Non-Hermitian interactions between harmonic oscillators, with applications to stable, Lorentz-violating quantum electrodynamics

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We examine a new application of the Holstein-Primakoff realization of the simple harmonic oscillator Hamiltonian. This involves the use of infinite-dimensional representations of the Lie algebra su(2). The representations contain nonstandard raising and lowering operators, which are nonlinearly related to the standard $a^\dagger$ and a. The new operators also give rise to a natural family of two-oscillator couplings. These nonlinear couplings are not generally self-adjoint, but their low-energy limits are self-adjoint, exactly solvable, and stable. We discuss the structure of a theory involving these couplings. Such a theory might have as its ultra-low-energy limit a Lorentz-violating Abelian gauge theory, and we discuss the extremely strong astrophysical constraints on such a model. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The simple harmonic oscillator is one of the best understood systems in quantum mechanics, with applications in essentially all areas of physics. However, there may remain many interesting properties of this system that have not been fully understood or elucidated (see Ref. 1, for instance). In this paper, we present an example of this. This example provides a possible way for nonlocal interactions to stabilize a Lorentz-violating modification to the free photon sector of the standard model.

We shall show how the Holstein-Primakoff realization of the angular momentum Lie algebra su(2) may be used in connection with the simple harmonic oscillator.[2] We first review the free oscillator, considered using the infinite-dimensional representations of this algebra. This leads naturally to a study of new nonlinear couplings between multiple identical harmonic oscillators. These couplings can be viewed in one of two ways. Taken at face value, the interactions are not self-adjoint, and the energy eigenvalues need not be real; however, the Hamiltonians in question do possess low-energy limits which are self-adjoint. The second possible viewpoint would be to take the formula which defines the real eigenvalues in the low-energy regime and extend that formula to cover the full range of the quantum numbers. This has the advantage of ensuring unitary evolution, but the additional complexity of the Hamiltonian is a corresponding disadvantage.

We shall describe how these new interactions may manifest themselves in a physical theory, with particular emphasis on couplings between the two polarization modes of the free electromagnetic field. However they are interpreted, the interactions we shall discuss may be relevant as part of a nonlocal, Lorentz-violating quantum field theory. Recently, there has been a great deal of interest in the possibility that Lorentz symmetry may not be exact in nature. A violation of this kind of fundamental symmetry could arise as part of the novel physics of the Planck scale. Relics of this violation would then persist even in the low-energy effective theory. The general local Lorentz-violating standard model extension (SME) has been developed,[3–5] and the stability[6] and

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renormalizability[7] of this extension have been studied. Lorentz violation is a very interesting area of theoretical physics, because even superficially simple questions about its physics may have subtle and even ambiguous answers. For example, the study of the gauge invariance properties of and finite radiative corrections to Lorentz-violating field theories has proven to be a fruitful source for new theoretical insights.[8–13]

One significant difficulty with Lorentz-violating quantum field theories is that they frequently exhibit problems with stability.[6,14] Yet it has been suggested that some form of nonlocality might overcome this problem.[6,15] The harmonic oscillator interactions we consider can provide a concrete example for how this stabilization might work, if we adopt the second interpretation of these interactions as described above. In the limit of very low energies, the nonlocal interactions may couple together the two polarization modes of a free photon in exactly the same way as would a local, renormalizable operator from the SME.[3,14] However, the nonlocality ensures that the theory remains stable, even for very large photon numbers. Weak forms on nonlocality have also been considered in other Lorentz-violating contexts.[16]

The kinds of infinite-dimensional representations of su(2) that we will consider have also been introduced in the context of the Dirac Coulomb problem[17,18] and in generalizations of the Dirac monopole,[19] where they provide useful insights. Moreover, other Lie algebras also possess infinite-dimensional representations that are not representations of any corresponding Lie group. These representations might be useful in the study of certain quantum-mechanical systems, through a generalization of the techniques used in Refs. 17–19 or developed in this paper.

II. SINGLE-OSCILLATOR OPERATORS

We shall begin by reviewing the Holstein-Primakoff realization of the harmonic oscillator raising and lowering algebra. Most frequently, when one studies the representations of su(2) in connection with quantum mechanics, one is interested only in the finite-dimensional representations, which are countable and parametrized by the total angular momentum ℓ. One considers an operator $\vec{J}=(J_1,J_2,J_3)=\left(\frac{1}{2}J_+ + \frac{1}{2}J_-, (1/2i)J_+ - (1/2i)J_-, J_3\right)$, with standard commutation relations. Beginning from a highest weight state $|\ell\rangle$, with $J_+|\ell\rangle=0$, one constructs each of the $2\ell+1$ states $|\ell-s\rangle$ by acting on $|\ell\rangle$ with J_- s times and normalizing appropriately.

When 2ℓ is a non-negative integer, there are only these $2\ell+1$ states, because $J_-|-\ell\rangle=0$. However, for more general values of the highest weight, the sequence of states does not terminate. Instead, one constructs an infinite tower of equally spaced states. This tower of states has a structure which is identical to that of the simple harmonic oscillator.

In fact, if we begin with a highest weight state $|\lambda\rangle$, with $J_3|\lambda\rangle=\lambda|\lambda\rangle$ (where 2λ is not a non-negative integer), we may construct states $|\lambda-n\rangle$ for all non-negative integers n, using $J_-|\lambda-n\rangle=\sqrt{\lambda(\lambda+1)-(\lambda-n)(\lambda-n-1)}|\lambda-n-1\rangle$. Then the Hamiltonian $H_\lambda=-\omega J_3+\omega\left(\lambda+\frac{1}{2}\right)$ has nondegenerate eigenvalues $\left(n+\frac{1}{2}\right)\omega$, which are precisely the energy eigenvalues of a harmonic oscillator (when we set $\hbar=1$). Since a quantum-mechanical system is entirely specified by its Hilbert space and the Hamiltonian acting on that space, this is equivalent to an alternate description of the harmonic oscillator. (Note that this description is completely distinct from Schwinger's development of the angular momentum algebra in terms of harmonic oscillator states.[20])

We should point out that the state space is a representation only of the Lie algebra su(2), not of the Lie group SU(2). That this is the case should be clear from an examination of the spectrum of the Hamiltonian $H_{\hat{n}}=\omega\hat{n}\cdot\vec{J}$. This would be a Zeeman effect Hamiltonian if the representation of $\vec{J}$ were finite dimensional, with $\vec{J}$ transforming in the adjoint representation of SU(2). The SU(2) symmetry would then dictate that the eigenenergies should be independent of the direction of $\hat{n}$. However, those energies are clearly not independent of $\hat{n}$ for the infinite-dimensional representations we are now considering. Specifically, if $\hat{n}=-\hat{e}_3$, then we have a harmonic oscillator system, but if $\hat{n}=+\hat{e}_3$, then the energy is not bounded from below. Therefore, the infinite-dimensional operators cannot form a representation of the group SU(2).

We shall now relabel our states, so that they match the usual harmonic oscillator nomencla-

ture. We make the replacement $|\lambda - n\rangle \rightarrow |n\rangle$. Now, in addition to the standard harmonic oscillator raising and lowering operators $a^\dagger$ and a, we have a new set of raising and lowering operators J_- and J_+, given by

$$J_-|n\rangle = \sqrt{\lambda(\lambda+1) - (\lambda - n)(\lambda - n - 1)}|n+1\rangle, \tag{1}$$

$$J_+|n\rangle = \sqrt{\lambda(\lambda+1) - (\lambda - n)(\lambda - n + 1)}|n-1\rangle, \tag{2}$$

or

$$J_- = a^\dagger \sqrt{2\lambda - a^\dagger a}, \tag{3}$$

$$J_+ = a\sqrt{2\lambda - a^\dagger a + 1}. \tag{4}$$

The square root operators are to be interpreted as having eigenvalues equal to the square roots of the eigenvalues of the operators inside, with the same eigenvectors. For a mechanical oscillator, we may further express the $J_\pm$ in terms of the position and momentum operators x and p, using the usual linear relations connecting x and p to $a^\dagger$ and a; however, this substitution must be made with the understanding that the proper interpretation of the $J_\pm$ operators requires the use of the discrete "number of quanta present" basis of states.

The $J_\pm$ give us a new family of raising and lowering operators, parametrized by λ. These operators are distinct from the $a^\dagger$ and a for all finite λ. This is clear from the differing commutation relations $[a, a^\dagger] = 1$ and $[J_+, J_-] = 2J_3$. In general, for large n (large in comparison with λ and unity), the matrix elements of $J_\pm$ are larger than those of a and $a^\dagger$ by a factor of $\mathcal{O}(\sqrt{n})$. However, the new operators do include the a and $a^\dagger$ as limiting cases. As $\lambda \rightarrow \infty$, $(J_+/\sqrt{2\lambda}) \rightarrow a$ and $(J_-/\sqrt{2\lambda}) \rightarrow a^\dagger$. (These limits are to be interpreted in terms of the matrix elements of the operators involved, and all half-integral values of λ must be avoided as the limit is taken.)

We can see from (3) and (4) that $J_+ \neq J_-^\dagger$ for finite, non-half-integral λ, because the square roots in (3) and (4) may become imaginary. This means that J_1 and J_2 are not self-adjoint, a difficulty which we glossed over when we discussed the Hamiltonian $H_{\hat{n}}$. The Casimir operator $\vec{J}^2$ is self-adjoint, however. Moreover, in the basis of eigenstates of J_3, $J_+ = J_-^T$. Since the matrix elements of J_- and $J_+^\dagger$ differ only by phase factors in the J_3 basis, there is no ambiguity in defining the entire state space starting from the ground state. Finally, we point out that if λ is large and positive, then the non-self-adjoint character of $\vec{J}$ does not become apparent unless n is at least comparable to 2λ. These facts will prove important when we discuss the coupling between two harmonic oscillators.

III. MULTIPLE COUPLED OSCILLATORS

We shall now consider a novel application of this description of the harmonic oscillator. We may determine the energy eigenvalues exactly for certain systems of coupled identical oscillators in which the couplings are nonlinear. Let us consider the Hamiltonian

$$H = H_\lambda + H_\mu + gH_{\text{int}} \tag{5}$$

$$H = \left[-\omega J_{A3} + \left(\lambda + \frac{1}{2}\right)\omega\right] + \left[-\omega J_{B3} + \left(\mu + \frac{1}{2}\right)\omega\right] + gH_{\text{int}}. \tag{6}$$

$\vec{J}_A$ and $\vec{J}_B$ are two independent vectors of operators of the type we have been considering, corresponding to the highest weights λ and μ, respectively. H_{int} is an interaction, whose form we shall discuss shortly. This Hamiltonian has three adjustable parameters. λ and μ determine the structure of the harmonic oscillator representations that we are using. However, like g, they may be seen as parameters describing the interaction, because we have shifted the total energy in such a way as to

make the spectrum of the free oscillators' Hamiltonian $H_\lambda + H_\mu$ independent of both λ and μ. These two parameters may be chosen freely, subject to the condition that neither 2λ nor 2μ is a non-negative integer.

We shall choose an interaction gH_{int} that is similar in form to $g\vec{J}_A \cdot \vec{J}_B$. If $g \neq 0$, $g\vec{J}_A \cdot \vec{J}_B$ is not self-adjoint; however, if λ and μ are large and positive, this problem will not be apparent in the vicinity of the ground state. So we take H_{int} to agree with $\vec{J}_A \cdot \vec{J}_B$ when $n_A + n_B + 1 < \min(2\lambda, 2\mu)$, where n_A and n_B are the principal quantum numbers of the two oscillators. We may then consider the effects of this interaction within this restricted ("low-energy") regime.

We may solve the *restricted* Hamiltonian using the ordinary techniques for the addition of angular momenta. The operator $\vec{J} = \vec{J}_A + \vec{J}_B$ has highest weights of the form $\lambda + \mu - i$ for all non-negative integers i, and each value of i corresponds to a single irreducible component of the representation. The Clebsch-Gordon coefficients for these representations can be calculated by the standard method of applying lowering operators and using Gram-Schmidt orthonormalization. However, our primary interest is in the energy levels.

The eigenvalues of $H_\lambda + H_\mu$ are just $(n_A + n_B + 1)\omega$. When we change the basis, to use the "total angular momentum" $\vec{J}$, this part of the Hamiltonian becomes

$$H_\lambda + H_\mu = -\omega J_3 + (\lambda + \mu + 1)\omega. \tag{7}$$

The eigenstates of the system are parametrized by the highest weight $\lambda + \mu - i$ and by the "number of quanta present" (that is, the number of applications of J_- on the highest weight state required to produce a given state), n. If we denote these states by $|i,n\rangle$, then it is clear that $(H_\lambda + H_\mu)|i,n\rangle = (i+n+1)\omega|i,n\rangle$. Since i and n have the same range as n_A and n_B (all must be non-negative integers), this verifies that the free system has the same spectrum in each basis.

The coupling term must be calculated in the $\vec{J}$ basis. This is easily done, using $\vec{J}_A \cdot \vec{J}_B = \frac{1}{2}(\vec{J}^2 - \vec{J}_A^2 - \vec{J}_B^2)$. For a state of specified i, $\vec{J}_A \cdot \vec{J}_B$ has the eigenvalue $\lambda\mu - (\lambda + \mu + \frac{1}{2})i + \frac{1}{2}i^2$. So the total energy is

$$E_{i,n} = \omega(i + n + 1) + g\left[\lambda\mu - \left(\lambda + \mu + \tfrac{1}{2}\right)i + \tfrac{1}{2}i^2\right]. \tag{8}$$

This formula holds exactly in the entire low-energy subspace.

We must now turn our attention to the general definition of H_{int}. There are two natural ways to define this interaction. The first possibility is that $H_{\text{int}} = \vec{J}_A \cdot \vec{J}_B$ exactly, and the fundamental Hamiltonian is not self-adjoint. The second possibility involves a less drastic modification of the structure of the theory. We simply take the exact Hamiltonian to be defined by its eigenvalues, which have the form (8). There is a complete set of states $\{|i,n\rangle\}$ corresponding to these eigenenergies, and for $i + n + 1 < \min(2\lambda, 2\mu)$, these states agree with the ones found above. The new Hilbert space is not equivalent to the old, two-oscillator Hilbert space, but the restricted, low-energy subspaces of these two Hilbert spaces are isomorphic. We shall henceforth adopt this second definition of H_{int} (although most of our statements will concern only the low-energy subspace, where the two definitions are equivalent).

A few words about the various parameters are now in order. Our coupled system is stable only if $g \geqslant 0$; if $g < 0$, the energy is not bounded below. We also see that the structure of the energy levels depends only on g and $\lambda + \mu$; the separate values of λ and μ only affect the zero-point energy.

This is a strongly nonlinearly coupled system. We may recover the more usual result for the spectrum in the presence of a linear coupling between the oscillators by setting $\lambda = \mu$ and expressing $a^\dagger$ and a in terms of the $\lambda \to \infty$ limits of J_+ and J_-. (Note that as $\lambda \to \infty$, there are no problems with the operators being self-adjoint.) The interaction $g(a_A a_B^\dagger + a_A^\dagger a_B)$ is the limit of $(g/\lambda)(\vec{J}_A \cdot \vec{J}_B - J_{A3}J_{B3})$ as λ approaches infinity. The two terms $(g/\lambda)\vec{J}_A \cdot \vec{J}_B$ and $(g/\lambda)J_{A3}J_{B3}$ each commute with the noninteracting Hamiltonian; and, although they do not commute with each other for finite values of λ, they do commute in the infinite limit. We may see this by evaluating the two operators

for finite λ in different bases. In the $\vec{J}$ basis, the first term is diagonal, with eigenvalues $g\{\lambda-[2+(1/2\lambda)]i+(1/2\lambda)i^2\}$, just as calculated above. The second term is diagonal in the J_A, J_B basis, with eigenvalues $(g/\lambda)(\lambda-n_A)(\lambda-n_B)$. As $\lambda\to\infty$, these eigenvalues become $g(\lambda-2i)$ and $g(\lambda-n_A-n_B)$, respectively. However, as we saw when we discussed the noninteracting case, the total number operator $n_A+n_B=n+i$ is diagonal in both bases, so $g(\lambda-n_A-n_B)=g(\lambda-n-i)$. Then the total energy shift, which is now the difference between $g(\lambda-2i)$ and $g(\lambda-n-i)$, becomes simply $g(n-i)$. That is, we have two decoupled oscillators with frequencies $\omega\pm g$, which is just the usual result.

More general interactions are also possible. We may replace $g\vec{J}_A\cdot\vec{J}_B$ with an arbitrary function of $\vec{J}_A\cdot\vec{J}_B$. Any such interaction will still commute with $H_\lambda+H_\mu$, and all the same considerations will still apply. Other generalizations are possible as well, through the use of other well-known properties of su(2). For example, we may generalize to the coupling of N identical oscillators, with the identity

$$\sum_{1\leqslant C<D\leqslant N}\vec{J}_C\cdot\vec{J}_D=\frac{1}{2}\left[\left(\sum_{C=1}^{N}\vec{J}_C\right)^2-\sum_{C=1}^{N}(\vec{J}_C)^2\right]. \tag{9}$$

However, it is important to keep in mind that many approximations that are typically used when one studies more than two interacting angular momenta will break down when working with infinite-dimensional representations of su(2).

IV. APPLICATION TO LORENTZ-VIOLATING QED

One of the simplest situations in which pairs of identical harmonic oscillators arise is in an Abelian gauge theory in 3+1 dimensions. An interaction of the form (6) might be relevant as a modification of the photon sector of quantum electrodynamics (QED). For the gauge sector alone, this interaction could be introduced separately at each value of the photon momentum. The selection of a specific basis of polarization states for each momentum, and the assignment of the couplings λ, μ, and g generally breaks Lorentz symmetry and may also break parity invariance. Moreover, the operators $J_\pm$ are nonlocal, since they involve the total energy present in a given mode of the electromagnetic field, and it is not possible to express this sort of interaction conveniently in terms of the ordinary electromagnetic field operators A^μ and $F^{\mu\nu}$. However, if we are willing to allow these modifications to the structure of the theory, the interaction is (in the absence of charges) exactly solvable. Since there is current interest in exotic modifications of QED, this type of interaction may be worthy of further investigation.

We must also say a word about the gauge invariance of this QED modification. The $\vec{J}_A\cdot\vec{J}_B$ interaction is formulated in terms of creation and annihilation operators (i.e., in the canonical quantization formalism), and so any discussion of gauge invariance will necessarily be complicated by the difficulties that are associated with the canonical quantization of gauge fields. However, at low energies, the interactions we have introduced are clearly consistent with gauge invariance in the following sense. If we specialize to the Coulomb gauge and quantize the transverse modes of the theory, then the low-energy interaction may be introduced without difficulty. It does not affect the number of polarization states (and is, in fact, strongly dependent upon this number), so it does not spoil gauge invariance in this fashion. However, it is possible that it may damage gauge invariance at higher energies or when interactions with matter are considered.

Although the interactions we are considering cannot be expressed simply in terms of the standard electromagnetic field operators, the ultra-low-energy limit of our theory could well be expressible in such a form. We shall shortly show that this is indeed the case for a particular class of models. The embedding of a ultra-low-energy Lorentz-violating effective field theory within the framework of our fundamental theory is attractive for several reasons. First, the interactions we have considered have eigenenergies that are exactly known. Second, although Lorentz-violating theories may exhibit stability problems, our theory does not; the i^2 term in (8) ensures this. This example shows that there can exist stable nonlocal interactions which have local, Lorentz-

violating Lagrangian theories as their ultra-low-energy limits. Third, such an embedding demonstrates the intriguing possibility that our conventional basis of polarization states may be inadequate for the description of the full Hilbert space of a more fundamental theory.

We shall therefore examine the ultra-low-energy behavior of our QED modification, to see to what sort of effective theory it may correspond. Since the energy-level differences depend only on $\lambda+\mu$, we shall set $\lambda=\mu$. We take λ to be a very large number, large in comparison with any relevant photon occupation number. (This is what we mean by "ultra-low-energy.") We may then neglect $a^\dagger a$ compared to λ in (3) and (4). It immediately follows that the energy eigenstates are approximately given by

$$|i,n\rangle \approx \frac{(a_A^\dagger - a_B^\dagger)^i (a_A^\dagger + a_B^\dagger)^n}{\sqrt{2^{i+n}(i!)(n!)}}|0,0\rangle. \tag{10}$$

Deviations from this expression are suppressed by a factor of $\mathcal{O}(\lambda^{-1/2})$. The corresponding energies, in the same approximation, are

$$E_{i,n} \approx (n+i)\omega + 2\lambda g i, \tag{11}$$

where we have dropped the zero-point energy.

These results imply that the polarization modes corresponding to $a_+^\dagger \equiv (1/\sqrt{2})(a_A^\dagger + a_B^\dagger)$ and $a_-^\dagger \equiv (1/\sqrt{2})(a_A^\dagger - a_B^\dagger)$ have different frequencies. The two frequencies are shifted from their mean value by $\pm\Delta\omega/2 \approx \pm g\lambda$, and the effective Hamiltonian is

$$H_{\text{eff}} = (\omega + 2\lambda g)a_-^\dagger a_- + \omega a_+^\dagger a_+. \tag{12}$$

This same effective Hamiltonian arises naturally in the context of a CPT-even, Lorentz-violating modification of the photon sector. For a theory with Lagrange density

$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} - \tfrac{1}{4}k_{\kappa\tau\mu\nu}F^{\kappa\tau}F^{\mu\nu} \tag{13}$$

(where $k_{\kappa\tau\mu\nu}$ has the symmetries of a Riemann tensor and is double traceless), the expressions for the photon modes' frequencies are (to leading order in $k_{\kappa\tau\mu\nu}$)[6,7,11]

$$\omega_\pm = (1 + \rho \pm \sigma)|\vec{p}|. \tag{14}$$

Here, $\vec{p}$ is the photons' 3-momentum, $\rho = -\frac{1}{2}\tilde{k}_\alpha{}^\alpha$, and $\sigma^2 = \frac{1}{2}\tilde{k}_{\alpha\beta}\tilde{k}^{\alpha\beta} - \rho^2$, with $\tilde{k}_{\alpha\beta} = k_{\alpha\mu\beta\nu}\hat{p}^\mu\hat{p}^\nu$ and $\hat{p}^\mu = (1, \vec{p}/|\vec{p}|)$. The approximate frequencies given by (14) and (12) correspond if $\rho = \sigma = g\lambda$. So any theory with $\rho = \sigma \geqslant 0$ for all $\vec{p}$ will reproduce the entire low-energy behavior of our modified theory. Theories with this property indeed exist; for example, if $k_{\kappa\tau\mu\nu}$ has the form

$$k_{\kappa\tau\mu\nu} = (v_\kappa u_\tau - v_\tau u_\kappa)(v_\mu u_\nu - v_\nu u_\mu) - \tfrac{1}{6}[v^2u^2 - (v\cdot u)^2](g_{\kappa\mu}g_{\tau\nu} - g_{\kappa\tau}g_{\mu\nu}) + (\kappa \leftrightarrow \mu), \tag{15}$$

then $\rho = \sigma = -w^2$, where $w^\mu = v^\mu(u\cdot\hat{p}) - u^\mu(v\cdot\hat{p})$. If $v^\mu = (V, \vec{0})$ and $u^\mu = (0, \vec{u})$, with $|\vec{u}| = 1$, then $\rho = V^2 \sin^2\theta$, where θ is the angle between $\vec{u}$ and $\vec{p}$. This particular model is parity-preserving, with three independent parameters.

Moreover, any theory with nonvanishing σ will demonstrate a splitting between polarization modes, as would arise in our su(2)-modified QED. There is therefore a large theoretical parameter space in which the theory given by (13) can be embedded in a su(2) coupling model.

These embeddings all require that, for a fixed direction $\hat{p}$, the coupling $g\lambda$ must be proportional to $|\vec{p}|$. It would seem most natural for λ, which represents the number of photons that must be present in a mode of the electromagnetic field in order for the failure of the polarization state basis to be apparent, to remain large for all values of $|\vec{p}|$. We therefore speculate that λ may be a $|\vec{p}|$-independent (or $\vec{p}$-independent) constant, while g scales with the magnitude of $\vec{p}$.

Based upon astrophysical experiments, the physical value of σ is strongly constrained, to parts in 10^{31} or better.[21,22] This represents an even stronger constraint on the su(2) model, because λ is

necessarily very large. It follows that $g=\sigma/\lambda$ is correspondingly smaller. Our modification of QED is thus physically reasonable only in a very, very small region of parameter space.

However, the formalism we have developed could be useful for developing an effective model in any situation in which there is a frequency splitting between polarization modes. For example, when the quantum corrections due to virtual electron exchange are considered, the effective Lagrange density for the electromagnetic field acquires nonlinear terms and becomes[23,24]

$$\mathcal{L}=\frac{1}{2}(\vec{E}^2-\vec{B}^2)+\frac{e^4}{360\pi^2m^4}[(\vec{E}^2-\vec{B}^2)+7(\vec{E}\cdot\vec{B})^2]. \tag{16}$$

In the presence of a large background magnetic field $\vec{B}_0$, the speed of light propagation will become dependent on the polarization vector. Specifically, if we write the magnetic field as $\vec{B}=\vec{B}_0+\vec{b}$ and keep only the relevant nonlinear terms with two powers of $\vec{B}_0$, then $\mathcal{L}$ becomes

$$\mathcal{L}\approx\frac{1}{2}(\vec{E}^2-\vec{b}^2)+\frac{e^4\vec{B}_0^2}{360\pi^2m^4}[(7\cos^2\theta_E-2)\vec{E}^2+(4\cos^2\theta_b+2)\vec{b}^2], \tag{17}$$

where θ_E and θ_b are the angles that $\vec{B}_0$ forms with $\vec{E}$ and $\vec{b}$, respectively. Waves polarized in the plane formed by the wave vector and $\vec{B}_0$ and those polarized normal to this plane propagate at different speeds. For a given direction, specified by θ_E and θ_b, the wave speed is

$$c=\left[\frac{1-\dfrac{e^4\vec{B}_0^2}{180\pi^2m^4}(4\cos^2\theta_b+2)}{1+\dfrac{e^4\vec{B}_0^2}{180\pi^2m^4}(7\cos^2\theta_E-2)}\right]^{1/2}. \tag{18}$$

Multiplying this by $|\vec{p}|$ gives the frequency, which can be inserted into the formalism we have developed.

V. CONCLUSIONS

In summary, we have studied an application of the Holstein-Primakoff realization of the simple harmonic oscillator operator algebra. This has involved the introduction of a set of raising and lowering operators that obey the angular momentum commutation relations. The properties of these operators allow us to solve exactly for the low-energy behavior of a theory with a particular nonlinear interaction. The high-energy extension of this model may involve either a non-self-adjoint Hamiltonian or a new basis of states.

This model has an interesting application in Lorentz-violating physics, where stability is typically a problem. The ultra-low-energy limit of the interaction we have considered resembles the effect of a small Lorentz-violating correction to free QED. At higher energies, the nonlocality of the special harmonic oscillator interactions we are considering can stabilize the Lorentz-violating theory. Physically, these kinds of effects are extremely strongly constrained by astronomical observations. However, this theory provides a useful insight into how nonlocality and Lorentz violation may combine to form a well-behaved theory.

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A bound on the mutual information, and properties of entropy reduction, for quantum channels with inefficient measurements

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The Holevo bound is a bound on the mutual information for a given quantum encoding. In 1996 Schumacher, Westmoreland, and Wootters [Phys. Rev. Lett. **76**, 3452 (1996)] derived a bound that reduces to the Holevo bound for complete measurements, but that is tighter for incomplete measurements. The most general quantum operations may be both incomplete and inefficient. Here we show that the bound derived by SWW can be further extended to obtain one that is yet again tighter for inefficient measurements. This allows us, in addition, to obtain a generalization of a bound derived by Hall, and to show that the average reduction in the von Neumann entropy during a quantum operation is concave in the initial state, for all quantum operations. This is a quantum version of the concavity of the mutual information. We also show that both this average entropy reduction and the mutual information for pure state ensembles, are Schur concave for unitarily covariant measurements; that is, for these measurements, information gain increases with initial uncertainty. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The celebrated Holevo bound, conjectured by Gordon[1] and Levitin[2] and proved by Holevo in 1973[3] gives a bound on the information that may be transmitted from A to B (strictly, the *mutual information*, M, between A and B) when A encodes information in a quantum system using a set of states $\{\rho_i\}$, chosen with probabilities $\{P(i)\}$, and B makes a subsequent measurement upon the system. The Holevo bound is

$$M(I{:}J) \leqslant \chi \equiv S(\rho) - \sum_i P(i)S(\rho_i), \tag{1}$$

where $\rho=\Sigma_i P(i)\rho_i$ (and which we will refer to as the *ensemble state*). We write the mutual information as $M(I:J)$ to signify that it is the mutual information between the random variables I and J, whose values i and j label, respectively, the encoding used by A, and the outcome of the measurement made by B. More recent proofs of the Holevo bound may be found in Refs. 4–6. The bound is achieved if and only if the encoding states, ρ_i, commute with each other, and the receiver, B, makes a von Neumann measurement in the basis in which they are diagonal. (A von Neumann measurement is one that projects the system onto one of a complete set of mutually orthogonal states. In this case the set of states is chosen to be the basis in which the coding states are diagonal.) With this choice of coding states and measurement the channel is classical, in that it can be implemented with a classical system. The Holevo bound takes into account that the sender may only be able to send mixed states, and this mixing reduces the amount of information that can be transmitted. However, if the receiver is not able to perform measurements that always project the system to a pure state (so-called *complete* measurements), then, in general, the information will be further reduced. In 1996 Schumacher, Westmoreland, and Wootters showed that when the receiv-

er's measurement is incomplete, it is possible to take this into account and derive a more stringent bound on the information. If the receiver's measurement is the POVM described by the operators $\{A_j\}$ (with $\Sigma_j A_j^\dagger A_j = 1$), so that the measurement outcomes are labeled by the index j, then the SWW bound is[6]

$$M(I{:}J) \leqslant \chi - \sum_j P(j)\chi_j, \tag{2}$$

where $P(j)$ is the probability of outcome j,[7] and χ_j is the Holevo quantity for the ensemble that the system remains in (from the point of view of the receiver), given outcome j. This bound can be at least partially understood by noting that if the system still remains in some ensemble of possible states after the measurement, then future measurements can potentially extract further information about the encoding, and so the information obtained by the first measurement must therefore be less than the maximum possible at least by this amount. What the SWW bound tells us is that the bound on the information is reduced not only by the amount of information that could be further extracted after outcome j has been obtained, but by the Holevo bound on this information, χ_j.

If the initial state of the system is ρ_i, then after outcome j the final state of the system is given by $\tilde{\rho}_{j|i} = A_j \rho_i A_j^\dagger / \mathrm{Tr}[A_j^\dagger A_j \rho_i]$. Thus the states that make up the final ensemble that remains after outcome j, are $\{\tilde{\rho}_{j|i}\}$, and the probability of each state in the ensemble is $P(i|j) = P(j|i)P(i)/P(j)$, with $P(j|i) = \mathrm{Tr}[A_j^\dagger A_j \rho_i]$. The Holevo quantity for ensemble j is thus

$$\chi_j = S(\tilde{\rho}_j) - \sum_i P(i|j) S(\tilde{\rho}_{j|i}), \tag{3}$$

where $\tilde{\rho}_j = A_j \rho A_j^\dagger / \mathrm{Tr}[A_j^\dagger A_j \rho]$. If at least one of the measurement operators A_j are higher than rank 1, then the measurement is incomplete. If the measurement is complete, then for each j all the final states $\tilde{\rho}_{j|i}$ are identical, χ_j is zero and the SWW bound reduces to the Holevo bound.

The most general kind of measurement can also be inefficient. A measurement is described as inefficient if the observer does not have full information regarding which of the outcomes actually occurred. The name *inefficient* comes from that fact that the need to consider such measurements first arose in the study of inefficient photo-detectors.[8] An inefficient measurement may be described by labeling the measurement operators with two indices, so that we have A_{kj}. The receiver has complete information about one of the indices, j, but no information about the other, k.[9] As a result, the final state for each j (given the value of i) is now

$$\rho'_{j|i} = \sum_k P(k|j) \frac{A_{kj} \rho_i A_{kj}^\dagger}{\mathrm{Tr}[A_{kj}^\dagger A_{kj} \rho_i]}. \tag{4}$$

Since inefficiency represents a loss of information, we wish to ask whether it is possible to take this into account and obtain a more stringent bound on the mutual information. If we merely apply the SWW bound to the measurement A_{kj}, then the bound involves the Holevo quantities of the ensembles that remain when both the values of k and j are known (the final ensembles that result from the efficient measurement). That is

$$M(I{:}J) \leqslant \chi - \sum_{kj} P(k,j)\chi_{kj}. \tag{5}$$

One therefore wishes to know whether it is possible to derive a bound that instead involves the Holevo quantities of the ensembles that remain after the inefficient measurement is made, that is, for the receiver who only has access to j.

In the first part of this paper we answer this question in the affirmative—for an inefficient measurement where the known outcomes are labeled by j, the bound given by Eq. (2) *remains true*, where now the χ_j are the Holevo quantities for the ensemble of states $\rho'_{j|i}$ that result from the inefficient measurement.

In the second part of the paper, we consider the average reduction in the von Neumann entropy induced by a measurement:

$$\langle \Delta S(\rho) \rangle \equiv S(\rho) - \sum_i P(j) S(\rho_j'). \tag{6}$$

Here ρ_j' is the state that results from outcome j, given that the initial state is ρ. Since the von Neumann entropy is a measure of how much we know about the state of the system, this is the difference between what we knew about the system state before we made the measurement, and what we know (on average) about the system state at the end of the measurement; it thus measures how much we learn about the final state of the system. Equivalently, it can be said to measure the degree of "state-reduction" that the measurement induces.

While it is the mutual information that is important for communication, the reduction in the von Neumann entropy is important for feedback control. Feedback control is the process of performing a sequence of measurements on a system, and applying unitary operations after each measurement in order control the evolution of the system. Such a procedure is useful for controlling systems that are driven by noise. If the ability to perform unitary operations is unlimited, then the von Neumann entropy provides a measure of the level of control that can be achieved: if the system has maximal entropy then the unitary operations have no effect on the system state whatsoever; conversely, if the state is pure then the system can be controlled precisely - that is, any pure state can be prepared. Thus the entropy measures the extent to which a pure state, or pure evolution can be obtained, and thus the level of predictability which can be achieved over the future behavior of the system.[10] The primary role of measurement in feedback control is therefore to reduce the entropy of the system. As such, the average reduction in von Neumann entropy provides a ranking of the effectiveness of different measurements for feedback control, other things being equal. Further details regarding quantum feedback control and von Neumann entropy can be found in Ref. 11.

The entropy reduction is also relevant to the transformation of pure-state entanglement, since the von Neumann entropy measures the entanglement of pure states. As a result this quantity gives the amount by which pure-state entanglement is broken by a local measurement.

We give two corollaries of the general information bound derived in the first part that involve $\langle \Delta S(\rho) \rangle$. The first is a generalization of a bound derived by Hall[12,13] to inefficient measurements. Hall's bound states that for efficient measurements the mutual information is bounded by $\langle \Delta S(\rho) \rangle$. We show that for inefficient measurements this becomes

$$M(I{:}J) \leqslant \langle \Delta S(\rho) \rangle - \sum_i P(i) \langle \Delta S(\rho_i) \rangle, \tag{7}$$

where $\langle \Delta S(\rho_i) \rangle$ is the average entropy reduction that would have resulted if the initial state had been ρ_i, and as above $\rho = \Sigma_i P(i) \rho_i$.

The second is the fundamental property that, for all quantum operations, the average reduction in von Neumann entropy is concave in the initial state ρ. That is,

$$\langle \Delta S(\rho) \rangle \geqslant \sum_i P(i) \langle \Delta S(\rho_i) \rangle. \tag{8}$$

Finally, in the third part of this paper, we use the above result to show that for measurements that are uniform in their sensitivity across state space (that is, measurements that are unitarily covariant), the amount that one learns about the final state always increases with the initial uncertainty, where this uncertainty is characterized by *majorization*. This is a quantum version of the much simpler classical result (which we also show) that the mutual information always increases with the initial uncertainty for classical measurements that are permutation symmetric. In addition, we show that, for unitarily covariant measurements, the mutual information for pure-state ensembles also has this property. One can sum up these results by saying that the statement

that information gain increases with initial uncertainty can fail to hold only if the measurement is asymmetric in its sensitivity.

II. AN INFORMATION BOUND FOR GENERAL QUANTUM OPERATIONS

We now show that the bound proved by SWW can be generalized to obtain a more stringent bound for channels in which the receiver's measurement is inefficient. To show this, it turns out that we can use the same method employed by SWW, but with the addition of an extra quantum system, which allows us to include the inefficiency of the measurement.

Theorem 1: *For a quantum channel in which the encoding ensemble is* $\epsilon=\{P(i),\rho_i\}$, *and the measurement performed by the receiver is described by operators* A_{kj} $(\Sigma_{kj}A_{kj}^\dagger A_{kj}=1)$, *where the measurement is, in general, inefficient so that the receiver knows j but not k; then the mutual information,* $M(I:J)$, *is bounded such that*

$$M(I:J) \leqslant \chi - \sum_j P(j)\chi_j, \tag{9}$$

where $P(j)$ *is the overall probability for outcome j,* $\chi=S(\rho)-\Sigma_i P(i)S(\rho_i)$ *is the Holevo quantity for the initial ensemble, and*

$$\chi_j = S(\sigma_j) - \sum P(i|j)S(\sigma_{j|i}), \tag{10}$$

is the Holevo quantity for the ensemble, ϵ_j, *that remains (from the point of view of the receiver) once the measurement has been made, so that the receiver has learned the outcome j, but not the value of k. Here the receiver's overall final state is*

$$\sigma_j = \frac{\sum_k A_{kj}\rho A_{kj}^\dagger}{P(j)} = \sum_{ik} P(i,k|j)\sigma_{kj|i}, \tag{11}$$

where $P(i,k|j)$ *is the probability for both i and outcome k given j, and* $\sigma_{kj|i}$ *is the final state that results given the initial state* ρ_i, *and both outcomes j and k. The remaining ensemble* $\epsilon_j=\{P(i|j),\sigma_{j|i}\}$, *where*

$$\sigma_{j|i} = \sum_k P(k|j,i)\sigma_{kj|i} = \frac{\sum_k A_{kj}\rho_i A_{kj}^\dagger}{P(j|i)}, \tag{12}$$

and where $P(k|j,i)$ *is the probability for outcome k given j and the initial state* ρ_i.

Proof: We begin by collecting various key facts. The first is that any efficient measurement on a system Q, described by $N=N_1N_2$ operators, A_{kj} $(j=1,\ldots,N_1$ and $k=1,\ldots,N_2)$ can be obtained by bringing up an auxiliary system A of dimension N, performing a unitary operation involving Q and A, and then making a von Neumann measurement on A.[14,15] If the initial state of Q is $\rho^{(Q)}$, then the final joint state of A and Q after the von Neumann measurement is

$$\sigma^{(AQ)} = |kj\rangle\langle kj|^{(A)} \otimes \frac{A_{kj}\rho^{(Q)}A_{kj}^\dagger}{P(k,j)}. \tag{13}$$

where $|kj\rangle$ is the state of A selected by the von Neumann measurement. The second fact is that the state that results from discarding all information about the measurement outcomes k and j can be obtained by performing a unitary operation between A and another system E that perfectly correlates the states $|kj\rangle$ of A with orthogonal states of E, and then tracing out E. The final key fact we require is a result proven by SWW,[6] which is that the Holevo χ quantity is nonincreasing under partial trace. That is, if we have two quantum systems A and B, and an ensemble of states $\rho_i^{(AB)}$ with associated probabilities P_i, then

$$\chi^{(A)} = S(\rho^{(A)}) - \sum_i S(\rho_i^{(A)}) \leqslant S(\rho^{(AB)}) - \sum_i S(\rho_i^{(AB)}) = \chi^{(AB)}, \tag{14}$$

where $\rho_i^{(A)} = \mathrm{Tr}_B[\rho_i^{(AB)}]$. To prove this result SWW use strong subadditivity.[16]

We now encode information in system Q using the ensemble $\boldsymbol{\epsilon}$, and consider the joint system that consists of the three systems Q, A, E and a forth system M, with dimension N_1. We now start with A, E and M in pure states, so that the Holevo quantity for the joint system is $\chi^{(QAEM)} = \chi^{(Q)}$. We then perform the required unitary operation between Q and A, and a unitary operation between A and E that perfectly correlates the states $|kj\rangle^{(A)}$ of A with orthogonal states of E. Unitary operations do not change the Holevo quantity. Then we trace over E, so that we are left with the state

$$|\psi\rangle\langle\psi|^{(M)} \otimes \sum_{jk} P(k,j)|k,j\rangle\langle k,j|^{(A)} \otimes \frac{A_{kj}\rho^{(Q)}A_{kj}^\dagger}{P(k,j)}. \tag{15}$$

After the two unitaries and the partial trace over E, the Holevo quantity for the remaining systems, which we will denote by $\chi'^{(QAM)}$, satisfies $\chi'^{(QAM)} \leqslant \chi^{(QAEM)} = \chi^{(Q)}$. We now perform one more unitary operation, this time between M and A, so that we correlate the states of M, which we denote by $|j\rangle\langle j|^{(M)}$ with the second index of the states of A, giving

$$\sum_j |j\rangle\langle j|^{(M)} \otimes \sum_k P(k,j)|k,j\rangle\langle k,j|^{(A)} \otimes \sigma_{kj}^{(Q)} \tag{16}$$

where $\sigma_{kj}^{(Q)} = A_{kj}\rho^{(Q)}A_{kj}^\dagger / P(k,j)$ is the final state resulting from knowing both outcomes k and j, with no knowledge of the initial choice of i. Finally we trace out A, leaving us with the state

$$\sigma^{(QM)} = \sum_j |j\rangle\langle j|^{(M)} \otimes \sum_k P(k,j)\sigma_{kj}^{(Q)}. \tag{17}$$

After this final unitary, and the partial trace over A, the Holevo quantity for the remaining systems Q and M, which we will denote by $\chi''^{(QM)}$, satisfies $\chi''^{(QM)} \leqslant \chi'^{(QAM)} \leqslant \chi^{(Q)}$. We have gone through the above process using the initial state ρ, but we could just as easily have started with any of the initial states, ρ_i, in the ensemble, and we will denote the final states that we obtain using the initial state ρ_i as $\sigma_i^{(QM)}$. Calculating $\chi''^{(QM)}$, we have

$$\chi''^{(QM)} = S(\sigma^{(QM)}) - \sum_i P(i)S(\sigma_i^{(QM)}) = H[J] - \sum_i P(i)H[J|i] + \sum_j P(j)\left[S(\sigma_j) - \sum_i P(i|j)\sigma_{j|i}\right] \tag{18}$$

$$= M(J{:}I) + \sum_j P(j)\chi_j^{(Q)} \leqslant \chi^{(Q)}. \tag{19}$$

Rearranging this expression gives the desired result. □

III. PROPERTIES OF ENTROPY REDUCTION

We now rewrite the above information bound using the fact that $P(i|j)P(j) = P(j|i)P(i)$. The result is

$$M(I{:}J) \leqslant \langle \Delta S(\rho)\rangle - \sum_i P(i)\langle \Delta S(\rho_i)\rangle, \tag{20}$$

where $\rho = \Sigma_i P_i\rho_i$. Ozawa has shown that for efficient measurements $\langle \Delta S(\rho)\rangle$ is always positive[17] (for more recent proofs of this result see Refs. 18 and 19). For efficient measurements, Eq. (20) is therefore in general stronger than, and gives immediately, Hall's bound,[12,13] which states that the mutual information is bounded by the reduction in the von Neumann entropy. The inequality in

Eq. (20) is then a generalization of Hall's bound to inefficient measurements. Since the mutual information is always positive, but for inefficient measurements the reduction in the von Neumann entropy can be negative (that is, the entropy of the quantum state can *increase* as a result of the measurement), the relation

$$M(I{:}J) \leqslant \langle \Delta S(\rho) \rangle \tag{21}$$

is not necessarily satisfied for such measurements. However, Eq. (20) tells us that if the entropy of the initial state, ρ, does increase, the average increase in the entropy for each of the coding states ρ_i is always *more* than this by at least the mutual information.

The second result that we obtain from Eq. (20) is that, because the mutual information is non-negative, we have

$$\langle \Delta S(\rho) \rangle \geqslant \sum_i P(i) \langle \Delta S(\rho_i) \rangle. \tag{22}$$

That is, the reduction in the von Neumann entropy is concave in the initial state. This parallels the fact that the mutual information is also concave in the initial state.

The fact that this is true for inefficient measurements means that once we have made an efficient measurement, no matter what information we throw away regarding the final outcomes (i.e., which outcomes we average over), $\langle \Delta S(\rho) \rangle$ is always greater than the average of the entropy reductions that would have been obtained through measurement in each of the coding states, when we throw away the same information regarding the measurement results.

IV. INFORMATION GATHERING AND STATE-SPACE SYMMETRY

In this section we show that measurements whose ability to extract information is uniform over the available state space (that is, does not vary from point to point in the state-space) always extract more information (strictly, never extract less information) the less that is known before the measurement is made. Thus, in this sense, one may regard "the more you know, the less you get" as a fundamental property of measurement. We will show that this is true both for the information obtained regarding the final state [being $\langle \Delta S(\rho) \rangle$], and the mutual information for a measurement on an ensemble of pure states. Here we will consider efficient measurements only; no doubt inefficient measurements will also have this property, but only if the information that is thrown away is also uniform with respect to the state space, and we do not wish to burden the treatment with this additional complication.

To proceed, we must make precise the notion that the sensitivity of a measurement is uniform over state space. This is captured by stating that such a measurement should be invariant under reversible transformations of the state space. For classical measurements (which are simply quantum measurements in which all operators and density matrices commute[20]) this means that the set of measurement operators is invariant under all permutations of the classical states: we will refer to these as *completely symmetric* measurements. Note that in this classical case, this is equivalent to saying that the measurement distinguishes all states from all other states equally well. The quantum generalization of this is invariance under all unitary transformations. Such measurements are referred to as being unitarily covariant.[21,22]

We must also quantify what we mean by the observer's lack of knowledge, or uncertainty, before the measurement is made. This is captured by the simple and elegant concept of *majorization*.[23,24] If two sets of probabilities $p \equiv \{P_i\}$ and $q \equiv \{Q_i\}$ satisfy the set of relations

$$\sum_{i=1}^{k} P_i \geqslant \sum_{i=1}^{k} Q_i, \quad \forall\, k, \tag{23}$$

where it is understood that the elements of both sets have been placed in decreasing order (e.g., $P_i > P_{i+1}, \ \forall\, i$), then p is said to majorize q, and this is written $q \prec p$. While at first Eq. (23) looks a little complicated, a few moments consideration reveals that it captures precisely what one

means by uncertainty—if p majorizes q, then p is more sharply peaked than q, and consequently describes a state of knowledge containing less uncertainty. What is more, majorization implies an ordering with Shannon entropy $H[\cdot]$. That is, if p majorizes q, then $H[p] \leqslant H[q]$.[23,24]

In a sense, majorization is a more basic notion of uncertainty than entropy in that it captures that concept alone—the Shannon entropy, on the other hand, characterizes the more specific notion of information. To characterize the uncertainty of a density matrix, we can apply majorization to the vector consisting of its eigenvalues. If ρ and σ are density matrices, then we will write $\sigma \prec \rho$ if ρ's eigenvalues majorize σ's. Various applications have been found for majorization in quantum information theory.[18,19,25–28]

We thus desire to show that for measurements with the specified symmetry, $\langle \Delta S(\sigma) \rangle \geqslant \langle \Delta S(\rho) \rangle$ whenever $\sigma \prec \rho$ (and similarly for the mutual information). Functions with this property [of which the von Neumann entropy, $S(\rho)$, is one example] are referred to as being *Schur concave*. To show that a function is Schur concave, it is sufficient to show that it is concave, and symmetric in its arguments,[23,24] which in our case are the eigenvalues of the density matrix ρ (if our functions did not depend only on the eigenvalues of ρ, then they could not be Schur concave, since the majorization condition only involves these eigenvalues).

The desired result for classical completely symmetric measurements is now immediate. In the classical case the mutual information is the unique measure of information gain, and $M(I:J) = \langle \Delta S(\rho) \rangle$. The mutual information is concave in the initial classical probability vector $\mathbf{P} = (P_1, \ldots, P_n)$ (being the vector of the eigenvalues of ρ in our quantum formalism), as is indeed implied by the concavity of $\langle \Delta S(\rho) \rangle$. Since all operators commute with the density matrix, $\langle \Delta S(\rho) \rangle$ is only a function of the $\{P_i\}$. From the form of $\langle \Delta S(\rho) \rangle$ we see that a permutation of the elements of $\mathbf{P}$ is equivalent to a permutation applied to the measurement operators, and since these are invariant under such an operation, $\langle \Delta S(\rho) \rangle$, and thus $M(I:J)$, is a symmetric function of its arguments. Thus $M(I:J)$ is Schur concave.

The Schur concavity of $\langle \Delta S(\rho) \rangle$ for unitarily covariant (UC) quantum measurements is just as immediate. Because of the unitary covariance of the measurement, we see from the form of $\langle \Delta S(\rho) \rangle$ that it is invariant under a unitary transformation of ρ. As a result, it only depends upon the eigenvalues of ρ. Since the permutations are a subgroup of the unitaries, it is also a symmetric function of its arguments (the eigenvalues), and thus Schur concave.

We wish finally to show that the mutual information is also Schur concave in ρ for unitarily covariant measurements on ensembles of pure states. This requires a little more work. First, we need to show that once we have fixed a set of encoding states, the mutual information is concave in the vector of the ensemble probabilities $P(i)$. This is straightforward if we first note that the mutual information, because it is, in fact, symmetric between i and j, can be written in the reverse form

$$M(I{:}J) = H[P(j)] - \sum_j P(i) H[P(j|i)]. \tag{24}$$

Since, for a fixed measurement, the mutual information is a function of the ensemble probabilities, we will write it as $M(\{P(i)\})$. Denoting the pure states in the encoding ensemble as $\rho_i = |\psi_i\rangle\langle\psi_i|$, and choosing the ensemble state $\rho = \Sigma_k P_k \sigma_k$, where the σ_k are built from the encoding states so that $\sigma_k = \Sigma_i P_{i|k} |\psi_i\rangle\langle\psi_i|$, then

$$\begin{aligned} M(\{P(i)\}) &= H\left[\sum_k P(k)P(j|k)\right] - \sum_i \sum_k P(i|k)P(k)H[P(j|i)] \\ &\geqslant \sum_k P(k)H[P(j|k)] - \sum_k P(k) \sum_i P(i|k)H[P(j|i)] \\ &= \sum_k P(k) M(\{P(i|k)\}), \end{aligned} \tag{25}$$

being the desired concavity relation. The inequality in the third line is merely a result of the

concavity of the Shannon entropy. Note that while we have written the measurement's outcomes explicitly as being discrete in the about derivation, the result also follows if they are a continuum (as in the case of UC measurements) by replacing the relevant sums with integrals.

Now we need to note some further points about UC measurements: A UC measurement may be generated by taking all unitary transformations of any single operator A, and dividing them by a common normalization factor. The resulting measurement operators are thus $A_U \propto UAU^\dagger$, where U ranges over all unitaries. The normalization for the A_U comes from $\int UA^\dagger AU^\dagger d\mu(U) = \mathrm{Tr}[A^\dagger A]I$, where $d\mu(U)$ is the (unitarily invariant) Haar measure[22,29] over unitaries.

It is not hard to show that all UC measurements can be obtained by *mixing* different UC measurements, each generated by a different operator. (Mixing a set of measurements means assigning to each a probability, and then making one measurement from the set at random based on these probabilities[30]).

Next, we need to show that for all UC measurements the mutual information depends only on the eigenvalues of the ensemble density matrix, and we state this as the following lemma.

Lemma 1: *The mutual information for a UC measurement on a pure-state ensemble*, $\epsilon = \{P(i), |\psi_i\rangle\}$ *depends on the ensemble only through the eigenvalues of the density matrix* $\rho = \Sigma_i P(i) |\psi_i\rangle\langle\psi_i|$.

Proof: We first show this for UC measurements generated from a single operator. Writing the mutual information in the reverse form, one has

$$M(I{:}J) = H[P(U)] - \sum_i P_i H[P(U|i)], \tag{26}$$

where U is the continuum index for the measurement operators (and thus the measurement outcomes) that are $A_U = UAU^\dagger$ for some appropriately normalized A. Naturally all this means is that $P(U|i)$ is a function of U, where U ranges over all unitaries. Since the measurement is unitarily covariant, $H[P(U|i)]$ is the same for all initial states $|\psi_i\rangle$, and therefore the second term is the same for all initial ensembles. Thus M depends only on the first term $H[P(U)] = H[\mathrm{Tr}[UA^\dagger AU^\dagger \rho]]$, which depends only on ρ, and is invariant under all unitary transformations of ρ. Thus M depends only on the eigenvalues of ρ. Since the mutual information for a mixture of measurements is merely a function of the respective mutual informations for each measurement (in particular, it is a linear combination of them), the result holds for all UC measurements. □

Since M depends only on ρ, in establishing the Schur concavity of M with respect to ρ, we need only consider one ensemble for each ρ. We therefore choose the eigenensemble $\{\lambda_i, |\phi_i\rangle\}$, where λ_i and $|\phi_i\rangle$ are the eigenvalues and eigenvectors of ρ, respectively. We know that the mutual information is concave in the vector of initial ensemble probabilities, and for the ensemble we have chosen, the initial probabilities are the eigenvalues of ρ. As a result, the mutual information is concave in the eigenvalues of ρ. Since M is invariant under unitary transformations, and since unitary transformations include permutations as a subgroup, it is also a symmetric function of the eigenvalues. Thus M is Schur concave.

V. CONCLUSION

In using a quantum channel, if there are limitations on the completeness (or alternatively the *strength*, in the terminology of Ref. 19) or efficiency of the measurements that the receiver can perform, then it is possible to give a bound on the mutual information that is stronger than the Holevo bound. Further, this bound has a very simple form in terms of the Holevo χ quantity, and the χ quantities of the ensembles, one of which remains after the measurement is made.

This bound also allows us to obtain a relationship between the mutual information and the average von Neumann entropy reduction induced by a measurement, and encompasses the fact that this von Neumann entropy reduction is concave in the initial state.

From the concavity of the mutual information and the von Neumann entropy reduction, it follows that these quantities are Schur concave (the former naturally for pure-state ensembles) for completely symmetric classical measurements, and for unitarily covariant quantum measurements.

Thus, the possibility that either of these kinds of information gain *decreases* with increasing initial uncertainty is associated with the asymmetry of the measurement in question.

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Entanglement monotones for multi-qubit states based on geometric invariant theory

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We construct entanglement monotones for multi-qubit states based on Plücker coordinate equations of Grassmann variety, which are a central notion in geometric invariant theory. As an illustrative example, we in detail investigate entanglement monotones of a three-qubit state. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The geometry of entanglement is a very interesting subject as much as quantification and classification of entanglement are.[1–6] It is possible to derive geometrical measures of entanglement invariant under stochastic local quantum operation and classical communication (SLOCC). All homogeneous positive functions of pure states that are invariant under determinant-one SLOCC operations are entanglement monotones.[7] In this paper, we will derive entanglement monotones based on a branch of the algebraic geometry called geometric invariant theory. In particular, let G be a group that acts on a set A, then the invariant theory is concerned with the study of the fixed points A^G and the orbits A/G associated to this action. The geometric invariant theory deals with the case where G is an algebraic group, e.g., a special linear group $\mathrm{SL}(r,\mathbf{C})$, that acts on a variety A via morphisms. Thus, based on the geometric invariant theory, we can construct a measure of entanglement that is invariant under action of $\mathrm{SL}(r,\mathbf{C})$ by construction. It has a well-defined geometrical structure called Grassmann variety or Grassmannian and it is generated by a quadratic polynomials called the Plücker coordinate equations. We will discuss our construction in detail in the following section. Recently, Lévay[8] has constructed a class of multi-qubit entanglement monotones, which was based on the construction of Emary.[9] His construction based on bipartite partitions of the Hilbert space and the invariants was expressed in terms of the Plücker coordinates of the Grassmannian. However, we do have different approaches and construction to solve the problem of quantifying multipartite states, but some of the results on entanglement monotones for multi-qubit states coincide. Now, let us start by denoting a general, pure, composite quantum system with m subsystems $\mathcal{Q}=\mathcal{Q}_m^p(N_1,N_2,\ldots,N_m)=\mathcal{Q}_1\mathcal{Q}_2\cdots\mathcal{Q}_m$, consisting of the pure state $|\Psi\rangle=\Sigma_{k_1=1}^{N_1}\Sigma_{k_2=1}^{N_2}\cdots\Sigma_{k_m=1}^{N_m}\ \alpha_{k_1,k_2,\ldots,k_m}|k_1,k_2,\ldots,k_m\rangle$ and corresponding to the Hilbert space $\mathcal{H}_\mathcal{Q}=\mathcal{H}_{\mathcal{Q}_1}\otimes\mathcal{H}_{\mathcal{Q}_2}\otimes\cdots\otimes\mathcal{H}_{\mathcal{Q}_m}$, where the dimension of the jth Hilbert space is given by $N_j=\dim(\mathcal{H}_{\mathcal{Q}_j})$. We are going to use this notation throughout this paper. In particular, we denote a pure two-qubit state by $\mathcal{Q}_2^p(2,2)$. Next, let $\rho_\mathcal{Q}$ denote a density operator acting on $\mathcal{H}_\mathcal{Q}$. The density operator $\rho_\mathcal{Q}$ is said to be fully separable, which we will denote by $\rho_\mathcal{Q}^{\mathrm{sep}}$, with respect to the Hilbert space decomposition, if it can be written as $\rho_\mathcal{Q}^{\mathrm{sep}}=\Sigma_{k=1}^{\mathrm{N}}p_k\otimes_{j=1}^m\rho_{\mathcal{Q}_j}^k$, $\Sigma_{k=1}^N p_k=1$ for some positive integer N, where p_k are positive real numbers and $\rho_{\mathcal{Q}_j}^k$ denotes a density operator on Hilbert space $\mathcal{H}_{\mathcal{Q}_j}$. If $\rho_\mathcal{Q}^p$ represents a pure state, then the quantum system is fully separable if $\rho_\mathcal{Q}^p$ can be written as $\rho_\mathcal{Q}^{\mathrm{sep}}=\otimes_{j=1}^m\rho_{\mathcal{Q}_j}$, where $\rho_{\mathcal{Q}_j}$ is the density operator on $\mathcal{H}_{\mathcal{Q}_j}$. If a state is not separable, then it is said to be an entangled state.

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The general references for the complex projective space are Refs. 10 and 11. So, let $\{f_1, f_2, \ldots, f_q\}$ be continuous functions $\mathbf{K}^n \to \mathbf{K}$, where $\mathbf{K}$ is the field of real $\mathbf{R}$ or complex numbers $\mathbf{C}$. Then we define real (complex) space as the set of simultaneous zeroes of the functions

$$\mathcal{V}_{\mathbf{K}}(f_1, f_2, \ldots, f_q) = \{(z_1, z_2, \ldots, z_n) \in \mathbf{K}^n : f_i(z_1, z_2, \ldots, z_n) = 0 \ \ \forall\ 1 \leqslant i \leqslant q\}. \tag{1}$$

These real (complex) spaces become topological spaces by giving them the induced topology from $\mathbf{K}^n$. Now, if all f_i are polynomial functions in coordinate functions, then the real (complex) space is called a real (complex) affine variety. A complex projective space $\mathbf{CP}^n$ is defined to be the set of lines through the origin in $\mathbf{C}^{n+1}$, that is, $\mathbf{CP}^n = (\mathbf{C}^{n+1} - 0)/\sim$, where $\sim$ is an equivalence relation define by $(x_1, \ldots, x_{n+1}) \sim (y_1, \ldots, y_{n+1}) \Leftrightarrow \exists \lambda \in \mathbf{C} - 0$, such that $\lambda x_i = y_i \forall\, 0 \leqslant i \leqslant n$. For $n = 1$ we have a one-dimensional complex manifold $\mathbf{CP}^1$, which is a very important one, since as a real manifold it is homeomorphic to the two-sphere $\mathbf{S}^2$, e.g., the Bloch sphere. Moreover, every complex compact manifold can be embedded in some $\mathbf{CP}^n$. In particular, we can embed a product of two projective spaces into the third one. Let $\{f_1, f_2, \ldots, f_q\}$ be a set of homogeneous polynomials in the coordinates $\{\alpha_1, \alpha_2, \ldots, \alpha_{n+1}\}$ of $\mathbf{C}^{n+1}$. Then the projective variety is defined to be the subset

$$\mathcal{V}(f_1, f_2, \ldots, f_q) = \{[\alpha_1, \ldots, \alpha_{n+1}] \in \mathbf{CP}^n : f_i(\alpha_1, \ldots, \alpha_{n+1}) = 0 \ \forall\ 1 \leqslant i \leqslant q\}. \tag{2}$$

We can view the complex affine variety $\mathcal{V}_{\mathbf{C}}(f_1, f_2, \ldots, f_q) \subset \mathbf{C}^{n+1}$ as a complex cone over the projective variety $\mathcal{V}(f_1, f_2, \ldots, f_q)$. We can also view $\mathbf{CP}^n$ as a quotient of the unit $2n+1$ sphere in $\mathbf{C}^{n+1}$ under the action of $U(1) = \mathbf{S}^1$, that is $\mathbf{CP}^n = \mathbf{S}^{2n+1}/U(1) = \mathbf{S}^{2n+1}/\mathbf{S}^1$, since every line in $\mathbf{C}^{n+1}$ intersects the unit sphere in a circle.

II. GRASSMANN VARIETY

In this section, we will define the Grassmann variety. However, the standard reference on geometric invariant theory is Ref. 12. Let $\mathrm{Gr}(r, d)$ be the Grassmann variety of the $r-1$-dimensional linear projective subspaces of $\mathbf{CP}^{d-1}$. Now, we can embed $\mathrm{Gr}(r, d)$ into $\mathbf{P}(\wedge^r(\mathbf{C}^d)) = \mathbf{CP}^{\mathcal{N}}$, $\mathcal{N} = \binom{d}{r} - 1$, by using the Plücker map $L \to \wedge^r(L)$, where the exterior product $\wedge^r(\mathbf{C}^d)$ for $1 \leqslant r \leqslant d$ is a subspace of $\mathbf{C}^{N_1} \otimes \cdots \otimes \mathbf{C}^{N_m}$, spanned by the antisymmetric tensors. The Plücker coordinates $P_{i_1, i_2, \ldots, i_r}, 1 \leqslant i_1 < \cdots < i_r \leqslant d$ are the projective coordinates in this projective space. Next, let $\mathbf{C}[\Lambda(r, d)]$ be a polynomial ring with the Plücker coordinatesP_J indexed by elements of the set $\Lambda(r, d)$ of ordered r-tuples in $\{1, 2, \ldots d\}$ as its variables. Then the image of the map $\kappa : \mathbf{C}[\Lambda(r, d)] \to \mathrm{Pol}(\mathrm{Mat}_{r,d})$, which assigns $P_{i_1 i_2 \ldots i_r}$ the bracket polynomial $[i_1, i_2, \ldots, i_r]$ (the bracket function on the $\mathrm{Mat}_{r,d}$, whose values on a given matrix is equal to the maximal minor formed by the columns from a set of $\{1, 2, \ldots, d\}$) is equal to the subring of the invariant of the polynomials. Moreover, the kernel $\mathcal{I}_{r,d}$ of the map κ is equal to the homogeneous ideal of the Grassmann in its Plücker embedding. Furthermore, the homogeneous ideal $\mathcal{I}_{r,d}$ defining $\mathrm{Gr}(r, d)$ in its Plücker embedding is generated by the quadratic polynomials

$$\mathcal{P}_{I,J} = \sum_{t=1}^{r+1} (-)^t P_{i_1, \ldots, i_{r-1}, j_t} P_{j_1 \ldots j_{t-1} j_{t+1}, \ldots, j_{r+1}}, \tag{3}$$

where $I = (i_1 \ldots i_{r-1}), 1 \leqslant i_1 < \cdots < i_{r-1} < j_i$, and $J = (j_1, \ldots, j_{r+1}), 1 \leqslant j_1 < \cdots < j_{r+1} \leqslant d$ are two increasing sequences of numbers from the set $\{1, 2, \ldots, d\}$. Note that the equations $\mathcal{P}_{I,J} = 0$ define the Grassmannian $\mathrm{Gr}(r, d)$ are called the Plücker coordinate equations. For example, for $\mathrm{Gr}(2, d)$ and $n = 2$, we have

$$\mathcal{P}_{I,J} = \sum_{t=1}^{4} (-)^t P_{i_1, j_t} P_{j_1 \ldots j_{t-1} j_{t+1}, \ldots, j_3} = -P_{i_1, j_1} P_{j_2, j_3} + P_{i_1, j_2} P_{j_1, j_3} - P_{i_1, j_3} P_{j_1, j_2}, \tag{4}$$

where $I = (i_1)$, and $J = (j_1, j_2, j_3)$. Note that, by its construction, the Grassmannian $\mathrm{Gr}(2, d)$ is invariant under $\mathrm{SL}(2, \mathbf{C})$.

III. PLÜCKER COORDINATES AND MULTIPARTITE ENTANGLEMENT

In this section, we will construct entanglement monotones based on Plücker coordinate equations of the Grassmannian. Let us consider a quantum system $\mathcal{Q}_m^p(2,2,\ldots,2)$ and let

$$\mathcal{E}_{I,J}(\mathrm{Mat}_{r,d}^j)=\sum_{t=1}^{r+2}(P_j^{i_1,\ldots,i_{r-1},j_t}\overline{P^j}_{i_1,\ldots,i_{r-1},j_t}+P_j^{j_1\cdots j_{t-1}j_{t+1},\ldots,j_{r+1}}\overline{P^j}_{j_1\cdots j_{t-1}j_{t+1},\ldots,j_{r+1}}), \tag{5}$$

where $I=(i_1\ldots i_{r-1}),1\leqslant i_1<\cdots<i_{r-1}<j_i$, and $J=(j_1,\ldots,j_{r+1}),1\leqslant j_1<\cdots<j_{r+1}\leqslant d$ are two increasing sequences of numbers from the set $\{1,2,\ldots,d\}$. For example, for $\mathrm{Gr}(2,d)$ and $r=2$, that is invariant under $\mathrm{SL}(2,\mathbf{C})$, we have

$$\mathcal{E}_{I,J}(\mathrm{Mat}_{2,d}^j)=\sum_{t=1}^{4}(P_j^{i_1,j_t}\overline{P^j}_{i_1,j_t}+P_j^{j_1\cdots j_{t-1}j_{t+1},\ldots,j_3}\overline{P^j}_{j_1\cdots j_{t-1}j_{t+1},\ldots,j_3})=P_j^{i_1,j_1}\overline{P^j}_{i_1,j_1}+P_j^{j_2,j_3}\overline{P^j}_{j_2,j_3}+P_j^{i_1,j_2}\overline{P^j}_{i_1,j_2}$$
$$+P_j^{j_1,j_3}\overline{P^j}_{j_1,j_3}+P_j^{i_1,j_3}\overline{P^j}_{i_1,j_3}+P_j^{j_1,j_2}\overline{P^j}_{j_1,j_2}, \tag{6}$$

where $I=(i_1)$, and $J=(j_1,j_2,j_3)$. Now, we can write the coefficient of a general multi-qubit state as follows:

$$\mathrm{Mat}_{2,d}^1=\begin{pmatrix}\alpha_{1,1,\ldots,1} & \alpha_{1,1,\ldots,2} & \cdots & \alpha_{1,2,\ldots,2}\\ \alpha_{2,1,\ldots,1} & \alpha_{2,1,\ldots,2} & \cdots & \alpha_{2,2,\ldots,2}\end{pmatrix},$$
$$\mathrm{Mat}_{2,d}^2=\begin{pmatrix}\alpha_{1,1,\ldots,1} & \alpha_{1,1,\ldots,2} & \cdots & \alpha_{2,1,\ldots,2}\\ \alpha_{1,2,\ldots,1} & \alpha_{1,2,\ldots,2} & \cdots & \alpha_{2,2,\ldots,2}\end{pmatrix}, \tag{7}$$
$$\vdots$$
$$\mathrm{Mat}_{2,d}^m=\begin{pmatrix}\alpha_{1,1,\ldots,1} & \alpha_{1,1,\ldots,1} & \cdots & \alpha_{2,2,\ldots,1}\\ \alpha_{1,1,\ldots,2} & \alpha_{1,1,\ldots,2} & \cdots & \alpha_{2,2,\ldots,2}\end{pmatrix},$$

where $d=2^{m-1}$ and $\mathrm{Mat}_{2,d}^j$, which we get by permutation of j for $1\leqslant j\leqslant m$. Moreover, we assume that the sequences I,J denote the columns of the $\mathrm{Mat}_{2,d}^j$. Then we can define entanglement monotones for the multi-qubit states by

$$\mathcal{E}(\mathcal{Q}_m^p(2,2,\ldots,2))=\left(\mathcal{N}\sum_{j=1}^{m}\mathcal{E}_{I,J}(\mathrm{Mat}_{2,2^{m-1}}^j)\right)^{1/2}. \tag{8}$$

As an example, let us consider the quantum system $\mathcal{Q}_3^p(2,2,2)$. For such three-qubit states, if e.g., the subsystem $\mathcal{Q}_1$ is unentangled with the $\mathcal{Q}_2\mathcal{Q}_3$ subsystems, then the separable set of this state is generated by the six 2-by-2 subdeterminants of

$$\mathrm{Mat}_{2,4}^1=\begin{pmatrix}\alpha_{1,1,1} & \alpha_{1,1,2} & \alpha_{1,2,1} & \alpha_{1,2,2}\\ \alpha_{2,1,1} & \alpha_{2,1,2} & \alpha_{2,2,1} & \alpha_{2,2,2}\end{pmatrix}. \tag{9}$$

$\mathrm{Mat}_{2,4}^2$ and $\mathrm{Mat}_{2,4}^3$ can be obtained in similar way. Then the partial entanglement monotones for $\mathrm{Mat}_{2,4}^1$ is given by

$$\mathcal{E}_{I,J}(\mathrm{Mat}_{2,d}^1)=P_1^{i_1,j_1}\overline{P^1}_{i_1,j_1}+P_1^{j_2,j_3}\overline{P^1}_{j_2,j_3}+P_1^{i_1,j_2}\overline{P}_{i_1,j_2}+P_1^{j_1,j_3}\overline{P^1}_{j_1,j_3}+P_1^{i_1,j_3}\overline{P^1}_{i_1,j_3}+P_1^{j_1,j_2}\overline{P^1}_{j_1,j_2}, \tag{10}$$

where the Plücker coordinates for $\mathrm{Mat}_{2,4}^1$ are given by

$$P_{1,2}^1=\alpha_{1,1,1}\alpha_{2,1,2}-\alpha_{1,1,2}\alpha_{2,1,1},\ P_{1,3}^1=\alpha_{1,1,1}\alpha_{2,2,1}-\alpha_{1,2,1}\alpha_{2,1,1},$$

$$P^1_{1,4} = \alpha_{1,1,1}\alpha_{2,2,2} - \alpha_{1,2,2}\alpha_{2,1,1},\ P^1_{2,3} = \alpha_{1,1,2}\alpha_{2,2,1} - \alpha_{1,2,1}\alpha_{2,1,2},$$

$$P^1_{2,4} = \alpha_{1,1,2}\alpha_{2,2,2} - \alpha_{1,2,2}\alpha_{2,1,2},\ P^1_{3,4} = \alpha_{1,2,1}\alpha_{2,2,2} - \alpha_{1,2,2}\alpha_{2,2,1}.$$

Thus, entanglement monotones for three-qubit states are given by

$$\mathcal{E}(\mathcal{Q}^p_m(2,2,2)) = \left(\mathcal{N}\sum_{j=1}^{3}\mathcal{E}_{I,J}(\mathrm{Mat}^j_{2,4})\right)^{1/2}. \tag{11}$$

Moreover, for matrices $\mathrm{Mat}^j_{2,4}$, we have $\mathcal{P}^j_{I,J} = -P^j_{1,2}P^j_{3,4} + P^j_{1,3}P^j_{2,4} - P^j_{1,4}P^j_{2,3} = 0$. For three-qubit states, this result coincides with construction of the Segre variety.[6] However, multi-qubit states needs further investigation. Now, as an example, let us consider the state $|\Psi_W\rangle = \alpha_{1,1,2}|1,1,2\rangle + \alpha_{1,2,1}|1,2,1\rangle + \alpha_{2,1,1}|2,1,1\rangle$. Then we have

$$\mathcal{C}(\mathcal{Q}_3(2,2,2)) = (2\mathcal{N}[|\alpha_{1,2,1}\alpha_{2,1,1}|^2 + |\alpha_{1,1,2}\alpha_{2,1,1}|^2 + |\alpha_{1,1,2}\alpha_{1,2,1}|^2])^{1/2}.$$

In particular, for $\alpha_{1,1,2} = \alpha_{1,2,1} = \alpha_{2,1,1} = 1/\sqrt{3}$, we get $\mathcal{C}(\mathcal{Q}_3(2,2,2)) = (\frac{2}{3}\mathcal{N})^{1/2}$.

IV. HYPERDETERMINANT AND PLÜCKER COORDINATE EQUATIONS

In this section, we will review some results of the construction of entanglement measure based on the hyperdeterminant for three-qubit states and the relation between the Plücker coordinate equations and the hyperdeterminant. We also discuss a generalization of this construction. The hyperdeterminant of the elements of $\mathbf{C}^{N_1}\otimes\mathbf{C}^{N_2}\otimes\cdots\otimes\mathbf{C}^{N_m}$ was introduced by Gelfand, Kapranov, and Zelevinsky in Ref. 13. They proved that the dual variety of Segre product $\mathbf{CP}^{N_1-1}\times\mathbf{CP}^{N_2-1}\times\cdots\times\mathbf{CP}^{N_m-1}$ is a hypersurface if and only if $N_j \leqslant \Sigma_{i\neq j}N_i$ for $j=1,2,\ldots,m$. Whenever the dual variety is a hypersurface its equation is called the hyperdeterminant of the format $N_1\times N_2\times\cdots\times N_m$ and denoted by Det. The hyperdeterminant is a homogeneous polynomial function over $\mathbf{C}^{N_1}\otimes\mathbf{C}^{N_2}\otimes\cdots\otimes\mathbf{C}^{N_m}$, so that the condition $\mathrm{Det}\,A\neq 0$ is meaningful for $\mathcal{A}\in\mathbf{CP}^{N_1N_2\cdots N_m-1}$. Moreover, the hyperdeterminant Det is $\mathrm{SL}(N_1,\mathbf{C})\times\mathrm{SL}(N_2,\mathbf{C}))\otimes\cdots\otimes\mathrm{SL}(N_m,\mathbf{C})$-invariant. For example, for $m=2$ we have $\mathrm{Det}\,\mathcal{A} = \alpha_{1,1}\alpha_{2,2} - \alpha_{1,2}\alpha_{2,1}$ and for $m=3$, we have

$$\begin{aligned}\mathrm{Det}\,\mathcal{A} = {} & \alpha^2_{1,1,1}\alpha^2_{2,2,2} + \alpha^2_{1,1,2}\alpha^2_{2,2,1} + \alpha^2_{1,2,1}\alpha^2_{2,1,2} + \alpha^2_{2,1,1}\alpha^2_{1,2,2} \\ & - 2(\alpha_{1,1,1}\alpha_{1,1,2}\alpha_{2,2,1}\alpha_{2,2,2} + \alpha_{1,1,1}\alpha_{1,2,1}\alpha_{2,1,2}\alpha_{2,2,2} + \alpha_{1,1,1}\alpha_{2,1,1}\alpha_{1,2,2}\alpha_{2,2,2} \\ & + \alpha_{1,1,2}\alpha_{1,2,1}\alpha_{2,1,2}\alpha_{2,2,1} + \alpha_{1,1,2}\alpha_{2,1,1}\alpha_{1,2,2}\alpha_{2,2,1} + \alpha_{1,2,1}\alpha_{2,1,1}\alpha_{1,2,2}\alpha_{2,1,2}) \\ & + 4(\alpha_{1,1,1}\alpha_{2,2,1}\alpha_{2,1,2}\alpha_{1,2,2} + \alpha_{2,2,2}\alpha_{2,1,1}\alpha_{1,2,1}\alpha_{1,1,2}).\end{aligned} \tag{12}$$

Now, let us introduce the Diophantine function. For any sequence of numbers $\gamma_1,\gamma_2,\gamma_3,\gamma_4$, and $\delta_1,\delta_2,\delta_3,\delta_4$ we have

$$\mathcal{P}(\gamma_1,\gamma_2,\gamma_3,\gamma_4,\delta_1,\delta_2,\delta_3,\delta_4) = (\gamma_1\delta_1 + \gamma_2\delta_2 - \gamma_3\delta_3 - \gamma_4\delta_4)^2 - 4(\gamma_1\gamma_2 + \delta_3\delta_4)(\gamma_3\gamma_4 + \delta_1\delta_2). \tag{13}$$

This equation is equal to the hyperdeterminant $\mathrm{Det}\,\mathcal{A}$. For the quantum system $\mathcal{Q}^p_3(2,2,2)$ we have

$$\mathrm{Det}\,\mathcal{A} = \mathcal{P}(-\alpha_{1,1,1},\alpha_{2,2,1},\alpha_{2,1,2},\alpha_{1,2,2},-\alpha_{2,2,2},\alpha_{1,1,2},\alpha_{1,2,1},\alpha_{2,1,1}). \tag{14}$$

For the quantum system $\mathcal{Q}^p_3(2,2,2,2)$, one can wonder if it would be possible to find a generalization of the polynomial $\mathcal{P}$ such that the hyperdeterminant $\mathrm{Det}\,\mathcal{A}$ could be give by $\mathcal{P}$. We can also construct the hyperdeterminant in terms of the Plücker coordinates. For example, Lévay[5] has constructed such Plücker coordinates for three-qubit states as follows. Let $\alpha^p,\beta^q,p,q=1,2,3,4$ be two-four component vectors defined as $\alpha_{1,k_1,k_2} = (1/\sqrt{2})\alpha_p\Sigma^{p,k_1,k_2}$, and $\alpha_{2,k_1,k_2} = (1/\sqrt{2})\beta_p\Sigma^{p,k_1,k_2}$, where $\Sigma^s = -i\sigma_s, s=1,2,3$, and $\Sigma^4 = I_2$, where σ_p are Pauli matrices. Then the hyperdeterminant is

given by Det $\mathcal{A}=2P_{p,q}P^{p,q}$, where the Plücker coordinates are given by $P_{p,q}=\alpha_p\beta_q-\alpha_q\beta_p$. Thus, this construction can be at least extended into multi-qubit states following our definition of the Plücker coordinates for the multi-qubit states and further extending the definition of two 2^{m-1} components vectors $\alpha^p,\beta^q,p,q=1,2,\ldots,2^{m-1}$. For further progress in this direction see Ref. 8.

V. CONCLUSION

In this paper, we have constructed entanglement monotones for multipartite states based on the Grassmannian $\mathrm{Gr}(r,d)$, which was defined in terms of the Plücker coordinate equations. In particular, we have given an explicit expression for entanglement monotones for multi-qubit states. Moreover, we have investigated entanglement monotones for three-qubit state as an illustrative example.

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Inequivalent quantizations of the $N=3$ Calogero model with scale and mirror-S_3 symmetry

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We study the inequivalent quantizations of the $N=3$ Calogero model by separation of variables, in which the model decomposes into the angular and the radial parts. Our inequivalent quantizations respect the "mirror-S_3" invariance (which realizes the symmetry under the cyclic permutations of the particles) and the scale invariance in the limit of vanishing harmonic potential. We find a two-parameter family of novel quantizations in the angular part and classify the eigenstates in terms of the irreducible representations of the S_3 group. The scale invariance restricts the quantization in the radial part uniquely, except for the eigenstates coupled to the lowest two angular levels for which two types of boundary conditions are allowed independently from all upper levels. It is also found that the eigenvalues corresponding to the singlet representations of the S_3 are universal (parameter-independent) in the family, whereas those corresponding to the doublets of the S_3 are dependent on one of the parameters. These properties are shown to be a consequence of the spectral preserving SU(2) (or its subgroup U(1)) transformations allowed in the family of inequivalent quantizations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The N-body Calogero model, which describes N particles interacting with each other by the combined inverse square and harmonic potential on a line, is exactly solvable and yet admits a diversity of mathematical extensions and physical applications. For the mathematical side, Calogero's analysis[1] for $N=3$ has been extended to general N[2,3] as well as to models with modified potentials[4,5] and Lie-algebraic structures[6] (see also Refs. 7–12, and references therein). For the physical side, its relevance to high energy physics has been argued, albeit in specific circumstances, in various areas, e.g., in the Yang-Mills theory,[13] two-dimensional QCD,[14] superstrings,[15] and black holes.[16] Moreover, its potential application has also been argued in condensed matter physics, e.g., for spin chains,[17] quantum Hall effect,[18] magnons,[19] and the electron-hole interaction.[20]

In considering the application to particles with anyon statistics, Veigy[21] made an important observation that, when the coupling constant of the interaction lies in a certain range, the Calogero model admits a wider class of solutions than those obtained by Calogero. Technically, the possibility of the extension is found in the treatment of the singularities in the inverse square potential, where a specific (the Dirichlet) boundary condition has conventionally been adopted, allowing for only bosons and fermions for the possible statistics of the particles. It is shown in Ref. 21 that, if one adopts a different boundary condition at the singularities in the *angular* part of the model, which arises after the separation of variables is implemented for the $N=3$ case, one indeed finds extra eigenstates that correspond neither to bosons nor fermions. More recently, it has also been shown in Refs. 22–24 that the model admits novel solutions if we consider a general class of

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boundary conditions for the *radial* part, even if the conventional boundary condition is adopted for the angular part.

To explore a fuller class of solutions available in the Calogero model, which amounts to exploring the possible *inequivalent quantizations* of the model, it is necessary to study the combined extension in the boundary conditions both in the angular and radial parts in more general terms, and this has been initiated in Ref. 25 for $N=3$. For the angular part, the class of boundary conditions considered in Ref. 25 forms a two-parameter family (containing the cases treated by Calogero and Veigy earlier) and respects a dihedral D_6 symmetry, which derives from the demand of indistinguishability of the particles. We found that the model can still be solvable, but the spectrum cannot be obtained explicitly except for a number of special cases such as the ones considered earlier. The purpose of the present paper is to provide another class of solutions allowed when we relax the demand from the D_6 symmetry to its subgroup S_3 and impose instead scale symmetry in the vanishing harmonic potential limit. In physical terms, the S_3 symmetry is equivalent to the invariance under cyclic permutations of the particles, while the additional scale symmetry ensures the smooth limit to the pure inverse square potential system at the quantum level. For the angular part, this leads to a novel two-parameter family of inequivalent quantizations, where the spectra can be obtained in closed form as well as the explicit solutions classified according to the irreducible representations of the group S_3. For the radial part, on the other hand, the scale symmetry specifies the quantization essentially uniquely to one obtained under the Dirichlet boundary condition, except for the eigenstates coupled to the lowest two angular levels for which the Neumann boundary condition is permitted as well. This allows us to have a number of possible combinations of boundary conditions for the angular and radial parts. We also observe that the levels which are singlets of S_3 are universal, i.e., independent of the parameters of the family, whereas the doublets of S_3 are dependent on one of the parameters. This will be seen as a consequence of the spectral preserving SU(2) (or its subgroup U(1)) transformations allowed in the family of inequivalent quantizations of the model.

The plan of the paper is as follows. We recapitulate in Sec. II the procedure of inequivalent quantizations of the $N=3$ Calogero model by separation of variables and present the symmetries we impose. We give a detailed discussion on the eigenstates and eigenvalues in the angular part in Sec. III. These results are then combined with the counterparts of the radial part discussed in Sec. IV to provide the solutions and the spectra of the entire system. Section V is devoted to the discussion of the universality of the S_3-singlets based on the spectral preserving $su(2)$ algebra found earlier.[26] Finally, our conclusion is presented in Sec. V.

II. THE $N=3$ CALOGERO MODEL

In the following we provide a framework for quantizing the $N=3$ Calogero model based on the separation of variables method, in which we split the model into the radial and angular parts. Concerning this, there are two important issues that require particular care, one of which is the treatment of the singularity in the potential and the other is the choice of the symmetry we shall adopt for our inequivalent quantizations.

A. Separation of variables

The N body Calogero model[2,3] is a system of N particles governed by the Hamiltonian,

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+\sum_{j=1}^{N}\sum_{i=j+1}^{N}\left\{\frac{g}{(x_i-x_j)^2}+\frac{1}{4}m\omega^2(x_i-x_j)^2\right\}, \tag{2.1}$$

where x_i, $i=1,\ldots,N$ represent the positions of the particles under interaction. As is well known, the system can be analyzed by the method of separation of variables (see, e.g., Ref. 25), which for the $N=3$ case begins with the use of the Jacobi coordinates,

$$x=\frac{x_1-x_2}{\sqrt{2}},\quad y=\frac{x_1+x_2-2x_3}{\sqrt{6}},\quad z=\frac{x_1+x_2+x_3}{\sqrt{3}},\tag{2.2}$$

and passes on to the polar coordinates $(x,y)=(r\sin\phi, r\cos\phi)$. In the unit $2m=1$, $\hbar=1$, this procedure brings the Hamiltonian to the separable form,

$$H=-\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}-\frac{\partial^2}{\partial z^2}+\frac{3}{8}\omega^2r^2+\frac{1}{r^2}\left\{-\frac{\partial^2}{\partial\phi^2}+\frac{g}{2}\frac{9}{\sin^2 3\phi}\right\}.\tag{2.3}$$

It is also known that, if $g<-\frac{1}{2}$, the model does not admit a ground state,[27] and if $\frac{3}{2}\leqslant g$, the Hamiltonian H is essentially self-adjoint and leads to a unique quantization. In the present paper, we consider the cases $-\frac{1}{2}<g<\frac{3}{2}$, $g\neq 0$, where H admits self-adjoint extensions allowing for inequivalent quantizations. Here, the two particular points $g=0$ and $g=-\frac{1}{2}$ are excluded because the model becomes a harmonic oscillator in the former case while it requires an independent treatment technically in the latter case. For our later convenience, instead of g we use ν introduced as

$$g=2\nu(\nu-1),\quad \tfrac{1}{2}<\nu<\tfrac{3}{2},\quad \nu\neq 1.\tag{2.4}$$

On account of the separable form (2.3), we have the Hamiltonian $H=H_0+H_{\rm rel}$ with H_0 describing the center of mass system and $H_{\rm rel}$ the relative motion. The latter splits further into $H_{\rm rel}=H_r+H_\Omega$, where H_r and H_Ω are the Hamiltonians for the radial and angular parts, respectively. Consider now the angular eigenvalue equation,

$$H_\Omega\psi_\lambda(\phi)=\lambda\psi_\lambda(\phi),\quad H_\Omega=-\frac{d^2}{d\phi^2}+\frac{9\nu(\nu-1)}{\sin^2 3\phi},\tag{2.5}$$

with eigenvalue λ. To each λ, we further consider the effective radial Hamiltonian $H_{r,\lambda}=H_r+\lambda/r^2$ and its eigenvalue equation,

$$H_{r,\lambda}\psi_E(r;\lambda)=E\psi_E(r;\lambda),\quad H_{r,\lambda}=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{3}{8}\omega^2r^2+\frac{\lambda}{r^2}.\tag{2.6}$$

The eigenfunction for the entire system (apart from that for the center-of-mass system in the z direction) with total energy E is obtained as $\psi_E(r;\lambda)\psi_\lambda(\phi)$ from the solutions of Eqs. (2.5) and (2.6).

B. Singularities and formal symmetries

In our quantization, an important point to note is that both the angular Hamiltonian H_Ω and the radial Hamiltonian $H_{r,\lambda}$ are ill-defined at the singular points of the potentials, i.e., at ϕ for which $\sin 3\phi=0$ and at $r=0$. Thus, to quantize the model properly and solve the eigenvalue equations, we need to consider self-adjoint extensions to each of the operators, that is, we provide an appropriate domain of definition in such a way that the entire Hamiltonian H be self-adjoint. In practice, this is accomplished by furnishing a set of connection conditions for the eigenfunctions at these singular points according to the general scheme for singular Hamiltonians (2.6) and (2.5), and in what follows we adopt the scheme presented in Ref. 28.

We start with the angular Hamiltonian, and for this we first note the formal symmetry of the operator H_Ω in (2.5). From the potential, it is clear that H_Ω is invariant under the reflections,

$$P_3:\phi\mapsto-\phi,\quad R_3:\phi\mapsto\frac{\pi}{3}-\phi,\tag{2.7}$$

and also under four other reflections P_i, R_i, $i=1,2$, analogously defined (see Fig. 1). It follows that the Hamiltonian is invariant under the rotation by angle $\pi/3$,

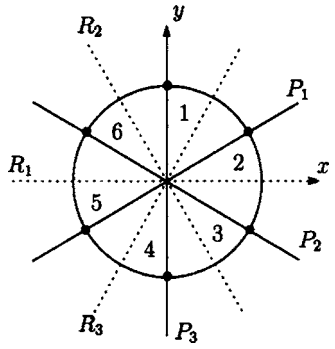

FIG. 1. Axes of reflections P_i, R_i, $i=1,2,3$, on the plane (x,y). The numbers $k=1,\ldots,6$ indicate the sectors $s_k=(\phi_{k-1},\phi_k)$ defined along the circle.

$$\mathcal{R}_{\pi/3}=R_3\circ P_3:\phi\mapsto\phi+\frac{\pi}{3}, \tag{2.8}$$

and hence under the successive ones $(\mathcal{R}_{\pi/3})^j$, $j=0,1,2,3,4,5$, as well. Combining all these reflections and rotations, we obtain a D_6 group as the group of the formal symmetry of H_Ω. On the angular wave function $\psi(\phi)$, the action of the operation $g\in D_6$ is realized by

$$\hat{g}\psi(\phi)=\psi(g^{-1}\phi). \tag{2.9}$$

It should be stressed, however, that the symmetry D_6 is still formal and the actual symmetry at the quantum level should be determined by taking account of the connection condition at the singularities.

In order to provide the connection condition at the singular points $\phi=\phi_k$,

$$\phi_k=\frac{k\pi}{3},\quad k=0,1,2,3,4,5, \tag{2.10}$$

we first focus on the singularity at $\phi=\phi_0=0$ and introduce the boundary vectors

$$B_0(\psi):=\begin{pmatrix}W[\psi,\varphi_1^0]_{0+}\\ W[\psi,\varphi_1^0]_{0-}\end{pmatrix},\quad B_0'(\psi):=\begin{pmatrix}W[\psi,\varphi_2^0]_{0+}\\ -W[\psi,\varphi_2^0]_{0-}\end{pmatrix}, \tag{2.11}$$

where $W[\psi_1,\psi_2]_{\phi\pm}=\lim_{\epsilon\to\pm0}W[\psi_1,\psi_2](\phi+\epsilon)$ are the limiting values of the Wronskian,

$$W[\psi_1,\psi_2]=\psi_1\frac{\mathrm{d}\psi_2}{\mathrm{d}\phi}-\psi_2\frac{\mathrm{d}\psi_1}{\mathrm{d}\phi}. \tag{2.12}$$

The functions φ_i^0 $(i=1,2)$ appearing in (2.11) are real eigenfunctions of H_Ω around $\phi=0$, called the "reference modes," which are normalized with respect to the Wronskian, $W[\varphi_1^0,\varphi_2^0]=1$. The most general form of the connection condition at $\phi=0$, which ensures the local continuity of the probability current there, is then given by

$$(U_0-\mathbf{1}_2)B_0(\psi)+i(U_0+\mathbf{1}_2)B_0'(\psi)=0, \tag{2.13}$$

where $U_0\in\mathrm{U}(2)$ is an arbitrary unitary matrix characterizing the connection condition (hence the singularity), and $\mathbf{1}_2$ is the identity matrix. In components, the condition (2.13) consists of two equations linear in ψ and its derivative $\mathrm{d}\psi/\mathrm{d}\phi$ at the singularity. The use of the Wronskians is to render the equations well-defined, since the quantities ψ and $\mathrm{d}\psi/\mathrm{d}\phi$ may be divergent at the singularity.

To provide the connection conditions at other singularities with $k=1,\ldots,5$ in (2.10) analogously to the case $k=0$, we need to choose the reference modes φ_i^k $(i=1,2)$ around each of the singularities ϕ_k. On account of the formal invariance of the Hamiltonian under D_6, these reference modes may simply be provided by the translations,

$$\varphi_i^k(\phi) := \varphi_i^0(\phi - \phi_k), \quad k=1,\ldots,5. \tag{2.14}$$

Note that, if we choose the reference modes for $k=0$ possessing the parity property,

$$\varphi_i^0(\phi) = (-1)^i \varphi_i^0(-\phi), \tag{2.15}$$

then (2.14) implies

$$\varphi_i^{k'}(\phi) = (-1)^i \varphi_i^k(R_l\phi), \tag{2.16}$$

which are fulfilled by the pair of reference modes at the two singular points ϕ_k and ϕ_k' mapped under the reflection R_l as

$$\phi_{k'} = R_l\phi_k. \tag{2.17}$$

With this choice of the reference modes, following (2.11) we introduce the boundary vectors

$$B_k(\psi) := \begin{pmatrix} W[\psi,\varphi_1^k]_{\phi_k+} \\ W[\psi,\varphi_1^k]_{\phi_k-} \end{pmatrix}, \quad B_k'(\psi) := \begin{pmatrix} W[\psi,\varphi_2^k]_{\phi_k+} \\ -W[\psi,\varphi_2^k]_{\phi_k-} \end{pmatrix}, \tag{2.18}$$

for $k=$even, and

$$B_k(\psi) := \begin{pmatrix} W[\psi,\varphi_1^k]_{\phi_k-} \\ W[\psi,\varphi_1^k]_{\phi_k+} \end{pmatrix}, \quad B_k'(\psi) := \begin{pmatrix} -W[\psi,\varphi_2^k]_{\phi_k-} \\ W[\psi,\varphi_2^k]_{\phi_k+} \end{pmatrix}, \tag{2.19}$$

for $k=$odd. As in (2.13), the connection conditions at $\phi=\phi_k$ for all k are provided by

$$(U_k - \mathbf{1}_2)B_k(\psi) + i(U_k + \mathbf{1}_2)B_k'(\psi) = 0, \tag{2.20}$$

with matrices $U_k \in \mathrm{U}(2)$ characterizing the singularities at $\phi=\phi_k$. We mention that (2.16) implies that these boundary vectors are related as

$$B_k(R_l\psi) = B_{k'}(\psi), \quad B_k'(R_l\psi) = B_{k'}'(\psi), \tag{2.21}$$

for the two singular points connected by (2.17).

Now, turning to the radial part, we introduce from the radial Hamiltonian $H_{r,\lambda}$ the new operator

$$\mathcal{H}_{r,\lambda} := \sqrt{r} \circ H_{r,\lambda} \circ \frac{1}{\sqrt{r}} = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{3}{8}\omega^2 r^2 + \frac{\lambda - \frac{1}{4}}{r^2}. \tag{2.22}$$

Note that the self-adjointness of $\mathcal{H}_{r,\lambda}$ with respect to the measure $\mathrm{d}r$ implies the self-adjointness of $H_{r,\lambda}$ with respect to the radial measure $r\,\mathrm{d}r$. It is known (see, *e.g.*, Ref. 25) that for $\lambda \geqslant 1$ the operator $\mathcal{H}_{r,\lambda}$ is essentially self-adjoint, while for $\lambda < 1$ it admits a $U(1)$ family of self-adjoint extensions. The family can be specified by the boundary condition for the radial wave function $\rho(r)$, which is given, using the Wronskian in the radial part, by

$$\frac{W[\rho,\varphi_1]_{0+}}{W[\rho,\varphi_2]_{0+}} = -\kappa(\lambda). \tag{2.23}$$

TABLE I. Character table of mirror-S_3.

Conjugacy class	$\{e\}$	$\{R_i\}$	$\{(\mathcal{R}_{\pi/3})^{\pm 2}\}$
Identity rep χ^+	1	1	1
Signature rep χ^-	1	−1	1
2-dim rep $\chi^{(2)}$	2	0	−1

Here, $\varphi_i(r)$ $(i=1,2)$ are the reference modes for the radial part which are eigenfunctions of $\mathcal{H}_{r,\lambda}$ and normalized as $W[\varphi_1,\varphi_2]=1$. Note that the real number $\kappa(\lambda)$ (which includes $\kappa(\lambda)=\infty$) characterizes the singularity at $r=0$ and is dependent on the angular eigenvalue λ in general.

C. Mirror-S_3 and scale invariant quantizations

In our scheme of quantization, we have the set of parameters in U_k, $k=0,\ldots,5$ and $\kappa(\lambda)$ which specify the connection/boundary conditions and thereby the self-adjoint extensions of the Hamiltonian. These conditions are subjected to the symmetry we wish to bestow with the quantized model. For the symmetry of the model, one may assume, for instance, that the three particles are identical physically. Since the three possible exchanges of the particles are generated by the reflections, P_i $(i=1,2,3)$, which form an S_3 group, the invariance under the reflections implies the "exchange-S_3" group as the symmetry of the model. One may further assume that the pairwise collision be physically independent of the position of the remaining spectator particle. This leads to the D_6 symmetry mentioned in Sec. I, and the quantizations with this symmetry have been presented in Ref. 25.

In this paper, we relax our demand and assume only the symmetry under the "mirror-S_3" group, which is generated by the reflections, R_i $(i=1,2,3)$, consisting of the elements $\{e,R_i,(\mathcal{R}_{\pi/3})^{\pm 2}\}$ with e being the identity. In physical terms, this demand ensures the invariance of the model under all cyclic permutations of the particles; for example, if $x_1<x_2<x_3$, the interaction in the limit $x_2\to x_1$ is identical to that in the limit $x_2\to x_3$ when the spectator particle is fixed. In our scheme, this is equivalent to the requirement that all U_k be identical, i.e.,

$$U_k = U, \quad k=0,1,2,3,4,5, \tag{2.24}$$

for some $U\in \mathrm{SU}(2)$. Indeed, when combined with (2.21), the property (2.24) ensures that the boundary conditions are compatible with all the reflections in the mirror-S_3 group. Once the mirror-S_3 is installed as a symmetry in the angular part, we can classify the eigenstates of the operator H_Ω in (2.5) in terms of the representations of the group S_3, which has two one-dimensional and one two-dimensional irreducible representations (see Table I).

Another property we wish to have comes from the observation that the Hamiltonian (2.3) acquires a formal scale invariance in the limit $\omega\to 0$. Namely, we demand that this scale symmetry be maintained in the limit in our inequivalent quantizations, so that our quantized model is smoothly connected to the model with a pure inverse square potential. Roughly speaking, the scale symmetry breaks down at the quantum level when we allow the parameters of self-adjoint extensions to bear nontrivial scale dimensions (see Ref. 28). For the mirror-S_3 invariant quantizations we are considering, a sufficient condition prohibiting such scale parameters is that

$$U=\pm \mathbf{1}_2, \quad \text{or} \quad U=V\sigma_3 V^{-1}, \quad V\in \mathrm{SU}(2), \tag{2.25}$$

for the angular part specified by (2.24), and that

$$\kappa(\lambda)=0, \quad \text{or} \quad \kappa(\lambda)=\infty \quad \text{for each } \lambda, \tag{2.26}$$

for the radial part (2.23). In the present paper, we shall restrict ourselves to the class of inequivalent quantizations fulfilling (2.24)–(2.26).

III. ANGULAR PART

We now discuss inequivalent quantizations for the angular part in detail. Among the scale invariant choices (2.25) the cases $U=\pm\mathbf{1}_2$, which are parity invariant, have already been treated in Ref. 25 and will not be discussed here. To analyze the remaining cases $U=V\sigma_3V^{-1}$, we consider V for which $U\neq\pm\sigma_3$ and $U=\pm\sigma_3$, separately. This separate treatment is required since for the latter case the angular part breaks into six sectors $s_k=(\phi_{k-1},\phi_k)$, $k=1,\ldots,6$, which are physically disconnected at the singular points (see Fig. 1). The treatment is based on a set of basic solutions, which are used to analyze both the connected and the separated cases later.

A. Basic solutions

For convenience, we first set $\lambda=9\mu^2$ allowing for complex μ for $\lambda<0$. The two independent solutions for (2.6) are given[25] by

$$v_{1,\mu}(\phi)=|\sin 3\phi|^{\nu}F\left(\frac{\nu+\mu}{2},\frac{\nu-\mu}{2},\nu+\frac{1}{2};\sin^2 3\phi\right), \tag{3.1}$$

$$v_{2,\mu}(\phi)=|\sin 3\phi|^{1-\nu}F\left(\frac{1-\nu-\mu}{2},\frac{1-\nu+\mu}{2},\frac{3}{2}-\nu;\sin^2 3\phi\right), \tag{3.2}$$

where $F(\alpha,\beta,\gamma;z)$ is the standard hypergeometric function. For the reference modes needed in the connection condition at the singularity $\phi=\phi_0$, we choose

$$\varphi_1^0(\phi)=\frac{1}{\sqrt{3(2\nu-1)}}v_{1,\mu_0}(\phi)[\Theta(\phi)-\Theta(-\phi)], \tag{3.3}$$

$$\varphi_2^0(\phi)=-\frac{1}{\sqrt{3(2\nu-1)}}v_{2,\mu_0}(\phi), \tag{3.4}$$

with some real μ_0, where $\Theta(\phi)$ is the Heaviside step function. The reference modes for the connection condition at the singularity $\phi=\phi_k$ are provided according to (2.14). We introduce the shorthand,

$$a_1(\mu)=v_{1,\mu}\left(\frac{\pi}{6}-0\right)=\frac{\Gamma\left(\nu+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\nu+\mu+1}{2}\right)\Gamma\left(\frac{\nu-\mu+1}{2}\right)}, \tag{3.5}$$

$$a_2(\mu)=v_{2,\mu}\left(\frac{\pi}{6}-0\right)=\frac{\Gamma\left(\frac{3}{2}-\nu\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(1-\frac{\nu+\mu}{2}\right)\Gamma\left(1-\frac{\nu-\mu}{2}\right)}, \tag{3.6}$$

$$b_1(\mu)=v'_{1,\mu}\left(\frac{\pi}{6}-0\right)=\frac{6\Gamma\left(\nu+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\nu+\mu}{2}\right)\Gamma\left(\frac{\nu-\mu}{2}\right)}, \tag{3.7}$$

$$b_2(\mu)=v'_{2,\mu}\left(\frac{\pi}{6}-0\right)=\frac{6\Gamma\left(\frac{3}{2}-\nu\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-\nu-\mu}{2}\right)\Gamma\left(\frac{1-\nu+\mu}{2}\right)}. \tag{3.8}$$

and

$$\alpha=\frac{a_1a_2}{3(2\nu-1)},\quad \beta=\frac{b_1b_2}{3(2\nu-1)},\quad \gamma=\frac{a_1b_2+a_2b_1}{3(2\nu-1)}=-\frac{\cos\pi\mu}{\cos\pi\nu}, \tag{3.9}$$

which fulfill the relation

$$\alpha\beta = \tfrac{1}{4}(\gamma^2 - 1). \tag{3.10}$$

In terms of these, as a set of basic solutions in sector s_1, we furnish the symmetric and antisymmetric eigenfunctions,

$$\eta^1_{+,\mu}(\phi) = \begin{cases} b_2(\mu)v_{1,\mu}(\phi) - b_1(\mu)v_{2,\mu}(\phi) & \left(0 < \phi \leqslant \dfrac{\pi}{6}\right) \\ b_2(\mu)v_{1,\mu}\left(\dfrac{\pi}{3} - \phi\right) - b_1(\mu)v_{2,\mu}\left(\dfrac{\pi}{3} - \phi\right) & \left(\dfrac{\pi}{6} \leqslant \phi < \dfrac{\pi}{3}\right) \\ 0 & \left(2\pi > \phi > \dfrac{\pi}{3}\right), \end{cases} \tag{3.11}$$

$$\eta^1_{-,\mu}(\phi) = \begin{cases} a_2(\mu)v_{1,\mu}(\phi) - a_1(\mu)v_{2,\mu}(\phi) & \left(0 < \phi \leqslant \dfrac{\pi}{6}\right) \\ -a_2(\mu)v_{1,\mu}\left(\dfrac{\pi}{3} - \phi\right) + a_1(\mu)v_{2,\mu}\left(\dfrac{\pi}{3} - \phi\right) & \left(\dfrac{\pi}{6} \leqslant \phi < \dfrac{\pi}{3}\right) \\ 0 & \left(2\pi > \phi > \dfrac{\pi}{3}\right). \end{cases} \tag{3.12}$$

Likewise, we also introduce the basic solutions in sector s_k from these by translation,

$$\eta^k_{\pm,\mu}(\phi) = \eta^1_{\pm,\mu}(\phi - \phi_{k-1}), \quad k = 2, \ldots, 6. \tag{3.13}$$

The general solution is then given by a linear combination of these basic solutions with appropriate coefficients $c^k_\pm$,

$$\psi_\mu(\phi) = \sum_{k=1}^{6} (c^k_+ \eta^k_{+,\mu}(\phi) + c^k_- \eta^k_{-,\mu}(\phi)). \tag{3.14}$$

Out of these basic solutions each having their support in one sector, we also introduce a set of solutions having supports on the sectors s_k with k odd or even only:

$$\eta_+ = \sum_{n=1}^{3} \eta^{2n-1}_{+,\mu}, \quad \tilde{\eta}_+ = \sum_{n=1}^{3} \eta^{2n}_{+,\mu}, \tag{3.15}$$

$$\eta_- = \sum_{n=1}^{3} (-1)^n \eta^{2n-1}_{-,\mu}, \quad \tilde{\eta}_- = \sum_{n=1}^{3} (-1)^n \eta^{2n}_{-,\mu}. \tag{3.16}$$

B. Connected case

To analyze the connected case

$$U = V\sigma_3 V^{-1}, \quad U \neq \pm\sigma_3, \tag{3.17}$$

we parametrize the characteristic matrix, using a real ξ and a complex ζ, as

$$U = \begin{pmatrix} \xi & \zeta \\ \zeta^* & -\xi \end{pmatrix}, \quad \xi^2 + |\zeta|^2 = 1. \tag{3.18}$$

In terms of the vectors defined from the coefficients in the general solutions (3.14),

$$C^k = \begin{pmatrix} c_+^k \\ c_-^k \end{pmatrix}, \tag{3.19}$$

we find that the connection conditions (2.20) become the matrix equations,

$$C^{2n} = T_+ C^{2n-1}, \quad C^{2n+1} = T_- C^{2n}, \tag{3.20}$$

with the transfer matrices defined at the singularities between odd-even and even-odd sectors,

$$T_+ = \frac{1}{\zeta}\begin{pmatrix} -\xi+\gamma & -2\alpha \\ -2\beta & \xi+\gamma \end{pmatrix}, \quad T_- = \frac{1}{\zeta^*}\begin{pmatrix} \xi+\gamma & -2\alpha \\ -2\beta & -\xi+\gamma \end{pmatrix}, \tag{3.21}$$

where α, β, and γ are given in (3.9). These relations lead to the consistency condition,

$$TC^1 = C^1, \quad T := T_- T_+ T_- T_+ T_- T_+. \tag{3.22}$$

From this we find $\det(T-I)=0$, which implies

$$\gamma^2 = 1 \quad \text{or} \quad \gamma^2 = \frac{1+3\xi^2}{4}. \tag{3.23}$$

These determine the spectrum μ in the angular part.

To examine the case $\gamma^2=1$ in (3.23), we note from (3.10) that the condition implies that either a_1, a_2, b_1 or b_2 must vanish. None of these are compatible with each other, and we consider them separately. First, we find that $a_1=0$ occurs when

$$\mu = \nu + 1 + 2m, \quad m = 0, 1, \ldots . \tag{3.24}$$

We then have

$$T = \begin{pmatrix} 1 & 0 \\ \dfrac{12\beta}{1-\xi} & 1 \end{pmatrix}, \tag{3.25}$$

and from this we find the coefficient vectors C^k to obtain, up to a constant, the corresponding eigenfunctions

$$\tilde{\psi}_-(\phi) = \frac{1-\xi}{\zeta^*}\eta_-(\phi) + \tilde{\eta}_-(\phi). \tag{3.26}$$

These eigenfunctions belong to the signature representation χ^- of S_3. Second, $a_2=0$ occurs when

$$\mu = 2m + 2 - \nu, \quad m = 0, 1, \ldots \tag{3.27}$$

and the transfer matrix is

$$T = \begin{pmatrix} 1 & 0 \\ -\dfrac{12\beta}{1+\xi} & 1 \end{pmatrix}. \tag{3.28}$$

The eigenfunctions are found to be

$$\psi_-(\phi) = \eta_-(\phi) - \frac{1-\xi}{\zeta}\tilde{\eta}_-(\phi), \tag{3.29}$$

which again belong to the signature representation χ^- of S_3. Third, $b_1=0$ occurs when

$$\mu = \nu + 2m, \quad m = 0,1, \ldots \ . \tag{3.30}$$

We then have

$$T = \begin{pmatrix} 1 & \dfrac{12\alpha}{1+\xi} \\ 0 & 1 \end{pmatrix}, \tag{3.31}$$

and the eigenfunctions

$$\tilde{\psi}_+(\phi) = -\frac{1-\xi}{\zeta^*}\eta_+(\phi) + \tilde{\eta}_+(\phi), \tag{3.32}$$

which belong to the identity representation χ^+ of S_3. Finally, if $b_2=0$, we find

$$\mu = |1 - \nu + 2m|, \quad m = 0,1,\ldots \tag{3.33}$$

and

$$T = \begin{pmatrix} 1 & -\dfrac{12\alpha}{1-\xi} \\ 0 & 1 \end{pmatrix}. \tag{3.34}$$

We obtain the eigenfunctions

$$\psi_+(\phi) = \eta_+(\phi) + \frac{1-\xi}{\zeta}\tilde{\eta}_+(\phi), \tag{3.35}$$

belonging to the identity representation χ^+ of S_3.

When the second condition $\gamma^2=(1+3\xi^2)/4$ in (3.23) holds, on the other hand, we have $T=\mathbf{1}_2$ and hence C^1 is left undetermined. For definiteness we may choose C^1 as an eigenvector of the rotation $\mathcal{R}^2_{\pi/3}$. The transfer matrix that corresponds to $\mathcal{R}^2_{\pi/3}$ is

$$T_-T_+ = \begin{pmatrix} -\dfrac{1}{2} & -\dfrac{4\alpha(\gamma+\xi)}{1-\xi^2} \\ -\dfrac{4\beta(\gamma-\xi)}{1-\xi^2} & -\dfrac{1}{2} \end{pmatrix}, \tag{3.36}$$

which has the eigenvectors

$$X_\pm = \begin{pmatrix} 2\alpha \\ \pm\sqrt{3}i(-\xi+\gamma) \end{pmatrix}. \tag{3.37}$$

With these eigenvectors, the vectors $C^k_\pm$ may be written as

$$C^{2n-1}_\pm = \mathrm{J}^{\mp n}X_\pm, \quad C^{2n}_\pm = \mathrm{J}^{\mp n}T_+X_\pm, \quad \mathrm{J} := \frac{-1+i\sqrt{3}}{2}. \tag{3.38}$$

If we denote by $\psi^{(\pm)}_1$ the eigenfunction corresponding to $C^k_\pm$ with $\gamma>0$, and similarly by $\psi^{(\pm)}_2$ the eigenfunction corresponding to $C^k_\pm$ with $\gamma<0$, then

$$\mathcal{R}^2_{\pi/3}\psi^{(\pm)}_i = \mathrm{J}^{\pm 1}\psi^{(\pm)}_i, \quad R_2\psi^{(\pm)}_i = \psi^{(\mp)}_i, \quad i = 1,2. \tag{3.39}$$

To find the spectrum of these eigenstates, we combine (3.23) and the last equation of (3.9) to obtain

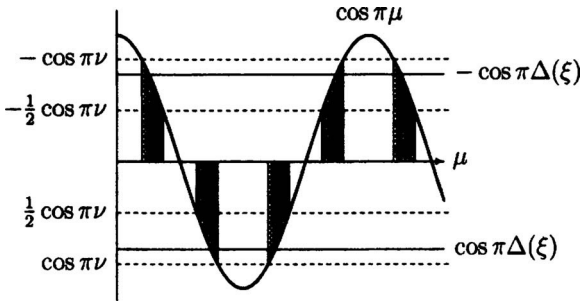

FIG. 2. Eigenvalues μ arise at the intersections of $\cos \pi\mu$ and the two lines $\pm\cos \Delta(\xi)$, which are shown here for the values $\nu=0.8$ and $\xi=\frac{5}{6}$. Dashed lines represent the upper and the lower limits of the lines, and the shaded regions indicate the allowed ranges of the eigenvalues.

$$\cos \pi\mu = \mp \cos \pi\Delta(\xi), \quad \Delta(\xi) := \frac{1}{\pi}\mathrm{Arccos}\left(\frac{\sqrt{1+3\xi^2}}{2}\cos \pi\nu\right). \tag{3.40}$$

The solutions for μ will furnish the eigenvalues, which occur periodically as displayed in Fig. 2. We then see that the eigenvalues for $\gamma>0$ are given by

$$\mu = \begin{cases} 2m+1-\Delta(\xi) \\ 2m+1+\Delta(\xi), \end{cases} \tag{3.41}$$

whereas the eigenvalues for $\gamma<0$ are

$$\mu = \begin{cases} 2m+2-\Delta(\xi) \\ 2m+\Delta(\xi), \end{cases} \tag{3.42}$$

where $m=0,1,\ldots$. Since $|\xi| \leqslant 1$, we find that $\Delta(\xi)$ stays in the range,

$$\Delta(0) \leqslant \Delta(\xi) \leqslant \Delta(1) = \nu. \tag{3.43}$$

The eigenvalues and eigenfunctions are summarized in Table II.

C. Separated case

Next we analyze the case

$$U = \sigma_3, \tag{3.44}$$

under which all the sectors s_k are physically separated from each other. (The other separated case $U=-\sigma_3$ can be dealt with similarly and will not be discussed here.) To proceed, we note that under the choice (3.44) the boundary condition (2.20) reads

TABLE II. Eigenvalues and eigenfunctions in the connected case.

Eigenvalue μ	Eigenfunction	Rep of S_3
$2m+1+\nu$	$\tilde{\psi}_-$	χ^-
$2m+2-\nu$	ψ_-	χ^-
$2m+\nu$	$\tilde{\psi}_+$	χ^+
$\lvert 2m+1-\nu\rvert$	ψ_+	χ^+
$2m+1-\Delta(\xi)$	$\psi_1^{(+)}, \psi_1^{(-)}$	$\chi^{(2)}$
$2m+1+\Delta(\xi)$		
$2m+2-\Delta(\xi)$	$\psi_2^{(+)}, \psi_2^{(-)}$	$\chi^{(2)}$
$2m+\Delta(\xi)$		

TABLE III. Eigenvalues and eigenfunctions in the separated case.

Eigenvalue μ	Eigenfunction	Rep of S_3
$2m+1+\nu$	$\tilde{\eta}_-$	χ^-
	$\tilde{\eta}_-^{(+)}, \tilde{\eta}_-^{(-)}$	$\chi^{(2)}$
$2m+\nu$	$\tilde{\eta}_+$	χ^+
	$\tilde{\eta}_+^{(+)}, \tilde{\eta}_+^{(-)}$	$\chi^{(2)}$
$2m+2-\nu$	η_-	χ^-
	$\eta_-^{(+)}, \eta_-^{(-)}$	$\chi^{(2)}$
$\lvert 2m+1-\nu \rvert$	η_+	χ^+
	$\eta_+^{(+)}, \eta_+^{(-)}$	$\chi^{(2)}$

$$b_2 C_+^{2n-1} = a_2 C_-^{2n-1} = b_1 C_+^{2n} = a_1 C_-^{2n} = 0. \tag{3.45}$$

As before, the vanishing conditions of a_1, a_2, b_1, and b_2 are not compatible, and we consider them separately. Recall, first, that $a_1=0$ is realized by μ in (3.24). The vectors C^k obtained in this case lead to the eigenfunctions $\tilde{\eta}_-$ belonging to the signature representation χ^-, and also

$$\tilde{\eta}_-^{(\pm)} = \sum_{n=1}^{3} \mathrm{J}^{\mp n} \eta_{-,\mu}^{2n}, \tag{3.46}$$

which belong to the doublet representation $\chi^{(2)}$. Second, $a_2=0$ is realized by μ in (3.27), and the corresponding eigenfunctions are given by η_- belonging to χ^-, and

$$\eta_-^{(\pm)} = \sum_{n=1}^{3} \mathrm{J}^{\mp n} \eta_{-,\mu}^{2n-1}, \tag{3.47}$$

which belong to $\chi^{(2)}$. Third, $b_1=0$ occurs when μ is given by (3.30). The eigenfunctions are found to be $\tilde{\eta}_+$ belonging to χ^+, and

$$\tilde{\eta}_+^{(\pm)} = \sum_{n=1}^{3} \mathrm{J}^{\mp n} \eta_{+,\mu}^{2n}, \tag{3.48}$$

which belong to $\chi^{(2)}$. Finally, $b_2=0$ occurs when μ is given by (3.33). The eigenfunctions are η_+ belonging to χ^+, and

$$\eta_+^{(\pm)} = \sum_{n=1}^{3} \mathrm{J}^{\mp n} \eta_{+,\mu}^{2n-1}, \tag{3.49}$$

which belong to $\chi^{(2)}$. These eigenvalues and the eigenfunctions are summarized in Table III. The spectral behavior of the two cases is shown in Fig. 3 (left).

At this point, we mention that the connected case discussed earlier has a smooth limit to the separated case, that is, the eigenfunctions in the former case can be obtained formally from those in the latter case by considering the limit $U \to \sigma_3$, even though the two cases require distinctive treatments. For the eigenstates which are singlets of the mirror-S_3, this can be seen at once since the eigenfunctions in the connected case reduce to

$$\psi_+ \to \eta_+, \quad \psi_- \to \eta_-, \quad \tilde{\psi}_+ \to \tilde{\eta}_+, \quad \tilde{\psi}_- \to \tilde{\eta}_-, \tag{3.50}$$

in the limit $\xi \to 1$, which is equivalent to $U \to \sigma_3$; see (3.18). To see that the same is true for the doublets, consider the case $a_1=0$ in which the eigenstates vanish $\psi_+^{(\pm)} \to 0$ in the limit. Nonvanishing outcomes in the limit may be obtained, however, by rescaling them properly as

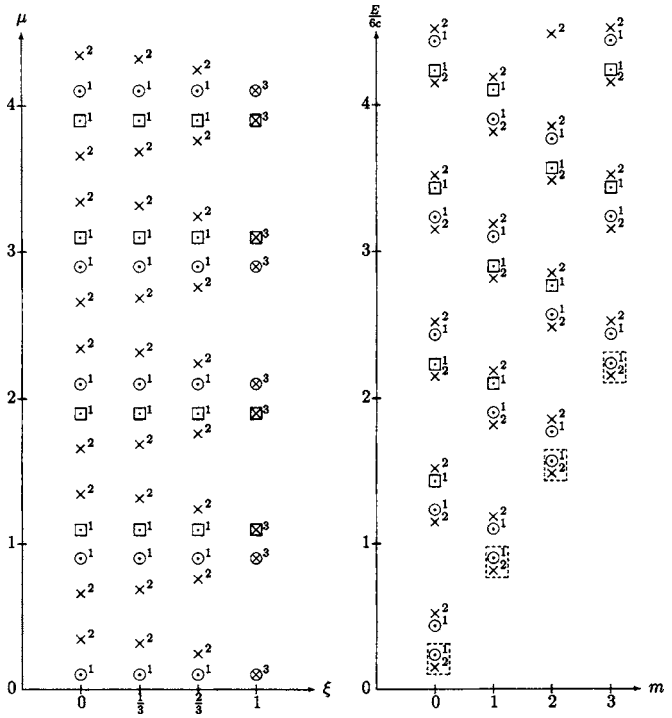

FIG. 3. The spectra of μ for various ξ (left), and the total energy E for $m=0,1,2,3$ (right). The spectra of μ are plotted for $\xi=0,\frac{1}{3},\frac{2}{3},1$ under $\nu=0.9$, which interpolate between $U=V^{-1}\sigma_3 V$ and $U=\sigma_3$. The energy spectrum of E (in units of $6c$) is obtained for $\nu=0.9$ and $\xi=\frac{5}{6}$. The signs inside the dashed squares for the lowest two levels to each m in the energy spectrum of E represent the levels arising for $\kappa(\lambda)=\infty$, which is allowed only for these two levels. All other levels are obtained for the choice $\kappa(\lambda)=0$. Symbols used to plot the levels show the representations of the mirror-S_3 group; the symbol $\odot$ stands for the identity representation χ^+, $\boxdot$ for the signature representation χ^-, and $\times$ for the two-dimensional representation $\chi^{(2)}$, respectively. (The superimposed symbols $\otimes$ and $\boxtimes$ indicate that the levels are degenerate by the corresponding distinct representations.) The numbers $1,2,3$ on the upper right of the symbols show the total multiplicities of the levels.

$$\frac{-8i}{\zeta^*\sqrt{3}}\psi_1^{(\pm)} \to \tilde{\eta}_-^{(\pm)}. \tag{3.51}$$

Similarly, for $a_2=0$, we find

$$\frac{i}{2\sqrt{3}}\psi_2^{(\pm)} \to \eta_-^{(\pm)}. \tag{3.52}$$

The continuity in the remaining cases $b_1=0$, $b_2=0$ can also be argued analogously.

IV. RADIAL PART AND THE TOTAL ENERGY SPECTRUM

A. Radial part

The eigenfunctions for the radial part can be obtained immediately, since there remain only two choices (2.26) for the inequivalent quantizations under the scale invariance we have imposed. Note that the radial Hamiltonian $\mathcal{H}_{r,\lambda}$ admits the two independent solutions,[25]

$$\rho_{E,1}(r) = (\sqrt{c}r)^{\sqrt{\lambda}+1/2} e^{-(1/2)cr^2} \Phi\left(\frac{1+\sqrt{\lambda}}{2} - \frac{E}{4c}, 1+\sqrt{\lambda}; cr^2\right), \tag{4.1}$$

$$\rho_{E,2}(r) = (\sqrt{c}r)^{-\sqrt{\lambda}+1/2} e^{-(1/2)cr^2} \Phi\left(\frac{1-\sqrt{\lambda}}{2} - \frac{E}{4c}, 1-\sqrt{\lambda}; cr^2 \right), \tag{4.2}$$

where $\Phi(a,b;z)$ is the confluent hypergeometric function and $c := \sqrt{(3/8)}\omega$. Since these two solutions diverge generically as $r \to \infty$, the square integrability requires that the eigenfunctions be proportional to their linear combination,

$$\rho_E(r) = \frac{\Gamma(1-\sqrt{\lambda})}{\Gamma\left(\frac{1-\sqrt{\lambda}}{2} - \frac{E}{4c} \right)} \rho_{E,1}(r) - \frac{\Gamma(1+\sqrt{\lambda})}{\Gamma\left(\frac{1+\sqrt{\lambda}}{2} - \frac{E}{4c} \right)} \rho_{E,2}(r), \tag{4.3}$$

which vanishes as $r \to \infty$.

To enforce (2.26), we choose the reference modes as

$$\varphi_1(r) = (2\sqrt{\lambda c})^{-1/2} \rho_{E,1}(r), \quad \varphi_2(r) = -(2\sqrt{\lambda c})^{-1/2} \rho_{E,2}(r). \tag{4.4}$$

With these the radial boundary condition (2.23) reads

$$\kappa(\lambda) = \frac{\Gamma(1+\sqrt{\lambda})\Gamma\left(\frac{1-\sqrt{\lambda}}{2} - \frac{E}{4c} \right)}{\Gamma(1-\sqrt{\lambda})\Gamma\left(\frac{1+\sqrt{\lambda}}{2} - \frac{E}{4c} \right)}. \tag{4.5}$$

For the case $\kappa(\lambda)=0$, the solutions and the energy eigenvalues are

$$\rho_E(r) = r^{\sqrt{\lambda}+1/2} e^{-(1/2)cr^2} L_m^{\sqrt{\lambda}}(cr^2), \quad E = E(m,\lambda) = 2c(2m+1+\sqrt{\lambda}), \tag{4.6}$$

for $m=0,1,\ldots$, where $L_m^{\sqrt{\lambda}}$ is the (generalized) Laguerre polynomial. Analogously, for the case $\kappa(\lambda)=\infty$ we find

$$\rho_E(r) = r^{-\sqrt{\lambda}+1/2} e^{-(1/2)cr^2} L_m^{-\sqrt{\lambda}}(cr^2), \quad E = E(m,\lambda) = 2c(2m+1-\sqrt{\lambda}), \tag{4.7}$$

for $m=0,1,\ldots$. As noted earlier, these two types of solutions arise only for $\lambda<1$; otherwise only the former solution (4.6) is allowed. This solution (4.6) is in fact the one used by Calogero[1] and also conventionally adopted by others[16,17,20] for all values of λ.

B. Total energy spectra

Having obtained the solutions for both the radial and the angular parts, we now construct the solutions for the entire (relative coordinates) system (2.5) by combining the solutions of the respective parts as

$$\psi_E(r;\lambda) = \frac{1}{\sqrt{r}} \rho_E(r) \psi_\mu(\phi), \quad E = E(m,\lambda = 9\mu^2), \tag{4.8}$$

where we have denoted the angular solutions by $\psi_\mu(\phi)$ collectively. These solutions $\rho_E(r)$ and $\psi_\mu(\phi)$ are dependent on the parameters $\kappa(\lambda)$ and ξ,ζ that specify the inequivalent quantizations of the respective part.

It is important, however, to note that not all combinations of them are allowed because the choice $\kappa(\lambda)=\infty$ is available only if $\lambda<1$. In fact, one can readily see that $\kappa(\lambda)=\infty$ is possible, at most, for the lowest two angular eigenvalues $\lambda=\lambda_1$ or $\lambda=\lambda_2$, where

$$\lambda_1 := 9(1-\nu)^2, \quad \lambda_2 := 9(1-\Delta)^2, \tag{4.9}$$

and that $\kappa(\lambda)=0$ for all other λ which are above the two. More explicitly, the case $\kappa(\lambda)=\infty$ is admitted for λ_1 if

TABLE IV. Possible choices of $\kappa(\lambda_1)$ and $\kappa(\lambda_2)$.

Range of ν	$\kappa(\lambda_1)$	$\kappa(\lambda_2)$
$\frac{1}{2}<\nu\leqslant\frac{2}{3}$	0	0
$\frac{2}{3}<\nu\leqslant 1-\nu_0$	0 or ∞	0
$1-\nu_0<\nu<1+\nu_0$	0 or ∞	0 or ∞
$1+\nu_0\leqslant\nu<\frac{4}{3}$	0 or ∞	0
$\frac{4}{3}\leqslant\nu<\frac{3}{2}$	0	0

$$\tfrac{2}{3}<\nu<\tfrac{4}{3}, \tag{4.10}$$

and for λ_2 if

$$1-\nu_0<\nu<1+\nu_0, \quad \nu_0=\frac{1}{\pi}|\arctan\sqrt{3}\xi|. \tag{4.11}$$

Since the condition (4.11) is stricter than (4.10), available choices for the inequivalent quantizations depend on the value of ν, as summarized in Table IV.

For illustration, we show in Fig. 3 the angular spectrum (left) for various values of ξ, and the total energy spectrum (right) for different choices of the $\kappa(\lambda)$ parameters. We observe that if $\kappa(\lambda)=0$ for all λ the energy levels are made of one single series, consisting of a regular pattern formed by four singlets and four doublets. The equispaced levels suggest that, for this case, the Calogero model may be solved by use of the ladder operator, as demonstrated for the special case[7,8] which amounts to $U=-I$ and $\kappa(\lambda)=0$ in our scheme.

V. SPECTRAL PRESERVING SU(2) AND THE ANGULAR SPECTRUM

The angular spectrum obtained in Sec. III is independent of the phase of the parameter ζ even though the eigenfunctions are dependent on it. In particular, the levels of the mirror-S_3 singlets depend on neither of the parameters ξ and ζ and hence are independent of the choice of V in $U=V\sigma_3V^{-1}$. In fact, these are a consequence of the spectral preserving SU(2) (or its subgroup U(1)) transformations[29] which are found in the family of inequivalent quantizations we are considering here.

To see this, let us first consider the reflection transformation Q_1 given by $Q_1:=P_3$ in (2.7). Observe that the action (2.9) on the states,

$$\psi(\phi)\to(Q_1\psi)(\phi)=\psi(-\phi), \tag{5.1}$$

is *spectrum-preserving* in the sense that if ψ_λ is an eigenstate of the angular operator H_Ω as in (2.5) with eigenvalue λ, then

$$H_\Omega(Q_1\psi_\lambda)(\phi)=\lambda(Q_1\psi_\lambda)(\phi), \tag{5.2}$$

on account of the formal invariance of the operator H_Ω under Q_1. Note that this does not imply that Q_1 is a symmetry unless it is compatible with the boundary conditions specified by U. For the boundary vectors, we find

$$B_k(Q_1\psi)=\sigma_1B_{6-k}(\psi), \quad B'_k(Q_1\psi)=\sigma_1B'_{6-k}(\psi), \tag{5.3}$$

for $k=0,\ldots,5$, with the identification $B_0=B_6$ and $B'_0=B'_6$. Thus, in effect, the transformation Q_1 induces in the connection conditions (2.20) the change

$$U\to\sigma_1U\sigma_1. \tag{5.4}$$

It follows that the operator H_Ω shares the same spectrum under the boundary conditions specified by U and $\sigma_1U\sigma_1$.

We next consider the "alternate reflection" defined by

$$\psi(x) \to (Q_3\psi)(\phi) := \begin{cases} \psi(\phi), & \phi_{2k} < \phi < \phi_{2k+1} \\ -\psi(\phi), & \phi_{2k+1} < \phi < \phi_{2k+2}. \end{cases} \tag{5.5}$$

Evidently, this is also spectral-preserving, and on the boundary vectors we have

$$B_k(Q_3\psi) = \sigma_3 B_k(\psi), \quad B'_k(Q_3\psi) = \sigma_3 B'_k(\psi). \tag{5.6}$$

Accordingly, we find that the alternate reflection (5.5) induces

$$U \to \sigma_3 U \sigma_3 \tag{5.7}$$

in the connection conditions (2.20). From Q_1 and Q_3 we further define the product transformation $Q_2 := iQ_1Q_3$ that yields

$$B_k(Q_2\psi) = \sigma_2 B_{6-k}(\psi), \quad B'_k(Q_2\psi) = \sigma_2 B'_{6-k}(\psi). \tag{5.8}$$

By construction, Q_2 is spectral-preserving and induces

$$U \to \sigma_2 U \sigma_2. \tag{5.9}$$

Consequently, we see that the connection conditions by U and $\sigma_i U \sigma_i$ for all $i=1,2,3$ give rise to the same spectrum for the operator H_Ω. Note that Q_i's form the $su(2)$ algebra,

$$[Q_i, Q_j] = 2i\epsilon^{ijk} Q_k. \tag{5.10}$$

Suppose, now that the state ψ is in a singlet representation of the mirror-S_3, i.e., it is an eigenstate of R_i with fixed eigenvalues ± 1 for all $i=1,2,3$. The state ψ is then a periodic function with period $2\pi/3$, and hence we have $B_k(\psi)=B_{-k}(\psi)$ and $B'_k(\psi)=B'_{-k}(\psi)$. The three relations (5.3), (5.6), and (5.8) can then be combined as

$$B_k(Q_i\psi) = \sigma_i B_k(\psi), \quad B'_k(Q_i\psi) = \sigma_i B'_k(\psi), \quad i = 1,2,3. \tag{5.11}$$

On account of the linearity of B_k and B'_k observed in (5.11) and the algebraic property (5.10), we find that a linear combination of the Q_i's,

$$Q = \sum_{i=1}^{3} c_i Q_i, \quad \sum_{i=1}^{3} c_i^2 = 1, \tag{5.12}$$

with arbitrary coefficients c_i fulfills $Q^2=I$ and is also spectral-preserving for singlet states. On the matrix U, this induces

$$U \to \sigma U \sigma, \quad \sigma = \sum_{i=1}^{3} c_i \sigma_i. \tag{5.13}$$

It can be shown[29] that by choosing c_i appropriately one finds σ such that $\sigma U \sigma = V^{-1}UV$ for any $V \in \mathrm{SU}(2)$. In other words, the transformation generated by Q in (5.12) yields the change

$$U \to V^{-1}UV, \tag{5.14}$$

without altering the spectrum. It then follows that, as far as the mirror-S_3 singlets are concerned, the operator H_Ω shares the same spectrum under $V^{-1}UV$ for any $V \in \mathrm{SU}(2)$. From this we see that for the scale invariant $U=V\sigma_3 V^{-1}$ we are considering, the spectrum of the mirror-S_3 singlets is independent of V, as we have observed in the last section.

This SU(2)-independence does not hold for the eigenstates in the doublet representation $\chi^{(2)}$ of the mirror-S_3, because for them the transformations Q_1 and Q_2 interchange different boundary vectors as seen in (5.3) and (5.8). However, the transformation Q_3 still maps the boundary vectors

to themselves as (5.6) and can be used to provide a one-parameter family of spectral-preserving transformations $e^{i\theta Q_3}$ for any real θ. On the matrix U, the transformations induce

$$U \to e^{-i\theta\sigma_3} U e^{i\theta\sigma_3}, \tag{5.15}$$

which form a U(1) subgroup of the SU(2) transformations (5.14). In parameters, this allows us to alter the phase of ζ in U freely, which implies that the whole spectrum depends only on $|\zeta|$ or ξ as seen earlier.

Finally, we mention that the universality in the spectrum is a general feature of a circle system with even number $2N$ of singularities that appears when it is quantized under mirror symmetries defined analogously to the present case $2N=6$.

VI. CONCLUSION

In the present paper we studied the inequivalent quantizations of the $N=3$ Calogero model based on the method of separation of variables. Our inequivalent quantizations respect both the mirror-S_3 invariance and the scale invariance. These quantizations are, in a sense, supplemental to the quantizations presented in Ref. 25 which respect the D_6 invariance, in view of the fact that the D_6 is restored when the scale invariance is exchanged for parity invariance in our case. Our symmetry requirement is that all the connection conditions at the singularities in the angular part are specified by a single matrix U of the form (2.26). For a system consisting of a line, this class of singularities is known as the scale invariant family and is given, except for the cases $U=\pm\mathbf{1}_2$, by an S^2 parameter space (see (3.18)). We mention that the scale invariant family supports the Berry phase (or anholonomy) when the singularities are tuned along a cycle on the scale invariant sphere S^2.[30]

In our inequivalent quantizations, we found the eigenstates and eigenvalues explicitly, both for the angular and radial parts that arise after the separation of variables is made. These eigenstates are classified in terms of the irreducible representations of the mirror-S_3 group. We observed that the eigenvalues corresponding to the singlets of the S_3 are independent of the choice of U in the family, whereas those corresponding to the doublets of the S_3 are dependent only on one parameter ξ which corresponds to the coordinate along a great circle on the S^2. We showed that these properties are due to the spectral-preserving SU(2) transformations or U(1) transformations that the scale invariant family possesses.

The scale invariance is strict enough to narrow the possible boundary conditions at $r=0$ in the radial part down to just two types, one given by the Dirichlet condition and the other by the Neumann condition. The Neumann condition is possible if $\lambda<1$, which occurs only for the eigenstates coupled to the lowest two angular levels. The possibility of the Neumann condition brings about a number of different spectra for the total energy, as we have seen in Fig. 3. When all the radial eigenstates adopt the Dirichlet condition irrespective of the eigenvalue λ of the radial level that couples to them, the energy spectrum exhibits a regular pattern consisting of a number of distinct sets of levels which are equispaced from each other. This suggests that for these cases we may also devise the method of the ladder operator to solve the model. In contrast, this seems to be impossible when the Neumann condition is adopted for the lower levels, where the regular pattern is broken at the lowest end of the spectrum. The appearance of the intriguing combination of inequivalent quantizations, which we found in the angular and radial parts in our model, is perhaps a generic feature to be observed in quantizing models of more than two dimensions in general frameworks.

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Scalar field theory at finite temperature in $D=2+1$

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We discuss the φ^6 theory defined in $D=2+1$-dimensional space-time and assume that the system is in equilibrium with a thermal bath at temperature β^{-1}. We use the $1/N$ expansion and the method of the composite operator (Cornwall, Jackiw, and Tomboulis) for summing a large set of Feynman graphs. We demonstrate explicitly the Coleman-Mermin-Wagner theorem at finite temperature. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2159068]

I. INTRODUCTION

The conventional perturbation theory in the coupling constant or in $\hbar$, i.e., the loop expansion can only be used for the study of small quantum corrections to classical results. When discussing quantum mechanical effects to any given order in such an expansion, one is not usually able to justify the neglect of yet higher order. In other words, for theories with a large N dimensional internal symmetry group, there exist another perturbation scheme, the $1/N$ expansion, which circumvents this criticism. Each term in the $1/N$ expansion contains an infinite subset of terms of the loop expansion. The $1/N$ expansion has the nice property that the leading-order quantum corrections are of the same order as the classical quantities. Consequently, the leading order which adequately characterizes the theory in the large N limit preserves much of the nonlinear structure of the full theory.

The scalar field $(\varphi^4)_{D=4}$ theory at finite temperature is of great interest in the field of phase transitions in the early universe and heavy ion collisions. When used as a simple model for the Higgs particle in the standard model of electroweak interactions, it may allow the study of symmetry breaking phase transitions in the early universe. For $N=4$ scalar fields, it is also a model of chiral symmetry breaking in QCD and hence is relevant for the theoretical study of heavy ion collisions. Moreover, this theory is an excellent theoretical laboratory in which analytic nonperturbative methods can be tested. Now for the case $D=3$ it has been shown that, in the large N limit, the φ^6 theory has a UV fixed point and therefore must have a second IR fixed point[1] and for this we could say that at least for large N the $(\varphi^6)_{D=3}$ theory is known to be qualitatively different from $(\varphi^4)_{D=4}$ theory. For other ways, theories in less than four space-time dimensions can offer interesting and complex behavior as well as tractability, and, for example, the case of three space-time dimensions, they can even be directly physical, describing various planar condensed matter systems. For example, the introduction of the φ^6 term generates a rich phase diagram, with the possibility of second order, first order phase transitions or even both transitions occurring simultaneously. This situation defines the tricritical phenomenon. For example, some systems such antiferromagnets in the presence of a strong external field or the He^3-He^4 mixture exhibits such behavior.

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FIG. 1. The 2PI vacuum graphs.

II. THE EFFECTIVE POTENTIAL

The theory for which we are interested is given by the Lagrangian,

$$\mathcal{L}(\varphi) = \frac{1}{2}(\partial_\mu \varphi)^2 - \frac{1}{2}m_0^2\varphi^2 - \frac{\lambda_0}{4!N}\varphi^4 - \frac{\eta_0}{6!N^2}\varphi^6, \tag{1}$$

is a theory of N real scalar fields with $O(N)$ symmetry.

For definiteness, we work at zero temperature; however, the finite temperature generalizations can be easily obtained.[2]

In this section we are going to use the method of composite operator developed by Cornwall, Jackiw, and Tomboulis (CJT)[3,4] in order to get the effective potential $\Gamma(\phi)$ at leading order in the $1/N$ expansion. The composite operator formalism reduces the problem to summing two particle irreducible (2PI) Feynman graphs by defining a generalized effective action $\Gamma(\phi, G)$ which is a functional not only of $\phi_a(x)$, but also of the expectation values $G_{ab}(x,y)$ of the time ordered product of quantum fields $\langle 0|T(\varphi(x)\varphi(y))|0\rangle$, i.e.,

$$\Gamma(\phi, G) = I(\phi) + \frac{i}{2}\mathrm{Tr\ Ln}\, G^{-1} + \frac{i}{2}\mathrm{Tr}\, D^{-1}(\phi)G + \Gamma_2(\phi, G) + \cdots, \tag{2}$$

where $I(\phi) = \int \mathrm{d}x^D\, \mathcal{L}(\phi)$, G and D are matrices in both the functional and the internal space whose elements are $G_{ab}(x,y)$, $D_{ab}(\phi; x, y)$, respectively, and D is defined by

$$iD^{-1} = \frac{\delta^2 I(\phi)}{\delta\phi(x)\,\delta\phi(y)}. \tag{3}$$

The quantity $\Gamma_2(\phi, G)$ is computed as follows. In the classical action $I(\varphi)$ we must shift the field φ by ϕ. The new action $I(\varphi+\phi)$ possesses terms cubic and higher in φ. This defines an interaction part $I_{\mathrm{int}}(\varphi, \phi)$ where the vertices depend on ϕ. $\Gamma_2(\phi, G)$ is given by sum of all (2PI) vacuum graphs in a theory with vertices determined by $I_{\mathrm{int}}(\varphi, \phi)$ and the propagators set equal to $G(x,y)$. The trace and logarithm in Eq. (2) are functional. After these procedures the interaction Lagrangian density becomes

$$\begin{aligned}\mathcal{L}_{\mathrm{int}}(\varphi, \phi) = &-\frac{1}{2}\left(\frac{\lambda_0\phi_a}{3N} + \frac{\eta_0\phi^2\phi_a}{30N^2}\right)\varphi_a\varphi^2 - \left(\frac{8\,\eta_0\phi_a\phi_b\phi_c}{6N^2}\right)\varphi_a\varphi_b\varphi_c - \frac{1}{4!N}\left(\lambda_0 + \frac{\eta_0\phi^2}{10N}\right)\varphi^4 \\ &- \left(\frac{12\,\eta_0\phi_a\phi_b}{6!N^2}\right)\varphi_a\varphi_b\varphi^2 - \frac{1}{5!}\left(\frac{\eta_0\phi_a}{N^2}\varphi_a\varphi^4\right) - \frac{\eta_0}{6!N^2}\varphi^6.\end{aligned} \tag{4}$$

The effective action $\Gamma(\phi)$ is found by solving for $G_{ab}(x,y)$ the equation

$$\frac{\delta\Gamma(\phi, G)}{\delta G_{ab}(x,y)} = 0, \tag{5}$$

and substituting the solution in the generalized effective action $\Gamma(\phi, G)$. The vertices in the above equation contain factors of $1/N$ or $1/N^2$, but a φ loop gives a factor of N provided the $O(N)$ isospin flows around it alone and not into another part of the graph. We usually call such loops bubbles. Then at leading order in $1/N$, the vacuum graphs are bubble trees with two or three bubbles at each vertex. The (2PI) graphs are shown in Fig. 1. It is straightforward to obtain

$$\Gamma_2(\phi,G)=\frac{-1}{4!N}\int d^Dx\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)[G_{aa}(x,x)]^2-\frac{\eta_0}{6!N^2}\int d^Dx[G_{aa}(x,x)]^3. \tag{6}$$

Therefore Eq. (5) becomes

$$\frac{\delta\Gamma(\phi,G)}{\delta G_{ab}(x,y)}=\frac{1}{2}(G^{-1})_{ab}(x,y)+\frac{i}{2}D^{-1}(\phi)-\frac{1}{12N}\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)[\delta_{ab}G_{cc}(x,x)]\delta^D(x-y)$$
$$-\frac{3\eta_0}{6!N}\delta_{ab}[G_{cc}(x,x)]^2\delta^D(x-y)=0. \tag{7}$$

Rewriting this equation, we obtain the gap equation

$$(G^{-1})_{ab}(x,y)=D^{-1}_{ab}(\phi;x,y)+\frac{i}{6N}\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)[\delta_{ab}G_{cc}(x,x)]\delta^D(x-y)$$
$$+\frac{i\eta_0}{5!N^2}\delta_{ab}[G_{cc}(x,x)]^2\delta^D(x-y). \tag{8}$$

Hence

$$\frac{i}{2}\mathrm{Tr}\,D^{-1}G=\frac{1}{12N}\int d^Dx\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)[G_{aa}(x,x)]^2+\frac{3\eta_0}{6!N^2}\int d^Dx[G_{aa}(x,x)]^3+cte. \tag{9}$$

Using Eqs. (8) and (9) in Eq. (6) we find the effective action

$$\Gamma(\phi)=I(\phi)+\frac{i}{2}\mathrm{Tr}[\mathrm{Ln}\,G^{-1}]+\frac{1}{4!N}\int d^Dx\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)[G_{aa}(x,x)]^2+\frac{2\eta_0}{6!N^2}\int d^Dx[G_{aa}(x,x)]^3, \tag{10}$$

where G_{ab} is given implicitly by Eq. (8). The trace in (10) are both the functional and the internal space. The last two terms on the right-hand side of Eq. (10) are the leading contribution to the effective action in the $1/N$ expansion. As usual we may simplify the situation by separating G_{ab} into transverse and longitudinal components, so

$$G_{ab}=\left(\delta_{ab}-\frac{\phi_a\phi_b}{\phi^2}\right)g+\frac{\phi_a\phi_b}{\phi^2}\tilde{g}, \tag{11}$$

in this form we can invert G_{ab},

$$(G)^{-1}_{ab}=\left(\delta_{ab}-\frac{\phi_a\phi_b}{\phi^2}\right)g^{-1}+\frac{\phi_a\phi_b}{\phi^2}\tilde{g}^{-1}. \tag{12}$$

Now we can take the trace with respect to the indices of the internal space,

$$G_{aa}=Ng+O(1),\quad (G)^{-1}_{aa}=Ng^{-1}+O(1). \tag{13}$$

From this equation at leading order in $1/N$, G_{ab} is diagonal in a,b. Substituting Eq. (13) into Eq. (10) and Eq. (8) and keeping only the leading order one finds that the daisy and superdaisy resumed effective potential for the φ^6 theory is given by

$$\Gamma(\phi)=I(\phi)+\frac{iN}{2}\mathrm{tr}(\ln g^{-1})+\frac{N}{4!}\int d^Dx\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)g^2(x,x)+\frac{2N\eta_0}{6!}\int d^Dxg^3(x,x)+O(1), \tag{14}$$

where the trace is only in the functional space, and the gap equation becomes

$$g^{-1}(x,y) = i\left[\Box + m_0^2 + \frac{\lambda_0}{6}\left(\frac{\phi^2}{N} + g(x,x)\right) + \frac{\eta_0}{5!}\left(\frac{\phi^2}{N} + g(x,x)\right)^2\right]\delta^D(x-y) + O\left(\frac{1}{N}\right). \quad (15)$$

It is important to point out that this calculation was done by Townsend.[5]

III. THE THEORY AT FINITE TEMPERATURE

In order to generalize these results to the case of finite temperature we are going to assume that the system is in equilibrium with a thermal bath a temperature $T=\beta^{-1}$. Since we are interested in the equilibrium situation it is convenient to use the Matsubara formalism (imaginary time). Consequently it is convenient to continue all momenta to Euclidean values ($p_0=ip_4$) and take the following Ansatz for $g(x,y)$:

$$g(x,y) = \int \frac{d^D p}{(2\pi)^D} \frac{\exp^{i(x-y)p}}{p^2 + M^2(\phi)}. \quad (16)$$

Substituting Eq. (16) in Eq. (15) we get the expression for the gap equation,

$$M^2(\phi) = m_0^2 + \frac{\lambda_0}{6}\left(\frac{\phi^2}{N} + F(\phi)\right) + \frac{\eta_0}{5!}\left(\frac{\phi^2}{N} + F(\phi)\right)^2, \quad (17)$$

where $F(\phi)$ is given by

$$F(\phi) = \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 + M^2(\phi)}, \quad (18)$$

and the effective potential in the D-dimensional Euclidean space can be written as

$$V(\phi) = V_0(\phi) + \frac{N}{2}\int \frac{d^D p}{(2\pi)^D} \ln[p^2 + M^2(\phi)] - \frac{N}{4!}\left(\lambda_0 + \frac{\eta_0\phi^2}{10N}\right)F(\phi)^2 - \frac{2N\eta_0 F(\phi)^3}{6!}, \quad (19)$$

where $V_0(\phi)$ is the tree approximation of the potential.

Replacing the continuous four momenta k_4 by discrete ω_n and the integration by a summation ($\beta=1/T$). The effective potential at finite temperature is

$$V_\beta(\phi) = V_0(\phi) + \frac{N}{2\beta}\sum_n^\infty \int \frac{d^{D-1}}{(2\pi)^{D-1}} \ln[\omega_n + p^2 + M_\beta^2(\phi)] - \frac{N}{4!}\left(\lambda_0 + \frac{\eta_0\phi^2}{10N}\right)F_\beta(\phi)^2 - \frac{2N\eta F_\beta(\phi)^3}{6!}, \quad (20)$$

where the expression $F_\beta(\phi)$ is the finite temperature generalization of $F(\phi)$, and is given by

$$F_\beta(\phi) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \frac{1}{\omega_n^2 + p^2 + M_\beta^2(\phi)}. \quad (21)$$

The gap equation for this theory at finite temperature is

$$M_\beta^2(\phi) = m_0^2 + \frac{\lambda_0}{6}\left(\frac{\phi^2}{N} + F_\beta(\phi)\right) + \frac{\eta_0}{5!}\left(\frac{\phi^2}{N} + F_\beta(\phi)\right)^2. \quad (22)$$

In order to regularize $F_\beta(\phi)$ given by Eq. (21), we use a mixing between dimensional regularization and analytic regularization. For this purpose we define the following expression:

$$I_\beta(D,s,m)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\int\frac{d^{D-1}k}{(2\pi)^{D-1}}\frac{1}{(\omega_n^2+k^2+m^2)^s}. \tag{23}$$

The analytic extension of the inhomogeneous Epstein zeta function can be done and the corresponding analytic extension of $I_\beta(D,s,m)$ is

$$I_\beta(D,s,m)=\frac{m^{D-2s}}{(2\pi^{1/2})^D\Gamma(s)}\left[\Gamma\left(s-\frac{D}{2}\right)+4\sum_{n=1}^{\infty}\left(\frac{2}{mn\beta}\right)^{D/2-s}K_{D/2-s}(mn\beta)\right], \tag{24}$$

where $K_\mu(z)$ is the modified Bessel function of the third kind. Fortunately for $D=2+1$ the analytic extension of the function $I_\beta(D,s=1,m=M_\beta(\phi))=F_\beta(\phi)$ is finite and can be expressed in a closed form[6]

$$F_\beta(\phi)=I_\beta(3,1,M_\beta(\phi))=-\frac{M_\beta(\phi)}{4\pi}\left(1+\frac{2\ln(1-e^{-M_\beta(\phi)\beta})}{M_\beta(\phi)\beta}\right). \tag{25}$$

We note that in $D=2+1$ we have no pole, at least in this approximation. To proceed to regularize the second term of Eq. (20), we define

$$LF_\beta(\phi)=\frac{1}{\beta}\sum_{n=1}^{\infty}\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\ln[\omega_n+p^2+M_\beta^2(\phi)] \tag{26}$$

then,

$$\frac{\partial LF_\beta(\phi)}{\partial M_\beta}=(2M_\beta)\frac{1}{\beta}\sum_{n=1}^{\infty}\int\frac{d^{D-1}p}{(2\pi)^{D-1}}\frac{1}{\omega_n+p^2+M_\beta^2(\phi)} \tag{27}$$

and from Eq. (21), we have that

$$\frac{\partial LF_\beta(\phi)}{\partial M_\beta}=(2M_\beta)F_\beta(\phi). \tag{28}$$

For $D=2+1$, $F_\beta(\phi)$ is finite and is given by Eq. (29) (Ref. 6) and integrating the Eq. (28), we obtain

$$LF_\beta(\phi)_R=-\frac{M_\beta(\phi)^3}{6\pi}-\frac{M_\beta(\phi)Li_2(e^{-M_\beta(\phi)\beta})}{\pi\beta^2}-\frac{Li_3(e^{-M_\beta(\phi)\beta})}{\pi\beta^3}. \tag{29}$$

The definition of general polylogarithm function $Li_n(z)$ can be found in Ref. 7.

The daisy and super daisy resummed effective potential at finite temperature for $D=2+1$ is then given by

$$V_\beta(\phi)=V_0(\phi)+\frac{N}{2}LF_\beta(\phi)_R-\frac{N}{4!}\left(\lambda_0+\frac{\eta_0\phi^2}{10N}\right)(F_\beta(\phi)_R)^2-\frac{2N\eta(F_\beta(\phi)_R)^2}{6!} \tag{30}$$

and the corresponding gap equation [see Eq. (22)]

$$M_\beta^2(\phi)=m_0^2+\frac{\lambda_0}{6}\left(\frac{\phi^2}{N}-\frac{M_\beta(\phi)}{4\pi}\left[1+\frac{2\ln(1-e^{-M_\beta(\phi)\beta})}{M_\beta(\phi)\beta}\right]\right)+\frac{\eta_0}{5!}\left(\frac{\phi^2}{N}-\frac{M_\beta(\phi)}{4\pi}\left[1+\frac{2\ln(1-e^{-M_\beta(\phi)\beta})}{M_\beta(\phi)\beta}\right]\right)^2. \tag{31}$$

From this expression we can deduce that there is no possible way to find a solution for M_β going to zero, because the terms in Eq. (31) containing the logarithm will not permit, and this situation is similar to the scalar theory with $O(N)$ symmetry in two dimensions (2D) at zero temperature.[8]

This result is in agreement with the the Coleman-Mermin-Wagner theorem,[9] which statement is related to the fact that it is impossible to construct a consistent theory of massless scalar in 2D. If a spontaneous breaking of continuous symmetry were to happen at finite T, then one would be faced with this problem at momentum scales below T_c, i.e., it would be impossible to construct an effective 2D theory of the Goldstone bosons zero modes.

IV. CONCLUSIONS

In this paper we have found the daisy and super daisy effective potential for the theory φ^6 in $D=2+1$-dimensional Euclidean space at finite temperature. The form of effective potential have been found explicitly using resummation method in the leading order $1/N$ approximation (Hartree-Fock approximation). We found that in this approximation there is no symmetry breaking for any temperature and this is clearly a manifestation of the Coleman-Mermin-Wagner theorem which stipulates that the spontaneous symmetry breaking of continuous symmetry cannot happen in $D=2+1$ at finite temperature.

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The Euclidean scalar Green function in the five-dimensional Kaluza-Klein magnetic monopole space-time

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In this paper we present, in a integral form, the Euclidean Green function associated with a massless scalar field in the five-dimensional Kaluza-Klein magnetic monopole superposed to a global monopole, admitting a nontrivial coupling between the field with the geometry. This Green function is expressed as the sum of two contributions: the first one related with uncharged component of the field, is similar to the Green function associated with a scalar field in a four-dimensional global monopole space-time. The second contains the information of all the other components. Using this Green function it is possible to study the vacuum polarization effects on this space-time. Explicitly we calculate the renormalized vacuum expectation value $\langle \Phi^{*}(x)\Phi(x)\rangle_{\mathrm{Ren}}$, which by its turn is also expressed as the sum of two contributions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A few years ago, Gross and Perry,[1] and Sorkin[2] presented a solitonlike solution of the five-dimensional Kaluza-Klein theory corresponding to an Abelian magnetic monopole. As the Dirac solution, their solutions describe a gauge-dependent string singularity line, if the fifth coordinate is conveniently compactified. Moreover, their solutions depend on the parameter m related with the physical magnetic charge g and the radius of the Kaluza-Klein circle R by

$$m = g\sqrt{\pi G} = R/8, \tag{1}$$

being G the Newton's constant. Also Gegenberg and Kunstatter[3] found another magnetic monopole solution. Their solutions were obtained by applying the static and Ricci-flat requirement on the field equations.

A global monopole is a heavy topological object formed in the phase transition of a system composed by self-coupling isoscalar field ϕ^a, whose original global O(3) symmetry of the physical system is spontaneously broken down to U(1). The scalar matter field plays the role of an order parameter which outside the monopole's core, acquires a nonvanishing value. The simplest model which gives rise to a global monopole has been proposed by Barriola and Vilenkin,[4] and is described by the Lagrangian density below

$$\mathcal{L} = -\tfrac{1}{2} g^{\mu\nu}\partial_\mu \phi^a \partial_\nu \phi^a - \tfrac{1}{4}\lambda(\phi^a\phi^a - \eta^2)^2 \tag{2}$$

with $a=1,2,3$ and η being the scale energy where the symmetry is broken. The field configuration which describes a monopole is

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$$\phi^a(x) = \eta f(r)\hat{x}^a, \tag{3}$$

where $\hat{x}^a\hat{x}^a = 1$. Coupling this matter field with the Einstein equation, a spherically symmetric regular metric tensor solution is obtained. Barriola and Vilenkin also show that for points outside the global monopole's core the geometry of the manifold can be approximately given by the line element

$$\mathrm{d}s^2 = -\,\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{\alpha^2} + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2) \tag{4}$$

with $\alpha^2 = 1 - 8\pi G\eta^2$. This line element represents a three-geometry with a solid angle deficit and a nonvanishing scalar curvature.

Recently a new solution for the Kaluza-Klein magnetic monopole in a five-dimensional global monopole space-time has been found.[5] This solution corresponds to a composite topological object, i.e., an Abelian magnetic monopole superposed to a pointlike global monopole. It was obtained by coupling the energy-momentum tensor associated with the five-dimensional generalization of the global monopole system, with the respective Einstein equation in the presence of an Abelian magnetic monopole. Due to the presence of the matter source, the Ricci-flat condition is no longer fulfilled. The solution can be expressed by the following line element in terms of the five-dimensional coordinates $x^A = (x^\mu, \Psi) = (t, r, \theta, \phi, \Psi)$,

$$\mathrm{d}\hat{s}^2 = -\,\mathrm{d}t^2 + V(r)\left(\frac{\mathrm{d}r^2}{\alpha^2} + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2)\right) + V(r)^{-1}(\mathrm{d}\Psi + 4m(1-\cos\theta)\mathrm{d}\phi)^2 \tag{5}$$

with

$$V(r) = 1 + \frac{4m}{\alpha r}. \tag{6}$$

As has been pointed out by Gross and Perry,[1] the gauge field associated with the magnetic monopole

$$A_\phi = 4m(1-\cos\theta), \tag{7}$$

presents a singularity at $\theta = \pi$. However, this singularity is gauge dependent if the period of the compactified coordinate Ψ is equal to $16\pi m$. This is the geometric description of the Dirac quantization. Adopting this period for the extra coordinate, it is possible to provide the Wu and Yang formalism[6] to describe the four-vector potential, A_μ, associated with the Abelian magnetic monopole without line of singularity. In order to do that it is necessary to construct two overlapping regions, R_a and R_b, which cover the whole space section of the manifold. Using spherical coordinate system, with the monopole at origin the only nonvanishing components for the vector potential are

$$\begin{aligned} (A_\phi)_a &= 4m(1-\cos\theta), \quad R_a\colon\ 0 \leqslant \theta < \tfrac{1}{2}\pi + \delta, \\ (A_\phi)_b &= -\,4m(1+\cos\theta), \quad R_b\colon\ \tfrac{1}{2}\pi - \delta < \theta \leqslant \pi, \end{aligned} \tag{8}$$

with $0 < \delta < \pi/2$. In the overlapping region, R_{ab}, the nonvanishing components are related by a gauge transformation. Using the appropriate normalization factor,[1] one can rewrite the above vector potential in terms of the physical one, A_ϕ^{ph}:

$$\sqrt{16\pi G}(A_{\phi}^{\mathrm{ph}})_a = \sqrt{16\pi G}\left[(A_{\phi}^{\mathrm{ph}})_b + \frac{i}{e}S\partial_{\phi}S^{-1}\right], \tag{9}$$

where $S=e^{2iq\phi}$, $q=eg=n/2$ in units $\hbar=c=1$ and g being the monopole strength. In terms of nonphysical vector potential this gauge transformation corresponds to subtract the quantity $8m$, which compensates the changing in the fifth coordinate $\Psi'=\Psi+8m\phi$.

Here, we shall consider the quantum analysis of a massless five-dimensional scalar field $\Theta(x)$ in the space-time described by (5). This field can be expanded in a Fourier series

$$\Theta(x) = \sum_{n=-\infty}^{\infty} e^{in\Psi/8m}\Theta^{(n)}(x^{\mu}) = \sum_{n=-\infty}^{\infty} e^{in\Psi/8m}e^{-iEt}R_n(r)Y_{lm}^{q}(\theta,\phi), \tag{10}$$

being $Y_{lm}^{q}(\theta,\phi)$, with $q=n/2$, the monopole harmonic[7] solution of the eigenvalue equations below

$$\vec{L}_q^2 Y_{lm}^{q} = l(l+1)Y_{lm}^{q} \quad \text{and } L_z Y_{lm}^{q} = mY_{lm}^{q}, \tag{11}$$

with $l=|q|, |q|+1, |q|+2,\ldots$, and $m=-l, -l+1,\ldots,l$. Where

$$\vec{L}_q = \vec{r}\times(\vec{p}-e\vec{A}) - q\hat{r}. \tag{12}$$

The Green function associated with the massless scalar field in this space-time can be obtained by solving the differential equation

$$(\Box + \xi R)G(x,x') = -\delta^{(5)}(x,x') = -\frac{\delta^{(5)}(x^A - x'^A)}{\sqrt{-g^{(5)}}}, \tag{13}$$

$g^{(5)}$ being the determinant of the metric tensor. Here we have introduced a nonminimal coupling between the field with the geometry, ξR, with ξ being an arbitrary constant and R the Ricci scalar curvature.

Green functions in a four-dimensional pointlike global monopole space-time have been obtained in Refs. 8 and 9 to massless scalar and fermionic fields, respectively. Also the effect of temperature on these functions has been considered in Ref. 10 More recently the Green function associated with a charged massless scalar field in the global monopole space-time superposed to an Abelian magnetic monopole, has been calculated in Ref. 11 The Green function is an important quantity to calculate vacuum polarization effects due to the presence of matter fields. Specifically for scalar field, the vacuum expectation value of the square of this field is formally given by

$$\langle\Phi^2(x)\rangle = \lim_{x'\to x} G(x',x). \tag{14}$$

So the objective of this paper is to calculate the Green function associated with a massless scalar field in the five-dimensional space-time, which takes into account the presence of the magnetic interaction between the matter field and the magnetic monopole in the unified formalism of Kaluza-Klein. Having this function, the next step is to calculate the vacuum polarization effect on this manifold, trying to understand the consequence of considering an extra compactified dimension.

This paper is organized as follows. In Sec. II, we explicitly calculate the Euclidean Green function associated with this system. As we shall see, this Green function, as the scalar field, will be expressed in terms of an infinite sum of all the Fourier components associated with the quantum number n. For the component $n=0$, the respective Green function, $G^{(0)}(x,x')$, is similar to the scalar Green function in a four-dimensional global monopole space-time. As to the other components, the respective Green function, $\overline{G}(x,x')$, will be expressed as the summation of all the $n\neq 0$ components $G^{(n)}(x,x')$. Although we have not found in the literature an explicit expression which provides to express $\overline{G}(x,x')$ in terms of any kind of special function, we were able to furnish an integral representation to it. In Sec. II A we calculate the renormalized vacuum expec-

tation value of the square of the scalar field, $\langle\Phi(x)^{*}\Phi(x)\rangle$. We show that this expectation value can be expressed as the sum of two contributions, the first, being given by the $n=0$ component of the total Green function, is associated with the uncharged component of the scalar field (10). The second contribution takes into account all the other Fourier components. In Sec. II B, we present a formal expression to the renormalized vacuum expectation value of the energy-momentum tensor, $\langle T_B^A(x)\rangle$. In Sec. III, we present our conclusions and the most important remarks about this system. In the Appendix we present the explicit calculation of the Green $\overline{G}(x',x)$ associated with the uncharged components of the field.

II. EUCLIDEAN GREEN FUNCTION

The Euclidean Green function can be obtained by the Schwinger-DeWitt formalism as follows:

$$G_E(x,x') = \int_0^\infty \mathrm{d}s\, K(x,x';s), \tag{15}$$

where $K(x,x';s)$ is the heat kernel, which can be expressed in terms of the sum over the complete normalized set of eigenstates of the Klein-Gordon operator. For the massless scalar field this operator reads

$$(\Box + \xi R)\Theta_\sigma(x) = -\sigma^2\Theta_\sigma(x). \tag{16}$$

So

$$K(x,x';s) = \sum_{\sigma^2} \Theta_\sigma^{*}(x')\Theta(x)_\sigma e^{-s\sigma^2}. \tag{17}$$

The covariant five-dimensional d'Alembertian operator

$$\Box = \frac{1}{\sqrt{-g^{(5)}}}\partial_A(\sqrt{-g^{(5)}}g^{AB}\partial_B), \tag{18}$$

in the space-time defined by (5) reads

$$\Box = -\partial_t^2 + \frac{1}{V(r)}\left\{\alpha^2\left(\partial_r^2 + \frac{2}{r}\partial_r\right) - \frac{\vec{L}^2}{r^2} - \frac{8m(1-\cos\theta)}{r^2\sin^2\theta}\partial_\phi\partial_\Psi + \frac{16m^2(1-\cos\theta)^2}{r^2\sin^2\theta}\partial_\Psi^2\right\} + V(r)\partial_\Psi^2. \tag{19}$$

On the other hand, the Ricci scalar curvature is

$$R = \frac{2(1-\alpha^2)}{V(r)r^2}. \tag{20}$$

Admitting to the eigenfunction $\Theta_\sigma(x)$ the form

$$\Theta_\sigma(x) = e^{-iEt}e^{in\Psi/8m}R_l^n(r)Y_{lm}^q(\theta,\phi) \tag{21}$$

and assuming $q=n/2$ it is possible to obtain the following differential equation:

$$\left\{-E^2 + \frac{1}{V(r)}\left[\alpha^2\left(\partial_r^2 + \frac{2}{r}\partial_r\right) - \frac{(\vec{L}_q^2 - q^2)}{r^2}\right] - \frac{q^2}{16m^2}V(r) + \frac{2\xi(\alpha^2-1)}{V(r)r^2}\right\}R_l^n(r)Y_{lm}^q(\theta,\phi)$$
$$= -\sigma^2 R_l^n(r)Y_{lm}^q(\theta,\phi), \tag{22}$$

where we identify

$$\vec{L}_q^2 = \vec{L}^2 + \frac{2iq(1-\cos\theta)}{\sin^2\theta}\partial_\phi + q^2\frac{(1-\cos\theta)^2}{\sin^2\theta} + q^2. \tag{23}$$

Admitting

$$\sigma^2 = E^2 + \alpha^2 p^2 + \frac{q^2}{16m^2} \tag{24}$$

we find the differential equation obeyed by the unknown radial function $R(r)$,

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{\mathrm{d}R(r)}{\mathrm{d}r} - \frac{\mu_{lq}}{r^2}R(r) - \gamma^2 V(r)^2 R(r) + \gamma^2 V(r)R(r) + p^2 V(r)R(r) = 0, \tag{25}$$

with

$$\gamma = \frac{q}{4m\alpha} \quad \text{and } \mu_{lq} = \frac{l(l+1) - q^2 - 2\xi(\alpha^2-1)}{\alpha^2}. \tag{26}$$

The solution to the above differential equation regular at origin is proportional to the Whittaker function[12] $M_{\lambda,\beta}(2ipr)$ with λ and β being given in terms of the parameters m and γ, and also in terms of the variable p. Unfortunately with this function it is not possible to present the Green function in a closed form. So at this point we should make an approximation in our calculations, we shall discard the terms proportional to m/r in (25). This means that we are considering points very far from the origin. [Discarding terms proportional to m/r does not reduce the system to a charged particle in the presence of an Abelian magnetic monopole.[11] Here the space-time remains five-dimensional, and this fact is present in the calculation of the heat kernel (17) where it is necessary to sum all the possible values for the parameter $q=n/2$.] In Ref. 1 an estimative value to the radius of the Kaluza-Klein circle is given, $R=3.7\times10^{-32}$ cm. So we are considering points at distance greater than 3.7×10^{-32} cm. Accepting this approximation (25) becomes

$$\frac{d^2R(r)}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}R(r)}{dr} - \frac{\mu_{lq}}{r^2}R(r) + p^2R(r) = 0. \tag{27}$$

The solution to the above equation regular at the origin is

$$R_l^n(r) = \frac{J_{\nu_{l,q}}(pr)}{\sqrt{pr}}, \tag{28}$$

where J_ν is the Bessel function of order

$$\nu_l^q = \frac{1}{\alpha}\sqrt{(l+1/2)^2 - q^2 - 2(\alpha^2-1)(\xi-1/8)}. \tag{29}$$

So the normalized eigenstate of the Klein-Gordon operator (16) is

$$\Theta_\sigma(x) = \frac{1}{4\pi}\sqrt{\frac{\alpha p}{2mr}}e^{-iEt}e^{in\Psi/8m}J_{\nu_l^q}(pr)Y_{lm}^q(\theta,\phi). \tag{30}$$

By making a Wick rotation, $t \to i\tau$, and according to (17) the Euclidean heat kernel is given by

$$K(x,x';s) = \int_{-\infty}^{\infty} \mathrm{d}E \sum_{n=-\infty}^{\infty} \int_0^{\infty} \mathrm{d}p \sum_{l,m} \Theta_\sigma(x)\Theta_\sigma^*(x') e^{-s\sigma^2}$$

$$= \frac{1}{256\pi^{5/2} m\alpha} \frac{1}{\sqrt{rr'}} \frac{e^{-(\Delta\tau\alpha^2 + r^2 + r'^2)/4\alpha^2 s}}{s^{3/2}} \sum_{n=-\infty}^{\infty} e^{-sn^2/64m^2} e^{in[(\Psi - \Psi')/8m]}$$

$$\times \sum_{l=|q|}^{\infty} I_{\nu_l^q}\left(\frac{rr'}{2\alpha^2 s}\right) \sum_{m=-l}^{l} Y_{lm}^q(\theta,\phi)(Y_{lm}^q(\theta',\phi'))^*, \tag{31}$$

I_ν being the modified Bessel function. In Ref. 13, Wu and Yang have derived some properties of the monopole harmonics, including the generalization of spherical harmonics addition theorem. However, because we are interested in calculating the renormalized value of the Green function in the coincidence limit, a simpler expression is obtained by taking $\theta = \theta'$ and $\phi = \phi'$ in (31). In Appendix A of Ref. 11 we have shown the simplified result to the sum of the product of monopole harmonics in coincidence limit in the angular variables,

$$\sum_{m=-l}^{l} Y_{lm}^q(\theta,\phi)(Y_{lm}^q(\theta,\phi))^* = \frac{(2l+1)}{4\pi}. \tag{32}$$

Moreover we shall take the coincidence limit in the fifth coordinate $\Psi' = \Psi$ and the Euclidean temporal coordinate $\tau' = \tau$ in (31). Doing this we get a simpler expression to the heat kernel which depends on the quantum number n in its second power.

Now according to (15) we get

$$G(x,x') = \frac{1}{256\pi^{5/2} m\alpha} \frac{1}{\sqrt{rr'}} \sum_{l=0}^{\infty} (2l+1) \int_0^{\infty} \mathrm{d}s\, s^{-3/2} e^{-\Omega/4\alpha^2 s} I_{\nu_l^0}(\sigma/s)$$

$$+ \frac{1}{128\pi^{5/2} m\alpha} \frac{1}{\sqrt{rr'}} \sum_{n=1}^{\infty} \sum_{l=q}^{\infty} (2l+1) \int_0^{\infty} \mathrm{d}s\, s^{-3/2} e^{-\Omega/4\alpha^2 s}$$

$$\times I_{\nu_l^q}(\sigma/s) e^{-sn^2/64m^2}, \tag{33}$$

where

$$\Omega = r^2 + r'^2 \quad \text{and} \quad \sigma = \frac{rr'}{2\alpha^2}. \tag{34}$$

As we can see the above Green function is composed by two contributions, the first one, $G^{(0)}$, corresponds to the Fourier component $n=0$ of the scalar field operator, and the second, $\overline{G}$ to the other components. By using Ref. 12 it is possible to develop the integral in s for the first contribution. So we get

$$G^{(0)}(r,r') = \frac{1}{128\pi^3 m} \frac{1}{rr'} \sum_{l=0}^{\infty} (2l+1) Q_{\nu_l^0 - 1/2}(\cosh u), \tag{35}$$

with $\cosh u = (r^2 + r'^2)/2rr'$ and Q_ν being the Legendre function, whose integral representation is

$$Q_{\nu-1/2}(\cosh u) = \frac{1}{\sqrt{2}} \int_u^{\infty} \mathrm{d}t \frac{e^{-\nu t}}{\sqrt{\cosh t - \cosh u}}. \tag{36}$$

This Green function is exactly $1/16\pi m = 1/2\pi R$ times the Green function obtained in a four-dimensional space-time (see Ref. 8).

As to the second contribution of (33), we did not find in the literature the explicit expression to the integral in the variable s. In the Appendix we give the procedure adopted to provide a simpler and workable expression to $\overline{G}$, which will be adopted by us in the analysis of the vacuum polarization effect. The result to this contribution is

$$\overline{G}(r,r') = \sum_{n=1}^{\infty} G^{(n)}(r,r') \tag{37}$$

with

$$G^{(n)}(r,r') = \frac{1}{128\pi^{5/2}m\alpha}\frac{1}{\sqrt{rr'}}\sum_{l=n/2}^{\infty}(2l+1)I_n \tag{38}$$

being

$$I_n = \frac{1}{\sqrt{\pi\sigma}}\int_u^{\infty}\frac{\mathrm{d}t\, e^{-\nu_l^q t}}{\sqrt{\cosh t-\cosh u}}\cos((n/4m)\sqrt{\sigma(\cosh t-\cosh u)}). \tag{39}$$

Finally we can write

$$G^{(n)}(r,r') = \frac{1}{64\sqrt{2}\pi^3 m}\frac{1}{rr'}\sum_{l=n/2}^{\infty}(2l+1)\int_u^{\infty}\frac{\mathrm{d}t\, e^{-\nu_l^q t}}{\sqrt{\cosh t-\cosh u}}\times\cos((n/4m)\sqrt{\sigma(\cosh t-\cosh u)}). \tag{40}$$

As the $n=0$ component of the Green function, Eq. (35), it is not possible to develop the integral above and provide a closed expression to $G^{(n)}$. The best we can do is to express it in an integral representation. Moreover (40) is similar to the $n=0$ component; however its coefficient is two times bigger than the coefficient multiplying the uncharged sector.

Another point that should be mentioned is that because of the nontrivial dependence of the parameter ν_l^q with α and q, it is not possible to develop exactly the sum in l in (40). On the other hand, for $\xi=1/8$, the geometric series in (35) can be performed, providing a simpler expression to $G^{(0)}$.

Having these Green functions, it is possible to calculate the vacuum polarization effect in the gravitational background of the composite five-dimensional Kaluza-Klein magnetic and global monopoles.

A. Computation of $\langle\Phi^*(x)\Phi(x)\rangle_{\mathrm{Ren}}$

In this section we discuss the calculation of the vacuum expectation value of the square of the massless scalar field operator. This quantity is formally obtained by calculating the complete Green function in the coincidence limit,

$$\langle\Phi^*(x)\Phi(x)\rangle = \lim_{x'\to x} G(x',x) = \lim_{r'\to r}[G^{(0)}(r',r)+\overline{G}(r',r)]. \tag{41}$$

However, this procedure provides a divergent result. In order to obtain a finite and well-defined result it is necessary to introduce some renormalization procedure. In this paper we shall apply the point-splitting renormalization procedure. The basic idea of this method consists to examine the singular behavior of the above limit, identify the divergent terms and subtract them off.[14] Let us apply this method separately for each component of (41).

We shall first start with the uncharged component of the vacuum expectation value,

$$\langle\Phi^2(x)\rangle^{(0)} = \lim_{x'\to x} G^{(0)}(x',x). \tag{42}$$

As we have already said $G^{(0)}$ is proportional to the Green function obtained by Mazzitelli and Lousto in Ref. 8. So the procedure to renormalize this component is by subtracting from $G^{(0)}$ the Hadamard function below

$$G_H(x',x) = \frac{1}{16\pi m}\left\{\frac{1}{16\pi^2}\left[\frac{2}{\sigma(x',x)} + \left(\xi - \frac{1}{6}\right)\mathcal{R}\,\ln\left(\frac{\mu^2\sigma(x',x)}{2}\right)\right]\right\}, \tag{43}$$

where μ is an arbitrary cutoff energy scale, $\mathcal{R}=2(1-\alpha^2)/r^2$ the scalar curvature in the four-dimensional global monopole space-time, and $\sigma(x',x)$ one-half of the square of the geodesic distance between x' and x. For the radial point splitting, in our approximation we have $\sigma=(r'-r)^2/2\alpha^2$.

Because the calculation of the vacuum expectation value (VEV) of the square of the massless scalar field operator has been developed in Ref. 8 for an arbitrary value of the nonminimal coupling ξ, up to the first order in the parameter $\eta^2=1-\alpha^2\ll 1$, and in an exact form for $\xi=1/8$, we shall not develop here the calculation of the VEV below,

$$\langle\Phi^2(x)\rangle^{(0)}_{\mathrm{Ren}} = \lim_{r'\to r}[G^{(0)}(r,r') - G_H(r,r')]. \tag{44}$$

We shall give only the result obtained for $\xi=1/8$,

$$\langle\Phi^2(x)\rangle = \frac{1}{512\pi^3 mr^2}\int_0^\infty \frac{\mathrm{d}t}{\sinh(t/2)}\left[\frac{\cosh(t/2\alpha)}{\sinh^2(t/2\alpha)} - \alpha^2\frac{\cosh(t/2)}{\sinh^2(t/2)} + \frac{(\alpha^2-1)}{6}e^{-t/2}\right]$$
$$+ \frac{1}{1536\pi^3 mr^2}(1-\alpha^2)\ln(\mu r/\alpha). \tag{45}$$

The new calculation is to obtain the VEV associated with all charged components of the Green function. In order to get some information on how we should proceed, we first analyze the singular behavior of each component $G^{(n)}(r',r)$. First of all, it is necessary to develop the summation on the angular quantum number l in (40),

$$S = \sum_{l=q}^{\infty}(2l+1)e^{-\nu_l^q t}. \tag{46}$$

Unfortunately it is not possible to develop this summation in an exact way even for $\xi=1/8$. Here it is necessary to adopt an approximation procedure, we shall develop an expansion of ν_l^q in powers of $q^2/(l+1/2)^2<1$. Moreover, developing an extra expansion in powers of parameter η^2, we get a very large expansion as shown in Ref. 11. So in order to obtain a more compact expression to the summation above, which allows us to proceed with the summation in the quantum number n to get $\overline{G}(r',r)$, we shall adopt $\xi=1/8$. So doing this we obtain, up to the first order in $q^2/(l+1/2)^2$, the following expression:

$$S = e^{-qt/\alpha}\left[\frac{q}{\sinh(t/2\alpha)} + \frac{\coth(t/2\alpha)}{2\sinh^2(t/2\alpha)} + \frac{q^2 t}{\alpha}\frac{1}{2\sinh(t/2\alpha)}\right], \tag{47}$$

with $q=n/2$. So $G^{(n)}$ becomes

$$G^{(n)}(r,r') = \frac{1}{64\sqrt{2}\pi^3 m}\frac{1}{rr'}\int_u^\infty \frac{\mathrm{d}t\cos((q/2m)\sqrt{\sigma(\cosh t-\cosh u)})}{\sqrt{\cosh t-\cosh u}} \times e^{-qt/\alpha}\left[\frac{q}{\sinh(t/2\alpha)}+\frac{\coth(t/2\alpha)}{2\sinh^2(t/2\alpha)}+\frac{q^2 t}{\alpha}\frac{1}{2\sinh(t/2\alpha)}\right]. \tag{48}$$

Analyzing $G^{(n)}$ in the limit $r'\to r$, it is possible to observe that this Green function presents effectively a four-dimensional Hadamard singular structure. So to renormalize the VEV of the square of the n-component of the scalar field, we should take the following Hadamard function:

$$G_H(x',x) = \frac{1}{8\pi m}\left\{\frac{1}{16\pi^2}\left[\frac{2}{\sigma(x',x)}+\overline{a_1}\ln\left(\frac{\mu^2\sigma(x',x)}{2}\right)\right]\right\}, \tag{49}$$

where $\overline{a_1}=(\xi-1/6)\mathcal{R}+(2q/R)^2$, with $\xi=1/8$. $\mathcal{R}$ is the scalar curvature and $R=8m$ is the radius of the circle in the fifth dimension. So, although the singular structure of the Green function is of the same type as the four-dimensional Hadamard one, the coefficient $\overline{a_1}$ in the above function presents an extra contribution proportional to the inverse of the square of the radius when compared with the expression given in the literature to this coefficient.[15]

After this discussion let us return to the VEV of the square of the n component of the scalar field,

$$\langle\Phi^*(x)\Phi(x)\rangle^{(n)}_{\mathrm{Ren}} = \lim_{r'\to r}[G^{(n)}(r,r')-G_H(r,r')] = \frac{1}{128\pi^3 mr^2}\int_0^\infty \frac{\mathrm{d}t}{\sinh(t/2)}\left\{\cos\left(\frac{qr}{2\alpha m}\sinh(t/2)\right)e^{-qt/\alpha} \times\left[q+\frac{\coth(t/2\alpha)}{2}+\frac{q^2 t}{2\alpha}\right]\frac{1}{\sinh(t/2\alpha)}-\frac{\alpha^2\coth(t/2)}{\sinh^2(t/2)}+\left(\frac{qr}{4m}\right)^2 e^{-t/2}-\frac{1-\alpha^2}{12}e^{-t/2}\right\} -\frac{q^2}{1024\pi^3 m^3}\ln\left(\frac{\mu r}{2}\right)+\frac{1-\alpha^2}{768\pi^3 m}\frac{1}{r^2}\ln\left(\frac{\mu r}{2}\right), \tag{50}$$

with $q=n/2$, being $n=1,2,3,\ldots$. So the above result is valid only for charged Fourier components of the scalar field.

Now let us return to the complete Green function. According to (37), $\overline{G}$ is given by developing the summation on the quantum number n in (48). Doing this we found

$$\overline{G}(r,r') = \frac{1}{256\sqrt{2}\pi^3 m}\frac{1}{r'r}\int_u^\infty \frac{\mathrm{d}t}{\sqrt{\cosh t-\cosh u}}\frac{1}{\sinh(t/2\alpha)}\frac{1}{\cosh(t/2\alpha)-\cos\gamma} \times\left\{\frac{\cosh(t/2\alpha)\cos\gamma-1}{\cosh(t/2\alpha)-\cos\gamma}-\cosh(t/2\alpha)(e^{-t/2\alpha}-\cos\gamma) +\frac{t}{8\alpha}\frac{[\cos\gamma\sinh(t/\alpha)+\cos(2\gamma)\sinh(t/2\alpha)-3\sinh(t/2\alpha)]}{(\cosh(t/2\alpha)-\cos\gamma)^2}\right\} \tag{51}$$

with

$$\gamma = \frac{1}{4\alpha m}\sqrt{\frac{r'r}{2}}\sqrt{\cosh t-\cosh u} \quad \text{and} \quad \cosh u = \frac{r^2+r'^2}{2rr'}. \tag{52}$$

Now, at this point, we must analyze the singular behavior of $\overline{G}$. Taking $r'\to r$, we observe that its singular behavior becomes more severe than for $G^{(n)}(r',r)$. In fact it is possible to show that in this limit we have

$$\overline{G}(r,r') \approx \frac{1}{\sigma^{3/2}} + \frac{1}{\sigma} + \frac{1}{\sigma^{1/2}} + \ln(\sigma), \tag{53}$$

with $\sigma=(r-r')^2/2\alpha^2$. So it contains the structure of the five-dimensional Hadamard function

$$G^{(5)}(r,r') \approx \frac{1}{\sigma^{3/2}} + \frac{1}{\sigma^{1/2}}, \tag{54}$$

and also the four-dimensional Hadamard function

$$G^{(4)}(r,r') \approx \frac{1}{\sigma} + \ln(\sigma), \tag{55}$$

at the same time. If we are inclined to provide a finite and well-defined vacuum expectation value of the square of the sum of all charged components of the scalar field operator, we must extract all the divergences of $\overline{G}$. We shall do this by subtracting from this Green function the "Hadamard" one which presents the same kind of singularity as given in (53). So we have

$$\langle \Phi^*(x)\Phi(x)\rangle_{\mathrm{Ren}} = \lim_{r'\to r}[\overline{G}(r',r) - \overline{G}_H(r',r)], \tag{56}$$

with

$$\overline{G}_H(r',r) = \frac{c_3}{(r'-r)^3} + \frac{c_2}{(r'-r)^2} + \frac{c_1}{(r'-r)} + \frac{c_0}{r^2}\ln\left(\frac{\mu^2(r'-r)^2}{4\alpha^2}\right). \tag{57}$$

The coefficients above will be determined appropriately by imposing that (56) be finite. Expressing all the singular terms by using the identities

$$\frac{1}{(r'-r)^d} = \frac{\sqrt{2}\Gamma\left(1+1/d\right)}{2^d(r'r)^{d/2}\sqrt{\pi}\Gamma\left(d/2\right)}\int_u^\infty \frac{\mathrm{d}t}{\sqrt{\cosh t-\cosh u}}\frac{\cosh(t/2)}{\sinh^d(t/2)} \tag{58}$$

and

$$\ln\left(\frac{\mu^2(r'-r)^2}{4\alpha^2}\right) = \ln\left(\frac{\mu^2(r'+r)^2}{4\alpha^2}\right) - \frac{2}{\sqrt{2}}\int_u^\infty \frac{\mathrm{d}t}{\sqrt{\cosh t-\cosh u}}e^{-t/2}, \tag{59}$$

it is possible to obtain all coefficients of (57) according to our requirement. These coefficients are long ones; however, because of the approximation adopted in the beginning of the calculation, they can be written shortly as

$$c_3 \approx -\frac{m\alpha^3}{4\pi^2\sqrt{r'r}},$$

$$c_2 \approx \frac{m\alpha^2}{2\pi^3 r'r},$$

$$c_1 \approx -\frac{7\alpha}{1536m\pi^2\sqrt{r'r}},$$

$$c_0 \approx -\frac{1}{3072m\pi^3}. \tag{60}$$

At this point two important remarks should be mentioned, (i) we did not find in the literature expressions to the coefficients of the adiabatic expansion of the Hadamard function for this five-dimensional space-time, which presents a compactified dimension. (ii) Consequently we do not have any geometric explanation to them. They have been found to provide a finite result to (56). The general structure to this VEV is

$$\langle \Phi^{*}(x)\Phi(x)\rangle_{\mathrm{Ren}} = \frac{A}{mr^2} + \frac{Bm}{r^4} + \frac{1}{1536m\pi^3}\frac{1}{r^2}\ln(\mu r/\alpha). \tag{61}$$

B. Dimensional analysis of $\langle T_A^B \rangle$

The energy-momentum tensor associated with scalar field in an n-dimensional curved space-time is given in Ref. 16. For this five-dimensional space-time, considering a massless field and $\xi = 1/8$ it reads

$$T_{AB}(x) = \tfrac{3}{4}\nabla_A\Phi\nabla_B\Phi - \tfrac{1}{4}g_{AB}g^{CD}\nabla_C\Phi\nabla_B\Phi - \tfrac{1}{4}(\nabla_A\nabla_B\Phi)\Phi + \tfrac{1}{32}g_{AB}\mathcal{R}\Phi^2 - \tfrac{1}{8}\mathcal{R}_{AB}\Phi^2, \tag{62}$$

where $\mathcal{R}_{AB}$ and $\mathcal{R}$ are the Ricci tensor and the scalar curvature, respectively.

The vacuum expectation value of the energy-momentum tensor operator is formally given by

$$\langle T_{AB}(x)\rangle = \lim_{x'\to x} \mathcal{D}_{AB'}(x,x')G(x',x). \tag{63}$$

The nonlocal bivector differential operator, $\mathcal{D}_{AB'}(x',x)$, for this case reads

$$\mathcal{D}_{AB'}(x',x) = \tfrac{3}{4}\nabla_A\nabla_{B'} - \tfrac{1}{4}g_{AB}(x)g^{CD}(x',x)\nabla_C\nabla_{D'} - \tfrac{1}{8}[\nabla_A\nabla_B + \nabla_{A'}\nabla_{B'}] + \tfrac{1}{32}g_{AB}\mathcal{R}(x) - \tfrac{1}{8}\mathcal{R}_{AB}(x). \tag{64}$$

The primes denote the derivative acting at x' rather than at x.

The calculation of the VEV above provides a divergent result. So in order to obtain a finite and well-defined result we must apply some renormalization procedure. Adopting the point-splitting renormalization one, we subtract from the Green function, $G(x',x)$, the Hadamard one, $G_H(x',x)$,

$$\langle T_{AB}(x)\rangle_{\mathrm{Ren}} = \lim_{x'\to x} \mathcal{D}_{AB'}(x,x')[G(x',x) - G_H(x',x)]. \tag{65}$$

This quantity must be conserved,

$$\nabla_A\langle T_B^A(x)\rangle_{\mathrm{Ren}} = 0. \tag{66}$$

As to the trace anomaly, in principle it exists only for even-dimensional space-time. In fact, as has been shown by Christensen[17] the trace of the renormalized VEV of the energy-momentum tensor is given by

$$\langle T_\mu^\mu(x)\rangle_{\mathrm{Ren}} = \frac{1}{(4\pi)^{n/2}}a_{n/2}(x), \tag{67}$$

for an even n-dimensional space-time. [The analysis of the vacuum polarization associated with massless scalar field in five- and six-dimensional global monopole space-time have been developed by us in Ref. 18. There it is explicitly written, up to the first order in the parameter $\eta^2 = 1 - \alpha^2$, the $a_3(x)$ coefficient, of the adiabatic expansion of the Hadamard function.] On the other hand, in our previous calculations, we have found that in this five-dimensional space-time, there appears a logarithmic term in the $\langle \Phi^{*}(x)\Phi(x)\rangle_{\mathrm{Ren}}$, which should be absent in an odd-dimensional space. So we conclude that although being five dimensional, this space-time with the fifth coordinate compactified with period $16\pi m$, and for distance r much greater than m, presents a four-dimensional characteristic. So it is expected to be a nonvanishing trace for this case, i.e.,

$$\langle T_A^A(x)\rangle_{\text{Ren}} \neq 0. \tag{68}$$

Another point that we want to mention is that (65) presents two contributions, the first one coming from the uncharged component of the scalar field, $\langle T_{AB}(x)\rangle_{\text{Ren}}^{(0)}$, and the second coming from the other components, $\langle \overline{T}_{AB}(x)\rangle_{\text{Ren}}$. The dimensional analysis of the renormalized vacuum expectation value of the energy-momentum tensor associated with a scalar field in a four-dimensional global monopole space-time has been developed in Ref. 8 considering this object as a pointlike one. Although the authors did not calculate explicitly this quantity, they present its general structure.

Here in this paper we also shall not calculate explicitly $\langle T_{AB}(x)\rangle_{\text{Ren}}$. However we can say that the general structure for this tensor is

$$\langle T_A^B(x)\rangle_{\text{Ren}} = \frac{1}{mr^4}[F_A^B(r/m,\alpha) + G_A^B(r/m,\alpha)\ln(\mu r/\alpha)], \tag{69}$$

where F_A^B and G_A^B are polynomials in the ratio r/m and depending on the parameter α which codify the presence of the global monopole.

III. CONCLUDING REMARKS

In this paper we have explicitly calculated the complete Green function associated with a massless scalar field in a five-dimensional Kaluza-Klein magnetic monopole superposed to a global monopole, for points very far from the monopole's center. This function is given in terms of two distinct contributions, one coming from the uncharged component of the scalar field, and the other from the other components,

$$G(x',x) = G^{(0)}(x',x) + \sum_{n=1}^{\infty} G^{(n)}(x',x) = G^{(0)}(x',x) + \overline{G}(x',x). \tag{70}$$

Having this function, it was possible to analyze the vacuum polarization effects due to this field in this gravitational background. Explicitly we analyzed the vacuum expectation value of the square of the field. This quantity is formally given by

$$\langle \Phi^*(x)\Phi(x)\rangle = \lim_{x'\to x} G(x',x) = \lim_{x'\to x}[G^{(0)}(x',x) + \overline{G}(x',x)]. \tag{71}$$

However because this quantity provides a divergent result, to obtain a finite and well-defined result, we must apply some renormalization procedure. We have applied the point-splitting renormalization procedure. As we have said before, the basic idea of this method consists to examine the singular behavior and subtract the divergent terms off, getting a finite result. We did this in a systematic way, by subtracting from the Green function the "Hadamard" one. This procedure has been developed separately for the two distinct contributions. For the first one, we observed that the singular behavior of $G^{(0)}(x',x)$ is similar to the four-dimensional Green function. However for the second contribution, the singular behavior of $\overline{G}(x',x)$ contains structure of the five- and four-dimensional Green function.

The Hadamard function for the first contribution could be constructed by knowing the Hadamard function for an ordinary four-dimensional space-time, $G_H^{(4)}(x',x)$; however the second case presents a new structure. So we must construct the respective Hadamard function in an appropriate way, $\overline{G}_H(x',x)$. So the renormalized vacuum expectation value of the square of the scalar field becomes

$$\langle \Phi^*(x)\Phi(x)\rangle_{\mathrm{Ren}} = \lim_{x'\to x}[G^{(0)}(x',x) - G_H^{(4)}(x',x)] + \lim_{x'\to x}[\overline{G}(x',x) - \overline{G}_H(x',x)]. \tag{72}$$

By these analyses we may conclude that although being five dimensional, because of the compactification of the fifth coordinates, with period $16\pi m$, and also because we are considering points at distance to the monopole, r, much greater than m, this space presents four-dimensional behavior in the singular behavior of the Green function. Consequently, there appears a logarithmic contribution in the above renormalized VEV, which presents an arbitrary energy scale μ.

We also analyze the general structure of the renormalized vacuum expectation value of the energy-momentum tensor, $\langle T_{AB}(x)\rangle_{\mathrm{Ren}}$. By dimensional arguments and also by the result obtained in previous analysis, we infer that this quantity behaves as

$$\langle T_A^B(x)\rangle_{\mathrm{Ren}} = \frac{1}{mr^4}[F_A^B(r/m,\alpha) + G_A^B(r/m,\alpha)\ln(\mu r/\alpha)].$$

Unfortunately we did not calculate the explicit expressions to the two tensors above. By inspection we can see that they present dependence on the ratio r/m up to second power.

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APPENDIX: CALCULATION OF THE SECOND CONTRIBUTION OF (33)

The second contribution to the Green function given by (33), $\overline{G}(r,r')$, is given by

$$\overline{G}(r,r') = \sum_{n=1}^{\infty} G^{(n)}(r,r') \tag{A1}$$

with

$$G^{(n)}(r,r') = \frac{1}{128\pi^{5/2}m\alpha}\frac{1}{\sqrt{rr'}}\sum_{l=q}^{\infty}(2l+1)I_n \tag{A2}$$

being

$$I_n = \int_0^{\infty} \mathrm{d}s\, s^{-3/2}e^{-\Omega/4\alpha^2 s}I_{\nu_l^q}(\sigma/s)e^{-sn^2/64m^2} \tag{A3}$$

with

$$\Omega = r^2 + r'^2 \quad \text{and } \sigma = \frac{rr'}{2\alpha^2}. \tag{A4}$$

Now let us first define a new variable $y=\sigma/s$. So we obtain

$$I_n = \frac{1}{\sigma^{1/2}}\int_0^{\infty}\frac{\mathrm{d}y}{\sqrt{y}}e^{-y(\Omega/4\alpha^2\sigma)}I_{\nu_l^q}(y)e^{-(\sigma/y)(n/8m)^2}. \tag{A5}$$

Unfortunately we did not find such integral in the literature. So in order to develop an expression to the Green function we expand $e^{-\sigma n^2/64m^2 y}$ in a series power getting

$$I_n = \frac{1}{\sigma^{1/2}} \sum_{k=0}^{\infty} \frac{[-(n/8m)^2\sigma]^k}{k!} \int_0^{\infty} dy\, y^{-k-1/2} e^{-y(\Omega/4\alpha^2\sigma)} I_{\nu_l^q}(y). \tag{A6}$$

On page 716 of Ref. 12, there is a similar formula for the above integral; however in that table there is a condition on the order of the modified Bessel function and the power of the variable y, that is not satisfied by the integrand of (A6), i.e., $\nu_l^q + 1/2 - k$ is not always a positive number. However adopting the correspondent formula, we obtain

$$I_n = \sqrt{\frac{2}{\sigma\pi}} \sum_{k=0}^{\infty} \frac{[(n/8m)^2\sigma]^k}{k!} Q^{-k}_{\nu_l^q - 1/2}(\cosh u) \sinh^k u. \tag{A7}$$

Now substituting the integral representation below to the Legendre function[12]

$$Q^{\mu}_{\nu}(\cosh u) = \sqrt{\frac{\pi}{2}} \frac{e^{\mu\pi i} \sinh^{\mu} u}{\Gamma(1/2-\mu)} \int_u^{\infty} \frac{dt e^{-(\nu+1/2)t}}{(\cosh t - \cosh u)^{\mu+1/2}}, \tag{A8}$$

we get

$$I_n = \frac{1}{\sqrt{\pi\sigma}} \sum_{k=0}^{\infty} \frac{[-(n/4m)^2\sigma]^k}{(2k)!} \int_u^{\infty} \frac{dt\, e^{-\nu_l^q t}}{\sqrt{\cosh t - \cosh u}} (\cosh t - \cosh u)^k. \tag{A9}$$

Although each integral of the series diverges for $k \geqslant \nu_l^q + 1/2$, interchanging the sum with the integral, we see that the total series obtained is the series of the cosine, so we finally get

$$I_n = \frac{1}{\sqrt{\pi\sigma}} \int_u^{\infty} \frac{dt\, e^{-\nu_l^q t}}{\sqrt{\cosh t - \cosh u}} \cos((n/4m)\sqrt{\sigma(\cosh t - \cosh u)}). \tag{A10}$$

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Partition functions of supersymmetric gauge theories in noncommutative $\mathbb{R}^{2D}$ and their unified perspective

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We investigate cohomological gauge theories in noncommutative $\mathbb{R}^{2D}$. We show that vacuum expectation values of the theories do not depend on noncommutative parameters, and the large noncommutative parameter limit is equivalent to the dimensional reduction. As a result of these facts, we show that a partition function of a cohomological theory defined in noncommutative $\mathbb{R}^{2D}$ and a partition function of a cohomological field theory in $\mathbb{R}^{2D+2}$ are equivalent if they are connected through dimensional reduction. Therefore, we find several partition functions of supersymmetric gauge theories in various dimensions are equivalent. Using this technique, we determine the partition function of the $\mathcal{N}=4$ U(1) gauge theory in noncommutative $\mathbb{R}^4$, where its action does not include a topological term. The result is common among (8-dim, $\mathcal{N}=2$), (6-dim, $\mathcal{N}=2$), (2-dim, $\mathcal{N}=8$) and the IKKT matrix model given by their dimensional reduction to 0-dim. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162127]

I. INTRODUCTION

The first break through of the recent calculation technology for $\mathcal{N}=2$ supersymmetric Yang-Mills theories is brought by Nekrasov.[21,23] After Ref. 21, many kinds of developments appear in $\mathcal{N}\geqslant 2$ supersymmetric Yang-Mills theories and string theories corresponding to them. From those analysis, it is found that different dimension theories are related to each other.[7,17,18,33,35] There are more examples that the different dimensional theories are connected to each other. For example, Dijkgraaf and Vafa show that some correlation functions in matrix theories and $\mathcal{N}=1$ Yang-Mills theories are equivalent.[5] It goes on and on. These facts imply the existence of some kind of unified perspectives. One of the ideas to explain the unification is the 'tHooft's large N gauge theory and string correspondence. Until now, many investigations from this point of view are reported. Meanwhile, the large N gauge theories are similar to noncommutative theories in the operator formalism in some infinite-dimensional Hilbert space with discrete basis. In this paper, we suggest a simple way to understand the reason why partition functions of various dimensional supersymmetric gauge theories are given as the same form or have relations with each other. The basic idea of the way is given in Refs. 28, 29, and 27. Cohomological gauge theories in Euclidian spaces are invariant under the noncommutative parameter shifting, as we will see in the next section. When we take the large noncommutative parameter limit, kinetic terms become irrelevant like dimensional reduction, then the partition function is essentially computable by using lower dimensional theories. From this fact, we will explain that partition functions in various dimensions are equivalent.

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Here is the organization of this paper. In Sec. II, invariance of cohomological field theories in noncommutative $\mathbb{R}^{2D}$ (NC $\mathbb{R}^{2D}$ for short) under deformation of noncommutative parameters will be proved formally. This invariance is not usual symmetry, because the action is deformed. Nevertheless, expectation values and partition functions are invariant. Particularly, we will treat the $\mathcal{N}=2$ and $\mathcal{N}=4$ Yang-Mills theories in NC $\mathbb{R}^4$ as examples. In Sec. III, universality of the partition functions will be investigated. By using the result of Sec. II, we will show that the several partition functions in different dimensions are equivalent. (In Appendix B, concrete discussions for some models will be given again.) In Sec. IV, by the technique of Sec. II we will calculate the partition function of the $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$ without the terms proportional to the instanton number $\int F\wedge F$. This partition function is equal to partition functions of several dimensions. In Sec. V, the moduli space of $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$ will be discussed. The partition function of $\mathcal{N}=4$ U(1) theory with $\int F\wedge F$ will be investigated, too. In Sec. VI, we will summarize this paper.

II. NC COHOMOLOGICAL YANG-MILLS THEORY

In this section, we investigate some important properties of the cohomological Yang-Mills theories in NC $\mathbb{R}^{2D}$ whose noncommutativity is defined as

$$[x^\mu,x^\nu]=i\theta^{\mu\nu}, \tag{1}$$

where the $\theta^{\mu\nu}$ is an element of an antisymmetric matrix and called noncommutative parameter.

Since action functionals of cohomological field theories are defined by BRS-exact functionals like $\hat{\delta}\Psi[\phi_i]$, where $\hat{\delta}$ is a some BRS operator and $\{\phi_i\}$ represent all considered fields and Ψ is a some fermionic functional, the partition function of the cohomological field theory is invariant under any infinitesimal variation δ' which commutes (or anticommutes) with the BRS transformation,

$$\hat{\delta}\delta' = \pm\,\delta'\hat{\delta},$$

$$\delta' Z_\theta=\int\prod_i \mathcal{D}\phi_i\,\delta'\left(-\int \mathrm{d}x^{2D}\,\hat{\delta}\Psi\right)\exp(-S_\theta)=\pm\int\prod_i \mathcal{D}\phi_i\,\hat{\delta}\left(-\int \mathrm{d}x^{2D}\delta'\Psi\right)\exp(-S_\theta)=0. \tag{2}$$

Let δ_θ be the infinitesimal deformation operator of the noncommutative parameter θ which operates as

$$\delta_\theta\theta^{\mu\nu}=\delta\theta^{\mu\nu}, \tag{3}$$

where $\delta\theta^{\mu\nu}$ are some infinitesimal antisymmetric two form elements. If δ_θ and BRS operator $\hat{\delta}$ commute each other, then the partition function is invariant. Indeed, there is some examples such that $\hat{\delta}\delta_\theta=\delta_\theta\hat{\delta}$, and partition functions are calculated by using this property.[28,29,27]

In this paper, cohomological Yang-Mills theories in noncommutative Euclidian spaces are discussed. If there is a gauge symmetry, the BRS-like transformation is slightly different from the one of nongauge theory. The BRS-like symmetry is not nilpotent but

$$\hat{\delta}^2=\delta_{g,\theta}, \tag{4}$$

where $\delta_{g,\theta}$ is a gauge transformation operator deformed by some noncommutative deformation method like the star product $*_\theta$. As occasion arises, the gauge transformation $\delta_{g,\theta}$ is defined as one including global symmetry transformations. The partition function of the noncommutative cohomological field theory is invariant under changing noncommutative parameters when the BRS transformation does not depend on the noncommutative parameters, because the BRS transformation $\hat{\delta}$ and the θ deformation δ_θ commute. Conversely, when the definition of the BRS-like

operator (4) depends on the noncommutative parameter θ, then $\hat{\delta}$ and δ_θ do not commute,

$$\delta_\theta \hat{\delta} \neq \hat{\delta}\delta_\theta \Rightarrow \delta_\theta \hat{\delta} = \hat{\delta}'\delta_\theta, \tag{5}$$

where $\hat{\delta}'$ is a BRS-like operator that generates the same transformations as the original BRS-like operator $\hat{\delta}$, except for the square. The square of $\hat{\delta}'$ is defined by

$$\hat{\delta}'^2 = \delta_{g,\theta+\delta\theta}. \tag{6}$$

Since the gauge symmetry is defined by using noncommutative parameter $\theta^{\mu\nu}+\delta\theta^{\mu\nu}$ after the δ_θ operation, this difference arises. This fact makes a little complex problem to prove the θ-shift invariance of noncommutative cohomological Yang-Mills theory in comparison with the case of nongauge theory.

Note that the essential point of this problem is not nilpotent property changing, but θ dependence of the definition of the BRS operator. (In fact, we can construct the BRS operator for the cohomological Yang-Mills theory as a nilpotent operator.[3])

However, we can prove the invariance of the partition function of cohomological Yang-Mills theory in NC $\mathbb{R}^{2D}$ under the noncommutative parameter deformation. For simplicity, we take

$$(\theta^{\mu\nu}) = \bigoplus_i \epsilon^{2i-1,2i}\theta = \theta\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

where $\epsilon^{2i-1,2i}$ is an antisymmetric tensor such that $\epsilon^{2i-1,2i} = -\epsilon^{2i,2i-1} = 1$, and we restrict the θ deformation to

$$\theta \to \theta + \delta\theta.$$

In the following, we only use operator formalisms to describe the noncommutative field theory, therefore the fields are operators acting on the Hilbert space $\mathcal{H}$. Then differential operators ∂_μ are expressed by using commutation brackets $-i\theta^{-1}_{\mu\nu}[x^\nu, *] \equiv [\hat{\partial}_\mu, *]$ and $\int d^{2D}x$ is replaced with $\det(\theta)^{1/2}\,\mathrm{Tr}_{\mathcal{H}}$. Therefore the noncommutative parameter deformation is equivalent with replacing $-i\theta^{-1}_{\mu\nu}[x^\nu,]$ and $\det(\theta)^{1/2}\,\mathrm{Tr}_{\mathcal{H}}$ by $-i(\theta+\delta\theta)^{-1}_{\mu\nu}[x^\nu,]$ and $\det(\theta+\delta\theta)^{1/2}\,\mathrm{Tr}_{\mathcal{H}}$, respectively.

Let us consider Donaldson-Witten theory (topological twisted $\mathcal{N}=2$ Yang-Mills theory) on NC $\mathbb{R}^4$.[36] This theory is constructed by bosonic fields $(A_\mu, H^+_{\mu\nu}, \bar{\phi}, \phi)$ and fermionic fields $(\psi_\mu, \chi^+_{\mu\nu}, \eta)$, where $(A_\mu, H^+_{\mu\nu}, \bar{\phi})$ and $(\psi_\mu, \chi^+_{\mu\nu}, \eta)$ are supersymmetric (BRS) pairs,

$$\begin{gathered} \chi^+_{\mu\nu}, H^+_{\mu\nu} \in \Omega^{2,+}(\mathbb{R}^4, \mathrm{ad}\,P), \quad \psi_\mu \in \Omega^1(\mathbb{R}^4, \mathrm{ad}\,P), \\ \eta, \bar{\phi}, \phi \in \Omega^0(\mathbb{R}^4, \mathrm{ad}\,P). \end{gathered} \tag{7}$$

Their ghost numbers are assigned as $(A_\mu, \chi^+_{\mu\nu}, H^+_{\mu\nu}, \psi_\mu, \eta, \bar{\phi}, \phi) = (0,-1,0,1,-1,-2,2)$. The BRS-like operator is defined by

$$\begin{gathered} \hat{\delta}A_\mu = \psi_\mu, \quad \hat{\delta}\chi^+_{\mu\nu} = H^+_{\mu\nu}, \\ \hat{\delta}\psi_\mu = D_\mu\phi, \quad \hat{\delta}H^+_{\mu\nu} = i[\chi^+_{\mu\nu}, \phi], \\ \hat{\delta}\phi = 0, \quad \hat{\delta}\bar{\phi} = \eta, \quad \hat{\delta}\eta = i[\bar{\phi}, \phi], \end{gathered} \tag{8}$$

where the covariant derivative is defined by $D_\mu * := [\hat{\partial}_\mu + iA_\mu, *]$ with $\hat{\partial}_\mu := -i\theta^{-1}_{\mu\nu}x^\nu$. When we consider only the case of NC $\mathbb{R}^{2D}$, field theories are expressed by the Fock space formalism (See Appendix A). In the Fock space representation, fields are expressed as A_μ

$=\Sigma A^{n_1 n_2}_{\mu_{m_1 m_2}} |n_1, n_2\rangle\langle m_1, m_2|$, $\psi_\mu = \Sigma \psi^{n_1 n_2}_{\mu_{m_1 m_2}} |n_1, n_2\rangle\langle m_1, m_2|$, etc. Therefore, the above BRS transformations are expressed as

$$\hat{\delta} A^{n_1 n_2}_{\mu_{m_1 m_2}} = \psi^{n_1 n_2}_{\mu_{m_1 m_2}}, \quad \ldots . \tag{9}$$

Let us define gauge fermions as

$$\begin{aligned} \Psi &= \left[2\chi^+_{\mu\nu} \left(-iF^{+\mu\nu} + \tfrac{1}{2} H^{+\mu\nu} \right) \right], \\ \Psi_{\text{proj}} &= -[\bar{\phi} D_\mu \psi^\mu], \end{aligned} \tag{10}$$

then the action functional is given by

$$\begin{aligned} S &= \mathrm{Tr}_{\mathcal{H}} L(A_\mu, \ldots; \hat{\partial}_{z_i}, \hat{\partial}_{\bar{z}_i}) = \mathrm{Tr}_{\mathcal{H}} \, \mathrm{tr} \, \hat{\delta}(\Psi + \Psi_{\text{proj}}) \\ &= \mathrm{Tr}_{\mathcal{H}} \, \mathrm{tr}(F^{+2} - 4i\chi^{+\mu\nu} D_\mu \psi_\nu - \eta D_\mu \psi^\mu + i\phi\{\chi^+_{\mu\nu}, \chi^{+\mu\nu}\} - i\bar{\phi}\{\psi_\mu, \psi^\mu\} - \bar{\phi} D_\mu D^\mu \phi), \end{aligned} \tag{11}$$

where tr is trace for gauge group. In this paper, we omit to note $\det(\theta)^{1/2}$ that is an overall factor, for economy of space. Let us change the dynamical variables as

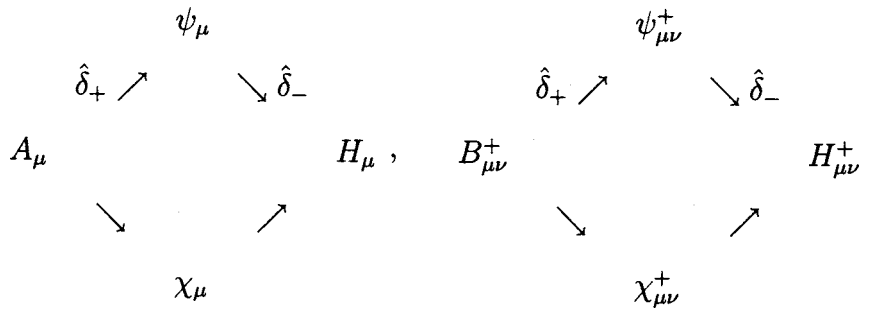
$$\begin{aligned} A_\mu \to \frac{1}{\sqrt{\theta}} \tilde{A}_\mu, \quad \psi_\mu \to \frac{1}{\sqrt{\theta}} \tilde{\psi}_\mu, \quad \bar{\phi} \to \frac{1}{\theta} \tilde{\bar{\phi}}, \quad \eta \to \frac{1}{\theta} \tilde{\eta}, \\ \chi^+_{\mu\nu} \to \frac{1}{\theta} \tilde{\chi}^+_{\mu\nu}, \quad H^+_{\mu\nu} \to \frac{1}{\theta} \tilde{H}^+_{\mu\nu}, \quad \phi \to \tilde{\phi}. \end{aligned} \tag{12}$$

Note that this changing does not cause nontrivial Jacobian from the path integral measure because of the BRS symmetry. Then, the action is rewritten as

$$S \to \frac{1}{\theta^2} \tilde{S}, \quad L(A_\mu, \ldots; \hat{\partial}_{z_i}, \hat{\partial}_{\bar{z}_i}) \to \frac{1}{\theta^2} L(\tilde{A}_\mu, \ldots; -a_i^\dagger, a_i). \tag{13}$$

Here the action on the left-hand side depends on θ because the derivative is given by $\partial_{z_i} = -\sqrt{\theta^{-1}}[a_i^\dagger,]$ and so on. In contrast, the action $\tilde{S}$ on the right-hand side does not depend on θ because all θ parameters are factorized out. Using the BRS symmetry or the fact of Eq. (2), it is proved that the partition function is invariant under the deformation of θ, because $\delta_\theta Z = -2(\delta\theta)\theta^{-3}\langle\tilde{S}\rangle = 0$. $\mathrm{Tr}_{\mathcal{H}_{2\ \mathrm{dim}}} \mathrm{tr}\left(\phi F + \frac{1}{2}\psi \wedge \psi\right)$ and $\mathrm{tr}\, \phi^n$ are known as observables of Donaldson-Witten theory. They are rewritten as $(1/\theta)\mathrm{Tr}_{\mathcal{H}} \mathrm{tr}\left(\tilde{\phi}\tilde{F} + \frac{1}{2}\tilde{\psi} \wedge \tilde{\psi}\right)$ and $\mathrm{tr}\, \tilde{\phi}^n$. We use O to represent such observables, then $\delta_\theta \langle O \rangle = 0$ are proved in a similar way to the proof of $\delta_\theta Z = 0$. Therefore, invariance of Donaldson-Witten theory under $\theta \to \theta + \delta\theta$ is proved.

We can discuss the topological twisted $\mathcal{N}=4$ Yang-Mills theory in noncommutative $\mathbb{R}^4$ similarly.[34] (There are many kinds of topological twisted theories of $\mathcal{N}=4$ Yang-Mills theory. We only consider Vafa-Witten-type theory.) There are additional fields $(B^+_{\mu\nu}, c, H_\mu)$ and $(\psi^+_{\mu\nu}, \bar{\eta}, \chi_\mu)$, where $(B^+_{\mu\nu}, c, H_\mu)$ are bosonic fields and $(\psi^+_{\mu\nu}, \bar{\eta}, \chi_\mu)$ are fermionic fields, where $B^+_{\mu\nu}, \psi^+_{\mu\nu} \in \Omega^{2,+}(\mathbb{R}^4, \mathrm{ad}\, P)$. They are supersymmetric partners, and the BRS multiplets are expressed by the following diagram:



There are two BRS-like operators $\hat{\delta}_+$ and $\hat{\delta}_-$ because of the R-symmetry of the $\mathcal{N}=4$. The $\hat{\delta}_+$ transformations are given by

$$\hat{\delta}_+ B^+_{\mu\nu} = \psi^+_{\mu\nu}, \quad \psi^+_{\mu\nu} = i[B^+_{\mu\nu}, \phi], \tag{14}$$

$$\hat{\delta}_+ \chi_\mu = H_\mu, \quad \hat{\delta}_+ H_\mu = i[\chi_\mu, \phi], \quad \hat{\delta}_+ c = \bar{\eta}, \quad \hat{\delta}_+ \bar{\eta} = i[c, \phi], \tag{15}$$

and the same transformations as (8) for other fields. The action of the topological twisted $\mathcal{N}=4$ Yang-Mills theory without the $\tau \int F \wedge F$ is

$$S = \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_+ \{\chi^+_{\mu\nu}(H^{+\mu\nu} - i(F^{+\mu\nu} - i[B^+_{\mu\rho}, B^+_{\nu\sigma}]\delta^{\rho\sigma} - i[B^+_{\mu\nu}, c]))\} + \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_+ \{\chi^\rho(H_\rho - i(-2D^\mu B^+_{\mu\rho} - D_\rho c))\} + \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_+ \{i[\phi, \bar{\phi}]\eta - i\bar{\eta}[c, \bar{\phi}] + i[B^{+\mu\nu}, \bar{\phi}]\psi^+_{\mu\nu} + (D_\mu \bar{\phi})\psi_\mu\}. \tag{16}$$

For this action, we change the variables as

$$B^+_{\mu\nu} \to \frac{1}{\sqrt{\theta}} \tilde{B}^+_{\mu\nu}, \quad \psi^+_{\mu\nu} \to \frac{1}{\sqrt{\theta}} \tilde{\psi}^+_{\mu\nu}, \quad c \to \frac{1}{\sqrt{\theta}} \tilde{c}, \quad \bar{\eta} \to \frac{1}{\sqrt{\theta}} \tilde{\bar{\eta}},$$

$$\chi_\mu \to \frac{1}{\theta} \tilde{\chi}_\mu, \quad H_\mu \to \frac{1}{\theta} \tilde{H}_\mu$$

with (12), then $S \to (1/\theta^2)\tilde{S}$, and $\tilde{S}$ does not depend on θ. At last, invariance of the $\mathcal{N}=4$ topological twisted theory under $\theta \to \theta + \delta\theta$ is proved as the same as the Donaldson-Witten theory.

It is worth commenting on the topological term $\int F \wedge F$ that exists in the usual Vafa-Witten theory but now is removed. This term is not written by a BRS exact term, so we cannot adapt the above discussion to the topological term. But, it is natural that we expect that $\int F \wedge F$ is invariant under the θ shift. Indeed, for instanton solutions constructed from noncommutative deformed ADHM data, we have proof of invariance of instanton number under θ shift.[14,26] This is why, we expect that the partition functions or vacuum expectation values are still invariants even if the action of the cohomological Yang-Mills theories include $\int F \wedge F$ (see also Sec. V).

By applying these facts for several physical models, some interesting information can be found. For example, as we will see soon, we can show that the partition function of the noncommutative cohomological gauge theory and the partition function of the IKKT matrix model have a correspondence. This correspondence is not only for certain classical background theory as we saw in Ref. 1. The reason is as follows. The IKKT matrix model is constructed as dimensional reduction of the 10-dimensional super U(N) Yang-Mills theory with large N limit.[2,12] This dimensional reduction is regarded as the large noncommutative parameter limit ($\theta \to \infty$ in Sec. IV). Taking the large N limit of the matrix model is similar to considering the Yang-Mills theories on noncommutative Moyal space, i.e., matrices are regarded as linear operators acting on the Hilbert space caused from noncommutativity. By the way, the noncommutative cohomological Yang-Mills model on Moyal space in the large θ limit is almost the same as the model of Moore, Nekrasov, and Shatashvili (MNS).[20] MNS show that the partition function is calculated by the cohomological

matrix model in Ref. 20 and related works are seen in Refs. 4, 11, and 31. This cohomological matrix model is almost equivalent to the IKKT matrix model. That is why we can produce similar result by using NC cohomological Yang-Mills theories. To show these facts concretely, we will calculate the partition function of $\mathcal{N}=4$, $d=4$ U(1) theory on NC $\mathbb{R}^4$ in Sec. IV by using the facts given in this section.

III. UNIVERSALITY OF PARTITION FUNCTIONS

In this section, we show that the large θ limit is equivalent to dimensional reduction. From this fact, we find the universal perspective for the partition functions of supersymmetric Yang-Mills theories in NC $\mathbb{R}^{2D}$.

In the preceding section, we consider the case of $\mathbb{R}^4$. There is two independent noncommutative parameters θ^1, θ^2 for the NC $\mathbb{R}^4$, that is to say, after choosing proper coordinate noncommutative parameters are expressed as

$$(\theta^{\mu\nu}) = \begin{pmatrix} 0 & \theta^1 & 0 & 0 \\ -\theta^1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \theta^2 \\ 0 & 0 & -\theta^2 & 0 \end{pmatrix}. \tag{17}$$

In the discussion of the preceding section, we take noncommutative parameter shift coincidently, that is $\theta^1=\theta^2=\theta\rightarrow\theta+\delta\theta$. However, we can shift θ^1, θ^2 independently without changing partition functions and vacuum expectations. Further, this discussion is extended to other dimensional theories.

Let us consider more general cases than NC $\mathbb{R}^4$. Let noncommutative parameter matrix of NC $\mathbb{R}^{2D}$ be $(\theta^{\mu\nu})=\oplus\theta^i\epsilon^{2i-1,2i}$. In the large θ^i limit, terms with derivative operators $\partial_{x_{2i}} := -i(\theta^i)^{-1}[x_{2i-1}, *]$ and $-\partial_{x_{2i-1}} := -i(\theta^i)^{-1}[x_{2i}, *]$ become irrelevant in Lagrangians. If the partition function and the VEV of arbitrary observables of the cohomological field theory are well defined, the terms including $\partial_{x_{2i}}$ or $\partial_{x_{2i-1}}$ are possible to be removed. (In Appendix B, concrete discussions and details are given.) In the complex coordinate expression, the terms including z_i and $\bar{z}_i$ derivatives are omitted. Meanwhile, an arbitrary operator is expressed as

$$\hat{\mathcal{O}} = \sum_{n_1,m_1} \cdots \sum_{n_D,m_D} \mathcal{O}^{n_1\cdots n_D}_{m_1\cdots m_D} |n_1, \ldots, n_D\rangle\langle m_1, \ldots, m_D|,$$

by using fock space basis (see Appendix A). We consider a quantum theory of infinite-dimensional matrix model, and $\mathcal{O}^{n_1\cdots n_D}_{m_1\cdots m_D}$ is a variable of path integration. Then we cannot distinguish dynamical variables

$$\mathcal{O}^{n_1\cdots n_{i-1}n_{i+1}\cdots n_D}_{m_1\cdots m_{i-1}m_{i+1}\cdots m_D} |n_1, \ldots, n_{i-1}, n_{i+1}, \ldots, n_D\rangle\langle m_1, \ldots, m_{i-1}, m_{i+1}, \ldots, m_D| \tag{18}$$

from $\mathcal{O}^{n_1\cdots n_D}_{m_1\cdots m_D}|n_1,\ldots,n_D\rangle\langle m_1,\ldots,m_D|$ because both of them are infinite-dimensional matrices. From the facts that there is no ∂_{z_i} or $\partial_{\bar{z}_i}$ and it is impossible to distinguish dynamical variables living in $\mathbb{R}^{2D}$ from variables in $\mathbb{R}^{2D-2}$, then we conclude that the large θ_i limit is equivalent to the dimensional reduction corresponding to x^{2i-1} and x^{2i} directions.

We must note two points, here. The first point is that naive path integrals contain zero mode integrals. To make the story precise, let us define the zero mode here. Let $\{\phi_i\}$ be a set of fields and $S[\phi_i]$ be an action functional of a considered theory. Here, we define the zero mode ϕ_i^0 by $S[\phi_i^0]=0$. To make the partition functions be well defined, we manage the zero modes, in general. But it is difficult that the dealing with the zero modes is discussed in general terms. To avoid this difficulty, the discussion of the zero mode integrals are taken up in the individual cases. In Sec. IV, we will closely study the handling of the zero modes for the case of $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$.

The second point is that there might be BPS solutions that become singular at $\theta^i \to \infty$ limit. To the authors' knowledge, such solutions have never been known until now, but we cannot deny their existence. Since we cannot estimate its contribution to the vacuum expectations when we calculate them at the large θ^i limit, we must rule out such singular configurations when we construct the correspondence between finite θ^i and infinite θ^i.

As a summary of these arguments, the following claim is obtained.

Claim: Let Z_{2D} *and* $\langle O \rangle_{2D}$ *be a partition function and vacuum expectation value of* O *of a cohomological field theory in* NC $\mathbb{R}^{2D}$ *with* $D \geqslant 1$ *such that* $\delta_\theta Z_{2D}=0$ *and* $\delta_\theta \langle O \rangle_{2D}=0$. *Here, zero mode integrals and contributions from BPS solutions that become singular at large noncommutative parameter limit are removed from the path integral of* Z_{2D} *and* $\langle O \rangle_{2D}$. *Let* Z_{2D-2} *and* $\langle O \rangle_{2D-2}$ *be the partition function and vacuum expectation value of* O *of a noncommutative cohomological field theory in* NC $\mathbb{R}^{2D-2}$, *where they are given by dimensional reduction of* Z_{2D} *and* $\langle O \rangle_{2D}$. *Then*,

$$Z_{2D} = Z_{2D-2}, \quad \langle O \rangle_{2D} = \langle O \rangle_{2D-2}, \tag{19}$$

i.e., the partition functions of such theories do not change under dimensional reduction from 2D *to* $2D-2$.

From this claim, we find that following partition functions of super Yang-Mills theories on NC $\mathbb{R}^{2D}$ are equivalent:

$$Z^{8\ \mathrm{dim}}_{\mathcal{N}=2} = Z^{6\ \mathrm{dim}}_{\mathcal{N}=2} = Z^{4\ \mathrm{dim}}_{\mathcal{N}=4} = Z^{2\ \mathrm{dim}}_{\mathcal{N}=8} = Z^{0\ \mathrm{dim}}_{***}, \tag{20}$$

where $Z^{I\ \mathrm{dim}}_{\mathcal{N}=J}$ is a partition function of the $\mathcal{N}=J$ super Yang-Mills theory in noncommutative $\mathbb{R}^I$ with arbitrary gauge group. They are obtained by dimensional reduction of the eight dimensional $\mathcal{N}=2$ super Yang-Mills theory. Note that the topological terms in the actions of the above theories should be removed because the topological term is not universal between the different dimensional theories. The proof of (20) is as follows. In the $\mathbb{R}^{2D}$, a topological twist exists at any time for $\mathcal{N} \geqslant 2$. Using the topological twist, the partition functions are described as the one of cohomological field theories. Therefore, $Z^{8\ \mathrm{dim}}_{\mathcal{N}=2}$ is invariant under θ-shift and satisfies the condition of the above claim. After all, Eq. (20) is obtained. We will calculate the partition functions concretely in the case of U(1) in the next section.

It is worth adding some comments about the above models. We consider noncommutative Euclidean spaces. $\mathcal{N}=4$ super Yang-Mills theory in NC $\mathbb{R}^4$ is given as follows. At first, we construct the four-dimensional $\mathcal{N}=4$ super Yang-Mills theory by dimensional reduction of the 10-dimensional $\mathcal{N}=1$ super Yang-Mills defined on Minkowski space with SO(9,1) symmetry. In four dimensions, spinor in Euclidean space is defined as well as the spinor in Minkowski space. Therefore, we can construct the $\mathcal{N}=4$ super Yang-Mills theory in $\mathbb{R}^4$ by formally replacing the metric, gamma matrices and so on. Since the θ-shift invariance of $Z^{4\ \mathrm{dim}}_{\mathcal{N}=4}$ was shown explicitly in Sec. II (see also Appendix B), theories connected to the $\mathcal{N}=4$ $d=4$ super Yang-Mills theory through the dimensional reduction appear in (20).

This discussion is valid not only for the $\mathcal{N}=4$ case. For example, we saw that the θ-shift invariance of $Z^{4\ \mathrm{dim}}_{\mathcal{N}=2}$ in Sec. II. Then, the similar relation should exist,

$$Z^{4\ \mathrm{dim}}_{\mathcal{N}=2} = Z^{2\ \mathrm{dim}}_{\mathcal{N}=4} = Z^{0\ \mathrm{dim}}_{***}. \tag{21}$$

Let us summarize this section. Universality of partition functions and vacuum expectation values of observables of NC cohomological field theories are discussed. From the claim, we found that $\mathcal{N} \geqslant 2$ supersymmetric models or cohomological field theories in NC $\mathbb{R}^{2D}$ are invariant under dimensional reduction from 2D to $2D-2$. In the following section, we will apply these facts to concrete calculations.

IV. $\mathcal{N}=4$ U(1) GAUGE THEORY IN NC $\mathbb{R}^4$

In this section, we calculate the partition function of the topological twisted $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$, without the topological term $\int F \wedge F$ in its action.

We perform the calculation in the $\theta\to\infty$ limit. The reason why we take this limit is as follows. As explained in Sec. II, the partition function and other correlation functions of cohomological field theories on noncommutative spaces are invariant under the shift transformation of the noncommutative parameter θ. So we obtain the exact result by taking $\theta\to\infty$ limit. Also this limit makes the calculation executable.

In the operator formalism, field theories in NC $\mathbb{R}^4$ are expressed as infinite dimensional matrix models whose symmetry is U(N) ($N\to\infty$). The size of matrices appearing in this model is infinite. To perform the calculation, we introduce a cutoff for the matrix size. In addition, this matrix model contains trace parts which correspond to zero modes in $\theta\to\infty$. Therefore we must carefully treat the trace parts to make the path integral well defined.

In Sec. IV A, we give the action of the topological twisted $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$ in the operator formalism, i.e., in terms of infinite-dimensional matrices. In Sec. IV B, we truncate the size of the matrices into finite size, a finite integer N. In Sec. IV C, we explain that the truncated $N\times N$ matrix model action obtained in the preceding section is equivalent to the dimension reduction of the 10 dimensional $\mathcal{N}=1$ U(N) super Yang-Mills action to 0 dimensions. This U(N) matrix model contains traceless parts and trace parts. In Sec. IV D, we calculate the partition function of the traceless sector. The traceless sector is a SU(N) matrix model. The partition function of this SU(N) matrix model was obtained by MNS.[20] By modifying their arguments, we evaluate the $N\to\infty$ limit of the partition function of the traceless sector. In Sec. IV E, we introduce extra parts into the matrices to handle the trace parts which are zero modes. The extra parts and trace parts are the next leading terms in the $1/\sqrt{\theta}$ expansion. In Sec. IV F, the calculation of the trace sector is performed. Our result is presented at the end of this section.

A. Setting

In the Fock space formalism, i.e., in terms of (infinite-dimensional) matrices, the action of the topological twisted $\mathcal{N}=4$ U(1) gauge theory on NC $\mathbb{R}^4$ is expressed as

$$S^{4\ \mathrm{dim}}_{\mathcal{N}=4}=\mathrm{Tr}_{\mathcal{H}}\ \hat{\delta}_+[+\chi^{+\mu\nu}\{H^+_{\mu\nu}-i(F^+_{\mu\nu}-i[B^+_{\mu\rho},B^+_{\nu\sigma}]\delta^{\rho\sigma}-i[B^+_{\mu\nu},c])\}+\chi^{\mu}\{H_\mu-i(-2D^\nu B^+_{\nu\mu}-D_\mu c)\}$$
$$+i[\phi,\bar{\phi}]\eta-i\bar{\eta}[c,\bar{\phi}]+i[B^{+\mu\nu},\bar{\phi}]\psi^+_{\mu\nu}+(D_\mu\bar{\phi})\psi_\mu]. \tag{22}$$

After acting $\hat{\delta}_+$, (22) is rewritten as

$$S^{4\ \mathrm{dim}}_{\mathcal{N}=4}=\mathrm{Tr}_{\mathcal{H}}[H^{+\mu\nu}\{H^+_{\mu\nu}-i(F^+_{\mu\nu}-i[B^+_{\mu\rho},B^+_{\nu\sigma}]\delta^{\rho\sigma}-i[B^+_{\nu\sigma},c])\}+\chi^{+\mu\nu}\{-i[\chi^+_{\mu\nu},\phi]+i(2D_\mu\psi_\nu$$
$$-2i[B^+_{\mu\rho},\psi^+_{\nu\sigma}]\delta^{\rho\sigma}-i[\psi^+_{\mu\nu},c]-i[B^+_{\mu\nu},\bar{\eta}])\}+H^\mu\{H_\mu-i(-2D^\nu B^+_{\nu\mu}-D_\mu c)\}+\chi^\mu\{-i[\chi_\mu,\phi]$$
$$-i(2D^\nu\psi^+_{\nu\mu}+2i[\psi^\nu,B^+_{\nu\mu}]-D_\mu\bar{\eta}+i[\psi_\mu,c])\}+[\phi,\bar{\phi}]^2+[c,\phi][c,\bar{\phi}]+[B^{+,\mu\nu},\bar{\phi}][B^+_{\mu\nu},\phi]$$
$$+D^\mu\bar{\phi}D_\mu\phi+i[\phi,\eta]\eta+i\bar{\eta}[\bar{\eta},\bar{\phi}]+i\bar{\eta}[c,\eta]+i[\psi^{+\mu\nu},\bar{\phi}]\psi^+_{\mu\nu}+i[B^{+\mu\nu},\eta]\psi^+_{\mu\nu}+D^\mu\eta\psi_\mu$$
$$+i[\psi^\mu,\bar{\phi}]\psi_\mu]. \tag{23}$$

From (22) or (23), we find the BPS equations. For example,

$$F^+_{\mu\nu}-i[B^+_{\mu\rho},B^+_{\nu\sigma}]\delta^{\rho\sigma}-i[B^+_{\mu\nu},c]=0,$$

$$-2D^\nu B^+_{\nu\mu}-D_\mu c=0. \tag{24}$$

In the following, we calculate the partition function $Z^{4\ \mathrm{dim}}_{\mathcal{N}=4}$ formally defined as

$$Z^{4\ \mathrm{dim}}_{\mathcal{N}=4}=\int\mathcal{D}f\,e^{-S^{4\ \mathrm{dim}}_{\mathcal{N}=4}[f]}, \tag{25}$$

where f represents all matrices $A_\mu, \psi_\mu, \ldots$. Also we use f_{boson} and f_{fermion} to denote bosonic matrices $A_\mu, H_\mu, \ldots$ and fermionic matrices $\psi_\mu, \chi_\mu, \ldots$, respectively.

In usual commutative spaces, U(1) gauge theories are free if all matters belong to the adjoint representation, because the gauge interactions between the fields belonging to the adjoint representation are described by commutators of matrices and all commutators vanish in the U(1) case. However, in noncommutative spaces, the noncommutativity of the multiplication induces the U(1) gauge theories to non-Abelian U(N) ($N\to\infty$) like gauge theories. This U(N) ($N\to\infty$) is identified with the unitary transformation group acting on state vectors of the Hilbert space $\mathcal{H}$. [It is a well-known fact that the U(∞) is different from $\lim_{N\to\infty}$ U(N), in the meaning of the topology. In this paper, we perform the calculation by using $\lim_{N\to\infty}$ U(N), and there is no denying that some extra collections appear from the difference. However, there is no doubt about validity of the calculation of U(N) ($N\to\infty$) as a good approximation even in this case.]

Let us consider to take the $\theta\to\infty$ limit in the calculation of the partition function $Z^{4\text{ dim}}_{\mathcal{N}=4}$. We can evaluate the partition function exactly in this limit, as explained in Sec. II. In the $\theta\to\infty$ limit we naively expect that all differential terms in the action vanish and dimensional reduction occurs as we saw in Sec. III. Therefore, we can perform the calculation by using a matrix model in 0-dimensional space whose symmetry is U(N) ($N\to\infty$). We define the action in 0-dimensional space-time as

$$S^{\infty}_{MM} = S^{4\text{ dim}}_{\mathcal{N}=4}\big|_{\theta\to\infty}: \quad \mathrm{U}(N)(N\to\infty) \text{ matrix model}, \tag{26}$$

then, we find $Z^{4\text{ dim}}_{\mathcal{N}=4}$ is equal to the partition function of the matrix model (26),

$$Z^{4\text{ dim}}_{\mathcal{N}=4} = \frac{1}{\mathrm{Vol\,U}(N)(N\to\infty)} \int \mathcal{D}f\, e^{-S^{\infty}_{MM}}. \tag{27}$$

To calculate the partition function of this infinite-dimensional U(N) ($N\to\infty$) matrix model (26), we need to overcome the following problems.

(i) The size of the matrices is infinite. To perform the calculation, we truncate the size of the matrices into a finite integer N.
(ii) The matrices contain trace parts. These trace parts play the role of zero modes. To make the path integral well defined, we must carefully treat the trace parts.

In the rest of this section, we solve these problems and obtain the partition function (27).

B. Cutoff for matrix size

In this section we truncate the size of the matrices, to calculate the partition function.

The Hilbert space of the $\mathcal{N}=4$ U(1) gauge theory on NC $\mathbb{R}^4$ is constructed by a Fock space

$$\mathcal{H} = \bigoplus_{n_1=0,n_2=0}^{n_1=\infty,n_2=\infty} \mathbb{C}|n_1,n_2\rangle. \tag{28}$$

We introduce a cutoff, a finite integer N_c, and truncate the Hilbert space into a finite-dimensional subspace $\mathcal{H}_N$ whose dimension is N. We can perform such truncation in several ways. For example, $\mathcal{H}_N$ is defined by

$$\mathcal{H}_N = \bigoplus_{n_1=0,n_2=0}^{n_1=N_c,n_2=N_c} \mathbb{C}|n_1,n_2\rangle. \tag{29}$$

For this case

$$\dim \mathcal{H}_{\mathcal{N}} = N = (N_c+1)^2, \tag{30}$$

and the unit matrix of $\mathcal{H}_N$ is given as

$$\mathbf{1}_N = \bigoplus_{n_1=0,n_2=0}^{n_1=N_c,n_2=N_c} |n_1,n_2\rangle\langle n_1,n_2|. \tag{31}$$

The results and calculations do not depend on the definition of the cutoff in the following discussion (see Appendix A). Therefore we do not use concrete expression of the example (29). By definition,

$$\mathrm{Tr}_{\mathcal{H}}\, \mathbf{1}_N = \dim \mathcal{H}_{\mathcal{N}} = N. \tag{32}$$

For later use, we define $\mathcal{I}$ as

$$\mathcal{I} = \frac{1}{\sqrt{N}}\mathbf{1}_N, \tag{33}$$

which satisfies

$$\mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}\mathcal{I} = 1. \tag{34}$$

We truncate the infinite-dimensional matrices appearing in (26) into finite-dimensional $N \times N$ matrices. We use the symbol f_N to denote the $N \times N$ truncation of f. For example, of (29), if

$$f = \sum_{n_i=0}^{\infty} \sum_{m_i=0}^{\infty} f^{n_1 n_2}_{m_1 m_2} |n_1,n_2\rangle\langle m_1,m_2|,$$

then

$$f_N = \sum_{n_i=0}^{N_c} \sum_{m_i=0}^{N_c} f^{n_1 n_2}_{m_1 m_2} |n_1,n_2\rangle\langle m_1,m_2|.$$

Now we consider the finite-dimensional $N \times N$ matrix model S^N_{MM} which is obtained by the truncation from (26)

$$S^N_{MM} = S^{\infty}_{MM}|_{N\times N \text{ truncation}}. \tag{35}$$

The partition function of the truncated matrix model (35) is defined by

$$Z^{4\ \dim}_{\mathcal{N}=4}|_N = \frac{1}{\mathrm{Vol}\ U(N)} \int \mathcal{D}f_N e^{-S^N_{MM}}. \tag{36}$$

$N \times N$ matrix f_N is decomposed into the traceless part and the trace part,

$$f_N = f^{\mathrm{su}} + f^{\mathrm{tr}}, \tag{37}$$

where f^{su} is the traceless part and f^{tr} is the trace part. The traceless part f^{su} is expanded by the generators of the Lie algebra su(N),

$$f^{\mathrm{su}} = \sum_{a=1}^{N^2-1} f_{(a)} \tau^a, \quad \tau^a \in \mathrm{su}(N), \tag{38}$$

and f^{tr} is proportional to $\mathcal{I}$,

$$f^{\mathrm{tr}} = f_{(1)}\mathcal{I}. \tag{39}$$

The basis, τ^a and $\mathcal{I}$, satisfy the following orthonormal conditions:

$$\mathrm{Tr}_{\mathcal{H}} \tau^a \tau^b = \delta^{ab}, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}\mathcal{I} = 1, \quad \mathrm{Tr}_{\mathcal{H}}\, \tau^a \mathcal{I} = 0. \tag{40}$$

In the naive $\theta \to \infty$ limit (i.e., 0-dimension reduction), Eq. (35) contains no trace part f^{tr},

$$Z^N_{MM} = Z^N_{MM}|_{\text{traceless}} \int \mathcal{D}f^{\text{tr}}, \tag{41}$$

where $Z^N_{MM}|_{\text{traceless}}$ is defined by

$$Z^N_{MM}|_{\text{traceless}} = \frac{1}{\text{Vol SU}(N)} \int \mathcal{D}f^{\text{su}} e^{-S^N_{MM}[f^{\text{su}}]}. \tag{42}$$

[Precisely speaking, the trace part of the auxiliary fields appear in (35). After integrating out the auxiliary fields, no trace part appears in (35).] So the trace part f^{tr} plays the role of the zero mode such that $S^N_{MM}[f^{\text{tr}}]=0$. To make the path integral well defined, we must carefully treat it. For other handling the zero modes, see, for example, Ref. 32. However we postpone this task for the moment. First, we concentrate on the traceless sector. Before the calculation of the traceless sector, we explain the equivalence between (35) and the action considered in Ref. 20 in the next section.

C. Relation to the work of MNS and IKKT

To explain that the equivalence between (35) and the action considered in Ref. 20, we first recall the fact that the dimensional reduction model from the $D=10$ $\mathcal{N}=1$ super Yang-Mills theory to 0 dimension can be reformulated into a cohomological matrix model.[11,20] The 0-dimension matrix model given by dimensional reduction from the $D=10$ $\mathcal{N}=1$ super Yang-Mills theory is expressed as

$$S^{10\to 0 \text{ dim}}_{\mathcal{N}=1} = \text{tr}\left(\frac{1}{4}[A_M, A_N]^2 + \frac{i}{2}\bar{\Psi}\Gamma^M[A_M, \Psi]\right), \tag{43}$$

where A_M is the gauge vector fields and M,N takes $1,\ldots,10$ for the 10-dimension Euclid space, or $0,1,\ldots,9$ for the 10-dimension Minkowski space-time. Ψ is a Majorana-Weyl spinor of the 10-dimension space-time. It contains real 16 components. (Note that there is no Majorana-Weyl spinor in 10-dimension Euclidean space. So, if we consider the 10 dimensional model, we should take Minkowski space-time. To obtain the low-dimensional Euclidean model, we first perform dimensional reduction from 10 dimensions to lower dimensions, and then carry out Wick rotation.)

In Refs. 11 and 20, it is shown that (43) can be reformulated into a cohomological matrix model. The mapping rules between them are as follows.[20] A_M are arranged into complex matrices ϕ and B_i $(i=1,\ldots,4)$,

$$\begin{aligned} B_i &= A_{2i-1} + iA_{2i} \quad (\text{for } i=1,2,3), \\ B_4 &= A_9 + iA_8, \\ \phi &= A_7 + iA_{10}, \end{aligned} \tag{44}$$

and Ψ are arranged as

$$\Psi \to (\psi_i, \psi_i^\dagger) \oplus \vec{\chi} \oplus \eta, \tag{45}$$

where $\vec{\chi}$ belongs to the **7** representation of Spin (7). Introducing the bosonic auxiliary matrices $\vec{H}$, we can rewrite (43) into a cohomological form,

$$S_{\text{MNS}} = \text{tr}\ \hat{\delta}\left(\frac{1}{16}\eta[\phi,\bar{\phi}] - i\vec{\chi}\cdot\vec{\mathcal{E}} + \vec{\chi}\cdot\vec{H} + \frac{1}{4}\sum_{a=1}^{8}\Psi_a[A_a,\bar{\phi}]\right), \tag{46}$$

where $\vec{\mathcal{E}}$ is defined by

$$\vec{\mathcal{E}} = \left([B_i, B_j] + \frac{1}{2}\epsilon_{ijkl}[B_k^\dagger, B_l^\dagger](i<j), \sum_i [B_i, B_i^\dagger] \right). \tag{47}$$

The BRS transformation rules are given as

$$\begin{gathered} \hat{\delta}A_a = \Psi_a, \quad \hat{\delta}\Psi_a = [\phi, A_a], \\ \hat{\delta}\vec{\chi} = \vec{H}, \quad \hat{\delta}\vec{H} = [\phi, \vec{\chi}], \\ \hat{\delta}\bar{\phi} = \eta, \quad \hat{\delta}\eta = [\phi, \bar{\phi}], \\ \hat{\delta}\phi = 0. \end{gathered} \tag{48}$$

From (46) and (48), the following BPS equations are obtained:

$$\vec{\mathcal{E}} = 0, \quad [\phi, \bar{\phi}] = 0, \quad [A_a, \phi] = 0. \tag{49}$$

One can show that (46) is equivalent to (26), by using the following correspondence rule:[16]

$$\begin{gathered} (\phi, c, \bar{\phi}) \Leftrightarrow \left(\sqrt{2}\varphi_{34}, i\frac{1}{\sqrt{2}}(\varphi_{14} - \varphi_{23}), \sqrt{2}\varphi_{12} \right), \\ (B_{\mu\nu}^+\sigma_{11}^{\mu\nu}, B_{\mu\nu}^+\sigma_{12}^{\mu\nu}, B_{\mu\nu}^+\sigma_{22}^{\mu\nu}) \Leftrightarrow \left(\sqrt{2}\varphi_{13}, -\frac{1}{\sqrt{2}}(\varphi_{14} + \varphi_{23}), \varphi_{24} \right), \end{gathered} \tag{50}$$

where φ is defined by

$$\varphi_{k4} = -\varphi_{4k} = \frac{1}{\sqrt{2}}(A_{k+4} + iA_{k+7}), \quad \varphi_{ij} = (\epsilon^{ijk}\varphi_{k4})^*, \quad k = 1,2,3. \tag{51}$$

Remark that the equivalence among (35), (43), and (46) holds for both U(N) group and SU(N) group.

By choosing gauge group SU(N) and setting N to be a finite integer, we obtain the equivalence between (35) and (46),

$$S_{MM}^N|_{\text{traceless}} = S_{\text{MNS}}|_{\text{gauge group:SU}(N)}^{N:\text{finite}}. \tag{52}$$

Therefore

$$Z_{MM}^N|_{\text{traceless}} = Z_{\text{MNS}}|_{\text{gauge group:SU}(N)}^{N:\text{finite}}, \tag{53}$$

where

$$Z_{\text{MNS}}|_{\text{gauge group:SU}(N)}^{N:\text{finite}} = \frac{1}{\text{Vol SU}(N)} \int \mathcal{D}f^{\text{su}} \exp\{ -S_{\text{MNS}}[f^{\text{su}}]|_{\text{gauge group:SU}(N)}^{N:\text{finite}} \}. \tag{54}$$

MNS obtained the partition function (54).[20] (See also Ref. 6 where the partition function of the D-instanton model was calculated.)

On the other hand, by choosing gauge group U(N) and taking the $N \to \infty$ limit, the action (43) becomes the IKKT matrix model,[12]

$$S_{\text{IKKT}} = \lim_{N\to\infty} S_{\mathcal{N}=1}^{10\to 0 \text{ dim}}|_{\text{gauge group:U}(N)}. \tag{55}$$

So, we obtain the equivalence between (26) and (55),

$$S_{MM}^{\infty} = S_{\mathrm{IKKT}}. \tag{56}$$

D. Calculation of traceless sector

As explained in the preceding section the partition function (42) is calculated in Ref. 20. Their result tells us that

$$Z_{MM}^{N}|_{\mathrm{traceless}} = \sum_{d|N} \frac{1}{d^2}, \tag{57}$$

where the summation is taken over all divisor d of the finite integer N.

One might expect that to obtain the contribution of the traceless part f^{su} to $Z_{\mathcal{N}=4}^{4\ \mathrm{dim}}$, one takes the $N\to\infty$ limit,

$$Z_{MM}^{\infty}|_{\mathrm{traceless}} = \lim_{N\to\infty} Z_{MM}^{N}|_{\mathrm{traceless}}. \tag{58}$$

However $N\to\infty$ limit on the right-hand side of (57) is not well defined. The reason is as follows. We see that the right-hand side of (57) is finite,

$$\sum_{d|N} \frac{1}{d^2} < \sum_{n=1}^{N} \frac{1}{n^2} < 1 + \int_1^{\infty} \mathrm{d}x \frac{1}{x^2} = 2. \tag{59}$$

But $\Sigma_{d|N}(1/d^2)$ is not a monotonically increasing function of N. So it does not converge. For example, if we constrain N to be prime numbers,

$$\lim_{N\to\infty} \sum_{d|N} \frac{1}{d^2} = \lim_{N\to\infty} (1 + N^{-2}) = 1. \tag{60}$$

If we constrain $N=2^{N'}$,

$$\lim_{N\to\infty} \sum_{d|N} \frac{1}{d^2} = \lim_{N\to\infty} \sum_{n=0}^{N'} 2^{-2n} = \frac{4}{3}. \tag{61}$$

Therefore, we must give the proper definition of $N\to\infty$ limit.

To find a prescription which leads the definite answer of the $N=\infty$ case, let us recall the argument of Ref. 20 where the result (57) is concluded for a finite N.

(i) The authors of Ref. 20 separated the coupling constant g to g, $\tilde{g}$ and $\hat{g}$ (on the right-hand side of (46), we omitted the coupling constant g),

$$S_{\mathrm{MNS}} \to \mathrm{tr}\ \hat{\delta}\left(\frac{1}{16\tilde{g}} \eta[\phi, \bar{\phi}] - i\vec{\chi}\cdot\vec{\mathcal{E}} + g\vec{\chi}\cdot\vec{H} + \frac{1}{4\hat{g}} \sum_{a=1}^{8} \Psi_a[A_a, \bar{\phi}] \right). \tag{62}$$

(ii) They deformed the action by redefining $\mathcal{E}_{ij}$, the $(\mathbf{6}\oplus\bar{\mathbf{6}})_r$ part of $\vec{\mathcal{E}}$, as

$$\begin{aligned} \mathcal{E}_{ij} &= \Phi_{ij} - \tfrac{1}{2}\epsilon_{ijkl}\Phi_{kl}^{\dagger}, \\ \Phi_{ij} &= [B_i, B_j] - m\epsilon_{ijk4}B_k, \end{aligned} \tag{63}$$

where m is a mass parameter. This mass deformation corresponds to the supersymmetry breaking from $\mathcal{N}=4$ to $\mathcal{N}=1$ in the picture of four dimensional space.

(iii) They again separated the coupling constants g and $\hat{g}$ as

$$g\vec{\chi}\cdot\vec{H}\to g'\sum_{i<j}\chi_{ij}H_{ij}+g''\chi_7H_7,$$
$$\frac{1}{4\hat{g}}\sum_{a=1}^{8}\Psi_a[A_a,\bar{\phi}]\to\frac{1}{4\hat{g}'}\sum_{a=1}^{6}\Psi_a[A_a,\bar{\phi}]+\frac{1}{4\hat{g}''}\sum_{a=7,8}\Psi_a[A_a,\bar{\phi}]. \tag{64}$$

(iv) Then, they took the following limit:

$$g'\to 0\quad\text{and}\ \hat{g}'\to 0. \tag{65}$$

Notice that each term in the action is BRS exact. So the partition function is independent of separated coupling constants $g',g'',\ldots$. By taking (65), the partition function is dominated by configurations around solutions of the following fixed point equations:

$$[B_i,B_j]=m\epsilon_{ijk4}B_k,\quad [B_4,B_i]=0,\quad [B_4,\phi]=0,\quad i=1,2,3, \tag{66}$$

where B_i, B_4 and ϕ are all $N\times N$ matrices.

(v) The solution of (66) is given by

$$(B_i)_{N\times N}=(L_i)_{a\times a}\otimes\mathbf{1}_{d\times d},$$
$$(B_4)_{N\times N}=\mathbf{1}_{a\times a}\otimes(B_4)_{d\times d},\quad (\phi)_{N\times N}=\mathbf{1}_{a\times a}\otimes\phi_{d\times d}, \tag{67}$$

where a is a divisor of N and d is the quotient of N by a, and $(L_i)_{a\times a}$ denotes the generator of the SU(2) group in the $a\times a$ representation. Of course, there are other solutions of (66),

$$(B_i)_{N\times N}=\left(\begin{array}{c|c|c} (L_i)_{a_1\times a_1}\otimes\mathbf{1}_{d_1\times d_1} & 0 & 0 \\ \hline 0 & \ddots & 0 \\ \hline 0 & 0 & (L_i)_{a_k\times a_k}\otimes\mathbf{1}_{d_k\times d_k}\end{array}\right),$$
$$(B_4)_{N\times N}=\left(\begin{array}{c|c|c} \mathbf{1}_{a_1\times a_1}\otimes(B_4)_{d_1\times d_1} & 0 & 0 \\ \hline 0 & \ddots & 0 \\ \hline 0 & 0 & \mathbf{1}_{a_k\times a_k}\otimes(B_4)_{d_k\times d_k}\end{array}\right),$$
$$(\phi)_{N\times N}=\left(\begin{array}{c|c|c} \mathbf{1}_{a_1\times a_1}\otimes\phi_{d_1\times d_1} & 0 & 0 \\ \hline 0 & \ddots & 0 \\ \hline 0 & 0 & \mathbf{1}_{a_k\times a_k}\otimes\phi_{d_k\times d_k}\end{array}\right), \tag{68}$$

where $N=\Sigma_{l=1}^{k}N_l$, $N_l=a_l\times d_l$. However as mentioned in Ref. 20 these solutions do not contribute to the partition function. The solutions (68) contain bosonic zero modes, corresponding to extra U(1) parts $\mathrm{tr}_{N_l}\phi,\ldots$, and they are accompanied by their fermionic partners. The fermionic partners play a role of fermionic zero modes, and they vanish the path integral. So the solutions (68) do not contribute to the partition function.

(vi) In the above coupling limit (65) the authors integrated out B_i and corresponding fermionic partners around the solutions (67) by the Gaussian integral. The Gaussian integrals from bosons and the one from fermions cancel each other, so they produce no nontrivial factor. The resulting *effective* action is a matrix model of $d\times d$ matrices, B_4, its fermionic partner and ϕ.

(vii) The partition function of this $d\times d$ matrix model, we call it Z_d, is given by

$$Z_d = \frac{1}{d^2}, \tag{69}$$

which is another result obtained in the same paper.[20] The partition function $Z^N_{MM}|_{\text{traceless}}$ is given by the sum of the contributions from the solutions, $Z_d=1/d^2$, so they concluded (57).

Now let us turn to the $N\to\infty$ case. Our basic strategy is that taking large N limit is done after calculations with finite N. However, the result depends on the definition of the large N limit as mentioned above. To find the proper definition of the large N limit, we consider a naive $N=\infty$ case. That is, we do not take the $N\to\infty$ limit after obtaining the result of the finite N case, but we take the matrices as $\infty\times\infty$ from the starting point for a moment. For the case of $\infty\times\infty$ matrix, the steps (i)–(iv) need no change, but the step (v) should be reconsidered. In $\infty\times\infty$ matrix, we can embed a solution which has a direct product of an arbitrary finite-dimensional matrix and an infinite-dimensional matrix. Therefore we obtain solutions,

$$\begin{aligned}(B_i)_{\infty\times\infty} &= (L_i)_{\infty\times\infty}\otimes 1_{d\times d},\\ (B_4)_{\infty\times\infty} &= \mathbf{1}_{\infty\times\infty}\otimes(B_4)_{d\times d},\quad (\phi)_{\infty\times\infty} = \mathbf{1}_{\infty\times\infty}\otimes\phi_{d\times d}.\end{aligned} \tag{70}$$

Now d takes all natural numbers, and $(L_i)_{\infty\times\infty}$ are the generator of the SU(2) group in the $\infty\times\infty$ representations. Solutions, like (68), again do not contribute to the partition function. Moreover, one can construct other types of solutions,

$$\begin{aligned}(B_i)_{\infty\times\infty} &= (L_i)_{a\times a}\otimes\mathbf{1}_{\infty\times\infty},\\ (B_4)_{\infty\times\infty} &= \mathbf{1}_{a\times a}\otimes(B_4)_{\infty\times\infty},\quad (\phi)_{\infty\times\infty} = \mathbf{1}_{a\times a}\otimes\phi_{\infty\times\infty},\end{aligned} \tag{71}$$

and

$$\begin{aligned}(B_i)_{\infty\times\infty} &= (L_i)_{\infty\times\infty}\otimes\mathbf{1}_{\infty\times\infty},\\ (B_4)_{\infty\times\infty} &= \mathbf{1}_{\infty\times\infty}\otimes(B_4)_{\infty\times\infty},\quad (\phi)_{\infty\times\infty} = \mathbf{1}_{\infty\times\infty}\otimes\phi_{\infty\times\infty}.\end{aligned} \tag{72}$$

The step (vi), integrating out of B_i and their fermionic partners, again produces no nontrivial factor, because the cancellation of the Gaussian integrals between bosons and fermions holds for the case of infinite-dimensional integral. Therefore the partition function Z^∞_{MM} is given by the sum of contributions from the solutions (70) and (71), and (72),

$$Z^\infty_{MM} = Z^{(\infty\times d)}_{MM} + Z^{(a\times\infty)}_{MM} + Z^{(\infty\times\infty)}_{MM}, \tag{73}$$

where the first term on the right-hand side comes from (70), the second from (71), and the third from (72). $Z^{(\infty\times d)}_{MM}$ is still given by the sum of $Z_d=1/d^2$, as the step (vii), but in this $N=\infty$ case d runs all natural numbers $\mathbb{N}$. On the other hand, it is natural to expect that $Z^{(a\times\infty)}_{MM}$ and $Z^{(\infty\times\infty)}_{MM}$ vanish, because

$$Z^{(a\times\infty)}_{MM} \sim \sum \lim_{d\to\infty}\frac{1}{d^2} = 0,\quad Z^{(\infty\times\infty)}_{MM} \sim \sum \lim_{d\to\infty}\frac{1}{d^2} = 0, \tag{74}$$

if (69) is valid for $d=\infty$. So we conclude

$$Z^\infty_{MM}|_{\text{traceless}} = \sum_{d\in\mathbb{N}}\frac{1}{d^2} = \zeta(2) = \frac{\pi^2}{6}. \tag{75}$$

From these considerations, we propose the following definition of the large N limit. Let $N(n_i,k)$ be

$$N(n_i,k) \equiv \prod_{i=1}^{k} P_i^{n_i}, \tag{76}$$

where P_i are ordered prime numbers, i.e., $P_1=2<P_2=3<\cdots<P_k$, and k and n_i are positive integers. We define the large N limit by

$$\lim_{N\to\infty} \equiv \lim_{k\to\infty} \lim_{n_i\to\infty}. \tag{77}$$

Using this definition, we reproduce the same result as (75),

$$Z_{MM}^{\infty}|_{\text{traceless}} = \lim_{k\to\infty} \lim_{n_i\to\infty} \sum_{l_i=0}^{n_i} \frac{1}{(\prod_{i=1}^{k} P_i^{l_i})^2} = \prod_{i=1}^{\infty} \frac{1}{1-P_i^{-2}} = \zeta(2) = \frac{\pi^2}{6}. \tag{78}$$

[It is well known and will be seen in Sec. V that the partition function of this case is the sum of the Euler number of the moduli space, $\chi(\mathcal{M}_k)$ which takes a rational number in general. So one may expect that $Z_{MM}^{\infty}|_{\text{traceless}}$ is given by a rational number. However the summation is an infinite one, then it could take an irrational number, $\pi^2/6$.]

E. Introduction of extra terms

In this section, we deal with the zero mode problem. The origin of this problem is the fact that no trace part appears in (35). The reason why all trace parts vanish in (35) is that we drop all differential terms in the $\theta\to\infty$ limit. To solve the zero mode problem, we keep the next leading terms including the trace parts in the $1/\sqrt{\infty}$ expansion.

Let us explain the outline of our calculation. To keep the next leading term, we bring back some extra part f^{ex} living in the outside of $\mathcal{H}_N$. The definition of f^{ex} is given later in this section. Roughly speaking, f^{ex} are matrices appearing in kinetic terms $(1/\theta)f^{\text{ex}}\Box f^{\text{tr}}$ in (23). By keeping f^{ex}, the part of (22) or (23) which includes the trace part f^{tr} does not vanish,

$$S_{\text{tr}\oplus\text{ex}}[f^{\text{tr}},f^{\text{ex}}] = S_{\mathcal{N}=4}^{4\ \text{dim}}|_{\text{trace part}} - O(1/\theta^{1+\epsilon}) \neq 0, \tag{79}$$

where ϵ is an arbitrary positive real number. Then the partition function of (79) is well defined,

$$Z_{\text{tr}\oplus\text{ex}} = \int \mathcal{D}f^{\text{tr}}\mathcal{D}f^{\text{ex}} e^{-S_{\text{tr}\oplus\text{ex}}[f^{\text{tr}},f^{\text{ex}}]}: \text{ well defined.} \tag{80}$$

We suppose f^{ex} has the following expansion form:

$$f^{\text{ex}} = \sum_{\mu=1}^{4} f_{(\mu)}\mathcal{T}_{\mu}. \tag{81}$$

$\mathcal{T}_{\mu}$ is essentially defined by the commutator of $\hat{\partial}_{\mu}$ and $\mathbf{1}_N$. The precise definition of $\mathcal{T}_{\mu}$ is as follows. First of all, we define T_{μ} as the commutator of $\hat{\partial}_{\mu}$ and $\mathbf{1}_N$, i.e.,

$$T_{\mu} = [\hat{\partial}_{\mu}, \mathbf{1}_N]. \tag{82}$$

In the Fock space formalism, $\hat{\partial}_{\mu}$ is given as

$$\hat{\partial}_1 = \frac{1}{\sqrt{2\theta^{\text{l}}}}(a_1 - a_1^{\dagger}), \quad \hat{\partial}_2 = \frac{-i}{\sqrt{2\theta^{\text{l}}}}(a_1 + a_1^{\dagger}), \tag{83}$$

$$\hat{\partial}_3 = \frac{1}{\sqrt{2\theta^2}}(a_2 - a_2^\dagger), \quad \hat{\partial}_4 = \frac{-i}{\sqrt{2\theta^2}}(a_2 + a_2^\dagger),$$

where a_i is the annihilation operator and $a_i^\dagger$ is the creation operator. Given the definition of $\mathbf{1}_N$, for example (31), we obtain

$$\begin{aligned}
T_1 &= \frac{\sqrt{N+1}}{\sqrt{2\theta^1}}\left(-\sum_{n_2=0}^{N}|N,n_2\rangle\langle N+1,n_2| - \sum_{n_2=0}^{N}|N+1,n_2\rangle\langle N,n_2|\right),\\
T_2 &= \frac{-i\sqrt{N+1}}{\sqrt{2\theta^1}}\left(-\sum_{n_2=0}^{N}|N,n_2\rangle\langle N+1,n_2| + \sum_{n_2=0}^{N}|N+1,n_2\rangle\langle N,n_2|\right),\\
T_3 &= \frac{\sqrt{N+1}}{\sqrt{2\theta^2}}\left(-\sum_{n_1=0}^{N}|n_1,N\rangle\langle n_1,N+1| - \sum_{n_1=0}^{N}|n_1,N+1\rangle\langle n_1,N|\right),\\
T_4 &= \frac{-i\sqrt{N+1}}{\sqrt{2\theta^2}}\left(-\sum_{n_1=0}^{N}|n_1,N\rangle\langle n_1,N+1| + \sum_{n_1=0}^{N}|n_1,N+1\rangle\langle n_1,N|\right).
\end{aligned} \tag{84}$$

Using (84), we can show

$$\mathrm{Tr}_{\mathcal{H}}\, T_\mu T_\nu = \frac{N}{\theta^{i(\mu)}}\delta_{\mu\nu}, \tag{85}$$

where $i(\mu)=[(\mu+1)/2]$ with the symbol [ ] indicating a Gaussian symbol. $\mathcal{T}_\mu$ is defined by

$$\mathcal{T}_\mu = \frac{\sqrt{\theta^{i(\mu)}}}{\sqrt{N}}T_\mu, \tag{86}$$

to satisfy

$$\mathrm{Tr}_{\mathcal{H}}\, \mathcal{T}_\mu \mathcal{T}_\nu = \delta_{\mu\nu}. \tag{87}$$

Here we list some formulas about $\mathcal{I}$ and $\mathcal{T}_\mu$, which will be used in the calculation of the partition function. They are

$$\mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}\mathcal{I} = 1, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{T}_\mu \mathcal{T}_\nu = \delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}\mathcal{T}_\mu = 0, \tag{88}$$

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}[\hat{\partial}_\mu, \mathcal{I}] = 0, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}[\hat{\partial}_\mu, \mathcal{T}_\nu] = -\frac{1}{\sqrt{\theta^{i(\mu)}}}\delta_{\mu\nu},\\
&\mathrm{Tr}_{\mathcal{H}}\, \mathcal{T}_\mu[\hat{\partial}_\nu, \mathcal{I}] = +\frac{1}{\sqrt{\theta^{i(\mu)}}}\delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{T}_\mu[\hat{\partial}_\nu, \mathcal{T}_\rho] = 0,
\end{aligned} \tag{89}$$

and

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}[\mathcal{I}, \mathcal{I}] = 0, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}[\mathcal{I}, \mathcal{T}_\mu] = 0,\\
&\mathrm{Tr}_{\mathcal{H}}\, \mathcal{I}[\mathcal{T}_\mu, \mathcal{T}_\nu] = +\frac{i\theta^{i(\mu)}}{\sqrt{N}}\theta^{-1}_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\, \mathcal{T}_\mu[\mathcal{T}_\nu, \mathcal{T}_\rho] = 0.
\end{aligned} \tag{90}$$

For the proof of (88)–(90), see Appendix A. Note that these formulas do not depend on the detail of the definition of the cutoff or (31).

Remark that, in the $N\to\infty$ limit, $\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\mathcal{T}_\mu,\mathcal{T}_\nu]$ vanishes,

$$\lim_{N\to\infty}\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\mathcal{T}_\mu,\mathcal{T}_\nu]=0. \tag{91}$$

We will use this $N\to\infty$ behavior to reduce the calculation of the partition function to the Gaussian integral.

F. Calculation of trace and extra sector

Now, let us calculate the partition function (80). First of all, we list the quantities appearing in the calculation. Because the model is constructed as a balanced topological field theory, it is natural to classify them into the BRS multiplets. For $\{A_\mu,H_\mu,\psi_\mu,\chi_\mu,H_\mu\}$,

$$\begin{array}{ccc} & \psi_{\mu(\mathbf{1})}\ ,\ \phi_{\mu(\alpha)} & \\ \hat{\delta}_+\nearrow & & \hat{\delta}_-\searrow \\ A_{\mu(\mathbf{1})}\ ,\ A_{\mu(\alpha)} & & H_{\mu(\mathbf{1})}\ ,\ H_{\mu(\alpha)} \\ \hat{\delta}_-\searrow & & \hat{\delta}_+\nearrow \\ & \chi_{\mu(\mathbf{1})}\ ,\ \chi_{\mu(\alpha)} & \end{array}\ , \tag{92}$$

and for $\{B^+_{\mu\nu},\psi^+_{\mu\nu},\chi^+_{\mu\nu},H^+_{\mu\nu}\}$,

$$\begin{array}{ccc} & \psi^+_{\mu\nu(\mathbf{1})}\ ,\ \psi^+_{\mu\nu(\alpha)} & \\ \hat{\delta}_+\nearrow & & \hat{\delta}_-\searrow \\ B^+_{\mu\nu(\mathbf{1})}\ ,\ B^+_{\mu\nu(\mu)} & & H^+_{\mu\nu(\mathbf{1})}\ ,\ H^+_{\mu\nu(\mu)} \\ \hat{\delta}_-\searrow & & \hat{\delta}_+\nearrow \\ & \chi^+_{\mu\nu(\mathbf{1})}\ ,\ \chi^+_{\mu\nu(\mu)} & \end{array}\ . \tag{93}$$

Note that $A_{\mu(\mathbf{1})}$ and $A_{\mu(\alpha)}$ are coefficients of $\mathcal{I}$ and $\mathcal{T}_\alpha$, i.e., $A_\mu=A_{\mu(\mathbf{1})}\mathcal{I}+\Sigma_{\mathrm{su}(N)}A_{\mu(a)}\tau^a+\Sigma A_{\mu(\alpha)}\mathcal{T}_\alpha$, and other fields are noted by similar manner.

It is necessary to comment on the net components of $\{A_{\mu(\alpha)},\psi_{\mu(\alpha)},\chi_{\mu(\alpha)},H_{\mu(\alpha)}\}$ in (92) and $\{B^+_{\mu\nu(\alpha)},\psi^+_{\mu\nu(\alpha)},\chi^+_{\mu\nu(\alpha)},H^+_{\mu\nu(\alpha)}\}$ in (93). In the following, we use the term (μ,ν) self-dual which means that $A_{\mu(\nu)}$ satisfies $A_{\mu(\nu)}=\frac{1}{2}\epsilon_{\mu\nu\rho\sigma}A_{\rho(\sigma)}$.

(i) $\{A_{\mu(\alpha)},\ldots\}$ have not 16 but four components. Three of them satisfy the self-dual relation and one is $A_{\mu(\mu)}$,

$$\left\{A_{\mu(\nu)}\middle|A_{\mu(\nu)}=\tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}A_{\rho(\sigma)}(\mu,\nu)\ \text{self-dual}\right\}\quad\text{and}\quad\left\{\sum_{\mu=1}^{4}A_{\mu(\mu)}\right\}. \tag{94}$$

(ii) $\{B^+_{\mu\nu(\mu)},\ldots\}$ have four components corresponding to $B^+_{\mu\nu(\mu)}$,

$$B^+_{\mu\nu(\mu)}=\sum_{\mu=1}^{4}B^+_{\mu\nu(\mu)}. \tag{95}$$

On the other hand, $\{\phi,c,\bar{\phi},\bar{\eta},\eta\}$ contain only trace parts

$$\begin{array}{ccc} \phi_{(\mathbf{1})} & & \\ & \hat{\delta}_- \searrow & \\ & & \overline{\eta}_{(\mathbf{1})} \\ & \hat{\delta}_+ \nearrow & \\ c_{(\mathbf{1})} & & \\ & \hat{\delta}_- \searrow & \\ & & \eta_{(1)} \\ & \hat{\delta}_+ \nearrow & \\ \overline{\phi}_{(\mathbf{1})} & & \end{array} . \tag{96}$$

Later we obtain the Gaussian action [(106)–(115), (119), and (120)]. For example, in (106) we find a term proportional to

$$\chi^+_{\mu\nu(\mathbf{1})}(A_{\nu(\mu)} - A_{\mu(\nu)}).$$

From this and other terms in (106)–(115), (119), and (120), we see that the net components (94)–(96) should be taken to remove the zero modes.

Taking the net components (94)–(96) and using (88)–(90), we obtain

$$\begin{aligned} S_{\mathrm{tr}\oplus\mathrm{ex}} = \mathrm{Tr}_{\mathcal{H}}\, \hat{\delta}_+[&+ \chi^{+\mu\nu}_{(\rho)}\mathcal{T}^p\{H^+_{\mu\nu(\sigma)}\mathcal{T}^\sigma - ([\hat{\partial}_\mu, A_{\nu(1)}\mathcal{I}] - [\hat{\partial}_\nu, A_{\mu(1)}\mathcal{I}])\} + \chi^{+\mu\nu}_{(1)}\mathcal{I}\{H^+_{\mu\nu(1)}\mathcal{I} - ([\hat{\partial}_\mu, A_{\nu(\rho)}\mathcal{T}^p] \\ &- [\hat{\partial}_\nu, A_{\mu(\rho)}\mathcal{T}^p])\} + \chi^{\mu}_{(\rho)}\mathcal{T}^p\{H_{\mu(\sigma)}\mathcal{T}^\sigma - (-2[\hat{\partial}^\nu, B^+_{\nu\mu(1)}\mathcal{I}] - [\hat{\partial}_\mu, c_{(1)}\mathcal{I}])\} + \chi^{\mu}_{(1)}\mathcal{I}\{H_{\mu(1)}\mathcal{I} \\ &- (-2[\hat{\partial}^\nu, B^+_{\nu\mu(\rho)}\mathcal{T}^p] - [\hat{\partial}_\mu, c_{(\rho)}\mathcal{T}^p])\} - [\hat{\partial}^\mu, \overline{\phi}_{(1)}\mathcal{I}]\psi_{\mu(\nu)}\mathcal{T}^\nu] + \mathcal{O}(N^{-1/2}). \end{aligned} \tag{97}$$

Note that $B^+_{\nu\mu(\rho)}$ may look like 12 components but only $B^+_{\nu\mu(\nu)}$ proportional terms survive in $\mathrm{Tr}_{\mathcal{H}}\, \chi^{\mu}_{(\mathbf{1})}\mathcal{I}[\hat{\partial}^\nu, B^+_{\nu\mu(\rho)}\mathcal{T}^p]$. In the $N\to\infty$ limit, only quadratic terms survive,

$$S^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}} = \lim_{N\to\infty} S_{\mathrm{tr}\oplus\mathrm{ex}}\text{:quadratic action}. \tag{98}$$

[Alternatively, we can take the weak coupling limit in the calculation. In general, partition functions of cohomological field theories are independent of coupling constants. So they can be evaluated exactly in the weak coupling limit.]

The action (98) has the following gauge symmetry:

$$\delta_{\mathrm{gauge}} A_{\mu(\nu)} = \frac{1}{\sqrt{\theta^{i(\mu)}}}\delta_{\mu\nu}\varphi_{(\mathbf{1})}. \tag{99}$$

Note that the gauge parameter φ contains only one component $\varphi_{(\mathbf{1})}$,

$$\varphi = \varphi_{(\mathbf{1})}\mathcal{I}. \tag{100}$$

Now we give the BRS transformation rules for $f_{(\mathbf{1})}$ and $f_{(\mu)}$. Except for $A_{\mu(\nu)}, \psi_{\mu(\nu)}$ and $A_{\mu(\mathbf{1})}, \psi_{\mu(\mathbf{1})}$,

$$\begin{gathered} \hat{\delta}_+\mathcal{B}_{(\nu)} = \mathcal{F}_{(\nu)}, \quad \hat{\delta}_+\mathcal{F}_{(\nu)} = 0, \\ \hat{\delta}^2_+\mathcal{B}_{(\nu)} = 0, \quad \hat{\delta}^2_+\mathcal{F}_{(\nu)} = 0, \end{gathered} \tag{101}$$

and

$$\hat{\delta}_+\mathcal{B}_{(\mathbf{1})}=\mathcal{F}_{(\mathbf{1})},\quad \hat{\delta}_+\mathcal{F}_{(\mathbf{1})}=0,$$
$$\hat{\delta}_+^2\mathcal{B}_{(\mathbf{1})}=0,\quad \hat{\delta}_+^2\mathcal{F}_{(\mathbf{1})}=0, \tag{102}$$

where $\mathcal{B}$ denotes the bosonic matrix and $\mathcal{F}$ denotes the fermionic one.

For $A_{\mu(\nu)},\psi_{\mu(\nu)}$ and $A_{\mu(\mathbf{1})},\psi_{\mu(\mathbf{1})}$,

$$\hat{\delta}_+A_{\mu(\nu)}=\psi_{\mu(\nu)},\quad \hat{\delta}_+\psi_{\mu(\nu)}=+\frac{1}{\sqrt{\theta^{i(\mu)}}}\delta_{\mu\nu}\phi_{(\mathbf{1})},$$

$$\hat{\delta}_+^2A_{\mu(\nu)}=+\frac{1}{\sqrt{\theta^{i(\mu)}}}\delta_{\mu\nu}\phi_{(\mathbf{1})},\quad \hat{\delta}_+^2\psi_{\mu(\nu)}=0, \tag{103}$$

and

$$\hat{\delta}_+A_{\mu(\mathbf{1})}=\psi_{\mu(\mathbf{1})},\quad \hat{\delta}_+\psi_{\mu(\mathbf{1})}=0,$$
$$\hat{\delta}_+^2A_{\mu(\mathbf{1})}=0,\quad \hat{\delta}_+^2\psi_{\mu(\mathbf{1})}=0. \tag{104}$$

For simplicity, in this section we set $\theta^1=\theta^2=\theta$ in the following. Using (88), (89), (103), (104), and (98) is shown to be

$$S^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}}=S^{\infty\ \mathrm{boson}}_{\mathrm{tr}\oplus\mathrm{ex}}+S^{\infty\ \mathrm{fermion}}_{\mathrm{tr}\oplus\mathrm{ex}}, \tag{105}$$

where

$$S^{\infty\ \mathrm{boson}}_{\mathrm{tr}\oplus\mathrm{ex}}=+H^{+\mu\nu}_{(\mathbf{1})}\left\{H^{+}_{\mu\nu(\mathbf{1})}+\frac{i}{\sqrt{\theta}}(A_{\nu(\mu)}-A_{\mu(\nu)})\right\} \tag{106}$$

$$+H^{+\mu\nu}_{(\alpha)}\left\{H^{+}_{\mu\nu(\alpha)}-\frac{i}{\sqrt{\theta}}(\delta^{\alpha}_{\mu}A_{\nu(\mathbf{1})}-\delta^{\alpha}_{\nu}A_{\mu(\mathbf{1})})\right\} \tag{107}$$

$$+H^{\mu}_{(\mathbf{1})}\left\{H_{\mu(\mathbf{1})}+\frac{i}{\sqrt{\theta}}(-2B^{+}_{\alpha\mu(\alpha)})\right\} \tag{108}$$

$$+H^{\mu}_{(\alpha)}\left\{H_{\mu(\alpha)}-\frac{i}{\sqrt{\theta}}(-2B^{+}_{\alpha\mu(\mathbf{1})}+\delta_{\mu\alpha}c_{(\mathbf{1})})\right\} \tag{109}$$

$$+\frac{4}{\theta}\bar{\phi}_{(\mathbf{1})}\phi_{(\mathbf{1})}, \tag{110}$$

and

$$S^{\infty\ \mathrm{fermion}}_{\mathrm{tr}\oplus\mathrm{ex}}=-\frac{i}{\sqrt{\theta}}\chi^{+\mu\nu}_{(\mathbf{1})}(\psi_{\nu(\mu)}-\psi_{\mu(\nu)}) \tag{111}$$

$$-\frac{2i}{\sqrt{\theta}}\chi^{+\mu\alpha}_{(\alpha)}\psi_{\mu(\mathbf{1})} \tag{112}$$

$$+\frac{i}{\sqrt{\theta}}\chi^{\mu}_{(\mathbf{1})}(2\psi^{+}_{\alpha\mu(\alpha)}) \tag{113}$$

$$-\frac{i}{\sqrt{\theta}}\chi^{\mu}_{(\alpha)}(2\psi^{+}_{\alpha\mu(\mathbf{1})}+\delta_{\mu\alpha}\bar{\eta}_{(\mathbf{1})}) \tag{114}$$

$$+\frac{i}{\sqrt{\theta}}\eta_{(\mathbf{1})}\psi^{\mu}_{(\mu)}. \tag{115}$$

Now we fix the gauge symmetry (99). We introduce the ghost ρ, the antighost $\bar{\rho}$ and the Nakanishi-Lautrup field b. Their ghost numbers are assigned as $(+1,-1,0)$ for $(\rho,\bar{\rho},b)$, respectively. BRS transformations for $\{\bar{\rho},b,\rho\}$ are defined as

$$\hat{\delta}_{+}b=\rho,\quad \hat{\delta}_{+}\rho=0,\quad \hat{\delta}_{+}\bar{\rho}=0. \tag{116}$$

Because the gauge symmetry is given by (99), $\{\bar{\rho},b,\rho\}$ contain only the trace parts.

Let us introduce a gauge fixing action by

$$S_{\mathrm{gf}}=\mathrm{Tr}_{\mathcal{H}}\,\hat{\delta}_{+}[\bar{\rho}_{(\mathbf{1})}\mathcal{I}(b_{(\mathbf{1})}\mathcal{I}+[\hat{\partial}^{\mu},A_{\mu(\nu)}\mathcal{T}^{\nu}])]. \tag{117}$$

To get the BRS exact action including the gauge fixing action, let us deform the BRS transformation rules for $A_{\mu(\nu)},\psi_{\mu(\nu)}$ (103) as

$$\begin{aligned}\hat{\delta}_{+}A_{\mu(\nu)}&=\psi_{\mu(\nu)}+\frac{1}{\sqrt{\theta}}\delta_{\mu\nu}\rho_{(\mathbf{1})},\\ \hat{\delta}_{+}\psi_{\mu(\nu)}&=+\frac{1}{\sqrt{\theta}}\delta_{\mu\nu}\phi_{(\mathbf{1})}.\end{aligned} \tag{118}$$

(117) is rewritten into

$$S_{\mathrm{gf}}=+b_{(\mathbf{1})}\left(b_{(\mathbf{1})}-\frac{1}{\sqrt{\theta}}A_{\mu,(\mu)}\right) \tag{119}$$

$$+\frac{4}{\theta}\bar{\rho}_{(\mathbf{1})}\rho_{(\mathbf{1})}+\frac{1}{\sqrt{\theta}}\bar{\rho}_{(\mathbf{1})}\psi_{\mu(\mu)}. \tag{120}$$

We list degrees of the Gaussian integral in (106)–(115), (119), and (120).

From bosons

degree			
3+3	$H^{+}_{\mu\nu(\mathbf{1})}$, $A_{\mu(\nu)}$ (μ,ν) self-dual	in (106)	
4+4	$H^{+\mu\nu}_{(\nu)}$, $A_{\mu(\mathbf{1})}$	in (107)	
4+4	$H^{\mu}_{(\mathbf{1})}$, $B^{+\alpha\mu}_{(\alpha)}$	in (108)	
3+1+3+1	$H_{\mu(\alpha)}$ (μ,α) self-dual, $H_{\mu(\mu)}$, $B^{+}_{\alpha\mu(\mathbf{1})}$, $c_{(\mathbf{1})}$	in (109)	
1+1	$\phi_{(\mathbf{1})}$, $\bar{\phi}_{(\mathbf{1})}$	in (110)	
1+1	$b_{(\mathbf{1})}$, $A_{\mu(\mu)}$	in (119)	(121)

	From fermions		
degree			
3+3	$\chi^{+}_{\mu\nu(\mathbf{1})}$, $\psi_{\nu(\mu)}$ (μ,ν) self-dual	in (111)	
4+4	$\chi^{+\mu\alpha}_{(\alpha)}$, $\psi_{\mu(\mathbf{1})}$	in (112)	
4+4	$\chi^{\mu}_{(\mathbf{1})}$, $\chi^{+\alpha\mu}_{(\alpha)}$	in (113)	
3+1+3+1	$\chi_{\mu(\nu)}$ (μ,ν) self-dual, $\chi^{\mu}_{(\mu)}$, $\chi^{+}_{\alpha\mu(\mathbf{1})}$, $\bar{\eta}_{(\mathbf{1})}$	in (114)	
1+1	$\eta_{(\mathbf{1})}$, $\psi^{\mu}_{(\mu)}$	in (115)	
1+1	$\rho_{(\mathbf{1})}$, $\bar{\rho}_{(\mathbf{1})}$	in (120)	(122)

From (121) and (122), we see that the path integral contains no zero mode, so we obtain a definite partition function. We adopt a standard path integral measure, which is largely expressed by

$$\mathcal{D}f = \prod \frac{\mathrm{d}f_{\mathrm{boson}}}{\sqrt{2\pi}} \prod \mathrm{d}f_{\mathrm{fermion}}, \tag{123}$$

where f_{boson} denotes a bosonic field and f_{fermion} denotes a fermionic field. For the precise definition of $\mathcal{D}f$ and the validity of this choice, see the next section and Appendix C. Then $Z^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}}$ is calculated as 1,

$$Z^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}} = \int \mathcal{D}f\, e^{-(S^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}}+S_{\mathrm{gf}})} = 1. \tag{124}$$

G. Results and remarks of this section

From (78) and (124), we conclude that the partition function of the $\mathcal{N}=4$ U(1) gauge theory on NC $\mathbb{R}^4$ is given by

$$Z^{4\ \mathrm{dim}}_{\mathcal{N}=4} = Z^{\infty}_{MM} = Z^{\infty}_{MM}|_{\mathrm{traceless}} Z^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}} = \frac{\pi^2}{6}. \tag{125}$$

We comment on the universality of partition function (20). Our calculation consists of largely two steps. In the first step the traceless part is treated, then in the second step the trace and extra parts are managed. The first step is manifestly dimensionally independent, because after the dimensional reduction to 0 dimensions all actions of (8-dim, $\mathcal{N}=2$), (6-dim, $\mathcal{N}=2$), (4-dim, $\mathcal{N}=4$), and (2-dim, $\mathcal{N}=8$) are the same as the IKKT matrix model action. On the other hand, the calculations in the second step may seem to depend on the dimension of the model, since we keep the derivatives, $\hat{\partial}_{\mu}$. However, the same result $Z^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}}=1$ is expected to be universal. The reason is as follows. The second step, introducing the extra part and fixing the gauge symmetry (99), is a kind of regularization of the zero mode integral. As expected from the other regularization method, for example, naively dropping the trace part, equivalent to dividing the path integral measure by the U(1) gauge volume, the regularization should produce a trivial factor 1. In our regularization method, this is implemented by the supersymmetry. Also, as explained in Appendix C, our regularization is valid for all of (8-dim, $\mathcal{N}=2$), (6-dim, $\mathcal{N}=2$), (4-dim, $\mathcal{N}=4$), and (2-dim, $\mathcal{N}=8$). Then we conclude

$$Z^{8\ \mathrm{dim}}_{\mathcal{N}=2} = Z^{6\ \mathrm{dim}}_{\mathcal{N}=2} = Z^{4\ \mathrm{dim}}_{\mathcal{N}=4} = Z^{2\ \mathrm{dim}}_{\mathcal{N}=8} = \frac{\pi^2}{6}. \tag{126}$$

Finally, we make a remark relating the mathematical significance of (126). In topological field theories, the path integral can be decomposed into finite-dimensional integrals of the moduli space defined by the BPS equations and infinite-dimensional integrals of fluctuations around each vacuum. The absolute value of the infinite-dimensional integrals of the fluctuations should be normalized to 1 to make the partition functions well defined, then only the integrals of the moduli

space remain (see also Appendix C). If the moduli space is compact, the remained moduli integrals produce a definite number, which is the Euler number of some vector bundle over the moduli space. In the case of this section, each $1/d^2$ in (75) corresponds to the Euler number. In this light, our prescription above, adopting the measure (123) to obtain (124), is an almost unique choice, though it may seem to be chosen by hand. Also, for the traceless part, the similar prescription is performed in Ref. 20. To conclude, the result $\pi^2/6$ is decided without ambiguity and has an absolute meaning as a topological invariant.

V. MODULI SPACE AND INSTANTON NUMBER

In this section, we concentrate on the relation between the moduli space of the Monads and the partition function of the $\mathcal{N}=4$ supersymmetric Yang-Mills theory. The partition function of Vafa-Witten theory is given by the generating function of the Euler number of some vector bundle over the moduli space with sign ± 1,

$$Z = \sum_{k=1} \epsilon_k \chi(\mathcal{M}_k) q^k, \tag{127}$$

$$q^k = e^{2\pi i k \tau}, \quad \epsilon_k = \pm 1. \tag{128}$$

Here τ is the complex coupling constant and $\mathcal{M}_k$ is the moduli space defined by

$$\{A,B,c | F^{+\mu\nu} - i[B^+_{\mu\rho}, B^{+\rho}_{\nu}] - i[B^+_{\mu\nu}, c] = 0, 2D^\mu B_{+\mu\rho} + D_\rho c = 0\}/\mathcal{G}, \tag{129}$$

where $\mathcal{G}$ is the gauge transformation group. In addition, if $\chi^{\mu\nu}, \chi^\mu$ zero modes are sections of the cotangent bundle of $\mathcal{M}_k$, then $\chi(\mathcal{M}_k)$ is the Euler number of $\mathcal{M}_k$. Particularly, the base four-fold satisfies the vanishing theorem in Ref. 34, then the moduli space is identified with the instanton moduli space with its instanton number k. Therefore, it is important to investigate the $\mathcal{M}_k$.

It is natural to assume that the topology of the moduli space does not change under the θ-shift. After dimensional reduction (large θ limit), let us replace variables as (44), (50), and (51). As operators, fields are infinite-dimensional matrices. If matrix size of these B_i is cut off at N, BPS Eqs. (24) are replaced by hyper-Kähler momentum maps,

$$\begin{aligned} \mu_{\mathbb{C}} &:= [B_i, B_j] + \tfrac{1}{2}\epsilon_{ijkl}[B_k^\dagger, B_l^\dagger] = 0, \\ \mu_{\mathbb{R}} &:= \sum_{i=1}^{4} [B_i, B_i^\dagger] = 0, \end{aligned} \tag{130}$$

then the moduli space is determined by

$$\mathcal{M}_N = (\mu_{\mathbb{C}}^{-1}(0) \cap \mu_{\mathbb{R}}^{-1}(0))/\mathrm{U}(N). \tag{131}$$

It is known that the solutions of Eqs. (130) include the solutions of simultaneous ADHM equations.[25] θ deformation realizes the continuous connection between (129) and (131). This is a direct correspondence between BPS equations of noncommutative field theory and Monads by means of changing the noncommutative parameter.

Turning now to the next issue, let us study the partition function whose action functional includes the topological term. In Sec. VI, we perform the calculation with the action functional which does not include the term of $\tau \int F \wedge F$ (or $\tau \mathrm{Tr}_{\mathcal{H}} F \wedge F$). In the MNS calculation, they use the mass deformation to decompose the theory to more simple ones whose partition function is given by $1/d^2$ in (57). (See Sec. 7 in Ref. 20 and Sec. IV D in this paper.) This mass deformation causes supersymmetry breaking from $\mathcal{N}=4$ to $\mathcal{N}=1$. B_1, B_2, B_3 become massive, and $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$ are left for massless fields. If we consider this mass deformation in the finite θ theory, we find that

gauge fields are given from $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$ as four-dimensional theory, because the massless fields correspond to the unbroken gauge fields. In the reduced theory after integrating out B_1, B_2, and B_3, fixed point loci are defined by

$$[B_4, B_4^\dagger] = 0, \quad [\phi, \bar{\phi}] = 0, \quad [B_4, \phi] = 0, \tag{132}$$

where $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$ are $d \times d$ matrices where d is a divisor of N and is appearing in the argument of (57). Furthermore, contributions for the partition function are given by isolated fixed points, as MNS mentioned in the end of Sec. V in Ref. 20. At least one of B_4 and ϕ is the rank d, when B_4 and ϕ are solutions of the fixed point equations and the fixed points contribute to the path integral. Because if rank $< d$ then there are zero modes of the equations

$$[\delta B_4, B_4^\dagger] + [B_4, \delta B_4^\dagger] = 0, \quad [\delta\phi, \bar{\phi}] + [\phi, \delta\bar{\phi}] = 0, \quad [\delta B_4, \phi] + [B_4, \delta\phi] = 0, \tag{133}$$

where these equations are given by variation of (132). These zero modes mean that the fixed point loci are nonzero dimension and path integrals vanish by the fermionic zero modes. With attention to these points, if we specify the instanton numbers corresponding to solutions of (132) labeled by d, then we determine the partition function whose action functional includes the topological term.

A hint to speculate the instanton number is ADHM correspondence. The solution of (132) is included in the set of solutions of noncommutative deformed ADHM equations corresponding to d instanton, i.e.,

$$[B_4, B_4^\dagger] + [\phi, \bar{\phi}] + II^\dagger - J^\dagger J = 0, \quad [B_4, \phi] + IJ = 0, \tag{134}$$

where I and $J^\dagger$ are d-dimensional. vectors. This is ADHM equations of noncommutative U(1) theories under the condition of noncommutativity $\theta^1 = -\theta^2$.[22,24] Here we must fix I and $J^\dagger$ to compare (134) with (132) as

$$I = 0_d, \quad J^\dagger = 0_d, \tag{135}$$

where 0_d is 0 vector of d-dimensions. Then, the solutions of (134) are given by the solutions of (132). From this observation, we find that the moduli space of $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$, which are gauge fields in this case, is the submanifold in instanton moduli space of instanton number d.

Therefore, someone might think it is not so strange to expect that the instanton number is given as $-[\det(\theta)^{1/2}/16\pi^2]\mathrm{Tr}_{\mathcal{H}} F \wedge F = d$, where the gauge fields correspond to $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$, and we conjecture that the partition function of the $\mathcal{N}=4$ U(1) gauge theory in noncommutative $\mathbb{R}^4$ with the topological term $\tau \int F \wedge F$ is given by $\tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,\tau} = \Sigma_{d=0}^{\infty}(1/d^2)e^{2\pi i \tau d}$. However, It would still be unwise to conclude $\tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,\tau} = \Sigma_{d=0}^{\infty}(1/d^2)e^{2\pi i \tau d}$, because the direct corresponding with the instanton number and $B_4, B_4^\dagger$ and $\phi, \bar{\phi}$ fixed point locus labeled by d is unknown. Meanwhile, it might be possible to investigate this conjecture from Montonen and Olive duality[19,34] if such a duality of noncommutative version exists (see also Ref. 8.) For example, if we assume that the partition function takes the form as

$$\tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,\tau} = \sum_{d=1}^{\infty} \frac{1}{d^2} e^{2\pi i \tau k(d)}, \tag{136}$$

where $k(d)$ is a instanton number depending on d, restriction to the modular like form

$$\tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,1/\tau} = \pm \left(\frac{\tau}{i}\right)^n \tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,\tau} \tag{137}$$

might determine $k(d)$, where n is some number. Unfortunately, we do not know how to choose a suitable modularlike form, and the above naive conjecture $\tilde{Z}^{4\,\mathrm{dim}}_{\mathcal{N}=4,\tau} = \Sigma_{d=0}^{\infty}(1/d^2)e^{2\pi i \tau d}$ does not sat-

isfy this condition. Anyway, further investigations are necessary to determine the contribution of the topological term.

At the end of this section, we consider the dimensional reduction of the theory with topological terms. In the discussions in Sec. III, we use cohomological field theory without topological terms like $\int F\wedge F$, and some of them are not supersymmetric gauge theories in the meaning of the usual supersymmetry. Now, let us consider the case including topological terms. As an example, let us consider the four-dimensional case whose action is given by cohomological terms and instanton number; $S=\int \mathrm{tr}\,\hat{\delta}\Psi+(i\vartheta/8\pi^2)\int \mathrm{tr}\,F\wedge F$. Let us consider perturbation around classical background fixed by instanton number, i.e., $A_\mu=A_\mu^{(k)}+\delta A_\mu^{(k)}$, $\int \mathrm{tr}\,F(A^{(k)})\wedge F(A^{(k)})=8\pi^2 k$. The partition function is given by

$$Z^{4\ \mathrm{dim}}=\sum_k e^{2\pi i\tau k}\int \mathcal{D}\delta A^{(k)}\cdots e^{-\int \mathrm{tr}\ \hat{\delta}\Psi_k},$$

where $\mathcal{D}\delta A^{(k)}\cdots$ is the path integral measure of the all fields and the functional Ψ_k depends on both $A_\mu^{(k)}$ and $\delta A_\mu^{(k)}$. The BRS transformations are induced from (8) and so on as $\hat{\delta}(\delta A_\mu^{(k)})=\psi_\mu^{(k)}$, etc. So we have

$$Z^{4\ \mathrm{dim}}=\sum_k e^{2\pi i\tau k}Z_k^{4\ \mathrm{dim}},$$

where $Z_k^{4\ \mathrm{dim}}$ is the perturbative partition function of the four-dimension theory without the topological term. The action $\hat{\delta}\Psi_k$ is still given by a BRS exact term. The arguments for the θ-shift invariance of the path integral are valid for $\int \mathcal{D}\delta A^{(k)}\cdots e^{-\int \mathrm{tr}\ \hat{\delta}\Psi_k}$. Then the dimensional reduction of the perturbative partition functions arises at the large θ limit,

$$Z_k^{4\ \mathrm{dim}}=Z_k^{2\ \mathrm{dim}}=Z_k^{0\ \mathrm{dim}}, \tag{138}$$

where $Z_k^{2\ \mathrm{dim}}$ and $Z_k^{0\ \mathrm{dim}}$ are possible to be described by partition functions of two- and 0-dimensional field theories, respectively. Therefore, we find that the universality of the perturbative partition functions $Z_k^{4\ \mathrm{dim}}$, $Z_k^{2\ \mathrm{dim}}$, and $Z_k^{0\ \mathrm{dim}}$, similar to the claim in Sec. III.

Now let us discuss the possibility that (138) means a universality of the partition functions of the usual supersymmetric theories in various dimensions. Consider the weighted sum of $Z_k^{4\ \mathrm{dim}}$, $Z_k^{2\ \mathrm{dim}}$, and $Z_k^{0\ \mathrm{dim}}$ with weight $e^{2\pi i\tau k}$,

$$\sum_k e^{2\pi i\tau k}Z_k^{4\ \mathrm{dim}}=\sum_k e^{2\pi i\tau k}Z_k^{2\ \mathrm{dim}}=\sum_k e^{2\pi i\tau k}Z_k^{0\ \mathrm{dim}}. \tag{139}$$

$\Sigma_k e^{2\pi i\tau k}Z_k^{4\ \mathrm{dim}}$ is equal to $Z^{4\ \mathrm{dim}}$, the partition of the four-dimension supersymmetric theory including the topological term. On the other hand, the meanings of the weighted sums $\Sigma_k e^{2\pi i\tau k}Z_k^{2\ \mathrm{dim}}$ and $\Sigma_k e^{2\pi i\tau k}Z_k^{0\ \mathrm{dim}}$ are obscure. It is unclear that they have the meaning of the partition functions of some lower dimension theories. If they can be interpreted as the partition functions of some supersymmetric theories in lower dimensions, (139) means a universality of the partition functions of supersymmetric theories in various dimensions. To answer whether this statement is true or not, we need to clarify the following questions.

(i) Is the number k expressed in terms of lower dimension theories?
(ii) Is the number k interpreted as a topological invariant? And does it characterize classical solutions of the lower dimension theories?
(iii) Is the total action, the sum of the action defining $Z_k^{2\ \mathrm{dim}}$ or $Z_k^{0\ \mathrm{dim}}$ and the action giving the number k, equivalent to a supersymmetric action in lower dimension?

At this time, we can only make a few comments on question (i). We calculated the large θ_2 limit of the elongated NC U(1) k-instanton, that is the reduction from four dimension to two dimension of the solution. [For construction of the elongated NC U(1) k-instanton, see Ref. 13.] For this case, we can show that k is expressed in terms of two-dimension theories,

$$\theta_1 \operatorname{Tr} F_{z_1,\bar{z}_1} = -k. \tag{140}$$

It may be that this fact implies that the number k is expressed in terms of lower dimension theories. However, we have no concrete answer to question (ii) and question (iii) at this time.

VI. CONCLUSIONS AND DISCUSSIONS

We investigated cohomological gauge theories in NC $\mathbb{R}^{2D}$. We saw that vacuum expectation values of the theories do not depend on noncommutative parameters, and the large noncommutative parameter limit is equivalent to the dimensional reduction. As a result of these facts, we showed that two types of cohomological theories defined in NC $\mathbb{R}^{2D}$ and NC $\mathbb{R}^{2D+2}$ are equivalent, if they are connected through dimensional reduction. Therefore, we found several partition functions of noncommutative supersymmetric Yang-Mills theories in various dimensions are equivalent, when they are connected by dimensional reduction from 2+2D to 2D. Using this technique and requiring some natural assumptions, we determine the partition function of the $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$, where the action does not include the topological term $\tau\int F\wedge F$, and the result is equivalent to the partition function of (8-dim, $\mathcal{N}=2$), (6-dim, $\mathcal{N}=2$), (2-dim, $\mathcal{N}=8$) and the IKKT matrix model given by their dimensional reduction to 0 dimensions. The case including the topological term was discussed, too.

Let us list some left over problems below. In this paper, concrete partition functions are given for the $\mathcal{N}=4$ U(1) gauge theory in NC $\mathbb{R}^4$ and the series connecting to it by dimensional reduction. So, we are interested in the NC non-Abelian cases. To calculate them, we must find some new formulation like MNS, because we know the partition function concerning su(N) but we need it for su(N)$\times$su(M) for U(M) theory.

Next, we had qualitative observation of $\mathcal{N}=2$ four-dimensional case but we do not do the quantitative approach. So, we must do the more detailed analysis for the $\mathcal{N}=2$ super Yang-Mills cases. We saw in Sec. V, after taking large θ limit, moduli space is described by Monads in $\mathcal{N}=4$ four-dimensional case. From the analogy with $\mathcal{N}=4$ four-dimensional case, direct and smooth connections between noncommutative instanton moduli spaces and ADHM spaces might be given in the $\mathcal{N}=2$ four-dimensional case.

Other important problems are applications to the various fuzzy spaces, T^d_θ, $\mathbb{C}P^d_N$, and so on. Since these noncommutative spaces are expressed by finite-dimensional Hilbert spaces, the dimensional reduction will not occur at the large θ limit despite omitting kinetic terms.

Wide spread applications of the technology of this paper are going to happen in many cases other than the above subjects. All of them are left for future works.

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APPENDIX A: FOCK SPACE

Let us consider NC $\mathbb{R}^{2D}$. First of all, we introduce the following operators:

$$a_i \equiv \frac{z_i}{\sqrt{\theta^{2i-1,2i}}}, \quad z_i \equiv \frac{1}{\sqrt{2}}(x^{2i-1} + ix^{2i}),$$

$$a_i^\dagger \equiv \frac{\bar{z}_i}{\sqrt{\theta^{2i-1,2i}}}, \quad \bar{z}_i \equiv \frac{1}{\sqrt{2}}(x^{2i-1} - ix^{2i}), \tag{A1}$$

where i runs from 1 to D, and a_i and $a_i^\dagger$ satisfy

$$[a_i, a_j^\dagger] = \delta_{ij}. \tag{A2}$$

We often use the symbol θ^i defined as

$$\theta^i = +\theta^{2i-1,2i} = -\theta^{2i,2i-1}. \tag{A3}$$

The Hilbert space is constructed as the Fock space,

$$\begin{gathered}\mathcal{H} = \oplus \mathbb{C}|n_1, \ldots, n_D\rangle, \\ |n_1, \ldots, n_D\rangle \equiv \frac{(a_1^\dagger)^{n_1} \cdots (a_D^\dagger)^{n_D}}{\sqrt{n_1! \cdots n_D!}}|0, \ldots, 0\rangle.\end{gathered} \tag{A4}$$

a_i and $a_i^\dagger$ operate on $|n_1, \ldots, n_D\rangle$ as follows:

$$\begin{gathered}a_i|n_1, \ldots, n_D\rangle = \sqrt{n_i}|n_1, \ldots, n_i - 1, \ldots, n_D\rangle, \\ a_i^\dagger|n_1, \ldots, n_D\rangle = \sqrt{n_i + 1}|n_1, \ldots, n_i + 1, \ldots, n_D\rangle.\end{gathered} \tag{A5}$$

$|n_1, \ldots, n_D\rangle$ are the eigenstates of the number operator $\hat{n}_i \equiv a_i^\dagger a_i$,

$$\hat{n}_i|n_1, \ldots, n_D\rangle = n_i|n_1, \ldots, n_D\rangle. \tag{A6}$$

The arbitrary operator has the following expression:

$$\hat{\mathcal{O}} = \sum_{n_1, m_1} \cdots \sum_{n_D, m_D} \mathcal{O}^{n_1 \cdots n_D}_{m_1 \cdots m_D}|n_1, \ldots, n_D\rangle\langle m_1, \ldots, m_D|.$$

Let us consider 2D=4 case. The Hilbert space $\mathcal{H}$ is expanded by the Fock basis $|n_1, n_2\rangle$,

$$\begin{gathered}\mathcal{H} = \oplus \mathbb{C}|n_1, n_2\rangle, \\ |n_1, n_2\rangle = \frac{(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}}{\sqrt{n_1! n_2!}}|0, 0\rangle.\end{gathered} \tag{A7}$$

$a_i^\dagger$ and a_i are expressed as

$$\begin{gathered}a_1^\dagger = \sum_{n_1=0}^{\infty} \sqrt{n_1 + 1}|n_1 + 1, n_2\rangle\langle n_1, n_2|, \quad a_2^\dagger = \sum_{n_2=0}^{\infty} \sqrt{n_2 + 1}|n_1, n_2 + 1\rangle\langle n_1, n_2|, \\ a_1 = \sum_{n_1=0}^{\infty} \sqrt{n_1 + 1}|n_1, n_2\rangle\langle n_1 + 1, n_2|, \quad a_2 = \sum_{n_2=0}^{\infty} \sqrt{n_2 + 1}|n_1, n_2\rangle\langle n_1, n_2 + 1|.\end{gathered} \tag{A8}$$

The finite-dimensional truncation $\mathcal{H}_N$ can be defined by several ways. One definition of $\mathcal{H}_N$ is given by

$$\mathcal{H}_N = \bigoplus_{n_1=0, n_2=0}^{n_1=N_c, n_2=N_c} \mathbb{C}|n_1, n_2\rangle, \tag{A9}$$

where N_c is a finite integer number. By the definition, we obtain

$$\text{dim. of } \mathcal{H}_N = (N_c + 1)^2 = N \tag{A10}$$

and

$$\mathbf{1}_N = \sum_{n_1=0,n_2=0}^{n_1=N_c,n_2=N_c} |n_1,n_2\rangle\langle n_1,n_2|. \tag{A11}$$

Another definition of $\mathcal{H}_N$ is given by

$$\mathcal{H}_N = \bigoplus_{n_1=0,n_2=0}^{n_1+n_2=N_c} \mathbb{C}|n_1,n_2\rangle. \tag{A12}$$

In this case,

$$\text{dim. of } \mathcal{H}_N = \frac{(N_c+1)(N_c+2)}{2} = N \tag{A13}$$

and

$$\mathbf{1}_N = \sum_{n_1=0,n_2=0}^{n_1+n_2=N_c} |n_1,n_2\rangle\langle n_1,n_2|. \tag{A14}$$

By using the definition of $\mathbf{1}_N$, (A11) or (A14), and the following expressions of the differential operators $\hat{\partial}_\mu$ in terms of $a_i^\dagger$ and a_i:

$$\begin{aligned} \hat{\partial}_1 &= \frac{1}{\sqrt{2\theta^1}}(a_1 - a_1^\dagger), \quad \hat{\partial}_2 = \frac{-i}{\sqrt{2\theta^1}}(a_1 + a_1^\dagger), \\ \hat{\partial}_3 &= \frac{1}{\sqrt{2\theta^2}}(a_2 - a_2^\dagger), \quad \hat{\partial}_4 = \frac{-i}{\sqrt{2\theta^2}}(a_2 + a_2^\dagger), \end{aligned} \tag{A15}$$

Given the definition of $\mathcal{H}_N$, for example, by (31), we obtain

$$\begin{aligned} [a_1,\mathbf{1}_N] &= -\sqrt{N+1}\sum_{n_2=0}^{N} |N,n_2\rangle\langle N+1,n_2|, \\ [a_1^\dagger,\mathbf{1}_N] &= +\sqrt{N+1}\sum_{n_2=0}^{N} |N+1,n_2\rangle\langle N,n_2|, \\ [a_2,\mathbf{1}_N] &= -\sqrt{N+1}\sum_{n_1=0}^{N} |n_1,N\rangle\langle n_1,N+1|, \\ [a_2^\dagger,\mathbf{1}_N] &= +\sqrt{N+1}\sum_{n_1=0}^{N} |n_1,N+1\rangle\langle n_1,N|. \end{aligned} \tag{A16}$$

From (A16) and (A15), we obtain

$$T_1 = \frac{1}{\sqrt{2\theta^1}}\left(-\sqrt{N+1}\sum_{n_2=0}^{N} |N,n_2\rangle\langle N+1,n_2| - \sqrt{N+1}\sum_{n_2=0}^{N} |N+1,n_2\rangle\langle N,n_2| \right),$$

$$T_2 = \frac{-i}{\sqrt{2\theta^1}}\left(-\sqrt{N+1}\sum_{n_2=0}^{N}|N,n_2\rangle\langle N+1,n_2| + \sqrt{N+1}\sum_{n_2=0}^{N}|N+1,n_2\rangle\langle N,n_2|\right),$$

$$T_3 = \frac{1}{\sqrt{2\theta^2}}\left(-\sqrt{N+1}\sum_{n_1=0}^{N}|n_1,N\rangle\langle n_1,N+1| - \sqrt{N+1}\sum_{n_1=0}^{N}|n_1,N+1\rangle\langle n_1,N|\right),$$

$$T_4 = \frac{-i}{\sqrt{2\theta^2}}\left(-\sqrt{N+1}\sum_{n_1=0}^{N}|n_1,N\rangle\langle n_1,N+1| + \sqrt{N+1}\sum_{n_1=0}^{N}|n_1,N+1\rangle\langle n_1,N|\right). \tag{A17}$$

Using (A11) and (A17), we can show

$$\mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N\mathbf{1}_N = N, \quad \mathrm{Tr}_{\mathcal{H}}\,T_\mu T_\nu = +\frac{1}{\theta^i}N\delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N T_\mu = 0. \tag{A18}$$

Also, we can obtain

$$\begin{gathered}\mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N[\hat{\partial}_\mu,\mathbf{1}_N] = 0, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N[\hat{\partial}_\mu,T_\nu] = -\frac{N}{\theta^i}\delta_{\mu\nu},\\ \mathrm{Tr}_{\mathcal{H}}\,T_\mu[\hat{\partial}_\nu,\mathbf{1}_N] = +\frac{N}{\theta^i}\delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\,T_\mu[\hat{\partial}_\nu,T_\rho] = 0,\end{gathered} \tag{A19}$$

and

$$\begin{gathered}\mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N[\mathbf{1}_N,\mathbf{1}_N] = 0, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N[\mathbf{1}_N,T_\mu] = 0,\\ \mathrm{Tr}_{\mathcal{H}}\,\mathbf{1}_N[T_\mu,T_\nu] = +iN\theta^{-1}_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\,T_\mu[T_\nu,T_\rho] = 0.\end{gathered} \tag{A20}$$

Let us define $\mathcal{I}$ and $\mathcal{T}_\mu$ as

$$\mathcal{I} = \frac{1}{\sqrt{N}}\mathbf{1}_N, \tag{A21}$$

and

$$\mathcal{T}_\mu = \frac{\sqrt{\theta_i}}{\sqrt{N}}T_\mu. \tag{A22}$$

By definition,

$$\mathcal{T}_\mu = \sqrt{\theta_i}[\hat{\partial}_\mu,\mathcal{I}]. \tag{A23}$$

Using $\mathcal{I}$ and $\mathcal{T}_\mu$, (A18)–(A20) are rewritten into

$$\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}\mathcal{I} = 1, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{T}_\mu\mathcal{T}_\nu = \delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}\mathcal{T}_\mu = 0, \tag{A24}$$

$$\begin{gathered}\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\hat{\partial}_\mu,\mathcal{I}] = 0, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\hat{\partial}_\mu,\mathcal{T}_\nu] = -\frac{1}{\sqrt{\theta^i}}\delta_{\mu\nu},\\ \mathrm{Tr}_{\mathcal{H}}\,\mathcal{T}_\mu[\hat{\partial}_\nu,\mathcal{I}] = +\frac{1}{\sqrt{\theta^i}}\delta_{\mu\nu}, \quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{T}_\mu[\hat{\partial}_\nu,\mathcal{T}_\rho] = 0,\end{gathered} \tag{A25}$$

and

$$\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\mathcal{I},\mathcal{I}]=0,\quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\mathcal{I},\mathcal{T}_\mu]=0,$$
$$\mathrm{Tr}_{\mathcal{H}}\,\mathcal{I}[\mathcal{T}_\mu,\mathcal{T}_\nu]=+\frac{i\theta^i}{\sqrt{N}}\theta^{-1}_{\mu\nu},\quad \mathrm{Tr}_{\mathcal{H}}\,\mathcal{T}_\mu[\mathcal{T}_\nu,\mathcal{T}_\rho]=0. \tag{A26}$$

The same formulas as (A24)–(A26) hold for the case of (A12). The difference between the definitions of $\mathcal{H}_N$'s, (A9) and (A12), are absorbed in dimensions of $\mathcal{H}_N$.

It is worthwhile to notice that the independence of the precise definitions of $\mathcal{H}_N$ holds generally. The proof is done by using the discrete version of Stokes's theorem for the boundary of the finite truncated Fock space.[14,26]

APPENDIX B: LARGE θ LIMIT

In this paper, we removed the terms including $\partial_\mu=-i\theta^{-1}_{\mu\nu}[x^\nu,*]$ in the Lagrangian when we calculated the partition function without zero mode integrals in the large θ limit. If we consider some specific fixed function $f(x)$, then expression of $\partial_\mu f(x)=-i\theta^{-1}_{\mu\nu}[x^\nu,f(x)]$ is not changed by taking large θ limit because $[x^\nu,f(x)]$ becomes large with θ. Therefore, someone might think that the process of removing terms including ∂_μ is not correct. However, we must recall that our Lagrangian is changed by θ variation and then the equations of motion and BPS equations, are changed. Then the solutions of the equations, which make much contribution to the partition functions and vacuum expectation values, are changed by θ changing. It follows that the terms including derivatives become irrelevant. In this section, we show concretely the validity of taking the terms including $\partial_\mu=-i\theta^{-1}_{\mu\nu}[x^\nu,*]$ away from Lagrangians at the large θ limit.

The BPS equations in this paper are given by differential equations of first order,

$$\sum_{i,I} c_{iI,k}\partial_{z_i}f_I+V_k(f_J)=0, \tag{B1}$$

where f_I are fields, $V_k(f_I)$ are some quadratic polynomial in f_I and $c_{iI,k}$ are some constants. $k=1,\ldots,n$, where n is the number of elements of f_I minus degree of gauge freedom. For example, BPS equations of $\mathcal{N}=4$ four-dimensional gauge theory are

$$F^{+\mu\nu}-i[B^+_{\mu\rho},B^{+\rho}_\nu]-i[B^+_{\mu\nu},c]=0,\quad 2D^\mu B^+_{\mu\rho}+D_\rho c=0. \tag{B2}$$

Let us consider (B1) by using the Fock basis,

$$B_k(\hat f_I,\theta)\equiv c^+_{iI,k}\frac{1}{\sqrt{\theta^i}}[a_i,\hat f_I]+c^-_{iI,k}\frac{1}{\sqrt{\theta^i}}[a_i^\dagger,\hat f_I]+V_k(\hat f_J)=d_{i,k}\frac{1}{\theta^i}. \tag{B3}$$

Here $d_{i,k}(1/\theta^i)$ are constants derived from $[\partial_{z_i},\partial_{\bar z_i}]$. For example, equations of $\mathcal{N}=4$ four-dimensional cases are given by

$$P^+_{\mu\nu\rho\tau}[\hat D^\rho,\hat D^\tau]+[B^+_{\mu\rho},B^{+\rho}_\nu]+[B^+_{\mu\nu},c]=i(P^+_{\mu\nu\rho\tau}(\theta^{-1})^{\rho\tau}), \tag{B4}$$

$$2[\hat D^\mu,B_{+\mu\rho}]+[\hat D_\rho,c]=0, \tag{B5}$$

where $P^+_{\mu\nu\rho\tau}$ is the self-dual projection operator and $\hat D_\mu=\hat\partial_\mu+iA_\mu$. When we take $\theta^{\mu\nu}$ as (17), the right-hand side of (B4) is rewritten as

$$P^+_{\mu\nu\rho\tau}(\theta^{-1})^{\rho\tau}=-\frac{\varepsilon_{\mu\nu}}{2}\left(\frac{1}{\theta^1}+\frac{1}{\theta^2}\right),$$

$$(\varepsilon_{\mu\nu}) \equiv \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & & \\ & & 0 & 1 \\ & & -1 & 0 \end{pmatrix}.$$

$\hat{f}_I$ is a operator representation of f_I, i.e., $\hat{f}_I = \Sigma (f_I)^{m_1,\ldots m_D}_{n_1,\ldots,n_D} |n_1,\ldots,n_D\rangle\langle m_1,\ldots,m_D|$. In this representation, the BPS equations are just simultaneous quadratic equations, and the noncommutative parameters θ^i appear in only the first two terms and the right-hand side of (B3). Note that solutions of (B3) depend on θ^i but variables $(f_I)^{m_1,\ldots,m_D}_{n_1,\ldots,n_D}$ themselves do not depend on θ. For this reason, BPS equations are truncated to

$$B_k(\hat{f}_I, \infty) \equiv V_k(\hat{f}_J) = 0, \tag{B6}$$

at the $\theta \to \infty$ limit. Such truncations have been discussed in many works, see for example, Refs. 10, 9, and 15. Thus, it becomes clear that terms including $\partial_\mu = -i\theta^{-1}_{\mu\nu}[x^\nu, *]$ in the Lagrangian become irrelevant at the large θ limit.

However, the above discussion is insufficient for the proof which justifies removing terms including ∂_μ. Because we assume the convergency of path integral which has not been confirmed when we formally prove that partition functions and vacuum expectation values of observables do not depend on θ. Therefore, we must check our models satisfying the convergency conditions. To understand this statement, let us consider the following example.

Let f_i be dynamical variables and assume that action functional take the following form:

$$S_\epsilon[f] = S_0 + \epsilon S_1, \tag{B7}$$

where ϵ is a some constant, S_0 and S_ϵ are BRS exact actions, and they do not depend on ϵ. Let us expand the partition function as

$$Z_\epsilon = \int \mathcal{D}f\, e^{-S_\epsilon} \tag{B8}$$

$$= \int \mathcal{D}f\, e^{-S_0}\left(1 - \epsilon S_1 + \frac{1}{2}\epsilon^2 S_1^2 - \cdots\right) \tag{B9}$$

and introduce

$$Z_0 \equiv \int \mathcal{D}f\, e^{-S_0}. \tag{B10}$$

If e^{-S_0} damp the integrand, the integral

$$\int \mathcal{D}f\, e^{-S_0}\epsilon^n S_1^n \quad \text{for } n \geqslant 1 \tag{B11}$$

is well defined. Then, Z_ϵ does not depend on ϵ, i.e.,

$$Z_\epsilon = Z_0,$$

because S_1^n is a BRS exact term and

$$\int \mathcal{D}f\, e^{-S_0}\epsilon^n S_1^n = 0 \quad \text{for } n \geqslant 1.$$

Therefore, we found that we must verify that (B10) is well defined and e^{-S_0} damp integrands for proof of ϵ independence.

To get a feeling for how all of this should work out, consider simple toy models. At first, let us consider the toy model given by Vafa and Witten in Sec. II of Ref. 34. Let x, y, H_1 and H_2 be real bosonic variables, and ψ_x, ψ_y, χ_1 and χ_2 be fermionic variables. We define BRS transformations by

$$\hat{\delta}x = \psi_x, \quad \hat{\delta}y = \psi_y, \quad \hat{\delta}\chi_1 = H_1, \quad \hat{\delta}\chi_2 = H_2. \tag{B12}$$

Consider the following action:

$$S_\epsilon^{\text{toy1}} = \hat{\delta}\{\chi_1(H_1 + 2i(x^2 - \epsilon - y^2)) + \chi_2(H_2 + 2i(2xy))\} = S_0^{\text{toy1}} + \epsilon S_1^{\text{toy1}}, \tag{B13}$$

where

$$S_0^{\text{toy1}} = \hat{\delta}\{\chi_1(H_1 + 2i(x^2 - y^2)) + \chi_2(H_2 + 2i(2xy))\},$$

$$S_1^{\text{toy1}} = \hat{\delta}\chi_1.$$

$e^{-S_0^{\text{toy1}}}$ makes the integral

$$\int \mathcal{D}f\, e^{-S_0^{\text{toy1}}} \epsilon^n (S_1^{\text{toy1}})^n \quad \text{for } n \geqslant 1 \tag{B14}$$

be well defined, and

$$Z_\epsilon^{\text{toy1}} = Z_0^{\text{toy1}} \equiv \int \mathcal{D}f\, e^{-S_0^{\text{toy1}}}. \tag{B15}$$

Indeed, we can easily perform the direct calculations of the partition functions Z_ϵ^{toy1} and Z_0^{toy1}, respectively, and their results reproduce (B15). Note that degeneracy of the solutions does not affect the independence of ϵ. In this case, when $\epsilon \neq 0$ equations are given by $x^2 - \epsilon - y^2 = 0$ and $2xy = 0$, then the solutions are given as $(x, y) = (\pm\sqrt{\epsilon}, 0)$. These two sets of solutions become degenerate in $\epsilon \to 0$. Despite such singularities, path integrals moderate them, and the partition function is smooth at $\epsilon = 0$.

As the second example, consider the following action:

$$S_\epsilon^{\text{toy2}} = \hat{\delta}\{\chi_1(H_1 + 2i(x^2 - \epsilon)) + \chi_2(H_2 + 2i(2xy))\} = S_0^{\text{toy2}} + \epsilon S_1^{\text{toy2}}, \tag{B16}$$

where

$$S_0^{\text{toy2}} = \hat{\delta}\{\chi_1(H_1 + 2i(x^2)) + \chi_2(H_2 + 2i(2xy))\},$$

$$S_1^{\text{toy2}} = \hat{\delta}\chi_1.$$

At first glance, the partition function Z_ϵ^{toy2} looks independent of ϵ from the formal discussion. But $e^{-S_0^{\text{toy2}}}$ does not damp the integrals in this case, then Z_ϵ^{toy2} depends on ϵ. Indeed,

$$Z_\epsilon^{\text{toy2}} = \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \frac{\mathrm{d}y}{\sqrt{2\pi}} \frac{\mathrm{d}H_1}{\sqrt{2\pi}} \frac{\mathrm{d}H_2}{\sqrt{2\pi}} \mathrm{d}\psi_x\, \mathrm{d}\psi_y\, \mathrm{d}\chi_1\, \mathrm{d}\chi_2 \exp(-S_\epsilon^{\text{toy2}}) = 1 + \frac{\epsilon}{2}\pi^{-1/2} + O(\epsilon^2). \tag{B17}$$

These observations show that we must check the convergency of e^{-S_0} where the action S_0 is the θ independent part of the total action, before removing terms including θ^{-1} from action.

Let us now attempt to investigate the specific case of $\mathcal{N}=4$ four dimensions. First we consider the case of $\theta^1 = -\theta^2$. This is a very special case and we can understand the validity of removing the terms including ∂_μ not from the above discussions but from the following discussions. Using $\theta^1 = -\theta^2$, the BPS Eqs. (B4) and (B5) are replaced by

$$P^{+}_{\mu\nu\rho\tau}[\hat{D}^{\rho},\hat{D}^{\tau}] + [B^{+}_{\mu\rho},B^{+\rho}_{\nu}] + [B^{+}_{\mu\nu},c] = 0, \tag{B18}$$

$$2[\hat{D}^{\mu},B_{+\mu\rho}] + [\hat{D}_{\rho},c] = 0. \tag{B19}$$

On the contrary, the BPS equations of the large θ limit are given by

$$-P^{+}_{\mu\nu\rho\tau}[A^{\rho},A^{\tau}] + [B^{+}_{\mu\rho},B^{+}_{\nu\tau}]\delta^{\tau\rho} + [B^{+}_{\mu\nu},c] = 0, \tag{B20}$$

$$2[A^{\mu},B^{+}_{\mu\rho}] + [A_{\rho},c] = 0. \tag{B21}$$

Equations (B20) and (B21) are equivalent to (B18) and (B19) with $1/\theta=0$. The correspondence of these and more general cases are already known in Refs. 1 and 30, that is, we can identify (B18) and (B19) with (B20) and (B21) by redefining

$$iA_{\mu} = \hat{D}_{\mu}. \tag{B22}$$

This is a trivial one-to-one correspondence between the large θ limit and finite $\theta^{1}=-\theta^{2}$ case. Under change of variables (B22), the path integral measure does not cause nontrivial Jacobian, the theory characterized (B18) and (B19) and the theory characterized (B20) and (B21) are equivalent quantum theories. From this correspondence, it is clear that we can remove the terms including ∂_{μ} from its action without changing.

Before investigating $\theta^{1}\neq-\theta^{2}$ case, let us consider

$$S_{\epsilon} = S_{0} + \epsilon S_{1},$$

$$S_{0} = \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_{+}\{\chi^{+}_{\mu\nu}(H^{+\mu\nu} - (P^{+}_{\mu\nu\rho\tau}[\hat{D}^{\rho},\hat{D}^{\tau}] + [B^{+}_{\mu\rho},B^{+}_{\nu\sigma}]\delta^{\rho\sigma} + [B^{+}_{\mu\nu},c]))\} + \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_{+}\{\chi^{\rho}(H_{\rho} - i($$
$$-2[\hat{D}^{\mu},B^{+}_{\mu\rho}] - [\hat{D}_{\rho},c]))\} + \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}_{+}\{i[\phi,\bar{\phi}]\eta - i\bar{\eta}[c,\bar{\phi}] + i[B^{+\mu\nu},\bar{\phi}]\psi^{+}_{\mu\nu} + ([\hat{D}_{\mu},\bar{\phi}])\psi_{\mu}\},$$

$$S_{1} = i\chi^{+}_{\mu\nu}\varepsilon^{\mu\nu}, \tag{B23}$$

and their partition functions

$$Z_{\mathcal{N}=4,\epsilon} = \int \mathcal{D}f\, e^{-S_{\epsilon}}, \quad Z_{\mathcal{N}=4,0} = \int \mathcal{D}f\, e^{-S_{0}}. \tag{B24}$$

Note that S_{0} is equivalent to the action of the Yang-Mills theory of $\theta^{1}=-\theta^{2}$ and IKKT matrix model when its gauge group is U(1). Therefore, it is natural to assume that $\exp(-S_{0})$ damp the path integral of an arbitrary observable. Indeed, this assumption is required in MNS too.[20] From the above discussion and this assumption, we can conclude that

$$Z_{\mathcal{N}=4,\epsilon} = Z_{\mathcal{N}=4,0}. \tag{B25}$$

In the next step, we consider the $\theta^{1}\neq-\theta^{2}$ case. Its action is equivalent to (B23) if

$$\epsilon = -\frac{1}{2}\left(\frac{1}{\theta^{1}} + \frac{1}{\theta^{2}}\right).$$

Under the above assumption that $\exp(-S_{0})$ damp integrands of path integrals, as we saw in (B25), $Z_{\mathcal{N}=4,\epsilon}$ does not depend on ϵ. Therefore, the partition function of $\theta^{1}\neq-\theta^{2}$ case is equal to the partition function of $\theta^{1}=-\theta^{2}$ whose BPS equations are given by (B18) and (B19), furthermore the partition function is equal to the partition function whose action functional is given by removing derivative terms and its BPS equations are given by (B20) and (B21).

In the above discussion, we have closely studied the case of dimensional reduction from $\mathcal{N}=4$ four dimensions to 0 dimensions. But it is clear that we can apply the above general discussion

to other dimensional cases or the cases of the $\mathcal{N}=2$ four-dimensional model and the series given by its dimensional reduction. All these things make it clear that it is proper procedure to remove the terms including $\partial_\mu = -i\theta^{-1}_{\mu\nu}[x^\nu, *]$ from Lagrangians at the large θ limit, in the calculations of this paper.

APPENDIX C: NORMALIZATION OF THE PARTITION FUNCTION

In this appendix, we give the precise definition of the path integral measure to decide the partition function without ambiguity.

As mentioned in Sec. IVG, the absolute value of the infinite-dimensional integrals of fluctuations around each vacuum should be normalized to be 1. This is implemented by virtue of the supersymmetry.

When we normalize fields appropriately the action of topological field theory has the following form:

$$S_{\mathrm{TFT}} = \int \hat{\delta}_+[\chi_i\{H_i - iM_{ij}A_j\}], \tag{C1}$$

here we have omitted terms including fields like $\phi, \bar{\phi}, \eta$, often called "Higgs sector," for simplicity. The normalization of the Higgs sector is possible to be managed similarly to other fields when usual gauge fixing is done by using Nakanishi-Lautrup field, ghost and antighost fields. We can see this fact in the latter half of this section devoted to trace and extra parts. Also we have kept only quadratic terms of fluctuations, because the path integral of topological field theories is estimated exactly in the weak coupling limit. M_{ij} in (C1) depends on backgrounds and parameters in general, but as seen below, the M_{ij} dependence does not appear in the result up to sign. The BRS transformation rules are given by

$$\begin{aligned} &\hat{\delta}_+ A_i = \psi_i, \quad \hat{\delta}_+ \psi_i = 0, \\ &\hat{\delta}_+ \chi_i = H_i, \quad \hat{\delta}_+ H_i = 0. \end{aligned} \tag{C2}$$

For $A_i, \ldots$, we adopt the following path integral measure:

$$\prod_i \frac{\mathrm{d}H_i}{\sqrt{2\pi}} \frac{\mathrm{d}A_i}{\sqrt{2\pi}} \mathrm{d}\chi_i \, \mathrm{d}\psi_i, \tag{C3}$$

then we obtain

$$\left| \int \prod_i \frac{\mathrm{d}H_i}{\sqrt{2\pi}} \frac{\mathrm{d}A_i}{\sqrt{2\pi}} \mathrm{d}\chi_i \, \mathrm{d}\psi_i \, e^{-S_{\mathrm{TFT}}} \right| = 1. \tag{C4}$$

The M_{ij} dependence does not appear due to the supersymmetry.

Now we give a detailed argument for calculations about the trace and extra parts of our model as an example. The action including the trace and extra parts $S^{\infty}_{\mathrm{tr}\oplus\mathrm{ex}} + S_{\mathrm{gf}}$ is decomposed into two parts, S_1 and S_2. S_1 consists of (106)–(109) and (111)–(114), and also S_2 consists of (110), (115), (119), and (120). S_2 involves the Higgs sector and also includes the gauge fixing terms. S_1 involves all the rest.

We start with the S_1 part. S_1 is represented in the same form as (C1), therefore we obtain

$$\int \prod_i \frac{\mathrm{d}H_i}{\sqrt{2\pi}} \frac{\mathrm{d}A_i}{\sqrt{2\pi}} \mathrm{d}\chi_i \, \mathrm{d}\psi_i \, e^{-S_1} = 1. \tag{C5}$$

As mentioned above, the θ-dependence does not appear.

Let us turn to the S_2 part. The action is given as

$$S_2 = \frac{4}{\theta}\bar{\phi}_{(\mathbf{1})}\phi_{(\mathbf{1})} \tag{C6}$$

$$+ \frac{i}{\sqrt{\theta}}\eta_{(\mathbf{1})}\psi^{\mu}_{(\mu)} \tag{C7}$$

$$+ b_{(\mathbf{1})}\left(b_{(\mathbf{1})} - \frac{1}{\sqrt{\theta}}A_{\mu(\mu)}\right) \tag{C8}$$

$$+ \frac{4}{\theta}\bar{\rho}_{(\mathbf{1})}\rho_{(\mathbf{1})} + \frac{1}{\sqrt{\theta}}\bar{\rho}_{(\mathbf{1})}\psi_{\mu(\mu)}. \tag{C9}$$

We adopt the following measure:

$$\frac{\mathrm{d}\bar{\phi}_{(\mathbf{1})}}{\sqrt{2\pi}}\frac{\mathrm{d}\phi_{(\mathbf{1})}}{\sqrt{2\pi}}\mathrm{d}\bar{\rho}_{(\mathbf{1})}\,\mathrm{d}\rho_{(\mathbf{1})}\frac{\mathrm{d}b_{(\mathbf{1})}}{\sqrt{2\pi}}\frac{\mathrm{d}A_{\mu(\mu)}}{\sqrt{2\pi}}\mathrm{d}\eta_{(\mathbf{1})}\,\mathrm{d}\psi^{\mu}_{(\mu)}, \tag{C10}$$

then we obtain

$$\int \frac{\mathrm{d}\bar{\phi}_{(\mathbf{1})}}{\sqrt{2\pi}}\frac{\mathrm{d}\phi_{(\mathbf{1})}}{\sqrt{2\pi}}\mathrm{d}\bar{\rho}_{(\mathbf{1})}\,\mathrm{d}\rho_{(\mathbf{1})}\frac{\mathrm{d}b_{(\mathbf{1})}}{\sqrt{2\pi}}\frac{\mathrm{d}A_{\mu(\mu)}}{\sqrt{2\pi}}\mathrm{d}\eta_{(\mathbf{1})}\,\mathrm{d}\psi^{\mu}_{(\mu)}e^{-S_2} = 1. \tag{C11}$$

Notice that the result (C11) is again a consequence of the supersymmetry.

As a result of these normalizations, partition functions of the cohomological field theories are defined as well-defined functions or finite values without ambiguity from infinite-dimensional integral.

At the end of this appendix, we should notice a fact relating the dimension-independence of partition function, (20). The gauge symmetry (99) and the gauge fixing term (117) are expected to have the same form for all cases of (8-dim, $\mathcal{N}=2$), (6-dim, $\mathcal{N}=2$), (4-dim, $\mathcal{N}=4$) and (2-dim, $\mathcal{N}=8$). So we expect that the trace and extra sector produce a trivial factor 1 for all of those cases.

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Gauged Wess–Zumino model in noncommutative Minkowski superspace

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We develop a gauged Wess–Zumino model in noncommutative Minkowski superspace. This is the natural extension of the work of Carlson and Nazaryan, which extended $N=1/2$ supersymmetry written over deformed Euclidean superspace to Minkowski superspace. We investigate the coupling of the vector and chiral superfields. Noncommutativity is implemented by replacing products with star products. Although, in general, our star product is nonassociative, we prove that it is associative to the first order in the deformation parameter C. We show that our model reproduces the $N=1/2$ theory in the appropriate limit, namely when the deformation parameters $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$. Essentially, we find the $N=1/2$ theory and a conjugate copy. As in the $N=1/2$ theory, a reparametrization of the gauge parameter, vector superfield, and chiral superfield are necessary to write standard C-independent gauge theory. However, our choice of parametrization differs from that used in the $N=1/2$ supersymmetry, which leads to some unexpected new terms. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162330]

I. INTRODUCTION

In the past several years there has been much discussion of noncommutative superspaces; see Refs. 1–13 for a partial account. Much recent discussion has been motivated by the observation that noncommutativity can result from certain string models. Of particular interest to this paper is the deformed Euclidean superspace constructed by Seiberg in Ref. 8. Seiberg found a deformation of Euclidean superspace that broke half the supersymmetry and yet preserved the usual superfield constructions. Because only half of the $N=1$ supersymmetry is found in Seiberg's theory, it is commonly referred to as $N=1/2$ supersymmetry. Generally, the literature following Seiberg has focused on superspace with a Euclidean signature. One reason for that is that it is not entirely straightforward to modify the construction of $N=1/2$ supersymmetry to the Minkowski case. However, Carlson and Nazaryan found in Ref. 11 how to construct a deformed Minkowski superspace very similar to Seiberg's deformed Euclidean space. In particular, Ref. 11 deformed superspace so that

$$\{\hat{\theta}^{\alpha},\hat{\theta}^{\beta}\}=C^{\alpha\beta},\quad \{\hat{\bar{\theta}}^{\dot{\alpha}},\hat{\bar{\theta}}^{\dot{\beta}}\}=\bar{C}^{\dot{\alpha}\dot{\beta}}, \tag{1}$$

where $(C^{\alpha\beta})^{*}=\bar{C}^{\dot{\alpha}\dot{\beta}}$. In their paper, they implemented superspace noncommutativity with a star product that was Hermitian, but not associative in general. Their star product reproduces the deformation of $N=1/2$ supersymmetry in the limit that $\bar{C}^{\dot{\alpha}\dot{\beta}}$ is identically zero. Additionally, they studied the Wess–Zumino model (only chiral superfields, no gauge interactions) and found results similar to that of Seiberg in Ref. 8. Our goal here is to continue the work of Carlson and Nazaryan by constructing the Wess–Zumino model with gauge interactions in the noncommutative Minkowski superspace they constructed. We will carefully study how the $N=1/2$ theory must be modified in the presence of the Minkowski metric. We will find the modification of the gauge theory is not entirely straightforward; subtle superfield component redefinitions must be made for

certain components in order to maintain deformation-independent gauge transformations.

We mention that after the completion of this work, the author learned that Ref. 12 and Ref. 13 also studied the Wess–Zumino model on deformed Minkowski superspaces in some detail. Both of these works employ a star product that is associative but not Hermitian. The star product studied here is Hermitian but not associative in general. We also note that Ref. 5 and Ref. 10 study some general aspects of deformed Minkowski superspace that have relevance to this work.

A. Deformed coordinate algebra

We begin by considering $N=1$ rigid Minkowski superspace where a typical point is $(x^m, \theta^\alpha, \bar{\theta}^{\dot{\alpha}})$. In the commutative case, we have

$$\begin{aligned} &[x^m, x^n] = 0 \qquad [x^m, \theta^\alpha] = 0, \\ &\{\theta^\alpha, \theta^\beta\} = 0 \qquad [x^m, \bar{\theta}^{\dot{\alpha}}] = 0, \\ &\{\bar{\theta}^{\dot{\alpha}}, \bar{\theta}^{\dot{\beta}}\} = 0 \qquad \{\theta^\alpha, \bar{\theta}^{\dot{\beta}}\} = 0. \end{aligned} \tag{2}$$

The coordinates x^m are identified with spacetime coordinates, whereas the θ^α and $\bar{\theta}^{\dot{\alpha}}$ are Grassman variables. We then construct noncommutative Minkowski superspace by replacing coordinate functions $(x^m, \theta^\alpha, \bar{\theta}^{\dot{\alpha}})$ with operators $(\hat{x}^m, \hat{\theta}^\alpha, \hat{\bar{\theta}}^{\dot{\alpha}})$. In particular, following the construction of Ref. 11, we deform $N=1$ rigid Minkowski superspace as follows:

$$\begin{aligned} &\{\hat{\theta}^\alpha, \hat{\theta}^\beta\} = C^{\alpha\beta}, \qquad [\hat{x}^m, \hat{\theta}^\alpha] = iC^{\alpha\beta}\sigma^m_{\beta\dot{\beta}}\hat{\bar{\theta}}^{\dot{\beta}}, \\ &\{\hat{\bar{\theta}}^{\dot{\alpha}}, \hat{\bar{\theta}}^{\dot{\beta}}\} = \bar{C}^{\dot{\alpha}\dot{\beta}}, \qquad [\hat{x}^m, \hat{\bar{\theta}}^{\dot{\alpha}}] = i\bar{C}^{\dot{\alpha}\dot{\beta}}\hat{\theta}^\beta\sigma^m_{\beta\dot{\beta}}, \\ &\{\hat{\theta}^\alpha, \hat{\bar{\theta}}^{\dot{\beta}}\} = 0, \qquad [\hat{x}^m, \hat{x}^n] = (C^{\alpha\beta}\hat{\bar{\theta}}^{\dot{\alpha}}\hat{\bar{\theta}}^{\dot{\beta}} - \bar{C}^{\dot{\alpha}\dot{\beta}}\hat{\theta}^\alpha\hat{\theta}^\beta)\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}, \end{aligned} \tag{3}$$

where $(C^{\alpha\beta})^* = \bar{C}^{\dot{\alpha}\dot{\beta}}$. This algebra was constructed in Ref. 11 so that the deformed chiral coordinates satisfy $\hat{y}^m = \hat{x}^m + i\hat{\theta}\sigma^m\hat{\bar{\theta}}$ and $\hat{\bar{y}}^m = \hat{x}^m - i\hat{\theta}\sigma^m\hat{\bar{\theta}}$ satisfy

$$\begin{aligned} &\{\hat{\theta}^\alpha, \hat{\theta}^\beta\} = C^{\alpha\beta}, \qquad [\hat{y}^m, \hat{\theta}^\alpha] = 0, \\ &\{\hat{\bar{\theta}}^{\dot{\alpha}}, \hat{\bar{\theta}}^{\dot{\beta}}\} = \bar{C}^{\dot{\alpha}\dot{\beta}}, \qquad [\hat{\bar{y}}^m, \hat{\bar{\theta}}^{\dot{\alpha}}] = 0, \\ &\{\hat{\theta}^\alpha, \hat{\bar{\theta}}^{\dot{\beta}}\} = 0. \end{aligned} \tag{4}$$

These relations will allow us to develop chiral and antichiral superfields in much the same way as in the commutative theory. In addition, we have

$$\begin{aligned} [\hat{\bar{y}}^m, \hat{\theta}^\alpha] &= 2iC^{\alpha\beta}\sigma^m_{\beta\dot{\beta}}\hat{\bar{\theta}}^{\dot{\beta}}, \\ [\hat{y}^m, \hat{\bar{\theta}}^{\dot{\alpha}}] &= 2i\bar{C}^{\dot{\alpha}\dot{\beta}}\hat{\theta}^\beta\sigma^m_{\beta\dot{\beta}}, \\ [\hat{y}^m, \hat{y}^n] &= (4\bar{C}^{\dot{\alpha}\dot{\beta}}\hat{\theta}^\alpha\hat{\theta}^\beta - 2C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}})\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}, \\ [\hat{\bar{y}}^m, \hat{\bar{y}}^n] &= (4C^{\alpha\beta}\hat{\bar{\theta}}^{\dot{\alpha}}\hat{\bar{\theta}}^{\dot{\beta}} - 2C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}})\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}, \\ [\hat{y}^m, \hat{\bar{y}}^n] &= 2C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}. \end{aligned} \tag{5}$$

In this deformation, all of the fermionic dimensions of superspace are deformed. A consequence of this is that Q and $\bar{Q}$ are broken symmetries (see the next section), so we say that this space has

$N=0$ supersymmetry. Despite this, the deformation still permits most of the usual superfield constructions just like the $N=1/2$ case.

B. Star product

The deformed coordinates have overcarets on them to emphasize that they are operators. The usual model is then deformed by simply putting an overcaret on all of the objects in the standard theory. In practice, we will not explicitly calculate anything in terms of these formal operators. Instead, we will find it useful to make the usual exchange of the operator product for the star product of ordinary functions of superspace;

$$\hat{F}\hat{G} \mapsto F * G. \tag{6}$$

This correspondence allows us to work out the details of noncommutative theory using ordinary calculus on superspace. In this sense we will obtain a noncommutative model by replacing ordinary products with star products.

The star product for our deformed Minkowski superspace is defined by

$$F * G = F(1+S)G, \tag{7}$$

where S is formed using the supercharges Q_α and $\bar{Q}_{\dot{\alpha}}$,

$$S = -\frac{1}{2}C^{\alpha\beta}\overleftarrow{Q}_\alpha\overrightarrow{Q}_\beta - \frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\overleftarrow{\bar{Q}}_{\dot{\alpha}}\overrightarrow{\bar{Q}}_{\dot{\beta}}$$

$$+\frac{1}{8}C^{\alpha\beta}C^{\gamma\delta}\overleftarrow{Q}_\alpha\overleftarrow{Q}_\gamma\overrightarrow{Q}_\delta\overrightarrow{Q}_\beta + \frac{1}{8}\bar{C}^{\dot{\alpha}\dot{\beta}}\bar{C}^{\dot{\gamma}\dot{\delta}}\overleftarrow{\bar{Q}}_{\dot{\alpha}}\overleftarrow{\bar{Q}}_{\dot{\gamma}}\overrightarrow{\bar{Q}}_{\dot{\delta}}\overrightarrow{\bar{Q}}_{\dot{\beta}}$$

$$+\frac{1}{4}C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}}(\overleftarrow{\bar{Q}}_{\dot{\alpha}}\overleftarrow{Q}_\alpha\overrightarrow{\bar{Q}}_{\dot{\beta}}\overrightarrow{Q}_\beta - \overleftarrow{Q}_\alpha\overleftarrow{\bar{Q}}_{\dot{\alpha}}\overrightarrow{Q}_\beta\overrightarrow{\bar{Q}}_{\dot{\beta}}).$$

It is straightforward to check that this star product does yield the deformed coordinate algebra of the preceding section, provided we use star products in place of the usual products. We follow the conventions of Wess and Bagger in Ref. 14 for supercharges. In the chiral coordinates $y^m=x^m+i\theta\sigma^m\bar{\theta}$, the supercharges have the following familiar forms. Note that the derivatives of θ^α and $\bar{\theta}^{\dot{\alpha}}$ are taken at fixed y^m:

$$\begin{aligned} Q_\alpha &= \left.\frac{\partial}{\partial\theta^\alpha}\right|_y, \\ \bar{Q}_{\dot{\alpha}} &= -\left.\frac{\partial}{\partial\bar{\theta}^{\dot{\alpha}}}\right|_y + 2i\theta^\alpha\sigma^m_{\alpha\dot{\alpha}}\frac{\partial}{\partial y^m}, \end{aligned} \tag{8}$$

whereas when the derivatives are taken at fixed antichiral coordinates $\bar{y}^m=x^m-i\theta\sigma^m\bar{\theta}$, we have

$$Q_\alpha = \left.\frac{\partial}{\partial\theta^\alpha}\right|_y - 2i\sigma^m_{\alpha\dot{\alpha}}\bar{\theta}^{\dot{\alpha}}\frac{\partial}{\partial\bar{y}^m}, \tag{9}$$

$$\bar{Q}_{\dot{\alpha}} = -\left.\frac{\partial}{\partial \bar{\theta}^{\dot{\alpha}}}\right|_{\bar{y}}.$$

We will not make explicit $|_y$ or $|_{\bar{y}}$ elsewhere, since they are to be understood implicitly. Many other formulas can be found in Ref. 11. Some properties of this star product on functions F, G, and H are

$$\begin{aligned} &\overline{F * G} = \bar{G} * \bar{F}, \qquad (F+G) * H = F * H + G * H, \\ &F * G \neq G * F, \qquad F * (G * H) \neq (F * G) * H. \end{aligned} \tag{10}$$

The noncommutativity and nonassociativity will require some attention in general. However, to the first order in the deformation parameter, we note that

$$F * (G * H) = (F * G) * H, \tag{11}$$

the star product is associative. A proof is given in the Appendix .

C. $N=0$ Supersymmetry

The formulas below are stated for the operators acting on functions of the deformed Minkowki superspace. In particular, they should be understood as statements about how the operators act on star products of functions. We define the star brackets as

$$\{A,B\}_* = A * B + B * A \quad \text{and} \quad [A,B]_* = A * B - B * A. \tag{12}$$

Then calculate

$$\begin{aligned} \{\theta^{\alpha}, \theta^{\beta}\}_* &= \theta^{\alpha} * \theta^{\beta} + \theta^{\beta} * \theta^{\alpha} = C^{\alpha\beta}, \\ \{\bar{\theta}^{\dot{\alpha}}, \bar{\theta}^{\dot{\beta}}\}_* &= \bar{\theta}^{\dot{\alpha}} * \bar{\theta}^{\dot{\beta}} + \bar{\theta}^{\dot{\beta}} * \bar{\theta}^{\dot{\alpha}} = \bar{C}^{\dot{\alpha}\dot{\beta}}. \end{aligned} \tag{13}$$

It is important to note that products of both θ^{α} and $\bar{\theta}^{\dot{\alpha}}$ are deformed. This has the consequence of breaking all of the supersymmetry. Starting with the canonical forms of the supercharges, we obtain

$$\begin{aligned} \{Q_{\alpha}, Q_{\beta}\}_* &= -4\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}\frac{\partial^2}{\partial \bar{y}^m\, \partial\, \bar{y}^n}, \\ \{\bar{Q}_{\dot{\alpha}}, \bar{Q}_{\dot{\beta}}\}_* &= -4C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}\sigma^n_{\beta\dot{\beta}}\frac{\partial^2}{\partial y^m\, \partial\, y^n}, \\ \{Q_{\alpha}, \bar{Q}_{\dot{\alpha}}\}_* &= 2i\sigma^m_{\alpha\dot{\alpha}}\frac{\partial}{\partial y^m}. \end{aligned} \tag{14}$$

Comparing this to Ref. 8, we note that when $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$, then Q_{α} is an unbroken symmetry, hence the label $N=1/2$ supersymmetry. The author proposes that we call the theory constructed by Carlson and Nazaryan $N=0$ supersymmetry to be consistent. Now, although the supercharges are broken, we still have

$$\{D_{\alpha}, Q_{\beta}\}_* = \{\bar{D}_{\dot{\alpha}}, Q_{\beta}\}_* = \{D_{\alpha}, \bar{Q}_{\dot{\beta}}\}_* = \{\bar{D}_{\dot{\alpha}}, \bar{Q}_{\dot{\beta}}\}_* = 0,$$

$$\{D_\alpha, D_\beta\}_* = \{\bar{D}_{\dot\alpha}, \bar{D}_{\dot\alpha}\}_* = 0. \tag{15}$$

These relations are crucial. We can still define the chiral (Φ) and antichiral ($\bar{\Phi}$) superfields by the constraints $\bar{D}_{\dot\alpha} * \Phi = 0$ and $D_\alpha * \bar{\Phi} = 0$ on noncommutative Minkowski superspace. Thus, most of the usual techniques in Wess and Bagger, Ref. 14, still apply for our discussion. The primary difference is that products will be replaced with star products.

II. VECTOR SUPERFIELDS

Our goal in this section is to construct a non-Abelian gauge theory on deformed Minkowski superspace. Thus, we consider a vector superfield V that carries some matrix representation of the gauge group and is subject to the usual covariant constraint: $\bar{V} = V$. In the standard super-Yang–Mills theory, it is convenient to use a reduced set of component fields called the Wess Zumino gauge. We will show in Section III A that the Wess Zumino gauge can be generalized to the current discussion provided we make some C-dependent shifts. But, for now, we let V take the canonical Wess–Zumino parametrization

$$V = -\theta\sigma^m\bar{\theta}v_m + i\theta\theta\bar{\theta}\bar{\lambda} - i\bar{\theta}\bar{\theta}\theta\lambda + \frac{1}{2}\theta\theta\bar{\theta}\bar{\theta}(D - i\,\partial_m v^m), \tag{16}$$

where the above is in chiral coordinates y^m. Physically this is not quite the correct parametrization because it does not naturally embed the usual gauge transformations on the component fields. Later we will find the parametrization that allows for standard deformation-independent gauge transformations on the component fields. We abstain from introducing that reparametrization at this point because it would only serve to complicate the expressions without need.

A. Star exponential of vector superfield

We define the star exponential of the vector superfield in the natural way:

$$e^V = 1 + V + \frac{1}{2}V * V + \frac{1}{3!}V * V * V + \cdots . \tag{17}$$

Our notation for the usual exponential will be $\exp(V)$ and powers are to be understood as ordinary powers—for example, $V^2 = VV$. In this paper, star products will be explicitly indicated.

The vector superfield is even, thus no new signs arise from pushing the Q_α or $\bar{Q}_{\dot\alpha}$ past V in the star product. Thus,

$$\begin{aligned} V * V &= V(1+S)V \\ &= V^2 - \frac{1}{2}C^{\alpha\beta}(Q_\alpha V)(Q_\beta V) - \frac{1}{2}\bar{C}^{\dot\alpha\dot\beta}(\bar{Q}_{\dot\alpha}V)(\bar{Q}_{\dot\beta}V) \\ &\quad + \frac{1}{8}C^{\alpha\beta}C^{\gamma\delta}(Q_\alpha Q_\gamma V)(Q_\delta Q_\beta V) + \frac{1}{8}\bar{C}^{\dot\alpha\dot\beta}\bar{C}^{\dot\gamma\dot\delta}(\bar{Q}_{\dot\alpha}\bar{Q}_{\dot\gamma}V)(\bar{Q}_{\dot\delta}\bar{Q}_{\dot\beta}V) \\ &\quad + \frac{1}{4}C^{\alpha\beta}\bar{C}^{\dot\alpha\dot\beta}((\bar{Q}_{\dot\alpha}Q_\alpha V)(\bar{Q}_{\dot\beta}Q_\beta V) - (Q_\alpha\bar{Q}_{\dot\alpha}V)(Q_\beta\bar{Q}_{\dot\beta}V)). \end{aligned}$$

We will now calculate these terms in chiral coordinates, starting with

$$\begin{aligned} Q_\alpha V &= \partial_\alpha\left(-\theta\sigma^m\bar{\theta}v_m + i\theta\theta\bar{\theta}\bar{\lambda} - i\bar{\theta}\bar{\theta}\theta\lambda + \frac{1}{2}\theta\theta\bar{\theta}\bar{\theta}(D - i\partial_m v^m)\right) \\ &= -\sigma^m_{\alpha\dot\alpha}\bar{\theta}^{\dot\alpha}v_m + 2i\theta_\alpha\bar{\theta}\bar{\lambda} + \bar{\theta}\bar{\theta}(-i\lambda_\alpha + \theta_\alpha(D - i\partial_m v^m)). \end{aligned} \tag{18}$$

Continuing, we find that

$$Q_\beta Q_\alpha V = \partial_\beta(-\sigma^m_{\alpha\dot\alpha}\bar\theta^{\dot\alpha}v_m + 2i\theta_\alpha\bar\theta\bar\lambda + \bar\theta\bar\theta(-i\lambda_\alpha + \theta_\alpha(D - i\partial_m v^m))) = -2i\epsilon_{\beta\alpha}\bar\theta\bar\lambda - \epsilon_{\beta\alpha}\bar\theta\bar\theta(D - i\partial_m v^m). \tag{19}$$

Next, we calculate $\bar Q_{\dot\alpha}V$,

$$\begin{aligned}\bar Q_{\dot\alpha}V &= (-\partial_{\dot\alpha} + 2i\theta^\alpha\sigma^n_{\alpha\dot\alpha}\partial_n)\left(-\theta\sigma^m\bar\theta v_m + i\theta\theta\bar\theta\bar\lambda - i\bar\theta\bar\theta\theta\lambda + \frac{1}{2}\theta\theta\bar\theta\bar\theta(D - i\,\partial_m v^m)\right)\\ &= -\theta^\alpha\sigma^m_{\alpha\dot\alpha}v_m + (-2i\bar\theta_{\dot\alpha} + 2\bar\theta\bar\theta\sigma^m_{\alpha\dot\alpha}\theta^\alpha\partial_m)\theta\lambda + \theta\theta\\ &\quad\times\left(i\bar\lambda_{\dot\alpha} + \bar\theta_{\dot\alpha}(D - i\partial_m v^m) + i\epsilon^{\alpha\beta}\sigma^m_{\alpha\dot\alpha}\sigma^n_{\beta\dot\beta}\bar\theta^{\dot\beta}\,\partial_m v_n\right).\end{aligned} \tag{20}$$

The next calculation is a bit longer.

$$\begin{aligned}\bar Q_{\dot\alpha}\bar Q_{\dot\beta}V &= (-\partial_{\dot\alpha} + 2i\theta^\alpha\sigma^m_{\alpha\dot\alpha}\partial_m)(\bar Q_{\dot\beta}V) = -2i\epsilon_{\dot\alpha\dot\beta}\theta\lambda + \theta\theta(\epsilon_{\dot\alpha\dot\beta}(D - i\partial_m v^m)\\ &\quad + i\epsilon^{\alpha\beta}(\sigma^m_{\alpha\dot\beta}\sigma^n_{\beta\dot\alpha} - \sigma^m_{\alpha\dot\alpha}\sigma^n_{\beta\dot\beta})\partial_m v_n + 2(\sigma^m_{\alpha\dot\alpha}\bar\theta^{\dot\beta} - \bar\theta^{\dot\alpha}\sigma^m_{\alpha\dot\beta})\partial_m\lambda^\alpha).\end{aligned} \tag{21}$$

Now, for the mixed supercharges, using the previous results, we find that

$$\begin{aligned}Q_\alpha\bar Q_{\dot\alpha}V &= \partial_\alpha(\bar Q_{\dot\alpha}V) = -\sigma^m_{\alpha\dot\alpha}v_m + 2i(\theta_\alpha\bar\lambda_{\dot\alpha} - \bar\theta_{\dot\alpha}\lambda_\alpha) + \theta_\alpha(2\bar\theta_{\dot\alpha}(D - i\partial_m v^m)\\ &\quad + 2i\bar\theta^{\dot\beta}\epsilon^{\sigma\beta}\sigma^m_{\sigma\dot\alpha}\sigma^n_{\beta\dot\beta}\partial_m v_n + 2\bar\theta\bar\theta\sigma^m_{\beta\dot\alpha}\partial_m\lambda^\beta).\end{aligned} \tag{22}$$

Similarly, we find that

$$\begin{aligned}\bar Q_{\dot\alpha}Q_\alpha V &= (-\partial_{\dot\beta} + 2i\theta^\alpha\sigma^m_{\alpha\dot\alpha}\partial_m)(Q_\alpha V)\\ &= \sigma^m_{\alpha\dot\alpha}v_m - 2i(\theta_\alpha\bar\lambda_{\dot\alpha} - \bar\theta_{\dot\alpha}\lambda_\alpha) + 2\theta_\alpha\bar\theta_{\dot\alpha}(D - i\,\partial_m v^m) - 2i\theta^\beta\bar\theta^{\dot\beta}\,\sigma^m_{\beta\dot\alpha}\sigma^n_{\alpha\dot\beta}\,\partial_m v_n\\ &\quad - 2\theta\theta\sigma^m_{\alpha\dot\alpha}\partial_m(\bar\theta\bar\lambda) + \bar\theta\bar\theta(2\theta^\beta\sigma^m_{\beta\dot\alpha}\,\partial_m\lambda_\alpha + i\theta\theta\sigma^m_{\alpha\dot\alpha}\partial_m(D - i\,\partial_m v^m)).\end{aligned} \tag{23}$$

The next task is to calculate the products of the terms above. In the product below, we have omitted from the beginning those terms with $\bar\theta\bar\theta$ because there is a $\bar\theta$ in each term.

$$\begin{aligned}\frac{1}{2}C^{\alpha\beta}Q_\alpha V Q_\beta V &= \frac{1}{2}C^{\alpha\beta}(-\sigma^m_{\alpha\dot\alpha}\bar\theta^{\dot\alpha}v_m + 2i\theta_\alpha(\bar\theta\bar\lambda))(-\sigma^n_{\beta\dot\beta}\bar\theta^{\dot\beta}v_n + 2i\theta_\beta(\bar\theta\bar\lambda))\\ &= \frac{1}{4}C^{\alpha\beta}\epsilon^{\dot\alpha\dot\beta}\sigma^m_{\alpha\dot\alpha}\sigma^n_{\beta\dot\beta}v_m v_n\bar\theta\bar\theta + \frac{i}{2}C^{\alpha\beta}\theta_\beta\sigma^m_{\alpha\dot\alpha}[v_m,\bar\lambda^{\dot\alpha}]\bar\theta\bar\theta\\ &= \left(\frac{1}{2}C^{mn}v_m v_n - \frac{i}{2}C^{\alpha\beta}\sigma^m_{\alpha\dot\alpha}\theta_\beta[v_m,\bar\lambda^{\dot\alpha}]\right)\bar\theta\bar\theta,\end{aligned} \tag{24}$$

where we have used the identity $C^{mn} = 1/2\,C^{\alpha\beta}\epsilon^{\dot\alpha\dot\beta}\sigma^m_{\alpha\dot\alpha}\sigma^n_{\beta\dot\beta}$, following the conventions of Ref. 8. Continuing to compute the products, since every term has a θ this time, we can ignore the $\theta\theta$ terms from the outset:

$$\frac{1}{2}\bar{C}^{\alpha\dot{\beta}}\bar{Q}_{\dot{\alpha}}V\bar{Q}_{\dot{\beta}}V=\frac{1}{2}\bar{C}^{\alpha\dot{\beta}}(-\theta^{\alpha}\sigma^{m}_{\alpha\dot{\alpha}}v_m-2i\bar{\theta}_{\dot{\alpha}}\theta\lambda)(-\theta^{\beta}\sigma^{n}_{\beta\dot{\beta}}v_n-2i\bar{\theta}_{\dot{\beta}}\theta\lambda)$$

$$=-\frac{1}{4}\bar{C}^{\alpha\dot{\beta}}\epsilon^{\beta\alpha}\sigma^{m}_{\alpha\dot{\beta}}\sigma^{n}_{\beta\dot{\alpha}}v_mv_n\theta\theta-\frac{i}{2}\bar{C}^{\alpha\dot{\beta}}\bar{\theta}_{\dot{\beta}}\sigma^{m}_{\alpha\dot{\alpha}}[v_m,\lambda^{\alpha}]\theta\theta$$

$$=\left(\frac{1}{2}\bar{C}^{mn}v_mv_n+\frac{i}{2}\bar{C}^{\alpha\dot{\beta}}\sigma^{m}_{\alpha\dot{\alpha}}\bar{\theta}_{\dot{\beta}}[v_m,\lambda^{\alpha}]\right)\theta\theta, \tag{25}$$

where we identified $\bar{C}^{mn}=-1/2\,\bar{C}^{\alpha\dot{\beta}}\epsilon^{\alpha\beta}\sigma^{m}_{\alpha\dot{\alpha}}\sigma^{n}_{\beta\dot{\beta}}$ following Ref. 11. Next, consider the second order in deformation parameter terms:

$$\frac{1}{8}C^{\alpha\beta}C^{\gamma\delta}(Q_{\alpha}Q_{\gamma}V)(Q_{\delta}Q_{\beta}V)=\frac{1}{8}C^{\alpha\beta}C^{\gamma\delta}\epsilon_{\alpha\gamma}\epsilon_{\beta\delta}(2i\bar{\theta}\bar{\lambda}+\bar{\theta}\bar{\theta}(D-i\,\partial_mv^m))^2$$

$$=-\frac{1}{8}|C|^2\bar{\lambda}\bar{\lambda}\bar{\theta}\bar{\theta},$$

where we use $|C|^2=4C^{\alpha\beta}C^{\gamma\delta}\epsilon_{\alpha\gamma}\epsilon_{\delta\beta}$. Similarly, we find that the next term is easily calculated due to a sizable cancellation, since we may omit a $\theta\theta$ term from the start:

$$\frac{1}{8}\bar{C}^{\dot{\alpha}\beta}\bar{C}^{\dot{\gamma}\dot{\delta}}(\bar{Q}_{\dot{\alpha}}\bar{Q}_{\dot{\gamma}}V)(\bar{Q}_{\dot{\delta}}\bar{Q}_{\beta}V)=\frac{1}{8}\bar{C}^{\dot{\alpha}\beta}\bar{C}^{\dot{\gamma}\dot{\delta}}\epsilon_{\dot{\alpha}\dot{\gamma}}\epsilon_{\beta\dot{\delta}}(-2i\theta\lambda)^2$$

$$=-\frac{1}{8}|\bar{C}|^2\lambda\lambda\,\theta\theta,$$

where we use $|\bar{C}|^2=4\bar{C}^{\dot{\alpha}\beta}\bar{C}^{\dot{\gamma}\dot{\delta}}\epsilon_{\dot{\alpha}\dot{\gamma}}\epsilon_{\beta\dot{\delta}}$. The remaining term to consider in $V*V$ is $1/4\,C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}}[(\bar{Q}_{\dot{\alpha}}Q_{\alpha}V)(\bar{Q}_{\dot{\beta}}Q_{\beta}V)-(Q_{\alpha}\bar{Q}_{\dot{\alpha}}V)(Q_{\beta}\bar{Q}_{\dot{\beta}}V)]$. We calculate

$$\frac{1}{4}C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}}((\bar{Q}_{\dot{\alpha}}Q_{\alpha}V)(\bar{Q}_{\dot{\beta}}Q_{\beta}V)-(Q_{\alpha}\bar{Q}_{\dot{\alpha}}V)(Q_{\beta}\bar{Q}_{\dot{\beta}}V))$$

$$=\frac{1}{4}C^{\alpha\beta}\bar{C}^{\dot{\alpha}\dot{\beta}}(\sigma^{m}_{\alpha\dot{\alpha}}\{v_m,4i(\bar{\theta}^{\dot{\beta}}\lambda_{\beta}-\theta^{\beta}\bar{\lambda}_{\dot{\beta}})\}-2i\sigma^{m}_{\alpha\dot{\alpha}}\{v_m,\partial_lv_k(\theta^{\gamma}\sigma^{l}_{\gamma\dot{\beta}}\sigma^{k}_{\beta\dot{\gamma}}\bar{\theta}^{\dot{\gamma}}+\theta^{\beta}\epsilon^{\sigma\gamma}\sigma^{l}_{\delta\dot{\beta}}\sigma^{k}_{\gamma\dot{\gamma}}\bar{\theta}^{\dot{\gamma}})\}$$

$$+2\sigma^{m}_{\alpha\dot{\alpha}}\bar{\theta}\bar{\theta}\sigma^{l}_{\gamma\dot{\beta}}\{v_m,\theta^{\gamma}\,\partial_l\lambda_{\beta}-\theta^{\beta}\,\partial_l\lambda^{\gamma}\}-2\sigma^{m}_{\alpha\dot{\alpha}}\theta\theta\sigma^{l}_{\beta\dot{\beta}}\{v_m,\partial_l(\bar{\theta}\bar{\lambda})\}+i\sigma^{m}_{\alpha\dot{\alpha}}\theta\theta\bar{\theta}\bar{\theta}\sigma^{l}_{\beta\dot{\beta}}\{v_m,\partial_l(D$$

$$-i\partial_mv^m)\}-4\theta_{\alpha}\theta^{\gamma}\sigma^{m}_{\gamma\dot{\beta}}\sigma^{n}_{\beta\dot{\gamma}}\bar{\theta}^{\dot{\gamma}}\{\bar{\lambda}_{\dot{\alpha}},\partial_mv_n\}+4\bar{\theta}_{\dot{\alpha}}\theta^{\gamma}\sigma^{m}_{\gamma\dot{\beta}}\sigma^{n}_{\beta\dot{\gamma}}\bar{\theta}^{\dot{\gamma}}\{\lambda_{\alpha},\partial_mv_n\}+4i\theta_{\alpha}\bar{\theta}\bar{\theta}\theta^{\gamma}\sigma^{m}_{\gamma\dot{\beta}}\{\bar{\lambda}_{\dot{\alpha}},\partial_m\lambda_{\beta}\}$$

$$+4i\theta_{\alpha}\theta\theta\theta^{\gamma}\sigma^{m}_{\beta\dot{\beta}}\{\lambda_{\alpha},\partial_m\bar{\lambda}_{\dot{\gamma}}\}-4i\theta_{\alpha}\bar{\theta}_{\dot{\alpha}}\theta^{\gamma}\sigma^{m}_{\gamma\dot{\beta}}\sigma^{n}_{\beta\dot{\gamma}}\bar{\theta}^{\dot{\gamma}}\{(D-i\,\partial_mv^m),\partial_mv_n\}$$

$$-4\theta^{\gamma}\bar{\theta}^{\dot{\gamma}}\theta^{\sigma}\bar{\theta}^{\dot{\sigma}}\sigma^{k}_{\gamma\dot{\sigma}}\sigma^{l}_{\alpha\dot{\gamma}}\sigma^{m}_{\sigma\dot{\beta}}\sigma^{n}_{\beta\dot{\sigma}}\partial_kv_l\partial_mv_n). \tag{26}$$

We can see from the expression above the full second-order calculations will be lengthy. Additionally, we would have to deal with the nonassociativity of the star product. At present, the author has only calculated portions of the theory to the second order, mostly for the purpose of comparing the present work with Ref. 8. We leave the complete development of the second-order deformed gauge theory to a later paper.

We shall now find the correction to $V*V*V$ to the first order in $C^{\alpha\beta}$. First, recall first that in the commutative theory, V^3 is zero in the Wess–Zumino gauge. Thus, any nontrivial term in $V*V*V$ must arise from the deformation

$$V*(V*V)=V(V*V)-\frac{1}{2}C^{\alpha\beta}(Q_\alpha V)Q_\beta(V*V)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}(\bar{Q}_{\dot{\alpha}}V)\bar{Q}_{\dot{\beta}}(V*V). \tag{27}$$

We can replace $V*V$ with V^2 as we are looking for the first order in $C^{\alpha\beta}$ terms:

$$V*(V*V)=V(V*V)-\frac{1}{2}C^{\alpha\beta}(Q_\alpha V)Q_\beta(V^2)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}(\bar{Q}_{\dot{\alpha}}V)\bar{Q}_{\dot{\beta}}(V^2)=V(V*V). \tag{28}$$

The two terms vanish because $Q_\alpha V$ and $\bar{Q}_{\dot{\alpha}}V$ have a $\bar{\theta}$ and θ in each term, respectively, while $Q_\beta(V^2)$ and $\bar{Q}_{\dot{\beta}}(V^2)$ are proportional to $\bar{\theta}\bar{\theta}$ and $\theta\theta$, respectively. To the first order, we have

$$V*(V*V)=\left(-\theta\sigma^m\bar{\theta}v_m+i\theta\theta\bar{\theta}\bar{\lambda}-i\bar{\theta}\bar{\theta}\theta\lambda+\frac{1}{2}\theta\theta\bar{\theta}\bar{\theta}(D-i\,\partial_m v^m)\right)(V*V). \tag{29}$$

Now, if we examine the first-order terms in $V*V$, we notice that each term either has $\theta\theta$ or $\bar{\theta}\bar{\theta}$; thus, the product with V that is proportional to θ and $\bar{\theta}$ vanishes. Therefore, to the first order in the deformation parameter,

$$V*(V*V)=0. \tag{30}$$

It is not hard to see that this extends to higher star products. Thus, $(V)_*^n=0$ for $n\geqslant 3$ to the first order in the deformation parameter. That is, to the first order in C, we have $e^V=1+V+1/2\,V*V$. This is nice but it will clearly be spoiled if we include the second-order terms. For example, if one examines the mixed second-order term, Eq. (26), the first few lines have only θ or $\bar{\theta}$. Hence, in the product with V they will not vanish like the first-order case, thus generating a nontrivial term in $V*(V*V)$. We will not complete the development of e^V to the second order in this paper. Next, we shall show that in the limit of $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$, we recover the terms found by Seiberg in Ref. 8.

Collecting the results of this section, we find that the star exponential of V in the canonical Wess–Zumino gauge is

$$\begin{aligned}e^V=1+V+\frac{1}{2}V*V=1&-\theta\sigma^m\bar{\theta}v_m+i\theta\theta\bar{\theta}\bar{\lambda}-i\bar{\theta}\bar{\theta}\theta^\alpha\lambda_\alpha+\frac{1}{2}\theta\theta\bar{\theta}\bar{\theta}(D-i\,\partial_m v^m)\\&-\left(\frac{1}{4}C^{mn}v_m v_n+\frac{i}{4}C^{\alpha\beta}\theta_\beta\sigma^m_{\alpha\dot{\alpha}}[\bar{\lambda}^{\dot{\alpha}},v_m]\right)\bar{\theta}\bar{\theta}-\left(\frac{1}{4}\bar{C}^{mn}v_m v_n+\frac{i}{4}\bar{C}^{\dot{\alpha}\dot{\beta}}\bar{\theta}_{\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}[v_m,\lambda^\alpha]\right)\theta\theta\\&-\frac{1}{16}|C|^2\bar{\lambda}\bar{\lambda}\bar{\theta}\bar{\theta}-\frac{1}{16}|\bar{C}|^2\lambda\lambda\theta\theta+\textit{other second-order terms containing }\bar{C}^{\dot{\alpha}\dot{\beta}}.\end{aligned} \tag{31}$$

B. $N=0$ verses $N=1/2$ star exponentials

To compare with the $N=1/2$ construction, we make the following dictionary:

$$\begin{aligned}m&\mapsto\mu\\v_m&\mapsto A_\mu\\\bar{\lambda}_{\dot{\alpha}}&\mapsto\bar{\lambda}_{\dot{\alpha}}\\\lambda_\alpha&\mapsto\lambda_\alpha+\frac{1}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^\mu_{\gamma\dot{\gamma}}\{\bar{\lambda}^{\dot{\gamma}},A_\mu\}\end{aligned} \tag{32}$$

$$(D - i\,\partial_m v^m) \mapsto D - i\,\partial_\mu A^\mu.$$

We use Greek indices for Euclidean spacetime and Latin indices for Minkowski spacetime. In Ref. 8, only products of θ were deformed. It is clear that we can recover this deformation by setting $\bar{C}^{\dot{\alpha}\dot{\beta}}$ to zero wherever it occurs. Using the dictionary and setting $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$, we have

$$\begin{aligned} e^V &= 1 + V + \frac{1}{2} V * V \\ &= 1 - \theta\sigma^\mu\bar{\theta}A_\mu + i\theta\theta\bar{\theta}\bar{\lambda} - i\bar{\theta}\bar{\theta}\theta^\alpha\left(\lambda_\alpha + \frac{1}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^\mu_{\gamma\dot{\gamma}}\{\bar{\lambda}^{\dot{\gamma}}, A_\mu\}\right) \\ &\quad + \frac{1}{2}\theta\theta\bar{\theta}\bar{\theta}(D - i\,\partial_\mu A^\mu) - \frac{1}{4}C^{\mu\nu}A_\mu A_\nu\bar{\theta}\bar{\theta} - \frac{i}{4}C^{\alpha\beta}\theta_\beta\sigma^\mu_{\alpha\dot{\alpha}}[A_\mu, \bar{\lambda}^{\dot{\alpha}}]\bar{\theta}\bar{\theta} - \frac{1}{16}|C|^2\bar{\lambda}\bar{\lambda}\bar{\theta}\bar{\theta}. \end{aligned} \tag{33}$$

This is precisely the exponential that Seiberg found on noncommutative Euclidean superspace in Ref. 8. This demonstrates again that the deformed Minkowski superspace of Ref. 11 truly is a natural extension of the $N=1/2$ theory to the Minkowski case.

III. GAUGE THEORY ON $N=0$ MINKOWSKI SUPERSPACE

In this section, we generalize super Yang–Mills theory to deformed Minkowski superspace. Most of the usual constructions hold and the approach is similar to Seiberg's $N=1/2$ super-Yang Mills theory in Ref. 8. We simply replace products in Ref. 14 with star products. The main subtlety is finding the correct parametrization of the vector superfield.

A. Gauge transformations

Our goal is to find a way to embed the usual C-independent gauge transformations into superfield equations on noncommutative Minkowski superspace. Since our spinors are built on Minkowski space, we are forced to relate θ and $\bar{\theta}$ by conjugation. This means that we cannot directly follow the construction of Ref. 8. In Ref. 8, we can see that $\overline{\theta^\alpha} \neq \bar{\theta}^{\dot{\alpha}}$, $\bar{V} \neq V$, and $\overline{\Lambda + \bar{\Lambda}} \neq \Lambda + \bar{\Lambda}$. These relations are sensible for Seiberg, who wrote them in a Euclidean superspace. On Minkowski space, these inequalities must become equalities. We will find that these reality conditions and the requirement that we recover $N=1/2$ theory in the $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$ limit almost uniquely fixes this construction.

Non-Abelian gauge transformations on the vector superfield are embedded into the following superfield equation on noncommutative Minkowski superspace:

$$e^V \mapsto e^{V\prime} = e^{-i\bar{\Lambda}} * e^V * e^{i\Lambda}. \tag{34}$$

This is the natural modification of the standard theory (see Ref. 14, for example). Infinitesimally, we have

$$\delta e^V = -i\bar{\Lambda} * e^V + i e^V * \Lambda. \tag{35}$$

The component fields of the vector superfield should transform in the adjoint representation of the gauge group as in the standard gauge theory. That is, under an infinitesimal gauge transformation, we should have

$$\begin{aligned} \delta v_m &= -2\,\partial_m\phi + i[\phi, v_m], \\ \delta\lambda_\alpha &= i[\phi, \lambda_\alpha], \end{aligned} \tag{36}$$

$$\delta D = i[\phi, D].$$

Our goal now is to find a suitable parametrization of the gauge parameter Λ and the vector superfield V such that Eq. (36) is embedded into Eq. (35). It is not surprising that the canonical Wess–Zumino gauge [Eq. (31)] does not work in the $N=0$ case, since it was also necessary for Ref. 8 to shift the λ component in the $N=1/2$ case. The reality of V requires that we cannot shift only λ; we must also shift $\bar{\lambda}$. To be precise, $\lambda \mapsto \lambda + A$ and $\bar{\lambda} \mapsto \bar{\lambda} + B$. We now determine what choice of A and B will preserve the reality of V while concurrently embedding Eq. (36). To the first order in C, we find under the above redefinitions that Eq. (31) becomes

$$e^V = 1 - \theta\sigma^m\bar{\theta}v_m - \frac{1}{4}\bar{C}^{mn}v_m v_n\theta\theta + \frac{1}{4}C^{mn}v_m v_n\bar{\theta}\bar{\theta} + \frac{1}{2}(D - i\,\partial_m v^m)\theta\theta\bar{\theta}\bar{\theta}$$
$$+ \bar{\theta}\bar{\theta}\theta^\alpha\left(-i\lambda_\alpha - iA + \frac{i}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot{\alpha}}[v_m, \bar{\lambda}^{\dot{\alpha}}]\right) + \theta\theta\bar{\theta}^{\dot{\alpha}}\left(-i\bar{\lambda}_{\dot{\alpha}} - iB - \frac{i}{4}\epsilon_{\dot{\alpha}\dot{\beta}}\bar{C}^{\dot{\beta}\dot{\gamma}}\sigma^m_{\alpha\dot{\gamma}}[v_m, \lambda^\alpha]\right). \tag{37}$$

Additionally, we make a C-dependent shift of the gauge parameter Λ similar to that of Ref. 8. For the moment, let us make a reasonably general ansatz for the gauge parameter in terms of a variable p:

$$\Lambda_p = -\phi + ip\,\theta\sigma^m\bar{\theta}\,\partial_m\phi + \frac{i}{2}\theta\theta\bar{C}^{mn}\{v_n, \partial_m\phi\} - (p+1)\,\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi$$
$$\bar{\Lambda}_p = -\phi + i(2-p)\,\theta\sigma^m\bar{\theta}\,\partial_m\phi - \frac{i}{2}\bar{\theta}\bar{\theta}C^{mn}\{\partial_m\phi, v_n\} - (p+1)\,\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi, \tag{38}$$

where everything is a function of y in the above. Notice that modulo the higher θ components in Λ, this reduces to the choice of gauge parameter in Ref. 8 when $p=0$. We now determine which choice of p will embed Eq. (36) in Eq. (35). We calculate that the $\bar{\theta}\bar{\theta}\theta^\alpha$ term on the rhs of Eq. (35) is

$$[\phi, \lambda_\alpha] + [\phi, A] - \frac{1}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot{\alpha}}([\phi, [\bar{\lambda}^{\dot{\alpha}}, v_m]] - 2i(p\bar{\lambda}^{\dot{\alpha}}\,\partial_m\phi + (2-p)\partial_m\phi\,\bar{\lambda}^{\dot{\alpha}})). \tag{39}$$

Similarly, the $\theta\theta\bar{\theta}^{\dot{\alpha}}$ term on the rhs of Eq. (35) is

$$[\phi, \bar{\lambda}_{\dot{\alpha}}] + [\phi, B] + \frac{1}{4}\bar{\epsilon}_{\dot{\alpha}\dot{\beta}}\bar{C}^{\dot{\beta}\dot{\gamma}}\sigma^m_{\alpha\dot{\gamma}}([\phi, [\lambda^\alpha, v_m]] + 2i(p\lambda^\alpha\,\partial_m\phi + (2-p)\partial_m\phi\lambda^\alpha)). \tag{40}$$

The $\bar{\theta}\bar{\theta}\theta^\alpha$ component of the lhs of Eq. (35) is

$$-i\,\delta\lambda_\alpha - i\,\delta A + \frac{i}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot{\alpha}}\delta[\bar{\lambda}^{\dot{\alpha}}, v_m]. \tag{41}$$

Similarly, the $\theta\theta\bar{\theta}^{\dot{\alpha}}$ component of the lhs of Eq. (35) is

$$-i\,\delta\bar{\lambda}_{\dot{\alpha}} - i\,\delta B - \frac{i}{4}\bar{\epsilon}_{\dot{\alpha}\dot{\beta}}\bar{C}^{\dot{\beta}\dot{\gamma}}\sigma^m_{\alpha\dot{\gamma}}\delta[\lambda^\alpha, v_m]. \tag{42}$$

It is not difficult to show [applying Eq. (36)] that

$$i\delta[\lambda^\alpha, v_m] + [\phi, [\lambda^\alpha, v_m]] = -2i[\lambda^\alpha, \partial_m\phi],$$
$$i\delta[\bar{\lambda}^{\dot{\alpha}}, v_m] + [\phi, [\bar{\lambda}^{\dot{\alpha}}, v_m]] = 2i[\bar{\lambda}^{\dot{\alpha}}, \partial_m\phi],$$
$$i\delta\{\bar{\lambda}^{\dot{\alpha}}, v_m\} + [\phi, \{\bar{\lambda}^{\dot{\alpha}}, v_m\}] = 2i\{\bar{\lambda}^{\dot{\alpha}}, \partial_m\phi\}, \tag{43}$$

$$i\delta(v_m\lambda^\alpha)+[\phi,v_m\lambda^\alpha]=2i\partial_m\phi\lambda^\alpha,$$
$$i\delta(\bar\lambda^{\dot\alpha}v_m)+[\phi,\bar\lambda^{\dot\alpha}v_m]=2i\bar\lambda^{\dot\alpha}\partial_m\phi.$$

Next, equate Eq. (41) and Eq. (39). Then require that $\delta\lambda^\alpha=i[\phi,\lambda^\alpha]$ so that Eq. (43) holds. Some terms cancel and we find that

$$-i\,\delta A-[\phi,A]=\frac{i}{2}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}((p+1)\bar\lambda^{\dot\alpha}\partial_m\phi+(1-p)\partial_m\phi\,\bar\lambda^{\dot\alpha}). \tag{44}$$

Likewise, equate Eq. (42) and Eq. (40). Then require that $\delta\bar\lambda^{\dot\alpha}=i[\phi,\bar\lambda^{\dot\alpha}]$ so that Eq. (43) holds. Some terms cancel, and we find that

$$-i\,\delta B-[\phi,B]=\frac{i}{2}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}((p-1)\lambda^\alpha\,\partial_m\phi+(3-p)\partial_m\phi\,\lambda^\alpha). \tag{45}$$

When $p=0$, we find that Eq. (44) becomes

$$-i\,\delta A-[\phi,A]=\frac{i}{2}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}\{\bar\lambda^{\dot\alpha},\partial_m\phi\}. \tag{46}$$

Hence, in view of Eq. (43), we can see why Ref. 8 shifted the λ_α component of the vector multiplet by $A=1/4\,\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}\{\bar\lambda^{\dot\alpha},v_m\}$. If we tried to use this choice of gauge parameter, we would destroy the reality of V because Eq. (45) would lead us to choose $B=1/4\,\bar\epsilon_{\dot\alpha\dot\beta}\bar C^{\dot\beta\dot\gamma}\sigma^m_{\alpha\dot\gamma}$ $(-\lambda^\alpha v_m+3v_m\lambda^\alpha)$. The correct choice is $p=1$. With this choice of gauge parameter, we find the following conditions for A and B from Eq. (44) and Eq. (45):

$$\begin{aligned}-i\,\delta A-[\phi,A]&=i\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}\bar\lambda^{\dot\alpha}\,\partial_m\phi\\ -i\,\delta B-[\phi,B]&=i\bar\epsilon_{\dot\alpha\dot\beta}\bar C^{\dot\beta\dot\gamma}\sigma^m_{\alpha\dot\gamma}\,\partial_m\phi\,\lambda^\alpha.\end{aligned} \tag{47}$$

These conditions are satisfied by

$$\begin{aligned}A&=\frac{1}{2}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}\bar\lambda^{\dot\alpha}v_m\\ B&=\frac{1}{2}\bar\epsilon_{\dot\alpha\dot\beta}\bar C^{\dot\beta\dot\gamma}\sigma^m_{\alpha\dot\gamma}v_m\lambda^\alpha.\end{aligned} \tag{48}$$

It is easy to see that $\bar A=B$ and $\bar B=A$, which is necessary in order to preserve $\bar V=V$. This is the only parametrization of the vector superfield and gauge parameter for noncommutative Minkowski superspace if we wish to stay in a generalized Wess Zumino gauge. In principle, we could use the other lower θ components of the vector superfield to do more complicated shifts. Fortunately, we will not need to do that. Define the vector superfield to be

$$\begin{aligned}V(y)=&-\theta\sigma^m\bar\theta v_m+\theta\theta\bar\theta^{\dot\alpha}\left(-i\bar\lambda_{\dot\alpha}+\frac{i}{2}\bar\epsilon_{\dot\alpha\dot\beta}\bar C^{\dot\beta\dot\gamma}\sigma^m_{\alpha\dot\gamma}v_m\lambda^\alpha\right)+\bar\theta\bar\theta\theta^\alpha\left(-i\lambda_\alpha-\frac{i}{2}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot\alpha}\bar\lambda^{\dot\alpha}v_m\right)\\ &+\frac{1}{2}\theta\theta\bar\theta\bar\theta(D-i\,\partial_m v^m).\end{aligned} \tag{49}$$

It should be evident from the calculations in this section that this parametrization of V embeds Eq. (36) in Eq. (35) while maintaining the reality of V. This, of course, requires that we define the gauge parameters as functions of y to be

$$\Lambda(y) = -\phi + i\theta\sigma^m\bar{\theta}\,\partial_m\phi + \frac{i}{2}\theta\theta\bar{C}^{mn}\{v_n,\partial_m\phi\} - 2\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi$$

$$\bar{\Lambda}(y) = -\phi + i\theta\sigma^m\bar{\theta}\,\partial_m\phi - \frac{i}{2}\bar{\theta}\bar{\theta}C^{mn}\{\partial_m\phi,v_n\} - 2\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi. \tag{50}$$

For the remainder of this paper, we will assume that the vector superfield is parametrized as in Eq. (49) and that the gauge parameter is parametrized as in Eq. (50). Explicitly in this parametrization, to the first order in C, Eq. (31) becomes

$$e^V = 1 - \theta\sigma^m\bar{\theta}v_m - \frac{1}{4}\bar{C}^{mn}v_mv_n\theta\theta + \frac{1}{4}C^{mn}v_mv_n\bar{\theta}\bar{\theta} + \frac{1}{2}(D - i\,\partial_m v^m)\,\theta\theta\bar{\theta}\bar{\theta}$$
$$+ \bar{\theta}\bar{\theta}\theta^\alpha\left(-i\lambda_\alpha - \frac{i}{4}\epsilon_{\alpha\beta}C^{\beta\gamma}\sigma^m_{\gamma\dot{\alpha}}\{\bar{\lambda}^{\dot{\alpha}},v_m\}\right) + \theta\theta\bar{\theta}^{\dot{\alpha}}\left(-i\bar{\lambda}_{\dot{\alpha}} - \frac{i}{4}\epsilon_{\dot{\alpha}\dot{\beta}}\bar{C}^{\dot{\beta}\dot{\gamma}}\sigma^m_{\alpha\dot{\gamma}}\{\lambda^\alpha,v_m\}\right). \tag{51}$$

The $\bar{\theta}\bar{\theta}\theta^\alpha$ and $\theta\theta\bar{\theta}^{\dot{\alpha}}$ components in the previous equation stand in contrast to what might be naively expected from $N=1/2$ theory.

B. Spinor superfields

Again, we will construct these as in the commutative theory except that everywhere that we had a product in the commutative theory, we place a star product here. Define

$$W_\alpha = -\frac{1}{4}\bar{D}_{\dot{\alpha}} * \bar{D}^{\dot{\alpha}} * e^{-V} * D_\alpha * e^V. \tag{52}$$

Conveniently, in chiral coordinates $y^m = x^m + i\theta\sigma^m\bar{\theta}$, several of the star products in the above are ordinary products. Thus,

$$W_\alpha = -\frac{1}{4}\bar{D}_{\dot{\alpha}}\bar{D}^{\dot{\alpha}}e^{-V} * D^\alpha * e^V. \tag{53}$$

Likewise, define

$$\bar{W}_{\dot{\alpha}} = -\frac{1}{4}D^\alpha * D_\alpha * e^{-V} * \bar{D}_{\dot{\alpha}} * e^V. \tag{54}$$

Similarly, in antichiral coordinates $\bar{y}^m = x^m - i\theta\sigma^m\bar{\theta}$, the above simplifies to

$$\bar{W}_{\dot{\alpha}} = -\frac{1}{4}D^\alpha D_\alpha e^{-V} * \bar{D}_{\dot{\alpha}} * e^V. \tag{55}$$

We must determine the component field content of W_α and $\bar{W}_{\dot{\alpha}}$. Referring to Eq. (51) and keeping only up to the first order in C, we obtain

$$W_\alpha = W_\alpha(C=0) + \theta\theta\left(\frac{1}{2}\bar{C}^{mn}\{F_{mn},\lambda_\alpha\} + \bar{C}^{mn}\left\{v_n,\mathcal{D}_m\lambda_\alpha - \frac{i}{4}[v_m,\lambda_\alpha]\right\}\right) + C^{\gamma\beta}\epsilon_{\beta\alpha}\theta_\gamma\bar{\lambda}\bar{\lambda}, \tag{56}$$

where, following Wess and Bagger's conventions in Ref. 14, the field strength and covariant derivative of the gaugino are

$$F_{mn} = \partial_m v_n - \partial_n v_m + \frac{i}{2}[v_m,v_n] \tag{57}$$

$$\mathcal{D}_m\lambda_\alpha = \partial_m\lambda_\alpha + \frac{i}{2}[v_m,\lambda_\alpha].$$

Additionally, the spinor superfield of ordinary superspace is

$$W_\alpha(C=0) = -i\lambda_\alpha + \theta_\alpha D - \sigma_\alpha^{mn\beta}\theta_\beta F_{mn} + \theta\theta\sigma^m_{\alpha\dot\beta}\mathcal{D}_m\bar\lambda^{\dot\beta}. \tag{58}$$

Notice that when we set $\bar C^{\dot\alpha\dot\beta}=0$, we recover the result of Seiberg Ref. 8 for W_α. Likewise, we find that

$$\bar W_{\dot\alpha} = \bar W_{\dot\alpha}(C=0) + \bar\theta\bar\theta\left(\frac{1}{2}C^{mn}\{F_{mn},\bar\lambda_{\dot\alpha}\} + C^{mn}\left\{v_n,\mathcal{D}_m\bar\lambda_{\dot\alpha} - \frac{i}{4}[v_m,\bar\lambda_{\dot\alpha}]\right\}\right) + \bar C^{\dot\gamma\dot\beta}\epsilon^{\dot\beta\dot\alpha}\bar\theta_{\dot\gamma}\lambda\lambda, \tag{59}$$

where

$$\bar W_{\dot\alpha}(C=0) = i\bar\lambda_{\dot\alpha} + \bar\theta_{\dot\alpha}D - \sigma_{\dot\alpha}^{mn\dot\beta}\bar\theta_{\dot\beta}F_{mn} + \bar\theta\bar\theta\bar\sigma^{m\dot\alpha\beta}\mathcal{D}_m\lambda^\beta. \tag{60}$$

Again, we reproduce the result of Ref. 8 upon setting $\bar C^{\dot\alpha\dot\beta}=0$.

The spinor superfield transforms as in the commutative theory. From the non-Abelian gauge transformation [Eq. (34)], it follows that

$$W_\alpha \mapsto W'_\alpha = e^{-i\bar\Lambda} * W_\alpha * e^{i\Lambda}. \tag{61}$$

This can be shown by modifying the calculation used in the commutative theory. We simply change products to star products and utilize the algebra given in Eq. (15).

IV. CHIRAL AND ANTICHIRAL SUPERFIELDS

Chiral (Φ) and antichiral ($\bar\Phi$) superfields are defined as usual:

$$\bar D_{\dot\alpha} * \Phi = 0, \quad D_\alpha * \bar\Phi = 0. \tag{62}$$

The stars deform any multiplications that result. However, as $D_\alpha=\partial_\alpha$ in the chiral coordinates $y^\mu=x^\mu+i\theta\sigma^m\bar\theta$ and $\bar D_{\dot\alpha}=\partial_{\dot\alpha}$ in the antichiral coordinates $\bar y^\mu=x^\mu-i\theta\sigma^m\bar\theta$, we find that the star products are ordinary products. Consequently, we find the well-known solutions,

$$\begin{aligned}\Phi(y,\theta) &= A(y) + \sqrt{2}\theta\psi(y) + \theta\theta F(y),\\ \bar\Phi(\bar y,\bar\theta) &= \bar A(\bar y) + \sqrt{2}\bar\theta\bar\psi(\bar y) + \bar\theta\bar\theta\bar F(\bar y).\end{aligned} \tag{63}$$

These solutions follow from the chain rule as in the standard commutative theory. This construction need not be modified on noncommutative Minkowski superspace because the anticommutation relations given in Eq. (15) are unspoiled by the deformation.

A. Parametrizing the chiral and antichiral superfields

The matter fields in the Wess–Zumino model should transform in the fundamental and antifundamental representations of the gauge group. This is naturally embedded into the following superfield equation written on noncommutative Minkowski superspace (as Araki, Ito, and Ohtsuka did for the Euclidean case in Ref. 15),

$$\Phi \mapsto \Phi' = e^{-i\Lambda} * \Phi, \qquad \bar\Phi \mapsto \bar\Phi' = \bar\Phi * e^{i\bar\Lambda}. \tag{64}$$

Infinitesimally, we have

$$\delta\Phi = -i\Lambda * \Phi, \qquad \delta\bar{\Phi} = i\bar{\Phi} * \bar{\Lambda}. \tag{65}$$

At the level of component fields, Eq. (65) should embed

$$\begin{aligned} \delta A(y) &= i\phi A(y), & \delta\bar{A}(\bar{y}) &= -i\bar{A}\phi(\bar{y}) \\ \delta\psi(y) &= i\phi\psi(y), & \delta\bar{\psi}(\bar{y}) &= -i\bar{\psi}\phi(\bar{y}) \\ \delta F(y) &= i\phi F(y), & \delta\bar{F}(\bar{y}) &= -i\bar{F}\phi(\bar{y}). \end{aligned} \tag{66}$$

It was necessary for Ref. 15 to shift the $\bar{F}$ term in $\bar{\Phi}$ to maintain the usual C-independent gauge transformations on the component fields. Similarly, we must modify both Φ and $\bar{\Phi}$ from the canonical form given in Eq. (63),

$$\begin{aligned} \Phi(y) &= A + \sqrt{2}\theta\psi + \theta\theta(F + \eta), \\ \bar{\Phi}(\bar{y}) &= \bar{A} + \sqrt{2}\bar{\theta}\bar{\psi} + \bar{\theta}\bar{\theta}(\bar{F} + \beta), \end{aligned} \tag{67}$$

where the shifts η and β must be chosen as to embed Eq. (66) in Eq. (65). Now Λ and $\bar{\Lambda}$ were given in Eq. (50), however, it will be convenient to view $\bar{\Lambda}$ as a function of $\bar{y}$ for this section:

$$\begin{aligned} \Lambda(y) &= -\phi + i\theta\sigma^m\bar{\theta}\,\partial_m\phi + \frac{i}{2}\theta\theta\bar{C}^{mn}\{v_n, \partial_m\phi\} - 2\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi, \\ \bar{\Lambda}(\bar{y}) &= -\phi - i\theta\sigma^m\bar{\theta}\,\partial_m\phi - \frac{i}{2}\bar{\theta}\bar{\theta}C^{mn}\{\partial_m\phi, v_n\} - 2\theta\theta\bar{\theta}\bar{\theta}\,\partial^2\phi. \end{aligned} \tag{68}$$

The $\theta\theta$ coefficient in Eq. (65) yields

$$\delta F + \delta\eta = i\phi F + i\phi\eta - 2i\bar{C}^{mn}\,\partial_m\phi\,\partial_n A + \frac{1}{2}\bar{C}^{mn}\{v_n, \partial_m\phi\}A. \tag{69}$$

Likewise, the $\bar{\theta}\bar{\theta}$ coefficient in Eq. (65) yields

$$\delta\bar{F} + \delta\beta = -i\bar{F}\phi - i\beta\phi - 2iC^{mn}\partial_n\bar{A}\,\partial_m\phi + \frac{1}{2}C^{mn}\bar{A}\{\partial_m\phi, v_n\}. \tag{70}$$

If we require that Eq. (66) holds, we then find that the following condition on β from Eq. (70) is

$$\delta\beta - i\phi\beta = -2iC^{mn}\,\partial_n\bar{A}\partial_m\phi + \frac{1}{2}C^{mn}\bar{A}\{\partial_m\phi, v_m\}. \tag{71}$$

Similarly, we find that the following condition on η from Eq. (69) is

$$\delta\eta - i\phi\eta = -2i\bar{C}^{mn}\partial_m\phi\,\partial_n A + \frac{1}{2}\bar{C}^{mn}\{v_n, \partial_m\phi\}A. \tag{72}$$

Following Ref. 15, we notice that

$$\begin{aligned} &\delta\left[iC^{mn}\partial_m(\bar{A}v_n) - \frac{1}{4}C^{mn}\bar{A}v_m v_n\right] + i\left[iC^{mn}(\partial_m\bar{A}v_n) - \frac{1}{4}C^{mn}\bar{A}v_m v_n\right]\phi \\ &\quad = -2iC^{mn}(\partial_m\bar{A})(\partial_n\phi) + \frac{1}{2}C^{mn}\bar{A}\{\partial_m\phi, v_n\}. \end{aligned} \tag{73}$$

Additionally, we note that

$$\delta\left[-i\bar{C}^{mn}\partial_m v_n A+\frac{1}{4}\bar{C}^{mn}v_m v_n A\right]-i\phi\left[-i\bar{C}^{mn}\partial_m(v_n A)+\frac{1}{4}\bar{C}^{mn}v_m v_n A\right]$$
$$=2i\bar{C}^{mn}(\partial_n\phi)(\partial_m A)+\frac{1}{2}\bar{C}^{mn}\{v_n,\partial_m\phi\}A. \tag{74}$$

Then, observe that Eq. (74) and Eq. (72) indicate that

$$\eta=-i\bar{C}^{mn}\partial_m(v_n A)+\frac{1}{4}\bar{C}^{mn}v_m v_n A. \tag{75}$$

Then, observe that Eq. (73) and Eq. (71) indicate that

$$\beta=iC^{mn}\partial_m(\bar{A}v_n)-\frac{1}{4}C^{mn}\bar{A}v_m v_n. \tag{76}$$

Thus, we define the chiral and antichiral superfields with respect to Eq. (50) as

$$\Phi=A+\sqrt{2}\theta\psi+\theta\theta\left(F-i\bar{C}^{mn}\partial_m(v_n A)+\frac{1}{4}\bar{C}^{mn}v_m v_n A\right),$$
$$\bar{\Phi}=\bar{A}+\sqrt{2}\bar{\theta}\bar{\psi}+\bar{\theta}\bar{\theta}\left(\bar{F}+iC^{mn}\partial_m(\bar{A}v_n)-\frac{1}{4}C^{mn}\bar{A}v_m v_n\right). \tag{77}$$

It should be clear from this section that this is the correct parametrization of the anti-(chiral) superfields. This definition embeds Eq. (66) in Eq. (65). This parametrization gives the component fields the standard C-independent gauge transformations.

V. GAUGED WESS–ZUMINO MODEL

We construct the gauge-invariant Lagrangian of the Wess–Zumino model on noncommutative Minkowski superspace:

$$\mathcal{L}=\frac{1}{16kg^2}\left(\int d^2\theta\,\mathrm{tr}\,W*W+\int d^2\bar{\theta}\,\mathrm{tr}\,\bar{W}*\bar{W}\right)+\int d^2\theta\,d^2\bar{\theta}\,\bar{\Phi}*e^V*\Phi. \tag{78}$$

Gauge invariance of $\mathcal{L}$ follows directly from the cyclicity of the trace and equations, Eq. (34), Eq. (61), and Eq. (64). Also, note that this Lagrangian is real as the star product has the property $\overline{F*G}=\bar{G}*\bar{F}$. To first order in the deformation parameter, we can calculate

$$\mathrm{tr}\,W*W|_{\theta\theta}=\mathrm{tr}\,W*W(C=0)|_{\theta\theta}-iC^{mn}\,\mathrm{tr}\,F_{mn}\bar{\lambda}\bar{\lambda}+i\bar{C}^{mn}\,\mathrm{tr}\,\lambda\lambda F_{mn},$$
$$\mathrm{tr}\,\bar{W}*\bar{W}|_{\bar{\theta}\bar{\theta}}=\mathrm{tr}\,\bar{W}*\bar{W}(C=0)|_{\bar{\theta}\bar{\theta}}-iC^{mn}\,\mathrm{tr}\,F_{mn}\bar{\lambda}\bar{\lambda}+i\bar{C}^{mn}\,\mathrm{tr}\,\lambda\lambda F_{mn}, \tag{79}$$

where

$$W*W(C=0)\Big|_{\theta\theta}=-2i\bar{\lambda}\bar{\sigma}^m\mathcal{D}_m\lambda-\frac{1}{2}F^{mn}F_{mn}+D^2+\frac{i}{4}F^{mn}F^{lk}\epsilon_{mnlk},$$
$$\bar{W}*\bar{W}(C=0)\Big|_{\bar{\theta}\bar{\theta}}=-2i\bar{\lambda}\bar{\sigma}^m\mathcal{D}_m\lambda-\frac{1}{2}F^{mn}F_{mn}+D^2-\frac{i}{4}F^{mn}F^{lk}\epsilon_{mnlk}. \tag{80}$$

To first order, these terms match those found by Ref. 8 if we set $\bar{C}^{mn}=0$. Next, consider the coupling of the vector and chiral multiplets. After some calculation, we find

$$\bar{\Phi} * e^V * \Phi \Big|_{\theta\theta\bar{\theta}\bar{\theta}} = \bar{F}F + i\sigma^m_{\alpha\dot{\alpha}}(\partial_m\bar{\psi}^{\dot{\alpha}})\psi^\alpha + \frac{1}{2}\bar{\psi}^{\dot{\alpha}}\sigma^m_{\alpha\dot{\alpha}}v_m\psi^\alpha + \frac{1}{2}\bar{A}(D - i\,\partial_m v^m)A - \frac{1}{4}\bar{A}v^m v_m A + (\partial^2\bar{A})A$$
$$- i(\partial_m\bar{A})v^m A + i\frac{\sqrt{2}}{2}\bar{A}\lambda\psi - i\frac{\sqrt{2}}{2}\bar{\psi}\bar{\lambda}A + iC^{mn}\partial_m(\bar{A}v_n)F - iC^{mn}(\partial_m\bar{A})v_n F$$
$$- i\bar{C}^{mn}\bar{F}\partial_m(v_n A) + i\bar{C}^{mn}\bar{F}v_n\partial_m A - \frac{1}{2}C^{mn}\bar{A}v_m v_n F + \frac{1}{2}\bar{C}^{mn}\bar{F}v_m v_n A$$
$$- i\frac{\sqrt{2}}{8}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}\bar{A}\{\bar{\lambda}^{\dot{\alpha}}, v_m\}\psi_\beta - i\frac{\sqrt{2}}{8}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\{\lambda^\alpha, v_m\}A - \frac{\sqrt{2}}{2}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}(\partial_m\bar{A})\bar{\lambda}^{\dot{\alpha}}\psi_\beta$$
$$- \frac{\sqrt{2}}{2}\bar{C}^{\dot{\alpha}\beta}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\lambda^\alpha\,\partial_m A. \tag{81}$$

We identify the terms without deformation parameters as the usual terms in the Wess Zumino model; that is, up to a total derivative we have

$$\bar{\Phi} * e^V * \Phi(C=0) \Big|_{\theta\theta\bar{\theta}\bar{\theta}} = \bar{F}F - i\bar{\psi}\bar{\sigma}^m\mathcal{D}_m\psi - (\mathcal{D}_m\bar{A})(\mathcal{D}^m A) + \frac{1}{2}\bar{A}DA + \frac{i}{\sqrt{2}}(\bar{A}\lambda\psi - \bar{\psi}\bar{\lambda}A), \tag{82}$$

where ψ and A are in the fundamental representation of the gauge group

$$\mathcal{D}_m\psi = \partial_m\psi + \frac{i}{2}v_m\psi, \quad \mathcal{D}_m A = \partial_m A + \frac{i}{2}v_m A. \tag{83}$$

In Eq. (81), we recover most of the terms found by Ref. 15 plus their conjugates. However, in comparison to the $N=1/2$ theory, terms that are linear in λ and $\bar{\lambda}$ are notably modified. The new shifts in the gauge parameters, Eq. (50), lead to the modification of the λ and $\bar{\lambda}$ components of the vector superfield V, which, in turn, give rise to the following terms in the Lagrangian $\mathcal{L}$:

$$- i\frac{\sqrt{2}}{8}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}\bar{A}\{\bar{\lambda}^{\dot{\alpha}}, v_m\}\psi_\beta - \frac{\sqrt{2}}{2}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}(\partial_m\bar{A})\bar{\lambda}^{\dot{\alpha}}\psi_\beta$$
$$- i\frac{\sqrt{2}}{8}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\{\lambda^\alpha, v_m\}A - \frac{\sqrt{2}}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\lambda^\alpha\,\partial_m A. \tag{84}$$

Using covariant derivatives, these terms become

$$- i\frac{\sqrt{2}}{8}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}\bar{A}[\bar{\lambda}^{\dot{\alpha}}, v_m]\psi_\beta - \frac{\sqrt{2}}{2}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}(\mathcal{D}_m\bar{A})\bar{\lambda}^{\dot{\alpha}}\psi_\beta$$
$$+ i\frac{\sqrt{2}}{8}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}[\lambda^\alpha, v_m]A - \frac{\sqrt{2}}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\lambda^\alpha\mathcal{D}_m A. \tag{85}$$

The term $-(\sqrt{2}/2)C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}(\mathcal{D}_m\bar{A})\bar{\lambda}^{\dot{\alpha}}\psi_\beta$ was also found in Ref. 15. However, the commutator terms result from the choice of gauge parameter we made in Eq. (50). We might naively have expected only the terms without the commutators. Let us summarize:

$$\mathcal{L} = \frac{1}{16kg^2}\,\mathrm{tr}(-4i\bar{\lambda}\bar{\sigma}^m\mathcal{D}_m\lambda - F^{mn}F_{mn} + 2D^2) + \bar{F}F - i\bar{\psi}\bar{\sigma}^m\mathcal{D}_m\psi - \mathcal{D}_m\bar{A}\mathcal{D}^mA + \frac{1}{2}\bar{A}DA$$
$$+ \frac{i}{\sqrt{2}}(\bar{A}\lambda\psi - \bar{\psi}\bar{\lambda}A) + \frac{1}{16kg^2}\,\mathrm{tr}(-2iC^{mn}F_{mn}\lambda\lambda + 2i\bar{C}^{mn}\bar{\lambda}\bar{\lambda}F_{mn}) + \frac{i}{2}C^{mn}\bar{A}F_{mn}F$$
$$- \frac{i}{2}\bar{C}^{mn}\bar{F}F_{mn}A - i\frac{\sqrt{2}}{8}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}\bar{A}[\bar{\lambda}^{\dot{\alpha}}, v_m]\psi_\beta - \frac{\sqrt{2}}{2}C^{\alpha\beta}\sigma^m_{\alpha\dot{\alpha}}(\mathcal{D}_m\bar{A})\bar{\lambda}^{\dot{\alpha}}\psi_\beta$$
$$+ i\frac{\sqrt{2}}{8}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}[\lambda^\alpha, v_m]A - \frac{\sqrt{2}}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\sigma^m_{\alpha\dot{\alpha}}\bar{\psi}_{\dot{\beta}}\lambda^\alpha\mathcal{D}_mA\,. \tag{86}$$

VI. CONCLUSIONS

We have developed a non-Abelian gauge theory over deformed Minkowski superspace. In this deformation, all of the fermionic dimensions are deformed and, as a result, all of the supersymmetry is broken. To be consistent with the $N=1/2$ terminology, we say that this deformed superspace has $N=0$ supersymmetry. Many of the results directly mirror the results of $N=1/2$ from Ref. 8 or Ref. 15. This is due to the fact that the deformation we consider in this paper reduces to the deformation of $N=1/2$ supersymmetry upon setting $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$. It is not surprising that we recover almost the same gauge theoretic results as Ref. 8 in the limit $\bar{C}^{\dot{\alpha}\dot{\beta}}=0$. The exception to this rule is the choice of gauge parameter introduced by Seiberg in Ref. 8. We found that it was not possible to use the same construction because it violated the hermiticity of the vector superfield. We fixed this by introducing a new gauge parameter that served to maintain both hermiticity and the C-independent gauge transformations on the component fields.

Next, we introduced the chiral superfield Φ. Again, we found it necessary to modify the canonical component field expansion in order to maintain the standard gauge transformations on the component fields. The modification is similar in spirit to that of Ref. 15. Essentially, what we found is the $N=1/2$ theory and conjugate copy, where all of the usual $N=1/2$ terms are accompanied by their conjugates due to the hermiticity properties of the star product used in this construction.

Finally, we constructed the Lagrangian that coupled the gauge and matter fields. The gauge invariance of $\mathcal{L}$ follows for reasons similar to the commutative theory. We simply modified the standard arguments for the gauged Wess–Zumino model by replacing products with star products. The primary obstacle to this construction was the task of finding the correct parametrization for the superfields. The Lagrangian is similar to that found by Ref. 15, however, there are several new terms. Most new terms come directly from the added deformation $\{\bar{\theta}^{\dot{\alpha}}, \bar{\theta}^{\dot{\beta}}\}_* = \bar{C}^{\dot{\alpha}\dot{\beta}}$ (which should have been expected from the outset). However, the reparametrization of the gauge parameter also led us to some terms that were not immediately obvious from the $N=1/2$ theory.

There is much work left to do. First, we should complete the program begun in this work to the second order in the deformation parameter. Nonassociativity will have to be addressed. It is likely that the constructions of this paper will need modification at the second order. Second, there are numerous papers, see Refs. 15–47, investigating $N=1/2$ supersymmetry. It would be interesting to find complementary results for the $N=0$ case where possible. We could try to find the dual results for, instantons as in Refs. 16–21, or renormalization as in Refs. 22–29, or the possibility of residual supersymmetry as in Ref. 30, or the Seiberg Witten map as in Ref. 31. We do not attempt to give a complete account of the $N=1/2$ developments; we just wish to point out the variety of novel directions future research might take. Finally, it would be interesting to derive the $N=0$ deformation from a string theoretical argument.

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APPENDIX: FIRST ORDER ASSOCIATIVITY OF STAR PRODUCT

Define the parity of F to be ϵ^F. If F is even, then $\epsilon^F=1$. If F is odd, then $\epsilon^F=-1$. We can express the star product to the first order as:

$$F*G=FG-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta G)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}G).$$

Let us then prove that the first order star product is associative. Consider:

$$\begin{aligned}(F*G)*H&=\left(FG-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta G)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}G)\right)*H\\&=FGH-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta G)H-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}G)H\\&\quad-\frac{1}{2}C^{\alpha\beta}\epsilon^{FG}(Q_\alpha FG)(Q_\beta H)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^{FG}(\bar{Q}_{\dot{\alpha}}FG)(\bar{Q}_{\dot{\beta}}H)\\&=FGH-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta G)H-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}G)H\\&\quad-\frac{1}{2}C^{\alpha\beta}\epsilon^{FG}[(Q_\alpha F)G+\epsilon^F F(Q_\alpha G)]Q_\beta H\\&\quad-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^{FG}[(\bar{Q}_{\dot{\alpha}}F)G+\epsilon^F F(\bar{Q}_{\dot{\alpha}}G)]\bar{Q}_{\dot{\beta}}H\\&=FGH-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta G)H-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}G)H\\&\quad-\frac{1}{2}C^{\alpha\beta}[\epsilon^F\epsilon^G(Q_\alpha F)G(Q_\beta H)+\epsilon^G F(Q_\alpha G)(Q_\beta H)]\\&\quad-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}[\epsilon^F\epsilon^G(\bar{Q}_{\dot{\alpha}}F)G(\bar{Q}_{\dot{\beta}}H)+\epsilon^G F(Q_\alpha G)(\bar{Q}_{\dot{\beta}}H)].\end{aligned}$$

Notice that we have used $\epsilon^{FG}=\epsilon^F\epsilon^G$ and $\epsilon^F\epsilon^F=1$ to complete the calculation above. Likewise, consider

$$\begin{aligned}F*(G*H)&=F*\left(GH-\frac{1}{2}C^{\alpha\beta}\epsilon^G(Q_\alpha G)(Q_\beta H)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^G(\bar{Q}_{\dot{\alpha}}G)(\bar{Q}_{\dot{\beta}}H)\right)\\&=FGH-\frac{1}{2}C^{\alpha\beta}\epsilon^G F(Q_\alpha G)(Q_\beta H)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^G F(\bar{Q}_{\dot{\alpha}}G)(\bar{Q}_{\dot{\beta}}H)\\&\quad-\frac{1}{2}C^{\alpha\beta}\epsilon^F(Q_\alpha F)(Q_\beta GH)-\frac{1}{2}\bar{C}^{\dot{\alpha}\dot{\beta}}\epsilon^F(\bar{Q}_{\dot{\alpha}}F)(\bar{Q}_{\dot{\beta}}GH)\end{aligned}$$

$$
\begin{aligned}
&= FGH - \frac{1}{2} C^{\alpha\beta} \epsilon^G F (Q_\alpha G)(Q_\beta H) - \frac{1}{2} \bar{C}^{\dot{\alpha}\dot{\beta}} \epsilon^G F (\bar{Q}_{\dot{\alpha}} G)(\bar{Q}_{\dot{\beta}} H) \\
&\quad - \frac{1}{2} C^{\alpha\beta} \epsilon^F (Q_\alpha F)[(Q_\beta G) H + \epsilon^G G (Q_\beta H)] \\
&\quad - \frac{1}{2} \bar{C}^{\dot{\alpha}\dot{\beta}} \epsilon^F (\bar{Q}_{\dot{\alpha}} F)[(\bar{Q}_{\dot{\beta}} G) H + \epsilon^G G (\bar{Q}_{\dot{\beta}} H)] \\
&= FGH - \frac{1}{2} C^{\alpha\beta} \epsilon^G F (Q_\alpha G)(Q_\beta H) - \frac{1}{2} \bar{C}^{\dot{\alpha}\dot{\beta}} \epsilon^G F (\bar{Q}_{\dot{\alpha}} G)(\bar{Q}_{\dot{\beta}} H) \\
&\quad - \frac{1}{2} C^{\alpha\beta} [\epsilon^F (Q_\alpha F)(Q_\beta G) H + \epsilon^F \epsilon^G (Q_\alpha F) G (Q_\beta H)] \\
&\quad - \frac{1}{2} \bar{C}^{\dot{\alpha}\dot{\beta}} [\epsilon^F (\bar{Q}_{\dot{\alpha}} F)(\bar{Q}_{\dot{\beta}} G) H + \epsilon^F \epsilon^G (Q_\alpha F) G (\bar{Q}_{\dot{\beta}} H)].
\end{aligned}
$$

Therefore, $F*(G*H)=(F*G)*H$ to the first order in the deformation parameter.

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Magnetic monopole in the loop representation

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We quantize, within the Loop Representation formalism, the electromagnetic field in the presence of a static magnetic pole. It is found that the loop-dependent physical wave functionals of the quantum Maxwell theory become multivalued, through a topological phase factor depending on the solid angle subtended at the monopole by a surface bounded by the loop. It is discussed how this fact generalizes what occurs in ordinary quantum mechanics in multiply connected spaces. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162333]

I. INTRODUCTION

Dirac found that the mere existence of a single monopole would explain the quantized nature of the electric charge.[1,2] He discovered a relation between the unit of electric charge and that of the magnetic pole, which is currently known as Dirac's quantization condition. In rationalized units $(c=\hbar=1)$ it reads as

$$\frac{eg}{4\pi}=\frac{1}{2}n, \tag{1}$$

where n is an integer and e (g) is the unit of electric (magnetic) charge. Besides this remarkable prediction, the Dirac theory of magnetic monopoles has been a source of inspiration for the development of new ideas in theoretical physics. Often, it occurs that different approaches to understanding the formulation of Dirac bring out novelties or unexpected relationships between old things.

Being a gauge theory, the Dirac theory of magnetic poles should be a candidate to admit a quantum geometric representation, such as the Loop Representation (LR) of Maxwell theory.[3–5] In this article we address this point to some extent. Concretely, we study the LR formulation of quantum Maxwell theory in the presence of an external magnetic pole, taking as a starting point a first-order action of Schwinger,[6] which is based on the earlier Dirac theory.[1,2] We shall see that the LR formulation of the Maxwell theory with a static monopole corresponds to that of the *free theory*, except by the fact that the loop-dependent wave functional acquires a topological dependence on the manner that the loop "winds" around the monopole. This dependence is manifested through a topological phase factor picked up by the wave functional when the loop undergoes an adiabatic excursion in the presence of the monopole. It could be said that loop-dependent wave functionals become multivalued in the presence of the monopole, in the same sense that in ordinary quantum mechanics wave functions are allowed to be multivalued whenever the configu-

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ration space is multiply connected.[7–9] These results are also related with previous studies about the quantum theory of strings in the presence of a Kalb–Ramond vortex,[10,11] where a generalization of the concept of anyons can be envisaged.

In the next section we present the model and discuss its quantization in the LR formulation. In the last section we study in which sense the magnetic monopole turns Maxwell theory into a loop-dependent theory with nontrivial boundary conditions in loop space.

II. QUANTIZATION AND LOOP REPRESENTATION

Electromagnetism with magnetic charges can be studied from the first-order Schwinger action,[6]

$$S = \int dx^4 \left(A_\mu J_e^\mu + B_\mu J_m^\mu - \frac{1}{2} F^{\mu\nu}(\partial_\mu A_\nu - \partial_\nu A_\mu) + \frac{1}{4} F^{\mu\nu} F_{\mu\nu} \right), \tag{2}$$

where B is given by

$$B_\mu(x) = \int dy^4 * F_{\mu\nu}(y) f^\nu(y - x) + \partial_\mu \lambda(x). \tag{3}$$

Here, f obeys

$$\partial_\mu f^\mu(y) = \delta^4(y), \tag{4}$$

and λ is an arbitrary function. The dual $*F$ is given by

$$* F_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\alpha\beta} F^{\alpha\beta}, \tag{5}$$

where $\epsilon_{\mu\nu\alpha\beta}$ is the completely antisymmetric symbol and J_e (J_m) denote the electric (magnetic) current density. The independent fields in (2) are A_ν and $F_{\mu\nu}$. Varying (2) with respect to A_μ gives

$$\partial_\nu F^{\mu\nu} = J_e^\mu, \tag{6}$$

whereas variations with respect to $F_{\mu\nu}$ yield

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - \frac{1}{2} \epsilon_{\mu\nu\alpha\beta} \int dy^4 \, J_m^\alpha(y) f^\beta(x - y), \tag{7}$$

which, with the use of Eqs. (3) and (4), implies

$$\partial_\nu * F^{\mu\nu} = J_m^\mu. \tag{8}$$

Thus, one obtains the Maxwell equations with both electric and magnetic currents. The duality electricity magnetism manifests through the invariance of the equations under the rotations

$$J_e \to \cos \phi J_e + \sin \phi J_m, \tag{9}$$

$$J_m \to - \sin \phi J_e + \cos \phi J_m, \tag{10}$$

$$F \to \cos \phi F + \sin \phi * F. \tag{11}$$

We are interested in studying how the presence of a magnetic monopole affects the loop-space formulation of the Maxwell field. Hence, we take $J_e = 0$ in Eq. (2) and restrict ourselves to consider a static monopole (we take it at the origin of space), which forces the magnetic current to be written as

$$J_m^\mu(x) = g\,\delta_0^\mu \delta^3(\vec{x}). \tag{12}$$

A convenient choice for f_μ [fulfilling Eq. (4)] is

$$f^\nu(y) = -\frac{1}{4\pi}\frac{y^i}{\vec{y}^3}\delta_i^\nu \delta(y_0). \tag{13}$$

The Hamiltonian formulation begins with the definition of the canonical momenta associated to A_0, F_{ij}, and A_i, which result to be

$$\Pi^0(x) \approx 0, \tag{14}$$

$$\Pi^{ij}(x) \approx 0, \tag{15}$$

$$\Pi^i(x) = -F^{0i}(x), \tag{16}$$

respectively. Equations (14), (15) are (primary) constraints in the sense of Dirac,[12] and we have introduced the weak equality symbol $\approx$ to mean that these equalities should not be used until Poisson brackets are calculated. Since F^{0i} is already a conjugate momentum, it is not necessary to treat it as a coordinate and to define its own canonical momentum.[13] Following Dirac's method to deal with constrained systems, one constructs the total Hamiltonian,[12]

$$H^* = H + \int d\vec{x}^3\, u(x)\Pi^0(x) + \int d\vec{x}^3\, u_{ij}(x)\Pi^{ij}(x), \tag{17}$$

where $u(x)$ and $u_{ij}(x)$ are Lagrange multipliers and H is the canonical Hamiltonian,

$$H = \int d\vec{x}^3 \left[\frac{1}{2}\Pi_i^2 - \frac{1}{4}F_{ij}^2 + \frac{1}{2}F_{ij}(f_{ij} - b_{ij})\right] + \int d\vec{x}^3\, \partial_i \Pi^i A_0. \tag{18}$$

Here we have defined

$$f_{ij}(x) = \partial_i A_j(x) - \partial_j A_i(x), \tag{19}$$

$$b_{ij}(x) = g\,\epsilon_{ijk} f^k(\vec{x}). \tag{20}$$

It is worth noticing that when the static monopole is absent, this Hamiltonian properly reduces to that of the conventional Maxwell theory, since in that case the magnetic field F_{ij} and the curl of the potential f_{ij} coincide.

The nonvanishing equal time canonical Poisson brackets are given by

$$\{F_{ij}(x), \Pi^{kl}(y)\} = \frac{1}{2}(\delta_i^k \delta_j^l - \delta_i^l \delta_j^k)\,\delta^3(\vec{x} - \vec{y}), \tag{21}$$

$$\{A_\alpha(x), \Pi^\beta(y)\} = \delta_\alpha^\beta \delta^3(\vec{x} - \vec{y}). \tag{22}$$

Following Dirac,[12] one must impose the time preservation of the constraints. From (14) one finds, as a secondary constraint, the Gauss Law,

$$\partial_i \Pi^i(x) \approx 0. \tag{23}$$

This constraint, in turn, has a vanishing Poisson bracket with the total Hamiltonian, hence, it does not produce further constraints. On the other hand, the time preservation of (15) gives the secondary constraint

$$K_{ij}(x) = F_{ij}(x) - f_{ij}(x) + b_{ij}(x) \approx 0. \tag{24}$$

Finally, the preservation of constraint (24) allows us to obtain the Lagrange multipliers u_{ij} in terms of the momenta Π^i,

$$u_{ij}(x) = -\frac{1}{2}(\partial_i F_{0j}(x) - \partial_j F_{0i}(x)), \tag{25}$$

which must be substituted into the expression for the total Hamiltonian.

It is found that constraints (23) and (14) are first class, while (15) and (24) are second class. Following Dirac's procedure, we must introduce Dirac brackets in order to obtain a quantum theory consistent with these second class constraints. Though it is not difficult to carry out the calculations of the matrix of the Poisson brackets between second class constraints and its inverse, which are the ingredients needed for building Dirac brackets, a simple argument suffices to obtain the result. Since Dirac brackets are going to be consistent with second class constraints, these may be put as strong equalities. Hence, we can write F_{ij} and its momentum Π^{ij} in terms of the remaining canonical variables, and substitute these expressions in the total Hamiltonian. Once this is done, we have only to consider Dirac brackets between the canonical variables that remain, which are A_i, A_0, and their canonical conjugates. But it is easy to see that these Dirac brackets just coincide with the Poisson ones. The net result is that we can eliminate F_{ij} and Π^{ij} using Eqs. (15) and (24), and continue using the Poisson brackets for the remaining variables.

At this point, it is also convenient to "eliminate" the constraint (14) of the formalism. This can be accomplished by fixing the temporal gauge $A_0=0$ and treating this equation as a new constraint, which, together with (14), can be considered as a pair of second class constraints. Then, we can put A_0 and Π^0 as strongly vanishing. As before, it can be seen that the new Dirac brackets are equal to the Poisson ones, as far as we consider only the remaining variables, namely A_i and their canonical conjugates.

Now we are ready to quantize the theory. First, promote canonical variables to operators obeying equal time canonical commutators,

$$[\hat{A}_i(x), \hat{A}_j(y)] = 0, \tag{26}$$

$$[\hat{\Pi}^i(x), \hat{\Pi}^j(y)] = 0, \tag{27}$$

$$[\hat{A}_i(x), \hat{\Pi}^j(y)] = i\delta_i^j \delta^3(\vec{x} - \vec{y}). \tag{28}$$

The first class constraints define the physical states $|\Psi>$ as those that satisfy

$$\partial_i \hat{\Pi}^i(x)|\Psi> 0. \tag{29}$$

On the physical subspace, the dynamics is given by the Schrödinger equation

$$i\partial_t|\Psi_t> = \hat{H}|\Psi_t> , \tag{30}$$

with

$$\hat{H} = \int d\vec{x}^3 \left[\frac{1}{2}\hat{\Pi}_i^2 + \frac{1}{4}(\partial_i \hat{A}_j - \partial_j \hat{A}_i - b_{ij})^2 \right]. \tag{31}$$

Thus, we obtain that the static monopole manifests in the theory just through the external field b_{ij}, which must be subtracted from the curl of the vector potential to give the magnetic field operator.

We are now prepared to discuss the LR of the model. We begin by recalling that the Abelian path space (PS) can be defined as the set of certain equivalence classes of curves γ in (for our purposes) R^3.[3–5,14] The equivalence relation is given by the so-called *form factor* $T^i(\vec{x}, \gamma)$ of the curve

$$T^i(\vec{x},\gamma)=\int_\gamma dy^i\ \delta(\vec{x}-\vec{y}), \tag{32}$$

as follows: γ and γ' are said to be equivalent (i.e., represent the same path) if their form factors coincide. Closed curves give rise to a subspace of the PS: the loop space. It can be seen that the usual composition of curves translates into a composition of paths that endows the PS with a group structure.

The path representation arises when one considers path-dependent wave functionals $\Psi[\gamma]$, and realizes the canonical field operators by means of operations onto these wave functionals.[3–5,14] We define the path and loop derivatives $\delta_i(\vec{x})$ and $\Delta_{ij}(\vec{x})$ by

$$(1+u^i(\vec{x})\delta_i(\vec{x}))\Psi[\gamma]=\Psi[\gamma\circ u], \tag{33}$$

$$\left(1+\frac{1}{2}\sigma^{ij}(\vec{x})\Delta_{ij}(\vec{x})\right)\Psi[\gamma]=\Psi[\gamma\circ \delta c], \tag{34}$$

where $\circ$ denotes the PS product.[4] The derivative $\delta_i(\vec{x})$ $(\Delta_{ij}(\vec{x}))$ measures the change in the path-dependent wave functional when an infinitesimal path δu (infinitesimal loop δc) is attached to its argument γ at the point $\vec{x}$. It is understood that these changes are considered up to first order in the infinitesimal vector u^i associated with the small path, or with the surface element,

$$\sigma^{ij}=u^iv^j-v^iu^j, \tag{35}$$

generated by the infinitesimal vectors $\vec{u}$ and $\vec{v}$ that define the small loop δc. It can be shown that both derivatives are related by[3–5,14]

$$\partial_i\delta_j(\vec{x})-\partial_j\delta_i(\vec{x})=\Delta_{ij}(\vec{x}). \tag{36}$$

With these tools at hand we represent the canonical field as operators acting on path-dependent wave functionals $\Psi[\gamma]$ by means of the prescriptions,

$$\hat{\Pi}^i(\vec{x})\to eT^i(\vec{x},\gamma), \tag{37}$$

$$\hat{A}_j(\vec{x})\to\frac{i}{e}\delta_j(\vec{x}). \tag{38}$$

It is readily seen that this realizes the algebra (26)–(28). We see that in this representation the form factor corresponds to Faraday lines of the electric field. The magnetic field operator, in turn, appends a small closed line of electric field to the argument of the wave functionals. The constant e is introduced to fix the scale of the Faradays lines of an electric field. In virtue of Gauss' law, e can at the same time be seen as the elementary unit of electric charge. In four dimensions (and using natural units) this constant is dimensionless (as well as the magnetic charge g).

Since the divergence of the form factor $T^i(\vec{x},\gamma)$ vanishes when the path is closed, the Gauss constraint (29) is identically satisfied if we restrict ourselves to deal with loop-dependent wave functionals.[3] Finally, the Schrödinger equation obeyed by the loop-dependent wave functional $\Psi[\gamma]$ that describes the Maxwell field quantized in the presence of the static external monopole can be written down as

$$i\,\partial_t\Psi[\gamma,t]=\int d\vec{x}^3\left[\frac{1}{2}e^2(T^i(\vec{x},\gamma))^2-\frac{1}{4e^2}(i\Delta_{ij}(\vec{x})-eb_{ij}(\vec{x}))^2\right]\Psi[\gamma,t]. \tag{39}$$

When $g=0$, this equation reduces to that corresponding to free electromagnetism in the LR,[3–5] as it should be.

The above formulation is empty unless an appropriate scalar product in loop space is defined. This is a rather subtle matter on which we shall just briefly comment. Nowadays it is known that

there exits a suitable integration measure in the quantum configuration space of gauge potentials (see Ref. 18 for a recent reference about this matter) that allows us to define an inner product in loop space for both Abelian and non-Abelian gauge theories. Moreover, it has also been understood how to relate the loop representation of Maxwell theory with its Fock representation,[19] which allows us to make contact with the familiar particle interpretation of field theory. This relationship between the "polymer-like" and photon-like representations heavily relies on the introduction of "smeared" Wilson loop operators, which, unlike the unsmeared ones, are well defined in Fock space. At last, it results that normalizable states in the Fock representation correspond to linear combinations of non-normalizable or distributional states of the loop representation.[19]

III. MULTIVALUED LOOP-DEPENDENT WAVE FUNCTIONALS

We have seen that introducing a static monopole in quantum Maxwell theory, in the LR, amounts to replacing the loop derivative $\Delta_{ij}(\vec{x})$ by a kind of "covariant derivative,"

$$i\Delta_{ij}(\vec{x}) \to i\Delta_{ij}(\vec{x}) - eb_{ij}(\vec{x}). \tag{40}$$

Now, we shall see that it is possible to recast the Schrödinger equation (39) as that corresponding to a *free* theory, provided that we deal with *multivalued loop-dependent* wave functionals. It should be emphasized that this *does not* mean that the Maxwell field plus a monopole is the same thing as that the Maxwell field alone. What this actually means is that one can convert the effect of the monopole into unusual boundary conditions for the wave functional.

To see how this happens we find it convenient to employ the space of surfaces framework,[15] which we summarize following very closely Ref. 16. One starts with the space of piecewise smooth oriented surfaces Σ in R^3. We define two surfaces as equivalent if they share the same "surface form factor,"

$$T^{ij}(\vec{x},\Sigma) = \int d\Sigma_y^{ij}\, \delta^{(3)}(\vec{x}-\vec{y}). \tag{41}$$

Here $d\Sigma_y^{ij}$ is the surface element,

$$d\Sigma_y^{ij} = \left(\frac{\partial y^i}{\partial s}\frac{\partial y^j}{\partial r} - \frac{\partial y^i}{\partial r}\frac{\partial y^j}{\partial s}\right) ds\, dr, \tag{42}$$

with s, r being surface parameters. Now we consider functionals $\Psi[\Sigma]$ and introduce the surface derivative $\delta_{ij}(\vec{x})$, that measures the response of $\Psi[\Sigma]$ when an element of surface whose infinitesimal area is σ_{ij} is attached to the argument Σ of $\Psi[\Sigma]$ at the point x, up to first order in σ_{ij}:

$$\Psi[\delta\Sigma \cdot \Sigma] = (1 + \sigma^{ij}\delta_{ij}(\vec{x}))\Psi[\Sigma]. \tag{43}$$

The surface derivative $\delta_{ij}(\vec{x})$ and the loop derivative $\Delta_{ij}(\vec{x})$ are different things. However, since in R^3 loop dependence is a particular case of surface dependence (a loop is always the boundary of an open surface in R^3), the loop derivative can be seen as the surface derivative restricted to loop-dependent functionals. Hence it makes sense to surface derive loop-dependent quantities. Soon we shall make use of the surface derivative of the form factor,

$$\delta_{ij}(\vec{x})T^{kl}(\vec{y},\Sigma) = \frac{1}{2}(\delta_i^k\delta_j^l - \delta_i^l\delta_j^k)\delta^{(3)}(\vec{x}-\vec{y}). \tag{44}$$

Turning back to our model, let us consider an open surface Σ whose boundary coincides with γ (i.e., $\partial\Sigma = \gamma$). Then define, from the path-dependent wave functional $\Psi[\gamma]$, the surface-dependent one,

$$\Psi[\Sigma] \equiv \exp\left(ie \int d\Sigma_{\vec{y}}^{km} b_{km}(\vec{y}) \right) \Psi[\gamma] = \exp\left(\frac{ieg}{4\pi} \Omega(\Sigma) \right) \Psi[\gamma], \tag{45}$$

where $\Omega(\Sigma)$ is the solid angle subtended by Σ, measured from the monopole. Using Eq. (44), it is easy to show that

$$\delta_{ij}(\vec{x}) \Psi[\Sigma] = \exp\left(\frac{ieg}{4\pi} \Omega(\Sigma) \right) (\Delta_{ij}(\vec{x}) + ieb_{ij}(\vec{x})) \Psi[\gamma]. \tag{46}$$

Then, the Schrödinger equation (39) of the model can also be written as

$$i\, \partial_t \Psi[\Sigma, t] = \int d\vec{x}^3 \left[\frac{1}{2} e^2 (T^i(\vec{x}, \partial\Sigma))^2 - \frac{1}{4e^2} (\delta_{ij}(\vec{x}))^2 \right] \Psi[\Sigma, t]. \tag{47}$$

[Unlike the loop dependence in Eq. (39), the surface dependence in Eq. (47) is not arbitrary: it is precisely given by the phase factor $\exp((ieg/4\pi)\Omega(\Sigma))$ carried by the wave functional, which just serves to compensate the contribution b_{ij} otherwise present in the Schrödinger equation. Hence, despite the appearances, we are not introducing extra degrees of freedom into the theory when working with surfaces instead of loops.]

Due to definition (45), we see that the properties of Σ that matter are the solid angle $\Omega(\Sigma)$ subtended at the monopole, and the boundary $\partial\Sigma$. This implies that the surface dependence of the wave functional $\Psi[\Sigma, t]$ is topological: if we replace Σ by another surface Σ' that has the same boundary γ, the wave functional changes as

$$\Psi[\Sigma'] = \exp(iegp) \Psi[\Sigma], \tag{48}$$

where p is the number of times that the closed surface $S = \Sigma' \circ (-\Sigma)$, that results from the composition of Σ' and the surface opposite to Σ, wraps around the monopole. Therefore we can rewrite Eq. (47) as the Schrödinger equation of the free Maxwell theory,

$$i\, \partial_t \Psi[\gamma, t] = \int d\vec{x}^3 \left[\frac{1}{2} e^2 (T^i(\vec{x}, \gamma))^2 - \frac{1}{4e^2} (\Delta_{ij}(\vec{x}))^2 \right] \Psi[\gamma, t], \tag{49}$$

provided that simultaneously we deal with nontrivial boundary conditions for the loop-dependent wave functionals: every time that the loop goes around a "closed trajectory" (i.e., a closed surface) that encloses p times the monopole, the wave function picks up the phase factor $\exp(iegp)$,

$$\Psi[[S] \,.\, \gamma] = \exp(iegp) \Psi[\gamma]. \tag{50}$$

In this equation, $[S].\gamma$ means that the loop γ has described a "closed trajectory" sweeping the closed surface S and wrapping p times to the monopole. The loop-dependent wave functional became multivalued due to the presence of the magnetic monopole.

This can be understood as a generalization of what occurs in ordinary quantum mechanics in multiply connected configuration spaces.[7–9] In such cases, multivaluedness of the wave function is allowed, being restricted to multiplication of the wave function by a phase factor carrying a representation of the fundamental group of the configuration space. But this is precisely what we have found in our study: since the configuration space of our quantum formulation is the space of loops in $R^3 - \{origin\}$, a "point" in the set is a loop, while the "closed curves" swept by loops will be closed surfaces, whose properties of contractibility in $R^3 - \{origin\}$ will define the fundamental group of the configuration space. Now, the phase factor $\exp(iegp)$ appearing in Eq. (48) just corresponds to a one-dimensional representation of this fundamental group, since it classifies the surfaces according to the manner in which they wrap the monopole.

Summarizing, we observe that there are three equivalent levels in the description of the model: (1) Eq. (39), where the wave functionals are loop dependent and single valued, and the interaction of the field with the monopole appears explicitly in the Hamiltonian. (2) Eq. (47), that uses a wave functional with a prescribed surface-dependence (45) that encodes the effect of the

monopole; and (3) the loop-dependent "free" equation (49), where the wave-functional carries a non trivial one-dimensional unitary representation of the fundamental group of the configuration space (which is the space of loops in $R^3-\{origin\}$) that takes into account the effect of the monopole.

To conclude, we should mention a feature that could look somewhat striking at first sight. If Dirac's quantization condition (1) holds, the topological phase factor appearing in (48) becomes unity and the dependence on the surface vanishes. But then the wave functional becomes single valued and the effect of the monopole seems to disappear at all!. What happens is that, in the absence of electrically charged particles, there is no need to quantize electric or magnetic charges. In fact, recall that in the formulation of Dirac, charge quantization arises when the wave function of the *charged particle* is asked to be single valued in the presence of the monopole. Or, alternatively, when the action functional of the *charge*-field-monopole system is asked to be independent of the string attached to the monopole [in our case, this corresponds to demanding that changing f^μ [given in (13)] by any other vector field obeying Eq. (4) does not modify the action]. Yet, there is another approach, which does not employ vector potentials, which derives charge quantization from the consistency of the Heisenberg equations of motion of a *charged* particle in the field of a magnetic monopole.[20] But in the absence of electric charges, all these requirements are automatically guaranteed, and Dirac's quantization condition is not required to have a consistent theory.

It would be interesting, in view of the above discussion, to study the LR formulation of the theory in the case with both charges and monopoles. Based on previous results about the LR of the Maxwell field coupled to dynamical point particles,[21] it can be expected in this case that the physical sector of loop space corresponds to both loops and open paths emanating or ending at the points where charges are located. This change in the configuration space of the quantum theory could modify the "striking consequence" regarding Dirac quantization condition discussed above.

The present approach could also be applied to the study of higher-rank Abelian theories, with their corresponding extended objects generalizing electric and magnetic charges.[17]

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Quiver gauge theory of non-Abelian vortices and noncommutative instantons in higher dimensions

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We construct explicit Bogomolnyi, Prasad, Sommerfeld (BPS) and non-BPS solutions of the Yang-Mills equations on the noncommutative space $\mathbb{R}^{2n}_\theta \times S^2$ which have manifest spherical symmetry. Using SU(2)-equivariant dimensional reduction techniques, we show that the solutions imply an equivalence between instantons on $\mathbb{R}^{2n}_\theta \times S^2$ and non-Abelian vortices on $\mathbb{R}^{2n}_\theta$, which can be interpreted as a blowing-up of a chain of $D0$-branes on $\mathbb{R}^{2n}_\theta$ into a chain of spherical $D2$-branes on $\mathbb{R}^{2n}_\theta \times S^2$. The low-energy dynamics of these configurations is described by a quiver gauge theory which can be formulated in terms of new geometrical objects generalizing superconnections. This formalism enables the explicit assignment of $D0$-brane charges in equivariant K-theory to the instanton solutions. © *2006 American Institute of Physics.*
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I. INTRODUCTION AND SUMMARY

One of the most basic questions that arises in trying to understand the nonperturbative structure of string theory concerns the classification of vector bundles over real and complex manifolds. In the presence of D-branes one encounters gauge theories in space-time dimensionalities up to 10. Already more than 20 years ago, BPS-type equations in higher dimensions were proposed[1,2] as a generalization of the self-duality equations in four dimensions. For non-Abelian gauge theory on a Kähler manifold the most natural BPS condition lies in the Donaldson-Uhlenbeck-Yau equations,[3] which arise, for instance, in compactifications down to four-dimensional Minkowski space-time as the condition for at least one unbroken supersymmetry.

While the criteria for solvability of these BPS equations are by now very well understood, in practice it is usually quite difficult to write down explicit solutions of them. One recent line of attack has been to consider noncommutative deformations of these field theories.[4–6] In certain instances, D-branes can be realized as noncommutative solitons,[7] which is a consequence[8,9] of the relationship between D-branes and K-theory.[10–13] All celebrated BPS configurations in field theories, such as instantons,[14] monopoles[15] and vortices,[16] have been generalized to the noncommutative case, originally in Ref. 17, in Refs. 18 and in Ref. 19, respectively (see Ref. 20 for reviews and further references). Solution generating techniques such as the Atiyah, Drinfeld, Hitchin, and Manin (ADHM) construction,[21] splitting,[22] and dressing[23] methods have also been generalized to the noncommutative setting in Refs. 17,24 and in Ref. 25. Solutions of the generalized self-duality equations[1,2] were investigated in Refs. 2 and 26, for example. Noncommutative instantons in

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higher dimensions and their interpretations as *D*-branes in string theory have been considered in Refs. 27–30. In all of these constructions the usual world volume description of *D*-branes emerges from the equivalence between analytic and topological formulations of *K*-homology.

In this paper we will complete the construction initiated in Refs. 29 and 30 of multi-instanton solutions of the Yang-Mills equations on the manifold which is the product of noncommutative Euclidean space $\mathbb{R}^{2n}_\theta$ with an ordinary two-sphere S^2. We consider both BPS and non-BPS solutions, and extend previous solutions to those which are explicitly SU(2)-equivariant for any value of the Dirac monopole charge characterizing the gauge field components along the S^2 directions. Dimensional reduction techniques are used to establish an equivalence between multi-instantons on $\mathbb{R}^{2n}_\theta \times S^2$ and non-Abelian vortices on $\mathbb{R}^{2n}_\theta$. The configurations can be interpreted in Type IIA superstring theory as *chains* of branes and antibranes with Higgs-type open string excitations between neighboring sets of *D*-branes. The equivalence between instantons and vortices may then be attributed to the decay of an unstable configuration of $D(2n)$-branes into a state of $D0$-branes (there are no higher brane charges induced because $\mathbb{R}^{2n}$ is equivariantly contractible). The $D0$-brane charges are classified by SU(2)-equivariant *K*-theory and the low-energy dynamics may be succinctly encoded into a simple quiver gauge theory. Unlike the standard brane-antibrane systems, the effective action cannot be recast using the formalism ofsuperconnections[31] but requires a more general formulation in terms of new geometrical entities that we call "graded connections." This formalism makes manifest the interplay between the assignment of *K*-theory classes to the explicit instanton solutions and their realization in terms of a quiver gauge theory.

The organization of this paper is as follows. The material is naturally divided into two parts. Sections II–V deal with *ordinary* gauge theory on a generic Kähler manifold of the form $M_{2n} \times \mathbb{C}P^1$ in order to highlight the geometric structures that arise due to dimensional reduction and which play a prominent role throughout the paper. Sections VI–X are then concerned with the noncommutative deformation $\mathbb{R}^{2n} \times \mathbb{C}P^1 \to \mathbb{R}^{2n}_\theta \times \mathbb{C}P^1$ and they construct explicit solutions of the dimensionally reduced Yang-Mills equations, emphasizing their interpretations in the context of equivariant *K*-theory, quiver gauge theory, and ultimately as states of *D*-branes. In Sec. II we introduce basic definitions and set some of our notation, and present the field equations that are to be solved. In Section III we write down an explicit ansatz for the gauge field which is used in the SU(2)-equivariant dimensional reduction. In Sec. IV we describe three different interpretations of the ansatz as configurations of *D*-branes, as charges in equivariant *K*-theory, and as field configurations in a quiver gauge theory (later on these three descriptions are shown to be equivalent). In Sec. V the dimensional reduction mechanism is explained in detail in the new language of graded connections and the resulting nonabelian vortex equations, arising from reduction of the Donaldson-Uhlenbeck-Yau equations, are written down. In Sec. VI we introduce the noncommutative deformations of all these structures. In Sec. VII we find explicit BPS and non-BPS solutions of the noncommutative Yang-Mills equations and show how they naturally realize representations of the pertinent quiver. In Sec. VIII we develop an SU(2)-equivariant generalization of the (noncommutative) Atiyah-Bott-Shapiro construction, which provides an explicit and convenient representation of our solution in terms of *K*-homology classes. In Sec. IX we compute the topological charge of our instanton solutions directly in the noncommutative gauge theory, and show that it coincides with the corresponding *K*-theory charge, which then allows us to assign $D0$-brane charges to the solutions from a world volume perspective. Finally, in Sec. X we construct some BPS solutions in the vacuum sectors of the noncommutative field theory and describe their relation to stable states of brane-antibrane systems.

II. YANG-MILLS EQUATIONS

In this section we will introduce the basic definitions and notation that will be used throughout this paper, as well as the pertinent field equations that we will solve.

The manifold $\mathcal{M}_q \times S^2$: Let $\mathcal{M}_q$ be a real q-dimensional Lorentzian manifold with nondegenerate metric of signature $(-+\cdots+)$, and $S^2 \cong \mathbb{C}P^1$ the standard two-sphere of constant radius R. We shall consider the manifold $\mathcal{M}_q \times S^2$ with local real coordinates $x' = (x^{\mu'}) \in \mathbb{R}^q$ on $\mathcal{M}_q$ and coordinates $\vartheta \in [0,\pi], \varphi \in [0,2\pi]$ on S^2. In these coordinates the metric on $\mathcal{M}_q \times S^2$ reads

$$\mathrm{d}\hat{s}^2 = g_{\hat{\mu}\hat{\nu}}\,\mathrm{d}x^{\hat{\mu}}\,\mathrm{d}x^{\hat{\nu}} = g_{\mu'\nu'}\,\mathrm{d}x^{\mu'}\,\mathrm{d}x^{\nu'} + R^2(d\vartheta^2 + \sin^2\vartheta\,\mathrm{d}\varphi^2), \tag{2.1}$$

where hatted indices $\hat{\mu},\hat{\nu},\ldots$ run over $0,1,\ldots,q+1$ while primed indices $\mu',\nu',\ldots$ run through $0,1,\ldots,q-1$. We use the Einstein summation convention for repeated space-time indices.

The Kähler manifold $M_{2n}\times\mathbb{C}P^1$: As a special instance of the manifold $\mathcal{M}_q$ we shall consider the product $\mathcal{M}_q=\mathbb{R}^1\times M_{2n}$ of dimension $q=2n+1$ with metric,

$$g_{\mu'\nu'}\,\mathrm{d}x^{\mu'}\,\mathrm{d}^{\nu'} = -(\mathrm{d}x^0)^2 + g_{\mu\nu}\,\mathrm{d}x^{\mu}\,\mathrm{d}x^{\nu}. \tag{2.2}$$

Here M_{2n} is a Kähler manifold of real dimension $2n$ with local real coordinates $x=(x^\mu)\in\mathbb{R}^{2n}$, where the indices $\mu,\nu,\ldots$ run through $1,\ldots,2n$. The Cartesian product $M_{2n}\times\mathbb{C}P^1$ is also a Kähler manifold with local complex coordinates $(z^1,\ldots,z^n,y)\in\mathbb{C}^{n+1}$ and their complex conjugates, where

$$z^a = x^{2a-1} - ix^{2a} \quad \text{and} \quad \overline{z^a} = x^{2a-1} + ix^{2a} \quad \text{with } a=1,\ldots,n \tag{2.3}$$

while

$$y = \frac{R\sin\vartheta}{1+\cos\vartheta}\exp(-i\varphi) \quad \text{and} \quad \overline{y} = \frac{R\sin\vartheta}{1+\cos\vartheta}\exp(i\varphi) \tag{2.4}$$

are stereographic coordinates on the northern hemisphere of S^2. In these coordinates the metric on $M_{2n}\times\mathbb{C}P^1$ takes the form

$$\mathrm{d}s^2 = g_{\mu\nu}\,\mathrm{d}x^{\mu}\,\mathrm{d}x^{\nu} + R^2(d\vartheta^2+\sin^2\vartheta\,\mathrm{d}\varphi^2) = 2g_{a\bar{b}}\mathrm{d}z^a\,\mathrm{d}\overline{z^b} + \frac{4R^4}{(R^2+y\overline{y})^2}\mathrm{d}y\,\mathrm{d}\overline{y}, \tag{2.5}$$

while the Kähler two-form ω is given by

$$\omega = \tfrac{1}{2}\omega_{\mu\nu}\,\mathrm{d}x^{\mu}\wedge\mathrm{d}x^{\nu} + R^2\sin\vartheta\,\mathrm{d}\vartheta\wedge\mathrm{d}\varphi = -2ig_{a\bar{b}}\mathrm{d}z^a\wedge\,\mathrm{d}\overline{z^b} - \frac{4iR^4}{(R^2+y\overline{y})^2}\mathrm{d}y\wedge\mathrm{d}\overline{y}. \tag{2.6}$$

Yang-Mills equations: Consider a rank k Hermitian vector bundle $\mathcal{E}\to\mathcal{M}_q\times S^2$ with gauge connection $\mathcal{A}$ of curvature $\mathcal{F}=\mathrm{d}\mathcal{A}+\mathcal{A}\wedge\mathcal{A}$. In local coordinates, wherein $\mathcal{A}=\mathcal{A}_{\hat{\mu}}\,\mathrm{d}x^{\hat{\mu}}$, the two-form $\mathcal{F}$ has components $\mathcal{F}_{\hat{\mu}\hat{\nu}}=\partial_{\hat{\mu}}\mathcal{A}_{\hat{\nu}}-\partial_{\hat{\nu}}\mathcal{A}_{\hat{\mu}}+[\mathcal{A}_{\hat{\mu}},\mathcal{A}_{\hat{\nu}}]$, where $\partial_{\hat{\mu}}:=\partial/\partial x^{\hat{\mu}}$. Both $\mathcal{A}_{\hat{\mu}}$ and $\mathcal{F}_{\hat{\mu}\hat{\nu}}$ take values in the Lie algebra $u(k)$. For the usual Yang-Mills Lagrangian (the Yang-Mills coupling constant g_{YM} can be introduced via the redefinition $\mathcal{A}\mapsto g_{\mathrm{YM}}\mathcal{A}$),

$$L_{\mathrm{YM}} = -\tfrac{1}{4}\sqrt{g}\,\mathrm{tr}_{k\times k}\,\mathcal{F}_{\hat{\mu}\hat{\nu}}\mathcal{F}^{\hat{\mu}\hat{\nu}} \tag{2.7}$$

the equations of motion are

$$\frac{1}{\sqrt{g}}\partial_{\hat{\mu}}(\sqrt{g}\mathcal{F}^{\hat{\mu}\hat{\nu}}) + [\mathcal{A}_{\hat{\mu}},\mathcal{F}^{\hat{\mu}\hat{\nu}}] = 0, \tag{2.8}$$

where $g=|\det(g_{\hat{\mu}\hat{\nu}})|$. The curvature two-form can be written in local coordinates on $\mathcal{M}_q\times\mathbb{C}P^1$ as

$$\mathcal{F} = \tfrac{1}{2}\mathcal{F}_{\mu'\nu'}\,\mathrm{d}x^{\mu'}\wedge\mathrm{d}x^{\nu'} + \mathcal{F}_{\mu' y}\,\mathrm{d}x^{\mu'}\wedge\mathrm{d}y + \mathcal{F}_{\mu'\bar{y}}\mathrm{d}x^{\mu'}\wedge\mathrm{d}\overline{y} + \mathcal{F}_{y\bar{y}}\mathrm{d}y\wedge\mathrm{d}\overline{y} \tag{2.9}$$

and the Yang-Mills Lagrangian becomes

$$L_{\mathrm{YM}} = -\tfrac{1}{4}\sqrt{g}\,\mathrm{tr}_{k\times k}\left[\mathcal{F}_{\mu'\nu'}\mathcal{F}^{\mu'\nu'} + \frac{(R^2+y\overline{y})^2}{R^4}g^{\mu'\nu'}(\mathcal{F}_{\mu' y}\mathcal{F}_{\nu'\bar{y}} + \mathcal{F}_{\mu'\bar{y}}\mathcal{F}_{\nu' y}) - \frac{1}{2}\left(\frac{(R^2+y\overline{y})^2}{R^4}\mathcal{F}_{y\bar{y}}\right)^2\right]. \tag{2.10}$$

Donaldson-Uhlenbeck-Yau equations: For static field configurations in the temporal gauge $\mathcal{A}_0=0$, the Yang-Mills equations (2.8) on $\mathbb{R}^1\times M_{2n}\times\mathbb{C}P^1$ reduce to equations on $M_{2n}\times\mathbb{C}P^1$. Their

stable solutions are provided by solutions of the Donaldson-Uhlenbeck-Yau (DUY) equations which can be formulated on any Kähler manifold.[3] The importance of these equations derives from the fact that they yield the BPS solutions of the full Yang-Mills equations.

The DUY equations on $M_{2n}\times\mathbb{C}P^1$ are

$$*\omega\wedge\mathcal{F}=0 \quad \text{and} \quad \mathcal{F}_{0,2}=0, \tag{2.11}$$

where * is the Hodge duality operator and $\mathcal{F}=\mathcal{F}^{2,0}+\mathcal{F}^{1,1}+\mathcal{F}^{0,2}$ is the Kähler decomposition of the gauge field strength. In the local complex coordinates (z^a,y) these equations take the form

$$g^{a\bar{b}}\mathcal{F}_{z^a\bar{z}^b}+\frac{(R^2+y\bar{y})^2}{2R^4}\mathcal{F}_{y\bar{y}}=0, \tag{2.12}$$

$$\mathcal{F}_{\bar{z}^a\bar{z}^b}=0=\mathcal{F}_{z^az^b}, \tag{2.13}$$

$$\mathcal{F}_{\bar{z}^a\bar{y}}=0=\mathcal{F}_{z^ay}, \tag{2.14}$$

where the indices $a,b,\ldots$ run through $1,\ldots,n$. Equation (2.12) is a Hermitian condition on the gauge field strength tensor, while Eqs. (2.13) and (2.14) are integrability conditions implying that the bundle $\mathcal{E}$ (and its connection $\mathcal{A}$) is holomorphic. It is easy to show that any solution of these $n(n+1)+1$ equations also satisfies the full Yang-Mills equations.

III. INVARIANT GAUGE FIELDS

In this section we shall write down the fundamental form of the gauge field $\mathcal{A}$ on $\mathcal{M}_q\times\mathbb{C}P^1$ that will be used later on to dimensionally reduce the Yang-Mills equations for $\mathcal{A}$ to equations on $\mathcal{M}_q$. This will be achieved by prescribing a specific $\mathbb{C}P^1$ dependence for $\mathcal{A}$, which we proceed to describe first.

Monopole bundles: Consider the Hermitian line bundle $\mathcal{L}^m\to\mathbb{C}P^1$ over the sphere with $\mathcal{L}^m:=(\mathcal{L})^{\otimes m}$ and unique SU(2)-invariant unitary connection a_m having, in the local complex coordinate y on $\mathbb{C}P^1$, the form

$$a_m=\frac{m}{2(R^2+y\bar{y})}(\bar{y}\,\mathrm{d}y-y\,\mathrm{d}\bar{y}), \tag{3.1}$$

where m is an integer. The curvature of this connection is

$$f_m=\mathrm{d}a_m=-\frac{mR^2}{(R^2+y\bar{y})^2}\mathrm{d}y\wedge\mathrm{d}\bar{y}. \tag{3.2}$$

The topological charge of this gauge field configuration is given by the first Chern number (equivalently the degree) of the associated complex line bundle as

$$\deg\mathcal{L}^m=\frac{i}{2\pi}\int_{\mathbb{C}P^1}f_m=m. \tag{3.3}$$

In terms of the spherical coordinates (ϑ,φ) the configuration (3.1) and (3.2) has the form

$$a_m=-\frac{im}{2}(1-\cos\vartheta)\mathrm{d}\varphi \quad \text{and} \quad f_m=\mathrm{d}a_m=-\frac{im}{2}\sin\vartheta\,\mathrm{d}\vartheta\wedge\mathrm{d}\varphi. \tag{3.4}$$

It describes $|m|$ Dirac monopoles or antimonopoles sitting on top of each other.

The m-monopole bundle is classified by the Hopf fibration $S^1\hookrightarrow S^3\to S^2$. For each $m\in\mathbb{Z}$ there is a one-dimensional representation $\boldsymbol{\nu}m=(\boldsymbol{\nu}_i)^{\otimes m}$ of the circle group $\mathrm{U}(1)\cong S^1$ defined by

$$\boldsymbol{\nu}_m : v \mapsto \zeta \cdot v = \zeta^m v \quad \text{with } \zeta \in S^1 \text{ and } v \in \mathbb{C}. \tag{3.5}$$

We denote this irreducible U(1)-module by $\underline{S}_m \cong \mathbb{C}$. Regarding the sphere as the homogeneous space $\mathbb{C}P^1 \cong \mathrm{SU}(2)/\mathrm{U}(1)$, the SU(2)-equivariant line bundle $\mathcal{L}^m \to \mathbb{C}P^1$ corresponds to the representation $\boldsymbol{\nu}_m$ in the sense that it can be expressed as

$$\mathcal{L}^m = \mathrm{SU}(2) \times_{\mathrm{U}(1)} \underline{S}_m, \tag{3.6}$$

where the quotient on $\mathrm{SU}(2) \times \underline{S}_m$ is by the U(1) action $\zeta \cdot (g, v) = (g\zeta^{-1}, \zeta^m v)$ for $g \in \mathrm{SU}(2), v \in \underline{S}_m$, and $\zeta \in \mathrm{U}(1)$. The action of SU(2) on $\mathrm{SU}(2) \times \underline{S}_m$ given by $g' \cdot (g, v) = (g'g, v)$ descends to an action on (3.6). Any SU(2)-equivariant Hermitian vector bundle over the sphere is a Whitney sum of bundles (3.6).

There is an alternative description in terms of the holomorphic line bundle $\mathcal{O}(m) \to \mathbb{C}P^1$ defined as the mth power of the tautological bundle over the complex projective line. The universal complexification of the Lie group SU(2) is $\mathrm{SL}(2,\mathbb{C})$, and we may regard the sphere as a projective variety through the natural diffeomorphism $\mathbb{C}P^1 \cong \mathrm{SU}(2)/\mathrm{U}(1) \cong \mathrm{SL}(2,\mathbb{C})/\mathrm{P}$, where P is the parabolic subgroup of lower triangular matrices in $\mathrm{SL}(2,\mathbb{C})$. The SU(2) action on (3.6) lifts to a smooth $\mathrm{SL}(2,\mathbb{C})$ action, and the complexification of (3.6) is realized as the $\mathrm{SL}(2,\mathbb{C})$-equivariant line bundle

$$\mathcal{O}(m) = \mathrm{SL}(2,\mathbb{C}) \times_{\mathrm{P}} \underline{S}_m \tag{3.7}$$

over $\mathbb{C}P^1$. Only the Cartan subgroup $\mathbb{C}^\times \subset P$ of nonzero complex numbers acts nontrivially on the modules $\underline{S}_m$, with the $\mathbb{C}^\times$ action defined analogously to (3.5). The two descriptions are equivalent after the introduction of a Hermitian metric on the fibers of $\mathcal{O}(m)$. This holomorphic line bundle has transition function y^m transforming sections from the northern hemisphere to the southern hemisphere of S^2. However, the monopole connection (3.1) is transformed on the intersection of the two patches covering $\mathbb{C}P^1$ via the transition function $(y/\overline{y})^{m/2}$, which is the unitary reduction of the holomorphic transition function y^m. Thus the bundle $\mathcal{O}(m)$ regarded as a Hermitian line bundle has transition function $(y/\overline{y})^{m/2}$ and can be substituted for the monopole bundle $\mathcal{L}^m$.

SU(2)-invariant gauge potential: The form of our ansatz for the gauge connection on $\mathcal{M}_q \times \mathbb{C}P^1$ is fixed by imposing invariance under the SU(2) isometry group of $\mathbb{C}P^1$ acting through rigid rotations of the sphere. Let $\mathcal{E} \to \mathcal{M}_q \times \mathbb{C}P^1$ be an SU(2)-equivariant U(k) bundle, with the group SU(2) acting trivially on $\mathcal{M}_q$ and in the standard way on $\mathbb{C}P^1 = \mathrm{SU}(2)/\mathrm{U}(1)$. Let $\mathcal{A}$ be a connection on $\mathcal{E}$. Imposing the condition of SU(2)-equivariance means that we should look for representations of the group SU(2) inside the U(k) structure group, i.e., for homomorphisms $\rho : \mathrm{SU}(2) \to \mathrm{U}(k)$. The ansatz for $\mathcal{A}$ is thus given by k-dimensional representations of SU(2). Up to isomorphism, for each positive integer d there is a unique irreducible SU(2)-module $\underline{V}_d \cong \mathbb{C}^d$ of dimension d. Therefore, for each positive integer m, the module

$$\underline{\mathcal{V}} = \bigoplus_{i=0}^{m} \underline{V}_{k_i}, \quad \text{with } \sum_{i=0}^{m} k_i = k \tag{3.8}$$

gives a representation ρ of SU(2) inside U(k). The total number of such homomorphisms is the number of partitions of the positive integer rank $(\mathcal{E}) = k$ into $\leqslant (m+1)$ components. The original U(k) gauge symmetry is then broken down to the centralizer subgroup of $\rho(\mathrm{SU}(2))$ in U(k) as

$$\mathrm{U}(k) \to \prod_{i=0}^{m} \mathrm{U}(k_i). \tag{3.9}$$

It is natural to allow for gauge transformations to accompany the SU(2) action,[32] and so some "twisting" can occur in the reduction of the connection $\mathcal{A}$ on $\mathcal{M}_q \times \mathbb{C}P^1$. The $\mathbb{C}P^1$ dependence in this case is uniquely determined by the above SU(2)-invariant Dirac monopole configurations.[33,34] The $u(k)$-valued gauge potential $\mathcal{A}$ thus splits into $k_i \times k_j$ blocks $\mathcal{A}^{ij}$,

$$\mathcal{A} = (\mathcal{A}^{ij}) \quad \text{with } \mathcal{A}^{ij} \in \mathrm{Hom}(\underline{V}_{k_j}, \underline{V}_{k_i}), \tag{3.10}$$

where the indices $i, j, \ldots$ run over $0, 1, \ldots, m, k_0 + k_1 + \cdots + k_m = k$ and

$$\mathcal{A}^{ii} = A^i(x') \otimes 1 + \mathbf{1}_{k_i} \otimes a_{m-2i}(y), \tag{3.11}$$

$$\mathcal{A}^{ii+1} =: \Phi_{i+1} = \phi_{i+1}(x') \otimes \overline{\beta}(y), \tag{3.12}$$

$$\mathcal{A}^{i+1i} = -(\mathcal{A}^{ii+1})^\dagger = -(\Phi_{i+1})^\dagger = -\phi_{i+1}^\dagger(x') \otimes \beta(y), \tag{3.13}$$

$$\mathcal{A}^{ii+l} = 0 = \mathcal{A}^{i+li} \quad \text{for } l \geqslant 2. \tag{3.14}$$

Here

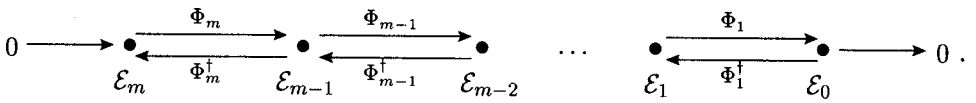
$$\beta = \frac{R\,\mathrm{d}y}{R^2 + y\overline{y}} \quad \text{and} \quad \overline{\beta} = \frac{R\,\mathrm{d}\overline{y}}{R^2 + y\overline{y}} \tag{3.15}$$

are the unique covariantly constant, SU(2)-invariant forms of type (1,0) and (0,1) such that the Kähler (1,1)-form on $\mathbb{C}P^1$ is $4R^2\beta\wedge\overline{\beta}$. They, respectively, take values in the bundles $\mathcal{L}^2$ and $\mathcal{L}^{-2}$.

It is easy to see that the gauge potential $\mathcal{A}$ given by (3.11)–(3.14) is anti-Hermitian and SU(2)-invariant. Note that we do not use the Einstein summation convention for the repeated indices i labelling the components of the irreducible representation $\underline{V}_{m+1} \cong \mathbb{C}^{m+1}$ of the group SU(2). Thus the gauge potential $\mathcal{A} \in u(k)$ decomposes into gauge potentials $A^i \in u(k_i)$ with $i = 0, 1, \ldots, m$ and a multiplet of scalar fields ϕ_{i+1} with $i = 0, 1, \ldots, m-1$ transforming in the bifundamental representations $\underline{V}_{k_i} \otimes \underline{V}_{k_i+1}^\vee$ of the subgroup $\mathrm{U}(k_i) \times \mathrm{U}(k_i+1)$ of the original $\mathrm{U}(k)$ gauge group. All fields (A^i, ϕ_{i+1}) depend only on the coordinates $x' \in \mathcal{M}_q$. Every SU(2)-invariant unitary connection $\mathcal{A}$ on $\mathcal{M}_q \times \mathbb{C}P^1$ is of the form given in (3.10)–(3.14),[34] which follow from the fact that the complexified cotangent bundle of $\mathbb{C}P^1$ is $\mathcal{L}^2 \otimes \mathcal{L}^{-2}$. This ansatz amounts to an equivariant decomposition of the original rank k SU(2)-equivariant bundle $\mathcal{E} \to \mathcal{M}_q \times \mathbb{C}P^1$ in the form

$$\mathcal{E} = \bigoplus_{i=0}^{m} \mathcal{E}_i \quad \text{with } \mathcal{E}_i = E_{k_i} \otimes \mathcal{L}^{m-2i}, \tag{3.16}$$

where $E_{ki} \to \mathcal{M}_q$ is a Hermitian vector bundle of rank k_i with typical fiber the module $\underline{V}_{ki}$, and $\mathcal{E}_i \to \mathcal{M}_q \times \mathbb{C}P^1$ is the bundle with fibers $(\mathcal{E}_i)_{(x',y,\overline{y})} = (E_{k_i})_{x'} \otimes (\mathcal{L}^{m-2i})_{(y,\overline{y})}$. By regarding $\Phi_i \in \mathrm{Hom}(\mathcal{E}_i, \mathcal{E}_{i-1}) \cong \mathrm{H}^0(\mathcal{M}_q \times \mathbb{C}P^1; \mathcal{E}_{i-1} \otimes \mathcal{E}_i^\vee)$ for $i = 1, \ldots, m$ and defining $\Phi_0 := 0 =: \Phi_{m+1}$, we can summarize our ansatz through the following chain of bundles:



(3.17)

Field strength tensor: The calculation of the curvature (2.9) for $\mathcal{A}$ of the form (3.10)–(3.14) yields,

$$\mathcal{F} = (\mathcal{F}^{ij}) \quad \text{with } \mathcal{F}^{ij} = \mathrm{d}\mathcal{A}^{ij} + \sum_{l=0}^{m} \mathcal{A}^{il} \wedge \mathcal{A}^{lj}, \tag{3.18}$$

where

$$\mathcal{F}^{ii} = F^i + f_{m-2i} + (\phi_{i+1}\phi_{i+1}^\dagger - \phi_i^\dagger\phi_i)\beta\wedge\overline{\beta}, \tag{3.19}$$

$$\mathcal{F}^{ii+1} = D\phi_{i+1}\wedge\overline{\beta}, \tag{3.20}$$

$$\mathcal{F}^{i+1i} = -(\mathcal{F}^{ii+1})^\dagger = -(D\phi_{i+1})^\dagger\wedge\beta, \tag{3.21}$$

$$\mathcal{F}^{ii+l} = 0 = \mathcal{F}^{i+li} \quad \text{for } l \geqslant 2. \tag{3.22}$$

Here we have defined $F^i := \mathrm{d}A^i + A^i\wedge A^i = \frac{1}{2}F^i_{\mu'\nu'}(x')\mathrm{d}x^{\mu'}\wedge\mathrm{d}x^{\nu'}$ and introduced the bifundamental covariant derivatives,

$$D\phi_{i+1} := \mathrm{d}\phi_{i+1} + A^i\phi_{i+1} - \phi_{i+1}A^{i+1}. \tag{3.23}$$

From (3.19)–(3.22) we find the nonvanishing field strength components

$$\mathcal{F}^{ii}_{\mu'\nu'} = F^i_{\mu'\nu'}, \tag{3.24}$$

$$\mathcal{F}^{ii+1}_{\mu'\overline{y}} = \frac{R}{R^2+y\overline{y}}D_{\mu'}\phi_{i+1} = -(\mathcal{F}^{i+1i}_{\mu' y})^\dagger, \tag{3.25}$$

$$\mathcal{F}^{ii}_{y\overline{y}} = -\frac{R^2}{(R^2+y\overline{y})^2}(m-2i+\phi_i^\dagger\phi_i - \phi_{i+1}\phi_{i+1}^\dagger). \tag{3.26}$$

IV. DESCRIPTION OF THE ANSATZ

In this section we shall clarify some features of the ansatz constructed in the preceding section from three different points of view. To set the stage for the string theory interpretations of the solutions that we will construct later on, we begin by indicating how the ansatz can be interpreted in terms of configurations of *D*-branes in Type II superstring theory. This leads into a discussion of how the ansatz is realized in topological *K*-theory, which classifies the Ramond-Ramond charges of these brane systems, and we will derive the decomposition (3.16) directly within the framework of SU(2)-equivariant *K*-theory. We will then explain how seeking explicit realizations of our ansatz is equivalent to finding representations of the A_{m+1} quiver. One of the goals of the subsequent sections will be to establish the precise link between these three descriptions, showing that they are all equivalent.

Physical interpretation: Before entering into the formal mathematical characterizations of the ansatz of the preceding section, let us first explain the physical situation which they will describe. Our ansatz implies an equivalence between brane-antibrane systems on $\mathcal{M}_q$ and wrapped branes on $\mathcal{M}_q\times\mathbb{C}P^1$. In the standard *D*-brane interpretation, our initial rank k Hermitian vector bundle $\mathcal{E}\to\mathcal{M}_q\times\mathbb{C}P^1$ corresponds to k coincident $D(q+1)$-branes wrapping the world volume manifold $\mathcal{M}_q\times\mathbb{C}P^1$. The condition of SU(2)-equivariance imposed on this bundle fixes the dependence on the coordinates of $\mathbb{C}P^1$ and breaks the gauge group U(k) as in (3.9). The rank k_i sub-bundle $E_{k_i}\to\mathcal{M}_q$ of this bundle is twisted by the Dirac multimonopole bundle $\mathcal{L}^{m-2i}\to\mathbb{C}P^1$. The system of k coincident $D(q+1)$-branes thereby splits into blocks of $k_0+k_1+\cdots+k_m=k$ coincident $D(q+1)$-branes, associated to irreducible representations of SU(2) and wrapping a common sphere $\mathbb{C}P^1$ with the monopole fields. This system is equivalent to a system of $k_0+k_1+\cdots+k_m=k$ $D(q-1)$-branes carrying different magnetic fluxes on their common world volume $\mathcal{M}_q$. The $D(q-1)$-branes which carry negative magnetic flux have opposite orientation with respect to the $D(q-1)$-branes with positive magnetic flux, i.e., they are antibranes. This will become evident

from the K-theory formalism, which will eventually lead to an explicit world volume construction, and also from the explicit calculation of the topological charges of the instanton solutions. In addition to the usual Chan-Paton gauge field degrees of freedom $A^i \in \mathrm{End}(E_{k_i})$ living on each block of branes, the field content on the brane configuration contains bifundamental scalar fields $\phi_{i+1} \in \mathrm{Hom}(E_{k_{i+1}}, E_{k_i})$ corresponding to massless open string excitations between neighboring blocks of k_i and k_{i+1} $D(q-1)$-branes. Other excitations are suppressed by the condition of SU(2)-equivariance.

However, as we shall see explicitly in the following, the fields ϕ_{i+1} should not be regarded as tachyon fields, but rather only as (holomorphic) Higgs fields responsible for the symmetry breaking (3.9). Only the brane-antibrane pairs whose constituents carry equal and opposite monopole charges are neutral and can thus annihilate to the vacuum, which carries no monopole charge (although it can carry a K-theory charge from the virtual Chan-Paton bundles over $\mathcal{M}_q$). Other brane pairs are stable because their overall nonvanishing Chern number over $\mathbb{C}P^1$ is an obstruction to decay, and the monopole bundles thereby act as a source of flux stabilization for such brane pairs by giving them a conserved topological charge. In particular, neighboring blocks of $D(q-1)$-branes are marginally bound by the massless open strings stretching between them. In this sense, the SU(2)-invariant reduction of D-branes on $\mathcal{M}_q \times \mathbb{C}P^1$ induces brane-antibrane systems on $\mathcal{M}_q$. Note that while the system on $\mathcal{M}_q$ is generically unstable, the original brane configuration on $\mathcal{M}_q \times \mathbb{C}P^1$ can be nonetheless stable.

K-theory charges: Given that the charges of configurations of D-branes in string theory are classified topologically by K-theory,[10,11,13] let us now seek the K-theory representation of the above physical situation. The one-monopole bundle $\mathcal{L}$ is a crucial object in establishing the Bott periodicity isomorphism

$$K(\mathcal{M}_q \times \mathbb{C}P^1) = K(\mathcal{M}_q) \tag{4.1}$$

in topological K-theory. The isomorphism is generated by taking the K-theory product of the tachyon field ϕ_1, $E_{k_1} \to E_{k_0}$ of a virtual bundle $[E_{k_0}, E_{k_1}; \phi_1] \in K(\mathcal{M}_q)$ with that of the class of the line bundle $\mathcal{L}$ which represents the Bott generator of $\widetilde{K}(\mathbb{C}P^1) = Z$.[11] The topological equivalence (4.1) then implies the equivalence of brane-antibrane systems on $\mathcal{M}_q \times \mathbb{C}P^1$ and $\mathcal{M}_q$. with the brane and antibrane systems each carrying a single unit of monopole charge. When they carry $m > 1$ units of charge, the isomorphism breaks down, and it is necessary to introduce the notion of "D-operations" to establish the relationship.[30] While these operations are natural, they are not isomorphisms and they reflect the fact that the explicit solutions in this setting are not SU(2)-invariant, so that the equivalence breaks downdue to spurious moduli dependences of the system of branes on the $\mathbb{C}P^1$ factor. In what follows we will derive a modification of the relation (4.1) in equivariant K-theory which will naturally give the desired isomorphism, reflecting the equivalence of the brane-antibrane systems for arbitrary monopole charge, and bypass the need for introducing D-operations. This is only possible by augmenting the basic brane-antibrane system to a *chain* of $(m+1)$ branes and antibranes with varying units of monopole charge as described above, and we will thereby arrive at an independent purely K-theoretic derivation of our ansatz.

The representation ring R_G of a group G (Ref. 35) is the Grothendieck ring of the category of finite-dimensional representations of G, with addition induced by direct sum of vector spaces, $[\underline{V}] + [\underline{V}'] := [\underline{V} \oplus \underline{V}']$, and multiplication induced by tensor product of modules, $[\underline{V}] \cdot [\underline{V}'] := [\underline{V} \otimes \underline{V}']$. As an Abelian group it is generated by the irreducible representations of G. Alternatively, since the isomorphism class of a G-module $\underline{V}$ is completely determined by its character $\chi_{\underline{V}} : G \to \mathbb{C}$, the map $\underline{V} \mapsto \chi_{\underline{V}}$ identifies R_G as a subring of the ring of G-invariant functions on G. If $\mathcal{M}_q$ is a G-space, then the Grothendieck group of G-equivariant bundles over $\mathcal{M}_q$ is called the G-equivariant K-theory group $K_G(\mathcal{M}_q)$. This group unifies ordinary K-theory with group representation theory, in the sense that for the trivial space $K_G(\mathrm{pt}) = R_G$ is the representation ring of G, while for the trivial group $K_{\mathrm{id}}(\mathcal{M}_q) = K(\mathcal{M}_q)$ is the ordinary K-theory of $\mathcal{M}_q$. The former property

implies that $K_G(\mathcal{M}_q)$ is an R_G-module and the coefficient ring in equivariant K-theory is R_G, rather than just $\mathbb{Z}$ as in the ordinary case. If the G-action on $\mathcal{M}_q$ is trivial, then any G-equivariant bundle $E\to\mathcal{M}_q$ may be decomposed as a finite Whitney sum

$$E=\bigoplus_{\underline{V}\in \mathrm{Rep}(G)} \mathrm{Hom}_G(\mathbb{1}_{\underline{V}},E)\otimes \mathbb{1}_{\underline{V}}, \tag{4.2}$$

where $\mathbb{1}_{\underline{V}}=\mathcal{M}_q\times \underline{V}$ is the trivial bundle over $\mathcal{M}_q$ with fiber the irreducible G-module $\underline{V}$. It follows that for trivial G-actions the equivariant K-theory takes the simple form

$$K_G(\mathcal{M}_q)=K(\mathcal{M}_q)\otimes R_G. \tag{4.3}$$

The K_G-functor behaves analogously to the ordinary K-functor, and in addition K_G is functorial with respect to group homomorphisms. A useful computational tool is the equivariant excision theorem. If F is a closed subgroup of G and $\mathcal{M}_q$ is an F-space, then the inclusion $\iota: F\hookrightarrow G$ induces an isomorphism[35]

$$\iota^*: K_G(G\times_F \mathcal{M}_q)\xrightarrow{\approx} K_F(\mathcal{M}_q), \tag{4.4}$$

where the quotient on $G\times\mathcal{M}_q$ is by the F-action $f\cdot(g,x')=(gf^{-1},f\cdot x')$ for $g\in G, x'\in\mathcal{M}_q$ and $f\in F$. The G-action on $G\times_F\mathcal{M}_q$ descends from that on $G\times\mathcal{M}_q$ given by $g'\cdot(g,x')=(g'g,x')$.

Let us specialize to our case of interest by taking $G=\mathrm{SU}(2)$, $F=\mathrm{U}(1)$ and the trivial action of SU(2) on the space $\mathcal{M}_q$. Using (4.3) and (4.4) we may then compute

$$K_{\mathrm{SU}(2)}(\mathcal{M}_q\times\mathbb{C}P^1)=K_{\mathrm{SU}(2)}(\mathrm{SU}(2)\times_{\mathrm{U}(1)}\mathcal{M}_q)=K_{\mathrm{U}(1)}(\mathcal{M}_q)=K(\mathcal{M}_q)\otimes R_{\mathrm{U}(1)}. \tag{4.5}$$

This K-theoretic equality asserts a one-to-one correspondence between classes of SU(2)-equivariant bundles over $\mathcal{M}_q\times\mathbb{C}P^1$ and classes of U(1)-equivariant bundles over $\mathcal{M}_q$ with U(1) acting trivially on $\mathcal{M}_q$. The isomorphism (4.5) of equivariant K-theory groups is constructed explicitly as follows.[35] Given an SU(2)-equivariant bundle $\mathcal{E}\to\mathcal{M}_q\times\mathbb{C}P^1$, we can induce a U(1)-equivariant bundle $E=i^*\mathcal{E}\to\mathcal{M}_q$ by restriction to the slice $\mathcal{M}_q\cong\mathcal{M}_q\times\mathrm{U}(1)/\mathrm{U}(1)\xrightarrow{\iota}\mathcal{M}_q\times\mathrm{SU}(2)/\mathrm{U}(1)$. Conversely, if $E\to\mathcal{M}_q$ is a U(1)-equivariant bundle, then $\mathcal{E}=\mathrm{SU}(2)\times_{\mathrm{U}(1)}E\to\mathcal{M}_q\times\mathbb{C}P^1$ is an SU(2)-equivariant bundle, where the quotient on $\mathrm{SU}(2)\times E$ is by the action of U(1) on both factors, $\zeta\cdot(g,e)=(g\zeta^{-1},\zeta\cdot e)$ for $g\in\mathrm{SU}(2), e\in E, \zeta\in\mathrm{U}(1)$, and the action of $g'\in\mathrm{SU}(2)$ on $\mathrm{SU}(2)\times_{\mathrm{U}(1)}E$ descends from that on $\mathrm{SU}(2)\times E$ given by $g'\cdot(g,e)=(g'g,e)$. This construction defines equivalence functors between the categories of SU(2)-equivariant vector bundles over $\mathcal{M}_q\times\mathbb{C}P^1$ and U(1)-equivariant vector bundles over $\mathcal{M}_q$, and hence the corresponding Grothendieck groups coincide, as in (4.5).

The role of the representation ring $R_{\mathrm{U}(1)}$ is unveiled by setting $\mathcal{M}_q=\mathrm{pt}$ in (4.5) to get

$$K_{\mathrm{SU}(2)}(\mathbb{C}P^1)=R_{\mathrm{U}(1)}, \tag{4.6}$$

which establishes a one-to-one correspondence between classes of homogeneous vector bundles over the sphere $\mathbb{C}P^1$ and classes of finite-dimensional representations of U(1). Since the corresponding irreducible representations are the $\boldsymbol{\nu}_m$ given by (3.5), the representation ring of U(1) is the ring of formal Laurent polynomials in the variable $\boldsymbol{\nu}_1$, $R_{\mathrm{U}(1)}=\mathbb{Z}[\boldsymbol{\nu}_1,\boldsymbol{\nu}_1^{-1}]$. Using (3.6) we can associate the monopole bundle $\mathcal{L}$ to the generator $\boldsymbol{\nu}_1$, and thereby identify (4.6) as the Laurent polynomial ring

$$K_{\mathrm{SU}(2)}(\mathbb{C}P^1)=\mathbb{Z}[\mathcal{L},\mathcal{L}^\vee]. \tag{4.7}$$

In particular, the relationship (4.5) can be expressed as

$$K_{\mathrm{SU}(2)}(\mathcal{M}_q \times \mathbb{C}P^1) = K(\mathcal{M}_q) \otimes \mathbb{Z}[\mathcal{L}, \mathcal{L}^\vee]. \tag{4.8}$$

This is the appropriate modification of the Bott periodicity isomorphism (4.1) to the present setting. The crucial difference now is that virtual bundles over $\mathcal{M}_q$ are multiplied by arbitrary powers of the one-monopole bundle, allowing us to extend the equivalence to arbitrary monopole charges $m \in \mathbb{Z}$. In the equivariant setting, there is no need to use external twists of the monopole bundle, nor the ensuing K-theory product as done in Ref. 30. The monopole fluxes are now naturally incorporated by the coefficient ring $R_{\mathrm{U}(1)}$ of the U(1)-equivariant K-theory, superseding the need for introducing D-operations.

It is instructive to see precisely how the correspondence (4.8) works. For this, it is convenient to work instead in the category of holomorphic $\mathrm{SL}(2,\mathbb{C})$-equivariant bundles.[34] If $\mathcal{E}$ is an SU(2)-equivariant vector bundle over $\mathcal{M}_q \times \mathbb{C}P^1$, then the action of SU(2) can be extended to an $\mathrm{SL}(2,\mathbb{C})$ action. Everything we have said above carries through by replacing the group SU(2) with its complexification $\mathrm{SL}(2,\mathbb{C})$ and the Cartan torus $\mathrm{U}(1) \subset \mathrm{SU}(2)$ with the subgroup $P \subset \mathrm{SL}(2,\mathbb{C})$ of lower triangular matrices. We are then interested in P-equivariant bundles over $\mathcal{M}_q$ with P acting trivially on $\mathcal{M}_q$. The Lie algebra $\mathrm{sl}(2,\mathbb{C})$ is generated by the three Pauli matrices,

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{4.9}$$

with the commutation relations

$$[\sigma_3, \sigma_\pm] = \pm 2\sigma_\pm \quad \text{and} \quad [\sigma_+, \sigma_-] = \sigma_3. \tag{4.10}$$

The Lie algebra of the subgroup P is generated by the elements σ_3 and σ_-, while the Cartan subgroup $\mathbb{C}^\times \subset P$ is generated by the element σ_3 with the corresponding irreducible representations being the $\boldsymbol{\nu}_m$ given by (3.5).

Since the manifold $\mathcal{M}_q$ carries a trivial action of the subgroup $\mathbb{C}^\times$, any $\mathbb{C}^\times$-equivariant bundle $E' \to \mathcal{M}_q$ can be written using (4.2) as a finite Whitney sum

$$E' = \bigoplus_{l \in \Delta(E')} E'_l \otimes \underline{S}_l, \tag{4.11}$$

where $\Delta(E') \subset \mathbb{Z}$ is the set of eigenvalues for the $\mathbb{C}^\times$-action on E' and $E'_l \to \mathcal{M}_q$ are bundles carrying the trivial $\mathbb{C}^\times$-action. The rest of the P-equivariant structure is determined by the generator σ_-. Since $[\sigma_3, \sigma_-] = -2\sigma_-$, the action of σ_- on $E'_l \otimes \underline{S}_l$ corresponds to holomorphic bundle morphisms $E'_l \to E'_{l-2}$ and the trivial σ_--action on the irreducible $\mathbb{C}^\times$-modules $\underline{S}_l$. Thus every indecomposable P-equivariant bundle $E' \to \mathcal{M}_q$ has weight set of the form $\Delta(E') = \{m_0, m_0 + 2, \ldots, m_{1-2}, m_1\}$ for some $m_0, m_1 \in \mathbb{Z}$ with $m_0 \leqslant m_1$. After an appropriate twist by a $\mathbb{C}^\times$-module and a relabelling, the σ_3-action is given by the $\mathbb{C}^\times$-equivariant decomposition,

$$E = \bigoplus_{i=0}^{m} E_{k_i} \otimes \underline{S}_{m-2i} \tag{4.12}$$

while the σ_--action is determined by a *chain*

$$0 \to E_{k_m} \xrightarrow{\phi_m} E_{k_{m-1}} \xrightarrow{\phi_{m-1}} \cdots \xrightarrow{\phi_2} E_{k_1} \xrightarrow{\phi_1} E_{k_0} \to 0 \tag{4.13}$$

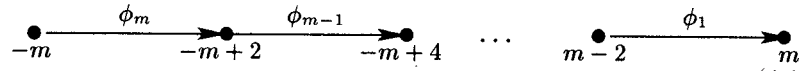
of holomorphic bundle maps between consecutive E_{k_i}'s. We can now consider the underlying U(1)-equivariant Hermitian vector bundle defined by the unitary $\mathrm{U}(k)$ reduction of the $\mathrm{GL}(k,\mathbb{C})$ structure group of the holomorphic bundle (4.12), after introducing a Hermitian metric on its fibers. Then the corresponding bundle $\mathcal{E} \to \mathcal{M}_q \times \mathbb{C}P^1$ is given by

$$\mathcal{E} = \mathrm{SU}(2) \times_{\mathrm{U}(1)} E. \tag{4.14}$$

Using (3.6) one finds that (4.14) coincides with the original equivariant decomposition (3.16). Conversely, given an SU(2)-equivariant bundle $\mathcal{E} \to \mathcal{M}_q \times \mathbb{C}P^1$, its restriction $E = \iota^* \mathcal{E}$ defines a U(l)-equivariant bundle over $\mathcal{M}_q$ which thereby admits an isotopical decomposition of the form (4.12) and $\mathcal{E}$ may be recovered from (4.14).

Quiver gauge theory: The ansatz for the gauge potential on $\mathcal{M}_q \times \mathbb{C}P^1$, represented symbolically by the bundle chain (3.17), corresponds to the disjoint union of two copies of the quiver,

A_{m+1} :



(4.15)

with the second copy obtained from (4.15) by reversing the directions of the arrows and replacing ϕ_i with $\phi_i^\dagger$ for each $i = 1, \ldots, m$. The vertices of the quiver are labelled by the degrees of the monopole bundles $\mathcal{L}^{m-2i}$, while the arrows correspond to module morphisms $\phi_i : \underline{V}_{k_i} \to \underline{V}_{k_{i-1}}$ (locally at each point $x' \in \mathcal{M}_q$). Equivalently, the vertices may be labelled by irreducible chiral representations of the group P. Thus our ansatz determines a representation of the quiver A_{m+1} in the category of complex vector bundles over the manifold $\mathcal{M}_q$.[36] Such a representation is called an A_{m+1}-bundle. Many properties of the explicit solutions that we construct later on find their most natural explanation in the context of such a quiver gauge theory, which provides a more refined description of the brane configurations than just their K-theory charges. This framework encompasses the algebraic and representation theoretic aspects of the problem.[37]

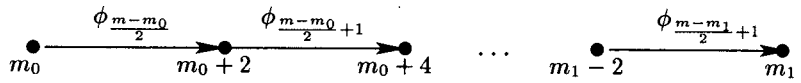
The quiver graph (4.15) is identical to the Dynkin diagram of the Lie algebra A_{m+1}. The adjacency matrix of the quiver has matrix elements specifying the number of links between each pair of vertices $m-2i$, $m-2j$, and in the case (4.15) it is given by $\mathrm{Adj}(\mathsf{A}_{m+1}) = (\delta_{i,j-1})_{i,j=0,1,\ldots,m}$. The matrix elements $C_{ij} = 2\delta_{ij} - \mathrm{Adj}(\mathsf{A}_{m+1})_{ij}$ are then identical to those of the Cartan matrix $C_{ij} = \vec{e}_i \cdot \vec{e}_j$, where $\vec{e}_i$, $i = 0, 1, \ldots, m$ are the simple roots of A_{m+1}. Corresponding to the gauge symmetry breaking (3.9), the dimension vector $\vec{k}_{\underline{V}} := (k_0, k_1, \ldots, k_m)$ can be regarded as a positive root of A_{m+1} associated with the Cartan matrix $C = (C_{ij})$ by writing it as

$$\vec{k}_{\underline{V}} = \sum_{i=0}^{m} k_i \vec{e}_i \quad \text{with } |\vec{k}_{\underline{V}}| := \sum_{i=0}^{m} k_i = k. \tag{4.16}$$

By Kac's theorem,[37] there is a one-to-one correspondence between the isomorphism classes of indecomposable representations of the quiver A_{m+1} and the set of positive roots of the Lie algebra A_{m+1}. This property is a consequence of the SU(2)-invariance of our ansatz.

Let us focus for a while on the case $\mathcal{M}_q = \mathrm{pt}$. In this case Eq. (3.16), with the m-monopole bundles $\mathcal{L}^m$ substituted everywhere by the holomorphic line bundles (3.7), gives a relation between the categories of homogeneous holomorphic vector bundles over $\mathbb{C}P^1 = \mathrm{SL}(2,\mathbb{C})/P$ and of finite-dimensional chiral representations of P, while the quiver representation further gives a relation with the Abelian category of finite-dimensional representations of A_{m+1}.[36] To describe this latter category, it is convenient to introduce the notion of a path P in A_{m+1}, which is generally defined as a sequence of arrows of the quiver which compose. In the present case any path is of the form

P :



(4.17)

with $-m \leq m_0 \leq m_1 \leq m$. We will denote it by the formal vector $|m_0, \ldots, m_1)$. The non-negative

integer $|\mathsf{P}| := 1/2(m_1 - m_0)$ is the length of the path (4.17). The trivial path of length 0 based at a single vertex m_0 is denoted $|m_0)$. The path algebra $\mathbb{C}\mathsf{A}_{m+1}$ of the quiver (4.15) is then defined as the algebra generated by all paths P of A_{m+1}, i.e., as the vector space

$$\mathbb{C}\mathsf{A}_{m+1} = \bigoplus_{\substack{m_0, m_1 = -m \\ m_0 \leq m_1}}^{m} \mathbb{C}|m_0, \dots, m_1) \tag{4.18}$$

together with the $\mathbb{C}$-linear multiplication induced by (left) concatenation of paths where possible,

$$|m_0, \dots, m_1) \cdot |n_0, \dots, n_1) = \delta_{m_1 n_0} |m_0, \dots, n_1). \tag{4.19}$$

This makes $\mathbb{C}\mathsf{A}_{m+1}$ into a finite-dimensional quasifree algebra. The path algebra has a natural $\mathbb{Z}_{m+1}$-grading by path length,

$$\mathbb{C}\mathsf{A}_{m+1} \bigoplus_{i=0}^{m} (\mathbb{C}\mathsf{A}_{m+1})_i \quad \text{with } (\mathbb{C}\mathsf{A}_{m+1})_i \bigoplus_{m_0 = -m}^{m-2i} \mathbb{C}|m_0, \dots, m_0 + 2i), \tag{4.20}$$

and can thereby be alternatively described as the tensor algebra over the ring

$$C_0 = \bigoplus_{i=0}^{m} \mathbb{C}|m - 2i) \cong \mathbb{C}^{m+1} \tag{4.21}$$

of the C_0-bimodule

$$C_1 = \bigoplus_{i=0}^{m} \mathbb{C}|m - 2i, m - 2i + 2). \tag{4.22}$$

The importance of the path algebra stems from the fact that the category of representations of the quiver A_{m+1} is equivalent to the category of (left) $\mathbb{C}\mathsf{A}_{m+1}$-modules.[37] Given a representation $\underline{W}_{m-2i} \to^{\eta_i} \underline{W}_{m-2i+2}$, $i = 1, \dots, m$, of A_{m+1}, the associated $\mathbb{C}\mathsf{A}_{m+1}$-module $\underline{\mathcal{W}}$ is

$$\underline{\mathcal{W}} = \bigoplus_{i=0}^{m} \underline{W}_{m-2i} \tag{4.23}$$

with multiplication extended $\mathbb{C}$-linearly from the definitions

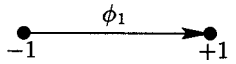
$$|m - 2i) \cdot w_j = \delta_{ij} w_j \quad \text{and} \quad |m - 2i, m - 2i + 2) \cdot w_j = \delta_{i,j+1} \eta_j(w_j) \tag{4.24}$$

for $w_j \in \underline{W}_{m-2j}$. Conversely, given a left $\mathbb{C}\mathsf{A}_{m+1}$-module $\underline{\mathcal{W}}$, we can set $\underline{W}_{m-2i} := |m-2i) \cdot \underline{\mathcal{W}}$ for $i = 0, 1, \dots, m$ and define $\eta_i : \underline{W}_{m-2i} \to \underline{W}_{m-2i+2}$ for $i = 1, \dots, m$ by

$$\eta_i(w_i) = |m - 2i, m - 2i + 2) \cdot w_i. \tag{4.25}$$

One can further show that morphisms of representations of A_{m+1} correspond to $\mathbb{C}\mathsf{A}_{m+1}$-module homomorphisms.[37] Thus, the problem of determining finite-dimensional representations of the quiver A_{m+1}, or equivalently homogeneous vector bundles over $\mathbb{C}P^1$, is equivalent to finding representations of its path algebra.

As an example, consider the A quiver,

A_2 : 

. (4.26)

It represents the standard brane-antibrane system, and as expected SU(2)-equivariance implies that it can only carry $m = 1$ unit of monopole charge.[30] The corresponding path algebra is

$$\mathbb{C}\mathsf{A}_2 = \mathbb{C}|-1) \oplus \mathbb{C}|+1) \oplus \mathbb{C}|-1,+1) = \begin{pmatrix} \mathbb{C} & \mathbb{C} \\ 0 & \mathbb{C} \end{pmatrix}. \tag{4.27}$$

Representations of this algebra yield the standard superconnections characterizing the low-energy field content on the world volume of a brane-antibrane system.[31] In the next section we will show how to generalize the superconnection formalism to account for representations of generic path algebras (4.18). Later on we shall write down explicit solutions with generic monopole charge $m \in \mathbb{Z}$ that also correspond to the basic brane-antibrane system.

Our technique for generating D-branes from a quiver gauge theory on $\mathcal{M}_q$ arises via a quotient with respect to a generalized SU(2)-action on Chan-Paton bundles over $\mathcal{M}_q \times \mathbb{C}P^1$. This new construction is rather different from the well-known quiver gauge theories that arise from orbifolds with respect to the action of a *discrete* group G.[38] In the latter case the nodes of a quiver represent the irreducible representation fractional branes into which a regular representation D-brane decays into when it is taken to an orbifold point of $\mathcal{M}_q/G$, and they can be thought of in terms of a projection of branes sitting on the leaves of the covering space $\mathcal{M}_q$. While our quiver gauge theory is fundamentally different, it shares many of the physical features of orbifold theories of D-branes. For instance, the blowing up of vortices on $\mathcal{M}_q$ into instantons on $\mathcal{M}_q \times \mathbb{C}P^1$ is reminescent of the blowing up of fractional $D(q-1)$-branes into $D(q+1)$-branes wrapping a noncontractible $\mathbb{C}P^1$that is used to resolve the orbifold singularity in $\mathcal{M}_q/G$. Our solutions provide explicit realizations of this blowing up phenomenon, but in a completely smooth setting.

V. DIMENSIONAL REDUCTION

The condition of SU(2)-equivariance uniquely prescribes a specific $\mathbb{C}P^1$ dependence for the gauge potential $\mathcal{A}$ and reduces the Yang-Mills equations (2.8) on $\mathcal{M}_q \times \mathbb{C}P^1$ to equations on $\mathcal{M}_q$. In this section we will formulate this reduction in detail and relate it to representations of the path algebra (4.18). This will be done by developing a new formalism of $\mathbb{Z}_{m+1}$-graded connections which describes the field content corresponding to the bundle chains (3.17) and (4.13), and which generalizes the standard superconnection field theories on the world volumes of brane-antibrane systems.[31] This formalism will be the crux to merging together the three interpretations of the preceding section.

Reduction of the Yang-Mills functional: The dimensional reduction of the Yang-Mills equations can be seen at the level of the Yang-Mills Lagrangian (2.7). Substituting (3.24)–(3.26) into (2.10) and performing the integral over $\mathbb{C}P^1$ we arrive at the action (a set of Yang-Mills coupling constants g^i_{YM}, $i=0,1,\ldots,m$ can be introduced via the redefinitions $A^i \mapsto g^i_{\mathrm{YM}} A^i$)

$$\begin{aligned} S_{\mathrm{YM}} := \int_{\mathcal{M}_q \times \mathbb{C}P^1} \mathrm{d}^{q+2}x L_{\mathrm{YM}} = \pi R^2 \int_{\mathcal{M}_q} \mathrm{d}^q x' \sqrt{g'} \sum_{i=0}^{m} \mathrm{tr}_{k_i \times k_i} \Big(& (F^i_{\mu'\nu'})^\dagger (F^{i\mu'\nu'}) + \frac{1}{R^2} (D_{\mu'} \phi_{i+1})(D^{\mu'} \phi_{i+1})^\dagger \\ & + \frac{1}{R^2} (D_{\mu'} \phi_i)^\dagger (D^{\mu'} \phi_i) + \frac{1}{2R^4} (m - 2i + \phi_i^\dagger \phi_i - \phi_{i+1} \phi_{i+1}^\dagger)^2 \Big), \end{aligned} \tag{5.1}$$

where $g' = |\det(g_{\mu'\nu'})|$. In the remainder of this paper we shall only consider static field configurations on $\mathcal{M}_q = \mathbb{R}^1 \times M_{2n}$ in the temporal gauge $\mathcal{A}_0 = 0$. In this case one can introduce the corresponding energy functional,

$$\begin{aligned} E_{\mathrm{YM}} = \pi R^2 \int_{M_{2n}} \mathrm{d}^{2n}x \sqrt{g_n} \sum_{i=0}^{m} \mathrm{tr}_{k_i \times k_i} \Big(& (F^i_{\mu\nu})^\dagger (F^{i\mu\nu}) + \frac{1}{R^2} (D_\mu \phi_{i+1})(D^\mu \phi_{i+1})^\dagger + \frac{1}{R^2} (D_\mu \phi_i)^\dagger (D^\mu \phi_i) \\ & + \frac{1}{2R^4} (m - 2i + \phi_i^\dagger \phi_i - \phi_{i+1} \phi_{i+1}^\dagger)^2 \Big), \end{aligned} \tag{5.2}$$

where $g_n = \det(g_{\mu\nu})$. The functional (5.2) is non-negative.

Graded connections: The energy functional (5.2) is analyzed most efficiently by introducing a

framework specific to connections on the rank k $\mathbb{Z}_{m+1}$-graded vector bundle,

$$E := \bigoplus_{i=0}^{m} E_{k_i} \tag{5.3}$$

over M_{2n} whose typical fiber is the module (3.8). The endomorphism algebra bundle corresponding to (5.3) is given by the direct sum decomposition,

$$\mathrm{End}(E) = \bigoplus_{i=0}^{m} \mathrm{End}(E_{k_i}) \oplus \bigoplus_{\substack{i,j=0 \\ i\neq j}}^{m} \mathrm{Hom}(E_{k_i}, E_{k_j}). \tag{5.4}$$

We may naturally associate to (5.4) a distinguished representation of the A_{m+1} quiver. For this, we note that the path algebra $\mathbb{C}\mathsf{A}_{m+1}$ is itself a $\mathbb{C}\mathsf{A}_{m+1}$-module, and that the elements $|m-2i) \in \mathbb{C}\mathsf{A}_{m+1}$ define a complete set of orthogonal projectors of the path algebra, i.e., $|m-2i)\cdot|m-2j) = \delta_{ij}|m-2i)$ for $i,j=0,1,\dots,m$ with $\Sigma_{i=0}^{m}|m-2i)=1$. Analogously to the construction of (4.23)–(4.25), we may thereby define a *projective* $\mathbb{C}\mathsf{A}_{m+1}$-module $\underline{\mathsf{P}}_i := |m-2i)\cdot\mathbb{C}\mathsf{A}_{m+1}$ for each $i=0,1,\dots,m$,[37] which is the subspace of $\mathbb{C}\mathsf{A}_{m+1}$ generated by all paths which start at the ith vertex of the quiver A_{m+1}. Then $(\underline{\mathsf{P}}_i)_{m-2j} \cong \mathbb{C}$ is the vector space generated by the path from the ith vertex to the jth vertex, and the corresponding dimension vector is

$$\vec{k}_{\underline{\mathsf{P}}_i} = \sum_{j=i}^{m} \vec{e}_j. \tag{5.5}$$

The modules $\underline{P}_i$, $i=0,1,\dots,m$ are exactly the set of all indecomposable projective representations of the A_{m+1} quiver,[37] with

$$\mathbb{C}\mathsf{A}_{m+1} = \bigoplus_{i=0}^{m} \underline{\mathsf{P}}_i. \tag{5.6}$$

The importance of this path algebra representation stems from the fact that, for any quiver representation (3.8), there is a natural isomorphism[37]

$$\mathrm{Hom}(\underline{\mathsf{P}}_i, \underline{\mathcal{V}}) \cong \underline{V}_{k_i}. \tag{5.7}$$

We may thereby identify $\mathrm{Hom}(\underline{V}_{k_j}, \underline{V}_{k_i})$ in terms of appropriate combinations of the spaces

$$\mathrm{Hom}(\underline{\mathsf{P}}_j, \underline{\mathsf{P}}_i) \cong |m-2j)\cdot\mathbb{C}\mathsf{A}_{m+1}\cdot|m-2i) \cong \mathbb{C}. \tag{5.8}$$

This is the vector space generated by the path from the ith vertex to the jth vertex of A_{m+1}. A natural representation of this path is by a matrix of dimension $(m+1)\times(m+1)$ with 1 in its (ij)th entry and 0's everywhere else. The path algebra (5.6) is thereby identified with the algebra of upper triangular $(m+1)\times(m+1)$ complex matrices.[37] For a given quiver representation (3.8), this algebra may be represented by assembling the chiral Higgs fields $\phi_1,\dots,\phi_m$ into the $k\times k$ matrix,

$$\boldsymbol{\phi}_{(m)} := \begin{pmatrix} 0 & \phi_1 & 0 & \dots & 0 \\ 0 & 0 & \phi_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \phi_m \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}, \tag{5.9}$$

with respect to the decomposition (5.3). This object generates a representation of the path algebra in the category of complex vector bundles over M_{2n}, corresponding to the off-diagonal $i<j$ components of the decomposition (5.4). The finite dimensionality of $\mathbb{C}\mathsf{A}_{m+1}$ is reflected in the property that generically

$$\boldsymbol{\phi}_{(m)}, (\boldsymbol{\phi}_{(m)})^2, \ldots, (\boldsymbol{\phi}_{(m)})^m \neq 0 \quad \text{but } (\boldsymbol{\phi}_{(m)})^{m+1} = 0. \tag{5.10}$$

The field configuration (5.9) generates the basic zero-form component of a geometric object that we shall refer to as a "$\mathbb{Z}_{m+1}$-graded connection" on M_{2n}. For $m=1$ it corresponds to a standard superconnection,[39] while for $m>1$ it is the appropriate entity that constructs representations corresponding to the enlargement of the path algebra $\mathbb{C}\mathsf{A}_{m+1}$. Its matrix form is similar to (3.10)–(3.14), but without the one-forms on $\mathbb{C}P^1$.

To formulate the definition precisely, we note that the algebra $\Omega(M_{2n},E)$ of differential forms on M_{2n} with values in the bundle (5.3) has a natural $\mathbb{Z}\times\mathbb{Z}_{m+1}$ grading, where the $\mathbb{Z}$-grading is by form degree. We can thereby induce a total $\mathbb{Z}_{m+1}$-grading by the decomposition

$$\Omega_\bullet(M_{2n},E) = \bigoplus_{p=0}^{m} \Omega_{(p)}(M_{2n},E) \quad \text{with } \Omega_{(p)}(M_{2n},E) = \bigoplus_{i+j\equiv_{m+1}p} \Omega^i(M_{2n},E_{k_j}), \tag{5.11}$$

where $\equiv_{m+1}$ denotes congruence modulo $(m+1)$. By using (5.4) and the usual tensor product grading, this induces a $\mathbb{Z}_{m+1}$-grading on the corresponding endomorphism algebra as

$$\Omega_\bullet(M_{2n},\mathrm{End}\,E) = \bigoplus_{p=0}^{m} \Omega_{(p)}(M_{2n},\mathrm{End}\,E) \tag{5.12}$$

with

$$\Omega_{(p)}(M_{2n},\mathrm{End}\,E) = \bigoplus_{i=0}^{m} \bigoplus_{a=0}^{p} \bigoplus_{i_a\equiv_{m+1}(p-a)} \Omega^{i_a}(M_{2n}) \otimes \mathrm{Hom}(E_{k_i},E_{k_{i+a}}). \tag{5.13}$$

A *graded connection* on (5.11) is defined to be a linear operator $\Omega_\bullet(M_{2n},E)\to\Omega_{\bullet+1}(M_{2n},E)$ which shifts the total $\mathbb{Z}_{m+1}$-grading by 1 modulo $(m+1)$, i.e., an element of

$$\Omega_{(1)}(M_{2n},\mathrm{End}\,E) = \bigoplus_{i=0}^{m}\Bigg(\bigoplus_{i_1\equiv_{m+1}1} \Omega^{i_1}(M_{2n}) \otimes \mathrm{End}(E_{k_i}) \oplus \bigoplus_{i_0\equiv_{m+1}0} \Omega^{i_0}(M_{2n}) \otimes \mathrm{Hom}(E_{k_i},E_{k_{i+1}})\Bigg), \tag{5.14}$$

and which satisfies the usual Leibniz rule on $\Omega(M_{2n})$. As in the standard cases, the $\mathbb{Z}_{m+1}$-graded connections form an affine space modelled on a set of local operators.

In our case we retain only the $i_0=0$ and $i_1=1$ components of (5.14) corresponding to the lowest lying massless degrees of freedom on the given configuration of D-branes. From the Leibniz rule it follows that the pertinent graded connections are then of the form $(d+\mathbf{A}^{(m)}+(\boldsymbol{\phi}_{(m)})+(\boldsymbol{\phi}_{(m)})^\dagger)$, where

$$\mathbf{A}^{(m)} := \sum_{i=0}^{m} A^i \otimes \Pi_i \tag{5.15}$$

and $\Pi_i : E\to E_{k_i}$ are the canonical orthogonal projections of rank 1,

$$\Pi_i\Pi_j = \delta_{ij}\Pi_i, \tag{5.16}$$

which may be represented, with respect to the decomposition (5.3), by diagonal matrices $\Pi_i = (\delta_{ji}\delta_{li})_{j,l=0,1,\ldots,m}$ of unit trace. In this geometric framework all ϕ_i are assumed to anticommute with a given local basis dx^μ of the cotangent bundle of the Kähler manifold M_{2n}, as if they were m basic odd complex elements of a superalgebra. This requisite property may be explicitly realized by extending the graded connection formalism to $M_{2n}\times\mathbb{C}P^1$. For this, we rewrite the ansatz (3.10)–(3.15) in terms of the above field configurations as

$$\mathcal{A}_\mu = (\mathbf{A}^{(m)})_\mu \otimes 1, \tag{5.17}$$

$$\mathcal{A}_y = \mathbf{1}_k \otimes (\mathbf{a}^{(m)})_y - (\boldsymbol{\phi}_{(m)})^\dagger \otimes \beta_y, \tag{5.18}$$

$$\mathcal{A}_{\overline{y}} = \mathbf{1}_k \otimes (\mathbf{a}^{(m)})_{\overline{y}} + (\boldsymbol{\phi}_{(m)}) \otimes \overline{\beta_{\overline{y}}}, \tag{5.19}$$

where

$$\mathbf{a}^{(m)} := \sum_{i=0}^{m} a_{m-2i} \otimes \Pi_i \tag{5.20}$$

and $\Pi_i : \mathcal{E} \to \mathcal{E}_i$ are the canonical projections on (3.16). The coupling of $\boldsymbol{\phi}_{(m)}$ to $\mathrm{d}\overline{y}$ in (5.19) yields the desired anticommutativity with $\mathrm{d}x^\mu$.

Alternatively, we may use the canonical isomorphism $\Omega(M_{2n} \times \mathbb{C}P^1) \cong C\ell(M_{2n} \times \mathbb{C}P^1)$ to map the cotangent basis $\mathrm{d}x^{\hat{\mu}} \mapsto \Gamma^{\hat{\mu}}$ onto the generators of the Clifford algebra

$$\Gamma^{\hat{\mu}}\Gamma^{\hat{\nu}} + \Gamma^{\hat{\nu}}\Gamma^{\hat{\mu}} = -2g^{\hat{\mu}\hat{\nu}}\mathbf{1}_{2^{n+1}} \quad \text{with } \hat{\mu}, \hat{\nu} = 1, \ldots, 2n+2. \tag{5.21}$$

The gamma matrices in (5.21) may be decomposed as

$$\{\Gamma^{\hat{\mu}}\} = \{\Gamma^\mu, \Gamma^y, \Gamma^{\overline{y}}\} \quad \text{with} \quad \Gamma^\mu = \gamma^\mu \otimes \mathbf{1}_2, \quad \Gamma^y = \gamma \otimes \gamma^y, \quad \text{and} \quad \Gamma^{\overline{y}} = \gamma \otimes \gamma^{\overline{y}}, \tag{5.22}$$

where the $2^n \times 2^n$ matrices $\gamma^\mu = -(\gamma^\mu)^\dagger$ act on the spinor module $\underline{\Delta}(M_{2n})$ over the Clifford algebra $C\ell(M_{2n})$,

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = -2g^{\mu\nu}\mathbf{1}_{2^n} \quad \text{with } \mu, \nu = 1, \ldots, 2n, \tag{5.23}$$

while

$$\gamma = \frac{i^n}{(2n)!\sqrt{g_n}}\epsilon_{\mu_1\cdots\mu_{2n}}\gamma^{\mu_1}\cdots\gamma^{\mu_{2n}} \quad \text{with } (\gamma)^2 = \mathbf{1}_{2^n} \quad \text{and} \quad \gamma\gamma^\mu = -\gamma^\mu\gamma \tag{5.24}$$

is the corresponding chirality operator. Here $\epsilon_{\mu_1\cdots\mu_{2n}}$ is the Levi-Civita symbol with $\epsilon_{12\cdots 2n} = +1$. The action of the Clifford algebra $C\ell(\mathbb{C}P^1)$ on the spinor module $\underline{\Delta}(\mathbb{C}P^1)$ is generated by

$$\gamma^y = \frac{1}{R^2}(R^2 + y\overline{y})\sigma^y \quad \text{and} \quad \gamma^{\overline{y}} = \frac{1}{R^2}(R^2 + y\overline{y})\sigma^{\overline{y}} \tag{5.25}$$

with constant 2×2 Pauli matrices $\sigma^{\overline{y}} = \sigma_-$ and $\sigma^y = -\sigma_+$ obeying $[\sigma^y, \sigma^{\overline{y}}] = -\sigma_3$. The gauge potential (3.10)–(3.14) may then be written in an algebraic form as

$$\hat{\mathcal{A}} := \Gamma^{\hat{\mu}}\mathcal{A}_{\hat{\mu}} = \gamma^\mu(\mathbf{A}^{(m)})_\mu \otimes \mathbf{1}_2 + (\boldsymbol{\phi}_{(m)})\gamma \otimes \gamma^{\overline{y}}\overline{\beta_{\overline{y}}} - (\boldsymbol{\phi}_{(m)})^\dagger\gamma \otimes \gamma^y\beta_y + \gamma \otimes (\gamma^y(\mathbf{a}^{(m)})_y + y^{\overline{y}}(\mathbf{a}^{(m)})_{\overline{y}}), \tag{5.26}$$

and the coupling of (5.9) with the chirality operator (5.24) realizes the desired anticommutativity with the one-form representatives γ^μ. Note that the products

$$(\boldsymbol{\phi}_{(m)})\gamma \otimes \gamma^{\overline{y}}\overline{\beta_{\overline{y}}} = \frac{1}{R}(\boldsymbol{\phi}_{(m)})\gamma \otimes \sigma^{\overline{y}} \quad \text{and} \quad (\boldsymbol{\phi}_{(m)})^\dagger\gamma \otimes \gamma^y\beta_y = \frac{1}{R}(\boldsymbol{\phi}_{(m)})^\dagger\gamma \otimes \sigma^y \tag{5.27}$$

are independent of the coordinates $(y, \overline{y}) \in \mathbb{C}P^1$.

The curvature $(d + \mathbf{A}^{(m)} + (\boldsymbol{\phi}_{(m)}) + (\boldsymbol{\phi}_{(m)})^\dagger)^2 \in \Omega_{(2)}(M_{2n}, \mathrm{End}\, E)$ of the graded connection is also most elegantly expressed through dimensional reduction from $M_{2n} \times \mathbb{C}P^1$. From (3.18)–(3.26) it is given by

$$\hat{\mathcal{F}} := \frac{1}{4}[\Gamma^{\hat{\mu}},\Gamma^{\hat{\nu}}]\mathcal{F}_{\hat{\mu}\hat{\nu}} = \frac{1}{4}[\gamma^{\mu},\gamma^{\nu}](\mathbf{F}^{(m)})_{\mu\nu}\otimes\mathbf{1}_2 - \frac{1}{R}\gamma(\gamma^{\mu}D_{\mu}\boldsymbol{\phi}_{(m)})^{\dagger}\otimes\sigma^{y} - \frac{1}{R}\gamma(\gamma^{\mu}D_{\mu}\boldsymbol{\phi}_{(m)})\otimes\sigma^{\overline{y}}$$
$$+ \frac{1}{2R^2}(\mathbf{\Upsilon}_{(m)} + (\boldsymbol{\phi}_{(m)})^{\dagger}(\boldsymbol{\phi}_{(m)}) - (\boldsymbol{\phi}_{(m)})(\boldsymbol{\phi}_{(m)})^{\dagger})\mathbf{1}_{2^n}\otimes\sigma_3, \tag{5.28}$$

where $\mathbf{F}^{(m)} := \mathrm{d}\mathbf{A}^{(m)} + \mathbf{A}^{(m)}\wedge\mathbf{A}^{(m)}$ and

$$\mathbf{\Upsilon}_{(m)} := \sum_{i=0}^{m}(m-2i)\Pi_i. \tag{5.29}$$

The contribution (5.29) is generated by the monopole connection on $\mathbb{C}P^1$ in (5.26), while the Higgs potentials in (5.28) are produced by (5.27). The graded curvature is independent of $(y,\overline{y}) \in \mathbb{C}P^1$, and the standard gamma-matrix trace formulas,

$$\mathrm{Tr}_{\mathbb{C}^{2n+1}}(\gamma^{\mu}\gamma^{\nu}\otimes\mathbf{1}_2) = -2^{n+1}g^{\mu\nu}, \tag{5.30}$$

$$\mathrm{Tr}_{\mathbb{C}^{2n+1}}(\gamma^{\mu}\gamma^{\nu}\gamma^{\lambda}\gamma^{\rho}\otimes\mathbf{1}_2) = 2^{n+1}(g^{\mu\nu}g^{\lambda\rho} + g^{\mu\rho}g^{\nu\lambda} - g^{\mu\lambda}g^{\nu\rho}), \tag{5.31}$$

$$\mathrm{Tr}_{\mathbb{C}^{2n+1}}([\gamma^{\mu},\gamma^{\nu}][\gamma^{\lambda},\gamma^{\rho}]\otimes\mathbf{1}_2) = 2^{n+3}(g^{\mu\rho}g^{\nu\lambda} - g^{\mu\lambda}g^{\nu\rho}), \tag{5.32}$$

$$\mathrm{Tr}_{\mathbb{C}^{2n+1}}(\gamma^{\mu}\gamma\gamma^{\nu}\gamma\otimes\sigma^{\overline{y}}\sigma^{y}) = -2^{n}g^{\mu\nu} = \mathrm{Tr}_{\mathbb{C}^{2n+1}}(\gamma^{\mu}\gamma\gamma^{\nu}\gamma\otimes\sigma^{y}\sigma^{\overline{y}}) \tag{5.33}$$

imply that the energy functional (5.2) can be compactly written in terms of (5.28) as

$$E_{\mathrm{YM}} = \frac{\pi R^2}{2^n}\int_{M_{2n}}\mathrm{d}^{2n}x\sqrt{g_n}\,\mathrm{tr}_{k\times k}\,\mathrm{Tr}_{\mathbb{C}^{2n+1}}\,\hat{\mathcal{F}}^2. \tag{5.34}$$

Non-Abelian coupled vortex equations: Let us now examine the reduction of the DUY equations on $M_{2n}\times\mathbb{C}P^1$ for a gauge potential of the form proposed in Sec. III (with static configurations in the gauge $\mathcal{A}_0=0$). Substituting (3.19)–(3.22) into (2.12)–(2.14), we obtain

$$g^{a\overline{b}}F^{i}_{a\overline{b}} = \frac{1}{2R^2}(m-2i+\phi_i^{\dagger}\phi_i - \phi_{i+1}\phi_{i+1}^{\dagger}), \tag{5.35}$$

$$F^{i}_{\overline{a}\overline{b}} = 0 = F^{i}_{ab}, \tag{5.36}$$

$$\overline{\partial}_{\overline{a}}\phi_{i+1} + A^{i}_{\overline{a}}\phi_{i+1} - \phi_{i+1}A^{i+1}_{\overline{a}} = 0, \tag{5.37}$$

for each $i=0,1,\ldots,m$, where $\phi_0 := 0 =: \phi_{m+1}$. Recall that there is no summation over i in these equations. We have abbreviated $F^{i}_{ab} := F^{i}_{z^a z^b}$, etc., and defined the derivatives $\partial_a := \partial_{z^a} = \frac{1}{2}(\partial_{2a-1} + i\partial_{2a})$ and $\partial_{\overline{a}} := \partial_{\overline{z^a}} = \frac{1}{2}(\partial_{2a-1} + i\partial_{2a})$ with $a,b=1,\ldots,n$. We shall call (5.35)–(5.37) the non-Abelian coupled vortex equations.

Equation (5.36) implies that the vector bundles $E_{k_i}\to M_{2n}$ are holomorphic, while Eq. (5.37) implies that the Higgs fields $\phi_{i+1}: E_{k_{i+1}}\to E_{k_i}$ are holomorphic maps. By using a Bogomolny-type transformation[33] one can show that solutions to these equations realize absolute minima of the energy functional (5.2). These field configurations describe supersymmetric BPS states of *D*-branes.

Seiberg-Witten monopole equations: For $n=2$, $m=1$, and $k_0=k_1=1$ (so that $k=k_0+k_1=2$), the equations (5.35)–(5.37) coincide with the perturbed Abelian Seiberg-Witten monopole equations on a Kähler four-manifold M_4.[40] In this case we have

$$A^0 = -A^1 =: A \in u(1), \quad F^0 = -F^1 =: F \quad \text{and} \quad \phi_1 =: \phi \in \mathbb{C}, \tag{5.38}$$

and the equations (5.35)–(5.37) reduce to

$$g^{a\bar{b}}F_{a\bar{b}} = \frac{1}{2R^2}(1 - \phi\bar{\phi}), \tag{5.39}$$

$$F_{\bar{a}\bar{b}} = 0 = F_{ab}, \tag{5.40}$$

$$\bar{\partial}_{\bar{a}}\phi + 2A_{\bar{a}}\phi = 0. \tag{5.41}$$

The perturbation, i.e., the term $1/2R^2$ in (5.39), is needed whenever M_4 has non-negative scalar curvature in order to produce a nontrivial and nonsingular moduli space of finite energy L^2 solutions. It is usually introduced into the Seiberg-Witten equations by hand. In the present context, it arises automatically from the extra space $\mathbb{C}P^1$ and the reduction from $M_4 \times \mathbb{C}P^1$ to M_4.

VI. NONCOMMUTATIVE GAUGE THEORY

To build further on the interpretation of our ansatz in terms of configurations of *D*-branes as described in Sec. IV, we should now proceed to construct explicit solutions of the reduced Yang-Mills equations on M_{2n}. Unfortunately, even solutions of the vortex equations (5.35)–(5.37) are difficult to come by and there is no known general method for explicitly constructing the appropriate field configurations. As we will demonstrate in the following, explicit realizations of these *D*-brane states are possible in the context of *noncommutative* gauge theory, which can be mapped afterwards onto commutative world volume configurations. For this, we will now specialize the Kähler manifold $M_{2n} \times \mathbb{C}P^1$ to be $\mathbb{R}^{2n} \times \mathbb{C}P^1$ with metric tensor $g_{\mu\nu} = \delta_{\mu\nu}$ on $\mathbb{R}^{2n}$ and pass to a noncommutative deformation of the flat part of the space, i.e., $\mathbb{R}^{2n} \times \mathbb{C}P^1 \to \mathbb{R}^{2n}_\theta \times \mathbb{C}P^1$. Note that the $\mathbb{C}P^1$ factor remains a commutative space throughout this paper. Then we will deform the Yang-Mills, DUY and non-Abelian coupled vortex equations, and in the subsequent sections construct various solutions of them.

Noncommutative deformation: Field theory on $\mathbb{R}^{2n}_\theta$ may be realized in an operator formalism which turns Schwartz functions f on $\mathbb{R}^{2n}$ into compact operators $\hat{f}$ acting on the n-harmonic oscillator Fock space $\mathcal{H}$.[6] The noncommutative space $\mathbb{R}^{2n}_\theta$ is then defined by declaring its coordinate functions $\hat{x}^1, \ldots, \hat{x}^{2n}$ to obey the Heisenberg algebra relations

$$[\hat{x}^\mu, \hat{x}^\nu] = i\theta^{\mu\nu} \tag{6.1}$$

with a constant real antisymmetric tensor $\theta^{\mu\nu}$. Via an orthogonal transformation of the coordinates, the matrix $\theta = (\theta^{\mu\nu})$ can be rotated into its canonical block-diagonal form with nonvanishing components

$$\theta^{2a-1\ 2a} = -\theta^{2a\ 2a-1} =: \theta^a \tag{6.2}$$

for $a = 1, \ldots, n$. We will assume for definiteness that all $\theta^a > 0$. The noncommutative version of the complex coordinates (2.3) has the nonvanishing commutators,

$$[\hat{z}^a, \hat{\bar{z}}^{\bar{b}}] = -2\delta^{a\bar{b}}\theta^a =: \theta^{a\bar{b}} = -\theta^{\bar{b}a} \leqslant 0. \tag{6.3}$$

Taking the product of $\mathbb{R}^{2n}_\theta$ with the commutative sphere $\mathbb{C}P^1$ means extending the noncommutativity matrix θ by vanishing entries along the two new directions.

The Fock space $\mathcal{H}$ may be realized as the linear span

$$\mathcal{H} = \bigoplus_{r_1,\ldots,r_n=0}^{\infty} \mathbb{C}|r_1, \ldots, r_n\rangle, \tag{6.4}$$

where the orthonormal basis states

$$|r_1, \ldots, r_n\rangle = \prod_{a=1}^{n} (2\theta^a r_a\,!\,)^{-1/2} (\hat{z}^a)^{r_a}|0, \ldots, 0 \tag{6.5}$$

are connected by the action of creation and annihilation operators subject to the commutation relations

$$\left[\frac{\hat{z}^{\bar{b}}}{\sqrt{2\theta^b}}, \frac{\hat{z}^a}{\sqrt{2\theta^a}}\right] = \delta^{a\bar{b}}. \tag{6.6}$$

In the Weyl operator realization $f \mapsto \hat{f}$, coordinate derivatives are given by inner derivations of the noncommutative algebra according to

$$\widehat{\partial_{z^a} f} = \theta_{a\bar{b}}[\hat{z}^{\bar{b}}, \hat{f}] =: \partial_{\hat{z}^a}\hat{f} \quad \text{and} \quad \widehat{\partial_{\bar{z}^a} f} = \theta_{\bar{a}b}[\hat{z}^b, \hat{f}] =: \partial_{\hat{\bar{z}}^a}\hat{f}, \tag{6.7}$$

where $\theta_{a\bar{b}}$ is defined via $\theta_{b\bar{c}}\theta^{\bar{c}a} = \delta_b^a$ so that $\theta_{a\bar{b}} = -\theta_{b\bar{a}} = \delta_{a\bar{b}}/2\theta^a$. On the other hand, integrals are given by traces over the Fock space $\mathcal{H}$ as

$$\int_{\mathbb{R}^{2n}} \mathrm{d}^{2n}x\, f(x) = \left(\prod_{a=1}^{n} 2\pi\theta^a\right) \mathrm{Tr}_{\mathcal{H}}\, \hat{f}. \tag{6.8}$$

The transition to the noncommutative Yang-Mills and DUY equations is trivially achieved by going over to operator-valued objects everywhere. In particular, vector bundles $E \to \mathbb{R}^{2n}$ whose typical fibers are complex vector spaces $\underline{V}$ are replaced by the corresponding (trivial) projective modules $\underline{V} \otimes \mathcal{H}$ over $\mathbb{R}^{2n}_\theta$. The field strength components along $\mathbb{R}^{2n}_\theta$ in (2.8) and (2.12)–(2.14) read $\hat{\mathcal{F}}_{\mu\nu} = \partial_{\hat{x}^\mu}\hat{\mathcal{A}}_\nu - \partial_{\hat{x}^\nu}\hat{\mathcal{A}}_\mu + [\hat{\mathcal{A}}_\mu, \hat{\mathcal{A}}_\nu]$, where $\hat{\mathcal{A}}_\mu$ are simultaneously $\mathrm{u}(k)$ and operator valued. To avoid a cluttered notation, we drop the hats over operators from now on. Thus all our equations have the same form as previously but are considered now as operator equations.

Noncommutative coupled vortex equations: By reducing the noncommutative version of the DUY equations on $\mathbb{R}^{2n}_\theta \times \mathbb{C}P^1$ to $\mathbb{R}^{2n}_\theta$ we obtain the noncommutative non-Abelian coupled vortex equations. Instead of working with the gauge potentials A^i_μ we shall use the operators X^i_μ defined by

$$X^i_a := A^i_a + \theta_{a\bar{b}}\bar{z}^{\bar{b}} \quad \text{and} \quad X^i_{\bar{a}} := A^i_{\bar{a}} + \theta_{\bar{a}b} z^b. \tag{6.9}$$

In terms of these operators the field strength tensor reads

$$F^i_{a\bar{b}} = [X^i_a, X^i_{\bar{b}}] + \theta_{a\bar{b}}, \quad F^i_{\bar{a}\bar{b}} = [X^i_{\bar{a}}, X^i_{\bar{b}}] \quad \text{and} \quad F^i_{ab} = [X^i_a, X^i_b], \tag{6.10}$$

while the bifundamental covariant derivatives become

$$D_{\bar{a}}\phi_{i+1} = X^i_{\bar{a}}\phi_{i+1} - \phi_{i+1}X^{i+1}_{\bar{a}} \quad \text{and} \quad D_a\phi_{i+1} = X^i_a\phi_{i+1} - \phi_{i+1}X^{i+1}_a. \tag{6.11}$$

The non-Abelian vortex equations (5.35)–(5.37) can then be rewritten as

$$\delta^{a\bar{b}}([X^i_a, X^i_{\bar{b}}] + \theta_{a\bar{b}}) = \frac{1}{4R^2}(m - 2i + \phi_i^\dagger\phi_i - \phi_{i+1}\phi_{i+1}^\dagger), \tag{6.12}$$

$$[X^i_{\bar{a}}, X^i_{\bar{b}}] = 0 = [X^i_a, X^i_b], \tag{6.13}$$

$$X_a^i\phi_{i+1} - \phi_{i+1}X_a^{i+1} = 0 \tag{6.14}$$

for $i=0,1,\ldots,m$. Note that for $m=1$ we obtain the equations

$$\delta^{ab}F^0_{ab} = \frac{1}{4R^2}(1-\phi_1\phi_1^\dagger) \quad \text{and} \quad F^0_{\bar{a}\bar{b}} = 0 = F^0_{ab}, \tag{6.15}$$

$$\delta^{ab}F^1_{ab} = -\frac{1}{4R^2}(1-\phi_1^\dagger\phi_1) \quad \text{and} \quad F^1_{\bar{a}\bar{b}} = 0 = F^1_{ab}, \tag{6.16}$$

$$\bar{\partial}_{\bar{a}}\phi_1 + A^0_{\bar{a}}\phi_1 - \phi_1 A^1_{\bar{a}} = 0 \tag{6.17}$$

which are considered in Refs. 29 and 30. In particular, for $n=2$ and $k_0=k_1=1$ the equations (6.15)–(6.17) coincide with the perturbed Seiberg-Witten $\mathrm{U}_+(1)\times\mathrm{U}_-(1)$ monopole equations on $\mathbb{R}^4_\theta$ as considered in Ref. 41.

VII. EXPLICIT SOLUTIONS OF THE NONCOMMUTATIVE YANG-MILLS EQUATIONS

We are now ready to construct solutions to the Yang-Mills equations on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$. We shall first present the generic non-BPS solutions of the full Yang-Mills equations, and then proceed to solve the non-Abelian coupled vortex equations (6.12)–(6.14), and thus the DUY equations on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$, which describe the stable BPS states. Our technique will make use of appropriate partial isometry operators T_{N_i} in the noncommutative space.

Ansatz for explicit solutions: Let us fix a monopole charge $m>0$ and an arbitrary integer $0<r\leqslant k$. Consider the ansatz

$$X_a^i = \theta_{a\bar{b}}T_{N_i}\bar{z}^{\bar{b}}T_{N_i}^\dagger \quad \text{and} \quad X_{\bar{a}}^i = \theta_{\bar{a}b}T_{N_i}z^bT_{N_i}^\dagger, \tag{7.1}$$

$$\phi_{i+1} = \alpha_{i+1}T_{N_i}T_{N_{i+1}}^\dagger \quad \text{and} \quad \phi_{i+1}^\dagger = \bar{\alpha}_{i+1}T_{N_{i+1}}T_{N_i}^\dagger, \tag{7.2}$$

for $i=0,1,\ldots,m$, where $\alpha_i\in\mathbb{C}$ are some constants with $\alpha_0=\alpha_{m+1}=0$. Denoting by $\mathcal{H}$ the n-oscillator Fock space, the Toeplitz operators $T_{N_i}:\mathbb{C}^r\otimes\mathcal{H}\to\underline{V}_{k_i}\otimes\mathcal{H}$ are partial isometries described by *rectangular* $k_i\times r$ matrices (with operator entries acting on $\mathcal{H}$) possessing the properties

$$T_{N_i}^\dagger T_{N_i} = \mathbf{1}_r \quad \text{while } T_{N_i}T_{N_i}^\dagger = \mathbf{1}_{k_i} - P_{N_i}, \tag{7.3}$$

where P_{N_i} is a Hermitian projector of finite rank N_i on the Fock space $\underline{V}_{k_i}\otimes\mathcal{H}$ so that

$$P_{N_i}^2 = P_{N_i} = P_{N_i}^\dagger \quad \text{and} \quad \mathrm{Tr}_{\underline{V}_{k_i}\otimes\mathcal{H}}P_{N_i} = N_i. \tag{7.4}$$

From (7.3) it follows that the operator T_{N_i} has a trivial kernel, while the kernel of $T_{N_i}^\dagger$ is the N_i-dimensional subspace of $\underline{V}_{k_i}\otimes\mathcal{H}$ corresponding to the range of P_{N_i}. Thus

$$\dim\ker T_{N_i} = 0 \quad \text{but } \dim\ker T_{N_i}^\dagger = N_i. \tag{7.5}$$

Substituted into (6.10) this ansatz yields the gauge field strength,

$$F^i_{ab} = \theta_{ab}P_{N_i} = \frac{1}{2\theta^a}\delta_{ab}P_{N_i} \quad \text{and} \quad F^i_{\bar{a}\bar{b}} = 0 = F^i_{ab}, \tag{7.6}$$

while from (6.11) one finds the covariant derivatives

$$D_{\bar{a}}\phi_{i+1} = 0 = D_a\phi_{i+1}. \tag{7.7}$$

Thus our ansatz describes *holomorphic* fields, and the projector P_{N_i} defines a noncommutative

gauge field configuration of rank N_i and constant curvature in the subspace $\ker T^\dagger_{N_i} \subset \underline{V}_{k_i} \otimes \mathcal{H}$. In particular, the Higgs fields ϕ_{i+1} are covariantly constant with

$$\phi_i^\dagger \phi_i = |\alpha_i|^2 (\mathbf{1}_{k_i} - P_{N_i}) \quad \text{and} \quad \phi_{i+1} \phi_{i+1}^\dagger = |\alpha_{i+1}|^2 (\mathbf{1}_{k_i} - P_{N_i}). \tag{7.8}$$

The ranks Ni are generically non-negative integers. If some $N_i = 0$, then we should formally set $P_{N_i} = 0$, $T_{N_i} = 1$, and $\phi_{i+1} = 0$ in the ith component of the ansatz, so that the noncommutative version of the bundle chain (4.13) collapses near the ith node to

$$\cdots \to \underline{V}_{k_{i+1}} \otimes \mathcal{H} \to 0 \to \underline{V}_{k_{i-1}} \otimes \mathcal{H} \to \cdots . \tag{7.9}$$

Then

$$X_a^i = \theta_{ab} \bar{z}^b \quad \text{and} \quad X_{\bar{a}}^i = \theta_{\bar{a}b} z^b \tag{7.10}$$

which leads to the vacuum gauge field configuration

$$A^i = 0 \quad \text{and} \quad F^i = 0. \tag{7.11}$$

These matter fields correspond to open strings with one end on a D-brane and the other end on the closed string vacuum.

Our ansatz has a natural interpretation in quiver gauge theory. Consider the module

$$\underline{\mathcal{T}} := \bigoplus_{i=0}^{m} \ker T^\dagger_{N_i} \quad \text{with } \vec{k}_{\underline{\mathcal{T}}} = \sum_{i=0}^{m} N_i \vec{e}_i \tag{7.12}$$

over the quiver A_{m+1}, which is a finite-dimensional submodule of the infinite-dimensional representation $\mathcal{V} \otimes \mathcal{H}$ of A_{m+1} given by the noncommutative quiver bundle. Let us fix an integer $0 \leqslant s \leqslant m$, and take $N_i \neq 0$ for all $i \leqslant s$ and $N_i = 0$ for all $i > s$. The quiver representation (7.12) is a combination of the indecomposable projective representations $\underline{\mathsf{P}}_i$ of A_{m+1} that we encountered in Sec. V. The $\underline{\mathsf{P}}_i$'s form a complete set of projective representations in the sense that any quiver representation has a projective resolution in terms of sums of them.[37] In particular, the canonical Ringel resolution of (7.12) is given by the exact sequence

$$0 \to \bigoplus_{i=1}^{s} \underline{\mathsf{P}}_{i-1} \otimes \ker T^\dagger_{N_i} \to \bigoplus_{i=0}^{s} \underline{\mathsf{P}}_i \otimes \ker T^\dagger_{N_i} \to \underline{\mathcal{T}} \to 0. \tag{7.13}$$

Solving the Yang-Mills equations: We shall now demonstrate that the field configurations (7.1)–(7.3) yield solutions of the full Yang-Mills equations on $\mathbb{R}^{2n}_\theta \times \mathbb{C}P^1$ for any values of m, $N_0, N_1, \ldots, N_m$ and $\alpha_1, \ldots, \alpha_m$. For this, we write the ansatz in the form

$$\mathcal{A}_a - \theta_{ab} \bar{z}^b = \sum_{i=0}^{m} X_a^i \otimes \Pi_i = \theta_{ab} \sum_{i=0}^{m} T_{N_i} \bar{z}^b T^\dagger_{N_i} \otimes \Pi_i, \tag{7.14}$$

$$\mathcal{A}_{\bar{a}} - \theta_{\bar{a}b} z^b = \sum_{i=0}^{m} X_{\bar{a}}^i \otimes \Pi_i = \theta_{\bar{a}b} \sum_{i=0}^{m} T_{N_i} z^b T^\dagger_{N_i} \otimes \Pi_i. \tag{7.15}$$

We also have

$$\mathcal{A}_y^{ii} = \frac{(m - 2i)\bar{y}}{2(R^2 + y\bar{y})} \mathbf{1}_{k_i}, \tag{7.16}$$

$$\mathcal{A}_{\overline{y}}^{ii} = -\frac{(m-2i)y}{2(R^2+y\overline{y})}\mathbf{1}_{k_i}, \tag{7.17}$$

$$\mathcal{A}_{\overline{y}}^{ii+1} = \frac{R}{R^2+y\overline{y}}\phi_{i+1} = \frac{R\alpha_{i+1}}{R^2+y\overline{y}}T_{N_i}T_{N_{i+1}}^{\dagger}, \tag{7.18}$$

$$\mathcal{A}_{y}^{i+1i} = -\frac{R}{R^2+y\overline{y}}\phi_{i+1}^{\dagger} = -\frac{R\overline{\alpha}_{i+1}}{R^2+y\overline{y}}T_{N_{i+1}}T_{N_i}^{\dagger}, \tag{7.19}$$

with

$$\mathcal{A}_{y}^{ij} = 0 = \mathcal{A}_{y}^{i+1j} \quad \text{for } j \neq i, i+1. \tag{7.20}$$

Thus for the ansatz (7.1)–(7.3) the field strength tensor is given by

$$\mathcal{F}_{a\overline{b}} = \theta_{a\overline{b}}\sum_{i=0}^{m} P_{N_i} \otimes \Pi_i, \tag{7.21}$$

$$\mathcal{F}_{y\overline{y}} = -\frac{R^2}{(R^2+y\overline{y})^2}\sum_{i=0}^{m}(m-2i+(|\alpha_i|^2-|\alpha_{i+1}|^2)(\mathbf{1}_{k_i}-P_{N_i}))\otimes\Pi_i, \tag{7.22}$$

with all other components of $\mathcal{F}_{\hat{\mu}\hat{\nu}}$ vanishing.

Let us now insert these expressions into the Yang-Mills equations (2.8) (for static configurations with $\mathcal{A}_0=0$). It is enough to consider the cases $\hat{\nu}=c$ and $\hat{\nu}=\overline{y}$, since the cases $\hat{\nu}=\overline{c}$ and $\hat{\nu}=y$ can be obtained by Hermitian conjugation of (2.8) due to the anti-Hermiticity of $\mathcal{A}_{\hat{\mu}}$ and $\mathcal{F}_{\hat{\mu}\hat{\nu}}$. For $\hat{\nu}=c$, Eq. (2.8) becomes

$$\delta^{\overline{c}a}\delta^{\overline{b}c}(\partial_{\overline{c}}\mathcal{F}_{a\overline{b}} + [\mathcal{A}_{\overline{c}}, \mathcal{F}_{a\overline{b}}]) = 0 \tag{7.23}$$

which is equivalent to

$$\delta^{\overline{c}a}\delta^{\overline{b}c}[\mathcal{A}_{\overline{c}} - \theta_{\overline{c}\overline{b}}z^b, \mathcal{F}_{a\overline{b}}] = 0. \tag{7.24}$$

Substituting (7.15) and (7.21), we see that (7.24) is satisfied due to the identities (5.16) and

$$T_{N_i}^{\dagger}P_{N_i} = P_{N_i}T_{N_i} = 0. \tag{7.25}$$

In the case $\hat{\nu}=\overline{y}$, Eq. (2.8) simplifies to

$$\partial_y(\sqrt{g}\mathcal{F}^{y\overline{y}}) + \sqrt{g}[\mathcal{A}_y, \mathcal{F}^{y\overline{y}}] = 0 \tag{7.26}$$

with $\sqrt{g}=2R^4/(R^2+y\overline{y})^2$. Substituting (7.16), (7.19), (7.20), (7.21), and (7.22), we find that (7.26) is also satisfied due to the identities (5.16) and (7.25). Hence, the Yang-Mills equations on $\mathbb{R}_{\theta}^{2n} \times \mathbb{C}P^1$ are solved by our choice of ansatz.

Finite-energy solutions: The arbitrary coefficients $\alpha_i \in \mathbb{C}$ can be fixed (up to a phase) by demanding that the solution (7.1)–(7.3) yield finite-energy field configurations. For this, we evaluate the energy functional (5.2) using (6.8). From (7.6) we may compute

$$(F_{\mu\nu}^i)^{\dagger}(F^{i\mu\nu}) = 8\,\delta^{a\overline{c}}\delta^{d\overline{b}}F_{ab}^{i}F_{d\overline{c}}^{i} = 2\left(\sum_{a=1}^{n}\frac{1}{(\theta^a)^2}\right)P_{N_i}, \tag{7.27}$$

and combining this with (7.7) and (7.8) we find the noncommutative Yang-Mills energy

$$E_{YM} = 2\pi R^2 \left(\prod_{a=1}^{n} 2\pi\theta^a \right) \sum_{i=0}^{m} \mathrm{Tr}_{\underline{V}_{k_i} \otimes \mathcal{H}} \left[\left(\sum_{b=1}^{n} \frac{1}{(\theta^b)^2} \right) P_{N_i} + \frac{1}{4R^4} (m - 2i + (|\alpha_i|^2 - |\alpha_{i+1}|^2)(\mathbf{1}_{k_i} - P_{N_i}))^2 \right]. \tag{7.28}$$

Because of the trace over the infinite-dimensional Fock space $\mathcal{H}$, the constant terms in (7.28) which are not proportional to the projectors P_{N_i} must all vanish in order for the energy to be finite. This leads to the finite-energy conditions

$$m - 2i + |\alpha_i|^2 - |\alpha_{i+1}|^2 = 0 \tag{7.29}$$

for each $i = 0, 1, \ldots, m$.

With $\alpha_0 = \alpha_{m+1} = 0$, the constraints (7.29) are solved by

$$|\alpha_{i+1}|^2 = (i+1)m - 2\sum_{j=0}^{i} j = (i+1)(m-i) \tag{7.30}$$

and the energy (7.28) can thereby be written as

$$E_{\mathrm{YM}} = 2\pi R^2 \left(\sum_{a=1}^{n} 2\pi\, \theta^a \right) \sum_{i=0}^{[m/2]} (N_i + N_{m-i}) \left[\left(\sum_{b=1}^{n} \frac{1}{(\theta^b)^2} \right) + \frac{(m-2i)^2}{4R^4} \right]. \tag{7.31}$$

We have naturally split the sum over nodes i into contributions from Dirac monopoles and anti-monopoles, which for each $i = 0, 1, \ldots, m$ have the same Yang-Mills energy on the sphere $\mathbb{C}P^1$. Later on we will see that this splitting corresponds to a $\mathbb{Z}_2$-grading of the chain of D-branes into brane-antibrane pairs. The monopole independent terms in (7.31) can be interpreted as the tension of $\Sigma_{i=0}^{m} N_i$ $D0$-branes inside a $D(2n)$-brane[42] in the Seiberg-Witten decoupling limit.[5]

BPS solutions: The solutions we have described generically yield non-BPS solutions of the full Yang-Mills equations on $\mathbb{R}^{2n}_{\theta} \times \mathbb{C}P^1$. On the other hand, the DUY equations on $\mathbb{R}^{2n}_{\theta} \times \mathbb{C}P^1$ are BPS conditions for the Yang-Mills equations. Inserting (7.1)–(7.3) and (7.6)–(7.8) into our non-Abelian vortex equations (6.12)–(6.14), we find that (6.13) and (6.14) are automatically satisfied. The vanishing of the constant term (not proportional to P_{N_i}) in (6.12) is precisely the finite-energy constraint (7.29), whose solution is given in (7.30). Equating the coefficients of P_{N_i} in (6.12) for each $N_i \neq 0$ leads to the additional constraints

$$\sum_{a=1}^{n} \frac{1}{\theta^a} = \frac{m-2i}{2R^2} \quad \text{with } i = 0, 1, \ldots, s. \tag{7.32}$$

For $s > 0$ the conditions (7.32) are incompatible with one another, implying that the ansatz (7.1)–(7.3) with $s > 0$ does not allow for BPS configurations. For $s = 0$, the equation (7.32) relates the radius R of the sphere to the noncommutativity parameters θ^a of $\mathbb{R}^{2n}_{\theta}$. In this case we obtain the explicit solutions of the noncommutative vortex and DUY equations parametrized by the partial isometry operators T_{N_0} as

$$X_a^0 = \theta_{a\bar{b}} T_{N_0} \bar{z}^{\bar{b}} T_{N_0}^{\dagger} \quad \text{and} \quad \phi_1 = \alpha_1 T_{N_0}, \tag{7.33}$$

$$X_a^i = \theta_{a\bar{b}} \bar{z}^{\bar{b}} \quad \text{and} \quad \phi_i = \alpha_i \mathbf{1}_{k_1} \text{ for } 0 < i \leq m. \tag{7.34}$$

The BPS conditions (6.12)–(6.14) force us to take $k_1 = \cdots = k_m$ corresponding to the gauge symmetry breaking $U(k) \to U(k_0) \times U(k_1)^m$, so that $r = k_1$, $k_0 + mk_1 = k$ with $k_0 > 0$ and $k_1 > 0$. The configurations with $i > 0$ correspond to the vacuum gauge fields (7.11) with trivial bundle maps ϕ_i given as multiplication by the complex numbers α_i satisfying (7.30). Using (7.32) and (7.31) we find that the energies of these BPS states are given by

$$E_{\mathrm{BPS}} = 2(2\pi)^{n+1}R^2\left(\sum_{\substack{b,c=1\\ b\leqslant c}}^{n}\prod_{\substack{a=1\\ a\neq b,c}}^{n}\theta^a\right)N_0. \tag{7.35}$$

These solutions have a natural physical interpretation along the lines described in Sec. IV. The original noncommutative DUY equations are fixed by the positive integers n and k. Our ansatz (3.10)–(3.14) and (7.1)–(7.3) is labelled by the collection of positive integers (m,k_i,N_i) with $i=0,1,\ldots,s$. According to the standard identification of D-branes as noncommutative solitons,[42] the configuration (7.33) and (7.34) with $s=0$ describes a collection of mN_0 BPS $D0$-branes as a stable bound state (i.e., a vortexlike solution on $\mathbb{R}^{2n}_\theta$) in a system of $k_0+mk_1=k$ $D(2n)$ branes and antibranes. But from the point of view of the initial branes wrapped on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$, they are spherical mN_0 $D2$-branes. This means that instantons on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$ are the spherical extensions of vortices which are points in $\mathbb{R}^{2n}_\theta$. For $s>0$ the configuration (7.1)–(7.3) describes an unstable system of $mN_0+|m-2|N_1+\cdots+|m-2s|N_s$ $D0$-branes (vortices) in a $D(2n)$ brane-antibrane system, because $\deg\mathcal{L}^{m-2i}=m-2i$ for each $i=0,1,\ldots,s$. Again they form a system of spherical $D2$-branes [i.e., an SU(2)-symmetric multi-instanton] in the initial brane-antibrane system on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$. Their orientation depends on the sign of the magnetic charge $m-2i$ for each $i=0,1,\ldots,s$, which determines whether we have $D2$-branes or $D2$-antibranes. If more than one $N_i\neq 0$ then the ansatz either describes pairs of $D0$-branes with overall nonvanishing monopole charges, or both $D0$-branes, and anti-$D0$-branes. Such systems cannot be stable, i.e., the corresponding configuration (7.1)–(7.3) cannot satisfy the noncommutative vortex and DUY equations.

The distinction between BPS versus non-BPS solutions is very natural in quiver gauge theory. The BPS configurations are described by the simple Schur representations $\underline{\mathsf{L}}_i$, $i=0,1,\ldots,m$ of the A_{m+1} quiver given by a one-dimensional vector space at vertex i with all maps equal to 0, i.e., the A_{m+1}-module with $(\underline{\mathsf{L}}_i)_{m-2j}=\delta_{ij}\,\mathbb{C}$ and dimension vector $\vec{k}_{\underline{\mathsf{L}}_i}=\vec{e}_i$. The BPS states constructed above then correspond to the quiver representations $(\underline{\mathsf{L}}_0)^{\oplus N_0}$. Together with the projective modules $\underline{\mathsf{P}}_i$, the Schur modules $\underline{\mathsf{L}}_i$ admit the projective resolutions

$$0\to\underline{\mathsf{P}}_0\to\underline{\mathsf{L}}_0\to 0, \tag{7.36}$$

$$0\to\underline{\mathsf{P}}_{i-1}\to\underline{\mathsf{P}}_i\to\underline{\mathsf{L}}_i\to 0\quad\text{for } i=1,\ldots,s \tag{7.37}$$

and satisfy the relations[37]

$$\mathrm{Hom}(\underline{\mathsf{L}}_i,\underline{\mathsf{L}}_j)=\delta_{ij}\mathbb{C}=\mathrm{Hom}(\underline{\mathsf{P}}_i,\underline{\mathsf{L}}_j). \tag{7.38}$$

The resolutions (7.13) and (7.36), (7.37) exhibit a sharp homological distinction between BPS and non-BPS solutions. The constituent D-branes at the vertices of the quiver A_{m+1} are associated with the basic representations $\underline{\mathsf{L}}_i$. Sums $(\underline{\mathsf{L}}_i)^{\oplus N_i}$ for fixed i correspond to BPS states, associated generally with the symmetry breaking $U(k)\to U(k_i)\times U(k_{i+1})^m$, which are constructed analogously to (7.33), (7.34) but with the vacuum Higgs configurations $\phi_j=\alpha_j\,\mathbf{1}_{k_i}$ for $j<i$ and $\phi_j=\alpha_j\,\mathbf{1}_{k_{i+1}}$ for $j>i$. A generic non-BPS state, associated to the quiver representation (7.12), corresponds to the decay of the original SU(2)-symmetric branes wrapped on $\mathbb{R}^{2n}_\theta\times\mathbb{C}P^1$ into the collection of constituent branes $(\underline{\mathsf{L}}_0)^{\oplus N_0}\oplus(\underline{\mathsf{L}}_1)^{\oplus N_1}\oplus\cdots\oplus(\underline{\mathsf{L}}_s)^{\oplus N_s}$ in $\mathbb{R}^{2n}_\theta$. For $s>0$ this collection is unstable. In the quiver gauge theory, we have thereby arrived at a natural construction of the unstable D-brane configurations in terms of stable BPS states of D-branes, which may be succinctly summarized through the sequence of distinguished triangles of quiver representations

$$\begin{array}{ccccccccccccc}
(\underline{\mathsf{L}}_0)^{\oplus N_0}= & \underline{\mathcal{T}}_0 & & \to & & \underline{\mathcal{T}}_1 & \to\ \cdots\ \to & \underline{\mathcal{T}}_{m-1} & & \to & & \underline{\mathcal{T}}_m & =\ \underline{\mathcal{T}} \\
& \nwarrow & & & \swarrow & & & \nwarrow & & & \swarrow & & \\
& & (\underline{\mathsf{L}}_1)^{\oplus N_1} & & & & \cdots & & & (\underline{\mathsf{L}}_m)^{\oplus N_m} & & & ,
\end{array} \tag{7.39}$$

where $\mathcal{T}_s:=\oplus_{i=0}^{s}\ker T^\dagger_{N_i}=\ker T^\dagger_{N_s}\oplus\underline{\mathcal{T}}_{s-1}$ and the horizontal maps are the canonical inclusions of submodules. This exact sequence expresses the fact that, for each $s=1,\ldots,m$, the non-BPS mod-

ule $\underline{\mathcal{T}}_s$ is an extension of the BPS module $(\underline{\mathsf{L}}_s)^{\oplus N_s}$ by the non-BPS module $\underline{\mathcal{T}}_{s-1}$.

VIII. GENERALIZED ATIYAH-BOTT-SHAPIRO CONSTRUCTION

In this section we shall construct an explicit realization of the basic partial isometry operators T_{N_i} which will be particularly useful for setting the *D*-brane interpretation of our noncommutative multi-instanton solutions on firmer ground. It is based on an SU(2)-equivariant generalization of the (noncommutative) Atiyah-Bott-Shapiro (ABS) construction of tachyon field configurations.[9–11]

Equivariant ABS construction: If G is a group and $C\ell_{2n} := C\ell(\mathbb{R}^{2n})$, we denote by $R_{\mathrm{spin}_G(2n)}$ the Grothendieck group of isomorphism classes of finite-dimensional $\mathbb{Z}_2$-graded $G \times C\ell_{2n}$ modules, i.e., Clifford modules possessing an even ($\mathbb{Z}_2$-degree preserving) G-action which commutes with the $C\ell_{2n}$-action. More precisely, we consider representations of $\mathbb{C}[G] \otimes C\ell_{2n}$ with $\mathbb{C}[G]$ the group ring of G. The inclusion $\iota(2n): C\ell_{2n} \hookrightarrow C\ell_{2n+1}$ of Clifford algebras induces a restriction map

$$\iota_G(2n)^*: R_{\mathrm{Spin}_G(2n+1)} \to R_{\mathrm{Spin}_G(2n)} \tag{8.1}$$

on equivariant Clifford modules. Following the standard ABS construction,[43] we may then obtain the G-equivariant K-theory $K_G(\mathbb{R}^{2n})$ (with compact support) through the descendent isomorphism

$$K_G(\mathbb{R}^{2n}) = \mathrm{coker}\ \iota_G(2n)^* = R_{\mathrm{Spin}_G(2n)} / \iota_G(2n)^* R_{\mathrm{Spin}_G(2n+1)}. \tag{8.2}$$

The image of $\iota_G(2n)^*$ in $R_{\mathrm{Spin}_G(2n)}$ contains classes of Clifford modules $[\underline{V}]$ which admit a $G \times C\ell_{2n}$-equivariant involution $\underline{V} \cong \underline{V}^\vee$, where $\underline{V}^\vee$ is the Clifford module $\underline{V}$ with its $\mathbb{Z}_2$-parity reversed.

In our case, we take $G = \mathrm{U}(1) \subset \mathrm{SU}(2)$ acting trivially on $\mathbb{R}^{2n}$, and thereby consider $\mathrm{U}(1) \times C\ell_{2n}$-modules with the U(1)-action commuting with the Clifford action. Any such module is a direct sum of tensor products of a U(1)-module and a spinor module, and hence

$$R_{\mathrm{Spin}_{\mathrm{U}(1)}(2n)} = R_{\mathrm{Spin}(2n)} \otimes R_{\mathrm{U}(1)} \quad \text{and} \quad \iota_{\mathrm{U}(1)}(2n)^* = \iota(2n)^* \otimes \mathbf{1}. \tag{8.3}$$

Since from the standard ABS construction one has the isomorphism[43]

$$K(\mathbb{R}^{2n}) = \mathrm{coker}\ \iota(2n)^* = R_{\mathrm{Spin}(2n)} / \iota(2n)^* R_{\mathrm{Spin}(2n+1)} \tag{8.4}$$

of Abelian groups, we can reduce (8.2) for $G = \mathrm{U}(1)$ to the isomorphism

$$K_{\mathrm{U}(1)}(\mathbb{R}^{2n}) = K(\mathbb{R}^{2n}) \otimes R_{\mathrm{U}(1)} \tag{8.5}$$

of $R_{\mathrm{U}(1)}$-modules, where $K(\mathbb{R}^{2n}) \cong \mathbb{Z}$ [note that the isomorphism $K_{\mathrm{U}(1)}(\mathbb{R}^{2n}) \cong \mathbb{R}_{\mathrm{U}(1)}$ also follows from the fact that $\mathbb{R}^{2n}$ is equivariantly contractible to a point]. We may describe the isomorphism (8.5) along the lines explained in Sec. IV. In particular, the spinor module $\underline{\Delta}_{2n} := \underline{\Delta}(\mathbb{R}^{2n})$ admits the isotopical decomposition

$$\underline{\Delta}_{2n} = \bigoplus_{i=0}^{m} \Delta_i \otimes \underline{S}_{m-2i} \quad \text{with } \Delta_i = \mathrm{Hom}_{\mathrm{U}(1)}(\underline{S}_{m-2i}, \underline{\Delta}_{2n}) \tag{8.6}$$

obtained by restricting $\underline{\Delta}_{2n}$ to representations of $\mathrm{U}(1) \subset \mathrm{Spin}(2n) \subset C\ell_{2n}$. The Δ_i's in (8.6) are the corresponding multiplicity spaces.

The most instructive and useful way to explicitly realize the decomposition (8.6) is to use the equivariant excision theorem (4.5) directly and consider the SU(2)-invariant dimensional reduction of spinors from $\mathbb{R}^{2n} \times \mathbb{C}P^1$ to $\mathbb{R}^{2n}$. For this, we introduce the twisted Dirac operator on $\mathbb{R}^{2n} \times \mathbb{C}P^1$ using the graded connection formalism of Sec. V to write the $\mathbb{Z}_{m+1}$-graded Clifford connection

$$\hat{\not{D}} := \Gamma^{\hat{\mu}} D_{\hat{\mu}} = \gamma^{\mu} D_{\mu} \otimes \mathbf{1}_2 + (\boldsymbol{\phi}_{(m)})\gamma \otimes \gamma^{\overline{y}} \beta_{\overline{y}} - (\boldsymbol{\phi}_{(m)})^{\dagger} \gamma \otimes \gamma^{y} \beta_{y} + \gamma \otimes \not{D}_{\mathbb{C}P^1}, \tag{8.7}$$

where

$$\not{D}_{\mathbb{C}P^1} := \gamma^{y} D_{y} + \gamma^{\overline{y}} D_{\overline{y}} = \gamma^{y} (\partial_{y} + \omega_{y} + (\mathbf{a}^{(m)})_{y}) + \gamma^{\overline{y}} (\partial_{\overline{y}} + \omega_{\overline{y}} + (\mathbf{a}^{(m)})_{\overline{y}}) \tag{8.8}$$

and $\omega_y, \omega_{\overline{y}}$ are the components of the Levi-Civita spin connection on the tangent bundle of $\mathbb{C}P^1$. From (8.7) we see that the monopole charges $m-2i$ in the Yang-Mills energy functional (5.2) can be understood as originating from the Dirac operator (8.8) on $\mathbb{C}P^1$. The operator (8.7) acts on spinors Ψ which are sections of the bundle

$$\Psi = \begin{pmatrix} \Psi^{+} \\ \Psi^{-} \end{pmatrix} \in \bigoplus_{i=0}^{m} (E_{k_i} \otimes \underline{\Delta}_{2n}) \otimes \begin{pmatrix} \mathcal{L}^{m-2i+1} \\ \mathcal{L}^{m-2i-1} \end{pmatrix} \tag{8.9}$$

over $\mathbb{R}^{2n} \times \mathbb{C}P^1$, where $\mathcal{L}^{m-2i+1} \oplus \mathcal{L}^{m-2i-1}$ are the twisted spinor bundles of rank 2 over the sphere $\mathbb{C}P^1$. We are therefore interested in the twisted spinor module $\underline{\Delta}_{\mathcal{V}}(\mathbb{R}^{2n} \times \mathbb{C}P^1)$ over the Clifford algebra $\mathrm{C}\ell(\mathbb{R}^{2n} \times \mathbb{C}P^1)$ which is the product of the spinor module $\underline{\Delta}_{2n} \otimes \underline{\Delta}(\mathbb{C}P^1)$ with the fundamental representation (3.8) of the gauge group $\mathrm{U}(k)$ broken as in (3.9).

The symmetric fermions on $\mathbb{R}^{2n}$ that we are interested in correspond to SU(2)-invariant spinors on $\mathbb{R}^{2n} \times \mathbb{C}P^1$. They belong to the kernel of the Dirac operator (8.8) on $\mathbb{C}P^1$ and will be massless on $\mathbb{R}^{2n}$. One can write

$$\not{D}_{\mathbb{C}P^1} = \bigoplus_{i=0}^{m} \not{D}_{m-2i} = \bigoplus_{i=0}^{m} \begin{pmatrix} 0 & \not{D}^{-}_{m-2i} \\ \not{D}^{+}_{m-2i} & 0 \end{pmatrix}, \tag{8.10}$$

where

$$\not{D}^{+}_{m-2i} = \frac{1}{R^2} \left((R^2 + y\overline{y}) \partial_{\overline{y}} - \frac{1}{2}(m-2i+1) y \right), \tag{8.11}$$

$$\not{D}^{-}_{m-2i} = -\frac{1}{R^2} \left((R^2 + y\overline{y}) \partial_{y} + \frac{1}{2}(m-2i-1) \overline{y} \right). \tag{8.12}$$

The operator (8.10) acts on sections of the bundle (8.9) which we write with respect to this decomposition as

$$\Psi = \bigoplus_{i=0}^{m} \begin{pmatrix} \psi^{+}_{(m-2i)} \\ \psi^{-}_{(m-2i)} \end{pmatrix}, \tag{8.13}$$

where $\psi^{\pm}_{(m-2i)}$ are sections of $\mathcal{L}^{m-2i\pm1}$ taking values in $\underline{\Delta}_{2n} \otimes \underline{V}_{k_i}$ with coefficients depending on $x \in \mathbb{R}^{2n}$.

To describe the kernel of the Dirac operator (8.10), we need to solve the differential equations

$$\not{D}^{+}_{m-2i} \psi^{+}_{(m-2i)} = 0 \quad \text{and} \quad \not{D}^{-}_{m-2i} \psi^{-}_{(m-2i)} = 0 \tag{8.14}$$

for the positive and negative chirality spinors $\psi^{+}_{(m-2i)}$ and $\psi^{-}_{(m-2i)}$ in $\ker \not{D}^{+}_{m-2i}$ and $\ker \not{D}^{-}_{m-2i}$. By recalling the form of the transition functions for the monopole bundles from Sec. III, one easily sees that the only solutions of these equations which are regular on both the northern and southern hemispheres of S^2 are of the form

$$\psi^{+}_{(m-2i)} = \frac{1}{(R^2 + y\overline{y})^{t_i/2}} \sum_{\ell=0}^{t_i} \psi^{+}_{(m-2i)\ell}(x) y^{\ell} \quad \text{and} \quad \psi^{-}_{(m-2i)} = 0 \quad \text{for } m-2i < 0 \tag{8.15}$$

and

$$\psi^-_{(m-2i)} = \frac{1}{(R^2+y\overline{y})^{t_i/2}} \sum_{\ell=0}^{t_i} \psi^-_{(m-2i)\ell}(x)\overline{y}^{\ell} \quad \text{and} \quad \psi^+_{(m-2i)} = 0 \quad \text{for } m-2i>0. \tag{8.16}$$

Here $t_i=|m-2i|-1$ and the component functions $\psi^{\pm}_{(m-2i)\ell}(x)$ on $\mathbb{R}^{2n}$ with $\ell=0,1,\ldots,t_i$ form the irreducible representation $\underline{V}_{t_i+1}\cong\mathbb{C}^{|m-2i|}$ of the group SU(2). Thus the chirality grading is by the sign of the magnetic charges.

This analysis is valid when the monopole charge m is an even or odd integer. However, when m is even there is precisely one term in (8.9) with $m=2i$ for which the sub-bundle $E_{k(m/2)}\to\mathbb{R}^{2n}$ is twisted by the ordinary spinor bundle $\mathcal{L}\oplus\mathcal{L}^{\vee}\to\mathbb{C}P^1$ of vanishing magnetic charge. This bundle admits an infinite-dimensional vector space of symmetric L^2-sections comprised of spinor harmonics $\Psi_{lq}\in\mathbb{C}^2$ with $l\in\mathbb{N}_0+\frac{1}{2}$, $q\in\{-l,-l+1,\ldots,l-1,l\}$ and $\not{D}_0\Psi_{lq}\neq 0$.[44] The spectrum of the (untwisted) Dirac operator $\not{D}_0$ consists of the eigenvalues $\pm\left(l+\frac{1}{2}\right)$, each of multiplicity $p+1=2l+1$. After dimensional reduction, this produces an infinite tower of massive spinors on $\mathbb{R}^{2n}$, and such fermions of zero magnetic charge have no immediate interpretation in the present context. However, one has $\dim\ker\not{D}_0=0$, and this will be enough for our purposes. We will therefore fix one of these vector spaces, such that after integration over $\mathbb{C}P^1$ it corresponds to the space

$$\underline{H}_p \cong \mathbb{C}^2\otimes\mathbb{C}^{p+1} \quad \text{with } p=1,3,5,\ldots. \tag{8.17}$$

All of our subsequent results will be independent of the particular choice of eigenspace (8.17).

We have thereby shown that the SU(2)-equivariant reduction of the twisted spinor representation of $C\ell(\mathbb{R}^{2n}\times\mathbb{C}P^1)$ decomposes as a $\mathbb{Z}_2$-graded bundle giving

$$\underline{\Delta}_{\underline{\mathcal{V}}}(\mathbb{R}^{2n}\times\mathbb{C}P^1)^{\mathrm{SU}(2)} = \underline{\Delta}_{2n}\otimes(\underline{\Delta}^+_{\underline{\mathcal{V}}}\otimes\underline{\Delta}^-_{\underline{\mathcal{V}}}) \quad \text{for } m \text{ odd}, \tag{8.18}$$

where

$$\underline{\Delta}^+_{\underline{\mathcal{V}}} = \bigoplus_{i=m_+}^{m} \underline{V}_{k_i}\otimes\underline{V}_{|m-2i|} \quad \text{and} \quad \underline{\Delta}^-_{\underline{\mathcal{V}}} = \bigoplus_{i=0}^{m_-} \underline{V}_{k_i}\otimes\underline{V}_{m-2i} \tag{8.19}$$

with $m_+=\lfloor(m+1)/2\rfloor$ and $m_-=\lfloor(m-1)/2\rfloor$. When m is an even integer, one should also couple the eigenspace (8.17) giving

$$\underline{\Delta}_{\underline{\mathcal{V}}}(\mathbb{R}^{2n}\times\mathbb{C}P^1)^{\mathrm{SU}(2)} = \underline{\Delta}_{2n}\otimes(\underline{\Delta}^+_{\underline{\mathcal{V}}}\otimes(\underline{V}_{k\frac{m}{2}}\otimes\underline{H}_p)\oplus\underline{\Delta}^-_{\underline{\mathcal{V}}}) \quad \text{for } m \text{ even} \tag{8.20}$$

with $m_+=\lfloor(m+3)/2\rfloor$ and $m_-=\lfloor(m+1)/2\rfloor$. It remains to work out the corresponding action of Clifford multiplication

$$\mu_{\underline{\mathcal{V}}}:\underline{\Delta}^-_{\underline{\mathcal{V}}}\to\underline{\Delta}^+_{\underline{\mathcal{V}}}. \tag{8.21}$$

For this, we recall from Sec. IV that the action of the generators of the parabolic subgroup $P\subset\mathrm{SL}(2,\mathbb{C})$ on the equivariant decomposition (8.18), (8.19) is given by $\sigma_3(\underline{V}_{k_i}\otimes\underline{V}_{|m-2i|})=(m-2i)(\underline{V}_{k_i}\otimes\underline{V}_{|m-2i|})$ and $\sigma_-:\underline{V}_{k_i}\otimes\underline{V}_{|m-2i|}\to\underline{V}_{k_{i-1}}\otimes\underline{V}_{|m-2i|}$. Since the Clifford action is required to commute with this action, the map (8.21) is thereby uniquely fixed on the isotopical components in the form

$$\mu_{\underline{\mathcal{V}}}\circ\Pi_i:\underline{V}_{k_i}\otimes\underline{V}_{|m-2i|}\to\underline{V}_{k_{i+\lfloor\frac{m}{2}\rfloor+1}}\otimes\underline{V}_{|m-2i|} \quad \text{for } i=0,1,\ldots,m_-. \tag{8.22}$$

Furthermore, since $\sigma_3(\underline{H}_p)=0$ for all p, the space of spinor harmonics must lie in the kernel of the Clifford map and one has

$$\mu_{\underline{\mathcal{V}}}\circ\Pi_{m/2}=0 \quad \text{for } m \text{ even}. \tag{8.23}$$

It is also illuminating to formulate this equivariant dimensional reduction from a dynamical point of view, as we did for the gauge fields in Sec. V. Using the gauged Dirac operator (8.7) we may define a fermionic energy functional on the space of sections of the bundle (8.9) by

$$E_D := \int_{\mathbb{R}^{2n}\times\mathbb{C}P^1} \mathrm{d}^{2n+2}x\sqrt{g}\Psi^\dagger \hat{\not{D}}\Psi . \tag{8.24}$$

One has

$$\Psi^\dagger(\gamma(\boldsymbol{\phi}_{(m)})\otimes\sigma^{\bar{y}} - \gamma(\boldsymbol{\phi}_{(m)})^\dagger\otimes\sigma^y)\Psi = ((\Psi^+)^\dagger(\Psi^-)^\dagger)\begin{pmatrix}\gamma(\boldsymbol{\phi}_{(m)})^\dagger(\Psi^-)\\ \gamma(\boldsymbol{\phi}_{(m)})(\Psi^+)\end{pmatrix}. \tag{8.25}$$

Substituting (8.10)–(8.16), we see that (8.25) vanishes on symmetric spinors and after integration over $\mathbb{C}P^1$ the energy functional (8.24) for m odd becomes

$$E_D = 4\pi R^2\int_{\mathbb{R}^{2n}}\mathrm{d}^{2n}x\left[\sum_{i=m_+}^{m}\sum_{\ell=0}^{|m-2i|-1}(\psi^+_{(m-2i)\ell})^\dagger\gamma^\mu D_\mu(\psi^+_{(m-2i)\ell}) + \sum_{i=0}^{m_-}\sum_{\ell=0}^{m-2i-1}(\psi^-_{(m-2i)\ell})^\dagger\gamma^\mu D_\mu(\psi^-_{(m-2i)\ell})\right]. \tag{8.26}$$

The symmetric fermion energy functional for m even also contains mass terms for fermions of vanishing magnetic charge which are proportional to the multiplicity $(p+1)$ of the spinor harmonics.

Explicit form of the operators: $\boldsymbol{T_{N_i}}$: The operators T_{N_i} parametrizing the solutions of the preceding section may be realized explicitly by appealing to a noncommutative version of the above construction. For this, we first note that the (trivial) action of $\mathrm{U}(1)\subset\mathrm{SU}(2)$ on $\mathbb{R}^{2n}$ induces an action on functions f on $\mathbb{R}^{2n}$ by $(\zeta\cdot f)(x) := f(\zeta^{-1}\cdot x)$ for $\zeta\in\mathrm{U}(1)$. This in turn defines an action of $\mathrm{U}(1)$ on the noncommutative space $\mathbb{R}^{2n}_\theta$ through automorphisms $\hat{f}\mapsto\widehat{\zeta\cdot f}$ of the Weyl operator algebra, i.e., a representation of $\mathrm{U}(1)$ in the automorphism group of the algebra. We will assume that the Fock space (6.4) carries a unitary representation of $\mathrm{U}(1)$. We can then decompose it into its isotopical components in the usual way as

$$\mathcal{H} = \bigoplus_{i=0}^{m}\mathcal{H}_i\otimes\underline{S}_{m-2i}. \tag{8.27}$$

For $\zeta\in\mathrm{U}(1)$ we denote the corresponding unitary operator on $\mathcal{H}$ by $\hat{\zeta}$. If we demand that the representations of $\mathrm{U}(1)$ above are covariant with respect to each other,[45]

$$\hat{\zeta}\hat{f}\hat{\zeta}^{-1} = \widehat{\zeta\cdot f}, \tag{8.28}$$

then they define a representation of the crossed-product of the algebra of Weyl operators with the group $\mathrm{U}(1)$. This defines the (trivial) noncommutative $\mathrm{U}(1)$-space $\mathbb{R}^{2n}_\theta\rtimes\mathrm{U}(1)$, and equivariant field configurations are operators belonging to the commutant of $\mathrm{U}(1)$ in the crossed-product algebra. In quiver gauge theory, the pertinent representation of A_{m+1} thus labels isotopical components of the Hilbert space of the noncommutative gauge theory. Since the $\mathrm{U}(1)$-action is trivial here, the isotopical components of the Fock space (8.27) are given by $\mathcal{H}_i\cong\mathcal{H}$ for each $i=0,1,\ldots,m$. Note that one has an isomorphism $(\mathcal{H})^{\otimes(m+1)}\cong\mathcal{H}$ by the usual Hilbert hotel argument.

We will now construct a representation on (8.27) of the partial isometry operators T_{N_i} in $\mathbb{R}^{2n}_\theta\rtimes\mathrm{U}(1)$. For this, let us set $r := 2^{n-1}$ and consider the operators[9]

$$\Sigma = (\sigma\cdot x)^\dagger \frac{1}{\sqrt{(\sigma\cdot x)(\sigma\cdot x)^\dagger}} \quad \text{and} \quad \Sigma^\dagger = \frac{1}{\sqrt{(\sigma\cdot x)(\sigma\cdot x)^\dagger}}(\sigma\cdot x), \tag{8.29}$$

where $\sigma\cdot x := \sigma_\mu x^\mu$, $\mu,\ \nu = 1,\dots,2n$ and the $r\times r$ matrices σ_μ are subject to the anticommutation relations

$$\sigma_\mu^\dagger\sigma_\nu + \sigma_\nu^\dagger\sigma_\mu = 2\delta_{\mu\nu}\mathbf{1}_r = \sigma_\mu\sigma_\nu^\dagger + \sigma_\nu\sigma_\mu^\dagger. \tag{8.30}$$

Equation (8.30) implies that the matrices

$$\gamma_\mu = \begin{pmatrix} 0 & \sigma_\mu^\dagger \\ -\sigma_\mu & 0 \end{pmatrix} \quad \text{with } \gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = -2\delta_{\mu\nu}\mathbf{1}_{2r} \tag{8.31}$$

generate the Clifford algebra $C\ell_{2n}$. Note that for $n=1$ we have $r=1$, $\sigma_1=1$, and $\sigma_2=i$, which yields

$$\Sigma^\dagger = \frac{1}{\sqrt{z^\dagger z}}z^\dagger = \sum_{\ell=1}^{\infty} |\,\ell-1\rangle\langle\ell\,| \tag{8.32}$$

and we obtain the standard shift operator $(\Sigma)^N$ on the Fock space $\mathcal{H}$ in this case. Generally, the operators (8.29) obey

$$(\Sigma^\dagger)^{N_i}(\Sigma)^{N_i} = \mathbf{1}_r \quad \text{and} \quad (\Sigma)^{N_i}(\Sigma^\dagger)^{N_i} = \mathbf{1}_r - \mathcal{P}_{N_i}, \tag{8.33}$$

where $\mathcal{P}_{N_i}$ is a projector of rank N_i on the vector space $\underline{\Delta}_{2n}^+\otimes\mathcal{H}$, and $\underline{\Delta}_{2n}^+\cong\mathbb{C}^r$ are the irreducible chiral spinor modules of dimension $r=2^{n-1}$ (with $\underline{\Delta}_{2n}=\underline{\Delta}_{2n}^+\oplus\underline{\Delta}_{2n}^-$) on which the matrices σ_μ act.

The partial isometry operators $(\Sigma)^{N_i}$ in $\mathbb{R}_\theta^{2n}$ do not act on the isotopical decomposition (8.27) and thus do not properly incorporate the SU(2)-equivariant reduction of the original system of D-branes. The desired operators T_{N_i} in $\mathbb{R}_\theta^{2n}\rtimes\mathrm{U}(1)$ are obtained by first projecting these partial isometries onto constituent brane subspaces. With Π_i the rank 1 projector onto the ith isotopical component in (8.27), we thereby define the $r\times r$ matrices

$$T_{N_i}^{(0)} = \mathbf{1}_r\otimes(1-\Pi_i) + (\Sigma)^{N_i}\otimes\Pi_i. \tag{8.34}$$

The operator $T_{N_i}^{(0)}$ acts as the shift operator $(\Sigma)^{N_i}$ on $\mathcal{H}_i$ and as the identity operator $\mathbf{1}_r$ on $\mathcal{H}_j$ for all $j\neq i$. It is easy to see that these matrices satisfy the equations

$$(T_{N_i}^{(0)})^\dagger(T_{N_i}^{(0)}) = \mathbf{1}_r \quad \text{and} \quad (T_{N_i}^{(0)})(T_{N_i}^{(0)})^\dagger = \mathbf{1}_r - \mathcal{P}_{N_i}^{(0)} \tag{8.35}$$

with

$$P_{N_i}^{(0)} = \mathcal{P}_{N_i}\otimes\Pi_i \tag{8.36}$$

a projector of rank N_i on the Fock space $\underline{\Delta}_{2n}^+\otimes\mathcal{H}$. They also satisfy the algebra

$$(T_{N_i}^{(0)})^N = T_{N_iN}^{(0)} \quad \text{and} \quad T_{N_i}^{(0)}T_{N_j}^{(0)} = T_{N_i}^{(0)} + T_{N_j}^{(0)} - \mathbf{1}_r = T_{N_j}^{(0)}T_{N_i}^{(0)} \quad \text{for } i\neq j. \tag{8.37}$$

The operator (8.34) may be regarded as a linear map

$$T_{N_i}^{(0)}:\underline{\Delta}_{2n}^-\otimes\mathcal{H}\to\underline{\Delta}_{2n}^+\otimes\mathcal{H}. \tag{8.38}$$

In particular, the map $(T_1^{(0)})$ has a trivial kernel, while $(T_1^{(0)})^\dagger$ has a one-dimensional kernel which is spanned by the vector $|\psi\rangle\otimes|0,\dots,0\rangle$ where $|\psi\rangle$ denotes the lowest-weight spinor of SO($2n$).

Finally, the desired *rectangular* $k_i\times r$ Toeplitz operators T_{N_i} may be realized in terms of the partial isometries (8.34) by appealing to the Hilbert hotel argument. For this, we introduce a lexicographic ordering $\mathbb{N}_0^n\sim\mathbb{N}_0$ on the Fock space $\mathcal{H}$ so that $|r_1,\dots,r_n\rangle=|q\rangle$ with $q=0,1,2,\dots$, and fix an orthonormal basis $\vec{\rho}_0,\vec{\rho}_1,\dots,\vec{\rho}_{r-1}$ of the chiral spinor representation space $\underline{\Delta}_{2n}^+\cong\mathbb{C}^r$.

Then $\vec{\rho}_a \otimes |q\rangle$, $a=0,1,\ldots,r-1$ is an orthonormal basis for $\underline{\Delta}^+_{2n} \otimes \mathcal{H}$ and there is a one-to-one correspondence $\vec{\rho}_a \otimes |q\rangle \leftrightarrow |rq+a\rangle$ of basis states. Similarly, by fixing an orthonormal basis $\vec{\lambda}^i_0, \vec{\lambda}^i_1, \ldots, \vec{\lambda}^i_{k_i-1}$ of the SU(2) representation space $\underline{V}_{k_i} \cong \mathbb{C}^{k_i}$, there is a one-to-one correspondence $\vec{\lambda}^i_{a_i} \otimes |q_i\rangle \leftrightarrow |k_i q_i + a_i\rangle$, $a_i=0,1,\ldots,k_i-1$ for the corresponding orthonormal basis of $\underline{V}_{k_i} \otimes \mathcal{H}$. Let us now introduce unitary isomorphisms $U_i : \underline{\Delta}^+_{2n} \otimes \mathcal{H} \to \underline{V}_{k_i} \otimes \mathcal{H}$ and $U_i^\dagger : \underline{V}_{k_i} \otimes \mathcal{H} \to \underline{\Delta}^+_{2n} \otimes \mathcal{H}$ by the formulas

$$U_i = \sum_{a=0}^{r-1} \sum_{a_i=0}^{k_i-1} \sum_{\substack{q,q_i=0 \\ rq+a=k_i q_i+a_i}}^{\infty} |k_i q_i + a_i\rangle\langle rq+a| = \sum_{a=0}^{r-1} \sum_{a_i=0}^{k_i-1} \sum_{\substack{q,q_i=0 \\ rq+a=k_i q_i+a_i}}^{\infty} \vec{\lambda}^i_{a_i} \vec{\rho}^\dagger_a \otimes |q_i\rangle\langle q|, \tag{8.39}$$

$$U_i^\dagger = \sum_{a=0}^{r-1} \sum_{a_i=0}^{k_i-1} \sum_{\substack{q,q_i=0 \\ rq+a=k_i q_i+a_i}}^{\infty} |rq+a\rangle\langle k_i q_i + a_i| = \sum_{a=0}^{r-1} \sum_{a_i=0}^{k_i-1} \sum_{\substack{q,q_i=0 \\ rq+a=k_i q_i+a_i}}^{\infty} \vec{\rho}_a \vec{\lambda}^{i\dagger}_{a_i} \otimes |q\rangle\langle q_i|. \tag{8.40}$$

By using the shift operators (8.34), we then define the operators

$$T_{N_i} = U_i(T^{(0)}_{N_i}) \quad \text{and} \quad T^\dagger_{N_i} = (T^{(0)}_{N_i})^\dagger U_i^\dagger \tag{8.41}$$

on $\underline{\Delta}^-_{2n} \otimes \mathcal{H} \to \underline{V}_{k_i} \otimes \mathcal{H}$ and $\underline{V}_{k_i} \otimes \mathcal{H} \to \underline{\Delta}^-_{2n} \otimes \mathcal{H}$. They satisfy the requisite equations (7.3), with the $k_i \times k_i$ matrix

$$P_{N_i} = U_i(\mathcal{P}_{N_i} \otimes \Pi_i) U_i^\dagger \tag{8.42}$$

a projector of rank N_i on the Fock space $\underline{V}_{k_i} \otimes \mathcal{H}$.

Notice that the rank $r=2^{n-1}$ used in this construction is an even integer for $n \geqslant 2$. To work with odd ranks r one may introduce the $(2^{n-1}+1) \times (2^{n-1}+1)$ matrices

$$T^{(0)\prime}_{N_i} = \begin{pmatrix} T^{(0)}_{N_{i-1}} & 0 \\ 0 & \Sigma'_1 \end{pmatrix}, \tag{8.43}$$

where $T^{(0)}_{N_i-1}$ is defined as above and

$$\Sigma'_1 = \sum_{\ell=1}^{\infty} |0,\ldots,0,\ell\rangle\langle\ell-1,0,\ldots,0| \tag{8.44}$$

is a shift operator on the Fock space $\mathcal{H}$. Then the operators (8.43) satisfy the equations (8.35) with

$$P^{(0)\prime}_{N_i} = \begin{pmatrix} \mathcal{P}_{N_i-1} \otimes \Pi_i & 0 \\ 0 & |0,\ldots,0\rangle\langle 0,\ldots,0| \end{pmatrix} \tag{8.45}$$

a projector of rank N_i on the Fock space $(\underline{\Delta}^+_{2n} \otimes \mathcal{H}) \oplus \mathcal{H} \cong \mathbb{C}^r \otimes \mathcal{H}$, where $r=2^{n-1}+1$. In this case the Toeplitz operators T_{N_i} are obtained by substituting (8.43) into (8.41) with the replacement $\underline{\Delta}^\pm_{2n} \to \underline{\Delta}^\pm_{2n} \oplus \mathbb{C}$.

Note also that the partial isometry operator

$$T^{(0)} := \prod_{i=0}^{m} T^{(0)}_{N_i} = \mathbf{1}_r + \sum_{i=0}^{m} (T^{(0)}_{N_i} - \mathbf{1}_r) = \mathbf{1}_r + \sum_{i=0}^{m} ((\Sigma)^{N_i} - \mathbf{1}_r), \tag{8.46}$$

together with the above representations of the U(1) group on the Weyl operator algebra of $\mathbb{R}^{2n}_\theta$ and on the Fock space $\mathcal{H}$, defines a cycle in the U(1)-equivariant analytic K-homology $K^a(\mathbb{R}^{2n}_\theta \rtimes \mathrm{U}(1)) \cong K^a_{\mathrm{U}(1)}(\mathbb{R}^{2n})$. After a twisting appropriate to the inclusion of the pertinent magnetic monopole bundles, it describes the SU(2)-invariant configurations of D-branes as branes on

the (trivial) quotient space $\mathbb{R}^{2n}/\mathrm{U}(1)$. The charge of this class is the same as that of the cocycle $[\underline{\Delta}_{\underline{\mathcal{V}}}^{+},\underline{\Delta}_{\underline{\mathcal{V}}}^{-};\mu_{\underline{\mathcal{V}}}]$ built earlier in the topological K-theory (8.5) from the standard ABS brane-antibrane class $[\underline{\Delta}_{2n}^{+},\underline{\Delta}_{2n}^{-};\mu]$ which is the generator of (8.4)[9–11,43]. The computation of the topological charge, as well as the equivalence between the commutative (topological) and noncommutative (analytic) K-homology descriptions of the D-brane configurations, will be presented in the next section.

Moduli space of solutions: The realization (8.34) can be generalized in order to introduce $2n\Sigma_{i=0}^{m}N_i$ real moduli into the solution which specify the locations of the various noncommutative solitons in $\mathbb{R}^{2n}$.[45] For this, one first must introduce "shifted ground states" centered at $(b_{\ell_i}^{i\mu})$, $\ell_i=1,\ldots,N_i$ for each $i=0,1,\ldots,m$. The operators (8.34) are rewritten as

$$T_{N_i}^{(0)}=\mathbf{1}_r\otimes(1-\Pi_i)+(\Sigma_1^i\Sigma_2^i\cdots\Sigma_{N_i}^i)\otimes\Pi_i, \tag{8.47}$$

where each $\Sigma_{\ell_i}^i$, $\ell_i=1,\ldots,N_i$, $i=0,1,\ldots,m$ is of the form of the shift operator Σ in (8.29) but with the coordinates x shifted to $x_{\ell_i}^i:=x-b_{\ell_i}^i$. They behave just like Σ except that now the kernel of $(\Sigma_{\ell_i}^i)^\dagger$ is spanned by the vector $|\psi\rangle\otimes|\overline{b_{\ell_i}^i}\rangle$, where $|\psi\rangle$ is the fermionic ground state and the shifted ground state $|\overline{b_{\ell_i}^i}\rangle$ is a coherent state in the n-oscillator Fock space $\mathcal{H}$, i.e., $\overline{z_{\ell_i}^{i\alpha}}|\overline{b_{\ell_i}^i}\rangle=0$. The states $|\psi\rangle\otimes|\overline{b_1^i}\rangle$ and $\Sigma_1^i\cdots\Sigma_{\ell_i-1}^i(|\psi\rangle\otimes|\overline{b_{\ell_i}^i}\rangle)$ for $\ell_i=2,\ldots,N_i$ span the kernel of the operator $(T_{N_i}^{(0)})^\dagger$ given by (8.47), and we find that the equations (8.35) are obeyed with $P_{N_i}^{(0)}$ the orthogonal projection onto $\ker(T_{N_i}^{(0)})^\dagger$.

The space of partial isometries (8.46) may thereby be described as the complex manifold $\Pi_{i=0}^{m}(\mathbb{C}^n)^{N_i}$. After a quotient by the appropriate discrete symmetry group, the moduli space for the full solution consisting of the rectangular Toeplitz operators (8.41) is given by

$$\mathcal{M}(n;\vec{k}_{\underline{\mathcal{V}}},\vec{k}_{\underline{\mathcal{I}}})=\mathcal{Q}(\vec{k}_{\underline{\mathcal{V}}})\times\prod_{i=0}^{m}\mathrm{Hilb}^{N_i}(\mathbb{C}^n), \tag{8.48}$$

where $\mathrm{Hilb}^{N_i}(\mathbb{C}^n)$ is the moduli space of N_i noncommutative solitons on $\mathbb{R}_\theta^{2n}$ (Ref. 46) which is given as the (singular) Hilbert scheme of N_i points in $\mathbb{C}^n$, i.e., the set of ideals $\mathcal{I}$ of codimension N_i in the polynomial ring $\mathbb{C}[b_1^i,\ldots,b_{N_i}^i]$. The factor $\mathcal{Q}(\vec{k}_{\underline{\mathcal{V}}})$ is the moduli space of isomorphism classes of quiver representations (3.8) of dimension[37]

$$\dim\mathcal{Q}(\vec{k}_{\underline{\mathcal{V}}})=1-\frac{1}{2}\vec{k}_{\underline{\mathcal{V}}}\cdot C\vec{k}_{\underline{\mathcal{V}}}=1+\sum_{i=0}^{m}k_i(k_{i+1}-k_i). \tag{8.49}$$

Note that real roots (having $\vec{k}_{\underline{\mathcal{V}}}\cdot C\vec{k}_{\underline{\mathcal{V}}}=2$) correspond to rigid representations of the quiver A_{m+1} with no moduli, while imaginary roots (having $\vec{k}_{\underline{\mathcal{V}}}\cdot C\vec{k}_{\underline{\mathcal{V}}}\leqslant 0$) carry moduli associated to the gauge symmetry breaking (3.9). The points of the moduli space (8.48) label the positions of well-separated D-branes, and it coincides in the low-energy limit with the moduli space of the commutative brane description.[45]

IX. *D*-BRANE CHARGES

In this section we will compute the topological charge of our multi-instanton solutions in essentially two distinct ways. The first one is a direct field theoretic calculation of the $(n+1)$th Chern number of our gauge field configurations on $\mathbb{R}_\theta^{2n}\times S^2$, which can also be computed using the $\mathbb{Z}_{m+1}$-graded connection formalism of Sec. V. The second one is a homological calculation of the index class of our solutions in K-theory, which is also equivalent to the Euler-Ringel character of the pertinent representations of the quiver A_{m+1}. The equivalence of these two calculations will then lead us directly into a world volume description whereby we can interpret the topological charge in terms of cycles in topological equivariant K-homology, yielding the claimed D-brane

interpretation of our solutions. The results of this section bridge together the descriptions presented in Sec. IV and justify the brane interpretations that have been given throughout this paper thus far.

Field theory calculation: We will first compute the topological charge of the configurations (7.1)–(7.3). For this, it is convenient to parametrize the two-sphere by the angular coordinates $0 \leqslant \varphi \leqslant 2\pi$ and $0 \leqslant \vartheta < \pi$ defined in (2.4). In these coordinates

$$\mathcal{F}_{y\overline{y}} = \left| \frac{\partial(\vartheta,\varphi)}{\partial(y,\overline{y})} \right| \mathcal{F}_{\vartheta\varphi} = \frac{1}{2i} \frac{\sin\vartheta}{y\overline{y}} \mathcal{F}_{\vartheta\varphi} = \frac{1}{2i} \frac{(1+\cos\vartheta)^2}{R^2 \sin\vartheta} \mathcal{F}_{\vartheta\varphi}, \tag{9.1}$$

and we have

$$\mathcal{F}_{2a-1\,2a} = 2i\mathcal{F}_{a\overline{a}} = -\frac{i}{\theta^a} \sum_{i=0}^{m} P_{N_i} \otimes \Pi_i, \tag{9.2}$$

$$\mathcal{F}_{\vartheta\varphi} = -i \frac{\sin\vartheta}{2} \sum_{i=0}^{m} (m-2i) P_{N_i} \otimes \Pi_i \tag{9.3}$$

giving

$$\begin{aligned} \mathcal{F}_{12}\mathcal{F}_{34}\cdots\mathcal{F}_{2n-12n}\mathcal{F}_{\vartheta\varphi} &= (-i)^{n+1} \frac{\sin\vartheta}{2\prod_{a=1}^{n} \theta^a} \left(\sum_{i=0}^{m} P_{N_i} \otimes \Pi_i \right)^n \left(\sum_{j=0}^{m} (m-2j) P_{N_j} \otimes \Pi_j \right) \\ &= (-i)^{n+1} \frac{\sin\vartheta}{2\prod_{a=1}^{n} \theta^a} \sum_{i=0}^{m} (m-2i) P_{N_i} \otimes \Pi_i, \end{aligned} \tag{9.4}$$

where we have used the definitions (7.4) and (5.16) of the projectors P_{N_i} and Π_i.

The instanton charge is then given by the $(n+1)$th Chern number

$$\begin{aligned} Q &:= \frac{1}{(n+1)!} \left(\frac{i}{2\pi} \right)^{n+1} \left(\prod_{a=1}^{n} 2\pi\theta^a \right) \int_{S^2} \mathrm{Tr}_{\underline{\mathcal{V}}\otimes\mathcal{H}} \underbrace{\mathcal{F} \wedge \cdots \wedge \mathcal{F}}_{n+1} \\ &:= \left(\frac{i}{2\pi} \right)^{n+1} \frac{(-i)^{n+1}}{2\prod_{b=1}^{n} \theta^b} \left(\prod_{a=1}^{n} 2\pi\theta^a \right) \sum_{i=0}^{m} (m-2i) N_i \int_{S^2} \sin\vartheta \, \mathrm{d}\vartheta \wedge \mathrm{d}\varphi. \end{aligned} \tag{9.5}$$

After splitting the sum over i into contributions from monopoles and antimonopoles analogously to (7.31), this becomes

$$Q = \sum_{i=0}^{[m/2]} (m-2i)(N_i - N_{m-i}), \tag{9.6}$$

where we recall that $N_i \geqslant 0$ for $i = 0, 1, \ldots, m$. The formula (9.6) clarifies the D-brane interpretation of the configuration (7.1)–(7.3). It describes a collection of $(m-2i)N_i$ $D0$-branes for $2i < m$ and $(2i-m)N_i$ anti-$D0$-branes for $2i > m$ as a bound state (i.e., a vortexlike configuration on $\mathbb{R}^{2n}_\theta$) in a

system of $k_0+k_1+\cdots+k_m=k$ $D(2n)$ branes and antibranes. However, from the point of view of the initial brane-antibrane system on $\mathbb{R}^{2n}_\theta\times S^2$, they are spherical $|m-2i|N_i$ $D2$-branes or $D2$-antibranes depending on the sign of the monopole charge $m-2i$. Note that the vortices with $2i=m$, which always exist for even m, have vanishing instanton charge since they couple with the trivial line bundle $\mathcal{L}^0=S^2\times\mathbb{C}$. Thus they are not extended to instantons on $\mathbb{R}^{2n}_\theta\times S^2$, but are rather unstable and simply decay into the vacuum.

The topological charge can be alternatively computed within the graded connection formalism of Sec. V. Recalling the equivariant ABS construction (8.18)–(8.20), we note that the $\mathbb{Z}_{m+1}$-graded vector space (3.8) [the fiber of the $\mathbb{Z}_{m+1}$-graded bundle (5.3)] also has a *natural* $\mathbb{Z}_2$-grading by the sign of the magnetic charge, i.e., by the involution $\epsilon:\underline{\mathcal{V}}\to\underline{\mathcal{V}}$ defined by $\epsilon(v_i):=\mathrm{sgn}(m-2i)\ v_i$ for $v_i\in\underline{V}_{k_i}$, where throughout we use the convention $\mathrm{sgn}(0):=0$. The corresponding supertrace is given by

$$\mathrm{str}_{k\times k}X:=\mathrm{tr}_{k\times k}(\epsilon\circ X)=\sum_{i=0}^{m}\mathrm{sgn}(m-2i)\ \mathrm{tr}_{k_i\times k_i}X_i \tag{9.7}$$

for any linear operator $X\in\mathrm{End}(\underline{\mathcal{V}})$ with block-diagonal components $X_i\in\mathrm{End}(\underline{\mathcal{V}}_{k_i})$. This extends to a supertrace $\mathrm{STr}_{\underline{\mathcal{V}}\otimes\mathcal{H}}:=\mathrm{Tr}_{\mathcal{H}}\,\mathrm{str}_{k\times k}$ which we may use to express the Chern number in terms of the graded curvature (5.28) as

$$Q=\frac{R^2}{2^n(n+1)!}\left(\frac{i}{2\pi}\right)^{n+1}\left(\prod_{a=1}^{n}2\pi\theta^a\right)\mathrm{STr}_{\underline{\mathcal{V}}\otimes\mathcal{H}}\mathrm{Tr}_{\mathbb{C}^{2n+1}}(\Gamma\hat{\mathcal{F}}^{n+1})_{\mathrm{asym}}, \tag{9.8}$$

where $\Gamma:=(2/\sqrt{g})\Gamma^1\cdots\Gamma^{2n+2}=\gamma\otimes\sigma_3$ and the antisymmetrized product of gamma matrices,

$$(\Gamma^{\hat\mu_1}\cdots\Gamma^{\hat\mu_q})_{\mathrm{asym}}:=\frac{1}{q!}\sum_{\pi\in S_q}\mathrm{sgn}(\pi)\Gamma^{\hat\mu_{\pi(1)}}\cdots\Gamma^{\hat\mu_{\pi(q)}} \tag{9.9}$$

mimicks the algebraic structure of the exterior product of differential forms. The formula (9.6) follows from (9.8) upon repeated application of the Clifford algebra and the trace identities (5.30)–(5.33), with the supertrace (9.7) giving the appropriate sign alternations.

K-theory calculation: The origin of the topological charge lies in the *graded Chern character* $\mathrm{ch}(\underline{\mathcal{V}}\otimes\mathcal{H}):=\mathrm{str}_{k\times k}\exp\hat{\mathcal{F}}/2\pi i$. Standard transgression arguments can be used to show that the cohomology class defined by this closed differential form is independent of the choice of graded connection.[39] In particular, we may either compute it by setting the off-diagonal Higgs fields $\phi_i=0$ or by setting the diagonal gauge fields $A^i=0$. It is instructive to recall how this works in the case $m=1$ corresponding to the basic brane-antibrane system represented by the chain (4.26).[8,31] In the former case we would obtain the difference $\mathrm{ch}(\underline{V}_{k_1}\otimes\mathcal{H})-\mathrm{ch}(\underline{V}_{k_0}\otimes\mathcal{H})$ of topological charges on the branes and antibranes. In the latter case we would compute the index of the tachyon field ϕ_1, or equivalently the Euler characteristic of the two-term complex $0\to\underline{V}_{k_1}\otimes\mathcal{H}\xrightarrow{\phi_1}\underline{V}_{k_0}\otimes\mathcal{H}\to 0$. The virtual Euler class generated by the cohomology of this complex is the analytic K-homology class $[\phi_1]\in K^{\mathrm{a}}(\mathbb{R}^{2n})$ of the brane configuration. The equivalence of the two computations is asserted by the index theorem.

The situation for $m>1$ is more subtle. The action of the graded connection zero-form (5.9) on the bundle (5.3) produces the holomorphic chain (4.13). In general this is *not* a complex because, according to (5.10), $(\boldsymbol{\phi}_{(m)})^2\neq 0$ for $m>1$, i.e., $\phi_i\phi_{i+1}\neq 0$. The only physical instance in which such a chain generates a complex is when it corresponds to an alternating sequence of branes and antibranes.[47] But if one has a tachyon field which is a holomorphic map from an antibrane to a brane, then the adjoint map is antiholomorphic. Recalling (5.37), we see that in our chain (4.13) all maps ϕ_i are *holomorphic* and thus do not represent tachyon fields between pairs of branes and antibranes. Furthermore, the maps ϕ_i obtained as solutions of the vortex equations, which can be

associated with the A_{m+1} quiver and are obtained by SU(2)-invariant reduction, can never satisfy the constraints $\phi_i\phi_{i+1}=0$.[34,36]

The solution to this problem is to fold the given holomorphic chain into maps between branes and antibranes. Let us first carry out the calculation in the case that the monopole Chern number m is an odd integer. By using the $\mathbb{Z}_2$-grading $\boldsymbol{\epsilon}:\underline{\mathcal{V}}\to\underline{\mathcal{V}}$ introduced above, we explicitly decompose (3.8) as a $\mathbb{Z}_2$-graded module into the ±1 eigenspaces of the involution $\boldsymbol{\epsilon}$ giving

$$\underline{\mathcal{V}}=\underline{\mathcal{V}}_+\otimes\underline{\mathcal{V}}_- \quad \text{with } \underline{\mathcal{V}}_+=\bigoplus_{i=0}^{m_-}\underline{V}_{k_i} \quad \text{and} \quad \underline{\mathcal{V}}_-=\bigoplus_{i=m_+}^{m}\underline{V}_{k_i}. \tag{9.10}$$

Using (5.9) and (5.10) we now introduce the operator

$$\mathbf{T}_{(m)}:=(\phi_{(m)})^{\lfloor m/2\rfloor+1}. \tag{9.11}$$

With respect to the $\mathbb{Z}_2$-grading (9.10), it is an odd map

$$\mathbf{T}_{(m)}:\underline{\mathcal{V}}_-\otimes\mathcal{H}\to\underline{\mathcal{V}}_+\otimes\mathcal{H} \quad \text{with } (\boldsymbol{T}_{(m)})^2=0. \tag{9.12}$$

Thus the triple $[\underline{\mathcal{V}}_+\otimes\mathcal{H},\underline{\mathcal{V}}_-\otimes\mathcal{H};\mathbf{T}_{(m)}]$ defines a two-term complex and represents a brane-antibrane system with tachyon field given in terms of the graded connection by (9.11). The corresponding index class $[\mathbf{T}_{(m)}]\in K^{\mathrm{a}}(\mathbb{R}^{2n})$ is thus the analytic K-homology class of our configuration of D-branes. In particular, on isotopical components one has

$$\mathbf{T}_{(m)}\circ\Pi_{i+1+\lfloor m/2\rfloor}=\phi_{i+1}\cdots\phi_{i+1+\lfloor m/2\rfloor}=(\alpha_{i+1}\cdots\alpha_{i+1+\lfloor m/2\rfloor})T_{N_i}T^\dagger_{N_{i+1+\lfloor m/2\rfloor}} \tag{9.13}$$

while $\mathbf{T}_{(m)}\circ\Pi_i=0$, where $i=0,1,\dots,m_-$. The tachyon field is thus a holomorphic map between branes of equal and opposite magnetic charge,

$$\mathbf{T}_{(m)}\circ\Pi_{i+\lfloor m/2\rfloor+1}:\underline{V}_{k_{i+\lfloor m/2\rfloor+1}}\otimes\mathcal{H}\to\underline{V}_{k_i}\otimes\mathcal{H}, \tag{9.14}$$

and from (7.5) it follows that it has a finite dimensional kernel and cokernel with

$$\dim\ker(\mathbf{T}_{(m)}\circ\Pi_{i+\lfloor m/2\rfloor+1})=N_{i+\lfloor m/2\rfloor+1} \quad \text{and} \quad \dim\ker(\mathbf{T}_{(m)}\circ\Pi_{i+\lfloor m/2\rfloor+1})^\dagger=N_i. \tag{9.15}$$

To incorporate the twistings by the magnetic monopole bundles, we use the ABS construction (8.18)–(8.23) to define the tachyon field

$$\boldsymbol{\mathcal{T}}_{(m)}:=\mathbf{T}_{(m)}\otimes\mathbf{1}:\underline{\Delta}^+_{\underline{\mathcal{V}}}\otimes\mathcal{H}\to\underline{\Delta}^-_{\underline{\mathcal{V}}}\otimes\mathcal{H}. \tag{9.16}$$

It behaves like a noncommutative version of Clifford multiplication $\underline{\mu}^\dagger_{\underline{\mathcal{V}}}$ in (8.21) and (8.22). Since $\dim\underline{V}_{|m-2i|}=|m-2i|$, from (9.15) it follows that the index of the tachyon field (9.16) is given by

$$\operatorname{index}\boldsymbol{\mathcal{T}}_{(m)}=\dim\ker(\boldsymbol{\mathcal{T}}_{(m)})-\dim\ker(\boldsymbol{\mathcal{T}}_{(m)})^\dagger=\sum_{i=m_+}^{m}|m-2i|N_i-\sum_{i=0}^{m_-}|m-2i|N_i=-Q. \tag{9.17}$$

Thus the K-theory charge of the noncommutative soliton configuration (7.1)–(7.3) coincides with the Yang-Mills instanton charge (9.5), (9.6) on $\mathbb{R}^{2n}_\theta\times S^2$.

When the monopole charge m is even, we introduce the tachyon field $\mathbf{T}_{(m)}$ by the same formula (9.11). The only difference now is that the subspace $\underline{V}_{k_{\frac{m}{2}}}\otimes\mathcal{H}$ is annihilated by both operators $(\mathbf{T}_{(m)})$ and $(\mathbf{T}_{(m)})^\dagger$ so that

$$\underline{V}_{k_{\frac{m}{2}}}\otimes\mathcal{H}\subset\ker(\boldsymbol{T}_{(m)})\cap\ker(\boldsymbol{T}_{(m)})^\dagger. \tag{9.18}$$

According to (8.20), this subspace should be coupled to the eigenspace (8.17) of spinor harmonics on $\mathbb{C}P^1$ when defining the extended tachyon field (9.16). Analogously to (8.23), one then has

$$\ker(\mathcal{T}_{(m)}\circ\Pi_{m/2})=\ker(\mathcal{T}_{(m)}\circ\Pi_{m/2})^{\dagger}=\underline{V}_{k_{m/2}}\otimes\underline{H}_p\otimes\mathcal{H}. \tag{9.19}$$

With a suitable regularization of the infinite dimensions of the kernel and cokernel of the operator $\mathcal{T}_{(m)}\circ\Pi_{m/2}$, these subspaces will make no contribution to the index (9.17). This statement will be justified below by the fact that index $\not{D}_0=0$ and that the index class of the noncommutative tachyon field coincides with that of the twisted SU(2)-invariant Dirac operator on $\mathbb{R}^{2n}\times\mathbb{C}P^1$.

We can give a more detailed picture of how the topological charge of the system of D-branes arises by relating the index to a homological computation in the corresponding quiver gauge theory, which shows precisely how the original brane configuration folds itself into branes and antibranes. Consider the A_{m+1}-module (7.12) defined by a generic (non-BPS) solution of the Yang-Mills equations on $\mathbb{R}^{2n}_{\theta}\times\mathbb{C}P^1$, and let

$$\underline{\mathcal{W}}=\bigoplus_{i=0}^{m}\underline{W}_i\quad\text{with }\vec{k}_{\underline{\mathcal{W}}}=\sum_{i=0}^{m}w_i\vec{e}_i \tag{9.20}$$

be any quiver representation. Applying the functor $\mathrm{Hom}(-,\underline{\mathcal{W}})$ to the projective resolution (7.13) gives a complex whose cohomology in the pth position defines the extension groups $\mathrm{Ext}^p(\underline{\mathcal{T}},\underline{\mathcal{W}})\cong H^p(\mathbb{R}^{2n}_{\theta};\underline{\mathcal{W}}\otimes\underline{\mathcal{T}}^{\vee})$, with $\mathrm{Ext}^0=\mathrm{Hom}$ and $\mathrm{Ext}^1=\mathrm{Ext}$. We may then define the relative Euler character between these two representations through the corresponding Euler form

$$\chi(\mathcal{T},\mathcal{W}):=\sum_{p\geqslant 0}(-1)^p\dim\mathrm{Ext}^p(\underline{\mathcal{T}},\underline{\mathcal{W}}). \tag{9.21}$$

Since the A_{m+1} quiver has no relations, one has $\mathrm{Ext}^p(\underline{\mathcal{T}},\underline{\mathcal{W}})=0$ for all $p\geqslant 2$ in the present case.[37]

By using (5.7), the resolution (7.13) induces an exact sequence of extension groups given by

$$0\to\mathrm{Hom}(\underline{\mathcal{T}},\underline{\mathcal{W}})\to\bigoplus_{i=0}^{s}\mathrm{Hom}(\ker T^{\dagger}_{N_i},\underline{\mathcal{W}}_i)\to\bigoplus_{i=0}^{s-1}\mathrm{Hom}(\ker T^{\dagger}_{N_{i+1}},\underline{\mathcal{W}}_i)\to\mathrm{Ext}(\underline{\mathcal{T}},\underline{\mathcal{W}})\to 0 \tag{9.22}$$

from which we may compute the Euler form (9.21) explicitly to get

$$\begin{aligned}\chi(\underline{\mathcal{T}},\underline{\mathcal{W}})&=\dim\mathrm{Hom}(\underline{\mathcal{T}},\underline{\mathcal{W}})-\dim\mathrm{Ext}(\underline{\mathcal{T}},\underline{\mathcal{W}})=\sum_{i=0}^{s}\dim\mathrm{Hom}(\ker T^{\dagger}_{N_i},\underline{W}_i)\\&\quad-\sum_{i=0}^{s-1}\dim\mathrm{Hom}(\ker T^{\dagger}_{N_{i+1}},\underline{W}_i)=\sum_{i=0}^{m}N_iw_i-\sum_{i=0}^{m-1}N_{i+1}w_i.\end{aligned} \tag{9.23}$$

Thus the relative Euler character depends only on the dimension vectors of the corresponding representations and coincides with the Ringel form $\langle\vec{k}_{\underline{\mathcal{T}}},\vec{k}_{\underline{\mathcal{W}}}\rangle$ on the representation ring $R_{\mathsf{A}_{m+1}}$ of the A_{m+1} quiver.[37] The map $[\underline{\mathcal{W}}]\mapsto\vec{k}_{\underline{\mathcal{W}}}$ gives a linear map $R_{\mathsf{A}_{m+1}}\to\mathbb{Z}^{m+1}$ which is an isomorphism of Abelian groups since $R_{\mathsf{A}_{m+1}}$ is generated by the Schur modules $\underline{\mathsf{L}}_i, i=0,1,\ldots,m$. By using (7.2) and (7.5) we can write this bilinear pairing in the suggestive form

$$\chi(\underline{\mathcal{T}},\underline{\mathcal{W}})=-\sum_{i=0}^{m}w_i\,\mathrm{index}(\phi_{i+1}). \tag{9.24}$$

The appropriate representation $\underline{\mathcal{W}}$ to couple with in the present case is dictated by the correct incorporation of magnetic charges. As before, the fact that the Higgs fields ϕ_{i+1} in (9.24) themselves are not tachyonic, i.e., do not generate a complex, means that we must fold the SU(2) representations $\underline{V}_{|m-2i|}$ appearing in the ABS construction (8.19) appropriately. The correct folding is expressed by the collection of distinguished triangles (7.39) which shows that we should couple and increasing sequence $\underline{W}_0\subset\underline{W}_1\subset\cdots\subset\underline{W}_m$ of representations as we move along the chain of constituent D-branes of the quiver, so that the SU(2)-module $\underline{W}_i$ gives an extension of the mono-

pole field carried by the elementary brane state at vertex i by the SU(2)-module $\underline{W}_{i-1}$. Thus we take $\underline{W}_i=\oplus_{j=0}^{i}\underline{V}_{|m-2j|}=\underline{V}_{|m-2i|}\oplus\underline{W}_{i-1}$ and embed its class into the representation ring $R_{\mathsf{A}_{m+1}}$ using the $\mathbb{Z}_2$-grading above as the element

$$[\underline{W}_i]=\sum_{j=0}^{i}\operatorname{sgn}(m-2j)[\underline{V}_{|m-2j|}]=\operatorname{sgn}(m-2i)[\underline{V}_{|m-2i|}]+[\underline{W}_{i-1}] \tag{9.25}$$

of virtual dimension

$$w_i=\sum_{j=0}^{i}(m-2j)=(i+1)(m-i) \tag{9.26}$$

for each $i=0,1,\dots,m$. In this case the Euler-Ringel form (9.23) becomes

$$\chi(\underline{\mathcal{T}},\underline{\mathcal{W}})=\sum_{i=0}^{m}(i+1)(m-i)(N_i-N_{i+1})=\sum_{i=0}^{m}(m-2i)N_i=Q \tag{9.27}$$

and it also coincides with the instanton charge of the gauge field configurations on $\mathbb{R}^{2n}_{\theta}\times S^2$. The equivalence of the relative Euler character with the index of the tachyon field above is a consequence of the Grothendieck-Riemann-Roch theorem.

World volume construction: We can now present a very explicit geometric description of the equivalence between the brane configurations on $\mathbb{R}^{2n}\times\mathbb{C}P^1$ and on $\mathbb{R}^{2n}$. The crux of the formulation is the well-known map in K-theory between analytic (noncommutative) and topological (commutative) descriptions.[9,12,30,48] If $\underline{\not{D}}:=-i\sigma\cdot\partial:L^2(\mathbb{R}^{2n},\underline{\Delta}^-_{2n})\to L^2(\mathbb{R}^{2n},\underline{\Delta}^+_{2n})$ is the usual Dirac operator on $\mathbb{R}^{2n}$, then its index coincides with that of the noncommutative ABS configuration (8.29) giving

$$\operatorname{index}\Sigma=\operatorname{index}\underline{\not{D}}. \tag{9.28}$$

This coincides with the K-theory charge of the Bott class $[\underline{\Delta}^+_{2n},\underline{\Delta}^-_{2n};\mu]\in K(\mathbb{R}^{2n})$ given by the ordinary ABS construction,[43] where $\mu_x=\sigma\cdot x/|x|:\underline{\Delta}^-_{2n}\to\underline{\Delta}^+_{2n}$ is Clifford multiplication by $x\in\mathbb{R}^{2n}$. In particular, the Dirac operator itself can be used to represent the analytic K-homology class $[\Sigma]=[\underline{\not{D}}]$ described by the noncommutative ABS field.

Let us represent a system of k Type IIA D-branes wrapped on $\mathbb{R}^{2n}\times\mathbb{C}P^1$ with virtual Chan-Paton bundle $\Xi\in K(\mathbb{R}^{2n}\times\mathbb{C}P^1)$ by the K-cycle $[\mathbb{R}^{2n}\times\mathbb{C}P^1,\Xi,\mathrm{id}]$ in the topological K-homology $\mathbf{K}^t(\mathbb{R}^{2n}\times\mathbb{C}P^1)$. Its equivalence class is invariant under the usual relations of bordism, direct sum and vector bundle modification.[12,30,48] There is an isomorphism $K^t(\mathbb{R}^{2n}\times\mathbb{C}P^1)\cong\mathbf{K}^a(\mathbb{R}^{2n}\times\mathbb{C}P^1)$ of Abelian groups which sends this K-cycle to the analytic K-homology class $[\hat{\not{D}}_\Xi]$ defined by the corresponding twisted Dirac operator on $\mathbb{R}^{2n}\times\mathbb{C}P^1$. Similarly, if $\xi\in K(\mathbb{R}^{2n})$ and $\iota:\mathbb{R}^{2n}\hookrightarrow\mathbb{R}^{2n}\times\mathbb{C}P^1$ is the slice induced by the inclusion $\mathrm{U}(1)\hookrightarrow\mathrm{SU}(2)$ of groups, then the topological K-cycle $[\mathbb{R}^{2n},\xi,\iota]\in K^t(\mathbb{R}^{2n}\times\mathbb{C}P^1)$ corresponds to the analytic K-homology class $\iota_*[\not{D}_\xi]\in K^a(\mathbb{R}^{2n}\times\mathbb{C}P^1)$, where $\not{D}_\xi$ is the twisted Dirac operator on $\mathbb{R}^{2n}$.

Now consider the SU(2)-equivariant reduction of these cycles. From the construction of the preceding section with $\boldsymbol{\phi}_{(m)}=0$ and the equivariant excision theorem of Sec. IV we have the equality

$$[\hat{\not{D}}_\Xi]^{\mathrm{SU}(2)}=\iota_*[\not{D}_{\iota^*\Xi}]^{\mathrm{U}(1)} \tag{9.29}$$

in $K^a_{\mathrm{SU}(2)}(\mathbb{R}^{2n}\times\mathbb{C}P^1)$ which leads to

$$[\mathbb{R}^{2n},\xi,\iota]=[\mathbb{R}^{2n}\times\mathbb{C}P^1,\Xi,\mathrm{id}]\quad\text{with }\Xi=\mathrm{SU}(2)\times_{\mathrm{U}(1)}\xi \tag{9.30}$$

in $K^t_{\mathrm{SU}(2)}(\mathbb{R}^{2n}\times\mathbb{C}P^1)$. The left-hand side of (9.30) corresponds to the class of $D(2n)$ brane-antibrane pairs wrapping $\mathbb{R}^{2n}$, while the right-hand side corresponds to $D(2n+2)$ brane-antibrane

pairs wrapping $\mathbb{R}^{2n}\times\mathbb{C}P^1$. This is just the equivalence between instantons on $\mathbb{R}^{2n}\times\mathbb{C}P^1$ and vortices on $\mathbb{R}^{2n}$. We note that in the case $m=1$, the monopole field is automatically spherically symmetric on $\mathbb{C}P^1$ and one can formulate the equivalence (9.30) using only the requirement of vector bundle modification in *ordinary* topological K-homology,[30] which is equivalent to Bott periodicity (4.1). In contrast, for $m>1$ one must appeal to an SU(2)-equivariant framework and the identification (9.30) of K-cycles is far more intricate. In this case it is a result of the equivariant excision theorem, and *not* of Bott periodicity in equivariant K-theory. It is this intricacy that leads to a more complicated brane-antibrane system when $m>1$.

Using the equivariant ABS construction of the preceding section, the K-homology class of the multi-instanton solution (7.1)–(7.3) is given by the left-hand side of (9.30) with

$$\xi=[\Delta_E^+,\Delta_E^-;\mu_{N_0,N_1,\ldots,N_m}], \tag{9.31}$$

where

$$\Delta_E^+=\bigoplus_{i=m_+}^{m} E_{k_i}\otimes \underline{V}_{|m-2i|} \quad\text{and}\quad \Delta_E^-=\bigoplus_{i=0}^{m_-} E_{k_i}\otimes \underline{V}_{m-2i} \tag{9.32}$$

while

$$\mu_{N_0,N_1,\ldots,N_m}=\prod_{i=0}^{m_-}(\mu_E\circ\Pi_i)^{N_i}\prod_{j=m_+}^{m}(\mu_E^\dagger\circ\Pi_j)^{N_j} \tag{9.33}$$

with $\mu_E:\Delta_E^+\to\Delta_E^+$ acting fiberwise as Clifford multiplication (8.21) and (8.22). The class (9.31) is the K-theory class of the noncommutative soliton field (8.46). The relation (9.30) equates the resulting K-homology class with that defined by

$$\Xi=[\mathrm{SU}(2)\times_{\mathrm{U}(1)}\Delta_E^+,\mathrm{SU}(2)\times_{\mathrm{U}(1)}\Delta_E^-;\pi^*\circ\mu_{N_0,N_1,\ldots,N_m}\circ\iota^*], \tag{9.34}$$

where the projection $\pi:\mathbb{R}^{2n}\times\mathbb{C}P^1\to\mathbb{R}^{2n}$ is a left inverse to the inclusion ι, i.e., $\pi\circ\iota=\mathrm{id}$. Through the standard process of tachyon condensation on the system of $D(2n+2)$ branes and antibranes wrapping $\mathbb{R}^{2n}$, the right-hand side of (9.30) then describes $\Sigma_{2i<m}(m-2i)N_i$ $D2$-branes and $\Sigma_{2i>m}|m-2i|N_i$ $D2$-antibranes. On the left-hand side of (9.30), these are instead $D0$-branes corresponding to vortices left over from condensation in the transverse space $\mathbb{R}^{2n}$.

One can also compute the topological charge in this world volume picture and explicitly demonstrate that the K-theory charges on both sides of (9.30) are the same. The natural charge of branes defined by elements of equivariant K-theory is given by the equivariant index $\mathrm{index}_{\mathrm{SU}(2)}\times(\hat{\not{D}}_\Xi)\in R_{\mathrm{SU}(2)}$, which may be computed by using the SU(2)-index theorem,[49]

$$\mathrm{index}_{\mathrm{SU}(2)}\hat{\not{D}}_\Xi=-\int_{\mathbb{R}^{2n}\times\mathbb{C}P^1}\mathrm{ch}_{\mathrm{SU}(2)}(\Xi)\wedge\hat{A}(\mathbb{R}^{2n}\times\mathbb{C}P^1), \tag{9.35}$$

where $\mathrm{ch}_{\mathrm{SU}(2)}:K_{\mathrm{SU}(2)}(\mathbb{R}^{2n}\times\mathbb{C}P^1)\to H^\bullet_{\mathrm{SU}(2)}(\mathbb{R}^{2n}\times\mathbb{C}P^1;\mathbb{Q})$ is the equivariant Chern character taking values in SU(2)-equivariant rational cohomology. Since this index depends only on the equivariant K-homology class of the Dirac operator on $\mathbb{R}^{2n}\times\mathbb{C}P^1$, we may explicitly use (9.29) and perform the dimensional reduction to write the index (9.35) as

$$\mathrm{index}_{\mathrm{SU}(2)}\hat{\not{D}}_\Xi=-\int_{\mathbb{R}^{2n}}\mathrm{ch}_{\mathrm{SU}(2)}(\xi). \tag{9.36}$$

Since the Chern character in (9.36) is a ring homomorphism between $K_{\mathrm{SU}(2)}(\mathbb{R}^{2n})\cong R_{\mathrm{SU}(2)}$ and $H^\bullet(\mathbb{R}^{2n};\mathbb{Q})\otimes R_{\mathrm{SU}(2)}$, upon substitution of (9.31), (9.32) we can use its additivity and multiplicativity to compute

$$\mathrm{ch}_{\mathrm{SU}(2)}(\xi)=\mathrm{ch}_{\mathrm{SU}(2)}(\Delta_E^+\ominus\Delta_E^-)=\sum_{i=m_+}^{m}\mathrm{ch}(E_{k_i})\otimes\chi_{\underline{V}_{|m-2i|}}-\sum_{i=0}^{m_-}\mathrm{ch}(E_{k_i})\otimes\chi_{\underline{V}_{|m-2i|}},\tag{9.37}$$

where $\chi_{\underline{V}_{|m-2i|}}:\mathrm{SU}(2)\to\mathbb{C}$ are the characters of the SU(2) representations $\underline{V}_{|m-2i|}\cong\mathbb{C}^{|m-2i|}$. This enables us to write the equivariant index on $\mathbb{R}^{2n}\times\mathbb{C}P^1$ in terms of ordinary indices on $\mathbb{R}^{2n}$ to get

$$\mathrm{index}_{\mathrm{SU}(2)}\,\hat{\not{D}}_\Xi=\sum_{i=0}^{m_-}\mathrm{index}(\not{D}_{E_{k_i}})\otimes\chi_{\underline{V}_{|m-2i|}}-\sum_{i=m_+}^{m}\mathrm{index}(\not{D}_{E_{k_i}})\otimes\chi_{\underline{V}_{|m-2i|}}.\tag{9.38}$$

We can turn (9.38) into a linear map $K_{\mathrm{SU}(2)}(\mathbb{R}^{2n}\times\mathbb{C}P^1)\to\mathbb{Z}$ by composing it with the projection $\pi_0:R_{\mathrm{SU}(2)}\to\mathbb{Z}$ onto the trivial representation. Acting on the character ring this gives

$$\pi_0(\chi_{\underline{V}_{|m-2i|}})=\chi_{\underline{V}_{|m-2i|}}(\mathrm{id})=\dim\underline{V}_{|m-2i|}=|m-2i|\tag{9.39}$$

and one finally arrives at

$$\pi_0(\mathrm{index}_{\mathrm{SU}(2)}\,\hat{\not{D}}_\Xi)=\sum_{i=0}^{m_-}|m-2i|\mathrm{index}(\not{D}_{E_{k_i}})-\sum_{i=m_+}^{m}|m-2i|\mathrm{index}(\not{D}_{E_{k_i}}).\tag{9.40}$$

Alternatively, one may arrive at the same formula by directly computing the *ordinary* index of the Dirac operator (8.7) with $\boldsymbol{\phi}_{(m)}=0$ using (8.10) and (8.14)–(8.16). Since

$$\mathrm{index}\,\not{D}_{m-2i}=\dim\ker\not{D}_{m-2i}^+-\dim\ker\not{D}_{m-2i}^-=-(m-2i),\tag{9.41}$$

the index of (8.7) acting on sections of the bundle (8.9) coincides with (9.40). For a gauge field configuration appropriate to the *K*-theory class defined by the tachyon field (9.33), these topological charges coincide with (9.6).

X. VACUUM SOLUTIONS

The extremal cases for which the Higgs fields have the configurations $\{\phi_{i+1}=0,\ i=0,1,\dots,m-1\}$ and $\{\partial_\mu\phi_{i+1}=0,\ i=0,1,\dots,m-1\}$, fall outside of the general scope of the previous analysis and are worth special consideration. They correspond to vacuum sectors of the noncommutative gauge theory and are associated with indecomposable representations of the quiver A_{m+1} that have no arrows. Nevertheless, these vacuum sectors admit nontrivial BPS solutions which signal the presence of stable *D*-branes attached to the closed string vacuum after condensation on the brane-antibrane system. We shall now study them in some detail.

Monopole vacuum: Let us first look at the case $\partial_\mu\phi_{i+1}=0$, $i=0,1,\dots,m-1$. The non-Abelian coupled vortex equations (6.12)–(6.14) then imply

$$A^0=A^1=\cdots=A^m=:A\quad\text{and}\quad F^0=F^1=\cdots=F^m=:F,\tag{10.1}$$

which is only possible in the equal rank case $r=k_0=k_1=\cdots=k_m$ corresponding to the gauge symmetry breaking pattern $\mathrm{U}(k)\to\mathrm{U}(r)^{m+1}$ with $k=(m+1)r$. Thus we take $\phi_{i+1}=\alpha_{i+1}\mathbf{1}_r$ and $\phi_{i+1}^\dagger=\overline{\alpha_{i+1}}\mathbf{1}r$ with $i=0,1,\dots,m-1$, where α_{i+1} are given in (7.30). In quiver gauge theory, the BPS conditions in this sector thus correspond to the representation of A_{m+1} which is r copies of the indecomposable quiver representation $\underline{\mathsf{L}}_0\oplus\underline{\mathsf{L}}_1\oplus\cdots\oplus\underline{\mathsf{L}}_m$. They also require

$$\delta^{a\bar{b}}F_{a\bar{b}}=0\quad\text{and}\quad F_{\bar{a}\bar{b}}=0=F_{ab},\tag{10.2}$$

which are simply the DUY equations on $\mathbb{R}_\theta^{2n}$. Note that (3.26) implies $\mathcal{F}_{y\bar{y}}=0$ in this case, giving the trivial dimensional reduction to $\mathbb{R}_\theta^{2n}$. After switching to matrix form via (6.9), we obtain

$$\delta^{a\bar{b}}[X_a,X_{\bar{b}}]+\delta^{a\bar{b}}\theta_{a\bar{b}}=0\quad\text{and}\quad[X_{\bar{a}},X_{\bar{b}}]=0=[X_a,X_b].\tag{10.3}$$

The obvious solution to (10.3) is the trivial one with $X_a=\theta_{a\bar{b}}\bar{z^b}$, giving $F_{a\bar{b}}=0$. This sector can be understood physically as the endpoint of tachyon condensation, wherein the Higgs fields ϕ_{i+1} have rolled to their minima at $\phi_{i+1}=\alpha_{i+1}\mathbf{1}_r$ and the fluxes have been radiated away to infinity. Here the $D0$-branes have been completely dissolved into the $D(2n)$-branes.

However, nontrivial solutions of the equations (10.3) also exist. For this, let us restrict ourselves to the Abelian case $r=1$ and simplify matters by taking $\theta^a=\theta$ for all $a=1,\ldots,n$. We fix an integer $l\geqslant 1$ and consider the ansatz[28]

$$X_a=\theta_{a\bar{c}}\Sigma_l^\dagger f(\mathcal{N})\bar{z^c}\Sigma_l \quad \text{and} \quad X_{\bar{a}}=\theta_{\bar{a}c}\Sigma_l^\dagger z^c f(\mathcal{N})\Sigma_l, \tag{10.4}$$

where f is a real function of the "total number operator"

$$\mathcal{N}:=\frac{1}{2\theta}\sum_{a=1}^{n} z^a\bar{z^a} \tag{10.5}$$

with the property that $f(r)=0$ for $r\leqslant l-1$. The shift operator Σ_l in (10.4) is defined to obey

$$\Sigma_l^\dagger\Sigma_l=1 \quad \text{while } \Sigma_l\Sigma_l^\dagger=1-P_l \tag{10.6}$$

with

$$P_l:=\sum_{|\vec{r}|\leqslant l-1}|r_1,\ldots,r_n\rangle\langle r_1,\ldots,r_n|, \tag{10.7}$$

where $\vec{r}=(r_1,\ldots,r_n)$ with $|\vec{r}|:=r_1+\cdots+r_n$. Note that

$$\Sigma_l^\dagger P_l=P_l\Sigma_l=0 \quad \text{and} \quad f(\mathcal{N})P_l=P_l f(\mathcal{N})=0, \tag{10.8}$$

and $\Sigma_l^\dagger$ projects all states with $|\vec{r}|<l$ out of the Fock space $\mathcal{H}$.

One easily sees that (10.4) fulfills the homogeneous equations in (10.3). Remembering that $\theta_{a\bar{b}}=-\theta_{\bar{b}a}=(1/2\theta)\delta_{a\bar{b}}$, we also obtain

$$\begin{aligned}[X_a,X_{\bar{b}}]&=\theta_{a\bar{c}}\theta_{\bar{b}d}\Sigma_l^\dagger\{f(\mathcal{N})\bar{z^c}(1-P_l)z^d f(\mathcal{N})-z^d f(\mathcal{N})(1-P_l)f(\mathcal{N})\bar{z^c}\}\Sigma_l\\&=-\frac{1}{4\theta^2}\delta_{a\bar{c}}\delta_{\bar{d}b}\Sigma_l^\dagger\{f^2(\mathcal{N})\bar{z^c}z^d-f^2(\mathcal{N}-1)z^d\bar{z^c}\}\Sigma_l\end{aligned} \tag{10.9}$$

with the help of the identities $\bar{z^c}P_l=P_{l-1}\bar{z^c}$ where $P_0:=0$. We have also used

$$\bar{z^c}f(\mathcal{N})=f(\mathcal{N}+1)\bar{z^c} \quad \text{and} \quad z^d f(\mathcal{N})=f(\mathcal{N}-1)z^d. \tag{10.10}$$

Substituting (10.9) into (10.3), we employ

$$\delta_{\bar{c}d}z^d\bar{z^c}=2\theta\mathcal{N} \quad \text{and} \quad \delta_{\bar{c}d}\bar{z^c}z^d=2\theta(\mathcal{N}+n) \tag{10.11}$$

to find the conditions

$$\begin{aligned}0=\delta^{a\bar{b}}[X_a,X_{\bar{b}}]+\delta^{a\bar{b}}\theta_{a\bar{b}}&=-\frac{1}{2\theta}\Sigma_l^\dagger\{f^2(\mathcal{N})(\mathcal{N}+n)-f^2(\mathcal{N}-1)\mathcal{N}\}\Sigma_l+\frac{n}{2\theta}\\&=\frac{1}{2\theta}\Sigma_l^\dagger\{\mathcal{N}f^2(\mathcal{N}-1)-(\mathcal{N}+n)f^2(\mathcal{N})+n\}\Sigma_l\end{aligned} \tag{10.12}$$

on the operator f. With the initial conditions $f(0)=f(1)=\cdots=f(l-1)=0$ and the finite-energy condition $f(r)\to 1$ as $r\to\infty$, these recursion relations are solved by

$$f^2(\mathcal{N}) = \left(1 - \frac{Qn!}{(\mathcal{N}+1)\cdots(\mathcal{N}+n)}\right)(1-P_l), \tag{10.13}$$

where

$$Q := \frac{l(l+1)\cdots(l+n-1)}{n!} \tag{10.14}$$

is the number of states in $\mathcal{H}$ with $\mathcal{N}\leqslant l-1$, i.e., the number of states removed by the operator $\Sigma_l^\dagger$.

We arrive finally at the nontrivial gauge field configuration given by

$$X_a = \frac{1}{2\theta}\Sigma_l^\dagger \sqrt{1 - \frac{Qn!}{(\mathcal{N}+1)\cdots(\mathcal{N}+n)}}(1-P_l)\,\delta_{a\bar{c}}\bar{z}^{\bar{c}}\Sigma_l. \tag{10.15}$$

The field strength F on $\mathbb{R}^{2n}_\theta$ obtained from (10.15) has finite nth Chern number Q.[28] The topological charge Q given by (10.14) is calculated here via an integral over $\mathbb{R}^{2n}_\theta$. However, the $(n+l)$th Chern number for this configuration considered as a gauge field on $\mathbb{R}^{2n}_\theta \times \mathbb{C}P^1$ with $\mathcal{F}_{y\bar{y}}=0=\mathcal{F}_{\vartheta\varphi}$ vanishes. Moreover, this configuration has finite energy (5.2) proportional to the topological charge,[28]

$$E_{\mathrm{BPS}} = (2\pi)^{n+1}R^2 n(n-1)Q, \tag{10.16}$$

as usual for a BPS instanton solution.

Higgs vacuum: The choice $\phi_{i+1}=0$ for all $i=0,1,\dots,m-1$ is somewhat more interesting since from (3.26) and (5.29) we then have $\mathcal{F}_{y\bar{y}}\neq 0$ with

$$\mathcal{F}_{y\bar{y}} = -\frac{R^2}{(R^2+y\bar{y})^2}\mathbf{\Upsilon}_{(m)}. \tag{10.17}$$

This configuration gives the local maximum of the Higgs potential corresponding to the open string vacuum containing D-branes. In this case the vortex equations (6.12)–(6.14) reduce to

$$\delta^{a\bar{b}}F^i_{a\bar{b}} = \frac{m-2i}{4R^2} \quad \text{and} \quad F^i_{a\bar{b}} = 0 = F^i_{ab}. \tag{10.18}$$

After switching to matrix form via (6.9) we obtain

$$\delta^{a\bar{b}}[X^i_a, X^i_{\bar{b}}] + \delta^{a\bar{b}}\left(1 - \frac{(m-2i)\theta}{2nR^2}\right)\theta_{a\bar{b}} = 0 \quad \text{and} \quad [X^i_{\bar{a}}, X^i_{\bar{b}}] = 0 = [X^i_a, X^i_b], \tag{10.19}$$

where we have used the formula $\theta_{a\bar{b}}=(1/2\theta)\delta_{a\bar{b}}$. Recall that there is no summation over the index $i=0,1,\dots,m$ in the equations (10.19).

By comparing (10.19) and (10.3), we conclude that (10.19) can be solved for each i by the same ansatz as for (10.3). For this, let us restrict ourselves again to the Abelian case for all nodes $i=0,1,\dots,m$ (so that $k=m+1$), and fix $m+1$ positive integers $l_0, l_1, \dots, l_m$. We take

$$X^i_a = \theta_{a\bar{c}}\Sigma^\dagger_{l_i} f_i(\mathcal{N})\bar{z}^{\bar{c}}\Sigma_{l_i} \quad \text{and} \quad X^i_{\bar{a}} = \theta_{\bar{a}c}\Sigma^\dagger_{l_i} z^c f_i(\mathcal{N})\Sigma_{l_i} \tag{10.20}$$

analogously to (10.4)–(10.7). Producing then the same calculations as before, we obtain the gauge field configuration

$$X^i_a = \frac{1}{2\theta^i}\Sigma^\dagger_{l_i}\sqrt{1 - \frac{Q_i n!}{(\mathcal{N}+1)\cdots(\mathcal{N}+n)}}(1-P_{l_i})\,\delta_{a\bar{c}}\bar{z}^{\bar{c}}\Sigma_{l_i}, \tag{10.21}$$

where

$$\theta^i := \frac{\theta}{\sqrt{1-\frac{(m-2i)\theta}{2nR^2}}} \tag{10.22}$$

and

$$Q_i = \frac{l_i(l_i+1)\cdots(l_i+n-1)}{n!}. \tag{10.23}$$

We have chosen the radius R of the sphere so that $R^2 > m\theta/2n$.

The solutions (10.21) coincide with those given by (10.15) if one assigns different noncommutativity parameters θ^i to the world volumes of $D(2n)$-branes carrying different magnetic fluxes proportional to $m-2i$. Then the field strength $F^i(\theta^i)$ on $\mathbb{R}^{2n}_{\theta^i}$ obtained from (10.21) will have finite topological charge Q_i given by (10.23) and corresponding finite BPS energy analogous to (10.16), and the configuration thus described extends to instantons on $\mathbb{R}^{2n}_{\theta}\times\mathbb{C}P^1$. The interesting idea of introducing distinct noncommutativity parameters on multiple coincident D-branes, generated by different magnetic fluxes on their world volumes,[50] was discussed in Ref. 51 as a means (among other things) of stabilizing brane-antibrane systems. This proposal gains support from our Higgs vacuum BPS solutions (10.21) which carry different magnetic fluxes on different branes.

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Fractional boundaries for fluid spheres

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A single Israel layer can be created when two metrics adjoin with no continuous metric derivative across the boundary. The properties of the layer depend only on the two metrics it separates. By using a fractional derivative match, a family of Israel layers can be created between the same two metrics. The family is indexed by the order of the fractional derivative. The method is applied to Tolman IV and V interiors and a Schwarzschild vacuum exterior. The method creates new ranges of modeling parameters for fluid spheres. A thin shell analysis clarifies pressure/tension in the family of boundary layers. © *2006 American Institute of Physics.*
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I. INTRODUCTION

There is long-standing interest in fluid sphere solutions, largely because of their astrophysical implications. An astrophysical model is often an interior fluid sphere metric matched to a Schwarzschild vacuum or Kottler exterior across a bounding surface. The standard technique matches metric functions and extrinsic curvatures on the boundary. When the extrinsic curvatures do not match, an Israel boundary layer[1,2] can be created. The layer depends only on the properties of the two bounding metrics. Methods that will create a family of surface layers between the bounds could prove useful in exploring models of spheres with variable crusts. One way of creating variable surface layers is to modify the boundary conditions at the fluid–vacuum interface.

While an extrinsic curvature match is the boundary condition currently most used, there are three types of boundary conditions that have been used to match analytic solutions across non-null boundaries. The three methods have been discussed by Bonnor and Vickers,[3] and they all involve derivatives of the metric functions. The boundary conditions can be generalized by broadening the idea of derivatives to include fractional derivatives.[4,5]

There are two simple ways to proceed with the generalization. The first is to assume a straight fractional derivative match on the boundary metrics and then to use the fractional relations in the usual formalism for the boundary stress energy. This would be a generalization of the Lichnerowicz boundary condition. It would not generalize the extrinsic curvature to fractional values. The second would be to use fractional derivatives to define a fractional extrinsic curvature and then use it to define a fractional boundary layer. This would be a generalization of the usual Lie derivative to fractional values. The use of fractional calculus is motivated by the possible fractional nature of the growth processes forming the boundary layer. Fractional transport processes are one of the main areas of application for fractional calculus, and boundary layers formed by these processes could reflect this fractional formation process.

Beyond the fractional generalizations of techniques and tensor functions, one must consider the various definitions of fractional differentiation. Use of fractional calculus in diverse areas of physics has increased enormously since fractional derivatives were first considered by Leibnitz and L'Hospital[4] in 1695. Many different definitions have been proposed for different applications. In this article we use the Caputo form of the Riemann–Liouville and Weyl definitions. The Caputo derivative is an integral transform of the regular partial derivative and preserves the zero fractional

derivative of a constant. While considering generalizations of relativistic gravity to include fractional calculus, the different definitions must be explored to determine their applicability.

This work has two goals: first to develop a variable layer model that could be applied to astrophysical problems, and second to better understand the role that fractional derivatives might play within a general relativistic framework. In this paper we will apply the first method and use fractional derivatives to create a family of Israel boundary layers between two bounding metrics. The family is parametrized by the order of the fractional derivative and may be used to model fluid spheres with variable crusts. Even when a regular derivative match is possible, the fractional match will broaden the parameter ranges for the fluid interior.

In the next section we discuss the metrics and describe the boundary layer. In the third section several models are considered: the Misner–Zapolsky (MZ) solution,[6,7] and Tolman's solutions IV and V.[8] The thin shell pressure balance is treated in the fourth section and some details of the fractional match are discussed in Sec. V. Details of the fractional derivatives and the standard fluid sphere formalism are given in the Appendices.

II. THEORETICAL FRAMEWORK

A. The space-time

The two regions to be considered are covered by an exterior Schwarzschild solution bounding an interior spherical fluid. The metrics are, with functions $\psi_{\rm Sch}=1-2m_0/y$, $\nu(r)$, $\lambda(r)$, $H(r)$:

$$\text{Exterior: } g^{\rm Sch}_{\alpha\beta}\,dx^\alpha\,dx^\beta=-\psi_{\rm Sch}\,dt^2+\psi^{-1}_{\rm Sch}\,dy^2+y^2\,d\Omega^2, \tag{1}$$

$$\text{Interior: } g^{\rm fluid}_{\alpha\beta}\,dx^\alpha\,dx^\beta=-e^{\nu}\,d\tau^2+e^{\lambda}\,dr^2+H^2\,d\Omega^2. \tag{2}$$

The bounding surface is located at $y=y_0$ in the exterior and $r=R_0$ in the interior. The corresponding normals to the surface are

$$\text{Exterior: } n^E_\mu\,dx^\mu=\psi^{-1/2}_{\rm Sch}\,dy, \tag{3}$$

$$\text{Interior: } n^I_\mu\,dx^\mu=e^{\lambda/2}\,dr. \tag{4}$$

Fractional derivatives leave these metrics unchanged. Our fractional extension provides a crust layer between the interior and exterior metrics.

B. Matching conditions

On the boundary, the metric match conditions are

$$(1-2m_0/R_0)=e^{\nu(R_0)},$$

$$R_0=H(R_0). \tag{5}$$

The second matching condition is the extrinsic curvature match, K^a_b, on the bounding surface. If the curvatures do not match, an Israel boundary layer is created. The stress–energy content of the Israel layer is constructed from the mismatch in the extrinsic curvatures. The stress–energy of the boundary layer is[2]

$$-8\pi S^a_b=\langle K^a_b\rangle-\langle K\rangle g^a_b. \tag{6}$$

Here $K=K^a_a$. The stress–energy components on the boundary are

$$-8\pi S^0_0=[\langle K^0_0\rangle-\langle K^0_0+2K^\theta_\theta\rangle g^0_0]=-2\langle K^\theta_\theta\rangle,$$

$$-8\pi S_\theta^\theta = -8\pi S_\phi^\phi = [\langle K_\theta^\theta\rangle - \langle K_0^0 + 2K_\theta^\theta\rangle g_\theta^\theta] = -[\langle K_\theta^\theta\rangle + \langle K_0^0\rangle],$$

and the stress–energy of the boundary is

$$8\pi S_0^0 = \frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{\theta\theta,y}^E}{g_{\theta\theta}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{\theta\theta,r}^I}{g_{\theta\theta}^I}$$

$$8\pi S_\theta^\theta = 8\pi S_\phi^\phi = \frac{1}{2}\left[\frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{\theta\theta,y}^E}{g_{\theta\theta}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{\theta\theta,r}^I}{g_{\theta\theta}^I}\right] + \frac{1}{2}\left[\frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{00,y}^E}{g_{00}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{00,r}^I}{g_{00}^I}\right]. \quad (7)$$

C. Match of fractional derivatives

The stress–energy of the Israel layer is evaluated on the boundary between the interior and exterior metrics. The actual finite thickness boundary layer is modeled by the single bounding surface at $r=R_0$. The stress–energy content is governed by regular derivatives of the metric functions. The metric match coupled with some derivative match of the metric on the layer, sets relations between the parameters of the interior and exterior solutions. With the usual extrinsic curvature or other derivative matches, the properties of the layer are set by the parameters of the bounding metric. With a fractional match, the order of the fractional derivative enters along with the other parameters and a family of fractional boundary layers is created. The fluid sphere examples considered in this paper have boundary metrics of the form

$$ds^2 = -F(r)dt^2 + r^2\, d\Omega^2.$$

The fractional match is applied only to the differing part of the Israel layer metric, the g_{00} metric potential. The actual calculation of the fractional derivatives involves a choice of definition. We use the Caputo definition (see Appendix A) with the $(0\leqslant r\leqslant R_0)$ Riemann–Liouville limits for the interior and the $(R_0\leqslant r\leqslant\infty)$ Weyl limits for the exterior. The limits themselves, as well as the choice of different limits for interior and exterior derivatives, reflect the nonlocality of the fractional derivative operation. Nonlocality in fractional time derivatives is an expression of system memory.[9] It has proven especially useful in modeling jump processes with long wait times.[10] Similarly, spatial nonlocality implies that the derivative on the boundary depends on values away from the boundary; fractional spatial derivatives have been useful in modeling processes with very large jump distances.[11] When the jump distance depends on the jump time, fractional time and spatial derivatives enter into the transport equations.[12] The examples discussed here are static, but the structure of the boundary layer could reflect the transport process. The fractional matching condition is

$$\frac{1}{\Gamma(n-\alpha)}\int_0^{R_0}\frac{d^nF_I(x)/dx^n}{(r-x)^{\alpha-n+1}}dx = \frac{(-1)^{n-1}}{\Gamma(n-\alpha)}\int_{R_0}^{\infty}\frac{d^nF_E(x)/dx^n}{(x-r)^{\alpha-n}}dx,$$

and is applied at $r=R_0$. We note that the single layer at $r=R_0$ only approximates a boundary of finite thickness and that using a nonlocal operator might be a better approximation to the actual match over a finite thickness than the usual derivative match over a zero thickness surface.

In the next sections, we apply the formalism to Tolman IV and V solutions.

III. MODEL CALCULATIONS

A. Tolman's Solution V

1. The solution

We consider a parametrization of Tolman's Vth solution.[8,13] The metric, with constants n and C, is

$$ds^2 = -(r/r_0)^{N_1}\,dt^2 + a(1-aCr^{2+b})^{-1}\,dr^2 + r^2\,d\Omega^2. \tag{8}$$

The parameters formed from n are

$$N_1 = 4n/(1+n), \qquad N_2 = 1+6n+n^2,$$

$$a = \frac{N_2}{(1+n)^2}, \qquad b = \frac{N_1(1-n)}{(1+3n)}.$$

The interior density and pressure for this solution are

$$\begin{aligned} 8\pi\rho &= \left(\frac{4n}{N_2}\right)\frac{1}{r^2} + C(3+b)r^b, \\ 8\pi P &= \left(\frac{4n^2}{N_2}\right)\frac{1}{r^2} - C\frac{(1+5n)}{1+n}r^b. \end{aligned} \tag{9}$$

For $C=0$, the solution reduces to the MZ solution.[6,7,15] This solution was originally used to describe neutron star models with equation of state $P=n\rho$. The solution with $C=0$ does not admit a zero-pressure boundary; the $C\neq 0$ solution does. Both solutions are singular at the origin and are used to represent an ultrahigh density core. The MZ solution, lacking a vacuum boundary, is generally matched to a gaseous envelope. It may be more realistic in some cases to match these solutions to a crust with surface stresses.

For $C\neq 0$, the zero-pressure boundary, R_z, relates constants C and n,

$$C = \frac{4n^2(1+n)}{(1+5n)N_2}\frac{1}{R_z^{2+b}}. \tag{10}$$

Substituting for C, the pressure and density can be written as

$$8\pi P_{C\neq 0} = \frac{4n^2}{N_2}\left(\frac{1}{r^2} - \frac{r^b}{R_z^{2+b}}\right), \tag{11}$$

$$8\pi\rho_{C\neq 0} = \frac{4n}{N_2}\left(\frac{1}{r^2}\right) + \frac{4n^2}{N_2}\frac{(n+3)}{(1+3n)}\left(\frac{r^b}{R_z^{2+b}}\right). \tag{12}$$

The condition $P_{C\neq 0}\geqslant 0$ requires

$$R_0 \leqslant R_z. \tag{13}$$

Fractional matching will allow a broader family of sphere sizes. Below, we graph values for the case $n=1/3$. For $C=0$, there is no zero-pressure boundary and no constraint.

2. Matching conditions

The matching conditions are the same for any C value. Matching the interior metric to vacuum Schwarzschild, we find

$$1 - 2m_0/R_0 = (R_0/r_0)^{N_1}$$

[recall $N_1=4n/(1+n)$],

$$\frac{2m_0}{R_0^{1+\alpha}}\Gamma(1+\alpha) = \left(\frac{R_0}{r_0}\right)^{N_1}\left(\frac{N_1}{R_0^{\alpha}}\right)\frac{\Gamma(N_1)}{\Gamma(N_1+1-\alpha)}.$$

Combining the two relations, we find that the scaled radius of the interior is

$$\frac{R_0}{2m_0} = 1 + \frac{\Gamma(1+\alpha)\Gamma(N_1+1-\alpha)}{\Gamma(1+N_1)}. \tag{14}$$

Note that the boundary radius is always greater than $2m_0$. For $\alpha<1$, there are no limits imposed by Eq. (14). For $\alpha\geqslant 1$ we require

$$1+N_1 > \alpha.$$

The metric parameter r_0 is described by

$$\left(\frac{r_0}{R_0}\right)^{N_1} = 1 + \frac{\Gamma(1+N_1)}{\Gamma(1+\alpha)\Gamma(N_1+1-\alpha)}. \tag{15}$$

The sizes of the fractional spheres are discussed in Sec. V.

3. The crust stress–energy

The stress–energy of the crust for general C is, with $\gamma_0 := \sqrt{1-2m_0/R_0}$,

$$8\pi S_0^0 = \frac{2}{R_0}\left[\gamma_0 - (1+n)N_2^{-1/2}\sqrt{1-aCR_0^{2+b}}\right]$$

$$8\pi S_\theta^\theta = 8\pi S_\phi^\phi = \frac{1}{2R_0}\left[\gamma_0 + 1/\gamma_0 - (1+n)(2+N_1)N_2^{-1/2}\sqrt{1-aCR_0^{2+b}}\right].$$

For $C\neq 0$, the boundary layer has a stress–energy content [recall $N_1=4n/(1+n)$, $N_2=1+6n+n^2$],

$$8\pi S_0^0 = \frac{2}{R_0}\left[\gamma_0 - (1+n)N_2^{-1/2}\sqrt{1-\frac{nN_1}{(1+5n)}(R_0/R_z)^{2+b}}\right],$$

$$8\pi S_\theta^\theta = 8\pi S_\phi^\phi = \frac{1}{2R_0}\left[\gamma_0 + 1/\gamma_0 - 2(1+3n)N_2^{-1/2}\sqrt{1-\frac{nN_1}{(1+5n)}(R_0/R_z)^{2+b}}\right]. \tag{16}$$

For $C=0$ the fluid energy density and stress are

$$8\pi S_0^0 = (2/R_0)\left[\gamma_0 - (1+n)N_2^{-1/2}\right]$$

$$= (2/R_0)\left[(R_0/r_0)^{2n/(1+n)} - (1+n)N_2^{-1/2}\right], \tag{17}$$

$$8\pi S_\theta^\theta = 8\pi S_\phi^\phi = (1/R_0)\left[(1-m_0/R_0)/\gamma_0 - (1+3n)N_2^{-1/2}\right],$$

and describe a much richer modeling environment.

B. Tolman's Solution IV

1. Metric and stress–energy

This solution describes an object with finite central presssure and density. A stiff fluid core is not possible in this model. The interior metric for this solution is, with constants A, B, and C,

$$ds^2 = -B^2(1+r^2/A^2)dt^2 + \frac{1+2r^2/A^2}{(1-r^2/C^2)(1+r^2/A^2)}dr^2 + r^2\,d\Omega^2. \tag{18}$$

The interior density and pressure are

$$8\pi\rho = \frac{1}{A^2}\left[\frac{1+3(A^2/C^2+r^2/C^2)}{1+2r^2/A^2} + 2\frac{1-r^2/C^2}{(1+2r^2/A^2)^2}\right], \tag{19}$$

$$8\pi P = \frac{1}{A^2}\left[\frac{1-(A^2/C^2+3r^2/C^2)}{1+2r^2/A^2}\right]. \tag{20}$$

Constants A and C can be expressed in terms of the central fluid values. We have

$$8\pi\rho_c = \frac{3}{A^2}\left[1+A^2/C^2\right],$$

$$8\pi P_c = \frac{1}{A^2}\left[1-A^2/C^2\right],$$

$$A^2 = \frac{2}{8\pi(\rho_c/3+P_c)},$$

$$C^2 = \frac{2}{8\pi(\rho_c/3-P_c)}.$$

Note that the central fluid equation of state (EOS) is constrained: $P_c < \rho_c/3$. The zero-pressure boundary that occurs in the regular derivative match has size

$$R_z^2 = C^2/3 - A^2/3. \tag{21}$$

2. Metric match

The match to vacuum Schwarzschild provides

$$B^2(1+R_0^2/A^2) = 1-2m_0/R_0. \tag{22}$$

The fractional match is

$$\frac{B^2}{A^2}\frac{1}{R_0^{\alpha-2}}\frac{1}{\Gamma(3-\alpha)} = \frac{m_0}{R_0^{1+\alpha}}\Gamma(1+\alpha),$$
$$B^2R_0^3 = A^2m_0\Gamma(3-\alpha)\Gamma(1+\alpha). \tag{23}$$

Combining with the metric match, we obtain

$$A^2 = R_0^2\frac{(R_0/m_0)-[2+\Gamma(3-\alpha)\Gamma(1+\alpha)]}{\Gamma(3-\alpha)\Gamma(1+\alpha)},$$

$$B^2 = \frac{m_0}{R_0}\left[\frac{R_0}{m_0}-[2+\Gamma(3-\alpha)\Gamma(1+\alpha)]\right], \tag{24}$$

$$R_0/m_0 > 2+\Gamma(3-\alpha)\Gamma(1+\alpha).$$

The boundary size depends on the central EOS as well as the order of the fractional derivative:

$$\left(\frac{R_0}{m_0}\right)^3 - \left(\frac{R_0}{m_0}\right)^2[2+\Gamma(3-\alpha)\Gamma(1+\alpha)] - \frac{\Gamma(3-\alpha)\Gamma(1+\alpha)}{4\pi m_0^2(P_c+\rho_c/3)} = 0. \tag{25}$$

3. Crust stress–energy

We introduce scaled parameters $r_A^2 := R_0^2/A^2$, $r_C^2 := R_0^2/C^2$, and $r_z^2 := R_z^2/A^2$.

$$8\pi S_0^0 = \frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{\theta\theta,y}^E}{g_{\theta\theta}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{\theta\theta,r}^I}{g_{\theta\theta}^I} = \frac{2}{R_0}\left[\sqrt{1-2m_0/R_0} - \sqrt{\frac{(1-r_C^2)(1+r_A^2)}{1+2r_A^2}}\right]$$
$$= \frac{2}{R_0}\sqrt{1+r_A^2}\left[B - \frac{A}{C}\sqrt{\frac{1+3r_z^2-r_A^2}{1+2r_A^2}}\right], \tag{26}$$

$$8\pi S_\theta^\theta = 8\pi S_\phi^\phi = \frac{1}{2}\left[\frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{\theta\theta,y}^E}{g_{\theta\theta}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{\theta\theta,r}^I}{g_{\theta\theta}^I}\right] + \frac{1}{2}\left[\frac{1}{(g_{yy}^E)^{1/2}}\frac{g_{00,y}^E}{g_{00}^E} - \frac{1}{(g_{rr}^I)^{1/2}}\frac{g_{00,r}^I}{g_{00}^I}\right]$$
$$= \frac{1}{R_0}\sqrt{1+r_A^2}\left[B - \frac{A}{C}\sqrt{\frac{1+3r_z^2-r_A^2}{1+2r_A^2}}\right] + \frac{1}{R_0\sqrt{1+r_A^2}}\left[\frac{m_0/R_0}{B} - (r_A^2)\sqrt{\frac{1-r_C^2}{1+2r_A^2}}\right]. \tag{27}$$

Some examples of radius variation and crust stress energy are given in Sec. V.

IV. EQUILIBRIUM IN THE PRESENCE OF SURFACE STRESSES

A. Stress–energy

The Israel layer is the zero-thickness idealization of a bounding layer with finite thickness, d. The physical crust runs from an outer boundary R_0 to an interior fluid boundary R_i with $d=R_0-R_i$. We know that the interior fluid solutions will satisfy the[22] Tolman–Oppenheimer-Volkov (TOV) equation. The Israel layers generated in this work are obtained by introducing a discontinuity in the derivative of g_{00}. The analog of the TOV equation for the layer, requiring that the solutions remain static, will provide relations among the model parameters. To develop the TOV analog for the layer, consider the general static spherical metric for an interior fluid with pressure P and density ρ,

$$ds^2 = -e^\nu dt^2 + e^\lambda dr^2 + r^2 d\Omega^2. \tag{28}$$

The details of the field equations are given in Appendix B. The covariant derivative of the general energy–momentum tensor provides the conservation equation

$$-\frac{\partial T_r^r}{\partial r} - \left(\frac{\nu'}{2} + \frac{2}{r}\right)T_r^r + \left(\frac{\nu'}{2}\right)T_0^0 + \left(\frac{2}{r}\right)T_\theta^\theta = 0. \tag{29}$$

For an isotropic fluid matched to vacuum, this is the usual TOV equation,

$$\frac{\partial P}{\partial r} + \frac{\nu'}{2}(P+\rho) = 0. \tag{30}$$

It is the analog of this equation that we want for the Israel layer.

B. The conservation equation over a limiting shell

Consider a bounding shell that will approximate a thin surface layer. The central radius of the shell is R with the outer boundary $R^{(+)}=R+d/2$, and the inner interior fluid boundary at $R^{(-)}=R-d/2$. d is the coordinate shell thickness. In the $d\to 0$ limit, $R\to R_0$. A general stress-energy T_j^i can be related to a surface stress–energy S_b^a by[2]

$$T_j^i = \delta(l) S_b^a e_a^i e_j^b, \tag{31}$$

where e_a^i is a tangent vector to the shell, and l the proper distance along a radial geodesic, $l = e^{\lambda/2}d$. The shell stress–energy has a perfect fluid analog,

$$S^{ij} = \sigma U^i U^j + \tau(h^{ij} + U^i U^j),$$

$$h^{ij} = g^{ij} - n^i n^j,$$

$$n^i = (0, e^{-\lambda}, 0, 0),$$

where $S_0^0/c^2 = -\sigma(\mathrm{g/cm^2})$ and $S_\theta^\theta = \pm\tau(\mathrm{dynes/cm})$. Following Poisson[2], we take $l=0$ on the hypersurface defined by R, with l negative for $r<R$ and positive on the vacuum side, $r>R$. The T_r^r content of the shell can be described using a Heaviside function, $\Theta(l)$, as

$$T_r^r = \Theta(l)T_r^{(+)r} + \Theta(-l)T_r^{(-)r} + \delta(l)S_r^r. \tag{32}$$

The last term will be zero for the 2+1 shell stress energy. Forming the derivative needed in the conservation equation, we have

$$\frac{\partial T_r^r}{\partial r} = \delta(l)\frac{dl}{dr}T_r^{(+)r} + \Theta(l)\frac{\partial T_r^{(+)r}}{\partial r} - \delta(l)\frac{dl}{dr}T_r^{(-)r} + \Theta(-l)\frac{\partial T_r^{(-)r}}{\partial r}.$$

In the $l\to 0$ limit we have

$$\frac{\partial T_r^r}{\partial r} = -\lim_{l\to 0}\left[\delta(l)\frac{dl}{dr}T_r^{(-)r}\right] = -\lim_{l\to 0}[\delta(l)\mathrm{Pe}^{\lambda/2}], \tag{33}$$

where the first term is zero with no radial pressure on the outer boundary. The stress–energy function evaluated at the inner boundary is P and $\lambda^{(-)}$ is an interior metric function. Substituting into the conservation equation in the $l\to 0$ hypersurface limit, we have

$$\mathrm{Pe}^{\lambda^{(-)}/2} + (\nu'/2)S_0^0 + (2/R_0)S_\theta^\theta = 0. \tag{34}$$

C. Evaluating $\partial_t g_{00}$

The derivative, ν', on the hypersurface, can be written as a difference equation,

$$\nu'(R) = \frac{\nu(R+d/2) - \nu(R-d/2)}{(R+d/2)-(R-d/2)} = \frac{\nu(R+d/2) - \nu(R) + \nu(R) - \nu(R-d/2)}{(R+d/2)-(R-d/2)}$$

$$= \frac{\nu(R+d/2) - \nu(R)}{d} + \frac{\nu(R) - \nu(R-d/2)}{d}.$$

Expanding, we can write

$$\nu(R \pm d/2) = \nu(R) \pm \nu'[R^{(\pm)}]\frac{d}{2} + \cdots.$$

Substituting in the thin shell limit, we have

$$\nu'(R) \approx \frac{\nu'[R^{(+)}] + \nu'[R^{(-)}]}{2}.$$

The first term follows from the Schwarzschild metric match and the second is given in Appendix B. We have

$$\nu'(R) \approx (2m/R^2 + 4\pi RP)(1-2m/R)^{-1},$$

where we have identified the Schwarzschild mass parameter with the interior mass of the fluid. Substituting into Eq. (34), we have

$$-P(1-2m/R)^{-1/2} = (m/R^2 + 2\pi RP)(1-2m/R)^{-1}S_0^0 + (2/R)S_\theta^\theta, \tag{35}$$

which describes the thin shell pressure balance. The classical limit of this equation follows from $c \to \infty$ and is

$$P - \sigma\frac{m}{R^2} = \left(\frac{2}{R}\right)(-\tau).$$

If the fluid pressure at the interior boundary dominates, this can be interpreted as a tension in the shell, balancing the outward interior fluid pressure at the boundary minus the inward pressure due to the gravitational attraction of the shell by the interior fluid. If the shell mass term dominates, the stress in the boundary layer will be a pressure. In the next section we explore the stress–energy structure of the boundary layer, and will see parameter ranges with both layer tension and pressure.

V. DETAILS OF THE FRACTIONAL MATCH

A. Sphere radii

The sizes of the sphere are described by

$$\text{TolmanV: } \frac{R_0}{2m_0} = 1 + \frac{\Gamma(1+\alpha)\Gamma(4n/(1+n)+1-\alpha)}{\Gamma(1+4n/(1+n))}, \tag{36}$$

$$\text{TolmanIV: } \left(\frac{R_0}{m_0}\right)^3 - \left(\frac{R_0}{m_0}\right)^2[2+\Gamma(3-\alpha)\Gamma(1+\alpha)] - \frac{\Gamma(3-\alpha)\Gamma(1+\alpha)}{4\pi m_0^2(P_c+\rho_c/3)} = 0. \tag{37}$$

The scaled boundary radius, R_0/m_0, for Tolman V is plotted as a function of alpha for various n in Fig. 1.

The overall effect of the fractional match is to increase the range of sphere sizes for a given EOS. The largest differences are for low- n fluids, where a very much smaller sphere radius is possible than for the zero-pressure match. The Buchdahl bound[14] limits the ratio of $2m_0/R_0$ for fluid spheres whose g_{00} component is continuous across the boundary and whose density is

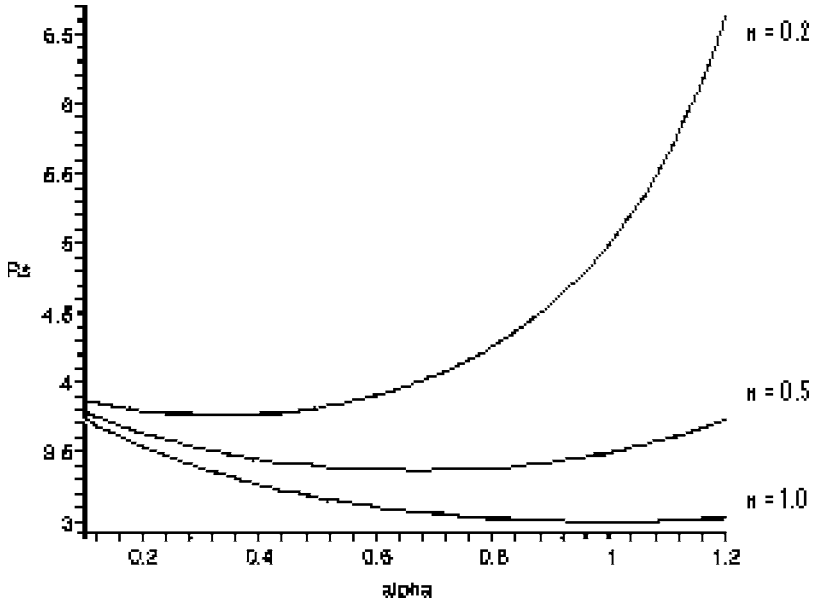

FIG. 1. Scaled radius versus fractional order.

decreasing outward. We have matched fractional derivatives rather than first derivatives and it is not clear that the conditions of the Buchdahl bound are satisfied, but from Fig. 1, it is seen that the Buchdahl bound, $2m_0/R_0 \leqslant 8/9$, is not violated.

The radius for Tolman IV is a cubic root of Eq. (37), but some general description can be given. The modeling term in the equation is the denominator of the last term. Consider the factor

$$c_1 \sim 4\pi m_0^2 \rho_c/3$$

describing an object with mass $m_0 = Nm_\odot = N(2\times 10^{30}\ \mathrm{kg})$, and central density and pressure of neutron star order, $\rho_c \sim 10^{17}\ \mathrm{kg/m^3}$, $P_c \sim 10^{33}$ Newton/$\mathrm{m^2}$. Numerical scaled radius values using these values are described in Table I for a range of N and alpha values. For $N \sim 100$ or larger, the last term in the cubic is negligible and the radius is essentially given by the limiting value

$$R_0/m_0 \sim 2 + \Gamma(3-\alpha)\Gamma(1+\alpha).$$

The masses for these radii are well out of the neutron star range. The reflection symmetry about $\alpha = 1$ is the result of a product equivalence of the two gamma functions for paired alpha values, i.e., $\alpha = (0.6, 1.4)$ give the same gamma function product. From Table I, it is clear that the low N values have masses and radii of neutron star orders of magnitude.[16] For example, for $N=1$, the radii are approximately $R_0 \sim 11.44 m_0 \sim 17$ km. Smaller central densities, describing more ordinary fluid objects, result in much larger fluid spheres. For a central density of $\rho_c \sim 10^{10}\ \mathrm{kg/m^3}$, the radii for $\alpha = 1$, $R_0(N)$ are $R_0(1) = 2228.33 m_0$, $R_0(10) = 480.87 m_0$, $R_0(100) = 104.39 m_0$, $R_0(1000) = 23.32 m_0$, with the values for larger and smaller α paired and increasing, just as for the larger central density.

TABLE I. R_0/M_0—Tolman IV—$\rho_c \sim 10^{17}\ \mathrm{kg/m^3}$.

α	$N=1$	$N=10$	$N=100$	$N=1000$
0.2	13.24	4.41	3.55	3.54
0.4	12.39	4.10	3.28	3.27
0.6	11.85	3.91	3.12	3.11
0.8	11.54	3.81	3.04	3.03
1	11.44	3.78	3.01	3
1.2	11.54	3.81	3.04	3.03
1.4	11.85	3.91	3.12	3.11
1.6	12.39	4.10	3.28	3.27

B. Crust stress–energy

Figures 2 and 3 describe the variation of the boundary energy density and pressure, in Tolman V, $n = 1/3$, as the size of the fluid sphere varies. Over a large part of the R_0/R_z range, a crust tension contains the interior fluid, with the tension increasing in size as the fluid sphere becomes smaller, essentially acting to squeeze the fluid into smaller volumes. The results are similar for $C=0$.

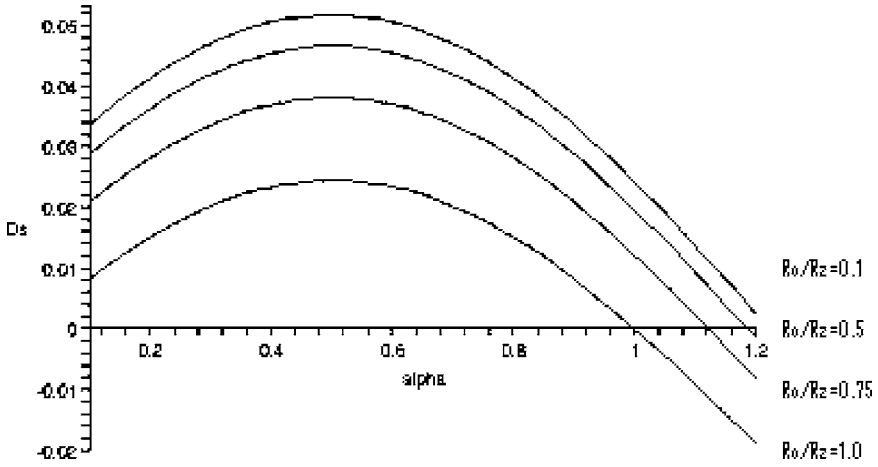

FIG. 2. $Ds=-8\pi m_0 S_0^0$ versus fractional order.

For Tolman IV, the crust energy density is

$$8\pi\sigma=\frac{2}{R_0}\left[-\sqrt{1-2m_0/R_0}+\sqrt{\frac{(1-R_0^2/C^2)(1+R_0^2/A^2)}{1+2R_0^2/A^2}}\right]$$

$$=\frac{2}{R_0}\left[-\sqrt{1-2m_0/R_0}+\sqrt{\frac{[1-4\pi R_0^2\rho_c(1/3-n)][1+4\pi\rho_c R_0^2(1/3+n)]}{1+R_0^2 8\pi\rho_c(1/3+n)}}\right].$$

The modeling factor of importance is the term

$$4\pi\frac{R_0^2}{m_0^2}\rho_c m_0^2=3c_1\frac{R_0^2}{m_0^2}.$$

For nuclear central densities, $\rho_c\sim 10^{14}$ g/cm^3, this is

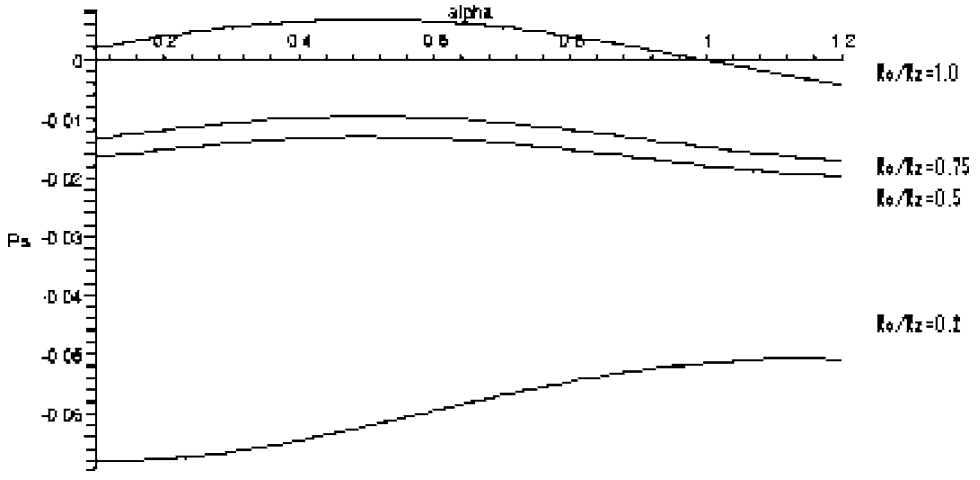

FIG. 3. $Ps=8\pi m_0 S_\vartheta^\vartheta$ versus fractional order.

$$20.35N^2 \times 10^{-4}\frac{R_0^2}{m_0^2}.$$

In order to have real values, we require

$$N=1, \quad R_0 \sim 12m_0, \quad [0.293 \times (1/3-n)] < 1,$$

$$N=10, \quad R_0 \sim 4m_0, \quad [3.26 \times (1/3-n)] < 1,$$

$$N=100, \quad R_0 \sim 3m_0, \quad [183 \times (1/3-n)] < 1.$$

It is clear that the broadest range of central equations of state for nuclear central densities is for the lower mass objects. Higher mass objects require a central EOS very close to the $1/3$ limit. For smaller values of the central density, the central EOS range is much broader. For a central density of $\rho_c \sim 10^7$ g/cm^3, the modeling factor is

$$4\pi\frac{R_0^2}{m_0^2}\rho_c m_0^2 = 20.35N^2 \times 10^{-11}\frac{R_0^2}{m_0^2},$$

and for real values require

$$N=1, \quad R_0 \sim 2228m_0, \quad [0.10 \times 10^{-2}(1/3-n)] < 1,$$

$$N=10, \quad R_0 \sim 480m_0, \quad [0.47 \times 10^{-2}(1/3-n)] < 1,$$

$$N=100, \quad R_0 \sim 104m_0, \quad [0.022 \times (1/3-n)] < 1,$$

$$N=1000, \quad R_0 \sim 23m_0, \quad [0.11 \times (1/3-n)] < 1.$$

VI. CONCLUSION

In this work we have examined a family of boundary layers created by matching fractional derivatives across a boundary.[17,18] The boundary layers considered have structure that depends on the order of the fractional derivative. One of the reasons that fractional calculus may be important for boundary layers is the mechanism by which a boundary layer is formed. One of the possible ways to build a variable density crust is by a diffusive process; a process whose underlying cause is Brownian motion. This motion, as analyzed by statistical mechanics, involves diffusion, dissipation, and the fluctuation-dissipation theorem. The dynamical model of Brownian motion was provided by Langevin in 1908 using a stochastic differential equation. It seems apparent from the nature of randomness that such macroscopic stochastic equations are incompatible with the continuous and differentiable character of microscopic Hamiltonian dynamics. (Think of the conventional diffusion equation, with the diffusion process described by a second-order spatial derivative.) Therefore, the mathematical description rests on either ordinary analytical functions describing the dynamics, or on conventional differential operators describing the phase space evolution. The differentiable nature of the macroscopic picture is, in a sense, a natural consequence of microscopic randomness. This means that use can be made of ordinary differential calculations on the macroscopic scale, even if the microscopic dynamics are incompatible with ordinary calculus methods. On the other hand, in the case where a time scale separation between macroscopic and microscopic levels of description does not exist, the nondifferentiable nature of the microscopic dynamics is transmitted to the macroscopic level. Since fractional calculus has been shown to provide a good description for a range of diffusive processes,[19] one might expect a boundary condition based on fractional calculus would reflect the fractional growth process. An

example, given by Allegrini, Grigolini, and West,[20] shows that a diffusion process generated by a fluctuation with no time scale at the macroscopic level generates a diffusion process well described by a fractional Laplacian.

While diffusion is a possible mechanism for generating a layer with structure, the method of generating the fractional family of layers is independent of the production mechanism and generates a family whose stress–energy and size depends on the order of the fractional derivative. The result is a much broader range in fluid sphere properties. For example, in Tolman V, a much larger range of spheres sizes can be described with the fractional layer than without, with the energy density of the layer decreasing as the size of the sphere increases. The $C \neq 0$ Tolman V spheres have a zero-pressure boundary solution. For spheres smaller than the zero-pressure sphere, the layer has a tension, while for spheres larger than the zero-pressure sphere, the layer has positive stress over much of the range of the fractional order. The fractional boundary could prove to be a valuable modeling tool in more realistic neutron star models.

The range of stress–energy in the fractional boundary layers implies differences in structure as a function of the fractional order. The differences in density could be modeled in several ways: for example, with different crust materials or different incomplete fluid coverings (tilings).[21] The layer itself is a model of a thin crust and there could be differences in the geometry of the $2+1$ shells that fill the real crust. The interior fluid geometry and the exterior Schwarzschild vacuum do not have to match for a crust with finite thickness.

The models presented in this paper matched an integral transform of the regular derivative across a spatial boundary. It is not a fractional generalization of general relativity, but a fractional generalization of a boundary condition. The next step is to explore the range of fractional generalizations of other sets of boundary conditions and other derivative definitions to applicable spacetimes.

APPENDIX A: DERIVATIVES

1. Regular

For functions f and F continuous on $[a,b] \in \mathit{Reals}$,

$$F(x) := \int_a^x f(t)dt,$$

$F(x)$ is differentiable such that $dF/dx = f$. The nth integer derivative is simply d^nF/dx^n. For example,

$$\frac{d^n}{dx^n}x^k = \frac{k!}{(k-n)!}x^{k-n}.$$

With the gamma function this is

$$\frac{d^n}{dx^n}x^\alpha = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-n+1)}x^{\alpha-n}.$$

The gamma function, $\Gamma(z)$, is defined as

$$\Gamma(z) = \int_0^\infty e^{-t}t^{z-1}\,dt, \quad \Gamma(1/2) = \sqrt{\pi}, \quad \Gamma(1) = 1,$$

$$\Gamma(n+1) = n\Gamma(n) = n\,!\,, \quad \text{for } n > 0.$$

2. Fractional

A. Riemann–Liouville

The Riemann-Liouville definition for the α fractional derivative of $f(x)$ is, with $\alpha \geqslant 0$,

$$D^{\alpha} f(x) = \frac{d^{\alpha}}{dx^{\alpha}} f(x) := \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_c^x \frac{f(t)}{(x-t)^{\alpha-n+1}} dt, \tag{A1}$$

where n is the smallest integer larger than α when it is fractional, that is, $n=[\alpha]+1$. In the $\alpha=1$ limit, the derivative produces the integer result. The constant c in the limit of the integral is usually set to 0 (Riemann definition) or to $-\infty$ (Liouville definition). For example, the Riemann–Liouville derivative of x^k for $\alpha \leqslant 1$ with $n=1$, we have

$$D^{\alpha} x^k = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x t^k (x-t)^{-\alpha}\, dt$$

$$= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x t^k x^{-\alpha} \left(1 - \frac{t}{x}\right)^{-\alpha} dt$$

$$= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^1 w^k x^{-\alpha+1+k} (1-w)^{-\alpha}\, dw.$$

Using the definition of the beta function,

$$\int_0^1 w^{p-1} (1-w)^{q-1}\, dw = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)},$$

we have

$$D^{\alpha} x^k = \frac{1}{\Gamma(1-\alpha)} \frac{dx^{-\alpha+1+k}}{dx} \frac{\Gamma(k+1)\Gamma(1-\alpha)}{\Gamma(k+2-\alpha)}$$

$$= (1+k-\alpha) x^{k-\alpha} \frac{\Gamma(k+1)}{\Gamma(k+2-\alpha)}$$

$$= x^{k-\alpha} \frac{\Gamma(k+1)}{\Gamma(k+1-\alpha)}.$$

For $\alpha=1$, this is the usual result $D^1 x^k = dx^{k-1}$. Note that, for $k=-1$, this operation fails. This is an example of one of the problems encountered in applying fractional derivatives to general relativity. Not all definitions of fractional derivatives work for all functions. The fractional derivative of x^k for $\alpha \geqslant 1$ is identical to the fractional derivative for $\alpha \leqslant 1$. For this function, the derivative is continuous across the $\alpha=1$ boundary.

$$D^{\alpha} x^k = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_0^x t^k x^{1-\alpha} \left(1 - \frac{t}{x}\right)^{1-\alpha} dt$$

$$= \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_0^1 w^k x^{k+2-\alpha} (1-w)^{1-\alpha}\, dw$$

$$= x^{k-\alpha}\frac{\Gamma(1+k)}{\Gamma(1+k-\alpha)}.$$

One should note that the Riemann–Liouville fractional derivative of a constant is not zero.

B. Caputo

The Caputo derivative is the integral transform of the regular derivative and is found by moving the derivative in the Riemann–Liouville definition inside the integral to act on the function. We have

$$D^{\alpha}f(x) = \frac{1}{\Gamma(n-\alpha)}\int_0^x \frac{\frac{d^n}{dt^n}f(t)}{(x-t)^{\alpha-n+1}}dt. \tag{A2}$$

Example: $f(x)=x^b$, $\beta \geqslant 0$,

$$D^{\alpha}(x-a)^k = \frac{1}{\Gamma(n-\alpha)}\int_0^x \frac{\frac{d^n}{dt^n}t^k}{(x-t)^{\alpha-n+1}}dt.$$

For $\alpha \leqslant 1$, $n=1$ we have

$$D^{\alpha}(x-a)^k = \frac{1}{\Gamma(1-\alpha)}\int_0^x kt^{k-1}(x-t)^{-\alpha}\,dt = \frac{kx^{k-\alpha}}{\Gamma(1-\alpha)}\int_0^1 w^{k-1}(1-w)^{-\alpha}\,dw = kx^{k-\alpha}\frac{\Gamma(k)}{\Gamma(k+1-\alpha)}, \tag{A3}$$

which is identical to the Riemann–Liouville derivative for this function. This derivative also is not defined for $k=-1$. In general relativity, one of the space-times one would like to treat is vacuum Schwarzschild, but the Riemann–Liouville derivative will not give finite answers for the $1/r$ structure. The derivative of $1/r$ can be taken with the Weyl derivative.

C. Weyl

The Weyl derivative differs from the Riemann–Liouville derivatives over the range of the fractional transform. To take the fractional derivatives of $1/r$ we use the Weyl derivative over the range (R_0, ∞). The Weyl derivative of $f(r)$ can be written as

$$D^{\alpha}f(r) = \frac{(-1)^{n-1}}{\Gamma(n-\alpha)}\int_r^{\infty} \frac{d^n f(t)}{dt^n}(t-r)^{n-\alpha}\,dt,$$

where n is the smallest integer above α when it is fractional. This paper is concerned with the fractional derivative across the boundary and the phase $(-1)^{n-1}$, was chosen to make D^{α} continuous across $\alpha=1$. Applying the derivative definition to $1/r$ for $\alpha \leqslant 1$ $(n=1)$ we find

$$D^{\alpha}r^{-1} = -r^{-(1+\alpha)}\Gamma(1+\alpha), \quad \alpha \leqslant 1. \tag{A4}$$

For $\alpha=1$, this gives the usual first derivative of $1/r$. For $\alpha>1$ $(n=2)$ the derivative is the same. One should be careful not to interpret the derivative for $\alpha=2$ as the second derivative. The second derivative would follow from a double application of D^{α}. For this function the single derivative at $\alpha=2$ is not the same as the double application of the derivative operator.

APPENDIX B: FLUID SPHERE FORMALISM

Consider the general static spherical metric over the interior fluid with $\nu(r)$ and $\lambda(r)$,

$$ds^2 = -e^{\nu}\,dt^2 + e^{\lambda}\,dr^2 + r^2\,d\Omega^2.$$

With Einstein's field equations as $G_{ij}=8\pi T_{ij}$, the energy–momentum components are

$$8\pi T_0^0 = -e^{-\lambda}(\lambda'/r - 1/r^2) - 1/r^2,$$

$$8\pi T_r^r = e^{-\lambda}(\nu'/r + 1/r^2) - 1/r^2,$$

$$8\pi T_\theta^\theta = 8\pi T_\phi^\phi = (e^{-\lambda}/2)[\nu^{\nu''} + (\nu'/2 + 1/r)(\nu' - \lambda')].$$

For the fluid interior, the energy–momentum, with four-velocity $U^i=(e^{\nu/2},0,0,0)$, is

$$T^{ij} = (\rho + P)U^iU^j + Pg^{ij}.$$

In the comoving frame the fluid stress energy is

$$T_0^0 = -\rho, \quad T_r^r = T_\theta^\theta = T_\phi^\phi = P.$$

It is common to use the function $m(r)$ in g_{rr} with

$$e^{\lambda} = [1 - 2m(r)/r]^{-1},$$

so that

$$\lambda' = 2(m'/r - m/r^2)(1 - 2m/r)^{-1}.$$

From the first field equation we have

$$m' = 4\pi r^2\rho.$$

The second field equation provides a relation between the fluid pressure, P, and ν',

$$\nu'/2 = (4\pi rP + m/r^2)(1 - 2m/r)^{-1}$$

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Colliding wave solutions from five-dimensional black holes and black *p*-branes

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We consider both the five-dimensional Myers-Perry and Reissner-Nordstrom black holes (BHs) and black *p*-branes in $(4+p)$-dimensions. By employing the isometry with the colliding plane waves (CPWs) we generate Cauchy-Horizon (CH) forming CPW solutions. From the five-dimensional vacuum solution through the Kaluza-Klein reduction the corresponding Einstein-Maxwell-dilaton solution is obtained. This CH forming cross polarized solution with the dilaton turns out to be a rather complicated nontype *D* metric. Since we restrict ourselves to the five-dimensional BHs we obtain exact solutions for colliding 2- and 3-form fields in $(p+4)$-dimensions for $p \geqslant 1$. By dualizing these forms we can obtain also colliding $(p+1)$- and $(p+2)$-forms which are important processes in the low energy limit of the string theory. All solutions obtained are CH forming, implying that an analytic extension beyond is possible. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Black holes (BHs) are known to have region isometric to the space of colliding plane waves (CPW).[1,2] This may be either in between the two horizons (i.e., inner and outer) or given the case with single horizon the inner region of the event horizon. Such an isometry renders it possible to generate CPW solutions from known solutions of BHs. In a recent paper[3] we gave a prescription for generating CPW solutions from an Einstein-Maxwell-Dilaton-Axion (EMDA) theory. In this theory the dilaton was linear and the BH was not asymptotically flat. In this solution the axion arises as the cross polarizing agent for the CPWs. This means that the limit of linear polarization removes the axion leaving behind only the Einstein-Maxwell-Dilaton (EMD) theory. Another solution with similar features but valid only in the zero dilaton limit was obtained previously.[4] Interesting physical property shared by both of these solutions is that the space-time subsequent to the collision of waves emerges free of physical singularities. Horizon forming CPW[1,2,5–7] solutions in the EMDA theory are naturally of utmost important to the string theory. Since the idea of higher dimensions has already gained enough momentum it is important to investigate the collision of waves in higher dimensions.[8,9] It is known already that the four-dimensional EMDA theory is equivalent to the six-dimensional Ricci flat, vacuum solution.[10,11]

In this paper we restrict ourselves to the five- (and four-) dimensional space-times and their extension through the brane world. We consider first the five-dimensional collision of gravitational (impulse and shock) waves obtained from the isometry with the Myer-Perry black hole (MPBH).[12,13] This particular BH contains two rotation parameters in addition to the mass. For simplicity we make the special choice in which the two angular momenta are equal. Then we identify the (r,θ) sector of the BH at hand with the null coordinates sector (u,v) of the colliding

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waves and accompany this with the necessary coordinate transformation. Inclusion of the Heaviside step functions along with the null coordinates must guarantee that no additional current sheets are created at the boundaries. In the standard Einstein and Einstein-Maxwell (EM) theories these are summarized in the O'Brian-Synge[14] boundary conditions, respectively. Similar arguments rightly follow in the higher dimensional space-times as well.

The static MPBH is transferred to the linearly polarized CPWs, which turns out to be a nonsingular type-*D* solution. The rotating MPBH transforms through the Kaluza-Klein (KK) reduction procedure to the CPW space-time with cross polarization in the four-dimensional EMD theory. This space-time is also regular but it does not belong to the type-*D* class. As a matter of fact the dilaton involved cross polarization (instead of axion, as it arises in the above-mentioned solutions) makes the space-time structure rather involved.

As a second example we consider the Reissner-Nordstrom (RN) BH[15] in five dimensions from which we obtain CPW solution in the five-dimensional EM theory. Similar to the CPW solution obtained from the MPBH this one also is singularity free. Our examples of five-dimensional BHs exclude the extremal limits because in such a limit which removes the isometric region of BHs with CPWs the equivalence fails to work. Under such circumstances an alternative transformation, analogous to the RN-Bertotti-Robinson equivalence, must be pursed which is out of our scope in this paper.

As a third example we consider the black-branes in the $(d+p)$-dimensional brane world. We find regular CPW solutions to colliding 3-form fields in higher dimensions. Another solution that we obtain from the same black-brane metric is colliding (EM) (2-form) fields in higher dimensions.

Our study may lay the foundation for promoting the string theory in approximation in low energies from single plane wave background to the more realistic CPW background. The regular initial data of CPWs provides a natural choice among the nonunique Penrose limits of space-times.[16–18] It is known that the incoming region of a CPW space-time admits automatically a Penrose limit of the interaction region. The advantage is that we have the double Penrose limits which are both well-defined initial data. Any Penrose limit does not qualify as an initial data toward construction of the interaction region.

Finally we wish to express the view that our technique can be extrapolated to higher dimensions provided some associated difficulties are overcome. The most important problem is the analytic integration of the radial coordinate (r) of BHs in terms of the prolate-type coordinate (τ) of CPWs. And as the second major difficulty we cite of the necessary proper representation of the higher dimensional spherical line element suitable for the ideals of the geometry of CPWs.

The organization of the paper is as follows. In Sec. II we obtain CPW solutions from the five-dimensional BHs, whose details are tabulated in Appendixes A, B, and C. Section III investigates the physical properties of the metrics obtained in Sec. II. Section IV contains solutions for colliding 3-form fields in higher dimensions and their KK reductions. Section V focuses attention on a class of by-product solutions of colliding EM shock waves in higher dimensions. We dualize our 2-form fields of Sec. V in Sec. VI to obtain colliding $(p+2)$-form fields in $(p+4)$-dimensions. Our conclusion and discussion is in Sec. VII.

II. CPW SOLUTIONS FROM FIVE-DIMENSIONAL BHs

In this section we concentrate on the two well-known types of BHs in five-dimensions. First we consider the MPBH and then RNBH. Our analysis applies, however, to any five-dimensional BHs that possesses two nonoverlapping horizons albeit the technical difficulties. We comment on this point at the end of the section in concentration with the Schwarzschild-de(-anti) Sitter BH.

(A) The MPBH in five dimensions with two equal angular momenta is given

$$ds_5^2 = \tilde{g}_{AB}\, dx^A\, dx^B \quad (A,B,\ldots = 0,\ldots 4),$$

$$ds_5^2 = dt^2 - \frac{\mu}{\rho^2}\left[dt + \frac{\overline{a}}{2}(d\varphi - \cos\theta\, d\eta)\right]^2 - \frac{\rho^4\, d\rho^2}{\rho^4 - \mu\rho^2 + \mu\overline{a}^2} - \rho^2\, d\Omega_3^2, \tag{1}$$

where μ and $\overline{a}$ are, respectively, proportional to the mass and angular momentum of the BH. We note that five-dimensional suffices are denoted by capital italic letters while four dimensional ones by greek letters. A tilde over specifies also the five-dimensional geometrical object. For the three-dimensional metric of S^3 we choose the representation

$$d\Omega_{(3)}^2 = \tfrac{1}{4}(d\theta^2 + d\eta^2 + d\varphi^2 - 2\cos\theta\, d\eta\, d\varphi), \tag{2}$$

where $0 < \theta < \pi$, and the angles η and φ are defined modulo 2π. The static MPBH corresponds to $a=0$, while the extreme case is defined by $\mu = 4\overline{a}^2$. The CPW form in five dimensions is obtained by imposing the identification of the (ρ, θ) sector in the above metric with the (τ, σ) sector of CPW as follows:[3]

$$\left(\frac{4\rho^2\, d\rho^2}{\mu\rho^2 - \rho^4 - \mu\overline{a}^2} - d\theta^2\right) = \left(\frac{d\tau^2}{1-\tau^2} - \frac{d\sigma^2}{1-\sigma^2}\right). \tag{3}$$

In the sequel, for simplicity we choose $\mu = 1$ leading us to the solution

$$\begin{gathered} 2\rho^2 = 1 + \sqrt{1 - 4\overline{a}^2}\tau, \\ \cos\theta = \sigma \end{gathered} \tag{4}$$

implying further that we impose $|\overline{a}| < \frac{1}{2}$. Supplementing this transformation with the identifications

$$\begin{gathered} t \to x, \\ \varphi \to y, \\ \eta \to z, \\ a_o^2 = 2\overline{a}^2 \end{gathered} \tag{5}$$

followed by an appropriate rescaling of coordinates we obtain the five-dimensional vacuum metric apt for CPWs:

$$ds_5^2 = F\left(\frac{d\tau^2}{\Delta} - \frac{d\sigma^2}{\delta}\right) - \frac{1}{F}[Z_o(dy - 2\sigma\, dz)dy + Z\, dz^2 + 4a_o(dy - \sigma\, dz)dx - (1 - k\tau)dx^2]. \tag{6}$$

Our abbreviations in this metric stand as follows:

$$\Delta = 1 - \tau^2,$$

$$\delta = 1 - \sigma^2,$$

$$F = 1 + k\tau,$$

$$Z = F^2 + 2a_o^2\sigma^2,$$

$$Z_o = F^2 + 2a_o^2,$$

$$k = \sqrt{1 - 2a_o^2},$$

$$0 < k \leqslant 1, \tag{7}$$

where the coordinates (τ, σ) are related to the null coordinates (u, v) through

$$\tau = \sin(au + bv),$$

$$\sigma = \sin(au - bv), \tag{8}$$

$$(a, b\text{:constants}).$$

Now, the crucial point toward the interpretation of this metric as a CPW metric is by making the substitutions

$$u \to u\,\theta(u),$$

$$v \to v\,\theta(v) \tag{9}$$

in the metric functions, where θ stands for the Heaviside unit step function. This process must not create currents (sources) on the null boundaries $u=0=v$. Alternatively this implies that the five-dimensional Ricci terms all vanish globally

$$\tilde{R}_{AB} = 0$$

$$(x^A\text{:}u, v, x, y, z). \tag{10}$$

The Riemann tensor components $\tilde{R}_{ABCD}$, however, involve Dirac delta functions, indicative of impulsive gravitational waves in addition to the shock waves required commonly by the step functions. In Appendix A we tabulate all components exhaustively from which we can easily identify the nonvanishing ones in the incoming regions. By setting $v<0 (u<0)$ we restrict ourselves to the incoming region II (III), comprising of five-dimensional gravitational plane waves alone. Obviously, for both $u<0$ and $v<0$ we obtain the region I which is a five-dimensional flat space-time given by

$$ds_5^2 = 4ab\,du\,dv - (1 + a_o^2)dy^2 - dz^2 - 4a_o\,dx\,dy - dx^2. \tag{11}$$

The Kretschmann scalar in the interaction region (region IV, $u>0, v>0$) turns out to be

$$K = \tilde{R}_{ABCD}\tilde{R}^{ABCD} = \frac{6}{(1 + k\tau)^6}[4k^2(k + \tau)^2 - (1 + k\tau)^2] \tag{12}$$

which is free of singularities.

We wish now to apply the KK reduction procedure to our five-dimensional metric (6) in order to obtain CPWs of the EMD theory in four dimensions. We follow the KK reduction procedure through the identification

$$\tilde{g}_{AB} = \phi^{-1/3}\begin{pmatrix} g_{\mu\nu} + 4\phi A_\mu A_\nu & 2\phi A_\mu \\ 2\phi A_\nu & -\phi \end{pmatrix}. \tag{13}$$

This makes it possible to read both the four-dimensional metric $g_{\mu\nu}$, as well as the dilaton ϕ, and the EM potential A_μ. The results are as follows:

$$ds_4^2 = (FZ)^{\frac{1}{2}}\left[\frac{d\tau^2}{\Delta} - \frac{d\sigma^2}{\delta} - \frac{1}{Z}\left(\frac{L}{F}dx^2 + \delta Z_o\,dy^2 - 4a_o\delta\,dx\,dy\right)\right],$$

$$\phi = \left(\frac{Z}{F}\right)^{\frac{3}{2}},$$

$$A_\mu = \frac{\sigma}{Z}\left(0,0,a_o,\frac{1}{2}Z_o\right), \tag{14}$$

where the notations are as in (7), and in addition we have labelled $L=2F-Z$. The action of the resulting four-dimensional EMD theory is

$$S = \frac{1}{16\pi}\int |g|^{\frac{1}{2}}\,\mathrm{d}x^4\left[-R-\phi F_{\mu\nu}F^{\mu\nu}+\frac{(\nabla\phi)^2}{6\phi^2}\right] \tag{15}$$

so that the dilaton and Maxwell equations take the respective forms

$$\Box(\ln\phi) = -3\phi F_{\mu\nu}F^{\mu\nu}, \tag{16}$$

$$\nabla_\alpha(\phi F^\alpha_\mu) = 0, \tag{17}$$

in which $\Box$ stands for the covariant Laplacian. To complete the set of Einstein equations we need also the Ricci tensor which is given by

$$R_{\mu\nu} = \frac{1}{6}\frac{\phi_{,\mu}\phi_{,\nu}}{\phi^2} - 2\phi\left(F_{\mu\alpha}F^\alpha_\nu - \frac{1}{4}g_{\mu\nu}F_{\alpha\beta}F^{\alpha\beta}\right). \tag{18}$$

We note that this representation of dilaton is different from the standard one expressed as an exponential function in the action. This more familiar latter form is related to the present one by the substitution

$$\phi = e^{-2a\sigma} \tag{19}$$

which casts the action into

$$S = \frac{1}{16\pi}\int |g|^{\frac{1}{2}}\,\mathrm{d}x^4[-R+2(\nabla\sigma)^2 - e^{-2a\sigma}F_{\mu\nu}F^{\mu\nu}], \tag{20}$$

where the dilatonic parameter is $\sqrt{3}$. The physical properties of the EMD space-time obtained hitherto will be studied in the next section.

(B) The five-dimensional RNBH is given by

$$\mathrm{d}s_5^2 = \left(1-\frac{m}{r^2}+\frac{q^2}{r^4}\right)\mathrm{d}t^2 - \left(1-\frac{m}{r^2}+\frac{q^2}{r^4}\right)^{-1}\mathrm{d}r^2 - r^2\,\mathrm{d}\Omega^2_{(3)}, \tag{21}$$

where m and q are, respectively, related to the mass and charge of the BH. The EM vector potential one-form is given by

$$A = A_\mu\,\mathrm{d}x^\mu = \frac{\sqrt{3}q}{2r^2}\mathrm{d}t. \tag{22}$$

Here also, similar to the MP case we choose the S^3 line element as in (2). The transition to the CPW metric is accomplished here by the identification

$$\frac{4\,\mathrm{d}r^2}{m-r^2-\frac{q^2}{r^2}} - \mathrm{d}\theta^2 = \frac{\mathrm{d}\tau^2}{1-\tau^2} - \frac{\mathrm{d}\sigma^2}{1-\sigma^2}. \tag{23}$$

A possible integral for $r(\tau)$ is readily available as

$$r^2 = \frac{m}{2}(1 + l\tau), \tag{24}$$

where

$$l = \sqrt{1 - \frac{4q^2}{m^2}} > 0.$$

By choosing $m=1$ in addition to the identifications

$$\sigma = \cos\theta = \sin(au - bv),$$

$$t \to x, \varphi \to y, \eta \to z,$$

$$\tau = \sin(au + bv),$$

$$(a,b = \text{constants}) \tag{25}$$

we obtain the metric (after rescaling of coordinates)

$$ds_5^2 = (1 + l\tau)(4ab\, du\, dv - dy^2 - dz^2 - 2\sin(au - bv)dy\, dz) - \frac{\Delta}{(1 + l\tau)^2}dx^2. \tag{26}$$

The EM vector potential one-form takes the form under the above transformation

$$A = \frac{\sqrt{3}q}{2\sqrt{2}l(1 + l\tau)}dx. \tag{27}$$

The interpretation of this metric as a CPW is completed by inserting the step functions into the null coordinates u and v. This metric represents collision of EM plane waves in five dimensions. For $l=1$ (or $q=0$) it reduces to the CPW metric of the five-dimensional pure gravity and coincides with the $a_o=0$ case of the metric (6). Thus, (26) is the EM extension while (6) was the rotational extension of the same CPW metric obtained from the five-dimensional Schwarzschild metric. The Riemann components of the metric (26) are given in Appendix B from which we compute the Kretschmann scalar to find (for $u>0$ and $v>0$).

$$K = \frac{127l^4 + 180l^3\tau - 2l^2 - 72\Delta l^2 + 19 - 36l\tau}{4(1 + l\tau)^4} \tag{28}$$

which is also regular to the future of the collision point $u=0=v$.

Finally we wish to comment on other BHs and corresponding CPW solutions in five dimensions. Although our method applies to any such BH that admits inner and outer horizons such that the region in between possesses two spacelike Killing vectors technically some cases are not tractable. As an example we cite the Schwarzschild-de(-anti) Sitter BH given by the line element

$$ds_5^2 = h(r)dt^2 - h(r)^{-1}\, dr^2 - r^2\, d\Omega_{(3)}^2, \tag{29}$$

where $h(r)=k-(m/r^2)\pm(r^2/l^2)$, in which $k=\pm 1$, m is related to mass and l to the cosmological constant. To obtain the associated CPW solution we demand now that

$$\int \frac{\mathrm{d}\rho}{\sqrt{\rho}\sqrt{m - k\rho \pm \frac{\rho^2}{l^2}}} = \pm \sin^{-1} \tau, \tag{30}$$

where we have used $\rho = r^2$. The inversion of such an elliptical integral seems to be beyond analytical calculation which must therefore be handled within the scope of numerical analysis.

III. PROPERTIES OF THE COLLIDING EMD SPACE-TIME

The linearly polarized CPW metric (14) is rather transparent so we restrict ourselves to the case $a_o = 0$, first. Upon rescaling of x and y we have the metric

$$\mathrm{d}s^2 = (1+\tau)^{\frac{3}{2}}\left(2\,\mathrm{d}u\,\mathrm{d}v - \frac{1-\tau}{(1+\tau)^2}\mathrm{d}x^2 - \delta\,\mathrm{d}y^2\right) \tag{31}$$

in which τ and σ are implied with the step functions. By the choice of Newman-Penrose (NP) null-tetrad basis one-forms,

$$l = (1+\tau)^{\frac{3}{4}}\,\mathrm{d}u,$$

$$n = (1+\tau)^{\frac{3}{4}}\,\mathrm{d}v,$$

$$\sqrt{2}m = (1-\tau)^{\frac{1}{2}}(1+\tau)^{-1/4}\,\mathrm{d}x + i\sqrt{\delta}(1+\tau)^{\frac{3}{4}}\,\mathrm{d}y, \tag{32}$$

we obtain all Ricci and Weyl components as tabulated in the Appendix C. It is observed by studying the Weyl scalars Ψ_o, Ψ_2, and Ψ_4 that the space-time is regular everywhere for $(u>0, v>0)$. On the boundaries, however, both Ψ_o and Ψ_4 suffer from singularities at $(u=0, bv=\pi/2)$ and $(v=0, au=\pi/2)$, respectively. These are the typical null singularities inherited from the problem of colliding EM shock waves, therefore such singularities in the present problem is not unexpected at all. From the metric (31) we observe that $\tau=1$ and $\sigma=1$ are spurious, removable coordinate singularities since they do not show up in the Weyl scalars. In particular, $\tau=1$ is the location of the horizon in the interaction region beyond which the metric can be extended analytically. The other coordinate singularity $\sigma=1$ is out of question since it does not belong to the interaction region. The incoming EMD waves prior to the collision can also be easily identified from Appendix C. In the region II we have

$$\begin{aligned}
\Psi_2 &= -\frac{3}{8}a^2\theta(u)\frac{(5+\sin(au))}{(1+\sin(au))^{\frac{5}{2}}}, \\
\Phi_{22} &= \frac{1}{16}a^2\theta(u)\frac{(7+\sin(au))}{(1+\sin(au))^{\frac{5}{2}}},
\end{aligned} \tag{33}$$

while in the region III we must replace $au \leftrightarrow bv$ to obtain Ψ_o and Φ_{oo}. The incoming waves that comprise Ricci components $\Phi_{22}(\Phi_{oo})$ is obviously constructed from both the EM and the dilaton parts. Inside the collision region we observe also that the condition

$$9\Psi_2^2 = \Psi_0\Psi_4 \tag{34}$$

holds among the Weyl scalars, showing its type-D character. Direct choice of a Kinnersley type tetrad eliminates both Ψ_o and Ψ_4 components of the Weyl scalars.[19] Such a tetrad is given by the basis one-forms

$$l = \frac{\sqrt{1+\tau}}{1-\tau}\mathrm{d}\tau - \mathrm{d}x,$$

$$2n = \mathrm{d}\tau + \frac{1-\tau}{\sqrt{1+\tau}}\mathrm{d}x,$$

$$\sqrt{2}m = (1+\tau)^{\frac{3}{4}}\left(\frac{\mathrm{d}\sigma}{\sqrt{\sigma}} - i\sqrt{\delta}\,\mathrm{d}y\right). \tag{35}$$

This choice gives now the only nonzero component

$$\psi_2 = -\frac{1}{8}\frac{(5+\tau)}{(1+\tau)^{\frac{5}{2}}} \tag{36}$$

verifying its manifestly type-D character.

Now returning to the general CPW metric (14) with $a_o \neq 0$, we can discuss again the interaction region alone. For this reason we omit all step functions and consider an NP tetrad basis one-form

$$\sqrt{2}l = (FZ)^{\frac{1}{4}}\left(\frac{\mathrm{d}\tau}{\sqrt{\Delta}} + \frac{\mathrm{d}\sigma}{\sqrt{\delta}}\right),$$

$$\sqrt{2}n = (FZ)^{\frac{1}{4}}\left(\frac{\mathrm{d}\tau}{\sqrt{\Delta}} - \frac{\mathrm{d}\sigma}{\sqrt{\delta}}\right),$$

$$\sqrt{2}m = \frac{\sqrt{L}}{(FZ)^{\frac{1}{4}}}\left[\mathrm{d}x + \left(\frac{a_o\delta F}{L} + i\sqrt{\frac{\delta F Z_o}{L}}\right)\mathrm{d}y\right]. \tag{37}$$

The results are rather tedious so we shall refrain from tabulating the Ricci and Weyl components. Instead, relying on a numerical computation we have verified that the condition (34) fails to hold in the present case. Thus, we have seen numerically at least that our space-time is not type-*D*. By the same numerical analysis we conclude that our space-time is not singular. Another approach to study this space-time is to search for a possible Kinnersley tetrad that serves to generalize (35). To attain this goal we define the null vector l^μ out of the geodesics equation. Unfortunately, in contrast to the BH case the choice $\theta = \theta_o = \text{constant}$ which used to simplify the problem significantly, remains ineffective. By this analysis we obtain a set of Kinnersley-type tetrad as follows:

$$l^\mu = \frac{\sqrt{F}}{\Delta}\{k\Delta S, 0, F, -a_o\},$$

$$2n^\mu = \frac{1}{k^2 F\sqrt{Z}S^2}\{k\Delta S, 0, -F, a_o\},$$

$$\sqrt{2}m^\mu = \frac{F^{\frac{1}{4}}}{\sqrt{\delta}Z^{\frac{3}{4}}S}\left\{0, -\delta S\sqrt{\frac{Z}{F}}, -ia_o\delta, i\right\}, \tag{38}$$

where $S = Z^{-1/2}(F - a_o^2\delta)^{\frac{1}{2}}$.

In the limit $a_o=0$, this tetrad reduces to (35), as it should. This fact that our space-time is not type-*D* reflects in the computation of the spin coefficients since none turn out to vanish.

In conclusion, we state that colliding cross-polarized EMD space-time obtained from the five-dimensional MPBH through the KK reduction procedure turns out to be nonsingular in spite of all its complication. This reflects the highly transcendental coupling between the dilaton and the other fields. Linear polarization limit removes all complication and we obtain a much simpler space-time structure.

IV. CPW SOLUTIONS FROM BLACK *p*-BRANES

A class of black *p*-brane solutions in *d*-dimensions of the action

$$S=\int d^{(d+p)}x\sqrt{-g}\left(R-\frac{2}{(d-p)!}F^2_{(d-2)}\right) \tag{39}$$

with

$$F_{(d-2)}=\frac{1}{(d-2)!}F_{\mu_1\cdots\mu_{(d-2)}}\,\mathrm{d}x^{\mu_1}\wedge\cdots\wedge\mathrm{d}x^{\mu_{d-2}}$$

is given by the metric.[20]

$$\mathrm{d}s^2_{(d+p)}=A_dB_d^{(1-p)/(1+p)}\mathrm{d}t^2-(A_dB_d)^{-1}\,\mathrm{d}r^2-B_d^{2/(p+1)}\mathrm{d}y\,\mathrm{d}y-r^2\,\mathrm{d}\Omega^2_{(d-2)} \tag{40}$$

in which

$$A_d=1-\left(\frac{r_+}{r}\right)^{d-3},$$

$$B_d=1-\left(\frac{r_-}{r}\right)^{d-3}.$$

We consider here only the nonextremal case $r_+>r_-$, where the region $r_-<r<r_+$ enables us to construct nonsingular CPW solutions. As examples we shall present solutions for $p=1$, $p=6$, and $p\to\infty$, however, our procedure applies for any $p\geqslant 1$. In particular, the six-dimensional magnetically charged metric (40) becomes

$$\mathrm{d}s^2_6=A_5\,\mathrm{d}t^2-(A_5B_5)^{-1}\,\mathrm{d}r^2-B_5\,\mathrm{d}y^2-r^2\,\mathrm{d}\Omega^2_{(3)},$$

$$F_{(3)}=Q\epsilon_3, \tag{41}$$

where ϵ_3 is the volume form on the 3-sphere and $Q^2=2(r_+r_-)^2$. By the KK reduction procedure the six-dimensional action is reduced to the five-dimensional one

$$S=\int d^5x\sqrt{-g}\left[R-2(\nabla\phi)^2-\frac{1}{3}e^{-2c\phi}F^2_{(3)}\right], \tag{42}$$

where $c=\sqrt{\frac{2}{3}}$ and the metric, dilaton and 3-form fields are

$$\mathrm{d}s^2_5=B_5^{\frac{1}{3}}[A_5\,\mathrm{d}t^2-(A_5B_5)^{-1}\,\mathrm{d}r^2-B_5\,\mathrm{d}y^2-r^2\,\mathrm{d}\Omega^2_{(3)}],$$

$$e^{c\phi}=B_5^{-\frac{1}{3}},$$

$$F_{(3)} = \sqrt{2}(r_+ r_-)\epsilon_3. \tag{43}$$

The corresponding CPW solutions are obtained by the transformation

$$r^2 = \tfrac{1}{2}(a_o + b_o\tau),$$

$$\cos\theta = \sigma,$$

$$t = 2x,$$

$$\varphi = z,$$

$$\eta = w, \tag{44}$$

in which we have adopted the representation for $d\Omega^2_{(3)}$ and introduced the abbreviations

$$a_o = r_+^2 + r_-^2,$$

$$b_o = r_+^2 - r_-^2. \tag{45}$$

The resulting CPW metric, dilaton and the 3-form fields are

$$ds_5^2 = \left(\frac{1+\tau}{k+\tau}\right)^{1/3}\left\{(k+\tau)\left[2\,du\,dv - dz^2 - dw^2 + 2\sigma\,dz\,dw - \frac{1-\tau}{k+\tau}dx^2\right]\right\},$$

$$e^{c\phi} = \left(\frac{1+\tau}{k+\tau}\right)^{-1/3},$$

$$F_{(3)uzw} = Qa\,\theta(u)\sqrt{\delta}, \tag{46}$$

$$F_{(3)vzw} = -Qb\,\theta(v)\sqrt{\delta},$$

where $Q=(1/\sqrt{2})(k^2-1)$ and $k=a_o/b_o>1$. Our notation for τ, σ, and δ are as in the preceding sections and in transforming (43) into (46) we used the freedom of rescaling of x and ds^2. This metric has the scalar curvature (for $u>0$, $v>0$)

$$R = \frac{4}{3}\frac{ab(k-1)}{(1+\tau)^{4/3}(k+\tau)^{5/3}} \tag{47}$$

which is regular in the interaction region. The colliding 3-form metric corresponding to (41) becomes

$$ds_6^2 = (k+\tau)(2\,du\,dv - dz^2 - dw^2 + 2\sigma\,dz\,dw) - \frac{1}{k+\tau}[(1-\tau)dx^2 + (1+\tau)dy^2], \tag{48}$$

whereas the 3-form field preserves its form. This metric represents the collision of 2-form fields in flat background. The 3-form field is obviously obtained from the 2-form potential by

$$F_{(3)} = dA_{(2)}, \tag{49}$$

where

$$A_{(2)} = \tfrac{1}{2}A_{zw}\,dz \wedge dw,$$

$$A_{zw} = Q \sin(au\theta(u) - bv\theta(v)).$$

By a similar analysis we obtain the collision of these 3-form fields in 11-dimensional space. The result is

$$ds_{11}^2 = (k+\tau)(2\,du\,dv - dz^2 - dw^2 + 2\sigma\,dz\,dw) - \left(\frac{1+\tau}{k+\tau}\right)^{\frac{2}{7}} \sum_{i=1}^{6} (dy^i)^2 - \left(\frac{1-\tau}{k+\tau}\right)\left(\frac{1+\tau}{k+\tau}\right)^{-5/7} dx^2 \tag{50}$$

which has the regular scalar curvature,

$$R = -\frac{5}{7}\frac{ab(k^2-1)}{(k+\tau)^3}. \tag{51}$$

The KK reduction of this 11-dimensional metric to the fifth dimension is expressed by

$$ds^2 = \left(\frac{1+\tau}{k+\tau}\right)^{\frac{4}{7}} \left\{ \begin{array}{c} (k+\tau)[2\,du\,dv - dz^2 - dw^2 + 2\sigma\,dz\,dw] \\ -\left(\frac{1-\tau}{k+\tau}\right)\left(\frac{1+\tau}{k+\tau}\right)^{\frac{-5}{7}} dx^2 \end{array} \right\},$$
$$e^{c\phi} = \left(\frac{1+\tau}{k+\tau}\right)^{-4/7}, \tag{52}$$

and $F_{(3)}$ components are as in (49).

V. COLLIDING EM WAVE SOLUTION IN ANY HIGHER DIMENSION

The action for the $(4+p)$-branes is given by

$$S = \int d^{(4+p)}x\sqrt{-g}(R - F_{(2)}^2), \tag{53}$$

in which $F_{(2)}$ stands for the EM 2-form.

Solution is given by[20]

$$ds_{4+p}^2 = AB^{(1-p)/(1+p)}\,dt^2 - B^{2/(p+1)}dy\,dy - (AB)^{-1}\,dr^2 - r^2\,d\Omega_{(2)}^2, \tag{54}$$

where

$$A = 1 - \frac{r_+}{r},$$

$$B = 1 - \frac{r_-}{r},$$

and

$$F = Q\epsilon_2.$$

Now, the transformation (with $r_+ = a_o + b_o$ and $r_- = a_o - b_o$)

$$r = a_o + b_o\tau,$$

$$\cos\theta = \sigma,$$

$$\varphi = z,$$

$$t = x, \tag{55}$$

yields the CPW metric,

$$ds_{4+p}^2 = (k+\tau)^2(2\,du\,dv - \delta\,dz^2) - \left(\frac{1+\tau}{k+\tau}\right)^{2/(p+1)} \sum_{i=1}^{p} (dy^i)^2 - \left(\frac{1-\tau}{k+\tau}\right)\left(\frac{1+\tau}{k+\tau}\right)^{(1-p)/(1+p)} dx^2 \tag{56}$$

in which we have introduced $k=a_o/b_o>1$, and rescaled the coordinates. The EM potential 1-form is given by

$$A = -Q\sin(au\theta(u) - bv\theta(v))dz.$$

So that the nonzero field 2-form components are

$$F_{uz} = -Qa\theta(u)\sqrt{\delta},$$
$$F_{vz} = Qb\theta(v)\sqrt{\delta}. \tag{57}$$

It is observed now, that it is a simple matter to obtain the CPW metrics for an arbitrary $p \geqslant 1$. In particular, for $p=1$ and $p=7$ we have

$$ds_5^2 = (k+\tau)^2(2\,du\,dv - \delta\,dz^2) - \frac{1}{k+\tau}[(1+\tau)dy^2 + (1-\tau)dx^2] \tag{58}$$

and

$$ds_{11}^2 = (k+\tau)^2(2\,du\,dv - \delta\,dz^2) - \left(\frac{1+\tau}{k+\tau}\right)^{\frac{1}{4}} \sum_{i=1}^{7} (dy^i)^2 - \left(\frac{1-\tau}{k+\tau}\right)\left(\frac{1+\tau}{k+\tau}\right)^{-3/4} dx^2, \tag{59}$$

respectively. By letting $p\to\infty$, we can easily obtain also the colliding EM wave solutions in the ∞-brane world. The KK reduction to the fourth dimension for an arbitrary p-brane is

$$ds_4^2 = \left(\frac{1+\tau}{k+\tau}\right)^{p/(p+1)} \left\{ (k+\tau)^2(2\,du\,dv - \delta\,dz^2) - \left(\frac{1-\tau}{k+\tau}\right)\left(\frac{1+\tau}{k+\tau}\right)^{(1-p)/(1+p)} dx^2 \right\} \tag{60}$$

with

$$e^{c\phi} = \left(\frac{1+\tau}{k+\tau}\right)^{-p/[2(p+1)]},$$

$$c = \sqrt{\frac{p}{p+2}},$$

$$F_{uz} = -Qa\theta(u)\sqrt{\delta},$$

$$F_{vz} = Qb\,\theta(v)\sqrt{\delta},$$

$$Q^2 = \frac{1}{2}(k^2-1)\left(\frac{p+2}{p+1}\right).$$

This metric describes the collision of dilaton coupled EM waves in four dimensions.

VI. COLLIDING $(p+2)$-FORMS IN $(p+4)$-DIMENSION

In Sec. V we have constructed CPW solutions for the 2-form fields in $(p+4)$-dimension. By applying the duality principle we can obtain $(p+2)$-form fields and consider their collision at equal ease. We define the duality

$$\tilde{F}^{\mu_1\cdots\mu_k} = \frac{|g|^{-1/2}}{(n-k)!}\epsilon^{\mu_1\cdots\mu_k\mu_{k+1}\cdots\mu_n}F_{\mu_{k+1}\cdots\mu_n}, \tag{61}$$

where $(n>k)$ and $F_{\mu_{k+1}\cdots\mu_n}$ is assumed known.

The permutation symbol $\epsilon^{\mu_1\cdots\mu_n}$ satisfies[21]

$$\epsilon^{\mu_1\cdots\mu_n}\epsilon_{\mu_1\cdots\mu_n} = (-1)^l n!\ , \tag{62}$$

where l=number of minus signs in $g_{\mu\nu}$. Since we have readily available 2-form at hand we define its dual

$$\tilde{F}^{\mu_1\cdots\mu_{p+2}} = \frac{1}{2!}|g_{p+4}|^{-1/2}\epsilon^{\mu_1\cdots\mu_{p+4}}F_{\mu_{p+3}\mu_{p+4}} \tag{63}$$

in $(p+4)$-dimension. The action of (gravity $+\tilde{F}_{p+2}$) is taken as

$$S = \int d^{4+p}x\sqrt{g}\left(R - \frac{2}{(p+2)!}\tilde{F}^2_{p+2}\right) \tag{64}$$

with the field equations

$$R_{\mu\nu} = \frac{2}{(p+2)!}\left(\tilde{F}_{\mu\mu_1\cdots\mu_{p+1}}\tilde{F}^{\mu_p\cdots\mu_{p+1}}_{\nu} - \frac{(p+1)}{(p+2)^2}g_{\mu\nu}\tilde{F}^2\right)$$

$$\partial_\mu(|g_{p+4}|^{1/2}\tilde{F}^{\mu\mu_1\cdots\mu_{p+1}}) = 0, \tag{65}$$

where $\tilde{F}^2 = \tilde{F}_{\mu_1\cdots\mu_{p+2}}\tilde{F}^{\mu_p\cdots\mu_{p+2}}$.

We proceed with two particular examples, $p=1$ and $p=6$.

(i) $p=1$ case. The 3-form field $\tilde{F}_3$ is from the metric (58) and $F_{uz}=-Qa\,\theta(u)\sqrt{\delta}$, $F_{vz}=-Qb\,\theta(v)\sqrt{\delta}$. It is given by

$$\tilde{F}_3 = \frac{Q\sqrt{\Delta}}{(k+\tau)^2}(a\,\theta(u)\mathrm{d}u + b\,\theta(v)\mathrm{d}v)\wedge\mathrm{d}x\wedge\mathrm{d}y \tag{66}$$

which can be associated through $\tilde{F}_3=\mathrm{d}\tilde{A}_2$ to the 2-form potential

$$\tilde{A}_2 = -\frac{Q}{(k+\tau)}\mathrm{d}x\wedge\mathrm{d}y. \tag{67}$$

The incoming region (II) metric and 3-form fields can also be expressed in the Brinkmann form since they are given here in the Rosen form. For this we define new coordinates (U,V,X,Y,Z) as follows:

$$U = \int (k + \sin au)^2 \, du,$$

$$X = A(u)x, \quad Y = B(u)y, \quad Z = C(u)z,$$

$$V = v + \frac{x^2}{2}AA_u + \frac{y^2}{2}BB_u + \frac{z^2}{2}CC_u,$$

where

$$A^2(u) = \frac{1 - \sin au\theta}{k + \sin au\theta},$$

$$B^2(u) = \frac{1 + \sin au\theta}{k + \sin au\theta},$$

$$C = (k + \sin au\theta)\cos au\theta. \tag{68}$$

The relation between U and u can be chosen as

$$U = \frac{3}{2}u + \frac{2}{a}(1 - \cos au) - \frac{1}{4a}\sin 2au, \tag{69}$$

so that $u=0$ and $U=0$ coincide. Further, the graph of $U(u)$ reveals that in the interval $0<au<\pi/2$, $u>0$ implies that $U>0$. However, as it is observed we cannot invert u in terms of U, and this enforces us to keep the Brinkman form in an implicit form. We have ultimately

$$ds^2 = 2\,dU\,dV - dX^2 - dY^2 - dZ^2 - 2H(u(U),X,Y,Z)dU^2,$$

where

$$H(u(U),X,Y,Z) = \frac{a}{2}\delta(U)\left[Y^2 - X^2 + \frac{1}{k}(2Z^2 - X^2 - Y^2)\right] + \frac{a^2\theta(U)}{4(k + \sin au)^2}[(k+1)(3 - k + 2\sin au)X^2 - (k-1)(3 + k - 2\sin au)Y^2 - (k + \sin au)(k + 4\sin au)Z^2]. \tag{70}$$

We recall that a general class of metrics given by

$$ds^2 = 2\,dU\,dV - \left(\sum_{i,j} A_{ij}(U)X^iX^j\right)du^2 - \sum_i (dX^i)^2,$$

where A_{ij}=constant, is known as Cahen-Wallach space.[22]

It is clear that we have $\nabla^2 H \neq 0$ in our case, indicating the presence of energy momentum for the 3-form field as it should. The 3-form field, in the Brinkman form for region II is

$$\tilde{F}_3 = \frac{aQ\theta(U)}{(k + \sin au)^3}dU \wedge dX \wedge dY, \tag{71}$$

where the inversion of the expression (69) is implied.

(ii) $p=6$ case. The 8-form field $\tilde{F}_8$ is found from the metric (56),

$$\tilde{F}_8 = \tilde{F}_{uxy^1\cdots y^6}\,du \wedge dx \wedge dy^1 \wedge \cdots \wedge dy^6 + \tilde{F}_{vxy^1\cdots y^6}\,dv \wedge dx \wedge dy^1 \wedge \cdots \wedge dy^6, \tag{72}$$

where

$$\tilde{F}^{uxy^1\cdots y^6} = \frac{Qb\,\theta(v)\sqrt{\delta}}{|g_{10}|^{1/2}},$$

$$\tilde{F}^{vxy^1\cdots y^6} = \frac{Qa\,\theta(u)\sqrt{\delta}}{|g_{10}|^{1/2}}$$

and we have chosen $\epsilon^{uvzxy^1\cdots y^6} = +1$. The corresponding 7-form potential is

$$\tilde{A}_7 = \frac{-Q}{k+\tau} \mathrm{d}x \wedge \mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^6 \tag{73}$$

which derives $\tilde{F}_8$ through $\tilde{F}_8 = \mathrm{d}\tilde{A}_7$.

It is seen that the collision problem of these 8-form fields is automatically solved with well-defined incoming states. The solutions, as we stated earlier are regular but our procedure does not allow at the moment to obtain the collision problem of arbitrary *n*-form fields. Our procedure limits itself only with the 2(3)-form fields and their duals. Different authors addressed themselves to the more general problem but they obtained only perturbative and singular solutions.[23,24]

VII. CONCLUSIONS

In this paper we have concentrated first on two five-dimensional BHs, namely Myers-Perry (MP) and Reissner-Nordstrom (RN). These are both extensions of the five-dimensional Schwarzschild BH, MP with rotation while RN with electric charge. The inherent isometry between the BHs and colliding plane waves (CPWs) yields regular, horizon forming solutions to the latter. By regular, throughout the paper we imply a Cauchy-Horizon (CH) forming space-time with finite curvature invariants. We have not attempted to extend our space-time beyond CH. Once this is done by Chandrasekhar and Xanthopoulos,[1] we may face various singularities ranging from timelike to spacelike ones or no singularities at all. Another issue that we have not addressed ourselves in the paper is the stability of the CH formed in the collision. There are strong arguments that under certain perturbations the CHs of the CPWs transform into curvature singularities.[25] Definitely this matter is far from being conclusive and requires further investigation. We note also that beside the BHs the more general Weyl solutions can be employed in the generating of CPWs.[26]

Our particular cross-polarized dilatonic non-type-*D* metric with CH provides an example to be taken into account other than the singular ones used in string theory.[27,28] Our procedure is extendible to higher dimensional BHs provided technical matters are overcome. One such problem is to find representation for the *n*-dimensional spherical line element which admits $(n-1)$-dimensional Abelian subspace. Equation (2) performs just this for the three-dimensional sphere. Although we obtain colliding 2(3)-form fields by our procedure through, employing five-dimensional BHs, we can dualize our forms and obtain colliding $(p+1)$- and $(p+2)$-form fields in $(p+4)$-dimensions. Extension of our work to arbitrary form fields will be the next stage of our study. Presumably all these metrics will find application in higher dimensional space-times and low energy limit of the string theory.

APPENDIX A

The nonzero components of the metric (6) are given below

$$\tilde{R}_{uvuv} = -2a^2b^2k^2\theta(u)\,\theta(v),$$

$$\tilde{R}_{uvyz} = -2abka_o^2\theta(u)\,\theta(v),$$

$$\tilde{R}_{uvzx} = 2abka_o\theta(u)\theta(v),$$

$$\tilde{R}_{uyvy} = abk^2a_o^2\theta(u)\theta(v),$$

$$\tilde{R}_{uyvx} = abk^2a_o^2\theta(u)\theta(v) = \tilde{R}_{uxvy},$$

$$\tilde{R}_{uzvy} = abka_o^2\theta(u)\theta(v) = -\tilde{R}_{uyvz},$$

$$\tilde{R}_{uzvz} = -aba_o^2\theta(u)\theta(v),$$

$$\tilde{R}_{uzvx} = abka_o\theta(u)\theta(v) = -\tilde{R}_{uxvz},$$

$$\tilde{R}_{uxvx} = abk^2\theta(u)\theta(v),$$

$$\tilde{R}_{yzyz} = -\left(\tfrac{1}{2} + 2a_o^4\right)\theta(u)\theta(v),$$

$$\tilde{R}_{yzzx} = 2a_o^3\theta(u)\theta(v),$$

$$\tilde{R}_{yxyx} = \tfrac{1}{2}k^2\theta(u)\theta(v),$$

$$\tilde{R}_{zxzx} = \left(k^2 - \tfrac{1}{2}\right)\theta(u)\theta(v),$$

$$\tilde{R}_{uyuy} = -a^2\theta(u)Y_1 + a\delta(u)\cos(bv\,\theta(v))Y_2,$$

$$\tilde{R}_{vyvy} = -b^2\theta(v)Y_1 + b\delta(v)\cos(au\,\theta(u))Y_2,$$

$$\tilde{R}_{uxux} = -2a^2\theta(u)Y_3 - \frac{2ak}{D^2}\delta(u)\cos(bv\,\theta(v)),$$

$$\tilde{R}_{vxvx} = -2b^2\theta(v)Y_3 - \frac{2bk}{D^2}\delta(v)\cos(au\,\theta(u)),$$

$$\tilde{R}_{uyux} = -a^2a_o\theta(u)Y_4 - \frac{2aa_ok}{D^2}\delta(u)\cos(bv\,\theta(v)),$$

$$\tilde{R}_{vyvx} = -b^2a_o\theta(v)Y_4 - \frac{2ba_ok}{D^2}\delta(v)\cos(au\,\theta(u)),$$

$$\tilde{R}_{uzuz} = a^2\theta(u)Y_5 + a\delta(u)\cos(bv\,\theta(v))Y_6,$$

$$\tilde{R}_{vzvz} = b^2\theta(v)Y_5 + b\delta(v)\cos(au\,\theta(u))Y_6,$$

$$\tilde{R}_{uzux} = -a^2 a_o \theta(u) Y_7 - 2aa_o \frac{(1+2k\tau)}{D^2} \delta(u) \cos(bv\,\theta(v)),$$

$$\tilde{R}_{vzvx} = b^2 a_o \theta(v) Y_7 + 2ba_o \frac{(1+2k\tau)}{D^2} \delta(v) \cos(au\,\theta(u)),$$

$$\tilde{R}_{uyuz} = -a^2 \theta(u) Y_8 - a\delta(u) \cos(bv\,\theta(v)) Y_9,$$

$$\tilde{R}_{vyvz} = b^2 \theta(v) Y_8 + b\delta(v) \cos(au\,\theta(u)) Y_9,$$

where we have used the following abbreviations:

$$D = 1 + k\tau,$$

$$Y_1 = \frac{1}{D^3}[4(1+k\tau - a_o^2) - k^2\Delta(3(1+a_o^2) + k\tau)],$$

$$Y_2 = \frac{k^2}{D^3}[\tau(k^2+2) + k(1+3\tau^2 + k\tau^3)],$$

$$Y_3 = \frac{a_o^2 - k^2\Delta}{D^3},$$

$$Y_4 = \frac{1}{D^3}[2(1+k\tau) - 3k^2\Delta],$$

$$Y_5 = \frac{1}{D^3}\{-4(1+k\tau - a_o^2) + \Delta[a_o^2(11+12k^2\tau^2) + k\tau(7-6k^2) - 3(1-2k^2)]\},$$

$$Y_6 = \frac{1}{D^3}[k + \tau(3-10a_o^2) + k\tau^2(3-16a_o^2) + k^2\tau^3(1-8a_o^2)],$$

$$Y_7 = \frac{1}{D^3}[2(k+\tau) - k\Delta(5+6k\tau)],$$

$$Y_8 = \frac{1}{D^3}[4(k + \tau(1-a_o^2)) + k\Delta(k^2\Delta - 5 - a_o^2 - 3k\tau(1+2a_o^2))],$$

$$Y_9 = \frac{1}{D^3}[(2-k^2)(1+3k\tau) + k^2\tau^2(5+k\tau - 2k^2)].$$

APPENDIX B

The nonzero Riemann components of the metric (26) are with the step functions inserted as follows:

$$\tilde{R}_{uvuv} = \frac{-2la^2b^2}{C}(l+\tau)\theta(u)\theta(v),$$

$$\tilde{R}_{uxux} = -\frac{a^2\theta(u)}{C^4}(3l^2+2l\tau-1) - \frac{2a}{C^3}\delta(u)\cos(bv\,\theta(v))(l+\tau),$$

$$\tilde{R}_{uxvx} = \frac{ab}{C^4}\theta(u)\theta(v)(2l^2+l\tau-1),$$

$$\tilde{R}_{uyuy} = -\frac{a^2\theta(u)}{4C}(3l^2+4l\tau+1) + a\delta(u)l\cos(bv\,\theta(v)),$$

$$\tilde{R}_{uyuz} = -\frac{a^2\theta(u)\sigma}{4C}(3l^2+4l\tau+1) + a\delta(u)\cos(bv\,\theta(v)),$$

$$\tilde{R}_{uyvy} = \frac{ab}{4C}(1-l^2)\theta(u)\theta(v),$$

$$\tilde{R}_{uyvz} = \frac{ab\sigma}{4C}(1-l^2)\theta(u)\theta(v),$$

$$\tilde{R}_{uzuz} = -\frac{a^2\theta(u)}{4C}(3l^2+4l\tau+1) + a\delta(u)l\cos(bv\,\theta(v)),$$

$$\tilde{R}_{uzvz} = \frac{ab}{4C}(1-l^2)\theta(u)\theta(v),$$

$$\tilde{R}_{vxvx} = -\frac{b^2\theta(v)}{C^4}(3l^2+2l\tau-1) - \frac{2b}{C^3}\delta(v)\cos(au\,\theta(u))(1+\tau),$$

$$\tilde{R}_{vyvy} = -\frac{b^2\theta(v)}{4C}(3l^2+4l\tau+1) + b\delta(v)l\cos(au\,\theta(u)),$$

$$\tilde{R}_{vyvz} = -\frac{b^2\theta(v)\sigma}{4C}(3l^2+4l\tau+1) - b\delta(v)\cos(au\,\theta(u)),$$

$$\tilde{R}_{vzvz} = -\frac{b^2\theta(v)}{4C}(3l^2+4l\tau+1) + b\delta(v)l\cos(au\,\theta(u)),$$

$$\tilde{R}_{xyxy} = \frac{l\Delta}{2C^4}\theta(u)\theta(v)(l+\tau),$$

$$\tilde{R}_{xyxz} = \frac{l\Delta\sigma}{2C^4}\theta(u)\theta(v)(l+\tau),$$

$$\tilde{R}_{xzxz} = \frac{l\Delta}{2C^4}\theta(u)\theta(v)(l+\tau),$$

$$\tilde{R}_{yzyz} = \frac{-\delta\theta(u)\theta(v)}{4C}(1+2l\tau+l^2),$$

where we have used $C=1+l\tau$.

APPENDIX C

The nonzero NP quantities for the metric (31) are

$$\Psi_2 = \frac{1}{8}ab\theta(u)\theta(v)\frac{(5+\tau)}{(1+\tau)^{\frac{5}{2}}},$$

$$\Psi_4 = -\frac{3}{8}a^2\theta(u)\frac{(5+\tau)}{(1+\tau)^{\frac{5}{2}}} + \frac{a}{4}\frac{\delta(u)}{\cos bv(\theta(v))}\frac{(3+\tau)}{(1+\tau)^{3/2}},$$

$$\Psi_0 = -\frac{3}{8}b^2\theta(v)\frac{(5+\tau)}{(1+\tau)^{\frac{5}{2}}} + \frac{b}{4}\frac{\delta(v)}{\cos au(\theta(u))}\frac{(3+\tau)}{(1+\tau)^{3/2}},$$

$$\Phi_{22} = \frac{1}{16}a^2\theta(u)\frac{(7+\tau)}{(1+\tau)^{\frac{5}{2}}},$$

$$\Phi_{00} = \frac{1}{16}b^2\theta(v)\frac{(7+\tau)}{(1+\tau)^{\frac{5}{2}}},$$

$$\Phi_{02} = -\frac{1}{4}\frac{ab\theta(u)\theta(v)}{(1+\tau)^{\frac{3}{2}}},$$

$$\Phi_{11} = \frac{3}{32}ab\theta(u)\theta(v)\frac{(1-\tau)}{(1+\tau)^{\frac{5}{2}}} = -3\Lambda.$$

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Explicit solutions of the classical Calogero and Sutherland systems for any root system

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Explicit solutions of the classical Calogero (rational with/without harmonic confining potential) and Sutherland (trigonometric potential) systems is obtained by diagonalization of certain matrices of simple time evolution. The method works for Calogero & Sutherland systems based on any root system. It generalizes the well-known results by Olshanetsky and Perelomov for the *A* type root systems. Explicit solutions of the (rational and trigonometric) higher Hamiltonian flows of the integrable hierarchy can be readily obtained in a similar way for those based on the classical root systems. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The classical and quantum integrability/solvability of Calogero-Moser systems[1–5] manifests itself in many guises; the existence of Lax pairs and/or Dunkl operators, algebraic linearization, quadratic algebras, associated integrable spin chains, "quantized" classical spectra, etc. Among them, a most intuitive understanding of solvability/integrability is provided by the fact that explicit solutions of the classical equations of motion are obtained by diagonalization of certain matrices having trivial time evolution, as shown by Olshanetsky and Perelomov[6] for the rational and trigonometric potential cases.[7] Their results are for the systems based on the *A*-type roots. Here we will show that the same results hold universally for systems based on any root system. To be more precise, for the rational potential (without/with harmonic confining potential) cases, the diagonalization method works for any root system, including the noncrystallographic ones. For the trigonometric and hyperbolic potential cases, we show that the explicit diagonalization method holds for any crystallographic root system based on the *universal* Lax pair.[8] A simpler form of explicit diagonalization is provided by the *minimal* Lax pair,[9,8] which exists only for those based on the *A*, *D*, E_6, and E_7 root systems. The basic idea of the explicit solution method is very closely related to the notion of algebraic linearization, proved universally for any root system by Caseiro–Françoise–Sasaki.[10] We will follow the notation of Ref. 10 throughout this paper and Eq. (a.b) of this paper will be cited as (Ia.b). Explicit solutions in terms of diagonalization is readily obtained for the *higher* (rational and trigonometric) *Hamiltonian flows* belonging to the integrable hierarchy. This works, however, only for those based on the classical root systems, *A*, *B*, *C*, and *D*. The conventional Lax pair in terms of the set of vector weights (*A*, *C*, and *D*) or the set of short roots (*B*) is indispensable.

This paper is organized as follows. In Sec. II, the historical background and the logical structure of the Calogero–Moser systems necessary for the present paper are briefly reviewed. The Hamiltonian and the universal Lax pair with rational potential are introduced. The explicit integration in terms of diagonalization is achieved by relating the Lax pair matrices *L* and *M* to a matrix *W* of the same size with trivial time evolution, $\ddot{W}=0$. Section III is devoted to the explicit solution of the systems with rational plus the harmonic confining potential. In Sec. IV, we show

the explicit solutions of the Sutherland systems, which have trigonometric/hyperbolic potentials. In Sec. IV A a simple form of explicit diagonalization is obtained by reinterpreting the formulas of the algebraic linearization method developed by Caseiro–Françoise–Sasaki.[10] This is based on the minimal Lax pair, which exists for those based on A, D, E_6, and E_7 root systems. A general treatment of explicit integration of the Sutherland systems in terms of the universal Lax pair is provided in Sec. IV B. This applies to any crystallographic root system. Sections V and VI are devoted to the problem of explicit integration of the higher Hamiltonian flows of the integrable hierarchy. The rational potential case is discussed in Sec. V and the trigonometric case in Sec. VI. The final section is for a summary and comments.

II. RATIONAL POTENTIAL

The integrability of the Calogero–Moser systems has a long history. First, various types of the integrable potentials are recognized; starting from the Calogero model[1] with rational $(1/q^2)$ plus a harmonic confining (q^2) potential followed by the Sutherland model[2] with a trigonometric $(1/\sin^2 q)$ potential. Then the pure rational potential $(1/q^2)$[3] and the hyperbolic $(1/\sinh^2 q)$[4] and the elliptic $[\wp(q)]$ potentials[5] are added to the list of the integrable potentials. As seen in many other subjects in mathematical physics, the quantum groups, the integrable spin chains, Yang–Baxter equations, etc., the elliptic case is the generic one, giving all the rest in various degenerations. However, each degenerate case, the rational, trigonometric, and the hyperbolic, has its own special properties and merits not shared by the more generic ones; for example, the algebraic linearization[10] of the degenerate Calogero–Moser systems and the quadratic algebras[11] for the quantum systems with the superintegrable rational $(1/q^2)$ potential. In the present article we deal with one of such properties of the degenerate Calogero–Moser systems and it is in fact very closely related to the algebraic linearization.[10] Second, the nature of the multiparticle interactions of the Calogero–Moser systems is recognized to be governed by the root systems associated with finite reflection (Coxeter/Weyl) groups.[12,13] The original models[1–5]are all based on the A-type root system related to the symmetric group S_N, with N being the number of the particles. The S_N is also the Weyl group of the special unitary group $SU(N)$. The integrability (the Lax pair) of the systems based on the classical root systems (A, B, C, and D) is noticed immediately by Olshanetsky and Perelomov,[12,13] but the actual demonstration of the integrability of the Calogero–Moser systems based on the exceptional[9,14] and noncrystallographic root systems[8] took more years. The classical universal Lax pair applicable for all types of potentials and for any root system[8] and the quantum universal Lax pair applicable for all degenerate potentials and for any root system[15] have been known for some years.

Let us denote by Δ a root system of rank r. It is a finite set of $\mathbf{R}^r$ vectors that is invariant under reflections in the hyperplane perpendicular to each vector in Δ. A reflection s_ρ in terms of a root ρ is defined by

$$s_\rho(x) = x - \rho(\rho^\vee \cdot x), \quad x \in \mathbf{R}^r, \tag{2.1}$$

in which $\rho^\vee = 2\rho/\rho^2$. Thus Δ is characterized by

$$s_\rho(\eta) \in \Delta, \quad \forall\, \rho, \eta \in \Delta. \tag{2.2}$$

The dynamical variables are the coordinates $q_i \in \mathbf{R}$, $i=1,\ldots,r$ and their canonically conjugate momenta $p_i \in \mathbf{R}$, $i=1,\ldots,r$, except for the A_r case in the ordinary embedding, in which the number of particles is $r+1$. The Hamiltonian for the classical Calogero–Moser system with the rational potential but without the harmonic confining potential is

$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\sum_{\rho\in\Delta_+} \frac{g_{|\rho|}^2 |\rho|^2}{(\rho\cdot q)^2}, \tag{2.3}$$

in which the real and positive coupling constants $g_{|\rho|}$ are defined on orbits of the corresponding Coxeter group. That is, for the simple Lie algebra cases $g_{|\rho|}=g$ for all roots in simply laced models and $g_{|\rho|}=g_L$ for long roots and $g_{|\rho|}=g_S$ for short roots in nonsimply laced models. In order to define Lax pair matrices L and M, let us choose a set of $\mathbf{R}^r$ vectors $\mathcal{R}=\{\alpha,\beta,\ldots,\}$, $\#\mathcal{R}=\mathcal{D}$, permuting under the action of the reflection group:

$$s_\rho(\alpha)\in\mathcal{R},\quad \forall\,\alpha\in\mathcal{R},\quad \forall\,\rho\in\Delta. \tag{2.4}$$

We demand that it consists of a single orbit of the Coxeter group, for irreducibility. Then we define $\mathcal{D}\times\mathcal{D}$ matrices indexed by the elements of $\mathcal{R}$:

$$p\cdot\hat{H}:\quad (p\cdot\hat{H})_{\alpha\beta}=(p\cdot\alpha)\delta_{\alpha\beta}, \tag{2.5}$$

$$\hat{s}_\rho:\quad (\hat{s}_\rho)_{\alpha\beta}=\delta_{\alpha,s_\rho(\beta)}. \tag{2.6}$$

Introduce next the $\mathcal{D}\times\mathcal{D}$ matrices X, L, and M:[9,8]

$$X=i\sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\hat{H})\frac{1}{(\rho\cdot q)}\hat{s}_\rho, \tag{2.7}$$

$$L=p\cdot\hat{H}+X, \tag{2.8}$$

$$M=-\frac{i}{2}\sum_{\rho\in\Delta_+} g_{|\rho|}\frac{|\rho|^2}{(\rho\cdot q)^2}\hat{s}_\rho, \tag{2.9}$$

and a *diagonal matrix*:

$$Q=q\cdot\hat{H}:\quad (Q)_{\alpha\beta}=(q\cdot\alpha)\delta_{\alpha\beta}. \tag{2.10}$$

Here L and Q are Hermitian $L^\dagger=L$, $Q^\dagger=Q$, and M is anti-Hermitian $M^\dagger=-M$.

As shown in Ref. 10, Eqs. (I2.7a), (I2.7b) the time evolution of the matrix L along the flow of the Hamiltonian (2.3) displays the following equations:

$$\frac{\partial L}{\partial t}=[L,M], \tag{2.11}$$

$$\frac{\partial Q}{\partial t}=[Q,M]+L. \tag{2.12}$$

Next let us define another $\mathcal{D}\times\mathcal{D}$ unitary matrix $U(t)$ by the linear equation and the initial condition:

$$\frac{\partial U}{\partial t}=UM,\quad U(0)=1_{\mathcal{D}}, \tag{2.13}$$

in which $1_{\mathcal{D}}$ is the $\mathcal{D}\times\mathcal{D}$ unit matrix. The final step is the introduction of $W(t)$:

$$W(t)\equiv U(t)Q(t)U^{-1}(t), \tag{2.14}$$

which has a simple time evolution

$$\dot{W} = U(\dot{Q} - [Q,M])U^{-1} = ULU^{-1}, \tag{2.15}$$

$$\ddot{W} = U(\dot{L} - [L,M])U^{-1} = 0. \tag{2.16}$$

The solution is

$$W(t) = W(0) + t\,\dot{W}(0), \tag{2.17}$$

with the initial values

$$W(0) = Q(0), \quad \dot{W}(0) = L(0), \tag{2.18}$$

which are determined by the initial values of the canonical variables $q_j(0)$, $p_j(0)$, $j=1,\ldots,r$. Due to the defining relation of $W(t)$ in terms of the *diagonal matrix* $Q(t)$ (2.14), the solution $\{q(t)\}$ of the canonical equations of motion,

$$\frac{\partial q_j}{\partial t} = \frac{\partial \mathcal{H}}{\partial p_j}, \quad \frac{\partial p_j}{\partial t} = -\frac{\partial \mathcal{H}}{\partial q_j}, \quad j = 1, \ldots, r, \tag{2.19}$$

with the above Hamiltonian (2.3), is simply obtained by *diagonalizing* the above matrix solution (2.17). The conjugate momenta $\{p(t)\}$ are obtained by differentiation $p_j(t) = \partial q_j(t)/\partial t$.

As promised, this is the universal proof applicable for any root system including the noncrystallographic one. The spectrum of $W(t)$ (2.17) is highly constrained, since its dimension $\mathcal{D}$ is usually much greater than the degree of freedom r. The high symmetry of the spectrum is guaranteed by the Coxeter invariance of the theory:

$$\mathcal{H}(s_\rho(p), s_\rho(q)) = \mathcal{H}(p,q), \quad \forall\, \rho \in \Delta, \tag{2.20}$$

$$L(s_\rho(p), s_\rho(q)) = \hat{s}_\rho L(p,q)\hat{s}_\rho, \quad M(s_\rho(q)) = \hat{s}_\rho M(q)\hat{s}_\rho. \tag{2.21}$$

The original proof of the explicit integration of the A type systems by Olshanetsky and Perelomov[6] is the very special case in which the spectrum of $W(t)$ (2.17) is not constrained. Our proof reduces to that of Ref. 6 when $\Delta = A_r$ and the set of vector weights is chosen as $\mathcal{R} = \mathbf{V}$, $\#\mathcal{R} = \mathcal{D} = r+1$.

III. RATIONAL WITH HARMONIC CONFINING POTENTIAL

The Hamiltonian is now

$$\mathcal{H}_\omega = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + \frac{1}{2}\sum_{\rho\in\Delta_+} \frac{g_{|\rho|}^2 |\rho|^2}{(\rho\cdot q)^2}. \tag{3.1}$$

With the same matrices introduced above in the preceding section, the time evolution displays (I3.2a), (I3.2b):

$$\dot{L} = [L,M] - \omega^2 Q, \tag{3.2}$$

$$\dot{Q} = [Q,M] + L. \tag{3.3}$$

With the same definition of the unitary matrix $U(t)$ as above (2.13), the matrix

$$W(t) \equiv U(t)Q(t)U^{-1}(t), \tag{3.4}$$

evolves harmonically in time:

$$\dot{W} = U(\dot{Q} - [Q,M])U^{-1} = ULU^{-1} \tag{3.5}$$

$$\ddot{W} = U(\dot{L} - [L,M])U^{-1} = -\omega^2 W. \tag{3.6}$$

The solution is

$$W(t) = \cos \omega t W(0) + \omega^{-1} \sin \omega t \dot{W}(0), \tag{3.7}$$

with the initial values

$$W(0) = Q(0), \quad \dot{W}(0) = L(0). \tag{3.8}$$

Again the explicit solution $\{q(t)\}$ is obtained by *diagonalizing* the above matrix $W(t)$ (3.7) with the harmonic time dependence.

IV. TRIGONOMETRIC POTENTIAL

The Hamiltonian of the trigonometric (Sutherland) model[2] is written as:

$$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\sum_{\rho \in \Delta_+} \frac{g_{|\rho|}^2 |\rho|^2}{\sin^2(\rho \cdot q)}. \tag{4.1}$$

In order to get the hyperbolic case, it suffices to change sin into sinh. In the following, we only demonstrate the explicit integration of the trigonometric case. The hyperbolic case can be deduced easily by the above replacement.

Two types of Lax pairs are known[9,8] for the trigonometric cases: the minimal and the universal Lax pairs. While the latter, the universal lax pair, applies to any crystallographic root system, the former, the minimal Lax pair, requires $\mathcal{R}$ to be the set of minimal weights, which exists only for the A, D, E_6, and E_7 root systems. Let us start with the minimal Lax pair, which has a simpler structure thanks to the restriction to the minimal weights, satisfying the condition

$$\mu\text{: minimal weight} \Leftrightarrow \alpha^\vee \cdot \mu = 0, \pm 1, \quad \forall\, \alpha \in \Delta. \tag{4.2}$$

A. Minimal Lax pair

We consider the matrices[9,8]

$$L = p \cdot \hat{H} + X, \tag{4.3}$$

$$X = i \sum_{\rho \in \Delta_+} g_{|\rho|} (\rho \cdot \hat{H}) \frac{1}{\sin(\rho \cdot q)} \hat{s}_\rho, \tag{4.4}$$

$$M = -\frac{i}{2} \sum_{\rho \in \Delta_+} g_{|\rho|} \frac{|\rho|^2 \cos(\rho \cdot q)}{\sin^2(\rho \cdot q)} (\hat{s}_\rho - 1_{\mathcal{D}}) + i \sum_{\rho \in \Delta_+} g_{|\rho|} \frac{(\rho \cdot \hat{H})^2}{\sin^2(\rho \cdot q)}, \tag{4.5}$$

and *diagonal matrices*:

$$Q = q \cdot \hat{H}: \quad (Q)_{\alpha\beta} = (q \cdot \alpha)\delta_{\alpha\beta}, \tag{4.6}$$

$$R = \mathrm{e}^{2iQ}. \tag{4.7}$$

Again L and Q are Hermitian $L^\dagger = L$, $Q^\dagger = Q$ and M is anti-Hermitian $M^\dagger = -M$. Thus R is unitary.

As shown in Ref. 10 (I5.3a), (I5.3b), when the root system admits a minimal representation, and $\mathcal{R}$ being the set of minimal weights, the time evolution along the flow of the Hamiltonian (4.1) displays

$$\frac{\partial L}{\partial t} = [L, M], \tag{4.8}$$

$$\frac{\partial R}{\partial t} = [R, M] + i(RL + LR). \tag{4.9}$$

With the same definition of the unitary matrix $U(t)$ as above (2.13),

$$\frac{\partial U}{\partial t} = UM, \quad U(0) = 1_{\mathcal{D}}, \tag{4.10}$$

we introduce a matrix

$$\mathcal{W}(t) = U(t)R(t)U(t)^{-1} = U(t)\mathrm{e}^{2iQ(t)}U(t)^{-1}. \tag{4.11}$$

It satisfies a simple first-order linear differential equation,

$$\frac{\partial \mathcal{W}}{\partial t} = U(\partial R/\partial t - [R, M])U^{-1} = iU(RL + LR)U^{-1} \tag{4.12}$$

$$= i(\mathcal{W}ULU^{-1} + ULU^{-1}\mathcal{W}), \tag{4.13}$$

since as in (2.15), (2.16), ULU^{-1} is a constant matrix:

$$\frac{\partial}{\partial t}(ULU^{-1}) = U(\partial L/\partial t - [L, M])U^{-1} = 0, \tag{4.14}$$

$$U(t)L(t)U(t)^{-1} = L(0). \tag{4.15}$$

The solution is

$$\mathcal{W}(t) = \mathrm{e}^{itL(0)}\mathrm{e}^{2iQ(0)}\mathrm{e}^{itL(0)}. \tag{4.16}$$

By *diagonalizing* the above matrix solution, we obtain the explicit solution $\{q(t)\}$ of the classical Sutherland model (4.1). One might naturally wonder if the coordinates $\{q(t)\}$ could be determined uniquely from the unitary matrix (4.16). The answer is affirmative since the motion is always restricted to one of the Weyl alcoves due to the periodicity and singularity of the potential. Near the boundary of a Weyl alcove, for example, at $\rho \cdot q = 0$, $\rho \in \Delta$, the singularity of the potential $\sim 1/(\rho \cdot q)^2$ can never be surpassed classically. Therefore if $\{q(0)\}$ is in the principal Weyl alcove,

$$PW_T = \{q \in \mathbf{R}^r | \rho \cdot q > 0, \quad \rho \in \Pi, \quad \rho_h \cdot q < \pi\}, \tag{4.17}$$

$\{q(t)\}$ will always remain there. Here Π is the set of the simple roots and ρ_h is the highest weight. This removes any ambiguity in determining $\{q(t)\}$ from the eigenvalues of (4.16). As in the rational potential cases, the spectrum of $\mathcal{W}(t)$ is highly constrained as a consequence of the Weyl invariance (2.20), (2.21).

B. Universal Lax pair

The universal Lax pair has $\cot(\rho \cdot q)$ function in L instead of $1/\sin(\rho \cdot q)$ in (4.4),

$$L = p \cdot \hat{H} + X, \tag{4.18}$$

$$X = i \sum_{\rho \in \Delta_+} g_{|\rho|} (\rho \cdot \hat{H}) \cot(\rho \cdot q) \hat{s}_\rho, \tag{4.19}$$

$$M = -\frac{i}{2} \sum_{\rho \in \Delta_+} g_{|\rho|} \frac{|\rho|^2}{\sin^2(\rho \cdot q)} (\hat{s}_\rho - 1_D), \tag{4.20}$$

which satisfy $\partial L/\partial t = [L,M]$ for the Hamiltonian flow, but the additional equation (4.9) takes a different form.

For $\mathcal{R}$ being the set of minimal weights, it reads as

$$\frac{\partial R}{\partial t} = [R,M] + i(R(L+K) + (L-K)R), \tag{4.21}$$

in which K is a non-negative constant matrix commuting with M:

$$K \equiv \sum_{\rho \in \Delta_+} g_{|\rho|} (\rho \cdot \hat{H})(\rho^\vee \cdot \hat{H}) \hat{s}_\rho, \quad [K,M] = 0. \tag{4.22}$$

It is a very important quantity in Calogero–Moser systems appearing in many contexts. For example, it is a commutator of Q (2.10) and the rational Lax matrix L (2.8), (2.7) [see (4.36) of Ref. 15 and (2.40) of Ref. 16):

$$[Q,L] = iK. \tag{4.23}$$

It should be noted that if K is defined as above, the expression (4.22) is *universal*, which is valid for any root system Δ and any choice of $\mathcal{R}$. Various properties of the K matrix, whose eigenvalues are all "integers," are discussed in detail by Corrigan-Sasaki, in the Appendix of Ref. 16.

For $\mathcal{R}$ being the set of all roots Δ (for the simply laced root systems) or the set of short roots Δ_S (for nonsimply laced root systems) and also the set of vector weights ($\mathbf{V}$) for the C, the relation corresponding to (4.9) and (4.21) reads as

$$\frac{\partial R}{\partial t} = [R,M] + i(R(L+\tilde{K}) + (L-\tilde{K})R), \tag{4.24}$$

in which $\tilde{K}$ is another constant matrix commuting with M,

$$\tilde{K} = \sum_{\rho \in \Delta_+} g_{|\rho|} |\rho \cdot \hat{H}| \hat{s}_\rho, \quad [\tilde{K},M] = 0, \tag{4.25}$$

introduced by Corrigan-Sasaki, as (5.32) of Ref. 16.

Now the explicit solution of the Sutherland system is achieved for any crystallographic root system, since one can choose at least one Lax pair satisfying (4.24). We proceed as before by defining the unitary matrix $U(t)$ by (4.10) and introduce a matrix

$$\mathcal{W}(t) = U(t)R(t)U(t)^{-1} = U(t)\mathrm{e}^{2iQ(t)}U(t)^{-1}. \tag{4.26}$$

It satisfies a simple first-order linear differential equation,

$$\frac{\partial \mathcal{W}}{\partial t} = U(\partial R/\partial t - [R,M])U^{-1} = iU(R(L+\tilde{K}) + (L-\tilde{K})R)U^{-1}, \tag{4.27}$$

$$= i(\mathcal{W}U(L+\tilde{K})U^{-1} + U(L-\tilde{K})U^{-1}\mathcal{W}), \tag{4.28}$$

since as in (2.15), (2.16), $U(L \pm \tilde{K})U^{-1}$ is a constant matrix:

$$\frac{d}{dt}(U(L\pm\tilde{K})U^{-1}) = U(\partial L/\partial t - [L,M])U^{-1} = 0, \tag{4.29}$$

$$U(t)(L(t)\pm\tilde{K})U(t)^{-1} = L(0)\pm\tilde{K}. \tag{4.30}$$

The solution is

$$\mathcal{W}(t) = \mathrm{e}^{it(L(0)-\tilde{K})}\mathrm{e}^{2iQ(0)}\mathrm{e}^{it(L(0)+\tilde{K})}. \tag{4.31}$$

By *diagonalizing* the above matrix solution, we obtain the explicit solution $\{q(t)\}$ of the classical Sutherland system (4.1) for any root system.

The very fact that $\tilde{K}$ (K) commutes with M simply means that a spectral parameter λ can be introduced trivially into the Lax pair for degenerate potentials:[8]

$$L_\lambda \equiv L + \lambda\tilde{K}, \quad \dot{L}_\lambda = [L_\lambda, M]. \tag{4.32}$$

V. RATIONAL HIGHER FLOWS

The integrable hierarchy of the Calogero–Sutherland systems consists of Hamiltonians generated by higher conserved quantities, which are constructed, for example, from the trace of the higher powers of the L matrix, $\mathcal{H}_n \propto \mathrm{Tr}(L^{2n})$. The method of explicit integration as described in the preceding sections applies also to these higher Hamiltonian flows, as shown by Suris[7] for the A-type root systems with the conventional Lax pair, $\mathcal{R}=\mathbf{V}$. However, in contrast to the basic Calogero–Sutherland flows, it works only for those systems based on the classical root systems, the A, B, C, and D. Let us denote by $\mathcal{R}$ the set of vector weights $\mathbf{V}$, for the A, C, and D root systems and the set of short roots Δ_S for the B root system. These particular sets $\mathcal{R}$ have a unique orthogonality property,

$$\text{if } \mu \neq \pm\nu, \quad \mu\cdot\nu = 0, \quad \forall\, \mu,\nu \in \mathcal{R}, \tag{5.1}$$

which endows a very special structure to the Lax pair represented on $\mathcal{R}$. The dimensions of the corresponding Lax matrices are $\mathcal{D}=r+1$ for the A_r and $\mathcal{D}=2r$ for the B_r, C_r, and D_r. It is through these special Lax matrices that the explicit integration of the higher rational and trigonometric flows is realized.

Let us start with the explicit forms of the rational L matrices:

$$(A)\colon L, \quad L_{jk} = p_j\delta_{jk} + ig(1-\delta_{jk})/(q_j - q_k), \tag{5.2}$$

$$(B)\colon L = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad A_{jk} = p_j\delta_{jk} + ig_L(1-\delta_{jk})/(q_j - q_k),$$

$$B_{jk} = i(g_S/q_j)\delta_{jk} + ig_L(1-\delta_{jk})/(q_j + q_k). \tag{5.3}$$

The rational C system will not be discussed since it is equivalent to the rational B system. The rational D system is obtained by constraining $g_S=0$ in the rational B system.

The higher Hamiltonians are

$$(A)\colon \mathcal{H}_n = \mathrm{Tr}(L^{n+1})/(n+1), \quad n \geqslant 1, \tag{5.4}$$

$$(B,D)\colon \mathcal{H}_n = \mathrm{Tr}(L^{2n})/(4n), \quad n \geqslant 1. \tag{5.5}$$

The lowest $\mathcal{H}_1$ is the original Hamiltonian (2.3). The basic idea is to rewrite the Hamiltonian flow,

$$\frac{\partial q_j}{\partial t_n} = \frac{\partial \mathcal{H}_n}{\partial p_j}, \quad \frac{\partial p_j}{\partial t_n} = -\frac{\partial \mathcal{H}_n}{\partial q_j}, \tag{5.6}$$

into equivalent matrix forms,

$$\frac{\partial L}{\partial t_n} = [L, M_n], \tag{5.7}$$

$$\frac{\partial Q}{\partial t_n} = [Q, M_n] + L^n \ (L^{2n-1}), \tag{5.8}$$

as in the lowest flow (2.11), (2.12).

In contrast to the lowest flow case in which the explicit form of M is given (2.9), we can interpret part of (5.7) and (5.8) as determining M_n. The diagonal part of the Q equation (5.8) is equivalent to the first half of the canonical equations (5.6). The off-diagonal part of the Q equation (5.8) determines the off-diagonal part of M_n completely:

$$(M_n)_{\mu\nu} = -(L^n)_{\mu\nu}/q\cdot(\mu-\nu), \quad (-(L^{2n-1})_{\mu\nu}/q\cdot(\mu-\nu)), \quad \mu \neq \nu. \tag{5.9}$$

Whereas the diagonal part of M_n does not enter the Q equation (5.8), it can be determined from the off-diagonal part of the Lax equation. The result is very simple:

$$(M_n)_{\mu\mu} = -\sum_{\nu\neq\mu} (M_n)_{\nu\mu} = -\sum_{\nu\neq\mu} (M_n)_{\mu\nu}, \quad M_n^\dagger = -M_n. \tag{5.10}$$

The proof that the diagonal part of the higher flow Lax equation (5.7) is equivalent to the second half of the canonical equations (5.6) goes almost parallel to that of the lowest flow.

After the equivalence of the canonical equations (5.6) with the two matrix equations (5.7) and (5.8) is established, the explicit integration by diagonalization is straightforward. Let us define a $\mathcal{D}\times\mathcal{D}$ unitary matrix $U_n(t_n)$ by the linear equation and the initial condition:

$$\frac{\partial U_n}{\partial t_n} = U_n M_n, \quad U_n(0) = 1_{\mathcal{D}}. \tag{5.11}$$

Then a matrix function $W_n(t_n)$, defined by

$$W_n(t_n) \equiv U_n(t_n) Q(t_n) U_n^{-1}(t_n), \tag{5.12}$$

has a simple time evolution,

$$\frac{\partial W_n}{\partial t_n} = U_n(\partial Q/\partial t_n - [Q, M_n])U_n^{-1} = (U_n L U_n^{-1})^n \quad ((U_n L U_n^{-1})^{2n-1}), \tag{5.13}$$

$$\frac{\partial}{\partial t_n}(U_n L U_n^{-1}) = U_n(\partial L/\partial t_n - [L, M_n])U_n^{-1} = 0, \tag{5.14}$$

$$\Rightarrow U_n(t_n) L(t_n) U_n(t_n)^{-1} = L(0). \tag{5.15}$$

The solution is

$$W_n(t_n) = W_n(0) + t_n\, \partial W_n(0)/\partial t_n, \tag{5.16}$$

with the initial values

$$W_n(0) = Q(0), \quad \partial W_n(0)/\partial t_n = L(0)^n \quad [L(0)^{2n-1}], \tag{5.17}$$

which are determined by the initial values of the canonical variables $q_j(0)$, $p_j(0)$, $j=1,\ldots,r$. Due

to the defining relation of $W_n(t_n)$ in terms of the *diagonal matrix* $Q(t_n)$ (5.12), the solution $\{q(t_n)\}$ of the canonical equations of motion (5.6) with the above Hamiltonian (5.4) or (5.5), is simply obtained by *diagonalizing* the above matrix solution (5.16). Determination of the conjugate momenta $\{p(t_n)\}$ requires a solution of the second half of the canonical equations of motion (5.6), which are now *algebraic* since $\{\partial q/\partial t_n\}$ are now known functions of time. An extension to the generic higher flows of the hierarchy

$$\mathcal{H} = \sum_n c_n \mathcal{H}_n, \quad c_n: \text{const}, \tag{5.18}$$

is straightforward since the matrix equations (5.7) and (5.8) are linear in M_n. However, some higher flows cannot be treated this way. For example, in the D_r (r: odd) theory, there exists another conserved quantity (Hamiltonian) of the form $p_1 p_2 \cdots p_r + \cdots$, which cannot be written as (5.18).

VI. TRIGONOMETRIC HIGHER FLOWS

The basic logics of the explicit integration of the trigonometric higher flows is almost the same as that of the rational higher flows, except that we have to consider two different types of Lax pairs; the minimal and the universal. So we just write down the key formulas without a detailed derivation.

A. Minimal Lax pair

We discuss the explicit integration of the trigonometric higher flows of the A and D theory in terms of the minimal Lax pair, although the formulation in terms of the universal Lax pair works well for them, too.

The explicit forms of the trigonometric minimal L matrices are

$$(A)\text{: } L, \quad L_{jk} = p_j \delta_{jk} + ig(1-\delta_{jk})/\sin(q_j - q_k), \tag{6.1}$$

$$(D)\text{: } L = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad A_{jk} = p_j \delta_{jk} + ig(1-\delta_{jk})/\sin(q_j - q_k),$$

$$B_{jk} = ig(1-\delta_{jk})/\sin(q_j + q_k). \tag{6.2}$$

The higher Hamiltonians take exactly the same form as (5.4) and (5.5). The lowest $\mathcal{H}_1$ is the original Hamiltonian (4.1). We rewrite the higher Hamiltonian flow (5.6) into equivalent matrix forms,

$$\frac{\partial L}{\partial t_n} = [L, M_n], \tag{6.3}$$

$$\frac{\partial R}{\partial t_n} = [R, M_n] + i(RL^n + L^n R) \quad (i(RL^{2n-1} + L^{2n-1}R)), \tag{6.4}$$

as in the lowest flow (4.8), (4.9). The off-diagonal part of M_n is

$$(M_n)_{\mu\nu} = -(L^n)_{\mu\nu} \cot[q\cdot(\mu-\nu)] \quad (-(L^{2n-1})_{\mu\nu} \cot[q\cdot(\mu-\nu)]), \quad \mu \neq \nu. \tag{6.5}$$

The diagonal part is

$$(M_n)_{\mu\mu} = \sum_{\nu\neq\mu} (L^n)_{\nu\mu}/\sin[q\cdot(\nu-\mu)] = \sum_{\nu\neq\mu} (L^n)_{\mu\nu}/\sin[q\cdot(\mu-\nu)], \quad M_n^\dagger = -M_n. \tag{6.6}$$

The $\mathcal{D}\times\mathcal{D}$ matrix $\mathcal{W}_n(t_n)$ obeys a simple time evolution:

$$\mathcal{W}_n(t_n) = U_n(t)R(t_n)U_n(t_n)^{-1} = U_n(t_n)\mathrm{e}^{2iQ(t_n)}U_n(t_n)^{-1}, \tag{6.7}$$

$$= \mathrm{e}^{it_nL(0)^n}\mathrm{e}^{2iQ(0)}\mathrm{e}^{it_nL(0)^n}(\mathrm{e}^{it_nL(0)^{2n-1}}\mathrm{e}^{2iQ(0)}\mathrm{e}^{it_nL(0)^{2n-1}}). \tag{6.8}$$

By *diagonalizing* the above matrix solution (6.8), we obtain the explicit solution $\{q(t_n)\}$ of the higher flows of the Sutherland system (5.4) and (5.5) for the A and D root systems.

B. Universal Lax pair

The explicit integration of the higher flows of the B and C Sutherland systems is achieved in terms of the universal Lax pairs based on the set of short roots ($\mathcal{R}=\Delta_S$) for B and the set of vector weights ($\mathcal{R}=\mathbf{V}$) for C. For the rank r system, both have $\mathcal{D}=2r$.

The Lax matrix L and the constant matrix $\widetilde{K}$ (4.25) are

$$L = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad \widetilde{K} = \begin{pmatrix} S & T \\ T & S \end{pmatrix}, \tag{6.9}$$

$$(B): A_{jk} = p_j\delta_{jk} + ig_L(1-\delta_{jk})\cot(q_j - q_k), \quad S_{jk} = g_L(1-\delta_{jk}), \tag{6.10}$$

$$B_{jk} = ig_S\cot q_j\delta_{jk} + ig_L(1-\delta_{jk})\cot(q_j + q_k), \quad T_{jk} = g_S\delta_{jk} + g_L(1-\delta_{jk}), \tag{6.11}$$

$$(C): A_{jk} = p_j\delta_{jk} + ig_S(1-\delta_{jk})\cot(q_j - q_k), \quad S_{jk} = g_S(1-\delta_{jk}), \tag{6.12}$$

$$B_{jk} = 2ig_L\cot 2q_j\delta_{jk} + ig_S(1-\delta_{jk})\cot(q_j + q_k), \quad T_{jk} = 2g_L\delta_{jk} + g_S(1-\delta_{jk}). \tag{6.13}$$

It is easy to see

$$\mathrm{e}^{iQ}(L+\widetilde{K})\mathrm{e}^{-iQ} = \mathrm{e}^{-iQ}(L-\widetilde{K})\mathrm{e}^{iQ}, \tag{6.14}$$

$$\Rightarrow \mathrm{Tr}(L+\widetilde{K})^n = \mathrm{Tr}(L-\widetilde{K})^n, \tag{6.15}$$

which are conserved quantities of the Sutherland flow (4.1). It differs from the usual one $\mathrm{Tr}(L^n)$ by a linear combination of lower-order conserved quantities. The canonical equations of the higher flow Hamiltonian,

$$\mathcal{H}_n = \mathrm{Tr}((L\pm\widetilde{K})^{2n})/(4n) \tag{6.16}$$

are equivalent to the matrix equations

$$\frac{\partial L}{\partial t_n} = [L, M_n], \tag{6.17}$$

$$\frac{\partial R}{\partial t_n} = [R, M_n] + i(R(L+\widetilde{K})^{2n-1} + (L-\widetilde{K})^{2n-1}R). \tag{6.18}$$

The off-diagonal part of M_n is

$$(M_n)_{\mu\nu} = -[e^{iq\cdot(\mu-\nu)}(L+\widetilde{K})^n_{\mu\nu} + e^{-iq\cdot(\mu-\nu)}(L-\widetilde{K})^n_{\mu\nu}]/\sin[q\cdot(\mu-\nu)], \quad \mu\neq\nu. \tag{6.19}$$

The diagonal part is

$$(M_n)_{\mu\mu} = -\sum_{\nu\neq\mu}(M_n)_{\nu\mu} = -\sum_{\nu\neq\mu}(M_n)_{\mu\nu}, \quad M_n^\dagger = -M_n. \tag{6.20}$$

The $\mathcal{D}\times\mathcal{D}$ matrix $\mathcal{W}_n(t_n)$ obeys simple time evolution:

$$\mathcal{W}_n(t_n) = U_n(t)R(t_n)U_n(t_n)^{-1} = U_n(t_n)\mathrm{e}^{2iQ(t_n)}U_n(t_n)^{-1}, \tag{6.21}$$

$$= \mathrm{e}^{it_n(L(0)-\tilde{K})^{2n-1}}\mathrm{e}^{2iQ(0)}\mathrm{e}^{it_n(L(0)+\tilde{K})^{2n-1}}. \tag{6.22}$$

By *diagonalizing* the above matrix solution (6.22), we obtain the explicit solution $\{q(t_n)\}$ of the higher flows of the Sutherland system (6.16) for the B and C root systems.

VII. SUMMARY AND COMMENTS

Explicit integration of the Calogero and Sutherland systems by means of diagonalization is demonstrated for any root system, the exceptional as well as the classical and the noncrystallographic. It is based on the universal Lax pair for the degenerate potentials, which is the rational with/without the harmonic confining potential and the trigonometric/hyperbolic potentials. As emphasized in the text, it is very closely related to the concept of algebraic linearization by Caseiro–Françoise–Sasaki.[10] The method is extended to the higher Hamiltonian flows of the rational and trigonometric/hyperbolic interactions. In contrast to the basic Calogero–Sutherland flows, the applicability is limited to those systems based on the classical root systems, the A, B, C, and D root systems.

The theory of explicit integration of higher Hamiltonian flows is very closely related to the dynamical r matrix[7,17,18] and the Hamiltonian reduction.[19,13] In the case of the most classical rational potential of the A type, the method of Hamiltonian reduction starts from the large phase space of the matrix dynamical variable W and its conjugate momentum variable Z, which are both assumed to be Hermitian. The Hamiltonians,

$$\mathcal{H}_n = \mathrm{Tr}(Z^{n+1})/(n+1), \tag{7.1}$$

generate the flows

$$\frac{\partial W}{\partial t_n} = Z^n, \quad \frac{\partial Z}{\partial t_n} = 0. \tag{7.2}$$

This Hamiltonian system is invariant under the action $(W,Z)\to(UWU^{-1},UZU^{-1})$ of unitary matrices U. The reduced phase space is obtained by imposing the constraint

$$[W,Z] = iK \tag{7.3}$$

and factoring out the constrained phase space by residual symmetries (i.e., by the group of unitary matrices that commute with K). The (Q,L) pair (4.23) is nothing but a representative of a point of the reduced phase space, which is connected with the point (W,Z) of the large phase space by a (t-dependent) unitary matrix U as

$$Q = U^{-1}WU, \quad L = U^{-1}ZU. \tag{7.4}$$

The linear flows of (W,Z) are thereby mapped to the Calogero flows of (Q,L). This is the way to understand the rational Calogero system of the A type as a Hamiltonian reduction;[19] a similar interpretation has been proposed for a few other cases.[13] The dynamical r matrix has been constructed in this framework of Hamiltonian reduction.[7] We expect that all the cases discussed in this paper can be treated in the same way.

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Fractional Lindstedt series

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The parametric equations of the surfaces on which highly resonant quasiperiodic motions develop (lower-dimensional tori) cannot be analytically continued, in general, in the perturbation parameter ε, i.e., they are not analytic functions of ε. However rather generally quasiperiodic motions whose frequencies satisfy only one rational relation ("resonances of order 1") admit formal perturbation expansions in terms of a fractional power of ε depending on the degeneration of the resonance. We find conditions for this to happen, and in such a case we prove that the formal expansion is convergent after suitable resummation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2157052]

I. INTRODUCTION

Resonances play an important role in the theory of dynamical systems. A possible application is provided by problems of celestial mechanics, such as the phenomenon of resonance locking between rotation and orbital periods of the satellites.[17] In fact, the presence of friction can select resonant motions which remain stable when friction (on astronomical time scales) becomes negligible. In such a case maximal KAM tori can be really observed only approximately and on very short time scale, whereas, on very large time scales one expects that only periodic motions survive. On intermediate time scales one can imagine that quasiperiodic motions, involving a number of frequencies less than the total number of degrees of freedom (and decreasing with time), describe most of the observed dynamics. This makes interesting and important to study quasiperiodic motions occurring on lower-dimensional tori for nearly integrable Hamiltonian systems. These quasiperiodic motions are characterized by frequencies satisfying s rational relations, with $r=N-s$ ranging between 1 (periodic motions) and the number N of degrees of freedom (KAM tori). The number s equals the number of normal frequencies appearing in the perturbed motions, whereas r is the number of independent components of the rotation vector.

The analysis of such motions is simpler under some (generic) nondegeneracy assumptions on the perturbations. On the contrary the situation becomes immediately very complicated if no restriction at all is made on the perturbation. Situations of this kind arise also in similar contexts, we can mention the conservation of KAM tori under perturbations for systems of N harmonic oscillators, proved for $N=2$ but conjectured to hold in general,[18,24] and the stability of Hill's equation under quasiperiodic perturbations.[14] In the case of lower-dimensional tori, the nondegeneracy assumption is that the normal frequencies become different from zero when the perturbation is switched on. If such an assumption is removed, then only partial results hold, and only in the case $s=1$, that is only in the case of one normal frequency.[2,3]

Starting from the work of Eliasson,[6] a new approach to KAM theory of quasiintegrable

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Hamiltonian systems arose, based on the analysis of cancellations in the "Lindstedt series" for the functions mapping unperturbed motions (uniform rotations, in suitable coordinates) into corresponding perturbed ones.

A convenient way to exploit cancellations to resolve apparent divergences in the Lindstedt series is through methods inspired by quantum field theory, consisting in graphical expansions, summation of classes of diverging subdiagrams, iterative study of the flow of the effective constants and the possible introduction of counterterms. With these techniques and ideas, a number of known results have been reproduced and new ones have been obtained; see Refs. 7, 11, 13, and 9 for some reviews.

In this paper we follow the latter approach to investigate the conservation of $(N-1)$-dimensional tori for systems with N degrees of freedom. More precisely we consider N degrees of freedom systems described by analytic Hamiltonians of the form

$$H(I,\varphi) = H_0(I) + \varepsilon f(I,\varphi), \tag{1.1}$$

with $(I,\varphi) \in \mathcal{D} \times \mathbb{T}^N$, where $\mathbb{T} = \mathbb{R} \backslash 2\pi\mathbb{Z}$ is the standard torus, $\mathcal{D}$ is an open subset of $\mathbb{R}^N$, ε is a real parameter, and the free Hamiltonian $H_0(I)$ is assumed to be uniformly convex, $\partial_I^2 H_0(I) \geqslant C > 0$ for all $I \in \mathcal{D}$.

Definition 1 (simple resonance): A simple Diophantine resonance *for the unperturbed system is a motion taking place on the torus* $\{I_0\} \times \mathbb{T}^N$ *with* $\omega_0 := \partial_I H_0(I_0)$ *satisfying a rational relation* $\omega_0 \cdot \nu_0 = 0$ *for some* $\nu_0 \in \mathbb{Z}^N$ *and* $|\omega_0 \cdot \nu| > C|\nu|^{-\tau}$ *for suitable* $C, \tau > 0$ *and for all* $0 \neq \nu \in \mathbb{Z}^N$ *not parallel to* ν_0.

Thus, if $\varepsilon = 0$, the motions with rotation velocity ω_0 will foliate the torus $\{I_0\} \times \mathbb{T}^N$ into a one parameter family of invariant tori of dimension $N-1$.

For $\varepsilon \neq 0$ invariant tori with dimension $N-1$ run by quasiperiodic motions with spectrum ω_0 will, in general, only continue to exist "close" to some of the unperturbed tori $\{I_0\} \times \mathbb{T}^N$. The problem is simpler under nondegeneracy assumptions on the average $\langle f \rangle$ of the perturbing function f on the torus $\{I_0\} \times \mathbb{T}^N$; it has been studied in Refs. 10 and 15 with techniques employed, under different assumptions on the perturbation, in this paper. Define the average of f on $\{I_0\} \times \mathbb{T}^N$ as

$$\langle f(\varphi) \rangle := \lim_{T \to \infty} \frac{1}{T} \int_0^T f(\varphi + \omega_0 t) \mathrm{d}t. \tag{1.2}$$

It depends nontrivially on φ in the sense that in general it is a nonconstant periodic function of φ. This is more easily visualized in coordinates *adapted* to the resonance: they are defined by a linear canonical transformation $(I,\varphi) := (I_0 + S^{-1}(\mathbf{A},B), S^T(\boldsymbol{\alpha},\beta))$, with S a nonsingular integer components $N \times N$ matrix with determinant $\det S = 1$ such that $\omega_0 \equiv S^T(\boldsymbol{\omega},0)$ with $\boldsymbol{\omega} \in \mathbb{R}^{N-1}$, $|\boldsymbol{\omega} \cdot \boldsymbol{\nu}| > C_0 |\boldsymbol{\nu}|^{-\tau_0}$ for *all* $\mathbf{0} \neq \boldsymbol{\nu} \in \mathbb{Z}^{N-1}$ and $\mathbf{A} \in \mathbb{R}^{N-1}$, $B \in \mathbb{R}$, $\boldsymbol{\alpha} \in \mathbb{T}^{N-1}$, $\beta \in \mathbb{T}$.

In the coordinates $(\mathbf{A},B,\boldsymbol{\alpha},\beta)$ the Hamiltonian becomes an analytic function of $(\mathbf{A},B)$, in the domain obtained from $\mathcal{D}$ under the transformation S, and $(\boldsymbol{\alpha},\beta) \in \mathbb{T}^{N-1} \times \mathbb{T}$. It will be of the form $H(\mathbf{A},B,\boldsymbol{\alpha},\beta) = H_0'(\mathbf{A},B) + \varepsilon f(\boldsymbol{\alpha},\beta)$, where $H_0'(\mathbf{A},B) = \boldsymbol{\omega} \cdot \mathbf{A} + H_0(\mathbf{A},B)$, with H_0 vanishing to second order at $\mathbf{A} = \mathbf{0}$, $B = 0$ and uniformly convex in the domain where it is defined. Of course the functions H, H_0, f have a different meaning with respect to those appearing in (1.1), but we prefer to use the same notation for simplicity. For the same reason we still shall use the notation (I,φ) to denote the new action-angle variables, by setting $I = (\mathbf{A},B)$ and $\varphi = (\boldsymbol{\alpha},\beta)$.

So in the new coordinates the Hamiltonian H, the rotation vector $\boldsymbol{\omega} \in \mathbb{R}^{N-1}$ and the average $f_{\mathbf{0}}(\mathbf{A},B,\beta)$ of the perturbing function can be supposed to be such that

$$H = \boldsymbol{\omega} \cdot \mathbf{A} + H_0(\mathbf{A},B) + \varepsilon f(\mathbf{A},B,\boldsymbol{\alpha},\beta), \quad |\boldsymbol{\omega} \cdot \boldsymbol{\nu}| \geqslant \frac{C_0}{|\boldsymbol{\nu}|^{\tau_0}} \quad \forall\, \mathbf{0} \neq \boldsymbol{\nu} \in \mathbb{Z}^{N-1},$$

$$f_0(\mathbf{A},B,\beta) := \int \frac{\mathrm{d}\alpha}{(2\pi)^{N-1}} f(\mathbf{A},B,\boldsymbol{\alpha},\beta) \quad \text{if } f(\mathbf{A},B,\boldsymbol{\alpha},\beta) = \sum_{\boldsymbol{\nu} \in \mathbb{Z}^{N-1}} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\alpha}} f_{\boldsymbol{\nu}}(\mathbf{A},B,\beta), \tag{1.3}$$

near the unperturbed resonance and *without any loss of generality*. The corresponding equations of motion for $X(t)\equiv(\mathbf{A}(t),B(t),\boldsymbol{\alpha}(t),\beta(t))$ are

$$\begin{aligned}&\dot{\mathbf{A}}=-\varepsilon\partial_{\boldsymbol{\alpha}}f,\\&\dot{B}=-\varepsilon\partial_{\beta}f,\\&\dot{\boldsymbol{\alpha}}=\boldsymbol{\omega}+\partial_{\mathbf{A}}H_0+\varepsilon\partial_{\mathbf{A}}f,\\&\dot{\beta}=\partial_{B}H_0+\varepsilon\partial_{B}f,\end{aligned}\qquad\text{or } \dot{X}=E\partial_X H(X),\quad\text{with } E=\begin{pmatrix}0&-1\\1&0\end{pmatrix},\tag{1.4}$$

where E is the standard $2N\times 2N$ symplectic matrix. We study the existence of motions which can be described by a constant β_0 and by functions $\mathbf{A}(\boldsymbol{\psi})$, $B(\boldsymbol{\psi})$, $\mathbf{a}(\boldsymbol{\psi})$, $b(\boldsymbol{\psi})$ of $\boldsymbol{\psi}\in\mathbb{T}^{N-1}$, which tend to 0 as $\varepsilon\to 0$, such that, by posing

$$\begin{gathered}\mathbf{A}(t)=\mathbf{A}(\boldsymbol{\psi}+\boldsymbol{\omega}t),\quad B(t)=B(\boldsymbol{\psi}+\boldsymbol{\omega}t),\\\boldsymbol{\alpha}(t)=\boldsymbol{\psi}+\boldsymbol{\omega}t+\mathbf{a}(\boldsymbol{\psi}+\boldsymbol{\omega}t),\quad \beta(t)=\beta_0+b(\boldsymbol{\psi}+\boldsymbol{\omega}t),\end{gathered}\tag{1.5}$$

one obtains, for all $\boldsymbol{\psi}\in\mathbb{T}^{N-1}$, solutions to the equations of motion (1.4). For brevity we shall sometimes write $X(t)$, instead of $X(\boldsymbol{\psi}+\boldsymbol{\omega}t)$, to indicate solutions of (1.4) of the form (1.5).

Note that, for $\varepsilon=0$, the motions (1.5) reduce to

$$\mathbf{A}^{(0)}(t)=\mathbf{0},\quad B^{(0)}(t)=0,\quad \boldsymbol{\alpha}^{(0)}(t)=\boldsymbol{\psi}+\boldsymbol{\omega}t,\quad \beta^{(0)}(t)=\beta_0,\tag{1.6}$$

where $\psi\in\mathbb{T}^{N-1}$ are arbitrary. The motions $X^{(0)}(t)=(\mathbf{A}^{(0)}(t),B^{(0)}(t),\boldsymbol{\alpha}^{(0)}(t),\beta^{(0)}(t))$ represent the unperturbed resonant motions filling a one parameter family of $N-1$ dimensional invariant tori (parametrized by β_0).

Given any function $G(\boldsymbol{\psi},\varepsilon)$ we shall denote by $G_{\boldsymbol{\nu}}$ the $\boldsymbol{\nu}$th Fourier component of its Fourier expansion in $\boldsymbol{\psi}$ and we shall call $[G]^k$ the kth order term obtained by expanding in ε the function G. Furthermore we shall denote by $[G]^k_{\boldsymbol{\nu}}$ the $\boldsymbol{\nu}$th Fourier component of the Fourier expansion of $[G]^k$ and by $G_{\neq\mathbf{0}}$ the function $G-G_{\mathbf{0}}$.

A formal solution of (1.4) and (1.5), as a power series in ε, $X(\boldsymbol{\psi})=X^{(0)}(\boldsymbol{\psi})+\varepsilon X^{(1)}(\boldsymbol{\psi})+\ldots$, is well known to exist if $\beta_0\in\mathbb{T}$ is a stationarity point for the average $f_{\mathbf{0}}(\mathbf{0},0,\beta)$ [i.e., a point such that $\partial_\beta f_{\mathbf{0}}(\mathbf{0},0,\beta_0)=0$] which is not degenerate [i.e., $\partial^2_\beta f_0(\mathbf{0},0,\beta_0)\neq 0$]; cf. for instance, Refs. 21, 19, and 10. *Here we consider explicitly the case in which the nondegeneracy condition on* $\partial^2_\beta f_{\mathbf{0}}(\mathbf{0},0,\beta_0)$ *fails to hold. This is a case in which in general no formal solution in powers of* ε *can be constructed.*

If β_0 is such that $\partial_\beta f_{\mathbf{0}}(\beta_0)=0$, then there exists a function X' such that $X^{(0)}+\varepsilon X'$ solves (1.4) up to terms of order ε^2 (excluded). Namely $X'(\boldsymbol{\psi})=(\mathbf{A}'(\boldsymbol{\psi}),B'(\boldsymbol{\psi}),\mathbf{a}'(\boldsymbol{\psi}),b'(\boldsymbol{\psi}))$ is obtained by applying the operator $(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^{-1}$ to the vector

$$(-\partial_\varphi f(\mathbf{0},0,\boldsymbol{\psi},\beta_0),\partial_I f(\mathbf{0},0,\boldsymbol{\psi},\beta_0)+\partial^2_I H_0(\mathbf{0},0)(\mathbf{A}'(\boldsymbol{\psi}),B'(\boldsymbol{\psi}))),\tag{1.7}$$

where $\partial_\varphi,\partial_I$ denote, respectively, the derivatives with respect to the angle and action variables. This means that one first determines $\mathbf{A}'(\boldsymbol{\psi})$ and $B'(\boldsymbol{\psi})$ by solving $(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})(\mathbf{A}'(\boldsymbol{\psi}),B'(\boldsymbol{\psi}))=-\partial_\varphi f(\mathbf{0},0,\boldsymbol{\psi},\beta_0)$; the (otherwise arbitrary) averages $\mathbf{A}'_0,B'_0$ are fixed by requiring that the operator $(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^{-1}$ can be applied to the vector formed by the last N components of (1.7), i.e., $\partial_I f_{\mathbf{0}}(\mathbf{0},0,\beta_0)+\partial^2_I H_0(\mathbf{0},0)(\mathbf{A}'_{\mathbf{0}},B'_{\mathbf{0}})=\mathbf{0}$. In this way also $\mathbf{a}'(\boldsymbol{\psi})$ and $b'(\boldsymbol{\psi})$ can be obtained. The averages of the angle variables will be chosen $\mathbf{a}'_{\mathbf{0}}=\mathbf{0}$ while we leave $b'_{\mathbf{0}}$ as a free parameter [to be suitably fixed at higher orders to make the equations (1.4) formally solvable].

There are, however other solutions which are correct up to order ε^2 (excluded). If $\partial^j_\beta f_{\mathbf{0}}(\mathbf{0},0,\beta_0)=0$ for all $j\leqslant k_0$ and $\partial^{k_0+1}_\beta f_{\mathbf{0}}(\mathbf{0},0,\beta_0)\neq 0$, one can imagine to add to the free parameter $b'_{\mathbf{0}}$ any polynomial in powers of $\eta=|\varepsilon|^{1/k_0}$ of degree $<k_0$. It can be checked (and it will be explicitly shown in next sections) that, for any choice of this polynomial, a solution of the equation of motions correct up to terms of order ε^2 (excluded) exists. This is, ultimately, the

reason why consistent expansions in powers of ε cannot in general be continued beyond first order. The consistency condition of the equations of motion necessary to improve (to second order included) the solution fixes one coefficient of such (*a priori* arbitrary) polynomials in η and, in general, this really forces the expansion to be an expansion in powers of η different from $\eta^{k_0}=\varepsilon$.

The analysis below shows that an expansion in η is actually possible at all orders if the following assumptions are satisfied.

Assumptions:

(a) *The constant* $a:=[\partial_\beta f(X^{(0)}+\varepsilon X_0')]_0^1$ *is* $a\neq 0$.
(b) *The matrix* $\partial_I^2 H_0(\mathbf{0},0)$ *is positive definite*.
(c) *There is* $k_0>0$ *such that* $\partial_\beta^j f_{\mathbf{0}}(\mathbf{0},0,\beta_0)=0$ *for all* $j\leqslant k_0$ *and* $c:=(1/k_0!)\partial_\beta^{k_0+1} f_{\mathbf{0}}(\mathbf{0},0,\beta_0)\neq 0$.

The constant a appearing in assumption (a), written explicitly, is

$$a := [\partial_{\beta,\varphi} f(X^{(0)}(\boldsymbol{\psi}))\cdot(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^{-1}(\partial_I f(X^{(0)}(\boldsymbol{\psi}))+\partial_I^2 H_0(\mathbf{0},0)(\mathbf{A}'(\boldsymbol{\psi}),B'(\boldsymbol{\psi})))_{\neq\mathbf{0}} - \partial_{\beta,I} f(X^{(0)}(\boldsymbol{\psi}))\cdot(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^{-1}\partial_\varphi f(X^{(0)}(\boldsymbol{\psi}))_{\neq\mathbf{0}}]_{\mathbf{0}}. \tag{1.8}$$

For instance if f depends only on the angle variables φ and $\partial_I^2 H(\mathbf{0},0)=\mathbb{1}$ the constant a is

$$a = \frac{1}{2}\partial_\beta \sum_{\boldsymbol{\nu}\neq\mathbf{0}} \frac{|\boldsymbol{\nu}|^2|f_{\boldsymbol{\nu}}(\beta)|^2+|\partial_\beta f_{\boldsymbol{\nu}}(\beta)|^2}{(\boldsymbol{\omega}\cdot\boldsymbol{\nu})^2}\Bigg|_{\beta=\beta_0}. \tag{1.9}$$

The number k_0 appearing in assumption (c) is a measure of the "degeneration" of the resonance, while the *order* of the resonance is the number of rational relations between the unperturbed frequencies, which is 1 in our case as the unperturbed motions have $N-1$ independent frequencies. The case $k_0=1$ was considered in Ref. 15 and we will not consider it again here. We shall focus on the case $k_0\geqslant 2$, in which case a formal power solution in ε to (1.4) does not exist. In fact, one checks that, as a consequence of assumptions (a) and (c), the average over $\boldsymbol{\psi}$ of the right-hand side (rhs) of the second equation in (1.4) is different from 0 at order ε^2, for any possible choice of the free parameter $b_{\mathbf{0}}'$ introduced after (1.7).

However, under the assumptions above, it is possible to find a formal solution to (1.4) such that the average of b is $b_{\mathbf{0}}=O(|\varepsilon|^{1/k_0})$: the average of b will be fixed in terms of the constants a and c in such a way that the average over $\boldsymbol{\psi}$ of the rhs of the second equation in (1.4) is 0 at all orders in $|\varepsilon|^{1/k_0}$.

The necessity of a fractional powers expansion can be seen by a heuristic argument sketched in Appendix A, the argument also suggests, as a conjecture, the forthcoming Theorem 1 and motivates the assumptions (a) *to* (c).

In Appendix A it is in fact shown that, in the simple case $H_0(\mathbf{A},B)=\frac{1}{2}(\mathbf{A}^2+B^2)$ and f depending only on the angles, a canonical transformation (explicitly constructed in Appendix A), defined in a neighborhood of $\{\mathbf{0}\}\times\{0\}\times\mathbb{T}^{N-1}\times\{\beta_0\}$, maps $\boldsymbol{\omega}\cdot\mathbf{A}+H_0(\mathbf{A},B)+\varepsilon f(\boldsymbol{\alpha},\beta)$ into

$$\boldsymbol{\omega}\cdot\mathbf{A}+H_0(\mathbf{A},B)+\frac{\varepsilon c}{k_0+1}(\beta-\beta_0)^{k_0+1}+\varepsilon^2 a(\beta-\beta_0)+O(\varepsilon(\beta-\beta_0)^{k_0+2})+O(\varepsilon^2(\beta-\beta_0)^2)+O(\varepsilon I^2) + O(\varepsilon^3). \tag{1.10}$$

As discussed in Appendix A, the Hamiltonian equations corresponding to (1.10) can be consistently solved to order ε^2. In particular, for some choices of the signs of ε,a,c, the angle β admits an approximate *quadratic* equilibrium point $O(|\varepsilon|^{1/k_0})$, whose stability depends again on the relative signs of ε,a,c. This second order computation suggests the conjecture that the unperturbed motion $X^{(0)}(t)$ can be continued at $\varepsilon\neq 0$, provided the average of β is chosen $O(|\varepsilon|^{1/k_0})$. The perturbed motion, if existing beyond second order, will take place on a torus (a small perturbation of the free one) which we shall call elliptic or hyperbolic, depending on the stability of the behavior of the linearization of the motion of β in the vicinity of its equilibrium point: if the

corresponding pair of nonzero Lyapunov exponents is imaginary then the torus will be said *elliptic*, if it is real it will be said *hyperbolic*.

In the following a *sparse Cantor set dense at* 0 will mean a set $\mathcal{E}$ contained in an interval $I=[-\varepsilon_0,0]$ or $I=[0,\varepsilon_0]$ with an open dense complement in I and with 0 as a density point in the sense of Lebesgue integration. In particular $\mathcal{E}$ will have positive measure.

Theorem 1: *Consider the system described by the Hamiltonian (1.3), under the assumptions* (a), (b), *and* (c). *There exists* $\varepsilon_0>0$ *such that for* $|\varepsilon|<\varepsilon_0$ *the following holds.*

(i) If k_0 *is odd and* $c\varepsilon<0$ *there is at least one hyperbolic invariant torus of dimension* $N-1$ *with rotation vector* $\boldsymbol{\omega}$. *If* $c\varepsilon>0$ *there is a sparse Cantor set* $\mathcal{E}\subset[-\varepsilon_0,0]$ *with the property that for* $\varepsilon\in\mathcal{E}$ *there is at least one elliptic torus of dimension* $(N-1)$ *with rotation vector* $\boldsymbol{\omega}$.

(ii) If k_0 *is even and* εc *has the same sign of* $-a$, *there is at least one hyperbolic invariant torus of dimension* $N-1$ *with rotation vector* $\boldsymbol{\omega}$. *Moreover, there is a sparse Cantor set* $\mathcal{E}$ *dense at* 0 *such that, if* $\varepsilon\in\mathcal{E}$ *and* εc *has the same sign of* $-a$, *there is at least one elliptic invariant torus of dimension* $N-1$ *with rotation vector* $\boldsymbol{\omega}$.

Remarks: (1) If assumption (c) is violated, since f is analytic in β, then $f_{\mathbf{0}}(\mathbf{0},0,\beta)\equiv 0$ as a function of β. In this case we can perform a canonical transformation removing the perturbation at order ε and casting the Hamiltonian into the form $H'=H_0'+\varepsilon^2 f'$, for some new analytic functions H_0' and f'. If f' satisfies the assumptions above we can apply Theorem 1 to H'. If H' satisfies assumption (c) and violates assumption (a) we cannot say much. If H' violates assumption (c) we can again remove the perturbation at lowest order through a new canonical transformation and cast the Hamiltonian into the new form $H''=H_0''+\varepsilon^4 f''$ and hope to be able to apply Theorem 1 to H''. And so on.

(2) Assumption (a) is essential and, if it does not hold, our expansion may fail to be convergent. In fact, in some cases (k_0 even), it is easy to show that if assumption (a) fails there cannot be perturbed motions of the form (1.5), see Appendix B for an example. If k_0 is odd, Ref. 2 proved existence of hyperbolic tori even if assumption (a) fails; in these cases we expect that a new perturbation parameter must be identified. The heuristic analysis in Appendix A concretely suggests plausible results to be expected if $a=0$ (under alternative assumptions).

(3) We expect that assumption (b) is not essential and that it could be weakened into the request that $\partial_I^2 H_0(\mathbf{0},0)$ is nondegenerate and that $\partial_{BB}^2 H_0(\mathbf{0},0)\neq 0$. Certainly the convexity assumption simplifies some of the estimates (see Appendix F) and we did not attempt to eliminate it.

(4) The only known result on the problems considered here is in Ref. 2, where conservation of $(N-1)$-dimensional "hyperbolic tori" is proved under weaker assumptions, although we study conservation of both hyperbolic and elliptic $(N-1)$-dimensional tori under assumptions (a) to (c) above.

(5) In principle one could proceed in a different way rather than following our approach. One could first perform the canonical transformation described in Appendix A and leading to the Hamiltonian (1.10), then study the system so obtained with other techniques, such as those in Refs. 5, 22, and 23 or 19. To this aim one should use that in the new coordinates the unperturbed Hamiltonian contains terms of order η^{2k_0-1}, while the perturbation is of order η^{2k_0}, hence has a further η.

(6) The analysis via Lindstedt series and summations of classes of diagrams is the main aspect of this work. Also the analyticity properties in η at $\boldsymbol{\omega}$ fixed are, to our knowledge, new.

(7) Technically the present work is strongly inspired by Refs. 10, 12, and 15. The proofs that can be taken literally from Ref. 15 will not be repeated here, hence familiarity with the latter reference is essential.

(8) The resummed series has manifest holomorphy properties which show that the set $\mathcal{E}$ is in the boundary of a complex domain where the functions $X(\boldsymbol{\psi})$ are analytic in ε, we do not discuss the details (see Refs. 10 and 15).

The paper is organized as follows. In Secs. II and III we prove formal solvability of the equation of motion in power series in $|\varepsilon|^{1/k_0}$ and we describe a graphical representation of the terms appearing in the formal power series. Such a representation involves labeled rooted trees, and is very similar to diagrammatic representations through Feynman diagrams arising in quantum

field theory. In Secs. IV–VI we describe an iterative resummation scheme which eliminates some classes of divergent subdiagrams and iteratively changes the power expansion, and we prove convergence of the resummed series. Some details of the proofs are deferred to the Appendixes.

II. LINDSTEDT SERIES

We define $\varepsilon=\sigma\eta^{k_0}$, with $\sigma\in\{\pm1\}$, $\eta>0$, and look for a family of formal solutions of the equations of motion in powers of η parametrized by $\boldsymbol{\psi}\in\mathbb{T}^{N-1}$, in the special form $X(t)=(\mathbf{A}(t),B(t),\boldsymbol{\alpha}(t),\beta(t))$

$$\mathbf{A}(t)=\sum_{k=k_0}^{\infty}\eta^k\sum_{\boldsymbol{\nu}\in\mathbb{Z}^{N-1}}e^{i\boldsymbol{\nu}\cdot(\boldsymbol{\psi}+\boldsymbol{\omega}t)}\mathbf{A}_{\boldsymbol{\nu}}^{(k)},$$

$$B(t)=\sum_{k=k_0}^{\infty}\eta^k\sum_{\boldsymbol{\nu}\in\mathbb{Z}^{N-1}}e^{i\boldsymbol{\nu}\cdot(\boldsymbol{\psi}+\boldsymbol{\omega}t)}B_{\boldsymbol{\nu}}^{(k)},$$

$$\boldsymbol{\alpha}(t)=\boldsymbol{\psi}+\boldsymbol{\omega}t+\mathbf{a}(t),\quad \mathbf{a}(t)=\sum_{k=k_0}^{\infty}\eta^k\sum_{\boldsymbol{\nu}\neq\mathbf{0}}e^{i\boldsymbol{\nu}\cdot(\boldsymbol{\psi}+\boldsymbol{\omega}t)}a_{\boldsymbol{\nu}}^{(k)},$$

$$\beta(t)=\beta_0+b(t),\quad b(t)=\sum_{k=k_0}^{\infty}\eta^k\sum_{\boldsymbol{\nu}\neq\mathbf{0}}e^{i\boldsymbol{\nu}\cdot(\boldsymbol{\psi}+\boldsymbol{\omega}t)}b_{\boldsymbol{\nu}}^{(k)}+\sum_{k=1}^{\infty}\eta^k b_{\mathbf{0}}^{(k)},\tag{2.1}$$

where all the involved functions have also a dependence on β_0 which has not been made explicit. The formal series (2.1) will be called *Lindstedt series* as it extends the corresponding notions already used in the theory of quasiperiodic motions on maximal tori.

In the following the average $b_{\mathbf{0}}^{(k)}$ will be abbreviated as β_k.

Remarks: (1) The functions $\mathbf{A},B,\mathbf{a}$ and $b-b_0$ have been chosen as power series in η starting with the k_0th order as the first nontrivial order; $\mathbf{a}$ has been chosen with zero average (this just corresponds to a redefinition of the origin of $\mathbb{T}^{N-1}$), while the average of b has been chosen as a series in η starting with the first order; the coefficients $\beta_k:=b_{\mathbf{0}}^{(k)}$ will be chosen in such a way that the Lindstedt series admits a formal solution.

(2) With the choices in (2.1), Eqs. (1.4) are identically solved for any order $k<k_0$ in η. The parameters β_k, $k<k_0$, are left as free parameters, to be explicitly chosen below.

To write the generic kth order of (1.4) we introduce the following definitions: given any function $\boldsymbol{\psi}\to F(X(\boldsymbol{\psi}))$, let $[F]^{(k)}$ be the kth order in the Taylor expansion of F in η and let $[F]_{\boldsymbol{\nu}}^{(k)}$ be the $\boldsymbol{\nu}$th Fourier component of the Fourier expansion of $[F]^{(k)}$. Note that this notation concerns expansions in η and is different from the one introduced after (1.6) which dealt with expansions in ε, with the new notation the quantity denoted $a=[\partial_\beta f(X^{(0)})+\varepsilon X')]_{\mathbf{0}}^{1}$ before (1.8) must be written as $a=\sigma[\partial_\beta f(X^{(0)}+\sigma\eta^{k_0}X')]_{\mathbf{0}}^{(k_0)}$ as the superscript k denotes kth order in ε while (k) denotes kth order in η. Then, if $\boldsymbol{\nu}\neq\mathbf{0}$ and $k\geqslant k_0$, the Eqs. (1.4) become

$$\begin{aligned}
(i\boldsymbol{\omega}\cdot\boldsymbol{\nu})\mathbf{A}_{\boldsymbol{\nu}}^{(k)}&=-\sigma[\partial_{\boldsymbol{\alpha}}f]_{\boldsymbol{\nu}}^{(k-k_0)},\\
(i\boldsymbol{\omega}\cdot\boldsymbol{\nu})B_{\boldsymbol{\nu}}^{(k)}&=-\sigma[\partial_\beta f]_{\boldsymbol{\nu}}^{(k-k_0)},\\
(i\boldsymbol{\omega}\cdot\boldsymbol{\nu})\mathbf{a}_{\boldsymbol{\nu}}^{(k)}&=[\partial_{\mathbf{A}}H_0]_{\boldsymbol{\nu}}^{(k)}+\sigma[\partial_{\mathbf{A}}f]_{\boldsymbol{\nu}}^{(k-k_0)},\\
(i\boldsymbol{\omega}\cdot\boldsymbol{\nu})b_{\boldsymbol{\nu}}^{(k)}&=[\partial_B H_0]_{\boldsymbol{\nu}}^{(k)}+\sigma[\partial_B f]_{\boldsymbol{\nu}}^{(k-k_0)},
\end{aligned}\tag{2.2}$$

and, since $\boldsymbol{\omega}$ satisfies the Diophantine property, they can be solved *provided*

$$\begin{aligned}
\mathbf{0} &= [\partial_{\boldsymbol{\alpha}} f]_{\mathbf{0}}^{(k-k_0)},\\
0 &= [\partial_{\beta} f]_{\mathbf{0}}^{(k-k_0)},\\
\mathbf{0} &= [\partial_{\mathbf{A}} H_0]_{\mathbf{0}}^{(k)} + \sigma[\partial_{\mathbf{A}} f]_{\mathbf{0}}^{(k-k_0)},\\
0 &= [\partial_{B} H_0]_{\mathbf{0}}^{(k)} + \sigma[\partial_{B} f]_{\mathbf{0}}^{(k-k_0)}.
\end{aligned} \tag{2.3}$$

If assumptions (a), (b), and (c) in Sec. I are satisfied, such a formal solution can be shown to exist provided the formal series for the average b_0 is suitably chosen.

Lemma 1: *Under the assumptions* (a), (b), *and* (c) *if k_0 is odd, a formal solution of (1.4) in the form (2.1) always exists; if k_0 is even, a formal solution of (1.4) in the form (2.1) exists if $\sigma ac<0$. When a formal solution exists, $\mathbf{A}^{(k)}, B^{(k)}, \mathbf{a}^{(k)}, b^{(k)}$ are uniquely fixed in the case k_0 odd. If k_0 is even, there are two possible such sequences corresponding to the choices $\beta_1 \equiv b_{\mathbf{0}}^{(1)} = \pm(-\sigma a/c)^{1/k_0}$.*

Proof: Let $X^{(0)}(\boldsymbol{\psi}) = (\mathbf{0}, 0, \boldsymbol{\psi}, \beta_0)$, $\varepsilon = \sigma\eta^{k_0}$ with $\sigma = \mathrm{sign}(\varepsilon)$ and $\eta > 0$, and look for a formal solution $t \to (\mathbf{A}(t), B(t), \boldsymbol{\alpha}(t), \beta(t))$ obtained by setting $\boldsymbol{\psi} = \boldsymbol{\psi} + \boldsymbol{\omega} t$ in

$$X(\boldsymbol{\psi}) = X^{(0)}(\boldsymbol{\psi}) + \sum_{k=k_0}^{\infty} \eta^k X^{(k)}(\boldsymbol{\psi}) + \sum_{k=1}^{\infty} \eta^k \xi^{(k)}, \tag{2.4}$$

where $\xi^{(k)} = (\mathbf{0}, 0, \mathbf{0}, \beta_k)$. Set $X^{(h)} \equiv 0$ for $0 < h < k_0$ and $\xi^{(0)} = 0$.

Suppose inductively that $X^{(h)}$ has been determined for $h = 0, 1, \ldots, k-1$, for $k \geqslant 1$. Consider a generic polynomial $Y(\boldsymbol{\psi}) := \sum_{h=0}^{k-1} \eta^h Y^{(h)}(\boldsymbol{\psi})$ and suppose, inductively, that if $Y^{(h)} = X^{(h)} + \xi^{(h)}$ the function $Y(\boldsymbol{\omega} t)$ solves the equation of motion $\dot{X} = E\partial_X H(X)$ up to order $k-1$. This is true for $k = 1$. Let $\Delta := (\boldsymbol{\omega} \cdot \partial_{\boldsymbol{\psi}})$ and remark that the identities $\int \sum_{j=1}^{2N} \partial_{\psi_i} Y_j \cdot \partial_{Y_j} H(Y) \mathrm{d}\boldsymbol{\psi} = 0$ and $\int \sum_{j=1}^{2N} \partial_{\psi_i} Y_j \cdot (E\Delta Y)_j \, \mathrm{d}\boldsymbol{\psi} = 0$ are identities *for all periodic functions* $Y(\boldsymbol{\psi})$.

Then $0 \equiv \int \Sigma_j \partial_{\psi_i} Y_j \cdot ((E\Delta Y)_j + \partial_{Y_j} H(Y)) \mathrm{d}\boldsymbol{\psi}$ and $\dot{Y} = E\partial_Y H(Y) + O(\eta^k)$ imply (note that Y has degree $< k$ in η) $\int \partial_{\psi_i} Y_j^{(0)} \cdot [\partial_{Y_j} H(Y)]^{(k)} \mathrm{d}\boldsymbol{\psi} = \mathbf{0}$, i.e., $\int [\partial_{\boldsymbol{\alpha}} H(Y)]^{(k)} \, \mathrm{d}\boldsymbol{\psi} = \mathbf{0}$ or

$$\left[\partial_{\boldsymbol{\alpha}} f \left(\sum_{h=0}^{k-1} \eta^h (X^{(h)} + \xi^{(h)}) \right) \right]_{\mathbf{0}}^{(k-k_0)} = \mathbf{0}, \tag{2.5}$$

which is the first of the compatibility conditions (2.3). This leaves $\mathbf{a}_{\mathbf{0}}^{(k)}$ as an arbitrary parameter: we can set $\mathbf{a}_{\mathbf{0}}^{(k)} = \mathbf{0}$. We also remark that, if $I \equiv (\mathbf{A}, B)$, the last two of the four equations in (2.3) have the form

$$(E\partial)_{\varphi} \partial_I H_0(\mathbf{0}, 0) I_{\mathbf{0}}^{(k)} + F^{(k)}(\{X^{(h)}, \xi^{(h)}\}_{0 \leqslant h \leqslant k-1}) = 0. \tag{2.6}$$

By assumption (b) in Sec. I, $\partial_I^2 H_0(\mathbf{0}, 0) \equiv (E\partial)_{\varphi} \partial_I H_0(\mathbf{0}, 0)$ is invertible; hence to impose the last two compatibility conditions in (2.3), it suffices to fix $I_{\mathbf{0}}^{(k)} = -[\partial_I^2 H_0(\mathbf{0}, 0)]^{-1} F^{(k)}(\{X^{(h)}, \xi^{(h)}\}_{0 \leqslant h \leqslant k-1})$, which is a known function of $\{X^{(h)}, \xi^{(h)}\}_{0 \leqslant h \leqslant k-1}$, for any possible choice of the functions $\{\xi^{(h)}\}_{0 \leqslant h \leqslant k-1}$.

So, to fulfill the compatibility conditions (2.3) and to continue the inductive construction of $X^{(k)}, \xi^{(k)}$, we are left with imposing the second of (2.3), which can only hold if β_{k-2k_0+1} satisfies certain compatibility properties. In fact if $k < 2k_0$ there is no requirement because the necessary condition that $[\partial_{\beta} f]_0^{(k-k_0)} = 0$ is automatically satisfied by assumption (c).

For $k = 2k_0$ the condition $[\partial_{\beta} f]_{\mathbf{0}}^{(k_0)} = 0$ can be expressed as follows. Let $c := (1/k_0!) \partial_{\beta}^{k_0+1} f_{\mathbf{0}}(\mathbf{0}, 0, \beta_0)$ and remark that with the notations leading to (1.8) it is $X^{(k_0)} \equiv \sigma X'$: then the second of (2.3) becomes

$$\left[\partial_{\beta X} f(X^{(0)}) \cdot X^{(k_0)} + \frac{1}{k_0!} \partial_\beta^{k_0+1} f(X^{(0)})(\beta_1)^{k_0} \right]_{\mathbf{0}} \equiv \sigma a + c\beta_1^{k_0} = 0, \tag{2.7}$$

which means

$$\beta_1 = \begin{cases} (-a\sigma/c)^{1/k_0} & \text{if } k_0 \text{ is odd,} \\ \pm(-a\sigma/c)^{1/k_0} & \text{if } k_0 \text{ is even and } a\sigma c < 0, \end{cases} \tag{2.8}$$

which is the compatibility condition to which β_1 must be subject.

For $k > 2k_0$ the second of (2.3) only involves a sum of quantities depending on $X^{(h)}$ with $h \leqslant k-k_0$ and on $\xi^{(h)}$ with $h \leqslant k-2k_0$ *with the exception of a single term*, proportional to $ck_0\beta_1^{k_0-1}\beta_{k-2k_0+1}$, involving $\xi^{(k-2k_0+1)}$. Therefore the second compatibility condition in (2.3) can be fulfilled by properly fixing β_{k-2k_0+1} in terms of $X^{(h)}$ with $h \leqslant k-k_0$ and of $\xi^{(h)}$ with $h \leqslant k-2k_0$, *provided* β_1 *exists and* $\beta_1 \neq 0$, i.e. *provided* $a \neq 0$ as assumed here.

This means that if k_0 is odd all β_k are uniquely determined while if k_0 is even there are two possible sequences β_k depending on the two choices for β_1 in (2.8). ■

Remarks: (1) For k_0 even the choice of β_k will be possible only if ε has sign σ such that $-\sigma a/c > 0$.

(2) With the notation (2.1) one has $X_{\mathbf{0}}^{(k)} = (\mathbf{A}_{\mathbf{0}}^{(k)}, B_{\mathbf{0}}^{(k)}, \mathbf{0}, 0)$ as $\mathbf{a}_{\mathbf{0}}^{(k)} = \mathbf{0}$ and $b_{\mathbf{0}}^{(k)} = \xi^{(k)}$.

III. TREE FORMALISM AND FORMAL SERIES

Given that the formal Lindstedt series is well defined, by proceeding as in Ref. 8 a graphical representation of the contributions to the perturbative series will be introduced. The idea to get the rules explained below is to start by representing the rhs of (2.2) as a power series in η by simply expanding the functions $\partial_\varphi f, \partial_I H$ in their arguments around $X^{(0)}(\boldsymbol{\psi})$ and then each argument again in powers until one obtains a power series in η.

Since the arguments of f depend on the $X^{(h)}$ with $h < k$ we obtain recursively a natural representation in terms of trees. Consider $(X_{\boldsymbol{\nu}}^{(k)})_\gamma$ where γ ranges in the symbols list

$$\mathcal{A} := \{A_1, \cdots, A_{N-1}, B, \alpha_1, \cdots, \alpha_{N-1}, \beta\}. \tag{3.1}$$

This notation is more convenient than the alternative one which would simply label the components with a label $\gamma = 1, 2, \ldots, N, N+1, \ldots, 2N$ because the first $N-1$ components play a very different role than the Nth or the remaining ones. It can be disturbing as the labels in (3.1) have the meaning of canonical variables when they do not appear as labels: hence the reader should keep this in mind in what follows. Occasionally, only in cases of possible confusion, we shall use the labels $1, \ldots, 2N$ instead of (3.1).

It will be convenient to call the first N labels *action components* and the last N *angle components;* the first $N-1$ of the two groups will be called, respectively, *fast actions* and *fast angles* component labels while the last will be called a *slow action* or, respectively, *slow angle* component label. When, occasionally, it will turn out to be useful, we shall denote the N action labels simply by I and the angle labels by φ. If $\gamma \in \mathcal{A}$ and γ is one of the first N labels (i.e., it is an action component), then $\gamma+N$ will indicate the corresponding label of the angle components and vice versa if $\gamma \in \mathcal{A}$ is an angle component then $\gamma-N$ will denote the corresponding label in the group of action components. With a slight abuse of notation, given $\gamma \in \mathcal{A}$, we shall write $\gamma \in I$ if γ is an action component and $\gamma \in \varphi$ if it is an angle component. If $\gamma, \gamma' \in \mathcal{A}$ then $\delta_{\gamma\gamma'}$ denotes the Kronecker delta; we shall also use the notation

$$\delta_{\gamma\varphi} = \begin{cases} 1 & \text{if } \gamma \in \varphi, \\ 0 & \text{if } \gamma \in I, \end{cases} \qquad \delta_{\gamma I} = \begin{cases} 1 & \text{if } \gamma \in I, \\ 0 & \text{if } \gamma \in \varphi. \end{cases} \tag{3.2}$$

Looking at (2.2) we see that, for $\boldsymbol{\nu} \neq \mathbf{0}$ and $k \geqslant k_0$, we can write it as

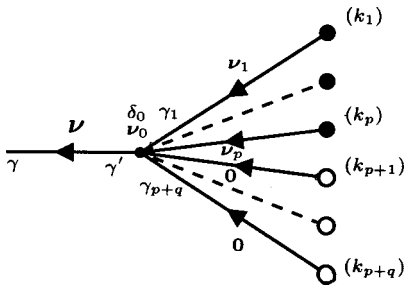


FIG. 1. Graphical representation of Eqs. (3.3) and (3.4). For $\boldsymbol{\nu}\neq\mathbf{0}$ the graph represents (3.3), while for $\boldsymbol{\nu}=\mathbf{0}$ it represents (3.4).

$$(X^{(k)}_{\boldsymbol{\nu}})_\gamma=\frac{\delta_{\gamma\gamma'}}{i\boldsymbol{\omega}\cdot\boldsymbol{\nu}}\Bigg[\sigma\sum_{p\geqslant 1}\sum_{\substack{\boldsymbol{\nu}_0+\boldsymbol{\nu}_1+\cdots+\boldsymbol{\nu}_p=\boldsymbol{\nu}\\ k_1+\cdots+k_p=k-k_0}}\frac{1}{p!}(E\partial)_{\gamma'}\partial_{\gamma_1\cdots\gamma_p}f_{\boldsymbol{\nu}_0}(\mathbf{0},0,\beta_0)\prod_{n=1}^{p}(X^{(k_n)}_{\boldsymbol{\nu}_n}+\xi^{(k_n)}\delta_{\boldsymbol{\nu}_n\mathbf{0}})_{\gamma_n}$$
$$+\sum_{p\geqslant 1}\sum_{\substack{\boldsymbol{\nu}_1+\cdots+\boldsymbol{\nu}_p=\boldsymbol{\nu}\\ \mathbf{k}_1+\cdots+k_p=k}}\frac{1}{p!}(E\partial)_{\gamma'}\partial_{\gamma_1\cdots\gamma_p}H_0(\mathbf{0},0)\prod_{n=1}^{p}(X^{(k_n)}_{\boldsymbol{\nu}_n})_{\gamma_n}\Bigg]. \tag{3.3}$$

Here the symbols ∂_γ must be interpreted as derivatives of $f_{\boldsymbol{\nu}}$ with respect to action arguments of f if γ is an action component, as derivatives with respect to β if $\gamma=\beta$ and as multiplications by $i\boldsymbol{\nu}_i$ if $\gamma=\alpha_i$, $i=1,\ldots,N-1$. *A summation convention is conveniently adopted for pairs of repeated component labels*. In the second line no $\xi^{(k_n)}$ appears because $\xi^{(h)}$ has only angle components but H_0 does not depend on the angles.

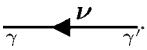
For $\boldsymbol{\nu}=\mathbf{0}$ and $\gamma\in I$ [i.e., γ an action component; cf. Remark (2) at the end of Sec. II], we use (2.6) and write

$$(X^{(k)}_{\mathbf{0}})_\gamma=-(\partial^2_I H_0(\mathbf{0},0)^{-1})_{\gamma,\gamma'-N}\delta_{\gamma'\varphi}\Bigg[\sum_{p=2}^{\infty}\sum_{\substack{k_1+\cdots k_p=k\\ \boldsymbol{\nu}_1+\cdots+\boldsymbol{\nu}_p=\mathbf{0}}}\frac{1}{p!}(E\partial)_{\gamma'}\partial_{\gamma_1\cdots\gamma_p}H_0(\mathbf{0},0)\prod_{n=1}^{p}(X^{(k_n)}_{\boldsymbol{\nu}_n})_{\gamma_n}$$
$$+\sigma\sum_{p=1}^{\infty}\sum_{\substack{k_1+\cdots k_p=k-k_0\\ \boldsymbol{\nu}_0+\boldsymbol{\nu}_1+\cdots+\boldsymbol{\nu}_p=\mathbf{0}}}\frac{1}{p!}(E\partial)_{\gamma'}\partial_{\gamma_1\cdots\gamma_p}f_{\boldsymbol{\nu}_0}(\mathbf{0},0,\beta_0)\prod_{n=1}^{p}(X^{(k_n)}_{\boldsymbol{\nu}_n}+\xi^{(k_n)}\delta_{\boldsymbol{\nu}_n\mathbf{0}})_{\gamma_n}\Bigg]. \tag{3.4}$$

For $\boldsymbol{\nu}=\mathbf{0}$ and γ an angle label the (2.2) are identically satisfied if the $\xi^{(h)}$ are determined as prescribed in Sec. II. The equation that fixes $\xi^{(h)}$ is again a relation of the type of (3.3) and (3.4) as we shall discuss in detail later.

Proceeding as in Refs. 8 and 10 we represent $(X^{(h)}_{\boldsymbol{\nu}})_\gamma$ as γ ◀—— $\boldsymbol{\nu}$ ● (k) and $\xi^{(h)}\equiv(\mathbf{0},0,\mathbf{0},\beta^{(k)})$ as γ ◀—— 0 ○ (k) and we realize that (3.3) and (3.4) can be very conveniently (as it turns out) represented by graphs of the type represented in Fig. 1.

The label $\delta_0=0,1$, that we call the *degree label* of the node to which it is associated, identifies the terms in (3.3) or (3.4) which contain inside the square brackets H_0 (then $\delta_0=0$) or f (then $\delta_0=1$). The other label attached to the first node indicates the harmonic $\boldsymbol{\nu}_0$ (mode label) selected in the terms with f (i.e., with $\delta_0=1$) and we take $\boldsymbol{\nu}_0=\mathbf{0}$ if $\delta_0=0$ (because H_0 does not depend on the angles). A further component label γ' is attached to the right extreme of the line exiting the central node in Fig. 1 and it indicates the derivative $(E\partial)_{\gamma'}$ in (3.3) and (3.4). We call a component label a "right" or "left" component label if it is attached at the beginning or at the end of the (oriented) line.

The component labels attached to the first node determine the components of the tensors defined by the derivatives of $f_{\boldsymbol{\nu}_0}$ or of H_0. The labels attached to the left extreme of each endline (to the right of the bifurcation point in the figure) determine which component of $(X^{(k_n)}_{\boldsymbol{\nu}_n})_{\gamma_n}$ is taken in the products of X's in (3.3) or (3.4). Finally the root line symbolizes the factor that is outside the square brackets in the expression (3.3) or in the expression (3.4): it will be called *propagator* of the line  . Hence the propagator of the line will be the matrix

$$\tilde{g}_{\gamma\gamma'}(\boldsymbol{\nu}) = \begin{cases} (i\boldsymbol{\omega}\cdot\boldsymbol{\nu})^{-1}\delta_{\gamma\gamma'} & \text{if } \boldsymbol{\nu}\neq\mathbf{0}, \\ -(\partial_I^2 H_0(\mathbf{0},0)^{-1})_{\gamma,\gamma'-N}\delta_{\gamma I}\delta_{\gamma'\varphi} & \text{if } \boldsymbol{\nu}=\mathbf{0}, \end{cases} \tag{3.5}$$

and $\boldsymbol{\nu}$ will be called the *momentum* of the line.

Finally the endpoints are divided into endpoints representing $X^{(h)}$ for some h, marked by bullets, and others representing $\xi^{(h)}$ marked by white disks that we shall call *leaves*.

It follows from the analysis of Sec. II that, setting β_1 equal to the constant in (2.8) and replacing $1/(k_0-1)!\partial_\beta^{k_0+1}f_{\mathbf{0}}(\mathbf{0},0,\beta_0)$ with $k_0 c$ by the definition of c before (2.7), the coefficients β_h with $h\geqslant 2$ can be derived in terms of β_1 from the relation

$$\beta_{k-2k_0+1} = \frac{1}{k_0 c\beta_1^{k_0-1}}\sum_{s\geqslant 1}\sum_{\substack{k_1+\cdots+k_s=k-k_0 \\ \boldsymbol{\nu}_0+\boldsymbol{\nu}_1+\cdots+\boldsymbol{\nu}_s=\mathbf{0}}}^{*}\frac{1}{s!}(E\partial)_B\partial_{\gamma_1\cdots\gamma_s}f_{\boldsymbol{\nu}_0}\prod_{m=1}^{s}(X^{(k_m)}_{\boldsymbol{\nu}_m}+\xi^{(k_m)}\delta_{\boldsymbol{\nu}_m\mathbf{0}})_{\gamma_m}, \tag{3.6}$$

where the derivatives of $f_{\boldsymbol{\nu}_0}$ are, as above, evaluated at $(\mathbf{0},0,\beta_0)$ and the $*$ on the sum recalls that we are excluding from the sum the contribution equal to $-k_0 c\beta_1^{k_0-1}\beta_{k-2k_0+1}$.

At this point we can repeat the construction and replace each endpoint of Fig. 1 ending in a node or in a leaf with a node into which merge several lines each of which comes out of a node or a leaf with some labels $(h),\boldsymbol{\nu},\gamma$ representing $(X^{(h)}_{\boldsymbol{\nu}})_\gamma$ for some $h,\boldsymbol{\nu},\gamma$ or, in the case of leaves, $(\xi^{(h)})_\gamma$.

Using also the relations (3.4) and (3.6), the construction can be iterated until we are left with a tree θ whose endpoints either carry a degree label 1 or are leaves representing β_1, we denote by $L(\theta)$ the set of endpoints representing such leaves. The constraint (3.6) can be automatically implied by imagining that the propagator of a line ℓ with momentum $\boldsymbol{\nu}$ is

$$g_{\gamma\gamma'}(\boldsymbol{\nu}) = \begin{cases} (i\boldsymbol{\omega}\cdot\boldsymbol{\nu})^{-1}\delta_{\gamma\gamma'} & \text{if } \boldsymbol{\nu}\neq\mathbf{0}, \\ \delta_{\gamma\gamma'} & \text{if } \boldsymbol{\nu}=\mathbf{0}, \quad \mathfrak{v}\in L(\theta), \\ -(\partial_I^2 H_0(\mathbf{0},0)^{-1})_{\gamma,\gamma'-N}\delta_{\gamma I}\delta_{\gamma'\varphi}+\dfrac{\delta_{\gamma\beta}\delta_{\gamma' B}}{\sigma\eta^{2k_0-1}k_0 c\beta_1^{k_0-1}} & \text{if } \boldsymbol{\nu}=\mathbf{0}, \quad \mathfrak{v}\notin L(\theta), \end{cases} \tag{3.7}$$

where $\mathfrak{v}$ is the node preceding ℓ on τ. We can write $(X_{\boldsymbol{\nu}})_\gamma$ as a formal power series in η, whose terms can be computed in terms of tree values. Let a tree θ be a tree diagram with nodes which look like the node drawn in Fig. 1 and let $V(\theta)$, $L(\theta)$, and $\Lambda(\theta)$ denote the sets of nodes, leaves and lines of θ, respectively. The *tree value* $\mathrm{Val}(\theta)$ will be a monomial in η obtained by multiplying

(1) a factor

$$\begin{aligned} [F(\boldsymbol{\nu}_{\mathfrak{v}})]_{\gamma'_{\ell_{\mathfrak{v}}},\boldsymbol{\gamma}(\mathfrak{v})} &= \sigma\eta^{k_0}(E\partial)_{\gamma'_{\ell_{\mathfrak{v}}}}\partial_{\gamma_{\mathfrak{v}1}\ldots\gamma_{\mathfrak{v}p_{\mathfrak{v}}}}f_{\boldsymbol{\nu}_{\mathfrak{v}}}(\mathbf{0},0,\beta_0) \quad \text{if } \delta_{\mathfrak{v}}=1, \\ [F(\boldsymbol{\nu}_{\mathfrak{v}})]_{\gamma'_{\ell_{\mathfrak{v}}},\boldsymbol{\gamma}(\mathfrak{v})} &= (E\partial)_{\gamma'_{\ell_{\mathfrak{v}}}}\partial_{\gamma_{\mathfrak{v}1}\ldots\gamma_{\mathfrak{v}p_{\mathfrak{v}}}}H_0(\mathbf{0},0) \quad \text{if } \delta_{\mathfrak{v}}=0, \end{aligned} \tag{3.8}$$

per each node $\mathfrak{v}\in V(\theta)$ into which merge $p_{\mathfrak{v}}\geqslant 1$ lines carrying component labels $\boldsymbol{\gamma}(\mathfrak{v})=(\gamma_{\mathfrak{v}1}\cdots\gamma_{\mathfrak{v}p_{\mathfrak{v}}})$ and emerges a line $\ell_{\mathfrak{v}}$ carrying a label $\gamma'_{\ell_{\mathfrak{v}}}$;

(2) a factor $\sigma\eta^{k_0}(E\partial)_{\gamma'_{\ell_\mathfrak{v}}} f_{\boldsymbol{\nu}_\mathfrak{v}}(\mathbf{0},0,\beta_0)$ per each endnode $\mathfrak{v}\notin L(\theta)$ (note that necessarily $\delta_\mathfrak{v}=1$); (3) a factor $\eta\beta_1$ per each leaf $\mathfrak{v}\in L(\theta)$ (note that necessarily $\boldsymbol{\nu}_\mathfrak{v}=\mathbf{0}$ and $\gamma_{\ell_\mathfrak{v}}=B$); (4) a factor $g_{\gamma_\ell\gamma'_\ell}(\boldsymbol{\nu})$ per line $\ell\in\Lambda(\theta)$, given by (3.7).

Note that the construction described above and in Sec. II forbids the presence in the tree diagrams of some configurations of nodes. More precisely, calling *trivial* the nodes $\mathfrak{v}$ with $p_\mathfrak{v}=1$ and $\boldsymbol{\nu}_\mathfrak{v}=\mathbf{0}$ and *b-trivial* the nodes $\mathfrak{v}$ with $p_\mathfrak{v}=k_0$, $\boldsymbol{\nu}_\mathfrak{v}=\mathbf{0}$, $\gamma'_{\ell_\mathfrak{v}}=B$ and immediately preceded by at least k_0-1 leaves, the following configurations of nodes:

(i) *trivial nodes with* $\delta_\mathfrak{v}=0$ *and the entering line with* $\mathbf{0}$ *momentum* and
(ii) *b-trivial nodes with the exiting line with* $\mathbf{0}$ *momentum and all the entering lines with left component labels equal to* β.

are not allowed, in the sense that $\mathrm{Val}(\theta)=0$ if θ contains such configurations of nodes. The reason why the trees containing such configurations of nodes are forbidden is a consequence of the use of the relations (3.4) and (3.6). Trees with no forbidden node will be called *allowed trees*

The result is that the perturbed motion runs on a $(n-1)$-dimensional torus whose equations are formally written as a sum of values of (allowed) tree diagrams, computable by using rules very similar to those listed in Ref. 10, with the value of an allowed tree θ defined as

$$\mathrm{Val}(\theta)=\frac{1}{|\Lambda(\theta)|!}\Big(\prod_{\mathfrak{v}\in V(\theta)}\varepsilon^{\delta_\mathfrak{v}}\Big)(\eta\beta_1)^{|L(\theta)|}\Big(\prod_{\mathfrak{v}\in V(\theta)}F_\mathfrak{v}\Big)\Big(\prod_{\ell\in\Lambda(\theta)}G_\ell\Big),\tag{3.9}$$

where $G_\ell:=g_{\gamma_\ell\gamma'_\ell}(\boldsymbol{\nu}_\ell)$ with $\boldsymbol{\nu}_\ell=\boldsymbol{\nu}_{\ell_\mathfrak{v}}=\Sigma_{\mathfrak{w}\preceq\mathfrak{v}}\boldsymbol{\nu}_\mathfrak{v}$, while $F_\mathfrak{v}$ is the node factor (a tensor) defined in items (1) and (2) above. In the product all the labels are summed over, except for the root label γ_{ℓ_0}, where ℓ_0 is the line entering the root. We call $\Theta^o_{k,\boldsymbol{\nu},\gamma}$ the set of trees with *degree* $|L(\theta)|+k_0\Sigma_{\mathfrak{v}\in V(\theta)}\delta_\mathfrak{v}-(2k_0-1)\Sigma_{\ell\in\Lambda(\theta)}\delta_{\boldsymbol{\nu}_\ell 0}\delta_{\gamma_\ell\beta}\delta_{\gamma'_\ell B}=k$, $\boldsymbol{\nu}_{\ell_0}=\boldsymbol{\nu}$ and $\gamma_{\ell_0}=\gamma$ (these are trees whose value is proportional to η^k). As in Ref. 15, we denote by $\Theta_{k,\boldsymbol{\nu},\gamma}$ the set of trees with k nodes, and with labels $\boldsymbol{\nu}_{\ell_0}=\boldsymbol{\nu}$ and $\gamma_{\ell_0}=\gamma$ associated with the root line.

The definitions above are given so that the formal series for X_γ is given by the sum

$$X^{(0)}_\gamma+\sum_{\boldsymbol{\nu}\in\mathbb{Z}^{N-1}}e^{i\boldsymbol{\nu}\cdot(\boldsymbol{\psi}+\boldsymbol{\omega}t)}\sum_{k=1}^{\infty}\sum_{\theta\in\Theta_{k,\boldsymbol{\nu},\gamma}}\mathrm{Val}(\theta).\tag{3.10}$$

The above rules give, order by order in powers of η, the solution of the perturbed equations of motion. In particular one can check that the trees contributing a monomial in η of degree $k\geq 1$ to the conjugating function have a number of lines that is bounded above and below proportionally to k. This is a property extensively used in the convergence analysis, for instance to show that the number of non-numbered trees of degree k is bounded by a constant to the power k; cf. Ref. 15 for details. An explicit bound is $\geq k/k_0$ and $\leq 3k_0k$, see Appendix C.

IV. ELIMINATION OF THE TRIVIAL NODES

The problem of proving convergence of the series just defined is very similar to that treated in Ref. 15. As in Ref. 15 the difficulty is that even exploiting the cancellations analogous to those of the maximal tori case, we are left with tree graphs containing chains of subdiagrams with one entering and one exiting lines, carrying the same momentum, that we call "self-energy (sub)diagrams." Naively such subdiagrams are the source of bad bounds on the kth the contribution proportional to η^k to the series. Proceeding as in in Ref. 15 we iteratively resum such chains into "renormalized propagators" and change step by step the structure of the perturbation series. At each step we define different rules to compute the tree values: we assign at each line ℓ a scale label $[n_\ell]$, with $n_\ell\geq -1$, depending on the size of its propagators, and, at the nth step ($n=0,1,\ldots$), we will not allow trees containing chains of self-energy diagrams on scale $\geq n-1$; at the same time we will assign to each line a propagator different from that in (3.7), depending on the value of its scale label, as explained below.

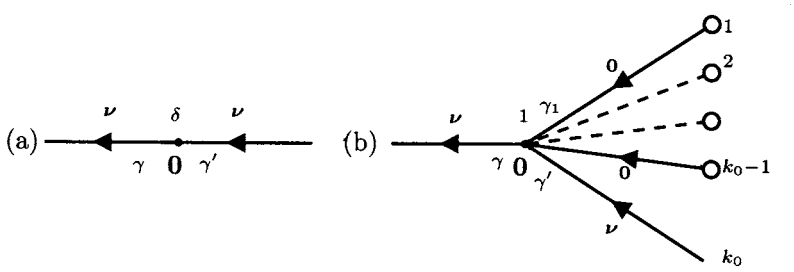


FIG. 2. Examples of lowest order self-energy clusters on scale $[-1]$. In (a) one has $\gamma=B$ and $\gamma' \in I$ or vice versa, while in (b) one has $\gamma=B$ and $\gamma'=\beta$. The order label δ in the first graph can be $\delta=0,1$. The leaves in the second graph represent factors β_1 so that they contribute to the order of the self-energy cluster with a power η^{k_0-1}.

The first step is the removal of the trivial nodes and of a class of few other subgraphs that can be present in *allowed trees*, see Sec. III, whose value is not 0. Assign, in a way similar to that described in Ref. 15, a scale label $[-1]$ to the $\mathbf{0}$-momentum propagator and let $\mathcal{S}^{\mathcal{R}}_{k,-1}$ be the set of self-energy clusters T on scale $[-1]$ and degree k (i.e. such that $k=|L(T)|+\Sigma_{\mathfrak{v}\in V(T)}\delta_{\mathfrak{v}}k_0-(2k_0-1)\Sigma_{\ell\in\Lambda(T)}\delta_{\boldsymbol{\nu}_\ell\mathbf{0}}\delta_{\gamma_\ell\beta}\delta_{\gamma'_\ell B}$), consistently with the notion of degree defined after (3.9).

A *cluster on scale* $[-1]$ is either a single node or a maximal connected set of nodes and lines, such that all the lines are on scale $[-1]$; the lines of nonzero momentum that enter or exit the nodes of the cluster are called *external lines*. A *self-energy cluster on scale* $[-1]$ is defined as a cluster on scale $[-1]$ such that there are only two external lines (one exiting and one entering), and they are connected to the same node of the cluster. This means that a self-energy cluster is formed by a node $\mathfrak{v}$ with $\mathbf{0}$-mode together with all lines (if any) of momentum $\mathbf{0}$, hence on scale $[-1]$, which are linked to $\mathfrak{v}$ by a path consisting of lines of momentum $\mathbf{0}$; see Fig. 2. *A cluster on scale* $[-1]$ *with only one exiting and one entering line, which are not connected to the same node, will not be considered a self-energy cluster on scale* $[-1]$.

The self-energy value, i.e., the value $\mathcal{V}_T(\eta)$ of the self-energy cluster T on scale $[-1]$, is defined, similarly to (3.9), as

$$\mathcal{V}_T(\eta)=\frac{1}{|\Lambda(T)|!}\Big(\prod_{\mathfrak{v}\in V(T)}\varepsilon^{\delta_{\mathfrak{v}}}\Big)(\eta\beta_1)^{|L(T)|}\Big(\prod_{\mathfrak{v}\in V(T)}F_{\mathfrak{v}}\Big)\Big(\prod_{\mathfrak{v}\in\Lambda(T)}G_\ell\Big), \tag{4.1}$$

where $V(T)$, $L(T)$, and $\Lambda(T)$ are the set of nodes, leaves, and lines, respectively, contained inside T. Then we can define

$$\mathcal{M}^{[0]}(\eta)=\sum_{k=k_0}^{\infty}\sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,-1}}\mathcal{V}_T(\eta), \tag{4.2}$$

where the sum runs over all the self-energy clusters on scale $[-1]$.

Remarks: (1) The clusters T in (4.1) and (4.2) with $k=k_0$ correspond to the trivial nodes appearing in the tree expansion of the preceding section. In the next section the general notion of cluster will be introduced.

(2) The clusters on scale $[-1]$ must contain only lines on scale $[-1]$ and there are infinitely many of them and (4.2) can be illustrated by the two clusters in Fig. 2. The self-energy values $\mathcal{V}_T(\eta)$ corresponding to the graphs in Fig. 2 give the lowest order (in powers of η) contributions to different entries of the matrix $\mathcal{M}^{[0]}$, as discussed in the caption of Fig. 2.

(3) Unlike the case in Ref. [15], Eq. (4.1), defining the matrix $\mathcal{M}^{[0]}(\eta)$, is really an infinite series; but it is still convergent, if η is sufficiently small. Convergence of the series defining $\mathcal{M}^{[0]}$ is a straightforward consequence of the fact that a self-energy cluster of degree k has a number of lines bounded by constant times k, see Appendix C, and of the fact that the propagators of the lines

with **0**-momentum can be bounded by an $O(1)$ constant if the line is preceded by a leaf or if $\gamma = I_i, \gamma' = \varphi_j$ and can be bounded by an $O(1)$ constant times η^{-2k_0+1} if the line is not preceded by a leaf and $\gamma = \beta, \gamma' = B$.

By construction, $\mathcal{M}^{[0]}(\eta)$ is real and has the following special structure:

$$\mathcal{M}^{[0]}(\eta) = \sum_{k=k_0}^{\infty} \sum_{T \in \mathcal{S}^{\mathcal{R}}_{k,-1}} \mathcal{V}_T = \begin{pmatrix} Q & R \\ P & -Q^\dagger \end{pmatrix}, \tag{4.3}$$

where the superscript dagger denotes Hermitian conjugation and P, Q, R are $N \times N$ matrices which to lowest order in η have the form [with a natural meaning of the symbols, in agreement with our convention on the component labels (3.1)]

$$P = \partial_I^2 H_0 + \varepsilon \partial_I^2 f_{\mathbf{0}}, \quad Q = \begin{pmatrix} 0 \\ -\varepsilon \partial_{\beta I} f_{\mathbf{0}} \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 \\ 0 & -\dfrac{\varepsilon \eta^{k_0-1}}{(k_0-1)!} \partial_\beta^{k_0+1} f_{\mathbf{0}} \beta_1^{k_0-1} \end{pmatrix}, \tag{4.4}$$

where $f_{\mathbf{0}}$ has $(\mathbf{0}, 0, \beta_0)$ as arguments. The complete expression, including the higher orders in η, simply replaces the *nonzero* terms in (4.4) by convergent series that we can write

$$P = \partial_I^2 H_0 + \varepsilon \bar{M}_{II}, \quad Q = \begin{pmatrix} 0 \\ -\varepsilon \bar{M}_{\beta I} \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 \\ 0 & -\varepsilon \eta^{k_0-1} \bar{M}_{\beta\beta} \end{pmatrix}, \tag{4.5}$$

where the entries $\bar{M}_{\gamma\gamma'}(\eta)$ are bounded uniformly in η, for η small enough. They can be computed order by order using the rules of the last section. *The vanishing entries of the matrix* $\mathcal{M}^{[0]}(\eta)$ *remain zero to all orders*: a property which simply follows from the definition of value of a self-energy cluster and from the remark that a derivative ∂_γ with $\gamma = \boldsymbol{\alpha}$ acting on f_0 must be interpreted as a multiplication by **0**. Note that, since P, Q, R are real and P, R are symmetric, $\mathcal{M}^{[0]}(\eta)$ satisfies the following symmetry properties:

$$E\mathcal{M}^{[0]}(\eta)E = [\mathcal{M}^{[0]}(\eta)]^T, \quad [\mathcal{M}^{[0]}(\eta)]^* = \mathcal{M}^{[0]}(\eta), \tag{4.6}$$

where $*$ denotes complex conjugation and T transposition. A consequence of (4.6) is that $\mathcal{M}^{[0]}E$ is Hermitian.

Now, we formally resum the chains of self-energy clusters on scale $[-1]$ into the new propagator

$$g^{[\geqslant 0]}(x; \eta) = \frac{1}{ix - \mathcal{M}^{[0]}(\eta)}, \tag{4.7}$$

where $x \neq 0$. This means that we modify the tree expansion described in the preceding section, the new expansion will involve only trees not containing self-energy graphs on scale $[-1]$ (and in particular containing neither trivial nor b-trivial nodes) and with the propagator of the lines with nonzero momentum replaced by (4.7). It is not clear at all that the new resummed series is well defined, on the contrary it will become clear that it is affected by divergence problems similar to those of the original series. In some sense, we just eliminated a few of the possible source of problems (that are actually an infinite class of divergent subdiagrams). However, the idea is to begin by eliminating this first few sources of problems and then, step by step, iteratively eliminate one after the other all possible sources of problems (first the less "dangerous" and then the more and more dangerous ones).

Certainly we must at least suppose that $ix - \mathcal{M}^{[0]}(\eta)$ can be inverted, otherwise the values of the trees representing the new series might even be meaningless. To give a meaning to $(ix - \mathcal{M}^{[0]}(\eta))^{-1}$ it is sufficient to impose $\det(ix - \mathcal{M}^{[0]}(\eta)) \neq 0$ for $x \neq 0$, by eliminating a denumer-

able dense set of values of η. One can compute the determinant of $(ix-\mathcal{M}^{[0]}(\eta))$, finding $\det(ix-\mathcal{M}^{[0]}(\eta))=-(ix)^{2(N-1)}\cdot[x^2+\varepsilon\eta^{k_0-1}\bar{M}_{\beta\beta}(\partial^2_{BB}H_0+\varepsilon\bar{M}_{BB})+\varepsilon^2|\bar{M}_{\beta B}|^2]$, so that the condition of invertibility of $(ix-\mathcal{M}^{[0]}(\eta))$ for $x\neq 0$ becomes

$$x^2+\varepsilon\eta^{k_0-1}\bar{M}_{\beta\beta}(\partial^2_{BB}H_0+\varepsilon\bar{M}_{BB})+\varepsilon^2|\bar{M}_{\beta B}|^2\neq 0 \tag{4.8}$$

for all $x=\boldsymbol{\omega}\cdot\boldsymbol{\nu}$, $\boldsymbol{\nu}\in\mathbb{Z}^{N-1}$. In computing $\det(ix-\mathcal{M}^{[0]}(\eta))$ the property $\bar{M}_{\beta B}=-\bar{M}_{B\beta}\in\mathbb{R}$ has been used.

If η is chosen according to (4.8), we have that the norm of $g^{[\geq 0]}(x;\eta)$ is equal to the eigenvalue of $[ix-\mathcal{M}^{[0]}(\eta)]E$ with smallest absolute value, this is because $\|ix-\mathcal{M}^{[0]}(\eta)\|=\|(ix-\mathcal{M}^{[0]}(\eta))E\|$ and, as remarked after (4.6), $(ix-\mathcal{M}^{[0]}(\eta))E$ is Hermitian. Here and in the following we use the uniform norm, given a $2N\times 2N$ complex matrix g, we define $\|g\|=\sup_{z\in\mathbb{C}^{2N},|z|=1}|gz|$, where $|z|=\Sigma_{i=1}^{2N}|z_i|$.

An approximate computation of the eigenvalues of $[ix-\mathcal{M}^{[0]}(\eta)]E$, see Appendix D, implies the following result.

Lemma 2: *There exists an* $O(1)$ *constant* $\rho>0$ *such that if* $x^2>\rho\eta^{2k_0-1}$ *then the resummed propagator* $g^{[\geq 0]}(x;\eta)$ *in (4.7) can be bounded as*

$$|g^{[\geq 0]}(x;\eta)|\leq\max\left\{\frac{2\mu_N^{(0)}}{x^2},\frac{2}{\mu_1^{(0)}}\right\}, \tag{4.9}$$

where $\mu_1^{(0)}$ *and* $\mu_N^{(0)}$ *are, respectively, the minimum and maximum eigenvalues of* P, *see (4.3) and (4.5).*

From now on we shall proceed following. Ref. [15]. First we assume that $|\varepsilon|$ is in an interval $(\bar{\varepsilon}/4,\bar{\varepsilon}]$ such that, by setting $\bar{\varepsilon}=\bar{\eta}^{k_0}$, we can define the integer n_0 through

$$C_0^2 2^{-2(n_0+1)}<\rho\bar{\varepsilon}\,\bar{\eta}^{k_0-1}\leq C_0^2 2^{-2n_0}, \tag{4.10}$$

with ρ as in Lemma 2.

In the first range of scales (in which $x^2\geq 2C_0^2 2^{-2n_0}$) the small denominators can be bounded by the "classical" small divisor x^2 and we proceed as described in the section "Non-resonant resummations" of Ref. [15].

For smaller scales we shall see below that the small divisor will bounded below by an $O(1)$ constant times $\min\{x^2,|x^2+\varepsilon\eta^{k_0-1}\lambda^{[n]}(x;\varepsilon)|\}$, with $\lambda^{[n]}(x;\varepsilon)$ a suitable $O(1)$ function. However here the distinction between the *hyperbolic* case $[\varepsilon\eta^{k_0-1}\lambda^{[n]}(x;\varepsilon)>0]$ and the *elliptic* one $[\varepsilon\eta^{k_0-1}\lambda^{[n]}(x;\varepsilon)<0]$ must be made, in the hyperbolic case the small divisors will be always bounded by an $O(1)$ constant times x^2, even for $x^2\leq O(\varepsilon\eta^{k_0-1})$, while in the elliptic case we will have to proceed differently, essentially as described in the section "Infrared resummations" of Ref. [15].

V. MULTISCALE ANALYSIS AND NONRESONANT RESUMMATION

The resummations will be defined via trees with no self-energy clusters on scale $[-1]$ and with lines bearing further labels. Moreover the definition of propagator will be changed, hence the values of the trees will be different from the ones in Sec. III, they are constructed recursively as follows.

We introduce a *multiscale decomposition* (see Ref. [15]), we call $\psi(D)$ a C^∞ nondecreasing compact support function defined for $D\geq 0$,

$$\psi(D)=1\quad\text{for } D\geq C_0^2,\quad \psi(D)=0\quad\text{for } D\leq C_0^2/4, \tag{5.1}$$

where C_0 is the Diophantine constant of $\boldsymbol{\omega}$, and let $\chi(D)=1-\psi(D)$. Define also $\psi_n(D)=\psi(2^{2n}D)$ and $\chi_n(D)=\chi(2^{2n}D)$ for all $n\geq 0$. Hence $\psi_0=\psi,\chi_0=\chi$ and

$$1 \equiv \psi_n(D(x)) + \chi_n(D(x)) \quad \text{for all } n \geqslant 0, \tag{5.2}$$

for all choices of the function $D(x) \geqslant 0$, in particular for $D(x) = x^2$, that we shall now use.

A simple way to represent the value of a tree as sum of many terms is to make use of the identity in (5.2). The resummed propagator $g^{[\geqslant 0]}(x;\eta) := (ix - \mathcal{M}^{[0]}(\eta))^{-1}$ of each line with non-zero momentum (hence with $x \neq 0$) is written as

$$g^{[\geqslant 0]}(x;\eta) = \psi_0(x^2) g^{[\geqslant 0]}(x;\eta) + \chi_0(x^2) g^{[\geqslant 0]}(x;\eta) := g^{[0]}(x;\eta) + g^{\{\geqslant 1\}}(x;\eta), \tag{5.3}$$

and we note that $g^{[0]}(x;\eta)$ vanishes if x^2 is smaller than $(C_0/2)^2$.

If we replace each $g^{[\geqslant 0]}(x;\eta)$ with the sum in (5.3) then the value of each tree with k nodes is split as a sum of up to 2^k terms which can be identified by affixing on each line with momentum $\boldsymbol{\nu} \neq \mathbf{0}$ a label $[0]$ or $\{\geqslant 1\}$. Further splittings of the tree values can be achieved as follows.

Definition 2 (Propagators): *Let n_0 be an integer, and for $1 \leqslant p < n_0$, give $2N \times 2N$ matrices $\mathcal{M}^{[p]}(x;\eta)$ satisfying the symmetry properties*,

$$E\mathcal{M}^{[p]}(x;\eta)E = [\mathcal{M}^{[p]}(-x;\eta)]^T, \quad [\mathcal{M}^{[p]}(x;\eta)]^* = \mathcal{M}^{[p]}(-x;\eta). \tag{5.4}$$

Let $\mathcal{M}^{[0]}(x;\eta) \equiv \mathcal{M}^{[0]}(\eta)$ and $\mathcal{M}^{[\leqslant n]}(x;\eta) = \Sigma_{p=0}^{n} \mathcal{M}^{[p]}(x;\eta)$. Define for $n_0 \geqslant n \geqslant 1$ the propagators

$$g^{[n-1]}(x;\eta) := \frac{\psi_n(x^2) \prod_{m=0}^{n-1} \chi_m(x^2)}{ix - \mathcal{M}^{[\leqslant n-1]}(x;\eta)},$$

$$g^{\{\geqslant n\}}(x;\eta) := \frac{\prod_{m=0}^{n-1} \chi_m(x^2)}{ix - \mathcal{M}^{[\leqslant n-1]}(x;\eta)},$$

$$g^{[\geqslant n]}(x;\eta) := \frac{\prod_{m=0}^{n-1} \chi_m(x^2)}{ix - \mathcal{M}^{[\leqslant n]}(x;\eta)}, \tag{5.5}$$

and $g^{[0]}(x;\eta) = \psi_0(x^2)(ix - \mathcal{M}^{[0]}(\eta))^{-1}$. We call the labels $[n], \{\geqslant n\}, [\geqslant n]$ scale labels.

Remarks: (1) The matrices $\mathcal{M}^{[p]}(x;\eta)$ will be defined recursively under the requirement that the functions $(\mathbf{A}, B, \mathbf{a}, b)$ defining the parametric equations (2.1) of the invariant torus will be expressed in terms of trees whose lines carry scale labels indicating that their values are computed with the propagators in (5.5).

(2) To have the propagators in (5.5) well defined, we must eliminate for each value of p a denumerable set of ε's, by imposing that $(ix - \mathcal{M}^{[\leqslant p]}(x;\eta))$ be invertible, in analogy with (4.8).

(3) So far n_0 can be any integer number. It will be fixed as prescribed after Lemma 2, in such a way that a bound like (4.9) will hold for all propagators $g^{[p]}$ with $p < n_0$.

To define recursively the matrices we introduce the notions of clusters and of self-energy clusters of a tree whose lines and nodes carry the same labels introduced so far and *in addition* each line carries a scale label which can be either $[-1]$, if the momentum of the line is zero, or $[p]$, with $0 \leqslant p < n_0$, or $[\geqslant n_0]$, with n_0 the same integer appearing in the statement of Definition 2 (still to be suitably fixed). Given a tree θ decorated in this way we give the following definition, for $n < n_0$.

Definition 3 (clusters): *(i) A cluster T on scale $[n]$, with $0 \leqslant n$, is a maximal set of nodes and lines connecting them with propagators on scales $[p]$, $p \leqslant n$, one of which, at least, on scale exactly $[n]$. We denote with $V(T)$, $L(T)$,* and $\Lambda(T)$ *the set of nodes, the set of leaves and the set of lines, respectively, contained in T. The number of nodes in T will be denoted by k_T.*

(ii) The $m_T \geqslant 0$ lines entering the cluster T and the possible line coming out of it (unique if existing at all) are called the external lines *of the cluster T.*

(iii) Given a cluster T on scale $[n]$, we shall call $n_T = n$ its scale.

Remarks: (1) The clusters on scale $[-1]$ were defined before (4.1), they can contain either only

lines with scale $[-1]$ or no line at all (i.e., they can contain just a single node).

(2) Here $n<n_0$. However the definition above is given in such a way that it will extend unchanged when also scales equal to or larger than n_0 will be introduced.

(3) The clusters of a tree can be regarded as sets of lines hierarchically ordered by inclusion and have hierarchically ordered scales.

(4) A cluster T is not a tree (in our sense); however we can uniquely associate a tree with it by adding the entering and the exiting lines and by imagining that the lower extreme of the exiting line is the root and that the highest extremes of the entering lines are nodes carrying a mode label equal to the momentum flowing into them (cf. Ref. [15], Fig. 3).

Definition 4 (self-energy clusters): A self-energy cluster *on scale* $[n]$, *with* $n\geqslant 0$, *of a tree* θ *will be any cluster* T *on scale* $[n]$ *with the following properties:*

(i) *T has only one entering line ℓ_T^2 and one exiting line ℓ_T^1;*
(ii) $\Sigma_{\mathbf{v}\in V(T)}\boldsymbol{\nu}_{\mathfrak{v}}=\mathbf{0}$;
(iii) *there is no line on scale $[-1]$ along the path connecting ℓ_T^2 to ℓ_T^1.*

We call k_T the number of nodes in $V(T)$.

Remarks: (1) The essential property of a self-energy cluster is that it has necessarily just one entering line and one exiting line, and both have *equal momentum* (because $\Sigma_{\mathfrak{v}\in V(T)}\nu_{\mathfrak{v}}=\mathbf{0}$). Note that both scales of the external lines of a self-energy cluster T are strictly larger than the scale of T regarded as a cluster, but they can be different from each other by just one unit.

(2) The self-energy clusters on scale $[-1]$ were defined before (4.1).

(3) For $n\geqslant 0$, the number of nodes of any self-energy cluster on scale $[n]$ is $\geqslant 2$, and the corresponding degree is $\geqslant 2k_0$. This can be seen as follows. Call T_0 the connected subset of T containing no line on scale $[-1]$ and containing the two nodes to which the external lines are attached. Then T_0 must have at least two nodes with $\delta=1$, and $T\backslash T_0$ is the union of subtrees with positive degree.

(4) The clusters which satisfy properties (i) and (ii), but not (iii) are not considered self-energy clusters. The same happened for the self-energy clusters on scale $[-1]$. The reason for such a definition is that the cancellation mechanisms that will imply the bounds needed on the derivatives of the self-energy values (see next definition and Lemma 3 below) can be derived only under such an extra condition. On the other hand, the clusters which verify only the first two properties, but contain lines on scale $[-1]$ along the path connecting the external lines, require no resummation, and can be dealt with in the same way as the other clusters which are not self-energy clusters. We note that in Ref. [15] property (iii) was explicitly required only for self-energy clusters on scale $[-1]$ but it was not mentioned any more for the others, the proofs in Ref. [15] however, implicitly used property (iii) also for the self-energy clusters on scale >-1.

Definition 5 (renormalized trees): Let $\Theta^{\mathcal{R}}_{k,\boldsymbol{\nu},\gamma}$ *be the set of trees with degree k [see comments after (3.9)], root line momentum* $\boldsymbol{\nu}$ *and root label* γ *which contain no self-energy clusters. Such trees will be called* renormalized trees.

Definition 6 (self-energy matrices): *(i) We denote with $\mathcal{S}^{\mathcal{R}}_{k,n}$ the set of self-energy clusters with degree k and scale $[n]$ which do not contain other self-energy clusters; we call them* renormalized self-energy clusters *on scale n.*

(ii) Given a self-energy cluster $T\in\mathcal{S}^{\mathcal{R}}_{k,n}$ we shall define the self-energy value *of T as the matrix*[1]

$$\mathcal{V}_T(\boldsymbol{\omega}\cdot\boldsymbol{\nu};\eta)=\frac{1}{|\Lambda(T)|!}\Big(\prod_{\mathfrak{v}\in V(T)}\varepsilon^{\delta_{\mathfrak{v}}}\Big)(\eta\beta_1)^{|L(T)|}\Big(\prod_{\mathfrak{v}\in V(T)}F_{\mathfrak{v}}\Big)\Big(\prod_{\ell\in\Lambda(T)}g_\ell^{[n_\ell]}\Big),\tag{5.6}$$

where $g_\ell^{[n_\ell]}=g^{[n_\ell]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\eta)$. Note that, necessarily, $n_\ell\leqslant n$. The k_T-1 lines of the self-energy cluster T will be imagined as distinct and to carry a number label ranging in $\{1,\dots,k_T-1\}$.

[1]This is a matrix because the self-energy cluster inherits the labels γ,γ' attached to the endnote of the entering line and to the initial node of the existing line

(iii) The self-energy matrices $\mathcal{M}^{[n]}(x;\eta)$, $n\geqslant 1$, *will be defined recursively as*

$$\mathcal{M}^{[n]}(x;\eta)=\left(\prod_{p=0}^{n-1}\chi_p(x^2)\right)\sum_{k=2k_0}^{\infty}\sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,n-1}}\mathcal{V}_T(x;\eta)\coloneqq\left(\prod_{p=0}^{n-1}\chi_p(x^2)\right)M^{[n]}(x;\eta), \tag{5.7}$$

where the self-energy values are evaluated by means of the propagators on scales $[p]$, *with* $p=-1,0,\ldots,n$.

The definition (5.7) makes sense because we have already defined the propagators on scale $[0]$ and the matrices $\mathcal{M}^{[0]}(x;\eta)\equiv\mathcal{M}^{[0]}(\eta)$ (cf. Definition 2). Of course we must still check that the series converges.

With the above new definitions let $h_{\boldsymbol{\nu},\gamma}$ with $\gamma=\mathbf{A},B,\boldsymbol{\alpha},\beta$ be the values of $A_{\boldsymbol{\nu}},B_{\boldsymbol{\nu}},\mathbf{a}_{\boldsymbol{\nu}},b_{\boldsymbol{\nu}}$. We have the formal identities

$$h_{\boldsymbol{\nu},\gamma}=\sum_{k=1}^{\infty}\sum_{\theta\in\Theta^{\mathcal{R}}_{k,\boldsymbol{\nu},\gamma}}\mathrm{Val}(\theta), \tag{5.8}$$

where we have redefined the *value* of a tree $\theta\in\Theta^{\mathcal{R}}_{k,\boldsymbol{\nu},\gamma}$ as

$$\mathrm{Val}(\theta)=\frac{1}{|\Lambda(\theta)|!}\left(\prod_{\mathfrak{v}\in V(\theta)}\varepsilon^{\delta_{\mathfrak{v}}}\right)(\eta\beta_1)^{|L(T)|}\left(\prod_{\ell\in\Lambda(\theta)}g^{[n_\ell]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\eta)\right)\left(\prod_{\mathfrak{v}\in V(\theta)}F_{\mathfrak{v}}\right), \tag{5.9}$$

with $[n_\ell]=[-1],[0],\ldots,[n_0-1],[\geqslant n_0]$. Note that (5.8) is not a power series in η.

The statement in (5.8) is checked to be an identity between formal series (as in the corresponding check in Ref. [15]).

As a first step to bypass the formal level, the series (5.7) defining $M^{[n]}(x;\eta)$ must be shown to be really convergent. This will be true because in the evaluation of $M^{[n]}(x;\eta)$ *the only involved propagators have scales* $[p]$ *with* $p\leqslant n-1$ so that, see the factors $\psi_n(x^2),\chi_n(x^2)$ in (5.5), their denominators not only do not vanish but have controlled sizes that can be bounded below proportionally to x^2 by (4.9), i.e., simply by a constant times $C_0^2|\boldsymbol{\nu}|^{-2\tau_0}$. Using this fact one can actually show that the matrices $M^{[n]}(x;\eta)$ are well defined and satisfy symmetry properties similar to (5.4).

Furthermore *cancellations* similar to the maximal KAM tori cancellations hold even in this case so that $M^{[n]}(x;\eta)$ has a special structure, as described in the following Lemma (see Appendixes E and F for a proof).

Lemma 3: *Let* $\bar{\varepsilon}<\varepsilon_0$ *with* ε_0 *small enough, and* $\varepsilon\in I(\bar{\varepsilon})=(\bar{\varepsilon}/4,\bar{\varepsilon}]$. *Define also* $\bar{\eta}$ *through* $\bar{\varepsilon}=\bar{\eta}^{k_0}$. *If* $1\leqslant n<n_0$, *with* n_0 *defined in (4.10), the following properties hold.*

(i) The series defining the matrices $\mathcal{M}^{[\leqslant n]}(x;\eta)$, $x=\boldsymbol{\omega}\cdot\boldsymbol{\nu}$, *converge and the matrices satisfy the same symmetry properties noted for* $\mathcal{M}^{(0)}$,

$$E\mathcal{M}^{[\leqslant n]}(x;\eta)E=[\mathcal{M}^{[\leqslant n]}(-x;\eta)]^T,\quad[\mathcal{M}^{[\leqslant n]}(x;\eta)]^*=\mathcal{M}^{[\leqslant n]}(-x;\eta), \tag{5.10}$$

where E *is the* $2N\times 2N$ *symplectic matrix (1.4). Hence, by (5.10),* $(ix-\mathcal{M}^{[\leqslant n]})E$ *is Hermitian.*

(ii) The matrix $\mathcal{M}^{[\leqslant n]}(x;\eta)$ *can be written in the form*

$$\begin{pmatrix} Q^{[\leqslant n]}(x;\eta) & R^{[\leqslant n]}(x;\eta)\\ P^{[\leqslant n]}(x;\eta) & -Q^{[\leqslant n]\dagger}(x;\eta)\end{pmatrix}, \tag{5.11}$$

where, if $\chi_{n-1}(x^2)\neq 0$,

$$P^{[\leqslant n]}(x;\eta)=\begin{pmatrix}\partial^2_{\mathbf{AA}}H_0+\varepsilon\bar{M}^{[\leqslant n]}_{\mathbf{AA}}(x;\eta) & \partial^2_{\mathbf{A}B}H_0+\varepsilon\bar{M}^{[\leqslant n]}_{\mathbf{A}B}(x;\eta)\\ \partial^2_{B\mathbf{A}}H_0+\varepsilon\bar{M}^{[\leqslant n]}_{B\mathbf{A}}(x;\eta) & \partial^2_{BB}H_0+\varepsilon\bar{M}^{[\leqslant n]}_{BB}(x;\eta)\end{pmatrix}=[P^{[\leqslant n]}(x;\eta)]^\dagger,$$

$$Q^{[\leqslant n]}(x;\varepsilon)=\begin{pmatrix} ix\varepsilon^2\bar{M}^{[\leqslant n]}_{\boldsymbol{\alpha}\boldsymbol{\Lambda}}(x;\eta) & ix\varepsilon^2\bar{M}^{[\leqslant n]}_{\boldsymbol{\alpha}B}(x;\eta) \\ \varepsilon\bar{M}^{[\leqslant n]}_{\beta\boldsymbol{\Lambda}}(x;\eta) & \varepsilon\bar{M}^{[\leqslant n]}_{\beta B}(x;\eta)\end{pmatrix}, \tag{5.12}$$

$$R^{[\leqslant n]}(x;\varepsilon)=\begin{pmatrix} x^2\varepsilon^2\bar{M}^{[\leqslant n]}_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(x;\eta) & ix\varepsilon^2\bar{M}^{[\leqslant n]}_{\boldsymbol{\alpha}\beta}(x;\eta) \\ -ix\varepsilon^2\bar{M}^{[\leqslant n]}_{\beta\boldsymbol{\alpha}}(x;\eta) & \varepsilon\eta^{k_0-1}\bar{M}^{[\leqslant n]}_{\beta\beta}(x;\eta)\end{pmatrix}=[R^{[\leqslant n]}(x;\eta)]^{\dagger}.$$

(iii) The entries $\bar{M}^{[\leqslant n]}_{\gamma,\gamma'}$ *are such that the corrections* $\bar{M}^{[n]}_{\gamma,\gamma'}(x;\eta)=\bar{M}^{[\leqslant n]}_{\gamma,\gamma'}(x;\eta)-\bar{M}^{[\leqslant n-1]}_{\gamma,\gamma'}(x;\eta)$ *are bounded, uniformly in* x *and* ε *for* ε *small enough, by* $Be^{-\kappa_1 2^{n/\tau}}$ *for* $n<n_0$ *and for suitable* n_0*-independent constants* $B,\kappa_1,\tau>0$; *one can take* $\tau=\tau_0$.

(iv) One has

$$\|\partial_x\mathcal{M}^{[\leqslant n]}(x,\eta)\|\leqslant B\varepsilon^2,\quad \|\partial_\varepsilon[\mathcal{M}^{[\leqslant n]}(x,\eta)-\mathcal{M}^{[0]}(x,\eta)]\|\leqslant B\varepsilon, \tag{5.13}$$

where the derivatives must be interpreted in the sense of Whitney and the constants $B,\kappa_1,\tau>0$ *can be taken the same as in item (iii).*

Remarks: (1) The symmetry property (5.10) is proved in Appendix E. Note that at the first step $\mathcal{M}^{[0]}(x;\eta)$ satisfies it, see (4.6).

(2) The key property in (5.12) is that some entries of $Q^{[\leqslant n]}(x;\eta)$ and $R^{[\leqslant n]}(x;\eta)$ are proportional to x or x^2, this is proved by exploiting cancellations among families of self-energy clusters, as described in detail in Appendix F; note that the single self-energy clusters contributing to $\mathcal{M}^{[\leqslant n]}(x;\eta)$ do not have in general the structure in (5.12) and only their sum has.

A crucial technical point in the proof of Lemma 3 is the fact that, if the scale n_ℓ of a line ℓ is smaller than n_0, as defined in (4.10), then the corresponding propagator admits a bound that is qualitatively the same as (4.9). More precisely the following result holds.

Lemma 4: *Let* $\varepsilon\in(\bar{\varepsilon}/4,\bar{\varepsilon}]$. *The propagator* $g^{[0]}(x;\eta)$ *admits the same bound as* $g^{[\leqslant 0]}(x;\eta)$ *in (4.9). For* $1\leqslant n<n_0$, *with* n_0 *given by (4.10), the propagator on scale* $[n]$ *can be bounded by*

$$|g^{[n]}(x;\eta)|\leqslant\frac{C}{x^2}, \tag{5.14}$$

for some positive constant C.

The proof of Lemma 4 proceeds as that of Lemma 2, in Appendix D, and we do not repeat it here. Once the bound (5.14) is established, the proof of convergence is the same as the one discussed in Appendix A3 of Ref. 15 and we do not repeat it here. Item (ii) of Lemma 3 simply follows from convergence and from the remark that $\mathcal{M}^{[\leqslant n]}(x;\eta)-\mathcal{M}^{[0]}(x;\eta)$ is of order ε^2 [cf. Remark (3) after Definition 4]. The bounds in items (iii) and (iv) of Lemma 3 also follow from the proof of convergence, see Appendix A3 of Ref. 15.

We have therefore constructed a new representation of the formal series for the parametric equations for the invariant torus, in it only trees with lines carrying a scale label $[-1],[0],\ldots,[n_0-1]$ or $[\geqslant n_0]$ and *no self-energy clusters* are present (note that, so far, self-energy clusters may have only scales $[n]$ with $n<n_0$). The above lemma will be the starting block of the construction that follows.

VI. RENORMALIZATION: THE INFRARED RESUMMATION

From the proof of Lemma 2 it is clear that for $x^2\leqslant\rho\eta^{2k_0-1}$ and $n\geqslant n_0$ it will not be possible to bound $g^{[n]}(x;\eta)$ by a constant times x^{-2}.

So, the first problem to face when reaching scales $n\geqslant n_0$ is the computation of the eigenvalues of $(ix-\mathcal{M}^{[\leqslant n]}(x;\eta))E$, in terms of which an estimate of the size of the propagator $g^{[n]}$ can be deduced.

If $\mathcal{M}^{[\leqslant n]}(x;\eta)$ does have the structure in (5.12) then an approximate computation of the eigenvalues of $(ix-\mathcal{M}^{[\leqslant n]})E$ leads to the following Lemma, proved in Appendix G.

Lemma 5: *Let* $n\geqslant n_0$ *and let us assign a matrix* $\mathcal{M}^{[\leqslant n]}(x;\eta)$ *satisfying the properties in (5.12)*

admitting right and left derivatives with respect to x and ε, *bounded as the derivatives in (5.13), and having the structure described by (5.12), with the entries* $\bar{M}^{[\le n]}_{\gamma,\gamma'}(x;\eta)$ *such that the corrections* $\bar{M}^{[n]}_{\gamma,\gamma'}(x;\eta)=\bar{M}^{[\le n]}_{\gamma,\gamma'}(x;\eta)-\bar{M}^{[\le n-1]}_{\gamma,\gamma'}(x;\eta)$ *can be bounded [as in item (iii) of Lemma 3] by* $|\bar{M}^{[n]}_{\gamma,\gamma'}(x;\eta)|\le Be^{-\kappa_1 2^{n/\tau_1}}$, *for suitable constants B,* κ_1, *and* τ_1. *Then the uniform norm of* $(ix-\mathcal{M}^{[\le n]}(x;\eta))$ *can be bounded below by*

$$\|ix-\mathcal{M}^{[\le n]}(x;\eta)\| \ge \frac{1}{4\mu}\min\{x^2,|x^2-\lambda^{[n]}(x;\eta)|\}, \tag{6.1}$$

where $\mu=\mu_N^{(0)}$ *is the largest eigenvalue of* $P^{[0]}$ *and* $\lambda^{[n]}(x;\eta)=\ell^{[n]}(x;\eta)\varepsilon\eta^{k_0-1}$ *is a real function with* $\ell^{[n]}(x;\eta)=ck_0\partial_{BB}^2 H_0\beta_1^{k_0-1}(1+O(\eta))$. *Furthermore* $\lambda^{[n]}(x;\eta)$ *is right and left differentiable in* ε *and x and the derivatives satisfy the following dimensional bounds:*

$$C^{-1}\eta^{k_0-1}\le|\partial_\varepsilon^{\pm}\lambda^{[n]}(x;\eta)|\le C\eta^{k_0-1},\quad |\partial_x^{\pm}\lambda^{[n]}(x;\eta)|\le C\eta^{k_0}, \tag{6.2}$$

for some positive constant C.

Remarks: (1) The bound (6.1) suggests to replace the classical small divisor x^2 used in the preceding sections by the (n-dependent) quantity $\min\{x^2,|x^2-\lambda^{[n]}(x;\eta)|\}$, that is essentially what we shall do below. In particular we shall replace the argument x^2 of the support functions ψ,χ by a quantity $\Delta^{[n]}(x;\eta)$, behaving like $\min\{x^2,|x^2-\lambda^{[n]}(x;\eta)|\}$, which will be the measure of the strength of the resonance for scales larger than n_0. With this choice we shall in general introduce a singularity in the definition of the propagators and self-energy matrices on scales $n\ge n_0$, this is due to the presence of a minimum and of an absolute value in the definition of $\Delta^{[n]}(x;\eta)$. This is ultimately why in (6.2) the right and left derivatives appear, rather than the plain derivatives, as in (5.13) above. This could be avoided by using a smoothed version of the quantity $\Delta^{[n]}(x;\eta)$ introduced below, but we shall not discuss it here.

(2) The bound on the derivatives of $\lambda^{[n]}(x;\eta)$ with respect to ε follows from the expression of $\mathcal{M}^{[0]}(\eta)$, in (4.3)–(4.5), and from the bounds (5.13), which allow to control the corrections. On the contrary the bound on the derivatives of $\lambda^{[n]}(x;\eta)$ with respect to x does not follow directly from (5.13), and it is explained in Appendix G.

Depending on the sign of ε, from now on, the analysis changes qualitatively. If ε is such that $c\varepsilon\beta_1^{k_0-1}<0$ [so that $\lambda^{[n]}(x;\eta)$ in (6.1) is negative], the minimum in (6.1) is always realized by the classical small divisor x^2. This implies that in this range of scales it is possible to proceed in the same way discussed above in Sec. V. We do not repeat the details, and we concentrate on the opposite case, namely ε with the sign such that $\lambda^{[n]}(x;\eta)>0$, which presents new difficulties.

In this case convergence problems can still arise from the propagators $g^{[\ge n_0]}(x;\eta)$, which become uncontrollably large for $x=\boldsymbol{\omega}\cdot\boldsymbol{\nu}$ close to the eigenvalue $\lambda^{[n]}(x;\eta)$ in (6.1).

We introduce a sequence of *self-energies* $\underline{\lambda}^{[n]}(\eta)$, Ref. 15 representing the locations of the singularities of $ix-\mathcal{M}^{[\le n]}(x;\eta)$ and, correspondingly, we introduce a sequence of *propagator divisors* $\Delta^{[n]}(x;\eta)$, which will give a bound for the size of the propagator on scale $n\ge n_0$. Then, we modify the scale decomposition, measuring the strength of the singularity in terms of $\Delta^{[n]}(x;\eta)$ rather than, as done in Sec. V, in terms of the classical small divisor x^2.

The choice of the scale decomposition will be done in such a way that the dimensional bounds for the propagators will be the same as for those with scales $n<n_0$, this will reduce the analysis of the infrared resummations to the same convergence proof discussed in Appendix C of Ref. 15.

We introduce the following definition.

Definition 7 (self-energies and propagator divisors): *Let the function* $\lambda^{[n]}(x;\eta)$ *be as in Lemma 5.*

(i) The sequence of self-energies $\underline{\lambda}^{[n]}(\eta)$ *is defined for* $n\ge n_0$ *by*

$$\underline{\lambda}^{[n]}(\eta):=\lambda^{[n]}(\sqrt{\underline{\lambda}^{[n-1]}(\eta)},\eta),\quad \underline{\lambda}^{[n_0]}(\eta):=\lambda^{[n_0]}(0;\eta), \tag{6.3}$$

provided $\underline{\lambda}^{[n]}(\eta)\ge 0$, $n\ge n_0$.

(ii) The propagator divisors *are defined for* $n\ge n_0$ by

$$\Delta^{[n]}(x;\eta) := \min\{x^2, |x^2 - \underline{\lambda}^{[n]}(\eta)|\}. \tag{6.4}$$

By repeating the analysis of Sec. V we can represent the function $X(\boldsymbol{\psi})$ via sums of values of trees whose lines can carry scale labels $[-1],[0],\dots,[n_0-1],[n_0],[n_0+1],\dots$, and which contain no self-energy clusters (i.e., they are renormalized trees; see Definition 5 in Sec. V). The new propagators will be defined by the same procedure used to eliminate the self-energy clusters on scales $[n]$ with $n \leqslant n_0-1$. However for $n \geqslant n_0$ the scale of a line will be determined in terms of the recursively defined $\Delta^{[n]}(x;\eta)$, (6.4), rather than in terms of x^2, see (5.2).

Set $X_{n_0-1}(x) := \Pi_{m=0}^{n_0-1}\chi_m(x^2)$, $Y_n(x;\eta) := \Pi_{m=n_0}^{n}\chi_m(\Delta^{[m]}(x;\eta))$ for $n \geqslant n_0$ and $Y_{n_0-1} \equiv 1$. The definition of the new propagators will be

$$\begin{aligned} g^{[n_0]} &:= X_{n_0-1}(x)\psi_{n_0}(\Delta^{[n_0]}(x;\eta))(x^2 - \mathcal{M}^{[\leqslant n_0]}(x;\eta))^{-1}, \\ g^{[n_0+1]} &:= X_{n_0-1}(x)\chi_{n_0}(\Delta^{[n_0]}(x;\eta))\psi_{n_0+1}(\Delta^{[n_0+1]}(x;\eta))(x^2 - \mathcal{M}^{[\leqslant n_0+1]}(x;\eta))^{-1}, \\ &\dots, \\ g^{[n]} &:= X_{n_0-1}(x)Y_{n-1}(x;\eta)\psi_n(\Delta^{[n]}(x;\eta))(x^2 - \mathcal{M}^{[\leqslant n]}(x;\eta))^{-1}, \end{aligned} \tag{6.5}$$

and so on, using indefinitely the identity $1 \equiv \psi_n(\Delta^{[n]}(x;\eta)) + \chi_n(\Delta^{[n]}(x;\eta))$ to generate the new propagators.

In this way we obtain a formal representation of $X(\boldsymbol{\psi})$ as a sum of tree values in which only renormalized trees appear and in which each line ℓ carries a *scale label* $[n_\ell]$. This means that we can formally write $X(\psi)$ as in (5.8), with $\mathrm{Val}(\theta)$ defined according to (5.9), but now the scale label $[n_\ell]$ is such that n_ℓ can assume all integer values $\geqslant -1$, and no line carries a scale label like $[\geqslant n]$: *only scale labels* $[n]$ *are possible*.

We can summarize the discussion above in the following definition.

Definition 8 (propagators and self-energy matrices): *Given a sequence of* $2N\times 2N$ *matrices* $\mathcal{M}^{[\leqslant m]}(x;\eta)$, $m \geqslant 1$, *let* $\mathcal{M}^{[n]}(x;\eta) = \mathcal{M}^{[\leqslant n]}(x;\eta) - \mathcal{M}^{[\leqslant n-1]}(x;\eta)$ *with* $\mathcal{M}^{[\leqslant 0]}(x;\eta) \equiv \mathcal{M}^{[0]}(\eta)$ [see (4.2)], *so that* $\mathcal{M}^{[\leqslant n]}(x;\eta) = \Sigma_{m=0}^{n}\mathcal{M}^{[m]}(x;\eta)$. *Setting* $\Delta^{[n]}(x;\eta) \equiv x^2$ *if* $n < n_0$, *define for all* $n \geqslant 0$

$$g^{[n]}(x;\eta) = \frac{\psi_n(\Delta^{[n]}(x;\eta))\prod_{m\geqslant 0}^{n-1}\chi_m(\Delta^{[m]}(x;\eta))}{x^2 - \mathcal{M}^{[\leqslant n]}(x;\eta)}. \tag{6.6}$$

[*for* $n=0$ *this means* $\psi_0(x^2)$ $(ix^2 - \mathcal{M}^{[0]}(\eta))^{-1}$]. *We say that* $g_\ell^{[n]} = g^{[n]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\varepsilon)$ *is a propagator on scale* $[n]$. *The matrices* $\mathcal{M}^{[m]}(x;\eta)$ *will be defined as in Sec. V for* $n < n_0$ *and will be defined recursively also for* $n \geqslant n_0$ *in terms of the self-energy clusters* $\mathcal{S}^{\mathcal{R}}_{k,n-1}$ *introduced in Definition 4, Sec. V, setting for* $n > n_0$ *[cf. (5.7)],*

$$\mathcal{M}^{[n]}(x;\eta) = \left(\prod_{m=0}^{n-1}\chi_m(\Delta^{[m]}(x;\eta))\right)\sum_{k=2}^{\infty}\sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,n-1}}\mathcal{V}_T(x;\eta), \tag{6.7}$$

where the self-energy values $\mathcal{V}_T(x;\eta)$ *are evaluated by means of propagators on scales less than* $[n]$. *Note that we have already defined [consistently with (6.7)] the matrices* $\mathcal{M}^{[\leqslant n]}$ *with* $n < n_0$ *and the propagators on scale* $[-1],[0],\dots,[n_0-1]$ *[so that (6.6) defines also* $g^{[n_0]}(x;\eta)$*].*

Of course the above definition makes sense only if the series (6.7) can be shown to be convergent for all n. For this purpose an inductive assumption on the propagators on the scales $[m]$, $0 \leqslant m < n$ is necessary.

Inductive assumption: *Let* n_0 *be fixed as in Lemma 3.*

(i) For $0 \leqslant m \leqslant n-1$ *the matrices* $\mathcal{M}^{[m]}(x;\eta)$ *are defined by convergent series for all* $|\varepsilon| \in I(\bar{\varepsilon}) = [\bar{\varepsilon}/4, \bar{\varepsilon}]$ *and, for all* x, *they satisfy the properties (i) and (iv) of Lemma 3. Moreover they*

can be represented as in (5.11), with $P^{[\leqslant n]}, Q^{[\leqslant n]}, R^{[\leqslant n]}$ *as in (5.12) and the entries* $\bar{M}^{[\leqslant n]}_{\gamma'\gamma}$ *bounded as described after (5.12).*

(ii) There exist $K>0$ *and open sets* $\mathcal{E}^o_m$, $m=0,\dots,n$, *with* $\mathcal{E}^o_m \subset I(\bar{\varepsilon})$, *such that, defining recursively* $\underline{\lambda}^{[m]}(\eta)$ *in terms of* $\underline{\lambda}^{[m-1]}(\eta)$ *for* $m=n_0,\dots,n-1$ *by (i) in Definition 7 above, while setting* $\underline{\lambda}^{[m]}(\eta)\equiv 0$ *for* $m=0,\dots,n_0-1$, *and defining* $\tau_1 := \tau_0(1+\delta_1)+N$, *with* $\delta_1>0$, *one has for* $\varepsilon \notin \mathcal{E}^o_m$,

$$\Gamma^{[m]}(x;\eta) := \left||x| - \sqrt{\underline{\lambda}^{[m]}(\eta)}\right| \geqslant 2^{-m/2}\frac{C_0}{|\boldsymbol{\nu}|^{\tau_1}},$$

$$|\mathcal{E}^o_m| \leqslant K 2^{-m/2}\bar{\varepsilon}\,\bar{\eta}^{\delta_1(k_0-1/2)}, \tag{6.8}$$

with $\bar{\varepsilon}=\bar{\eta}^{k_0}$, *for all* $m\leqslant n-1$ *and all* x.

Remark: As in Ref. 15, a key point is checking that $\Delta^{[n]}(x;\eta)$ can be used to bound below the denominators of the nonvanishing propagators on scale $[n]$. If x has scale $[n]$, with $n\geqslant n_0$, one has

$$\begin{aligned}
|x^2-\lambda^{[n]}(x;\eta)| &\geqslant |x^2-\underline{\lambda}^{[n]}(\eta)| - |\underline{\lambda}^{[n]}(\eta)-\lambda^{[n]}(x;\eta)| \\
&\geqslant \frac{1}{2}|x^2-\underline{\lambda}^{[n]}(\eta)| + 2^{-(n+2)}C_0 - |\lambda^{[n]}(\sqrt{\underline{\lambda}^{[n-1]}(\eta)},\eta)-\lambda^{[n]}(x;\eta)| \\
&\geqslant \frac{1}{2}|x^2-\underline{\lambda}^{[n]}(\eta)| \Rightarrow \|x^2-\mathcal{M}^{[n]}(x,\eta)\| \geqslant \frac{1}{8\mu}\Delta^{[n]}(x;\eta),
\end{aligned} \tag{6.9}$$

having used the lower cutoff $\psi_n(\Delta^{[n]}(x;\eta))$ in the propagator [see (6.5)] to obtain the first two terms in the second line while the upper cutoff $\chi_{n-1}(\Delta^{[n-1]}(x;\eta))$ has been used to obtain positivity of the difference between the second and third terms in the second line, after applying the second inequality in (6.2), so that the last term in the second line of (6.9) can be bounded above proportionally to $\varepsilon 2^{-n}C_0$.

The inequality (6.9) allows us a complete word by word reduction of the proof of the inductive assumption above to the corresponding inductive assumption of Ref. 15. The symbols here and in Ref. 15 have been chosen to coincide so that the analysis in Sec. VI and Appendix A3 of Ref. 15 can be taken over and reinterpreted, with no change, as proofs of the above inductive hypothesis, apart for the check of the measure $\mathcal{E}^0_m$ in (6.8), which in the present case is slightly different from the corresponding computation in Ref. 15. The estimate (6.8) of the measure of $\mathcal{E}^0_m$ is explicitly given in Appendix H.

We can summarize the previous discussion into the following lemma.

Lemma 6: *There is* ε_0 *small enough such that for* $\bar{\varepsilon}<\varepsilon_0$ *and* $\varepsilon \in I(\bar{\varepsilon})$, *if the inductive hypothesis is assumed for* $0\leqslant m\leqslant n-1$ *then it holds for* $m=n$.

The series for $X(\psi)$ is now fully "renormalized" and its terms are well defined for ε in a set $\mathcal{E}$ whose measure is large (near 0). The series is expressed as a sum of renormalized tree values of tree graphs without any self-energy graph. Therefore the series is convergent (by Siegel's lemma); see the corresponding discussion in Appendix A3 of Ref. 15.

In the derivation geometric series with ratio $z>1$ have been considered and the rule $\Sigma_{k=0}^{\infty}z^k = (1-z)^{-1}$ has been repeatedly used, this is not mathematically rigorous and therefore an *a posteriori* check must be made that the function $X(\boldsymbol{\psi})$, via (1.5), actually does satisfy the equations (1.4). The check, however, is a repetition of the corresponding (essentially algebraic) check in Appendix A5 of Ref. 15.

Therefore the proof of Theorem 1 is complete.

VII. CONCLUSIONS

We conclude by mentioning some problems that seem to us of interest.

(1) First we note that the proof of Theorem 1 also provided some information about the analyticity properties in η, hence in ε, of the surviving lower-dimensional tori; cf. Refs. 10 and 15 for further details. As in the quoted papers, it can be interesting to further investigate such properties, and related ones, such as Borel summability.

(2) The uniqueness of the resonant tori appears to be a hard problem. Even a proof of Borel summability would not resolve the problem as there could be solutions which are not Borel summable. Just as in the maximal tori case analyticity is not sufficient to guarantee uniqueness. The very recent Ref. 1 does not settle the question, as it proves uniqueness of the C^∞ diffeomorphism mapping the unperturbed invariant tori which are conserved into those which are explictly constructed, but it does not eliminate the possibility that other nearby quasiperiodic motions with the same rotation vectors exist.

(3) Another open problem concerns the possibility of removing the assumptions we made in this paper. We have been able to do this in several particular cases but we did not find a satisfactory general formulation, for instance can something be said in general in the case in which the average of the perturbation vanishes identically?

(4) Finally, it would be interesting to understand what happens in the case of n-dimensional tori, with n strictly less than $N-1$ (that is in the case of several normal frequencies), by relaxing the assumptions on the perturbing potential with respect the results existing in literature, as done here and in Cheng's paper[2,3] for $n=N-1$. This is a substantially more difficult endeavour with respect to that considered here and in Cheng's quoted papers.

VIII. ACKNOWLEDGMENT

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APPENDIX A: HEURISTIC ANALYSIS LEADING TO FRACTIONAL SERIES

Consider the simple case $H(\mathbf{A},B,\boldsymbol{\alpha},\beta)=\boldsymbol{\omega}\cdot\mathbf{A}+\frac{1}{2}(\mathbf{A}^2+B^2)+\varepsilon f(\boldsymbol{\alpha},\beta)$, and let assumptions (a) and (c) in Sec. I be satisfied by f. Let us consider the generating function,

$$\Gamma(\mathbf{A}',B',\boldsymbol{\alpha},\beta)=\boldsymbol{\alpha}\cdot\mathbf{A}'+\beta B'+\varepsilon\Psi_1(\mathbf{A}',B',\boldsymbol{\alpha},\beta)+\varepsilon^2\Psi_2(\mathbf{A}',B',\boldsymbol{\alpha},\beta)+\varepsilon^2\boldsymbol{\alpha}\cdot\boldsymbol{\zeta}+\varepsilon^2\beta\rho, \tag{A1}$$

where, if $\Delta:=\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\alpha}}$,

$$\Psi_1(\mathbf{A}',B',\boldsymbol{\alpha},\beta):=-\Delta^{-1}[1-(\mathbf{A}'\cdot\partial_{\boldsymbol{\alpha}}+B'\partial_\beta)\Delta^{-1}]f_{\neq\mathbf{0}}(\boldsymbol{\alpha},\beta), \tag{A2}$$

and, if $\Phi(\mathbf{A}',B',\boldsymbol{\alpha},\beta)=\frac{1}{2}[(\partial_{\boldsymbol{\alpha}}\Psi_1)^2+(\partial_\beta\Psi_1)^2]$,

$$\begin{aligned}\Psi_2(\mathbf{A}',B',\boldsymbol{\alpha},\beta)&:=-\Delta^{-1}[1-(\mathbf{A}'\cdot\partial_{\boldsymbol{\alpha}}+B'\partial_\beta)\Delta^{-1}]\boldsymbol{\Phi}_{\neq\mathbf{0}}(\mathbf{A}',B',\boldsymbol{\alpha},\beta),\\ \boldsymbol{\zeta}&=-\partial_{\mathbf{A}'}\boldsymbol{\Phi}_{\mathbf{0}}(\mathbf{A}',0,\beta_0)|_{\mathbf{A}'=\mathbf{0}},\quad \rho=-\partial_{B'}\boldsymbol{\Phi}_{\mathbf{0}}(\mathbf{0},B',\beta_0)|_{B'=0}.\end{aligned} \tag{A3}$$

The canonical map $(\mathbf{A},B,\boldsymbol{\alpha},\beta)\leftrightarrow(\mathbf{A}',B',\boldsymbol{\alpha}',\beta')$ generated by $\Gamma(\mathbf{A}',B',\boldsymbol{\alpha},\beta)$ transforms the Hamiltonian $H(\mathbf{A},B,\boldsymbol{\alpha},\beta)$ into

$$\begin{aligned}H'(\mathbf{A}',B',\boldsymbol{\alpha}',\beta')=\boldsymbol{\omega}\cdot\mathbf{A}'+\tfrac{1}{2}(\mathbf{A}'^2+B'^2)+\varepsilon f_{\mathbf{0}}(\beta')-\varepsilon^2\partial_{\beta'}f_{\mathbf{0}}(\beta')\cdot\Delta^{-2}\partial_{\beta'}f_{\neq\mathbf{0}}(\boldsymbol{\alpha}',\beta')\\ +\varepsilon^2\boldsymbol{\Phi}_{\mathbf{0}}(\mathbf{0},0,\beta')+O(\varepsilon I'^2)+O(\varepsilon^3).\end{aligned} \tag{A4}$$

Writing the Hamiltonian equations generated by (A4), we realize that in a small neighborhood of β_0 the evolution equation for β' takes the form

$$\ddot{\beta}' = -c\varepsilon(\beta' - \beta_0)^{k_0} - \varepsilon^2 a + \varepsilon^2 a'(\beta - \beta_0) + O(\varepsilon(\beta' - \beta_0)^{k_0+1}) + O(\varepsilon^2(\beta' - \beta_0)^2) + O(\varepsilon^3), \tag{A5}$$

where $a = \partial_{\beta'} \mathbf{\Phi_0}(\mathbf{0}, 0, \beta_0)$ is the same constant defined in (1.9) and a' is a suitable constant.

Therefore, under the assumption that both a and c are nonzero, the perturbed equilibrium of the angle β' is equal, *up to high order corrections*, to $\beta_0' = \beta_0 + \delta\beta_0$, with

$$\delta\beta_0 = \begin{cases} (-a\varepsilon/c)^{1/k_0} & \text{if } k_0 \text{ is odd,} \\ \pm(-a\varepsilon/c)^{1/k_0} & \text{if } k_0 \text{ is even and } a\varepsilon/c < 0. \end{cases} \tag{A6}$$

If k_0 is odd and $c\varepsilon > 0$ the approximate perturbed equilibrium point β_0' is quadratically stable, while if $c\varepsilon < 0$ β_0' is quadratically unstable: hence we shall say that the resonant invariant torus is elliptic if $c\varepsilon > 0$ and hyperbolic if $c\varepsilon < 0$. The center of oscillations is displaced by $O(\varepsilon^{1/k_0})$ so that a fractional series in powers of $\eta = \varepsilon^{1/k_0}$ has to be expected (at best).

If k_0 is even the unperturbed equilibrium point β_0 can be continued into a perturbed equilibrium $\beta_0' = \beta_0 + \delta\beta_0$ (with $\delta\beta_0$ vanishing as $\varepsilon \to 0$) *only if* $a\varepsilon c < 0$. In this case, if $c\varepsilon\delta\beta_0 > 0$ the approximate perturbed equilibrium point β_0' is quadratically stable, while if $c\varepsilon\delta\beta_0 < 0$ β_0' it is quadratically unstable: hence we shall say that the resonant invariant torus is elliptic if $c\varepsilon\delta\beta_0 > 0$ and hyperbolic if $c\varepsilon\delta\beta_0 < 0$. Given the results known for elliptic and hyperbolic resonances Theorem 1 becomes a natural conjecture.

If $c \neq 0$ and $a = 0$ the theory depends on the corrections in (A5), for instance if $a' \neq 0$ a natural conjecture is that the new equilibrium point for β' is approximately $\beta_0' + \delta\beta_0$, with $\delta\beta_0$ satisfying the equation $(\delta\beta_0)^{k_0 - 1} = \varepsilon a'/c$, whenever this equation is solvable. The stability of this equilibrium point can be again analyzed in terms of the relative signs of ε, a, c. If $a' = 0$ one expects that the higher order terms must be studied in details.

APPENDIX B: ON ASSUMPTION (a)

Here we want to show that assumption (a) is not a purely technical assumption; that is we want to show that generically a Hamiltonian of the form (1.3) violating assumption (a) cannot admit quasiperiodic motions of codimension 1 continuously connected to an unperturbed motion of the form (1.6) in the limit $\varepsilon \to 0$. We show this by producing an explicit example, given by a Hamiltonian of the form (1.3), satisfying assumptions (c) and (b) and violating assumption (a), for which we can prove absence of quasiperiodic motions of codimension 1 tending to an unperturbed motion of the form (1.6) as $\varepsilon \to 0$.

The counterexample is given by the following Hamiltonian:

$$H = A + \frac{1}{2}A^2 + \frac{1}{2}B^2 + \varepsilon\left(\frac{\sin^3\beta}{3} + \sin\beta\cos\alpha\right), \tag{B1}$$

where $A, B \in \mathbb{R}^1$ and $\alpha, \beta \in \mathbb{T}^1$. If $\varepsilon = 0$ the Hamiltonian (B1) is strictly convex [then it satisfies assumption (b)] and it admits the unperturbed periodic motions

$$A(t) = 0, \quad \alpha(t) = t, \quad B(t) = 0, \quad \beta(t) = \beta_0, \tag{B2}$$

parametrized by the choice of $\beta_0 \in \mathbb{T}^1$. Choosing $\beta_0 = 0$, we see that $f_{\mathbf{0}}(0) = \partial_\beta f_{\mathbf{0}}(0) = \partial_\beta^2 f_{\mathbf{0}}(0) = 0$ and $\partial_\beta^3 f_{\mathbf{0}}(0) = 2 \neq 0$ [so that assumption (c) is satisfied with $k_0 = 2$]. Using the fact that f is independent of the action variables and that $f(\alpha, \beta = 0) = \partial_\beta^2 f(\alpha, \beta = 0) \equiv 0$, we see that the quantity a defined in (1.8) is identically 0: this means that assumption (a) is violated in the case under analysis.

We now investigate the possible existence of periodic motions of the form

$$\alpha(t) = t + a(t;\varepsilon), \quad A(t) = \dot{a}(t;\varepsilon), \quad \beta(t) = \eta(\varepsilon) + b(t;\varepsilon), \quad B(t) = \dot{b}(t;\varepsilon), \tag{B3}$$

where $\eta(\varepsilon)$ is a continuous function of ε such that $\lim_{\varepsilon\to 0}\eta(\varepsilon)=0$ and $a(t;\varepsilon), b(t;\varepsilon)$ are 0 average periodic functions of t of period 2π. We want to show that it is impossible that a motion of the form (B3) satisfies the Hamiltonian equations of motion

$$\begin{aligned} \ddot{a}(t;\varepsilon) &= \varepsilon \sin(t + a(t;\varepsilon))\sin(\eta + b(t;\varepsilon)), \\ \ddot{b}(t;\varepsilon) &= -\varepsilon[\sin^2(\eta + b(t;\varepsilon))\cos(\eta + b(t;\varepsilon)) + \cos(t + a(t;\varepsilon))\cos(\eta + b(t;\varepsilon))]. \end{aligned} \tag{B4}$$

In fact a 0 average periodic solution to (B4) is necessarily of the form

$$a(t;\varepsilon) = -\varepsilon\left(\eta \sin t + \frac{\varepsilon}{4}\sin t \cos t\right) + \varepsilon^2 O(\varepsilon^2 + \eta^2),$$

$$b(t;\varepsilon) = \varepsilon \cos t + \varepsilon O(\varepsilon^2 + \eta^2). \tag{B5}$$

Averaging over t the second of (B4) we find

$$\int_0^{2\pi} \frac{\mathrm{d}t}{2\pi}(\cos(t + a(t;\varepsilon))\cos(\eta + b(t;\varepsilon)) + \sin^2(\eta + b(t;\varepsilon))\cos(\eta + b(t;\varepsilon))) = 0. \tag{B6}$$

Now, using the expressions (B5), we see that (B6) is equal to $\eta^2 + (\varepsilon^2/2)$, plus terms of order at least $\eta^4 + \varepsilon^4$, and this leads to a contradiction.

APPENDIX C: COUNTING THE NUMBER OF TREES LINES

We want to show that the number of lines of a tree contributing to $\mathbf{A}^{(k)}$, $B^{(k)}$, $\mathbf{a}^{(k)}$ or $b^{(k)}$ can be bounded, above and below, by an $O(1)$ constant times k. A lower bound k/k_0 is an immediate consequence of the definitions.

We proceed by induction, using that

(1) the trees contributing to $\mathbf{A}^{(k_0)}$ and $B^{(k_0)}$ have one line [see (2.2)]; those contributing to $\mathbf{A}^{(k_0+1)}$ and $B^{(k_0+1)}$ have two lines;
(2) the trees contributing to $\mathbf{a}_{\boldsymbol{\nu}}^{(k_0)}$ and $b_{\boldsymbol{\nu}}^{(k_0)}$, with $\boldsymbol{\nu}\neq\mathbf{0}$, have at most two lines and those contributing to $\mathbf{a}_{\boldsymbol{\nu}}^{(k_0+1)}$ and $b_{\boldsymbol{\nu}}^{(k_0+1)}$, with $\boldsymbol{\nu}\neq\mathbf{0}$, have at most three lines;
(3) $b_{\mathbf{0}}^{(1)} \equiv \beta_1$ is represented by a trivial tree (i.e., a tree with one line) and the trees contributing to $b_{\mathbf{0}}^{(2)} \equiv \beta_2$ have at most k_0+2 lines.

We introduce the following definitions:
$B_k(I)$ is the maximum number of lines of the trees contributing to $\mathbf{A}^{(k)}$, $B^{(k)}$,
$B_k(\varphi)$ is the maximum number of lines of the trees contributing to $\mathbf{a}_{\boldsymbol{\nu}}^{(k)}$, $b_{\boldsymbol{\nu}}^{(k)}$, $\boldsymbol{\nu}\neq\mathbf{0}$,
$B_k(b_0)$ is the maximum number of lines of the trees contributing to $b_0^{(k)} \equiv \beta_k$.

We shall make the following inductive assumption:

$$\begin{aligned} B_k(I) &\leqslant 3k_0(k - k_0 + 1) - 4k_0 - 2, \quad k \geqslant k_0 + 1, \\ B_k(\varphi) &\leqslant 3k_0(k - k_0 + 1) - 4k_0 - 1, \quad k \geqslant k_0 + 1, \\ B_{k-k_0+1}(b_0) &\leqslant 3k_0(k - k_0 + 1) - 4k_0, \quad k \geqslant k_0 + 1. \end{aligned} \tag{C1}$$

By the remarks above and the fact that $k_0 \geqslant 2$ it follows that at the first step (that is $k=k_0+1$) the inequalities above are verified.

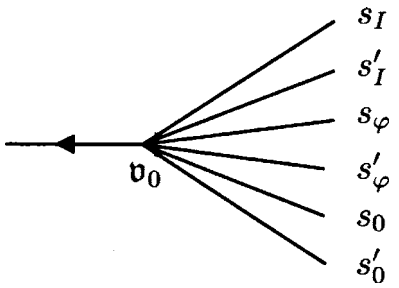

FIG. 3. The lines entering v_0 represent *symbolically* the bundle of subtrees entering $\mathfrak{v}_0$ and with root lines of types $I^{(k)}, I^{(k_0)}, \varphi^{(k)}_{\boldsymbol{\nu}}, \varphi^{(k_0)}_{\boldsymbol{\nu}}$, with $k \geq k_0+1$, and β_k, β_1, with $k \geq 2$. The number of subtrees in each bundle is indicated by the right labels.

Assume inductively the inequalities in (C1) for $k_0+1 \leq k \leq h-1$ and let us prove them for $k = h \geq k_0+2$. Let us start with the third inequality. We call $\mathfrak{v}_0$ the first node preceding the root. By the rules explained in Sec. III we have that the sum of the orders of the $s = s_{\mathfrak{v}_0}$ subtrees entering $\mathfrak{v}_0$ must be h. So, using the inductive assumptions, and calling (see Fig. 3)
s_I the number of subtrees of type $I^{(k)}$, $k \geq k_0+1$, entering $\mathfrak{v}_0$,
s'_I the number of subtrees of type $I^{(k_0)}$ entering $\mathfrak{v}_0$,
s_φ the number of subtrees of type $\varphi^{(k)}_{\boldsymbol{\nu}}$, $k \geq k_0+1$, $\boldsymbol{\nu} \neq \mathbf{0}$, entering $\mathfrak{v}_0$,
s'_φ the number of subtrees of type $\varphi^{(k_0)}_{\boldsymbol{\nu}}$, $\boldsymbol{\nu} \neq \mathbf{0}$, entering $\mathfrak{v}_0$,
s_0 the number of subtrees of type $b^{(k)}_{\mathbf{0}}$, $k \geq 2$, entering $\mathfrak{v}_0$,
s'_0 the number of subtrees of type $b^{(1)}_0$ entering $\mathfrak{v}_0$,
$B_{h-k_0+1}(b_{\mathbf{0}})$ can be bounded by the maximum over the choices of $s_I, s'_I, s_\varphi, s'_\varphi, s_0, s'_0$ of

$$1 + 3k_0 h - \{(3k_0^2 + k_0 + 2)s_I + (3k_0^2 - 1)s'_I + (3k_0^2 + k_0 + 1)s_\varphi + (3k_0^2 - 2)s'_\varphi + 4k_0 s_0 + (3k_0 - 1)s'_0\}. \tag{C2}$$

Let us first consider the case $s_I + s'_I + s_\varphi + s'_\varphi \geq 1$.

In this case, if $s=1$, since $h \geq k_0+2$, we must have that either s_φ or s_I is $=1$, and, in both cases, we can bound (C2) by $1+3k_0h-(3k_0^2+k_0+1)$, that is the desired bound; if, on the contrary, $s \geq 2$, then (C2) can be bounded by $1+3k_0h-(3k_0^2-2)-(3k_0-1) \leq 3k_0h-3k_0^2-k_0$. Let us now consider the case $s_I+s'_I+s_\varphi+s'_\varphi=0$, in which case $s=s_0+s'_0$ and necessarily $s \geq k_0$ [note that in this case the $s+1$ derivatives in (3.6) must be derivatives with respect to β so that $s \geq k_0$]. If $s \geq k_0+0$, then (C2) can be bounded by $1+3k_0h-(k_0+1)(3k_0-1) \leq 3k_0h3k_0^2-k_0$. If $s=k_0$, by the rules in Sec. III it must be $s'_0 \leq k_0-2$, so that (C2) can be bounded by $1+3h_0h-4k_0(k_0-s'_0)-(3k_0-1)s'_0 \leq 1+3k_0h-4k_0^2 +(k_0-2)(k_0+1)$ that implies the desired inductive bound.

Let us now consider the first of the three inequalities in (C1). By the rules explained in Sec. III we have that the sum of the degrees of the s subtrees entering $\mathfrak{v}_0$ is $h-k_0$ or h if, respectively, $\delta_{\mathfrak{v}_0}=1,0$. If $\delta_{\mathfrak{v}_0}=1$, $B_h(I)$ can be bounded by the maximum over the choices of $s_I, s'_I, s_\varphi, s'_\varphi, s_0, s'_0$ of $1+3k_0(h-k_0)-\{\cdots\}$, where the brackets include the same expression as in (C2), and we can bound this number by $1+3k_0h-3k_0^2-(3k_0-1)$ that is even better than the desired bound. If $\delta_{\mathfrak{v}_0} =0$, one must have $s=s_I+s'_I \geq 2$ (as $s=1$ corresponds to a not allowed tree graph) and $B_h(I)$ can be bounded by $1+3k_0h-2(3k_0^2-1)$, that is even better than the desired bound.

We finally consider the second of the three inequalities in (C1). By the rules explained in Sec. III we have that the sum of the orders of the s subtrees entering $\mathfrak{v}_0$ must be $h-k_0$ or h, if, respectively, $\delta_{\mathfrak{v}_0}=1,0$. If $\delta_{\mathfrak{v}_0}=1$ the number of lines of the corresponding trees can be bounded in the same way as we proceeded above for the first inequality in (C1). If $\delta_{\mathfrak{v}_0}=0$, only lines of type I can enter $\mathfrak{v}_0$, and then the corresponding trees have a number of lines bounded by $1+3k_0h$ $-\{(3k_0^2+k_0+2)s_I+(3k_0^2-1)s'_I\}$. So, if $s_I \geq 1$ the desired bound follows. If $s_I=0$, since $h \geq k_0+2$, we must have $s'_I \geq 2$, and again the bound follows.

APPENDIX D: PROOF OF LEMMA 2

To estimate the eigenvalues of $(ix-\mathcal{M}^{[0]}(\eta))E$, we start by rewriting $(ix-\mathcal{M}^{[0]}(\eta))E$ in the form

$$(ix-\mathcal{M}^{[0]}(\eta))E=\begin{pmatrix} -R & -ix+Q \\ ix+Q^{\dagger} & P \end{pmatrix}. \tag{D1}$$

Note that, by the strict convexity of the Hessian of H_0 if ε is small enough, P admits N positive eigenvalues $0<\mu_1^{(0)}\leqslant\cdots\leqslant\mu_N^{(0)}\equiv\mu$. Let $v_\alpha(x;\eta)=\binom{u}{v}$ be an eigenvector of $(ix-\mathcal{M}^{[0]})E$ with eigenvalue α (here u and v are two column vectors of dimension N),

$$\begin{pmatrix} -R & -ix+Q \\ ix+Q^{\dagger} & P \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}=\begin{pmatrix} -Ru+(-ix+Q)v \\ (ix+Q^{\dagger})u+Pv \end{pmatrix}=\alpha\begin{pmatrix} u \\ v \end{pmatrix}. \tag{D2}$$

Now, either $|\alpha|\geqslant\mu_1^{(0)}/2$ or $P/2<P-\alpha<3P/2$. In the latter case $(P-\alpha)$ is invertible, $2/(3\mu_N^{(0)})\leqslant(P-\alpha)^{-1}\leqslant 2/\mu_1^{(0)}$, and we can rewrite (D2) as

$$v=-(P-\alpha)^{-1}(ix+Q^{\dagger})u,\quad -Ru-(-ix+Q)(P-\alpha)^{-1}(ix+Q^{\dagger})u=\alpha u. \tag{D3}$$

The second equation in (D3) is of the form

$$[-x^2(P-\alpha)^{-1}+O(\varepsilon x)+O(\varepsilon\eta^{k_0-1})]u=\alpha u, \tag{D4}$$

so that $|\alpha|\geqslant(2/3\mu)x^2+O(\varepsilon x)+O(\varepsilon\eta^{k_0-1})$. If $x^2\geqslant\rho|\varepsilon|\eta^{k_0-1}$, for ρ large enough, the latter estimate implies $|\alpha|\geqslant(1/2\mu)x^2$, and Lemma 2 is proven.

APPENDIX E: SYMMETRY PROPERTIES OF THE SELF-ENERGY MATRICES

In this section we discuss the symmetry properties (5.10) of $\mathcal{M}^{[\leqslant n]}(x;\eta)$.

We begin with proving (5.10) for $\mathcal{M}^{[n]}(x;\eta)$. We inductively suppose that the same symmetry properties hold for both $\mathcal{M}^{[p]}(x;\eta)$ and $g^{[p]}(x;\eta)$, for $0\leqslant p<n$,

$$Eg^{[p]}(x;\eta)E=[g^{[p]}(-x;\eta)]^T,\quad [g^{[p]}(x;\eta)]^*=g^{[p]}(-x;\eta), \tag{E1}$$

where the $*$ denotes complex conjugation and T transposition. Note that if $p=0$, $\mathcal{M}^{[0]}(\eta)$ and $g^{[0]}(x;\eta)$ satisfy the desired symmetry properties, as discussed in Sec. IV.

Consider the representation of $\mathcal{M}^{[n]}(x;\eta)$ given by (5.6) and (5.7) in the following confusion between T denoting transposition and T denoting a self-energy cluster will be avoided by renaming the cluster T with a new symbol D. Note that $F^*(\boldsymbol{\nu}_{\mathfrak{v}})=F(-\boldsymbol{\nu}_{\mathfrak{v}})$, so that, using the second of (E1), $[\mathcal{V}_D(x;\eta)]^*$ can be written as[2]

$$\begin{aligned}[\mathcal{V}_D(x;\eta)]^* &= \frac{(\eta\beta_1)^{|L(D)|}}{|\Lambda(D)|!}\Big(\prod_{\mathfrak{v}\in V(D)}\varepsilon^{\delta_{\mathfrak{v}}}\Big)\Big(\prod_{\mathfrak{v}\in V(D)}F^*(\boldsymbol{\nu}_{\mathfrak{v}})\Big)\Big(\prod_{\ell\in\Lambda(D)}[g^{[n_\ell]}(x_\ell;\eta)]^*\Big)\\ &= \frac{(\eta\beta_1)^{|L(D)|}}{|\Lambda(D)|!}\Big(\prod_{\mathfrak{v}\in V(D)}\varepsilon^{\delta_{\mathfrak{v}}}\Big)\Big(\prod_{\mathfrak{v}\in V(D)}F(-\boldsymbol{\nu}_{\mathfrak{v}})\Big)\Big(\prod_{\ell\in\Lambda(D)}g^{[n_\ell]}(-x_\ell;\eta)\Big)=\mathcal{V}_{D^*}(-x;\varepsilon),\end{aligned} \tag{E2}$$

where D^* is a cluster topologically equivalent to D, with opposite mode labels (clearly the correspondence $D\leftrightarrow D^*$ is one-to-one). Summing over the choices of D [see (5.7)] the second of (5.10) follows.

[2]We stress that we use the convention that the internal γ indices of D are summed over, while the momentum labels are not summed over; in this way the value $\mathcal{V}_D$ explicitly depends only on the momenta of the internal nodes, the external momentum, and the two γ labels associated to the incoming and outcoming lines.

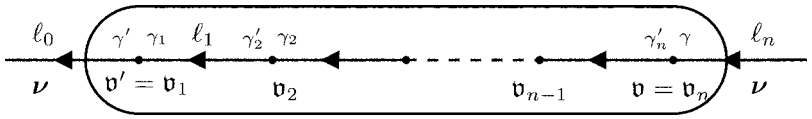

FIG. 4. A self-energy cluster D and the path $\mathcal{L}$ connecting its external lines. The subtrees internal to D with root on $\mathcal{L}$ are not drawn.

To prove the first of (5.10), it is convenient to shorten notations; see Fig. 4 for a pictorial representation of the symbols. Given a self-energy cluster D, let us denote by $\mathfrak{v}$ and $\mathfrak{v}'$ the nodes such that the exiting line of D comes out from $\mathfrak{v}'$ and the entering line of D enters $\mathfrak{v}$.

(1) Let $\mathfrak{v}' \equiv \mathfrak{v}_1, \dots, \mathfrak{v}_n \equiv \mathfrak{v}$ be the nodes on the path $\mathcal{L} \equiv \mathcal{L}(D)$ joining $\mathfrak{v}$ to $\mathfrak{v}'$, and $\boldsymbol{\nu}_j$ be their mode labels; let also $\ell_j = (\mathfrak{v}_{j+1}\mathfrak{v}_j)$ be the line joining the two successive nodes $\mathfrak{v}_{j+1}$ and $\mathfrak{v}_j$ in $\mathcal{L}$; let γ'_j, γ_j be the component labels at the beginning of the line in $\mathcal{L}$ exiting from $\mathfrak{v}_j$ and at the end of the line in $\mathcal{L}$ entering the node $\mathfrak{v}_j$ (they are, respectively, the lines ℓ_{j-1} and ℓ_j). Recall that, by definition of self-energy cluster, any propagator g_j associated to the lines $\ell_j \in \mathcal{L}$ has a scale $[n_{\ell_j}]$, with $n_{\ell_j} \geqslant 0$, i.e., there cannot be $\mathbf{0}$-momentum propagators along the path $\mathcal{L}$.

(2) Let $\boldsymbol{\vartheta}_j$ be the (possibly empty) family of subtrees of D with root in $\mathfrak{v}_j$ and with no line in common with $\mathcal{L}$ (not represented in Fig. 4, $\boldsymbol{\vartheta}_j$ can be imagined to be a set of trees with the root line ending in $\mathfrak{v}_j$ or, possibly, $\boldsymbol{\vartheta}_j$ may consist just in $\mathfrak{v}_j$).

(3) Let N_j be the $N \times N$ symmetric matrix $\partial_{\gamma'_j \gamma_j} f_{\boldsymbol{\nu}_j}(\beta_0, \boldsymbol{\vartheta}_j)$, where $f_{\boldsymbol{\nu}_j}(\beta_0, \boldsymbol{\vartheta}_j)$ is a function depending only on the set of trees $\boldsymbol{\vartheta}_j$ and on $f_{\boldsymbol{\nu}_j}(\beta)$ [it can be read off (5.6) and (5.7)] and $\partial_{\gamma'}$, ∂_{γ} must be interpreted as explained after (3.2).

(4) The momentum flowing in a generic line ℓ of the graph D will be the sum of the momentum $\boldsymbol{\nu}^0_\ell$ that would flow on the line if the entering line momentum $\boldsymbol{\nu}$ was $\mathbf{0}$ plus $\boldsymbol{\nu}$ if the line is on the path $\mathcal{L}$; then the propagator matrix g_j associated to the line ℓ_j of $\mathcal{L}$ is equal to $g^{[n_{\ell_j}]} \times (x^0_j + x; \eta)$, where x^0_j is the scalar product of $\boldsymbol{\omega} \cdot \boldsymbol{\nu}^0_{\ell_j}$ and $x = \boldsymbol{\omega} \cdot \boldsymbol{\nu}$.

Then the matrix $\mathcal{V}_D(x; \eta)$, see (E1), can be concisely written as

$$(\mathcal{V}_D(x;\eta))_{\gamma'\gamma} = (EN_1 g_1 EN_2 g_2 \cdots g_{n-2} EN_{n-1} g_{n-1} EN_n)_{\gamma'\gamma}. \tag{E3}$$

Interchanging the external lines (i.e., having $\mathfrak{v}'$ as entering node and $\mathfrak{v}$ as exiting node) generates a new self-energy cluster D' in which the momenta flowing in the lines of the subtrees $\boldsymbol{\vartheta}_j$ with roots on the nodes $\mathfrak{v}_j \in \mathcal{L}$ are unchanged while the momentum on the line $\ell_j \in \mathcal{L}$ changes from $\boldsymbol{\nu}^0_{\ell_j} + \boldsymbol{\nu}$, with $\boldsymbol{\nu}^0_{\ell_j}$ equal to the momentum which would flow on ℓ_j if the external momentum $\boldsymbol{\nu}$ was set equal to $\mathbf{0}$, to a new value $-\boldsymbol{\nu}^0_{\ell_j} + \boldsymbol{\nu}$.

The matrix $\mathcal{V}_{D'}(x; \eta)$ can therefore be written as

$$(\mathcal{V}_{D'}(x;\eta))_{\gamma'\gamma} = (EN_n g'_{n-1} EN_{n-1} g'_{n-2} \cdots g'_2 EN_2 g'_1 EN_1)_{\gamma'\gamma}, \tag{E4}$$

where $g'_j = g^{[n_{\ell_j}]}(-x^0_{\ell_j} + x; \eta)$. Inserting $\mathbb{1} \equiv E^T E$ after $N_n, \dots, N_2$ and using the symmetry of $N_1, \dots, N_n$, the inductive validity of the first of (E1) and the transposition rules for matrix products, we get

$$(\mathcal{V}^T_{D'}(x;\eta))_{\gamma'\gamma} = (N_1 g''_1 EN_2 g''_2 \cdots g''_{n-2} EN_{n-1} g''_{n-1} EN_n E^T)_{\gamma'\gamma}, \tag{E5}$$

where $g''_j \equiv g^{[n_{\ell_j}]}(x^0_{\ell_j} - x; \eta)$. Hence $E\mathcal{V}^T_{D'}(x;\eta)E \equiv \mathcal{V}_D(-x;\eta)$ completing the inductive proof of (E1), because $\mathcal{M}^{[n]}(x;\eta)$ is defined as a sum over D of the values $\mathcal{V}_D$ [see (5.7)].

Remark: From (5.10) and (E1) follows that $g^{[\geqslant n]}(x;\eta)$ satisfies the same symmetry properties as $\mathcal{M}^{[n]}(x;\eta)$,

$$Eg^{[\geqslant n]}(x;\eta)E = [g^{[\geqslant n]}(-x;\eta)]^T, \quad [g^{[\geqslant n]}(x;\eta)]^* = g^{[\geqslant n]}(-x;\eta). \tag{E6}$$

APPENDIX F: CANCELLATIONS

In this section we discuss the cancellations needed to show that $\mathcal{M}^{[\le n]}(x;\eta)$ has the structure described in (5.11) and (5.12). In particular we want to show that the elements $(\mathcal{M}^{[n]}(x;\eta))_{\gamma'\gamma}$ with either $\gamma'=A_i$ or $\gamma=\alpha_j$ are proportional to x, while the elements with $\gamma'=A_i$ and $\gamma=\alpha_j$ are proportional to x^2, for $x^2\le\rho\eta^{2k_0-1}$.

As in, Ref. 15 the contributions to $\mathcal{M}^{[n]}(x;\eta)$ coming from clusters such that

$$\sum_{\mathfrak{v}\in V(T)}|\boldsymbol{\nu}_{\mathfrak{v}}|\ge(C_0/2^6|x|)^{1/\tau_0} \tag{F1}$$

require no cancellations, in fact the exponential decay as $\boldsymbol{\nu}_{\mathfrak{v}}\to\infty$ of the node functions implies that the contributions coming from clusters satisfying (F1) are smaller than Cx^2, for some constant $C>0$.

When (F1) does not hold we need to exploit cancellations, because *a priori* there is no reason for some of the entries of $\mathcal{M}^{[n]}(x;\eta)$ to be proportional to x or x^2 for small x. Following the same strategy used in Appendix A2 of Ref. 15 (and of Appendix A4 of Ref. 10), the necessary cancellations can be checked to occur by collecting clusters violating condition (F1) into families. Such cancellations are due to the same mechanism pointed out first in Refs. 7, 8, and 4. The following analysis follows Ref. 16.

Given a self-energy cluster D on scale $[n-1]$, let us call D_0 the connected subset of D containing no line on scale $[-1]$ and containing the nodes $\mathfrak{v}$ and $\mathfrak{v}'$ to which the entering and exiting lines are attached. By definition $\Sigma_{\mathfrak{v}\in D_0}\boldsymbol{\nu}_{\mathfrak{v}}=\mathbf{0}$. Note also that, if the path $\mathcal{L}$ connecting $\mathfrak{v}$ and $\mathfrak{v}'$ is nontrivial (i.e., $\mathfrak{v}\ne\mathfrak{v}'$), $\mathcal{L}$ is completely contained into D_0; moreover, if D does not contain lines on scale $[-1]$, then $D_0\equiv D$. We define the family $\mathcal{F}\equiv\mathcal{F}_D$ as the set of self-energy clusters obtained from D by shifting the entering and exiting lines by reattaching them to the nodes of D_0 in all possible ways. We then consider the sum

$$\mathcal{V}_{\mathcal{F}}(x;\eta)=\sum_{D\in\mathcal{F}}\mathcal{V}_D(x;\eta), \tag{F2}$$

contributing to the rhs of (5.7). When summing $\mathcal{V}_{\mathcal{F}}(x;\eta)$ over all distinct families of clusters on scale $[n-1]$, we recover the quantity $M^{[n]}(x;\eta)$ defined in (5.7). To prove that $\mathcal{M}^{[\le n]}$ has the structure described by (5.11) and (5.12), we proceed in the following way. We first note that, by the same analysis of Sec. VI of Ref. 15, $\mathcal{V}_{\mathcal{F}}(x;\eta)$ is differentiable with respect to x in the sense of Whitney; then, we show that $(\mathcal{V}_{\mathcal{F}}(0;\eta))_{\gamma'\gamma}=0$ if $\gamma'=A_i$ or $\gamma=\alpha_j$ and $(\partial_x\mathcal{V}_{\mathcal{F}}(0;\eta))_{\gamma'\gamma}=0$ if $\gamma'=A_i$ and $\gamma=\alpha_j$.

Let us begin with proving that $(\mathcal{V}_{\mathcal{F}}(0;\eta))_{\gamma'\gamma}=0$ if $\gamma'=A_i$ or $\gamma=\alpha_j$, and to be definite let us assume that $\gamma=\alpha_j$ for some $j=1,\dots,N-1$. Recall that, employing the notation of Appendix E, we can write each matrix $\mathcal{V}_D(x;\eta)$ appearing in the sum (F2) in the form (E3). By the explicit expression of (E3) and of the matrices N_j, we see that, when computing $\mathcal{V}_D(x;\eta)$ in $x=0$, we find $(\mathcal{V}_D(0;\eta))_{\gamma'\alpha_j}=O(\mathcal{F},\mathfrak{v}',\eta)_{\gamma'}(\boldsymbol{\nu}_{\mathfrak{v}})_j$ for some function $O(\mathcal{F},\mathfrak{v}',\eta)_{\gamma'}$ *independent* of the choice of the node $\mathfrak{v}$ to which the entering line with label $\gamma=\alpha_j$ is attached to.

If we change D within $\mathcal{F}$ by attaching the entering line to all possible nodes in D_0 (keeping $\mathfrak{v}'$ fixed), we see that the global contribution from such self-energy clusters is equal to $O(\mathcal{F},\mathfrak{v}',\eta)_{\gamma'}\cdot\cdot\Sigma_{\mathfrak{v}\in D_0}(\boldsymbol{\nu}_{\mathfrak{v}})_j$, which is 0 by the property $\Sigma_{\mathfrak{v}\in D_0}(\boldsymbol{\nu}_{\mathfrak{v}})_j=\mathbf{0}$. So, if $\gamma=\alpha_j$, the proof of the fact that $(\mathcal{V}_{\mathcal{F}}(0;\eta))_{\gamma'\gamma}=0$ is complete. In the case that $\gamma'=A_i$ the proof is completely analogous and we do not repeat it here.

Let us now turn to the proof of the fact that, if $\gamma'=A_i$ and $\gamma=\alpha_j$, then $(\partial_x\mathcal{V}_{\mathcal{F}}(0;\eta))_{\gamma'\gamma}=0$. First note that, by the explicit form (E3) of the value $\mathcal{V}_D(x;\eta)$ and in particular by the fact that $\mathcal{V}_D(x;\eta)$ depends on x only through the propagators along the path $\mathcal{L}$, we find that, when differentiating $\mathcal{V}_D(x;\eta)$ with respect to x, the effect of the derivative is as follows:

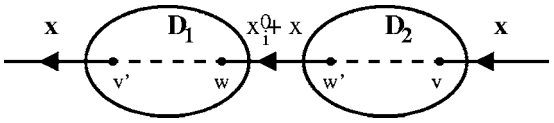

FIG. 5. Subdiagrams D_1 and D_2 in a self-energy cluster D. The drawn lines connected to $\mathbf{v}$ and $\mathbf{v}'$ are the external lines of D.

$$\partial_x \mathcal{V}_D(x;\eta) = \sum_{i=1}^{n-1} (EN_1 g_1 \cdots g_{i-1} EN_i)\partial_x g_i (EN_{i+1} g_{i+1} \cdots g_{n-1} EN_n). \tag{F3}$$

Given the line $\ell_i \in D_0$, we call D_1 and D_2 the two connected distinct subsets of D_0 obtained from D_0 by detaching the line ℓ_i and such that D_1 contains the node $\mathfrak{v}'$ to which the line exiting from D is attached, while D_2 contains the node $\mathfrak{v}$ to which the line entering D is attached. D_1 and D_2 are two subgraphs of D with two external lines, one coinciding with one of the external lines of D, the other coinciding with ℓ_i, see Fig. 5.

If we define the values of D_1, D_2 by formulas analogous to (E3), we can rewrite each term under the sum in (F3) as $\mathcal{V}_{D_1}(x;\eta)\partial_x g^{[n_{\ell_i}]}(x_i^0+x;\eta)\mathcal{V}_{D_2}(x;\eta)$, where, with the same notations of Appendix E, we defined $x_i^0 = \boldsymbol{\vartheta}\cdot\boldsymbol{\nu}_{\ell_i}^0$, with $\boldsymbol{\nu}_{\ell_i}^0$ equal to the momentum which would flow on ℓ_i if the external momentum $\boldsymbol{\nu}$ was set equal to $\mathbf{0}$.

In particular let us consider the value $(\mathcal{V}_{D_1}(0;\eta)\partial_x g^{[n_{\ell_i}]}(x_i^0;\eta)\mathcal{V}_{D_2}(0;\eta))_{A_i\alpha_j}$ at $x=0$, that is one of the contributions we are interested in, and again note that by the very definition of $\mathcal{V}_{D_1}$ and $\mathcal{V}_{D_2}$, it holds that $(\mathcal{V}_{D_1}(0;\eta))_{A_i\gamma_1} = (\boldsymbol{\nu}_{\mathfrak{v}'})_i \Omega(\mathfrak{w})_{\gamma_1}$ and $(\mathcal{V}_{D_2}(0;\eta))_{\gamma_2\alpha_j} = \Omega(\mathfrak{w}')_{\gamma_2}(\boldsymbol{\nu}_{\mathfrak{v}})_j$, where $\mathfrak{w}$, $\mathfrak{w}'$ are the two nodes where ℓ_i enters into and exists from, see Fig. 5, and $\Omega(\mathfrak{w})_{\gamma_1}$, $\Omega(\mathfrak{w}')_{\gamma_2}$ are two functions depending on the structure of D_1 and D_2, *but not on the choices of* $\mathfrak{v}'$, $\mathfrak{v}$ within D_1, D_2.

This implies that if we change D within $\mathcal{F}$ by attaching the entering line to all possible nodes in $D_2 \cap D_0$ and by attaching the exiting line to all possible nodes in $D_1 \cap D_0$, keeping ℓ_i fixed, the sum of the contributions of the form $(\mathcal{V}_{D_1}(0;\eta)\partial_x g^{[n_{\ell_i}]}(x_i^0;\eta)\mathcal{V}_{D_2}(0;\eta))_{A_i\alpha_j}$ from this class of graphs is equal to

$$\left(\sum_{\mathfrak{v}'\in D_1\cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}'})_i\right)\Omega(\mathfrak{w})_{\gamma_1}(\partial_x g^{[n_{\ell_i}]}(x_i^0;\eta))_{\gamma_1\gamma_2}\Omega(\mathfrak{w}')_{\gamma_2}\left(\sum_{\mathfrak{v}\in D_2\cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}})_j\right). \tag{F4}$$

Note that, given any graph D with the structure in Fig. 5, the graph D' in which the entering and exiting lines are interchanged (so that the external lines enter in $\mathfrak{v}'$ and exit from $\mathfrak{v}$, see Fig. 6) the momentum through the line ℓ_i changes from $\boldsymbol{\nu}_{\ell_i^0}+\boldsymbol{\nu}$ to $-\boldsymbol{\nu}_{\ell_i^0}+\boldsymbol{\nu}$.

At $x=0$, if we change D into D', the value $\mathcal{V}_{D_1}(0;\eta)\partial_x g^{[n_{\ell_i}]}(x_i^0;\eta)\mathcal{V}_{D_2}(0;\eta)$ is changed into $\mathcal{V}_{D_2'}(0;\eta)\partial_x g^{[n_{\ell_i}]}(-x_i^0;\eta)\mathcal{V}_{D_1'}(0;\eta)$. In analogy with the results of Appendix E, employing the symmetry relations (E1), we find $\mathcal{V}_{D_2'}(0;\eta) = E[\mathcal{V}_{D_2}(0;\eta)]^T E$ and $\mathcal{V}_{D_1'}(0;\eta) = E[\mathcal{V}_{D_1}(0;\eta)]^T E$. Using also the symmetry $E\partial_x g^{[n_{\ell_i}]}(-x_i^0;\eta)E = -\partial_x[g^{[n_{\ell_i}]}]^T(x_i^0;\eta)$, we find that the element (A_i,α_j) of the contribution corresponding to the graph in Fig. 6 can be written as

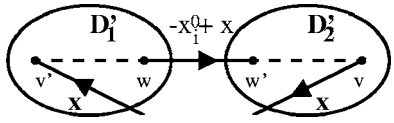

FIG. 6. The self-energy cluster D' obtained from D by interchanging the external lines of D, the exiting line is attached to a node $\mathbf{v}\in D_2'$ and the entering line is attached to a node $\mathbf{v}\in D_1'$.

$$(\mathcal{V}_{D_2'}(0;\eta)\partial_x g^{[n\ell_i]}(-x_i^0;\eta)\mathcal{V}_{D_1'}(0;\eta))_{A_i\alpha_j} = -(E[\mathcal{V}_{D_2}(0;\eta)]^T\partial_x[g^{[n\ell_i]}]^T(x_i^0;\eta)\mathcal{V}_{D_1}^T(0;\eta)E)_{A_i\alpha_j}$$
$$= -(E\mathcal{V}_{D_1}(0;\eta)\partial_x g^{[n\ell_i]}(x_i^0;\eta)\mathcal{V}_{D_2}(0;\eta)E)_{\alpha_j A_i}$$
$$= -(\mathcal{V}_{D_1}(0;\eta)\partial_x g^{[n\ell_i]}(x_i^0;\eta)\mathcal{V}_{D_2}(0;\eta))_{A_j\alpha_i}. \tag{F5}$$

Repeating the discussion leading to (F4) we see that, if we sum (F5) over the graphs obtained by attaching the entering line to all possible nodes $\mathfrak{v}' \in D_1' \cap D_0$ and attaching the exiting line to all possible nodes $\mathfrak{v} \in D_2' \cap D_0$, we get

$$-\left(\sum_{\mathfrak{v}' \in D_1' \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}'})_j\right)\Omega(\mathfrak{w})_{\gamma_1}(\partial_x g^{[n\ell_i]}(x_i^0;\eta))_{\gamma_1\gamma_2}\Omega(\mathfrak{w}')_{\gamma_2}\left(\sum_{\mathfrak{v} \in D_2' \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}})_i\right). \tag{F6}$$

Now, using the fact that $\Sigma_{\mathfrak{v} \in D_0}\boldsymbol{\nu}_{\mathfrak{v}} = \mathbf{0}$ and that D_1', D_2' and D_1, D_2 are topologically equivalent, we also find that

$$\sum_{\mathfrak{v}' \in D_1' \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}'})_j = -\sum_{\mathfrak{v} \in D_2 \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}})_j, \qquad \sum_{\mathfrak{v} \in D_2' \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}})_i = -\sum_{\mathfrak{v}' \in D_1 \cap D_0} (\boldsymbol{\nu}_{\mathfrak{v}'})_i, \tag{F7}$$

so that (F4) and (F6) sum up to 0.

This completes the proof of the fact that

$$\sum_{D \in \mathcal{F}} \mathcal{V}_D(\varepsilon;0)_{A_i\alpha_j} = 0, \quad \partial_x \sum_{D \in \mathcal{F}} \mathcal{V}_D(\varepsilon;x)_{A_i\alpha_j}\big|_{x=0} = 0. \tag{F8}$$

Remark: It can be checked that the symmetry (E1) "only" implies that, if we define $C_{ij}(x) := \Sigma_{D \in \mathcal{F}}\mathcal{V}_D(\varepsilon;x)_{A_i\alpha_j}$, it holds $C_{ij}(x) = C_{ji}(-x) = C_{ji}^*(x)$: therefore the cancellation to second order (in x), expressed by (F7), *is not a parity cancellation* [unless $i=j$ where by the self-adjointness of the matrix C it follows that $C_{ii}(x)$ is real and, hence, even in x]. If the coefficients $f_{\boldsymbol{\nu}}(\beta)$ are assumed real then the self-adjointness property (E1) implies that $C_{ij}(x)$ is even in x and the second order cancellation at $x=0$ is an obvious parity cancellation and the proof above is greatly simplified, as remarked in the simple cases considered in Refs. 7 and 8.

Having proved that $(\mathcal{M}^{[n]}(0;\eta))_{\gamma'\gamma}=0$ if either $\gamma'=A_i$ or $\gamma=\alpha_j$ and that $(\partial_x\mathcal{M}^{[n]}(0;\eta))_{\gamma'\gamma}=0$ if $\gamma'=A_i$ and $\gamma=\alpha_j$, it must still be shown that the elements $(\mathcal{M}^{[n]}(x;\eta))_{\gamma'\gamma}$ (with the suitable choices of γ' and γ) satisfy appropriate bounds once the factors x determining the order of zero at $x=0$ are extracted. From convergence one expects that the bounds on the rests of the Taylor series in x around $x=0$ should still be proportional to ε^2.

This is in fact true, *under the condition that* (F1) *does not hold*, if (F1) does not hold, then changing the nodes where the external lines are attached to *does not change the scale* of the internal lines. And this implies that the bounds on the derivatives with respect to x are qualitatively the same as the bounds on $\mathcal{M}^{[n]}(x;\eta)$ and boundedness of the entries of $\bar{M}^{[\le n]}$ follows, see (5.12).

APPENDIX G: BOUNDS ON THE PROPAGATOR

In this section we want to get a lower bound for the norm of $(ix-\mathcal{M}^{[n]}(x;\eta))E$, by an approximate computation of its eigenvalue which is lowest in absolute value, for $x^2 \le \rho\eta^{2k_0-1}$, with ρ the same constant appearing in Lemma 3. Moreover we want to prove dimensional bounds for the derivatives in x and ε of the approximate lowest eigenvalue.

Write $(ix-\mathcal{M}^{[\le n]}(x;\eta))E$ as

$$(ix-\mathcal{M}^{[\le n]}(x;\eta))E = \begin{pmatrix} -R^{[\le n]}(x;\eta) & -ix+Q^{[\le n]}(x;\eta) \\ ix+Q^{[\le n]\dagger}(x;\eta) & P^{[\le n]}(x;\eta) \end{pmatrix},$$

where $P^{[\le n]}, Q^{[\le n]}, R^{[\le n]}$ are the matrices defined in (5.12).

The N eigenvalues of $P^{[\leqslant n]}(x;\eta)$ are of order 1 and positive; call them $\mu_1^{(n)} \leqslant \cdots \leqslant \mu_N^{(n)}$. Since $P^{[\leqslant n]}(x;\eta)$ differs from $P^{[0]}(x;\eta)$ by $O(\varepsilon^2)$, the eigenvalues $\mu_i^{(n)}$ can be written as $\mu_i^{(n)} = \mu_i^{(0)}(1 + O(\varepsilon^2))$.

To estimate the smallest eigenvalue of $(ix - \mathcal{M}^{[\leqslant n]}(x;\eta))E$ we can follow a strategy adapted from the proof of Lemma 2. Let $v_\alpha(x;\eta) = \binom{u}{v}$ be an eigenvector of $(ix - \mathcal{M}^{[\leqslant n]}(x;\eta))E$ with eigenvalue α (here u and v are two column vectors of dimension N),

$$\begin{pmatrix} -R^{[\leqslant n]}(x;\eta) & -ix + Q^{[\leqslant n]}(x;\eta) \\ ix + Q^{[\leqslant n]\dagger}(x;\eta) & P^{[\leqslant n]}(x;\eta) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -R^{[\leqslant n]}u + (-ix + Q^{[\leqslant n]})v \\ (ix + Q^{[\leqslant n]\dagger})u + P^{[\leqslant n]}v \end{pmatrix} = \alpha \begin{pmatrix} u \\ v \end{pmatrix}. \tag{G1}$$

To estimate the eigenvalue α with smallest absolute value, we restrict attention to the case $P^{[\leqslant n]} - \alpha \geqslant P^{[\leqslant n]}/2$, as in the opposite case $|\alpha| > \mu_1^{(n)}/2$. Then $(P^{[\leqslant n]} - \alpha)$ is invertible, $(P^{[\leqslant n]} - \alpha)^{-1} = [P^{[\leqslant n]}]^{-1} + O(\alpha)$ and we can rewrite (G1) as

$$\begin{aligned} v &= -(P^{[\leqslant n]} - \alpha)^{-1}(ix + Q^{[\leqslant n]\dagger})u, \\ -R^{[\leqslant n]} &- (-ix + Q^{[\leqslant n]})(P^{[\leqslant n]} - \alpha)^{-1}(ix + Q^{[\leqslant n]\dagger})u = \alpha u. \end{aligned} \tag{G2}$$

From the second of (G2) we see that α must solve an equation of the form

$$\det[N^{[\leqslant n]} - \alpha(1 + O(x) + O(\varepsilon))] = 0, \tag{G3}$$

where we defined $N^{[\leqslant n]} := -R^{[\leqslant n]} - (-ix + Q^{[\leqslant n]})[P^{[\leqslant n]}]^{-1}(ix + Q^{[\leqslant n]\dagger})$ and we used that $Q^{[\leqslant n]} = O(\varepsilon)$. This means that α is an eigenvalue of a Hermitian matrix of the form $N^{[\leqslant n]}(1 + O(x) + O(\varepsilon))$, so that, calling $\lambda_i^{[n]}$ the eigenvalues of $N^{[\leqslant n]}$, we have (see Ref. 20)

$$\alpha = \lambda_i^{[n]}(1 + O(x) + O(\varepsilon)), \tag{G4}$$

for some $i = 1, \ldots, N$. The conclusion of the previous discussion is that the problem of computing the smallest eigenvalue of $(ix - \mathcal{M}^{[n]}(x;\eta))E$ is essentially equivalent to the problem of computing the smallest eigenvalue of $N^{[\leqslant n]}$.

An explicit computation of $N^{[\leqslant n]}$ shows that it can be written in the form

$$\begin{aligned} N^{[\leqslant n]} &= -x^2\mathcal{H}_0^{-1} + \{-R^{[\leqslant n]} + x^2\mathcal{H}_0^{-1} - (-ix + Q^{[\leqslant n]})[P^{[\leqslant n]}]^{-1}(ix + Q^{[\leqslant n]\dagger})\} \\ &= -x^2\mathcal{H}_0^{-1} + \begin{pmatrix} 0 & i\varepsilon x D(\eta) \\ -i\varepsilon x D^\dagger(\eta) & -\varepsilon\eta^{k_0-1}\tilde{M}_{\beta\beta}(\eta) \end{pmatrix} + O(\varepsilon x^2), \end{aligned} \tag{G5}$$

where

$$\mathcal{H}_0 := \begin{pmatrix} \partial_{\mathbf{A}\mathbf{A}}^2 H_0 & \partial_{\mathbf{A}B}^2 H_0 \\ \partial_{B\mathbf{A}}^2 H_0 & \partial_{BB}^2 H_0 \end{pmatrix}, \quad \tilde{M}_{\beta\beta}(\eta) = -ck_0\beta_1^{k_0-1}(1 + O(\eta)), \quad \text{and } D(\eta) = D_0 + O(\eta),$$

with

$$\begin{pmatrix} D_0 \\ 0 \end{pmatrix} := -\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\mathcal{H}_0^{-1}\begin{pmatrix} \partial_{\mathbf{A}\beta}^2 f_{\mathbf{0}}(\beta_0) \\ \partial_{B\beta}^2 f_{\mathbf{0}}(\beta_0) \end{pmatrix}. \tag{G6}$$

The off-diagonal $O(\varepsilon x)$ elements can be eliminated through a small rotation of $N^{[\leqslant n]}$. In fact, defining the Hermitian matrix Z as

$$Z = \begin{pmatrix} 0 & [\tilde{M}_{\beta\beta}(\eta)]^{-1}D(\eta) \\ [\tilde{M}_{\beta\beta}(\eta)]^{-1}D(\eta) & 0 \end{pmatrix}, \tag{G7}$$

a computation shows that

$$e^{ix\eta^{-k_0+1}Z}N^{[\leqslant n]}e^{-ix\eta^{-k_0+1}Z} \equiv -x^2\mathcal{H}_0^{-1} + \delta N^{[\leqslant n]} = -x^2\mathcal{H}_0^{-1} + \begin{pmatrix} 0 & 0 \\ 0 & -\varepsilon\eta^{k_0-1}\tilde{M}_{\beta\beta}(\eta) \end{pmatrix} + O(\eta^{1/2}x^2), \tag{G8}$$

where we used the property $x\eta^{-k_0+1} \leqslant (\rho\eta)^{1/2}$, if $x^2 \leqslant \rho\varepsilon\eta^{k_0-1}$. Multiplying the rhs of (G8) times $\mathcal{H}_0^{1/2}$ both from the left and from the right [remark that $\mathcal{H}_0^{1/2}$ is a well-defined positive $O(1)$ operator] we see that the norm of $N^{[\leqslant n]}$ can be bounded above and below by an $O(1)$ constant times the norm of

$$-x^2 + \mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2}. \tag{G9}$$

Finally, using the explicit structure of $\delta N^{[\leqslant n]}$, see (G8), $N-1$ of the eigenvalues of (G9) are equal to $-x^2(1+O(\eta^{1/2}))$, while the last one is $-x^2(1+O(\eta^{1/2}))-\varepsilon\eta^{k_0-1}\tilde{M}_{\beta\beta}(\varepsilon)\partial_B^2 H_0$.

From this computation, the bound (6.1) of Lemma 5 follows. To address the differentiability of $\lambda^{[n]}(x;\eta)$ with respect to ε and x, we note that $\mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2}$ is C^∞ in the sense of Whitney (because such is $\mathcal{M}^{[\leqslant n]}$, see the corresponding discussion in Appendix A3 of Ref. 15) and its derivatives admit the following dimensional bounds:

$$\|\partial_\varepsilon(\mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2})\| \leqslant C\eta^{k_0-1}, \quad \|\partial_x(\mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2})\| \leqslant C\eta^{k_0}. \tag{G10}$$

Given this and the fact that the last eigenvalue of $\mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2}$ is isolated [it is nondegenerate and its distance from the others is $O(\varepsilon\eta^{k_0-1})$], we can represent $\lambda^{[n]}(x;\eta)$ in the form

$$\lambda^{[n]}(x;\eta) = -\eta^{2k_0-1}\,\mathrm{Tr}\left(\frac{1}{2\pi i}\oint_\gamma \frac{z\,dz}{z-\eta^{1-2k_0}\mathcal{H}_0^{1/2}\delta N^{[\leqslant n]}\mathcal{H}_0^{1/2}}\right), \tag{G11}$$

where z is a complex variable *independent of* ε, x, and γ is a circle in the complex plane around $\tilde{M}_{\beta\beta}(\eta)\partial_B^2 H_0$ not surrounding the origin, with ε-independent radius. The derivatives of $\lambda^{[n]}(x;\eta)$ with respect to ε and x can be computed differentiating the rhs of (G11) and, using the dimensional bounds (G10), we find the same dimensional bounds for the derivatives of $\lambda^{[n]}(x;\eta)$,

$$|\partial_\varepsilon\lambda^{[n]}(x;\eta)| \leqslant C\eta^{k_0-1}, \quad |\partial_x\lambda^{[n]}(x;\eta)| \leqslant C\eta^{k_0}. \tag{G12}$$

The proof of Lemma 5 is concluded.

APPENDIX H: EXCLUDED VALUES OF THE PERTURBATION PARAMETER

In this section we want to check that, by imposing the first condition in (6.8), the measure of excluded values of ε can be bounded by the second of (6.8). To estimate the measure of the excluded ε's we proceed as in Appendix A2 of Ref. 15. We present a proof valid for any $n \geqslant n_0$. The dimensional bounds (6.2) and the property $|\lambda^{[n]}(\eta)-\lambda^{[n-1]}(\eta)| \leqslant Ce^{-\kappa_1 2^{n/\tau_1}}$ (see Lemma 5) implies the following dimensional bound for the derivative of $\sqrt{\lambda^{[n]}(\eta)}$:

$$|\partial_\varepsilon\sqrt{\lambda^{[n]}(\eta)}| \leqslant C'\eta^{-1/2}. \tag{H1}$$

Then the first condition in (6.8) excludes, for each $\boldsymbol{\nu}$, a subinterval of $I(\bar{\varepsilon})$ whose measure is bounded by

$$\frac{C_0 2^{-m/2}\eta^{1/2}}{C'|\boldsymbol{\nu}|^{\tau_1}.} \tag{H2}$$

The Diophantine condition on $\boldsymbol{\omega}$ implies that if the first condition in (6.8) is invalid then $|\boldsymbol{\nu}|$ cannot be too small,

$$\frac{C_0 2^{-m/2}}{|\boldsymbol{\nu}|^{\tau_1}} + \sqrt{\lambda^{[n]}(\eta)} \geqslant |x| \geqslant C_0 |\boldsymbol{\nu}|^{-\tau_0}. \tag{H3}$$

Therefore $C_0/2|\boldsymbol{\nu}|^{\tau_0} \geqslant C'' \eta^{k_0-1/2}$, hence in this case we only have to consider the values of $\boldsymbol{\nu}$ such that $|\boldsymbol{\nu}|^{\tau_0} \geqslant (C_0/2C'')\eta^{1/2-k_0}$. Summing (H2) over the $\boldsymbol{\nu}$'s satisfying this constraint, and using the definition $\tau_1 = \tau_0(1+\delta_1)+N$ we find that the total measure of excluded ε's can be bounded by

$$\frac{C_0 2^{-m/2}\eta^{1/2}}{C'}\left(\frac{2C''\eta^{k_0-1/2}}{C_0}\right)^{1+\delta_1} \sum_{|\boldsymbol{\nu}|\neq 0} \frac{1}{|\boldsymbol{\nu}|^N} \equiv K C_0 2^{-m/2} |\varepsilon| \eta^{\delta_1(k_0-1/2)}, \tag{H4}$$

which is in fact the second inequality in (6.8).

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Covariant irreducible parametrization of electromagnetic fields in arbitrary space-time

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We present a new unified covariant description of electromagnetic field properties for an arbitrary space-time. We derive a complete set of irreducible components describing a six-dimensional electromagnetic field from the Maxwell and metric tensors using the symmetry group SL(2,C). For the special case of a flat space-time metric the components are shown to correspond to the scalar invariants of the electromagnetic field, the energy-momentum-stress tensor and in addition, three new tensors expressing physical observables of rank two and four, respectively. We make a physical interpretation of one of the new rank two tensor as describing a classical intrinsic spin of the electromagnetic field. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162107]

I. INTRODUCTION

The electromagnetic field in Maxwells theory is since long known to satisfy important symmetries and consequently satisfy conservation laws. For example, the conservation law $T^{\alpha\beta}{}_{,\beta}=0$ where $T^{\alpha\beta}$ is the usual energy-momentum-stress tensor expresses the conservation of energy, momentum (Poynting) and stress densities of the electromagnetic field in a (local) Minkowski space. However, these are not the only symmetries and conserved quantities of physical relevance. In Minkowski space the Maxwell equations are invariant under the important inhomogeneous Lorentz group, or as sometimes called, the Poincaré group. The flat space-time of Minkowski space exhibits the maximum degree of symmetry one can obtain.

Moving to the curved space-time of general relativity many of the symmetries are lost, and conservation laws applies only locally. A group arising naturally in the study of general relativity is the group SL(2,C), the group of complex unimodular 2×2 matrices. There exist a homomorphism between SL(2,C) and the proper, orthochronous homogeneous Lorentz group L,

$$\mathrm{SL}(2,\mathrm{C}) \rightarrow \mathrm{L}, \tag{1}$$

reflecting the fact that SL(2,C) is the covering group of L and indicating how local Lorentz invariance is retained.

In this paper we present a new unified treatment of the symmetries of the electromagnetic field in a general Riemannian space-time by calculating the irreducible components of the covariant spectral density tensor. By performing a Fourier transform in time and considering the complex spectral densities we have further generalized to wave fields.

In Sec. II we define the problem of finding the irreducible components by expressing the possible bilinear forms of the electromagnetic field in terms of the covariant spectral density. We then translate this to an equivalent problem under the group SL(2,C) by transforming to the tangent spinor space. After decomposing the spectral density spinor into irreducible components under SL(2,C) we transform back to the equivalent tensors in Riemann space. In Sec. III we study the important special case of a flat space-time and calculate the components explicitly. Some of

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them are shown to correspond to well-known objects in Maxwells theory, while other components obtained have not previously been found in the literature. Finally, in Sec. IV we discuss our conclusions and present ideas for future work.

II. SL(2,C) THEORY OF WAVE FIELD SPECTRAL DENSITIES

A. Covariant spectral density tensor

The fundamental physical object describing the electromagnetic field is the electromagnetic field tensor $f_{\mu\nu}$ which is skew-symmetric in its two indices,

$$f_{\mu\nu} = -f_{\nu\mu}. \tag{2}$$

It is comprised of the six components of the electromagnetic field. We wish to categorize an electromagnetic *wave* field and therefore decompose the electric and magnetic fields in their spectral components. Let $\mathbf{f}(t,\mathbf{r})$ denote either the electric field $\mathbf{E}$ or magnetic field $\mathbf{B}$ at a point in space and time,

$$\mathbf{f}(t,\mathbf{r}) = \begin{pmatrix} f_x(t,\mathbf{r}) \\ f_y(t,\mathbf{r}) \\ f_z(t,\mathbf{r}) \end{pmatrix}. \tag{3}$$

The Fourier transform in time, denoted by capital letters, is then given by

$$\mathbf{F}(\omega,\mathbf{r}) = \int_{-\infty}^{\infty} \mathbf{f}(t,\mathbf{r}) e^{i\omega t}. \tag{4}$$

In the following we assume that the fields $\mathbf{E}$, $\mathbf{B}$, and hence the tensor $F_{\mu\nu}$ are Fourier transformed according to (4). This implies that the tensor $F_{\mu\nu}(\omega,\mathbf{r})$ is now complex. We form all possible bilinear forms of the electromagnetic field by constructing the outer product

$$S = F \otimes F^{\dagger} \tag{5}$$

which in tensor notation becomes

$$S_{\alpha\beta\gamma\delta} = F_{\alpha\beta}\overline{F_{\delta\gamma}}, \tag{6}$$

where the bar denotes complex conjugate. We call the complex tensor $S_{\alpha\beta\gamma\delta}$ in Eq. (6) the *covariant spectral density tensor*. From its definition and the skew-symmetry of $F_{\mu\nu}$, Eq. (2), the symmetries of $S_{\alpha\beta\gamma\delta}$ follows as

$$S_{\alpha\beta\gamma\delta} = -S_{\beta\alpha\gamma\delta} = -S_{\alpha\beta\delta\gamma} = S_{\beta\alpha\delta\gamma}, \tag{7a}$$

$$S_{\alpha\beta\gamma\delta} = \overline{S_{\gamma\delta\alpha\beta}}. \tag{7b}$$

Note that the decomposition in this section is not dependent on the particular transform used, but rather on the local structure and symmetry of the tensor $S_{\alpha\beta\gamma\delta}$. This tensor has $4^4 = 256$ complex components, but only 36 of these are independent due to the symmetries expressed in Eq. (7a). This number is further decreased to half by the symmetry in Eq. (7b). Accordingly, we find that $S_{\alpha\beta\gamma\delta}$ behaves as a six-dimensional Hermitian matrix and has 36 independent real valued components. To find these we will find it convenient to reduce $S_{\alpha\beta\gamma\delta}$ into its irreducible parts. This will be done in the spinor formalism of SL(2,C).

B. Spinor representation of spectral density

Spinors arise in the representation theory of the group SL(2,C). For a short review of the theory of spinors, see the Appendix, or a general reference such as Ref. 1. According to Eq. (A7) we find the spinor equivalent of the covariant spectral density tensor to be given by

$$S_{AB'CD'EF'GH'} = \sigma^{\alpha}_{AB'}\sigma^{\beta}_{CD'}\sigma^{\gamma}_{EF'}\sigma^{\delta}_{GH'}S_{\alpha\beta\gamma\delta}, \tag{8}$$

where the $\sigma^{\mu}_{AB'}$ matrices are the Infeld van der Waerden symbols, related to the metric tensor $g_{\mu\nu}$ by Eq. (A2). We call the spinor $S_{AB'CD'EF'GH'}$ the *spectral density spinor*. The symmetry condition Eq. (7a) and Eq. (8) implies

$$S_{AB'CD'EF'GH'} = -S_{CD'AB'EF'GH'} = -S_{AB'CD'GH'EF'}. \tag{9a}$$

Since $S_{\alpha\beta\gamma\delta}$ is complex, the spectral density spinor is not Hermitian in its indices. To find how $S_{AB'CD'EF'GH'}$ transforms under complex conjugation we consider Eq. (8) and Eqs. (7) with the result

$$S_{AB'CD'EF'GH'} = \overline{S_{HG'FE'DC'BA'}} = \overline{S}_{H'GF'ED'CB'A}. \tag{9b}$$

To find the decomposition of the spectral density spinor we make the observation that the equivalent spectral density tensor satisfies some of the same symmetries, Eq. (7a), as the Riemann tensor. We therefore let Refs. 1 and 2 inspire us in the decomposition and make use of the identities Eqs. (A11) and (A12). Writing the spectral density spinor in a symmetric form

$$S_{AB'CD'EF'GH'} = \tfrac{1}{2}(S_{AB'CD'EF'GH'} - S_{CB'AD'EF'GH'}) + \tfrac{1}{2}(S_{CB'AD'EF'GH'} - S_{CD'AB'EF'GH'}) \tag{10}$$

and applying Eq. (A12) gives

$$S_{AB'CD'EF'GH'} = \tfrac{1}{2}(\varepsilon_{AC}S_{IB'}{}^{I}{}_{D'EF'GH'} + S_{CJ'A}{}^{J'}{}_{EF'GH'}\varepsilon_{B'D'}). \tag{11}$$

Writing Eq. (11) in symmetric form and using Eq. (A12) once more on each term results in

$$\begin{aligned} S_{AB'CD'EF'GH'} = {} & \tfrac{1}{4}\varepsilon_{AC}(S_{IB'}{}^{I}{}_{D'JF'}{}^{J}{}_{H'}\varepsilon_{EG} + S_{IB'}{}^{I}{}_{D'EK'G}{}^{K'}\varepsilon_{F'H'}) \\ & + \tfrac{1}{4}(S_{AI'C}{}^{I'}{}_{JF'}{}^{J}{}_{H'}\varepsilon_{EG} + S_{AI'C}{}^{I'}{}_{EK'G}{}^{K'}\varepsilon_{F'H'})\varepsilon_{B'D'}. \end{aligned} \tag{12}$$

For the spinors in the last three terms in Eq. (12) we introduce the notation

$$\Gamma_{B'D'EG} = \tfrac{1}{4}S_{IB'}{}^{I}{}_{D'EK'G}{}^{K'}, \tag{13}$$

$$\Delta_{ACF'H'} = \tfrac{1}{4}S_{AI'C}{}^{I'}{}_{JF'}{}^{J}{}_{H'}, \tag{14}$$

$$\Sigma_{ACEG} = \tfrac{1}{4}S_{AI'C}{}^{I'}{}_{EK'G}{}^{K'}. \tag{15}$$

From Eq. (9a) and Eqs. (13)–(15) it follows that the symmetries of the decomposed spinors are

$$\Gamma_{B'D'EG} = \Gamma_{D'B'EG} = \Gamma_{B'D'GE}, \tag{16}$$

$$\Delta_{ACF'H'} = \Delta_{CAF'H'} = \Delta_{ACH'F'}, \tag{17}$$

$$\Sigma_{ACEG} = \Sigma_{CAEG} = \Sigma_{ACGE}. \tag{18}$$

For the first term in Eq. (12) we obtain

$$\tfrac{1}{4}S_{IB'\ D'JF'\ H'}^{\ \ I\ \ \ \ J} = \tfrac{1}{4}\overline{S_{FJ'H\ \ BI'D}^{\ \ \ J'\ \ \ \ I'}} = \overline{\Sigma}_{F'H'B'D'}, \tag{19}$$

where we have used Eqs. (9) and Eq. (15). The Γ and Δ spinors in the second and third terms of Eq. (12) both contain mixed indices and do not satisfy a relation similar to Eq. (19). Instead they transform under complex conjugation as

$$\Gamma_{B'D'EG} = \overline{\Gamma_{E'G'BD}} = \overline{\Gamma}_{EGB'D'}, \tag{20}$$

$$\Delta_{ACF'H'} = \overline{\Delta_{FHA'C'}} = \overline{\Delta}_{F'H'AC}, \tag{21}$$

where we have used Eqs. (9). Hence, Eq. (12) can be written as

$$S_{AB'CD'EF'GH'} = \varepsilon_{AC}(\overline{\Sigma}_{F'H'B'D'}\varepsilon_{EG} + \Gamma_{B'D'EG}\varepsilon_{F'H'}) + (\Delta_{ACF'H'}\varepsilon_{EG} + \Sigma_{ACEG}\varepsilon_{F'H'})\varepsilon_{B'D'}. \tag{22}$$

C. Number of independent parameters

From Eq. (22) we may find the number of independent parameters needed to fully describe an electromagnetic wave field. Introducing the notation $(1,2,3)=(00,01=10,11)$ we can write the components of the Σ_{ACEG} spinor as $\Sigma_{0000}=\Sigma_{11}$, $\Sigma_{1000}=\Sigma_{0100}=\Sigma_{21}$, $\Sigma_{1100}=\Sigma_{31}$, and similarily for the other components. From the symmetries in Eq. (18) we can then view the components of Σ_{ACEG} as a matrix $\boldsymbol{\Sigma}$ with nine independent complex components

$$\boldsymbol{\Sigma} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix} \tag{23}$$

or equivalently 18 real independent components. The $\Delta_{ACF'H'}$ and $\Gamma_{B'D'EG}$ spinors in addition to Eq. (16) and Eq. (17) also satisfies Eq. (21) and Eq. (20). Hence the corresponding matrices behave like Hermitian 3×3 matrices $\Delta_{ij}=\overline{\Delta}_{ji}$, $\Gamma_{ij}=\overline{\Gamma}_{ji}$ where $(i,j)\in(1,2,3)$, i.e., $\Delta=\Delta^\dagger$, $\Gamma=\Gamma^\dagger$. Therefore the spinor $\Delta_{ACF'H'}$ has three real components $\Delta_{11},\Delta_{22},\Delta_{33}$ and three complex components $\Delta_{12},\Delta_{13},\Delta_{23}$, in total nine real independent components. The same applies to the $\Gamma_{B'D'EG}$ spinor. In total we find $18+9+9=36$ real independent components describing the wave electromagnetic field in the spinor formulation, in accordance with the discussion following Eq. (7).

D. Irreducible spinor representation

Equation (22) is still not on an irreducible form. To find the first irreducible component we form the contracted spinor

$$S_{AB'CD'} = S^{EF'}{}_{AB'EF'CD'} = \varepsilon_{AC}\varepsilon_{B'D'}\tfrac{1}{2}(\lambda + \lambda^*) - \Gamma_{B'D'AC} - \Delta_{ACB'D'}, \tag{24}$$

where we have defined λ as the trace of the Σ spinor,

$$\lambda = \Sigma_{AE}^{\ \ AE} \tag{25}$$

and used

$$\Sigma_{AE\ C}^{\ E} = \frac{\lambda}{2}\varepsilon_{AC}, \tag{26}$$

$$\overline{\Sigma}_{D'F'\ B'}^{\ \ F'} = \frac{\lambda^*}{2}\varepsilon_{D'B'}. \tag{27}$$

The trace S of the contracted spinor $S_{AB'CD'}$,

$$S = S_{AB'}{}^{AB'} = \varepsilon^{AG}\varepsilon^{B'H'}S_{AB'GH'} = 2(\lambda + \lambda^*) - \Gamma_{B'}{}^{B'}{}_{A}{}^{A} - \Delta_{A}{}^{A}{}_{B'}{}^{B'} = 2(\lambda + \lambda^*) \tag{28}$$

is thus real. We now form the spinor

$$M_{AB'CD'} = S_{AB'CD'} - \tfrac{1}{4}g_{AB'CD'}S \tag{29}$$

which is traceless by construction and hence irreducible. From its definition we find the relations

$$M_{AB'CD'} = -\Gamma_{B'D'AC} - \Delta_{ACB'D'}, \tag{30}$$

$$M_{AB'CD'} = M_{CD'AB'}, \tag{31}$$

$$M_{AB'CD'} = \overline{M_{BA'DC'}}. \tag{32}$$

Calculating the trace of the terms involving the Γ and Δ spinors in Eq. (22) we find

$$M_{AB'CD'} = \varepsilon^{EG}\varepsilon^{F'H'}(\varepsilon_{GA}\varepsilon_{F'D'}\Gamma_{H'B'EC} + \varepsilon_{EC}\varepsilon_{H'B'}\Delta_{GAF'D'}). \tag{33}$$

We therefore write these terms in a form symmetric and antisymmetric in exchange of the first and second against the third and fourth pair of indices with the result

$$\begin{aligned}&\varepsilon_{AC}\varepsilon_{F'H'}\Gamma_{B'D'EG} + \varepsilon_{EG}\varepsilon_{B'D'}\Delta_{ACF'H'}\\ &\quad = \tfrac{1}{2}(\varepsilon_{EG}\varepsilon_{B'D'}D_{AF'CH'} - \varepsilon_{AC}\varepsilon_{F'H'}D_{EB'GD'} - \varepsilon_{AC}\varepsilon_{F'H'}M_{EB'GD'} - \varepsilon_{EG}\varepsilon_{B'D'}M_{AF'CH'}),\end{aligned} \tag{34}$$

where we have also defined

$$D_{AB'CD'} = -\Gamma_{B'D'AC} + \Delta_{ACB'D'} \tag{35}$$

which has the same symmetries as $M_{AB'CD'}$ and is also traceless.

It remains to find the irreducible parts of the Σ spinors in Eq. (22). To this end we write Σ in a form utilizing the symmetries expressed in Eq. (18),

$$\begin{aligned}\Sigma_{ABCD} = \Psi_{ABCD} &+ \frac{1}{3!}(\Sigma_{ABCD} - \Sigma_{DABC}) + \frac{1}{3!}(\Sigma_{ABCD} - \Sigma_{CDAB}) + \frac{1}{3!}(\Sigma_{ABCD} - \Sigma_{BCDA})\\ &+ \frac{1}{3!}(\Sigma_{ABCD} - \Sigma_{DBAC}) + \frac{1}{3!}(\Sigma_{ABCD} - \Sigma_{ACDB}),\end{aligned} \tag{36}$$

where

$$\Psi_{ABCD} = \frac{1}{3!}(\Sigma_{ABCD} + \Sigma_{DABC} + \Sigma_{CDAB} + \Sigma_{BCDA} + \Sigma_{DBAC} + \Sigma_{ACDB}) \tag{37}$$

is a completely symmetric spinor,

$$\Psi_{ABCD} = \Psi_{BACD} = \Psi_{ABDC} = \Psi_{ACBD}. \tag{38}$$

Using Eqs. (A12) and (26) on the remaining terms of Eq. (36) we find

$$\Sigma_{ABCD} = \Psi_{ABCD} + \frac{\lambda}{6}(\varepsilon_{AC}\varepsilon_{BD} + \varepsilon_{AD}\varepsilon_{BC}) + \xi_{ABCD} \tag{39}$$

where we have defined the spinor

$$\xi_{ABCD} = \tfrac{1}{6}(\Sigma_{ABCD} - \Sigma_{CDAB}) \tag{40}$$

satisfying the symmetries

$$\xi_{ABCD} = \xi_{BACD} = \xi_{ABDC} = -\xi_{CDAB}. \tag{41}$$

Inserting Eq. (39) and its complex conjugate equivalent into (22) and using (34) finally gives

$$\begin{aligned} S_{AB'CD'EF'GH'} = C_{AB'CD'EF'GH'} &+ \frac{\lambda}{6}\varepsilon_{B'D'}\varepsilon_{F'H'}(\varepsilon_{AE}\varepsilon_{CG} + \varepsilon_{AG}\varepsilon_{CE}) + \frac{\lambda^*}{6}\varepsilon_{AC}\varepsilon_{EG}(\varepsilon_{F'B'}\varepsilon_{H'D'} \\ &+ \varepsilon_{F'D'}\varepsilon_{H'B'}) + \frac{1}{2}(\varepsilon_{EG}\varepsilon_{B'D'}D_{AF'CH'} - \varepsilon_{AC}\varepsilon_{F'H'}D_{EB'GD'} - \varepsilon_{AC}\varepsilon_{F'H'}M_{EB'GD'} \\ &- \varepsilon_{EG}\varepsilon_{B'D'}M_{AF'CH'}). \end{aligned} \tag{42}$$

The spinor $C_{AB'CD'EF'GH'}$ is defined by

$$C_{AB'CD'EF'GH'} = A_{AB'CD'EF'GH'} + B_{AB'CD'EF'GH'}, \tag{43}$$

where

$$A_{AB'CD'EF'GH'} = \Psi_{ACEG}\varepsilon_{F'H'}\varepsilon_{B'D'} + \overline{\Psi}_{F'H'B'D'}\varepsilon_{AC}\varepsilon_{EG}, \tag{44}$$

and

$$B_{AB'CD'EF'GH'} = \xi_{ACEG}\varepsilon_{F'H'}\varepsilon_{B'D'} + \overline{\xi}_{F'H'B'D'}\varepsilon_{AC}\varepsilon_{EG}. \tag{45}$$

The decomposition of $C_{AB'CD'EF'GH'}$ into A and B is equivalent to a decomposition of the spinor into real and imaginary parts, $A_{AB'CD'EF'GH'} = \Re(C_{AB'CD'EF'GH'})$ and $B_{AB'CD'EF'GH'} = \Im(C_{AB'CD'EF'GH'})$. The spinor $A_{AB'CD'EF'GH'}$ is identically zero when contracted over the first and third pair of indices,

$$A^{EF'}{}_{AB'EF'CD'} = 0, \tag{46}$$

due to its symmetries and real valuedness which is readily verified after some straightforward algebra. The spinor $B_{AB'CD'EF'GH'}$ can be contracted to form

$$\Upsilon_{AB'CD'} = B^{EF'}{}_{AB'EF'CD'} \tag{47}$$

satisfying

$$\Upsilon_{AB'CD'} = -\Upsilon_{CD'AB'} = \overline{\Upsilon}_{CD'AB'} \tag{48}$$

and which is traceless in turn

$$\Upsilon^{AB'CD'}{}_{AB'CD'} = 0. \tag{49}$$

Equations (42)–(47) is comprised only of scalars or traceless spinors and hence is the sought irreducible representation of the spectral density spinor. In summary the decomposition is

$$S_{AB'CD'EF'GH'} = A_{AB'CD'EF'GH'} \oplus \Upsilon_{AB'CD'} \oplus M_{AB'CD'} \oplus D_{AB'CD'} \oplus \lambda. \tag{50}$$

Counting components we find that Eq. (43) has 5 plus 3 complex components from Ψ and ξ, respectively, which follows from the symmetries. From the discussion in Sec. II C we know that the Γ and Δ spinors have nine real components each which implies that M and D have 18 real components in total. Together with the complex invariant λ it adds up to 36 independent real components, in agreement with the above discussion.

E. Relation to the Riemann tensor

We may note that if the covariant spectral density tensor was real and satisfied $S_{\alpha\beta\gamma\delta}=S_{\gamma\delta\alpha\beta}$ instead of Eq. (7b) it would satisfy the same symmetries as the Riemann tensor, $S_{\alpha\beta\gamma\delta}=R_{\alpha\beta\gamma\delta}$. Indeed in such a case $D_{AB'CD'}=0$, $\xi_{AB'CD'}=0$, $\Gamma_{AB'CD'}=\overline{\Delta}_{CD'AB'}$ so that $M_{AB'CD'}=2\Delta_{AB'CD'}$ would be the traceless Ricci spinor, $A_{AB'CD'EF'GH'}=\Psi_{ACEG}\varepsilon_{F'H'}\varepsilon_{B'D'}+\overline{\Psi}_{F'H'B'D'}\varepsilon_{AC}\varepsilon_{EG}$ the traceless Weyl spinor and $\lambda=\lambda^{*}=R$ would be the Ricci scalar curvature. Hence Eq. (42) would be completely analogous to the irreducible spinor representation of the Riemann curvature tensor.

F. Irreducible tensor representation

It is interesting to transform Eq. (42) to its tensor form, using the relation between a spinor and its equivalent tensor, given by Eq. (A9). In summary, we can write this decomposition of the covariant spectral density tensor into its irreducible components symbolically as

$$S_{\alpha\beta\gamma\delta}=A_{\alpha\beta\gamma\delta}\oplus\Upsilon_{\alpha\beta}\oplus M_{\alpha\beta}\oplus D_{\alpha\beta}\oplus\lambda, \tag{51}$$

with the number of independent components $10+6+9+9+2=36$. In connection to this it is worthwhile noting that the complex scalar invariant λ, the only quantity of the electromagnetic field different observers agree on, satisfies

$$\Re(\lambda)=\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}, \tag{52}$$

$$\Im(\lambda)=-\tfrac{1}{8}F_{\mu\nu}{}^{*}F^{\mu\nu}, \tag{53}$$

where ${}^{*}F^{\mu\nu}$ is the dual tensor

$${}^{*}F^{\mu\nu}=\tfrac{1}{2}\varepsilon^{\mu\nu\rho\sigma}F_{\rho\sigma}. \tag{54}$$

Hence, we recover the two scalar invariants of electromagnetic field theory as the real and imaginary parts of the complex scalar invariant of the covariant spectral density tensor.

III. SPECIAL CASE: FLAT SPACE-TIME

In this section we treat the important special case of a flat space-time in the absence of gravitation, with the prescribed metric given by

$$g_{\mu\nu}=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}. \tag{55}$$

The electromagnetic field tensor is represented by

$$F_{\mu\nu}=\begin{pmatrix}0&-E_x&-E_y&-E_z\\E_x&0&B_z&-B_y\\E_y&-B_z&0&B_x\\E_z&B_y&-B_x&0\end{pmatrix} \tag{56}$$

in natural units where we have put $c=1$.

The solution to Eq. (A2) for the given Minkowskian metric Eq. (55) gives the Infeld van der Waerden symbols

$$\sigma^0_{AB'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^1_{AB'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\sigma^2_{AB'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma^3_{AB'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{57}$$

proportional to the Pauli matrices.[1] We now follow the following scheme:

(1) Form the spectral density tensor Eq. (6).
(2) Calculate the spectral density spinor Eq. (8) using Eq. (57).
(3) Calculate Γ, Σ, Δ using Eqs. (13)–(15).
(4) Calculate the irreducible spinor components λ from Eq. (25), $M_{AB'CD'}$ from Eq. (30), $D_{AB'CD'}$ from Eq. (35), Ψ from Eq. (37) and ξ using Eq. (40).
(5) Transform the spinors obtained to their irreducible tensor counterparts using Eq. (A9) and the spinorally contravariant form of Eq. (57).

A. Fundamental objects as irreducible components

By following the above scheme we find the SL(2,C) irreducible tensor components that comprise the spectral density tensor according to Eq. (51). The first tensor, the complex scalar invariant λ is found to be

$$\lambda = \tfrac{1}{2}[|\mathbf{E}|^2 - |\mathbf{B}|^2] + i\Re(\mathbf{E}\cdot\mathbf{B}^*). \tag{58}$$

We identify the real and imaginary parts as the scalar Lagrangian invariant and the pseudoscalar invariant (here expressed in complex form since the fields are Fourier transformed). As is well known, these are the only two invariants that exist in Maxwells theory. This is verified here by the fact that only scalars are true invariants under a general spin frame transformation.

Calculating the components of the first rank two tensor $M_{\alpha\beta}$ we find

$$M_{\alpha\beta} = \begin{pmatrix} \sigma & P_x & P_y & P_z \\ P_x & T_{xx} & T_{xy} & T_{xz} \\ P_y & T_{yx} & T_{yy} & T_{yz} \\ P_z & T_{zx} & T_{zy} & T_{zz} \end{pmatrix}, \tag{59}$$

where we have used the notation

$$\sigma = \tfrac{1}{2}(|\mathbf{E}|^2 + |\mathbf{B}|^2), \tag{60}$$

$$P_x = \tfrac{1}{2}[\Re(E_y B_z^*) - \Re(B_y^* E_z)], \tag{61}$$

$$P_y = \tfrac{1}{2}[\Re(E_z B_x^*) - \Re(B_z^* E_x)], \tag{62}$$

$$P_z = \tfrac{1}{2}[\Re(E_x B_y^*) - \Re(B_x^* E_y)], \tag{63}$$

$$T_{ij} = -\Re[E_i E_j^* + B_i B_j^*] + \delta_{ij}\sigma. \tag{64}$$

We immediately recognize Eq. (59) as the energy-momentum-stress tensor in Maxwells theory, here obtained as one of the irreducible components of the spectral density tensor under SL(2,C). We identify as usual σ as the energy density of the electromagnetic field, $(P_x, P_y, P_z) = \frac{1}{2}\Re(\mathbf{E}\times\mathbf{B}^*)$ as the complex Poynting vector and T_{ij} as the three-dimensional Maxwell stress tensor.

Turning our attention to the second rank two irreducible tensor $D_{\alpha\beta}$ we find analogously

$$D_{\alpha\beta}=\begin{pmatrix} K & Q_x & Q_y & Q_z \\ Q_x & U_{xx} & U_{xy} & U_{xz} \\ Q_y & U_{yx} & U_{yy} & U_{yz} \\ Q_z & U_{zx} & U_{zy} & U_{zz} \end{pmatrix}, \tag{65}$$

where we have used the notation

$$K=-\Im(\mathbf{E}\cdot\mathbf{B}^*), \tag{66}$$

$$\mathbf{Q}=-\frac{i}{2}(\mathbf{E}\times\mathbf{E}^*+\mathbf{B}\times\mathbf{B}^*), \tag{67}$$

$$U_{ij}=-\Im[E_i^*B_j-B_i^*E_j]+\delta_{ij}K. \tag{68}$$

We identify the D_{00} component as the imaginary part of the pseudoscalar invariant of the electromagnetic field. Since also, e.g., $Q_x=-\Im(E_zE_y^*+B_zB_y^*)$ we note that all components of the tensor $D_{\alpha\beta}$ can be written as imaginary parts. In analogy with σ, the energy density Eq. (60), we may denote Eq. (66) the spin density of the electromagnetic field. This is because **Q**, Eq. (67), is only different from zero in the case when the electromagnetic field is elliptically (i.e., not linearly) polarized. We call **Q** the "spin flux density."

Finally we calculate the components of the remaining rank four tensor $C_{\alpha\beta\gamma\delta}$. Its real part $A_{\alpha\beta\gamma\delta}$ is traceless

$$A^{\gamma}{}_{\alpha\gamma\beta}=0 \tag{69}$$

when contracted. This tensor has 10 independent components. In order to write this rank four tensor on a compact form, we introduce the bijective mapping of the index pairs $(1,0)\leftrightarrow(1)$, $(2,0)\leftrightarrow(2)$, $(3,0)\leftrightarrow(3)$, $(3,2)\leftrightarrow(4)$, $-(3,1)\leftrightarrow(5)$, $(2,1)\leftrightarrow(6)$. We can then construct the column sixtors A_k, where, for example, the first vector is $A_1=(A_{1010},A_{1020},A_{1030},A_{1032},-A_{1031},A_{1021})^T$. The tensor $A_{\alpha\beta\gamma\delta}$ is then equivalent to the 6×6 matrix $A_{kl}=(A_1A_2A_3A_4A_5A_6)$. In index notation it becomes

$$A_{\alpha\beta\gamma\delta}\leftrightarrow\begin{pmatrix} E & F \\ F & -E \end{pmatrix}, \tag{70}$$

where the two block matrices

$$E=E_{ij}=-\tfrac{1}{2}\Re(E_i^*E_j-B_i^*B_j)+\tfrac{2}{6}\Re(\lambda)\delta_{ij} \tag{71}$$

and

$$F=F_{ij}=-\tfrac{1}{2}\Re(E_i^*B_j+B_i^*E_j)+\tfrac{2}{6}\Im(\lambda)\delta_{ij} \tag{72}$$

each contains five independent components.

The contracted imaginary part of $C_{\alpha\beta\gamma\delta}$ behaves as an antisymmetric Hermitian matrix and have the components

$$\Upsilon_{\alpha\beta}=\begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ S_x & 0 & \cdot & \cdot \\ S_y & V_{yx} & 0 & \cdot \\ S_z & V_{zx} & V_{zy} & 0 \end{pmatrix}, \tag{73}$$

where

$$S = (S_x, S_y, S_z) = -\frac{i}{3}\Im(\mathbf{E} \times \mathbf{B}^*) \tag{74}$$

is the imaginary part of the complex Poynting vector and

$$V_{ij} = -\frac{i}{3}\Im(E_i^* E_j - B_i^* B_j) \tag{75}$$

is a three-tensor.

B. Physical interpretation

Interestingly, as we noted above, the real part of the scalar invariant Eq. (58) of the electromagnetic field would play the role of the Ricci scalar curvature in the case of real valued fields. Similarly the energy-momentum-stress tensor $M_{\alpha\beta}$ would play the role of the Ricci tensor, while the rank four tensor $A_{\alpha\beta\gamma\delta}$ would be analogous to the Weyl conformal tensor. While we could proceed with the analogy of curvature of space-time to the "curvature" of the electromagnetic field, we will not pursue this topic further in the present paper.

The fact that the two possible true invariants of the electromagnetic field are found as the real and imaginary parts of the complex scalar invariant is natural, since all inertial observers should agree upon their measured values. That the energy-momentum-stress tensor is found to be an irreducible component under SL(2,C) is encouraging and stress its importance in Maxwells theory.

More surprising is the (pseudo-) tensor $D_{\alpha\beta}$ found as the second irreducible rank two component. To the authors knowledge, this rank two tensor has not been written down explicitly in this form before.[3] We stress that this tensor is obtained on equal footing and occur as naturally as the energy-momentum stress tensor in our analysis. The components of $D_{\alpha\beta}$ represents observables, with a clear physical meaning of classical "spin". The new rank four tensor $C_{\alpha\beta\gamma\delta}$ is complex valued. Although the contracted imaginary part $\Upsilon_{\alpha\beta}$ is containing the imaginary part of the complex Poynting vector its physical interpretation is not yet clear and is left for a future study.

IV. CONCLUSIONS AND OUTLOOK

We have considered all possible bilinear forms of the electromagnetic Fourier transformed field for an arbitrary time-independent metric in Riemannian space-time. The constructed spectral density tensor was decomposed into irreducible components by considering the spectral density spinor in the complex tangent space introduced under the group SL(2,C). The spectral density was found to be comprised of the following irreducible components: a complex scalar invariant corresponding to the two known invariants of the electromagnetic field, the rank two energy-momentum-stress tensor, another new rank two tensor expressing the spin (polarization) properties of the electromagnetic field, another rank two tensor, containing the imaginary part of the complex Poynting vector, and finally a new rank four tensor. This decomposition is expressed in Eqs (50) and (51). While the first two tensors (scalar and stress tensor) are well-known important objects in Maxwells theory, the new rank two and rank four tensors are very little or not at all previously studied. Since they are irreducible components under the group transformations we propose that they also are conserved quantities of the electromagnetic field. Considering how they arise as naturally and inevitably as the ususal energy-momentum-stress tensor, they certainly deserve further study. We leave the detailed study of the discovered components and their conservation laws to a future investigation.

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APPENDIX: SPINOR REPRESENTATION OF THE GROUP SL(2,C) IN CURVED SPACE-TIME

In this appendix we review the theory of spinors and how they are applied to general relativity. In a Riemannian space one can to each point in space-time introduce a complex two-dimensional tangent space. For every tensor in Riemannian space there is then a corresponding complex spinor in the tangent spinor space. For every tensor index labeled with greek letters running over 0, 1, 2, 3 there are then two spinor indices labeled with capital letters running over 0, 1. Primed spinor indices belong to the complex conjugate spinor space and and runs over $0',1'$. Spinors originate from the representation theory of the group SL(2,C). We use a matrix representation in which a typical element g of the group SL(2,C) is represented by the matrix

$$g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad ad-bc=1 \tag{A1}$$

with determinant unity.

The correspondence between tensors and spinors are established by the Infeld van der Waerden symbols, a set of four 2×2 Hermitian matrices $\sigma^{\mu}_{AB'}(x^{\nu})$, which are functions of space-time. These objects transform as a tensor in greek indices, and as a spinor in italic indices. They satisfy the relation

$$g_{\mu\nu}\sigma^{\mu}_{AB'}\sigma^{\nu}_{CD'}=\varepsilon_{AC}\varepsilon_{B'D'} \tag{A2}$$

relating the Infeld van der Waerden symbols to the metric tensor of Riemannian space and the Levi-Cevita symbols, represented by

$$\varepsilon_{AC}=\varepsilon_{B'D'}=\varepsilon^{AC}=\varepsilon^{B'D'}=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{A3}$$

The Levi-Cevita symbols play the spinor role analog to the metric tensors. The operation of raising and lowering spinor indices are accomplished by

$$\eta^{A}=\varepsilon^{AB}\eta_{B}, \quad \eta_{A}=\eta^{B}\varepsilon_{BA} \tag{A4}$$

and analogously for primed indices

$$\xi^{A'}=\varepsilon^{A'B'}\xi_{B'}, \quad \xi_{A'}=\xi^{B'}\varepsilon_{B'A'}. \tag{A5}$$

One can easily check that the spinor of the metric tensor satisfies

$$g_{AB'CD'}=\varepsilon_{AC}\varepsilon_{B'D'}. \tag{A6}$$

The relation between a tensor $T_{\mu\nu}$ and the corresponding spinor is given by

$$T_{AB'CD'}=\sigma^{\mu}_{AB'}\sigma^{\nu}_{CD'}T_{\mu\nu} \tag{A7}$$

and analogously for tensors with more indices. If the tensor is real valued, the spinor equivalent is Hermitian, e.g., the real valued vector A_{μ} has an equivalent Hermitian spinor

$$A_{AB'}=\overline{A_{BA'}}=\overline{A}_{B'A}. \tag{A8}$$

If the tensor is complex the hermicity condition of the spinor does not hold. This is the case for most spinors encountered in this paper. Finally, given a spinor $T_{AB'CD'}$ its tensor equivalent $T_{\mu\nu}$ is given by

$$\sigma^{AB'}_{\mu}\sigma^{CD'}_{\nu}T_{AB'CD'}=T_{\mu\nu}. \tag{A9}$$

We also list the following useful spinor relations:

$$\varepsilon^{AB}\varepsilon_{CA} = -\,\delta_C^{\ B}, \tag{A10}$$

$$\xi_{AB} - \xi_{BA} = \xi_C^{\ C}\varepsilon_{AB} = \varepsilon^{CD}\xi_{CD}\varepsilon_{AB}, \tag{A11}$$

$$\psi_{ABCD} - \psi_{BACD} = \psi_F^{\ F}{}_{CD}\varepsilon_{AB} = \varepsilon^{FG}\psi_{FGCD}\varepsilon_{AB}. \tag{A12}$$

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Some mathematical properties of Maxwell's equations for macroscopic dielectrics

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We consider a number of mathematical properties of Maxwell's equations for linear dispersive and absorptive dielectric media using the auxiliary field method developed earlier by the author [A. Tip, Phys. Rev. A **57**, 4818 (1998)]. Here the fields are interpreted as square integrable functions of $\mathbf{x} \in \mathbb{R}^3$. In case the susceptibility $\chi(\mathbf{x},t)$ is piecewise constant in $\mathbf{x}$, we show rigorously that a decomposition into independent equations for longitudinal and transverse fields can be made. We point out its relevance for the study of spectral properties of photonic crystals. Again, for the piecewise constant case we discuss the usual boundary conditions at interfaces and discuss the different nature of those for the longitudinal and transverse fields. Then we consider energy conservation for dispersive, nonabsorptive, media. We show that additional contributions to the free field energy density, as given in the literature, are associated with the energy stored in the auxiliary field modes. Finally, we show that also for nonlinear dielectrics it is possible to obtain a conserved energy by introducing auxiliary fields. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In the present paper we discuss some mathematical properties of the classical phenomenological Maxwell's equations for linear dielectrics, considering the fields as square integrable functions. Indeed, outside the realm of electrostatics, the propagation of electromagnetic waves is a major issue and it can be advantageous to employ a Hilbert space formulation. Then concepts known from the Schrödinger case can be taken over, notably for scattering and spatially periodic systems. In the first Møller (wave) operators naturally appear, whereas in the second the Bloch–Floquet decomposition is a convenient tool to study the spectral band structure of photonic crystals (PCs). A basic observation is here that the energy

$$\mathcal{E}_{\mathrm{em}}(t) = \frac{1}{2}\int d\mathbf{x}\{\mathbf{E}(\mathbf{x},t)^2 + \mathbf{B}(\mathbf{x},t)^2\} \tag{1.1}$$

of an electromagnetic system in vacuum, is a conserved quantity, so Eq. (1.1) can be used to introduce a norm and associated Hilbert space, leading to a unitary time evolution. However, macroscopic dielectrics have a more complicated structure and the situation is not as straightforward. The main obstacle is the appearance of a time convolution in the constitutive equation relating the displacement $\mathbf{D}(\mathbf{x},t)$ and electric field $\mathbf{E}(\mathbf{x},t)$,

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$$\mathbf{D}(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t) + \mathbf{P}(\mathbf{x},t), \quad \mathbf{P}(\mathbf{x},t) = \int_{t_0}^{t} ds\, \chi(\mathbf{x},t-s)\mathbf{E}(\mathbf{x},s). \tag{1.2}$$

Nevertheless, as shown earlier by the author,[1] it is possible, by introducing two auxiliary fields, to obtain once more a description as a unitary time evolution in an appropriate Hilbert space. In a subsequent paper, with Moroz and Combes,[2] a mathematically precise theory of photonic crystals made up from general dispersive or absorptive dielectric material was given.

In the present work, after introducing the general formalism for macroscopic absorptive and dispersive systems, the emphasis will be on systems where the electric susceptibility $\chi(\mathbf{x},t)$ is piecewise constant as a function of $\mathbf{x}$, which is the typical situation for the scattering of electromagnetic waves from a homogeneous dielectric object and for PCs. For this case we show that an exact decomposition into separate sets of equations of motion for the transverse and longitudinal field components is possible. Here we use the momentum space definition of longitudinal and transverse components, valid for general square integrable fields, which reduces to the usual characterizations $\partial_{\mathbf{x}} \cdot \mathbf{f} = 0$ for transverse and $\partial_{\mathbf{x}} \times \mathbf{f} = 0$ for longitudinal fields for sufficiently smooth $\mathbf{f}$.

We then turn to the discussion of initial and boundary conditions. Although in electrostatics the continuity across interfaces of the normal component of the displacement $\mathbf{D}$ and the tangential components of the electric field $\mathbf{E}$ are often treated in a similar way, using Gauss' and Stokes' theorems, we show that they are of a different nature. The first is actually an initial condition on the system, whereas the second is not required at all for the existence of a time evolution, but makes its appearance in the differential form of Maxwell's equations and in eigenvalue problems. In this connection we note that we are dealing with elements of a Hilbert space, which are equivalence classes of square integrable functions. Within this context, continuity means that the equivalence class contains a continuous element.

Next we consider the conservation of energy for dispersive dielectrics. Although energy is expected to be conserved in the absence of absorption, it depends on which energy is actually considered. We show that the existing approximate expressions for the conserved energy density in fact consist of the sum of the electromagnetic one and the part contained in the auxiliary field modes.

Since the existence of a conserved energy plays an important role in the development of the theory presented here, we finally show that it is also possible to define a conserved energy for nonlinear dielectrics. Here we take the opportunity to discuss an alternative, equivalent, method to introduce auxiliary fields.

II. MAXWELL'S EQUATIONS AND THE LINEAR SUSCEPTIBILITY

A. Maxwell's equations

Here we summarize our earlier results[1] and start off by proceeding formally, but in the next section will end up with a precise setting where Maxwell's equations are recast as a unitary time evolution on a Hilbert space. As said this is *a priori* not evident in view of the time convolution in Eq. (1.2).

The macroscopic Maxwell's equations pertaining to absorptive and dispersive dielectrics are (we set $\varepsilon_0 = \mu_0 = 1$ and, in quantum situations, also $\hbar = 1$)

$$\partial_t \mathbf{D}(\mathbf{x},t) = \partial_{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t), \quad \partial_t \mathbf{B}(\mathbf{x},t) = -\partial_{\mathbf{x}} \times \mathbf{E}(\mathbf{x},t),$$

$$\partial_{\mathbf{x}} \cdot \mathbf{D}(\mathbf{x},t) = \partial_{\mathbf{x}} \cdot \mathbf{B}(\mathbf{x},t) = 0, \quad \mathbf{D}(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t) + \mathbf{P}(\mathbf{x},t), \tag{2.1}$$

where, in the isotropic linear case considered here, the polarization field $\mathbf{P}(\mathbf{x},t)$ is related to the electric field according to

$$\mathbf{P}(\mathbf{x},t) = \int_{t_0}^{t} ds\, \chi(\mathbf{x},t-s)\mathbf{E}(\mathbf{x},s), \quad \chi(\mathbf{x},t) = 0, \quad t \leqslant 0, \tag{2.2}$$

with $\chi(\mathbf{x},t)$ the electric susceptibility, which we consider as a given quantity. We are primarily concerned with the situation where the dielectric of interest fills the part of space outside of which we have a vacuum or an isotropic, spatially homogeneous, background medium, characterized by the dielectric constant $\varepsilon_{\mathrm{bg}}$, so $\mathbf{D}(\mathbf{x},t)=\varepsilon_{\mathrm{bg}}\mathbf{E}(\mathbf{x},t)$ for $\mathbf{x}$ in the background. By a simple rescaling, both cases can be treated in the same way. In Ref. 1 the situation where $\varepsilon_{\mathrm{bg}}$ depends on $\mathbf{x}$ was also considered.

We assume that $\chi(\mathbf{x},t)$ is measurable in $\mathbf{x}$ and differentiable in t [we denote $\partial_t\chi(\mathbf{x},t) = \chi'(\mathbf{x},t)$], satisfying

$$\chi(\mathbf{x},t) = 0, \quad t < 0, \quad \chi(\mathbf{x},0) = 0, \quad |\chi'(\mathbf{x},t)| \leqslant c' < \infty, \quad \forall\, \mathbf{x},t. \tag{2.3}$$

The vanishing of $\chi(\mathbf{x},t)$ for negative times is a consequence of causality, whereas its vanishing at $t=0$ excludes nonphysical initial surges in the current density $\mathbf{J}(\mathbf{x},t)=\partial_t\mathbf{P}(\mathbf{x},t)$.

An important special case is the situation where the material is contained in a set $\mathcal{A}\subset\mathbb{R}^3$, surrounded by the background medium, where $\mathcal{A}$ may be made up from a collection of nonoverlapping subsets, $\mathcal{A}=\cup_j\mathcal{A}_j$, $\mathcal{A}_j\cap\mathcal{A}_h=\varnothing$, $j\neq h$, with the boundaries of the subsets having certain regularity properties (spheres, cubes, a set of parallel layers or a half-space). In order to keep the bookkeeping simple, we assume that the susceptibility is homogeneous over each $\mathcal{A}_j$, so

$$\chi(\mathbf{x},t) = \sum_j \mathbf{I}_{\mathcal{A}_j}(\mathbf{x}) g_j(t), \tag{2.4}$$

where $\mathbf{I}_{\mathcal{M}}(\mathbf{x})$ is the characteristic function for the set $\mathcal{M}$, $\mathbf{I}_{\mathcal{M}}(\mathbf{x})=1$, $\mathbf{x}\in\mathcal{M}$, and vanishes otherwise. For PCs (see Sec. IV) the $\mathcal{A}_j$'s are identical sets with identical positions in the unit cells with the same $g(t)$.

Definition: We refer to the situation given by Eq. (2.4) as the piecewise constant case.

B. The susceptibility

We now turn to the general properties of the electric susceptibility $\chi(\mathbf{x},t)$. First we recast the first of Eqs. (2.1) according to

$$\partial_t\mathbf{E}(\mathbf{x},t) = \partial_{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t) - \mathbf{J}(\mathbf{x},t), \quad \mathbf{J}(\mathbf{x},t) = \int_{t_0}^{t} ds\, \chi'(\mathbf{x},t-s)\mathbf{E}(\mathbf{x},s). \tag{2.5}$$

With $\mathcal{E}_{\mathrm{em}}(t)$ as given by Eq. (1.1), we noted in Ref. 5 that, adapting to the present notation,

$$\Delta\mathcal{E}_{\mathrm{em}}(t) \equiv \mathcal{E}_{\mathrm{em}}(t) - \mathcal{E}_{\mathrm{em}}(t_0) = -\int d\mathbf{x} \int_{t_0}^{t} ds \int_{t_0}^{t} du\, \chi'(\mathbf{x},s-u)\mathbf{E}(\mathbf{x},u)\cdot\mathbf{E}(\mathbf{x},s). \tag{2.6}$$

Denoting Laplace transforms with an overcaret,

$$\hat{f}(z) = \int_0^\infty dt\, \exp[izt] f(t), \quad \mathrm{Im}\, z > 0, \quad f(t) = \frac{1}{2\pi}\int d\omega\, \exp[-i(\omega+i\delta)t]\hat{f}(\omega+i\delta), \quad \delta > 0, \tag{2.7}$$

we then have, since $\chi(\mathbf{x},0)=0$,

$$\hat{\chi}'(\mathbf{x},z) = -iz\hat{\chi}(\mathbf{x},z), \tag{2.8}$$

and both $\hat{\chi}(\mathbf{x},z)$ and $\hat{\chi}'(\mathbf{x},z)$ are analytic in the open upper complex half-plane $\mathbb{C}^+$. In addition, we note that, in view of Eqs. (2.3), for $y>0$,

$$y|\hat{\chi}'(\mathbf{x},iy)| \leqslant c'. \tag{2.9}$$

We now write

$$\begin{aligned}\Delta\mathcal{E}_{\mathrm{em}}(t) &= -\frac{1}{2\pi}\int d\mathbf{x}\int d\omega\,\hat{\chi}'(\mathbf{x},\omega+i\delta)\left|\int_{t_0}^{t} ds\,\exp[-i(\omega+i\delta)s]\mathbf{E}(\mathbf{x},s)\right|^2 \\ &= -\frac{1}{2\pi}\int d\mathbf{x}\int d\omega\,\mathrm{Re}\,\hat{\chi}'(\mathbf{x},\omega+i\delta)\left|\int_{t_0}^{t} ds\,\exp[-i(\omega+i\delta)s]\mathbf{E}(\mathbf{x},s)\right|^2. \end{aligned}\tag{2.10}$$

Definition: We define the class of dispersive and absorptive systems as that for which $\Delta\mathcal{E}_{\mathrm{em}}(t)$ is nonincreasing.

For such systems $\mathrm{Re}\,\hat{\chi}'(\mathbf{x},z)\geqslant 0$, $z\in\mathbb{C}^+$, and taking the other properties of $\hat{\chi}'(\mathbf{x},z)$ into account, we conclude that $i\hat{\chi}'(\mathbf{x},z)$ is a Herglotz function (for a useful summary of the properties of Herglotz functions, see Ref. 4). Hence, $\hat{\chi}'(\mathbf{x},z)$ can be represented as

$$\hat{\chi}'(\mathbf{x},z) = -i\int \nu(\mathbf{x},d\lambda)\frac{1}{\lambda-z}, \tag{2.11}$$

where $\nu(\mathbf{x},d\lambda)$ is a non-negative measure with finite total measure $\nu(\mathbf{x},\mathbb{R})$. Then $\chi'(\mathbf{x},t)=\int\nu(\mathbf{x},d\lambda)\exp[-i\lambda t]$ and since $\chi'(\mathbf{x},t)$ is real, we can, without loss of generality, assume that $\nu(\mathbf{x},d\lambda)$ is even in λ. We discussed these matters before in Ref. 5, but in a more roundabout way. We now decompose $\nu(\mathbf{x},d\lambda)$ into parts that are absolutely continuous and singular continuous with respect to Lebesgue measure and a pure point (discrete) part,

$$\nu(\mathbf{x},d\lambda) = \nu_{ac}(\mathbf{x},d\lambda)+\nu_{\mathrm{sing}}(\mathbf{x},d\lambda)+\nu_p(\mathbf{x},d\lambda) = \nu(\mathbf{x},\lambda)d\lambda+\nu_{\mathrm{sing}}(\mathbf{x},d\lambda)+\sum_n \nu_n(\mathbf{x})\delta(\lambda-\omega_n)d\lambda. \tag{2.12}$$

We shall dismiss $\nu_{\mathrm{sing}}(\mathbf{x},d\lambda)$ since it has no apparent physical applications, and in the sequel we shall absorb the point measure part in $\nu(\mathbf{x},\lambda)d\lambda$, so

$$\chi'(\mathbf{x},t) = \int d\lambda\ \nu(\mathbf{x},\lambda)\cos\lambda t, \quad t\geqslant 0, \quad \nu(\mathbf{x},\lambda) = \frac{1}{\pi}\int_0^\infty dt\ \chi'(\mathbf{x},t)\cos\lambda t,$$

$$\hat{\chi}(\mathbf{x},z) = \int d\lambda\ \nu(\mathbf{x},\lambda)\frac{1}{\lambda^2-z^2}, \quad \hat{\chi}'(\mathbf{x},z) = -iz\int d\lambda\ \nu(\mathbf{x},\lambda)\frac{1}{\lambda^2-z^2},$$

$$\mathrm{Re}\,\hat{\chi}'(\mathbf{x},\omega+i0) = \omega\,\mathrm{Im}\,\hat{\chi}(\mathbf{x},\omega+i0) = \pi\nu(\mathbf{x},\omega),$$

$$\Delta\mathcal{E}_{\mathrm{em}}(t) = -\frac{1}{2}\int d\mathbf{x}\int d\lambda\ \nu(\mathbf{x},\lambda)\left|\int_{t_0}^{t} ds\,\exp[i\lambda s]\mathbf{E}(\mathbf{x},s)\right|^2. \tag{2.13}$$

Definition: Absorptive systems are those for which $\nu(\mathbf{x},\lambda)$ is absolutely continuous and dispersive systems those for which it is a set of point measures. Obviously we can refine this to absorptive and dispersive intervals.

The general Drude–Lorentz susceptibility in a space region where $\chi(\mathbf{x},t)$ does not depend on $\mathbf{x}$, is

$$\hat{\chi}(z) = -\frac{\Omega_0^2}{z^2 + i\gamma_0 z} - \sum_{n=1}^{\infty} \frac{\Omega_n^2}{z^2 + i\gamma_n z - \omega_n^2}, \quad \Omega_0, \Omega_n, \omega_n, \gamma_n > 0. \tag{2.14}$$

The point measure case is then obtained by setting $\gamma_n = 0$, i.e., the dispersive Drude–Lorentz susceptibility is

$$\hat{\chi}(z) = -\frac{\Omega_0^2}{z^2} - \sum_{n=0}^{\infty} \frac{\Omega_n^2}{z^2 - \omega_n^2}, \quad \chi(t) = \Omega_0^2 t + \sum_{n=1}^{\infty} \Omega_n^2 \frac{\sin \omega_n t}{\omega_n}, \quad \chi'(t) = \Omega_0^2 + \sum_{n=1}^{\infty} \Omega_n^2 \cos \omega_n t, \quad t \geqslant 0. \tag{2.15}$$

The dispersive Drude case, $\hat{\chi}(z) = -\Omega_0^2/z^2$, is somewhat pathological, $\chi(t)$ growing linearly in t. But it still fits into the formalism we are going to develop.

Returning to our original notation, it follows from

$$\partial_z\{z\hat{\chi}(\mathbf{x}, z)\} = \int d\lambda\ \nu(\mathbf{x}, \lambda) \frac{\lambda^2 + z^2}{(\lambda^2 - z^2)^2}, \tag{2.16}$$

that in the dispersive case, for real $\omega \neq \omega_n$,

$$\partial_\omega\{\omega\hat{\chi}(\mathbf{x}, \omega)\} = \sum_n \nu_n(\mathbf{x}) \frac{\omega^2 + \omega_n^2}{(\omega^2 - \omega_n^2)^2} \geqslant 0, \tag{2.17}$$

a quantity that occurs in work concerning the energy of dispersive dielectrics,[6,7] as discussed later on.

C. The Helmholtz equation

If $t_0 = 0$, so $\mathbf{D}(\mathbf{x}, 0) = \mathbf{E}(\mathbf{x}, 0)$, we can Laplace transform Maxwell's equations, resulting in the inhomogeneous Helmholtz equation

$$[z^2\varepsilon(\mathbf{x}, z) - \mathbf{h}] \cdot \hat{\mathbf{E}}(\mathbf{x}, z) = iz\mathbf{E}(\mathbf{x}, 0) - \partial_{\mathbf{x}} \times \mathbf{B}(\mathbf{x}, 0), \quad \operatorname{Im} z > 0, \tag{2.18}$$

where

$$\hat{\mathbf{D}}(\mathbf{x}, z) = \varepsilon(\mathbf{x}, z)\hat{\mathbf{E}}(\mathbf{x}, z), \quad \varepsilon(\mathbf{x}, z) = 1 + \hat{\chi}(\mathbf{x}, z), \quad \mathbf{h} = \partial_{\mathbf{x}} \times (\partial_{\mathbf{x}} \times \cdots). \tag{2.19}$$

But if $t_0 = -\infty$ this becomes problematic since then there is an additional term $\hat{\chi}(\mathbf{x}, z)\int_{-\infty}^{0} dt \exp[izt]\mathbf{E}(\mathbf{x}, t)$, which can be infinite. In this case we can try to Fourier transform Maxwell's equations. Proceeding formally, we find for

$$\tilde{\mathbf{E}}(\mathbf{x}, \omega) = (2\pi)^{-1/2} \int dt \exp[i\omega t]\mathbf{E}(\mathbf{x}, t), \tag{2.20}$$

that $[\varepsilon(\mathbf{x}, \omega) = 1 + \hat{\chi}(\mathbf{x}, \omega + i0)$, so $\operatorname{Im} \omega\varepsilon(\mathbf{x}, \omega) = \pi\nu(\mathbf{x}, \omega) \geqslant 0]$

$$[\omega^2\varepsilon(\mathbf{x}, \omega) - \mathbf{h}] \cdot \tilde{\mathbf{E}}(\mathbf{x}, \omega) = 0. \tag{2.21}$$

Assuming $\tilde{\mathbf{E}}(\mathbf{x}, \omega)$ to be locally square integrable in $\mathbf{x}$, we have for a bounded measurable set $\mathcal{M} \subset \mathbb{R}^3$,

$$\operatorname{Im} \int_{\mathcal{M}} d\mathbf{x}\{[\omega^2\varepsilon(\mathbf{x}, \omega) - \mathbf{h}] \cdot \tilde{\mathbf{E}}(\mathbf{x}, \omega)\} \cdot \overline{\tilde{\mathbf{E}}(\mathbf{x}, \omega)} = \pi\omega \int_{\mathcal{M}} d\mathbf{x}\ \nu(\mathbf{x}, \omega)|\tilde{\mathbf{E}}(\mathbf{x}, \omega)|^2 = 0. \tag{2.22}$$

For a dispersive system this becomes

$$\pi\omega\sum_n \delta(\omega-\omega_n)\int_{\mathcal{M}} d\mathbf{x}\ \nu_n(\mathbf{x})|\tilde{\mathbf{E}}(\mathbf{x},\omega_n)|^2=0, \tag{2.23}$$

so $\tilde{\mathbf{E}}(\mathbf{x},\omega_n)=0$, for all $\mathbf{x}$ for which $\nu_n(\mathbf{x})\neq 0$, i.e., Eq. (2.20) has no solutions for $\omega=\omega_n$. Then, letting $t_0\to-\infty$ and $t\to\infty$,

$$\Delta\mathcal{E}_{\rm em}=\mathcal{E}_{\rm em}(\infty)-\mathcal{E}_{\rm em}(-\infty)=-\frac{1}{2}\int d\mathbf{x}\int d\lambda\ \nu(\mathbf{x},\lambda)|\tilde{\mathbf{E}}(\mathbf{x},\lambda)|^2=-\frac{1}{2}\sum_n\ \int d\mathbf{x}\ \nu_n(\mathbf{x})|\tilde{\mathbf{E}}(\mathbf{x},\omega_n)|^2=0, \tag{2.24}$$

so $\Delta\mathcal{E}_{\rm em}=0$ for dispersive systems, justifying the above definition. Thus, although $\Delta\mathcal{E}_{\rm em}(t)$ is time dependent, asymptotically it turns back to its initial value. Note that the above manipulations are of a formal nature. But, as shown later on for the PC case, the result can be rigorously justified. For the absorptive PC case, as we showed in Ref. 2, Eq. (2.20) has no solutions for real ω in frequency intervals, where $\mathrm{Im}\,\varepsilon(\mathbf{x},\omega)\neq 0$. This can also be obtained in a formal manner from Eq. (2.21). It implies that the Fourier expansion, Eq. (2.20), does not exist. This situation is rather unsatisfactory, but it can be improved by using the auxiliary field formalism to which we turn now.

III. THE AUXILIARY FIELD FORMALISM

A. Absorptive case

We define for the absorptive case, where we can write $\nu(\mathbf{x},\lambda)=\sigma(\mathbf{x},\lambda)^2$, $\sigma(\mathbf{x},\lambda)\geqslant 0$,

$$\mathbf{F}_1(\mathbf{x},t)=\mathbf{E}(\mathbf{x},t),\quad \mathbf{F}_3(\mathbf{x},t)=\mathbf{B}(\mathbf{x},t),$$

$$\mathbf{F}_2(\mathbf{x},\lambda,t)=\sigma(\mathbf{x},\lambda)\int_{t_0}^{t} ds\,\sin\lambda(t-s)\mathbf{E}(\mathbf{x},s),$$

$$\mathbf{F}_4(\mathbf{x},\lambda,t)=\sigma(\mathbf{x},\lambda)\int_{t_0}^{t} ds\,\cos\lambda(t-s)\mathbf{E}(\mathbf{x},s). \tag{3.1}$$

Then, omitting $\mathbf{x}$ and λ dependencies for brevity, denoting

$$\mathbf{F}(t)=\begin{pmatrix}\mathbf{F}_e(t)\\ \mathbf{F}_m(t)\end{pmatrix}=\begin{pmatrix}\mathbf{F}_1(t)\\ \mathbf{F}_2(t)\\ \mathbf{F}_3(t)\\ \mathbf{F}_4(t)\end{pmatrix}, \tag{3.2}$$

we have

$$\partial_t\mathbf{F}(t)=-i\mathbf{K}\mathbf{F}(t), \tag{3.3}$$

where ($\boldsymbol{\epsilon}=\{\epsilon_{klm}\}$ is the Levi-Civita symbol, $\epsilon_{123}=1$ and ϵ_{klm} changes sign under the interchange of each two subscripts, so $(\boldsymbol{\epsilon}\cdot\mathbf{a})\cdot\mathbf{b}=-\mathbf{a}\times\mathbf{b}$, whereas $\mathbf{p}=-i\partial_{\mathbf{x}}$ is the generator of translations, i.e., the momentum operator of quantum mechanics),

$$\mathbf{K}=\begin{pmatrix}0 & \mathbf{K}_{em}\\ \mathbf{K}_{me} & 0\end{pmatrix},\quad \mathbf{K}_{em}=\begin{pmatrix}\boldsymbol{\epsilon}\cdot\mathbf{p} & -i\int d\lambda\ \sigma(\mathbf{x},\lambda)\dots\\ 0 & i\lambda\end{pmatrix},\quad \mathbf{K}_{me}=\begin{pmatrix}-\boldsymbol{\epsilon}\cdot\mathbf{p} & 0\\ i\sigma(\mathbf{x},\lambda) & -i\lambda\end{pmatrix}. \tag{3.4}$$

We note that Eq. (3.3) is equivalent to Maxwell's equations, provided

$$\mathbf{F}_2(\mathbf{x},t_0)=\mathbf{F}_4(\mathbf{x},t_0)=0, \tag{3.5}$$

where it is understood that the limits $t_0\to-\infty$ are meant in case $t_0=-\infty$. Let $\mathcal{H}=\oplus_{j=1}^4\mathcal{H}_j$, $\mathcal{H}_1=\mathcal{H}_3=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)$, $\mathcal{H}_2=\mathcal{H}_4=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)\otimes L^2(\mathbb{R},d\lambda)$, so we have for the inner product and norm squared,

$$\begin{aligned}(\mathbf{f},\mathbf{g})&=\int d\mathbf{x}[\mathbf{f}_1(\mathbf{x})\cdot\overline{\mathbf{g}_1(\mathbf{x})}+\mathbf{f}_3(\mathbf{x})\cdot\overline{\mathbf{g}_3(\mathbf{x})}+\int d\lambda\{\mathbf{f}_2(\mathbf{x},\lambda)\cdot\overline{\mathbf{g}_2(\mathbf{x},\lambda)}+\mathbf{f}_4(\mathbf{x},\lambda)\cdot\overline{\mathbf{g}_4(\mathbf{x},\lambda)}\}]\\&=\sum_{j=1}^4(\mathbf{f}_j,\mathbf{g}_j)_j,\end{aligned}$$

$$\|\mathbf{f}\|^2=\sum_{j=1}^4(\mathbf{f}_j,\mathbf{f}_j)_j=\sum_{j=1}^4\|\mathbf{f}_j\|_j^2. \tag{3.6}$$

As already noted in Ref. 7, $\mathbf{K}$ defines a self-adjoint operator in $\mathcal{H}$. To see this we write $\mathbf{K}=\mathbf{K}_0+\mathbf{K}_1$, with

$$\mathbf{K}_0=\begin{pmatrix}0&\mathbf{K}_{0em}\\\mathbf{K}_{0me}&0\end{pmatrix},\quad \mathbf{K}_{0em}=\begin{pmatrix}\boldsymbol{\epsilon}\cdot\mathbf{p}&0\\0&i\lambda\end{pmatrix},\quad \mathbf{K}_{0me}=\begin{pmatrix}-\boldsymbol{\epsilon}\cdot\mathbf{p}&0\\0&-i\lambda\end{pmatrix}. \tag{3.7}$$

In Fourier (momentum) space $\mathbf{K}_0$ is a matrix multiplication operator, which is easily seen to have a unique self-adjoint extension, whereas a simple estimate, using $|\chi'(\mathbf{x},0)|\leqslant c'$, shows that $\mathbf{K}_1$ is a bounded self-adjoint operator. We note further that

$$\mathbf{K}^2=\begin{pmatrix}\mathbf{H}_e&0\\0&\mathbf{H}_m\end{pmatrix},\quad \mathbf{H}_e=\begin{pmatrix}\mathbf{h}+\chi'(\mathbf{x},0)&-\int d\lambda\,\lambda\sigma(\mathbf{x},\lambda)\ldots\\-\lambda\sigma(\mathbf{x},\lambda)&\lambda^2\end{pmatrix}, \tag{3.8}$$

$$\mathbf{H}_m=\begin{pmatrix}\mathbf{h}&i\boldsymbol{\epsilon}\cdot\mathbf{p}\int d\lambda\,\sigma(\mathbf{x},\lambda)\ldots\\i\sigma(\mathbf{x},\lambda)\boldsymbol{\epsilon}\cdot\mathbf{p}&\lambda^2\end{pmatrix}.$$

Here, in dyadic notation, with $\mathbf{U}$ the unit 3×3 matrix,

$$\mathbf{h}=\mathbf{p}^2\mathbf{U}-\mathbf{pp}=\mathbf{p}^2\boldsymbol{\Delta}_\mathbf{p},\quad \boldsymbol{\Delta}_\mathbf{p}=\mathbf{U}-\mathbf{e}_\mathbf{p}\mathbf{e}_\mathbf{p},\quad \mathbf{e}_\mathbf{p}=\mathbf{p}/|\mathbf{p}|=\mathbf{p}/p, \tag{3.9}$$

so $\mathbf{h}\cdot\mathbf{f}(\mathbf{x})=\partial_\mathbf{x}\times(\partial_\mathbf{x}\times\mathbf{f}(\mathbf{x}))$ for sufficiently smooth $\mathbf{f}(\mathbf{x})$. Thus we have obtained a precise setting for Maxwell's equations for an absorptive dielectric as a unitary time evolution for a set of square integrable functions in a Hilbert space $\mathcal{H}$ under the assumption $\mathbf{F}_2(\mathbf{x},\lambda,t_0)=\mathbf{F}_4(\mathbf{x},\lambda,t_0)=0$. We note in passing that it is an appropriate starting point for a quantized theory as discussed fully in Ref. 1. Since there the fields become operators the initial condition $\mathbf{F}_2(\mathbf{x},\lambda,t_0)=\mathbf{F}_4(\mathbf{x},\lambda,t_0)=0$ loses its meaning and is dropped.

$\mathbf{K}$ being self-adjoint, it has the spectral decompositions

$$\mathbf{K}=\int\omega\mathbf{E}(d\omega). \tag{3.10}$$

Then, if $\mathbf{K}$ possesses an eigenfunction expansion (α labels a possible degeneracy),

$$\mathbf{E}(d\omega)=\sum_\alpha|\mathbf{u}_{\omega\alpha}\rangle\langle\mathbf{u}_{\omega\alpha}|d\omega,\quad \langle\mathbf{u}_{\omega\alpha}|\mathbf{u}_{\mu\beta}\rangle=\mathbf{U}\delta(\omega-\mu)\delta_{a\beta}, \tag{3.11}$$

the Fourier transform $\tilde{\mathbf{F}}(\omega)$ satisfies the eigenvalue equation

$$\mathbf{K}\tilde{\mathbf{F}}(\omega) = \omega\tilde{\mathbf{F}}(\omega), \tag{3.12}$$

or,

$$\mathbf{H}_e\tilde{\mathbf{F}}_e(\omega) = \omega^2\tilde{\mathbf{F}}_e(\omega), \tag{3.13}$$

which, in contrast to Eq. (2.21), make sense for real ω. Thus the problem noted at the end of Sec. II can be circumvented. We shall not go into the proof of the existence of eigenfunction expansions. In scattering situations $\mathbf{H}_e$ is not very different from the Schrödinger operator case with a simple bounded potential, see Ref. 8, but here we also encounter the variable $\lambda \in \mathbb{R}$. In the dispersive case, see below, we deal with a discrete set of ω_n's and for PCs the problem can be reduced by means of a Bloch–Floquet decomposition to one involving square integrable eigenfunctions.

B. Dispersive case

In the dispersive case we can no longer write $\nu(\mathbf{x},\lambda)=\sigma(\mathbf{x},\lambda)^2$ and the formalism needs modification. In Ref. 1 a general formulation was given, with $\nu(\mathbf{x},\lambda)$ as a weight function in the inner product. But we can also proceed by writing

$$\mathbf{J}(\mathbf{x},t) = \sum_n \nu_n(\mathbf{x})\int_{t_0}^{t} ds\, \cos\,\omega_n(t-s)\mathbf{E}(\mathbf{x},s) = \sum_n \sigma_n(\mathbf{x})\mathbf{F}_{4n}(\mathbf{x},t), \quad \nu_n(\mathbf{x}) = \sigma_n(\mathbf{x})^2, \quad \sigma_n(\mathbf{x}) \geqslant 0. \tag{3.14}$$

Thus, with

$$\mathbf{F}_1(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t), \quad \mathbf{F}_3(\mathbf{x},t) = \mathbf{B}(\mathbf{x},t),$$

$$\mathbf{F}_{2n}(\mathbf{x},t) = \sigma_n(\mathbf{x})\int_{t_0}^{t} ds\, \sin\,\omega_n(t-s)\mathbf{E}(\mathbf{x},s),$$

$$\mathbf{F}_{4n}(\mathbf{x},t) = \sigma_n(\mathbf{x})\int_{t_0}^{t} ds\, \cos\,\omega_n(t-s)\mathbf{E}(\mathbf{x},s), \tag{3.15}$$

we have

$$\partial_t\mathbf{F}_1(\mathbf{x},t) = -i\left[(\boldsymbol{\epsilon}\cdot\mathbf{p})\mathbf{F}_3(\mathbf{x},t) - i\sum_n \sigma_n(\mathbf{x})\mathbf{F}_{4n}(\mathbf{x},t)\right],$$

$$\partial_t\mathbf{F}_{2n}(\mathbf{x},t) = -i[i\omega_n\mathbf{F}_{4n}(\mathbf{x},t)],$$

$$\partial_t\mathbf{F}_3(\mathbf{x},t) = -i[-(\boldsymbol{\epsilon}\cdot\mathbf{p})\mathbf{F}_1(\mathbf{x},t)],$$

$$\partial_t\mathbf{F}_{4n}(\mathbf{x},t) = -i[i\sigma_n(\mathbf{x})\mathbf{F}_1(\mathbf{x},t) - i\omega_n\mathbf{F}_{2n}(\mathbf{x},t)]. \tag{3.16}$$

We can now define $\mathbf{K}$ acting in $\mathcal{H}=\oplus_j\mathcal{H}_0$, $\mathcal{H}_0=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)$. Of particular interest is the case of a single n and $\sigma_n(\mathbf{x})=\Omega P_{\mathcal{A}}$, where $P_{\mathcal{A}}$ is the projector associated with $\mathbf{I}_{\mathcal{A}}(\mathbf{x})$. Then, setting $\omega_n = \omega_0$,

$$\mathbf{K} = \begin{pmatrix} 0 & \mathbf{K}_{em} \\ \mathbf{K}_{me} & 0 \end{pmatrix}, \quad \mathbf{K}_{em} = \begin{pmatrix} \boldsymbol{\epsilon}\cdot\mathbf{p} & -i\Omega P_{\mathcal{A}} \\ 0 & i\omega_0 \end{pmatrix}, \quad \mathbf{K}_{me} = \begin{pmatrix} -\boldsymbol{\epsilon}\cdot\mathbf{p} & 0 \\ i\Omega P_{\mathcal{A}} & -i\omega_0 \end{pmatrix},$$

$$\mathbf{H}_e = \begin{pmatrix} \mathbf{h} + \Omega^2 P_{\mathcal{A}} & -\omega_0 \Omega P_{\mathcal{A}} \\ -\omega_0 \Omega P_{\mathcal{A}} & \omega_0^2 \end{pmatrix}, \quad \mathbf{H}_m = \begin{pmatrix} \mathbf{h} & i\boldsymbol{\epsilon}\cdot\mathbf{p}\Omega P_{\mathcal{A}} \\ i\Omega P_{\mathcal{A}}\boldsymbol{\epsilon}\cdot\mathbf{p} & \omega_0^2 + \Omega^2 P_{\mathcal{A}} \end{pmatrix}. \tag{3.17}$$

The Drude case is obtained by setting $\omega_0 = 0$, leading to

$$\mathbf{H}_e = \begin{pmatrix} \mathbf{h} + \Omega^2 P_{\mathcal{A}} & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{H}_m = \begin{pmatrix} \mathbf{h} & i\boldsymbol{\epsilon}\cdot\mathbf{p}\Omega P_{\mathcal{A}} \\ i\Omega P_{\mathcal{A}}\boldsymbol{\epsilon}\cdot\mathbf{p} & \Omega^2 P_{\mathcal{A}} \end{pmatrix}. \tag{3.18}$$

Here the properties of $\mathbf{H}_e$ are essentially those of $\mathbf{h}+\Omega^2 P_{\mathcal{A}}$, its transverse part (see below) $\mathbf{p}^2 + \Omega^2 P_{\mathcal{A}}$ being the Schrödinger operator for a potential consisting of a number of humps. In the piecewise constant case with randomly placed $\mathcal{A}_j$'s and Ω^2 sufficiently large, it cannot be ruled out that spectral intervals showing Anderson localization exist.

IV. PHOTONIC CRYSTALS

Three-dimensional photonic crystals are dielectrics with spatial periodicity,

$$\chi(\mathbf{x},t) = \chi\left(\mathbf{x} + \sum_{j=1}^{3} n_j \mathbf{a}_j, t\right), \quad n_j \in \mathbb{Z}, \tag{4.1}$$

with the $\mathbf{a}_j$'s three linearly independent real vectors (other cases are those with only two independent $\mathbf{a}_j$'s or only a single one). In practice, the dielectric fills an identical region $\mathcal{A}_j$ in each unit cell $\mathcal{C}_j$ over which $\chi(\mathbf{x},t)$ is homogeneous in $\mathbf{x}$ (piecewise constant case). Then a Bloch–Floquet decomposition can be made, so that $\mathbf{K}$ is reduced to $\mathbf{K}(\boldsymbol{\kappa})$ on $\mathcal{H}_{\mathcal{C}}$, where in the $\mathcal{H}_j$'s of Sec. III the $\mathbf{x}$ integration is restricted to the unit cell $\mathcal{C}\subset\mathbb{R}^3$ containing the origin. The vector $\boldsymbol{\kappa}\in\mathcal{B}$, the first Brillouin zone, labels the (Bloch) boundary conditions on $\partial_{\mathcal{C}}$. For details, see Ref. 2. In this case the operator $\mathbf{h}$ changes into $\mathbf{h}(\boldsymbol{\kappa})$, the closure of $-\partial_{\mathbf{x}}^2\mathsf{U}+\partial_{\mathbf{x}}\partial_{\mathbf{x}}$ with Bloch boundary conditions on $\partial_{\mathcal{C}}$. Instead of Eq. (2.21) we then have

$$[\omega^2\varepsilon(\mathbf{x},\omega) - \mathbf{h}(\boldsymbol{\kappa})]\cdot\tilde{\mathbf{E}}(\mathbf{x},\boldsymbol{\kappa},\omega) = 0, \tag{4.2}$$

In dispersive intervals, i.e., intervals over which $\varepsilon(\mathbf{x},\omega)$ is real, the transverse parts of the corresponding $\mathbf{K}(\boldsymbol{\kappa})$ and $\mathbf{H}_e(\boldsymbol{\kappa})$ have a discrete point spectrum, each eigenvalue having finite multiplicity. As in the solid state case, band gaps (intervals containing no eigenvalues for any $\boldsymbol{\kappa}\in\mathcal{B}$) are possible. In the absorptive case there are resonances rather than eigenvalues, giving rise to a complex band spectrum.[2] A practical consequence is that now Eq. (4.2) has solutions with complex $\omega=\omega(\boldsymbol{\kappa})$ in the lower complex half-plane $\mathbb{C}^-$. After complex dilatation, letting $\boldsymbol{\kappa}$ run through $\mathcal{B}$, we obtain the spectrum of the complex dilated original operator $\mathbf{K}$, a set of islands in $\mathbb{C}^-$. In Ref. 9 we calculated the latter for a two-dimensional case with dielectric cylinders. It is possible that in other cases the situation is similar but this may be hard to establish since here we could first deal with the situation for a single $\boldsymbol{\kappa}$ and then reconstruct the full spectrum, which is not possible in general. In the sequel, when referring to a photonic crystal, we mean the arrangement sketched above.

V. DECOMPOSITION INTO LONGITUDINAL AND TRANSVERSE COMPONENTS

The piecewise constant case, Eq. (2.4), is often encountered in practical situations, in particular PCs. In the absence of external charges and currents the Laplace transform,

$$\hat{\mathbf{D}}(\mathbf{x},z) = \varepsilon(\mathbf{x},z)\hat{\mathbf{E}}(\mathbf{x},z), \tag{5.1}$$

satisfies $\partial_{\mathbf{x}}\cdot\hat{\mathbf{D}}(\mathbf{x},z)=0$, so $\hat{\mathbf{D}}(\mathbf{x},z)$ is transverse. Then

$$\varepsilon(\mathbf{x},z)\partial_{\mathbf{x}}\cdot\hat{\mathbf{E}}(\mathbf{x},z)=-\{\partial_{\mathbf{x}}\varepsilon(\mathbf{x},z)\}\cdot\hat{\mathbf{E}}(\mathbf{x},z), \tag{5.2}$$

which is, in general, nonzero, so $\hat{\mathbf{E}}(\mathbf{x},z)$ can have both longitudinal and transverse components. But here $\partial_{\mathbf{x}}\varepsilon(\mathbf{x},z)$ is nonzero only on the boundary $\partial_{\mathcal{A}}$ of $\mathcal{A}$, where it is, in fact, singular. Thus $\hat{\mathbf{E}}(\mathbf{x},z)$ is transverse except on a set of measure zero in $\mathbb{R}^3$ and, since it is square integrable, we expect this to be irrelevant. But in order to proceed we first have to define the decomposition into longitudinal and transverse components for general square integrable fields. Thus let $\mathbf{f}(\mathbf{x})\in L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)$ with Fourier transform $\tilde{\mathbf{f}}(\mathbf{k})$. Then we can write, indicating longitudinal fields by $\|$ and transverse ones by $\perp$,

$$\tilde{\mathbf{f}}(\mathbf{k})=\mathbf{e}_{\mathbf{k}}\mathbf{e}_{\mathbf{k}}\cdot\tilde{\mathbf{f}}(\mathbf{k})+\boldsymbol{\Delta}_{\mathbf{k}}\cdot\tilde{\mathbf{f}}(\mathbf{k})=P^{\|}\tilde{\mathbf{f}}(\mathbf{k})+P^{\perp}\tilde{\mathbf{f}}(\mathbf{k})=\tilde{\mathbf{f}}^{\|}(\mathbf{k})+\tilde{\mathbf{f}}^{\perp}(\mathbf{k}), \tag{5.3}$$

so $\tilde{\mathbf{f}}^{\|}(\mathbf{k})$ is along $\mathbf{k}$ and $\tilde{\mathbf{f}}^{\perp}(\mathbf{k})$ orthogonal to $\mathbf{k}$. This defines the corresponding decomposition in coordinate space. It is easily verified that, for sufficiently smooth $\mathbf{f}(\mathbf{x})$, indeed $\partial_{\mathbf{x}}\cdot\mathbf{f}^{\perp}(\mathbf{x})=0$ and $\partial_{\mathbf{x}}\times\mathbf{f}^{\|}(\mathbf{x})=0$.

For a general absorptive dielectric,

$$\sigma(\mathbf{x},\lambda)=\sum_j \mathbf{l}_{\mathcal{A}_j}(\mathbf{x})s_j(\lambda)=\sum_j P_j s_j(\lambda), \tag{5.4}$$

where $P_j=P_{\mathcal{A}_j}$ is the projector associated with $\mathbf{l}_{\mathcal{A}_j}(\mathbf{x})$. Let the longitudinal and transverse projectors on $\mathcal{H}$ be defined by

$$\mathbf{E}^{\|}=P^{\|}\mathbf{V},\quad \mathbf{E}^{\perp}=P^{\perp}\mathbf{V},\quad \mathcal{H}^{\|}=\mathbf{E}^{\|}\mathcal{H},\quad \mathcal{H}^{\perp}=\mathbf{E}^{\perp}\mathcal{H}, \tag{5.5}$$

with $\mathbf{V}$ the unit 4×4 matrix. We are interested in the commutation properties of $\mathbf{E}^{\|}$ and $\mathbf{K}$. We first consider the commutation properties of $P^{\|}$ and $P_{\mathcal{A}}$.

Lemma: On $\mathcal{H}_0=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)$ the operators $P_{\mathcal{A}}$ and $P^{\|}$ (and hence also $P_{\mathcal{A}}$ and $P^{\perp}$) commute.

Proof: Let $\mathcal{F}\subset\mathcal{H}_0$ be the dense subset of compactly supported smooth functions that vanish in a neighborhood of $\partial_{\mathcal{A}}$. Then $\mathcal{G}=\{\mathbf{g}=\mathbf{p}^2\mathbf{f}\,|\,\mathbf{f}\in\mathcal{F}\}$ also has these properties. Now let $\mathbf{g}=\mathbf{p}^2\mathbf{f}\in\mathcal{G}$. Then $(P^{\|}\mathbf{g})(\mathbf{x})=(\mathbf{pp}\cdot\mathbf{f})(\mathbf{x})=-\partial_{\mathbf{x}}\partial_{\mathbf{x}}\cdot\mathbf{f}(\mathbf{x})$ and noting that $\mathbf{f}(\mathbf{x})$ vanishes in a neighborhood of $\partial_{\mathcal{A}}$,

$$(P_{\mathcal{A}}P^{\|}\mathbf{g})(\mathbf{x})=-\mathbf{l}_{\mathcal{A}}(\mathbf{x})\partial_{\mathbf{x}}\partial_{\mathbf{x}}\cdot\mathbf{f}(\mathbf{x})=-\partial_{\mathbf{x}}\partial_{\mathbf{x}}\cdot\mathbf{l}_{\mathcal{A}}(\mathbf{x})\mathbf{f}(\mathbf{x})=(\mathbf{pp}\cdot P_{\mathcal{A}}\mathbf{f})(\mathbf{x})=(P^{\|}\mathbf{p}^2P_{\mathcal{A}}\mathbf{f})(\mathbf{x}). \tag{5.6}$$

But

$$(\mathbf{p}^2P_{\mathcal{A}}\mathbf{f})(\mathbf{x})=-\partial_{\mathbf{x}}^2\mathbf{l}_{\mathcal{A}}(\mathbf{x})\mathbf{f}(\mathbf{x})=-\mathbf{l}_{\mathcal{A}}(\mathbf{x})\partial_{\mathbf{x}}^2\mathbf{f}(\mathbf{x})=(P_{\mathcal{A}}\mathbf{p}^2\mathbf{f})(\mathbf{x})=(P_{\mathcal{A}}\mathbf{g})(\mathbf{x}), \tag{5.7}$$

so $(P_{\mathcal{A}}P^{\|}\mathbf{g})(\mathbf{x})=(P^{\|}P_{\mathcal{A}}\mathbf{g})(\mathbf{x})$. Since $\mathcal{G}$ is dense in $\mathcal{H}_0$ and $P^{\|}$ and $P_{\mathcal{A}}$ are bounded operators, we conclude that they commute and hence so do $P^{\perp}$ and $P_{\mathcal{A}}$. ■

Remark: The above result sensitively depends on the topology. In the proof the existence of a dense set of functions, vanishing in a neighborhood of $\partial_{\mathcal{A}}$ is essential. The result is somewhat surprising since, in contrast to $P_{\mathcal{A}}$, $P^{\|}$ and $P^{\perp}$ are not obviously local operators in coordinate space.

We now turn to functions from the domain $\mathcal{D}(\mathbf{K})$ of $\mathbf{K}$. Noting that $\mathcal{D}(\mathbf{K})=\mathcal{D}(\mathbf{K}_0)$ and $\mathbf{f}\in\mathcal{D}(\mathbf{K}_0)$ can be written as

$$\mathbf{f}=[z-\mathbf{K}_0]^{-1}\mathbf{g}=[z+\mathbf{K}_0][z^2-\mathbf{K}_0^2]^{-1}\mathbf{g}, \tag{5.8}$$

where $\mathrm{Im}\,z\neq0$ and $\mathbf{g}\in\mathcal{H}$, we have, using $(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot[z^2-\mathbf{h}]^{-1}=(\boldsymbol{\epsilon}\cdot\mathbf{p})[z^2-\mathbf{p}^2]^{-1}=[z^2-\mathbf{p}^2]^{-1}(\boldsymbol{\epsilon}\cdot\mathbf{p})$,

$$\mathbf{f}_1=z[z^2-\mathbf{h}]^{-1}\mathbf{g}_1-[z^2-\mathbf{p}^2]^{-1}(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathbf{g}_3,\quad \mathbf{f}_2=z[z^2-\lambda^2]^{-1}\mathbf{g}_2+i\lambda[z^2-\lambda^2]^{-1}\mathbf{g}_4, \tag{5.9}$$

and similar for the other components. Since $P^{\perp}\mathbf{h}=P^{\perp}\mathbf{p}^2=\mathbf{p}^2P^{\perp}$ and $\boldsymbol{\epsilon}\cdot\mathbf{p}=P^{\perp}\boldsymbol{\epsilon}\cdot\mathbf{p}=\boldsymbol{\epsilon}\cdot\mathbf{p}P^{\perp}$, we have

$$P^{\perp}\mathbf{f}_1 = P^{\perp}[z^2 - \mathbf{p}^2]^{-1}\{z\mathbf{g}_1 - (\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathbf{g}_3\}, \tag{5.10}$$

and it follows that $\mathbf{f}_1^{\perp}$ and $\mathbf{f}_3^{\perp}$ are in $\mathcal{D}(\boldsymbol{\epsilon}\cdot\mathbf{p})$. Also, since $P^{\parallel}\boldsymbol{\epsilon}\cdot\mathbf{p}=0$, $P^{\parallel}\mathsf{h}=0$,

$$P^{\parallel}\mathbf{f}_1 = \frac{1}{z}P^{\parallel}\mathbf{g}_1, \quad P^{\parallel}\mathbf{f}_3 = \frac{1}{z}P^{\parallel}\mathbf{g}_3, \tag{5.11}$$

so there are no restrictions on the longitudinal parts $\mathbf{f}_1^{\parallel}$ and $\mathbf{f}_3^{\parallel}$. As to $\mathbf{f}_2$ and $\mathbf{f}_4$, we note that there is only a square integrability requirement in λ. Let now $\mathbf{F}\in\mathcal{D}(\mathbf{K})$. Then, in view of the lemma and the above remarks, we find that

$$\mathbf{E}^{\perp}\mathbf{K}\mathbf{F} = \mathbf{K}\mathbf{E}^{\perp}\mathbf{F} = \mathbf{K}^{\perp}\mathbf{E}^{\perp}\mathbf{F}, \quad \mathbf{E}^{\parallel}\mathbf{K}\mathbf{F} = \mathbf{K}\mathbf{E}^{\parallel}\mathbf{F} = \mathbf{K}^{\parallel}\mathbf{E}^{\parallel}\mathbf{F}, \tag{5.12}$$

where $\mathbf{K}^{\perp}$ has the same form as $\mathbf{K}$, but in $\mathbf{K}^{\parallel}$ the $\boldsymbol{\epsilon}\cdot\mathbf{p}$ terms are missing, so it reduces to a matrix-valued multiplication operator only depending on $\mathbf{x}$. In summary:

Proposition: The operators $\mathbf{E}^{\perp}$ and $\mathbf{E}^{\parallel}$ reduce $\mathbf{K}$.

We note, furthermore, that there is a corresponding decomposition of $\mathbf{H}_e$ acting in $\mathcal{H}_e=\mathcal{H}_1\oplus\mathcal{H}_2=\mathcal{H}_e^{\perp}\oplus\mathcal{H}_e^{\parallel}$ and similar for $\mathbf{H}_m$. Thus

$$\mathbf{H}_e^{\perp} = \begin{pmatrix} \mathbf{p}^2 + P_{\mathcal{A}}g'(0) & -P_{\mathcal{A}}\int d\lambda\, \lambda s(\lambda)\ldots \\ -\lambda s(\lambda)P_{\mathcal{A}} & \lambda^2 \end{pmatrix}, \quad \mathbf{H}_e^{\parallel} = \begin{pmatrix} P_{\mathcal{A}}g'(0) & -P_{\mathcal{A}}\int d\lambda\, \lambda s(\lambda)\ldots \\ -\lambda s(\lambda)P_{\mathcal{A}} & \lambda^2 \end{pmatrix}. \tag{5.13}$$

We observe that $\mathbf{H}_e^{\perp}$ and $\mathbf{H}_m^{\perp}$ have empty null space [note that $g'(0)=\int d\lambda s(\lambda)^2$ and consider the inner product $(\mathbf{H}_j^{\perp}\mathbf{f},\mathbf{f})=0$]. In the same way we obtain the decomposition for the dispersive case.

VI. INITIAL AND BOUNDARY CONDITIONS

Since we are dealing with a unitary time evolution any $\mathbf{F}\in\mathcal{H}$ is acceptable as an initial set of fields. On the other hand, boundary conditions for normal and tangential field components often appear in piecewise constant situations. Here we shall discuss how this comes about. It turns out that the two types of conditions are of a different nature. As we show below, the first are basically an initial condition, whereas the second type only comes into play if we require the fields to satisfy Maxwell's equations in the usual differential equation form.

We start with determining $\mathcal{N}(\mathbf{K})$, the null space of $\mathbf{K}$. Let $\mathbf{f}\in\mathcal{N}(\mathbf{K})$, i.e., $\mathbf{K}\mathbf{f}=0$. It then follows in the absorptive case (the dispersive case goes similarly) that $\mathbf{f}_4=0$, $(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathbf{f}_3=0$, implying that $\mathbf{f}_3=P^{\parallel}\mathbf{g}_3$, $(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathbf{f}_1=0$, so $\mathbf{f}_1=P^{\parallel}\mathbf{g}_1$, and $\mathbf{f}_2=\lambda^{-1}\sigma(\mathbf{x},\lambda)P^{\parallel}\mathbf{g}_1$ or

$$\mathbf{f} = \begin{pmatrix} P^{\parallel}\mathbf{g}_1 \\ \dfrac{\sigma(\mathbf{x},\lambda)}{\lambda}P^{\parallel}\mathbf{g}_1 \\ P^{\parallel}\mathbf{g}_3 \\ 0 \end{pmatrix}, \tag{6.1}$$

where $\mathbf{g}\in\mathcal{H}$ is arbitrary. Setting $\mathbf{f}=\mathbf{M}\mathbf{g}$, we have, for the projector $\mathbf{E}_0$ on $\mathcal{N}(\mathbf{K})$, $\mathbf{E}_0=\mathbf{M}(\mathbf{M}^*\mathbf{M})^{-1}\mathbf{M}^*$. Working things out, using $1+\int d\lambda(\sigma(\mathbf{x},\lambda)^2/\lambda^2)=1+\hat{\chi}(\mathbf{x},0)=\varepsilon(\mathbf{x},0)=\varepsilon_{\mathrm{stat}}(\mathbf{x})$, the static permeability [we exclude Drude contributions for which $\varepsilon_{\mathrm{stat}}(\mathbf{x})$ does not exist and a slightly different approach is needed],

$$\mathbf{E}_0 = \begin{pmatrix} \mathbf{E}_{0e} & 0 \\ 0 & \mathbf{E}_{0m} \end{pmatrix}, \quad \mathbf{E}_{0e} = \begin{pmatrix} 1 & 0 \\ \dfrac{\sigma(\mathbf{x},\lambda)}{\lambda} & 0 \end{pmatrix} P^{\parallel}[P^{\parallel}\varepsilon_{\mathrm{stat}}(\mathbf{x})P^{\parallel}]^{-1}P^{\parallel}\begin{pmatrix} 1 & \displaystyle\int d\lambda\frac{\sigma(\mathbf{x},\lambda)}{\lambda}\ldots \\ 0 & 0 \end{pmatrix}, \tag{6.2}$$

$$\mathbf{E}_{0m} = \begin{pmatrix} P^{\|} & 0 \\ 0 & 0 \end{pmatrix}.$$

Remark: We have $\mathcal{N}(\mathbf{K}) \subset \mathcal{H}^{\|}$ but, in general, $\mathcal{N}(\mathbf{K}) \neq \mathcal{H}^{\|}$. Thus time-dependent longitudinal solutions of Eqs. (2.1) can exist.

We note that $\mathbf{E}_0\mathbf{F}(t)$ is conserved in time, leading to the conservation of $P^{\|}\{\mathbf{F}_1(t) + \int d\lambda(\sigma(\mathbf{x},\lambda)/\lambda)\mathbf{F}_2(\lambda,t)\}$ and $P^{\|}\mathbf{F}_3(t)$. Since

$$\mathbf{F}_1(\mathbf{x},t) + \int d\lambda \frac{\sigma(\mathbf{x},\lambda)}{\lambda}\mathbf{F}_2(\mathbf{x},\lambda,t) = \mathbf{D}(\mathbf{x},t), \tag{6.3}$$

we see that $\mathbf{D}^{\|}(\mathbf{x},t) = \mathbf{D}^{\|}(\mathbf{x})$ and $\mathbf{B}^{\|}(\mathbf{x},t) = \mathbf{B}^{\|}(\mathbf{x})$ are time independent. Note that here no differentiability conditions are required but that continuity of the longitudinal fields at the initial time implies continuity for all later times, so continuity is basically an initial condition. The standard, heuristic, procedure to obtain such a result, follows from Maxwell's equations,

$$\partial_t \partial_{\mathbf{x}} \cdot \mathbf{D}(\mathbf{x},t) = 0, \quad \partial_t \partial_{\mathbf{x}} \cdot \mathbf{B}(\mathbf{x},t) = 0, \tag{6.4}$$

so, formally,

$$\partial_{\mathbf{x}} \cdot \mathbf{D}(\mathbf{x},t) = \rho_e(\mathbf{x}), \quad \partial_{\mathbf{x}} \cdot \mathbf{B}(\mathbf{x},t) = \rho_m(\mathbf{x}), \tag{6.5}$$

where $\rho_m(\mathbf{x}) \equiv 0$ since magnetic charges are absent. Thus $\mathbf{B}^{\|}(\mathbf{x}) \equiv 0$. In the absence of free electric charges, also $\mathbf{D}^{\|}(\mathbf{x}) = 0$. In the literature (see, for instance, Ref. 3) Gauss' theorem is sometimes applied to Eq. (6.5) to obtain the continuity of the normal component of $\mathbf{D}(\mathbf{x})$ across an interface in electrostatics. Note that in more general situations, where transverse components are present, it is a statement about $\mathbf{D}^{\|}(\mathbf{x})$. Also, since the procedure works for any surface and not only an interface between two regions with different electric permeability, the result is that $\mathbf{D}^{\|}(\mathbf{x})$ is continuous. But there seems to be some circularity in the argument since the starting point is a relation for the divergence of $\mathbf{D}^{\|}(\mathbf{x})$, which already requires the existence of its space derivatives.

A similar matter is the application of Stokes' theorem to the relation

$$\partial_{\mathbf{x}} \times \mathbf{E}(\mathbf{x},t) = \partial_{\mathbf{x}} \times \mathbf{E}^{\perp}(\mathbf{x},t) = -\partial_t \mathbf{B}(\mathbf{x},t), \tag{6.6}$$

to obtain the continuity of the tangential components of $\mathbf{E}^{\perp}(\mathbf{x},t)$ across an interface.

In our approach there are no conditions on $\mathbf{E}^{\perp}(\mathbf{x},t_0)$ except its square integrability. This seems to be different from what is commonly found in textbooks. However, if we consider the differential equation $\partial_t \mathbf{F}(t) = -i\mathbf{K}\mathbf{F}(t)$, we must have $\mathbf{F}(t) \in \mathcal{D}(\mathbf{K})$, which is true if $\mathbf{F}(t_0) \in \mathcal{D}(\mathbf{K})$ since $\exp[-i\mathbf{K}t]\mathcal{D}(\mathbf{K}) = \mathcal{D}(\mathbf{K})$. As we noted earlier, this requires $\mathbf{E}^{\perp}(t_0) \in \mathcal{D}(\boldsymbol{\epsilon}\cdot\mathbf{p})$. Thus, dropping t_0,

$$\begin{aligned} \mathbf{E}^{\perp} &= [1 + i\boldsymbol{\epsilon}\cdot\mathbf{p}]^{-1}\mathbf{f}^{\perp} = [1+\mathbf{h}]^{-1}[1 - i\boldsymbol{\epsilon}\cdot\mathbf{p}]\mathbf{f}^{\perp} = [1+\mathbf{p}^2]^{-1}[1 - i\boldsymbol{\epsilon}\cdot\mathbf{p}]\mathbf{f}^{\perp} \\ &= [i-p]^{-1}[1 - i\boldsymbol{\epsilon}\cdot\mathbf{p}][-i-p]^{-1}\mathbf{f}^{\perp} = [i-p]^{-1}\mathbf{g}^{\perp}, \end{aligned} \tag{6.7}$$

with $\mathbf{f}^{\perp}$ an arbitrary square integrable transverse function (note that $[1 - i\boldsymbol{\epsilon}\cdot\mathbf{p}][-i-p]^{-1}$ is a bounded operator, so $\mathbf{g}^{\perp}$ is square integrable). Now

$$\mathbf{E}^{\perp}(\mathbf{x}) = ([i-p]^{-1}\mathbf{g}^{\perp})(\mathbf{x}) = (2\pi i)^{-1}\int d\mathbf{y} \frac{\exp[-y]}{y}\mathbf{g}^{\perp}(\mathbf{x}+\mathbf{y}), \tag{6.8}$$

and Young's inequality gives $\mathbf{E}^{\perp}(\mathbf{x}) \in L^2(\mathbb{R}^3, d\mathbf{x}; \mathbb{C}^3) \cap L^{\infty}(\mathbb{R}^3, d\mathbf{x}; \mathbb{C}^3)$. A further estimate results in

$$|\mathbf{E}^{\perp}(\mathbf{x}+\mathbf{a}) - \mathbf{E}^{\perp}(\mathbf{x})| \leqslant (2\pi)^{1/2}[2\|\mathbf{g}^{\perp}\|^2 - (\exp[i\mathbf{p}\cdot\mathbf{a}]\mathbf{g}^{\perp}, \mathbf{g}^{\perp}) - (\mathbf{g}^{\perp}, \exp[i\mathbf{p}\cdot\mathbf{a}]\mathbf{g}^{\perp})], \tag{6.9}$$

where the right-hand side tends to 0 with $\mathbf{a}$, so $\mathbf{E}^{\perp}(\mathbf{x})$ is continuous. Obviously we have the same result for $\mathbf{B}^{\perp}(\mathbf{x}) = \mathbf{B}(\mathbf{x})$. In eigenvalue problems, even stronger conditions hold. Thus, if H is a self-adjoint operator in a Hilbert space $\mathcal{H}$ and $Hf = \lambda f$, then $H^n f = \lambda^n f$ so $f \in \mathcal{D}(H^n)$. This applies

directly to dispersive PC's, where the Bloch-decomposed spectrum is discrete and the eigenvectors at nonzero eigenvalues are transverse.

VII. PHOTONIC CRYSTALS, THE PIECEWISE CONSTANT CASE

In Ref. 2 the presence of a nonempty null space of $\mathbf{H}_e$ gave rise to complications in applying the analytic Fredholm theorem in a discussion of spectral properties. But in the piecewise constant case the present results allow us to concentrate directly on $\mathbf{H}_e^{\perp}$, thus avoiding this problem. In the Bloch-decomposed situation on the unit cell either the definitions of $P^{\parallel}$ and $P^{\perp}$ must be modified[2] or a direct Bloch decomposition of $P^{\parallel}$ and $P^{\perp}$ can be made with the same result. An important observation is that the Bloch-decomposed projectors do not depend on $\boldsymbol{\kappa}$.

Let us now consider the transverse eigenvalue problem for the dispersive piecewise constant, case,

$$\mathbf{K}^{\perp}(\boldsymbol{\kappa})\cdot\mathbf{F}=\lambda\mathbf{F},\quad \mathbf{H}_e^{\perp}(\boldsymbol{\kappa})\cdot\mathbf{F}_e=\lambda^2\mathbf{F}_e. \tag{7.1}$$

Then

$$\left[\mathbf{p}^2(\boldsymbol{\kappa})+\sum_n \sigma_n(\mathbf{x})^2\right]\mathbf{F}_1-\sum_n \omega_n\sigma_n(\mathbf{x})\mathbf{F}_{2n}=[\mathbf{p}^2(\boldsymbol{\kappa})+\chi'(\mathbf{x},0)]\mathbf{F}_1-\sum_n \omega_n\sigma_n(\mathbf{x})\mathbf{F}_{2n}=\lambda^2\mathbf{F}_1,$$

$$-\omega_n\sigma_n(\mathbf{x})\mathbf{F}_1+\omega_n^2\mathbf{F}_{2n}=\lambda^2\mathbf{F}_{2n}. \tag{7.2}$$

We observed earlier that $\mathbf{H}_e^{\perp}$ has an empty null space, so $\lambda\neq 0$. Setting $\lambda=\omega_n$ the second equation implies that $\mathbf{F}_1=0$ for $\mathbf{x}\in\mathcal{A}$. Also, from the first, $\omega_n^2\mathbf{F}_1=\mathbf{p}^2(\boldsymbol{\kappa})\mathbf{F}_1$, $\mathbf{x}\notin\mathcal{A}$. Then the continuity conditions on $\partial_{\mathcal{A}}$ imply that $\mathbf{F}_1$ vanishes everywhere (see Ref. 2 Sec. IV), i.e., ω_n is not an eigenvalue.

VIII. ENERGY CONSERVATION FOR DISPERSIVE SYSTEMS

A. The conserved energy

Since we found that $\mathcal{E}=\mathcal{E}_{\mathrm{em}}+\mathcal{E}_{\mathrm{aux}}$ is conserved in time, this is the proper conserved energy and, in fact, becomes the Hamiltonian in a quantized theory.[1] Also, in view of the above result that ω_n is not an eigenvalue of $\mathbf{K}^{\perp}$ in the dispersive PC case, we rigorously have [see Eq. (2.23)] that in this case $\Delta\mathcal{E}_{\mathrm{em}}=0$. But also in the general piecewise constant transverse case, provided an eigenfunction expansion exists, considering a single dispersive Lorentz term for simplicity, we obtain from

$$\mathbf{H}_e^{\perp}\tilde{\mathbf{F}}_e(\omega)=\omega^2\tilde{\mathbf{F}}_e(\omega), \tag{8.1}$$

that

$$[\mathbf{p}^2+\Omega^2P_{\mathcal{A}}]\tilde{\mathbf{F}}_1(\omega)-\omega_0\Omega P_{\mathcal{A}}\tilde{\mathbf{F}}_2(\omega)=\omega^2\tilde{\mathbf{F}}_1(\omega),$$

$$-\omega_0\Omega P_A\tilde{\mathbf{F}}_1(\omega)+\omega_0^2\tilde{\mathbf{F}}_2(\omega)=\omega^2\tilde{\mathbf{F}}_2(\omega). \tag{8.2}$$

So, once more,

$$\mathbf{p}^2\tilde{\mathbf{F}}_1(\mathbf{x},\omega_0)=\omega_0^2\tilde{\mathbf{F}}_1(\mathbf{x},\omega_0),\quad \mathbf{x}\notin\mathcal{A},\quad \tilde{\mathbf{F}}_1(\mathbf{x},\omega_0)=0,\quad \mathbf{x}\in\mathcal{A}, \tag{8.3}$$

and again continuity across $\partial_{\mathcal{A}}$ implies that $\tilde{\mathbf{F}}_1(\mathbf{x},\omega_0)$ and hence $\tilde{\mathbf{F}}(\omega_0)$ vanishes everywhere. The situation remains the same in the general dispersive situation.

Next we consider, again for the piecewise constant case and transverse fields, the situation where $t_0=-\infty$, so, according to Eq. (3.15),

$$\mathbf{F}_{0n}(\mathbf{x},t)=\mathbf{F}_{4n}(\mathbf{x},t)+i\mathbf{F}_{2n}(\mathbf{x},t)=\lim_{\delta\downarrow 0}\sigma_n(\mathbf{x})\int_{-\infty}^{t}ds\,\exp[-\delta|s|]\exp[i\omega_n(t-s)]\mathbf{E}(\mathbf{x},s). \tag{8.4}$$

In terms of Fourier transforms,

$$\mathbf{F}(\mathbf{x},t)=\int d\omega\,\exp[-i\omega t]\widetilde{\mathbf{F}}(\mathbf{x},\omega), \tag{8.5}$$

we then obtain

$$\mathbf{F}_{0n}(\mathbf{x},t)=\lim_{\delta\downarrow 0}\sigma_n(\mathbf{x})\exp[i\omega_n t]\int d\omega\, i[\{[\omega+\omega_n+i\delta]^{-1}-[\omega+\omega_n-i\delta]^{-1}\}+i[\omega+\omega_n-i\delta]^{-1}$$
$$\times\exp[-\delta t]\exp[-i(\omega+\omega_n)t]]\widetilde{\mathbf{E}}(\mathbf{x},\omega). \tag{8.6}$$

Letting $\delta\downarrow 0$, the first term on the right gives the δ function $\delta(\omega+\omega_n)$, which does not contribute since $\widetilde{\mathbf{F}}(\mathbf{x},\pm\omega_n)=0$. Next, we make the technical assumption that $[\omega+\omega_n-i\delta]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega)=[\omega+\omega_n-i\delta]^{-1}\{\widetilde{\mathbf{E}}(\mathbf{x},\omega)-\widetilde{\mathbf{E}}(\mathbf{x},\omega_n)\}$ has an absolutely integrable limit as $\delta\downarrow 0$, denoted as $[\omega+\omega_n]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega)$. This is, for instance, trivially the case if we assume that $\widetilde{\mathbf{E}}(\mathbf{x},\omega)$ vanishes in a neighborhood of each ω_n. Then, noting that $\widetilde{\mathbf{E}}(\mathbf{x},\omega)=\widetilde{\mathbf{E}}(\mathbf{x},-\omega)$,

$$\mathbf{F}_{0n}(\mathbf{x},t)=i\sigma_n(\mathbf{x})\int d\omega\,\exp[-i\omega t][\omega+\omega_n]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega),$$

$$\mathbf{F}_{2n}(\mathbf{x},t)=-\sigma_n(\mathbf{x})\int d\omega\,\omega_n\exp[-i\omega t][\omega^2-\omega_n^2]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega),$$

$$\mathbf{F}_{4n}(\mathbf{x},t)=\sigma_n(\mathbf{x})\int d\omega\, i\omega\exp[-i\omega t][\omega^2-\omega_n^2]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega). \tag{8.7}$$

According to the above assumption, $[\omega+\omega_n]^{-1}\widetilde{\mathbf{E}}(\mathbf{x},\omega)$ is absolutely integrable and hence the auxiliary fields vanish as $t\to\pm\infty$ by the Riemann–Lebesgue lemma (recall that $t_0=-\infty$). This applies to the situation where an electromagnetic wave packet is scattered from a finite piece of dielectric material. Then the wave packet is initially freely moving in the direction of the material and becomes free again as $t\to\infty$.

For a monochromatic field,

$$\mathbf{E}(\mathbf{x},t)=\mathbf{E}_0(\mathbf{x})\cos\omega t,\quad \mathbf{B}(\mathbf{x},t)=\mathbf{B}_0(\mathbf{x})\sin\omega t,\quad 0\neq\omega\neq\omega_n, \tag{8.8}$$

we obtain

$$\mathbf{F}_{2n}(\mathbf{x},t)=-\frac{\omega_n\sigma_n(\mathbf{x})}{\omega^2-\omega_n^2}\mathbf{E}_0(\mathbf{x})\cos\omega t,\quad \mathbf{F}_{4n}(\mathbf{x},t)=\frac{\omega\sigma_n(\mathbf{x})}{ega^2-\omega_n^2}\mathbf{E}_0(\mathbf{x})\sin\omega t. \tag{8.9}$$

In this case, the energy $\mathcal{E}$ is infinite but the energy density,

$$U_\omega(\mathbf{x},t)=\frac{1}{2}\left[\mathbf{F}_1(\mathbf{x},t)^2+\mathbf{F}_3(\mathbf{x},t)^2+\sum_n\{\mathbf{F}_{2n}(\mathbf{x},t)^2+\mathbf{F}_{4n}(\mathbf{x},t)^2\}\right], \tag{8.10}$$

still makes sense. Taking the time average over a field period $2\pi/\omega$ (cycle averaging), using some results from Sec. II, we arrive at

$$U_\omega(\mathbf{x}) = \langle U_\omega(\mathbf{x},t)\rangle = \frac{1}{4}[\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega)\}\mathbf{E}_0(\mathbf{x})^2 + \mathbf{B}_0(\mathbf{x})^2]. \tag{8.11}$$

We see by comparison with the vacuum case that the contribution to the energy density from the auxiliary fields is given by

$$\frac{1}{4}[\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega)\} - 1]\mathbf{E}_0(\mathbf{x})^2. \tag{8.12}$$

However, the use of monochromatic fields is somewhat unsatisfactory since the current density $\mathbf{J}(\mathbf{x},t)$ remains oscillating as $t\to-\infty$, which is usually not the case for actual physical systems. To remedy this, we have to use wave packets containing a continuous range of ω's, but then cycle averaging loses its meaning. However, if $\widetilde{\mathbf{E}}(\mathbf{x},\omega)$ is strongly peaked around some value ω_0 and $\varepsilon(\mathbf{x},\omega)$ has no sharp peaks in a neighborhood of ω_0, then $U_{\omega_0}(\mathbf{x})$ is approximately conserved.

For longitudinal fields the situation is quite different. As can be seen from Eq. (3.17), which refers to a single Lorentz contribution inside the dielectric material,

$$\mathbf{H}^{\parallel}_{e\mathcal{A}} = \begin{pmatrix} \Omega^2 & -\omega_0\Omega \\ -\omega_0\Omega & \omega_0^2 \end{pmatrix} P_{\mathcal{A}}, \tag{8.13}$$

which has the eigenvalues 0 and $\pm\sqrt{\Omega^2+\omega_0^2}$. Thus $\mathbf{F}^{\parallel}_{\mathcal{A}}(t)$ is a sum of constant and harmonic functions, which is also true in the general case. This means that we cannot set $t_0=-\infty$. But $t_0=0$ is a possible choice. In the above case we then obtain, for $\mathbf{x}\in\mathcal{A}$, applying the inverse Laplace transform to the longitudinal component of Eq. (2.18), the explicit expressions

$$\mathbf{E}^{\parallel}(\mathbf{x},t) = [\Omega^2+\omega_0^2]^{-1}[\omega_0^2 + \Omega^2\cos\sqrt{\Omega^2+\omega_0^2}t]\mathbf{E}^{\parallel}(\mathbf{x},0),$$

$$\mathbf{F}^{\parallel}_0(\mathbf{x},t) = \Omega[\Omega^2+\omega_0^2]^{-1}[i\omega_0\{1-\cos\sqrt{\Omega^2+\omega_0^2}t\} + \sqrt{\Omega^2+\omega_0^2}\sin\sqrt{\Omega^2+\omega_0^2}t]\mathbf{E}^{\parallel}(\mathbf{x},0), \tag{8.14}$$

resulting in $U(\mathbf{x},t)=\frac{1}{2}\mathbf{E}^{\parallel}(\mathbf{x},0)^2$, which is time independent and differs in form from the expression for the transverse fields. In fact, a difference is to be expected since longitudinal fields are not propagating waves. Note that the contributions of the auxiliary fields must be taken into account to obtain the above result.

B. Other approaches

Let us consider once more a situation where the material is confined to $\mathcal{A}\subset\mathbb{R}^3$ over which $\chi(\mathbf{x},t)$ is homogeneous in $\mathbf{x}$ and given by the absorptive Lorentz expression, Eq. (2.15). Then, for $\mathbf{x}\in\mathcal{A}$,

$$\mathbf{P}(\mathbf{x},t) = \sum_n \mathbf{P}_n(\mathbf{x},t), \mathbf{P}_n(\mathbf{x},t) = \int_{t_0}^{t} ds\ \chi_n(\mathbf{x},t-s)\mathbf{E}(\mathbf{x},s). \tag{8.15}$$

A little calculation then results in

$$\partial_t^2\mathbf{P}_n(\mathbf{x},t) + 2\gamma_n\,\partial_t\mathbf{P}_n(\mathbf{x},t) + \omega_n^2\mathbf{P}_n(t) = \Omega_n^2\mathbf{E}(\mathbf{x},t). \tag{8.16}$$

Note that this expression is similar to the one obtained by Loudon,[6] who started from a damped oscillator model. He then went on by considering

$$-\partial_{\mathbf{x}}\cdot\mathbf{S}(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t)\cdot\partial_t x\mathbf{D}(\mathbf{x},t) + \mathbf{H}(\mathbf{x},t)\cdot\partial_t\mathbf{B}(\mathbf{x},t), \tag{8.17}$$

where $\mathbf{S}(\mathbf{x},t)=\mathbf{E}(\mathbf{x},t)\times\mathbf{H}(\mathbf{x},t)$ is the Poynting vector, a relation that is generally valid for sufficiently smooth fields. The aim is here to try to write the right-hand side as a time derivative so that a continuity equation is obtained. Note that in our case $\mathbf{H}(\mathbf{x},t)=\mathbf{B}(\mathbf{x},t)$. Next, we write

$$\mathbf{E}(\mathbf{x},t)\cdot\partial_t\mathbf{D}(\mathbf{x},t)+\mathbf{H}(\mathbf{x},t)\cdot\partial_t\mathbf{B}(\mathbf{x},t)=\partial_t\frac{1}{2}\{\mathbf{E}(\mathbf{x},t)^2+\mathbf{B}(\mathbf{x},t)^2\}+\mathbf{E}(\mathbf{x},t)\cdot\partial_t\mathbf{P}(\mathbf{x},t)$$
$$=\partial_t U_{\mathrm{em}}(\mathbf{x},t)+\mathbf{E}(\mathbf{x},t)\cdot\partial_t\mathbf{P}(\mathbf{x},t), \tag{8.18}$$

where $U_{\mathrm{em}}(\mathbf{x},t)$ is the electromagnetic energy density. Inside $\mathcal{A}$,

$$\mathbf{E}(t)\cdot\partial_t\mathbf{P}(t)=\sum_n\mathbf{E}(t)\cdot\partial_t\mathbf{P}_n(t)=\sum_n\frac{1}{\Omega_n^2}\{\partial_t^2\mathbf{P}_n(t)+\gamma_n\,\partial_t\mathbf{P}_n(t)+\omega_n^2\mathbf{P}_n(t)\}\cdot\partial_t\mathbf{P}_n(t)$$
$$=\partial_t\sum_n\frac{1}{2\Omega_n^2}\{\partial_t\mathbf{P}_n(t)^2+\omega_n^2\mathbf{P}_n(t)^2\}+\sum_n\frac{\gamma_n}{\Omega_n^2}\partial_t\mathbf{P}_n(t)^2, \tag{8.19}$$

so

$$-\partial_{\mathbf{x}}\cdot\mathbf{S}(\mathbf{x},t)=\partial_t\left[U_{\mathrm{em}}(\mathbf{x},t)+\mathbf{l}_{\mathcal{A}}(\mathbf{x})\sum_n\frac{1}{2\Omega_n^2}\{\partial_t\mathbf{P}_n(\mathbf{x},t)^2+\omega_n^2\mathbf{P}_n(\mathbf{x},t)^2\}\right]+\sum_n\frac{\gamma_n}{\Omega_n^2}\partial_t\mathbf{P}_n(\mathbf{x},t)^2. \tag{8.20}$$

In the dispersive case, $\gamma_n\equiv 0$, so

$$\partial_t U(\mathbf{x},t)+\partial_{\mathbf{x}}\cdot\mathbf{S}(\mathbf{x},t)=0,$$

$$U(\mathbf{x},t)=U_{\mathrm{em}}(\mathbf{x},t)+\mathbf{l}_{\mathcal{A}}(\mathbf{x})\sum_n\frac{1}{2\Omega_n^2}\{\partial_t\mathbf{P}_n(\mathbf{x},t)^2+\omega_n^2\mathbf{P}_n(\mathbf{x},t)^2\}]. \tag{8.21}$$

Then, for a harmonic field, as given by Eq. (8.8), we have

$$\mathbf{P}_n(\mathbf{x},t)=-\frac{\Omega_n^2}{\omega^2-\omega_n^2}\mathbf{E}_0(\mathbf{x})\cos\,\omega t,\quad \mathbf{B}(\mathbf{x},t)=\mathbf{B}_0(\mathbf{x})\sin\,\omega t, \tag{8.22}$$

so

$$U_\omega(\mathbf{x},t)=\frac{1}{2}\left[\mathbf{E}_0(\mathbf{x})^2\cos^2\,\omega t+\mathbf{B}_0(\mathbf{x})^2\sin^2\,\omega t+\mathbf{l}_{\mathcal{A}}(\mathbf{x})\sum_n\frac{\Omega_n^2}{(\omega^2-\omega_n^2)^2}\right.$$
$$\left.\times\{\omega^2\sin^2\,\omega t+\omega_n^2\cos^2\,\omega t\}\mathbf{E}_0(\mathbf{x})^2\right], \tag{8.23}$$

and upon cycle averaging we obtain $\langle\partial_t\mathbf{S}(\mathbf{x},t)\rangle=0$, whereas the averaged energy density is

$$U_\omega(\mathbf{x})=\langle U_\omega(\mathbf{x},t)\rangle=\frac{1}{4}\left[\left\{1+\mathbf{l}_{\mathcal{A}}(\mathbf{x})\sum_n\frac{\Omega_n^2(\omega^2+\omega_n^2)}{(\omega^2-\omega_n^2)^2}\right\}\mathbf{E}_0(\mathbf{x})^2+\mathbf{B}_0(\mathbf{x})^2\right]$$
$$=\frac{1}{4}[\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega\,\}\mathbf{E}_0(\mathbf{x})^2+\mathbf{B}_0(\mathbf{x})^2], \tag{8.24}$$

a result obtained earlier by various authors (see Ref. 6 and references cited) and that coincides with Eq. (8.11). Since we used the general expression for the dispersive susceptibility χ, this expression is generally valid. Thus we see that the contribution $\frac{1}{4}[\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega\,\}-1]\mathbf{E}_0(\mathbf{x})^2$ is precisely the energy stored in the auxiliary field modes.

Loudon also applies the averaging procedure to the absorptive situation but this does not seem to be correct since then harmonic solutions of Maxwell's equations with real ω do not exist. The same issue is encountered in Ref. 10, where once more a harmonic dependence is assumed for the absorptive case. In Refs. 2 and 9 we found that for absorptive PC's transverse solutions of the

Helmholtz equation generically exist only for a set of complex frequencies $\zeta=\omega-i\gamma$, $\gamma>0$, contained in the spectral islands in $\mathbb{C}^-$; see Sec. IV. Thus, for given ω, there is, in general, a whole interval of allowed γ's. Then a specific solution has the form

$$\mathbf{E}(\mathbf{x},t)=\mathbf{E}_0(\mathbf{x})\exp[-\gamma t]\cos(\omega t-\delta), \quad t\geqslant 0, \tag{8.25}$$

which gives a significantly more complicated form for $\mathbf{P}_n(\mathbf{x},t)$. In addition a cycle average over the interval $[t,t+2\pi/\omega]$ now depends on t. Actually it is rather obvious that a damping factor should be present in Eq. (8.25) since the field amplitudes will decrease in time due to absorption.

Landau and Lifshits,[7] considering the dispersive case, took a slightly different approach. They considered fields with Fourier components sharply peaked around a central frequency ω_0, $\mathbf{E}(t)=\mathbf{E}_0(t)\cos\omega_0 t$ with $\mathbf{E}_0(t)$ only slowly time dependent on the scale set by ω_0. A crucial point in their development is the expansion of $\hat{\chi}(\omega_0+\alpha)$ to first order in α. But this is questionable if there is a sharp peak in $\hat{\chi}(\omega)$ in ω_1 close to ω_0. Here again an average over $2\pi/\omega_0$ is taken, once more resulting in the contribution $\frac{1}{4}\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega\,\}\mathbf{E}_0(\mathbf{x})^2$ to the averaged energy density.

We note that cycle averaging can be relevant in experimental situations where the detection time interval extends over a large number of periods of the field. But in phase-sensitive cases, the situation may become different.

IX. ENERGY CONSERVATION FOR NONLINEAR DIELECTRICS

In this section we consider the conserved energy for nonlinear systems. We use an alternative method, also applicable to the linear case, featuring an additional time variable u rather than a frequency λ.

A. The conserved energy

We consider nonlinear dielectrics, characterized by a set of nonlinear susceptibilities $\{\boldsymbol{\chi}_n(\mathbf{x},t_1,\ldots,t_n)\}$, where $n\in\mathbb{N}$ but, in practice, only the first few n play a role. Thus ($\odot$ indicates an n-fold tensorial contraction with the object following it)

$$\mathbf{P}(\mathbf{x},t)=\sum_{n=1}^{\infty}\mathbf{P}_n(\mathbf{x},t),$$

$$\mathbf{P}_n(\mathbf{x},t)=\int_{t_0}^{t}ds_1\ldots\int_{t_0}^{t}ds_n\,\boldsymbol{\chi}_n(\mathbf{x},t-s_1,\ldots,t-s_n)\odot\mathbf{E}(\mathbf{x},s_1)\ldots\mathbf{E}(\mathbf{x},s_n). \tag{9.1}$$

We make the following assumptions for the susceptibilities $\boldsymbol{\chi}_n$ (see Ref. 11 for detailed information about nonlinear susceptibilities):

A: $\boldsymbol{\chi}_n(\mathbf{x},t_1,\ldots,t_n)=0$ if at least one $t_j<0$, which is a causality requirement.

B: $\boldsymbol{\chi}_n(\mathbf{x},0,t_2\ldots,t_n)=0$, which excludes sudden surges in the current density at the initial time.

C: The rank $n+1$ tensors $\boldsymbol{\chi}_n(\mathbf{x},t_1,\ldots,t_n)$ possess the symmetry property (cf. Ref. 11)

$$(\boldsymbol{\chi}_n)_{kk_1\ldots k_n}(\mathbf{x},t_1,\ldots,t_n)=(\boldsymbol{\chi}_n)_{kk'_1tsk'_n}(\mathbf{x},t'_1,\ldots,t'_n), \tag{9.2}$$

with $\{(k'_1,t'_1),\ldots(k'_n,t'_n)\}$ any permutation of $\{(k_1,t_1),\ldots(k_n,t_n)\}$, i.e., $(\boldsymbol{\chi}_2)_{kk_1k_2}(\mathbf{x},t_1,t_2)=(\boldsymbol{\chi}_2)_{kk_2k_1}(\mathbf{x},t_2,t_1)$, etc.

D: $(\boldsymbol{\chi}_1)_{kl}(\mathbf{x},t)=(\boldsymbol{\chi}_1)_{lk}(\mathbf{x},t)$.

These properties can be verified for material systems subject to a time-dependent external field by expanding the expectation of the polarization in powers of the driving field. Property D holds if the system Hamiltonian is real (time-reversal invariant). Here we note that time reversal invariance apparently does not lead to useful additional relations between the components of the higher-order $\boldsymbol{\chi}_n$'s.

The polarization current density $\mathbf{J}(\mathbf{x},t)$ is now given by

$$\mathbf{J}(\mathbf{x},t) = \partial_t \mathbf{P}(\mathbf{x},t) = \sum_{n=1}^{\infty} \mathbf{J}_n(\mathbf{x},t),$$

$$\mathbf{J}_n(\mathbf{x},t) = \int_{t_0}^{t} ds_1 \ldots \int_{t_0}^{t} ds_n \, \boldsymbol{\chi}_n'(\mathbf{x},t-s_1,\ldots,t-s_n) \odot \mathbf{E}(\mathbf{x},s_1)\ldots\mathbf{E}(\mathbf{x},s_n), \tag{9.3}$$

where

$$\boldsymbol{\chi}_n'(\mathbf{x},t_1,\ldots,t_n) = (\partial_{t_1} + \ldots \partial_{t_n})\boldsymbol{\chi}_n(\mathbf{x},t_1,\ldots,t_n). \tag{9.4}$$

We have

$$\partial_t \mathcal{E}_{\mathrm{em}}(t) = -\int d\mathbf{x}\, \mathbf{E}(\mathbf{x},t)\cdot\mathbf{J}(\mathbf{x},t) = -\sum_{n=1}^{\infty} \int d\mathbf{x}\mathbf{E}(\mathbf{x},t)\cdot\mathbf{J}_n(\mathbf{x},t) \tag{9.5}$$

and we define

$$\mathcal{E}(t) = \mathcal{E}_{\mathrm{em}}(t) + \int_{t_0}^{t} ds \int d\mathbf{x}\, \mathbf{E}(\mathbf{x},s)\cdot\mathbf{J}(\mathbf{x},s) = \mathcal{E}_{\mathrm{em}}(t) + \mathcal{E}_{\mathrm{aux}}(t), \tag{9.6}$$

where

$$\mathcal{E}_{\mathrm{aux}}(t) = \sum_{n=1}^{\infty} \mathcal{E}_n(t), \quad \mathcal{E}_n(t) = \int_{t_0}^{t} ds \int d\mathbf{x}\, \mathbf{E}(\mathbf{x},s)\cdot\mathbf{J}_n(\mathbf{x},s). \tag{9.7}$$

We shall refer to $\mathcal{E}(t)$ as the energy of the system. However, note that, as in the linear case, it does not depend on the fields at time t only. As before we remedy this by introducing auxiliary fields. Dropping $\mathbf{x}$ in the various objects for brevity, we have

$$\begin{aligned}
\mathcal{E}_n(t) &= \int d\mathbf{x} \int_{t_0}^{t} ds_0\, \mathbf{E}(s_0)\cdot\int_{t_0}^{s_0} ds_1\ldots ds_n\, \boldsymbol{\chi}_n'(s_0-s_1,\ldots,s_0-s_n)\odot\mathbf{E}(s_1)\ldots\mathbf{E}(s_n) \\
&= \int d\mathbf{x}\int_{t_0}^{t} ds_0\ldots ds_n \mathbf{E}(s_0)\cdot\boldsymbol{\chi}_n'(s_0-s_1,\ldots,s_0-s_n)\odot\mathbf{E}(s_1)\ldots\mathbf{E}(s_n) = \int d\mathbf{x}\int ds_0\ldots ds_n \\
&\quad \Theta(t-s_0)\Theta(s_0-t_0)\mathbf{E}(s_0)\cdot\boldsymbol{\chi}_n'(s_0-s_1,\ldots,s_0-s_n)\odot\Theta(s_0-s_1)\Theta(s_1-t_0)\mathbf{E}(s_1)\ldots\Theta(s_0-s_n) \\
&\quad \Theta(s_n-t_0)\mathbf{E}(s_n), \quad t>t_0,
\end{aligned} \tag{9.8}$$

or, with $u_j = t - s_j$,

$$\begin{aligned}
\mathcal{E}_n(t) &= \int d\mathbf{x}\int du_0\ldots du_n\, \Theta(u_0)\Theta(t-t_0-u_0)\mathbf{E}(t-u_0)\cdot\boldsymbol{\chi}_n'(u_1-u_0,\ldots,u_n-u_0)\odot\Theta(u_1) \\
&\quad \Theta(t-t_0-u_1)\mathbf{E}(t-u_1)\ldots\Theta(u_n)\Theta(t-t_0-u_n)\mathbf{E}(t-u_n) = \int d\mathbf{x}\int_0^{\infty} du_0\ldots du_n\, \Theta(t-t_0-u_0) \\
&\quad \times \mathbf{E}(t-u_0)\cdot\boldsymbol{\chi}_n'(u_1-u_0,\ldots,u_n-u_0)\odot\Theta(t-t_0-u_1)\mathbf{E}(t-u_1)\ldots\Theta(t-t_0-u_n)\mathbf{E}(t-u_n).
\end{aligned} \tag{9.9}$$

Now let

$$\mathbf{F}_0(u,t) = \Theta(u)\Theta(t-t_0-u)\mathbf{E}(t-u). \tag{9.10}$$

Then

$$\mathcal{E}_n(t) = \int d\mathbf{x} \int du_0 \dots du_n \, \mathbf{F}_0(u_0,t) \cdot \boldsymbol{\chi}_n'(u_1-u_0, \dots, u_n-u_0) \odot \mathbf{F}_0(u_1,t) \dots \mathbf{F}_0(u_n,t). \tag{9.11}$$

Similarly, for the current density,

$$\mathbf{J}_n(\mathbf{x},t) = \int du_1 \dots du_n \, \boldsymbol{\chi}_n'(u_1, \dots, u_n) \odot \mathbf{F}_0(u_1,t) \dots \mathbf{F}_0(u_n,t). \tag{9.12}$$

Note that

$$\mathbf{F}_0(u,t) = 0, \quad t < t_0,$$

$$\mathbf{F}_0(u,t_0) = 0, \quad u \neq 0,$$

$$\mathbf{F}_0(0,t) = \Theta(t-t_0)\mathbf{E}(t)\{=\mathbf{E}(t), t \geqslant t_0\}, \tag{9.13}$$

and $\mathbf{F}_0(u,t)$ satisfies the differential equation

$$\partial_t \mathbf{F}_0(u,t) = -\partial_u \mathbf{F}_0(u,t) + \delta(u)\mathbf{E}(t). \tag{9.14}$$

It is easily checked, using the equations of motion for the electromagnetic fields with Eq. (9.12) for the current densities and Eq. (9.14) for $\mathbf{F}_0(u,t)$ that indeed $\mathcal{E}$, expressed in terms of the fields at time t, is a constant of the motion.

B. The equation of motion for $\mathbf{F}_0(u,t)$

We note that in the previous section only $u \geqslant 0$ enter the formalism, so we consider Eq. (9.14) as an equation of motion for $\mathbf{F}_0(u,t)$ in the real Hilbert space $\mathcal{H}=L_r^2([0,\infty),du)$, interpreting $\delta(u)du$ as the unit point measure concentrated in $0 \in [0,\infty)$. In this space the operator $-\partial_u$ is antisymmetric when acting upon smooth functions with compact support avoiding zero. It has a unique anti-self-adjoint extension $\mathbf{L}$, with the property that the functions in its domain vanish in $u=0$ and

$$(\exp[\mathbf{L}t]f)(u) = \begin{cases} f(u-t), & u \geqslant t \\ 0, & u < t \end{cases} = \Theta(u-t)f(u-t), \tag{9.15}$$

so Eq. (9.14) becomes

$$\partial_t \mathbf{F}_0(u,t) = \mathbf{L}\mathbf{F}_0(u,t) + \delta(u)\Theta(t-t_0)\mathbf{E}(t). \tag{9.16}$$

Its general solution for $t > t_0$ is

$$\begin{aligned} \mathbf{F}_0(u,t,t_0) &= \exp[\mathbf{L}(t-t_0)]\mathbf{F}_0^{\text{in}}(u,t_0) + \int_{t_0}^{t} ds \, \exp[\mathbf{L}(t-s)]\delta(u)\Theta(s-t_0)\mathbf{E}(s) \\ &= \Theta(u-t+t_0)\mathbf{F}_0^{\text{in}}(u-t+t_0,t_0) + \int_{t_0}^{t} ds \, \delta(u-t+s)\Theta(s-t_0)\mathbf{E}(s) \\ &= \Theta(u-t+t_0)\mathbf{F}_0^{\text{in}}(u-t+t_0,t_0) + \Theta(t-t_0-u)\mathbf{E}(t-u), \end{aligned} \tag{9.17}$$

where the initial field $\mathbf{F}_0^{\text{in}}(u,t_0)$ is arbitrary, square integrable in u. Note that this solution reduces to the earlier one if we require $\mathbf{F}_0(u,t_0,t_0)=0$ since then $\mathbf{F}_0^{\text{in}}(u,t_0)$ must vanish.

C. Connection with earlier approach

The Fourier transform $\widetilde{\mathbf{F}}_0(\lambda,t)$ of $\mathbf{F}_0(u,t)$ is

$$\widetilde{\mathbf{F}}_0(\lambda,t)=\int_0^\infty du\,\exp[-i\lambda u]\mathbf{F}_0(u,t)=\exp[-i\lambda(t-t_0)]\int_0^\infty du\,\exp[-i\lambda u]\mathbf{F}_0^{\mathrm{in}}(u,t_0)$$
$$+\int_{t_0}^t ds\,\exp[-i\lambda(t-s)]\mathbf{E}(s), \tag{9.18}$$

which reduces to

$$\widetilde{\mathbf{F}}_0(\mathbf{x},\lambda,t)=\int_{t_0}^t ds\,\exp[-i\lambda(t-s)]\mathbf{E}(\mathbf{x},s)=\widetilde{\mathbf{F}}_4(\mathbf{x},\lambda,t)+i\widetilde{\mathbf{F}}_2(\mathbf{x},\lambda,t), \tag{9.19}$$

in the Maxwell case, $\mathbf{F}_0(u,t_0)=0$. Note that, apart from the factors $\sigma(\mathbf{x},\lambda)$, these are the fields $\mathbf{F}_{2,4}(\mathbf{x},\lambda,t)$ introduced earlier in Eqs. (3.1). Note also that $\sigma(\mathbf{x},\lambda)$ is specific for the absolutely continuous linear case and it makes no sense to introduce it here. In our earlier discussion we could have dropped the condition (we omit the overtildes from now on for notational simplicity) $\mathbf{F}_{2,4}(\mathbf{x},\lambda,t_0)=0$ leading to a term $\exp[-i\lambda(t-t_0)]\mathbf{F}_0(\mathbf{x},\lambda,t_0)$ but here we have a bonus since it follows from Eq. (9.18) that $\mathbf{F}_0(\mathbf{x},\lambda,t_0)$ and $\mathbf{F}_0(\mathbf{x},\lambda,t)$ are analytic upon continuation in $\mathbb{C}^-$, the open lower complex half-plane. This can be of importance in a quantization procedure since there the initial fields can no longer be set equal to zero.

We can also express $\mathcal{E}$ in terms of the Fourier transformed fields. Setting **($\boldsymbol{\lambda}=(\lambda_1,\ldots\lambda_n)$, $\mathbf{t}=(t_1,\ldots t_n)$, $\int_a^b d\mathbf{t}$ means that each t_j is integrated over $[a,b)$)**

$$\boldsymbol{\chi}_n'(\mathbf{x},\mathbf{t})=\int d\boldsymbol{\lambda}\,\exp[-i\boldsymbol{\lambda}\cdot\mathbf{t}]\boldsymbol{\mu}_n(\mathbf{x},\boldsymbol{\lambda}),$$

$$\boldsymbol{\mu}_n(\mathbf{x},\boldsymbol{\lambda})=(2\pi)^{-n}\int_0^\infty d\mathbf{t}\,\exp[i\boldsymbol{\lambda}\cdot\mathbf{t}]\boldsymbol{\chi}_n'(\mathbf{x},\mathbf{t}), \tag{9.20}$$

we arrive at

$$\mathcal{E}_n(t)=\int d\mathbf{x}\int d\boldsymbol{\lambda}\,\bar{\mathbf{F}}_0(\lambda_1+\ldots\lambda_n,t)\cdot\boldsymbol{\mu}_n(\boldsymbol{\lambda})\odot\mathbf{F}_0(\lambda_1,t)\ldots\mathbf{F}_0(\lambda_n,t). \tag{9.21}$$

We can once more check the time independence of $\mathcal{E}$ expressed in terms of the Fourier transformed fields by using the equations of motion. In doing so we also need

$$\int d\lambda_j\,\bar{\mathbf{F}}_0(\lambda_1+\ldots+\lambda_n,t)\cdot\boldsymbol{\mu}_n(\boldsymbol{\lambda})=0,$$

$$\int d\lambda_j\ldots d\lambda_r\,\bar{\mathbf{F}}_0(\lambda_1+\ldots+\lambda_n,t)\cdot\boldsymbol{\mu}_n(\boldsymbol{\lambda})\bar{\mathbf{F}}_0(\lambda_j,t)\ldots\bar{\mathbf{F}}_0(\lambda_r,t)=0, \tag{9.22}$$

which are a consequence of the analyticity properties of $\boldsymbol{\mu}_n(\boldsymbol{\lambda})$ and those of $\mathbf{F}_0(\mathbf{x},\lambda,t)$ that follow from Eq. (9.18). Note that, in particular, $\mathbf{F}_0(\mathbf{x},\lambda,t_0)$ has this analyticity property. Starting from the Fourier transformed formalism, this would not have followed.

It is interesting to note that if $\mathbf{F}_0(\lambda,t)$ has harmonic time dependence, $\mathbf{F}_0(\lambda,t)=\exp[-i\omega t]\mathbf{F}_0(\lambda,0)$ (which is true if we decouple the electromagnetic and auxiliary fields) that each $\mathcal{E}_n(t)$ is conserved in time, i.e., all $\mathcal{E}_n$'s are constants of the motion. However, the construction of a Lagrange–Hamilton setup and its quantization are at present open problems. Finding such a formalism is an important issue since nonlinear equations of motion are usually based on models

starting from an *ad hoc* Hamiltonian with the appropriate number of higher-order terms in creation and annihilation operators.

X. DISCUSSION

A. Summary of results

In the present work we discussed an number of issues connected with the macroscopic Maxwell's equations for dispersive and absorptive dielectrics with the emphasis on systems where the electric susceptibility $\chi(\mathbf{x},t)$ is a piecewise constant function of $\mathbf{x}$. This covers the important cases of scattering from finite objects and photonic crystals. A complicating factor is here the time convolution in the relation

$$\mathbf{P}(\mathbf{x},t) = \int_{t_0}^{t} ds\, \chi(\mathbf{x},t-s)\mathbf{E}(\mathbf{x},s), \tag{10.1}$$

between the polarization and the electric field. However, the existence of an equivalent unitary time evolution in an enlarged Hilbert space made it possible to treat the problem by standard Hilbert space methods. We showed rigorously that in the piecewise constant case the equations of motion for longitudinal and transverse field components decouple. This gives a significant simplification in the discussion of band structure of, in general absorptive, photonic crystals. In our original setup[2] quite a number of steps were necessary to remove an infinite-dimensional null space in an application of the analytic Fredholm theorem. With the present results we can directly concentrate on the transverse case where the null space is empty.

We then considered boundary and initial value problems, again for the piecewise constant case. We found that continuity of the longitudinal component of the displacement, in particular, the continuity of the normal component across an interface, enters as a condition at the initial time t_0. Without it the time evolution still exists for general square integrable fields. Since magnetic charges are absent, $\mathbf{B}^{\parallel}=0$, as is also the case for $\mathbf{D}^{\parallel}$ if there are no external electric charges. But if a static external charge distribution $\rho_e(\mathbf{x}) \in L^1(\mathbb{R}^3,d\mathbf{x}) \cap L^{6/5}(\mathbb{R}^3,d\mathbf{x})$ is present, it is easily verified that $\mathbf{D}^{\parallel}(\mathbf{x},t_0)$ is continuous in $\mathbf{x}$ and then this is also true at all later times. We can also deal with nonstationary external charge and current distributions, but then a corresponding external current must be added in Eqs. (2.1). There are no conditions on the initial transverse fields $\mathbf{E}^{\perp}(\mathbf{x},t_0)$ and $\mathbf{B}^{\perp}(\mathbf{x},t_0)=\mathbf{B}(\mathbf{x},t_0)$, but in the usual differential form of Maxwell's equations these fields must be in the domain of the generator of the time evolution, and this implies their continuity in $\mathbf{x}$, which is then true for all times. This also applies to eigenvalue problems, thus recovering the usual boundary conditions.

We also considered energy conservation for dispersive, nonabsorptive systems. It is expected that, since no absorption takes place, the electromagnetic energy $\mathcal{E}_{\mathrm{em}}$ is conserved. This turns out to be asymptotically true ($t_0=-\infty$, $t\to\infty$), implying conservation in scattering problems, but, in general, $\mathcal{E}_{\mathrm{em}}(t)$ oscillates for finite t. In the literature an approximate conserved energy is obtained for harmonic motion by cycle averaging. In Sec. VIII we identified the excess energy associated with $\partial_\omega\{\omega\varepsilon(\mathbf{x},\omega)\}-1$ as the energy stored in the auxiliary field modes. Somewhat surprisingly, the energy density associated with the longitudinal modes, including the auxiliary ones, is constant in time. This seems not to have been noted before. In this case, since there is no differential operator in the relevant Helmholtz equation, everything is strictly local in $\mathbf{x}$. Although oscillating modes can exist inside dispersive dielectrics it is not obvious how to excite the latter since an external current inside the dielectric is required.

A quite unexplored subject is the mathematical description of nonlinear dielectrics. We showed that here once more a conserved energy exists. We took the opportunity to introduce an alternative setup for the auxiliary fields, also applicable to the linear case, which involves an additional time variable rather than a frequency λ.

In closing this part we note that the initial time t_0 can be $-\infty$ or a finite time. In the second case there is no loss in generality in setting $t_0=0$. In the first case, if the dielectric material is confined to a bounded space region $\mathcal{A}\subset\mathbb{R}^3$ or a half-space we can have a situation where the electromag-

netic fields constitute a wave packet that is initially away from the material and propagates toward it. Thus the front of the wave packet will reach the material at some finite time before which the polarization vanishes. This is typical for a scattering situation, which was studied earlier by the author.[1] But in other cases, such as PCs, the material is spread out through all space and the above argument breaks down. Here we encounter a problem that is specific for infinite systems. Production and detection apparatus must necessarily be embedded in the system, and this does not correspond to actual physical situations. In practice, a PC is a finite object and in usual experiments radiation is produced and observed outside it. This can involve elastic scattering but also the incoming radiation can be absorbed and reemitted, possibly at a different frequency. However, it is advantageous to consider infinite PCs since the spatial periodicity allows a Bloch–Floquet decomposition, reducing the spectral problem to that of an operator on the unit cell. For a sufficiently large PC the actual spectral properties will not deviate much from those of an infinite one.

B. Related work

The construction of a formalism without time convolutions from one that has this property is in itself an interesting issue. In a recent publication, Figotin and Schenker[12] give a mathematical analysis of this matter. In particular, they addressed the matter of uniqueness of the auxiliary field formalism.

C. Outlook

Most of the results obtained here were for the piecewise constant case. If $\chi(\mathbf{x},t)$ is a smooth function of $\mathbf{x}$, longitudinal and transverse modes become coupled and the situation changes. This complicates the eigenvalue problem for photonic crystals and also the approximate expressions for energy conservation need revision. A more challenging problem is the possible existence of a Hamiltonian formulation for nonlinear systems. Although it is straightforward in the linear case,[1] it is far from obvious that an affirmative result exists in case quadratic or cubic terms are added to the polarization.

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Auger effect in the generalized kinetic theory of electrons and holes

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In this paper we propose a model for a proper kinetic description of the Auger effect as a generation/recombination mechanism for electrons and holes in a bipolar device. Boltzmann-type equations for the two-species population in a phonon background are presented, and equilibria and their stability are investigated. Particles and quasiparticles are allowed to obey generalized statistics, in order to possibly include nonstandard or nonextensive effects. The macroscopic recombination/generation rate is recovered as hydrodynamic limit. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161020]

I. INTRODUCTION

Analytical and numerical investigation of Boltzmann-type equations in semiconductors is a subject of growing interest in the scientific literature (see, for instance, Refs. 1 and 2). On the other hand, it is well known that emission/absorption phenomena must be taken into account in the interaction of electrons and positively charged carriers (holes) with phonons in bipolar devices.[3,4] Another important effect to be accounted for, essential in driving the process, is generation/recombination of a pair electron-hole, which may occur in several ways.[5] On the other hand, as pointed out by Koponen, fractal or inverse power law distributions are of interest in modelling various meaningful situations in solid state physics. An example, treated in Ref. 6, is the thermalization of a nonequilibrium electron-phonon system. Until recently, however, there has been little guidance on how to generalize the kinetic theory of electrons and phonons obeying non-Gibbsian statistics. An attempt in this direction has been performed in Refs. 7 and 8, where the kinetic theory of electrons and phonons has been generalized in the sense that electrons and phonons do not obey necessarily Fermi-Dirac and Bose-Einstein, respectively, but also other, generalized, statistics are allowed to them. The case of electrons and holes interacting with a phonon background has been treated in a generalized way and the band-trap capture and emission has been included in the model.[9]

Another important generation/recombination mechanism, that cannot be neglected when both the electron and hole densities are not too small, is the Auger effect.[5] This is what is dealt with in this paper, which moves in the frame of the mathematical methods of kinetic theory,[10] and follows the lines of Ref. 9, so that proofs that are only slight modifications of those given there will be skipped. In our opinion, in fact, a kinetic approach is needed in order to investigate rigorously the whole process and to possibly deduce, in some continuum limit, the macroscopic implications of practical relevance. In the present work (necessarily confined to a formal level, at this stage) we introduce Boltzmann-type equations for interacting populations of electrons (distribution function f_e) and holes (distribution function f_h) in a phonon background in local thermodynamical equi-

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librium, and include specific three-body collision terms for the Auger recombination/generation. Collision integrals are represented in terms of suitable transition probabilities, and the investigation, based on their structure and general properties only, leads to the determination of collision invariants and collision equilibria, and to the proof of an H theorem.[10] Hydrodynamic limit is studied by a preliminary asymptotic procedure with respect to the proper Knudsen numbers.

The Auger effect consists of two different processes and their inverse.

(a) Electron capture, an electron fills a hole. Its energy is transferred to another electron, and vice versa,

$$e + e + h \rightleftharpoons e^{\sharp},$$

where $\sharp$ means "more energetic."

(b) Hole capture, a hole is filled by an electron. Its energy is transferred to another hole, and vice versa,

$$h + h + e \rightleftharpoons h^{\sharp}.$$

The governing equations for the two interacting species in the phonon background are presented in Sec. II under general statistics. Mathematical results on equilibrium and stability are given in Sec. III in terms of an appropriate Lyapunov functional. Finally, in Sec. IV, a very simple zero-order singular perturbation approach is employed for deriving, as hydrodynamic limit in the low density approximation, the macroscopic recombination/generation rate, recovering well-known classical results available in the literature.[5]

II. KINETIC EQUATIONS

Consider two populations, conduction band (CB) electrons [quasi-momentum (QM) $\mathbf{p}$, energy $\epsilon_e(\mathbf{p})$] and holes [QM $\mathbf{k}$, energy $\epsilon_h(\mathbf{k})$], in a phonon background [QM $\mathbf{q}$, energy $\omega(\mathbf{q})$] in thermal equilibrium at temperature T. The distribution functions are normalized in such a way that the concentrations and the energy densities are given by

$$n_\alpha(\mathbf{x},t) = \int f_\alpha(\mathbf{p},\mathbf{x},t) 2\, \mathrm{d}\mathbf{p}, \quad E_\alpha(\mathbf{x},t) = \int f_\alpha(\mathbf{p},\mathbf{x},t)\epsilon_\alpha(\mathbf{p}) 2\, \mathrm{d}\mathbf{p} \tag{1}$$

($\alpha = e,h$), respectively (the factor 2 inside these integrals accounts for degeneracy). Interaction mechanisms to be taken into account are the following:

(i) Absorption and emission of a phonon by a CB electron,
(ii) Absorption and emission of a phonon by a hole,
(iii) Auger recombination/generation.

All processes are assumed to satisfy microreversibility and to fulfill their specific laws of transformation between pre- and post-collision momenta and energies. For the sake of generality, all types of particles are allowed to obey a given statistics, defined by a pair of suitable smooth functions $(\varphi_\alpha, \psi_\alpha)$, $\alpha = e,h$, describing saturation or enhancement effects in the departure/arrival state, respectively. These functions depend on the relevant distribution functions, and appear in the collision terms given below, in the gain and loss terms. Specifically, fermions are characterized by the option $\varphi_\alpha(f_\alpha) = f_\alpha$, $\psi_\alpha(f_\alpha) = 1 - f_\alpha$, whereas the choice underlying the Bose-Einstein statistics would be $\varphi_\alpha(f_\alpha) = f_\alpha$, $\psi_\alpha(f_\alpha) = 1 + f_\alpha$. Other expressions (generalized or fractional statistics) have been found recently to be in order for nonextensive systems with nonadditive entropies,[11,12] occurring for instance in electronic plasmas, anomalous diffusion, galaxy clusters, long-range memory effects. Quantities like $\varphi_e[f_e(\mathbf{p})]$ will be written as $\varphi_e(\mathbf{p})$ for brevity. By following Ref. 7, we assume that $\varphi_\alpha/\psi_\alpha$ is monotonically increasing as a function of f_α, as it occurs in all physical situations of interest. Phonons belong to the various branches g of the phonon spectrum, and their statistics is defined by the pair of functions Φ_g and Ψ_g, functions of the distribution function f_g. Their equilibrium distribution f_g^* (a star is meant to label equilibria throughout) is defined by[9]

$$\ln \frac{\Phi_g^*}{\Psi_g^*} = -\frac{\omega_g(\mathbf{q})}{T}. \tag{2}$$

For simplicity, only the space homogeneous version of the kinetic equations will be considered here, and dependence on t will not be explicitly shown, unless strictly necessary.

Taking into account the processes in which a specific species may be gained or lost, the kinetic equations read as

$$\frac{\partial f_e}{\partial t} = \left(\frac{\partial f_e}{\partial t}\right)_{ep} + \left(\frac{\partial f_e}{\partial t}\right)_A, \quad \frac{\partial f_h}{\partial t} = \left(\frac{\partial f_h}{\partial t}\right)_{hp} + \left(\frac{\partial f_h}{\partial t}\right)_A, \tag{3}$$

where subscripts αp and A are used to label interactions with phonons and Auger effect, respectively. Like in Ref. 9 the collision terms relevant to phonons read as

$$\left(\frac{\partial f_\alpha}{\partial t}\right)_{\alpha p}(\mathbf{p}) = \sum_g \int\int [G^g_{\alpha p}(\mathbf{p}',\mathbf{q};\mathbf{p}) - G^g_{\alpha p}(\mathbf{p},\mathbf{q};\mathbf{p}')]\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{p}', \tag{4}$$

where the kernels G are given by

$$G^g_{\alpha p}(\mathbf{p}',\mathbf{q};\mathbf{p}) = V^g_{\alpha p}(\mathbf{p}',\mathbf{q};\mathbf{p})[\Phi^*_g(\mathbf{q})\varphi_\alpha(\mathbf{p}')\psi_\alpha(\mathbf{p}) - \varphi_\alpha(\mathbf{p})\psi_\alpha(\mathbf{p}')\Psi^*_g(\mathbf{q})] \tag{5}$$

in terms of the transition probabilities V. The latter must be understood in the sense of distributions, and account for momentum and energy balance. More precisely,

$$V^g_{\alpha p}(\mathbf{p}',\mathbf{q};\mathbf{p}) = \mathcal{V}^g_{\alpha p}(\mathbf{p}',\mathbf{q};\mathbf{p})\,\delta(\mathbf{p}-\mathbf{p}'-\mathbf{q}+\mathbf{b})\,\delta[\epsilon_\alpha(\mathbf{p}) - \epsilon_\alpha(\mathbf{p}') - \omega_g(\mathbf{q})], \tag{6}$$

where δ denotes Dirac's delta measure, $\mathbf{b}$ is a suitable vector of the reciprocal lattice, and $\mathcal{V}^g_{\alpha p}$ are positive smooth functions. Of course, delta functions are used to mean that integrations in (4) actually range only on the appropriate two-dimensional manifolds of the whole six-dimensional domain.

In a similar fashion the Auger contributions can be written as

$$\begin{aligned}\left(\frac{\partial f_e}{\partial t}\right)_A(\mathbf{p}) = {} & \int\int\int G^A_e(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{p}_1\,\mathrm{d}\mathbf{p}_2 - 2\int\int\int G^A_e(\mathbf{k},\mathbf{p},\mathbf{p}_2;\mathbf{p}_1)\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{p}_1\,\mathrm{d}\mathbf{p}_2 \\ & - \int\int\int G^A_h(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2,\end{aligned} \tag{7}$$

$$\begin{aligned}\left(\frac{\partial f_h}{\partial t}\right)_A(\mathbf{k}) = {} & \int\int\int G^A_h(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2 - 2\int\int\int G^A_h(\mathbf{p},\mathbf{k},\mathbf{k}_2;\mathbf{k}_1)\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2 \\ & - \int\int\int G^A_e(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}_1\,\mathrm{d}\mathbf{p}_2,\end{aligned} \tag{8}$$

with kernels

$$\begin{aligned}G^A_e(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) &= W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})[\varphi_h(\mathbf{k})\varphi_e(\mathbf{p}_1)\varphi_e(\mathbf{p}_2)\psi_e(\mathbf{p}) - \psi_h(\mathbf{k})\psi_e(\mathbf{p}_1)\psi_e(\mathbf{p}_2)\varphi_e(\mathbf{p})] \\ G^A_h(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}) &= U(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})[\varphi_e(\mathbf{p})\varphi_h(\mathbf{k}_1)\varphi_h(\mathbf{k}_2)\psi_h(\mathbf{k}) - \psi_e(\mathbf{p})\psi_h(\mathbf{k}_1)\psi_h(\mathbf{k}_2)\varphi_h(\mathbf{k})].\end{aligned} \tag{9}$$

The Auger transition probabilities are once more distributions and account for momentum and energy balance,

$$W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) = \mathcal{W}(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})\,\delta(\mathbf{p}-\mathbf{k}-\mathbf{p}_1-\mathbf{p}_2+\mathbf{b}_e)\,\delta[\epsilon_e(\mathbf{p}) - \epsilon_h(\mathbf{k}) - \epsilon_e(\mathbf{p}_1) - \epsilon_e(\mathbf{p}_2)], \tag{10}$$

$$U(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}) = \mathcal{U}(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})\,\delta(\mathbf{k}-\mathbf{p}-\mathbf{k}_1-\mathbf{k}_2+\mathbf{b}_h)\,\delta\left[\epsilon_h(\mathbf{k})-\epsilon_e(\mathbf{p})-\epsilon_h(\mathbf{k}_1)-\epsilon_h(\mathbf{k}_2)\right],$$

where $\mathbf{b}_\alpha$ are appropriate vectors in the reciprocal lattice and $\mathcal{W}$ and $\mathcal{U}$ are smooth positive functions. Again, delta functions mean that ninefold integrations in (7) and (8) actually collapse to fivefold.

As usual in kinetic theory, the weak form of the kinetic equations (3) is essential for any further development. So, take a string of two smooth test functions $(\gamma_e(\mathbf{p}),\gamma_h(\mathbf{k}))$ and multiply each of them by the corresponding collision operator appearing in (3). Then integrate each pair with respect to the relevant kinetic variable and sum them up (after multiplication by 2 because of degeneracy), to get, as usual, a functional $F(\gamma_e,\gamma_h)$.

It is possible to prove, after suitable rearrangement and some algebra, not reported here since they follow closely similar steps in Ref. 9, the following important result.

Proposition 1: For any test function $(\gamma_e(\mathbf{p}),\gamma_h(\mathbf{k}))$ *we have*

$$\begin{aligned} F(\gamma_e,\gamma_h) = &\int\int\int\int G_e^A(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})[\gamma_e(\mathbf{p})-\gamma_h(\mathbf{k})-\gamma_e(\mathbf{p}_1)-\gamma_e(\mathbf{p}_2)]\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}_1\,\mathrm{d}\mathbf{p}_2 \\ &+\int\int\int\int G_h^A(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})[\gamma_h(\mathbf{k})-\gamma_e(\mathbf{p})-\gamma_h(\mathbf{k}_1)-\gamma_h(\mathbf{k}_2)]\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2 \\ &+\sum_\alpha\sum_g\int\int\int G_{\alpha p}^g(\mathbf{p}',\mathbf{q};\mathbf{p})[\gamma_\alpha(\mathbf{p}')-\gamma_\alpha(\mathbf{p})]\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'. \end{aligned} \tag{11}$$

From a physical point of view, F represents the net production by collision of the molecular property defined by the string $\{\gamma_\alpha\}$. Collision invariants are determined by the condition of remaining constant through all possible collisions, and make then the functional F vanish. It is easily seen that this amounts to requiring that indeed all square brackets in (11) vanish identically with respect to their independent variables. Such a strong constraint implies immediately that both γ_α must be constant, and that they must take opposite values. Since the space of these invariants is linear, we can conclude that it is one dimensional, and the unique independent collision invariant may be chosen as the string $(-1,1)$, representing electric charge. Notice that energy, namely the string $(\epsilon_e(\mathbf{p}),\epsilon_h(\mathbf{k}))$, would be conserved by the Auger collision integrals [first two addends in (11)], thanks to the δ functions present in (10). It is clear that it cannot be conserved in the whole process, since it is actually exchanged with the lattice. In conclusion we may state the following.

Proposition 2: Collision invariants constitute a one-dimensional linear space, exhausted by the strings of test functions proportional to

$$(-1,1), \tag{12}$$

representing (*dimensionless*) *electric charge*.

III. EQUILIBRIUM AND STABILITY

The structure of (11) suggests that it is useful to introduce a new functional $\mathcal{D}$ as a suitable specialization of F,

$$\mathcal{D}(f_e,f_h) = F\left[\ln\left(\frac{\varphi_e(\mathbf{p})}{\psi_e(\mathbf{p})}\exp\left(\frac{\epsilon_e(\mathbf{p})}{T}\right)\right),\ln\left(\frac{\varphi_h(\mathbf{k})}{\psi_h(\mathbf{k})}\exp\left(\frac{\epsilon_h(\mathbf{k})}{T}\right)\right)\right], \tag{13}$$

since we get, after some algebra,

$$\mathcal{D}(f_e,f_h)=\int\int\int\int G_e^A(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p})\ln\frac{\psi_h(\mathbf{k})\psi_e(\mathbf{p}_1)\psi_e(\mathbf{p}_2)\varphi_e(\mathbf{p})}{\varphi_h(\mathbf{k})\varphi_e(\mathbf{p}_1)\varphi_e(\mathbf{p}_2)\psi_e(\mathbf{p})}\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}_1\,\mathrm{d}\mathbf{p}_2$$
$$+\int\int\int\int G_h^A(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k})\ln\frac{\psi_e(\mathbf{p})\psi_h(\mathbf{k}_1)\psi_h(\mathbf{k}_2)\varphi_h(\mathbf{k})}{\varphi_e(\mathbf{p})\varphi_h(\mathbf{k}_1)\varphi_h(\mathbf{k}_2)\psi_h(\mathbf{k})}\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{k}_1\,\mathrm{d}\mathbf{k}_2$$
$$+\sum_\alpha\sum_g\int\int\int G_{\alpha p}^g(\mathbf{p}',\mathbf{q};\mathbf{p})\ln\frac{\varphi_\alpha(\mathbf{p})\psi_\alpha(\mathbf{p}')\Psi_g^*(\mathbf{q})}{\psi_\alpha(\mathbf{p})\varphi_\alpha(\mathbf{p}')\Phi_g^*(\mathbf{q})}\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'. \tag{14}$$

In each logarithmic function of (14) numerator and denominator are exactly the two addends that are subtracted in the square brackets of the corresponding kernels G_e^A, G_h^A, and $G_{\alpha p}^g$, respectively, as given by (9) and (5). Therefore, once the integrations are restricted to lower dimensional smooth integrals by the delta measures, the usual convexity arguments of kinetic theory may be applied. In particular, all addends making up $\mathcal{D}$ turn out to be nonpositive and therefore $\mathcal{D}$ is definite in sign. Moreover, it vanishes if and only if all integrals in (14) vanish, and, since $(1-x)\ln x\leqslant 0$ with equal sign only for $x=1$, this occurs if and only if all arguments of the logarithmic functions are unity. In other words we have a sort of Boltzmann lemma.

Proposition 3: $\mathcal{D}\leqslant 0$ *for any admissible distribution function* (f_e,f_h). *In particular* $\mathcal{D}=0$ *iff*

$$\varphi_h(\mathbf{k})\varphi_e(\mathbf{p}_1)\varphi_e(\mathbf{p}_2)\psi_e(\mathbf{p})=\psi_h(\mathbf{k})\psi_e(\mathbf{p}_1)\psi_e(\mathbf{p}_2)\varphi_e(\mathbf{p}),$$

$$\varphi_e(\mathbf{p})\varphi_h(\mathbf{k}_1)\varphi_h(\mathbf{k}_2)\psi_h(\mathbf{k})=\psi_e(\mathbf{p})\psi_h(\mathbf{k}_1)\psi_h(\mathbf{k}_2)\varphi_h(\mathbf{k}), \tag{15}$$

$$\psi_\alpha(\mathbf{p})\varphi_\alpha(\mathbf{p}')\Phi_g^*(\mathbf{q})=\varphi_\alpha(\mathbf{p})\psi_\alpha(\mathbf{p}')\Psi_g^*(\mathbf{q}),$$

for all admissible values of the independent variables in each of the relevant collisions.

But now it is clear from (14) and from Proposition 3 that $\mathcal{D}=0$ implies (and then is equivalent to) vanishing of the whole collision operator in (3). On the other hand, (15) may be reformulated in terms of logarithms and, bearing in mind (9), (5), and (2), this shows that the string

$$\left(\ln\frac{\varphi_e(\mathbf{p})}{\psi_e(\mathbf{p})}+\frac{\epsilon_e(\mathbf{p})}{T},\ln\frac{\varphi_h(\mathbf{k})}{\psi_h(\mathbf{k})}+\frac{\epsilon_h(\mathbf{k})}{T}\right) \tag{16}$$

must be a collision invariant. We may state then a detailed balance principle.

Proposition 4: The collision equilibrium condition,

$$\left(\frac{\partial f_e}{\partial t}\right)_{ep}+\left(\frac{\partial f_e}{\partial t}\right)_A=0,\quad \left(\frac{\partial f_h}{\partial t}\right)_{hp}+\left(\frac{\partial f_h}{\partial t}\right)_A=0, \tag{17}$$

for all admissible distribution functions, *is equivalent to the requirement that (16) be a collision invariant*.

At this point, Proposition 2 applies, which means that there is exactly one one-parameter family of equilibria, given by

$$\ln\frac{\varphi_e^*}{\psi_e^*}=\frac{\mu-\epsilon_e}{T},\quad \ln\frac{\varphi_h^*}{\psi_h^*}=\frac{-\mu-\epsilon_h}{T}, \tag{18}$$

for all real μ. Solvability of the transcendental equations (18) is discussed in Ref. 9. Notice that, in terms of the chemical potentials μ_α,[5] equilibrium is characterized by

$$\mu_e=-\mu_h=\mu. \tag{19}$$

Concerning stability of the above equilibria, it is possible to establish an H theorem, again along the lines of kinetic theory. Introduce the functional

$$H = H_e + H_h + \int \frac{\epsilon_e(\mathbf{p}) f_e(\mathbf{p}) + \epsilon_h(\mathbf{p}) f_h(\mathbf{p})}{T} \mathrm{d}\mathbf{p}, \tag{20}$$

where

$$H_\alpha = \int \mathcal{H}_\alpha[f_\alpha(\mathbf{p})]\mathrm{d}\mathbf{p}, \quad \frac{\mathrm{d}\mathcal{H}_\alpha(x)}{\mathrm{d}x} = 2 \ln \frac{\varphi_\alpha(x)}{\psi_\alpha(x)}. \tag{21}$$

Notice that in our assumptions all $\mathcal{H}_\alpha$ are convex functions of their argument because of the monotonicity assumption on the ratios $\varphi_\alpha/\psi_\alpha$. The additional integral in (20) is due to the fact that our system is not closed, but interacts with the background lattice. We can then prove the H theorem.

Proposition 5: H is a strict Lyapunov functional for the initial value problem (3).

For a sketch of the proof, which goes along the same lines as in Ref. 9, we first remark that, following a solution of (3), the time derivative of H coincides exactly with $\mathcal{D}$, and therefore it has the required definiteness in sign. Then, the conclusion follows by usual convexity arguments provided we are able to show that

$$\sum_\alpha \int \left(\frac{\partial \mathcal{H}_\alpha}{\partial f_\alpha}\right)^* (f_\alpha - f_\alpha^*)(\mathbf{p})\mathrm{d}\mathbf{p} + \int \frac{\epsilon_e(f_e - f_e^*) + \epsilon_h(f_h - f_h^*)}{T} \mathrm{d}\mathbf{p} = 0, \tag{22}$$

and it is not difficult to verify that this is true thanks to the expressions of $(\ln(\varphi_\alpha/\psi_\alpha))^*$ and to charge conservation (see Proposition 2).

IV. RECOMBINATION/GENERATION RATE

In kinetic theory it is appropriate to introduce a convenient scaling in Eq. (3), also in order to derive, by a suitable asymptotic procedure, macroscopic equations at a hydrodynamic level. In our case, the most significant macroscopic quantity needed for practical applications is the Auger recombination/generation rate.[5] We shall deduce a formula for such a rate in a very simple way from the kinetic level as a suitable asymptotic limit. We perform our scaling according to the fact that the microscopic relaxation times of the considered interaction mechanisms are typically much shorter than the pertinent macroscopic time. Upon adimensionalization, this leads to the appearance of a small parameter ε, ratio of the two time scales (the Knudsen number), downstairs in front of the collision terms, making the initial value problem of singular perturbation type. The limiting form when $\varepsilon \to 0$ of the evolution equations (3) are just the equilibrium equations (17). If we then restrict ourselves to the low density limit of Gibbsian statistics $\varphi_\alpha(f_\alpha) = f_\alpha$ and $\psi_\alpha(f_\alpha) = 1$, the limiting solution is the Maxwellian-type equilibrium,

$$f_e^*(\mathbf{p}) = \exp\left(\frac{\mu - \epsilon_e(\mathbf{p})}{T}\right) = n_e M_e(\mathbf{p}), \quad f_h^*(\mathbf{k}) = \exp\left(-\frac{\mu + \epsilon_h(\mathbf{k})}{T}\right) = n_h M_h(\mathbf{k}), \tag{23}$$

where the normalized shape functions M_α are

$$M_e(\mathbf{p}) = \frac{\exp(-\epsilon_e(\mathbf{p})/T)}{\int \exp(-\epsilon_e(\mathbf{p})/T)\mathrm{d}\mathbf{p}}, \quad M_h(\mathbf{k}) = \frac{\exp(-\epsilon_h(\mathbf{k})/T)}{\int \exp(-\epsilon_h(\mathbf{k})/T)\mathrm{d}\mathbf{k}}. \tag{24}$$

By multiplying the two equilibrium distributions in (23) and integrating then over both momenta $\mathbf{p}$ and $\mathbf{k}$, we see that the chemical equilibrium condition $\mu_e^* + \mu_h^* = 0$ may be cast as

$$n_e^* n_h^* = \int \exp(-\epsilon_e(\mathbf{p})/T)\mathrm{d}\mathbf{p} \int \exp(-\epsilon_h(\mathbf{k})/T)\mathrm{d}\mathbf{k} = \mathcal{K}, \tag{25}$$

(where $\mathcal{K}$ is an intrinsic constant depending only on the energy functions ϵ and on the lattice temperature) which can be regarded as a sort of mass action law. For the general evolution problem, we see that, from Proposition 2, the only macroscopic conservation equation which is in order for (3) is charge conservation, obtained after integration over the kinetic variables and subtraction, which reads as

$$n_e(t) - n_h(t) = B, \tag{26}$$

where B is a constant depending only on initial conditions. The only equilibrium which is compatible with given initial conditions is then easily obtained by combining Eqs. (25) and (26), which leads to

$$n_e^* = \frac{B}{2} + \left(\frac{B^2}{4} + \mathcal{K}\right)^{1/2}, \quad n_h^* = -\frac{B}{2} + \left(\frac{B^2}{4} + \mathcal{K}\right)^{1/2}. \tag{27}$$

The most important physical information is constituted by the evolution equations for densities, which are obtained instead by simple separate integrations of (3). They are of course exact but not closed, and the simplest hydrodynamic closure is represented by the relevant Euler equations, zero order approximation of any asymptotic technique, which may be deduced by approximating the distribution functions appearing in the collision terms by the equilibria (23). We get in this way

$$\dot{n}_e = \dot{n}_h = -A_{21} n_e^2 n_h + A_{10} n_e - A_{12} n_e n_h^2 + A_{01} n_h, \tag{28}$$

where

$$\begin{aligned}
A_{21} &= \int\int\int\int W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) M_h(\mathbf{k}) M_e(\mathbf{p}_1) M_e(\mathbf{p}_2) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{p}_1\, \mathrm{d}\mathbf{p}_2\, \mathrm{d}\mathbf{p}, \\
A_{10} &= \int\int\int\int W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) M_e(\mathbf{p}) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{p}_1\, \mathrm{d}\mathbf{p}_2\, \mathrm{d}\mathbf{p}, \\
A_{12} &= \int\int\int\int U(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}) M_e(\mathbf{p}) M_h(\mathbf{k}_1) M_h(\mathbf{k}_2) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{k}_1\, \mathrm{d}\mathbf{k}_2\, \mathrm{d}\mathbf{p}, \\
A_{01} &= \int\int\int\int U(\mathbf{p},\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}) M_h(\mathbf{k}) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{k}_1\, \mathrm{d}\mathbf{k}_2\, \mathrm{d}\mathbf{p}.
\end{aligned} \tag{29}$$

Making explicit use of (24) and (25), we can write now

$$\begin{aligned}
A_{21}\mathcal{K} \int \exp(-\epsilon_e(\mathbf{p})/T)\mathrm{d}\mathbf{p} = \int\int\int\int W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) \exp[-(\epsilon_h(\mathbf{k}) + \epsilon_e(\mathbf{p}_1) \\
+ \epsilon_e(\mathbf{p}_2))/T] \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{p}_1\, \mathrm{d}\mathbf{p}_2\, \mathrm{d}\mathbf{p},
\end{aligned}$$

$$A_{10} \int \exp(-\epsilon_e(\mathbf{p})/T)\mathrm{d}\mathbf{p} = \int\int\int\int W(\mathbf{k},\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}) \exp(-(\epsilon_e(\mathbf{p})/T) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{p}_1\, \mathrm{d}\mathbf{p}_2\, \mathrm{d}\mathbf{p}, \tag{30}$$

and similarly for A_{12} and A_{01}. Then, thanks to energy conservation in the Auger effect, accounted for by the δ functions in W and U, we finally end up with

$$A_{10} = \mathcal{K} A_{21}, \quad A_{01} = \mathcal{K} A_{12}. \tag{31}$$

In conclusion, the macroscopic Auger generation/recombination rate[5]

$$\dot{n}_e = \dot{n}_h = -(C_e n_e + C_h n_h)(n_e n_h - C_i^2) \tag{32}$$

is recovered, as first approximation deduced from kinetic theory, by putting together (28) and (31), with specification of coefficients as $C_i^2 = \mathcal{K}$, $C_e = A_{21}$, and $C_h = A_{12}$.

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Determinant representation of correlation functions for the $U_q(\mathrm{gl}(1|1))$ free Fermion model

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With the help of the factorizing F-matrix, the scalar products of the $U_q(\mathrm{gl}(1|1))$ free fermion model are represented by determinants. By means of these results, we obtain the determinant representations of correlation functions of the model.
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I. INTRODUCTION

The computation of correlation functions is one of the challenging problems in the theory of quantum integrable lattice models.[1,2] In this paper, we compute the correlation functions of the free fermion model by means of the algebraic Bethe ansatz method.[1–3] Our computations are based on the recent progress on the Drinfeld twists. Working in the F-bases provided by the F-matrices (Drinfeld twists), the authors in Refs. 4 and 5 managed to derive the determinant representations of the form factors and correlation functions of the XXX and XXZ models in the framework of algebraic Bethe ansatz.

Recently we have constructed the Drinfeld twists for both the rational $\mathrm{gl}(m|n)$ and the quantum $U_q(\mathrm{gl}(m|n))$ supersymmetric models and resolved the hierarchy of their nested Bethe vectors in the F-basis.[6–8] These results serve as the basis of our computation in this paper of the correlation functions of the $U_q(\mathrm{gl}(1|1))$ free Fermion model.

Correlation functions of the free Fermion model based on the $XX0$ spin chain (XY model[9]) with periodic boundary condition were studied in Refs. 10–15. As is seen in Sec. VI, by using the Jordan-Wigner transform, our $U_q(\mathrm{gl}(1|1))$ free Fermion model is equivalent to a twisted $XX0$ model, and the one-point functions we obtained [see Eqs. (5.5) and (5.7) below] give the m-point correlation functions of the twisted $XX0$ model [see e.g., Eq. (6.6)].

The present paper is organized as follows. In Sec. II, we review the background of the $U_q(\mathrm{gl}(1|1))$ model and its algebraic Bethe ansatz. In Sec. III, we construct the Drinfeld twists for the model. In Sec. IV, we obtain the determinant representation of the scalar products of the $U_q(\mathrm{gl}(1|1))$ Bethe states. Then in Sec. V, we compute correlation functions of the local Fermionic operators of the model. We conclude the paper by offering some discussions in Sec. VI.

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II. $U_q(\mathrm{gl}(1|1))$ FREE FERMION MODEL

A. The background of the model

Let V be the two-dimensional $U_q(\mathrm{gl}(1|1))$-module and $R \in \mathrm{End}(V \otimes V)$ the R-matrix associated with this module. V is Z_2-graded, and in the following we choose the FB grading for V, i.e., $[1]=1$, $[2]=0$. The R-matrix depends on the difference of two spectral parameters u_1 and u_2 associated with the two copies of V, and is, in the FB grading, given by

$$R_{12}(u_1,u_2) = R_{12}(u_1-u_2) = \begin{pmatrix} c_{12} & 0 & 0 & 0 \\ 0 & a_{12} & b_{12}^{+} & 0 \\ 0 & b_{12}^{-} & a_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{2.1}$$

where

$$a_{12} = a(u_1,u_2) \equiv \frac{\sinh(u_1-u_2)}{\sinh(u_1-u_2+\eta)}, \quad b_{12}^{\pm} = b^{\pm}(u_1,u_2) \equiv \frac{e^{\pm(u_1-u_2)}\sinh\eta}{\sinh(u_1-u_2+\eta)},$$

$$c_{12} = c(u_1,u_2) \equiv \frac{\sinh(u_1-u_2-\eta)}{\sinh(u_1-u_2+\eta)} \tag{2.2}$$

with $\eta \in C$ being the crossing parameter. One can easily check that the R-matrix satisfies the unitary relation

$$R_{21}R_{12} = 1. \tag{2.3}$$

Here and throughout $R_{ij} \equiv R_{ij}(u_i,u_j)$. The R-matrix satisfies the graded Yang-Baxter equation (GYBE)

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}. \tag{2.4}$$

In terms of the matrix elements defined by

$$R(u)(v^{i'} \otimes v^{j'}) = \sum_{i,j} R(u)_{ij}^{i'j'}(v^i \otimes v^j), \tag{2.5}$$

the GYBE reads

$$\sum_{i',j',k'} R(u_1-u_2)_{ij}^{i'j'} R(u_1-u_3)_{i'k}^{i''k'} R(u_2-u_3)_{j'k'}^{j''k''}(-1)^{[j']([i']+[i''])}$$
$$= \sum_{i',j',k'} R(u_2-u_3)_{jk}^{j'k'} R(u_1-u_3)_{ik'}^{i'k''} R(u_1-u_2)_{i'j'}^{i''j''}(-1)^{[j']([i]+[i'])}. \tag{2.6}$$

The quantum monodromy matrix $T(u)$ of the free Fermion model on a lattice of length N is defined as

$$T_0(u) = R_{0N}(u,z_N)R_{0N-1}(u,z_{N-1})\cdots R_{01}(u,z_1), \tag{2.7}$$

where the index 0 refers to the auxiliary space and $\{z_i\}$ are arbitrary inhomogeneous parameters depending on site i. $T(u)$ can be represented in the auxiliary space as the 2×2 matrix whose elements are operators acting on the quantum space $V^{\otimes N}$,

$$T_0(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}_{(0)}. \tag{2.8}$$

By using the GYBE, one may prove that the monodromy matrix satisfies the GYBE,

$$R_{12}(u-v)T_1(u)T_2(v) = T_2(v)T_1(u)R_{12}(u-v) \tag{2.9}$$

or in matrix form

$$\sum_{i',j'} R(u-v)_{ij}^{i'j'} T(u)_{i'}^{i''} T(v)_{j'}^{j''} (-1)^{[j']([i']+[i''])} = \sum_{i',j'} T(v)_j^{j'} T(u)_i^{i'} R(u-v)_{i'j'}^{i''j''} (-1)^{[j']([i]+[i'])}. \tag{2.10}$$

Define the transfer matrix $t(u)$

$$t(u) = \mathrm{str}_0\, T_0(u), \tag{2.11}$$

where str_0 denotes the supertrace over the auxiliary space. With the help of the GYBE, one may check that the transfer matrix satisfies the commutation relation $[t(u),t(v)]=0$, ensuring the integrability of the system. The transfer matrix gives the Hamiltonian of the system,

$$\begin{aligned} H &= \left.\frac{d \ln t(u)}{du}\right|_{u=0} \\ &= \frac{1}{\sinh \eta} \sum_{j=1}^{N} (E_{(j)}^{12} E_{(j+1)}^{21} + E_{(j)}^{21} E_{(j+1)}^{12} - 2\cosh \eta E_{(j)}^{11} E_{(j+1)}^{11} - (e^{\eta} E_{(j)}^{11} E_{(j+1)}^{22} + e^{-\eta} E_{(j)}^{22} E_{(j+1)}^{11})), \end{aligned} \tag{2.12}$$

where $E_{(k)}^{ij}$ are generators, which act on the kth space, of the superalgebra $U_q(\mathrm{gl}(1|1))$.

Using the standard Fermionic representation

$$E_{(k)}^{12} = c_k, \quad E_{(k)}^{21} = c_k^{\dagger}, \quad E_{(k)}^{11} = 1 - n_k, \quad E_{(k)}^{22} = n_k, \quad n_k = c_k^{\dagger} c_k, \tag{2.13}$$

the Hamiltonian can be rewritten as

$$H = \frac{1}{\sinh \eta} \sum_{j=1}^{N} (c_j c_{j+1}^{\dagger} + c_j^{\dagger} c_{j+1} - 2\cosh \eta (1 - n_j)). \tag{2.14}$$

B. Algebraic Bethe ansatz

The transfer matrix (2.11) can be diagonalized by using the algebra Bethe ansatz. Define the Bethe state of the system

$$\Phi_N(v_1, v_2, \ldots, v_n) = \prod_{i=1}^{n} C(v_i)|0\rangle, \tag{2.15}$$

where $|0\rangle$ is the pseudovacuum,

$$|0\rangle = \prod_{k=1}^{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{(k)} \tag{2.16}$$

and the index (k) indicates the kth space.

Applying the elements of the monodromy matrix (2.8) to the pseudovacuum $|0\rangle$ and its dual, we easily obtain

$$B(u)|0\rangle = 0, \quad \langle 0|C(u) = 0, \quad D|0\rangle = |0\rangle, \quad \langle 0|D(u) = \langle 0|,$$

$$A(u)|0\rangle = \prod_{i=1}^{N} a(u,z_i)|0\rangle, \quad \langle 0|A(u) = \prod_{i=1}^{N} a(u,z_i)\langle 0|. \tag{2.17}$$

With the help of the GYBE (2.9), we obtain the commutation relations between the elements of the monodromy matrix,

$$C(u)C(v) = -c(u,v)C(v)C(u), \tag{2.18}$$

$$D(u)D(v) = D(v)D(u), \tag{2.19}$$

$$A(u)C(v) = \frac{c(u,v)}{a(u,v)}C(v)A(u) + \frac{b^+(u,v)}{a(u,v)}C(u)A(v), \tag{2.20}$$

$$D(u)C(v) = \frac{1}{a(v,u)}C(v)D(u) - \frac{b^-(v,u)}{a(v,u)}C(u)D(v), \tag{2.21}$$

$$\begin{aligned} B(u)C(v) &= -C(v)B(u) + \frac{b^+(u,v)}{a(u,v)}[D(v)A(u) - D(u)A(v)] \\ &= -C(v)B(u) + \frac{b^+(u,v)}{a(u,v)}[D(u)t(v) - D(v)t(u)]. \end{aligned} \tag{2.22}$$

Thus applying the transfer matrix $t(u)=D(u)-A(u)$ to the Bethe state and using the commutation relations repeatedly, we obtain the eigenvalues of $t(u)$ as

$$t(u)\Phi_N = \Lambda(u,\{v_k\})\Phi_N = \left[\prod_{k=1}^{n}\frac{1}{a(v_k,u)} - \prod_{j=1}^{N}a(u,z_j)\prod_{k=1}^{n}\frac{c(u,v_k)}{a(u,v_k)}\right]\Phi_N \tag{2.23}$$

providing v_k $(k=1,2,\ldots,n)$ satisfying the Bethe ansatz equations (BAE),

$$\prod_{j=1}^{N}a(v_k,z_j) = 1. \tag{2.24}$$

For late use, we define the state of the free Fermion chain of length N,

$$|a_1a_2\cdots a_N\rangle = |a_1\rangle_{(1)}|a_2\rangle_{(2)}\cdots|a_N\rangle_{(N)} \tag{2.25}$$

and its dual

$$|a_1a_2\cdots a_N\rangle^\dagger = \langle a_N|_{(N)}\langle a_{N-1}|_{(N-1)}\cdots\langle a_1|_{(1)} \equiv \langle a_Na_{N-1}\cdots a_1|. \tag{2.26}$$

III. DRINFELD TWISTS OF THE MODEL

A. Factorizing *F*-matrix and its inverse

Following Ref. 4, we now introduce the notation $R^{\sigma}_{1,\ldots,N}$, where σ is any element of the permutation group $\mathcal{S}_N$. We note that we may rewrite the GYBE as

$$R^{\sigma_{23}}_{23}T_{0,23} = T_{0,32}R^{\sigma_{23}}_{23}, \tag{3.1}$$

where $T_{0,23}\equiv R_{03}R_{02}$ and σ_{23} is the transposition of space labels (2,3). It follows that $R^{\sigma}_{1,\ldots,N}$ is a product of elementary R-matrices,[4,6] corresponding to a decomposition of σ into elementary transpositions. With the help of the GYBE, one may generalize (3.1) to a N-fold tensor product of spaces,

$$R^{\sigma}_{1,\ldots,N}T_{0,1,\ldots,N} = T_{0,\sigma(1,\ldots,N)}R^{\sigma}_{1,\ldots,N}, \tag{3.2}$$

where $T_{0,1,\ldots,N} \equiv R_{0N}\cdots R_{01}$. This implies the "decomposition" law

$$R^{\sigma'\sigma}_{1,\ldots,N} = R^{\sigma}_{\sigma'(1,\ldots,N)} R^{\sigma'}_{1,\ldots,N}, \tag{3.3}$$

for a product of two elements in $\mathcal{S}_N$. Note that $R^{\sigma}_{\sigma'(1,\ldots,N)}$ satisfies the relation

$$R^{\sigma}_{\sigma'(1,\ldots,N)} T_{0,\sigma'(1,\ldots,N)} = T_{0,\sigma'\sigma(1,\ldots,N)} R^{\sigma}_{\sigma'(1,\ldots,N)}. \tag{3.4}$$

Let us write the elements of $R^{\sigma}_{1,\ldots,N}$ as

$$(R^{\sigma}_{1,\ldots,N})^{\alpha_{\sigma(N)}\cdots\alpha_{\sigma(1)}}_{\beta_N\cdots\beta_1}, \tag{3.5}$$

where the labels in the upper indices are permuted relative to the lower indices according to σ.

We proved in Refs. 6–8 that for the R-matrix $R^{\sigma}_{1,\ldots,N}$, there exists a nondegenerate lower-diagonal F-matrix (the Drinfeld twist) satisfying the relation

$$F_{\sigma(1,\ldots,N)}(z_{\sigma(1)}, \ldots, z_{\sigma(N)}) R^{\sigma}_{1,\ldots,N}(z_1, \ldots, z_N) = F_{1,\ldots,N}(z_1, \ldots, z_N). \tag{3.6}$$

Explicitly,

$$F_{1,\ldots,N} = \sum_{\sigma\in\mathcal{S}_N} \sum_{\alpha_{\sigma(1)}\cdots\alpha_{\sigma(N)}}^{*} \prod_{j=1}^{N} P^{\alpha_{\sigma(j)}}_{\sigma(j)} S(c,\sigma,\alpha_\sigma) R^{\sigma}_{1,\ldots,N}, \tag{3.7}$$

where the sum Σ^* is over all nondecreasing sequences of the labels $\alpha_{\sigma(i)}$,

$$\alpha_{\sigma(i+1)} \geqslant \alpha_{\sigma(i)}, \quad \text{if } \sigma(i+1) > \sigma(i),$$

$$\alpha_{\sigma(i+1)} > \alpha_{\sigma(i)}, \quad \text{if } \sigma(i+1) < \sigma(i), \tag{3.8}$$

and the c-number function $S(c,\sigma,\alpha_\sigma)$ is given by

$$S(c,\sigma,\alpha_\sigma) \equiv \exp\left\{ \frac{1}{2} \sum_{l>k=1}^{N} (1-(-1)^{[\alpha_{\sigma(k)}]}) \delta_{\alpha_{\sigma(k)},\alpha_{\sigma(l)}} \ln(1+c_{\sigma(k)\sigma(l)}) \right\}. \tag{3.9}$$

The inverse of the F-matrix is given by

$$F^{-1}_{1,\ldots,N} = F^{*}_{1,\ldots,N} \prod_{i<j} \Delta^{-1}_{ij} \tag{3.10}$$

with

$$\Delta_{ij} = \mathrm{diag}((1+c_{ij})(1+c_{ji}), a_{ji}, a_{ij}, 1) \tag{3.11}$$

and

$$F^{*}_{1,\ldots,N} = \sum_{\sigma\in\mathcal{S}_N} \sum_{\alpha_{\sigma(1)}\cdots\alpha_{\sigma(N)}}^{**} S(c,\sigma,\alpha_\sigma) R^{\sigma^{-1}}_{\sigma(1,\ldots,N)} \prod_{j=1}^{N} P^{\alpha_{\sigma(j)}}_{\sigma(j)}, \tag{3.12}$$

where the sum Σ^{**} is taken over all possible α_i which satisfies the following nonincreasing constraints:

$$\alpha_{\sigma(i+1)} \leqslant \alpha_{\sigma(i)} \quad \text{if } \sigma(i+1) < \sigma(i),$$

$$\alpha_{\sigma(i+1)} < \alpha_{\sigma(i)} \quad \text{if } \sigma(i+1) > \sigma(i). \tag{3.13}$$

B. Symmetric representation of the Bethe state

The nondegeneracy of the F-matrix means that its column vectors form a complete basis, which is called the F-basis. By the procedure in Ref. 8, we find that in the F-basis, the simple generators of the superalgebra $U_q(\mathrm{gl}(1|1))$ have the symmetric form,

$$\tilde{E}^{12} = F_{12,\ldots,N} E^{12} F^{-1}_{12,\ldots,N} = \sum_{i=1}^{N} E^{12}_{(i)} \otimes_{j\neq i} \mathrm{diag}(2e^{-\eta}\cosh\,\eta, e^{-\eta})_{(j)}, \tag{3.14}$$

$$\tilde{E}^{21} = F_{12,\ldots,N} E^{21} F^{-1}_{12,\ldots,N} = \sum_{i=1}^{N} E^{12}_{(i)} \otimes_{j\neq i} \mathrm{diag}(e^{\eta}(2a_{ji}\cosh\,\eta)^{-1}, e^{\eta}a_{ji}^{-1})_{(j)}. \tag{3.15}$$

Similarly, the diagonal element $D(u)$ of the monodromy matrix in the F-basis is given by

$$\tilde{D}(u) = F_{12,\ldots,N} D(u) F^{-1}_{12,\ldots,N} = \otimes_{j=1}^{N} \mathrm{diag}(a_{0j}, 1), \tag{3.16}$$

where $a_{0j} \equiv a(u, z_j)$.

Then, the creation and annihilation operators $C(u)$ and $B(u)$ read, in the F-basis,

$$\begin{aligned}\tilde{C}(u) &= F_{12,\ldots,N} C(u) F^{-1}_{12,\ldots,N} = (q^{-1}\tilde{E}^{12}_{(i)}\tilde{D}(u) - \tilde{D}(u)\tilde{E}^{12}_{(i)}) q^{-\Sigma_{i=1}^{N} h_{(i)}} \\ &= \sum_{i=1}^{N} b_{0i}^{-} E^{12}_{(i)} \otimes_{j\neq i} \mathrm{diag}(2a_{0j}\cosh\,\eta, 1)_{(j)},\end{aligned} \tag{3.17}$$

$$\begin{aligned}\tilde{B}(u) &= F_{12,\ldots,N} B(u) F^{-1}_{12,\ldots,N} = q^{\Sigma_{i=1}^{N} h_{(i)}} (\tilde{E}^{21}\tilde{D} - q\tilde{D}\tilde{E}^{21}) \\ &= -\sum_{i=1}^{N} b_{0i}^{+} E^{21}_{(i)} \otimes_{j\neq i} \mathrm{diag}(a_{0j}(2a_{ji}\cosh\,\eta)^{-1}, a_{ji}^{-1})_{(j)},\end{aligned} \tag{3.18}$$

where $b^{\pm}_{0j} \equiv b^{\pm}(u, z_j)$, $q = e^{\eta}$, and $h \equiv -E^{11} - E^{22}$.

Acting the F-matrix (3.7) on the state (2.16), one sees that the pseudovacuum is invariant. Therefore in the F-basis, the Bethe state (2.15) becomes

$$\tilde{\Phi}_N(v_1, v_2, \ldots, v_n) \equiv F_{1,\ldots,N} \Phi_N(v_1, \ldots, v_n) = \prod_{i=1}^{n} \tilde{C}(v_n)|0\rangle. \tag{3.19}$$

Substituting (3.17) into (3.19), we obtain

$$\tilde{\Phi}_N(v_1, \ldots, v_n) = (2\cosh\,\eta)^{[n(n-1)]/2} \sum_{i_1<\cdots<i_n} B_n^{-}(v_1, \ldots, v_n | z_{i_1}, \ldots, z_{i_n}) E^{12}_{(i_1)} \cdots E^{12}_{(i_n)}|0\rangle, \tag{3.20}$$

where

$$B_n^{\pm}(v_1, \ldots, v_n | z_{i_1}, \ldots, z_{i_n}) = \sum_{\sigma\in\mathcal{S}_n} \mathrm{sign}(\sigma) \prod_{k=1}^{n} b^{\pm}(v_k, z_{i_{\sigma(k)}}) \prod_{l=k+1}^{n} a(v_k, z_{i_{\sigma(l)}}) = \det \mathcal{B}^{\pm}(\{v_k\}, \{z_j\}) \tag{3.21}$$

with $\mathcal{B}^{\pm}(\{v_i\}, \{z_j\})$ being a $n \times n$ matrix with matrix elements,

$$\mathcal{B}^{\pm}_{\alpha\beta} = b^{\pm}(v_\alpha, z_\beta) \prod_{\gamma=1}^{\alpha-1} a(v_\gamma, z_\beta). \tag{3.22}$$

Similarly, acting $\widetilde{B}(u_n)\cdots\widetilde{B}(u_1)$ on the dual pseudovacuum state, we have

$$\langle 0|\widetilde{B}(u_n)\cdots\widetilde{B}(u_1) = (-1)^n(2\cosh\eta)^{[-n(n-1)]/2}\sum_{i_1<\cdots<i_n}\prod_{l=1}^{n}\prod_{k=1,\neq i_l}^{N}a^{-1}(z_k,z_{i_l}) \times \det\mathcal{B}^{+}(\{v_k\},\{z_{i_j}\})\langle 0|E^{21}_{(i_n)}\cdots E^{21}_{(i_1)}. \tag{3.23}$$

IV. DETERMINANT REPRESENTATION OF THE SCALAR PRODUCT OF THE BETHE STATES

In Refs. 2 and 5 the authors gave the determinant representation of the scalar product of the Bethe state for the spin-1/2 *XXZ* model. In this section, we derive the determinant representation of the scalar product of the $U_q(\mathrm{gl}(1|1))$ Bethe states defined by

$$S_n(\{u_j\},\{v_k\}) = \langle 0|B(u_n)\cdots B(u_1)C(v_1)\cdots C(v_n)|0\rangle. \tag{4.1}$$

The F-invariance of the pseudovacuum state $|0\rangle$ and its dual state $\langle 0|$ leads to

$$S_n(\{u_j\},\{v_k\}) = \langle 0|\widetilde{B}(u_n)\cdots\widetilde{B}(u_1)\widetilde{C}(v_1)\cdots\widetilde{C}(v_n)|0\rangle. \tag{4.2}$$

Following Ref. 5, we define

$$G^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n) = \langle i_n,\ldots,i_{m+1}|\widetilde{B}(u_m)\cdots\widetilde{B}(u_1)\widetilde{C}(v_1)\cdots\widetilde{C}(v_n)|0\rangle, \tag{4.3}$$

where i_k $(k=m+1,\ldots,n)$, ordered as $i_{m+1}<\cdots<i_n$, indicate the positions having state $\binom{1}{0}$, and other positions have state $\binom{0}{1}$. One sees that when $m=n$, $G^{(n)}=S_n$. Inserting a complete set and noticing (3.18) and (4.3) becomes

$$G^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n) = \sum_{j\neq i_{m+1},\ldots,i_n}^{N}\langle i_n,\ldots,i_{m+1}|\widetilde{B}(u_m)|i_{m+1},\ldots,i_{m+p},j,i_{m+p+1},\ldots,i_n\rangle \times G^{(m-1)}(\{v_k\},u_1,\ldots,u_{m-1},i_{m+1},\ldots,i_{m+p},j,i_{m+p+1},\ldots,i_n). \tag{4.4}$$

In view of (3.18), we have

$$\langle i_n,\ldots,i_{m+1}|\widetilde{B}(u_m)|i_{m+1},\ldots,i_{m+p},j,i_{m+p+1},\ldots,i_n\rangle = -(2\cosh\eta)^{-(n-m)} \times(-1)^p b^{+}(u_m,z_j)\prod_{k\neq j}^{N}a^{-1}(z_k,z_j)\prod_{l=m+1}^{n}a(u_m,z_{i_l}). \tag{4.5}$$

With the help of (3.20), we obtain $G^{(0)}$,

$$G^{(0)}(\{v_k\},i_1,\ldots,i_n) = \langle i_n,\ldots,i_1|\prod_{k=1}^{n}\widetilde{C}(v_k)|0\rangle = (2\cosh\eta)^{[n(n-1)]/2}\det\mathcal{B}^{-}(\{v_k\},\{z_{i_l}\}). \tag{4.6}$$

We now compute $G^{(1)}$ by using the recursion relation (4.4). Substituting (4.5) and (4.6) into (4.4), we obtain

$$G^{(1)}(\{v_k\},u_1,i_2,\ldots,i_n)=\sum_{j\neq i_2,\ldots,i_n}^{N}\langle i_n,\ldots,i_2|\tilde{B}(u_1)|i_2,\ldots,i_{p+1},j,i_{p+2},\ldots,i_n\rangle$$
$$\times G^{(0)}(\{v_k\},i_2,\ldots,i_{p+1},j,i_{p+2},\ldots,i_n)$$
$$=-(2\cosh\eta)^{[(n-1)(n-2)]/2}\sum_{j\neq i_2,\ldots,i_n}^{N}(-1)^p b^+(u_1,z_j)\prod_{k\neq j}^{N}a^{-1}(z_k,z_j)\prod_{l=2}^{n}a(u_1,z_{i_l})$$
$$\times\det\mathcal{B}^-(\{v_k\},z_{i_2},\ldots,z_{i_{p+1}},z_j,z_{i_{p+2}},\ldots,z_{i_n})\quad(k=1,\cdots,n).\tag{4.7}$$

Let v_k $(k=1,\ldots,n)$ label the row and z_l $(l=i_2,\ldots,j,\ldots,i_n)$ label the column of the matrix $\mathcal{B}^-$. From (4.6), one sees that the column indices in (4.7) satisfy the sequence $i_2<\cdots<j<\cdots<i_n$. Therefore, moving the column j in the matrix $\mathcal{B}^-$ to the first column, we have

$$G^{(1)}(\{v_k\},u_1,i_2,\ldots,i_n)=-(2\cosh\eta)^{[(n-1)(n-2)/2]}\sum_{j\neq i_1,\ldots,i_n}^{N}b^+(u_1,z_j)\prod_{k\neq j}^{N}a^{-1}(z_k,z_j)\prod_{l=2}^{n}a(u_1,z_{i_l})$$
$$\times\det\mathcal{B}(\{v_k\},z_j,z_{i_2},\ldots,z_{i_n})$$
$$=-(2\cosh\eta)^{[(n-1)(n-2)/2]}\det(\mathcal{B}^-)^{(1)}(\{v_k\},u_1,z_{i_2},\ldots,z_{i_n}),\tag{4.8}$$

where the matrix $(\mathcal{B}^-)^{(1)}(\{v_k\},u_1,z_{i_2},\ldots,z_{i_n})$ is given by

$$(\mathcal{B}^-_{\alpha\beta})^{(1)}=a(u_1,z_{i_\beta})\mathcal{B}^-_{\alpha\beta}\quad\text{for }\beta\geqslant 2,\tag{4.9}$$

$$(\mathcal{B}^-_{\alpha 1})^{(1)}=\sum_{j\neq i_2,\ldots,i_n}^{N}b^+(u_1,z_j)b^-(v_\alpha,z_j)\prod_{\gamma=1}^{\alpha-1}a(v_\gamma,z_j)\prod_{k=1,\neq j}^{N}a^{-1}(z_k,z_j).\tag{4.10}$$

Using the properties of determinant, one finds that if $j=i_2,\ldots,i_n$, the corresponding terms in (4.10) contribute zero to the determinant. Thus, we may rewrite (4.10) as

$$(\mathcal{B}^-_{\alpha 1})^{(1)}=\sum_{j=1}^{N}\frac{e^{u_1-v_\alpha}\sinh^2\eta}{\sinh(u_1-z_j+\eta)\sinh(v_\alpha-z_j+\eta)}\prod_{\gamma=1}^{\alpha-1}\frac{\sinh(v_\gamma-z_j)}{\sinh(v_\gamma-z_j+\eta)}\prod_{k=1,\neq j}^{N}\frac{\sinh(z_k-z_j+\eta)}{\sinh(z_k-z_j)}$$
$$\equiv e^{u_1}f(u_1).\tag{4.11}$$

Thanks to the Bethe ansatz equation (2.24), we may construct the function

$$\mathcal{M}^{\pm}_{\alpha\beta}=e^{\mp u_\beta}g(u_\beta)=\frac{e^{\pm(v_\alpha-u_\beta)}\sinh\eta}{\sinh(v_\alpha-u_\beta)}\prod_{\gamma=1}^{\alpha-1}\frac{\sinh(v_\gamma-u_\beta-\eta)}{\sinh(v_\gamma-u_\beta)}\left\{1-\prod_{k=1}^{N}\frac{\sinh(u_\beta-z_k)}{\sinh(u_\beta-z_k+\eta)}\right\}.\tag{4.12}$$

Comparing $f(u_1)$ in (4.11) with $g(u_1)$ in (4.12), one finds that as functions of u_1, they have the same residues at the simple pole $u_1=z_j-\eta\,\mathrm{mod}(i\pi)$, and that when $u_1\to\infty$, they are bounded. Moreover, one may prove that the residues of $g(u_1)$ at $u_1=v_\nu\,\mathrm{mod}(i\pi)$ $(\nu=1,\ldots,\alpha)$ are zero because v_ν are solutions of the Bethe ansatz equation (2.24). Therefore, we have

$$(\mathcal{B}^-_{\alpha 1})^{(1)}=\mathcal{M}^-_{\alpha 1}=\frac{b^-(v_\alpha,u_1)}{a(v_\alpha,u_1)}\prod_{\gamma=1}^{\alpha-1}a^{-1}(u_1,v_\gamma)\left(1-\prod_{k=1}^{N}a(u_1,z_k)\right).\tag{4.13}$$

Then, by using the function $G^{(0)}$, $G^{(1)}$ and the intermediate function (4.4) repeatedly, we obtain $G^{(m)}$ as

$$G^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n)=(-1)^m(2\cosh\eta)^{[n(n-1)-m(2n-m-1)]/2}\prod_{1\leqslant j<k\leqslant m}a^{-1}(u_k,u_j)$$
$$\times\det(\mathcal{B}^-)^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n) \tag{4.14}$$

with the matrix elements

$$(\mathcal{B}^-_{\alpha\beta})^{(m)}=\prod_{k=1}^{m}a(u_k,z_{i_\beta})\mathcal{B}^-_{\alpha\beta},\quad \text{for } \beta>m,$$

$$(\mathcal{B}^-_{\alpha\beta})^{(m)}=\mathcal{M}^-_{\alpha\beta}\quad \text{for } \beta\leqslant m. \tag{4.15}$$

Equation (4.14) can be proved by induction. First from (4.8), (4.9), (4.13), and (4.14) is true for $m=1$. Assume (4.14) for $G^{(m-1)}$. Let us show (4.14) for general m. Substituting $G^{(m-1)}$ and (4.5) into intermediate function (4.4), we have

$$\begin{aligned}
&G^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n)\\
&=\sum_{j\neq i_{m+1},\ldots,i_n}^{N}\langle i_n,\ldots,i_{m+1}|\tilde{B}(u_m)|i_{m+1},\ldots,i_{m+p},j,i_{m+p+1},\ldots,i_n\rangle\\
&\quad\times G^{(m-1)}(\{v_k\},u_1,\ldots,u_{m-1},i_{m+1},\ldots,i_{m+p},j,i_{m+p+1},\ldots,i_n)\\
&=-(2\cosh\eta)^{-(n-m)}\sum_{j\neq i_{m+1},\ldots,i_n}^{N}b^+(u_m,z_j)\prod_{k\neq j}^{N}a^{-1}(z_k,z_j)\prod_{l=m+1}^{n}a(u_m,z_{i_l})\\
&\quad\times G^{(m-1)}(\{v_k\},u_1,\ldots,u_{m-1},j,i_{m+1},\ldots,i_n)\\
&=(-1)^m(2\cosh\eta)^{[n(n-1)-m(2n-m-1)]/2}\prod_{1\leqslant j<k\leqslant m-1}a^{-1}(u_k,u_j)\\
&\quad\times\det\mathcal{B}'^{(m)}(\{v_k\},u_1,\ldots,u_m,i_{m+1},\ldots,i_n),
\end{aligned} \tag{4.16}$$

where the matrix elements $\mathcal{B}'^{(m)}_{\alpha\beta}$ are given by

$$\mathcal{B}'^{(m)}_{\alpha\beta}=\prod_{k=1}^{m}a(u_k,z_{i_\beta})\mathcal{B}^-_{\alpha\beta}\quad \text{for } \beta>m,$$

$$\mathcal{B}'^{(m)}_{\alpha\beta}=\mathcal{M}^-_{\alpha\beta}\quad \text{for } \beta<m,$$

$$\mathcal{B}'^{(m)}_{\alpha m}=\prod_{i=1}^{m-1}a(u_i,z_j)\sum_{j\neq i_{m+1},\ldots,i_n}b^+(u_m,z_j)b^-(v_\alpha,z_j)\prod_{\gamma=1}^{\alpha-1}a(v_\gamma,z_j)\prod_{k=1,\neq j}^{N}a^{-1}(z_k,z_j). \tag{4.17}$$

Thus, by the procedure leading to $(\mathcal{B}^-_{\alpha\beta})^{(1)}$, we can prove

$$\mathcal{B}'^{(m)}_{\alpha m}=\prod_{i=1}^{m-1}a^{-1}(u_m,u_i)\mathcal{M}^-_{\alpha m}. \tag{4.18}$$

Then one sees that $\mathcal{B}'^{(m)}_{\alpha\beta}=\mathcal{B}^{(m)}_{\alpha\beta}$. Therefore we have proved that (4.14) holds for all m.

When $m=n$, we obtain the scalar product $S_n(\{u_i\},\{v_j\})$,

$$S_n(\{u_i\},\{v_j\})=(-1)^n\prod_{k>l}^{n}a^{-1}(u_k,u_l)\det\mathcal{M}^-(\{v_j\},\{u_i\}), \tag{4.19}$$

where the matrix elements of $\mathcal{M}^-$ are given by

$$\mathcal{M}^{\pm}_{\alpha\beta}=\frac{b^{\pm}(v_\alpha,u_\beta)}{a(v_\alpha,u_\beta)}\prod_{\gamma=1}^{\alpha-1}a^{-1}(u_\beta,v_\gamma)\left(1-\prod_{k=1}^{N}a(u_\beta,z_k)\right). \tag{4.20}$$

By using the expression of the eigenvalues of the system (2.23), the scalar product (4.19) can be rewritten as

$$S_n(\{u_i\},\{v_j\})=(-1)^n\prod_{k>l}^{n}a^{-1}(u_k,u_l)\det\hat{\mathcal{M}}^{-}(\{v_j\},\{u_i\}) \tag{4.21}$$

with the matrix $\hat{\mathcal{M}}^{\pm}$ being

$$\hat{\mathcal{M}}^{\pm}_{\alpha\beta}=e^{\pm(v_\alpha-u_\beta)}\sinh(u_\beta-v_\alpha)\prod_{\mu\neq\alpha}a(v_\mu,u_\beta)\prod_{\gamma=1}^{\alpha-1}a^{-1}(u_\alpha,v_\gamma)\frac{\partial\Lambda(u_\beta,\{v_\alpha\})}{\partial v_\alpha}. \tag{4.22}$$

Remark: In the derivation of (4.19), the parameters v_i in the state $\tilde{C}(v_1)\cdots\tilde{C}(v_n)|0\rangle$ are required to satisfy the BAE (2.24). However, the parameters u_j $(j=1,\ldots,n)$ in the dual state $\langle 0|\tilde{B}(u_n)\cdots\tilde{B}(u_1)$ do not need to satisfy the BAE.

On the other hand, if we compute the scalar product by starting from the dual state $\langle 0|B(v_n)\cdots B(v_1)$, then by using the same procedure, we have

$$S_n(\{v_i\},\{u_j\})=\langle 0|\tilde{B}(v_n)\cdots\tilde{B}(v_1)\tilde{C}(u_1)\cdots\tilde{C}(u_n)|0\rangle=(-1)^n\prod_{k>l}^{n}a^{-1}(u_k,u_l)\det\mathcal{M}^{+}(\{v_i\},\{u_j\}). \tag{4.23}$$

In the above equation, we have assumed that $\{v_i\}$ satisfy the BAE.

Noticing the BAE (2.24), one sees that the scalar product $S_n(\{u_i\},\{v_j\})=0$ if both parameter sets $\{u_i\}$ and $\{v_j\}(\{v_j\}\neq\{u_i\}i,j=1,\ldots,n)$ in (4.19) and (4.23) satisfy the BAE.

Let $u_\alpha\to v_\alpha$ $(\alpha=1,\ldots,n)$ in (4.19), we obtain the Gaudin formula for the norm of the $U_q(\mathrm{gl}(1|1))$ Bethe state,

$$\begin{aligned}\mathcal{S}_n&=S_n(\{v_j\},\{v_k\})=\langle 0|B(v_n)\cdots B(v_1)C(v_1)\cdots C(v_n)|0\rangle\\&=(-1)^n\sinh^n\eta\prod_{k>j}^{n}\frac{\sinh^2(v_k-v_j+\eta)}{\sinh^2(v_k-v_j)}\left[\prod_{\alpha=1}^{n}\frac{1}{v_\alpha-u_\alpha}\left(1-\prod_{l=1}^{N}\frac{\sinh(u_\alpha-z_l)}{\sinh(u_\alpha-z_l+\eta)}\right)\right]_{u_\alpha\to v_\alpha}\\&=(-1)^n\sinh^n\eta\prod_{k>j}^{n}\frac{\sinh^2(v_k-v_j+\eta)}{\sinh^2(v_k-v_j)}\left[\prod_{\alpha=1}^{n}\frac{\partial}{\partial u_\alpha}\ln\left(\prod_{l=1}^{N}\frac{\sinh(u_\alpha-z_l)}{\sinh(u_\alpha-z_l+\eta)}\right)\right]_{u_\alpha\to v_\alpha}\\&=(-1)^n\sinh^{2n}\eta\prod_{k>j}^{n}\frac{\sinh^2(v_k-v_j+\eta)}{\sinh^2(v_k-v_j)}\prod_{\alpha=1}^{n}\sum_{l=1}^{N}\frac{1}{\sinh(v_\alpha-z_l)\sinh(v_\alpha-z_l+\eta)},\end{aligned} \tag{4.24}$$

where we have used the BAE (2.24).

V. CORRELATION FUNCTIONS

Having obtained the scalar product and the norm, we are now in the position to compute the k-point correlation functions of the model. In general, a k-point correlation function is defined by

$$F_n^{\epsilon^1,\ldots,\epsilon^k}=\langle 0|B(u_n)\cdots B(u_1)\epsilon^1_{i_1}\cdots\epsilon^k_{i_k}C(v_1)\cdots C(v_n)|0\rangle, \tag{5.1}$$

where $\epsilon^j_{i_j}$ stand for the local Fermion operators c_{i_j}, $c^{\dagger}_{i_j}$ or n_{i_j}, and the lower indices i_j indicate the positions of the Fermion operators.

The authors in Ref. 16 proved that the local spin and field operators of the fundamental graded models can be represented in terms of monodromy matrix. Specializing to the current system, we obtain

$$c_j^\dagger = \prod_{k=1}^{j-1} (-A(z_k) + D(z_k)) \cdot B(z_j) \cdot \prod_{k=j+1}^{N} (-A(z_k) + D(z_k)), \tag{5.2}$$

$$c_j = \prod_{k=1}^{j-1} (-A(z_k) + D(z_k)) \cdot C(z_j) \cdot \prod_{k=j+1}^{N} (-A(z_k) + D(z_k)), \tag{5.3}$$

$$n_j = \prod_{k=1}^{j-1} (-A(z_k) + D(z_k)) \cdot D(z_j) \cdot \prod_{k=j+1}^{N} (-A(z_k) + D(z_k)). \tag{5.4}$$

A. One-point functions

In this section, we compute the one-point functions for the local operators $c_m^\dagger$, c_m, and n_m, respectively.

We first calculate $c_m^\dagger$. Noticing that the Bethe state and its dual are eigenstates of the transfer matrix under the constraint of the BAE, we have, from (5.2),

$$\begin{aligned}
F_n^-(\{u_j\},z_m,\{v_k\}) &= \langle 0|B(u_n)\cdots B(u_1)c_m^\dagger C(v_1)\cdots C(v_{n+1})|0\rangle \\
&= \phi_{m-1}(\{u_j\})\phi_m^{-1}(\{v_k\})\langle 0|B(u_n)\cdots B(u_1)B(z_m)C(v_1)\cdots C(v_{n+1})|0\rangle \\
&= \phi_{m-1}(\{u_j\})\phi_m^{-1}(\{v_k\})\langle 0|\widetilde{B}(u_n)\cdots \widetilde{B}(u_1)\widetilde{B}(z_m)\widetilde{C}(v_1)\cdots \widetilde{C}(v_{n+1})|0\rangle \\
&= \phi_{m-1}(\{u_j\})\phi_m^{-1}(\{v_k\})S_{n+1}(u_n,\ldots,u_1,z_m,\{v_j\}) \\
&= (-1)^{n+1}\phi_{m-1}(\{u_j\})\phi_m^{-1}(\{v_k\})\prod_{k>j}^{n} a^{-1}(u_k,u_j)\prod_{l=1}^{n} a^{-1}(u_l,z_m) \\
&\quad \times \det \mathcal{M}^-(\{v_j\},z_m,u_1,\ldots,v_n),
\end{aligned} \tag{5.5}$$

where $\phi_i(\{u_j\})=\Pi_{k=1}^{i}\Pi_{l=1}^{n}a(u_l,u_k)$. As mentioned in the remark of the preceding section, $F_n^-=0$ if the parameter set $\{u_i\}$ $(i=1,\ldots,n)$ is not a subset of $\{v_j\}$ $(j=1,\ldots,n+1)$. When $\{u_i\}\subset\{v_j\}$, (5.5) can be simplified to a simple function. For example, if $u_i=v_{i+1}$ $(i=1,\ldots,n)$, the one-point function F^- becomes

$$\begin{aligned}
&F_n^-(v_{n+1},\ldots,v_2,z_m,v_1,\ldots,v_{n+1}) \\
&\quad = (-1)^{n+1}\frac{\phi_{m-1}(\{u_j\})}{\phi_m(\{v_k\})}\frac{e^{-(v_1-z_m)}\sinh^{2n+1}\eta}{\sinh(v_1-z_m)}\prod_{k>j=2}^{n+1}\frac{\sinh^2(v_k-v_j+\eta)}{\sinh^2(v_k-v_j)} \\
&\qquad \times\prod_{j=2}^{n+1}\frac{\sinh(v_j-z_m+\eta)}{\sinh(v_j-z_m)}\prod_{j=2}^{n+1}\frac{\sinh(v_j-v_1+\eta)}{\sinh(v_j-v_1)}\prod_{\alpha=2}^{n+1}\sum_{l=1}^{N}\frac{1}{\sinh(v_\alpha-z_l)\sinh(v_\alpha-z_l+\eta)}.
\end{aligned} \tag{5.6}$$

Similarly, when $\{u_i\}\subset\{v_j\}$, we obtain the one-point function involving the operator c_m,

$$
\begin{aligned}
F_n^+(\{v_k\},z_m,\{u_j\}) &= \langle 0|B(v_{n+1})\cdots B(v_1)c_m C(u_1)\cdots C(u_n)|0\rangle \\
&= \phi_{m-1}(\{v_j\})\phi_m^{-1}(\{u_k\})S_{n+1}(\{v_j\},z_m,u_1,\ldots,u_n) \\
&= (-1)^{n+1}\phi_{m-1}(\{v_j\})\phi_m^{-1}(\{u_k\})\prod_{k>j}^{n} a^{-1}(u_k,u_j)\prod_{l=1}^{n} a^{-1}(u_l,z_m) \\
&\quad \times \det \mathcal{M}^+(\{v_j\},z_m,u_1,\ldots,v_n). \qquad (5.7)
\end{aligned}
$$

F_n^+ is nonvanishing if $\{u_i\}\subset\{v_j\}$. When $\{u_i\}\subset\{v_j\}$, (5.7) can also be simplified to a simple function. In the case $u_i=v_{i+1}$ $(i=1,\ldots,n)$, the one-point function F^+ becomes

$$
\begin{aligned}
&F_n^+(v_{n+1},\ldots,v_2,z_m,v_1,\ldots,v_{n+1}) \\
&= (-1)^{n+1}\frac{\phi_{m-1}(\{v_j\})}{\phi_m(\{u_k\})}\frac{e^{(v_1-z_m)}\sinh^{2n+1}\eta}{\sinh(v_1-z_m)}\prod_{k>j=2}^{n+1}\frac{\sinh^2(v_k-v_j+\eta)}{\sinh^2(v_k-v_j)} \\
&\quad \times\prod_{j=2}^{n+1}\frac{\sinh(v_j-z_m+\eta)}{\sinh(v_j-z_m)}\prod_{j=2}^{n+1}\frac{\sinh(v_j-v_1+\eta)}{\sinh(v_j-v_1)}\prod_{\alpha=2}^{n+1}\sum_{l=1}^{N}\frac{1}{\sinh(v_\alpha-z_l)\sinh(v_\alpha-z_l+\eta)}. \qquad (5.8)
\end{aligned}
$$

The one-point function involving the operator n_m is defined by

$$
F_n^{n_m}(\{u_j\},z_m,\{v_k\}) = \langle 0|B(u_n)\cdots B(u_1)n_m C(v_1)\cdots C(v_n)|0\rangle. \qquad (5.9)
$$

Substituting (5.4) into the above equation and considering the BAE, we have

$$
\begin{aligned}
F_n^{n_m}(\{u_j\},z_m,\{v_k\}) &= \langle 0|B(u_n)\cdots B(u_1)n_m C(v_1)\cdots C(v_n)|0\rangle \\
&= \frac{\phi_{m-1}(\{u_j\})}{\phi_{m-1}(\{v_k\})}\langle 0|\tilde{B}(u_n)\cdots\tilde{B}(u_1)\tilde{D}(z_m)\tilde{C}(v_1)\cdots\tilde{C}(v_n)|0\rangle. \qquad (5.10)
\end{aligned}
$$

With the help of (2.21), we see

$$
\begin{aligned}
D(z_m)C(v_1)\cdots C(v_n)|0\rangle &= \prod_{k=1}^{n} a^{-1}(v_k,z_m)C(v_1)\cdots C(v_n)|0\rangle \\
&\quad -\sum_{j=1}^{n}\frac{b^-(v_j,z_m)}{a(v_j,z_m)}\prod_{l=1}^{j-1}\frac{c(v_l,v_j)}{c(v_l,z_m)}\prod_{k=1,\neq j}^{n} a^{-1}(v_k,v_j) \\
&\quad \times C(v_1)\cdots C(v_{j-1})C(z_m)C(v_{j+1})\cdots C(v_n)|0\rangle. \qquad (5.11)
\end{aligned}
$$

Therefore, substituting (5.11) into (5.10), we obtain

$$
\begin{aligned}
F_n^{n_m}(\{u_j\},z_m,\{v_k\}) &= \frac{\phi_{m-1}(\{u_j\})}{\phi_{m-1}(\{v_k\})}\prod_{k=1}^{n} a^{-1}(v_k,z_m)S_n(\{u_i\},\{v_j\}) \\
&\quad -\sum_{j=1}^{n}\frac{b^-(v_j,z_m)}{a(v_j,z_m)}\prod_{l=1}^{j-1}\frac{c(v_l,v_j)}{c(v_l,z_m)}\prod_{k=1,\neq j}^{n} a^{-1}(v_k,v_j)S_n(\{u_i\},v_1,\ldots,v_{j-1},z_m,v_{j+1},\ldots,v_n) \\
&= (-1)^n\frac{\phi_{m-1}(\{u_j\})}{\phi_{m-1}(\{v_k\})}\prod_{k=1}^{n} a^{-1}(v_k,z_m)\prod_{k>j} a^{-1}(v_k,v_j)\det[M^+(\{u_i\},\{v_j\}) \\
&\quad -\mathcal{N}(\{u_i\},\{v_j\},z_m)], \qquad (5.12)
\end{aligned}
$$

where $\mathcal{N}$ is a rank-one matrix with the following matrix elements:

$$\mathcal{N}_{\alpha\beta}(\{u_i\},\{v_j\},z_m)=\frac{e^{u_\alpha-v_\beta}\sinh^2\eta}{\sinh(u_\alpha-z_m)\sinh(v_\beta-z_m+\eta)}\prod_{i=1}^{\alpha-1}\frac{\sinh(z_m-u_i+\eta)}{\sinh(z_m-u_i)}. \tag{5.13}$$

In the above derivation, we have used the following property of determinant: If $\mathcal{A}$ is an arbitrary $n\times n$ matrix and $\mathcal{B}$ is a rank-one $n\times n$ matrix, then the determinant of $\mathcal{A}+\mathcal{B}$ is given by

$$\det(\mathcal{A}+\mathcal{B})=\det\mathcal{A}+\sum_{i=1}^{n}\det\mathcal{A}^{(i)}, \tag{5.14}$$

where

$$\mathcal{A}^{(i)}_{\alpha\beta}=\mathcal{A}_{\alpha\beta}\quad\text{for }\beta\neq i,$$

$$\mathcal{A}^{(i)}_{\alpha i}=\mathcal{B}_{\alpha i}.$$

B. Correlation function of two adjacent operators

In this section, we compute the correlation function of two adjacent operators c_m and c_{m+1} defined by

$$F_n^{-+}(\{u_i\},z_m,z_{m+1},\{v_j\})=\langle 0|B(u_n)\cdots B(u_1)c_m c^\dagger_{m+1}C(v_1)\cdots C(v_n)|0\rangle. \tag{5.15}$$

Substituting (5.3) and (5.2) into the above definition and considering the fact $\Pi_{k=1}^N t(z_k)=1$, we have

$$F_n^{-+}(\{u_i\},\{v_j\},z_m,z_{m+1})=\frac{\phi_{m-1}(\{u_i\})}{\phi_{m+1}(\{v_j\})}\langle 0|\tilde{B}(u_n)\cdots\tilde{B}(u_1)\tilde{C}(z_m)\tilde{B}(z_{m+1})\tilde{C}(v_1)\cdots\tilde{C}(v_n)|0\rangle. \tag{5.16}$$

By using the commutation relation (2.22), we obtain

$$\begin{aligned}B(z_{m+1})C(v_1)\cdots C(v_n)|0\rangle&=(-1)^nC(v_1)\cdots C(v_n)B(z_{m+1})|0\rangle\\&+\sum_{j=1}^{n}(-1)^{j+1}\frac{b^+(z_{m+1},v_j)}{a(z_{m+1},v_j)}C(v_1)\cdots C(v_{j-1})D(z_{m+1})t(v_j)C(v_{j+1})C(v_n)|0\rangle\\&+\sum_{j=1}^{n}(-1)^{j}\frac{b^+(z_{m+1},v_j)}{a(z_{m+1},v_j)}C(v_1)\cdots C(v_{j-1})t(z_{m+1})D(v_j)C(v_{j+1})C(v_n)|0\rangle,\end{aligned} \tag{5.17}$$

where $\tilde{t}(u)\equiv F_{1\cdots N}t(u)F^{-1}_{1\cdots N}$. On the right-hand side (rhs) of the above equation, one easily finds that the first term is zero. Using the BAE, one may check that the second term also equals zero. Therefore, only the third term survives on the rhs of the above equation and we have

$$\begin{aligned}&B(z_{m+1})C(v_1)\cdots C(v_n)|0\rangle\\&=\sum_{j=1}^{n}(-1)^j\frac{b^+(z_{m+1},v_j)}{a(z_{m+1},v_j)}\prod_{k=j+1}^{n}a^{-1}(v_k,z_{m+1})\prod_{l=j+1}^{n}a^{-1}(v_l,v_j)\\&\quad\times C(v_1)\cdots C(v_{j-1})C(v_{j+1})C(v_n)|0\rangle\\&\quad+\sum_{j=1}^{n}(-1)^{j+1}\frac{b^+(z_{m+1},v_j)}{a(z_{m+1},v_j)}\prod_{k=j+1}^{n}a^{-1}(v_k,z_{m+1})\end{aligned}$$

$$\times \sum_{l=j+1}^{n} \frac{b^{-}(v_l,v_j)}{a(v_l,v_j)} \prod_{m=j+1}^{l-1} \frac{c(v_m,v_l)}{c(v_m,v_j)} \prod_{i=j+1,\neq l}^{n} a^{-1}(v_i,v_l)$$

$$\times C(v_1)\cdots C(v_{j-1})C(v_{j+1})\cdots C(v_{l-1})C(v_j)C(v_{l+1})\cdots C(v_n)|0\rangle$$

$$\equiv \sum_{j=1}^{n} M_j C(v_1)\cdots C(v_{j-1})C(v_{j+1})C(v_n)|0\rangle$$

$$+ \sum_{j=1}^{n}\sum_{l=j+1}^{n} M_{j,l} C(v_1)\cdots C(v_{j-1})C(v_{j+1})\cdots C(v_{l-1})C(v_j)C(v_{l+1})\cdots C(v_n)|0\rangle. \quad (5.18)$$

Substituting (5.18) into (5.16), we obtain two-point correlation function F_n^{-+},

$$F_n^{-+}(\{u_i\},z_m,z_{m+1},\{v_j\}) = \frac{\phi_{m-1}(\{u_i\})}{\phi_{m+1}(\{v_j\})}\Bigg[\sum_{j=1}^{n} M_j S_n(\{u_i\},z_m,v_1,\ldots,v_{j-1},v_{j+1},v_n)$$

$$+ \sum_{j=1}^{n}\sum_{l=j+1}^{n} M_{j,l} S_n(\{u_i\},z_m,v_1,\ldots,v_{j-1},v_{j+1},\ldots,v_{l-1},v_j,v_{l+1},\ldots,v_n)\Bigg]. \quad (5.19)$$

VI. DISCUSSION

In this paper, with the help of the factorizing F-matrix (F-basis), we have obtained the determinant representations of the scalar products and correlation functions of the $U_q(\mathrm{gl}(1|1))$ free Fermion model.

In Refs. 10–15, the authors studied the correlation Functions of the free Fermion model based on the finite $XX0$ spin chain (XY model[9]) with periodic boundary condition

$$H_{XX0} = \sum_{j=1}^{N} (\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + h\sigma_j^z), \quad (6.1)$$

where σ^{ϵ} ($\epsilon = x,y,z$) are the Pauli matrices and h is an external classical magnetic field. The equivalence between the free Fermion model and the $XX0$ model can be proved by using the Jordan-Wigner transform

$$c_k = \exp[i\pi Q_{k-1}]\sigma_k^{+}, \quad (6.2)$$

$$c_k^{\dagger} = \sigma_k^{-}\exp[i\pi Q_{k-1}], \quad (6.3)$$

where $\sigma^{\pm} = \frac{1}{2}(\sigma^x \pm \sigma^y)$, $Q_k = \sum_{j=1}^{k}\frac{1}{2}(1-\sigma_k^z)$. Because of the periodic boundary condition of the finite $XX0$ spin chain, we have

$$\sigma_{N+1}^{\pm} = \sigma_1^{\pm}. \quad (6.4)$$

Substituting the Jordan-Wigner transforms into the above relation, we obtain

$$c_{N+1} = \exp[i\pi Q_N]c_1, \quad c_{N+1}^{\dagger} = c_1^{\dagger}\exp[i\pi Q_N]. \quad (6.5)$$

Thus, comparing the above boundary condition with that of the $U_q(\mathrm{gl}(1|1))$ free Fermion model (2.14), we find that the free Fermion model arising from the $XX0$ model has a twisted boundary condition which depends on the operator $\sigma^z = \sum_{i=1}^{N}\sigma_i^z$.

On the other hand, by means of the Jordan-Wigner transform, the $U_q(\mathrm{gl}(1|1))$ free Fermion model is equivalent to a twisted $XX0$ model, and the one-point correlation functions (5.5) and (5.7) give rise to the m-point correlation functions of the twisted $XX0$ model. For example, substituting (6.3) into (5.5), we obtain

$$\begin{aligned} F_n^-(\{u_j\},z_m,\{v_k\}) &= \langle 0|B(u_n)\cdots B(u_1)c_m^\dagger C(v_1)\cdots C(v_{n+1})|0\rangle \\ &= \langle 0|B(u_n)\cdots B(u_1)\sigma_1^z\cdots\sigma_{m-1}^z\sigma_m^- C(v_1)\cdots C(v_{n+1})|0\rangle. \end{aligned} \tag{6.6}$$

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The equivalence problem for fourth order differential equations under fiber preserving diffeomorphisms

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In the present work we use the method of equivalence to determine necessary and sufficient conditions for a general fourth order ordinary differential equation to be equivalent to the flat model under a fiber preserving transformation. As a result, explicit and simple conditions are obtained. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Introduced and developed by Élie Cartan in the beginning of the 1920s, the method of equivalence is a systematic procedure that allows one to decide whether two systems of differential equations can be mapped one to each other by a transformation taken in a given pseudogroup. For instance, the method of equivalence answers questions like: find necessary and sufficient conditions on f such that

$$y'' = f\left(x, y, \frac{dy}{dx}\right)$$

can be mapped to

$$\frac{d^2Y}{dX} = 0$$

under a point transformation $X=X(x,y)$, $Y=Y(x,y)$.

Thanks to C. Erhesmann and S. Chern who introduced two important concepts to the method of equivalence: jets spaces and G-structures. Actually a G-structure on manifold is a G-subbundle of the frame bundle. Applying the equivalence method leads to $\{e\}$-structure, which is invariantly associated to the given equation.

In the 1960s, Singer, Sternberg, Guillemin, Kuranishi, Kodaira, and Spencer made major contributions making the equivalence method more rigorous. We refer the reader to Refs. 4,3 or even to Cartan paper[1] for detailed exposition.

In recent years, with the help of algebraic computers, many authors have successfully used the method of equivalence to many interesting problems: classifications of differential equations (Kamran, Olver and Fels), holonomy groups (Bryant), inverse variational problems (Fels), general relativity (Newman).

In this paper we completely characterize the fourth order differential equations which are equivalent to the flat model under fiber preserving transformations.

II. MAIN RESULT

Consider the fourth order equation

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$$y^{(4)} = f(x,y,y',y'',y''') \tag{1}$$

and let Φ be a fiber preserving transformation from J^3 to J^3 with $\mathrm{x} := (x,y,p=y',q=y'',r=y''') \in \mathbb{R}^5$ as local coordinates. Recall that a map Φ is said to be fiber preserving if there exists a map $\phi:\mathbb{R}\to\mathbb{R}$ such that

$$\phi \circ (\mathrm{proj}) = (\mathrm{proj}) \circ \Phi.$$

Thus in terms of local coordinates on J^0, we have

$$\begin{cases} \bar{x} \circ \Phi = \phi(x), \\ \bar{y} \circ \Phi = \psi(x,y). \end{cases} \tag{2}$$

The main result of the paper is

Thorem 1: *The following propositions for a fourth order ordinary differential equation* $y^{(4)} = f(x,y,p,q,r)$ *are equivalent*

(i) *The equation is equivalent to the flat model* $y^{(4)}=0$ *under a fiber preserving transformation.*

(ii) *The equation admits an eight dimensional symmetry group of fiber preserving transformations.*

(iii) f *satisfies*

$$f_{rr} = 0, \quad f_{qr} = 0,$$

$$-f_r^{\,3} + 6D_x f_r f_r - 4f_q f_r - 8f_p + 8D_x f_q - 4D_x^{\,2} f_r = 0,$$

$$\begin{aligned} &1512 D_x f_r f_r^{\,2} - 1440 f_r D_x^{\,2} f_r + 832 f_q D_x f_r + 2000 D_x f_q f_r - 1600 f_p f_r - 808 f_q f_r^{\,2} - 1120 D_x^{\,2} f_q \\ &\quad + 480 D_x^{\,3} f_r + 1600 D_x f_p - 864 (D_x f_r)^2 - 1600 f_y - 144 f_q^{\,2} - 189 f_r^{\,4} = 0, \end{aligned} \tag{3}$$

$$-800 D_x^{\,2} f_r + 1600 D_x f_q - 200 f_r^{\,3} - 1600 f_p + 1200 D_x f_r f_r - 800 f_q f_r = 0$$

where $D_x = \partial_x + p\partial_y + q\partial_p + r\partial_q + f(x,y,p,q,r)\partial_r$ *is the total derivative.*

III. PROBLEM FORMULATION

Any fiber preserving diffeomorphism has a standard lift to J^3 (called the *third prolongation*) which preserves the Pfaffian system

$$\omega^1 = -f(x,y,p,q,r)\mathrm{d}x + \mathrm{d}r, \quad \omega^2 = -p\mathrm{d}x + \mathrm{d}y, \quad \omega^3 = -q\mathrm{d}x + \mathrm{d}p, \quad \omega^4 = -r\mathrm{d}x + \mathrm{d}q. \tag{4}$$

In local coordinates, the equivalence of $y^{(4)}=f(x,y,p,q,r)$ and $\bar{y}^{(4)}=\bar{f}(\bar{x},\bar{y},\bar{p},\bar{q},\bar{r})$ under fiber preserving transformations is expressed as local equivalence problem for G-structures B and $\bar{B}$ given by

$$\underbrace{\begin{pmatrix} \bar{a}_1 & \bar{a}_2 & \bar{a}_3 & \bar{a}_4 & 0 \\ 0 & \bar{a}_5 & 0 & 0 & 0 \\ 0 & \bar{a}_6 & \bar{a}_7 & 0 & 0 \\ 0 & \bar{a}_8 & \bar{a}_9 & \bar{a}_{10} & 0 \\ 0 & 0 & 0 & 0 & \bar{a}_{11} \end{pmatrix}}_{S(\bar{a})\in G} \bar{\omega}(\bar{x}) = \underbrace{\begin{pmatrix} a_1 & a_2 & a_3 & a_4 & 0 \\ 0 & a_5 & 0 & 0 & 0 \\ 0 & a_6 & a_7 & 0 & 0 \\ 0 & a_8 & a_9 & a_{10} & 0 \\ 0 & 0 & 0 & 0 & a_{11} \end{pmatrix}}_{S(a)\in G} \omega(\mathrm{x}) \tag{5}$$

where $\omega=(\omega^1,\ldots,\omega^5)^t$ and $\omega^5=\mathrm{d}x$.

IV. SOLUTION

According to Cartan we take the lifts $\theta=S(a)\omega$ and $\bar{\theta}=S(\bar{a})\bar{\omega}$. By differentiation we obtain the following *structure equations*

$$\begin{pmatrix} \mathrm{d}\theta^1 \\ \mathrm{d}\theta^2 \\ \mathrm{d}\theta^3 \\ \mathrm{d}\theta^4 \\ \mathrm{d}\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^1 & \pi^2 & \pi^3 & \pi^4 & 0 \\ 0 & \pi^5 & 0 & 0 & 0 \\ 0 & \pi^6 & \pi^7 & 0 & 0 \\ 0 & \pi^8 & \pi^9 & \pi^{10} & 0 \\ 0 & 0 & 0 & 0 & \pi^{11} \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} \tag{6}$$

$$+ \begin{pmatrix} I_1\theta^1\wedge\theta^5 + I_2\theta^2\wedge\theta^5 + I_3\theta^3\wedge\theta^5 + I_4\theta^4\wedge\theta^5 \\ I_5\theta^2\wedge\theta^5 + I_6\theta^3\wedge\theta^5 \\ I_7\theta^2\wedge\theta^5 + I_8\theta^3\wedge\theta^5 + I_9\theta^4\wedge\theta^5 \\ I_{10}\theta^1\wedge\theta^5 + I_{11}\theta^2\wedge\theta^5 + I_{12}\theta^3\wedge\theta^5 + I_{13}\theta^4\wedge\theta^5 \\ 0 \end{pmatrix}. \tag{7}$$

The torsion of the pseudoconnection π is $T_\pi := T^i_{jk} v_i \otimes v^j \wedge v^k \in \Gamma(B, V\otimes\wedge^2 V^*)$ (here $V=\mathbb{R}^5$) and we are less interested in T_π than in the intrinsic torsion which is independent of any choice of π. Recall that (see Ref. 2) the intrinsic torsion of a linear Pfaffian system with tableau $A\subseteq W\otimes V^*$ lies in $H^{0,2}(A)=(W\otimes\wedge^2 V^*)/\delta(A\otimes V^*)$, where δ is the skew-symmetrization map. In the theory of the equivalence problems we have $W=V$ and $A=\mathfrak{g}$ the Lie algebra of G.

Lemma 1: $H^{0,2}(\mathfrak{g})\neq 0$. Indeed, the absorption of the apparent torsion (that is, factorizing the above structure equations according to the $\{\theta^j\}$ and renaming the new forms of the pseudoconnection such that $\pi^\rho := \pi^\rho + \lambda^\rho_j \theta^j$) yields

$$\begin{pmatrix} \mathrm{d}\theta^1 \\ \mathrm{d}\theta^2 \\ \mathrm{d}\theta^3 \\ \mathrm{d}\theta^4 \\ \mathrm{d}\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^1 & \pi^2 & \pi^3 & \pi^4 & 0 \\ 0 & \pi^5 & 0 & 0 & 0 \\ 0 & \pi^6 & \pi^7 & 0 & 0 \\ 0 & \pi^8 & \pi^9 & \pi^{10} & 0 \\ 0 & 0 & 0 & 0 & \pi^{11} \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} 0 \\ I_1\theta^3\wedge\theta^5 \\ I_2\theta^4\wedge\theta^5 \\ I_3\theta^1\wedge\theta^5 \\ 0 \end{pmatrix}. \tag{8}$$

Now, define the structure map $\tau: B\to H^{0,2}(\mathfrak{g})$ such that for every $p=(x,u)\in B$ we have $\tau(p)=[T_p]$. The torsion lies in a single orbit of G in $H^{0,2}(\mathfrak{g})$. Thus we can can choose a normal form T_0 in the image of the structure map so that $B_1 := \{p\in B: \tau(p)=T_0\}$ and $G_1 := \{g\in G: \forall p \in B, \tau(p.g)=\tau(p)\}$ define a normalization of *first order constant type*, i.e., B_1 is G_1-structure. G_1 is the matrix group defined by normalizing a_5, a_7, a_{10} in the following manner:

$$I_1 = -\frac{a_5}{a_7 a_{11}} = -1, \quad I_2 = -\frac{a_7}{a_{10}a_{11}} = -1, \quad I_3 = -\frac{a_{10}}{a_1 a_{11}} = -1.$$

Let us denote by $\mathfrak{g}_1$ the new Lie algebra and we continue to denote by π the pull back of the pseudoconnection. The calculations give

$$\begin{pmatrix} d\theta^1 \\ d\theta^2 \\ d\theta^3 \\ d\theta^4 \\ d\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^{10}-\pi^{11} & \pi^2 & \pi^3 & \pi^4 & 0 \\ 0 & \pi^{10}+2\pi^{11} & 0 & 0 & 0 \\ 0 & \pi^6 & \pi^{10}+\pi^{11} & 0 & 0 \\ 0 & \pi^8 & \pi^9 & \pi^{10} & 0 \\ 0 & 0 & 0 & 0 & \pi^{11} \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} I_1\theta^1\wedge\theta^5 + I_2\theta^2\wedge\theta^5 + I_3\theta^3\wedge\theta^5 + I_4\theta^4\wedge\theta^5 \\ I_5\theta^2\wedge\theta^5 - \theta^3\wedge\theta^5 \\ I_6\theta^2\wedge\theta^5 + I_7\theta^3\wedge\theta^5 - \theta^4\wedge\theta^5 \\ -\theta^1\wedge\theta^5 + I_8\theta^2\wedge\theta^5 + I_9\theta^3\wedge\theta^5 + I_{10}\theta^4\wedge\theta^5 \\ 0 \end{pmatrix} \tag{9}$$

Lemma 2: $H^{0,2}(\mathfrak{g}_1)\neq 0$. Indeed since we can absorb the apparent torsion to obtain

$$\begin{pmatrix} d\theta^1 \\ d\theta^2 \\ d\theta^3 \\ d\theta^4 \\ d\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^7-\pi^8 & \pi^1 & \pi^2 & \pi^3 & 0 \\ 0 & \pi^7+2\pi^8 & 0 & 0 & 0 \\ 0 & \pi^4 & \pi^7+\pi^8 & 0 & 0 \\ 0 & \pi^5 & \pi^6 & \pi^7 & 0 \\ 0 & 0 & 0 & 0 & \pi^8 \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} 0 \\ I_1\theta^2\wedge\theta^5 \\ -\theta^4\wedge\theta^5 \\ -\theta^1\wedge\theta^5 + I_2\theta^4\wedge\theta^5 \\ 0 \end{pmatrix}.$$

Again the torsion lies in single orbit of G_1 in $H^{0,2}(\mathfrak{g}_1)$ thus we can define B_2 by setting $I_1=I_2=0$ where

$$I_1 = -\frac{1}{2}\frac{-5a_6+3a_9a_{11}+{a_{11}}^2f_{,}a_1+{a_{11}}^2a_4}{a_1{a_{11}}^3}$$

and

$$I_2 = \frac{1}{2}\frac{-3a_9a_{11}+3{a_{11}}^2a_4+a_6+{a_{11}}^2f_{,}a_1}{a_1{a_{11}}^3}.$$

This normalizes (a_6,a_9) and gives a new Lie algebra $\mathfrak{g}_2$.

Lemma 3: $H^{0,2}(\mathfrak{g}_2)\neq 0$. In the same manner as above the precesses of absorption of torsion leads

$$\begin{pmatrix} d\theta^1 \\ d\theta^2 \\ d\theta^3 \\ d\theta^4 \\ d\theta^5 \end{pmatrix} = \begin{pmatrix} pi^6+\pi^5 & \pi^1 & \pi^2 & \frac{3}{4}\pi^4 & 0 \\ 0 & \pi^5+2\pi^6 & 0 & 0 & 0 \\ 0 & \frac{3}{4}\pi^4 & \pi^5+\pi^6 & 0 & 0 \\ 0 & \pi^3 & \pi^4 & \pi^5 & 0 \\ 0 & 0 & 0 & 0 & \pi^6 \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} I_1\theta^1\wedge\theta^4 + I_2\theta^4\wedge\theta^5 \\ -\theta^3\wedge\theta^5 \\ I_3\theta^1\wedge\theta^2 + I_4\theta^2\wedge\theta^4 - \theta^4\wedge\theta^5 \\ -\theta^1\wedge\theta^5 \\ 0 \end{pmatrix}.$$

New normalization is possible:

$$I_2 = \frac{118a_{11}a_4f_ra_1 - 48a_{11}f_q{a_1}^2 - 84a_3a_1a_{11} + 32a_{11}{a_4}^2 + 18D_xf_r{a_1}^2a_{11} + 36a_8a_1 - 9a_{11}f_r{}^2{a_1}^2)}{48{a_1}^2{a_{11}}^3} = 0,$$

$$I_5 = -\frac{132a_{11}{a_4}^2 + 38a_{11}a_4f_ra_1 - 84a_8a_1 + 6D_xf_r{a_1}^2a_{11} + 9a_{11}f_r{}^2{a_1}^2 + 36a_3a_1a_{11})}{48{a_1}^2{a_{11}}^3} = 0.$$

The normalized parameters are (a_8, a_3) and Lie algebra is now reduced to $\mathfrak{g}_3$. Thus the absorbed structure equations read

$$\begin{pmatrix} d\theta^1 \\ d\theta^2 \\ d\theta^3 \\ d\theta^4 \\ d\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^3 - \pi^4 & \pi^1 & 0 & \frac{3}{4}\pi^2 & 0 \\ 0 & \pi^3 + 2\pi^4 & 0 & 0 & 0 \\ 0 & \frac{3}{4}\pi^2 & \pi^3 + \pi^4 & 0 & 0 \\ 0 & 0 & \pi^2 & \pi^3 & 0 \\ 0 & 0 & 0 & 0 & \pi^4 \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} I_1\theta^1 \wedge \theta^4 + I_2\theta^3 \wedge \theta^5 \\ -\theta^3 \wedge \theta^5 \\ I_3\theta^1 \wedge \theta^2 + I_4\theta^2 \wedge \theta^4 - \theta^4 \wedge \theta^5 \\ I_5\theta^1 \wedge \theta^2 - \theta^1 \wedge \theta^5 + I_6\theta^2 \wedge \theta^5 \\ I_7\theta^2 \wedge \theta^5 + I_8\theta^3 \wedge \theta^5 \end{pmatrix}.$$

This proves the following lemma

Lemma 4: $H^{0,2}(\mathfrak{g}_3) \neq 0$.

We arrive at the last normalization of the parameter a_2: $I_2 = \frac{1}{720}(54{a_1}^2{f_r}^2a_4 - 396f_q{a_1}^3f_1 + 240a_1f_r{a_4}^2 + 432f_r{a_1}^3D_xf_r - 81{f_r}^3{a_1}^3 - 720f_p{a_1}^3 - 216f_q{a_1}^2a_4 - 720a_2{a_1}^2 + 160{a_4}^3 + 144a_4D_xf_r{a_1}^2 - 216{a_1}^3D_x^2f_r + 504{a_1}^3D_xf_q)/({a_{11}}^3{a_1}^3) = 0$ and just as before, $\mathfrak{g}_4$ is the new lie algebra.

We can absorb the torsion to get

$$\begin{pmatrix} d\theta^1 \\ d\theta^2 \\ d\theta^3 \\ d\theta^4 \\ d\theta^5 \end{pmatrix} = \begin{pmatrix} \pi^2 - \pi^3 & 0 & 0 & \frac{3}{4}\pi^1 & 0 \\ 0 & \pi^2 + 3\pi^3 & 0 & 0 & 0 \\ 0 & \frac{3}{4}\pi^1 & \pi^2 + \pi^3 & 0 & 0 \\ 0 & 0 & \pi^1 & \pi^2 & 0 \\ 0 & 0 & 0 & 0 & \pi^3 \end{pmatrix} \wedge \begin{pmatrix} \theta^1 \\ \theta^2 \\ \theta^3 \\ \theta^4 \\ \theta^5 \end{pmatrix} + \begin{pmatrix} I_1\theta^2 \wedge \theta^3 + I_2\theta^2 \wedge \theta^4 + I_3\theta^2 \wedge \theta^5 \\ -\theta^3 \wedge \theta^5 \\ I_4\theta^1 \wedge \theta^2 + I_5\theta^2 \wedge \theta^4 + I_6\theta^3 \wedge \theta^4 - \theta^4 \wedge \theta^5 \\ I_7\theta^1 \wedge \theta^2 - \theta^1 \wedge \theta^5 + I_8\theta^2 \wedge \theta^4 + I_9\theta^2 \wedge \theta^5 \\ I_{10}\theta^2 \wedge \theta^5 + I_{11}\theta^3 \wedge \theta^5 + I_{12}\theta^4 \wedge \theta^5 \end{pmatrix}. \tag{10}$$

The Cartan characters are $s_1 = 3$, $s_2 = 0$, $s_3 = 0$ and the indetermination degree is 0 thus the involution test fails:

Lemma 5: The above system is not in involution.

In this circumstances we define $\hat{V} = \mathfrak{g}_4 \oplus V$ and $\mathfrak{g}^{(1)} = (\mathfrak{g}_4 \otimes V^*) \cap (V \otimes S^2V^*)$ the *prolongation* of $\mathfrak{g}_4$. In fact, $\mathfrak{g}^{(1)}$ is just the Lie algebra of the Lie group formed by the λ_ρ^j remaining arbitrary after

the last absorption. Since the indetermination degree is 0, $\mathfrak{g}^{(1)}$ is reduced to the identity which means that $\mathfrak{g}$ is of finite type. Thus the necessary and sufficient condition for the G_4-structure B_4 to be locally flat is that the structure functions of all prolongations of $\mathfrak{g}_4$ must vanish. On the other hand, the Cartan's lemma applied to (10) gives

$$\begin{cases} \mathrm{d}\pi^1 = I_{13}\theta^1\wedge\theta^2 + I_{14}\theta^1\wedge\theta^3 + I_{15}\theta^1\wedge\theta^4 + I_{16}\theta^1\wedge\theta^5 + I_{17}\theta^2\wedge\theta^3 \\ \quad + I_{18}\theta^2\wedge\theta^4 + I_{19}\theta^2\wedge\theta^5 + I_{20}\theta^2\wedge\pi^1 + I_{21}\theta^3\wedge\theta^4 + I_{22}\theta^3\wedge\theta^5 \\ \quad + I_{23}\theta^4\wedge\theta^5 + I_{24}\theta^4\wedge\pi^1 + \pi^1\wedge\pi^3, \\ \mathrm{d}\pi^2 = I_{25}\theta^1\wedge\theta^2 + I_{26}\theta^1\wedge\theta^3 + I_{27}\theta^1\wedge\theta^4 + I_{28}\theta^1\wedge\theta^5 + I_{29}\theta^2\wedge\theta^3 \\ \quad + I_{30}\theta^2\wedge\theta^4 + I_{31}\theta^2\wedge\theta^5 + I_{32}\theta^3\wedge\theta^4 + I_{33}\theta^3\wedge\theta^5 + I_{34}\theta^4\wedge\theta^5 \\ \quad - \frac{1}{4}\theta^5\wedge\pi^1, \\ \mathrm{d}\pi^3 = I_{35}\theta^1\wedge\theta^2 + I_{36}\theta^1\wedge\theta^3 + I_{37}\theta^1\wedge\theta^4 + I_{38}\theta^1\wedge\theta^5 + I_{39}\theta^2\wedge\theta^3 \\ \quad + I_{40}\theta^2\wedge\theta^4 + I_{41}\theta^2\wedge\theta^5 + I_{42}\theta^2\wedge\pi^1 + I_{43}\theta^3\wedge\theta^4 + I_{44}\theta^3\wedge\theta^5 \\ \quad + I_{45}\theta^4\wedge\theta^5 + \frac{1}{2}\theta^5\wedge\pi^1 \end{cases}. \tag{11}$$

Now the degree of indetermination is 0 and the Cartan characters are $s_1=0$, $s_2=0$. Thus we obtain the involution

Proposition 1: The system (10) and (11) is in involution.

Going back to our main result, the achievement of the proof is due to the fundamental identity $d^2=0$. Indeed, we prove that

Proposition 2: All the structure functions vanish if and only if

$$I_4 = \frac{f_{rr}}{a_1 a_{11}}, \quad I_{34} = \frac{f_{qr}a_1 - f_{rr}a_4}{{a_{11}}^2 {a_1}^2},$$

$$I_9 = (-{f_r}^3 + 6D_x f_r f_r - 4f_q f_r - 8f_p + 8D_x f_q - 4{D_x}^2 f_r)/{a_{11}}^3,$$

$$\begin{aligned} I_3 = ((&1512D_x f_r {f_r}^2 - 1440 f_r {D_x}^2 f_r + 832 f_q D_x f_r + 2000 D_x f_q f_r - 1600 f_p f_r - 808 f_q {f_r}^2 - 1120 {D_x}^2 f_q \\ &+ 480 {D_x}^3 f_r + 1600 D_x f_p - 864 (D_x f_r)^2 - 1600 f_y - 144 {f_q}^2 - 189 {f_r}^4) a_1 + (-800 {D_x}^2 f_r + 1600 D_x f_q \\ &- 200 {f_r}^3 - 1600 f_p + 1200 D_x f_r f_r - 800 f_q f_r) a_4)/(a_1 {a_{11}}^4) \end{aligned}$$

vanish.

Again $d^2=0$ shows that if the invariants are constant then they must vanish. Combining this with the fact that the dimension of the symmetry group is equal to the dimension of the coframing $\{\theta^i, \pi^j\}$ minus the rank of the coframing (actually the number of functionally independent invariants), we prove the equivalence between *(ii)* and *(iii)*. The equivalence between *(i)* and *(iii)* is straightforward.

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Possible quantum kinematics

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The quantum group and space theory is reformulated from the standard skew-symmetric basis to an arbitrary one. The N-dimensional quantum Cayley–Klein spaces are described in Cartesian basis and the quantum analogs of $(N-1)$-dimensional constant curvature spaces are introduced. Part of the four-dimensional constant curvature spaces are interpreted as the noncommutative analogs of $(1+3)$ space-time models. As a result the quantum (anti) de Sitter, Minkowski, Newton, Galilei, Carroll kinematics with the fundamental length and the fundamental time are suggested. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Space-time is a fundamental conception that underlines the most significant physical theories. Therefore the analysis of a possible space-time model (or kinematics) has the fundamental meaning for physics. Space and time in nonrelativistic physics were regarded as independent what mathematically is connected with the fiber property of Galilei kinematics. In special relativity it was determined that space and time depend on each other and must be regarded as an integrated object, namely flat Minkowski space-time with a pseudo-Euclidean metric. The notion of curvature was introduced in physics by general relativity. Anti-de Sitter and de Sitter kinematics with constant positive and negative curvature, respectively, are the simplest relativistic space-time models with curvature. Possible kinematics, which satisfy the natural physical postulates: space is isotropic and rotations in space-time planes form a noncompact subgroup, were described in Ref. 1 on the level of Lie algebras. From the point of view of geometry these kinematics are realized as constant curvature spaces, which can be obtained from the spherical space by contractions and analytical continuations known as a Cayley–Klein (CK) scheme.[2]

The Snyder quantized space-time coordinates[3] or, respectively, the curved momentum space, are the oldest example of using the noncommutative geometry in physics. The simplest curved de Sitter geometry with constant curvature was used instead of flat Minkowski space in different generalizations of quantum field theory[4–7] as a momentum space model. The universal constant, the fundamental length l, or fundamental mass M, related to l by $l=\hbar/Mc$, where $\hbar$ is the Plank constant and c is the velocity of light, enters necessarily into the theory.[4,6,7]

A new possibility for construction of the noncommutative space-time models is provided by quantum groups and quantum vector spaces.[8] According to Dirac[9] from the early 30s, "The most powerful method of advance that can be suggested at present is to employ all the resources of pure mathematics in attempts to perfect and generalize the mathematical formalism that forms the existing basis of theoretical physics, and *after* each success in this direction, to try to interpret the new mathematical features in terms of physical entities." Similar views were expressed by Faddeev,[10] where we found this cite. The quantum Poincaré group related to the κ-Poincaré algebra as well as the κ-Minkowski kinematics were suggested.[11–13] A general formalism that allows the construction of field theory in κ-Minkowski space-time was developed.[14]

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On the other hand, the quantum deformations can be useful in the large-scale limit, in particular, for a dark matter problem. If one uses a so-called Maslanka mapping,[15]

$$\widetilde{P}_0 = 2\kappa \operatorname{arcsinh} \frac{P_0}{2\kappa},$$

where P_0 ($\widetilde{P}_0$) is the energy of the particle for Minkowski (κ-Minkowski) kinematics, then, as it was pointed out by Bacry,[16] the energy of a system S composed of two subsystems, $S_{(1)}$ and $S_{(2)}$, reads as

$$2\kappa \sinh \frac{\widetilde{P}_0}{2\kappa} = 2\kappa \sinh \frac{\widetilde{P}_{0(1)}}{2\kappa} + 2\kappa \sinh \frac{\widetilde{P}_{0(2)}}{2\kappa},$$

rather then $P_0 = P_{0(1)} + P_{0(2)}$. Actually, the above implies that $\widetilde{P}_0 < \widetilde{P}_{0(1)} + \widetilde{P}_{0(2)}$. It means that the total energy of the universe is not proportional to the number of particles it contains. Hence there is no need for dark matter due to the kinematical reason.

Our purpose in this paper is to obtain the noncommutative (quantum) analogs of the possible kinematics. It is made just in the same way as for the commutative case, with the exception of the initial Euclidean space, which is substituted by the quantum Euclidean space associated with the quantum orthogonal group. The CK scheme of contractions and analytical continuations was developed in the Cartesian basis, whereas the standard quantum group theory[8] was formulated in a different skew-symmetric one. Therefore, first of all, this theory is reformulated in the Cartesian basis; then the noncommutative analogs of constant curvature spaces (CCS) including fiber (or flag) spaces are investigated and some of them are interpreted as noncommutative kinematics.

The paper is organized as follows. In Sec. II, we briefly recall the description of the classical commutative kinematics as spaces of constant curvature. In Sec. III, the general formalism of quantum Cayley–Klein orthogonal groups and associated spaces is developed. Section IV is devoted to the investigation of noncommutative four-dimensional space-time models.

II. COMMUTATIVE KINEMATICS

Classical four-dimensional space-time models can be obtained[2] by the physical interpretation of the orthogonal coordinates of the most symmetric spaces, namely constant curvature spaces. All 3^N N-dimensional CCS are realized on the spheres,

$$S_N(j) = \{\xi_1^2 + j_1^2\xi_2^2 + \ \dots\ + (1,N+1)^2\xi_{N+1}^2 = 1\}, \tag{1}$$

where

$$(i,k) = \prod_{l=\min(i,k)}^{\max(i,k)-1} j_l, \quad (k,k) \equiv 1, \tag{2}$$

and each of parameters j_k takes the values $1, \iota_k, i$, $k=1,\dots,N$. Here ι_k are nilpotent generators $\iota_k^2=0$, with commutative law of multiplication $\iota_k\iota_m = \iota_m\iota_k \neq 0$, $k \neq m$.

The intrinsic Beltrami coordinates $x_k = \xi_{k+1}\xi_1^{-1}$, $k=1,2,\dots,N$ present the coordinate system in CCS, which coordinate lines $x_k=$const are geodesic. CCS has positive curvature for $j_1=1$, negative for $j_1=i$, and it is flat for $j_1=\iota_1$. For a flat space the Beltrami coordinates coincide with the Cartesian ones. Nilpotent values $j_k=\iota_k$, $k>1$ correspond to a fiber (flag) spaces and imaginary values $j_k=i$ correspond to pseudo-Riemannian spaces.

Classical (1+3) kinematics[1] are obtained from CCS for $N=4$, $j_1=1,\iota_1,i$, $j_2=\iota_2,i$, $j_3=j_4=1$ if one interprets x_1 as the time axis $t=\xi_2\xi_1^{-1}$ and the rest as the space axes $r_k=\xi_{k+2}\xi_1^{-1}$, $k=1,2,3$.

The standard de Sitter kinematics $S_4^{(-)}$ with constant negative curvature is realized for $j_1=j_2=i$, anti-de Sitter kinematics $S_4^{(+)}$ with positive curvature—for $j_1=1$, $j_2=i$. Relativistic flat Minkowski kinematics M_4 appears for $j_1=\iota_1$, $j_2=i$. Nonrelativistic Newton $N_4^{(\pm)}$ and Galilei G_4 kinematics correspond to $j_2=\iota_2$, $j_1=1$, i and $j_1=\iota_1$, respectively.

If one interprets three first Beltrami coordinates as space axes, while the last one as a time axis, and puts $j_2=j_3=1,j_4=\iota_4$, then three exotic Carroll kinematics[1,17] are obtained, namely C_4^0 for $j_1=\iota_1$, with zero curvature, $C_4^{\pm}$ for $j_1=1,i$, with positive and negative curvature. The Carroll space and time have contrary properties as compared with those of Galilei kinematics. The Galilei time is absolute, i.e., two events simultaneous in some reference frame remain simultaneous in any reference frame that is obtained by Galilei boost (or space-time rotation) from the initial one. On the contrary, in Carroll kinematics the space is absolute, i.e. two events with the equal spatial coordinates in some reference frame have the same spatial coordinates in any reference frame that is obtained from the initial one by space-time rotation.

III. QUANTUM ORTHOGONAL GROUPS AND QUANTUM CAYLEY–KLEIN SPACES

According to FRT theory,[8] the algebra function on quantum orthogonal group $Fun(SO_q(N))$ [or simply quantum orthogonal group $SO_q(N)$] is the algebra of noncommutative polynomials of n^2 variables t_{ij}, $i,j=1,\ldots,n$, that are the subject of commutation relations,

$$R_qT_1T_2=T_2T_1R_q, \tag{3}$$

and additional relations of q orthogonality,

$$TCT^t=C,\quad T^tC^{-1}T=C^{-1}. \tag{4}$$

Here $T_1=T\otimes I$, $T_2=I\otimes T\in M_{n^2}(\mathbf{C}\langle t_{ij}\rangle)$, $T=(t_{ij})_{i,j=1}^n\in M_n(\mathbf{C}\langle t_{ij}\rangle)$, I is the unit matrix in $M_n(\mathbf{C})$, $C=C_0q^{\rho}$, $\rho=\mathrm{diag}(\rho_1,\ldots,\rho_N)$, $(C_0)_{ij}=\delta_{i'j}$, $i'=N+1-i$, $i,j=1,\ldots,N$, that is, $(C)_{ij}=q^{\rho_{i'}}\delta_{i'j}$ and $C^{-1}=C$,

$$(\rho_1,\ldots,\rho_N)=\begin{cases}\left(n-\frac{1}{2},n-\frac{3}{2},\ldots,\frac{1}{2},0,-\frac{1}{2},\ldots,-n+\frac{1}{2}\right), & N=2n+1,\\ (n-1,n-2,\ldots,1,0,0,-1,\ldots,-n+1), & N=2n.\end{cases} \tag{5}$$

The numerical matrix R_q is the well-known solution[8] of Yang–Baxter equation and its elements fulfils the role of the structure constant of quantum group generators.

Let us remind the definition of the quantum vector space.[8] An algebra $O_q^N(\mathbf{C})$ with generators $x_1,\ldots,x_N$ and commutation relations

$$\hat{R}_q(x\otimes x)=qx\otimes x-\frac{q-q^{-1}}{1+q^{N-2}}x^tCxW_q, \tag{6}$$

where $\hat{R}_q=PR_q$, $Pu\otimes v=v\otimes u$, $\forall u,v\in\mathbf{C}^n$, $W_q=\sum_{i=1}^N q^{\rho_{i'}}e_i\otimes e_{i'}$,

$$x^tCx=\sum_{i,j=1}^N x_iC_{ij}x_j=\epsilon x_{n+1}^2+\sum_{k=1}^n\left(q^{-\rho_k}x_kx_{k'}+q^{\rho_k}x_{k'}x_k\right), \tag{7}$$

$\epsilon=1$ for $N=2n+1$, $\epsilon=0$ for $N=2n$ and vector $(e_i)_k=\delta_{ik}$, $i,k=1,\ldots,N$ is called the algebra of functions on N-dimensional quantum Euclidean space (or simply the quantum Euclidean space) $O_q^N(\mathbf{C})$.

The coaction of the quantum group $SO_q(N)$ on the noncommutative vector space $O_q^N(\mathbf{C})$ is given by

$$\delta(x) = T\dot{\otimes}x, \quad \delta(x_i) = \sum_{k=1}^{n} t_{ik} \otimes x_k, \quad i = 1, \ldots, n, \tag{8}$$

and quadratic form (7) is invariant $\mathrm{inv}=x^tCx$ with respect to this coaction.

The matrix C has nonzero elements only on the secondary diagonal. They are equal to unity in the commutative limit $q=1$. Therefore the quantum group $SO_q(N)$ and the quantum vector space $O_q^N(\mathbf{C})$ are described by equations (3), (4), (6), (7) in a skew-symmetric basis, where for $q=1$ the invariant form $\mathrm{inv}=x^tC_0x$ is given by the matrix C_0 with the only nonzero elements on the secondary diagonal that are all equal to real units.

New generators $y=D^{-1}x$ of the vector space $O_q^N(\mathbf{C})$ in *arbitrary* basis are obtained[18,19] with the help of nondegenerate matrix $D \in M_N$ and they are subject of the commutation relations,

$$\hat{R}(y \otimes y) = qy \otimes y - \frac{\lambda}{1+q^{N-2}} y^t C' y W, \tag{9}$$

where $\hat{R}=(D\otimes D)^{-1}\hat{R}_q(D\otimes D)$, $W=(D\otimes D)^{-1}W_q$, $C'=D^tCD$. The corresponding quantum group $SO_q(N)$ is generated in arbitrary basis by $U=(u_{ij})_{i,j=1}^N$, where $U=D^{-1}TD$. The commutation relations of the new generators are

$$\tilde{R}U_1U_2 = U_2U_1\tilde{R} \tag{10}$$

and q-orthogonality relations look as follows:

$$U\tilde{C}U^t = \tilde{C}, \quad U^t(\tilde{C})^{-1}U = (\tilde{C})^{-1}, \tag{11}$$

where $\tilde{R}=(D\otimes D)^{-1}R_q(D\otimes D)$, $\tilde{C}=D^{-1}C(D^{-1})^t$.

In the case of kinematics, the most natural basis is the Cartesian basis, where the invariant form $\mathrm{inv}=y^ty$ is given by the unit matrix I. The transformation from the skew-symmetric basis x to the Cartesian basis y is described by the matrix D, which is a solution of the following equation:

$$D^tC_0D = I. \tag{12}$$

This equation has many solutions. Take one of these, namely

$$D = \frac{1}{\sqrt{2}} \begin{pmatrix} I & 0 & -i\tilde{C}_0 \\ 0 & \sqrt{2} & 0 \\ \tilde{C}_0 & 0 & iI \end{pmatrix}, \quad N = 2n+1, \tag{13}$$

where $\tilde{C}_0$ is the $n\times n$ matrix with real units on the secondary diagonal. For $N=2n$ the matrix D is given by (13) without the middle column and row. The matrix (13) provides one of the possible combinations of the quantum group structure and the CK scheme of group contractions. All other similar combinations are given by the matrices $D_\sigma=DV_\sigma$, obtained from (13) by the right multiplication on the matrix $V_\sigma \in M_N$ with elements $(V_\sigma)_{ik}=\delta_{\sigma_i,k}$, where $\sigma \in S(N)$ is a permutation of the Nth order.[20] The matrices D_σ are solutions of Eq. (12).

We derive the quantum Cayley–Klein spaces with the same transformation of the Cartesian generators $y=\psi\xi$, $\psi=\mathrm{diag}[1,(1,2),\ldots,(1,N)] \in M_N$, as in the commutative case.[2,19] The transformation $z=Jv$ of the deformation parameter $q=e^z$ should be added in the quantum case. The commutation relations of the Cartesian generators of the quantum N-dimensional Cayley–Klein space are given by the equations

$$\hat{R}_\sigma(j)\xi \otimes \xi = e^{Jv}\xi \otimes \xi - \frac{2shJv}{1+e^{Jv(N-2)}} \xi^t C_\sigma(j) \xi W_\sigma(j),$$

where

$$\hat{R}_\sigma(j) = \Psi^{-1}\hat{R}_\sigma\Psi, \quad W_\sigma(j) = \Psi^{-1}W_\sigma,$$

$$C_\sigma(j) = \psi D^t_\sigma C D_\sigma \psi = \psi V^t_\sigma D^t C D V_\sigma \psi, \quad \Psi = \psi \otimes \psi, \tag{14}$$

and in explicit form are

$$\xi_{\sigma_k}\xi_{\sigma_m} = \xi_{\sigma_m}\xi_{\sigma_k}\cosh Jv - i\xi_{\sigma_m}\xi_{\sigma_{k'}}(1,\sigma_{k'})(1,\sigma_k)^{-1}\sinh Jv, \quad k<m<k', \quad k\neq m',$$

$$\xi_{\sigma_k}\xi_{\sigma_m} = \xi_{\sigma_m}\xi_{\sigma_k}\cosh Jv - i\xi_{\sigma_{m'}}\xi_{\sigma_k}(1,\sigma_{m'})(1,\sigma_m)^{-1}\sinh Jv, \quad m'<k<m, \quad k\neq m',$$

$$[\xi_{\sigma_k},\xi_{\sigma_{k'}}] = 2i\epsilon\sinh\left(\frac{Jv}{2}\right)(\cosh Jv)^{n-k}\xi^2_{\sigma_{n+1}}\frac{(1,\sigma_{n+1})^2}{(1,\sigma_k)(1,\sigma_{k'})}$$
$$+ i\frac{\sinh(Jv)}{(\cosh Jv)^{k+1}(1,\sigma_k)(1,\sigma_{k'})}\sum_{m=k+1}^{n}(\cosh Jv)^m[(1,\sigma_m)^2\xi^2_{\sigma_m} + (1,\sigma_{m'})^2\xi^2_{\sigma_{m'}}], \tag{15}$$

where $k,m=1,2,\ldots,n$. The invariant form of the Cayley–Klein space $O^N_v(j;\sigma;\mathbf{C})$ is written as

$$\mathrm{inv}(j) = \cosh(Jv\rho_1)\left(\epsilon(1,\sigma_{n+1})^2\xi^2_{\sigma_{n+1}}\frac{(\cosh Jv)^n}{\cosh(Jv/2)} + \sum_{k=1}^{n}((1,\sigma_k)^2\xi^2_{\sigma_k} + (1,\sigma_{k'})^2\xi^2_{\sigma_{k'}})(\cosh Jv)^{k-1}\right). \tag{16}$$

The multiplier J in the transformation $z=Jv$ of the deformation parameter is chosen as $J=\cup^n_{k=1}(\sigma_k,\sigma_{k'})$. This is the minimal multiplier, which guarantees the existence of the Hopf algebra structure for the associated quantum group $SO_v(N;j;\sigma)$. The "union" $(\sigma_k,\sigma_p)\cup(\sigma_m,\sigma_r)$ is understood as the first power multiplication of all parameters j_k, which occur at least in one multiplier (σ_k,σ_p) or (σ_m,σ_r), for example, $(j_1j_2)\cup(j_2j_3)=j_1j_2j_3$.

The quantum orthogonal Cayley–Klein sphere $S^{(N-1)}_v(j;\sigma)$ is obtained as the quotient of $O^N_v(j;\sigma)$ by $\mathrm{inv}(j)=1$. The quantum analogs of the intrinsic Beltrami coordinates on this sphere are given by the sets of independent right or left generators,

$$r_{\sigma_i-1} = \xi_{\sigma_i}\xi_1^{-1}, \quad \hat{r}_{\sigma_i-1} = \xi_1^{-1}\xi_{\sigma_i}, \quad i=1,\ldots,N, \quad i\neq k, \quad \sigma_k = 1. \tag{17}$$

In the case of quantum Euclidean spaces $O^N_q(\mathbf{C})$, the use of different D_σ for $\sigma\in S(N)$ makes no sense, because all similarly obtained quantum spaces are isomorphic. However, the situation is radically different for the quantum Cayley–Klein spaces. In this case the Cartesian generators ξ_k are multiplied by $(1,k)$ and for nilpotent values of all or some parameters j_k this isomorphism of quantum vector spaces is destroyed. The necessity of using different D_σ arises as well if there is some physical interpretation of generators. In this case physically different generators may be confused by permutations σ, for example, time and space generators of kinematics. Mathematically isomorphic kinematics may be physically nonequivalent.

IV. QUANTUM KINEMATICS

For $N=5$ the thorough analysis of the multiplier $J=(\sigma_1,\sigma_5)\cup(\sigma_2,\sigma_4)$, which appears in the transformation of the deformation parameter $z=Jv$, and commutation relations (15) of the quantum space generators for different permutations allowed to find three permutations giving different J and a physically nonequivalent kinematics, namely $\sigma_0=(1,2,3,4,5)$, $\sigma'=(1,4,3,5,2)$, $\tilde{\sigma}=(2,3,1,4,5)$.

In order to clarify the relation with the standard Inonu–Wigner contraction procedure,[21] the mathematical parameter j_1 is replaced by the physical one $\tilde{j}_1T^{-1}$, and the parameter j_2 is replaced

by ic^{-1}, where $\tilde{j}_1=1,i$. The limit $T\to\infty$ corresponds to the contraction $j_1=\iota_1$, and the limit $c\to\infty$ corresponds to $j_2=\iota_2$. The parameter T is interpreted as the curvature radius and has the physical dimension of time $[T]=[\text{time}]$, the parameter c is the light velocity $[c]=[\text{length}]\times[\text{time}]^{-1}$.

As far as the generator ξ_1 does not commute with others, it is convenient to introduce right and left time $t=\xi_2\xi_1^{-1}$, $\hat{t}=\xi_1^{-1}\xi_2$ and space $r_k=\xi_{k+2}\xi_1^{-1}$, $\hat{r}_k=\xi_1^{-1}\xi_{k+2}$, $k=1,2,3$, generators. The reason for this definition is the simplification of expressions for commutation relations of quantum kinematics. It is possible to use only, say, right generators, but its commutators are cumbersome in the case of the (anti-)de Sitter kinematics. The commutation relations of the independent generators are obtained (see Ref. 22 for details) in the form

$$S_v^{4(\pm)}(\sigma_0)=\left\{t,\mathbf{r}|\hat{t}r_1=\hat{r}_1t\cos\frac{\tilde{j}_1v}{cT}+i\hat{r}_1r_2\frac{1}{c}\sin\frac{\tilde{j}_1v}{cT},\ \hat{t}r_2-\hat{r}_2t=-2i\hat{r}_1r_1\frac{1}{c}\sin\frac{\tilde{j}_1v}{2cT},\ \hat{t}r_3=\hat{r}_3t\cos\frac{\tilde{j}_1v}{cT}\right.$$
$$\left.-it\frac{cT}{\tilde{j}_1}\sin\frac{\tilde{j}_1v}{cT},\ \hat{r}_1r_2=\hat{r}_2r_1\cos\frac{\tilde{j}_1v}{cT}-i\hat{t}r_1c\sin\frac{\tilde{j}_1v}{cT},\ \hat{r}_pr_3=\hat{r}_3r_p\cos\frac{\tilde{j}_1v}{cT}-ir_p\frac{cT}{\tilde{j}_1}\sin\frac{\tilde{j}_1v}{cT}\right\},\tag{18}$$

where the right and left generators are connected as follows:

$$r_3-\hat{r}_3=2i\frac{\tilde{j}_1}{cT}\left(\left(\hat{t}t-\frac{1}{c^2}\hat{r}_2r_2\right)\cos\frac{\tilde{j}_1v}{2cT}-i\frac{1}{c^2}\hat{r}_1r_1\cos\frac{\tilde{j}_1v}{cT}\right)\sin\frac{\tilde{j}_1v}{2cT},$$

$$\hat{r}_p=r_p\cos\frac{\tilde{j}_1v}{cT}-i\hat{r}_3r_p\frac{\tilde{j}_1}{cT}\sin\frac{\tilde{j}_1v}{cT},\quad p=1,2,\tag{19}$$

$$\hat{t}=t\cos\frac{\tilde{j}_1v}{cT}-i\hat{r}_2t\frac{\tilde{j}_1}{cT}\sin\frac{\tilde{j}_1v}{cT}.$$

$$S_v^{4(\pm)}(\sigma')=\left\{t,\mathbf{r}|\hat{r}_kt=\hat{t}r_k\cosh\frac{\tilde{j}_1v}{T}-ir_k\frac{T}{\tilde{j}_1}\sinh\frac{\tilde{j}_1v}{T},\ \hat{r}_2r_1=\hat{r}_1r_2\cosh\frac{\tilde{j}_1v}{T}-i\hat{r}_1r_3\sinh\frac{\tilde{j}_1v}{T},\ \hat{r}_1r_3\right.$$
$$\left.=\hat{r}_3r_1\cosh\frac{\tilde{j}_1v}{T}-i\hat{r}_2r_1\sinh\frac{\tilde{j}_1v}{T},\ \hat{r}_2r_3-\hat{r}_3r_2=2i\hat{r}_1r_1\sinh\frac{\tilde{j}_1v}{2T}\right\},\tag{20}$$

where the right and left generators are connected as

$$\hat{r}_k=r_k\cosh\frac{\tilde{j}_1v}{T}+i\hat{t}r_k\frac{\tilde{j}_1}{T}\sinh\frac{\tilde{j}_1v}{T},$$

$$\hat{t}=t+2i\frac{\tilde{j}_1}{c^2T}\left(\hat{r}_1r_1\cosh\frac{\tilde{j}_1v}{T}+(\hat{r}_2r_2+\hat{r}_3r_3)\cosh\frac{\tilde{j}_1v}{2T}\right)\sinh\frac{\tilde{j}_1v}{2T},\tag{21}$$

$$S_v^{4(\pm)}(\tilde{\sigma})=\left\{t,\mathbf{r}|\hat{t}r_p=\hat{r}_pt\cos\frac{v}{c}+i\hat{r}_pr_3\frac{1}{c}\sin\frac{v}{c},\ \hat{t}r_3-\hat{r}_3t=2i\frac{cT^2}{\tilde{j}_1^2}\left(\cos\frac{v}{c}-\frac{\tilde{j}_1^2}{c^2T^2}(\hat{r}_1r_1+\hat{r}_2r_2)\cos\frac{v}{2c}\right)\right.$$

$$\times \sin\frac{v}{2c},\ \hat{r}_p r_3 = \hat{r}_3 r_p \cos\frac{v}{c} - i\hat{t} r_p c \sin\frac{v}{c},\ \hat{r}_1 r_2 - \hat{r}_2 r_1 = 2\frac{c^2 T^2}{\widetilde{j}_1^2}\sin\frac{v}{2c}\Bigg\} \tag{22}$$

where $k=1,2,3$, $p=1,2$, and the left and right generators are connected by the following relations:

$$\hat{t} = t\cos\frac{v}{c} + ir_3\frac{1}{c}\sin\frac{v}{c}, \quad \hat{r}_1 = r_1\cos\frac{v}{c} + r_2\sin\frac{v}{c},$$
$$\hat{r}_2 = r_2\cos\frac{v}{c} - r_1\sin\frac{v}{c}, \quad \hat{r}_3 = r_3\cos\frac{v}{c} + itc\sin\frac{v}{c}. \tag{23}$$

In the case of the identical permutation σ_0, deformation parameter v for the system units, where $\hbar=1$, has the physical dimension of length $[v]=[cT]=[\text{length}]$ and may be interpreted as the fundamental length. For the permutation σ', the quantum (anti-) de Sitter kinematics (20) are characterized by the fundamental time $[v]=[\text{time}]$ and for the permutation $\widetilde{\sigma}$ are characterized by the fundamental velocity $[v]=[\text{velocity}]$. Recall that the same physical dimensions of the deformation parameter have been obtained for the quantum algebras $so_v(3;j;\sigma)$ and corresponding $(1+1)$ kinematics for different permutations.[23]

As it follows from (22), (23), both contractions $T\to\infty$, $c\to\infty$ are not permitted, therefore the quantum (anti-) de Sitter kinematics $S_v^{4(\pm)}(\widetilde{\sigma})$ do not have Minkowski, Newton, and Galilei kinematics as limiting cases.

In the zero curvature limit $T\to\infty$ two quantum Minkowski kinematics are obtained,

$$M_v^4(\sigma_0) = \{t,\mathbf{r}|[t,r_p]=0,\ [r_3,t]=ivt,\ [r_2,r_1]=0,\ [r_3,r_p]=ivr_p,\ p=1,2,\},$$
$$M_v^4(\sigma') = \{t,\mathbf{r}|[t,r_k]=ivr_k,\ [r_i,r_k]=0,\ i,k=1,2,3\}. \tag{24}$$

The first one is isomorphic to the tachyonic κ-Minkowski kinematics, the second one to the standard κ-deformation.[11–13] For both κ-Minkowski kinematics in the system units $\hbar=c=1$, the deformation parameter $\Lambda=\kappa^{-1}$ has the physical dimension of length and is interpreted as the fundamental length. But in the system units $\hbar=1$ the deformation parameter has different dimensions, namely v is the fundamental length for $M_v^4(\sigma_0)$ and v is the fundamental time for $M_v^4(\sigma')$.

As far as the commutation relations (24) do not depend on c, they do not change in the limit $c\to\infty$, therefore the generators of the quantum Galilei kinematics $G_v^4(\sigma_0)$ and $G_v^4(\sigma')$ are the subject of the same commutation relations. The only difference consists in the following statement: for the Galilei kinematics there are two invariants $\text{inv}_1=t^2$, $\text{inv}_2=r_1^2+r_2^2+r_3^2$ with respect to the coaction of the corresponding quantum groups, whereas for the Minkowski kinematics there is only one invariant $\text{inv}=t^2-(r_1^2+r_2^2+r_3^2)$. Thereby the quantum deformations of the flat kinematics are identical up to the coaction of the corresponding quantum groups for both relativistic and nonrelativistic kinematics.

In the nonrelativistic limit $c\to\infty$ there are two noncommutative analogs of the Newton kinematics:

$$N_v^{4(\pm)}(\sigma_0) = \left\{t,\mathbf{r}|[t,r_p]=0,\ [r_3,t]=ivt\left(1+\widetilde{j}_1^2\frac{t^2}{T^2}\right),\ [r_1,r_2]=0,\ [r_3,r_p]=ivr_p\left(1+\widetilde{j}_1^2\frac{t^2}{T^2}\right),\ p=1,2\right\},$$

$$N_v^{4(\pm)}(\sigma') = \left\{t,\mathbf{r}|[t,r_k]=i\left(r_k+\frac{\widetilde{j}_1^2}{T^2}tr_k t\right)\frac{T}{\widetilde{j}_1}\tanh\frac{\widetilde{j}_1 v}{T},\ r_2r_1 = r_1r_2\cosh\frac{\widetilde{j}_1 v}{T} - ir_1r_3\sinh\frac{\widetilde{j}_1 v}{T},\ r_1r_3\right.$$
$$\left. = r_3r_1\cosh\frac{\widetilde{j}_1 v}{T} - ir_2r_1\sinh\frac{\widetilde{j}_1 v}{T},\ [r_2,r_3]=2ir_1^2\sinh\frac{\widetilde{j}_1 v}{2T}\right\}, \tag{25}$$

where in the last case the deformation parameter is not transformed under contraction. The mul-

tiplier T^{-1} appears as the result of the physical interpretation of the quantum space generators. For nonzero curvature kinematics commutation relations of generators depend on c and are different for relativistic and nonrelativistic cases, unlike Minkowski and Galilei kinematics.

The exotic Carroll kinematics are also realized as constant curvature spaces, but with different interpretation of the Beltrami coordinates, namely $r_k=\xi_{k+1}\xi_1^{-1}$, $k=1,2,3$ are the space generators and $t=\xi_5\xi_1^{-1}$ is the time generator. Due to this interpretation the new physical dimensions of the contraction parameters appear: the parameter j_1 is replaced by $\tilde{j}_1 R^{-1}$, where $R\to\infty$ corresponds to $j_1=\iota_1$ and $[R]=[\text{length}]$; the parameter j_4 is replaced by c, where $c\to 0$ corresponds to $j_4=\iota_4$ and $[c]=[\text{velocity}]$. There are three noncommutative analogs of the exotic nonzero curvature Carroll kinematics:

$$C_v^{4(\pm)}(\sigma_0)=\left\{t,\mathbf{r}|[t,r_k]=iv r_k\left(1+\frac{\tilde{j}_1^2}{R^2}\mathbf{r}^2\right),\ [r_i,r_k]=0,\right\},$$

$$C_v^{4(\pm)}(\sigma')=\left\{t,\mathbf{r}|[t,r_1]=0,\ [t,r_2]=iv\frac{\tilde{j}_1}{R}r_3r_2,\ [r_3,t]=iv\frac{\tilde{j}_1}{R}r_1^2,\ [r_i,r_k]=0,\right\}, \tag{26}$$

$$C_v^{4(\pm)}(\tilde{\sigma})=\left\{t,\mathbf{r}|[t,r_p]=0,\ [r_i,r_k]=0,\ [r_1,t]=iv\left(\frac{R^2}{\tilde{j}_1^2}+\mathbf{r}^2\right)\right\}.$$

Two quantum analogs of the zero curvature Carroll kinematics are achieved in the limit $R\to\infty$ and are as follows:

$$\begin{aligned} C_v^{4(0)}(\sigma_0)&=\{t,\mathbf{r}|[t,r_k]=iv r_k,\ [r_i,r_k]=0,\ i,k=1,2,3\},\\ C_v^{4(0)}(\sigma')&=\{t,\mathbf{r}|[t,r_k]=0,\ [r_i,r_k]=0,\ i,k=1,2,3\}. \end{aligned} \tag{27}$$

For the permutations σ_0, σ' the deformation parameter $v=Rc^{-1}$ has the physical dimension of time $[v]=[\text{time}]$ and is interpreted as the fundamental time. For the permutation $\tilde{\sigma}$ the deformation parameter $v=c^{-1}$ has the dimension of inverse velocity $[v]=[\text{velocity}]^{-1}$ and may be interpreted as the fundamental velocity.

V. CONCLUSION

We have reformulated the quantum orthogonal group $SO_q(N)$ and the corresponding q-Euclidean space O_q^N in Cartesian coordinates and then used the standard trick with real, complex, and dual numbers in order to define the quantum Cayley–Klein spaces of constant curvature $O_q^N(j;\sigma)$ uniformly, using a q analog of Beltrami coordinates. The different combinations of quantum structure and CK scheme of contractions and analytical continuations are described with the help of permutations σ. As a result, for $N=5$, the quantum deformations of (anti-) de Sitter, Minkowski, Newton, Galilei, and Carroll kinematics are obtained.

We have found two types of the noncommutative realistic space-time models with fundamental length and fundamental time, which admit nonrelativistic and zero curvature limits and one type of the (anti-) de Sitter kinematics with fundamental velocity, where both limits are forbidden. For the exotic Carroll kinematics there are two types with fundamental time, which admit zero curvature limit and one type with fundamental velocity, where this limit is forbidden.

The quantum Galilei kinematics $G_v^4(\sigma_0)$ and $G_v^4(\sigma')$ have the same commutation relations (24) as the quantum Minkowski kinematics $M_v^4(\sigma_0)$ and $M_v^4(\sigma')$. In other words, the quantum deformations of the flat kinematics are identical up to the coaction of the corresponding quantum groups, whereas for nonzero curvature kinematics commutation relations of generators are different for relativistic and nonrelativistic cases.

In spite of the fact that the commutation relations of generators of Carroll $C_v^{4(0)}(\sigma_0)$ (27) and Minkowski $M_v^4(\sigma')$ (24) kinematics are identical, both kinematics are physically different. Mathematically isomorphic kinematics may be physically nonequivalent.

Noncommutative kinematics are obtained by the interpretation of some mathematical constructions associated with quantum groups and quantum spaces. The deformation parameter is free parameter of these models. Which type of model is more appropriate and what is the value of deformation parameter are questions of experimental study.

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The equation for time-like extremal surfaces in Minkowski space $\mathbb{R}^{2+n}$

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In this paper we investigate the equation for time-like extremal surfaces in the Minkowski space $\mathbb{R}^{2+n}$, and show that this kind of equation enjoys many interesting properties nonstrict hyperbolicity, constant multiplicity of eigenvalues, boundedness of characteristic propagation speeds, linear degeneracy of all characteristic fields, richness, etc. Without any smallness assumption of initial data, we give the necessary and sufficient condition on the global existence of classical solutions of the Cauchy problem. Based on this, we prove some global existence theorems on classical solutions of the Dirichlet problem and Neumann problem for this kind of equation. Finally, we present an explicit exact representation, involving two independent arbitrary functions of general solution. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2158435]

I. INTRODUCTION AND MAIN RESULTS

Let (t,x,y) be points in the $(1+2)$-dimensional Minkowski space. A time-like surface takes the form

$$y = \phi(t,x). \tag{1.1}$$

This surface is called to be *extremal surface* if ϕ is the critical point of the area functional,

$$I_1 = \int\int \sqrt{1+\phi_x^2-\phi_t^2}\,dx\,dt. \tag{1.2}$$

The corresponding Euler–Lagrange equation is

$$\left(\frac{\phi_t}{\sqrt{1+\phi_x^2-\phi_t^2}}\right)_t - \left(\frac{\phi_x}{\sqrt{1+\phi_x^2-\phi_t^2}}\right)_x = 0. \tag{1.3}$$

Recently, Brenier[1] discussed an equation for generalized extremal surfaces in the five-dimensional Minkowski space, from which the Vlasov-Maxwell system of classical electrodynamics can be formlly derived. Similar to the geometric ideas of the Born-Infeld nonlinear theory of the electromagnetic field (see Ref. 2), Brenier[3] tried to design a nonlinearly cutoff theory for classical electrodynamics, instead of considering springs linking two particles of opposite charges, he considered surfaces $(t,s)\to X(t,s)$ spanning curves $t\to X_-(t)$ and $t\to X_+(t)$ followed by two particles of opposite charge, so that $X(s=-1,t)=X_-(t)$ and $X(s=1,t)=X_+(t)$, $s\in[-1,1]$ standing for the *interpolation* parameter between the two trajectories. Just by prescribing (t,s)

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$\rightarrow (t,s,X(t,s))$ to be an extremal surface in the five-dimensional Minkowski space (t,s,x_1,x_2,x_3) with the signature $(-,+,+,+,+)$, he got the building block of the model: the individual action of each surface is

$$I_3 = \int\int \sqrt{1+|\partial_s X|^2 - |\partial_t X|^2 - |\partial_s X \times \partial_t X|^2}\, ds\, dt, \tag{1.4}$$

which is basically the Nambu–Goto action of classical string theory. The Euler–Lagrange equation corresponding to the functional (1.4) is

$$\left(\frac{\phi_t}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t\times\phi_x|^2}}\right)_t - \left(\frac{\phi_x}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t\times\phi_x|^2}}\right)_x + \left(\frac{\phi_x\times(\phi_t\times\phi_x)}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t\times\phi_x|^2}}\right)_t - \left(\frac{\phi_t\times(\phi_t\times\phi_x)}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t\times\phi_x|^2}}\right)_x = 0, \tag{1.5}$$

where x stands for s in (1.4) and $\phi=(\phi_1,\phi_2,\phi_3)^T$ represents X in (1.4).

More generally, we consider a vector function $\phi=(\phi_1,\ldots,\phi_n)^T$, which is the critical point of the area functional,

$$I_n = \int\int \sqrt{1+|\phi_x|^2-|\phi_t|^2|\phi_x|^2+\langle\phi_t,\phi_x\rangle^2}\, dx\, dt, \tag{1.6}$$

where $\langle\cdot,\cdot\rangle$ stands for the inner product. The Euler–Lagrange equation is

$$\left(\frac{\phi_t+|\phi_x|^2\phi_t-\langle\phi_t,\phi_x\rangle\phi_x}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t|^2|\phi_x|^2+\langle\phi_t,\phi_x\rangle^2}}\right)_t - \left(\frac{\phi_x+\langle\phi_t,\phi_x\rangle\phi_t-|\phi_t|^2\phi_x}{\sqrt{1+|\phi_x|^2-|\phi_t|^2-|\phi_t|^2|\phi_x|^2+\langle\phi_t,\phi_x\rangle^2}}\right)_x = 0. \tag{1.7}$$

Remark 1.1: When $n=1$, *the equation (1.7) is nothing but the equation (1.3); moreover, if*

$$1+\phi_x^2-\phi_t^2>0, \tag{1.8}$$

i.e., the surface is time-like, then (1.3) is just the Born–Infeld equation (see Ref. 2). The Born–Infeld as well as the hydrodynamic version of the equation has been considered by Arik et al.[4] *On the other hand, when* $n=3$, *the equation (1.7) goes back to the equation (1.5).*

(1.7) is the equation for time-like extremal surfaces in the Minkowski space $\mathbb{R}^{2+n}$. The extremal surfaces in the Minkowski space are C^2 surfaces with vanishing mean curvature. The time-like case have been investigated by several authors (e.g., Refs. 5 and 6). Barbashov, Nesterenko, and Chervyakov[5] studied the nonlinear differential equations describing in differential geometry the minimal surfaces in the pseudo-Euclidean space. The geometric nature of these equations allows one to obtain explicitly their general solutions. Milnor[6] described all entire time-like minimal surfaces in the three-Minkowski space via a kind of Weierstrass representation. Gu[7–10] studied the extremal surfaces of mixed type in the n-dimensional Minkowski space (Refs. 11, 7, and 9 for the case $n=3$). Under the assumptions that the surfaces is C^3 (C^2 for the case $n=3$), and the gradient of the square of the area density does not vanish on the light-like points of the surface, by linearizing the equation via the Legendre transformation or the generalized isothermal coordinates, Gu obtained the general explicit expression of the surface and proved that (i) the time-like part and space-like part are separated by a null curve; (ii) the surface is analytic not only on the space-like part but also in some mixed region. Moreover, many complete extremal surfaces of mixed type in the three-Minkowski space are constructed with explicit expressions (see Ref. 10). In addition, the multidimensional versions of the system (1.7) has been addressed recently and successfully by Lindblad[12] and, later, by Chae and Huh[13] in a more general framework. They proved the existence of global smooth solutions for small initial data, using the null forms in the style of Christodoulou and Klainerman style (see Refs. 14 and 15).

In the present paper, we study the equation (1.7) using a different method and obtain a complete result on global classical solutions of the Cauchy problem, Dirichlet problem, and Neumann problem for this kind of equation. Moreover, we also present an explicit exact representation, involving two independent arbitrary functions, of a general solution of the equation (1.7). Here we particularly emphasize that, in our arguments, we do not require the smallness of the initial data.

Let

$$u = \phi_x, \quad v = \phi_t, \tag{1.9}$$

where $u=(u_1,\ldots,u_n)^T$ and $v=(v_1,\ldots,v_n)^T$. Then (1.7) can be equivalently rewritten as

$$u_t - v_x = 0,$$

$$\left(\frac{v+|u|^2v-\langle u,v\rangle u}{\sqrt{1+|u|^2-|v|^2-|v|^2|u|^2+\langle u,v\rangle^2}}\right)_t - \left(\frac{u+\langle u,v\rangle v-|v|^2u}{\sqrt{1+|u|^2-|v|^2-|v|^2|u|^2+\langle u,v\rangle^2}}\right)_x = 0, \tag{1.10}$$

for classical solutions. In this paper, we investigate many interesting properties enjoyed by the system (1.10) such as nonstrict hyperbolicity, constant multiplicity of eigenvalues, boundedness of characteristic propagation speeds, linear degeneracy of all characteristic fields, richness, etc. Based on this, we prove some global existence theorems on classical solutions of the Cauchy problem, Dirichlet problem, and Neumann problem for the equation (1.7), and present an explicit exact representation, involving two independent arbitrary functions, of the general solution of (1.7).

Let

$$\Delta(u,v) = 1+|u|^2-|v|^2-|v|^2|u|^2+\langle u,v\rangle^2. \tag{1.11}$$

Our main results are the following Theorem 1.1 and Theorem 1.2.

Theorem 1.1: *Suppose* $n\geqslant 2$ *and suppose furthermore that on the domain under consideration*,

$$\Delta(u,v) > 0, \tag{1.12}$$

holds, then (1.10) is a nonstrictly hyperbolic system with two n-constant multiple eigenvalues; moreover, the characteristic propagation speeds are bounded (not larger than the light speed), all characteristic fields are linearly degenerate in the sense of Lax (see Ref. 16) and the system (1.10) is rich in the sense of Serre (see Ref. 17).

Remark 1.2: For the case $n=1$, *if (1.8) is satisfied, then as pointed out in Remark 1.1, (1.7) is nothing but the Born–Infeld equation. In this case, it is easy to verify that the system (1.10) is a* 2×2 *strictly hyperbolic system, and both characteristic fields are linearly degenerate. Moreover, the richness of the system (1.10) becomes trivial in the present situation.*

Remark 1.3: In fact, the assumption (1.12) is nothing but the condition which guarantees that the surface is timelike. When $n=1$, *(1.12) is just (1.8). Thus, for every timelike surface the conclusion of Theorem 1.1 is always true.*

We next consider the Cauchy problem for Eq. (1.7) with the initial data

$$\phi(0,x) = f(x), \quad \phi_t(0,x) = g(x), \tag{1.13}$$

where f is a given C^2 vector-valued function and g is a given C^1 vector-valued function. Define

$$\Lambda_\pm(x) = \frac{1}{1+|f'(x)|^2}\left[-\langle f'(x),g(x)\rangle \pm \sqrt{\Delta(f'(x),g(x))}\right]. \tag{1.14}$$

We assume that

$$\Lambda_+(x) > \Lambda_-(y), \quad \forall\, x,y \in \mathbb{R}. \tag{1.15}$$

In Sec. III, we shall prove the following global existence theorem.

Theorem 1.2: *The Cauchy problem [(1.7) and (1.13)] admits a unique global C^2 solution $\phi=\phi(t,x)$ on $\mathbb{R}^+\times\mathbb{R}$ if and only if* (1.15) *is satisfied. Moreover, if the global classical solution $\phi=\phi(t,x)$ exists, then it satisfies*

$$\Delta(\phi_x(t,x),\phi_t(t,x)) > 0, \quad \forall\, (t,x) \in \mathbb{R}^+\times\mathbb{R}. \tag{1.16}$$

Remark 1.4: The assumption (1.15) guarantees the validity of the hypothesis (1.12). That is, under the assumption (1.15) the surface is timelike. If (1.15) is not satisfied, then the solution may enlarge in finite time and singularities will appear. In this case, Eq. (1.7) loses the hyperbolicity at the points where the fast characteristic meets the slow characteristic. In geometry, this corresponds to the fact that the surface is no longer timelike at these points.

Remark 1.5: Theorem 1.2 solves an open problem of Brenier (see [6]).

The paper is organized as follows. In Sec. II, we first simplify the system (1.10) and then give the eigenvalues, the left and right eigenvectors of the system (1.10); based on this, we investigate many interesting properties enjoyed by the system (1.10) and then prove Theorem 1.1. Section III is devoted to the proof of Theorem 1.2. Based on Theorem 1.2, in Sec. IV, we study the global existence of the classical C^2 solutions of the Dirichlet and Neumann problems for Eq. (1.7). In Sec. V, we present an explicit exact representation, involving two independent arbitrary functions, of general solution of Eq. (1.7). Finally, the global existence of the classical solutions is discussed in Sec. VI for the inhomogeneous Dirichlet problem for (1.7).

II. PROPERTIES ENJOYED BY THE SYSTEM (1.10)—PROOF OF THEOREM 1.1

This section is devoted to the study on many interesting properties enjoyed by the system (1.10).

To do so, we first simplify (1.10). Let

$$\Phi = (1+|u|^2)v - \langle u,v\rangle u, \quad \Psi = (1-|v|^2)u + \langle u,v\rangle v. \tag{2.1}$$

The second equation in (1.10) can be rewritten as

$$\left(\frac{\Phi}{\sqrt{\Delta(u,v)}}\right)_t - \left(\frac{\Psi}{\sqrt{\Delta(u,v)}}\right)_x = 0, \tag{2.2}$$

namely,

$$\Phi\frac{\partial\Delta(u,v)}{\partial t} - \Psi\frac{\partial\Delta(u,v)}{\partial x} + 2\Delta(u,v)(\Psi_x - \Phi_t) = 0. \tag{2.3}$$

Substituting (1.11) and (2.1) into (2.3) gives

$$(1+|u|^2)O - 2\langle u,v\rangle P - (1-|v|^2)Q = 0, \tag{2.4}$$

where

$$\begin{aligned}
O &= \Delta(u,v)v_t + (1+|u|^2)\langle v,v_t\rangle v - \langle u,v\rangle\langle u,v_t\rangle v - \langle u,v\rangle\langle v,v_t\rangle u - (1-|v|^2)\langle u,v_t\rangle u,\\
P &= \Delta(u,v)v_x + (1+|u|^2)\langle v,v_x\rangle v - \langle u,v\rangle\langle u,v_x\rangle v - \langle u,v\rangle\langle v,v_x\rangle u - (1-|v|^2)\langle u,v_x\rangle u,\\
Q &= \Delta(u,v)u_x + (1+|u|^2)\langle v,u_x\rangle v - \langle u,v\rangle\langle u,u_x\rangle v - \langle u,v\rangle\langle v,u_x\rangle u - (1-|v|^2)\langle u,u_x\rangle u.
\end{aligned} \tag{2.5}$$

We can write the system (2.4) as the following matrix equation:

$$M\mathbf{v}_t - \frac{2\langle u,v\rangle}{1+|u|^2}M\mathbf{v}_x - \frac{1-|v|^2}{1+|u|^2}M\mathbf{u}_x = 0, \tag{2.6}$$

where

$$M = \Delta(u,v)I_{n\times n} + (1+|u|^2)vv^T - \langle u,v\rangle vu^T - \langle u,v\rangle uv^T - (1-|v|^2)uu^T, \tag{2.7}$$

$$\mathbf{v} = \begin{bmatrix} v_1 & 0 & \cdots & 0 & 0 \\ 0 & v_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & v_{n-1} & 0 \\ 0 & 0 & \cdots & 0 & v_n \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} u_1 & 0 & \cdots & 0 & 0 \\ 0 & u_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & u_{n-1} & 0 \\ 0 & 0 & \cdots & 0 & u_n \end{bmatrix}. \tag{2.8}$$

Therefore, the system (1.10) can be equivalently rewritten as

$$u_t - v_x = 0,$$

$$M\mathbf{v}_t - \frac{2\langle u,v\rangle}{1+|u|^2}M\mathbf{v}_x - \frac{1-|v|^2}{1+|u|^2}M\mathbf{u}_x = 0. \tag{2.9}$$

Lemma 2.1: If A is a nonsingular $m_1\times m_1$ square matrix, D is a nonsingular $m_2\times m_2$ square matrix, B is a $m_1\times m_2$ matrix, and C is a $m_2\times m_1$ matrix, where m_1, m_2 are two positive integers, then it holds that

$$|A|\cdot|D - CA^{-1}B| = |D|\cdot|A - BD^{-1}C|. \tag{2.10}$$

Proof: In fact, (2.10) follows from the following identities directly:

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = \begin{vmatrix} A & B \\ 0 & D - CA^{-1}B \end{vmatrix} = \begin{vmatrix} A - BD^{-1}C & B \\ 0 & D \end{vmatrix}.$$

■

Lemma 2.2: If

$$\Delta(u,v) > 0, \tag{2.11}$$

then

$$|M| = (\Delta(u,v))^{n-1} > 0. \tag{2.12}$$

Proof: By (1.11), we have

$$\Delta(u,v) = (1+|u|^2)(1-|v|^2) + \langle u,v\rangle^2. \tag{2.13}$$

On the other hand, it follows from (2.7) that

$$M = \Delta(u,v)I_{n\times n} + [u,v]\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} u^T \\ v^T \end{bmatrix}, \tag{2.14}$$

where

$$a = -(1-|v|^2), \quad b = c = -\langle u,v\rangle, \quad d = 1+|u|^2. \tag{2.15}$$

Noting (2.13) and (2.15) gives

$$\Delta(u,v) = bc - ad. \tag{2.16}$$

Let

$$A=\Delta(u,v)I_{n\times n},\quad B=[u,v],\quad C=\begin{bmatrix}u^T\\ v^T\end{bmatrix},\quad D=-\begin{bmatrix}a & b\\ c & d\end{bmatrix}^{-1}. \tag{2.17}$$

By (2.11) and (2.16), we find that A is a nonsingular $n\times n$ matrix, D is a nonsingular 2×2 matrix. On the other hand, it follows from (2.14) that

$$|M|=|A+B(-D)^{-1}C|=|A-BD^{-1}C|=\frac{1}{|D|}\cdot|D|\cdot|A-BD^{-1}C|. \tag{2.18}$$

We now apply Lemma 2.1 and obtain

$$|M|=\frac{1}{|D|}\cdot|A|\cdot|D-CA^{-1}B|. \tag{2.19}$$

Substituting (2.17) into (2.19) and noting (2.15) yields

$$\begin{aligned}|M|&=\frac{|\Delta(u,v)I_{n\times n}|}{\left|-\begin{bmatrix}a & b\\ c & d\end{bmatrix}^{-1}\right|}\left|-\begin{bmatrix}a & b\\ c & d\end{bmatrix}^{-1}-\begin{bmatrix}u^T\\ v^T\end{bmatrix}(\Delta(u,v)I_{n\times n})^{-1}[u,v]\right|\\ &=\frac{(\Delta(u,v))^n}{(-\Delta(u,v))^{-1}}\left|\frac{1}{\Delta(u,v)}\begin{bmatrix}d & -b\\ -c & a\end{bmatrix}-\frac{1}{\Delta(u,v)}\begin{bmatrix}u^Tu & u^Tv\\ v^Tu & v^Tv\end{bmatrix}\right|\\ &=-(\Delta(u,v))^{n-1}\begin{vmatrix}d-u^Tu & -b-u^Tv\\ -c-v^Tu & a-v^Tv\end{vmatrix}=-(\Delta(u,v))^{n-1}\begin{vmatrix}1 & 0\\ 0 & -1\end{vmatrix}=(\Delta(u,v))^{n-1}>0.\end{aligned} \tag{2.20}$$

Thus, the proof of Lemma 2.2 is completed. ■

Remark 2.1: In particular, when $n=1$, we have $|M|=1$.

Throughout this section, we always assume that (2.11) is satisfied. Thus, by Lemma 2.2, the system (2.9) can be simplified as

$$u_t-v_x=0,$$

$$v_t-\frac{2\langle u,v\rangle}{1+|u|^2}v_x-\frac{1-|v|^2}{1+|u|^2}u_x=0. \tag{2.21}$$

Let

$$U=(u_1,\ldots,u_n,v_1,\ldots,v_n)^T. \tag{2.22}$$

Then, we can rewrite (2.21) as

$$\frac{\partial U}{\partial t}+\mathbf{A}(U)\frac{\partial U}{\partial x}=0, \tag{2.23}$$

where

$$\mathbf{A}(U)=\begin{bmatrix}0 & -I_{n\times n}\\ -\dfrac{1-|v|^2}{1+|u|^2}I_{n\times n} & -\dfrac{2\langle u,v\rangle}{1+|u|^2}I_{n\times n}\end{bmatrix}. \tag{2.24}$$

By a direct calculation, the eigenvalues of $\mathbf{A}(U)$ are

$$\lambda_1\equiv\cdots\equiv\lambda_n=\lambda_-,\quad \lambda_{n+1}\equiv\cdots\equiv\lambda_{2n}=\lambda_+, \tag{2.25}$$

where

$$\lambda_{\pm}=\frac{1}{1+|u|^2}(-\langle u,v\rangle\pm\sqrt{1+|u|^2-|v|^2-|v|^2|u|^2+\langle u,v\rangle^2}). \tag{2.26}$$

The right eigenvector corresponding to $\lambda_i(i=1,\ldots,2n)$ can be chosen as

$$r_i=(e_i^T,-\lambda_- e_i^T)^T\ (i=1,\ldots,n),\quad r_i=(e_{i-n}^T,-\lambda_+ e_{i-n}^T)^T\ (i=n+1,\ldots,2n), \tag{2.27}$$

where

$$e_\alpha=(0,\ldots,0,\overset{(\alpha)}{1},0,\ldots,0)^T\ (\alpha=1,\ldots,n); \tag{2.28}$$

while the left eigenvector corresponding to $\lambda_i(i=1,\ldots,2n)$ can be taken as

$$l_i=(\lambda_+ e_i^T,e_i^T)\ (i=1,\ldots,n),\quad l_i=(\lambda_- e_{i-n}^T,e_{i-n}^T)\ (i=n+1,\ldots,2n). \tag{2.29}$$

Thus we have proved the following Property 2.1.

Property 2.1: Under the assumption of Theorem 1.1, (1.10) is a nonstrictly hyperbolic system with two n-constant multiple eigenvalues [see (2.25)], and the right (resp., left) eigenvectors can be chosen as (2.27) [resp., (2.29)].

Property 2.2: Under the assumption (1.12), the characteristic propagation speeds $\lambda_\pm$ *satisfy*

$$\lambda_+\in(-1,1],\quad \lambda_-\in[-1,1). \tag{2.30}$$

Proof: Let

$$r=|u|,\quad s=|v|. \tag{2.31}$$

Then

$$\langle u,v\rangle=rs\cos\theta, \tag{2.32}$$

where $\theta\in[0,\pi]$ is the angle between vectors u and v. Thus, we have

$$\lambda_{\pm}=\frac{1}{1+r^2}(-rs\cos\theta\pm\sqrt{1+r^2-s^2-r^2s^2\sin^2\theta}), \tag{2.33}$$

where

$$\theta\in[0,\pi],\quad 1+r^2-s^2-r^2s^2\sin^2\theta>0. \tag{2.34}$$

We only prove the first part in (2.30). The proof of the second part in (2.30) is similar. Noting (2.33), we have

$$(1+r^2)\lambda_+=-rs\cos\theta+\sqrt{1+r^2-s^2-r^2s^2\sin^2\theta}, \tag{2.35}$$

that is,

$$(1+r^2)\lambda_++rs\cos\theta=\sqrt{1+r^2-s^2-r^2s^2\sin^2\theta}. \tag{2.36}$$

Squaring both sides of (2.36) yields

$$(1+r^2)^2\lambda_+^2+2(1+r^2)\lambda_+rs\cos\theta+r^2s^2\cos^2\theta=1+r^2-s^2-r^2s^2\sin^2\theta. \tag{2.37}$$

Dividing (2.37) by $1+r^2$ leads to

$$(\lambda_+r\cos\theta+s)^2+\lambda_+^2r^2\sin^2\theta=1-\lambda_+^2. \tag{2.38}$$

This implies

$$\lambda_+^2\leqslant 1. \tag{2.39}$$

We now claim that $\lambda_+ \neq -1$.

In fact, if $\lambda_+ = -1$, then it follows from (2.38) that

$$r \sin\theta = 0, \quad s - r\cos\theta = 0. \tag{2.40}$$

Case I: If $r=0$, then it follows from the second equation in (2.40) that $s=0$. In this case, noting (2.33), we have

$$\lambda_+ = 1. \tag{2.41}$$

This contradicts the assumption that $\lambda_+ = -1$.

Case II: If $r \neq 0$, then $\theta = 0, \pi$, and then $s = \pm r$. In the present situation, by (2.33) we have

$$\lambda_+ = \frac{1 \pm r^2}{1 + r^2} > -1. \tag{2.42}$$

This also contradicts the assumption that $\lambda_+ = -1$.

Therefore, noting (2.39), we obtain the first part in (2.30). Thus, the proof of Property 2.2 is completed. ■

Property 2.3: Under the assumption (1.12), the characteristic fields $\lambda_\pm$ are linearly degenerate in the sense of Lax, that is, the system (1.10) is linearly degenerate in the sense of Lax.

Proof: We calculate the invariants $\nabla\lambda_- \cdot r_\alpha (\alpha = 1, \ldots, n)$ and $\nabla\lambda_+ \cdot r_\beta (\beta = n+1, \ldots, 2n)$.

For every $\alpha \in \{1, \ldots, n\}$, by a direct calculation, we have

$$\nabla\lambda_- \cdot r_\alpha = \left(\frac{\partial\lambda_-}{\partial u}, \frac{\partial\lambda_-}{\partial v}\right) \cdot (e_\alpha^T, -\lambda_- e_\alpha^T)^T = \left(\frac{\partial\lambda_-}{\partial u} - \lambda_- \frac{\partial\lambda_-}{\partial v}\right) \cdot e_\alpha = 0. \tag{2.43}$$

Similarly, we can prove

$$\nabla\lambda_+ \cdot r_\beta \equiv 0, \quad \forall\, \beta \in \{n+1, \ldots, 2n\}. \tag{2.44}$$

Thus, the proof of Property 2.3 is finished. ■

Remark 2.2: When $n \geqslant 2$, the linear degeneracy of $\lambda_\pm$ follows from Boillat[18] and Freistühler[11] directly.

Property 2.4: Under the assumption (1.12), the system (1.10) is rich in the sense of Serre.

Remark 2.3: The rich systems (see page 144 in Ref. 17 for the definition) generalize the class of 2×2 systems while preserving their essential properties:

(1) *diagonalization with the help of the strict Riemann invariants*;
(2) *the infinite dimension of the entropy space*.

Proof of Property 2.4: On the domain under consideration, we consider the following linear system:

$$\nabla w \cdot r_\mu = 0 \quad (\mu = 1, \ldots, n), \tag{2.45}$$

where $w = w(u,v)$ is the unknown function of (u,v); r_μ are given by (2.27). In the $2n$-dimensional U space, the system (2.45) has n linearly independent solutions denoted by $R_\alpha = R_\alpha(U)(\alpha = 1, \ldots, n)$. Similarly, let $R_\beta = R_\beta(U)(\beta = n+1, \ldots, 2n)$ be the linearly independent solutions of the following linear system:

$$\nabla w \cdot r_\nu = 0 \quad (\nu = n+1, \ldots, 2n), \tag{2.46}$$

where r_ν are defined by (2.27). Noting (2.27) and (2.29), we have

$$\nabla R_\alpha = \sum_{\nu=n+1}^{2n} c_{\alpha,\nu} l_\nu \ (\alpha = 1, \ldots, n), \quad \nabla R_\beta = \sum_{\mu=1}^{n} c_{\beta,\mu} l_\mu \ (\beta = n+1, \ldots, 2n), \tag{2.47}$$

with

$$\det(c_{\alpha,\nu}) \neq 0 \quad \text{and} \quad \det(c_{\beta,\mu}) \neq 0, \tag{2.48}$$

where $c_{\alpha,\nu}=c_{\alpha,\nu}(U)$, $c_{\beta,\mu}=c_{\beta,\mu}(U)$ are smooth functions of U, and $l_i(i=1,\ldots,2n)$ are given by (2.29). Notice that

$$l_\mu\left(\frac{\partial U}{\partial t} + \lambda_- \frac{\partial U}{\partial x}\right) = 0 \ (\mu = 1, \ldots, n). \tag{2.49}$$

Multiplying (2.49) by $c_{\beta,\mu}$ and summing up them with respect to μ gives

$$\nabla R_\beta\left(\frac{\partial U}{\partial t} + \lambda_- \frac{\partial U}{\partial x}\right) = 0 \ (\beta = n+1, \ldots, 2n),$$

that is,

$$\frac{\partial R_\beta}{\partial t} + \lambda_- \frac{\partial R_\beta}{\partial x} = 0 \ (\beta = n+1, \ldots, 2n). \tag{2.50}$$

Similarly, we have

$$\frac{\partial R_\alpha}{\partial t} + \lambda_+ \frac{\partial R_\alpha}{\partial x} = 0 \ (\alpha = 1, \ldots, n). \tag{2.51}$$

Take $R_i=R_i(U)(i=1,\ldots,2n)$ as the new unknown functions. Then, (2.50) and (2.51) show that the system (1.10) can be diagonalized (at least in a local domain). On the other hand, since the system (1.10) is in a conservative form, it follows from Ref. 17 that it is rich. Thus, the proof of Property 2.4 is completed. ■

Remark 2.4: The system (2.50) and (2.51) is called the Riemann-invariant representation of the system (1.10).

Introduce

$$R_i = v_i + \lambda_- u_i, \quad R_{i+n} = v_i + \lambda_+ u_i \ (i = 1, \ldots, n). \tag{2.52}$$

It is easy to verify that R_i (resp., R_{i+n}) are Riemann invariants corresponding to λ_+ (resp., λ_-), and then they satisfy

$$\frac{\partial R_i}{\partial t} + \lambda_+ \frac{\partial R_i}{\partial x} = 0, \quad \frac{\partial R_{i+n}}{\partial t} + \lambda_- \frac{\partial R_{i+n}}{\partial x} = 0 \ (i = 1, \ldots, n). \tag{2.53}$$

On the other hand, λ_- (resp., λ_+) is also a Riemann invariant corresponding to λ_+ (resp., λ_-), and $\lambda_\pm$ satisfy

$$\frac{\partial \lambda_-}{\partial t} + \lambda_+ \frac{\partial \lambda_-}{\partial x} = 0, \quad \frac{\partial \lambda_+}{\partial t} + \lambda_- \frac{\partial \lambda_+}{\partial x} = 0. \tag{2.54}$$

The systems (2.53) and (2.54) play an important role in the proof of Theorem 1.2.

Proof of Theorem 1.1: Theorem 1.1 follows from Properties (2.1)–(2.4) directly. ■

III. GLOBAL EXISTENCE OF CLASSICAL SOLUTIONS OF THE CAUCHY PROBLEM—PROOF OF THEOREM 1.2

In this section, we prove Theorem 1.2.

Proof of Theorem 1.2: By (2.54), the necessity comes from Theorem 2.1 in Kong and Tsuji[19] directly. (Here we have made use of Property 2.2.)

In what follows, we prove the sufficiency and (1.16).

As a matter of fact, the C^2 solution of the Cauchy problem (1.7) and (1.13) is equivalent to the C^1 solution of the Cauchy problem for the system (1.10) with the following initial data:

$$t=0: u=f'(x),\ v=g(x). \tag{3.1}$$

Therefore, in order to prove Theorem 1.2, it suffices to prove that, under the assumption of Theorem 1.2, the Cauchy problem (1.10) and (3.1) has a unique global C^1 solution $U=(u^T,v^T)^T$ on $\mathbb{R}^+\times\mathbb{R}$; moreover, it holds that

$$\Delta(u(t,x),v(t,x))>0, \quad \forall\,(t,x)\in\mathbb{R}^+\times\mathbb{R}. \tag{3.2}$$

For any given interval $\mathbb{I}=[x_1,x_2]\subset\mathbb{R}$, define the *strong determinate region*,

$$\Delta_{\mathbb{I}}=\{(t,x)|t\geqslant 0, x_1+t\leqslant x\leqslant x_2-t\}, \tag{3.3}$$

where x_1,x_2 are arbitrary given real numbers with $x_1<x_2$. Thus, in order to prove that the Cauchy problem (1.10) and (3.1) has a unique global C^1 solution $U=(u^T,v^T)^T$ with (3.2) on $\mathbb{R}^+\times\mathbb{R}$; it suffices to prove that, under the assumption of Theorem 1.2, for any given interval $\mathbb{I}\subset\mathbb{R}$ the Cauchy problem for the system (1.10) with the initial data

$$t=0: u=f'(x),\ v=g(x), \quad \forall\, x\in\mathbb{I} \tag{3.1a}$$

has a unique C^1 solution $U=(u^T,v^T)^T$ on the domain $\Delta_{\mathbb{I}}$; moreover, it holds that

$$\Delta(u(t,x),v(t,x))>0, \quad \forall\,(t,x)\in\Delta_{\mathbb{I}}. \tag{3.4}$$

To do so, we first consider the Cauchy problem for the system (2.54) with the initial data

$$t=0: \lambda_{\pm}=\Lambda_{\pm}(x), \quad \forall\, x\in\mathbb{I}, \tag{3.5}$$

on the domain $\Delta_{\mathbb{I}}$.

In the present situation, noting the assumption (1.15), we have

$$\|\Lambda_{\pm}(x)\|_{C^1(\mathbb{I})}\leqslant c_{\mathbb{I}}, \quad \inf_{x\in\mathbb{I}}\Lambda_+(x)-\sup_{x\in\mathbb{I}}\Lambda_-(x)\triangleq\delta_{\mathbb{I}}>0, \tag{3.6}$$

where $c_{\mathbb{I}}$, $\delta_{\mathbb{I}}$ are two positive constants. Under the condition (3.6), by the existence and uniqueness of local C^1 solution of Cauchy problem for quasilinear hyperbolic system (see Ref. 20), there exists a positive number τ such that the Cauchy problem (2.54) and (3.5) has a unique C^1 solution, denoted by $(\lambda_-,\lambda_+)=(\lambda_-^{\mathbb{I}}(t,x),\lambda_+^{\mathbb{I}}(t,x))$, on the domain

$$\Delta_{\mathbb{I}}(\tau)=\{(t,x)|0\leqslant t\leqslant\tau, x_1+t\leqslant x\leqslant x_2-t\}. \tag{3.7}$$

It is easy to see that, on the existence domain of the classical solution of the Cauchy problem (2.54) and (3.5),

$$\sup\lambda_{\pm}=\sup_{x\in\mathbb{I}}\Lambda_{\pm}(x), \quad \inf\lambda_{\pm}=\inf_{x\in\mathbb{I}}\Lambda_{\pm}(x), \tag{3.8}$$

and then by (3.6),

$$\lambda_+(t,x) - \lambda_-(t',x') \geqslant \delta_{\mathbb{I}} > 0, \tag{3.9}$$

where (t,x) (t',x') stand for two arbitrary points in the existence domain of classical solution. Thus, by Ref. 21, the Cauchy problem (2.54) and (3.5) has a unique global C^1 solution, still denoted by $(\lambda_-,\lambda_+)=(\lambda_-^{\mathbb{I}}(t,x),\lambda_+^{\mathbb{I}}(t,x))$, on the domain $\Delta_{\mathbb{I}}$; moreover it holds that

$$\sup_{(t,x)\in\Delta_{\mathbb{I}}} \lambda_\pm^{\mathbb{I}}(t,x) = \sup_{x\in\mathbb{I}} \Lambda_\pm(x), \qquad \inf_{(t,x)\in\Delta_{\mathbb{I}}} \lambda_\pm^{\mathbb{I}}(t,x) = \inf_{x\in\mathbb{I}} \Lambda_\pm(x) \tag{3.10}$$

and

$$\lambda_+^{\mathbb{I}}(t,x) - \lambda_-^{\mathbb{I}}(t',x') \geqslant \delta_{\mathbb{I}} > 0, \quad \forall\, (t,x),(t',x') \in \Delta_{\mathbb{I}}. \tag{3.11}$$

We next consider the Cauchy problem for the following linear system:

$$\frac{\partial R_i}{\partial t} + \lambda_+^{\mathbb{I}}(t,x)\frac{\partial R_i}{\partial x} = 0, \quad \frac{\partial R_{i+n}}{\partial t} + \lambda_-^{\mathbb{I}}(t,x)\frac{\partial R_{i+n}}{\partial x} = 0 \ (i=1,\ldots,n), \tag{3.12}$$

with the initial data

$$t=0: \begin{cases} R_i = g_i(x) + \Lambda_-(x) f_i'(x) \triangleq R_i^0(x) \\ R_{i+n} = g_i(x) + \Lambda_+(x) f_i'(x) \triangleq R_{i+n}^0(x) \end{cases} \quad (i=1,\ldots,n), \quad \forall\, x \in \mathbb{I}, \tag{3.13}$$

on the domain $\Delta_{\mathbb{I}}$, where f_i (resp., g_i) is the ith component of f (resp., g).

Noting the assumptions on $f(x)$ and $g(x)$, we have

$$\|R_j^0(x)\|_{C^1(\mathbb{I})} \leqslant c_{\mathbb{I}}' \quad (j=1,\ldots,2n), \tag{3.14}$$

where $c_{\mathbb{I}}'$ is a positive constant. On the other hand, noting (1.14) and (3.10), and using (2.30), we have

$$-1 \leqslant \lambda_\pm^{\mathbb{I}}(t,x) \leqslant 1, \quad \forall\, (t,x) \in \Delta_{\mathbb{I}}. \tag{3.15}$$

Thus, noting (3.14) and (3.15) and using the method of characteristics, we can easily prove that the Cauchy problem (3.12) and (3.13) has a unique global C^1 solution, denoted by $(R_1,\ldots,R_{2n})^T = (R_1^{\mathbb{I}}(t,x),\ldots,R_{2n}^{\mathbb{I}}(t,x))^T$, on the domain $\Delta_{\mathbb{I}}$.

By (2.52), the C^1 solution of the Cauchy problem (1.10) and (3.1a) on the domain $\Delta_{\mathbb{I}}$ is uniquely determined by

$$u_i = \frac{R_{i+n}^{\mathbb{I}}(t,x) - R_i^{\mathbb{I}}(t,x)}{\lambda_+^{\mathbb{I}}(t,x) - \lambda_-^{\mathbb{I}}(t,x)}, \quad v_i = \frac{\lambda_+^{\mathbb{I}}(t,x)R_i^{\mathbb{I}}(t,x) - \lambda_-^{\mathbb{I}}(t,x)R_{i+n}^{\mathbb{I}}(t,x)}{\lambda_+^{\mathbb{I}}(t,x) - \lambda_-^{\mathbb{I}}(t,x)} \ (i=1,\ldots,n). \tag{3.16}$$

Moreover, (3.4) comes from (3.11) directly. Thus, the proof of Theorem 1.2 is completed. ■

Remark 3.1: If (1.15) is not satisfied, then the solution must blow up in finite time and singularities will appear. In this case, the equation (1.7) loses the hyperbolicity at the points where $\lambda_+=\lambda_-$. *In geometry, this corresponds to the fact that the surface is no longer time-like at these points. In the forthcoming paper, we shall investigate the blowup phenomena of the solution.*

IV. GLOBAL EXISTENCE OF CLASSICAL SOLUTIONS OF THE DIRICHLET AND NEUMANN PROBLEMS

Here, we study the global existence of the classical C^2 solutions, $\phi=\phi(t,x)$, satisfying (1.7) on a time–space region of the form $[0,\infty)\times[0,L]$ and obeying either the Dirichlet boundary condition

$$\phi(t,x)\Big|_{x=L}^{x=0} = 0, \quad \text{for } t>0, \tag{4.1}$$

or the Neumann boundary condition

$$\frac{\partial \phi}{\partial x}(t,x)\Big|_{x=L}^{x=0} = 0, \quad \text{for } t > 0, \tag{4.2}$$

on the sidewalls, together with the initial conditions

$$\phi(0,x) = f(x), \quad \phi_t(0,x) = g(x), \tag{4.3}$$

where $(f,g) \in C^2([0,L]) \times C^1([0,L])$. In order for ϕ to belong to $C^2([0,\delta] \times [0,L])$ for arbitrarily small $\delta > 0$, the initial data f and g must necessarily satisfy the compatibility conditions

$$f(x)\Big|_{x=L}^{x=0} = f''(x)\Big|_{x=L}^{x=0} = 0, \quad g(x)\Big|_{x=L}^{x=0} = 0, \quad \text{for the Dirichlet conditions;} \tag{4.4}$$

$$\frac{\partial f}{\partial x}(t,x)\Big|_{x=L}^{x=0} = 0, \quad \frac{\partial g}{\partial x}(t,x)\Big|_{x=L}^{x=0} = 0, \quad \text{for the Neumann conditions.} \tag{4.5}$$

We have the following consequences of Theorem 1.2.

Theorem 4.1: (I) *Suppose that the compatibility conditions in (4.4) are satisfied and suppose furthermore that*

$$\min\{\inf_{x\in[0,L]} \Gamma_+(\pm f(x), g(x))\} > \max\{\sup_{x\in[0,L]} \Gamma_-(\pm f(x), g(x))\}, \tag{4.6}$$

where $\Gamma_\pm$ *are defined by*

$$\Gamma_\pm(\mu(x), \nu(x)) = \frac{1}{1+|\mu'(x)|^2}[-\langle \mu'(x), \nu(x)\rangle \pm \sqrt{\Delta(\mu'(x), \nu(x))}]. \tag{4.7}$$

Then the Dirichlet problem for (1.7) with the initial data (4.3) admits a unique global C^2 *solution* $\phi = \phi(t,x)$ *on* $[0,\infty) \times [0,L]$; *moreover, it holds that*

$$\Delta(\phi_x(t,x), \phi_t(t,x)) > 0, \quad \forall\, (t,x) \in [0,\infty) \times [0,L]. \tag{4.8}$$

(II) *Suppose that the compatibility conditions in (4.5) are satisfied and suppose furthermore that (4.6) holds. Then the Neumann problem for (1.7) with the initial data (4.3) admits a unique global* C^2 *solution* $\phi = \phi(t,x)$ *on* $[0,\infty) \times [0,L]$; *moreover, (4.8) still holds.*

Remark 4.1: As a special case, if

$$\Gamma_+(f(x), g(x)) > 0 > \Gamma_-(f(y), g(y)), \quad \forall\, x,y \in [0,L], \tag{4.6a}$$

then the hypothesis (4.6) *is satisfied, and then the conclusions of Theorem 4.1 hold.*

Proof of Theorem 4.1. For the Dirichlet problem for (1.7), we extend any C^2 solution $\phi = \phi(t,x)$ to the interval $[-L,L]$ by

$$\phi(t,x) = -\phi(t,-x), \quad \text{for } x \in [-L,0], \tag{4.9}$$

and then extend $\phi(t,x)$ to be $2L$ periodic. One easily checks that if the given initial data has the form in (4.3), the extended initial data is $2L$ periodic and given by

$$\tilde{f} \triangleq \phi(0,x) = \begin{cases} -f(-x), & \text{for } x \in [-L,0], \\ f(x), & \text{for } x \in [0,L], \end{cases} \qquad \tilde{g} \triangleq \phi_t(0,x) = \begin{cases} -g(-x), & \text{for } x \in [-L,0], \\ g(x), & \text{for } x \in [0,L]. \end{cases} \tag{4.10}$$

When the compatibility conditions in (4.4) are satisfied, this extended ϕ is a C^2 solution of (1.7) with the initial data $(\tilde{f}, \tilde{g})$. Therefore, under the assumptions of Theorem 4.1(I), we may make use of Theorem 1.2 and obtain the following lemma.

Lemma 4.1: Under the assumptions of Theorem 4.1(I), the Cauchy problem for (1.7) with the following $2L$*-periodic initial data:*

$$\phi(0,x)=\tilde{f}(x),\quad \phi_t(0,x)=\tilde{g}(x) \tag{4.11}$$

admits a unique global C^2 *solution* $\phi=\tilde{\phi}(t,x)$ *on* $\mathbb{R}^+\times\mathbb{R}$; *moreover, it holds that*

$$\Delta(\tilde{\phi}_x(t,x),\tilde{\phi}_t(t,x))>0,\quad \forall\,(t,x)\in\mathbb{R}^+\times\mathbb{R}. \tag{4.12}$$

Let $\phi(t,x)$ be the restriction of $\tilde{\phi}(t,x)$ on the region $[0,\infty)\times[0,L]$. It is obvious that $\phi(t,x)$ is the unique global C^2 solution of the Dirichlet problem for (1.7) with the initial data (4.3). On the other hand, (4.8) comes from (4.12) directly. This proves Theorem 4.1(I).

Similarly, for the Neumann problem, we extend ϕ by

$$\phi(t,x)=\phi(t,-x),\quad \text{for } x\in[-L,0]. \tag{4.13}$$

Then, $\phi(t,x)$ can be extended to be a classical $2L$-periodic C^2 solution of the equation (1.7) with $2L$-periodic initial data given by

$$\tilde{f}\equiv\phi(0,x)=\begin{cases} f(-x), & \text{for } x\in[-L,0],\\ f(x), & \text{for } x\in[0,L],\end{cases}\qquad \tilde{g}\equiv\phi_t(0,x)=\begin{cases} g(-x), & \text{for } x\in[-L,0],\\ g(x), & \text{for } x\in[0,L].\end{cases} \tag{4.14}$$

When the compatibility conditions in (4.5) are satisfied, by a similar argument as used above, we can prove Theorem 4.1(II). Thus, the proof of Theorem 4.1 is completed. ■

V. EXPLICIT EXACT REPRESENTATION OF GENERAL SOLUTIONS

In this section we present an explicit exact representation, involving two independent arbitrary functions, of general solution of the equation (1.7).

To do so, we consider the global C^2 solution of the Cauchy problem (1.7) and (1.13). As pointed out in Sec. III, the C^2 solution of the Cauchy problem (1.7) and (1.13) is equivalent to the C^1 solution of the Cauchy problem (1.10) and (3.1). Thus, it suffices to give an explicit exact representation of the C^1 solution of the Cauchy problem (1.10) and (3.1).

As before, throughout this section we assume that the condition (1.15) is satisfied.

We now solve the Cauchy problem for the system (2.54) with the following initial data:

$$t=0{:}\lambda_\pm=\Lambda_\pm(x). \tag{5.1}$$

Following Peng,[22] we define

$$Y_0(x)=\int_0^x\frac{2}{\Lambda_+(\xi)-\Lambda_-(\xi)}d\xi \tag{5.2}$$

and let $x=X_0(y)$ be the inverse function of $y=Y_0(x)$. Similarly, define

$$X(t,y)=\frac{1}{2}\int_0^{y+t}\Lambda_+(X_0(\xi))d\xi-\frac{1}{2}\int_0^{y-t}\Lambda_-(X_0(\xi))d\xi \tag{5.3}$$

and let $y=Y(t,x)$ be the inverse function of $x=X(t,y)$. Similar to Ref. 22, the solution of the Cauchy problem (2.54) and (5.1) can be explicitly given by

$$\lambda_\pm(t,x)=\Lambda_\pm(X_0(Y(t,x)\pm t)), \tag{5.4}$$

provided that the hypothesis (1.15) is satisfied.

We next solve the Cauchy problem for the following linear system:

$$\frac{\partial R_i}{\partial t}+\lambda_+(t,x)\frac{\partial R_i}{\partial x}=0,\quad \frac{\partial R_{i+n}}{\partial t}+\lambda_-(t,x)\frac{\partial R_{i+n}}{\partial x}=0\ (i=1,\ldots,n),\tag{5.5}$$

with the initial data

$$t=0:\begin{cases}R_i=g_i(x)+\Lambda_-(x)f_i'(x)\triangleq R_i^0(x),\\ R_{i+n}=g_i(x)+\Lambda_+(x)f_i'(x)\triangleq R_{i+n}^0(x)\end{cases}\quad (i=1,\ldots,n),\tag{5.6}$$

where $\lambda_\pm(t,x)$ are given by (5.4), and f_i and g_i are the ith component of f and g, respectively.

Consider the following initial value problems for ODEs:

$$\frac{d\zeta_\pm}{d\tau}=\lambda_\pm(\tau,\zeta_\pm(\tau)),\quad \zeta_\pm(t)=x.\tag{5.7}$$

Let $\zeta_\pm=\zeta_\pm(\tau;t,x)$ be the solutions of the above initial value problems and define

$$\alpha_\pm(t,x)=\zeta_\pm(0;t,x).\tag{5.8}$$

Noting (5.4) and using (2.54) yields

$$\alpha_\pm(t,x)=X_0(Y(t,x)\mp t).\tag{5.9}$$

By the method of characteristics, the solution of the Cauchy problem (5.5) and (5.6) is given by

$$R_i(t,x)=R_i^0(\alpha_+(t,x)),\quad R_{i+n}(t,x)=R_{i+n}^0(\alpha_-(t,x))\ (i=1,\ldots,n),\tag{5.10}$$

that is,

$$R_i(t,x)=R_i^0(X_0(Y(t,x)-t)),\quad R_{i+n}(t,x)=R_{i+n}^0(X_0(Y(t,x)+t))\ (i=1,\ldots,n).\tag{5.11}$$

Noting (1.15) and using (2.52), we obtain the solution of the Cauchy problem (1.10) and (3.1)

$$u_i=\frac{R_{i+n}(t,x)-R_i(t,x)}{\lambda_+(t,x)-\lambda_-(t,x)},\quad v_i=\frac{\lambda_+(t,x)R_i(t,x)-\lambda_-(t,x)R_{i+n}(t,x)}{\lambda_+(t,x)-\lambda_-(t,x)}\ (i=1,\ldots,n),\tag{5.12}$$

where $\lambda_\pm(t,x)$ and $R_j(t,x)(j=1,\ldots,2n)$ are given by (5.4) and (5.11), respectively. Therefore, the solution of the Cauchy problem (1.7) and (1.13) is

$$\phi(t,x)=f(x)+\int_0^t v(s,x)ds,\tag{5.13}$$

where $v=(v_1,\ldots,v_n)^T$ in which v_i are defined in (5.12). By the assumption (1.15), $\phi(t,x)$ is well defined for all $(t,x)\in\mathbb{R}\times\mathbb{R}$.

(5.13) gives an explicit exact representation, involving two independent arbitrary functions $f(x)$ and $g(x)$, of general solution of the equation (1.7), where $f(x)$ and $g(x)$ are chosen such that the condition (1.15) is satisfied.

Remark 5.1: The referee kindly points out that, using the hodograph transform, Barbashov and Chernikov[23] *derived the solution representation.*

VI. INHOMOGENEOUS DIRICHLET PROBLEM

Inhomogeneous Dirichlet problem for the equation (1.7) plays an important role in the Breniers theory (see Ref. 1) and other physical problems. In this section, we investigate the global existence of the classical C^2 solutions, $\phi=\phi(t,x)$, satisfying (1.7) on a time-space region of the form $[0,\infty)\times[0,L]$ and obeying inhomogeneous Dirichlet boundary conditions,

$$\phi(t,0)=\varphi_0(t),\quad \phi(t,L)=\varphi_L(t),\quad \text{for } t>0\tag{6.1}$$

on the sidewalls together with the initial conditions

$$\phi(0,x) = F(x), \quad \phi_t(0,x) = G(x), \quad \forall\, x \in [0,L], \tag{6.2}$$

where $F \in C^2([0,L])$ and $G \in C^1([0,L])$. In order for ϕ to belong to $C^2([0,\delta]\times[0,L])$ for arbitrarily small $\delta>0$, the initial data F and G must necessarily satisfy certain compatibility conditions (here we omit them).

Stimulated by (1.15), we assume that

$$\min_{x\in[0,L]} \tilde{\Lambda}_+(x) > \max_{x\in[0,L]} \tilde{\Lambda}_-(x), \tag{6.3}$$

where

$$\tilde{\Lambda}_\pm(x) = \frac{1}{1+|F'(x)|^2}[-\langle F'(x), G(x)\rangle \pm \sqrt{\Delta(F'(x), G(x))}]. \tag{6.4}$$

Define two functions on $\mathbb{R}$, still denoted by f and g, which satisfy the following:

$$(i)\ f \in C^2, \quad g \in C^1;$$

$$(ii)\ f(x) = F(x), \quad \text{on } [0,L]; \quad g(x) = G(x), \quad \text{on } [0,L];$$

$$(iii)\ \Lambda_+(x) > \Lambda_-(y), \quad \forall\, x,y \in \mathbb{R},$$

where $\Lambda_\pm(x)$ are defined by (1.14). Noting the condition (*iii*), for such functions f,g, we know that the Cauchy problem (1.7) and (1.13) has a unique global C^2 solution, moreover this solution can be explicitly exactly given by (5.13).

Definition 6.1: The boundary conditions (φ_0,φ_L) *are said to be globally solvable if there exist two functions f and g satisfying (i)–(iii), such that*

$$\phi(t,0) = \varphi_0(t), \quad \phi(t,L) = \varphi_L(t), \quad \text{for } t > 0, \tag{6.5}$$

where $\phi(t,x)$ *is defined by (5.13).*

Theorem 6.1: *Suppose that certain compatibility conditions and (6.3) are satisfied. Then the inhomogeneous Dirichlet problem (1.7), (6.1), and (6.2) has a unique global* C^2 *solution if and only if the boundary condition* (φ_0,φ_L) *is globally solvable.*

Proof: The sufficiency is obvious. In order to prove the necessity, it suffices to interchange the role of t and x variables, then solve two Cauchy problems that initial data are given on two half-lines, $x=0$ and $x=L$ with $t\geqslant 0$, respectively. After that, we can easily construct the desired functions f and g. Thus, the proof is completed. ■

Remark 6.1: For globally solvable boundary conditions (φ_0,φ_L), *the functions* (f,g) *may not be unique.*

Remark 6.2: It follows from Sec. IV that, under the hypotheses (4.4) and (4.6), the homogeneous boundary conditions (0,0) are globally solvable.

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Blow-up, blow-up rate and decay of the solution of the weakly dissipative Camassa-Holm equation

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In this paper, we mainly study several problems on the weakly dissipative periodic Camassa-Holm equation. At first, the local well-posedness of the equation is obtained by Kato's theorem, a necessary and sufficient condition of the blow-up of the solution and some criteria guaranteeing the blow-up of the solution are established. Then, the blow-up rate of the solution is discussed. Moreover, we prove that the equation has global solutions and these global solutions decay to zero as time goes to infinite provided the potentials associated to their initial date are of one sign. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2158437]

I. INTRODUCTION

The Camassa-Holm equation

$$u_t - u_{txx} + 3uu_x = 2u_x u_{xx} + uu_{xxx}, \quad t > 0,\ x \in \mathbf{R}$$

is a model for wave motion on shallow water, where $u(t,x)$ represents the fluid's free surface above a flat bottom (or equivalently, the fluid velocity at time $t \geqslant 0$ in the spatial x direction).

Since the equation was derived physically by Camassa and Holm (see Refs. 3 and 4), many researchers have paid extensive attention to it. The equation has a bi-Hamiltonian structure[15] and is completely integrable (see Refs. 1, 4, 6, and 16). Its solitary waves are peaked,[6] and they are orbitally stable and interact like solitons (see Refs. 2, 13, and 14). There are also numerous papers devoted recently to study this equation on the other issues, such as local well-posedness, global existence and blow-up of strong solutions, the existence and uniqueness of global weak solutions (see Refs. 5, 7–12, 18, 20, 21, 23–25, and 28, etc.).

In Ref. 11, Constantin and Escher give a quite detailed description of the blow-up phenomenon for the periodic Camassa-Holm equation. They find that the equation offers a very nice picture of the wave-breaking phenomena. Namely, if the maximal existence time $T < \infty$, they have

$$\lim_{t \to T} \left(\min_{x \in \mathbf{S}} \{u_x(t,x)\} \right) = -\infty$$

and the exact blow-up rate is

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$$\lim_{t\to T}\left((T-t)\min_{x\in\mathbf{S}}\{u_x(t,x)\}\right)=-2.$$

Furthermore, the authors show that for a large class of odd initial data the waves break at a discrete set of points and anything "bad" at breaking time is not observed elsewhere.

In general, it is difficult to avoid energy dissipation mechanisms in a real world. For example, Ott and Sudan[22] investigated how KdV equation was modified by the presence of dissipation and the effect of such dissipation on the solitary solution of KdV equation, and Ghidaglia[17] investigated the long time behavior of solutions to the weakly dissipative KdV equation as a finite-dimensional dynamical system.

Similarly, we would like to consider the dissipative Camassa-Holm equation,

$$u_t-u_{txx}+3uu_x+L(u)=2u_xu_{xx}+uu_{xxx},\quad t>0,\ x\in\mathbf{R},$$

where $L(u)$ is a dissipative term, L can be a differential operator or a quasidifferential operator according to different physical situations. We are interested in the effect of the weakly dissipative term on the Camassa-Holm equation. In the paper, we mainly consider the following weakly dissipative periodic Camassa-Holm equation:

$$y_t+uy_x+2u_xy+\lambda y=0,\quad t>0,\quad x\in\mathbf{R},$$

$$y=u-u_{xx},\quad t>0,\quad x\in\mathbf{R},$$

$$u(0,x)=u_0(x),\quad x\in\mathbf{R},$$

$$u(t,x+1)=u(t,x),\quad t>0,\quad x\in\mathbf{R},\tag{1.1}$$

where $\lambda y=\lambda(I-\partial_{xx})u$ is the weakly dissipative term, $\lambda>0$ is a constant, u_0 is a given periodic initial value.

We find that the behaviors of the equation (1.1) are similar to the Camassa-Holm equation in a finite interval of time, such as, the local well-posedness and the blow-up phenomena. But there are considerable differences between the equation (1.1) and the Camassa-Holm equation in their long time behaviors. Global solution of the equation (1.1) decays to zero as time goes to infinite provided the potential $y_0=(I-\partial_{xx})u_0$ is of one sign. This long time behavior is an important feature that the Camassa-Holm equation does not possess. It is well known that the Camassa-Holm equation has peaked traveling wave solutions. Lemma 2.2 in the sequel shows that any global solution decays in the H^1 norm. This means that there are no traveling wave solutions of the equation (1.1). This is also another considerable difference between the equation (1.1) and the Camassa-Holm equation in their long time behaviors.

It is very interesting that the equation (1.1) has the same blow-up rate as the Camassa-Holm equation does when the blow-up occurs. This fact shows that the blow-up rate of the Camassa-Holm equation are not affected by the weakly dissipative term. But the occurrence of blow-up of the equation (1.1) is affected by the dissipative parameter.

It should be noticed that the equation (1.1) does not have the conservation laws

$$I_1=\int_{\mathbf{S}}u\,\mathrm{d}x,\quad I_2=\int_{\mathbf{S}}(u^2+u_x^2)\mathrm{d}x,$$

which play an important role in the study of the Camassa-Holm equation.

II. LOCAL WELL-POSEDNESS AND BLOW-UP

We first state Kato's theorem so as to obtain the local well-posedness of the equation (1.1). Consider the abstract quasilinear evolution equation,

$$\frac{dv}{dt} + A(v)v = f(v), \quad t \geqslant 0, \quad v(0) = v_0. \tag{2.1}$$

Let X and Y be Hilbert spaces such that Y is continuously and densely embedded in X and let $Q: Y \to X$ be a topological isomorphism. $L(Y,X)$ denotes the space of all bounded linear operators from Y to X [$L(X)$, if $X=Y$]. Assume that

(i) $A(y) \in L(Y,X)$ for $y \in X$ with

$$\|(A(y) - A(z))w\|_X \leqslant \mu_1 \|y - z\|_X \|w\|_Y, \quad y,z,w \in Y,$$

and $A(y) \in G(X,1,\beta)$ [i.e., $A(y)$ is quasi-m-accretive], uniformly on bounded sets in Y.

(ii) $QA(y)Q^{-1} = A(y) + B(y)$, where $B(y) \in L(X)$ is bounded, uniformly on bounded sets in Y. Moreover,

$$\|(B(y) - B(z))w\|_X \leqslant \mu_2 \|y - z\|_Y \|w\|_X, \quad y,z \in Y, \quad w \in X.$$

(iii) $f: Y \to Y$ and extends also to a map from X into X. f is bounded on bounded sets in Y, and

$$\|f(y) - f(z)\|_Y \leqslant \mu_3 \|y - z\|_Y, \quad y,z \in Y,$$

$$\|f(y) - f(z)\|_X \leqslant \mu_4 \|y - z\|_X, \quad y,z \in Y.$$

Here μ_1, μ_2, μ_3, and μ_4 depend only on $\max\{\|y\|_Y, \|z\|_Y\}$.

Theorem 2.1 (*Kato's theorem*[19]*): Assume that* (*i*), (*ii*), *and* (*iii*) *hold. Given* $v_0 \in Y$, *there is a maximal* $T > 0$ *depending only on* $\|v_0\|_Y$ *and a unique solution* v *to Eq. (2.1) such that*

$$v = v(\cdot, v_0) \in C([0,T);Y) \cap C^1([0,T);X).$$

Moreover, the map $v_0 \mapsto v(\cdot, v_0)$ *is continuous from* Y *to* $C([0,T);Y) \cap C^1([0,T);X)$.

In order to apply Kato's theorem, we reformulate now Eq. (1.1).

First, we identify all spaces of periodic functions with function spaces over the unit circle **S** in **R**, where $\mathbf{S} = \mathbf{R}/\mathbf{Z}$; for simplicity, we drop **S** from our notation. Additionally, we denote by $\|\cdot\|_r$ the norm in the Sobolev spaces H^r, $r \geqslant 0$.

We note that if

$$G(x) = \frac{\cosh\left(x - [x] - \frac{1}{2}\right)}{2\sinh\left(\frac{1}{2}\right)},$$

here $[x]$ stands for the integer part of $x \in \mathbf{R}$, then $(1 - \partial_x^2)^{-1} f = G * f$ for all $f \in L^2(\mathbf{S})$ and $G * y = u$, we denote by * the convolution. Using this identity, we can rewrite the equation (1.1) as follows:

$$u_t + uu_x = -\partial_x\left(G * \left(u^2 - \lambda u_x + \tfrac{1}{2}u_x^2\right)\right) - \lambda G * u, \quad t > 0, \quad x \in \mathbf{R},$$

$$u(0,x) = u_0(x), \quad x \in \mathbf{R},$$

$$u(t,x+1) = u(t,x), \quad t > 0, \quad x \in \mathbf{R}, \tag{2.2}$$

or the equivalent form:

$$u_t + uu_x = -\partial_x(1 - \partial_x^2)^{-1}\left(u^2 - \lambda u_x + \tfrac{1}{2}u_x^2\right) - \lambda(1 - \partial_x^2)^{-1}u, \quad t > 0, \quad x \in \mathbf{R},$$

$$u(0,x) = u_0(x), \quad x \in \mathbf{R},$$

$$u(t,x+1)=u(t,x), \quad t>0, \quad x\in \mathbf{R}. \tag{2.3}$$

Set $A(u)=u\partial_x$, $f(u)=-\partial_x(1-\partial_x^2)^{-1}\left(u^2-\lambda u_x+\frac{1}{2}u_x^2\right)-\lambda(1-\partial_x^2)^{-1}u$, $Y=H^r$, $X=H^{r-1}$, $r>\frac{3}{2}$, and $Q=(1-\partial_x^2)^{\frac{1}{2}}$. Obviously, Q is an isomorphism of Y onto X. Analogous to the proofs in Ref. 26 or Ref. 27, we can prove that $A(u)$ and $f(u)$ satisfy the conditions (i)–(iii). Hence, we obtain the following theorem for the local well-posedness of Eq. (1.1) [or Eq. (2.3)].

Theorem 2.2: *Given $u_0\in H^r$, $r>\frac{3}{2}$, there exist a maximal $T=T(\lambda,\|u_0\|_r)>0$, and a unique solution u to Eq. (1.1) [or Eq. (2.3)], such that*

$$u=u(\cdot,u_0)\in C([0,T);H^r)\cap C^1([0,T);H^{r-1}),$$

and the solution depends continuously on the initial data, i.e., the mapping $u\to u(\cdot,u_0):H^r\to C([0,T);H^r)\cap C^1([0,T);H^{r-1})$ is continuous. Moreover, T may be chosen independent of r in the following sense: if

$$u=u(\cdot,u_0)\in C([0,T);H^r)\cap C^1([0,T);H^{r-1})$$

to Eq. (1.1), and if $u_0\in H^{r'}$ for some $r'\neq r$, $r'>\frac{3}{2}$, then

$$u\in C([0,T);H^{r'})\cap C^1([0,T);H^{r'-1})$$

with the same T.

The following results are only proved with regard to $r=3$, since we can obtain the same conclusion for general case $r>\frac{3}{2}$ by using denseness.

We prove now a necessary and sufficient condition of the blow-up of the solution for Eq. (1.1).

Theorem 2.3: *Given $u_0\in H^3$, the solution of Eq. (1.1) blows up in a finite time $T>0$ if and only if*

$$\lim_{t\uparrow T}\inf\left\{\inf_{x\in \mathbf{S}}[u_x(t,x)]\right\}=-\infty.$$

Proof: Notice that

$$\int_{\mathbf{S}} uyy_x\,dx=-\frac{1}{2}\int_{\mathbf{S}} u_xy^2\,dx, \quad \int_{\mathbf{S}} uy_xy_{xx}\,dx=-\frac{1}{2}\int_{\mathbf{S}} u_xy_x^2\,dx,$$

$$\int_{\mathbf{S}} u_{xx}yy_x\,dx=-\frac{1}{2}\int_{\mathbf{S}} u_xy^2\,dx.$$

Then, we have by Eq. (1.1),

$$\frac{d}{dt}\int_{\mathbf{S}} y^2\,dx=2\int_{\mathbf{S}} yy_t\,dx=-4\int_{\mathbf{S}} u_xy^2\,dx-2\int_{\mathbf{S}} uyy_x\,dx-2\lambda\int_{\mathbf{S}} y^2\,dx=-3\int_{\mathbf{S}} u_xy^2\,dx-2\lambda\int_{\mathbf{S}} y^2\,dx. \tag{2.4}$$

If $u_0\in H^4$, we can obtain by Eq. (1.1)

$$\begin{aligned}\frac{d}{dt}\int_{\mathbf{S}} y_x^2\,dx&=2\int_{\mathbf{S}} y_xy_{xt}\,dx=-4\int_{\mathbf{S}} u_{xx}yy_x\,dx-6\int_{\mathbf{S}} u_xy_x^2\,dx-2\int_{\mathbf{S}} uy_xy_{xx}\,dx-2\lambda\int_{\mathbf{S}} y_x^2\,dx\\&=-5\int_{\mathbf{S}} u_xy_x^2\,dx+2\int_{\mathbf{S}} u_xy^2\,dx-2\lambda\int_{\mathbf{S}} y_x^2\,dx.\end{aligned} \tag{2.5}$$

As for $u_0 \in H^3$, we will show that (2.5) still holds. In fact, we can approximate u_0 in H^3 by function $u_0^n \in H^4$. Moreover, we write $u^n = u^n(\cdot, u_0^n)$ for the solution of Eq. (1.1) with initial data u_0^n.

By Theorem 2.2, we know that

$$u^n \in C([0,T_n);H^4) \cap C^1([0,T_n);H^3), \quad n \geqslant 1,$$

$$y^n = u^n - u^n_{xx} \in C([0,T_n);H^2) \cap C^1([0,T_n);H^1), \quad n \geqslant 1,$$

$u^n \to u$ in H^3 and $T_n \to T$ as $n \to \infty$.

Due to $u_0^n \in H^4$, we have by (2.5)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbf{S}} (y_x^n)^2 \,\mathrm{d}x = -5\int_{\mathbf{S}} u_x^n (y_x^n)^2 \,\mathrm{d}x + 2\int_{\mathbf{S}} u_x^n (y^n)^2 \,\mathrm{d}x - 2\lambda \int_{\mathbf{S}} (y_x^n)^2 \,\mathrm{d}x.$$

Since $u^n \to u$ in H^3 as $n \to \infty$, it follows that $u_x^n \to u_x$ in L^∞ as $n \to \infty$. Note also that $y^n \to y$ in H^1 and $y_x^n \to y_x$ in L^2 as $n \to \infty$. Letting n go to infinity in the above equation, we can easily deduce that (2.5) holds for $u_0 \in H^3$.

Adding (2.4) and (2.5), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\mathbf{S}} y^2 \,\mathrm{d}x + \int_{\mathbf{S}} y_x^2 \,\mathrm{d}x\right) = -5\int_{\mathbf{S}} u_x y_x^2 \,\mathrm{d}x - \int_{\mathbf{S}} u_x y^2 \,\mathrm{d}x - 2\lambda\left(\int_{\mathbf{S}} y^2 \,\mathrm{d}x + \int_{\mathbf{S}} y_x^2 \,\mathrm{d}x\right). \tag{2.6}$$

If u_x is bounded from below on $[0,T)$, for example, $u_x \geqslant -k$, k is a positive constant, we get by (2.6) and Gronwall's inequality

$$\|y\|_1^2 \leqslant e^{(5k-2\lambda)t}\|y(0)\|_1^2,$$

it means that the H^3-norm of the solution u of Eq. (1.1) does not blow up in finite time. □

In the following, we provide two blow-up criteria for Eq. (1.1) guaranteeing the occurrence of this phenomenon.

Let us first introduce the following two useful lemmas:

Lemma 2.1 (Ref. 8): Let $T>0$ and $v \in C^1([0,T);H^2)$, then for every $t \in [0,T)$ there exists at least one point $\xi(t) \in \mathbf{S}$ with

$$m(t) := \inf_{x \in \mathbf{S}}[v_x(t,x)] = v_x(t,\xi(t)).$$

The function $m(t)$ is almost everywhere differentiable on $(0,T)$ with

$$\frac{\mathrm{d}m}{\mathrm{d}t} = v_{tx}(t,\xi(t)), \quad \text{a.e. on } (0,T).$$

Lemma 2.2: Let $u_0 \in H^1$, then, as long as the solution $u(t)$ given by Theorem 2.2 exists, we have

$$\|u\|_1^2 = e^{-2\lambda t}\|u_0\|_1^2, \quad \forall\, t \in [0,T).$$

Proof: Taking the scalar product of Eq. (1.1) with u in $L^2(\mathbf{S})$, and noting that

$$\int_{\mathbf{S}} u^2 y_x \,\mathrm{d}x + 2\int_{\mathbf{S}} u u_x y \,\mathrm{d}x = 0,$$

we obtain

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbf{S}}(u^2+u_x^2)dx+\lambda\int_{\mathbf{S}}(u^2+u_x^2)dx=0,$$

or

$$\frac{d}{dt}\|u\|_1^2+2\lambda\|u\|_1^2=0.$$

By integration between 0 and t, we have

$$\|u\|_1^2=e^{-2\lambda t}\|u_0\|_1^2,\quad \forall\, t\in[0,T).$$

Hence, the lemma is proved. □

Theorem 2.4: *Let $u_0\in H^3$, and assume that there exists $x_0\in\mathbf{S}$ such that*

$$u_0'(x_0)<-\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}.$$

Then the corresponding solution of Eq. (1.1) blows up in finite time.

Proof: Let $T>0$ be the existence time of the solution $u(t,\cdot)$ of Eq. (1.1) [or Eq. (2.2)] with the initial data u_0. Differentiating Eq. (2.2) with respect to x, we get

$$u_{tx}=-u_x^2-uu_{xx}-\partial_x^2G*\left(u^2+\tfrac{1}{2}u_x^2\right)-\lambda\partial_xG*(u-u_{xx}).$$

Note that

$$\partial_x^2G*\left(u^2+\tfrac{1}{2}u_x^2\right)=G*\left(u^2+\tfrac{1}{2}u_x^2\right)-\left(u^2+\tfrac{1}{2}u_x^2\right),\quad G*(u-u_{xx})=u.$$

Thus, we have

$$u_{tx}=-\tfrac{1}{2}u_x^2-uu_{xx}+u^2-G*\left(u^2+\tfrac{1}{2}u_x^2\right)-\lambda u_x. \tag{2.7}$$

We infer from Theorem 2.2 and Lemma 2.1 that for every $t\in[0,T)$, there exists at least one point $\xi(t)\in\mathbf{S}$ with $u_x(t,\xi(t))=\inf_{x\in\mathbf{S}}[u_x(t,x)]$. Let $m(t)=u_x(t,\xi(t))=\inf_{x\in\mathbf{S}}[u_x(t,x)]$, then $u_{xx}(t,\xi(t))=0$, $\forall t\in[0,T)$. Hence we have from (2.7)

$$\frac{dm}{dt}=-\frac{1}{2}m^2(t)+u^2(t,\xi(t))-\left[G*\left(u^2+\frac{1}{2}u_x^2\right)\right](t,\xi(t))-\lambda m(t)\quad \text{a.e. on } (0,T). \tag{2.8}$$

Note that $G*\left(u^2+\frac{1}{2}u_x^2\right)\geqslant 0$, $t\in[0,T)$, and (by the Sobolev imbedding theorem and Lemma 2.2)

$$\|u(t,\cdot)\|_{L^\infty}^2\leqslant\tfrac{1}{2}\|u(t,\cdot)\|_1^2\leqslant\tfrac{1}{2}\|u_0\|_1^2. \tag{2.9}$$

Then, we obtain

$$\frac{dm}{dt}\leqslant-\frac{1}{2}(m^2(t)+2\lambda m(t)-\|u_0\|_1^2)$$

$$=-\frac{1}{2}(m(t)+\lambda-\sqrt{\lambda^2+\|u_0\|_1^2})(m(t)+\lambda+\sqrt{\lambda^2+\|u_0\|_1^2}).$$

From the hypothesis, we have $m(0)<-\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}$, thus $dm/dt|_{t=0}<0$. By continuity with respect to t of $m(t)$, we have $dm/dt<0$, $\forall t\in[0,T)$. Therefore, $m(t)<-\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}$, $\forall t\in[0,T)$. So, we can solve the above inequality to obtain

$$\frac{m(0)+\lambda+\sqrt{\lambda^2+\|u_0\|_1^2}}{m(0)+\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}}e^{(\sqrt{\lambda^2+\|u_0\|_1^2}t)}-1\leqslant\frac{2\sqrt{\lambda^2+\|u_0\|_1^2}}{m(t)+\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}}\leqslant 0.$$

Since

$$0<\frac{m(0)+\lambda+\sqrt{\lambda^2+\|u_0\|_1^2}}{m(0)+\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}}<1,$$

there exists T,

$$T\leqslant\frac{1}{\sqrt{\lambda^2+\|u_0\|_1^2}}\ln\left(\frac{m(0)+\lambda-\sqrt{\lambda^2+\|u_0\|_1^2}}{m(0)+\lambda+\sqrt{\lambda^2+\|u_0\|_1^2}}\right),$$

such that $\lim_{t\uparrow T}m(t)=-\infty$. Hence, the above theorem is proved according to Theorem 2.3. □

Theorem 2.5: *Assume that* $u_0\in H^3$ *is odd,* $u_0'(0)<-2\lambda$. *Then the corresponding solution of Eq.* (1.1) *blows up infinite time.*

Proof: Let $T>0$ be the existence time of the solution $u(t,\cdot)$ of Eq. (1.1) [or Eq. (2.2)] with the initial data u_0. AS one can check, the function

$$v(t,x):=-u(t,-x),\quad t\in[0,T),\ x\in\mathbf{R},$$

is also a solution of Eq. (1.1) in $C([0,T);H^3)]\cap C^1([0,T);H^2)$ with initial data u_0. By uniqueness we conclude that $v\equiv u$ and therefore $u(t,\cdot)$ is odd for any $t\in[0,T)$. In particular, by continuity with respect to the spatial variable of u and u_{xx}, we get

$$u(t,0)=u_{xx}(t,0)=0,\quad t\in[0,T). \tag{2.10}$$

Define $g(t):=u_x(t,0)$ for $t\in[0,T)$ and note that $g\in C^1([0,T),\mathbf{R})$. From (2.7) and (2.10), we get

$$\frac{\mathrm{d}g}{\mathrm{d}t}(t)=-\frac{1}{2}g^2(t)-\lambda g(t)-\int_{\mathrm{S}}G(x-\eta)\left(u^2+\frac{1}{2}u_x^2\right)\mathrm{d}\eta$$

$$\leqslant-\frac{1}{2}(g(t)+2\lambda)g(t),\quad t\in[0,T).$$

From the hypothesis, we have $g(0)<-2\lambda$. Therefore, $g(t)<-2\lambda$, $\forall t\in[0,T)$. Solving the above inequality, we get

$$1-\frac{g(0)}{g(0)+2\lambda}e^{-\lambda t}\leqslant\frac{2\lambda}{g(t)+2\lambda}\leqslant 0.$$

Since

$$\frac{g(0)}{g(0)+2\lambda}>1,$$

we conclude that there exists T,

$$T\leqslant-\frac{1}{\lambda}\ln\frac{g(0)+2\lambda}{g(0)},$$

such that $\lim_{t\uparrow T}g(t)=-\infty$. We complete the proof of the above theorem by Theorem 2.3. □

III. BLOW-UP RATE

In this section, we give more insight into the blow-up mechanism for the wave-breaking solutions to Eq. (1.1).

Theorem 3.1: *Let $u_0 \in H^3$, and let $T>0$ be the maximal existence time of the corresponding solution to Eq. (1.1). If T is finite, we have*

$$\lim_{t\to T}(T-t)\min_{x\in\mathbf{S}} u_x(t,x) = -2.$$

Proof: We already know by Theorem 2.3 that

$$\liminf_{t\to T}\min_{x\in\mathbf{S}} u_x(t,x) = -\infty. \tag{3.1}$$

Define now $m(t) := \min_{x\in\mathbf{S}}[u_x(t,x)]$, $t\in[0,T)$, and let $\xi(t)\in\mathbf{S}$ be a point where this minimum is attained. Clearly $u_{xx}(t,\xi(t))=0$ since $u(t,\cdot)\in H^3\subset C^2$. From (2.8) we have

$$\frac{\mathrm{d}m}{\mathrm{d}t}+\frac{1}{2}m^2(t)+\lambda m(t) = u^2(t,\xi(t)) - \left[G*\left(u^2+\frac{1}{2}u_x^2\right)\right](t,\xi(t)) \quad \text{a.e. on } (0,T). \tag{3.2}$$

By Young's inequality and Lemma 2.2, we have for $t\in[0,T)$ that

$$\left\|G*\left(u^2+\frac{1}{2}u_x^2\right)(t,\cdot)\right\|_{L^\infty} \le \|G\|_{L^\infty}\left\|u^2+\frac{1}{2}u_x^2\right\|_{L^1} \le \frac{\cosh\left(\frac{1}{2}\right)}{2\sinh\left(\frac{1}{2}\right)}\|u(t,\cdot)\|_1^2 \le \frac{\cosh\left(\frac{1}{2}\right)}{2\sinh\left(\frac{1}{2}\right)}\|u_0\|_1^2. \tag{3.3}$$

Then, we infer from (2.9) and (3.3) that

$$\left|u^2(t,\xi(t)) - \left[G*\left(u^2+\frac{1}{2}u_x^2\right)\right](t,\xi(t))\right| \le \left(\frac{1}{2}+\frac{\cosh\left(\frac{1}{2}\right)}{2\sinh\left(\frac{1}{2}\right)}\right)\|u_0\|_1^2.$$

Set

$$K = \left(\frac{1}{2}+\frac{\cosh\left(\frac{1}{2}\right)}{2\sinh\left(\frac{1}{2}\right)}\right)\|u_0\|_1^2.$$

We infer from (3.2) that

$$-K \le \frac{\mathrm{d}m}{\mathrm{d}t}+\frac{1}{2}m^2(t)+\lambda m(t) \le K \quad \text{a.e. on } (0,T).$$

Hence,

$$-K-\frac{1}{2}\lambda^2 \le \frac{\mathrm{d}m}{\mathrm{d}t}+\frac{1}{2}(m(t)+\lambda)^2 \le K+\frac{1}{2}\lambda^2 \quad \text{a.e. on } (0,T). \tag{3.4}$$

Let $\epsilon\in\left(0,\frac{1}{2}\right)$. Since $\lim_{t\to T}\inf(m(t)+\lambda)=-\infty$ [by (3.1)], there is some $t_0\in(0,T)$ with $m(t_0)+\lambda<0$ and

$$(m(t_0)+\lambda)^2 > \frac{1}{\epsilon}\left(K+\frac{1}{2}\lambda^2\right).$$

We claim that

$$(m(t)+\lambda)^2 > \frac{1}{\epsilon}\left(K+\frac{1}{2}\lambda^2\right), \quad t \in [t_0,T). \tag{3.5}$$

In fact, since $m(t)$ is locally Lipschitz [it belongs to $W^{1,\infty}_{\mathrm{loc}}(\mathbf{R})$ by Lemma 2.1] there is some $\delta > 0$ such that

$$(m(t)+\lambda)^2 > \frac{1}{\epsilon}\left(K+\frac{1}{2}\lambda^2\right), \quad t \in (t_0,t_0+\delta).$$

From (3.4), we have

$$\frac{\mathrm{d}m}{\mathrm{d}t} < \left(\epsilon-\frac{1}{2}\right)(m(t)+\lambda)^2 < 0 \quad \text{a . e . on } (t_0,t_0+\delta).$$

Being locally Lipschitz, the function $m(t)$ is absolutely continuous. Therefore, by integrating the above relation on $[t_0,t_0+\delta]$, we obtain that $m(t_0+\delta) \leqslant m(t_0)$. Thus,

$$m(t_0+\delta)+\lambda \leqslant m(t_0)+\lambda < 0.$$

By the above inequality, we have

$$(m(t_0+\delta)+\lambda)^2 \geqslant (m(t_0)+\lambda)^2 > \frac{1}{\epsilon}\left(K+\frac{1}{2}\lambda^2\right).$$

The relation (3.5) is proved by continuous extension.

A combination of (3.4) and (3.5) enables us to infer

$$-\frac{1}{2}-\epsilon < \frac{\frac{\mathrm{d}m}{\mathrm{d}t}}{(m(t)+\lambda)^2} < -\frac{1}{2}+\epsilon \quad \text{a . e . on } (t_0,T). \tag{3.6}$$

For $t \in (t_0,T)$, integrating (3.6) on (t,T), we obtain

$$-\frac{1}{2}-\epsilon < \frac{1}{(m(t)+\lambda)(T-t)} < -\frac{1}{2}+\epsilon, \quad t \in (t_0,T).$$

Letting ϵ goes to zero, we obtain

$$\lim_{t\to T}[m(t)(T-t)+\lambda(T-t)] = -2,$$

that is

$$\lim_{t\to T}(T-t)m(t) = -2.$$

So, the proof of the above theorem is completed. □

Remark 3.1: Although the occurrence of blow-up of strong solutions to Eq. (1.1) is affected by the dissipative parameter (*see Theorems 2.4 and 2.5*), *Theorem 3.1 shows that the blow-up rate of strong solutions to the Camassa-Holm equation is not affected by the weakly dissipative term.*

IV. GLOBAL SOLUTION AND ITS DECAY

In this section we will show that there exist global strong solutions to the equation (1.1) provided the initial data u_0 satisfying certain sign conditions and some global solutions decay to zero at time goes to infinite provided the dissipative parameter being in a certain range.

Given a strong solution u to Eq. (1.1) with initial data $u_0 \in H^3$ and with maximal existence time $T>0$, we can associate it with the differential equation

$$q_t = u(t,q), \quad t \in (0,T),$$

$$q(0,x)=x, \quad x\in \mathbf{R}. \tag{4.1}$$

Lemma 4.1: Let $u_0\in H^3$ and let $T>0$ be the maximal existence time of the corresponding solution u to Eq. (1.1). *Then Eq.* (4.1) *has a unique solution $q\in C^1([0,T)\times\mathbf{R},\mathbf{R})$. Moreover, for each fixed $t\in[0,T)$, the map $q(t,\cdot)$ in an increasing diffeomorphism of $\mathbf{R}$ with $q_x(t,x)>0$ for $(t,x)\in[0,T)\times\mathbf{R}$.*

The proof of the above lemma is similar to the proof of Lemma 2 in Ref. 11, so we omit it.□

Lemma 4.2: Let $u_0\in H^3$ and let $T>0$ be the maximal existence time of the corresponding solution u to (1.1). *Then we have*

$$y(t,q(t,x))q_x^2(t,x)=y_0(x)e^{-\lambda t},$$

where $y_0=u_0-\partial_x^2u_0$.

Proof: Differentiation of the system (4.1) with respect to x yields

$$\frac{d}{dt}q_x=u_x(t,q)q_x, \quad t\in(0,T),$$

$$q_x(0,x)=1, \quad x\in\mathbf{R}. \tag{4.2}$$

Let $p(t,x)=y(t,q(t,x))q_x^2(t,x)$, and we infer from (1.1) and (4.1) and (4.2) that

$$\frac{d}{dt}p(t,x)=-\lambda p(t,x),$$

we integrate the above relation between 0 and t and complete the proof. □

Theorem 4.1: *Assume that $u_0\in H^3$ does not change sign ($y_0\geqslant 0$ or $y_0\leqslant 0$ on $\mathbf{S}$), then the corresponding solution u to (1.1) exists globally. Moreover, the global solution decays to 0 as time goes to infinite.*

Proof: We consider first the case when $y_0(x)\geqslant 0$, $x\in\mathbf{S}$. Let $T>0$ be the existence time of the solution u with initial data u_0 given by Theorem 2.2. By Lemma 4.2, we obtain for $t\in[0,T)$ that $y(t,x)\geqslant 0$, $x\in\mathbf{S}$.

From Sec. II we know that

$$u(t,x)=\int_{\mathbf{S}}G(x-\eta)y(t,\eta)\,d\eta, \quad (t,x)\in[0,T)\times\mathbf{S},$$

where $G(x):=\cosh\left(x-[x]\frac{1}{2}\right)/2\sinh\left(\frac{1}{2}\right)$, $x\in\mathbf{S}$.

Fix $(t,x)\in[0,T)\times\mathbf{S}$ and let $\sigma:=1/4\sinh\left(\frac{1}{2}\right)$. We have

$$\begin{aligned}u(t,x)=&\sigma e^x\int_0^x e^{-\eta-1/2}y(t,\eta)\,d\eta+\sigma e^{-x}\int_0^x e^{\eta+1/2}y(t,\eta)\,d\eta+\sigma e^x\int_x^1 e^{-\eta+1/2}y(t,\eta)\,d\eta\\&+\sigma e^{-x}\int_x^1 e^{\eta-1/2}y(t,\eta)\,d\eta.\end{aligned} \tag{4.3}$$

Differentiation with respect to x yields for $(t,x)\in[0,T)\times\mathbf{S}$,

$$\begin{aligned}u_x(t,x)=&\sigma e^x\int_0^x e^{-\eta-1/2}y(t,\eta)\,d\eta-\sigma e^{-x}\int_0^x e^{\eta+1/2}y(t,\eta)\,d\eta+\sigma e^x\int_x^1 e^{-\eta+1/2}y(t,\eta)\,d\eta\\&-\sigma e^{-x}\int_x^1 e^{\eta-1/2}y(t,\eta)\,d\eta.\end{aligned} \tag{4.4}$$

From (4.3) and (4.4), (2.9) and Lemma 2.2, we infer that

$$-u_x(t,x) \leqslant u(t,x) \leqslant \|u\|_{L^\infty} \leqslant \frac{e^{-\lambda t}}{\sqrt{2}}\|u_0\|_1. \tag{4.5}$$

So, by Theorem 2.3 we know that $T=\infty$.

By (4.5), we obtain that $-u_x \leqslant \lambda/5$ for sufficiently large t. This yields in combination with (2.6) and Gronwall's inequality,

$$\|y\|_1^2 \leqslant Ce^{-\lambda t}$$

for large t, where C is a positive constant. Hence, the second conclusion of the above theorem is proved.

For the case when $y_0(x) \leqslant 0$, $x \in \mathbf{S}$, we can repeat the above proof to get the desired result.□

Remark 4.1: Note that the global solution to the Camassa-Holm equation does not generally decay to zero as time goes to infinite. Theorem 4.1 shows that there is a considerable difference between the equation (1.1) and the Camassa-Holm equation in their long time behaviors. More precisely, the energy dissipation will affect the long time behavior of global solutions to the Camassa-Holm equation.

Remark 4.2: It is well-known the Camassa-Holm equation has peaked traveling wave solutions. Theorem 4.1 shows that global H^3 solutions with y_0 of one sign decay in the H^3 norm. Lemma 2.2 shows that any global solution decays in the H^1 norm. This means that there are no traveling wave solutions of the dissipative equation (1.1) . This is also another considerable difference between the equation (1.1) and the Camassa-Holm equation in their long time behaviors.

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The approximation of the transmutation kernel

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The transformation operator plays an important role in the direct and inverse spectral theory of Sturm-Liouville operators. In this paper we would like to approximate the kernel of the transformation operator used in the Gelfand-Levitan theory. The analytic properties of the solution allows for its representation by either a Taylor series about the diagonal or a Fourier cosine series. Example illustrating how the coefficients can be computed are provided. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2159067]

I. INTRODUCTION

We are concerned with the approximation of the kernel $K(x,t)$ appearing in the transformation operator[2–4,6,7]

$$y(x,\lambda)=\cos(x\lambda)+\int_0^x K(x,t)\cos(t\lambda)\mathrm{d}t, \tag{1.1}$$

where y is the eigensolution of the singular Sturm-Liouville operator L,

$$\begin{gathered} L(y):=-y''(x,\lambda)+q(x)y(x,\lambda)=\lambda^2 y(x,\lambda), \quad x\in[0,\infty), \\ hy(0,\lambda)-y'(0,\lambda)=0. \end{gathered} \tag{1.2}$$

The transformation operator $1+\mathbf{K}$ in (1.1) links the eigensolutions of (1.2) to $\cos(x\lambda)$ which are also eigensolutions of (1.2) when $q=h=0$. Its kernel K stores all the spectral information of the operator L (1.2) and consequently plays a fundamental role in the direct and inverse spectral theory of L.[6] For example, the Gelfand-Levitan theory is based on the solution of the linear integral equation which is defined by

$$F(x,t)+\int_0^x K(x,s)F(s,t)\mathrm{d}s=-K(x,t), \tag{1.3}$$

where

$$F(x,t)=\int_0^\infty \cos(x\lambda)\cos(t\lambda)\mathrm{d}\sigma(\lambda^2)+\int_{-\infty}^0 \cosh(x\lambda)\cosh(t\lambda)\mathrm{d}\rho(-\lambda^2) \tag{1.4}$$

and $\sigma(\lambda)=\rho(\lambda)-(2/\pi)\sqrt{\lambda_+}$. In (1.4), the measure ρ is the spectral function of the operator L in (1.2), and its support is the spectrum of the operator. If ρ is absolutely continuous and supp $\rho\subset[0,\infty)$ then

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$$\left(2\lambda\rho'(\lambda^2)-\frac{2}{\pi}\right)\cos(t\lambda)=\frac{2}{\pi}\int_0^\infty F(x,t)\cos(x\lambda)\mathrm{d}x \tag{1.5}$$

and letting $t\to 0$, formally yields

$$\lambda\rho'(\lambda)=\frac{1}{\pi}+\frac{1}{\pi}\int_0^\infty F(x,0)\cos(x\lambda)\mathrm{d}x. \tag{1.6}$$

A more direct method using operational calculus and the kernel of the inverse transmutation can be found in Ref. 1. Thus the first step towards computing the function F, ρ or the solution $y(x,\lambda)$ is obviously to start with the kernel K, which is the main objective of this paper.

Another possible application of (1.1) is to express the solution of a singular Sturm-Liouville operator,

$$\begin{gathered}-\varphi''(x)+q(x)\varphi(x)=f(x),\quad \text{where } x\geqslant 0,\\ \varphi(0)=1\quad\text{and}\quad \varphi'(0)=h.\end{gathered} \tag{1.7}$$

Since $(1+\mathbf{K})$ is a transmutation,[3] we have

$$[-D^2+q(x)](1+\mathbf{K})=(1+\mathbf{K})(-D^2)$$

and the solution of (1.7) is then given by $\varphi(x)=(1+\mathbf{K})s(x)$ where $-s''(x)=(1+\mathbf{K})^{-1}f$. Once the operators $(1+\mathbf{K})$ and its inverse are known, the solution φ can be computed symbollically.

The Fourier transform provides yet another way for (1.7). Define $\varphi(x)=\int_0^\infty(1/\lambda)\hat{f}(\lambda)y(x,\lambda)\mathrm{d}\rho(\lambda)$, where $\hat{f}(\lambda)=\int_0^\infty f(x)y(x,\lambda)\mathrm{d}x$, $y(x,\lambda)$ is given by (1.1) and ρ by (1.5). Thus there are many ways where the kernel K can be used to solve computational problems related to the Sturm-Liouville theory.

Recall that Povzner and Marchenko,[7] to prove the existence of the kernel K, used a fixed point argument, since the kernel K solves a hyperbolic equation,

$$\begin{gathered}\frac{\partial^2}{\partial x^2}K(x,t)-\frac{\partial^2}{\partial t^2}K(x,t)=q(x)K(x,t),\quad 0\leqslant t\leqslant x,\\ \frac{\mathrm{d}}{\mathrm{d}x}K(x,x)=\frac{1}{2}q(x),\\ \frac{\partial}{\partial t}K(x,0)=0.\end{gathered}$$

Unfortunately, the idea of successive approximations cannot easily be implemented numerically, since the iterates involve two-dimensional integrals. Finite differences also are difficult to use since the domain is a sector.

We briefly mention a different numerical method of approximating ρ directly by Fulton and Pruess.[5] Their algorithm approximates ρ by step functions by computing the integral $\int_0^N|y(x,\lambda)|^2\,\mathrm{d}x$ for large values of N. For example, if λ belongs to the continuous spectrum then we know that $\lim_{N\to\infty}\int_0^N|y(x,\lambda)|^2\,\mathrm{d}x=\infty$ and so $\rho(\lambda+)-\rho(\lambda-)=(\lim_{N\to\infty}\int_0^N|y(x,\lambda)|^2\,\mathrm{d}x)^{-1}=0$, i.e., ρ is continuous. On the other hand, if λ is an eigenvalue then $\rho(\lambda+)-\rho(\lambda-)=(\lim_{N\to\infty}\int_0^N|y(x,\lambda)|^2\,\mathrm{d}x)^{-1}\neq 0$ and so ρ has a jump at λ. This idea can also be implemented by our method since we approximate symbollically the solution $y(x,\lambda)$ when $\lambda\neq 0$.

II. PRELIMINARIES

We first prove the following.

Proposition 1: *Assume that* $q^{(m)}\in L^{\mathrm{loc}}[0,\infty)$ *for* $m\geqslant 1$, *then there exists* α_k *and* β_k *such that*

$$y(x,\lambda)=\cos(x\lambda)\sum_{k=0}^{[m/2]}\frac{\alpha_k(x)}{\lambda^{2k}}+\sin(x\lambda)\sum_{k=0}^{[(m-1)/2]}\frac{\beta_k(x)}{\lambda^{2k+1}}+\frac{1}{\lambda^{m+1}}\epsilon(x,m+1,\lambda), \tag{2.1}$$

where $\alpha_k^{(m+2-2k)}$, $\beta_k^{(m+1-2k)}\in L^{\mathrm{loc}}[0,\infty)$ *and* $\epsilon(x,m+1,\lambda)=o(1)$ *as* $\lambda\to\infty$.

Proof: From the Gelfand-Levitan-Gasymov theorem we recall that,[6] if $q^{(m)}\in L^{\mathrm{loc}}[0,\infty)$ then $\partial_t^{m+1}K(x,.)\in L(0,x)$. Thus for each fixed x, we can integrate by parts at least m times in t, say $m=2n+1$ is odd,

$$\begin{aligned}\int_0^x K(x,t)\cos(t\lambda)\mathrm{d}t &= K(x,x)\frac{1}{\lambda}\sin(x\lambda)-K_t(x,x)\frac{1}{\lambda^2}\cos(x\lambda)+K_t(x,0)\frac{1}{\lambda^2}-\int_0^x K_{tt}(x,t)d\frac{1}{\lambda^3}\sin(t\lambda)\\ &=\cos(x\lambda)\sum_{k=0}^{2n}\frac{\alpha_k(x)}{\lambda^{2k}}+\sin(x\lambda)\sum_{k=1}^{2n}\frac{\beta_k(x)}{\lambda^{2k+1}}+\sum_{k=1}^{2n}\frac{\gamma_k(x)}{\lambda^{2k}}\\ &\quad+\frac{1}{\lambda^{2n+2}}\int_0^x\frac{\partial^{2n+2}}{\partial t^{2n+2}}K(x,t)\cos(t\lambda)\mathrm{d}t.\end{aligned} \tag{2.2}$$

Clearly, by Riemann-Lebesgue's theorem, we have

$$\epsilon(x,m+1,\lambda)=\int_0^x\frac{\partial^{m+1}}{\partial t^{m+1}}K(x,t)\cos(t\lambda)\mathrm{d}t=o(1)\quad\text{as }\lambda\to\infty\,. \tag{2.3}$$

From (2.2), $\sin(x\lambda)$ appears with odd powers of $1/\lambda$ while $\cos(x\lambda)$ with even powers of $1/\lambda$. If we denote by

$$\beta_k(x)=(-1)^k\frac{\partial^{2k}}{\partial t^{2k}}K(x,x)\quad\text{and}\quad\alpha_k(x)=(-1)^k\frac{\partial^{2k-1}}{\partial t^{2k-1}}K(x,x) \tag{2.4}$$

then $\alpha_k^{(m+2-2k)}$, $\beta_k^{(m+1-2k)}\in L^{\mathrm{loc}}[0,\infty)$. The next step we need to show that in (2.2),

$$\gamma_{2k}(x)=\frac{\partial^{2k-1}}{\partial t^{2k-1}}K(x,0)=0$$

for $k=0,\ldots,m$. This can be done directly by looking at the linear integral equation (1.3). Since $(\partial^{2k+1}/\partial t^{2k+1})F(x,t)=(-1)^k\lambda^{2k+1}\int\cos(x\lambda)\sin(t\lambda)\mathrm{d}\sigma(\pm\lambda^2)$ we have $(\partial^{2k+1}/\partial t^{2k+1})F(x,0)=0$ and hence (1.3) implies

$$\frac{\partial^{2k+1}}{\partial t^{2k+1}}K(x,0)=0\Rightarrow\gamma_{2k}(x)=0. \tag{2.5}$$

By checking (2.2) when m is even, we deduce the upper bounds of the sum in (2.1). □

Remark: In Ref. 8, Sec. 2.8, Olver works out a formal infinite series solution, which is similar to (2.1), with $\exp(x\lambda)$ instead of $\sin(x\lambda)$ and $\cos(x\lambda)$. However the Gelfand-Levitan theory makes the argument plain and explains how the number of terms in the expansion depends on the smoothness of q, and thus cannot in general be an infinite series; moreover it yields an explicit error term.

III. COMPUTING THE COEFFICIENTS α_k, β_k

Equation (2.4) shows that we can recover the partial derivative of K, if we can compute the coefficients α_k, β_k. To this end use the fact that

$$L(fg)=-f''g-2f'g'+fLg$$

to obtain

$$L(\cos(x\lambda)\alpha_n) = \lambda^2 \cos(x\lambda)\alpha_n + 2\lambda \sin(x\lambda)\alpha_n' + \cos(x\lambda)L\alpha_n,$$

$$L(\sin(x\lambda)\beta_n) = \lambda^2 \sin(x\lambda)\beta_n - 2\lambda \cos(x\lambda)\beta_n' + \sin(x\lambda)L\beta_n.$$

Thus from (2.1), it follows

$$\begin{aligned} Ly &= \cos(x\lambda)\sum_{n=0}^{N}\left(\frac{\alpha_n}{\lambda^{2n-2}} + \frac{L\alpha_n - 2\beta_n'}{\lambda^{2n}}\right) + \sin(x\lambda)\sum_{n=0}^{N}\left(\frac{\beta_n + 2\alpha_n'}{\lambda^{2n-1}} + \frac{L\beta_n}{\lambda^{2n+1}}\right) \\ &= \cos(x\lambda)\sum_{n=0}^{N}\left(\frac{\alpha_n - 2\beta_{n-1}' + L\alpha_{n-1}}{\lambda^{2n-2}}\right) + \sin(x\lambda)\sum_{n=0}^{N}\left(\frac{\beta_n + 2\alpha_n' + L\beta_{n-1}}{\lambda^{2n-1}}\right) \end{aligned} \tag{3.1}$$

with the understanding that $\alpha_{-1}=\beta_{-1}=0$. Since

$$Ly = \lambda^2 y = \cos(x\lambda)\sum_{n=0}^{N-2}\frac{\alpha_n}{\lambda^{2n-2}} + \sin(x\lambda)\sum_{n=0}^{N-2}\frac{\beta_n}{\lambda^{2n-1}} \tag{3.2}$$

by identifying the different coefficients in (3.1) and (3.2), we end up with for $n \geqslant 1$,

$$-2\beta_{n-1}' + L\alpha_{n-1} = 0$$

$$2\alpha_n' + L\beta_{n-1} = 0$$

or

$$\beta_{n-1}(x) = \beta_{n-1}(0) + \frac{1}{2}\int_0^x L\alpha_{n-1}(t)\mathrm{d}t,$$

$$\alpha_n(x) = \alpha_n(0) - \frac{1}{2}\int_0^x L\beta_{n-1}(t)\mathrm{d}t.$$

The constants $\alpha_n(0)$ and $\beta_n(0)$ are obtained from the asymptotic behavior of y (1.2),

$$y(x,\lambda) = 1 + xh + o(x^2) \quad \text{as } x \to 0$$

while the representation (2.1) as $x \to 0$, reduces to

$$y(x,\lambda) \approx \sum_{n=0}\frac{\alpha_n(0)}{\lambda^{2n}} + x\sum_{n=0}\frac{\beta_n(0)}{\lambda^{2n}},$$

$$\alpha_0(0) = 1, \quad \beta_0(0) = h, \tag{3.3}$$

$$\alpha_n(0) = 0 \quad \text{and} \quad \beta_n(0) = 0 \quad \text{for } n \geqslant 1.$$

The algorithm is easy to see, taking into account that $\alpha_{-1}=\beta_{-1}=0$,

$$\begin{aligned} &\alpha_0(x) = 1 && \alpha_1(x) = -\frac{1}{2}\int_0^x L\beta_0(t)\mathrm{d}t && \alpha_2(x) = -\frac{1}{2}\int_0^x L\beta_1(t)\mathrm{d}t \\ &\beta_0(x) = h + \frac{1}{2}\int_0^x q(x)\mathrm{d}t \Rightarrow && \beta_1(x) = \frac{1}{2}\int_0^x L\alpha_1(t)\mathrm{d}t && \Rightarrow \quad \beta_2(x) = \frac{1}{2}\int_0^x L\alpha_2(t)\mathrm{d}t \end{aligned} \tag{3.4}$$

$$\beta_n(x) = \frac{1}{2}\left(\alpha_n'(0) - \alpha_n'(x) + \int_0^x q(t)\alpha_n(t)\mathrm{d}t\right).$$

$$\alpha_n(x) = \frac{-1}{2}\left(\beta_{n-1}'(0) - \beta_{n-1}'(x) + \int_0^x q(t)\beta_{n-1}(t)\mathrm{d}t\right),$$

In this case we need only one derivation and a simple integration that could be performed symbolically. For a faster algorithm, we can combine both sequences (α_n) and (β_n) into one

$$\alpha_0 \to \beta_0 \to \alpha_1 \to \beta_1 \to \alpha_2 \to \beta_2 \to \cdots \to \alpha_n \to \beta_n \to \alpha_{n+1} \to \cdots .$$

Let $\{c_n\}$ be a new sequence defined by

$$c_{2n}(x) = \alpha_n(x) \quad \text{while } c_{2n+1}(x) = \beta_n(x)$$

then it can be defined recursively for $n \geqslant 3$ by

$$c_n(x) = \frac{(-1)^{n-1}}{2}\int_0^x Lc_{n-1}(t)\mathrm{d}t. \tag{3.5}$$

Proposition 1 reduces to the following.

Proposition 2: *Assume that* $q^{(m)} \in L^{\mathrm{loc}}[0,\infty)$ *for* $m \geqslant 1$, *then*

$$y(x,\lambda) = \cos(x\lambda)\sum_{k=0}^{[m/2]}\frac{c_{2k}(x)}{\lambda^{2k}} + \sin(x\lambda)\sum_{k=0}^{[(m-1)/2]}\frac{c_{2k+1}(x)}{\lambda^{2k+1}} + \frac{1}{\lambda^{m+1}}\epsilon(x,m+1,\lambda), \tag{3.6}$$

where $\epsilon(x,m+1,\lambda) = o(1)$ *as* $\lambda \to \infty$ *and the sequence* c_n *can be computed iteratively by* (3.5).

Since our solution starts with $\cos(x\lambda)$, we have $c_0(x) = 1$ while $c_1(x) = h + \int_0^x q(t)\mathrm{d}t$. The second independent solution, can be generated by

$$\varphi(0,\lambda) = 0 \quad \text{and} \quad \varphi'(0,\lambda) = 1$$

represented by[6]

$$\varphi(x,\lambda) = \frac{\sin(x\lambda)}{\lambda} + \int_0^x L(x,t)\frac{\sin(t\lambda)}{\lambda}\mathrm{d}t,$$

and so by comparing with (2.1), we see that it starts with $\sin(x\lambda)/\lambda$, which means $c_0(x) = 0$ and $c_1(x) = 1$.

Having the coefficients c_k we now show how to approximate the kernel $K(x,t)$ close to the region $x = t$.

Proposition 3: *Assume that* $q^{(m)} \in L^{\mathrm{loc}}(0,\infty)$, *then the kernel K can be approximated by*

$$K(x,t) = \sum_{n=0}^{m} a_n(x)\frac{1}{n!}(x-t)_+^n + \epsilon_m(x,t),$$

where

$$\alpha_{2k}(x) = (-1)^k c_{2k+1}(x), \quad \alpha_{2k-1}(x) = (-1)^k c_{2k}(x),$$

and the remainder

$$\epsilon_m(x,t) = (1/m\,!)\int_x^t \partial_t^{m+1}K(x,n)(t-\eta)^m\mathrm{d}\eta.$$

Proof: Since $\partial_t^{m+1}K(x,\eta)\in L(0,x)$, for any fixed $x>0$, its Taylor expansion yields for $0\leqslant t\leqslant x$,

$$K(x,t)=\sum_{n=0}^{m}\partial_t^n K(x,x)\frac{1}{n!}(x-t)_+^n+\epsilon_m(x,t).$$

The functions $\partial_t^n K(x,x)$ were already found in terms of α_k and β_k (2.4). □

IV. THE COSINE SERIES

For any fixed $x>0$, we can recover $K(x,t)$, which is continuous for $t\in(0,x)$, by a cosine series expansion

$$K(x,t)=\frac{1}{2}\hat{K}(x,0)+\sum_{n\geqslant 1}\hat{K}(x,n)\cos\left(nt\frac{\pi}{x}\right)\quad\text{for } t\in(0,x),$$

where the Fourier coefficients are readily available when $n\neq 0$,

$$\begin{aligned}\hat{K}(x,n)&=\frac{2}{x}\int_0^x K(x,t)\cos\left(tn\frac{\pi}{x}\right)\mathrm{d}t=\frac{2}{x}\left[y\left(x,n\frac{\pi}{x}\right)-\cos(n\pi)\right]=\frac{2}{x}\cos(n\pi)\sum_{j=1}^{[m/2]}\frac{c_{2j}(x)}{\left(n\frac{\pi}{x}\right)^{2j}}\\&+\frac{2}{x}\frac{x^{m+1}}{(n\pi)^{m+1}}\epsilon\left(x,m+1,n\frac{\pi}{x}\right)=(-1)^n 2\sum_{j=1}^{[m/2]}\frac{c_{2j}(x)}{(n\pi)^{2j}}x^{2j-1}+\frac{2x^m}{n^{m+1}\pi^{m+1}}\epsilon\left(x,m+1,n\frac{\pi}{x}\right),\end{aligned}\tag{4.1}$$

where $\epsilon(x,m+1,n(\pi/x))=o(1)$ as $n\to\infty$ is the truncation error defined by (2.3). For the remaining coefficient $n=0$, use

$$\frac{1}{2}\hat{K}(x,0)=\frac{1}{x}(y(x,0)-1)$$

which can be easily computed independently since it does not contain the parameter λ. For example, successive approximations to solve

$$y(x,0)=1+xh+\int_0^x(x-t)q(t)y(t,0)\mathrm{d}t\tag{4.2}$$

yields (4.2), $y(x,0)=1+xh+\int_0^x(x-t)q(t)(1+th)\mathrm{d}t+\cdots$.

Proposition 4: *If* $q^{(m)}\in L^{\mathrm{loc}}[0,\infty)$, *then the kernel* K *can be approximated for* $t\in(0,x)$, $x>0$ *by*

$$K(x,t)=\frac{1}{x}(y(x,0)-1)+\sum_{n\geqslant 1}(-1)^n 2\sum_{j=1}^{[m/2]}\frac{c_{2j}(x)}{(n\pi)^{2j}}x^{2j-1}\cos\left(nt\frac{\pi}{x}\right)+C(m),$$

where

$$C(m)=\sum_{n\geqslant 1}\frac{2x^m}{n^{m+1}\pi^{m+1}}\epsilon\left(x,m+1,n\frac{\pi}{x}\right)\cos\left(nt\frac{\pi}{x}\right)\to 0\quad\text{as } m\to\infty.$$

The kernel can then be approximated by combining (4.1) and a solution of (4.2),

$$K(x,t)=\frac{1}{2}\hat{K}(x,0)+\sum_{n\geqslant 0}\hat{K}(x,n)\cos\left(nt\frac{\pi}{x}\right).$$

Observe that a simple formula can be obtained from the convergence of the Fourier series at the endpoint $t=x$.

Corollary 1: *We have*

$$K(x,0)=-h-1-\frac{1}{2}\int_0^x q(\eta)\mathrm{d}\eta+y(x,0)+\frac{4}{x}\sum_{n\geqslant 0}(-1)^n\left(y\left(x,n\frac{\pi}{x}\right)-\cos(xn)\right).$$

V. EXAMPLES

It is enough to see that the true solution $y(x,\lambda)$ and its approximation are close for $\lambda>0$.

Example 1: Consider $-y''+\cos(x)y=\lambda^2 y$, where $y(0,\lambda)=1$ and $y'(0,\lambda)=-2$. The exact solution is

$$y_e(x,\lambda)=\mathrm{MathieuC}(4\mu^2,2,1/2x)-4\mathrm{MathieuS}(4\mu^2,2,1/2x).$$

The coefficients are easily computed,

$$a[0]=1,$$

$$a[1]=-2+1/2\sin(x),$$

$$a[2]=1/4\cos(x)+\sin(x)-1/8\sin(x)^2-1/4,$$

$$a[3]=-1/2\cos(x)+3/16\cos(x)\sin(x)+1/16x-1/4\cos(x)^2-1/48\sin(x)^3+1/2+1/4+1/48,$$

$$a[4]=-1/24\sin(x)-3/16\sin(x)^2+3/8\cos(x)\sin(x)+1/8x-1/96\cos(x)\sin(x)^2$$
$$-5/96\cos(x)+5/96\cos(x)^3-1/32\sin(x)x+1/24\cos(x)^2\sin(x)+1/384\sin(x)^4$$
$$+5/96-5/96.$$

Here we compare few values from $y(3,n)$, $n=1,\ldots,36$,

−0.748 175 9807	1.163 419 958	−1.142 541 067	1.083 920 209	−0.999 452 0843
0.894 915 0519	−0.774 048 1629	0.639 976 5749	−0.495 688 4404	0.3441844722
−0.188 508 0895	0.317 272 989$e-1$	0.123 104 5542	−0.272 997 4445	0.415 076 9273
−0.546 636 6709	0.6651 890 699	−0.768 512 3266	0.854 692 7372	−0.922 161 1523
0.969 722 7807	−0.996 579 6800	1.002 345 451	−0.987 051 8211	0.951 146 9772
−0.895 485 6744	0.821 311 3179	−0.730 230 3749	0.624 179 6300	−0.505 386 9379

and their approximations

0.167 443 0785$e14$	−18.635 141 80	−1.125 120 026	1.074 961 786	−0.994 041 1660
0.891 348 4130	−0.771 566 0093	0.638 186 0079	−0.494 365 0076	0.343 190 2959
−0.187 753 6293	0.311 517 829$e-1$	0.123 543 8801	−0.273 331 5660	0.415 328 8682
−0.546 823 9036	0.665 325 0926	−0.768 607 7264	0.854 755 9242	−0.922 198 8779
0.969 740 5119	−0.996 581 8730	1.002 3357 56	−0.987 033 2372	0.951 121 9718
−0.895 456 2764	0.821 279 1906	−0.730 196 8755	0.624 145 8567	−0.505 353 7692

Example 2: Consider $-y''+xy=\lambda^2 y$, with $y(0,\lambda)=1$ and $y'(0,\lambda)=3$. The exact solution is

$$y(x,\mu) = c(\mu)\text{Airy Ai}(x-\mu^2) + d(\mu)\text{Airy Bi}(x-\mu^2),$$

$$c(\mu) = \frac{-(3\ \text{Airy Bi}(-\mu^2) - \text{Airy Bi}(1,-\mu^2))}{(-\text{Airy Bi}(-\mu^2)\text{Airy Ai}(1,-\mu^2) + \text{Airy Bi}(1,-\mu^2)\text{Airy Ai}(-\mu^2))},$$

$$d(\mu) = \frac{(3\text{Airy Ai}(-\mu^2) - \text{Airy Ai}(1,-\mu^2))}{(-\text{Airy Bi}(-\mu^2)\text{Airy Ai}(1,-\mu^2) + \text{Airy Bi}(1,-\mu^2)\text{Airy Ai}(-\mu^2))},$$

$$a[0] = 1,$$

$$a[1] = 3 + 1/4x^2,$$

$$a[2] = 1/4x - 1/32x^4 - 3/4x^2,$$

$$a[3] = 5/48x^3 + 3/4x - 1/384x^6 - 3/32x^4,$$

$$a[4] = 5/32x^2 - 7/384x^5 - 5/16x^3 + 1/6144x^8 + 1/128x^6.$$

We can compare few values between $y(4,n)$, $n=1,\ldots,35$,

−121.675 2146	−1.542 623 760	−0.232 618 3437	1.190 754 717	−0.746 224 3562
−0.341 321 5597	1.043 099 355	−0.835 041 5628	−0.037 893 0074	0.854 225 5264
−0.992 844 0701	0.375 265 9630	0.514 655 7178	−1.012 088 021	0.759 688 2042
0.046 090 2340	−0.812 971 6401	0.987 483 9651	−0.449 896 0328	−0.408 335 0581
0.971 349 3754	−0.839 583 4697	0.110 615 7287	0.695 147 8309	−1.006 400 897
0.604 834 8112	0.223 439 5774	−0.892 768 4890	0.931 937 0240	−0.314 938 7262
−0.522 867 2854	0.992 396 1517	−0.764 716 4534	0.000 729 6130	0.763 166 2083

and its approximation $y_a(4,n)$, $n=1,\ldots 35$,

−0.322 422 204	−1.532 733 809	−0.235 509 6315	1.190 079 810	−0.745 065 2802
−0.341 883 1913	1.043 060 296	−0.834 750 3038	−0.038 132 2011	0.854 290 1206
−0.992 769 0014	0.375 152 6849	0.514 723 6304	−1.012 084 876	0.759 639 5448
0.046 140 0680	−0.812 991 4709	0.987 470 0399	−0.449 866 2059	−0.408 358 0246
0.971 352 8141	−0.839 569 9001	0.110 597 6148	0.695 158 0462	−1.006 398 438
0.604 823 8579	0.223 450 3635	−0.892 772 2668	0.931 932 6936	−0.314 930 5316
−0.522 873 4089	0.992 396 6261	−0.764 711 9144	0.000 723 7982	0.763 169 3436

.

Example 3: Consider $-y''+\sin(x)y=\lambda^2 y$, $y(0,\lambda)=1$, and $y'(0,\lambda)=6$,

$$y_e(x,y) = \frac{-(12\text{MS}(4\lambda^2,2,\pi/4) + \text{MSP}(4\lambda^2,2,\pi/4))\text{MC}(4\lambda^2,2,\arccos(1/2\sqrt{2\sin(x)+2}))}{(\text{MS}(4\lambda^2,2,\pi/4)\text{MCP}(4\lambda^2,2,\pi/4) - \text{MSP}(4\lambda^2,2,\pi/4)\text{MC}(4\lambda^2,2,\pi/4))}$$

$$+ \frac{(12\text{MC}(4\lambda^2,2,\pi/4) + \text{MCP}(4\lambda^2,2,\pi/4))\text{MS}(4\lambda^2,2,\arccos(1/2\sqrt{2\sin(x)+2}))}{(\text{MSS}(4\lambda^2,2,\pi/4)\text{MCP}(4\lambda^2,2,\pi/4) - \text{MSP}(4\lambda^2,2,\pi/4)\text{MC}(4\lambda^2,2,\pi/4))},$$

where the functions MS is MathieuS, MSP is MathieuSprime, MC is MathieuC, MCP is MathieuCprime, the sequence $c_n(x)$ is given by

$$c_0(x) = 1,$$

$$c_1(x) = 6 - 1/2\cos(x) + 1/2,$$

$$c_2(x) = 1/4\sin(x) + 13/4\cos(x) - 1/8\cos(x)^2 - 13/4 + 1/8,$$

$$c_3(x) = 23/16\cos(x) + 13/8\sin(x) - 3/16\sin(x)\cos(x) - 13/16\cos(x)^2$$

$$+ 1/48\cos(x)^3 + 1/16x - 23/16 + 13/16 - 1/48,$$

Here are few values. $y(1,n)$, $n=1,\ldots,30$,

6.154 887 033	2.686 340 637	−0.552 612 7710	−1.794 216 234	−0.932 806 7024
0.636 401 0418	1.321 948 590	0.629 621 7057	−0.611 762 7914	−1.168 450 847
−0.562 712 0822	0.557 951 1189	1.102 551 938	0.577 070 0830	−0.485 371 8233
−1.065 348 923	−0.626 533 2182	0.397 830 3214	1.034 591 044	0.691 350 0662
−0.297 928 7750	−0.999 996 1806	−0.760 924 1610	0.188 149 2214	0.956 313 8733
0.828 544 8431	−0.070 929 5701	−0.900 846 9644	−0.889 590 9568	−0.051 175 2417

and their corresponding approximations

−1.359 708 560 10	12.009 765 65	−0.550 356 7325	−1.797 145 576	−0.934 797 8934
0.636 028 9944	1.322 414 114	0.630 110 6212	−0.611 612 5445	−1.168 582 633
−0.562 900 6564	0.557 870 8830	1.102 598 044	0.577 160 3441	−0.485 322 6859
−1.065 365 683	−0.626 582 0311	0.397 797 7152	1.034 596 076	0.691 378 4867
−0.297 951 5535	−0.999 996 2206	−0.760 906 8620	0.188 165 6944	0.956 316 1424
0.828 534 0647	−0.070 941 7673	−0.900 850 1472	−0.889 584 2056	−0.051 166 0655

As expected, apart from the first two, all the other values agree.

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Compatible Lie brackets related to elliptic curve

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For the direct sum of several copies of sl_n, a family of Lie brackets compatible with the initial one is constructed. The structure constants of these brackets are expressed in terms of θ functions associated with an elliptic curve. The structure of Casimir elements for these brackets is investigated. A generalization of this construction to the case of vector-valued θ-functions is presented. A different procedure for constructing compatible Lie brackets based on the argument shift method for quadratic Poisson brackets is discussed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2158434]

I. INTRODUCTION

Two Lie brackets $[\cdot,\cdot]_1$ and $[\cdot,\cdot]_2$, defined on the same finite-dimensional vector space $\mathbf{V}$, are said to be compatible if

$$[\cdot,\cdot]_u=[\cdot,\cdot]_1+u[\cdot,\cdot]_2 \tag{1.1}$$

is a Lie bracket for any constant u. As a matter of fact, this notion coincides with the concept of two compatible linear Poisson structures (see Ref. 1). Indeed, the formula

$$\{x_i,\ x_j\}=c_{ij}^k x_k,\quad i,j=1,\ldots,N \tag{1.2}$$

defines a Poisson bracket iff c_{ij}^k are structural constants of a Lie algebra and the compatibility of two Poisson brackets of this form is equivalent to the compatibility of the two corresponding Lie structures.

The Casimir functions of the Poisson bracket $\{\cdot,\cdot\}_u$ corresponding to (1.1) are polynomials in u, whose coefficients commute with respect to both Poisson brackets. This way for constructing completely integrable Hamiltonian dynamical systems of compatible Poisson brackets is called the Lenard–Magri scheme.[1,2] Pairs of compatible Lie brackets have been considered in this context in Refs. 3 and 4.

However, possible applications of compatible pairs of Lie algebras in the integrability theory are not exhausted by this construction. For example, it was shown in Ref. 5 that the system of nonlinear hyperbolic equations,

$$U_x=[U,V]_1,\quad V_y=[V,U]_2,\quad U,V\in\mathbf{V},$$

is integrable for compatible Lie brackets. If the brackets $[\cdot,\cdot]_{1,2}$ coincide, this system is just the principal chiral model.

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Compatible Lie brackets also are closely related to decompositions of infinite-dimensional Lie algebras into a vector direct sum of two subalgebras.[6–8] Furthermore, it was shown in Ref. 9 that any pair of compatible Lie brackets having a common quadratic Casimir function produces a (nonconstant) solution of the classical Yang–Baxter equation.

The following classification problem arises: to describe all possible brackets $[\cdot,\cdot]_2$ on a vector space $\mathbf{V}$, compatible with a given semisimple bracket $[\cdot,\cdot]_1$. Since any semisimple Lie algebra is rigid, the bracket (1.1) is isomorphic to $[\cdot,\cdot]_1$ for almost all values of the parameter u. It is well known that for the semisimple case the second bracket $[\cdot,\cdot]_2$ is given by the formula

$$[X,Y]_2=[R(X),Y]_1+[X,R(Y)]_1-R([X,Y]_1),$$

where R is a linear operator on $\mathbf{V}$.

Some examples of compatible brackets are known (see Refs. 4 and 5). Similar to solutions of classical Yang–Baxter equations (Ref. 10), these examples are (in some sense) rational, trigonometric, or elliptic.

In this paper, we construct a class of compatible semisimple Lie brackets related to an elliptic curve. By analogy with other "elliptic" models in integrability theory, one can expect that a very wide class of compatible Lie brackets can be obtained by different degenerations of these basic "elliptic" pairs and by deformations of degenerate pairs, which are usually not as rigid as the elliptic models.

The paper is organized as follows. In Sec. II we present a construction of compatible elliptic $\oplus_{i=1}^{m} sl_n$-Lie brackets. The initial date for our construction is a pair of θ functions of order m without common zeros on an elliptic curve $\mathcal{E}$. To demonstrate the main idea, let us consider a slightly different situation of two compatible associative structures.

Let $\mathbf{V}$ be the k-dimensional vector space of all polynomials of degree $\leqslant k-1$ in one variable, let μ_1 and μ_2 be given polynomials of degree k without common roots. It is clear that any polynomial Z, where $\deg Z\leqslant 2k-1$, can be uniquely represented in the form $Z=\mu_1 P+\mu_2 Q$, where $P,Q\in\mathbf{V}$. The explicit form of P and Q can be found with the help of the Lagrange interpolation formula. Let us define two multiplications $\circ$ and $\star$ on $\mathbf{V}$ by the formula

$$XY=\mu_1(X\circ Y)+\mu_2(X\star Y),\quad X,Y\in\mathbf{V}.$$

It can be checked that any linear combination of these two products is associative. We consider an analog of this construction for Lie algebras replacing polynomials by θ functions on $\mathcal{E}$ with values in sl_n.

In Sec. III we investigate properties of the Lie algebra $\mathcal{G}_u$ with the bracket (1.1) constructed in Sec. II. Since for generic u the Lie algebra $\mathcal{G}_u$ is isomorphic to $\oplus_{i=1}^{m} sl_n$, we know that the center of the universal enveloping algebra $\mathbf{U}(\mathcal{G}_u)$ is generated by $m(n-1)$ elements of $\mathbf{U}(\mathcal{G}_u)$. More precisely, we have m generators of degree p, where $p=2,3,\ldots,n$. Usually the elements of the center are called the Casimir elements.

Since (1.1) is linear in u, the Casimir elements can be chosen to be polynomial in u. It turns out that for each p there exists one Casimir element $K_{p,1}$ of degree $p-2$ in u, $m-2$ Casimir elements $K_{p,2},\ldots,K_{p,m-1}$ of degree $p-1$ and one element $K_{p,m}$ of degree p. In particular, there exists one quadratic Casimir element, which does not depend on u. This element can be regarded as an invariant bilinear form, common for both brackets $[\cdot,\cdot]_{1,2}$.

This picture is in accordance with general results and conjectures by Gelfand and Zakharevich[11] about "good" bi-Hamiltonian structures that in our case states, in particular, that $\Sigma_{i,j}(2\deg_u K_{ij}+1)$ should be equal to $\dim \mathcal{G}_u=m(n^2-1)$.

In Sec. III we find explicit formulas for of all these Casimir elements K_{ij}.

In Sec. IV we generalize the results of Sec. II to the case of vector-valued θ functions or, which is the same, to the case of l-dimensional indecomposable holomorphic vector bundles over the elliptic curve. As the result, we get an $(l+1)$-dimensional vector space of pairwise compatible Lie brackets.[11]

In Sec. V we discuss a different way for constructing compatible linear Poisson brackets starting with a quadratic Poisson bracket of Sklyanin type. This construction is based on the argument shift method. We conjecture that the family of compatible brackets thus obtained coincides with the brackets constructed in Sec. IV.

II. COMPATIBLE LIE BRACKETS RELATED TO SCALAR θ-FUNCTIONS

Let $\Gamma \subset \mathbb{C}$ be a lattice generated by 1 and τ, where $\operatorname{Im}\tau > 0$. Let $m \in \mathbb{N}$. We denote by $\Theta_m(\tau)$ the vector space of holomorphic functions $\phi: \mathbb{C} \to \mathbb{C}$, such that

$$\phi(z+1) = \phi(z), \quad \phi(z+\tau) = (-1)^m \exp(-2\pi i m z)\phi(z).$$

Elements of this vector space are called θ functions of order m. Properties of θ functions are described, for example, in the Appendix to the review.[12] In particular, the dimension of $\Theta_m(\tau)$ is equal to m. We fix a generator of $\Theta_1(\tau)$ and denote it by $\theta(z)$. It is known that any element $f \in \Theta_m(\tau)$ has m roots modulo Γ and the sum of these roots is equal to zero modulo Γ. In particular, $\theta(z)$ has only one root modulo Γ at $z=0$. If $x_1, \ldots, x_m$ are all roots of $f \in \Theta_m(\tau)$, then $f(z) = c\,\theta(z-x_1)\cdots\theta(z-x_m)$, where c is a constant.

Let us fix relatively prime natural numbers k and n such that $1 \leqslant k < n$. Let $\mathbf{a}$ and $\mathbf{b}$ be $n \times n$ matrices, such that

$$\mathbf{a}^n = \mathbf{b}^n = 1, \quad \mathbf{ba} = \exp\left(\frac{2\pi i k}{n}\right)\mathbf{ab}. \tag{2.1}$$

Note that such a pair of matrices $(\mathbf{a}, \mathbf{b})$ is a necessary ingredient of several "elliptic" constructions related to sl_n (see Refs. 10, 13, and 14). It is clear that the matrices $\mathbf{a}^\alpha \mathbf{b}^\beta$, where $\alpha, \beta = 0, \ldots, n-1$, $(\alpha, \beta) \neq (0,0)$, form a basis in sl_n. The commutator relations between these matrices are given by

$$[\mathbf{a}^{\alpha_1}\mathbf{b}^{\beta_1},\ \mathbf{a}^{\alpha_2}\mathbf{b}^{\beta_2}] = \left[\exp\left(\frac{2\pi i k \beta_1 \alpha_2}{n}\right) - \exp\left(\frac{2\pi i k \beta_2 \alpha_1}{n}\right)\right]\mathbf{a}^{\alpha_1+\alpha_2}\mathbf{b}^{\beta_1+\beta_2}. \tag{2.2}$$

We denote by $\mathbf{V}_m$ the vector space of holomorphic functions $f: \mathbb{C} \to sl_n$ satisfying the following quasiperiodic conditions:

$$f(z+1) = \mathbf{a} f(z) \mathbf{a}^{-1}, \quad f(z+\tau) = (-1)^m \exp(-2\pi i m z)\mathbf{b} f(z) \mathbf{b}^{-1}. \tag{2.3}$$

Note that if $f_1 \in \mathbf{V}_{m_1}$ and $f_2 \in \mathbf{V}_{m_2}$, then $f_1 f_2 \in \mathbf{V}_{m_1+m_2}$. It follows from (2.3) that if

$$f(z) = \sum f_{\alpha,\beta}(z)\mathbf{a}^\alpha \mathbf{b}^\beta,$$

then

$$f_{\alpha,\beta}(z+1) = \exp\left(-\frac{2\pi i k \beta}{n}\right) f_{\alpha,\beta}(z),$$

$$f_{\alpha,\beta}(z+\tau) = (-1)^m \exp\left(-2\pi i m z + \frac{2\pi i k \alpha}{n}\right) f_{\alpha,\beta}(z). \tag{2.4}$$

These identities imply that

$$f_{\alpha,\beta}(z) = \exp\left(-\frac{2\pi i k \beta}{n} z\right) g_{\alpha,\beta}\left(z - \frac{k\alpha}{mn} - \frac{k\beta}{mn}\tau\right), \tag{2.5}$$

where $g_{\alpha,\beta}(z)$ belongs to $\Theta_m(\tau)$.

Lemma 1: *Let $\mu_1, \mu_2 \in \Theta_m(\tau)$ be a pair of θ functions that have no common zeros. Then any element $Z \in \mathbf{V}_{2m}$ can be uniquely represented in the form*

$$Z = \mu_1 P + \mu_2 Q, \quad P, Q \in \mathbf{V}_m.$$

Proof: Consider a linear mapping $L: \mathbf{V}_m \oplus \mathbf{V}_m \to \mathbf{V}_{2m}$ given by the formula

$$L(P,Q) = \mu_1 P + \mu_2 Q.$$

We should prove that L is an isomorphism. Since $\dim(\mathbf{V}_m \oplus \mathbf{V}_m) = \dim \mathbf{V}_{2m} = 2m(n^2-1)$, it suffices to prove that $\operatorname{Ker} L = 0$. Substituting

$$P = \sum P_{\alpha,\beta}(z)\mathbf{a}^\alpha \mathbf{b}^\beta, \quad Q = \sum Q_{\alpha,\beta}(z)\mathbf{a}^\alpha \mathbf{b}^\beta$$

into $L(P,Q)=0$, we find that $\mu_1(z)P_{\alpha,\beta}(z) + \mu_2(z)Q_{\alpha,\beta}(z) = 0$ for all $(\alpha,\beta) \neq 0$. Since $\mu_1(z)$ and $\mu_2(z)$ have no common roots, we see that any root of $\mu_1(z)$ is a root of $Q_{\alpha,\beta}(z)$. We know that $\mu_1(z) \in \Theta_m(\tau)$ has exactly m zeros modulo Γ and the sum of all these zeros equals 0. It follows from (2.5) that if $Q_{\alpha,\beta}(z) \not\equiv 0$, then $Q_{\alpha,\beta}(z)$ also has exactly m zeros, but their sum is equal to $k\alpha/n + (k\beta/n)\tau$. Hence $Q_{\alpha,\beta}(z) \equiv 0$, which implies that $Q \equiv P \equiv 0$. □

Using Lemma 1, for any $f_1, f_2 \in \mathbf{V}_m$, we define $[f_1,f_2]_1$ and $[f_1,f_2]_2$ by the formula

$$[f_1,f_2] = \mu_1[f_1,f_2]_1 + \mu_2[f_1,f_2]_2. \tag{2.6}$$

Proposition 1: *The bilinear operations* $[f_1,f_2]_1$ *and* $[f_1,f_2]_2$ *are compatible Lie brackets on* $\mathbf{V}_m$.

Proof: It is clear that the standard bracket $[f_1,f_2] = f_1 f_2 - f_2 f_1$ is a Lie bracket on the vector space $\oplus_{p>0}\mathbf{V}_p$. Lemma 1 shows that $[\cdot,\cdot]_{1,2}$ are well-defined brackets on $\mathbf{V}_m$. Substituting (2.6) into the antisymmetricity condition $[f_1,f_2]+[f_2,f_1]=0$ for the standard bracket, we get $\mu_1([f_1,f_2]_1+[f_2,f_1]_1)+\mu_2([f_1,f_2]_2+[f_2,f_1]_2)=0$. It follows from Lemma 1 that $[f_1,f_2]_i+[f_2,f_1]_i = 0$ for $i=1,2$. Substituting (2.6) into the Jacobi identity for the standard bracket, we obtain an identity of the form $\mu_1^2 P + \mu_1\mu_2 Q + \mu_2^2 R = 0$ for some $P,Q,R \in \mathbf{V}_m$. Using the same argument as in the proof of Lemma 1, one can prove that $P \equiv Q \equiv R \equiv 0$. It is easy to verify that the identities $P=0$ and $R=0$ coincide with the Jacobi identity for the brackets $[\cdot,\cdot]_1$ and $[\cdot,\cdot]_2$, respectively. The identity $Q=0$ is equivalent to the compatibility of the brackets $[\cdot,\cdot]_{1,2}$. □

Let $x_i(u)$ be all roots of $\mu_2(z) - u\mu_1(z)$:

$$\mu_2(z) - u\mu_1(z) = c(u)\,\theta(z - x_1(u)) \cdots \theta(z - x_m(u)).$$

If $x_1(u), \ldots, x_m(u)$ are distinct modulo Γ, we say that u is regular. For brevity, we use the notation x_j instead of $x_j(u)$.

Now we are going to prove that the linear combination,

$$[f_1,f_2]_u = [f_1,f_2]_1 + u[f_1,f_2]_2, \tag{2.7}$$

of brackets (2.6) is isomorphic to $\oplus_{i=1}^m sl_n$ for all regular values of u.

Consider the following elements $v_{\alpha,\beta,\gamma}(u,z) \in \mathbf{V}_m$, defined by

$$v_{\alpha,\beta,\gamma}(u,z) = P_{\alpha,\beta,\gamma}(u)\, g_{\alpha,\beta,\gamma}(u,z), \tag{2.8}$$

where

$$P_{\alpha,\beta,\gamma}(u) = \frac{\mu_1(x_\gamma)}{\theta(x_\gamma - x_1)\cdots\hat{\gamma}\cdots\theta(x_\gamma - x_m)\,\theta\left(-\dfrac{k\alpha}{n} - \dfrac{k\beta}{n}\tau\right)} \tag{2.9}$$

and

$$g_{\alpha,\beta,\gamma}(u,z)=\exp\left(-\frac{2\pi ik\beta}{n}z\right)\theta(z-x_1)\cdots\hat{\gamma}\cdots\theta(z-x_m)\times\theta\left(z-x_\gamma-\frac{k\alpha}{n}-\frac{k\beta}{n}\tau\right)\mathbf{a}^\alpha\mathbf{b}^\beta. \tag{2.10}$$

Here the symbol $\hat{\gamma}$ means that the factor $\theta(z-x_\gamma)$ is omitted in the product, $\alpha,\beta=0,\ldots,n-1$, where $(\alpha,\beta)\neq(0,0)$ and $\gamma=1,\ldots,m$.

Theorem 1: *The elements* $v_{\alpha,\beta,\gamma}(u)$ *satisfy the following commutator relations*;

$$[v_{\alpha_1,\beta_1,\gamma_1},v_{\alpha_2,\beta_2,\gamma_2}]_u=0, \tag{2.11}$$

for $\gamma_1\neq\gamma_2$ *and* [cf. (2.2)]

$$[v_{\alpha_1,\beta_1,\gamma},v_{\alpha_2,\beta_2,\gamma}]_u=\left[\exp\left(\frac{2\pi ik\beta_1\alpha_2}{n}\right)-\exp\left(\frac{2\pi ik\beta_2\alpha_1}{n}\right)\right]v_{\alpha_1+\alpha_2,\beta_1+\beta_2,\gamma}. \tag{2.12}$$

The proof of Theorem 1 is based on the following.

Lemma 2: *Suppose* $x_1,\ldots,x_m\in\mathbb{C}$ *are distinct modulo* Γ *and* $x_1+\cdots+x_m\neq k\alpha/n+(k\beta/n)\tau$ *modulo* Γ *for* $0\leqslant\alpha,\beta<n$, $(\alpha,\beta)\neq(0,0)$. *Then for any* $\sigma_1,\ldots,\sigma_m\in sl_n$ *there exists a unique element* $f\in\mathbf{V}_m$ *such that* $f(x_\delta)=\sigma_\delta$ for $\delta=1,\ldots,m$.

Proof of Lemma 2: Consider a linear mapping $M:\mathbf{V}_m\to\oplus_{i=1}^m sl_n$ given by the formula $M(f)=(f(x_1),\ldots,f(x_m))$. Since $\dim\mathbf{V}_m=\dim\oplus_{i=1}^m sl_n=m(n^2-1)$, it suffices to prove that $\operatorname{Ker}M=0$. Suppose $M(f)=0$, where $f=\Sigma_{\alpha,\beta}f_{\alpha,\beta}(z)\mathbf{a}^\alpha\mathbf{b}^\beta$. Then $f_{\alpha,\beta}(x_\delta)=0$ for all α,β,δ. But it follows from (2.5) that if $f_{\alpha,\beta}\not\equiv 0$, then the sum of all zeros for $f_{\alpha,\beta}$ is equal to $k\alpha/n+(k\beta/n)\tau$. □

Proof of Theorem 1: The basic idea is to verify that the identities (2.11), (2.12) hold if we substitute $z=x_\delta$, $\delta=1,\ldots,m$. Then Lemma 2 concludes the proof. It is easy to check that

$$\begin{aligned}[g_{\alpha_1,\beta_1,\gamma_1},g_{\alpha_2,\beta_2,\gamma_2}]=&\exp\left(-\frac{2\pi ik(\beta_1+\beta_2)}{n}z\right)\theta(z-x_1)\cdots\hat{\gamma}_1\cdots\theta(z-x_m)\\&\times\theta(z-x_1)\cdots\hat{\gamma}_2\cdots\theta(z-x_m)\times\theta\left(z-x_{\gamma_1}-\frac{k\alpha_1}{n}-\frac{k\beta_1}{n}\tau\right)\\&\times\theta\left(z-x_{\gamma_2}-\frac{k\alpha_2}{n}-\frac{k\beta_2}{n}\tau\right)\left[\exp\left(\frac{2\pi ik\beta_1\alpha_2}{n}\right)-\exp\left(\frac{2\pi ik\beta_2\alpha_1}{n}\right)\right]\\&\times\mathbf{a}^{\alpha_1+\alpha_2}\mathbf{b}^{\beta_1+\beta_2}.\end{aligned} \tag{2.13}$$

Using the formula

$$[\cdot,\cdot]=\mu_1[\cdot,\cdot]_u+(\mu_2-u\mu_1)[\cdot,\cdot]_2, \tag{2.14}$$

we find that

$$[g_{\alpha_1,\beta_1,\gamma_1},g_{\alpha_2,\beta_2,\gamma_2}]_u(x_\delta)=0,$$

for $\gamma_1\neq\gamma_2$, which implies (2.11) by Lemma 2. If $\gamma_1=\gamma_2=\gamma$, then it follows from (2.13), (2.14) that

$$[g_{\alpha_1,\beta_1,\gamma},\ g_{\alpha_2,\beta_2,\gamma}]_u(x_\delta)=0,$$

for $\delta\neq\gamma$. This proves that (2.12) holds for $z=x_\delta$, $\delta\neq\gamma$. A simple straightforward computation shows that (2.12) also holds for $z=x_\gamma$. □

Remark 1: Suppose the functions $\mu_1(z)$ and $\mu_2(z)$ have distinct roots modulo Γ; then the points $u=0$ and $u=\infty$ are regular and the brackets $[\cdot,\cdot]_1$ and $[\cdot,\cdot]_2$ correspond to the Lie algebra isomorphic to $\oplus_{i=1}^m sl_n$.

Remark 2: It is possible to construct "trigonometric" and "rational" degenerations of the

elliptic brackets described above. Namely, in the trigonometric case one should replace $\theta(z)$ by $1-\exp(2\pi i z)$, the space $\Theta_m(\tau)$ by the space of functions of the form

$$a_0 + a_1 \exp(2\pi i z) + \cdots + a_m \exp(2\pi i m z),$$

such that $a_m=(-1)^m a_0$, and the space $\mathbf{V}_m$ by the space of $sl(n)$-valued functions of the form

$$\sum c_{\alpha,\beta} \exp\left(2\pi i \frac{\beta}{n} z\right) \mathbf{a}^\alpha \mathbf{b}^\beta, \quad 0 \leqslant \alpha \leqslant n, \quad 0 \leqslant \beta \leqslant mn,$$

where $c_{\alpha,0}=(-1)^m c_{\alpha,mn}$. In this formula we assume that $\mathbf{a}^n=\mathbf{b}^n=1$, $\mathbf{ba}=\exp(2\pi i/n)\mathbf{ab}$. We should also modify the definitions of $P_{\alpha,\beta,\gamma}(u)$ and $g_{\alpha,\beta,\gamma}(u)$ given by (2.9) and (2.10) in the following way:

$$P_{\alpha,\beta,\gamma}(u) = \frac{\mu_1(x_\gamma)}{\theta_t(x_\gamma - x_1)\cdots \hat{\gamma} \cdots \theta_t(x_\gamma - x_m)\theta_t\left(-\frac{\alpha}{n}\right)},$$

$$g_{\alpha,\beta,\gamma}(u,z) = \exp\left(-\frac{2\pi i \beta}{n} z\right) \theta_t(z-x_1)\cdots \hat{\gamma} \cdots \theta_t(z-x_m)$$

$$\times \theta_t\left(z - x_\gamma - \frac{\alpha}{n}\right) \mathbf{a}^\alpha \mathbf{b}^\beta,$$

if $\alpha \neq 0$ and

$$P_{0,\beta,\gamma}(u) = \frac{\mu_1(x_\gamma)}{\theta_t(x_\gamma - x_1)\cdots \hat{\gamma} \cdots \theta_t(x_\gamma - x_m)},$$

$$g_{0,\beta,\gamma}(u,z) = \exp\left(-\frac{2\pi i \beta}{n} z\right) \theta_t(z-x_1)\cdots \hat{\gamma} \cdots \theta_t(z-x_m)\mathbf{b}^\beta.$$

Here $\theta_t(z)=1-\exp(2\pi i z)$.

In the rational case $\theta(z)$ has to be replaced by z, the space $\Theta_m(\tau)$ by the space of polynomials of the form $\Sigma_{i=0}^m c_\alpha z^\alpha$, $c_{m-1}=0$, and $\mathbf{V}_m$ by the space of polynomials $\Sigma_{i=0}^{m-1} g_\alpha z^\alpha$, $g_\alpha \in sl_n$. In this case

$$P_{\alpha,\beta,\gamma}(u) = \frac{\mu_1(x_\gamma)}{(x_\gamma - x_1)\cdots \hat{\gamma} \cdots (x_\gamma - x_m)},$$

$$g_{\alpha,\beta,\gamma}(u,z) = (z-x_1)\cdots \hat{\gamma} \cdots (z-x_m) \times \mathbf{a}^\alpha \mathbf{b}^\beta.$$

In both cases $v_{\alpha,\beta,\gamma}(u,z)$ is defined by (2.8).

III. STRUCTURE OF CASIMIR ELEMENTS

A. Casimir elements for sl_n

Let $\mathbf{e}_\alpha$, $\alpha=1,\ldots,n^2-1$, be a basis in sl_n, and let $\mathbf{e}^\alpha$ be the dual basis with respect to the invariant form $<X,Y>=\mathrm{tr}(XY)$. Then the Casimir elements,

$$C_p = \sum_{1 \leqslant \alpha_1, \ldots \alpha_p \leqslant n^2-1} \mathrm{tr}(\mathbf{e}^{\alpha_1}\cdots \mathbf{e}^{\alpha_p}) \mathbf{e}_{\alpha_1} \circ \cdots \circ \mathbf{e}_{\alpha_p}, \quad p=2,\ldots,n,$$

where $\circ$ denotes the multiplication in the universal enveloping algebra $\mathbf{U}(sl_n)$, generate the center of $\mathbf{U}(sl_n)$.

Let us take $\mathbf{t}_{\alpha,\beta}=\mathbf{a}^{\alpha}\mathbf{b}^{\beta}$ for a basis in sl_n, where $\mathbf{a},\mathbf{b}$ are defined by (2.1), $0\leqslant\alpha,\beta<n$, and $(\alpha,\beta)\neq(0,0)$. Then, up to a common multiplicative constant, the dual basis is given by

$$\mathbf{t}^{\alpha,\beta}=\exp\left(\frac{2\pi ik\alpha\beta}{n}\right)\mathbf{t}_{-\alpha,-\beta}.$$

In this basis the Casimir elements have the form

$$C_p=\sum_{\mathbb{D}_p}\exp\left(\frac{2\pi ik}{n}\sum_{1\leqslant j_1\leqslant j_2\leqslant p}\alpha_{j_1}\beta_{j_2}\right)\mathbf{t}_{\alpha_1,\beta_1}\circ\cdots\circ\mathbf{t}_{\alpha_p,\beta_p},$$

where

$$\mathbb{D}_p=\{(\alpha_1,\ldots,\alpha_p,\beta_1,\ldots\beta_p)|\quad 0\leqslant\alpha_i,\beta_j<n,\quad(\alpha_j,\beta_j)\neq(0,0),\quad\alpha_1+\cdots+\alpha_p\equiv 0 \bmod n,$$
$$\beta_1+\cdots+\beta_p\equiv 0 \bmod n\}.$$

In particular, the quadratic Casimir element is given by

$$C_2=\sum_{\alpha,\beta}\exp\left(\frac{2\pi ik\alpha\beta}{n}\right)\mathbf{t}_{\alpha,\beta}\circ\mathbf{t}_{-\alpha,-\beta}.$$

B. Polynomial Casimir elements for $\mathcal{G}_u$

In the previous section, we have equipped the vector space $\mathbf{V}_m$ with the Lie bracket (2.7). For generic u the corresponding Lie algebra $\mathcal{G}_u$ is isomorphic to $\oplus_{i=1}^{m}sl_n$.

It was shown that the vector space $\mathbf{V}_m$ is isomorphic to $\oplus_{\alpha,\beta}\mathbf{F}_{\alpha,\beta}$, where $\mathbf{F}_{\alpha,\beta}$ is the vector space of holomorphic functions satisfying (2.4). Denote by $\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ the vector space of holomorphic functions of variables $z_1,\ldots,z_p$ satisfying the conditions

$$f(z_1,\ldots,z_j+1,\ldots,z_p)=\exp\left(-\frac{2\pi ik\beta_j}{n}\right)f(z_1,\ldots,z_p),$$
$$f(z_1,\ldots,z_j+\tau,\ldots,z_p)=(-1)^m\exp\left(-2\pi imz_j+\frac{2\pi ik\alpha_j}{n}\right)f(z_1,\ldots,z_p). \tag{3.1}$$

Calculating the number of free coefficients in the Fourier decomposition of a function satisfying (3.1), we find that $\dim\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}=m^p$. In particular, $\dim\mathbf{F}_{\alpha,\beta}=m$. Hence, the vector space $\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ is spanned by the products $f_1(z_1)\cdots f_p(z_p)$, where $f_i(z)\in\mathbf{F}_{\alpha_i,\beta_i}$. In other words, $\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ is isomorphic to $\mathbf{F}_{\alpha_1,\beta_1}\otimes\cdots\otimes\mathbf{F}_{\alpha_p,\beta_p}$.

We use functions from $\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ to represent elements of the universal enveloping algebra $\mathbf{U}(\mathcal{G}_u)$. Namely, to the product $f_1(z_1)\cdots f_p(z_p)\in\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ we assign the element $f_1(z)\mathbf{t}_{\alpha_1,\beta_1}\bullet\cdots\bullet f_p(z)\mathbf{t}_{\alpha_p,\beta_p}\in\mathbf{U}(\mathcal{G}_u)$, where $\bullet$ is the multiplication in $\mathbf{U}(\mathcal{G}_u)$. Denote the corresponding linear mapping from $\oplus_{\mathbb{D}_p}\mathbf{F}_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}$ to $\mathbf{U}(\mathcal{G}_u)$ by σ_p.

Suppose u is regular, that is, all roots $x_1,\ldots,x_m$ of the function $\mu_2(z)-u\mu_1(z)$ are distinct. Let $v_{\alpha,\beta,\gamma}(u,z)=s_{\alpha,\beta,\gamma}(u,z)\mathbf{t}_{\alpha,\beta}$ be the basis of $\mathbf{V}_m$ given by (2.8)–(2.10).

By Theorem 1, for each γ the elements of this basis satisfy the same commutator relations as $\mathbf{t}_{\alpha,\beta}$. Hence, the center of $\mathbf{U}(\mathcal{G}_u)$ is generated by

$$C_{\gamma,p}=\sum_{\mathbb{D}_p}\exp\left(\frac{2\pi ik}{n}\sum_{1\leqslant j_1\leqslant j_2\leqslant p}\alpha_{j_1}\beta_{j_2}\right)\sigma_p(f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p,\gamma}), \tag{3.2}$$

where $f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p,\gamma}(z_1,\dots,z_p)=s_{\alpha_1,\beta_1,\gamma}(u,z_1)\cdots s_{\alpha_p,\beta_p,\gamma}(u,z_p)$.

Now our goal is to find linear combinations of generators (3.2) that are polynomial in u. Let $W_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}\subset\mathbf{F}_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ be the vector subspace spanned by $f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p,\gamma}$, where $\gamma=1,\dots,m$. The following statement gives us an inner description of this subspace.

Lemma 3: *The vector space* $W_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ *consists of holomorphic functions* $f(z_1,\dots,z_p)$ *satisfying* (3.1) *and vanishing on the surfaces* $\{z_{j_1}=x_{\delta_1}$ *and* $z_{j_2}=x_{\delta_2}\}$ *for all* $j_1\neq j_2$ *and* $\delta_1\neq\delta_2$.

Proof: It is clear that the functions $f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p,\gamma}(z_1,\dots,z_p)$ enjoy these properties. On the other hand, since $\{s_{\alpha,\beta,\gamma}(z),\ \gamma=1,\dots,m\}$ is a basis in $\mathbf{F}_{\alpha,\beta}$, the products $s_{\alpha_1,\beta_1,\gamma_1}(z_1)\cdots s_{\alpha_p,\beta_p,\gamma_p}(z_p)$, where $\gamma_j=1,\dots,m$, $j=1,\dots,p$, form a basis in $\mathbf{F}_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$. Suppose a function

$$f(z_1,\dots,z_p)=\sum a_{\gamma_1,\dots,\gamma_p}s_{\alpha_1,\beta_1,\gamma_1}(z_1)\cdots s_{\alpha_p,\beta_p,\gamma_p}(z_p) \tag{3.3}$$

satisfies the conditions of Lemma 3. We have to prove that $a_{\gamma_1,\dots,\gamma_p}=0$ if $\gamma_{j_1}\neq\gamma_{j_2}$. To show this, it suffices to substitute $x_{\gamma_{j_1}}$ and $x_{\gamma_{j_2}}$ for z_{j_1} and z_{j_2} in (3.3) and to take into account formulas (2.8)–(2.10). □

Let $W_p\subset\oplus_{\mathbb{D}_p}W_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ be the vector space spanned by $\{\oplus_{\mathbb{D}_p}f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p,\gamma},\ \gamma=1,\dots,m\}$. Similar to the proof of Lemma 3, one can prove the following.

Lemma 4: *The vector space* W_p *consists of elements of the form* $\oplus_{\mathbb{D}_p}g_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$, *where* $g_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}(z_1,\dots,z_p)$ *satisfies the conditions of Lemma 3 and, in addition*,

$$\exp\left(\frac{2\pi ik}{n}x_\gamma(\beta_1+\cdots+\beta_p)\right)g_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}(x_\gamma,\dots,x_\gamma)$$

$$=\exp\left(\frac{2\pi ik}{n}x_\gamma(\beta_1'+\cdots+\beta_p')\right)g_{\alpha_1',\beta_1',\dots,\alpha_p',\beta_p'}(x_\gamma,\dots,x_\gamma),$$

for any $\alpha_1,\beta_1,\dots,\alpha_p,\beta_p$, $\alpha_1',\beta_1',\dots,\alpha_p',\beta_p'$ *and* $\gamma=1,\dots,m$.

Using Lemmas 3,4, we construct polynomials in u that span W_p for generic u.

Theorem 2: *For arbitrary* $g(z)\in\Theta_m(\tau)$, *put*

$$f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}(z_1,\dots,z_p)=\exp\left[-\frac{2\pi ik}{n}(\beta_1z_1+\cdots+\beta_pz_p)\right]\sum_{1\leqslant t\leqslant p}g(z_t)\theta\left(\frac{k\alpha_t}{n}+\frac{k\beta_t}{n}\tau\right)$$
$$\times\prod_{1\leqslant j\leqslant p,j\neq t}\frac{\theta\left(z_t-z_j+\frac{k\alpha_j}{n}+\frac{k\beta_j}{n}\tau\right)}{\theta(z_t-z_j)}\prod_{1\leqslant j\leqslant p,j\neq t}(\mu_2(z_j)-u\mu_1(z_j)). \tag{3.4}$$

Then $\oplus_{\mathbb{D}_p}f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ *belongs to* W_p *and, therefore, the formula*

$$\sum_{\mathbb{D}_p}\exp\left(\frac{2\pi ik}{n}\sum_{1\leqslant j_1\leqslant j_2\leqslant p}\alpha_{j_1}\beta_{j_2}\right)\sigma_p(f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p})$$

defines a Casimir element in $\mathbf{U}(\mathcal{G}_u)$.

Proof: We must prove that $f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ satisfies the assumptions of Lemmas 3,4. Using the quasiperiodic properties of the functions $\mu_1(z),\mu_2(z)\in\Theta_m(\tau)$ and $\theta(z)\in\Theta_1(\tau)$, one can verify condition (3.1) by a simple computation. To prove that $f_{\alpha_1,\beta_1,\dots,\alpha_p,\beta_p}$ is holomorphic, one can check that the only possible pole at $z_t=z_j$ is cancelled after summation. It is clear that if we put $z_{j_1}=x_{\delta_1}$ and $z_{j_2}=x_{\delta_2}$, where $\delta_1\neq\delta_2$, then all summands in (3.4) vanish. Thus the assumptions of

Lemma 3 hold. The assumption of Lemma 4 can be checked by a straightforward computation.□

Remark 3: If $g(z) \in \Theta_m(\tau)$ does not depend on u, then the function (3.4) is polynomial in u, of degree $p-1$.

Remark 4: Since the Casimir function given by (3.4) is linear in $g(z)$, we have constructed a linear map $T: \Theta_m(\tau) \to$ center of $\mathbf{U}(\mathcal{G}_u)$.

Lemma 5: *The kernel of T is generated by the element* $g(z)=\mu_2(z)-u\mu_1(z)$ *and, therefore,* dim Ker $T=1$.

Proof: It follows from (3.4) that

$$T(\mu_2(z)-u\mu_1(z)) = \prod_{1\leqslant j\leqslant p}(\mu_2(z_j)-u\mu_1(z_j))\exp\left[-\frac{2\pi ik}{n}(\beta_1 z_1+\cdots+\beta_p z_p)\right]$$

$$\times \sum_{1\leqslant t\leqslant p}\theta\left(\frac{k\alpha_t}{n}+\frac{k\beta_t}{n}\tau\right)\prod_{1\leqslant j\leqslant p, j\neq t}\frac{\theta\left(z_t-z_j+\frac{k\alpha_j}{n}+\frac{k\beta_j}{n}\tau\right)}{\theta(z_t-z_j)}.$$

Consider the function

$$\frac{T(\mu_2(z)-u\mu_1(z))}{\prod_{1\leqslant j\leqslant p}(\mu_2(z_j)-u\mu_1(z_j))}.$$

It can be checked that this function is holomorphic and satisfies (3.1) with $m=0$. Analyzing its Fourier decomposition, we see that such a function is identically zero. Hence $T(\mu_2(z)-u\mu_1(z))=0$. Suppose now that $T(g(z))=0$. Substituting a root x of $\mu_2(z)-u\mu_1(z)$ for z in (3.4), we see that $g(x)=0$. Since $g(z)$ has exactly m zeros mod Γ, the function $g(z)$ is proportional to $\mu_2(z)-u\mu_1(z)$. □

It follows from Lemma 5 that $T(\mu_2)$ is a polynomial of degree $p-2$ in u. Therefore, formula (3.4) yields an $(m-1)$-dimensional subspace in the m-dimensional vector space W_p such that one generator of this subspace is the polynomial $T(\mu_2)$ of degree $p-2$ and $m-2$ generators are polynomials of degree $p-1$ in u.

In the following statement we construct a remaining generator of W_p.

Theorem 3: *Let*

$$h_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p}(z_1,\ldots,z_p) = \sum_{1\leqslant t\leqslant p}A_t\times(\mu_2'(z_t)-u\mu_2'(z_t))\prod_{1\leqslant j\leqslant p, j\neq t}(\mu_2(z_j)-u\mu_1(z_j))$$

$$-B\times\prod_{1\leqslant j\leqslant p}(\mu_2(z_j)-u\mu_1(z_j)),$$

where A_t *is given by*

$$A_t=\exp\left[-\frac{2\pi ik}{n}(\beta_1 z_1+\cdots+\beta_p z_p)\right]\theta\left(\frac{k\alpha_t}{n}+\frac{k\beta_t}{n}\tau\right)\prod_{1\leqslant j\leqslant p, j\neq t}\frac{\theta\left(z_t-z_j+\frac{k\alpha_j}{n}+\frac{k\beta_j}{n}\tau\right)}{\theta(z_t-z_j)}$$

and B is defined by the formula

$$B=\frac{m}{n}\exp\left[-\frac{2\pi ik}{n}(\beta_1 z_1+\cdots+\beta_p z_p)\right](B_1+B_2),$$

where

$$B_1 = \sum_{1\leqslant t\leqslant p, 1\leqslant j\leqslant p, j\neq t} \theta\left(\frac{k\alpha_t}{n}+\frac{k\beta_t}{n}\tau\right)\frac{\theta'\left(z_t-z_j+\frac{k\alpha_j}{n}+\frac{k\beta_j}{n}\tau\right)}{\theta(z_t-z_j)}$$

$$\times \prod_{1\leqslant l\leqslant p, l\neq j,t} \frac{\theta\left(z_t-z_l+\frac{k\alpha_l}{n}+\frac{k\beta_l}{n}\tau\right)}{\theta(z_t-z_l)}$$

$$B_2 = \sum_{1\leqslant t\leqslant p} \theta'\left(\frac{k\alpha_t}{n}+\frac{k\beta_t}{n}\tau\right) \prod_{1\leqslant l\leqslant p, l\neq t} \frac{\theta\left(z_t-z_l+\frac{k\alpha_l}{n}+\frac{k\beta_l}{n}\tau\right)}{\theta(z_t-z_l)}.$$

Then the formula

$$\sum_{\mathbb{D}_p} \exp\left(\frac{2\pi i k}{n} \sum_{1\leqslant j_1\leqslant j_2\leqslant p} \alpha_{j_1}\beta_{j_2}\right)\sigma_p(h_{\alpha_1,\beta_1,\ldots,\alpha_p,\beta_p})$$

defines a Casimir element in $\mathbf{U}(\mathcal{G}_u)$.

The proof is similar to the proof of Theorem 2.

Remark 5: It is clear that the Casimir element constructed in Theorem 3 is polynomial in u, of degree p.

Remark 6: We have constructed the Casimir elements for $\mathbf{U}(\mathcal{G}_u)$, whereas in the Lenard–Magri scheme Casimir functions of the corresponding Poisson algebra are needed. However, these two kinds of Casimirs are given by the same formulas. Indeed, if a Casimir element is written in such a way that it is homogeneous with respect to elements of Lie algebra, then the same formula defines also a Casimir function of the corresponding Poisson algebra.

IV. FAMILIES OF COMPATIBLE LIE BRACKETS ASSOCIATED WITH VECTOR θ FUNCTIONS

In this section we generalize the construction in Sec. II replacing the usual θ functions by vector-valued θ functions. All proofs are similar to those in Sec. II.

Let $\Gamma\subset\mathbb{C}$ be a lattice spanned by 1 and τ, where $\operatorname{Im}\tau>0$. Our general construction will depend on $d,l,m\in\mathbb{N}$, such that $1\leqslant l<m$ and m, l are relatively prime. Denote by $V\Theta^d_{m/l}$ the vector space consisting of holomorphic functions $f:\mathbb{C}^{l+1}\to\mathbb{C}$ of variables z, $x_0,\ldots,x_{l-1}$, possessing the following properties:

- $f(z,x_0,\ldots,x_{l-1})$ is a homogeneous polynomial of degree d in variables $x_0,\ldots,x_{l-1}$,
- $$f(z+1,x_0,\ldots,x_{l-1}) = f(z,\mathbf{p}(x_0),\ldots,\mathbf{p}(x_{l-1})),$$
- $$f(z+\tau,x_0,\ldots,x_{l-1}) = \exp\left[-2\pi i\left(\frac{m}{l}z+\frac{m-l-1}{2l}\right)d\right]f(z,\mathbf{q}(x_0),\ldots,\mathbf{q}(x_{l-1})),$$

where

$$\mathbf{p}(x_\alpha) = \exp\left(-2\pi i\frac{m}{l}\alpha\right)x_\alpha, \quad \mathbf{q}(x_\alpha) = x_{\alpha+1}, \quad \alpha\in\mathbb{Z}/l\mathbb{Z}.$$

Lemma 6:

$$\dim V\Theta^d_{m/l} = m\frac{(l+1)\cdots(l+d-1)}{(d-1)!}.$$

It follows from this formula that in the case $d=1$, which is of most importance for us, $\dim V\Theta^1_{m/l}=m$.

Remark 7: Our space $V\Theta^d_{m/l}$ is a space of holomorphic sections of an indecomposable vector bundle of degree m and rank l on the elliptic curve. The classification of holomorphic vector bundles on elliptic curves was obtained in the paper of Ref. 15.

Let $1\leqslant k<n$ and let k,n be relatively prime. Denote by $\mathbf{V}^d_{m,l}$ the vector space of all holomorphic functions $f:\mathbb{C}^{l+1}\to sl_n$ such that we have the following.

- $f(z,x_0,\ldots,x_{l-1})$ is a homogeneous polynomial of degree d in variables $x_0,\ldots,x_{l-1}$,
- $$f(z+1,x_0,\ldots,x_{l-1}) = \mathbf{a}f(z,\mathbf{p}(x_0),\ldots,\mathbf{p}(x_{l-1}))\mathbf{a}^{-1}$$
- $$f(z+\tau,x_0,\ldots,x_{l-1}) = \exp\left[-2\pi i\left(\frac{m}{l}z+\frac{m-l-1}{2l}\right)d\right]\mathbf{b}f(z,\mathbf{q}(x_0),\ldots,\mathbf{q}(x_{l-1}))\mathbf{b}^{-1},$$

where $\mathbf{a}$ and $\mathbf{b}$ satisfy (2.1).

Lemma 7: *Suppose* $\mu_1,\ldots,\mu_{l+1}\in V\Theta^1_{m/l}$ *have no common zeros for* $(x_0,\ldots,x_{l-1})\neq 0$. *Then any element* $Z\in\mathbf{V}^2_{m,l}$ *can be uniquely represented in the form*

$$Z=\mu_1P_1+\cdots+\mu_{l+1}P_{l+1},\quad P_i\in\mathbf{V}^1_{m,l}.$$

It is clear that if $f,g\in\mathbf{V}^1_{m,l}$, then $fg-gf$ belongs to $\mathbf{V}^2_{m,l}$. Using Lemma 7, we define $[\cdot,\cdot]_1,\ldots,[\cdot,\cdot]_{l+1}$ by the formula

$$f_1f_2-f_2f_1=\mu_1[f_1,f_2]_1+\cdots+\mu_{l+1}[f_1,f_2]_{l+1},\quad f_1,f_2\in\mathbf{V}^1_{m,l}.$$

Proposition 2: *The bilinear operations* $[\cdot,\cdot]_1,\ldots,[\cdot,\cdot]_{l+1}$ *are Lie brackets on the m-dimensional vector space* $\mathbf{V}^1_{m,l}$. *All these Lie brackets are pairwise compatible*.

It is clear that any linear combination of brackets from Proposition 2 is a Lie bracket. We call a d-dimensional vector space of pairwise compatible Lie brackets a *d-Lie structure*.

Remark 8: Suppose that one of the sections $\mu_1,\ldots,\mu_{l+1}\in V\Theta^1_{m/l}$, say, μ_{l+1}, is nonzero for each z. In this case the subbundle generated by μ_{l+1} is trivial. Consider the quotient bundle modulo this subbundle. It has degree m and rank $l-1$. It is clear that the l-Lie structure obtained from this quotient bundle is a substructure of our $(l+1)$-Lie structure. The counting of parameters shows that any generic l-Lie structure is obtained in this way. Therefore, any $(l+1)$-Lie structure constructed in this section is embedded into an m-Lie structure corresponding to $l=m-1$.

Remark 9: Any l-Lie structure yields a family of l compatible linear Poisson brackets. We don't know whether the Lenard–Magri scheme can be generalized to the case $l>2$. However, applying the Lenard–Magri scheme to two generic Poisson brackets from the family, we get an integrable system containing $2l$ parameters. It is clear that we can reduce the number of parameters to l, bringing one of the brackets to a canonical form. But the remaining l parameters turn out to be essential parameters of the model.

V. ARGUMENT SHIFT METHOD FOR QUADRATIC POISSON BRACKETS

The standard argument shift method allows one to get a family of constant Poisson brackets compatible with any linear Poisson bracket (1.2). Namely, if we perform a shift of coordinates $x_i\mapsto x_i+ua_i$, where a_i are arbitrary constants, we will have as the result an inhomogeneous linear bracket of the form $\{\cdot,\cdot\}_u=\{\cdot,\cdot\}+u\{\cdot,\cdot\}_1$, where the operation $\{\cdot,\cdot\}_1$ is a constant Poisson bracket depending on the shift vector $\mathbf{a}=(a_1,\ldots,a_N)$. Moreover, since the shift vector $\mathbf{a}$ is arbitrary, we

have got an N-dimensional vector space of constant Poisson brackets such that each of these brackets is compatible with (1.2) and any two of them are pairwise compatible.

Consider now the case of a finite-dimensional quadratic Poisson bracket. Suppose we have a Poisson bracket of the form

$$\{x_i,x_j\}=\Gamma_{i,j}^{p,q}x_px_q,\quad i,j=1,\ldots,N. \tag{5.1}$$

The shift $x_i\to x_i+ua_i$ yields a Poisson bracket of the form $\{\cdot,\cdot\}_u=\{\cdot,\cdot\}+u\{\cdot,\cdot\}_1+u^2\{\cdot,\cdot\}_2$. If the coefficient of u^2 is equal to zero, then this formula defines a compatible pair consisting of the quadratic bracket (5.1) and a linear Poisson bracket. This means that the shift vector **a** is not arbitrary one but satisfies the following overdetermined system of algebraic equations:

$$\Gamma_{i,j}^{p,q}a_pa_q=0,\quad i,j=1,\ldots,N. \tag{5.2}$$

Such a vector is said to be *admissible*. It is clear that the set of admissible vectors coincides with the set of zero-dimensional symplectic leaves of the Poisson structure (5.1). Note that if the set of admissible vectors contains a p-dimensional vector space, then shifting by vectors from this space we obtain p compatible linear brackets, and each of them is compatible with the quadratic bracket (5.1).

Let us apply this construction to quadratic elliptic Poisson structures (see Ref. 12). For most of these brackets, the system of equations (5.2) has no nontrivial solutions. Nevertheless, for some important brackets of Sklyanin type non-trivial admissible vectors exist.

Example: Consider the following quadratic Poisson brackets between variables $x_0,\ldots,x_7$ (subscripts are taken modulo 8):

$$\begin{aligned}
\{x_i,x_{i+1}\}&=p_1x_ix_{i+1}+k_1x_{i+2}x_{i+7}-2k_2x_{i+3}x_{i+6}+p_2x_{i+4}x_{i+5},\\
\{x_i,x_{i+2}\}&=p_3(x_{i+1}^2-x_{i+5}^2),\\
\{x_i,x_{i+3}\}&=p_1x_ix_{i+3}+k_1x_{i+5}x_{i+6}-2k_2x_{i+1}x_{i+2}+p_2x_{i+4}x_{i+7},\\
\{x_i,x_{i+4}\}&=p_4(x_{i+1}x_{i+3}-x_{i+5}x_{i+7}),
\end{aligned} \tag{5.3}$$

where

$$p_1=-\frac{1}{2}k_1^{1/2}k_2^{-1/2}(4k_2^2+k_1^2)^{1/2},\quad p_2=k_2^{1/2}k_1^{-1/2}(4k_2^2+k_1^2)^{1/2},$$

$$p_3=k_2^{1/4}k_1^{1/4}(4k_2^2+k_1^2)^{1/4},\quad p_4=k_2^{-1/4}k_1^{-1/4}(4k_2^2+k_1^2)^{3/4};$$

k_1,k_2 are arbitrary parameters. These brackets depend on the only essential parameter k_1/k_2.

Brackets (5.3) possess the following four Casimir functions:

$$C_i=k_2(x_i^2+x_{i+4}^2)+p_3(x_{i+3}x_{i+5}+x_{i+1}x_{i+7})+k_1x_{i+2}x_{i+6},\quad i=0,1,2,3.$$

The admissible vectors are given by

$$\mathbf{a}_\pm=(t_1,0,t_2,0,\pm t_1,0,\pm t_2,0),\quad \mathbf{b}_\pm=(0,t_1,0,t_2,0,\pm t_1,0,\pm t_2),$$

where t_1,t_2 are arbitrary parameters. We see that the admissible vectors form four two-dimensional vector spaces such that $\mathbb{R}^8$ is their direct sum.

Consider the shift of coordinates defined by $\mathbf{a}_+$. As the result, we get a linear bracket $\{\cdot,\cdot\}_a=t_1\{\cdot,\cdot\}_1+t_2\{\cdot,\cdot\}_2$. Hence, we obtain a pair of compatible linear Poisson brackets $\{\cdot,\cdot\}_{1,2}$. For generic t_1,t_2, the bracket $\{\cdot,\cdot\}_a$ is isomorphic to $gl_2\oplus gl_2$. It is easy to verify that the bracket $\{\cdot,\cdot\}_a$ has two linear Casimir functions $K_1=x_0+x_4$ and $K_2=x_2+x_6$. After reducting the linear brackets to the surface $K_1=K_2=0$, we get a pair of compatible $sl_2\oplus sl_2$ brackets. It is important to mention

that the initial quadratic bracket (5.3) cannot be restricted to the surface $K_1=K_2=0$ since K_i are not Casimir functions for (5.3). One can check that the Lenard–Magri scheme applied to the reduced brackets $\{\cdot,\cdot\}_{1,2}$ produces the so(4) Schottky–Manakov top.

In the paper,[12] the Poisson algebra (5.3) is denoted by $q_{8,3}$. It turns out that the situation is the same for a wide class of quadratic elliptic Poisson algebras. Namely, let n and k be coprime positive integers such that $1\leqslant k<n$. Let $\tau\in\mathbb{C}$, where $\operatorname{Im}\tau>0$. Let us define a Poisson algebra $q_{n,k}(\tau)$ on the space of polynomials in x_i, $i\in\mathbb{Z}/n\mathbb{Z}$ as follows:

$$\{x_i,x_j\}=\left(\frac{\theta'_{j-i}(0)}{\theta_{j-i}(0)}+\frac{\theta'_{k(j-i)}(0)}{\theta_{k(j-i)}(0)}-2\pi i n\right)x_ix_j+\theta'_0(0)\sum_{r\in\mathbb{Z}/n\mathbb{Z},r\neq 0,j-i}\frac{\theta_{j-i+r(k-1)}(0)}{\theta_{kr}(0)\theta_{j-i-r}(0)}x_{j-r}x_{i+r}.$$

Here $\theta_\alpha(z)$ are defined by

$$\theta_\alpha(z)=\theta\left(z+\frac{\alpha}{n}\tau\right)\theta\left(z+\frac{1}{n}+\frac{\alpha}{n}\tau\right)\cdots\theta\left(z+\frac{n-1}{n}+\frac{\alpha}{n}\tau\right)e^{2\pi i(\alpha z+\alpha(\alpha-n)/2n\tau+\alpha/2n)}.$$

It can be readily seen that $\theta_{\alpha+n}(z)=\theta_\alpha(z)$, $\theta_\alpha(-z)=-e^{-2\pi i(nz-\alpha/n)}\theta_{-\alpha}(z)$, and

$$\theta_\alpha\left(z+\frac{1}{n}\right)=e^{2\pi i\alpha/n}\theta_\alpha(z),\quad \theta_\alpha\left(z+\frac{1}{n}\tau\right)=e^{-2\pi i(z+1/2n-(n-1)/2n\tau)}\theta_{\alpha+1}(z).$$

Using these relations, one can check that the bracket described above satisfies the Jacobi identity (see Refs. 12 and 16 for details).

Theorem 4: *For the quadratic Poisson algebras $q_{mn^2,kmn-1}(\tau)$, the set of admissible vectors is a union of n^2 components which are m-dimensional vector spaces. The space of generators of the algebra is the direct sum of these spaces.*

Theorem 4 can be proved using the so-called functional realization of these Poisson algebras (see Refs. 16 and 12). The proof will be given in another publication. The case $m=1$ was considered in detail in Refs. 17–19.

It is clear that for any m-dimensional vector space of admissible vectors for the quadratic Poisson algebra $q_{mn^2,kmn-1}(\tau)$ we obtain m compatible linear Poisson structures shifting the quadratic bracket by these vectors.

Conjecture 1: Each of the corresponding Lie algebras is isomorphic to $\oplus_{i=1}^m gl_n$. Moreover, all these Lie algebras have a common center. After factorization with respect to the center, one obtains m compatible $\oplus_{i=1}^m sl_n$ brackets. These m-Lie structures are isomorphic to the one constructed in Sec. IV, where $l=m-1$.

Conjecture 2: Each of the $(l+1)$-Lie structures constructed in Sec. III is a substructure of this m-Lie structure.

Remark 10: The Lenard–Magri scheme applied to the pair of compatible linear brackets described in Secs. II and III gives rise to an integrable model with the $\oplus_{i=1}^m sl_n$ Poisson brackets. Probably this integrable system is nothing but the elliptic Gaudin model.[17,18] However, the family of integrals for the $\oplus_{i=1}^m sl_2$-Gaudin model considered in Ref. 18 contains one parameter related to the elliptic curve plus $m-1$ additional constant parameters. In our construction, we have $2m-2$ additional parameters. But if Conjectures 1 and 2 are true, then all these additional parameters are inessential in the following sense. The complete set of integrals is given by the Casimir functions of the quadratic brackets. These integrals depend on the elliptic curve only. Furthermore, there exist linear brackets $\{\cdot,\cdot\}_1,\ldots,\{\cdot,\cdot\}_m$ that depend on the elliptic curve only such that any linear combination of these brackets is a Poisson bracket as well. The integrals commute with respect to the whole family of these brackets. If we choose two generic brackets,

$$\sum_{i=1}^{m} c_i\{\cdot,\cdot\}_i \quad \text{and} \quad \sum_{i=1}^{m} \bar{c}_i\{\cdot,\cdot\}_i,$$

and bring the first one to the canonical form $\oplus_{i=1}^{m} sl_n$ by a linear transformation, then the coefficients c_i appear as parameters in the integrals and the second bracket becomes dependent on parameters $c_i, \bar{c}_i$.

Remark 11: One more construction of families of compatible linear Poisson brackets is known.[6] It would be interesting to understand whether these families coincide with those described in our paper or not.

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Recursive parametrization and invariant phases of unitary matrices

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We present further properties of a previously proposed recursive scheme for parametrization of n-by-n unitary matrices. We show that the factors in the recursive formula may be introduced in any desired order. The method is used to study the invariant phases of unitary matrices. The case of four-by-four unitary matrices is investigated in detail. We also address the question of how to construct symmetric unitary matrices (i.e., unitary matrices U that satisfy the condition $U_{ij}=U_{ji}$) using the recursive approach. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Unitary matrices play a central role in physics. For example, the standard model of particle physics is defined by a $SU(3)\times SU(2)\times U(1)$ symmetry group and many popular grand unified models are again based on unitary symmetries. Indeed explicit representations of unitary matrices are often so badly needed that there is already a vast literature on the subject (see, for example, Ref. 1 and references therein).

Recently we have presented a simple-looking recursive parametrization of general n-by-n unitary matrices,[2] applicable also, of course, to subcategories such as special unitary matrices and orthogonal matrices which are of great importance in physics.

In recent publications Fujii and his collaborators[3] have found that the parametrization in Ref. 2 looks interesting for constructing unitary gates for quantum computation but for that purpose more study is needed. In this paper we present further results on the structure of the recursive parametrization hoping that it will be useful for future applications. You use the method to study the "invariant phases" (to be defined below) of unitary matrices, by considering the symmetries of the recursive parametrization. Subsequently, we give detailed attention to the case of four-by-four unitary matrices.

It should be emphasized that *all* parametrization of a general n-by-n unitary matrix are equivalent to each another. However, for a specific application a certain parametrization may be more convenient than others. Therefore, it is important to provide new parametrizations, a topic which has been addressed by other authors as well. See, for example, Ref. 4, a paper which contains an extended list of references and presents yet another representation of unitary matrices.

II. THE PARAMETRIZATION

A general n-by-n unitary matrix $X^{(n)}$ may be expressed as a product of three unitary matrices,

$$X^{(n)}=\Phi^{(n)}(\vec{\alpha})V^{(n)}\Phi^{(n)}(\vec{\beta}), \tag{1}$$

where the matrices Φ are diagonal unitary matrices,

$$\Phi^{(n)}(\vec{\alpha})=\mathrm{diag}(e^{i\alpha_1},e^{i\alpha_2},\ldots,e^{i\alpha_n}) \tag{2}$$

$\Phi(\vec{\beta})$ is defined analogously, the α's and β's being real. We shall refer to Φ's as external (pure phase) matrices.

The matrix $X^{(n)}$ has n^2 real parameters. The quantities $\vec{\alpha}$ and $\vec{\beta}$ take care of $2n-1$ of these parameters because only the sums $\alpha_i+\beta_j$ enter, where i and j run from 1 to n. The remaining $(n-1)^2$ real parameters reside in the nontrivial matrix $V^{(n)}$ which was the subject of the study presented in Ref. 2 and will be further investigated in this paper. For simplicity, whenever no confusion may arise, we refer to $V^{(n)}$ as the most general n-by-n unitary matrix leaving out the qualifying statement that this is only true modulo the external matrices $\Phi(\vec{\alpha})$ and $\Phi(\vec{\beta})$. In Ref. 2 it was shown that the matrix $V^{(n)}$ may be written in the form (note that the notations in this paper are a simplified version of that in Ref. 2)

$$V^{(n)} = A_{n,2}A_{n,3}\ldots A_{n,n-1}A_{n,n}, \tag{3}$$

where the $A_{n,k}$ are unitary matrices defined by

$$A_{n,k} = \begin{pmatrix} \mathbb{A}^{(k)} & 0 \\ 0 & I_{n-k} \end{pmatrix}. \tag{4}$$

Here I_{n-k} is the unit matrix of order $n-k$. For $k=n$ this unit matrix is absent. $\mathbb{A}^{(k)}$ is a k-by-k unitary matrix,

$$\mathbb{A}^{(k)} \equiv \begin{pmatrix} I_{k-1} - (1-c_k)|A^{(k)}\rangle\langle A^{(k)}| & s_k|A^{(k)}\rangle \\ -s_k\langle A^{(k)}| & c_k \end{pmatrix}. \tag{5}$$

Here c_k and s_k stand for cosine and sine of an angle denoted by θ_k. Furthermore, $|A^{(k)}\rangle$ is a $k-1$ dimensional complex vector normalized to one,

$$|A^{k)}\rangle = \begin{pmatrix} a_1^{(k)} \\ a_2^{(k)} \\ \cdots \\ \cdots \\ a_{k-1}^{(k)} \end{pmatrix}, \quad \langle A^{k)}|A^{k)}\rangle = 1 \tag{6}$$

and $(|A^{(k)}\rangle\langle A^{(k)}|)_{ij} = a_i^{(k)}a_j^{(k)\star}$. We shall refer to $|A^{(k)}\rangle$ as the characteristic vector of order k.

The parameter counting was presented in Ref. 2 where it was shown that $V^{(n)}$, thus obtained, is the most general n-by-n unitary matrix, again modulo the external matrices Φ. The essential point is that $|A^{k)}\rangle$ introduces $2(k-2)$ real parameters and not $2(k-1)$, the reason being that it is normalized and its overall phase can be absorbed into the definition of the external matrices Φ.

To summarize, in this recursive parametrization the n-by-n unitary matrix is represented by a product of $n-1$ unitary matrices, each with its own angle θ and characteristic vector $|A\rangle$ while, for example, in the conventional approach in particle physics one would write the matrix as a product of at least $n(n-1)/2$ matrices, these being Euler rotation matrices, $(n-1)(n-2)/2$ of them modified by phases (see, for example, Ref. 5 and references therein). Note also that in Ref. 4 the matrix is parametrized by a product of n diagonal unitary matrices interlaced with $n-1$ orthogonal matrices.

A. Reordering of the factors

At the first sight, the recursive parametrization appears highly ordered and rigid. In Eq. (3), the two-by-two structure is immediately followed by the three-by-three and so on. Actually, we may write these factors *in any order* we wish by observing that the order of factors in a given product, $A_{n,r}A_{n,s}$, may be flipped as follows. For $r<s$ we have

$$A_{n,r}A_{n,s} = (A_{n,r}A_{n,s}A_{n,r}^{\dagger})A_{n,r} \equiv A'_{n,s}A_{n,r}, \tag{7}$$

where $A'_{n,s}$ has the same form as $A_{n,s}$. The two characteristic vectors appearing in these matrices are related by a unitary rotation,

$$|A'^{(s)}\rangle = \hat{\mathbb{A}}^{(r)}|A^{(s)}\rangle, \tag{8}$$

$$\hat{\mathbb{A}}^{(r)} = \begin{pmatrix} \mathbb{A}^{(r)} & 0 \\ 0 & I_{s-1-r} \end{pmatrix}. \tag{9}$$

For the case $s<r$ we have

$$A_{n,r}A_{n,s} = A_{n,s}(A^{\dagger}_{n,s}A_{n,r}A_{n,s}) \equiv A_{n,s}A''_{n,r}, \tag{10}$$

where now the two characteristic vectors are related by

$$|A''^{(r)}\rangle = \hat{\mathbb{A}}^{\dagger(s)}|A^{(r)}\rangle. \tag{11}$$

Obviously, by inserting as many factors $A^{\dagger}_{n,j}A_{n,j}=1$ as needed in the recursion formula, Eq. (3), one may move the factors around as one wishes. The upshot is that in the reordering process a factor of lower rank simply "tunnels" through that of a higher rank without being affected but induces a unitary rotation of the characteristic vector of the latter. Thus the ensuing parametrization remains the most general one. Note that the angles θ_k remain invariant under reordering.

The recursive parametrization looks highly asymmetric. However, using the above reordering procedure, one may construct manifestly symmetric unitary matrices (see the Appendix).

B. Further properties of the recursive parametrization

We wish to study, in more detail, the properties of the matrices $\mathbb{A}^{(k)}$ in Eq. (5) as these are the building blocks of the recursive parametrization.

To begin with we simplify the notation, to avoid indices, and introduce a generic matrix $\mathbb{A}$ defined by

$$\mathbb{A} \equiv \begin{pmatrix} I-(1-c)|A\rangle\langle A| & s|A\rangle \\ -s\langle A| & c \end{pmatrix}. \tag{12}$$

Here, as usual, I denotes the appropriate unit matrix and c and s stand for cosine and sine of an angle, respectively. The angle itself will be denoted by θ. Defining

$$Y \equiv |A\rangle\langle A| \tag{13}$$

we have that Y is Hermitian and satisfies

$$Y|A\rangle = |A\rangle, \quad Y^2 = Y, \quad \text{tr } Y = 1, \quad \det Y = 0, \tag{14}$$

where the vanishing of the determinant is, of course, only valid when Y is a matrix and not just a number as is the case when $|A\rangle$ is one dimensional. Following Fujii,[3] we introduce a matrix $\mathbb{G}$ which generates $\mathbb{A}$,

$$\mathbb{G} \equiv \begin{pmatrix} 0 & -i|A\rangle \\ i\langle A| & 0 \end{pmatrix}. \tag{15}$$

This matrix is hermitian and satisfies $\mathbb{G}^3=\mathbb{G}$. A simple computation, using Eqs. (14), yields

$$\mathbb{A} = e^{i\theta\mathbb{G}} = I + is\mathbb{G} - (1-c)\mathbb{G}^2. \tag{16}$$

This relation is reminiscent of the expansion of exponentials containing Pauli matrices σ (in a short-hand notation, $e^{i\theta\sigma}=c+is\sigma$). The essential point here is that the series expansion of $e^{i\theta\mathbb{G}}$, for arbitrarily $\mathbb{G}$, terminates rapidly and does not continue for ever as the exponentials often tend to do. Furthermore we have

$$\mathrm{tr}\,\mathbb{G}=0,\quad \mathrm{tr}\,\mathbb{G}^2=2,\quad \det\mathbb{A}=1. \tag{17}$$

Note also that, for a fixed $\mathbb{G}$, the matrix $\mathbb{A}$ is Abelian with respect to θ,

$$\mathbb{A}(\theta_i)\mathbb{A}(\theta_j)=\mathbb{A}(\theta_i+\theta_j) \tag{18}$$

and

$$\mathbb{A}^{-1}(\theta)=\mathbb{A}(-\theta). \tag{19}$$

To rewrite the recursion formula, Eq. (3), in terms of $\mathbb{G}$ and $\mathbb{A}$ we must attach appropriate indices to our generic $\mathbb{G}$ (or $\mathbb{A}$) to distinguish the relevant factors. We introduce

$$\mathbb{G}_{n,k}=\begin{pmatrix}\begin{pmatrix}0 & -i|A^{(k)}\rangle\\ i\langle A^{(k)}| & 0\end{pmatrix} & 0\\ 0 & 0\end{pmatrix}, \tag{20}$$

where the required number of zeros have been added to make $\mathbb{G}_{n,k}$ an n-by-n matrix. This yields that the factor $A_{n,k}$ in the recursion formula Eq. (3) is given by

$$A_{n,k}\equiv e^{i\theta_k\mathbb{G}_{n,k}}=I_n+is_k\mathbb{G}_{n,k}-(1-c_k)\mathbb{G}_{n,k}^2. \tag{21}$$

III. INVARIANT PHASES OF UNITARY MATRICES

The invariant phases of a unitary n-by-n matrix V^n are defined as those phases of the matrix that cannot be "removed" with any choice of the external phase matrices Φ in Eq. (1). These phases play an important role in particle physics as they are measurable quantities related to CP violation (for a review see, for example, Ref. 6).

Given a unitary matrix, the simplest way to detect the presence of invariant phases in it is to construct

$$(\alpha\beta;jk)\equiv \mathrm{Im}(V_{\alpha j}V_{\beta k}V_{\alpha k}^{\star}V_{\beta j}^{\star}), \tag{22}$$

where we have suppressed the superscript n. The symbols α,β and j,k now refer to rows and columns of the matrix and the indices are not summed. These imaginary parts are manifestly invariant under multiplication by the external phase matrices. Therefore if any of them is nonzero that would be a signal of the presence of a nonremovable phase in the matrix. We refer to these imaginary parts as invariant phases of the matrix instead of calling them invariants of the matrix that contain nonremovable phases. One may easily construct higher order invariants, containing properly chosen, six or more, elements of the matrix but these are in general reducible to the above set unless the matrix would have vanishing elements. For example, for $V_{\beta j}\neq 0$,

$$\mathrm{Im}(V_{\alpha j}V_{\beta k}V_{\gamma l}V_{\alpha k}^{\star}V_{\beta l}^{\star}V_{\gamma j}^{\star})=\frac{1}{|V_{\beta j}|^2}\,\mathrm{Im}\{(V_{\alpha j}V_{\beta k}V_{\alpha k}^{\star}V_{\beta j}^{\star})(V_{\beta j}V_{\gamma l}V_{\beta l}^{\star}V_{\gamma j}^{\star})\} \tag{23}$$

$$=\frac{1}{|V_{\beta j}|^2}\{(\alpha\beta,jk)\langle\beta\gamma,jl\rangle+\langle\alpha\beta,jk\rangle(\beta\gamma,jl)\}, \tag{24}$$

where none of the indices is summed and

$$\langle\alpha\beta;jk\rangle\equiv \mathrm{Re}[V_{\alpha j}V_{\beta k}V_{\alpha k}^{\star}V_{\beta j}^{\star}]. \tag{25}$$

These real parts are also invariant under the action of the external matrices. The above reduction would not work if $V_{\alpha j}=0$ but then the analysis is much simpler to begin with (see below) as the matrix contains fewer invariant phases.

Returning to the simplest invariant phases, there are altogether $[n(n-1)/2]^2$ quantities $(\alpha\beta;jk)$, because these are antisymmetric under the interchange of the row indices, $\alpha\leftrightarrow\beta$, as well as under the interchange of the column indices, $j\leftrightarrow k$. However, we know that the most general $V^{(n)}$ has "only" $(n-1)(n-2)/2$ independent invariant phases. One may therefore look for $(n-1)\times(n-2)/2$ independent $(\alpha\beta;jk)$'s and use them as a basis for expressing the remaining ones.

As mentioned above, the invariants in Eq. (22) play an essential role in the n-family version of the standard model of particle physics as they are measurable quantities related to CP violation. For the case of $n=3$ there is only one such quantity

$$(\alpha\beta;jk) \equiv J\sum_{\gamma,i} \epsilon_{\gamma\alpha\beta}\epsilon_{ijk}. \tag{26}$$

The row and column unitarity conditions for a three-by-three unitary matrix define six triangles. One may show that[7] all these triangles have the same area and this unique area equals $J/2$.

For $n=4$ there are 36 possible invariants $(\alpha\beta;jk)$ but only three independent ones. In Ref. 8 an attempt was made to find an appropriate basis and carry through the above program. The treatment of this issue is much simpler in the recursive parametrization, as will be shown in the next section.

A. Invariant phases of four-by-four unitary matrices

For $n=4$ we have from Eq. (3)

$$V^{(4)} = A_{4,2}A_{4,3}A_{4,4}, \tag{27}$$

where each factor comes with its own θ and characteristic vector $|A\rangle$. We denote the latter by

$$|A^{(2)}\rangle = 1, \quad |A^{(3)}\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad |A^{(4)}\rangle = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \tag{28}$$

remembering that x's and y's are complex numbers and $\langle A^{(k)}|A^{(k)}\rangle=1$, $k=2,3,4$. We shall now spell out this four-by-four matrix in order to exhibit its symmetries in a manifest fashion. This will also enable us to understand the general case of n-by-n matrices. Equation (3) yields

$$V^{(4)} = \begin{pmatrix} c_2 & s_2 & 0 & 0 \\ -s_2 & c_2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1-(1-c_3)x_1x_1^\star & -(1-c_3)x_1x_2^\star & s_3x_1 & 0 \\ -(1-c_3)x_2x_1^\star & 1-(1-c_3)x_2x_2^\star & s_3x_2 & 0 \\ -s_3x_1^\star & -s_3x_2^\star & c_3 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
$$\times \begin{pmatrix} 1-(1-c_4)y_1y_1^\star & -(1-c_4)y_1y_2^\star & -(1-c_4)y_1y_3^\star & s_4y_1 \\ -(1-c_4)y_2y_1^\star & 1-(1-c_4)y_2y_2^\star & -(1-c_4)y_2y_3^\star & s_4y_2 \\ -(1-c_4)y_3y_1^\star & -(1-c_4)y_3y_2^\star & 1-(1-c_4)y_3y_3^\star & s_4y_3 \\ -s_4y_1^\star & -s_4y_2^\star & -s_4y_3^\star & c_4 \end{pmatrix}. \tag{29}$$

We now focus on the symmetries of this matrix. By symmetries we mean transformations that leave $V^{(4)}$ invariant modulo the external matrices Φ in Eq. (1). A simple inspection shows that this matrix has two such symmetries, denoted by S_1 and S_2 and defined by

$$S_1, \quad \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to e^{i\phi_2}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad y_3 \to e^{-i\phi_2}y_3, \tag{30}$$

$$S_2, \quad \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \to e^{i\phi_3} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \tag{31}$$

where ϕ_2 and ϕ_3 are arbitrary phases. The indices are to remind us of the dimension of the corresponding vector. Therefore the three independent phases in $V^{(4)}$ can be chosen to be

$$\omega_1 = \phi(x_2) - \phi(x_1),$$

$$\omega_2 = \phi(y_2) - \phi(y_1), \tag{32}$$

$$\omega_3 = \phi(x_2) + \phi(y_3) - \phi(y_2).$$

Here $\phi(x_j)$ and $\phi(y_k)$ denote the phases of the corresponding parameters. These phases are not invariant under the above symmetries and thus cannot appear as independent entities in computations of invariants of $V^{(4)}$. Allowed to appear are the ω's or any combination of them because these are invariant under the action of both S_1 and S_2. We may, if we so wish, use the symmetry S_1 to rotate the phase of x_2 to zero, and then employ the symmetry S_2 to do the same with the ensuing y_3 whereby x_2 and y_3 may be taken to be real and say positive. The invariant phases in this "frame" are then $\phi(x_1)$, $\phi(y_1)$, and $\phi(y_2)$. These constitute the maximum number of independent phases that $V^{(4)}$ can possess. By imposing further relations on the angles or the x's and y's this number could be smaller as shall be considered further below.

B. Generalization to larger *n*

Going one order higher to $n=5$, we must introduce the relevant characteristic vector

$$|A^{(5)}\rangle \equiv \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}. \tag{33}$$

The corresponding matrix $V^{(5)}$ has three symmetries given by

$$S_1, \quad \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to e^{i\phi_2} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad y_3 \to e^{-i\phi_2} y_3, \quad z_3 \to e^{-i\phi_2} z_3, \tag{34}$$

$$S_2, \quad \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \to e^{i\phi_3} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \quad z_4 \to e^{-i\phi_3}, \tag{35}$$

$$S_3, \quad \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix} \to e^{i\phi_4} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}. \tag{36}$$

In this case there are six invariant phases. These may be chosen as

$$\omega_1 = \phi(x_2) - \phi(x_1),$$

$$\omega_2 = \phi(y_2) - \phi(y_1),$$

$$\omega_3 = \phi(z_2) - \phi(z_1),$$

$$\omega_4 = \phi(x_2) + \phi(y_3) - \phi(y_2), \tag{37}$$

$$\omega_5 = \phi(x_2) + \phi(z_3) - \phi(z_2),$$

$$\omega_6 = \phi(y_3) + \phi(z_4) - \phi(z_3).$$

As before, we may use S_1 to remove the phase of x_2 followed by S_2 and S_3 to rotate the ensuing y_3 and z_4 to be real and say positive. The invariant phases are then the phases of x_1, y_1, y_2, z_1, z_2, and z_3. Note that, from the very beginning we chose the angle θ_2 not to be accompanied by a phase, i.e., $|A^{(2)}\rangle = 1$. One can, of course, leave the phase of $|A^{(2)}\rangle$ arbitrary. This will introduce an extra symmetry which we have not bothered to write down as it is trivial.

The above procedure may be generalized to arbitrary order n. Without loss of generality, we may take, for example, the last component of all the characteristic vectors $|A^{(k)}\rangle$ to be real. The invariant phases are then the phases of the remaining components. For an n-by-n matrix there are then $1+2+\cdots+(n-2)=(n-1)(n-2)/2$ such independent phases as expected.

C. The "panel" approach to invariant phases

Another approach to constructing the invariant phases of a matrix is to consider the latter as a lattice. For the case of $n=4$, considered from now on, the matrix can be visualized as shown

$$\begin{array}{ccccccc}
\bullet & & \bullet & & \bullet & & \bullet \\
 & P_{11} & & P_{12} & & P_{13} & \\
\bullet & & \bullet & & \bullet & & \bullet \\
 & P_{21} & & P_{22} & & P_{23} & \\
\bullet & & \bullet & & \bullet & & \bullet \\
 & P_{31} & & P_{32} & & P_{33} & \\
\bullet & & \bullet & & \bullet & & \bullet
\end{array} . \tag{38}$$

The bullets denote the sites where the matrix elements are situated. For example, the bullets on the first row stand for V_{11}, V_{12}, V_{13}, and V_{14} and so on. The P's denote minipanels of the matrix, to be described here below. The invariants of interest to us are again

$$(\alpha\beta;jk) \equiv \mathrm{Im}[V_{\alpha j} V_{\beta k} V^{\star}_{\alpha k} V^{\star}_{\beta j}], \tag{39}$$

$$\langle\alpha\beta;jk\rangle \equiv \mathrm{Re}[V_{\alpha j} V_{\beta k} V^{\star}_{\alpha k} V^{\star}_{\beta j}]. \tag{40}$$

As mentioned before, there are 36 quantities $(\alpha\beta;jk)$ (six possible combinations of α,β multiplied by as many combinations of j,k) and we are looking for a set of three of them such that all the others can be expressed as functions of them and the real parts $\langle\alpha\beta;jk\rangle$. This problem was treated long time ago[8] and was found to be rather involved. Here we provide some simplification. Nine of these invariants (the nearest neighbors) are explicitly exhibited on our lattice. Their analytic form may easily be read off from their locations. For example,

$$P_{11} \equiv V_{11} V_{22} V^{\star}_{12} V^{\star}_{21},$$

$$P_{12} \equiv V_{12} V_{23} V^{\star}_{13} V^{\star}_{22},$$

$$P_{22} \equiv V_{22} V_{33} V^{\star}_{23} V^{\star}_{32},$$

$$P_{32} \equiv V_{32}V_{43}V_{33}^{\star}V_{42}^{\star},$$

and so on. Furthermore

$$P_{ab} = R_{ab} + iJ_{ab}, \tag{41}$$

where R and J denote the real and imaginary parts of the corresponding P. Thus the imaginary parts, in the notation employed earlier, are given by

$$J_{11} = (12;12), \quad J_{12} = (12;23), \quad J_{22} = (23;23), \quad J_{32} = (34;23) \tag{42}$$

and so forth. Similar expressions may be written down for the real parts.

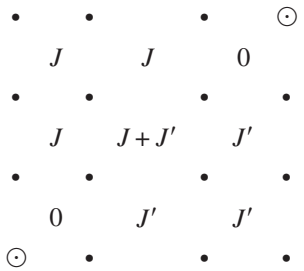
Suppose that none of the matrix elements vanishes. Using unitarity conditions we then find

$$\begin{aligned}
J_{13} - \left(1 + \frac{R_{11}}{|V_{12}V_{22}|^2}\right)J_{12} &= \frac{R_{12}}{|V_{12}V_{22}|^2}J_{11}, \\
J_{13} - \left(1 + \frac{R_{33}}{|V_{33}V_{34}|^2}\right)J_{23} &= \frac{R_{23}}{|V_{33}V_{34}|^2}J_{33}, \\
J_{31} - \left(1 + \frac{R_{11}}{|V_{21}V_{22}|^2}\right)J_{21} &= \frac{R_{21}}{|V_{21}V_{22}|^2}J_{11}, \\
J_{31} - \left(1 + \frac{R_{33}}{|V_{33}V_{43}|^2}\right)J_{32} &= \frac{R_{32}}{|V_{33}V_{43}|^2}J_{33}, \\
J_{12} - \frac{R_{22}}{|V_{32}V_{33}|^2}J_{32} &= \left(1 + \frac{R_{32}}{|V_{32}V_{33}|^2}\right)J_{22}, \\
J_{21} - \frac{R_{22}}{|V_{23}V_{33}|^2}J_{23} &= \left(1 + \frac{R_{23}}{|V_{23}V_{33}|^2}\right)J_{22}.
\end{aligned} \tag{43}$$

In principle, we may take the set J_{11}, J_{22}, J_{33} to constitute a basis and determine the remaining six J's in terms of them. These equations are rather complicated and need further thought concerning special cases. For example, if the matrix is symmetric we only have three equations but, of course, also only three unknown, say J_{12}, J_{13}, and J_{23}. We are not allowed to divide by vanishing matrix elements and so forth. Here below, we shall consider a simple and yet nontrivial example to demonstrate the technique and to compare it with the recursive approach which is much simpler and does not require thinking about the possible pitfalls.

D. A simple example

For simplicity we consider the case where two of the elements of the four-by-four matrix are zero, and where these elements are neither on the same row nor on the same column. All other elements of the matrix are assumed to be nonzero. Without loss of generality we may take the two vanishing elements to be V_{14} and V_{41} which in particle physics would correspond to the case where the mixing of the first and the fourth families is negligible. Our lattice, with its nine minipanels, now looks as follows:



(44)

Here the ⊙'s indicate where the vanishing matrix elements are situated and we have defined

$$J = J_{11} \equiv (12,12), \quad J' = J_{33} \equiv (34,34). \tag{45}$$

A simple computation, using unitarity relations, gives the imaginary parts of the minipanels as marked in the lattice. Computing all the imaginary parts, we find that 19 of the 36 invariants $(\alpha\beta, jk)$ vanish. The nonvanishing ones, in addition to J and J' defined in Eq. (45), are

$$\begin{aligned} &-(12,13) = (12,23) = -(13,12) = (13,13) = -(13,23) = (23,12) = -(23,13) = J, \\ &-(23,24) = (23,34) = -(24,23) = (24,24) = -(24,34) = (34,23) = -(34,24) = J', \end{aligned} \tag{46}$$

and

$$(23,23) = J + J' \tag{47}$$

as exhibited in the corresponding panel. Moreover, we find

$$\frac{J'^2}{J^2} = \left|\frac{V_{24}V_{34}}{V_{21}V_{31}}\right|^2 = \left|\frac{V_{42}V_{43}}{V_{12}V_{13}}\right|^2 = \left(\frac{|V_{24}|^2 + |V_{34}|^2}{|V_{12}|^2 + |V_{13}|^2}\right)^2 = \left(\frac{|V_{42}|^2 + |V_{43}|^2}{|V_{21}|^2 + |V_{31}|^2}\right)^2. \tag{48}$$

It is amusing to note that the unitarity relations for the above matrix define eight triangles. Using the method in Ref. 7 one finds that four of these have each an area equal to $J/2$ while the area of the other four is $J'/2$.

We would now like to compute J and J'. For this purpose we turn to the recursive parametrization. It turns out that the calculations are simpler if we take $V_{34}=V_{43}=0$ instead of the above choice $V_{14}=V_{41}=0$. The two choices are equivalent as they are related to one another by interchanges in rows and columns. This amounts to a relabeling of the matrix elements which obviously cannot affect the results. After finishing the computations we can simply revert to the former case by interchanging rows one and three as well as columns one and three.

In the recursive parametrization, Eq. (29), the conditions $V_{34}=V_{43}=0$ give

$$y_3 = x_1 y_1^\star + x_2 y_2^\star = 0. \tag{49}$$

These conditions tell us that $|y_1|=|x_2|$, $|y_2|=|x_1|$ and that x_1 and y_1 are relatively real in the frame where x_2 and y_2 are taken to be real. Therefore, there is only one invariant phase, in this example. We introduce the lattice again

$$
\begin{array}{cccccc}
\bullet & & \bullet & & \bullet & & \bullet \\
& \hat{J} & & \hat{J} & & 0 & \\
\bullet & & \bullet & & \bullet & & \bullet \\
& \hat{J} & & \hat{J} & & 0 & \\
\bullet & & \bullet & & \bullet & & \odot \\
& 0 & & 0 & & 0 & \\
\bullet & & \bullet & & \odot & & \bullet
\end{array}
\quad . \tag{50}
$$

$\odot$'s indicate where the vanishing matrix elements are situated. Furthermore, we have exhibited the imaginary parts of the minipanels starting with the definition

$$\hat{J} = (12,12). \tag{51}$$

Taking into account the permutations, we find that $\hat{J}$ here is identical with our previous J that we wanted to compute. Using the recursive parametrization we find

$$
\begin{aligned}
J &= c_2 c_3 c_4 s_2 s_3^2 \,\mathrm{Im}(x_1^\star x_2), \\
J' &= -\, c_2 c_3 c_4 s_2 s_4^2 \,\mathrm{Im}(x_1^\star x_2).
\end{aligned} \tag{52}
$$

Thus

$$\frac{J'}{J} = -\,\frac{s_4^2}{s_3^2}. \tag{53}$$

For comparison, note that for a general three-by-three matrix [which we may obtain from Eq. (29) by setting $\theta_4 = 0$] the unique invariant is given by $J^{(3\text{-fam})} = c_2 c_3 s_2 s_3^2 \,\mathrm{Im}(x_1^\star x_2)$.

The recursive parametrization allows us to compute all the imaginary parts for the most general case, i.e., irrespectively of whether the matrix has zeros or not. We find, for the general four-by-four matrix, parametrized as in Eq. (29),

$$
\begin{aligned}
(34,34) &= c_3 c_4 s_3 s_4^2 |y_3| \{ |x_2 y_2| \sin\omega_3 + |x_1 y_1| \sin(\omega_3 + \omega_2 - \omega_1) \}, \\
(34,24) &= c_4 s_3 s_4^2 |x_2 y_2| \{ s_3 |x_1 y_1| \sin(\omega_1 - \omega_2) - c_3 |y_3| \sin\omega_3 \},
\end{aligned} \tag{54}
$$

where the angles ω_j are as defined in Eq. (32). We thus see that, as expected, only the invariant phases appear in these relations. We do not quote the remaining imaginary parts $(\alpha\beta, jk)$. The important point is that all of them are functions of $|x_j|$, $|y_j|$ and the three ω's, as expected.

IV. CONCLUSIONS

In this paper, we have presented further properties of the recursive parametrization of unitary matrices proposed in Ref. 2, where the matrix is written as a product of $n-1$ matrices each with its own angle θ and characteristic vector $|A\rangle$. We have found that the factors in the recursive formula may be introduced in any desired order.

Encouraged by the convenience of the recursive method, we have taken a fresh look at the issue of invariant phases of unitary matrices. After having exhibited the symmetries of the parametrization, we have shown how the invariant phases of n-by-n matrices can be identified. Subsequently, we have paid particular attention to the case $n=4$ and have compared the results with those of an earlier approach based on "panels" of the matrix.

The recursive parametrization has some really nice features because in some cases it allows the "new physics" to be introduced in a gentle manner through the last factor in the recursion formula, a topic which we are currently studying.

In an earlier study,[9] we found that there is a parametrization that allows one to introduce, in a simple way, any desired angle of any of the so-called unitarity triangles as one of the parameters in the quark mixing matrix for three families in the standard model of particle physics. The same parametrization allowed us to choose the expansion parameter in this matrix to be λ^2 instead of λ that one usually uses.[5] Indeed λ is not so small ($\lambda=0.2$). Therefore, the recursive parametrization may be convenient whenever expansion in the above parameter is required, for example, in model building or for construction of quark and lepton mass matrices. It turned out that the parametrization found in Ref. 9, with the above nice features, is indeed nothing but the order $n=3$ version of the recursive parametrization discussed in this paper and in Ref. 2.

Finally, in the Appendix of this paper, we deal with the question of how to construct manifestly symmetric unitary matrices in the recursive framework.

APPENDIX: SYMMETRIC UNITARY MATRICES

A matrix X is defined to be symmetric if $X_{ij}=X_{ji}$. We write the symmetric unitary matrix in the form

$$X^{(n)\mathrm{sym}} = \Phi^{(n)}(\vec{\alpha}) V^{(n)\mathrm{sym}} \Phi^{(n)}(\vec{\alpha}) \tag{A1}$$

requiring $V^{(n)\mathrm{sym}}$ to be symmetric, as indicated by its superscript, and that the external matrices be the same [see Eq. (1)]. A general symmetric unitary matrix has $n(n+1)/2$ real parameters. The external matrix Φ takes care of n of them. Thus $n(n-1)/2$ real parameters reside in $V^{(n)\mathrm{sym}}$.

For a general $V^{(n)}$, we have (see Sec. II B) that the factors in the recursion formula Eq. (3) may be written as

$$A_{n,k} = e^{i\theta_k \mathbb{G}_{n,k}}, \tag{A2}$$

where the generating matrix $\mathbb{G}_{n,k}$ is Hermitian. In order to obtain a symmetric $A_{n,k}$ we must impose the additional requirement that the generating matrix be symmetric. This means that the corresponding characteristic vector is purely imaginary. For example, for $k=2$ we obtain

$$V^{(2)\mathrm{sym}} \equiv A^{\mathrm{sym}}_{n,2} = \begin{pmatrix} c_2 & is_2 & 0 \\ is_2 & c_2 & 0 \\ 0 & 0 & I_{n-2} \end{pmatrix} \tag{A3}$$

and for $k=3$,

$$A^{\mathrm{sym}}_{n,3} \begin{pmatrix} 1-(1-c_3)x_1^2 & -(1-c_3)x_1x_2 & is_3x_1 & 0 \\ -(1-c_3)x_1x2_1 & 1-(1-c_3)x_2^2 & is_3x_2 & 0 \\ is_3x_1 & is_3x_2 & c_3 & 0 \\ 0 & 0 & 0 & I_{n-3} \end{pmatrix}. \tag{A4}$$

We have set $|A\rangle = i|x\rangle$, where the x's are real. Thus, the construction of symmetric factors in the recursion formula is a trivial task. But, of course, the product of these factors will not be symmetric. This defect is easily remedied by invoking the reordering procedure described in Sec. II A in which we showed that the reordering of the factors in the recursion formula only amounts to a redefinition of the characteristic vectors. Therefore, we may write

$$V^{(n)\mathrm{sym}} = A^{\mathrm{sym}}_{n,2} A^{\mathrm{sym}}_{n,3} \cdots A^{\mathrm{sym}}_{n,n-1} A^{\mathrm{sym}}_{n,n} A^{\mathrm{sym}}_{n,n-1} \cdots A^{\mathrm{sym}}_{n,3} A^{\mathrm{sym}}_{n,2}, \tag{A5}$$

$V^{(n)\mathrm{sym}}$ thus obtained is manifestly unitary and symmetric. We must now count the number of its independent parameters. Each order k introduces $k-1$ real parameters, these being the angle θ_k and $k-2$ components of the corresponding characteristic vector (one component being redundant because the vector is normalized). Therefore the total number of parameters in $V^{(n)\mathrm{sym}}$ is

$$\sum_{k=2}^{n}(k-1)=n(n-1)/2 \tag{A6}$$

as expected. Adding into this number the n parameters coming from the external matrices amounts to the total of $n(n+1)/2$ real parameters, as required.

Note that it would be somewhat more elegant to call the angles in the above factors $\theta_k/2$ instead of θ_k, except the angle θ_n of the factor $A^{\mathrm{sym}}_{n,n}$. The reason being that $A^{\mathrm{sym}}_{n,n}$ appears only once while the others appear twice.

The chain in Eq. (A5) looks long and perhaps a bit frightening. However, if needed for practical applications, it can be somewhat simplified as we shall now describe.

Consider the case $n=3$, where we introduce

$$V^{(3)\mathrm{sym}}\equiv V^{(2)\mathrm{sym}}(\theta_2/2)A^{(3)\mathrm{sym}}V^{(2)\mathrm{sym}}(\theta_2/2), \tag{A7}$$

where $V^{(2)\mathrm{sym}}$ is as defined in Eq. (A3), for $n=3$. Multiplying the factors, we find

$$V^{(3)\mathrm{sym}}=\begin{pmatrix} c_2-(1-c_3)u_1^2 & is_2-(1-c_3)u_1u_2 & is_3u_1 \\ is_2-(1-c_3)u_1u_2 & c_2-(1-c_3)u_2^2 & is_3u_2 \\ is_3u_1 & is_3u_2 & c_3 \end{pmatrix}. \tag{A8}$$

Here

$$u_1=c_2'x_1+is_2'x_2,\quad u_2=c_2'x_2+is_2'x_1 \tag{A9}$$

$c_2'=\cos(\theta_2/2)$ and $s_2'=\sin(\theta_2/2)$. Moreover, the x's are as introduced in Eq. (A4).

The essential point is that we may set aside the question of the origin of the u's and their relationship with the x's and simply consider them as our new variables, as two complex numbers that satisfy

$$|u_1|^2+|u_2|^2=1 \tag{A10}$$

and, of course, $c_2'u_1-is_2'u_2$ as well as $c_2'u_2-is_2'u_1$ must be real as these are x_1 and x_2 in the above equations. Going to the next order, $n=4$, we may use the identity

$$A_2^{\mathrm{sym}}A_3^{\mathrm{sym}}A_4^{\mathrm{sym}}A_3^{\mathrm{sym}}A_2^{\mathrm{sym}}=A_2^{\mathrm{sym}}A_3^{\mathrm{sym}}A_2^{\mathrm{sym}}[(A_2^{\mathrm{sym}})^{-1}A_4^{\mathrm{sym}}(A_2^{\mathrm{sym}})^{-1}]A_2^{\mathrm{sym}}A_3^{\mathrm{sym}}A_2^{\mathrm{sym}}=V^{(3)\mathrm{sym}}[A_4'^{\mathrm{sym}}]V^{(3)\mathrm{sym}},$$

$$A_4'^{\mathrm{sym}}\equiv(A_2^{\mathrm{sym}})^{-1}A_4^{\mathrm{sym}}(A_2^{\mathrm{sym}})^{-1}. \tag{A11}$$

Here $V^{(3)\mathrm{sym}}$ is as found in Eq. (A8). From our earlier results, we have

$$A_4^{\mathrm{sym}}=\begin{pmatrix} 1-(1-c_4)y_1^2 & -(1-c_4)y_1y_2 & -(1-c_4)y_1y_3 & is_4y_1 \\ -(1-c_4)y_1y_2 & 1-(1-c_4)y_2^2 & -(1-c_4)y_2y_3 & is_4y_2 \\ -(1-c_4)y_1y_3 & -(1-c_4)y_2y_3 & 1-(1-c_4)y_3^2 & is_4y_3 \\ is_4y_1 & is_4y_2 & is_4y_3 & c_4 \end{pmatrix}, \tag{A12}$$

where y's are real. Therefore, we may immediately write down the factor $A_4'^{\mathrm{sym}}$, without having to do any calculations. The first two components of the vector y get "rotated" but y_3 is untouched. We find

$$A_4^{\mathrm{sym}\prime}=\begin{pmatrix} c_2-(1-c_4)v_1^2 & -is_2-(1-c_4)v_1v_2 & -(1-c_4)v_1v_3 & is_4v_1 \\ -is_2-(1-c_4)v_1v_2 & c_2-(1-c_4)v_2^2 & -(1-c_4)v_2v_3 & is_4v_2 \\ -(1-c_4)v_1v_3 & -(1-c_4)v_2v_3 & 1-(1-c_4)v_3^2 & is_4v_3 \\ is_4v_1 & is_4v_2 & is_4v_3 & c_4 \end{pmatrix}, \tag{A13}$$

where

$$v_1 = c_2' y_1 - i s_2' y_2, \quad v_2 = c_2' y_2 - i s_2' y_1, \quad v_3 = y_3. \tag{A14}$$

Again the vector v has unit norm and we may, as before, forget about the y's and just use v's, keeping in mind that v_1 and v_2 are complex numbers.

As a final example, we wish to compute the quantity J for the case of a three-by-three symmetric matrix, where

$$(\alpha\beta;jk) \equiv J \sum_{\gamma,i} \epsilon_{\gamma\alpha\beta}\epsilon_{ijk} \tag{A15}$$

and $V^{(3)\mathrm{sym}}$ is as given in Eq. (A8). A glance at this matrix yields

$$J = c_2 c_3 s_3^2 \,\mathrm{Im}\,(u_2)^2 = c_2 c_3 s_2 s_3^2 x_1 x_2. \tag{A16}$$

This resembles our earlier result in Sec. III D where we found $J^{(3-\mathrm{fam})} = c_2 c_3 s_2 s_3^2 \,\mathrm{Im}(x_1^\star x_2)$. The meaning of the x's in the two cases are, of course, different. Note that a general $V^{(3)}$ has four parameters while $V^{(3)\mathrm{sym}}$ has one less. Equation (A16) is telling us that the symmetry requirement does not remove the invariant phase of the matrix. In the language of Euler rotations, where $V^{(3)}$ would be parametrized with three rotation angles and one phase, the requirement that the matrix be symmetric keeps the phase but removes one of the rotation angles. Note that the new phase and angles will be functions of the former phase and angles.

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Distributed Gaussian polynomials as *q*-oscillator eigenfunctions

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Karabulut and Sibert [J. Math. Phys. **38**, 4815 (1997)] have constructed an orthogonal set of functions from linear combinations of equally spaced Gaussians. In this paper we show that they are actually eigenfunctions of a *q*-oscillator in coordinate representation. We also reinterpret the coordinate representation example of *q*-oscillator given by Macfarlane as the functions orthogonal with respect to an unusual inner product definition. It is shown that the eigenfunctions in both *q*-oscillator examples are infinitely degenerate. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161022]

I. INTRODUCTION

Distributed Gaussians are a set of equally spaced Gaussians, $g_n(x)=e^{-c^2(x-n)^2}$ where $(n=-\infty,\ldots,\infty)$. A finite chain of them is often used in variational calculations as a basis set. They are a very flexible and efficient basis set often yielding very accurate variational results. Calculating the potential matrix elements are often the most difficult part of a variational calculation. Because of their compactness it is very easy to calculate potential energy matrix elements with a few point Gauss-Hermite quadrature very accurately which is a major advantage of using this basis.

We need orthogonal functions for variational calculations and the distributed Gaussians are not orthogonal. In a 1997 paper Karabulut and Sibert[1] constructed a set of orthogonal functions from distributed Gaussians and they studied the underlying Gaussian quadrature. They called these functions distributed Gaussian polynomials (DG polynomials briefly). Their motivation was entirely practical and they were not looking for an algebraic structure behind these functions. Later Karabulut[2] showed how to normalize them and used these functions to construct a Wannier function set from distributed Gaussians.

While searching for an operator that admits the DG polynomials as eigenfunctions the author came across a seminal paper by Macfarlane[3] in which he constructed a coordinate representation of his *q*-oscillator algebra (the same *q*-oscillator was also studied by Biederharn[4] but he did not have the explicit coordinate representation example that Macfarlene gave). Eigenfunctions of Macfarlene were a linear combination of distributed Gaussians and it involved the *q*-binomial coefficients just like the DG polynomials. They looked similar to the DG polynomials but they were not the same. Following his example, the author constructed another coordinate representation of the *q*-oscillator algebra that yields the DG polynomials as eigenfunctions. The *q*-oscillator turns out to be a coordinate representation example of the Arik-Coon oscillator.[5] Macfarlane gave an inner product definition for his functions in term of Rogers-Szegö polynomials. The author of this paper also found a simpler inner product definition for the Macfarlane functions and reinterpreted his results.

The outline of the paper is the following. Section II gives a summary of the basic results about the DG polynomials and discusses its links to Rogers-Szegö polynomials. Section III derives the DG polynomials from the *q*-oscillator algebra. Section IV discusses Macfarlane's example to his *q*-oscillator and reinterprets its eigenfunctions. Finally, Sec. V gives a summary and discussion.

II. DISTRIBUTED GAUSSIAN POLYNOMIALS AND THEIR PROPERTIES

We will mostly denote the Gaussians $e^{-c^2x^2}$ as q^{x^2} where $q=e^{-c^2}$ and c^{-1} is related to the width of the Gaussians. DG polynomials are defined as

$$\Phi_n(x) = \sum_{k=0}^{n} C_k^n (-1)^k q^{-k/2} q^{(x-k)^2}. \tag{1}$$

The C_k^n are the well-known q-binomial coefficients

$$C_k^n = \frac{(q,q)_n}{(q,q)_k (q,q)_{n-k}}, \tag{2}$$

where $(q,q)_n$ is defined as

$$(q,q)_n = (1-q)(1-q^2)\cdots(1-q^n), \tag{3}$$

and $(q,q)_0=1$. They satisfy the following orthogonality relation:[2]

$$\int_{-\infty}^{\infty} \Phi_n(x)\Phi_m(x)\mathrm{d}x = \|\Phi_n(x)\|^2 \delta_{nm}, \tag{4}$$

where the norm $\|\Phi_n(x)\|$ is given as

$$\|\Phi_n(x)\| = \left(\frac{\pi}{2c^2}\right)^{1/4} q^{-n/2}\sqrt{(q,q)_n}. \tag{5}$$

We will denote the normalized functions with lowercase ϕ,

$$\phi_n = \frac{\Phi_n(x)}{\|\Phi_n(x)\|} = \frac{\alpha}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} C_k^n (-1)^k q^{(n-k)/2} q^{(x-k)^2}, \tag{6}$$

where

$$\alpha = \left(\int_{-\infty}^{\infty} q^{2x^2}\,\mathrm{d}x\right)^{-1/2} = \left(\frac{2c^2}{\pi}\right)^{1/4}. \tag{7}$$

We defined α this way for later convenience.

Karabulut and Sibert[1] also found that the DG polynomials yield harmonic oscillator eigenfunctions in a particular limit as

$$\lim_{c\to 0} \frac{\Phi_n(s/\sqrt{2}c)}{(-c/\sqrt{2})^n} = e^{-s^2/2} h_n(s), \tag{8}$$

where $h_n(s)$ are the standard Hermite polynomials. We will refer to this limit later.

DG polynomials are related Stieltjes-Wigert polynomials. Let us write the orthogonality relation as follows:

$$\int_{-\infty}^{\infty} \Phi_n(x-s)\Phi_m(x-s)\mathrm{d}x = 0, \quad (n \neq m). \tag{9}$$

If we denote $u=q^{-2x}$ then $\Phi_n(x-s)$ is written as

$$\Phi_n(x-s) = e^{-(\ln u)^2/(-4\ln q)} u^s P_n(u;s), \tag{10}$$

where the polynomials $P_n(u;s)$ are

$$P_n(u;s)=\sum_{k=0}^{n} C_k^n(-1)^k q^{(k+s)^2-k/2}u^k. \tag{11}$$

Then the orthogonality relation becomes

$$\int_{-\infty}^{\infty} e^{-(\ln u)^2/(-2\ln q)}u^{2s-1}P_n(u;s)P_m(u;s)\mathrm{d}x=0, \quad (n\neq m). \tag{12}$$

Evidently the polynomials $P_n(u;s)$ are orthogonal with respect to the weight function

$$W(u)=e^{-(\ln u)^2/(-2\ln q)}u^{2s-1}. \tag{13}$$

For $s=1/2$ the weight function is the lognormal distribution and the corresponding polynomials are known as the Stieltjes-Wigert polynomials. So the $P_n(u;1/2)$ are proportional to Stieltjes-Wigert polynomials.

The above connection to the Stieltjes Wigert polynomials were noted in Karabulut and Sibert.[1] Later Atakishiyev and Nagiyev[6] found a connection between the Stieltjes-Wigert polynomials and Rogers-Szegö polynomials through the Fourier transform which implied that DG polynomials are also connected to the Rogers-Szegö polynomials. Here we note this connection.

We take the convention for the Fourier transform as

$$f(\theta)=\int_{-\infty}^{\infty} e^{i2\pi\theta x}f(x)\mathrm{d}x. \tag{14}$$

Using the Parseval relation of the Fourier transforms

$$\int_{-\infty}^{\infty} F^*(x)G(x)\mathrm{d}x=\int_{-\infty}^{\infty} F^*(\theta)G(\theta)\mathrm{d}\theta, \tag{15}$$

we write Eq. (4) as

$$\int_{-\infty}^{\infty} \Phi_n^*(\theta)\Phi_m(\theta)\mathrm{d}\theta=\left(\frac{\pi}{2c^2}\right)^{1/2} q^{-n}(q,q)_n\delta_{nm}, \tag{16}$$

where $\Phi_n(\theta)$ is the Fourier transform of $\Phi_n(x)$ given as

$$\Phi_n(\theta)=\left(\frac{\pi}{c^2}\right)^{1/2} e^{-(\pi/c)^2\theta^2}\sum_{k=0}^{n} C_k^n(-q^{-1/2}e^{i2\pi\theta})^k. \tag{17}$$

The polynomials

$$H_n(x)=\sum_{k=0}^{n} C_k^n x^k \tag{18}$$

are known as Rogers-Szegö polynomials.[6–8] Using them the orthogonality relation is written as

$$\int_{-\infty}^{\infty} H_n(-q^{-1/2}e^{-i2\pi\theta})H_n(-q^{-1/2}e^{i2\pi\theta})e^{-2(\pi/c)^2\theta^2}\,\mathrm{d}\theta=\left(\frac{c^2}{2\pi}\right)^{1/2} q^{-n}(q,q)_n\delta_{nm}. \tag{19}$$

A form of the Poisson summation formula reads

$$\int_{-\infty}^{\infty} f(x)\mathrm{d}x=\int_0^1\left(\sum_{k=-\infty}^{\infty} f(x+k)\right)\mathrm{d}x, \tag{20}$$

which is valid when $\Sigma_{k=-\infty}^{\infty} f(x+k)$ exists (in our case it does). Using this, Eq. (19) is expressed as

$$\int_0^1 H_n(-q^{-1/2}e^{-i2\pi\theta})H_n(-q^{-1/2}e^{i2\pi\theta})\left(\sum_{k=-\infty}^{\infty} e^{-2(\pi/c)^2(\theta+k)^2}\right)\mathrm{d}\theta = \left(\frac{c^2}{2\pi}\right)^{1/2} q^{-n}(q,q)_n \delta_{nm}. \quad (21)$$

The sum in parentheses is periodic with period unity and it is a form of theta function. We can expand it in Fourier series. The Fourier coefficients can be calculated using the Poisson summation formula as

$$\sum_{k=-\infty}^{\infty} e^{-2(\pi/c)^2(\theta+k)^2} = \sqrt{\frac{c^2}{2\pi}} \sum_{k=-\infty}^{\infty} q^{n^2/2} e^{i2\pi n\theta}. \quad (22)$$

Using the Jacobi ϑ_3 function[9] defined as

$$\vartheta_3(\theta;q) = \sum_{n=-\infty}^{\infty} q^{n^2/2} e^{in\theta}, \quad (23)$$

the orthogonality is written as follows:

$$\int_0^1 H_n(-q^{-1/2}e^{-i2\pi\theta})H_m(-q^{-1/2}e^{i2\pi\theta})\,\vartheta_3(2\pi\theta;q)\mathrm{d}\theta = q^{-n}(q,q)_n \delta_{nm}. \quad (24)$$

This relation is the well-known orthogonality of the Rogers-Szegö polynomials on the unit circle. Clearly it is the same thing as the orthogonality of the DG polynomials and one can be expressed in terms of the other. This is also of interest because Macfarlane[3] expressed orthogonality of his q-oscillator eigenfunctions in terms of orthogonality of Rogers-Szegö polynomials on the unit circle.

III. DG POLYNOMIALS AS A q-OSCILLATOR EIGENFUNCTIONS

A. Algebraic derivation of DG polynomials

Let us define the translation operator T^s as $T^s = e^{s(\partial/\partial x)}$. It has the effect of shifting a function to the left by s, $T^s f(x) = f(x+s)$. We define the creation and destruction operators $\hat{a}$ and $\hat{a}^\dagger$ as

$$\hat{a} = \frac{1}{\sqrt{1-q}} T^{1/2}[q^{x+1/4} - T^{1/2}], \quad (25)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{1-q}} [q^{x+1/4} - T^{-1/2}]T^{-1/2}. \quad (26)$$

Our inner product is the usual one

$$(f,g) = \int_{-\infty}^{\infty} f^*(x)g(x)\mathrm{d}x, \quad (27)$$

and the conjugate operator is defined as $(f,\hat{O}g) = (\hat{O}^\dagger f, g)$. According to this $(q^x)^\dagger = q^x$ and $(\partial/\partial x)^\dagger = -(\partial/\partial x)$ and $\hat{a}^\dagger$ given above is the right one. The $\hat{a}$ and $\hat{a}^\dagger$ satisfy the commutation relation

$$\hat{a}\hat{a}^\dagger - q\hat{a}^\dagger\hat{a} = 1. \quad (28)$$

This is the commutation relation satisfied by the Arik-Coon oscillator.[5]

We look for the eigenstates of the $\hat{a}^\dagger\hat{a}$,

$$\hat{a}^\dagger \hat{a} A_n(x) = \lambda_n A_n(x). \tag{29}$$

We start from a ground state $A_0(x)$ that satisfies $\hat{a}A_0(x)=0$ which yields the functional equation,

$$A_0(x+1/2) = q^{(x+1/4)} A_0(x). \tag{30}$$

If we set $A_0(x)=(\text{const})w(x)q^{x^2}$ in this equation we get $w(x+1/2)=w(x)$. Therefore the normalized ground state is

$$A_0(x) = \alpha_w w(x) q^{x^2}, \tag{31}$$

where $w(x)$ is any (in general complex) function satisfying $w(x+1/2)=w(x)$ periodicity condition and α_w is the normalization coefficient,

$$\alpha_w = \left(\int_{-\infty}^{\infty} |w(x)|^2 q^{2x^2} \, dx \right)^{-1/2}. \tag{32}$$

For $w(x)=1$ we denote α_w as just α whose value is given in Eq. (7). We choose normalization of our eigenfunctions as $(A_n,A_n)=1$ and taking $w(x)=1$ with this normalization will lead us to the normalized DG polynomials.

Next we build the states $(\hat{a}^\dagger)^n A_0(x)$. Using the commutation relation one can easily show that if $(\hat{a}^\dagger)^n A_0(x)$ is an eigenfunction of $\hat{a}^\dagger\hat{a}$ with the eigenvalue λ_n then the $(\hat{a}^\dagger)^{n+1} A_0(x)$ is an eigenfunction of the $\hat{a}^\dagger\hat{a}$ with eigenvalue λ_{n+1} and one obtains a recursion relation for the eigenvalues

$$\lambda_{n+1} = q\lambda_n + 1. \tag{33}$$

Since $\hat{a}A_0(x)=0$, then $A_0(x)$ is an eigenfunction of $\hat{a}^\dagger\hat{a}$ with the eigenvalue $\lambda_0=0$ and by induction it follows that all $(a^\dagger)^n A_0(x)$ are eigenfunctions. Using the recursion relation in Eq. (33) and $\lambda_0=0$ we get the eigenvalues as

$$\lambda_n = \frac{1-q^n}{1-q}. \tag{34}$$

In exactly the same way that we do in solving the harmonic oscillator algebraically, we can easily obtain the following relations:

$$\hat{a}A_n(x) = \sqrt{\lambda_n} A_{n-1}(x), \tag{35}$$

$$\hat{a}^\dagger A_n(x) = \sqrt{\lambda_{n+1}} A_{n+1}(x). \tag{36}$$

Then $A_n(x)$ can be written as

$$A_n(x) = \sqrt{\frac{(1-q)^n}{(q,q)_n}} (\hat{a}^\dagger)^n A_0(x). \tag{37}$$

Instead of applying $\hat{a}^\dagger$ n times, the following recursive relation is easier. Define $A_n(x)$ as

$$A_n(x) = \frac{\alpha_w w(x)}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} D_k^n (-1)^k q^{(n-k)/2} q^{(x-k)^2}. \tag{38}$$

Then if we apply $\hat{a}^\dagger/\sqrt{\lambda_{n+1}}$ to obtain $A_{n+1}(x)$ and compare the coefficients we get the recursion relation for the D_k^n coefficients. In this process $w(x)$ completely commutes with $\hat{a}^\dagger$ because of periodicity, $T^{-1/2}w(x)=w(x-1/2)=w(x)$. The recursion relation we obtain is

$$D_k^{n+1} = q^k D_k^n + D_{k-1}^n. \tag{39}$$

Together with the conditions $D_0^0=1$ and $D_{-1}^n=D_{n+1}^n=0$ this completely determines the D_k^n. As can be shown easily, the q-binomial coefficients C_k^n satisfy this recursion relation and the boundary conditions and therefore

$$D_k^n = C_k^n = \frac{(q,q)_n}{(q,q)_k(q,q)_{n-k}}. \tag{40}$$

This shows that

$$A_n(x) = \frac{\alpha_w w(x)}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} C_k^n (-1)^k q^{(n-k)/2} q^{(x-k)^2}, \tag{41}$$

are the normalized eigenfunctions and they reduce to the normalized DG polynomials $\phi_n(x)$ when $w(x)=1$.

Now let us see how the q-oscillator algebra reduces to harmonic oscillator algebra in the limit $q\to 0 (c\to 0)$. The limit in Eq. (8) shows us how to do it. First define the new variable $z=cx$. With this variable, the $\hat{a}$ will look like

$$\hat{a} = \frac{1}{\sqrt{1-e^{-c^2}}} e^{(c/2)(\partial/\partial z)} [e^{-c^2/4} e^{-cz} - e^{(c/2)(\partial/\partial z)}], \tag{42}$$

and in the limit $c\to 0$ this reduces to

$$\hat{a} \to -\frac{1}{2}\frac{\partial}{\partial z} - z. \tag{43}$$

Similarly, $\hat{a}^\dagger$ reduces to

$$\hat{a}^\dagger \to \frac{1}{2}\frac{\partial}{\partial z} - z, \tag{44}$$

which, together with $\hat{a}$, are the destruction and creation operators for the harmonic oscillator problem

$$\left(-\frac{1}{4}\frac{\partial}{\partial z^2} + z^2\right)\psi(z) = E\psi(z). \tag{45}$$

B. Further discussion on $w(x)$ degeneracy

Although the algebraic solution seems flawless, it is still very surprising that the $A_n(x)$ are orthogonal for all the functions $w(x)$ satisfying $w(x+1/2)=w(x)$. Here we give a separate proof of it.

When we multiply two of our parent Gaussians $g_n(x)=q^{(x-n)^2}$ we get daughter Gaussians $G_n(x)=q^{2(x-n/2)^2}$ as

$$g_n(x)g_m(x) = q^{(n-m)^2/2} G_{n+m}(x). \tag{46}$$

The parent Gaussians are centered at integers whereas the daughter Gaussians are centered at both integers and half-integers. Therefore the $\phi_n(x)\phi_m(x)$ product of the normalized DG polynomials

$$\phi_n(x) = \frac{\alpha}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} C_k^n (-1)^k q^{(n-k)/2} q^{(x-k)^2}, \tag{47}$$

can be written as a linear combination of daughter polynomials as

$$\phi_n^*(x)\phi_m(x) = \alpha^2 \sum_{k=0}^{n+m} d_k^{nm} q^{2(x-k/2)^2}. \tag{48}$$

If we integrate this we should get δ_{nm} due to the orthogonality of normalized DG polynomials. The integrals $\int_{-\infty}^{\infty} q^{2(x-k/2)^2}\,dx$ are independent of k (just shift the integral by $k/2$) and have the value $1/\alpha^2$. Therefore we get the relation

$$\sum_{k=0}^{n+m} d_k^{nm} = \delta_{nm}. \tag{49}$$

Now, the $A_n^*(x)A_m(x)$ product of the $A_n(x)$ functions

$$A_n(x) = \frac{\alpha_w w(x)}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} C_k^n (-1)^k q^{(n-k)/2} q^{(x-k)^2}, \tag{50}$$

can be expressed as

$$A_n^*(x)A_m(x) = |\alpha_w|^2 \sum_{k=0}^{n+m} d_k^{nm} (|w(x)|^2 q^{2(x-k/2)^2}). \tag{51}$$

If we integrate this we get

$$\int_{-\infty}^{\infty} A_n^*(x)A_m(x)\,dx = \sum_{k=0}^{n+m} d_k^{nm} \left(|\alpha_w|^2 \int_{-\infty}^{\infty} |w(x)|^2 q^{2(x-k/2)^2}\,dx \right). \tag{52}$$

The integral in parentheses can be shifted by $k/2$ as

$$\int_{-\infty}^{\infty} |w(x)|^2 q^{2(x-k/2)^2}\,dx = \int_{-\infty}^{\infty} |w(x+k/2)|^2 q^{2x^2}\,dx. \tag{53}$$

Because of the periodicity of $w(x)$, we have $w(x+k/2)=w(x)$ and all the integrals are independent of k and they have the value $1/|\alpha_w|^2$. This yields

$$\int_{-\infty}^{\infty} A_n^*(x)A_m(x)\,dx = \sum_{k=0}^{n+m} d_k^{nm} = \delta_{nm}, \tag{54}$$

which follows from Eq. (49). Therefore the orthogonality holds for any $w(x)$ satisfying the periodicity requirement.

We actually found more than the DG polynomials from the algebraic treatment. We found an infinite set of orthogonal functions.

IV. A DIFFERENT INTERPRETATION OF q-OSCILLATOR EXAMPLE OF MACFARLANE

In a seminal and widely cited paper Macfarlane constructed a different coordinate representation of the q-oscillator. His definition of the creation and destruction operators are

$$\hat{b} = e^{2x} - e^x e^{s(\partial/\partial x)}, \tag{55}$$

$$\hat{b}^{\dagger} = e^{-2x} - e^{s(\partial/\partial x)}e^{-x}. \tag{56}$$

Obviously, according to the usual definition of the inner product in Eq. (27) the $\hat{b}^{\dagger}$ is not right. Macfarlane himself goes on to construct eigenstates of $\hat{b}^{\dagger}\hat{b}$ without discussing the inner product and orthogonality relation first. After finding the eigenfunctions he states inner product and orthogonality relations in terms of orthogonality of Rogers-Szegö polynomials on the unit circle. The functions we find do not agree with the functions he found and apparently his formula for the eigenfunctions contains some error. Therefore we redo the problem with a different inner product definition here.

We define the inner product as

$$(f,g) = \int_{-\infty}^{\infty} (\hat{P}f^{*}(x))g(x)\mathrm{d}x. \tag{57}$$

$$= \int_{-\infty}^{\infty} f^{*}(-x)g(x)\mathrm{d}x, \tag{58}$$

where $\hat{P}$ is the usual parity operator. For an operator $\hat{O}$, its conjugate $\hat{O}^{\dagger}$ is defined by the relation

$$(f,\hat{O}g) = (\hat{O}^{\dagger}f,g), \tag{59}$$

The $\hat{b}^{\dagger}$ expression in Eq. (56) is right if one defines the inner product this way because $(e^{x})^{\dagger} = e^{-x}$ and $(d/\mathrm{d}x)^{\dagger} = d/\mathrm{d}x$. Notice that this definition of the inner product does not satisfy $(f,f) \geqslant 0$ condition. But we will not use this property of the inner product in our development. We will use the conjugacy definition in Eq. (59) in a few places.

In order to obtain functions as a linear combination of the Gaussians centered at non-negative integers we change the variable $x=-c^2(y+1/4)$ and $s=-c^2/2$ and we take $q=e^{-c^2}$ as before. We will also divide $\hat{b}$ and $\hat{b}^{\dagger}$ by $\sqrt{q(1-q)}$ which does not change the eigenfunctions (only eigenvalues), but in the limit of the harmonic oscillator $(q\to 1)$ it helps to get the right results. The new $\hat{b}$ and $\hat{b}^{\dagger}$ are

$$\hat{b} = (q^{2y+1/2} - q^{y+1/4}T^{1/2})/\sqrt{q(1-q)}, \tag{60}$$

$$\hat{b}^{\dagger} = (q^{-2y+1/2} - T^{1/2}q^{-y+1/4})/\sqrt{q(1-q)}, \tag{61}$$

where $T^{1/2} = e^{\frac{1}{2}(\partial/\partial y)}$. They satisfy the commutation relation

$$\hat{b}^{\dagger}\hat{b} - q\hat{b}\hat{b}^{\dagger} = 1. \tag{62}$$

Note that this is somewhat different than the commutation relation in Eq. (28).

Again we want to find the eigenfunctions of the operator $\hat{b}^{\dagger}\hat{b}$,

$$\hat{b}^{\dagger}\hat{b}B_n(y) = \lambda_n B_n(y). \tag{63}$$

We again start from a ground state that satisfies $\hat{b}B_0(y)=0$ (hence $\lambda_0=0$). $\hat{b}B_0(y)=0$ yields the same functional equation that $A_0(x)$ satisfy

$$B_0(y+1/2) = q^{y+1/4}B_0(y), \tag{64}$$

which we already know has the solution $B_0(y)=\alpha_w w(y)q^{y^2}$ where $w(y)$ satisfies the $w(y+1/2) = w(y)$ periodicity condition. The infinite degeneracy of the states appear here too. Note that this time α_w is defined as

$$\alpha_w = \left(\int_{\infty}^{-\infty} w^*(-y) w(y) q^{2y^2} \mathrm{d}y \right)^{-1/2}. \tag{65}$$

Next we build the unnormalized states $(\hat{b}^\dagger)^n B_0(y)$. Using the commutation relation we can easily show that if the $(\hat{b}^\dagger)^n B_0$ is an eigenfunction of $\hat{b}^\dagger \hat{b}$ with an eigenvalue λ_n then $(\hat{b}^\dagger)^{n+1} B_0$ is an eigenfunction with the eigenvalue λ_{n+1} where λ_{n+1} is related to the λ_n as

$$q\lambda_{n+1} = \lambda_n - 1. \tag{66}$$

Since $B_0(y)$ is an eigenfunction, by induction all $(\hat{b}^\dagger)^n B_0$ are eigenfunctions too. Starting from $\lambda_0 = 0$, this recursion relation yields

$$\lambda_n = -q^{-n} \left(\frac{1-q^n}{1-q} \right). \tag{67}$$

Notice that the eigenvalues are negative.

To obtain relations similar to Eqs. (35) and (36). We form the inner product

$$\lambda_n (B_n, B_n) = (B_n, \hat{b}^\dagger \hat{b} B_n) = (\hat{b} B_n, \hat{b} B_n). \tag{68}$$

Taking $\hat{b} B_n = \mu_n B_{n-1}$ we get

$$\lambda_n = |\mu_n|^2 \frac{(B_{n-1}, B_{n-1})}{(B_n, B_n)}. \tag{69}$$

Since $|\mu_n|^2$ is positive and λ_n is negative, the (B_{n-1}, B_{n-1}) and (B_n, B_n) must have opposite signs. This looks surprising but we should remember that in our definition of the inner product the (f, f) can be negative. Therefore we will take our normalization as

$$(B_n, B_n) = (-1)^n. \tag{70}$$

With this normalization we obtain $\mu_n = \sqrt{-\lambda_n}$,

$$\hat{b} B_n = \sqrt{-\lambda_n} B_{n-1}. \tag{71}$$

Starting from

$$\lambda_{n+1} B_{n+1} = \hat{b}^\dagger \hat{b} B_{n+1} = \sqrt{-\lambda_{n+1}} \hat{b}^\dagger B_n, \tag{72}$$

we also obtain

$$\hat{b}^\dagger B_n = -\sqrt{-\lambda_{n+1}} B_{n+1}. \tag{73}$$

This result is also a little unusual because of the sign in front. It is a consequence of negative λ_n eigenvalues.

Since we started from an unusual inner product definition there might be doubts on orthogonality of the B_n. Consider the inner product

$$(B_m, \hat{b}^\dagger \hat{b} B_n) = (\hat{b}^\dagger \hat{b} B_m, B_n). \tag{74}$$

Using $\hat{b}^\dagger \hat{b} B_k = \lambda_k B_k$ we get

$$(\lambda_n - \lambda_m)(B_m, B_n) = 0, \tag{75}$$

which yields $(B_m, B_n) = 0$ when $m \neq n$. We added this common proof to emphasize that the orthogonality does not depend on the $(f, f) \geqslant 0$ property of the usual inner products. We just used the conjugacy relation Eq. (59) in this proof of orthogonality. But unlike the case of usual definition

inner product given in Eq. (27), $(f,f)=0$ does not imply $f=0$ when we do not have $(f,f)\geqslant 0$ property.

To complete the discussion we obtain the eigenfunctions $B_n(y)$. It makes things easier to figure out the coefficient of Gaussian centered at zero (q^{y^2}) first. The $\hat{b}^\dagger$

$$\hat{b}^\dagger = (q^{-2y+1/2} - T^{1/2}q^{-y+1/4})/\sqrt{q(1-q)}, \tag{76}$$

has two parts that do different things. When $q^{-2y+1/2}$ acts on $q^{(y-k)^2}$ it produces the next Gaussian $q^{(y-k-1)^2}$ and multiplies it with a constant. When $T^{1/2}q^{-y+1/4}$ act on $q^{(y-k)^2}$ it gives $q^{(y-k)^2}$ back and multiplies with a constant. Here are the precise relations

$$q^{-2y+1/2}q^{(y-k)^2} = q^{-2k-1/2}q^{(y-k-1)^2}, \tag{77}$$

$$T^{1/2}q^{-y+1/4}q^{(y-k)^2} = q^{-k}q^{(y-k)^2}. \tag{78}$$

From the second relation we have $T^{1/2}q^{-y+1/4}q^{y^2}=q^{y^2}$ which means this operator leaves q^{y^2} as it is. The other operator $q^{-2y+1/2}$ creates $k=1$ Gaussian $(q^{(y-1)^2})$ from it. Since we produce higher eigenfunctions by applying $-\hat{b}^\dagger/\sqrt{-\lambda_n}$ successively, after each application the coefficient of $k=0$ Gaussian changes by a factor $1/\sqrt{q(1-q)(-\lambda_n)}$. We denote the coefficient of $k=0$ Gaussian in $B_n(y)$ by ζ_n and it should be

$$\zeta_n = \alpha_w \frac{1}{\sqrt{q^n(1-q)^n}} \frac{1}{\sqrt{(-\lambda_1)(-\lambda_2)\cdots(-\lambda_n)}} = \alpha_w \frac{q^{n(n-1)/4}}{\sqrt{(q,q)_n}}. \tag{79}$$

Now let us take the $B_n(y)$ of the form

$$B_n(y) = w(x)\zeta_n \sum_{k=0}^{n} E_k^n q^{(y-k)^2}, \tag{80}$$

where $E_0^n=1$ by construction. We can use Eq. (72) to generate a recursion relation for E_k^n as before. To show a different and easier way of doing things we will use Eq. (70) relation this time. The $\hat{b}$ has the effect of shifting each Gaussian to the left by one unit

$$\hat{b}q^{(y-k)^2} = -\frac{q^{k-1/2}(1-q^k)}{\sqrt{q(1-q)}} q^{(y-k+1)^2}, \tag{81}$$

and it also destroys the leftmost Gaussian (the $k=0$ Gaussian centered at zero). Therefore the equality

$$\hat{b}[(\zeta_n E_k^n)q^{(y-k)^2}] = \sqrt{-\lambda_n}[(\zeta_{n-1}E_{k-1}^{n-1})q^{(y-k+1)^2}] \tag{82}$$

should hold for each Gaussian. This yields the recursion relation for the E_k^n as

$$E_k^n = -E_{k-1}^{n-1}\left(\frac{1-q^n}{1-q^k}\right)q^{-n-k+3/2}. \tag{83}$$

Together with the condition $E_0^n=1$ this is enough information to solve the E_k^n. The quotient in parentheses tells us that the q binomial coefficients C_k^n are involved. If we set $E_k^n=(-1)^k C_k^n q^{u(n,k)}$ we get the recursion relation for $u(n,k)$ as

$$u(n,k) - u(n-1,k-1) = -n-k+3/2. \tag{84}$$

Together with the condition $u(n,0)=0$ (which follows from $E_0^n=1$) this is uniquely solved as $u(n,k)=-nk+k/2$. Therefore the $B_n(y)$ should be

$$B_n(y) = \alpha_w w(x) \frac{q^{n(n-1)/4}}{\sqrt{(q,q)_n}} \sum_{k=0}^{n} C_k^n (-1)^k q^{-(n-1/2)k} q^{(y-k)^2}. \tag{85}$$

This formula does not agree with the result of Macfarlane even after setting $c^2=-2s$ and $y=-1/4+x/2s$ back in $B_n(y)$ above. To be sure that we have the right formula we have checked numerically if the $B_n(y)$ satisfy the orthogonality relation

$$\int_{-\infty}^{\infty} B_n(-y) B_m(y) \mathrm{d}y = (-1)^n \delta_{nm}. \tag{86}$$

They satisfy it perfectly and we are sure that we have the right formula. Apparently Macfarlane's paper contains an error.

The harmonic oscillator limit is as straightforward as it is in the DG polynomials case. We change variable $y=z/c$ and take the limit $c \to 0$ which yields

$$\hat{b} \to z - \frac{1}{2} \frac{\partial}{\partial z}, \tag{87}$$

$$\hat{b}^\dagger \to -z - \frac{1}{2} \frac{\partial}{\partial z}. \tag{88}$$

Then $\hat{b}^\dagger \hat{b} B_n = \lambda_n B_n$ reduces to ($\lambda_n \to -n$ in this limit)

$$\left(-\frac{1}{4} \frac{\partial^2}{\partial z^2} + z^2 \right) \Psi_n = (n + 1/2) \Psi_n. \tag{89}$$

The fact that the inner product is defined differently makes no difference in this limit because the harmonic oscillator eigenfunctions are either even or odd. The harmonic oscillator eigenfunctions satisfy the normalization condition

$$\int \Psi_n^*(-y) \Psi_m(y) \mathrm{d}y = (-1)^n \delta_{nm} \tag{90}$$

as can be verified easily using parity of the wave functions.

Now, just as the DG polynomials, the orthogonality of the $B_n(y)$ can be expressed as an orthogonality relation of the Rogers-Szegö polynomials on the unit circle. We will take $w(x)=1$ and $\alpha_w = \alpha$ for this. By Fourier transforming the orthogonality relation Eq. (85) we get the relation

$$\int_{-\infty}^{\infty} B_n^*(-\theta) B_m(\theta) \mathrm{d}\theta = (-1)^n \delta_{nm}, \tag{91}$$

where $B_n(\theta)$ is the Fourier transform of the $B_n(y)$,

$$B_n(\theta) = \left(\frac{\pi}{c^2} \right)^{1/2} \zeta_n e^{-(\pi/c)^2 \theta^2} \sum_{k=0}^{n} C_k^n (-q^{-(n-1/2)} e^{i2\pi\theta})^k. \tag{92}$$

Here θ is the Fourier transform variable just as before. Using the Poisson summation formula in Eq. (20) the orthogonality relation can be expressed as

$$\int_0^1 H_n(-q^{-(n-1/2)} e^{i2\pi\theta}) H_m(-q^{-(m-1/2)} e^{i2\pi\theta}) \left(\sum_{k=-\infty}^{\infty} e^{-2(\pi/c)^2(\theta+k)^2} \right) \mathrm{d}\theta = \frac{c^2}{\pi} \frac{(-1)^n}{\zeta_n^2} \delta_{nm}. \tag{93}$$

Setting the sum in parentheses from Eqs. (22) and (23) we obtain

$$\int_0^1 H_n(-q^{-(n-1/2)}e^{i2\pi\theta})H_m(-q^{-(m-1/2)}e^{i2\pi\theta})\vartheta_3(2\pi\theta;q)\mathrm{d}\theta = q^{-n(n-1)/2}(q,q)_n(-1)^n\delta_{nm}. \quad (94)$$

This is again some form of the orthogonality relation of the Rogers-Szegö polynomials on the circle. This is a new set of orthogonality relations and we are not aware of its existence in mathematical literature.

V. SUMMARY

In this study we found that the DG polynomials that Karabulut and Sibert discovered before are actually eigenfunctions of coordinate representation of the Arik-Coon q-oscillator. We derived the DG polynomials from q-oscillator algebra. We also indicated that orthogonality of the DG polynomials can be cast into orthogonality of the Rogers-Szegö polynomials on the unit circle and the two are equivalent.

We showed that the example given by Macfarlane can be interpreted with an unusual inner product definition and we constructed the corresponding orthogonal functions. Their orthogonality can be recast into a form of orthogonality relation for the Rogers-Szegö polynomials on the unit circle. We were not able to find this result in mathematical literature and it is probably a new result.

A very interesting result of this work is that the eigenstates of the q-oscillators we solved turned out to be infinitely degenerate. We know that algebraic solution of the one dimensional harmonic oscillator is nondegenerate. In the usual algebraic solution of the harmonic oscillator we base our arguments on the commutation relations and the algebra has nothing in it that implies nondegenerate states. But the ground state $\hat{a}\phi_0=0$ yields a unique solution for the harmonic oscillator because it is a differential equation and nondegeneracy of the excited states follows from this. For our q-oscillator examples we have a first order difference equation for the $\hat{a}\phi_0=0$ and such equations together with the boundary conditions do not uniquely define a function. It defines a function on all real axis if its values in a $1/2$ wide interval are known.

Finally, the freedom to choose $w(x)$ arbitrarily gives us possibility of constructing orthogonal function sets more general than the DG polynomials. Consider a set of functions $w_0(x), w_1(x), w_2(x), \ldots$ satisfying the periodicity condition $w_n(x+1/2)=w_n(x)(n=0,1,2,\ldots)$ and the orthogonality relation

$$\int_{-\infty}^{\infty} w_n^*(x)w_m(x)q^{2x^2}\,\mathrm{d}x = \delta_{nm}. \quad (95)$$

Then the set of functions

$$\Gamma_{nm}(x) = \frac{\alpha(w_n)}{\alpha} w_n(x)\phi_m(x) \quad (96)$$

will satisfy an orthogonality relation of the form

$$\int_{-\infty}^{\infty} \Gamma_{nm}^*(x)\Gamma_{ij}(x)\mathrm{d}x = \delta_{ni}\delta_{mj}. \quad (97)$$

Here $\alpha(w_n)$ is the α_w for $w=w_n(x)$ given in Eq. (32) and α is given in Eq. (7). This gives us much freedom to construct orthogonal function sets useful as basis sets in variational calculations. This possibility should be investigated in future research.

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responsible for the creation of the work presented here, he kindly declined to coauthor this paper on the grounds that his contribution was minimal. The author is indebted to Professor Robert G. Littlejohn for suggesting the problem addressed in this paper.

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The decomposition of an orthogonal transformation as a product of reflections

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In this work, an algorithm to decompose a given orthogonal transformation as a product of reflections through hyperplanes is presented. This in fact constitutes a constructive proof of a Cartan theorem, valid over any field $K=\mathbb{Q}$, $\mathbb{R}$ or $\mathbb{C}$. Clifford algebras are used to explicitly calculate the reflections that decompose a given orthogonal transformation. Our algorithm may have application in fields such as computer graphics or crystallography, and can also play an important role in orthogonal elimination and the solution of equations systems. An explicit example is provided and we apply our results to the crystallographic problem of coincidence lattices. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161072]

I. INTRODUCTION

This work is concerning the decomposition of a given orthogonal transformation in $\mathbb{R}^n$ as a product of simple reflections (reflections by hyperplanes). This problem is directly related to a Cartan theorem,[1] which asserts that every orthogonal transformation can be written as the product of at most n reflections with respect to hyperplanes. The original proofs of this theorem, of around 70 years ago, were nonconstructive; for a given orthogonal transformation the existence of such reflections was demonstrated. In Ref. 2, for instance, a proof based on the Raleigh quotient is presented. Constructive ways by the induction method have been given in different contexts; when computing over $\mathbb{R}$ or $\mathbb{C}$, and by using Householder matrices, it was proved that any real (or complex) orthogonal (or unitary) matrix can be written as the product of at most n Householder matrices, derived constructively from the original matrix.[3] The importance of this proof relies in the fact that Householder matrices are relevant in numerical linear algebra.[3,4] Also, there exists a constructive derivation of the analog of the Cartan theorem for symplectic matrices.[5]

Here, we present a constructive proof of the Cartan theorem, valid for n-dimensional linear spaces with inner product over any field $K=\mathbb{Q}$, $\mathbb{R}$ or $\mathbb{C}$, which produces an algorithm for the factorization of a given orthogonal transformation into a product of simple reflections. We have found that this factorization is greatly simplified by using Clifford algebras, where reflections and rotations are handled in a convenient way. These algebras have proved to be a powerful mathematical language for expressing geometric ideas and have been relevant not only in several mathematical areas but also in physics, engineering and computer science (see, for example, Ref. 6 and references therein). The use of Clifford algebras to prove the Cartan theorem do not obscure but enhances the geometrical meaning, yielding an algorithm which can be relevant in several

fields since it offers a simple way to decompose any arbitrary orthogonal transformation as a product of simple reflections. In particular, we have shown that Clifford algebras are suitable for calculations in n-dimensional crystallographic lattices.[7,8] In these works, it was conjectured that any coincidence transformation of the lattice $\mathbb{Z}^n$ (see Sec. V) can be written as the product of coincidence reflections. The conjecture was proved in two dimensions[8] and here, as an application of our results, we prove the conjecture for $\mathbb{Z}^n$ (Sec. V, Theorem 20).

This paper is organized as follows. In Sec. II we provide a brief introduction to real orthogonal spaces and Clifford algebras. In Sec. III, we present a constructive proof of the Cartan theorem that produces an algorithm to calculate the simple reflections that decompose a given orthogonal transformation. An explicit example is given in Sec. IV and applications to coincidence transformation are presented in Sec. V. Section VI is devoted to conclusions and discussions.

II. REAL ORTHOGONAL SPACES AND CLIFFORD ALGEBRAS

To set the background and fix notation, in this section we first introduce several basic concepts and the basis of Clifford algebras. Most of the results are presented without proofs, and interested readers are referred to Refs. 9 and 10.

Definition 1: The pair $(\mathcal{X},\mathcal{B})$ *is called a n-dimensional real orthogonal space if* $\mathcal{X}$ *is a n-dimensional vector space and* $\mathcal{B}$: $\mathcal{X}\times\mathcal{X}\to\mathbb{R}$ *is an inner product.*

If $\mathcal{W}\subset\mathcal{X}$ is a vector subspace of $\mathcal{X}$ ($\mathcal{W}<\mathcal{X}$), the orthogonal complement of $\mathcal{W}$ in $\mathcal{X}$ is the set

$$\mathcal{W}^{\perp}=\{u\in\mathcal{X}|\mathcal{B}(v,u)=0,\ \text{for all } v\in\mathcal{W}\}.$$

Clearly $\mathcal{W}^{\perp}<\mathcal{X}$. Furthermore, we have the following.

Proposition 2: Let $(\mathcal{X},\mathcal{B})$ *be a n-dimensional real orthogonal space and let* $\mathcal{W}<\mathcal{X}$. *Then* $\mathcal{X}=\mathcal{W}\oplus\mathcal{W}^{\perp}$.

In particular, for a given $a\in\mathcal{X}$ such that $\mathcal{B}(a,a)\neq 0$ we have that $\mathcal{X}=\mathbb{R}a\oplus(\mathbb{R}a)^{\perp}$, and the element $a\in\mathcal{X}$ is called *invertible*. Moreover,

$$a^{-1}=\frac{a}{a^2}=\frac{a}{\mathcal{B}(a,a)}.$$

The $(n-1)$-dimensional subspace $H_a=(\mathbb{R}a)^{\perp}<\mathcal{X}$ is called the hyperplane associated with the invertible element $a\in\mathcal{X}$. Now, since each $v\in\mathcal{X}$ allows a unique decomposition $v=\lambda a+b$, where $\lambda\in\mathbb{R}$ and $b\in(\mathbb{R}a)^{\perp}=H_a$, then the map $\varphi_a(v)=-\lambda a+b$ is orthogonal. Thus φ_a represents a reflection with respect to the hyperplane H_a, which is called a simple reflection.

To end this brief section, we introduce some basic concepts of Clifford algebra. It is important to remark that there are several constructions of Clifford algebras[11–14] and here we choose the approach by Porteous.[10]

Definition 3: Let $(\mathcal{X},\mathcal{B})$ *be a n-dimensional real orthogonal space and let* $\mathcal{A}$ *be a real associative algebra with identity* 1 *such that*

(*C*1) $\mathcal{A}$ *contains copies of* $\mathbb{R}$ *and* $\mathcal{X}$ *as linear subspaces.*

(*C*2) *For all* $v\in\mathcal{X}$ *we have that* $v^2=\mathcal{B}(v,v)$.

(*C*3) $\mathcal{A}$ *is generated as a ring by the copies of* $\mathbb{R}$ *and* $\mathcal{X}$ *or, equivalently as a real algebra by* $\{1\}$ *and* $\mathcal{X}$.

Then $\mathcal{A}$ *is said to be a real Clifford algebra for* $(\mathcal{X},\mathcal{B})$ *and it is denoted by* $\mathcal{A}=\mathcal{C}(\mathcal{X})$.

Axiom (C2) contains the relationship between Clifford algebras and bilinear forms thus holding, as we shall see below, the geometrical interpretation of the Clifford algebra.

If $e=\{e_1,e_2,\ldots,e_n\}$ is an orthonormal basis of $(\mathcal{X},\mathcal{B})$, from the condition (C2) it follows that

$$e_i^2=1,\quad i=1,2,\ldots,n$$

$$e_ie_j+e_je_i=0,\quad i\neq j.$$

In general, for all v, $w\in\mathcal{X}$ we have that

$$\mathcal{B}(v,w) = \tfrac{1}{2}(vw + wv), \tag{1}$$

as it is inferred from $\mathcal{B}(v+w,v+w)=(v+w)^2$. Notice that from (1) it readily follows that two vectors u, $v \in \mathcal{X}$ anticommute if and only if they are orthogonal.

If u, $v \in \mathcal{X}$, then we have

$$uv = \tfrac{1}{2}(uv + vu) + \tfrac{1}{2}(uv - vu) = \mathcal{B}(u,v) + u \wedge v,$$

where

$$u \wedge v = \tfrac{1}{2}(uv - vu)$$

is called the *exterior* product. Moreover, it turns out that $u \wedge v = 0$ if and only if u, v are parallel or linearly dependent vectors.

Notice that since $\mathcal{C}(\mathcal{X})$ is generated by $\{1\}$ and $\mathcal{X}$ then, in terms of the orthonormal basis e, a typical element a of $\mathcal{C}$ is

$$a = \sum_A \lambda_A e_{\alpha_1}^{n_1} e_{\alpha_2}^{n_2} \cdots e_{\alpha_s}^{n_s},$$

where $\lambda_A \in \mathbb{R}$ and $n_j = 1, 0$.

There is an obvious upper bound to the linear dimension of a Clifford algebra for a n-dimensional real orthogonal space. More specifically, $\dim \mathcal{C}(\mathcal{X}) = 2^{n-1}$ or $\dim \mathcal{C}(\mathcal{X}) = 2^n$. In this work, we shall restrict ourselves to Clifford algebras of dimension 2^n, which are called *universal* Clifford algebras.

III. THE CARTAN THEOREM

Before formulating the Cartan theorem, it is useful to first briefly discuss how the algebraic properties of Clifford algebra provide us with a convenient framework for representing orthogonal transformations (linear transformations that preserve the bilinear form).

Suppose $a \in \mathcal{X}$ is a nonzero vector and let H_a be its orthogonal complement.

Lemma 4: Let $\mathcal{C}(\mathcal{X})$ be a Clifford algebra for a n-dimensional real orthogonal space $(\mathcal{X},\mathcal{B})$. If $a \in \mathcal{X}$ is invertible, then the map $T_a: \mathcal{X} \to \mathcal{X}$, defined by

$$T_a(x) = -axa^{-1},$$

is an orthogonal transformation. Moreover, T is a simple reflection.

Proof: T_a is linear, as a consequence of the distributive property of the algebra. To see that T_a is a reflection by the hyperplane H_a it is enough to prove that $T_a(a) = -a$ and $T_a(w) = w$ for all $w \in H_a$. Indeed,

$$T_a(a) = -aaa^{-1} = -a,$$

$$T_a(w) = -awa^{-1} = -(-wa)a^{-1} = w,$$

where we use the fact that $aw = -wa$ since $\mathcal{B}(a,w) = 0$. T_a is an orthogonal transformation since $T_a(v)^2 = v^2$ for all $v \in \mathcal{X}$.

■

Clearly the inverse of a simple reflection is a simple reflection itself

$$T_a(x) = -axa^{-1} = -ax\frac{a}{a^2} = -\frac{a}{a^2}xa = a^{-1}x(a^{-1})^{-1} = T_{a^{-1}}(x).$$

The following Lemma not only displays a simple geometrical fact discussed below, but turns out to be fundamental for the proof of the Cartan theorem proposed here (cf. with Ref. 10, p. 34).

Lemma 5: Let $\mathcal{C}(\mathcal{X})$ be a Clifford algebra for a n-dimensional real orthogonal space $(\mathcal{X},\mathcal{B})$.

If $a,b \in \mathcal{X}$ *are invertible vectors and* $a^2=b^2 \neq 0$, *then there exists a simple reflection* $\varphi:\mathcal{X}\to\mathcal{X}$ *such that*

$$\varphi(a) = b.$$

Proof: For the trivial case $a=b$, it is enough to take $\varphi=I$, where $I:\mathcal{X}\to\mathcal{X}$ is the identity transformation. If $a \neq b$ we shall first prove that the vectors $a-b$ and $a+b$ are orthogonal. Indeed,

$$2\mathcal{B}(a-b,a+b) = (a-b)(a+b) + (b+a)(a-b) = (a^2 - ba + ab - b^2) + (ba + a^2 - ab - b^2) = 0.$$

Now, since

$$(a+b)^2 + (a-b)^2 = (a^2 + ab + ba + b^2) + (a^2 - ab - ba + b^2) = 4a^2 \neq 0,$$

we conclude that $a-b$ is invertible. We can thus define the following orthogonal transformation:

$$\varphi_{a-b}(x) = -(a-b)x(a-b)^{-1},$$

which satisfies $\varphi_{a-b}(a)=b$, as it can be easily verified:

$$\varphi_{a-b}(a) = -(a-b)\left(\frac{1}{2}(a-b) + \frac{1}{2}(a+b)\right)(a-b)^{-1}$$

$$= -\frac{1}{2}(a-b)(a-b)(a-b)^{-1} - \frac{1}{2}(a-b)(a+b)(a-b)^{-1} = -\frac{1}{2}(a-b) + \frac{1}{2}(a+b) = b.$$

Thus, $\varphi(x)$ can be expressed as

$$\varphi(x) = \begin{cases} I & \text{if } a = b, \\ \varphi_{a-b}(x) & \text{if } a \neq b. \end{cases}$$

■

The geometric meaning of the previous lemma can be explained if we consider two vectors, a and b, such that $a^2=b^2\neq 0$. The diagonals of the rhombuses ($a+b$ and $a-b$) are perpendicular and thus the orthogonal complement of $a-b$ is $a+b$ and vice versa. Consequently, if we construct the reflection by using the vector $a-b$, the operation $\varphi_{a-b}(a)$ produces the reflection of a through the hyperplane H_{a-b}, which obviously gives b. The recurrent application of Lemma 5 produces an algorithm to decompose any given orthogonal transformation as the composition of simple reflections. For this goal, it is enough to adequately choose the vectors a and b at each step of the algorithm. This constitutes the Cartan theorem and therefore a constructive proof can now be given.

Theorem 6 (Cartan): *Any orthogonal transformation, in a n-dimensional real orthogonal space* $(\mathcal{X},\mathcal{B})$, *can be written as the product of at most n simple reflections*.

Proof: Let $T:\mathcal{X}\to\mathcal{X}$ be an orthogonal transformation in a n-dimensional real orthogonal space $(\mathcal{X},\mathcal{B})$, and assume that $\{w_1,\ldots,w_n\}$ is an orthogonal basis of $(\mathcal{X},\mathcal{B})$ such that $w_i^2 \neq 0$ for $i=1,\ldots,n$.

Consider w_1, $T(w_1)$ (which play the role of a and b, respectively, in the proof of Lemma 5) and the transformation $\varphi_1:\mathcal{X}\to\mathcal{X}$ defined by

$$\varphi_1(x) = \begin{cases} I & \text{if } T(w_1) = w_1, \\ -c_1 x c_1^{-1} & \text{if } T(w_1) \neq w_1, \end{cases}$$

where $c_1=T(w_1)-w_1$. As it follows from Lemma 5, $\varphi_1(x)$ has the following properties:

$$\varphi_1 T(w_1) = w_1,$$

$$\varphi_1 T(w_l) \in \mathrm{Span}\{w_2,\ldots,w_n\} \quad \text{for } l = 2,\ldots,n.$$

Now, consider w_2, $\varphi_1 T(w_2)$ and the transformation $\varphi_2: \mathcal{X} \to \mathcal{X}$ defined by

$$\varphi_2(x) = \begin{cases} I & \text{if } \varphi_1 T(w_2) = w_2, \\ -c_2 x c_2^{-1} & \text{if } \varphi_1 T(w_2) \neq w_2, \end{cases}$$

where $c_2 = \varphi_2 T(w_2) - w_2$. We already know that $\varphi_2 \varphi_1 T(w_2) = w_2$, and since $c_1 \in \mathrm{Span}\{w_2, w_3, \ldots, w_n\}$, it can be verified that $\varphi_2 \varphi_1 T(w_1) = w_1$. Then we have that

$$\varphi_2 \varphi_1 T(w_i) = w_i \quad \text{for } i = 1,2,$$

$$\varphi_2 \varphi_1 T(w_l) \in \mathrm{Span}\{w_3, w_4, \ldots, w_n\}, \quad \text{for } l = 3,4, \ldots, n.$$

Accordingly, now consider w_3, $\varphi_2 \varphi_1 T(w_3)$ and $\varphi_3: \mathcal{X} \to \mathcal{X}$ defined by

$$\varphi_3(x) = \begin{cases} I & \text{if } \varphi_2 \varphi_1 T(w_3) = w_3, \\ -c_3 x c_3^{-1} & \text{if } \varphi_2 \varphi_1 T(w_3) \neq w_3, \end{cases}$$

where $c_3 = \varphi_2 \varphi_1 T(w_3) - w_3$. We also already know that $\varphi_3 \varphi_2 \varphi_1 T(w_2) = w_2$, and since $c_3 \in \mathrm{Span}\{w_3, \ldots, w_n\}$, it follows that $\varphi_2 \varphi_1 T(w_i) = w_i$, $i = 1,2$. Thus we have that

$$\varphi_3 \varphi_2 \varphi_1 T(w_i) = w_i \quad \text{for } i = 1,2,3,$$

$$\varphi_3 \varphi_2 \varphi_1 T(w_l) \in \mathrm{Span}\{w_4, \ldots, w_n\} \quad \text{for } l = 4, \ldots, n.$$

This procedure can be straightforwardly continued up to n steps, to obtain $\varphi_1, \varphi_2, \ldots, \varphi_n$ orthogonal transformations such that

$$\varphi_n \varphi_{n-1} \cdots \varphi_1 T(w_i) = w_i \quad \text{for } i = 1, \ldots, n, \tag{2}$$

where

$$\varphi_{k+1}(x) = \begin{cases} I & \text{if } \varphi_k \varphi_{k-1} \cdots \varphi_1 T(w_{k+1}) = w_{k+1}, \\ -c_{k+1} x c_{k+1}^{-1} & \text{if } \varphi_k \varphi_{k-1} \ldots \varphi_1 T(w_{k+1}) \neq w_{k+1}, \end{cases}$$

and

$$c_{k+1} = \varphi_k \varphi_{k-1} \cdots \varphi_1 T(w_{k+1}) - w_{k+1}.$$

Notice that

$$\varphi_{k+1}^{-1}(x) = \begin{cases} I & \text{if } \varphi_k \varphi_{k-1} \cdots \varphi_1 T(w_{k+1}) = w_{k+1}, \\ -c_{k+1} x c_{k+1}^{-1} & \text{if } \varphi_k \varphi_{k-1} \ldots \varphi_1 T(w_{k+1}) \neq w_{k+1}. \end{cases}$$

By (2) we obtain

$$T(x) = \varphi_1^{-1} \cdots \varphi_n^{-1}(x),$$

and since each $\varphi_k^{-1}(x)$ is a simple refelction, then the orthogonal transformation T is written as the product of at most n reflections by hyperplanes. Moreover, we can find $a_1, a_2, \ldots, a_s \in \mathcal{X}$ such that

$$T(x) = (-1)^s a_1 a_2 \cdots a_s x a_s^{-1} \cdots a_2^{-1} a_1^{-1},$$

where $s \leqslant n$.

■

IV. EXAMPLE

The following example illustrates the procedure to decompose a particular orthogonal transformation in $\mathbb{R}^3$ as a product of simple reflections. The computations were done with a *Mathematica* Clifford algebra package.[15]

Let $T:\mathbb{R}^3\to\mathbb{R}^3$ be an orthogonal transformation with the following associated matrix, with respect to the canonical basis $\{e_1,e_2,e_3\}$:

$$\mathcal{T}=\begin{pmatrix} \frac{6}{7} & \frac{2}{7} & \frac{3}{7} \\ \frac{2}{7} & \frac{3}{7} & -\frac{6}{7} \\ -\frac{3}{7} & \frac{6}{7} & \frac{2}{7} \end{pmatrix}.$$

By following step by step the procedure used in the proof of the Cartan theorem (Theorem 6), we have that

$$c_1 = T(e_1) - e_1 = \begin{pmatrix} -\frac{1}{7} \\ \frac{2}{7} \\ -\frac{3}{7} \end{pmatrix},$$

and thus $\phi_1(x)=-c_1xc_1^{-1}$. Now

$$c_2 = \phi_1(T(e_2)) - e_2 = -c_1T(e_2)c_1^{-1} - e_2 = 0,$$

that is, $\phi_2(x)=x$, the identity. Finally

$$c_3 = \phi_2(\phi_1(T(e_3))) - e_3 = -c_1T(e_3)c_1^{-1} - e_3 = \begin{pmatrix} 0 \\ 0 \\ -2 \end{pmatrix},$$

and $\phi_3(x)=-c_3xc_3^{-1}$. Consequently, T is decomposed as

$$T(x) = \phi_1(\phi_2(\phi_3(x))) = a_1a_3xa_3^{-1}a_1.$$

If Φ_i denotes the matrix associated to ϕ_i, with respect to the canonical basis, these are given by

$$\Phi_1 = \frac{1}{7}\begin{pmatrix} -6 & -2 & 3 \\ -2 & -3 & -6 \\ 3 & -6 & 2 \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \Phi_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and we can easily verify that $\mathcal{T}=\Phi_1\Phi_2\Phi_3$.

V. AN APPLICATION TO THE COINCIDENCE SITE LATTICE THEORY

Coincidence site lattice theory has provided partial answers to the complex problems that arise in the description of grain and twin boundaries.[16] Mathematically, the problem can be stated as follows:

Let Λ be a lattice in $\mathbb{R}^n$ and let $T\in O(\mathbb{R}^n)$, T is called a coincidence transformation if $\Lambda\cap T\Lambda$ is a sublattice of Λ. The problem is therefore to identify and characterize coincidence transformations of a given lattice Λ.

Here, by considering simple reflections as primitive transformation, we analyze this problem by finding conditions under which a given transformation is of coincidence. In a previous work,[7] it was conjectured that any arbitrary coincidence transformation can be decomposed as product of coincidence reflections by vectors of the lattice Λ. This conjecture was proved in two dimensions[8] and here, as an application of our results, we prove the conjecture for $\mathbb{Z}^n$ (Theorem 20).

We first introduce the basic concepts related to lattices and coincidence lattices, by following the formalization of the coincidence problem given by Baake.[17] Henceforth $\mathcal{B}(x,y)$ represents the canonical scalar product in $\mathbb{R}^n$, denoted by $x\cdot y$.

Definition 7: A discrete subset $\Lambda\subset\mathbb{R}^n$ is called a lattice, of dimension n, if it is spanned as $\Lambda=\oplus_{i=1}^{n}\mathbb{Z}a_i$, with $\{a_1,\ldots,a_1\}$ a set linearly independent vectors of $\mathbb{R}^n$. These vectors form a basis of the lattice.

The lattice Λ is isomorphic to the free Abelian group of order n. It allows us to define the concept of sublattice.

Definition 8: Let $\Lambda\subset\mathbb{R}^n$ be a lattice. A subset $\Lambda_1\subset\Lambda$ is called a sublattice of Λ if it is a subgroup of finite order, i.e., $[\Lambda,\Lambda_1]<\infty$ (the number of the right cosets is finite).

The following two definitions are central for the coincidence problem.

Definition 9: Two lattices Λ_1 and Λ_2 are called commensurate, denoted by $\Lambda_1\sim\Lambda_2$ if and only if $\Lambda_1\cap\Lambda_2$ is a sublattice of both Λ_1 and Λ_2.

Definition 10: An orthogonal transformation $T\in O(\mathbb{R}^n)$ is called a coincidence transformation if and only if $T\Lambda\sim\Lambda$. The integer $\Sigma(T)=[\Lambda:T\Lambda\cap\Lambda]$ is called the coincidence index of T with respect to Λ. If T is not a coincidence transformation then $\Sigma(T):=\infty$. Two useful sets are also defined,

$$OC(\Lambda) := \left\{T\in O(n)\middle|\sum(T)<\infty\right\},$$

$$SOC(\Lambda) := \{T\in O(n)|\det T=1\}.$$

Coincidence transformations are usually worked out using matrices. In what follows, we recall this approach in order to state a result that will be used later.

Definition 11: Let Λ be a lattice in $\mathbb{R}^n$ with basis $\{a_1,\ldots,a_n\}$. The structure matrix N of Λ is defined through the relation $a_i=Ne_i=\Sigma_{j=1}^{n}N_{ji}e_j$, where $\{e_1,\ldots,e_n\}$ is the canonical basis of $\mathbb{R}^n$.

Theorem 12 (Grimmer): *Let Λ_1 and Λ_2 be two lattices in $\mathbb{R}^n$, with structure matrices N_1 and N_2, respectively. Then, $\Lambda_1\sim\Lambda_2$ if and only if $N_1^{-1}N_2$ has rational entries.*

Theorem 13: *Let $\Lambda\subset\mathbb{R}^n$ be a lattice and let T be an orthogonal transformation. Then, $T\in OC(\Lambda)$ if and only if its associated matrix, with respect to the basis of the lattice, has rational entries.*

A consequence of this theorem is the following.

Proposition 14: Let $\Lambda=\oplus_{i=1}^{n}\mathbb{Z}a_i$ and T be a lattice and an orthogonal transformation in $\mathbb{R}^n$, respectively. Then $T\in OC(\Lambda)$ if and only if for any a_i there exists $m_i\in\mathbb{N}$ such that $m_ia_i\in T(\Lambda)$.

With this background, we can formulate the problem of coincidences between two lattices by using the language of Clifford algebras. By simplicity, in some cases we restrict our treatment to the case of hypercubic lattices $\mathbb{Z}^n$.

Let $\mathbb{Z}^n=\oplus_{i=1}^{n}\mathbb{Z}e_i$ be a n-dimensional hypercubic lattice equipped with a canonical basis $\{e_1,\ldots,e_n\}$. As we have seen, the simple reflection R of a vector x can be written as

$$R(x)=-sxs^{-1}=-\lambda sx(\lambda s)^{-1},$$

where $\lambda\neq 0$ and the reflection hyperplane is $H_s=\{s\}^{\perp}$. We shall find conditions under which R is a coincidence reflection.

Proposition 15: Let $\Lambda=\oplus_{i=1}^{n}\mathbb{Z}a_i$ be a lattice in $\mathbb{R}^n$ and consider a vector $s\in\mathbb{R}^n$. If the transformation $R(x)=-sxs^{-1}$ is a coincidence reflection, i.e., *$R(x)\in OC(\Lambda)$, then there exists a vector $t\in\Lambda$ such that $R(x)=-sxs^{-1}=-txt^{-1}$.*

Proof: Let R be a reflection and assume $R\in OC(\Lambda)$. Given this last assumption, for a given $a\in\Lambda$ we can always find $m\in\mathbb{N}$ such that $mR(a)=R(ma)\in\Lambda$. Thus, for a given $x\in\Lambda$ the vector $y=R(x)$ belongs to the lattice Λ, that is, for some $s\in\mathbb{R}^n$ we have that

$$y=-sxs^{-1}\in\Lambda.$$

Now, since $ys=-sx$,

$$y \cdot s = -s \cdot x$$

$$y \wedge s = -s \wedge x = x \wedge s,$$

and therefore

$$(y - x) \wedge s = 0.$$

Consequently, since $x, y \in \Lambda$, there exists $\lambda \in \mathbb{R}$ such that $y - x = \lambda s \in \Lambda$. By taking $t = \lambda s \in \Lambda$, we conclude that $R(x) - sxs^{-1} = -txt^{-1}$.

■

The contrary is true for hypercubic lattices $\Lambda = \mathbb{Z}^n$.

Proposition 16: Consider $c \in \mathbb{Z}^n$ with $c \neq 0$. Then $R(x) = -cxc^{-1} \in OC(\mathbb{Z}^n)$.

Proof: If $c, x \in \mathbb{Z}^n$ then

$$R(x) = -cxc^{-1} = -2\frac{x \cdot c}{c^2}c + x,$$

since $B(x,c)/c^2 \in \mathbb{Q}$. Then by taking $m = c^2 \in \mathbb{N}$ we obtain

$$mR(x) = -2(x \cdot c)c + mx,$$

which belongs to $\mathbb{Z}^n$ and thus $R(x) \in OC(\mathbb{Z}^n)$.

■

Consequently, for hypercubic lattices the previous results can be summarized as follows.

Theorem 17: *Let R be a reflection by a hyperplane in $\mathbb{R}^n$. Then $R \in OC(\mathbb{Z}^n)$ if and only if it can be written as*

$$R(x) = -cxc^{-1},$$

where $c \in \mathbb{Z}^n$.

Now, we are interested in decomposing any arbitrary coincidence orthogonal transformation into a product of coincidence reflections. First consider the following.

Lemma 18: Let $T \in OC(\mathbb{Z}^n)$ be a coincidence orthogonal transformation. Let also $a \in \mathbb{Z}^n$ and $b \in T(Z^n)$ be two lattice vectors of the same length, that is $a^2 = b^2$. Then, there exists a map $S \in OC(\mathbb{Z}^n)$ such that $S(a) = b$.

Proof: Let $a \in \mathbb{Z}^n$ be a lattice vector and let $T \in OC(\mathbb{Z}^n)$ be a coincidence orthogonal transformation. If $b \in T(\mathbb{Z}^n)$ is a vector in the transformed lattice, then there exists an integer m such that $m(a-b) \in \mathbb{Z}^n$. Thus, the reflection defined by

$$S(x) = -(ma - mb)x(ma - mb)^{-1} = -(a - b)x(a - b)^{-1},$$

belongs to $OC(\mathbb{Z}^n)$, and then it follows that

$$S(a) = b.$$

■

An immediate consequence is the following.

Corollary 19: Consider the hypercubic lattice $\mathbb{Z}^n$ and let $T \in OC(\mathbb{Z}^n)$ be a coincidence orthogonal transformation. Let also $a \in \mathbb{Z}^n$ and $b \in T(\mathbb{Z}^n)$ be vectors of the same length $(a^2 = b^2)$ belonging to the lattice and to the transformed lattice, respectively. Then there exists $c \in \mathbb{Z}^n$ such that $S(a) = b$, where $S(x) = -cxc^{-1}$.

The following theorem allows us to formulate our main result, namely that any arbitrary coincidence transformation can be written as product of coincidence reflections by vectors of the lattice $\mathbb{Z}^n$.

Theorem 20: *Let $\mathbb{Z}^n$ be a hypercubic lattice, and consider $T \in OC(\mathbb{Z}^n)$. Then, for some integer*

l, $0<l\leqslant n$, *there exist reflections* $R_1,R_2,\ldots,R_l\in OC(\mathbb{Z}^n)$ *such that* T *can be written as* $T=R_1R_2\cdots R_l$.

Proof: We will proceed by induction by first considering $n=1$. In this case, the only available orthogonal transformations in $\mathbb{Z}$ are $I(x)=x$ and $S(x)=-x$. If $b\in\mathbb{Z}$ and $b\neq 0$, we have that $S(x)=-bxb^{-1}$ and $I(x)=S^2(x)$. These transformations belong to $OC(\mathbb{Z})$, as follows from Theorem 16, and thus the theorem is valid for $n=1$.

Assume now that the theorem is valid for $n=k$. Let $\mathbb{Z}^k$ be a k-dimensional hypercubic lattice and let $T\in OC(\mathbb{Z}^{k+1})$ be an orthogonal coincidence transformation. Suppose that $\{e_1,\ldots,e_n\}$ is an orthonormal basis of $\mathbb{Z}^n$ and consider the vectors $T(e_{k+1})$ and e_{k+1}. According to Lemma 18, there exists a reflection $S\in OC(\mathbb{Z}^{k+1})$, such that $S(T(e_{k+1}))=e_{k+1}$. Clearly $ST\in OC(\mathbb{Z}^{k+1})$ but $ST|_{\mathbf{Z}^k}\in OC(\mathbb{Z}^n)$. Then, for some integer $l>0$, by the induction hypothesis we have that $ST=R_1R_2\cdots R_l$, where $R_1,R_2,\ldots,R_l\in OC(\mathbb{Z}^k)$ are reflections. Consequently

$$T=S^{-1}R_1R_2\cdots R_l.$$

■

Theorem 21: *Let* $\mathbb{Z}^n=\oplus_{i=1}^n\mathbb{Z}e_i$ *be a hypercubic lattice. Then an orthogonal transformation* T *is of coincidence*, i.e., $T\in OC(\mathbb{Z}^n)$, *if and only if there exist lattice vectors* $c_1,c_2,\ldots,c_k\in\mathbb{Z}^n$ *such that*

$$T(x)=(-1)^k(c_1c_2\cdots c_k)x(c_1c_2\cdots c_k)^{-1},$$

where $k\leqslant n$.

VI. CONCLUSIONS

In this work we provide a simple algorithm to explicitly calculate the reflections in which a particular orthogonal transformation is decomposed. This algorithm constitutes a constructive proof of the Cartan theorem. Albeit we have assumed that the underlying field is $\mathbb{R}$, the proofs of and theorems are also valid for $\mathbb{Q}$ or $\mathbb{C}$.

The approach given here can also be useful for solving equations systems and orthogonal elimination. In this case, Householder matrices replaces the reflections through hyperplanes derived from the Cartan theorem here presented. Also we can generalize the proof of this theorem to the Cartan-Dieudonné theorem.[18] This work is under way.

As an application, the crystallographic problem of coincidence lattices is formulated in terms of reflections. We show that any arbitrary coincidence transformation for the lattice $\mathbb{Z}^n$ can be written as product of coincidence reflections in vectors of the lattice.

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The generalized Davey-Stewartson equations, its Kac-Moody-Virasoro symmetry algebra and relation to Davey-Stewartson equations

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We compute the Lie symmetry algebra of the generalized Davey-Stewartson (GDS) equations and show that under certain conditions imposed on parameters in the system it is infinite-dimensional and isomorphic to that of the standard integrable Davey-Stewartson equations which is known to have a very specific Kac-Moody-Virasoro loop algebra structure. We discuss how the Virasoro part of this symmetry algebra can be used to construct new solutions, which are of vital importance in demonstrating existence of blow-up profiles, from known ones using Lie subgroup of transformations generated by three-dimensional subalgebras, namely $\mathrm{sl}(2,\mathbb{R})$. We further discuss integrability aspects of GDS equations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162147]

I. INTRODUCTION

A system of nonlinear partial differential equations in $2+1$ dimensions as a model of wave propagation in a bulk medium composed of an elastic material with couple stresses has recently been derived in Ref. 1, namely

$$\begin{aligned} &i\psi_t+\delta\psi_{xx}+\psi_{yy}=\chi|\psi|^2\psi+\gamma(w_x+\phi_y)\psi,\\ &w_{xx}+n\phi_{xy}+m_2w_{yy}=(|\psi|^2)_x,\\ &nw_{xy}+\lambda\phi_{xx}+m_1\phi_{yy}=(|\psi|^2)_y, \end{aligned} \tag{1.1}$$

with the condition $(\lambda-1)(m_1-m_2)=n^2$. Here $\psi(t,x,y)$ is a complex function, $w(t,x,y)$ and $\phi(t,x,y)$ are real functions and $\delta,n,m_1,m_2,\lambda,\chi,\gamma$ are real constants. The authors of Ref. 1 showed that if the parameters are related by

$$n=1-\lambda=m_1-m_2, \tag{1.2}$$

then (1.1) can be reduced to the standard Davey-Stewartson (DS) equations (in general not integrable) by a noninvertible point transformation of dependent variables. Therefore, they called (1.1) the generalized Davey-Stewartson (GDS) equations. Below, we justify this naming from a group-theoretical point of view. Also, in Ref. 1 some travelling type solutions of (1.1) in terms of elementary and elliptic functions are obtained. Based on some physically obvious Noetherian symmetries (time-space translations and constant change of phase), global existence and nonexistence results are given in Ref. 2. In another recent work,[3] under some constraints on the physical parameters, the so-called hyperbolic-elliptic-elliptic case of the system (1.1) [in Ref. 3 the system is classified into different types according to the signs of parameters (δ,m_1,m_2,λ)] was shown to

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admit singular solutions that blow up in a finite time. To do this, inspired by the (pseudo) conformal invariance of the DS system, they used the fact that time-dependent $\mathrm{SL}(2,\mathbb{R})$ invariant solutions can be generated from stationary radial solutions for an appropriate choice of coefficients.

The purpose of this paper is to study GDS equations from a group theoretical point of view. For our purposes, we find it more convenient to consider the differentiated form of (1.1). Thus, differentiating the last two equations of (1.1) with respect to x and y, respectively, and then making the substitution $w_x \to w$, $\phi_y \to \phi$ and rewriting the corresponding system in a real form by separating $\psi = u + iv$ into real and imaginary parts, we obtain a system of four real partial differential equations,

$$\begin{aligned} u_t + \delta v_{xx} + v_{yy} &= \chi v(u^2 + v^2) + \gamma v(w + \phi), \\ -v_t + \delta u_{xx} + u_{yy} &= \chi u(u^2 + v^2) + \gamma u(w + \phi), \\ w_{xx} + n\phi_{xx} + m_2 w_{yy} &= 2(u_x^2 + uu_{xx} + v_x^2 + vv_{xx}), \\ nw_{yy} + \lambda\phi_{xx} + m_1\phi_{yy} &= 2(u_y^2 + uu_{yy} + v_y^2 + vv_{yy}). \end{aligned} \tag{1.3}$$

In the sequel, we shall call (1.3) the GDS equations.

The main result of the paper is to show that, when some conditions on physical parameters $\delta, n, m_1, m_2, \lambda$ are imposed, the Lie algebra of the symmetry group of the GDS system has a Kac-Moody-Virasoro (KMV) loop structure which is shared by the symmetry algebras of all known integrable equations in $2+1$ dimensions such as the Kadomtsev-Petviashvilli (KP) equation[4,5] and the usual integrable DS equations.[6] The corresponding special case is a candidate for being integrable. Moreover, we show that this algebra is isomorphic to that of DS equations[6]

$$\begin{aligned} i\psi_t + \delta_1\psi_{xx} + \psi_{yy} &= \delta_2|\psi|^2\psi + w\psi, \\ \varepsilon_1 w_{xx} + w_{yy} &= \varepsilon_2(|\psi|^2)_{yy}, \end{aligned} \tag{1.4}$$

with $\delta_1 = \pm 1$, $\delta_2 = \pm 1$. In the special case when $\delta_1 + \varepsilon_1 = 0$, this system which is one of the rare systems in more than $1+1$ dimensions for which the Cauchy initial value problem is solvable by the inverse spectral transform (IST) technique becomes completely integrable. The Lie algebra of the symmetry group of the integrable DS system is referred to as the DS algebra. This isomorphism (a necessary condition for two different systems to be transformable into each other) should motivate one to look for point transformations taking the Lie algebras into each other. We expect such transformations to transform the systems into each other as well.

In Sec. II we compute the Lie symmetry algebra of (1.3) and identify its structure. In particular, we show that for a special choice of parameters it is a centerless Kac-Moody-Virasoro algebra.

II. THE SYMMETRY GROUP OF THE GDS EQUATIONS AND STRUCTURE OF ITS LIE ALGEBRA

We apply the standard infinitesimal procedure[7] to find the symmetry algebra L and hence the symmetry group G of (1.3). We write the GDS equations as a system $\Delta_i(t,x,y,u,v,w,\phi) = 0$, $i = 1,2,3,4$. A general element of the algebra is represented by a vector field

$$\mathbf{V} = \tau\partial_t + \xi\partial_x + \eta\partial_y + \varphi_1\partial_u + \varphi_2\partial_v + \varphi_3\partial_w + \varphi_4\partial_\phi, \tag{2.1}$$

where the coefficients $\tau, \xi, \eta, \varphi_i, i = 1,2,3,4$ are functions of t,x,y,u,v,w,ϕ. According to the general theory for symmetries of differential equations, to find these functions we prolong the vector field (2.1) to second order derivatives and require that the second prolonged vector field annihilates Δ_i on the solution manifold of the system, namely

$$\mathrm{pr}^{(2)}\,\mathbf{V}(\Delta_i(t,x,y,u,v,w,\phi))\big|_{\Delta_i=0}=0,\quad i=1,2,3,4, \tag{2.2}$$

where $\mathrm{pr}^{(2)}\,\mathbf{V}$ is the second prolongation of the vector field $\mathbf{V}$. This condition provides us with a quite complicated system of determining equations (a system of linear partial differential equations) for the coefficients. This step is entirely algorithmic and is implemented on several computer algebra packages like REDUCE, MATHEMATICA, MAPLE (see Ref. 8 for a survey of symbolic softwares for symmetry). The final step of integrating the determining equations is less algorithmic. Solving these huge numbers of determining equations we find that the general element can be written as

$$\mathbf{V}=T(f)+X(g)+Y(h)+W(m), \tag{2.3}$$

where

$$\begin{aligned}
T(f)&=f(t)\partial_t+\frac{1}{2}f'(t)(x\partial_x+y\partial_y-u\partial_u-v\partial_v-2w\partial_w-2\phi\partial_\phi)\\
&\quad-\frac{(x^2+\delta y^2)}{8\delta}\left[f''(t)(v\partial_u-u\partial_v)+\frac{f'''(t)}{2\gamma}(\partial_w+\partial_\phi)\right],\\
X(g)&=g(t)\partial_x-\frac{x}{2\delta}\left[g'(t)(v\partial_u-u\partial_v)+\frac{g''(t)}{2\gamma}(\partial_w+\partial_\phi)\right],\\
Y(h)&=h(t)\partial_y-\frac{y}{2}\left[h'(t)(v\partial_u-u\partial_v)+\frac{h''(t)}{2\gamma}(\partial_w+\partial_\phi)\right],\\
W(m)&=m(t)(v\partial_u-u\partial_v)+\frac{m'(t)}{2\gamma}(\partial_w+\partial_\phi).
\end{aligned} \tag{2.4}$$

The functions $g(t)$, $h(t)$, and $m(t)$ are arbitrary functions of class $C^\infty(I)$, $I\subseteq\mathbb{R}$. The function $f(t)$ is arbitrary if

$$m_2\delta+n+1=0,\quad m_1\delta+n\delta+\lambda=0, \tag{2.5}$$

otherwise $f(t)=c_2t^2+c_1t+c_0$. We mention that these conditions come from the fact that two of the determining equations are

$$(m_2\delta+n+1)f'''(t)=0,\quad (m_1\delta+n\delta+\lambda)f'''(t)=0,$$

whereas the remaining ones are solved without any constraints on g, h, and m.

We mainly focus on the case when $f(t)$ is allowed to be arbitrary. The symmetry algebra realized by the vector fields (2.3) and (2.4) is then infinite dimensional and more important has the structure of a Kac-Moody-Virasoro algebra as we shall see below. More interestingly, it is generic among the symmetry algebras of a few 2+1-dimensional integrable partial differential equations (the KP equation, the modified KP equation, the potential KP equation, the integrable three-wave resonant equations and the integrable DS equations). Henceforth, we shall call this the GDS symmetry algebra and the corresponding system the GDS system.

Note that sometimes it is more convenient to use the polar decomposition $u+iv=\mathrm{Re}^{i\sigma}$ so that in (2.4) we can write

$$u\partial_u+v\partial_v=R\partial_R,\quad -(v\partial_u-u\partial_v)=\partial_\sigma.$$

The commutation relations for the GDS algebra are easily obtained as follows:

$$[T(f_1),T(f_2)]=T(f_1f_2'-f_1'f_2),$$

$$[T(f),X(g)] = X\left(fg' - \tfrac{1}{2}f'g\right),$$

$$[T(f),Y(h)] = Y\left(fh' - \tfrac{1}{2}f'h\right),$$

$$[T(f),W(m)] = W(fm'), \tag{2.6}$$

$$[X(g_1),X(g_2)] = -\frac{1}{2\delta}W(g_1g_2' - g_1'g_2),$$

$$[Y(h_1),Y(h_2)] = -\tfrac{1}{2}W(h_1h_2' - h_1'h_2),$$

$$[X(g),Y(h)] = [X(g),W(m)] = [Y(h),W(m)] = [W(m_1),W(m_2)] = 0.$$

From (2.6) we see that the GDS system has a Lie symmetry algebra L isomorphic to that of the DS symmetry algebra.[6] Indeed, it allows a Levi decomposition

$$L = S \oplus N, \tag{2.7}$$

where $S=\{T(f)\}$ is a simple infinite-dimensional Lie algebra and

$$N = \{X(g),Y(h),W(m)\}$$

is a nilpotent ideal (nilradical). Here, $\oplus$ denotes a semidirect sum. The algebra $\{T(f)\}$ is isomorphic to the Lie algebra corresponding to the Lie group of diffeomorphisms of a real line.

We remark that a similar isomorphism between the symmetry algebras of a class of (integrable) generalized cylindrical KP (GCKP) equation and of the KP equation was pointed out in Ref. 9.

Expanding the arbitrary functions f, g, h, and m into Laurent polynomials and considering each monomial t^n (n not necessarily positive integer) separately, we obtain a realization of a KMV algebra without central extension. Here the factor subalgebra S is the Virasoro part, the nilpotent subalgebra N is the Kac-Moody part of the GDS algebra.[10] We refer for different realizations of the Virasoro algebras to Ref. 11. Furthermore, just as the DS algebra[6] it can be shown that the GDS algebra with (2.5) can be imbedded into a Kac-Moody-type loop algebra.

Theorem 2.1: *The system* (1.3) *is invariant under an infinite-dimensional Lie point symmetry group, the Lie algebra of which has a Kac-Moody-Virasoro structure isomorphic to the DS algebra if and only if the conditions* (2.5) *hold.*

Let us mention that the GDS equations are also invariant under a group of discrete transformations generated by

$$t \to t, \quad x \to -x, \quad y \to y, \quad \psi \to \psi, \quad w \to w, \quad \phi \to \phi,$$

$$t \to t, \quad x \to x, \quad y \to -y, \quad \psi \to \psi, \quad w \to w, \quad \phi \to \phi,$$

$$t \to t, \quad x \to x, \quad y \to y, \quad \psi \to -\psi, \quad w \to w, \quad \phi \to \phi,$$

$$t \to -t, \quad x \to x, \quad y \to y, \quad \psi \to \psi^*, \quad w \to w, \quad \phi \to \phi. \tag{2.8}$$

The obvious physical symmetries L_p of the GDS equations are obtained by restricting all the functions f, g, h, and m to be first order polynomials. Indeed, we have

$$T = T(1) = \partial_t, \quad P_1 = X(1) = \partial_x, \quad P_2 = Y(1) = \partial_y,$$

$$W_0 = W(1) = v\partial_u - u\partial_v,$$

$$D = T(t) = t\partial_t + \tfrac{1}{2}(x\partial_x + y\partial_y - u\partial_u - v\partial_v - 2w\partial_w - 2\phi\partial_\phi), \tag{2.9}$$

$$B_1 = X(t) = t\partial_x - \frac{x}{2\delta}(v\partial_u - u\partial_v), \quad B_2 = Y(t) = t\partial_y - \frac{y}{2}(v\partial_u - u\partial_v),$$

$$W_1 = W(t) = t(v\partial_u - u\partial_v) + \frac{1}{2\gamma}(\partial_w + \partial_\phi).$$

We see that T, P_1, P_2 generate translations, D dilations, B_1 and B_2 Galilei boosts in the x and y directions, respectively. Finally, W_0 and W_1 generate a constant change of phase of ψ and a change of phase of ψ, linear in t, plus constant shifts in w and ϕ, respectively.

The generators (2.9) form a basis of an eight-dimensional solvable Lie algebra $L_p = \{D, T, P_1, P_2, B_1, B_2, W_0, W_1\}$. It has a seven-dimensional nilpotent ideal (the nilradical) $N = \{T, P_1, P_2, B_1, B_2, W_0, W_1\}$.

Another finite-dimensional algebra, not contained in L_p is obtained by restricting $f(t)$ to quadratic polynomials. We obtain $T=T(1)$, $D=T(t)$ as in (2.9), and in addition

$$C = T(t^2) = t^2\partial_t + tD - \frac{(x^2 + \delta y^2)}{4\delta}(v\partial_u - u\partial_v). \tag{2.10}$$

The commutation relations are

$$[T,D] = T, \quad [T,C] = 2D, \quad [D,C] = C,$$

so that we have obtained the algebra $\mathrm{sl}(2,\mathbb{R})$ with C generating conformal type of transformations

$$\tilde{t} = \frac{t}{1-pt}, \quad \tilde{x} = \frac{x}{1-pt}, \quad \tilde{y} = \frac{y}{1-pt},$$

$$\tilde{R} = (1-pt)R, \quad \tilde{\sigma} = \frac{p(x^2 + \delta y^2)}{4\delta(1-pt)} + \sigma, \tag{2.11}$$

$$\tilde{w} = (1-pt)^2 w, \quad \tilde{\phi} = (1-pt)^2\phi,$$

where p is the group parameter. Further, composing (2.11) with time translations generated by T and dilations generated by D we obtain the $\mathrm{SL}(2,\mathbb{R})$ group generated by actions on the space of independent and depend variables. It should be mentioned that any finite-dimensional subalgebra of the Virasoro algebra of 2+1 dimensional integrable equations is isomorphic to $\mathrm{sl}(2,\mathbb{R})$ or one of its subalgebras. The transformed variables and the new solution in terms of the original ones are given by the formulas

$$\tilde{t} = \frac{c+dt}{a+bt}, \quad \tilde{x} = \frac{x}{a+bt}, \quad \tilde{y} = \frac{y}{a+bt}, \quad ad - bc = 1,$$

$$\tilde{\psi} = (a+bt)^{-1} \exp\left\{\frac{ib(x^2 + \delta y^2)}{4\delta(a+bt)}\right\}\psi(\tilde{t},\tilde{x},\tilde{y}),$$

$$\tilde{w} = (a+bt)^{-2} w(\tilde{t},\tilde{x},\tilde{y}),$$

$$\tilde{\phi} = (a+bt)^{-2}\phi(\tilde{t},\tilde{x},\tilde{y}). \tag{2.12}$$

Here a,b,c are the group parameters of $\mathrm{SL}(2,\mathbb{R})$. These are exactly the formulas which played an essential role in the construction of analytic blow-up profiles[3] in which the authors made use of stationary radial solutions (ψ,w,ϕ) to generate new solutions (time dependent) $(\tilde{\psi},\tilde{w},\tilde{\phi})$ of the GDS equations. More generally, the elements of the connected part of the full symmetry group of the GDS equations can be obtained by integrating the vector fields (2.3) and (2.4). We refer the reader to Ref. 6 for the general Lie group of transformations of DS algebra.

Let us now return to the isomorphic GDS and DS symmetry algebras, and transform the GDS vector fields (2.1) by the point transformation $q=w+\phi-|\psi|^2$. It is easy to see that the component $\frac{1}{2}(\partial_w+\partial_\phi)$ transforms to ∂_q, and $D\to x\partial_x+y\partial_y-u\partial_u-v\partial_v-2q\partial_q$, and the rest remains unaltered, namely the DS symmetry algebra is obtained. This means that the functions (ψ,q) satisfy the DS equations whenever (ψ,w,ϕ) satisfy the GDS equations, but not vice versa. At this time, it remains open whether it is possible to construct an invertible point transformation relating these two systems.

We conclude by making several comments. As is well illustrated by the results of this paper, knowing that a nonlinear partial differential equation (or system) admits a KMV algebra as a symmetry algebra can serve as a useful criterion of identifying integrable equations. In particular, this fact can be used to pick out an integrable equation from a class of generically nonintegrable ones. For instance, for all values of parameters not satisfying (2.5), the Virasoro part $T(f)$ of the GDS algebra is not present. The first author of the present paper and Winternitz[12] used the same approach to identify all subclasses invariant under a KMV algebra and its subalgebras containing up to three arbitrary functions of time from a rather general class of KP-type equations involving nine arbitrary functions of one or two variables. On the other hand, a classification of all one- and two-dimensional subalgebras of the DS algebra into conjugacy classes under the adjoint action of the DS group (including the discrete transformations) is performed in Ref. 6. The GDS algebra will have the same conjugacy classes of subalgebras as the DS algebra. Depending on which of the functions $g(t)$, $h(t)$, and $m(t)$ are nonzero, precisely six conjugacy classes of one-dimensional subalgebras exist,

$$L_{1,1}=\{T(1)\},\quad L_{1,2}^{a}=\{X(1)+aY(1)\},\quad L_{1,3}(h)=\{X(1)+Y(h)\},\quad a\geqslant 0,$$

$$L_{1,4}=\{Y(1)\},\quad L_{1,5}=\{W(t)\},\quad L_{1,6}=\{W(1)\}.$$

They can be used to reduce the integrable GDS system to integrable one in two variables and thus to obtain subgroup invariant solutions. There will be four type of reductions since only the first four subgroups corresponding to $(L_{1,1},L_{1,2}^{a},L_{1,3}(h),L_{1,4})$ will generate actions on the coordinate space (t,x,y). The remaining two $(L_{1,5},L_{1,6})$ generate purely vertical (or gauge) transformations changing phases only and thus lead to no reductions. For example, one can show that all the travelling wave solutions obtained in Ref. 1 can be extracted from those of representative reduced equations by applying appropriate symmetry group transformations. We note that these types of physically important solutions are invariant under translational subgroups alone.

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The Faraday effect revisited: General theory

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This paper is the first in a series revisiting the Faraday effect, or more generally, the theory of electronic quantum transport/optical response in bulk media in the presence of a constant magnetic field. The independent electron approximation is assumed. At zero temperature and zero frequency, if the Fermi energy lies in a spectral gap, we rigorously prove the Widom-Streda formula. For free electrons, the transverse conductivity can be explicitly computed and coincides with the classical result. In the general case, using magnetic perturbation theory, the conductivity tensor is expanded in powers of the strength of the magnetic field B. Then the linear term in B of this expansion is written down in terms of the zero magnetic field Green function and the zero field current operator. In the periodic case, the linear term in B of the conductivity tensor is expressed in terms of zero magnetic field Bloch functions and energies. No derivatives with respect to the quasimomentum appear and thereby all ambiguities are removed, in contrast to earlier work. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162148]

I. INTRODUCTION

In sharp contrast with the zero magnetic field case, the analysis of properties of electrons in periodic or random potentials subjected to external magnetic fields is a very challenging problem. The difficulty is rooted in the singular nature of the magnetic interaction: due to a linear increase of the magnetic vector potential, the naive perturbation theory breaks down even at arbitrarily small fields.

To our best knowledge, only the periodic case has been considered in connection with the Faraday effect for bulk systems. The first full scale quantum computation was done by Roth[30] (for a review of earlier attempts[4–6] we direct the reader to this paper). The physical experiment starts by sending a monochromatic light wave, parallel to the $0z$ direction and linearly polarized in the plane $x0z$. When the light enters the material, the polarization plane can change; in fact, there exists a linear relation between the angle θ of rotation of the plane of polarization per unit length and the transverse component of the conductivity tensor σ_{xy} [see formula (1) in Ref. 30]. The material is chosen in such a way that when the magnetic field is zero, this transverse component

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vanishes. When the magnetic field B is turned on, the transverse component is no longer zero. For weak fields one expands the conductivity tensor to first order in B and obtains a formula for the Verdet constant.

Therefore the central object is $\sigma_{xy}(B)$, which depends among other things on temperature, density of the material, and frequency of light. Using a modified Bloch representation, Roth was able to obtain a formula for $(\mathrm{d}\sigma_{xy}/\mathrm{d}B)(0)$, and studied how this first order term behaves as a function of frequency, both for metals and semiconductors.

However, the theory in Ref. 30 is not free of difficulties. First, it seems almost hopeless to estimate errors or to push the computation to higher orders in B. Second, even the first order formula contains terms which are singular at the crossings of the Bloch bands. Accordingly, at the practical level this theory only met a moderate success and alternative formalisms have been used, as for example the celebrated Kohn-Luttinger effective many band Hamiltonian (see Refs. 17, 31, and 28 and references therein), or tight-binding models.[25] Since all these methods have limited applicability, a more flexible approach was still needed.

In the zero magnetic field case, a very successful formalism (see, e.g., Refs. 2, 9, 16, and 27 and references therein) is to use the Green function method. This is based on the fact that the traces involved in computing various physical quantities can be written as integrals involving Green functions. The main aim of our paper is to develop a Green function approach to the Faraday effect, i.e., for the conductivity tensor when a magnetic field is present. Let us point out that the use of Green functions (albeit different from the ones used below) goes back at least to Sondheimer and Wilson[33] in their theory of diamagnetism of Bloch electrons. Aside from the fact that the Green function (i.e., the integral kernel of the resolvent or the semigroup) is easier to compute and control, the main point is that by factorizing out the so-called nonintegrable phase factor (or magnetic holonomy) from the Green function, one can cope with the singularities introduced by the increase at infinity of the magnetic vector potentials. In addition (as it has already been observed by Schwinger[32] in a QED context), after factorizing out the magnetic holonomy one remains with a gauge invariant quantity which makes the problem of gauge fixing irrelevant. The observation (going back at least to Peierls[26]) that one can use these magnetic phases in order to control the singularity of the magnetic perturbation has been used many times in various contexts (see, e.g., Refs. 19 and 33). We highlight here the results of Nedoluha[20] where a Green function approach for the magneto-optical phenomena at zero temperature and with the Fermi level in a gap has been investigated.

But the power of this method has only recently been fully exploited in Refs. 11 and 12 and developed as a general gauge invariant magnetic perturbation theory in Ref. 22. Applied to the case at hand, this theory gives an expansion of the conductivity tensor in terms of the zero magnetic field Green functions. Moreover, it is free of any divergences. A key ingredient in controlling divergences is the exponential decrease of the Green functions with the distance between the arguments, for energies outside the spectrum.[10,21] We stress the fact that since no basis is involved, periodicity is not needed and the theory can also be applied to random systems. Finite systems and/or special geometries (layers) are also allowed. The content of the paper is as follows.

In Sec. II we give a derivation of the conductivity tensor from first principles in the linear response theory. We include it to point out that it coincides with various formulas used before. Although in physics establishing the Kubo formula is considered somehow a triviality, from a mathematical point of view it remains a serious challenge (see Ref. 7).

Section III contains the precise formulation of the thermodynamic limit, stated in Theorem 3.1. We do not give its proof here, but we try to explain why it is true.

Section IV shows that at the thermodynamic limit, at zero temperature, zero frequency, and for the Fermi energy in a spectral gap, we reobtain a formula of Streda[34] for the transverse component of the conductivity tensor, known from the integral quantum Hall effect (IQHE). A precise statement and its proof are contained in Theorem 4.1. Moreover, under the proviso that exponentially localized Wannier function exist (see Theorem 4.2), this transverse component vanishes (see also Refs. 35 and 3 for related results). We stress that this result holds for the *whole* $\sigma_{xy}(B)$ as long as

the magnetic field is not too large, not just for $(\mathrm{d}\sigma_{xy}/\mathrm{d}B)(0)$. The vanishing of its first order correction was in fact claimed in formula (50) in Ref. 30.

Section V contains the exact quantum computation of $\sigma_{xy}(B)$ for free electrons; in spite of the fact that such a result might be known (and it is known at zero frequency), we were not able to find it in the literature. Interestingly enough, the quantum computation gives the same result as the well-known classical computation (when the relaxation time is infinite).

Section VI contains the core of the paper, which includes the derivation of $(\mathrm{d}\sigma_{xy}/\mathrm{d}B)(0)$ for general Bloch electrons. As in the zero magnetic field case, its formula only contains zero magnetic field Green functions and current operators.

Section VII deals with periodic systems, and the result of the preceding section is written down in terms of zero magnetic field Bloch functions and bands.

At the end we have some conclusions.

The main goal of this paper is to present the strategy, state the results concerning the Verdet constant, and to outline future theoretical and practical problems. Detailed proofs of the thermodynamic limit and of other technical estimates will be given elsewhere.

II. PRELIMINARIES: THE CONDUCTIVITY TENSOR IN THE LINEAR RESPONSE REGIME

We begin by fixing the notation used in the description of independent electrons subjected to a constant magnetic field. The units are chosen so that $\hbar=1$. Since we consider spin $1/2$ particles, the one particle Hilbert space for a nonconfined particle is

$$\mathcal{H}_\infty = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$$

with the standard scalar product. Accordingly, all operators below and their integral kernels are 2×2 matrices in the spin variable. We choose the constant magnetic field of strength B to be oriented along the z axis. Then the one particle Hamiltonian with the spin-orbit coupling included is (see, e.g., Ref. 30)

$$H_\infty(B) = \frac{1}{2m}\mathbf{P}(B)^2 + V + g\mu_b B\sigma_3, \tag{2.1}$$

with

$$\mathbf{P}(B) = -i\nabla - b\mathbf{a} + \frac{1}{2mc^2}\mathbf{s}\wedge(\nabla V) = \mathbf{P}(0) - b\mathbf{a}, \tag{2.2}$$

where

$$b = -\frac{e}{c}B$$

and $\mathbf{a}(\mathbf{x})$ is an arbitrary smooth magnetic vector potential which generates a magnetic field of intensity $B=1$, i.e., $\nabla\wedge\mathbf{a}(\mathbf{x})=(0,0,1)$. The most frequently used magnetic vector potential is the symmetric gauge,

$$\mathbf{a}_0(\mathbf{x}) = \tfrac{1}{2}\mathbf{n}_3\wedge\mathbf{x}, \tag{2.3}$$

where $\mathbf{n}_3$ is the unit vector along z axis.

In the periodic case we denote by $\mathcal{L}$ the underlying Bravais lattice, by Ω its elementary cell and by Ω^* the corresponding Brillouin zone. $|\Omega|$ and $|\Omega^*|$ stand for the volumes of the elementary cell and Brillouin zone, respectively. In the absence of the magnetic field one has the well-known Bloch representation in terms of Bloch functions,

$$\Psi_j(\mathbf{x},\mathbf{k}) = \frac{1}{\sqrt{|\Omega^*|}} e^{i\mathbf{k}\cdot\mathbf{x}} u_j(\mathbf{x},\mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^3, \tag{2.4}$$

where $u_j(\mathbf{x},\mathbf{k})$ are the normalized to one eigenfunctions of the operator

$$h(\mathbf{k})u_j(\mathbf{x},\mathbf{k}) = \lambda_j(\mathbf{k})u_j(\mathbf{x},\mathbf{k}), \tag{2.5}$$

$$h(\mathbf{k}) = \frac{1}{2m}\left(-i\nabla_p + \frac{1}{2mc^2}\mathbf{s}\wedge(\nabla V) + \mathbf{k}\right)^2 + V = \frac{1}{2m}(\mathbf{p}+\mathbf{k})^2 + V, \quad \mathbf{k} \in \Omega^*,$$

$$\mathbf{p} = -i\nabla_p + \frac{1}{2mc^2}\mathbf{s}\wedge(\nabla V), \tag{2.6}$$

defined in $L^2(\Omega)\oplus L^2(\Omega)$ with periodic boundary conditions. We label $\lambda_j(\mathbf{k})$ in increasing order. We have to remember that, as functions of $\mathbf{k}$, $\lambda_j(\mathbf{k})$, and $u_j(\mathbf{x},\mathbf{k})$ are not differentiable at the crossing points. Since the $\Psi_j(\mathbf{x},\mathbf{k})$'s form a basis of generalized eigenfunctions, the Green function (i.e., the integral kernel of the resolvent) writes as

$$G_\infty^{(0)}(\mathbf{x},\mathbf{y};z) = \int_{\Omega^*}\sum_{j\geqslant 1}\frac{|\Psi_j(\mathbf{x},\mathbf{k})\rangle\langle\Psi_j(\mathbf{y},\mathbf{k})|}{\lambda_j(\mathbf{k})-z}\mathrm{d}\mathbf{k}, \tag{2.7}$$

and it is seen as a matrix in the spin variables. The above formula must be understood in the formal sense since the series on the right-hand side is typically not absolutely convergent, and care is to be taken when interchanging the sum with the integral. Notice however that $G_\infty^{(0)}(\mathbf{x},\mathbf{x}';z)$ is a well behaved matrix valued function.

We consider a system of noninteracting electrons in the grand-canonical ensemble. More precisely, we consider a box $\Lambda_1 \subset \mathbb{R}^3$, which contains the origin, and a family of scaled boxes

$$\Lambda_L = \{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x}/L \in \Lambda_1\}. \tag{2.8}$$

The thermodynamic limit will mean $L\to\infty$, that is when Λ_L tends to fill out the whole space. The one particle Hilbert space is $\mathcal{H}_L := L^2(\Lambda_L)\oplus L^2(\Lambda_L)$. The one particle Hamiltonian is denoted by $H_L(B)$ and is given by (2.1) with Dirichlet boundary conditions [i.e., the wave functions in the domain of $H_L(B)$ vanish at the surface $\partial\Lambda_L$]. More precisely, we first define it on $C_0^\infty(\Lambda_L)\oplus C_0^\infty(\Lambda_L)$, and then $H_L(B)$ will be the Friedrichs extension of this minimal operator. This is indeed possible, because our operator can be written as (up to some irrelevant constants) $-\Delta_D I_2 + W$, where Δ_D is the Dirichlet Laplacian and W is a first order differential operator, relatively bounded to $-\Delta_D I_2$ (remember that $L<\infty$) with relative bound zero. The form domain of $H_L(B)$ is the Sobolev space $H_0^1(\Lambda_L)\oplus H_0^1(\Lambda_L)$, while the operator domain is

$$\mathrm{Dom}(H_L(B)) = D_L \oplus D_L, \quad D_L := H^2(\Lambda_L)\cap H_0^1(\Lambda_L). \tag{2.9}$$

Moreover, $H_L(B)$ is essentially self-adjoint on $C_{(0)}^\infty(\overline{\Lambda_L})$, i.e., functions with support in $\overline{\Lambda_L}$ and indefinitely differentiable in Λ_L up to the boundary.

We assume that the temperature $T=1/(k\beta)$ and the chemical potential μ are fixed by a reservoir of energy and particles. We work in a second quantized setting with an antisymmetric Fock space denoted by $\mathcal{F}_L$. Denote the operators in the Fock space with a hat and borrow some notation from the book of Bratelli and Robinson,[8] if A is an operator defined in $\mathcal{H}_L$, we denote by $\hat{A}=\mathrm{d}\Gamma(A)$ its second quantization in the Fock space. At $t=-\infty$ the system is supposed to be in the grand-canonical equilibrium state of temperature T and chemical potential μ, i.e., the density matrix is

$$\hat{\rho}_e = \frac{1}{\mathrm{Tr}(e^{-\beta\hat{K}_\mu})} e^{-\beta\hat{K}_\mu}, \tag{2.10}$$

where

$$\hat{K}_\mu = \mathrm{d}\Gamma(H_L(B) - \mu \cdot \mathrm{Id}) \tag{2.11}$$

is the "grand-canonical Hamiltonian."

The interaction with a classical electromagnetic field is described by a time-dependent electric potential

$$V(\mathbf{x},t) := (e^{i\omega t} + e^{-i\bar{\omega}t}) e\mathbf{E} \cdot \mathbf{x}, \quad t \leqslant 0, \quad \mathbf{x} \in \Lambda_L. \tag{2.12}$$

so the total time-dependent one-particle Hamiltonian is

$$H(t) = H_L(B) + V(t). \tag{2.13}$$

Notice that e near $\mathbf{E}$ is the positive elementary charge. Here we take $\mathrm{Im}\ \omega < 0$ which plays the role of an adiabatic parameter, and insures that there is no interaction in the remote past. Finally, the one-particle current operator is as usual

$$\mathbf{J} = -ei[H_L(B), \mathbf{X}] = -\frac{e}{m}\mathbf{P}(B), \tag{2.14}$$

where $\mathbf{X}$ is the multiplication by $\mathbf{x}$. Note that $\mathbf{J}$ is a well-defined operator on the domain of $H_L(B)$, because multiplication by any component of $\mathbf{X}$ leaves this domain invariant [see (2.9)]. Moreover, since $L < \infty$, $\mathbf{X}$ is a bounded operator. In fact, $\mathbf{X}$ is the true physical self-adjoint observable, while $\mathbf{P}(B)$ (or $\mathbf{J}$) appear when one differentiates the map $t \mapsto e^{itH_L(B)}\mathbf{X}e^{-itH_L(B)}$ in the strong sense on the domain of $H_L(B)$.

We assume that the state of our system is now described by a time-dependent density matrix, $\hat{\rho}(t)$, obtained by evolving $\hat{\rho}_e$ from $-\infty$ up to the given time, i.e.,

$$i\partial_t \hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)], \quad \hat{\rho}(-\infty) = \hat{\rho}_e. \tag{2.15}$$

Going to the interaction picture and using the Dyson expansion up to the first order, one gets

$$\hat{\rho}(t=0) = \hat{\rho}_e - i\int_{-\infty}^{0} [\mathrm{d}\Gamma(\widetilde{V}(s), \hat{\rho}_e\ ]\mathrm{d}s + \mathcal{O}(\mathbf{E}^2), \tag{2.16}$$

where

$$\widetilde{V}(s) := e^{isH_L(B)} V(s) e^{-isH_L(B)}. \tag{2.17}$$

The current density flowing through our system at $t=0$ is given by [see (2.16)]:

$$\mathbf{j} = \frac{1}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{F}_L}(\hat{\rho}(0)\hat{\mathbf{J}}) = \frac{1}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{F}_L}(\hat{\rho}_e\hat{\mathbf{J}}) - \frac{i}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{F}_L}\left(\int_{-\infty}^{0} [\mathrm{d}\Gamma(\widetilde{V}(s)), \hat{\rho}_e]\hat{\mathbf{J}}\,\mathrm{d}s\right) + \mathcal{O}(\mathbf{E}^2). \tag{2.18}$$

In evaluating the right-hand side (rhs) of (2.18) we use the well-known fact that traces over the Fock space can be computed in the one-particle space (see Proposition 5.2.23 in Ref. 8),

$$\mathrm{Tr}_{\mathcal{F}_L}\{\hat{\rho}_e\,\mathrm{d}\Gamma(A)\} = \mathrm{Tr}_{\mathcal{H}_L}\{f_{\mathrm{FD}}(H_L(B))A\}, \tag{2.19}$$

where f_{FD} is the Fermi-Dirac one-particle distribution function,

$$f_{\mathrm{FD}}(x) := \frac{1}{e^{\beta(x-\mu)}+1}, \quad x \in \mathbb{R}, \quad \beta > 0, \quad \mu \in \mathbb{R}. \tag{2.20}$$

Plugging (2.19) into (2.18), the identity $[\mathrm{d}\Gamma(A),\mathrm{d}\Gamma(B)]=\mathrm{d}\Gamma([A,B])$, the invariance of trace under cyclic permutations and ignoring the quadratic correction in $\mathbf{E}$ one arrives at

$$\mathbf{j} = \frac{1}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\{f_{\mathrm{FD}}(H_L(B))\mathbf{J}\} - \frac{i}{|\Lambda_L|}\frac{e}{m}\mathrm{Tr}_{\mathcal{H}_L}\left(\int_{-\infty}^{0}[\tilde{V}(s),\mathbf{P}(B)]f_{\mathrm{FD}}(H_L(B))\mathrm{d}s\right). \tag{2.21}$$

The first term in (2.21) is always zero because of the identity (trace cyclicity again)

$$\mathrm{Tr}_{\mathcal{H}_L}\{[H_L(B),\mathbf{X}]f_{\mathrm{FD}}(H_L(B))\} = \mathrm{Tr}_{\mathcal{H}_L}\{[f_{\mathrm{FD}}(H_L(B)),H_L(B)]\mathbf{X}\} = 0 \tag{2.22}$$

which is nothing but the fact that the current vanishes on an equilibrium state. Note that these operations under the trace sign are quite delicate, since unbounded operators are involved. Let us for once give a complete proof to (2.22). We have the identity between bounded operators (consider the first component X_1),

$$[H_L(B),X_1]f_{\mathrm{FD}}(H_L(B)) = H_L(B)X_1 f_{\mathrm{FD}}(H_L(B)) - X_1 H_L(B) f_{\mathrm{FD}}(H_L(B)). \tag{2.23}$$

Remember that X_1 is a bounded operator in the box, and preserves the domain of $H_L(B)$. This means that the operator $O_L=(H_L(B)+i)X_1(H_L(B)+i)^{-1}$ is bounded. Hence we can write

$$H_L(B)X_1 f_{\mathrm{FD}}(H_L(B)) = [1 - i(H_L(B)+i)^{-1}]O_L[H_L(B)+i]f_{\mathrm{FD}}(H_L(B)).$$

Now the operator $[H_L(B)+i]f_{\mathrm{FD}}(H_L(B))$ still is trace class due to the exponential decay of f_{FD}, while $[1-i(H_L(B)+i)^{-1}]$ and O_L are bounded. Thus $H_L(B)X_1 f_{\mathrm{FD}}(H_L(B))$ is trace class and we can compute its trace using the complete eigenbasis of $H_L(B)$, which gives the same result as for the other operator $X_1 H_L(B) f_{\mathrm{FD}}(H_L(B))$. Thus (2.22) is proved.

Using (2.12) and (2.17) one can write

$$j_\alpha = \sum_{\beta=1}^{3}\{\sigma_{\alpha\beta}(\omega) + \sigma_{\alpha\beta}(-\bar{\omega})\}E_\beta, \quad \alpha \in \{1,2,3\}, \quad \Im(\omega) < 0, \tag{2.24}$$

where the conductivity tensor is given by

$$\sigma_{\alpha\beta}(B,\omega) = -\frac{i}{|\Lambda_L|}\frac{e^2}{m}\mathrm{Tr}_{\mathcal{H}_L}\int_{-\infty}^{0}[e^{isH_L(B)}x_\beta e^{-isH_L(B)},P_\alpha(B)]f_{\mathrm{FD}}(H_L(B))e^{is\omega}\,\mathrm{d}s. \tag{2.25}$$

Performing an integration by parts, using the formulas $i[H_L(B),x_\beta]=P_\beta(B)/m$ and $i[P_\alpha(B),x_\beta]=\delta_{\alpha\beta}$ one arrives at

$$\sigma_{\alpha\beta}(B,\omega) = \frac{1}{|\Lambda_L|}\frac{e^2}{im\omega}\left\{\delta_{\alpha\beta}\,\mathrm{Tr}(f_{\mathrm{FD}}(H_L(B))) + \frac{i}{m}\mathrm{Tr}\int_{-\infty}^{0} e^{is(\omega+H_L(B))}P_\beta(B)e^{-isH_L(B)} \times[P_\alpha(B),f_{\mathrm{FD}}(H_L(B))]\mathrm{d}s\right\}, \tag{2.26}$$

and this coincides (at least at the formal level) with formula (5) in Ref. 30. Notice that from now on, we write just Tr when we perform the trace, since we only work in the one-particle space.

Since we are interested in the Faraday effect, and we assume that the magnetic field $\mathbf{B}$ is parallel with the z axis, we will only consider the transverse conductivity $\sigma_{12}(B,\omega)$. Hence the first term vanishes. We now perform the integral over s with the help of Stone's formula followed by a deformation of the contour [paying attention not to hit the singularities of $f_{\mathrm{FD}}(z)$ or to make the integral over s divergent]

$$f_{\mathrm{FD}}(H_L(B))e^{is(H_L(B)+\eta)} = \frac{i}{2\pi}\int_{\Gamma_\omega} f_{\mathrm{FD}}(z)e^{is(z+\eta)}(H_L(B)-z)^{-1}\,\mathrm{d}z, \tag{2.27}$$

where η is either 0 or ω, the contour is counter-clockwise oriented and given by

$$\Gamma_\omega = \{x \pm i\mathrm{d}: a \leqslant x < \infty\} \cup \{a + iy: -\mathrm{d} \leqslant y \leqslant \mathrm{d}\} \tag{2.28}$$

with

$$\mathrm{d} = \min\left\{\frac{\pi}{2\beta}, \frac{|\mathrm{Im}\ \omega|}{2}\right\}, \tag{2.29}$$

and $a+1$ lies below the spectrum of $H_L(B)$. As a final result one gets

$$\sigma_{12}(B,\omega) = -\frac{e^2}{2\pi m^2 \omega|\Lambda_L}\mathrm{Tr}\int_{\Gamma_\omega} f_{\mathrm{FD}}(z)\{P_1(B)(H_L(B)-z)^{-1}P_2(B)(H_L(B)-z-\omega)^{-1}$$
$$+ z \to z-\omega\}\mathrm{d}z =: \frac{e^2}{m^2\omega}a_L(B,\omega), \tag{2.30}$$

where "$z \to z-\omega$" means a similar term where we exchange z with $z-\omega$. Now one can see that by inserting the eigenbasis of $H_L(B)$ one obtains the well-known formula derived from semiclassical radiation theory [see, e.g., formula (4) in Ref. 30].

III. GAUGE INVARIANCE AND EXISTENCE OF THE THERMODYNAMIC LIMIT

Up to now the system was confined in a box Λ_L. As is well known (see, e.g., Ref. 30) a direct evaluation of (2.30) [or previous formulas equivalent to it including formula (4) in Roth's paper] is out of reach: the eigenvalues and eigenstates of $H(B)$ are rather complicated (even in the thermodynamic limit $\Lambda_L \to \mathbb{R}^3$) and at the same time the Bloch representation is plagued by singular matrix elements of the magnetic vector potential. Roth used a modified magnetic Bloch representation in Ref. 29 and derived a formula for the linear term in B of (2.30) in terms of the zero magnetic field Bloch representation. Still, her procedure is not free of difficulties since it involves $\nabla_{\mathbf{k}} u_j(\mathbf{x},\mathbf{k})$ which might not exist at crossing points. In addition, it seems almost hopeless to control the errors or to push computations to the second order in B which would describe the Cotton-Mouton effect for example.

In what follows, we shall outline another route of evaluating (2.30) which is mathematically correct, systematic, and completely free of the above difficulties. There are two basic ideas involved. The first one (going back at least to Sondheimer and Wilson[33] in their theory of diamagnetism) consists in writing the trace in (2.30) as integrals over Λ_L of corresponding integral kernels. This is nothing but the well-known Green function approach (see, e.g., Ref. 15) which has been very successful in computing optical and magneto-optical properties of solids (see, e.g., Refs. 2, 16, and 27) in the absence of an external magnetic field. The point is that the integral kernels are on the one hand easier to control and compute, and on the other hand they do not require periodicity. Moreover, this approach proved to be essential in deriving rigorous results concerning the diamagnetism of free electrons[1,11] and actually we expect the methods of the present paper to simplify the theory of diamagnetism of Bloch electrons as well.

However, when applying Green function approach in the presence of an external magnetic field one hits again the divergences caused by the linear increase of the magnetic vector potential: naively, at the first sight $a_L(B,\omega)$ is not bounded in the thermodynamic limit $L \to \infty$ but instead grows like the second power of L. It was already observed in Ref. 1 that these divergent terms vanish identically due to some identities coming from gauge invariance.

This is indeed the case and the main point of this paper is to show, following the developments in Refs. 11, 12, and 22 that factorizing the so-called nonintegrable phase factor from the Green function [the integral kernel of $(H_L(B)-\zeta)^{-1}$] allows, at the same time, to eliminate the

divergences coming from the increase of the magnetic vector potential and to obtain a controlled expansion in powers of B. In addition, this leads to expressions of $a_L(B,\omega)$ which are manifestly gauge invariant.

For an arbitrary pair of points $\mathbf{x}$, $\mathbf{y} \in \Lambda_L$ consider the "magnetic phase" associated with the magnetic vector potential $\mathbf{a}(\mathbf{u})$ defined as the path integral on the line linking $\mathbf{y}$ and $\mathbf{x}$,

$$\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y}) = \int_{\mathbf{y}}^{\mathbf{x}} \mathbf{a}(\mathbf{u}) \cdot \mathrm{d}\mathbf{u}. \tag{3.1}$$

The magnetic phase satisfies the following crucial identity: for every fixed $\mathbf{c}$,

$$e^{-ib\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})}\mathbf{P}(B)e^{ib\phi_{\mathbf{a}}(\mathbf{x},\mathbf{c})} = \mathbf{P}(0) - b\mathbf{A}(\mathbf{x}-\mathbf{c}), \tag{3.2}$$

where $\mathbf{A}(\mathbf{x}) = \frac{1}{2}\mathbf{n}_3 \wedge \mathbf{x}$, i.e., irrespective of the choice of $\mathbf{a}(\mathbf{x})$,

$$\mathbf{A}(\mathbf{x}-\mathbf{c}) = \tfrac{1}{2}\mathbf{n}_3 \wedge (\mathbf{x}-\mathbf{c}) \tag{3.3}$$

is the symmetric (transverse, Poincaré) gauge with respect to $\mathbf{c}$.

Write now the Green function (as a 2×2 matrix in the spin space)

$$G_L(\mathbf{x},\mathbf{y};\zeta) = (H_L - \zeta)^{-1}(\mathbf{x},\mathbf{y}) \tag{3.4}$$

in the factorized form

$$G_L(\mathbf{x},\mathbf{y};\zeta) = e^{ib\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}K_L(\mathbf{x},\mathbf{y};\zeta). \tag{3.5}$$

It is easy to check that while $G_L(\mathbf{x},\mathbf{y};\zeta)$ is gauge dependent, $K_L(\mathbf{x},\mathbf{y};\zeta)$ is gauge independent, i.e., the whole gauge dependence of $G_L(\mathbf{x},\mathbf{y};\zeta)$ is contained in the phase factor $e^{ib\phi_{\mathbf{a}}(\mathbf{x},\mathbf{y})}$. Plugging the factorization (3.5) into the integrand of the rhs of (2.30), using (3.2) and (3.3), one obtains that its integral kernel writes as

$$\begin{aligned}\mathcal{A}^L_{s,s'}(\mathbf{x},\mathbf{x}') = e^{ib\phi_{\mathbf{a}}(\mathbf{x},\mathbf{x}')}\int_{\Gamma_\omega} \mathrm{d}z\, f_{\mathrm{FD}}(z)\sum_{\sigma=1}^{2}\int_{\Lambda_L}\mathrm{d}\mathbf{y}\, e^{ib\Phi(\mathbf{x},\mathbf{y},\mathbf{x}')}\{[(P_{1,\mathbf{x}}(0) - bA_1(\mathbf{x}-\mathbf{y}))K_L(\mathbf{x},\mathbf{y};z)]_{s,\sigma}\\ \times [(P_{2,\mathbf{y}}(0) - bA_2(\mathbf{x}-\mathbf{y}))K_L(\mathbf{y},\mathbf{x}';z+\omega)]_{\sigma,s'} + z \to z-\omega\},\end{aligned} \tag{3.6}$$

where

$$\Phi(\mathbf{x},\mathbf{y},\mathbf{x}') = \phi_{\mathbf{a}}(\mathbf{x},\mathbf{y}) + \phi_{\mathbf{a}}(\mathbf{y},\mathbf{x}') + \phi_{\mathbf{a}}(\mathbf{x}',\mathbf{x})$$

is the flux of the magnetic field (0, 0, 1) through the triangle $\Delta(\mathbf{x},\mathbf{y},\mathbf{x}')$. Now the fact that there are no long range divergences in the formula for $\mathcal{A}_{s,s'}(\mathbf{x},\mathbf{x}')$ follows from the exponential decay of Green functions[10] (see also Ref. 21): for ζ outside the spectrum of H there exists $m(\zeta)>0$ such that as $|\mathbf{x}-\mathbf{y}|\to\infty$

$$|K_L(\mathbf{x},\mathbf{y};\zeta)| = |G_L(\mathbf{x},\mathbf{y};\zeta)| \sim e^{-m(\zeta)|\mathbf{x}-\mathbf{y}|}. \tag{3.7}$$

It can be proved (the technical details which are far from being simple will be given elsewhere) that $\mathcal{A}^L_{s,s'}(\mathbf{x},\mathbf{x}')$ is jointly continuous and moreover outside a thin region near the surface of Λ_L one can replace it by the integral kernel $\mathcal{A}^\infty_{s,s'}(\mathbf{x},\mathbf{x}')$ of the corresponding operator on the whole $\mathbb{R}^3$. Accordingly, up to surface corrections,

$$a_L(B,\omega) \approx -\frac{1}{2\pi|\Lambda_L|}\sum_{s=1}^{2}\int_{\Lambda_L}\mathcal{A}^\infty_{s,s}(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x}. \tag{3.8}$$

Notice that due to the fact that $\Phi(\mathbf{x},\mathbf{y},\mathbf{x}) = \phi_{\mathbf{a}}(\mathbf{x},\mathbf{x}) = 0$ the phase factors appearing in (3.6) reduce to unity in (3.8).

In the periodic case, from the fact that in the symmetric gauge the Hamiltonian $H_\infty(B)$ commutes with the magnetic translations [actually one can define magnetic translations for an arbitrary gauge, just first make the gauge transformation relating $\mathbf{a}(\mathbf{x})$ to $\mathbf{A}(\mathbf{x})$] generated by $\mathcal{L}$, it follows that for $\vec{\gamma} \in \mathcal{L}$ we have

$$K_\infty(\mathbf{x}+\vec{\gamma},\mathbf{y}+\vec{\gamma};\zeta) = K_\infty(\mathbf{x},\mathbf{y};\zeta),$$

which implies that

$$\mathcal{A}^\infty_{s,s}(\mathbf{x}+\vec{\gamma},\mathbf{x}+\vec{\gamma}) = \mathcal{A}^\infty_{s,s}(\mathbf{x},\mathbf{x})$$

is periodic with respect to $\mathcal{L}$, hence up to surface corrections

$$a_L(B,\omega) \approx a(B,\omega) = -\frac{1}{2\pi|\Omega|}\sum_{s=1}^{2}\int_\Omega \mathcal{A}^\infty_{s,s}(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x}. \tag{3.9}$$

Therefore, the transverse conductivity writes as

$$\sigma_{12}(B,\omega) = \frac{e^2}{m^2\omega}a(B,\omega) \tag{3.10}$$

with $a(B,\omega)$ given by the rhs of (3.9).

A precise formulation of this result is contained in the following theorem.

Theorem 3.1: *Assume for simplicity that* Ω *is the unit cube in* $\mathbb{R}^3$. *The above defined transverse component of the conductivity tensor admits the thermodynamic limit; more precisely* as follows.

(i) *The following operator defined by a* $B(L^2\oplus L^2)$*-norm convergent Riemann integral*,

$$F_L := -\frac{1}{2\pi}\int_{\Gamma_\omega} f_{\mathrm{FD}}(z)\{P_1(B)(H_L(B)-z)^{-1}P_2(B)(H_L(B)-z-\omega)^{-1} + z\to z-\omega\}\mathrm{d}z, \tag{3.11}$$

is in fact trace-class, and $\sigma^{(L)}_{12}(B,\omega) = (e^2/m^2\omega|\Lambda_L|)\mathrm{Tr}(F_L)$.

(ii) *Consider the operator* F_∞ *defined by the same integral but with* $H_\infty(B)$ *instead of* $H_L(B)$, *and defined on the whole space. Then* F_∞ *is an integral operator, with a kernel* $\mathcal{A}^\infty_{s,s'}(\mathbf{x},\mathbf{x}')$ *jointly continuous on its spatial variables. Moreover, the function defined by* $\mathbb{R}^3 \ni \mathbf{x} \to s_B(\mathbf{x}) := \Sigma^2_{s=1}\mathcal{A}^\infty_{s,s}(\mathbf{x},\mathbf{x}) \in \mathbb{C}$ *is continuous and periodic with respect to* $\mathbb{Z}^3$.

(iii) *The thermodynamic limit exists*,

$$\sigma^{(\infty)}_{12}(B,\omega) := \lim_{L\to\infty}\sigma^{(L)}_{12}(B,\omega) = \frac{e^2}{m^2\omega|\Omega|}\int_\Omega s_B(\mathbf{x})\mathrm{d}\mathbf{x}. \tag{3.12}$$

The proof of this theorem will be given elsewhere.[13]

IV. THE ZERO FREQUENCY LIMIT AT $T=0$: A RIGOROUS PROOF OF THE WIDOM-STREDA FORMULA FOR SEMICONDUCTORS

Doing some very formal computations one can show that at $T=0$ and $\omega=0$, $\sigma_{12}(B,\omega)$ as given by (3.9) and (3.10) coincide with the formula for the quantized Hall conductivity [see, e.g., formulas (5) and (6) in Ref. 34] which in turn gives (again at the heuristic level) the well-known Widom-Streda formula. The original derivation has little mathematical rigor, in particular because it assumes some very strong assumptions on the existence and regularity of $(H_\infty(B)-\lambda+i0)^{-1}$ as a function of $\lambda\in\mathbb{R}$. These assumptions are clearly not true in many situations.

Here we will show how the Widom-Streda formula can be rigorously obtained when the Fermi energy lies in a spectral gap. The problem in which the Fermi energy is in the spectrum, remains

open. Now assume that for some B, the chemical potential μ lies in a spectral gap of $H_\infty(B)$. More precisely, throughout this section we suppose that $(d_1,d_2)\subset\rho(H_\infty(B))$ with $d_1<d_2$, and take $\mu\in(d_1,d_2)$. For simplicity, assume that $\mu=(d_1+d_2)/2$. This is the typical situation for semiconductors and/or isolators. In the absence of spin, the Widom-Streda formula roughly states that

$$\sigma_{12}(B,T=0,\omega=0)=ec\left.\frac{\partial N(B,E)}{\partial B}\right|_{E=\mu}, \tag{4.1}$$

where $N(B,E)$ is the integrated density of states up to the energy E. When the spin is present (this was not considered by Streda), this formula is slightly changed. If we denote by B_1 the B multiplying the spin matrix σ_3 in our Hamiltonian (2.1), and with B_2 the B near $\mathbf{A}$, then in fact we have

$$\sigma_{12}(B,T=0,\omega=0)=ec\left.\frac{\partial N(B_1,B_2,E)}{\partial B_2}\right|_{E=\mu,B_1=B_2=B}. \tag{4.2}$$

In the rest of this section we give a rigorous (but still not fully technical) proof of (4.2).

Theorem 4.1: *Consider the conductivity at the thermodynamic limit given in* (3.12), *and drop the superscript* ∞. *Then if we first take the limit* $T\searrow 0$, *and after that* $\omega\to 0$, *we get*

$$\lim_{\omega\to 0}\lim_{T\to 0}\sigma_{12}(B,T,\omega)=ec\frac{\partial}{\partial B_2}\left.\frac{1}{|\Omega|}\sum_{s=1}^{2}\int_\Omega \Pi^B_{s,s}(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x}\right|_{B_1=B_2=B}, \tag{4.3}$$

where

$$\Pi^B=\frac{i}{2\pi}\int_\Gamma\frac{1}{H_\infty(B)-z}\mathrm{d}z \tag{4.4}$$

with a positively oriented contour Γ *enclosing the spectrum of* $H_\infty(B)$ *below* μ, *i.e.*, Π^B *is the Fermi projection onto the subspace of "occupied" states at* $T=0$.

Remarks:

(1) Streda did not consider spin in his work[34] and in this case the derivative with respect to the magnetic field appears on the rhs of (4.3).

(2) While it is not clear that $\Pi^B(\mathbf{x},\mathbf{x})$ is well defined $[(H_\infty(B)-z)^{-1}(\mathbf{x},\mathbf{x})$ does not exist] this can be seen by writing for some $a\in\rho(H_\infty(B))$,

$$\begin{aligned}\Pi^B&=\frac{1}{2\pi}\int_\Gamma((H_\infty(B)-z)^{-1}\ -(H_\infty(B)-a)^{-1}\,\mathrm{d}z\\&=\frac{1}{2\pi}\int_\Gamma(z-a)(H_\infty(B)-z)^{-1}(H_\infty(B)-a)^{-1}\,\mathrm{d}z.\end{aligned} \tag{4.5}$$

Each resolvent has a polar integral kernel with a $1/|\mathbf{x}-\mathbf{x}'|$ singularity, and the product of two resolvents will have a continuous kernel. In fact we can repeat this trick and obtain products of as many resolvents as we want, thus further improving the regularity of the integral kernel. Technical details will be given elsewhere. Actually this kind of argument can be used to show that all operators defined by integrals over complex contours have jointly continuous integral kernels.

(3) Although the order of limits in (4.3) is important for the argument below, it might be possible [at least under additional conditions on the spectrum of $H_\infty(B)$] to interchange the order of limits. The important fact is that the thermodynamic limit must be taken first: great care is to be taken when defining currents in the static limit for finite systems (for a discussion of this point in a related context see Ref. 24).

(4) The result is valid for arbitrary magnetic field B and establishes the connection between the Hall conductivity and the Faraday effect. However, the quantum Hall effect requires high magnetic fields while the Faraday effect is usually considered at low magnetic fields.

Proof: We start from the conductivity in the thermodynamic limit as given by Theorem 3.1,

$$\sigma_{12}(B,T,\omega) = -\frac{e^2}{2\pi m^2 \omega |\Omega|} \sum_{s=1}^{2} \int_{\Omega} \left[\int_{\Gamma_{\beta,\omega}} f_{\mathrm{FD}}(z) \Sigma(z,\omega) \mathrm{d}z \right]_{s,s} (\mathbf{x},\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{4.6}$$

where

$$\Sigma(z,\omega) := P_1(B)(H_\infty(B)-z)^{-1} P_2(B)(H_\infty(B)-z-\omega)^{-1} + (z \to z-\omega). \tag{4.7}$$

Since we made the assumption that $(d_1,d_2) \subset \rho(H_\infty(B))$, then for $|\omega| < (d_2-d_1)/4$ the integral over z on the contour $\Gamma_{\beta,\omega}$ can be replaced with the integral on the contour $\Gamma^1_{\beta,\omega} \cup \Gamma^2_{\beta,\omega}$ where [see also (2.28) and (2.29)],

$$\Gamma^1_{\beta,\omega} = \left\{ x \pm id : a \leqslant x \leqslant d_1 + \frac{d_2-d_1}{4} \right\} \cup \{ a+iy : -d \leqslant y \leqslant d \} \cup \left\{ d_1 + \frac{d_2-d_1}{4} + iy : -d \leqslant y \leqslant d \right\} \tag{4.8}$$

and

$$\Gamma^2_{\beta,\omega} = \left\{ x \pm id : x \geqslant d_2 - \frac{d_2-d_1}{4} \right\} \cup \left\{ d_2 - \frac{d_2-d_1}{4} + iy : -d \leqslant y \leqslant d \right\}. \tag{4.9}$$

Accordingly, one can rewrite $\sigma_{12}(B,T,\omega)$ as

$$\begin{aligned} \sigma_{12}(B,T,\omega) = -\frac{e^2}{2\pi m^2 \omega |\Omega|} \sum_{s=1}^{2} \int_{\Omega} \Bigg\{ & \int_{\Gamma^1_{\beta,\omega}} \Sigma(z,\omega) \mathrm{d}z + \int_{\Gamma^1_{\beta,\omega}} (f_{\mathrm{FD}}(z)-1) \Sigma(z,\omega) \mathrm{d}z \\ & + \int_{\Gamma^2_{\beta,\omega}} f_{\mathrm{FD}}(z) \Sigma(z,\omega) \mathrm{d}z \Bigg\}_{s,s} (\mathbf{x},\mathbf{x}) \mathrm{d}\mathbf{x}. \end{aligned} \tag{4.10}$$

Note that since the singularities of $f_{\mathrm{FD}}(z)$ lie on $(c+d)/2+iy, y \in (-\infty,\infty)$, one can take $\Gamma^j_{\beta,\omega}$ independent of β, i.e., one can take $d = |\Im(\omega)|/2$ in (2.29). At this point we take the limit $\beta \to \infty$. Since on Γ^2_ω we have $|f_{\mathrm{FD}}(z)| \leqslant 2\exp[-\beta(x-(d_1+d_2)/2)]$, and on Γ^1_ω we have that $|f_{\mathrm{FD}}(z)-1| \leqslant 2\exp[-\beta((d_1+d_2)/2-x)]$, the last two terms in (4.10) vanish in the zero temperature limit (full details about the control of various integral kernels will be given elsewhere). Hence we get

$$\sigma_{12}(B,T=0,\omega) = -\frac{e^2}{2\pi m^2 \omega |\Omega|} \sum_{s=1}^{2} \int_{\Omega} \left\{ \int_{\Gamma^1_\omega} \Sigma(z,\omega) \mathrm{d}z \right\}_{s,s} (\mathbf{x},\mathbf{x}) \mathrm{d}\mathbf{x}. \tag{4.11}$$

An application of the Cauchy residue theorem shows that the two terms of $\Sigma(z,\omega)$ [see (4.7)] will combine in the above integral and give

$$\begin{aligned} \sigma_{12}(B,T=0,\omega) = -\frac{e^2}{2\pi m^2 \omega} \frac{1}{|\Omega|} \sum_{s=1}^{2} \int_{\Omega} \Bigg[& \int_{\Gamma} P_1(B)(H_\infty(B) \\ & - z + \omega/2)^{-1} P_2(B)(H_\infty(B) - z - \omega/2)^{-1} \Bigg]_{s,s} (\mathbf{x},\mathbf{x}) \mathrm{d}\mathbf{x}, \end{aligned} \tag{4.12}$$

where Γ is any finite contour such that $\Gamma \subset \rho(H_\infty(B)+\omega)$ for all $|\omega| < |d_2-d_1|/4$ and only enclosing the spectrum of $H_\infty(B)$ below $(d_1+d_2)/2$. Now the integrand in (4.12) is analytic in ω in a neighborhood of the origin. By expanding the resolvents one obtains

$$\sigma_{12}(B,T=0,\omega)=-\frac{e^2}{2\pi m^2}\frac{1}{|\Omega|}\sum_{s=1}^{2}\int_{\Omega}\left\{\int_{\Gamma}\frac{1}{\omega}P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-1}\right.$$
$$+\frac{1}{2}[P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-2}$$
$$\left.-P_1(B)(H_\infty(B)-z)^{-2}P_2(B)(H_\infty(B)-z)^{-1}]\right\}_{s,s}(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x}+\mathcal{O}(\omega). \tag{4.13}$$

Apparently we have a first order pole at $\omega=0$. But we now prove that the singular term on the rhs of (4.13) is identically zero. Namely (when no spin variables appear the integral kernels below must be understood as matrices in the spin space):

$$\left\{\int_{\Gamma}P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-1}\,\mathrm{d}z\right\}(\mathbf{x},\mathbf{x})=0. \tag{4.14}$$

Using the magnetic perturbation theory and the trick from (4.5) one can prove that even though the integrand in (4.14) has a quite singular kernel, after integration with respect to z one gets a smooth kernel, exponentially localized near the diagonal (details will be given elsewhere).

Let us notice an operator equality which makes sense on compactly supported functions,

$$\frac{1}{m}(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-1}=i[X_2,(H_\infty(B)-z)^{-1}], \tag{4.15}$$

because the resolvent $(H_\infty(B)-z)^{-1}$ sends compactly supported functions into exponentially decaying functions [see (3.7)], which are in the domain of X_2. In fact, the operator on the right-hand side has a nice integral kernel, given by

$$\{i[X_2,(H_\infty(B)-z)^{-1}]\}(\mathbf{x},\mathbf{y})=i(x_2-y_2)G_\infty(\mathbf{x},\mathbf{y};z), \tag{4.16}$$

which is no longer singular at the diagonal and still exponentially localized near the diagonal, thus defining a bounded operator on the whole Hilbert space. After integration we get

$$\frac{i}{2\pi}\int_{\Gamma}P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-1}\,\mathrm{d}z=\frac{im}{2\pi}\int_{\Gamma}P_1(B)[(H_\infty(B)-z)^{-1},X_2]\mathrm{d}z$$
$$=m[P_1(B)\Pi^B,X_2], \tag{4.17}$$

where we used that $P_1(B)$ and X_2 commute. Note that the magnetic perturbation theory states that the integral kernel of $P_1(B)\Pi^B$ is smooth and exponentially localized near the diagonal. Therefore $[P_1(B)\Pi^B,X_2]$ will have the integral kernel

$$\{[P_1(B)\Pi^B,X_2]\}(\mathbf{x},\mathbf{y})=(y_2-x_2)\{P_1(B)\Pi^B\}(\mathbf{x},\mathbf{y}) \tag{4.18}$$

which is identically zero at the diagonal and proves (4.14). We can conclude at this point that

$$\lim_{\omega\to 0}\sigma_{12}(B,T=0,\omega)=-\frac{e^2}{4\pi m^2}\frac{1}{|\Omega|}\sum_{s=1}^{2}\int_{\Omega}\{P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z)^{-2}$$
$$-P_1(B)(H_\infty(B)-z)^{-2}P_2(B)(H_\infty(B)-z)^{-1}\}_{s,s}(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x}. \tag{4.19}$$

Now consider the rhs of (4.3). Since the magnetic field multiplying the spin will not change, our notation will only refer to B_2. Due to the stability of the spectrum against small variations of the magnetic field, for sufficiently small ΔB, $\Pi^{B_2+\Delta B}$ still exists and

$$\Pi^{B_2+\Delta B} - \Pi^{B_2} = \frac{i}{2\pi}\int_\Gamma ((H_\infty(B_2+\Delta B) - z)^{-1} - (H_\infty(B_2) - z)^{-1})\mathrm{d}z. \tag{4.20}$$

By using the magnetic perturbation theory[22] with respect to ΔB [see also the discussion around (6.2)] one obtains

$$[\Pi^{B_2+\Delta B} - \Pi^{B_2}](\mathbf{x},\mathbf{x}) = \frac{ie\Delta B}{2\pi mc}\int_\Gamma \left\{ \int_{\mathbb{R}^3} \mathrm{d}\mathbf{y}(H_\infty(B_2) - z)^{-1}(\mathbf{x},\mathbf{y}) \right.$$
$$\left. \times[\mathbf{P}_\mathbf{y}(B_2)\cdot\mathbf{A}(\mathbf{y}-\mathbf{x})](H_\infty(B_2) - z)^{-1}(\mathbf{y},\mathbf{x}) \right\}\mathrm{d}z + \mathcal{O}((\Delta B)^2). \tag{4.21}$$

Now a very important identity is [see (3.3), (4.15), and (4.16)]

$$\mathbf{A}(\mathbf{y}-\mathbf{x})(H_\infty(B_2) - z)^{-1}(\mathbf{y},\mathbf{x}) = -\frac{i}{2m}\mathbf{n}_3 \wedge [(H_\infty(B_2) - z)^{-1}\mathbf{P}(B_2)(H_\infty(B_2) - z)^{-1}](\mathbf{y},\mathbf{x}). \tag{4.22}$$

The remainder in $(\Delta B)^2$ will have a smooth integral kernel after the integration with respect to z, hence we obtain

$$\frac{\partial}{\partial B_2}\frac{1}{|\Omega|}\int_\Omega \Pi^B(\mathbf{x},\mathbf{x})\mathrm{d}\mathbf{x} = -\frac{e}{4\pi m^2 c}$$
$$\times \int_\Omega \left\{ \int_\Gamma [(H_\infty(B) - z)^{-1}P_1(B)(H_\infty(B) - z)^{-1}P_2(B)(H_\infty(B) - z)^{-1} \right.$$
$$\left. - (H_\infty(B) - z)^{-1}P_2(B)(H_\infty(B) - z)^{-1}P_1(B)\ (H_\infty(B) - z)^{-1})\mathrm{d}z] \right\}(\mathbf{x},\mathbf{x}). \tag{4.23}$$

From (4.23) and (4.19) we see that (4.3) follows if we can prove that one can circularly permute the operators under the integral sign in (4.23). One can prove this by interpreting (4.23) as the thermodynamic limit of the corresponding expression on finite volume and then using the invariance of the trace under cyclic permutations. Alternatively one can prove it directly and in what follows we outline the proof.

Due to the smoothing effect of the integral with respect to z, we can always restrict ourselves to considering a product of only two integral operators which commute with the discrete magnetic translations, and have kernels $e^{ib\phi_\mathbf{a}(\mathbf{x},\mathbf{y})}K_1(\mathbf{x},\mathbf{y})$ and $e^{ib\phi_\mathbf{a}(\mathbf{y},\mathbf{x}')}K_2(\mathbf{y},\mathbf{x}')$. We therefore look at an absolutely convergent integral of the form [the antisymmetric magnetic phases disappear when we look at the diagonal, see (3.1)]

$$\int_\Omega \mathrm{d}\mathbf{x}\int_{\mathbb{R}^3}\mathrm{d}\mathbf{y}\ K_1(\mathbf{x},\mathbf{y})K_2(\mathbf{y},\mathbf{x}) \tag{4.24}$$

with

$$K_{1,2}(\mathbf{x},\mathbf{y}) = K_{1,2}(\mathbf{x}+\vec{\gamma},\mathbf{y}+\vec{\gamma}).$$

Then

$$\int_\Omega d\mathbf{x}\int_{\mathbb{R}^3} d\mathbf{y}\, K_1(\mathbf{x},\mathbf{y})K_2(\mathbf{y},\mathbf{x}) = \sum_{\vec{\gamma}\in\mathcal{L}}\int_\Omega d\mathbf{x}\int_\Omega d\mathbf{y}\, K_1(\mathbf{x},\mathbf{y}+\vec{\gamma})K_2(\mathbf{y}+\vec{\gamma},\mathbf{x})$$

$$= \sum_{\vec{\gamma}\in\mathcal{L}}\int_\Omega d\mathbf{x}\int_\Omega d\mathbf{y}\, K_1(\mathbf{x}-\vec{\gamma},\mathbf{y})K_2(\mathbf{y},\mathbf{x}-\vec{\gamma})$$

$$= \int_\Omega d\mathbf{y}\int_{\mathbb{R}^3} d\mathbf{x}\int_{\mathbb{R}^3} K_2(\mathbf{y},\mathbf{x})K_1(\mathbf{x},\mathbf{y}) \tag{4.25}$$

which gives the needed "trace cyclicity" and the theorem is proved. □

We now turn to the question whether the limit in (4.3) actually vanishes as is suggested by some heuristic arguments (see, e.g., Ref. 30). We start by recalling some results about Wannier functions. Let $\sigma_0(B_0)$ be an isolated part of the spectrum of $H_\infty(B_0)$ and $\Pi_0^{B_0}$ the corresponding spectral projection. We say that $\Pi_0^{B_0}$ has a basis of exponentially localized (magnetic) Wannier functions if there exist $\alpha>0$, $w_j\in L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3)$, $j=1,2,\ldots,p<\infty$ satisfying [we denote by $w_j(\mathbf{x},s)\in\mathbb{C}$ the values of w_j in $\mathbf{x}\in\mathbb{R}^3$ and $s\in\{1,2\}$]

$$\sum_{s=1}^{2}\int_{\mathbb{R}^3}|w_j(\mathbf{x},s)|^2 e^{2\alpha|\mathbf{x}|}\,d\mathbf{x}\leqslant M<\infty, \tag{4.26}$$

such that the set of functions $\{w_{j,\vec{\gamma}}\}_{j=1,2,\ldots,p,\vec{\gamma}\in\mathcal{L}}$ with

$$w_{j,\vec{\gamma}}(\mathbf{x},s) = e^{ib\phi_{\mathbf{a}}(\mathbf{x},\vec{\gamma})}w_j(\mathbf{x}-\vec{\gamma},s)$$

is a basis in the range of the projection $\Pi_0^{B_0}(L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3))$. If the spin is neglected, it has been proved in Ref. 21 that the existence of bases of exponentially localized Wannier functions is stable against small values of the magnetic field (i.e., $B_0=0$). More precisely, if σ_0 is an isolated part of the spectrum of $-\Delta+V$ and the corresponding subspace has a basis of exponentially localized Wannier functions then, for sufficiently small B, $\sigma_0(B)$ is still isolated and the corresponding spectral subspace has a basis of exponentially localized magnetic Wannier functions. The methods in Ref. 23 together with the magnetic perturbation theory[11,12,22] allow one to generalize the above result to arbitrary B_0 and presence of the spin (as far as the spin-orbit term is sufficiently small).[14] Now the existence of exponentially localized magnetic Wannier functions for an isolated part of the spectrum and for the value of the magnetic field B_2 in an interval around B_0 allows one to write

$$\sum_{s=1}^{2}\int_\Omega \Pi^B_{0;s,s}(\mathbf{x},\mathbf{x})d\mathbf{x} = \int_\Omega \sum_{j,\vec{\gamma}}\sum_{s=1}^{2}|w_{j,\vec{\gamma}}(\mathbf{x},s)|^2\,d\mathbf{x}$$

$$= \sum_{j,\vec{\gamma}}\sum_{s=1}^{2}\int_\Omega d\mathbf{x}|w_j(\mathbf{x}-\vec{\gamma},s)|^2 = \sum_{j=1}^{p}\sum_{s=1}^{2}\int_{\mathbb{R}^3}d\mathbf{x}|w_j(\mathbf{x},s)|^2 = p. \tag{4.27}$$

Thus the integrated density of states corresponding to the Fermi projection is constant in B_2 in a small interval around B_0, hence this band gives no contribution on the rhs of (4.3).

For small fields, the above discussion can be summarized in the following.

Theorem 4.2: *Suppose* $(d_1,d_2)\subset\rho(-\Delta+V)$, $d_2>d_1$, *and that the spectral subspace corresponding to* $(-\infty,d_1]$ *admits a basis of exponentially localized Wannier functions. Suppose that the spin-orbit interaction* [*see* (2.2)] *is small enough such that as* c^2 *decreases from* ∞ *to its actual value, we have that* $(d_1+d_2)/2\in\rho(H_\infty(0))$. *Then for sufficiently small* B,

$$\lim_{\omega\to 0}\lim_{T\to 0}\sigma_{12}(B,T,\omega)=0. \tag{4.28}$$

In particular all the derivatives of $\sigma_{12}(B,0)$ vanish for $B=0$, and this substantiates Roth's result [formula (50) in Ref. 30] for the first-order correction in B at zero frequency.

V. A CLOSED FORMULA FOR FREE ELECTRONS

If $V=0$ it turns out that the conductivity tensor can be explicitly computed for all values of B and ω. The formula does not depend on whether we work in two or three dimensions. More precisely, we will show in this section that

$$\sigma_{12}(B,\omega)=\frac{e^3 n}{m^2 c}\frac{B}{\omega^2-\dfrac{B^2e^2}{m^2c^2}}, \tag{5.1}$$

where $n=n(T,\mu,B)$ is the grand-canonical density. The formula (5.1) is well known in classical physics and goes back at least to Drude but we are not aware of a known fully quantum derivation. The coincidence of classical and quantum formulas can be understood taking into account that the Hamiltonians involved (choose the symmetric gauge) are quadratic and it is known that for this class of operators classical and quantum computations coincide in many instances. While it is possible to derive (5.1) by using the explicit form of the Green function or alternatively of eigenvalues and eigenprojections for the Landau Hamiltonian (see, e.g., Ref. 18) we shall obtain it below only using resolvent and commutation identities.

Let us only notice that when $\omega=0$ we reobtain formula (18) in Ref. 34, while for a fixed frequency we get

$$\frac{\partial\sigma_{12}}{\partial B}(0,\omega)=\frac{e^3 n}{m^2 c\omega^2}$$

which is "the high frequency limit" or what Roth also calls "the free electron Faraday effect" in formula (51) from Ref. 30.

We begin by listing a few identities which are valid for a free electron on the entire space,

$$\begin{aligned}
i[P_1(B),P_2(B)]&=\frac{Be}{c},\\
i[H_\infty(B),P_1(B)]&=-\frac{Be}{mc}P_2(B),\\
i[H_\infty(B),P_2(B)]&=\frac{Be}{mc}P_1(B),\\
[H_\infty(B),[H_\infty(B),P_1(B)]]&=\frac{B^2e^2}{m^2c^2}P_1(B),\\
[H_\infty(B),[H_\infty(B),P_2(B)]]&=\frac{B^2e^2}{m^2c^2}P_2(B).
\end{aligned} \tag{5.2}$$

Next, since in this case $\mathcal{A}^{\infty}_{s,s}(\mathbf{x},\mathbf{x})$ does not depend upon $\mathbf{x}$ one has

$$\begin{aligned}
a(B,\omega)=-\frac{1}{2\pi}\sum_{s=1}^{2}\left\{\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)[P_1(B)(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z-\omega)^{-1}+z\to z-\omega]\right\}\\
\times(\vec{0},s;\vec{0},s).
\end{aligned} \tag{5.3}$$

Commuting $(H_\infty(B)-z-\omega)^{-1}$ with $P_2(B)$ in the first term, and $P_1(B)$ with $(H_\infty(B)-z+\omega)^{-1}$ in the second one, we obtain

$$a(B,\omega) = -\frac{1}{2\pi|\Omega|}\sum_{s=1}^{2}\left\{\int_{\Gamma_\omega} \mathrm{d}z\, f_{\mathrm{FD}}(z)[P_1(B)(H_\infty(B)-z)^{-1}(H_\infty(B)-z-\omega)^{-1}P_2(B)+P_1(B)\right.$$
$$\times (H_\infty(B)-z)^{-1}(H_\infty(B)-z-\omega)^{-1}[H_\infty(B),P_2(B)](H_\infty(B)-z-\omega)^{-1}+(H_\infty(B)$$
$$-z+\omega)^{-1}P_1(B)P_2(B)(H_\infty(B)-z)^{-1}+(H_\infty(B)-z+\omega)^{-1}[H_\infty(B),P_1(B)]$$
$$\left.\times (H_\infty(B)-z+\omega)^{-1}P_2(B)(H_\infty(B)-z)^{-1}]\right\}(\vec{0},s;\vec{0},s) = \mathrm{I}+\mathrm{II}+\mathrm{III}+\mathrm{IV}. \tag{5.4}$$

Now I+III can easily be computed. Indeed, by cyclic permutations [see (4.25)] one can cluster the two resolvents and then by the resolvent identity

$$(A-z_1)^{-1}(A-z_2)^{-1} = (z_1-z_2)^{-1}[(A-z_1)^{-1}-(A-z_2)^{-1}], \tag{5.5}$$

one obtains four terms. Two of them vanish after the integration over z due to the analyticity of the integrand while the other two give

$$\mathrm{I}+\mathrm{III} = \frac{1}{2\pi}\sum_{s=1}^{2}\left\{\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\frac{1}{\omega}[P_2(B),P_1(B)](H_\infty(B)-z)^{-1}\right\}(\vec{0},s;\vec{0},s) \tag{5.6}$$

$$= \frac{Be}{\omega}\sum_{s=1}^{2}\{f_{\mathrm{FD}}(H_\infty(B))\}(\vec{0},s;\vec{0},s) =: \frac{Be}{\omega}n(T,\mu,B). \tag{5.7}$$

In an analogous manner

$$\mathrm{III}+\mathrm{IV} = \frac{1}{2\pi\omega}\sum_{s=1}^{2}\left\{\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\{(H_\infty(B)-z)^{-1}[H_\infty(B),P_2(B)](H_\infty(B)-z-\omega)^{-1}P_1(B)\right.$$
$$\left.-(H_\infty(B)-z)^{-1}[H_\infty(B),P_1(B)](H_\infty(B)-z+\omega)^{-1}P_2(B)\}\right\}(\vec{0},s;\vec{0},s). \tag{5.8}$$

At this point we commute $[H_\infty(B),P_2(B)]$ with $(H_\infty(B)-z-\omega)^{-1}$ in the first term, and $[H_\infty(B),P_1(B)]$ with $(H_\infty(B)-z+\omega)^{-1}$ in the second term and use (3.3) again. Some of the terms vanish after performing the integration over z and the remaining ones write as

$$-\frac{1}{\omega}(H_\infty(B)-z)^{-1}[H_\infty(B),P_2(B)]P_1(B)-\frac{1}{\omega}(H_\infty(B)-z)^{-1}[H_\infty(B),[H_\infty(B),P_2(B)]](H_\infty(B)$$
$$-z-\omega)^{-1}P_1(B)-\frac{1}{\omega}(H_\infty(B)-z)^{-1}[H_\infty(B),P_1(B)]P_2(B)$$
$$-\frac{1}{\omega}(H_\infty(B)-z)^{-1}[H_\infty(B),[H_\infty(B),P_1(B)]](H_\infty(B)-z+\omega)^{-1}P_2(B). \tag{5.9}$$

Taking into account (5.2) the first and the third terms in (5.9) combine to

$$-\frac{1}{\omega}(H_\infty(B)-z)^{-1}[H_\infty(B),P_1(B)P_2(B)]$$

which after integration over z is proportional to

$$f_{\mathrm{FD}}(H_\infty(B))i[H_\infty(B),P_1(B)P_2(B)]=\frac{Be}{mc}\{f_{\mathrm{FD}}(H_\infty(B))P_1(B)^2-f_{\mathrm{FD}}(H_\infty(B))P_2(B)^2\}, \quad (5.10)$$

where we used the second and third identities in (5.2). Consider the unitary operator U which implements the coordinate change $(Uf)(x_1,x_2,x_3)=f(x_2,-x_1,x_3)$. Then one can prove that $UP_1(B)U^*=-P_2(B)$, $UP_2(B)U^*=P_1(B)$, and $UH_\infty(B)U^*=H_\infty(B)$. This implies that

$$Uf_{\mathrm{FD}}(H_\infty(B))P_1(B)^2U^*=f_{\mathrm{FD}}(H_\infty(B))P_2(B)^2.$$

Since both operators have a smooth integral kernel, and because the rotation with U does not change the diagonal value of the integral kernel on the left-hand side, it means that the contribution given by (5.10) is zero.

Therefore we only remain with the second and fourth terms in (5.9). Using (5.2), they become

$$\begin{aligned}&-\frac{B^2e^2}{m^2c^2\omega}(H_\infty(B)-z)^{-1}P_2(B)(H_\infty(B)-z-\omega)^{-1}P_1(B),\\&-\frac{B^2e^2}{m^2c^2\omega}(H_\infty(B)-z)^{-1}P_1(B)(H_\infty(B)-z+\omega)^{-1}P_2(B).\end{aligned} \quad (5.11)$$

Using once more the cyclicity of the trace and comparing with the starting point (5.3), we obtain the remarkable identity

$$\mathrm{II}+\mathrm{IV}=\frac{B^2e^2}{m^2c^2\omega^2}a(B,\omega). \quad (5.12)$$

Setting together (5.4), (5.6), and (5.12), we obtain the equation

$$a(B,\omega)=\frac{Be}{c\omega}n+\frac{B^2e^2}{m^2c^2\omega^2}a(B,\omega),$$

which gives (5.1) [see (3.10)].

VI. MAGNETIC PERTURBATION THEORY AND THE LINEAR TERM IN *B*

When $V\neq 0$ it is no longer possible to obtain a closed formula for $\sigma_{12}(B,\omega)$. Since in most physical applications the external magnetic field can be considered weak, an expansion in B up to the first or second order would be sufficient. In this section we show that $a_L(B,\omega)$ has an expansion in B to any order and write down the expressions of the first two terms. The first one gives the transverse conductivity at zero magnetic field and the second which is linear in B provides the Verdet constant. From (3.6) and (3.8) (in what follows by tr we mean the trace over the spin variable),

$$\begin{aligned}a_L(B,\omega)=-\frac{1}{2\pi|\Lambda_L|}\int_{\Lambda_L}\mathrm{d}\mathbf{x}\ \Bigg\{\mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\,f_{\mathrm{FD}}(z)\int_{\Lambda_L}\mathrm{d}\mathbf{u}\{[(P_{\mathbf{x},1}(0)-bA_1(\mathbf{x}-\mathbf{u}))K_L(\mathbf{x},\mathbf{u};z)]\\\times[(P_{\mathbf{u},2}(0)-bA_2(\mathbf{u}-\mathbf{x}'))K_L(\mathbf{u},\mathbf{x}';z+\omega)]+[(P_{\mathbf{x},1}(0)-bA_1(\mathbf{x}-\mathbf{u}))K_L(\mathbf{x},\mathbf{u};z-\omega)]\\\times[(P_{\mathbf{u},2}(0)-bA_2(\mathbf{u}-\mathbf{x}'))K_L(\mathbf{u},\mathbf{x}';z)]\}\Bigg\}\Bigg|_{\mathbf{x}=\mathbf{x}'}.\end{aligned} \quad (6.1)$$

Let us mention here that one cannot interchange the order of the above integrals. First one performs the integral with respect to $\mathbf{u}$, then the integral in z, then we can set $\mathbf{x}=\mathbf{x}'$ since the resulting kernel is smooth, and finally one integrates with respect to $\mathbf{x}$ over Λ_L.

When considering the expansion in b of $a_L(B,\omega)$ we are left with the problem of the expansion of $K_{\Lambda_L}(\mathbf{x},\mathbf{y};\zeta)$. This expansion is provided by the magnetic perturbation theory as developed in Ref. 22. Following the steps in Ref. 22 in the case at hand one obtains

$$\begin{aligned} K_L(\mathbf{x},\mathbf{y};z) &= G_L^{(0)}(\mathbf{x},\mathbf{y};z) + \frac{b}{m}\int_{\Lambda_L} G_L^{(0)}(\mathbf{x},\mathbf{u};z)[\mathbf{P}_\mathbf{u}(0)\mathbf{A}(\mathbf{u}-\mathbf{y})G_L^{(0)}(\mathbf{u},\mathbf{y};z)]\mathrm{d}\mathbf{u} \\ &\quad + b\frac{gc\mu_b}{e}\int_{\Lambda_L} G_L^{(0)}(\mathbf{x},\mathbf{u};z)\sigma_3 G_L^{(0)}(\mathbf{u},\mathbf{y};z)\mathrm{d}\mathbf{u} + \mathcal{O}(b^2) \\ &= G_L^{(0)}(\mathbf{x},\mathbf{y};z) + bG_L^{(\mathrm{orbit})}(\mathbf{x},\mathbf{y};z) + bG_L^{(\mathrm{spin})}(\mathbf{x},\mathbf{y};z) + \mathcal{O}(b^2). \end{aligned} \tag{6.2}$$

The above integrands are matrices in the spin variable, that is why the spin does not appear explicitly. The error term $\mathcal{O}(b^2)$ can also be fully controlled with the magnetic perturbation theory (actually arbitrary order terms can be computed; see Ref. 22 for details). Plugging the expansion into (6.2) and collecting the terms of zero and first order one obtains

$$a_L(B,\omega) = a_L(0,\omega) + ba_{L,1}(\omega) + \mathcal{O}(b^2), \tag{6.3}$$

where the zeroth order term is

$$\begin{aligned} a_L(0,\omega) = -\frac{1}{2\pi|\Lambda_L|}\int_{\Lambda_L}\mathrm{d}\mathbf{x}\ \Bigg\{\mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\{P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z+\omega)^{-1} \\ + (z\to z-\omega)\}\Bigg\}\Bigg|_{\mathbf{x}=\mathbf{x}'}, \end{aligned} \tag{6.4}$$

while the first order correction reads as

$$a_{L,1}(\omega) = a_{L,1}^{\mathrm{orbit}}(\omega) + a_{L,1}^{\mathrm{spin}}(\omega), \tag{6.5}$$

where

$$\begin{aligned} a_{L,1}^{\mathrm{orbit}}(\omega) = -\frac{1}{2\pi|\Lambda_L|}\int_{\Lambda_L}\mathrm{d}\mathbf{x}\ \Bigg\{\mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\int_{\Lambda_L}\mathrm{d}\mathbf{u}\{-[A_1(\mathbf{x}-\mathbf{u})G_L^{(0)}(\mathbf{x},\mathbf{u};z)] \\ \times[P_{\mathbf{u},2}(0)G_L^{(0)}(\mathbf{u},\mathbf{x}';z+\omega)] - [P_{\mathbf{x},1}(0)G_L^{(0)}(\mathbf{x},\mathbf{u};z)][A_2(\mathbf{u}-\mathbf{x}')G_L^{(0)}(\mathbf{u},\mathbf{x}';z+\omega)] \\ + [P_{\mathbf{x},1}(0)G_L^{(\mathrm{orbit})}(\mathbf{x},\mathbf{u};z)][P_{\mathbf{u},2}(0)G_L^{(0)}(\mathbf{u},\mathbf{x}';z+\omega)] + [P_{\mathbf{x},1}(0)G_L^{(0)}(\mathbf{x},\mathbf{u};z)] \\ \times[P_{\mathbf{u},2}(0)G_L^{(\mathrm{orbit})}(\mathbf{u},\mathbf{x}';z+\omega)] + (z\to z-\omega)\}\Bigg\}\Bigg|_{\mathbf{x}=\mathbf{x}'}, \end{aligned} \tag{6.6}$$

$$\begin{aligned} a_{L,1}^{\mathrm{spin}}(\omega) = -\frac{1}{2\pi|\Lambda_L|}\int_{\Lambda_L}\mathrm{d}\mathbf{x}\ \Bigg\{\mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\int_{\Lambda_L}\mathrm{d}\mathbf{u}\{[P_{\mathbf{x},1}(0)G_L^{(\mathrm{spin})}(\mathbf{x},\mathbf{u};z)][P_{\mathbf{u},2}(0)G_L^{(0)}(\mathbf{u},\mathbf{x}';z \\ + \omega)] + [P_{\mathbf{x},1}(0)G_L^{(0)}(\mathbf{x},\mathbf{u};z)][P_{\mathbf{u},2}(0)G_L^{(\mathrm{spin})}(\mathbf{u},\mathbf{x}';z+\omega)] + (z\to z-\omega)\}\Bigg\}\Bigg|_{\mathbf{x}=\mathbf{x}'}. \end{aligned} \tag{6.7}$$

Now consider the expression $\mathbf{A}(\mathbf{x}-\mathbf{y})G_L^{(0)}(\mathbf{x},\mathbf{y};z)$ appearing in the formula for $a_{L,1}(\omega)$. Observing that it represents a commutator [see (3.3)] one has the identity

$$\begin{aligned}\mathbf{A}(\mathbf{x}-\mathbf{y})G_L^{(0)}(\mathbf{x},\mathbf{y};z) &= \left(\frac{1}{2}\mathbf{n}_3 \wedge (\mathbf{x}-\mathbf{y})\right) G_L^{(0)}(\mathbf{x},\mathbf{y};z) \\ &= \left(\frac{1}{2}\mathbf{n}_3 \wedge [\mathbf{X},(H_L(0)-z)^{-1}]\right)(\mathbf{x},\mathbf{y}) \\ &= -\frac{i}{2m}\{(H_L(0)-z)^{-1}(\mathbf{n}_3 \wedge P)(H_L(0)-z)^{-1}\}(\mathbf{x},\mathbf{y}), \end{aligned} \tag{6.8}$$

where $\mathbf{X}$ denotes the multiplication operator with $\mathbf{x}$. By a straightforward (but somewhat tedious) computation one arrives at

$$a_{L,1}(\omega) = a_{L,1}^{\text{orbit},1}(\omega) + a_{L,1}^{\text{orbit},2}(\omega) + a_{L,1}^{\text{spin}}(\omega), \tag{6.9}$$

where

$$\begin{aligned} a_{L,1}^{\text{orbit},1}(\omega) = \frac{i}{4m\pi\omega|\Lambda_L|}\int_{\Lambda_L} d\mathbf{x}\Bigg\{ \text{tr}\int_{\Gamma_\omega} dz\, f_{\text{FD}}(z)\Bigg[&\sum_{\alpha=1}^{2} P_\alpha(0)(H_L(0)-z)^{-1}P_\alpha(0)(H_L(0)-z-\omega)^{-1} \\ &+ \sum_{\alpha=1}^{2} P_\alpha(0)(H_L(0)-z)^{-1}P_\alpha(0)(H_L(0)-z+\omega)^{-1} \\ &- \sum_{\alpha=1}^{2} P_\alpha(0)(H_L(0)-z)^{-1}P_\alpha(0)(H_L(0)-z)^{-1}\Bigg]\Bigg\}(\mathbf{x},\mathbf{x}), \end{aligned} \tag{6.10}$$

$$\begin{aligned} a_{L,1}^{\text{orbit},2}(\omega) = \frac{i}{4\pi m^2|\Lambda_L|}\int_{\Lambda_L} d\mathbf{x}\Bigg\{ \text{tr}\int_{\Gamma_\omega} dz\, f_{\text{FD}}(z)\{ &- P_1(0)(H_L(0)-z)^{-1}P_1(0)(H_L(0)-z)^{-1} \\ &\times P_2(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1} + P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z)^{-1} \\ &\times P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1} - P_1(0)(H_L(0)-z+\omega)^{-1}P_1(0) \\ &\times (H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z)^{-1} \\ &+ P_1(0)(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z+\omega)^{-1}P_1(0)(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0) \\ &- z)^{-1} - P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1}P_1(0)(H_L(0)-z-\omega)^{-1}P_2(0)(H_L(0) \\ &- z-\omega)^{-1} + P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1}P_1(0) \\ &\times (H_L(0)-z-\omega)^{-1} - P_1(0)(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z)^{-1} \\ &\times P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z)^{-1} + P_1(0)(H_L(0)-z+\omega)^{-1} \\ &\times P_2(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z)^{-1}P_1(0)(H_L(0)-z)^{-1}\}\Bigg\}(\mathbf{x},\mathbf{x}), \end{aligned} \tag{6.11}$$

and

$$a^{\mathrm{spin}}_{L,1}(\omega) = -\frac{gc\mu_b}{2e\pi|\Lambda_L|}\int_{\Lambda_L} \mathrm{d}\mathbf{x}\Bigg\{ \mathrm{tr}\int_{\Gamma_\omega} \mathrm{d}z\, f_{\mathrm{FD}}(z)\{[P_1(0)(H_L(0)-z)^{-1}\sigma_3(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1}] + [P_1(0)(H_L(0)-z)^{-1}P_2(0)(H_L(0)-z-\omega)^{-1}\sigma_3(H_L(0)-z-\omega)^{-1}] + [P_1(0)(H_L(0)-z+\omega)^{-1}\sigma_3(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z)^{-1}] + [P_1(0)(H_L(0)-z+\omega)^{-1}P_2(0)(H_L(0)-z)^{-1}\sigma_3(H_L(0)-z)^{-1}]\}\Bigg\}(\mathbf{x},\mathbf{x}). \tag{6.12}$$

VII. THE PERIODIC CASE

Now consider the case when V is periodic. In this case, after taking the thermodynamic limit one can replace [see (3.9)] $(1/|\Lambda_L|)\int_{\Lambda_L}$ with $(1/|\Omega|)\int_\Omega$ and rewrite (6.10)–(6.12) as integrals over the Brillouin zone,

$$\begin{aligned} a^{\mathrm{orbit},1}_{\infty,1}(\omega) = \frac{i}{4m\pi\omega|\Omega|}\int_{\Omega^*}\mathrm{d}\mathbf{k}\int_\Omega \mathrm{d}\mathbf{x}\Bigg\{ \mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z) \\ \times\sum_{\alpha=1}^{2}(p_\alpha+k_\alpha)(h(\mathbf{k})-z)^{-1}(p_\alpha+k_\alpha)(h(\mathbf{k})-z-\omega)^{-1} \\ +\sum_{\alpha=1}^{2}(p_\alpha+k_\alpha)(h(\mathbf{k})-z)^{-1}(p_\alpha+k_\alpha)(h(\mathbf{k})-z+\omega)^{-1} \\ -\sum_{\alpha=1}^{2}(p_\alpha+k_\alpha)(h(\mathbf{k})-z)^{-1}P_\alpha(0)(h(\mathbf{k})-z)^{-1}\Bigg\}(\mathbf{x},\mathbf{x}), \end{aligned} \tag{7.1}$$

$$\begin{aligned} a^{\mathrm{orbit},2}_{\infty,1}(\omega) = \frac{i}{4\pi m^2|\Omega|}\int_{\Omega^*}\mathrm{d}\mathbf{k}\int_\Omega \mathrm{d}\mathbf{x}\Bigg\{ \mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z) \\ \times\{-(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_1+k_1)(h(\mathbf{k})-z)^{-1}\times(p_2+k_2)(h(\mathbf{k})-z)^{-1} \\ \times(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}+(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1} \\ \times(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}-(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1}(p_1+k_1) \\ \times(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}+(p_1+k_1)(h(\mathbf{k})-z \\ +\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z+\omega)^{-1}(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}-(p_1+k_1) \\ \times(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}(p_1+k_1)(h(\mathbf{k})-z-\omega)^{-1} \\ \times(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}+(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}(p_2+k_2) \\ \times(h(\mathbf{k})-z-\omega)^{-1}(p_1+k_1)(h(\mathbf{k})-z-\omega)^{-1}-(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2) \\ \times(h(\mathbf{k})-z)^{-1}(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}+(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1} \\ \times(p_2+k_2)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}(p_1+k_1)(h(\mathbf{k})-z)^{-1}\}\Bigg\}(\mathbf{x},\mathbf{x}), \end{aligned} \tag{7.2}$$

and

$$a_{\infty,1}^{\mathrm{spin}}(\omega) = -\frac{gc\mu_b}{2e\pi|\Omega|}\int_{\Omega^*}\mathrm{d}\mathbf{k}\int_{\Omega}\mathrm{d}\mathbf{x}\Bigg\{\mathrm{tr}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)\{[(p_1+k_1)(h(\mathbf{k})-z)^{-1}\sigma_3(h(\mathbf{k})-z)^{-1}(p_2+k_2)$$
$$\times(h(\mathbf{k})-z-\omega)^{-1}] + [(p_1+k_1)(h(\mathbf{k})-z)^{-1}(p_2+k_2)(h(\mathbf{k})-z-\omega)^{-1}\sigma_3(h(\mathbf{k})-z-\omega)^{-1}]$$
$$+ [(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1}\sigma_3(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}]$$
$$+ [(p_1+k_1)(h(\mathbf{k})-z+\omega)^{-1}(p_2+k_2)(h(\mathbf{k})-z)^{-1}\sigma_3(h(\mathbf{k})-z)^{-1}]\}\Bigg\}(\mathbf{x},\mathbf{x}). \tag{7.3}$$

Finally, for the convenience of the reader only interested in applying the theory to the case when one assumes that the Bloch bands and functions are known (as, for example, from Kohn-Luttinger type models), we write (7.1)–(7.3) in terms of Bloch functions and energies. The important thing here is that no derivatives with respect to the quasimomentum appear. With the usual notation (here $\langle,\rangle$ denotes the scalar product over the spin variables)

$$\hat{\pi}_{ij}(\alpha,\mathbf{k}) = \int_{\Omega}\langle u_i(\mathbf{x},\mathbf{k}),(p_\alpha+\mathbf{k}_\alpha)u_j(\mathbf{x},\mathbf{k})\rangle\mathrm{d}\mathbf{x}, \tag{7.4}$$

and after some rearrangements, the terms coming from the orbital magnetism are

$$a_{\infty,1}^{\mathrm{orbit},1}(\omega) = \frac{1}{2m\omega(2\pi)^3}\sum_{\alpha=1}^{2}\int_{\Omega^*}\mathrm{d}\mathbf{k}\Bigg\{\sum_{j\geqslant 1}|\hat{\pi}_{jj}(\alpha,\mathbf{k})|^2 f'_{\mathrm{FD}}(\lambda_j(\mathbf{k}))$$
$$-\omega^2\sum_{j\neq l}|\hat{\pi}_{lj}(\alpha,\mathbf{k})|^2\frac{f_{\mathrm{FD}}(\lambda_j(\mathbf{k}))-f_{\mathrm{FD}}(\lambda_l(\mathbf{k}))}{[(\lambda_j(\mathbf{k})-\lambda_l(\mathbf{k}))^2-\omega^2](\lambda_j(\mathbf{k})-\lambda_l(\mathbf{k}))}\Bigg\}, \tag{7.5}$$

$$a_{\infty,1}^{\mathrm{orbit},2}(\omega) = \frac{1}{2m^2(2\pi)^3}\int_{\Omega^*}\mathrm{d}\mathbf{k}\sum_{n_1,n_2,n_3,n_4\geqslant 1}\frac{1}{2\pi i}\int_{\Gamma_\omega}\mathrm{d}z\, f_{\mathrm{FD}}(z)$$
$$\times\Bigg\{\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(1,\mathbf{k})\hat{\pi}_{n_2n_3}(2,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\lambda_{n_1}(\mathbf{k}))(z-\lambda_{n_2}(\mathbf{k}))(z-\lambda_{n_3}(\mathbf{k}))(z+\omega-\lambda_{n_4}(\mathbf{k}))}$$
$$-\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(2,\mathbf{k})\hat{\pi}_{n_2n_3}(1,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\lambda_{n_1}(\mathbf{k}))(z-\lambda_{n_2}(\mathbf{k}))(z-\lambda_{n_3}(\mathbf{k}))(z+\omega-\lambda_{n_4}(\mathbf{k}))}$$
$$+\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(1,\mathbf{k})\hat{\pi}_{n_2n_3}(2,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\omega-\lambda_{n_1}(\mathbf{k}))(z-\omega-\lambda_{n_2}(\mathbf{k}))(z-\omega-\lambda_{n_3}(\mathbf{k}))(z-\lambda_{n_4}(\mathbf{k}))}$$
$$-\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(2,\mathbf{k})\hat{\pi}_{n_2n_3}(1,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\omega-\lambda_{n_1}(\mathbf{k}))(z-\omega-\lambda_{n_2}(\mathbf{k}))(z-\omega-\lambda_{n_3}(\mathbf{k}))(z-\lambda_{n_4}(\mathbf{k}))}$$
$$+\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(2,\mathbf{k})\hat{\pi}_{n_2n_3}(1,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\lambda_{n_1}(\mathbf{k}))(z+\omega-\lambda_{n_2}(\mathbf{k}))(z+\omega-\lambda_{n_3}(\mathbf{k}))(z+\omega-\lambda_{n_4}(\mathbf{k}))}$$
$$-\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(2,\mathbf{k})\hat{\pi}_{n_2n_3}(2,\mathbf{k})\hat{\pi}_{n_3n_4}(1,\mathbf{k})}{(z-\lambda_{n_1}(\mathbf{k}))(z+\omega-\lambda_{n_2}(\mathbf{k}))(z+\omega-\lambda_{n_3}(\mathbf{k}))(z+\omega-\lambda_{n_4}(\mathbf{k}))}$$
$$+\frac{\hat{\pi}_{n_4n_1}(1,\mathbf{k})\hat{\pi}_{n_1n_2}(2,\mathbf{k})\hat{\pi}_{n_2n_3}(1,\mathbf{k})\hat{\pi}_{n_3n_4}(2,\mathbf{k})}{(z-\omega-\lambda_{n_1}(\mathbf{k}))(z-\lambda_{n_2}(\mathbf{k}))(z-\lambda_{n_3}(\mathbf{k}))(z-\lambda_{n_4}(\mathbf{k}))}$$

$$- \frac{\hat{\pi}_{n_4 n_1}(1,\mathbf{k})\hat{\pi}_{n_1 n_2}(2,\mathbf{k})\hat{\pi}_{n_2 n_3}(2,\mathbf{k})\hat{\pi}_{n_3 n_4}(1,\mathbf{k})}{(z-\omega-\lambda_{n_1}(\mathbf{k}))(z-\lambda_{n_2}(\mathbf{k}))(z-\lambda_{n_3}(\mathbf{k}))(z-\lambda_{n_4}(\mathbf{k}))} \Bigg\}. \tag{7.6}$$

As for the spin contribution, with the notation

$$\hat{s}_{ij}(\mathbf{k}) := \int_\Omega \langle u_i(\mathbf{x},\mathbf{k}), \sigma_3 u_j(\mathbf{x},\mathbf{k})\rangle \mathrm{d}\mathbf{x}, \tag{7.7}$$

one has

$$\begin{aligned} a^{\mathrm{spin}}_{\infty,1}(\omega) = & -\frac{gc\mu_b}{(2\pi)^4 e}\int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{n_1,n_2,n_3\geqslant 1} \frac{1}{2\pi i}\int_{\Gamma_\omega} \mathrm{d}z\, f_{\mathrm{FD}}(z) \\ & \times \Bigg\{ \frac{\hat{\pi}_{n_1 n_2}(1,\mathbf{k})\hat{s}_{n_2 n_3}(\mathbf{k})\hat{\pi}_{n_3 n_1}(2,\mathbf{k})}{(\lambda_{n_2}(\mathbf{k})-z)(\lambda_{n_3}(\mathbf{k})-z)(\lambda_{n_1}(\mathbf{k})-z-\omega)} \\ & + \frac{\hat{\pi}_{n_1 n_2}(1,\mathbf{k})\hat{\pi}_{n_2 n_3}(2,\mathbf{k})\hat{s}_{n_3 n_1}(\mathbf{k})}{(\lambda_{n_2}(\mathbf{k})-z)(\lambda_{n_3}(\mathbf{k})-z-\omega)(\lambda_{n_1}(\mathbf{k})-z-\omega)} \\ & + \frac{\hat{\pi}_{n_1 n_2}(1,\mathbf{k})\hat{s}_{n_2 n_3}(\mathbf{k})\hat{\pi}_{n_3 n_1}(2,\mathbf{k})}{(\lambda_{n_2}(\mathbf{k})-z+\omega)(\lambda_{n_3}(\mathbf{k})-z+\omega)(\lambda_{n_1}(\mathbf{k})-z)} \\ & + \frac{\hat{\pi}_{n_1 n_2}(1,\mathbf{k})\hat{\pi}_{n_2 n_3}(2,\mathbf{k})\hat{s}_{n_3 n_1}(\mathbf{k})}{(\lambda_{n_2}(\mathbf{k})-z+\omega)(\lambda_{n_3}(\mathbf{k})-z)(\lambda_{n_1}(\mathbf{k})-z)} \Bigg\}. \end{aligned} \tag{7.8}$$

VIII. CONCLUSIONS

We presented in the present paper a method which shed new light on the quantum dynamics/optical response in bulk media in the presence of a constant magnetic field. We applied the gauge invariant magnetic perturbation theory and gave a clear and very general way of dealing with long range magnetic perturbations.

The formal connection with the integer quantum Hall effect was established in (4.2). Equations (6.9)–(6.12) and (7.4)–(7.8) contain our main result concerning the Verdet constant and the Faraday effect: it gives the linear term in B of the transverse conductivity in terms of the zero magnetic field Green function. They open the way of using the recently developed Green function techniques for the calculation of optical and magneto-optical properties of solids, to the case when an external magnetic field is present. Our method can be applied to ordered, as well as to random systems (with the appropriate average over configurations). Of course, in the last case one must assume ergodicity properties in order to insure convergence of results in the thermodynamic limit. Layers or other geometries can also be considered.

There are many subtle and difficult mathematical questions left aside in this paper, as those related to the thermodynamic limit, the convergence of infinite series over Bloch bands, and the low frequency limit when the Fermi energy lies in the spectrum. Another open problem is to consider self-interacting electrons and to investigate the exciton influence on the Faraday effect. These questions will be addressed elsewhere.

Our results are not only theoretical. In a future presentation we will use the residue theorem in Eqs. (7.4)–(7.8) to calculate the Verdet constant for various finite band models, and compare our results with the existing experimental data. Moreover, our results will be shown to imply those of Roth[30] and Nedoluha.[20]

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Fine grading of $\mathrm{sl}(p^2,\mathbb{C})$ generated by tensor product of generalized Pauli matrices and its symmetries

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Study of the normalizer of the MAD-group corresponding to a fine grading offers the most important tool for describing symmetries in the system of nonlinear equations connected with contraction of a Lie algebra. One fine grading that is always present in any Lie algebra $\mathrm{sl}(n,\mathbb{C})$ is the Pauli grading. The MAD-group corresponding to it is generated by generalized Pauli matrices. For such MAD-group, we already know its normalizer; its quotient group is isomorphic to the Lie group $\mathrm{SL}(2,\mathbb{Z}_n)\times\mathbb{Z}_2$. In this paper, we deal with a more complicated situation, namely that the fine grading of $\mathrm{sl}(p^2,\mathbb{C})$ is given by a tensor product of the Pauli matrices of the same order p, p being a prime. We describe the normalizer of the corresponding MAD-group and we show that its quotient group is isomorphic to $\mathrm{Sp}(4,\mathbb{F}_p)\times\mathbb{Z}_2$, where $\mathbb{F}_p$ is the finite field with p elements. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162149]

I. INTRODUCTION

A grading Γ of a Lie algebra L is a decomposition $\Gamma: L=\oplus_{i\in J}L_i$ into nontrivial subspaces L_i such that, for each pair of indices $i,j\in J$, there exists an index $k\in J$ fulfilling the property $[L_i,L_j]\subset L_k$. Among all the gradings of a Lie algebra, the most important ones are fine gradings, since any grading is created from some fine grading.

It was shown in Ref. 10 that there is a one-to-one correspondence between fine gradings of a simple Lie algebra over $\mathbb{C}$ and maximal Abelian groups of diagonalizable automorphisms (so-called MAD-groups) in Aut L. Each fine grading of a simple Lie algebra over $\mathbb{C}$ is obtained as a decomposition of L into eigensubspaces of automorphisms from a MAD group. In Ref. 4, all MAD-groups of Aut $\mathrm{sl}(n,\mathbb{C})$ were described.

Let us recall that the Lie algebra $\mathrm{sl}(n,\mathbb{C})$ has inner and outer automorphisms. An inner automorphism is given by a nonsingular matrix A of order n by the prescription

$$\mathrm{Ad}_A X := A^{-1}XA \quad \text{for } X\in \mathrm{sl}(n,\mathbb{C}).$$

An outer automorphism is connected with a nonsingular matrix A of order n as well, and it is given by the prescription

$$\mathrm{Out}_A X := -(A^{-1}XA)^{\mathsf{T}} \quad \text{for } X\in \mathrm{sl}(n,\mathbb{C}),$$

where A^{T} denotes the transposed matrix.

An important role in the description of MAD-groups without outer automorphism is played by generalized Pauli matrices. They were introduced in Ref. 11.

Definition 1.1: For a given $n\in\mathbb{N}$, set $\omega=\omega_n=e^{2\pi i/n}$. A group of matrices

$$\mathcal{P}_n := \{\omega^j P_n^k Q_n^l | j,k,l\in\{0,1,\ldots,n-1\}\}, \quad \text{where}$$

$$P_n = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & \omega & 0 & \dots & 0 \\ 0 & 0 & \omega 2 & \dots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \dots & \omega^{n-1} \end{pmatrix} \in \mathbb{C}^{n\times n} \quad \text{and } Q_n = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \end{pmatrix} \in \mathbb{C}^{n\times n},$$

is called the Pauli group of order n; P_n and Q_n are the generalized Pauli matrices of order n.

Let us note that the matrices P_n and Q_n do not commute, since $Q_nP_n=\omega P_nQ_n$. Nevertheless, the inner automorphisms corresponding to these matrices do commute, $\mathrm{Ad}_{Q_n}\mathrm{Ad}_{P_n}=\mathrm{Ad}_{P_n}\mathrm{Ad}_{Q_n}$.

In order to describe MAD-groups of the algebra $\mathrm{sl}(n,\mathbb{C})$, we need further notation:

The group of nonsingular diagonal matrices of order n will be denoted by $\mathcal{D}_n$, i.e.,

$$\mathcal{D}_n = \{\mathrm{diag}(\alpha_1,\alpha_2,\dots,\alpha_n)|\alpha_1,\alpha_2,\dots,\alpha_n \in \mathbb{C}\setminus\{0\}\}.$$

If G_1 and G_2 are groups of matrices, then $G_1\otimes G_2$ denotes the group of all tensor products $A\otimes B$, where $A\in G_1$ and $B\in G_2$. [If $A\in\mathbb{C}^{n\times n}$ and $B\in\mathbb{C}^{m\times m}$, then the tensor product $A\otimes B\in\mathbb{C}^{nm\times nm}$ is defined by $(A\otimes B)_{IJ}=A_{i_1i_2}B_{j_1j_2}$, where $i_1,i_2\in\{0,1,\dots,n-1\}$, $j_1,j_2\in\{0,1,\dots,m-1\}$, $I,J\in\{0,1,\dots,mn-1\}$ and $I=i_1m+j_1$, $J=i_2m+j_2$.]

The MAD-groups of $\mathrm{Aut}\,\mathrm{sl}(n,\mathbb{C})$ can be divided into two classes, depending whether or not they contain an outer automorphism. It is proved in Ref. 4 that any MAD-group in the automorphism group $\mathrm{Aut}\,\mathrm{sl}(n,\mathbb{C})$ containing only inner automorphisms is isomorphic to a group of the following form:

$$\mathcal{G} = \{\mathrm{Ad}_A|A \in \mathcal{P}_{n_1}\otimes\mathcal{P}_{n_2}\otimes\cdots\otimes\mathcal{P}_{n_{r-1}}\otimes\mathcal{D}_{n_r}\},$$

where $n_1n_2\cdots n_r=n$ and n_{i-1} divides n_i for any $i=2,3,\dots,r-1$.

A grading $\Gamma: L=\oplus_{i\in J}L_i$ of a Lie algebra L is a starting point for searching for graded contractions of the Lie algebra. This method for finding contractions of Lie algebras was used by several authors.[1,3,7] In this type of contraction, we define new Lie brackets by prescription

$$[x,y]_{\mathrm{new}} := \varepsilon_{jk}[x,y], \quad \text{where } x\in L_j,\ y\in L_k.$$

The complex or real parameters ε_{jk}, for $j,k\in J$, must be determined in such way that the vector space L with the binary operation $[.,.]_{\mathrm{new}}$ forms again a Lie algebra. Antisymmetry of Lie brackets demands that $\varepsilon_{jk}=\varepsilon_{kj}$. Compliance with the Jacobi identity, however, already implies that the coefficients ε_{jk} fulfill a complicated system of quadratic equations, which is in general difficult to solve. For description of symmetries of this system, it is important to know the symmetries of the original grading Γ. By a symmetry of a grading of the Lie algebra L we mean such an automorphism $g\in\mathrm{Aut}\,L$ that

$$\text{for each } j\in J \text{ there exists } k\in J \text{ fulfilling } gL_j=L_k. \tag{1}$$

Let us suppose that a fine grading $\Gamma:\mathrm{sl}(n,\mathbb{C})=\oplus_{j\in J}L_j$ corresponds to a MAD-group $\mathcal{G}\subset\mathrm{Aut}\,\mathrm{sl}(n,\mathbb{C})$. It means that

$$hL_k=L_k \quad \text{for all } h\in\mathcal{G} \quad \text{and } k\in J. \tag{2}$$

Combining (2) and (1), we obtain

$$ghg^{-1}L_j=L_j \quad \text{for any } j\in J.$$

The maximality of $\mathcal{G}$ implies that $ghg^{-1}\in\mathcal{G}$ for any $h\in\mathcal{G}$. This means, in other words, that the symmetries of the grading Γ corresponding to the MAD-group $\mathcal{G}$ form a group

$$\mathcal{N}(\mathcal{G}) = \{g \in \mathrm{Aut}\,\mathrm{sl}(n,\mathbb{C}) | g\mathcal{G}g^{-1} \subseteq \mathcal{G}\}.$$

This group is usually called the normalizer of the subgroup $\mathcal{G}$ in $\mathrm{Aut}\,\mathrm{sl}(n,\mathbb{C})$.

The definition of the normalizer $\mathcal{N}(\mathcal{G})$ implies that $\mathcal{G} \subset \mathcal{N}(\mathcal{G})$. Moreover, $\mathcal{G}$ is a normal subgroup of $\mathcal{N}(\mathcal{G})$. Thus, when describing $\mathcal{N}(\mathcal{G})$, it is sufficient to inspect the quotient group $\mathcal{N}(\mathcal{G})/\mathcal{G}$.

Reference 5 shows the study of the normalizer of one MAD-group of $\mathrm{sl}(n,\mathbb{C})$, namely

$$\mathcal{G} = \{\mathrm{Ad}_A | A \in \mathcal{P}_n\}.$$

It was shown that $\mathcal{N}(\mathcal{G})/\mathcal{G}$ is isomorphic to the matrix group $\{A \in \mathbb{Z}_n^{2\times 2} | \det A = \pm 1\}$, $\mathbb{Z}_n$ being a cyclic group of order n. This result was used for obtaining all the graded contractions (see Ref. 6) of Lie algebra $\mathrm{sl}(3,\mathbb{C})$ that arise from the Pauli grading

$$\mathrm{sl}(3,\mathbb{C}) = \oplus_{(j,k)\in J}\{P_3^j Q_3^k\}_{\mathrm{lin}}, \quad J = \mathbb{Z}_3 \times \mathbb{Z}_3 \setminus \{(0,0)\}.$$

In this paper, we are going to study the symmetries of the grading corresponding to the MAD-group,

$$\mathcal{G} = \{\mathrm{Ad}_A | A \in \mathcal{P}_n \otimes \mathcal{P}_n\} \subset \mathrm{Aut}\,\mathrm{sl}(n^2,\mathbb{C}), \quad n \text{ prime}. \tag{3}$$

In the sequel we will use notation P and Q instead of P_n and Q_n, and by the letter $\mathcal{G}$ we will denote only the group given by (3).

If n and m are coprime integers, then the tensor product $\mathcal{P}_n \otimes \mathcal{P}_m$ of the Pauli groups $\mathcal{P}_n$ and $\mathcal{P}_m$ is isomorphic to the Pauli group $\mathcal{P}_{nm}$, therefore it is a natural step in investigation of symmetries of gradings to devote attention to the MAD-group given by $\mathcal{P}_n \otimes \mathcal{P}_n$.

II. THE NORMALIZER OF THE MAD-GROUP CORRESPONDING TO THE TENSOR PRODUCT $\mathcal{P}_n \otimes \mathcal{P}_n$

If $(g_i)_{i\in I}$ is a set of generators of a group $\mathcal{H} \subset \mathrm{Aut}\,L$, then $\varphi \in \mathrm{Aut}\,L$ belongs to the normalizer $\mathcal{N}(\mathcal{H})$ if and only if $\varphi g_i \varphi^{-1} \in \mathcal{H}$ for all the generators g_i. Since $\mathcal{P}_n \otimes \mathcal{P}_n = \{P^i Q^j \otimes P^k Q^l\}$, our MAD-group

$$\mathcal{G} = \{\mathrm{Ad}_{P^i Q^j \otimes P^k Q^l} | i,j,k,l \in \mathbb{Z}_n\}$$

has four generators (we use the letter I for unit matrix of order n),

$$\mathrm{Ad}_{A_1}, \quad \text{where } A_1 = P \otimes I,$$

$$\mathrm{Ad}_{A_2}, \quad \text{where } A_2 = Q \otimes I,$$

$$\mathrm{Ad}_{A_3}, \quad \text{where } A_3 = I \otimes P,$$

$$\mathrm{Ad}_{A_4}, \quad \text{where } A_4 = I \otimes Q.$$

Any element of the MAD-group $\mathcal{G}$ is characterized by a quadruple of indices in $\mathbb{Z}_n$. We know that an automorphism $\varphi \in \mathrm{Aut}\,\mathrm{sl}(n^2,\mathbb{C})$ belongs to $\mathcal{N}(\mathcal{G})$ if and only if $\varphi \mathrm{Ad}_{A_i} \varphi^{-1} \in \mathcal{G}$ for $i = 1,2,3,4$. Thus each $\varphi \in \mathcal{N}(\mathcal{G})$ is characterized by a set of 16 coefficients $(a_{ij})_{i,j=1}^4$ such that

$$\varphi\, \mathrm{Ad}_{A_j}\, \varphi^{-1} = \mathrm{Ad}_{P^{a_{1j}} Q^{a_{2j}} \otimes P^{a_{3j}} Q^{a_{4j}}} = \mathrm{Ad}_{A_1^{a_{1j}} A_2^{a_{2j}} A_3^{a_{3j}} A_4^{a_{4j}}} \quad \text{for } j = 1,2,3,4.$$

We order these 16 parameters into a matrix $C(\varphi) \in \mathbb{Z}_n^{4\times 4}$ as follows:

$$\varphi \mapsto C(\varphi) = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}. \tag{4}$$

Remark 2.1: Obviously, the assignment $\varphi \mapsto C(\varphi)$ implies that $C(\varphi)=I_4$ if and only if φ commutes with each generator of the MAD-group $\mathcal{G}$, and thus with the whole MAD-group. This means that φ necessarily belongs to $\mathcal{G}$ (due to the maximality of $\mathcal{G}$). Shortly, we have

$$C(\varphi) = I_4 \Leftrightarrow \varphi \in \mathcal{G}. \tag{5}$$

The advantage of such ordering of the 16 coefficients corresponding to $\varphi \in \mathcal{N}(\mathcal{G})$ is obvious from the following statement.

Proposition 2.2: Let $\varphi, \psi \in \mathcal{N}(\mathcal{G})$. *Then* $C(\varphi\psi)=C(\varphi)C(\psi)$.

Proof: We denote the coefficient matrices by $C(\varphi)=(a_{ij})_{i,j=1}^4$, and $C(\psi)=(b_{ij})_{i,j=1}^4$. Let us apply the automorphism $\varphi\psi$ on an element $\mathrm{Ad}_{A_p} \in \mathcal{G}$ as follows:

$$\begin{aligned}(\varphi\psi)\mathrm{Ad}_{A_p}(\varphi\psi)^{-1} &= \varphi(\psi\,\mathrm{Ad}_{A_p}\psi^{-1})\varphi^{-1} = \varphi(\mathrm{Ad}_{A_1^{b_{1p}}A_2^{b_{2p}}A_3^{b_{3p}}A_4^{b_{4p}}})\varphi^{-1} \\ &= (\varphi\,\mathrm{Ad}_{A_4}\,\varphi^{-1})^{b_{4p}}(\varphi\,\mathrm{Ad}_{A_3}\,\varphi^{-1})^{b_{3p}}(\varphi\,\mathrm{Ad}_{A_2}\,\varphi^{-1})^{b_{2p}}(\varphi\,\mathrm{Ad}_{A_1}\,\varphi^{-1})^{b_{1p}} \\ &= (\mathrm{Ad}_{A_1^{a_{14}}A_2^{a_{24}}A_3^{a_{34}}A_4^{a_{44}}})^{b_{4p}}(\mathrm{Ad}_{A_1^{a_{13}}A_2^{a_{23}}A_3^{a_{33}}A_4^{a_{43}}})^{b_{3p}}(\mathrm{Ad}_{A_1^{a_{12}}A_2^{a_{22}}A_3^{a_{32}}A_4^{a_{42}}})^{b_{2p}}(\mathrm{Ad}_{A_1^{a_{11}}A_2^{a_{21}}A_3^{a_{31}}A_4^{a_{41}}})^{b_{1p}}.\end{aligned}$$

Since $A_jA_k=\mathrm{const}\,A_kA_j$, we have $\mathrm{Ad}_{A_jA_k}=\mathrm{Ad}_{A_kA_j}$ for any $j,k=1,2,3,4$. Therefore

$$(\varphi\psi)\mathrm{Ad}_{A_p}(\varphi\psi)^{-1} = \mathrm{Ad}_{A_1^{c_{1p}}A_2^{c_{2p}}A_3^{c_{3p}}A_4^{c_{4p}}},$$

where

$$c_{1p} = a_{11}b_{1p} + a_{12}b_{2p} + a_{13}b_{3p} + a_{14}b_{4p},$$

$$c_{2p} = a_{21}b_{1p} + a_{22}b_{2p} + a_{23}b_{3p} + a_{24}b_{4p},$$

$$c_{3p} = a_{31}b_{1p} + a_{32}b_{2p} + a_{33}b_{3p} + a_{34}b_{4p},$$

$$c_{4p} = a_{41}b_{1p} + a_{42}b_{2p} + a_{43}b_{3p} + a_{44}b_{4p}.$$

This means, in brief notation, that $C(\varphi\psi)=C(\varphi)C(\psi)$. □

We prove below that the matrix $C(\varphi)$ assigned to the element φ of the normalizer $\mathcal{N}(\mathcal{G})$ characterizes a coset belonging to the quotient group $\mathcal{N}(\mathcal{G})/\mathcal{G}$.

Proposition 2.3: Let φ, ψ *belong to the normalizer* $\mathcal{N}(\mathcal{G})$ *of the MAD-group* $\mathcal{G}$. *Then* $C(\varphi)=C(\psi)$ *if and only if there exists* $h \in \mathcal{G}$ *such that* $\varphi=h\psi$.

Proof: Let $\varphi, \psi \in \mathcal{N}(\mathcal{G})$ such that $C(\varphi)=C(\psi)$. Since $\psi^{-1} \in \mathcal{N}(\mathcal{G})$ as well, we obtain from Proposition 2.2,

$$C(\varphi\psi^{-1}) = C(\varphi)C(\psi^{-1}) = C(\psi)C(\psi^{-1}) = C(\psi\psi^{-1}) = C(Id) = I_4.$$

By Remark 2.1, $\varphi\psi^{-1}$ commutes with all elements of $\mathcal{G}$, which is only possible when $\varphi\psi^{-1} \in \mathcal{G}$.

The opposite implication follows directly from Remark 2.1. □

Lemma 2.4: The outer automorphism Out_I *belongs to the normalizer* $\mathcal{N}(\mathcal{G})$, *and*

$$C(\mathrm{Out}_I) = \mathrm{diag}(-1,1,-1,1).$$

Proof: Let us denote $\varphi_0=\mathrm{Out}_I$. As φ_0 is given by the prescription $\varphi_0 X=-X^{\mathsf{T}}$, clearly $\varphi_0^{-1}=\varphi_0$. We can derive for any inner automorphism Ad_A that

$$(\varphi_0 \operatorname{Ad}_A \varphi_0^{-1})(X) = (\varphi_0 \operatorname{Ad}_A)(-X^{\mathsf{T}}) = \varphi_0(-A^{-1}X^{\mathsf{T}}A)$$
$$= (A^{-1}X^{\mathsf{T}}A)^{\mathsf{T}} = A^{\mathsf{T}}XA^{-\mathsf{T}} = (A^{-\mathsf{T}})^{-1}XA^{-\mathsf{T}} = \operatorname{Ad}_{A^{-\mathsf{T}}}(X),$$

where we used abbreviated notation $A^{-\mathsf{T}}$ instead of $(A^{-1})^{\mathsf{T}}$. This notation is used in the sequel as well.

Thus we have shown that the action of Out_I on any inner automorphism Ad_A is

$$\mathrm{Out}_I \operatorname{Ad}_A \mathrm{Out}_I^{-1} = \operatorname{Ad}_{A^{-\mathsf{T}}}. \tag{6}$$

Now, for each generator Ad_{A_j}, $j=1,2,3,4$, of the MAD-group $\mathcal{G}$, we prove that $\varphi_0 \operatorname{Ad}_{A_j} \varphi_0^{-1}$ belongs to $\mathcal{G}$:

Let us recall the following trivial properties of matrices P and Q and the properties of tensor product:

(i) $(A\otimes B)^{-1}=A^{-1}\otimes B^{-1}$;
(ii) $(A\otimes B)^{\mathsf{T}}=A^{\mathsf{T}}\otimes B^{\mathsf{T}}$;
(iii) $P^{\mathsf{T}}=P$, as P is diagonal;
(iv) $Q^{-1}=Q^{\mathsf{T}}$, as Q is a permutation matrix.

Using these relations, we obtain

(1) $A_1^{-\mathsf{T}}=(P\otimes I)^{-\mathsf{T}}=P^{-\mathsf{T}}\otimes I=P^{-1}\otimes I=(P\otimes I)^{-1}=A_1^{-1}$;
(2) $A_2^{-\mathsf{T}}=(Q\otimes I)^{-\mathsf{T}}=Q^{-\mathsf{T}}\otimes I=Q\otimes I=A_2$;
(3) $A_3^{-\mathsf{T}}=(I\otimes P)^{-\mathsf{T}}=I\otimes P^{-\mathsf{T}}=I\otimes P^{-1}=(I\otimes P)^{-1}=A_3^{-1}$;
(4) $A_4^{-\mathsf{T}}=(I\otimes Q)^{-\mathsf{T}}=I\otimes Q^{-\mathsf{T}}=I\otimes Q=A_4$.

Statements (1)–(4) together with Eq. (6) already prove the lemma. □

Remark 2.5: Product of two outer automorphisms is an inner automorphism. Thus, when describing the set of all automorphisms in $\mathcal{N}(\mathcal{G})$, we can focus on the subgroup $\mathcal{N}_{\mathrm{in}}(\mathcal{G})$ containing all the inner automorphisms in $\mathcal{N}(\mathcal{G})$. The whole $\mathcal{N}(\mathcal{G})$ can then be described as

$$\mathcal{N}(\mathcal{G}) = \mathcal{N}_{\mathrm{in}}(\mathcal{G}) \cup \mathrm{Out}_I \mathcal{N}_{\mathrm{in}}(\mathcal{G}).$$

The following theorem shows the connection between normalizers of these MAD-groups and the symplectic groups over finite field which were introduced in Ref. 2.

Theorem 2.6: *Let* Ad_A *be an inner automorphism contained in the normalizer* $\mathcal{N}(\mathcal{G})$ *of the MAD-group* $\mathcal{G}$, *and let* $C(\mathrm{Ad}_A)$ *be the coefficient matrix corresponding to* Ad_A. *Then*

$$C(\mathrm{Ad}_A) \in \mathrm{Sp}(4,\mathbb{Z}_n) := \{X \in \mathbb{Z}_n^{4\times 4} | X^{\mathsf{T}}JX = J\}, \tag{7}$$

where

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} = I_2 \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Proof: Let us denote $C(\mathrm{Ad}_A)=(a_{ij})_{i,j=1}^4$. The definition of the matrix $C(\mathrm{Ad}_A)$ implies that

$$\operatorname{Ad}_A \operatorname{Ad}_{A_p}(\operatorname{Ad}_A)^{-1} = \operatorname{Ad}_{A^{-1}A_pA} = \operatorname{Ad}_{A_1^{a_{1p}}A_2^{a_{2p}}A_3^{a_{3p}}A_4^{a_{4p}}} \quad \text{for } p=1,2,3,4. \tag{8}$$

As $\mathrm{Ad}_K=\mathrm{Ad}_H$ if and only if $K=\alpha H$ for some $\alpha\in\mathbb{C}-\{0\}$, we obtain from (8) existence of four nonzero constants $\alpha_p, p=1,2,3,4$, such that

$$A_p = \alpha_p A A_1^{a_{1p}} A_2^{a_{2p}} A_3^{a_{3p}} A_4^{a_{4p}} A^{-1}. \tag{9}$$

We derive easily from the basic relation $QP=\omega PQ$ that

$$A_1A_2 = \omega^{-1}A_2A_1, \tag{10}$$

$$A_3A_4 = \omega^{-1}A_4A_3. \tag{11}$$

The remaining pairs A_i, A_j commute

$$A_1A_3 = A_3A_1, \tag{12}$$

$$A_1A_4 = A_4A_1, \tag{13}$$

$$A_2A_3 = A_3A_2, \tag{14}$$

$$A_2A_4 = A_4A_2. \tag{15}$$

By inputting A_1, A_2 expressed in the form (9) into the relation (10), we obtain

$$\alpha_1 A A_1^{a_{11}} A_2^{a_{21}} A_3^{a_{31}} A_4^{a_{41}} A^{-1} \alpha_2 A A_1^{a_{12}} A_2^{a_{22}} A_3^{a_{32}} A_4^{a_{42}} A^{-1}$$
$$= \omega^{-1} \alpha_2 A A_1^{a_{12}} A_2^{a_{22}} A_3^{a_{32}} A_4^{a_{42}} A^{-1} \alpha_1 A A_1^{a_{11}} A_2^{a_{21}} A_3^{a_{31}} A_4^{a_{41}} A^{-1},$$

and, after simplification and using relations (10)–(15),

$$\omega^{a_{21}a_{12}+a_{41}a_{32}} A_1^{a_{11}+a_{12}} A_2^{a_{21}+a_{22}} A_3^{a_{31}+a_{32}} A_4^{a_{41}+a_{42}} = \omega^{-1+a_{22}a_{11}+a_{42}a_{31}} A_1^{a_{11}+a_{12}} A_2^{a_{21}+a_{22}} A_3^{a_{31}+a_{32}} A_4^{a_{41}+a_{42}}.$$

This implies that $\omega^{a_{21}a_{12}+a_{41}a_{32}} = \omega^{-1+a_{22}a_{11}+a_{42}a_{31}}$, and therefore

$$1 = a_{11}a_{22} - a_{21}a_{12} + a_{31}a_{42} - a_{41}a_{32} \pmod{n}. \tag{16}$$

Analogously, the equations (11)–(15) result in

$$1 = a_{13}a_{24} - a_{14}a_{23} + a_{33}a_{44} - a_{34}a_{43} \pmod{n}, \tag{17}$$

$$0 = a_{11}a_{23} - a_{13}a_{21} + a_{31}a_{43} - a_{33}a_{41} \pmod{n}, \tag{18}$$

$$0 = a_{11}a_{24} - a_{14}a_{21} + a_{31}a_{44} - a_{34}a_{41} \pmod{n}, \tag{19}$$

$$0 = a_{12}a_{23} - a_{13}a_{22} + a_{32}a_{43} - a_{33}a_{42} \pmod{n}, \tag{20}$$

$$0 = a_{12}a_{24} - a_{14}a_{22} + a_{32}a_{44} - a_{34}a_{42} \pmod{n}. \tag{21}$$

It can be easily verified (by a direct calculation) that the matrix $(a_{ij})_{i,j=1}^4$ belongs to the group $\mathrm{Sp}(4,\mathbb{Z}_n)$ if and only if the matrix elements a_{ij} fulfill equations (16)–(21). □

Remark 2.7: We were notified[9] that the set $\mathrm{Sp}(4,\mathbb{Z}_n)$ defined analogously to (7) is a group even in the case when $\mathbb{Z}_n$ is not a field. All our previous considerations hold therefore for any positive integer n. But our deductions in the sequel already need n to be a prime number.

We are going to prove that the mapping given by (4) is in fact the mapping on the whole symplectic group $\mathrm{Sp}(4,\mathbb{F}_n)$. To show it we need to find for any element of $\mathrm{Sp}(4,\mathbb{F}_n)$ its preimage, or equivalently for any generator of $\mathrm{Sp}(4,\mathbb{F}_n)$ its preimage.

To simplify the proof we need to find the smallest possible set of generators of $\mathrm{Sp}(4,\mathbb{F}_n)$. In Ref. 8 a set of generators of the group $\mathrm{Sp}(2m,K)$ over a finite field K is described. In case $m=2$, the set of generators contains n^4-n^2+n+1 elements, where n is the cardinality of K. As we show in Appendix B, it is possible to reduce the number of generators of the group $\mathrm{Sp}(4,\mathbb{F}_n)$ to four matrices. In formal notation

$$\mathrm{Sp}(4,\mathbb{F}_n)=\langle D_1,D_2,D_3,D_4\rangle,$$

where

$$D_1=\begin{pmatrix}1&1&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad D_2=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$D_3=\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix},\quad \text{and}\quad D_4=\begin{pmatrix}1&0&0&0\\0&1&0&-1\\1&0&1&0\\0&0&0&1\end{pmatrix}. \tag{22}$$

(We recall that for elements $k_1,k_2,\ldots,k_s$ of a group G, the notation $\langle k_1,k_2,\ldots,k_s\rangle$ means the smallest subgroup of the group G containing $k_1,k_2,\ldots,k_s$.) We show that these four matrices are images of inner automorphisms which belong to the normalizer of the group $\mathcal{G}$.

Proposition 2.8: Let n be a prime. Then for the four matrices D_j as introduced in (22), there exist inner automorphisms $\varphi_j=\mathrm{Ad}_{B_j}\in\mathcal{N}_{\mathrm{in}}(\mathcal{G})$ such that $D_j=C(\varphi_j)=C(\mathrm{Ad}_{B_j})$.

The proof is postponed to the Appendix A since it is rather technical and we do not want to interrupt coherency in the content of the paper.

The immediate consequence of the previous proposition is the following main result of the paper.

Theorem 2.9: *Let n be a prime. The mapping $\varphi\mapsto C(\varphi)$ defined in (4) is an isomorphism between groups*

$$\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}\simeq\mathrm{Sp}(4,\mathbb{F}_n)=\{X\in\mathbb{Z}_n^{4\times4}|X^{\mathsf{T}}JX=J\},$$

and

$$\mathcal{N}(\mathcal{G})/\mathcal{G}\simeq\{X\in\mathbb{Z}_n^{4\times4}|X^{\mathsf{T}}JX=\pm J\},$$

where

$$J=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&1\\0&0&-1&0\end{pmatrix}=I_2\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix}.$$

Proof:

(i) The mapping $\varphi\mapsto C(\varphi)$ from $\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}$ to $\mathrm{Sp}(4,\mathbb{F}_n)$ is a homomorphism, as $C(\varphi\psi)=C(\varphi)C(\psi)$, which was proved in Proposition 2.2.

(ii) The mapping $\varphi\mapsto C(\varphi)$ from $\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}$ to $\mathrm{Sp}(4,\mathbb{F}_n)$ is injective, as shown in Proposition 2.3.

(iii) The group $\mathrm{Sp}(4,\mathbb{F}_n)$ is generated by four matrices D_1,D_2,D_3,D_4 (see Theorem 3.1 in Appendix B).

(iv) All the matrices D_j, $j=1,2,3,4$, have their inverse images $\varphi_j\in\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}$, such that $C(\varphi_j)=D_j$ (see Proposition 2.8). This implies that the mapping $\varphi\mapsto C(\varphi)$ is also surjective.

In total, we see that the mapping $\varphi\mapsto C(\varphi)$ is an isomorphism from $\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}$ onto $\mathrm{Sp}(4,\mathbb{F}_n)$.

To show isomorphism between $\mathcal{N}(\mathcal{G})/\mathcal{G}$ and $\mathrm{Sp}(4,\mathbb{F}_n)\otimes\mathbb{Z}_2$, it is enough to use Remark 2.5 and the fact that the matrix $M:=C(\mathrm{Out}_I)=\mathrm{diag}(-1,1,-1,1)$ corresponding to the outer automorphisms $\mathrm{Out}_I\in\mathcal{N}(\mathcal{G})$ satisfies the equality $M^{\mathsf{T}}JM=-J$. □

III. CONCLUSIONS

Let us summarize the content of the paper:

(1) The normalizer $\mathcal{N}(\mathcal{G})$ of the MAD-group $\mathcal{G}=\{\mathrm{Ad}_{P^iQ^j\otimes P^kQ^l} | i,j,k,l\in\mathbb{Z}_n\}\subset \mathrm{Aut}\ \mathrm{sl}(n^2,\mathbb{C})$ consists of two subsets,

$$\mathcal{N}_{\mathrm{in}}(\mathcal{G}) \quad \text{the group of all inner automorphisms in } \mathcal{N}(\mathcal{G}),$$

$$\mathrm{Out}_I\mathcal{N}_{\mathrm{in}}(\mathcal{G}) \quad \text{the set of all outer automorphisms in } \mathcal{N}(\mathcal{G}).$$

(2) We provide an explicit expression of the four generators of $\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}$, namely the inner automorphisms Ad_{B_j}, $j=1,2,3,4$ (see Proposition 2.8).

(3) Altogether, we can write the set of generators

$$\mathcal{G}=\langle \mathrm{Ad}_{P\otimes I},\mathrm{Ad}_{Q\otimes I},\mathrm{Ad}_{I\otimes P},\mathrm{Ad}_{I\otimes Q}\rangle,$$

$$\mathcal{N}_{\mathrm{in}}(\mathcal{G})/\mathcal{G}=\langle \mathrm{Ad}_{B_1},\mathrm{Ad}_{B_2},\mathrm{Ad}_{B_3},\mathrm{Ad}_{B_4}\rangle,$$

$$\mathcal{N}(\mathcal{G})=\mathcal{N}_{\mathrm{in}}(\mathcal{G})\cup \mathrm{Out}_I\mathcal{N}_{\mathrm{in}}(\mathcal{G}).$$

(4) Thus, one can generate each element of the normalizer from the set $\{\mathrm{Ad}_{B_1},\mathrm{Ad}_{B_2},\mathrm{Ad}_{B_3},\mathrm{Ad}_{B_4},\mathrm{Out}_I,\mathrm{Ad}_{P\otimes I},\mathrm{Ad}_{Q\otimes I},\mathrm{Ad}_{I\otimes P},\mathrm{Ad}_{I\otimes Q}\}$. In formal notation,

$$\mathcal{N}(\mathcal{G})=\langle \mathrm{Ad}_{B_1},\mathrm{Ad}_{B_2},\mathrm{Ad}_{B_3},\mathrm{Ad}_{B_4},\mathrm{Out}_I,\mathrm{Ad}_{P\otimes I},\mathrm{Ad}_{Q\otimes I},\mathrm{Ad}_{I\otimes P},\mathrm{Ad}_{I\otimes Q}\rangle,$$

where the matrices B_j were defined in the proof of Proposition 2.8.

The description of the normalizer as done in this article was only possible for n prime. For n nonprime, the problem is still open.

It was shown previously that for the Pauli grading, the normalizer of the respective MAD-group is isomorphic to $\mathrm{SL}(2,\mathbb{Z}_n)$, which is isomorphic to $\mathrm{Sp}(2,\mathbb{Z}_n)$, for any positive integer $n>1$. This suggests that in the case of a MAD-group formed by inner automorphisms generated by

$$\underbrace{\mathcal{P}_n\otimes\mathcal{P}_n\otimes\ \ldots\ \otimes\mathcal{P}_n}_{k\text{–times}},$$

the normalizer may be isomorphic to $\mathrm{Sp}(2k,\mathbb{Z}_n)$.

Let us mention that the normalizer has not yet been described for any MAD-group containing outer automorphisms.

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APPENDIX A

This section contains a proof of Proposition 2.8. The matrices D_j's considered in the proof are defined by (22).

Proof: In order to prove that an automorphism $\varphi_j=\mathrm{Ad}_{B_j}$ is an inverse image of D_j, we must express the action of φ_j on the basis elements $P\otimes I,Q\otimes I,I\otimes P,I\otimes Q$ of $\mathcal{G}$ again in terms of $P\otimes I,Q\otimes I,I\otimes P,I\otimes Q$. The coefficients a_{kl} describing the action of φ_j [as introduced in (4)] then form the matrix D_j. In the following we set the four matrices B_j, and verify that each satisfies the equation $D_j=C(\mathrm{Ad}_{B_j})$.

Throughout the proof, we use the coefficient ω, which is, as defined previously, the nth root of unity, $\omega=\omega_n=e^{2\pi i/n}$. We also shorten the notation of I_n to I.

And, finally, the elements of matrices P,Q (whose indices are also counted modulo n) can be written in terms of the Kronecker symbol as

$$P_{ij}=\delta_{ij}\omega^j,\quad Q_{ij}=\delta_{i(j-1)},\quad Q^{\mathsf{T}}_{ij}=\delta_{i(j+1)}. \tag{A1}$$

(1) We define $\varphi_1=\mathrm{Ad}_{B_1}$, where

$$B_1=\widetilde{B}_1\otimes I,\quad \widetilde{B}_1=\mathrm{diag}(b_0,b_1,\ldots,b_{(n-1)}),\quad b_j=\varepsilon^j\omega^{j(j-1)/2},\quad \varepsilon=\omega^{-(n-1)/2}.$$

As $\widetilde{B}_1$, $\widetilde{B}_1^{-1}$, and P are diagonal, they all mutually commute, and thus $B_1^{-1}(P\otimes I)B_1=(\widetilde{B}_1\otimes I)^{-1}(P\otimes I)(\widetilde{B}_1\otimes I)=(\widetilde{B}_1^{-1}\otimes I)(P\widetilde{B}_1\otimes I)=(\widetilde{B}_1^{-1}P\widetilde{B}_1)\otimes I=(\widetilde{B}_1^{-1}\widetilde{B}_1P)\otimes I=P\otimes I$. In other words,

$$\varphi_1\,\mathrm{Ad}_{P\otimes I}\,\varphi_1^{-1}=\mathrm{Ad}_{B_1}\,\mathrm{Ad}_{P\otimes I}\,\mathrm{Ad}_{B_1^{-1}}=\mathrm{Ad}_{B_1^{-1}(P\otimes I)B_1}=\mathrm{Ad}_{P\otimes I},$$

which means, according to the definition of $C(\varphi_1)$, that the first column of the matrix $C(\varphi_1)$ is

$$(a_{11},a_{21},a_{31},a_{41})^{\mathsf{T}}=(1,0,0,0)^{\mathsf{T}}.$$

Now we apply φ_1 on the second generator of the group $\mathcal{G}$, which is the inner automorphism defined by the matrix $Q\otimes I$. In fact, we need to express $B_1^{-1}(Q\otimes I)B_1$ in terms of the basis matrices $P\otimes I,Q\otimes I,I\otimes P,I\otimes Q$. Using the notation of elements of P and Q introduced in (A1), we obtain

$$\begin{aligned}(\widetilde{B}_1^{-1}Q\widetilde{B}_1)_{ij}&=\sum_{k=0}^{n-1}\sum_{l=0}^{n-1}(\widetilde{B}_1^{-1})_{ik}Q_{kl}(\widetilde{B}_1)_{lj}\\&=\sum_{k=0}^{n-1}\sum_{l=0}^{n-1}\delta_{ik}\varepsilon^{-k}\omega^{-k(k-1)/2}\delta_{k(l-1)}\delta_{lj}\varepsilon^j\omega^{j(j-1)/2}\\&=\sum_{k=0}^{n-1}\delta_{ik}\varepsilon^{j-k}\omega^{[j(j-1)-k(k-1)]/2}\delta_{k(j-1)}\\&=\varepsilon\,\delta_{i(j-1)}\omega^{j-1}\end{aligned}$$

$$(PQ)_{ij}=\sum_{k=0}^{n-1}P_{ik}Q_{kj}=\sum_{k=0}^{n-1}\delta_{ik}\omega^k\delta_{k(j-1)}=\delta_{i(j-1)}\omega^{j-1}.$$

We see that the matrix $B_1^{-1}(Q\otimes I)B_1$ is just an ε multiple of PQ, and it follows that

$$\varphi_1\,\mathrm{Ad}_{Q\otimes I}\,\varphi_1^{-1}=\mathrm{Ad}_{B_1}\,\mathrm{Ad}_{Q\otimes I}\,\mathrm{Ad}_{B_1^{-1}}=\mathrm{Ad}_{B_1^{-1}(Q\otimes I)B_1}=\mathrm{Ad}_{(\tilde{B}_1^{-1}Q\tilde{B}_1)\otimes I}=\mathrm{Ad}_{(\varepsilon PQ)\otimes I}=\mathrm{Ad}_{PQ\otimes I}.$$

The second column of the matrix $C(\varphi_1)$ is thus equal to

$$(a_{12},a_{22},a_{32},a_{42})^{\mathsf{T}}=(1,1,0,0)^{\mathsf{T}}.$$

By simple matrix multiplication, we see that $B_1^{-1}(I\otimes P)B_1=(\widetilde{B}_1^{-1}\otimes I)(I\otimes P)(\widetilde{B}_1\otimes I)=(\widetilde{B}_1^{-1}\widetilde{B}_1)\otimes P=I\otimes P$; which means $\varphi_1\,\mathrm{Ad}_{I\otimes P}\,\varphi_1^{-1}=\mathrm{Ad}_{B_1}\,\mathrm{Ad}_{I\otimes P}\,\mathrm{Ad}_{B_1^{-1}}=\mathrm{Ad}_{B_1^{-1}(I\otimes P)B_1}=\mathrm{Ad}_{I\otimes P}$, and therefore

$$(a_{13},a_{23},a_{33},a_{43})^{\mathsf{T}}=(0,0,1,0)^{\mathsf{T}}.$$

Analogously, setting Q on the place of P, we have $B_1^{-1}(I\otimes Q)B_1=(\widetilde{B}_1^{-1}\otimes I)(I\otimes Q)(\widetilde{B}_1\otimes I)=(\widetilde{B}_1^{-1}\widetilde{B}_1)\otimes Q=I\otimes Q$; which means $\varphi_1\,\mathrm{Ad}_{I\otimes Q}\,\varphi_1^{-1}=\mathrm{Ad}_{B_1}\,\mathrm{Ad}_{I\otimes Q}\,\mathrm{Ad}_{B_1^{-1}}=\mathrm{Ad}_{B_1^{-1}(I\otimes Q)B_1}=\mathrm{Ad}_{I\otimes Q}$, and therefore

$$(a_{14},a_{24},a_{34},a_{44})^{\mathsf{T}} = (0,0,0,1)^{\mathsf{T}}.$$

Thus, we have shown that

$$C(\varphi_1) = D_1 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

(2) We define $\varphi_2 = \mathrm{Ad}_{B_2}$, where

$$B_2 = \widetilde{B}_2 \otimes I, \quad (\widetilde{B}_2)_{ij} = \omega^{ij}, \quad i,j = 0,1,\ldots,n-1.$$

Note that $\widetilde{B}_2$ is the famous Sylvester matrix.

In preparation for describing the action of Ad_{B_2}, we apply the matrix $\widetilde{B}_2$ on P, Q, and Q^{T} from both right and left,

$$(P\widetilde{B}_2)_{ij} = \sum_{k=0}^{n-1} P_{ik}(\widetilde{B}_2)_{kj} = \sum_{k=0}^{n-1} \delta_{ik}\omega^k\omega^{kj} = \omega^i\omega^{ij} = \omega^{i(j+1)},$$

$$(\widetilde{B}_2Q^{\mathsf{T}})_{ij} = \sum_{k=0}^{n-1} (\widetilde{B}_2)_{ik}(Q^{\mathsf{T}})_{kj} = \sum_{k=0}^{n-1} \omega^{ik}\delta_{k(j+1)} = \omega^{i(j+1)},$$

$$(Q\widetilde{B}_2)_{ij} = \sum_{k=0}^{n-1} Q_{ik}(\widetilde{B}_2)_{kj} = \sum_{k=0}^{n-1} \delta_{i(k-1)}\omega^{kj} = \omega^{(i+1)j},$$

$$(\widetilde{B}_2P)_{ij} = \sum_{k=0}^{n-1} (\widetilde{B}_2)_{ik}P_{kj} = \sum_{k=0}^{n-1} \omega^{ik}\delta_{kj}\omega^j = \omega^{ij}\omega^j = \omega^{(i+1)j}.$$

We easily conclude that

$$P\widetilde{B}_2 = \widetilde{B}_2Q^{\mathsf{T}} \Rightarrow \widetilde{B}_2^{-1}P\widetilde{B}_2 = Q^{\mathsf{T}} = Q^{-1},$$

$$Q\widetilde{B}_2 = \widetilde{B}_2P \Rightarrow \widetilde{B}_2^{-1}Q\widetilde{B}_2 = P.$$

Using these relations, the way to find the coefficients of $C(\varphi_2) = C(\mathrm{Ad}_{B_2})$ is quite straightforward as follows:

$$B_2^{-1}(P\otimes I)B_2 = (\widetilde{B}_2\otimes I)^{-1}(P\otimes I)(\widetilde{B}_2\otimes I) = (\widetilde{B}_2^{-1}\otimes I)(P\widetilde{B}_2\otimes I) = (\widetilde{B}_2^{-1}P\widetilde{B}_2)\otimes I = Q^{-1}\otimes I.$$

Therefore, $\varphi_2\,\mathrm{Ad}_{P\otimes I}\,\varphi_2^{-1} = \mathrm{Ad}_{B_2^{-1}(P\otimes I)B_2} = \mathrm{Ad}_{(Q\otimes I)^{-1}}$, and we have found the coefficients

$$(a_{11},a_{21},a_{31},a_{41})^{\mathsf{T}} = (0,-1,0,0)^{\mathsf{T}};$$

$$B_2^{-1}(Q\otimes I)B_2 = (\widetilde{B}_2\otimes I)^{-1}(Q\otimes I)(\widetilde{B}_2\otimes I) = (\widetilde{B}_2^{-1}\otimes I)(Q\widetilde{B}_2\otimes I) = (\widetilde{B}_2^{-1}Q\widetilde{B}_2)\otimes I = P\otimes I.$$

Therefore, $\varphi_2\,\mathrm{Ad}_{Q\otimes I}\,\varphi_2^{-1}=\mathrm{Ad}_{B_2^{-1}(Q\otimes I)B_2}=\mathrm{Ad}_{(P\otimes I)}$, and the respective coefficients of D_2 are

$$(a_{12},a_{22},a_{32},a_{42})^{\mathsf{T}}=(1,0,0,0)^{\mathsf{T}};$$

$B_2^{-1}(I\otimes P)B_2=(\tilde{B}_2\otimes I)^{-1}(I\otimes P)(\tilde{B}_2\otimes I)=(\tilde{B}_2^{-1}\otimes I)(\tilde{B}_2\otimes P)=(\tilde{B}_2^{-1}\tilde{B}_2)\otimes P=I\otimes P$. In this case, $\varphi_2\,\mathrm{Ad}_{I\otimes P}\,\varphi_2^{-1}=\mathrm{Ad}_{B_2^{-1}(I\otimes P)B_2}=\mathrm{Ad}_{(I\otimes P)}$, and the respective coefficients of D_2 are

$$(a_{13},a_{23},a_{33},a_{43})^{\mathsf{T}}=(0,0,1,0)^{\mathsf{T}};$$

$B_2^{-1}(I\otimes Q)B_2=(\tilde{B}_2\otimes I)^{-1}(I\otimes Q)(\tilde{B}_2\otimes I)=(\tilde{B}_2^{-1}\otimes I)(\tilde{B}_2\otimes Q)=(\tilde{B}_2^{-1}\tilde{B}_2)\otimes Q=I\otimes Q$. So lastly, we obtain $\varphi_2\,\mathrm{Ad}_{I\otimes Q}\,\varphi_2^{-1}=\mathrm{Ad}_{B_2^{-1}(I\otimes Q)B_2}=\mathrm{Ad}_{(I\otimes Q)}$, and obviously,

$$(a_{14},a_{24},a_{34},a_{44})^{\mathsf{T}}=(0,0,0,1)^{\mathsf{T}}.$$

Thus, the matrix $C(\varphi_2)$ is equal to

$$C(\varphi_2)=D_2=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}.$$

(3) We define $\varphi_3=\mathrm{Ad}_{B_3}$, where

$$(B_3)_{pq}=\delta_{p_1q_2}\delta_{p_2q_1},\quad p=p_1n+p_2,\quad q=q_1n+q_2,\quad p_1,p_2,q_1,q_2\in\{0,1,\ldots,n-1\}.$$

(One can easily verify by a direct calculation that $B_3^{-1}=B_3$.)

In order to satisfy the relation $C(\varphi_3)=C(\mathrm{Ad}_{B_3})=D_3$, it is sufficient to show that the matrix B_3 fulfills the following equations:

$$B_3^{-1}(P\otimes I)B_3=I\otimes P,\quad B_3^{-1}(I\otimes P)B_3=P\otimes I,$$

$$B_3^{-1}(Q\otimes I)B_3=I\otimes Q,\quad B_3^{-1}(I\otimes Q)B_3=Q\otimes I.$$

In fact, we have found B_3 such that even a more general relation is satisfied,

$$B_3^{-1}(K\otimes L)B_3=L\otimes K\ \text{for any matrices}\ K,L\in\mathbb{C}^{n\times n}. \tag{A2}$$

The matrix elements of B_3 are $\delta_{p_1q_2}\delta_{p_2q_1}$ as introduced above. In order to prove Eq. (A2), it is sufficient to express the (pq)th element of the tensor product $K\otimes L$ as $(K\otimes L)_{pq}=K_{p_1q_1}L_{p_2q_2}$, and proceed by

$$\begin{aligned}[B_3^{-1}(K\otimes L)B_3]_{pq}&=[B_3^{-1}(K\otimes L)B_3]_{(p_1n+p_2)(q_1n+q_2)}\\&=\sum_{r_1,r_2=0}^{n-1}(B_3^{-1})_{(p_1n+p_2)(r_1n+r_2)}[(K\otimes L)B_3]_{(r_1n+r_2)(q_1n+q_2)}\\&=\sum_{r_1,r_2=0}^{n-1}\sum_{s_1,s_2=0}^{n-1}(B_3^{-1})_{(p_1n+p_2)(r_1n+r_2)}(K\otimes L)_{(r_1n+r_2)(s_1n+s_2)}(B_3)_{(s_1n+s_2)(q_1n+q_2)}\\&=\sum_{r_1,r_2=0}^{n-1}\sum_{s_1,s_2=0}^{n-1}\delta_{p_1r_2}\delta_{p_2r_1}K_{r_1s_1}L_{r_2s_2}\delta_{s_1q_2}\delta_{s_2q_1}\\&=K_{p_2q_2}L_{p_1q_1}=L_{p_1q_1}K_{p_2q_2}=(L\otimes K)_{pq}.\end{aligned}$$

(4) We define $\varphi_4=\mathrm{Ad}_{B_4}$, where

$$(B_4)_{pq} = \delta_{(p_1-p_2)q_1}\delta_{p_2q_2}, \quad p = p_1 n + p_2, \quad q = q_1 n + q_2, \quad p_1,p_2,q_1,q_2 \in \{0,1,\ldots,n-1\}.$$

Remember that, with the matrix coefficients p_1, p_2, q_1, q_2, we count modulo n.

We first express the matrices relevant for the proof by means of their pqth elements,

$$(P \otimes I)_{pq} = \omega^{p_1}\delta_{p_1q_1}\delta_{p_2q_2},$$

$$(P \otimes P)_{pq} = \omega^{p_1+p_2}\delta_{p_1q_1}\delta_{p_2q_2},$$

$$(I \otimes P)_{pq} = \omega^{p_2}\delta_{p_1q_1}\delta_{p_2q_2},$$

$$(Q \otimes I)_{pq} = \delta_{(p_1+1)q_1}\delta_{p_2q_2},$$

$$(Q^{-1} \otimes Q)_{pq} = \delta_{p_1(q_1+1)}\delta_{(p_2+1)q_2},$$

$$(I \otimes Q)_{pq} = \delta_{p_1q_1}\delta_{(p_2+1)q_2}.$$

Then, we proceed by showing that the elements of matrix D_4 indeed reflect the action of the automorphism $\varphi_4 = \mathrm{Ad}_{B_4}$,

$$\begin{aligned}
[(P \otimes I)B_4]_{pq} &= \sum_{r_1,r_2=0}^{n-1} (P \otimes I)_{(p_1n+p_2)(r_1n+r_2)}(B_4)_{(r_1n+r_2)(q_1n+q_2)} \\
&= \sum_{r_1,r_2=0}^{n-1} \omega^{p_1}\delta_{p_1r_1}\delta_{p_2r_2}\delta_{(r_1-r_2)q_1}\delta_{r_2q_2} \\
&= \omega^{p_1}\delta_{(p_1-p_2)q_1}\delta_{p_2q_2},
\end{aligned}$$

$$\begin{aligned}
[B_4(P \otimes P)]_{pq} &= \sum_{r_1,r_2=0}^{n-1} (B_4)_{(p_1n+p_2)(r_1n+r_2)}(P \otimes P)_{(r_1n+r_2)(q_1n+q_2)} \\
&= \sum_{r_1,r_2=0}^{n-1} \delta_{(p_1-p_2)r_1}\delta_{p_2r_2}\omega^{r_1+r_2}\delta_{r_1q_1}\delta_{r_2q_2} \\
&= \delta_{(p_1-p_2)q_1}\delta_{p_2q_2}\omega^{q_1+q_2} = \omega^{p_1}\delta_{(p_1-p_2)q_1}\delta_{p_2q_2}.
\end{aligned}$$

Thus we have shown that $(P \otimes I)B_4 = B_4(P \otimes P)$, and consequently, $B_4^{-1}(P \otimes I)B_4 = P \otimes P$, which gives the coefficients

$$(a_{11},a_{21},a_{31},a_{41})^{\mathsf{T}} = (1,0,1,0)^{\mathsf{T}},$$

$$\begin{aligned}
[(Q \otimes I)B_4]_{pq} &= \sum_{r_1,r_2=0}^{n-1} (Q \otimes I)_{(p_1n+p_2)(r_1n+r_2)}(B_4)_{(r_1n+r_2)(q_1n+q_2)} \\
&= \sum_{r_1,r_2=0}^{n-1} \delta_{(p_1+1)r_1}\delta_{p_2r_2}\delta_{(r_1-r_2)q_1}\delta_{r_2q_2} \\
&= \delta_{p_2q_2}\delta_{(p_1+1)(q_1+q_2)},
\end{aligned}$$

$$[B_4(Q\otimes I)]_{pq} = \sum_{r_1,r_2=0}^{n-1} (B_4)_{(p_1n+p_2)(r_1n+r_2)}(Q\otimes I)_{(r_1n+r_2)(q_1n+q_2)}$$
$$= \sum_{r_1,r_2=0}^{n-1} \delta_{(p_1-p_2)r_1}\delta_{p_2r_2}\delta_{(r_1+1)q_1}\delta_{r_2q_2}$$
$$= \delta_{p_2q_2}\delta_{(p_1-p_2)(q_1-1)} = \delta_{p_2q_2}\delta_{(p_1+1)(q_1+q_2)}.$$

Combining the two equations, we obtain $(Q\otimes I)B_4=B_4(Q\otimes I)$, and $B_4^{-1}(Q\otimes I)B_4$. In terms of the matrix coefficients of D_4, it writes as

$$(a_{12},a_{22},a_{32},a_{42})^{\mathsf{T}} = (0,1,0,0)^{\mathsf{T}},$$

.

$$[(I\otimes P)B_4]_{pq} = \sum_{r_1,r_2=0}^{n-1} (I\otimes P)_{(p_1n+p_2)(r_1n+r_2)}(B_4)_{(r_1n+r_2)(q_1n+q_2)}$$
$$= \sum_{r_1,r_2=0}^{n-1} \omega^{p_2}\delta_{p_1r_1}\delta_{p_2r_2}\delta_{(r_1-r_2)q_1}\delta_{r_2q_2}$$
$$= \omega^{p_2}\delta_{(p_1-p_2)q_1}\delta_{p_2q_2},$$

$$[B_4(I\otimes P)]_{pq} = \sum_{r_1,r_2=0}^{n-1} (B_4)_{(p_1n+p_2)(r_1n+r_2)}(I\otimes P)_{(r_1n+r_2)(q_1n+q_2)}$$
$$= \sum_{r_1,r_2=0}^{n-1} \delta_{(p_1-p_2)r_1}\delta_{p_2r_2}\omega^{r_2}\delta_{r_1q_1}\delta_{r_2q_2}$$
$$= \omega^{p_2}\delta_{(p_1-p_2)q_1}\delta_{p_2q_2}.$$

From $(I\otimes P)B_4=B_4(I\otimes P)$ we obtain $B_4^{-1}(I\otimes P)B_4=I\otimes P$, i.e., the matrix $I\otimes P$ remains intact by the action of Ad_{B_4}, which means that

$$(a_{13},a_{23},a_{33},a_{43})^{\mathsf{T}} = (0,0,1,0)^{\mathsf{T}},$$

$$[(I\otimes Q)B_4]_{pq} = \sum_{r_1,r_2=0}^{n-1} (I\otimes Q)_{(p_1n+p_2)(r_1n+r_2)}(B_4)_{(r_1n+r_2)(q_1n+q_2)}$$
$$= \sum_{r_1,r_2=0}^{n-1} \delta_{p_1r_1}\delta_{(p_2+1)r_2}\delta_{(r_1-r_2)q_1}\delta_{r_2q_2}$$
$$= \delta_{(p_2+1)q_2}\delta_{p_1(q_1+q_2)},$$

$$[B_4(Q^{-1}\otimes Q)]_{pq} = \sum_{r_1,r_2=0}^{n-1} (B_4)_{(p_1n+p_2)(r_1n+r_2)}(Q^{-1}\otimes Q)_{(r_1n+r_2)(q_1n+q_2)}$$
$$= \sum_{r_1,r_2=0}^{n-1} \delta_{(p_1-p_2)r_1}\delta_{p_2r_2}\delta_{r_1(q_1+1)}\delta_{(r_2+1)q_2}$$
$$= \delta_{(p_2+1)q_2}\delta_{(p_1-p_2)(q_1+1)}$$

$$= \delta_{(p_2+1)q_2}\delta_{p_1(q_1+q_2)}.$$

Here, we see the action of Ad_{B_4} on the last of the four matrices generating $\mathcal{G}$: $(I\otimes Q)B_4 = B_4(Q^{-1}\otimes Q)$ is equivalent to $B_4^{-1}(I\otimes Q)B_4 = Q^{-1}\otimes Q$. As a result,

$$(a_{14},a_{24},a_{34},a_{44})^{\mathsf{T}} = (0,-1,0,1)^{\mathsf{T}}.$$

Thus, we have shown that

$$C(\varphi_4) = D_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

□

APPENDIX B

Theorem 3.1: *Let n be a prime. Then the four matrices*

$$D_1 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad D_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$D_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \text{and} \quad D_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

generate the group $\mathrm{Sp}(4,\mathbb{F}_n)$.

For a better overview, we first sketch the main framework of the proof, and only afterwards we prove the individual steps in detail.

Remark 3.2: The fact that n is a prime ensures that $\mathbb{Z}_n$ is a field $\mathbb{F}_n$, and consequently that the set $\mathrm{Sp}(4,\mathbb{F}_n)=\{X\in\mathbb{Z}_n^{4\times 4} \mid X^{\mathsf{T}}JX=J\}$, where $J=\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)\oplus\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, is a group.

Remark 3.3: It is a well known fact that, for any integer n, the two matrices $\left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ generate the group $\mathrm{SL}(2,\mathbb{Z}_n)=\{A\in\mathbb{Z}_n^{2\times 2} \mid \det A=1\}$ (see Ref. 5).

Remark 3.4: It is easy to verify that D_1, D_2, D_3, and D_4 belong to $\mathrm{Sp}(4,\mathbb{F}_n)$.

For a group $\mathcal{K}$ and any group elements $k_1,k_2,\ldots,k_r\in\mathcal{K}$, we denote by $\langle k_1,\ldots,k_r\rangle$ the smallest subgroup of $\mathcal{K}$ containing $k_1,\ldots,k_r$.

Under the framework of this notation and Remark 3.3, we have

$$\langle D_1,D_2\rangle = \left\{ \begin{pmatrix} A & 0 \\ 0 & I_2 \end{pmatrix} \middle| A \in \mathrm{Sl}(2,\mathbb{Z}_n) \right\},$$

$$\langle D_1,D_2,D_3\rangle = \left\{ \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}, \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix} \middle| A,B \in \mathrm{Sl}(2,\mathbb{Z}_n) \right\}.$$

Our aim is to prove that $\langle D_1,D_2,D_3,D_4\rangle=\mathrm{Sp}(4,\mathbb{Z}_n)$. For this purpose, it is enough to verify statements of the next two steps.

Step 1: Let us note $\mathcal{H}:=\langle D_1,D_2,D_3\rangle$ and $M\in\mathrm{Sp}(4,\mathbb{F}_n)$, $M\notin\mathcal{H}$. There exist $k\in\mathbb{Z}_n$ and matrices $G_1,G_2\in\mathcal{H}$ such that $G_1MG_2=S(k)$, where

$$S(k) := \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & k & 0 & 1-k \\ k-1 & 0 & k & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}.$$

Step 2: The matrix $S(k)$ belongs to $\langle D_1, D_2, D_3, D_4 \rangle$ for any $k \in \mathbb{Z}_n$.

Lemma 3.5: Let n be a prime and $A = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathbb{Z}_n^{2\times 2}$, $A \neq \left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$. *Then there exist*

(i) *matrices* $B, C \in \mathrm{SL}(2, \mathbb{Z}_n)$ *such that* $BAC = \left(\begin{smallmatrix} 1 & 0 \\ 0 & k \end{smallmatrix}\right)$, *where* $k = \det A$;

(ii) *matrices* $D, E \in \mathrm{SL}(2, \mathbb{Z}_n)$ *such that* $DAE = \left(\begin{smallmatrix} k & 0 \\ 0 & 1 \end{smallmatrix}\right)$, *where* $k = \det A$.

Moreover, if $\det A = k \neq 0$, *then we have* $C = E = I_2$.

Proof: (a) First, we consider the case $\det A = k \neq 0$.

(i) We assume, without loss of generality, that $a \neq 0$ [otherwise, we would consider matrix $A\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right) = \left(\begin{smallmatrix} -b & a \\ -d & c \end{smallmatrix}\right) = \left(\begin{smallmatrix} -b & 0 \\ -d & c \end{smallmatrix}\right)$, as $b \neq 0$ when $a = 0$]. The desired matrices B and C are as follows:

$$B = B_3 B_2 B_1 = \begin{pmatrix} 1 & -ba^{-1}k^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -ac & 1 \end{pmatrix} \begin{pmatrix} a^{-1} & 0 \\ 0 & a \end{pmatrix},$$

$$C = I_2,$$

$$BAC = B_3 B_2 \begin{pmatrix} a^{-1} & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = B_3 \begin{pmatrix} 1 & 0 \\ -ac & 1 \end{pmatrix} \begin{pmatrix} 1 & a^{-1}b \\ ac & ad \end{pmatrix}$$
$$= \begin{pmatrix} 1 & -ba^{-1}k^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & a^{-1}b \\ 0 & k \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & k \end{pmatrix}.$$

(ii) Alternatively, we multiply the result by one more matrix, in order to obtain the desired matrix $\left(\begin{smallmatrix} k & 0 \\ 0 & 1 \end{smallmatrix}\right)$,

$$D = \begin{pmatrix} k & 0 \\ 0 & k^{-1} \end{pmatrix} B,$$

$$E = C = I_2,$$

$$DAE = \begin{pmatrix} k & 0 \\ 0 & k^{-1} \end{pmatrix} BAC = \begin{pmatrix} k & 0 \\ 0 & k^{-1} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & k \end{pmatrix} = \begin{pmatrix} k & 0 \\ 0 & 1 \end{pmatrix}.$$

(b) Second, we have the situation $\det A = k = 0$, but still $A \neq 0$.

(i) If $a \neq 0$, we set

$$B = B_2 B_1,$$

$$C = \begin{pmatrix} 1 & -a^{-1}b \\ 0 & 1 \end{pmatrix},$$

$$BAC = B_2\begin{pmatrix} a^{-1} & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix}C = \begin{pmatrix} 1 & 0 \\ -ac & 1 \end{pmatrix}\begin{pmatrix} 1 & a^{-1}b \\ ac & ad \end{pmatrix}C$$
$$= \begin{pmatrix} 1 & a^{-1}b \\ 0 & k \end{pmatrix}\begin{pmatrix} 1 & -a^{-1}b \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & k \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

If $a=0$, then at least one of the remaining three matrix elements is nonzero. Thus, we can analogously work with one of the matrices

$$A\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}A, \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}A\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{B1}$$

namely with the one whose element in the first row and first column is nonzero.

(ii) Again, without loss of generality, we assume that $d \neq 0$ [otherwise we would transform A into one of the three matrices given in (B1); one of which would have a nonzero element in its second row and second column]. We set

$$D = D_2D_1 = \begin{pmatrix} 1 & -bd \\ 0 & 1 \end{pmatrix}\begin{pmatrix} d & 0 \\ 0 & d^{-1} \end{pmatrix},$$

$$E = \begin{pmatrix} 1 & 0 \\ -cd^{-1} & 1 \end{pmatrix},$$

$$DAE = D_2\begin{pmatrix} d & 0 \\ 0 & d^{-1} \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix}E = \begin{pmatrix} 1 & -bd \\ 0 & 1 \end{pmatrix}\begin{pmatrix} da & db \\ d^{-1}c & 1 \end{pmatrix}E$$
$$= \begin{pmatrix} k & 0 \\ d^{-1}c & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -cd^{-1} & 1 \end{pmatrix} = \begin{pmatrix} k & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

□

Proof of Step 1: Let us express a matrix $M \in \mathrm{Sp}(4,\mathbb{F}_n)$ in blocks:

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, \quad \text{where } M_{ij} \in \mathbb{Z}_n^{2\times 2}.$$

The equality (17) means that $\det M_{12} + \det M_{22} = 1$. We denote $\det M_{22} = k$, and consequently $\det M_{12} = 1-k$.

(i) Let us assume that $k \neq 0$. We take matrices $B, C \in \mathrm{SL}(2,\mathbb{Z}_n)$ as described in Lemma 3.5, so as to obtain $BM_{12}C = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1-k \end{smallmatrix}\right)$. Afterwards, we apply Lemma 3.5 on matrix $M_{22}C$, whose determinant is $\det(M_{22}C) = (\det M_{22})(\det C) = k \cdot 1 = k \neq 0$. Thus, we find $D \in \mathrm{SL}(2,\mathbb{Z}_n)$ such that $DM_{22}C = \left(\begin{smallmatrix} k & 0 \\ 0 & 1 \end{smallmatrix}\right)$. At this moment, we are able to transform M by means of matrices $F_1 = \left(\begin{smallmatrix} B & 0 \\ 0 & D \end{smallmatrix}\right)$, $F_2 = \left(\begin{smallmatrix} I_2 & 0 \\ 0 & C \end{smallmatrix}\right)$ into the following:

$$F_1MF_2 = \begin{pmatrix} B & 0 \\ 0 & D \end{pmatrix}\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} I_2 & 0 \\ 0 & C \end{pmatrix} = \begin{pmatrix} BM_{11} & BM_{12} \\ DM_{21} & DM_{22} \end{pmatrix}\begin{pmatrix} I_2 & 0 \\ 0 & C \end{pmatrix}$$
$$= \begin{pmatrix} BM_{11} & BM_{12}C \\ DM_{21} & DM_{22}C \end{pmatrix} = \begin{pmatrix} \tilde{m}_{11} & \tilde{m}_{12} & 1 & 0 \\ \tilde{m}_{21} & \tilde{m}_{22} & 0 & 1-k \\ \tilde{m}_{31} & \tilde{m}_{32} & k & 0 \\ \tilde{m}_{41} & \tilde{m}_{42} & 0 & 1 \end{pmatrix} = \tilde{M},$$

where we denote matrices $BM_{11}=\left(\begin{smallmatrix}\tilde{m}_{11} & \tilde{m}_{12}\\ \tilde{m}_{21} & \tilde{m}_{22}\end{smallmatrix}\right)$ and $DM_{21}=\left(\begin{smallmatrix}\tilde{m}_{31} & \tilde{m}_{32}\\ \tilde{m}_{41} & \tilde{m}_{42}\end{smallmatrix}\right)$ by $\tilde{M}_{11},\tilde{M}_{21}$, respectively. As the matrix $\tilde{M}$ is a multiple of F_1, F_2, and M, which all belong to $\mathrm{Sp}(4,\mathbb{F}_n)$, then also $\tilde{M}$ is an element of $\mathrm{Sp}(4,\mathbb{F}_n)$, and so its elements fulfill equations (18)–(21),

$$0=-\tilde{m}_{21}-k\tilde{m}_{41} \pmod{n},$$

$$0=(1-k)\tilde{m}_{11}+\tilde{m}_{31} \pmod{n},$$

$$0=-\tilde{m}_{22}-k\tilde{m}_{42} \pmod{n},$$

$$0=(1-k)\tilde{m}_{12}+\tilde{m}_{32} \pmod{n}.$$

These relations ensure that we can transform $\tilde{M}$ into $S(k)$ by means of matrix $N=\left(\begin{smallmatrix}\tilde{m}_{11} & \tilde{m}_{12}\\ -\tilde{m}_{41} & -\tilde{m}_{42}\end{smallmatrix}\right)$,

$$\begin{pmatrix}1 & 0\\ 0 & k\end{pmatrix}N=\begin{pmatrix}\tilde{m}_{11} & \tilde{m}_{12}\\ -k\tilde{m}_{41} & -k\tilde{m}_{42}\end{pmatrix}=\begin{pmatrix}\tilde{m}_{11} & \tilde{m}_{12}\\ \tilde{m}_{21} & \tilde{m}_{22}\end{pmatrix}=\tilde{M}_{11},$$

$$\begin{pmatrix}k-1 & 0\\ 0 & -1\end{pmatrix}N=\begin{pmatrix}(k-1)\tilde{m}_{11} & (k-1)\tilde{m}_{12}\\ \tilde{m}_{41} & \tilde{m}_{42}\end{pmatrix}=\begin{pmatrix}\tilde{m}_{31} & \tilde{m}_{32}\\ \tilde{m}_{41} & \tilde{m}_{42}\end{pmatrix}=\tilde{M}_{21}.$$

Therefore, $\tilde{M}_{11}N^{-1}=\left(\begin{smallmatrix}1 & 0\\ 0 & k\end{smallmatrix}\right)$, $\tilde{M}_{21}N^{-1}=\left(\begin{smallmatrix}k-1 & 0\\ 0 & -1\end{smallmatrix}\right)$, and consequently

$$\tilde{M}\begin{pmatrix}N^{-1} & 0\\ 0 & I_2\end{pmatrix}=\begin{pmatrix}\tilde{m}_{11} & \tilde{m}_{12} & 1 & 0\\ \tilde{m}_{21} & \tilde{m}_{22} & 0 & 1-k\\ \tilde{m}_{31} & \tilde{m}_{32} & k & 0\\ \tilde{m}_{41} & \tilde{m}_{42} & 0 & 1\end{pmatrix}\begin{pmatrix}N^{-1} & 0\\ 0 & I_2\end{pmatrix}=S(k).$$

As an element of $\mathrm{Sp}(4,\mathbb{F}_n)$, the matrix $\tilde{M}$ also fulfills Eq. (16), which implies that $\det\tilde{M}_{11}+\det\tilde{M}_{21}=1=k\det N+(1-k)\det N=\det N$, and thus $N\in\mathrm{SL}(2,\mathbb{Z}_n)$. Hence, we have found the desired matrices $G_1=F_1=B\oplus D$, $G_2=F_2(N^{-1}\oplus I_2)=N^{-1}\oplus C$, transforming M into $G_1MG_2=S(k)$.

(ii) The case when $k=0$, we treat as follows. First, we find D, $E\in\mathrm{SL}(2,\mathbb{Z}_n)$ such that $DM_{22}E=\left(\begin{smallmatrix}k & 0\\ 0 & 1\end{smallmatrix}\right)$ and $B\in\mathrm{SL}(2,\mathbb{Z}_n)$ such that $BM_{21}E=\left(\begin{smallmatrix}1 & 0\\ 0 & 1-k\end{smallmatrix}\right)$, according to Lemma 3.5. Analogously to the case $k\neq 0$, we set $G_1=F_1=B\oplus D$, $G_2=F_2(N^{-1}\otimes I_2)=N^{-1}\oplus E$, and we reach the result $G_1MG_2=S(k)$.

Proof of Step 2: We need to express each matrix $S(k)$ as an element of $\langle D_1,D_2,D_3,D_4\rangle$. We begin by showing (by induction) that

$$D_4^j=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & -j\\ j & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & -1\\ 1 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & -j+1\\ j-1 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}=D_4D_4^{j-1}.$$

We make use of the fact that $J=\left(\begin{smallmatrix}0 & 1\\ -1 & 0\end{smallmatrix}\right)\oplus\left(\begin{smallmatrix}0 & 1\\ -1 & 0\end{smallmatrix}\right)\in\mathcal{H}$, $J^{\mathsf{T}}\in\mathcal{H}$, and $D_4^{\mathsf{T}}=D_3D_4D_3\in\mathrm{Sp}(4,\mathbb{F}_n)$ (this can be verified by a simple matrix multiplication); and we generate $S(k)$ from D_4 and elements from $\mathcal{H}$,

$$J^{\mathsf{T}}(D_4^{1-k})^{\mathsf{T}}JD_4^{\mathsf{T}} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1-k & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & k-1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 1-k & 0 \\ 0 & 1-k & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & k & 0 & 1-k \\ k-1 & 0 & k & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix} = S(k).$$

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Standard and nonstandard extensions of Lie algebras

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We study the problem of quadruple extensions of simple Lie algebras. We find that, adding a new simple root α_{+4}, it is not possible to have an extended Kac-Moody algebra described by a Dynkin-Kac diagram with simple links and no loops between the dots, while it is possible if α_{+4} is a Borcherds imaginary simple root. We also comment on the root lattices of these new algebras. The folding procedure is applied to the simply laced triple extended Lie algebras, obtaining all the non-simply laced ones. Nonstandard extension procedures for a class of Lie algebras are proposed. It is shown that the two-extensions of E_8, with a dot simply linked to the Dynkin-Kac diagram of E_9, are rank 10 subalgebras of E_{10}. Finally the simple root systems of a set of rank 11 subalgebras of E_{11}, containing as sub-algebra E_{10}, are explicitly written. © *2006 American Institute of Physics.*
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I. INTRODUCTION

It has been conjectured by Peter West[1] that the still elusive M-Theory possesses a rank 11 Kac-Moody symmetry algebra, called E_{11}, that is the triple extended or very extended E_8 algebra. Very extended algebras can be defined for any finite-dimensional Lie algebra $\mathcal{G}$.[2] So it is tempting to argue that other theories, which are associated with other triple extensions of Lie algebras, may exist. Indeed the same analysis was applied to a conjectured extension of the eleven dimensional supergravity.[3,4] More generally, it has been proposed that the closed bosonic string in D dimensions and type I supergravity and pure gravity theories exhibit a Kac-Moody symmetry algebra, respectively, identified as the triple extensions of the D and A series.[5–7] This conjecture is supported by dimensional reduction and by the so-called cosmological billiards.[8–10] Then it is natural to look for a more general symmetry algebra which can include all these Kac-Moody algebras as particular cases. So we address the question of how to go beyond $\mathcal{G}^{+++}$ algebras; we find that the adjoint of a new simple root α_{+4} introduces multiple links and loops in the structure of the 4-extended algebra, if α_{+4} is an ordinary Kac-Moody simple root, while the "simple-links" structure is preserved if we allow α_{+4} is a Borcherds (imaginary) simple root.

The (first) extension of a finite-dimensional Lie algebra is the construction of (untwisted) affine Kac-Moody algebras, which are obtained adding to the simple roots of any finite-dimensional Lie algebra $\mathcal{G}$ a root α_0 that is the opposite of the highest root (h.r.) plus a light-like vector k_+, in order to make α_0 linearly independent from the system of the simple roots of $\mathcal{G}$, keeping unchanged its length, and are denoted as $\mathcal{G}^+$ or $\hat{\mathcal{G}}$ or $\mathcal{G}^1$. This procedure for the simply laced algebras of the D_N and E_N series can be formulated as the addition to the simple root system of $\mathcal{G}$ of another root α_0, that is the opposite of the unique fundamental weight of length 2, which is in the root lattice of the algebra, plus a light-like vector k_+. The light-like vector can be considered to belong to a 2-dim. Lorentzian lattice, usually denoted $\mathrm{II}^{1,1}$, and the double extension or overextension of $\mathcal{G}$, denoted $\mathcal{G}^{++}$, is obtained by adding a new simple root, of length 2, which

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is formed by the sum of the two light like vectors $k_{\pm}$, $(k_+,k_-)=1$, spanning $\mathrm{II}^{1,1}$. The triple extended or very extended $\mathcal{G}$, denoted $\mathcal{G}^{+++}$, is obtained adding a new simple root of length 2, which belongs to a new copy of the lattice $\mathrm{II}^{1,1}$, plus k_+. In this way, an indefinite Kac-Moody or Lorentzian algebra of rank $r+3$ is obtained whose roots belong to a Lorentzian lattice of dimension $r+4$, so it is natural to wonder if an indefinite Kac-Moody algebra of rank $r+4$ can be obtained by a further extension. Moreover, let us notice that in the lattice $\mathrm{II}^{1,1}$ vectors of negative length do exist (see Appendix A). From this remark one can make an extension of $\mathcal{G}$ adding a new root, that is the opposite of any fundamental weight, that can be written as linear combination with integer coefficients of the simple roots of the algebra, plus a suitable element of the lattice $\mathrm{II}^{1,1}$ in order to have an independent new simple root of length 2. This construction will be discussed in the following. It has been pointed out in Ref. 11 that the structure of subalgebras of hyperbolic Kac-Moody, in general of two-extended (overextended) Lie algebras, is very rich and surprising. Some of the results of that paper can be generalized to more general extensions and we comment on this point in the following. This paper is organized as follows. In Sec. II, to make the paper self-contained, we recall the well-known construction of the three-extended Lie algebras. We show that the four-extended algebras are described by Dynkin-Kac diagrams with loops and multiple links (so their structure is quite different from that of the one-, two-, and three-extended algebras). In particular, we show that we cannot have a situation in which the new (fourth) simple root α_{+4} is simply linked to α_{+3}, unless we let α_{+4} be a Borcherds simple root (with squared norm zero or negative). So we also study the possibility to have a Borcherds extension of the $\mathcal{G}^{+++}$ algebras, but this extension has sense only when the algebra $\mathcal{G}$ is simply-laced (see Appendix B for the definition of a Borcherds algebra[12]). In Sec. III, we show that all the nonsimply laced three-extended Lie algebras can be obtained by *folding* the simply-laced ones. In Sec. IV, we discuss nonstandard extension procedures, discussing in detail a few examples which may be of physical interest. In Sec. V, we show that the algebras obtained by some general nonstandard procedure, but not for all the procedures, are indeed subalgebras, of the same rank, of the standard triple extended algebras. In particular we prove that any nonstandard one-extension of E_9, with a root simply linked to a simple roots of E_9, is a subalgebra of E_{10}. The simple root systems of a set of rank 11 subalgebras of E_{11}, containing as subalgebra E_{10}, are explicitly written. Finally we present a few conclusions and perspectives. To make the paper self-contained two very short Appendices are added to recall the main features of the 2-dim Lorentzian lattice $\mathrm{II}^{1,1}$ and of Borcherds algebras.

II. ON EXTENSIONS OF $\mathcal{G}^{+++}$ ALGEBRAS

An excellent discussion of the mechanism of standard extensions of Lie algebras can be found in Ref. 2, here we briefly recall the essential points, mainly to introduce the notation and to make the paper self-consistent. [Let us remember that the standard extension for G_2 does not work, because G_2 is the only finite Lie algebra for which it is not possible to normalize the highest root θ such that $(\theta,\theta)=2$. However, it's possible to extend G_2 with the following choice of the extended roots: $\alpha_{+1}=k_+-\theta$, $\alpha_{+2}=-(k_++3k_-)$ and $\alpha_{+3}=-(l_++3l_-)+k_+$. Anyway, G_2^{+++} can be obtained by folding D_4^{+++} (see Sec. III).] Let $\mathcal{G}$ be a simple Lie algebra of rank r, with simple root system α_i $(i=1,\ldots,r)$ and root lattice $\Lambda_{\mathcal{G}}=\oplus_{i=1}^{r}\mathbb{Z}\alpha_i$ (for the roots and fundamental weights we use the notation of Ref. 13). Let us consider also two copies of the lattice $\mathrm{II}^{1,1}$, which we indicate with $\mathrm{II}^{1,1}_{k_\pm}$ and $\mathrm{II}^{1,1}_{l_\pm}$. In the following, we consider indefinite Kac-Moody algebras with root lattice included in the direct sum $\Lambda_{\mathcal{G}}\oplus\mathrm{II}^{1,1}_{k_\pm}\oplus\mathrm{II}^{1,1}_{l_\pm}$.

Let $\mathcal{G}^+$ be the extended Lie algebra (or affine Kac-Moody algebra), with simple root system $\{\alpha_i,\alpha_0\equiv\alpha_{r+1}\equiv\alpha_{+1}=-\mathrm{h.r.}+k_+\}$ $(i=1,\ldots,r)$, where h.r. denotes the highest root of $\mathcal{G}$ (which is $\theta\equiv\mathrm{h.r.}=\Sigma_{i=1}^{r}a_i\alpha_i$ where a_i are Kac marks, see Ref. 13), and

$$(k_+,k_+)=(k_+,\alpha_i)=0. \tag{1}$$

Let $\mathcal{G}^{++}$ be the double extended or overextended Lie algebra (actually a Lorentzian Kac-Moody algebra), with simple root system $[\alpha_j,\alpha_{r+2}\equiv\alpha_{+2}=-(k_++k_-)\}$ $(j=1,\ldots,r+1)$, where

$$(k_+,k_-)=1, \quad (k_-,k_-)=(k_-,\alpha_i)=0. \tag{2}$$

Let us note that the root lattice of $\mathcal{G}^+$ is properly contained in the direct sum $\Lambda_{\mathcal{G}}\oplus \mathrm{II}^{1,1}_{k_\pm}$, whereas the root lattice of $\mathcal{G}^{++}$ coincides with the direct sum. To see this, it is enough to obtain k_+ and k_- from the other roots α_j $(j=1,\ldots,r+2)$. In fact,

$$k_+=\theta+\alpha_{+1}=\sum_{i=1}^{r} a_i\alpha_i+\alpha_{+1}, \tag{3}$$

$$k_-=-k_+-\alpha_{+2}=-\theta-\alpha_{+1}-\alpha_{+2} \tag{4}$$

so k_+ and k_- are linear combinations (with integer coefficients) of the $r+2$ simple roots of the $\mathcal{G}^{++}$ algebra. This means that with a change of basis (in the lattice), we can pass from $\{\alpha_j\ (j=1,\ldots,r+2)\}$ to $\{\alpha_i\ (i=1,\ldots,r);k_+,k_-\}$, that is the lattice $\Lambda_{\mathcal{G}}\oplus\mathbb{Z}\alpha_{+1}\oplus\mathbb{Z}\alpha_{+2}$ coincides with $\Lambda_{\mathcal{G}}\oplus \mathrm{II}^{1,1}_{k_\pm}$.

Now, let $\mathcal{G}^{+++}$ be the triple extended Lie algebra (still a Lorentzian Kac-Moody algebra), with simple root system $\{\alpha_k,\alpha_{r+3}\equiv\alpha_{+3}=-(l_++l_-)+k_+\}$ $(k=1,\ldots,r+2)$, where

$$(\alpha_i,l_\pm)=(k_\pm,l_\pm)=(k_\mp,l_\pm)=(l_\pm,l_\pm)=0, \quad (l_\mp,l_\pm)=1. \tag{5}$$

In this way starting from the r-dim. Euclidean lattice $\Lambda_{\mathcal{G}}$, we have build up a $(r+4)$-dim. Lorentzian lattice $\mathbf{\Lambda}\equiv\Lambda_{\mathcal{G}}\oplus \mathrm{II}^{1,1}_{k_\pm}\oplus \mathrm{II}^{1,1}_{l_\pm}$, with signature $+\ldots+--$ ($r+2$ plus signs). The simple root system of $\mathcal{G}^{+++}$ clearly spans a $(r+3)$-dim sublattice of $\mathbf{\Lambda}$ (because α_{+3} only takes the direction l_++l_- in the second lattice $\mathrm{II}^{1,1}$, so the orthogonal direction is lacking), so it is natural to wonder if it is possible to extend further the $\mathcal{G}^{+++}$ algebra and *fill in* $\mathbf{\Lambda}$.

Motivated by the previous steps, one would just add another node at the Dynkin diagram of a $\mathcal{G}^{+++}$ algebra, with a simple link to the root α_{+3}; in this way, as it happens in the case of the $\mathcal{G}^{++}$ algebra, one would expect that this construction fills the root lattice $\Lambda_{\mathcal{G}}\oplus \mathrm{II}^{1,1}_{k_\pm}\oplus \mathrm{II}^{1,1}_{l_\pm}$. In the following, we show that actually this is not the case. (Our discussion does not account for the introduction of another lattice $\mathrm{II}^{1,1}$, which solves the question only partially, because it moves the problem to fill this new lattice.)

As we already mentioned, the simple root α_{+3} contains only the combination l_++l_-, so if we want to span completely also the second lattice $\mathrm{II}^{1,1}$, we need a new simple root α_{+4} which allows us to obtain l_+ and l_- separately. In this way, we are guaranteed that the root lattice of the new algebra also contains all vectors which are integer multiples of l_+ or l_-, so this lattice coincides with $\mathbf{\Lambda}$. In the following, let us choose for α_{+4} the more general form:

$$\alpha_{+4}\equiv al_++bl_-+ck_++dk_-, \tag{6}$$

which allows us to make many considerations about the possible extensions of the $\mathcal{G}^{+++}$ algebras. (As it happens also for α_{+2} and α_{+3}, here we do not consider the situation in which α_{+4} is also linked with the simple roots α_i of $\mathcal{G}$. However this simple choice does not really change the conclusions of our analysis.) First of all, let us obtain the expression for l_+ and l_- using the definition of α_{+3} and α_{+4}:

$$(a-b)l_+=(d-b-c)\theta+(d-b-c)\alpha_{+1}+d\alpha_{+2}+b\alpha_{+3}+\alpha_{+4}, \tag{7}$$

$$(b-a)l_-=(d-a-c)\theta+(d-a-c)\alpha_{+1}+d\alpha_{+2}+a\alpha_{+3}+\alpha_{+4}. \tag{8}$$

We see then that it is possible to obtain l_+ and l_- as linear combinations (over $\mathbb{Z}$) of the simple roots if and only if $|a-b|=1$. Only in this case we are guaranteed that we actually catch all the vectors in the lattice $\mathrm{II}^{1,1}_{l_\pm}$. With this in mind, let us find the other relations a,b,c,d have to satisfy, that is let us compute the norm of α_{+4} and the scalar products with the other simple roots (here we write only the relevant elements a_{ij} of the generalized Cartan matrix):

$$(\alpha_{+4})^2 = 2(ab + cd), \tag{9}$$

$$a_{+4,+1} \equiv 2\frac{(\alpha_{+4}, \alpha_{+1})}{(\alpha_{+4}, \alpha_{+4})} = \frac{d}{ab + cd}, \quad a_{+4,+2} \equiv 2\frac{(\alpha_{+4}, \alpha_{+2})}{(\alpha_{+4}, \alpha_{+4})} = \frac{-c - d}{ab + cd}, \tag{10}$$

$$a_{+4,+3} \equiv 2\frac{(\alpha_{+4}, \alpha_{+3})}{(\alpha_{+4}, \alpha_{+4})} = \frac{d - a - b}{ab + cd}. \tag{11}$$

Let us limit ourselves to consider the case $(\alpha_{+4})^2=2$ (to look for a "natural extension") and let all four coefficients be different from zero; we must have

$$ab + cd = 1, \tag{12}$$

$$d < 0, \quad c \geqslant -d > 0, \quad d \leqslant a + b, \tag{13}$$

because only with these constraints α_{+4} is an acceptable simple root (à la Kac-Moody). In particular, the product cd must be negative, and as Eq. (12) holds, the product ab must be positive (actually, it must be at least 2), that is a and b must have the same sign. A simple solution, pointed out to us by C. Helfgott, to Eqs. (12) and (13) is the following:

$$a = 2, \quad b = 1, \quad c = 1, \quad d = -1, \tag{14}$$

where α_{+4} has norm 2 and the scalar products are $(\alpha_{+4}, \alpha_{+1})=-1$, $(\alpha_{+4}, \alpha_{+2})=0$ and $(\alpha_{+4}, \alpha_{+3})=-4$. Furthermore, this solution verifies also the condition $a-b=1$, so its root lattice is precisely $\mathbf{\Lambda}$, but it presents one loop and a multiple link with the (last) root α_{+3}, so its structure is very different from the other previous extensions. [A. Kleinschmidt suggested another solution to us $\alpha_{+4}=\alpha+3k_+-2k_--2l_+-3l_-$ in which α_{+4} is also linked to the only simple root α of su(2); this solution too presents loops and multiple links.] This situation is common to all solutions of Eqs. (12) and (13): it is not possible (we stress: without adding any $\mathrm{II}^{1,1}$ or different lattice) to have a simple link with α_{+4} and no loops (for example the equation $d-a-b=-1$ is never satisfied if a and b are both positive, because d is at least -1, and goes in contradiction with the other relations if a and b are both negative). In this sense, the procedure of standard extension stops at the third step ($\mathcal{G}^{+++}$).

It is clear that there exist infinite solutions to Eqs. (12) and (13) [for example, it is enough to take a, b both positive, $d=-1$ and an opportune value of c to satisfy Eq. (12) and the second equation of Eq. (13)], but only those with $|a-b|=1$ have the property that their root lattice coincides with $\mathbf{\Lambda}$. We can also try (in α_{+4}) to put one coefficient equal to zero and to explore more specific cases. An investigation, case by case, shows that:

- $d=0$: the scalar products imply $ab=1$ and $a+b>0$, that is $a=b=1$, but the case $a=b$ is not acceptable because, in this case, α_{+4} is a linear combination of the other simple roots.
- $c=0$: the scalar products with α_{+1} and α_{+2} are, respectively, proportional to d and $-d$, so one of the two is positive and has the wrong sign, or $d=0$ and then α_{+4} is a linear combination of the other simple roots.
- $a=0$: this case implies $c=-1$, but then $d=-1$ too and the scalar product with α_{+2} is positive.
- $b=0$: it has the same problem as the case $a=0$.

If we put equal to zero two coefficients, the only possibility is to have $c=d=0$ (we cannot take equal to zero a coefficient of l_+ or l_- and a coefficient of k_+ or k_-, because α_{+4} would have vanishing norm), but in this case, as already discussed, we have problems.

So far, we have seen that it is never possible to add a (Kac-Moody) simple root in order to have a simple link with α_{+3}; besides this, the possible solutions which span the whole lattice $\mathbf{\Lambda}$ are

restricted to the condition $|a-b|=1$. Yet, if we abandon the condition that α_{+4} is a Kac-Moody simple root and let it be a Borcherds (imaginary) simple root, the situation changes. In fact, we can easily find an imaginary root of the kind:

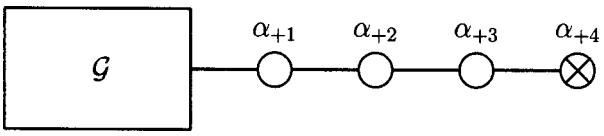
$$\alpha_{+4} = al_+ + bl_-, \tag{15}$$

which has scalar product equal to -1 with α_{+3}: it is only necessary that $b=1-a$, that is $\alpha_{+4}=al_+ +(1-a)l_-$, with norm $2a(1-a)$. Then if $a=0$ or $a=1$, α_{+4} has norm zero, in all the other cases its norm is negative, that is α_{+4} is a good Borcherds simple root. If we want to fill in $\mathbf{\Lambda}$ with the introduction of a Borcherds simple root, we have always to fulfill the condition $|a-b|=1$ (this condition is independent from the norm of α_{+4}), but now it is possible to have both $(\alpha_{+4},\alpha_{+3})=-1$ and, at the same time, to span the whole lattice $\mathbf{\Lambda}$. In fact the values $a=1$, $b=0$ (and vice versa $a=0$, $b=1$), which correspond to $\alpha_{+4}=l_+$ ($\alpha_{+4}=l_-$), are the only ones which allow one to have

$$\Lambda_{\text{roots}}(\mathcal{BG}^{+++}) \equiv \Lambda_{\text{roots}}(\mathcal{G}^{++}) \oplus \text{II}^{1,1}_{l_\pm} = \mathbf{\Lambda}, \tag{16}$$

$$(\alpha_{+4},\alpha_{+3}) = -1, \tag{17}$$

as opposite to the Kac-Moody case, where, as we already said, it is never possible to satisfy Eq. (17) and only some solutions allow one to fill in $\mathbf{\Lambda}$ (we have called $\mathcal{BG}^{+++}$ the Borcherds extension of $\mathcal{G}^{+++}$ corresponding to $\alpha_{+4}=l_+$ or $\alpha_{+4}=l_-$). Denoting by a crossed dot the Borcherds simple root α_{+4}, we can draw the Dynkin diagram of this Borcherds algebra in the following way:



Actually, this construction makes sense if $\mathcal{G}$ is simply laced, because otherwise the Cartan matrix is not well-defined. In fact, if α_{+4} is an imaginary (isotropic) root, we cannot define the extended Cartan matrix as $2(\alpha_i,\alpha_j)/(\alpha_i,\alpha_i)$ for all α_i because $\alpha_{+4}^2=0$. We have the same problem if we add an imaginary simple root with negative squared norm (as previously recalled, in $\text{II}^{1,1}$ there are infinite vectors whose squared norm is negative), because we shall have positive elements out of the principal diagonal. The solution is then to consider a $\mathcal{G}$ simply laced and define the extended Cartan matrix by the scalar products between all the simple roots: $b_{i,j}:=(\alpha_i,\alpha_j)$. So, while the extension of $\mathcal{G}$ is possible up to $\mathcal{G}^{+++}$ for any finite $\mathcal{G}$, in the case of a Borcherds extension it is necessary to choose for $\mathcal{G}$ a simply laced algebra (in fact, a Borcherds algebra is defined only on a symmetric Cartan matrix). To summarize our result, we have proven the following.

Proposition 1: The extension of $\mathcal{G}^{+++}$ algebra, whose simple root system spans completely $\mathbf{\Lambda}$ and whose Dynkin-Kac diagram has no loops and only simple links between the dots, is the Borcherds algebra $\mathcal{BG}^{+++}$ (with $\mathcal{G}$ simply laced).

The particular solution $a=1$, $b=0$ (or vice versa) looks like the same construction of $\mathcal{G}^+$ and $\mathcal{G}^{++}$, as the role of $k_\pm$ is now played by $l_\pm$, with the difference that α_{+1} contains also a root of a simple Lie algebra, while α_{+4} does not. This observation suggests that it is possible to fuse together two (finite) simple Lie algebras, let's say $\mathcal{G}$ and $\mathcal{G}'$, adding the highest root θ' of $\mathcal{G}'$ to α_{+4}. In this way, $\alpha'_{+4}\equiv\alpha_{+4}-\theta'$ is again a Kac-Moody simple root, indeed the affine root of $\mathcal{G}'^{+}$. Anyway, we do not insist on this point, because there are many possible ways to fuse together two (or more) finite dimensional simple Lie algebras (with or without the introduction of intermediate Kac-Moody or Borcherds algebras).

Remark: In this section, we have seen that triple extended Lie algebras $\mathcal{G}^{+++}$ have their root lattice properly included in $\mathbf{\Lambda}=\Lambda_{\mathcal{G}}\oplus\text{II}^{1,1}\oplus\text{II}^{1,1}$ (in particular, their root lattice is Lorentzian with just one negative eigenvalue). Among the four-extensions we considered in this section, we have shown that there are many algebras (of Kac-Moody or generalized Kac-Moody type) whose root

lattice coincides with $\mathbf{\Lambda}$, which is Lorentzian in a more general sense (it has two negative eigenvalues). These seem to be the first algebras obtained in literature with this kind of lattice, together with some similar algebras studied by Harvey and Moore in Refs. 14 and 15 (strictly speaking, their algebras are not Borcherds algebras, because they could not satisfy some grading conditions in the characterization of generalized Kac-Moody algebras, while our Borcherds algebras are *true* Borcherds algebras because we have constructed them from an acceptable generalized Cartan matrix). Our result is not in contrast with the statement of Ref. 16, according to which algebras of physical states, whose root lattices are of the kind $\Gamma^{p,q}$, i.e., with a signature with more than one negative sign (obtained through a vertex operator construction) cannot be described in terms of generators and relations of Kac-Moody or Borcherds algebras and belong to a new class of Lie algebras. Indeed our algebras are defined by a Cartan matrix and do not satisfy the root structure and multiplicities of the physical state algebra; this last condition seems, indeed, too strong and incompatible with the algebras constructed by us.

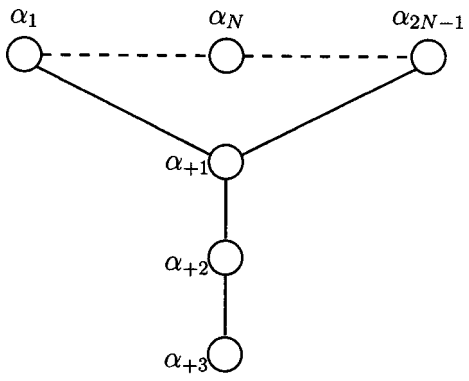
III. FOLDING OF TRIPLE EXTENDED LIE ALGEBRAS

The *folding* technique is a simple and powerful method to find class of singular subalgebras of finite Lie algebras as well as of affine or indefinite Kac-Moody algebras. The starting point is to use the symmetry τ of the Dynkin diagram, corresponding to an exterior automorphism of the algebra $\mathcal{G}$. In the finite case all the Dynkin diagrams of simply laced algebras show an automorphism of order $k=2$, except the case of D_4 where the order is 3. Let α_i be a simple root of $\mathcal{G}$. Using the automorphism τ of order k, we obtain

$$\beta_i := \alpha_i + \tau(\alpha_i) + \cdots + \tau^{k-1}(\alpha_i), \tag{18}$$

which form the simple root system of a singular subalgebra $\mathcal{H}$ of $\mathcal{G}$. The generators of $\mathcal{G}$, corresponding to the simple roots α_i, left unchanged by τ, become generators of $\mathcal{H}$, while the other ones transform according to a relation analogous to Eq. (18). In the following we apply the folding method to the triple extended Lie algebras, obtaining all the nonsimply laced triple extended algebras, as in the finite case. The automorphism of the three-extended Dynkin diagram acts on the standard way upon the roots of the finite classical subalgebras and trivially on the extended roots $\alpha_{+1}, \alpha_{+2}, \alpha_{+3}$. This property has to hold if we want to preserve the structure of the triple extension of the nonsimply laced algebras. (Indeed, also the nonsimply laced G^{++} algebras can be obtained with the same folding technique from the simply laced $\mathcal{G}^{++}$, while a different kind of folding applied to the $\mathcal{G}^{+}$ algebras allows one to get all the twisted affine algebras.) Let us enumerate all the cases.

A. $A^{+++}_{2N-1} \to C^{+++}_{N}$



The Cartan matrix of A^{+++}_{2N-1} can be written, in block form, as

$$A = (a_{ij}) = (\alpha_i, \alpha_j) = \begin{pmatrix} & & & -1 & 0 & 0 \\ & A_{A_{2N-1}} & & \vdots & \vdots & \vdots \\ & & & -1 & 0 & 0 \\ -1 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{19}$$

The not trivial action of τ on the simple roots gives

$$\beta_1 := \alpha_1 + \tau(\alpha_1) = \alpha_1 + \alpha_{2N-1}, \tag{20}$$

$$\beta_2 := \alpha_2 + \tau(\alpha_2) = \alpha_2 + \alpha_{2N-2} \ldots, \tag{21}$$

$$\beta_{N-1} := \alpha_{N-1} + \tau(\alpha_{N-1}) = \alpha_{N-1} + \alpha_{N+1}, \tag{22}$$

$$\beta_N := \alpha_N + \tau(\alpha_N) = 2\alpha_N, \tag{23}$$

$$\beta_{+1} := \alpha_{+1} + \tau(\alpha_{+1}) = 2\alpha_{+1}, \tag{24}$$

$$\beta_{+2} := \alpha_{+2} + \tau(\alpha_{+2}) = 2\alpha_{+2}, \tag{25}$$

$$\beta_{+3} := \alpha_{+3} + \tau(\alpha_{+3}) = 2\alpha_{+3}, \tag{26}$$

the length of the simple roots is

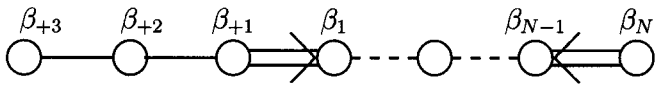
$$\beta_1^2 = \ldots = \beta_{N-1}^2 = 4, \tag{27}$$

$$\beta_{+3}^2 = \beta_{+2}^2 = \beta_{+1}^2 = \beta_N^2 = 8. \tag{28}$$

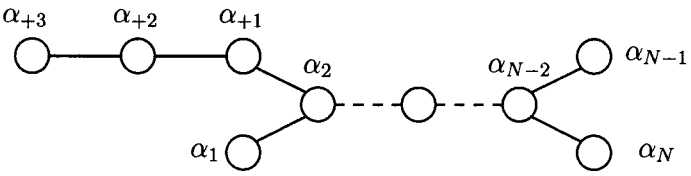
The corresponding Cartan matrix is

$$B = (b_{ij})_{i,j} = 2\frac{(\beta_i, \beta_j)}{(\beta_i, \beta_i)} = \begin{pmatrix} & & & -2 & 0 & 0 \\ & A_{C_N} & & \vdots & \vdots & \vdots \\ & & & 0 & 0 & 0 \\ -1 & \cdots & 0 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{29}$$

So we get the three-extended Lie algebra C_N^{+++} with Dynkin diagram



B. $\mathbf{D}_N^{+++} \longrightarrow \mathbf{B}_{N-1}^{+++}$



The Cartan matrix can be written as

$$A=(a_{ij})_{i,j}=(\alpha_i,\alpha_j)=\begin{pmatrix} & & & & 0 & 0 & 0 \\ & & & & -1 & \vdots & \vdots \\ & & A_{D_N} & & \vdots & \vdots & \vdots \\ & & & & 0 & 0 & 0 \\ 0 & -1 & \cdots & 0 & 2 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{30}$$

The nontrivial action of τ is

$$\tau(\alpha_{N-1})=\alpha_N, \quad \tau(\alpha_N)=\alpha_{N-1}. \tag{31}$$

The new simple roots are

$$\beta_{N-1}:=\alpha_{N-1}+\tau(\alpha_{N-1})=\alpha_{N-1}+\alpha_N, \tag{32}$$

$$\beta_{N-2}:=\alpha_{N-2}+\tau(\alpha_{N-2})=2\alpha_{N-2}\ldots, \tag{33}$$

$$\beta_1:=\alpha_1+\tau(\alpha_1)=2\alpha_1, \tag{34}$$

$$\beta_{+1}:=\alpha_{+1}+\tau(\alpha_{+1})=2\alpha_{+1}, \tag{35}$$

$$\beta_{+2}:=\alpha_{+2}+\tau(\alpha_{+2})=2\alpha_{+2}, \tag{36}$$

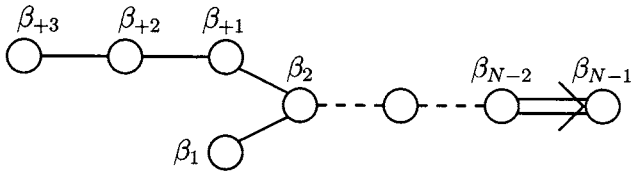
$$\beta_{+3}:=\alpha_{+3}+\tau(\alpha_{+3})=2\alpha_{+3}, \tag{37}$$

where

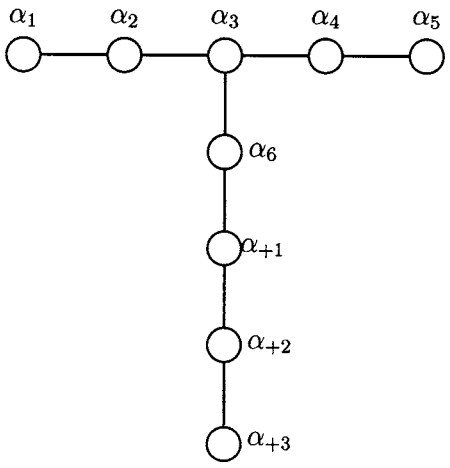
$$\beta_{N-1}^2=4, \quad \beta_{+3}^2=\beta_{+2}^2=\ldots=\beta_{N-2}^2=8. \tag{38}$$

The Cartan matrix and the corresponding Dynkin diagram of B_{N-1}^{+++} are

$$B=(b_{ij})_{i,j}=2\frac{(\beta_i,\beta_j)}{(\beta_i,\beta_i)}=\begin{pmatrix} & & & & 0 & 0 & 0 \\ & & & & -1 & \vdots & \vdots \\ & & A_{B_{N-1}} & & \vdots & \vdots & \vdots \\ & & & & 0 & 0 & 0 \\ 0 & -1 & \cdots & 0 & 2 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{39}$$



c. $\mathbf{E}_6^{+++} \longrightarrow \mathbf{F}_4^{+++}$



The Cartan matrix of E_6^{+++} is

$$A = (a_{ij})_{i,j} = (\alpha_i, \alpha_j) = \begin{pmatrix} & & & 0 & 0 & 0 \\ & A_{E_6} & & \vdots & \vdots & \vdots \\ & & & -1 & 0 & 0 \\ 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{40}$$

The simple roots are given by

$$\beta_1 := \alpha_1 + \tau(\alpha_1) = \alpha_1 + \alpha_5, \tag{41}$$

$$\beta_2 := \alpha_2 + \tau(\alpha_2) = \alpha_2 + \alpha_4, \tag{42}$$

$$\beta_3 := \alpha_3 + \tau(\alpha_3) = 2\alpha_3, \tag{43}$$

$$\beta_4 := \alpha_6 + \tau(\alpha_6) = 2\alpha_6 \tag{44}$$

$$\beta_{+1} := 2\alpha_{+1}, \quad \beta_{+2} := 2\alpha_{+2} \tag{45}$$

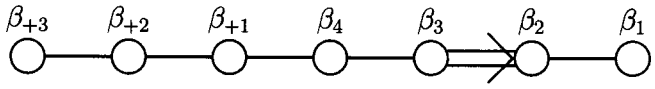
$$\beta_{+3} := 2\alpha_{+3}, \tag{46}$$

and

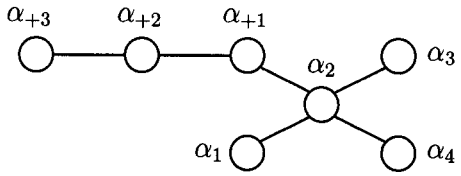
$$\beta_1^2 = \beta_2^2 = 4, \quad \beta_{+3}^2 = \beta_{+2}^2 = \ldots = \beta_3^2 = 8. \tag{47}$$

One gets the three-extended algebra F_4^{+++}, with Cartan matrix and Dynkin diagram

$$B = (b_{ij})_{i,j} = 2\frac{(\beta_i,\beta_j)}{(\beta_i,\beta_i)} = \begin{pmatrix} & & & 0 & 0 & 0 \\ & A_{F_4} & & \vdots & \vdots & \vdots \\ & & & -1 & 0 & 0 \\ 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{48}$$



D. $D_4^{+++} \longrightarrow G_2^{+++}$



The Cartan matrix of D_4^{+++} is

$$A = (a_{ij})_{i,j} = (\alpha_i,\alpha_j) = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & -1 & -1 & 0 & 0 \\ 0 & -1 & 2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 2 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{49}$$

The action of τ on the simple roots gives

$$\beta_1 := \alpha_1 + \tau(\alpha_1) + \tau^2(\alpha_1) = \alpha_1 + \alpha_3 + \alpha_4, \tag{50}$$

$$\beta_2 := 3\alpha_2, \tag{51}$$

$$\beta_{+1} := 3\alpha_{+1}, \quad \beta_{+2} := 3\alpha_{+2}, \tag{52}$$

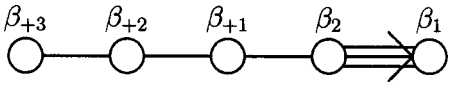
$$\beta_{+3} := 3\alpha_{+3} \tag{53}$$

and

$$\beta_1^2 = 6, \quad \beta_{+3}^2 = \ldots = \beta_2^2 = 18. \tag{54}$$

One gets the extended algebra G_2^{+++} with Cartan matrix and Dynkin diagram:

$$B = (b_{ij})_{i,j} = 2\frac{(\beta_i,\beta_j)}{(\beta_i,\beta_i)} = \begin{pmatrix} 2 & -3 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}. \tag{55}$$



Let us remark that, in general, by applying the folding procedure to an algebra $\mathcal{G}$, defined by the Cartan matrix A and Dynkin diagram $S(A)$, we obtain the Cartan matrix B and the corresponding Dynkin diagram $S(B)$ of another algebra $\mathcal{H}$. However we have to check that the new generators, defined in function of the generators of $\mathcal{G}$ satisfy all the defining relations of the algebra $\mathcal{H}$. Let us see how the new generators are obtained. Let α_i be a simple root of $\mathcal{G}$ and h_i, e_i, f_i the associated generators. Let us denote by β_i, respectively, h_i', e_i', f_i', the roots and the associated generators transformed under the action of τ, which we identify, respectively, as the simple roots and the associated generators of $\mathcal{H}$. If the action of τ is trivial, that is $\beta_i = k\alpha_i$ (where k is the order of the automorphism τ, $\tau^k = 1$) then the generators are not transformed $h_i' = h_i$, $e_i' = e_i$ and $f_i' = f_i$. If the action of τ is not trivial, that is $\beta_i = \alpha_i + \tau(\alpha_i) + \ldots + \tau^{k-1}(\alpha_i)$, we obtain $h_i' = h_i + h_{\tau(\alpha_i)} + \ldots + h_{\tau^{k-1}(\alpha_i)}$, $e_i' = e_i + e_{\tau(\alpha_i)} + \ldots + e_{\tau^{k-1}(\alpha_i)}$ and $f_i' = f_i + f_{\tau(\alpha_i)} + \ldots + f_{\tau^{k-1}(\alpha_i)}$. We have to verify that the generators h_i', e_i', f_i' satisfy the defining relations

$$[e_i', f_j'] = \delta_{ij} h_j',$$

$$[h_i', e_j'] = b_{ij} e_j', \quad [h_i', f_j'] = -b_{ij} f_j',$$

$$[h_i', h_j'] = 0,$$

$$(\text{ad } e_i')^{1-b_{ij}} e_j' = 0, \quad (\text{ad } f_i')^{1-b_{ij}} f_j' = 0, \quad (i \neq j).$$

We do not report here the explicit calculations, but everything works nicely. Finally it should be remarked that the folding procedure for indefinite Kac-Moody algebra, when applicable, always gives rise to indefinite Kac-Moody algebra, as it happens for the finite, affine, hyperbolic Kac-Moody algebras. On the contrary other reduction procedures, as the orbifolding, do not preserve the kind of algebras. Indeed as remarked in Ref. 17, the orbifolding of E_{10}, to which the folding procedure cannot be applied, gives rise to non Kac-Moody algebras.

IV. NONSTANDARD EXTENSIONS OF LIE ALGEBRAS

In this section we present a nonstandard construction of extended Lie algebras; as stated in Sec. I, the idea of the nonstandard extension is to add to the simple root system $\{\alpha_i\}$ of a simple Lie algebra $\mathcal{G}$ new roots, which are formed by those fundamental weights of the algebra that are linear combinations with integer coefficients of α_i, plus a suitable combination of vectors belonging to the Lorentzian lattice $\text{II}^{1,1}_{k_\pm}$ and/or $\text{II}^{1,1}_{l_\pm}$. The new roots have to satisfy the requirements that their squared norms are equal to 2 and that are suitably linked with the previous ones. Let us remark that the roots of the nonstandard extension do not generally span the whole lattice $\mathbf{\Lambda} = \Lambda_{\mathcal{G}} \oplus \text{II}^{1,1}_{k_\pm} \oplus \text{II}^{1,1}_{l_\pm}$ and that, moreover, the structure of the added simple root is, by no way, unique. Of course one can add more than two 2-dim. Lorentzian lattices, but these extensions will not be considered in the present paper, where we add at most three new roots. Also we shall not discuss the case where the squared norm of the added roots is not equal to 2. So, given a simple Lie algebra $\mathcal{G}$, we add to the root lattice $\Lambda_{\mathcal{G}}$ a new simple root $\alpha_{r+1} \equiv \alpha_{+1}$, which is formed by the opposite of a fundamental weight $-\Lambda_i$ and by a suitable linear combination, with integer coefficients, of the vectors $k_\pm$, in order to have $\alpha_{+1}^2 = 2$, as Λ_i^2 is not necessarily 2. Let us remember that the fundamental weights have the property $2(\Lambda_i, \alpha_j)/(\alpha_j, \alpha_j) = \delta_{i,j}$; they span the weight lattice $P = \oplus_{i=1}^r \mathbb{Z}\Lambda_i$, which is dual to the coroot lattice $\Lambda_{\mathcal{G}}^\vee = \oplus_{i=1}^r \mathbb{Z}\alpha_i^\vee$ where $\alpha_i^\vee = 2\alpha_i/(\alpha_i, \alpha_i)$ are the coroots. So while it is always true that $P = (\Lambda_{\mathcal{G}}^\vee)^*$, in general we have $\Lambda_{\mathcal{G}} \subseteq P$. This means that for each $\mathcal{G}$, only some Λ_i belong to the root lattice; so, in defining α_{+1} we choose the $\Lambda_i \in \Lambda_{\mathcal{G}}$. Since Λ_i is only linked with the simple root α_i, we have $(\alpha_{+1}, \alpha_j) = -\delta_{+1,i}$. So the first extension is made by adding the root $\alpha_{r+1} \equiv \alpha_{+1} \equiv := -\Lambda_i + k_+ - ak_-$, where $a \in \mathbf{Z}_+$ is fixed by the condition $\alpha_{+1}^2 = \Lambda_i^2$

$-2a=2$. At this point, we add the simple root $\alpha_{r+2}\equiv\alpha_{+2}:=-\theta+bk_--l_-$, where θ is the highest root of $\mathcal{G}$ and $b\in\mathbf{Z}$ is a coefficient chosen in order to have $(\alpha_{+2},\alpha_{+1})=(\Lambda_i,\theta)-b=0$. In this way, we have $\alpha_{+2}^2=2$ and α_{+2} behaves like an affine root (that is, it is linked with the simple roots of $\mathcal{G}$ in a way completely analogous as the affine root of the algebras $\hat{\mathcal{G}}$). At the end, we add the third simple root $\alpha_{r+3}\equiv\alpha_{+3}:=l_++l_-$ with the property that $(\alpha_{+3},\alpha_{+2})=-1$ and $(\alpha_{+3},\alpha_i)=0$ for $i=1,\ldots,r,r+1$. As $(\Lambda_i,\Lambda_j)\in\mathbf{Z}_>$ for the Lie algebra $\mathcal{G}$ below considered, this procedure is completely general and the extended algebra contains as subalgebra the affine extension of $\mathcal{G}$ (so sometimes we shall call this a *nonstandard affine extension*). Clearly the lightlike vector l_- can be hanged up to any other simple root, producing another indefinite Kac-Moody. We shall comment on this point in Sec. V. This construction leads to indefinite Kac-Moody algebras, one-, two-, and three-extended, whose (symmetric) Cartan matrix $2(\alpha_i,\alpha_j)/(\alpha_i,\alpha_i)$ (for $i,j=1,\ldots,r+3$) has Lorentzian signature $(+\ldots+-)$ with $r+2$ plus signs and 1 minus sign. The root lattice of the three-extended algebra is properly contained in $\Lambda_{\mathcal{G}}\oplus\mathrm{II}^{1,1}_{k_\pm}\oplus\mathrm{II}^{1,1}_{l_\pm}$. For these algebras, one can make similar discussions as those in Sec. II on eventual further extensions. Now we want to discuss another possible extension, which cannot be performed for any fundamental weight Λ_i belonging to the root lattice of $\mathcal{G}$. The first extension is performed as before, but as second extension we add the root $\alpha_{+2}:=-\Lambda_j+k_+-bk_--l_-$ $(i\neq j)$, where $b\in\mathbf{Z}_+$ is such that $\alpha_{+2}^2=2$ and $(\alpha_{+1},\alpha_{+2})=(\Lambda_i,\Lambda_j)-a-b=0$. In the following we shall show that, for $\mathcal{G}\neq E_6$, for any i $(\Lambda_i\neq\theta)$, at least one j exists which satisfies the above condition. In the following, we discuss only some examples of the general construction, we called *affine extension*; in particular we concentrate on the simply laced algebras, but it is possible to consider also the other cases paying attention at the choice of the fundamental weight.

Looking at the fundamental weights of simply laced-Lie algebras, see Ref. 13, one realizes that the fundamental weights which can be written as

$$\Lambda_i=\sum_n c_n\alpha_n,\quad c_n\in\mathbf{Z} \tag{56}$$

are

1. for $D_N=so(2N)$ $(N\geqslant 4)$, the weights Λ_i with i even number $(N-2\geqslant i\geqslant 2)$,
2. for E_6, only the weights Λ_i $(i=3,6)$,
3. for E_7, only the weights Λ_i $(i=1,2,3,5)$,
4. for E_8, all the weights Λ_i, which is just a consequence of the E_8-lattice being a self-dual one.

In the following we discuss some of the possible nonstandard extensions, with the aim to illustrate the procedure in a few examples which may be relevant for their subalgebras content. Let us emphasize that the discussed extensions as well their subalgebras content are not at all exhaustive, being the choice of the extended simple roots not unique, in general.

A. $D_N=so(2N)$

In order to illustrate the general procedure, we discuss in some detail the case of $D_6=so(12)$, which is the first algebra of the even orthogonal series which admits a nonstandard extension. We add the simple root

$$\alpha_{+1}:=-\Lambda_4+k_+-k_-,\quad \alpha_{+1}^2=2, \tag{57}$$

where Λ_4 is the fundamental weight (the ε_i are unit ortho-normal vectors in $\mathbb{R}^6$)

$$\Lambda_4=\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4,\quad \Lambda_3^2=4, \tag{58}$$

Clearly we have

$$(\alpha_{+1},\alpha_i)=-\delta_{4,i}. \tag{59}$$

We add now the root

$$\alpha_{+2} := -\text{h.r.} - 2k_- - l_- = -(\varepsilon_1 + \varepsilon_2) - 2k_- - l_-, \tag{60}$$

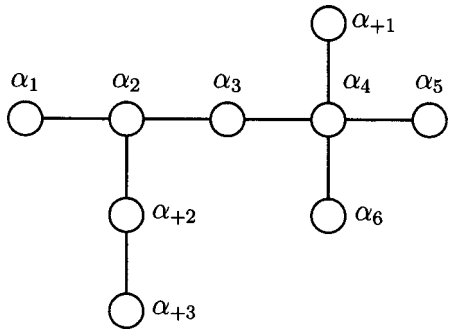
$$(\alpha_{+2}, \alpha_j) = -\delta_{2,j}, \tag{61}$$

and

$$\alpha_{+3} := l_+ + l_-, \tag{62}$$

$$(\alpha_{+3}, \alpha_k) = -\delta_{+2,k}, \tag{63}$$

with Dynkin diagram:



Let's observe that the first extension of D_6 is the same algebra as D_4^{+++}, so folding α_{+1}, α_5, and α_6 we re-obtain G_2^{+++}. Clearly the choice of the extended simple roots is not unique. One can easily see that:

- A nonstandard extension of $so(4N)$ admits as subalgebra the affine extension of $so(4N)$ and $so(4(N-1))$. Indeed one adds to the roots of $so(4N)$ the root of the affine extension

  $$\alpha_{+1} := -\Lambda_2 + k_+ \tag{64}$$

  and the new nonstandard root

  $$\alpha_{+2} := -\Lambda_4 + l_+ - l_-. \tag{65}$$

  Taking away the roots α_{+1}, α_j $(j=1,2)$ one gets the algebra $so(4(N-1))^{(1)}$. Let us remark that if we add the root

  $$\alpha_{+2} := -\Lambda_6 + l_+ - 2l_- \tag{66}$$

  and then we take away the roots α_{+1}, α_j $(j=1,\ldots,4)$ one gets the algebra $so(4(N-2))^{(1)}$.
- The nonstandard extension of $so(24)$ is the smallest extension of the orthogonal series which contains as subalgebra E_{11}. Indeed adding to the roots of $so(24)$ the nonstandard root

  $$\alpha_{+1} := -\Lambda_8 + k_+ - 3k_- \tag{67}$$

  and deleting α_{11}, α_{12} one gets E_{11}.

Let us call $\hat{\Lambda}_{2n} = -\Lambda_{2n} + k_+ - (n-1)k_-$, where $n \in \mathbb{Z}_+$ and $\Lambda_{2n} = \Sigma_{i=1}^{2n} \varepsilon_i$ is a fundamental weight. Clearly we have

$$\hat{\Lambda}_{2n}^2 = 2 \quad (\hat{\Lambda}_{2n}, \hat{\Lambda}_{2n+2}) = 0. \tag{68}$$

B. E_6

Let us add to the simple root system of E_6 the root

$$\alpha_{+1} := -\Lambda_3 + k_+ - 2k_-, \quad \alpha_{+1}^2 = 2, \tag{69}$$

where Λ_3 is the fundamental weight

$$\Lambda_3 = \varepsilon_3 + \varepsilon_4 + \varepsilon_5 + \varepsilon_8 - \varepsilon_7 - \varepsilon_6, \quad \Lambda_3^2 = 6. \tag{70}$$

Clearly we have

$$(\alpha_{+1}, \alpha_i) = -\delta_{3,i}. \tag{71}$$

We add now the root

$$\alpha_{+2} := -\text{h.r.} - 3k_- - l_- = -\tfrac{1}{2}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + \varepsilon_5 - \varepsilon_6 - \varepsilon_7 + \varepsilon_8) - 3k_- - l_-, \tag{72}$$

$$(\alpha_{+2}, \alpha_j) = -\delta_{6,j}, \tag{73}$$

and

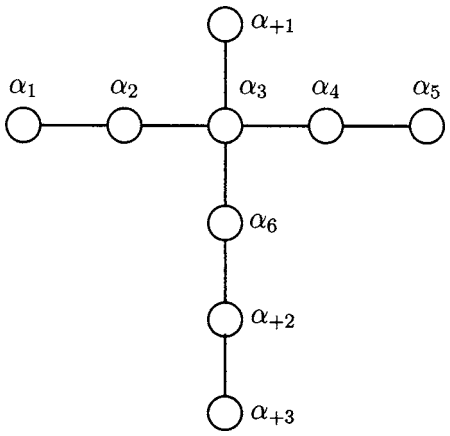
$$\alpha_{+3} := l_+ + l_-, \quad (\alpha_{+3}, \alpha_k) = -\delta_{+2,k}. \tag{74}$$

Alternatively we can add the roots

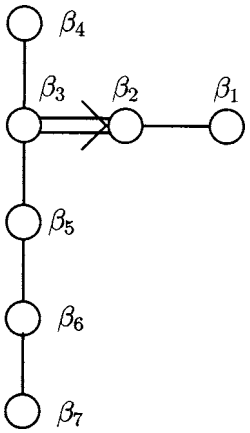
$$\alpha_{+2} := k_- + k_+ - l_-, \quad (\alpha_{+2}, \alpha_j) = -\delta_{+1,j}, \tag{75}$$

$$\alpha_{+3} := l_+ + l_-, \quad (\alpha_{+3}, \alpha_k) = -\delta_{+2,k}, \tag{76}$$

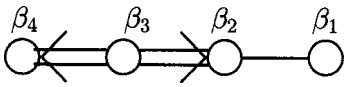
and we obtain the same Dynkin diagram:



where in the second construction the roles of α_{+1} and α_6 are exchanged. Let's observe that many nonstandard (simply laced) Dynkin diagrams can be folded to obtain other (nonsimply laced) Dynkin diagrams. For example, in the case of E_6, we can identify the roots α_1 and α_2 with α_5 and α_4, respectively (so the new simple roots are $\beta_1 = \alpha_1 + \alpha_5$, $\beta_2 = \alpha_2 + \alpha_4$ and $\beta_i = 2\alpha_i$ for $i = 3, +1, +2, +3$), obtaining the following folded Dynkin diagram:



Actually, if we consider only the first extension of E_6, then we can identify also α_{+1} with α_6 and we obtain:



C. E_7

In this case we could use the fundamental weights Λ_1, Λ_2, Λ_3, and Λ_5. To illustrate the procedure, let's consider the weight Λ_5 $((\Lambda_5,\Lambda_5)=4)$ and add the simple roots:

$$\alpha_{+1} := -\Lambda_5 + k_+ - k_-, \quad \alpha_{+1}^2 = 2, \quad (\alpha_{+1},\alpha_i) = -\delta_{5,i}, \tag{77}$$

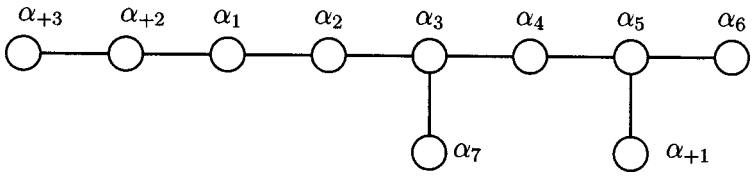
with

$$\Lambda_5 = \varepsilon_5 + \varepsilon_6 - \varepsilon_7 + \varepsilon_8, \quad \Lambda_5^2 = 4. \tag{78}$$

Then

$$\alpha_{+2} := -\text{h.r.} - 2k_- - l_- = \varepsilon_7 - \varepsilon_8 - 2k_- - l_-, \quad \alpha_{+3} = l_+ + l_-, \tag{79}$$

with $(\alpha_{+2},\alpha_k)=-\delta_{k,1}$ and $(\alpha_{+3},\alpha_j)=-\delta_{j,+2}$. In this way we obtain the Dynkin diagram:



Let us call $\hat{\Lambda}_i := -\Lambda_i + k_+ - ak_-$, where $a \in \mathbb{Z}_+$ and Λ_i, $i=1,2,3,5$, is a fundamental weight. We have

$$\hat{\Lambda}_i^2 = 2 \quad (\hat{\Lambda}_3,\hat{\Lambda}_5) = 0. \tag{80}$$

D. E_8

E_8 root lattice is self-dual, so it coincides with the weight lattice. The nonstandard extension can be made adding to the simple root system a root equal to the opposite of any weight Λ_i ($i=1,\ldots,8$) plus some combination of k_+ and k_-. In this way we have eight different extensions of E_8, with the nodes +2, +3 always in the same position (that is $(\alpha_{+2},\alpha_7)=-1$ and $(\alpha_{+3},\alpha_{+2})=-1$), while the node +1 moves from the node 1 to the node 8, when i runs from 1 to 8, respectively. Actually, this situation is general for the nonstandard extensions.

Let us emphasize again that the choice of the extended simple roots is not unique at all. Motivated by this consideration, we observe that classically we have $E_6 \subset E_7 \subset E_8$, while this inclusion is lost when we consider the corresponding affine algebras (and the same thing is true for the double and the triple extensions). So we look for an algebra that may contain all the E series and the $E^{(1)}$ series. This is possible considering the following nonstandard extension of E_8 (in which the new simple roots are linked to those of E_8 using different fundamental weights). We add the new simple root:

$$\alpha_{+1} := -\text{h.r.} + k_+ + l_+ = -(\varepsilon_7 + \varepsilon_8) + k_+ + l_+, \quad \alpha_{+1}^2 = 2, \tag{81}$$

Then we add the two simple roots:

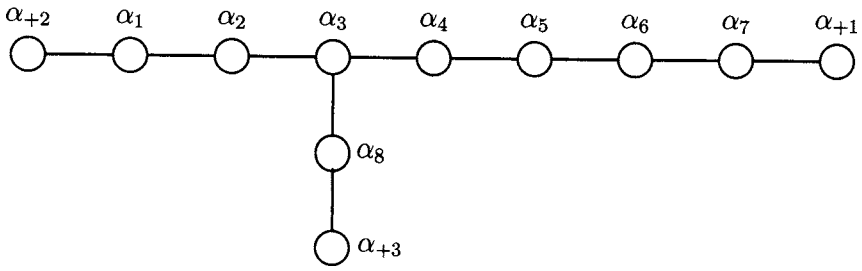
$$\Lambda_1 = 2\varepsilon_8, \quad \Lambda_8 = \frac{1}{2}\left(\sum_{i=1}^{7} \varepsilon_i + 5\varepsilon_8\right), \tag{82}$$

$$\alpha_{+2} := -\Lambda_1 - k_- + l_+ - l_-, \quad \alpha_{+1}^2 = 2, \tag{83}$$

and

$$\alpha_{+3} := -\Lambda_8 + k_+ + l_+ - 3l_-, \quad \alpha_{+3}^2 = 2, \tag{84}$$

so that the only nonzero scalar products are: $(\alpha_{+1}, \alpha_7) = -1$, $(\alpha_{+2}, \alpha_1) = -1$ and $(\alpha_{+3}, \alpha_8) = -1$ and we have the following Dynkin diagram:



This algebra contains E_8 (then also E_7 and E_6) and all the affinizations $E_{6,7,8}^{(1)}$, so it seems to be interesting for its content in subalgebras. Let us call $\hat{\Lambda}_i = -\Lambda_i + k_+ - ak_-$, where $a \in \mathbb{Z}_+$ and Λ_i, is any fundamental weight. We have $(\hat{\Lambda}_i^2 = 2)$

$$(\hat{\Lambda}_1, \hat{\Lambda}_2) = (\hat{\Lambda}_1, \hat{\Lambda}_5) = 0,$$

$$(\hat{\Lambda}_4, \hat{\Lambda}_8) = 0 (\hat{\Lambda}_2, \hat{\Lambda}_3) = (\hat{\Lambda}_2, \hat{\Lambda}_4) = (\hat{\Lambda}_2, \hat{\Lambda}_5) = (\hat{\Lambda}_2, \hat{\Lambda}_6) = 0,$$

$$(\hat{\Lambda}_2, \hat{\Lambda}_3) = (\hat{\Lambda}_2, \hat{\Lambda}_4) = (\hat{\Lambda}_2, \hat{\Lambda}_5) = (\hat{\Lambda}_2, \hat{\Lambda}_6) = 0. \tag{85}$$

We have proposed a procedure to build nonstandard triple extended Lie algebras, which we have illustrated with a number of relevant examples. As already recalled, Kac-Moody or Borcherds extensions can be defined for these Lie algebras too. On the light of the remarks of Ref. 11, it is natural to wonder if these or some of these algebras are not really subalgebras of the standard triple extended Lie algebras. This point will be discussed in the next section, where we discuss also a few examples of subalgebras which point out the intriguing and surprising structure of the subalgebras.

V. SUBALGEBRAS OF EXTENDED LIE ALGEBRAS

First of all, let us discuss another nonstandard procedure to extend a Lie algebras of rank r. If one adds to the simple roots of $\mathcal{G}$ the opposite of the h.r. $\alpha_0 \equiv \alpha_{r+1}$ and, to recover the linear independence of the simple root system, one glues the light like vector k_+ to a simple root α_i $(1 \leqslant i \leqslant r)$, one gets exactly the affine $\mathcal{G}$. As next step one adds the new root, which belongs to $\mathrm{II}_k^{1,1}$, $\alpha_{r+2} = -(k_+ + k_-)$. From the Feingold-Nicolai theorem,[11] it is easy to realize that in this way one obtains a generalized Kac-Moody algebra which is really a subalgebra of the standard overextended Lie algebra $\mathcal{G}^{++}$. Things may be different if one considers simple root systems, obtained by analogous procedure, in the lattice $\Lambda_{\mathcal{G}} \oplus \mathrm{II}_k^{1,1} \oplus \mathrm{II}_l^{1,1}$. Indeed indefinite Kac-Moody algebras are obtained which, in general, are described by Dynkin-Kac diagrams not equivalent to the ones obtained by the standard and not standard procedure described in the previous section. A general discussion of these algebras is beyond the aim of this paper and we limit ourselves to state a few properties and to present some examples. Let us start with the following

Proposition 2: The roots $\hat{\Lambda}_i$ defined in Sec. IV are roots of the standard overextended $\mathcal{G}^{++}$.

Proof: We shall explicitly write $\hat{\Lambda}_i$ in terms of the simple roots of $\mathcal{G}^{++}$. Let us remark that, by construction, $\mathcal{G}^{++}$ contains two affine $\mathcal{G}$, i.e., $\mathcal{G}^{+}$, whose real root system is formed by the roots of $\mathcal{G}$ plus nk_+, respectively, nk_-, $(n \in \mathbf{Z})$. Clearly the following decomposition in roots is not all unique.

1. $so(2N)$

$$\begin{aligned}\hat{\Lambda}_{2m} &= -(-\varepsilon_1 - \varepsilon_2 + k_+) + (-\varepsilon_3 - \varepsilon_4 - k_-) + \ \ldots \ + (-\varepsilon_{2m-1} - \varepsilon_{2m} - k_-) \\ &= -\Lambda_{2m} + k_+ - (m-1)k_-. \end{aligned} \tag{86}$$

2. E_6

$$\begin{aligned}\hat{\Lambda}_3 &= \frac{1}{2}\left[-\sum_{i\neq 6,7} \varepsilon_i + \varepsilon_6 + \varepsilon_7 + k_+\right] + \frac{1}{2}[\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4 - \varepsilon_5 + \varepsilon_6 + \varepsilon_7 - \varepsilon_8 - 2k_-] \\ &= -\Lambda_3 + k_+ - 2k_-. \end{aligned} \tag{87}$$

3. E_7

$$\hat{\Lambda}_2 = \frac{1}{2}[\varepsilon_1 - \varepsilon_2 - \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - \varepsilon_6 + \varepsilon_7 - \varepsilon_8 + k_+] + (\varepsilon_7 - \varepsilon_8 - 2k_-) = -\Lambda_2 + k_+ - 2k_-, \tag{88}$$

$$\begin{aligned}\hat{\Lambda}_3 &= (-\varepsilon_3 + \varepsilon_7 + k_+) + (-\varepsilon_4 + \varepsilon_7 - 2k_-) + (-\varepsilon_5 - \varepsilon_8 - k_-) + (-\varepsilon_6 - \varepsilon_8 - 2k_-) \\ &= -\Lambda_3 + k_+ - 5k_-, \end{aligned} \tag{89}$$

$$\hat{\Lambda}_5 = (-\varepsilon_3 - \varepsilon_6 + k_+) + (-\varepsilon_7 + \varepsilon_8 - k_-) = -\Lambda_5 + k_+ - k_-. \tag{90}$$

4. E_8

$$\hat{\Lambda}_1 = (-\varepsilon_i - \varepsilon_8 + k_+) + (\varepsilon_i - \varepsilon_8 - k_-) = -\Lambda_1 + k_+ - k_- \quad (i \neq 8),$$

$$\begin{aligned}\hat{\Lambda}_2 &= \frac{1}{2}[(\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 - \varepsilon_5 - \varepsilon_6 - \varepsilon_7 - \varepsilon_8) + k_+] + (-\varepsilon_3 - \varepsilon_8 - k_-) + (-\varepsilon_4 - \varepsilon_8 - 2k_-) \\ &\quad + (-\varepsilon_5 - \varepsilon_8 - 3k_-) = -\Lambda_2 + k_+ - 6k_-, \end{aligned}$$

$$\hat{\Lambda}_3 = (-\varepsilon_3 - \varepsilon_8 + k_+) + (-\varepsilon_4 - \varepsilon_8 - 2k_-) + (-\varepsilon_5 - \varepsilon_8 - 3k_-) + (-\varepsilon_6 - \varepsilon_8 - 4k_-) + (-\varepsilon_7 - \varepsilon_8 - 5k_-) = -\Lambda_3 + k_+ - 14k_-,$$

$$\hat{\Lambda}_4 = (-\varepsilon_4 - \varepsilon_8 + k_+) + (-\varepsilon_5 - \varepsilon_8 - 2k_-) + (-\varepsilon_6 - \varepsilon_8 - 3k_-) + (-\varepsilon_7 - \varepsilon_8 - 4k_-) = -\Lambda_4 + k_+ - 9k_-,$$

$$\hat{\Lambda}_5 = (-\varepsilon_5 - \varepsilon_8 + k_+) + (-\varepsilon_6 - \varepsilon_8 - 2k_-) + (-\varepsilon_7 - \varepsilon_8 - 3k_-) = -\Lambda_5 + k_+ - 5k_-,$$

$$\hat{\Lambda}_6 = (-\varepsilon_6 - \varepsilon_8 + k_+) + (-\varepsilon_7 - \varepsilon_8 - 2k_-) = -\Lambda_6 + k_+ - 2k_-,$$

$$\hat{\Lambda}_8 = \frac{1}{2}[(-\varepsilon_1 - \varepsilon_2 - \varepsilon_3 - \varepsilon_4 - \varepsilon_5 - \varepsilon_6 + \varepsilon_7 + \varepsilon_8) + k_+] + (-\varepsilon_6 - \varepsilon_8 - k_-) + (-\varepsilon_7 - \varepsilon_8 - 2k_-) = -\Lambda_8 + k_+ - 3k_-. \tag{91}$$

Therefore, the considered combinations of the fundamental weights with the vectors of the Lorentzian lattices $\mathrm{II}^{1,1}_k$ do belong to the root system of the overextended Lie algebras, even if the considered fundamental weights do not belong to the root system of the native Lie algebra. (One can recover the generators by the change $\alpha \to E_\alpha$ and $\alpha+\beta \to [E_\alpha, E_\beta]$.) It follows that the double nonstandard extensions (called previously *affine extensions*) are all subalgebras, of the same rank, of $\mathcal{G}^{++}$. Indeed it is easy to verify that the differences $\beta_i - \beta_j$ $(\forall i,j; i \neq j)$ of the simple roots β_i of the nonstandard double extension of $\mathcal{G}$ do not belong to the root system, therefore satisfying the conditions of the Feingold-Nicolai theorem. In particular we have

Proposition 3: The indefinite Kac-Moody algebras of rank 10 described by the Dynkin-Kac diagrams, obtained by adding to the diagram of the affine algebra E_8, i.e., E_9, a dot, connected with a simple link to the jth dot of E_9 $(1 \leqslant j \leqslant 9)$, is a subalgebra of E_{10}.

The simple root systems of these subalgebras is formed by the simple roots of E_8, by a root $\hat{\Lambda}_i$ given by Eq. (91) and by the root $-\theta + ak_-$ where a is a positive integer such that $(\hat{\Lambda}_i, -\theta + ak_-) = 0$.

One can naturally ask if an analogous theorem holds for E_{11}, that is if the triple nonstandard extensions of E_8 form Lorentzian algebras of rank 11, subalgebra of E_{11}. We have:

Proposition 4: The indefinite Kac-Moody algebras of rank 11 obtained by adding to the simple root system of the algebra E_8 three roots: $\alpha_{+1} = \hat{\Lambda}_j$, connected with a simple link to the jth dot of E_8 $(1 \leqslant j \leqslant 8, j \neq 7)$; $\alpha_{+2} = -\theta - ak_-$, where a is a positive integer such that $(\alpha_{+2}\alpha_{+1}) = 0$ and $\alpha_{+3} = l_+ + l_- - k_-$, simply linked with α_{+1}, is a subalgebra of E_{11}.

The proof is straightforward using the explicit expressions of $\hat{\Lambda}_j$, given in Eq. (91). Let us remark that these subalgebras do not have as subalgebra E_{10}. In the following we give the simple roots systems of a set (not exhaustive) of rank eleven subalgebra E_{11}, which contains as subalgebra E_{10}. Let us consider the following simple root system of E_{11}: α_i $(1 \leqslant i \leqslant 8)$ are the simple roots of E_8, $\alpha_9 = -\alpha_0 - k_+$, $\alpha_{10} = k_+ + k_-$ and $\alpha_{11} = (l_+ + l_-) - k_+$. We follow the convention of Ref. 13 and, for the reader convenience, we explicitly write here the E_8 simple root system and the root system Δ:

$$\alpha_1 = \frac{1}{2}\left(\varepsilon_1 + \varepsilon_8 - \sum_{j=2}^{7} \varepsilon_j\right), \quad \alpha_i = \varepsilon_i - \varepsilon_{i-1} \; i = 2, \ldots, 7$$

$$\alpha_8 = \varepsilon_1 + \varepsilon_2, \quad \text{h.r.} := \alpha_0 = \varepsilon_7 + \varepsilon_8, \tag{92}$$

$$\Delta = \left\{ \tfrac{1}{2}(\pm\varepsilon_1 \pm \varepsilon_2 \pm \varepsilon_3 \pm \varepsilon_4 \pm \varepsilon_5 \pm \varepsilon_6 \pm \varepsilon_7 \pm \varepsilon_8), \pm\varepsilon_i \pm \varepsilon_j \right\}, \tag{93}$$

where the total number of + signs (or − signs) in the first expression is an even number. Let us consider the E_{10} Dynkin-Kac diagram obtained by the E_{11} diagram, deleting the dot corresponding to 11th simple root. Let us denote by $E_{10}^{(j)}$ the algebra of rank 11 whose Dynkin-Kac diagram is obtained by the E_{10} diagram adding a dot (in the following denoted by +1) with a simple link to the jth dot ($1 \leqslant j \leqslant 10$) and by $\beta_i^{(j)}$ ($i = 1, \ldots, 10, +1$) the simple roots of $E_{10}^{(j)}$. In the following we do not explicitly write the upper label j in the roots. Clearly $E_{10}^{(10)} = E_{11}$ and, in this case, $\beta_{+1} = \alpha_{11}$. We make the following (not unique) choice for the simple root system of $E_{10}^{(j)}$ ($1 \leqslant j \leqslant 9$):

- $j=9$)

$$\beta_1 = \alpha_1 - k_+, \quad \beta_i = \alpha_i, \quad i = 2, \ldots, 7, 8,$$

$$\beta_9 = -\varepsilon_7 + \varepsilon_8 + k_-, \quad \beta_{10} = -\alpha_0 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{94}$$

- $j=7$)

$$\beta_i = \alpha_i, \quad i = 1, \ldots, 6, 8, \quad \beta_7 = \alpha_7 - k_+,$$

$$\beta_9 = \alpha_{10}, \quad \beta_{10} = \alpha_{11}, \quad \beta_{+1} = -\alpha_0. \tag{95}$$

- $j=6$)

$$\beta_i = \alpha_i, \quad i = 1, \ldots, 5, 7, 8, \quad \beta_6 = \alpha_6 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = \varepsilon_7 + \varepsilon_6 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{96}$$

- $j=5$)

$$\beta_i = \alpha_i, \quad i = 1,2,3,4,6,7,8, \quad \beta_5 = \alpha_5 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = \varepsilon_5 + \varepsilon_8 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{97}$$

- $j=4$)

$$\beta_i = \alpha_i, \quad i = 1,2,3,5,6,7,8, \quad \beta_4 = \alpha_4 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = \varepsilon_4 + \varepsilon_8 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{98}$$

- $j=3$)

$$\beta_i = \alpha_i, \quad i = 1,2, \ldots, 7, 8, \quad \beta_3 = \alpha_3 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = \varepsilon_3 + \varepsilon_8 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{99}$$

- $j=2$)

$$\beta_i = \alpha_i, \quad i = 1,3, \ldots, 7, 8, \quad \beta_2 = \alpha_2 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = -\varepsilon_1 + \varepsilon_8 - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{100}$$

- $j=1$)

$$\beta_1 = -\frac{1}{2}\sum_{i=i}^{8} \varepsilon_i + k_-, \quad \beta_2 = \alpha_8, \quad \beta_i = \alpha_i, \quad i = 3, \ldots, 6, \quad \beta_8 = \alpha_2,$$

$$\beta_7 = \alpha_7, \quad \beta_9 = -\varepsilon_7 + \varepsilon_8, \quad \beta_{10} = -\alpha_1 + k_+, \quad \beta_{+1} = \alpha_{11}. \tag{101}$$

- $j=8$)

$$\beta_i = \alpha_i, \quad i = 1, \ldots, 7, \quad \beta_8 = \alpha_8 + k_-,$$

$$\beta_9 = -\alpha_0, \quad \beta_{10} = \frac{1}{2}\sum_{i=1}^{8} \varepsilon_i - k_+, \quad \beta_{+1} = \alpha_{11}. \tag{102}$$

It is easy to verify that the roots β_i belong to the roots systems of E_{11}. Actually they belong, except for α_{11}, to the root system of affine $E_8=E_9$ which is a regular subalgebra of E_{11}—while the differences $\beta_i-\beta_j$ $(\forall i,j;i\neq j)$ $(|\beta_i-\beta_j|^2\geqslant 4)$ do not belong, therefore satisfying the conditions of the Feingold-Nicolai theorem. The Dynkin-Kac diagrams describing these algebras contain loops except for $j=7$. This algebra has been considered in Ref. 14, where it has been denoted EE_{11}, and it has been shown to be a subalgebra of E_{11} by explicitly constructing the generators by commutation of the E_{11} generators. The Dynkin-Kac diagrams for these algebras are easily drawn by adding to the E_{10} diagram a dot simply connected with the jth dot and then connecting, with a simple link, the following dots: $j=9$) 7–10; $j=6$) 1–10; $j=5$) 6–10; $j=4$) 5–10; $j=3$) 4–10; $j=2$) 8–10; $j=1$) 7–10, 8–10; $j=8$) 1–10. Of course, these subalgebras do not exhaust the set of 11 dimensional indefinite Kac-Moody subalgebras of E_{11}. In particular we have not considered the subalgebras which do appear as invariant algebras with respect to an involution of the generators of E_{11}, see Refs. 18 and 19.

VI. CONCLUSIONS AND FUTURE DEVELOPMENTS

In studying four-extended Lie algebras, we have seen that Borcherds algebras seem to emerge naturally. This remark raises the question: which are the fingerprints of a theory which exhibits a symmetry under a Borcherds algebra? This question is indeed interesting on the light of the remark that many dualities have a group-theoretical origin in the Weyl group of the algebra. The Weyl group of the Borcherds algebra has peculiar properties as the reflection with respect to the imaginary vanishing roots is not defined. Some particular properties related to this kind of algebras have already been discussed in Ref. 20. The nonstandard extension introduced in this paper has peculiar features, which deserve further investigation, on both their mathematical structure and their possible physical relevance. A classification of these algebras is beyond the aim of this paper, where we present only a few representative examples. As, however, very little is known on Lorentzian Kac-Moody algebras, we believe that any new information is interesting. In the cited literature on the physical role of the very extended Lie algebras, nonlinear realizations of the indefinite Kac-Moody algebras are used. How does a Chevalley realization of this algebra look like? In Ref. 21 a procedure to build up vertex realization of Lorentzian algebra with only a lattice $\mathrm{II}^{1,1}$ has been proposed and applied to the very simple case of the overextended A_1 algebra. It seems possible to generalize that procedure to the triple extended Lie algebras. Moreover, it has also been argued by West[22] that $sl(32)$ is contained in the Cartan invariant subalgebra of E_{11}. At first sight the rank of $sl(32)$ is too large to be a subalgebra, so it seems that very extended algebras, at least in the nonlinear realization, admit finite dimensional subalgebras which naively could not be there. The investigation of the finite Lie subalgebras of the indefinite Kac-Moody algebras requires new methods beyond the very familiar ones used in the case of finite Lie algebra, which are essentially based on the Dynkin methods. This feature is not completely unrelated with the property, noted in Ref. 11, that the set of infinite dimensional subalgebras of Lorentzian algebras is quite rich and surprising. We have illustrated this feature in Sec. V iscussing a class of subalgebras of E_{11}, but it would be useful to dispose of techniques to build up explicitly or to identify classes of these subalgebras or to dispose of further examples.

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APPENDIX A: SOME FACTS ABOUT THE LATTICE $II^{1,1}$

We review some basic facts about the lattice $II^{1,1}$, which is the only Lorentzian even self-dual lattice in dimension two. The points in this lattice can be described as the vectors:

$$(n,m) \tag{A1}$$

with $n,m \in \mathbb{Z}$ and Gram matrix $\left(\begin{smallmatrix} 0 & -1 \\ -1 & 0 \end{smallmatrix}\right)$, with eigenvalues ± 1. In this way, the scalar product between two vectors $a=(a_+,a_-)$ and $b=(b_+,b_-)$ can be written as: $a\cdot b=-a_+b_--a_-b_+$. We can take $k_+ \equiv (1,0)$ and $k_- \equiv (0,-1)$ as basis vectors in $II^{1,1}$; with this choice, we have

$$k_\pm \cdot k_\pm = 0, \quad k_\pm \cdot k_\mp = 1. \tag{A2}$$

All the vectors in $II^{1,1}$ can be written as $v=pk_+ + qk_-$ (with $p,q \in \mathbb{Z}$); in particular there are only two vectors of squared norm 2, $\pm(k_+ + k_-)$, but infinite vectors of positive ($\geqslant 4$) and negative ($\leqslant -2$) squared norm, being $v^2=2pq$.

APPENDIX B: DEFINITION OF BORCHERDS ALGEBRAS

The best way to think of a Borcherds algebra is to consider it as a generalization of a finite-dimensional simple Lie algebra. The definition is based on the Serre-Chevalley construction of finite-dimensional algebras; we follow Ref. 12. These algebras always have a symmetric matrix and their structure is very similar to that of ordinary Kac-Moody algebras, the only major difference is that generalized Kac-Moody algebras allow the presence of imaginary simple roots. Let $A=(a_{i,j})$ a $n \times n$ (real) symmetric matrix satisfying the following properties:

- $a_{ii}=2$ or $a_{ii} \leqslant 0$,
- $a_{ij} \leqslant 0$ if $i \neq j$,
- $a_{ij} \in Z$ if $a_{ii}=2$.

Then the Borcherds algebra $\mathcal{G}(A)$ associated with the Cartan matrix A is the Lie algebra given by the following generators and relations.

$3n$ *Generators*: e_i, f_i and h_i

Relations:

- $[h_i,h_j]=0$,
- $[e_i,f_j]=\delta_{ij}h_i$,
- $[h_i,e_j]=a_{ij}e_j$, $[h_i,f_j]=-a_{ij}e_j$,
- $e_{ij} := (\mathrm{ad}e_i)^{1-a_{ij}}e_j=0$, $f_{ij} := (\mathrm{ad}f_i)^{1-a_{ij}}f_j=0$ if $a_{ii}=2$ and $i \neq j$,
- $e_{ij} := [e_i,e_j]=0$, $f_{ij} := [f_i,f_j]=0$ if $a_{ii} \leqslant 0$, $a_{jj} \leqslant 0$ and $a_{ij}=0$.

The elements h_i form a basis for an abelian subalgebra of $\mathcal{G}(A)$, called Cartan subalgebra $\mathcal{H}(A)$; as it happens for Kac-Moody algebras, $\mathcal{G}(A)$ has the triangular decomposition:

$$\mathcal{G}(A) = \mathcal{N}_- \oplus \mathcal{H}(A) \oplus \mathcal{N}_+ \tag{B1}$$

and has many of the properties of the usual Kac-Moody algebras (real and imaginary roots, etc.). In particular, in this paper, we have considered Borcherds algebras with just one imaginary simple root (with squared norm 0), which we have added by hand. A rank 2 Borcherds algebra in the lattice $II^{1,1}$ can be constructed as follows: the Cartan matrix is given by

$$A = \begin{pmatrix} 0 & -1 \\ -1 & 2 \end{pmatrix}. \tag{B2}$$

A possible choice for the simple roots is

$$\alpha_1 = k_+, \quad \alpha_2 = -(k_+ + k_-), \tag{B3}$$

with Weyl vector $\rho = -k_+$ (defined by $(\rho, \alpha_i) = 1/2(\alpha_i, \alpha_i)$).

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Singular solutions to the Seiberg-Witten and Freund equations on flat space from an iterative method

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Although it is well known that the Seiberg-Witten equations do not admit nontrivial L^2 solutions in flat space, singular solutions to them have been previously exhibited—either in $\mathbb{R}^3$ or in the dimensionally reduced spaces $\mathbb{R}^2$ and $\mathbb{R}^1$—which have physical interest. In this work, we employ an extension of the Hopf fibration to obtain an iterative procedure to generate particular singular solutions to the Seiberg-Witten and Freund equations on flat space. Examples of solutions obtained by such method are presented and briefly discussed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2162823]

I. INTRODUCTION

Given a physical system defined on a configuration space M, there are various instances where it is useful to employ (extensions of) fibrations $P \to M$ to lift the corresponding equations of motion from M to P. For instance, the natural extension of the Hopf fibration $S^3 \to S^2$ to $\mathbb{R}^4 \to \mathbb{R}^3$ (defining the so-called Kustaanheimo-Stiefel transformation[1,2]) can be used to map the Kepler problem in $\mathbb{R}^3$ to a harmonic oscillator problem in $\mathbb{R}^4$. This construction has been recurrently employed to regularize and calculate orbits of celestial objects, besides giving rise to various applications in atomic physics (see, e.g., Ref. 3, and references therein). In this work, we apply this idea to the case when M, instead of representing the configuration space of a particle, is the target space of a given field theory. Specifically, we show that by lifting the equations of magnetostatics (in the sense above), it is possible to obtain the Seiberg-Witten equations (SWE) on $\mathbb{R}^3$ provided that a certain constraint is imposed on the resulting fields. Moreover, we show that such constraint naturally gives rise to an iterative method to generate particular solutions to the SWE and Freund equations on $\mathbb{R}^3$ and its dimensionally reduced spaces.

It should be kept in mind that the SWE do not admit nontrivial L^2 solutions in flat space[4] (the same is not true for the Freund equations[5]). However, singular solutions to the SWE in flat space do exist,[5,6] with physical interest. Another point to be emphasized is that the lifting procedure considered here (Sec. II) is not new since it is implicit in the pioneer work of Loss and Yau on zero modes of the three-dimensional Dirac operator[7] (it is also known that, by applying the Kustaanheimo-Stiefel transformation to the vector potential coupled to a Dirac spinor, one recovers the *ansatz* of Loss and Yau[8]). In fact, our formulas for the relevant Abelian potential A_k and wave function $|\psi\rangle$ are the same as those of Ref. 7, where A_k and $|\psi\rangle$ are given in terms of a generating vector field, but with the differences that, in our case, such generating vector field satisfies a certain constraint and that, due to the singular nature of the present problem, we do not demand that the associated fields be square integrable.

It is precisely such constraint that gives rise, in our approach, to the aforementioned iterative method to the SWE and Freund equations on $\mathbb{R}^3$. This is considered in Sec. III, where we also show that application of such method recovers some known solutions to the SWE and Freund

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equations and yields, to the best of our knowledge, previously unnoticed solutions to the SWE. In particular, we obtain an axisymmetric singular solution to the SWE on $\mathbb{R}^3$. We conclude by presenting some final remarks in Sec. IV.

II. LIFTING THE MAGNETOSTATICS EQUATIONS

We start from the equations of magnetostatics,

$$\nabla \cdot \boldsymbol{H} = 0, \tag{1a}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J}, \tag{1b}$$

where $\boldsymbol{J}$ is the steady current associated with the magnetic field $\boldsymbol{H}$ (we use Heaviside-Lorentz units with $c=1$). Let $|\psi\rangle$ be a two-component spinor such that

$$H^k = \langle\psi|\sigma^k|\psi\rangle, \quad k=1,2,3, \tag{2}$$

where $\sigma^1,\sigma^2,\sigma^3$ are the Pauli matrices. For each $\boldsymbol{r}\in\mathbb{R}^3$, $\boldsymbol{H}(\boldsymbol{r})$ can be formally regarded as the "polarization vector" or "spin density" associated with $|\psi(\boldsymbol{r})\rangle\in\mathbb{C}^2$, as in quantum mechanics textbooks.[9] The general solution of Eq. (2) for $|\psi\rangle$ in terms of $\boldsymbol{H}$ is given by

$$|\psi\rangle = e^{-i\chi}\frac{1}{\sqrt{2(H+H^3)}}\begin{pmatrix} H+H^3 \\ H^1+iH^2 \end{pmatrix}, \tag{3}$$

where $H=\|\boldsymbol{H}\|$ and $e^{-i\chi}$ is an arbitrary phase factor. In spherical coordinates, Eq. (3) assumes the familiar form

$$|\psi\rangle = e^{-i\chi}\sqrt{H}\begin{pmatrix} \cos(\alpha/2) \\ e^{i\beta}\sin(\alpha/2) \end{pmatrix},$$

where $\boldsymbol{H}=H(\sin\alpha\cos\beta,\sin\alpha\sin\beta,\cos\alpha)$. It is interesting to note that this is a (trivial) application of what has been termed the inversion theorem,[11] an useful result (especially in four dimensions[12,13]) when one wants to reconstruct a given spinor, apart from arbitrary phases, from its bilinear covariants.

Before transferring the dynamics (Eq. (1)) from $\boldsymbol{H}$ to $|\psi\rangle$, we briefly consider the geometry underlying Eqs. (2) and (3). Let S^n_a denote the n-sphere of radius a in $\mathbb{R}^{n+1}$, and consider the map $\pi_a: S^3_a \to S^2_{a^2}$ taking a two-component spinor $|\phi\rangle\in S^3_a\subset\mathbb{C}^2$ into the vector $\boldsymbol{s}\in S^2_{a^2}$ with components $s^k=\langle\phi|\sigma^k|\phi\rangle$. Here $|\phi\rangle=\binom{z_1}{z_2}\in S^3_a\subset\mathbb{C}^2$ means that $|z_1|^2+|z_2|^2=a^2$. This defines a principal fiber bundle $U(1)\cdots S^3_a\to S^2_{a^2}$ which is essentially the first Hopf bundle (where one usually takes $a=1$).[10] More generally, one can drop the requirement that $|\phi\rangle$ belongs to a sphere of fixed radius and consider the map $\pi:\mathbb{R}^4\to\mathbb{R}^3$ taking $|\phi\rangle\in\mathbb{C}^2\cong\mathbb{R}^4$ into $s^k=\langle\phi|\sigma^k|\phi\rangle$. In this way, π is a natural extension of the Hopf map $S^3\to S^2$ to $\mathbb{R}^4\to\mathbb{R}^3$, in which each sphere of radius $a>0$ in $\mathbb{R}^4$ is mapped into the sphere $S^2_{a^2}\subset\mathbb{R}^3$, and the origin of $\mathbb{R}^4$ is mapped into the origin of $\mathbb{R}^3$. Such map defines the so-called Kustaanheimo-Stiefel transformation[1,2] (this no longer gives rise to a principal fiber bundle, since the fiber over the origin is just a point). Note that, in our case, Eq. (2) defines a Kustaanheimo-Stiefel transformation on the corresponding *target spaces*, relating, for each $\boldsymbol{r}$, the vector $\boldsymbol{H}(\boldsymbol{r})\in\mathbb{R}^3$ to the spinor $|\psi(\boldsymbol{r})\rangle\in\mathbb{C}^2\cong\mathbb{R}^4$. We also note that Eq. (3) yields, for each fixed $\boldsymbol{r}$, a local section of the bundle $U(1)\cdots S^3_H\to S^2_{H^2}$ over $S^2_{H^2}\backslash\{\text{south pole}\}$. A related local section over $S^2_{H^2}\backslash\{\text{north pole}\}$ can be similarly obtained.

Going back to Eq. (3), it is easy to see that the density matrix associated with $|\psi\rangle$ is given by

$$|\psi\rangle\langle\psi| = \tfrac{1}{2}(H\mathbb{1} + H^k\sigma_k), \tag{4}$$

where $\mathbb{1}$ is the identity 2×2 matrix (notice that we are working with Cartesian coordinates in Euclidean flat space, so that indices can be freely raised and lowered). For what follows, it is useful to define the following matrix-valued functions:

$$\mathsf{H}(\boldsymbol{r}) = H^k(\boldsymbol{r})\sigma_k, \tag{5a}$$

$$\mathsf{J}(\boldsymbol{r}) = J^k(\boldsymbol{r})\sigma_k. \tag{5b}$$

Then, it is easily seen that Eq. (1) can be equivalently written, in terms of H and J, as

$$\partial\mathsf{H} = i\mathsf{J}, \tag{6}$$

where $\partial = \sigma^k\partial_k$ (this follows at once from the relationship $\sigma^i\sigma^j = \delta^{ij}\mathbb{1} + i\epsilon^{ijk}\sigma_k$ satisfied by the Pauli matrices, where ϵ^{ijk} is the totally antisymmetric symbol with $\epsilon^{123}=1$).

We now transfer the dynamics defined by Eq. (1) from $\boldsymbol{H}$ to $|\psi\rangle$. From Eq. (4):

$$\mathsf{H} = 2|\psi\rangle\langle\psi| - H\mathbb{1},$$

which leads, upon substitution into Eq. (6), to

$$\sigma^k\left[\partial_k|\psi\rangle\langle\psi| + |\psi\rangle\partial_k\langle\psi| - \frac{1}{2}\partial_k H - \frac{i}{2}J_k\right] = 0.$$

Our aim is to obtain a differential equation governing the dynamics of $|\psi\rangle$. To that end, we right-multiply the above equation by $|\psi\rangle$ and use the fact that $\langle\psi|\psi\rangle = H$. This yields

$$\sigma^k\left[\partial_k + \frac{1}{2H}\partial_k H - \frac{1}{H}\langle\psi|\partial_k|\psi\rangle - \frac{i}{2H}J_k\right]|\psi\rangle = 0. \tag{7}$$

The term $\langle\psi|\partial_k|\psi\rangle$ can be computed by a straightforward calculation; it follows from Eq. (2) that

$$\langle\psi|\partial_k|\psi\rangle = \frac{1}{2}\partial_k H + \frac{i}{2(H+H^3)}(H^1\partial_k H^2 - H^2\partial_k H^1) - iH\partial_k\chi.$$

Upon substitution into Eq. (7), this leads to

$$\sigma^k\left[\partial_k + i\left(\partial_k\chi - \frac{1}{2H(H+H^3)}(H^1\partial_k H^2 - H^2\partial_k H^1) - \frac{1}{2H}J_k\right)\right]|\psi\rangle = 0.$$

Defining

$$A_k := -\frac{1}{2H(H+H^3)}(H^1\partial_k H^2 - H^2\partial_k H^1) - \frac{1}{2H}J_k, \tag{8}$$

which can be fully expressed in terms of $\boldsymbol{H}$ (through Eq. (1b)) as

$$A_k = -\frac{1}{2H(H+H^3)}(H^1\partial_k H^2 - H^2\partial_k H^1) - \frac{1}{2H}(\nabla\times\boldsymbol{H})_k, \tag{9}$$

we finally get

$$i\sigma^k(\partial_k + iA_k + i\partial_k\chi)|\psi\rangle = 0. \tag{10}$$

Therefore, $|\psi\rangle$ satisfies the Weyl equation with the Abelian potential A_k (i.e., the massless Dirac equation for two-component spinors representing states of definite chirality). Note that χ enters Eqs. (3) and (9) simply as a gauge parameter.

It is interesting to note that Eq. (1b) enters the derivation above merely as a bookkeeping device. In fact, Eq. (10) follows as long as $\boldsymbol{H}$ satisfies Eq. (1a), regardless of any interpretation of the right-hand side of Eq. (1b) as an external current. In any case, it should be noted that Eq. (1b) does affect the form of Eq. (10) through A_k.

An important observation for what follows is that the field strength B_k associated with A_k,

$$\boldsymbol{B} := \nabla \times \boldsymbol{A}, \tag{11}$$

does not have to bear any relation to the magnetic field $\boldsymbol{H}$ we started with.

III. SEIBERG-WITTEN AND FREUND EQUATIONS

Let us summarize what has been done above. We started from the equations of magnetostatics, expressed the magnetic field $\boldsymbol{H}$ in terms of the associated spinor field $|\psi\rangle$, and then lifted the dynamics from $\boldsymbol{H}$ to $|\psi\rangle$. As a result, the following set of equations (Eqs. (2), (10), and (11)) was obtained:

$$\langle\psi|\sigma^k|\psi\rangle = H^k, \tag{12a}$$

$$i\sigma^k(\partial_k + iA_k)|\psi\rangle = 0, \tag{12b}$$

$$\epsilon^{ijk}\partial_i A_j = B^k, \tag{12c}$$

where we chose to suppress the terms associated with the gauge parameter χ. The SWE and Freund equations in three dimensions have been discussed in detail in Ref. 5 (see especially its Eqs. (3.5) and (3.6)) from where we note a remarkable similarity with Eq. (12). More precisely:

1. Eqs. (12a)–(12c) are the Seiberg-Witten equations on $\mathbb{R}^3$ *provided that* $H_k = +B_k$;
2. Eqs. (12a)–(12c) are the Freund equations on $\mathbb{R}^3$ *provided that* $H_k = -B_k$.

Therefore, the constraint

$$\boldsymbol{H} = \pm \boldsymbol{B} \tag{13}$$

yields a natural *ansatz* for obtaining solutions to the Seiberg-Witten and Freund equations for $\boldsymbol{A}$, $\boldsymbol{B}$, and $|\psi\rangle$ on $\mathbb{R}^3$. Using Eq. (9), this amounts to solving

$$\boldsymbol{H} = \pm \nabla \times \left(-\frac{1}{2H(H+H^3)}(H^1 \nabla H^2 - H^2 \nabla H^1) - \frac{1}{2H} \nabla \times \boldsymbol{H} \right) \tag{14}$$

for $\boldsymbol{H}$. This equation has been recently studied from a group-theoretical perspective in Ref. 14 to examine the Lie symmetries of the SWE and Freund equations on $\mathbb{R}^3$.

It is interesting to note that, given a solution of Eq. (14), with the + or − sign, respectively, one immediately obtains $|\psi\rangle$, A_k, and B_k from Eqs. (3), (9), and (13):

$$|\psi\rangle = \frac{1}{\sqrt{2(H+H^3)}} \begin{pmatrix} H+H^3 \\ H^1 + iH^2 \end{pmatrix}, \tag{15a}$$

$$\boldsymbol{A} = -\frac{1}{2H(H+H^3)}(H^1 \nabla H^2 - H^2 \nabla H^1) - \frac{1}{2H} \nabla \times \boldsymbol{H}, \tag{15b}$$

$$\boldsymbol{B} = \pm \boldsymbol{H}. \tag{15c}$$

As noted in Sec. I, the above expressions for $|\psi\rangle$ and $\boldsymbol{A}$ in terms of a generating vector field (which is given, in this case, by $\boldsymbol{H}$) were first obtained in the study of zero modes of the massless Dirac operator in Ref. 7.

A. An iterative procedure.

We now show how Eq. (14) can serve as a basis for an iterative procedure for obtaining $\boldsymbol{H}$, and thus $|\psi\rangle$, $\boldsymbol{A}$ and $\boldsymbol{B}$ satisfying the SWE or Freund equations on flat space. The procedure goes as follows. Choose an initial guess $\boldsymbol{H}_{(0)}$ for $\boldsymbol{H}$; substitute $\boldsymbol{H}_{(0)}$ into the right-hand side of Eq. (14) and consider the result as a second estimate $\boldsymbol{H}_{(1)}$ for $\boldsymbol{H}$; then substitute $\boldsymbol{H}_{(1)}$ into the right-hand side of Eq. (14), and so on. If the sequence $\boldsymbol{H}_{(k)}$ converges, its limit is a solution to Eq. (14). It is important to note that this procedure does fail in most cases, either by computational or mathematical difficulties (we come back to this point in Sec. IV). Nevertheless, when it succeeds, we end up with a solution to the Seiberg-Witten or Freund equations. In the remainder of this section, we show representative results of a limited experiment in algebraic computation, performed with the software MATHEMATICA, implementing such iterative procedure.

Example 1: Starting with $\boldsymbol{H}_{(0)}=\pm(x,y,z)$, we obtain the solution

$$\boldsymbol{B}=\mp\frac{1}{2r^3}(x,y,z), \tag{16a}$$

$$\boldsymbol{A}=\frac{1}{2r(r\pm z)}(y,-x,0), \tag{16b}$$

$$|\psi\rangle=\frac{1}{2r\sqrt{r(r\pm z)}}\begin{pmatrix} r\pm z \\ \pm(x+iy)\end{pmatrix} \tag{16c}$$

to the Freund equations, where $r=\sqrt{x^2+y^2+z^2}$. A monopole solution of this kind was first obtained in Ref. 15 (see also Ref. 5, where the authors discuss in detail how the Freund equations are related to the SWE on $\mathbb{R}^3$).

Example 2: Starting with $\boldsymbol{H}_{(0)}=\pm(\sinh\kappa y,0,0)$, we obtain the solution

$$\boldsymbol{B}=\mp\frac{\kappa^2}{\sinh^2\kappa y}\mathbf{e}_x, \tag{17a}$$

$$\boldsymbol{A}=\pm\kappa\coth\kappa y\mathbf{e}_z, \tag{17b}$$

$$|\psi\rangle=\frac{\kappa}{\sqrt{2}\sinh\kappa y}\begin{pmatrix} 1 \\ \mp 1\end{pmatrix} \tag{17c}$$

to the Seiberg-Witten equations (in order to avoid dealing with the absolute value function in the algebraic computation procedure of Examples 2 and 3, it is useful to first restrict attention to the domain given by $x>0$, $y>0$, and $z>0$, and later extend the obtained solution to any nonzero x, y, and z). This solution is essentially the same as the effectively one-dimensional solution to the SWE found in Ref. 6. On the other hand, if we start with $\boldsymbol{H}_{(0)}=\pm(\cosh\kappa y,0,0)$, we obtain the solution

$$\boldsymbol{B}=\pm\frac{\kappa^2}{\cosh^2\kappa y}\mathbf{e}_x,$$

$$\boldsymbol{A}=\pm\kappa\tanh\kappa y\mathbf{e}_z,$$

$$|\psi\rangle = \frac{\kappa}{\sqrt{2}\cosh \kappa y}\begin{pmatrix} 1 \\ \mp 1 \end{pmatrix}$$

to the Freund equations. We note that similar expressions were also obtained in Ref. 6 through analytic continuation of the aforementioned one-dimensional solution to the SWE.

Example 3: Starting with $\boldsymbol{H}_{(0)} = \pm(xyz, 0, 0)$, we obtain the solution

$$\boldsymbol{B} = \mp\left(\frac{1}{y^2} + \frac{1}{z^2}, 0, 0\right), \tag{18a}$$

$$\boldsymbol{A} = \pm\frac{1}{y^2 + z^2}\left(0, -\frac{y^2}{z}, \frac{z^2}{y}\right), \tag{18b}$$

$$|\psi\rangle = \sqrt{\frac{1}{2y^2} + \frac{1}{2z^2}}\begin{pmatrix} 1 \\ \mp 1 \end{pmatrix} \tag{18c}$$

to the Seiberg-Witten equations.

For solutions of this kind, in which $\boldsymbol{B}(\boldsymbol{r})$ is always parallel to some fixed vector $\mathbf{n}$ and only depends on coordinates (u, v) of a plane orthogonal to $\mathbf{n}$, the quantity $\omega = \frac{1}{2}\ln B$ is known[6] to satisfy the Liouville equation $4\partial_z\partial_{\bar{z}}\omega = e^{2\omega}$, where z now denotes the complex coordinate $z = u + iv$ and $B = \|\boldsymbol{B}\|$ [it should be clear from the context when z refers to the complex coordinate $z = u + iv$ or to the Cartesian coordinate in (x, y, z)]. Using the *ansatz*

$$\omega = \frac{1}{2}\ln\frac{4(\mathrm{d}g/\mathrm{d}z)(\mathrm{d}\bar{g}/\mathrm{d}\bar{z})}{(1 - g\bar{g})^2}, \tag{19}$$

with $g(z)$ an arbitrary analytic function, the authors of Ref. 6 construct a family of effectively two-dimensional solutions to the SWE with interesting properties. We note, however, that the above solution (18a) apparently does not belong to such family, obtained via *ansatz* (19). In any case, we show in the Appendix that the alternative *ansatz*

$$\omega = \frac{1}{2}\ln\frac{(\mathrm{d}g/\mathrm{d}z)(\mathrm{d}\bar{g}/\mathrm{d}\bar{z})}{[\Im(g)]^2}, \tag{20}$$

where $\Im(g)$ denotes the imaginary part of g, does yield the above solution. In fact, as discussed in the Appendix, (18a) is the $n = 2$ case of a family of two-dimensional singular solutions generated by the choice $g(z) = z^n$ in (20), with $n = \frac{1}{2}, 1, \frac{3}{2}, \ldots$ [it should be noted that both (19) and (20) are particular cases of the well-known general solution of the Liouville equation[16] (see Appendix)].

Example 4: Starting with $\boldsymbol{H}_{(0)} = \pm(y, -x, 0)$, we obtain the axisymmetric solution

$$\boldsymbol{B} = \pm\frac{1}{2\rho^2}\mathbf{e}_\phi, \tag{21a}$$

$$\boldsymbol{A} = -\frac{1}{2\rho}\mathbf{e}_\phi \pm \frac{1}{2\rho}\mathbf{e}_z, \tag{21b}$$

$$|\psi\rangle = \frac{1}{2\rho}\begin{pmatrix} 1 \\ \pm ie^{i\phi} \end{pmatrix} \tag{21c}$$

to the Seiberg-Witten equations, where cylindrical coordinates ρ, ϕ, z, with $\rho = \sqrt{x^2 + y^2}$ and $\phi = \arctan(y/x)$, were used. Such $\boldsymbol{B}$ is similar (but different in the ρ-dependence) to the magnetic field $\boldsymbol{B} \propto (1/\rho)\mathbf{e}_\phi$ produced by a steady current along the z axis. The integral curves of $\boldsymbol{A}$ are

helices of constant ρ going upward (downward) with respect to the z axis. We note that the first term $\boldsymbol{A}_{AB}=-(1/2\rho)\mathbf{e}_{\phi}$ of $\boldsymbol{A}$ is in fact an Aharonov-Bohm potential, with holonomy given by

$$\int_{\gamma} \boldsymbol{A}_{\mathrm{AB}}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} = -\pi, \tag{22}$$

where γ is any loop winding once around the z axis. Note that the Aharonov-Bohm term $\boldsymbol{A}_{\mathrm{AB}}$ is actually *implied* by $\boldsymbol{B}$ [through Eq. (15b)] even though $\boldsymbol{B}$ in Eq. (21a) does not receive any contribution from the curl of $\boldsymbol{A}_{\mathrm{AB}}$ (which is actually zero for $\rho \neq 0$). In this way, the purely azimuthal magnetic field of Eq. (21a), defined away from the z axis, unavoidably gives rise, through $\boldsymbol{A}_{\mathrm{AB}}$, to the "additional" singular magnetic field $-\pi\delta(x)\delta(y)\mathbf{e}_z$ along the z axis (which is the same as the magnetic field of an infinitely long and infinitesimally thin solenoid at the z axis).

It is also interesting to note that, although the two solutions to the SWE in Eq. (21a) (given, respectively, by its plus and minus signs) wind in opposite directions with respect to the xy plane, their associated potentials both wind clockwise, with identical Aharonov-Bohm terms, the only difference residing in their z components.

IV. CLOSING REMARKS

In all the examples above, the final solution for $\boldsymbol{H}$ is obtained in *exact form* after very few iterations. On the other hand, some experience with the above computational experiment shows that a generic initial condition for $\boldsymbol{H}$ typically leads to an increasingly complicated algebraic expression at each iteration, thereby requiring further investigation on convergence issues related to such method. A natural question to ask is what are the initial conditions under which the sequence $\boldsymbol{H}_{(k)}$ may be guaranteed to converge since, under such circumstances, the approach presented here could be used to define classes of solutions to the SWE and Freund equations iteratively.

Finally, we note that the approach presented here suggests a natural generalization to the four-dimensional case, where one may try to lift the whole set of (Euclidean) Maxwell equations to obtain (singular) solutions to the SWE on $\mathbb{R}^4$. This is the subject of work in progress.

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APPENDIX

The general solution to the Liouville equation,

$$4\partial_z\partial_{\bar{z}}\omega = e^{2\omega},$$

was first given by Liouville in Ref. 16 (where the author considers, in fact, the corresponding equation for $\lambda=e^{2\omega}$, and with real variables). It is given by

$$\omega(z,\bar{z}) = \frac{1}{2}\ln\frac{4(\mathrm{d}g(z)/\mathrm{d}z)(\mathrm{d}h(\bar{z})/\mathrm{d}\bar{z})}{[1-g(z)h(\bar{z})]^2}, \tag{A1}$$

where $g(z)$ and $h(\bar{z})$ are arbitrary analytic and antianalytic functions, respectively. The *ansatz* of Ref. 6, given by Eq. (19), is recovered from Eq. (A1) if the natural choice $h(\bar{z})=\overline{g(z)}$ is made. However, as mentioned in Example 3 of Sec. III, the solution given by $B=1/u^2+1/v^2$ is apparently not recovered by such *ansatz* (recall that B is related to ω by $B=e^{2\omega}$, where $B=\|\boldsymbol{B}\|$ and now z denotes the complex coordinate $z=u+iv$). This motivates the search for an alternative *ansatz* for such B. Generalizing the above choice of h in terms of g to $h(\bar{z})=\overline{g(z)}^{\nu}$, it is not hard to show that,

in general, the requirement that ω be real restricts ν to $+1$ or -1, which yield Eq. (19) and Eq. (20), respectively. Therefore, the alternative *ansatz* (20) is given by the choice $h(\bar{z})=1/\overline{g(z)}$ in (A1). The solution of Example 3 is recovered from such *ansatz* for $g(z)=z^2$, as a direct calculation shows.

More generally, choosing $g(z)=z^n$ in Eq. (20) leads to the solution $B=n^2/(\rho^2 \sin^2 n\phi)$, where polar coordinates $z=\rho e^{i\phi}$ were used. The requirement that B be single-valued restricts n to $n=\frac{1}{2},1,\frac{3}{2},\ldots$ (note that B is insensitive to the change $n\to -n$). In this way, the solution of Example 3 is the $n=2$ case of such family of two-dimensional singular solutions. Note that the solution corresponding to a given n is singular along $2n$ lines starting at the origin and passing through the roots of unity of order $2n$.

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The spectrum minimum for random Schrödinger operators with indefinite sign potentials

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This paper sets out to study the spectral minimum for an operator belonging to the family of random Schrödinger operators of the form $H_{\lambda,\omega}=-\Delta+W_{\text{per}}+\lambda V_\omega$, where we suppose that V_ω is of Anderson type and the single site is assumed to be with an indefinite sign. Under some assumptions we prove that there exists $\lambda_0>0$ such that for any $\lambda\in[0,\lambda_0]$, the minimum of the spectrum of $H_{\lambda,\omega}$ is obtained by a given realization of the random variables. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Among the most investigated and dealt with operators in the field of mathematical physics problems are random Schrödinger operators of the form

$$H_\omega=-\Delta+W_{\text{per}}+V_\omega=H_0+V_\omega, \tag{1.1}$$

where W_{per} is a $\mathbb{Z}^d$-periodic function and V_ω is a random potential having the Anderson form, i.e., $V_\omega(\cdot)=\Sigma_{\gamma\in\mathbb{Z}^d}\omega_\gamma f(\cdot-\gamma)$. See Refs. 2 and 12 for the physical motivations.

Here we consider H_ω as a family of self-adjoint operators in $L^2(\mathbb{R}^d)$ with some appropriate domain. In fact, we are not dealing with a single Schrödinger operator, but with rather large family of operators H_ω, indexed by the random parameter $\omega\in\Omega$. Nevertheless, from the general theory of ergodic operators, which applies to H_ω, it is known[9] that the spectrum of H_ω is *almost surely deterministic*, i.e., there exists a set $\Sigma\subset\mathbb{R}$ such that the spectrum $\sigma(H_\omega)$ coincides with Σ for $\mathbb{P}$-almost every $\omega\in\Omega$. (Here $\mathbb{P}$ is the probability measure on the probability space Ω.)

The study of the spectral theory of operators of the form (1.1) has drawn the attention of many researchers for the importance of the related results. In fact, it is linked to the systems evolutions for which the Hamiltonian is described by (1.1). The goal of this paper is to discuss one of the problems that remain unsolved: the spectrum location of H_ω, precisely the spectrum infimum. This will be carried out in the case when the single site f does not have a definite sign.

As the main object is to study the location of the spectrum, let us recall the following basic results already known on this subject and stated by Kirsch and Martinelli:[2,3]

Theorem 1.1:

$$\Sigma(H_\omega)=\overline{\bigcup_{(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}\in\mathcal{P}}\Sigma\left(-\Delta+W_{\text{per}}+\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma f(x-\gamma)\right)}. \tag{1.2}$$

Here $\mathcal{P}$ is the set of all periodic sequences $\{\omega_\gamma\}_{\gamma\in\mathbb{Z}^d}$, with an arbitrary period such that ω_γ is in the support of μ for all γ and $\Sigma(H)$ is the spectrum of H.

As has been said above the proof of Theorem 1.1 exists in Refs. 2 and 3 and is based on Weyl sequences and probabilistic arguments. Notice that this theorem reduces the determination of the

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spectra of random Schrödinger operators for the case of periodic Schrödinger operators. As it is well known[10] that the spectrum of periodic operators have a band structure, this will be the case for $\Sigma(H_\omega)$ with the possibility to close gaps.

Under additional assumptions on f more is known:

Theorem 1.2: *If f has a fixed sign, i.e., $f\leqslant 0$ or $f\geqslant 0$ and if μ is supported in $[\omega^-,\omega^+]$, then*

$$\Sigma(H_\omega)=\bigcup_{\omega\in[\omega^-,\omega^+]}\Sigma\left(-\Delta+W_{\mathrm{per}}+\omega\sum_{\gamma\in\mathbb{Z}^d}f(x-\gamma)\right). \tag{1.3}$$

In particular,

$$\inf\Sigma(H_\omega)=\begin{cases}\inf\Sigma\left(-\Delta+W_{\mathrm{per}}+\omega^+\sum_{\gamma\in\mathbb{Z}^d}f(x-\gamma)\right) & \text{if } f\leqslant 0\\ \inf\Sigma\left(-\Delta+W_{\mathrm{per}}+\omega^-\sum_{\gamma\in\mathbb{Z}^d}f(x-\gamma)\right) & \text{if } f\geqslant 0.\end{cases} \tag{1.4}$$

Theorem 1.2 is a simple consequence of Theorem 1.1. Indeed, using (1.2) and the fact that constant sequences $\{\omega_\gamma=\omega\in\operatorname{supp}\mu\}\subset\mathcal{P}$, we get that the right-hand side of (1.3) is naturally contained in $\Sigma(H_\omega)$. For the inverse inclusion, let $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}\in\mathcal{P}$ be k-periodic and let $[a,b]$ be the nth band of the k periodic operator $H_{\omega,k}=-\Delta+W_{\mathrm{per}}+\Sigma_{\gamma\in\mathbb{Z}^d}\omega_\gamma f(x-\gamma)$. Let $[a_1,b_2]$ and $[a_2,b_2]$ be the nth bands of, respectively, $-\Delta+W_{\mathrm{per}}+\omega^-\Sigma_{\gamma\in\mathbb{Z}^d}f(x-\gamma)$ and $-\Delta+W_{\mathrm{per}}+\omega^+\Sigma_{\gamma\in\mathbb{Z}^d}f(x-\gamma)$ (both seen as k-periodic operators). By the min-max principle we have $a_1\leqslant a\leqslant a_2$ and $b_1\leqslant b\leqslant b_2$. As the bands of $-\Delta+W_{\mathrm{per}}+\omega\Sigma_{\gamma\in\mathbb{Z}^d}f(x-\gamma)$ depend continuously on ω, we deduce that $\Sigma(-\Delta+W_{\mathrm{per}}+\Sigma_{\gamma\in\mathbb{Z}^d}\omega_\gamma f(x-\gamma))$ is contained in the r.h.s of (1.3). The proof of (1.3) is ended by taking into account the fact that these sets are closed.

For (1.4) it is a simple consequence of monotonicity of the model, it is increasing when $f\geqslant 0$ and decreasing when $f\leqslant 0$. indeed if $f\leqslant 0$, and $\widetilde{\omega}_\gamma\leqslant\hat{\omega}_\gamma$ for any $\gamma\in\mathbb{Z}^d$ then in the sense form we have

$$-\Delta+W_{\mathrm{per}}+\sum_{\gamma\in\mathbb{Z}^d}\hat{\omega}_\gamma f(x-\gamma)\leqslant-\Delta+W_{\mathrm{per}}+\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma f(x-\gamma).$$

The situation is more complicated and different when the single site f changes the sign, as the monotonicity property is not true in this case. We notice that recently Lott and Stolz have conjectured[6] that in dimension one, the spectral minimum of random displacement models is realized through the pair formation of the single site.

A. The model

Our basic object of study is the so-called *Anderson model*, a random Schrödinger operator of the form

$$H_{\lambda,\omega}=-\sum_{i=1}^{d}\frac{\partial^2}{\partial x_i^2}+W_{\mathrm{per}}+\lambda\sum_{\gamma\in\mathbb{Z}^d}\omega_\gamma f(x-\gamma), \tag{1.5}$$

where

- W_{per} is a $\mathbb{Z}^d$-periodic and bounded function.
- λ is a positive parameter
- $(\omega_\gamma)_{\gamma\in\mathbb{Z}^d}$ is a family of independent, identically distributed random variables taking values in $[\omega^-,\omega^+]$. We denote by μ the probability distribution.
- For $C_0=\left[-\frac{1}{2},\frac{1}{2}\right]^d$, the single site potential $f\in C_0^\infty(C_0)$ such that $f\in l^1(L^p(\mathbb{R}^d))$, with $p=2$ if $d\leqslant 3$, $p>2$ if $d=4$ and $p=d/2$ if $d\geqslant 5$ and $f=f^+ +f^-$, with $f^+\geqslant 0$, $f^-\leqslant 0$, and $f^+\cdot f^-=0$.

By Refs. 2 and 9, we know that $H_{\lambda,\omega}$ is an essentially self-adjoint operator on $L^2(\mathbb{R}^d)$ with the domain $C_0^\infty(\mathbb{R}^d)$, we denote by $H_{\lambda,\omega}$ its self-adjoint extension.

It is an ergodic operator so, according to Refs. 2 and 9, we know that there exist $\Sigma_\lambda, \Sigma_{\lambda,\mathrm{pp}}, \Sigma_{\lambda,\mathrm{ac}}$, and $\Sigma_{\lambda,\mathrm{sc}}$ closed and nonrandom sets of $\mathbb{R}$ such that Σ_λ is the spectrum of $H_{\lambda,\omega}$ with probability one and such that if σ_{pp} (respectively, σ_{ac} and σ_{sc}) design the pure point spectrum (the absolutely continuous and singular continuous spectrum, respectively) of $H_{\lambda,\omega}$, then $\Sigma_{\lambda,\mathrm{pp}} = \sigma_{\mathrm{pp}}, \Sigma_{\lambda,\mathrm{ac}} = \sigma_{\mathrm{ac}}$ and $\Sigma_{\lambda,\mathrm{sc}} = \sigma_{\mathrm{sc}}$ with probability one.

B. The result

Let us introduce the following operators:

$$H_{\lambda,\omega^-} = -\sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} + W_{\mathrm{per}} + \lambda \sum_{\gamma\in\mathbb{Z}^d} \omega^- f(x-\gamma),$$

and

$$H_{\lambda,\omega^+} = -\sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} + W_{\mathrm{per}} + \lambda \sum_{\gamma\in\mathbb{Z}^d} \omega^+ f(x-\gamma).$$

We denote by $\Sigma_{\lambda,\omega^-}$ and $\Sigma_{\lambda,\omega^+}$ the spectrum of H_{λ,ω^-} and H_{λ,ω^+}, respectively.

As we will see (Sec. II A) $H_{\lambda,\omega}$ can be considered as a perturbation of the periodic operator H_{λ,ω^-}. Let $\varphi_{\lambda,1}(x,\theta(\lambda))$ be the Floquet eigenfunction associated to the first Floquet eigenvalue $E_1(\lambda,\theta)$ of H_{λ,ω^-}. Let $(\theta_k(\lambda))_{1\leqslant k\leqslant m}$ be the points where $E_1(\lambda,\theta)$ attains its minimum. We set

$$A(0) = (\langle f\varphi_{0,1}(\cdot,\theta_k(0)), \varphi_{0,1}(\cdot,\theta_{k'}(0))\rangle_{L^2(C_0)})_{1\leqslant k,k'\leqslant m}.$$

We prove that

Theorem 1.3: *Let $H_{\lambda,\omega}$ be the operator defined by* (1.5).

If the matrix $A(0)$ is positive-definite, then there exists $\lambda_0>0$ such that for any $\lambda\in[0,\lambda_0]$ we have

$$\inf(\Sigma_\lambda) = \inf(\Sigma_{\lambda,\omega^-}).$$

If the matrix $A(0)$ is negative-definite, then there exists $\lambda_0>0$ such that for any $\lambda\in[0,\lambda_0]$ we have

$$\inf(\Sigma_\lambda) = \inf(\Sigma_{\lambda,\omega^+}).$$

Remark 1.4: *Theorem* 1.3 *is stated for the infimum of the spectrum. Under some additional assumptions the same result is still true for the internal edges of the spectrum.*

The result remains true if we replace $\mathbb{Z}^d$ by any nondegenerate d-dimensional lattice $\Gamma = \oplus_{i=1}^d \mathbb{Z}e_i$, with $(e_1,\ldots,e_d)$ some basis of $\mathbb{R}^d$.

The analogous problem for the random magnetic Schrödinger operator is considered and studied in Ref. 1.

Theorem 1.3 *can be considered as a first step toward the physically motivated applications. One of them is the study of the so-called Lifshitz tails of the integrated density of states. This could be done under some additional assumptions on the behavior of the random variables in the vicinity of ω^- or ω^+.*[4,7,8] *Another one is the spectral localization.*[12,13]

The proof of Theorem 1.3, is given in Sec. III. It is based on the reduction procedure. This powerful technique was predicted by Klopp[4] and used in several works.[1,7,8]

As stated the proof of Theorem 1.3 can be divided naturally into two parts, we shall discuss them separately.

Indeed, if $A(0)$ is positive-definite we will conjugate H_ω with $\Pi_{\lambda,0}$, the spectral projection for H_{λ,ω^-} on the first band. Then we prove that

$$\Pi_{\lambda,0} H_{\lambda,\omega} \Pi_{\lambda,0} \geqslant E_{\lambda,\omega^-} \Pi_{\lambda,0}.$$

Here E_{λ,ω^-} is the bottom of the spectrum of the periodic operator H_{λ,ω^-}.

If $A(0)$ is negative-definite we will conjugate H_ω with $\Pi_{\lambda,0}$, the spectral projection for H_{λ,ω^+} on the first band. Then we prove

$$\Pi_{\lambda,0} H_{\lambda,\omega} \Pi_{\lambda,0} \geqslant E_{\lambda,\omega^+} \Pi_{\lambda,0}.$$

Here E_{λ,ω^+} is the bottom of the spectrum of the periodic operator H_{λ,ω^+}.

II. PRELIMINARY

Let us consider the following periodic operator:

$$H_{\lambda,\omega^-} = -\Delta + W_{\text{per}} + \lambda \sum_{\gamma \in \mathbb{Z}^d} \omega^- f(\cdot - \gamma). \tag{2.1}$$

For this, it is convenient to consider $H_{\lambda,\omega}$ as a perturbation of H_{λ,ω^-}. Indeed, we have

$$H_{\lambda,\omega} = H_{\lambda,\omega^-} + \lambda \sum_{\gamma \in \mathbb{Z}^d} (\omega_\gamma - \omega^-) f(\cdot - \gamma).$$

For this for $\gamma \in \mathbb{Z}^d$, we set $\widetilde{\omega}_\gamma = \omega_\gamma - \omega^-$ and $V_{\widetilde{\omega}}(\cdot) = \Sigma_{\gamma \in \mathbb{Z}^d} \widetilde{\omega}_\gamma f(\cdot - \gamma)$. We notice that according to the definition of $(\omega_\gamma)_{\gamma \in \mathbb{Z}^d}$ we get that $(\widetilde{\omega}_\gamma)_{\gamma \in \mathbb{Z}^d}$ is a family of random positive and bounded variables.

A. Some Floquet theory

For $\gamma \in \mathbb{Z}^d$, we denote by τ_γ the translation by γ operator, i.e., $(\tau_\gamma \varphi)(x) = \varphi(x - \gamma)$. We have, for any $\gamma \in \mathbb{Z}^d$,

$$\tau_\gamma H_{\lambda,\omega^-} \tau_\gamma^* = \tau_\gamma^* H_{\lambda,\omega^-} \tau_\gamma = H_{\lambda,\omega^-}.$$

Then the so-called Floquet Theory can be used to study H_{λ,ω^-}. For this, we review some standard facts from the Floquet theory for periodic operators. Basic references for this material are Refs. 5, 10, and 11. Let $\mathbb{T}^* = \mathbb{R}^d / (2\pi\mathbb{Z}^d)$. We define $\mathcal{H}$ by

$$\mathcal{H} = \{u(x,\theta) \in L^2_{\text{loc}}(\mathbb{R}^d) \otimes L^2(\mathbb{T}^*);\ \forall\ (x,\theta,\gamma) \in \mathbb{R}^d \times \mathbb{T}^* \times \mathbb{Z}^d; u(x+\gamma,\theta) = e^{i\gamma\theta} u(x,\theta)\}.$$

$\mathcal{H}$ is equipped with the norm

$$\frac{1}{\text{vol}(\mathbb{T}^*)} \int_{\mathbb{T}^*} \|u(x,\theta)\|^2_{L^2(C_0)} \mathrm{d}\theta.$$

For $\theta \in \mathbb{R}^d$ and $u \in \mathcal{S}(\mathbb{R}^d)$; the Schwartz space of rapidly decreasing functions we define

$$(Uu)(x,\theta) = \sum_{\gamma \in \mathbb{Z}^d} e^{i\gamma\cdot\theta} u(x-\gamma).$$

U can be extended as a unitary isometry from $L^2(\mathbb{R}^d)$ to $\mathcal{H}$. Its inverse is given by the formula,

$$\text{for } u \in \mathcal{H}, \quad (U^* u)(x) = \frac{1}{\text{vol}(\mathbb{T}^*)} \int_{\mathbb{T}^*} u(x,\theta) \mathrm{d}\theta.$$

U is a unitary isometry from $L^2(\mathbb{R}^d)$ to $\mathcal{H}$ and $H_{\lambda,\omega}$ admits the Floquet decomposition[5,11]

$$UH_{\lambda,\omega^-}U^* = \int_{\mathbb{T}^*}^{\oplus} H_{\lambda,\omega^-}(\theta)\mathrm{d}\theta.$$

Here $H_{\lambda,\omega^-}(\theta)$ is the operator H_{λ,ω^-} acting on $\mathcal{H}_\theta$, defined by

$$\mathcal{H}_\theta = \{u \in L^2_{\mathrm{loc}}(\mathbb{R}^d);\ \forall\ \gamma \in \mathbb{Z}^d, u(x+\gamma) = e^{i\gamma\theta}u(x)\}.$$

As H_{λ,ω^-} is elliptic, we know that, $H_{\lambda,\omega^-}(\theta)$ has a compact resolvent; hence its spectrum is discrete.[10] We denote its eigenvalues, called Floquet eigenvalues of H_{λ,ω^-}, by

$$E_1(\lambda,\theta) \leqslant E_2(\lambda,\theta) \leqslant \cdots \leqslant E_n(\lambda,\theta) \leqslant \cdots .$$

The corresponding Floquet eigenfunctions are denoted by $(\varphi_{\lambda,j}(x,\cdot))_{j\in\mathbb{N}^*}$. The functions $(\theta \to E_n(\lambda,\theta))_{n\in\mathbb{N}^*}$ are Lipshitz-continuous, and we have

$$E_n(\lambda,\theta) \to +\infty \quad \text{as } n \to +\infty \text{ uniformly in } \theta.$$

The spectrum $\Sigma_{\lambda,\omega^-}$ of H_{λ,ω^-} is made of bands (i.e., $\Sigma_{\lambda,\omega^-} = \cup_{n\in\mathbb{N}^*} E_n(\lambda,\mathbb{T}^*)$.)

Let us note by E_{λ,ω^-} the bottom of the spectrum of $\Sigma_{\lambda,\omega^-}$, i.e., $E_{\lambda,\omega^-} = \inf_{\theta\in\mathbb{T}^d} E_1(\lambda,\theta)$.

It is a well-known fact that, in any dimension, the bottom (the first band) of the spectrum of periodic Schrödinger operators is given by a simple Floquet eigenvalue and that the minimum of this Floquet eigenvalue is nondegenerate and quadratic. More precisely let $\theta(\lambda)$ be an element of

$$Z_\lambda = \{\theta \in \mathbb{T}^*;\ E_1(\lambda,\theta) = E_{\lambda,\omega^-}\}.$$

Then there exist $C>0$ and $\delta>0$ such that

$$\forall |\theta-\theta(\lambda)| \leqslant \delta, \quad \frac{1}{C}|\theta-\theta(\lambda)|^2 \leqslant E_1(\lambda,\theta) - E_{\lambda,\omega^-} \leqslant C|\theta-\theta(\lambda)|^2.$$

Hence, the points where $E_1(\lambda,\theta)$ reaches E_{λ,ω^-} are isolated and as $\mathbb{T}^*$ is compact, one concludes that Z_λ contains only finitely many of the elements. Let m be the cardinal of Z_λ and let us denote them by $(\theta_k(\lambda))_{1\leqslant k\leqslant m}$. One can check that $\theta_k(\lambda)$ depends continuously on λ. For the sake of brevity, we use the notation $\theta_k = \theta_k(\lambda)$.

For $1 \leqslant k \leqslant m$ and $\theta \in \mathbb{T}^*$, we set

$$\zeta_{k,\lambda}(\theta) = \sum_{1\leqslant i\leqslant d} (\theta_i - \theta_{k,i})^2. \tag{2.2}$$

We notice that for any $1 \leqslant k \leqslant m$,

$$\theta \mapsto \varphi_{\lambda,1}(x,\theta)$$

is analytic in a neighborhood of θ_k.

B. Wannier basis

We recall concepts used in Ref. 4. Let $\mathcal{E} \subset L^2(\mathbb{R}^d)$ be a closed subspace invariant by the $\mathbb{Z}^d$-translations, i.e., such that $\Pi^{\mathcal{E}}$, the orthogonal projection on $\mathcal{E}$, satisfies

$$\forall\ \gamma \in \mathbb{Z}^d, \quad \Pi^{\mathcal{E}} = \tau_{-\gamma}\Pi^{\mathcal{E}}\tau_\gamma.$$

Following the computations done in Sec. I B of Ref. 4, we see that there exists an orthonormal system of vectors $(\widetilde{\varphi}_{j,0})_{j\in N}$ such that for $\widetilde{\varphi}_{j,\gamma} = \tau_\gamma(\widetilde{\varphi}_{j,0})$; $(\widetilde{\varphi}_{j,\gamma})_{(j\in N;\gamma\in\mathbb{Z}^d)}$ is an orthonormal basis of $\mathcal{E}$. Such a system is called the ***Wannier basis*** of $\mathcal{E}$. The vectors $(\widetilde{\varphi}_{n,0})_{n\in N}$ are called ***Wannier generators*** of $\mathcal{E}$.

Let $\mathcal{E} \subset L^2(\mathbb{R}^d)$ be a space which is translation-invariant. $\mathcal{E}$ is said to be of finite energy for $H_{\lambda,\omega}$ if $\Pi^{\mathcal{E}}H_{\lambda,\omega}\Pi^{\mathcal{E}}$ is a bounded operator. In this case, $\mathcal{E}$ admits a finite set of Wannier generators.

Let $\Pi_{\lambda,0}(\theta)$ (respectively, $\Pi_{\lambda,+}(\theta)$) be the orthogonal projection in $\mathcal{H}_\theta$ on the vector space generated by $\varphi_{\lambda,1}(\cdot,\theta)$ (respectively by $(\varphi_{\lambda,j}(\cdot,\theta))_{j\geqslant 2}$). These projections are two-by-two orthogonal and their sum is the identity for all $\theta\in\mathbb{T}^*$. One defines

$$\Pi_{\lambda,\alpha}=U^{-1}\left(\int_{\mathbb{T}^*}\Pi_{\lambda,\alpha}(\theta)\mathrm{d}\theta\right)U:L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d),$$

where $\alpha\in\{0,+\}$. $\Pi_{\lambda,\alpha}$ is an orthogonal projection on $L^2(\mathbb{R}^d)$ and for all $\gamma\in\mathbb{Z}^d$, we have $\tau_\gamma^*\Pi_{\lambda,\alpha}\tau_\gamma=\Pi_{\lambda,\alpha}$.

For $\alpha\in\{0,+\}$, we set $\mathcal{E}_{\lambda,\alpha}=\Pi_{\lambda,\alpha}(L^2(\mathbb{R}^d))$. These spaces are translation-invariant. Moreover $\mathcal{E}_{\lambda,0}$ is of finished energies for H_{λ,ω^-}. The reduction procedure consists in decomposing the operator H_{λ,ω^-} according to various translation-invariants subspaces. The random operators thus obtained are reference operators.

III. THE PROOF OF THEOREM 1.3

As we have indicated, our aim in this section is to prove Theorem 1.3, but first, let us introduce some notations and useful lemma.

For $u\in L^2(\mathbb{T}^*)$, let

$$\mathcal{T}_{\varphi_{\lambda,1}}(u)=U^*(u\varphi_{\lambda,1}(x,\theta))=\int_{\mathbb{T}^*}u(\theta)\varphi_{\lambda,1}(x,\theta)\mathrm{d}\theta. \tag{3.1}$$

So, $\mathcal{T}_{\varphi_{\lambda,1}}$ define a unitary transformation from $L^2(\mathbb{T}^*)$ to $\mathcal{E}_{\lambda,0}$ and if to simplify the computation we set $\mathrm{vol}(\mathbb{T}^*)=1$, then for $v\in\mathcal{E}_{\lambda,0}$ we have

$$\mathcal{T}^*_{\varphi_{\lambda,1}}(v)=\langle(Uv)(\cdot,\theta),\varphi_{\lambda,1}(\cdot,\theta)\rangle.$$

For $1\leqslant k\leqslant m$ and $(x,\theta)\in\mathbb{R}^d\times\mathbb{T}^*$, let

$$\widetilde{\varphi}_{\lambda,1,k}(x,\theta)=\varphi_{\lambda,1}(\theta_k(\lambda),x)e^{(\theta-\theta_k)\cdot x}.$$

We set,

$$\delta\varphi_{\lambda,1,k}(x,\theta)=\frac{1}{\sqrt{\zeta_{k,\lambda}(\theta)}}(\varphi_{\lambda,1}-\widetilde{\varphi}_{\lambda,1,k}(x,\theta)).$$

By this, for any $u\in L^2(\mathbb{T}^*)$, we have

$$\mathcal{T}_{\varphi_{\lambda,1}}(u)=\mathcal{T}_{\widetilde{\varphi}_{\lambda,1,k}}(u)+\mathcal{T}_{\delta\varphi_{\lambda,1,k}}(\sqrt{\zeta_{k,\lambda}}u). \tag{3.2}$$

For $v\in\mathcal{H}^2_\theta=\{v\in H^2_{\mathrm{loc}}(\mathbb{R}^d);v(\cdot-\gamma)=e^{-i\gamma\cdot\theta}u(\cdot)\}$ one defines the following norms:

$$\sup_{\theta\in\mathbb{T}^*}\{\|v(\cdot,\theta)\|^2_{L^2(C_0)}\}=\|v\|^2_{1,\infty},$$

and

$$\sup_{\theta\in\mathbb{T}^*}(\|H_{\lambda,\omega^-}(\theta)u(\cdot,\theta)\|^2_{L^2(C_0)}+\|v(\cdot,\theta)\|^2_{L^2(C_0)})=\|v\|_{H_{\lambda,\omega^-},\infty}.$$

Remark 3.1: *The functions* $\widetilde{\varphi}_{\lambda,1,k}$ *and* $\delta\varphi_{\lambda,1,k}$ *are well defined and*

$$\|\widetilde{\varphi}_{\lambda,1,k}\|_{1,\infty},\quad \|\widetilde{\varphi}_{\lambda,1,k}\|_{H_{\lambda,\omega^-},\infty}\|\delta\widetilde{\varphi}_{\lambda,1,k}\|_{1,\infty},\quad \textit{and}\quad \|\delta\widetilde{\varphi}_{\lambda,1,k}\|_{H_{\lambda,\omega^-},\infty}$$

are finished (*see Ref.* 4).

The following Lemma is of use. It will be proven at the end of this section.

Lemma 3.2: *For* $\theta_k,\theta_{k'}\in\mathbb{T}^*$ *and* $\varphi\in L^2(\mathbb{T}^*,\mathcal{H}^2)$ *let* $\varphi_k=e^{i(\theta-\theta_k)x}\varphi(x,\theta_k)$, $\varphi_{k'}=e^{i(\theta-\theta_{k'})x}$

$\varphi(x,\theta_{k'})$, *and* $a_{\varphi,k,k'}(x)=f(x)\varphi(x,\theta_k)\varphi(x,\theta_{k'})$. *If* $\|\varphi\|_{1,\infty}<\infty$ (*respectively*, $\|\varphi\|_{H_{\lambda,\omega^-},\infty}<\infty$) *then* $\mathcal{T}_\varphi \in \mathcal{L}(L^2(\mathbb{T}^*),L^2(\mathbb{R}^d))$ (*respectively*, $V_{\tilde{\omega}}\cdot\mathcal{T}_\varphi \in \mathcal{L}(L^2(\mathbb{T}^*),L^2(\mathbb{R}^d))$) *and there exist* $C,\beta>0$ *such that for all* $u,v\in L^2(\mathbb{T}^*)$, *we have*

$$\left|\langle V_{\tilde{\omega}}\mathcal{T}_{\varphi_k}(u),\mathcal{T}_{\varphi_{k'}}(v)\rangle - \left(\int_{C_0} a_{\varphi,k,k'}(x)\mathrm{d}x\right)\cdot\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma\hat{u}(\gamma)\overline{\hat{v}(\gamma)}\right| \leqslant C\beta\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma(|\hat{u}(\gamma)|^2+|\hat{v}(\gamma)|^2)$$
$$+C(1+1/\beta)(\langle\zeta_{k,\lambda}u,u\rangle_{L^2(\mathbb{T}^*)}+\langle\zeta_{k',\lambda}v,v\rangle_{L^2(\mathbb{T}^*)}), \tag{3.3}$$

$$\|V_{\tilde{\omega}}\mathcal{T}_{\varphi_k}(u)\|^2_{L^2(\mathbb{R}^d)} \leqslant C\left(\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma|\hat{u}(\gamma)|^2+\langle\zeta_{k,\lambda}u,u\rangle_{L^2(\mathbb{T}^*)}\right). \tag{3.4}$$

A. If $A(0)$ is positive-definite

We set

$$H^0_{\lambda,\omega}=\Pi_{\lambda,0}H_{\lambda,\tilde{\omega}}\Pi_{\lambda,0}=\Pi_{\lambda,0}H_{\lambda,\omega^-}\Pi_{\lambda,0}+\Pi_{\lambda,0}V_{\tilde{\omega}}\Pi_{\lambda,0}.$$

Theorem 3.3: *Assume that the matrix* $A(0)$ *is positive-definite. Then there exists* $\lambda_0>0$ *such that for any* $\lambda\in[0,\lambda_0]$ *we have*

$$\Pi_{\lambda,0}(H_{\lambda,\omega}-E_{\lambda,\omega^-})\Pi_{\lambda,0} \quad \textit{is a positive operator}.$$

The proof of Theorem 3.3 is the object of the following section.

1. The proof of Theorem 3.3

Using (3.1), we get that $H^0_{\lambda,\omega}$ is unitarily equivalent to the operator

$$h^0_{\lambda,\omega}=\mathcal{T}^*_{\varphi_{\lambda,1}}H^0_{\lambda,\omega}\mathcal{T}_{\varphi_{\lambda,1}},$$

acting on $L^2(\mathbb{T}^*)$ and written as

$$h^0_{\lambda,\omega}=h^0_{\lambda,\omega^-}+\lambda V^0_{\lambda,\tilde{\omega}}.$$

h^0_{λ,ω^-} is the multiplication operator by $E_1(\lambda,\theta)$ and $V^0_{\lambda,\tilde{\omega}}$ is an integral operator with the kernel

$$V_{\lambda,\tilde{\omega}}(\theta,\theta')=\langle V_{\tilde{\omega}}\varphi_{\lambda,1}(\cdot,\theta),\varphi_{\lambda,1}(\cdot,\theta')\rangle.$$

Let V_k be a neighborhood of θ_k, such that if $\theta_{k'}\in Z$ and $k\neq k'$ then $\theta\notin\overline{V_k}$ and $V_k\cap V_{k'}=\emptyset$. As $\mathbb{T}^*$ is compact, one can cover it by $(V_k)_{1\leqslant k\leqslant m}$ (i.e., $\cup_{1\leqslant k\leqslant m}V_k=\mathbb{T}^*$). For $1\leqslant k\leqslant m$ let χ_k be the characteristic function of V_k.

For simplicity for $u\in L^2(\mathbb{T}^*)$, we will denote $\chi_k u$ as u_k in the following. We consider u as a system of m columns denoted by $(u_k)_{1\leqslant k\leqslant m}$. We endow $L^2(\mathbb{T}^*)\otimes\mathbb{C}^m$ with the scalar product generating the following Euclidean norm:

$$\|u\|^2_{L^2(\mathbb{T}^*)\otimes\mathbb{C}^m}=\sum_{k=1}\|u_k\|^2_{L^2(\mathbb{T}^*)}.$$

2. The lower bound of h^0_{λ,ω^-}

Proposition 3.4: *There exists* $C>0$ *such that for any* $u\in L^2(\mathbb{T}^*)$, *we have*

$$\langle h^0_{\lambda,\omega^-}u,u\rangle \geqslant \sum_{1\leqslant k\leqslant m}E_1(\lambda,\theta_k(\lambda))\|u_k\|^2_{L^2(\mathbb{T}^*)}+\frac{1}{C}\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.5}$$

Proof: For $u \in L^2(\mathbb{T}^*)$, one computes

$$\langle h^0_{\lambda,\omega^-} u,u\rangle = \int_{\mathbb{T}^*} E_1(\lambda,\theta)|u(\theta)|^2 \mathrm{d}\theta = \sum_{1\leqslant k\leqslant m} \int_{\mathbb{T}^*} E_1(\lambda,\theta)\chi_k(\theta)|u(\theta)|^2 \mathrm{d}\theta.$$

As for any θ in V_k the support of χ_k, there exists $C>0$ such that we have

$$E_1(\lambda,\theta_k(\lambda)) + \frac{1}{C}\zeta_{k,\lambda}(\theta) \leqslant E_1(\lambda,\theta),$$

we get the result. □

3. The lower bound of $V^0_{\lambda,\widetilde{\omega}}$

Proposition 3.5: *There exists* $C_1, C_2 > 0$, *and* λ_0 *such that for all* $\lambda \in [0,\lambda_0]$ *and* $u \in L^2(\mathbb{T}^*)$ *we have*

$$\langle V^0_{\lambda,\widetilde{\omega}} u,u\rangle \geqslant C_1 \sum_{1\leqslant k\leqslant m,\,\gamma\in\mathbb{Z}^d} \widetilde{\omega}_\gamma |(\hat{u_k})(\gamma)|^2 - C_2 \sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k, u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.6}$$

Proof of Theorem 3.3: Let us notice that, by combining the results of Propositions 3.4 and 3.5, one gets that there exists $\lambda_0>0$ such that for any $\lambda \in [0,\lambda_0]$ and for any $u \in L^2(\mathbb{T}^*)$ we have

$$\langle h^0_{\lambda,\omega} u,u\rangle \geqslant \sum_{1\leqslant k\leqslant m} E_1(\lambda,\theta_k(\lambda))\|u_k\|^2_{L^2(\mathbb{T}^*)} + \frac{1}{C}\left(\sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k, u_k\rangle_{L^2(\mathbb{T}^*)} + \lambda \sum_{1\leqslant k\leqslant m} \sum_{\gamma\in\mathbb{Z}^d} \widetilde{\omega}_\gamma |\hat{u_k}(\gamma)|^2 \right)$$

$$\geqslant E_{\lambda,\omega^-}\|u\|^2_{L^2(\mathbb{T}^*)} + \frac{1}{C}\left(\sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k, u_k\rangle_{L^2(\mathbb{T}^*)} + \lambda \sum_{1\leqslant k\leqslant m} \sum_{\gamma\in\mathbb{Z}^d} \widetilde{\omega}_\gamma |\hat{u_k}(\gamma)|^2 \right).$$

This gives that

$$\langle (h^0_{\lambda,\widetilde{\omega}} - E_{\lambda,\omega^-})u,u\rangle \geqslant \frac{1}{C}\left(\sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k, u_k\rangle_{L^2(\mathbb{T}^*)} + \lambda \sum_{1\leqslant k\leqslant m} \sum_{\gamma\in\mathbb{Z}^d} \widetilde{\omega}_\gamma |\hat{u_k}(\gamma)|^2 \right). \tag{3.7}$$

This ends the proof of Theorem 3.3. □

Remark 3.6: *We notice that even if we know that the bottom of the spectrum of* H_ω *coincides with the bottom of the spectrum of* H_{λ,ω^-} *we cannot consider* $\Pi_{\lambda,0}(H_{\lambda,\omega} - H_{\lambda,\omega^-})\Pi_{\lambda,0}$ *as a positive operator*.

Proof of Proposition 3.5: Let us start by expanding $\langle V^0_{\lambda,\widetilde{\omega}} u,u\rangle$,

$$\langle V^0_{\lambda,\widetilde{\omega}} u,u\rangle = \sum_{1\leqslant k,k'\leqslant m} \langle V^0_{\lambda,\omega} \mathcal{T}_{\widetilde{\varphi}_{\lambda,1,k}}(u_k), \mathcal{T}_{\widetilde{\varphi}_{\lambda,1,k'}}(u_{k'})\rangle_{L^2(\mathbb{R}^d)}$$

$$+ \sum_{1\leqslant k,k'\leqslant m} \langle V^0_{\lambda,\widetilde{\omega}} \mathcal{T}_{\delta\widetilde{\varphi}_{\lambda,1,k}}(\sqrt{\zeta_{k,\lambda}}u_k), \mathcal{T}_{\delta\widetilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}$$

$$+ 2 \sum_{1\leqslant k,k'\leqslant m} \Re(\langle V^0_{\lambda,\widetilde{\omega}} \mathcal{T}_{\widetilde{\varphi}_{\lambda,1,k}}(u_k), \mathcal{T}_{\delta\widetilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}).$$

We start by estimating the three sums of the last equation.

For the second sum, using Cauchy Schwartz inequality and Lemma 3.2, we get that for any $1\leqslant k,k'\leqslant m$, there exists $C>0$ such that we have

$$|\langle V^0_{\lambda,\tilde{\omega}}\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k}}(\sqrt{\zeta_{k,\lambda}}u_k),\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}| \leqslant \tfrac{1}{2}(\|V^0_{\lambda,\tilde{\omega}}\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k}}(\sqrt{\zeta_{k,\lambda}}u_k)\|^2_{L^2(\mathbb{R}^d)} + \|\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\|^2_{L^2(\mathbb{R}^d)}) \leqslant C\cdot(\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)} + \langle\zeta_{k',\lambda}u_{k'},u_{k'}\rangle_{L^2(\mathbb{T}^*)}).$$

So there exists $C>0$ such that we have

$$\sum_{1\leqslant k,k'\leqslant m}|\langle V^0_{\lambda,\tilde{\omega}}\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k}}(\sqrt{\zeta_{k,\lambda}}u_k),\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}| \leqslant C\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.8}$$

For the third sum, using the Cauchy-Schwartz inequality once more, we get that for $1\leqslant k\leqslant m$ there exists $\beta>0$ such that we have

$$|\langle V^0_{\lambda,\tilde{\omega}}\mathcal{T}_{\tilde{\varphi}_{\lambda,1,k}}(u_k),\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}| \leqslant \beta\|V^0_{\tilde{\omega}}\mathcal{T}_{\tilde{\varphi}_{\lambda,1,k}}(u_k)\|^2_{L^2(\mathbb{R}^d)} + 1/(4\beta)\|\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k,\lambda}}u_{k'})\|^2_{L^2(\mathbb{R}^d)}. \tag{3.9}$$

Using Eq. (3.4), one gets that there exist $\widetilde{C}_1,\widetilde{C}_2,\beta>0$ such that

$$\sum_{1\leqslant k,k'\leqslant m}|\langle V^0_{\lambda,\tilde{\omega}}\mathcal{T}_{\tilde{\varphi}_{\lambda,1,k}}(u_k),\mathcal{T}_{\delta\tilde{\varphi}_{\lambda,1,k'}}(\sqrt{\zeta_{k',\lambda}}u_{k'})\rangle_{L^2(\mathbb{R}^d)}| \leqslant \widetilde{C}_1\beta\sum_{1\leqslant k\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma|\hat{u_k}(\gamma)|^2 + \widetilde{C}_2(\beta+1/\beta)\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.10}$$

For the first sum, using (3.3), we get that there exist $C_1',C_2',\beta>0$ such that

$$\left|\sum_{1\leqslant k,k'\leqslant m}\langle V^0_{\tilde{\omega}}\mathcal{T}_{\tilde{\varphi}_{\lambda,1,k}}(u_k),\mathcal{T}_{\tilde{\varphi}_{\lambda,1,k'}}(u_{k'})\rangle_{L^2(\mathbb{R}^d)} - \sum_{1\leqslant k,k'\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma\left(\int_{C_0}a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)(\hat{u_k})(\gamma)\overline{(\hat{u_{k'}})(\gamma)}\right| \leqslant C_1'\beta\sum_{1\leqslant k\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma|\hat{u_k}(\gamma)|^2 + C_2'(1+1/\beta)\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.11}$$

Now Eqs. (3.8), (3.10), and (3.11) give that there exist $K_1,K_2,\beta>0$ such that

$$\left|\langle V^0_{\lambda,\tilde{\omega}}u,u\rangle - \sum_{1\leqslant k,k'\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma\left(\int_{C_0}a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)(\hat{u_k})(\gamma)\overline{(\hat{u_{k'}})(\gamma)}\right| \leqslant K_1\beta\sum_{1\leqslant k\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma|(\hat{u_k})(\gamma)|^2 + K_2(1+1/\beta)\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.12}$$

Now, if the matrix

$$A(0)=\left(\int_{C_0}a_{\varphi_{0,1},k,k'}(x)\mathrm{d}x\right)_{1\leqslant k,k'\leqslant m}$$

is positive-definite, one gets that $\inf\sigma(A(0))=C>0$ satisfies

$$CI_m\leqslant A.$$

Let $A(\lambda)$ be the matrix,

$$\left(\int_{C_0}a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)_{1\leqslant k,k'\leqslant m}.$$

Notice that for any $1\leqslant k,k'\leqslant m$, the functions

$$f_{k,k'}:\lambda \to \int_{C_0} a_{\varphi_{\lambda,1},\theta_k(\lambda),\theta_{k'}(\lambda)}(x)\mathrm{d}x$$

are continuous in λ. So there exists $\lambda_0>0$ such that for any $\lambda \in [0,\lambda_0]$,

$$\frac{C}{2} I_m \leqslant A(\lambda).$$

This gives that for any $u \in L^2(\mathbb{T}^*)$,

$$\frac{C}{2} \sum_{1\leqslant k\leqslant m} \sum_{\gamma\in\mathbb{Z}^d} \tilde{\omega}_\gamma |(\hat{u_k})(\gamma)|^2 \leqslant \sum_{1\leqslant k,k'\leqslant m} \sum_{\gamma\in\mathbb{Z}^d} \tilde{\omega}_\gamma \left(\int_{C_0} a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)(\hat{u_k})(\gamma)\overline{(\hat{u_{k'}})(\gamma)}. \quad (3.13)$$

Now using the expanation of $\langle V^0_{\lambda,\tilde{\omega}} u,u\rangle$ and Eq. (3.12), we get that there exist $K_1,K_2>0$ and $\beta>0$ such that

$$\langle V^0_{\lambda,\tilde{\omega}} u,u\rangle \geqslant \left(\frac{C_1'}{2} - K_1\beta\right) \sum_{1\leqslant k\leqslant m;\gamma\in\mathbb{Z}^d} \tilde{\omega}_\gamma |(\hat{u_k})(\gamma)|^2 - K_2(1+1/\beta) \sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \quad (3.14)$$

So, for $\beta>0$ well chosen we get that there exist constants $C_1,C_2>0$ such that

$$\langle V^0_{\lambda,\tilde{\omega}} u,u\rangle \geqslant \frac{C_1}{3} \sum_{1\leqslant k\leqslant m;\gamma\in\mathbb{Z}^d} \tilde{\omega}_\gamma |(\hat{u_k})(\gamma)|^2 - C_2 \sum_{1\leqslant k\leqslant m} \langle \zeta_{k,\lambda} u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \quad (3.15)$$

This ends the proof of Proposition 3.5. □

B. If $A(0)$ is negative-definite

We recall that H_{λ,ω^+} is the following operator:

$$H_{\lambda,\omega^+} = -\Delta + W_{\mathrm{per}} + \lambda \sum_{\gamma\in\mathbb{Z}^d} \omega^+ f(\cdot-\gamma).$$

As H_{λ,ω^+} is a $\mathbb{Z}^d$-periodic operator, the analysis given in Sec. II A for H_{λ,ω^-} is still true in the present case. For $(E_j(\lambda,\theta))_{j\in\mathbb{N}^*}$, the Floquet eigenvalue of H_{λ,ω^+} let us set $E_{\lambda,\omega^+}=\inf_{\theta\in\mathbb{T}^*} E_1(\lambda,\theta)$.

Theorem 3.7: *Assume that the matrix $A(0)$ is negative-definite. Then there exists $\lambda_0>0$ such that for any $\lambda\in[0,\lambda_0]$ we have*

$$\Pi_{\lambda,0}(H_{\lambda,\omega} - E_{\lambda,\omega^+})\Pi_{\lambda,0} \quad \textit{is a positive operator}.$$

The result of Theorem 3.7 can be proved in the same way as we did for Theorem 3.3 in the previous section. Indeed, $H_{\lambda,\omega}$ can be seen as a perturbation of H_{λ,ω^+} as follows:

$$H_{\lambda,\omega} = H_{\lambda,\omega^+} + V_{\bar{\omega}}.$$

With $V_{\bar{\omega}}(\cdot)=\Sigma_{\gamma\in\mathbb{Z}^d}\bar{\omega}_\gamma f(\cdot-\gamma)$ and for any $\gamma\in\mathbb{Z}^d$, $\bar{\omega}_\gamma=\omega_\gamma-\omega^+$. Notice that in this case $(\bar{\omega}_\gamma)_{\gamma\in\mathbb{Z}^d}$ is a family of bounded and negative random variables. Using an analogous unitary transformation to (3.1), one gets that $H^0_{\lambda,\omega}$ is unitarily equivalent to

$$h^0_{\lambda,\omega} = h^0_{\lambda,\omega^+} + V^0_{\lambda,\bar{\omega}}.$$

The lower bound of h_{λ,ω^+} can be derived easily. As all arguments used to lower bound $V^0_{\tilde{\omega}}$ remain valid, we lower bound $V^0_{\lambda,\bar{\omega}}$ using the same computation done in Sec. III A.

So we get that there exist $K_1,K_2,\beta>0$ such that

$$\left|\langle V^0_{\lambda,\bar{\omega}}u,u\rangle - \sum_{1\leqslant k,k'\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\bar{\omega}_\gamma\left(\int_{C_0}a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)(\hat{u_k})(\gamma)\overline{(\hat{u_{k'}})(\gamma)}\right|$$

$$\leqslant K_1\beta(\omega^+-\omega^-)\sum_{1\leqslant k\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}|(\hat{u_k})(\gamma)|^2+K_2(1+1/\beta)\sum_{1\leqslant k\leqslant m}\langle\zeta_{k,\lambda}u_k,u_k\rangle_{L^2(\mathbb{T}^*)}. \tag{3.16}$$

When $A(0)$ is negative-definite, there exists $C<0$ and $\lambda_0>0$ such that for any $\lambda\in[0,\lambda_0]$, we have

$$A(\lambda)\leqslant CI_m.$$

As the random variables $(\bar{\omega}_\gamma)_{\gamma\in\mathbb{Z}^d}$ are negative, we get that

$$C\sum_{1\leqslant k\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\bar{\omega}_\gamma|(\hat{u_k})(\gamma)|^2\leqslant\sum_{1\leqslant k,k'\leqslant m}\sum_{\gamma\in\mathbb{Z}^d}\bar{\omega}_\gamma\left(\int_{C_0}a_{\varphi_{\lambda,1},k,k'}(x)\mathrm{d}x\right)(\hat{u_k})(\gamma)\overline{(\hat{u_{k'}})(\gamma)}. \tag{3.17}$$

This and Eq. (3.16) give the desired result on the lower bound of $V_{\bar{\omega}}$. This ends the proof of Theorem 3.7. □

Proof of Lemma 3.2: As $V_{\tilde{\omega}}$ is H_{λ,ω^-}-relatively bound uniformly on $\tilde{\omega}_\gamma$, there exists $c>0$ such that for any $u\in L^2(\mathbb{T}^*)$ we have

$$\|V_{\tilde{\omega}}\mathcal{T}_\varphi(u)\|\leqslant c(\|H_{\lambda,\omega^-}\mathcal{T}_\varphi(u)\|^2+\|\mathcal{T}_\varphi(u)\|^2)$$

$$\leqslant c\int_{\mathbb{T}^*}(\|H_{\lambda,\omega^-}(\theta)\varphi(\cdot,\theta)\|^2_{L^2(C_0)}+\|\varphi(\cdot,\theta)\|^2_{L^2(C_0)})|u(\theta)|^2\mathrm{d}\theta$$

$$\leqslant c\|\varphi\|^2_{H_{\lambda,\omega^-,\infty}}\cdot\|u\|^2_{L^2(\mathbb{T}^*)}.$$

One computes

$$\begin{aligned}&\langle V^0_{\tilde{\omega}}\mathcal{T}_{\varphi_k}(u),\mathcal{T}_{\varphi_{k'}}(v)\rangle_{L^2(\mathbb{R}^d)}\\&=\int_{\mathbb{R}^d}V_{\tilde{\omega}}(x)\varphi_k(x,\theta_k)\overline{\varphi_{k'}(x,\theta_{k'})}\cdot\left(\int_{\mathbb{T}^*}e^{(\theta-\theta_k)x}u(\theta)\mathrm{d}\theta\cdot\overline{\int_{\mathbb{T}^*}e^{(\theta-\theta_{k'})x}v(\theta)\mathrm{d}\theta}\right)\mathrm{d}x\\&=\sum_{\gamma\in\mathbb{Z}^d}\tilde{\omega}_\gamma\int_{C_0}f(x)\varphi_k(x,\theta_k)\overline{\varphi_{k'}(x,\theta_{k'})}\cdot\left(\int_{\mathbb{T}^*}e^{(\theta-\theta_k)x}e^{i\gamma\cdot\theta}u(\theta)\mathrm{d}\theta\cdot\overline{\int_{\mathbb{T}^*}e^{(\theta-\theta_{k'})x}e^{i\gamma\cdot\theta}v(\theta)\mathrm{d}\theta}\right)\mathrm{d}x.\end{aligned}$$

Let

$$\hat{u}(\gamma)=\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}u(\theta)\mathrm{d}\theta.$$

For any $(x,\theta)\in\mathbb{R}^d\times\mathbb{T}^*$ and $1\leqslant k\leqslant m$, we set

$$g_k(x,\theta)=\frac{e^{i(\theta-\theta_k)\cdot x}-1}{\sqrt{\zeta_{k,\lambda}(\theta)}}. \tag{3.18}$$

As $\theta_k(\lambda)$ is the only zero of $\zeta_{k,\lambda}$ and as it is nondegenerate, there exist $C>0$ such that, for $(x,\theta)\in\mathbb{R}^d\times\mathbb{T}^*$, and $1\leqslant k\leqslant m$, we have

$$|g_k(x,\theta)|\leqslant C(1+|x|). \tag{3.19}$$

We have $e^{i(\theta-\theta_k)x}=\sqrt{\zeta_{k,\lambda}}g_k(x,\theta)+1$. So using this and expanding $\langle V_{\widetilde{\omega}}\mathcal{T}_{\varphi_k}(u),\mathcal{T}_{\varphi_{k'}}(v)\rangle_{L^2(\mathbb{R}^d)}$, we get

$$\begin{aligned}
&\langle V_{\widetilde{\omega}}\mathcal{T}_{\varphi_k}(u),\mathcal{T}_{\varphi_{k'}}(v)\rangle_{L^2(\mathbb{R}^d)}-\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\left(\int_{C_0}a_{\varphi,k,k'}(x)\mathrm{d}x\right)\cdot u(\gamma)\cdot\overline{v(\gamma)}\\
&=\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\int_{C_0}a_{\varphi,k,k'}(x)\cdot\left(\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_k(x,\theta)\sqrt{\zeta_{k,\lambda}(\theta)}u(\theta)\mathrm{d}\theta\cdot\overline{\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_{k'}(x,\theta)\sqrt{\zeta_{k',\lambda}(\theta)}v(\theta)\mathrm{d}\theta}\right)\mathrm{d}x\\
&\quad+\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\hat{u}(\gamma)\int_{C_0}a_{\varphi,k,k'}(x)\cdot\left(\overline{\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_{k'}(x,\theta)\sqrt{\zeta_{k',\lambda}(\theta)}v(\theta)\mathrm{d}\theta}\right)\mathrm{d}x\\
&\quad+\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\overline{\hat{v}(\gamma)}\int_{C_0}a_{\varphi,k,k'}(x)\cdot\left(\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_k(x,\theta)\sqrt{\zeta_{k,\lambda}(\theta)}u(\theta)\mathrm{d}\theta\right)\mathrm{d}x. \qquad (3.20)
\end{aligned}$$

Now using the fact that the family $(\widetilde{\omega}_\gamma)_{\gamma\in\mathbb{Z}^d}$ is bounded, Cauchy-Schwartz inequality and Perseval identity and Eq. (3.19), we get that there exists $C,\beta>0$ such that

$$\begin{aligned}
&\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\int_{C_0}a_{\varphi,k,k'}(x)\cdot\left(\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_k(x,\theta)\sqrt{\zeta_{k,\lambda}(\theta)}u(\theta)\mathrm{d}\theta\cdot\overline{\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_{k'}(x,\theta)\sqrt{\zeta_{k',\lambda}(\theta)}v(\theta)\mathrm{d}\theta}\right)\mathrm{d}x\\
&\quad\leqslant C\langle\zeta_{k,\lambda}u,u\rangle_{L^2(\mathbb{T}^*)}+\langle\zeta_{k',\lambda}v,v\rangle_{L^2(\mathbb{T}^*)}, \qquad (3.21)
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\hat{u}(\gamma)\int_{C_0}a_{\varphi,k,k'}(x)\cdot\overline{\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_{k'}(x,\theta)\sqrt{\zeta_{k',\lambda}(\theta)}v(\theta)\mathrm{d}\theta}\mathrm{d}x\leqslant C\beta\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma|\hat{u}(\gamma)|^2\\
&\qquad+\frac{C}{4\beta}\langle\zeta_{k',\lambda}v,v\rangle_{L^2(\mathbb{T}^*)}. \qquad (3.22)
\end{aligned}$$

The same argument gives

$$\begin{aligned}
&\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma\overline{\hat{v}(\gamma)}\int_{C_0}a_{\varphi,k,k'}(x)\cdot\int_{\mathbb{T}^*}e^{i\gamma\cdot\theta}g_k(x,\theta)\sqrt{\zeta_{k,\lambda}(\theta)}u(\theta)\mathrm{d}\theta\,\mathrm{d}x\leqslant C\beta\sum_{\gamma\in\mathbb{Z}^d}\widetilde{\omega}_\gamma|\hat{v}(\gamma)|^2\\
&\qquad+\frac{C}{4\beta}\langle\zeta_{k,\lambda}u,u\rangle_{L^2(\mathbb{T}^*)}. \qquad (3.23)
\end{aligned}$$

So from (3.20)–(3.23) we get (3.3).

The proof of (3.4) follows by changing $\mathcal{T}_{\varphi_{\lambda,1}}(u)$ using (3.2) and following the same steps as (3.3).

This ends the proof of Lemma 3.2. □

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Remarkable identities related to the (quantum) elliptic Calogero-Sutherland model

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We present remarkable functional identities related to the elliptic Calogero-Sutherland (eCS) system. We derive them from a second quantization of the eCS model within a quantum field theory model of anyons on a circle and at finite temperature. The identities involve two eCS Hamiltonians with arbitrary and, in general, different particle numbers N and M, and a particular function of $N+M$ variables arising as anyon correlation function of N particles and M antiparticles. In addition to identities obtained from anyons with the same statistics parameter λ, we also obtain "dual" relations involving "mixed" correlation functions of anyons with two different statistics parameters λ and $1/\lambda$. We also give alternative, elementary proofs of these identities by direct computations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2167807]

I. BACKGROUND AND RESULT

The elliptic Calogero-Sutherland (eCS) system is a quantum mechanical model of an arbitrary number, N, of particles moving on a circle of length 2π and interacting with two-body potentials given by the Weierstrass elliptic functions $\wp$.[2,15,13] More specifically, this model is defined by the differential operator

$$H = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\lambda(\lambda-1) \sum_{1\leqslant j<k\leqslant N} V(x_j - x_k), \tag{1}$$

where $-\pi \leqslant x_j \leqslant \pi$ are coordinates on the circle, $\lambda > 0$ is a real parameter determining the coupling strength, and

$$V(r) = \sum_{m\in\mathbb{Z}} \frac{1}{4\sin^2[(r+i\beta m)/2]}, \quad \beta > 0 \tag{2}$$

is essentially the Weierstrass elliptic function $\wp$ with periods 2π and $i\beta$,

$$V(z) = \wp(z) + c_0, \quad c_0 = \frac{1}{12} - \sum_{m=1}^{\infty} \frac{1}{2\sinh^2[(\beta m)/2]} \tag{3}$$

(see Appendix A 1. in Ref. 12, for example).

In this paper we obtain and prove various remarkable identities involving eCS Hamiltonians and special functions of many variables constructed from the following building block:

$$\theta(z) = \sin(z/2)\prod_{n=1}^{\infty}(1-2q^{2n}\cos(z)+q^{4n}), \quad q = e^{-\beta/2}, \tag{4}$$

which is essentially the Jacobi theta function ϑ_1,

$$\theta(z) = \frac{1}{2q^{1/4}\prod_{n=1}^{\infty}(1-q^{2n})}\vartheta_1\left(\frac{1}{2}z\right) \tag{5}$$

(see Sec. 21.3 in Ref. 17, for example). We derive these results from the quantum field theory construction in Ref. 11 We collect all these identities in the following theorem.

Theorem: *Let*

$$F_{N,M}(\mathbf{x};\mathbf{y}) = \frac{\prod_{1\leqslant j<k\leqslant N}\theta(x_k-x_j)^{\lambda}\prod_{1\leqslant j<k\leqslant M}\theta(y_j-y_k)^{\lambda}}{\prod_{j=1}^{N}\prod_{k=1}^{M}\theta(x_j-y_k)^{\lambda}} \tag{6}$$

with $\mathbf{x}\in\mathbb{C}^N$ *and* $\mathbf{y}\in\mathbb{C}^M$ *and* $\theta(z)$ *defined in Eq. (4). This function obeys the identity*

$$\left[H_{\lambda,N}(\mathbf{x}) - H_{\lambda,M}(\mathbf{y}) + 2(N-M)\lambda\frac{\partial}{\partial\beta} - c_{N,M}\right]F_{N,M}(\mathbf{x};\mathbf{y}) = 0 \tag{7}$$

with $H=H_{\lambda,N}(\mathbf{x})$ *the eCS Hamiltonian in Eq. (1) and the constant*

$$c_{N,M} = \lambda^2[N(N-1)-M(M-1)]c_0 + (N-M)\lambda^2[N(N-1)+M(M-1)-2NM]c_1, \tag{8}$$

where

$$c_0 = \frac{1}{12} - \sum_{n=1}^{\infty}\frac{2q^{2n}}{(1-q^{2n})^2}, \quad c_1 = \frac{1}{12}. \tag{9}$$

Moreover, a similar identity holds true for the function

$$\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y}) = \prod_{1\leqslant j<k\leqslant N}\theta(x_k-x_j)^{\lambda}\prod_{1\leqslant j<k\leqslant M}\theta(y_j-y_k)^{1/\lambda}\prod_{j=1}^{N}\prod_{k=1}^{M}\theta(x_j-y_k), \tag{10}$$

namely

$$\left[H_{\lambda,N}(\mathbf{x}) + \lambda H_{1/\lambda,M}(\mathbf{y}) + 2(\lambda N+M)\frac{\partial}{\partial\beta} - \widetilde{c}_{N,M}\right]\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y}) = 0 \tag{11}$$

with

$$\begin{aligned}\widetilde{c}_{N,M} = {}& [\lambda^2 N(N-1) + M(M-1)/\lambda + (1+\lambda)NM]c_0 \\ & + (\lambda N+M)[\lambda N(N-1) + M(M-1)/\lambda + 2NM]c_1.\end{aligned} \tag{12}$$

It is interesting to note that there are corresponding identities for the first order differential operators

$$P_N(\mathbf{x}) = \sum_{j=1}^{N} i\frac{\partial}{\partial x_j} \tag{13}$$

equal to the total momentum operator for the eCS system, namely

$$[P_N(\mathbf{x}) + P_M(\mathbf{y})]F_{N,M}(\mathbf{x};\mathbf{y}) = 0 \tag{14}$$

[this is easily proven by observing that $F_{N,M}(\mathbf{x};\mathbf{y})$ is invariant under common shifts $(x_j,y_k) \to (x_j+a,y_k+a)$ for arbitrary real a], and similarly

$$[P_N(\mathbf{x}) + P_M(\mathbf{y})]\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y}) = 0. \tag{15}$$

It is natural to conjecture that similar identities hold true for all commuting differential operators $H^{(j)}=H_N^{(j)}(\mathbf{x})$, $j=1,2,,\ldots$, which are known to exist for the eCS model[13] (since $H^{(j)}$ for $j=1$ and 2 are equal to the total momentum operator and the Hamiltonian of the eCS system, respectively).

Remark 1.1: Note that the constant c_0 in Eq. (9) is identical to the one in Eq. (3). Moreover, the constant c_1 appears in the following from:

$$c_1 = \frac{1}{8} - \sum_{n=1}^{\infty} \frac{nq^{2n}}{1-q^{2n}} - \frac{c_0}{2},$$

but due to the identity

$$\sum_{n=1}^{\infty} \frac{nq^{2n}}{1-q^{2n}} = \sum_{m=1}^{\infty} \frac{q^{2m}}{(1-q^{2m})^2} \tag{16}$$

one gets $c_1=1/12$.

Remark 1.2: It is interesting to note that by redefining the elliptic functions by β-dependent constants as follows:

$$V(r) \to V(r) + b_0,$$

$$\theta(r) \to B_1\theta(r) \quad \text{with } \frac{\partial \ln(B_1)}{\partial\beta} = b_1,$$

the constants in our identities are changed as follows:

$$c_{N,M} \to c_{N,M} - \lambda(\lambda-1)[N(N-1) - M(M-1)]b_0 - (N-M)\lambda^2[N(N-1) + M(M-1) - 2NM]b_1$$

and

$$\widetilde{c}_{N,M} \to \widetilde{c}_{N,M} - [\lambda(\lambda-1)N(N-1) + (1/\lambda - 1)M(M-1)]b_0 + (\lambda N + M)[\lambda N(N-1) + M(M-1)/\lambda + 2NM]b_1.$$

In particular, choosing $b_0=c_0$ and $b_1=c_1$ we can simplify these constants significantly,

$$\begin{aligned} c_{N,M} &\to \lambda[N(N-1) - M(M-1)]c_0, \\ \widetilde{c}_{N,M} &\to [\lambda N(N-1) + M(M-1) + (1+\lambda)MN]c_0. \end{aligned} \tag{17}$$

This latter simple choice amounts to replacing

$$\begin{aligned} V(r) &\to \wp(r), \\ \theta(r) &\to \vartheta_1\left(\tfrac{1}{2}r\right). \end{aligned} \tag{18}$$

This shows that if one uses the standard elliptic functions one gets somewhat simpler formulas. However, our choice has the advantage that the trigonometric limit $q=0$ is not singular. Moreover, it removes a trivial contribution from the eigenvalues of the eCS model.[12] □

It is useful to write the constants above as follows:

$$c_{N,M} = \tfrac{1}{12}\lambda^2(N-M)[(N-M)^2-1] + 2\lambda^2(N-M)(N+M-1)c_2 \tag{19}$$

and

$$\widetilde{c}_{N,M} = \tfrac{1}{12}[\lambda^2 N^3 + M^3/\lambda + 3NM(\lambda N + M) - (\lambda^2 N + M/\lambda)] - 2[\lambda^2 N^2 + M^2/\lambda - (\lambda^2 N + M/\lambda) + (\lambda + 1)MN]c_2 \tag{20}$$

with

$$c_2 = \sum_{n=1}^{\infty} \frac{nq^{2n}}{1-q^{2n}}. \tag{21}$$

In Refs. 9 and 11 we obtained the special case $N=M$ of the identity in Eq. (7) using a second quantization of the eCS model in a quantum field theory (QFT) of anyons on a circle and at finite temperature $1/\beta$, and in Ref. 12, Appendix A 3, we gave an alternative, elementary proof by straightforward but rather tedious computations. In this paper we show that the QFT results in Ref. 11 naturally imply all the identities in the theorem above. To be convincing also for readers not familiar with QFT we will also give elementary proofs by direct computations which are, however, not so illuminating. These direct proofs are based on three functional identities of the functions $V(r)$ and $\theta(r)$ introduced above: First,

$$V(r) = -\frac{d^2}{dr^2} \ln \theta(r), \tag{22}$$

second,

$$\phi(x)\phi(y) + \phi(x)\phi(z) + \phi(y)\phi(z) = f(x) + f(y) + f(z) \quad \text{if } x+y+z=0, \tag{23}$$

where

$$\phi(x) = \frac{d}{dx} \ln \theta(x), \quad f(x) = \frac{1}{2}[V(x) - \phi(x)^2 - c_0], \tag{24}$$

and third,

$$f(x) = -\frac{\partial}{\partial\beta} \ln \theta(x) + c_1 \tag{25}$$

with the constants c_0 and c_1 in Eq. (9). The (elementary) proofs (22) and (23) can be found in Ref. 12, Appendix A 1 and A 2, respectively; (25) follows readily from

$$\vartheta_1(x/2) = \sum_{n=1}^{\infty} (-1)^{n-1} q^{(n-1/2)^2} \sin[(n-1/2)x]$$

(see Section 21.22 in Ref. 17, for example) and Eq. (5), using the observation made in Remark 1.1 above. To avoid misunderstanding we stress that the functional identities needed to prove our results are classical and known for a long time.

An interesting special case of our result is for $M=0$ in which case the identities reduce to

$$H_{\lambda,N}(\mathbf{x})\Psi_0(\mathbf{x}) = \left[c_{N,0} - 2N\lambda\frac{\partial}{\partial\beta}\right]\Psi_0(\mathbf{x}), \tag{26}$$

where $\Psi_0(\mathbf{x}) = F_{N,0}(\mathbf{x},\mathbf{y})$, i.e.,

$$\Psi_0(\mathbf{x}) = \prod_{1\leqslant j<k\leqslant N} \theta(x_k - x_j)^{\lambda}. \tag{27}$$

In the limiting case $\beta\to\infty$ the β-derivative term disappears, and we recover the well-known eigenvalue equation for the ground state of the Sutherland model. It is interesting to note that the elliptic generalization of this identity which we find here does *not* give the ground state of the eCS

model, which is why Sutherland's solution[15] of the Sutherland model does not generalize to the elliptic case. For $N=2$, $M=0$ our identities reduce to

$$\left[-2\frac{\partial^2}{\partial x^2}+4\lambda\frac{\partial}{\partial\beta}-c_{2,0}\right]\theta(x)^\lambda=0,$$

which for $\lambda=1$ is (essentially) the heat equation obeyed by ϑ_1 ($x=x_1-x_2$). Other interesting special cases will be discussed in Sec. III.

It is worth noting that original motivation to study the QFT model of anyons in Ref. 3 was its relation to the fractional quantum Hall effect,[16] and it is remarkable that this physics relation proved to be helpful for finding the generalization in Refs. 9 and 11. However, one can regard this construction also pragmatically as a useful generating function technique for deriving interesting identities which, once found, can also be proven by direct computations. Since we believe that there are other identities to be found along similar lines, we hope it is nevertheless of some interest to not only give the direct proof but also the detailed QFT derivation.

We also mention that the QFT construction in Ref. 11 seems closely related to earlier work on conformal field theory on the torus[1,5,4,6,7] also finding and exploiting interesting relations to the eCS model. The approach in Ref. 11 and here is, however, rather different in spirit and technique.

The plan of this paper is as follows. In Sec. II we give an outline of how to derive our identities from the QFT results in Refs. 9 and 11, emphasizing the physical interpretation and deferring computational details to Appendix A. In this discussion we clarify this QFT construction, in particular the interpretation of the representation we use as finite temperature representation (which, since not needed there, was only discussed in an Appendix in Ref. 11). Section III contains our conclusions, including a comparison with previous results and a short discussion of possible applications of our identities. The elementary, alternative proofs can be found in Appendix B.

II. QUANTUM FIELD THEORY DERIVATION

In this section we explain how the identities in our theorem are obtained from our results in Refs. 9 and 11. Some computational details are deferred to Appendix A.

1. Second quantization of the eCS model

We first briefly summarize the construction of anyons.[11]

Anyons (for us) are operator valued distributions $\phi_\nu(x)$ parametrized by a coordinate on the unit circle, $-\pi\leqslant x\leqslant\pi$, and depending on a real parameter ν determining their commutator relations as follows:

$$\phi_\nu(x)\phi_\nu(y)=e^{\pm i\pi\nu^2}\phi_\nu(y)\phi_\nu(x)\quad\text{for } x\neq y \tag{28}$$

[see the Definition in Sec. 2.2 in Ref. 11; note that what we denote as $\phi_\nu(x)$ here is identical with $\lim_{\varepsilon\downarrow}\phi^1_\varepsilon(x)$ there; we ignore the regularization parameter ε here but indicate the parameter ν determining the statistics instead: see also Remark 2.1 below]. We constructed a particular representation of these anyons on a Fock space $\mathcal{F}$ generated from a "vacuum" Ω such that

$$\langle\Omega,\phi_\nu(x)^*\phi_\nu(y)\Omega\rangle=\text{const }\theta(x-y)^{-\nu^2} \tag{29}$$

where $\theta(r)$ is the elliptic function in Eq. (4); $\langle\cdot,\cdot\rangle$ is the Hilbert space inner product and $*$ the Hilbert space adjoint. This representation is characterized by a parameter $\beta>0$ which determines the modulus of the elliptic functions as $q=\exp(-\beta/2)$ and which, as we showed, has a natural physical interpretation as inverse temperature. We then constructed a self-adjoint operator $\mathcal{H}$ in $\mathcal{F}$ which has remarkable commutator relations with products of an arbitrary number N of anyon fields

$$\Phi_\nu^N(\mathbf{x}) := \phi_\nu(x_1)\cdots\phi_\nu(x_N), \tag{30}$$

namely

$$[\mathcal{H},\Phi_\nu^N(\mathbf{x})]\Omega = H_{N,\lambda}(\mathbf{x})\Phi_\nu^N(\mathbf{x})\Omega, \tag{31}$$

where $H=H_{\lambda,N}(\mathbf{x})$ is the eCS Hamiltonian given in Eq. (1) with the coupling determined by the statistic parameter as follows:

$$\lambda = \nu^2. \tag{32}$$

These relations suggest to regard $\mathcal{H}$ as a second quantization of the eCS Hamiltonian. Another important property of $\mathcal{H}$ is the following:

$$\langle\Omega,[A,\mathcal{H}]\Omega\rangle = 0, \tag{33}$$

which is true for a large class of operators A on $\mathcal{F}$ (see Lemma 4 in Ref. 11 for the precise statement), including arbitrary products of anyons.

Remark 2.1: A main technical point in Ref. 11 was to give precise mathematical meaning to this operator valued distributions $\phi_\nu(x)$ by introducing approximate anyons depending on a regularization parameter $\varepsilon>0$ such that, for $\varepsilon>0$, they are well-defined operator, and the anyons are obtained as a limit $\varepsilon\downarrow 0$ (see Sec. 2.2 in Ref. 11). This is a useful method to treat QFT divergences. However, in the present paper we can ignore this technicality except for one instance in Appendix A.

Remark 2.2: It is worth noting that, at zero temperature, the "vacuum" is a highest weight state annihilated by $\mathcal{H}$, but this property is lost at finite temperature. The relation in Eq. (33) is a weaker substitute for this highest weight conditions which holds true also at finite temperature. A similar remark applies to the operator $\check{W}^2$ discussed below.

2. Identities: a special case

In Refs. 9 and 11 we observed that the relations above imply that the anyon correlation function

$$G_{N,N}(\mathbf{x},\mathbf{y}) \equiv \langle\Omega,\Phi_\nu^N(\mathbf{x})^*\Phi_\nu^N(\mathbf{y})\Omega\rangle \tag{34}$$

satisfies the following remarkable identity:

$$[H_{\lambda,N}(\mathbf{x}) - H_{\lambda,N}(\mathbf{y})]G_{N,N}(\mathbf{x},\mathbf{y}) = 0. \tag{35}$$

The argument is simple: using Eq. (33) for $A=\Phi_\nu^N(\mathbf{x})^*\Phi_\nu^N(\mathbf{y})$ we get

$$\langle[\mathcal{H},\Phi_\nu^N(\mathbf{x})]\Omega,\Phi_\nu^N(\mathbf{y})\Omega\rangle - \langle\Omega,\Phi_\nu^N(\mathbf{x})^*[\mathcal{H},\Phi_\nu^N(\mathbf{y})]\Omega\rangle = 0, \tag{36}$$

where we used $[\Phi_\nu^N(\mathbf{x})^*,\mathcal{H}]=[\mathcal{H},\Phi_\nu^N(\mathbf{x})]^*$ which holds true since $\mathcal{H}$ is self-adjoint. Inserting Eq. (31) twice, moving the eCS Hamiltonians in front of the Hilbert inner product, and using (34) we get Eq. (35). Computing $G_{N,N}(\mathbf{x},\mathbf{y})$ one finds that it is equal to $F_{N,N}(\mathbf{x},\mathbf{y})$ in Eq. (6) [see Proposition 1 in Ref. 11 or Eqs. (42) and (43) below], and we thus obtain the special case $N=M$ of the identity in Eq. (7).

3. Other correlation functions

It is natural to try to generalize this identity by considering generalized anyon correlation functions which are vacuum expectation values of

$$\Phi_\nu^N(\mathbf{x})^* \Phi_\mu^M(\mathbf{y}),$$

allowing also for different particle numbers in $\mathbf{x}$ and $\mathbf{y}$ and/or different anyon parameters ν and μ. To construct and compute nontrivial such functions we need to recall a few more details of the anyon construction in Ref. 11

The explicit form of the anyons is

$$\phi_\nu(x) = {}^{\times}_{\times} R \exp\left(- i\nu^2 Q x - \nu \sum_{n\neq 0} \frac{1}{n} \rho(n) e^{inx} \right)^{\times}_{\times}, \tag{37}$$

where the $\rho(n)$, $n \in Z$, and R are generators of the Heisenberg algebra defined by the following relations:

$$[\rho(n), \rho(m)] = n\delta_{n,-m}, \quad [\rho(n), R] = \delta_{n,0} R \tag{38}$$

and

$$\rho(n)^* = \rho(-n), \quad R^* = R^{-1}, \tag{39}$$

where

$$\rho(0) = Q \tag{40}$$

has the physical interpretation of a *charge operator*. A important point here is the definition of normal ordering ${}^{\times}_{\times} \cdot {}^{\times}_{\times}$ which is not the standard one; see Lemma 1 in Ref. 11 for a detailed characterization. The operator Q satisfies, by definition,

$$Q\Omega = 0, \tag{41}$$

and this has important consequences: we say that an operator A on $\mathcal{F}$ has charge q iff $[Q, A] = qA$, and the definitions above imply that only operators A with charge zero can have a nonzero vacuum expectation value, and that $R^{\pm 1}$ changes the charge by ± 1. We therefore need to insert an appropriate power of R to get a nontrivial vacuum expectation value, and the natural correlation function to consider is

$$G_{\nu,\mu;N,M}(\mathbf{x};\mathbf{y}) = \langle \Omega, \Phi_\nu^N(\mathbf{x})^* R^{N-M} \Phi_\mu^M(\mathbf{y}) \Omega \rangle. \tag{42}$$

By straightforward computations we obtain (for details see Appendix A 1)

$$G_{\nu,\mu;N,M}(\mathbf{x};\mathbf{y}) = e^{i(p_1 X - p_2 Y)} \frac{\prod_{1\leq j<k\leq N} \theta(x_j - x_k)^{\nu^2} \prod_{1\leq j<k\leq M} \theta(y_k - y_j)^{\mu^2}}{\prod_{j=1}^N \prod_{k=1}^M \theta(x_j - y_k)^{\nu\mu}}, \tag{43}$$

where the exponential factor gives the dependence of the center-of-mass coordinates,

$$X = \sum_{j=1}^N x_j, \quad Y = \sum_{j=1}^M y_j, \tag{44}$$

and the center-of-mass momenta are determined by the statistics parameters of the anyons as follows:

$$p_1 = \tfrac{1}{2}(\nu^2 N - \nu\mu M), \quad p_2 = \tfrac{1}{2}(\mu^2 M - \nu\mu N). \tag{45}$$

Note that, up to the exponential factors, these correlation functions for $\mu = \nu = \sqrt{\lambda}$ and $\nu = -1/\mu = \sqrt{\lambda}$ are equal to the functions in Eq. (6) and (10), respectively.

In the following we give a simplified derivation of Eqs. (7) and (11), ignoring less interesting terms which only contribute to the constants $c_{N,M}$ and $\tilde{c}_{N,M}$, respectively, and which we indicate by dots. This simplifies the argument considerably. The complete equations including all terms are given in Appendix A 3 and A 4, respectively.

4. Derivation of the identity in Eq. (7)

We now consider the function

$$G_{N,M}(\mathbf{x};\mathbf{y}) \equiv G_{\nu,\nu;N,M}(\mathbf{x};\mathbf{y}), \quad \nu = \sqrt{\lambda} \tag{46}$$

and try to use a similar argument as above. If we now use the identity in Eq. (33) for $A = \Phi_\nu^N(\mathbf{x})^* R^{N-M} \Phi_\nu^M(\mathbf{y})$ and use Eq. (31) twice we obtain

$$[H_{\lambda,N}(\mathbf{x}) - H_{\lambda,M}(\mathbf{y})] G_{N,M}(\mathbf{x},\mathbf{y}) = \langle \Omega, \Phi_\nu^N(\mathbf{x})^* [\mathcal{H}, R^{N-M}] \Phi_\nu^M(\mathbf{y}) \Omega \rangle, \tag{47}$$

where we now get an additional term. It is a rather surprising that it is possible to compute this term in a simple manner: this is due to a "miracle" which we now describe.

For that we need to recall the explicit form of the second quantized eCS Hamiltonian $\mathcal{H}$,

$$\mathcal{H} = \nu \breve{W}^3 + (1-\nu^2)\mathcal{C} + 2\nu^2 \breve{W}^2 Q + \tfrac{1}{3}\nu^4 Q^3 - \nu^4 c_0 Q, \tag{48}$$

with the constant c_0 in Eq. (9),

$$\breve{W}^s = \frac{1}{s}\int_0^{2\pi} \frac{\mathrm{d}x}{2\pi} {}^{\times}_{\times} \left(\sum_{n\neq 0} \rho(n) e^{inx} \right)^s {}^{\times}_{\times} \quad \text{for } s = 2,3, \tag{49}$$

and $\mathcal{C}$ is some (known) operator satisfying

$$[\mathcal{C}, R] = 0, \quad \mathcal{C}\Omega = 0 \tag{50}$$

[see Proposition 2 in Ref. 11; the formula given there looks different but is equivalent, as is seen by a simple computation and the identity in Eq. (16)].

Remark 2.3: The charge operator Q [equal to the zero mode $\rho(0)$] plays an even more important role here than in Ref. 11, and it is therefore more natural now to write $\mathcal{H}$ in terms of the operators $\breve{W}^s$ with all zero modes removed: since these operators obviously commute with the charge-rising operator R,

$$\breve{W}^2 = \frac{1}{2}{\sum_n}' {}^{\times}_{\times} \rho(n)\rho(-n) {}^{\times}_{\times},$$

$$\breve{W}^3 = \frac{1}{3}{\sum_{n,m}}' {}^{\times}_{\times} \rho(n)\rho(m)\rho(-n-m) {}^{\times}_{\times} \tag{51}$$

with the prime on the sums indicating that all terms with at least one factor $\rho(0)$ are left out, it thus becomes easier to compute the commutator of $\mathcal{H}$ with R. It is gratifying to see that this also simplifies the formula for $\mathcal{H}$ [compare Eq. (48) above with Eq. (57) in Ref. 11].

We thus get

$$[\mathcal{H}, R^{N-M}] = 2(N-M)\lambda R^{N-M} \breve{W}^2 + \cdots, \tag{52}$$

with the dots less interesting terms which we ignore for simplicity (they are given in Appendix 2.3). The "miracle" is that this commutator is proportional to the operator $\breve{W}^2$ which plays an important twofold role in the anyon QFT: first, $\breve{W}^2$ is (essentially) the second quantization of the total momentum operator,

$$[\breve{W}^2, \Phi_\nu^N(\mathbf{x})] = P_N(\mathbf{x})\Phi_\nu^N(\mathbf{x}) + \cdots \tag{53}$$

with $P_N(\mathbf{x})$ defined in Eq. (13) is the generator of translations [see Eq. (68) in Ref. 11], and second, $\breve{W}^2$ is (essentially) identical with the many-body Hamiltonian used to construct the temperature representation (see Proposition 4 in Appendix B.2 of Ref. 11) which implies

$$\langle \Omega, A\breve{W}^2\Omega\rangle = -\frac{\partial}{\partial\beta}\langle\Omega, A\Omega\rangle + \cdots . \tag{54}$$

Remark 2.4: Equation (54) is the key to our identities. While the first term on the right-hand-side (rhs) is easy to understand from what we said above, the computation of the terms "$\cdots$" proportional to $\langle A\rangle$ is somewhat subtle. This computation clarifies some interesting aspects of our finite temperature representation not mentioned in Ref. 11. They are discussed in Appendix A 2.

Using Eqs. (53) and (54) we can compute

$$\begin{aligned}\langle \Omega, \Phi_\nu^N(\mathbf{x})^*[\mathcal{H}, R^{N-M}]\Phi_\nu^M(\mathbf{y})\Omega\rangle &= 2\lambda(N-M)\langle\Omega, \Phi_\nu^N(\mathbf{x})^* R^{N-M}([\breve{W}^2, \Phi_\nu^M(\mathbf{y})] + \Phi_\nu^M(\mathbf{y})\breve{W}^2)\Omega\rangle + \cdots \\ &= 2\lambda(N-M)\left(P_M(\mathbf{y}) - \frac{\partial}{\partial\beta}\right)G_{N,M}(\mathbf{x};\mathbf{y}) + \cdots ,\end{aligned}$$

and inserting this in Eq. (47) we obtain

$$[H_{\lambda,N}(\mathbf{x}) - H_{\lambda,M}(\mathbf{y})]G_{N,M}(\mathbf{x},\mathbf{y}) = 2\lambda(N-M)\left(P_M(\mathbf{y}) - \frac{\partial}{\partial\beta}\right)G_{N,M}(\mathbf{x};\mathbf{y}) + \cdots . \tag{55}$$

From Eqs. (46), (43), and (6) we see that $G_{N,M}(\mathbf{x};\mathbf{y})$ is equal to $F_{N,M}(\mathbf{x};\mathbf{y})$ up to a phase factor depending only on center-of-mass coordinates X and Y, and using

$$e^{-ipX}H_N(\mathbf{x})e^{ipX} = H_N(\mathbf{x}) + Np^2 - 2pP_N(\mathbf{x})$$

$$e^{-ipX}P_N(\mathbf{x})e^{ipX} = P_N(\mathbf{x}) - Np \tag{56}$$

the identity in Eq. (55) turns into a similar identity for $F_{N,M}(\mathbf{x};\mathbf{y})$. Remarkably we can use Eq. (14) to cancel all terms involving $P_N(\mathbf{x})$ and $P_M(\mathbf{y})$. This proves the identity in Eq. (7) up to the precise value of the constant $c_{N,M}$.

As mentioned, the missing details to also compute the constant $c_{N,M}$ are given in Appendices A 2 and A 3.

5. Derivation of the identity in Eq. (11)

In general, the argument above does not work for correlation functions in Eq. (42) if the anyon parameters ν and μ are different. However, there is one such case where it does work: from the explicit formula for the second quantization of the eCS Hamiltonian in Eq. (48) we observe that replacing ν by $-1/\nu$ gives back essentially the same operator up to a constant factor,

$$\mathcal{H}^{(\nu)} = -\lambda\mathcal{H}^{(-1/\nu)} + 2(\lambda+1)\breve{W}^2Q + (\lambda^2 + 1/\lambda)\left(\tfrac{1}{3}Q^3 - c_0Q\right), \quad \lambda = \nu^2, \tag{57}$$

where we now indicate also the anyon parameter ν. This suggests that we should be able to also get an identity for the correlation functions

$$\widetilde{G}_{N,M}(\mathbf{x};\mathbf{y}) \equiv G_{\nu,-1/\nu;N,M}(\mathbf{x};\mathbf{y}), \quad \nu = \sqrt{\lambda} \tag{58}$$

defined in Eq. (42). Indeed, by a similar computation as above we obtain

$$0 = \langle \Omega, [\Phi_\nu^N(\mathbf{x})^* R^{N-M} \Phi_{-1/\nu}^M(\mathbf{y}), \mathcal{H}^{(\nu)}]\Omega\rangle = [H_{\lambda,N}(\mathbf{x}) + \lambda H_{1/\lambda,M}(\mathbf{y})]\widetilde{G}_{N,M}$$
$$- \langle \Omega, \Phi_\nu^N(\mathbf{x})^* ([\mathcal{H}^{(\nu)}, R^{N-M}] - 2(\lambda+1)MR^{N-M}\check{W}^2)\Phi_{-1/\nu}^M(\mathbf{y})\Omega\rangle + \cdots ,$$

where we used Eqs. (33) and (57) and twice Eq. (31). As mentioned, the dots indicate less interesting terms specified in Appendix A 4. Inserting Eqs. (52) and (53) we get, similarly as above,

$$(H_{\lambda,N}(\mathbf{x}) + \lambda H_{1/\lambda,M}(\mathbf{y}))\widetilde{G}_{N,M}(\mathbf{x};\mathbf{y}) = \left(2(N-M)P_M(\mathbf{y}) - 2(\lambda N + M)\frac{\partial}{\partial\beta}\right)\widetilde{G}_{N,M}(\mathbf{x};\mathbf{y}) + \cdots . \tag{59}$$

Since $\widetilde{G}_{N,M}(\mathbf{x};\mathbf{y})$ is equal to $\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y})$ up to the center-of-mass phase factor [cf. Eqs. (58), (43), and (10)] we can use Eq. (56) to obtain a similar identity for $\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y})$. Again all terms involving $P_N(\mathbf{x})$ and $P_M(\mathbf{y})$ cancel due to Eq. (15), and we obtain the identity in Eq. (11) up to the value of the constant $\widetilde{c}_{N,M}$.

The details of this computation can be found in Appendix A 4.

III. CONCLUSIONS

It is interesting to note that by introducing the operators

$$L_{N,\lambda}(\mathbf{x}) = 2\lambda N\frac{\partial}{\partial\beta} + H_{N,\lambda}(\mathbf{x}) \tag{60}$$

one can write the identities in Eqs. (7) and (11) as follows:

$$(L_{\lambda,N}(\mathbf{x}) - L_{M,\lambda}(\mathbf{y}) - c_{N,M})F_{N,M}(\mathbf{x};\mathbf{y}) = 0 \tag{61}$$

and

$$(L_{\lambda,N}(\mathbf{x}) + \lambda L_{1/\lambda,M}(\mathbf{y}) - \widetilde{c}_{N,M})\widetilde{F}_{N,M}(\mathbf{x};\mathbf{y}) = 0, \tag{62}$$

respectively. The operator L_N seems to be a special case of one introduced by Bernard;[1] see Eq. (6.1) in Ref. 5. The results in Ref. 1 suggests that it should be possible to interpret Eqs. (61) and (62) as Ward identities of some conformal field theory on the torus; see Refs. 6 and 7. We also note that the special case $M=0$ of Eq. (7) seems to be identical with an identity given in the Remark after Theorem 4.1 in Ref. 7.

We finally discuss possible applications of these identities. We first discuss the trigonometric limit $\beta\to\infty$ in which case the derivative terms proportional to $\partial/\partial\beta$ in Eqs. (7) and (11) are absent. In particular, for $M=0$ we recover the well-known eigenvalue equation for the ground state of the Sutherland model which is the starting point of Sutherland's solution of this model,[15] as already mentioned in Sec. I. Another interesting special case is the identity in Eq. (7) for $N=M$: it seems to give an alternative construction of the Q-operator playing a central role in Ref. 8 deriving interesting explicit results for the solution of the Sutherland system. Moreover, this very identity is also the starting point of an alternative solution algorithm for the Sutherland model.[10] Our generalization of this identity to $M\neq N$ might allow to construct a generalized Q-operator relating eigenfunctions of the Sutherland model for different particle numbers and/or different coupling parameters λ and $1/\lambda$. For the general elliptic case $\beta<\infty$ the identity $N=M$ in Eq. (7) was used as a starting point for a perturbative algorithm to solve the eCS model as a formal power series in q^2.[12] We speculate that it might be possible to also find elliptic generalizations of the results in Ref. 8 using our identities (this is suggested to us by the interesting results on the 3-particle eCS system in Sec. 7 of Ref. 14).

APPENDIX A: QFT DERIVATION. DETAILS

In this Appendix we provide the details of the quantum field theory derivation of the identities summarized in our theorem.

1. Computation of the anyon correlation functions

Here we give more details of how to compute $G_{\nu,\mu;N,M}(\mathbf{x};\mathbf{y})$ defined in Eq. (42) and obtain Eq. (43).

We know that

$$\Phi_\nu^N(\mathbf{y}) = b_N(\mathbf{x})^{\nu^2 \times}_{\times} \Phi_\nu^N(\mathbf{x})^{\times}_{\times}, \quad b_N(\mathbf{x}) = \prod_{1\leqslant j<k\leqslant N} \theta(x_j - x_k) \tag{A1}$$

and thus

$$\begin{aligned}\left\langle \Omega, {}^{\times}_{\times}\Phi_\nu^N(\mathbf{x})^{*\times}_{\times} R^{N-M} {}^{\times}_{\times}\Phi_\mu^M(\mathbf{y})^{\times}_{\times}\Omega \right\rangle &= \langle \Omega, e^{i\nu^2 X/2} R^{-N} e^{i\nu^2 X/2} R^N R^{-M} e^{-i\mu^2 Y/2} R^M e^{-i\mu^2 Y/2}\Omega\rangle(*) \\ &= e^{i(N\nu^2 X - M\mu^2 Y)/2}(*)\end{aligned} \tag{A2}$$

[see Eqs. (50), (16), and (17) and in Ref. 11 we also used $R^{-1}QR = Q+1$ following from Eqs. (11) in Ref. 11] where

$$(*) = \prod_{j,k} e^{\nu\mu C(x_j - y_k)} = \prod_{j,k} \theta(x_j - x_k)^{-\nu\mu} e^{-i\nu\mu(x_j - y_k)/2} = e^{-i\nu\mu(MX - NY)/2} \prod_{j,k} \theta(x_j - x_k)^{-\nu\mu}$$

are the other contributions [see Eq. (44) in Ref. 11]. By simple computations this yields Eq. (43).

2. Finite temperature correlations functions

Equation (54) is a crucial step in the QFT derivation of our identities. As discussed in the main text, it is a consequence of β being equal to the inverse temperature and $\breve{W}^2$ being (essentially) the Hamiltonian used to construct the finite temperature representation of our QFT model. We now discuss this relation in more detail.

In Ref. 11 Appendix B.1, we proved that the vacuum expectation value of (essentially) any operator A is equal to its thermal expectation as follows:

$$\langle \Omega, A\Omega\rangle = \frac{1}{\mathcal{Z}} \lim_{a\to\infty} \mathrm{Tr}(e^{-\beta H_0} A_0), \tag{A3}$$

where

$$H_0 = aQ_0^2 + \sum_{n=1}^{\infty} \rho_0(n)\rho_0(-n) \tag{A4}$$

and the subscripts 0 are to indicate that these operators are in the standard (=zero temperature) representation;

$$\mathcal{Z} = \prod_{n=1}^{\infty} \frac{1}{(1-q^{2n})}, \quad q = e^{-\beta/2} \tag{A5}$$

is the partition function [see Proposition 4 and Eq. (B16) in Ref. 11]. Remarkably,

$$\frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \beta} = -c_2 \tag{A6}$$

with c_2 the constant in Eq. (21), and thus Eq. (A3) implies

$$\langle\Omega,AH\Omega\rangle = -\left(\frac{\partial}{\partial\beta} - c_2\right)\langle\Omega,A\Omega\rangle \tag{A7}$$

with $H=aQ^2+\Sigma_{n=1}^{\infty}\rho(-n)\rho(n)$. Since H is (essentially) equal to $aQ^2+\breve{W}^2$ this implies Eq. (54).

However, there is a subtle point we need to take into account to make this relation precise: the normal ordering prescription used in Ref. 11 is β-dependent, and $aQ^2+\breve{W}^2$ is therefore *not* equal to H (which is defined by zero temperature normal ordering) but differs from it by a constant. This difference can be computed as follows: by definition of the normal ordering in the thermal state [see Eq. (25) in Ref. 11], $\langle\Omega,\breve{W}^2\Omega\rangle=0$, whereas Eq. (A7) for $A=\mathbf{1}$ gives $\langle\Omega,H\Omega\rangle=c_2$. We conclude that $\breve{W}^2=H-aQ^2-c_2$, and thus

$$\langle\Omega,A\breve{W}^2\Omega\rangle = -\frac{\partial}{\partial\beta}\langle\Omega,A\Omega\rangle \tag{A8}$$

with the normal ordering difference taking away precisely the constant c_2 in Eq. (A7).

It is also important to note that also the anyon operators are defined using normal ordering. More explicitly, as explained in Remark 2.6 after Eq. (46) in Ref. 11, normal ordering of the anyon field $\phi_\nu(x)$ amounts to a multiplication with the constant

$$\left[(1-e^{-2\varepsilon})\prod_{m=1}^{\infty}(1-q^{2m}e^{-2\varepsilon})^2\right]^{-\nu^2/2}$$

in the limit $\varepsilon\downarrow 0$ [see Eq. (A4) in Ref. 11]; since the divergent factor is β independent, the factor accounting for the difference in normal ordering has a finite limit as $\varepsilon\downarrow 0$ which is identical with $\mathcal{Z}^{\nu^2}$. Thus

$$\langle\Omega,\Phi_\nu^N(\mathbf{x})^* R^{N-M}\Phi_\mu^M(\mathbf{y})\Omega\rangle = \mathcal{Z}^{N\nu^2+M\mu^2-1}\lim_{a\to\infty}\mathrm{Tr}(e^{-\beta H_0}\Phi_{\nu,0}^N(\mathbf{x})^* R_0^{N-M}\Phi_{\mu,0}^M(\mathbf{y})). \tag{A9}$$

We conclude that

$$\langle\Omega,\Phi_\nu^N(\mathbf{x})^* R^{N-M}\Phi_\mu^M(\mathbf{y})\breve{W}^2\Omega\rangle = -\left(\frac{\partial}{\partial\beta} + (N\nu^2+M\mu^2)c_2\right)G_{\nu,\mu;N,M}(\mathbf{x};\mathbf{y}) \tag{A10}$$

[we used Eq. (42)] which is the equation we need.

3. Detailed derivation of Eq. (7)

In our derivation of Eq. (7) in the main text we ignored terms proportional to $G_{N,M}(\mathbf{x};\mathbf{y})$ (indicated by dots), to simplify the argument. Here we give the full derivation, with all terms included.

Using Eq. (48) we obtain

$$[\mathcal{H},R^{N-M}] = (2\lambda\breve{W}^2 - c_0\lambda^2)(N-M)R^{N-M} + \tfrac{1}{3}\lambda^2[Q^3,R^{N-M}], \tag{A11}$$

implying

$$\begin{aligned}\langle\Omega,\Phi_\nu^N(\mathbf{x})^*[\mathcal{H},R^{N-M}]\Phi_\nu^M(\mathbf{y})\Omega\rangle &= 2\lambda(N-M)\langle\Omega,\Phi_\nu^N(\mathbf{x})^*\breve{W}^2 R^{N-M}\Phi_\nu^M(\mathbf{y})\Omega\rangle \\ &\quad + \lambda^2\left[\tfrac{1}{3}(N^3-M^3) - c_0(N-M)\right]G_{N,M}(\mathbf{x},\mathbf{y}).\end{aligned} \tag{A12}$$

We now use

$$\left[\breve{W}^2+\tfrac{1}{2}\lambda Q^2,\Phi_\nu^N(\mathbf{x})\right]=P_N(\mathbf{x})\Phi_\nu^N(\mathbf{x}) \tag{A13}$$

with $P_N(\mathbf{x})$ defined in Eq. (13) [see Eqs. (68) in Ref. 11; there is an error in this latter formula: $(\nu-1)(\nu-3)$ should be replaced by (ν^2-1)]. Using that and (A10) for $\nu=\mu$ [recall Eq. (49)] we obtain

$$\langle\Omega,\Phi_\nu^N(\mathbf{x})^*\breve{W}^2R^{N-M}\Phi_\nu^M(\mathbf{y})\Omega\rangle=\left(P_M(\mathbf{y})-\tfrac{1}{2}\lambda M^2-\frac{\partial}{\partial\beta}-\lambda(N+M)c_2\right)G_{N,M}(\mathbf{x},\mathbf{y}). \tag{A14}$$

Putting the equations above together we obtain

$$\left[H_{\lambda,N}(\mathbf{x})-H_{\lambda,M}(\mathbf{y})+2\lambda(N-M)\frac{\partial}{\partial\beta}\right]G_{N,M}(\mathbf{x},\mathbf{y})=\left(\lambda^2\left[\tfrac{1}{3}(N^3-M^3)-c_0(N-M)\right]+2\lambda(N-M)\times\left[P_M(\mathbf{y})-\tfrac{1}{2}\lambda M^2-\lambda(N+M)c_2\right]\right)G_{N,M}(\mathbf{x},\mathbf{y}). \tag{A15}$$

To get from this an identity for $F_{N,M}(\mathbf{x},\mathbf{y})$ we recall Eqs. (42), (43), (46), and (6), implying

$$G_{N,M}(\mathbf{x},\mathbf{y})=e^{ip(X+Y)}F_{N,M}(\mathbf{x},\mathbf{y}),\quad p=\tfrac{1}{2}(N-M)\lambda. \tag{A16}$$

Using the identities in Eq. (56) this gives

$$\left[H_{\lambda,N}(\mathbf{x})-H_{\lambda,M}(\mathbf{y})+2\lambda(N-M)\frac{\partial}{\partial\beta}\right]F_{N,M}(\mathbf{x},\mathbf{y})=\left(\lambda^2\left[\tfrac{1}{3}(N^3-M^3)-c_0(N-M)\right]+2\lambda(N-M)\times\left[P_M(\mathbf{y})-Mp-\tfrac{1}{2}\lambda M^2-\lambda(N+M)c_2\right]-(N-M)p^2+2p[P_N(\mathbf{x})-P_M(\mathbf{y})]\right)F_{N,M}(\mathbf{x},\mathbf{y}).$$

Inserting $p=\frac{1}{2}\lambda(N-M)$ and using Eq. (15) we see that all terms involving $P_N(\mathbf{x})$ and $P_M(\mathbf{y})$ on the rhs cancel, and we obtain the identity in Eq. (7) with

$$c_{N,M}=\lambda^2\left(\tfrac{1}{3}(N^3-M^3)-c_0(N-M)\right)-\lambda(N-M)(M\lambda(N-M)+\lambda M^2+2\lambda(N+M)c_2)-\tfrac{1}{4}(N-M)^3\lambda^2, \tag{A17}$$

identical with the constant in Eq. (8).

4. Detailed derivation of Eq. (11)

We now consider the functions defined in Eq. (58). Equations (42), (43), and (10) imply

$$\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y})=e^{i(p_1X-p_2Y)}\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y}),\quad p_1=\tfrac{1}{2}(\lambda N+M),\quad p_2=\tfrac{1}{2}(N+M/\lambda). \tag{A18}$$

Using Eq. (57) we can compute

$$\begin{aligned}0=&\langle\Omega,[\Phi_\nu^N(\mathbf{x})^*R^{N-M}\Phi_{-1/\nu}^M(\mathbf{y}),\mathcal{H}^{(\nu)}]\Omega\rangle=\langle[\mathcal{H}^{(\nu)},\Phi_\nu^N(\mathbf{x})]^*\Omega,R^{N-M}\Phi_M^{-1/\nu}(\mathbf{y})\Omega\rangle\\&+\langle\Omega,\Phi_{\nu,N}(\mathbf{x})^*[R^{N-M},\mathcal{H}^{(\nu)}]\Phi_M^{-1/\nu}(\mathbf{y})\Omega\rangle+\left\langle\Omega,\Phi_{\nu,N}(\mathbf{x})^*R^{N-M}\left[\lambda\mathcal{H}^{(-1/\nu)}-2(\lambda+1)\breve{W}^2Q\right.\right.\\&\left.\left.-(\lambda^2+1/\lambda)\left(\tfrac{1}{3}Q^3-c_0Q\right),\Phi_M^{-1/\nu}(\mathbf{y})\Omega\right\rangle=\left[H_{\lambda,N}(\mathbf{x})+\lambda H_{1/\lambda,M}(\mathbf{y})-(\lambda^2+1/\lambda)\left(\tfrac{1}{3}M^3-Mc_0\right)\right]\widetilde{G}_{N,M}\\&-\langle\Omega,\Phi_{\nu,N}(\mathbf{x})^*[\mathcal{H}^{(\nu)},R^{N-M}]\Phi_M^{-1/\nu}(\mathbf{y})\Omega\rangle-2(\lambda+1)M\langle\Omega,\Phi_{\nu,N}(\mathbf{x})^*\breve{W}^2R^{N-M}\Phi_M^{-1/\nu}(\mathbf{y})\Omega\rangle.\end{aligned}$$

As above,

$$\langle\Omega,\Phi_\nu^N(\mathbf{x})^*[\mathcal{H}^{(\nu)},R^{N-M}]\Phi_{-1/\nu}^M(\mathbf{y})\Omega\rangle = 2\lambda(N-M)\langle\Omega,\Phi_\nu^N(\mathbf{x})^*R^{N-M}\breve{W}^2\Phi_{-1/\nu}^M(\mathbf{y})\Omega\rangle + \lambda^2\left[\tfrac{1}{3}(N^3-M^3)-c_0(N-M)\right]\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y})$$

which yields

$$\left[H_{\lambda,N}(\mathbf{x})+\lambda H_{1/\lambda,M}(\mathbf{y})-\lambda^2\left(\tfrac{1}{3}N^3-Nc_0\right)-\left(\tfrac{1}{3}M^3-Mc_0\right)/\lambda\right]\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y}) = 2(\lambda N+M)\langle\Omega,\Phi_\nu^N(\mathbf{x})^*\breve{W}^2R^{N-M}\Phi_{-1/\nu}^M(\mathbf{y})\Omega\rangle. \tag{A19}$$

Moreover, Eq. (A10) gives

$$\langle\Omega,\Phi_\nu^N(\mathbf{x})^*\breve{W}^2R^{N-M}\Phi_{-1/\nu}^M(\mathbf{y})\Omega\rangle = \left(P_M(\mathbf{y})-\tfrac{1}{2}M^2/\lambda-\frac{\partial}{\partial\beta}-(\lambda N+M/\lambda)c_2\right)\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y}), \tag{A20}$$

and with that we obtain

$$\left[H_{\lambda,N}(\mathbf{x})+\lambda H_{1/\lambda,M}(\mathbf{y})+2(N\lambda+M)\frac{\partial}{\partial\beta}\right]\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y}) = \left[\lambda^2\left(\tfrac{1}{3}N^3-c_0N\right)+\left(\tfrac{1}{3}M^3-Mc_0\right)/\lambda + 2(N\lambda+M)\left[P_M(\mathbf{y})-\tfrac{1}{2}M^2/\lambda-(\lambda N+M/\lambda)c_2\right]\right]\widetilde{G}_{N,M}(\mathbf{x},\mathbf{y}),$$

or equivalently

$$\left[H_{\lambda,N}(\mathbf{x})+\lambda H_{1/\lambda,M}(\mathbf{y})+2(N\lambda+M)\frac{\partial}{\partial\beta}\right]\widetilde{F}_{N,M}(\mathbf{x},\mathbf{y}) = \left[\lambda^2\left(\tfrac{1}{3}N^3-c_0N\right)+\left(\tfrac{1}{3}M^3-Mc_0\right)/\lambda + 2(N\lambda+M)\left[P_M(\mathbf{y})+Mp_2-\tfrac{1}{2}M^2/\lambda-(\lambda N+M/\lambda)c_2\right]-Np_1^2+2p_1P_N(\mathbf{x})-\lambda Mp_2^2 - 2\lambda p_2P_M(\mathbf{y})\right]\widetilde{F}_{N,M}(\mathbf{x},\mathbf{y}), \tag{A21}$$

where we used Eqs. (A18) and (56). Using Eq. (15) we see that, again, all derivative terms involving $P_N(\mathbf{x})$ and $P_M(\mathbf{y})$ cancel, and we obtain the identity in Eq. (11) with

$$\widetilde{c}_{N,M} = \lambda^2\left(\tfrac{1}{3}N^3-c_0N\right)+\left(\tfrac{1}{3}M^3-Mc_0\right)/\lambda+(N\lambda+M)[M(N+M/\lambda)-M^2/\lambda-2(\lambda N+M/\lambda)c_2] - \tfrac{1}{4}N(N\lambda+M)^2-\tfrac{1}{4}\lambda M(N+M/\lambda)^2 \tag{A22}$$

identical with the constant in Eq. (12).

APPENDIX B: ELEMENTARY PROOFS OF THE IDENTITIES

We define the function

$$G(\mathbf{x};\mathbf{y}) = \frac{\prod_{1\le j<k\le N}\theta(x_k-x_j)^{\lambda_1}\prod_{1\le J<K\le M}\theta(y_J-y_K)^{\lambda_2}}{\prod_{j=1}^N\prod_{K=1}^M\theta(x_j-y_K)^{\lambda_3}} \tag{B1}$$

and compute

$$W := \frac{1}{G}\left(\sum_{j=1}^N\frac{\partial^2}{\partial x_j^2}-A\sum_{J=1}^M\frac{\partial^2}{\partial y_J^2}\right)G \tag{B2}$$

with parameters λ_1, λ_2, λ_3, and A to be determined. We find it convenient to use in this appendix two different kinds of indices: small letters $j,k,\ell=1,2,\ldots,N$ and capital letters $J,K,L=1,2,\ldots,M$. Obviously,

$$\frac{\partial G}{\partial x_j} = \left[\sum_{j \neq k} \lambda_1 \phi(x_j - x_k) - \sum_K \lambda_3 \phi(x_j - y_K) \right] G \tag{B3}$$

and

$$\frac{1}{G} \frac{\partial^2}{\partial x_j^2} G = \sum_{k \neq j} \lambda_1 \phi'(x_j - x_k) + \sum_{k,\ell \neq j} \lambda_1^2 \phi(x_j - x_k) \phi(x_j - x_\ell) - \sum_K \lambda_3 \phi'(x_j - y_K) + \sum_{K,L} \lambda_3^2 \phi(x_j - y_K) \phi(x_j - y_L) - 2 \sum_{k \neq j, K} \lambda_1 \lambda_3 \phi(x_j - x_k) \phi(x_j - y_K), \tag{B4}$$

and similarly for the y_J-derivatives. We collect the terms in eight different groups as follows:

$$W = W_1 + W_2 + W_3 + W_4, \quad W_s = W_s^{(1)} - W_s^{(2)} \tag{B5}$$

with

$$W_1^{(1)} = \sum_{j,k \neq j} [\lambda_1 \phi'(x_j - x_k) + \lambda_1^2 \phi(x_j - x_k)^2], \tag{B6}$$

$$W_1^{(2)} = A \sum_{J,K \neq J} [\lambda_2 \phi'(y_J - y_K) + \lambda_2^2 \phi(y_J - y_K)^2], \tag{B7}$$

$$W_2^{(1)} = \sum_{j \neq k \neq \ell} \lambda_1^2 \phi(x_j - x_k) \phi(x_j - x_\ell), \tag{B8}$$

where $\Sigma_{j \neq k \neq \ell}$ is short for the sum over all j, k, ℓ with the constraints $j \neq k$ and $j \neq \ell$ and $k \neq \ell$,

$$W_2^{(2)} = A \sum_{J \neq K \neq L} \lambda_2^2 \phi(y_J - y_K) \phi(y_J - y_L), \tag{B9}$$

$$W_3 = (1 - A) \sum_{j,K} [-\lambda_3 \phi'(x_j - y_K) + \lambda_3^2 \phi(x_j - y_K)^2], \tag{B10}$$

since obviously $W_3^{(2)} = -A W_3^{(1)}$, and the rest

$$W_4 = \sum_{j,K \neq L} \lambda_3^2 \phi(x_j - y_K) \phi(x_j - y_L) - A \sum_{J,k \neq \ell} \lambda_3^2 \phi(y_J - x_k) \phi(y_J - x_\ell) - \sum_{j,k \neq j,K} 2\lambda_1 \lambda_3 \phi(x_j - x_k) \phi(x_j - y_K) + A \sum_{J,K \neq J,k} 2\lambda_2 \lambda_3 \phi(y_J - y_K) \phi(y_J - x_k). \tag{B11}$$

We insert $\phi'(x) = -V(x)$ and $\phi(x)^2 = V(x) - c_0 - 2f(x)$ [see Eqs. (23) and (24)] in Eq. (B6) and obtain

$$\begin{aligned} W_1^{(1)} &= \sum_{j,k \neq j} [\lambda_1(\lambda_1 - 1) V(x_j - x_k) - \lambda_1^2 c_0 - 2\lambda_1^2 f(x_j - x_k)] \\ &= -N(N-1)\lambda_1^2 c_0 + \sum_{j<k} [2\lambda_1(\lambda_1 - 1) V(x_j - x_k) - 4\lambda_1^2 f(x_j - x_k)], \end{aligned}$$

where we used that the functions V and f are even, and similarly

$$W_1^{(2)} = -AM(M-1)\lambda_2^2 c_0 + A \sum_{J<K} [2\lambda_2(\lambda_2 - 1) V(y_J - y_K) - 4\lambda_2^2 f(y_J - y_K)].$$

Renaming summation indices and using that ϕ is odd we then write

$$W_2^{(1)} = \sum_{j\neq k\neq \ell} \frac{1}{3}(-\lambda_1^2)[\phi(x_k - x_j)\phi(x_j - x_\ell) + \phi(x_j - x_\ell)\phi(x_\ell - x_k) + \phi(x_\ell - x_k)\phi(x_k - x_j)].$$

Inserting the identity in Eq. (23) with $x=x_k-x_j$, $y=x_j-x_\ell$, and $z=x_\ell-x_k$ gives

$$W_2^{(1)} = \sum_{j\neq k\neq \ell} \frac{1}{3}(-\lambda_1^2)[f(x_k - x_j) + f(x_j - x_\ell) + f(x_\ell - x_k)] = -2\lambda_1^2(N-2)\sum_{j<k} f(x_j - x_k),$$

where we again renamed summation indices and used that f is even. Similarly,

$$W_2^{(2)} = -2A\lambda_2^2(M-2)\sum_{J<K} f(y_J - y_K).$$

Inserting Eq. (23) in Eq. (B10) we obtain

$$W_3 = (1-A)\lambda_3(\lambda_3+1)\sum_{j,K} V(x_j - y_K) - (1-A)\lambda_3^2\left(NMc_0 + 2\sum_{j,K} f(x_j - y_K)\right).$$

The first term in this expression mixes $\mathbf{x}$ and $\mathbf{y}$ in a intolerable way, and in order to get a useful relation it must disappear. This leads to the following important restriction on parameters:

$$(1-A)\lambda_3(\lambda_3+1) = 0. \tag{B12}$$

Next we try to simplify W_4. We write $W_4 = W_4^{(1)} - W_4^{(2)}$ with

$$W_4^{(1)} = \sum_{j,K\neq L} [-\lambda_3^2\phi(y_K - x_j)\phi(x_j - y_L) - A\lambda_2\lambda_3\phi(y_K - y_J)\phi(y_J - x_j) - A\lambda_2\lambda_3\phi(y_J - y_K)\phi(y_K - x_j)],$$

where we used that ϕ is odd and wrote the same term in two different ways renaming summation indices. Similarly,

$$W_4^{(2)} = \sum_{J,k\neq \ell} [-A\lambda_3^2\phi(x_k - y_J)\phi(y_J - x_\ell) - \lambda_1\lambda_3\phi(x_k - x_j)\phi(x_j - y_K) - \lambda_1\lambda_3\phi(x_j - x_k)\phi(x_k - y_K)].$$

We now see that we can use the identity in Eq. (23) to simplify W_4 provided the parameters obey the following conditions:

$$\lambda_3 = A\lambda_2 \quad \text{and } A\lambda_3 = \lambda_1, \tag{B13}$$

and this is another important restriction on parameters. If and only if this holds true we get

$$\begin{aligned} W_4^{(1)} &= \sum_{j,K\neq L} (-\lambda_3^2)[f(y_K - x_j) + f(y_J - y_K) + f(x_j - y_J)] \\ &= -2(M-1)\lambda_3^2\sum_{j,K} f(y_K - x_j) - 2N\lambda_3^2\sum_{J<K} f(y_J - y_K), \end{aligned}$$

and similarly

$$W_4^{(2)} = -2A(N-1)\lambda_3^2\sum_{J,k} f(x_k - y_J) - 2MA\lambda_3^2\sum_{j<k} f(x_j - x_k).$$

Assuming the conditions in Eqs. (B12) and (B13) hold true we thus obtain

$$W = 2\lambda_1(\lambda_1 - 1)\sum_{j<k} V(x_j - x_k) - A2\lambda_2(\lambda_2 - 1)\sum_{J<K} V(y_J - y_K) - [N(N-1)\lambda_1^2 - AM(M-1)\lambda_2^2 + (1-A)\lambda_3^2 NM]c_0 + 2(-N\lambda_1^2 + AM\lambda_3^2)\sum_{j<k} f(x_j - x_k) + 2(AM\lambda_2^2 - N\lambda_3^2)\sum_{J<K} f(y_J - y_K) + 2[-(1-A) - (M-1) + A(N-1)]\lambda_3^2\sum_{j,K} f(x_j - y_K), \tag{B14}$$

or equivalently,

$$\left[H_{\lambda_1,N}(\mathbf{x}) - AH_{\lambda_2,M}(\mathbf{x}) - C_0 - C_1\sum_{j<k} f(x_j - x_k) - C_2\sum_{J<K} f(x_J - x_K) + C_3\sum_{j,K} f(x_j - y_K)\right]G = 0 \tag{B15}$$

with

$$C_1 = 2(N\lambda_1^2 - AM\lambda_3^2), \quad C_2 = 2(N\lambda_3^2 - AM\lambda_2^2), \quad C_3 = 2[AN - M] \tag{B16}$$

and

$$C_0 = [N(N-1)\lambda_1^2 - AM(M-1)\lambda_2^2 + (1-A)\lambda_3^2 NM]c_0. \tag{B17}$$

Using the identity in (25) we now compute

$$\frac{1}{G}\frac{\partial G}{\partial \beta} = \lambda_1\sum_{j<k}[c_1 - f(x_j - x_k)] + \lambda_2\sum_{J<K}[c_1 - f(y_J - y_K)] - \lambda_3\sum_{j,K}[c_1 - f(x_j - y_K)] = \frac{1}{2}[N(N-1)\lambda_1 + M(M-1)\lambda_2 - 2NM\lambda_3]c_1 - \lambda_1\sum_{j<k} f(y_J - y_K) - \lambda_2\sum_{J<K} f(y_J - y_K) + \lambda_3\sum_{j,K} f(x_j - y_K). \tag{B18}$$

We thus see that we can write Eq. (B15) in the following form:

$$\left[H_{\lambda_1,N}(\mathbf{x}) - AH_{\lambda_2,M}(\mathbf{y}) - \tilde{C}_0 + C\frac{\partial}{\partial \beta}\right]G = 0 \tag{B19}$$

provided that

$$C_i = C\lambda_i \quad \text{for } i = 1,2,3. \tag{B20}$$

In this case

$$\tilde{C}_0 = C_0 + C\tfrac{1}{2}[N(N-1)\lambda_1 + M(M-1)\lambda_2 - 2NM\lambda_3]c_1. \tag{B21}$$

Interestingly, the conditions in (B12), (B13), and (B20) have two nontrivial solutions. First,

$$A = 1, \quad \lambda_1 = \lambda_2 = \lambda_3 \equiv \lambda, \tag{B22}$$

with $C=2(N-M)\lambda$ and $\tilde{C}_0=c_{N,M}$ given in Eq. (8), and second,

$$A = -\lambda, \quad \lambda_1 = \lambda, \quad \lambda_2 = 1/\lambda, \quad \lambda_3 = -1 \tag{B23}$$

with $C=2(\lambda N+M)$ and $\tilde{C}_0=\tilde{c}_{N,M}$ in Eq. (12). Obviously these two cases correspond to the identities given in Eqs. (6)–(11), and we have completed our proof. □

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Optimal estimation of quantum observables

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We consider the problem of estimating the ensemble average of an observable on an ensemble of equally prepared identical quantum systems. We show that, among all kinds of measurements performed jointly on the copies, the optimal unbiased estimation is achieved by the usual procedure that consists in performing independent measurements of the observable on each system and averaging the measurement outcomes. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168122]

I. INTRODUCTION

The astonishing precision of measurements currently available in quantum optics[1] along with the growing demand of quantum devices of the new information technology[2,3] have revived the interest in the theory of quantum measurements.[4] The outcome statistics of a quantum measurement for all possible input states is described by a positive operator valued measure (POVM). The general optimization approach of quantum estimation theory[5] is to maximize over all possible POVM's an appropriate cost function, which depends on the context and on the specific use of the measurement. The output statistics can then be improved by using multiple copies of the same quantum system, all prepared in the same state, and performing a suitable *ensemble measurement* over the copies.

The experimental complexity of ensemble measurements is roughly classified by dividing them into three main categories: (a) *independent*, (b) *separable*, and (c) *entangled* measurements. Category (a) is described by tensor products of independent POVM's; (b) by POVM's with separable elements only; (c) by POVM's where some elements are entangled. Notice that the separability of POVM's generally does not correspond to a physical separability of measuring apparatuses [there exist separable measurements that cannot be performed by separate measuring apparatuses, i.e., by local operations and classical communication (LOCC)], and this classification remains essentially mathematical in nature. However, at least one can say that category (b) contains all *adaptive* measurements (in which the choice of the measuring apparatus on the nth copy depends on the outcomes of previous measurements), whereas category (c) contains those measurements that need quantum interactions between copies, implying that all copies during the measuring time must be at the same physical location, or, otherwise, that a "quantum memory" is available.

Among the three categories of ensemble measurements, the category (c) of entangled POVM's discloses the full exponential growth of the Hilbert space dimension versus the number of copies N for a virtually unlimited optimization of the statistical efficiency of the measurement, with the

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possibility of largely surpassing the performance of categories (a) and (b).[6–9] Indeed, over the last few years, it has been recognized that entangled measurements are usually more efficient than independent measurements, and the optimal measurement scheme is almost always entangled.[10–13] However, in some situations it has been also shown that asymptotically for $N\to\infty$ an equivalently optimal estimation may be achieved using just independent measurements over the copies.[14–17]

In the above scenario it is natural to ask if the *canonical procedure* of averaging the outcomes of repeated measurements of an observable A over equally prepared systems is the best way of estimating the ensemble average $\langle A\rangle$ of A, or, instead, if a joint entangled measurement over the copies can improve the estimation. As we will see it turns out that the canonical procedure is indeed optimal, however, the derivation of this result is nontrivial, and offers a general warning against easy assumptions and generalizations when evaluating statistical efficiencies of ensemble measurements.

Let us be more precise, and fix precisely the scenario of the quantum estimation. Suppose one has a finite number N of equally prepared distinguishable identical d-dimensional quantum systems, which are described by the state $\rho^{\otimes N}$, and one wants to estimate the ensemble average $\langle A\rangle_\rho \equiv \mathrm{Tr}[\rho A]$ of the observable A. Suppose now that one has unlimited technology at one's disposal, including measuring apparatus that can achieve any desired entangled POVM on all N systems jointly. The question is which is the best measuring apparatus to choose in order to estimate $\langle A\rangle_\rho$ with the minimum statistical error? What we will prove in the present paper is that the best estimation strategy is just the canonical procedure, which consists in averaging the outcomes of repeated measurements of the observable A over the equally prepared quantum systems.

II. PERMUTATIONALLY INVARIANT POLARIZATION IDENTITIES

In the derivation of our main result the following lemma will play a crucial role.

Lemma 1: Any permutationally invariant operator X on $\mathsf{H}^{\otimes N}$ is completely determined by all ensemble averages $\mathrm{Tr}[X\rho^{\otimes N}]$ on identical equally prepared systems.

Proof: The statement of the lemma is equivalent to the following logical implication:

$$X\in\mathcal{P}_N(\mathsf{H}),\quad \forall\,\rho\in\mathcal{S}(H),\quad \mathrm{Tr}[X\rho^{\otimes N}]=0\Rightarrow X=0, \tag{1}$$

where $\mathcal{S}(H)$ denotes the set of states on H, and $\mathcal{P}_N(\mathsf{H})$ the algebra of permutationally invariant operators on $\mathsf{H}^{\otimes N}$. Indeed, statement (1) is equivalent to the statement that if $\mathrm{Tr}[X\rho^{\otimes N}]=\mathrm{Tr}[Y\rho^{\otimes N}]$ for all states ρ, then $X\equiv Y$.

Consider the following special states of the form

$$\rho_\lambda=\sum_{j=1}^{N}\lambda_j|\psi_j\rangle\langle\psi_j|,\quad \lambda_j>0,\lambda_j\neq\lambda_i,i\neq j, \tag{2}$$

with $\{\psi_j\}_N$ any set of N unequal states (not necessarily orthogonal). The trace $\mathrm{Tr}[X\rho_\lambda^{\otimes N}]$ is a polynomial in $\Pi_{j=1}^N\lambda_j^{x_j}$, with $\Sigma_{j=1}^N x_j=N$ and $x_j\geqslant 0$ integers. Now, in order to have $\mathrm{Tr}[X\rho_\lambda^{\otimes N}]=0$ for arbitrary ρ_λ, all coefficients of the polynomial must vanish. In particular, the coefficient of $\Pi_{j=1}^N\lambda_j$ is given by

$$\sum_\sigma\langle\psi_1|\ldots\langle\psi_N|\Pi_\sigma X\Pi_\sigma^\dagger|\psi_1\rangle\ldots|\psi_N\rangle\equiv 0, \tag{3}$$

where Π_σ are the permutations of the N systems. By hypothesis we have $\Pi_\sigma X\Pi_\sigma^\dagger=X$, then the vanishing of $\mathrm{Tr}[X\rho_\lambda^{\otimes N}]$ for all states ρ_λ implies

$$\langle\psi_1|\ldots\langle\psi_N|X|\psi_1\rangle\ldots|\psi_N\rangle=0, \tag{4}$$

for all sets $\{\psi_j\}_N$. If we take $|\psi_k\rangle=\alpha|\phi\rangle+\beta|\phi_\perp\rangle$, by arbitrariness of α and β we have

$$\begin{aligned}\langle\psi_1|\cdots\langle\phi|\cdots\langle\psi_N|X|\psi_1\rangle\cdots|\phi\rangle\cdots|\psi_N\rangle &= \langle\psi_1|\cdots\langle\phi|\cdots\langle\psi_N|X|\psi_1\rangle\cdots|\phi_\perp\rangle\cdots|\psi_N\rangle \\ &= \langle\psi_1|\cdots\langle\phi_\perp|\cdots\langle\psi_N|X|\psi_1\rangle\cdots|\phi\rangle\cdots|\psi_N\rangle \\ &= \langle\psi_1|\cdots\langle\phi_\perp|\cdots\langle\psi_N|X|\psi_1\rangle\cdots|\phi_\perp\rangle\cdots|\psi_N\rangle = 0. \quad (5)\end{aligned}$$

By repeating the same argument for different values of k and choosing ϕ and $\phi_\perp$ as all possible elements of an orthonormal basis $\{\phi_j\}$ we get

$$\langle\phi_{j_1}|\cdots\langle\phi_{j_N}|X|\phi_{k_1}\rangle\cdots|\phi_{k_N}\rangle = 0, \quad \forall\,\{j_i\},\{k_i\}. \quad (6)$$

Since all the matrix elements of X on an orthonormal basis are null, one has that $X\equiv 0$. ■

Notice that the proof of the previous lemma contains the following interesting corollary.

Corollary 1: For any operator X on $\mathsf{H}^{\otimes N}$ the diagonal elements on factorized states completely determine X.

This is a kind of *factorized* polarization identity for permutation invariant operators.

III. THE MAIN RESULT

Let us now come back to the original problem of determining the optimal measurement for estimating the ensemble average of an observable. Consider a generic joint POVM $P(r)$ on $\mathsf{H}^{\otimes N}$, with outcome r providing an estimate of the expectation $\langle A\rangle_\rho$ of the observable A on N identical systems all in the same state ρ. Clearly, one has $\lambda_m \leqslant r \leqslant \lambda_M$, with λ_m and λ_M minimum and maximum eigenvalues of A, respectively. The POVM $P(r)$ provides an estimate of the expectation $\langle A\rangle_\rho$ if the conditional probability $p(r|\rho)$ of estimating expectation value r for actual value $\mathrm{Tr}[A\rho]$ is expressed via the Born rule as follows:

$$p(r|\rho)\mathrm{d}r = \mathrm{Tr}[P(r)\rho^{\otimes N}]\mathrm{d}r. \quad (7)$$

Since the state $\rho^{\otimes N}$ is permutation invariant, we can consider permutation invariant POVM's. Indeed, using invariance of $\rho^{\otimes N}$ under permutations, one has

$$p(r|\rho)\mathrm{d}r = \frac{1}{N!}\sum_\sigma \mathrm{Tr}[\Pi_\sigma\rho^{\otimes N}\Pi_\sigma^\dagger P(r)]\mathrm{d}r = \mathrm{Tr}\left[\rho^{\otimes N}\frac{1}{N!}\sum_\sigma(\Pi_\sigma^\dagger P(r)\Pi_\sigma)\right]\mathrm{d}r = \mathrm{Tr}[\Pi'(r)\rho^{\otimes N}]\mathrm{d}r, \quad (8)$$

where the POVM

$$P'(r) \equiv \frac{1}{N!}\sum_\sigma \Pi_\sigma^\dagger P(r)\Pi_\sigma \quad (9)$$

is permutation invariant by construction. This means that for any POVM there is a permutation invariant one giving the same probability distributions for all states $\rho^{\otimes N}$. Therefore, without loss of generality, in the following we can assume that $P(r)$ is permutation invariant. We will consider now the case in which the POVM is *unbiased*, that is the averaging over r coincides with the value to be estimated. Mathematically this means that for all states ρ the following identity holds:

$$\int_{\lambda_m}^{\lambda_M}\mathrm{d}r\, rp(r|\rho) = \mathrm{Tr}[A\rho]. \quad (10)$$

The statistical error in the estimate is given by the rms of the probability distribution

$$\epsilon_N(A) \doteq \left[\int_{\lambda_m}^{\lambda_M}\mathrm{d}r(r-\langle A\rangle_\rho)^2 p(r|\rho)\right]^{1/2}, \quad (11)$$

which for unbiased estimation equals

$$\epsilon_N(A) \doteq \left[\int_{\lambda_m}^{\lambda_M} \mathrm{d}r[r^2 p(r|\rho)] - \langle A \rangle_\rho^2 \right]^{1/2}. \tag{12}$$

Since the only part which depends on the POVM is the conditional probability $p(r|\rho)$, the optimization of the error resorts to minimize the quantity

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, r^2 \,\mathrm{Tr}[P(r)\rho^{\otimes N}], \tag{13}$$

with the constraints

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, P(r) = I, \tag{14}$$

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, r\, \mathrm{Tr}[P(r)\rho^{\otimes N}] = \langle A \rangle_\rho. \tag{15}$$

Using the following identity:

$$\langle A \rangle_\rho = \mathrm{Tr}\left[\rho^{\otimes N} \frac{1}{N!} \sum_\sigma \Pi_\sigma (A \otimes I^{\otimes (N-1)}) \Pi_\sigma^\dagger \right] = \mathrm{Tr}\left[\rho^{\otimes N} \frac{1}{N} \sum_{k=1}^N A^{(k)} \right] \tag{16}$$

with $A^{(k)} \doteq I^{\otimes (k-1)} \otimes A \otimes I^{\otimes N-k}$, by virtue of Lemma 1 we can recast Eq. (15) as follows:

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, rP(r) = \frac{1}{N} \sum_{k=1}^N A^{(k)} \doteq \Theta. \tag{17}$$

The operator $\Delta \geqslant 0$ defined as

$$\Delta \doteq \int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, r^2 P(r), \tag{18}$$

allows to reexpress the statistical error as follows:

$$\epsilon_N(A)^2 = \mathrm{Tr}[\Delta \rho^{\otimes N}] - \langle A \rangle_\rho^2. \tag{19}$$

In the representation in which Δ is diagonal, the constraints (14) and (15) become

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, P(r)_{lk} = \delta_{lk}, \tag{20}$$

$$\int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, rP(r)_{lk} = \Theta_{lk}, \tag{21}$$

whereas the error (12) becomes

$$\epsilon_N(A)^2 = \sum_n (\rho^{\otimes N})_{nn} \int_{\lambda_m}^{\lambda_M} \mathrm{d}r\, r^2 P(r)_{nn} - \langle A \rangle_\rho^2. \tag{22}$$

From Eqs. (20) and (21) it follows that the diagonal elements $P(r)_{nn}$ are probability densities in r over $[\lambda_m, \lambda_M]$, with average Θ_{nn}. Denoting the variance of $P(r)_{nn}$ by σ_n^2, we can write

$$\epsilon_N(A)^2 = \sum_n (\rho^{\otimes N})_{nn}(\sigma_n^2 + \Theta_{nn}^2) - \langle A\rangle_\rho^2. \tag{23}$$

Therefore, $\epsilon_N(A)^2$ is minimized by taking $\sigma_n^2=0$, corresponding to $P(r)_{nn} \equiv \delta(\Theta_{nn}-r)$. This implies that the outcomes of the optimal POVM are actually discrete, corresponding to $r_n=\Theta_{nn}$. In this discrete version, the POVM has $P(r_n)_{nm}=\delta_{nm}$ [which also implies that $\Theta_{nm}=\delta_{nm}\Theta_{nn}$ via Eq. (21)], that is $P(r_n)$ is projection valued on the nth eigenvector of Δ (when it happens that $\Theta_{nn}=\Theta_{mm}$ for some $m \neq n$, then the projector has rank equal to the number of equal diagonal elements). We have finally

$$\epsilon_N(A)^2 = \sum_n (\rho^{\otimes N})_{nn}\Theta_{nn}^2 - \langle A\rangle_\rho^2. \tag{24}$$

Moreover, we have

$$I = \sum_n P(r_n), \tag{25}$$

$$\Theta = \sum_n \Theta_{nn} P(r_n), \tag{26}$$

$$\Delta = \sum_n \Theta_{nn}^2 P(r_n). \tag{27}$$

Since optimization makes Θ and Δ jointly diagonal, one has $\Sigma_n \Theta_{nn}^2(\rho^{\otimes N})_{nn}=\mathrm{Tr}[\Theta^2\rho^{\otimes N}]$, and using Eqs. (17) and (24) we can write the following expression for the minimal error:

$$\epsilon_N(A)^2 = \frac{1}{N^2}\sum_{i,j=1}^{N} \mathrm{Tr}[A^{(i)}A^{(j)}\rho^{\otimes N}] - \langle A\rangle_\rho^2. \tag{28}$$

Notice that the sum in the first term contains N terms with $i=j$ equal to $\mathrm{Tr}[A^2\rho]$ and $N(N-1)$ with $i \neq j$ equal to $\langle A\rangle_\rho^2$, resulting in

$$\epsilon_N(A) = \sqrt{\frac{\langle A^2\rangle_\rho - \langle A\rangle_\rho^2}{N}}, \tag{29}$$

that is the optimal error equals the statistical error occurring when measuring A separately on all the identical quantum systems in the state ρ, and then averaging. Indeed, the optimal POVM coincides with the spectral resolution of $\Theta=(1/N)\Sigma_n A^{(n)}$ on $\mathsf{H}^{\otimes N}$.

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Regge trajectories of the Coulomb potential in the space of constant negative curvature ${}^1S_3$

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Analytic properties of the scattering amplitude for Coulomb potential on the background of the space of constant negative curvature are studied. Special attention is given to the comparison of the Regge trajectories for curved and flat spaces. We show that there exist considerably differences in the behavior of the Regge trajectories in these spaces. © *2006 American Institute of Physics.*
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I. INTRODUCTION

As is well known one of the central roles in high energy physics plays Regge concept[1–4] based on the analytical extension of the scattering amplitudes in the complex angular momentum plane. One of the most distinctive features of this technique are the Regge trajectories. Regge trajectories are very generic in hadronic physics. For example, they are well established for mesons, baryons, and soft Pomeron.[5–8] Recently a lot of activity has been dedicated to various studies of the Regge trajectories.[7,9,10]

In recent years a revival interest to the Regge approach in the high energy physics is seen.[11,12] At present time, Regge approach is applied with success for description of the hadrons at high energies.[13–15] We note that, in the series of the works the idea of the generalized Pomeron (vacuum Regge trajectory which determine asymptotic behavior of the scattering amplitudes at high energies)—the BFKL (Balitsky-Fadin-Kuraev-Lipatov) Pomeron is applied with success for description of the processes at high energy.[16] Recently, the Regge concept is applied to astrophysics problems.[17,18] For example, in cosmology it is demonstrated[17] that the use of the Regge trajectories makes it possible to explain the problem of the rotation of cosmic objects.[19,20]

Also in recent years the quantum-mechanical models based on the geometry of spaces of constant curvature have attracted considerable attention due to their interesting mathematical features[21–24] as well as the possibility of applications to physical problems.[25] For example, these models are used for the description of the bound states in nuclear and elementary particle physics[24] Thus, Kepler problem on the sphere S_3 has been used as a model for description of quarkonium spectrum,[26] also it was used as a model for description of the spectra electrons, holes, and excitons confined in semiconductor quantum dots.[27,28] Also, integrable models on a sphere S_3 are used for construction of model potential for quantum dots.[29]

In this paper we apply the Regge analysis to the Coulomb scattering problem in the space of constant negative curvature ${}^1S_3$. The analytic properties of the scattering amplitude for Coulomb potential in the complex angular momentum plane in the three-dimensional space of constant negative curvature ${}^1S_3$ are discussed. In Refs. 4 and 30 the analytic properties of the Coulomb scattering amplitude in the complex angular momentum plane for flat space are discussed. Special attention is given to the comparison of the Regge trajectories for curved and flat spaces.

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II. REGGE ANALYSIS OF THE COULOMB PROBLEM IN THE SPACE OF CONSTANT NEGATIVE CURVATURE

As is known in the case of space of constant negative curvature, both finite and infinite motions of a particle are possible. The corresponding Schrödinger equation has both discrete and continuous spectra. Therefore it is possible to formulate the Coulomb scattering problem.

We use embedding of the space of constant negative curvature in four-dimensional pseudo-Euclidean space with coordinates $x_\mu, \mu=1,2,3,4$, given by the formulas

$$x_\mu x_\mu = \mathbf{x}^2 + x_4^2 = \mathbf{x}^2 - x_0^2 = -\rho^2,$$
$$\mathbf{x} = \{x_1, x_2, x_3\}, \quad x_4 = ix_0. \tag{1}$$

The Coulomb potential in the ${}^1S_3$ space reads

$$U = -\frac{\alpha}{\rho}\frac{x_0}{|\mathbf{x}|}, \tag{2}$$

where $\alpha > 0$ for the attractive potential.

The Schrödinger equation for the attractive Coulomb potential (2) is

$$H\Psi = E\Psi, \quad H = \frac{1}{4\rho^2}M_{\mu\nu}M_{\mu\nu} - \frac{\alpha}{\rho}\frac{x_0}{|\mathbf{x}|},$$
$$M_{\mu\nu} = x_\mu\partial_\nu - x_\nu\partial_\mu. \tag{3}$$

We use the system of units such that $\hbar = m = 1$.

The exact solution of the Coulomb scattering problem in the space of constant negative curvature was found in the work.[31] The S-matrix element for energy E, angular momentum l and curvature ρ in the ${}^1S_3$ space is given by

$$S(E,l,\rho) = \frac{\Gamma(1 - i\gamma_+ + i\gamma_- + l)}{\Gamma(1 + i\gamma_+ - i\gamma_- + l)}, \tag{4}$$

where

$$\gamma_\pm = \sqrt{\frac{(E\rho^2 \pm \alpha\rho)}{2} - \frac{1}{4}}. \tag{5}$$

The S-matrix element for the Coulomb problem in the flat space is

$$S(E,l) = \frac{\Gamma\left(1 + l - \frac{i}{\sqrt{2E}}\right)}{\Gamma\left(1 + l + \frac{i}{\sqrt{2E}}\right)}. \tag{6}$$

We note that in the limit of the flat space, i.e., when $\rho \to \infty$ we have

$$\lim_{\rho\to\infty}(\gamma_+ - \gamma_-) = \frac{\alpha}{\sqrt{2E}}, \tag{7}$$

and expression for the S matrix in the ${}^1S_3$ space (4) transforms to (6).

It is well known from quantum mechanics that the scattering amplitude may be expanded in Legendre polynomials. This is called partial wave expansion. In our case partial wave expansion of the scattering amplitude[31] is given by

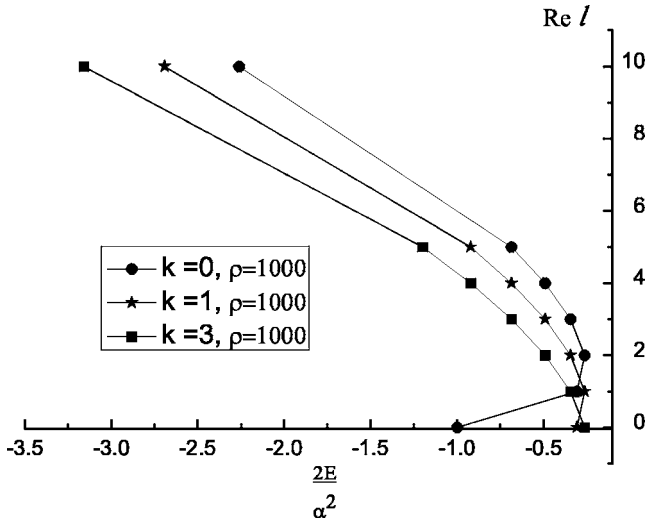

FIG. 1. The first three Regge trajectories in the space of constant negative curvature. The symbols on the plot correspond to bound states of the system.

$$f(\theta,\rho) = \frac{\rho}{2i(\gamma_+ + \gamma_-)} \times \sum_l (2l+1)\frac{\Gamma(1 - i\gamma_+ + i\gamma_- + l)}{\Gamma(1 + i\gamma_+ - i\gamma_- + l)} P_l(\cos\theta), \tag{8}$$

where θ is the scattering angle.

As is known, the Regge poles are determined by the position of singularities of the scattering amplitude at complex plane of angular momentum. Since $\Gamma(z)$ is a meromorphic function in the finite z plane with poles at $z=0,-1,-2,\ldots$, therefore the Regge poles are the poles of the gamma function $\Gamma(1-i\gamma_+ + i\gamma_- + l)$.

Thus, the position of kth Regge pole $l=\alpha_k(E,\rho)$ is given by

$$\alpha_k(E,\rho) = -k + \alpha_0(E,\rho) \quad (\text{for } k = 0,1,2,\ldots), \tag{9}$$

where

$$\alpha_0(E,\rho) = -1 + i\gamma_+ - i\gamma_-. \tag{10}$$

When we vary the energy, the poles $\alpha_k(E)$ move in the l plane along Regge trajectories. The first three Regge trajectories are shown in Fig. 1.

We see from Figs. 2 and 3 there exist differences in the Regge trajectories for curved and flat spaces. From these figures it follows that there are such values of the angular momentum l and quantum number k for which no differences exist. But with the increase of l and k considerable differences in the Regge trajectories appear.

The plot of the dependence $\mathrm{Im}[\alpha_k(E,\rho)]$ on $\mathrm{Re}[\alpha_k(E,\rho)]$ is also called Regge trajectory. We can now trace the Regge trajectory of that type in the l plane as we vary the energy along the real axis (see Figs. 4 and 5). Also from these figures we can observe that with the growth of the radius of curvature ρ we have the plane case.

The energy at which the kth Regge pole crosses a physical l value is given by

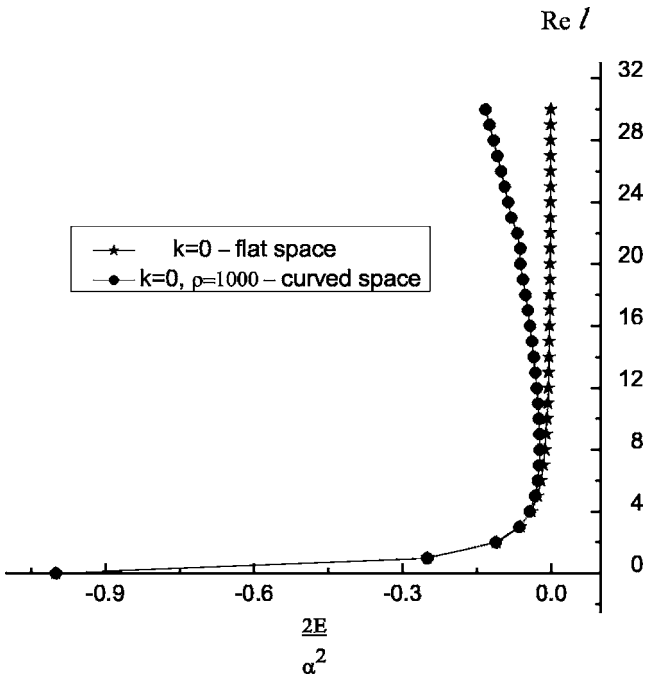

FIG. 2. The comparison of the Regge trajectories for $k=0$.

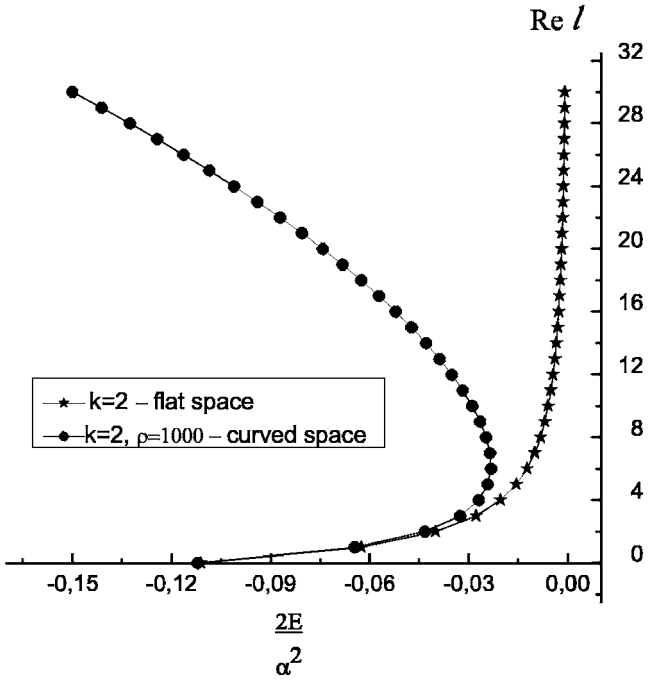

FIG. 3. The comparison of the Regge trajectories for $k=2$.

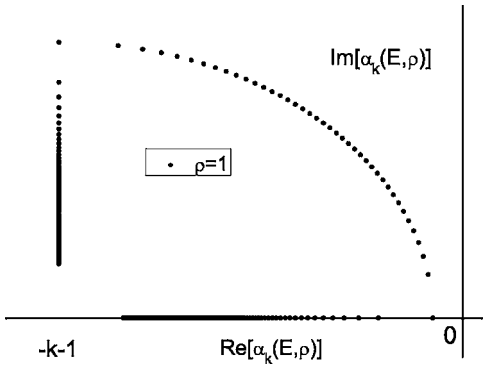

FIG. 4. The trajectory with energy (real) of the kth Regge pole for attractive Coulomb potential in the space of constant negative curvature for $\rho=1$.

$$E=-\frac{1}{2}\left[\frac{\alpha^2}{(k+l+1)^2}+\frac{(k+l+1)^2-1}{\rho^2}\right]. \tag{11}$$

These values are just the energies of the bound states for the attractive Coulomb field in the ${}^1S_3$ space.

As is known, the function $\alpha_k(E)=l+1-i/\sqrt{2E}$ in the flat space is a real analytical in E with a branch point at $E=0$. From (9) it follows

$$\alpha_m(0,\rho)=-k-1+i\left(\sqrt{\frac{\alpha\rho}{2}-\frac{1}{4}}-\sqrt{\frac{-\alpha\rho}{2}-\frac{1}{4}}\right),$$

that is in the space of constant negative curvature the function $\alpha_k(E,\rho)$ has not a branch point at $E=0$. Instead, in the space of constant negative curvature the function $\alpha_k(E,\rho)$ has two branch points in E,

$$E_1(\rho)=\frac{1-2\alpha\rho}{2\rho^2} \text{ and } E_2(\rho)=\frac{1+2\alpha\rho}{2\rho^2}. \tag{12}$$

The branch points move as the curvature ρ varies. For any ρ the value $E_2(\rho)>0$, if $\rho<1/2\alpha$ then $E_1(\rho)>0$ too. When $\rho-\to\infty$ the branch points $E_1(\rho)$ and $E_2(\rho)$ transform to $E=0-\epsilon$ and $E=0+\epsilon$, respectively.

In Ref. 31 the explicit expression for the scattering amplitude

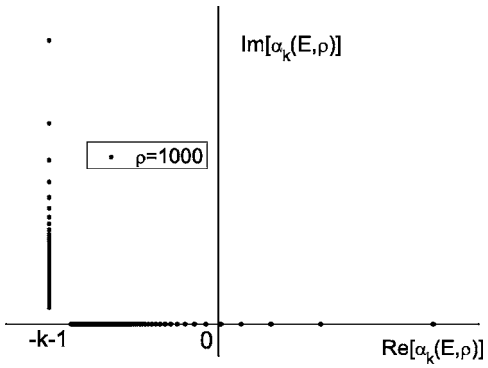

FIG. 5. The trajectory with energy (real) of the kth Regge pole for attractive Coulomb potential in the space of constant negative curvature for $\rho=1000$.

$$f(\theta,\rho)=\frac{\rho(\gamma_+-\gamma_-)}{(\gamma_++\gamma_-)}\frac{\Gamma(1-i\gamma_++i\gamma_-)}{\Gamma(1+i\gamma_+-i\gamma_-)}\times 2^{-i(\gamma_+-\gamma_-)}(1-\cos\theta)^{i\gamma_+-i\gamma_--1} \tag{13}$$

was found.

Using the recurrence formula $\Gamma(1+z)=z\Gamma(z)$ and (10) we may rewrite the scattering amplitude (13) in the Regge representation

$$f(\theta,\rho)=\frac{\rho}{2i(\gamma_++\gamma_-)}\frac{\Gamma[-\alpha_0(E,\rho)]}{\Gamma[1+\alpha_0(E,\rho)]}\times\left(\frac{1-\cos\theta}{2}\right)^{\alpha_0(E,\rho)}. \tag{14}$$

With the use of the variable

$$t=-2E(1-\cos\theta), \tag{15}$$

Eq. (14) can be written as

$$f(t,E,\rho)=\frac{\rho}{2i(\gamma_++\gamma_-)}\frac{\Gamma[-\alpha_0(E,\rho)]}{\Gamma[1+\alpha_0(E,\rho)]}\times\left(-\frac{t}{4E}\right)^{\alpha_0(E)}. \tag{16}$$

We see from (16) that the asymptotic of the scattering amplitude $f(t,E,\rho)$ when $t\to\infty$ is determined of the poles (9) and has behavior of the Regge type

$$f(t,E,\rho)\big|_{t\to\infty}\approx g(E,\rho)t^{\alpha_0(E,\rho)}. \tag{17}$$

Thus, at the very high energies the scattering amplitude is determined mainly by the zero Regge pole.

III. CONCLUSION

The Regge analysis for Coulomb problem in the space of constant negative curvature has been given. We have the following results:

(a) As in the case of the three-dimensional Euclidean space for the Coulomb scattering problem in the space of constant negative curvature to each value of energy corresponds to the finite number of the Regge trajectories. This fact is underlaid by the existence of additional conserved quantity, the Runge-Lentz vector.

(b) The Regge poles considered as a function of energy E in the ${}^1S_3$ space has two branch points and are directly proportional to the square from the energy. While in the three-dimensional Euclidean space the Regge trajectories are inversely proportional to the square from the energy and has a branch point at $E=0$.

In conclusion, we note that the Regge trajectories are nonlinear trajectories for potential scattering in the flat space. At that time, when we vary the radius of curvature ρ the Regge trajectories may be a straight line in the entire energy interval in the curved space. This fact can be used for description of the bound states in particle physics and will be a subject of further study. In this approach the radius of curvature ρ will be connected with the size of particles.[32,33]

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Quantum and Fisher information from the Husimi and related distributions

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The two principal/immediate influences—which we seek to interrelate here—upon the undertaking of this study are papers of Życzkowski and Słomczyński [J. Phys. A **34**, 6689 (2001)] and of Petz and Sudár [J. Math. Phys. **37**, 2262 (1996)]. In the former work, a metric (the Monge one, specifically) over generalized Husimi distributions was employed to define a distance between two arbitrary density matrices. In the Petz-Sudár work (completing a program of Chentsov), the quantum analog of the (classically unique) Fisher information (monotone) metric of a probability simplex was extended to define an uncountable infinitude of Riemannian (also monotone) metrics on the set of positive definite density matrices. We pose here the questions of what is the specific/*unique* Fisher information metric for the (classically defined) Husimi distributions and how does it relate to the *infinitude* of (quantum) metrics over the density matrices of Petz and Sudár? We find a highly proximate (small relative entropy) relationship between the probability distribution (the quantum Jeffreys' prior) that yields quantum universal data compression, and that which (following Clarke and Barron) gives its classical counterpart. We also investigate the Fisher information metrics corresponding to the *escort* Husimi, positive-*P* and certain Gaussian probability distributions, as well as, in some sense, the discrete Wigner *pseudoprobability*. The *comparative noninformativity* of prior probability distributions—recently studied by Srednicki [Phys. Rev. A **71**, 052107 (2005)]—formed by normalizing the volume elements of the various information metrics, is also discussed in our context. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The two-level quantum systems (TLQS) are describable (nonclassically) in terms of 2×2 density matrices (ρ)—Hermitian non-negative definite matrices of trace unity. These matrices can be parametrized by points in the unit ball [Bloch ball/sphere (Ref. 1, p. 10244)] in Euclidean 3-space. On the other hand, the TLQS can be described in a *classical* manner using a generalization of the Husimi distribution[2] (Ref. 3, Sec. 4.1) (cf. Refs. 4–9). "The Husimi function is a function on phase space, and takes only non-negative values while the Wigner function can be negative and is usually violently oscillating. Hence the Husimi function can be regarded as a probability distribution in phase space, and its order of delocalization can be a measure of chaoticity of quantum states."[10] (Note that the original Husimi distribution was defined only for density operators in *separable* Hilbert space—one which admits a countable orthonormal basis—while the distribution studied here is defined over a finite-dimensional Hilbert space.)

There is an (uncountable) *infinitude* (Ref. 11, Sec. 16.7) of (quantum monotone) Riemannian metrics that can be attached to the Bloch ball of TLQS. Contrastingly, in the classical context of the Husimi distribution, there is not an infinitude, but rather a *single* distinguished (up to a constant multiple) monotone Riemannian metric—the *Fisher information* metric.[12–14] ["In the

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classical case, decision theory provides a unique monotone metric, namely, the Fisher information. In the quantum case, there are infinitely many monotone metrics on the state space" (Ref. 15, p. 2672).] So, it appears to be an question of obvious interest—which we seek to address here—of how one reconciles/deals with this phenomenon of classical uniqueness and quantum nonuniqueness, as applied to essentially the *same* objects (that is, the TLQS).

II. MONOTONE METRICS

The monotone metrics are all *stochastically monotone*.[15] That is, geodesic distances (as well as relative entropies) between density matrices *decrease* under coarse-grainings [completely positive trace-preserving maps, satisfying the Schwarz inequality: $T(a^*a) \geqslant T(a)^*T(a)$]. These metrics can be used for purposes of statistical distinguishability.[15] The monotone metrics for the TLQS have been found to be rotationally invariant over the Bloch ball, depending only on the radial coordinate r, that is the distance of the state in question from the origin (0,0,0)—corresponding to the fully mixed state. They are splittable into radial and tangential components of the form [Ref. 15, Eq. (3.17),

$$\mathrm{d}s^2_{\mathrm{monotone}} = \frac{1}{1-r^2}\mathrm{d}r^2 + \left((1+r)f\left(\frac{1-r}{1+r}\right)\right)^{-1}\mathrm{d}n^2. \tag{1}$$

Here, using spherical coordinates (r,θ_1,θ_2), one has $\mathrm{d}n^2 = r^2\,\mathrm{d}\theta_1^2 + r^2\sin^2\theta_1\,\mathrm{d}\theta_2^2$. Further, $f:\mathbb{R}^+ \to \mathbb{R}^+$ is an operator monotone function such that $f(t)=tf(t^{-1})$ for every $t>0$. [A function is operator monotone if the relation $0 \leqslant K \leqslant H$, meaning that $H-K$ is nonnegative definite, implies $0 \leqslant f(K) \leqslant f(H)$ for any such matrices K and H of any order.] The radial component is *independent* of the function f, and in the case of the Bures (minimal monotone) metric [corresponding to the particular choice $f_{\mathrm{Bures}}(t)=(1+t)/2$], the tangential component is independent of r.[16]

In the classical context of the Husimi distribution, there is not an infinitude, but rather a *single* distinguished (to a constant multiple) monotone metric—the *Fisher information* metric.[12–14] (The counterpart here to stochastic mappings—which are the appropriate morphisms in the category of quantum state spaces—are stochastic *matrices*.[15]) The ij entry of the Fisher information matrix (tensor) is the expected value with respect to the probability distribution in question of the product of the *first* derivative of the logarithm of the probability with respect to its ith parameter times the analogous first derivative with respect to its jth parameter. [Under certain regularity conditions, the Fisher information matrix is equal to the "second derivative matrix for the informational divergence (relative entropy)" (Ref. 17, pp. 455–456, Ref. 18, p. 43).] The volume element of the Fisher information metric can be considered—in the framework of Bayesian theory—as a prior distribution (Jeffreys' prior[17,19,20]) over, for our purposes here, the Bloch ball of TLQS.

Fisher information metric for the Husimi distribution: We have found (having to make use of numerical, as well as symbolic MATHEMATICA procedures in our quest) that for the Husimi distribution over the TLQS, the Fisher information metric takes the specific form [cf. (2)],

$$\mathrm{d}s^2_{\mathrm{Fisher_{Hus}}} = \frac{-2r - \ln\left(\frac{1-r}{1+r}\right)}{2r^3}\mathrm{d}r^2 + \left((1+r)f_{\mathrm{Hus}}\left(\frac{1-r}{1+r}\right)\right)^{-1}\mathrm{d}n^2. \tag{2}$$

Here,

$$f_{\mathrm{Hus}}(t) = \frac{(t-1)^3}{t^2 - 2t\ln t - 1}. \tag{3}$$

Now, a plot (Fig. 1) shows $f_{\mathrm{Hus}}(t)$ to be, in fact, a *monotone* function. [$f_{\mathrm{Hus}}(t)$ is "almost" equal to $(t-1)^3/(t^2-2t-1) = t-1$.] It has a singularity at $t=1$, corresponding to the fully mixed state ($r=0$), where $f_{\mathrm{Hus}}(1+\Delta t) \approx 3+3\Delta t/2$, though we have not attempted to confirm its *operator* monotonicity. Also, $f_{\mathrm{Hus}}(t)$ fulfills the self-adjointness condition $f(t)=tf(t^{-1})$ of Petz and Sudár (Ref. 15, p. 2667), at least at $t \neq 1$. For the pure states, that is $t=0$, $r=1$, we have $\lim_{t\to 0} f_{\mathrm{Hus}}(t)=1$.

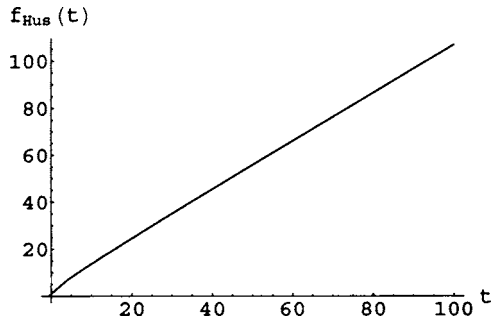

FIG. 1. The monotone function $f_{\mathrm{Hus}}(t)$ that yields the *tangential* component of the Fisher information metric over the trivariate Husimi probability distributions for the two-level quantum systems.

We further have the relation,

$$c_{\mathrm{Hus}}(p,q) = \frac{1}{q f_{\mathrm{Hus}}\left(\frac{p}{q}\right)} = \frac{q^2 - p^2 - 2pq \ln \frac{q}{p}}{(q-p)^3}, \tag{4}$$

where $c_{\mathrm{Hus}}(p,q)$ is a specific "Morozova-Chentsov" function. There exist one-to-one correspondences between Morozova-Chentsov functions, monotone metrics and operator means (Ref. 21, Corollary 6). "Operator means are binary operations on positive operators which fulfill the main requirements of monotonicity and the transformer inequality."[21]

We can write (1) more explicitly as

$$\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}} = \frac{-2r - \ln\left(\frac{1-r}{1+r}\right)}{2r^3}\mathrm{d}r^2 + \frac{2r + (1-r^2)\ln\left(\frac{1-r}{1+r}\right)}{4r^3}\mathrm{d}n^2. \tag{5}$$

Certainly, $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$ does not have—in terms of the radial component—the specific form (1) required of a monotone metric (cf. Ref. 22). In Fig. 2 we show both the *radial* components of (any) $\mathrm{d}s^2_{\mathrm{monotone}}$ and of $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$. Petz (Ref. 23, p. 934) attributes the unvarying nature $[1/(1-r^2)]$ of the radial component of the (quantum) monotone metrics to the (classical) Chentsov uniqueness (of Fisher information) theorem.[12,13] "Loosely speaking, the unicity [sic] result in the [probability] simplex case survives along the diagonal and the off-diagonal provides new possibilities for the definition of a stochastically invariant metric" (Ref. 15, p. 2664).

If we (counterfactually) equate the volume element of $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$ to that of a generic monotone

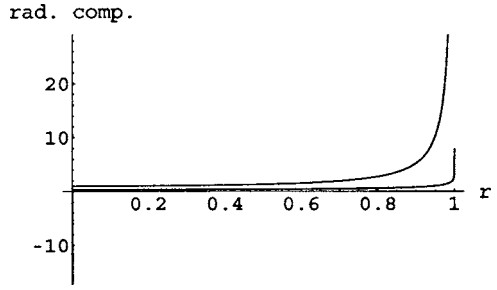

FIG. 2. The radial components of *any* monotone metric and that of the Fisher information metric derived from the family of trivariate Husimi distributions over the TLQS. The one for the (nondenumerably infinite) class $\mathrm{d}s^2_{\mathrm{monotone}}$ dominates that for $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$.

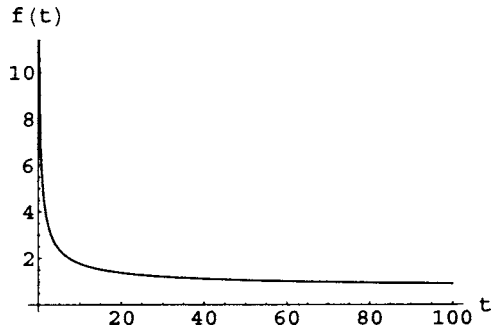

FIG. 3. Monotonically *decreasing* function $f_{\text{counter factual}}$ obtained by equating the volume element of $ds^2_{\text{Fisher}_{\text{Hus}}}$ to that of a generic monotone metric (1).

metric (1), and solve for $f(t)$, we obtain a monotonically *decreasing* function (Fig. 3) (cf. Ref. 22),

$$f_{\text{counter factual}}(t) = \frac{\sqrt{2}(-1+t)^{9/2}}{t(1+t)\sqrt{(-1+t^2-2t\ln(t))^2(2-2t+(1+t)\ln(t))}}. \tag{6}$$

Converting to (Cartesian coordinates (x,y,z), the *trace* of $ds^2_{\text{Fisher}_{\text{Hus}}}$ can be simply expressed as $-\ln[(1-R)/(1+R)]/(2R)$, where $R=\sqrt{x^2+y^2+z^2}$ (cf. Refs. 14 and 24). Also, at the fully mixed state $(x=y=z=0)$, the metric is simply *flat*, that is

$$ds^2_{\text{Fisher}_{\text{Hus}}} = \tfrac{1}{3}(dx^2+dy^2+dz^2). \tag{7}$$

(The Riemann and Ricci tensors evaluated at the fully mixed state have no nonzero entries.)

Numerical evidence indicates that the Fisher information matrix for the Husimi distribution over the TLQS is bounded by the corresponding information matrices for the (quantum) monotone metrics, in the sense that the monotone metric tensors minus the Fisher-Husimi information tensor are positive definite.

We can normalize the volume element of $ds^2_{\text{Fisher}_{\text{Hus}}}$ to a probability distribution p_{Hus} by dividing by the Fisher information metric volume $\approx 1.393\,509\,893\,676\,60$. If we generate a "hybridized-Husimi" (quantum[15]) monotone metric, $ds^2_{\text{HYB}_{\text{Hus}}}$, *via* the formula (1), using $f_{\text{Hus}}(t)$, then the volume of the Bloch ball of TLQS in terms of this newly generated monotone metric is $\frac{1}{2}\pi^2(4-\pi)\approx 4.236\,07 > 1.393\,51$. Using this as a normalization factor, we obtain a probability distribution $(p_{\text{HYB}_{\text{Hus}}})$ of interest over the TLQS.

III. COMPARATIVE NONINFORMATIVITIES

Let us compare p_{Hus}—in the manner employed in Refs. 25 and 26 (cf. Refs. 27 and 28, Sec. VI)—with the prior probability distribution (p_{Bures}). The latter is obtained by normalizing the volume element of the well-studied *minimal* monotone (Bures) metric [Ref. 29, Eq. (7)] [Ref. 30, Eq. (16)], that is,

$$p_{\text{Bures}} = \frac{r^2 \sin\theta_1}{\pi^2\sqrt{1-r^2}}, \tag{8}$$

generated from (1) using the operator monotone function $f_{\text{Bures}}(t)=(1+t)/2$. (We avoid the specific designations $f_{\min}(t)$ and $f_{\max}(t)$ because these are usually, confusingly, considered to generate the maximal and minimal monotone metrics, respectively [Ref. 15, Eq. (3.21)]. Our integrations of probability distributions are conducted over $r\in[0,1]$, $\theta_1\in[0,\pi]$ and $\theta_2\in[0,2\pi]$.)

The *relative entropy* (Kullback-Leibler distance) of p_{Bures} with respect to p_{Hus} [which we denote $S_{\text{KL}}(p_{\text{Bures}},p_{\text{Hus}})$]—that is, the *expected* value with respect to p_{Bures} of $\ln p_{\text{Bures}}/p_{\text{Hus}}$—is 0.130 845 "nats" of information. (We use the *natural* logarithm, and not 2 as a base, with one nat

equalling 0.531 bits.) Let us note that the Shannon entropy (S_{Shannon}) of the Husimi distribution is the Wehrl entropy (S_{Wehrl}) of the corresponding quantum state. Explicitly implementing [Ref. 31, Eq. (6)], we have for the TLQS,

$$S_{\text{Wehrl}} = \frac{1}{4r}\left(2r + 4r\ln 2 + (1+r^2)\ln\left(\frac{1-r}{1+r}\right) - 2r\ln(1-r^2)\right). \tag{9}$$

S_{Wehrl} is always greater than the von Neumann entropy, $S_{\text{vN}} = -\text{Tr}\,\rho\ln\rho$, which for the TLQS is expressible as

$$S_{\text{vN}} = \frac{1}{2}\left(2\ln 2 + r\ln\left(\frac{1-r}{1+r}\right) - \ln(1-r^2)\right). \tag{10}$$

[We, of course, notice the omnipresence in these last two formulas, as well as in (5) and further formulas below of the term $W \equiv \ln[(1-r)/(1+r)]$. The two eigenvalues $(\lambda_1, \lambda_2 = 1-\lambda_1)$ of ρ are $(1\pm r)/2$, so W is expressible as $\ln(\lambda_1/\lambda_2)$.] Each monotone metric can be obtained in the form of a "contrast functional" for a certain convex subset of relative entropies.[32,33]

A. Bures prior

Now, let us convert p_{Bures} to a *posterior* probability distribution ($\text{post}_{\text{Bures}}$) by assuming the performance of *six* measurements, *two* (with one outcome "up" and the other "down") in each of the x, y, and z directions. Normalizing the product of the prior p_{Bures} and the *likelihood* function corresponding to the six measurement outcomes (Ref. 25, p. 3),

$$\text{post}_{\text{Bures}} = \frac{192\,p_{\text{Bures}}(1-x^2)(1-y^2)(1-z^2)}{71}, \tag{11}$$

we find $S_{\text{KL}}(\text{post}_{\text{Bures}}, p_{\text{Hus}}) = 0.091\,2313 < 0.130\,845$. [The Cartesian coordinates in (11) are transformed to the spherical ones employed in our analysis.] So, in this sense p_{Bures} is *more* noninformative than p_{Hus}, the relative entropy being *reduced* by *adding* information to p_{Bures}. On the other hand, p_{Bures}—corresponding to the *minimal* monotone metric—is itself the *least* noninformative of the monotone-metric priors (p_{monotone}).[25] (Luo has established an inequality between the [monotone metric] Wigner-Yanase *skew information* and its minimal monotone counterpart.[34])

Reversing the arguments of the relative entropy functional, we obtain $S_{\text{KL}}(p_{\text{Hus}}, p_{\text{Bures}}) = 0.081\,8197$. But now, following the same form of posterior construction, we find $S_{\text{KL}}(\text{post}_{\text{Hus}}, p_{\text{Bures}}) = 0.290\,405 > 0.081\,8197$, further supportive of the conclusion that p_{Bures} is *more* noninformative than p_{Hus}. In some sense, then, p_{Bures} assumes *less* about the data than p_{Hus}. But this diminishability of the relative entropy is limited. If we convert p_{Bures} to a new posterior $\text{Post}_{\text{Bures}}$ using the *square* of the likelihood function above—that is, assuming 12 measurements, *four* (with two outcomes "up" and the other two "down") in each of the x, y, and z directions, giving

$$\text{Post}_{\text{Bures}} = \frac{21\,504\,p_{\text{Bures}}[(1-x^2)(1-y^2)(1-z^2)]^m}{3793}, \quad m = 2, \tag{12}$$

then $S_{\text{KL}}(\text{Post}_{\text{Bures}}, p_{\text{Hus}}) = 0.292\,596 > 0.130\,845$. To much the same effect, if we use a likelihood based on the *optimal/nonseparable* set of measurements for *two* qubits, consisting of five possible measurement outcomes, given in Ref. 35, Eq. (8), to convert p_{Bures} to a new posterior, then the relative entropy reaches higher still, that is from 0.130 845 to 0.623 855. (Employing a likelihood based on the optimal/nonseparable set of measurements for *three* qubits, consisting of eight possible measurement outcomes [Ref. 35, Eq. (9)], the relative entropy with respect to p_{Hus} increases further to 1.513 65.) Actually, if we *formally* take $m = \frac{1}{2}$ in Eq. (12), and renormalize to a new posterior, we obtain a superior reduction, that is, to $0.071\,67 < 0.091\,2313$. (Further, with $m = \frac{5}{8}$, we get 0.070 2389 and 0.073 2039, with $m = \frac{3}{4}$.)

B. Morozova-Chentsov prior

In Ref. 25, it was found that the ("Morozova-Chentsov") prior distribution,

$$p_{\mathrm{MC}} = \frac{0.005\,132\,99\left[\ln\left(\frac{1-r}{1+r}\right)\right]^2 \sin\theta_1}{\sqrt{1-r^2}}, \tag{13}$$

that is, the normalized volume element of the monotone metric (1) based on the operator monotone function,

$$f_{\mathrm{MC}}(t) = \frac{2(t-1)^2}{(1+t)(\ln t)^2}, \tag{14}$$

was apparently the *most* noninformative of those (normalizable) priors based on the operator monotone functions that had been explicitly discussed in the literature. Now, $S_{\mathrm{KL}}(p_{\mathrm{MC}}, p_{\mathrm{Hus}}) = 1.379\,91$, that is, quite large. This can be reduced to 0.893 996 if, into p_{MC}, one incorporates $m=6$ measurements of the type described above; diminished further to 0.561 901 with $m=12$; and further still to 0.471 852—the greatest reduction of this type—with $m=18$. (For $m=24$, it starts to rise to 0.652 441.)

But, if we again use the likelihood based on the optimal nonseparable measurement of two qubits [Ref. 25, Eq. (8)], with just five measurements, the relative entropy of the corresponding posterior form of p_{MC} with respect to p_{Hus} is reduced to 0.342 124, which is the *smallest* we have achieved so far along these lines. (For the mentioned optimal nonseparable measurement scheme for *three* qubits, the reduction is quite minor, only to 1.334 92 nats.) We obtained intermediate-sized reductions to 0.455 24 and 0.492 979, respectively, by using for our measurements, 20 projectors oriented to the vertices (Ref. 36, Secs. 9 and 10) of a dodecahedron and of an icosahedron. (The primary measurement scheme used above, and in Ref. 25, with six measurements oriented along three orthogonal directions, is tantamount to the use of an *octahedron*.)

C. Hilbert-Schmidt prior

The prior distribution generated by normalizing the volume element of the Hilbert-Schmidt metric over the Bloch sphere is [Ref. 25, Eq. (10)] [Ref. 16, Eq. (31)]

$$p_{\mathrm{HS}} = 3\frac{r^2 \sin\theta_1}{4\pi}, \tag{15}$$

which is simply the uniform distribution over the unit ball. The Hilbert-Schmidt volume element can be reproduced using the formula (1) for a quantum monotone metric, making use of $f_{\mathrm{HS}} = (1+t)^2/\sqrt{t}$, but this function is neither monotone increasing nor decreasing over $t \in [0,1]$ (cf. Ref. 37).

We have that $S_{\mathrm{KL}}(p_{\mathrm{Hus}}, p_{\mathrm{HS}}) = 0.057\,9239$ and $S_{\mathrm{KL}}(p_{\mathrm{HS}}, p_{\mathrm{Hus}}) = 0.054\,43$. Now, in terms of our usual posterior distributions based on six measurements, $S_{\mathrm{KL}}(\mathrm{post}_{\mathrm{Hus}}, p_{\mathrm{HS}}) = 0.023\,6596$ and $S_{\mathrm{KL}}(\mathrm{post}_{\mathrm{HS}}, p_{\mathrm{Hus}}) = 0.278\,953$, so we can conclude that the Husimi prior p_{Hus} is more noninformative than the Hilbert-Schmidt prior p_{HS}.

IV. UNIVERSAL DATA COMPRESSION

Employing p_{Hus} as a prior distribution (Jeffreys' prior) over the family (Riemannian manifold) of Husimi qubit probability distributions, the (classical) *asymptotic minimax/maximin redundancy of universal data compression* is equal to [Ref. 18, Eq. (2.4)],[17]

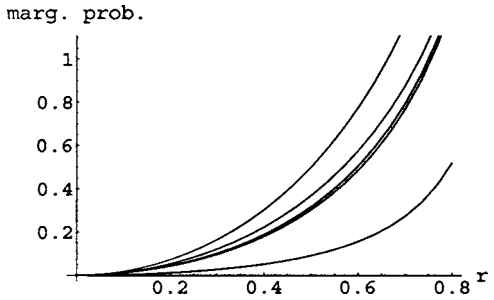

FIG. 4. Plots of one-dimensional marginal probability distributions over the radial coordinate r of p_{Bures}, $p_{\mathrm{HYB}_{\mathrm{Hus}}}$, p_{GKS}, p_{Hus}, and p_{MC}. The order of dominance of the curves is $p_{\mathrm{Hus}} > p_{\mathrm{Bures}} > p_{\mathrm{GKS}} > p_{\mathrm{HYB}_{\mathrm{Hus}}} > p_{\mathrm{MC}}$. The marginal distributions of $p_{\mathrm{HYB}_{\mathrm{Hus}}}$ and p_{GKS} are quite close, as reflected in their small relative entropy (≈ 0.0004).

$$\frac{3}{2}\ln\frac{n}{2\pi e}+\ln 1.393\,509\,893\,676\,60=\frac{3}{2}\ln\frac{n}{2\pi e}+0.331\,826=\frac{3}{2}\ln n-3.924\,99, \tag{16}$$

where n is the sample size (the number of qubits [TLQS]) and we used the before-mentioned volume of $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$. ["Suppose that X is a discrete random variable whose distribution is in the parametric family $\{P_\theta : \theta \in \Theta\}$ and we want to encode a block of data for transmission. It is known that a lower bound on the expected codeword length is the entropy of the distribution. Moreover, this entropy bound can be achieved, within one bit, when the distribution is known. Universal codes have expected length near the entropy no matter which member of the parametric family is true. The redundancy of a code is defined to be the difference between its expected length and its entropy" (Ref. 17, p. 459).]

For the *quantum*/nonclassical counterpart[38] (cf. Refs. 39–41), let us consider the use of the "Grosse-Krattenthaler-Slater" ("quasi-Bures") probability distribution [Ref. 35, Eq. (33)],

$$p_{\mathrm{GKS}}=\frac{0.083\,2258e}{1-r^2}\left(\frac{1-r}{1+r}\right)^{1/2r} r^2\sin\theta_1. \tag{17}$$

This is the normalized form of the monotone metric (1) associated with the (presumably operator) monotone function,

$$f_{\mathrm{GKS}}(t)=\frac{t^{t/(t-1)}}{e}. \tag{18}$$

[Taking limits, we have for the fully mixed state, $f_{\mathrm{GKS}}(1)=1$ and for the pure states, $f_{\mathrm{GKS}}(0)=e^{-1}$.] It appears[42] (though not yet fully rigorously established) that the (quantum) asymptotic minimax/maximin redundancy, employing p_{GKS} as a prior probability distribution over the 2×2 density matrices [*and* their n-fold tensor products (cf. Ref. 43)], is $\frac{3}{2}\ln n - 1.770\,62$. This is *greater* than the classical (Husimi-Fisher-information-based) analog (16) by 2.200 95 nats of information. It would seem that this difference is attributable to the greater dimensionality (2^n) of an n-qubit Hilbert space, as opposed to a dimensionality of $3n$ for n trivariate Husimi probability distributions over the TLQS.

We further note that $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{\mathrm{Hus}}})=0.006\,360\,46$ and $S_{\mathrm{KL}}(p_{\mathrm{HYB}_{\mathrm{Hus}}}, p_{\mathrm{Bures}})=0.006\,2714$, both being very small. Smaller still, $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{GKS}})=0.003\,590\,93$ and $S_{\mathrm{KL}}(p_{\mathrm{GKS}}, p_{\mathrm{Bures}})=0.003\,545\,79$—whence the designation $p_{\text{quasi-Bures}} \equiv p_{\mathrm{GKS}}$. But then, even more strikingly, we computed that $S_{\mathrm{KL}}(p_{\mathrm{GKS}}, p_{\mathrm{HYB}_{\mathrm{Hus}}})=0.000\,397\,852$ and $S_{\mathrm{KL}}(p_{\mathrm{HYB}_{\mathrm{Hus}}}, p_{\mathrm{GKS}})=0.000\,396\,915$. In Fig. 4 we show the *one*-dimensional marginal probability distributions over the radial coordinate r of the five distributions p_{Bures}, $p_{\mathrm{HYB}_{\mathrm{Hus}}}$, p_{Hus}, p_{GKS}, and p_{MC}, with those for $p_{\mathrm{HYB}_{\mathrm{Hus}}}$ and p_{GKS} being—as indicated—particularly proximate.

Substitution of $p_{\mathrm{HYB}_{\mathrm{Hus}}}$ for p_{GKS} into the quantum asymptotic (maximin) redundancy formula that has to be *maximized* over all possible prior probability distributions [Ref. 42, Eq. (4.3)],

$$\frac{3}{2}\ln n-\frac{1}{2}-\frac{3}{2}\ln 2-\frac{3}{2}\ln\pi+4\pi\int_0^1\left(-\ln(1-r^2)+\frac{1}{2r}\ln\left(\frac{1-r}{1+r}\right)-\ln w(r)\right)r^2w(r)\mathrm{d}r, \tag{19}$$

leads to a very slightly decreased (and hence suboptimal) redundancy, $\frac{3}{2}\ln n-1.771\,01$ vs $\frac{3}{2}\ln n-1.770\,62$. (Use of p_{Bures} as a quantum prior over the 2×2 density matrices gives us a constant term of $-1.774\,21$, use of p_{Hus}, $-1.882\,79$ and use of p_{MC}, $-2.156\,67$.) To obtain the appropriate form of $w(r)$ to use in (19), we take our probability distributions [such as (8) and (13)], divide them by $4\pi r^2$ and integrate the results over $\theta_1\in[0,\pi]$ and $\theta_2\in[0,2\pi]$. [Thus, we must have $4\pi\int_0^1 w(r)r^2\,\mathrm{d}r=1$.] The *minimax* objective function is

$$\min_w\max_{0\leqslant r\leqslant 1}\left(\frac{3}{2}\ln n-\frac{1}{2}-\frac{3}{2}\ln 2-\frac{3}{2}\ln\pi-\ln(1-r^2)+\frac{1}{2r}\ln\left(\frac{1-r}{1+r}\right)-\ln w(r)\right). \tag{20}$$

The minimax is also achieved using the $w(r)$ formed from p_{GKS}.

We can, additionally, achieve an extremely good fit to p_{Hus} by proceeding in somewhat an *opposite* fashion to that above—*reversing* our hybridization procedure. Employing $f_{\mathrm{GKS}}(t)$, rather than $f_{\mathrm{Hus}}(t)$ in the expression (2) for $\mathrm{d}s^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$ and obtaining the corresponding normalized (dividing by 4.002 77) volume element ($p_{\mathrm{H\tilde{Y}B}_{\mathrm{GKS}}}$), we find $S_{\mathrm{KL}}(p_{\mathrm{H\tilde{Y}B}_{\mathrm{GKS}}},p_{\mathrm{Hus}})=0.000\,316\,927$. (Interchanging the arguments of the relative entropy functional, we get 0.000 317 754.) It is quite surprising, then, that a joint plot of $f_{\mathrm{GKS}}(t)$ and $f_{\mathrm{Hus}}(t)$ readily shows them to be substantially *different* in character [for example, $f_{\mathrm{Hus}}(50)=55.8161$ and $f_{\mathrm{GKS}}(50)=19.9227$], since they have been shown here to generate two pairs of such highly similar probability distributions, one pair composed of (quantum) monotone (p_{GKS} and $p_{\mathrm{HYB}_{\mathrm{Hus}}}$), and the other pair of (quantum) nonmonotone metrics ($p_{p_{\mathrm{H\tilde{Y}B}_{\mathrm{GKS}}}}$ and p_{Hus}).

V. ESCORT-HUSIMI DISTRIBUTIONS

For the *escort*-Husimi distributions,[44] we raise the probability element of the Husimi distribution to the qth power, and renormalize to a new probability distribution. (Of course, the Husimi distribution itself corresponds to $q=1$. If we set $\alpha=2q-1$, we recover the α-family of Amari.[33,45,46]) To normalize the qth power of the Husimi distribution, one must divide by

$$\frac{2^{-q}(-(1-r)^{1+q}+(1+r)^{1+q})}{r+qr}. \tag{21}$$

A. The case $q=2$

For (entropic index) $q=2$, the Fisher information metric takes the form

$$\mathrm{d}s^2_{\mathrm{Fisher}_{q=2}}=\frac{2}{(3+r^2)^2}\mathrm{d}r^2+\left((1+r)f_{q=2}\left(\frac{1-r}{1+r}\right)\right)\mathrm{d}n^2, \tag{22}$$

where

$$f_{q=2}(t)=\frac{t^2+t+1}{2(t+1)}. \tag{23}$$

We have $f_{q=2}(1)=\frac{3}{4}$ and $f_{q=2}(0)=\frac{1}{2}$.

Relative entropies: Further, the relative entropies $S_{\mathrm{KL}}(p_{\mathrm{Hus}},p_{\mathrm{Esc}_{q=2}})=0.011\,4308$ and $S_{\mathrm{KL}}(p_{\mathrm{Bures}},p_{\mathrm{Esc}_{q=2}})=0.429\,64$, So, it appears that $p_{\mathrm{Esc}_{q=2}}$ is even less noninformative than p_{Hus} [recalling that $S_{\mathrm{KL}}(p_{\mathrm{Bures}},p_{\mathrm{Hus}})=0.130\,845<0.429\,64$], which in turn we found above was less noninformative than the prior probabilities formed from any of the (quantum) monotone metrics. We also note that $S_{\mathrm{KL}}(\mathrm{post}_{\mathrm{Bures}},p_{\mathrm{Esc}_{q=2}})=0.125\,159<0.429\,64$. If we "hybridize" $\mathrm{d}s^2_{\mathrm{Fisher}_{q=2}}$ by

modifying its radial component into that required of a (quantum) monotone metric, then we find that $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=2}}) = 0.002\,460\,31 (< (S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{\mathrm{Hus}}}) = 0.006\,360\,46)$ is quite small.

B. The cases $q>2$

For the escort-Husimi probability distribution with $q=3$, the Fisher information metric takes the form

$$\mathrm{d}s^2_{\mathrm{Fisher}_{q=3}} = \frac{3-r^2}{(1+r^2)^2}\mathrm{d}r^2 + \left((1+r) f_{q=3}\left(\frac{1-r}{1+r}\right)\right)\mathrm{d}n^2, \tag{24}$$

where

$$f_{q=3}(t) = \frac{t^2+1}{3(t+1)}. \tag{25}$$

Now, $f_{q=3}(1) = f_{q=3}(0) = \frac{1}{3}$ and a plot of $f_{q=3}(t)$ clearly manifests monotonic behavior also. (The monotonically decreasing scalar curvature of $\mathrm{d}s^2_{\mathrm{Fisher}_{q=3}}$ equals $\frac{4}{3}$ at $r=0$.) We have that $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{Esc}_{q=3}}) = 0.637\,05 > S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{Esc}_{q=2}}) = 0.429\,64$, so the informativity (noninformativity) of the escort-Husimi prior probabilities *appears* to increase (decrease) with q.

For $q=4$,

$$\mathrm{d}s^2_{\mathrm{Fisher}_{q=4}} = \frac{80(5-2r^2+r^4)}{3(5+10r^2+r^4)^2}\mathrm{d}r^2 + \left((1+r) f_{q=4}\left(\frac{1-r}{1+r}\right)\right)^{-1}\mathrm{d}n^2, \tag{26}$$

where

$$f_{q=4}(t) = \frac{3(t^4+t^3+t^2+t+1)}{4(t+1)(3t^2+4t+3)}. \tag{27}$$

For $q=5$,

$$\mathrm{d}s^2_{\mathrm{Fisher}_{q=5}} = \frac{3(5-r^2)(5+3r^4)}{(3+10r^2+3r^4)^2}\mathrm{d}r^2 + \left((1+r) f_{q=5}\left(\frac{1-r}{1+r}\right)\right)^{-1}\mathrm{d}n^2, \tag{28}$$

where

$$f_{q=5}(t) = \frac{2(t^4+t^2+1)}{5(t++1)(2t^2+t+2)}. \tag{29}$$

We have (as found by Krattenthaler, making use of explicit MATHEMATICA computations of ours for $q=2,3,\ldots,40$) (cf. Ref. 47, Sec. 3.2, Ref. 48),

$$f_q(t) = \frac{(q-1)\sum_{i=0}^{q} t^i}{q(t+1)\sum_{i=0}^{q-1} i(q-i)t^{i-1}}. \tag{30}$$

[For *odd* q some simplification in the resulting expression occurs due to cancellation by a factor of $(t+1)$.]

In Fig. 5 we plot $f_{q=i}(t)$, $i=1,\ldots,30$, revealing their common monotonically increasing behavior. [Of course, we have $f_{q=1}(t) \equiv f_{\mathrm{Hus}}(t)$, shown already in Fig. 1. The steepness of the curves *decreases* with increasing q.]

Let us further note that in addition to $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{\mathrm{Hus}}}) = 0.006\,360\,46$ and $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=2}}) = 0.002\,460\,43$, we have $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=3}}) = 0.013\,2258$, $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=4}}) = 0.023\,8858$ and $S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=5}}) = 0.032\,7578$. [We have also been able to compute that

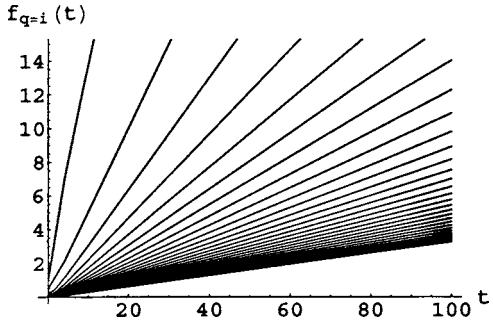

FIG. 5. The monotone functions $f_{q=i}(t)$, $i=1,\ldots,30$ that yield the *tangential* components of the Fisher information metric over the escort-Husimi ($q=i$) probability distributions. The steepness of the graphs decreases as q increases.

$S_{\mathrm{KL}}(p_{\mathrm{Bures}}, p_{\mathrm{HYB}_{q=1000}})=0.096\,9315$ and $S_{\mathrm{KL}}(p_{\mathrm{GKS}}, p_{\mathrm{HYB}_{q=1000}})=0.127\,027$.] So, the best of these fits of p_{Bures} to the prior probabilities for the hybridized-escort-Husimi probability distributions is for $q=2$.

C. Tangential components

Now, we can reexpress the formula (30) *without* summations, making use of the binomial theorem, as

$$f_q(t)=\frac{(-1+q)(-1+t)^2(-1+t^{1+q})}{q(1+t)(1-q+t+qt-t^q-qt^q-t^{1+q}+qt^{1+q})}. \tag{31}$$

So, we could study hybridized escort-Husimi metrics based on *non*integral q using this formula. [We note that (31), in fact, yields $\lim_{q\to 1} f_q(t)\equiv f_{\mathrm{Hus}}(t)$.] For example,

$$f_{q=1/2}(t)=6+6\sqrt{t}+2t-\frac{4}{1+t}. \tag{32}$$

Thus, (31) gives us [following the formulation (1)] the tangential components of the escort-Husimi Fisher information metrics for arbitrary q. (Pennini and Plastino[44] have argued, though, that in a *quantal* regime, q can be no less than 1. Tsallis statistics with an entropic index of $q=\frac{3}{2}$, Beck has contended, correctly describes the small-scale statistics of Lagrangian turbulence.[49])

D. Radial components

We do not have, at this point, a comparable complete formula for the *radial* components. However, Krattenthaler has shown—making use of explicit computations of ours for the cases $q=2,3,\ldots,18$—that the *denominators* of the functions giving the radial components are simply proportional to

$$u(q)=\left(\sum_{i=0}^{q}\frac{\mathrm{Pochhammer}[q-2i+1,2i+1]r^{2i}}{2(2i+1)!}\right)^2. \tag{33}$$

(The Pochhammer symbol is synonymous with the rising or ascending factorial. The obtaining of comparable formulas for the *numerators* of the radial components might be possible using the "Rate.m" program available from the website of Krattenthaler [http://www.mat.univie.ac.at/kratt/], if we had available additional explicit computations beyond the $q=18$.) As way of illustration, the radial component of $\mathrm{d}s^2_{\mathrm{Fisher}_{q=8}}$ is expressible as

$$\frac{144(21+42r^2+135r^4+28r^6+35r^8-6r^{10}+r^{12})}{7u(8)}. \tag{34}$$

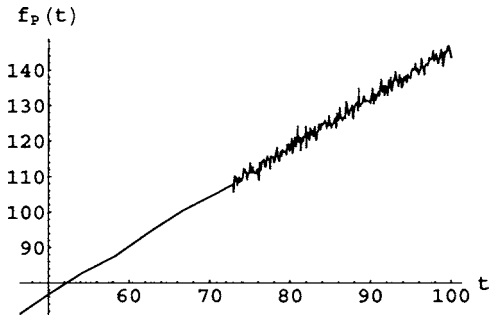

FIG. 6. *Approximation* to the presumed operator monotone function $f_P(t)$ yielding the *tangential* component of $\mathrm{d}s^2_{\mathrm{Fisher}_P}$ for the positive P representation over the two-level quantum systems.

VI. POSITIVE *P*-REPRESENTATION FOR TLQS

Braunstein, Caves, and Milburn focused on a specific choice of *positive P*-representation which they called the canonical form and which is always well defined [Ref. 50, Eq. (3.3)] (cf. Ref. 51, Sec. 6.4):

$$P_{\mathrm{can}}(\alpha,\beta^*) \equiv \frac{1}{4\pi^2}\exp\left(-\frac{1}{4}|\alpha+\beta|^2\right)\left\langle \frac{1}{2}(\alpha+\beta)\left|\hat{\rho}\right|\frac{1}{2}(\alpha+\beta)\right\rangle$$
$$= \frac{1}{4\pi^2}\exp\left(-\frac{1}{4}|\alpha-\beta|^2\right)Q\left(\frac{1}{2}(\alpha+\beta)\right). \tag{35}$$

"The canonical form is clearly positive, and…it is essentially the Q-function [Husimi distribution]."[50]

We sought to implement this model, choosing for α and β *independent* two-dimensional representations of the spin-$\frac{1}{2}$ coherent states (while for the Husimi distribution or Q-function, only, say α, need be employed). [The "positive P representation achieves [its] considerable success by doubling the number of degrees of freedom of the system, i.e., doubling the number of dimensions of the phase space" (Ref. 50, p. 1153). More typically, in the positive P representation, α and β are allowed to vary independently over the *entire* complex plane.] However, then our result—using this choice of α and β—was *not* normalized to a probability distribution in the manner indicated in (35).

We noted that Braunstein, Caves, and Milburn had commented that a "positive P representation can be defined for a large class of operators. We restrict ourselves here to those that are built up from the standard annihilation and creation operators of a harmonic oscillator. In particular, our work does not apply to generalizations of the positive P representation that include spin or pseudospin operators often used to describe a two-level atom" (Ref. 50, p. 1155). [We are not aware, however, of any specific applications reported in the literature of the positive P representation to n-level (finite-dimensional) quantum systems.]

We did not perceive how to exactly (re)normalize the distribution (35) for our particular choices of α and β. So, we expanded just the exponential term of (35) into a power series in third order in the four *phase* variables and exactly normalized the product of this series with the remaining unmodified factor (the Q-function or Husimi distribution) to obtain a new (presumed) probability distribution. We then fit (numerically) the resultant tangential component of the associated Fisher information metric to the form (1) required of a monotone metric. In Fig. 6 we show what we (gratifyingly) obtained in this manner for $f_P(t)$. In Fig. 7 we show an approximation to the radial component of $\mathrm{d}s^2_{\mathrm{Fisher}_P}$, similarly obtained. [The positive P function "seems to possess some interesting properties and may deserve close inspection" (Ref. 52, p. 175).] It would be of interest to see how near the associated probability distributions (p_P and p_{HYB_P}) would be to the probability distributions (already discussed above) p_{GKS}, p_{Hus}, $p_{\mathrm{HYB}_{\mathrm{Hus}}}$, and $p_{\mathrm{H\tilde{Y}B}_{\mathrm{GKS}}}$. Most press-

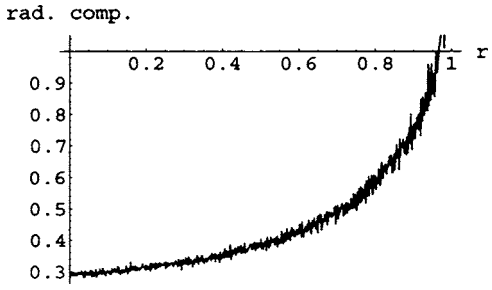

FIG. 7. *Approximation* to the *radial* component of $ds^2_{\mathrm{Fisher}_P}$ for the positive P-representation over the two-level quantum systems.

ing, though, is the question of whether or not the concept of a positive P representation does, in fact, have a meaningful and natural theoretical application to the n-level quantum systems.

VII. GAUSSIAN DISTRIBUTION

An approach quite distinct from that of the Husimi probability distributions, but still *classical* in nature, to modeling quantum systems has been presented in Refs. 4–8 (cf. Ref. 9). Here the family of probability distributions is taken as that of the Gaussian (complex multivariate normal distributions) having covariance matrix equal to the density matrix. For the TLQS, Slater [Ref. 53, Eq. (13)] [Ref. 54, Eq. (16)] derived the corresponding Fisher information metric. This is representable as

$$ds^2_{\mathrm{Fisher}_{\mathrm{Gauss}}} = \frac{2(1+r^2)}{(1-r^2)^2}dr^2 + \frac{2}{1-r^2}dn^2. \tag{36}$$

The tangential component can be reproduced, following the basic formula (1), by choosing $f_{\mathrm{Gauss}}(t)=t/(1+t)$. This is simply *one-half* of that—$f_{\mathrm{YL}}(t)=2f_{\mathrm{Gauss}}(t)=2t/(1+t)$—associated with the *maximal* monotone (Yuen-Lax) metric.[55] Like that metric, the metric (36) yields a *non*-normalizable volume element (so one cannot immediately apply—without some preliminary truncation—the comparative noninformativity/relative entropy test we have used above[25,26]). Of course, the radial component of (36) is also not consistent with the requirement for a monotone metric. In fact, it rises much *more* steeply than $1/(1-r^2)$, in opposite behavior to that for $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$. In Fig. 8 we show this phenomenon.

VIII. DISCRETE WIGNER FUNCTION FOR A QUBIT

The discrete Wigner function (pseudoprobability) W, in the simplest case of a qubit, is defined on a 2×2 array, with four components $W_{i,j}$, $i, j=1,2$ [Ref. 56, Eqs. (14)–(17)]. The sum of W_{ij} in each "line" λ is the probability p_{ij} of projecting the state onto the basis vector $|\alpha_{ij}\rangle$, where i

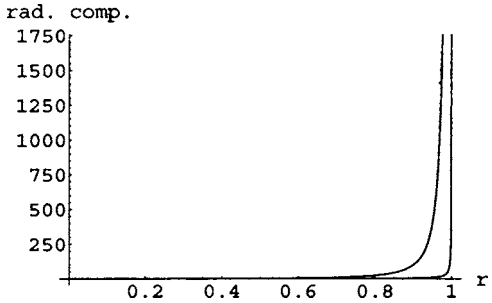

FIG. 8. Radial components of ds^2_{monotone} and $ds^2_{\mathrm{Fisher}_{\mathrm{Gauss}}}$. The latter dominates the former.

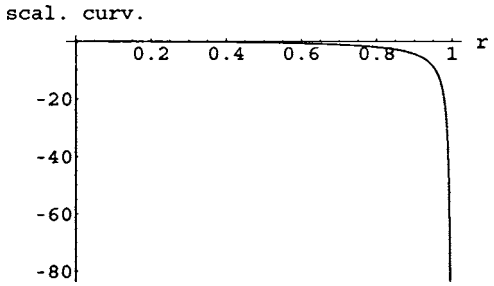

FIG. 9. Scalar curvature of the Fisher information metric for the family of Husimi distributions.

$\in\{1,2,3\}$ indexes a set of three mutually unbiased bases (MUB) for a qubit and $j\in\{1,2\}$ indexes the basis vector in each MUB. Choosing the MUB to be the eigenstates of the three Pauli operators, and using our cartesian coordinates, one can obtain three one-dimensional *marginal* (binomial) probability distributions over the x, y, and z axes, of the form $((1+x)/2,(1-x)/2),\ldots$(cf. Refs. 57 and 58). Now, the corresponding Jeffreys' prior for the one-dimensional family of such binomial distribution is simply the *beta* distribution $p_\beta(x)=1/\pi\sqrt{1-x^2}$. (Let us note that the one-dimensional marginal distributions obtained for p_{Bures} are of another form, that is, $2\sqrt{1-x^2}/\pi$.)

Let us take the product of $p_\beta(x)$, $p_\beta(y)$, and $p_\beta(z)$, which naturally forms a (prior) probability distribution,

$$p_{\text{product}}=\frac{1}{\pi^3\sqrt{(1-x^2)(1-y^2)(1-z^2)}},\tag{37}$$

over the hypercube with vertices $(\pm1,\pm1,\pm1)$ and renormalize/truncate it to a probability distribution over the Bloch sphere,

$$p_{\text{Wigner}}=\frac{1}{6.614\,555\,161\,01\sqrt{(1-x^2)(1-y^2)(1-z^2)}}.\tag{38}$$

(Thus, the quantum-mechanically *inaccessible* region lying outside the Bloch ball, but within the hypercube is disregarded—assigned null measure—in the new normalization.)

Now, we found—strictly following the notation, formulas and line of argument above in Sec. III—that $S_{\text{KL}}(p_{\text{Wigner}},p_{\text{Hus}})=0.014\,9831$ and $S_{\text{KL}}(p_{\text{Hus}},p_{\text{Wigner}})=0.015\,6225$, so these two distributions are rather close in nature. Of course, p_{Hus} is rotationally symmetric over the Bloch sphere, while p_{Wigner} is not, so it seems to make little sense to try to compute some function $f_{\text{Wigner}}(t)$ to generate the tangential component. We found it problematical, using our usual (relative entropy) approach, to designate either p_{Hus} or p_{Wigner} as more or less noninformative. [The "Husimi function is a kind of...coarse-grained Wigner function" (Ref. 48, p. 3).]

IX. SCALAR CURVATURE

In Fig. 9, we plot the *scalar curvature* of $\mathrm{d}s^2_{\text{Fisher}_{\text{Hus}}}$. The formula for this scalar curvature is

$$K^{n=2}_{\text{Hus}}=\frac{r(-6r+W(-3+r^2))(-4r^2(-3+r^2)+6Wr(2-3r^2+r^4)+W^2(3-8r^2+5r^4))}{(W+2r)^2(-1+r^2)(-2r+W(-1+r^2))^2},\tag{39}$$

where $W=\ln(1-r)/(1+r)$. Also, expanding about $r=0$,

$$K^{n=2}_{\text{Hus}}\approx\frac{-6r^2}{5}-\frac{138r^4}{125}-\frac{32\,094r^6}{30\,625}-\frac{154\,474r^8}{153\,125}-\frac{57\,710\,054r^{10}}{58\,953\,125}.\tag{40}$$

The *nonpositive* monotonically *decreasing* scalar curvature (Fig. 9) has its *maximum* at $r=0$, corresponding to the fully mixed state, indicative of a *flat* metric there [cf. (7)] (and is $-\infty$ at the pure states, $r=1$). For the minimal monotone (Bures) metric, the *non-negative* scalar curvature is *constant*, that is $K^{n=2}_{\min}=6$, over the Bloch ball, and for the (n^2-1)-dimensional convex set of $n \times n$ density matrices, $n>2$, achieves its *minimum* of $K^{n}_{\min}=(5n^2-4)(n^2-1)/8$ at the fully mixed state $[\rho=(1/n)I]$.[59] [In Ref. 59, the metric used is one-quarter of that corresponding to (1), used here, so the results we compute here differ from those there by such a factor. For the *maximal* monotone metric, $K^{n=2}_{\max}=8(r^2-6)/(1-r^2)$, which is monotonically *decreasing* as r increases, as is $K^{n=2}_{\mathrm{Hus}}$.]

For the two-level quantum systems, Andai[60] has constructed a family of monotone metrics with *non*monotone scalar curvature, and given a condition for a monotone metric to have a local minimum at the maximally mixed state.

Metrics of constant scalar curvature: The metric $\mathrm{d}s^2_{\mathrm{Fisher}_{q=2}}$ has *constant* scalar curvature, $K^{n=2}_{q=2}=\frac{3}{2}$ while, as previously noted, $K^{n=2}_{\min}=6$. Let us note that $K^{n}_{\mathrm{WY}}=\frac{1}{4}(n^2-1)(n^2-2)$, which is also $\frac{3}{2}$ for $n=2$. Here, WY denotes the Wigner-Yanase metric—the only pull-back metric among the quantum monotone metrics—and $f_{\mathrm{WY}}(t)=\frac{1}{4}(\sqrt{t}+1)^2$, which is the only *self-dual* operator monotone function.[61] "It is not known at the moment if there are other monotone metrics of constant sectional and scalar curvature" (Ref. 61, p. 3760). It is a theorem that the "set of two-dimensional normalized density matrices equipped with the Bures metric is isometric to one closed-half of the three-sphere with radius $\frac{1}{2}$."[62] The WY-metric "looks locally like a sphere of radius 2 of dimension (n^2-1)" (Ref. 61, p. 3759). If we transform to spherical coordinates on the 3-sphere, then, the metric tensor for $\mathrm{d}s^2_{\min}$ is diagonal in character, while the two other (constant scalar curvature) metrics are not (cf. Ref. 63).

The three metrics $\mathrm{d}s^2_{\min}$, $\mathrm{d}s^2_{\mathrm{WY}}$, and $\mathrm{d}s^2_{\mathrm{Fisher}_{q=2}}$ are *Einstein*. If we *scale* these metrics so that they are all of *unit* volume,[64] then $K^{n=2}_{\mathrm{min/scaled}}=6\pi^2\approx 59.2176$, $K^{n=2}_{\mathrm{WY/scaled}}=6\pi(\pi-2)\approx 21.5185$ and $K^{n=2}_{q=2/\mathrm{scaled}}=4\pi^2-6\sqrt{3}\pi\approx 6.830\,03$. The constant scalar curvatures of (unit-volume) *Yamabe* metrics are bounded above, and their least upper bound is a real number equal to $n(n-1)V_n^{2/n}$, where V_n is the volume of the standard metric on S^n, and in our (Bloch sphere) case, $n=3$, so the bound is $242^{1/3}\pi^{4/3}\approx 139.13$.[64]

X. DISCUSSION

Luo[24] (cf. Ref. 44, Sec. 2.4 and Refs. 19, 20, and 65) has calculated the Fisher information matrix of the Husimi distribution in the Fock-Bargmann representation of the quantum harmonic oscillator with one degree of freedom. He found that the Fisher information of the position and that of the momentum move in opposite directions, and that a weighted trace of the Fisher information matrix is a constant independent of the wave function, and thus has an upper bound. (Luo did not consider the possibility of generating prior probability distributions by normalizing the volume element of the Fisher information metric.)

Gnutzmann and Życzkowski noted that one "is tempted to think of the Husimi function as a probability density on the phase space. However, the rules for calculating expectation values of some observable using the Husimi function are nonclassical" (Ref. 47, Sec. 2.1) (cf. Ref. 66, p. 548). Gardiner and Zoller remarked that the "main problem of the Q-function is that not all positive normalizable Q-functions correspond to positive normalizable density operators" (Ref. 51, p. 109).

Further, the comparison of distances between Husimi distributions for arbitrary quantum states based on the Fisher information metric with those employing the Monge distance,[3] might be investigated. For the TLQS studied here, the Monge distance is, in fact, "consistent with the geometry of the Bloch ball induced by the Hilbert-Schmidt or the trace distance" (Ref. 3, p. 6716). [The trace distance is monotone, but *not* Riemannian, while the Hilbert-Schmidt distance, contrastingly, is Riemannian, but *not* monotone (Ref. 67, p. 10083).[37]] For n-dimensional quantum systems ($n>2$), unlike the trace, Hilbert-Schmidt or Bures distance, the Monge distance of ρ to the fully mixed state—which provides information concerning the *localization* of ρ in the classical

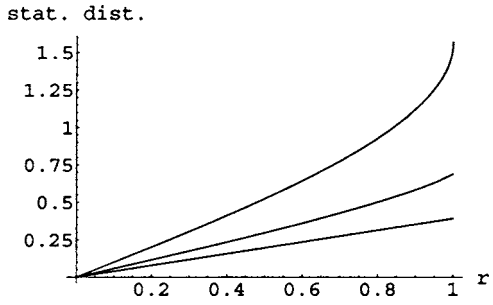

FIG. 10. Statistical distance as a function of distance from the origin of the Bloch ball—corresponding to the fully mixed state—for any monotone metric, for $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$, and for the Monge (or equivalently, for $n=2$, Hilbert-Schmidt) metric. The monotone-metric curve dominates that for $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$, which dominates the linear curve for the Monge metric.

phase space—is *not* the same for all pure states.[3] The only monotone metrics for which explicit distance formulas are so-far available are the Bures (minimal monotone) and Wigner-Yanase ones.[61]

In Fig. 10 we show how the distance from the fully mixed state ($r=0$) increases as r increases, for any monotone metric and for $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$, and (linearly) for the Monge (or Hilbert-Schmidt) metric. The first-mentioned distance—taking the functional form $\arcsin r$ (equalling $\pi/2$ for $r=1$)—dominates the second-mentioned distance (equalling $\pi/4.555\,153\,216\,7057$ for $r=1$), which in turns dominates the third [Ref. 3, Eq. (4.10)], which takes the value $\pi/8$ for $r=1$.

Let us bring to the attention of the reader, a recent preprint, which introduces a concept of escort *density operators* and a related one of *generalized* Fisher information[68] (cf. Refs. 46 and 69).

We have been consistently able above to find (apparently operator) monotone functions to generate the tangential components of (classical) Fisher information metrics for (rotationally symmetric) probability distributions over the TLQS. We suspect the existence of some (yet not formally demonstrated) theorem to this effect. Also, it would be of interest to formally test the various monotone functions presented above for the property (requisite for a *quantum* monotone metric[15,21] of *operator* monotonicity.

We have "hybridized" $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$ above to a (quantum) monotone metric $ds^2_{\mathrm{HYB}_{\mathrm{Hus}}}$ by replacing its radial component by that required $[1/(1-r^2)]$ while retaining its tangential component [formed from $f_{\mathrm{Hus}}(t)$]. But it appears that we could also convert it by appropriately scaling (a *conformal* transformation) the entire metric (tangential *and* radial components) by some suitable function. If we do so, we find that—by explicit construction—the new metric ($ds^2_{\mathrm{conformal}_{\mathrm{Hus}}}$) has the required radial component, while the tangential component is generated by a function

$$f_{\mathrm{conformal}_{\mathrm{Hus}}}(t) = f_{\mathrm{Hus}}(t) - t - 1, \tag{41}$$

which also appears to be operator monotone. [We note that $f_{\mathrm{conformal}_{\mathrm{Hus}}}(1)=1$ and $\lim_{t\to 0} f_{\mathrm{conformal}_{\mathrm{Hus}}}(t)=0$.] But now, we have the large relative entropies $S_{\mathrm{KL}}(p_{\mathrm{GKS}}, p_{\mathrm{conformal}_{\mathrm{Hus}}}) = 50.4636$ and $S_{\mathrm{KL}}(p_{\mathrm{conformal}_{\mathrm{Hus}}}, p_{\mathrm{GKS}}) = 54.2601$. At $r=0$, $ds^2_{\mathrm{conformal}_{\mathrm{Hus}}}$ is not flat, as is $ds^2_{\mathrm{Fisher}_{\mathrm{Hus}}}$, but has a (limiting) scalar curvature of $-\frac{24}{5}$.

Further questions: Motivated by the analyses above, we would like to pose the question of whether there exists a family of trivariate *probability* distributions parametrized by the points of the Bloch ball, for which the associated [classically *unique* (up to a constant multiple)] Fisher information metric *fully*—both in terms of tangential *and* radial components—has the requisite form (1) for a monotone metric. Also, the *volume elements* (and hence associated prior probabilities) of the monotone metrics are expressible as the *product* of Haar measure and measures over the eigenvalues.[16] To what extent, if any, does this hold true for prior probabilities *not* arising from monotone metrics? Are there any nonmonotone metrics which give rise to prior probabilities *more* noninformative than (at the very least) the minimal monotone (Bures) one? What are suitable

counterparts to formula (1) for n-level quantum systems ($n>2$)? Are there any monotone metrics which are flat at the fully mixed state, as is $ds^2_{\text{Fisher}_{\text{Hus}}}$ (7)?

XI. SUMMARY

In a *classical* context, for the family of Husimi *probability* distributions over the three-dimensional Bloch ball of two-level quantum systems (TLQS), we derived the (flat-at-the-fully-mixed-state) Fisher information metric [$ds^2_{\text{Fisher}_{\text{Hus}}}$, given by (2)]. Its tangential—but *not* its radial (r)—component conformed to that of one of the (uncountably) *infinite* class of (quantum) monotone metrics. The *prior* probability distribution (p_{Hus}) formed by normalizing the volume element of $ds^2_{\text{Fisher}_{\text{Hus}}}$ was found (Sec. III) to be considerably *less* noninformative than the priors formed from *any* of the (quantum) monotone metrics, even that (p_{Bures}) based on the (relatively informative) *minimal* monotone (Bures) metric. However, if we replaced the radial component of $ds^2_{\text{Fisher}_{\text{Hus}}}$ by that required $[1/(1-r^2)]$ of *all* (quantum) monotone metrics, the resultant "hybridized-Husimi" prior probability ($p_{\text{HYB}_{\text{Hus}}}$) became very close (in the sense of relative entropy ≈ 0.006 "nats") to p_{Bures}, and thus comparably informative in nature, but even nearer (≈ 0.0004) to another quantum-monotone-metric-based ("Grosse-Krattenthaler-Slater" or "quasi-Bures") probability distribution (p_{GKS}) that has been conjectured to yield the asymptotic minimax/maximin redundancy for universal *quantum* coding. The analogous (Bayesian) role in universal (classical) coding—by a well-known result of Clarke and Barron[17,18]—is played by Jeffreys' prior (cf. Refs. 19 and 20). This takes the specific (original, nonhybridized) form p_{Hus} for the family (manifold) of trivariate Husimi qubit probability distributions under study. We also studied the Fisher information metric for the *escort*-Husimi (Sec. V), positive-P (Sec. VI) and certain Gaussian probability distributions (Sec. VII), as well as, in some sense, the discrete Wigner pseudoprobability (Sec. VIII). Additionally, we applied the Clarke comparative noninformativity test[25,26] to quantum priors (Sec. III). Evidence that this test is consistent with the recently stated criterion of "biasedness to pure states" of Srednicki[27] has been presented.[28]

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Rigorous bra-ket formalism and wave function operator for one particle quantum mechanics

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Following previous works dedicated to the mathematical meaning of the "bra-ket" formalism [I. M. Gel'fand and G. E. Shilov, Generalized Functions (Academic, New York, 1964), Vol. I; J. P. Antoine, J. Math. Phys. **10**, 53 (1969); Yu. M. Berezanskii, Expansions of Self-adjoint Operators (American Mathematical Society, Providence, RI 1968); E. Prugovečki, J. Math. Phys. **14**, 1410 (1973); J. P. Antoine and A. Grossmann, J. Funct. Anal. **23**, 369 (1976); **23**, 379 (1976)], we develop a new rigorous mathematical approach, based on an operator representation of bras and kets. This leads to a formalism very similar to second quantization. Well-defined operators associated with local observables can be exhibited, intimately related to previous works of E. Prugovečki [Stochastic Quantum Mechanics and Quantum Space-Time (Reidel, Dordrecht, 1986)]. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2157053]

I. INTRODUCTION

Since the early years of quantum mechanics, different mathematical studies have been led to give a rigorous meaning to the symbolic "bra-ket" formalism used in most quantum mechanical papers. Quantum mechanics (for a spinless particle) is mathematically represented on the Hilbert space $\mathcal{H}=L^2(\mathbb{R}^3)$ over position space equipped with the inner product $(\phi|\psi)=\int_{\mathbb{R}^3}d^3\vec{q}\ \phi^*(\vec{q})\psi(\vec{q})$; but most of quantum mechanics books also introduce "the states $|\vec{q}\rangle$, $|\vec{p}\rangle$," the "inner product" $\langle\vec{q}|\psi\rangle$ or use the formula $|\phi\rangle=\int_{\mathbb{R}^3}d^3\vec{q}\ \phi(\vec{q})|\vec{q}\rangle$, while "the vectors $|\vec{q}\rangle$" do not belong to $\mathcal{H}$. So different structures have been developed to give a right mathematical meaning to these objects. We can quote two different procedures. The first one is based on the construction of "super-Hilbert" spaces, such as the rigged,[1,2] equipped,[3] extended,[4] or nested[5] Hilbert spaces. The second approach is essentially the reverse of the previous ones and is based on the definition of a new mathematical structure: the partial inner product spaces,[6] that unifies the previous constructions.

In this paper we study how the symbolic expressions and calculations of the bra-ket formalism are justified, if we represent bras and kets by operators. Our approach is practical: we do not start from a general abstract structure, and we study the concrete case of a spinless particle in standard nonrelativistic quantum mechanics. Of course our construction crosses the previous works by several ways.

First of all, we focus on the "basis" $\{|\vec{q}\rangle\}$ and then we assign a special role to the position operator. In the abstract context of previous works, this means that the position coordinates correspond to *labeled observables*.[2,7] To give a right mathematical meaning to the vectors $|\vec{q}\rangle$, we map them into bounded operators $\mathbf{\Phi}_{\vec{q}}$ on $\mathcal{H}$, and the symbolic integral $\int_{\mathbb{R}^3}d^3\vec{q}\phi(\vec{q})|\vec{q}\rangle$ over $\mathbb{R}^3$ becomes a true (operator valued) integral (Sec. II). The $\mathbf{\Phi}_{\vec{q}}$ are obtained thanks to the introduction of a C^∞ function ξ of compact support that we call the *dressing function*: it plays a central role in our procedure. Then we show that bounded bras and kets are realized as Hilbert-Schmidt operators, and the standard inner product is mapped into the Hilbert-Schmidt inner product (Secs. III and IV). Moreover this bra-ket representation can be extended to a large family of "unbounded"

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bras and kets corresponding to possibly unbounded operators (Sec. V). The representation of all objects in terms of operators is an old idea that can be found in Foias's papers.[8] More precisely, he defined the concept of an integral decomposition of some vector space in terms of eigenoperators associated with a self-adjoint operator. In the symbolic language of the bra-ket formalism, these eigenoperators correspond to distributions as $\delta(\mathbf{P}-p)=|\vec{p}\rangle\langle\vec{p}|$. We recover this formalism with the representation of unbounded bra-kets and the properties of the momentum observable (Secs. V and X). Moreover the definition of a generalized inner product for unbounded bras and kets leads us to the definition of a partial inner product (Sec. V).

Then we look at how to represent observables and symmetries with our formalism (Secs. VI–XI). In fact quantum observables are represented as self-adjoint operators acting on the standard Hilbert space $\mathcal{H}$ or as superoperators acting on the Hilbert space $\mathcal{L}_{\mathrm{HS}}$ of Hilbert-Schmidt operators. This representation gives a right mathematical representation for the symbolic objects $|\vec{q}_1\rangle\langle\vec{q}_2|$. We analyze in Sec. VIII the physical meaning of these representations and the role of the dressing function ξ.

Furthermore, we find that the operator $\mathbf{\Phi}_{\vec{q}}$ can be interpreted as a "wave function operator," and the quantum mechanical observables (for one particle) are expressed in a very similar way to second quantization. Nevertheless we do not think that this similarity hides some deeper direct connection, but rather that it is a consequence of the common mathematical structure shared by both formalisms, kets (creating operators), bras (annihilating operators), and observables (one particle observables) are elements of the same algebra, moreover in both cases we have a linear mapping from the initial Hilbert space into some algebra.

Finally the "wave function operator" allows us to define local observables, and we show that these operators are intimately related to previous works of Prugovečki[9] (positive operator valued measures). We also recover "the proper wave function" of a particle that cannot be pointlike. This special point was also derived in our previous paper.[10]

In the remainder we call the $\mathcal{H}$ Hilbert space $L^2(\mathbb{R}^3)$ over position space, $\mathcal{L}_{\mathcal{H}}$ the set of bounded operators on $\mathcal{H}$, and $\mathcal{L}_{\mathcal{HS}}$ the Hilbert space of Hilbert-Schmidt operators and the paper is organized as follows:

(i) First, we define the "wave function operator" $\mathbf{\Phi}_{\vec{q}}$ and the representation of $\mathcal{H}$ into $\mathcal{L}_{\mathcal{H}}$, allowing us to give a precise mathematical definition of "kets" in the q-basis (Sec. II). Then we show that "bounded kets" are in fact represented by Hilbert-Schmidt operators and we show that the representation of $\mathcal{H}$ into $\mathcal{L}_{\mathcal{HS}}$ is in fact an isometry (Sec. III). This allows us to give the representation of "bras." We also study the reverse mapping from $\mathcal{L}_{\mathcal{HS}}$ onto $\mathcal{H}$ (Sec. IV). In Sec. V, we generalize the previous definitions to "unbounded kets and bras."
(ii) We continue with the representation of symmetries and quantum observables in this new framework (Secs. VI and VII).
(iii) In Sec. VIII, we summarize the mathematical results and their physical meanings.
(iv) Then we study in details different observables, the position (Sec. IX), the momentum (Sec. X), and local observables (Sec. XI). Section XII is devoted to the Schrödinger equation.
(v) Finally we conclude this paper by Sec. XIII.

Remark: We specify that operator valued integrals are defined in the weak operator topology and bold letters stand for operators.

II. MAPPING $\mathcal{H}$ INTO $\mathcal{L}_{\mathcal{H}}$

In this section we introduce the operators $\mathbf{\Phi}_{\vec{q}}$ that allow us to map $\mathcal{H}$ into $\mathcal{L}_{\mathcal{H}}$. We call $\mathbf{\Phi}_{\vec{q}}$ the "wave function operator."

A. Definition of the wave function operator and first properties

We define the operators $\mathbf{\Phi}_{\vec{q}}$ on $\mathcal{H}$ as

$$\forall \varphi \in \mathcal{H}, \quad \forall \vec{q},\vec{x} \in \mathbb{R}^3, \quad \mathbf{\Phi}_{\vec{q}}(\varphi)(\vec{x}) = \xi(\vec{x}-\vec{q})\varphi(\vec{x}-\vec{q}), \tag{1}$$

where ξ is a given radial real function $\xi(\vec{x})=F(\|\vec{x}\|)$; and we assume ξ to be a C^∞ function with compact support.

Moreover ξ is normalized as

$$\int_{\mathbb{R}^3} d^3\vec{x}\ \xi(\vec{x})^2 = 1. \tag{2}$$

If we introduce the quantum operators $\vec{\mathbf{Q}}$ and $\vec{\mathbf{P}}=-i\hbar\,\partial_{\vec{q}}$, the operators $\mathbf{\Phi}_{\vec{q}}$ can be written

$$\mathbf{\Phi}_{\vec{q}} = \exp[-(i/\hbar)\vec{\mathbf{P}}\cdot q]\xi(\vec{\mathbf{Q}}), \tag{3}$$

so

$$\|\mathbf{\Phi}_{\vec{q}}\|_\infty \leqslant \|\xi\|_\infty. \tag{4}$$

We deduce that the adjoint $\mathbf{\Phi}_{\vec{q}}^\dagger$ verifies

$$\forall \varphi \in \mathcal{H}, \quad \forall \vec{q},\vec{x} \in \mathbb{R}^3, \quad \mathbf{\Phi}_{\vec{q}}^\dagger(\varphi)(\vec{x}) = \xi(\vec{x})\varphi(\vec{x}+\vec{q}),$$

$$\mathbf{\Phi}_{\vec{q}}^\dagger = \xi(\vec{\mathbf{Q}})\exp[(i/\hbar)\mathbf{P}\cdot\vec{q}]. \tag{5}$$

Finally, we conclude this part with the following important property.

Theorem: For any vectors φ and ψ of $\mathcal{H}$, the functions $\vec{q}\to\|\mathbf{\Phi}_{\vec{q}}^\dagger(\psi)\|_{\mathcal{H}}$ and $\vec{q}\to(\varphi|\mathbf{\Phi}_{\vec{q}}\psi)$ belong to $\mathcal{H}$.

Proof: We have

$$\|\mathbf{\Phi}_{\vec{q}}^\dagger(\psi)\|_{\mathcal{H}}^2 = \int_{\mathbb{R}^3} d^3\vec{x}\ \xi(\vec{x})^2|\psi(\vec{x}+\vec{q})|^2, \tag{6}$$

so

$$\int_{\mathbb{R}^3} d^3\vec{q}\|\mathbf{\Phi}_{\vec{q}}^\dagger(\psi)\|_{\mathcal{H}}^2 = \|\psi\|_{\mathcal{H}}^2\int_{\mathbb{R}^3} d^3\vec{x}\ \xi(\vec{x})^2 = \|\psi\|_{\mathcal{H}}^2. \tag{7}$$

Moreover we can write $(\varphi|\mathbf{\Phi}_{\vec{q}}\psi)$ as being $(\psi|\mathbf{\Phi}_{\vec{q}}^\dagger\varphi)^*$, then using the Schwarz inequality and the previous result we find

$$\int_{\mathbb{R}^3} d^3\vec{q}|(\varphi|\mathbf{\Phi}_{\vec{q}}\psi)|^2 \leqslant \|\varphi\|_{\mathcal{H}}^2\|\psi\|_{\mathcal{H}}^2. \tag{8}$$

B. The representation of kets in the *q*-basis

The previous theorem shows that for any $f\in\mathcal{H}$, the quantity $B_f(\varphi,\psi)=\int_{\mathbb{R}^3}d^3\vec{q}\ f(\vec{q})(\varphi|\mathbf{\Phi}_{\vec{q}}\psi)$ defines a continuous sesquilinear form on $\mathcal{H}$, so we know[11] that there exists some bounded operator $\hat{\mathbf{f}}$ on $\mathcal{H}$ such that $B_f(\varphi,\psi)=(\varphi|\hat{\mathbf{f}}\psi)$. By construction $\hat{\mathbf{f}}$ is the operator valued integral,

$$\hat{\mathbf{f}} = \int_{\mathbb{R}^3} d^3\vec{q}\ f(\vec{q})\mathbf{\Phi}_{\vec{q}}. \tag{9}$$

$\hat{\mathbf{f}}$ is a bounded operator, moreover we find

$$\|\hat{\mathbf{f}}^{\dagger}(\varphi)\|_{\mathcal{H}} \leqslant \int_{\mathbb{R}^3} d^3\vec{q}\,|f(\vec{q})|\|\mathbf{\Phi}^{\dagger}_{\vec{q}}(\varphi)\|_{\mathcal{H}} \leqslant \|f\|_{\mathcal{H}}\|\varphi\|_{\mathcal{H}}, \tag{10}$$

so

$$\|\hat{\mathbf{f}}\|_{\infty} = \|\hat{\mathbf{f}}^{\dagger}\|_{\infty} \leqslant \|f\|_{\mathcal{H}}. \tag{11}$$

We deduce that the mapping $\mathcal{U}: f \to \hat{\mathbf{f}}$ from $\mathcal{H}$ into the set $\mathcal{L}_{\mathcal{H}}$ of bounded operators on $\mathcal{H}$ is a continuous linear mapping.

Then we have the following correspondence between the ket formalism and its operator representation on $\mathcal{L}_{\mathcal{H}}$:

$$\text{for } f \in \mathcal{H}, \quad \begin{cases} |\vec{q}\rangle \mapsto \mathbf{\Phi}_{\vec{q}}, \\ |f = \int_{\mathbb{R}^3} d^3\vec{q}\, f(\vec{q})|\vec{q} \mapsto \hat{\mathbf{f}} = \int_{\mathbb{R}^3} d^3\vec{q}\, f(\vec{q})\mathbf{\Phi}_{\vec{q}}. \end{cases} \tag{12}$$

The same correspondence is formally used in second quantization (up to the replacement $\mathbf{\Phi}_{\vec{q}} \to \mathbf{\Phi}^{\dagger}_{\vec{q}}$). So we can think that $\mathbf{\Phi}_{\vec{q}}$ (or $\mathbf{\Phi}^{\dagger}_{\vec{q}}$) represents in our formalism some analogous of the "wave function operator," but in the unusual framework of one particle equations. This idea is confirmed by our first theorem, since the expectation value $f(\vec{q}) = (\varphi|\mathbf{\Phi}_{\vec{q}}\varphi)$ defines a vector of $\mathcal{H}$. We will see in the following that a great number of results agrees with this interpretation of $\mathbf{\Phi}_{\vec{q}}$.

III. INNER PRODUCT AND BRAS

We call $\mathcal{L}_{\mathcal{HS}}$ the Hilbert space of Hilbert-Schmidt operators on $\mathcal{H}$ equipped with the inner product $(\mathbf{A}|\mathbf{B})_{\mathcal{HS}} = \mathrm{Tr}(\mathbf{A}^{\dagger}\mathbf{B})$.

A. Isometric mapping from $\mathcal{H}$ into $\mathcal{L}_{\mathcal{HS}}$

We have the following theorem that specifies the isometry.

Theorem: For any $\phi \in \mathcal{H}$, $\hat{\boldsymbol{\phi}} \in \mathcal{L}_{\mathcal{HS}}$, and $\|\hat{\boldsymbol{\phi}}\|_{\mathcal{HS}} = \|\phi\|_{\mathcal{H}}$. So $(\hat{\boldsymbol{\varphi}}|\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\hat{\boldsymbol{\psi}}) = (\varphi|\psi)_{\mathcal{H}}$.

Proof: First we remark from Eq. (5) that $\hat{\boldsymbol{\phi}}$ is defined by a kernel K_{ϕ},

$$\forall \varphi \in \mathcal{H}, \quad \forall \vec{x} \in \mathbb{R}^3, \quad \hat{\boldsymbol{\phi}}(\varphi)(\vec{x}) = \int_{\mathbb{R}^3} d^3\vec{q}\; \phi(\vec{q})\xi(\vec{x}-\vec{q})\varphi(\vec{x}-\vec{q}), \tag{13}$$

then

$$\hat{\boldsymbol{\phi}}(\varphi)(\vec{x}) = \int_{\mathbb{R}^3} d^3\vec{q}\; K_{\phi}(\vec{x},\vec{q})\varphi(\vec{q}),$$

$$K_{\phi}(\vec{x},\vec{q}) = \phi(\vec{x}-\vec{q})\xi(\vec{q}). \tag{14}$$

Moreover $K_{\phi} \in L^2(\mathbb{R}^6)$ since

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} d^3\vec{x}\, d^3\vec{q}\,|K_{\phi}(\vec{x},\vec{q})|^2 = \|\phi\|^2_{\mathcal{H}}, \tag{15}$$

where we use the condition of normalization on the field ξ.

This shows that $\hat{\boldsymbol{\phi}}$ is a Hilbert-Schmidt operator and

$$\|\hat{\boldsymbol{\phi}}\|_{\mathcal{HS}} = \|\phi\|_{\mathcal{H}}. \tag{16}$$

Then, from the polarization identity we deduce that

$$\forall \varphi, \quad \psi \in \mathcal{H}, \quad (\hat{\boldsymbol{\varphi}}|\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\hat{\boldsymbol{\psi}}) = (\varphi|\psi)_{\mathcal{H}}. \tag{17}$$

We have shown that the linear mapping $\mathcal{U}$: $\phi \to \hat{\boldsymbol{\phi}}$ is an isometry from the Hilbert space $\mathcal{H}$ into a closed subspace $\hat{\mathcal{H}} = \mathcal{U}(\mathcal{H})$ of $\mathcal{L}_{\mathrm{HS}}$.

B. The bra representation in the *q*-basis

From the relation $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\hat{\boldsymbol{\psi}}) = (\varphi|\psi)_{\mathcal{H}}$, we deduce that we have the following correspondence between the bra formalism and its operator representation on $\mathcal{L}_{\mathcal{H}}$:

$$\text{for } f \in \mathcal{H}, \quad \begin{cases} \langle \vec{q}| \mapsto \boldsymbol{\Phi}_{\vec{q}}^{\dagger} \\ \langle f| = \displaystyle\int_{\mathbb{R}^3} d^3\vec{q} f(\vec{q})^* \langle \vec{q}| \mapsto \hat{\mathbf{f}}^{\dagger} = \int_{\mathbb{R}^3} d^3\vec{q} f(\vec{q})^* \boldsymbol{\Phi}_{\vec{q}}^{\dagger}. \end{cases} \tag{18}$$

Then the set of bras and the set of kets are represented as two different subspaces of bounded (or Hilbert-Schmidt) operators and the symmetry bra-ket is given by the conjugate antilinear mapping $\mathbf{A} \to \mathbf{A}^{\dagger}$. So, in this formalism bras and kets are elements of a same space of operators.

IV. REVERSE MAPPING FROM $\mathcal{L}_{\mathcal{HS}}$ ONTO $\mathcal{H}$

Since $\hat{\mathcal{H}} = \mathcal{U}(\mathcal{H})$ is a closed subspace of the Hilbert space $\mathcal{L}_{\mathcal{HS}}$, we can formally define the superprojector Π from $\mathcal{L}_{\mathcal{HS}}$ onto $\hat{\mathcal{H}}$ as Π: $\mathbf{K} \in \mathcal{L}_{\mathcal{HS}} \to \Pi(\mathbf{K}) = \int_{\mathbb{R}^3} d^3\vec{q}\, \boldsymbol{\Phi}_{\vec{q}} \mathrm{Tr}(\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\mathbf{K})$, where it is assumed that $\mathrm{Tr}(\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\hat{\boldsymbol{\phi}}) = \phi(\vec{q})$ and then $\Pi(\hat{\boldsymbol{\phi}}) = \hat{\boldsymbol{\phi}}$. Unfortunately $\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\mathbf{K}$ for $\mathbf{K} \in \mathcal{L}_{\mathcal{HS}}$ is not always (for any $\vec{q}$) a trace class operator, so $\mathrm{Tr}(\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\mathbf{K})$ is not a well-defined mathematical quantity. Nevertheless, we will see with the following theorem that the kernel integral deduced from the symbolic expression of $\mathrm{Tr}(\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\mathbf{K})$ is almost everywhere defined.

Theorem: For $\mathbf{K} \in \mathcal{L}_{\mathcal{HS}}$ represented by its kernel $K(\vec{x},\vec{y})$, we define the function $\breve{\mathbf{K}}: \vec{q} \to \int_{\mathbb{R}^3} d^3\vec{x}\, \xi(\vec{x}) K(\vec{x}+\vec{q},\vec{x})$ [corresponding to the symbolic expression $\mathrm{Tr}(\boldsymbol{\Phi}_{\vec{q}}\mathbf{K})$]. $\breve{\mathbf{K}}$ is an almost everywhere defined function that belongs to $\mathcal{H}$, and $\mathbf{K} \to \breve{\mathbf{K}}$ corresponds to a continuous linear extension to $\mathcal{L}_{\mathcal{HS}}$ of the reverse mapping $\mathcal{U}^{-1}$ from $\hat{\mathcal{H}}$ onto $\mathcal{H}$.

Proof: So let us prove that $\breve{\mathbf{K}}$ is an almost everywhere defined square integrable function. From the Scharwz inequality and the normalization of ξ we have

$$\int_{\mathbb{R}^3} d^3\vec{q} \left(\int_{\mathbb{R}^3} d^3\vec{x} |\xi(\vec{x})| |K(\vec{x}+\vec{q},\vec{x})| \right)^2 \leqslant \|\mathbf{K}\|_{\mathcal{HS}}^2. \tag{19}$$

This shows that $\breve{\mathbf{K}}(\vec{q})$ is almost everywhere defined and that $\breve{\mathbf{K}} \in \mathcal{H}$. Moreover

$$\|\breve{\mathbf{K}}\|_{\mathcal{H}} \leqslant \|\mathbf{K}\|_{\mathcal{HS}}, \tag{20}$$

then $\mathbf{K} \to \breve{\mathbf{K}}$ is continuous.

Finally, the kernel K_{ϕ} corresponding to $\hat{\boldsymbol{\phi}} \in \hat{\mathcal{H}}$ is given by

$$K_{\phi}(\vec{x},\vec{y}) = \phi(\vec{x}-\vec{y})\xi(\vec{y}), \tag{21}$$

so

$$\breve{\hat{\boldsymbol{\phi}}} = \phi. \tag{22}$$

Conclusion: We deduce that the superprojector Π previously mentioned from $\mathcal{L}_{\mathcal{HS}}$ onto $\hat{\mathcal{H}}$ possesses the well-defined expression

$$\forall \mathbf{K} \in \mathcal{L}_{\mathcal{HS}}, \quad \Pi(\mathbf{K}) = \int_{\mathbb{R}^3} d^3\vec{q}\, \breve{\mathbf{K}}(\vec{q})\mathbf{\Phi}_{\vec{q}}. \tag{23}$$

V. GENERALIZED BRAS, KETS AND THEIR INNER PRODUCT

In this section we extend the definition of bras and kets to be able to define the kets $|\vec{p}\rangle$, for example.

A. Generalized bras and kets

The previous representation of bounded kets and bras suggests that we can define generalized objects by relaxing the condition on f in the operator valued integral $\hat{\mathbf{f}}=\int_{\mathbb{R}^3} d^3\vec{q}\, f(\vec{q})\mathbf{\Phi}_{\vec{q}}$. The simplest way is to use a complex Baire measure μ and to define $\hat{\boldsymbol{\mu}}=\int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})\mathbf{\Phi}_{\vec{q}}$. Generally $\hat{\boldsymbol{\mu}}$ is an unbounded operator on $\mathcal{H}$.

We introduce the Gel'fand triplet $\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$, where $\mathcal{H}_+=\{f \in L^\infty(\mathbb{R}^3)$ with a compact support$\}$ and $\mathcal{H}_-$ is the Frechet space of locally summable functions on $\mathbb{R}^3$ with its directed family of seminorms $\|f\|_n=\int_{\|\vec{q}\|\leq n} d^3\vec{q}\,|f(\vec{q})|$. $\mathcal{H}_+$ is a dense subset of $\mathcal{H}$ and is related to $\mathcal{H}_-$ by the duality $\mathcal{H}_-^*=\mathcal{H}_+$.

Theorem: For any Baire measure μ, the operator valued integral $\hat{\boldsymbol{\mu}}=\int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})\mathbf{\Phi}_{\vec{q}}$ is a continuous linear mapping from $\mathcal{H}$ into $\mathcal{H}_-$. Moreover, the operator $\hat{\boldsymbol{\mu}}^\dagger$ defined as $\hat{\boldsymbol{\mu}}^\dagger = \int_{\mathbb{R}^3} \mathrm{d}\mu^*(\vec{q})\mathbf{\Phi}_{\vec{q}}^\dagger$ is a linear mapping from $\mathcal{H}_+$ into $\mathcal{H}$. Then $\hat{\boldsymbol{\mu}}$ and $\hat{\boldsymbol{\mu}}^\dagger$ are special cases of mappings from $\mathcal{H}_+$ into $\mathcal{H}_-$.

Proof: Since any complex measure μ can be split into $\mu=\mu_1+i\mu_2$ where μ_1 and μ_2 are real, and since any real measure μ can be written as $\mu=\mu_+-\mu_-$ where μ_+ and μ_- are positive, we only need to analyze the case of positive Baire measures. So, let μ be a positive measure and $\varphi \in \mathcal{H}$. We study the function $\psi(\vec{x})=\hat{\mu}(\varphi)(\vec{x})=\int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})\mathbf{\Phi}_{\vec{q}}(\varphi)(\vec{x})$.

From the Eq. (5) we have

$$\psi(\vec{x}) = \int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})\xi(\vec{x}-\vec{q})\varphi(\vec{x}-\vec{q}). \tag{24}$$

Let us prove that ψ is an almost everywhere defined, locally summable function.

We call K_n the compact set $K_n=\{\vec{q}/\|\vec{q}\| \leq n\}$; using the Schwarz inequality we have

$$\int_{K_n} d^3\vec{x} \int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})|\xi(\vec{x}-\vec{q})\varphi(\vec{x}-\vec{q})| \leq C_n\|\varphi\|_{\mathcal{H}} \tag{25}$$

with

$$C_n = \int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q}) \left(\int_{K_n} d^3\vec{x}\, \xi(\vec{x}-\vec{q})^2 \right)^{1/2}. \tag{26}$$

Since ξ is a C^∞ function with a compact support, $F(\vec{q})=\int_{K_n} d^3\vec{x}\, \xi(\vec{x}-\vec{q})^2$ is a continuous function with compact support, then $\int_{\mathbb{R}^3} \mathrm{d}\mu(\vec{q})\sqrt{F(\vec{q})}$ is finite (μ is a Baire measure). This shows that ψ is a locally summable function, and

$$\|\hat{\mu}(\varphi)\|_n \leq C_n\|\varphi\|. \tag{27}$$

So $\hat{\boldsymbol{\mu}}$ is a continuous linear mapping from $\mathcal{H}$ into $\mathcal{H}_-$.

Moreover, since functions of $\mathcal{H}_+$ define continuous linear functionals on $\mathcal{H}_-$, we have for any $\eta \in \mathcal{H}_+$ and any $\varphi \in \mathcal{H}$,

$$<\eta^*, \hat{\boldsymbol{\mu}}(\varphi)> = \int_{\mathbb{R}^3} d^3\vec{x}\, \eta^*(\vec{x})\hat{\boldsymbol{\mu}}(\varphi)(\vec{x}) = \int_{\mathbb{R}^3} \mathrm{d}\mu_{\vec{q}}(\eta|\mathbf{\Phi}_{\vec{q}}\varphi)_{\mathcal{H}}. \tag{28}$$

By duality, we deduce that the operator $\hat{\boldsymbol{\mu}}^\dagger = \int_{\mathbf{R}^3} d\mu^*(\vec{q}) \boldsymbol{\Phi}_{\vec{q}}^\dagger$ is a well-defined linear mapping from $\mathcal{H}_+ = \mathcal{H}_-^*$ into $\mathcal{H} = \mathcal{H}^*$, and

$$\forall\, \eta \in \mathcal{H}_+,\ \hat{\boldsymbol{\mu}}^\dagger(\eta)(\vec{x}) = \xi(\vec{x}) \int_{\mathbb{R}^3} \mathrm{d}\mu^*(\vec{q})\, \eta(\vec{x}+\vec{q}),$$

$$\forall\, \eta \in \mathcal{H}_+,\ \forall\, \varphi \in \mathcal{H}, \quad (\varphi | \hat{\boldsymbol{\mu}}^\dagger \eta)_{\mathcal{H}} = \int_{\mathbb{R}^3} \mathrm{d}\mu^*(\vec{q}) (\varphi | \boldsymbol{\Phi}_{\vec{q}}^\dagger \eta)_{\mathcal{H}}. \tag{29}$$

B. Generalized inner product

For any complex Baire measures μ and ν, the above paragraph shows that $\hat{\boldsymbol{\mu}} \cdot \hat{\boldsymbol{\nu}}^\dagger$ is a well-defined operator from $\mathcal{H}_+$ into $\mathcal{H}_-$; but $\hat{\boldsymbol{\nu}}^\dagger \cdot \hat{\boldsymbol{\mu}}$ is generally undefined. So, if M is the set of complex Baire measures, we define the subset Ω of $M \times M$ as being the set of pairs (ν, μ) such that $\hat{\boldsymbol{\nu}}^\dagger \cdot \hat{\boldsymbol{\mu}}$ is a well-defined trace class operator on $\mathcal{H}$. We define a generalized inner product on Ω as

$$\forall (\nu, \mu) \in \Omega, \quad (\hat{\boldsymbol{\nu}} | \hat{\boldsymbol{\mu}}) = \mathrm{Tr}(\hat{\boldsymbol{\nu}}^\dagger \cdot \hat{\boldsymbol{\mu}}). \tag{30}$$

By construction, this definition generalized the Hilbert-Schmidt inner product $(\hat{\boldsymbol{\varphi}} | \hat{\boldsymbol{\psi}})_{\mathcal{HS}}$ previously defined and this structure corresponds to a partial inner product.[6]

C. Practical examples

We introduce the Dirac measure $\delta_{\vec{q}}$ and the Fourier measure $\mu_{\vec{k}}$ such that $\mathrm{d}\mu_{\vec{k}}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) d^3\vec{x}$ with $\phi_{\vec{k}}(\vec{x}) = \exp(i\vec{k} \cdot \vec{x})$; we also define the correspondent operators $\hat{\boldsymbol{\delta}}_{\vec{q}}$ and $\hat{\boldsymbol{\phi}}_{\vec{k}}$. Obviously we have

$$\hat{\boldsymbol{\delta}}_{\vec{q}} = \boldsymbol{\Phi}_{\vec{q}} \quad \text{and} \quad \hat{\boldsymbol{\delta}}_{\vec{q}}^\dagger = \boldsymbol{\Phi}_{\vec{q}}^\dagger \tag{31}$$

then $\hat{\boldsymbol{\delta}}_{\vec{q}}$ and $\hat{\boldsymbol{\delta}}_{\vec{q}}^\dagger$ define bounded operators on $\mathcal{H}$. Moreover

$$\forall\, \varphi \in \mathcal{H}, \quad \hat{\boldsymbol{\phi}}_{\vec{k}}(\varphi)(\vec{x}) = \int_{\mathbb{R}^3} d^3\vec{q}\, \exp(i\vec{k} \cdot \vec{q}) \xi(\vec{x} - \vec{q}) \varphi(\vec{x} - \vec{q}), \tag{32}$$

so

$$\forall\, \varphi \in \mathcal{H}, \quad \begin{cases} \hat{\boldsymbol{\phi}}_{\vec{k}}(\varphi)(\vec{x}) = F(\vec{k}) \phi_{\vec{k}}(\vec{x}), \\ F(\vec{k}) = \displaystyle\int_{\mathbb{R}^3} d^3\vec{q}\, \exp(-i\vec{k} \cdot \vec{q}) \xi(\vec{q}) \varphi(\vec{q}). \end{cases} \tag{33}$$

But $\vec{x} \to \boldsymbol{\Phi}_{\vec{q}}(\phi_{\vec{k}})(\vec{x}) = \exp(i\vec{k} \cdot \vec{q}) \xi(\vec{x}) \exp(i\vec{k} \cdot \vec{x})$ is a well-defined function of $\mathcal{H}$, then the operator $\hat{\boldsymbol{\delta}}_{\vec{q}}^\dagger \cdot \hat{\boldsymbol{\mu}}_{\vec{k}}$ is a bounded operator on $\mathcal{H}$ defined by the kernel K,

$$K(\vec{x}, \vec{y}) = \exp(i\vec{k} \cdot \vec{q}) \psi^*(\vec{x}) \psi(\vec{y}),$$

$$\psi(\vec{y}) = \xi(\vec{y}) \exp(-i\vec{k} \cdot \vec{y}). \tag{34}$$

This corresponds to a trace class operator and we have the generalized inner product,

$$(\hat{\boldsymbol{\delta}}_{\vec{q}} | \hat{\boldsymbol{\phi}}_{\vec{k}}) = \int_{\mathbb{R}^3} d^3\vec{x}\, K(\vec{x}, \vec{x}) = \exp(i\vec{k} \cdot \vec{q}). \tag{35}$$

We can easily check that $\hat{\boldsymbol{\phi}}_{\vec{k}}^\dagger \cdot \hat{\boldsymbol{\delta}}_{\vec{q}}$ also is a trace class operator and

$$(\hat{\boldsymbol{\phi}}_{\vec{k}}|\hat{\boldsymbol{\delta}}_{\vec{q}}) = \exp(-i\vec{k}\cdot\vec{q}). \tag{36}$$

This reasoning can be extended to any $\hat{\mathbf{f}}$ where f is a bounded continuous function,

$$(\hat{\boldsymbol{\delta}}_{\vec{q}}|\hat{\mathbf{f}}) = f(\vec{q}) \quad \text{and} \quad (\hat{\mathbf{f}}|\hat{\boldsymbol{\delta}}_{\vec{q}}) = f(\vec{q})^*. \tag{37}$$

Furthermore, let us assume ϕ to be a C^∞ function of rapid decrease, then $\hat{\boldsymbol{\delta}}^\dagger_{\vec{q}}\cdot\hat{\boldsymbol{\phi}}$ and $\hat{\boldsymbol{\phi}}^\dagger_{\vec{k}}\cdot\hat{\boldsymbol{\phi}}$ are trace class operators and

$$(\hat{\boldsymbol{\delta}}_{\vec{q}}|\hat{\boldsymbol{\phi}}) = \phi(\vec{q}),$$

$$(\hat{\boldsymbol{\phi}}_{\vec{k}}|\hat{\boldsymbol{\phi}}) = \int_{\mathbb{R}^3} d^3\vec{x}\,\exp(-i\vec{k}\cdot\vec{x})\,\phi(\vec{x}). \tag{38}$$

After this study on the representation of bras and kets, we can look for the representation of operators used in the bra-ket formalism.

VI. LOWERING AND RAISING THE BRA-KET FORMALISM

The bra-ket formalism used on $\mathcal{H}$ can be also employed on $\mathcal{L}_{\mathcal{HS}}$. Let us analyze in this section the symbolic expressions resulting from this simultaneous utilization.

We write down $|\varphi\rangle$ for the kets of $\mathcal{H}$ and $|\hat{\boldsymbol{\varphi}}\rangle$ for the kets of $\hat{\mathcal{H}}$. This notation extends to operators from $\mathcal{H}$ to $\mathcal{H}_-$ and the formula,

$$|\hat{\boldsymbol{\varphi}}\rangle = \int_{\mathbb{R}^3} d^3\vec{q}\;\varphi(\vec{q})|\boldsymbol{\Phi}_{\vec{q}} \tag{39}$$

becomes meaningful. Moreover we have seen that $\langle\boldsymbol{\Phi}_{\vec{q}}|\hat{\boldsymbol{\varphi}}\rangle = \mathrm{Tr}(\boldsymbol{\Phi}^\dagger_{\vec{q}}\hat{\boldsymbol{\varphi}})$ is an almost everywhere defined function and $\langle\boldsymbol{\Phi}_{\vec{q}}|\hat{\boldsymbol{\varphi}}\rangle = \varphi(\vec{q})$ (almost everywhere) then the symbolic closure relation $\int_{\mathbb{R}^3} d^3\vec{q}\,|\boldsymbol{\Phi}_{\vec{q}}\rangle\langle\boldsymbol{\Phi}_{\vec{q}}| = \mathbf{1}$ is justified. Now let us investigate more symbolic expressions.

We can write $|\hat{\boldsymbol{\varphi}}\rangle = \int_{\mathbb{R}^3} d^3\vec{q}\langle\vec{q}\,|\,\varphi\rangle|\boldsymbol{\Phi}_{\vec{q}}\rangle$, then our mapping $\mathcal{U}$ is $\mathcal{U} = \int_{\mathbb{R}^3} d^3\vec{q}\,|\boldsymbol{\Phi}_{\vec{q}}\rangle\langle\vec{q}|$ and $\mathcal{U}^{-1} = \int_{\mathbb{R}^3} d^3\vec{q}\,|\vec{q}\rangle\langle\boldsymbol{\Phi}_{\vec{q}}|$. If we are interested in the representation of operators different possibilities appear.

Let us assume that $\mathbf{A}$ is an operator, given in the bra-ket formalism of $\mathcal{H}$ by $\mathbf{A} = \int d^3\vec{q}\;d^3\vec{q}\,'\langle\vec{q}\,|\mathbf{A}\,|\vec{q}\,'\rangle|\vec{q}\rangle\langle\vec{q}\,'|$.

We can first lift up $\mathbf{A}$ in a superoperator

$$\mathbf{A}^{(S)} = \mathcal{U}\mathbf{A}\mathcal{U}^{-1} = \int d^3\vec{q}\;d^3\vec{q}\,'\langle\vec{q}|\mathbf{A}|\vec{q}\,'\rangle|\boldsymbol{\Phi}_{\vec{q}}\rangle\langle\boldsymbol{\Phi}_{\vec{q}\,'}|. \tag{40}$$

This corresponds to the isometric representation. But this is not the unique solution.

$\mathbf{A}$ possesses a natural action on the operators $\hat{\boldsymbol{\varphi}} \in \hat{\mathcal{H}}$ by $\hat{\boldsymbol{\varphi}} \to \mathbf{A}\cdot\hat{\boldsymbol{\varphi}}$, but $\mathbf{A}\cdot\hat{\boldsymbol{\varphi}}$ is not an element of $\hat{\mathcal{H}}$. If we remark that the matrix elements $(\hat{\boldsymbol{\psi}}|\,\mathbf{A}\cdot\hat{\boldsymbol{\varphi}})_{\mathcal{HS}}$ are the only important quantities, we find another (nonequivalent) representation of $\mathbf{A}$ as a new superoperator,

$$\hat{\mathbf{A}} = \int d^3\vec{q}\;d^3\vec{q}\,'\;\mathrm{Tr}(\boldsymbol{\Phi}^\dagger_{\vec{q}}\mathbf{A}\boldsymbol{\Phi}_{\vec{q}\,'})|\boldsymbol{\Phi}_{\vec{q}}\rangle\langle\boldsymbol{\Phi}_{\vec{q}\,'}|. \tag{41}$$

The interesting point of this representation is the relation

$$\langle\hat{\boldsymbol{\psi}}|\hat{\mathbf{A}}|\hat{\boldsymbol{\varphi}}\rangle = \mathrm{Tr}(\hat{\boldsymbol{\psi}}^\dagger\mathbf{A}\hat{\boldsymbol{\varphi}}) \tag{42}$$

that reproduces the symmetric notation of the bra-ket formalism.

Finally we have a third representation. The symbolic expression $|\vec{q}\rangle\langle\vec{q}'|$ represents an operator by some "tensorial product," but if we do the substitutions $|\vec{q}\rangle \to \mathbf{\Phi}_{\vec{q}}$ and $\langle\vec{q}'| \to \mathbf{\Phi}^{\dagger}_{\vec{q}'}$ the quantity $\mathbf{\Phi}_{\vec{q}}\mathbf{\Phi}^{\dagger}_{\vec{q}'}$ is well defined as a product of operators. Then we deduce a new representation on $\mathcal{H}$ by

$$\widetilde{\mathbf{A}} = \int d^3\vec{q}'\ d^3\vec{q}\langle\vec{q}|\mathbf{A}|\vec{q}'\rangle\mathbf{\Phi}_{\vec{q}}\,\mathbf{\Phi}^{\dagger}_{\vec{q}'}. \tag{43}$$

The interest of this representation is the substitution of the ket-bra tensorial product by the usual operator product $|\varphi\rangle\langle\psi| \to \hat{\boldsymbol{\varphi}}\hat{\boldsymbol{\psi}}^{\dagger}$.

In the following we study in details the representations $\hat{\mathbf{A}}$ and $\widetilde{\mathbf{A}}$.

VII. BOUNDED OPERATORS IN THE NEW REPRESENTATION

A. Representation of symmetries

1. Definition

Symmetries on $\mathcal{H}$ are given by unitary operators $\mathbf{U}$ and they represent, either a change of mathematical basis, or the change of state associated with a physical change of frame. So it is natural to lift up directly the action of $\mathbf{U}$ on $\mathcal{H}$ into an unitary superoperator $\mathbf{U}^{(S)}$ acting on $\hat{\mathcal{H}} = \mathcal{U}(\mathcal{H})$ as

$$\mathbf{U}^{(S)} = \mathcal{U}\mathbf{U}\mathcal{U}^{-1}. \tag{44}$$

Then

$$\forall\,\varphi \in \mathcal{H}, \quad \mathbf{U}^{(S)}(\hat{\boldsymbol{\varphi}}) = \widehat{\mathbf{U}(\varphi)}. \tag{45}$$

Moreover,

$$\forall\,\varphi, \quad \psi \in \mathcal{H}, \quad (\hat{\boldsymbol{\varphi}}|\mathbf{U}^{(S)}(\hat{\boldsymbol{\psi}}))_{\mathrm{HS}} = (\varphi|\mathbf{U}(\psi))_{\mathcal{H}}. \tag{46}$$

Another equivalent definition is obtained by postulating that symmetries are superunitary operators on $\mathcal{L}_{\mathcal{HS}}$ that have $\hat{\mathcal{H}}$ invariant.

2. Geometrical symmetries: Rotations, translations, and parity

The unitary transforms $\mathbf{R}_{\vec{\omega}}, \mathbf{T}_{\vec{a}}$, and $\mathbf{K}_P$ of rotation, translation, and parity are defined on $\mathcal{H}$ as

$$\mathbf{R}_{\vec{\omega}}(\varphi)(\vec{x}) = \varphi(\mathcal{R}^{-1}_{\vec{\omega}}(\vec{x})),$$

$$\mathbf{T}_{\vec{a}}(\varphi)(\vec{x}) = \varphi(\vec{x} - \vec{a}),$$

$$\mathbf{K}_P(\varphi)(\vec{x}) = \varphi(-\vec{x}), \tag{47}$$

where $\mathcal{R}_{\vec{\omega}}$ is a geometric rotation.

Since the function ξ is radial, we find

$$\mathbf{R}_{\vec{\omega}}\mathbf{\Phi}_{\vec{q}}\mathbf{R}^{\dagger}_{\vec{\omega}} = \mathbf{\Phi}_{\mathcal{R}_{\vec{\omega}}(\vec{q})},$$

$$\mathbf{T}_{\vec{a}}\,\mathbf{\Phi}_{\vec{q}} = \mathbf{\Phi}_{\vec{q}-\vec{a}},$$

$$\mathbf{K}_P\mathbf{\Phi}_{\vec{q}}\mathbf{K}_P = \mathbf{\Phi}_{-\vec{q}}. \tag{48}$$

From the expression $\hat{\boldsymbol{\varphi}}=\int_{\mathbb{R}^3} d^3\vec{q}\ \varphi(\vec{q})\boldsymbol{\Phi}_{\vec{q}}$, we deduce that for any $\varphi\in\mathcal{H}$, we have

$$\widehat{\mathbf{R}_{\vec{\omega}}(\varphi)}=\mathbf{R}_{\vec{\omega}}\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{R}_{\vec{\omega}}^{\dagger},$$

$$\widehat{\mathbf{T}_{\vec{a}}(\varphi)}=\mathbf{T}_{\vec{a}}\cdot\hat{\boldsymbol{\varphi}},$$

$$\widehat{\mathbf{K}_P(\varphi)}=\mathbf{K}_P\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{K}_P. \tag{49}$$

So, the superunitary operators $\mathbf{R}_{\vec{\omega}}^{(S)}$, $\mathbf{T}_{\vec{a}}^{(S)}$, and $\mathbf{K}_P^{(S)}$ on $\hat{\mathcal{H}}$ are defined as

$$\mathbf{R}_{\vec{\omega}}^{(S)}(\hat{\boldsymbol{\varphi}})=\mathbf{R}_{\vec{\omega}}\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{R}_{\vec{\omega}}^{\dagger},$$

$$\mathbf{T}_{\vec{a}}^{(S)}(\hat{\boldsymbol{\varphi}})=\mathbf{T}_{\vec{a}}\cdot\hat{\boldsymbol{\varphi}},$$

$$\mathbf{K}_P^{(S)}(\hat{\boldsymbol{\varphi}})=\mathbf{K}_P\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{K}_P. \tag{50}$$

3. Kinematical symmetry: Galilei boost

This symmetry $\mathbf{G}_{\vec{k}}$ is defined on $\mathcal{H}$ as

$$\mathbf{G}_{\vec{k}}(\varphi)(\vec{x})=\exp(i\vec{k}\cdot\vec{x})\varphi(\vec{x}), \tag{51}$$

so

$$\mathbf{G}_{\vec{k}}\boldsymbol{\Phi}_{\vec{q}}\mathbf{G}_{\vec{k}}^{\dagger}=\exp(i\vec{k}\cdot\vec{q})\boldsymbol{\Phi}_{\vec{q}}. \tag{52}$$

From the expression $\hat{\boldsymbol{\varphi}}=\int_{\mathbb{R}^3} d^3\vec{q}\ \varphi(\vec{q})\boldsymbol{\Phi}_{\vec{q}}$, we deduce that for any $\varphi\in\mathcal{H}$, we have

$$\widehat{\mathbf{G}_{\vec{k}}(\varphi)}=\mathbf{G}_{\vec{k}}\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{G}_{\vec{k}}^{\dagger}. \tag{53}$$

So the superunitary operator $\mathbf{G}_{\vec{k}}^{(S)}$ is defined as

$$\mathbf{G}_{\vec{k}}^{(S)}(\hat{\boldsymbol{\varphi}})=\mathbf{G}_{\vec{k}}\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{G}_{\vec{k}}^{\dagger}. \tag{54}$$

4. The special case of antiunitary transform: Time reversal

This antiunitary symmetry $\mathbf{K}_T$ is defined on $\mathcal{H}$ as

$$\mathbf{K}_T(\varphi)(\vec{x})=\varphi(\vec{x})^*. \tag{55}$$

Since ξ is real, we find

$$\mathbf{K}_T\cdot\boldsymbol{\Phi}_{\vec{q}}\cdot\mathbf{K}_T=\boldsymbol{\Phi}_{\vec{q}},$$

$$\mathbf{K}_T\cdot\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\cdot\mathbf{K}_T=\boldsymbol{\Phi}_{\vec{q}}^{\dagger}. \tag{56}$$

From the expression $\hat{\boldsymbol{\varphi}}=\int_{\mathbb{R}^3} d^3\vec{q}\ \varphi(\vec{q})\boldsymbol{\Phi}_{\vec{q}}$, we deduce that for any $\varphi\in\mathcal{H}$, we have

$$\widehat{\mathbf{K}_T(\varphi)}=\mathbf{K}_T\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{K}_T. \tag{57}$$

We deduce that $\mathbf{K}_T$ can be lifted into an antiunitary superoperator $\mathbf{K}_T^{(S)}$ acting on $\hat{\mathcal{H}}$ as

$$\mathbf{K}_T^{(S)}(\hat{\boldsymbol{\varphi}})=\mathbf{K}_T\cdot\hat{\boldsymbol{\varphi}}\cdot\mathbf{K}_T. \tag{58}$$

B. Representation of observables

1. Definition and first properties

Since $\mathcal{L}_{\mathcal{HS}}$ is an ideal of $\mathcal{L}_{\mathcal{H}}$, we have a natural representation of $\mathcal{L}_{\mathcal{H}}$, on $\mathcal{L}_{\mathcal{HS}}$, as $L_{\mathbf{A}}:\mathbf{B} \in \mathcal{L}_{\mathcal{HS}} \rightarrow \mathbf{A}\cdot\mathbf{B} \in \mathcal{L}_{\mathcal{HS}}$ for bounded operator $\mathbf{A}$. Moreover if Π is the superprojector on the closed subspace $\hat{\mathcal{H}}=\mathcal{U}(\mathcal{H})$ of $\mathcal{L}_{\mathcal{HS}}$, we can define the superoperator $\hat{\mathbf{A}}$ on $\mathcal{L}_{\mathcal{HS}}$ that maps $\hat{\mathcal{H}}$into $\hat{\mathcal{H}}$ as

$$\hat{\mathbf{A}} = \Pi L_{\mathbf{A}} \Pi. \tag{59}$$

Obviously

$$(\hat{\mathbf{A}})^{\dagger} = \widehat{\mathbf{A}^{\dagger}},$$

$$\mathbf{A} \geqslant \mathbf{0} \Rightarrow \hat{\mathbf{A}} \geqslant 0. \tag{60}$$

Moreover we have the following relation for inner product:

$$\forall\, \varphi, \psi \in \mathcal{H}, \quad (\hat{\boldsymbol{\varphi}}|\hat{\mathbf{A}}(\hat{\boldsymbol{\psi}}))_{\mathcal{HS}} = (\hat{\boldsymbol{\varphi}}|\mathbf{A}\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}}). \tag{61}$$

Since results of experiments are given by expectation values, the previous equation gives a very natural way to represent observables in the new representation. Moreover we recover in $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}})$ the complete symmetric expression $\langle\varphi|\,\mathbf{A}\,|\psi\rangle$ used in the bra-ket formalism.

Furthermore, we can build the sesquilinear form B_A on $\mathcal{H}$ as

$$\forall\, \varphi,\ \psi \in \mathcal{H}, \quad B_A(\varphi,\psi) = (\hat{\boldsymbol{\varphi}}|\hat{\mathbf{A}}(\hat{\boldsymbol{\psi}}))_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}}). \tag{62}$$

B_A is continuous since

$$B_A(\varphi,\psi) \leqslant \|\mathbf{A}\|_{\infty}\|\varphi\|_{\mathcal{H}}\|\psi\|_{\mathcal{H}}. \tag{63}$$

So for any operator $\mathbf{A} \in \mathcal{L}_{\mathcal{H}}$, there exists some bounded operator $\widetilde{\mathbf{A}}$ on $\mathcal{H}$ such that

$$(\hat{\boldsymbol{\varphi}}|\mathbf{A}\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}}) = (\varphi|\widetilde{\mathbf{A}}\psi)_{\mathcal{H}}. \tag{64}$$

This shows that

$$\hat{\mathbf{A}}(\hat{\boldsymbol{\varphi}}) = \widehat{\widetilde{\mathbf{A}}(\varphi)}. \tag{65}$$

Since we know that

$$\|\widetilde{\mathbf{A}}\|_{\infty} = \sup_{\varphi,\psi\in\mathcal{H}} \frac{|(\varphi|\widetilde{\mathbf{A}}\psi)_{\mathcal{H}}|}{\|\varphi\|_{\mathcal{H}}\|\psi\|_{\mathcal{H}}} \tag{66}$$

and

$$|(\hat{\boldsymbol{\varphi}}|\mathbf{A}\hat{\boldsymbol{\psi}})_{\mathrm{HS}}| \leqslant \|\mathbf{A}\|_{\infty}\|\hat{\boldsymbol{\varphi}}\|_{\mathrm{HS}}\|\hat{\boldsymbol{\psi}}\|_{\mathrm{HS}}, \tag{67}$$

we find

$$\|\widetilde{\mathbf{A}}\|_{\infty} \leqslant \|\mathbf{A}\|_{\infty}. \tag{68}$$

We deduce a new continuous mapping $\mathcal{V}:\mathbf{A}\rightarrow\widetilde{\mathbf{A}}$ from $\mathcal{L}_{\mathcal{H}}$ into itself. Moreover,

$$(\widetilde{\mathbf{A}})^\dagger = \widetilde{\mathbf{A}^\dagger},$$

$$\mathbf{A} \geqslant \mathbf{0} \Rightarrow \widetilde{\mathbf{A}} \geqslant 0. \tag{69}$$

Finally, using the functional calculus, the Eq. (65) implies that for any bounded Borel function f, we have

$$f(\hat{\mathbf{A}})(\hat{\boldsymbol{\varphi}}) = \widehat{f(\widetilde{\mathbf{A}})(\varphi)}. \tag{70}$$

2. Analytical expression of $\tilde{\mathbf{A}}$ for Hilbert-Schmidt operators

(a) Kernel representation: Let us assume that $\mathbf{A} \in \mathcal{L}_{\mathcal{HS}}$ is represented by its kernel $A(\vec{x},\vec{y}), [A(\vec{x},\vec{y}) \in L^2(\mathbb{R}^6)]$, and that $\hat{\boldsymbol{\psi}}, \hat{\boldsymbol{\varphi}}^\dagger$ are defined by their kernels K_ψ and $K_{\varphi^\dagger}$,

$$K_\psi(\vec{x},\vec{y}) = \xi(\vec{y})\psi(\vec{x}-\vec{y}),$$

$$K_{\varphi^\dagger}(\vec{x},\vec{y}) = \xi(\vec{x})\varphi^*(\vec{y}-\vec{x}). \tag{71}$$

Then $\hat{\boldsymbol{\varphi}}^\dagger \mathbf{A} \hat{\boldsymbol{\psi}}$ is given by the kernel K,

$$K(\vec{x},\vec{y}) = \xi(\vec{x})\xi(\vec{y}) \int_{\mathbb{R}^3\times\mathbb{R}^3} d^3\vec{q}\, d^3\vec{q}_1\, \varphi^*(\vec{q}-\vec{x}) A(\vec{q},\vec{q}_1)\psi(\vec{q}_1-\vec{y}), \tag{72}$$

or

$$K(\vec{x},\vec{y}) = \xi(\vec{x})\xi(\vec{y}) \int_{\mathbb{R}^3\times\mathbb{R}^3} d^3\vec{q}\, d^3\vec{q}_1\, \varphi^*(\vec{q})\psi(\vec{q}_1) A(\vec{q}+\vec{x},\vec{q}_1+\vec{y}). \tag{73}$$

So

$$(\varphi|\widetilde{\mathbf{A}}\psi)_{\mathcal{H}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^\dagger \mathbf{A} \hat{\boldsymbol{\psi}}) = \int_{\mathbb{R}^3} d^3\vec{x}\, K(\vec{x},\vec{x}). \tag{74}$$

From Eqs. (73) and (74), we find that $\widetilde{\mathbf{A}}$ is given by a kernel $\widetilde{A}(\vec{x},\vec{y})$,

$$\widetilde{A}(\vec{x},\vec{y}) = \int_{\mathbb{R}^3} d^3\vec{q}\, \xi(\vec{q})^2 A(\vec{q}+\vec{x},\vec{q}+\vec{y}). \tag{75}$$

If $\mathbf{A}$ is a trace class operator, then

$$\widetilde{A}(\vec{x},\vec{y}) = \mathrm{Tr}(\boldsymbol{\Phi}_{\vec{x}}^\dagger \mathbf{A} \boldsymbol{\Phi}_{\vec{y}}). \tag{76}$$

(The previous expression cannot be defined for any $\vec{x}$ and $\vec{y}$ if $\mathbf{A}$ is only a Hilbert-Schmidt operator.)

Remark: Using the Schwarz inequality and the normalization of ξ we have

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} d^3\vec{x}\, d^3\vec{y} |\widetilde{A}(\vec{x},\vec{y})|^2 \leqslant \|\mathbf{A}\|^2_{\mathcal{HS}}. \tag{77}$$

This shows that $\mathcal{V}: \mathbf{A} \to \widetilde{\mathbf{A}}$ maps $\mathcal{L}_{\mathcal{HS}}$ into $\mathcal{L}_{\mathcal{HS}}$.

(b) Explicit formula with operator valued integral: We notice that

$$(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}\psi)_{\mathcal{H}}=\int_{\mathbb{R}^3}d^3\vec{q}\;\xi(\vec{q})^2\varphi^*(\vec{q}+\vec{x})\psi(\vec{q}+\vec{y}),\tag{78}$$

and since ξ is radial, we have $\xi(\vec{q})=\xi(-\vec{q})$, so

$$(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}\psi)_{\mathcal{H}}=\int_{\mathbb{R}^3}d^3\vec{q}\;\xi(\vec{q})^2\varphi^*(\vec{x}-\vec{q})\psi(\vec{y}-\vec{q}).\tag{79}$$

Moreover using the Scharwz inequality we find

$$\int_{\mathbb{R}^3\times\mathbb{R}^3}d^3\vec{x}\,d^3\vec{y}|(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}\psi)|^2\leqslant\|\varphi\|_{\mathcal{H}}^2\|\psi\|_{\mathcal{H}}^2.\tag{80}$$

So the function $(\vec{x},\vec{y})\to(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}\psi)$ belongs to $L^2(\mathbb{R}^6)$.

From Eqs. (72), (74), and (79) we find

$$(\varphi|\widetilde{\mathbf{A}}\psi)=\int_{\mathbb{R}^3\times\mathbb{R}^3}d^3\vec{x}\,d^3\vec{y}\,A(\vec{x},\vec{y})(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}\psi).\tag{81}$$

We deduce that the operator $\widetilde{\mathbf{A}}$ is given by the following operator valued integral (well-defined for Hilbert-Schmidt operators)

$$\widetilde{\mathbf{A}}=\int_{\mathbb{R}^3\times\mathbb{R}^3}d^3\vec{x}\,d^3\vec{y}\,A(\vec{x},\vec{y})\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}.\tag{82}$$

(c) Correspondence with the bra-ket formalism: When $\mathbf{A}$ belongs to $\mathcal{L}_{\mathcal{HS}}$, $\mathbf{A}$ allows to define a correspondence between the bra-ket symbolic formula and its well-defined mathematical representation,

$$|\vec{x}\rangle\langle\vec{y}|\mapsto\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger},$$

$$\int_{\mathbb{R}^3\times\mathbb{R}^3}d^3\vec{x}\,d^3\vec{y}\,A(\vec{x},\vec{y})|\vec{x}\rangle\langle\vec{y}|\mapsto\widetilde{\mathbf{A}}=\int_{\mathbb{R}^3\times\mathbb{R}^3}d^3\vec{x}\,d^3\vec{y}\,A(\vec{x},\vec{y})\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{y}}^{\dagger}.\tag{83}$$

Moreover if $\mathbf{A}$ is a trace class operator, we have the correspondence

$$\langle\vec{x}|\mathbf{A}|\vec{y}\rangle\to\widetilde{\mathbf{A}}(\vec{x},\vec{y})=\mathrm{Tr}(\mathbf{\Phi}_{\vec{x}}^{\dagger}\mathbf{A}\mathbf{\Phi}_{\vec{y}}).\tag{84}$$

Finally we notice

$$\mathbf{A}=\text{“}|\varphi\rangle\langle\psi|\text{”}\mapsto\widetilde{\mathbf{A}}=\hat{\boldsymbol{\varphi}}\cdot\hat{\boldsymbol{\psi}}^{\dagger}.\tag{85}$$

We will see in the next section how to generalize Eq. (83).

3. The representation of bounded operators and the closure relation

We start from the preceding section with $\mathbf{A}\in\mathcal{L}_{\mathcal{HS}}$. The kernel representation of Eq. (75) gives the following relation for any $\varphi,\psi\in\mathcal{H}$:

$$(\varphi|\widetilde{\mathbf{A}}\psi)=\int_{\mathbb{R}^3}d^3\vec{q}\;\xi(\vec{q})^2(\varphi|\exp[(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]\mathbf{A}\exp[-(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]\psi).\tag{86}$$

We deduce that for any $\mathbf{A}\in\mathcal{L}_{\mathcal{HS}}$,

$$\widetilde{\mathbf{A}} = \int_{\mathbb{R}^3} d^3\vec{q}\ \xi(\vec{q})^2 \exp[(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]\mathbf{A}\exp[-(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]. \tag{87}$$

Since ξ is square integrable, this relation can be extended to all bounded operators $\mathbf{A}\in\mathcal{L}_{\mathcal{H}}$. Moreover $\widetilde{\mathbf{A}}\to\mathbf{A}$ if $\xi^2\to\delta$.

Remark: ξ is a radial function, then $\xi(\vec{q})=\xi(-\vec{q})$ and the previous equation becomes

$$\widetilde{\mathbf{A}} = \int_{\mathbb{R}^3} d^3\vec{q}\ \xi(\vec{q})^2 \exp[-(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]\mathbf{A}\exp[(i/\hbar)\vec{\mathbf{P}}\cdot\vec{q}]. \tag{88}$$

Now we can explain the relation $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^\dagger\mathbf{A}\hat{\boldsymbol{\psi}})=(\varphi|\widetilde{\mathbf{A}}\psi)_{\mathcal{H}}$. From Eqs. (87) and (88), we find $\mathrm{Tr}(\widetilde{\mathbf{A}}\mathbf{B})=\mathrm{Tr}(\mathbf{A}\widetilde{\mathbf{B}})$. If we choose $\mathbf{B}=$"$|\psi\rangle\langle\varphi|$," taking into account Eq. (85), we recover $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^\dagger\mathbf{A}\hat{\boldsymbol{\psi}})=(\varphi|\widetilde{\mathbf{A}}\psi)_{\mathcal{H}}$.

Now, if $\{\phi_n\}$ is an orthonormal basis of $\mathcal{H}$, and if we call π_n the orthogonal projector "$|\phi_n\rangle\langle\phi_n|$," we have the closure relation on $\mathcal{H}$,

$$\sum_{n=0}^{\infty}\pi_n = \mathbf{1}_{\mathcal{H}}, \tag{89}$$

where the limit holds in the weak operator topology.

The mapping $\mathbf{A}\to\widetilde{\mathbf{A}}$ is continuous, so

$$\sum_{n=0}^{\infty}\widetilde{\pi}_n = \widetilde{\mathbf{1}}_{\mathcal{H}} = \mathbf{1}_{\mathcal{H}} \tag{90}$$

in the weak operator topology.

From Eq. (85) we deduce

$$\sum_{n=0}^{\infty}\hat{\phi}_n\hat{\phi}_n^\dagger = \mathbf{1}_{\mathcal{H}}. \tag{91}$$

We recover the symbolic notation $\Sigma_{n=0}^{\infty}|\phi_n\rangle\langle\phi_n| = \mathbf{1}_{\mathcal{H}}$.

This reasoning naturally extends to bounded self-adjoint operators $\mathbf{A}=\Sigma_{n=0}^{\infty}a_n\pi_n$ where $\{a_n\}$ are the (bounded) eigenvalues,

$$\widetilde{\mathbf{A}} = \sum_{n=0}^{\infty}a_n\hat{\phi}_n\hat{\phi}_n^\dagger. \tag{92}$$

But generally $\widetilde{\mathbf{A}}\neq\mathbf{A}$, and the eigenvalues (eigenvectors) of $\widetilde{\mathbf{A}}$ are not a_n (ϕ_n).

The physical meaning of this last result seems obscure, so let us return to quantum axiomatic.

VIII. QUANTUM AXIOMATIC IN THE NEW FRAMEWORK

We summarize in this paragraph the results previously obtained and their connection with quantum axiomatic:

(i) From the usual quantum framework on $\mathcal{H}$, we have developed a new mathematical framework that supports the symbolic manipulations of bras and kets as elements of an algebra of operators.

(ii) A particle must be associated with $\varphi\in\mathcal{H}$ or with $\hat{\boldsymbol{\varphi}}\in\hat{\mathcal{H}}$, and the bra-ket formalism on $\hat{\mathcal{H}}$ possesses a well-defined mathematical representation as seen above [Eqs. (12) and (18)]. Unbounded states are realized as operators that do not belong to $\hat{\mathcal{H}}$.

(iii) Symmetries are represented by unitary operators on $\mathcal{H}$ or by superunitary operators on $\hat{\mathcal{H}}$ [Eq. (45)] and the practical cases of geometrical symmetries and Galilei boosts are given in Eqs. (50) and (54).

(iv) We have a natural method to lift up observables $\mathbf{A}$ as superoperators $\hat{\mathbf{A}}$ [Eq. (59)] such that the symmetric bra-ket notation $\langle\varphi|\mathbf{A}|\psi\rangle$ can be mapped into the well-defined symmetric expression $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}})$. Furthermore this procedure leads to the definition of a new operator $\tilde{\mathbf{A}}$ on $\mathcal{H}$ such that $\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\psi}})=(\varphi|\tilde{\mathbf{A}}\psi)_{\mathcal{H}}$, where $\tilde{\mathbf{A}}$ possesses a well-defined integral representation [Eqs. (82) and (87)] very similar to the bra-ket expression of $\mathbf{A}$ [Eqs. (83)]. But the eigenvalues and eigenvectors of $\mathbf{A}$ are not those of $\tilde{\mathbf{A}}$.

The physical interpretation: A simple picture of these results can be given if we introduce the idea of two categories of objects in our quantum formalism: "the bare objects" and "the dressed ones." Usual objects introduced by the bra-ket formalism of quantum mechanics are in fact "bare objects" that have to be dressed. A state $\varphi\in\mathcal{H}$ is a bare wave function, while $\hat{\boldsymbol{\varphi}}\in\hat{\mathcal{H}}$ is its dressed version. In the same way, we must think about the definition of all usual quantum observables $\mathbf{A}$ in the bra-ket formalism as being "bare objects" that have to be dressed into new observables $\tilde{\mathbf{A}}$ acting on $\mathcal{H}$ (or superoperators $\hat{\mathbf{A}}$ acting on $\hat{\mathcal{H}}$).

In fact we have a duality of frameworks for physical calculations (expectation values):

(i) On $\hat{\mathcal{H}}$ we must use dressed wave functions $\hat{\boldsymbol{\varphi}}$ to represent states and standard self-adjoint operators $\mathbf{A}$ (bare) for observables, $\langle\mathbf{A}\rangle=\mathrm{Tr}(\hat{\boldsymbol{\varphi}}^{\dagger}\mathbf{A}\hat{\boldsymbol{\varphi}})$. This corresponds to the rigorous form of the symmetric bra-ket notation.

(ii) On $\mathcal{H}$ we must use standard wave functions φ (bare) and dressed observables $\tilde{\mathbf{A}}$: $\langle\mathbf{A}\rangle=(\varphi|\tilde{\mathbf{A}}\varphi)_{\mathcal{H}}$.

This reasoning implies that the physical eigenvalues and eigenvectors are those of $\tilde{\mathbf{A}}$ on $\mathcal{H}$ (or $\hat{\mathbf{A}}$ on $\hat{\mathcal{H}}$).

We obtain the same result differently from the relation $\mathrm{Tr}(\tilde{\mathbf{A}}\mathbf{B})=\mathrm{Tr}(\mathbf{A}\tilde{\mathbf{B}})$ (Sec. VI). Let us assume that $\boldsymbol{\rho}$ is any statistical density operator and $\mathbf{A}$ an observable, usual quantum mechanics says that the expectation value of $\mathbf{A}$ is $\langle\mathbf{A}\rangle=\mathrm{Tr}(\boldsymbol{\rho}\mathbf{A})$. Our formalism says that we must modify this formula according to $\langle\mathbf{A}\rangle=\mathrm{Tr}(\boldsymbol{\rho}\tilde{\mathbf{A}})=\mathrm{Tr}(\tilde{\boldsymbol{\rho}}\mathbf{A})$. Moreover $\tilde{\boldsymbol{\rho}}$ also is a density operator (for a pure state φ, $\tilde{\boldsymbol{\rho}}=\hat{\boldsymbol{\varphi}}\hat{\boldsymbol{\varphi}}^{\dagger}$) and $\tilde{\mathbf{A}}$ is an observable. So, with purely mathematical arguments, we cannot choose between the modification of $\boldsymbol{\rho}$ and the modification of $\mathbf{A}$. But this is not true on the physical level, because the mapping $\boldsymbol{\rho}\rightarrow\tilde{\boldsymbol{\rho}}$ is not "onto:" $\tilde{\boldsymbol{\rho}}$ cannot be a pure state ($\hat{\boldsymbol{\varphi}}\hat{\boldsymbol{\varphi}}^{\dagger}$ is not a projector). If we say that the physical observable is $\mathbf{A}$, then the particle can never be in a pure state: this is a too strong modification. If we say that the physical observable is $\tilde{\mathbf{A}}$, of course the "bare" observable $\mathbf{A}$ is possibly modified, but all statistical properties of usual quantum mechanics are preserved.

The physical meaning of the dressing function: Let us start with an observable $\mathbf{A}$ and a density operator $\boldsymbol{\rho}$ defined with the bra-ket formalism. From the previous paragraph the usual formula for expectation value must be modified according to $\langle\mathbf{A}\rangle=\mathrm{Tr}(\boldsymbol{\rho}\tilde{\mathbf{A}})=\mathrm{Tr}(\tilde{\boldsymbol{\rho}}\mathbf{A})$, and the symmetry $\mathrm{Tr}(\boldsymbol{\rho}\tilde{\mathbf{A}})=\mathrm{Tr}(\tilde{\boldsymbol{\rho}}\mathbf{A})$ allows us to preserve the set of all possible densities (and then the Hilbert space structure) by choosing to change $\mathbf{A}$ in $\tilde{\mathbf{A}}$. However, this choice could be a simple technical trick that allows us to bypass a supplementary difficulty (the disappearance of pure states), while preventing us to see the real physical meaning of the transformation $\boldsymbol{\rho}\rightarrow\tilde{\boldsymbol{\rho}}$. So let us analyze what kind of physical process can produce this modification. In fact since $\tilde{\boldsymbol{\rho}}$ is a true density operator, there exists a unique well-known process: a *decoherence* one. Furthermore if the transformation $\boldsymbol{\rho}\rightarrow\tilde{\boldsymbol{\rho}}$ is real, it must be applied in all circumstances; this means that we are looking for an *intrinsic decoherence process*. Of course we cannot find the origin of such a phenomenon in the framework of nonrelativistic quantum mechanics, but an explanation exists in the framework of quantum field theory.

We know that any particle (quantum field) possesses at least one way to interact with other ones and this interaction is described by a coupling with another quantum field. So the complete quantum description of a free particle is in fact some intricate state that describes the degrees of freedom of the particle and the vacuum of some associated quantum field. Looking at the degrees of freedom of the particle (and only them) is obtained by some partial trace on the degrees of freedom of the quantum field, and this corresponds to a decoherence process. The decoherence is intrinsic in the sense that the coupling with an external quantum field is intrinsic. Moreover since field interactions always take place in space-time (and not in momentum space), we can understand that this decoherence effect essentially acts on the position operator and then on the states $|\vec{q}\rangle$. Of course this effect cannot be measured in the framework of nonrelativistic quantum mechanics, but this does not mean that the mathematical structure of the theory is not sensitive to this effect. This is exactly what we find through the dressing function ξ that introduces some length scale λ: λ can be as small as you want but it cannot be removed everywhere in the formalism. In fact the limit $\lambda \to 0$ is only possible for the computation of expectation values, because these quantities are in fact weighted integrals depending on the function ξ^2 (ξ^2 is similar to a point spread function). The limit $\lambda \to 0$ corresponds to $\xi^2 \to \delta$.

In conclusion, the dressing function ξ can be related to some decoherence effect that transforms bare operators into dressed ones; but thanks to the symmetry $\langle \mathbf{A} \rangle = \mathrm{Tr}(\boldsymbol{\rho}\widetilde{\mathbf{A}}) = \mathrm{Tr}(\tilde{\boldsymbol{\rho}}\mathbf{A})$ we can preserve the Hilbert space structure by modifying observables (dressed observables) rather than densities.

The following section analyzes the effect of the dressing function on the position operator.

IX. THE POSITION OPERATOR

A. The projection valued measure

The projection valued measure (pvm) associated with the quantum operator $\vec{\mathbf{Q}}$ of position is given by the family of orthogonal projectors $\{\chi_A(\vec{\mathbf{Q}})\}_{A \in \mathcal{B}(\mathbb{R}^3)}$ [where $\mathcal{B}(\mathbb{R}^3)$ is the family of Borel sets and χ_A is characteristic function of A].

Computing $(\hat{\boldsymbol{\varphi}}|\chi_A(\vec{\mathbf{Q}})\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \mathrm{Tr}(\hat{\boldsymbol{\varphi}}^\dagger \chi_A(\vec{\mathbf{Q}})\hat{\boldsymbol{\psi}})$ with the kernel method previously seen, we obtain

$$(\hat{\boldsymbol{\varphi}}|\chi_A(\vec{\mathbf{Q}})\hat{\boldsymbol{\psi}})_{\mathrm{HS}} = \int_{\mathbb{R}^3} d^3\vec{q}\ \varphi^*(\vec{q})\psi(\vec{q}) \int_{\mathbb{R}^3} d^3\vec{x}\ \chi_A(\vec{x})\xi(\vec{q}-\vec{x})^2. \tag{93}$$

We deduce that the operator $\widetilde{\chi_A(\vec{\mathbf{Q}})}$ is given by

$$\widetilde{\chi_A(\vec{\mathbf{Q}})} = F_A(\vec{\mathbf{Q}}),$$

$$F_A(\vec{q}) = \int_A d^3\vec{x}\ \xi(\vec{q}-\vec{x})^2. \tag{94}$$

But using Eqs. (93) and (79) we also find

$$(\hat{\boldsymbol{\varphi}}|\chi_A(\vec{\mathbf{Q}})\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = \int_{\mathbb{R}^3} d^3\vec{x}\ \chi_A(\vec{x})(\varphi|\boldsymbol{\Phi}_{\vec{x}}\boldsymbol{\Phi}_{\vec{x}}^\dagger\psi)_{\mathcal{H}}. \tag{95}$$

So

$$\widetilde{\chi_A(\vec{\mathbf{Q}})} = \int_A d^3\vec{x}\, \mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger. \tag{96}$$

Moreover $\chi_{\mathbf{R}^3}(\vec{\mathbf{Q}}) = \mathbf{1}$ and $(\hat{\boldsymbol{\varphi}}|\hat{\boldsymbol{\psi}})_{\mathcal{HS}} = (\varphi|\psi)_{\mathcal{H}}$, so

$$\widetilde{\mathbf{1}}_{\mathcal{H}} = \mathbf{1}_{\mathcal{H}} = \int_{\mathbb{R}^3} d^3\vec{x}\, \mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger. \tag{97}$$

We deduce that the family of operators $\{\widetilde{\chi_A(\vec{\mathbf{Q}})}\}_{A \in \mathcal{B}(\mathbb{R}^3)}$ corresponds to a positive operator valued measure (pov). This pov is used in different works of Prugovečki.[9,12] Moreover these studies show that the mathematical field ξ must be interpreted as the "proper wave function" of the particle (the particle cannot be pointlike). This idea was previously introduced by Landé[13] and Born.[14]

B. Related operators

From functional calculus, we can generalize the previous result to a real bounded or unbounded function of $\vec{\mathbf{Q}}$ as

$$\widetilde{F(\vec{\mathbf{Q}})} = \int_{\mathbb{R}^3} d^3\vec{x}\, F(\vec{x}) \mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger,$$

$$\widetilde{F(\vec{\mathbf{Q}})} = \widetilde{F}(\vec{\mathbf{Q}}),$$

$$\widetilde{F}(\vec{q}) = \int_{\mathbb{R}^3} d^3\vec{x}\, \xi(\vec{q} - \vec{x})^2 F(\vec{x}). \tag{98}$$

In the particular case $F(\vec{x}) = \vec{x}$, we have

$$\widetilde{F}(\vec{q}) = \int_{\mathbb{R}^3} d^3\vec{x}\, \xi(\vec{x})^2 (\vec{x} + \vec{q}). \tag{99}$$

Since ξ is a (normalized) radial function, ξ is even, so

$$\widetilde{F}(\vec{q}) = \vec{q}. \tag{100}$$

We deduce

$$\widetilde{\vec{\mathbf{Q}}} = \vec{\mathbf{Q}} = \int_{\mathbb{R}^3} d^3\vec{x}\, \vec{x} \mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger. \tag{101}$$

We see that the well-defined bounded operator $\mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger = \xi(\vec{\mathbf{Q}} - \vec{x})^2$ represents the symbolic expression $|\vec{x}\rangle\langle\vec{x}|$ used in the bra-ket formalism. Moreover the Eq. (101) shows that the observable $\vec{\mathbf{Q}}$ is unchanged in our framework.

Furthermore, the expression $|\vec{x}\rangle\langle\vec{x}| = \delta(\vec{\mathbf{Q}} - \vec{x})$ corresponds to the "density operator" (or the probability density). So we find that $\mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger = \delta_{\vec{x}}(\vec{\mathbf{Q}})$ is the mathematically well-defined observable (dressed operator) associated with the probability density. This interpretation is consistent with the fact that $\int_{\mathbb{R}^3} d^3\vec{x} (\varphi|\mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger \varphi)_{\mathcal{H}} = 1$ if φ is a normalized vector of $\mathcal{H}$. Moreover since $(\varphi|\mathbf{\Phi}_{\vec{x}} \mathbf{\Phi}_{\vec{x}}^\dagger \varphi)_{\mathcal{H}} = ||\mathbf{\Phi}_{\vec{x}}^\dagger(\varphi)||_{\mathcal{H}}^2 \leqslant ||\xi||_\infty^2$ [Eq. (4)], we see that the probability density is always bounded; then the particle cannot be localized "at the point $\vec{x}$." A punctual localization corresponds to the limit $\xi(\vec{x})^2 \to \delta(\vec{x})$.

Finally, if $(\varphi|\mathbf{\Phi}_{\vec{x}}\mathbf{\Phi}_{\vec{x}}^{\dagger}\varphi)_{\mathcal{H}}$ is the effective probability density, it is natural to say that $(\varphi|\mathbf{\Phi}_{\vec{x}}\varphi)_{\mathcal{H}}$ is the "wave function expectation value," and then we recover that $\mathbf{\Phi}_{\vec{x}}$ is the "wave function operator." We also remark that the expression of the density operator is formally the same in second quantization. Of course all this reasoning cannot be induced from usual quantum mechanical axioms.

X. THE MOMENTUM OPERATOR

We are interested in the family of operators $\{\chi_A(\vec{\mathbf{P}})\}_{A\in\mathcal{B}(\mathbb{R}^3)}$. Using Eq. (87) and the normalization of ξ we find

$$\widetilde{\chi_A(\vec{\mathbf{P}})} = \chi_A(\vec{\mathbf{P}}). \tag{102}$$

By extension, this equation remains valid for any Borel function f,

$$\widetilde{f(\vec{\mathbf{P}})} = f(\vec{\mathbf{P}}). \tag{103}$$

This last result can be reformulated on $\hat{\mathcal{H}}$ as

$$\forall\,\varphi\in\mathcal{H},\quad \widehat{f(\vec{\mathbf{P}})}(\hat{\varphi}) = f(\vec{\mathbf{P}})\cdot\hat{\varphi}. \tag{104}$$

Now using Eq. (33), we find that the unbounded kets $\hat{\boldsymbol{\phi}}_{\vec{k}}$ are the eigenstates of $\vec{\mathbf{P}}$,

$$\vec{\mathbf{P}}\hat{\boldsymbol{\phi}}_{\vec{k}} = \hbar\,\vec{k}\hat{\boldsymbol{\phi}}_{\vec{k}}. \tag{105}$$

Moreover if φ and ψ are two C^{∞} functions of rapid decrease $(\varphi|\,\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}\psi)$ is well-defined and we have

$$\int_{\mathbb{R}^3}\frac{d^3\vec{k}}{(2\pi)^3}(\varphi|\,\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}\psi) = (\varphi|\psi) \tag{106}$$

and

$$\int_{\mathbb{R}^3}\frac{d^3\vec{k}}{(2\pi)^3}\,\hbar\,\vec{k}(\varphi|\,\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}\psi) = (\varphi|\vec{\mathbf{P}}\psi). \tag{107}$$

In fact $\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}$ is the distribution $2\pi\hbar\,\delta(\vec{\mathbf{P}}-\hbar\vec{\mathbf{k}})$ corresponding to $|\vec{k}\rangle\langle\vec{k}|$. In Foias's approach[8] these distributions are the eigenoperators of $\vec{\mathbf{P}}$ and Eq. (106) represents the spectral decomposition of the space of C^{∞} functions of rapid decrease. But in our formalism the true eigenoperators (eigenstates) are the $\hat{\boldsymbol{\phi}}_{\vec{k}}$ in agreement with the bra-ket formalism. The dressing function ξ explains this difference. In terms of distributions, we can write $\hat{\boldsymbol{\phi}}_{\vec{k}}=2\pi\hbar\,\delta(\vec{\mathbf{P}}-\hbar\vec{\mathbf{k}})\xi(\vec{\mathbf{Q}})$ or $\hat{\boldsymbol{\phi}}_{\vec{k}}=|\vec{k}\rangle\langle\vec{k}|\,\xi(\vec{\mathbf{Q}})$ and then $\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}=2\pi\hbar\,\delta(\vec{\mathbf{P}}-\hbar\vec{\mathbf{k}})F(\vec{\mathbf{k}})$ with $F(\vec{\mathbf{k}})=\langle\vec{k}|\,\xi(\vec{\mathbf{Q}})^2\,|\vec{k}\rangle$. But the normalization of ξ gives $F(\vec{\mathbf{k}})=1$ and then $\hat{\boldsymbol{\phi}}_{\vec{k}}\hat{\boldsymbol{\phi}}_{\vec{k}}^{\dagger}=2\pi\hbar\,\delta(\vec{\mathbf{P}}-\hbar\vec{\mathbf{k}})$. So the dressing function allows us to define some "square root" of the distribution $\delta(\vec{\mathbf{P}}-\hbar\vec{\mathbf{k}})$ that gives the true eigenstates of $\vec{\mathbf{P}}$ corresponding to the bra-ket formula.

XI. LOCAL OBSERVABLES

We have shown that the probability density is $\boldsymbol{\rho}_{\vec{q}}=\mathbf{\Phi}_{\vec{q}}\mathbf{\Phi}_{\vec{q}}^{\dagger}$. Now we are interested in the current density.

Let us call $\mathcal{S}$ the dense subset of $\mathcal{H}$ of C^∞ functions of rapid decrease. The operators $\mathbf{\Phi}_{\vec{q}}$ and $\mathbf{\Phi}^\dagger_{\vec{q}}$ map $\mathcal{S}$ into $\mathcal{S}$, and the unbounded operators $\partial_{\vec{q}}\mathbf{\Phi}_{\vec{q}}$ and $\partial_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}$ are defined on $\mathcal{S}$,

$$-i\hbar\,\partial_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}} = \mathbf{\Phi}^\dagger_{\vec{q}}\vec{\mathbf{P}},$$

$$i\hbar\,\partial_{\vec{q}}\mathbf{\Phi}_{\vec{q}} = \vec{\mathbf{P}}\mathbf{\Phi}_{\vec{q}}. \tag{108}$$

Using Eq. (97) we deduce that

$$\vec{\mathbf{P}} = \int_{\mathbb{R}^3} d^3\vec{q}\;\mathbf{\Phi}_{\vec{q}}(-i\hbar\,\partial_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}) = \int_{\mathbb{R}^3} d^3\vec{q}(i\hbar\,\partial_{\vec{q}}\mathbf{\Phi}_{\vec{q}})\mathbf{\Phi}^\dagger_{\vec{q}}. \tag{109}$$

The same arguments show that

$$\vec{\mathbf{P}}^2 = \int_{\mathbb{R}^3} d^3\vec{q}\;\mathbf{\Phi}_{\vec{q}}(-\hbar^2\Delta_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}) = \int_{\mathbb{R}^3} d^3\vec{q}(-\hbar^2\Delta_{\vec{q}}\mathbf{\Phi}_{\vec{q}})\mathbf{\Phi}^\dagger_{\vec{q}}. \tag{110}$$

(where $\Delta_{\vec{q}}$ is the Laplacian), or in a symmetric form

$$\vec{\mathbf{P}}^2 = \int_{\mathbb{R}^3} d^3\vec{q}\;\hbar^2(\partial_{\vec{q}}\mathbf{\Phi}_{\vec{q}})\cdot(\partial_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}). \tag{111}$$

Moreover, starting from Eq. (109) and if we call m the mass of the particle, we can define the local (unbounded) observable of current density $\vec{\mathbf{J}}(\vec{q})$ as

$$\vec{\mathbf{J}}(\vec{q}) = \frac{i\hbar}{2m}((\partial_{\vec{q}}\mathbf{\Phi}_{\vec{q}})\mathbf{\Phi}^\dagger_{\vec{q}} - \mathbf{\Phi}_{\vec{q}}(\partial_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}})). \tag{112}$$

From Eq. (108) we find

$$\vec{\mathbf{J}}(\vec{q}) = \frac{1}{2m}(\mathbf{\Phi}_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}\vec{\mathbf{P}} + \vec{\mathbf{P}}\mathbf{\Phi}_{\vec{q}}\mathbf{\Phi}^\dagger_{\vec{q}}) \tag{113}$$

and

$$\vec{\mathbf{P}} = m\int_{\mathbb{R}^3} d^3\vec{q}\;\vec{\mathbf{J}}(\vec{q}). \tag{114}$$

We recover in formula (109) and (112) the expressions used in second quantization, $\mathbf{\Phi}^\dagger_{\vec{q}}$ being the wave function operator. This parallel leads us to study the integral $m\int d^3\vec{q}\;\vec{q}\wedge\vec{\mathbf{J}}(\vec{q})$ that usually gives the field angular momentum. Using Eqs. (113) and (101) we find

$$m\int_{\mathbb{R}^3} d^3\vec{q}\;\vec{q}\wedge\vec{\mathbf{J}}\cdot(\vec{q}) = \vec{\mathbf{Q}}\wedge\vec{\mathbf{P}} = \vec{\mathbf{L}}. \tag{115}$$

So the observable of angular momentum $\vec{\mathbf{L}}$ is really obtained as in second quantization. Moreover we can verify that $\vec{\mathbf{L}} = \vec{\mathbf{L}}$.

These definitions of local observables for one particle can be also found in Prugovečki's monograph,[9] but they are not build with this formalism.

XII. THE SCHRÖDINGER EQUATION

A. The evolution operator

The evolution with time of a vector $\varphi \in \mathcal{H}$ is given by $\varphi(t)=\mathbf{U}_t(\varphi_0)$ where $\mathbf{U}_t$ is the unitary operator $\mathbf{U}_t=\exp(-(i/\hbar)\mathbf{H}t)$, where $\mathbf{H}$ is the standard quantum Hamiltonian. So the evolution on $\mathcal{H}$ is naturally defined as $\hat{\boldsymbol{\varphi}}(t)=\widehat{\varphi(t)}$. This implies that $\mathbf{U}_t$ must be lifted up into the superunitary operator $\mathbf{U}_t^{(S)}$ acting on $\hat{\mathcal{H}}$ as defined in Sec. VII A 1

$$\hat{\boldsymbol{\varphi}}(t) = \mathbf{U}_t^{(S)}(\hat{\boldsymbol{\varphi}}_0) = \widehat{\mathbf{U}_t(\varphi_0)}. \tag{116}$$

Furthermore, the standard quantum Hamiltonian $\mathbf{H}$ is a physical observable, so following our general point of view $\mathbf{H}$ "has to be dressed" into $\widetilde{\mathbf{H}}$ that represents the "true" physical observable on $\mathcal{H}$. Consequently, if the true physical observable is $\widetilde{\mathbf{H}}$, we must use $\widetilde{\mathbf{H}}$ and not $\mathbf{H}$ into the definition of $\mathbf{U}_t$, so we define in fact

$$\mathbf{U}_t = \exp(-(i/\hbar)\widetilde{\mathbf{H}}t), \tag{117}$$

where $\mathbf{H}$ is the standard Hamiltonian; $\hat{\boldsymbol{\varphi}}(t)$ is defined as in Eq. (116). Now, from Eq. (70), we deduce that

$$\mathbf{U}_t^{(S)} = \exp(-(i/\hbar)\hat{\mathbf{H}}t). \tag{118}$$

B. The Schrödinger equation

On the dense subset $\mathcal{S}$ of functions of rapid decrease, Eqs. (116) and (118) lead to the Schrödinger equation,

$$i\hbar\frac{\partial\hat{\boldsymbol{\varphi}}}{\partial t} = \hat{\mathbf{H}}(\hat{\boldsymbol{\varphi}}) = \widetilde{H(\vec{\varphi})}. \tag{119}$$

C. The free particle

The standard Hamiltonian is $\mathbf{H}_0=\vec{\mathbf{P}}^2/2m$ and from Eq. (103) we know that $\widetilde{\mathbf{H}}_0=\mathbf{H}_0$ because $\mathbf{H}_0$ only depends on $\vec{\mathbf{P}}$. Moreover using Eqs. (110) and (111) we find

$$\widetilde{\mathbf{H}}_0 = \mathbf{H}_0 = \int_{\mathbb{R}^3} d^3\vec{q}\,\boldsymbol{\Phi}_{\vec{q}}\left(-\frac{\hbar^2}{2m}\Delta_{\vec{q}}\,\boldsymbol{\Phi}_{\vec{q}}^{\dagger}\right) = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} d^3\vec{q}(\partial_{\vec{q}}\,\boldsymbol{\Phi}_{\vec{q}})\cdot(\partial_{\vec{q}}\,\boldsymbol{\Phi}_{\vec{q}}^{\dagger}), \tag{120}$$

and we formally recover the expression used in second quantization.

Furthermore, always from Eq. (103), the superunitary operator $\mathbf{U}_t^{(S)}$ acts on $\hat{\mathcal{H}}$ as

$$\mathbf{U}_t^{(S)}(\hat{\boldsymbol{\varphi}}) = \mathbf{U}_t\hat{\boldsymbol{\varphi}},$$

$$\mathbf{U}_t = \exp((-i/\hbar)\mathbf{H}_0t). \tag{121}$$

Remark: The observables that generate the Galilei group $(\vec{\mathbf{Q}},\vec{\mathbf{P}},\vec{\mathbf{L}},\mathbf{H}_0)$ verify $\mathbf{A}=\mathbf{A}$. Then the dressing function ξ introduces no modification of quantum equations for the natural observables of the free particle.

XIII. CONCLUSION

This procedure shows how the definition of a dressing function ξ for a particle and the associated wave function operator $\boldsymbol{\Phi}_{\vec{q}}$, can be related to a rigorous development of the bra-ket formalism. Moreover we show that the new quantum framework contains "bare" and "dressed"

quantities and we find that local observables are now well defined, while these objects are singular in the usual quantum context. Finally the function ξ can be seen as a perturbative effect that "regularizes" the bra-ket formalism in such a way that all standard formula correspond to the limit $\xi^2 \to \delta$.

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Large-order behavior of the perturbation energies for the hydrogen atom in magnetic field

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Large-order behavior for the perturbation energies of the hydrogen atom in magnetic field is derived. By means of the dispersion relations, the large-order behavior of the series is determined by calculating the lifetime of the quasistationary states in an imaginary magnetic field. This problem is treated by means of the modified multidimensional WKB method. The asymptotic formula for the perturbation energies derived by Avron is generalized to the states with an arbitrary degeneracy. The first order correction to the resulting formula is also found. Thus, the multidimensional WKB method is for the first time explicitly carried out beyond the leading approximation. The analytical results are verified numerically and an excellent agreement between the two is found. The connection between our and conventional semiclassical approximation is also briefly discussed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168689]

I. INTRODUCTION

The problem of the hydrogen atom in the magnetic field is elementary but difficult and great deal of effort has been devoted to its solution over the years (see, e.g., Refs. 1–21and references given therein). Except for its own importance, it has been used as a relatively simple problem to answer some more general questions, as for example determination of the large-order behavior of the perturbation energies and related problem of the multidimensional WKB approximation,[1,3,4] summation of the divergent perturbation series,[2,7,21] application of the perturbation theory in the degenerate case,[8] determination of the lower bounds to the eigenvalues[9,14] and so on.

In this paper, we are interested in the problem of the hydrogen atom in magnetic field mainly from the point of view of the multidimensional WKB approximation and related problem of the asymptotic behavior of the corresponding divergent perturbation series. The multidimensional WKB method is important in many areas of physics ranging from the theory of chemical reactions to cosmology, for review see Ref. 22. Knowledge of the large-order behavior of the divergent perturbation series can be used in the summation of the series[1,2,21,23] and checking correctness of calculated perturbation energies. The latter application is especially important when treating the degenerate states where the perturbation theory is difficult to apply.

Schrödinger equation for the hydrogen atom in a constant magnetic field $\vec{B}=(0,0,B)$ with fixed nucleus and neglecting the spin effects reads

$$\left[-\frac{\nabla^2}{2}-\frac{1}{r}+\frac{BL_z}{2}+\frac{B^2}{8}(x^2+y^2)\right]\psi=E\psi, \tag{1}$$

where the atomic units are used. The Hamiltonian commutes with the projection of the angular momentum operator $\vec{L}$ onto the direction of the magnetic field and with the parity operator. In the following, we shall restrict ourselves to the states of the zero projection of the angular momentum onto the z axis and even parity.

The energy E has the following perturbation expansion:

$$E = \sum_{n=0}^{\infty} E_n \left(\frac{B^2}{8} \right)^n . \tag{2}$$

This perturbation series is divergent. The reason is that the energy E is not an analytic function in the vicinity of point $B=0$. This can be understood as follows. We consider analytic continuation of the energy E for complex magnetic fields $E=E(B^2)$. In the upper half of the complex plane we take $B^2=|B^2|e^{i\ \arg(B^2)}$ and in the lower half of the complex plane we take $B^2=|B^2|e^{-i\ \arg(B^2)}$, $\arg(B^2) \in (0,\pi)$. For real magnetic fields, Eq. (1) is solved with the boundary condition $\psi(\rho \to \infty) \to e^{-(B^2/8)^{1/2}\rho^2}$, where $\rho^2=x^2+y^2$. For complex magnetic fields, Eq. (1) is solved with the analytic continuation of this boundary condition. Now, approaching the value $-|B^2|$ from the upper half of the complex plane leads to the boundary condition $\psi(\rho \to \infty) \to e^{-i|B^2/8|^{1/2}\rho^2}$,while approaching this value from the lower half of the complex plane leads to the boundary condition $\psi(\rho \to \infty) \to e^{+i|B^2/8|^{1/2}\rho^2}$. These different boundary conditions yield different signs of the imaginary part of the energy $\Im[E(B^2)]$. Therefore, the energy E has for real negative values of B^2 the discontinuity $2i\Im[E(-|B^2|+i\varepsilon)]$, $\varepsilon>0$. Using Cauchy theorem one can show that the perturbation energies E_n are related to the imaginary part of the energy for the imaginary values of the magnetic fields via the dispersion relation[1,24–26]

$$E_n = \frac{(-1)^{n+1}(2N^2)^n}{\pi} \int_0^{\infty} \mathrm{d}\lambda \frac{\Im[E(\lambda)]}{\lambda^{n+1}}, \tag{3}$$

where a new coupling constant λ has been introduced via equation

$$\frac{B^2}{8} = -\frac{\lambda}{2N^2}. \tag{4}$$

Here, $N=1,2,3,\ldots$ denotes the principal quantum number of the hydrogen atom. The imaginary part of the energy is one-half of the inverse lifetime of the quasistationary states in the potential in Eq. (1) with the imaginary magnetic field B.

It is seen from Eq. (3) that the behavior of the perturbation energies E_n for very large n is given by the lifetime of the quasistationary states for small values of the coupling constant λ. Thus, provided we are able to calculate this lifetime, Eq. (3) enables precise determination of the degree of the divergence of the series (2).

Expression for the imaginary part of the energy can be derived as follows. First, since Eq. (1) has an axial symmetry we introduce the cylindric coordinates $x=\rho\cos\varphi$, $y=\rho\sin\varphi$, $z=z$. Since the states with the zero projection of the angular momentum are independent of the coordinate φ, Eq. (1) reads

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2} \right] \psi = [V(\rho,z) - 2E]\psi, \tag{5}$$

where

$$V(\rho,z) = -\frac{2}{(\rho^2+z^2)^{1/2}} - \frac{\lambda}{N^2}\rho^2. \tag{6}$$

Equation (5) is solved with the boundary condition $\psi(\rho \to \infty) \to e^{-i\lambda^{1/2}\rho^2/N}$. Further, we multiply Eq. (5) by $\rho\psi^*$. We take complex conjugate of Eq. (5) and multiply it by $\rho\psi$. Then we subtract the two equations and integrate the resulting equation over the whole space, i.e., over z from $-\infty$ to ∞ and over ρ from 0 to ∞. Finally, we integrate this equation by parts and obtain the time-independent version of the continuity equation for the probability density

$$\Im[E] = \frac{J}{2\langle\psi|\psi\rangle}, \tag{7}$$

where the probability flux J in the ρ direction equals

$$J = -\frac{1}{2i}\int_{-\infty}^{\infty} \mathrm{d}z \lim_{\rho\to\infty}\rho\left[\psi^*\frac{\partial}{\partial\rho}\psi - \psi\frac{\partial}{\partial\rho}\psi^*\right] \tag{8}$$

and the norm of the wave function reads

$$\langle\psi|\psi\rangle = \int_0^{\infty}\mathrm{d}\rho\int_{-\infty}^{\infty}\mathrm{d}z\,\rho|\psi|^2. \tag{9}$$

To calculate the imaginary part of the energy from Eq. (7) we proceed as follows.[24] Inside the potential well, we approximate the wave function by means of the Rayleigh-Schrödinger perturbation theory (RSPT). Since the dominant contribution to the norm of the wave function describing the quasistationary state comes from the interior of the well we replace the exact wave function in the denominator of Eq. (7) by the perturbation wave function. In the tunneling region and outside the potential well we approximate the wave function by the WKB wave function. Since the dominant contribution to the probability current comes from the tunneling, classically forbidden region we replace the exact wave function in Eq. (8) by the WKB wave function. The same normalization of the RSPT and the WKB wave functions is guaranteed by the asymptotic matching of these functions in the overlap region of their mutual validity.

The main obstacle in carrying out the program described above is the construction of the WKB wave function. The standard formulation of the WKB approximation as applied to Eq. (5) leads to the nonseparable nonlinear partial differential equation that is difficult to solve.

The simplification of the problem used here comes out from the fact that the tunneling of the particle takes place in the neighborhood of the line $z=0$, see Eq. (5). Consequently, we do not need to know the wave function in all space, but only in the neighborhood of this line. The situation is further greatly simplified by the fact that the minimum of the potential is the straight line (compare it with the case of the curved lines[27,28]). This simplification was for the first time realized in Ref. 29 for the problem of the coupled oscillators and later used in Ref. 1 to derive the imaginary part of the energy in Eq. (5) at the leading approximation. However, it seems that the full content of the simplification was not appreciated so far. Indeed, none from the multidimensional WKB calculations for the straight escape paths performed so far[1,4,29,30] shows how to extend the calculation beyond the leading approximation.

In this paper we show how the WKB wave function for Eq. (5) and the outgoing probability flux can be obtained to the desired accuracy. Our method is not bound to the problem considered here and with appropriate modifications it can be extended to all problems involving multidimensional tunneling along the straight escape paths.

The paper is organized as follows. In Sec. II the modified multidimensional WKB method is suggested and used to calculate the outgoing probability flux, Eq. (8), with accuracy to the order $\lambda^{1/2}$. In Sec. III the calculation of the perturbation energies in Eq. (2) is described. The perturbation wave function is used to calculate the norm of the wave function (9). In Sec. IV the results of the preceding two sections are put together and inserted into Eq. (3) to get the asymptotics of the perturbation energies. Numerical verification of the derived formula is made and an excellent agreement between the analytical and numerical calculation is found. In the Conclusions the perspectives of further applications of the proposed WKB approximation are briefly outlined. In the Appendix the connection between the suggested and conventional WKB method is discussed.

II. WKB METHOD

There are two facts stressed in the next two paragraphs that simplify the calculations enormously and that were not explicitly realized so far. The first one is the approximation of the wave function in the coordinate z by the wave function of the anharmonic oscillator, Eq. (11). The second one is the scaling in the coordinate ρ, Eq. (15).

A. Approximation of the wave function in the transversal direction

First, in the vicinity of the ρ axis the potential $V(\rho,z)$ given by Eq. (6) can be expanded as

$$V(\rho,z) = V_0(\rho) + V_2(\rho)z^2 + V_4(\rho)z^4 + \cdots . \tag{10}$$

Then, the wave function of the particle in the direction transversal to tunneling can be written as

$$\psi(\rho,z) = e^{f(\rho)+h(\rho)z^2+q(\rho)z^4+\cdots} . \tag{11}$$

Physically, this says nothing else than close to the minimum of the potential in the direction perpendicular to tunneling we can approximate the exact wave function by the wave function of the harmonic oscillator. This approximation can be further improved by considering anharmonic terms.

Inserting the expansions (10) and (11) into Eq. (5) and comparing the terms of the same order of z we get

$$f'(\rho)^2 + f''(\rho) + \frac{f'(\rho)}{\rho} + 2h(\rho) = -2E - \frac{\lambda}{N^2}\rho^2 - \frac{2}{\rho} \tag{12}$$

at the zeroth order,

$$2f'(\rho)h'(\rho) + h''(\rho) + \frac{h'(\rho)}{\rho} + 4h(\rho)^2 + 12q(\rho) = \frac{1}{\rho^3} \tag{13}$$

at the second order and

$$2f'(\rho)q'(\rho) + h'(\rho)^2 + q''(\rho) + \frac{q'(\rho)}{\rho} + 16h(\rho)q(\rho) = -\frac{3}{4\rho^5} \tag{14}$$

at the fourth order of z. Here, the prime denotes the differentiation with respect to ρ.

B. Approximation of the wave function in the longitudinal direction

Second, in the direction of the tunneling we approximate the wave function as follows. In the classically forbidden region the terms $-2E_0$ and $-(\lambda/N^2)\rho^2$ are of the same order of magnitude.[31] To make these terms of the same order in λ we make the scaling in the coordinate ρ,

$$\rho = \lambda^{-1/2}u, \tag{15}$$

and expand the real part of the energy in the series (2). Equations (12)–(14) then read

$$\lambda\left(f'(u)^2 + f''(u) + \frac{f'(u)}{u}\right) + 2h = \frac{1-u^2}{N^2} - \frac{2\lambda^{1/2}}{u} - 2\sum_{n=1}^{\infty} E_n\left(-\frac{\lambda}{2N^2}\right)^n, \tag{16}$$

$$\lambda\left(2f'(u)h'(u) + h''(u) + \frac{h'(u)}{u}\right) + 4h(u)^2 + 12q(u) = \frac{\lambda^{3/2}}{u^3} \tag{17}$$

and

$$\lambda\left(2f'(u)q'(u)+h'(u)^2+q''(u)+\frac{q'(u)}{u}\right)+16h(u)q(u)=-\frac{3\lambda^{5/2}}{4u^5}, \tag{18}$$

where the prime denotes now differentiation with respect to u. To get a clue how to expand the functions $f(u)$, $h(u)$, and $q(u)$ in the powers of $\lambda^{1/2}$ we use the fact that for $u\to 0$ we must recover the wave function of the hydrogen atom. For example, it reads for the ground state

$$\psi_{1s}=e^{-r}=e^{-\sqrt{\rho^2+z^2}}=e^{-\rho-z^2/(2\rho)-z^4/(8\rho^3)+\cdots}=e^{-u/\lambda^{1/2}-\lambda^{1/2}z^2/(2u)-\lambda^{3/2}z^4/(8u^3)+\cdots}. \tag{19}$$

Therefore we expand the functions $f(u)$, $h(u)$, and $q(u)$ as follows:

$$f(u)=\frac{f_0(u)}{\lambda^{1/2}}+f_1(u)+f_2(u)\lambda^{1/2}+\cdots, \tag{20}$$

$$h(u)=h_0(u)\lambda^{1/2}+h_1(u)\lambda+\cdots, \tag{21}$$

and

$$q(u)=q_0(u)\lambda^{3/2}+\cdots. \tag{22}$$

C. Equations for the WKB wave function

Comparing the terms of the order λ^0 in Eq. (16), of the order λ in Eq. (17) and of the order $\lambda^{1/2}$ in Eq. (16) we get equations for the functions $f_0(u)$, $h_0(u)$, and $f_1(u)$,

$$f_0'(u)=\frac{\pm\sqrt{1-u^2}}{N}, \tag{23}$$

$$2f_0'(u)h_0'(u)+4[h_0(u)]^2=0 \tag{24}$$

and

$$2f_0'(u)f_1'(u)+f_0''(u)+\frac{1}{u}f_0'(u)+2h_0(u)=-\frac{2}{u}, \tag{25}$$

respectively. Since we want to calculate the imaginary part of the energy beyond the leading approximation, we have to determine also the functions $q_0(u)$, $h_1(u)$, and $f_2(u)$. Comparing the terms of the order λ^2 in Eq. (18), of the order $\lambda^{3/2}$ in Eq. (17) and of the order λ in Eq. (16) we get equations for the functions $q_0(u)$, $h_1(u)$, and $f_2(u)$,

$$2f_0'(u)q_0'(u)+[h_0'(u)]^2+16h_0(u)q_0(u)=0, \tag{26}$$

$$2f_0'(u)h_1'(u)+2f_1'(u)h_0'(u)+h_0''(u)+\frac{1}{u}h_0'(u)+8h_0(u)h_1(u)+12q_0(u)=\frac{1}{u^3}, \tag{27}$$

and

$$2f_0'(u)f_2'(u)+[f_1'(u)]^2+f_1''(u)+\frac{1}{u}f_1'(u)+2h_1(u)=\frac{E_1}{N^2}, \tag{28}$$

respectively. The solution of the above equations is determined uniquely by requirement that for u going to zero, the WKB wave function must match the bound state function. This will be discussed in detail below. Before actual solution of the equations given above, let us show that the proposed approximation to the wave function yields systematic approximation to the outgoing probability flux.

D. Approximation to the outgoing probability flux

To calculate the outgoing probability flux from Eq. (8) we need to know the behavior of the wave function for large ρ. Integration of Eq. (25) yields

$$f_1(u) = -\tfrac{1}{2}\ln(uf_0'(u)) + F_1(u), \tag{29}$$

where the second term is given as

$$F_1(u) = -\frac{N}{2}\ln\frac{1+(1-u^2)^{1/2}}{1-(1-u^2)^{1/2}} + \frac{1}{2}\ln(h_0(u)) - A_1. \tag{30}$$

The integration constant A_1 is determined from the requirement of the matching of the WKB and bound state functions. Here, we took the solution of Eq. (23) with the minus sign, see discussion after Eq. (37) below.

Thus, the behavior of the wave function (11) for large ρ is given as

$$\psi(\rho,z) = \frac{\exp\{f_0(\rho)/\lambda^{1/2} + F_1(\rho) + \lambda^{1/2}f_2(\rho) + \cdots + h(\rho)z^2 + q(\rho)z^4 + \cdots\}}{[\rho f_0'(\rho)]^{1/2}}, \tag{31}$$

where we inserted the expansion (20). Differentiation of the function (31) with respect to ρ yields

$$\frac{\partial\psi(\rho,z)}{\partial\rho} \sim \frac{[f_0'(\rho)]^{1/2}}{[\rho\lambda]^{1/2}}\exp\left\{\frac{f_0(\rho)}{\lambda^{1/2}} + F_1(\rho) + \lambda^{1/2}f_2(\rho) + + h(\rho)z^2 + q(\rho)z^4 + \cdots\right\}. \tag{32}$$

Differentiation of the terms $F_1(\rho)$, $\lambda^{(1/2)}f_2(\rho)$ and so on yields the contribution to the probability flux that vanishes for ρ approaching infinity. For large ρ the particle moves in the classically allowed region and $f_0'(\rho)$ is purely imaginary, see Eq. (23). Thus it follows from Eqs. (8), (31), and (32) that the nonvanishing contribution to the probability flux for ρ going to infinity is given as[29,30]

$$\begin{aligned} J = {} & \frac{1}{\lambda^{1/2}}\exp\{2\Re[f_0(u\to\infty)/\lambda^{1/2} + F_1(u\to\infty) + \lambda^{1/2}f_2(u\to\infty) + \cdots]\} \\ & \times\int_{-\infty}^{\infty} dz\,\exp\{2z^2\Re[\lambda^{1/2}h_0(u\to\infty) + \lambda h_1(u\to\infty)] + 2z^4\Re[\lambda^{3/2}q_0(u\to\infty)] + \cdots\}, \end{aligned} \tag{33}$$

where $\Re$ denotes the real part. Here we inserted the expansions (21) and (22) and made the substitution (15). This can be done since the real parts of the functions $f_i(u)$, $h_i(u)$ and so on, goes to the constants for u going to infinity. Therefore, it does not matter if we calculate it in the variable u or ρ.

The integration over the transversal direction can be performed easily. Expanding the above equation in the powers of $\lambda^{1/2}$ as

$$\begin{aligned} J = {} & \frac{1}{\lambda^{1/2}}\exp\{2\Re[f_0(u\to\infty)/\lambda^{1/2} + F_1(u\to\infty)]\}(1 + 2\lambda^{1/2}\Re[f_2(u\to\infty)] + \cdots) \\ & \times\int_{-\infty}^{\infty} dz\,\exp\{2z^2\Re[\lambda^{1/2}h_0(u\to\infty)]\}(1 + 2z^2\lambda\Re[h_1(u\to\infty)] + 2z^4\lambda^{3/2}\Re[q_0(u\to\infty)] + \cdots) \end{aligned} \tag{34}$$

we are left with the Gaussian integrals. The outgoing probability flux accurate up to the first order of $\lambda^{1/2}$ then reads

$$J = \exp\{2\Re[f_0(u \to \infty)/\lambda^{1/2} + F_1(u \to \infty)]\} \frac{\sqrt{\pi}}{\lambda^{3/4}(\Re[-2h_0(u \to \infty)])^{1/2}} (1 + \lambda^{1/2} R_1 + \lambda R_2 + \cdots), \tag{35}$$

where the first correction coefficient R_1 equals

$$R_1 = 2\Re[f_2(u \to \infty)] + \frac{\Re[h_1(u \to \infty)]}{\Re[-2h_0(u \to \infty)]} + \frac{3\Re[q_0(u \to \infty)]}{2(\Re[-2h_0(u \to \infty)])^2}. \tag{36}$$

It is clear from the above equations that the suggested approximation of the wave function provides systematic approximation to the outgoing probability flux in the form of the series in powers of $\lambda^{1/2}$. It is well known that the WKB approximation fails in the vicinity of the turning point corresponding here to $u=1$, see Eq. (23). There is a number of papers dealing with the approximation of the wave function in the neighborhood of the turning points, see, e.g., Refs. 32–36. It is clear from the above equations that what we actually need is the behavior of the WKB approximation for u going to infinity. The proper normalization of the WKB wave function is guaranteed by matching it to the bound state function for u going to zero. In this region the WKB wave function is valid as an asymptotic expansion. Therefore, we do not have to care at all about the divergence of the WKB approximation at the turning point, see also Ref. 31.

E. Solution of equations

1. Boundary conditions

As becomes apparent during the calculation it is possible and advantageous to normalize the bound state wave function in such a way that it behaves in the overlap region as

$$\psi_0(\rho \to \infty, z \to 0) \sim e^{-\rho/N - z^2/(2N\rho) - z^4/(8N\rho^3) - \cdots} \rho^{N-1} \left(1 + \frac{Cz^2}{\rho^2} + \cdots\right), \tag{37}$$

where C is a constant depending on the form of the bound state wave function and it will be precisely determined in Sec. III. It is seen from Eq. (19) that for the ground state

$$C_{1s} = 0. \tag{38}$$

The solution of Eqs. (23)–(28) is determined uniquely by the requirement that the WKB wave function has this behavior for small u.

2. Calculation of the first approximation

Since for $u>1$ the integrand in Eq. (23) is purely imaginary we can stop the integration at the turning point $u=1$. We start the integration at the point $u=0$ and take the minus sign in Eq. (23) to get the first term in the argument of exponential function on the right-hand side of Eq. (37) for small u

$$\Re[f_0(u \to \infty)] = -\int_0^1 du \frac{\sqrt{1-u^2}}{N} = -\frac{\pi}{4N}. \tag{39}$$

Equation (24) is nonlinear first order differential equation whose solution reads

$$h_0(u) = -\frac{1}{2N \arcsin u}, \tag{40}$$

where the integration constant was set to zero to get the second term in the argument of exponential function on the right-hand side of Eq. (37) for small u. We note that for $u>1$, the function $\arcsin(u)$ is complex and two-valued with the branch point at $u=1$,

$$\arcsin(u) = \frac{\pi}{2} + i \ln(u \pm \sqrt{u^2 - 1}). \tag{41}$$

These two values correspond to the incoming (+) and outgoing (−) waves. Taking the solution with the minus sign we get

$$\Re[h_0(u \to \infty)] = h_0(u = 1) = -\frac{1}{N\pi}. \tag{42}$$

For u going to zero the function $f_1(u)$ given by Eq. (29) behaves as

$$f_1(u \to 0) \to -\frac{2N+1}{2} \ln 2 + (N-1)\ln(u) - A_1 = -\frac{2N+1}{2} \ln 2 + \frac{N-1}{2} \ln \lambda + (N-1)\ln \rho - A_1, \tag{43}$$

where we substituted for u from Eq. (15). To get the leading power term in Eq. (37) we obviously must set

$$A_1 = -\frac{2N+1}{2} \ln 2 + \frac{N-1}{2} \ln \lambda. \tag{44}$$

Using Eqs. (40) and (41) in Eq. (30) we get

$$\Re[F_1(u \to \infty)] = -\frac{1}{2} \ln N\pi - A_1 = -\frac{1}{2} \ln N\pi - \frac{N-1}{2} \ln \lambda + \frac{2N+1}{2} \ln 2. \tag{45}$$

Now we are ready to calculate the outgoing probability flux at the leading order of $\lambda^{1/2}$ from Eq. (35). By inserting Eqs. (39), (42), and (45) into Eq. (35) we obtain

$$J = \frac{2^{2N+1}}{\lambda^{N-1/4}(2N)^{1/2}} e^{-\pi/(2N\lambda^{1/2})}(1 + R_1\lambda^{1/2} + \cdots). \tag{46}$$

3. Calculation of the second approximation

To calculate the coefficient R_1 we must determine the functions $q_0(u)$, $h_1(u)$, and $f_2(u)$.

Equation (26) is inhomogenous linear differential equation for $q_0(u)$. We first solve the homogenous part and then use the variation of a constant. We obtain the function $q_0(u)$ as

$$q_0(u) = [h_0(u)]^4 Q_0(u), \tag{47}$$

where

$$Q_0(u) = N^3 \frac{2u}{(1-u^2)^{1/2}}. \tag{48}$$

The integration constant was set to zero to get the third term in the argument of the exponential function on the right-hand side of Eq. (37). By virtue of Eqs. (42) and (48) the real part of the function $q_0(u)$ vanishes for u going to infinity

$$\Re[q_0(u \to \infty)] = \Re[Q_0(u \to \infty)] = 0. \tag{49}$$

The function $h_1(u)$ is obtained similarly as the function $q_0(u)$,

$$h_1(u) = [h_0(u)]^2 H_1(u), \tag{50}$$

where for the function $H_1(u)$ we obtain using Eqs. (24), (25), (47), (48) and integrating by parts

$$H_1'(u) = -\frac{2}{[f_0'(u)]^3} + \frac{1}{2u^3 f_0'(u)[h_0(u)]^2} + \left(3Q_0(u)h_0(u) + \frac{1}{[f_0'(u)]^2}\right)'. \tag{51}$$

Inserting now the explicit form of the functions $f_0'(u)$ and $h_0(u)$, Eqs. (23) and (40), the integration of the last equation yields

$$H_1(u) = 3Q_0(u)h_0(u) + \frac{1}{[f_0'(u)]^2} + 2N^3\left[\frac{1}{(1-u^2)^{1/2}} + \frac{(1-u^2)^{1/2}}{2u^2}\arcsin^2(u) + \frac{\arcsin(u)}{u} - \int_0^u \frac{\arcsin^2(t)}{t(1-t^2)^{1/2}}dt\right] - A_2. \tag{52}$$

To determine the integration constant A_2 we note that for u going to zero we get from Eqs. (48), (50), and (52),

$$\lambda h_1(u \to 0) \to \frac{\lambda}{(2N)^2u^2}(5N^3 - 2N^2 - A_2) = \frac{1}{(2N)^2\rho^2}(5N^3 - 2N^2 - A_2), \tag{53}$$

where we substituted for u from Eq. (15). To get the last term on the right-hand side of Eq. (37), we obviously must set

$$A_2 = 4N^2\left(\frac{5N-2}{4} - C\right). \tag{54}$$

The real part of the asymptotics of the function $h_1(u)$ is by virtue of Eqs. (42) and (48) given as

$$\Re[h_1(u \to \infty)] = h_0(u=1)\Re[H_1(u \to \infty)] = h_0(u=1)\left\{-A_2 - 2N^3\Re\left[\int_0^u \frac{\arcsin^2(t)}{t(1-t^2)^{1/2}}\mathrm{d}t\right]\right\}. \tag{55}$$

Finally, the integration of Eq. (28) is substantially simplified by the identity

$$\frac{f_1''(u)}{2f_0'(u)} = \left(\frac{f_1'(u)}{2f_0'(u)}\right)' + \frac{f_1'(u)f_0''(u)}{2[f_0'(u)]^2}. \tag{56}$$

We note that this identity substantially simplifies the calculation of the higher orders of the WKB approximation in general. Further, it is useful to separate the part of $f_2(u)$ denoted as $F_2(u)$ that depends on the function $h_0(u)$ and the part denoted as $\phi_2(u)$ that is independent of it,

$$f_2(u) = F_2(u) + \phi_2(u). \tag{57}$$

The function $\phi_2(u)$ is integrated easily without any tricks. The real part of its asymptotics is given as

$$\Re[\phi_2(u \to \infty)] = -\frac{E_1\pi}{4N}. \tag{58}$$

For the part $F_2(u)$ we find using Eqs. (24), (25), and (51) and integrating by parts

$$F_2'(u) = -\frac{1}{4u^3 f_0'(u)h_0(u)} + \left(\frac{H_1(u)h_0(u)}{2} - \frac{3Q_0(u)h_0(u)^2}{4}\right)'. \tag{59}$$

The real part of the asymptotics of the function $F_2(u)$ is by virtue of Eqs. (23), (40), and (48) given as

$$\Re[F_2(u\to\infty)]=h_0(u=1)\frac{H_1(u\to\infty)}{2}+\lim_{u\to\infty}\frac{N^2}{4}\left\{\frac{(1-u^2)^{1/2}\arcsin(u)}{u^2}+\frac{1}{u}-\Re\left[\int_0^u\frac{\mathrm{d}t\arcsin(t)}{t(1-t^2)^{1/2}}\right]\right\}. \tag{60}$$

By inserting Eqs. (49), (54), (55), (57), (58), and (60) into Eq. (36) we obtain

$$R_1=-\frac{E_1\pi}{2N}+\frac{A_2}{2N\pi}+\frac{N^2}{2\pi}\int_0^1\frac{\arcsin^2(u)-\pi\arcsin(u)}{u(1-u^2)^{1/2}}\mathrm{d}u=-\frac{E_1\pi}{2N}+\frac{2N}{\pi}\left(\frac{5N-2}{4}-C\right)-N^2\frac{7\zeta(3)}{4\pi}, \tag{61}$$

where $\zeta(z)$ denotes Riemann zeta function. The first order perturbation energy E_1 as well as the constant C will be determined in the next section.

III. PERTURBATION METHOD

To calculate the norm of the wave function in Eq. (9) accurate up to the first order in $\lambda^{1/2}$ it is sufficient to take the wave function of the unperturbed hydrogen atom. For the excited states, the unperturbed wave function is degenerate and we must use the first order perturbation theory to determine the correct linear combination of the unperturbed functions. Since we need to calculate the perturbation energies up to the large order for numerical verification of the analytic formulas we describe the application of the perturbation method to Eq. (1) in greater detail.

The method described here is an extension of the method suggested in Ref. 29 for the coupled oscillators. The alternative way of calculation of the perturbation energies for the problem considered here is described for example in Ref. 10 for the ground state energy and in Refs. 8 and 37 for the excited states.

A. Derivation of difference equations

We transform Eq. (1) into the spherical coordinates, $x=r\sin\theta\cos\varphi$, $y=r\sin\theta\sin\varphi$ and $z=r\cos\theta$, multiply it by r, write the wave function in the form

$$\psi(r,\theta)=e^{-r/n}\sum_{k=0}\varphi_k(r,\theta)\left(\frac{B^2}{8}\right)^k, \tag{62}$$

insert the expansion (2) for the energy and compare the terms of the same order of $(B^2/8)$. Equation (1) then reads

$$\left\{-\frac{r}{2}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{\partial^2}{\partial\theta^2}\right)\right]+\frac{r}{N}\frac{\partial}{\partial r}+\frac{1-N}{N}\right\}\varphi_k+r^3\sin^2\theta\varphi_{k-1}=r\sum_{l=1}^{k}E_l\varphi_{k-l}. \tag{63}$$

Further, we expand the perturbation functions φ_k in the form of the double series

$$\varphi_k=\sum_{i=0}\sum_{j=0}g_{i,j}^{(k)}r^i\sin^{2j}\theta, \tag{64}$$

where the upper bounds of the summations will be determined later, insert it into Eq. (63) and compare the terms of the same order of r and $\sin^2\theta$. As a result we get the difference equations for the coefficients $g_{i,j}^{(k)}$,

$$-\frac{1}{2}g^{(k)}_{i+1,j}[(i+1)(i+2)-2j(j+1)]-2(j+1)^2 g^{(k)}_{i+1,j+1}+\frac{i+1-N}{N}g^{(k)}_{i,j}+g^{(k-1)}_{i-3,j-1}=\sum_{l=1}^{k}E_l g^{(k-l)}_{i-1,j}. \tag{65}$$

These equations can be used for the calculation of the perturbation energies as follows. The calculation for the ground state is not difficult and does not differ from that described in Refs. 2 and 29. In the first order of the perturbation theory we get

$$E_1^{1s}=2. \tag{66}$$

For the excited states, the situation is a bit more complicated because the unperturbed state is degenerate. We describe calculation of the perturbation energies for the $3s$-$3d$ state in detail.

B. Solution of equations for the 3*s*-3*d* state

The unperturbed wave function of the $3s$-$3d$ state reads

$$\psi_{3s\text{-}3d}=s\psi_{3s}+d\psi_{3d}, \tag{67}$$

where s and d denotes the coefficients of the linear combination and the unperturbed wave functions of $3s$ and $3d$ states read

$$\psi_{3s}=e^{-r/3}\left(1-\frac{2r}{3}+\frac{2r^2}{27}\right) \tag{68}$$

and

$$\psi_{3d}=e^{-r/3}r^2(1-3\cos^2\theta), \tag{69}$$

respectively. Thus, we set $g^{(0)}_{0,0}=s$, $g^{(0)}_{1,0}=-2s/3$, $g^{(0)}_{2,0}=(2s/27)-2d$, $g^{(0)}_{2,1}=3d$, and $g^{(0)}_{i,j}=0$ otherwise. We express the third term in Eq. (65), $g^{(k)}_{i,j}$, set $g^{(k)}_{i,k+2}=0$, $g^{(k)}_{3k+3,j}=0$ and solve Eq. (65) with $N=3$ for k starting from 1. For given k we solve Eq. (65) for j descending from $k+1$ to 0 and for i descending from $3k+2$ to 3. For $i=2$ the third term in Eq. (65) vanishes. Therefore, for $i=2$ we solve Eq. (65) for j descending from k to 1 to get equations for the coefficients $g^{(k)}_{2,k-1}$. For $i=2$ and $j=0$ we get the equation for the perturbation energies E_k. Finally, for i descending from 1 to 0 we again express $g^{(k)}_{i,j}$ and solve Eqs. (65) for j descending from $k+1$ to 0. The perturbation coefficients calculated in this way agree with those given in Ref. 8.

For the sake of transparency we illustrate this procedure of solving Eqs. (65) for $i=2$ on the first two orders of the perturbation theory. In the first order, $k=1$, we get for $j=1$,

$$30s+(1620-27E_1)d=0 \tag{70}$$

and for $j=0$

$$(72-2E_1/3)s+18E_1 d=0. \tag{71}$$

From Eq. (70) we get

$$d=\frac{10s}{9(E_1-60)}. \tag{72}$$

By inserting this value into Eq. (71) we obtain a quadratic equation for E_1. Two roots of this equation equal

$$(E_1^{3s\text{-}3d})_{1,2}=99\pm 9\sqrt{41}. \tag{73}$$

In the second order of the perturbation theory, $k=2$, we get for $j=2$,

$$g_{2,2}^{(1)} = 0, \tag{74}$$

for $j=1$,

$$766\,908s + 15\,549\,570d - (5616s + 167\,670d)E_1 + 1701/2E_1^2 d - 405g_{2,0}^{(1)} + (9E_1 - 810)g_{2,1}^{(1)} + 27E_2 d = 0 \tag{75}$$

and finally for $j=0$,

$$1\,308\,798s + 1\,296\,4536d - (14\,310s + 29\,160d)E_1 + (57s - 567d)E_1^2 + (9E_1 - 972)g_{2,0}^{(1)} - 648g_{2,1}^{(1)} + (2s/3 - 18d)E_2 = 0. \tag{76}$$

We solve Eq. (75) to get the coefficient $g_{2,1}^{(1)}$ and insert it into Eq. (76) to get E_2. We note that the values of the coefficients s and $g_{2,0}^{(1)}$ are not given by the perturbation theory. We also note that Eq. (76) for E_2 is linear. It means that after splitting of the degenerate energy level at the first order, there is only one solution for given E_1 for higher order perturbation energies E_2, E_3, and so on.

Since the coefficient s is not given by the perturbation theory, it can be used to normalize the bound state function to behave as in Eq. (37) for large ρ and small z. The function (67) behaves in this region as

$$\psi_{3s\text{-}3d} \sim e^{-\rho/3 - z^2/(6\rho)}\rho^2\left\{\frac{2s}{27} + d + \frac{z^2}{\rho^2}\left(\frac{2s}{27} - 2d\right) + \cdots\right\}. \tag{77}$$

It is seen that to get required behavior (37) we must set

$$\frac{2s}{27} + d = 1 \tag{78}$$

and that the constant C in Eq. (37) equals

$$C_{3s\text{-}3d} = \frac{2s}{27} - 2d. \tag{79}$$

C. Solution of equations for the state 5*s*-5*d*-5*g*

Only slight modifications of the above procedure are necessary for the $5s$-$5d$-$5g$ state. The unperturbed wave function in this case equals

$$\psi_{5s\text{-}5d\text{-}5g} = \mathrm{s}\psi_{5s} + \mathrm{d}\psi_{5d} + g\psi_{5g}, \tag{80}$$

where the wave functions of the $5s$, $5d$, and $5g$ states read

$$\psi_{5s} = e^{-r/5}\left(1 - \frac{4r}{5} + \frac{4r^2}{25} - \frac{4r^3}{375} + \frac{2r^4}{9375}\right), \tag{81}$$

$$\psi_{5d} = e^{-r/5}r^2\left(1 - \frac{2r}{15} + \frac{2r^2}{525}\right)(1 - 3\cos^2\theta) \tag{82}$$

and

$$\psi_{5g} = e^{-r/5}r^4\left(1 - 10\cos^2\theta + \frac{35}{3}\cos^4\theta\right), \tag{83}$$

respectively.

In the first order of the perturbation theory we get from Eqs. (65) the following three energies:

$$(E_1^{5s\text{-}5d\text{-}5g})_{1,2,3} = 550,775 \pm 25\sqrt{481}. \tag{84}$$

Further we get the expression for the coefficients d and g,

$$d = \frac{2s(7E_1 - 2850)}{(E_1 - 300)(E_1 - 750)} \tag{85}$$

and

$$g = \frac{12s}{7(E_1 - 300)(E_1 - 750)}. \tag{86}$$

To get required behavior (37) we set

$$\frac{2s}{9375} + \frac{2d}{525} + g = 1 \tag{87}$$

and the constant C equals

$$C_{5s\text{-}5d\text{-}5g} = \frac{4s}{9375} - \frac{2d}{525} - 8g. \tag{88}$$

D. Calculation of the norm of the wave function

The norm of the function (19) is calculated from Eq. (9):

$$\langle \psi_{1s} | \psi_{1s} \rangle = \int_0^\infty \mathrm{d}r \int_0^\pi \mathrm{d}\theta r^2 \sin\theta |\psi_{1s}|^2 = 1/2, \tag{89}$$

where we made change of the variables $\rho = r \sin\theta$ and $z = r\cos\theta$. Further, the norm of the wave functions (67) and (80) equals

$$\langle \psi_{3s\text{-}3d} | \psi_{3s\text{-}3d} \rangle = 19\,683d^2 + \frac{27s^2}{2} \tag{90}$$

and

$$\langle \psi_{5s\text{-}5d\text{-}5g} | \psi_{5s\text{-}5d\text{-}5g} \rangle = \frac{125s^2}{2} + \frac{390\,625d^2}{7} + 136\,718\,750\,000g^2, \tag{91}$$

respectively.

IV. LARGE-ORDER BEHAVIOR OF THE PERTURBATION SERIES

By inserting Eq. (46) into Eq. (7) and the latter equation into Eq. (3) we obtain the large-order behavior of the perturbation energies,

$$E_n = E_n^{\mathrm{asy}} \left(1 + \frac{R_1 \pi}{2N\left(2n + 2N - \frac{3}{2}\right)} + \cdots \right), \tag{92}$$

where the leading term of the large-order behavior reads

TABLE I. Comparison of the numerical and analytical values of the coefficient R_1. See the text after Eq. (94) for details.

State	E_1	R_1, Eq. (94)	R_1, Eq. (61)
$1s$	2	−3.333 724 367 368 66	−3.333 724 367 368 65
$3s$-$3d$	$99+9\sqrt{41}$	−82.969 565 723 945	−82.969 565 723 942
$3s$-$3d$	$99-9\sqrt{41}$	−47.079 674 497 78	−47.079 674 497 77
$5s$-$5d$-$5g$	550	−273.083 854 65	−273.083 854 64
$5s$-$5d$-$5g$	$775+25\sqrt{481}$	−417.562 256 273	−417.562 256 272
$5s$-$5d$-$5g$	$775-25\sqrt{481}$	−212.681 342 928	−212.681 342 920

$$E_n^{\mathrm{asy}} = \frac{2^{4N}N^{2N-1}}{\pi^{2N+1/2}\langle\psi|\psi\rangle}(-1)^{n+1}\left(\frac{2^{3/2}N^2}{\pi}\right)^n \Gamma\left(2n+2N-\frac{1}{2}\right). \tag{93}$$

Here, the norm of the wave function $\langle\psi|\psi\rangle$ is given by Eqs. (89)–(91) for $1s$, $3s$-$3d$, and $5s$-$5d$-$5g$ states, respectively. The coefficients s and d in Eq. (90) are given by Eqs. (72) and (78), respectively. The coefficients s, d, and g in Eq. (91) are given by Eqs. (85)–(87), respectively.

The coefficient R_1 in Eq. (92) is given by Eq. (61). The first order perturbation energies in this equation are given by Eqs. (66), (73), and (84) for $1s$, $3s$-$3d$, and $5s$-$5d$-$5g$ states, respectively. The constant C in Eq. (61) is given by Eqs. (38), (79), and (88) for $1s$, $3s$-$3d$, and $5s$-$5d$-$5g$ states, respectively.

Formula (93) for $N=1$ and $N=3$ was for the first time given in Ref. 1 and for $N=1$ rederived in Refs. 3 and 4. The first correction (61) is given here for the first time. To check its correctness we calculated numerically

$$R_1 = \left(\frac{E_n}{E_n^{\mathrm{asy}}} - 1\right)\frac{2N\left(2n+2N-\frac{3}{2}\right)}{\pi}, \tag{94}$$

where E_n are the exact perturbation energies calculated from Eqs. (65) by means of the language MAPLE and E_n^{asy} is the leading term of the large-order behavior given by Eq. (93). For $1s$ state we calculated first 80 perturbation coefficients in the rational form. Numerical values in Eq. (94) were extrapolated by means of the Thiele-Padé extrapolation from the interval $n=70-80$ to infinity. For $3s$-$3d$ and $5s$-$5d$-$5g$ states we calculated first 100 coefficients in 200 digits accuracy for both energies in Eq. (73) and all three energies in Eq. (84). Numerical values were extrapolated from the interval $n=90-100$ to infinity. The extrapolated values are compared with the values given by Eq. (61) in Table I. Agreement between numerical and WKB results is excellent and confirms soundness of both the perturbation and WKB methods suggested in this paper.

V. CONCLUSIONS

In this paper the large-order behavior of the perturbation series for the energy of the hydrogen atom in the magnetic field was derived by means of the modified WKB approximation. The asymptotic formula derived by Avron in Ref. 1 was generalized to describe the states of higher than twofold degeneracies. On the other hand, we restricted ourselves to the states of zero projection of the angular momentum and even parity, while in Ref. 1 this restriction was not done. The first correction to the asymptotic formula was given here for the first time. The analytic results were compared with numerical ones and an excellent agreement between the two was found. The calculation of further terms in the expansions (35) and (92), though straightforward in principle, is very tedious. We note that in this case we must take also the correction to the norm of the wave function.[24,31,33,34] On the basis of the experience with one-dimensional problems[33,34] we expect that the series (35) and (92) are only asymptotic, i.e., hold for sufficiently small λ and large n only.

The most immediate further application of the WKB method suggested in this paper is the calculation of the ionization rate of the atoms in the weak electric field. The standard calculation of this rate for the many-electron atoms is based on the calculation for the hydrogen atom.[38] The latter is based on the separability of the Schrödinger equation in the parabolic coordinates.[33,35,36,39] However, the separation of the Schrödinger equation for the motion of the electron in the binding potential and applied electric field holds only in the case of a purely Coulombic binding potential. Arbitrarily small perturbation from the other electrons destroys the separability of Schrödinger equation. Even for the hydrogen atom, the separability is lost once the relativistic effects are considered. Only slight modifications of the procedure described here are necessary to derive the ionization rate of the hydrogen atom in the weak electric field without invoking the separability of the Schrödinger equation.

Finally, we note that the WKB approximation suggested here is not bound to the problem of the calculation of the lifetime of quasistationary states. It is a local approximation of the wave function and it can be used, for example, to describe motion of the bound electron in the intense laser field or to estimate forward scattering amplitude for the elastic scattering of the electrons on the atoms.

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APPENDIX

In this Appendix we discuss the relation between the WKB method suggested in Sec. II and the usual semiclassical approximation.

Let us consider the Schrödinger equation where we included the reduced Planck constant $\hbar$,

$$\hbar^2\left[\frac{\partial^2}{\partial\rho^2}+\frac{\partial^2}{\partial z^2}\right]\psi=[V(\rho,z)-E]\psi, \tag{A1}$$

and let us assume that the potential behaves in the vicinity of ρ axis as in Eq. (10). Then we can write the wave function of the particle in the vicinity of ρ axis in the form of Eq. (11). In general case there is no parameter λ associated with the external field driving the particle out of the potential well. Nevertheless, by the scaling

$$z=\hbar\,\eta \tag{A2}$$

the WKB approximation, very similar to that suggested for Eq. (5), can be obtained. Physically, the scaling (A2) implies that while the longitudinal motion is treated semiclassicaly, the transversal motion is treated in fully quantum manner. Proceeding then in accordance with the considerations leading to Eq. (35), it can be shown that the expansion of Eq. (A1) in the powers of η and $\hbar$ provides systematic approximations to the probability flux in the ρ direction in form of the series in the reduced Planck constant $\hbar$.

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Mathematical analysis of a Bohr atom model

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Bohr proposed in 1913 a model for atoms and molecules by synthesizing Planck's quantum hypothesis with classical mechanics. When the atom number Z is small, his model provides good accuracy for the ground-state energy. When Z is large, his model is not as accurate in comparison with the experimental data but still provides a good trend agreeing with the experimental values of the ground-state energy of atoms. The main objective of this paper is to provide a rigorous mathematical analysis for the Bohr atom model. We have established the following: (1) An existence proof of the global minimizer of the ground-state energy through scaling. (2) A careful study of the critical points of the energy function. Such critical points include both the stable steady-state electron configurations as well as unstable saddle-type configurations. (3) Coplanarity of certain electron configurations. Numerical examples and graphics are also illustrated. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168396]

I. INTRODUCTION

In 1913, Bohr presented a series of three papers[1–3] describing his approach for modeling atoms and molecules by synthesizing Planck's quantum hypothesis with classical mechanics. Bohr tried to explain the hydrogen spectral lines with a radical "planetary" model of electrons orbiting around a nucleus. He made a set of assumptions to quantify his model, leading to the existence in the atom a discrete set of stable, stationary orbits for electrons:

(1) The dynamical equilibrium of the stationary orbits is achieved by balancing the electrostatic Coulomb forces of attraction against the centrifugal effect and the interelectronic repelling of the orbital motion in classical mechanics.
(2) Stationary states satisfy the quantization condition that the ratio of the total kinetic energy of the electron to its orbital frequency be an integral multiple of $\pi\hbar$. For circular orbits, this signifies that the angular momentum of the electron is restricted to integral multiples of $\hbar$.

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(3) Energy is emitted only when an electron makes a "jump" (i.e., noncontinuous) transition between two stationary orbits, and the frequency of such a radiation emission is determined by $\Delta E/2\pi\hbar$, where ΔE is the energy difference between the two orbits where the transition occurs.

From now on, vectors will be denoted by bold letters. For the hydrogen atom, Bohr's assumptions work as follows. The total energy of the electron on a circular orbit with radius r and velocity $\mathbf{v}$ is

$$E = \text{kinetic energy} + \text{potential energy} = \frac{m_e v^2}{2} - \frac{Ze^2}{r}, \tag{1.1}$$

where

$$m_e = \text{the mass of the electron},$$

$$e = \text{the charge of the electron},$$

$$Ze = \text{the positive charge of the nucleus}.$$

Since

$$\mathbf{L} = \text{the angular momentum} = \mathbf{r} \times \mathbf{p} \quad (\mathbf{p} \equiv \text{the linear momentum} = m_e \mathbf{v}),$$

$$|\mathbf{L}| = L = m_e v r, \tag{1.2}$$

which, in turn, by Bohr's quantization assumption, satisfies

$$L = n\hbar. \tag{1.3}$$

From (1.1)–(1.3), we now have

$$E = \frac{m_e^2 v^2 r^2}{2m_e r^2} - \frac{Ze^2}{r} = \frac{L^2}{2m_e r^2} - \frac{Ze^2}{r} = \frac{n^2\hbar^2}{2m_e r^2} - \frac{Ze^2}{r} = \frac{1}{2}\frac{n^2}{r^2} - \frac{Z}{r}, \tag{1.4}$$

in atomic units (by setting $e=1$, $\hbar^2/m_e=1$).

Minimizing $E=E(r,n,Z)$ with respect to r for $n=1,2,3,\ldots$, for fixed Z, we obtain

$$\hat{E}_n \equiv \min_{r>0} E(r,n,Z) = -\frac{1}{2}\frac{Z^2}{n^2}, \quad n = 1,2,3, \ldots . \tag{1.5}$$

These values and their differences totally determine the hydrogen atom's spectral lines.

Sommerfeld later in 1916 generalized Bohr's theory by allowing noncircular orbits and by incorporating relativistic effects, leading to the Bohr-Sommerfeld (old) quantum theory of the hydrogen atom. However, for other atoms, including the simple helium, there are difficulties unaccountable by the Bohr-Sommerfeld theory; see, e.g., Refs. 6 and 7. Heisenberg worked under both Bohr and Sommerfeld trying to resolve such difficulties, eventually he gave up but in the process invented the matrix mechanics during the 1920s.

The objective of the present paper is to analyze, mathematically, a Bohr atom model for the ground states of general atoms. Such a general Bohr model seems to be well understood by atomic physicists (see, e.g., the pictorials on the website of Patton[11]) but we could not provide an exact citation. The model that we are going to describe below is communicated to us by our colleague, Dr. S. A. Chin.[4] Consider a neutral atom with atom number Z. There are Z electrons. The kinetic energy of an electron i moving around a circular orbit of radius r_i on the nth shell, $n_i = 1,2,3,\ldots$, is

TABLE I. Assignment of quantum numbers n_i for the ground state of an atom with atom number Z from $Z=1$ to 108.

Electron numbers i	Electron shells names	Assigned quantum numbers n_i
$1 \leqslant i \leqslant 2$	K	1
$3 \leqslant i \leqslant 8$	L	2
$9 \leqslant i \leqslant 18$	M	3
$19 \leqslant i \leqslant 36$	N	4
$37 \leqslant i \leqslant 54$	O	5
$55 \leqslant i \leqslant 86$	P	6
$87 \leqslant i \leqslant 108$	Q	7

$$T_i = -\tfrac{1}{2} n_i^2 / r_i^2 \quad [r_i = |\mathbf{r}_i|, \mathbf{r}_i = (x_i, y_i, z_i) \in \mathbb{R}^3 \text{ is the position vector of electron } i]. \tag{1.6}$$

For a heuristic derivation of (1.6), see Ref. 6, Appendix. The potential energy is attributed to the Coulomb interactions of electron j with the nucleus and electrons j for $j \neq i$,

$$P_i = -\frac{Z}{r_i} + \sum_{\substack{j=1 \\ j \neq i}}^{Z} \frac{1}{r_{ij}} \quad (r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|). \tag{1.7}$$

Thus the total energy of the atom is

$$E = E(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z) = \sum_{j=1}^{Z} (T_j + P_j) = \sum_{i=1}^{Z} \left(\frac{n_i^2}{2r_i^2} - \frac{Z}{r_i} \right) + \sum_{\substack{i,j=1 \\ i \neq j}}^{Z} \frac{1}{2r_{ij}}. \tag{1.8}$$

We now pack these Z electrons into the various "electron shells" by the *Aufbau principle* by assigning the values of n_i according to Table I. (The packing of electrons into electron shells by the Aufbau principle involves also *subshells* p, d, f, etc. Since here we are only dealing with ground states of atoms, we pack electrons only into the *principal s* shells.) These designated integral values of n_i give us the Bohr atom model in this paper.

The stable stationary orbit or electron configuration, denoted as $(\mathbf{r}_1^*, \mathbf{r}_2^*, \ldots, \mathbf{r}_Z^*)$, and the associated ground state energy $E(\mathbf{r}_1^*, \mathbf{r}_2^*, \ldots, \mathbf{r}_Z^*)$, can now be obtained by

$$\min_{\mathbf{R} \in \mathbb{R}^{3Z}} E(\mathbf{R}) \equiv E(\mathbf{R}^*), \quad \mathbf{R}^* \equiv (\mathbf{r}_1^*, \mathbf{r}_2^*, \ldots, \mathbf{r}_Z^*). \tag{1.9}$$

In Table II, we have listed the ground-state energy of all the atoms calculated from (1.9) as well as the known ("exact") experimental values. The reader may find some agreement between these two sets of values, especially when Z is small.

The Bohr model of atoms was derived by Bohr in an *ad hoc* way at first. The rigorous, wave-mechanical model is the following Schrödinger-Born-Oppenheimer equation describing the many-particle quantum-mechanical behavior

$$\left(-\frac{1}{2} \sum_{k=1}^{Z} \nabla_k^2 + \frac{1}{2} \sum_{\substack{k,k'=1 \\ k \neq k'}}^{Z} \frac{1}{r_{kk'}} - \sum_{k=1}^{Z} \frac{Z}{r_k} \right) \phi(\mathbf{R}) = E \phi(\mathbf{R}). \tag{1.10}$$

As Bohr's model appears to be something of the history, why does it still warrant any attention? The reasons that motivate our study here are threefold:

(i) Recently, through the *dimensional scaling* (D-scaling) method,[9] Svidzinsky, Scully, and

TABLE II. Comparison of ground-state energies of atoms' ground-state energies in hartrees (htr) with atom number Z: $2 \leqslant Z \leqslant 30$, between experimental values and Bohr's energies. When Z is small, there is a better agreement, and the trend is basically sound. But none of Bohr's energies are within the *chemical accuracy* of five decimal places.

Z	Experiment	Bohr
2.0	−2.903	−3.0615
3.0	−7.478	−7.6889
4.0	−14.667	−14.8377
5.0	−24.652	−24.7906
6.0	−37.842	−37.8128
7.0	−54.584	−54.1540
8.0	−75.059	−74.1726
9.0	−99.719	−97.9746
10.0	−128.919	−125.5152
11.0	−162.233	−156.9173
12.0	−200.026	−192.3112
13.0	−242.315	−231.7757
14.0	−289.322	−275.4952
15.0	−341.208	−323.5122
16.0	−398.601	−376.0176
17.0	−460.102	−433.0846
18.0	−527.494	−494.9136
19.0	−599.924	−561.4195
20.0	−677.558	−632.8097
21.0	−760.575	−709.3828
22.0	−849.285	−791.0756
23.0	−943.804	−878.0731
24.0	−1044.315	−970.5907
25.0	−1150.866	−1068.6207
26.0	−1263.483	−1172.1997
27.0	−1382.494	−1281.5093
28.0	−1507.990	−1396.5737
29.0	−1640.123	−1517.7809
30.0	−1779.048	−1644.9630

Hershbach[12,13] have arrived at Bohr's model from the totally quantum-mechanical (Schrödinger-Born-Oppenheimer) model via asymptotics. This has stirred surprise, excitement, and interests,[15] especially among the researchers in the Institute for Quantum Studies at Texas A&M and has rekindled efforts in trying to understand the synergism between D-scaling, the Schrödinger-Born-Oppenheimer model and the Bohr model for atoms and molecules.

(ii) The Schrödinger-Born-Oppenheimer model (1.10) involves large-scale numerical computation and is rather theoretically intractable, while the Bohr model (1.8) and (1.9) requires only desk-top computing, producing outcomes of electron configurations highly valuable and intuitive for atomic experiments and molecular modeling, especially with the incorporation of the Hartree-Fock and other refinement techniques (e.g., Refs. 6, 7, 5, 8, and 14).

(iii) Mathematically speaking, even though Bohr's atom model is nearly 90 years old, historically it has not attracted due attention in the mathematics community and, thus, has not undergone rigorous mathematical analysis it rightfully deserves. Many relevant interesting mathematical problems are worth investigation. We hope our mathematical analysis carried out here will improve the understanding of Bohr's atomic model and that of atoms in

general at a more fundamental level, with an ultimate goal of improving the modeling and compution of molecules or even building new molecular models.

II. EXISTENCE AND ALGORITHM FOR THE GLOBAL MINIMIZER

The following problems are of significant mathematical interests, which also have physical importance:

(i) a rigorous existence proof of ground-state energies;
(ii) *stable* as well as *unstable* electron steady-state orbits;
(iii) geometric configurations: coplanarity and symmetries of electron locations.

We discuss them through a sequence of lemmas and theorems.

From now on, to simplify notation, we often write

$$\sum_{i=1}^{n} \text{ as } \sum_{i}, \quad \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \text{ as } \sum_{i\neq j},$$

unless more clarity of the summation index is deemed necessary.

We begin by letting Z be a positive number and n be a positive integer; $n=1,2,3,\ldots$, define

(1) For $n=1$,

$$E_1^Z:\mathbb{R}^3 \to \mathbb{R}, \quad E_1^Z(\mathbf{r}_1) = \frac{n_1^2}{2r_1^2} - \frac{Z}{r_1}, \quad \mathbf{r}_1 \in \mathbb{R}^3.$$

(2) For $n \geqslant 2$ and $Z \geqslant n$, $E_n^Z:\mathbb{R}^{3n} \to \mathbb{R}$,

$$E_n^Z(\mathbf{R}) = \sum_{i=1}^{n} \left(\frac{n_i^2}{2r_i^2} - \frac{Z}{r_i} \right) + \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \frac{1}{2r_{ij}}, \tag{2.1}$$

where $\mathbf{R}=(\mathbf{r}_1,\ldots,\mathbf{r}_n)$, $\mathbf{r}_i \in \mathbb{R}^3$, r_i and r_{ij} are defined as in (1.6) and (1.7). The domain of E_n^Z is then given by $\mathbb{R}^{3n}\backslash\mathcal{S}_n$, where $\mathcal{S}_n$ is the singularity manifold of E_n^Z given by

$$\mathcal{S}_n = \{\mathbf{R}=(\mathbf{r}_1,\ldots,\mathbf{r}_n) \in \mathbb{R}^{3n} | \mathbf{r}_j = \mathbf{0} \text{ or } \mathbf{r}_j - \mathbf{r}_k = 0, \quad \text{for some } j,k, 1 \leqslant j,k \leqslant n, j \neq k\}.$$

E_n^Z is obviously in $C^\infty(\mathbb{R}^{3n}\backslash\mathcal{S}_n)$. We are interested in the existence of $\mathbf{R}^* \in \mathbb{R}^{3n}\backslash\mathcal{S}_n$ such that

$$E_n^Z(\mathbf{R}^*) = \inf_{\mathbf{R}\in\mathbb{R}^{3n}\backslash\mathcal{S}_n} E_n^Z(\mathbf{R}), \quad \text{for } n \geqslant 2.$$

Note that the case of $n=1$ is already solved in (1.6). From now on, we will abbreviate E_n^Z as E if no ambiguities should arise. Throughout the rest of the section, the reader may find that in all of the proofs given, as long as $n_i>0$ for $i=1,2,\ldots,n$, the proofs go through without any problem, i.e., n_i's do not have to follow the designated values as in Table I. We further define

$$\mathcal{S}_Z^n = \left\{ \mathbf{R} \in \mathbb{R}^{3n}\backslash\mathcal{S}_n \middle| \sum_i \frac{Z}{r_i} - \sum_{i\neq j} \frac{1}{2r_{ij}} > 0 \right\}.$$

Lemma 1 (scaling along a ray): Let $\mathbf{R} \in \mathcal{S}_Z^n$. The function $g:\mathbb{R}_+ \equiv (0,\infty) \to \mathbb{R}$, $g(t) \equiv E(t\mathbf{R})$ has a unique global minimum at

$$t^* = t^*(\mathbf{R}) = \arg \min_{t\neq 0, t\in\mathbb{R}} E(t\mathbf{R}), \tag{2.2}$$

where

$$t^* > 0, g'(t^*) = 0, \quad g''(t^*) > 0, \tag{2.3}$$

$$E(t^*\mathbf{R}) = -\frac{1}{2}\sum_i \frac{n_i^2}{r_i^2}\frac{1}{t^{*2}} = -\frac{1}{2}\left(\sum_i \frac{Z}{r_i} - \sum_{i\neq j}\frac{1}{r_{ij}}\right)^2 \Bigg/ \left(\sum_i \frac{n_i^2}{r_i^2}\right) < 0. \tag{2.4}$$

Proof: First, we note that $\mathcal{S}_Z^n$ is a nonempty unbounded open set of $\mathbb{R}^{3Z}$. It is easy to see that if $\mathbf{R} \in \mathcal{S}_Z^n$, then $t\mathbf{R} \in \mathcal{S}_Z^n$ for any $t \neq 0$, i.e., $\mathcal{S}_Z^n$ is star shaped. For $t > 0$, we have

$$g(t) = \frac{1}{t^2}\sum_i \left(\frac{n_i^2}{2r_i^2}\right) + \frac{1}{t}\left(-\sum_i \frac{Z}{r_i} + \sum_{i\neq j}\frac{1}{2r_{ij}}\right), \tag{2.5}$$

$$g'(t) = -\frac{2}{t^3}\sum_i \frac{n_i^2}{2r_i^2} + \frac{1}{t^2}\left(\sum_i \frac{Z}{r_i} - \sum_{i\neq j}\frac{1}{2r_{ij}}\right). \tag{2.6}$$

Set $g'(t^*)=0$ to get the *only* zero of g' at

$$t^* = \frac{\sum_i n_i^2/r_i^2}{\sum_i Z/r_i - \sum_{i\neq j} 1/2r_{ij}}. \tag{2.7}$$

Note that the denominator in (2.7) is positive since $\mathbf{R} \in \mathcal{S}_Z^n$. So t^* is well defined. Next, we have

$$g''(t) = \frac{6}{t^4}\sum_i \frac{n_i^2}{2r_i^2} - \frac{2}{t^3}\left(\sum_i \frac{Z}{r_i} - \sum_{i\neq j}\frac{1}{2r_{ij}}\right),$$

$$g''(t^*) = \frac{1}{t^{*4}}\sum_i \frac{n_i^2}{r_i^2} > 0.$$

Therefore $g(t)$ has only a global minimum at $t^* > 0$, and $\phi(t^*) = E(t^*\mathbf{R})$ is given as in (2.4). □

Remark 1: If $\mathbf{R} \notin \mathcal{S}_n \cup \mathcal{S}_Z^n$, then for $t > 0$,

$$g(t) = E(t\mathbf{R}) = \frac{1}{t^2}\sum_i \frac{n_i^2}{r_i^2} + \frac{1}{t}\left(-\sum_i \frac{Z}{r_i} + \sum_{i\neq j}\frac{1}{2r_{ij}}\right).$$

This function $g(t)$ is always *positive* and monotonic for $t \in (0,\infty)$ such that $g'(t)=0$ has no solution $t \in \mathcal{R}_+$. In fact, $g'(t) < 0$ on $\mathbb{R}_+$, i.e., g is strictly decreasing. Since $g(t)$ is smooth on $\mathbb{R}_+$, $\lim_{t\to 0} g(t) = +\infty$ and $\lim_{t\to\infty} g(t) = 0$, we have $g(t) \geqslant 0$ for any $t \in \mathbb{R}_+$. □

From (2.1), by completing the square we have

$$E(\mathbf{R}) = \sum_i \left(\frac{n_i}{\sqrt{2}r_i} - \frac{\sqrt{2}Z}{n_i}\right)^2 + \sum_{i\neq j}\frac{1}{2r_{ij}} - \sum_i \frac{2Z^2}{n_i^2} \geqslant -\sum_i \frac{2Z^2}{n_i^2},$$

therefore $E(\mathbf{R})$ is bounded from below, its infimum exists and we have

$$\mu_n^Z := \inf_{\mathbf{R}\in\mathbb{R}^{3n}\setminus\mathcal{S}_n} E_n^Z(\mathbf{R}) = \inf_{\mathbf{R}\in\mathcal{S}_Z^n} E_n^Z(\mathbf{R}) < 0. \tag{2.8}$$

We introduce the following gradient notation: Let $f(x_1, x_2, \ldots, x_n)$ be any scalar valued function of n variables. For any variables $x_{i_1} x_{i_2}, \ldots, x_{i_k}$, where $1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant n$, we denote the gradient of f with respect to these variables as

$$D_{(x_{i_1}x_{i_2},\ldots,x_{i_k})}f(x_1,x_2,\ldots,x_n)=\left[\frac{\partial f}{\partial x_{i_1}}(x_1,x_2,\ldots,x_n),\frac{\partial f}{\partial x_{i_2}}(x_1,x_2,\ldots,x_n),\ldots,\frac{\partial f}{\partial x_{i_k}}(x_1,x_2,\ldots,x_n)\right]^T,$$

(where T means transpose) which is regarded as a column vector. If $(x_{i_1},x_{i_2},\ldots,x_{i_k})=(x_1,x_2,\ldots,x_n)$, i.e., all the variables $x_1,x_2,\ldots,x_n$ are included, then we simply write the above as Df, i.e.,

$$Df=[\partial f/\partial x_1\ \partial f/\partial x_2\cdots\partial f/\partial x_n]^T.$$

A point $\mathbf{y}\in\mathbb{R}^n$ is said to be a *critical point* of f if $Df(y)=\mathbf{0}$. Obviously, any local maximum or minimum of E is a critical point, but many critical points of E may be of the saddle type which are *physically unstable*.

Later, we will also need to utilize the *Hessian matrix* of f,

$$D^2f=\left[\frac{\partial^2 f}{\partial x_i\partial x_j}\right]_{1\leqslant i,j\leqslant n}. \tag{2.9}$$

A critical point $\mathbf{R}^\dagger\in\mathbb{R}^{3Z}$ of $E(\mathbf{R})$ is defined by $DE(\mathbf{R}^\dagger)=0$. Thus, at a critical point we obtain the set of gradient (vector) equations

$$D_{\mathbf{r}_j}E(\mathbf{R}^\dagger)=\mathbf{0}\quad\text{for } j=1,2,\ldots,n, \tag{2.10}$$

i.e.,

$$\left(\frac{n_j^2}{r_j^{\dagger 4}}-\frac{Z}{r_j^{\dagger 3}}\right)\mathbf{r}_j^\dagger+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\mathbf{r}_{kj}^\dagger=\mathbf{0}\in\mathbf{R}^3,\quad j=1,2,\ldots,n. \tag{2.11}$$

Using $\mathbf{r}_{kj}^\dagger=\mathbf{r}_k^\dagger-\mathbf{r}_j^\dagger$, we can write (2.11) alternatively as

$$\left(\frac{n_j^2}{r_j^{\dagger 4}}-\frac{Z}{r_j^{\dagger 3}}+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\right)\mathbf{r}_j^\dagger-\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{2r_{kj}^{\dagger 3}}\mathbf{r}_k^\dagger=\mathbf{0},\quad j=1,2,\ldots,n. \tag{2.12}$$

These constitute the equations for the *steady states* of electron orbits, based on the Bohr model. In particular, if $\mathbf{R}^*$ is a global minimum of E established in the preceding section, then $\mathbf{R}^*$ is necessarily a critical point and so the equations in (2.11) or (2.12) hold, with the "†" signs therein replaced by "*."

Theorem 1 (Virial): *Let* $\mathbf{R}^\dagger=(\mathbf{r}_1^\dagger,\mathbf{r}_2^\dagger,\ldots,\mathbf{r}_n^\dagger)$ *be a critical point of E satisfying* $DE(\mathbf{R}^\dagger)=\mathbf{0}\in\mathbb{R}^{3n}$, *then so is* $\mathcal{R}\mathbf{R}^\dagger$ *for any 3D rotation* $\mathcal{R}$, *and* $\mathbf{R}^\dagger\in\mathcal{S}_Z^n$. *The ground-state energy value is given by*

$$E(\mathbf{R}^\dagger)=-\sum_{i=1}^{n}\frac{n_i^2}{2r_i^{\dagger 2}}<0. \tag{2.13}$$

In addition, along the ray $t\mathbf{R}^\dagger$ *for* $t>0$, $E(t\mathbf{R}^\dagger)$ *attains its global minimum at* $t=1$.

Proof: The energy $E(\mathbf{R})$ is invariant under any 3D rotation $\mathcal{R}$, where for $\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)$, $\mathcal{R}\mathbf{R}=(\mathcal{R}\mathbf{r}_1,\mathcal{R}\mathbf{r}_2,\ldots,R\mathbf{r}_n)$. Thus, if $\mathbf{R}^\dagger$ is a critical point, so is $\mathcal{R}\mathbf{R}^\dagger$.

Consider, for $t\neq 0$,

$$E(t\mathbf{R}^\dagger)=\sum_{i=1}^{n}\left(\frac{n_i^2}{2t^2r_i^{\dagger 2}}-\frac{Z}{tr_i^\dagger}\right)+\sum_{\substack{i,j=1\\i\neq j}}^{2}\frac{1}{2tr_{ij}^\dagger}.$$

Then, because $DE(\mathbf{R}^\dagger)=\mathbf{0}$, we have

$$\frac{d}{dt}E(t\mathbf{R}^\dagger)\big|_{t=1} = DE(\mathbf{R}^\dagger)\cdot\mathbf{R}^\dagger = 0,$$

i.e.,

$$\sum_i \left(-\frac{n_i^2}{r_i^{\dagger 2}} + \frac{Z}{r_i^\dagger}\right) - \sum_{i\neq j}\frac{1}{2r_{ij}^\dagger} = 0, \tag{2.14}$$

and

$$\sum_i \frac{Z}{r_i^\dagger} - \sum_{i\neq j}\frac{1}{2r_{ij}^\dagger} = \sum_i \frac{n_i^2}{r_i^{\dagger 2}} > 0,$$

and, hence, $\mathbf{R}^\dagger \in S_Z^n$. Therefore

$$E(\mathbf{R}^\dagger) = \sum_i \left(\frac{n_i^2}{2r_i^{\dagger 2}} - \frac{Z}{r_i^\dagger}\right) + \sum_{i\neq j}\frac{1}{2r_{ij}^\dagger} = \left[\sum_i \left(\frac{n_i^2}{r_i^{\dagger 2}} - \frac{Z}{r_i^\dagger}\right) + \sum_{i\neq j}\frac{1}{2r_{ij}}\right] - \sum_i \frac{n_i^2}{2r_i^{\dagger 2}} = -\sum_{i=1}^{Z}\frac{n_i^2}{2r_i^{\dagger 2}}.$$

But from the proof of Lemma 1, the derivative of function $g(t)=E(t\mathbf{R}^\dagger)$, $g'(t)$, has only one zero t^* satisfying $g'(t^*)=0$. Thus $t^*=1$, and $t^*=1$ necessarily corresponds to the global minimum of $g(t)$.

The proof is complete. □

Corollary 1: Let $R^\dagger=(\mathbf{r}_1^\dagger,\ldots,\mathbf{r}_n^\dagger)$ *be a critical point of E satisfying Theorem 1. Define an* $n\times n$ *matrix* $M^\dagger$ whose (j,k)*-entries* M_{jk} *are given by*

$$M_{jk}^\dagger = \begin{cases} -\dfrac{1}{2r_{kj}^{\dagger 3}}, & k\neq j, \\ \dfrac{n_k^2}{r_k^{\dagger 4}} - \dfrac{Z}{r_k^{\dagger 3}} + \displaystyle\sum_{\substack{i=1\\ i\neq k}}^{Z}\frac{1}{2r_{ki}^{\dagger 3}}, & j=k. \end{cases} \tag{2.15}$$

Then $\det M^\dagger = 0$.

Proof: Note that these $M_{jk}^\dagger$'s are the coefficients appearing in (2.12). As the matrix equation $M^\dagger\boldsymbol{\alpha}=\mathbf{0}\in\mathbb{R}^n$ has at least a nontrivial solution $\boldsymbol{\alpha}\in\mathbb{R}^n$, $\boldsymbol{\alpha}\neq 0$, where $\boldsymbol{\alpha}$ is a vector formed by all of the ith components of the vectors in $(\mathbf{r}_1^\dagger,\mathbf{r}_2^\dagger,\ldots,\mathbf{r}_n^\dagger)$, with $i=1$, or 2, or 3, we must have the determinant of $M^\dagger$ equal to 0. □

From (2.14), we obtain that the set

$$\mathcal{N}_Z^n = \left\{\mathbf{R}=(\mathbf{r}_1,\ldots,\mathbf{r}_n)\in\mathbb{R}^{3n}\setminus\mathcal{S}_n \Big| \sum_{k=1}^{n}\left[\frac{Z}{r_k} - \frac{n_i^2}{r_k^2}\right] = \sum_{\substack{j,k=1\\ j\neq k}}^{n}\frac{1}{2r_{jk}}\right\}, \tag{2.16}$$

contains all critical points of E_n^Z. $\mathcal{N}_Z^n$ is a closed nonempty subset of $\mathbb{R}^{3n}$, and $\mathcal{N}_Z^n\subset S_Z^n$. We then have

$$\inf_{\mathbf{R}\in\mathcal{S}_Z^n} E_n^Z(\mathbf{R}) = \inf_{\mathbf{R}\in\mathcal{N}_Z^n} E_n^Z(\mathbf{R}). \tag{2.17}$$

Furthermore, we obtain from (2.4)

$$E_n^Z(\mathbf{R}) = -\frac{1}{2}\sum_{i=1}^{n}\frac{n_i^2}{r_i^2} < 0, \quad \forall\,\mathbf{R}=(\mathbf{r}_1,\ldots,\mathbf{r}_n)\in\mathcal{N}_Z^n. \tag{2.18}$$

When $n=1$, define $\mathcal{N}_Z^1=\{\mathbf{r}_1\in\mathbb{R}^3 | r_1=n_1^2/Z\}$. For any $\mathbf{r}\in\mathcal{N}_Z^1$,

$$E_1^Z(\mathbf{r}) = -\frac{Z^2}{2n_1^2} = \inf_{\mathbf{r}_1 \in \mathbb{R}^3 \setminus \mathcal{S}_1} E_1^Z(\mathbf{r}_1).$$

Lemma 2: Let $n \geqslant 2$ and $Z=n$, then

$$\mu_n^Z \leqslant \mu_k^Z, \quad \forall\, k\colon 1 \leqslant k \leqslant n-1.$$

If $\mu_k^Z = E_k^Z(\mathbf{r}_1^*, \ldots, \mathbf{r}_k^*)$ for some $(\mathbf{r}_1^*, \ldots, \mathbf{r}_k^*) \in (\mathbb{R}^3)^k$, then

$$\mu_n^Z < \mu_k^Z, \quad \forall\, 1 \leqslant k \leqslant n-1.$$

Proof: For any $(\mathbf{r}_1, \ldots, \mathbf{r}_k) \in S_Z^k$ and $(\mathbf{r}_{k+1}, \ldots, \mathbf{r}_n) \in S_{Z-k}^{n-k}$, we have

$$\begin{aligned} E_n^Z(\mathbf{r}_1, \ldots, \mathbf{r}_k, t\mathbf{r}_{k+1}, \ldots, t\mathbf{r}_n) &= \left\{ \sum_{j=1}^{k} \left[\frac{n_j^2}{2r_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=1 \\ j \neq i}}^{k} \frac{1}{2r_{ij}} \right\} \\ &\quad + \left\{ \sum_{j=k+1}^{n} \left[\frac{n_j^2}{2t^2 r_j^2} - \frac{Z}{t r_j} \right] + \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2tr_{ij}} + \sum_{j=k+1}^{n} \sum_{i=1}^{k} \frac{1}{|t\mathbf{r}_j - \mathbf{r}_i|} \right\} \\ &\equiv \Delta_1 + \frac{1}{t}\Delta_2. \end{aligned}$$

Note that

$$\lim_{t\to\infty} \Delta_2 = \lim_{t\to\infty} \left\{ \sum_{j=k+1}^{n} \left[\frac{n_j^2}{2tr_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2r_{ij}} + \sum_{j=k+1}^{n} \sum_{i=1}^{k} \frac{t}{|t\mathbf{r}_j - \mathbf{r}_i|} \right\} = -\left(\sum_{j=k+1}^{n} \frac{Z-k}{r_j} - \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2r_{ij}} \right).$$

In the special case when $k=n-1$, we have $\mathbf{r}_n \in S_{Z-n+1}^1$ and then

$$\lim_{t\to\infty} \Delta_2 = -\frac{Z-n+1}{r_n} < 0;$$

but if $1 \leqslant k \leqslant n-2$, which occurs only when $n \geqslant 3$, then $(\mathbf{r}_{k+1}, \ldots, \mathbf{r}_n) \in S_{Z-k}^{n-k}$ implies

$$\lim_{t\to\infty} \Delta_2 = -\left(\sum_{j=k+1}^{n} \frac{Z-k}{r_j} - \sum_{\substack{j,i=k+1 \\ j \neq i}}^{n} \frac{1}{2r_{ij}} \right) < 0. \tag{2.19}$$

Thus we obtain, for any $(\mathbf{r}_{k+1}, \ldots, \mathbf{r}_n) \in S_{Z-k}^{n-k}$,

$$\frac{1}{t}\Delta_2 < 0, \quad \text{for } t \text{ sufficiently large.}$$

Hence, we have for any $(\mathbf{r}_1, \ldots, \mathbf{r}_k) \in S_Z^k$, for t sufficiently large,

$$\mu_n^Z \leqslant E_n^Z(\mathbf{r}_1, \ldots, \mathbf{r}_k, t\mathbf{r}_{k+1}, \ldots, t\mathbf{r}_n) < \left(\sum_{j=1}^{k} \left[\frac{n_j^2}{2r_j^2} - \frac{Z}{r_j} \right] + \sum_{\substack{j,i=1 \\ j \neq i}}^{k} \frac{1}{2r_{ij}} \right). \tag{2.20}$$

Thus

$$\mu_n^Z \leqslant \mu_k^Z.$$

If $\mu_k^Z = E_k^Z(\mathbf{r}_1^*, \ldots, \mathbf{r}_k^*)$ for some $(\mathbf{r}_1^*, \ldots, \mathbf{r}_k^*) \in (\mathbb{R}^3)^k$, then (2.19) and (2.20) leads to

$$\mu_n^Z < \mu_k^Z.$$

□

Theorem 2: *Let $Z=n$. There exists an $\mathbf{R}^*=(\mathbf{r}_1^*,\ldots,\mathbf{r}_n^*)\in\mathbb{R}^{3n}$ such that*

$$E_n^Z(\mathbf{R}^*) = \inf_{\mathbf{R}\in\mathbb{R}^{3n}\setminus\mathcal{S}_n} E_n^Z(\mathbf{R}).$$

Proof: Since the case of $n=1$ is trivial, we assume $n\geqslant 2$. From (2.8) and (2.17), we only need to prove that there exists an $\mathbf{R}^*=(\mathbf{r}_1^*,\ldots,\mathbf{r}_n^*)\in\mathcal{N}_Z^n$ such that

$$E_n^Z(\mathbf{R}^*) = \inf_{\mathbf{R}\in\mathcal{N}_Z^n} E_n^Z(\mathbf{R}) = \mu_n^Z.$$

Let $\{\mathbf{R}_m\}\subset\mathcal{N}_Z^n$ be a minimizing sequence such that $E_n^Z(\mathbf{R}_m)\to\mu_n^Z$ as $m\to\infty$. We first show that $\{\mathbf{R}_m\}$ is bounded.

Suppose $\{\mathbf{R}_m\}$ is unbounded. Let $\mathbf{R}_m=(\mathbf{r}_1^m,\ldots,\mathbf{r}_n^m)$. By replacing $\{\mathbf{R}_m\}$ with its subsequence, if necessary, essentially two cases need to be considered:

(a) $|\mathbf{r}_k^m|\to+\infty$, $1\leqslant k\leqslant n$; and
(b) there exist $M>0$ and k_0: $1\leqslant k_0\leqslant n-1$, such that

$$r_k^m\to+\infty,\quad 1\leqslant k\leqslant k_0,$$

$$r_k^m\leqslant M,\quad k_0+1\leqslant k\leqslant n.$$

In general, the index set $\{1,2,\ldots,n\}$ has two disjoint subsets such that $r_k^m\to\infty$ and $r_k^m<M$, respectively, as $m\to\infty$ for k in each of these two index subsets. But the proof is the same.

For case (a), since $\{\mathbf{R}_m\}\subset\mathcal{N}_Z^n$ and (2.18), we have

$$\mu_n^Z = \lim_{m\to\infty} E_n^Z(\mathbf{R}_m) = \lim_{m\to\infty}\left\{-\frac{1}{2}\sum_{i=1}^n \frac{n_i^2}{r_i^m}\right\} = 0.$$

This contradicts $\mu_n^Z<0$ from (2.8). Thus, case (a) is impossible.

For case (b), we can further assume that $\mathbf{r}_k^m\to\mathbf{r}_k^*$ for $k_0+1\leqslant k\leqslant n$. Then we have

$$\begin{aligned}\mu_n^Z &= \lim_{m\to\infty} E_n^n(\mathbf{R}_m) = \lim_{m\to\infty}\left\{\sum_{i=1}^n\left(\frac{n_i^2}{2(r_i^m)^2}-\frac{Z}{r_i^m}\right)+\sum_{\substack{i,j=1\\ i\neq j}}^n\frac{1}{2r_{ij}^m}\right\}\\ &= \left\{\sum_{k=k_0+1}^n\left[\frac{n_k^2}{2(r_k^*)^2}-\frac{Z}{r_k^*}\right]+\sum_{\substack{j,k=k_0+1\\ j\neq k}}^n\frac{1}{2r_{jk}^*}\right\}+\lim_{m\to\infty}\sum_{\substack{j,k=1\\ j\neq k}}^{k_0}\frac{1}{2r_{jk}^m}\geqslant\mu_{n-k_0}^Z+\lim_{m\to\infty}\sum_{\substack{j,k=1\\ j\neq k}}^{k_0}\frac{1}{2r_{jk}^m}\geqslant\mu_{n-k_0}^Z.\end{aligned}$$

By applying the first part of Lemma 2, we must have

$$\lim_{m\to\infty}\sum_{\substack{j,k=1\\ j\neq k}}^{k_0}\frac{1}{r_{jk}^m}=0$$

and

$$\mu_n^Z = \mu_{n-k_0}^Z = \sum_{k=k_0+1}^{n} \left[\frac{n_i^2}{2(r_k^*)^2} - \frac{Z}{r_k^*} \right] + \sum_{\substack{j,k=k_0+1 \\ j\neq k}}^{n} \frac{1}{2r_{jk}^*},$$

which contradicts the second part of Lemma 2. Thus, case (b) is also impossible.

Therefore $\{\mathbf{R}_m\}$ is bounded and contains a convergent subsequence, denoted by $\{\mathbf{R}_m\}$ again, such that $\mathbf{R}_m \to \mathbf{R}^* \in \mathbb{R}^{3n}$. Since $\mathcal{N}_Z^n$ is a closed subset of $\mathbb{R}^{3n}$, we have $\mathbf{R}^* \in \mathcal{N}_Z^n$, and

$$E_n^n(\mathbf{R}^*) = \mu_n^Z = \inf_{\mathbf{R}\in\mathbb{R}^{3n}\setminus\mathcal{S}_n} E_n^Z(\mathbf{R}).$$

□

Corollary 2: Let $Z=n$. For any nontrivial subspace V of $\mathbb{R}^3$, the energy function E_n^Z defined in (2.1) attains a minimum in V^n. □

III. CRITICAL POINTS OF THE ENERGY E: STABLE AND UNSTABLE ELECTRON CONFIGURATIONS

From here throughout the rest of the paper for all practical interest we assume $n=Z$ for E_n^Z, which will be written simply as E.

In order to distinguish any global (or, possibly local) minimizer $\mathbf{R}^*$ from a saddle-type critical point $\mathbf{R}^\wedge$ of E, we need to examine whether the $(3Z)\times(3Z)$ Hessian matrix D^2E [cf. (2.9)] is (semi-) positive-definite at $\mathbf{R}^*$, as the second order Taylor approximation gives

$$E(\mathbf{R}) = E(\mathbf{R}^*) + DE(\mathbf{R}^*)\cdot(\mathbf{R}-\mathbf{R}^*) + \frac{1}{2}(\mathbf{R}-\mathbf{R}^*)^T\cdot D^2E(\mathbf{R}^*)\cdot(\mathbf{R}-\mathbf{R}^*) + \mathcal{O}(|\mathbf{R}-\mathbf{R}^*|^3)$$

$$= E(\mathbf{R}^*) + \frac{1}{2}(\mathbf{R}-\mathbf{R}^*)^T\cdot D^2E(\mathbf{R}^*)\cdot(\mathbf{R}-\mathbf{R}^*) + \mathcal{O}(|\mathbf{R}-\mathbf{R}^*|^3), \quad \text{for } |\mathbf{R}-\mathbf{R}^*| \text{ small},$$

requiring that

$$\mathbf{R}^T\cdot D^2E(\mathbf{R}^*)\cdot\mathbf{R} \geqslant 0 \quad \text{for any } \mathbf{R}\in\mathbb{R}^{3Z},$$

for $\mathbf{R}^*$ to be a local or global minimum.

Following the terminology of calculus of variations, we say that a critical point $\mathbf{R}^\wedge$ is *nondegenerate* if $D_{\mathbf{R}}^2E(\mathbf{R}^\wedge)$ is an invertible (i.e., nonsingular) $(3Z)\times(3Z)$ matrix. Otherwise, $\mathbf{R}^\wedge$ is said to be a *degenerate* critical point. Thus, a critical point is degenerate if and only if $D_{\mathbf{R}}^2E(\mathbf{R}^\wedge)$ has 0 as its eigenvalue. Here all the critical points are degenerate according to the following, due to the rotational invariance of the critical points (Theorem 1).

Theorem 3 (degeneracy of critical points): *Any critical point $\mathbf{R}^\wedge$ of $E(\mathbf{R})$ is degenerate. The dimension of degeneracy is at least 2.*

Proof: Any critical point $\mathbf{R}_0^\wedge$ satisfies (2.10) and, according to Theorem 1, $\mathcal{R}\mathbf{R}^\wedge$ is also a critical point for any 3D rotation $\mathcal{R}$,

$$DE(\mathcal{R}\mathbf{R}_0^\wedge) = \mathbf{0} \in \mathbb{R}^{3Z}. \tag{3.1}$$

From the theory of Lie groups in $\mathbb{R}^3$, we know that the rotation group SO(3) (i.e., the special orthogonal group) in $\mathbb{R}^3$ can be (essentially) parametrized by two independent parameters (θ_1,θ_2). So we may write $\mathcal{R}=\mathcal{R}(\theta_1,\theta_2)$ and define

$$\mathbf{R}^\wedge(\theta_1,\theta_2) \equiv \mathcal{R}(\theta_1,\theta_2)\mathbf{R}_0^\wedge. \tag{3.2}$$

Then by (3.1),

$$DE(\mathbf{R}^{\wedge}(\theta_1,\theta_2))=\mathbf{0} \quad \text{for all } \theta_1 \text{ and } \theta_2. \tag{3.3}$$

Thus, by the chain rule,

$$\frac{\partial}{\partial\theta_j}DE(\mathbf{R}^{\wedge}(\theta_1,\theta_2))=D^2E(\mathbf{R}^{\wedge}(\theta_1,\theta_2))\cdot\left[\frac{\partial}{\partial\theta_j}\mathbf{R}^{\wedge}(\theta_1,\theta_2)\right]=\mathbf{0}, \quad j=1,2. \tag{3.4}$$

Since

$$\frac{\partial}{\partial\theta_j}\mathbf{R}^{\wedge}(\theta_1,\theta_2)\neq\mathbf{0} \quad \text{for } j=1,2, \tag{3.5}$$

and $(\partial/\partial\theta_1)\mathbf{R}^{\wedge}(\theta_1,\theta_2)$ and $(\partial/\partial\theta_2)\mathbf{R}^{\wedge}(\theta_1,\theta_2)$ are linearly independent, because by holding $\theta_1=\theta_1^0$ and $\theta_2=\theta_2^0$, $\mathbf{R}^{\wedge}(\theta_1,\theta_2^0)$ and $\mathbf{R}^{\wedge}(\theta_1^0,\theta_2)$ form two independent trajectories when only one of θ_1 and θ_2 is allowed to vary, and $(\partial/\partial\theta_1)\mathbf{R}^{\wedge}(\theta_1,\theta_2^0)$ and $(\partial/\partial\theta_2)\mathbf{R}^{\wedge}(\theta_1^0,\theta_2)$ are the tangent vectors along these two independent trajectories. We conclude from (3.4) that the Hessian matrix $D^2E(\mathbf{R}^{\wedge})$ has two linearly independent eigenvectors corresponding to the eigenvalue 0. The proof is complete. □

The determination of *all* critical point $\mathbf{R}^{\dagger}$ from either (2.11) or analytically is no easy task. The following two theorems provide a systematic way to construct (unstable) saddle-type critical points which are not global minima.

Define a subset $\mathbb{R}_x^{3Z}$ of $\mathbb{R}^{3Z}$ by

$$\mathbb{R}_x^{3Z}=\{\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_Z)\in\mathbb{R}^{3Z}|\mathbf{r}_j=(x_j,y_j,z_j)^T=(x_j,0,0), \text{ for } j=1,2,\ldots,Z;x_j\in\mathbb{R}\}. \tag{3.6}$$

So $\mathbb{R}_x^{3Z}$ is a Z-dimensional subspace of $\mathbb{R}^{3D}$. The subspaces $\mathbb{R}_y^{3Z}$ and $\mathbb{R}_z^{3Z}$ can be defined likewise.

Theorem 4: *The minimization problem*

$$\min_{\mathbf{R}\in\mathbb{R}_x^{3Z}} E(\mathbf{R}) \tag{3.7}$$

has at least a (global) minimizer $\mathbf{R}_x^*\in\mathbf{R}_x^{3Z}$. *This* $\mathbf{R}_x^*$ *is also a critical point of* E *in* $\mathbb{R}^{3Z}$, *i.e.*, $DE(\mathbf{R}_x^*)=\mathbf{0}$. *In fact, any critical point* $\mathbf{R}_x^{\dagger}$ *of* $E(\mathbf{R})$ *in* $\mathbb{R}_x^{3Z}$ *is also a critical point of* E *in* $\mathbb{R}^{3Z}$, *i.e.*, $DE(\mathbf{R}_x^{\dagger})=\mathbf{0}$. *The same is true if* $\mathbb{R}_x^{3Z}$ *is replaced by* $\mathbb{R}_y^{3Z}$ *or* $\mathbb{R}_z^{3Z}$.

Proof: Because $\mathbb{R}_x^{3Z}$ is a closed subspace of $\mathbb{R}^{3Z}$, we can establish that (3.7) has a minimizer $\mathbf{R}_x^*$ in $\mathbb{R}_x^{3Z}$ by Corollary 2. The same conclusion follows for $\mathbb{R}_{y_x}^{3Z}$ and $\mathbb{R}_y^{3Z}$.

We now show how $\mathbf{R}_x^*$ satisfies $DE(\mathbf{R}_x^*)=\mathbf{0}$. Since $\mathbf{R}_x^*$ solves (3.7), we have the gradient equations

$$\frac{\partial}{\partial x_j}E(\mathbf{R})\big|_{\mathbf{R}=\mathbf{R}_x^*}=0, \quad \text{for } j=1,2,\ldots,Z; \text{ cf. (3.6) for } x_j.$$

The above gives

$$\left(\frac{n_j^2}{x_j^{*4}}-\frac{Z}{x_j^{*3}}+\sum_{\substack{k=1\\k\neq j}}^{Z}\frac{1}{2|x_k^*-x_j^*|^3}\right)x_j^*-\sum\frac{1}{2|x_k^*-x_j^*|^3}x_k^*=0, \quad j=1,2,\ldots,Z, \tag{3.8}$$

where x_j^*'s are the first components of $\mathbf{r}_j^*$, with $\mathbf{R}_x^*=(\mathbf{r}_1^*,\mathbf{r}_2^*,\ldots,\mathbf{r}_Z^*)$. Note that (3.8) just represents the first component (i.e., related to x) of the vector equations (2.12), with "†" therein replaced by "*." But the second and third components (related to y and z) are automatically satisfied because $y_j=z_j=0$ for $j=1,2,\ldots,Z$. □

Next, define the following subsets of $\mathbb{R}^{3Z}$:

$$\mathbb{R}_{x,y}^{3Z}=\{\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_Z)\in\mathbb{R}^{3Z}|\mathbf{r}_j=(x_j,y_j,z_j)=(x_j,y_j,0), \text{ for } j=1,2,\ldots,Z;x_j,y_j\in\mathbb{R}\},$$

$$\mathbb{R}^{3Z}_{x,z} = \{\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_z) \in \mathbb{R}^{3Z} | \mathbf{r}_j = (x_j, y_j, z_j) = (x_j, 0, z_j), \text{ for } j = 1,2, \ldots, Z; x_j, z_j \in \mathbb{R}\},$$

$$\mathbb{R}^{3Z}_{y,z} = \{\mathbb{R} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z) \in \mathbb{R}^{3Z} | \mathbf{r}_j = (x_j, y_j, z_j) = (0, y_j, z_j), \text{ for } j = 1,2, \ldots, Z; y_j, z_j \in \mathbb{R}\}.$$

Theorem 5: *The minimization problem*

$$\min_{\mathbf{R} \in \mathbb{R}^{3Z}_{x,y}} E(\mathbf{R})$$

has at least a (global) minimizer $\mathbf{R}^*_{x,y} \in \mathbb{R}^{3Z}_{x,y}$. *This* $\mathbf{R}^*_{x,y}$ *is a critical point of* $E(\mathbf{R})$ *in* $\mathbb{R}^{3Z}$, *i.e.*, $DE(\mathbf{R}^*_{x,y}) = \mathbf{0}$. *In fact, any critical point* $\mathbf{R}^\dagger_{x,y}$ *of* $E(\mathbf{R})$ *in* $\mathbb{R}^{3Z}_{x,y}$ *is also a critical point of* $E(\mathbf{R})$ *in* $\mathbb{R}^{3Z}$, *i.e.*, $DE(\mathbf{R}^\dagger_{x,y}) = \mathbf{0}$. *The same theorem holds if we replace* $\mathbb{R}^{3D}_{x,y}$ *above by* $\mathbb{R}^{3D}_{x,z}$ *or* $\mathbb{R}^{3D}_{y,z}$.

Proof: Same as that for Theorem 4. □

Corollary 3: Let V be a (coordinate) subspace of $\mathbb{R}^3$ *with dimension 1 or 2. Then any critical point of E on* V^Z *is a critical point of E on* $\mathbb{R}^{3Z}$.

Proof: Any such V can be obtained by a rotation from $\mathbb{R}^{3Z}_x$ or $\mathbb{R}^{3Z}_{x,y}$, respectively, if V has dimension of, respectively, 1 and 2. The corollary follows because E is rotationally invariant. □

Remark 2:

(i) Due to the rotational invariance of the critical points, there is *nonuniqueness* of the global minimum of $E(\mathbf{R})$. Thus, a *quotient space* needs to be used (or considered) if one wishes to have any uniqueness of the global minimum of E. Computationally, this 3D rotational congruence is avoided by setting up a coordinate frame using (5.1) in Sec. V.

(ii) According to Lemma 1, for any critical point $\mathbf{R}^\wedge$, the direction along the ray $\mathbf{R}^\wedge$ is a direction of increase for E. Therefore, $D^2_{\mathbf{R}} E(\mathbf{R}^\wedge)$ has *at least one positive eigenvalue*.

(iii) According to the numerical computation in Examples 2 and 3 in Sec. V, critical points computed by utilizing Theorems 4 and 5 and Corollary 3 all have some *negative eigenvalues* for the Hessian $D^2_R(E)$ at those critical points. Thus, in view of (ii) above, those critical points are all *saddle-type* unstable critical points. □

We conjecture that the energy function E as defined in Table I and (1.6) and (1.9) has only finitely many critical points $\mathbf{R}^\dagger$ satisfying $DE(\mathbf{R}^\dagger) = \mathbf{0}$, which are not rotationally equivalent. But we do not yet have a proof.

IV. COPLANARITY OF STABLE OR UNSTABLE ELECTRON CONFIGURATIONS

Numerical results (see Example in Sec. V) indicate that for $Z=3$ and 4, the stable electron configuration (corresponding to a global minimizer of E) has all electrons coplanar with the origin. For $Z=1$ and 2, the coplanarity is trivial. For $Z \geqslant 5$, numerical evidence suggests that coplanarity no longer holds.

Theorem 6 (co-planarity of the electrons with the origin, $Z=3$): Let $Z=3$. If $\mathbf{R}^\dagger = (\mathbf{r}^\dagger_1, \mathbf{r}^\dagger_2, \mathbf{r}^\dagger_3)$ *is a critical point of* $E(\mathbf{R})$ (*including the global minimizer* $\mathbf{R}^*$), *then* $\mathbf{r}^\dagger_1, \mathbf{r}^\dagger_2, \mathbf{r}^\dagger_3$, and $\mathbf{0}$ *are coplanar in* $\mathbb{R}^3$.

Proof: For clarity, we write out the system of equations (2.12),

$$\left(\frac{1}{r^{\dagger 4}_1} - \frac{3}{r^{\dagger 3}_1} + \frac{1}{r^{\dagger 3}_{12}} + \frac{1}{r^{\dagger 3}_{13}}\right)\mathbf{r}^\dagger_1 - \frac{1}{r^{\dagger 3}_{12}}\mathbf{r}^\dagger_2 - \frac{1}{r^{\dagger 3}_{13}}\mathbf{r}^\dagger_3 = \mathbf{0},$$

$$\left(\frac{1}{r^{\dagger 4}_2} - \frac{3}{r^{\dagger 3}_2} + \frac{1}{r^{\dagger 3}_{12}} + \frac{1}{r^{\dagger 3}_{23}}\right)\mathbf{r}^\dagger_2 - \frac{1}{r^{\dagger 3}_{12}}\mathbf{r}_1 - \frac{1}{r^{\dagger 3}_{23}}\mathbf{r}^\dagger_3 = \mathbf{0},$$

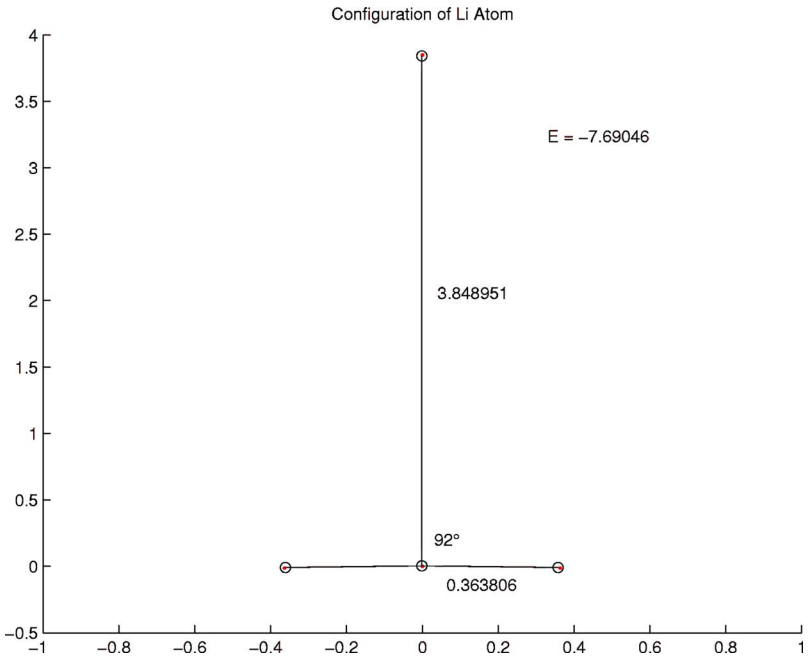

FIG. 1. For lithium (Li), $Z=3$. The electron configuration is shown. We have $r_1=r_2=0.363\,806$, $r_3=3.848\,951$, $\theta_2=1.605\,660=91.997\,541\,43^\circ\neq\pi/2$, $\theta_3=1.605\,660=91.997\,541\,31^\circ\neq\pi/2$, $\phi_3=\pi$, $E=-7.690\,46$(htr); htr=hartree.

$$\left(\frac{4}{r_3^{\dagger 4}}-\frac{3}{r_3^{\dagger 3}}+\frac{1}{r_{13}^{\dagger 3}}+\frac{1}{r_{23}^{\dagger 3}}\right)\mathbf{r}_3^{\dagger}-\frac{1}{r_{13}^{3}}\mathbf{r}_1^{\dagger}-\frac{1}{r_{23}^{\dagger 3}}\mathbf{r}_2^{\dagger}=\mathbf{0}. \tag{4.1}$$

If any single equation in (4.1) has all three coefficients of $\mathbf{r}_1^{\dagger}$, $\mathbf{r}_2^{\dagger}$, and $\mathbf{r}_3^{\dagger}$ to be nonzero, then any one vector in $\{\mathbf{r}_1^{\dagger},\mathbf{r}_2^{\dagger},\mathbf{r}_3^{\dagger}\}$ can be expressed as a linear combination of the other two vectors, and

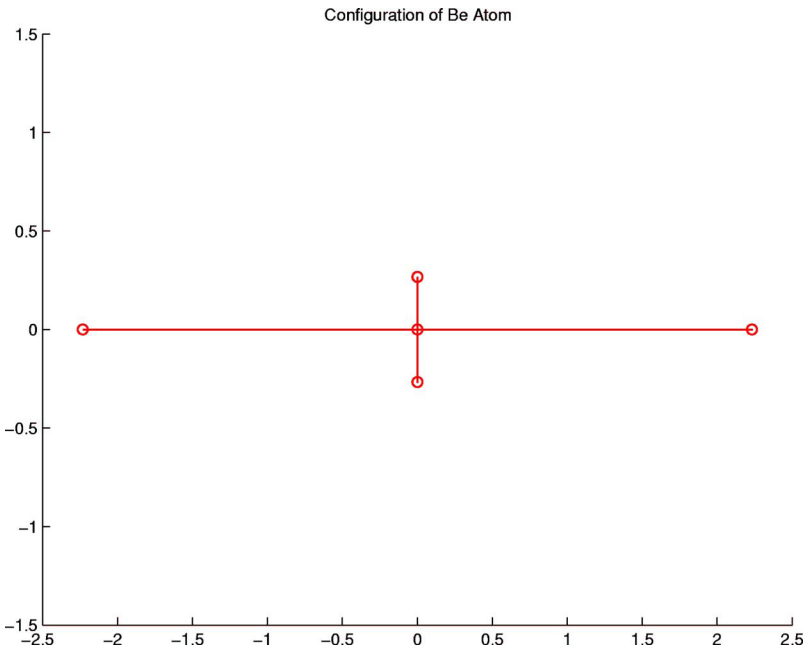

FIG. 2. (Color online) For beryllium (Be), $Z=4$. We have $r_1=r_2=0.266\,90$, $\theta_2=3.141\,59=\pi$, $r_3=r_4=2.231\,96$, $\theta_3=\theta_4=1.570\,80=\pi/2$, $\phi_3=\phi_4=3.141\,59=\pi$, $E=-14.840\,35$(htr).

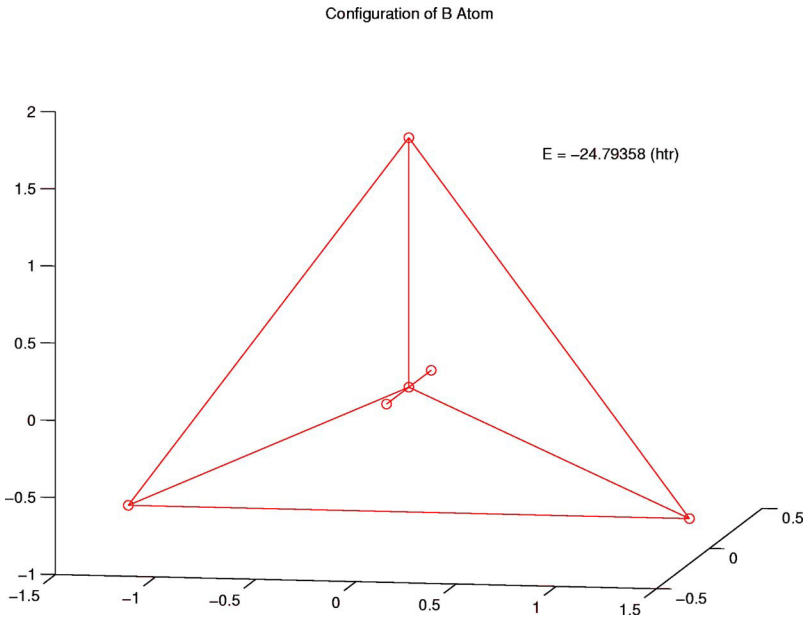

FIG. 3. (Color online) For boron (B), $Z=5$. We have $r_1=r_2=0.210\,81$, $r_3=r_4=r_5=1.617\,77$, $\theta_2=2.094\,40=2\pi/3$, $\theta_3=2.094\,40=2\pi/3$, $\phi_3=3.141\,59=\pi$, $\theta_4=1.570\,80=\pi/2$, $\phi_4=1.570\,80=\pi/2$, $\theta_5=1.570\,80=\pi/2$, $\phi_5=-1.570\,80=-\pi/2$, $E=-24.793\,58$(htr).

thus the proof follows. Therefore, the only possibility that $\mathbf{r}_1^\dagger$, $\mathbf{r}_2^\dagger$, $\mathbf{r}_3^\dagger$ and $\mathbf{0}$ are not coplanar is when

$$\frac{n_i^2}{r_i^{\dagger 4}} - \frac{3}{r_i^{\dagger 3}} - \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{1}{r_{ij}^\dagger} = 0 \quad \text{for } i = 1,2,3. \tag{4.2}$$

But the above implies, from (4.2), that

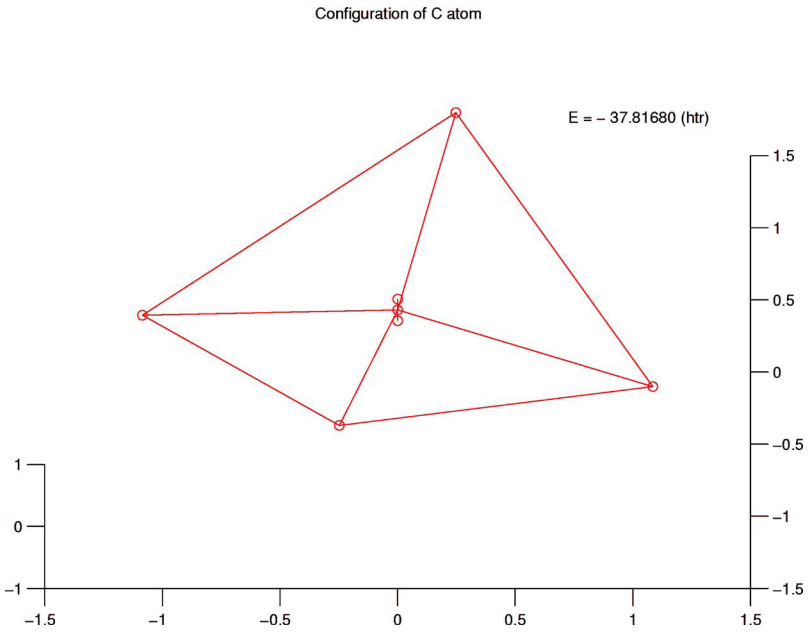

FIG. 4. (Color online) For carbon (C), $Z=6$. We have $r_1=r_2=0.173\,98$, $r_3=r_4=r_5=r_6=1.293\,53$, $\theta_2=3.141\,59=\pi$, $\theta_3=2.106\,38$, $\phi_3=-0.224\,66$, $\theta_4=1.035\,22$, $\phi_4=1.346\,14$, $\theta_5=2.106\,38$, $\phi_5=2.916\,93$, $\theta_6=1.035\,22$, $\phi_6=-1.795\,46$, $E=-37.816\,80$(htr).

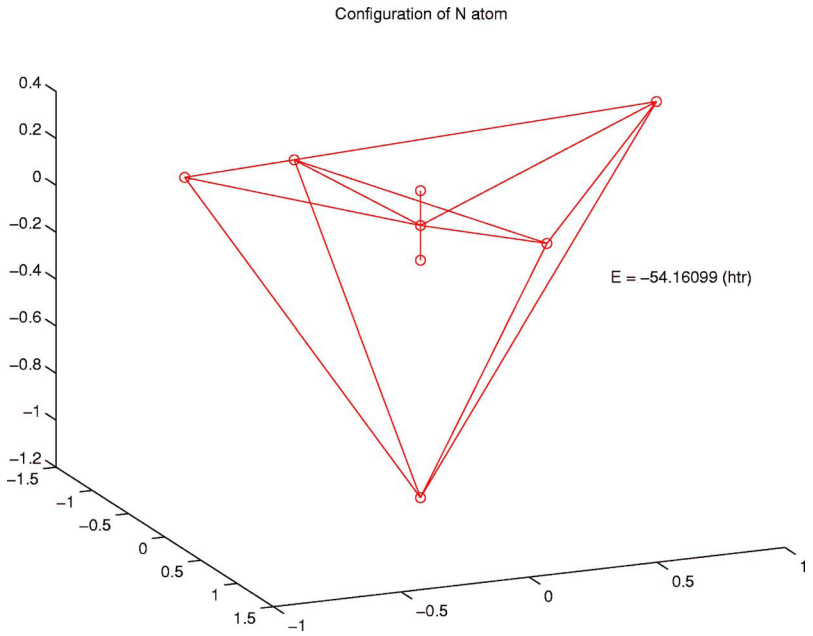

FIG. 5. (Color online) For nitrogen (N), $Z=7$. We have $r_1=r_2=0.148\,22$, $r_3=r_6=1.060\,95$, $r_4=r_5=1.051\,75$, $r_7=1.158\,87$, $\theta_2=3.141\,59=\pi$, $\theta_3=-\theta_6=1.218\,01$, $\phi_3=\phi_6=-0.195\,28$, $\theta_4=\theta_5=1.474\,08$, $\phi_4=1.375\,51$, $\phi_5=-1.766\,08$, $\theta_7=3.141\,59=\pi$, $\phi_7=0.328\,85$, $E=-54.160\,99$(htr).

$$\frac{1}{r_{12}^{\dagger 3}}\mathbf{r}_2^{\dagger}+\frac{1}{r_{13}^{\dagger 3}}\mathbf{r}_3^{\dagger}=\mathbf{0},\quad \frac{1}{r_{12}^{\dagger 3}}\mathbf{r}_1^{\dagger}+\frac{1}{r_{23}^{\dagger 3}}\mathbf{r}_3^{\dagger}=\mathbf{0},\quad \frac{1}{r_{12}^{\dagger 3}}\mathbf{r}_1^{\dagger}+\frac{1}{r_{23}^{\dagger 3}}\mathbf{r}_2^{\dagger}=\mathbf{0}.$$

Adding up the three equations in (4.2), we have

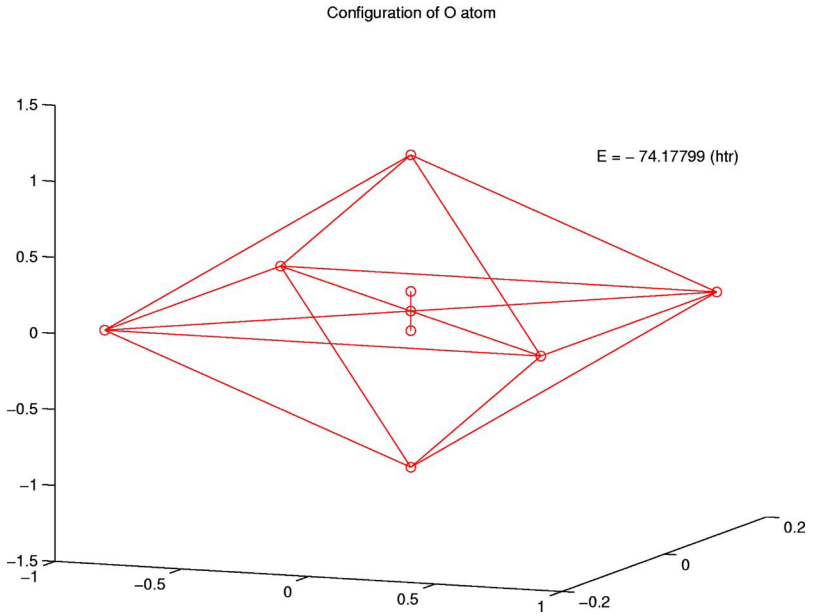

FIG. 6. (Color online) For oxygen (O), $Z=8$. We have $r_1=r_2=0.129\,10$, $r_3=r_4=r_5=r_6=0.877\,70$, $r_7=r_8=1.026\,74$, $\theta_2=\theta_8=\pi$, $\theta_3=\theta_4=\theta_5=\theta_6=\pi/2$, $\theta_7=0$, $\phi_3=-0.197\,20$, $\phi_4=1.373\,60$, $\phi_5=2.944\,40$, $\phi_6=-1.768\,00$, $\phi_7=-0.482\,03$, $\phi_8=-0.737\,23$, $E=-74.177\,99$(htr).

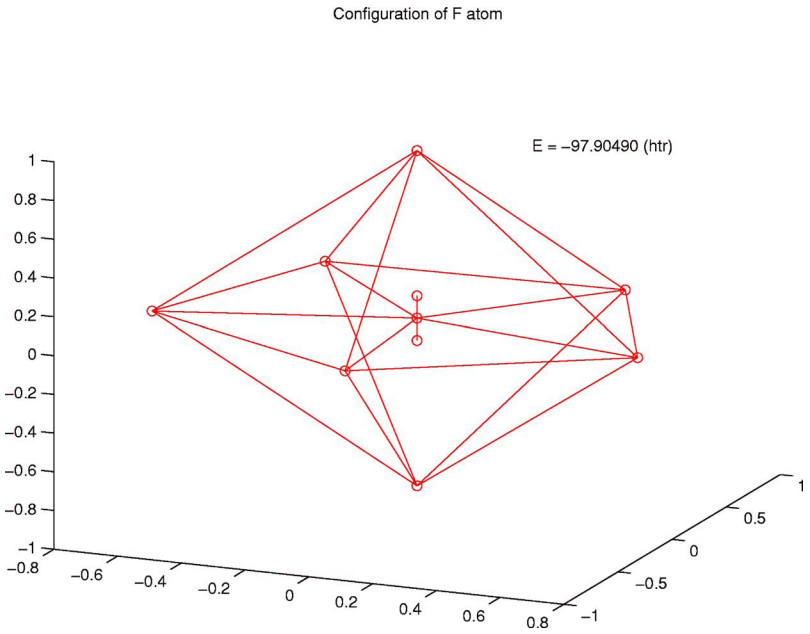

FIG. 7. (Color online) For fluorine (F), $Z=9$. We have $r_1=r_2=0.114\,35$, $r_3=r_4=r_5=r_6=r_7=0.78\,23$, $r_8=r_9=0.865\,58$, $\theta_2=\theta_9=\pi$, $\theta_3=\theta_4=\theta_5=\theta_6=\theta_7=\pi/2$, $\theta_8=0$, $\phi_3=-0.261\,52$, $\phi_4=0.995\,12$, $\phi_5=2.251\,76$, $\phi_6=3.508\,39$, $\phi_7=4.765\,03$, $\phi_8=-0.213\,56$, $\phi_9=-0.021\,96$, $E=-97.904\,90$(htr).

$$\sum_{i=}^{3}\left(\sum_{\substack{j=1\\ j\neq i}}^{3}\frac{1}{r_{ij}^{\dagger 3}}\right)\mathbf{r}_i^{\dagger}=\mathbf{0}.$$

Once again, any $\mathbf{r}_i^{\dagger}$ can be expressed as a linear combination of $\mathbf{r}_j^{\dagger}$ for $j\neq i$. Therefore, $\mathbf{r}_1^{\dagger}$, $\mathbf{r}_2^{\dagger}$, $\mathbf{r}_3^{\dagger}$ and $\mathbf{0}$ are coplanar. □

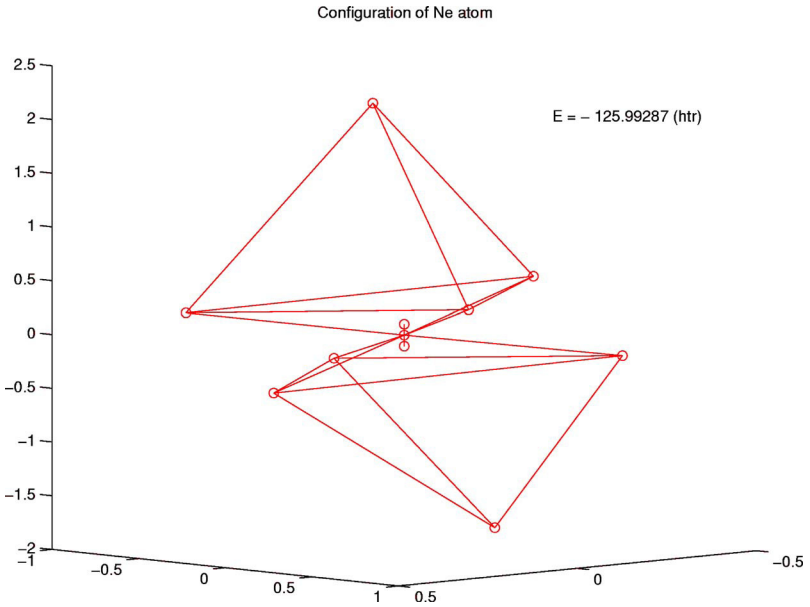

FIG. 8. (Color online) For neon (NE), $Z=10$. We have $r_1=r_2=0.102\,63$, $r_3=2.146\,17$, $r_4=0.637\,26$, $r_5=0.632\,88$, $r_6=0.633\,87$, $r_7=0.633\,55$, $r_8=0.630\,08$, $r_9=0.624\,96$, $r_{10}=1.870\,83$, $\theta_2=3.139\,87(\neq\pi)$, $\theta_3=-0.063\,17$, $\theta_4=0.990\,93$, $\theta_5=1.069\,46$, $\theta_6=0.985\,91$, $\theta_7=2.138\,22$, $\theta_8=2.114\,86$, $\theta_9=2.040\,94$, $\theta_{10}=3.016\,75$, $\phi_3=-0.168\,95$, $\phi_4=0.141\,27$, $\phi_5=2.172\,93$, $\phi_6=4.253\,46$, $\phi_7=1.110\,58$, $\phi_8=3.258\,05$, $\phi_9=-0.948\,26$, $\phi_{10}=-1.325\,32$, $E=-125.992\,87$(htr).

TABLE III. Locations of four critical points of problem (5.4). Note that only $\mathbf{R}_2^\dagger$ and $\mathbf{R}_3^\dagger$ are true minimizers for (5.4), while $\mathbf{R}_1^\dagger$, $\mathbf{R}_4^\dagger$, and $\mathbf{R}_5^\dagger$ are just local minima for (5.4).

	Coordinates [cf. (5.3)] (set $\phi_2=\pi$)					
Critical points	r_1	r_2	r_3	θ_1	θ_2	Energies
$\mathbf{R}_1^\dagger$	1.0334	0.3133	7.2778	0	0	−5.5985
$\mathbf{R}_2^\dagger$	0.3622	0.3647	4.1865	0	π	−7.6837
$\mathbf{R}_3^\dagger$	0.3647	0.3622	4.1865	π	0	−7.6837
$\mathbf{R}_4^\dagger$	1.0967	0.3174	2.2462	π	π	−5.7752
$\mathbf{R}_5^\dagger$	0.3174	1.0967	2.2462	π	π	−5.7752

At this time, we are not yet able to prove the coplanarity property for the case $Z=4$, which as Fig. 2 in the next section indicates, is true from numerical computation.

V. NUMERICAL EXAMPLES AND DATA

We first list in Table II the comparison between the experimental values of atoms' ground-state energies and those of the Bohr energies, for atom numbers between 2 and 30. There is a reasonable agreement between these values when Z is small. When the value of Z increases, the deviations also grow. Nevertheless, the *trend* of Bohr's atom energies look good.

We now provide several examples to illustrate stable as well as unstable electron configurations according to Bohr's model, by utilizing Theorems 4 and 5 and Corollary 3.

Example 1 (*stable electron configurations for the ground state of the Bohr atom model, with* $Z: 3 \leqslant Z \leqslant 10$): We set up the problem as follows. In order to avoid the 3D rotational congruence as stated in Theorem 1, we fix the direction of $\mathbf{r}_1$ along the positive z axis and that of $\mathbf{r}_2$ on the (x,z)-plane, as follows:[10]

$$\mathbf{r}_1 = r_1\mathbf{k},$$

$$\mathbf{r}_2 = r_2 \sin\theta_2\mathbf{i} + r_2\cos\theta_2\mathbf{k},$$

$$\mathbf{r}_i = r_i \sin\theta_i\cos\phi_i\mathbf{i} + r_i\sin\theta_i\sin\phi_i\mathbf{j} + r_i\cos\theta_i\mathbf{k}, \quad i \geqslant 3,$$

$$0 \leqslant \theta_i \leqslant \pi, \quad 0 \leqslant \phi_i \leqslant 2\pi, \quad i \geqslant 2. \tag{5.1}$$

Then the relative distances become

$$r_{1i} = (r_1^2 - r_i^2 - 2r_1r_i\cos\theta_i)^{1/2}, \quad 2 \leqslant i \leqslant Z,$$

$$r_{2i} = [r_2^2 + r_i^2 - 2r_2r_i(\sin\theta_2\sin\theta_i\cos\phi_i + \cos\theta_2\cos\phi_i)]^{1/2}, \quad 3 \leqslant i \leqslant Z,$$

TABLE IV. Eigenvalues of the Hessian with respect to the angular variables θ_1 and θ_2.

Point	Two eigenvalues of Hessian $[\partial^2 E/\partial\theta_i\partial\theta_j]$	Eigenvectors
$\mathbf{R}_1^\dagger$	−1.7530, −0.0187	$(-0.7120,-0.7022)^T$, $(0.7022,-0.7120)^T$
$\mathbf{R}_2^\dagger$	−0.0061, 0.6831	$(-0.7290,0.685)^T$, $(0.6845,0.7290)^T$
$\mathbf{R}_3^\dagger$	−0.0061, 0.6831	$(0.6845,-0.7290)^T$, $(-0.7290,-0.6845)^T$
$\mathbf{R}_4^\dagger$	−1.4170, 0.0542	$(0.7014,0.7128)^T$, $(-0.7128,0.7014)^T$
$\mathbf{R}_5^\dagger$	−1.4170, 0.0542	$(0.7014,0.7128)^T$, $(-0.7128,0.7014)$

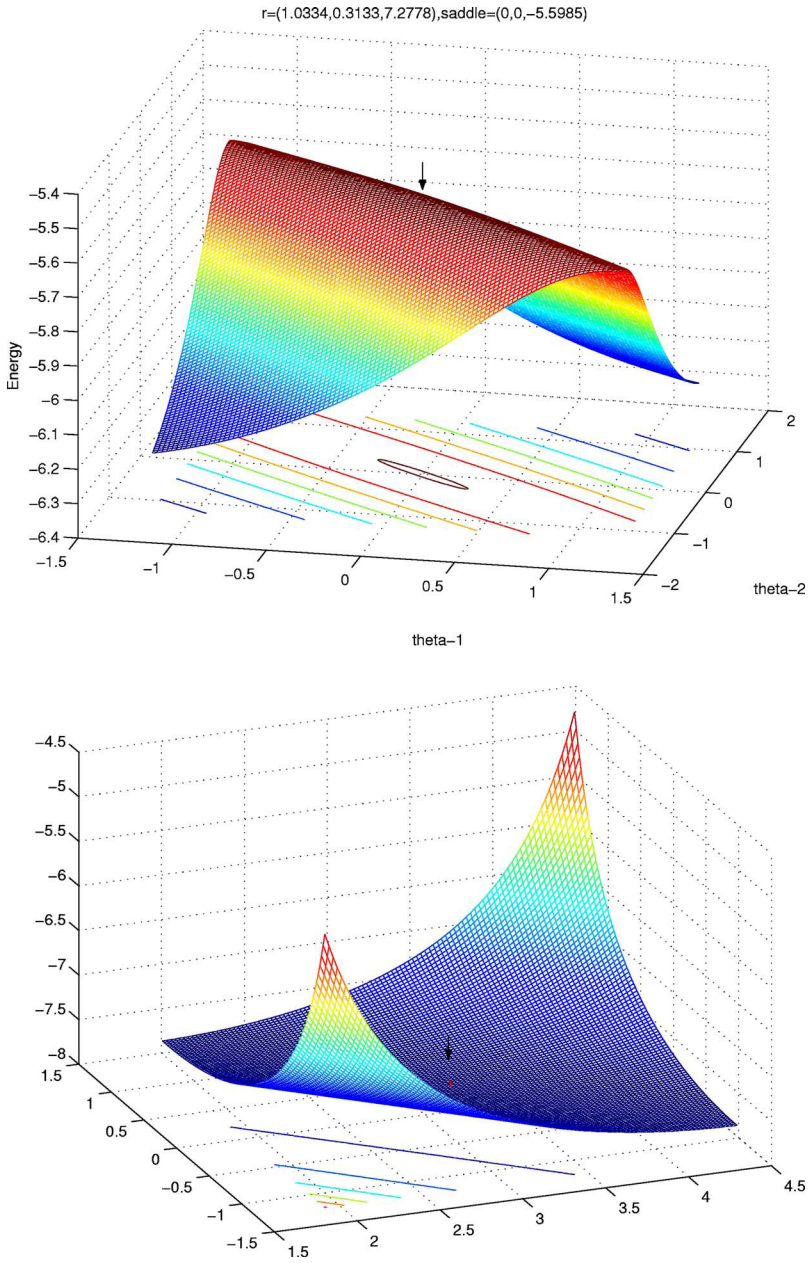

FIG. 9. (Color online) The energy surface E plotted against the angular variables θ_1 and θ_2 [cf. (5.3)] near the critical points $\mathbf{R}_i^{\dagger}$, $i=1,2,3,4,5$ (cf. Table III) in sequential order, whose locations are pin-pointed by an arrow. These surfaces are all of the saddle type.

$$r_{ij}=[r_i^2+r_j^2-2r_ir_j(\sin\,\theta_i\sin\,\theta_j\cos(\phi_i-\phi_j)+\cos\,\theta_i\cos\,\theta_j)]^{1/2},\quad 3\leqslant i<j<Z. \tag{5.2}$$

The stable electron configurations corresponding to minimal ground-state energy are shown in Figs. 1–8, along with the data given in the captions.

Example 2 (*saddle-type unstable colinear electron configurations,* $Z=3$): Consider the case of Li, $Z=3$. Write

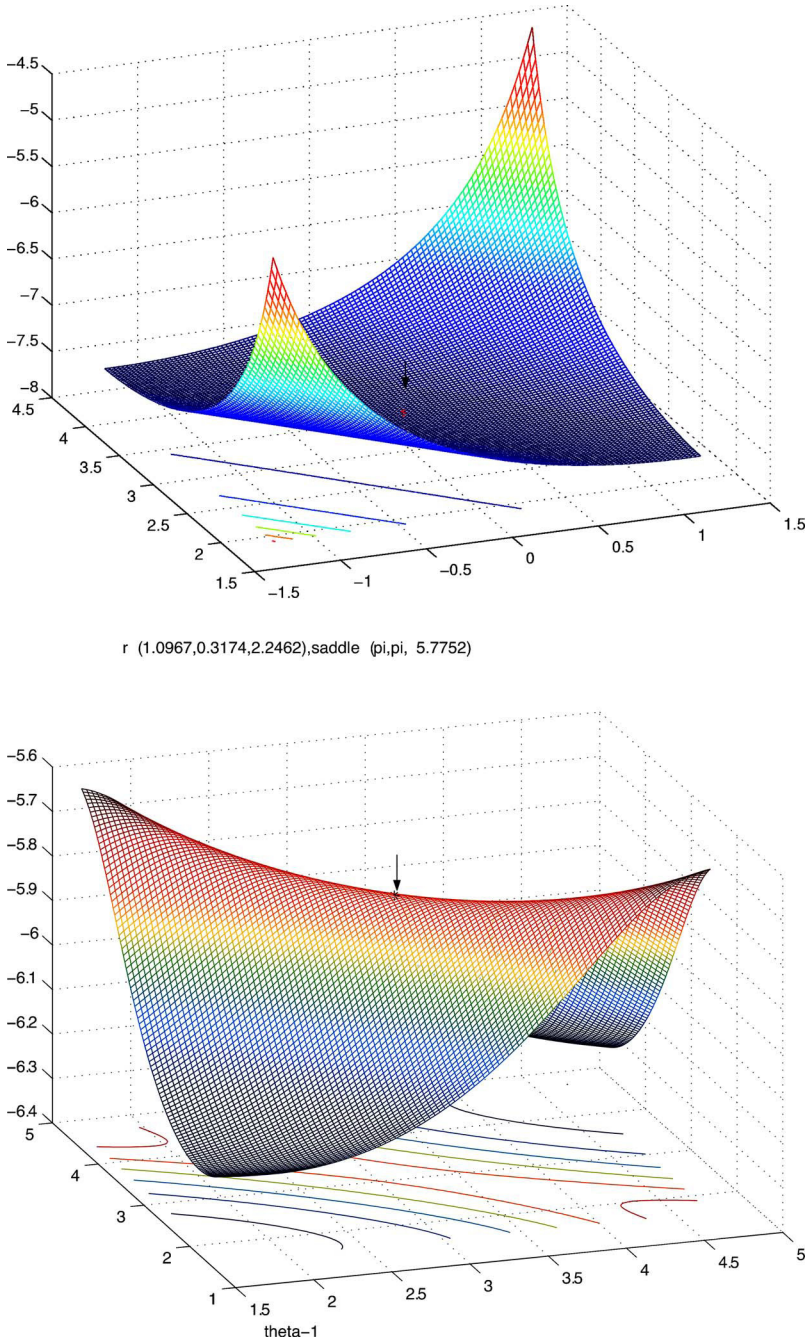

FIG. 9. (*Continued*).

$$\mathbf{r}_3 = r_3\mathbf{k}, \mathbf{r}_1 = r_1 \sin\theta_1\mathbf{i} + r_1 \cos\theta_1\mathbf{k},$$

$$\mathbf{r}_2 = r_2 \cos\theta_2\mathbf{k} + r_2 \sin\theta_2 \cos\phi_2\mathbf{i} + r_2 \sin\theta_2 \sin\phi_2\mathbf{j}. \tag{5.3}$$

We consider

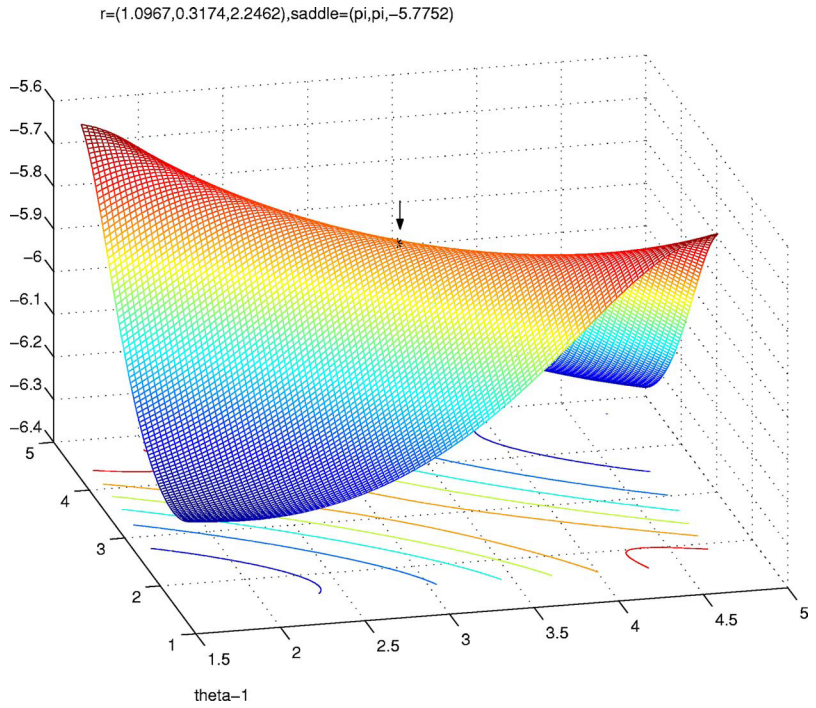

FIG. 9. (*Continued*).

$$\min_{\mathbf{R}\in\mathbb{R}^9_z} E(\mathbf{R}), \quad \mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\left(\begin{bmatrix}0\\0\\r_1\end{bmatrix},\begin{bmatrix}0\\0\\r_2\end{bmatrix},\begin{bmatrix}0\\0\\r_3\end{bmatrix}\right), \tag{5.4}$$

i.e., all three vectors $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are required to be colinear on the z axis. This can be done by setting $\phi_2=\pi$ and by requiring θ_1 and θ_2 to be equal to either 0 or π in (5.3).

For problem (5.4), we have found five critical points $\mathbf{R}_i^\dagger$, $i=1,2,3,4,5$, with respect to the three scalar variables r_1, r_2, and r_3. See Table III.

Note that by Theorem 4, all these points $\mathbf{R}_i^\dagger$, $i=1,2,3,4,5$, are critical points of E on $\mathbb{R}^{3Z}$. On the other hand, fix $\phi_2=\pi$ only. Then $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ are coplanar and

$$E(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\frac{1}{2r_1}+\frac{1}{2r_2}+\frac{4}{2r_3}-\sum_{i=1}^{3}\frac{3}{r_i}+\left(\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_3|}+\frac{1}{|\mathbf{r}_2-\mathbf{r}_3|}\right)\equiv E(r_1,r_2,r_3,\theta_1,\theta_2). \tag{5.5}$$

Numerical computations of the Hessian matrix $H=[\partial^2 E/\partial\theta_i\partial\theta_j]_{1\leqslant i,j\leqslant 2}$ and Lemma 1 show that, indeed, these $\mathbf{R}_i^\dagger$ are saddle-type critical points. See Table IV.

In Fig. 9, we plot the energy surfaces of E with respect to the angular variables θ_1 and θ_2 in a neighborhood of these critical points $\mathbf{R}_i^\dagger$.

It is quite interesting to note from Fig. 1 earlier that the global minimum value of E on $\mathbb{R}^9$ is −7.690 46 htr, while the global minimum value of E in (5.4) by restricting all $\mathbf{r}_i$, $i=1,2,3$, to lie on the z axis is −7.6837 htr (cf. Table III), which differs from −7.690 46 by less than 0.1%. □

Example 3 (*saddle type unstable coplanar electron configurations*, $Z=5$): In order to find unstable coplanar electron configurations, Z must be greater than or equal to 5, as Sec. IV has proved that $Z=3$ can only have stable configurations and Fig. 1 has provided a numerical evidence that $Z=4$ also has stable coplanar electron configurations. For $Z=5$, we apply Theorem 6 to find

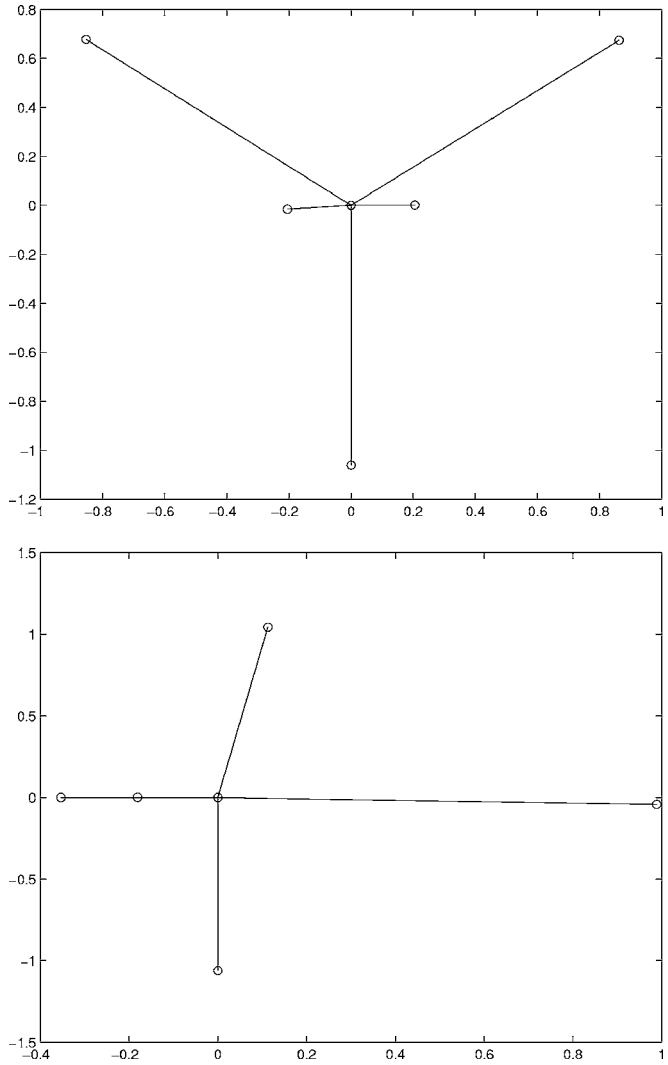

FIG. 10. For $Z=5$ (boron), the above three configurations are obtained according to Theorem 6 by finding critical points of E on the (x,y)-plane numerically. They should be contrasted with the one in Fig. 3. Coordinates of the five vectors, as well as the corresponding energy values, given from top to bottom for these three configurations, are $(-0.2045, -0.0156, 0)$, $(0.2050, 0.0014, 0)$, $(0.8625, 0.6741, 0)$, $(-0.8524, 0.6777, 0)$, $(0., -1.0604, 0)$ with $E_{\min}=-28.9146$; $(-0.3532, 0, 0)$, $(-0.1808, 0.0011, 0)$, $(0.9884, -0.0419, 0)$, $(0.1128, 1.0034, 0)$, $(0., -1.0610, 0)$ with $E_{\min}=-24.9439$; $(0.0661, 0.1942, 0)$, $(0.0628, -0.1781, 0)$, $(-6.4876, 0.3784, 0)$, $(-0.9024, 0.2594, 0)$, $(0., -1.5647, 0)$ with $E_{\min}=-27.5713$.

coplanar configurations, which must be of the saddle type and unstable, as Fig. 3 shows that a stable configuration cannot be coplanar. Several unstable configurations can be seen in Fig. 10.

VI. CONCLUSIONS

In this paper, we have conducted basic mathematical analysis for existence of minimal energy configurations and certain properties of critical points for the Bohr energy function. Relevant numerical results are also developed and presented.

There are still interesting problems remaining open. One among them is the *coplanarity* of the stable electron configuration for $Z=4$, which we have not yet been able to prove in Sec. IV. Also, the determination of the many symmetries manifested in Figs. 1–8 has not been achieved.

Bohr's original model for *molecules*[3] (which generalized the atomic case studied here) had

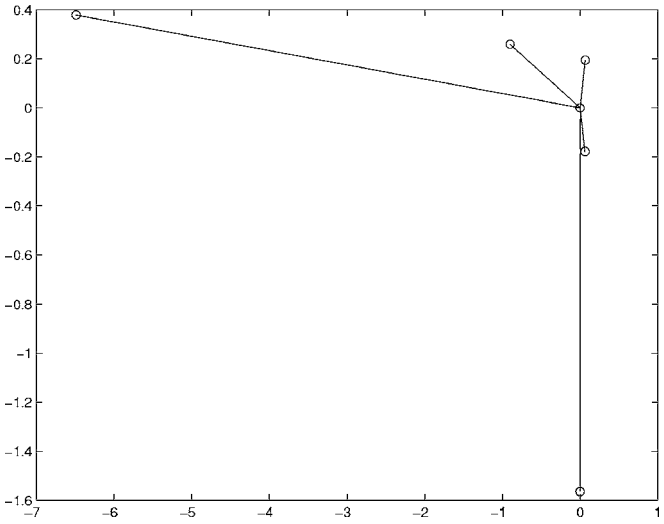

FIG. 10. (*Continued*).

some difficulties which has recently been improved by Svidzinsky, Scully, and Hershbach.[13] It has many interesting mathematical features therein worth investigation and we hope to be able to do it in the near future.

ACKNOWLEDGMENTS

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New families of finite coherent orthoalgebras without bivaluations

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In the present paper we study the following problem: how to construct a coherent orthoalgebra which has only a finite number of elements, but at the same time does not admit a bivaluation (i.e., a morphism with a codomain being an orthoalgebra with just two elements). This problem is important in the perspective of Bell-Kochen-Specker theory, since one can associate such an orthoalgebra to every saturated noncolorable finite configuration of projective lines. The first result obtained in this paper provides a general method for constructing finite orthoalgebras. This method is then applied to obtain a new infinite family of finite coherent orthoalgebras that do not admit bivaluations. The corresponding proof is combinatorial and yields a description of the groups of symmetries for these orthoalgebras. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2171691]

I. INTRODUCTION

Mackey formulated in his book[7] the axiomatics of nonrelativistic quantum mechanics based on the notion of an *orthomodular poset*. That is just a partially ordered set equipped with an involution, such that certain axioms hold. These axioms are chosen such that the elements of this poset may be identified with binary observables of a quantum system. Compared to the traditional axiomatics in terms of linear operators on Hilbert spaces,[11] this system focuses on the *logical* aspects of quantum theory. In fact, the Hilbert space is introduced only at the final stage in a completely *ad hoc* manner.

In alternative terminology, an orthomodular poset is called a *coherent orthoalgebra*, and an orthoalgebra is a particular case of an *effect algebra*. Let us provide some motivation for the introduction of these notions. Consider a Hilbert space $\mathcal{H}$ over $\mathbb{C}$, and denote by $L(\mathcal{H})$ a collection of closed linear manifolds in it. For every $U \in L(\mathcal{H})$, we have an orthogonal projector $\hat{\pi}_U$ on U, which represents an observable with two possible values, 0 and 1. Two observables represented by $\hat{\pi}_U$ and $\hat{\pi}_{U_1}$, $U, U_1 \in L(\mathcal{H})$, are *compatible* iff their commutator $[\hat{\pi}_U, \hat{\pi}_{U_1}]=0$. The first step towards the notion of an effect algebra is based on the following remark. The mentioned commutator vanishes iff $\mathcal{H}$ splits into an orthogonal sum $\mathcal{H}=Z\oplus V\oplus V_1\oplus W$, such that $Z\oplus V=U$ and $Z\oplus V_1=U_1$. The idea is to reformulate everything in terms of orthogonal decomposition.

Consider $\cdot\oplus\cdot$ as a partially defined binary operation on $L(\mathcal{H})$ with domain of definition consisting of all pairs (U, U_1) such that $U_1 \subset U^\perp$. Note that $U_1 \subset U^\perp$ is equivalent to $U \subset U_1^\perp$. Consider $L(\mathcal{H})$ as a partially ordered set with respect to inclusion $\subset$. Then the map $U \mapsto U^\perp$ is an involution on $L(\mathcal{H})$, since $U^{\perp\perp}=U$ and for all U and U_1 we have $U \subset U_1 \Leftrightarrow U^\perp \supset U_1^\perp$. Note, that it is possible to express the partial order $\subset$ in terms of the $\cdot\oplus\cdot$ operation: $U \subset U_1$ iff $\exists V: V\oplus U = U_1$. The involution $(\cdot)^\perp: L(\mathcal{H}) \to L(\mathcal{H})$, admits a similar characterization. For every U, there exists a unique U_1, such that $U_1 \oplus U = \mathcal{H}$; this U_1 is precisely $U^\perp$.

Take any $U, U_1 \in L(\mathcal{H})$. If the corresponding two observables are compatible, then the following formulas are valid:

$$\inf\{U,U_1\}\oplus U^{\perp}=U_1\oplus\sup\{U,U_1\}^{\perp},$$
$$\inf\{U,U_1\}\oplus U_1^{\perp}=U\oplus\sup\{U,U_1\}^{\perp}. \tag{1}$$

Moreover, it is not difficult to prove that $\hat{\pi}_U$ and $\hat{\pi}_{U_1}$ are compatible exactly when these two equalities (1) are valid. Which properties of $\cdot\oplus\cdot$ are actually needed in this proof? It turns out that it is convenient to capture these properties within the notion of an *effect algebra*.

Let S be a set, and $R\subset S\times S$ a relation on S. Let $\cdot\oplus\cdot:R\to S$, $(x,y)\mapsto x\oplus y$, be a map. Let $\mathbf{0}$ and $\mathbf{1}$ be two elements in S, such that $\mathbf{1}\neq\mathbf{0}$. The algebraic structure $(S,\oplus,\mathbf{0},\mathbf{1})$ is called an *effect algebra* if for all $x,y,z\in S$ the following conditions are satisfied:

(1) if $x\oplus y$ is defined, then $y\oplus x$ is defined and $y\oplus x=x\oplus y$;
(2) if $(x\oplus y)\oplus z$ is defined, then $x\oplus(y\oplus z)$ is defined and $x\oplus(y\oplus z)=(x\oplus y)\oplus z$;
(3) $x\oplus\mathbf{0}=x$;
(4) if $x\oplus y=x\oplus z$, then $y=z$;
(5) there exists $x^*\in S$, such that $x^*\oplus x=\mathbf{1}$;
(6) if $x\oplus\mathbf{1}$ is defined, then $x=\mathbf{0}$.

Note that for each x, the element x^* is uniquely defined. Hence, to every effect algebra $X=(S,\oplus,\mathbf{0},\mathbf{1})$ one associates a map $(\cdot)^*:S\to S$, $x\mapsto x^*$. The set S is termed the *ground* set of X.

An effect algebra is called an *orthoalgebra*, if for any element x of the ground set, such that $x\oplus x$ is defined, we have $x=\mathbf{0}$. Note that this property together with the first five axioms, implies the sixth axiom. An othoalgebra is called *coherent* if for all x, y, and z in the ground set, such that $x\oplus y$, $y\oplus z$, and $z\oplus x$ are defined, the $x\oplus y\oplus z$ is defined.

The basic example of an effect algebra is, of course, the following: $S=L(\mathcal{H})$, $\oplus$ is the orthogonal sum defined for all (U,U_1) such that $U_1\subset U^{\perp}$, $\mathbf{0}=\theta_{\mathcal{H}}$ is the trivial subspace of $\mathcal{H}$, and $\mathbf{1}=\mathcal{H}$. Denote this effect algebra by $\mathbb{L}(\mathcal{H})$. In fact, it is a coherent orthoalgebra. Just as for $\mathbb{L}(\mathcal{H})$, one can define for every effect algebra $X=(S,\oplus,\mathbf{0},\mathbf{1})$ a partial order $\preccurlyeq$ on the ground set S (termed the *standard* partial order): $\forall x,y\in S: x\preccurlyeq y:\Leftrightarrow\exists x_1: x_1\oplus x=y$. The map $(\cdot)^*$ is an involution with respect to $\preccurlyeq$. It is possible to imitate the notion of compatibility on any effect algebra as follows: call two elements $U,U_1\in S$ *compatible*, if the set $\{U,U_1\}$ has infimum and supremum (with respect to the standard partial order), and the formulas of the form (1) (with $\perp$ replaced by *) are valid. Such a definition of compatibility, is additionally justified by the following fact: for any compatible U and U_1, there exists a decomposition of $\mathbf{1}$ of the form $\mathbf{1}=Z\oplus V\oplus V_1\oplus W$, such that $Z\oplus V=U$ and $Z\oplus V_1=U_1$.

Since the notion of a coherent orthoalgebra captures up to certain extent the essential properties of $L(\mathcal{H})$, it presents special interest to investigate the case when the ground set is *finite*. By that one may try to imitate quantum mechanics on a finite set. The latter is not only conceptually interesting, but also can be important for the computational methods. Of course, it is necessary to have a "complicated enough" example for this case.

It is natural to introduce a category of effect algebras $\mathcal{E}$ with morphisms $f:(S,\oplus,\mathbf{0},\mathbf{1})\to(S',\oplus',\mathbf{0}',\mathbf{1}')$ being the maps $\bar{f}:S\to S'$ such that $\bar{f}(\mathbf{0})=\mathbf{0}'$, $\bar{f}(\mathbf{1})=\mathbf{1}'$, and $\bar{f}(x\oplus y)=\bar{f}(x)\oplus'\bar{f}(y)$, whenever $x\oplus y$ is defined. The composition of morphisms is defined by the composition of the corresponding maps. Consider the most simple effect algebra that can be—the effect algebra with only two elements—$\mathbf{0}$ and $\mathbf{1}$. This is an initial object in the category of effect algebras. There is only one way to define $\oplus$ in this case $\mathbf{0}\oplus\mathbf{0}:=\mathbf{0}$, $\mathbf{0}\oplus\mathbf{1}=\mathbf{1}\oplus\mathbf{0}:=\mathbf{1}$, and $\mathbf{1}\oplus\mathbf{1}$—undefined. Denote this object by $\mathbb{B}$ and call it the *minimal Boolean* effect algebra. The other example of an effect algebra that has been described above is $\mathbb{L}(\mathcal{H})$. Call it the *Hilbert* effect algebra. Is it possible to have an arrow from $\mathbb{L}(\mathcal{H})$ to $\mathbb{B}$ in the category $\mathcal{E}$? The answer is well known from functional analysis (Gleason's theorem) and is negative. At the same time there is another important example of an effect algebra $(S,\oplus,\mathbf{0},\mathbf{1})$, for which such an arrow exists. Let $S=\mathcal{F}$, where $\mathcal{F}$ is some σ-algebra of subsets of a set Ω. Define $U\oplus U_1$ as $U\cup U_1$ for all *disjoint* $U,U_1\in\mathcal{F}$. Set $\mathbf{0}=\varnothing$ and $\mathbf{1}=\Omega$. This defines an effect algebra, denoted by $\mathbb{W}(\mathcal{F})$ and called *Kolmogorov* effect algebra. Any

$\mathbb{W}(\mathcal{F})$ admits a morphism f to $\mathbb{B}$: one may fix any $\omega \in \Omega$ and for each $U \in \mathcal{F}$ set $\bar{f}(U)=\mathbf{1}$ if $U \ni \omega$, and $\mathbf{0}$—otherwise.

The Kolmogorov and Hilbert effect algebras, $\mathbb{W}(\mathcal{F})$ and $\mathbb{L}(\mathcal{H})$, are different, and this is clear if one looks at all morphisms ending in the minimal Boolean effect algebra $\mathbb{B}$. This motivates the following mathematical problem. For any $X \in \mathcal{E}$, let us call an arrow $f: X \to \mathbb{B}$ (if it exists) a *bivaluation*. Denote by *for* the forgetful functor from $\mathcal{E}$ to the category of sets, $for: \mathcal{E} \to \mathbf{Sets}$. One is required to find in $\mathcal{E}$ such objects X, which do not admit a bivaluation, but have a finite ground set *for* (X). In the present paper an infinite family of such objects is constructed.

Let us make several bibliographical remarks to conclude the introduction. The analysis of logical foundations of quantum mechanics has been initiated in the famous paper by Birkhoff and von Neumann.[1] The new wave of interest to this subject is motivated by the recent developments in quantum computing technology. For an up to date discussion of effect algebras, orthoalgebras, and similar structures, one should refer to the monograph.[2] The terms effect algebra and orthoalgebra were suggested in Refs. 3 and 4, respectively. The importance of orthoalgebras is also clear in the perspective of the consistent histories approach to quantum theory.[5]

The results obtained in the present paper are related to the results of Refs. 10 and 11, and may be viewed as their generalization. The orthoalgebras described below yield a family of "indeterministic objects" in the terminology of Ref. 9. Every saturated (in the sense of Ref. 10) Kochen-Specker-type configuration of projective lines naturally yields a finite orthoalgebra not admitting a bivaluation.

II. GENERAL CONSTRUCTION

How to construct a *finite* orthoalgebra, which will look "similar" to the Hilbert orthoalgebra? The starting point can be the following. Consider a Hilbert space $\mathcal{H}$ over $\mathbb{C}$ of finite dimension d. Let $\mathbb{P}(\mathcal{H})$ denote the set of projective lines in $\mathcal{H}$. Consider the set $\mathcal{P}_\perp(\mathbb{P}(\mathcal{H}))$ consisting of all subsets $U \subset \mathbb{P}(\mathcal{H})$ satisfying the condition $\forall l, l_1 \in U: l_1 \neq l \Rightarrow l \perp l_1$. Note, that the empty set and any subset with only one element, belong to $\mathcal{P}_\perp(\mathbb{P}(\mathcal{H}))$. There is a natural equivalence relation $\sim$ on this set: $U \sim U_1 :\Leftrightarrow \operatorname{span} U_1 = \operatorname{span} U$ (the span of the empty set is $\theta_\mathcal{H}$ by definition). It is clear, that the set $\mathcal{L}(\mathcal{H}) := \mathcal{P}_\perp(\mathbb{P}(\mathcal{H}))/\sim$ is in natural bijection with $L(\mathcal{H})$. Hence, the structure of orthoalgebra on $L(\mathcal{H})$ induces a structure of orthoalgebra on $\mathcal{L}(\mathcal{H})$. For $[U],[U_1] \in \mathcal{L}(\mathcal{H})$ ($[\cdot]$ denotes the equivalence class with respect to $\sim$), the value of $[U] \oplus [U_1]$ is defined iff $U \cap U_1 = \varnothing$ and $U \cup U_1 \in \mathcal{P}_\perp(\mathbb{P}(\mathcal{H}))$, and it is equal to $[U \cup U_1]$.

This leads to the first (naive) idea of how to construct examples of finite orthoalgebras. Take a *finite* set A equipped with some relation $T \subset A \times A$, which is thought to imitate the orthogonality relation $\perp$. In analogy with $\mathcal{L}(\mathcal{H})$, consider the set

$$\mathcal{P}_T(A) := \{U \subset A \mid \forall\, l, l_1 \in U: l_1 \neq l \Rightarrow (l, l_1) \in T\},$$

and try to find an equivalence relation $\sim$ on it, such that the formula $[U] \oplus [U_1] := [U \cup U_1]$ yields the structure of an orthoalgebra. It is necessary to describe this equivalence relation in terms of T. After that one faces the difficulty to find some reasonable conditions on T, entailing the axioms of an effect algebra.

It turns out that there is a better idea. For *any* $B \subset A$, denote

$$B^T := \{l \in A \mid \forall\, l_1 \in A: l_1 \in B \Rightarrow (l_1, l) \in T\}.$$

Consider a map $\tau: \mathcal{P}_T(A) \to \mathcal{P}(A)$, $U \mapsto U^T$, and look at the image of this map,

$$\mathcal{P}^T(A) := \operatorname{Im}(\mathcal{P}_T(A) \ni U \mapsto U^T). \tag{2}$$

Take it as a ground set for the future orthoalgebra. Note, that if one specializes A to $\mathbb{P}(\mathcal{H})$, and T to the orthogonality relation $\perp$, then for $U, U_1 \in \mathcal{P}_T(A)$ one has $\tau(U) = \tau(U_1)$, whenever $\operatorname{span} U_1 = \operatorname{span} U$. It is natural to try to define the $\oplus$ operation by the formula

$$Q \oplus Q_1 := (Q \cup Q_1)^{TT}, \tag{3}$$

for all $Q, Q_1 \in \mathcal{P}^T(A)$, such that $Q_1 \subset Q^T$. Of course, it is necessary to impose some conditions on T, which ensure that $\oplus$ is well defined, since the right-hand side is not *a priori* in $\mathcal{P}^T(A)$. The axioms of an orthoalgebra will induce the other conditions on T.

First, since T is supposed to imitate the orthogonality relation $\perp$, one needs to require for all $l, l_1 \in A$, $l_1 \neq l$, the following:

$$(l, l_1) \in T \Leftrightarrow (l_1, l) \in T, \tag{4}$$

$$(l, l) \in T. \tag{5}$$

Impose one more condition,

$$\forall M \in \mathrm{Max}(\mathcal{P}_T(A); \subset)\ \forall B \subset M: B^T = (M \setminus B)^{TT}, \tag{6}$$

where Max(−) means taking the *set* of all maximal subsets of the partially ordered set. Note that this condition is valid for the case $A = \mathbb{P}(\mathcal{H})$ and $T = \perp$. Let us say that T is *saturated* if it satisfies (6).

Theorem 1: *Let A be a finite nonempty set and T be a relation on A. Let $\mathcal{P}^T(A)$ be defined by* (2). *If T satisfies the three conditions* (4)–(6), *then*

(1) *A and $\varnothing$ belong to $\mathcal{P}^T(A)$;*
(2) *$\oplus$ is well-defined by the formula* (3);
(3) *$(\mathcal{P}^T(A), \oplus, \varnothing, A)$ is a coherent orthoalgebra.*

Proof: (1) Since $\varnothing \in \mathcal{P}_T(A)$, and $\varnothing^T = A$, one has $A \in \mathcal{P}^T(A)$. Now, take any $M \in \mathrm{Max}(\mathcal{P}_T(A); \subset)$, set $B = M$, and apply the third condition on T above. This yields $M^T = (M \setminus M)^{TT} = \varnothing^{TT} = A^T$. If A^T is not empty, then one can take any $l \in A^T$ and applying the definition of $(\cdot)^T$ claim, that $(l, l) \in T$. But this contradicts the first condition on T above. Hence, $A^T = \varnothing$. Therefore, $\varnothing = M^T \in \mathcal{P}^T(A)$.

(2) Take any $Q, Q_1 \in \mathcal{P}_T(A)$, such that $Q_1 \subset Q^T$. It is necessary to show that $(Q \cup Q_1)^{TT} \in \mathcal{P}^T(A)$. Invoking the main condition on T, represent Q and Q_1 in the form $Q = U^T = (M \setminus U)^{TT}$, and $Q_1 = U_1^T = (M_1 \setminus U_1)^{TT}$, where $U, U_1 \in \mathcal{P}_T(A)$, $M, M_1 \in \mathrm{Max}(\mathcal{P}_T(A); \subset)$, and $M \supset U$, $M_1 \supset U_1$. Since $Q_1 \subset Q^T$, for any $l \in (M \setminus U)^{TT}$ and any $l_1 \in (M_1 \setminus U_1)^{TT}$, one has $(l, l_1) \in T$. Note, that due to the symmetry of T, for all $B \subset A$ there is an inclusion $B^{TT} \supset B$. Indeed, take any $\lambda_0 \in B$. In order to show, that $\lambda_0 \in B^{TT}$, one must show that $\forall \lambda_1 \in B^T: (\lambda_1, \lambda_0) \in T$. But the definition of B^T implies that $\forall \lambda \in B\, \forall \lambda_1 \in B^T: (\lambda, \lambda_1) \in T$. Since T is symmetric, the order of appearance of λ and λ_1 in $(\lambda, \lambda_1) \in T$ is unimportant, and one obtains $B \subset B^{TT}$. Now, return to Q and Q_1. One has $Q = U^T = (M \setminus U)^{TT}$, and $Q_1 = U_1^T = (M_1 \setminus U_1)^{TT}$. Take any $l \in M \setminus U$, and any $l_1 \in M_1 \setminus U_1$. Since $M \setminus U \subset (M \setminus U)^{TT}$, and $M_1 \setminus U_1 \subset (M_1 \setminus U_1)^{TT}$, the elements l and l_1 are in Q and Q_1, respectively. From $Q_1 \subset Q^T$, one obtains $(l, l_1) \in T$. Therefore, $(M \setminus U) \cup (M_1 \setminus U_1) \in \mathcal{P}_T(A)$. Now note, that for any $B, B_1 \subset A$, the definition of $(\cdot)^T$, without any assumptions on T, implies $(B \cup B_1)^T = B^T \cap B_1^T$. This together with the main condition, yields

$$(Q \cup Q_1)^{TT} = (Q^T \cap Q_1^T)^T = (U^{TT} \cap U_1^{TT})^T = ((M \setminus U)^T \cap (M_1 \setminus U_1)^T)^T = ((M \setminus U) \cup (M_1 \setminus U_1))^{TT}.$$

Before proceeding further, let us prove two simple auxiliary facts. Recall, that $A, \varnothing \in \mathcal{P}^T(A)$, and we have $\varnothing^T = A$, $A^T = \varnothing$. Therefore $\varnothing^{TT} = \varnothing$, $A^{TT} = A$. Let us show that for any $Q_0 \in \mathcal{P}^T(A)$, the element $Q_0^T \in \mathcal{P}^T(A)$, and $Q_0^{TT} = Q_0$. Indeed, take any Q_0 and represent it in the form $Q_0 = U_0^T$, $U_0 \in \mathcal{P}_T(A)$. For any $M_0 \supset U_0$, $M_0 \in \mathrm{Max}(\mathcal{P}_T(A); \subset)$, the main condition implies $Q_0^T = U_0^{TT} = (M_0 \setminus U_0)^T$. Since $M_0 \setminus U_0 \in \mathcal{P}_T(A)$, one has $Q_0^T \in \mathcal{P}^T(A)$. Now, for Q_0^{TT}, we have $Q_0^{TT} = (U_0^{TT})^T = ((M_0 \setminus U_0)^T)^T = (M_0 \setminus U_0)^{TT} = U_0^T = Q_0$ (we have used the main condition once more).

Specializing $Q_0 \in \mathcal{P}^T(A)$ to $((M \setminus U) \cup (M_1 \setminus U_1))^T = (M \setminus U)^T \cap (M_1 \setminus U_1)^T = U^{TT} \cap U_1^{TT} = (U^T \cup U_1^T)^T = (Q \cup Q_1)^T$, we obtain $\mathcal{P}^T(A) \ni Q_0^T = (Q \cup Q_1)^{TT}$, i.e., $\oplus$ is well defined.

(3) Let us start with the axioms of an effect algebra. Consider the first axiom. Take any $Q,Q_1\in\mathcal{P}^T(A)$ such that $Q_1\subset Q^T$. The latter inclusion means, that for any $l\in Q$ and any $l_1\in Q_1$, the pair $(l,l_1)\in T$. Since T is symmetric, $(l_1,l)\in T$. Hence, $Q_1\subset Q^T$ is equivalent to $Q\subset Q_1^T$, i.e., $Q\oplus Q_1$ is defined iff $Q_1\oplus Q$ is defined. We have $Q\oplus Q_1=(Q\cup Q_1)^{TT}=(Q_1\cup Q)^{TT}=Q_1\oplus Q$.

Next, let us verify the second axiom. Take any $Q,Q_1,Q_2\in\mathcal{P}^T(A)$, and assume that $(Q\oplus Q_1)\oplus Q_2$ is defined. We have

$$(Q\oplus Q_1)\oplus Q_2=((Q\cup Q_1)^{TT}\cup Q_2)^{TT}=((Q\cup Q_1)^{TTT}\cap Q_2^T)^T=((Q\cup Q_1)^T\cap Q_2^T)^T$$
$$=(Q^T\cap Q_1^T\cap Q_2^T)^T=(Q\cup Q_1\cup Q_2)^{TT}.$$

Hence, if we can prove that $Q\oplus(Q_1\oplus Q_2)$ is defined as well, then $Q\oplus(Q_1\oplus Q_2)=(Q_1\oplus Q_2)\oplus Q=(Q_1\cup Q_2\cup Q)^{TT}$, and then the second axiom is established. So, we assume $Q_1\subset Q^T$ and $Q_2\subset(Q\oplus Q_1)^T$, and need to verify two inclusions, $Q_2\subset Q_1^T$ and $Q\subset(Q_1\oplus Q_2)^T$. Recall that whenever $Q\oplus Q_1$ is defined, we know that $(Q\cup Q_1)^T\in\mathcal{P}^T(A)$. Derive, $Q_2\subset(Q\oplus Q_1)^T=((Q\cup Q_1)^{TT})^T=(Q\cup Q_1)^T=Q^T\cap Q_1^T$. In particular $Q^T\cap Q_1^T\subset Q_1^T$ and therefore $Q_2\subset Q_1^T$, i.e., the first inclusion is valid, i.e., $Q_1\oplus Q_2$ is defined. Note, that we also have $Q_2\subset Q^T$, or, what is the same, $Q\subset Q_2^T$. Now, invoke the assumption $Q_1\subset Q^T$, or, equivalently, $Q\subset Q_1^T$. Combining this with the previous fact, we obtain $Q\subset Q_1^T\cap Q_2^T=(Q_1\cup Q_2)^T=(Q_1\cup Q_2)^{TTT}=(Q_1\oplus Q_2)^T$. Hence, the second inclusion is valid and by that the second axiom is established.

Consider the third axiom. The candidate for $\mathbf{0}$ is $\varnothing$. For any $Q\in\mathcal{P}^T(A)$, $Q\oplus\mathbf{0}$ is defined, since $\varnothing\subset Q^T$. We have $Q\oplus\mathbf{0}=(Q\cup\varnothing)^{TT}=Q^{TT}=Q$. The third axiom is established.

Before considering the fourth axiom, let us prove another general auxiliary fact. We know, that any $Q\in\mathcal{P}^T(A)$ can be represented in the form $Q=V^{TT}$, where $V\in\mathcal{P}_T(A)$ [take $U\in\mathcal{P}_T(A)$ and $M\in\mathrm{Max}(\mathcal{P}_T(A);\subset)$ such that $M\supset U$, and set $V=M\backslash U$]. The element Q^T is in $\mathcal{P}^T(A)$ as well. Hence, $Q^T=W^{TT}$, for some $W\in\mathcal{P}_T(A)$. Claim, that $V\cup W\in\mathrm{Max}(\mathcal{P}_T(A);\subset)$. Indeed, since $Q^{TT}=Q$, we have, in particular, $Q\subset(Q^T)^T$, and so $Q\oplus Q^T$ is defined. Next, $Q\oplus Q^T=(V^{TT}\cup W^{TT})^{TT}=(V^{TTT}\cap W^{TTT})^T=(V^T\cap W^T)^T=(V\cup W)^{TT}$. If $V\cup W$ is not maximal, then there exists $l_0\in(V\cup W)^T$. At the same time, $(V\cup W)^T=(V\cup W)^{TTT}=(Q\oplus Q^T)^T=(Q\cup Q^T)^{TTT}=(Q\cap Q^T)^{TT}$. But $Q\cap Q^T=\varnothing$, due to the first condition on T. Therefore, we continue, $(Q\cap Q^T)^{TT}=\varnothing^{TT}=\varnothing$. Hence, l_0 cannot exist, and $V\cup W$ is maximal. Note, that we also have $(Q\oplus Q^T)^T=\varnothing$, and as a corollary $Q\oplus Q^T=(Q\oplus Q^T)^{TT}=\varnothing^T=A$.

Now for the fourth axiom, take any $Q,Q_1,Q_2\in\mathcal{P}^T(A)$, and assume that $Q\oplus Q_1=Q\oplus Q_2$. It is necessary to show, that $Q_1=Q_2$. Represent Q, Q_1, and Q_2 in the form $Q=V^{TT}$, $Q_1=V_1^{TT}$, and $Q_2=V_2^{TT}$, where $V,V_1,V_2\in\mathcal{P}_T(A)$. Denote $Q_0:=Q\oplus Q_1=Q\oplus Q_2$, and write it in the form $Q_0=U_0^T$, where $U_0\in\mathcal{P}_T(A)$. Hence, $Q_0^T=U_0^{TT}$. We claim that both $(V\cup V_1)\cup U_0$ and $(V\cup V_2)\cup U_0$ are in $\mathrm{Max}(\mathcal{P}_T(A);\subset)$. Since $V\subset V^{TT}=Q\subset Q_1^T=V_1^{TTT}=V_1^T$, due to the first condition, the sets V and V_1 are disjoint. Similarly, $V\cap V_2=\varnothing$. We also have $Q_0=Q\oplus Q_1=(V^{TT}\cup V_1^{TT})^{TT}=(V^{TTT}\cap V_1^{TTT})^T=(V^T\cap V_1^T)^T=(V\sqcup V_1)^{TT}$, and $Q_0^T=U_0^{TT}$. Since $Q_0\oplus Q_0^T$ is defined, we similarly conclude that $V\sqcup V_1$ and U_0 are disjoint. Moreover, we already know, that in this case $(V\sqcup V_1)\sqcup U_0$ is maximal. Similarly, $(V\sqcup V_2)\sqcup U_0$ is maximal. Applying the main condition, one obtains $V_1^{TT}=(V\cup U_0)^T=V_2^{TT}$, i.e., $Q_1=Q_2$. Hence the fourth axiom is established.

Consider the fifth axiom. The candidate for $\mathbf{1}$ is A. It is easy to guess, that for $Q\in\mathcal{P}^T(A)$ it is necessary to set $Q^*:=Q^T$. We already know, that $Q^T\oplus Q=A$, and since A plays the role of $\mathbf{1}$, we obtain $Q^*\oplus Q=\mathbf{1}$. The fifth axiom is established.

Finally, it remains to consider the sixth axiom. Note, that since $\mathbf{1}=A$, $\mathbf{0}=\varnothing$, and A is not empty, one has $\mathbf{1}\neq\mathbf{0}$. Take any $Q\in\mathcal{P}^T(A)$, and assume that $Q\oplus\mathbf{1}$ is defined. This implies, that $Q\subset\mathbf{1}^T=A^T=\varnothing$. Hence, $Q=\varnothing$, i.e., $Q=\mathbf{0}$. The last axiom is established, and we have an effect algebra.

It is not difficult to verify, that in fact this effect algebra is an orthoalgebra, and, moreover, a coherent orthoalgebra. Indeed, if we take any $Q\in\mathcal{P}^T(A)$, and assume, that $Q\oplus Q$ is defined, then this implies $Q\subset Q^T$. Hence, $Q=Q\cap Q^T$. But $Q\cap Q^T=\varnothing$ due to the first condition. Therefore $Q=\mathbf{0}$ ($\mathbf{0}:=\varnothing$), i.e., our effect algebra is an orthoalgebra. Now, consider $Q,Q_1,Q_2\in\mathcal{P}^T(A)$, and assume, that $Q\oplus Q_1$, $Q_1\oplus Q_2$, and $Q_2\oplus Q$ are defined. We have $Q\subset Q_1^T$ and $Q\subset Q_2^T$. Hence,

$Q \subset Q_1^T \cap Q_2^T$. Apply the $(\cdot)^T$ operation, $Q^T \supset (Q_1^T \cap Q_2^T)^T = (Q_1 \cup Q_2)^{TT} = Q_1 \oplus Q_2$. Therefore $Q \oplus (Q_1 \oplus Q_2)$ is defined. The orthoalgebra is coherent. □

III. THE GROUP OF SYMMETRY

We have just three conditions on $T \subset A \times A$, which, when valid, allow to construct a coherent orthoalgebra. The first two are very simple, but the verification of the third one (the main condition), may be nontrivial. The main problem is, that there can be many elements in $\mathrm{Max}(\mathcal{P}_T(A); \subset)$. First, it is necessary to *characterize* them all, and then, for every $M \in \mathrm{Max}(\mathcal{P}_T(A); \subset)$ and every $B \subset M$ verify the property $B^T = (M \backslash B)^{TT}$. A straightforward computation can become very complicated.

The general approach to deal with this problem is to find some group of symmetry of A. Look at all bijections $\beta: A \xrightarrow{\sim} A$, which respect the T relation on A, i.e., $\forall l, l_1 \in A: (l_1, l) \in T \Rightarrow (\beta(l_1), \beta(l)) \in T$. Denote the group of all such bijections as $Bij_T(A)$. Every $\beta \in Bij_T(A)$ induces a bijective map from $\mathrm{Max}(\mathcal{P}_T(A); \subset)$ to itself. Suppose, we are able to describe some subgroup $\mathcal{G} \subset Bij_T(A)$, such that its natural action on $\mathrm{Max}(\mathcal{P}_T(A); \subset)$ has "large" orbits. Since it suffices to pick from each orbit just one representative, and verify the main condition on T only for these, the verification of the main condition becomes more feasible.

Let us now describe A, T, and $\mathcal{G}$ for the examples given below. Note, that these constructions clarify the combinatorics of the formulas present in Ref. 10. Let V be a finite set, such that $N := \#V$ is divisible by 4. Our construction will involve two collections of parameters with values in $\mathbb{Z}/2$. The first collection is indexed by $U \in \mathcal{P}(V)$ and the corresponding parameters are denoted as $b_U \in \mathbb{Z}/2$. The second collection is indexed by $U, U_1 \in \mathcal{P}(V)$, $U \neq U_1$, and the parameters are denoted by c_{U,U_1}. It is assumed that $c_{U,U_1} = c_{U_1,U}$. Look at all maps $V \to \mathbb{Z}/2$, and for every $U \in \mathcal{P}(V)$ denote

$$L_b(U) := \left\{ \phi: V \to \mathbb{Z}/2 \,\middle|\, \sum_{v \in V} \phi(v) = b_U \right\}, \tag{7}$$

where the index b in the notation $L_b(\cdot)$ stands for $b := \{b_U\}_U$. Set

$$A_b := \bigsqcup_{U \in \mathcal{P}(V)} L_b(U). \tag{8}$$

Denote by $i_U^b: L_b(U) \rightarrowtail A_b$, $U \in \mathcal{P}(V)$, the canonical injections. Now define some relation T_c on A_b, making use of the second collection of parameters $c := \{c_{U,U_1}\}_{U,U_1}$. For any $U, U_1 \in \mathcal{P}(V)$, $U \neq U_1$, and any $\phi, \phi' \in L(U)$ and $\phi_1 \in L(U_1)$, set

$$\begin{aligned} (i_U^b(\phi), i_U^b(\phi')) \in T_c &:\Leftrightarrow \phi \neq \phi', \\ (\phi, \phi_1) \in T_c &:\Leftrightarrow \sum_{s \in U \Delta U_1} (\phi(z) + \phi_1(z)) \neq c_{U,U_1}, \end{aligned} \tag{9}$$

where Δ denotes the symmetric difference of two subsets.

We are going to apply with respect to (A_b, T_c) the general construction of the preceding section, i.e., substitute $A = A_b$, $T = T_c$, and try to adjust the parameters b_U and c_{U,U_1} in order to satisfy the three conditions. The main result of the present paper can now be outlined as follows: if the number of points N in V is divisible by 4, then it is possible to choose the parameters b_U and c_{U,U_1} in such a way, that the assumptions of the proposition above are satisfied. Hence a new family of orthoalgebras is constructed. Moreover, it is possible to choose c_{U,U_1} and b_U in such a way, that the corresponding orthoalgebras do not admit bivaluations. It is interesting to stress the observed periodicity by 4. Without $4 \mid N$, the construction does not work.

Let us describe the group $\mathcal{G}$. Note, that the set of functions from V to $\mathbb{Z}/2$ may be viewed as a N-dimensional vector space over a field with two elements $\mathbb{F}_2$. Denote this vector space by $\mathbb{F}_2^N$. The number of elements in $\mathbb{F}_2^N$ is 2^N. The sum of two vectors corresponds to a symmetric differ-

ence of two subsets. Look at the group of all automorphisms of this vector space, i.e., the general linear group $\mathrm{GL}(N,\mathbb{F}_2)$ of $N\times N$ matrices with coefficients in $\mathbb{F}_2$. Let us describe a system of generators of this group (not a minimal one). For every $S\in\mathcal{P}(V)$, define a map $T_S:\mathcal{P}(V)\to\mathcal{P}(V)$,

$$T_S(U) := \begin{cases} U & \text{if } \#(U\cap S) \text{ is even,} \\ \overline{U\Delta S} & \text{if } \#(U\cap S) \text{ is odd,} \end{cases} \tag{10}$$

where U varies over $\mathcal{P}(V)$. Note, that these maps in the case of $N=4$ have been introduced in Ref. 10. Hence, in order to compute $T_S(U)$, one needs to look at $S\cap U$. Observe, that $S\cap T_S(U)=S\cap U$. This implies, that $T_S^2=\mathrm{id}$. In particular, T_S is a bijection. Moreover, for all $S,U,U_1\in\mathcal{P}(V)$, we have

$$T_S(U\Delta U_1)=T_S(U)\Delta T_S(U_1).$$

In order to prove the latter formula, note, that

$$\#(S\cap(U\Delta U_1))=\#(S\cap U)+\#(S\cap U_1)-2\#(S\cap U\cap U_1).$$

Therefore $\#_2(S\cap(U\Delta U_1))$ ($\#_2$ denotes the cardinality of a set viewed in $\mathbb{Z}/2$) is determined by $\#_2(S\cap U)$ and $\#_2(S\cap U_1)$. Hence the T_S correspond to *linear* bijective maps of $\mathbb{F}_2^N$, i.e., T_S corresponds to an element $\hat{T}_S\in\mathrm{GL}(N,\mathbb{F}_2)$. The range of possible values of S—the set $\mathcal{P}(V)$—may be identified with $\mathbb{F}_2^N$. We denote by $|S\rangle$ an element of $\mathbb{F}_2^N$ corresponding to S. Note, that there exists a formula $\hat{T}_S|U\rangle=|T_S(U)\rangle$, where $U,S\in\mathcal{P}(V)$.

Proposition 1: Let T_S, $|S\rangle\in\mathbb{F}_2^N$, *be the set of reflections defined by the formula* (10). *Then* $\{\hat{T}_S\}_S$ *generates the whole group* $\mathrm{GL}(N,\mathbb{F}_2)$.

Proof: For particular N small enough it is easy to verify the statement on computer in GAP. Let us provide a proof for all N. Note, that $T_\varnothing=T_V=\mathrm{id}$. Take any $S\in\mathcal{P}(V)$, $S\neq\varnothing,V$, and select $w\in\overline{S}:=V\backslash S$. There is a useful formula:

$$(T_S T_{S\cup\{w\}} T_S)(\{v\}) = \begin{cases} \{v\} & \text{if } v\neq w, \\ \overline{S} & \text{if } v\neq w. \end{cases} \tag{11}$$

It allows to prove (by induction) that the standard basis in $\mathbb{F}_2^N$ transforms into any other basis by a sequence of $\hat{T}_S$. Hence, the group is indeed $\mathrm{GL}(N,\mathbb{F}_2)$. □

Note, that the fact that $\hat{T}_S$ are reflections, and the fact that they generate the whole general linear group, is obtained without using the assumption $4|N$.

We shall describe some bijections $A_b\xrightarrow{\sim}A_b$, which respect the relation $T_c\subset A_b\times A_b$. The group $\mathcal{G}$ will be generated by these bijections. Before considering the general case, first look at the case where all the parameters b_U and c_{U,U_1} are set to $0\in\mathbb{Z}/2$. Write A_0 and T_0 in this case instead of A_b and T_c, respectively. For every $S\in\mathcal{P}(V)$, define the maps $\theta_S:\mathrm{Maps}(V,\mathbb{Z}/2)\to\mathrm{Maps}(V,\mathbb{Z}/2)$ by the formulas,

$$\theta_S(\varphi)(v) := \begin{cases} \varphi(v) & \text{if } v\in\overline{S}, \\ \varphi(v)+\displaystyle\sum_{w\in\overline{S}}\varphi(w) & \text{if } v\in S, \end{cases} \tag{12}$$

where $\varphi:V\to\mathbb{Z}/2$, $\overline{S}:=V\backslash S$. The latter can be expressed more compactly by $\theta_S(\varphi)(v)=\Sigma_{z\in T_S(\{v\})}\varphi(z)$. A straightforward computation shows, that

$$\theta_S^2=\mathrm{id},$$

and that for any $S,U\in\mathcal{P}(V)$, and any $\varphi:V\to\mathbb{Z}/2$, the following formula is valid:

$$\sum_{v\in T_S(U)} \theta_S(\varphi)(v) = \sum_{v\in U} \varphi(v). \tag{13}$$

This implies for any $U,S\in\mathcal{P}(V)$, that $\varphi\in L_0(U)$ yields $\theta_S(\varphi)\in L_0(T_S(U))$. It means that there exist induced maps

$$\theta_{S,U}: L_0(U)\to L_0(T_S(U)).$$

For every $S\in\mathcal{P}(V)$, the collection $\{\theta_{S,U}\}_U$, $U\in\mathcal{P}(V)$, defines a bijective map

$$\hat{\theta}_S: A_0 \xrightarrow{\sim} A_0,$$

[recall, $A_0=\sqcup_{U\in\mathcal{P}(V)}L_0(U)$]. The bijectivity follows from $\theta_S^2=\mathrm{id}$. Of course, $\hat{\theta}_S^2=\mathrm{id}$ itself as well. Invoking that for any $S,U,U_1\in\mathcal{P}(V)$, we have $T_S(U\Delta U_1)=T_S(U)\Delta T_S(U_1)$, it is not difficult to verify that all $\hat{\theta}_S$ respect the relation $T_0\subset A_0\times A_0$, or, equivalently, the relation $(A_0\times A_0)\backslash T_0$. Consider $U,U_1\in\mathcal{P}(V)$ and $\varphi\in L_0(U)$, $\varphi_1\in L_0(U_1)$, such that $(i^0_U(\varphi), i^0_{U_1}(\varphi_1))\notin T_0$ (i^0_U and $i^0_{U_1}$ denote the canonical injections into A_0). If $U_1=U$, then the fact mentioned is implied by the bijectivity of $\hat{\theta}_S$. If $U\neq U_1$, then we have $\Sigma_{v\in U\Delta U_1}(\varphi(v)+\varphi_1(v))=0$. Therefore, $\Sigma_{v\in T_S(U\Delta U_1)}\times(\theta_S(\varphi)(v)+\theta_S(\varphi_1)(v))=0$. Since $T_S(U\Delta U_1)=T_S(U)\Delta T_S(U_1)$, the pair of elements in A_0 that correspond to $\theta_S(\varphi)\in L_0(T_S(U))$ and $\theta_S(\varphi_1)\in L_0(T_S(U_1))$, is in relation $(A_0\times A_0)\backslash T_0$.

Now let us generalize the construction of the maps $\hat{\theta}_S$. We have the collections of parameters $b=\{b_U\}_U$, and $c=\{c_{U,U_1}\}_{U,U_1}$. For every $U,S\in\mathcal{P}(V)$, we need to describe some maps $L_b(U)\to L_b(T_S(U))$. In the case considered above, these were the maps $\theta_{S,U}$. For every fixed S, the whole collection $\{\theta_{S,U}\}_U$ stemmed just from one "global" function θ_S. Now, let us not assume this property. Take an arbitrary collection of $\mathbb{Z}/2$-valued parameters $\{a_{S,U}(v)\}_{S,U,v}$, $S,U\in\mathcal{P}(V)$, $v\in V$, and try to define some maps $\theta^{(a)}_{S,U}: L_b(U)\to L_b(T_S(U))$ by the formula

$$\theta^{(a)}_{S,U}(\varphi)(v) := \theta_S(\varphi)(v) + a_{S,U}(v), \tag{14}$$

where $\varphi\in L_b(U)$, $v\in V$. The case considered above corresponds to all $a_{S,U}(v)=0$. It is necessary to ensure, that $\theta^{(a)}_{S,U}(\varphi)(v)\in L_b(T_S(U))$. This yields a condition on $a_{S,U}(v)$,

$$\sum_{v\in U}\theta^{(a)}_{S,U}(\varphi)(v) = b_{T_S(U)},$$

where $\varphi\in L_b(U)$. Expanding the definitions of $L_b(U)$ and $\theta^{(a)}_{S,U}$, one reduces this equality just to $0=b_{T_S(U)}$, if $\#(S\cap U)$ is even, and to $b_U+\Sigma_{v\in\overline{U\Delta S}}a_{S,U}(v)=b_{T_S(U)}$, if $\#(S\cap U)$ is odd. Both cases are captured by one formula,

$$\sum_{v\in T_S(U)} a_{S,U}(v) = b_{T_S(U)} + b_U, \tag{15}$$

where S and U vary over $\mathcal{P}(V)$. Assume, that this condition is satisfied. Hence, we have well-defined maps $\theta^{(a)}_{S,U}: L_b(U)\to L_b(T_S(U))$. Since $\theta_{S,U}$ are bijections, so are $\theta^{(a)}_{S,U}$. For every fixed $S\in\mathcal{P}(V)$, the collection $\{\theta^{(a)}_{S,U}\}_U$ defines a bijective map

$$\hat{\theta}^{(a)}_S: A_b \xrightarrow{\sim} A_b.$$

Impose a requirement, that $\hat{\theta}^{(a)}_S$ respects the relation $T_c\subset A_b\times A_b$. This yields another condition on the parameters $a_{S,U}(v)$. Take any $U,U_1\in\mathcal{P}(V)$. Since $\hat{\theta}^{(a)}_S$ is bijective, the requirement is satisfied if $U_1=U$. Let $U_1\neq U$. Take any $\varphi\in L_b(U)$, $\varphi_1\in L_b(U_1)$, and assume that $\Sigma_{v\in U\Delta U_1}(\varphi(v)+\varphi_1(v))=c_{U,U_1}$. This should imply $\Sigma_{v\in T_S(U)\Delta T_S(U_1)}(\theta^{(a)}_{S,U}(\varphi)(v)+\theta^{(a)}_{S,U_1}(\varphi_1)(v))=c_{T_S(U),T_S(U_1)}$. Taking into account, that $T_S(U)\Delta T_S(U_1)=T_S(U\Delta U_1)$, expanding the definitions (14) of $\theta^{(a)}_{S,U}$ and $\theta^{(a)}_{S,U_1}$, and taking into account the mentioned formula (13) for θ_S, one reduces this requirement to the form

$$\sum_{v \in T_S(U \Delta U_1)} (a_{S,U}(v) + a_{S,U_1}(v)) = c_{U,U_1} + c_{T_S(U),T_S(U_1)}, \tag{16}$$

where S, U, and U_1 vary over $\mathcal{P}(V)$, and $U_1 \neq U$.

We have an overdetermined system of linear equations (15) and (16), with respect to the indeterminates $a_{S,U}(v) \in \mathbb{Z}/2$. The quantities b_U and c_{U,U_1} are parameters. It is necessary to solve this system of equations, and then obtain a condition of solvability in terms of b_U and c_{U,U_1}. After that b_U and c_{U,U_1} become indeterminates themselves, and one needs to find at least some solutions of the solvability equations. Assume all this is accomplished. Then we obtain a collection of bijective maps $\hat{\theta}_S^{(a)}: A_b \xrightarrow{\sim} A_b$, which respect the relation T_c. They generate some group $\mathcal{G}_a \subset Bij_{T_c}(A_b)$. In what follows, it is this group that will be used to establish the main condition on T_c, that allows to construct the orthoalgebra. Moreover, that parameters b_U and c_{U,U_1} can be chosen in such a way, that the corresponding orthoalgebra does not admit a bivaluation (this is the easy part).

IV. THE SOLUTIONS

Let us rewrite Eq. (16) as follows. This equation contains a sum over $v \in T_S(U \Delta U_1)$. This is the same as the sum over $v \in T_S(U) \Delta T_S(U_1)$. Since the terms in this sum are $\mathbb{Z}/2$-valued, it can be split as $\Sigma_{v \in T_S(U)} + \Sigma_{v \in T_S(U_1)}$. Perform this action upon Eq. (16), and then use twice Eqs. (15) corresponding to $U_0 = U$ and $U_0 = U_1$. It is convenient to denote

$$c_{U,U_1}^{(S)} := c_{U,U_1} + b_U + b_{U_1} + c_{T_S(U),T_S(U_1)} + b_{T_S(U)} + b_{T_S(U_1)},$$

$$b_{U_0}^{(S)} := b_{U_0} + b_{T_S(U_0)}.$$

The system of Eqs. (15) and (16), is equivalent to

$$\sum_{v \in T_S(U_1)} a_{S,U}(v) + \sum_{v \in T_S(U)} a_{S,U_1}(v) = c_{U,U_1}^{(S)}, \tag{17}$$

$$\sum_{v \in T_S(U_0)} a_{S,U_0}(v) = b_{U_0}^{(S)}. \tag{18}$$

Let us express all $a_{S,Q}(v)$ with $\#Q \geqslant 2$ via the indeterminates of the form $a_{S,\{z\}}(v)$. Let $Q \in \mathcal{P}(V)$ be any subset such that $\#Q \geqslant 2$, and $u \in S$ and $w \in \bar{S}$ be any points. Look at the equation (17). Set $U = Q$ and $U_1 = \{w\}$. This allows to find $a_{S,Q}(w)$,

$$a_{S,Q}(w) = \sum_{v \in T_S(Q)} a_{S,\{w\}}(v) + c_{Q,\{w\}}^{(S)}, \quad w \in \bar{S}.$$

Next, set $U = Q$ and $U_1 = \{u\}$. Since $T_S(\{u\}) = \{u\} \cup \bar{S}$, the resulting expression on the left-hand side will contain a sum of $a_{S,Q}(v)$ over $v \in \{u\} \cup \bar{S}$. For all values of v, except $v = u$, we already can express $a_{S,Q}(v)$. Hence, it is possible to find $a_{S,Q}(u)$,

$$a_{S,Q}(u) = \sum_{w' \in \bar{S}} a_{S,Q}(w') + \sum_{v \in T_S(Q \Delta \{u\})} a_{S,\{u\}}(v) + c_{Q,\{u\}}^{(S)}, \quad u \in S.$$

Now consider the case where the sets U_0, U, and U_1, are singletons. Let $u, u_1 \in S$ and $w, w_1 \in \bar{S}$ be any points. Equations (18) corresponding to $U_0 = \{w\}$ and $U_0 = \{u\}$, respectively, yield

$$a_{S,\{w\}}(w) = 0,$$

$$a_{S,\{u\}}(u) = b^{(S)}_{\{u\}} + \sum_{w' \in \bar{S}} a_{S,\{u\}}(w').$$

For the c-equations, it is necessary to consider the following three cases: (1) $U=\{w\}$, $U_1=\{w_1\}$; (2) $U=\{u\}$, $U_1=\{w\}$; (3) $U=\{u\}$, $U_1=\{u_1\}$. They yield

$$a_{S,\{w\}}(w_1) + a_{S,\{w_1\}}(w) = 0,$$

$$a_{S,\{u\}}(w) + a_{S,\{w\}}(u) = c^{(S)}_{\{u\},\{u_1\}} + \sum_{w' \in \bar{S}} a_{S,\{w\}}(w'),$$

$$a_{S,\{u\}}(u_1) + a_{S,\{u_1\}}(u) = c^{(S)}_{\{u\},\{u_1\}} + \sum_{w' \in \bar{S}} (a_{S,\{u\}}(w') + a_{S,\{u_1\}}(w')).$$

For every fixed $S \in \mathcal{P}(V)$, one may view the latter five equalities as a system of linear equations with respect to $a_{S,\{z\}}(v) \in \mathbb{Z}/2$, $v, z \in V$. It is not difficult to verify, that the corresponding *homogeneous* system of equations has many solutions. Redenote the indeterminates in this system as $\alpha_{S,\{z\}}(v)$, $v, z \in V$. Denote $\mathcal{E}(V) := \{U \subset V \mid \#U=2\}$. Write vz instead of $\{v, z\}$ for the elements of $\mathcal{E}(V)$. Take any function $\mu: \mathcal{E}(V) \to \mathbb{Z}/2$, and denote

$$\chi^{Q}_{\mu}(v) := \sum_{z \in Q \setminus \{v\}} \mu(vz),$$

where $Q \in \mathcal{P}(V)$, $v \in V$. It is not difficult to verify in a straightforward manner, that $\alpha_{\{z\}}(v) = \chi^{T_S(\{z\})}_{\mu}(v)$ defines a solution of the homogeneous system. We just remark, that $\chi^{T_S(\{w\})}_{\mu}(v) = \mu(vw)$ for $w \in \bar{S}$, $\chi^{T_S(\{u\})}_{\mu}(v) = \mu(uv) + \Sigma_{w' \in \bar{S}} \mu(vw')$ for $u \in S$, and it is convenient to accept a formal agreement $\mu(vv)=0$ in order to perform this computation.

We need a solution of the nonhomogeneous system. Let $u, u_1 \in S$ and $w, w_1 \in \bar{S}$ be any points. Set

$$\bar{a}_{S,\{w\}}(w_1) := \begin{cases} 0 & \text{if } w \prec w_1, \\ c^{(S)}_{\{w\},\{w_1\}} & \text{if } w_1 \prec w, \\ b^{(S)}_{\{w\}} & \text{if } w_1 = w; \end{cases}$$

$$\bar{a}_{S,\{u\}}(u_1) := \begin{cases} 0 & \text{if } u \prec u_1, \\ c^{(S)}_{\{u\},\{u_1\}} & \text{if } u_1 \prec u, \\ b^{(S)}_{\{u\}} & \text{if } u_1 = u; \end{cases}$$

$$\bar{a}_{S,\{w\}}(u) := b^{(S)}_{\{w\}} + c^{(S)}_{\{u\},\{w\}} + \sum_{\substack{w' \in \bar{S}, \\ w' \prec w}} c^{(S)}_{\{w'\},\{w\}},$$

$$\bar{a}_{s,\{u\}}(w) := 0.$$

A straightforward computation shows that $a_{S,\{z\}}(v) = \bar{a}_{S,\{z\}}(v)$ is a solution. Moreover, any other solution $a_{S,\{z\}}(v) = \hat{a}_{S,\{z\}}(v)$ can be represented in the form

$$\hat{a}_{S,\{z\}}(v) = \bar{a}_{S,\{z\}}(v) + \chi_{\hat{\mu}}^{T_S(\{z\})}(v),$$

for some $\hat{\mu}: \mathcal{E}(V) \to \mathbb{Z}/2$. For any $u, u \in S$, $u \neq u_1$, and $w, w_1 \in \bar{S}$, $w \neq w_1$, the values of $\hat{\mu}(ww_1)$, $\hat{\mu}(uu_1)$, and $\hat{\mu}(uw)$ are given by the formulas

$$\hat{\mu}(ww_1) := \begin{cases} \hat{a}_{S,\{w\}}(w_1) & \text{if } w \prec w_1, \\ \hat{a}_{S,\{w_1\}}(w) & \text{if } w_1 \prec w, \end{cases}$$

$$\hat{\mu}(uu_1) := \begin{cases} \hat{a}_{S,\{u\}}(u_1) & \text{if } u \prec u_1, \\ \hat{a}_{S,\{u_1\}}(u) + \sum\limits_{w' \in \bar{S}} \hat{a}_{S,\{u\}}(w') & \text{if } u_1 \prec u, \end{cases}$$

and

$$\hat{\mu}(uw) := \hat{a}_{S,\{u\}}(w) + \sum_{\substack{w' \in \bar{S}, \\ w' \prec w}} \hat{a}_{S,\{w'\}}(w) + \sum_{\substack{w' \in \bar{S}, \\ w' \succ w}} \hat{a}_{S,\{w\}}(w').$$

The verification is straightforward. Therefore, *any* solution of the homogeneous system is of the form $\alpha_{S,\{z\}}(v) = \chi_{\mu}^{T_S(\{z\})}(v)$, μ is some function. One can now take a solution for $a_{S,\{z\}}(v)$, and compute the rest of the $a_{S,Q}(v)$ according to the formulas derived above. Note, that the transformation $\alpha_{\{z\}}(v) = \chi_{\mu}^{T_S(\{z\})}(v) \to \alpha_{\{z\}}(v) = \chi_{\mu}^{T_S(\{z\})}(v) + \chi_{\mu}^{T_S(\{z\})}(v)$ induces the transformation of $a_{S,Q}(v)$ of the form $a_{S,Q}(v) \to a_{S,Q}(v) + \chi_{\mu}^{T_S(Q)}(v)$, i.e., there is a gauge symmetry group of transformations for the system of equations for $a_{S,Q}(v)$.

We have the expressions for all $a_{S,Q}(v)$, but we did not use all the equations of the system. Take any $S \in \mathcal{P}(V)$, and any $Q, Q_1 \in \mathcal{P}(V)$, $Q_1 \neq Q$. Substituting these expressions into the equations, one obtains the conditions,

$$c_{Q,Q_1}^{(S)} + \sum_{z_1 \in Q_1} c_{Q,\{z_1\}}^{(S)} + \sum_{z \in Q} c_{\{z\},Q_1}^{(S)} = \sum_{z_1 \in Q_1} \sum_{v \in T_S(Q)} a_{S,\{z_1\}}(v) + \sum_{z \in Q} \sum_{v_1 \in T_S(Q_1)} a_{S,\{z\}}(v_1)$$

and

$$b_Q^{(S)} + \sum_{z \in Q} c_{Q,\{z\}}^{(S)} = \sum_{z \in Q} \sum_{v \in T_S(Q)} a_{S,\{z\}}(v).$$

Denote the right-hand sides of these equalities by $X_a(S,Q,Q_1)$ and $Y_a(S,Q,Q_1)$, respectively. Note, that these two quantities are invariant under the gauge transformation $a_{S,\{z\}}(v) \to a_{S,\{z\}}(v) + \chi_{\mu}^{T_S(\{z\})}(v)$, ($\mu$ is any function). It remains to substitute $a_{S,\{z\}}(v) = \bar{a}_{S,\{z\}}(v)$ and compute the corresponding $X_{\bar{a}}$ and $Y_{\bar{a}}$.

In order to compute $Y_{\bar{a}}$ it is necessary to consider two cases, $\#(Q \cap S)$ is even, and $\#(Q \cap S)$ is odd. The computation in the first case is a little bit easier, but it turns out, that in both cases the result is the same

$$Y_{\bar{a}}(S,Q,Q_1) = \sum_{z \in Q} b_{\{z\}}^{(S)} + \sum_{\substack{z,z' \in Q, \\ z \prec z'}} c_{\{z\},\{z'\}}^{(S)}.$$

The value of the sum on the right-hand side does not depend on $\prec$, due to the symmetry $c_{U,U_1}^{(S)} = c_{U_1,U}^{(S)}$, which is implied by the assumption $c_{U,U_1} = c_{U_1,U}$.

In order to compute $X_{\bar{a}}(S,Q,Q_1)$, it is necessary to investigate the following three cases: (1) both $\#(Q \cap S)$ and $\#(Q_1 \cap S)$ are even; (2) $\#(Q \cap S)$ is odd, and $\#(Q_1 \cap S)$ is even; (3) both $\#(Q \cap S)$ and $\#(Q_1 \cap S)$ are odd. In all three cases, one obtains the same expression,

$$X_{\bar{a}}(S,Q,Q_1) = \sum_{\substack{z\in Q, z_1\in Q_1,\\ z\neq z_1}} c^{(S)}_{\{z\},\{z_1\}}.$$

Therefore, we obtain the following conditions:

$$c^{(S)}_{Q,Q_1} + \sum_{z_1\in Q_1} c^{(S)}_{Q,\{z_1\}} + \sum_{z\in Q} c^{(S)}_{\{z\},Q_1} + \sum_{\substack{z\in Q, z_1\in Q_1,\\ z\neq z_1}} c^{(S)}_{\{z\},\{z_1\}} = 0 \tag{19}$$

and

$$\sum_{z\in Q} c^{(S)}_{Q,\{z\}} + \sum_{\substack{z,z'\in Q,\\ z<z'}} c^{(S)}_{\{z'\},\{z\}} = b^{(S)}_{Q} + \sum_{z\in Q} b^{(S)}_{\{z\}}. \tag{20}$$

Recall that S, Q, and Q_1 vary over $\mathcal{P}(V)$, $Q_1 \neq Q$. By definition, we set formally $c^{(S)}_{Q,Q}=0$. Note, that if $\#Q=1$, then the second condition (20) turns into an identity. Similarly, if at least one of the sets Q or Q_1 has cardinality 1, then the first condition (19) trivializes as well. These two conditions are the conditions of the solvability of the system of equations for $\{a_{S,U}(v)\}_{v,U,S}$.

V. PERIODICITY BY FOUR

Is it possible to satisfy the obtained solvability conditions (20) and (19)? We shall not try to describe all the solutions, but construct some. The crucial assumption is the following. Let us search for c_{U,U_1} and b_U in the form

$$\begin{aligned} c_{U,U_1} &= c(\#_4(U\Delta U_1)),\\ b_U &= b(\#_4 U), \end{aligned} \tag{21}$$

where $U, U_1 \in \mathcal{P}(V)$, $U_1 \neq U$, $\#_4(\cdot)$ denotes the cardinality of the subset viewed in $\mathbb{Z}/4$, and $c(\cdot):\mathbb{Z}/4\to\mathbb{Z}/2$ and $b(\cdot):\mathbb{Z}/4\to\mathbb{Z}/2$ are unknown functions. A not quite trivial property of the solvability system of equations (19) and (20), is that it admits such an anzats if the number of points N in V is divisible by 4.

Take any S, and look at the quantity $b^{(S)}_{\{z\}}$, $z\in V$. Observe, that since $b_U=b(\#_4 U)$, its value depends only on whether $z\in S$ or $z\notin S$. In other words, one may take *any* $u_0\in S$ and $w_0\in\bar{S}$, and claim that $b^{(S)}_{\{z\}}=b^{(S)}_{\{u_0\}}$, if $z\in S$, and $b^{(S)}_{\{z\}}=b^{(S)}_{\{w_0\}}$, if $z\in\bar{S}$. Similar statements may be made about the quantities of the form $c^{(S)}_{Q,\{z_1\}}$, $c^{S}_{\{z\},Q_1}$, and $c^{(S)}_{\{z\},\{z_1\}}$.

Choose any S, and Q, Q_1 such that $Q_1\neq Q$. Look at the set S. It gets partitioned into four subsets,

$$S = (S\cap Q\cap Q_1)\sqcup(S\cap\bar{Q}\cap Q_1)\sqcup(S\cap Q\cap\bar{Q}_1)\sqcup(S\cap\bar{Q}\cap\bar{Q}_1).$$

In each of the subsets, if nonempty, choose a point (it does not matter which one): $\xi_0 \in S\cap Q\cap Q_1$, $\xi_1\in S\cap\bar{Q}\cap Q_1$, $\xi_2\in S\cap Q\cap\bar{Q}_1$, and $\xi_3\in S\cap\bar{Q}\cap\bar{Q}_1$. Denote the cardinalities of these four subsets by m_0, m_1, m_2, and m_3, respectively. Next, perform a similar process with respect to $\bar{S}$, i.e., choose arbitrary four points η_0, η_1, η_2, and η_3, such that $\eta_0\in\bar{S}\cap Q\cap Q_1$, $\eta_1 \in\bar{S}\cap\bar{Q}\cap Q_1$, $\eta_2\in\bar{S}\cap Q\cap\bar{Q}_1$, and $\eta_3\in\bar{S}\cap\bar{Q}\cap\bar{Q}_1$. (If a set is empty, the corresponding point will not be needed.) Denote the cardinalities of these subsets as n_0, n_1, n_2, and n_3, respectively. Note, that $c^{(S)}_{\{z\},\{z_1\}}=0$, if both z and z_1 are in S, or both are in $\bar{S}$. With this remark, the solvability equation (19) after the described anzats, acquires the form,

$$c^{(S)}_{Q,Q_1} + (m_0 c^{(S)}_{Q,\{\xi_0\}} + n_0 c^{(S)}_{Q,\{\eta_0\}} + m_1 c^{(S)}_{Q,\{\xi_1\}} + n_1 c^{(S)}_{Q,\{\eta_1\}}) + [m_0 c^{(S)}_{Q_1,\{\xi_0\}} + n_0 c^{(S)}_{Q_1,\{\eta_0\}} + m_2 c^{(S)}_{Q_1,\{\xi_2\}} + n_2 c^{(S)}_{Q_1,\{\eta_2\}}]$$
$$+ \{m_0 n_1 + n_0 m_1 + m_0 n_2 + n_0 m_2 + m_1 n_2 + n_1 m_2\} c^{(S)}_{\{\xi_3\},\{\eta_3\}} = 0.$$

Note, that the values of m_i and n_i $(i=0,1,2,3)$ depend on the sets S, Q, and Q_1. Of course, $\Sigma_{i=0}^{3}(m_i+n_i)=N$. Note, that it suffices to know only the images of m_i and n_i $(i=0,1,2,3)$ in $\mathbb{Z}/2$.

The solvability condition (20) is reduced in a similar way. This time we do not need the set Q_1. Take any S and Q, choose any points $\zeta \in Q \cap S$, $\omega \in Q \cap \bar{S}$, and then any $\zeta' \in Q \cap S$, $\zeta' \neq \zeta$, and $\omega' \in Q \cap \bar{S}$, $\omega' \neq \omega$ (if some of these points cannot be chosen, they are not needed). Denote $k := \#(Q \cap S)$ and $l := \#(Q \cap \bar{S})$. The condition reduces to the form

$$k c^{(S)}_{Q,\{\zeta\}} + l c^{(S)}_{Q,\{\omega\}} + \frac{k(k-1)}{2} c^{(S)}_{\{\zeta\},\{\zeta'\}} + \frac{l(l-1)}{2} c^{(S)}_{\{\omega\},\{\omega'\}} + kl c^{(S)}_{\{\zeta\},\{\omega\}} = b^{(S)}_{Q} + k b^{(S)}_{\{\zeta\}} + l b^{(S)}_{\{\omega\}}.$$

Note, that each time, when the corresponding points cannot be chosen, the term that contains this point contains a factor equal to zero. The values of k and l depend on the sets S and Q. Note that it suffices to know only the image of l in $\mathbb{Z}/2$, and the image of k in $\mathbb{Z}/4$ (not $\mathbb{Z}/2$)!

It remains to perform the mentioned anzats in these equations and simplify them. It is convenient to use the following formulas:

$$\#_4(U \Delta U_1) = \#_4 U + \#_4 U_1 - 2\#_4(U \cap U_1),$$

$$\forall i \in \mathbb{Z}/4 : [i]_2 = 0 \Rightarrow 2i = 0,$$

$$\forall i \in \mathbb{Z}/4 : [i]_2 = 1 \Rightarrow 2i = 2,$$

where $[i]_2$ denotes the canonical image of i in $\mathbb{Z}/2$, U and U_1 are any subsets of V. We shall also need the assumption that the number N of points in V is divisible by 4. In this case, for all $U \in \mathcal{P}(V)$, the following formula is valid:

$$\#_4 \bar{U} = -\#_4 U.$$

First look at Eq. (20). Recall, that $\zeta \in S \cap Q$, and $\omega \in \bar{S} \cap Q$. We have

$$b^{(S)}_{Q} = b(\#_4 Q) + b(\#_4 T_S(Q)),$$

$$b^{(S)}_{\{\zeta\}} = b(\#_4\{\zeta\}) + b(\#_4 T_S(\{\zeta\})) = b(1) + b(-\#_4 S + 1),$$

$$b^{(S)}_{\{\omega\}} = b(\#_4\{\omega\}) + b(\#_4 T_S(\{\omega\})) = 0.$$

Similar computations yield

$$c^{(S)}_{Q,\{\zeta\}} = b^{(S)}_{Q} + b^{(S)}_{\{\zeta\}} + c(\#_4 Q - 1) + c(\#_4 T_S(Q \Delta \{\zeta\})),$$

$$c^{(S)}_{Q,\{\omega\}} = b^{(S)}_{Q} + b^{(S)}_{\{\omega\}} + c(\#_4 Q - 1) + c(\#_4 T_S(Q \Delta \{\omega\})),$$

$$c^{(S)}_{\{\zeta\},\{\zeta'\}} = 0,$$

$$c^{(S)}_{\{\zeta\},\{\omega\}} = b(1) + b(-\#_4 S + 1) + c(2) + c(-\#_4 S),$$

$$c^{(S)}_{\{\omega\},\{\omega'\}} = 0.$$

We need to compute $\#_4 T_S(Q)$, $\#_4 T_S(Q\Delta\{\zeta\})$, and $\#_4 T_S(Q\Delta\{\omega\})$. Set

$$s := \#_4 S, \quad q := \#_4 Q, \quad t := \#_4(Q \cap S).$$

If $\#(Q \cap S)$ is even, (i.e., $t=0,2$), then

$$\#_4 T_S(Q) = q,$$

$$\#_4 T_S(Q\Delta\{\zeta\}) = -s - q - 1,$$

$$\#_4 T_S(Q\Delta\{\omega\}) = q - 1.$$

If $\#(Q \cap S)$ is odd, (i.e., $t=1,3$), then

$$\#_4 T_S(Q) = -s - q + 2,$$

$$\#_4 T_S(Q\Delta\{\zeta\}) = q - 1,$$

$$\#_4 T_S(Q\Delta\{\omega\}) = -s - q - 1.$$

Hence, it suffices to know the values of these parameters $s,q,t \in \mathbb{Z}/4$ in order to compute the left-hand and right-hand expressions of Eq. (20). (Of course, $[k]_4 = t$, and $[l]_4 = q - t$.) It turns out (this can be easily verified on a computer in Maple, or by a straightforward computation), that for each of the 4^3 possible variants of (s,q,t), the reduced equation acquires only one of the following types: either it becomes an identity $0=0$, or one of the two equations,

$$\begin{aligned} c(0) + c(2) &= b(0) + b(2), \\ c(1) + c(3) &= b(1) + b(3), \end{aligned} \tag{22}$$

or their sum $\Sigma_{i=0}^{3}(c(i)+b(i))=0$. One may assign arbitrary values, say to all $c(i)$ and to $b(0)$, $b(1)$, and then determine $b(2)$ and $b(3)$.

Equations (19) are reduced in a similar way, and in the final stage it is best to compute in Maple. Let us describe all the preparatory work. Look at $c^{(S)}_{Q,Q_1}$. We have $c^{(S)}_{Q,Q_1} = b^{(S)}_{Q} + b^{(S)}_{Q_1} + c(\#_4(Q\Delta Q_1)) + c(\#_4 T_S(Q\Delta Q_1))$. In particular, it is necessary to know $\#_2 S \cap (Q\Delta Q_1)$. Since $\#S \cap (Q\Delta Q_1) = \#(S \cap Q) + \#(S \cap Q_1) - 2\#(S \cap Q \cap Q_1)$, and the latter term is even, one has

$$\#_2 S \cap (Q\Delta Q_1) = \#_2(S \cap Q) + \#_2(S \cap Q_1).$$

Denote

$$s := \#_4 S, \quad q := \#_4 Q, \quad q_1 := \#_4 Q_1,$$

$$t := \#_4(S \cap Q), \quad t_1 := \#_4(S \cap Q_1),$$

$$p := \#_4(Q \cap Q_1), \quad r := \#_4(S \cap Q \cap Q_1).$$

With this notation, $\#_2 S \cap (Q\Delta Q_1) = [t + t_1]_2$. Therefore $\#_4(Q\Delta Q_1) = q + q_1 - 2p$, and

$$\#_4 T_S(Q\Delta Q_1) = \begin{cases} q+q_1-2p & \text{if } [t+t_1]_2 = 0, \\ -s-(q+q_1-2p)+2 & \text{if } [t+t_1]_2 = 1. \end{cases}$$

Taking into account these formulas, one can reduce $c^{(S)}_{Q,Q_1}$ to the following form. If $[t]_2=0$ and $[t_1]_2=0$, then $c^{(S)}_{Q,Q_1}=0$. If $[t]_2=1$ and $[t_1]_2=0$, then $c^{(S)}_{Q,Q_1}=b(q)+b(-q-s+2t)+c(q+q_1-2p)+c(-s-(q+q_1-2p)+2)$. Similarly, if $[t]_2=0$ and $[t_1]_2=1$, then $c^{(S)}_{Q,Q_1}=b(q_1)+b(-q_1-s+2t_1)+c(q+q_1-2p)+c(-s-(q+q_1-2p)+2)$. Finally, if $[t]_2=1$ and $[t_1]_2=1$, then $c^{(S)}_{Q,Q_1}=b(q)+b(-q-s+2t)+b(q_1)+b(-q_1-s+2t_1)$. The other computations are easier.

If $\#(Q\cap S)$ is even, i.e., $t=0,2$, then

$$c^{(S)}_{Q,\{\xi_0\}} = b(1)+b(-s+1)+c(q-1)+c(-s-q+2t-1),$$

$$c^{(S)}_{Q,\{\eta_0\}} = 0,$$

$$c^{(S)}_{Q,\{\xi_1\}} = b(1)+b(-s+1)+c(q+1)+c(-s-q+2t+1),$$

$$c^{(S)}_{Q,\{\eta_1\}} = 0.$$

If $t=1,3$, then

$$c^{(S)}_{Q,\{\xi_0\}} = b(q)+b(-s-q+2t)+b(1)+b(-s+1),$$

$$c^{(S)}_{Q,\{\eta_0\}} = b(q)+b(-s-q+2t)+c(q-1)+c(-s-q+2t+1),$$

$$c^{(S)}_{Q,\{\xi_1\}} = b(q)+b(-s-q+2t)+b(1)+b(-s+1),$$

$$c^{(S)}_{Q,\{\eta_1\}} = b(q)+b(-s-q+2t)+c(q+1)+c(-s-q+2t-1).$$

There are similar expressions corresponding to Q_1. If $\#(Q_1\cap S)$ is even, i.e., $t_1=0,2$, then

$$c^{(S)}_{Q_1,\{\xi_0\}} = b(1)+b(-s+1)+c(q_1-1)+c(-s-q_1+2t_1-1),$$

$$c^{(S)}_{Q_1,\{\eta_0\}} = 0,$$

$$c^{(S)}_{Q_1,\{\xi_2\}} = b(1)+b(-s+1)+c(q_1+1)+c(-s-q_1+2t_1+1),$$

$$c^{(S)}_{Q_1,\{\eta_2\}} = 0.$$

If $t_1=1,3$, then

$$c^{(S)}_{Q_1,\{\xi_0\}} = b(q_1)+b(-s-q_1+2t_1)+b(1)+b(-s+1),$$

$$c^{(S)}_{Q_1,\{\eta_0\}} = b(q_1)+b(-s-q_1+2t_1)+c(q_1-1)+c(-s-q_1+2t_1+1),$$

$$c^{(S)}_{Q_1,\{\xi_2\}} = b(q_1)+b(-s-q_1+2t_1)+b(1)+b(-s+1),$$

$$c^{(S)}_{Q_1,\{\eta_2\}} = b(q_1) + b(-s-q_1+2t_1) + c(q_1+1) + c(-s-q_1+2t_1-1).$$

Finally, $c^{(S)}_{\{\xi_3\},\{\eta_3\}}$ reduces to the form

$$c^{(S)}_{\{\xi_3\},\{\eta_3\}} = b(1) + b(-s+1) + c(2) + c(-s).$$

For the cardinalities m_0, m_1, m_2, and m_3, we have

$$[m_0]_4 = r, \quad [m_1]_4 = t_1 - r, \quad [m_2]_4 = t - r, \quad [m_3]_4 = s - t - t_1 + r,$$

where $[\cdot]_4$ denotes the canonical image of an integer number in $\mathbb{Z}/4$. Similarly, for the cardinalities n_0, n_1, n_2, and n_3, we have

$$[n_0]_4 = p - r, \quad [n_1]_4 = (q_1 - t_1) - (p - r), \quad [n_2]_4 = (q - t) - (p - r),$$

$$[n_3]_4 = (-s) - (q - t) - (q_1 - t_1) + (p - r).$$

Therefore it remains to investigate what happens to Eq. (19) as the parameters s, q, q_1, t, t_1, p, and r, vary over $\mathbb{Z}/4$. There are finitely many options, and the corresponding computation is easily implemented in Maple. In fact, it is possible to perform it manually, if one uses some symmetry of Eq. (19). The result is similar to the case of Eq. (20), i.e., every variant reduces to a linear combination of the simple equalities (22) mentioned above. It means, that we have established the fact that the solvability system of Eqs. (19) and (20), has solutions, and we have identified at least some of them (21).

VI. THE ORBITS

We are able to construct the group $\mathcal{G}_a$ in two steps. First, verify the main condition on T_c for some of the elements of $\mathrm{Max}(\mathcal{P}_{T_c}(A_b), \subset)$, and then compute the orbits of these elements under the action of $\mathcal{G}_a$. One needs enough such elements, so that the orbits cover the whole set $\mathrm{Max}(\mathcal{P}_{T_c}(A_b), \subset)$. The proof is essentially combinatorial.

Recall, that for every $U, S \in \mathcal{P}(V)$ we have defined the maps $\theta^U_S : L_b(U) \to L_b(T_S(U))$:

$$\theta^U_S(\varphi)(v) = \sum_{z \in T_S(\{v\})} \varphi(z) + a^U_S(v),$$

where $\varphi \in L_b(U)$, $v \in V$. There is also a collection of maps $I^U_\mu : L_b(U) \to L_b(U)$, $U \in \mathcal{P}(V)$, corresponding to the gauge transformation with function $\mu : \mathcal{E}(V) \to \mathbb{Z}/2$, defined by the formula

$$I^U_\mu(\varphi)(v) \coloneqq \varphi(v) + \chi^U_\mu(v),$$

where $\varphi \in L_b(U)$, $v \in V$, and $\chi^U_\mu(\cdot)$ is as in the preceding section.

Look at the diagram (in **Sets**),

$$\begin{array}{ccc} L_b(U) & \xrightarrow{\theta^U_S} & L_b(T_S(U)) \\ {\scriptstyle I^U_\nu}\,\vdots & & \downarrow{\scriptstyle I^{T_S(U)}_\mu} \\ L_b(U) & \xrightarrow{\theta^U_S} & L_b(T_S(U)) \end{array}$$

It turns out, that for every $U, S \in \mathcal{P}(V)$ and every $\mu : \mathcal{E}(V) \to \mathbb{Z}/2$, there exists a unique $\nu : \mathcal{E}(V) \to \mathbb{Z}/2$, rendering this diagram commutative. Denote this ν by $\tau_S(\mu)$. We have

$$I^{T_S(U)}_\mu \circ \theta^U_S = \theta^U_S \circ I^U_{\tau_S(\mu)},$$

where

$$\tau_S(\mu)(vv_1) := \mu(vv_1) + \sum_{z\in T_S(\{v\})} \mu(zv_1) + \sum_{z_1\in T_S(\{v_1\})} \mu(vz_1),$$

for vv_1 varying over $\mathcal{E}(V)$.

Now select some sets in $\mathrm{Max}(\mathcal{P}_{T_c}(A_b), \subset)$, and verify the main condition for them. The most simple case is $M=\{i^b_U(\varphi)\}_{\varphi\in L_b(U)}$. It is almost obvious, that $M\in\mathrm{Max}(\mathcal{P}_{T_c}(A_b), \subset)$. Choose any point in V and denote it by e, $e\in V$. Set $U=\{e\}$. Take any $B\subset M$, and write it as $B=\{i^b_{\{e\}}(\sigma)\}_{\sigma\in S}$, S is some subset of $L_b(\{e\})$. For $C:=M\backslash B$ we have $C=\{i^b_{\{e\}}(\sigma)\}_{\sigma\in S'}$, where $S'=L_b(\{e\})\backslash S$. It is necessary to show, that if $l\in B^{T_c}$ and $l_1\in C^{T_c}$, then $(l,l_1)\in T_c$. We have, $B^{T_c}=C\sqcup(B^{T_c}\backslash C)$ and $C^{T_c}=B\sqcup(C^{T_c}\backslash B)$. If $l\in C$ or $l_1\in B$, then the requirement is satisfied. The nontrivial case is $l\in B^{T_c}\backslash C$ and $l_1\in C^{T_c}\backslash B$. Assume, that such l and l_1 exist, and let $l=i^b_U(\varphi)$, $\varphi\in L_b(U)$, and $l_1=i^b_{U_1}(\varphi_1)$, $\varphi_1\in L_b(U_1)$. Note, that $U, U_1\neq\{e\}$. Invoking the explicit description (9) of the relation T_c, we conclude, that such l and l_1 exist iff

$$\exists\lambda\in\mathbb{Z}/2\ \forall\,\sigma\in S:\ \sum_{v\in\{e\}\Delta U}\sigma(v)=\lambda,$$

$$\exists\lambda'\in\mathbb{Z}/2\ \forall\,\sigma\in S':\ \sum_{v\in\{e\}\Delta U_1}\sigma(v)=\lambda'.$$

There exist two possibilities (1) $U=U_1$; (2) $U\neq U_1$. Consider the possibility $U=U_1$. In this case one must have

$$S=\left\{\sigma\in L_b(\{e\})\middle|\ \sum_{v\in\{e\}\Delta U}\sigma(v)=\lambda\right\},$$

since otherwise S' cannot satisfy the condition above. The parameter λ' corresponding to S' is, of course, $\lambda'=1+\lambda$. For $l=i^b_U(\varphi)$, using the description of T_c, we obtain, $\varphi(e)=\lambda+b(\#U)+c(\#(\{e\}\Delta U))+1$. Similarly, for l_1 we have $\varphi_1(e)=\lambda'+b(\#U_1)+c(\#(\{e\}\Delta U_1))+1=1+\varphi(e)$. Hence, $\varphi_1(\cdot)\neq\varphi(\cdot)$, and $(l,l_1)\in T_c$. Now look at the possibility $U_1\neq U$. This implies that the sets $\{e\}\Delta U$ and $\{e\}\Delta U_1$ are also different. Hence, there exists a point z, belonging to one of these sets, and not belonging to the other. Without loss of generality, let $z\in\{e\}\Delta U_1$ and $z\notin\{e\}\Delta U$. First, assume, that it is possible to choose them so that $z\neq e$. In this case, take any σ such that $\Sigma_{v\in\{e\}\Delta U_1}\sigma(v)=1+\lambda'$. Look at $\Sigma_{v\in\{e\}\Delta U}\sigma(v)$. If it is equal to λ, then modify the value of $\sigma(\cdot)$ in the point z by adding 1. This does not change the sum with U_1, and we obtain $\Sigma_{v\in\{e\}\Delta U}\sigma(v)=1+\lambda$. This σ belongs neither to S, nor to S'. But this is a contradiction, since S and S' partition the set $L_b(\{e\})$ of all possible σ. Therefore, the pair (l,l_1) cannot exist. It remains to consider the case when the only option for z is $z=e$. We have $U\not\ni e$ and $U_1=\{e\}\sqcup U$. Then the parameters λ and λ' associated to S and S' may be written as $\lambda=b(1)+\Sigma_{v\in U}\sigma(v)$, σ—any element of S, and $\lambda'=\Sigma_{v\in U}\sigma'(v)$, σ'—any element of S'. Since S and S' partition $L(\{e\})$, S' must coincide with the set of *all* σ' such that $\Sigma_{v\in U}\sigma'(v)=\lambda'$ (otherwise it is impossible to define λ for S). Therefore, for every $\sigma\in S$ we have $\Sigma_{v\in U}\sigma(v)=1+\lambda'$, and one obtains $\lambda=b(1)+1+\lambda'$. Since $l=i^b_U(\varphi)$ is in relation T_c with every $i^v_{\{e\}}(\sigma)$, invoking the definition of $L(U)$ and the description of T_c, it follows that $\varphi(e)+b(\#_4U)+\lambda=c(\#_4U+1)+1$. Similarly, for $\varphi_1\in L(\{e\}\Delta U)$, we arrive at $\varphi_1(e)+b(\#_4U+1)+[1+\lambda+b(1)]=c(\#_4U)+1$. Hence,

$$\varphi(e)+\varphi_1(e)=1+b(1)+b(\#_4U)+b(\#_4U+1)+c(\#_4U)+c(\#_4U+1).$$

On the other hand, the requirement $(i^b_U(\varphi), i^b_{U_1}(\varphi_1))$ implies, that $\varphi(e)+\varphi_1(e)=1+c(1)$. Therefore, one obtains a condition

$$b(1)+c(1)+b(\#_4U)+c(\#_4U)+b(\#_4U+1)+c(\#_4U+1)=0.$$

Since this must be valid for generic U, we obtain

$$b(0)+c(0)=0,\quad b(2)+c(2)=0,$$
$$b(1)+c(1)+b(3)+c(3)=0. \tag{23}$$

The latter is the equation we already have, and the first two imply the other equation, but are not equivalent to it. Hence, under these conditions, the main property of T_c for the set $M=\{i^b_{\{e\}}(\sigma)\}_{\sigma\in L_b(\{e\})}$ is established.

Let us consider some other subsets $M\in \mathrm{Max}(\mathcal{P}_{T_c}(A_b),\subset)$. There exists a natural map $\eta: A_b\to\mathcal{P}(V)$, $i^b_U(\varphi)\mapsto U$. For every $B\subset A_b$, call the set $\{\eta(l)\}_{l\in B}$ the *shadow* of B. Take any nonempty subset $\Omega\subset V$. Under some additional assumptions on $b(\cdot)$ and $c(\cdot)$, it will be shown that there exist sets $M\in\mathrm{Max}(\mathcal{P}_{T_c}(A_b),\subset)$ of the form

$$M=\bigsqcup_{U\in\mathcal{P}_{\mathrm{odd}}(\Omega)}\{i^b_U(\varphi)\}_{\varphi\in Q_U},$$

where Q_U are some subsets of $L_b(U)$, and

$$\mathcal{P}_{\mathrm{odd}}(\Omega):=\{U\subset\Omega\,|\,\#U \text{ is odd}\}.$$

Similarly, one may introduce the set $\mathcal{P}_{\mathrm{even}}(\Omega)$ consisting of all subsets of Ω of even cardinality. We will impose such conditions of $b(\cdot)$ and $c(\cdot)$, that the following statement will be true: if $B\subset A_b$ has a shadow which contains a subset being an element of $\mathcal{P}_{\mathrm{even}}(\Omega)$, then it does not belong to $\mathcal{P}_{T_c}(A_b)$.

More precisely, take any $\Omega\subset V$, such that $\#\Omega$ is even. Assume that $b(\cdot)$ and $c(\cdot)$ satisfy the conditions (23). Is it possible to have a set $B\in\mathcal{P}_{T_c}(A_b)$ consisting of $\#\Omega+1$ elements, such that $\#\Omega$ of them are of the form $i^b_{\{v\}}(\sigma_v)$, $\sigma_v\in L_b(\{v\})$, $v\in\Omega$, and the other element is of the form $i^b_\Omega(\varphi)$, $\varphi\in L_b(\Omega)$? Denote $\mathcal{E}(\Omega):=\{U\subset\Omega\,|\,\#U=2\}$. Assume that $i^b_{\{v\}}(\sigma_v)$, $\sigma_v\in L_b(\{v\})$, $v\in\Omega$, are pairwise in relation T_c. For $z\neq v$ we have $\sigma_z(v)+\sigma_v(z)=1+c(2)$. Choose and fix any order $\prec$ on V and associate to this collection of elements a function $\tau:\mathcal{E}(\Omega)\to\mathbb{Z}/2$, $\tau(zw):=\sigma_v(z)$, $v\prec z$. Hence, for any $vv_1\in\mathcal{E}(\Omega)$,

$$\sigma_v(v_1)=\begin{cases}\tau(vv_1) & \text{if } v\prec v_1,\\ \tau(vv_1)+1+c(2) & \text{if } v\succ v_1.\end{cases}$$

Now investigate what this means for φ. For every $v\in\Omega$, the definition of T_c yields,

$$\sum_{z\in\{v\}\Delta\Omega}(\sigma_v(z)+\varphi(z))=c(\#_4\Omega-1)+1.$$

The fact $\Sigma_{z\in\Omega}\varphi(z)=b(\#_4\Omega)$ yields

$$\varphi(v)=\sum_{z\in\Omega\setminus\{v\}}\sigma_v(z)+b(\#_4\Omega)+c(\#_4\Omega-1)+1,$$

where $v\in\Omega$. Apply summation over $v\in\Omega$ and invoke once more the mentioned fact to obtain

$$\frac{m(m-1)}{2}(c(2)+1)+m[b(m)+c(m-1)+1]=b(m),$$

where $m:=\#_4\Omega$. If this were true for generic Ω, one would have the following four equalities corresponding to $m=0,1,2,3$, respectively, $b(0)=0$, $c(0)+1=0$, $(c(2)+1)+b(2)=0$, and $(c(2)+1)+c(2)+1=0$. The latter is just an identity. The third one is not valid, since we already have a condition $b(2)+c(2)=0$. Moreover, since $b(0)+c(0)=0$, either the first or the second equality is not valid as well. Set $b(0)=c(0)=1$. Hence, m cannot be 0 or 2, i.e., $\#\Omega$ cannot be even. We have

$$b(0)=1,\quad c(0)=1,$$

$$b(2)+c(2)=0, \tag{24}$$

$$b(1)+c(1)+b(3)+c(3)=0.$$

It is impossible to have a collection consisting of elements of A_b of the form $i_v^b(\sigma_v)$, $v\in\Omega$, and $i_\Omega^b(\varphi)$, if $\#\Omega$ is even. In case $\#\Omega$ is odd, the values of $\varphi(\cdot)$ are determined by the function $\tau:\mathcal{E}(\Omega)\to\mathbb{Z}/2$, associated to $\sigma_v(\cdot)$, $v\in\Omega$. The values on the points of $V\backslash\Omega$ can be chosen arbitrary.

Now suppose one has a collection of elements $l_1,l_2,\ldots,l_n\in A_b$ which are pairwise in relation T_c. Denote $U_i:=\eta(l_i)$, $i=1,2,\ldots,m$, where $\eta:A_b\to\mathcal{P}(V)$ is the natural map mentioned above. Some of these sets may have cardinality 1, and some may contain more points. Denote by Ω the union of all U_i such that $\#U_i=1$. Note, that it is possible that Ω is empty. There exists a bijection $A_b\tilde{\to}A_b$ which respects the relation T_c, which transforms this collection into a collection with the following property: every U_i is a subset of Ω. Indeed, we have constructed the maps $\hat{\theta}_S^{(\bar{a})}$. These maps respect the relation T_c on A_b. If $l\in A_b$ satisfies $\eta(l)=U$, then $l'=\hat{\theta}_S^{(\bar{a})}(l)$ satisfies $\eta(l')=T_S(U)$. Let $l_1,l_2,\ldots,l_n\in A_b$ be as above. Denote $U_i:=\eta(l_i)$, $i=1,2,\ldots,n$, and construct the corresponding Ω. If there exists U_{i_0}, which is not a subset of Ω, then one can take a point $v_0\in U_0\backslash\Omega$. Look at the composition $T_{\bar{U}_{i_0}}\circ T_{\bar{U}_{i_0}\sqcup\{v_0\}}\circ T_{\bar{U}_{i_0}}$. This map transfers U_{i_0} into a one-point set $\{v_0\}$, and at the same time leaves all the one point-sets $\{v\}$, $v\in\Omega$, fixed. Therefore, if one applies a composition $\hat{\theta}^{(a)}_{\bar{U}_{i_0}}\circ\hat{\theta}^{(a)}_{\bar{U}_{i_0}\sqcup\{v_0\}}\circ\hat{\theta}^{(a)}_{\bar{U}_{i_0}}$ to each $l_1,l_2,\ldots,l_n$, one increases the number of points in Ω by 1. Proceeding this way we arrive at the situation where all U_i are subsets of the corresponding Ω. Of course, in this case, all U_i will have odd cardinalities. Note, that the cardinality of Ω need not be odd.

Take any $l_1,l_2,\ldots,l_n$, such that $\eta(l_i)=\{e_i\}$, $i=1,2,\ldots,n$, $e_i\in V$ some points, such that $e_i\neq e_j$ for $i\neq j$. Assume that $(l_i,l_j)\in T_c$, $i\neq j$. Hence $\Omega=\{e_1,e_2,\ldots,e_n\}$. Take any $U\subset\Omega$ and try to construct $l\in A_b$ of the form $l=i_U^b(\varphi)$, $\varphi\in L_b(U)$, such that for all i, $(l,l_i)\in T_c$. The cardinality $\#U$ needs to be odd. Let $U=\{e_i\}_{i\in I}$, where $I\subset\{1,2,\ldots,n\}$, $\#I$ is odd. The elements l_k, $k=1,2,\ldots,n$, are of the form $l_k=i^b_{\{e_k\}}(\sigma_k)$, the σ_k element of $L_b(\{e_k\})$. The requirement that $(l_i,l)\in T_c$ for every $i\in I$, yields

$$\varphi(e_i)=\sum_{i'\in I\backslash\{i\}}\sigma_i(e_{i'})+b(\#_4I)+c(\#_4I-1)+1.$$

Similarly, the requirement that for every $q\in\{1,2,\ldots,n\}\backslash I$, the pair $(l_q,l)\in T_c$, yields,

$$\varphi(e_q)=\sum_{i\in I}\sigma_q(e_i)+b(1)+b(\#_4I)+c(\#_4I+1)+1.$$

Therefore, the values of $\varphi(\cdot)$ on the points of Ω are determined, and on the points of $V\backslash\Omega$ remain arbitrary. Now take any $W\subset\Omega$, $W\neq U$, $\#W$ is odd. Let $W=\{e_j\}_{j\in J}$, $J\subset\{1,2,\ldots,n\}$. There exists $l'\in A_b$ of the form $l'=i_W^b(\psi)$, $\psi\in L_b(W)$, which is in relation T_c with every $l_1,l_2,\ldots,l_n$. The values of the function $\psi(\cdot)$ on the points of Ω are given by formulas similar to the ones above, and on $V\backslash\Omega$ can be assigned in an arbitrary way. Is it possible to have $(l',l)\in T_c$? It turns out, that l and l' are *always* in T_c. Note, that the condition for $(l,l')\in T_c$ involves only the values of $\varphi(\cdot)$ and $\psi(\cdot)$ in the points of Ω (more precisely, only in e_s, $s\in I\Delta J$). For these values one has the corresponding expressions via $\sigma_k(\cdot)$, $k=1,2,\ldots,n$. Substitute them into the mentioned condition and take into account, that $\sigma_k(e_{k'})+\sigma_{k'}(e_k)=c(2)+1$. After simplification, the expression reduces to

$$\frac{\#(I\Delta J)(\#(I\Delta J)-1)}{2}(c(2)+1)+c(\#_4(I\Delta J))+1+\#(I\cap\bar{J})\{c(\#_4 I-1)+c(\#_4 J+1)\}$$

$$+\#(J\cap\bar{I})\{c(\#_4 J-1)+c(\#_4 I+1)\}+\#(I\Delta J)[b(1)+b(\#_4 I)+b(\#_4 J)]=0.$$

In order to compute the value of the left-hand side it suffices to know $\#_4 I$, $\#_4 J$, and $\#_4(I\cap J)$. Recall, that $\#I$ and $\#J$ are odd. Hence, it remains to run through all the $2\times 2\times 4=16$ (in fact, even 8, due to the symmetry with respect to permutation of I and J) possibilities and look at what happens to the equation above. A straightforward (Maple) computation shows that each time one obtains either an identity $0\equiv 0$, or an equality $c(0)=1$. The latter is already present in the list of assumptions (24) concerning $b(\cdot)$ and $c(\cdot)$ above. Therefore, indeed $(l,l')\in T_c$.

Associate to the set $l_1,l_2,\ldots,l_n$ the function $\tau:\mathcal{E}(\Omega)\to\mathbb{Z}/2$ as explained above. One may write all formulas in terms of this function. Construct from it a function $\hat{\tau}:\Omega\times\Omega\to\mathbb{Z}/2$ of two arguments,

$$\hat{\tau}(v,v_1):=\begin{cases}\tau(vv_1) & \text{if } v\prec v_1,\\ b(1) & \text{if } v=v_1,\\ \tau(vv_1)+c(2)+1 & \text{if } v\succ v_1.\end{cases} \tag{25}$$

Note, that for $v\neq v_1$, one has $\hat{\tau}(v,v_1)=\hat{\tau}(v_1,v)+c(2)+1$. Next, construct a function $\tilde{\tau}:\mathcal{P}_{\mathrm{odd}}(\Omega)\times\Omega\to\mathbb{Z}/2$, as follows. Set $\tilde{\tau}(\{v\},v):=\hat{\tau}(v,v)=b(1)$, and for $U\neq\{v\}$ set

$$\tilde{\tau}(U,v):=\sum_{z\in U}\hat{\tau}(v,z)+b(\#_4 U)+b(1)+c(\#_4(U\Delta\{v\}))+1. \tag{26}$$

It is convenient to rewrite the formulas obtained above using this notation. For $l_i=i^b_{\{e_i\}}(\sigma_i)$, $i=1,2,\ldots,n$, we have

$$\forall z\in\Omega:\sigma_i(z)=\tilde{\tau}(\{e_i\},z).$$

For an element l of the form $l=i^b_U(\varphi)$, $\varphi\in L_b(U)$, $U\subset\Omega$, $\#U$ is odd, which is in relation T_c with every l_i, we have

$$\forall z\in\Omega:\varphi(z)=\tilde{\tau}(U,z).$$

The values of $\sigma_i(w)$ and $\varphi(w)$ in $w\in V\backslash\Omega$ remain arbitrary.

Now, take any nonempty $\Omega\subset V$, and take any function $\tau:\mathcal{E}(\Omega)\to\mathbb{Z}/2$. Define $\tilde{\tau}$ corresponding to τ by the formulas (25) and (26). For every $U\in\mathcal{P}_{\mathrm{odd}}(\Omega)$, denote

$$Q_U:=\{\varphi\in L_b(U)\,|\,\forall z\in\Omega:\varphi(z)=\tilde{\tau}(U,z)\}. \tag{27}$$

Note, that every $\varphi\in Q_U$ should satisfy $\Sigma_{z\in U}\tilde{\tau}(U,z)=b(\#_4 U)$. This yields the following condition:

$$\frac{\#U(\#U-1)}{2}(c(2)-1)+\#Uc(\#_4 U-1)-1=0.$$

The value of the left-hand side is determined by $\#_4 U$. Since $\#U$ is odd, it is necessary to consider just two cases, $\#_4 U=1$ and $\#_4 U=3$. In the first case one obtains $c(0)=1$, i.e., the condition we already have above, and the second case reduces to $0\equiv 0$.

Consider now the following set (for some Ω and τ):

$$M:=\bigsqcup_{U\in\mathcal{P}_{\mathrm{odd}}(\Omega)}\{i^b_U(\varphi)\}_{\varphi\in Q_U}. \tag{28}$$

The elements of M are pairwise in relation T_c. The cardinality of Ω is n, and the cardinality of V is N. On the points of $V\backslash\Omega$ a function $\varphi\in Q_U$ may take any value. In total there are 2^{N-n} possibilities for that. The number of all subsets of Ω is 2^n, and among them the number of those with odd cardinality is 2^{n-1}. Hence $\#M=2^{n-1}\times 2^{N-n}=2^{N-1}$. This number coincides with $\#L_b(W)$

for every nonempty $W \subset V$. It is not difficult to show that $M \in \mathrm{Max}(\mathcal{P}_{T_c}(A_b), \subset)$. Indeed, if $\Omega = V$, then it is impossible to have an element of the form $i^b_W(\psi)$ which is in relation T_c with every element of M, since if $\#W$ is odd, then such element is already in M, and the case $\#W$ being even is excluded due to conditions above. Consider a proper nonempty Ω. For the same reasons, W cannot be a subset of Ω. Hence, there exists a point $w \in W \backslash \Omega$. Consider $\theta' := \theta^{(\bar{a})}_{\bar{W}} \circ \theta^{(\bar{a})}_{\bar{W \sqcup \{w\}}} \circ \theta^{(\bar{a})}_{\bar{W}}$. Apply θ' to every element of M and to $i^b_W(\psi)$. The set M will still be of the form as above, but, perhaps, corresponding to a different τ, and the image of $i^b_W(\psi)$ after θ' is projected by the natural map $\eta: A_b \to \mathcal{P}(V)$ into the point $\{w\}$. Therefore, it suffices to consider just the case $W = \{w\}$. Take any $z \in \Omega$ and look at $\{i^b_{\{z\}}(\varphi)\}_{\varphi \in Q_{\{z\}}}$. As φ varies over $Q_{\{z\}}$, its value in w sweeps up the whole $\mathbb{Z}/2$. Therefore, it is impossible to satisfy $(i^b_{\{z\}}(\varphi), i^b_{\{w\}}(\psi)) \in T_c$ simultaneously for all φ. Hence, M is maximal.

Choose and fix any $B \subset M$. One has

$$B = \bigsqcup_{U \in \mathcal{P}_{\mathrm{odd}}(\Omega)} \{i^b_U(\varphi)\}_{\varphi \in S_U}, \tag{29}$$

where $S_U \subset Q_U$ are subsets (some of S_U, or even all, may be empty). Take any $i^b_W(\psi)$, $W \in \mathcal{P}(V)$, $\psi \in L_b(W)$, and look at what the condition $i^b_W(\psi) \in B^{T_c}$ means. It is necessary to consider different possibilities for W. Start with the case where W is a subset of Ω, and the number of elements in it is even. For any $U \in \mathcal{P}_{\mathrm{odd}}(\Omega)$ and any $\varphi \in S_U$, one must have $\Sigma_{z \in U \Delta W}(\psi(z) + \varphi(z)) = c(\#_4(U \Delta W)) + 1$. This is equivalent to

$$\sum_{z \in U} \psi(z) = \sum_{z \in W} \varphi(z) + b(\#_4 W) + b(\#_4 U) + c(\#_4(U \Delta W)) + 1.$$

Since $W \subset \Omega$, the values of $\varphi(z)$ are known, $\varphi(z) = \tilde{\tau}(U, z)$. Therefore, in the case $W \in \mathcal{P}_{\mathrm{even}}(\Omega)$, the requirement $i^b_W(\psi) \in B^{T_c}$ is rewritten as follows:

$$\begin{aligned}(i^b_W(\psi) \in B^{T_c}) = \bigwedge_{U \in \mathcal{P}_{\mathrm{odd}}(\Omega)} \Bigg(& S_U = \varnothing \ \text{ or } \sum_{z \in U} \psi(z) = \sum_{z \in W} \tilde{\tau}(U, z) + b(\#_4 W) \\ & + b(\#_4 U) + c(\#_4(U \Delta W)) + 1 \Bigg).\end{aligned} \tag{30}$$

There is a similar expression in case $W \in \mathcal{P}_{\mathrm{odd}}(\Omega)$, but special care is needed for the variant $U = W$,

$$\begin{aligned}(i^b_W(\psi) \in B^{T_c}) = (\psi \notin S_W) \quad \text{and} \quad \bigwedge_{\substack{U \in \mathcal{P}_{\mathrm{odd}}(\Omega) \\ U \neq W}} \Bigg(& S_U = \varnothing \ \text{ or } \sum_{z \in U} \psi(z) \\ & = \sum_{z \in W} \tilde{\tau}(U, z) + b(\#_4 W) + b(\#_4 U) + c(\#_4(U \Delta W)) + 1 \Bigg).\end{aligned} \tag{31}$$

Finally, there is a more complicated case, when W contains a part outside Ω, i.e., $W \cap \bar{\Omega} \neq \varnothing$. In this case we must deal with the sum $\Sigma_{z \in W} \varphi(z)$, but only part of $\varphi(z)$ are known, i.e., those that correspond to $z \in W \cap \Omega$, can be expressed as $\tilde{\tau}(U, z)$. Instead of the equality above, we obtain

$$\begin{aligned}(i^b_W(\psi) \in B^{T_c}) = \bigwedge_{U \in \mathcal{P}_{\mathrm{odd}}(\Omega)} \Bigg(& S_U = \varnothing \ \text{ or } \sum_{z \in U} \psi(z) = \sum_{z \in W \cap \Omega} \tilde{\tau}(U, z) + \sum_{z \in W \cap \bar{\Omega}} (\text{any } \varphi \in S_U)(z) \\ & + b(\#_4 W) + b(\#_4 U) + c(\#_4(U \Delta W)) + 1 \Bigg).\end{aligned} \tag{32}$$

The sum on the right-hand side containing φ should not depend on the choice of $\varphi \in S_U$, so we have a condition on S_U ensuring the existence of $i^b_W(\psi) \in B^{T_c}$ with such W.

First, consider in more detail the term $\psi \notin S_W$, $W \in \mathcal{P}_{\text{odd}}(\Omega)$ in the formula (31). Since $S_W \subset Q_W$, it splits into a disjunction $(\psi \in Q_W \setminus S_W) \vee (\psi \notin Q_W)$. The case that is described by the second term means that there exists a nontrivial $\chi: \Omega \to \mathbb{Z}/2$, such that $\psi(z) = \tilde{\pi}(W,z) + \chi(z)$, $z \in \Omega$. Since $\psi \in L_b(W)$, χ must satisfy $\Sigma_{z \in W} \chi(z) = 0$. It is convenient to view χ as an indicator function χ_Z of some nonempty subset $Z \in \mathcal{P}(\Omega)^\times := \mathcal{P}(\Omega) \setminus \{\varnothing\}$. Therefore, we have

$$(\psi \notin S_W) = (\psi \in Q_W \setminus S_W) \vee (\psi \notin Q_W),$$

while

$$(\psi \notin Q_W) = \bigvee_{\substack{Z \in \mathcal{P}(\Omega)^\times, \\ \#_2(Z \cap W) = 0}} [\psi(z \in \Omega) = \tilde{\pi}(W,z) + \chi_Z(z)].$$

Note that the cardinality of Z need not be odd.

The expression for $i^b_W(\psi) \in B^{T_c}$, $W \in \mathcal{P}_{\text{odd}}(\Omega)$, reduces to

$$(i^b_W(\psi) \in B^{T_c}) = (\psi \in Q_W \setminus S_W) \quad \text{or} \bigvee_{\substack{Z \in \mathcal{P}(\Omega)^\times, \\ \#_2(Z \cap W) = 0}} \left\{ [\psi(z \in \Omega) = \tilde{\pi}(W,z) + \chi_Z(z)] \quad \text{and} \right.$$
$$\left. \bigwedge_{\substack{U \in \mathcal{P}_{\text{odd}}(\Omega), \\ \#_2(U \cap Z) = 1}} (S_U = \varnothing) \right\}. \tag{33}$$

Note, that for the conjunction on the right-hand side of the formula one first obtains the range of possible values of U in the form $U \in \mathcal{P}_{\text{odd}}(\Omega)$, $\#_2((U \Delta W) \cap Z) = 1$, but since $\#_2(Z \cap W) = 0$, one has $\#_2((U \Delta W) \cap Z) = \#_2(U \cap Z)$.

Now one needs to consider arbitrary $i^b_W(\psi) \in B^{T_c}$ and $i^b_{W_1}(\psi_1) \in (M \setminus B)^{T_c}$, and then verify that $i^b_{W_1}(\psi_1)$ is in relation T_c with $i^b_W(\psi)$. The formulas for $i^b_{W_1}(\psi_1)$ are similar, except that it is necessary to replace all S_U with $Q_U \setminus S_U$. We must establish the following implication:

$$(i^b_W(\psi) \in B^{T_c}) \quad \text{and} \quad (i^b_{W_1}(\psi_1) \in (M \setminus B)^{T_c}) \Rightarrow (i^b_W(\psi), i^b_{W_1}(\psi_1)) \in T_c. \tag{34}$$

There are three possibilities for W and three possibilities for W_1 described above. In total, due to the symmetry of T_c, this yields $3 + 3(3-1)/2 = 6$ combinations. Each needs to be investigated separately verifying whether a strengthening of the conditions on $b(\cdot)$ and $c(\cdot)$ results. The result is the following.

Theorem 2: *Assume that the number N of points in V is divisible by 4. Let* $b, c: \mathbb{Z}/4 \to \mathbb{Z}/2$ *be two functions, such that* $b(0) = c(0) = 1$, $b(2) + c(2) = 0$, *and* $\Sigma_{i=1,3}(b(i) + c(i)) = 0$. *Define the finite set* A_b *and the relation* T_c *on* A_b *by (8) and (9) using (21). Then the relation* T_c *is saturated.*

Proof: The aim is to establish the implication (34). The proof splits naturally into six parts, corresponding to the six combinations mentioned above.

(1) The case $W, W_1 \in \mathcal{P}_{\text{odd}}(\Omega)$. We have a formula (31) for W, and there exists a similar formula for W_1 obtained after replacing S_U by $Q_U \setminus S_U$. If $W = W_1$, then one needs to show that $\psi(\cdot) \neq \psi_1(\cdot)$. In this case, for some $Z \in \mathcal{P}(\Omega)^\times$, $\psi(z \in \Omega) = \tilde{\pi}(W,z) + \chi_Z(z)$, and for all $U \in \mathcal{P}_{\text{odd}}(\Omega)$ such that $\#((U \Delta W) \cap Z)$ is odd, $S_U = \varnothing$. Similarly, for some $Z_1 \in \mathcal{P}(\Omega)^\times$, $\psi_1(z \in \Omega) = \tilde{\pi}(W,z) + \chi_{Z_1}(z)$, and for all $U_1 \in \mathcal{P}_{\text{odd}}(\Omega)$ such that $\#((U_1 \Delta W) \cap Z_1)$ is odd, $Q_{U_1} \setminus S_{U_1} = \varnothing$. If $Z \neq Z_1$, then $\psi(\cdot) \neq \psi_1(\cdot)$, since $\chi_Z(\cdot) \neq \chi_{Z_1}(\cdot)$. Hence, the implication holds. If $Z = Z_1$, then for every of the mentioned U, we have $S_U = \varnothing$ and $Q_U \setminus S_U = \varnothing$. Since Q_U is not empty, this possibility cannot occur. So the implication is established for $W = W_1$. Now assume, that $W \neq W_1$. One needs to verify that $\Sigma_{z \in W \Delta W_1}(\psi(z) + \psi_1(z)) = c(\#_4(W \Delta W_1)) + 1$. Observe that from the definition of M, and the property that relates Q_U and $\tilde{\pi}(U,z)$, for any $U, U_1 \in \mathcal{P}_{\text{odd}}(\Omega)$, we have

$$\sum_{z\in U\Delta U_1}(\tilde{\pi}(U,z)+\tilde{\pi}(U_1,z))=c(\#_4(U\Delta U_1))+1.$$

Hence, if $\psi\in Q_W\backslash S_W\subset Q_W$ and $\psi_1\in S_{W_1}\subset Q_{W_1}$, the requirement is satisfied. Now let $\psi\notin Q_W$, but $\psi_1\in S_{W_1}$. For $\psi(\cdot)$ we have a nonempty $Z\subset\Omega$, such that $\psi(z\in\Omega)=\tilde{\pi}(W,z)+\chi_Z(z)$. Moreover, whenever $U\in\mathcal{P}_{\text{odd}}(\Omega)$ and $\#((U\Delta W)\cap Z)$ is odd, one has $S_U=\emptyset$. For $\psi_1(\cdot)$ we have $\psi_1(z\in\Omega)=\tilde{\pi}(W,z)$. Therefore, the required equality holds iff $\Sigma_{z\in W\Delta W_1}\chi_Z(z)=0$, i.e., $\#((W\Delta W_1)\cap Z)$ is even. But $\#((W\Delta W_1)\cap Z)$ cannot be odd, since then (specializing U to W_1) one obtains $S_{W_1}=\emptyset$, i.e., $\psi_1(\cdot)$ does not exist. Hence, in this case the implication is established. The dual case, i.e., $\psi\in Q_W\backslash S_W$ and $\psi_1\notin Q_{W_1}$, is completely similar. It remains to investigate the possibility $\psi\notin Q_W$ and $\psi_1\notin Q_{W_1}$. For some nonempty $Z\subset\Omega$, $\#(Z\cap W)$ even, one has $\psi(z\in\Omega)=\tilde{\pi}(W,z)+\chi_Z(z)$. Similarly, for some nonempty $Z_1\subset\Omega$, $\#(Z_1\cap W_1)$ even, one has $\psi_1(z\in\Omega)=\tilde{\pi}(W_1,z)+\chi_{Z_1}(z)$. One needs an equality $\Sigma_{z\in W\Delta W_1}(\chi_Z(z)+\chi_{Z_1}(z))=0$, i.e., $\#((W\Delta W_1)\cap Z)$ and $\#((W\Delta W_1)\cap Z_1)$ are either both odd, or both even. To establish it, use the conjunctions over U and U_1 present in the corresponding formulas. Note, that $Z\cap Z_1$ needs to be empty. Indeed, otherwise one may take any $v\in Z\cap Z_1$ and set $U=U_1=\{v\}$. Since for these U and U_1, $\#_2(U\cap Z)=\#_2(U_1\cap Z_1)=1$, we have $S_{\{v\}}=\emptyset$ and $S_{\{v\}}=Q_{\{v\}}$, this contradicts $Q_{\{v\}}\neq\emptyset$. Hence, $Z\cap Z_1=\emptyset$. Moreover, Z and Z_1 should partition Ω, since otherwise one can set $U=U_1=\{v,v_1,w\}$, where $v\in Z$, $v_1\in Z_1$, and $w\in\Omega\backslash(Z\sqcup Z_1)$. For these, U and U_1 again have intersections with Z and Z_1, respectively, of odd cardinalities, and one obtains a contradiction between $S_{\{v,v_1,w\}}=\emptyset$ and $S_{\{v,v_1,w\}}=Q_{\{v,v_1,w\}}$ results. Now, we obtain $\Sigma_{z\in W\Delta W_1}(\chi_Z(z)+\chi_{Z_1}(z))=\Sigma_{z\in W\Delta W_1}\chi_\Omega(z)=\#_2(W\Delta W_1)=\#_2W+\#_2W_1$. Since $\#_2W=\#_2W_1=1$, this sum vanishes. This completes the proof of the implication (34) for $W,W_1\in\mathcal{P}_{\text{odd}}(\Omega)$.

(2) Now consider the case where both $W,W_1\in\mathcal{P}_{\text{even}}(\Omega)$. First look at the expression (30) corresponding to $i^b_W(\psi)\in B^{T_c}$. We have a conjunction over $U\in\mathcal{P}_{\text{odd}}(\Omega)$ on the right-hand side. In particular, U can be equal to $\{v\}$, where $v\in W$. Is it possible to have $\forall v\in W: S_{\{v\}}\neq\emptyset$? We claim that the answer is no. Indeed, if $S_{\{v\}}$ is not empty, then we have $\Sigma_{z\in\{v\}\Delta W}(\psi(z)+\tilde{\pi}(\{v\},z))=c(\#_4W-1)+1$. Apply summation over $v\in W$ and infer that $\tilde{\pi}(\{v\},z)=\hat{\pi}(v,z)$ and $\hat{\pi}(v,z)+\hat{\pi}(z,w)=c(2)+1$. This yields $(\#W-1)b(\#_4W)+(\#_4W(\#_4W-1)/2)(c(2)+1)=0$. If $\#_4W=0$, then one obtains $b(0)=0$, which is impossible, since we already have a condition $b(0)=1$. If $\#_4W=2$, then $b(2)+c(2)+1=0$, again contradicting the earlier assumption $b(2)+c(2)=0$. Therefore, there always exists $v\in W$, such that $S_{\{v\}}=\emptyset$. Similarly, we may analyze the expression for $i^b_{W_1}(\psi_1)\in(M\backslash B)^{T_c}$, and conclude that there exists $v_1\in W_1$, such that $S_{\{v_1\}}=W_{\{v_1\}}$. Start with the case $W_1=W$. Is it possible to have $\psi(\cdot)=\psi_1(\cdot)$? Suppose that ψ and ψ_1 coincide. For every $v\in W$, if $S_{\{v\}}\neq\emptyset$, then we have $\psi(v)=\Sigma_{z\in W}\hat{\pi}(v,z)+b(\#_4W)+b(1)+c(\#_4W-1)+1$. If $S_{\{v\}}=\emptyset$, then $S_{\{v\}}\neq Q_{\{v\}}$, and this implies $\psi_1(v)=\Sigma_{z\in W}\hat{\pi}(v,z)+b(\#_4W)+b(1)+c(\#_4W-1)+1$. But $\psi_1(v)=\psi(v)$, so we have the same expression for $\psi(v)$ in all $v\in W$. For the same reasons as mentioned above, the condition $\Sigma_{v\in W}\psi(b)=b(\#_4W)$ yields a contradiction. Therefore, $\psi(\cdot)$ and $\psi_1(\cdot)$ cannot be equal, and the implication of the form (34) for $W=W_1$ is established. Now assume, that $W_1\neq W$. It is necessary to show, that $\Sigma_{z\in W\Delta W_1}(\psi(z)+\psi_1(z))=c(\#_4(W\Delta W_1))+1$, whenever $i^b_W(\psi)\in B^{T_c}$ and $i^b_{W_1}(\psi_1)\in(M\backslash B)^{T_c}$ exist. Look at the expression (30) for $i^b_W(\psi)\in B^{T_c}$. Specialize U to a one-point set $U=\{u\}$, $u\in\Omega$. If $S_{\{u\}}\neq\emptyset$, then the value of $\psi(u)$ is known. How do we find the values of $\psi(\cdot)$ in other points of Ω? Actually, we do not need to know the value of $\psi(z)$ for each $z\in\Omega$, but just the sum $\Sigma_{z\in W\Delta W_1}\psi(z)$.

Let us establish an auxiliary fact first. We have $W\in\mathcal{P}_{\text{even}}(\Omega)$. Take any $U\in\mathcal{P}_{\text{odd}}(\Omega)$. Then $U\Delta W$ is a subset of Ω, and, moreover, $U\Delta W\in\mathcal{P}_{\text{odd}}(\Omega)$, since $\#_2U\Delta W=\#_2U+\#_2W$. Suppose, that $S_U\neq\emptyset$. Is it possible to have $S_{U\Delta W}\neq\emptyset$ as well? Suppose, that it is. For $U',U''\in\mathcal{P}(V)$, denote

$$g_{b,c}(U',U'')\coloneqq b(\#_4U')+b(\#_4U'')+c(\#_4(U'\Delta U''))+1.$$

One has

$$\sum_{z\in U}\psi(z)=\sum_{z\in W}\tilde{\pi}(W,z)+g_{b,c}(U,W),$$

$$b(\#_4 W) + \sum_{z \in U} \psi(z) = \sum_{z \in W} \tilde{\tau}(U \Delta W, z) + g_{b,c}(U \Delta W, W).$$

Sum the two equations and regroup the terms

$$\sum_{z \in W} [\tilde{\tau}(U,v) + \tilde{\tau}(U \Delta W, v)] = b(\#_4 W) + g_{b,c}(U,W) + g_{b,c}(U \Delta W, W).$$

Since $\tilde{\tau}(U,v) = \Sigma_{z \in U} \hat{\tau}(v,z) + g_{b,c}(U, \{v\})$, and, similarly, $\tilde{\tau}(U \Delta W, v) = \Sigma_{z \in U \Delta W} \hat{\tau}(v,z) + g_{b,c}(U \Delta W, \{v\})$, we obtain

$$\tilde{\tau}(U,v) + \tilde{\tau}(U \Delta W, v) = \sum_{z \in W} \hat{\tau}(v,z) + b(\#_4 U) + b(\#_4(U \Delta W)) + c(\#_4(U \Delta \{v\})) + c(\#_4(U \Delta W \Delta \{v\})).$$

It remains to sum over $v \in W$, and reduce the sum with $\hat{\tau}(v,z)$ on the right-hand side, taking into account that $\hat{\tau}(v,v) \equiv b(1)$, and $\hat{\tau}(v,z) + \hat{\tau}(z,v) = c(2) + 1$, $z \neq v$. Since $\#W$ is even, expressing $\#(U \Delta W)$ in terms of $\#U$, $\#W$, and $\#(U \cap W)$, yields

$$\frac{m(m-1)}{2}(c(2)+1) + t\{c(n-1) + c(n+m-2t+1) + c(n+1) + c(n+m-2t-1)\} + c(n) + c(n+m-2t) = b(n) + b(m) + b(n+m-2t),$$

where $m := \#_4 W$, $n := \#_4 U$, and $t := \#_4(U \cap W)$. This equation should be valid for generic W and U. The value of m can be 0 or 2, the value of n can be 1 or 3, and the value of t can be 0, 2, or 3. In total this yields $2 \times 2 \times 4 = 16$ variants. A straightforward (Maple) computation shows, that each of the variants reduces to one of the following four equations: either $b(0) = 0$, or $1 + b(2) + c(2) = 0$, or $b(0) + \Sigma_{i=1,3}(b(i) + c(i)) = 0$, or $1 + \Sigma_{i=1,2,3}(b(i) + c(i)) = 0$. Each of the four equations contradicts the already imposed assumptions on $b(\cdot)$ and $c(\cdot)$. Therefore, the following fact is established (recall, that $\#W$ is even):

$$\forall U \in \mathcal{P}_{\text{odd}}(\Omega) : (S_U \text{ or } S_{U \Delta W}) = \varnothing .$$

In a similar way (recall, that $\#W_1$ is also even), one obtains

$$\forall U \in \mathcal{P}_{\text{odd}}(\Omega) : S_U = Q_U \text{ or } S_{U \Delta W_1} = Q_{U \Delta W_1}.$$

Since $W \neq W_1$, there exists $e \in W \Delta W_1$. Take such e. Observe, that $\#(\{e\} \Delta W)$ and $\#(\{e\} \Delta W_1)$ are odd. Specializing U to $\{e\} \Delta W$, one obtains two facts: (1) $S_{\{e\} \Delta W} = \varnothing$ or $S_{\{e\}} = \varnothing$; (2) $S_{\{e\} \Delta W} = Q_{\{e\} \Delta W}$ or $S_{\{e\} \Delta W \Delta W_1} = Q_{\{e\} \Delta W \Delta W_1}$. Similarly, specializing U to $\{e\} \Delta W_1$, one obtains two more facts: (3) $S_{\{e\} \Delta W_1} = \varnothing$ or $S_{\{e\} \Delta W \Delta W_1} = \varnothing$; (4) $S_{\{e\} \Delta W_1} = Q_{\{e\} \Delta W_1}$ or $S_{\{e\}} = Q_{\{e\}}$. Look at the set $S_{\{e\}}$. It is either empty, or nonempty. If $S_{\{e\}} = \varnothing$, then, due to the fourth fact, $S_{\{e\} \Delta W_1} = Q_{\{e\} \Delta W_1}$. This, together with the third fact, implies $S_{\{e\} \Delta W \Delta W_1} = \varnothing$. From the second fact, $S_{\{e\} \Delta W} = Q_{\{e\} \Delta W}$. Now consider the second possibility, $S_{\{e\}} \neq \varnothing$. The first fact then implies $S_{\{e\} \Delta W} = \varnothing$. Hence, due to the second fact, $S_{\{e\} \Delta W \Delta W_1} = Q_{\{e\} \Delta W \Delta W_1}$. From the third fact, $S_{\{e\} \Delta W_1} = \varnothing$. Then the fourth fact yields $S_{\{e\}} = Q_{\{e\}}$. Therefore, we have an alternative, either

$$S_{\{e\}} = \varnothing , \quad S_{\{e\} \Delta W \Delta W_1} = \varnothing ,$$

$$S_{\{e\} \Delta W} = Q_{\{e\} \Delta W}, \quad S_{\{e\} \Delta W_1} = Q_{\{e\} \Delta W_1},$$

or

$$S_{\{e\}} = Q_{\{e\}}, \quad S_{\{e\} \Delta W \Delta W_1} = Q_{\{e\} \Delta W \Delta W_1},$$

$$S_{\{e\}\Delta W} = \varnothing, \quad S_{\{e\}\Delta W_1} = \varnothing.$$

In both cases there is a way to compute the sums $\Sigma_{z\in W\Delta W_1}\psi(z)$ and $\Sigma_{z\in W\Delta W_1}\psi_1(z)$. In the first case, the values of $\Sigma_{z\in\{e\}\Delta W\Delta W_1}\psi_1(z)$ and $\psi_1(e)$ are known. Their sum yields $\Sigma_{z\in W\Delta W_1}\psi_1(z)$. The sum $\Sigma_{z\in W\Delta W_1}\psi(z)$ should be computed as the sum of $\Sigma_{z\in\{e\}\Delta W}\psi(z)$ and $\Sigma_{z\in\{e\}\Delta W_1}\psi(z)$. The second case is dual to the first one (the roles of ψ and ψ_1 must be interchanged). So we always know $\Sigma_{z\in W\Delta W_1}(\psi(z)+\psi_1(z))$. It remains to compute this value, and then, using the assumptions about $b(\cdot)$ and $c(\cdot)$, verify that it reduces to $c(\#_4(W\Delta W_1))+1$. This is done by a straightforward computation. Consider, for example, the first option. One has

$$\sum_{z\in\{e\}\Delta W}\psi(z) = \sum_{v\in W}\tilde{\pi}(\{e\}\Delta W, v) + g_{b,c}(\{e\}, W),$$

$$\sum_{z\in\{e\}\Delta W_1}\psi(z) = \sum_{v\in W}\tilde{\pi}(\{e\}\Delta W_1, v) + g_{b,c}(\{e\}\Delta W_1, W).$$

This yields

$$\sum_{z\in W\Delta W_1}\psi(z) = \sum_{v\in W}[\tilde{\pi}(\{e\}\Delta W, v) + \tilde{\pi}(\{e\}\Delta W_1, v)] + c(1) + c(\#_4(W\Delta W_1) - 1) + b(\#_4(\{e\}\Delta W)) + b(\#_4(\{e\}\Delta W_1)).$$

Expanding the definitions of $\tilde{\pi}(\cdot,\cdot)$ in the square brackets, and then taking into account that $\#W$ is even, we obtain

$$\sum_{z\in W\Delta W_1}\psi(z) = \sum_{v\in W}\sum_{z\in W\Delta W_1}\hat{\pi}(v,z) + b(\#_4(\{e\}\Delta W)) + b(\#_4(\{e\}\Delta W_1)) + c(1) + c(\#_4(W\Delta W_1) - 1) + \sum_{v\in W}[c(\#_4(\{e\}\Delta W\Delta\{v\})) + c(\#_4(\{e\}\Delta W_1\Delta\{v\}))].$$

A similar computation yields

$$\sum_{z\in W\Delta W_1}\psi_1(z) = \sum_{v\in W_1}\sum_{z\in W\Delta W_1}\hat{\pi}(v,z) + c(\#_4(\{e\}\Delta W)) + c(\#_4(\{e\}\Delta W_1)) + b(1) + b(\#_4(W\Delta W_1) - 1) + \sum_{v\in W_1}[c(\#_4(\{e\}\Delta\{v\})) + c(\#_4(\{e\}\Delta W\Delta W_1\Delta\{v\}))].$$

Now, sum these equalities. On the right-hand side a sum of the form $\Sigma_{z,v\in W\Delta W_1}\hat{\pi}(v,z)$ appears; it is easily computed using $\hat{\pi}(v,v)\equiv b(1)$, and for $z\neq v$, $\hat{\pi}(v,z)+\hat{\pi}(z,v)=c(2)+1$. Hence an expression for $\Sigma_{z\in W\Delta W_1}(\psi(z)+\psi_1(z))$ in terms of $b(\cdot)$ and $c(\cdot)$ is obtained. On the other hand, we must verify that it is equal to $c(\#_4(W\Delta W_1))+1$. Denote $m := \#_4 W$, $m_1 := \#_4 W_1$, and $t := \#_4(W\cap W_1)$. Equate the two expressions mentioned and simplify the result taking into account, that $\#W$ and $\#W_1$ are even. It is necessary to consider the cases, $e\in W\setminus W_1$ and $e\in W_1\setminus W$, but in the end the result is the same,

$$\frac{m+m_1-2t}{2}[c(2)+1] + c(m) + c(m_1) + c(m+2) + c(m_1+2) + t\{c(m_1) + c(m_1+2) + c(m+m_1-2t) + c(m+m_1-2t+2)\} + b(m-1) + b(m_1+1) + b(1) + b(m+m_1-2t-1) + c(m-1) + c(m_1+1) + c(1) + c(m+m_1-2t-1) = c(m+m_1-2t) + 1.$$

It is straightforward to verify (best of all in Maple), that for all $m,m_1=0,2$ and all $t=0,1,2,3$, this equation reduces to one of the following: $1+c(0)=0$, of $\Sigma_{i=1,3}(b(i)+c(i))=0$, or $1+c(0)+\Sigma_{i=1,3}(b(i)+c(i))=0$, or $0=0$. Due to the assumptions above, this always holds. Hence, it is

established that if $W, W_1 \in \mathcal{P}_{\text{even}}(\Omega)$, then any $i^b_W(\psi) \in B^{T_c}$ is in relation T_c with any $i^b_{W_1}(\psi_1) \in (M\backslash B)^{T_c}$.

(3) Now consider the third possibility: let W and W_1 both contain points outside Ω, i.e., $W \cap \bar{\Omega} \neq \varnothing$ and $W_1 \cap \bar{\Omega} \neq \varnothing$. Take any $i^b_W(\psi) \in B^{T_c}$ and $i^b_{W_1}(\psi_1) \in (M\backslash B)^{T_c}$. Then we need to show, that $\psi_1(\cdot) \neq \psi(\cdot)$. There is an expression (32) for ψ and the expression for ψ_1 is similar. For every $U \in \mathcal{P}_{\text{odd}}(\Omega)$, such that $S_U \neq \varnothing$, the following quantity needs to be well defined: $\lambda_U := \Sigma_{z \in W \cap \bar{\Omega}} \varphi(z)$, where φ is an element of S_U. Similarly, if $S_U \neq Q_U$, then the following quantity is well defined: $\mu_U := \Sigma_{z \in W_1 \cap \bar{\Omega}} \varphi_1(z)$, where φ_1 is an element of $Q_U \backslash S_U$. Let us start with the case $W_1 = W$. Note, that the set of values of $\Sigma_{z \in U \cap \bar{\Omega}} \phi(z)$ as ϕ varies over the entire Q_U is $\mathbb{Z}/2$. Therefore, if $S_U \neq \varnothing$ and $S_U \neq Q_U$, then one has $\mu_U = 1 + \lambda_U$. Is it possible to have $S_U = \varnothing$ or $S_U = Q_U$ at all? If $S_U = \varnothing$, then, in particular, $S_U \neq Q_U$, and, μ_U needs to be well defined. At the same time, the corresponding sum $\Sigma_{z \in W_1 \cap \bar{\Omega}} \varphi_1$ ranges over $\mathbb{Z}/2$ as φ_1 varies over $Q_U \backslash S_U = Q_U$. Hence, μ_U is not defined, and therefore, S_U cannot be empty. For similar reasons, S_U cannot be equal to Q_U. So, we have $\forall U \in \mathcal{P}_{\text{odd}}(\Omega) : S_U \neq \varnothing, Q_U$. If $W_1 = W$, we must show, that $\psi(\cdot) \neq \psi_1(\cdot)$. This follows from the fact, that $\Sigma_{z \in U} \psi(z) + \Sigma_{z \in W} \tilde{\pi}(U, z) + g_{b,c}(U, W)$ should be equal to λ_U and $\mu_U = 1 + \lambda_U$ at the same time, a contradiction! Now let $W_1 \neq W$. One needs to compute the sum $\Sigma_{z \in W \Delta W_1}(\psi(z) + \psi_1(z))$. We can say nothing about the values of $\psi(z)$ and $\psi_1(z)$ in the points $z \notin \Omega$. Let us show, that these values are not needed, i.e., we show, that $W \Delta W_1 \subset \Omega$. The latter is equivalent to the statement, that the sets $K := W \cap \bar{\Omega}$ and $K_1 := W_1 \cap \bar{\Omega}$ coincide. Indeed, for every $U \in \mathcal{P}_{\text{odd}}(\Omega)$ the quantities $\lambda_U = \Sigma_{z \in K} \varphi(z)$ and $\mu_U = \Sigma_{z \in K_1} \varphi_1(z)$ are defined ($\varphi \in S_U$, $\varphi_1 \in Q_U \backslash S_U$). The definition (27) of Q_U implies, that the values of $\phi \in Q_U$ in the points outside Ω are not restricted by any condition. Hence, if $K \neq K_1$, there exists $\phi \in Q_U$, such that $\Sigma_{z \in K} \phi(z) = 1 + \lambda_U$ and $\Sigma_{z \in K_1} \phi(z) = 1 + \mu_U$. But such $\phi \notin S_U$, $Q_U \backslash S_U$, a contradiction! Hence, $K = K_1$, and $W \Delta W_1 \subset \Omega$. Since $K = K_1$, it follows that $\mu_U = 1 + \lambda_U$, $U \in \mathcal{P}_{\text{odd}}(\Omega)$. Take any $u \in \Omega$, and specialize U to $\{u\}$. This yields

$$\psi(u) = \sum_{v \in W \cap \Omega} \tilde{\pi}(\hat{u}, v) + \lambda_{\hat{u}} + g_{b,c}(\{u\}, W),$$

$$\psi_1(u) = \sum_{v \in W_1 \cap \Omega} \tilde{\pi}(\hat{u}, v) + (1 + \lambda_{\hat{u}}) + g_{b,c}(\{u\}, W_1).$$

Sum these two equalities, and then preform summation over $u \in W \Delta W_1$. The result should be $c(\#_4(W \Delta W_1)) + 1$. Note, that on the other hand, the terms with $\tilde{\pi}(\hat{u}, v)$ on the right-hand side are of the form $\Sigma_{u,v \in W \Delta W_1} \tilde{\pi}(\hat{u}, v)$, and this sum can be expressed in terms of $b(\cdot)$ and $c(\cdot)$ as above. Denote $m := \#_4 W$, $m_1 := \#_4 W_1$, and $t := \#_4(W \cap W_1)$. After simplifications, the result can be written in the form,

$$\frac{q(q-1)}{2}[c(2) + 1] + q(1 + b(1) + b(m) + b(m_1)) + (m - t)\{c(m - 1) + c(m_1 + 1)\} + (m_1 - t) \times \{c(m + 1) + c(m_1 - 1)\} + c(q) + 1 = 0,$$

where $q := m + m_1 - 2t$. The variables m, m_1, and t, vary over $\mathbb{Z}/4$. It remains to verify (easiest in Maple) that for each of the possible $4 \times 4 \times 4 = 64$ variants this equality is true. Each time the left-hand side reduces to one of the following variants: $1 + c(0)$, $1 + b(0)$, $b(2) + c(2)$, $b(1) + b(3) + c(1) + c(3)$, or a linear combination of the mentioned ones. Hence, due to the imposed conditions, the equality is always valid. This means, that $(i^b_W(\psi), i^b_{W_1}(\psi_1)) \in T_c$ in case $W \cap \bar{\Omega} \neq \varnothing$ and $W_1 \cap \bar{\Omega} \neq \varnothing$.

(4) Now it is necessary to consider three mixed cases. Start with $W \in \mathcal{P}_{\text{even}}(\Omega)$ and $W_1 \in \mathcal{P}_{\text{odd}}(\Omega)$. Assume, that $i^b_W(\psi) \in B^{T_c}$ and $i^b_{W_1}(\psi_1) \in (M\backslash B)^{T_c}$. For ψ_1 there are two possibilities. The first one is that $\psi_1 \in S_W$, and hence $\psi_1(z) = \tilde{\pi}(W_1, z)$, $z \in \Omega$. The other is that $\psi_1(\cdot)$ in the points $z \in \Omega$ is of the form $\psi_1(z) = \tilde{\pi}(W_1, z) + \chi_Z(z)$, where Z is some nonempty subset of Ω, such that

$\#(Z\cap W)$ is even. In the latter case, for all $U\in\mathcal{P}_{\mathrm{odd}}(\Omega)$ such that $\#(U\cap Z)$ is odd, $S_U=Q_U$. Concerning $\psi(\cdot)$ one can say, that for all $U\in\mathcal{P}_{\mathrm{odd}}(\Omega)$, either $S_U=\varnothing$, or $\Sigma_{z\in U}\psi(z)=\Sigma_{z\in W}\tilde{\tau}(U,z)+g_{b,c}(U,W)$. Consider the first possibility for ψ_1. In particular this implies that $S_{W_1}\neq\varnothing$. Hence the sum $\Sigma_{z\in W_1}\psi(z)$ is known. On the other hand, since $\psi_1\in S_W\subset Q_W$, one has $\psi_1(z\in\Omega)=\tilde{\tau}(W_1,z)$. From this $\Sigma_{z\in W_1}\psi(z)=\Sigma_{z\in W}\psi_1(z)+g_{b,c}(W,W_1)$, i.e., $(i^b_W(\psi),i^b_{W_1}(\psi_1))\in T_c$ follows. Now consider the second possibility for ψ_1 (the one with Z). Observe, that $\#_2(W\Delta W_1)=\#_2W+\#_2W_1=1$, i.e., $W\Delta W_1\in\mathcal{P}_{\mathrm{odd}}(\Omega)$. Look at $(W\Delta W_1)\cap Z$. We have $\#_2(W\Delta W_1)\cap Z=\#_2((W\cap Z)\Delta(W_1\cap Z))=\#_2(W\cap Z)$. Therefore, if $\#(W\cap Z)$ is odd, take $U=W\Delta W_1$ and obtain $S_{W\Delta W_1}=Q_{W\Delta W_1}$. In particular, $S_{W\Delta W_1}\neq\varnothing$, leading to the expression for $\Sigma_{z\in W\Delta W_1}\psi(z)$. The values of $\psi_1(z)$ are known at all points $z\in\Omega$, so there is no problem to compute $\Sigma_{z\in W\Delta W_1}\psi_1(z)$. Taking into account, that $\Sigma_{v\in W\Delta W_1}\chi_Z(v)=\#((W\Delta W_1)\cap Z)=1$, and then expressing $\tilde{\tau}$ via $\hat{\tau}$ and $g_{b,c}$, we obtain

$$\sum_{z\in W\Delta W_1}[\psi(z)+\psi_1(z)]=1+\sum_{v,z\in W}\hat{\tau}(v,z)+\sum_{v,z\in W_1}\hat{\tau}(v,z)+\sum_{v\in W}g_{b,c}(\{v\},W\Delta W_1)+\sum_{v\in W\Delta W_1}g_{b,c}(\{v\},W_1)+g_{b,c}(W\Delta W_1,W).$$

On the other hand, this sum should be equal to $c(\#_4(W\Delta W_1))+1$. Expressing the sums with $\hat{\tau}(v,z)$ in terms of $b(\cdot)$ and $c(\cdot)$, one obtains the following equality:

$$\begin{aligned}(m+m_1)b(1)+\left(\frac{m(m-1)}{2}+\frac{m_1(m_1-1)}{2}\right)[c(2)+1]+(m-t)c(q-1)+tc(q+1)\\+m\{b(1)+b(q)+1\}+(m-t)c(m_1+1)+(m_1-t)c(m_1-1)+q\{b(1)+b(m_1)+1\}+b(q)\\+b(m)+c(m_1)+c(q)+1=0,\end{aligned}$$

where $m:=\#_4W$, $m_1:=\#_4W_1$, $t:=\#_4(W\cap W_1)$, $q:=m+m_1-2t$. It is necessary to verify that this equality is true for every $m=0,2$, every $m_1=1,3$, and $t=0,1,2,3$. This is done by a straightforward computation (in Maple). In each variant, the left-hand side reduces to a linear combination of the expressions $1+b(0)$, $1+c(0)$, $b(2)+c(2)$, and $\Sigma_{i=1,3}(b(i)+c(i))$. Due to the conditions on $b(\cdot)$ and $c(\cdot)$ imposed above, the equality is always true, so one has $(i^b_W(\psi),i^b_{W_1}(\psi_1))\in T_c$ for $W\in\mathcal{P}_{\mathrm{even}}(\Omega)$, $W_1\in\mathcal{P}_{\mathrm{odd}}(\Omega)$.

(5) Now consider the next case. Suppose that there exist $i^b_W(\psi)\in B^{T_c}$, $i^b_{W_1}(\psi_1)\in(M\backslash B)^{T_c}$, where $W_1\cap\bar{\Omega}\neq\varnothing$ and $W\in\mathcal{P}_{\mathrm{even}}(\Omega)$. Take any $U\in\mathcal{P}_{\mathrm{odd}}(\Omega)$. For ψ we have $S_U=\varnothing$ or $\Sigma_{z\in U}\psi(z)=\Sigma_{v\in W}\tilde{\tau}(U,v)+g_{b,c}(U,W)$. For ψ_1 we have $S_U=Q_U$ or $\Sigma_{z\in U}\psi_1(z)=\Sigma_{v\in W_1\cap\Omega}\tilde{\tau}(U,v)+\mu_U+g_{b,c}(U,W_1)$, where $\mu_U=\Sigma_{z\in W_1\cap\bar{\Omega}}\varphi(z)$, φ being an element of $Q_U\backslash S_U$. Observe, that S_U cannot be empty, since either $S_U=Q_U$, or μ_U is defined. Therefore, we always know the sum $\Sigma_{z\in U}\psi(z)$. In particular, U can be of the form $\{w\}$, where $w\in W$, then $\psi(w)=\Sigma_{v\in W}\tilde{\tau}(w,v)+b(\#_4W)+b(1)+c(\#_4(W\Delta\{w\}))+1$. Sum over all $w\in W$, and use the fact that $\#W$ is even. This yields $\Sigma_{w\in W}\psi(w)=\Sigma_{v,w\in W}\tilde{\tau}(w,v)$. On the other hand, this sum should be equal to $b(\#_4W)$. Hence one derives $b(m)=(m(m-1)/2)[c(2)+1]$, $m:=\#_4W$. If $m=0$, one obtains $b(0)=0$, and if $m=2$, one obtains $b(2)=c(2)+1$. In both cases this contradicts the assumptions on $b(\cdot)$ and $c(\cdot)$. This means, that the pair $(i^b_W(\psi),i^b_{W_1}(\psi_1))$ cannot exist.

(6) It remains to investigate just the case where one of the sets W or W_1 is an odd subset of Ω, and the other contains at least one point outside Ω. Let $W\in\mathcal{P}_{\mathrm{odd}}(\Omega)$ and $W_1\cap\bar{\Omega}\neq\varnothing$. Suppose, that $i^b_W(\psi)\in B^{T_c}$ and $i^b_{W_1}(\psi_1)\in(M\backslash B)^{T_c}$. First look at the condition for ψ_1. For any $U\in\mathcal{P}_{\mathrm{odd}}(\Omega)$, the set S_U cannot be empty, since one has either $S_U=Q_U$ or the quantity $\mu_U:=\Sigma_{z\in W_1\cap\bar{\Omega}}\varphi(z)$ needs to be defined (φ is an element of $Q_U\backslash S_U$; if φ varies over the entire Q_U, the sum ranges over the entire $\mathbb{Z}/2$ and μ_U is undefined). Now look at the condition for ψ. First investigate the possibility $\psi(z)=\tilde{\tau}(W,z)+\chi_Z(z)$, $z\in\Omega$, for some nonempty $Z\subset\Omega$, with $\#(Z\cap W)$ even. If $\#Z$ is odd, then take $U=Z$. This yields $S_Z=\varnothing$, contradicting the previous fact. If $\#Z$ is even, then since $\#W$ is odd, there always exist a point $e\in W\backslash Z$. [This is implied by the facts that $\#W$ is odd and $\#(W\cap Z)$ is even,

and therefore $\#(W\backslash Z)$ is odd.] Set $U=\{e\}\sqcup Z$. This yields $S_{\{e\}\sqcup Z}=\varnothing$, again a contradiction. Hence the only possibility that remains for ψ is $\psi\in Q_W\backslash S_W$. For this case the values of $\psi(\cdot)$ are known in every point of Ω. Since such ψ is assumed to exist, $S_W\neq Q_W$. Now, set $U=W$ in the condition for ψ_1 [one can do it since $W\in\mathcal{P}_{\mathrm{odd}}(\Omega)$]. This yields $\Sigma_{z\in W}\psi_1(z)=\Sigma_{z\in W_1\cap\Omega}\tilde{\pi}(W,z)+\mu_U+g_{b,c}(W,W_1)$. But $\tilde{\pi}(W,z)$ is just the value of $\psi(z)$. Recall, that the definition of μ_U contains an arbitrary function $\varphi\in Q_U\backslash S_U$. Take $\varphi=\psi$. In the result, one obtains $\Sigma_{z\in W}\psi_1(z)=\Sigma_{z\in W_1}\psi(z)+g_{b,c}(W,W_1)$, i.e., $(i^b_W(\psi),i^b_{W_1}(\psi_1))\in T_c$. This completes the proof that T_c satisfies the main condition (6). Applying the described construction to the set A_b and relation T_c, one obtains a coherent orthoalgebra. □

VII. ABSENSE OF BIVALUATIONS

Recall, that we have made the following assumptions in order to construct an orthoalgebra: N is divisible by 4, $b(0)=1$, $c(0)=1$, $b(2)+c(2)=0$, and $\Sigma_{i=1,3}(b(i)+c(i))=0$. Let us show that such orthoalgebra cannot admit bivaluations. Take $N+1$ elements of $\mathrm{Max}(\mathcal{P}_{T_c}(A_b),\subset)$: N elements $B_v:=\{i^b_{\{v\}}(\sigma)\}_{\sigma\in L_b(\{v\})}$, $v\in V$, and an element $\hat{B}:=\{i^b_V(\pi)\}_{\pi\in L_b(V)}$. Note, that $\hat{B}$ is transformed into B_v if one applies $\hat{\theta}^{(\bar{a})}_{\{v\}}\hat{\theta}^{(\bar{a})}_V\hat{\theta}^{(\bar{a})}_{\{v\}}$ to each of its elements. Recall, that the ground set of our orthoalgebra is $\mathcal{P}^{T_c}(A_b)$. Every singleton $\{l\}$, where $l\in(\sqcup_{v\in V}B_v)\sqcup\hat{B}$ is in this ground set, $\{l\}\in\mathcal{P}^{T_c}(A_b)$. For every $v\in V$ the sum $\oplus_{l\in B_v}\{l\}$ is defined and equals A_b, i.e., the $\mathbf{1}$ of the orthoalgebra. Also, $\oplus_{l\in\hat{B}}\{l\}=\mathbf{1}$. Assume that there exists a bivaluation $f:X_{b,c}\to\mathbb{B}$, where $X_{b,c}$ denotes the constructed orthoalgebra. One has the following equalities in $\mathbb{B}$: $\oplus_{l\in B_v}f(\{l\})=\mathbf{1}$, $v\in V$, and $\oplus_{l\in\hat{B}}f(\{l\})=\mathbf{1}$. Since $\oplus$ in $\mathbb{B}$ is defined just in three cases, $\mathbf{0}\oplus\mathbf{0}$, $\mathbf{1}\oplus\mathbf{0}$, and $\mathbf{0}\oplus\mathbf{1}$, one derives two statements: (1) $\forall v\in V\exists!\,l\in B_v:f(l)=\mathbf{1}$; (2) $\exists!\,l\in\hat{B}:f(l)=\mathbf{1}$. Denote these uniquely defined elements by $l_v\in B_v$, $v\in V$, and $\hat{l}\in\hat{B}$, respectively. Any pair (l,l'), $l'\neq l$, of these elements cannot be in T_c. Indeed, then $l\oplus l'$ would have been defined. Applying to it f, $f(l)\oplus f(l')=\mathbf{1}\oplus\mathbf{1}$, follows a contradiction. Write $l_v=i^b_{\{v\}}(\sigma_v)$, $\sigma_v\in L_b(\{v\})$, and $\hat{l}=i^b_V(\hat{\pi})$, $\hat{\pi}\in L_b(V)$. The definition of T_c yields, for any $v,v_1\in V$, $v\neq v_1$, that

$$\sigma_v(v_1)+\sigma_{v_1}(v)=c(2),$$

$$\sum_{z\in V\backslash\{v\}}(\pi(z)+\sigma_v(z))=c(3).$$

Take the sum over $v\in V$ for the second equality. Using the definition of $L_b(V)$ one obtains

$$(N-1)b(0)+\sum_{\substack{z,v\in V,\\ z\prec v}}(\sigma_z(v)+\sigma_v(z))=Nc(3),$$

where $\prec$ is any order on V. Now, using the first equality, and then the fact that N is divisible by 4, one arrives at $b(0)=0$. This contradicts the assumption $b(0)=1$. Therefore, a bivaluation of $X_{b,c}$ cannot exist.

VIII. ISOMORPHIC ORTHOALGEBRAS

There are several options for the choice of $b(\cdot)$ and $c(\cdot)$ satisfying the conditions of the theorem. Let us derive a *sufficient* condition for two orthoalgebras of the form $X_{b,c}$ to be isomorphic. Select any (b,c) satisfying the conditions of the theorem, and any (b',c') satisfying the same conditions. Construct $A_b:=\sqcup_{U\in\mathcal{P}(\Omega)}L_b(U)$ and $A_{b'}:=\sqcup_{U\in\mathcal{P}(\Omega)}L_{b'}(U)$, and define the relations T_c and $T_{c'}$ on A_b and $A_{b'}$, respectively. Denote by $i^b_U:L_b(U)\rightarrowtail A_b$ and $i^{b'}_U:L_{b'}(U)\rightarrowtail A_{b'}$ the canonical injections. Suppose that there exists a bijective map $\hat{t}:A_b\xrightarrow{\sim}A_{b'}$, such that $(l,l_1)\in T_c$ implies $(\hat{t}(l),\hat{t}(l_1))\in T_{c'}$. Then this map induces a bijection $\mathcal{P}^{T_c}(A_b)\xrightarrow{\sim}\mathcal{P}^{T_{c'}}(A_{b'})$, which establishes an isomorphism of the orthoalgebras $X_{b,c}$ and $X_{b',c'}$. Let us try to construct such a map and investigate what kind of relations between b, c, b', and c', emerge.

The map $\hat{t}$ is defined by a collection of bijections $\{t_U\}_{U\in\mathcal{P}(V)}$, where $t_U: L_b(U)\tilde{\to}L_{b'}(U)$. Let us search for t_U in the form

$$t_U(\psi)(v) = \psi(v) + \alpha_U(v),$$

where $\alpha_U(v)$ are some $\mathbb{Z}/2$-valued parameters, $U\in\mathcal{P}(V)$, $v\in V$. Denote

$$\tilde{b}_U := b(\#_4 U) + b'(\#_4 U),$$

$$\tilde{c}_{U,U_1} := c(\#_4(U\Delta U_1)) + c'(\#_4(U\Delta U_1)) + \tilde{b}_U + \tilde{b}_U.$$

The requirement that $\Sigma_{v\in U}\psi(v)=b(\#_4 U)\Rightarrow\Sigma_{v\in U}t_U(\psi)(v)=b'(\#_4 U)$, yields for every $U\in\mathcal{P}(V)$ an equation on $\alpha_U(\cdot)$,

$$\sum_{v\in U}\alpha_U(v) = \tilde{b}_U.$$

Similarly, for every $U,U_1\in\mathcal{P}(V)$, $U\neq U_1$, the requirement that for any $\psi\in L_b(U)$, $\psi_1\in L_b(U_1)$, $\Sigma_{v\in U\Delta U_1}(\psi(v)+\psi_1(v))=c(\#_4(U\Delta U_1))+1\Rightarrow\Sigma_{v\in U\Delta U_1}(t_U(\psi)(v)+t_U(\psi_1)(v))=c'(\#_4(U\Delta U_1))+1$, yields an equation

$$\sum_{v_1\in U_1}\alpha_U(v_1) + \sum_{v\in U}\alpha_{U_1}(v) = \tilde{c}_{U,U_1}.$$

These equations are similar to Eqs. (17) and (18), for $a_{S,U}(v)$ derived above. It is not difficult to solve them. First consider the case, $\#U=1$ and $\#U_1=1$. From this it follows, that $\alpha_{\{v\}}(z)$ is a solution of the corresponding system iff it is of the form $\alpha_{\{v\}}(z)=\alpha^{(\nu)}_{\{v\}}(z)$, where

$$\alpha^{(\nu)}_{\{v\}}(z) := \begin{cases} \nu(zv) & \text{if } z\prec v,\\ \tilde{b}_{\{v\}} & \text{if } z=v,\\ \nu(zv)+\tilde{c}_{\{z\},\{v\}} & \text{if } z\succ v,\end{cases}$$

where $\nu:\mathcal{E}(V)\to\mathbb{Z}/2$ is an arbitrary function, and $\prec$ is some chosen and fixed order on V. The other $\alpha_Q(v)$, $\#Q\geqslant 2$, may be found from the specialization $U=\{v\}$, $U_1=Q$, in the equation with $\tilde{c}_{U,U_1}$. This yields $\alpha_Q(v)=\alpha^{(\nu)}_Q(v)$, where

$$\alpha^{(\nu)}_Q(v) = \tilde{c}_{\{v\},Q} + \sum_{z\in Q}\alpha^{(\nu)}_{\{v\}}(z).$$

Now consider the equations with $\tilde{b}_U$, corresponding to $U=Q$, $\#Q\geqslant 2$, and the equations with $\tilde{c}_{U,U_1}$, corresponding to $U=Q$, $U_1=Q_1$, with $\#Q,\#Q_1\geqslant 2$. This leads to the following solvability conditions:

$$\tilde{c}_{Q,Q_1} + \sum_{z\in Q}\tilde{c}_{\{z\},Q_1} + \sum_{z_1\in Q_1}\tilde{c}_{Q,\{z_1\}} + \sum_{\substack{z\in Q,\\ z_1\in Q_1}}\tilde{c}_{\{z\},\{z_1\}} = 0, \tag{35}$$

$$\sum_{v\in Q}\tilde{c}_{\{v\},Q} + \sum_{\substack{v,z\in Q,\\ z\succ v}}\tilde{c}_{\{v\},\{z\}} = \tilde{b}_Q + \sum_{v\in Q}\tilde{b}_{\{v\}}. \tag{36}$$

Note that if one formally takes Q or Q_1 of cardinality 1, the corresponding equality trivializes. Note also that this system of equations becomes the system of equations (19) and (20), for $c^{(S)}_{Q,Q_1}$ and $b^{(S)}_Q$ investigated above, if one formally replaces $\tilde{c}_{Q,Q_1}$ with $c^{(S)}_{Q,Q_1}$, and $\tilde{b}_Q$ with $b^{(S)}_Q$. From the

definition of $\tilde{b}_U$, it is clear that its value is determined by $\#_4 U$, i.e., $\tilde{b}_U = \beta(\#_4 U)$, where $\beta: \mathbb{Z}/4 \to \mathbb{Z}/2$ is some function. Similarly, $\tilde{c}_{U,U_1}$ can be written as $\tilde{c}_{U,U_1} = \gamma(\#_4(U \Delta U_1)) + \beta(\#_4 U) + \beta(\#_4 U_1)$, where $\gamma: \mathbb{Z}/4 \to \mathbb{Z}/2$ is some function. It is necessary to substitute these expressions into the solvability conditions (35) and (36), above. The values of the resulting expressions are determined by $m := \#_4 Q$, $m_1 := \#_4 Q_1$, and $t := \#_4(Q \cap Q_1)$. Analyzing the $4 \times 4 \times 4 = 64$ corresponding variants, we should discover which assumptions on $\beta(\cdot)$ and $\gamma(\cdot)$ emerge. The equation with four $\tilde{c}$ yields

$$\{\gamma(m + m_1 - 2t) + \beta(m) + \beta(m_1)\} + (m - t)\gamma(m_1 + 1) + t\gamma(m_1) + m[\beta(1) + \beta(m_1)] + (m_1 - t)\gamma(m + 1) + t\gamma(m) + m_1[\beta(1) + \beta(m)] + \left(\frac{t(t-1)}{2} + (m - t)t + (m_1 - t)t + (m - t)(m_1 - t)\right)\gamma(2) = 0.$$

The equation with $\tilde{b}$ yields

$$m\{\gamma(m - 1) + \beta(1) + \beta(m)\} + \frac{m(m-1)}{2}\gamma(2) = \beta(m) + m\beta(1).$$

A straightforward (Maple) computation shows, that all these equalities hold iff

$$\gamma(0) = 0, \quad \gamma(2) = 0, \quad \gamma(1) + \gamma(3) = 0,$$

$$\beta(0) = 0, \quad \beta(2) = 0, \quad \beta(1) + \beta(3) = 0.$$

Recall that $b'(i) = b(i) + \beta(i)$, $c'(i) = c(i) + \gamma(i)$, $i \in \mathbb{Z}/4$. Hence, if the additions $\beta(\cdot)$ and $\gamma(\cdot)$ satisfy these conditions, the corresponding orthoalgebras are isomorphic.

IX. THE PROJECTIVE LINES

Let $N=4$. Set $b(0) = c(0) = 1$ and the other $b(i) = c(i) = 0$, $i = 1, 2, 3$. We have the set A_b and the relation $T_c \subset A_b \times A_b$. Let us write just A and T in this case. Let us show how (only in this particular case) the main condition on T may be established in a different way (not combinatorial, but geometric).

Take a Hilbert space $\mathcal{H}$ of finite dimension $d = 2^{N-1} = 8$ over $\mathbb{C}$. Consider $\mathbb{P}(\mathcal{H})$ equipped with the orthogonality relation $\perp$. Suppose, that there exists an *injective* map $\mu: A \rightarrowtail \mathbb{P}(\mathcal{H})$, such that $\forall x, x_1 \in A: (x, x_1) \in T \Leftrightarrow \mu(x) \perp \mu(x_1)$. Then the main property for T can be easily established. Indeed, take any $M \in \mathrm{Max}(\mathcal{P}_T(A), \subset)$, and then any $B \subset M$. The map μ sends M into a set of d pairwise orthogonal projective lines. An element $x \in A$ falls into B^T iff its image $\mu(x)$ is orthogonal to every $\mu(y)$, $y \in B$. The latter is equivalent to $\mu(x) \in (\mathrm{span}\{\mu(y) \,|\, y \in B\})^{\perp} =: P_1$. Similarly, $x \in A$ falls into $(M \backslash B)^T$ iff $\mu(x) \in (\mathrm{span}\{\mu(y) \,|\, y \in M \backslash B\})^{\perp} =: P_2$. Since $\mu(y)$, $y \in M$, are pairwise orthogonal and the span over them is the whole space $\mathcal{H}$, the subspaces P_1 and P_2 have trivial intersection and are mutually orthogonal. For any $x_1 \in B$ and any $x_2 \in M \backslash B$, we have $\mu(x_1) \in P_1$ and $\mu(x_2) \in P_2$. Hence $\mu(x_2) \perp \mu(x_1)$, and this is equivalent to $(x_1, x_2) \in T$. So the main property of T is established.

In case $N=4$ the map μ mentioned can be constructed. This fact relies on the results of Ref. 10. Set $\mathcal{H} = (\mathbb{C}^2)^{\otimes 3}$. Take any orthonormal basis $\{\varphi_\alpha\}_\alpha$ in $\mathbb{C}^2$ indexed by $\alpha \in \mathbb{Z}/2$. Define a map $u: (\mathbb{Z}/2)^2 \to \mathbb{R}$ as follows: $u(1,1) := -1$ and $u(i,j) := 1$ for $(i,j) \neq (1,1)$. Construct another orthonormal basis $\{\psi_\beta\}_{\beta \in \mathbb{Z}/2}$ in $\mathbb{C}^2$ by defining $\psi_\beta := (1/\sqrt{2}) \Sigma_\alpha u(\alpha, \beta) \varphi_\alpha$. Recall that $A = \sqcup_{U \in \mathcal{P}(V)} L(U)$, where $L(U)$ consists of all functions $\phi: V \to \mathbb{Z}/2$, such that $\Sigma_{z \in U} \phi(z) = b(\#_4 U)$. Note that since we have $b(0) = 1$, the set $L(\varnothing)$ is empty. Hence the latter disjoint union can be viewed as being taken over $U \in \mathcal{P}(V)^{\times} := \mathcal{P}(V) \backslash \{\varnothing\}$. Denote by $i_U: L(U) \rightarrowtail A$ the canonical injections. The elements $\mu(i_U(\phi)) \in \mathbb{P}(\mathcal{H})$, $U \in \mathcal{P}(V)^{\times}$, $\phi \in L(U)$, are defined as follows. In Ref. 10 there were defined 120 projective lines in $\mathcal{H}$ denoted by Ψ^v_σ, $X^{vw}_\varkappa$, Φ^v_ρ, and F_π, where $v, w \in V$, $w \neq v$, and the indices σ, $\varkappa$, ρ, and π vary over the sets S_v, K_{vw}, R_v, and Λ, respectively, defined as follows:

$$S_v := \mathrm{Maps}(\{\{v,z\}|z \in V\setminus\{v\}\} \to \mathbb{Z}/2),$$

$$K_{vw} := \mathrm{Maps}(\{\{v,w\}\} \sqcup (V\setminus\{v,w\}) \to \mathbb{Z}/2),$$

$$R_v := \mathrm{Maps}(\{\{z,w\}|z,w \in V\setminus\{v\}, z \neq w\} \to \mathbb{Z}/2),$$

$$\Lambda := \left\{ \pi \in \mathrm{Maps}(V \to \mathbb{Z}/2) | \sum_{z\in V} \pi(z) = 1 \right\}.$$

The corresponding formulas for the projective lines are given in terms of φ_α, ψ_β, and $u(\alpha,\beta)$ $(\alpha,\beta \in \mathbb{Z}/2)$, and discussed in more detail in that paper. Note that the index sets S_v, K_{vw}, R_v, and Λ, all have cardinality $2^3=8$.

Let us establish bijections $\alpha_v : L(\{v\}) \tilde{\to} S_v$, $\beta_{vw} : L(\{v,w\}) \tilde{\to} K_{vw}$, $\gamma_v : L(V\setminus\{v\}) \tilde{\to} R_v$, and $\lambda : L(V) \tilde{\to} \Lambda$. For $v \in V$ and $\phi \in L(\{v\})$, set

$$\alpha_v(\phi)(vz) := \phi(z), \quad z \in V\setminus\{v\}.$$

For $v,w \in V$, $w \neq v$, and $\phi \in L(\{v,w\})$, set

$$\beta_{vw}(\phi)(vw) := \phi(v) = \phi(w),$$

$$\beta_{vw}(\phi)(z) := \phi(t), \quad \beta_{vw}(\phi)(t) := \phi(z),$$

where z and t are the two different elements of $V\setminus\{v,w\}$. [Note, that $\phi(v)=\phi(w)$, since $b(2)=0$.] For every $v \in V$ and $\phi \in L(V\setminus\{v\})$, set

$$\gamma_v(\phi)(V\setminus\{v,z\}) := 1 + \phi(v) + \phi(z), \quad z \in V\setminus\{v\}.$$

Finally, for every $\phi \in L(V)$, set

$$\lambda(\phi)(v) := 1 + \phi(v), \quad v \in V.$$

The collection of bijections α_v, β_{vw}, γ_v, and λ, define an injective map $\mu : A \rightarrowtail \mathbb{P}(\mathcal{H})$ by the formulas $i_{\{v\}}(\phi_1) \mapsto \Psi^v_{\alpha_v(\phi_1)}$, $i_{\{v,w\}}(\phi_2) \mapsto X^{vw}_{\beta_{vw}(\phi_2)}$, $i_{V\setminus\{v\}}(\phi_3) \mapsto \Phi^v_{\gamma_v(\phi_3)}$, and $i_V(\phi_0) \mapsto F_{\lambda(\phi_0)}$, where $\phi_1 \in L(\{v\})$, $\phi_2 \in L(\{v,w\})$, $\phi_3 \in L(V\setminus\{v\})$, and $\phi_0 \in L(V)$. It is straightforward to verify that it transforms a pair $(i_U(\phi), i_W(\phi')) \in T$ $(\phi \in L(U), \phi' \in L(W), U,W \in \mathcal{P}(V)^\times)$, into a pair of orthogonal projective lines. Note, that the only facts needed in order to prove this, are the following four properties of $u(\cdot,\cdot)$: (1) $u(\alpha,\beta)=u(\beta,\alpha)$; (2) $u(\alpha,\beta+\gamma)=u(\alpha,\beta)u(\alpha,\gamma)$; (3) $\Sigma_{\beta\in\mathbb{Z}/2} u(\alpha,\beta)u(\beta,\alpha)=2\delta_{\alpha,\gamma}$; (4) $u(\alpha,1+\alpha) \equiv 1$. Therefore T satisfies the main condition.

Let us mention, how to obtain in principle the formulas for the projective lines (for $N=4$). The result will be just the 120 projective lines constructed in Ref. 10. The configuration of these lines is saturated (i.e., every subset of pairwise orthogonal lines is contained in a set of eight pairwise orthogonal lines) and has a Kochen-Specker-type property.[6] More precisely, this set contains a subset of $40=5\times 8$ projective lines, which are implicitly present in the no-hidden-variables argument due to Mermin.[8] Denote the lines as l^U_ϕ, $U \in \mathcal{P}(V)^\times$, $\phi \in L(U)$. It is convenient to view the set of four points V as a disjoint union of the ground set of $\mathbb{Z}/3$ and a singleton $\{*\}$, where $*$ is a formal symbol. Write $\mathbb{Z}/3$ additively, and denote its elements as 0, 1, and 2. For $\xi \in L(\{*\})$, set

$$l^{\{*\}}_\xi := \mathbb{C} \bigotimes_{i\in\mathbb{Z}/3}^{2i} \varphi_{\xi(i)},$$

where the upper indices denote the ordering of the factors in the tensor product. Let $\{\varphi_\alpha\}_\alpha$ and $\{\psi_\beta\}_\beta$ be the orthonormal bases in $\mathbb{C}^2$ as above. For $k \in \mathbb{Z}/3$ and $\xi \in L(\{k\})$, set

$$l_{\xi}^{\{k\}} := \mathbb{C}\left\{ \varphi_{\xi(*)}^{2k} \otimes \bigotimes_{j\in(\mathbb{Z}/3)\setminus\{k\}} \psi_{\xi(j)}^{k+j} \right\}.$$

For any $U\in\mathcal{P}(V)$, $\#U\geqslant 2$, one can search for the projective line corresponding to $\eta\in L(U)$ in the form

$$l_{\eta}^{U} := \sum_{\xi\in L(\{*\})} B_{\eta}^{U}(\xi) \bigotimes_{i\in\mathbb{Z}/3} \varphi_{\xi(i)}^{2i},$$

where $B_{\eta}^{U}(\xi)\in\mathbb{C}$ are some coefficients. The conditions

$$\sum_{z\in U\Delta\{v\}} (\eta(z)+\xi(z)) = c(\#_4(U\Delta\{v\}))+1 \Rightarrow l_{\xi}^{\{v\}} \perp l_{\eta}^{U},$$

where v varies over V, and ξ varies over $L(\{v\})$, yield (for every U and η) a system of equations on $\{B_{\eta}^{U}(\xi)\}_{\xi}$. This system is homogeneous and linear, but overdetermined. Nevertheless, it turns out that it has nontrivial solutions. Moreover, for every $U\in\mathcal{P}(V)$, the obtained projective lines $\{l_{\eta}^{U}\}_{\eta\in L(U)}$ are pairwise orthogonal, and for every $U,U_1\in\mathcal{P}(V)$, if $U\neq U_1$, then $l_{\eta}^{U}\neq l_{\eta_1}^{U_1}$, where $\eta\in L(U)$, $\eta_1\in L(U_1)$. A straightforward computation shows, that the orthogonality relation between the lines corresponding to different $U,U_1\in\mathcal{P}(V)^{\times}$, $U\neq U_1$, is described by the formula

$$l_{\eta}^{U} \perp l_{\eta_1}^{U_1} \Leftrightarrow \sum_{z\in U\Delta U_1} (\eta(z)+\eta(z_1)) = c(\#_4(U\Delta U_1))+1,$$

where $\eta\in L(U)$, $\eta_1\in L(U_1)$. It remains to define the injection $\mu: A\rightarrowtail\mathbb{P}(\mathcal{H})$ by the formula $\mu(i_U(\phi)) := l_{\phi}^{U}$, $U\in\mathcal{P}(V)^{\times}$, $\phi\in L(U)$.

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Upper and lower bounds for an eigenvalue associated with a positive eigenvector

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When an eigenvector of a semibounded operator is positive, we show that a remarkably simple argument allows to obtain upper and lower bounds for its associated eigenvalue. This theorem is a substantial generalization of Barta-type inequalities and can be applied to non-necessarily purely quadratic Hamiltonians. An application for a magnetic Hamiltonian is given and the case of a discrete Schrödinger operator is also discussed. It is shown how this approach leads to some explicit bounds on the ground-state energy of a system made of an arbitrary number of attractive Coulombian particles. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In most situations, the principal eigenvalue of a semibounded operator cannot be obtained explicitly whereas it plays a crucial role in physics: the smallest vibration frequency of an elastic system, the fundamental mode of an electromagnetic cavity, the ground-state energy of a quantum system with a finite number of degrees of freedom, the energy of the vacuum in a quantum field theory, the equilibrium state at zero temperature in statistical physics, etc. There are actually very few ways—which are usually specific to a restricted class of systems[1]—to obtain accurate approximations of an eigenvalue with a rigorous control on the errors and a reasonable amount of numerical computations. For instance, in a typical Dirichlet-Laplacian problem defined for an open connected set $\mathcal{Q}\subset\mathbb{R}^d$; $d\in\mathbb{N}$; Barta's inequalities (Barta, 1937) allow to bound to the lowest eigenvalue e_0: The determination of a lower (respectively, upper) bound requires the finding of the absolute minimum (respectively, maximum) of a smooth function defined on $\mathcal{Q}$. Compared to the general and traditional methods like the Rayleigh-Schrödinger perturbative series and the Rayleigh-Ritz or Temple variational methods, an advantage of Barta's approach is not only to naturally provide both an upper and a lower bound, but also does not involve the calculation of any integral. Therefore, generalizations of Barta's inequalities can lead to interesting spectral information. This generalization has been carried out in two directions:

(i) For Laplacian operators acting on square integrable functions defined on a Riemannian manifold (for a recent work on this subject, see Bessa and Montenegro, 2004).

(ii) For Schrödinger operators of the form $-\Delta+V$ acting on square integrable functions defined on an open set of $\mathbb{R}^d$ (Barnsley, 1978; Baumgartner, 1979; Thirring, 1979; Crandall and Reno, 1982; Schmutz, 1985) or more generally second order elliptic operators (Protter and Weinberger, 1966; Berestycki *et al.*, 1994; Harrell II, 2005).

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[1]Finding lower bounds for the smallest eigenvalue of a typical Hamiltonian is far more difficult than finding upper bounds. For successful attempts, see for instance the moment method proposed by Handy and Bessis, 1985, the Riccati-Padé method proposed in Fernández *et al.*, 1989 and the lower bounds obtained for few-body systems by Benslama *et al.*, 1998.

In both cases, the proofs of Barta's inequalities involve the use of a Kato-type inequality and therefore rely extensively on the somehow specific properties of the purely quadratic differential operator. In this paper, we propose a significant extension of Barta's inequalities that will rely on the properties of one eigenvector only. More precisely, with a remarkably simple argument, we will show that we can obtain upper and lower bounds for the eigenvalue e_0 associated with the eigenvector Φ_0 of an operator, under the only hypothesis that Φ_0 is real and non-negative. This result includes cases (i) and (ii) because the Krein-Rutman theorem guarantees the positivity of Φ_0 (Reed and Simon, 1978a, Sec. XIII.12) for the smallest eigenvalue e_0,[2] but also applies for a much wider class of operators including the following.

(iii) the Schrödinger operators involving a magnetic field, e.g., the hydrogen atom in a Zeeman configuration;

(iv) discrete Hamiltonians, e.g., the one occurring in the Harper model;[3]

(v) some integral or pseudodifferentiable operators, e.g., the Klein-Gordon or spinless Salpeter Hamiltonians.

The next section fixes the notations, proves the main general results (theorems 1 and 2). Section III shows how the original argument given in Sec. II actually embraces and generalizes the Barta-type inequalities that have been already obtained in the literature and furnishes guidelines to numerically improve the bounds on e_0. Sections IV and V provide two applications in the differentiable case (many-body problem) and in the discrete case, respectively.

II. BOUNDING THE PRINCIPAL EIGENVALUE WITH THE LOCAL ENERGY

A. General inequalities

In the following, $\mathcal{Q}$ will be a locally compact space endowed with a positive Radon measure μ. $\langle\psi|\varphi\rangle$ will denote the scalar product between two elements ψ and φ belonging to the Hilbert space of the square integrable complex functions $\mathsf{L}^2(\mathcal{Q},\mu)$,

$$\langle\psi|\varphi\rangle = \int_{\mathcal{Q}} \bar{\psi}(q)\varphi(q)\mathrm{d}\mu(q).$$

$\mathsf{D}(H)$ will denote the domain of the operator H acting on $\mathsf{L}^2(\mathcal{Q},\mathrm{d}\mu)$. The crucial hypothesis on H is the following.

Hypothesis 1: The operator H is symmetric and has one real eigenvector $\Phi_0 \in \mathsf{D}(H)$ *such that* $\Phi_0 \geqslant 0$ (*almost everywhere with respect to* μ) *on* $\mathcal{Q}$.

If e_0 stands for the eigenvalue of H associated with Φ_0, the symmetry of H implies that, for all $\varphi \in \mathsf{D}(H)$, we have $\langle\Phi_0|(H-e_0)\varphi\rangle=0$ that is

$$\forall\,\varphi \in \mathsf{D}(H), \quad \int_{\mathcal{Q}} \overline{\Phi_0}(q)(H-e_0)\varphi(q)\mathrm{d}\mu(q) = 0.$$

Taking the real part of the integral, we can see that the support of $q\mapsto \mathrm{Re}[\overline{\Phi_0}(q)(H-e_0)\varphi(q)]$ either is empty, either contains two disjoints open sets $\mathcal{Q}_\pm$ such that $\mathrm{Re}(\overline{\Phi_0}(H-e_0)\varphi) \gtrless 0$ and $\mu(\mathcal{Q}_\pm)>0$. The hypothesis of positivity of Φ_0 implies that on $\mathcal{Q}_\pm$, we have $\mathrm{Re}[(H-e_0)\varphi] \gtrless 0$. The last results motivates the following definition.

Definition 1 (*local energy*): *For any* φ *in* $\mathsf{D}(H)$, *the* local energy *is the function* $E_\varphi: \mathcal{Q}\to\bar{\mathbb{R}}$ *defined by*

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[2]The positivity of Φ_0 is also required for the traditional proofs of Barta's inequalities; this explains why, in case (i) and (ii), they concern the lowest eigenvalue only.

[3]After the first version of this paper was written, the author became aware of the paper by Barnsley and Duffin, 1980 where a similar argument as the one presented here was proposed (Theorem 7) for the bounds on an eigenvalue of a finite matrix.

$$E_\varphi(q) = \frac{\mathrm{Re}(H\varphi(q))}{\mathrm{Re}(\varphi(q))}. \tag{1}$$

Therefore from what precedes, we have obtained the main theorem.

Theorem 1: *For any symmetric operator H on $\mathsf{L}^2(\mathcal{Q},\mu)$ having an eigenvalue e_0 whose corresponding eigenfunction is non-negative almost everywhere on $\mathcal{Q}$, we have*

$$\forall \varphi \in \mathsf{D}(H) \text{ such that } \mathrm{Re}(\varphi) \geqslant 0, \quad \inf_{\mathcal{Q}}(E_\varphi) \leqslant e_0 \leqslant \sup_{\mathcal{Q}}(E_\varphi). \tag{2}$$

Actually, for a nonsymmetric operator K, we can keep working with its adjoint K^* and easily generalize the above argument.

Theorem 2: *Let K being an operator on $\mathsf{L}^2(\mathcal{Q},\mu)$ having an eigenvalue k_0 whose corresponding eigenfunction is real and non-negative almost everywhere on $\mathcal{Q}$, we have $\forall \varphi \in \mathsf{D}(K^*)$ such that $\varphi > 0$,*

$$\inf_{\mathcal{Q}}\left[\frac{\mathrm{Re}(K^*\varphi)}{\varphi}\right] \leqslant \mathrm{Re}(k_0) \leqslant \sup_{\mathcal{Q}}\left[\frac{\mathrm{Re}(K^*\varphi)}{\varphi}\right], \tag{3a}$$

$$\inf_{\mathcal{Q}}\left[-\frac{\mathrm{Im}(K^*\varphi)}{\varphi}\right] \leqslant \mathrm{Im}(k_0) \leqslant \sup_{\mathcal{Q}}\left[-\frac{\mathrm{Im}(K^*\varphi)}{\varphi}\right]. \tag{3b}$$

This generalization may be of physical relevance. There are some models (e.g., the so-called "kicked" systems, or quantized maps) where the dynamics are described "stroboscobically", i.e., implemented by a unitary operator (the Floquet evolution operator) that cannot be constructed from a smooth Hamiltonian. However, we will not consider this possibility here, and up to the end of this paper, H will denote a symmetric operator.

B. Optimization strategy

Since generally, the eigenfunction Φ_0 is not known exactly, it will be approximated with the help of test functions that belong to a trial space $\mathsf{T}(H) \subset \mathsf{D}(H)$, very much like the variational method. Since we want a test function to mimic Φ_0 at best, we will restrict $\mathsf{T}(H)$ to functions that respect the *a priori* known properties of Φ_0: its positivity, its boundary conditions and its symmetries if there are any. For each test function the error on e_0 is controlled by inequalities (2). Therefore, the strategy for obtaining reasonable approximations is clear: First, we must choose or construct φ to eliminate all the singularities of the local energy in order to work with a bounded function and second, perturb the test function in the neighborhood of the absolute minimum (respectively, maximum) of the local energy in order to increase (respectively, decrease) its value. For practical and numerical computations, this perturbation will be implemented by constructing a diffeomorphism $\Lambda \to \mathsf{T}(H), \lambda \mapsto \varphi_\lambda$ from a finite dimensional differentiable real manifold Λ of control parameters λ and the optimized bounds for e_0 will be

$$\sup_{\Lambda}\inf_{\mathcal{Q}}(E_{\varphi_\lambda}) \leqslant e_0 \leqslant \inf_{\Lambda}\sup_{\mathcal{Q}}(E_{\varphi_\lambda}). \tag{4}$$

III. INEQUALITIES IN THE DIFFERENTIABLE CASE: OLD AND NEW

A. General considerations

When H is a local differential operator, i.e., involves a finite number of derivatives in an appropriate representation (for instance in position or in momentum representation), one can therefore construct an algorithm that does not require any integration but differential calculus only. In an analytic and in a numerical perspective, this may be a significant advantage on the pertur-

bative or variational methods even though it is immediate to see[4] that the upper bound given by (2) is always larger than $\langle\varphi|H\varphi\rangle/\langle\varphi|\varphi\rangle$. The global analysis appears only through the determination of the singularities and the *absolute* extrema of the local energy that may have bifurcated when the control parameter λ varies smoothly. For a Schrödinger operator, the possible singularities of the potential on $\bar{\mathcal{Q}}$ like a Coulombian divergence or an unbounded behavior at infinite distances may furnish a strong guideline for constructing relevant test functions (see Sec. III D below). We have given in Mouchet, 2005, some heuristic and numerical arguments to show how this strategy can be fruitful. In the present paper, the main focus will concern rigorous results and will explain how some of them can be obtained with great simplicity even for systems as complex as those involved in the many-body problem.

B. Case (i) Barta's inequalities

They immediately appear as a particular case of Theorem 1.

Theorem 3 (Barta, 1937): *Let $\mathcal{Q}$ be a connected bounded Riemannian manifold endowed with the metric g and H, the opposite of the Laplacian Δ_g acting on the functions in $\mathsf{L}^2(\mathcal{Q},\mu)$ that satisfy Dirichlet boundary conditions on the boundary $\partial\mathcal{Q}$. The lowest eigenvalue e_0 of H is such that, for all positive $\varphi\in\mathcal{C}^2(\mathcal{Q})$,*

$$\inf_{\mathcal{Q}}\left(-\frac{\Delta_g\varphi}{\varphi}\right)\leqslant e_0\leqslant\sup_{\mathcal{Q}}\left(-\frac{\Delta_g\varphi}{\varphi}\right). \tag{5}$$

Proof: It follows directly from Theorem 1, with the local energy given by $E_\varphi=-\Delta_g\varphi/\varphi$: The spectrum of H is discrete and the Krein-Rutman theorem assures that Hypothesis 1 is fulfilled for e_0 being the lowest (and simple) eigenvalue. ■

Remark 1: The Dirichlet boundary conditions are not essential and can be replaced by any other type of boundary conditions provided that Hypothesis 1 remains fulfilled. However, as explained in Sec. II B, *for obtaining interesting bounds on e_0 extending $\mathsf{T}(H)$ to test functions that do not fulfill the boundary conditions* (*as proposed by Duffin, 1947*) *seems not appropriate*.

C. Case (ii) Duffin-Barnsley-Thirring inequalities

Extensions of Barta's inequalities for Schrödinger operators have been obtained partially by Duffin (Duffin, 1947) and Barnsley (Barnsley, 1978) (for the lower bound only) and completely (lower and upper bound) by Thirring (Thirring, 1979) using Kato's inequalities (see also Schmutz, 1985).

Theorem 4 (Duffin, 1947; Barnsley, 1978; Thirring, 1979): *Let $H=-\Delta+V$ be a Schrödinger operator acting on $\mathsf{L}^2(\mathbb{R}^d)$ having an eigenvalue below the essential spectrum. Then the lowest eigenvalue e_0 of H is such that for any strictly positive $\varphi\in\mathsf{D}(H)$,*

$$\inf_{\mathbb{R}^d}\left(V-\frac{\Delta\varphi}{\varphi}\right)\leqslant e_0\leqslant\sup_{\mathbb{R}^d}\left(V-\frac{\Delta\varphi}{\varphi}\right). \tag{6}$$

The proof is similar to the one presented above with the local energy being now $E_\varphi=V-\Delta\varphi/\varphi$. This argument has the advantage on the existing ones that it does not involve the specific properties of the Laplacian and can be immediately transposed to the larger class of the differential operators (not necessarily of second order) that fulfill Hypothesis 1.

D. Case (iii) magnetic Schrödinger operators

In the presence of a magnetic field, Schrödinger operators take the form $H=(\mathrm{i}\partial_q+A(q))^2+V(q)$ with $A:\mathcal{Q}\to\mathbb{R}^d$ being a smooth magnetic potential vector and $V:\mathcal{Q}\to\mathbb{R}$ a smooth scalar

[4]For each positive φ, it follows from $\langle\varphi|H\varphi\rangle=\mathrm{Re}[\langle\varphi|H\varphi\rangle]=\int_{\mathcal{Q}}\varphi(q)\mathrm{Re}[H\varphi(q)]\mathrm{d}\mu(q)=\int_{\mathcal{Q}}\varphi^2(q)E_\varphi(q)\mathrm{d}\mu(q)\leqslant\langle\varphi|\varphi\rangle\sup_{\mathcal{Q}}(E_\varphi(q))$.

potential. The Krein-Rutman theorem may not apply whereas there still exists a non-negative real eigenfunction (e_0 may be not simple nor the lowest eigenvalue) (Helffer *et al.*, 1999).

In the particular case of the hydrogen atom in a constant and uniform magnetic field, Hypothesis 1 is fulfilled for all values of the magnetic field (Avron *et al.*, 1977; Avron *et al.*, 1978) and indeed concerns the lowest eigenvalue. Therefore Theorem 1 applies and furnishes relevant analytical bounds that can be improved numerically as shown in (Mouchet, 2005).

Proposition 1: The smallest eigenvalue e_0 of the (3d-)Zeeman Hamiltonian

$$H = \frac{1}{2}\left(-i\vec{\nabla} + \frac{1}{2}\vec{r}\times\vec{B}\right)^2 - \frac{1}{r} \tag{7}$$

is such that

$$\forall B \geqslant 0, \quad e_0 \leqslant -1/2 + B/2. \tag{8}$$

Proof: In cylindrical coordinates (ρ, θ, z) where the magnetic field is $\vec{B}=B\vec{u}_z$, the test function of the form $\varphi=\exp(-\sqrt{\rho^2+z^2}-B\rho^2/4)$ is constructed, according to the strategy explained in Sec. II B, in order to respect the rotational invariance of the ground state (Avron *et al.*, 1977) and eliminate both singularities at $r\to 0$ and at $\rho\to\infty$. Indeed such a choice leads straightforwardly to the bounded local energy

$$E_\varphi = -1/2 + B/2 - \frac{\rho^2 B}{2\sqrt{\rho^2+z^2}}. \tag{9}$$

The upper bound follows. ■

IV. APPLICATION TO THE MANY-BODY PROBLEM

A. Expression of the local energy in terms of two-body functions

We will consider in this section a N-body nonrelativistic bosonic system in d dimensions; $(d,N)\in(\mathbb{N}\backslash\{0,1\})^2$; whose Hamiltonian is given by

$$\tilde{H} = \sum_{i=0}^{N-1} -\frac{1}{2m_i}\Delta_i + V(\vec{r}_0, \ldots, \vec{r}_{N-1}) \tag{10}$$

acting on $\mathsf{L}^2(\mathbb{R}^{Nd})$, endowed with the canonical Lebesgue measure, and where $\forall i\in\{0,\ldots,N-1\}$, $\vec{r}_i\in\mathbb{R}^d$. Δ_i is the Laplacian in the $\vec{r}_i$ variables and $m_i\in\mathbb{R}^+\backslash\{0\}$ the mass of the ith particle. The spinless bosons interact only by the two-body radial potentials $v_{ij}=v_{ji}:\mathbb{R}\to\mathbb{R}$, i.e., V is given by

$$V = \sum_{\substack{i,j=0\\ i<j}}^{N-1} v_{ij}(r_{ij}), \tag{11}$$

where $r_{ij}=r_{ji}=\|\vec{r}_j-\vec{r}_i\|$. Once the center of mass is removed, the Hamiltonian $\tilde{H}$ leads to a reduced Hamiltonian H acting on $\mathsf{L}^2(\mathbb{R}^{(N-1)d})$ [see for instance Sec. XI.5 of (Reed and Simon, 1978b)] and we will suppose in the following that H has at least one eigenvector.[5] Therefore, Hypothesis 1 is fulfilled for e_0 being the lowest (and simple) eigenvalue. A natural choice for test functions is to consider factorized ones of the form

[5]Physically, this can be achieved with a confining external potential (a "trap" is currently used in experiments involving cold atoms). Formally, this can be obtained in the limit of one mass, say m_0, being much larger than the others. The external potential appears to be the $v_{0,i}$'s, created by such an infinitely massive motionless device. It will trap the remaining $N-1$ particles in some bounded states if the $v_{0,i}$'s increase sufficiently rapidly with the $r_{0,i}$'s.

$$\varphi(\vec{r}_0,\ldots,\vec{r}_{N-1}) = \prod_{\substack{i,j=0\\ i<j}}^{N-1} \phi_{ij}(r_{ij}), \tag{12}$$

where $\phi_{ij} \in \mathsf{L}^2(\mathbb{R}^+)$ and $\phi_{ji}=\phi_{ij}>0$. One can check easily that the total momentum of such a test function vanishes. The corresponding local energy (1) is given by

$$E_\varphi(q_N) = \sum_{\substack{i,j=0\\ i<j}}^{N-1} \left[\frac{-1}{2m_{ij}\phi_{ij}(r_{ij})} \left(\phi''_{ij}(r_{ij}) + \frac{d-1}{r_{ij}} \phi'_{ij}(r_{ij}) \right) + v_{ij}(r_{ij}) \right] - \sum_{(\widehat{j,i,k})} \frac{1}{m_i} S'_{ij}(r_{ij}) S'_{ik}(r_{ik}) \cos(\widehat{j,i,k}), \tag{13}$$

where $q_N \in \mathcal{Q}_N = \mathbb{R}^{(N-1)d}$ stands for the $(N-1)d$ relative coordinates $(\vec{r}_1-\vec{r}_0,\ldots,\vec{r}_{N-1}-\vec{r}_0)$, m_{ij} for the reduced masses $m_i m_j/(m_i+m_j)$, S'_{ij} is the derivative of $S_{ij}=\ln(\phi_{ij})$. The last sum involves all the $N(N-1)(N-2)/2$ angles $(\widehat{j,i,k})$ between $\vec{r}_j-\vec{r}_i$ and $\vec{r}_k-\vec{r}_i$ that can be formed with all the triangles made of three distinct particles.

Whenever each v_{ij} allows for a two-body bounded state, we can choose ϕ_{ij} to be the eigenvector of $-(2m_{ij})^{-1}\Delta+v_{ij}$ having the smallest eigenvalue $\epsilon^{(2)}_{ij}$. Moreover, if $v_{ij}(r)$ is bounded when $r\to\infty$, from an elementary semiclassical analysis [see for instance (Maslov and Fedoriuk, 1981)] it follows that S'_{ij} is also bounded since asymptotically we have $S'_{ij}(r)\sim_{r\to\infty} -\sqrt{2m_{ij}[v_{ij}(r)-\epsilon^{(2)}_{ij}]}$. It follows that the local energy is also bounded and finite lower and upper bounds on e_0 can be found. For instance, directly from expression (13), we have the following.

Proposition 2: If, for all $(i,j)\in\{0,\ldots,N-1\}^2$, $i\neq j$, $v_{ij}(r)$ *is bounded when* $r\to\infty$ *and* $-(2m_{ij})^{-1}\Delta+v_{ij}$ *has a smallest eigenvalue* $\epsilon^{(2)}_{ij}$ *obtained for* $\phi_{ij}=\exp S_{ij}$, *then the smallest eigenvalue* e_0 *of the N-body Hamiltonian in the center-of-mass frame is bounded by*

$$\sum_{\substack{i,j=0\\ i<j}}^{N-1} \epsilon^{(2)}_{ij} - \frac{s^2}{2m} N(N-1)(N-2) \leqslant e_0 \leqslant \sum_{\substack{i,j=0\\ i<j}}^{N-1} \epsilon^{(2)}_{ij} + \frac{s^2}{2m} N(N-1)(N-2), \tag{14}$$

where $m=\min_i m_i$ *and* $s=\max_{i,j} \sup_{\mathbb{R}^+} |S'_{ij}|$.

For potentials that are relevant in physics [see for instance the effective power-law potentials of the form $v_{ij}(r)=\mathrm{sign}(\beta) r^\beta$; $\beta\in\mathbb{R}$; between massive quarks as studied by Benslama *et al.*, 1998], the analytic form of the two-body eigenvector is not known in general and some numerical computations are required to obtain the absolute maximum and minimum of the local energy (13).

B. The local energy for a general Coulombian problem

When N is large, the estimation (14) is quite rough, in particular it does not take into account the constraints between the several angles. More precise results are obtained for the Coulombian problem where $v_{ij}(r)=e_{ij}/r$ with $e_{ij}\in\mathbb{R}$ and $d>1$. In that case, provided a bounded state exists and that we keep the test function (12) in $\mathsf{L}^2(\mathbb{R}^{(N-1)d})$, we choose a constant derivative $S'_{ij}=2e_{ij}m_{ij}/(d-1)$ in order to get rid of the Coulombian singularities of V. We obtain a bounded local energy given by

$$E_\varphi(q_N) = \sum_{\substack{i,j=0\\ i<j}}^{N-1} -\frac{2m_{ij}e_{ij}^2}{(d-1)^2} - \frac{4}{(d-1)^2} \sum_{(\widehat{j,i,k})} \frac{m_{ij}m_{ik}e_{ij}e_{ik}}{m_i} \cos(\widehat{j,i,k}). \tag{15}$$

C. Identical purely attractive Coulombian particles

The case where all the N particles are identical and attract each other, i.e., when $\forall(i,j)\in\{0,\ldots,N-1\}^2$, $i\neq j$, $m_i=1$ and $e_{ij}=-1$, has been extensively studied in the literature, in particular the asymptotic behavior of e_0 with large N may have some dramatic consequences on the

thermodynamical limit (Fisher and Ruelle, 1966; Lenard and Dyson, 1967; Lévy-Leblond, 1969; Lieb, 2005). The local energy method allows to obtain in a much simpler way energy bounds that are comparable to those already obtained by other methods. Actually, (15) simplifies to

$$E_\varphi(q_N) = -\frac{1}{(d-1)^2}\left[\tfrac{1}{2}N(N-1) + F_N(q_N)\right] \tag{16}$$

with $F_2 \equiv 0$ and for $N \geqslant 3$,

$$F_N(q_N) = \sum_{\widehat{(j,i,k)}} \cos(\widehat{j,i,k}). \tag{17}$$

The angular function F_N depends only on the geometrical configuration of the N vertices $(\vec{r}_0, \ldots, \vec{r}_{N-1})$, i.e., it is invariant under the group of Euclidean isometries and the scale invariance of the Coulombian interaction makes it invariant under dilations as well.

Lemma 1: $\inf_{\mathcal{Q}_3} F_3 = 1$ *is obtained when the three points are aligned.* $\sup_{\mathcal{Q}_3} F_3 = 3/2$ *is obtained when the three points make an equilateral triangle.*

Proof: The extrema of F_3 correspond to the extrema of the function defined by $(\theta_0, \theta_1, \theta_2) \mapsto \cos\theta_0 + \cos\theta_1 + \cos\theta_2$ under the constraint $\theta_0 + \theta_1 + \theta_2 = \pi$ for $(\theta_0, \theta_1, \theta_2)$ being the three angles $\widehat{(1,0,2)}$, $\widehat{(0,1,2)}$, $\widehat{(0,2,1)}$, respectively. The Lagrange multiplier method leads to the determination of the extrema of the function $[0;\pi]^3 \to \mathbb{R}$ defined by $(\theta_0, \theta_1, \theta_2) \mapsto \cos\theta_0 + \cos\theta_1 + \cos\theta_2 + l(\theta_0 + \theta_1 + \theta_2 - \pi)$; $l \in \mathbb{R}$. We immediately obtain that the extremal points are located at $(\theta_0, \theta_1, \theta_2) = (\pi/3, \pi/3, \pi/3)$ and $(\theta_0, \theta_1, \theta_2) = (0, 0, \pi)$ together with the solutions that are obtained by circular permutations. It is easy to check that the first solution provides an absolute maximum for F_3 and the second ones an absolute minimum. ■

An immediate consequence of the preceding lemma is the following.

Proposition 3: The lowest energy e_0 *of* $N \geqslant 2$ *identical attractive Coulombian spinless particles in* $d > 1$ *dimensions is such that*

$$e_0 \leqslant -\frac{1}{(d-1)^2}\frac{1}{6}N(N-1)(N+1) \tag{18}$$

when the individual masses equal to unity and the attractive potential is $-1/r$.

Proof: The sum on the angles that defines F_N in (17) can be written as a sum of $N(N-1)(N-2)/6$ F_3-terms calculated for all the triangles that belong to the N-uplet made of the N vertices. Since, from Lemma 1 the absolute minimum of F_3 is obtained for a flat configuration, when all the N points are aligned all the F_3-terms reach their absolute minimum simultaneously and the absolute minimum of F_N is obtained. We have

Lemma 2: $\inf_{\mathcal{Q}_N} F_N = \frac{1}{6}N(N-1)(N-2)$ *is obtained when all the N points are aligned.*

The upper bound (18) follows from (16). ■

More generally, for a given N-uplet (i.e., a set of exactly N points), clustering the sum (17) in M-uplets $(N \geqslant M \geqslant 3)$ allows to find bounds on F_N from bounds on F_M. Indeed, we can write

$$F_N(q_N) = \sum_{q_M} \frac{(M-3)!\,(N-M)!}{(N-3)!} F_M(q_M), \tag{19}$$

where the sum is taken on all the M-uplets, labeled by the coordinates q_M, that belong to the given N-uplet. This sum involves exactly $N!/(M!\,(N-M)!)$ terms and we have, therefore,

Lemma 3: $\forall (N,M) \in \mathbb{N}^2$ *such that* $N \geqslant M \geqslant 3$,

$$\sup_{\mathcal{Q}_N} F_N \leqslant \frac{N(N-1)(N-2)}{M(M-1)(M-2)} \sup_{\mathcal{Q}_M} F_M. \tag{20}$$

For a given N, $\sup_{\mathcal{Q}_N} F_N$ is not known exactly but the ordered sequence

$$\frac{\sup_{\mathcal{Q}_N} F_N}{N(N-1)(N-2)} \leqslant \frac{\sup_{\mathcal{Q}_{N-1}} F_{N-1}}{(N-1)(N-2)(N-3)} \leqslant \cdots \leqslant \frac{\sup_{\mathcal{Q}_M} F_M}{M(M-1)(M-2)} \leqslant \cdots \leqslant \frac{\sup_{\mathcal{Q}_3} F_3}{3.2.1} = \frac{1}{4} \tag{21}$$

shows that in order to improve the lower bounds on (16), we must try to find $\sup_{\mathcal{Q}_M} F_M$ with M being the largest as possible. However, when considering identity (19) for $N=4$ and $M=3$ together with Lemma 1 we have the following.

Lemma 4: $\sup_{\mathcal{Q}_4} F_4=6$ *is obtained when the four points make a regular tetrahedron.*

Then $\sup_{\mathcal{Q}_4} F_4/(4.3.2)=\sup_{\mathcal{Q}_3} F_3/(3.2.1)=1/4$ and no better estimate is obtained when considering $M=4$ rather than $M=3$. Numerical investigations lead to the following conjectures.

Conjecture 1: (C_5) *When* $d=3$,

$$\sup_{\mathcal{Q}_5} F_5 = \frac{9}{2} + \frac{6(h_0+1)}{\sqrt{h_0^2+\frac{1}{3}}} - \frac{1}{h_0^2+\frac{1}{3}} \simeq 14.591\,594$$

with

$$6h_0 = 1 + \sqrt{-1 + \sqrt[3]{7+4\sqrt{3}} + \frac{1}{\sqrt[3]{7+4\sqrt{3}}}} + \sqrt{-2 - \sqrt[3]{7+4\sqrt{3}} - \frac{1}{\sqrt[3]{7+4\sqrt{3}}} + 8\frac{1}{\sqrt{-1+(7+4\sqrt{3})^{1/3}+(7+4\sqrt{3})^{-1/3}}}} \tag{22}$$

is obtained when the five points make two mirror-symmetric tetrahedrons sharing one common equilateral basis, their other faces being six isosceles identical triangles.

Remark 2: The only free parameter of the specific configuration can be chosen to be the height h of one tetrahedron (the length of the edges of the common equilateral basis being fixed to one). The maximum of $h\mapsto F_5$ *is reached for* h_0 *being the greatest solution of* $9h^4-6h^3+3h^2-2h+1/3$ *that is precisely given by* (22).

Remark 3: The pyramidal configurations with a squared basis leads to a local maximum that gives $F_5=15/2+5\sqrt{2}\simeq 14.57$.

Conjecture 2: (C_6) *When* $d=3$, $\sup_{\mathcal{Q}_6} F_6=12(1+\sqrt{2})$ *is obtained when the six points make a regular octahedron.*

Conjecture 3: (C_8) *When* $d=3$,

$$\sup_{\mathcal{Q}_8} F_8 = 16\left[\frac{4}{5} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{5}} + \frac{4(1+\sqrt{2})}{\sqrt{5}\sqrt{5+4\sqrt{2}}} + \frac{3+2\sqrt{2}}{\sqrt{5+4\sqrt{2}}} - \frac{1}{5+4\sqrt{2}}\right] \simeq 79.501$$

is obtained when the eight points make two identical squares (whose edges have length one) lying in two parallel planes separated by a distance $h=\sqrt{1+2\sqrt{2}}/2$. *The axis joining the centers of the two squares is perpendicular to the squares and the two squares are twisted one from the other by a relative angle of* $\pi/4$.

Remark 4: The cube corresponds to $F_8=8(3\sqrt{2}+\sqrt{3}+3/2+\sqrt{6})\simeq 79.393$.

Conjecture 4: (C_∞) *When* $d=3$ *and* $N\to\infty$, *the configuration that maximizes* F_N *corresponds to N points uniformly distributed on a sphere and* $\sup_{\mathcal{Q}_N} F_N \sim \frac{2}{9}N^3+o(N^3)$.

Remark 5: The ambiguity of distributing N points uniformly on a sphere (Saff and Kuijlaars, 1997 and references therein) vanishes for large N as far as a uniform density is obtained. Assuming such a uniform density, the continuous limit of F_N/N^3 *is a triple integral on the sphere than can be computed exactly to* $2/9$.

The upper bound (18) for $d=3$ is slightly above the one obtained by Lévy-Leblond, 1969, Eq. (17), p. 807, namely $-(5/8)^2N(N-1)^2/8$, and the numerical estimate $-0.0542N(N-1)^2$ by Basdevant *et al.*, 1990, Eq. (16), p. 63. For the lower bounds, from Lemmas 1 or 4, we have obtained the following.

Proposition 4: The lowest energy e_0 of $N \geqslant 2$ identical attractive Coulombian spinless particles in $d > 1$ dimensions is such that

$$-\frac{1}{(d-1)^2}\frac{1}{4}N^2(N-1) \leqslant e_0 \tag{23}$$

when the individual masses equal to unity and the attractive potential is $-1/r$.

The same result has been obtained for $d=3$ by Basdevant *et al.*, 1990, Eq. (11), p. 62 and is slightly better than $-N(N-1)^2/8$ given by Lévy-Leblond, 1969 Eq. (13), p. 807. For $N \geqslant M \geqslant 4$, this lower bound can be improved to

$$-\frac{1}{(d-1)^2}N(N-1)\left(\frac{1}{2}+\alpha_M(N-2)\right) \leqslant e_0 \tag{24}$$

with

$$\alpha_M = \frac{\sup_{\mathcal{Q}_M} F_M}{M(M-1)(M-2)} \leqslant \frac{1}{4}. \tag{25}$$

If conjecture (C_5) [respectively (C_6), (C_8), and (C_∞)] is correct we get, when $d=3$, $\alpha_5 \simeq 0.2432$ (respectively, $\alpha_6 \simeq 0.2414$, $\alpha_8 \simeq 0.2366$, and $\alpha_\infty \sim 2/9$) and the lower bounds are, therefore, improved.

Some numerical investigations, in particular a systematic comparison with the lower bounds obtained with variational methods in (Benslama *et al.*, 1998) for $N=3$ and $N=4$ Coulombian particles will be given elsewhere (Mouchet, 2006).

V. APPLICATION TO DISCRETE HAMILTONIANS

Where $q \in \mathbb{Z}^d$; $d \in \mathbb{N}$; the discretized analog of a local differential operator corresponds to a Hamiltonian that couples at most a finite number of basis vectors (e.g., the nearest neighbors on the lattice $\mathbb{Z}^d$). For instance, when $d=1$, it can be seen as a Hermitian band matrix (finite or infinite) of finite half-width in an appropriate basis. Possibly with renumbering the q's, on $\ell^2(\mathbb{Z}^d)$ H has the form:

$$(H\varphi)_q = \sum_{\substack{\nu \in \mathbb{Z}^d \\ |\nu|_\infty \leqslant N_b}} H_{q,q+\nu}\varphi_{q+\nu}, \tag{26}$$

where $N_b \in \mathbb{N}$, $\forall (q,q') \in \mathbb{Z}^d \times \mathbb{Z}^d$, $H_{q',q} = \bar{H}_{q,q'} \in \mathbb{C}$ and $|\nu|_\infty$ stands for $\max(|\nu_1|,\ldots,|\nu_d|)$. φ will be taken as a discrete set of real strictly positive numbers, and the local energy $E_\varphi(q)$ is computed, for a given q, with elementary algebraic operations whose number is finite and all the smaller than N_b are small: its value at a given q depends on $(2N_b)^d+1$ components of φ at most. Under hypothesis 1,[6] if, say, for a given test vector φ, the absolute maximum of E_φ occurs only at a unique finite q_m, one can immediately improve the upper bound by a finite amount, for instance just by varying φ_{q_m} only, until $E_\varphi(q_m)$ is not an absolute maximum anymore. Only $(2N_b)^d+1$ values of the local energy will be affected by the variation of just one component of φ. One can see easily that this approach leads to a wide variety of algorithms where a sequence of optimization steps is constructed; each step involves a number of optimization parameters and functions that is usually much smaller [of order $(2N_b)^d$ or less] than the dimension of the original matrix.

Discrete Schrödinger operators are important particular cases of Hamiltonians (26) with $N_b = 1$. They are relevant models for the description of quantum (quasi-) particles evolving in periodic crystals. For $d=1$, they can be written as

[6]We have seen at the end of Sec. II A that the symmetry hypothesis can be relaxed.

$$(H\varphi)_q = -\varphi_{q+1} - \varphi_{q-1} + V(q)\varphi_q, \tag{27}$$

where the potential V is a real bounded function on $\mathbb{Z}$. By possibly subtracting a constant positive real number to V, the bounded operator $-H$ can be made positive and ergodic: First, for any positive and non-identically vanishing φ and φ' in $\ell^2(\mathbb{Z})$, $-H\varphi$ remains positive. Second, $\langle\varphi'|(-H)^{|q'-q|}\varphi\rangle = \varphi'_{q'}\varphi_q + (\text{positive terms}) \neq 0$ for any given pair of strictly positive components $\varphi'_{q'}$ and φ_q with $q' \neq q$. [In the marginal case where φ and φ' both vanish everywhere but on the same point, we have $\langle\varphi'|(-H)\varphi\rangle) \neq 0$. Therefore Theorem XIII.43 of (Reed and Simon, 1978a) applies: if H has indeed one eigenvalue, hypothesis 1 is fulfilled for e_0 being the smallest eigenvalue of H. In that case, inequalities (2) takes the following form:

Proposition 5: When the discrete Schrödinger operator (27) *admits at least one eigenvalue and when V is bounded, then the smallest eigenvalue* e_0 *is such that,* $\forall\varphi \in \ell^2(\mathbb{Z})$ *such that* $\varphi > 0$,

$$\inf_{q\in\mathbb{Z}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q)\right) \leqslant e_0 \leqslant \sup_{q\in\mathbb{Z}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q)\right). \tag{28}$$

When V is actually a N-periodic real function, the spectral problem (see Reed and Simon, 1978a for instance) leads to the search of complex series $(u_q)_{q\in\mathbb{Z}}$ such that

$$\forall\,\eta = (\eta_1, \eta_2) \in [0;1[^2 \quad \begin{cases} -u_{q+1} - u_{q-1} + V(q+\eta_2)u_q = e(\eta)u_q, \\ u_{q+N} = e^{i2\pi\eta_1}u_q. \end{cases} \tag{29}$$

The spectrum of H is the bounded set $\sigma(H) = \{e(\eta)\,|\,\eta \in [0;1[^2\} \subset \mathbb{R}$. It is given by the reunion for all η's of the N eigenvalues of finite $N\times N$ Hermitian matrices $H^{(\eta)}$ obtained after transforming (29) with the one-to-one mapping $u_q \mapsto u_q \exp(-\mathrm{i}2\pi q\eta_1/N)$. As far as positive solutions of (29) are concerned, we will take $\eta_1 = 0$ and will look for the smallest eigenvalue $e_0(\eta_2)$ of

$$H^{(0,\eta_2)} = \begin{pmatrix} V(\eta_2) & -1 & 0 & \cdots & 0 & -1 \\ -1 & V(1+\eta_2) & -1 & 0 & \cdots & 0 \\ 0 & -1 & V(2+\eta_2) & -1 & \cdots & \cdots \\ 0 & \cdots & \cdots & & \cdots & \cdots \\ -1 & 0 & \cdots & 0 & -1 & V(N-1+\eta_2) \end{pmatrix}. \tag{30}$$

Remark 6: The (rational) Harper model (Harper, 1955b; Harper, 1955a) [*also called the almost Mathieu equation (Bellissard and Simon, 1982)*] *corresponds to* $V(q) = -V_0\cos(2\pi qM/N)$ *where* $V_0 > 0$, (M,N) *being strictly positive coprimes integers. For a given N and M,* $\sigma(H)$ *appears to be made of N bands. The union of these bands for each rational number* M/N *between 0 and 1 produces the so-called Hofstadter butterfly (Hofstadter, 1976).*

We are therefore able to produce two nontrivial bounds on the lowest eigenvalue $e_0(\eta_2)$ without any diagonalization:

Proposition 6: When V is N-periodic, $\forall\,\eta_2 \in [0;1[$, *the smallest eigenvalue* $e_0(\eta_2)$ *of* (30) *is such that* $\forall\varphi \in (\mathbb{R}^+\backslash\{0\})^N$,

$$\min_{q\in\{0,\ldots,N-1\}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q+\eta_2)\right) \leqslant e_0(\eta_2) \tag{31a}$$

and

$$e_0(\eta_2) \leqslant \max_{q\in\{0,\ldots,N-1\}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q+\eta_2)\right) \tag{31b}$$

(the indices labeling the components of φ *are taken modulo N).*

Therefore, we can bound the bottom of the Hofstadter butterfly with the help of any test function.

Corollary 1: For the rational Harper Hamiltonian

$$H\varphi_q = -\varphi_{q+1} - \varphi_{q-1} - V_0 \cos\left(2\pi q \frac{M}{N}\right)\varphi_q, \tag{32}$$

we have $\forall \varphi \in (\mathbb{R}^+\backslash\{0\})^N$

$$\min_{q\in\{0,\ldots,N-1\}}\left[-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} - V_0 \cos\left(2\pi q \frac{M}{N}\right)\right] \leqslant \inf[\sigma(H)] \tag{33a}$$

and

$$\inf[\sigma(H)] \leqslant \max_{q\in\{0,\ldots,N-1\}}\left[-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} - V_0 \cos\left(2\pi q \frac{M}{N}\right)\right]. \tag{33b}$$

Proof: In the Harper model, for each rational number M/N, the lowest eigenvalue is obtained for $\eta=(0,0)$. It is a direct application of Reed and Simon, 1978a, Theorem XIII.89(e) and thus inequalities (33) follow directly from (31). ■

Choosing for φ, at first guess, semiclassical approximations (i.e., corresponding to large N) constructed from Mathieu functions are therefore expected to provide numerical reasonable bounds.

VI. CONCLUSION

It has been shown on various examples how theorem 1 can be used to obtain rigorous estimates on the principal value of any symmetric operator. Its simplicity, its low cost in computations and its wide domain of applications make the method presented in this article a powerful tool for controlling bounds. In many situations, it provides nontrivial complementary information to those obtained by traditional or more system-dependent methods. Unfortunately, this paper does not extend the method to fermionic systems (see for instance, Sigal, 1995 and references therein) where the spatial wave function of the ground state has generically nontrivial nodes (Ceperley, 1991) that cannot be known *a priori* even with some considerations on symmetries.

This paper presents some clues for further developments of optimization algorithms. However it remains an open question whether such algorithms really bear the potential of an efficient treatment and will overcome the possible difficulties one may face in realistic problems.

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Covariant canonical formalism for four-dimensional BF theory

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The covariant canonical formalism for four-dimensional BF theory is performed. The aim of the paper is to understand in the context of the covariant canonical formalism both the reducibility that some first class constraints have in Dirac's canonical analysis and also the role that topological terms play. The analysis includes also the cases when both a cosmological constant and the second Chern character are added to the pure BF action. In the case of the BF theory supplemented with the second Chern character, the presymplectic 3-form is different to the one of the BF theory in spite of the fact both theories have the same equations of motion while on the space of solutions they both agree to each other. Moreover, the analysis of the degenerate directions shows some differences between diffeomorphisms and internal gauge symmetries. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161805]

I. INTRODUCTION

In the path integral quantization of a given field theory one needs to sum the exponential of the classical action weighted with a suitable factor over all possible configurations of the fields under consideration. If the theory under study is a gauge theory one needs, in addition, to factor out the gauge transformations in such a way that the sum includes only equivalence classes of gauge transformed fields. So, intuitively, it is expected that any change in the action principle, yielding the same classical equations of motion, provides a completely different quantum theory. For instance, if the Yang-Mills Lagrangian density $\mathrm{tr}\, F\wedge\star F$ is modified adding the term $\theta\,\mathrm{tr}\, F\wedge F$ the resulting quantum theory is sensitive to this contribution even when it does not modify the classical equations of motion.[1] One way to understand, at the classical level, the cause of having a different quantum theory for the Yang-Mills field is to realize that, in the generic case, the specification of the Lagrangian density is equivalent to specify the symplectic geometry in the various phase spaces associated with the classical theory. Thus, if the Lagrangian density changes, the symplectic geometry also does generically. If one accepts that what defines a dynamical system is its equations of motion then this knowledge is not enough to specify the symplectic geometry on the various phase spaces involved. If, on the other hand, one accepts that what defines a dynamical system is its equations of motion plus an action principle (which provides its equations of motion), then one is in a different situation. The difference is that, as we have already mentioned, the specification of the Lagrangian density provides a symplectic structure. Thus, an action principle plays a double role: (1) it provides the equations of motion and also (2) provides the symplectic geometry. Before going into the analysis of the BF theory, which is the subject of

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this paper, let us emphasize this point with a very simple example borrowed from dynamical systems with a finite number of degrees of freedom. The equations of motion for the two-dimensional isotropic harmonic oscillator $\ddot{x}+\omega^2 x=0$ and $\ddot{y}+\omega^2 y=0$ can be obtained from the Lagrangian $\mathcal{L}(x,y,\dot{x},\dot{y})=m(\dot{x}\dot{y}-\omega^2 xy)$ or from $\mathcal{L}_{\text{usual}}(x,y,\dot{x},\dot{y})=\frac{1}{2}m(\dot{x}^2+\dot{y}^2-\omega^2x^2-\omega^2y^2)$. Moreover, $\mathcal{L}\neq\mathcal{L}_{\text{usual}}+\mathrm{d}F(x,y,t)/\mathrm{d}t$. Note also that we are not making a change of coordinates, which are the same for both cases. The symplectic structures coming from these Lagrangians are very distinct to each other even when they both provide the same equations of motion.[2] Coming back to field theory, it has been shown, in the context of Dirac's canonical analysis, that the symplectic potential changes if one adds topological terms to the Lagrangian density of tetrad gravity.[3] On the other hand, using the covariant canonical formalism, it has been shown that the inclusion of topological terms in Lagrangians for string theory also modifies the original symplectic potential.[4,5]

In this paper, in the context of the covariant canonical formalism,[6–9] we perform the covariant canonical analysis of four-dimensional BF theory, BF theory plus a cosmological constant Λ, and BF plus the second Chern character $F^{IJ}\wedge F_{IJ}$. These theories are topological in the sense that there is no fixed background metric g on the four-dimensional manifold $\mathcal{M}$ in which they are defined. In addition, they are topological in the sense that they have no local degrees of freedom. A more detailed analysis of the covariant canonical formalism for BF theory can be found in Ref. 10. Of course, the inclusion of the second Chern character does not modify the equations of motion while the cosmological constant does. However, the aim of the paper is to study the symplectic geometry involved. It must be emphasized that Dirac's canonical analysis for BF theory has been already done[11,12] (see also the Appendix). In Ref. 12 it is shown that the first class constraints $\tilde{\Psi}^a{}_{IJ}:=\frac{1}{2}\tilde{\eta}^{abc}F_{bcIJ}(A)\approx 0$ are reducible. Dirac's canonical analysis for BF theory with a cosmological constant is reported in the Appendix, where it is shown that now the reducibility equations involve both the Gauss constraints $\tilde{\Psi}^{IJ}$ and the other set of first class constraints $\tilde{\Psi}^a{}_{IJ}:=\frac{1}{2}\tilde{\eta}^{abc}F_{bcIJ}-\Lambda\epsilon_{IJKL}\tilde{\Pi}^{aKL}\approx 0$. This is so because of the cosmological constant Λ. In both cases, the reducibility equations in Dirac's canonical analysis come from the Bianchi identities $DF_{IJ}=0$. So, the covariant canonical formalism is an opportunity to understand the role these identities play on this formalism.

II. BF THEORY

The four-dimensional BF theory with SO(3,1) as the internal relevant group is defined by the equations of motion

$$F_{IJ}=0,\quad DB^{IJ}=0, \tag{1}$$

where $F_{IJ}(A)=\mathrm{d}A_{IJ}+A_{IK}\wedge A^K{}_J$ is the curvature of the Lorentz connection 1-form A_{IJ}, $B^{IJ}=\frac{1}{2}B^{IJ}_{\alpha\beta}\,\mathrm{d}x^\alpha\wedge\mathrm{d}x^\beta$ is a set of six 2-forms, $DB^{IJ}:=\mathrm{d}B^{IJ}+A^I{}_K\wedge B^{KJ}+A^J{}_K\wedge B^{IK}$ is the covariant derivative of B^{IJ}; $I,J=0,1,2,3$ are Lorentz indexes which are raised and lowered with the Minkowski metric η_{IJ}. Even though the analysis will be restricted to a Lorentz BF theory, the results are generic in the sense that hold for any BF theory in 4-space-time dimensions. The choice of the Lorentz group is only to fix the notation that might be used for the case of BF gravity.

In the context of the covariant canonical formalism, the *kinematical* phase space $\mathcal{F}$ of the theory is defined as the space formed by all smooth Lorentz connections A_{IJ} and B^{IJ} fields. Any generic point of $\mathcal{F}$ is not required to satisfy the equations of motion of the BF theory. The space of solutions to the equations of motion $\bar{\mathcal{F}}$ is considered as submanifold of $\mathcal{F}$ and is formed by all points of $\mathcal{F}$ that satisfy the equations of motion of Eq. (1). The reduced (or physical) phase space for the theory is reached by making the quotient of $\bar{\mathcal{F}}$ by the gauge transformations of the theory.[6,7] Even though the term "phase space" has been used to name these different manifolds, it must be emphasized that, at this stage, $\mathcal{F}$, $\bar{\mathcal{F}}$, and the reduced phase space carry no intrinsic symplectic geometry. Thus, although the equations of motion of Eq. (1) are used to define $\bar{\mathcal{F}}$, they are not enough to uniquely endow the various phase spaces for the theory already mentioned with sym-

plectic geometry. Where does symplectic geometry come from then? One possibility is from action principles, specifying the Lagrangian density.[13] The equations of motion of Eq. (1) are usually obtained from the action[11]

$$S[A,B] = \int_{\mathcal{M}} B^{IJ} \wedge F_{IJ}[A] \tag{2}$$

(see also Refs. 14 and 15 for alternative choices of the action). To get the geometry, one needs to proceed along the following lines. The first order variation of the Lagrangian 4-form $\mathbf{L}[A,B] = B^{IJ} \wedge F_{IJ}[A]$ is

$$\delta\mathbf{L}[A,B] = (\delta B^{IJ}) \wedge F_{IJ} - (DB^{IJ}) \wedge \delta A_{IJ} + \mathrm{d}\boldsymbol{\Theta}(B,\delta A), \tag{3}$$

from which the *presymplectic potential* 3-form

$$\boldsymbol{\Theta}(B,\delta A) := B^{IJ} \wedge \delta A_{IJ}, \tag{4}$$

is read off. Now, by taking into account an arbitrary smooth two-parameter family of field configurations and computing the antisymmetric combination of the variations in $\mathbf{L}[A,B],[\delta_1,\delta_2]\mathbf{L}[A,B]=0$ yields[8]

$$\mathrm{d}\omega(\delta_1 A,\delta_1 B,\delta_2 A,\delta_2 B) = (\delta_1 B^{IJ}) \wedge \delta_2 F_{IJ} - (\delta_2 DB^{IJ}) \wedge \delta_1 A_{IJ} - (\delta_1 \leftrightarrow \delta_2), \tag{5}$$

where

$$\omega(\delta_1 A,\delta_1 B,\delta_2 A,\delta_2 B) = (\delta_1 B^{IJ} \wedge \delta_2 A_{IJ} - \delta_2 B^{IJ} \wedge \delta_1 A_{IJ}) \tag{6}$$

is the *presymplectic* 3-form.[16]

A. "Fundamental" set of local gauge transformations

(i) *Local Lorentz transformations*: The action is fully gauge invariant under any arbitrary finite local Lorentz transformation. The infinitesimal version of this transformation is

$$\delta_\epsilon A_{IJ} = D\epsilon_{IJ},$$

$$\delta_\epsilon B^{IJ} = -\epsilon^I{}_K B^{KJ} - \epsilon^J{}_K B^{IK}, \tag{7}$$

where ϵ_{IJ} are the infinitesimal gauge parameters. The change of the Lagrangian $\mathbf{L}[A,B]$ induced by the infinitesimal variation of the fields, given in Eq. (7), is

$$\delta_\epsilon \mathbf{L}[A,B] = \delta_\epsilon B^{IJ} \wedge F_{IJ} + B^{IJ} \wedge \delta_\epsilon F_{IJ} = 0. \tag{8}$$

Therefore, from Eqs. (3) and (8) the *Noether current* 3-form $\mathbf{J}_N[A,B,\epsilon]$ (Ref. 8) associated with the symmetry (7) is[17]

$$\mathbf{J}_N[A,B,\epsilon] = \boldsymbol{\Theta}(B,D\epsilon_{IJ}) = B^{IJ} \wedge D\epsilon_{IJ}, \tag{9}$$

which can be rewritten as

$$\mathbf{J}_N[A,B,\epsilon] = \mathrm{d}\mathbf{Q}[B,\epsilon] - \epsilon_{IJ} \wedge DB^{IJ}, \tag{10}$$

with

$$\mathbf{Q}[B,\epsilon] := \epsilon_{IJ} B^{IJ}, \tag{11}$$

the corresponding *Noether current potential* 2-form. Equation (10) has the *same* structure that appears in the Noether current associated with infinitesimal diffeomorphisms in theories with dynamical background metric in the sense that the right-hand side of Eq. (10) is the exterior derivative of the Noether current potential 2-form $\mathbf{Q}[B,\epsilon]$ plus a term proportional to (one set of)

the equations of motion.[18] There is *a priori* no reason for an internal symmetry, like (7), behaves in the same manner as diffeomorphisms.

Degenerate directions: These can be obtained from the symplectic inner product between the gauge transformation δ_ϵ and an arbitrary variation δ by taking $\delta_1 \equiv \delta$ and $\delta_2 = \delta_\epsilon$. From Eqs. (6) and (7),

$$\omega(\delta A, \delta B, \delta_\epsilon A, \delta_\epsilon B) = \mathrm{d}(\epsilon_{IJ}\delta B^{IJ}) - \epsilon_{IJ}\delta(DB^{IJ}) = \mathrm{d}(\delta \mathbf{Q}[B,\epsilon]) - \epsilon_{IJ}\delta(DB^{IJ}). \tag{12}$$

Note that on the right-hand side of Eq. (12) appears one term involving the linearized Eulerian derivative, $\delta(DB^{IJ})$, but no terms proportional to Eulerian derivatives themselves appear explicitly. As it will be seen, later on, this is a difference with respect to infinitesimal diffeomorphisms (see Sec. II B). Thus, we have

$$\Omega_\Sigma(\delta A, \delta B, \delta_\epsilon A, \delta_\epsilon B) \coloneqq \int_\Sigma \omega(\delta A, \delta B, \delta_\epsilon A, \delta_\epsilon B) = -\int_\Sigma \epsilon_{IJ}\delta DB^{IJ} + \int_{\delta\Sigma} (\epsilon_{IJ}\delta B^{IJ}). \tag{13}$$

The integral over Σ depends on the gauge parameters ϵ_{IJ}, the fields (A_{IJ}, B^{KL}) and their variations while the integral over $\delta\Sigma$ depends only on the gauge parameters ϵ_{IJ} and the variation of the B^{IJ} fields, δB^{IJ}. Both integrals, in general, do not vanish and therefore the gauge transformation of Eq. (7) does not qualify as a degenerate direction unless additional assumptions are imposed. In particular, one has the following.

Proposition: If the linearized Eulerian derivative $\delta(DB^{IJ})$ vanishes, $\delta(DB^{IJ}) = 0$, and the arbitrary variations δB^{IJ} have compact support in the interior of Σ, $\delta B^{IJ}|_{\delta\Sigma} = 0$, then

$$\Omega_\Sigma(\delta A, \delta B, \delta_\epsilon A, \delta_\epsilon B) = 0, \tag{14}$$

without imposing any additional restrictions on the gauge parameters ϵ_{IJ}. Note that (A_{IJ}, B^{KL}) need not be a point of the space of solutions to the equations of motion $\bar{\mathcal{F}}$ in order for Eq. (14) to hold (see also Ref. 19). Nevertheless, it is a common fact to restrict the analysis to $\bar{\mathcal{F}}$ and also to take $(\delta A_{IJ}, \delta B^{KL})$ as tangent vectors to $\bar{\mathcal{F}}$. Of course, the integral over $\partial\Sigma$ in Eq. (13) also vanishes if the gauge parameters ϵ_{IJ} vanish at $\partial\Sigma$, i.e., if the infinitesimal gauge transformation of Eq. (7) is the identity at $\partial\Sigma$.

Canonical transformations:

Proposition: The infinitesimal gauge transformation of Eq. (7) is a canonical transformation.

Proof: From the gauge transformation of Eq. (7),

$$A'_{IJ} = A_{IJ} + D\epsilon_{IJ},$$

$$B'^{IJ} = B^{IJ} - \epsilon^I{}_K B^{KJ} - \epsilon^J{}_K B^{IK}, \tag{15}$$

we can compute two arbitrary variations of the gauge-transformed fields of Eq. (15) (Ref. 7),

$$\delta_i A'_{IJ} = \delta_i A_{IJ} - \delta_i A^K{}_I \epsilon_{KJ} - \delta_i A^K{}_J \epsilon_{IK},$$

$$\delta_i B'^{IJ} = \delta_i B^{IJ} - \epsilon^I{}_K \delta_i B^{KJ} - \epsilon^J{}_K \delta_i B^{IK}. \tag{16}$$

So,

$$\begin{aligned}\omega' \coloneqq (\delta_1 B'^{IJ} \wedge \delta_2 A'_{IJ} - \delta_2 B'^{IJ} \wedge \delta_1 A'_{IJ}) &= (\delta_1 B^{IJ} - \epsilon^I{}_K \delta_1 B^{KJ} - \epsilon^J{}_K \delta_1 B^{IK}) \wedge (\delta_2 A_{IJ} - \delta_2 A^K{}_I \epsilon_{KJ} \\ &- \delta_2 A^K{}_J \epsilon_{IK}) - (\delta_2 B^{IJ} - \epsilon^I{}_K \delta_2 B^{KJ} - \epsilon^J{}_K \delta_2 B^{IK}) \wedge (\delta_1 A_{IJ} - \delta_1 A^K{}_I \epsilon_{KJ} - \delta_1 A^K{}_J \epsilon_{IK}) = \omega,\end{aligned} \tag{17}$$

exactly, i.e., without using any additional conditions. Therefore,

$$\Omega'_\Sigma \coloneqq \int_\Sigma \omega(\delta_1 A', \delta_1 B', \delta_2 A', \delta_2 B') = \int_\Sigma \omega(\delta_1 A, \delta_1 B, \delta_2 A, \delta_2 B) = \Omega_\Sigma. \tag{18}$$

(ii) *B's transform like connections*: The infinitesimal version of this gauge transformation is

$$\delta_\chi A_{IJ} = 0,$$

$$\delta_\chi B^{IJ} = D\chi^{IJ}, \tag{19}$$

where the gauge parameters χ^{IJ} are 1-forms. However, this symmetry is peculiar in the sense that it does not satisfy the definition of symmetry in a strict sense.[8] To see this, the variation of the Lagrangian $\mathbf{L}[A,B]$ induced by the variation of the fields is computed

$$\delta_\chi \mathbf{L}[A,B] = D\chi^{IJ} \wedge F_{IJ}, \tag{20}$$

which has not the desired form in the sense that the right-hand side of Eq. (20) is not of the form $\mathrm{d}\boldsymbol{\alpha}$. To continue, we must rewrite the right-hand side of the last equation,

$$\delta_\chi \mathbf{L}[A,B] = \mathrm{d}(\chi^{IJ} \wedge F_{IJ}) + \chi^{IJ} \wedge DF_{IJ}. \tag{21}$$

Thus, the right-hand side of Eq. (21) is not, in a strict sense, of the form $\mathrm{d}\boldsymbol{\alpha}$. It acquires this form just if the Bianchi identities $DF_{IJ}=0$ are used. However, when computing the transformation of the Lagrangian $\mathbf{L}[A,B]$ induced by the transformation of the fields it is not allowed to use the equations of motion in order to check if the transformation of the fields does (or does not) qualify as a gauge symmetry. A purist might say that the second term on the right-hand side of Eq. (21) involves no equations of motion simply because the Bianchi identities do *not* qualify as equations of motion in the sense that they do not appear when the first order variation of the Lagrangian is computed [see Eq. (3)].

Therefore, from Eqs. (3) and (21),

$$\mathrm{d}(\chi^{IJ} \wedge F_{IJ}) + \chi^{IJ} \wedge DF_{IJ} = (D\chi^{IJ}) \wedge F_{IJ}, \tag{22}$$

and so

$$\mathrm{d}\mathbf{J}_N[A,\chi] = -\chi^{IJ} \wedge DF_{IJ} + (D\chi^{IJ}) \wedge F_{IJ}, \tag{23}$$

with[17]

$$\mathbf{J}_N[A,\chi] := \chi^{IJ} \wedge F_{IJ}, \tag{24}$$

the Noether current associated with the local symmetry (19). Note that $\mathbf{J}_N[A,\chi]$ is proportional to the Eulerian derivative F_{IJ}. Note that if the equations of motion hold (i.e., if $F_{IJ}=0$ hold) and the Bianchi identities hold (i.e., if $DF_{IJ}=0$ hold) then the Noether current is identically conserved. Moreover, note that $\mathbf{J}_N[A,\chi]$ identically vanishes on-shell, i.e., $\mathbf{J}_N=0$ if $F_{IJ}=0$.

Degenerate directions: Again, from the symplectic inner product between the gauge transformation δ_χ and an arbitrary variation δ and Eqs. (6) and (19),

$$\omega(\delta A, \delta B, \delta_\chi A, \delta_\chi B) = \mathrm{d}(\delta(-\chi^{IJ} \wedge A_{IJ})) - \chi^{IJ} \wedge \delta F_{IJ}. \tag{25}$$

Note that on the right-hand side of Eq. (25) appears the linearized Eulerian derivative δF_{IJ} but not the Eulerian derivatives themselves in contrast to what happens with diffeomorphisms (see Sec. II B). Thus, we have

$$\Omega_\Sigma(\delta A, \delta B, \delta_\chi A, \delta_\chi B) := \int_\Sigma \omega(\delta A, \delta B, \delta_\chi A, \delta_\chi B) = -\int_\Sigma \chi^{IJ} \wedge \delta F_{IJ} - \int_{\partial\Sigma} (\chi^{IJ} \wedge \delta A_{IJ}). \tag{26}$$

Again, the integral over Σ depends on the gauge parameters χ^{IJ}, the field A_{IJ} and its first order variations δA_{IJ} while the integral over $\partial\Sigma$ depends only on the gauge parameters χ^{IJ} and the variations of the field A_{IJ}, δA_{IJ}. Both integrals, in general, do not vanish and therefore the gauge transformation of Eq. (19) does not qualify as a degenerate direction unless additional assumptions are imposed. In particular, one has the following.

Proposition: If the linearized Eulerian derivative δF_{IJ} vanishes, $\delta F_{IJ}=0$, and the arbitrary variations δA_{IJ} have compact support in the interior of Σ, $\delta A_{IJ}|_{\partial\Sigma}=0$, then

$$\Omega_\Sigma(\delta A, \delta B, \delta_\chi A, \delta_\chi B) = 0, \tag{27}$$

without imposing any additional conditions on the gauge parameters χ^{IJ}. Note also that in order for Eq. (27) to hold it is not necessary that the point (A_{IJ}, B^{KL}) belongs to the space of solutions to the equations of motion $\bar{\mathcal{F}}$. Nevertheless, it is a common fact to restrict the analysis to this case and also to take $(\delta A_{IJ}, \delta B^{KL})$ as tangent vectors to $\bar{\mathcal{F}}$. Of course, the integral over $\partial\Sigma$ in Eq. (26) also vanishes if the gauge parameters χ^{IJ} vanish at $\partial\Sigma$, i.e., if the infinitesimal gauge transformation of Eq. (19) is the identity at $\partial\Sigma$.

Canonical transformations:

Proposition: The transformation induced by the gauge symmetry of Eq. (19) is an infinitesimal canonical transformation.

Proof: In fact, from Eq. (19),

$$A'_{IJ} = A_{IJ},$$

$$B'^{IJ} = B^{IJ} + D\chi^{IJ}, \tag{28}$$

we can compute two arbitrary variations of the gauge-transformed fields[7]

$$\delta_i A'_{IJ} = \delta_i A_{IJ},$$

$$\delta_i B'^{IJ} = \delta_i B^{IJ} + \delta_i A^I{}_K \wedge \chi^{KJ} + \delta_i A^J{}_K \wedge \chi^{IK}, \quad i = 1,2. \tag{29}$$

So,

$$\omega' := (\delta_1 B'^{IJ} \wedge \delta_2 A'_{IJ} - \delta_2 B'^{IJ} \wedge \delta_1 A'_{IJ}) = (\delta_1 B^{IJ} + \delta_1 A^I{}_K \wedge \chi^{KJ} + \delta_1 A^J{}_K \wedge \chi^{IK}) \wedge \delta_2 A_{IJ} - (\delta_2 B^{IJ} + \delta_2 A^I{}_K \wedge \chi^{KJ} + \delta_2 A^J{}_K \wedge \chi^{IK}) \wedge \delta_1 A_{IJ} = \omega, \tag{30}$$

exactly, i.e., without using any additional conditions. Therefore,

$$\Omega'_\Sigma := \int_\Sigma \omega(\delta_1 A', \delta_1 B', \delta_2 A', \delta_2 B') = \int_\Sigma \omega(\delta_1 A, \delta_1 B, \delta_2 A, \delta_2 B) = \Omega_\Sigma, \tag{31}$$

under the infinitesimal gauge transformation of Eq. (19).

B. Diffeomorphisms

The gauge symmetries discussed in Sec. II A can also be obtained by using Dirac's canonical analysis. In addition, Dirac's canonical analysis shows that the full set of constraints are first class. There are no second class constraints in the theory. However, the first class constraints $\tilde{\Psi}^a{}_{IJ}$ (which generate the δ_χ symmetry) are *reducible* on account of the Bianchi identities $DF_{IJ}=0$ which imply the reducibility equation $D_a\tilde{\Psi}^a{}_{IJ}=0$. Once reducibility is taken into account the counting of the local degrees of freedom is zero, showing that the theory has only global degrees of freedom (see, for instance, Ref. 12 and the Appendix). Moreover, it is also known that the theory is diffeomorphism covariant. Therefore, the transformation of the fields induced by diffeomorphisms must be built from the "fundamental" set of gauge transformations (7) and (19). (The quotation marks in the word "fundamental" emphasize the fact that the gauge transformations are not independent on account of the reducibility of the constraints.) In fact, a diffeomorphism induces a change in the fields A_{IJ} given by

$$\delta_\xi A_{IJ} = \mathcal{L}_\xi A_{IJ} = \xi \cdot F_{IJ} + D\epsilon_{IJ} = \xi \cdot F_{IJ} + \delta_\epsilon A_{IJ}, \tag{32}$$

as well as in the fields B^{IJ},

$$\delta_\xi B^{IJ} = \mathcal{L}_\xi B^{IJ} = \xi \cdot DB^{IJ} - \epsilon^I{}_K B^{KJ} - \epsilon^J{}_K B^{IK} + D\chi^{IJ} = \xi \cdot DB^{IJ} + \delta_\epsilon B^{IJ} + \delta_\chi B^{IJ}, \tag{33}$$

where $\epsilon_{IJ} := \xi \cdot A_{IJ}$ is a set of 0-forms and $\chi^{IJ} := \xi \cdot B^{IJ}$ is a set of 1-forms.

Noether current: The *Noether current* 3-form associated with diffeomorphisms is[17]

$$\mathbf{J}_N[A,B,\xi] = \mathbf{\Theta}(B,\mathcal{L}_\xi A) - \xi \cdot \mathbf{L} = \mathrm{d}\mathbf{Q}[A,B,\xi] - (\xi \cdot A_{IJ})DB^{IJ} - (\xi \cdot B^{IJ}) \wedge F_{IJ}, \tag{34}$$

where

$$\mathbf{Q}[A,B,\xi] = (\xi \cdot A_{IJ})B^{IJ}, \tag{35}$$

is the *Noether current potential* 2-form. If (A_{IJ}, B^{IJ}) is a point of the space of solutions to the equations of motion $\bar{\mathcal{F}}$ then $\mathbf{J}_N[A,B,\xi]$ can be obtained from the Noether current potential $\mathbf{J}_N[A,B,\xi] = \mathrm{d}\mathbf{Q}[A,B,\xi]$. The *Noether charge* $\mathcal{Q}_\Sigma(\xi)$ associated with infinitesimal diffeomorphisms is given by the integral of $\mathbf{J}_N[A,B,\xi]$ over Σ,

$$\mathcal{Q}_\Sigma(\xi) := \int_\Sigma \mathbf{J}_N[A,B,\xi] = \int_{\partial\Sigma} \mathbf{Q}[A,B,\xi] - \int_\Sigma [(\xi \cdot A_{IJ})DB^{IJ} + (\xi \cdot B^{IJ}) \wedge F_{IJ}]. \tag{36}$$

Proposition: If (A_{IJ}, B^{IJ}) is a point in $\bar{\mathcal{F}}$ then the Noether charge just has a contribution from the boundary of Σ,

$$\mathcal{Q}_\Sigma(\xi) = \int_{\partial\Sigma} \mathbf{Q}[A,B,\xi] = \int_{\partial\Sigma} (\xi \cdot A_{IJ})B^{IJ}. \tag{37}$$

Canonical transformation induced by diffeomorphisms: The transformation of the fields induced by a diffeomorphism is

$$A'_{IJ} = A_{IJ} + \mathcal{L}_\xi A_{IJ},$$

$$B'^{IJ} = B^{IJ} + \mathcal{L}_\xi B^{IJ}, \tag{38}$$

and so[7]

$$\delta_i A'_{IJ} = \delta_i A_{IJ} + \delta_i(\mathcal{L}_\xi A_{IJ}) = \delta_i A_{IJ} + \mathcal{L}_\xi(\delta_i A_{IJ}),$$

$$\delta_i B'^{IJ} = \delta_i B^{IJ} + \delta_i(\mathcal{L}_\xi B^{IJ}) = \delta_i B^{IJ} + \mathcal{L}_\xi(\delta_i B^{IJ}). \tag{39}$$

Therefore, at first order in the gauge parameters,

$$\omega' := (\delta_1 B'^{IJ} \wedge \delta_2 A'_{IJ} - \delta_2 B'^{IJ} \wedge \delta_1 A'_{IJ}) = \omega + \mathcal{L}_\xi \omega. \tag{40}$$

Finally,

$$\Omega'_\Sigma := \int_\Sigma \omega' = \int_\Sigma \omega + \int_\Sigma (\xi \cdot \mathrm{d}\omega + \mathrm{d}(\xi \cdot \omega)) = \Omega_\Sigma + \int_\Sigma (\xi \cdot \mathrm{d}\omega + \mathrm{d}(\xi \cdot \omega)). \tag{41}$$

If the linearized Eulerian derivatives vanish, i.e., if $\delta_i(F_{IJ}) = 0$ and $\delta_i(DB^{IJ}) = 0$, $i = 1,2$ then $\mathrm{d}\omega = 0$, and so

$$\Omega'_\Sigma = \Omega_\Sigma + \int_\Sigma \mathrm{d}(\xi \cdot \omega) = \Omega_\Sigma + \int_{\partial\Sigma} \xi \cdot \omega. \tag{42}$$

Note that A_{IJ} and B^{IJ} in $\delta_i(F_{IJ})=0$ and $\delta_i(DB^{IJ})=0$ are *not* required to be solutions to the equations of motion $F_{IJ}=0$ and $DB^{IJ}=0$, i.e., $\delta_i A_{IJ}$ and $\delta_i B^{IJ}$ are tangent to $\mathcal{F}$ but not to $\bar{\mathcal{F}}$. Thus, if

$$\int_{\partial\Sigma} \xi \cdot \omega = 0, \tag{43}$$

then

$$\Omega'_\Sigma = \Omega_\Sigma. \tag{44}$$

This result can be summarized in the following:

Proposition: If the linearized Eulerian derivatives $\delta_i(F_{IJ})=0$ and $\delta_i(DB^{IJ})=0$ hold then Eq. (43) is a necessary and sufficient condition for Ω_Σ be invariant under the transformation associated with infinitesimal diffeomorphisms, i.e., if the linearized Eulerian derivatives $\delta_i(F_{IJ})=0$ and $\delta_i(DB^{IJ})=0$ hold then Eq. (43) is a necessary and sufficient condition for infinitesimal diffeomorphisms to be canonical transformations.

It is clear that in the particular case when Σ has no boundary, i.e., $\partial\Sigma=\emptyset$ then Eq. (43) holds without any additional restrictions on ξ.

Degenerate directions: The starting point is the expression for the presymplectic 3-form with $\delta_1=\delta$ an arbitrary variation and δ_2 is taken as the variation induced by the Lie derivative on the dynamical fields. From Eqs. (6) and (38),

$$\omega(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) = (\delta B^{IJ} \wedge \mathcal{L}_\xi A_{IJ} - \mathcal{L}_\xi(B^{IJ} \wedge \delta A_{IJ}) + B^{IJ} \wedge \delta(\mathcal{L}_\xi A_{IJ})). \tag{45}$$

Now, by taking $\delta=\mathcal{L}_\xi$ in the expression for the presymplectic current potential 3-form of Eq. (4) and computing its variation one has

$$\delta\mathbf{\Theta}(B, \mathcal{L}_\xi A) = \delta B^{IJ} \wedge \mathcal{L}_\xi A_{IJ} + B^{IJ} \wedge \delta(\mathcal{L}_\xi A_{IJ}). \tag{46}$$

Inserting the right-hand side of Eq. (46) into the right-hand side of Eq. (45) one gets

$$\omega(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) = \delta\mathbf{\Theta}(B, \mathcal{L}_\xi A) - \mathcal{L}_\xi(B^{IJ} \wedge \delta A_{IJ}) = \delta\mathbf{\Theta}(B, \mathcal{L}_\xi A) - \mathcal{L}_\xi\mathbf{\Theta}(B, \delta A). \tag{47}$$

On the other hand, the variation of the Noether current 3-form is

$$\begin{aligned}\delta\mathbf{J}_N[A,B,\xi] &= \delta\mathbf{\Theta}(B,\mathcal{L}_\xi A) - \xi\cdot\delta\mathbf{L} = \delta\mathbf{\Theta}(B,\mathcal{L}_\xi A) - \xi\cdot((\delta B^{IJ})\wedge F_{IJ} - (DB^{IJ})\wedge\delta A_{IJ} + \mathrm{d}\mathbf{\Theta}(B,\delta A))\\ &= \omega(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B) + \mathcal{L}_\xi\mathbf{\Theta}(B,\delta A) - \xi\cdot((\delta B^{IJ})\wedge F_{IJ} - (DB^{IJ})\wedge\delta A_{IJ})\\ &\quad - \xi\cdot\mathrm{d}\mathbf{\Theta}(B,\delta A) = \omega(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B) - \xi\cdot((\delta B^{IJ})\wedge F_{IJ} - (DB^{IJ})\wedge\delta A_{IJ})\\ &\quad + \mathrm{d}(\xi\cdot\mathbf{\Theta}(B,\delta A)).\end{aligned} \tag{48}$$

To get the second line on the right-hand side, Eq. (3) was used while Eq. (47) was used to get the third line. Inserting the explicit expression for $\delta\mathbf{J}_N[A,B,\xi]$ given in Eq. (34) into the left-hand side of Eq. (48) one has

$$\begin{aligned}\omega(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B) &= \mathrm{d}(\delta\mathbf{Q}_N[A,B,\xi] - \xi\cdot\mathbf{\Theta}(B,\delta A)) - (\xi\cdot A_{IJ})\,\delta DB^{IJ} - (\xi\cdot B^{IJ})\wedge\delta F_{IJ}\\ &\quad + (\delta B^{IJ})\wedge(\xi\cdot F_{IJ}) - (\xi\cdot DB^{IJ})\wedge\delta A_{IJ}.\end{aligned} \tag{49}$$

Note that, in contrast to Eqs. (12) and (25), in the case of diffeomorphisms the symplectic inner product between δ_ξ and an arbitrary variation δ involves both Eulerian derivatives and the linearized Eulerian derivatives. One has the following:

Proposition: Let (A_{IJ},B^{IJ}) be a point in $\bar{\mathcal{F}}$; let $(\delta A_{IJ},\delta B^{IJ})$ be a solution to the linearized Eulerian derivatives at (A_{IJ},B^{IJ}) [i.e., $(\delta A_{IJ},\delta B^{IJ})$ are such that $\delta(DB^{IJ})=0$ and $\delta F_{IJ}=0$ and are tangent to $\bar{\mathcal{F}}$ at (A_{IJ},B^{IJ})]. Then, we have

$$\omega(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) = \mathrm{d}(\delta \mathbf{Q}_N[A,B,\xi] - \xi \cdot \mathbf{\Theta}(B, \delta A)), \tag{50}$$

and thus, integrating on Σ,

$$\Omega_\Sigma(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) \coloneqq \int_\Sigma \omega(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) = \oint_{\partial\Sigma} (\delta \mathbf{Q}_N[A,B,\xi] - \xi \cdot \mathbf{\Theta}(B, \delta A)). \tag{51}$$

Inserting the explicit expressions for $\mathbf{Q}_N[A,B,\xi]$ and $\mathbf{\Theta}(B,\delta A)$ one has

$$\Omega_\Sigma(\delta A, \delta B, \mathcal{L}_\xi A, \mathcal{L}_\xi B) = \oint_{\partial\Sigma} [\delta((\xi \cdot A_{IJ})B^{IJ}) - \xi \cdot (B^{IJ} \wedge \delta A_{IJ})] = \oint_{\partial\Sigma} [(\xi \cdot A_{IJ})\delta B^{IJ} - (\xi \cdot B^{IJ}) \wedge \delta A_{IJ}]. \tag{52}$$

Some remarks follow: (1) first of all, Eq. (52) tells us that, in the context of the covariant canonical formalism, not all diffeomorphisms are to be regarded as gauge because the right-hand side of (52) will *not* vanish for any ξ, (2) note that if $(A_{IJ}, B^{IJ}) \in \bar{\mathcal{F}}$ then $\xi \cdot A_{IJ} \neq 0$ and $\xi \cdot B^{IJ} \neq 0$ in the generic case. Moreover, note that the right-hand side of (52) vanishes for all (A_{IJ}, B^{IJ}) of $\bar{\mathcal{F}}$ and for all tangent variation $(\delta A_{IJ}, \delta B^{IJ})$ to $\bar{\mathcal{F}}$ in (A_{IJ}, B^{IJ}) if and only if ξ vanishes at the boundary $\partial\Sigma$, $\xi|_{\partial\Sigma} = 0$. Thus, just those diffeomorphisms which are the identity at $\partial\Sigma$ must be regarded as gauge. One could say that the gauge transformation is broken at $\partial\Sigma$ in the sense that $\xi|_{\partial\Sigma} = 0$. However, from that perspective one would be *a priori* assuming that all diffeomorphisms are gauge which as the previous analysis shows is not the case. Let ζ be a diffeomorphism such that it does not vanish at $\partial\Sigma$. The full set of these ζ's span the *boundary symmetry group*. Thus, the covariant canonical formalism tells us *boundary symmetry group* is *not* a gauge group (see also Ref. 9 understand the role of diffeomorphisms in the case of general relativity).

Existence of a Hamiltonian: For variations δA_{IJ} with compact support in the interior of Σ, i.e., $\delta A_{IJ}|_{\partial\Sigma} = 0$,

$$\Omega_\Sigma = \delta \oint_{\partial\Sigma} (\zeta \cdot A_{IJ}) B^{IJ} = \delta \oint_{\partial\Sigma} \mathbf{Q}[A,B,\zeta], \tag{53}$$

which means that a Hamiltonian conjugate to ζ on Σ exists and that its Hamiltonian density is precisely the Noether potential $\mathbf{Q}[A,B,\zeta]$. We have assumed that ζ does *not* vanish at $\partial\Sigma$ and thus, by definition, ζ is not a degenerate direction.

On the other hand, for variations δB_{IJ} with compact support in the interior of Σ, i.e., $\delta B^{IJ}|_{\partial\Sigma} = 0$,

$$\Omega_\Sigma = \delta \oint_{\partial\Sigma} -(\zeta \cdot B^{IJ}) \wedge A_{IJ}, \tag{54}$$

so there exists a Hamiltonian conjugate to ζ on Σ.

Relationship between the Noether currents: It is possible to compare the Noether current associated with diffeomorphisms, $\mathbf{J}_N[A,B,\xi]$, with the currents associated to the fundamental set of gauge symmetries

$$\begin{aligned}\mathbf{J}_N[A,B,\xi] &= B^{IJ} \wedge \mathcal{L}_\xi A_{IJ} - \xi \cdot (B^{IJ} \wedge F_{IJ}) = B^{IJ} \wedge [\xi \cdot F_{IJ} + D\epsilon_{IJ}] - (\xi \cdot B^{IJ}) \wedge F_{IJ} - B^{IJ} \wedge (\xi \cdot F_{IJ}) \\ &= B^{IJ} \wedge D\epsilon_{IJ} - \chi^{IJ} \wedge F_{IJ} = \mathbf{J}_N[A,B,\epsilon] - \mathbf{J}_N[A,\chi].\end{aligned} \tag{55}$$

In a more appropriate notation

$$\mathbf{J}_N[A,B,\xi] = (\mathbf{J}_N[A,B,\epsilon] - \mathbf{J}_N[A,\chi])\big|_{\epsilon_{IJ}=\xi\cdot A_{IJ}, \chi^{IJ}=\xi\cdot B^{IJ}}. \tag{56}$$

Note also that $\mathbf{J}_N[A,B,\xi] = \mathbf{J}_N[A,B,\epsilon]$ because $\mathbf{J}_N[A,\chi] = 0$ on shell (i.e., if $F_{IJ} = 0$). Moreover, note that

$$\mathbf{Q}[A,B,\xi]=(\xi\cdot A_{IJ})B^{IJ}=\epsilon_{IJ}B^{IJ}=\mathbf{Q}[B,\epsilon]. \tag{57}$$

III. BF THEORY PLUS A COSMOLOGICAL CONSTANT

The four-dimensional BF theory with SO(3,1) as the internal group and supplemented with a cosmological constant Λ is defined by the equations of motion

$$F_{IJ}=2\Lambda\ {}^*B_{IJ},\quad DB_{IJ}=0, \tag{58}$$

where ${}^*B_{IJ}=\frac{1}{2}\varepsilon_{IJKL}B^{KL}$ is the dual of B^{IJ}. If SO(4) were taken as the internal group then $\eta_{IJ}\rightarrow\delta_{IJ}$, the connection were valued in the Lie algebra of SO(4) and ${}^{*2}=+1$. Equations (58) can be obtained from the action principle[11,20]

$$S[A,B]=\int_{\mathcal{M}}B^{IJ}\wedge F_{IJ}[A]-\Lambda\int_{\mathcal{M}}B^{IJ}\wedge\ {}^*B_{IJ}. \tag{59}$$

Thus, in contrast to BF theory, the space of solutions to the equations of motion $\bar{\mathcal{F}}_{BF+\Lambda}$ is now defined by Eq. (58). To get the geometry, one needs to compute the first order variation of the Lagrangian 4-form $\mathbf{L}[A,B]=B^{IJ}\wedge F_{IJ}[A]-\Lambda B^{IJ}\wedge {}^*B_{IJ}$,

$$\delta\mathbf{L}[A,B]=(\delta B^{IJ})\wedge(F_{IJ}-2\Lambda\ {}^*B_{IJ})-(DB^{IJ})\wedge\delta A_{IJ}+\mathrm{d}\mathbf{\Theta}(B,\delta,A), \tag{60}$$

from which the *presymplectic potential* 3-form

$$\mathbf{\Theta}(B,\delta A):=B^{IJ}\wedge\delta A_{IJ}, \tag{61}$$

is read off. Therefore, the presymplectic 3-form ω is the same of the BF theory. The symplectic structure induced on $\bar{\mathcal{F}}_{BF+\Lambda}$ is simply the pullback to $\bar{\mathcal{F}}_{BF+\Lambda}$ of the curl of $\mathbf{\Theta}$ on the kinematical phase space.

Degenerate directions:

(1) The symplectic inner product between $\delta_1=\delta$ and $\delta_2=\delta_\epsilon$, $\omega(\delta A,\delta B,\delta_\epsilon A,\delta_\epsilon B)$, has the same analytical form of the BF theory.

(2) The symplectic inner product between $\delta_1=\delta$ and $\delta_2=\delta_\chi$ where $\delta_\chi A_{IJ}=\Lambda\epsilon_{IJKL}\chi^{KL}$ and $\delta_\chi B^{IJ}=D\chi^{IJ}$ (Ref. 17) is now

$$\omega(\delta A,\delta B,\delta_\chi A,\delta_\chi B)=\mathrm{d}(\delta(-\chi^{IJ}\wedge A_{IJ}))-\chi^{IJ}\wedge\delta(F_{IJ}-2\Lambda\ {}^*B_{IJ}). \tag{62}$$

(3) The Noether current associated with diffeomorphisms acquires the form[17]

$$\mathbf{J}_N[A,B,\xi]=\mathrm{d}\mathbf{Q}_N[A,B,\xi]-(\xi\cdot A_{IJ})DB^{IJ}-(\xi\cdot B^{IJ})\wedge(F_{IJ}-2\Lambda\ {}^*B_{IJ}), \tag{63}$$

with the Noether current potential 2-form $\mathbf{Q}_N[A,B,\xi]$ having the same analytical form than the one of the BF theory. Due to the fact that $\omega(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B)=\mathrm{d}(\delta\mathbf{Q}_N[A,B,\xi]-\xi\cdot\mathbf{\Theta}(B,\delta A))$ if the equations of motion and the linearized Eulerian derivatives hold and because $\mathbf{Q}_N[A,B,\xi]$ and $\mathbf{\Theta}(B,\delta A)$ have the same form of the BF theory, then analysis of the degenerate directions is the same of the BF theory. Finally, note that now $\delta_\xi,\delta_\epsilon$, and δ_χ are not related by (32) but by $\delta_\xi A_{IJ}=\xi\cdot(F_{IJ}-2\Lambda\ {}^*B_{IJ})+\delta_\epsilon A_{IJ}+\delta_\chi A_{IJ}$ while $\delta_\xi B^{IJ}=\xi\cdot DB^{IJ}+\delta_\epsilon B^{IJ}+\delta_\chi B^{IJ}$ retains his form with $\epsilon_{IJ}=\xi\cdot A_{IJ},\chi^{IJ}=\xi\cdot B^{IJ}$.

IV. BF THEORY PLUS THE SECOND CHERN CHARACTER

Now, the action we consider is the action for BF theory supplemented with the second Chern character

$$S[A,B]=\int_{\mathcal{M}} B^{IJ}\wedge F_{IJ}[A]+\theta\int_{\mathcal{M}} F^{IJ}[A]\wedge F_{IJ}[A], \tag{64}$$

with θ a parameter. The first order variation of the Lagrangian 4-form $\mathbf{L}[A,B]=B^{IJ}\wedge F_{IJ}+\theta F^{IJ}\wedge F_{IJ}$ is

$$\delta\mathbf{L}[A,B]=\delta B^{IJ}\wedge F_{IJ}-(DB^{IJ}+2\theta DF^{IJ})\wedge\delta A_{IJ}+\mathrm{d}\mathbf{\Theta}, \tag{65}$$

where

$$\mathbf{\Theta}=(B^{IJ}+2\theta F^{IJ})\wedge\delta A_{IJ}, \tag{66}$$

is the presymplectic potential 3-form [cf. Eq. (4)]. From Eq. (65), it is clear that the equations of motion $F_{IJ}=0$ and $DB^{IJ}+2\theta DF^{IJ}=0$ coming from Eq. (64) reduce to those of the BF theory because the Bianchi identities $DF_{IJ}=0$ always hold. Thus, the inclusion of the second Chern character does not modify the classical dynamics of the BF theory, as expected. This means that the space of solutions to the equations of motion $\bar{\mathcal{F}}$ is the same for both theories. Nevertheless, in spite of the fact that the equations of motion are the same, the presymplectic 3-form changes. For the present case one has

$$\omega=\delta_1(B^{IJ}+2\theta F^{IJ})\wedge\delta_2 A_{IJ}-\delta_2(B^{IJ}+2\theta F^{IJ})\wedge\delta_1 A_{IJ} \tag{67}$$

[cf. Eq. (6)]. Therefore, the presymplectic 3-forms coming from Eqs. (2) and (64) are distinct. On the space of solutions $\bar{\mathcal{F}}$, the symplectic structure of Eq. (67) is the same as the symplectic structure of Eq. (6), of course (see also Ref. 15).

Degenerate directions:

(1) The symplectic inner product between $\delta_1=\delta$ and $\delta_2=\delta_\epsilon$ is now

$$\omega(\delta A,\delta B,\delta_\epsilon A,\delta_\epsilon B)=\mathrm{d}(\epsilon_{IJ}\delta B^{IJ}+2\theta\delta A^{IJ}\wedge D\epsilon_{IJ})-\epsilon_{IJ}\delta(DB^{IJ}) \tag{68}$$

and so

$$\Omega_\Sigma(\delta A,\delta B,\delta_\epsilon A,\delta_\epsilon B)=-\int_\Sigma \epsilon_{IJ}\delta DB^{IJ}+\int_{\partial\Sigma}(\epsilon_{IJ}\delta B^{IJ}+2\theta\delta A^{IJ}\wedge D\epsilon_{IJ}). \tag{69}$$

Therefore, if the linearized Eulerian derivative $\delta(DB^{IJ})$ vanishes, $\delta(DB^{IJ})=0$, and the arbitrary variations $(\delta A^{IJ},\delta B^{IJ})$ have compact support in the interior of Σ, $\delta A^{IJ}|_{\partial\Sigma}=0$ and $\delta B^{IJ}|_{\partial\Sigma}=0$, then

$$\Omega_\Sigma(\delta A,\delta B,\delta_\epsilon A,\delta_\epsilon B)=0, \tag{70}$$

without imposing any additional restrictions on the gauge parameters ϵ_{IJ}. The integral over $\partial\Sigma$ in Eq. (69) also vanishes if both the gauge parameters ϵ_{IJ} vanish and satisfy $D\epsilon_{IJ}=0$ at $\partial\Sigma$.

(2) The symplectic inner product between $\delta_1=\delta$ and $\delta_2=\delta_\chi$ is the same as the one of the BF theory.

(3) Now, we consider diffeomorphisms. The Noether current associated with diffeomorphisms acquires the form

$$\mathbf{J}_N[A,B,\xi]=\mathrm{d}\mathbf{Q}_N[A,B,\xi]-(\xi\cdot A_{IJ})(DB^{IJ}+2\theta DF^{IJ})-(\xi\cdot B^{IJ})\wedge F_{IJ}, \tag{71}$$

where

$$\mathbf{Q}_N[A,B,\xi]=(\xi\cdot A_{IJ})(B^{IJ}+2\theta F^{IJ}), \tag{72}$$

is the *Noether current potential* 2-form. Therefore, the Noether charge is the same as in the BF theory if the equations of motion are satisfied. Moreover, if both the equations of

motion and the linearized equations of motion hold, then symplectic inner product between $\delta_1=\delta$ and $\delta_2=\delta_\xi$ becomes

$$\Omega_\Sigma(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B)=\oint_{\partial\Sigma}(\delta\mathbf{Q}_N[A,B,\xi]-\xi\cdot\mathbf{\Theta}(B,\delta A)). \tag{73}$$

Inserting the explicit expressions for $\mathbf{Q}_N[A,B,\xi]$ and $\mathbf{\Theta}(B,\delta A)$ one has

$$\begin{aligned}\Omega_\Sigma(\delta A,\delta B,\mathcal{L}_\xi A,\mathcal{L}_\xi B)&=\oint_{\partial\Sigma}[\delta(\xi\cdot A_{IJ}(B^{IJ}+2\theta F^{IJ}))-\xi\cdot((B^{IJ}+2\theta F^{IJ})\wedge\delta A_{IJ})]\\&=\oint_{\partial\Sigma}[(\xi\cdot A_{IJ})\delta B^{IJ}-(\xi\cdot B^{IJ})\wedge\delta A_{IJ}],\end{aligned} \tag{74}$$

because $F^{IJ}=0$ and $\delta F^{IJ}=0$, by hypothesis. Last equation has the same analytical form as the one of the BF theory. Therefore, the inclusion of the second Chern character does not modify the degenerate directions in the case of diffeomorphisms.

V. CONCLUSIONS AND PERSPECTIVES

To conclude, we emphasize the role that the Bianchi identities $DF_{IJ}=0$ play in four-dimensional BF theories. On the one hand, they are the cause of having the symmetry δ_χ in the various four-dimensional BF theories already discussed. On the other hand, in the case of the BF theory with a nonvanishing cosmological constant Λ the combination of the Bianchi identities together with the equation of motion $F_{IJ}=2\Lambda*B_{IJ}$ "generates" dynamics for the B^{IJ} fields in the sense that they imply $DB_{IJ}=0$. This fact is the origin of the reducibility of the corresponding first class constraints of the theory in Dirac's canonical analysis. This same phenomenon appears, in essence, in the action[17]

$$S[A,B,\phi]=\int_{\mathcal{M}}B^{IJ}\wedge F_{IJ}-\frac{1}{2}\phi_{IJKL}B^{IJ}\wedge B^{KL}, \tag{75}$$

with $\phi_{IJKL}=-\phi_{JIKL}=-\phi_{IJLK}=\phi_{KLIJ}$ where the combination of the Bianchi identities and the equations of motion $F_{IJ}=\phi_{IJKL}B^{KL}$ and $DB^{IJ}=0$ generates dynamics for the ϕ_{IJKL} fields in the sense that these equations imply $(D\phi_{IJKL})\wedge B^{KL}=0$. From the lesson learned from the case of the BF theory plus a cosmological constant Λ, we would expect that the theory defined by Eq. (75) has also reducibility in the constraints in the context of Dirac's analysis. We consider the present analysis as a first step towards the covariant canonical analysis of BF gravity.[21]

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APPENDIX: REVIEW OF DIRAC'S CANONICAL ANALYSIS FOR FOUR-DIMENSIONAL BF THEORY

To compare some results of this Appendix with some results of the covariant canonical formalism one must make the changes $\epsilon_{IJ}\to-\epsilon_{IJ}$ and $\epsilon_a^{IJ}\to-\chi_a^{IJ}$ in this Appendix.

(1) *BF theory*: By making the $3+1$ decomposition, a straightforward computation shows that the action (2) acquires the form

$$S[A_{aIJ},\tilde{\Pi}^{aIJ},\lambda_{IJ},\lambda_a{}^{IJ}]=\int_{\mathcal{M}} d^4x\left[\dot{A}_{aIJ}\tilde{\Pi}^{aIJ}-\lambda_{IJ}D_a\tilde{\Pi}^{aIJ}-\lambda_a{}^{IJ}\left(\frac{1}{2}\tilde{\eta}^{abc}F_{bcIJ}\right)\right]+\int_{\mathcal{M}} d^4x\partial_a(\lambda_{IJ}\tilde{\Pi}^{aIJ}), \tag{A1}$$

where the phase space variables $(A_{aIJ},\tilde{\Pi}^{bKL})$ and Lagrange multipliers λ_{IJ} and $\lambda_a{}^{IJ}$ are defined in terms of the initial configuration variables as $\tilde{\Pi}^{aIJ}:=\frac{1}{2}\tilde{\eta}^{abc}B_{bc}{}^{IJ}$, $\lambda_{IJ}:=-A_{0IJ}$, $\lambda_a{}^{IJ}:=-B_{0a}{}^{IJ}$, $D_a\tilde{\Pi}^{aIJ}:=\partial_a\tilde{\Pi}^{aIJ}+A_a{}^I{}_K\tilde{\Pi}^{aKJ}+A_a{}^J{}_K\tilde{\Pi}^{aIK}$. If the space-time $\mathcal{M}$ has the topology $\mathcal{M}=\Sigma\times R$ and Σ has no boundary the second integral on the right-hand side of (A1) can be neglected. The lowercase letters a,b are space ones and run from 1 to 3. Notice that the Lorentz indices I,J are not split holding in this way the full Lorentz group. The variation of Eq. (A1) with respect to the phase space variables yields the equations of motion

$$\dot{A}_{aIJ}=-D_a\lambda_{IJ},$$

$$\dot{\tilde{\Pi}}^{aIJ}=2\lambda^{[I}{}_K\tilde{\Pi}^{aKJ]}-\tilde{\eta}^{abc}D_b\lambda_c{}^{IJ}, \tag{A2}$$

with $D_a\lambda_{IJ}=\partial_a\lambda_{IJ}-A_a{}^K{}_I\lambda_{KJ}-A_a{}^K{}_J\lambda_{IK}$. The variation with respect to the Lagrange multipliers gives the constraints

$$\tilde{\Psi}^{IJ}:=D_a\tilde{\Pi}^{aIJ}\approx 0,\quad \tilde{\Psi}^a{}_{IJ}:=\frac{1}{2}\tilde{\eta}^{abc}F_{bcIJ}(A)\approx 0, \tag{A3}$$

which are first class. The infinitesimal gauge transformation generated by the Gauss constraint $\tilde{\Psi}^{IJ}$ is

$$A'_{aIJ}=A_{aIJ}-D_a\epsilon_{IJ},\quad \widetilde{\Pi'}^{aIJ}=\tilde{\Pi}^{aIJ}+\epsilon^{IM}\tilde{\Pi}^a{}_M{}^J-\epsilon^{JM}-\tilde{\Pi}^a{}_M{}^I, \tag{A4}$$

and

$$A'_{aIJ}=A_{aIJ},\quad \widetilde{\Pi'}^{aIJ}=\tilde{\Pi}^{aIJ}-\tilde{\eta}^{abc}D_b\epsilon^{IJ}{}_c, \tag{A5}$$

is the gauge transformation generated by the constraint $\tilde{\Psi}^a{}_{IJ}$. However, even though the constraints $\tilde{\Psi}^{IJ}$ are irreducible the constraints $\tilde{\Psi}^a{}_{IJ}$ are not, i.e., they are *reducible*. This is so because the Bianchi identities $DF_{IJ}=0$ imply the relationship among the $\tilde{\Psi}^a{}_{IJ}$'s,

$$\tilde{\Phi}_{IJ}:=D_a\tilde{\Psi}^a{}_{IJ}=0. \tag{A6}$$

The counting of physical degrees of freedom is as follows. There are $3\times 6=18$ configuration variables A_{aIJ} and $6+[(3\times 6)-6]=18$ *independent* first class constraints. Therefore, the system has no local degrees of freedom.[12] Alternatively, the independent number of gauge parameters is $18=6$ (the ϵ_{IJ}'s) $+12$ $(=18-6$ independent gauge parameters from $\epsilon_a^{IJ})$.

(2) *BF theory plus a cosmological constant*: By performing the $3+1$ decomposition the action (59) can be written as

$$S[A_{aIJ},\tilde{\Pi}^{aIJ},\lambda_{IJ},\lambda_a{}^{IJ}]=\int d^4x\left[\dot{A}_{aIJ}\tilde{\Pi}^{aIJ}-\lambda_{IJ}D_a\tilde{\Pi}^{aIJ}-\lambda_a{}^{IJ}\left(\tfrac{1}{2}\tilde{\eta}^{abc}F_{bcIJ}-\Lambda\epsilon_{IJKL}\tilde{\Pi}^{aKL}\right)\right]. \tag{A7}$$

The equations of motion are

$$\dot{A}_{aIJ}=-D_a\lambda_{IJ}-\Lambda\epsilon_{IJKL}\lambda_a{}^{KL},$$

$$\dot{\tilde{\Pi}}^{aIJ} = 2\lambda^{[I}{}_K\tilde{\Pi}^{aKJ]} - \tilde{\eta}^{abc}D_b\lambda_c{}^{IJ}. \tag{A8}$$

The constraints are

$$\tilde{\Psi}^{IJ} := D_a\tilde{\Pi}^{aIJ}, \quad \tilde{\Psi}^a{}_{IJ} := \tfrac{1}{2}\tilde{\eta}^{abc}F_{bcIJ} - \Lambda\epsilon_{IJKL}\tilde{\Pi}^{aKL}. \tag{A9}$$

The evolution of the constraints provides no more constraints. To compute the algebra of constraints it is convenient to smear them

$$\Psi[u] := \int d^3x u_{IJ}\tilde{\Psi}^{IJ}, \quad \Psi[N] := \int d^3x N^{IJ}{}_a\tilde{\Psi}^a_{IJ}. \tag{A10}$$

The constraint algebra is

$$\{\Psi[u],\Psi[v]\} = \Psi[[u,v]], \quad \{\Psi[u],\Psi[N]\} = \Psi[[u,N]], \quad \{\Psi[N],\Psi[M]\} = 0, \tag{A11}$$

with $[u,v]_{IJ} := u_I{}^M v_{MJ} - u_J{}^M v_{MI}$, $[u,N]^{IJ}{}_a = u^I{}_K N^{KJ}{}_a - u^J{}_K N^{KI}{}_a$. The infinitesimal gauge transformation generated by the Gauss constraint $\tilde{\Psi}^{IJ}$ is

$$A'_{aIJ} = A_{aIJ} - D_a\epsilon_{IJ}, \quad \tilde{\Pi}'^{aIJ} = \tilde{\Pi}^{aIJ} + \epsilon^{IM}\tilde{\Pi}^a{}_M{}^J - \epsilon^{JM}\tilde{\Pi}^a{}_M{}^I, \tag{A12}$$

and

$$A'_{aIJ} = A_{aIJ} - \Lambda\epsilon_{IJKL}\epsilon^{KL}{}_a, \quad \tilde{\Pi}'^{aIJ} = \tilde{\Pi}'^{aIJ} = \tilde{\Pi}^{aIJ} - \tilde{\eta}^{abc}D_b\epsilon^{IJ}{}_c, \tag{A13}$$

is the infinitesimal gauge transformation generated by the constraint $\tilde{\Psi}^a{}_{IJ}$. Again, the Bianchi identities imply that the constraints are reducible

$$D_a\tilde{\Psi}^a{}_{IJ} + \Lambda\epsilon_{IJKL}\tilde{\Psi}^{KL} = 0. \tag{A14}$$

Like in pure BF gravity the system has $3\times 6=18$ configuration variables and $6+[(3\times 6)-6]=18$ independent first class constraints. Therefore, the system has no local degrees of freedom, as expected because the addition of a cosmological constant does not add local degrees of freedom. However, a key difference with respect to the case without cosmological constant Λ is that there the constraints $\tilde{\Psi}^a{}_{IJ}$ and $\tilde{\Psi}^{IJ}$ are independent while in the present case they are related through the reducibility equation given in Eq. (A14). Moreover, due to the fact the reducibility equation involves now the Gauss constraints too, there are 18 independent gauge parameters among the 6 of ϵ_{IJ}'s and the 18 of ϵ_a^{IJ}'s. One can take these independent number of gauge parameters as the 18 of the ϵ_a^{IJ}'s. By doing this, one might say that the local Lorentz transformation is redundant if a cosmological constant is present.

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Instability of coherent states of a real scalar field

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We investigate stability of both localized time-periodic coherent states (pulsons) and uniformly distributed coherent states (oscillating condensate) of a real scalar field satisfying the Klein-Gordon equation with a logarithmic nonlinearity. The linear analysis of time-dependent parts of perturbations leads to the Hill equation with a singular coefficient. To evaluate the characteristic exponent we extend the Lindemann-Stieltjes method, usually applied to the Mathieu and Lamé equations, to the case that the periodic coefficient in the general Hill equation is an unbounded function of time. As a result, we derive the formula for the characteristic exponent and calculate the stability-instability chart. Then we analyze the spatial structure of the perturbations. Using these results we show that the pulsons of any amplitudes, remaining well-localized objects, lose their coherence with time. This means that, strictly speaking, all pulsons of the model considered are unstable. Nevertheless, for the nodeless pulsons the rate of the coherence breaking in narrow ranges of amplitudes is found to be very small, so that such pulsons can be long-lived. Further, we use the obtained stability-instability chart to examine the Affleck-Dine-type condensate. We conclude the oscillating condensate can decay into an ensemble of the nodeless pulsons. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Nonlinear localized field configurations, nontopological solitons, are currently considered as models of various physical objects, from elementary particles to giant lumps of dark matter in the form of soliton stars and galactic halos.[1–3] Stability properties of solitons were investigated by many authors, and a number of important results has been obtained (see, e.g., Ref. 4 and references therein). In particular, Hobart[5] and Derrick[6] have proved that static multidimensional scalar solitons are energetically unstable, and, hence, these objects cannot last in a real world for a long time. One way to avoid this theorem is to invoke time dependence. Along this line main efforts were focused on the stability analysis of the stationary states, i.e., coherent states of a complex scalar field oscillating harmonically in time. It turned out, however, that for a wide class of relativistic models these states can be only conditionally stable, i.e., stable with respect to a certain type of perturbations (e.g., conserving the scalar charge).[4] As to the time-periodic states of a more general form, both complex and real, there are presently no strong analytical results on their stability.

In this paper we examine stability of time-periodic configurations of the form

$$\phi = \phi_0(t,\mathbf{r}) = a(t)u(\mathbf{r}) \tag{1}$$

satisfying the nonlinear Klein-Gordon equation

$$\phi_{tt} - \Delta\phi + U'(\phi) = 0. \tag{2}$$

These are coherent states in the sense the field oscillates synchronously at all spatial points. It is necessary to stress that we consider real solutions, so that the energy density oscillates as well [in

contrast to the stationary states for which $a(t) \propto e^{i\omega t}$]. Solitons with oscillating energy density are usually called pulsons.

It turns out that for real ϕ the ansatz (1) determines uniquely the potential $U(\phi)$ in Eq. (2). Namely, if neither $a(t)$ nor $u(\mathbf{r})$ are constants, the only potential admitting such solutions will have the form[7]

$$U(\phi) = \tfrac{1}{2}\phi^2[m^2 + \lambda(1 - \ln \phi^2)], \tag{3}$$

where m^2 and λ are arbitrary constants.

Originally, the Klein-Gordon equation with a logarithmic potential of this type has been introduced in the quantum field theory by Rosen.[8] Later on Bialynicki-Birula and Mycielski[9] have rediscovered this equation and also considered its nonrelativistic version, the nonlinear Schrödinger equation.[10]

In inflationary cosmology and in modern supersymmetric field theories the logarithmic nonlinearities appear naturally when quantum corrections to effective potentials are allowed for.[11–14] In this context the expression in the square brackets of Eq. (3) can be treated as a dynamic inflaton mass term m_S^2 that is the bare inflaton mass term m^2 plus the logarithmic correction. It can be represented in the commonly considered form[14–21] by the substitution $\ln \phi^2 = 1 + \ln(\Phi/M)^2$, $\lambda/m^2 = -K$, where Φ is an inflaton scalar field, M is a large mass scale, K is a constant (usually negative and small). Thus our consideration is also relevant to dynamics of the pulson exitations of a real inflaton field oscillating around a vacuum value.

Note that the multidimensional pulsons probably exist in other scalar models as well. Thus the long-living oscillating spherically symmetric localized states were numerically found in the sine-Gordon, ϕ^4, and $\phi^3 - \phi^4$ models[22–26] (see Ref. 27 for a review). Unfortunately, the analytic form of these solutions is so far unknown.

The model (2) and (3) is unique in the sense it has a whole family of exact pulson solutions of the form (1), all existing in any number of spatial dimensions.[7] This is also true for complex version of the model.[28,29] The real pulsons we are dealing with are the limiting states of the complex ones, when the scalar charge tends to zero. Other limiting states are Q-balls[15,16] for which $a(t) \propto e^{i\omega t}$. It is believed that Q-balls can arise due to fragmentation of the Affleck-Dine condensate.[18–21] We will see below that the parametric instability of the oscillating condensate leads to the resonant fragmentation that can give rise to the pulson formation at the nonlinear stage. Like Q-balls,[17] pulsons interact elastically or inelastically in collisions depending on their relative velocities, phases, and rest masses.[30,31] Thus, in model (2) and (3) the light pulsons with given relative velocities interact always elastically, independently of their phases. In contrast, the collisions of heavy pulsons can result in formation of the so-called explosons, localized states with exponentially growing amplitude.[30] For the intermediate masses the picture depends essentially on the phases of the colliding pulsons and impact velocity determining the duration of the interaction.[31]

The above results suggest that there is a domain of parameters where pulsons are stable, at least in short time interactions. But in what sense? How long a pulson conserves its characteristic features once interaction ends? If pulsons are long-lived objects they will be interesting candidates for the dark matter constituents having time-dependent density. What is known about stability of an isolated pulson at the long time scale? Surprisingly, but very few. In Ref. 29 it was argued in favor of its perfect stability. No deviations from the exact solution (1) were found after about 1000 oscillations. However, our preliminary numerical experiments[32,33] have shown that the pulsons of certain amplitudes, even perturbed by computer round-off errors only, gradually lose their coherency, remaining well-localized oscillating objects. This has motivated the closer examination.

In the present paper we clarify how long the pulsons can conserve the coherency depending on their parameters. For this purpose we investigate stability of the spherically symmetric pulson solutions (1) with respect to small initial perturbations of an arbitrary form.

The paper is organized as follows. In Sec. II the main properties of the real pulsons of the model considered are reviewed. Section III is wholly devoted to the linear stability analysis. We arrive at the singular Hill equation and generalize the Lindemann-Stieltjes method to evaluate the

characteristic exponent. On this basis we examine stability of the pulsons and discuss fragmentation of the oscillating Affleck-Dine-type condensate. In Sec. IV we make some remarks concerning the complex pulsons and summarize the main results.

II. PULSONS AS COHERENT STATES

Assuming λ positive, let us first eliminate the constants m^2 and λ from consideration by the scaling $t \to \lambda^{-1/2} t$, $\mathbf{r} \to \lambda^{-1/2}\mathbf{r}$, $\phi \to \phi \exp(m^2/2\lambda)$. In the new variables the field ϕ may be thought of as satisfying Eq. (2) with the potential

$$U(\phi) = \tfrac{1}{2}\phi^2(1 - \ln \phi^2). \tag{4}$$

It is the potential we will deal with. It has local minimum at $\phi=0$ and two maxima at $\phi=\pm 1$, at the minimum the potential having the singularity: its second derivative tends to infinity as $\phi \to 0$.

The substitution of the ansatz (1) into Eq. (2) leads then to two independent equations,

$$a_{tt} = -\frac{d}{da}\left[\frac{1}{2}a^2(1 - \ln a^2)\right], \tag{5}$$

$$\Delta u = -\frac{d}{du}\left[\frac{1}{2}u^2(\ln u^2 - 1)\right]. \tag{6}$$

Note that the potentials in the square brackets of Eqs. (5) and (6) have the same form as the potential (4) taken with plus and minus signs, respectively. The existence of the oscillating localized solutions (1) is thus apparent from consideration of motion of a mechanical particle in these potentials.

Let us consider in more detail the oscillatory solutions of Eq. (5). Using the Hamiltonian and denoting $\xi = a/a_{\max}$ ($0 < a_{\max} < 1$, $-1 \leqslant \xi \leqslant 1$), we obtain

$$\xi_t^2 = \omega_0^2(1 - \xi^2) + \xi^2 \ln \xi^2, \tag{7}$$

where

$$\omega_0^2 = 1 - \ln a_{\max}^2 > 1. \tag{8}$$

In the case of small amplitudes, $a_{\max}^2 \ll 1$, $\omega_0^2 \gg 1$, Eq. (7) gives

$$\xi(t) \approx \cos \omega_0 t. \tag{9}$$

Thus, we have quasiharmonic high-frequency oscillations which are however nonlinear since their period,

$$T \approx \frac{2\pi}{|\ln a_{\max}^2|^{1/2}}, \tag{10}$$

depends on the amplitude.[33] In the next approximation from Eq. (7) we find

$$T = \frac{2\pi}{\omega_0}\left[1 + \frac{0.307}{\omega_0^2} + O\left(\frac{1}{\omega_0^4}\right)\right]. \tag{11}$$

In the case of near-critical amplitudes, when $a_{\max}^2 \to 1$, the oscillations become almost rectangular and have the period

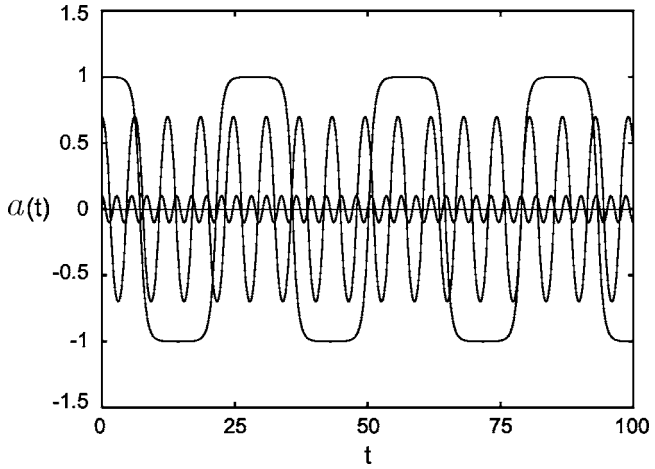

FIG. 1. Oscillatory solutions of Eq. (5) for $a_{\max}=0.1$, $a_{\max}=0.7$, and $a_{\max}=0.9999$.

$$T \approx 2\sqrt{2} \ln \frac{1}{1-a_{\max}^2}. \tag{12}$$

Examples of solutions of Eq. (5) are shown in Fig. 1.

The spatial structure of a pulson is determined by Eq. (6). In the spherically symmetric case this equation has a discrete spectrum of localized N-nodal solutions $u_N(r)$ with the first derivatives vanishing at the origin[34] (see Fig. 2). The simplest of them, the nodeless solution, has a Gaussian-type shape,

$$u_0(r) = e^{(3-r^2)/2}, \tag{13}$$

and is usually called gausson.[8–10] It is agreed that its effective radius equals $\sqrt{2}$. In the multinodal solutions, as r increases, the field undergoes spatial oscillations of the half-wavelength $L \lesssim 2\sqrt{2}$ and then decays as

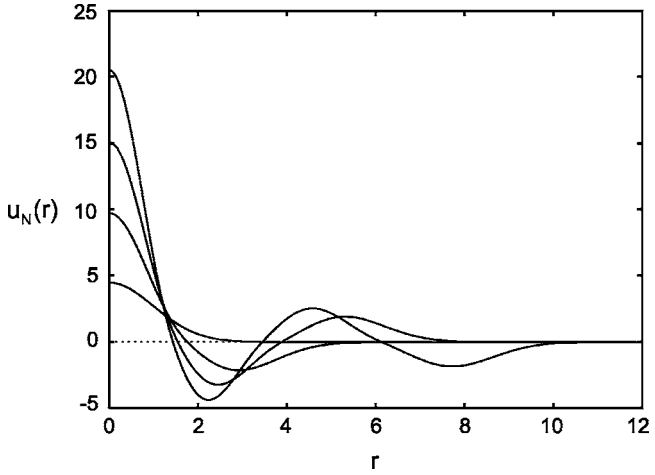

FIG. 2. Spectrum of the spherically symmetric N-nodal solutions $u_N(r)$ of Eq. (6): $u_0(0)=e^{3/2}$, $u_1(0)=9.726$, $u_2(0)=15.084$, $u_3(0)=20.526,\ldots$.

$$u_N(r) \approx C_N e^{-(r-\rho_N)^2/2} \quad (r \gg r-\rho_N,\ N \gg 1), \tag{14}$$

where C_N is the value of the last extremum of $u_N(r)$ attained at $r=\rho_N$, $C_N \to (-1)^N e^{1/2} (N \to \infty)$, $\rho_N \sim NL$. Thus, the pulsons of the model (2) and (4) are well-localized states of the inhomogeneity length L, at all points the field oscillating coherently with the period T. (To return to the physical units these scales should be multiplied by $\lambda^{-1/2}$.) In our dimensionless variables the pulsons are characterized by two parameters only: the amplitude $a_{\max}$ and the number of the nodes N [or T and $u_N(0)$, respectively].

It should be stressed that, due to nonanalyticity of $U(\phi)$ at $\phi=0$, the right-hand sides of Eqs. (5) and (6) are nonanalytic when a and u become zero. Hence, the solutions $a(t)$ and $u(r)$ themselves become nonanalytic at those points t and r where they pass through zero. Thus in the solution (9) we have dropped the terms which are small (of the order of ω_0^{-2}) but nonanalytic when $\xi(t)=0$. In the general case from Eq. (7) it follows that $\xi(t)$ passes through zero at $t=t_m$ as

$$\underset{t \to t_m}{\xi(t)} = \pm\, \omega_0 (t-t_m)\left[1 + \tfrac{1}{6}(t-t_m)^2 \ln(t-t_m)^2 + O((t-t_m)^2)\right], \tag{15}$$

where $\pm$ sign is taken for $\xi_t(t_m) \gtrless 0$. It is seen that ξ_{ttt} becomes infinite as $t \to t_m$. Similarly, one can show that in the vicinity of the nth node $(n=1,\ldots,N)$,

$$\underset{r \to r_n}{u(r)} = u_r(r_n)(r-r_n)\left[1 - \frac{r-r_n}{r_n} - \frac{1}{6}(r-r_n)^2 \ln(r-r_n)^2 + O((r-r_n)^2)\right]. \tag{16}$$

As we will see below, the nonanalyticity of $U(\phi)$ gives rise to some specific features of the stability analysis.

III. THE LINEAR STABILITY ANALYSIS

Consider a small fluctuation $\eta(t,\mathbf{r})$ around the spherically symmetric pulson (1), $\phi=\phi_0(t,r) + \eta(t,\mathbf{r})$. In the linear approximation the equation for η reads

$$\eta_{tt} - \Delta\eta - (2 + \ln \phi_0^2)\eta = 0. \tag{17}$$

Seeking a solution in the form $\eta(t,\mathbf{r}) \propto X(t)\Psi(\mathbf{r})$ we arrive at the equations

$$X_{tt} + (E - 2 - \ln a^2)X = 0, \tag{18}$$

$$\Delta\Psi + (E + \ln u^2)\Psi = 0, \tag{19}$$

where E is some constant.

The expression in the parentheses of Eq. (17) is $-U''(\phi_0)$. It becomes infinite, as well as the expressions in the parentheses of Eqs. (18) and (19), at the points t_m and r_n where $a(t)$ and $u(r)$ become zero. Thus we need to analyze the second order differential equations with singular coefficients. We begin with Eq. (18) which has the periodic singular coefficient $\ln a^2(t)$ and hence belongs to the class of Hill equations.

A. Singular Hill equation and generalized Lindemann-Stieltjes method

It turns out to be very useful to look at the problem as a whole, considering first the Hill equation of a general form

$$X_{tt} + h(z(t))X = 0. \tag{20}$$

We will assume that $h(z)$ is an integral function of z, while $z(t)$ is a real-valued periodic (of a period τ) even function of t, having, in general, singularities, but such, that $h(z(t))$ remains still integrable.

It is well known that the Hill equation describes the physical systems in which the parametric resonance can occur. In the context of our stability analysis we will be interested in real resonant solutions of Eq. (20). In accordance with the Floquet theory (see, e.g., Ref. 35), any one of these solutions can be represented as a linear combination of the fundamental solutions

$$X_+(t) = \varphi(t)e^{\mu t}, \quad X_-(t) = \varphi(-t)e^{-\mu t}, \tag{21}$$

where $\varphi(t)$ is a τ-periodic or τ-antiperiodic real function, $\mu > 0$ is the characteristic exponent. In the case that $z(t)$ is unbounded it is impossible to obtain the solutions and evaluate μ by expansions in Fourier series, following the standard Hill approach. Another way is to apply the Lindemann-Stieltjes method.[36] In some cases it allows one to obtain the results in a closed analytical form.[37–40] We first outline this method in the context of the general Hill equation (20) with an extension to the case that the periodic function $z(t)$ is unbounded. In doing so we follow Ref. 39 where the method was used to construct the resonant solutions of the Lamé equation.

The main idea is as follows. Let us treate z as a new "time" variable instead of t. In each interval of monotonicity of $z(t)$ we define

$$y(z) = X(t). \tag{22}$$

Assume that the periodic function $z(t)$ satisfies the equation

$$z_t^2 = g(z), \tag{23}$$

where $g(z)$ is an integral function of z. Equation (20) then becomes

$$g(z)y'' + \tfrac{1}{2}g'(z)y' + h(z)y = 0 \tag{24}$$

(hereinafter the prime denotes $d/\mathrm{d}z$).

Let us first suppose $z(t)$ is bounded. Equation (23) then shows that it is differentiable. Zeros of the function $g(z)$ on the complex z plane, taken to be isolated, are singular points of Eq. (24). Since $z(t)$ is periodic and real-valued, among singular points there are two, ζ_1 and ζ_2, lying on the real axis and being minimal and maximal values which $z(t)$ acquires at the endpoints of the intervals of monotonicity. Also, it follows that $g'(\zeta_{1,2}) \neq 0$. Physically, this is well understood, since ζ_1 and ζ_2 can be treated as turning points in periodic motion of a mechanical particle, e.g., of a nonlinear oscillator, under the action of the force $g'/2$. From Eq. (23) it is clear that the interval $[\zeta_1, \zeta_2]$ does not contain other singular points of Eq. (24).

For example, in the case of the Mathieu equation we have $z(t) = \cos^2 t$, $g(z) = 4z(1-z)$, so that Eq. (24) has the regular singular points $z = \zeta_1 = 0$, $z = \zeta_2 = 1$, both being the turning points. In addition, the equation has an irregular singularity at infinity. For the Lamé equation $z(t) = \mathrm{sn}^2(t, \varkappa)$, $g(z) = 4z(1-z)(1-\varkappa^2 z)$. Equation (24) then has the regular singular points $z = \zeta_1 = 0$, $z = \zeta_2 = 1$, $z = \varkappa^{-2} > 1$, first two of them being the turning points, and a regular singularity at infinity.

In general, it is easy to verify that the turning points $\zeta_{1,2}$ are regular singular points of Eq. (24), the exponents at each being 0 and 1/2. This implies that in the vicinity of each turning point ζ there exist two independent solutions of Eq. (24), $y^{(0)}(z;\zeta)$ and $y^{(1/2)}(z;\zeta)$, having asymptotics $1 + O(z-\zeta)$ and $(z-\zeta)^{1/2}[1 + O(z-\zeta)]$, correspondingly.

Now let us consider any one interval of monotonicity of the τ-periodic even function $z(t)$. Denote as $y_1(z)$ and $y_2(z)$ those two linearly independent solutions of Eq. (24) one of which coinsides, by Eq. (22), with the increasing solution (21), $X_+(t)$, and another with the decreasing one, $X_-(t)$, on the interval chosen. Since $\varphi(t)$ is either τ-periodic or τ-antiperiodic, the product $\varphi(t)\varphi(-t) = X_+X_- = y_1y_2 = w(z)$ is always τ-periodic even function defined on the whole t axis. Hence, at the endpoints of the intervals of monotonicity of $z(t)$, i.e., at $t_m = m\tau/2 (m = 0, \pm 1, \ldots)$, the derivative $[(X_+X_-)_t]_{t=t_m} = 0$ or, what is the same,

$$(w'\sqrt{g})_{z=\zeta_{1,2}} = 0. \tag{25}$$

In the vicinity of a turning point ζ the solutions y_1 and y_2 can be represented as linear combinations of the solutions $y^{(0)}$ and $y^{(1/2)}$. Consequently, the singularity $(z-\zeta)^{1/2}$ is the only one which the function $w(z)=y_1y_2$ might have. But its existence is in contradiction with Eq. (25), because $g'(\zeta)\neq 0$ and, hence, $g(z)_{z\to\zeta}\sim g'(\zeta)(z-\zeta)$. Therefore, the product y_1y_2 is analytic at $z=\zeta_{1,2}$. Recall now that the interval $[\zeta_1,\zeta_2]$ does not contain other singular points of Eq. (24) and the singular points are assumed to be isolated. We thus conclude that on the complex z plane there exists a vicinity of the interval $[\zeta_1,\zeta_2]$, i.e., an open domain $D\supset[\zeta_1,\zeta_2]$, in which y_1y_2 is an analytic function of z. In addition, it follows that y_1^2 and y_2^2 of necessity have singularities of the type $(z-\zeta)^{1/2}$ and, thus, cannot satisfy Eq. (25).

Now consider the case that one of the turning points or both are at infinity. This implies that at the corresponding instants t_m the functions $z(t)$ and $z_t(t)$ become unbounded, the latter changing the sign. Nevertheless, we assume that in the vicinities of t_m the function $h(z(t))$ in Eq. (20) is integrable and X is continuous, whence it follows that X_t and, therefore, w_t are also continuous. Hence, as before, $(w_t)_{t=t_m}=0$ due to evenness and periodicity, so that we arrive at Eq. (25) again, where $\zeta_1=-\infty$ and/or $\zeta_2=+\infty$.

It is easy to verify that the bilinear combinations y_1^2, y_1y_2, and y_2^2 constitute the fundamental system of solutions of the third-order differential equation

$$g(z)w''' + \tfrac{3}{2}g'(z)w'' + \left(\tfrac{1}{2}g''(z) + 4h(z)\right)w' + 2h'(z)w = 0. \tag{26}$$

Equation (25) is thus a common criterion for selection of the solution

$$w = y_1y_2 \tag{27}$$

from the set of solutions of Eq. (26). In the case that $z(t)$ is bounded, Eq. (25) is the equivalent to the requirement that a solution of Eq. (26) be analytic in D. If $z(t)$ is unbounded, Eq. (25) will give the boundary conditions at infinity which must be satisfied in solving Eq. (26). In this case $w(z)$ will be analytic in a vicinity D of one of the intervals $(-\infty,\zeta_2]$, $[\zeta_1,\infty)$, $(-\infty,\infty)$.

Thus, in a neighborhood of any one point $\zeta\in D$ we can write the expansions

$$\begin{pmatrix} w(z) \\ g(z) \\ h(z) \end{pmatrix} = \sum_{n=0}^{\infty} \begin{pmatrix} w_n \\ g_n \\ h_n \end{pmatrix} (z-\zeta)^n. \tag{28}$$

Substitution of (28) into Eq. (26) leads to the following set of equations for the coefficients:

$$m\sum_{n=1}^{m+2} n(m+n)g_{m-n+2}w_n + 4\sum_{n=0}^{m}(m+n)h_{m-n}w_n = 0 \tag{29}$$

$(m=1,2,\ldots)$. Thus for $m=1$ we have

$$6g_0w_3 + 3g_1w_2 + (g_2+4h_0)w_1 + 2h_1w_0 = 0. \tag{30}$$

Assuming $w(\zeta)\neq 0$, we normalize $w(z)$ by $w_0=1$. Then, at given w_1 and w_2 the remaining coefficients w_n are determined from Eqs. (29). The choice of w_1 and w_2 is not arbitrary but determined by Eq. (25). Thus, setting $\zeta=\zeta_1$ and, hence, $g_0=0$, we must choose w_1 in such a way that the series (28) for w (or its continuation) converges at the second turning point ζ_2, or satisfies the boundary condition at infinity (25) if $\zeta_2=+\infty$. For the Mathieu and Lamé equations this leads to the function $w(z)$ which is an integral one, for the latter it is a polynomial.[36] In these cases the domain D is evidently the z plane with $|z|<\infty$.

Let us suppose the function $w(z)$ (27) is found. Return now to Eqs. (20)–(24). Denote as W the Wronskian of the solutions (21),

$$X_+X_{-t} - X_{+t}X_- = W = \text{const}. \tag{31}$$

Setting

$$\begin{aligned} y_1 &= X_+, \quad y_2 = X_- \quad (z_t \geqslant 0), \\ y_1 &= X_-, \quad y_2 = X_+ \quad (z_t \leqslant 0), \end{aligned} \tag{32}$$

we then obtain

$$y_1 y_2' - y_1' y_2 = W/\sqrt{g}, \tag{33}$$

where $\sqrt{g} \geqslant 0$ is assumed. The system of equations (27) and (33) can be easily solved, which gives

$$y_{1,2}^2 = \exp \int \frac{f_\mp}{w\sqrt{g}} \mathrm{d}z, \tag{34}$$

where

$$f_\pm = w'\sqrt{g} \pm W. \tag{35}$$

Now let us insert $y_{1,2}$ (34) back into Eq. (24). We obtain

$$2gww'' + g'ww' - gw'^2 + 4hw^2 + W^2 = 0. \tag{36}$$

By this formula one can find the constant W^2 from a knowledge of $w(z)$ in a vicinity of any point z. Thus, calculating (36) at any one finite turning point ζ we obtain [in terms of expansions (28) with normalization $w_0 = 1$]

$$W^2 = -4h_0 - g_1 w_1. \tag{37}$$

Alternatively, one can take zeros z_i of $w(z)$. [The functions $g(z)$ and $w(z)$ do not have common zeros because otherwise the Wronskian (31) would be zero.] Then we find

$$W^2 = g(z_i)w'^2(z_i). \tag{38}$$

The requirement for positivity of W^2 determines the values of parameters of Eq. (20) (resonance zones) for which the resonant solutions exist.

Let us construct these solutions. Consider the intervals of monotonicity $t_1 \leqslant t \leqslant t_2 (z_t \geqslant 0)$, $t_2 \leqslant t \leqslant t_3 (z_t \leqslant 0)$, etc. According to (32) and (34) we can write

$$\begin{aligned} X_\pm^2(t)_{t_1 \leqslant t \leqslant t_2} &= X_\pm^2(t_1) \exp \int_{\zeta_1}^{z} \frac{f_\mp}{w\sqrt{g}} \mathrm{d}z, \\ X_\pm^2(t)_{t_2 \leqslant t \leqslant t_3} &= X_\pm^2(t_2) \exp \int_{\zeta_2}^{z} \frac{f_\pm}{w\sqrt{g}} \mathrm{d}z, \text{etc}. \end{aligned} \tag{39}$$

To find the characteristic exponent μ consider, e.g., the growing solution $X_+(t)$. Setting $t = t_2$, $z(t_2) = \zeta_2$ in the first equation of (39) and $t = t_3$, $z(t_3) = \zeta_1$ in the second one, we can express $X_+^2(t_3)$ through $X_+^2(t_1)$. Using Eq. (21) and taking into account that $t_3 = t_1 + \tau$, $\varphi(t+\tau) = \pm\varphi(t)$, we thus obtain

$$\mu = -\frac{W}{\tau} \int_{\zeta_1}^{\zeta_2} \frac{\mathrm{d}z}{w\sqrt{g}}. \tag{40}$$

Recall that τ is the period of $z(t)$, the constant W is determined from Eq. (37) or Eq. (38), its sign being taken opposite to that of the integral in (40) to provide for positivity of μ. Since $w(z)$ has

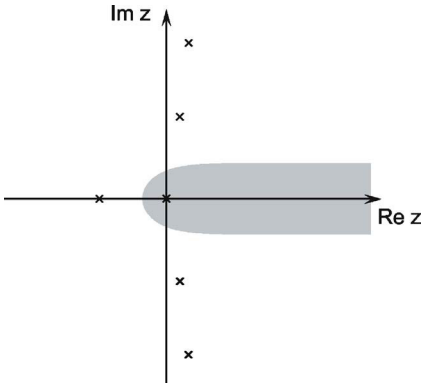

FIG. 3. The layout of zeros of $g(z)$ (43) on the complex z plane. The vicinity D (shaded) of the interval $[0,\infty)$ belongs to the domain of analyticity of $w(z)$.

zeros, the integrals in Eqs. (39) and (40) are understood as their principal values. Formula (40) is a simple generalization of the ones used previously in Refs. 37–40.

B. Evaluation of the characteristic exponent

Let us return to Eq. (18). It can be written in the form of Eq. (20) if we set

$$z(t) = -\ln(a/a_{\max})^2, \quad z(0) = 0, \tag{41}$$

$$h(z) = E - 3 + \omega_0^2 + z. \tag{42}$$

Equation (7) then immediately gives

$$g(z) = 4[\omega_0^2(e^z - 1) - z]. \tag{43}$$

Zeros of this function are shown in Fig. 3. Since $\xi(t)=a/a_{\max}$ oscillates with the period T in the interval $-1\leqslant\xi\leqslant 1$ [see Eqs. (7)–(12)], the function $z(t)$ (41) oscillates with the period $\tau=T/2$ between the turning points $\zeta_1=0$ and $\zeta_2=+\infty$. To calculate the characteristic exponent by the formula (40) we need to know the function $w(z)$ which is the solution of Eq. (26) with boundary conditions (25). Unfortunately, for given $h(z)$ (42) and $g(z)$ (43), Eq. (26) cannot be solved analytically. We solve it numerically[33] for various values of the parameters E and $\omega_0^2=1-\ln a_{\max}^2$. Doing so, we use the conditions (25) in the following way. As discussed above, the fulfillment of (25) at a finite turning point means analyticity of $w(z)$ in some vicinity of this point. Therefore, we can use the expansions (28) setting there $\zeta=\zeta_1=0$, $g_0=0$, $g_1=4(\omega_0^2-1)$, $g_n=4\omega_0^2/n!(n=2,3,\ldots)$, $h_0=E+\omega_0^2-3$, $h_1=1$. Equation (30) then gives

$$w_2 = -\frac{1 + (2E + 3\omega_0^2 - 6)w_1}{6(\omega_0^2 - 1)}. \tag{44}$$

We thus solve Eq. (26) with the following conditions at $z=0$: $w(0)=1$, $w'(0)=w_1$, $w''(0)=2w_2$. Given values of E and ω_0^2, we choose w_1 so as to satisfy the condition (25) at infinity,

$$(w'\sqrt{g})_{z\to+\infty} \to 0. \tag{45}$$

At the same time, since μ is assumed to be real, the values of E, ω_0^2, and w_1 must provide for positivity of W^2,

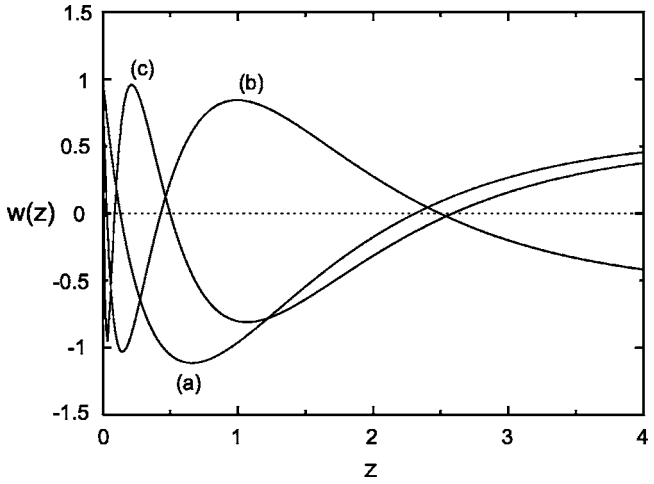

FIG. 4. Behavior of $w(z)$ for $E=4$ in the different resonance zones: (a) zone Z_1, $a^2_{\max}=0.5625$, (b) zone Z_2, $a^2_{\max}=0.9025$, (c) zone Z_3, $a^2_{\max}=0.9598$. The values of $a^2_{\max}$ chosen correspond to the centers of zones where μ achieves its maxima. One can see that the number of zeros of $w(z)$ is unit above the number of a zone.

$$W^2 = 4[3 - E - \omega_0^2 - (\omega_0^2 - 1)w_1] > 0 \tag{46}$$

[see Eqs. (37) and (40)]. Conditions (45) and (46) determine the resonance zones in the space of parameters E and ω_0^2 (or $a^2_{\max}$). Hereinafter the zones will be referred to as Z_j and numbered sequentially as E grows (with $a^2_{\max}$ fixed) starting with $j=-1$ in the region $E<0$. Figure 4 shows the solutions $w(z)$ for zones Z_1, Z_2, and Z_3 lying in the region $E>2$. Now, knowing $w(z)$, we can calculate the integral in (40). Because $w(z)$ has zeros, we first transform the integrand with the help of Eq. (36) extracting the total derivative. Owing to the condition (45), the latter does not contribute to the principal value of the integral, while the remaining terms give

$$\int_0^\infty \frac{dz}{w\sqrt{g}} = -\frac{1}{2W^2}\int_0^\infty [\sqrt{g}(w'\sqrt{g})' \ln w^2 + 8hw]\frac{dz}{\sqrt{g}}. \tag{47}$$

The integrand on the right-hand side of Eq. (47) is more convenient for numerical integration because its singularities are all integrable. We perform the integration in (47), calculate W^2 by the formula (46), and find the period $T=2\tau$ by integration of Eq. (7). These procedures are carried out numerically for a set of grid points in every resonance zone. In this way from (40) we obtain the characteristic exponent μ as a function of E and $a^2_{\max}$.

To check this result we derive $\mu(E, a^2_{\max})$ directly from analysis of numerical solutions of Eq. (18). Examples of these solutions for resonance zones Z_1, Z_2, and Z_3 are shown in Fig. 5. The growth of the amplitude with time is clearly seen. The function $\mu(E, a^2_{\max})$ so derived is found to be fully coincident with the one obtained by the formula (40).

The resulting stability-instability chart is presented in Fig. 6. Figure 6(a) shows the region $E>2$. There is an infinite series of narrow resonance zones $Z_1, Z_2, Z_3, \ldots$, the first one having the highest magnitude (≈ 0.08 at the maximum). All these zones originate from the point $E=2$, $a^2_{\max}=1$ at which $\mu=0$ [see Eqs. (40) and (46)]. In the region $E\leqslant 2$ we have two zones, Z_0 and Z_{-1}, lying in the ranges $0<E<2$ and $E<0$, correspondingly. Since in these zones the values of μ proved to be much greater than in $Z_1, Z_2, \ldots$, we depict the surface $\mu(E, a^2_{\max})$ for this region separately, in Fig. 6(b).

C. Spatial structure of the perturbation

Consider now Eq. (19). It has the form of the Schrödinger equation for a quantum particle of the energy E moving in the potential $-\ln u^2$. Since the potential tends to $+\infty$ with growing r [as r^2,

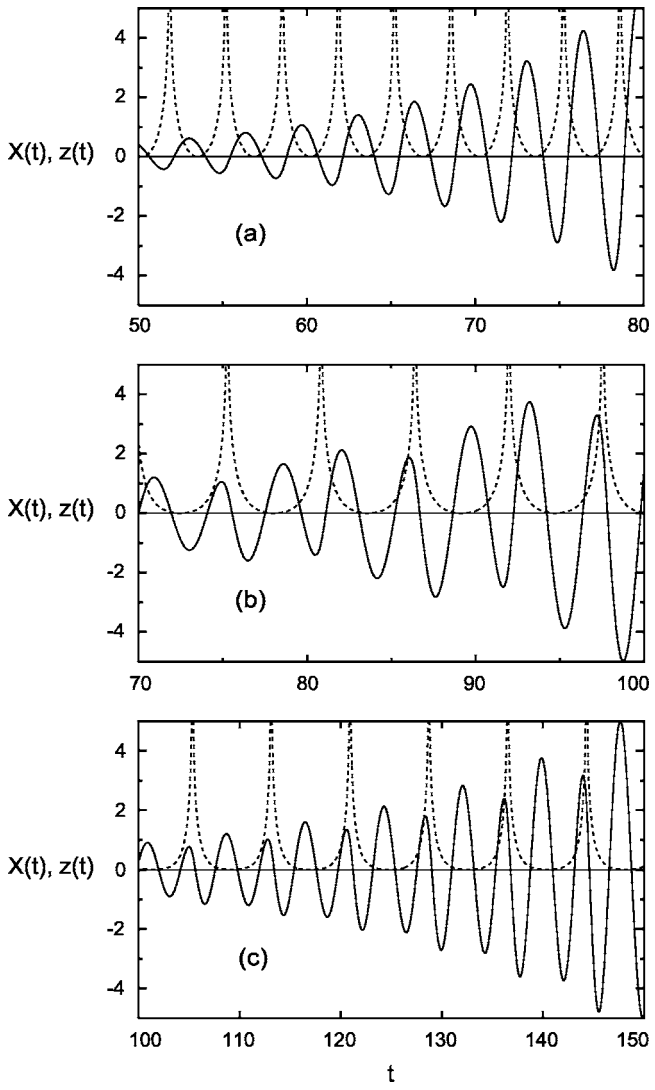

FIG. 5. Resonant solutions of Eq. (18), $X(t)\sim X_+(t)=\varphi(t)e^{\mu t}$, (solid lines) and the function $z(t)=-\ln(a/a_{\max})^2$ (dashed lines): (a) zone Z_1, (b) zone Z_2, (c) zone Z_3. The initial conditions are: $a(0)=a_{\max}$, $a_t(0)=0$, $X_t(0)=0$, $X(t)$ is normalized in a proper way. The values of E and $a_{\max}^2$ in each zone are the same as in Fig. 4. It is seen that $\varphi(t)$ is τ-periodic in Z_1, τ-antiperiodic in Z_2, τ-periodic in Z_3, and so on, in accordance with the solutions (39) [see Eqs. (35) and (38) and Fig. 4].

see Eqs. (13) and (14)], the energy spectrum is discrete, $E=E_n$, and the corresponding eigenfunctions $\Psi_n(\mathbf{r})$ are all localized. In the case of the nodeless pulson (13) we have the isotropic harmonic oscillator. Its eigenfunctions are well known (see, e.g., Ref. 41). We write them as follows:

$$\Psi_n(\mathbf{r})=\sum_{l=0}^{n}[1+(-1)^{n-l}]R_{nl}(r)Y_l(\theta,\varphi), \tag{48}$$

$$R_{nl}(r)=r^l e^{-r^2/2}\Phi\left(-\frac{n-l}{2},l+\frac{3}{2},r^2\right), \tag{49}$$

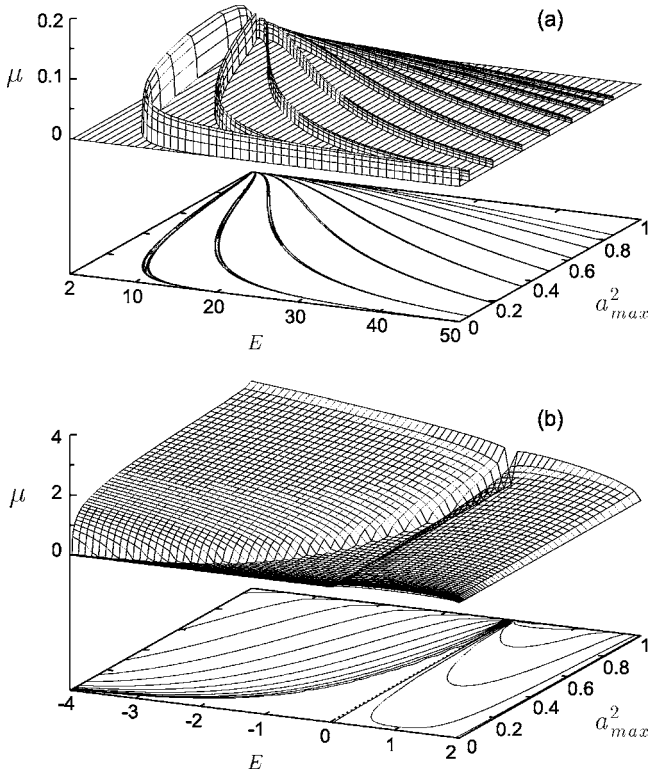

FIG. 6. The stability-instability chart: (a) $E>2$, first 10 zones are shown, (b) $E\leqslant 2$.

$$Y_l(\theta,\varphi)=\sum_{m=-l}^{l} c_{l,m}P_l^{|m|}(\cos\theta)e^{im\varphi}. \tag{50}$$

Here $\Phi(\alpha,\gamma,x)$ is the Kummer function, $P_\nu^\mu(x)$ are the associated Legendre functions, $c_{l,m}$ are constants, $c_{l,-m}=c_{l,m}^*$. The energy spectrum is given by

$$E=E_n=2n \quad (n=0,1,2,\dots). \tag{51}$$

(Our energy levels are shifted with respect to the conventional ones since the minimum of the potential $-\ln u_0^2$ is -3.)

In the case of the nodal pulsons the picture becomes more complicated due to the loss of the orbital degeneracy. The corresponding eigenfunctions and eigenvalues can be calculated only numerically. As an example, in Fig. 7 is shown the energy spectrum for perturbations of the one-nodal pulson.

Note that there always exist the eigenvalues $E=0$, $l=0$ and the corresponding eigenfunction $\Psi_0(r)\propto u(r)$. This fact immediately follows from the comparison of Eqs. (6) and (19). The corresponding $X_0(t)$ in $\eta(t,\mathbf{r})$ is an oscillating function with the amplitude growing linearly with time. It is easy to see, however, that this mode is physically meaningless. Indeed, it will formally appear if we perturb the pulson by a small variation of its amplitude $a_{\max}$ but not the form $u(r)$. Due to nonlinearity, this results in a pulson with slightly shifted frequency. Then the difference of the perturbed and unperturbed pulsons, i.e., $\eta(t,r)$, will have the form of beats generated by two oscillations with close frequencies and the same profile $u(r)$. The function $X_0(t)$ approximates the initial, linearly growing part of a beat. We exclude this mode from the subsequent consideration, since it belongs to the class of perturbations that conserve a pulson as a whole. Next, for the nodal pulsons only, there is a mode with $E=0$, $l=1$ (see Fig. 7). Since this mode cannot grow faster than linearly in time, we also do not take it into account. Further, we should exclude the mode resulting

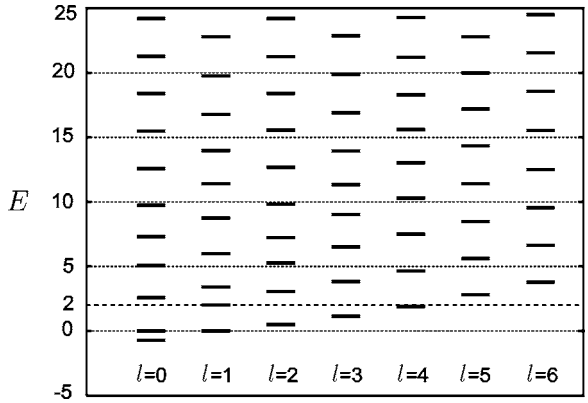

FIG. 7. The energy levels for the perturbations with different orbital numbers l. The case of the one-nodal pulson.

from a small translation of the pulson. The corresponding eigenfunction is proportional to $\mathbf{n}\nabla u$, where $\mathbf{n}$ is a displacement vector. Using Eqs. (6) and (19) one can easily show that this mode corresponds to $E=2$, $l=1$. Thus the resulting perturbation is written as

$$\eta(t,\mathbf{r}) = \sum_n X_n(t)\Psi_n(\mathbf{r}), \tag{52}$$

where X_n is a solution of Eq. (18) with $E=E_n$, $E_n \neq 0,2$. If E_n and $a^2_{\max}$ are in a resonance zone, $X_n(t)$ will be represented as a linear combination of the solutions (21) and, hence, will grow with time as $e^{\mu(E_n,a^2_{\max})t}$.

D. Instability of the pulsons

The arrangement of the resonance zones on the $(E,a^2_{\max})$ plane indicates that for any spectrum E_n there always exist the ranges of $a^2_{\max}$ where pulsons are unstable. But do the values of $a^2_{\max}$ exist for which the pulsons are stable? To answer this question let us return to the surface $\mu(E,a^2_{\max})$ depicted in Fig. 6. Take, at first, the spectrum for the nodeless pulson. We choose the sections $\mu_n(a^2_{\max})$ of the surface $\mu(E,a^2_{\max})$ by $E=2n$ and project them on the $(\mu,a^2_{\max})$ plane. As a result, the pattern shown in Fig. 8(a) emerges. It is clearly seen the tendency to the total filling of the interval $0<a^2_{\max}<1$ by the resonant peaks as the successively higher energy levels are accounted for. This implies that for any given $a^2_{\max}$ there always exists an unstable mode with $\mu=\mu_n(a^2_{\max})$, i.e., strictly speaking, all nodeless pulsons are unstable. On the other hand, the figure shows that there are domains of $a^2_{\max}$ where the peaks are very small. These domains are the gaps between the main peaks originated from the low-energy cross sections of the surface $\mu(E,a^2_{\max})$ over a few first zones. In the gaps the exponent μ is small, so that the corresponding pulsons are long-lived. For example, in Ref. 33 we observed numerically the nodeless pulson with $a^2_{\max}=0.49$ that conserved its coherency against the radially symmetric perturbations over the course of several hundreds of periods.

Further, the above projective procedure is performed using the spectrum of the one-nodal pulson (Fig. 7). The main contribution here is made by the sections with the energies $E_n=-0.7142$ ($l=0$), 0.4833 ($l=2$), 1.1222 ($l=3$), and 1.8996 ($l=4$) falling into zones Z_{-1} and Z_0, the projections of the first and the third sections overlapping the other ones. The result is presented in Fig. 8(b). We see that $a^2_{\max}$ axis is totally full. Thus, the one-nodal pulson has neither stability nor even quasistability domains. It seems likely that things will get worse, not better, if one goes to the multinodal pulsons. We thus conclude that, strictly speaking, all pulsons of the model considered are unstable. But nodeless pulsons can be quasistable in narrow ranges of amplitudes. It is the

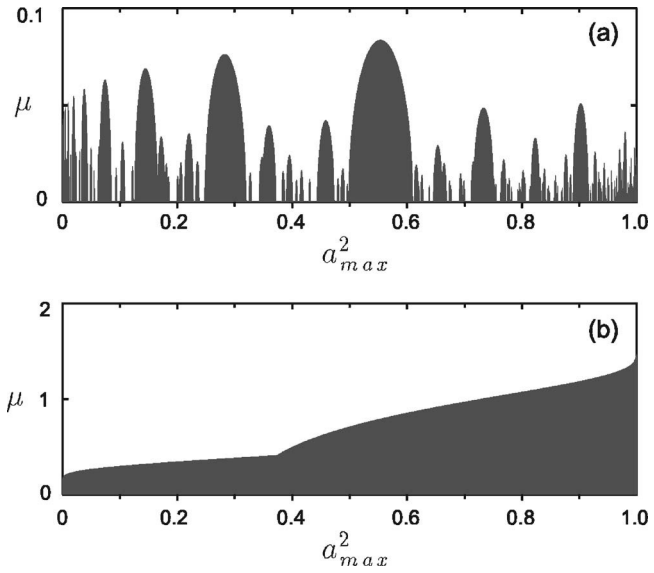

FIG. 8. Superposition of the sections $\mu_n(a^2_{\max})$ of the surface $\mu(E,a^2_{\max})$: (a) the nodeless pulson, $E_n=4,6,8,\ldots,50$, ($n=2,3,4,\ldots,25$), (b) the one-nodal pulson, $E_n=-0.7142,0.4833,1.1222,1.8996,\ldots$.

long-lived pulsons that can be of astrophysical and cosmological interest. If the dark matter consists of scalar particles, such pulsons will be realistic candidates for the dark matter objects having oscillating density.[42]

E. On the instability of the Affleck-Dine-type condensate

The obtained stability-instability chart turns out to be appropriate for the stability analysis of the nonlocalized coherent states as well. As an example, we consider a uniformly distributed background $\phi_0(t)$, a scalar condensate, oscillating around the minimum of the potential (4) at $\phi=0$. This state can be formally obtained from Eq. (1) if we set there $u(\mathbf{r})\equiv 1$. We thus assume that $\phi_0(t)$ obeys Eq. (5). Taking the perturbed state $\phi=\phi_0(t)+\eta(t,\mathbf{r})$, in the linear approximation from Eqs. (2) and (4) we readily obtain

$$A_{tt}+(k^2-2-\ln\phi_0^2)A=0, \tag{53}$$

where $A(t,\mathbf{k})$ is the Fourier amplitude of the perturbation, and $k=|\mathbf{k}|$. It is seen that the real and imaginary parts of this equation have the form of Eq. (20) with $h(z)$ given by Eq. (42), $z=-\ln(\phi_0/\phi_{0\,\max})^2$, $\omega_0^2=1-\ln\phi_{0\max}^2$, and $E=k^2$. Returning to the stability-instability chart (Fig. 6) we note that in the region $E\geqslant 0$ maximal values of μ are attained in the zone Z_0 for which $0<E<2$. Interestingly, this band exactly coincides with the one obtained in Ref. 20 for the power-law potential approximating (3) when $\lambda\ll 1$. In the interior of Z_0 the exponent μ depends almost not at all on the amplitude of the condensate oscillations and is a sufficiently smooth function of k^2 with a maximum at $k^2=k_0^2\approx 1$ where $\mu\approx 0.5$. Therefore, if the initial power spectrum $|A(0,\mathbf{k})|^2$ lies in the region $0\lesssim|\mathbf{k}|\lesssim\sqrt{2}$ and, in addition, its characteristic width along $\mathbf{k}$ is small, $\Delta k\ll\sqrt{2}$, then the growth of the perturbation amplitude will not be accompanied by significant changes in the structure of the perturbation. The limiting case of such perturbations is a harmonic wave. Otherwise, if $\Delta k\gtrsim\sqrt{2}$, the shape of the power spectrum will vary with time so that a maximum will appear at $k_0\approx 1$. As a result, the effective width of the spectrum will become smaller, $\Delta k\lesssim 1$. In this case, if the initial spectrum is sufficiently isotropic in $\mathbf{k}$ space, the parametric amplification of the perturbations will result in the emergence of the localized field configurations of the characteristic size $\Delta r\sim 1/\Delta k\gtrsim 1$ that agrees with the radius of the gausson (see Sec. II). At this scale the field practically does not undergo spatial oscillations since the corresponding wavelength

$2\pi/k_0 \gtrsim 1$. We thus expect that at the nonlinear stage these configurations will turn into the nodeless pulsons. Their period will be equal to the period of the condensate oscillations since in the zone Z_0 the parametric amplification proceeds at the basic frequency. Gradually, the energy of the oscillating condensate will go to ensemble of the arising pulsons, this process resulting in the damping of the background oscillations. As to the pulsons themselves, they can be long-lived or short-lived depending on their amplitudes, in accordance with the results of the preceding subsection.

Note, that numerical simulations performed for the complex version of the model (2) and (3) have shown the fragmentation of both the rotating[18,19] and oscillating[20] Affleck-Dine condensate. The localized configurations arising in the condensate have been identified with Q-balls. We belive, however, that the configurations observed in the oscillating condensate are in fact the complex pulsons (see Sec. IV), rather than the usual Q-balls. This possibility was early discussed in Ref. 15 where an attempt to simulate the complex pulson has been made.

The resonant exitation of the pulsons was also observed in the two-vacuum $\phi^4-\phi^6$ model within a regularly oscillating background[39] and in the ϕ^4 model within an initially thermalized background.[43] Note that in two-vacuum models the pulsons can play the role of nuclei of a new phase. In Ref. 39 the general suggestion has been made that the parametric resonance can underlie the mechanism responsible for the first-order phase transitions in nonlinear nondissipative systems. This conjecture turns out to be in agreement with recent results of Ref. 44 where the resonant nucleation within the thermalized background have been numerically observed in the $\phi^3-\phi^4$ model. Note, in addition, that the dynamical nucleation can also take place in the nonlinear Schrödinger equation.[45]

IV. CONCLUDING REMARKS

In this paper we have examined only the linear stage of instability at which small deformations of the pulson's shape result in loss of the coherence. There is numerical evidence that in time the growth of the perturbations becomes saturated due to nonlinear effects.[33] We thus suggest that in the model considered the pulsons, while unstable, remain well localized objects with no tendency for spreading or collapsing.

Further, we dealt with a real scalar field. It would be interesting to perform the similar analysis for a complex scalar field too. It is believed that the existence of the scalar charge can stabilize a field lump. For Q-balls this fact is well established (so-called Q-theorem[2,4,27]). In contrast, for the complex pulsons this is an open question. As it was shown in Refs. 28 and 29, the field equation (2) with $U'=-\phi\ln(\phi\phi^*)$ admits the exact pulson solutions of the form $\phi_0(t,r)=a(t)u(r)e^{i\theta(t)}$, where $a(t)$, $u(r)$, and $\theta(t)$ are real. The function $u(r)$ satisfies Eq. (6) as before, while $a(t)$ oscillates with a period T in accordance with the equation

$$a_{tt}=-\frac{d}{da}\left[\frac{1}{2}a^2(1-\ln a^2)+\frac{q^2}{2a^2}\right], \tag{54}$$

where q is a real constant, $q^2<(2e)^{-1}$, and $\theta_t=qa^{-2}$. The constant q is proportional to the charge of the scalar field. In contrast to Eq. (5), the potential in the square brackets of Eq. (54) prevents $a(t)$ from being zero. Without loss of generality one may assume $a(t)$ positive, so that the oscillations occur arround the minimum of the potential at $a=a_0$, where a_0 is the least positive root of the equation $a^4\ln a^2=-q^2$. If a is at rest in this minimum, then $\theta(t)=qa_0^{-2}t+\theta(0)$, and we have the standard Q-ball. Physically, Eq. (54) describes the motion of a mechanical particle with an angular momentum q in the potential $(a^2/2)(1-\ln a^2)$. The condition for its trajectory to be closed is $\theta(T)-\theta(0)=2\pi m/n$, where m and n are arbitrary integers (see, e.g., Ref. 46). In fact, it relates the energy of the particle and its angular momentum whereby such trajectories exist. In our case this means periodicity of the solution $\phi_0(t,r)$ with the period nT. Obviously, there is an infinity of such solutions. Taking $\phi_0(t,r)$ and considering the partial perturbation $\eta\propto X(t)\Psi(\mathbf{r})$ one can find that the function $\Psi(\mathbf{r})$, assumed to be real, satisfies Eq. (19) as before, while $X(t)$ obeys the equation

$$X_{tt} + (E - 1 - \ln a^2)X = e^{2i\theta}X^*, \tag{55}$$

where E is a real constant. This equation can be represented as a system of four real first-order equations with periodic coefficients of the periods T and nT. It is significant that, since $a(t) \neq 0$, these coefficients are bounded in time, so that one can attempt to estimate the characteristic exponent of the system using the standard methods.[47]

Also, it would be interesting to examine stability of a self-gravitating pulson. Hopefully, gravitation can expand the domains of (quasi)stability, as it is the case for Q-balls.[4] These are possible subjects of our future work.

In the present paper we have investigated stability of both the coherent localized states (pulsons) and nonlocalized states (uniformly oscillating scalar condensate) of the real scalar field. Our main analytical result is the generalization of the Lindemann-Stieltjes method to the case that the periodic coefficient in the Hill equation is unbounded in time. Our main numerical result is the stability-instability chart with the values of characteristic exponent calculated in the resonance zones. Using this chart we have found the gaps in the set of the pulson amplitude values in which the real nodeless pulsons conserve the coherency for an extremely long time. Also, considering the oscillating scalar condensate, we have detemined the wavelength of the most unstable mode. This wavelength turned out to be equal to the characteristic size of the nodeless pulson. We thus suggest the pulsons can be formed due to resonant fragmentation of the scalar condensate. These are our main physical results.

ACKNOWLEDGMENTS

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Integrability from an Abelian subgroup of the diffeomorphisms group

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It has been known for some time that for a large class of nonlinear field theories in Minkowski space with two-dimensional target space the complex eikonal equation defines integrable submodels with infinitely many conservation laws. These conservation laws are related to the area-preserving diffeomorphisms on target space. Here we demonstrate that for all these theories there exists, in fact, a weaker integrability condition which again defines submodels with infinitely many conservation laws. These conservation laws will be related to an Abelian subgroup of the group of area-preserving diffeomorphisms. As this weaker integrability condition is much easier to fulfill, it should be useful in the study of those nonlinear field theories. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168400]

I. INTRODUCTION

Recently there has been rising interest in nonlinear field theories which allow for the existence of knotlike solitons. The probably best known of these models, the Faddeev-Niemi model,[1,2] for example, finds some applications in condensed matter physics.[3,4] Further, some versions of it are discussed as possible candidates for a low-energy effective theory of Yang-Mills theory.[5,6] In addition, there is some intrinsical mathematical interest in theories with knot solitons. Generally, these models are described by a complex field $u:\mathbb{R}^3\times\mathbb{R}\to\mathcal{M}:(\vec{x},t)\to u(\vec{x},t)$ where $\mathcal{M}$ is a two-dimensional target space manifold and u plays the role of a complex coordinate on this manifold.

The Faddeev-Niemi model has the two-sphere as target space and is given by the Lagrangian density

$$\mathcal{L}_{\mathrm{FN}}=\mathcal{L}_2-\lambda\mathcal{L}_4, \tag{1}$$

where λ is a dimensionful coupling constant, $\mathcal{L}_2$ is

$$\mathcal{L}_2=4\frac{\partial_\mu u\partial^\mu\overline{u}}{(1+u\overline{u})^2}, \tag{2}$$

and $\mathcal{L}_4$ is

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$$\mathcal{L}_4 = 4\frac{(\partial^\mu u \partial_\mu \overline{u})^2 - (\partial^\mu u \partial_\mu u)(\partial^\nu \overline{u} \partial_\nu \overline{u})}{(1+u\overline{u})^4}. \tag{3}$$

Two more models which support solitons and can be constructed from the two Lagrangian densities $\mathcal{L}_2$ and $\mathcal{L}_4$ separately, are the AFZ (Aratyn, Ferreira, and Zimerman) model[7,8]

$$\mathcal{L}_{\mathrm{AFZ}} = -(\mathcal{L}_4)^{\frac{3}{4}} \tag{4}$$

and the Nicole model[9]

$$\mathcal{L}_{\mathrm{Ni}} = (\mathcal{L}_2)^{\frac{3}{2}}. \tag{5}$$

Here the noninteger powers for the Lagrangian densities have been chosen appropriately to avoid Derrick's theorem. More models together with some explicit soliton solutions have been constructed, e.g., in Refs. 10 and 11.

Among these models the AFZ model is special, because it has infinitely many symmetries and, as a consequence, infinitely many conservation laws.[12,13] Further, infinitely many soliton solutions can be found by an explicit integration for a special ansatz (separation of variables in toroidal coordinates), which realizes the concept of integrability in a rather explicit way. The other models do not have infinitely many symmetries, but, nevertheless, "integrable" subsectors with infinitely many conserved currents can be defined.[14,15] The condition which defines these integrable subsectors is the complex eikonal equation

$$u^\mu u_\mu = 0, \tag{6}$$

where $u_\mu \equiv \partial_\mu u$. The infinitely many conserved currents J^G_μ (defined in Sec. III) for these submodels are parametrized by an arbitrary, real function $G(u,\overline{u})$ and are, in fact, just the Noether currents for the area-preserving diffeomorphisms on target space.[12,16] [Some more ("generalized") integrability conditions, which, however, depend on the Lagrangian, have been introduced in Refs. 17 and 16.]

Here we want to demonstrate that there exists, instead of the complex eikonal equation, a weaker condition which again defines submodels with infinitely many conservation laws. Further, these integrable submodels can be defined for all Lagrangians for which the complex eikonal equation defines integrable submodels. Explicitly this condition reads

$$\overline{u}^2 u_\mu^2 - u^2 \overline{u}_\mu^2 = 0. \tag{7}$$

The infinitely many conserved currents J^G_μ for these submodels are as above, but with the additional restriction that now $G = G(u\overline{u})$. They are the Noether currents for an Abelian subgroup of the group of area-preserving diffeomorphisms on target space.

The meaning of condition (7) becomes especially transparent when we reexpress u in terms of its modulus and phase like

$$u = \exp(\Sigma + i\phi). \tag{8}$$

Then the complex eikonal equation is equivalent to the two real equations

$$\Sigma_\mu^2 = \phi_\mu^2 \tag{9}$$

and

$$\Sigma^\mu \phi_\mu = 0, \tag{10}$$

whereas the weaker condition (7) becomes Eq. (10) alone or, for time-independent u,

$$(\nabla\Sigma)\cdot(\nabla\phi) = 0. \tag{11}$$

The integrability condition (7) might be quite useful, for instance, in the case of the Faddeev-Niemi model. For the Faddeev-Niemi model soliton solutions are only known numerically up to now.[2,18–21] No solutions which solve the complex eikonal equation, as well, are known and there are even arguments against the existence of such solutions. On the other hand, it is perfectly possible that there exist solutions which solve the weaker integrability condition (7) and that this condition helps in the search for analytic solutions.

The condition (7) is in fact quite weak, i.e., quite easy to fulfill. For instance, many commonly used separation-of-variable ansätze, like the ansatz $u=\rho(r,\theta)e^{im\varphi}$ in spherical polar coordinates, or the ansatz $u=\rho(\eta)e^{i(m\varphi+n\xi)}$ in toroidal coordinates (both ρ are real), identically obey condition (7) due to the orthogonality of the corresponding basis vectors. On the other hand, for the eikonal equation these ansätze lead to a differential equation for the profile function ρ which only allows for very specific solutions, therefore providing a much stronger restriction, see, e.g., Refs. 22 and 23. In short, condition (7) applies to a rather large class of field configurations and, therefore, we believe that it will be useful for the study of nonlinear field theories with a two-dimensional target space, like the Faddeev-Niemi or the Nicole model, or the other models mentioned above.

In Sec. II we discuss the algebra of generators of area-preserving diffeomorphisms and their Abelian subalgebra on a two-dimensional manifold. Further we define the Noether charges corresponding to these generators. In Sec. III we show that condition (7) defines subsectors with infinitely many conservation laws for a very general class of Lagrangians (which cover all Lagrangians given above). Further we demonstrate that the corresponding conserved currents are indeed the Noether currents of the Abelian area-preserving diffeomorphisms.

II. ABELIAN AREA-PRESERVING DIFFEOMORPHISMS

Here we describe area-preserving diffeomorphisms and an Abelian subgroup contained within them for a two-dimensional manifold $\mathcal{M}$ which later on will be identified with the target space of the nonlinear field theories which we want to study. Concretely, we choose real coordinates (ξ^1,ξ^2) or the complex coordinate $u=\xi^1+i\xi^2$ and allow for the class of metrics

$$ds^2 = g(a)[(d\xi^1)^2+(d\xi^2)^2] = g(a)du\,d\overline{u}, \tag{12}$$

where

$$a = (\xi^1)^2+(\xi^2)^2 = u\overline{u} \tag{13}$$

and

$$du\,d\overline{u} \equiv \tfrac{1}{2}(du\otimes d\overline{u}+d\overline{u}\otimes du), \tag{14}$$

$$du\wedge d\overline{u} \equiv \tfrac{1}{2}(du\otimes d\overline{u}-d\overline{u}\otimes du). \tag{15}$$

The corresponding area two-form is

$$\Omega \equiv g(a)d\xi^1\wedge d\xi^2 = \frac{g(a)}{2i}d\overline{u}\wedge du. \tag{16}$$

The choice of conformally flat metrics does not mean a restriction in two dimensions, because any metric on a two-dimensional manifold may be chosen conformally flat by an appropriate choice of coordinates. On the other hand, the functional dependence for the metric function $g=g(a)$ is a restriction, which is however sufficiently general for our purposes. In principle, one could skip this restriction, which would just complicate the subsequent discussion without adding substantial new structures (see the remark at the end of Sec. III).

An area-preserving diffeomorphism is a transformation $u\to v(u,\overline{u})$ such that the area form (16) remains invariant (see also Refs. 12, 13, and 15),

$$\Omega \equiv \frac{1}{2i} g(u\overline{u}) \mathrm{d}\overline{u} \wedge \mathrm{d}u = \frac{1}{2i} g(v\overline{v}) \mathrm{d}\overline{v} \wedge \mathrm{d}v. \tag{17}$$

For infinitesimal transformations $v = u + \epsilon$ it is easy to see that the condition of invariance of the area form leads to

$$\epsilon_u + \overline{\epsilon_{\overline{u}}} = -\frac{g'}{g}(\overline{u}\overline{\epsilon} + u\overline{\epsilon}), \tag{18}$$

where $\epsilon_u \equiv \partial_u \epsilon$ and $g' \equiv \partial_a g(a)$. Defining

$$\epsilon = g^{-1}\delta, \quad \delta = F_{\overline{u}} \tag{19}$$

the above equation for ϵ simplifies to

$$\partial_u \partial_{\overline{u}} (F + \overline{F}) = 0. \tag{20}$$

The general solution to this equation is

$$F + \overline{F} = \zeta(u) + \overline{\zeta(\overline{u})} \tag{21}$$

but for our purposes an imaginary F,

$$F + \overline{F} = 0, \tag{22}$$

serves as a general solution, because for any F which solves (21) there exists a $\widetilde{F} = F - \zeta(u)$ which is imaginary and leads to the same $\delta = F_{\overline{u}} = \widetilde{F}_{\overline{u}}$, i.e., to the same area-preserving diffeomorphism.

Introducing the real function G via $F = iG$, the area-preserving diffeomorphisms are therefore generated by the vector fields

$$v^G = ig^{-1}(G_{\overline{u}}\partial_u - G_u \partial_{\overline{u}}) \tag{23}$$

which obey the Lie algebra

$$[v^{G_1}, v^{G_2}] = v^{G_3}, \quad G_3 = ig^{-1}(G_{1,\overline{u}} G_{2,u} - G_{1,u} G_{2,\overline{u}}). \tag{24}$$

Now we want to find an Abelian subalgebra of this Lie algebra of vector fields. It is easy to see that the commutator (24) vanishes if both $G_i, i = 1, 2$ are of the form

$$G = G(u\overline{u}). \tag{25}$$

In addition, this gives a maximal Abelian subalgebra in the sense that if $G_1 = G_1(u\overline{u})$ then $G_3 = 0 \Leftrightarrow G_2 = G_2(u\overline{u})$. These issues may be seen especially easily by introducing the modulus and phase of u, $u = \sqrt{a}e^{i\phi}$. Then the vector field v^G for $G = G(a)$ is

$$v^G = H(a)\partial_\phi, \quad H(a) \equiv g^{-1}G' \tag{26}$$

and the above statements follow immediately. In short, the G of the form $G = G(u\overline{u})$ generate a maximal Abelian subgroup of the group of area-preserving diffeomorphisms.

Due to the Abelian nature of this subgroup it is trivial to integrate the infinitesimal transformations to reach finite ones. The result is that the transformations

$$u \to e^{i\Lambda(u\overline{u})} u \tag{27}$$

form a subgroup of Abelian area-preserving diffeomorphisms, where $\Lambda = \Lambda(a)$ is an arbitrary function of its argument. In fact, these transformations leave invariant the two terms $g(a)$ and $\mathrm{d}\overline{u} \wedge \mathrm{d}u$ separately.

Finally, let us describe how these transformations are implemented for field theories. For fields $u:\mathbb{R}^d\times\mathbb{R}\to\mathcal{M}:(\vec{x},t)\to u(\vec{x},t)$ the generators of area-preserving diffeomorphisms are given by Noether charges which are constructed with the help of the canonical momenta π, $\overline{\pi}$ of the fields u and $\overline{u}$. Concretely, they read

$$Q^G = i\int d^d\mathbf{x} g^{-1}(\overline{\pi}G_u - \pi G_{\overline{u}}) \tag{28}$$

and act on functions of $u,\overline{u},\pi,\overline{\pi}$ via the Poisson bracket, where the fundamental Poisson bracket is (with $x^0=y^0$)

$$\{u(\mathbf{x}),\pi(\mathbf{y})\} = \{\overline{u}(\mathbf{x}),\overline{\pi}(\mathbf{y})\} = \delta^d(\mathbf{x}-\mathbf{y}) \tag{29}$$

as usual. The generators Q^{G_i} close under the Poisson bracket, $\{Q^{G_1},Q^{G_2}\}=Q^{G_3}$ where G_3 is as in (24). Specifically, for $G=G(a)$ they generate the Abelian area-preserving diffeomorphisms, as above.

III. INTEGRABLE SUBSECTORS

In this section we want to show that for a wide class of Lagrangian densities integrable subsectors can be defined which have infinitely many conserved Noether currents which may be related to the Abelian diffeomorphisms of the above section. The discussion in this section in some respect resembles the discussion in Ref. 16. However, the integrability condition which we shall derive here has not been discussed in that reference. We introduce the class of Lagrangian densities

$$\mathcal{L}(u,\overline{u},u_\mu,\overline{u}_\mu) = \mathcal{F}(a,b,c), \tag{30}$$

where

$$a = u\overline{u}, \quad b = u_\mu\overline{u}^\mu, \quad c = (u_\mu\overline{u}^\mu)^2 - u_\mu^2\overline{u}_\nu^2 \tag{31}$$

and $\mathcal{F}$ is at this moment an arbitrary real function of its arguments. That is to say, we allow for Lagrangian densities which depend on the fields and on their first derivatives, are Lorentz invariant, real, and obey the phase symmetry $u\to e^{i\lambda}u$ for a constant $\lambda\in\mathbb{R}$. We could relax the last condition and allow for real Lagrangian densities which depend on u and $\overline{u}$ independently, but this would just complicate the subsequent discussion without adding anything substantial. Further, all models we want to cover fit into the general framework provided by the class of Lagrangian densities (30), therefore we restrict our discussion to this class.

The canonical four-momentum for this class of models is

$$\pi_\mu \equiv \mathcal{L}_{u^\mu} = \overline{u}^\mu\mathcal{F}_b + 2(u^\lambda\overline{u}_\lambda\overline{u}_\mu - \overline{u}_\lambda^2 u_\mu)\mathcal{F}_c \tag{32}$$

and the equation of motion reads

$$\partial^\mu\pi_\mu = \mathcal{L}_u = \overline{u}\mathcal{F}_a \tag{33}$$

together with its complex conjugate.

We introduce the infinitely many currents

$$J_\mu^G = if(a)(G_u\overline{\pi}_\mu - G_{\overline{u}}\pi_\mu), \tag{34}$$

where $f(a)$ is an arbitrary but fixed real function of its argument. Further, G is an arbitrary real function of u and $\overline{u}$, and $G_u\equiv\partial_u G$. Comparing with the Noether charge (28) it is tempting to identify $f=g^{-1}$ and J_μ^G with the Noether currents of area-preserving diffeomorphisms, and we will see in a moment that for a large subclass of Lagrangian densities this identification can be made, indeed.

In a first step, let us investigate which conditions make the divergence of the above current vanish, $\partial^\mu J^G_\mu = 0$. We find after a simple calculation

$$\partial^\mu J^G_\mu = if([(M'\overline{u}G_u + G_{uu})u_\mu^2 - (M'uG_{\overline{u}} + G_{\overline{uu}})\overline{u}_\mu^2]\mathcal{F}_b + (uG_u - \overline{u}G_{\overline{u}})[M'(b\mathcal{F}_b + 2c\mathcal{F}_c) + \mathcal{F}_a]), \tag{35}$$

where

$$M \equiv \ln f \tag{36}$$

and the prime denotes the derivative with respect to a.

The condition that the second term on the right-hand side (rhs) of Eq. (35) vanishes requires that either

$$uG_u - \overline{u}G_{\overline{u}} = 0 \tag{37}$$

or

$$M'(b\mathcal{F}_b + 2c\mathcal{F}_c) + \mathcal{F}_a = 0. \tag{38}$$

Assuming condition (37) we find the general solution

$$G(u,\overline{u}) = G(u\overline{u}) \equiv G(a) \tag{39}$$

which is exactly equal to the condition (25) which restricts the generators of area-preserving diffeomorphisms to the Abelian subalgebra.

The condition that the first term on the rhs of Eq. (35) vanishes requires that either

$$\mathcal{F}_b = 0 \tag{40}$$

or that

$$[(M'\overline{u}G_u + G_{uu})u_\mu^2 - (M'uG_{\overline{u}} + G_{\overline{uu}})\overline{u}_\mu^2] = 0. \tag{41}$$

Condition (40) may, e.g., be satisfied by assuming $\mathcal{F}_b \equiv 0 \Rightarrow \mathcal{F} = \mathcal{F}(a,c)$. It follows that theories with Lagrangians $\mathcal{L} = \mathcal{F}(a,c)$ have infinitely many conserved currents (34), where G is restricted to (39). Of the models mentioned in the Introduction, only the AFZ model falls into this class. However, the AFZ model also obeys condition (38), therefore the restriction (39) is unnecessary and the J^G_μ are conserved for all G.

Alternatively we may make the first term on the rhs of Eq. (35) vanish by imposing Eq. (41). For an unrestricted G this leads to a condition on the field u,

$$u_\mu^2 = 0, \tag{42}$$

i.e., the complex eikonal equation, which, therefore, defines a submodel for which there exist infinitely many conserved currents provided that one of the two conditions (37) or (38) is imposed, in addition.

However, by invoking condition (39) we may reexpress condition (41) like

$$(M'G' + G'')F_b[\overline{u}^2 u_\mu^2 - u^2\overline{u}_\mu^2] \tag{43}$$

and, therefore, we find, instead of the complex eikonal equation, the weaker integrability condition

$$\overline{u}^2 u_\mu^2 - u^2\overline{u}_\mu^2 = 0, \tag{44}$$

i.e., Eq. (7). Therefore, for *all* Lagrangians $\mathcal{L} = \mathcal{F}(a,b,c)$ condition (44) defines submodels which have infinitely many conserved currents (34), where G is restricted to (39), again. All models mentioned in the Introduction belong to this class.

Finally, we want to investigate what happens if we impose condition (38), either alternatively or in addition to condition (39) [we want to remark that condition (38) is fulfilled by all models mentioned in the Introduction]. Equation (38) can be solved easily by the method of characteristics and has the general solution

$$\mathcal{F}(a,b,c) = \mathcal{F}\left(\frac{b}{f}, \frac{c}{f^2}\right). \tag{45}$$

This solution allows us to interpret the Lagrangian in terms of the target space geometry and to identify the currents (34) with the Noether currents of the area-preserving diffeomorphisms of Sec. II, as we want to demonstrate briefly. Indeed, trading the complex u field for two real target space coordinates ξ^α, $u \to (\xi^1, \xi^2)$, the expressions on which $\mathcal{F}$ may depend can be expressed as follows. The first term is

$$\frac{b}{f} = \frac{u_\mu \overline{u^\mu}}{f} = g_{\alpha\beta}(\xi)\partial^\mu \xi^\alpha \partial_\mu \xi^\beta, \tag{46}$$

where $\alpha = 1, 2$, etc., and the target space metric $g_{\alpha\beta}$ is diagonal and conformally flat for the coordinate choice $\xi^1 = \mathrm{Re}\, u$, $\xi^2 = \mathrm{Im}\, u$, i.e.,

$$g_{\alpha\beta} = g(a)\,\delta_{\alpha\beta} \equiv f^{-1}\delta_{\alpha\beta}. \tag{47}$$

For the second term we get

$$\frac{c}{f^2} = \tilde{\epsilon}_{\alpha\beta}\tilde{\epsilon}_{\gamma\delta}\partial^\mu \xi^\alpha \partial_\mu \xi^\gamma \partial^\nu \xi^\beta \partial_\nu \xi^\delta, \tag{48}$$

where

$$\tilde{\epsilon}_{\alpha\beta} = g\epsilon_{\alpha\beta}, \quad g = f^{-1} = \det{}^{1/2}(g_{\gamma\delta}) \tag{49}$$

and $\epsilon_{\alpha\beta}$ is the usual antisymmetric symbol in two dimensions. We remark that the two terms are different in that the first one, b/f, depends on the target space metric, whereas the second one only depends on the determinant of the target space metric. For this class of Lagrangians the currents (34) are the Noether currents of area-preserving diffeomorphisms on target space, and the condition $G = G(a)$ defines these Noether currents for the subgroup of Abelian area-preserving diffeomorphisms defined in Sec. II, as announced.

Remark: The Abelian subalgebra spanned by generators of the form $G = G(u\overline{u})$ is by no way the only Abelian subalgebra that exists for the algebra of vector fields v^G of Eq. (24). In fact, any subset of G of the form $G(u,\overline{u}) = \tilde{G}_i[h(u,\overline{u})]$ where h is an arbitrary but fixed function forms an Abelian subalgebra, i.e., $[v^{\tilde{G}_1}, v^{\tilde{G}_2}] = 0$. This follows from the fact that for an area-preserving diffeomorphism the vector field $v^{\tilde{G}}$ must be perpendicular to the (target space) gradient of h, i.e., it must point into the direction $h = \mathrm{const}$. Indeed,

$$v^{\tilde{G}}h = i\tilde{G}'(h_{\overline{u}}\partial_u - h_u\partial_{\overline{u}})h = i\tilde{G}'(h_{\overline{u}}h_u - h_u h_{\overline{u}}) = 0. \tag{50}$$

However, these Abelian subalgebras for $h \neq u\overline{u}$ do not play a special role in our discussion, i.e., they do not produce new integrability conditions. The reason why $h = u\overline{u}$ plays a special role lies in the fact that our metric function (Weyl factor) g depends on it, $g = g(u\overline{u})$. Had we chosen a different functional dependence $g = g[h(u,\overline{u})]$ for the metric function, then the corresponding generators $\tilde{G}_i[h(u,\overline{u})]$ of an Abelian subalgebra would define a nontrivial new integrability condition. For example, in the case $g = g(\xi^1) \equiv g[(u+\overline{u})/2]$ we find the integrability condition

$$u_\mu^2 - \vec{u}_\mu^2 = 0 \quad \text{or } (\xi^1)_\mu (\xi^2)^\mu = 0. \tag{51}$$

A target space with a metric of the form $g=g(\xi^1)$, however, does not have the topology of the two-sphere (but rather the topology of $\mathbb{R}^2$ or of a cylinder). Therefore, the corresponding field theory does not have a nontrivial Hopf index and, consequently, does not give rise to knot solitons. In this sense it is, therefore, less interesting.

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Global visibility of naked singularities

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Global visibility of naked singularities is analyzed here for a class of spherically symmetric spacetimes, extending previous studies—limited to inhomogeneous dust cloud collapse—to more physical valid situations in which pressures are non-vanishing. Existence of nonradial geodesics escaping from the singularity is shown, and the observability of the singularity from far-away observers is discussed.
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I. INTRODUCTION

The study of gravitational collapse of spherically symmetric solutions in general relativity led to many examples of locally naked singularities, starting from pioneering works in the early 1980's—a quite exhaustive and updated list of references can be found in Refs. 1 and 2. Most of these papers concentrate on the aim to find photons emanated from the singularity and escaping the Schwarzschildian trapped region at least locally. Moreover, the analysis has been always limited to the study of *radial* null geodesics, quite simplifying then the system to study, which remains not defined at the singular point, but fully decouples.

However, in order to study the effects of these photons for a distant observer, global behavior of null geodesics must be studied in full generality, since *nonradial* geodesics, with nonzero angular momentum, determine the angular diameter of the central naked singularity as seen by the observers, giving the measure of the "size" of the singularity. In this direction there are in literature quite detailed studies of Tolman-Bondi self-similar dust cloud collapse. In Refs. 3 and 4 necessary conditions—which actually turn out to be sufficient—for nonradial geodesics existence are derived, and behavior at infinity of these photons is numerically studied for some particular case. Further, a complete result of nonradial geodesic existence but under the assumption of self-similarity of the dust solution is fully proved in Ref. 5, and considerations about topology of the singularity are derived.

Of course, the dust model cannot be considered as a good physical model of singularity formation, because pressures are expected to occur during the collapse. In this paper we extend the results on dust models to a wide class of solutions, found in Ref. 6, for which local nakedness results from a suitable choice of initial data. This class represents the wider set found so far of locally naked singularities in the gravitational collapse of elastic materials. Since these models are not pressureless, and in particular radial pressure does not generally vanish along a timelike hypersurface, a junction between a solution from this class and a anisotropic generalization of de Sitter space-time discussed in Ref. 7 is performed to construct a global model. It is found that properties satisfied by dust solution and showed in previously cited works remains qualitatively valid for this wider class of collapsing space-times.

The paper is organized as follows. Interior and exterior solutions are described in Sec. II, and local existence of nonradial geodesic—which are continued in the exterior space-time using junc-

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tion conditions—is derived in Sec. III. The resulting behavior for a distant observer is analyzed in Sec. IV, together with some remarks about photons with infinite redshift. Last, Sec. V is devoted to overall conclusions.

II. COLLAPSE OF SPHERICAL ANISOTROPIC MATTER

In this part we briefly review the model we will deal with for the rest of the paper. The space-time will be made by two different solutions to Einstein field equations: an interior part, that collapses until singularity forms, and an exterior part, that is matched with the former at a timelike hypersurface in order to satisfy Israel-Darmois conditions;[8] it amounts to say that both first and second fundamental forms induced by the two solutions on this hypersurface, respectively, coincide. The interior part is described by the collapsing anisotropic solutions found in Ref. 6, which will be matched with the de Sitter generalizations discussed in Ref. 7 (see also references therein).

A. Interior region

The interior region is provided by a class of anisotropic collapsing matter. To describe it, the use of area-radius coordinates, first introduced by Ori,[9] turns out to be more useful than the usual comoving reference frame

$$\mathrm{d}s^2 = -e^{2\nu}\mathrm{d}t^2 + \frac{1}{\eta}\mathrm{d}r^2 + R^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2). \tag{2.1}$$

Indeed, as well known,[10] the general spherical matter distribution can be given assigning energy density ϵ and pressures p_r and p_t as suitable functions of the triple (r,R,η). Under the assumption $\partial p_r/\partial\eta=0$, in Ref. 6 it is shown that the metric takes the form

$$\mathrm{d}s^2 = -A(r,R)\mathrm{d}r^2 - 2B(r,R)\mathrm{d}R\,\mathrm{d}r - C(r,R)\mathrm{d}R^2 + R^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2), \tag{2.2a}$$

where

$$A = \left(1 - \frac{2\Psi}{R}\right)G^2, \quad B = -G\frac{Y}{u}, \quad C = \frac{1}{u^2}. \tag{2.2b}$$

In (2.2b), the two functions $\Psi(r,R)$ and $Y(r,R)$ are arbitrary (positive) functions while

$$u^2 = Y^2 + \frac{2\Psi}{R} - 1, \tag{2.2c}$$

and the function G is given in terms of a quadrature,

$$G(r,R) = \int_R^r \frac{1}{Y(r,\sigma)}\frac{\partial(1/u)}{\partial r}(r,\sigma)\,\mathrm{d}\sigma + \frac{1}{Y(r,r)u(r,r)}. \tag{2.2d}$$

In particular, the function Ψ represents Misner–Sharp mass. Conditions on Taylor developments of the above quantities may be given to characterize complete collapse and naked singularity formation, that we summarize in the following theorem.

Theorem 2.1 (Ref. 6):

(1) *In the space-time described by the metric* (2.2a), (2.2b), (2.2c), and (2.2d), *the singularity forms at the center* $r=0$ *in a finite amount of comoving time if Taylor development of the function* Ru^2 *is as follows*:

$$Ru^2 = \alpha r^3 + \beta r^2 R + \gamma r R^2 + \delta R^3 + o(r^2+R^2)^{3/2} \quad (\alpha > 0). \tag{2.3}$$

(2) *Under the above condition, and introduced the Taylor development of the* (*regular*) *function* $G(r,0)$

$$G(r,0) = \xi r^{n-1} + o(r^{n-1}), \tag{2.4}$$

then the central singularity is (*locally*) *naked if*, $n=1$, $n=2$, *or* $n=3$ *and* $\xi > \alpha\omega_{\text{crit}}$ *where* $\omega_{\text{crit}} = (26+15\sqrt{3})/2$.

We also remark that this model possesses nonvanishing anisotropic pressures, which are given by[6]

$$p_r = -\frac{1}{4\pi R^2}\frac{\partial \Psi}{\partial R}, \tag{2.5}$$

$$p_t = -\frac{1}{8\pi u R G}\left(\frac{1}{Y}\frac{\partial^2 \Psi}{\partial r\, \partial R} - \frac{1}{Y^2}\frac{\partial \Psi}{\partial r}\frac{\partial Y}{\partial R} + u\, G\frac{\partial^2 \Psi}{\partial R^2}\right), \tag{2.6}$$

and in this sense the model can be considered physically more reasonable than Tolman-Bondi dust collapsing sphere, where the space-time is ruled by the pressureless equation of state $p_r = p_t = 0$.

B. Exterior region

In our model, since the internal source is given by (2.2a), one cannot hope, in general, that radial pressure vanishes at some timelike hypersurface $\Sigma = \{(t, r, \theta, \phi) : r = r_b\}$. This is a quite restrictive feature of dust cloud collapsing model[11] or also nonvanishing radial pressure models,[10] that here arise only as very special cases, that happen when $\Psi = \Psi(r)$. Therefore, it cannot be possible to consider Schwarzschild vacuum solution as external region, if we want Israel–Darmois condition to be satisfied.

Hence, we perform a junction between the internal source satisfying conditions stated in Theorem 2.1, and the anisotropic generalization of de Sitter space-time, which are a class of spherically symmetric solutions of Einstein equation satisfying the condition $\epsilon + p_r = 0$ and admitting a particular G_4 group of motions (see Ref. 7). A coordinate transformation exists, that brings the line element in the form

$$\mathrm{d}s^2 = -\chi(R)\mathrm{d}T^2 + \chi(R)^{-1}\,\mathrm{d}R^2 + R^2\,\mathrm{d}\Omega^2, \quad \chi(R) = 1 - \frac{2M(R)}{R}, \tag{2.7}$$

thereby obtaining a family of solutions as Misner-Sharp mass $M(R)$ varies. In Ref. 12 it is shown that, actually, *any* spherically symmetric line element (2.1) can be matched with a metric of this family at a timelike hypersurface Σ as before, under the condition of continuity of mass only. Therefore, it suffices to choose

$$M(R) = \Psi(r_b, R), \quad \forall\, R \in [0, r_b]$$

and junction conditions will be certainly satisfied for all (comoving) times $t \geqslant 0$. The value of the external mass for bigger values of R depends on the internal space-time at comoving times prior to observation starting, and we will suppose that it is chosen such that

$$\limsup_{R \to +\infty} M(R) < +\infty\,. \tag{2.8}$$

C. Energy condition

In order to deal with a physically reasonable class of solutions, we impose the weak energy condition (WEC) on the energy-momentum tensor T of the space-time. Basically, this means $T(v, v) \geqslant 0$ for all timelike vectors v, and it is easily seen[6] that it holds in the internal region if, for each $r \in [0, r_b]$, the two functions of the variable R only

$$R \mapsto \frac{1}{Y(r,R)} \frac{\partial \Psi}{\partial r}(r,R), \quad R \mapsto \frac{\partial \Psi}{\partial R}(r,R) \tag{2.9}$$

are non-negative subsolutions of the *same* ODE,

$$\frac{\mathrm{d}F}{\mathrm{d}R} \leqslant \frac{2}{R} F(R) \tag{2.10}$$

for $R>0$. In particular, for $r=r_b$, the above condition ensures WEC in the external region also [see Ref. 12, Eq. (4.6)].

Models of internal solutions satisfying (2.3), (2.8) and WEC can be easily found: for instance, the choice

$$\Psi(r,R) = \int_0^r \gamma(s) s^2 \, \mathrm{d}s + \int_0^R \chi(\sigma) \sigma^2 \, \mathrm{d}\sigma, \quad Y = Y(r), \tag{2.11}$$

with $\gamma(s)$ and $\chi(\sigma)$ positive and not increasing in $[0,+\infty)$, allows for (2.3) and the weak energy condition to be satisfied. As an example, one may take

$$\chi(\sigma) = \frac{1}{(1+R^3)^4}$$

in order to satisfy also (2.8). Note that, with the choice of χ=constant, the space-time coincides with the so-called Tolman-Bondi-de Sitter (TBdS), and that is the reason why, in Ref. 6, the models arising from the above choice (2.11) are termed *anisotropysations of TBdS space-time*.

III. NULL GEODESICS FROM THE SINGULARITY

A. Geodesic equations

As stated in Theorem 2.1, conditions on the metric functions allow to determine when the central singularity is locally naked. This is made by showing the existence of a future pointing radial null geodesic which lies in the region $R>2\Psi$ and may be traced back to the central singularity. In Ref. 6 it is shown that, to obtain violations of cosmic censorship in spherical symmetry, one may restrict oneself in looking for null geodesic which are radial only. In other words, if a singularity is radially censored, it is censored all the way. Nevertheless, if one wants to study visibility under a more general point of view, also nonradial light rays should be taken into account.

Let κ be the affine parameter of the null geodesic. Without loss of generality, we will suppose that the geodesic lies in the hypersurface $\theta=\pi/2$, and then the angular components of tangent vector along the geodesic read

$$\kappa^\theta := \frac{\mathrm{d}\theta}{\mathrm{d}\kappa} = 0, \quad \kappa^\phi := \frac{\mathrm{d}\phi}{\mathrm{d}\kappa} = \frac{\ell}{R^2}, \tag{3.1}$$

where ℓ is the (conserved) angular momentum. Let us also introduce a function q such that

$$\kappa^r := \frac{\mathrm{d}r}{\mathrm{d}\kappa} = \frac{1}{qRG}. \tag{3.2}$$

Then, expressing R, θ, and ϕ as functions of r instead of κ, the equations for null geodesics can be given in the following form:

$$\frac{\mathrm{d}R}{\mathrm{d}r} = uG\left[Y - u\sqrt{1+\left(\frac{\ell q}{u}\right)^2} \right], \tag{3.3a}$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}r}=0, \quad \frac{\mathrm{d}\phi}{\mathrm{d}r}=\frac{\ell qG}{R}, \tag{3.3b}$$

and

$$-\frac{1}{q}\frac{\mathrm{d}q}{\mathrm{d}r}-\frac{1}{G}\frac{\mathrm{d}G}{\mathrm{d}r}-\frac{1}{R}\frac{\mathrm{d}R}{\mathrm{d}r}-\frac{CA_{,r}+B(A_{,R}-2B_{,r})}{2G^2}-\frac{CA_{,R}-BC_{,r}}{G^2}\frac{\mathrm{d}R}{\mathrm{d}r}+\frac{BC_{,R}+C(C_{,r}-2B_{,R})}{2G^2}\left(\frac{\mathrm{d}R}{\mathrm{d}r}\right)^2$$
$$+\ell^2\frac{q^2B}{R}=0, \tag{3.3c}$$

and A,B,C are given in (2.2b). Dealing with radial geodesics results in vanishing of ℓ, and so (3.3a), which is found imposing that the geodesic is null, becomes an ODE in the R function only, which is enough to study at least the existence of corresponding pregeodesics. On the other side, when $\ell\neq 0$, also (3.3c) must be studied.

Before to state and show results, we restrict the analysis hereafter to the case when n in (2.4) is equal to 3. As it will be cleared in Remark 3.4, this particular situation—that, as seen in the statement of Theorem 2.1, has a sort of "endstate transition"—corresponds to a so–called *strong curvature* singularity, unlike $n=1,2$ cases—at least along null radial geodesics. We refer the reader to Remark 3.4 below and, for instance, to Refs. 13–15 for a general insight about strong curvature conditions.

B. Null geodesics existence

Existence of null radial geodesics has already been proved in Ref. 6, using comparison arguments in ODE. We here complete the analysis about the asymptotic behavior of the geodesics finding also an existence result for nonradial geodesics.

Remark 3.1: In the forthcoming Proposition it will be shown that the null geodesic equation can be put in the form

$$\frac{\mathrm{d}y}{\mathrm{d}r}=\frac{1}{r}f(y)+g(r,y), \tag{3.4}$$

where $y(r)\in\mathbb{R}^n$ and $f:\mathbb{R}^n\to\mathbb{R}$, $g:\mathbb{R}^{n+1}\to\mathbb{R}$ are $\mathcal{C}^1$ functions; introducing a new independent variable s such that $\mathrm{d}r/\mathrm{d}s=-r(s)$ then, from (3.4), we obtain the system

$$\frac{\mathrm{d}y}{\mathrm{d}s}=-f(y(s))-r(s)g(r(s),y(s)),$$
$$\frac{\mathrm{d}r}{\mathrm{d}s}=-r(s), \tag{3.5}$$

whose solutions describe parametrizations of solutions of (3.4) by the parameter s. Equilibria of the above system (as $s\to+\infty$) are given by points $(y_0,0)$ where y_0 is a root of $f(y)=0$, and searching for these equilibria amounts to search for admissible solutions of the so-called *root equation*, first introduced in Ref. 16 for the study of radial light rays.

The key point is that these equilibria for the null geodesic equation will be shown to be hyperbolic—see, e.g., Ref. 17 for basic concepts about hyperbolic dynamical systems—and that is the reason why the root equation solution's existence is a necessary but also sufficient condition for light rays existence.

Proposition 3.2: *Under the hypotheses of Theorem 2.1, when, with reference to equation* (2.4), $n=3$ *and* $\xi>\alpha\omega_{\mathrm{crit}}$, *there exists infinite null geodesics emanating from the central singularity and escaping from the trapped region* $\{R>2\Psi\}$. *In particular, there exists three numbers* x_1, x_2, x_c, *depending on* α *and* ξ, *with* $x_c>x_2>x_1>\alpha$, *such that these geodesics can be divided in the following classes*:

(1) *infinite radial and nonradial geodesics such that* $R(r)=x_1r^3+o(r^3)$,
(2) *infinite nonradial null geodesic such that* $R(r)=x_2r^3+o(r^3)$, *and*
(3) *a radial geodesic (Cauchy horizon) such that* $R_c(r)=x_cr^3+o(r^3)$, *which bounds from above any geodesic in classes* (1) *and* (2), *in the sense that* $R_c(r)>R_g(r)$, $\forall\, r>0$, *for any other geodesic* $R_g(r)$.

Moreover, the nonradial geodesic of case (1) *have finite* $\lim_{r\to 0^+}\phi(r)$, *whereas nonradial geodesics of case* (2) *are such that* $\lim_{r\to 0^+}\phi(r)=-\infty$.

Proof: Let us consider system (3.3a), (3.3b), and (3.3c). We are interested in determining existence of solutions such that $R(r)$ lies above the apparent horizon $R_h(r)$, which is known (see Ref. 6 for details) to have the behavior $R_h(r)=\alpha r^3+o(r^3)$. Then, we first introduce a new unknown function $z(r)$ in place of R, which is defined as

$$z(r)=\sqrt{\frac{R(r)}{\alpha r^3}}, \tag{3.6}$$

and we will study the system made by the first and the last equation above, in the unknown functions $(z(r),q(r))$—with $q(r)$ given by (3.2)—since the equation for ϕ can be decoupled from these. Moreover, note that since ℓ appears in (3.3a), (3.3b), and (3.3c) as a factor of the quantity ℓq only, we will consider $\ell q(r)$ instead of $q(r)$ as variable.

We first observe that $z(r)$ and $q(r)$ must be bounded from below by 1 and 0, respectively, in order for the solution to be physically acceptable. Then, estimates of terms involved in (3.3a) will be performed, under the additional hypothesis that $z(r)$ is also bounded from below, and Eqs. (3.3a) and (3.3c) become, with the further position

$$\omega=\frac{\xi}{\alpha},$$

$$\frac{\mathrm{d}z}{\mathrm{d}r}=\frac{1}{r}w(z,\ell\, q)+g_1(r,z,\ell\, q), \tag{3.7a}$$

$$\ell\frac{\mathrm{d}q}{\mathrm{d}r}=\frac{1}{r}[\ell\, q(k(z)-(\ell q)^2h(z)+w(z,\ell\, q)\tilde{k}(z))]+\ \ell\, qg_2(r,z,\ell\, q), \tag{3.7b}$$

where

$$w(z,\ell\, q)=-\frac{2z^4+\sqrt{1+(\ell q)^2z^2}z^3-\omega z+\sqrt{1+(\ell q)^2z^2}\omega}{2z^3}, \tag{3.7c}$$

$$k(z)=\frac{\omega^2-10z^3\omega-2z^6}{2z^3(\omega+z^3)}, \tag{3.7d}$$

$$h(z)=\frac{\omega+z^3}{z}, \tag{3.7e}$$

$$\tilde{k}(z)=-\frac{z^3+4\omega}{z(\omega+z^3)}, \tag{3.7f}$$

and $g_i(r,z,\ell q)$, $i=1,2$ are continuous functions.

Let us check equilibria of (3.7a) and (3.7b), using the idea from Remark 3.1. The following cases happen:

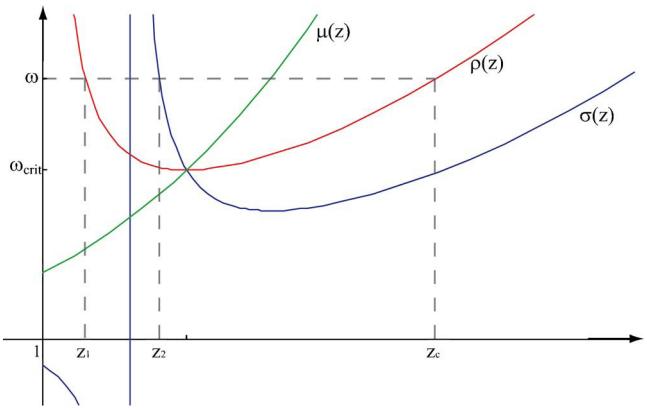

FIG. 1. (Color online) The curves $\rho(z)$ (3.9), $\sigma(z)$ (3.12), and $\mu(z)$ intersect each other at the local minimum of $\rho(z)$, attained for $z=(1+\sqrt{3})/2$, $\rho(z)=\omega_{\text{crit}}$ (see Theorem 2.1).

(a) $\ell q=0, z$ such that $w(z,0)=0$;

(b) $\ell q=\sqrt{k(z)/h(z)}, z$ such that $w(z,\sqrt{k(z)/h(z)})=0$.

First, in both cases it can be seen that $(g_1(r,z,\ell q),\ell q g_2(r,z,\ell q))$ is regular in a neighborhood of $(0,z,\ell q)$ where $(z,\ell q)$ is an equilibrium as above. Let us now discuss the character of these equilibria.

In case (a), the situation goes as follows. With reference to the notation of Remark 3.1, the Jacobian computed in the equilibrium $(z,0)$ is given by

$$J_{(z,0)}f=\begin{pmatrix}\dfrac{\partial w}{\partial z}(z,0) & \dfrac{\partial w}{\partial q}(z,0)\\ 0 & k(z),\end{pmatrix}, \tag{3.8}$$

and one finds that there exists a *root function*

$$\rho(z)=\frac{2z^4+z^3}{z-1}, \tag{3.9}$$

such that

$$w(z,0)=0 \;\Leftrightarrow\; \rho(z)=\omega, \tag{3.10a}$$

$$\frac{\partial w}{\partial z}(z,0)=-\frac{1}{2z^2}\rho'(z). \tag{3.10b}$$

Moreover, $k(z)>0$ if and only if $\omega>\mu(z):=(5+\sqrt{27})z^3$. The curves $\rho(z)$ and $\mu(z)$ are depicted in Fig. 1. For the acceptable range of ω, that is $\omega>\omega_{\text{crit}}$ (see Theorem 2.1), there exists a unique value z_1 that satisfies (3.10a) and such that $k(z_0)>0$. From (3.10b), we have that also $(\partial w/\partial z)\times(z_1,0)>0$. This means that the Jacobian (3.8) has two positive eigenvalues and therefore we have part (1) of the claim, with an infinite number of radial geodesics tending to this equilibrium point, for every $\ell\geqslant 0$. Note that this situation (1) covers also radial geodesic existence, that is when $\ell=0$. Using (3.6), the curves $R(r)$ behaves like $R(r)=\alpha z_1^2 r^3+o(r^3)$.

If $\omega>\omega_{\text{crit}}$, from Fig. 1 we see that there exists another value of $z=z_c$ satisfying $\rho(z_c)=\omega$. In this case we have two negative eigenvalues of (3.8). With reference to the system put in the form (3.5), the equilibrium is again hyperbolic, but the stable manifold has dimension 1, and therefore a single null geodesic tending to the equilibrium exists. Actually, it can be shown that this geodesic is radial, since it can be seen that at least a radial null geodesic tending to the equilibrium exists.

Indeed, radial geodesics are solutions of the ODE (3.7a) under the assumption $\ell=0$. We can easily see that $z=z_c$ is an equilibrium of (3.7a), such that there exist a unique solution tending to this equilibrium. Since radial geodesics are solutions of (3.7a) and (3.7b) with $\ell q\equiv 0$, we conclude that the (unique) solution of (3.7a) and (3.7b) must be radial. The corresponding $x=\alpha z_c^2$ represents *Cauchy horizon* direction.

We also note that the corresponding function $R_c(r)$ must bound from above any other geodesic $R_g(r)$. Of course, this must be true for any other radial geodesic near $r=0$, and therefore for any other value of r by uniqueness of Cauchy problem solution. Let us show that this also holds true for nonradial geodesic. By contradiction, let $R_g(r)$ be a nonradial geodesic, such that its projection on the (r,R) plane bounds from above $R_c(r)$ for some r_*, that is $R_g(r_*)>R_c(r_*)$. Since $R_g(r)$ is a subsolution of radial null geodesic equation, and $R_c(r)$ is a solution of the same ODE, therefore we can find a radial null geodesic $R_n(r)$ with initial data $R_n(r_*)\in]R_c(r_*),R_g(r_*)[$, and trace it back until $R_n(0)=0$, obtaining a radial geodesic $R_n(r)>R_c(r)$ in a right neighborhood of $r=0$, which as said before is absurd, and claim (3) is complete.

Let us now discuss case (b) to get claim (2) of the Proposition.

We first observe that this time it must be $k(z)>0$ otherwise we have no equilibria. Arguing as in the previous case, we find that the determinant of the Jacobian in the equilibrium—say $(z_2,\sqrt{k(z_2)/h(z_2)})$—is given by

$$-2k(z_2)\frac{\mathrm{d}w(z,\sqrt{k(z)/h(z)})}{\mathrm{d}z}\Big|_{z=z_2}. \tag{3.11}$$

The root function in this case is given by

$$\sigma(z)=\frac{4z^5}{2z^2-3}, \tag{3.12}$$

which has the properties

$$w\left(z_2,\sqrt{\frac{k(z_2)}{h(z_2)}}\right)=0 \;\Leftrightarrow\; \sigma(z_2)=\omega, \tag{3.13a}$$

$$\frac{\partial w}{\partial z}\left(z_2,\sqrt{\frac{k(z_2)}{h(z_2)}}\right)=-\gamma^2\sigma'(z_2), \tag{3.13b}$$

where γ is some nonvanishing constant. The situation is depicted in Fig. 1. For any $\omega>\omega_{\mathrm{crit}}$ there exists a unique value of z_2 satisfying (3.13a) with $k(z_2)>0$. Using (3.13b), we get that the quantity (3.11) is negative and then there exists one and only one positive eigenvalue of the Jacobian, which results in the existence of infinite nonradial null geodesic such that the corresponding $R(r)$ behaves like $R(r)=\alpha z_2^2 r^3+o(r^3)$. Indeed, the stable manifold of the system put in the form (3.5) has dimension 2.

Notice that, in this case, there are no other choices available since the other root of the equation $\sigma(z)=\omega$ lies in the $\{k<0\}$ region.

To complete the proof, let us now analyze the behavior of the angular function $\phi(r)$. Using (3.3b), and the above estimates,

$$\frac{\mathrm{d}\phi}{\mathrm{d}r}\cong \ell\left(\frac{h(z)}{z}\right)\frac{q}{r}. \tag{3.14}$$

For a nonradial geodesic from case (1), $q\to 0$ as $r\to 0^+$, and then, from (3.7b), $\mathrm{d}q/\mathrm{d}r\cong k(z_1)\times(q/r)$, from which $q(r)\cong r^{k(z_1)}$, and then, using (3.14), $\phi(r)$ has a finite limit as $r\to 0^+$.

For a nonradial geodesic from case (2) conversely, q tends to a finite positive value and then the function $\phi(r)$ goes like kr^{-1}, which determines a negative diverging behavior of the function $\phi(r)$. □

Remark 3.3: These results are completely consistent with the analysis carried out in Refs. 4 and 5, which have established a double topological nature of the naked singularity in the particular case of dust solution under self-similarity assumption. In particular, case (1) corresponds to a region of the singularity foliated by a 2-sphere, whereas case (2) corresponds to a topologically pointwise singular region.

Remark 3.4: If we look at the behavior of the quantity $k^2R_{\alpha\beta}K^\alpha K^\beta$ along null radial geodesics, where $R_{\alpha\beta}$ is Ricci tensor, $K^\alpha=\mathrm{d}x^\alpha/\mathrm{d}k$ is the tangent vector of the geodesic with parameter k, we get

$$k^2R_{\alpha\beta}K^\alpha K^\beta=\frac{k^2\Psi_{,r}}{4\pi R^2u^3GY}(K^R)^2. \tag{3.15}$$

In view of the above theorem, Eqs. (3.2) and (3.3a) ensure that there exists $\lim_{k\to 0^+}K^R$, then $(k/R)K^R$ tends to a finite nonzero limit value. Since both G and $\Psi_{,r}$ goes like r^2, and Y,u tends to a finite nonzero limit along the geodesics, the quantity in (3.15) goes to a finite nonzero value. It follows that these null geodesics terminate in a strong curvature singularity in the sense of Tipler[14].

IV. FARAWAY VISIBILITY OF THE SINGULARITY

A. Size of the singularity

In the following, we will study the behavior at infinity of null geodesics emanating from the singularity. We have already seen that there exists an infinite number of light rays escaping from the trapped region; these geodesics arrives at the boundary of the collapsing sphere of anisotropic matter with some value $R(r_b)$, and they must be continued by studying the behavior of null geodesics in the external region (2.7) escaping from the boundary and such that $R=R(r_b)$.

The equation for null geodesics—that, without loss of generality, we will suppose to lie in the subspace $\{\theta=\pi/2\}$—is given by

$$\frac{\mathrm{d}T}{\mathrm{d}\kappa}=\frac{\omega}{\chi(R)},\quad \frac{\mathrm{d}R}{\mathrm{d}\kappa}=\omega\sqrt{1-\frac{\chi(R)}{R^2}\left(\frac{\ell}{\omega}\right)^2},\quad \frac{\mathrm{d}\theta}{\mathrm{d}\kappa}=0,\quad \frac{\mathrm{d}\phi}{\mathrm{d}\kappa}=\frac{\ell}{R^2}, \tag{4.1}$$

where κ denotes as usual the affine parameter and ℓ and ω are constant of motion.

As explained in Ref. 4, since the metric (2.7) does not depend on T we can uniquely associate to an observer $R=R_0$ an orthonormal basis of the tangent space to a point (T,R_0,θ,ϕ) of the outer region [i.e., such that $R_0>2M(R_0)$], which will be denoted by

$$\{e_{(T)}=\chi(R_0)^{-1/2}\partial_T, e_{(R)}=\chi(R_0)^{1/2}\partial_R, e_{(\theta)}=R_0^{-1}\partial_\theta, e_{(\phi)}=(R_0\sin\theta)^{-1}\partial_\phi\}.$$

Then, if we consider a null geodesic with affine parameter κ emanating from the singularity passing for $R=R_0$, and denote by $\kappa^\alpha=\mathrm{d}X^\alpha/\mathrm{d}\kappa$ its tangent vector, this observer measures an angle δ between the light ray and the radial direction equal to

$$\delta=\arctan\left(\frac{g_{\mu\alpha}e^\mu_{(\phi)}\kappa^\alpha}{g_{\mu\alpha}e^\mu_{(R)}\kappa^\alpha}\right)=\frac{\ell}{\omega}\sqrt{\frac{\chi(R_0)}{R_0^2-(\ell/\omega)^2\chi(R_0)}}. \tag{4.2}$$

The above quantity depends on the geodesic, and therefore the supremum made among the set $\mathfrak{S}$ of all singular geodesics detected at $R=R_0$ gives a measure of the singularity detected by the observer. One can conceive the right-hand side above, fixing R_0, as a function in (ℓ/ω) which results to be increasing. Therefore, the "size" of the singularity detected by the faraway observer is related to the quantity

$$b:=\sup_{\mathfrak{S}}\frac{\ell}{\omega},$$

which can be regarded[4] as a sort of *impact parameter*.

Using this definition, it is not hard to prove an extension of the result already proved for the particular case studied in Ref. 4.

Proposition 4.1: If the boundary of the interior region $r=r_b$ is sufficiently small, then the nonradial geodesics of largest impact parameters emanating from the singularity are such that the angular function $\phi\to-\infty$ in the approach to the singularity [*case* (2) *of Proposition 3.2, see also Remark 3.3*].

Proof: Of course, we will consider only nonradial geodesics, when $\ell\neq 0$.

Using continuity of the metric along the junction hypersurface, one gets

$$\frac{\mathrm{d}T}{\mathrm{d}\kappa}=\frac{\mathrm{d}T}{\mathrm{d}R}\frac{\mathrm{d}R}{\mathrm{d}\kappa}+\frac{\mathrm{d}T}{\mathrm{d}r}\frac{\mathrm{d}r}{\mathrm{d}\kappa}=\left[-\frac{Y}{\chi u}\frac{\mathrm{d}R}{\mathrm{d}r}+G\right]\frac{\mathrm{d}r}{\mathrm{d}\kappa}, \tag{4.3}$$

and using (4.1), together with (3.2), (3.3a), and (3.3b) one finds the angular frequency ω and therefore the impact parameter b, which is given by

$$b=\sup_{\mathfrak{S}}\left(\frac{R(r)\,\ell\,q(r)}{Y(r,R(r))\sqrt{u^2(r,R(r))+(\ell\,q(r))^2}-u^2(r,R(r))}\right)\Big|_{r=r_b}. \tag{4.4}$$

With reference to the cases listed in Proposition 3.2, let $R_1(r)$ be a nonradial geodesic from case (1), and let $R_2(r)$ a (necessarily nonradial) geodesic from case (2). It is easy to verify that, as $r\to 0^+$, the quantity in round brackets in (4.4) tends to 0 along $R_1(r)$ and tends to a finite nonzero value along $R_2(r)$. Then, if r_b is sufficiently small, we can suppose that this quantity, along R_2, bounds from above the same quantity computed along R_1 until $r=r_b$. □

B. Redshift

Following Ref. 18, the frequency shift z between a source and an observer, respectively, located at events P_1 and P_2, connected by a null geodesic with tangent vector $\vec{\kappa}$ with respect to the affine parameter, is defined as

$$1+z=\frac{g_{P_1}(\vec{\kappa},u_{(s)})}{g_{P_2}(\vec{\kappa},u_{(o)})}. \tag{4.5}$$

where $u_{(s)}$ and $u_{(o)}$ are the 4-velocities of the source and the observer, respectively.

To determine the redshift associated to the singular geodesics, the numerator above will be replaced by a limit expression as P_1 approaches the central singularity. Let us therefore consider a singular geodesic passing at event P_2 in the exterior space such that $R(P_2)=R_0$. Using the basis (4.3), together with (4.1), it is easy to see that the denominator in (4.5) is given by $-\chi(R_0)^{1/2}\omega$, which under the hypothesis (2.8) is always finite also if R_0 tends to infinity. On the other side, the velocity field in the interior space-time is given by $-u(r,R)\partial_R$, and using (3.2) and (3.3a) one finds that the absolute value of the numerator in (4.5) is given by

$$\lim_{r\to 0^+}\frac{1}{R(r)}\left[\left(\frac{u(r,R(r))}{q(r)}\right)^2+\ell^2\right]^{1/2}=+\infty, \tag{4.6}$$

which results in an infinite frequency shift. Actually we can observe that calculation of (4.6) above seems a feature of all singular spherically symmetric models, at least for nonradial geodesics, when $\ell\neq 0$. In the case under our study, moreover, (4.6) holds also for *radial* geodesic since, using Proposition 3.2 and Eq. (2.2c), $u(r,R(r))\cong u_0\neq 0$, and both $R(r)$ and $q(r)$ are infinitesimal. It appears also to be possible the study of the limit in (4.6) in a even more general framework, and work in this direction is in progress.

All in all, these models show the same feature described in Ref. 18 for dust solutions: in the case corresponding to a strong naked singularity (along radial geodesic), null geodesics are infinitely redshifted. (As pointed out in Ref. 18, it can be possible that the strength of the singularity

may have a directional behavior, that is the singularity is weak—in the sense explained in Remark 3.4—along some geodesics, and strong among others.) Therefore, it can be said that there exists a form of weak censorship for such class of solutions, at least at the classical level. Of course however, quantum phenomena might change this scenario, as suggested by some authors (see Refs. 4 and 11).

V. DISCUSSION AND CONCLUSIONS

In this paper we have studied visibility of the naked singularity for a faraway observer, investigating global behavior of null (radial and nonradial) geodesics in a class of spherically symmetric singular space-times. The interior part belongs to a wide class of anisotropic solutions; as known from the analysis carried out in Ref. 6, the end state of the central singularity is determined by the lower order term n of Taylor development of a quantity determined by the metric. In this paper we considered the case $n=3$, which has a special interest since (i) the end state is determined by the value of a certain parameter ξ/α, that causes a sort of "phase transition" between naked singularity and black hole situations, and (ii) radial geodesics terminates into a strong curvature singularity, as observed in Remark 3.4.

The exterior part belongs to the class of anisotropic generalization of de Sitter solution discussed in Ref. 7. The form of the metric closely resembles the Schwarzschild line element, but the mass here depends on the areal coordinate R since a constant mass would not properly match an interior solution with nonvanishing radial pressures. Indeed, if Misner-Sharp masses for both solutions (interior and exterior) coincide at a hypersurface $r=\text{const}$, this ensures Darmois junction conditions to hold along this hypersurface.

Existence of nonradial geodesics is crucial to investigate global visibility. The system of ODE satisfied by the nonradial geodesics does not decouple and the most suitable way seems to study equilibrium points of this system. It turns out that there are two values $x_1<x_2$, depending on the data of the space-time, such that there is an infinite number of nonradial geodesic $R(r)$ emanating with "direction" x_1 [i.e., such that $\lim_{r\to 0} R(r)/r^3=x_1$] and infinite nonradial geodesics with direction x_2. This result is not in contrast with previous results regarding self-similar collapse[5] where one has infinite geodesic with direction x_1 vs only one geodesic with direction x_2. Indeed, as the proof of Proposition 3.2 points out, the stable manifold of the equilibrium has dimension 3 in the first case and 2 in the second one. Self-similarity assumption simplifies the geometry of these stable manifolds, shrinking them by one dimension.

It must be remarked that a crucial fact is that ODE system can be brought in the form (3.4), where the equilibria are all hyperbolic. This is a feature of all collapsing matter models known in literature, which excluded pathological situations such as the ones outlined in Ref. 11, and explains why the so-called *root equation* method repeatedly exploited in previous works—based on the existence of a certain limit which in principle cannot be taken for granted (see for instance Refs. 3, 16, and 4)—leads all the same to the conclusions one would expect.

The analysis of the ODE system allowed us to determine a sort of "impact parameter" that characterizes the "size" of the singularity as it is seen by a faraway observer. It turns out that photons emanated by the naked singularity are infinitely redshifted also when pressures are present, as has been already shown (see Ref. 18) for the pressureless Tolman-Bondi collapse.

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Killing vectors in asymptotically flat space-times. II. Asymptotically translational Killing vectors and the rigid positive energy theorem in higher dimensions

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We show that the borderline cases in the proof of the positive energy theorem for initial data sets, on spin manifolds, in dimensions $n \geqslant 3$, are only possible for initial data arising from embeddings in Minkowski space-time. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2167809]

I. INTRODUCTION

Witten's proof of the positive energy theorem[10] shows that, under appropriate conditions, the time-component of the energy-momentum vector p is non-negative. For various reasons it is of interest to understand precisely the borderline cases, with a vanishing, or perhaps lightlike, p. In the context of initial data sets this has been done in detail in an accompanying paper[5] in space-dimension three. It is the purpose of this work to generalize the results proved there to all spin initial data manifolds of dimension $n \geqslant 3$.

The argument presented in Ref. 5 proceeds as follows: in the borderline cases, Witten's proof provides one or more covariantly constant "KIDs" (by definition, those are the initial data counterparts of space-time Killing vectors).[4] A careful study of such KIDs shows that their existence implies the vanishing of mass, and then flatness of space-time along the initial data. One then concludes by showing that the Killing development of the initial data set is flat.

Not unexpectedly, all those arguments can be extended to higher dimensions, after adjustment of the rates of decay of the fields. The only part of the proof where essential work is needed is the algebra proving existence of KIDs. This is based on Ref. 8, and presented in Sec. III. On the other hand, the analysis of the KIDs is essentially identical to that in Ref. 5, so we will (mainly) only present the statements of the results needed for the positive energy theorem here.

The notation and conventions of Ref. 5 are used throughout. We assume that the space-dimension n is larger than or equal to three.

Our main results can be summarized as follows.

Theorem 1.1: *Let* $(\mathcal{M}, g_{\mu\nu})$ *be an* $(n+1)$*-dimensional space-time,* $n \geqslant 3$*, with a Killing vector field which is asymptotically null along an (appropriately regular, see Sec. II below) asymptotically flat spacelike hypersurface* $\mathcal{J}$*. Then the ADM energy-momentum vector of* $\mathcal{J}$ *vanishes.*

The precise hypotheses needed for Theorem 1.1 are the conditions on the asymptotic behavior of (g, K) in (2.18) and (2.19) below, together with the matter decay conditions (2.20) and (2.22). Theorem 1.1 is a special case of Theorem 2.5 below.

Theorem 1.2 (Timelike "future-pointing" energy-momentum theorem): *Under natural regu-*

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larity and matter-energy conditions (see the conditions of Theorem 3.2 below), the ADM energy-momentum vector p^μ of a spin initial-data manifold $\mathcal{J}$ satisfies

$$p^0 > \sqrt{\sum_{i=1}^{n} (p^i)^2},$$

unless $(\mathcal{J}, g_{ij}, K_{ij})$ are initial data for Minkowski space-time.

Theorem 1.1 is a loose rephrasing of Theorem 3.2 below.

There are well-known counterparts of this with trapped boundaries, which are of no concern to us here because they always lead to a strict inequality.

It would be natural to extend the result to cover the Bondi mass, both in three and higher dimensions. The starting point of the calculations of the proof of Theorem 3.2 is the existence of a parallel spinor, which follows from the analysis in Ref. 7 when the Bondi mass is null in space-dimension three. The calculations that follow apply without modifications, yielding a parallel isotropic KID. One expects that this is incompatible with a nonvanishing Trautman-Bondi mass, but a complete analysis of this has not been carried out so far.

II. KIDs IN *n*-DIMENSIONAL ASYMPTOTICALLY FLAT INITIAL DATA SETS, $n \geqslant 3$

We have the following string of propositions, which are the building stones of the proof of Theorem 2.5 below.

Proposition 2.1: Let $R>0$ and let (g_{ij}, K_{ij}) be initial data on $\mathcal{J}_R \equiv \mathbb{R}^n \backslash B(R)$ satisfying

$$g_{ij} - \delta_{ij} = O_k(r^{-\alpha}), \quad K_{ij} = O_{k-1}(r^{-1-\alpha}), \tag{2.1}$$

with some $k>1$ and some $\alpha>0$. Let N be a C^2 scalar field and Y^i a C^2 vector field on $\mathcal{J}_R$ such that

$$2NK_{ij} + \mathcal{L}_Y g_{ij} = 0. \tag{2.2}$$

Define ρ, J^i, and τ_{ij} by the equations

$$2\rho = {}^nR + (K^i_{\ i})^2 - K^{ij}K_{ij}, \tag{2.3}$$

$$J^i = D_j(K^{ij} - K^k_{\ k} g^{ij}), \tag{2.4}$$

$$\tau_{ij} - \tfrac{1}{2} g^{k\ell}\tau_{k\ell} g_{ij} = {}^nR_{ik} + K^k_{\ k}K_{ij} - 2K_{ik}K^k_{\ j} - N^{-1}(\mathcal{L}_Y K_{ij} + D_i D_j N) - \tfrac{\rho}{2} g_{ij}, \tag{2.5}$$

and assume that ρ and τ_{ij} satisfy

$$\rho = O_{k-2}(r^{-2-\alpha}), \quad \tau_{ij} = O_{k-2}(r^{-2-\alpha}). \tag{2.6}$$

Then there exists numbers $\Lambda_{\mu\nu} = \Lambda_{[\mu\nu]}$ such that we have, for r large,

$$D_i Y_j - \Lambda_{ij} = O_{k-1}(r^{-\alpha}), \quad Y^i - \Lambda_{ij}x^j = \begin{cases} O(r^{1-\alpha}), & \alpha \neq 1, \\ O(\ln r), & \alpha = 1, \end{cases} \tag{2.7}$$

$$D_i N - \Lambda_{i0} = O_{k-1}(r^{-\alpha}), \quad N - \Lambda_{i0}x^i = \begin{cases} O(r^{1-\alpha}), & \alpha \neq 1, \\ O(\ln r), & \alpha = 1. \end{cases} \tag{2.8}$$

If $\Lambda_{\mu\nu}=0$, then there exist numbers A^μ such that we have

$$Y^i - A^i = O_k(r^{-\alpha}), \quad N - A^0 = O_k(r^{-\alpha}). \tag{2.9}$$

If $\Lambda_{\mu\nu}=A^\mu=0$, then $Y^i \equiv N \equiv 0$.

Proof: See Sec. II and Appendix C of Ref. 5.

Proposition 2.2: Let $R>0$ and let (g_{ij},K_{ij}) be initial data on $\mathcal{J}_R$ satisfying

$$g_{ij}-\delta_{ij}=O_2(r^{-\alpha}),\quad K_{ij}=O_1(r^{-1-\alpha}),\quad \alpha>(n-2)/2, \tag{2.10}$$

$$J^i=O(r^{-n-\epsilon}),\quad \rho=O(r^{-n-\epsilon}),\quad \epsilon>0. \tag{2.11}$$

Let N be a C^1 scalar field and Y^i a C^1 vector field on $\mathcal{J}_R$ such that

$$N-A^0=O_1(r^{-\alpha}),\quad Y^i\to_{r\to\infty}A^i, \tag{2.12}$$

for some set of constants $(A^\mu)\not\equiv 0$, satisfying

$$2NK_{ij}+\mathcal{L}_Y g_{ij}=O_1(r^{-(n-1)-\epsilon}). \tag{2.13}$$

Let p^μ be the ADM energy-momentum of $\mathcal{J}_R$. Then

(1) *If $A^0=0$, then $p^0=0$.*
(2) *If $A^0\neq 0$, then p^μ is proportional to A^μ.*

Proof: See the proof of Proposition 3.1 in Ref. 5. □

Proposition 2.3: Under the hypotheses of Proposition 2.2, suppose further that N is C^2 and that

$$\tau_{ij}=O(r^{-n-\epsilon}). \tag{2.14}$$

If

$$(A^0)^2<\sum_i A^iA^i, \tag{2.15}$$

then p^μ vanishes.

Proof: See the proof of Proposition 3.2 in Ref. 5. □

Proposition 2.4: Under the hypotheses of Proposition 2.2, assume moreover that N is C^2, that (2.14) holds and that

$$NK_{ij}+D_iY_j=O_1(r^{-(n-1)-\epsilon}), \tag{2.16}$$

$$K_{ij}Y^j+D_iN=O_1(r^{-(n-1)-\epsilon}), \tag{2.17}$$

$$A^\mu A_\mu\neq 0.$$

Then the ADM energy-momentum p^μ vanishes.

Proof: See the proof of Proposition 3.3 in Ref. 5. Note that the proof in Ref. 5 uses the equality of the Komar and the ADM masses for translational, asymptotically timelike Killing vectors, while Proposition 2.3 shows that one only needs to consider timelike A^μ's to complete the proof. The equality of those masses, which is well known in space-dimension three,[3] can also be established in higher dimensions by an asymptotic analysis of the stationary Einstein equations when the sources decay sufficiently fast. □

The notation used in the next theorem is explained in the Appendix.

Theorem 2.5: *Let $R>0$ and let (g_{ij},K_{ij}) be initial data on $\mathcal{J}_R=\mathbb{R}^n\backslash B(R)$ satisfying*

$$g_{ij}-\delta_{ij}=O_{3+\lambda}(r^{-\alpha}),\quad K_{ij}=O_{2+\lambda}(r^{-1-\alpha}), \tag{2.18}$$

$$\alpha>\begin{cases}1/2, & n=3,\\ n-3, & n\geqslant 4,\end{cases}\qquad \epsilon>0,\quad 0<\lambda<1. \tag{2.19}$$

$$J^i = O_{1+\lambda}(r^{-n-\epsilon}), \quad \rho = O_{1+\lambda}(r^{-n-\epsilon}). \tag{2.20}$$

Let N be a scalar field and Y^i a vector field on $\mathcal{J}_R$ such that

$$N \to_{r\to\infty} A^0, \quad Y^i \to_{r\to\infty} A^i, \quad A^\mu A_\mu = 0,$$

for some constants $A^\mu \not\equiv 0$. Suppose further that

$$2NK_{ij} + \mathcal{L}_Y g_{ij} = O_{3+\lambda}(r^{-(n-1)-\epsilon}), \tag{2.21}$$

$$\tau_{ij} = O_{1+\lambda}(r^{-n-\epsilon}), \tag{2.22}$$

Then the ADM energy-momentum of $\mathcal{J}_R$ vanishes.

Proof: See the proof of Theorem 3.4 in Ref. 5. We note that in our context, Ref. 5, Eq. (3.40) reads as follows:

$$g_{nA} = \begin{cases} C_{AB}(x^n)\partial_B \ln \rho + O_{(1)}(\rho^{-1-\epsilon} \ln \rho), & n = 3, \\ C_{AB}(x^n)\partial_B \dfrac{1}{\rho^{n-3}} + O_{(1)}(\rho^{-(n-2)-\epsilon}), & n \geqslant 4. \end{cases} \tag{2.23}$$

Similarly instead of Ref. 5, Eq. (3.47) we have

$$\frac{\partial g_{AB}}{\partial x^n} = \begin{cases} D_{ABCD}\partial_C\partial_D \ln \rho + O_{(1)}(\rho^{-2-\epsilon} \ln \rho), & n = 3, \\ D_{ABCD}\partial_C\partial_D \dfrac{1}{\rho^{n-3}} + O_{(1)}(\rho^{-(n-1)-\epsilon}), & n \geqslant 4. \end{cases} \tag{2.24}$$

Finally, there are misprints in the definitions of the quantities Ω and Ω' in the proof there; the correct definitions, in all dimensions, are

$$\Omega = \lim_{\rho\to\infty} \sum_C \int_{S^{n-2}(\rho,x^n)} (x^A \partial_C g_{nA} - g_{nC}) \mathrm{d}S_C,$$

$$\Omega' = \lim_{\rho\to\infty} \int_{S^{n-2}(\rho,x^n)} ((n-1)(x^A x^B \partial_C \partial_n g_{AB} - 2x^B \partial_n g_{CB}) - x^A x^A \partial_C \partial_n g_{BB} + 2x_C \partial_n g_{AB}) \mathrm{d}S_C,$$

where summation over every repeated occurrence of indices is implicitly understood, regardless of their positions. [We take this opportunity to point out that Eq. (2.20) of Ref. 5 should be replaced by $\rho = O_{k-2}(r^{-2-\alpha})$, $\tau_{ij} = O_{k-2}(r^{-2-\alpha})$. Furthermore, Eqs. (2.15) and (3.34) of Ref. 5 are mutually incompatible; the correct one is (2.15).] Here $\rho^2 = (x^1)^2 + \cdots + (x^{n-1})^2$, while $S^{n-2}(\rho,a)$ is a sphere (or circle, when $n=3$) of radius ρ centered at $x^1 = \cdots = x^{n-1} = 0$ lying in the plane $x^n = a$. Finally the $\mathrm{d}S_C$'s are the usual surface forms $\mathrm{d}S_C = \partial_C \rfloor (\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^{n-1})$, and $\rfloor$ denotes contraction. □

III. THE RIGID POSITIVE ENERGY THEOREM

The following strengthens somewhat Theorem 4.1 of Ref. 5 in the case $n=3$, and generalizes that theorem to higher dimensions; the calculations here are closely related to those in Ref. 8.

Theorem 3.1 [(rigid) positive energy theorem]: *Consider a data set $(\mathcal{J}, g_{ij}, K_{ij})$, with $(\mathcal{J}, g_{ij})$ a complete Riemannian spin manifold of dimension $n \geqslant 3$, and with $g_{ij} \in C^2$, $K_{ij} \in C^1$. Suppose that $\mathcal{J}$ contains an asymptotically flat end $\mathcal{J}_R$ diffeomorphic to $\mathbb{R}^n \backslash B(R)$ for some $R > 0$, with $B(R)$—a coordinate ball of radius R, where the fields (g, K) satisfy*

$$|g_{ij} - \delta_{ij}| + |r\partial_k g_{ij}| + |rK_{ij}| \leqslant Cr^{-\alpha}, \tag{3.1}$$

for some constants $C > 0$ and $\alpha > \max(1/2, n-3)$, with $r = \sqrt{\sum_{i=1}^n (x^i)^2}$. Suppose moreover that the quantities ρ and J,

$$2\rho := {}^3R + (K^k{}_k)^2 - K^{ij}K_{ij}, \tag{3.2}$$

$$J^k := D_l(K^{kl} - K^k{}_k g^{kl}), \tag{3.3}$$

satisfy

$$\sqrt{g_{ij}J^iJ^j} \leqslant \rho \leqslant C(1+r)^{-n-\epsilon}, \quad \epsilon > 0. \tag{3.4}$$

Then the ADM energy-momentum (m, p^i) *of any of the asymptotic ends of* $\mathcal{J}$ *satisfies*

$$m \geqslant \sqrt{p_i p^i}. \tag{3.5}$$

If $m=0$, *then* $\rho \equiv J^i \equiv 0$, *and there exists an isometric embedding* i *of* $\mathcal{J}$ *into Minkowski space-time* $(\mathbb{R}^{n+1}, \eta_{\mu\nu})$ *such that* K_{ij} *represents the extrinsic curvature tensor of* $i(\mathcal{J})$ *in* $(M, \eta_{\mu\nu})$. *Moreover* $i(\mathcal{J})$ *is an asymptotically flat Cauchy surface in* $(\mathbb{R}^{n+1}, \eta_{\mu\nu})$.

Theorem 3.1 has been formulated under differentiability requirements which are stronger than necessary, compare Refs. 2 and 9. Unfortunately our proof that ADM energy-momentum cannot be null requires even more differentiability and asymptotic decay conditions.

Theorem 3.2: *Under the hypotheses of Theorem 3.1, suppose moreover that*

$$g_{ij} - \delta_{ij} = O_{3+\lambda}(r^{-\alpha}), \quad K_{ij} = O_{2+\lambda}(r^{-1-\alpha}), \tag{3.6}$$

$$\rho = O_{1+\lambda}(r^{-n-\epsilon}), \tag{3.7}$$

with some $0 < \lambda < 1$. *Then the ADM energy-momentum cannot be null.*

Proofs of Theorems 3.1 and 3.2: We use a Witten-type argument, as follows. Let $(\mathfrak{S}, \langle\cdot,\cdot\rangle)$ be any Riemannian bundle of real spinors over (M, g) with scalar product $\langle\cdot,\cdot\rangle$, such that Clifford multiplication (which we denote by $X\cdot$) is antisymmetric. We suppose that there exists a bundle isomorphism $\gamma_0 : \mathfrak{S} \to \mathfrak{S}$ with the following properties:

$$\gamma_0^2 = 1, \tag{3.8a}$$

$$\forall X \in TM, \quad \gamma_0 X\cdot = -X\cdot\gamma_0, \tag{3.8b}$$

$${}^t\gamma_0 = \gamma_0, \tag{3.8c}$$

$$D\gamma_0 = \gamma_0 D, \tag{3.8d}$$

where ${}^t\gamma_0$ denotes the transpose of γ_0 with respect to $\langle\cdot,\cdot\rangle$, and D is the usual Riemannian spinorial connection associated with the metric g.

[Such a map always exists if $\mathfrak{S}$ is obtained by pulling-back a space-time spinor bundle, using an externally oriented isometric embedding of (M, g) in a Lorentzian space-time. Then the Clifford product $n\cdot$, where n is the field of Lorentzian unit normals to the image of M, has the required properties. If, however, such a map does not exist, we proceed as follows: let $\mathfrak{S}' = \mathfrak{S} \oplus \mathfrak{S}$ be the direct sum of two copies of $\mathfrak{S}$, equipped with the direct sum metric $\langle\cdot,\cdot\rangle_\oplus$:

$$\langle(\psi_1,\psi_2),(\varphi_1,\varphi_2)\rangle_\oplus := \langle\psi_1,\varphi_1\rangle + \langle\psi_2,\varphi_2\rangle. \tag{3.9}$$

We set, for $X \in TM$,

$$\gamma_0(\psi_1,\psi_2) := (\psi_2,\psi_1), \tag{3.10a}$$

$$X\cdot(\psi_1,\psi_2) := (X\cdot\psi_1, -X\cdot\psi_2), \tag{3.10b}$$

$$D_X(\psi_1,\psi_2) := (D_X\psi_1, D_X\psi_2). \tag{3.10c}$$

One readily verifies that (3.10b) defines a representation of the Clifford algebra on $\mathfrak{S}'$, and that (3.8) holds.]

Given an initial data set (M, g, K), a vector field X, and a spinor field ξ we set

$$K(X) := K_i{}^j X^i e_j \cdot , \tag{3.11}$$

$$\nabla_X \xi := D_X \xi + \tfrac{1}{2} K(X) \gamma_0 \xi. \tag{3.12}$$

Here e_i is a local orthonormal basis of TM; it is straightforward to check that (3.11) does not depend upon the choice of this basis. (To make things clear, (3.12) defines ∇ in terms of the Riemannian spin connection D and of the extrinsic curvature tensor K_{ij}. If the spin bundle arises from a space-time bundle, then ∇ coincides with the canonical space-time spinorial derivative, when restricted to space directions.)

We will need an explicit expression for the curvature of ∇.

Proposition 3.3: For every $X, Y \in \Gamma(T\mathcal{J})$ we have

$$R_{X,Y} = {}^n R_{X,Y} + \tfrac{1}{2} \mathrm{d}^D K(X,Y) \gamma_0 - \tfrac{1}{4} (K(X)K(Y) - K(Y)K(X)), \tag{3.13}$$

where R is the curvature of ∇, ${}^n R$ is that of D, and

$$\mathrm{d}^D K(e_i, e_j) = (K^k{}_{j;i} - K^k{}_{i;j}) e_k.$$

Proof: We have

$$\begin{aligned}
\nabla_X \nabla_Y \psi &= \left(D_X + \tfrac{1}{2} K(X) \gamma_0\right)\left(D_Y \psi + \tfrac{1}{2} K(Y) \gamma_0 \psi\right) \\
&= D_X D_Y \psi + \tfrac{1}{2} K(X) \gamma_0 D_Y \psi + \tfrac{1}{2} ((D_X K)(Y) \gamma_0 \psi + K(D_X Y) \gamma_0 \psi + K(Y) \gamma_0 D_X \psi) \\
&\quad + \tfrac{1}{4} K(X) \gamma_0 K(Y) \gamma_0 \psi \\
&= D_X D_Y \psi + \tfrac{1}{2} (K(X) \gamma_0 D_Y \psi + K(Y) \gamma_0 D_X \psi) + \tfrac{1}{2} ((D_X K)(Y) \gamma_0 \psi + K(D_X Y) \gamma_0 \psi) \\
&\quad - \tfrac{1}{4} K(X) K(Y) \psi,
\end{aligned}$$

so that

$$\begin{aligned}
R_{X,Y} \psi &= \nabla_X \nabla_Y \psi - \nabla_Y \nabla_X \psi - \nabla_{[X,Y]} \psi \\
&= D_X D_Y \psi - D_Y D_X \psi - D_{[X,Y]} \psi - \tfrac{1}{2} K([X,Y]) \gamma_0 \psi \\
&\quad + \tfrac{1}{2} (((D_X K)(Y) - (D_Y K)(X)) \gamma_0 \psi + K(D_X Y - D_Y X) \gamma_0 \psi) \\
&\quad - \tfrac{1}{4} (K(X)K(Y) - K(Y)K(X)) \psi,
\end{aligned}$$

and the vanishing of the torsion of the Levi-Civita connection gives the result. □

We now run the usual Witten argument (see, e.g., Ref. 2) using the connection ∇ and the associated Dirac operator $\mathcal{D} = e^i \cdot \nabla_i$. Under the current conditions the ADM energy-momentum of $\mathcal{J}$ is finite and well defined,[1,6] and the Witten boundary integral reproduces the ADM energy-momentum. The arguments in Ref. 2 shows that, again under the current conditions, for every spinor field $\mathring{\psi}$, with constant entries in the natural spin frame in the asymptotic region, one can find a solution ψ to the Witten equation which asymptotes to $\mathring{\psi}$. Witten's identity subsequently implies that

$$\langle \mathring{\psi}, p \cdot \mathring{\psi} \rangle \geqslant 0, \tag{3.14}$$

where

$$p\cdot := m\gamma_0 + p^i e_i\cdot ,$$

and $p=(m,p^i)$ is the ADM momentum. This gives (3.5).

The equality case, which is the main interest here, is only possible if p is lightlike or vanishes. In either case one obtains a spinor field $\psi\in\Gamma(\mathfrak{S})$ which is asymptotic to $\mathring{\psi}$, and satisfies

$$\nabla\psi = 0, \tag{3.15}$$

$$\langle\psi,\mathcal{R}\psi\rangle = 0. \tag{3.16}$$

Here

$$\mathcal{R} := \tfrac{1}{2}(\rho + J^i e_i\cdot\gamma_0)$$

is the (non-negative) spinorial endomorphism which appears in the identity

$$\mathcal{D}^*\mathcal{D} = \nabla^*\nabla + \mathcal{R}.$$

The idea of the calculations that follow is to show, roughly speaking, that the space-time is a *pp*-wave space-time, perhaps with matter decaying at infinity, with a null Killing vector, which by the results in the preceding section is only possible if we are in Minkowski space-time. We start with an analysis of the curvature tensor.

As ψ is ∇-parallel we have $R_{XY}\psi=0$, and from Proposition 3.3 one finds, for all $X,Y\in T\mathcal{J}$,

$$\langle {}^nR_{X,Y}\psi,\psi\rangle - \tfrac{1}{2}\langle \mathrm{d}^D K(X,Y)\cdot\gamma_0\psi,\psi\rangle - \tfrac{1}{4}\langle (K(X)K(Y)-K(Y)K(X))\psi,\psi\rangle = 0.$$

Both the first and third term vanish since the spinorial curvature can be written as

$${}^nR_{XY}\psi = -\frac{1}{2}\sum_{i<j} {}^nR(X,Y,e_i,e_j)e_i\cdot e_j\cdot\psi,$$

and since the Clifford product of two distinct elements of an ON basis is antisymmetric. [We use the conventions

$${}^nR(e_i,e_j)e_k = D_{e_i}D_{e_j}e_k - D_{e_j}D_{e_i}e_k - D_{[e_i,e_j]}e_k = {}^nR^s{}_{kij}e_s = {}^nR(e_m,e_k,e_i,e_j)g^{sm}e_s,$$

$${}^nR_{ij} = {}^nR^k{}_{ikj},$$

where ${}^nR_{ij}$ is the Ricci tensor of g.] Thus we obtain

$$\langle \mathrm{d}^D K(X,Y)\gamma_0\psi,\psi\rangle = 0. \tag{3.17}$$

Let us denote by N the function

$$N = \langle\psi,\psi\rangle, \tag{3.18}$$

and by Y the real 1-form defined as

$$Y(X) = -\langle\gamma_0 X\cdot\psi,\psi\rangle. \tag{3.19}$$

Using this notation, (3.17) can be rewritten as

$$K_{ki;j}Y^k = K_{kj;i}Y^k. \tag{3.20}$$

We continue with the following calculation:

$$\sum_{k=1}^{n} e_k \cdot R_{e_s,e_k} = \sum_{k=1}^{n} e_k \cdot \left({}^n R_{e_s,e_k} - \frac{1}{4}(K(e_s)K(e_k) - K(e_k)K(e_s)) + \frac{1}{2}\mathrm{d}^D K(e_s,e_k)\gamma_0 \right)$$

$$= -\frac{1}{4}({}^n R_s{}^{kij} + K_s{}^i K^{kj} - K^{ki}K_s{}^j)e_k \cdot e_i \cdot e_j \cdot + \frac{1}{2}(K^{mk}{}_{;k} - K^m{}_s{}^{;k})e_k \cdot e_m \cdot \gamma_0. \tag{3.21}$$

In order to analyze the curvature terms in the before-last line of (3.21), recall the convenient identity [to prove (3.22), note first that the result is clearly true if all indices are distinct or equal; the final formula follows by inspection of the remaining possibilities].

$$e_k \cdot e_i \cdot e_j \cdot = e_{[k} \cdot e_i \cdot e_{j]} \cdot - g_{ki} e_j \cdot + g_{ij} e_k \cdot - g_{kj} e_i \cdot \ . \tag{3.22}$$

(Square brackets around indices denote antisymmetrization, and parentheses denote symmetrization.) The Bianchi identity ${}^n R_s{}^{[kij]} = 0$ immediately implies

$${}^n R_s{}^{kij} e_k \cdot e_i \cdot e_j \cdot = 2 {}^n R_s{}^i e_i \cdot .$$

Next, the undifferentiated extrinsic curvature terms in next-to-last line of (3.21) can be manipulated as

$$K_s{}^i K^{kj} \underbrace{e_k \cdot e_i \cdot}_{-2g_{ki} - e_i \cdot e_k \cdot} e_j \cdot - K_s{}^j \underbrace{K^{ki} e_k \cdot e_i \cdot}_{-K^{ki} g_{ki}} e_j \cdot = -2K_s{}^i K^{kj} g_{ki} e_j \cdot - K_s{}^i e_i \cdot \underbrace{K^{kj} e_k \cdot e_j \cdot}_{-K^{ki} g_{kj}} + K_s{}^j K^{ki} g_{ki} e_j \cdot$$

$$= 2(-K^{kj}K_{sk} + K^k{}_k K_s{}^j) e_j \cdot ,$$

which results in

$$({}^n R_s{}^{kij} + K_s{}^i K^{kj} - K^{ki} K_s{}^j) e_k \cdot e_i \cdot e_j \cdot = 2({}^n R_s{}^i + K^k{}_k K_s{}^i - K^{ki} K_{sk}) e_i \cdot =: 2E_s{}^i e_i \cdot =: 2E(e_s). \tag{3.23}$$

Using again that ψ is ∇-parallel we have $\Sigma_{k=1}^n e_k \cdot R_{e_s,e_k}\psi = 0$. Equations (3.21) and (3.23) show that

$$(E(e_s) - (K^{mk}{}_{;s} - K^m{}_s{}^{;k}) e_k \cdot e_m \cdot \gamma_0)\psi = 0.$$

Multiplying by $e_r \cdot$ and taking a scalar product with ψ we obtain

$$-NE_{rs} = (K^{mk}{}_{;s} - K^m{}_s{}^{;k}) \langle \psi, \underbrace{e_r \cdot e_k \cdot e_m \cdot}_{= e_{[r} \cdot e_k \cdot e_{m]} \cdot - g_{rk} e_m \cdot + g_{rm} e_k \cdot - g_{km} e_r \cdot} \gamma_0 \psi \rangle$$

$$= (K^{mk}{}_{;s} - K^m{}_s{}^{;k}) \langle \psi, (-g_{rk} e_m \cdot + g_{rm} e_k \cdot - g_{km} e_r \cdot) \gamma_0 \psi \rangle$$

$$= (K^{mk}{}_{;s} - K^m{}_s{}^{;k})(-g_{rk} Y_m + g_{rm} Y_k - g_{km} Y_r) = -(K_{rs;k} - K_{ks;r}) Y^k + J_s Y_r, \tag{3.24}$$

where we have used the fact that the products $e_r \cdot e_m \cdot$ and $e_r \cdot e_k \cdot e_m \cdot \gamma_0$ are antisymmetric when all indices are distinct, and therefore give no contribution in (3.24). Hence

$$N({}^n R_{ij} + K^k{}_k K_{ij} - K_{ik} K^k{}_j) = (K_{ij;k} - K_{kj;i}) Y^k - J_j Y_i. \tag{3.25}$$

Taking a trace implies

$$N\rho = -J^i Y_i. \tag{3.26}$$

Antisymmetrizing (3.25) in i and j and using (3.20) one finds

$$J_i = \sigma Y_i \tag{3.27}$$

for some function σ.

We wish, now, to show that the pair (N, Y^i) defined by (3.18) and (3.19) satisfies (2.2). It is convenient to choose an ON basis $\{e_i\}_{i=1}^n$ which satisfies $e_i=\partial_i$ and $D_{e_i}e_j=0$ at the point under consideration, then

$$\begin{aligned}
-D_iY_j &= \partial_i\langle\gamma_0 e_j\cdot\psi,\psi\rangle = \langle\gamma_0 e_j\cdot D_i\psi,\psi\rangle + \langle\gamma_0 e_j\cdot\psi, D_i\psi\rangle \\
&= 2\langle\gamma_0 e_j\cdot \underbrace{D_i\psi}_{-\frac{1}{2}K_i^k e_k\cdot\gamma_0\psi},\psi\rangle \\
&= -K_i^k\langle e_j\cdot e_k\cdot\psi,\psi\rangle = -K_i^k\underbrace{\langle e_{[j}\cdot e_{k]}\cdot\psi,\psi\rangle}_{0} - K_i^k\underbrace{\langle e_{(j}\cdot e_{k)}}_{-g_{jk}}\cdot\psi,\psi\rangle \\
&= NK_{ij},
\end{aligned}$$

as desired.

Next,

$$D_iN = \partial_i\langle\psi,\psi\rangle = 2\langle\psi, D_i\psi\rangle = -\langle\psi, K_i^k e_k\gamma_0\psi\rangle = -K_{ik}Y^k$$

[compare (2.17)]. For further use we note that $d(N^2-|Y|^2)=0$, and as $N^2-|Y|^2\to_{r\to\infty}0$ [since equality is attained in (3.14)] we conclude that

$$N^2 = |Y|^2.$$

Further differentiation yields

$$D_iD_jN = N(K\circ K)_{ij} - D_iK_{jk}Y^k.$$

Inserting this into (2.5) and using the relations above leads to our key formula

$$N^2\tau_{ij} = \rho Y_iY_j. \tag{3.28}$$

Note that $N\to_{r\to\infty}0$ implies $Y\to_{r\to\infty}0$. The last part of Proposition 2.1 gives then $N\equiv 0$, hence $\psi=0$, contradicting the fact that we have a nontrivial solution of the Witten equation. Thus N approaches a nonzero constant at infinity by (2.9), and our hypothesis on the decay of ρ provides decay of τ_{ij}. We can therefore apply Proposition 2.4 and Theorem 2.5 to conclude that the ADM momentum vanishes. But then for any $\mathring{\psi}$ there exists an associated ∇-parallel ψ. Let $\mathring{\psi}_a$, $a=1,\ldots,m$, form a basis and let ψ_a be the parallel spinor that asymptotes to $\mathring{\psi}_a$. Now,

$$\nabla\langle\psi_a,\psi_b\rangle = 0,$$

which implies that the ψ_a's form a basis of $\mathfrak{S}_p$ at every $p\in\mathcal{J}$. It follows that $R_{XY}\psi_a=0$ for a collection of spinors forming a basis at each point, hence

$$R_{XY} = 0. \tag{3.29}$$

Choose $\mathring{\psi}$ so that $N\to 1$ and $Y\to 0$. [If no such $\mathring{\psi}$ exists, we pass to $\mathfrak{S}'$ with the structures defined by (3.9) and (3.10), choose any $\mathring{\chi}$ with norm one-half, then $\mathring{\psi}=(\mathring{\chi},\mathring{\chi})$ will have the desired property.] Let $\widetilde{\mathcal{J}}$ be the universal covering space of $\mathcal{J}$ with corresponding data $(\widetilde{\mathcal{J}},\widetilde{g}_{ij},\widetilde{K}_{ij},\widetilde{N},\widetilde{Y}^j)$, and consider the *Killing development* thereof: by definition, this is $\widetilde{\mathcal{M}}=\mathbb{R}\times\widetilde{\mathcal{J}}$ endowed with the metric

$$\tilde{g}_{\mu\nu} = -\tilde{N}^2\,\mathrm{d}u^2 + \tilde{g}_{ij}(\mathrm{d}x_i + \tilde{Y}^i\,\mathrm{d}u)(\mathrm{d}x_j + \tilde{Y}^j\,\mathrm{d}u),$$

where $\tilde{N}(u,x)=\tilde{N}(x)$, $\tilde{g}_{ij}(u,x)=\tilde{g}_{ij}(x)$, $\tilde{Y}^j(u,x)=\tilde{Y}^j(x)$. Similarly let $(\mathcal{M},g_{\mu\nu})$ be the Killing development of $(\mathcal{J},g_{ij},K_{ij},N,Y^j)$. It should be clear that $(\tilde{\mathcal{M}},\tilde{g}_{\mu\nu})$ is the universal pseudo-Riemannian covering of $(\mathcal{M},g_{\mu\nu})$.

Equations (3.26)–(3.29) and the Codazzi-Mainardi embedding equations [compare (3.13)] show then that both $(\tilde{\mathcal{M}},\tilde{g}_{\mu\nu})$ and $(\mathcal{M},g_{\mu\nu})$ are flat. The remaining arguments of the proof of Ref. 5 Theorem 4.1 apply to show that $(\tilde{\mathcal{M}},\tilde{g}_{\mu\nu})=(\mathcal{M},g_{\mu\nu})=(\mathbb{R}^{n+1},\eta_{\mu\nu})$, as desired. □

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APPENDIX: WEIGHTED HÖLDER SPACES

Consider a function f defined on $\mathcal{J}_R\equiv\mathbb{R}^n\backslash B(R)$, where $B(R)$ is a closed ball of radius $R>0$. We shall write $f=O_k(r^\beta)$ if there exists a constant C such that we have

$$0\leqslant i\leqslant k,\quad |\partial^i f|\leqslant Cr^{\beta-i}.$$

For $\sigma\in(0,1)$ we shall write $f=O_{k+\sigma}(r^\beta)$ if $f=O_k(r^\beta)$ and if there exists a constant C such that we have

$$|y-x|\leqslant r(x)/2 \Rightarrow |\partial^k f(x)-\partial^k f(y)|\leqslant C|x-y|^\sigma r^{\beta-k-\sigma}.$$

Let us note that $f=O_{k+1}(r^\beta)$ implies $f=O_{k+\sigma}(r^\beta)$ for all $\sigma\in(0,1)$, so that the reader unfamiliar with Hölder type spaces might wish to simply replace, in the hypotheses of our theorems, the $k+\sigma$ by $k+1$ wherever convenient.

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A systematic derivation of the Riemannian Barrett-Crane intertwiner

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The Barrett-Crane intertwiner for the Riemannian general relativity is systematically derived by solving the quantum Barrett-Crane constraints corresponding to a tetrahedron (except for the nondegeneracy condition). It was shown by Reisenberger that the Barrett-Crane intertwiner is the unique solution. The systematic derivation can be considered as an alternative proof of the uniqueness. The new element in the derivation is the rigorous imposition of the cross-simplicity constraint. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168397]

I. INTRODUCTION

A quantization of a four-simplex for the Riemannian general relativity was proposed by Barrett and Crane.[1] It was built on the idea of the Barrett-Crane intertwiner. It was shown by Reisenberger[2] that the Barrett-Crane intertwiner is the unique solution to the Barrett-Crane constraints corresponding a tetrahedron (except for the nondegeneracy condition). Here we present an alternative proof of uniqueness by systematically deriving the Barrett-Crane intertwiner by imposing the Barrett-Crane constraints.

II. REVIEW

The bivectors B_i associated with the 10 triangles of a four-simplex in a flat Riemannian space satisfy the following properties called the Barrett-Crane constraints:[1]

(1) The bivector changes sign if the orientation of the triangle is changed.
(2) Each bivector is simple.
(3) If two triangles share a common edge, then the sum of the bivectors is also simple.
(4) The sum of the bivectors corresponding to the edges of any tetrahedron is zero. This sum is calculated taking into account the orientations of the bivectors with respect to the tetrahedron.
(5) The six bivectors of a four-simplex sharing the same vertex are linearly independent.
(6) The volume of a tetrahedron calculated from the bivectors is real and non-zero.

The items two and three can be summarized as follows:

$$B_i \wedge B_j = 0 \quad \forall\, i,j,$$

where $A \wedge B = \varepsilon_{IJKL} A^{IJ} B^{KL}$ and the i,j represents the triangles of a tetrahedron. If $i=j$, it is referred to as the simplicity constraint. If $i \neq j$ it is referred as the cross-simplicity constraints.

Barrett and Crane have shown[1] that these constraints are sufficient to restrict a general set of 10 bivectors E_b so that they correspond to the triangles of a geometric four-simplex up to translations and rotations in a four dimensional flat Riemannian space.

A quantum four-simplex for Riemannian general relativity is defined by quantizing the Barrett-Crane constraints.[1] The bivectors B_i are promoted to the Lie operators $\hat{B}_i$ on the representation space of the relevant group and the Barrett-Crane constraints are imposed at the quantum level. The last two constraints are inequalities and they are difficult to impose. For these reasons

here after we refer to a state sum model that satisfies only the first four constraints as an *essential Barrett-Crane model*, while a state sum model that satisfies all the six constraints as a *rigorous Barrett-Crane model*. The Barrett-Crane intertwiner corresponds to essential Barrett-Crane model only. We will do a systematic derivation of the essential Barrett-Crane model here.

A. The simplicity constraint

Our treatment of the simplicity constraints is basically a review of work done before.[1,3] The group $SO(4,R)$ is isomorphic to $SU(2)\times SU(2)/Z_2$. An element B of the Lie algebra of $SO(4)$ can be split into the left-handed and the right-handed $SU(2)$ components,

$$B = B_L + B_R. \tag{1}$$

There are two Casimir operators for $SO(4)$ which are

$$\varepsilon_{IJKL}B^{IJ}B^{KL}$$

and

$$\delta_{IK}\delta_{JL}B^{IJ}B^{KL},$$

where η_{IK} is the flat Euclidean metric. In terms of the left- and right-handed split we can expand the Casimir operators as

$$\varepsilon_{IJKL}B^{IJ}B^{KL} = B_L \cdot B_L - B_R \cdot B_R$$

and

$$\delta_{IK}\delta_{JL}B^{IJ}B^{KL} = B_L \cdot B_L + B_R \cdot B_R,$$

where the dot products are the trace in the $SU(2)$ Lie algebra coordinates.

The bivectors are to be quantized by promoting the Lie algebra vectors to Lie operators on the unitary representation space of $SO(4)\cong SU(2)\times SU(2)/Z_2$. The relevant unitary representations of $SO(4)$ are labeled by a pair (J_L,J_R) of unitary representations of $SU(2)$. The elements of the representation space $D_{J_L}\otimes D_{J_R}$ are the eigenstates of the Casimirs and on them the operators reduce to the following:

$$\varepsilon_{IJKL}\hat{B}^{IJ}\hat{B}^{KL} = \frac{J_L(J_L+1) - J_R(J_R+1)}{2}\hat{I} \tag{2}$$

and

$$\delta_{IK}\delta_{JL}\hat{B}^{IJ}\hat{B}^{KL} = \frac{J_L(J_L+1) + J_R(J_R+1)}{2}\hat{I}. \tag{3}$$

The equation (2) implies that on $D_{J_L}\otimes D_{J_R}$ the simplicity constraint $B\wedge B=0$ is equivalent to the condition $J_L=J_R$. We would like to find a representation space on which the representations of $SO(4)$ are restricted precisely by $J_L = J_R$.

In Ref. 3 it has been shown for $SO(N,R)$ that the simplicity constraint reduces the Hilbert space associated to a triangle to that of the L^2 functions on S^{N-1}. Consider a square integrable function $f(x)$ on the sphere S^3 defined by

$$x \cdot x = 1, \quad \forall\, x \in \mathbf{R}^4.$$

It can be Fourier expanded in the representation matrices of $SU(2)$ using the isomorphism $S^3 \cong SU(2)$,

$$f(x) = \sum_J d_J \,\mathrm{Tr}(F_J T_J(\mathfrak{g}(x)^{-1})), \tag{4}$$

where $\mathfrak{g}: S^3 \to \mathrm{SU}(2)$ is an isomorphism from S^3 to $\mathrm{SU}(2)$, $F^{m_1}_{m_2 J}$ the Fourier coefficients, $T^{m_1}_{m_2 J}(g)$ are the matrix elements of spin J representation of an element $g \in \mathrm{SU}(2)$ and d_J the dimension of the J representation. The group action of $g=(g_L, g_R) \in \mathrm{SO}(4)$ on $x \in S^3$ is given by

$$\mathfrak{g}(gx) = g_L^{-1}\mathfrak{g}(x)g_R. \tag{5}$$

Using Eq. (4) we can consider the $T_J(\mathfrak{g}(x))(m_1, m_2)$ as the basis functions of L^2 functions on S^3. The matrix elements of the action of g on S^3 is given by

$$\int \overline{T^{m_1}_{m_2' J'}}(\mathfrak{g}(x)) T^{m_1}_{m_2 J}(\mathfrak{g}(gx))\mathrm{d}x = \frac{1}{d_J}\overline{T^{m_1}_{m_1' J'}}(g_L) T^{m_2'}_{m_2 J}(g_R)\delta(J' - J).$$

The representation matrices are precisely those of SO(4) only restricted by the constraint $J_L = J_R$. Since we have all the simple representations included in the representation, the simplicity constraint effectively reduces the Hilbert space H to the space of L^2 functions on S^3.

B. The cross-simplicity constraints

Next we quantize the cross-simplicity constraint part of the Barrett-Crane constraint. Consider the quantum state space associated with a pair of triangles 1 and 2 of a tetrahedron. A general quantum state that just satisfies the simplicity constraints $B_1 \wedge B_1 = 0$ and $B_2 \wedge B_2 = 0$ is of the form $f(x_1, x_2) \in L^2(S^3 \times S^3)$, $x_1, x_2 \in S^3$.

On the elements of $L^2(S^3 \times S^3)$ the action $B_1 \wedge B_2$ is equivalent to the action of $(B_1 + B_2) \wedge (B_1 + B_2)$. [Please notice that $(\hat{B}_1 + \hat{B}_2) \wedge (\hat{B}_1 + \hat{B}_2) = \hat{B}_1 \wedge \hat{B}_1 + \hat{B}_2 \wedge \hat{B}_2 + 2B_1 \wedge \hat{B}_2$. But since $\hat{B}_1 \wedge \hat{B}_1 = \hat{B}_2 \wedge \hat{B}_2 = 0$ on $f(x_1, x_2)$ we have $(\hat{B}_1 + \hat{B}_2) \wedge (\hat{B}_1 + \hat{B}_2) f(x_1, x_2) = \hat{B}_1 \wedge \hat{B}_2 f(x_1, x_2)$.] This implies that the cross-simplicity constraint $B_1 \wedge B_2 = 0$ requires the simultaneous rotation of x_1, x_2 involve only the $J_L = J_R$ representations. The simultaneous action of $g=(g_L, g_R)$ on the arguments of $f(x_1, x_2)$ is

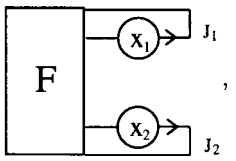
$$gf(x_1, x_2) = f(g_L^{-1} x_1 g_R, g_L^{-1} x_2 g_R). \tag{6}$$

The harmonic expansion of $f(x_1, x_2)$ in terms of the basis function $T_J(\mathfrak{g}(x))(m_1, m_2)$ is

$$f(x_1, x_2) = \sum_J F^{m_1' m_2'}_{m_1 m_2 J_1 J_2} T^{m_1}_{m_1' J_1}(\mathfrak{g}(x_1)) T^{m_2}_{m_2' J_2}(\mathfrak{g}(x_2)).$$

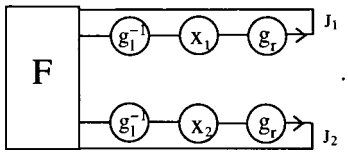
The rest of the calculations can be understood graphically. The last equation can be graphically written as follows:

$$f(x_1, x_2) = \sum_{J_1 J_2}$$



where the box F represents the Fourier coefficient $F^{m_1' m_2'}_{m_1 m_2 J_1 J_2}$. The action of $g \in \mathrm{SO}(4)$ on f is

$$gf(x_1,x_2)=\sum_{J_1J_2}$$



(7)

Now for any $h\in \mathrm{SU}(2)$,

$$T^{b_1}_{a_1J_1}(h)T^{b_2}_{a_2J_1}(h)=\sum_{J_3} C^{b_1b_2J_3}_{J_1J_2b_3}\overline{C}^{J_1J_2a_3}_{a_1a_2J_3}T^{b_3}_{a_3J_3}(h),$$

where C's are the Clebsch-Gordan coefficients of SU(2).[4] We have assumed all the repeated indices are either integrated or summed over for the previous and the next two equations. Using this we can rewrite the g_L and g_R parts of the result (7) as follows:

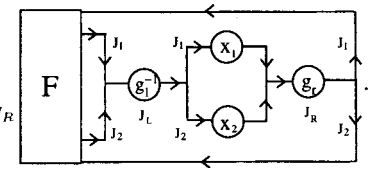
$$T^{m_1}_{a_1J_1}(g_L^{-1})T^{m_2}_{a_2J_2}(g_L^{-1})=\sum_{J_L} C^{m_1m_2J_L}_{J_1J_2m_3}\overline{C}^{J_1J_2a_3}_{a_1a_2J_L}T^{m_3}_{a_3J_L}(g_L^{-1}) \tag{8}$$

and

$$T^{b_1}_{\acute{m}_1J_1}(g_R)T^{b_2}_{\acute{m}_2J_2}(g_R)=\sum_{J_L} C^{b_1b_2J_R}_{J_1J_2b_3}\overline{C}^{J_1J_2\acute{m}_3}_{\acute{m}_1\acute{m}_2J_R}T^{b_3}_{\acute{m}_3J_R}(g_R). \tag{9}$$

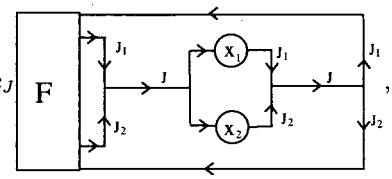
Now we have

$$gf(x_1,x_2)=\sum_{J_1J_2J_LJ_R}$$



To satisfy the cross-simplicity constraint the expansion of $gf(x_1,x_2)$ must have contribution only from the terms with $J_L=J_R$. Let me remove all the terms which do not satisfy $J_L=J_R$. Also let me set $g=I$. Now we can deduce that the functions denoted by $\tilde{f}(x_1,x_2)$ obtained by reducing $f(x_1,x_2)$ using the cross-simplicity constraints must have the expansion,

$$\tilde{f}(x_1,x_2)=\sum_{J_1J_2J} c_J$$



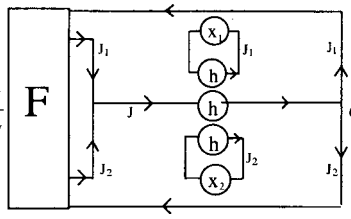
(10)

where the coefficients c_J introduced depends on the precise definition of the cross-simplicity projector. But as we will see, the final answer does not depend on the c_J's. Now the Clebsch-Gordan coefficient terms in the expansion can be reexpressed using the following equation:

$$C^{m_1m_2J}_{J_1J_2m_3}\overline{C}^{J_1J_2\acute{m}_3}_{\acute{m}_1\acute{m}_2J}=\frac{1}{d_J}\int_{\mathrm{SU}(2)} T^{m_1}_{\acute{m}_1J_1}(h)T^{m_2}_{\acute{m}_2J_2}(h)\overline{T}^{m_3}_{m_3J}(h)\mathrm{d}h, \tag{11}$$

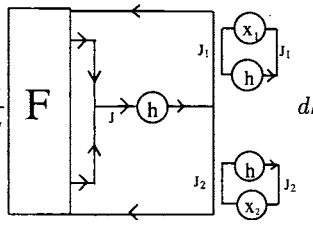
where h, $\tilde{h}\in \mathrm{SU}(2)$ and dh the bi-invariant measure on SU(2). Using this in the two middle Clebsch-Gordan coefficients of $\tilde{f}(x_1,x_2)$ we get

$$\tilde{f}(x_1,x_2)=\sum_{J_1J_2J}\int_{SU(2)}\frac{c_J}{d_J}$$



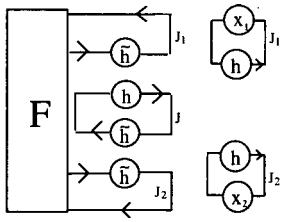
This result can be rewritten for clarity as

$$\tilde{f}(x_1,x_2)=\sum_{J_1J_2J}\int_{SU(2)}\frac{c_J}{d_J}$$



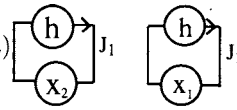
Once again applying Eq. (11) to the remaining two Clebsch-Gordan coefficients we get

$$\tilde{f}(x_1,x_2)=\sum_{J_1J_2J}c_J\iint_{SU(2)\times SU(2)}\left(\frac{1}{d_J}\right)^2$$



By rewriting the above expression, we deduce that a general function $\tilde{f}(x_1,x_2)$ that satisfies the cross-simplicity constraint must be of the form

$$\tilde{f}(x_1,x_2)=\sum_{J_1J_2}\int_{SU(2)}F_{J_1J_2}(h)$$



$$dh,$$

$$=\sum_{J_1J_2}\int_{SU(2)}F_{J_1J_2}(h)tr(T_{J_1}(\mathfrak{g}(x_1)h)tr(T_{J_2}(\mathfrak{g}(x_2)h)dh,$$

where $F_{J_1J_2}(h)$ is arbitrary.

If $\Psi(x_1,x_2,x_3,x_4)$ is the quantum state of a tetrahedron that satisfies all of the simplicity constraints and the cross-simplicity constraints, it must be of the form

$$\Psi(x_1,x_2,x_3,x_4) \tag{12}$$

$$=\sum_{J_1J_2J_3J_4}F_{J_1J_2J_3J_4}(h)\mathrm{tr}(T_{J_1}(\mathfrak{g}(x_1)h)\mathrm{tr}(T_{J_2}(\mathfrak{g}(x_2)h)$$

$$\mathrm{tr}(T_{J_3}(\mathfrak{g}(x_3)h)\mathrm{tr}(T_{J_4}(\mathfrak{g}(x_4)h)\mathrm{d}h.$$

This general form is deduced by requiring that for every pair of variables with the other two fixed, the function must be the form of the right-hand side of Eq. (12)

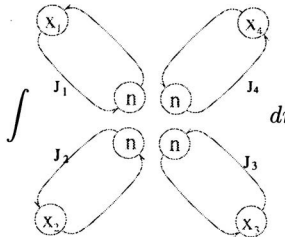
C. The SO(4) Barrett-Crane intertwiner

Now the quantization of the fourth Barrett-Crane constraint demands that Ψ is invariant under the simultaneous rotation of its variables. This is achieved if $F_{J_1J_2J_3J_4}(h)$ is a constant function of h. Therefore the quantum state of a tetrahedron is spanned by

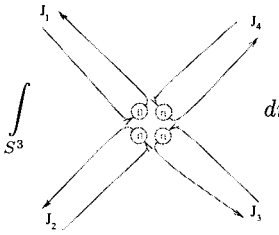
$$\Psi_{J_1J_2J_3J_4}(x_1,x_2,x_3,x_4) = \int_{n\in S^3} \prod_i T_{J_i}(\mathfrak{g}(x_i)\mathfrak{g}(n))\mathrm{d}n, \tag{13}$$

where the measure dn on S^3 is derived from the bi-invariant measure on SU(2).

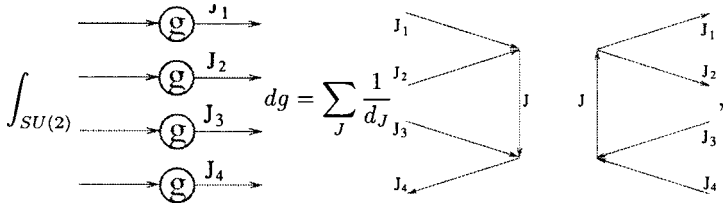
The quantum state can be diagrammatically represented as follows:

$\Psi_{J_1J_2J_3J_4}(x_1,x_2,x_3,x_4) =$  $dn.$

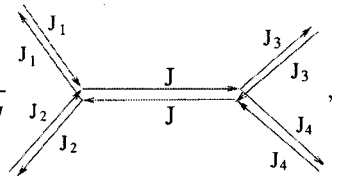
A unitary representation T_J of $SU(2)$ can be considered as an element of $D_J \otimes D_J^*$ where D_J^* is the dual representation of D_J. So using this the Barrett-Crane intertwiner can be written as an element $|\Psi_{J_1J_2J_3J_4}\rangle \in \otimes_i D_{J_i} \otimes D_{J_i}^*$ as follows:

$\Psi_{J_1J_2J_3J_4}\rangle =$  $dn.$

Since $SU(2) \approx S^3$, using the following graphical identity:



the Barrett-Crane solution can be rewritten as

$|\Psi_{J_1J_2J_3J_4}\rangle =$ 

which emerges as an intertwiner in the familiar form in which Barrett and Crane proposed it for the Riemannian general relativity.

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Analysis of a particle antiparticle description of a soliton cellular automaton

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We present a derivation of a formula that gives dynamics of an integrable cellular automation associated with crystal bases. This automaton is related to type D affine Lie algebra and contains usual box-ball systems as a special case. The dynamics is described by means of such objects as carriers, particles, and antiparticles. We derive it from an analysis of a recently obtained formula of the combinatorial R (an intertwiner between tensor products of crystals) that was found in a study of geometric crystals. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161390]

I. INTRODUCTION

The crystal basis theory[10,11] has played an important role in studies of solvable lattice models and integrable systems since more than a decade. In this context Ref. 9 by Kang, Kashiwara, and Misra has provided useful families of crystal bases associated with affine Lie algebras $A_n^{(1)}$, $B_n^{(1)}$, $C_n^{(1)}$, $D_n^{(1)}$, $A_{2n-1}^{(2)}$, $A_{2n}^{(2)}$, and $D_{n+1}^{(2)}$. We call the first algebra *type A* and the fourth one *type D*. In Ref. 3 we have obtained a formula of the *combinatorial R* (an intertwiner of the crystals) associated with the type A algebra. From the viewpoint of integrable systems an intriguing fact in Ref. 3 is that this formula has been derived from a discrete soliton equation (the nonautonomous discrete KP equation) by a procedure known as the ultradiscretization. Since then there has been progress which goes beyond the type A case. In a study of geometric crystals associated with the type D algebra we have obtained an explicit formula of a *tropical R*, an intertwiner of geometric crystals.[13] The tropical R is a birational map between totally positive rational functions, while the combinatorial R is a bijective map between finite sets. Further analysis of this tropical R and the combinatorial R derived from it should be an important task in studies of integrable systems, since they are connected with discrete and ultradiscrete soliton equations of type D Lie algebra symmetry.[14]

The purpose of this paper is to investigate a *piecewise linear formula* of the above-mentioned combinatorial R for the type D crystals in Ref. 13. Our main result is the derivation of the limit of the formula that leads to the *particle antiparticle description* of an integrable cellular automaton (Theorem 13). This description was recently obtained[15] by using a *factorization of the combinatorial R into Weyl group operators*, a property that had been found and proved in Ref. 7. We emphasize that the result proves a nontrivial fact that the factorization of the combinatorial R can be conducted in two different ways, via the Weyl operator description and via the piecewise linear formula. This point is new even in the type A case (Theorem 3).

We briefly explain the background to our problem. There were studies on one dimensional cellular automata known as the box-ball systems.[17–21] It was found that dynamics in these automata was controlled by the combinatorial R of the type A crystals.[2,3] Based on the families of crystals in Ref. 9 integrable cellular automata associated with crystals of the other types were also constructed.[5,6] A question about such generalized automata arose as to whether we could give a description of their dynamics as box-ball-like systems. To answer this question the particle antiparticle description was found.[8,15]

In Ref. 15 it was found that the automata associated with crystal bases of any types of affine

Lie algebra in Ref. 9 can be embedded into the type D case. Thus one can obtain the particle antiparticle description of these automata from that of the type D case. This is the reason why we devote ourselves into this particular case.

The plan of this paper is as follows. In Sec. II the automaton associated with the type A crystals is reviewed. The piecewise linear formula of the combinatorial R is presented. The particle description of the automaton is proved in terms of the piecewise linear formula. In Sec. III we discuss the piecewise linear formula of the combinatorial R of the type D crystals. Its reduction to the type A case is also shown. The automaton associated with the type D crystals is explained in Sec. IV. The formula of a factorized dynamics of an inhomogeneous automaton (Theorem 13) is reviewed. This formula is proved in Sec. V using the piecewise linear formula of the combinatorial R. Proofs of several lemmas are given in the Appendix.

II. $A^{(1)}_{n-1}$ CASE

A. Combinatorial R

We begin with type A case. Instead of $A^{(1)}_n$ we adopt $A^{(1)}_{n-1}$ crystals because it enables us to compare the results with those in the $D^{(1)}_n$ crystals. For the notation we use overlines to distinguish the symbols from those in the type D case, writing $\bar{B}$ for a crystal, $\bar{R}$ for the combinatorial R and so on.

As a set the $A^{(1)}_{n-1}$ crystal $\bar{B}_l$ (l is any positive integer) is given by

$$\bar{B}_l = \left\{ (x_1, \ldots, x_n) \in \mathbb{Z}^n_{\geqslant 0} \,\middle|\, \sum_{i=1}^{n} x_i = l \right\}. \tag{1}$$

The other properties of this crystal are available in Ref. 9. In this paper we use no other property of $\bar{B}_l$. We will write simply $\bar{B}$ or $\bar{B}'$ for $\bar{B}_l$ with arbitrary l.

Definition 1: Given a pair of variables $x=(x_1,\ldots,x_n)\in\bar{B}$, $y=(y_1,\ldots,y_n)\in\bar{B}'$, let $\bar{R}:(x,y)\mapsto(x',y')$ be the piecewise linear map defined by $x'=(x'_1,\ldots,x'_n)$, $y'=(y'_1,\ldots,y'_n)$ where

$$x'_i = y_i + P_{i+1} - P_i,$$

$$y'_i = x_i + P_i - P_{i+1}.$$

Here P_i is given by

$$P_i = \max_{1\leqslant j\leqslant n}\left(\sum_{k=1}^{j-1}(y_{k+i-1}-x_{k+i-1}) + y_{j+i-1}\right). \tag{2}$$

The indices herein involved are interpreted in modulo n.

Except for the notation this formula is the same one as defined in Proposition 4.1 of Ref. 3. The normalization of (2) is so chosen as the P_1 to take the same expression as the formula in Theorem 5.1 of Ref. 9. The property of $\bar{R}$ to intertwine the actions of Kashiwara operators in the crystal basis theory was essentially proved in Sec. I of Ref. 13. It ensures that the (x',y') falls into $\bar{B}'\times\bar{B}$.

We note that there exist other ways to present the combinatorial R (e.g., Refs. 4 and 16) but which are not used in this paper.

B. Automaton

Now we consider the automaton. In Ref. 3 the space of automaton extends infinitely towards both ends

$$\cdots \times \bar{B}_{l_{i-1}} \times \bar{B}_{l_i} \times \bar{B}_{l_{i+1}} \times \cdots .$$

For our purposes it is sufficient to consider a finite size system like

$$\bar{B}_{l_1} \times \cdots \times \bar{B}_{l_N}. \tag{3}$$

Let $L(\gg \Sigma_{i=1}^{N} l_i)$ be an integer. We call a particular letter for the ground state of the automaton a *vacuum*. We can use any letter in $\{1, \ldots, n\}$ as a vacuum of the automaton.[15] Throughout this paper we adopt n as the letter for the vacuum. As in Ref. 7 we define

$$\bar{B}_L[n] = \{(x_1, \ldots, x_n) \in \bar{B}_L | x_n \gg x_a \text{ for any } a \neq n\}.$$

We write $\bar{B} \times \bar{B}' \simeq \bar{B}' \times \bar{B}$ for correspondence by $\bar{R}$. Take any $x \in \bar{B}_L[n]$. Applying $\bar{R}$ successively we have

$$\bar{B}_L[n] \times (\bar{B}_{l_1} \times \cdots \times \bar{B}_{l_N}) \simeq (\bar{B}_{l_1} \times \cdots \times \bar{B}_{l_N}) \times \bar{B}_L[n],$$

$$x \times Y \mapsto X' \times y', \tag{4}$$

that gives the following.

Definition 2: The time evolution operator $\bar{T}$ of the automaton is given by

$$\bar{T}: Y \mapsto X'.$$

It means that we regard Y and X' in (4) as two automaton states before and after the time evolution. We note that the operator $\bar{T}$ actually depends on x.

C. Particle description

There is an interpretation of the automaton that we call a particle description. It is the description of the box-ball systems in Refs. 17–20. Suppose we have balls with index $a(1 \leqslant a \leqslant n-1)$ that we call *a-balls*. For $x=(x_1, \ldots, x_n) \in \bar{B}_{l_i}$ we associate a box of capacity l_i that has x_a a-balls $(1 \leqslant a \leqslant n-1)$ in it. Then an element of $\bar{B}_{l_1} \times \cdots \times \bar{B}_{l_N}$ is regarded as a one dimensional array of boxes of capacities $l_1, \ldots, l_N$ with these balls. For any $a(1 \leqslant a \leqslant n-1)$ we consider a carrier of a-balls that we call an *a-carrier*. We assume that the a-carrier has a sufficiently large capacity, so that it can carry arbitrary number of a-balls at a time.

First we suppose $l_i=1$ for all i. We call the associated automaton *basic*.[15] In this case the x represents a box with an a-ball if $x_a=1$ for $a \neq n$. It represents an empty box if $x_n=1$. For any a we write $\boxed{a}$ for x with $x_a=1$. The carrier goes along the array of boxes. Then there are four actions in the loading-unloading process by the a-carrier:

(1) If the carrier has at least one ball and meets an empty box, we unload a ball from the carrier and put it into the box.
(2) If the carrier meets a box with an a-ball, we pick up the ball and load it into the carrier.
(3) If the carrier meets a box with a b-ball $(b \neq a)$, we do nothing.
(4) If the carrier has no ball and meets an empty box, we do nothing.

These actions are depicted by the left four pictures in Fig. 1. For any $a(1 \leqslant a \leqslant n-1)$ let $\mathcal{K}_a$ be a *particle motion operator* that acts on the space of automaton (array of boxes) and does the actions in the loading-unloading process explained above. We assume that the $\mathcal{K}_a$ depends on x in (4) in such a way that the a-carrier has x_a balls in it at the beginning where x_a is the ath element of the x. Then for the basic automaton we have[2,3]

$$\bar{T} = \mathcal{K}_1 \mathcal{K}_2 \cdots \mathcal{K}_{n-1}.$$

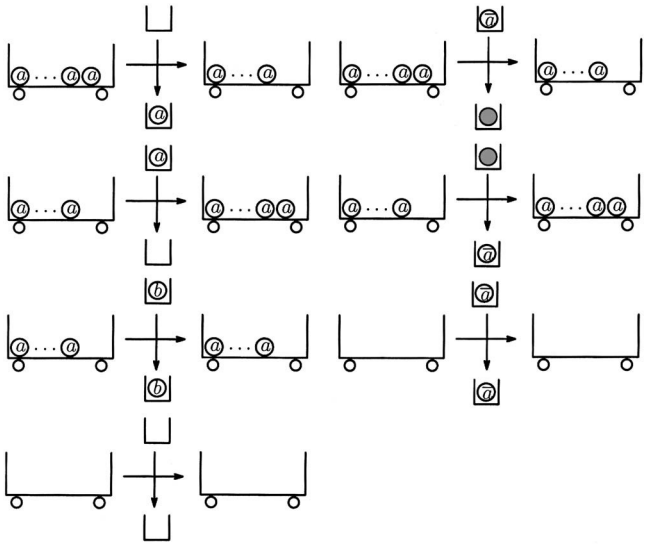

FIG. 1. The loading and unloading process by the carrier of balls with index a. A gray ball represents the bound state of a particle and an antiparticle. It is assumed that $b \neq a, \bar{a}$.

Now we consider a not necessarily basic case which we call *inhomogeneous*.[15] We denote by $\mathcal{P}$ the operator that reduces the automaton into a basic one, and by $\mathcal{Q}$ the operator that makes a rearrangement of balls.[15] To explain them we first let $N=1$ in (4),

$$\bar{B}_L[n] \times \bar{B}_l \simeq \bar{B}_l \times \bar{B}_L[n].$$

Then let

$$\mathcal{P}:\bar{B}_l \to \underbrace{\bar{B}_1 \times \cdots \times \bar{B}_1}_{l}$$

be the operator which sends $y=(y_1, \ldots, y_n) \in \bar{B}_l$ into

$$\underbrace{\boxed{n} \times \cdots \times \boxed{n}}_{y_n} \times \cdots \times \underbrace{\boxed{1} \times \cdots \times \boxed{1}}_{y_1}.$$

Its inverse $\mathcal{P}^{-1}$ can be defined only on such arrays in which the letters are arranged in decreasing order. Let

$$\mathcal{Q}:\underbrace{\bar{B}_1 \times \cdots \times \bar{B}_1}_{l} \to \underbrace{\bar{B}_1 \times \cdots \times \bar{B}_1}_{l}$$

be the operator which packs $\boxed{n}$'s into the left end. Next we consider the case $N>1$. We insert walls between the $\bar{B}_{l_i}$'s in (3) to mark their positions. Then by $\mathcal{P}$ we denote the operator that applies the above $\mathcal{P}$ on each $\bar{B}_{l_i}$, and by $\mathcal{Q}$ or $\mathcal{P}^{-1}$ those that applies the above $\mathcal{Q}$ or $\mathcal{P}^{-1}$ on each $\bar{B}_1 \times \cdots \times \bar{B}_1$ between the walls. Now we have[1,15] the following.

Theorem 3: *The time evolution operator of the inhomogeneous automaton is given by*

$$\bar{T} = \mathcal{P}^{-1}\mathcal{Q}\mathcal{K}_1\mathcal{K}_2 \cdots \mathcal{K}_{n-1}\mathcal{P}. \tag{5}$$

This theorem means that the time evolution of the inhomogeneous automaton can be reduced into that of the basic one only by inserting a simple rearrangement.

D. Proof of the particle description

The reduction of an inhomogeneous automaton to a basic one (Theorem 3) was first presented by Fukuda.[1] We gave another proof of this theorem (and its generalization to type D case) in Ref. 15. Here we show still another proof of this theorem that uses the piecewise linear formula in Definition 1. This is the proof that was inferred in Sec. II D of Ref. 3 but was not explicitly given there. Let $p_i=\lim_{x_n\to\infty} P_i$. Then by (2) we have

$$p_i = \max_{1\leqslant j\leqslant n+1-i}\left(\sum_{k=1}^{j-1}(y_{k+i-1}-x_{k+i-1})+y_{j+i-1}\right). \tag{6}$$

From Definition 1 and (6) we obtain $p_n=y_n$ and

$$p_i = \max\{y_i, y_i - x_i + p_{i+1}\}, \tag{7}$$

$$x_i' = \min\{p_{i+1}, x_i\}. \tag{8}$$

Note that the relation (7) is a descending recursion formula for p_i's on i. Let $x\in \bar{B}_L[n]$ and $y \in \bar{B}_l$ be a pair of variables. Let $\mathcal{K}_a$ be the particle motion operator introduced in Section II C. Then it is easy to see that the p_i's (respectively, x_i''s) for $1\leqslant i\leqslant n-1$ obtained by (7) [respectively by (8)] denote the number of *empty boxes* (respectively, the number of *boxes with balls with index i*) in the automaton state $\mathcal{K}_i\cdots\mathcal{K}_{n-1}\mathcal{P}y$. We also see that the a-carrier finally has $y_a'=x_a+y_a-x_a'$ balls in it. This proves the factorization of $\bar{T}$ in (5) for the case $N=1$ in (4). The assertion of the theorem for the case $N>1$ follows immediately by repeated use of this case, where we adopt the final states of the carriers for $\bar{B}_{l_i}$ in (3) as their initial states for $\bar{B}_{l_{i+1}}$.

III. $D_n^{(1)}$ COMBINATORIAL R

A. Piecewise linear formula

As a set the $D_n^{(1)}$ crystal B_l (l is any positive integer) is given by

$$B_l = \left\{(x_1,\ldots,x_n,\bar{x}_n,\ldots,\bar{x}_1)\in \mathbb{Z}_{\geqslant 0}^{2n} \mid x_n\bar{x}_n=0, \sum_{i=1}^{n}(x_i+\bar{x}_i)=l\right\}. \tag{9}$$

The other properties of this crystal are available in a preprint version of Ref. 11 (Kyoto Univ., RIMS-887, 1992) or in, e.g., Ref. 12. In this paper we use no other property of B_l. We will write simply B or B' for B_l with arbitrary l.

Definition 4: Let $x=(x_1,\ldots,\bar{x}_1)\in B$, $y=(y_1,\ldots,\bar{y}_1)\in B'$ be a pair of variables. The involutive automorphisms $*$, σ_1, σ_n, on x,y are defined by

$$*: x_i \leftrightarrow \bar{y}_i, \bar{x}_i \leftrightarrow y_i \quad (1\leqslant i\leqslant n),$$

$$\sigma_1: x_1 \leftrightarrow \bar{x}_1, y_1 \leftrightarrow \bar{y}_1,$$

$$\sigma_n: x_n \leftrightarrow \bar{x}_n, y_n \leftrightarrow \bar{y}_n.$$

For any function $F=F(x,y)$ we denote by F^a the function obtained from F by applying $a=(*,\sigma_1,\sigma_a)$ to it. For $x\in B_l$ we write $\ell(x)$ for l.

Definition 5: Given a pair of variables $x=(x_1,\ldots,\bar{x}_1)\in B$, $y=(y_1,\ldots,\bar{y}_1)\in B'$, let $R:(x,y)\mapsto(x',y')$ be the piecewise linear map defined by $x'=(x_1',\ldots,\bar{x}_1')$, $y'=(y_1',\ldots,\bar{y}_1')$ where

$$x_1' = y_1 + V_0^{\sigma_1} - V_1,$$

$$x_i' = y_i + V_{i-1} - V_i + W_i - W_{i-1} \quad (2 \leqslant i \leqslant n-1),$$

$$x_n' = y_n + V_{n-1} - V_n^{\sigma_n},$$

$$\bar{x}_i' = \bar{y}_i + V_{i-1} - V_i \quad (1 \leqslant i \leqslant n),$$

$$y_i' = x_i + V_{i-1}^* - V_i^* \quad (1 \leqslant i \leqslant n),$$

$$\bar{y}_1' = \bar{x}_1 + V_0^{\sigma_1} - V_1^*,$$

$$\bar{y}_i' = \bar{x}_i + V_{i-1}^* - V_i^* + W_i - W_{i-1} \quad (2 \leqslant i \leqslant n-1),$$

$$\bar{y}_n' = \bar{x}_n + V_{n-1}^* - V_n^{\sigma_n}. \tag{10}$$

Here V_i and W_i are given by

$$V_i = \max_{1 \leqslant j \leqslant n-1} \{\alpha_{i,j}, \alpha_{i,j}'\}, \tag{11}$$

$$W_i = \max(V_i + V_{i-1}^* - y_i, V_{i-1} + V_i^* - \bar{x}_i) + \min(x_i, \bar{y}_i) \quad (1 \leqslant i \leqslant n-2), \tag{12}$$

$$W_{n-1} = V_n + V_n^{\sigma_n}. \tag{13}$$

The functions $\alpha_{i,j} = \alpha_{i,j}(x,y)$ and $\alpha_{i,j}' = \alpha_{i,j}'(x,y)$ in (11) are given by

$$\alpha_{i,j}(x,y) = \max(\delta_{j,n-1}\beta_i, \bar{y}_j - x_j) + \begin{cases} \ell(x) + \sum_{k=j+1}^{i} (\bar{y}_k - \bar{x}_k) & \text{for } j \leqslant i, \\ \ell(y) + \sum_{k=i+1}^{j} (\bar{x}_k - \bar{y}_k) & \text{for } j > i, \end{cases} \tag{14}$$

$$\alpha_{i,j}'(x,y) = \max(\delta_{j,n-1}\beta_i', x_j - \bar{y}_j) + \ell(x) + \sum_{k=1}^{i} (\bar{y}_k - \bar{x}_k) + \sum_{k=1}^{j} (y_k - x_k), \tag{15}$$

where

$$\beta_i = \begin{cases} x_n - \bar{y}_n & \text{for } i \neq n-1, n, \\ 0 & \text{for } i = n-1, \\ \bar{x}_n - y_n & \text{for } i = n, \end{cases}$$

$$\beta_i' = \begin{cases} \bar{y}_n - x_n & \text{for } i \neq n-1, n, \\ \max(y_n - 2\bar{x}_n, \bar{y}_n - 2x_n) & \text{for } i = n-1, \\ y_n - \bar{x}_n & \text{for } i = n. \end{cases}$$

The map R is the combinatorial R for the $D_n^{(1)}$ crystals. The property of R to intertwine the actions of Kashiwara operators in the crystal basis theory was proved in Theorem 4.28 of Ref. 13. It ensures that the (x', y') falls into $B' \times B$.

Remark 6: We have changed the notation from Ref. 13 since our present formalism uses both x_n and $\bar{x}_n$. The changes are listed in Table I.

TABLE I. The correspondence of the notation between this paper and in Ref. 13 for the piecewise linear formula of the $D_n^{(1)}$ combinatorial R. The z in the first column denotes x, y, x', or y'. It is assumed that $i \neq n-1$, n in the last two columns.

This paper	Reference 13	This paper	Reference 13	This paper	Reference 13
z_n	$\max(z_n,0)$	V_n	V_{n-1}	$\alpha_{i,j(\neq n-1)}$	$\max(\theta_{i,j},\eta_{i,j})$
$\bar{z}_n$	$\max(-z_n,0)$	$V_n^{\sigma_n}$	V_{n-1}^*	$\alpha'_{i,j(\neq n-1)}$	$\max(\theta'_{i,j},\eta'_{i,j})$
z_{n-1}	$z_{n-1}+\min(z_n,0)$	V_{n-1}, V_{n-1}^*		$\alpha_{i,n-1}$	$\max(\eta_{i,n-1},\eta_{i,n})$
$\bar{z}_{n-1}$	$\bar{z}_{n-1}+\min(z_n,0)$	$*$	$*\circ\sigma_n$	$\alpha'_{i,n-1}$	$\max(\eta'_{i,n-1},\eta'_{i,n})$

According to the correspondence in Table I one of the formulas in Eq. (4.66) of Ref. 13 is now translated into

$$x'_n = y_n + \max(V_n - \bar{y}_n, V_n^{\sigma_n} - y_n) - V_n^{\sigma_n},$$

$$\bar{x}'_n = \bar{y}_n + \max(V_n - \bar{y}_n, V_n^{\sigma_n} - y_n) - V_n.$$

In order to make them coincide with the relations in (10) we should define the V_{n-1} as $\max(V_n - \bar{y}_n, V_n^{\sigma_n} - y_n)$. Actually the above definition of V_{n-1} is equivalent to this. In other words we have the following.

Lemma 7: The following relation holds:

$$V_{n-1} = \max(V_n - \bar{y}_n, V_n^{\sigma_n} - y_n). \tag{16}$$

Proof: We have

$$\alpha_{n-1,j} = \max(\alpha_{n,j} - \bar{y}_n, \alpha_{n,j}^{\sigma_n} - y_n),$$

$$\alpha'_{n-1,j} = \max(\alpha'_{n,j} - \bar{y}_n, (\alpha'_{n,j})^{\sigma_n} - y_n),$$

for $1 \leqslant j \leqslant n-1$. In order to check these relations we can use $\max(-x_n,-\bar{x}_n)=\max(-y_n,-\bar{y}_n)=0$. The claim of the lemma follows immediately from these relations. □

Remark 8: The transformation properties of the piecewise linear functions V_i and W_i under the automorphisms σ_1, $*$, and σ_n will be used afterwards, so we list them in Table II. It was quoted from Ref. 13 and adjusted by the correspondence in Table I.

Some more relations on the piecewise linear functions will be used later. We give them at the beginning of the Appendix.

B. Reduction of the $A_{n-1}^{(1)}$ case

We realize that the piecewise linear formula in type D case has a rather bulky expression in contrast with its type A counterpart: See Definitions 1 and 5. In order to understand its structure it

TABLE II. The transformation of the piecewise linear functions V_i and W_i in Definition 5 by the automorphisms σ_1, $*$, and σ_n in Definition 4.

	V_0	$V_i(1 \leqslant i \leqslant n-1)$	V_n	$W_i(1 \leqslant i \leqslant n-1)$
σ_1	$V_0^{\sigma_1}$	v_i	V_n	W_i
$*$	V_0	V_i^*	V_n	W_i
σ_n	V_0	V_i	$V_n^{\sigma_n}$	W_i

is worth trying to study some special limits of the formula. Here we consider a reduction to the type A case. We observe that the piecewise linear map R in Definition 5 for the $D_n^{(1)}$ crystals becomes the intertwiner of the $A_{n-1}^{(1)}$ crystals under the reduction.

Theorem 9: *Set*

$$\bar{x}_i = y_i = 0 \quad \text{for } 1 \leqslant i \leqslant n. \tag{17}$$

Then the map $R:(x,y)\mapsto(x',y')$ *in Definition 5 reduces to*

$$x_i' = y_i + P_{i+1} - P_i,$$

$$y_i' = x_i + P_i - P_{i+1},$$

$$\bar{x}_i' = 0,$$

$$\bar{y}_i' = 0,$$

where P_i *was defined by (2).*

This theorem follows from Lemma 10 below.

Lemma 10: Under the specialization (17) the following relations hold:

$$V_i = \ell(x) + P_1, \quad V_i^* = \ell(x) + P_{i+1} \quad (0 \leqslant i \leqslant n),$$

$$V_0^{\sigma_1} = \ell(x) + P_2, \quad V_n^{\sigma_n} = \ell(x) + P_n,$$

$$W_i = 2\ell(x) + P_1 + P_{i+1} \quad (1 \leqslant i \leqslant n-1).$$

We shall give a proof of this lemma in the Appendix.

We note that the reduction from type D to type A (Theorem 9) itself can also be obtained from the description of the combinatorial R in Ref. 4 since the insertion algorithms for types A and D in Ref. 4 coincide under the condition (17).

IV. $D_n^{(1)}$ AUTOMATON

A. Definition

We now present a brief definition of the $D_n^{(1)}$ automaton using the crystals and the combinatorial R. For a more complete definition, see Refs. 5 and 6. We consider a finite size system like

$$B_{l_1} \times \cdots \times B_{l_N}.$$

Let $L(\geqslant \Sigma_{i=1}^N l_i)$ be an integer. We define

$$B_L[n] = \{(x_1, \ldots, x_n, \bar{x}_n, \ldots, \bar{x}_1) \in B_L | x_n \gg x_a \text{ for any } a \neq n\}. \tag{18}$$

Take any $x \in B_L[n]$. Applying the combinatorial R successively we have

$$B_L[n] \times (B_{l_1} \times \cdots \times B_{l_N}) \simeq (B_{l_1} \times \cdots \times B_{l_N}) \times B_L[n],$$

$$x \times Y \mapsto X' \times y', \tag{19}$$

that gives the following.

Definition 11: The time evolution operator T of the automaton is given by

$$T: Y \mapsto X'.$$

Remarks similar to those after Definition 2 also apply here.

B. Particle antiparticle description

We consider a particle antiparticle description of this automation.[8,15] This is a generalization of the particle description in Sec. III C. Suppose we have balls with index a and $\bar{a}$, $(1 \leqslant a \leqslant n-1)$ that we call an a-ball and an $\bar{a}$-ball respectively. The a-ball and the $\bar{a}$-ball are regarded as a particle and an antiparticle one another. We introduce a pair annihilation process in which a pair of particle and antiparticle makes a bound state, and a pair creation process where the bound state breaks up into a pair of particle and antiparticle of another kind. To each $x = (x_1, \ldots, x_n, \bar{x}_n, \ldots, \bar{x}_1) \in B_{l_i}$ we associate a box of capacity l_i that has x_a a-balls, $\bar{x}_a$ $\bar{a}$-balls $(1 \leqslant a \leqslant n-1)$, and $\bar{x}_n$ bound states in it. Then any element of $B_{l_1} \times \cdots \times B_{l_N}$ can be regarded as a one dimensional array of boxes of capacities $l_1, \ldots, l_N$ with the balls and the bound states. For any $a(1 \leqslant a \leqslant n-1)$ we introduce the notion of an a-carrier as in Sec. III C, and that of a carrier for $\bar{a}$-balls that we call an *$\bar{a}$-carrier*. Assume that their capacities are sufficiently large.

First we consider a basic case, i.e., we suppose $l_i = 1$ for all i. In this case the x represents a box with an a-ball if $x_a = 1$ and a box with an $\bar{a}$-ball if $\bar{x}_a = 1$ for $a \neq n$. It represents an empty box if $x_n = 1$ and a box with a bound state if $\bar{x}_n = 1$. We write $\boxed{a}$ for x with $x_a = 1$ and write $\boxed{\overline{a}}$ for x with $\bar{x}_a = 1$.

Remark 12: In what follows we write a also for a number with an overline as well as that without an overline. We interpret $\bar{\bar{a}} = a$ and $x_{\bar{a}} = \bar{x}_a$. We call $\bar{x}_a$ the $\bar{a}$th element of x.

Besides the four actions in the loading-unloading process in Sec. III C we have three additional actions by the a-carrier:

(5) If the carrier has at least one ball and meets a box with an $\bar{a}$-ball, we unload a ball from the carrier and make a bound state in the box.
(6) If the carrier meets a box with a bound state, we extract an a-ball from the bound state, load it into the carrier, and leave an $\bar{a}$-ball in the box.
(7) If the carrier has no ball and meets a box with an $\bar{a}$-ball, we do nothing.

These actions are depicted by the right three pictures in Fig. 1.

For any $a \in \{1, \ldots, n-1\} \cup \{\overline{n-1}, \ldots, \overline{1}\}$ (see Remark 12) let $\mathcal{K}_a$ be a particle motion operator[8,15] that acts on the space of automaton and does the actions in the loading-unloading process explained above. We assume that the $\mathcal{K}_a$ depends on x in (19) in such a way that the a-carrier has x_a balls in it at the beginning, where x_a is the ath element of x. Then for the basic automaton we have[8]

$$T = \mathcal{K}_{\overline{n-1}} \cdots \mathcal{K}_{\bar{2}} \mathcal{K}_{\bar{1}} \mathcal{K}_1 \mathcal{K}_2 \cdots \mathcal{K}_{n-1}.$$

Now we consider an inhomogeneous case. We define the operators $\mathcal{P}$ and $\mathcal{Q}$ as in Sec. III C but modify them to be suitable for the type D case.[15] To define them we first set $N = 1$ in (19),

$$B_L[n] \times B_l \simeq B_l \times B_L[n]. \tag{20}$$

Then let

$$\mathcal{P}: B_l \to \underbrace{B_1 \times \cdots \times B_1}_{l}$$

be the operator which sends $y = (y_1, \ldots, y_n, \bar{y}_n, \ldots, \bar{y}_1) \in B_l$ into

$$\underbrace{\boxed{\bar{1}}\times\cdots\times\boxed{\bar{1}}}_{\bar{y}_1}\times\cdots\times\underbrace{\boxed{\bar{n}}\times\cdots\times\boxed{\bar{n}}}_{\bar{y}_n}\times\underbrace{\boxed{n}\times\cdots\times\boxed{n}}_{y_n}\times\cdots\times\underbrace{\boxed{1}\times\cdots\times\boxed{1}}_{y_1}. \tag{21}$$

Its inverse $\mathcal{P}^{-1}$ can be defined only on such arrays in which the letters are arranged as in (21). Let

$$\mathcal{Q}:\underbrace{B_1\times\cdots\times B_1}_{l}\to\underbrace{B_1\times\cdots\times B_1}_{l}$$

be the operator which packs $\boxed{n}$'s into the left end and $\boxed{\bar{n}}$'s into the right end. For the case $N>1$ we generalize the definitions of these operators in the same way as in Sec. III C. Now we have the following.

Theorem 13: *The time evolution operator of the inhomogeneous automaton is given by*

$$T=\mathcal{P}^{-1}\mathcal{K}_{\overline{n-1}}\cdots\mathcal{K}_{\bar{2}}\mathcal{K}_{\bar{1}}\mathcal{Q}\mathcal{K}_1\mathcal{K}_2\cdots\mathcal{K}_{n-1}\mathcal{P}. \tag{22}$$

In Ref. 15 a proof of this theorem was given by means of the factorization of the combinatorial R in Ref. 7. In the remaining part of this paper we give another proof of this theorem that uses the piecewise linear formula of the combinatorial R in Definition 5.

V. PROOF OF THE PARTICLE ANTIPARTICLE DESCRIPTION

A. Limit of the piecewise linear formula

We study a limit of the piecewise linear formula of the map R in Definition 5. Let $F=F(x,y)$ be any function of $(x,y)\in B\times B'$. The limit we consider here is to adopt the $B_L[n]$ in (18) as the B. We introduce the following normalized limits:

$$\lim_{\star}F=\lim_{x_n\to\infty,\bar{x}_n\to 0}(F(x,y)-\ell(x)), \tag{23}$$

$$\lim_{\star\star}F=\lim_{x_n\to\infty,\bar{x}_n\to 0}(F(x,y)-2\ell(x)). \tag{24}$$

First we consider the limit (23) of V_i. For the sake of notational simplicity we denote $\lim_{\star}V_i$ by v_i. For $a=\sigma_1$, σ_n or $*$ we denote $\lim_{\star}V_i^a$ by v_i^a. Note that if $a=\sigma_n$ or $*$ the v_i^a is not necessarily equal to the function that is obtained from v_i by applying a to it, whereas if $a=\sigma_1$ it is. Next we consider the limit (24) of W_i. We shall denote $\lim_{\star\star}W_i$ by w_i.

The relations in Lemma 23 in the Appendix become recursion relations in the limit (23). We let $(x)_+$ denote $\max(x,0)$.

Lemma 14: *For $F=V_i$, V_i^*, $V_0^{\sigma_1}$ or $V_n^{\sigma_n}$ the limit $\lim_{\star}F$ exists. Moreover the following relations hold:*

$$v_n^{\sigma_n}=v_{n-1}^*=y_n-\bar{y}_n, \tag{25}$$

$$v_{n-1}^*=y_i-x_i+\max\{v_i^*,(x_i-\bar{y}_i)_+\}\quad(1\leqslant i\leqslant n-1), \tag{26}$$

$$v_i=\max\{\bar{y}_i-\bar{x}_i+v_{i-1},(\bar{y}_i-x_i)_+\}\quad(1\leqslant i\leqslant n-1), \tag{27}$$

$$v_n=\bar{y}_n-y_n+\max\{y_n+\bar{y}_{n-1}-\bar{x}_{n-1}+v_{n-2},(y_n+\bar{y}_{n-1}-x_{n-1})_+\}. \tag{28}$$

We consider the limit (24) of the defining relations of W_i [(12) and (13)].

Lemma 15: *The following relation holds:*

$$w_i=v_i+v_i^*-\min\{v_i^*-v_{i-1}^*+y_i,v_i-v_{i-1}+\bar{x}_i\}+\min\{x_i,\bar{y}_i\}\quad(1\leqslant i\leqslant n-1). \tag{29}$$

These lemmas will be used in proofs of Lemmas 20 and 21. We shall give their proofs in the Appendix.

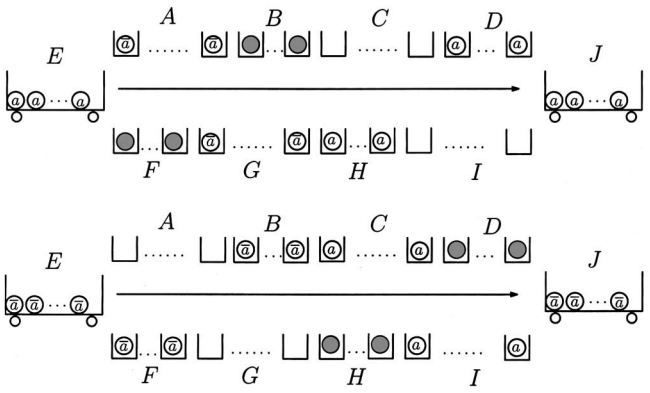

FIG. 2. The meaning of the map γ in Definition 16 by the particle antiparticle description of the automaton.

B. Analysis of the particle antiparticle description

We now consider a recursion formula satisfied by the numbers of items in the particle antiparticle description. For this purpose we introduce the following.

Definition 16: For any non-negative integers A,B,C,D,E, define the piecewise linear map

$$\gamma:(A,B,C,D,E) \mapsto (F,G,H,I,J)$$

by

$$F = \min(A,E),$$

$$G = B + (A-E)_+,$$

$$H = \min(C,B + (E-A)_+),$$

$$I = D + (C - B - (E-A)_+)_+,$$

$$J = D + (B - C + (E-A)_+)_+.$$

The identities $F+G=A+B$, $H+I=C+D$, and $F+H+J=B+D+E$ can be checked easily and will be used afterwards. We give an interpretation of the map γ in the particle antiparticle description that is illustrated in Fig. 2. Recall the seven actions in the loading-unloading process by the a-carrier (Fig. 1) that were explained in Secs. II C and IV B. We write *act-i* for the action with number i in the lists. Note that the a can represent an overlined number in Fig. 1. In Fig. 2 the boxes with b-balls ($b \neq a, \bar{a}$) have been omitted because of act-3. In the upper picture of Fig. 2 we are applying act-5 (or act-7 if $E=0$), act-6, act-1 [or act-4 if $B+(E-A)_+=0$], and act-2 from left to right. In the lower picture we are applying act-1 (or act-4 if $E=0$), act-2, act-5 [or act-7 if $B+(E-A)_+=0$], and act-6.

In what follows we always assume

$$x_n \gg 0 \quad \text{and } \bar{x}_n = 0. \tag{30}$$

Let B and B' be the $D_n^{(1)}$ crystals.

Definition 17: For each pair of variables $x=(x_1,\ldots,\bar{x}_1) \in B$, $y=(y_1,\ldots,\bar{y}_1) \in B'$, define the set of variables $z^{(i)}, \bar{z}^{(i)} (0 \leqslant i \leqslant 2n-2)$, $y_i^{\circ}, \bar{y}_i^{\circ} (1 \leqslant i \leqslant n-1)$, $x_i', \bar{x}_i', y_i', \bar{y}_i' (1 \leqslant i \leqslant n)$ as follows.

(1) Set

$$\bar{z}^{(0)} = \bar{y}_n, \quad z^{(0)} = y_n. \tag{31}$$

TABLE III. The correspondence between the variables in Definition 17 and the items in the particle antiparticle description.

Variables	Items at time t_i	Variables	Items at time $\bar{t}_i$
$z^{(n-i)}$	Empty boxes	$z^{(n-1+i)}$	Empty boxes
$\bar{z}^{(n-i)}$	Boxes with bound states	$\bar{z}^{(n-1+i)}$	Boxes with bound states
$y_i^{\bigcirc}$	Boxes with i-balls	x_i'	Boxes with i-balls
$\bar{y}_i^{\bigcirc}$	Boxes with $\bar{i}$-balls	$\bar{x}_i'$	Boxes with $\bar{i}$-balls
y_i'	Balls in the i-carrier	$\bar{y}_i'$	Balls in the $\bar{i}$-carrier

(2) Define $z^{(n-i)}, \bar{z}^{(n-i)}, y_i^{\bigcirc}, \bar{y}_i^{\bigcirc} y_i' (1 \leqslant i \leqslant n-1)$ as

$$\gamma(\bar{y}_i,\ \bar{z}^{(n-1-i)},\ z^{(n-1-i)},\ y_i,\ x_i) = (\bar{z}^{(n-i)},\ \bar{y}_i^{\bigcirc},\ y_i^{\bigcirc},\ z^{(n-i)},\ y_i'), \tag{32}$$

by descending recursion on i. Here the function γ is given by Definition 16.

(3) Define $z^{(n-1+i)}, \bar{z}^{(n-1+i)}, x_i', \bar{x}_i', \bar{y}_i' (1 \leqslant i \leqslant n-1)$ as

$$\gamma(z^{(n-2+i)},\ \bar{y}_i^{\bigcirc},\ y_i^{\bigcirc},\ \bar{z}^{(n-2+i)},\ \bar{x}_i) = (\bar{x}_i',\ z^{(n-1+i)},\ \bar{z}^{(n-1+i)},\ x_i',\ \bar{y}_i'), \tag{33}$$

by recursion on i.

(4) Set

$$x_n' = z^{(2n-2)}, \quad \bar{x}_n' = \bar{z}^{(2n-2)}, \quad y_n' = \ell(x) - \sum_{i=1}^{n-1} (y_i' + \bar{y}_i'), \quad \bar{y}_i' = 0. \tag{34}$$

Remark 18: Let us consider the case when $x \in B_L[n]$ and $y \in B_l$. Then the numbers represented by the variables $z^{(i)}$, etc., in Definition 17 are equal to the numbers of items in the particle antiparticle description in Sec. IV B. More precisely these items appear within the time evolution process by T in Theorem 13 for the case $N=1$. See Table III. In the table t_i and $\bar{t}_i$ are defined as follows: For $1 \leqslant i \leqslant n-1$ we let t_i (respectively, $\bar{t}_i$) denote the time just after the i-carrier (respectively, $\bar{i}$-carrier) has passed, where the automaton state is given by $\mathcal{K}_i \cdots \mathcal{K}_{n-1} \mathcal{P} y$ (respectively, $\mathcal{K}_{\bar{i}} \cdots \mathcal{K}_{\bar{1}} \mathcal{Q} \mathcal{K}_1 \cdots \mathcal{K}_{n-1} \mathcal{P} y$).

C. Proof

We now give the proof of Theorem 13 that we have promised at the end of Sec. IV. It is obtained from the following.

Theorem 19: *Let $x=(x_1, \ldots, \bar{x}_1) \in B$, $y=(y_1, \ldots, \bar{y}_1) \in B'$ be a pair of variables, and suppose the condition* (30) *on x. Let $v_i, w_i, v_i^*, v_0^{\sigma_1}, v_n^{\sigma_n}$ be the functions defined in Sec. V A, and let $x_i', \bar{x}_i', y_i', \bar{y}_i' (1 \leqslant i \leqslant n)$ be the variables given by Definition 17. Then the following relations hold:*

$$x_1' = y_1 + v_0^{\sigma_1} - v_1,$$

$$x_i' = y_i + v_{i-1} - v_i + w_i - w_{i-1} \quad (2 \leqslant i \leqslant n-1),$$

$$x_n' = y_n + v_{n-1} - v_n^{\sigma_n},$$

$$\bar{x}_i' = \bar{y}_i + v_{i-1} - v_i \quad (1 \leqslant i \leqslant n),$$

$$y_i' = x_i + v_{i-1}^* - v_i^* \quad (1 \leqslant i \leqslant n),$$

$$\bar{y}_i' = \bar{x}_1 + v_0^{\sigma_1} - v_1^*,$$

$$\bar{y}_i' = \bar{x}_i + v_{i-1}^* - v_i^* + w_i - w_{i-1}, \quad (2 \leqslant i \leqslant n-1),$$

$$\bar{y}_n' = \bar{x}_n + v_{n-1}^* - v_n^{\sigma_n}. \tag{35}$$

A proof of Theorem 19 will be given after the following two lemmas.

Lemma 20: Let $A=\bar{y}_i$, $B=\min(x_{i+1},\bar{y}_{i+1})$, $C=v_i^*+\min(x_{i+1},\bar{y}_{i+1})$, $D=y_i$ *and* $E=x_i$ *in* $\gamma:(A,B,C,D,E)\mapsto(F,G,H,I,J)$. *Then*

$$F = \min(x_i,\bar{y}_i),$$

$$G = \bar{y}_i - \min(x_i,\bar{y}_i) + \min(x_{i+1},\bar{y}_{i+1}),$$

$$H = -\min(x_i,\bar{y}_i) + \min(x_{i+1},\bar{y}_{i+1}) + y_i + v_i^* - v_{i-1}^*,$$

$$I = v_{i-1}^* + \min(x_i,\bar{y}_i),$$

$$J = x_i + v_{i-1}^* - v_i^*,$$

for $1 \leqslant i \leqslant n-1$.

In what follows we set $w_0=2v_0$. Note that we have $v_0^*=v_0$ from Table II and $w_1=v_0+v_0^{\sigma_1}$ from Lemma 22 in the Appendix.

Lemma 21: Let $A=v_{i-1}+\min(x_i,\bar{y}_i)$, $B=\bar{y}_i-\min(x_i,\bar{y}_i)+\min(x_{i+1},\bar{y}_{i+1})$, $C=-\min(x_i,\bar{y}_i)+\min(x_{i+1},\bar{y}_{i+1})+y_i+v_i^*-v_{i-1}^*$, $D=\min(x_i,\bar{y}_i)+v_{i-1}+v_{i-1}^*-w_{i-1}$, *and* $E=\bar{x}_i$ *in* $\gamma:(A,B,C,D,E)\mapsto(F,G,H,I,J)$. *Then*

$$F = \bar{y}_i + v_{i-1} - v_i,$$

$$G = v_i + \min(x_{i+1},\bar{y}_{i+1}),$$

$$H = \min(x_{i+1},\bar{y}_{i+1}) + v_i + v_i^* - w_i,$$

$$I = y_i + w_i - w_{i-1} - v_i + v_{i-1},$$

$$J = \bar{x}_i + w_i - w_{i-1} - v_i^* + v_{i-1}^*,$$

for $1 \leqslant i \leqslant n-1$.

We shall give proofs of these lemmas in the Appendix.

Proof of Theorem 19: Suppose $i=n-1$ in Lemma 20. Then we have $B=\bar{y}_n=\bar{z}^{(0)}$ and $C=y_n=z^{(0)}$ because of (25), (30), and (31). Then by comparing (32) with Lemma 20 we see that $\bar{z}^{(1)}$, $\bar{y}_{n-1}^{\bigcirc}$, $y_{n-1}^{\bigcirc}$, $z^{(1)}$, and y_{n-1}' in (32) should be equal to F, G, H, I, and J. Thus the expression for y_{n-1}' was obtained. The expressions for $y_i'(1 \leqslant i \leqslant n-2)$, as well as those for $\bar{z}^{(n-i)}$, $\bar{y}_i^{\bigcirc}$, $y_i^{\bigcirc}$, $z^{(n-i)}$ will be obtained by descending recursion on i, where one uses F and I as B and C in the next step.

Since B and C in Lemma 21 are equal to G and H in Lemma 20, we have $B=\bar{y}_i^{\bigcirc}$ and $C=y_i^{\bigcirc}$ in Lemma 21. We also see that when $i=1$ we have $A=z^{(n-1)}$ and $D=\min(x_1,\bar{y}_1)=\bar{z}^{(n-1)}$ in Lemma 21, from the result obtained in the preceding paragraph. Then by comparing (33) with Lemma 21 we see that $\bar{x}_1'$, $z^{(n)}$, $\bar{z}^{(n)}$, x_1', and $\bar{y}_1'$ in (33) are equal to F, G, H, I, and J in Lemma 21 if $i=1$. Thus the expressions for $x_1', \bar{x}_1', y_1'$ were obtained. The expressions for $x_i', \bar{x}_i', y_i'(2 \leqslant i \leqslant n-2)$ will be obtained by recursion on i, where one uses G and H as A and D in the next step.

Then from (34) we can obtain the expressions for x'_n and $\bar{x}'_n$ in (35) since we have (30) and (25). It is clear that the relation $\bar{y}'_n=0=\bar{x}_n+v^*_{n-1}-v^{\sigma_n}_n$ holds. Then the expression for y'_n in (35) is obtained from the condition $\ell(y')=\ell(x)$. The proof is completed. □

Finally we give the proof of Theorem 13.

Proof of Theorem 13: If we impose the condition (30) on the defining relations (10) in Definition 5 then their right-hand sides become those of (35) because of the existence of the limiting functions defined in the Appendix. Then Theorem 19 tells that the numbers represented by $x'_i, \bar{x}'_i, y'_i, \bar{y}'_i$ in Definition 5 are equal to those by the same symbols in Definition 17 under this condition. Then according to Remark 18 we see that the time evolution T by Definition 11 is identical to the T in Theorem 13 for the case $N=1$. The assertion for the case $N>1$ follows immediately by repeated use of this case, where we adopt the final states of the carriers for B_{l_i} in (19) as their initial states for $B_{l_{i+1}}$. □

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APPENDIX: PROOFS OF THE LEMMAS

Before giving the proofs we present some relations between piecewise linear functions. They are used in the main text and in this Appendix. These relations have been essentially obtained in Ref. 13.

Ultradiscretization[18,20,21] is a procedure to derive an equation of piecewise linear functions from an equation of totally positive (i.e., having no minus sign) rational functions. It is realized as a transformation that replaces $+$, $\times$, and / by max(min), $+$ and $-$, respectively. As the ultradiscretization of Lemma 4.12 of Ref. 13 we have the following.

Lemma 22: The following relation holds:

$$W_1 = V_0 + V_0^{\sigma_1}. \tag{A1}$$

This lemma is used just above Lemma 21. The next lemma is obtained from the formulas $(4.23)^*$, (4.23), and (4.24) of Ref. 13 by the ultradiscretization.

Lemma 23: The following relations hold:

$$\max\{V^*_i, \ell(x), \ell(x)+x_i-\bar{y}_i\} = \max\{x_i-y_i+V^*_{i-1}, \ell(y), \ell(y)+x_i-\bar{y}_i\}, \tag{A2}$$

$$\max\{V_i, \ell(y), \ell(y)+\bar{y}_i-x_i\} = \max\{\bar{y}_i-\bar{x}_i+V_{i-1}, \ell(x), \ell(x)+\bar{y}_i-x_i\}, \tag{A3}$$

$$\max\{V_n, \ell(y)+X\} = \max\{\bar{y}_{n-1}+\bar{y}_n-\bar{x}_{n-1}-\bar{x}_n+V_{n-2}, \ell(x)+X\}, \tag{A4}$$

where $1\leqslant i\leqslant n-2$ *and* $X=\bar{y}_n-y_n+(\bar{y}_{n-1}+y_n-x_{n-1}-\bar{x}_n)_+$.

Here we write $(x)_+$ for $\max(x,0)$. This lemma will be used in the proof of Lemma 14.

Proof of Lemma 10

Proof: We derive the expression for V_i. First we suppose $i\neq n-1,n$. Then under the specialization (17) we have $V_i=\max_{1\leqslant j\leqslant n-1}\{\alpha_{i,j}, \alpha'_{i,j}\}$ with

$$\alpha_{i,j} = x_n\delta_{j,n-1} + \begin{cases} \ell(x) & \text{for } j\leqslant i, \\ \ell(y) & \text{for } j>i, \end{cases}$$

$$\alpha'_{i,j} = \ell(x) + \sum_{k=1}^{j-1} (y_k - x_k) + y_j.$$

Since $\alpha_{i,j(\leqslant i)} \leqslant \alpha'_{i,1}$ and $\alpha_{i,j(>i)} \leqslant \alpha_{i,n-1}$, we can drop off $\alpha_{i,j(\neq n-1)}$ in the max. Thus we obtain the desired result from (2) with $i=1$. Now we suppose $i=n-1$ or n. Then we have

$$\alpha_{i,j} = \ell(x) + \begin{cases} 0 & \text{for } i = n-1, \\ \max(-y_n, -x_{n-1}) & \text{for } i = n, \end{cases}$$

$$\alpha'_{i,j} = \ell(x) + \sum_{k=1}^{j-1} (y_k - x_k) + y_j + \delta_{j,n-1} \max(y_n - x_{n-1}, 0).$$

Since $\alpha_{i,j} \leqslant \alpha'_{i,1}$, we can drop off $\alpha_{i,j}$ in the max and obtain the desired result.

We derive the expression for V_i^*. Note that if $i=0,n$ it has already been proved since $V_i^* = V_i$ for $i=0,n$. Suppose $i \neq 0,n$. Then under the specialization (17) we have $V_i^* = \max_{1 \leqslant j \leqslant n-1}\{\alpha_{i,j}^*, (\alpha'_{i,j})^*\}$ with

$$\alpha_{i,j}^* = x_j + \begin{cases} \ell(y) + \sum_{k=j+1}^{i} (x_k - y_k) & \text{for } j \leqslant i, \\ \ell(x) + \sum_{k=i+1}^{j} (y_k - x_k) & \text{for } j > i, \end{cases}$$

$$(\alpha'_{ij})^* = \delta_{j,n-1} x_n + \ell(y) + \sum_{k=1}^{i} (x_k - y_k).$$

Since $(\alpha'_{i,j(\neq n-1)})^* \leqslant \alpha'_{i,1}$, we can drop off $(\alpha_{i,j(\neq n-1)})^*$ in the max. The remaining candidates are

$$\alpha_{i,i+1}^* = \ell(x) + y_{i+1},$$

$$\alpha_{i,i+2}^* = \alpha_{i,i+1}^* - x_{i+1} + y_{i+2},$$

$$\cdots,$$

$$\alpha_{i,n-1}^* = \alpha_{i,n-2}^* - x_{n-2} + y_{n-1},$$

$$(\alpha'_{i,n-1})^* = \alpha_{i,n-1}^* - x_{n-1} + y_n,$$

$$\alpha_{i,1}^* = (\alpha'_{i,n-1})^* - x_n + y_1,$$

$$\alpha_{i,2}^* = \alpha_{i,1}^* - x_1 + y_2,$$

$$\cdots,$$

$$\alpha_{i,i}^* = \alpha_{i,i-1}^* - x_{i-1} + y_i.$$

Thus we obtain the desired result.

We derive the expression for $V_0^{\sigma_1}$. Under the specialization (17) we have $V_0^{\sigma_1} = \max_{1 \leqslant j \leqslant n-1}\{\alpha_{0,j}^{\sigma_1}, (\alpha'_{0,j})^{\sigma_1}\}$ with

$$\alpha_{0,j}^{\sigma_1} = \ell(y) + x_1 - (1 - \delta_{j,1})y_1 + \delta_{j,n-1}x_n,$$

$$(\alpha'_{0,j})^{\sigma_1} = \ell(x) + \sum_{k=2}^{j} (y_k - x_k) + (1 - \delta_{j,1})x_j.$$

Since $\alpha_{0,j(\neq n-1)}^{\sigma_1} \leqslant \alpha_{0,1}^{\sigma_1}$ and $(\alpha'_{0,1})^{\sigma_1} \leqslant (\alpha'_{0,2})^{\sigma_1}$, we can drop off $\alpha_{0,j(\neq 1,n-1)}^{\sigma_1}$ and $(\alpha'_{0,1})^{\sigma_1}$ in the max and obtain the desired result.

We derive the expression for $V_n^{\sigma_n}$. Under the specialization (17) we have $V_n^{\sigma_n} = \max_{1 \leqslant j \leqslant n-1}\{\alpha_{n,j}^{\sigma_n}, (\alpha'_{n,j})^{\sigma_n}\}$ with

$$\alpha_{n,j}^{\sigma_n} = \ell(x) + y_n - (1 - \delta_{j,n-1})x_n,$$

$$(\alpha'_{n,j})^{\sigma_n} = \ell(x) + y_n - x_n + \sum_{k=1}^{j-1} (y_k - x_k) + y_j.$$

Since $\alpha_{n,j(\neq n-1)}^{\sigma_n} \leqslant (\alpha'_{n,1})^{\sigma_n}$, we can drop off $\alpha_{n,j(\neq n-1)}^{\sigma_n}$ in the max and obtain the desired result.

The expression for W_{n-1} is derived from (13), and that for $W_{i(\neq n-1)}$ is from (12) and the following lemma. □

Lemma 24: Let P_i be the function that was defined by (2). Then

$$P_{i+1} \geqslant P_i - y_i.$$

Proof: It is easy to see that

$$P_i - y_i = \max_{1 \leqslant j \leqslant n} \{A_j\}, \quad P_{i+1} = \max_{2 \leqslant j \leqslant n+1} \{x_i + A_j\},$$

where

$$A_j = \sum_{k=1}^{j-1} (y_{i+k} - x_{i+k-1}).$$

The claim of the lemma holds since we have $x_i \geqslant 0$ and $x_i + A_2 = y_{i+1} \geqslant 0 = A_1$. □

Proof of Lemma 14

Proof: By definition we have $V_n^{\sigma_n} = \max_{1 \leqslant j \leqslant n-1}\{\alpha_{n,j}^{\sigma_n}, (\alpha'_{n,j})^{\sigma_n}\}$, where

$$(\alpha_{n,j})^{\sigma_n} = \max(\delta_{j,n-1}(x_n - \bar{y}_n), \bar{y}_j - x_j) + \ell(x) + \sum_{k=j+1}^{n-1} (\bar{y}_k - \bar{x}_k) + y_n - x_n,$$

$$(\alpha'_{n,j})^{\sigma_n} = \max(\delta_{j,n-1}(\bar{y}_n - x_n), x_j - \bar{y}_j) + \ell(x) + \sum_{k=1}^{n-1} (\bar{y}_k - \bar{x}_k) + \sum_{k=1}^{j} (y_k - x_k) + y_n - x_n.$$

In the limit $\lim_\star$ the only element that survives in the max is $(\alpha_{n,n-1})^{\sigma_n}$, which yields $v_n^{\sigma_n} = y_n - \bar{y}_n$. In the same way the relation

$$v_{n-2}^* = y_{n-1} + y_n - x_{n-1} + (x_{n-1} - \bar{y}_{n-1} + y_n)_+, \tag{A5}$$

can be obtained by a direct calculation. Then from (A2) we see that the v_i^*'s exist and the relation (26) holds for $1 \leqslant i \leqslant n-2$ by descending induction on i. Since $V_0 = V_0^*$ (Table II) we have $v_0 = v_0^*$. Then from (A3) and (A4) we see that v_i's exist for $i \neq n-1$, and that the relations (27) for $1 \leqslant i \leqslant n-2$ and (28) hold, by induction on i. Since v_n and $v_n^{\sigma_n}$ exist, we see by (16) that the function v_{n-1} also exists and equals to $\max\{v_n - \bar{y}_n, -\bar{y}_n\}$. Substituting (28) into $v_{n-1} = \max\{v_n$

$-\bar{y}_n,-\bar{y}_n\}$ we obtain (27) for $i=n-1$. From $*$ of (16) we obtain $v^*_{n-1}=y_n-\bar{y}_n$. Then from (A5) and $\max\{-y_n,-\bar{y}_n\}=0$ we obtain (26) for $i=n-1$. From σ_1 of (A2) the existence of $v_0^{\sigma_1}$ can be verified. The proof is completed. □

Proof of Lemma 15

Proof: For $1\leqslant i\leqslant n-2$ the relations follow immediately from (12). We consider the case $i=n-1$. We obtain $w_{n-1}=v_n+v_n^{\sigma_n}$ from (13). First we suppose $x_{n-1}\leqslant\bar{y}_{n-1}$. Then from Lemma 14 we obtain $v_{n-1}=\bar{y}_{n-1}+\max\{-\bar{x}_{n-1}+v_{n-2},-x_{n-1}\}$. It yields the relations $v_n+v_n^{\sigma_n}=v_{n-1}+y_n$ and

$$\text{RHS of (29)} = v_{n-1}+y_n-\bar{y}_n+x_{n-1}-\min\{x_{n-1}-\bar{y}_n,\bar{x}_{n-1}-v_{n-2}-v_{n-1}\}=v_{n-1}+y_n-\min\{0,\bar{y}_n+(\bar{y}_{n-1}-x_{n-1})+(\bar{x}_{n-1}-x_{n-1}-v_{n-2})_+\}=v_{n-1}+y_n.$$

Thus the assertion of the lemma was proved in this case. Now we suppose $x_{n-1}>\bar{y}_{n-1}$. Then

$$\text{RHS of (29)} = v_{n-1}+y_n-\bar{y}_n+\bar{y}_{n-1}-\min\{x_{n-1}-(x_{n-1}-\bar{y}_{n-1}-y_n)_+-\bar{y}_n,\bar{x}_{n-1}-v_{n-2}-v_{n-1}\}=\max\{(y_n+\bar{y}_{n-1}-x_{n-1})_+ +v_{n-1},v_{n-2}+\bar{y}_{n-1}-\bar{x}_{n-1}+y_n-\bar{y}_n\}.$$

From Lemma 14 we have $v_{n-1}=(\bar{y}_{n-1}-\bar{x}_{n-1}+v_{n-2})_+$. Therefore

$$\text{RHS of (29)} = \max\{(y_n+\bar{y}_{n-1}-x_{n-1})_+,\bar{y}_{n-1}-\bar{x}_{n-1}+y_n+v_{n-2}+\max\{-y_n,-\bar{y}_n,\bar{y}_{n-1}-x_{n-1}\}\}.$$

The last expression gives $v_n+v_n^{\sigma_n}$ since the inner max vanishes. The proof is completed. □

Proof of Lemma 20

Proof: The expressions for F and G are given by definition. The expression for I is given by $I=C+D-H$, and that for J is by $J=I+B-C+E-F$. Thus it suffices to prove H. We have

$$H=\min(C,B+E-F)=\min(x_{i+1},\bar{y}_{i+1})+\min\{v_i^*,-\min(x_i,\bar{y}_i)+x_i\}=\min(x_{i+1},\bar{y}_{i+1})+v_i^*-\min(x_i,\bar{y}_i)+x_i-\max\{v_i^*,-\min(x_i,\bar{y}_i)+x_i\}.$$

Then by (26) we obtain the desired result. □

Proof of Lemma 21

Proof: The expression for G is given by $G=A+B-F$, that for I is by $I=C+D-H$, and that for J is by $J=I+B-C+E-F$. Thus it suffices to prove F and H. For F we have

$$F=\min(A,E)=\bar{y}_i+v_{i-1}+\min\{\min(x_i,\bar{y}_i)-\bar{y}_i,\bar{x}_i-\bar{y}_i-v_{i-1}\}=\bar{y}_i+v_{i-1}-\max\{-\min(x_i,\bar{y}_i)+\bar{y}_i,-\bar{x}_i+\bar{y}_i+v_{i-1}\}.$$

Then by (27) we obtain the desired result. For H we have

$$H=\min(C,B+E-F)=\min(x_{i+1},\bar{y}_{i+1})-\min(x_i,\bar{y}_i)+\min\{v_i^*-v_{i-1}^*+y_i,v_i-v_{i-1}+\bar{x}_i\}.$$

Then by (29) we obtain the desired result. □

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Positive Lyapunov exponents for continuous quasiperiodic Schrödinger equations

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We prove that the continuous one-dimensional Schrödinger equation with an analytic quasi-periodic potential has positive Lyapunov exponents in the bottom of the spectrum for large couplings. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this short paper we study the one-dimensional Schrödinger equation with a quasi-periodic potential:

$$(H_\theta u)(t) \equiv -u''(t) + \lambda V(t, \theta + \omega t)u(t) = Eu(t). \tag{1.1}$$

Here $V: \mathbb{T} \times \mathbb{T}^d \to \mathbb{R}$ $(\mathbb{T} = \mathbb{R}/\mathbb{Z}, d \geqslant 1)$ is assumed to be a real-analytic function which attains its minimum value at most finitely many points in $\mathbb{T}^{d+1}$. Moreover, the frequency vector $\omega \in \mathbb{R}^d$ satisfies the Diophantine condition $(\mathrm{DC})_{\kappa,\tau}$,

$$\|\omega \cdot n\| \geqslant \frac{\kappa}{|n|^\tau} \quad \forall\, n \in \mathbb{Z}^d \setminus \{0\}$$

for some constants $\kappa > 0, \tau > d$. The coupling constant λ is positive and the phase θ is in $\mathbb{T}^d$. We shall study the behavior of the solutions to (1.1) for energies E in the bottom of the spectrum of the operator H_θ in the regime of large coupling constants λ. Recall that the spectrum of H_θ, which we denote by $\sigma(H_\theta)$, as a set, is independent of the phase θ.

Writing (1.1) as the system

$$X'(t) = \begin{pmatrix} 0 & 1 \\ \lambda V(t, \theta + \omega t) - E & 0 \end{pmatrix} X(t), \quad X(t) = \begin{pmatrix} u(t) \\ u'(t) \end{pmatrix}, \tag{1.2}$$

we denote by $M_t(\theta, E)$ its fundamental solution. Since the above matrix lies in $sl(2, \mathbb{R})$ for all t, it is clear that $M_t(\theta, E) \in SL(2, \mathbb{R})$ for all t. The Lyapunov exponent is defined as

$$L(E) = \lim_{t \to \infty} \frac{1}{t} \int_{\mathbb{T}^d} \ln \|M_t(\theta, E)\| \mathrm{d}\theta \geqslant 0.$$

We leave the dependence on λ implicit.

By adding a constant to V if needed, we can without loss of generality assume that $\min V = 0$.

Our main result is the following.

Theorem 1: *There is a constant $c_0 = c_0(V) > 0$ and a $\lambda_0 = \lambda_0(V, \kappa, \tau) > 0$ such that for all $\lambda > \lambda_0$,*

$$L(E) \geqslant c_0 \sqrt{\lambda},$$

for all $E \in [0, \lambda^{2/3}]$.

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This theorem generalizes the Sorets-Spencer result.[4] It is likely that the spectrum of H_θ in $[0,\lambda^{2/3}]$ is pure-point (for a.e. θ) with exponentially decaying eigenfunctions, i.e., there is a situation of Anderson localization. See Ref. 2 for an example when this is the case.

It is well known that $\min\{E:E\in\sigma(H_\theta)\}\leqslant \text{const}\ \sqrt{\lambda}$, where the constant depends on the shape of the minimum of V and the modulus of the frequency vector ω (recall that we have assumed that $\min V=0$). Hence our result indeed covers energies in the spectrum, provided that λ is sufficiently large.

From Eliasson's result[1] we know that there is an $E_0>0$ such that the spectrum in $\sigma(H_\theta)\cap[E_0,\infty)$ is purely absolutely continuous, and $L(E)=0$ on the spectrum. Hence, as the energy increases, the dynamics undergo a dramatic change. It is still unknown what is happening in the transition region, i.e., for energies $\lambda^{2/3}<E<E_0$.

For a more detailed introduction to the subject, we refer to Refs. 1–4, and the references therein.

II. PROOF OF THEOREM 1

The proof of Theorem 1 is based on a method developed by Goldstein and Schlag in Ref. 3, where they, among many other things, prove an analog of Theorem 1 for the discrete Schrödinger equation. This method relies on two tools: a large deviation estimate and the so-called avalanche principle. Below we will apply this method to the present problem.

We assume that the frequency vector $\omega\in\mathbb{R}^d$ satisfies the Diophantine condition $(\text{DC})_{\kappa,\tau}$ for some $\kappa,\tau>0$. Moreover, the energy E is always assumed to be in the interval $[0,\lambda^{2/3}]$, and λ should be sufficiently large, depending on V and the Diophantine condition.

As above, we let $M_t(\theta,E)$ denote the fundamental solution to (1.2). We introduce the matrix

$$A(\theta,E)=M_1(\theta,E)\in \mathrm{SL}(2,\mathbb{R}),\quad \theta\in\mathbb{T}^d,$$

i.e., we integrate time-one. In view of system (1.2), we have the relation

$$M_n(\theta,E)=A(\theta+(n-1)\omega,E)\cdots A(\theta+\omega,E)A(\theta,E)$$

for $n=1,2,3,\ldots$.

Let

$$L_n(E)=\frac{1}{n}\int_{\mathbb{T}^d}\ln\|M_n(\theta,E)\|\mathrm{d}\theta$$

be the approximated Lyapunov exponents. By definition

$$L(E)=\lim_{n\to\infty}L_n(E).$$

Since V is analytic, it is clear that $A(\cdot,E)$ is analytic in some complex neighborhood of $\mathbb{T}^d$. Consequently,

$$f_n(\theta)=\frac{1}{n}\ln\|M_n(\theta,E)\|$$

is a bounded plurisubharmonic function in some neighborhood of $\mathbb{T}^d$.

We note that we have the following upper bound:

$$\sup_{\theta\in\mathbb{T}^d}\|A(\theta,E)\|\leqslant\exp(c_2\sqrt{\lambda}),$$

where the constant $c_2>0$ only depends on V. This follows easily from (1.1): if $\|(u(0),u'(0))\|=1$, then $\|(u(1),u'(1))\|$ cannot be larger than $\exp(c_2\sqrt{\lambda})$. In particular, this implies that we have the upper bounds

$$|f_n(\theta)| \leqslant c_2\sqrt{\lambda} \quad \text{and } L_n(E) \leqslant c_2\sqrt{\lambda} \quad \text{for } n = 1,2,3,\ldots . \tag{2.1}$$

From the fact that $M_n(\theta+\omega)=A(\theta+n\omega)M_n(\theta)A(\theta)^{-1}$ we deduce that

$$\sup_{\theta\in\mathbb{T}^d}|f_n(\theta+\omega)-f_n(\theta)| \leqslant \frac{\text{const}}{n},$$

where the constant only depends on the norm of $A(\theta)$. By applying Proposition 9.1 in Ref. 3, Sec. 9 we obtain the large deviation estimate

$$\int_{\mathbb{T}^d}\left|\frac{1}{n}\ln\|M_n(\theta,E)\|-L_n(E)\right| \leqslant c_0\sqrt{\lambda}n^{-\sigma},$$

where the constants $c_0>0$ and $\sigma>0$ only depend on V, κ, and τ. Combining this estimate with the avalanche principle (Ref. 3, Proposition 2.2) one gets the following (see Lemma 11.1 in Ref. 3): There is an integer $l_0=l_0(c_0,\sigma)>0$ such that if

$$L_l(E) > \sqrt{\lambda}l^{-\sigma/4} \quad \text{and } L_l(E)-L_{2l}(E) < \frac{L_l(E)}{8} \tag{2.2}$$

for some $l\geqslant l_0$, then $L(E)\geqslant L_l(E)/2$.

Thus, to prove the statement of Theorem 1, i.e., that $L(E)>c_0\sqrt{\lambda}$, we only have to establish $L_l(E)>2c_0\sqrt{\lambda}$ and (2.2) for some $l>l_0$. The main tool is the following lemma.

Lemma 2.1: There exists a constant $c_1=c_1(V)>0$ such that for any integer $n>0$ there is a $\lambda_1=\lambda_1(V,d,n)>0$ such that

$$L_n(E) > c_1\sqrt{\lambda}$$

for all $E\in[0,\lambda^{2/3}]$ and for all $\lambda\geqslant\lambda_1$.

Proof: For simplicity we assume that V has a unique minimum. The case with finitely many minimum points is treated similarly. Below we always assume that $\lambda>0$ is sufficiently large, depending only on n, d, and V. Since $V:\mathbb{T}\times\mathbb{T}^d\to\mathbb{R}$ has the unique minimum 0, at $(x_0,y_0)\in\mathbb{T}\times\mathbb{T}^d$ say, there exists a $\delta>0$ such that $V(x,y)>3\delta$ for all $|x-x_0|>1/100$ and all $y\in\mathbb{T}^d$.

Define

$$G_n=\left\{\theta\in\mathbb{T}^d:\inf_{0\leqslant t\leqslant n}\lambda V(t,\theta+t\omega)-\lambda^{2/3}>0\right\}.$$

Clearly $\text{mes}(G_n)\to 1$ as $\lambda\to\infty$, so for large λ we have

$$\text{mes}(G_n) > 1/2. \tag{2.3}$$

For any $\theta\in G_n$ and any $E\in[0,\lambda^{2/3}]$ it now follows from the above definitions that for $0\leqslant t\leqslant n$,

$$\lambda V(t,\theta+t\omega)-E > \begin{cases} 2\lambda\delta & \text{if } \inf_{p\in\mathbb{Z}}|t-x_0-p|>1/100,\\ 0 & \text{otherwise.}\end{cases}.$$

Thus one verifies easily that the solution $u(t)$ to the equation

$$-u''(t)+(\lambda V(t,\theta+t\omega)-E)u(t)=0, \quad u(0)=1, \quad u'(0)=0$$

satisfies $u(n)\geqslant\exp(n\sqrt{\delta\lambda})$. Since $u(n)$ is one of the entries of the matrix $M_n(\theta,E)$, this implies that

$$\|M_n(\theta,E)\| \geqslant \exp(n\sqrt{\delta\lambda}), \quad \theta\in G_n, E\in[0,\lambda^{2/3}].$$

From this, (2.3) and the fact that M_n is in $\text{SL}(2,\mathbb{R})$, so $\|M_n(\theta,E)\|\geqslant 1$, we get

$$L_n(E) = \frac{1}{n}\int_{\mathbb{T}^d} \ln\|M_n(\theta,E)\|\mathrm{d}\theta \geqslant \frac{1}{n}\int_{G_n} \ln\|M_n(\theta,E)\|\mathrm{d}\theta \geqslant \sqrt{\delta\lambda}/2.$$

This ends the proof of the lemma. □

We now have all the pieces to complete the proof of Theorem 1. As above we assume that $\lambda > 0$ is sufficiently large, depending on V, κ, and τ. Take $\tilde{l} > l_0$, where $l_0 = l_0(c_0, \sigma) > 0$ is as above, so large that $c_1 > l^{-\sigma/4}$. Let

$$k = \left[\frac{\ln(c_2/c_1)}{\ln(8/7)}\right] + 1.$$

An application of Lemma 2.1 with $n = 2^k\tilde{l}$ yields

$$L_{2^k\tilde{l}} > c_1\sqrt{\lambda}.$$

Then there is an integer $j \in [0,2,\ldots,k]$ such that $L_{2^{j+1}\tilde{l}} > \frac{7}{8}L_{2^j\tilde{l}}$, i.e., such that

$$L_{2^{j+1}\tilde{l}} - L_{2^j\tilde{l}} < \frac{L_{2^j\tilde{l}}}{8}. \tag{2.4}$$

Indeed, since if $L_{2^{j+1}\tilde{l}} \leqslant \frac{7}{8}L_{2^j\tilde{l}}$ for all $j = 0,1,\ldots,k$, then we would have, making use of the trivial upper bound (2.1),

$$c_1\sqrt{\lambda} < L_{2^k\tilde{l}} \leqslant \left(\frac{7}{8}\right)^k L_{\tilde{l}} < \left(\frac{7}{8}\right)^k c_2\sqrt{\lambda},$$

contradicting the definition of k.

Finally, since the sequence $\{nL_n\}$ is subadditive, we also have the following estimate (since $k \geqslant j$):

$$L_{2^j\tilde{l}} \geqslant L_{2^{j+1}\tilde{l}} \geqslant \cdots \geqslant L_{2^k\tilde{l}} > c_1\sqrt{\lambda} > \tilde{l}^{-\sigma/4}\sqrt{\lambda} > (2^j\tilde{l})^{-\sigma/4}\sqrt{\lambda}. \tag{2.5}$$

Thus, (2.4) and (2.5) show that condition (2.2) holds with $l = 2^j\tilde{l} \geqslant l_0$.

Consequently,

$$L \geqslant \frac{L_l}{2} = \frac{L_{2^j\tilde{l}}}{2} \geqslant \frac{L_{2^k\tilde{l}}}{2} > \frac{c_1}{2}\sqrt{\lambda}.$$

Letting $c_0 = c_1/2$ finishes the proof of Theorem 1.

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Novel solvable variants of the goldfish many-body model

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A recent technique to identify *solvable* many-body problems in two-dimensional space yields, via a new twist, new many-body problems of "goldfish" type. Some of these models are *isochronous*, namely their *generic* solutions are *completely periodic* with a fixed period (independent of the initial data). The investigation of the behavior of some of these isochronous systems in the vicinity of their equilibrium configurations yields some amusing diophantine relations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2167917]

I. INTRODUCTION AND MAIN RESULTS

Recently a novel technique to manufacture *solvable* many-body problems has been introduced, and some many-body problems obtained in this manner have been investigated.[5–8,10] The *solvable* character of these N-body models is manifested by the possibility to reduce the solution of their initial-value problem to algebraic operations, indeed generally just to finding the N eigenvalues of an $N \otimes N$ matrix whose time evolution is explicitly known. Some of these models are extensions of the so-called "goldfish" many-body problem, a particularly neat (hence its name)[3] Hamiltonian model interpretable as a (rotation- and translation-invariant) many-body problem in the horizontal plane. In this paper we take advantage of a new twist of this technique to manufacture a novel *solvable* model, that provides a one-parameter extension of that treated in Ref. 10, itself a one-parameter extension of the goldfish model. A further extension is also outlined, but it is also noted that it is relatively trivial, inasmuch as it is reducible to just a simple variant of the preceding treatment.

The main idea of this approach is to take as starting point a *solvable* $N \otimes N$ *matrix* evolution equation, and to then focus on the time evolution of the N *eigenvalues* of the matrix whose *explicit* time dependence is obtained by solving the initial-value problem for this matrix evolution equation. One often finds that this time evolution of the N eigenvalues is naturally interpretable as a Newtonian N-body problem: indeed this evolution is generally determined by a system of N second-order ODEs in which the "accelerations" of these N moving points (thereby interpreted as the coordinates of N "point particles") are proportional to "one- and two-body forces." However, the two-body forces generally feature time-dependent "coupling constants," whose time evolution is determined by an additional system of first-order ODEs. One can interpret these "coupling constants" as additional degrees of freedom of the problem: indeed in some cases it is possible to attribute also to them a "physical" interpretation as internal degrees of freedom of the moving particles, possibly associated with "spin" variables. Another possibility, which however emerges only exceptionally, is to find some appropriate *ansatz* for the "coupling constants," whereby a subclass of solutions of the equations of motion can be identified for which the time dependence of these quantities can be gotten rid of, obtaining thereby a more standard N-body problem involving only the coordinates of the N moving particles. All the models previously treated by this

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approach[5–8,10] were characterized by the occurrence of such a "miracle," which is as well featured by the models introduced and discussed in this paper.

But before describing our new findings let us review tersely previous results, thereby also introducing our notation. We do not however elaborate here on the previous history of this approach, nor report the relevant references, since this has already been done in preceding papers of this series.[5–8,10]

The "goldfish" N-body problem is characterized by the Newtonian equations of motion

$$\ddot{z}_n = 2 \sum_{m=1, m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m}. \tag{1}$$

Notation: here and throughout this paper N is an arbitrary positive integer (generally $N \geqslant 2$), and indices such as n, m, ℓ are understood to run from 1 to N unless otherwise indicated; t is the *independent* variable, and superimposed dots denote differentiations with respect to this, generally *real*, variable ("time"); the *dependent* variables $z_n \equiv z_n(t)$ are instead generally *complex* numbers. In the case of this model, (1), the dependent variables $z_n(t)$ could be *real*, namely the motion could take place along the *real* axis in the *complex* z-plane; in some of the models considered below this is not possible; but in any case the motions in the *complex* z-plane are much more interesting than those restricted to the *real* axis, not only because for motions in the *complex* z-plane particle collisions are *not* generic (they only occur for a lower-dimensional set of initial data), but also because it is often possible to identify the *complex* z-plane with a *real* (say, horizontal) plane and to thereby reformulate the models under consideration as "physical" many-body problems characterized by *real* (and *rotation-invariant*) Newtonian equations determining the motion of N "physical" point particles moving in the *real* horizontal plane.[2,4] Such a reformulation is indeed possible in all the models reported and introduced in this paper and it contributes nontrivially to their interest; but we forsake to exhibit the relevant "physical" equations of motion, since obtaining them is a simple task well explained in the literature[2,4] that can therefore be left as an exercise for the diligent reader.

An interesting *solvable* variant[4] of the goldfish N-body problem (1) is characterized by the following Newtonian equations of motion:

$$\ddot{z}_n - (2\lambda + 1) i\omega \dot{z}_n - \lambda(\lambda + 1)\omega^2 z_n = 2 \sum_{m=1, m\neq n}^{N} \frac{(\dot{z}_n - i\lambda\omega z_n)(\dot{z}_m - i\lambda\omega z_m)}{z_n - z_m}. \tag{2}$$

Notation: here and hereafter i denotes the *imaginary* unit ($i^2 = -1$), ω is a *positive* constant which could be rescaled away but that we prefer to keep in evidence and to which we associate the basic period

$$T = \frac{2\pi}{\omega}, \tag{3}$$

and λ is a arbitrary dimensionless number. However we hereafter generally assume λ to be *real* and *rational*, these restrictions being sufficient to guarantee that *all the nonsingular* solutions of this N-body problem, (2), are *isochronous*, namely *completely periodic* with a period that is a *rational* multiple of the basic period (3). Note that the motions take now necessarily place in the *complex* z-plane and that the *singular* solutions are *not* generic, being characterized by the occurrence of a collision of two or more of the point particles $z_n(t)$ [they correspond to sets of initial data having lower dimensionality than the full $(4N)$-dimensional real phase space]. The Hamiltonian character of this model, and of other many-body *isochronous* problems, will be discussed in a separate paper by one of us (F.C.) and François Leyvraz.[11]

This *isochronous* model, (2), is related to the standard goldfish model (1), via the following simple change of dependent and independent variables[1] (generally referred to as "the trick"):[4–10]

$$z_n(t) = \exp(i\lambda\omega t)\zeta_n(\tau), \quad \tau = \frac{\exp(i\omega t) - 1}{i\omega}. \tag{4}$$

Indeed, this change of variables clearly implies that if the N (*complex*) coordinates $z_n(t)$ satisfy the system of N ODEs (2), then the N (*complex*) coordinates $\zeta_n(\tau)$ satisfy the system of N ODEs,

$$\zeta_n'' = 2\sum_{m=1,m\neq n}^{N} \frac{\zeta_n'\zeta_m'}{\zeta_n - \zeta_m}, \tag{5}$$

and vice versa. And it is plain that this system of N ODEs, (5), coincides with the standard goldfish model (1), up to a trivial, now merely notational, change of variables (here and hereafter appended primes denote of course derivation with respect to the argument of the functions they are appended to).

Note that, as the *real* time variable t evolves, the corresponding *complex* variable τ, see (4), travels round and round on the circle whose diameter, of length $2/\omega$, lies on the upper *imaginary* axis in the *complex* τ-plane, with its lower end at the origin ($\tau=0$) and its upper end at $\tau=2i/\omega$; clearly this fact is at the origin of the *isochronous* character of the many-body (2) (for more details see for instance Ref. 4).

The Newtonian equations of motion of the main *solvable* many-body problem introduced and discussed in Ref. 10 read as follows:

$$\ddot{z}_n = 2a\dot{z}_n z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - az_n^2)(\dot{z}_m - az_m^2)}{z_n - z_m}, \tag{6}$$

and their *isochronous* variant, obtained by first rewriting these equations of motion via the merely notational change of variables consisting in the replacement of the independent variable t with τ and of the dependent variables $z_n(t)$ with $\zeta_n(\tau)$ and by then applying the trick (4) with $\lambda=1$, read[10]

$$\ddot{z}_n - 3i\omega\dot{z}_n - 2\omega^2 z_n = 2a(\dot{z}_n - i\omega z_n)z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - i\omega z_n - az_n^2)(\dot{z}_m - i\omega z_m - az_m^2)}{z_n - z_m}. \tag{7}$$

Notation: here and hereafter a denotes an *arbitrary* constant, that could generally be rescaled away but that we prefer to keep in evidence. Of course for $a=0$ these two models, (6), respectively, (7), reduce to the standard goldfish model and to its *isochronous* variant, (1), respectively, (2) (with $\lambda=1$).

The (*autonomous*) Newtonian equations of motion of the first one of the *solvable* many-body problems introduced and discussed in this paper read as follows:

$$\ddot{z}_n = 2a\dot{z}_n z_n + b[\dot{z}_n - az_n^2] + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n - az_n^2][\dot{z}_m - az_m^2]}{z_n - z_m}. \tag{8}$$

Here b is an *arbitrary* constant; clearly for $b=0$ this model reduces to (6). The solution of this model is given in Sec. III (see in particular Proposition 1 and Sec. III A).

Another *solvable* N-body problem, the solution of which is provided in Sec. IV (see in particular Proposition 2 in Sec. IV A), is characterized by the following equations of motion:

$$\ddot{z}_n - (3+k)i\omega\dot{z}_n - (2+k)\omega^2 z_n = a[2\dot{z}_n - (2+k)i\omega z_n]z_n + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n - i\omega z_n - az_n^2][\dot{z}_m - i\omega z_m - az_m^2]}{z_n - z_m}. \tag{9}$$

Here k is also an *arbitrary* constant, but our main interest is in the case when k is a (*positive* or *negative*) *integer*, since this model is then *isochronous*, with the single exception of the case $k=$

-2, when the solutions are instead *multiply periodic* [and note that this model reduces to (7) for $k=0$].

Alternative formulations of these *solvable* models, (8) and (9), are provided and discussed in Sec. V. The corresponding *solvable* systems of ODEs read as follows:

$$\ddot{c}_m - 2am\dot{c}_{m+1} + (2ac_1 - b)\dot{c}_m + a^2(m+2)(m-1)c_{m+2} + a[b - m(2ac_1 - b)]c_{m+1} + a[2ac_2 - bc_1]c_m = 0, \tag{10}$$

$$\ddot{c}_m - 2ma\dot{c}_{m+1} + [2ac_1 - (2m+k+1)i\omega]\dot{c}_m + (m+2)(m-1)a^2c_{m+2} + [-2ma^2c_1 + (m+1)(2m+k)i\omega a]c_{m+1} + [2a^2c_2 - (2m+k)i\omega ac_1 - m(m+k+1)\omega^2]c_m = 0. \tag{11}$$

Notation: in each of these two dynamical systems the N dependent variables are denoted as $c_m \equiv c_m(t)$, and the rest of the notation is, we trust, self-explanatory. The index m ranges as usual from 1 to N, while the quantities c_{N+1} and c_{N+2} by definition vanish,

$$c_{N+1} = c_{N+2} = 0. \tag{12}$$

It can be moreover noted that, for each of these systems, the equation with $m=0$ is identically satisfied, provided one sets $c_0=1$. These systems look superficially linear; but they are in fact *nonlinear*, due to the presence of the dependent variables $c_1(t)$ and $c_2(t)$ in the equations of motion for the dependent variable $c_m(t)$. The second of these models, (11), is *isochronous*, namely its *generic* solutions are completely periodic with period T [see (3)],

$$c_m(t+T) = c_m(t), \tag{13}$$

provided k is an integer different from -2.

In Sec. VI we discuss the behavior of some of these systems in the neighborhood of their equilibrium configurations, focusing of course on those that do possess such (nontrivial) configurations and which are moreover *isochronous:* then the requirement that these behaviors be consistent with the *isochronous* character of these models entails some amusing *diophantine* relations, for instance determinantal formulas such as

$$\begin{vmatrix} \tilde{\mu}^2+3\tilde{\mu}-4 & 2\tilde{\mu}+8 & 0 & 0 & 0 \\ 40\beta & \tilde{\mu}^2+\tilde{\mu}-6 & 4\tilde{\mu}+6 & 4 & 0 \\ -90\beta & -20\beta & \tilde{\mu}^2-\tilde{\mu}-6 & 6\tilde{\mu} & 10 \\ 78\beta & 30\beta & 0 & \tilde{\mu}^2-3\tilde{\mu}-4 & 8\tilde{\mu}-10 \\ -24\beta & -12\beta & 0 & 0 & \tilde{\mu}^2-5\tilde{\mu} \end{vmatrix} = \prod_{j=-4}^{5} (\tilde{\mu}-j). \tag{14}$$

Here β is an arbitrary number, and there are such formulas for determinants of arbitrary order, see Sec. V (see in particular Theorem 2 and Conjecture 2).

In Sec. VII we tersely outline a generalization of the models treated in the preceding sections, but we also point out that in fact it does not represent a really substantial extension of them.

The paper is completed by two Appendixes that contain some developments, and report some formulas, whose inclusion in the main text of the paper would have disrupted the flow of the presentation.

II. A MATRIX ODE AND ITS SOLUTION

The starting point of our treatment is the following simple system of two coupled *matrix* ODEs:

$$\dot{U}(t) = a[U(t)]^2 + V(t), \quad \dot{V}(t) = b(t)V(t). \tag{15}$$

Notation: the dependent variables $U(t)$ and $V(t)$ are $N\otimes N$ matrices, the independent variable is the scalar t ("time," but occasionally we will replace below t with the *complex* variable τ), superimposed dots indicate time-differentiations, a is an arbitrary *scalar* constant (that could be rescaled away, but we prefer to keep it; note that throughout this paper we assume that a does not vanish, $a\neq 0$, because the results for the $a=0$ case are not new), and $b(t)$ is a *scalar* function of time which we reserve to assign later.

The second of these two matrix ODEs can of course be easily solved,

$$V(t)=\varphi(t)C, \tag{16a}$$

$$\varphi(t)=\exp\left[\int_0^t \mathrm{d}t'\; b(t')\right], \tag{16b}$$

$$C=V(0), \tag{16c}$$

and the system of two matrix ODEs (15) can thereby be rewritten as the single $N\otimes N$ matrix ODE,

$$\dot{U}(t)=a[U(t)]^2+\varphi(t)C. \tag{17}$$

The reason for writing the system first in the form (15) will become clear later. Note that for $b(t)=0$, $\varphi(\tau)=1$, this matrix evolution equation, (17), reduces to the matrix evolution equation that provided the starting point for the treatment given in Ref. 10.

To solve the matrix ODE (17) we set

$$U(t)=-a^{-1}\dot{W}(t)[W(t)]^{-1}, \tag{18}$$

and we thereby obtain for the $N\otimes N$ matrix $W(t)$ the following *linear* second-order ODE:

$$\ddot{W}(t)+a\varphi(t)CW(t)=0. \tag{19}$$

We now introduce the *scalar* second-order ODE,

$$\ddot{w}(\alpha;t)+\alpha\varphi(t)w(\alpha;t)=0, \tag{20}$$

where α is a *scalar* constant, and we denote with $w_{\pm}(\alpha;t)$ the two independent solutions of this ODE characterized by the initial conditions

$$w_+(\alpha;0)=1,\quad \dot{w}_+(\alpha;0)=0, \tag{21a}$$

$$w_-(\alpha;0)=0,\quad \dot{w}_-(\alpha;0)=1. \tag{21b}$$

Let us note for future reference that as a consequence of (20) and (21) there holds the Wronskian relation

$$w_+(\alpha;t)\dot{w}_-(\alpha;t)-\dot{w}_+(\alpha;t)w_-(\alpha;t)=1. \tag{22}$$

It is now clear that the solution of the initial-value problem for the *matrix* ODE (19) is provided by the formula

$$W(t)=w_+(aC;t)W(0)+w_-(aC;t)\dot{W}(0). \tag{23}$$

Note that there is no ordering ambiguity in the definition of the two $N\otimes N$ matrices $w_{\pm}(aC;t)$, since each of them only depends on the single matrix C, that of course commutes with itself [while it need not commute with $W(0)$ or $\dot{W}(0)$].

The insertion of this expression of the $N\otimes N$ matrix $W(t)$ in (18) yields, after a bit of elementary matrix algebra, the following solution of the original ODE (15):

$$U(t) = [\dot{w}_-(aC;t)U(0) - a^{-1}\dot{w}_+(aC;t)][w_+(aC;t) - aw_-(aC;t)U(0)]^{-1}, \tag{24a}$$

with the constant matrix C defined as follows [see (15) and (16c)]:

$$C = \dot{U}(0) - a[U(0)]^2. \tag{24b}$$

The matrix system (15) is considered *solvable* inasmuch as the explicit solution of the initial-value problem for it is given by these formulas, (24), that require of course knowledge of the two *scalar* solutions $w_\pm(\alpha;t)$ of the *scalar* second-order ODE (20). In the following we will consider specific cases in which this *scalar* ODE (20) can be explicitly solved in terms of standard special functions (such as, say, Bessel functions, see below).

But before ending this section let us also report the more explicit form that the solution (24) takes in the special case (that will be of interest to us, see below) in which the $N \otimes N$ matrix C is *dyadic* indeed proportional to an $N \otimes N$ projection matrix P,

$$C = cP, \quad P_{nm} = p_n p_m, \quad \sum_{n=1}^{N} p_n^2 = 1, \quad P^2 = P. \tag{25}$$

Then, after a considerable amount of tedious if trivial algebra, the solution formula (24a) with (25) can be rewritten as follows:

$$\begin{aligned} U(t) = \{U(0) + [v(t)]^{-1}\{f(t)P + g(t)PU(0) + U(0)[1 - atU(0)]^{-1}P[1 - w_+(ac;t) \\ + a[w_-(ac;t) - t]U(0)]\}\}[1 - atU(0)]^{-1}, \end{aligned} \tag{26a}$$

$$f(t) = -a^{-1}\dot{w}_+(ac;t)v(t) + [w_+(ac;t) - 1]u(t), \tag{26b}$$

$$g(t) = [\dot{w}_-(ac;t) - 1]v(t) - a[w_-(ac;t) - t]u(t), \tag{26c}$$

$$v(t) = \sum_{n,m=1}^{N} p_n\{[w_+(ac;t) - aw_-(ac;t)U(0)][1 - atU(0)]^{-1}\}_{nm}p_m, \tag{26d}$$

$$u(t) = \sum_{n,m=1}^{N} p_n\{[a^{-1}\dot{w}_+(ac;t) + [1 - \dot{w}_-(ac;t)]U(0)][1 - atU(0)]^{-1}\}_{nm}p_m. \tag{26e}$$

Note that the only matrices appearing on the right-hand sides of these formulas, (26), are $U(0)$ and P: the functions $w_\pm(ac;t)$ are now *scalars*, in contrast to the $N \otimes N$ *matrices* $w_\pm(aC;t)$ appearing on the right-hand side of (24a). Moreover, an additional simplification will be entailed below by the fact that, in the cases of interest to us, the matrix $U(0)$ will be *diagonal*, entailing that the matrix inversions involving only this matrix can be performed trivially [in contrast to what is the case for the matrix inversion on the right-hand side of (24a)]. To obtain this simplified version of the solution we took advantage of the following standard identity valid for any projection matrix P, see (25):

$$h(XPY) = h(0) + \frac{h(z) - h(0)}{z}XPY, \tag{27a}$$

with

$$PYXP = zP, \quad z = \sum_{n,m,\ell=1}^{N} p_n Y_{nm} X_{m\ell} p_\ell. \tag{27b}$$

This identity holds for any two matrices X and Y and for any *scalar* function $h(z)$ for which these formulas make good sense.

Remark: The expression (26) of the solution of the matrix evolution equation (17) is valid provided the formulas (25) hold with a finite (nonvanishing) value of the constant c. This is not the case if the $N\otimes N$ matrix C is *nilpotent*, $C^p=0$ for some positive integer value of p. The treatment of this special case is left as an instructive exercise for the diligent reader.

■

III. A NEW GOLDFISH MANY-BODY PROBLEM

To derive new solvable many-body problems of goldfish type from the solvable system of two $N\otimes N$ matrix ODEs (15) we use a (minor modification of a) by now standard technique.[5–8,10] Hence we set

$$U(t) = R(t)Z(t)[R(t)]^{-1}, \quad Z(t) = \mathrm{diag}[z_n(t)], \tag{28a}$$

$$V(t) = R(t)G(t)[R(t)]^{-1}, \quad [G(t)]_{nm} = \delta_{nm}g_n(t) + (1-\delta_{nm})g_{nm}(t), \tag{28b}$$

so that

$$\dot{U}(t) = R(t)\{\dot{Z}(t) + [M(t),Z(t)]\}[R(t)]^{-1}, \tag{29a}$$

$$\dot{V}(t) = R(t)\{\dot{G}(t) + [M(t),G(t)]\}[R(t)]^{-1}, \tag{29b}$$

where

$$M(t) = [R(t)]^{-1}\dot{R}(t), \tag{29c}$$

$$[M(t)]_{nm} = (1-\delta_{nm})\mu_{nm}(t). \tag{29d}$$

Note that the formulas (28a) imply that the N (generally *complex*) numbers $z_n(t)$ are the N eigenvalues of the $N\otimes N$ matrix $U(t)$, and that the $N\otimes N$ matrix $R(t)$ is the matrix that diagonalizes the $N\otimes N$ matrix $U(t)$. Moreover, for simplicity, we are assuming here [see (29d)] that the diagonal elements of the $N\otimes N$ matrix $M(t)$, defined in terms of $R(t)$ by (29c), *all* vanish: the legitimacy of such a choice is a well-known fact.[5–8,10]

Insertion of these formulas in (15) yields the following two $N\otimes N$ matrix ODEs:

$$\dot{Z}(t) + [M(t),Z(t)] = a[Z(t)]^2 + G(t), \tag{30a}$$

$$\dot{G}(t) + [M(t),G(t)] = b(t)G(t). \tag{30b}$$

By writing out separately the *diagonal* and *off-diagonal* parts of these matrix equations we get the following equations:

$$\dot{z}_n(t) = az_n^2(t) + g_n(t), \tag{31a}$$

$$\dot{g}_n(t) + \sum_{m=1,m\neq n}^{N} [\mu_{nm}(t)g_{mn}(t) - g_{nm}(t)\mu_{mn}(t)] = b(t)g_n(t), \tag{31b}$$

$$\mu_{nm}(t)[z_n(t) - z_m(t)] = -g_{nm}(t), \quad n \neq m, \tag{31c}$$

$$\dot{g}_{nm}(t) = \mu_{nm}(t)[g_n(t) - g_m(t)] + b(t)g_{nm}(t) - \sum_{\ell=1;\ell\neq n,m}^{N} [\mu_{n\ell}(t)g_{\ell m}(t) - g_{n\ell}(t)\mu_{\ell m}(t)], \quad n \neq m. \tag{31d}$$

By solving the first of these equations for $g_n(t)$ and the third for $\mu_{nm}(t)$ and by then inserting the results in the second and the fourth we get

$$\ddot{z}_n(t) = 2a\dot{z}_n(t)z_n(t) + b(t)[\dot{z}_n(t) - az_n^2(t)] + 2\sum_{m=1,m\neq n}^{N} \frac{g_{nm}(t)g_{mn}(t)}{z_n(t) - z_m(t)}, \tag{32a}$$

$$\frac{\dot{g}_{nm}(t)}{g_{nm}(t)} = -\frac{[\dot{z}_n(t) - az_n^2(t)] - [\dot{z}_m(t) - az_m^2(t)]}{z_n(t) - z_m(t)} + b(t) + \sum_{\ell=1;\ell\neq n,m}^{N} \left\{ \frac{g_{n\ell}(t)g_{\ell m}(t)}{g_{nm}(t)} \left[\frac{1}{z_n(t) - z_\ell(t)} + \frac{1}{z_m(t) - z_\ell(t)} \right] \right\}, \quad n \neq m. \tag{32b}$$

We now take advantage of the following *miraculous* fact: as the diligent reader will easily verify,

$$g_{nm}(t) = [\dot{z}_n(t) - az_n^2(t)]^{1/2}[\dot{z}_m(t) - az_m^2(t)]^{1/2} \tag{33}$$

provides a solution to (32b) [which has been written above in a format appropriate to facilitate checking that this is indeed true: differentiate logarithmically this formula, (33) and use (32a)]. Hence the insertion of this expression of $g_{nm}(t)$ in (32a) entails that the N-body problem characterized by the following system of N coupled Newtonian equations of motion:

$$\ddot{z}_n(t) = 2a\dot{z}_n(t)z_n(t) + b(t)[\dot{z}_n(t) - az_n^2(t)] + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n(t) - az_n^2(t)][\dot{z}_m(t) - az_m^2(t)]}{z_n(t) - z_m(t)}, \tag{34}$$

is *solvable*, to the extent the $N\otimes N$ matrix ODE (15) is itself *solvable* (as discussed in the preceding Sec. II). It is moreover clear that the substantial simplification, see above, associated with the *dyadic* nature of the constant matrix C is applicable in this case, since this $N\otimes N$ matrix is now given by the simple *dyadic* expression

$$C_{nm} = [\dot{z}_n(0) - az_n^2(0)]^{1/2}[\dot{z}_m(0) - az_m^2(0)]^{1/2}. \tag{35}$$

This formula, (35), follows from (16), (33), and (31a) via (28b) with $R(0)=\mathbf{1}$, this last assignment being a permissible one; a different assignment would cause a unitary transformation of the matrices $U(t)$ and $V(t)$, with no effect on the eigenvalues $z_n(t)$ of $U(t)$. Note that this assignment, $R(0)=\mathbf{1}$, also implies via (28a) that the $N\otimes N$ matrix $U(0)$ is *diagonal*,

$$U(0) = \mathrm{diag}[z_n(0)]. \tag{36}$$

The fact that the matrix C is *dyadic*, see (35), entails the validity of (25) with the quantities p_n and c given now in terms of the initial data $z_n(0)$, $\dot{z}_n(0)$ as follows:

$$p_n = \left[\frac{\dot{z}_n(0) - az_n^2(0)}{c} \right]^{1/2}, \quad c = \sum_{n=1}^{N} [\dot{z}_n(0) - az_n^2(0)]; \tag{37}$$

and moreover (36) entails that the scalars $v(t)$ and $u(t)$, see (26d) and (26e), are now given in terms of the initial data as follows:

$$v(t) = \sum_{n=1}^{N} p_n^2 \frac{w_+(ac;t) - a w_-(ac;t) z_n(0)}{1 - a t z_n(0)}, \tag{38a}$$

$$u(t) = \sum_{n=1}^{N} p_n^2 \frac{a^{-1}\dot{w}_+(ac;t) + [1 - \dot{w}_-(ac;t)] z_n(0)}{1 - a t z_n(0)}. \tag{38b}$$

It is also easily seen, using (22), that some additional simplifications occur in the expressions of $f(t)$ and $g(t)$, see (26b) and (26c), that may now be rewritten as follows:

$$f(t) = \sum_{n=1}^{N} p_n^2 \frac{-a^{-1}\dot{w}_+(ac;t) + [w_+(ac;t) + \dot{w}_-(ac;t) - 2] z_n(0)}{1 - a t z_n(0)}, \tag{38c}$$

$$g(t) = \sum_{n=1}^{N} p_n^2 \frac{1 - w_+(ac;t) + t\dot{w}_+(ac;t) + [1 - \dot{w}_-(ac;t)] a t z_n(0)}{1 - a t z_n(0)}. \tag{38d}$$

In conclusion there holds the following

Proposition 1: The solution $z_n(t)$ of the initial-value problem for the system of N ODEs (34) is given by the following prescription:

$$z_n(t) = \text{eigenvalues of } U(t), \tag{39}$$

[see (28a)], where the $N \otimes N$ matrix $U(t)$ is given by the formula (26a) with the constant $N \otimes N$ matrix $U(0)$, the projection matrix $P_{nm} = p_n p_m$, as well as the scalar constant c, respectively, the scalar functions $f(t)$, $g(t)$, and $v(t)$ defined in terms of the initial data by (36) and (37), respectively, (38), and with the *scalar* functions $w_\pm(\alpha;t)$ defined as the solutions characterized by the initial conditions (21) of the second-order ODE (20) with (16b). ■

This proposition demonstrates the *solvability* of the system of N ODEs (34) for the N dependent variables $z_n(t)$ by reducing its initial-value problem to the purely algebraic task of finding the N eigenvalues $z_n(t)$ of an $N \otimes N$ matrix $U(t)$ given in terms of the initial data by a quite explicit formula, see (26) with (38) and (37), the time dependence of which is encoded in the solutions of the *scalar* ODE (20) with (16b). This is a *linear* second-order ODE, generally simple enough to be explicitly solvable in terms of well-known special functions, see below.

The system of N ODEs (34) for the N dependent variables $z_n(t)$ is generally *nonautonomous* due to the explicit time dependence of the function $b(t)$, which we are still free to assign. In the following section we focus on the *autonomous* case that obtains by assuming this function $b(t)$ to be just a constant. In the sequent Sec. IV, by assigning a specific time dependence to the function $b(t)$, we obtain, via an appropriate change of *dependent* and *independent* variables, another *autonomous* version of the goldfish system which, for appropriate values of the arbitrary constants it features, has the property to be *isochronous*.

A. Autonomous case

The many-body model (34) contains the *scalar* function $b(t)$, which we are still free to assign. Of course if one sets $b(t) = 0$ one gets back to the model treated in Ref. 10. In this section we treat the case in which

$$b(t) = b \tag{40}$$

is an *arbitrary* (of course *scalar*) *constant*, entailing that the equations of motion (34) become *autonomous* [see (8)],

$$\ddot{z}_n(t) = 2a\dot{z}_n(t)z_n(t) + b[\dot{z}_n(t) - az_n^2(t)] + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n(t) - az_n^2(t)][\dot{z}_m(t) - az_m^2(t)]}{z_n(t) - z_m(t)}. \tag{41}$$

The treatment given above entails that the solution $z_n(t)$ of the initial-value problem for this problem is given by Proposition 1, with the following specific assignment of the two scalar functions $w_\pm(\alpha;t)$:

$$w_+(\alpha;t) = \frac{Y_0'[x(0)]J_0[x(t)] - J_0'[x(0)]Y_0[x(t)]}{Y_0'[x(0)]J_0[x(0)] - J_0'[x(0)]Y_0[x(0)]}, \tag{42a}$$

$$w_-(\alpha;t) = \frac{4\{-Y_0[x(0)]J_0[x(t)] + J_0[x(t)]Y_0[x(t)]\}}{\alpha^{1/2}\{Y_0'[x(0)]J_0[x(0)] - J_0'[x(0)]Y_0[x(0)]\}}, \tag{42b}$$

where

$$x(t) = \frac{\alpha^{1/2}}{2b}\exp\left[\frac{bt}{2}\right] \tag{42c}$$

and $J_0(x)$ and $Y_0(x)$ are the standard Bessel functions of order zero (see for instance Ref. 12). Indeed these two functions, see (42), are the solutions characterized by the initial conditions (21) of the second-order ODE,

$$\ddot{w}(\alpha;t) + \alpha\exp(bt)w(\alpha;t) = 0, \tag{43}$$

that clearly corresponds to (20) with (16b) and (40). An explicit expression of the time dependence of these two functions is provided by the following two formulas:

$$J_0[x(t)] = \sum_{k=0}^{\infty} \frac{1}{(k!)^2}\left[\frac{-\alpha\exp(bt)}{16}\right]^k, \tag{44a}$$

$$Y_0[x(t)] = \left(\frac{2}{\pi}\right)\sum_{k=0}^{\infty} \frac{1}{(k!)^2}\left[\frac{-\alpha\exp(bt)}{16}\right]^k\left[bt + \frac{1}{2}\ln\left(\frac{\alpha}{4b^2}\right) + \gamma_k\right], \tag{44b}$$

$$\gamma_k = -\sum_{\ell=1}^{k}\ln\left(\frac{1+\ell}{\ell}\right) + \sum_{\ell=k+1}^{k}\left[\frac{1}{\ell} - \ln\left(\frac{1+\ell}{\ell}\right)\right]. \tag{44c}$$

These expressions clearly entail that, if $\mathrm{Re}(b) < 0$, in the remote future $(t \to +\infty)$

$$J_0[x(t)] = 1 + O[\exp(bt)], \tag{45a}$$

$$Y_0[x(t)] = \left(\frac{2}{\pi}\right)\left[bt + \frac{1}{2}\ln\left(\frac{\alpha}{4b^2}\right) + \gamma\right] + O[t\exp(bt)], \tag{45b}$$

$$\gamma = \gamma_0 = \sum_{\ell=1}^{\infty}\left[\frac{1}{\ell} - \ln\left(\frac{1+\ell}{\ell}\right)\right]. \tag{45c}$$

Using these formulas it is easily shown that, if $\mathrm{Re}(b) < 0$, in the remote future *all* the particles tend to the origin,

$$z_n(t) \to 0 \quad \text{as } t \to +\infty. \tag{46}$$

This outcome obtains for *generic* initial data: note that the asymptotic configuration with all

particles sitting at the origin is an equilibrium configuration, albeit not a *genuine* one (see below). The exceptional (i.e., *nongeneric*) case is when the particles are in equilibrium, which can only happen for $N=2$ and $N=3$ and entails that the constant c, see (37), vanishes, see the next section.

If $\mathrm{Re}(b)\geqslant 0$ the asymptotic behavior as $t\to\infty$ is somewhat less trivial, and we just mention qualitatively the *generic* outcome here, which obtains because asymptotically the matrix $U(t)$ equals—up to a time-dependent factor—the projection operator P (the diligent reader will verify). Then all particles but one converge to the origin, while if $\mathrm{Re}(b)=0$ that one approaches a limit cycle trajectory which circles around the origin with period $T=4\pi/|b|$ (we are of course assuming $b\neq 0$, the $b=0$ having being treated in Ref. 10), while if $\mathrm{Re}(b)>0$ it spirals exponentially towards infinity.

B. Equilibrium configuration

It is easy to show (see Appendix A) that this N-body problem, (41), has no *genuine* equilibrium configuration for $N>3$ (here and hereafter we denote as *genuine* the equilibrium configurations in which no two particles sit at the same position, namely such that $z_n\neq z_m$ for $n\neq m$). For $N=2$ the equilibrium configuration is unique (up to permutations; this obvious *caveat* applies of course to *all* equilibrium configurations, and will not be repeated below):

$$z_1=-\frac{(1+i)b}{2a},\quad z_2=-\frac{(1-i)b}{2a}. \tag{47}$$

For $N=3$ the configuration, again unique, is the same, see (47), complemented by $z_3=0$.

Note that in both these cases the constant c, see (37), vanishes (see the *Remark* at the end of Sec. II).

IV. NEW ISOCHRONOUS GOLDFISH MODEL

To manufacture another *solvable* and *autonomous* variant of the goldfish many-body problem we take as starting point the model (34) with

$$b(t)=\frac{ik\omega}{1+i\omega t} \tag{48a}$$

entailing [see (28b)]

$$\varphi(t)=(1+i\omega t)^k. \tag{48b}$$

Here and throughout ω is a *positive* constant that sets the time scale via the associated period (3); and k is an *arbitrary* dimensionless constant, but we shall see below that it is convenient, in order to obtain *isochronous* models, to assume that k is an *integer* [but different from -2; and note that, as already mentioned above, for $k=0$, i.e., $b(\tau)=0$, one obtains again the model treated in Ref. 10]. A hint of the reason why such values have a special significance is provided by (20) with (48); but we will return to this question below, so for the moment k can be considered just an arbitrary number.

With this assignment (48) the equations of motion (34) become

$$\zeta_n''(\tau)=2a\zeta_n'(\tau)\zeta_n(\tau)+\frac{ik\omega}{1+i\omega\tau}[\zeta_n'(\tau)-a\zeta_n^2(\tau)]+2\sum_{m=1,m\neq n}^{N}\frac{[\zeta_n'(\tau)-a\zeta_n^2(\tau)][\zeta_m'(\tau)-a\zeta_m^2(\tau)]}{\zeta_n(\tau)-\zeta_m(\tau)}. \tag{49}$$

Note that we made (for reasons that will be immediately clear) a trivial, *merely notational*, change [we wrote the independent variable as τ rather than t, and the dependent variables as $\zeta_n(\tau)$ rather than $z_n(t)$]: accordingly appended primes indicate here differentiations of the dependent variables $\zeta_n(\tau)$ with respect to the independent variable τ.

A. An isochronous model

We now make the following change of *dependent* and *independent* variables:

$$z_n(t) = \exp(i\omega t)\zeta_n(\tau), \tag{50a}$$

$$\tau = \frac{\exp(i\omega t) - 1}{i\omega}, \quad \exp(i\omega t) = 1 + i\omega\tau, \tag{50b}$$

entailing the relation

$$\dot{z}_n(t) - i\omega z_n(t) = \exp(i\omega t)\zeta_n'(\tau), \tag{50c}$$

hence as well

$$\dot{z}_n(0) = -i\omega z_n(0) = \zeta_n'(0). \tag{50d}$$

Note that this coincides with the trick (4), with the specific assignment $\lambda = 1$.

It is thereby easily seen that the (*nonautonomous*) system (49) becomes via (50) the following *autonomous* system, that we hereafter interpret as a many-body problem describing the motion in the *complex* z-plane of the N points $z_n(t)$ evolving as functions of the (*real*) variable t ("time"):

$$\ddot{z}_n(t) - (3+k)i\omega\dot{z}_n(t) - (2+k)\omega^2 z_n(t) = a[2\dot{z}_n(t) - (2+k)i\omega z_n(t)]z_n(t) + 2\sum_{m=1, m\neq n}^{N} \frac{[\dot{z}_n(t) - i\omega z_n(t) - az_n^2(t)][\dot{z}_m(t) - i\omega z_m(t) - az_m^2(t)]}{z_n(t) - z_m(t)}. \tag{51}$$

For $k=0$ this system reduces of course to (7), while for $k \neq 0$ it coincides with (9).

The solution of the initial-value problem for this system is then given, via (50) and (48b), by the following

Proposition 2: The solution $z_n(t)$ of the initial-value problem for this N-body problem, (51), is given by the following prescription:

$$z_n(t) = \text{eigenvalues of } \widetilde{U}(t), \tag{52a}$$

$$\widetilde{U}(t) = \exp(i\omega t)\{\widetilde{U}(0) + [\widetilde{v}(\tau)]^{-1}\{\widetilde{f}(\tau)\widetilde{P} + \widetilde{g}(\tau)\widetilde{P}\widetilde{U}(0) + \widetilde{U}(0)[1 - a\tau\widetilde{U}(0)]^{-1}\widetilde{P}[1 - \widetilde{w}_+(ac;k;\tau) + a[\widetilde{w}_-(ac;k;\tau) - \tau]\widetilde{U}(0)]\}\}[1 - a\tau\widetilde{U}(0)]^{-1}, \tag{52b}$$

$$\widetilde{U}(0) = \text{diag}[z_n(0)]. \tag{52c}$$

$$\widetilde{v}(\tau) = \sum_{n,m=1}^{N} \widetilde{p}_n^2 \frac{\widetilde{w}_+(ac;k;\tau) - a\widetilde{w}_-(ac;k;\tau)z_n(0)}{1 - a\tau z_n(0)}, \tag{52d}$$

$$\widetilde{f}(t) = \sum_{n,m=1}^{N} \widetilde{p}_n^2 \frac{-a^{-1}\widetilde{w}_+'(ac;k;\tau) + [\widetilde{w}_+(ac;k;\tau) + \widetilde{w}_-'(ac;k;\tau) - 2]z_n(0)}{1 - a\tau z_n(0)}, \tag{52e}$$

$$\widetilde{g}(t) = \sum_{n,m=1}^{N} \widetilde{p}_n^2 \frac{1 - \widetilde{w}_+(ac;k;\tau) + \tau\widetilde{w}_+'(ac;k;\tau) + [1 - \widetilde{w}_-'(ac;k;\tau)]a\tau z_n(0)}{1 - a\tau z_n(0)}, \tag{52f}$$

$$\tilde{p}_n = \left[\frac{\dot{z}_n(0) - i\omega z_n(0) - a z_n^2(0)}{\tilde{c}} \right]^{1/2}, \tag{52g}$$

$$\tilde{c} = \sum_{n=1}^{N} [\dot{z}_n(0) - i\omega z_n(0) - a z_n^2(0)]. \tag{52h}$$

The two *scalar* functions $\tilde{w}_{\pm}(\alpha;k;\tau)$ that characterize the time dependence of the $N \otimes N$ matrix $\tilde{U}(t)$ are the two solutions of the second-order ODE,

$$\tilde{w}''(\alpha;k;\tau) + \alpha(1 + i\omega\tau)^k \tilde{w}(\alpha;k;\tau) = 0, \tag{53a}$$

[see (20) with (48b)] characterized by the initial conditions

$$\tilde{w}_+(\alpha;k;0) = 1, \quad \tilde{w}'_+(\alpha;k;0) = 0, \tag{53b}$$

$$\tilde{w}_-(\alpha;k;0) = 0, \quad \tilde{w}'_-(\alpha;k;0) = 1 \tag{53c}$$

[see (21)]; and the variable τ appearing in these equations, see (52) and (53), is related to the independent variable t ("time") by (50b). ■

The *solvability* of this model is underscored by the possibility to write in explicit form the functions $\tilde{w}_{\pm}(\alpha;k;\tau)$,

$$\tilde{w}_+(\alpha;k;\tau) = \left[\frac{\xi(\tau)}{\xi(0)} \right]^{\nu} \frac{I_{1-\nu}[\xi(0)] I_{\nu}[\xi(\tau)] - I_{\nu-1}[\xi(0)] I_{-\nu}[\xi(\tau)]}{I_{1-\nu}[\xi(0)] I_{\nu}[\xi(0)] - I_{\nu-1}[\xi(0)] I_{-\nu}[\xi(0)]}, \tag{54a}$$

$$\tilde{w}_-(\alpha;k;\tau) = (-\alpha)^{-1/2} \left[\frac{\xi(\tau)}{\xi(0)} \right]^{\nu} \frac{-I_{-\nu}[\xi(0)] I_{\nu}[\xi(\tau)] + I_{\nu}[\xi(0)] I_{-\nu}[\xi(\tau)]}{I_{1-\nu}[\xi(0)] I_{\nu}[\xi(0)] - I_{\nu-1}[\xi(0)] I_{-\nu}[\xi(0)]}, \tag{54b}$$

$$\xi(t) = 2\nu \left(\frac{\alpha}{\omega^2} \right)^{1/2} (1 + i\omega\tau)^{1/(2\nu)} = \frac{2\alpha^{1/2}(1 + i\omega\tau)^{1+(k/2)}}{\omega(2+k)}, \tag{54c}$$

$$\nu = \frac{1}{2+k}, \tag{54d}$$

where $I_{\nu}(\xi)$ is the Bessel functions of the second kind (see, for instance, Ref. 12). Note that these formulas, which are valid for any value of the parameter k except $k=-2$, imply

$$\left[\frac{\xi(\tau)}{\xi(0)} \right]^{\nu} = (1 + i\omega\tau)^{1/2}, \tag{55}$$

and, more importantly for the following, that the functions $\tilde{w}_{\pm}(\alpha;k;\tau)$ are *entire* functions of the (*complex*) variable τ if k is an integer larger than -2, and that they are as well singularity free in the entire *complex* τ-plane if k is a negative integer smaller than -2 except for an essential singularity at $\tau = i/\omega$. The more direct way to verify the validity of these assertions is to note that the formulas (54c) with (54d), as well as the definition of the Bessel functions $I_{\pm\nu}(\xi)$,[12] entail

$$[\xi(\tau)]^{\nu} I_{\nu}[\xi(\tau)] = \left[\frac{2\alpha}{(2+k)^2\omega^2} \right]^{\nu} \sum_{j=0}^{\infty} \frac{1 + i\omega\tau}{j!\Gamma(j+1+\nu)} \left[\frac{\alpha(1 + i\omega\tau)^{2+k}}{(2+k)^2\omega^2} \right]^j, \tag{56a}$$

$$[\xi(\tau)]^{\nu} I_{-\nu}[\xi(\tau)] = \left[\frac{\alpha}{2(2+k)^2\omega^2} \right]^{\nu} \sum_{j=0}^{\infty} \frac{1}{j!\Gamma(j+1-\nu)} \left[\frac{\alpha(1 + i\omega\tau)^{2+k}}{(2+k)^2\omega^2} \right]^j. \tag{56b}$$

It is therefore clear that if k is a *arbitrary integer* (different from -2), the $N\otimes N$ matrix $\widetilde{U}(t)$ is *periodic* in t with period T, see (50b) and (3),

$$\widetilde{U}(t+T)=\widetilde{U}(t), \tag{57}$$

and therefore its eigenvalues $z_n(t)$ are as well periodic functions of t with a period which is a finite integer multiple J of T [due to the possibility that the eigenvalues of $\widetilde{U}(t)$ exchange their roles through the motion; but of course J cannot exceed $N!$, indeed it is generally much smaller].[13] The conclusions reported above about the *isochronicity* of the N-body problem (51) are therefore confirmed for *all integer* values of the parameter k, be they *positive* or *negative*, with the single exception of the value $k=-2$.

In the exceptional case $k=-2$ clearly [see (53)]

$$\widetilde{w}_+(\alpha;-2;\tau)=\tfrac{1}{2}(1+i\omega\tau)^{1/2}[(1+i\omega\tau)^{\Delta}+(1+i\omega\tau)^{-\Delta}], \tag{58a}$$

$$\widetilde{w}_-(\alpha;-2;\tau)=\frac{1}{2i\omega\Delta}(1+i\omega\tau)^{1/2}[(1+i\omega\tau)^{\Delta}-(1+i\omega\tau)^{-\Delta}], \tag{58b}$$

$$\Delta=\frac{1}{2}\left(1+\frac{4\alpha}{\omega^2}\right)^{1/2}, \tag{58c}$$

entailing that the functions $\widetilde{w}_{\pm}(\alpha;-2;\tau)$ have a branch point at $\tau=i/\omega$. Hence in this case the *generic* solution of the many-body model (51) is *not* completely periodic: it is *multiply periodic*, its time evolution being a nonlinear superposition of two periodic time evolutions with two periods which are integer multiples, respectively, of $T/2$ and of

$$\widetilde{T}=\frac{T}{\Delta}=2T\left(1+\frac{4a\widetilde{c}}{w^2}\right)^{-1/2}=4\pi(\omega^2+4a\widetilde{c})^{-1/2}. \tag{59}$$

Note that, in contrast to the period T, see (3), this second period $\widetilde{T}$ does depend on the initial data, see (59) with (52h); of course the solution is *completely periodic* whenever $\widetilde{T}$ and T are *congruent*.

The formulas written above remain valid for *arbitrary* (even *complex*) values of the parameter k, but in this paper we do not discuss such cases.

B. Equilibrium configurations

In this section we report tersely some simple results for the equilibrium configurations of the solvable *isochronous* system defined above. An outline of the derivation of these simple findings is provided in Appendix A. More information on the equilibrium configurations (when they exist for the N-body problem with *arbitrary* N) are provided in Sec. VI.

For $N=2$ the only *genuine* equilibrium configuration of the model (51) is $z_1=0$ and $z_2=\omega/ia$; this equilibrium configuration exists for all values of the parameter k. For $N>2$ there exist *genuine* equilibrium configurations in which none of the coordinates z_n takes one of these two values (namely such that $z_n\neq 0$ and $z_n\neq\omega/ia$) only if $k=-(N+1)$ or $k=N-3$. The first case is characterized by the relations

$$\sum_{n=1}^{N} z_n=0, \tag{60a}$$

$$\sum_{n=1}^{N} z_n^2 = 0; \tag{60b}$$

the second is instead characterized by the relations

$$\sum_{n=1}^{N} z_n = \frac{N\omega}{ia}, \quad \sum_{n=1}^{N} z_n^2 = -N\left(\frac{\omega}{a}\right)^2. \tag{61}$$

Moreover there are two corresponding *genuine* equilibrium configurations of the $(N+1)$-body problem with the same values of the N coordinates z_n and with $z_{N+1}=0$ (provided $z_n \neq 0$), respectively, $z_{N+1}=\omega/ia$ (provided $z_n \neq \omega/ia$); and there is a corresponding *genuine* equilibrium configuration of the $(N+2)$-body problem with the same values of the coordinates z_n and with $z_{N+1}=0$, $z_{N+2}=\omega/ia$ (provided $z_n \neq 0$ and $z_n \neq \omega/ia$).

V. ALTERNATIVE FORMULATIONS

Alternative formulations of the *solvable* many-body problems reported above can be obtained by introducing the time-dependent monic polynomial $\psi(z,t)$, of degree N in z, whose N zeros $z_n(t)$ evolve according to the *solvable* models described above,

$$\psi(z,t) = \prod_{n=1}^{N} [z - z_n(t)] = z^N + \sum_{m=1}^{N} c_m(t) z^{N-m} \tag{62a}$$

$$= \sum_{m=0}^{N} c_m(t) z^{N-m}, \quad c_0 = 1, \tag{62b}$$

and by then considering the systems of ODEs characterizing the time evolution of the N coefficients $c_m(t)$ of this polynomial. These systems of N ODEs for the N coefficients $c_m(t)$ constitute then new, and clearly no less *solvable*, dynamical systems. To obtain these results the formulas collected in Appendix B are quite useful, and they allow us to report without further ado the relevant results.

Remark: Clearly whenever the N numbers $z_n(t)$ are identified as the N eigenvalues of an $N \otimes N$ matrix $U(t)$, the polynomial $\psi(z,t)$ is given by the formula

$$\psi(z,t) = \det[z - U(t)]. \tag{63}$$

■

It is now easily seen that, if the N zeros $z_n(t)$ evolve according to the Newtonian equations of motion (8), the polynomial $\psi(z,t)$ satisfies the PDE,

$$\psi_{tt} + 2az^2\psi_{zt} + a^2z^4\psi_{zz} + [2ac_1(t) - b - 2(N-1)az]\psi_t + az^2[2ac_1(t) - b - 2(N-2)az]\psi_z + a\{2ac_2(t) - bc_1(t) + [bN - 2(N-1)ac_1(t)]z + N(N-3)az^2\}\psi = 0, \tag{64}$$

and this clearly entails that the coefficients $c_m(t)$ evolve according to the following system of N ODEs:

$$\ddot{c}_m - 2ma\dot{c}_{m+1} + (2ac_1 - b)\dot{c}_m + (m+2)(m-1)a^2c_{m+2} + [b - m(2ac_1 - b)]ac_{m+1} + [2ac_2 - bc_1]ac_m = 0. \tag{65}$$

The special case of this system with $b=0$ (as well as its *isochronous* version) have been already discussed in Ref. 10.

Likewise, if the N zeros $z_n(t)$ evolve according to the Newtonian equations of motion (9), the polynomial $\psi(z,t)$ satisfies the PDE,

$$\psi_{tt} + 2(i\omega + az)z\psi_{zt} + (i\omega + az)^2 z^2 \psi_{zz} + [2ac_1(t) - (2N + k + 1)i\omega - 2(N-1)az]\psi_t + \{(2N+k)\omega^2 + 2i\omega a c_1(t) + [2a^2 c_1(t) - (4N + k - 4)i\omega a]z - 2(N-2)a^2 z^2\} z\psi_z + \{2a^2 c_2(t) - (2N+k)i\omega a c_1(t) - N(N+k+1)\omega^2[-2(N-1)a^2 c_1(t) + N(2N+k-2)i\omega a]z + N(N-3)a^2 z^2\}\psi = 0, \tag{66}$$

and this clearly entails that the coefficients $c_m(t)$ evolve according to the following system of N ODEs:

$$\ddot{c}_m - 2ma\dot{c}_{m+1} + [2ac_1 - (2m + k + 1)i\omega]\dot{c}_m + (m+2)(m-1)a^2 c_{m+2} + [-2ma^2 c_1 + (m+1)(2m+k)i\omega a]c_{m+1} + [2a^2 c_2 - (2m+k)i\omega a c_1 - m(m+k+1)\omega^2]c_m = 0. \tag{67}$$

Note that, in writing these two systems of ODEs (65) and (67) satisfied by the dependent variables $c_m(t)$, we always assume, consistently with our notational prescriptions, that the index m ranges from 1 to N, with the "boundary conditions"

$$c_{N+1} = c_{N+2} = 0; \tag{68}$$

but in fact in both these two cases the equations of motion are also identically satisfied for $m = 0$ with $c_0 = 1$, consistently with (62b).

Consistently with the rescaled notation of Appendix A we now set

$$c_m(t) = \left(\frac{\omega}{ia}\right)^m \gamma_m(t), \tag{69}$$

and we thereby rewrite the system of ODEs (67) as follows:

$$\ddot{\gamma}_m + 2mi\omega\dot{\gamma}_{m+1} - [2\gamma_1 + 2m + k + 1]i\omega\dot{\gamma}_m - (m+2)(m-1)\omega^2\gamma_{m+2} + [2m\gamma_1 + (m+1)(2m+k)]\omega^2\gamma_{m+1} - [2\gamma_2 + (2m+k)\gamma_1 + m(m+k+1)]\omega^2\gamma_m = 0, \tag{70a}$$

$$\gamma_{N+1} = \gamma_{N+2} = 0. \tag{70b}$$

VI. EQUILIBRIUM CONFIGURATIONS, BEHAVIOR IN THEIR VICINITY, DIOPHANTINE RELATIONS

The results of Appendix A entail that, via the rescaled definition

$$z_n = \frac{\omega u_n}{ia}, \tag{71}$$

the N equilibrium positions of the model characterized by the Newtonian equations of motion (9) (which is *isochronous* for all integer values of k except $k = -2$) are characterized as the solutions of the two sets of N algebraic equations

$$s(N-1) = 2\sum_{m=1, m\neq n}^{N} \frac{u_m^{(s)}(1 - u_m^{(s)})}{u_n^{(s)} - u_m^{(s)}}, \quad s = \pm \tag{72}$$

[see (A7b) and (A10)]. We moreover know that these two sets of equilibrium configurations, corresponding to the two signs of the parameter s, are characterized by the values of the parameters k respectively σ_1 and σ_2 [see (9), respectively, (A8)] related to N by the simple expressions (A10). [Other equilibrium configurations of the N-body problem can be obtained from the solutions of (72) with N replaced by $N-1$ and either $u_N^{(s)} = 0$ or $u_N^{(s)} = 1$, or from (72) with N replaced by $N-2$ and $u_{N-1}^{(s)} = 0$, $u_N^{(s)} = 1$; as explained in Sec. IV C.]

Remark 6.1: The solutions of these two systems of algebraic equations, (72), are clearly related by the simple formula

$$u_n^{(s)} = 1 - u_n^{(-s)}. \tag{73}$$

■

Hence we can hereafter restrict consideration to the simpler case with $s=-1$, setting for notational convenience $u_n^{(-)}=u_n$. This entails $\sigma_1=\sigma_2=0$, see (A8) and (A10), as well as

$$k = -(N+1) \tag{74}$$

and

$$1 - N = 2 \sum_{m=1, m\neq n}^{N} \frac{u_m(1-u_m)}{u_n - u_m}. \tag{75a}$$

■

By replacing the numbers u_m with $(u_m-u_n)+u_n$ in the numerator on the right-hand side of this system we rewrite, after some elementary algebra, this system of N algebraic equations as follows:

$$N - 1 - 2(N-2)u_n = 2 \sum_{m=1, m\neq n}^{N} \frac{u_n(1-u_n)}{u_n - u_m}. \tag{75b}$$

It is now convenient to introduce the polynomial $\varphi(u)$, of degree N in the variable u, that has the N numbers u_n, solutions of this system of N algebraic equations, (75), as its N zeros,

$$\varphi(u) = \prod_{n=1}^{N} (u - u_n) = \sum_{m=0}^{N} \alpha_m u^{N-m}, \quad \alpha_0 = 1. \tag{76}$$

It is then easy, using the formulas of Appendix B [see in particular (B2a), (B2b), (B2f), and (B2h)], to conclude from (75b) that the polynomial $\varphi(u)$ is characterized by the second-order linear differential ODE,

$$u^2\varphi'' - 2(N-2)u\varphi' + N(N-3)\varphi = u\varphi'' - (N-1)\varphi'. \tag{77}$$

Remark 6.2: This ODE coincides with that characterizing the Jacobi polynomial $P_N^{(\alpha,\beta)}(2u-1)$ via the identification $\alpha=-N+2$, $\beta=-N$. But this observation is somewhat misleading because the Jacobi polynomial $P_N^{(\alpha,\beta)}$ (see Ref. 12) is not properly defined when its parameters α and β are *negative integers*, as it is indeed the case here. ■

Remarkably (as the diligent reader will verify), the *general* solution of the ODE (77) is the following polynomial:

$$\varphi(u) = (1-\beta)u^N + \beta\left[(u-1)^N + N(u-1)^{N-1} + \tfrac{1}{2}N(N-1)(u-1)^{N-2}\right], \tag{78}$$

where β is an *arbitrary* constants [and we adjusted the second *arbitrary* constant featured by the *general* solution of the second-order ODE (77) by imposing that the polynomial $\varphi(u)$ be *monic*, see (76)]. Note that, with this choice, the coefficients α_m, see (76), are defined by the following formula:

$$\alpha_0 = 1, \quad \alpha_m = (-)^m \frac{\beta(m-1)(m-2)N!}{2[m!(N-m)!]}, \quad m = 1, \ldots, N. \tag{79}$$

Note that these formulas entail

$$\alpha_1 = \alpha_2 = 0. \tag{80}$$

Correspondingly the numbers u_n are the N zeros of this polynomial (78),

$$\varphi(u_n) = 0, \tag{81}$$

see (76).

A. Behavior near equilibrium

Let us now consider the behavior of the *isochronous* system (51), respectively, (11) in the neighborhood of their equilibrium configurations, see Appendix A, respectively, just above.

We treat first the system (51). Consistently with the notation of Appendix A [see (A6)] we now set

$$z_n(t) = \left(\frac{\omega}{ia}\right) u_n + \varepsilon w_N(t), \tag{82}$$

and by treating ε as a small parameter we obtain for the N-vector $\underline{w} \equiv (w_1, \ldots, w_N)$ the system of N linear ODEs,

$$\ddot{\underline{w}} + i\omega \underline{A}\, \dot{\underline{w}} + \omega^2 \underline{B}\, \underline{w} = 0, \tag{83}$$

with the two $N \otimes N$ matrices $\underline{A}$ and $\underline{B}$ defined as follows:

$$A_{nm} = \delta_{nm}(2u_n - 1) + 2(1 - \delta_{nm}) \frac{u_n(1 - u_n)}{u_n - u_m}, \tag{84a}$$

$$B_{nm} = -2\delta_{nm} \sum_{m=1, m\neq n}^{N} \frac{u_n u_m (1 - u_n)(1 - u_m)}{(u_n - u_m)^2} + 2(1 - \delta_{nm}) \frac{u_n(1 - u_n)(u_m^2 - 2u_n u_m + u_n)}{(u_n - u_m)^2}. \tag{84b}$$

Note that in this section we denote N-vectors, respectively, $N \otimes N$ matrices by underlined lower-case, respectively, upper-case (italic) letters. To obtain these expressions of the matrices $\underline{A}$ and $\underline{B}$ we also used the formula (A7b). Remarkably, the number N does not appear explicitly in the definitions of these two matrices, except to the extent of defining their rank and the upper limit of the sum in (84b); but its value does of course influence the values of the N numbers u_n, see above.

Clearly the *general* solution of the N-vector second-order ODE (83) reads

$$\underline{w}(t) = \sum_{j=1}^{2N} [\, \eta_j \exp(i\mu_j \omega t) \underline{w}^{(j)}], \tag{85a}$$

where the $2N$ constants η_j are *arbitrary*, while the $2N$ numbers μ_j, respectively, the $2N$ (time-independent) N-vectors $\underline{w}^{(j)}$ are the eigenvalues, respectively, the eigenvectors of the (generalized) eigenvalue equation

$$(\mu_j^2 + \mu_j \underline{A} - \underline{B}) \underline{w}^{(j)} = 0, \quad j = 1, 2, \ldots, 2N. \tag{85b}$$

But we know that the system (51) is *isochronous*, namely its *generic* solution is *completely periodic* with period T, see (3). Hence the solution (85) must also possess this property, and this clearly entails the following *diophantine*

Theorem 1: Let the N numbers $u_n \equiv u_n(\beta)$ be the N zeros of the polynomial $\varphi(u)$ [see (78), and note the arbitrariness of the constant β], and let the two $N \otimes N$ matrices $\underline{A}$ and $\underline{B}$ be defined in terms of these N numbers by the formulas (84); then the $2N$ eigenvalues μ_j of the generalized eigenvalue equation (85b) are *all integers*. ■

We have verified this finding by performing some numerical computations, and we are thereby led to proffer the following (more specific) *diophantine*

Conjecture 1: Let the N numbers $u_n \equiv u_n(\beta)$ be the N zeros of the polynomial $\varphi(u)$ [see (78),

and note the arbitrariness of the constant β], and let the two $N\otimes N$ matrices $\underline{A}$ and $\underline{B}$ be defined in terms of these N numbers by the formulas (84); then

$$\det[\mu^2+\mu\underline{A}-\underline{B}]=\prod_{j=1-N}^{N}(\mu-j). \tag{86}$$

■

Let us now proceed and treat analogously the *isochronous* system (11), or rather its rescaled version (70a). Hence we set

$$\gamma_m=\alpha_m+\varepsilon\rho_m(t), \tag{87}$$

where the numbers α_m characterize the equilibrium configuration and we will treat again ε as a small parameter. Clearly the numbers α_m satisfy the linear recursion relations

$$-(m+2)(m-1)\alpha_{m+2}-(m+1)(N+1-2m)\alpha_{m+1}+m(N-m)\alpha_m=0, \tag{88a}$$

with the additional conditions

$$\alpha_{N+1}=\alpha_{N+2}=0, \tag{88b}$$

which obtain, to the lowest order in ε, by inserting (87) in the system of ODEs (70) satisfied by the dependent variables $\gamma_m(t)$. Note that, to simplify these equations, (88a), we also used the fact that α_1 and α_2 vanish, see (80), as well of course as the fact that we are restricting attention to the value $k=-(N+1)$, see (74). As implied by their definition and by the treatment given above these numbers α_m are given by the explicit formulas (79), as the diligent reader will verify

To the next order in ε we get the linearized system of ODEs,

$$\begin{aligned}&\ddot{\rho}_m+2mi\omega\dot{\rho}_{m+1}+(N-2m)i\omega\dot{\rho}_m-(m+2)(m-1)\omega^2\rho_{m+2}-(m+1)(N+1-2m)\omega^2\rho_{m+1}\\&\quad+2m\alpha_{m+1}\omega^2\rho_1+m(N-m)\omega^2\rho_m-2\alpha_m\omega^2\rho_2+(N+1-2m)\alpha_m\omega^2\rho_1=0,\end{aligned} \tag{89a}$$

which has again been simplified by taking advantage of (80) and (74). We now rewrite this system in more compact form as follows:

$$\ddot{\underline{\rho}}+i\omega\underline{\tilde{A}}\dot{\underline{\rho}}-\omega^2\underline{\tilde{B}}\underline{\rho}=0, \tag{89b}$$

where the N-vector $\underline{\rho}\equiv\underline{\rho}(t)$ has of course the components $\rho_m\equiv\rho_m(t)$ and the two $N\otimes N$ matrices $\underline{\tilde{A}}$ and $\underline{\tilde{B}}$ are defined (componentwise) as follows:

$$\tilde{A}_{m,n}=(N-2m)\delta_{m,n}+2m\delta_{m+1,n}, \tag{90}$$

$$\begin{aligned}\tilde{B}_{m,n}&=m(N-m)\delta_{m,n}-(m+1)(N+1-2m)\delta_{m+1,n}-(m+2)(m-1)\delta_{m+2,n}\\&\quad+[2m\alpha_{m+1}+(N+1-2m)\alpha_m]\delta_{1,n}-2\alpha_m\delta_{2,n},\end{aligned} \tag{91a}$$

where the numbers α_m are of course defined by (79) with (88b). Hence, proceeding in close analogy with the treatment given above we arrive at the following findings.

Theorem 2: Let the two $N\otimes N$ matrices $\underline{\tilde{A}}$ and $\underline{\tilde{B}}$ be defined by (90) and (91a) with (79) and (88b). Then the $2N$ eigenvalues $\tilde{\mu}_j$ of the generalized eigenvalue equation

$$(\tilde{\mu}_j^2+\tilde{\mu}_j\underline{A}-\underline{B})\underline{\tilde{w}}^{(j)}=0,\quad j=1,2,\ldots,2N \tag{91b}$$

are all integer numbers. ■

Conjecture 2: Let the two $N\otimes N$ matrices $\underline{\tilde{A}}$ and $\underline{\tilde{B}}$ be defined by (90) and (91a) with (79) and (88b). Then

$$\det[\tilde{\mu}^2 + \tilde{\mu}\underline{\tilde{A}} - \underline{\tilde{B}}] = \prod_{j=1-N}^{N} (\tilde{\mu} - j). \tag{92}$$

■

For small values of N this conjecture can of course be easily verified by explicit computation. For instance for $N=5$ it yields the result (14).

VII. A FURTHER EXTENSION

A further extension of our results obtains if we take as starting point of our treatment, instead of the *solvable* matrix evolution equation (15), the following (more general, but still *solvable*) matrix evolution equation:

$$\dot{U}(t) = a[U(t)]^2 + V(t), \quad \dot{V}(t) = b(t)V(t) + f(t)[V(t)]^2. \tag{93}$$

Here $f(t)$ is an *arbitrary* (*scalar*) function. Of course this equation reduces back to (15) for $f(t) = 0$.

The developments of Secs. II and III can then be repeated and they lead to the following, apparently more general, variant of (34):

$$\begin{aligned}\ddot{z}_n(t) = {} & 2a\dot{z}_n(t)z_n(t) + b(t)[\dot{z}_n(t) - az_n^2(t)] + f(t)[\dot{z}_n(t) - az_n^2(t)]^2 \\ & + \sum_{m=1, m\neq n}^{N} ([\dot{z}_n(t) - az_n^2(t)][\dot{z}_m(t) - az_m^2(t)]\{f(t) + 2[z_n(t) - z_m(t)]^{-1}\}),\end{aligned} \tag{94}$$

which can however clearly be rewritten in the following equivalent form:

$$\ddot{z}_n(t) = 2a\dot{z}_n(t)z_n(t) + \tilde{b}(t)[\dot{z}_n(t) - az_n^2(t)] + 2\sum_{m=1, m\neq n}^{N} \frac{[\dot{z}_n(t) - az_n^2(t)][\dot{z}_m(t) - az_m^2(t)]}{z_n(t) - z_m(t)}, \tag{95a}$$

with

$$\tilde{b}(t) = b(t) + f(t)\sum_{n=1}^{N} [\dot{z}_n(t) - az_n^2(t)]. \tag{95b}$$

It is thereby clear that the system of N Newtonian equations of motion (94) is identical to the system (34), up to the replacement of the *arbitrary* (*scalar*) function $b(t)$ with the function $\tilde{b}(t)$, see (95b). Moreover, by summing (95a) over n from 1 to N one notes that

$$\frac{d}{dt}\sum_{n=1}^{N} [\dot{z}_n(t) - az_n^2(t)] = \tilde{b}(t)\sum_{n=1}^{N} [\dot{z}_n(t) - az_n^2(t)] \tag{96}$$

entailing

$$\sum_{n=1}^{N} [\dot{z}_n(t) - az_n^2(t)] = c\exp\left[\int_0^t dt'\ \tilde{b}(t')\right] \tag{97a}$$

with

$$c = \sum_{n=1}^{N} [\dot{z}_n(0) - az_n^2(0)] \tag{97b}$$

[see, incidentally, (37)], so that the function $\tilde{b}(t)$ turns out, see (95b), to be related to the (*a priori arbitrary*) function $b(t)$ by the formula

$$\tilde{b}(t) = b(t) + cf(t)\exp\left[\int_0^t \mathrm{d}t'\ \tilde{b}(t')\right], \tag{98a}$$

which is easily inverted to read

$$\tilde{b}(t) = b(t) + [\tilde{b}(0) - b(0)]\frac{f(t)}{f(0)}\exp\left[\int_0^t \mathrm{d}t'\ b(t')\right]. \tag{98b}$$

One therefore concludes that, in spite of the additional generality of the matrix evolution equation (93) with respect to the matrix evolution (15), the *solvable* Newtonian system one finally arrives at starting from (93) is not really more general than that, see (34), obtained in Secs. II and III starting from (15). Hence we do not pursue this generalization in this paper.

APPENDIX A: EQUILIBRIUM CONFIGURATIONS

In this appendix we outline the calculations that yield the results about the equilibrium configurations of the many-body problems (41) and (51), as reported above.

To treat the first case, (41), we set, for notational convenience,

$$Z \equiv \sum_{n=1}^{N} z_n, \quad S \equiv \sum_{n=1}^{N} z_n^2. \tag{A1}$$

The equilibrium configuration of this system (41) is clearly characterized by the following set of N algebraic equations:

$$baz_n^2 = 2a^2 \sum_{m=1, m\neq n}^{N} \frac{z_n^2 z_m^2}{z_n - z_m}. \tag{A2a}$$

Here we assume $a \neq 0$, and as well $z_n \neq 0$, hence we replace the above system with the following one:

$$b = 2a \sum_{m=1, m\neq n}^{N} \frac{z_m^2}{z_n - z_m}. \tag{A2b}$$

Note that the structure of the above equations, see (A2), entails that, to every *genuine* equilibrium configuration of N points z_n satisfying (A2b) and such that $z_n \neq 0$, there also corresponds a *genuine* equilibrium configuration of $N+1$ points with the same N values z_n and with $z_{N+1}=0$.

Summing (A2a) over n from 1 to N we clearly get

$$S = 0, \tag{A3}$$

since the sum on the right-hand side vanishes due to the antisymmetry of the summand under the exchange of the two dummy indices n and m. Likewise, summing (A2b) over n from 1 to N and taking advantage of the possibility to exchange in the double sum on the right-hand side the two dummy indices n and m we easily get

$$Z = -\frac{Nb}{2(N-1)a}. \tag{A4}$$

Finally, multiplying (A2b) by z_n and then summing over n from 1 to N, taking again advantage of the possibility to exchange in the double sum on the right-hand side the two dummy indices n and m and using (A3) we easily get

$$bZ = -aZ^2, \tag{A5}$$

and it is then immediately seen, via (A4), that this yield $N=2$ (in addition to the unacceptable result $N=0$).

To analyze the equilibrium configuration of the second system, (51), it is convenient to rescale the dependent variables by setting

$$z_n = \frac{\omega u_n}{ia}, \tag{A6}$$

assuming hereafter that neither one of the two constants a, ω vanish. The equilibrium configuration is then clearly characterized by the following set of N algebraic equations:

$$(2+k)u_n(u_n-1) = -2u_n(u_n-1)\sum_{m=1,m\neq n}^{N}\frac{u_m(u_m-1)}{u_n-u_m}. \tag{A7a}$$

We now restrict consideration to equilibrium configurations of N points z_n such that $u_n \neq 0$ and $u_n \neq 1$: note that the structure of these algebraic equations implies then the possibility to extend our findings for the N-body system (51) to analogous $(N+1)$-body and $(N+2)$-body systems, as reported in Sec. IV C. We therefore rewrite these algebraic equations as follows:

$$2+k = 2\sum_{m=1,m\neq n}^{N}\frac{u_m(1-u_m)}{u_n-u_m}. \tag{A7b}$$

It is now convenient, proceeding in close analogy to what we did just above, to introduce the two quantities

$$\sigma_1 = \sum_{n=1}^{N} u_n, \quad \sigma_2 = \sum_{n=1}^{N} u_n^2, \tag{A8}$$

and to thereby obtain [by summing (A7b) over n from 1 to N after multiplying it, respectively, by $u_n\,(1-u_n)$, by 1, and by u_n] the three relations

$$\sigma_1 = \sigma_2, \tag{A9a}$$

$$2(N-1)\sigma_1 = N(N+k+1), \tag{A9b}$$

$$(2+k)\sigma_1 = \sigma_1^2 - \sigma_2. \tag{A9c}$$

It is then a matter of trivial algebra to obtain the formulas

$$k = s(N-1)-2, \quad \sigma_1 = \sigma_2 = \frac{N(1+s)}{2}, \quad s = \pm 1, \tag{A10}$$

which entail the results reported in Sec. IV C, and are the basis for the further developments reported in Sec. VI.

APPENDIX B: SOME USEFUL POLYNOMIAL IDENTITIES

We report here some useful identities: several of them are copied from Sec. 2.3.2 of Ref. 4, a few are analogous to those explicitly given there (and their proofs are sufficiently standard to be forsaken).

Let $\psi(z,t)$ be a monic polynomial of degree N in z, and let us denote with $c_m(t)$ its N coefficients and with $z_n(t)$ its N zeros,

$$\psi(z,t) = z^N + \sum_{m=1}^{N} c_m(t) z^{N-m} = \prod_{n=1}^{N} [z - z_m(t)], \tag{B1a}$$

so that clearly

$$\sum_{n=1}^{N} z_n(t) = -c_1(t), \quad \sum_{n=1}^{N} [z_n(t)]^2 = [c_1(t)]^2 - 2c_2(t), \tag{B1b}$$

and so on. Then clearly

$$z\psi_z(z,t) = Nz^N + \sum_{m=1}^{N} (N-m) c_m(t) z^{N-m}, \tag{B1c}$$

$$z^2\psi_{zz}(z,t) = N(N-1)z^N + \sum_{m=1}^{N} (N-m)(N-m-1) c_m(t) z^{N-m}, \tag{B1d}$$

and so on;

$$\psi_t(z,t) = \sum_{m=1}^{N} \dot{c}_m(t) z^{N-m}, \tag{B1e}$$

$$\psi_{tt}(z,t) = \sum_{m=1}^{N} \ddot{c}_m(t) z^{N-m}, \tag{B1f}$$

and so on.

Likewise,

$$\psi_z(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1}, \tag{B2a}$$

$$z\psi_z(z,t) - N\psi(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} \{z_n(t)\}, \tag{B2b}$$

$$z^2\psi_z(z,t) + [c_1(t) - Nz]\psi(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} \{[z_n(t)]^2\}, \tag{B2c}$$

$$\psi_t(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} \{-\dot{z}_n(t)\}, \tag{B2d}$$

$$z\psi_t(z,t) - \dot{c}_1(t)\psi(t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} \{-\dot{z}_n(t) z_n(t)\}, \tag{B2e}$$

$$\psi_{zz}(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} \left\{ \sum_{m=1, m\neq n}^{N} \frac{2}{z_n(t) - z_m(t)} \right\}, \tag{B2f}$$

$$z\psi_{zz}(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2z_n(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2g}$$

$$z^2\psi_{zz}(z,t) - N(N-1)\psi(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2z_n^2(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2h}$$

$$z^2\psi_{zz}(z,t) - 2(N-1)z\psi_z(z,t) + N(N-1)\psi(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2z_n(t)z_m(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2i}$$

$$z^3\psi_{zz}(z,t) - Z(N-1)z\psi(z,t) + 2(N-1)c_1(t)\psi(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2z_n^3(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2j}$$

$$z[z^2\psi_{zz}(z,t) - 2(N-1)z\psi_z(z,t) + N(N-1)\psi(z,t)] = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2[z_n(t)]^2z_m(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2k}$$

$$\begin{aligned} &z^3\psi_{zz}(z,t) - 2(N-2)z^2\psi_z(z,t) + 2c_1(t)z\psi_z(z,t) + N(N+1)z\psi(z,t) - 2(N-1)c_1(t)\psi(z,t) \\ &\quad = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1;m\neq n}^{N}\frac{2z_n(t)z_m^2(t)}{z_n(t)-z_m(t)}\right\}, \end{aligned} \tag{B2l}$$

$$\begin{aligned} &z^4\psi_{zz}(z,t) - N(N-1)z^2\psi(z,t) + 2(N-1)c_1(t)z\psi(z,t) - 2(N-1)[c_1(t)]^2\psi(z,t) + 2(2N-3)c_2(t)\psi(z,t) \\ &\quad = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2z_n^4(t)}{z_n(t)-z_m(t)}\right\}, \end{aligned} \tag{B2m}$$

$$\begin{aligned} &z^4\psi_{zz}(z,t) - 2(N-2)z^3\psi_z(z,t) + 2c_1(t)z^2\psi_z(z,t) + [N(N-3)z^2 - 2(N-1)c_1(t)z + 2c_2(t)]\psi(t) \\ &\quad = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{\sum_{m=1,m\neq n}^{N}\frac{2[z_n(t)]^2[z_m(t)]^2}{z_n(t)-z_m(t)}\right\}, \end{aligned} \tag{B2n}$$

$$\psi_{zt}(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{-\sum_{m=1,m\neq n}^{N}\frac{\dot z_n(t)+\dot z_m(t)}{z_n(t)-z_m(t)}\right\}, \tag{B2o}$$

$$z\psi_{zt}(z,t) = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{-\sum_{m=1,m\neq n}^{N}\frac{z_n(t)[\dot z_n(t)+\dot z_m(t)]}{z_n(t)-z_m(t)}\right\}, \tag{B2p}$$

$$\begin{aligned} &z^2\psi_{zt}(z,t) + [c_1(t) - (N-2)z]\psi_t(z,t) - \dot c_1(t)\psi(z,t) \\ &\quad = \psi(z,t)\sum_{n=1}^{N}[z-z_n(t)]^{-1}\left\{-\sum_{m=1,m\neq n}^{N}\frac{\dot z_n(t)z_m^2(t)+\dot z_m(t)z_n^2(t)}{z_n(t)-z_m(t)}\right\}, \end{aligned} \tag{B2q}$$

$$\psi_{tt}(z,t) = \psi(z,t)\sum_{n=1}^{N}[z - z_n(t)]^{-1}\left\{-\ddot{z}_n(t) + \sum_{m=1,m\neq n}^{N}\frac{2\dot{z}_n(t)\dot{z}_m(t)}{z_n(t) - z_m(t)}\right\}. \tag{B2r}$$

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Formal and analytical integrability of the Bianchi IX system

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In this paper we provide a complete description of the first integrals of the classical Bianchi IX system that can be described by a general class of formal power series. As a corollary we also obtain a complete description of some of its analytic first integrals in a neighborhood of the origin. In particular, we prove that the system is not completely integrable by analytic first integrals. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2168123]

I. INTRODUCTION TO THE PROBLEM

The Bianchi IX model can be written as the Hamiltonian system (see Ref. 4):

$$\begin{aligned}
\dot{q}_1 &= F_1(q,p) = 12q_1(p_1q_1 - p_2q_2 - p_3q_3),\\
\dot{q}_2 &= F_2(q,p) = 12q_2(-p_1q_1 + p_2q_2 - p_3q_3),\\
\dot{q}_3 &= F_3(q,p) = 12q_3(-p_1q_1 - p_2q_2 + p_3q_3),\\
\dot{p}_1 &= F_4(q,p) = -12p_1(p_1q_1 - p_2q_2 - p_3q_3) - \tfrac{1}{3}(q_1 - q_2 - q_3),\\
\dot{p}_2 &= F_5(q,p) = -12p_2(-p_1q_1 + p_2q_2 - p_3q_3) - \tfrac{1}{3}(-q_1 + q_2 - q_3),\\
\dot{p}_3 &= F_6(q,p) = -12p_3(-p_1q_1 - p_2q_2 + p_3q_3) - \tfrac{1}{3}(-q_1 - q_2 + q_3),
\end{aligned} \tag{1}$$

with the Hamiltonian

$$\begin{aligned}
H = {} & 6(p_1^2q_1^2 + p_2^2q_2^2 + p_3^2q_3^2 - 2p_1q_1p_2q_2 - 2p_1q_1p_3q_3 - 2p_2q_2p_3q_3)\\
& + \tfrac{1}{6}(q_1^2 + q_2^2 + q_3^2 - 2q_1q_2 - 2q_1q_3 - 2q_2q_3).
\end{aligned}$$

Of course, here (q,p) denotes $(q_1,q_2,q_3,p_1,p_2,p_3)$.

The solutions which lie in the zero level set of the Hamiltonian H, provide a model for describing the evolution of the universe, see for instance, Ref. 6. Furthermore, the set defined as

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$$C = \{(q,p) \in \mathbb{R}^6 | q_i \geqslant 0, i = 1,2,3,\ q_1 q_2 q_3 = 0\},$$

is the phase space gravitational collapse set. It should noted that since $q_i=0$ are invariant under the flow of (1), the phase space gravitational collapse set C is invariant under the flow given by (1). We note that in our study of the first integrals of system (1), the invariant sets $q_i=0$, will play a main role.

Recently, this system has been intensively investigated from the point of view of integrability by using different methods. One of these methods is the Painlevé test (see, for instance, Refs. 7 and 3) where the authors prove that the solutions of the equation of motion do not have movable critical points and conjecture that system (1) is not integrable. Another method is the numerical computation of the Lyapunov exponents (see Ref. 2), where the authors also conjecture the nonintegrability of system (1). In Ref. 4 the authors, by means of symplectic geometrical techniques, study the local integrability of system (1). In Ref. 11 it is shown that system (1) is not completely integrable in the Birkhoff sense. In Ref. 12 the author proves that the Hamiltonian system (1) is not completely integrable with rational first integrals using techniques from the differential Galois theory. Moreover, in Ref. 10, the authors, applying the Darboux theory of integrability, provide a complete description of the Darboux polynomials, exponential factors, rational first integrals and Darbouxian first integrals for this model.

The aim of this paper is to study the existence of first integrals of system (1) that can be described by formal series. We use these tools for proving similar results to the ones of this paper for the Lorenz system and for the Einstein-Yang-Mills system, see Refs. 8 and 9. But the use of formal series in the study of differential equations and, in particular, in the existence of their first integrals is a classical tool. Indeed, for instance, solutions described by formal series around singularities have been studied by Seidenberg,[15] the existence of first integrals given by formal series have been studied by Nemytskii and Stepanov,[14] Moussu.[13] etc. However, the greatest success in using formal series to study differential equations has been achieved by Écalle[5] who used them to prove the Dulac's conjecture.

In this paper we say that a *formal first integral* $f=f(q,p)$ of system (1) is a formal power series in the variables q and p such that

$$\sum_{k=1}^{3} \left(\frac{\partial f}{\partial q_i} F_i(q,p) + \frac{\partial f}{\partial p_i} F_{i+3}(q,p) \right) = 0,$$

is different from a polynomial. In Ref. 10 the authors have proved that all polynomial first integrals of system (1) are polynomial functions in the variable H. The first main result of this paper is the following.

Theorem 1: *All formal first integrals of the Bianchi IX model* (1) *are formal series in the variable H.*

Here an *analytic first integral* of system (1) is an analytic function in the variables q and p which is constant over the trajectories of system (1) and it is different from a polynomial. The second main result of this paper is the following.

Theorem 2: *All analytic first integrals of the Bianchi IX model* (1) *in a neighborhood of the origin are analytic functions in the variable H.*

Theorems 1 and 2 are an immediate consequence of Theorems 3 and 4 stated below. We first observe that since $\dot{H}=0$, we can rewrite system (1) as the following system in the seven variables $(q_1,q_2,q_3,p_1,p_2,p_3,H)$:

$$\dot{q}_1 = F_1(q,p) = 12q_1(p_1q_1 - p_2q_2 - p_3q_3),$$

$$\dot{q}_2 = F_2(q,p) = 12q_2(-p_1q_1 + p_2q_2 - p_3q_3),$$

$$\dot{q}_3 = F_3(q,p) = 12q_3(-p_1q_1 - p_2q_2 + p_3q_3),$$

$$\dot{p}_1 = F_4(q,p) = -12p_1(p_1q_1 - p_2q_2 - p_3q_3) - \tfrac{1}{3}(q_1 - q_2 - q_3),$$

$$\dot{p}_2 = F_5(q,p) = -12p_2(-p_1q_1 + p_2q_2 - p_3q_3) - \tfrac{1}{3}(-q_1 + q_2 - q_3),$$

$$\dot{p}_3 = F_6(q,p) = -12p_3(-p_1q_1 - p_2q_2 + p_3q_3) - \tfrac{1}{3}(-q_1 - q_2 + q_3),$$

$$\dot{H} = F_7(q,p) = 0. \tag{2}$$

We say that a formal first integral $f=f(q_1,q_2,q_3,p_1,p_2,p_3,H)$ of system (2) is a formal power series in the variables q, p, and H such that

$$\sum_{k=1}^{3}\left(\frac{\partial f}{\partial q_i}F_i(q,p) + \frac{\partial f}{\partial p_i}F_{i+3}(q,p)\right) + \frac{\partial f}{\partial H}F_7(q,p) = 0.$$

Theorem 3: *All formal first integrals of system* (2) *are formal series in the variable H.*

Here an *analytic first integral* of system (2) is an analytic function in the variables q, p, and H which is constant over the trajectories of system (2).

Theorem 4: *All analytic first integrals of system* (2) *in a neighborhood of the origin are analytic functions in the variable H.*

The proofs of Theorems 3 and 4 are given in Sec. III.

We say that the functions $F_1,\ldots,F_n$ are in *involution* if $\{F_i,F_j\}=0$ for all $i\neq j$, where $\{\cdot,\cdot\}$ denotes the Poisson bracket. Moreover, they are *independent* if the one-forms $dF_1,\ldots,dF_n$ are linearly independent over a full Lebesgue measure subset of the common definition domain of F_j for $j=1,\ldots,n$. By definition, a Hamiltonian system with n degrees of freedom having n independent first integrals in involution is *completely integrable*, see for more details Ref. 1.

As a direct consequence of Theorem 2, we have the next result.

Corollary 5: The Bianchi IX model (1) *is not completely integrable by analytic first integrals.*

The paper is organized as follows. In Sec. II we provide some auxiliary results that will be used all through the paper and will be crucial to prove Theorem 3. Finally, in Sec. III we provide the proofs of Theorems 3 and 4.

II. AUXILIARY RESULTS

In this section we provide some auxiliary results that will be used along the paper.

Lemma 6: Let x and y be one-dimensional variables. Given a formal power series $f(x)$, there exists a formal power series $g(x,y)$ such that

$$f(x) + f(y) = f(x+y) + f(0) - xyg(x,y).$$

Proof: We write $f(z)=f(0)+\Sigma_{j=1}^{\infty}f_jz^j$. Then, using Newton's binomial formula,

$$f(x+y) + f(0) = 2f(0) + \sum_{j=1}^{\infty} f_j(x+y)^j = 2f(0) + \sum_{j=1}^{\infty} f_j \sum_{k=0}^{j}\binom{j}{k}x^k y^{j-k} = f(x) + f(y)$$

$$+ xy\sum_{j=2}^{\infty} f_j \sum_{k=0}^{j-2}\binom{j}{k+1}x^k y^{j-2-k} = f(x) + f(y) + xyg(x,y).$$

■

Lemma 7: Let x_k be one-dimensional variables for $k=1,\ldots,n$ with $n>1$. Let $f=f(x_1,\ldots,x_n)$ be a formal power series such that in $x_l=c_0$, $f(x_1,\ldots,x_n)|_{x_l=c_0}=\bar{f}$, where c_0 is a constant, f is a formal power series in the variables $x_1,\ldots,x_{l-1}$, $x_{l+1},\ldots,x_n$ and $l\in\{1,\ldots,n\}$. Then, there exists a formal series $g=g(x_1,\ldots,x_n)$ such that $f=\bar{f}+(x_l-c_0)g$.

Proof: We denote by $\mathbb{Z}^+$ the set of all non-negative integers. We write

$$f=\sum_{(k_1,\ldots,k_n)\in(\mathbb{Z}^+)^n} f_{k_1,\ldots,k_n}x_1^{k_1}\cdots x_n^{k_n}.$$

Without loss of generality we can assume $l=1$. Then, writing $x_1=c_0+(x_1-c_0)$, we have

$$f=\sum_{(k_1,\ldots,k_n)\in(\mathbb{Z}^+)^n} f_{k_1,\ldots,k_n}(c_0+(x_1-c_0))^{k_1}x_2^{k_2}\cdots x_n^{k_n}.$$

Now, by the Newton's binomial formula we have

$$\begin{aligned}f&=\sum_{(k_1,\ldots,k_n)\in(\mathbb{Z}^+)^n} f_{k_1,\ldots,k_n}\sum_{j=0}^{k_1}\binom{k_1}{j}c_0^j(x_1-c_0)^{k_1-j}x_2^{k_2}\cdots x_n^{k_n}\\&=\sum_{(k_1,\ldots,k_n)\in(\mathbb{Z}^+)^n} f_{k_1,\ldots,k_n}c_0^{k_1}x_2^{k_2}\ldots x_n^{k_n}\\&\quad+(x_1-c_0)\sum_{(k_1,\ldots,k_n)\in(\mathbb{Z}^+)^n} f_{k_1,\ldots,k_n}\sum_{j=0}^{k_1-1}\binom{k_1}{j}c_0^j(x_1-c_0)^{k_1-j-1}x_2^{k_2}\cdots x_n^{k_n}\\&=f(c_0,x_2,\ldots,x_n)+(x_1-c_0)g(x_1,\ldots x_n)=\bar{f}+(x_1-c_0)g,\end{aligned}$$

which finishes the proof of the lemma. ■

The following lemmas are auxiliary results, that will be used in the proof of Proposition 13, Proposition 15, and Theorem 1.

Proposition 8: Any analytic first integral f of the differential system

$$\dot{x}=12xu,\quad \dot{y}=12yu+\tfrac{1}{3},\quad \dot{z}=12zu+\tfrac{1}{3},\quad \dot{u}=-12u^2-\tfrac{1}{3},\tag{3}$$

in $\mathbb{R}^4$ *is an analytic function* $f=f(F_1(x,u),F_2(y,u),F_3(z,u))$ *in the variables* $(F_1(x,u),F_2(u,y),F_3(u,z))$, *where*

$$F_1(x,u)=x^2(1+36u^2),\quad F_2(y,u)=6\sqrt{1+36u^2}y+\arcsin(6u)\tag{4}$$

and

$$F_3(z,u)=6\sqrt{1+36u^2}z+\operatorname{arcsinh}(6u).\tag{5}$$

Proof: Since $F_1(x,u)$, $F_2(y,u)$, and $F_3(z,u)$ are three functionally independent analytical first integrals of the four-dimensional system (3), any other analytical first integral must be an analytic function of them. ■

From Proposition 8 it follows the next result.

Corollary 9: Any formal first integral f of system (3) *is a formal power series in the variables* $F_1(x,u)$, $f_2(y,u)$, *and* $f_3(u,z)$, *where* $f_2(y,u)$ *and* $f_3(u,z)$ *are, respectively, the power series of* $F_2(y,u)$ *and* $F_3(u,z)$ *in a neighborhood of the origin.*

We observe that since

$$\sqrt{1+36u^2}=1+18u^2+O(u^4),\quad \operatorname{arcsinh}(u)=u\left[1-\frac{u^2}{6}+O(u^4)\right]$$

we get

$$\begin{aligned}f_2(y,u)&=6y(1+18u^2+O(u^4))+6u(1-6u^2+O(u^4)),\\f_3(z,u)&=6z(1+18u^2+O(u^4))+6u(1-6u^2+O(u^4)).\end{aligned}\tag{6}$$

Proposition 10: Any analytic first integral f of the differential system

$$\dot{x} = 12xu, \quad \dot{y} = 12yu, \quad \dot{z} = 12zu + \tfrac{1}{3}, \quad \dot{u} = -12u^2 - \tfrac{1}{3}, \tag{7}$$

in $\mathbb{R}^4$ *is an analytic function* $f=f(F_1(x,u),F_3(y,u),F_4(z,u))$ *in the variables* $(F_1(x,u),F_3(y,u),F_4(z,u))$, *where* $F_1(x,u)$ *was introduced in* (4), $F_3(z,u)$ *was introduced in* (5) *and* $F_4(y,u)=y^2(1+36u^2)$.

Proof: Since $F_1(x,u)$, $F_3(y,u)$, and $F_4(z,u)$ are three functionally independent analytical first integrals of the four-dimensional system (7), any other analytical first integral must be an analytic function of them. ■

From Proposition 10 it follows the next result.

Lemma 11: Any analytic first integral f *of system* (7) *in* $x\neq 0$ *of the form* $f=g/x^{2m}$, *where* m *is a positive integer and* g *is a formal power series, can be written in the form*

$$f = \frac{y^{2m}}{x^{2m}} \sum_{k,l,n\geqslant 0} f_{k,m+l,n} F_1(x,u)^k F_4(y,u)^l f_3(z,u)^n.$$

Proof: Since f is an analytic first integral of system (7) in $x\neq 0$, we have from Proposition 10 that in $x\neq 0$, $f=f(F_1(x,u),F_3(z,u),F_4(y,u))$. Since f is of the form $f=g/x^{2m}$ with g being a formal series, and only $F_1(x,u)$ depends on x (in the form x^2), we obtain

$$f = \frac{1}{F_1(x,u)^m} \sum_{k,l,n\geqslant 0} f_{k,l,n} F_1(x,u)^k F_4(y,u)^l f_3(z,u)^n.$$

Using that $F_1=x^2F_4/y^2$ we get

$$f = \frac{y^{2m}}{x^{2m}F_4(y,u)^m} \sum_{k,l,n\geqslant 0} f_{k,l,n} F_1(x,u)^k F_4(y,u)^l f_3(z,u)^n, \tag{8}$$

and since f must be analytic in $x\neq 0$, we have that the sum in (8) with $l=0,1,\ldots,m-1$ must be zero, i.e.,

$$\sum_{k,n\geqslant 0} \sum_{l=0}^{m-1} f_{k,l,n} F_1(x,u)^k F_4(y,u)^l f_3(z,u)^n = 0,$$

and thus, (8) becomes

$$f = \frac{y^{2m}}{x^{2m}} \sum_{k,l,n\geqslant 0} f_{k,m+l,n} F_1(x,u)^k F_4(y,u)^l f_3(z,u)^n,$$

which finishes the proof of the lemma. ■

Let $\tau,\sigma:\mathbb{C}[q_1,q_2,q_3,p_1,p_2,p_3,H]\to\mathbb{C}[q_1,q_2,q_3,p_1,p_2,p_3,H]$ be the automorphism

$$\tau(q_i) = -q_i, \quad \tau(p_i) = -p_i, \quad i=1,2,3, \quad \tau(H) = H;$$

$$\sigma(q_1) = q_2, \sigma(q_2) = q_3, \sigma(\sigma_3) = q_1, \sigma(p_1) = p_2, \sigma(p_2) = p_3, \sigma(p_3) = p_1, \sigma(H) = H.$$

Then, the following proposition holds.

Proposition 12: Let g *be a formal first integral of system* (2).

(a) *Then* $f=(g\cdot\sigma g\cdot\sigma^2 g)\cdot\tau(g\cdot\sigma g\cdot\sigma^2 g)$ *is another formal first integral of system* (2) *invariant by* τ *and* σ. *Here* $\cdot$ *denotes multiplication*.

(b) *Moreover, the monomials of* f *are of the form* $q_1^{j_1}q_2^{j_2}q_3^{j_3}p_1^{l_1}p_2^{l_2}p_3^{l_3}H^m$ *with* $j_1+j_2+j_3+l_1+l_2+l_3$ *even*.

Proof: Statement (a) of the proposition follows taking into account that system (2) is invariant under τ, σ, and σ^2. To prove statement (b) we write f in formal power series of its variables as

$$f=\sum_{(j_1,j_2,j_3,l_1,l_2,l_3,m)\in(\mathbb{Z}^+)^7} f_{j_1,j_2,j_3,l_1,l_2,l_3,m}q_1^{j_1}q_2^{j_2}q_3^{j_3}p_1^{l_1}p_2^{l_2}p_3^{l_3}H^m.$$

Then, since f is invariant by τ, it must hold that $f-\tau(f)=0$. That is, the formal power series

$$\sum_{(j_1,j_2,j_3,l_1,l_2,l_3,m)\in(\mathbb{Z}^+)^7}(1-(-1)^{j_1+j_2+j_3+l_1+l_2+l_3})f_{j_1,j_2,j_3,l_1,l_2,l_3,m}q_1^{j_1}q_2^{j_2}q_3^{j_3}p_1^{l_1}p_2^{l_2}p_3^{l_3}H^m$$

must be zero. This implies that $j_1+j_2+j_3+l_1+l_2+l_3$ must be even. ■

Proposition 13: Let $n\in\{1,2,3\}$. System (2) *restricted to $q_n=0$ has the two first integrals*

$$H_{2n-1}=6(p_mq_m-p_rq_r)^2+\tfrac{1}{6}(q_m-q_r)^2,\quad H_{2n}=q_mq_r,$$

where $\{m,n,r\}=\{1,2,3\}$. If g is a formal first integral of system (2) *invariant by τ and σ, then $f=g_{|q_n=0}$ is a formal power series in the variables H_{2n-1} and H_{2n}.*

Proof: We shall prove only the case $n=1$ since the other two cases can be proved in the same way. In this case, we can consider $m=2$ and $r=3$. It is easy to check that H_1 and H_2 are first integrals of system (2) restricted to $q_1=0$.

Let $f=f(q_2,q_3,p_1,p_2,p_3,H_1)$ be the restriction of g to $q_1=0$. Then, f is a formal first integral of system (2) restricted to $q_1=0$. We write f as

$$f=\sum_{k\geqslant 0}f_kH_1^k,\quad f_k=f_k(q_2,q_3,p_1,p_2,p_3),\tag{9}$$

where f_k are formal series in their variables. From the fact that f is a formal first integral of system (2) restricted to $q_1=0$, it satisfies

$$12q_2(p_2q_2-p_3q_3)\frac{\partial f}{\partial q_2}-12q_3(p_2q_2-p_3q_3)\frac{\partial f}{\partial q_3}+\left(12p_1(p_2q_2+p_3q_3)+\frac{1}{3}(q_2+q_3)\right)\frac{\partial f}{\partial p_1}$$
$$-\left(12p_2(p_2q_2-p_3q_3)+\frac{1}{3}(q_2-q_3)\right)\frac{\partial f}{\partial p_2}+\left(12p_3(p_2q_2-p_3q_3)+\frac{1}{3}(q_2-q_3)\right)\frac{\partial f}{\partial p_3}=0.$$

We denote by $\bar{f}$ the restriction of f to the set

$$F=\{q_2=0,\ H_1=0\}=\{q_2=0,q_3^2(p_3^2+1/36)=0\}.$$

We note that on $q_2=q_3=0$ all the points $(0,0,p_1,p_2,p_3)$ are singular points of system (2) restricted to $q_1=0$, and thus we do not obtain any information on $\bar{f}$ by restricting f to the subset $q_2=q_3=0$ of F. We shall compute the restriction $\hat{f}$ of f to $q_2=0$ $q_3\neq 0$. In this case, $\hat{f}$ is a formal power series that satisfy, after dividing by q_3,

$$12q_3p_3\frac{\partial\hat{f}}{\partial q_3}+\left(12p_1p_3+\frac{1}{3}\right)\frac{\partial\hat{f}}{\partial p_1}+\left(12p_2p_3+\frac{1}{3}\right)\frac{\partial\hat{f}}{\partial p_2}-\left(12p_3^2+\frac{1}{3}\right)\frac{\partial\hat{f}}{\partial p_3}=0.$$

Then, $\hat{f}$ is a formal first integral of system (3) (setting $x=q_3$, $u=p_3$, $y=p_1$ and $z=p_2$) and from Corollary 9 we get

$$\hat{f}=\sum_{k,l,n\leqslant 0}\hat{f}_{k,l,n}F_1(q_3,p_3)^kf_2(p_1,p_3)^lf_3(p_2,p_3)^n\tag{10}$$

with $F_1(q_3,p_3)$ introduced in (4) and $f_2(p_1,p_3)$, $f_3(p_2,p_3)$ were introduced in Corollary 9. Now, by definition $\bar{f}$ is the restriction of $\hat{f}$ to $F_1(q_3,p_3)=0$. Thus, from (10), we have

$$\bar{f} = \sum_{l,n\geqslant 0} \hat{f}_{0,l,n} f_2(p_1,p_3)^l f_3(p_2,p_3)^n = \sum_{l,n\geqslant 0} \bar{f}_{l,n} f_2(p_1,p_3)^l f_3(p_2,p_3)^n.$$

Now, let f^* be the restriction of g to $H=0$. Then, f^* is a formal power series and since g and H are invariant by σ, $\sigma(f^*)=f^*$. Furthermore, if we denote by f_1^* the restriction of f^* to $q_1=q_2=q_3=0$, we have that f_1^* is equal to the restriction of $\bar{f}$ to $q_3=0$, and since $\bar{f}$ does not depend on q_3, $\bar{f}$ is invariant by σ. So, $\sigma(\bar{f})=\bar{f}$ and $\sigma^2(\bar{f})=\bar{f}$. This implies that

$$\bar{f} = \sum_{l,n\geqslant 0} \bar{f}_{l,n} f_2(p_1,p_3)^l f_3(p_2,p_3)^n = \sum_{l,n\geqslant 0} \bar{f}_{l,n} f_2(p_2,p_1)^l f_3(p_3,p_1)^n = \sum_{l,n\geqslant 0} \bar{f}_{l,n} f_2(p_3,p_2)^l f_3(p_1,p_2)^n. \tag{11}$$

Now, we will prove by induction that

$$\bar{f}_{l,n} = 0 \quad \text{for } l,n \geqslant 0, \quad (l,n) \neq (0,0). \tag{12}$$

Setting $p_3=0$ in the three equalities of (11) and using the form of f_2 and f_3 in (6) we get

$$\begin{aligned} \sum_{l,n\geqslant 0} \bar{f}_{l,n}(6p_1)^l(6p_2)^n &= \sum_{l,n\geqslant 0} \bar{f}_{l,n}(6p_1 + 6p_2 + O(p_2p_1^2) + O(p_1^3))^l(6p_1 + O(p_1^3))^n \\ &= \sum_{l,n\geqslant 0} \bar{f}_{l,n}(6p_2 + O(p_2^3))^l(6p_1 + 6p_2 + O(p_1p_2^2) + O(p_2^3))^n. \end{aligned} \tag{13}$$

We first compute in (13) the terms of degree 1 and we get, after dividing by 6,

$$\bar{f}_{1,0}p_1 + \bar{f}_{0,1}p_2 = \bar{f}_{1,0}(p_1+p_2) + \bar{f}_{0,1}p_1 = \bar{f}_{1,0}p_2 + \bar{f}_{0,1}(p_1+p_2),$$

which clearly implies $\bar{f}_{1,0}=\bar{f}_{0,1}=0$. This proves (12) for $l,n\geqslant 0$ with $l+n=1$.

Now we proceed by induction over the degree $l+n=k$. We assume (12) is true for $k=1,\ldots,N-1$ and we will prove it for $k=N$. By induction hypothesis, the terms of degree N in (13) are, after dividing by 6^N,

$$\sum_{l=0}^{N} \bar{f}_{l,N-l} p_1^l p_2^{N-l} = \sum_{l=0}^{N} \bar{f}_{l,N-l}(p_1+p_2)^l p_1^{N-l} = \sum_{l=0}^{N} \bar{f}_{l,N-l} p_2^l (p_1+p_2)^{N-l}. \tag{14}$$

Using the Newton's Binomial formula we can rewrite (14) as

$$\sum_{l=0}^{N} \bar{f}_{l,N-l} p_1^l p_2^{N-l} = \sum_{l=0}^{N} \bar{f}_{l,N-l} \sum_{j=0}^{l} \binom{l}{j} p_2^j p_1^{N-j} = \sum_{l=0}^{N} \bar{f}_{l,N-l} \sum_{j=0}^{N-l} \binom{N-l}{j} p_1^j p_2^{N-j}. \tag{15}$$

We will prove by induction that

$$\begin{aligned} \bar{f}_{l,N-1} = f_{N-l,l} = 0 \quad &\text{for } l = 0,\ldots,[N/2], \\ \bar{f}_{l+1,N-1} = f_{N-l-1,l+1} \quad &\text{for } l = 0,\ldots,[(N-2)/2], \end{aligned} \tag{16}$$

where $[\cdot]$ denotes the integer part function. To prove (16) for $l=0$ we first observe that if we set $p_1=0$ in the first equality of (15) we obtain $\bar{f}_{0,N}p_2^N=\bar{f}_{N,0}p_2^N$, i.e., $\bar{f}_{0,N}=\bar{f}_{N,0}$. Furthermore, if we compute in the first equality of (15) the coefficient of $p_1p_2^{N-1}$ we get

$$\bar{f}_{1,N-1} = \bar{f}_{N-1,1} + N\bar{f}_{N,0}, \tag{17}$$

and if we compute in the first and third terms of identity (15) the coefficient of $p_1^{N-1}p_2$ we get

$$\bar{f}_{N-1,1} = \bar{f}_{1,N-1} + N\bar{f}_{0,N}. \tag{18}$$

Equations (17) and (18) together with the fact that $\bar{f}_{0,N}=\bar{f}_{N,0}$ imply that $\bar{f}_{0,N}=\bar{f}_{N,0}=0$ and $\bar{f}_{1,N-1}=\bar{f}_{N-1,1}$. This finishes the proof of (16) for $l=0$.

Now, we assume that (16) is true for $l=0,\ldots,m-1$ ($m<[(N-2)/2]$) and we will prove it for $l=m$. By induction hypothesis we can write (15) as

$$\sum_{l=m}^{N} \bar{f}_{l,N-l} p_1^l p_2^{N-l} = \sum_{l=m}^{N} \bar{f}_{l,N-l} \sum_{j=0}^{l} \binom{l}{j} p_2^j p_1^{N-j} = \sum_{l=m}^{N} \bar{f}_{l,N-l} \sum_{j=0}^{N-l} \binom{N-l}{j} p_1^j p_2^{N-j}, \tag{19}$$

and we also have that $\bar{f}_{m,N-m}=\bar{f}_{N-m,m}$. Now, computing in the first equality of (19) the coefficients of $p_1^{m+1}p_2^{N-m-1}$ we get

$$\bar{f}_{m+1,N-m-1} = \bar{f}_{N-m,m+1} + (N-m)\bar{f}_{N-m,m},$$

and computing in the first and third terms of equality (19) the coefficients of $p_1^{N-m-1}p_2^{m+1}$ we get

$$\bar{f}_{N-m-1,m+1} = \bar{f}_{m+1,N-m-1} + (N-m)\bar{f}_{m,N-m}.$$

These two equalities imply, taking into account that $\bar{f}_{m,N-m}=\bar{f}_{N-m,m}$, that $\bar{f}_{N-m,m}=f_{m,N-m}=0$ and $\bar{f}_{m+1,N-m-1}=\bar{f}_{N-m-1,m+1}$. Thus, (16) is proved for $l=0,\ldots,[(N-2)/2]$.

Now, by induction hypothesis, for $l=[N/2]$ we have the following.

Case 1: if N is even then, from (14) we get

$$\bar{f}_{N/2,N/2} p_1^{N/2} p_2^{N/2} = \bar{f}_{N/2,N/2}(p_1+p_2)^{N/2} p_1^{N/2} = \bar{f}_{N/2,N/2} p_2^{N/2}(p_1+p_2)^{N/2},$$

which clearly implies $\bar{f}_{N/2,N/2}=0$. Thus, (16) is true in this case.

Case 2: if N is odd then, again from (14) we obtain

$$\begin{aligned}
&\bar{f}_{(N-1)/2,(N+1)/2}[p_1^{(N-1)/2}p_2^{(N+1)/2} + p_1^{(N+1)/2}p_2^{(N-1)/2}] \\
&\quad = \bar{f}_{(N-1)/2,(N+1)/2}[(p_1+p_2)^{(N-1)/2}p_1^{(N+1)/2} + (p_1+p_2)^{(N+1)/2}p_1^{(N-1)/2}] \\
&\quad = \bar{f}_{(N-1)/2,(N+1)/2}[p_2^{(N+1)/2}(p_1+p_2)^{(N-1)/2} + p_2^{(N-1)/2}(p_1+p_2)^{(N+1)/2}],
\end{aligned}$$

which clearly implies $\bar{f}_{(N-1)/2,(N+1)/2}=0$. Thus, (16) is true. Consequently, (12) holds. Therefore, from (11) we get that $\bar{f}=\bar{f}_{0,0}:=d_0$, being d_0 is a constant.

Therefore, if we denote by g_1 the restriction of f to $H_1=0$, then g_1 is a formal power series and since $\bar{f}$ is the restriction of g_1 to $q_2=0$, from Lemma 7, we get that $g_1=d_0+q_2h_3$ where $h_3=h_3(q_2,q_3,p_1,p_2,p_3)$ is a formal power series in its variables.

Now, making the restriction of f to $H_1=0$, $q_3=0$, and proceeding as for the restriction of f to $H_1=0$, $q_2=0$, we get that g_1 can also be written as $g_1=c_0+q_3h_4$, where c_0 is a constant and $h_4=h_4(q_2,q_3,p_1,p_2,p_3)$ is a formal power series in its variables.

Equating the two expressions for g_1, we get that $d_0=c_0$ and there exists a formal power series h_5 such that $h_3=q_3h_5$ and $h_4=q_2h_5$. Thus, g_1 can be written as $g_1=c_0+q_2q_3h_5$. Since g_1 and q_2q_3 are formal first integrals of system (2) restricted to $q_1=0$ and $H_1=0$, we get that h_5 is also a formal first integral of system (2) restricted to $q_1=0$ and $H_1=0$. Then, proceeding as we did for g_1 we get that $h_5=c_1+q_2q_3h_6$, for some formal power series h_6. Since this argument can be repeated infinitely many times, we get that g_1 is a formal power series in $H_2=q_2q_3$ and thus $g_1=g_1(H_2)$. Then, from (9) we have that $f_0=g_1(H_2)$ and thus, $f=g_1(H_2)+H_1g_2$, with $g_2=\Sigma_{k\geqslant 1}f_kH_1^{k-1}$. Thus, since f, H_2, and H_1 are formal first integrals of system (2) restricted to $q_1=0$, g_2 is also a formal first integral of system (2) restricted to $q_1=0$. Repeating the argument that we did for f_0 infinitely many times, the proposition follows. ■

Proposition 14: Any formal first integral $f=f(q_1,q_2,q_3,p_1,p_2,p_3)$ of system (2) *invariant by τ and σ can be written as*

$$f = f^1(H) + H_2 f^2(H,H_2) + H_4 f^2(H,H_4) + H_6 f^2(H,H_6) + q_1 q_2 q_3 f^3(q_1,q_2,q_3,p_1,p_2,p_3), \quad (20)$$

where f^1, f^2, and f^3 are formal power series in their variables, $H_2=q_2q_3$, $H_4=q_1q_3$, and $H_6=q_1q_2$. Furthermore, $f^3=\sigma(f^3)$ and $f^3=-\tau(f^3)$.

Proof: From Proposition 13 and Lemma 7, there exists nine formal power series $g_1,\ldots,g_9$ such that f can be written in the following three forms:

$$f = g_1(H_1) + H_2 g_2(H_1,H_2) + q_1 q_3,$$

$$f = g_4(H_3) + H_4 g_5(H_3,H_4) + q_2 g_6,$$

$$f = g_7(H_5) + H_6 g_8(H_5,H_6) + q_3 g_9.$$

Since

$$H = H_1 + 6(p_1^2 q_1^2 - 2p_1q_1p_2q_2 - 2p_1q_1p_3q_3) + \tfrac{1}{6}(q_1^2 - 2q_1q_2 - 2q_1q_3) = H_1 + q_1 h_1,$$

by Lemma 6, there exist formal power series T, T_0, and T_1 such that

$$g_1(H_1) = g_1(H) - g_1(q_1h_1) + g_1(0) - H_1q_1h_1T(H_1,q_1h_1) = g_1(H) + q_1h_1T_0(H_1,q_1,h_1) = g_1(H) + q_1T_1.$$

Using the same arguments for $g_4(H_3)$ and $g_7(H_5)$, we get that f can be written as

$$f = g_1(H) + H_2 g_2(H_1,H_2) + q_1\bar{T}_1,$$

$$f = g_4(H) + H_4 g_5(H_3,H_4) + q_2\bar{T}_2, \quad (21)$$

$$f = g_7(H) + H_6 g_8(H_5,H_6) + q_3\bar{T}_3.$$

The three equations of (21) must be equal. Thus, restricting the first and second equations of (21) to $q_1=q_2=0$ and equating them, we have that $g_1(\hat{H})=g_4(\hat{H})$, where $\hat{H}$ is the restriction of H to $q_1=q_2=0$. Thus, $g_4=g_1$. In the same way, restricting the first and third equations of (21) to $q_1=q_3=0$, we obtain that $g_7=g_1$. Since f is invariant by σ, $f=\sigma(f)$, and then the first expression of f in (21) can be written as

$$f = g_1(H) + H_4 g_2(H_3,H_4) + q_2\sigma(T_1).$$

This relation for f must coincide with the second expression of f in (21) and thus,

$$0 = H_4(g_2(H_3,H_4) - g_5(H_3,H_4)) + q_2(\sigma(\bar{T}_1) - \bar{T}_2).$$

Taking $q_2=0$ in the above equation we obtain that $g_5=g_2$. In a similar way, since $f=\sigma^2(f)$, proceeding as above for σ, we get that $g_8=g_2$.

Restricting the first and second equations of (21) to $q_2=0$, and decomposing $\bar{T}_1$ as $\bar{T}_1=T_{1,0}+q_2T_{1,1}$, with $T_{1,0}$, $T_{1,1}$ formal power series and $T_{1,0}$ not depending on q_2 (see Lemma 7), we get that $q_1T_{1,0}=H_4g_2(H_3,H_4)$ and thus, the first relation of (21) can be written as

$$f = g_1(H) + H_2 g_2(H_1,H_2) + H_4 g_2(H_3,H_4) + q_1q_2T_{1,1}. \quad (22)$$

Now, writing $T_{1,1}=T_{1,1,0}+q_3T_{1,1,1}$ with $T_{1,1,0}$, $T_{1,1,1}$ formal series and $T_{1,1,0}$ not depending on q_3, we get that restricting the third relation of (21) to $q_3=0$ and restricting (22) to $q_3=0$, we obtain that $q_1q_2T_{1,1,0}=H_6g_2(H_5,H_6)$. Thus, f can be written as

$$f = g_1(H) + H_2 g_2(H_1,H_2) + H_4 g_2(H_3,H_4) + H_6 g_2(H_5,H_6) + q_1 q_2 q_3 T_{1,1,1}. \tag{23}$$

Now, using Lemma 7, we decompose $g_2 = g_2(H_1,H_2)$ as

$$g_2(H_1,H_2) = \sum_{k\geqslant 0} c_k(H_1) H_2^k, \tag{24}$$

where c_k are formal power series in the variable H_1. Then, since $H_1 = H - q_1 h_1$, from (24) and Lemma 6, we have

$$\begin{aligned} g_2(H_1,H_2) &= \sum_{k\geqslant 0} c_k(H - q_1 h_1) H_2^k = \sum_{k\geqslant 0} c_k(H) H_2^k + q_1 \sum_{k\geqslant 0} \tilde{c}_k(q_1,q_2,q_3,p_1,p_2,p_3) H_2^k \\ &= g_2(H,H_2) + q_1 \tilde{g}_2(q_1,q_2,q_3,p_1,p_2,p_3), \end{aligned}$$

where $\tilde{g}_2$ is a formal power series in its variables. Doing the same with $g_2(H_3,H_4)$ and $g_2(H_5,H_6)$, we get that

$$g_2(H_3,H_4) = g_2(H,H_4) + q_2 \tilde{g}_5(q_1,q_2,q_3,p_1,p_2,p_3),$$

$$g_2(H_5,H_6) = g_2(H,H_6) + q_3 \tilde{g}_8(q_1,q_2,q_3,p_1,p_2,p_3),$$

being $\tilde{g}_5$ and $\tilde{g}_8$ formal series in their variables. Therefore, those relations together with (23) imply that f can be written as in (20) if one takes $f^1 = g_1$, $f^2 = g_2$, and $f^3 = T_{1,1,1} + \tilde{g}_2 + \tilde{g}_5 + \tilde{g}_8$.

From (20) and using that f is invariant by σ, we get that

$$\sigma(f) = f^1(H) + H_2 f^2(H,H_2) + H_4 f^2(H,H_4) + H_6 f^2(H,H_6) + q_1 q_2 q_3 \sigma(f^3).$$

Since this equation must coincide with (20) we get that $f^3 = \sigma(f^3)$. Furthermore, using that f is invariant by τ, we get that

$$\tau(f) = f^1(H) + H_2 f^2(H,H_2) + H_4 f^2(H,H_4) + H_6 f^2(H,H_6) - q_1 q_2 q_3 \tau(f^3).$$

Since this equation must coincide with (20) we get that $f^3 = -\tau(f^3)$. ■

Proposition 15: Let f be a formal power series restricted to $H=0$ satisfying $f=\sigma(f)$, $f=(-1)^m \tau(f)$ for a positive integer m such that

$$\frac{\mathrm{d}f}{\mathrm{d}t} = 12m(p_1 q_1 + p_2 q_2 + p_3 q_3) f, \tag{25}$$

where the derivatives are evaluated along a solution of system (2) *restricted to $H=0$. Then, $f = q_1 q_2 q_3 f_1$, for some formal power series f_1 restricted to $H=0$.*

Proof: Note that from hypothesis, f only contains monomials $q_1^{j_1} q_2^{j_2} q_3^{j_3} p_1^{l_1} p_2^{l_2} p_3^{l_3}$ such that the parity of $l_1+l_2+l_3+j_1+j_2+j_3$ is equal to the parity of m. Note that since $f=\sigma(f)$, if q_1 divides f, then, q_2 and q_3 must divide f and thus, it is enough to prove that the restriction of f to $q_1=0$ is equal to zero. We will prove it by contradiction. We denote by g_1 the restriction of f to $q_1=0$. Then, g_1 is a formal power series satisfying

$$\frac{\mathrm{d}g_1}{\mathrm{d}t} = 12m(p_2 q_2 + p_3 q_3) g_1, \tag{26}$$

where the derivatives are evaluated along a solution of system (2) restricted to $q_1 = H_1 = 0$. We assume that $g_1 \neq 0$ and we consider two different cases.

Case 1: g_1 is not divisible by $q_2 q_3$. We introduce the formal power series $g_2 = g_1 q_2^m$. Then, g_2 is a formal power series satisfying

$$\frac{dg_2}{dt} = 24mp_2q_2g_2, \tag{27}$$

where the derivatives are evaluated along a solution of system (2) restricted to $q_1=H=0$.

Now, we restrict (27) to $q_3=0$ and denote by g_2^* the restriction of g_2 to $q_3=0$. We consider $g_2^*\neq 0$ and we will reach a contradiction. If $g_2^*\neq 0$, then g_2^* satisfies (27) restricted to $q_3=0$ and since for system (2) restricted to $q_1=q_3=H=0$ and $q_2\neq 0$ we have $12p_2q_2=(dq_2/dt)/q_2$, then, on $q_2\neq 0$, we have that (27) restricted to $q_3=0$ is equivalent to $dg_2^*/g_2^*=2m\,dq_2/q_2$. That is, $g_2^*=q_2^{2m}g_3^*$ where g_3^* is a first integral of system (2) restricted to $q_1=q_3=H=0$, $q_2\neq 0$, i.e., of system

$$\dot{q}_2 = 12p_2q_2, \quad \dot{p}_1 = 12p_1p_2 + \tfrac{1}{3}, \quad \dot{p}_2 = -12p_2^2 - \tfrac{1}{3}, \quad \dot{p}_3 = 12p_3p_2 + \tfrac{1}{3},$$

after dividing by q_2. Furthermore, $g_3^*=g_2^*/q_2^{2m}$ where g_2^* is a formal power series. Introducing the change of variables

$$x = q_2, \quad y = p_1 - p_3, \quad z = p_3, \quad u = p_2, \tag{28}$$

we have that $g_3^*(q_2,p_1,p_2,p_3)=h(x,y,z,u)$, where h is a first integral of system (7). Furthermore with this change of variables $g_2^*(q_2,p_1,p_2,p_3)=h^*(x,y,z,u)$. Then, $h^*(x,y,z,u)$ is a formal power series and $h=h^*/x^{2m}$. Therefore, h satisfies the hypothesis of Lemma 11 and thus, from Lemma 11 and the change of variables (28) we have

$$g_3^* = \frac{(p_1-p_3)^{2m}}{q_2^{2m}} \sum_{k,l,n\geq 0} g^*_{3,k,m+l,n}(q_2^2(36p_2^2+1))^k((p_1-p_3)^2(36p_2^2+1))^l f_3(p_3,p_2)^n$$

which yields

$$g_2^* = (p_1-p_3)^{2m} \sum_{k,l,n\geq 0} g^*_{3,k,m+l,n}(q_2^2(36p_2^2+1)^k((p_1-p_3)^2(36p_2^2+1))^l f_3(p_3,p_2)^n \ . \tag{29}$$

However, we already know that g_2^* is also restricted to $q_2^2(36p_2^2+1)=0$ and then, from (29) we get

$$\begin{aligned} g_2^* &= (p_1-p_3)^{2m} \sum_{l,n\geq 0} g^*_{3,0,m+l,n}((p_1-p_3)^2(36p_2^2+1))^l f_3(p_3,p_2)^n \\ &= (p_1-p_3)^{2m} \sum_{l,n\geq 0} g^*_{2,l,n}((p_1-p_3)^2(36p_2^2+1))^l f_3(p_3,p_2)^n, \end{aligned} \tag{30}$$

which clearly is a formal power series.

By (30) we have that the restriction of g_2^* to $q_2=0$ is equal to g_2^*. Furthermore, the restriction of g_2^* to $q_2=0$ is also equal to the restriction of g_2 to $q_3=q_2=0$ and by definition it is equal to zero. Using (30) this implies that $g^*_{2,l,n}=0$ for $l,n\geq 0$ and thus $g_2^*=0$, a contradiction.

Then, $g_2^*=0$ and since g_2^* is the restriction of g_2 to $q_3=0$, by Lemma 7, we get that $g_2=q_3h_2$ for some formal power series $h_2=h_2(q_2,q_3,p_1,p_2,p_3)$. Furthermore, since g_2 has q_2^m as a factor, it holds that $h_2=q_2^mh_3$ for some formal power series $h_3=h_3(q_2,q_3,p_1,p_2,p_3)$. Then, using that $g_1=g_2/q_2^m$, we obtain

$$g_1 = q_3h_3. \tag{31}$$

Now, if we introduce the formal power series $g_3=g_1q_3^m$, we get that g_3 satisfies

$$\frac{dg_3}{dt} = 24mp_3q_3g_3,$$

where the derivative is evaluated along a solution of system (2) restricted to $q_1=H=0$. Then, repeating the same arguments for g_3 as we did for g_2, we obtain that g_1 can be written as

$$g_1 = q_2 h_4, \tag{32}$$

for some formal power series $h_4 = h_4(q_2, q_3, p_1, p_2, p_3)$.

Finally, equating the expressions (31) and (32) for g_1 we obtain that there exists a formal power series $h_5 = h_5(q_2, q_3, p_1, p_2, p_3)$ such that $h_3 = q_2 h_5$ and $h_4 = q_3 h_5$. Then, g_1 can be written as $g_1 = q_2 q_3 h_5$, a contradiction with the fact that g_1 was not divisible by $q_2 q_3$.

Case 2: g_1 is divisible by $q_2 q_3$. In this case, we write $g_1 = (q_2 q_3)^j h_1$, where $j \geqslant 1$ and h_1 is a formal power series which is not divisible by $q_2 q_3$. Furthermore, since $q_2 q_3$ is a first integral of system (2) restricted to $q_1 = 0$, we get that h_1 also satisfies (26). Then, the same arguments used in Case 1 for g_1 can be applied to h_1 and we shall obtain a contradiction. Hence, the proposition is proved. ■

III. PROOF OF THE THEOREMS

Now we prove Theorems 3 and 4.

Proof of Theorem 3: Let g be a formal first integral of system (2). If g is a formal first integral in the variable H the theorem is proved. So, we can assume that g is not a formal power series in the variable H. Moreover, without loss of generality the formal power series g has no independent term. We also can assume that g is not divisible by any formal power series $T(H)$ depending on H; otherwise if $T(H)$ divides g, then we can take $g/T(H)$ instead of g as a new formal first integral. By Proposition 12, we have that

$$f = (g \cdot \sigma g \cdot \sigma^2 g) \cdot \tau(g \cdot \sigma g \cdot \sigma^2 g) \tag{33}$$

is invariant by τ and σ and thus, f has all its monomials $q_1^{j_1} q_2^{j_2} q_3^{j_3} p_1^{l_1} p_2^{l_2} p_3^{l_3} H^m$ satisfying that $j_1 + j_2 + j_3 + l_1 + l_2 + l_3$ is even. Moreover, from Proposition 14, we have that f can be written as in (20). We write

$$\begin{aligned} f &= \sum_{l \geqslant 0} f_l(q_1, q_2, q_3, p_1, p_2, p_3) H^l, \\ f^1(H) &= \sum_{l \geqslant 0} f_l^1 H^l, \\ f^2(H, H_j) &= \sum_{k,l \geqslant 0} f_{k,l}^2 H_j^k H^l, \quad j = 2,4,6, \\ f^3 &= \sum_{l \geqslant 0} g_l(q_1, q_2, q_3, p_1, p_2, p_3) H^l, \end{aligned} \tag{34}$$

where f_l and g_l are formal power series in their variables not divisible by H, for $l \geqslant 0$, $k \geqslant 0$, f_l^1, $f_{k,l}^2$ are constants. Then, from (20), we have

$$f_0 = f_{|H=0} = f_0^1 + \sum_{k \geqslant 0} f_{k,0}^2 (H_2^{k+1} + H_4^{k+1} + H_6^{k+1}) + q_1 q_2 q_3 g_0. \tag{35}$$

Note that since f^3 satisfies $f^3 = \sigma(f^3)$ and we get that g_0 satisfies $g_0 = \sigma(g_0)$. Furthermore, $f^3 = -\tau(f^3)$ and thus $g_0 = -\tau(g_0)$.

Taking into account that the derivatives of H_2, H_4, and H_6 evaluated along a solution of system (2) satisfy

$$\frac{dH_2}{dt} = -24 p_1 q_1 H_2, \quad \frac{dH_4}{dt} = -24 p_2 q_2 H_4, \quad \frac{dH_6}{dt} = -24 p_3 q_3 H_6,$$

then, after dividing by $q_1 q_2 q_3$, the derivative of f_0 along a solution of system (2) is given by

$$24\sum_{k\geqslant 0}(1+k)f_{k,0}^2(p_1H_2^k+p_2H_4^k+p_3H_6^k)+12(p_1q_1+p_2q_2+p_3q_3)g_0=\frac{\mathrm{d}g_0}{\mathrm{d}t}, \tag{36}$$

where the derivatives are taken along a solution of system (2) and relation (36) is taken restricted to $H=0$.

Now, restricting (36) to $q_1=q_2=q_3=0$ (note that then $H=0$), and taking into account that this is a singular point of system (2), we obtain that $f_{0,0}^2(p_1+p_2+p_3)=0$ and thus, $f_{0,0}^2=0$. Then, (36) can be written as

$$24\sum_{k\geqslant 1}(1+k)f_{k,0}^2(p_1H_2^k+p_2H_4^k+p_3H_6^k)+12(p_1q_1+p_2q_2+p_3q_3)g_0=\frac{\mathrm{d}g_0}{\mathrm{d}t}, \tag{37}$$

where the derivatives are evaluated along a solution of system (2) and this relation is restricted to $H=0$.

Now, we denote by $\bar{g}_1$ the restriction of g_0 to $q_1=0$. Then, $\bar{g}_1$ satisfies

$$24p_1\sum_{k\geqslant 1}(1+k)f_{k,0}^2H_2^k+12(p_2q_2+p_3q_3)\bar{g}_1=\frac{\mathrm{d}\bar{g}_1}{\mathrm{d}t}, \tag{38}$$

where the derivatives are evaluated along a solution of system (2) and this relation is restricted to $q_1=H=0$.

Now, taking into account that on $q_1=q_2=0$ or $q_1=q_3=0$ we have $H_2=0$, we can proceed exactly in the same way as in the proof of Case 1 in Proposition 15 and we get that $\bar{g}_1$ must be divisible by q_2q_3, i.e., $\bar{g}_1=q_2q_3h$ for some formal series h. Furthermore, from (38) and since $H_2=q_2q_3$ is a first integral of system (2) restricted to $q_1=0$ and $H=0$, we get that, after dividing by q_2q_3, h satisfies

$$24p_1\sum_{k\geqslant 1}(1+k)f_{k,0}^2H_2^{k-1}+12(p_2q_2+p_3q_3)h=\frac{\mathrm{d}h}{\mathrm{d}t}, \tag{39}$$

with this equation restricted to $H=0$. Evaluating (39) on $q_2=q_3=0$, taking into account that those are singular points of the system (2) restricted to $q_1=0$, we obtain that $-48p_1f_{1,0}^2=0$, which clearly implies $f_{1,0}^2=0$. Hence, (39) becomes

$$24p_1H_2\sum_{k\geqslant 2}(1+k)f_{k,0}^2H_2^{k-2}+12(p_2q_2+p_3q_3)h=\frac{\mathrm{d}h}{\mathrm{d}t}$$

which is of the same kind as (38). Now, repeating the reasoning we did for $\bar{g}_1$ infinitely many times, we have that $f_{k,0}^2=0$ for all $k\geqslant 0$. Therefore, (37) becomes

$$\frac{\mathrm{d}g_0}{\mathrm{d}t}=12(p_1q_1+p_2q_2+p_3q_3)g_0,$$

where the derivative is evaluated along a solution of system (2) restricted to $H=0$. We want to prove that $g_0=0$. We will proceed by contradiction. We assume $g_0\neq 0$ and consider two different cases.

Case 1: g_0 is not divisible by $q_1q_2q_3$. It is clear that g_0 satisfies $g_0=\sigma(g_0)=\sigma^2(g_0)$ and $\tau(g_0)=-g_0$, then from Proposition 15 with $m=1$, we get that $g_0=q_1q_2q_3h_5$ for some formal series h_5, a contradiction with the fact that g_0 was not divisible by $q_1q_2q_3$.

Case 2: g_0 is divisible by $q_1q_2q_3$. In this case we write $g_0=(q_1q_2q_3)^jh_j$ with $j\geqslant 1$, $h_j\neq 0$ is not divisible by $q_1q_2q_3$. Furthermore, h_j satisfies

$$\frac{dh_j}{dt} = 12(j+1)(p_1q_1 + p_2q_2 + p_3q_3)h_j,$$

where the derivative is evaluated along a solution of system (2) restricted to $H=0$. Furthermore, $h_j=\sigma(h_j)$ and since $\tau(g_0)=-g_0$ we get that $\tau(h_j)=(-1)^{j+1}h_j$. Then, applying Proposition 15 with $m=j+1$, we get that $h_j=q_1q_2q_3h_{j+1}$ with h_{j+1} a formal series, a contradiction with the fact that h_j is not divisible by $q_1q_2q_3$.

Hence, $g_0=0$ and from (35), we have obtained that $f_0=f_0^1$, a constant and thus, from the first relation in (34) we have that

$$f = f_0^1 + H\sum_{l\geqslant 1} f_l(q_1,q_2,q_3,p_1,p_2,p_3)H^{l-1}.$$

Since H is a first integral of system (2), we get that $\Sigma_{l\geqslant 1}f_l(q_1,q_2,q_3,p_1,p_2,p_3)H^{l-1}$ is also a first integral of system (2). Then, the same arguments used for f_0 imply that $f_1=f_1^1$, a constant since this argument can be repeated infinitely many times, we get that for all $k\geqslant 0$, $f_k=f_k^1$, constants, and thus, the first equation in (34) implies that $f=f(H)=\Sigma_{l\geqslant 0}f_l^1H^l=f(H)$.

Hence, from (33) we get that f must be reducible, that is, there exist formal series $T=T(H)$ and $T_1=T_1(H)$ such that $f=T(H)T_1(H)$. Furthermore, we can assume that T is irreducible. Then, from (33) we get that $T(H)$ divides $g\cdot\sigma g\cdot\sigma^2 g$ or $\tau(g\cdot\sigma g\cdot\sigma^2 g)$. In the first case, we also can assume that divides σg or $\sigma^2 g$; otherwise we reach a contradiction with the assumptions on g. Thus, if $T(H)$ divides σg then $\sigma g=T(H)T_2$ for some formal series $T_2=T_2(q_1,q_2,q_3,p_1,p_2,p_3)$ and thus

$$g = \sigma^3 g = \sigma^2 T(H)\cdot\sigma^2 T_2$$

a contradiction with the assumptions on g. Now, we can assume that $T(H)$ divides $\sigma^2 g$. With similar arguments to those used for the case in which $T(H)$ divides σg we reach a contradiction with the assumptions on g.

Now, we assume that $T(H)$ divides $\tau(g\cdot\sigma g\cdot\sigma^2 g)$. With similar arguments to those used for the case in which $T(H)$ divides $g\cdot\sigma g\cdot\sigma^2 g$ we reach a contradiction with the assumptions on g. Thus, Theorem 3 is proved. ■

Proof of Theorem 4: Since H is an analytic first integral of system (2), it is clear that any analytic function in a neighborhood of zero in the variable H is an analytic first integral of system (2) in a neighborhood of zero. To prove that these are the only ones, we proceed by contradiction. Assume that g is an analytic first integral of system (2) which is not a function of H. Then, there exists a neighborhood $U\subset\mathbb{R}^6$ of the origin such that $g_{|U}$ is an analytic first integral of system (2) which is not a series in H. Clearly, $g_{|U}$ can be written as a formal power series which turns out to be convergent. Hence, in U, g is a formal first integral which is not a series in H, a contradiction with Theorem 3. Thus, Theorem 4 is proved. ■

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Discrete dynamical systems embedded in Cantor sets

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While the notion of chaos is well established for dynamical systems on manifolds, it is not so for dynamical systems over discrete spaces with N variables, as binary neural networks and cellular automata. The main difficulty is the choice of a suitable topology to study the limit $N \to \infty$. By embedding the discrete phase space into a Cantor set we provided a natural setting to define topological entropy and Lyapunov exponents through the concept of error profile. We made explicit calculations both numerical and analytic for well-known discrete dynamical models.
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I. INTRODUCTION

For motions on differentiable manifolds, the commonly accepted notion of chaos identifies it with the so-called *sensitive dependence* on *initial conditions* and the latter with the existence of positive Lyapunov exponents signaling exponential separation of initially close trajectories.[1] In this sense, chaotic motion means unstable behavior; there is, however, an equivalent interpretation of chaos in terms of information production.[2] This is due to a celebrated theorem by Pesin which says that, for sufficiently regular ergodic systems, the sum of the positive Lyapunov exponents coincides with the *Kolmogorov-Sinai dynamical (KS-)entropy* associated with the dynamics. The KS-entropy measures the long run unpredictability of the motion with respect to an invariant state. Further, a variational principle states that the maximal KS-entropy with respect to all possible invariant states of a homeomorphism on a compact metric space is Bowen's *topological entropy* which gives a state-independent description of the degree of chaos based on how open sets change during the motion.

Roughly speaking, in standard dynamical system contexts, chaos reveals itself through the exponential increase of errors or, equivalently, via not-less-than linear information production.

On the contrary, there is no definite agreement about what chaos should mean in discrete dynamical systems, such as binary neural networks or cellular automata, where one cannot directly appeal to differentiability and thus to the standard definition of Lyapunov exponents.

However, inspired by the equivalent manifestations of chaos, briefly sketched above, one may try to overcome the lack of differentiable structures by looking at entropylike quantities.

In the following, we shall investigate how far chaos in discrete system can be identified with the exponential increase of initial errors or with (topological) information production.

Discrete, deterministic dynamical systems, consisting of N binary variables, have finite, even though very large (2^N), number of states.[3–9] This means that their dynamics is eventually going to end up in a periodic cycle. Due to this fact, there is no room for chaotic behavior as it is usually intended, unless the number of states $N \to \infty$.

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In numerical studies of continuous systems one needs to discretize the manifold in order to solve physical models based on differential equations.[10] Once the space has been discretized, the number of available states is finite and one has no longer a chaotic system since the motion eventually becomes periodic. However the discretized systems inherit the natural distance of their continuous limit, so that, if the number of states goes to infinity, one expects to smoothly retrieve the continuous structure with all its dynamical properties. The problem with discrete dynamical systems is that the "natural" distance, the so-called Hamming distance is ill-defined in the limit $N \to \infty$.[9]

To overcome these difficulties in this work we try to resort to topological techniques. On compact sets, one may define the concept of sensitive dependence on initial conditions (together with topological transitivity) by only topological means and no differentiable structure. So, we define the topology of a Cantor set and endow it with compatible metrics that remain well defined in the limit of infinitely many states.[9] Then we look at the various dynamical patterns that appear and try to characterize them by adapting standard tools from ergodic theory as, Lyapunov exponents and topological entropy.[1,11–14]

In Sec. II, we review the concept of sensitive dependence on initial conditions formulated in a topological way. We endow the space with the topology of a Cantor set and introduce metrics compatible with it. In Sec. III, Lyapunov exponents in discrete systems are defined by means of metrics and also in terms of the derivative of suitable embedding homeomorphisms into the reals. In Sec. IV, the topological entropy is formulated in terms of spanning sets; while in Sec. V, Lyapunov exponents and topological entropy are related to an appropriate indicator of error propagation, that we call *error profile*. In Sec. VI, some concrete calculations are presented and in Sec. VII conclusions are drawn and future directions of investigation briefly mentioned.

II. DEFINING CHAOS ON DISCRETE SYSTEMS

We shall study discrete systems described in the following way:[3–9] a phase space is defined by a set Ω of states $\mathbf{S}$ consisting of N bits $S_i = \{0,1\}$; $i = 1, \ldots, N$, which evolve according to binary functions $f: \Omega \to \Omega$,

$$S_i(n+1) = f_i(\mathbf{S}(n)), \tag{1}$$

that update each bit $S_i(n)$ at each stroke of time n.

In neural networks and cellular automata, in general, all bits have an equally important role in the development of the system with time. When the number N of bits is finite, the metric most suited to this state of affairs is the Hamming distance[4,5,9] given by

$$d_H(\mathbf{S},\mathbf{S}') = \sum_{i=1}^{N} |S_i - S_i'|, \tag{2}$$

for any two states $\mathbf{S}, \mathbf{S}' \in \Omega$. Note that Hamming distance counts the number of different bits between $\mathbf{S}$ and $\mathbf{S}'$, but it is not sensitive to where the differences occur.

The usual way of identifying chaos in the evolution law (1) is to study the so-called *damage spreading*.[5–7,15] One follows the dynamical development of two states with initial Hamming distance equal to one and studies how it increases with time n. The speed of damage spreading is then defined by[15]

$$v(S,S') = \lim_{n \to \infty} \frac{d_H(\mathbf{S}(n),\mathbf{S}'(n))}{n}. \tag{3}$$

Two observations are necessary at this point. The first is that the above definition does not correspond to the identification of an exponential increase of an initial small error, but only discriminates between sublinear, linear, and superlinear increase of the Hamming distance.

The second is that, in the definition, it is implicit that the number N of binary variables is infinite, otherwise there will be recurrences and the limit in (3) would automatically vanish.

However, when $N\to\infty$, the Hamming distance makes no sense since there are infinitely many states with infinite d_H, and then it fails to be a properly defined distance function.

Remark 2.1: We stress that if one wants to think of binary systems as discretizations of continuous ones, so that asymptotic quantities like (3) make sense, then the metric of the space should be well defined when $N\to\infty$. There are two alternatives: either binary systems are taken as intrinsically discrete, in such a case formula (3) is to be investigated as a possible behavior over finite time scales.[16] Or the number of states is allowed to go to infinity, in such a case, appropriate metrics that are well defined for $N\to\infty$ must be chosen in order to look at the dynamics from a topological point of view.

In this paper we are going to explore the topological point of view. Let us take $N\to\infty$ and introduce the base of open sets[17]

$$\mathcal{N}(\mathbf{S},q)=\{\mathbf{S}'\in\Omega|S_k=S'_k,1\leqslant k<q\}. \tag{4}$$

It is well known that they generate the topology of a Cantor set on Ω.[9,11,12]

Definition 2.1: A Cantor set is a topological space such that[11]

(i) it is *totally disconnected*;
(ii) *perfect*, that is, it is closed and all its points are accumulation points;
(iii) *compact*.

The main issue in what follows is the identification of chaotic behaviors in discrete systems with a Cantor structure. As observed in the introduction, the lack of differentiability excludes that one may recognize any exponential separation of trajectories from the analysis of the tangent map.

Before trying to explore the possible existence of an exponential increase of initial small errors, one may start from a weaker form of instability than the usual one and identify a minimal degree of chaoticity with the following topological definition.[9]

Definition 2.2: Let $f:\Omega\to\Omega$ be a continuous map; we say that it shows *weak sensitive dependence on initial conditions* (WSDIC) if there exists a $p\in\mathbb{N}$ such that for any $\mathbf{S}$ and any $\mathcal{N}(\mathbf{S},q)$, there exists a $\mathbf{S}'\in\mathcal{N}(\mathbf{S},q)$ and a $k\in\mathbb{N}$ such that $f^k(\mathbf{S}')\notin\mathcal{N}(f^k(\mathbf{S}),p)$.

Remark 2.2: Note that the only requisite to define WSDIC is to have a topology on Ω. Which one? It depends not on mathematical arguments, but on physical considerations. That is, which properties do we want to measure and with how much accuracy? As extreme examples, in the *trivial topology* (given by $\{\emptyset,\Omega\}$) the dynamics is going to be trivial; while, in the *discrete topology* (where any subset of Ω is an open set) all systems show WSDIC.

There are several metrics compatible with the topology generated by the base (4), the more popular is[11,12]

$$\tilde{d}(\mathbf{S},\mathbf{S}')=\sum_{i=1}^{\infty}\frac{1}{2^{i-1}}|S_i-S'_i|.$$

However, for the purpose of this work we are going to use, for any $0<\beta<1$, the following ones:

$$d_\beta(\mathbf{S},\mathbf{S}')=\beta^m \quad \text{if } S_k=S'_k \quad \forall\, 1\leqslant k<m \quad \text{and } S_m\neq S'_m, \tag{5}$$

in terms of which the base (4) can be expressed as

$$\mathcal{N}(\mathbf{S},q)=\{\mathbf{S}'\in\Omega|d_\beta(\mathbf{S},\mathbf{S}')\leqslant\beta^q\}. \tag{6}$$

Remarks 2.3:

(i) We can view the embedding process of a finite discrete system into the Cantor set as follows: Let $\mathcal{F}$ be the set of all the continuous functions $f:\Omega\to\Omega$ on the Cantor set. Then any finite discrete dynamical system with N bits described by equations (1) is an element of the set

$$\mathcal{F}_N=\{f\in\mathcal{F}|\ \forall\ \mathbf{S}\in\Omega f(\mathcal{N}(\mathbf{S},N))=\mathcal{N}(f(\mathbf{S}),N)\}.$$

(ii) There is a price to pay for working with the base (4) and their associated metrics (5). Indeed, some of the binary variables contribute more than others. At first sight, this looks as a major problem since typical binary systems such as the ones constructed with random couplings[8,18,19] evolve through functions f_i's where all the variables contribute on an equal footing to the dynamics and so, apparently, there is no reason to "dismiss" some and "privilege" others as the distances (5) do. However, if we make a permutation $\pi:\mathbb{N}\to\mathbb{N}$ of the automata's indexes, and thus reenumerate them, the induced mapping $\hat{\pi}:\Omega\to\Omega$, such that

$$\hat{\pi}(S_1,S_2,\dots)=(S_{\pi^{-1}(1)},S_{\pi^{-1}(2)},\dots), \tag{7}$$

is, as we show below, an homeomorphism and so the Cantor topology is preserved despite the fact that the new metrics are not going to be Lipschitz equivalent.[13] From this it follows that, since WSDIC is a topological property, it does not depend in which way we have numerated the automata.

Let us now show that $\hat{\pi}$ is an homeomorphism: By construction the function is a bijection so we only need to show that it is continuous. Given $\varepsilon>0$ choose $M\in\mathbb{N}$ such that $\beta^M<\varepsilon$. Now take $m\in\mathbb{N}$ such that $\pi^{-1}(i)<m$ for any $1\leqslant i<M$. Then,

$$d_\beta(\mathbf{S},\mathbf{S}')<\beta^m\Rightarrow d_\beta(\hat{\pi}(\mathbf{S}),\hat{\pi}(\mathbf{S}'))\leqslant\beta^M<\varepsilon,$$

hence continuity.

Remarks 2.4:

(i) The metrics (5) seem to establish a preferred direction along the network. However, one can always reverse it by means of the permutation

$$\hat{\pi}(S_1,S_2,\dots,S_N)=(S_N,S_{N-1},\dots,S_2,S_1)$$

and, then, take the limit $N\to\infty$ in the metrics (5).

(ii) The metrics (5) are suited to semi-infinite networks. However, when expanding to infinity finite networks with periodic boundary conditions, as we will see in the examples, more symmetric metrics are preferable. These are achieved by means of two-sided sequences $\mathbf{S}=(\dots,S_{-2},S_{-1},S_0,S_1,S_2,\dots)$ and using the metrics

$$\hat{d}_\beta(\mathbf{S},\mathbf{S}')=\beta^m\quad\text{if } S_k=S'_k\quad\forall\ |k|<m$$

$$\text{with}\quad S_m\neq S'_m\quad\text{or } S_{-m}\neq S'_{-m}$$

which also define a Cantor topology.

III. LYAPUNOV EXPONENTS

Since Definition 2.2 is a topological one, and the metrics (5) all define the same topology, we can use any of them (by fixing a β) to check if there is WSDIC or not.

However, in continuous dynamics there is a definition of *sensitive dependence on initial conditions*, which we shall refer to as *strong* (SSDIC) in comparison with the previous one (WSDIC), which is based on the concept of positive Lyapunov exponents; that is, on the expo-

nential separation of initially close trajectories.[1,11,13] Such a behavior is usually associated with exponential increase of initial small errors. We propose two different natural definitions of Lyapunov exponents. The first one is based on the metrics (5), the second one is via an embedding of Ω into the continuum, where the notion of derivative can be used.

The metrics (5) offer a natural means to measure the increase of errors in Cantor sets. In fact, given d_β, one can define Lyapunov exponents as follows:

$$\lambda_M(\mathbf{S}) = \limsup_{n\to\infty} \lim_{d_\beta(\mathbf{S},\mathbf{S}')\to 0} \frac{1}{n} \log_{\beta^{-1}} \frac{d_\beta(f^n(\mathbf{S}),f^n(\mathbf{S}'))}{d_\beta(\mathbf{S},\mathbf{S}')}. \tag{8}$$

The quantity $\lambda_M(\mathbf{S})$ depends in general on $\mathbf{S}$, it amounts to identify separation of trajectories with the following behavior:

$$d_\beta(f^n(\mathbf{S}),f^n(\mathbf{S}')) \simeq \beta^{-n\lambda_M(\mathbf{S})} d_\beta(\mathbf{S},\mathbf{S}').$$

Remarks 3.1:

(i) In (8), we have used lim sup as we do not know whether the limit for $n\to\infty$ exist as it is the case for smooth dynamical systems by Oseledec's multiplicative theorem.[2] Also, the limit when $d_\beta(\mathbf{S},\mathbf{S}')\to 0$ may very well diverge as is the case when discrete dynamical systems exhibit nearly stochastic behavior such as random Boolean networks or binary neural networks with long range connections among the variables.[8,9,15,18]

(ii) Since the distances depend on β, we use a logarithm base β^{-1} to make $\lambda_M(\mathbf{S})$ β independent.

(iii) Due to the presence of a positive λ_M because of the exponential separation of trajectories, however close to each other initially, it turns out that the SSDIC property implies the weaker WSDIC property.

One may also try a kind of differential approach to the notion of exponential instability which is based on an appropriate embedding of the Cantor set Ω into the reals (compare, the abstract mathematical approach in Ref. 20). Let us consider the following commutative diagram:

$$\begin{array}{ccc} \Omega & \overset{f}{\to} & \Omega \\ \phi\downarrow & & \downarrow\phi \\ \Xi & \overset{\tilde{f}}{\to} & \Xi \end{array} \tag{9}$$

which defines the function $\tilde{f}$, by means of a homeomorphism ϕ, with Ξ being a Cantor set embedded in the reals ($\Xi\subset\mathbb{R}$). It is important to observe that due to the commutativity of the diagram (9), the dynamics generated by f and $\tilde{f}$ are intrinsically the same because of *topological conjugacy*.[11,12] Since Ω is an uncountable compact Abelian topological group, there are uncountably many ways of constructing a homeomorphism $\phi:\Omega\to\Xi$ (for instance, by suitable translations).[21] We will consider a ϕ that is suited to the metrics (5). Explicitly, let

$$\phi(\mathbf{S}) = \sum_{k=1}^{\infty} \gamma_k S_k, \tag{10a}$$

where

$$\gamma_k = h^k(h^{-1}-1) = \left(\frac{1-\alpha}{2}\right)^k \frac{1+\alpha}{1-\alpha}, \tag{10b}$$

with

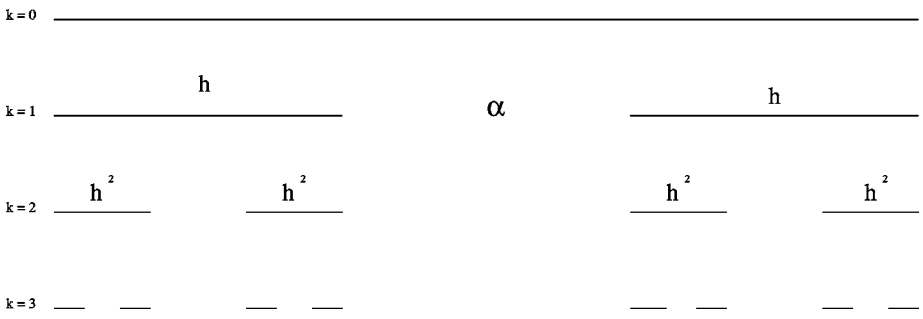


FIG. 1. Some steps in the construction of the Cantor set, with $h=(1-\alpha)/2$.

$$h = \frac{1-\alpha}{2} \quad \text{and } 0 < \alpha < 1,$$

sets the scale of the Cantor set by suppressing intervals in the proportion α (the standard choice being $\alpha = 1/3$). Figure 1 explains the idea of the construction of the Cantor set in a graphical way. Note that the self-similar nature of the Cantor set is reflected by the fact that the coefficients γ_k satisfy the following recursion relation:

$$\gamma_{k+m} = h^m \gamma_k. \tag{11}$$

Now, given any continuous function $f:\Omega \to \Omega$, we define the function $\delta_h f:\Omega \to \mathbb{R}$ by

$$\delta_h f(\mathbf{S}) = \lim_{\mathbf{S}' \to \mathbf{S}} \frac{\phi \circ f(\mathbf{S}') - \phi \circ f(\mathbf{S})}{\phi(\mathbf{S}') - \phi(\mathbf{S})}, \tag{12}$$

which has the typical properties of a derivative. In particular it maps to the vector space $\mathbb{R}$. Indeed, (12) is nothing but the derivative of the conjugate map $\tilde{f}$. Of course the actual value of $\delta_h f(\mathbf{S})$ is α-dependent, for if one wants to give the instantaneous rate of change of a function, one needs a scale. Similarly, if one wants to speak about the Hausdorff dimension of a Cantor set, one needs to embed it into $\mathbb{R}$ and the result is going to be scale dependent.

From (12), there naturally comes the following proposal of Lyapunov exponent associated with the derivative

$$\lambda_D(\mathbf{S}) = \limsup_{n \to \infty} \frac{1}{n} \log_{h^{-1}} |\delta_h f^n(\mathbf{S})|. \tag{13}$$

IV. ENTROPY

In ergodic theory, one approaches the notion of entropy from two different perspectives: the first one is statistical and based on the presence of an invariant measure, the other is topological. We shall consider the latter point of view which leads to the notion of topological entropy.[1,13,14]

Topological entropy: In the topological case, the fundamental objects are the open sets (4). We shall calculate $h_{\text{top}}(f)$ following standard techniques,[1,13] namely the so-called (n,ε)-*spanning set*. For this we need the dynamics-dependent distances

$$d_{\beta,n}(\mathbf{S},\mathbf{S}') = \max_{0 \leqslant k \leqslant n} d_\beta(f^k(\mathbf{S}), f^k(\mathbf{S}')),$$

and the corresponding open balls

$$\mathcal{B}_\beta(\mathbf{S},\varepsilon,n) = \{\mathbf{S}' \in \Omega | d_{\beta,n}(\mathbf{S},\mathbf{S}') < \varepsilon\}. \tag{14}$$

A subset $E(n,\varepsilon) \subseteq \Omega$ is called (n,ε)-spanning if

$$\Omega = \bigcup_{\mathbf{S} \in E(n,\varepsilon)} \mathcal{B}_\beta(\mathbf{S},\varepsilon,n). \tag{15}$$

That is, any (n,ε)-spanning set corresponds to an open cover of Ω. Because of the compactness of Ω, there will always be an (n,ε)-spanning set containing finitely many states $\mathbf{S}$; therefore, the minimal cardinality

$$\mathcal{S}(\varepsilon,n) = \min_{E(n,\varepsilon)} \quad \#E(n,\varepsilon)$$

of (n,ε)-spanning sets is finite.

The topological entropy $h_{\text{top}}(f)$ is defined by

$$h_{\text{top}}(f) = \lim_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{1}{n} \ln \mathcal{S}(\varepsilon,n), \tag{16}$$

where the logarithm is in base 2.

Since the topological entropy $h_{\text{top}}(f)$ reflects the way open sets change in time under $f:\Omega \to \Omega$ given by (1), $h_{\text{top}}(f)$ will not depend on β. This is Bowen's definition and is based on using metrics.[13] The intrinsically topological nature of the notion rests on the fact that Bowen's formulation is equivalent to the one of Adler, Konheim, and McAndrew based on open covers.[1,13,14]

Remark 4.1: The topological entropy $h_{\text{top}}(f)$ is related by a variational principle to the metric or dynamical entropy of Kolmogorov, $h_\mu(f)$,

$$h_{\text{top}}(f) = \sup_{\mu \in \mathcal{M}(\Omega,f)} h_\mu(f), \tag{17}$$

where $\mathcal{M}(\Omega,f)$ is the space of invariant measures in Ω under the dynamics f. To establish (17) one needs a measurable structure to be defined on Ω, which is easily achieved by considering the σ-algebra generated by the open sets (4). What is more difficult to obtain is a measure μ on the σ-algebra being invariant under the dynamics: $\mu(f^{-1}(C))=\mu(C)$ for all measurable subsets $C \subseteq \Omega$. This is the meaning of the request $\mu \in \mathcal{M}(\Omega,f)$. Such a problem will be a matter of further investigation and will not be of concern in this work.

V. ERROR PROFILE AND CHAOTIC BEHAVIOR

Now we are going to study how Lyapunov exponents (8) and (13) and the topological entropy (16) are related to error propagation along the ordering defined by the metrics (5) over the network.

Let us take two near states $\mathbf{S}$ and $\mathbf{S}'$ with initial distance

$$d_\beta(\mathbf{S},\mathbf{S}') = \beta^q. \tag{18a}$$

Their evolution in time can always be written as

$$d_\beta(f^n(\mathbf{S}),f^n(\mathbf{S}')) = \beta^{q-L_n(\mathbf{S},\mathbf{S}')}, \tag{18b}$$

where $L_n(\mathbf{S},\mathbf{S}') \in \mathbb{Z}$ measures the length traveled to the left ($L_n>0$), or to the right ($L_n<0$), by the errors at the nth time step. The behavior of $L_n(\mathbf{S},\mathbf{S}')$, numerically measurable, reflects the properties of the network dynamics and is not necessarily monotonically increasing with time.

Remark 5.1: It is to be emphasized that $L_n(\mathbf{S},\mathbf{S}')$ does not correspond to the Hamming distance, since $q-L_n(\mathbf{S},\mathbf{S}')$ locates the first error that appears in the automaton ordering associated with the metrics (5). Such an error may very well be the only one, in such a case, $d_H(f^n(\mathbf{S}),f^n(\mathbf{S}'))=1$.

Thus, the picture we have in mind is as follows. Let us assume $L_n>0$, at time $n=0$, take two states $\mathbf{S}$, $\mathbf{S}'$ which agree upon the first $q-1$ bits, at time $n=1$ they agree upon the first

$q-L_1(\mathbf{S},\mathbf{S}')-1$ bits, at time $n=2$ upon the first $q-L_2(\mathbf{S},\mathbf{S}')-1$ bits, and so on. In this way, after n iterations of the dynamics (1), the first error will have propagated from position q to position $q-1-L_n(\mathbf{S},\mathbf{S}')$.

Remark 5.2: If $L_n<0$, then the initial error moves further and further away to the right with two consequences: first, it need not be the first error and thus need not appear at the exponent in (18b); second, it may become smaller and smaller contrary to the expectation that instability should amplify initial small errors. However, this is due to a preferred direction inherent in the choice of the metrics (5) as discussed in Remark 2.4(i). This also means that we can always consider $L_n>0$ in (18b) up to a reflection: this argument particularly applies to the behavior of the rule 30 in Wolfram's classification (see the examples) which seems otherwise to contradict instability.

Definition 5.1: We define the $\mathbf{S}$ *error profile* by the following limit:

$$\Lambda_n(\mathbf{S}) = \limsup_{d_\beta(\mathbf{S},\mathbf{S}')\to 0} L_n(\mathbf{S},\mathbf{S}'), \tag{19}$$

measures the length traveled by the errors at the nth time step due to two infinitesimally closed initial states.

Remark 5.3: The idea behind the previous definition is that, in physical instances, $L_n(\mathbf{S},\mathbf{S}') \approx \Lambda_n(\mathbf{S})$ once spurious boundary effects are eliminated by $\mathbf{S}'\to\mathbf{S}$ in the Cantor topology defined by the metrics (5). Numerically, the limit in (19), will be later handled by considering $\mathbf{S}$ and $\mathbf{S}'$ with $d_\beta(\mathbf{S},\mathbf{S}')$ sufficiently small.

We are now going to see how the error profile is related with the concepts introduced in the preceding sections. First, we deal with the Lyapunov exponents introduced in Sec. III.

A. Lyapunov exponents

Concerning metric-based Lyapunov exponents λ_M defined in (8), Eqs. (18) and (19) yield

$$\lambda_M(\mathbf{S}) = \limsup_{n\to\infty} \frac{\Lambda_n(\mathbf{S})}{n}. \tag{20}$$

Concerning derivative-based Lyapunov exponents λ_D defined in (13), we first calculate the derivative of a generic continuous function $f:\Omega\to\Omega$.

Consider two closed points $\mathbf{S},\mathbf{S}'\in\Omega$ with distance β^m, they are of the form [see Eq. (5)]

$$\mathbf{S} = (S_1S_2S_3\cdots S_{m-1}S_mS_{m+1}\cdots) \tag{21a}$$

and

$$\mathbf{S}' = (S_1S_2S_3\cdots S_{m-1}S'_mS'_{m+1}\cdots), \tag{21b}$$

where $S_m\neq S'_m$. Applying the homeomorphism (10a), we get

$$\Delta\mathbf{S} \equiv \phi(\mathbf{S}') - \phi(\mathbf{S}) = \sum_{k=m}^{\infty} \gamma_k(S'_k - S_k). \tag{21c}$$

The images of $\mathbf{S}$ and $\mathbf{S}'$ after the nth time-step $f^n:\Omega\mapsto\Omega$ are, in a short-hand notation,

$$f^n(\mathbf{S}) = (\zeta_1\zeta_2\zeta_3\cdots\zeta_{p_n-1}\zeta_{p_n}\zeta_{p_n+1}\cdots)$$

and

$$f^n(\mathbf{S}') = (\zeta_1\zeta_2\zeta_3\cdots\zeta_{p_n-1}\zeta'_{p_n}\zeta'_{p_n+1}\cdots),$$

where $\zeta_{p_n}\neq\zeta'_{p_n}$, with $p_n=p_n(m)$ being a function, of the initial error position m in (21). From (21c), we have that

$$\Delta \mathbf{S} = \gamma_m \mu_m + R_m,$$

where $\mu_m \equiv S'_m - S_m = \pm 1$ and $R_m \equiv \Sigma_{k=m+1}^{\infty} \gamma_k \mu_k$. Now, by means of (10b) and (11) follows that $|R_m| \leqslant \Sigma_{k=m+1}^{\infty} \gamma_k = h^m$. So that $R_m \sim \mathcal{O}(h^m)$ which gives

$$\Delta \mathbf{S} = h^m (h^{-1} - 1) \mu_m (1 + \mathcal{O}(h)).$$

An analogous expression is obtained for $\Delta f^n \equiv f^n(\mathbf{S}) - f^n(\mathbf{S}')$ giving

$$\Delta f^n = h^{p_n(m)} (h^{-1} - 1) \mu_{p_n(m)} (1 + \mathcal{O}(h)).$$

Therefore,

$$\delta_h f^n(\mathbf{S}) = \lim_{m \to \infty} \frac{\Delta f^n}{\Delta \mathbf{S}} = \lim_{m \to \infty} \mu_m \mu_{p_n(m)} h^{p_n(m) - m} (1 + \mathcal{O}(h)).$$

If the limit exists; we obtain

$$\delta_h f^n(\mathbf{S}) = \pm h^{-\Lambda_n(\mathbf{S})} (1 + \mathcal{O}(h)),$$

where

$$\Lambda_n(\mathbf{S}) \equiv \lim_{m \to \infty} (m - p_n(m)),$$

which, if exists, it is the error propagation at time n as seen through the embedding (9).

Inserting the above result into (13) yields

$$\lambda_D(\mathbf{S}) = \lim_{n \to \infty} \frac{\Lambda_n(\mathbf{S})}{n}, \tag{22}$$

which, if it exists, equals (20).

Remark 5.4: As observed in Remark 3.1(ii), the metric and derivative definitions of Lyapunov exponents do not depend on the specific scale used. The velocity of leftward propagation of errors should be a dynamical effect independent of the scale, which is exactly what turns out from above, whence the coincidence of (20) and (22).

B. Topological entropy

Consider Eqs. (18) and let us define

$$L_n^*(\mathbf{S}, \mathbf{S}') \equiv \max_{0 \leqslant k \leqslant n} L_k(\mathbf{S}, \mathbf{S}'). \tag{23}$$

From (14) it follows that

$$\mathcal{B}_\beta(\mathbf{S}, \varepsilon, n) = \{\mathbf{S}' \in \Omega | \beta^{q - L_n^*(\mathbf{S}, \mathbf{S}')} < \varepsilon\}.$$

In the particular case where the dynamics (1) is such that L_n^* is independent of $\mathbf{S}$ and $\mathbf{S}'$ let us define

$$\theta_n \equiv L_n^*(\mathbf{S}, \mathbf{S}') \tag{24}$$

and take $\varepsilon = \beta^p$. From (6) and (14) it follows that

$$\mathcal{B}_\beta(\mathbf{S}, \beta^p, n) = \{\mathbf{S}' \in \Omega | \beta^q < \beta^{p + \theta_n}\} = \{\mathbf{S}' \in \Omega | d_\beta(\mathbf{S}, \mathbf{S}') \leqslant \beta^{p + \theta_n + 1}\} = \mathcal{N}(\mathbf{S}, r_{n,p}),$$

where

$$r_{n,p} = p + \theta_n + 1.$$

Since $\mathcal{N}(\mathbf{S}, r_{n,p})$ are elements of the base (4), it follows that

$$E(n,\beta^p) = \{\mathbf{S} \in \Omega | S_k = 0 \ \forall \ k > r_{n,p}\}$$

is an (n,β^p)-spanning set with cardinality $2^{r_{n,p}}$; which, by construction, is minimal. From (16) we obtain

$$h_{\text{top}}(f) = \lim_{p\to\infty} \limsup_{n\to\infty} \frac{r_{n,p}}{n}.$$

So that,

$$h_{\text{top}}(f) = \limsup_{n\to\infty} \frac{\theta_n}{n}. \tag{25}$$

In the general case (24) is not valid and the behavior of $L_n^*(\mathbf{S},\mathbf{S}')$ depends on the fine details of the dynamics (1). In such cases, it is still possible to set an upper bound to the value of the topological entropy. Let us define

$$\eta(n) \equiv \max_{\mathbf{s},\mathbf{s}'} L_n^*(\mathbf{S},\mathbf{S}'),$$

with $\mathbf{S}$ and $\mathbf{S}'$ subject to the constraint (18a). Then [using (6) and (14)],

$$\mathcal{B}_\beta(\mathbf{S},\beta^p,n) = \{\mathbf{S}' \in \Omega | \beta^{q-L_n^*(\mathbf{S},\mathbf{S}')} < \beta^p\} \supseteq \{\mathbf{S}' \in \Omega | \beta^{q-\eta(n)} < \beta^p\} \supseteq \{\mathbf{S}' \in \Omega | d_\beta(\mathbf{S},\mathbf{S}') \leqslant \beta^{p+\eta(n)+1}\} \supseteq \mathcal{N}(\mathbf{S}, t_{n,p}),$$

where

$$t_{n,p} = p + \eta(n) + 1.$$

Now

$$E(n,\beta^p) = \{\mathbf{S} \in \Omega | S_k = 0 \ \forall \ k > t_{n,p}\},$$

is again an (n,β^p)-spanning set with cardinality $2^{t_{n,p}}$, but we cannot assure that it is minimal. So, from (16) we obtain

$$h_{\text{top}}(f) \leqslant \limsup_{n\to\infty} \frac{\eta(n)}{n},$$

which assures that, if $\eta(n)$ does not increase as n or faster, the topological entropy vanishes.

VI. EXAMPLES

A. The shift map

We begin applying the ideas developed so far to the v-shift map σ_v defined by

$$\sigma_v(S_1 S_2 S_3 \cdots) = (S_{1+v} S_{2+v} S_{3+v} \cdots).$$

Consider two points $\mathbf{S},\mathbf{S}' \in \Omega$ with distance $d_\beta(\mathbf{S},\mathbf{S}') = \beta^q$. Applying σ_v^n we obtain

$$d_\beta(\mathbf{S}(n),\mathbf{S}'(n)) = \beta^{q-vn}.$$

According to (18), (23) and (24), we see that $\theta_n = vn$; thus, from (25) we have

TABLE I. Boolean rules.

S_{i-1}	S_i	S_{i+1}	30	73	90	167
0	0	0	0	1	0	1
0	0	1	1	0	1	1
0	1	0	1	0	0	1
0	1	1	1	1	1	0
1	0	0	1	0	1	0
1	0	1	0	0	0	1
1	1	0	0	1	1	0
1	1	1	0	0	0	1

$$h_{\mathrm{top}}(f) = \upsilon > 0.$$

It is also evident that the topological entropy coincides with the Lyapunov exponents $\lambda_M = \lambda_D$ [see Eqs. (20) and (22)].

B. Networks with three inputs

We study now the evolution rule (1) in the case of interactions involving three nearest neighbors and impose periodic boundary conditions; specifically

$$S_i(n+1) = f(S_{i-1}(n), S_i(n), S_{i+1}(n)) \quad \text{for } i = 2,3,\ldots,N-1, \tag{26a}$$

$$S_1(n+1) = f(S_N(n), S_1(n), S_2(n)), \tag{26b}$$

and

$$S_N(n+1) = f(S_{N-1}(n), S_N(n), S_1(n)), \tag{26c}$$

where the transfer function f is the same for all the bits.

Due to the periodic boundary conditions, the infinite limit of these networks requires the symmetric metrics discussed in Remark 2.4(ii): this context accommodates errors propagating both to the left and to the right.

We are going to study the Boolean rules numbered 30, 73, 90, and 167 according to Wolfram's which[5–7] which we explicitly list in Table I. The first three columns give the values of three adjacent bits and the remaining columns show the corresponding bits for the two rules. We stress that the rule 90 is the XOR rule in the two adjacent bits and it is well known as "chaotic" in Wolfram's terminology.

We have considered an automaton consisting of $N = 1000$ bits and start with a random initial state. After a transient of length N^2 we let the dynamics reach a state $\mathbf{S}$. Then we choose a state $\mathbf{S}'$ which differs from $\mathbf{S}$ in the 499, 500, and 501 bits, and start to measure the speed of error profile Λ_n/n and the speed of damage spreading $d_H(\mathbf{S}(\mathbf{n}), \mathbf{S}'(\mathbf{n}))/n$. The main results are plotted in Figs. 2–4.

Figure 2 shows the spread of errors as the states $\mathbf{S}$, $\mathbf{S}'$ evolve in time, each cross corresponding to a different bit in the two configurations.

Figure 3 shows the speed of error profile as a function of time. According to (20) and (22), they exhibit, for $n \gg 1$ a Lyapunov exponent $\lambda = 1$ for all the rules but the rule 73 which shows $\lambda = 0$. The same conclusions can be extracted from the topological entropy.

Figure 4 shows the evolution in time of the speed of damage spreading. One can see that no clear behavior emerges for $n \gg 1$ that may help evaluate the damage spreading according to (3); moreover, even when, according to the Lyapunov and entropic analysis, the behavior is complex as is the case with rule 90, there is instead a clear tendency of the damage spreading to go to zero.

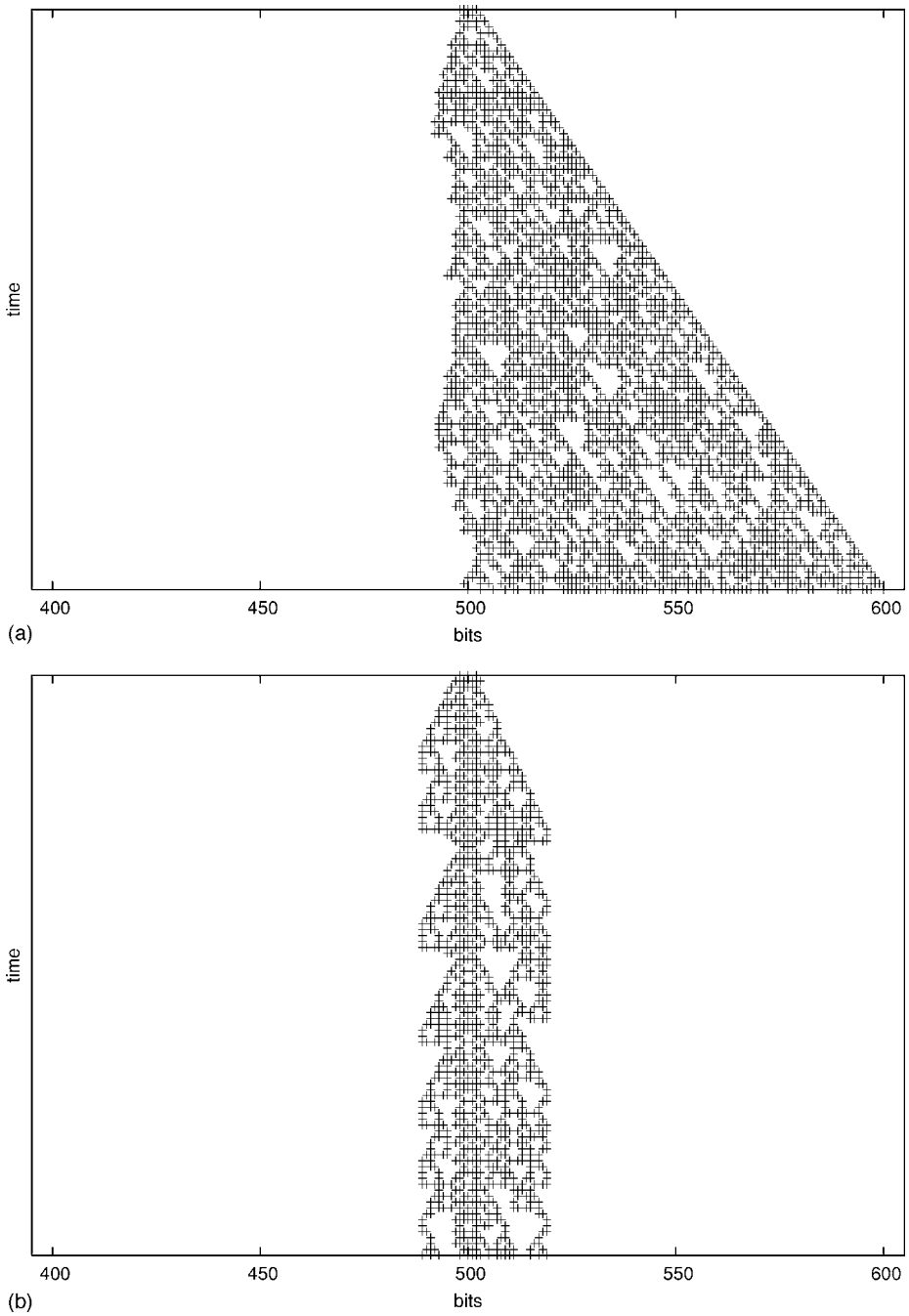


FIG. 2. (a) Spread of errors for rule 30. Starting from two states **S**, **S**′ which differ in the 499, 500, and 501 bits. A cross is plotted when the bits are different. Time goes from top to bottom for 100 iterations. (b) Spread of errors for rule 73. Starting from two states **S**, **S**′ which differ in the 499, 500, and 501 bits. A cross is plotted when the bits are different. Time goes from top to bottom for 100 iterations. (c) Spread of errors for rule 90. Starting from two states **S**, **S**′ which differ in the 499, 500, and 501 bits. A cross is plotted when the bits are different. Time goes from top to bottom for 100 iterations. (d) Spread of errors for rule 167. Starting from two states **S**, **S**′ which differ in the 499, 500, and 501 bits. A cross is plotted when the bits are different. Time goes from top to bottom for 100 iterations.

It is important to observe from Fig. 2(b) that rule 73 shows a complex behavior. However it is localized in the sense that it does not grow with N, so for $N\to\infty$, **S** and **S**′ are on a periodic attractor and so the dynamics is not chaotic. In contrast the other rules, which are chaotic, spread the errors along all the bits.

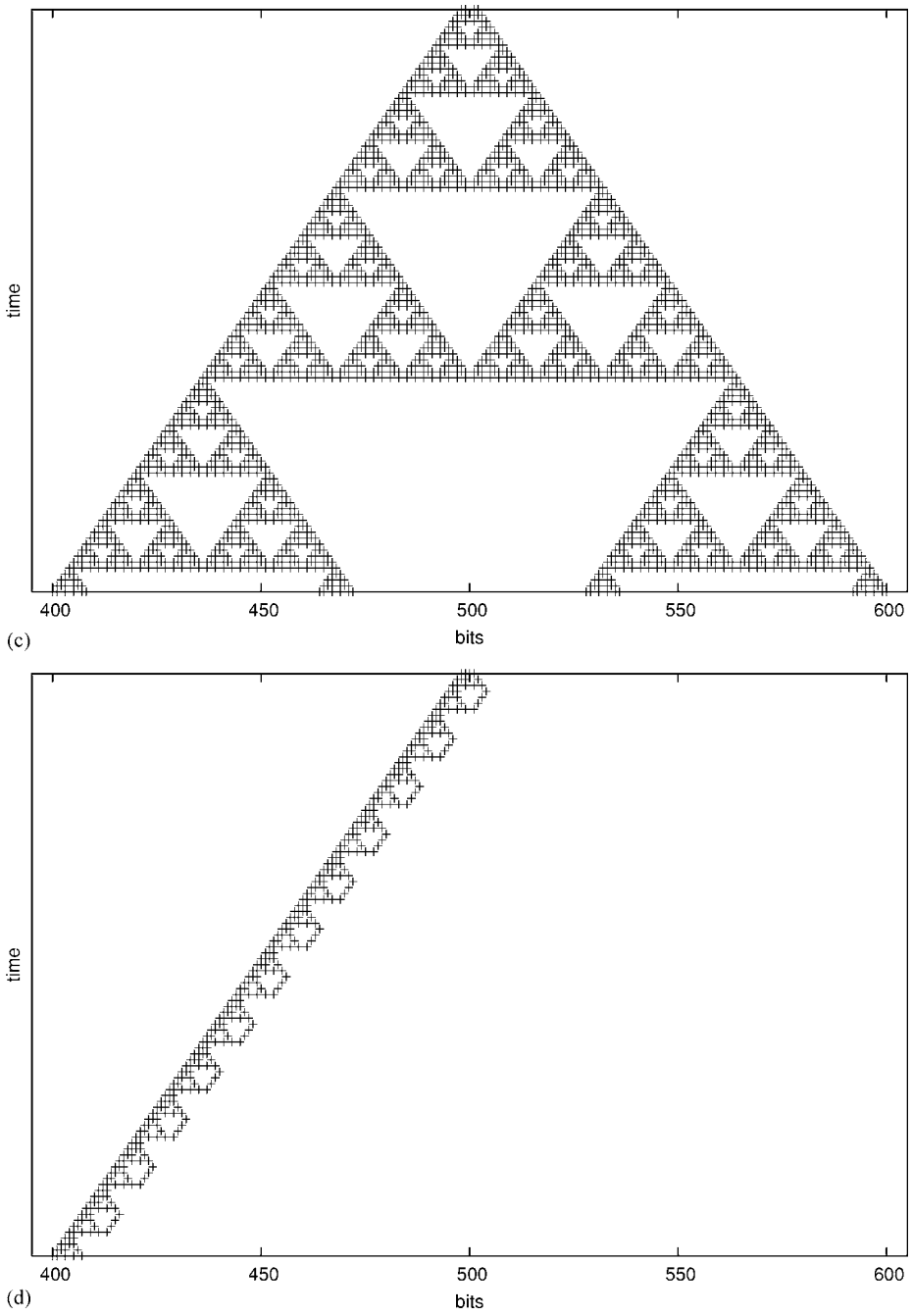


FIG. 2. (*Continued*).

VII. CONCLUSIONS

We have endowed the phase space of binary variables with the topology of the Cantor set in the limit when the number of variables N goes to infinity. This embedding of the phase space permits us to understand the dynamical behavior of binary dynamical systems, much on the same footing as the ones over differentiable manifolds providing a mathematically solid framework for discrete systems. One of the advantages of this approach is the fact that the distance function (5)

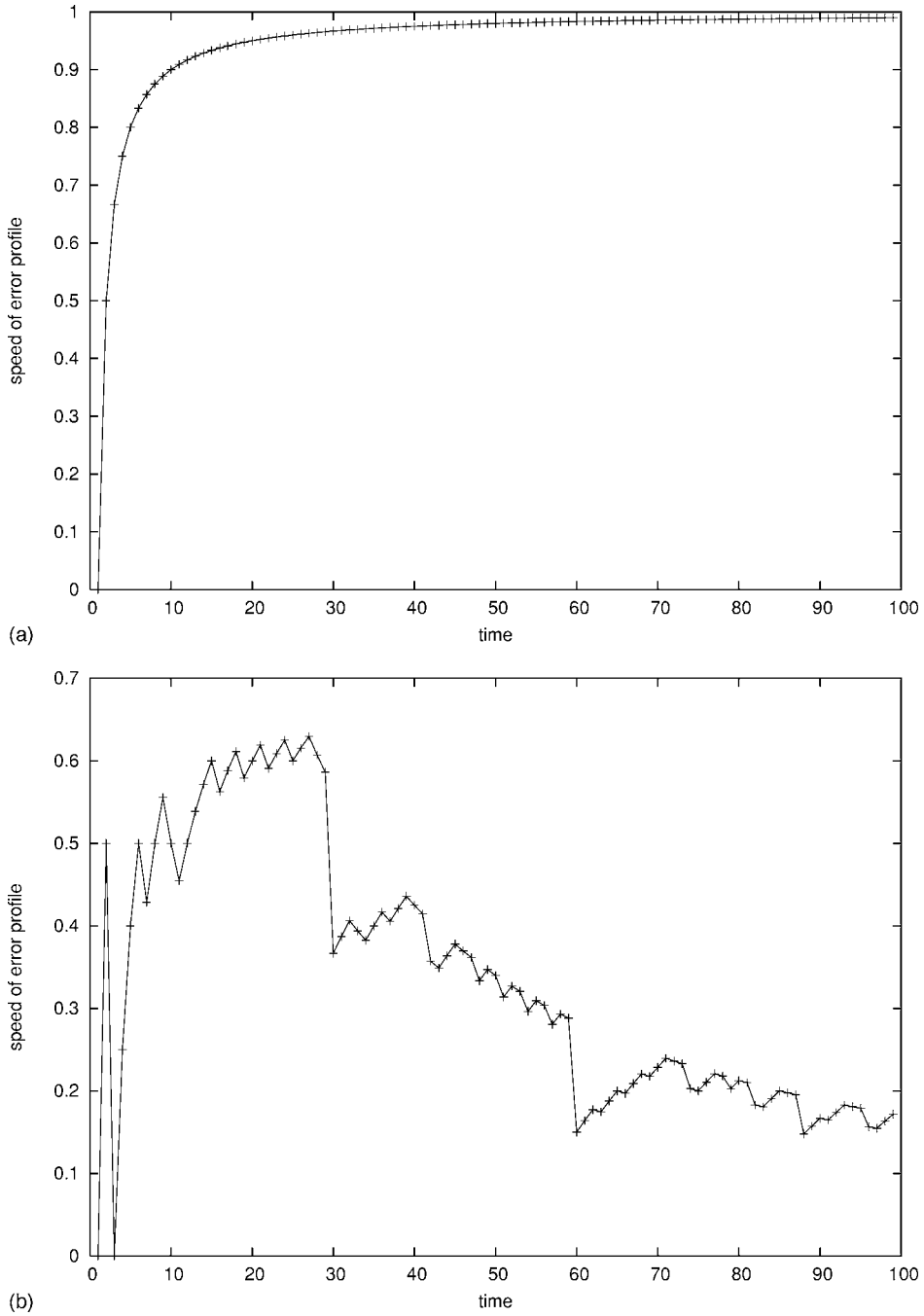
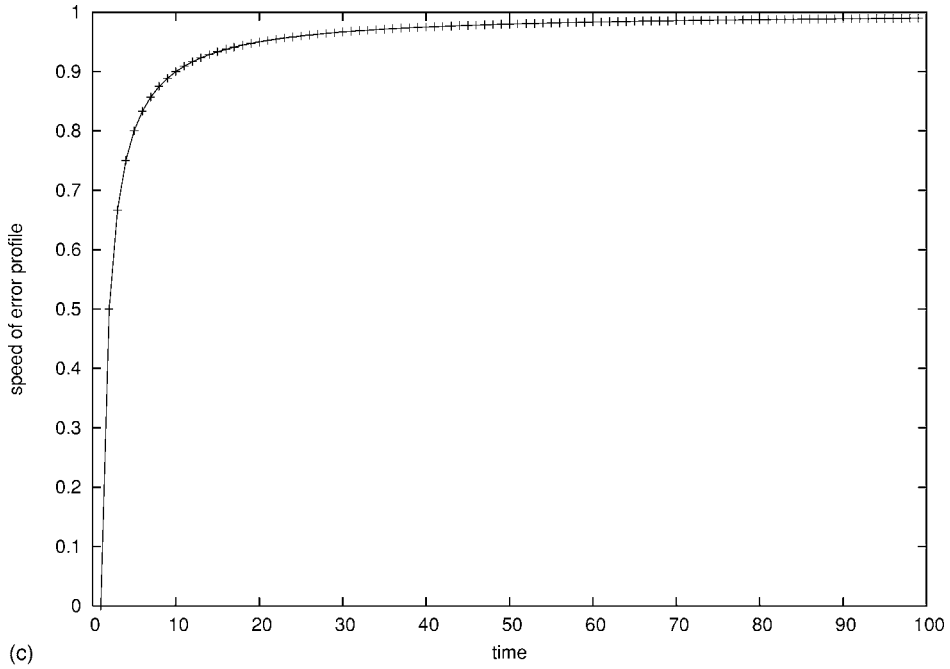
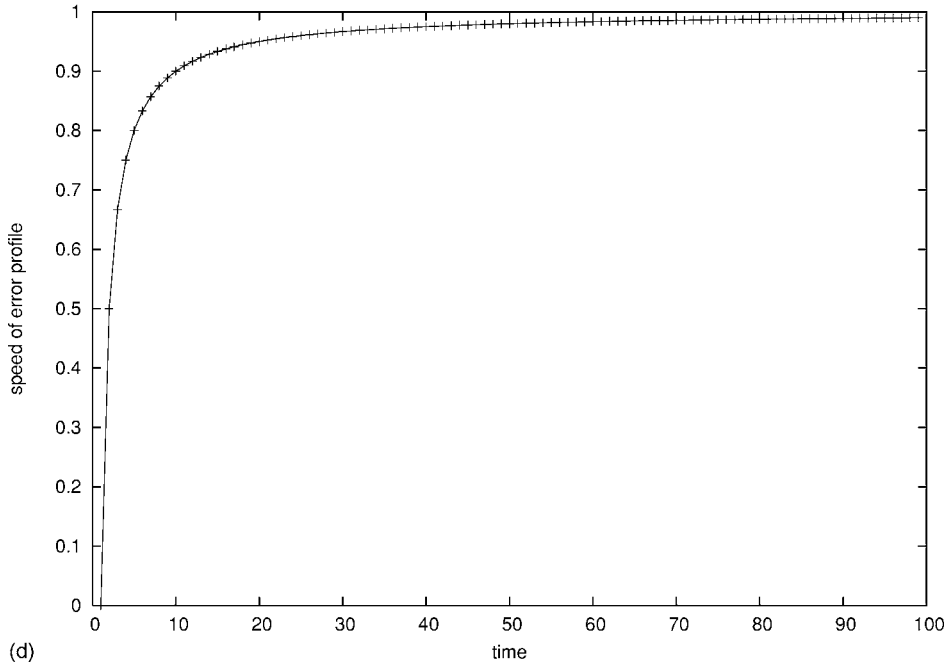


FIG. 3. (a) Evolution of the speed of error profile Λ_n/n in function of time for rule 30 showing for $n \gg 1$ a Lyapunov exponent $\lambda=1$. (b) Evolution of the speed of error profile Λ_n/n in function of time for rule 73 showing for $n \gg 1$ a Lyapunov exponent $\lambda=0$. (c) Evolution of the speed of error profile Λ_n/n in function of time for rule 90 showing for $n \gg 1$ a Lyapunov exponent $\lambda=1$. (d) Evolution of the speed of error profile Λ_n/n in function of time for rule 167 showing for $n \gg 1$ a Lyapunov exponent $\lambda=1$.

is well defined for finite or infinite N. Despite being the Hamming distance (2), the most natural distance function over the space of binary variables Ω, it has the disadvantage of being divergent as $N \to \infty$ on states differing on an infinite number of binary variables.



(c)



(d)

FIG. 3. (*Continued*).

We have formalized the notion of Lyapunov exponents for discrete systems in two related ways: by resorting to metrics compatible with the Cantor topology and by suitably embedding the Cantor structure into a differentiable one.

Guided by the connections between Lyapunov exponents and topological entropy in continuous system, we have also computed the topological entropy and compared it with the Lyapunov exponents calculated according to the given prescriptions. This has been done in Sec. V where we

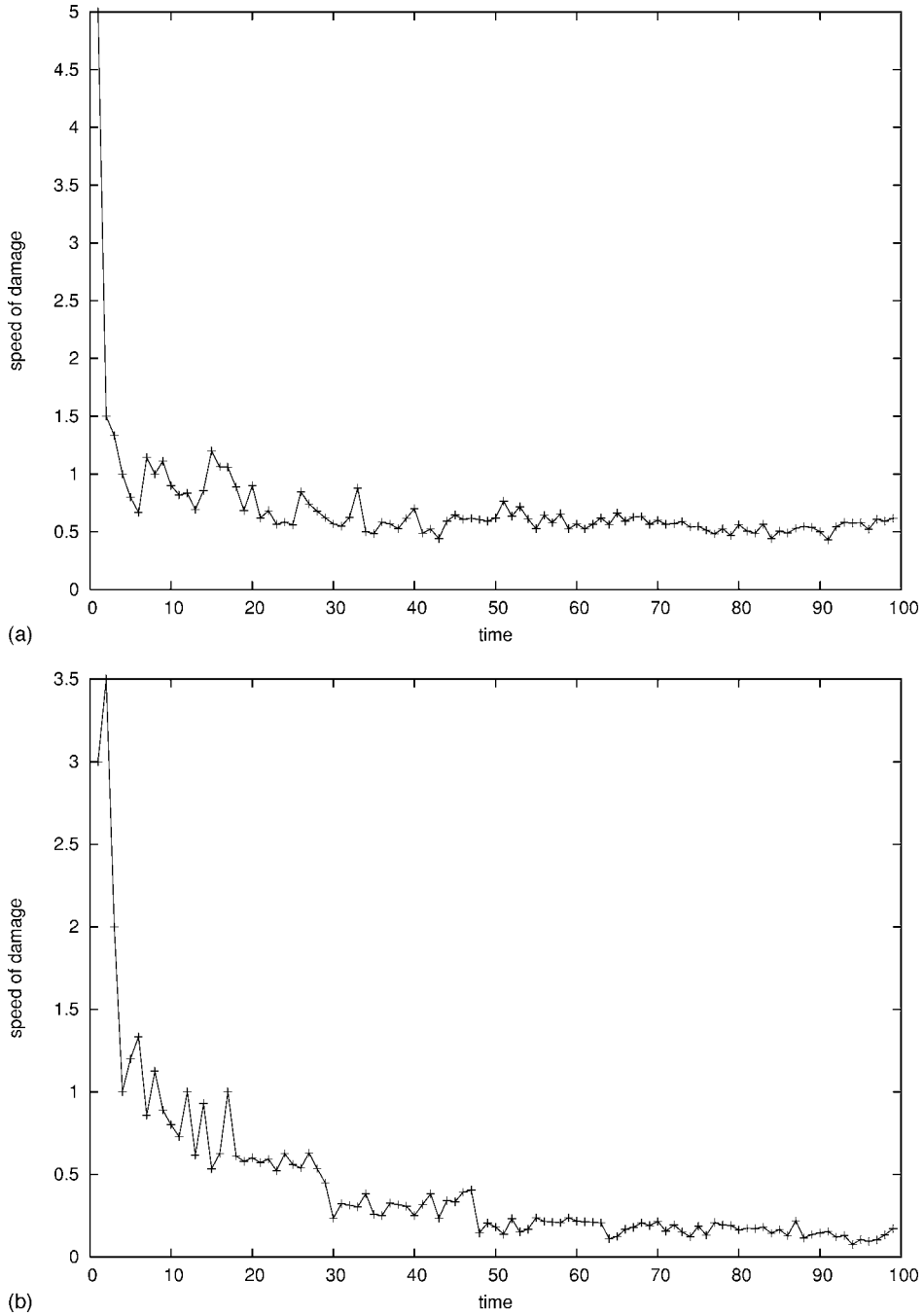
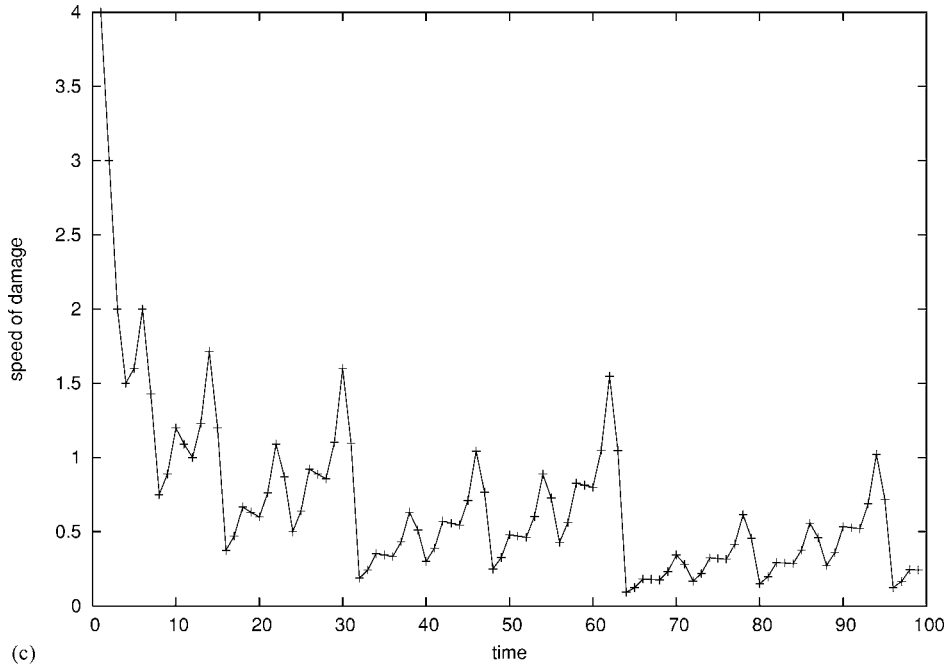
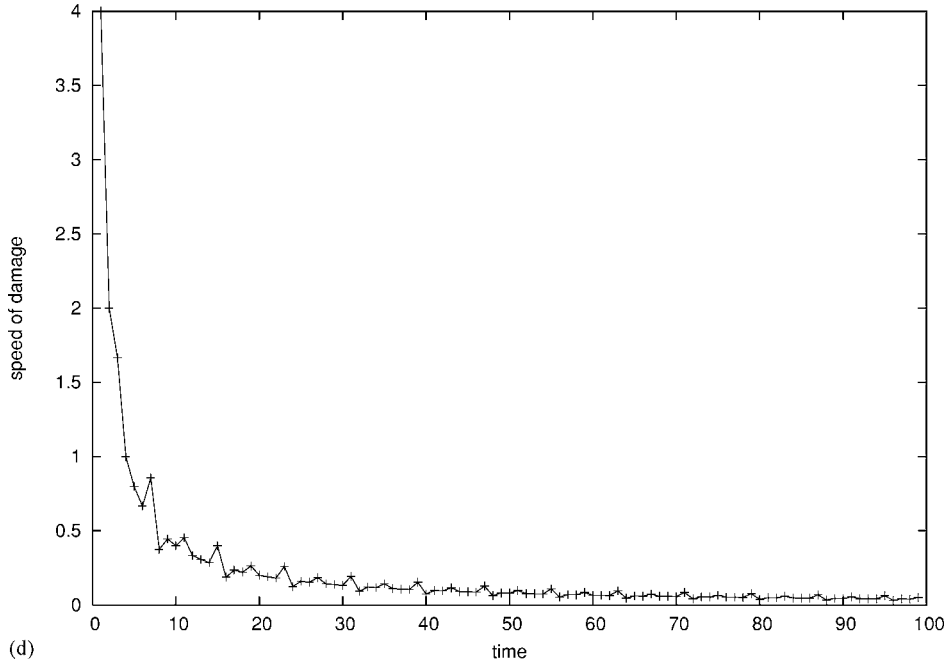


FIG. 4. (a) Evolution of the speed of damage spreading $d_H(\mathbf{S}(\mathbf{n}),\mathbf{S}'(\mathbf{n}))/n$ in function of time for rule 30. There is not a clear behavior for $n \gg 1$ which help to make an evaluation of the damage spreading. (b) Evolution of the speed of damage spreading $d_H(\mathbf{S}(\mathbf{n}),\mathbf{S}'(\mathbf{n}))/n$ in function of time for rule 73. There is not a clear behavior for $n \gg 1$ which help to make an evaluation of the damage spreading. (c) Evolution of the speed of damage spreading $d_H(\mathbf{S}(\mathbf{n}),\mathbf{S}'(\mathbf{n}))/n$ in function of time for rule 90. There is not a clear behavior for $n \gg 1$ which help to make an evaluation of the damage spreading and is tending to zero for a complex rule. (d) Evolution of the speed of damage spreading $d_H(\mathbf{S}(\mathbf{n}),\mathbf{S}'(\mathbf{n}))/n$ in function of time for rule 167. There is not a clear behavior for $n \gg 1$ which help to make an evaluation of the damage spreading and is tending to zero for a rule which has a positive Lyapunov exponent in our scheme.

related both notions to the concept of error profile which is a phenomenological quantity that can be accessed numerically and has a self-evident physical interpretation. We have illustrated all these concepts by examples in Sec. VI.



(c)



(d)

FIG. 4. (*Continued*).

Further points that deserve to be studied are

(i) The problem of the concept of a derivative. Here we have introduced it with the aid of the homeomorphism (10) which is compatible with the metrics (5). However, from the mathematical point of view it would be better if one could construct a meaningful "discrete derivative" which is homeomorphism free.

(ii) The construction of an invariant measure for the definition of the metric entropy (17), as sketched in Remark 4.1.

(iii) The application of the methods presented above to the treatment of Kauffman's models of cellular automata with connectivity K and random couplings which show a transition from an ordered phase for $K \leqslant 2$ where the length of the attractors grows as $\sqrt{N}$, to a disordered one, termed chaotic, for $K > 2$ with lengths growing as e^N.[3,5,18]

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New four-dimensional solutions of the Jacobi equations for Poisson structures

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A four-dimensional family of skew-symmetric solutions of the Jacobi equations for Poisson structures is characterized. As a consequence, previously known types of Poisson structures found in a diversity of physical situations appear to be obtainable as particular cases of new family of solutions. Additionally, it is possible to apply constructive methods for the explicit determination of fundamental properties of those solutions, such as their Casimir invariants, symplectic structure and the algorithm for the reduction to the Darboux canonical form, which have been reported only for a limited sample of known finite-dimensional Poisson structures. Moreover, the results developed are valid globally in phase space, thus ameliorating the usual scope of Darboux theorem which is of local nature. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2161804]

I. INTRODUCTION

Poisson structures[1,2] are present in many different domains of mathematical physics, such as fluid dynamics,[3] plasma physics,[4] field theory,[5] continuous media,[6] etc. In particular, finite-dimensional Poisson structures (to which this work is devoted) are relevant in the study of very different kinds of nonlinear systems, including population dynamics,[7–12] mechanics,[13–16] electromagnetism,[17] optics,[18] or plasma physics,[19] to cite a sample. The association of a finite-dimensional Poisson structure to a differential system (which is still an open problem[16,20–22]) is not only mathematically appealing, but also very useful through the use of a plethora of specialized techniques which include the development of perturbative solutions,[17] numerical algorithms,[23] stability analysis by means of the energy-Casimir[24] and energy-momentum[25] methods, characterization of invariants,[26] reductions,[2,27] analysis of integrability properties,[28] establishment of variational principles,[29] study of bifurcation properties and chaotic behavior,[18,30] etc.

When expressed in terms of a system of local coordinates on an n-dimensional manifold, finite-dimensional Poisson structures take the form

$$\dot{x}_i = \sum_{j=1}^{n} J_{ij}\partial_j H, \quad i = 1, \ldots, n. \tag{1}$$

Here and in what follows $\partial_j \equiv \partial/\partial x_j$. The C^1 real-valued function $H(x)$ in (1) is a constant of motion of the system playing the role of Hamiltonian. The $J_{ij}(x)$, called structure functions, are also C^1 and real valued and constitute the entries of an $n \times n$ structure matrix $\mathcal{J}$. The $J_{ij}(x)$ are characterized by two properties. The first one is that they are skew-symmetric,

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$$J_{ij} = -J_{ji} \quad \text{for all } i,j. \tag{2}$$

And second, they are solutions of the Jacobi equations,

$$\sum_{l=1}^{n} (J_{il}\partial_l J_{jk} + J_{kl}\partial_l J_{ij} + J_{jl}\partial_l J_{ki}) = 0, \tag{3}$$

where indices i,j,k run from 1 to n in Eqs. (2) and (3).

One of the reasons justifying the importance of the Poisson representation is the local equivalence between Poisson systems and classical Hamiltonian systems, as stated by Darboux theorem[1,2] which demonstrates that if an n-dimensional Poisson manifold has constant rank of value $2r$ everywhere, then at each point of the manifold there exist local coordinates $(p_1,\ldots,p_r,q_1,\ldots,q_r,z_1,\ldots,z_{n-2r})$ in terms of which the equations of motion become

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1,\ldots,r,$$

$$\dot{z}_j = 0, \quad j = 1,\ldots,n-2r.$$

As mentioned above, the problem of recasting a given vector field not explicitly written in the form (1) in terms of a finite-dimensional Poisson system is an open issue of fundamental importance in this context to which important efforts have been devoted in past years in a variety of approaches and situations.[7–22] This explains, together with the intrinsic mathematical interest of the problem, the permanent attention deserved in the literature by the obtainment and classification of skew-symmetric solutions of the Jacobi equations.[7–22,31–38] Given that Eqs. (3) constitute a set of coupled nonlinear partial differential equations, the characterization of solutions of (2) and (3) has proceeded by means of either suitable *ansatzs*[7–11,32,37] or through a diversity of other approaches.[12–16,20–22,31,38] These efforts have led to the determination of certain families of solutions of increasing nonlinearity such as the constant ones (of which the symplectic matrices are just a particular case), as well as linear[2,33] (i.e., Lie-Poisson), affine-linear,[34] quadratic,[7–11,15,35,36] and cubic[37] structures, together with solutions which comprise arbitrary functions.[12–14,16,20–22,31,32,38] Simultaneously, the growing complexity of the Jacobi equations (3) as the dimension n increases has determined that the analysis is often focused on three-dimensional solutions,[9,10,12,20,21,32,37,38] while the characterization of families of dimensions four,[13] five,[14] six,[17] etc., is less frequent. In addition, some wide families of n-dimensional solutions have also been analyzed in the literature.[8,11,31,33–36]

In this work a four-dimensional family of solutions of the Jacobi equations (3) is characterized. This contribution presents several interesting features. First, it is worth noting that previously known types of Poisson structures appearing in a diversity of physical situations and systems can be seen to be obtainable as particular cases of the family of solutions, as it will be seen in the examples section. Second, in spite of their generality the solutions to be considered in what follows are amenable to explicit and detailed analysis, since it is possible to characterize globally their Casimir invariants and symplectic structure, as well as to globally provide the reduction to the Darboux canonical form. This constitutes a significant amelioration of the usual scope of Darboux theorem, which does only guarantee in principle a local reduction.[1,2] In addition, the achievement of such reduction is relevant as far as the explicit determination of the Darboux coordinates is often a complicated task, only known for a limited sample of finite-dimensional Poisson structures.[2,8,27,31,38]

The structure of the paper is as follows. In Sec. II the solutions are characterized. The symplectic structure and the constructive reduction to the Darboux canonical form are investigated in Sec. III. Examples and comments on the relationship with some previously known results are provided in Sec. IV. The work concludes in Sec. V with some final remarks.

II. CHARACTERIZATION OF THE FAMILY OF SOLUTIONS

We begin with one of the main results.

Theorem 2.1: Consider the family of functions of the form

$$J_{ij}(x) = \sigma_{ij}\eta(x)\psi_i(x_i)\psi_j(x_j)\sum_{k,l=1}^{4}\epsilon_{ijkl}\phi_l(x_l), \quad i,j=1,\ldots,4 \tag{4}$$

defined in an open domain $\Omega \subset \mathbb{R}^4$, where ϵ_{ijkl} denotes the Levi-Civita symbol and such that

(a) Constants $\sigma_{ij} \in \mathbb{R}$ are defined for every pair (i,j), $i \neq j$.
(b) $\sigma_{ij} = \sigma_{ji}$ for every pair (i,j), $i \neq j$.
(c) $\sigma_{ij} \neq 0$ for at least one pair (i,j), $i \neq j$.
(d) $\eta(x)$, $\psi_i(x_i)$, and $\phi_i(x_i)$ are $C^1(\Omega)$ functions of their respective arguments for every i.
(e) $\eta(x)$ and $\psi_i(x_i)$ are nonvanishing in Ω for every i.
(f) The differences $[\phi_i(x_i) - \phi_j(x_j)]$ are nonvanishing in Ω for every pair (i,j), $i \neq j$.

Then the set of functions $J_{ij}(x)$ defined in (4) constitutes a skew-symmetric solution of the four-dimensional Jacobi identities

$$\sum_{l=1}^{4}(J_{il}\partial_l J_{jk} + J_{kl}\partial_l J_{ij} + J_{jl}\partial_l J_{ki}) = 0, \quad i,j,k=1,\ldots,4 \tag{5}$$

and therefore $\mathcal{J}=(J_{ij})$ is a four-dimensional structure matrix, if and only if

$$\sigma_{12}\sigma_{34} = \sigma_{13}\sigma_{24} = \sigma_{14}\sigma_{23}. \tag{6}$$

Proof: Consider first functions (4) in the case $\eta=1$. Substitution of (4) in Eq. (5) of indexes (i,j,k) leads after some algebra to

$$\begin{aligned}
\sum_{l=1}^{4}(J_{il}\partial_l J_{jk} + J_{kl}\partial_l J_{ij} + J_{jl}\partial_l J_{ki}) &= \psi_i\psi_j\psi_k \sum_{r_1,r_2,s_1,s_2=1}^{4}\{(\sigma_{ij}\sigma_{jk}\epsilon_{ijr_1r_2}\epsilon_{jks_1s_2} + \sigma_{kj}\sigma_{ij}\epsilon_{kjr_1r_2}\epsilon_{ijs_1s_2}) \\
&\quad \times(\partial_j\psi_j)\phi_{r_2}\phi_{s_2} + (\sigma_{ki}\sigma_{ij}\epsilon_{kir_1r_2}\epsilon_{ijs_1s_2} + \sigma_{ji}\sigma_{ki}\epsilon_{jir_1r_2}\epsilon_{kis_1s_2})(\partial_i\psi_i)\phi_{r_2}\phi_{s_2} \\
&\quad + (\sigma_{ik}\sigma_{jk}\epsilon_{ikr_1r_2}\epsilon_{jks_1s_2} + \sigma_{jk}\sigma_{ki}\epsilon_{jkr_1r_2}\epsilon_{kis_1s_2})(\partial_k\psi_k)\phi_{r_2}\phi_{s_2} \\
&\quad + (\sigma_{is_2}\sigma_{jk}\epsilon_{is_2r_1r_2}\epsilon_{jks_1s_2} + \sigma_{ks_2}\sigma_{ij}\epsilon_{ks_2r_1r_2}\epsilon_{ijs_1s_2} \\
&\quad + \sigma_{js_2}\sigma_{ki}\epsilon_{js_2r_1r_2}\epsilon_{kis_1s_2})\psi_{s_2}\phi_{r_2}(\partial_{s_2}\phi_{s_2})\} \\
&= \psi_i\psi_j\psi_k \sum_{r_1,r_2,s_1,s_2=1}^{4}\{(\sigma_{is_2}\sigma_{jk}\delta_{jks_1s_2}^{is_2r_1r_2} + \sigma_{ks_2}\sigma_{ij}\delta_{ijs_1s_2}^{ks_2r_1r_2} \\
&\quad + \sigma_{js_2}\sigma_{ki}\delta_{kis_1s_2}^{is_2r_1r_2})\psi_{s_2}\phi_{r_2}(\partial_{s_2}\phi_{s_2})\}
\end{aligned} \tag{7}$$

where the δ symbol denotes the generalized Kronecker delta according to its standard definition, namely, given q superindexes $(i_1,\ldots,i_q)$ and q subindexes $(j_1,\ldots,j_q)$ all of them taking values in the range $(1,\ldots,n)$, then $\delta_{j_1\cdots j_q}^{i_1\cdots i_q}$ is defined by the properties: (a) it is totally antisymmetric in the superindexes; (b) it is totally antisymmetric in the subindexes; (c) if the superindexes are all different (this is, $i_{a_1} \neq i_{a_2}$ if $a_1 \neq a_2$) and the subindexes are a permutation of the superindexes, then $\delta_{j_1\cdots j_q}^{i_1\cdots i_q}$ takes the value $+1$ (respectively, -1) if $(i_1,\ldots,i_q)$ and $(j_1,\ldots,j_q)$ are permutations of the same (of different) sign; (d) the value of $\delta_{j_1\cdots j_q}^{i_1\cdots i_q}$ is zero otherwise. Consequently, it can be verified that the expression in (7) vanishes if two of the three indexes (i,j,k) are equal. Consider then the case in which i, j, and k are different. If m is the integer, $1 \leqslant m \leqslant 4$, such that (i,j,k,m) is a permutation of $(1,2,3,4)$, we arrive at

$$\sum_{l=1}^{4} (J_{il}\partial_l J_{jk} + J_{kl}\partial_l J_{ij} + J_{jl}\partial_l J_{ki})$$
$$= \psi_i\psi_j\psi_k\psi_m(\partial_m\phi_m)\{\sigma_{im}\sigma_{jk}(\phi_k - \phi_j) + \sigma_{km}\sigma_{ij}(\phi_j - \phi_i) + \sigma_{jm}\sigma_{ki}(\phi_i - \phi_k)\}$$
$$= \psi_i\psi_j\psi_k\psi_m(\partial_m\phi_m)\{(\sigma_{jm}\sigma_{ki} - \sigma_{km}\sigma_{ij})\phi_i + (\sigma_{km}\sigma_{ij} - \sigma_{im}\sigma_{jk})\phi_j + (\sigma_{im}\sigma_{jk} - \sigma_{jm}\sigma_{ki})\phi_k\}. \tag{8}$$

Now let p, where $0 \leqslant p \leqslant 4$, be the number of functions ϕ_i which have constant value everywhere in Ω. Taking into account hypothesis (f) of the theorem, there are five different possibilities to be examined for Eq. (8).

$p=0$, in this case it is straightforward that (8) vanishes if and only if (6) holds.

$p=1$, the analysis and the result are similar to those of the case $p=0$.

$p=2$, assume without loss of generality that ϕ_k and ϕ_m are constant in Ω while ϕ_i and ϕ_j are not. Then expression (8) vanishes if and only if

$$\sigma_{im}\sigma_{jk} - \sigma_{jm}\sigma_{ik} = (\sigma_{im}\sigma_{jk} - \sigma_{ij}\sigma_{km})\phi_k + (\sigma_{ij}\sigma_{km} - \sigma_{im}\sigma_{jk})\phi_m = 0.$$

Given that $\phi_k \neq \phi_m$, these equations are equivalent to (6).

$p=3$, suppose without loss of generality that ϕ_i, ϕ_j, and ϕ_k are constant in Ω, while ϕ_m is not. Then expression (8) is equal to zero if and only if

$$\{(\sigma_{jm}\sigma_{ki} - \sigma_{km}\sigma_{ij})\phi_i + (\sigma_{km}\sigma_{ij} - \sigma_{im}\sigma_{jk})\phi_j + (\sigma_{im}\sigma_{jk} - \sigma_{jm}\sigma_{ki})\phi_k\}\partial_m\phi_m = 0.$$

Taking into account that $\partial_m\phi_m$ does not vanish everywhere in Ω, and that ϕ_i, ϕ_j, and ϕ_k are arbitrary [as far as hypothesis (f) of the theorem is respected] the outcome is again that (6) is necessary and sufficient for the vanishing of (8).

$p=4$, Eqs. (8) vanish because $\partial_m\phi_m=0$ for all possible values of m. This is to be expected because in this case we are dealing with a separable structure.[31]

Then conditions (6) are necessary and sufficient for the vanishing of (8) when $0 \leqslant p \leqslant 3$. For $p=4$ expression (8) is always zero. This concludes the analysis of the case $\eta=1$. Let us now turn to the general form (4) of the solution, namely to general η. To analyze this case, consider an arbitrary four-dimensional skew-symmetric solution $J_{ij}(x)$ of the Jacobi equations. If such solution is multiplied by a $C^1(\Omega)$ function $\eta(x)$ the resulting set of functions $J^*_{ij}(x) = \eta(x)J_{ij}(x)$ will be a skew-symmetric solution of (5) if and only if η verifies

$$(J_{im}J_{jk} + J_{km}J_{ij} + J_{jm}J_{ki})\partial_m\eta = 0, \tag{9}$$

where again (i,j,k,m) denotes every permutation of $(1,2,3,4)$. We now apply condition (9) to the functions J_{ij} in (4) for which $\eta=1$, just considered in the first part of this proof. It can thus be seen that

$$J_{im}J_{jk} + J_{km}J_{ij} + J_{jm}J_{ki} = \psi_i\psi_j\psi_k\psi_m \sum_{p,q,r,s=1}^{4} \phi_q\phi_s\{\sigma_{im}\sigma_{jk}\delta^{jkrs}_{impq} + \sigma_{ij}\sigma_{km}\delta^{ijrs}_{kmpq} + \sigma_{jm}\sigma_{ki}\delta^{kirs}_{jmpq}\}. \tag{10}$$

To evaluate this expression, consider first the cases $0 \leqslant p \leqslant 3$, which are verified if and only if (6) is valid. In such situations Eq. (10) becomes

$$J_{im}J_{jk} + J_{km}J_{ij} + J_{jm}J_{ki} = \psi_i\psi_j\psi_k\psi_m\sigma_{im}\sigma_{jk} \sum_{p,q,r,s=1}^{4} \phi_q\phi_s\{\delta^{jkrs}_{impq} + \delta^{ijrs}_{kmpq} + \delta^{kirs}_{jmpq}\} = 0$$

and the result is demonstrated. For the remaining case $p=4$ it can be seen after some algebra that (10) amounts to

$$J_{im}J_{jk}+J_{km}J_{ij}+J_{jm}J_{ki}=\psi_i\psi_j\psi_k\psi_m\{(\sigma_{im}\sigma_{jk}-\sigma_{jm}\sigma_{ki})(\phi_i\phi_j+\phi_k\phi_m)$$
$$+(\sigma_{ij}\sigma_{km}-\sigma_{im}\sigma_{jk})(\phi_i\phi_k+\phi_j\phi_m)+(\sigma_{jm}\sigma_{ki}-\sigma_{ij}\sigma_{km})(\phi_i\phi_m+\phi_j\phi_k)\}. \tag{11}$$

This expression must vanish everywhere in Ω if (4) is to be a solution for arbitrary η in this case. Since $p=4$ (namely all ϕ_i are constant in Ω) then hypothesis (f) implies that there are two possibilities: either $\phi_i\neq 0$ for every $i=1,\ldots,4$; or $\phi_i=0$ for just one value of i. It can be shown in both situations that (11) vanishes if and only if (6) is verified. Consequently, the inclusion of function η implies that conditions (6) are also necessary and sufficient in the case $p=4$. This completes the proof of Theorem 2.1. Q.E.D.

Therefore the family of Poisson structures just characterized has the matrix form

$$\mathcal{J}=\eta\cdot\begin{pmatrix} 0 & \sigma_{12}\psi_1\psi_2(\phi_4-\phi_3) & \sigma_{13}\psi_1\psi_3(\phi_2-\phi_4) & \sigma_{14}\psi_1\psi_4(\phi_3-\phi_2)\\ \sigma_{12}\psi_1\psi_2(\phi_3-\phi_4) & 0 & \sigma_{23}\psi_2\psi_3(\phi_4-\phi_1) & \sigma_{24}\psi_2\psi_4(\phi_1-\phi_3)\\ \sigma_{13}\psi_1\psi_3(\phi_4-\phi_2) & \sigma_{23}\psi_2\psi_3(\phi_1-\phi_4) & 0 & \sigma_{34}\psi_3\psi_4(\phi_2-\phi_1)\\ \sigma_{14}\psi_1\psi_4(\phi_2-\phi_3) & \sigma_{24}\psi_2\psi_4(\phi_3-\phi_1) & \sigma_{34}\psi_3\psi_4(\phi_1-\phi_2) & 0 \end{pmatrix} \tag{12}$$

where additionally $\sigma_{12}\sigma_{34}=\sigma_{13}\sigma_{24}=\sigma_{14}\sigma_{23}$. For what is to follow, the next definition will be necessary.

Definition 2.2: For every open domain $\Omega\subset\mathbb{R}^4$, the set of Poisson structures defined in Ω and of the kind (4) characterized in Theorem 2.1 will be denoted $\Theta(\Omega)$.

To provide the basis for the analysis of the symplectic structure and Darboux reduction in Sec. III and also in order to complete the description of these structures, the following result is important.

Proposition 2.3: Let $\Omega\subset\mathbb{R}^4$ be an open set, then every Poisson structure $\mathcal{J}\in\Theta(\Omega)$ has constant rank of value 2 everywhere in Ω.

Proof: The determinant of $\mathcal{J}$ in (12) is

$$|\mathcal{J}|=\eta(\psi_1\psi_2\psi_3\psi_4)^2[(\sigma_{14}\sigma_{23}-\sigma_{13}\sigma_{24})(\phi_1\phi_2+\phi_3\phi_4)+(\sigma_{12}\sigma_{34}-\sigma_{14}\sigma_{23})(\phi_1\phi_3+\phi_2\phi_4)$$
$$+(\sigma_{13}\sigma_{24}-\sigma_{12}\sigma_{34})(\phi_1\phi_4+\phi_2\phi_3)]^2.$$

Due to identities (6) the result is that $|\mathcal{J}|=0$. Therefore the rank cannot be 4, but only 2 or 0. The fact that the rank is 2 everywhere in Ω is implied by conditions (c), (e), and (f) of Theorem 2.1. Q.E.D.

Proposition 2.3 provides the basis for the explicit determination of the symplectic structure and Darboux reduction of these structures. This is the purpose of the next section.

III. SYMPLECTIC STRUCTURE AND DARBOUX CANONICAL FORM

Before developing the main issues of this section it is necessary to recall a known definition[38] that will be needed for their establishment.

Definition 3.1: Let $\Omega\subset\mathbb{R}^4$ be an open set. A reparametrization of time is defined as a transformation of the form

$$d\tau=\frac{1}{\mu(x)}dt, \tag{13}$$

where t is the initial time variable, τ is the new time and $\mu(x):\Omega\to\mathbb{R}$ is a $C^1(\Omega)$ function which does not vanish in Ω.

The sense of this definition is the following: let

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \mathcal{J} \cdot \nabla H \tag{14}$$

be an arbitrary four-dimensional Poisson structure defined in an open domain $\Omega \subset \mathbb{R}^4$. Then, every reparametrization of time of the form (13) leads from (14) to the differential system,

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = \mu \mathcal{J} \cdot \nabla H. \tag{15}$$

Note however that such transformation often destroys the Poisson structure for systems of dimension higher than three,[38] because for a given $\mathcal{J}$ which is a structure matrix, $\mu\mathcal{J}$ is not necessarily a solution of (2) and (3) as it has been discussed in the proof of Theorem 2.1 in connection with the four-dimensional case.

The main purpose of this section is the investigation of the symplectic structure of family $\Theta(\Omega)$. The central result in this sense corresponds to the next theorem, for which the proof is constructive and completely classifies the different cases arising in the explicit determination of the Casimir invariants and the global reduction to the Darboux canonical form for the members of $\Theta(\Omega)$.

Theorem 3.2: For every four-dimensional Poisson system

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \mathcal{J} \cdot \nabla H$$

defined in an open domain $\Omega \subset \mathbb{R}^4$ and such that $\mathcal{J} \in \Theta(\Omega)$, both a complete set of $C^2(\Omega)$ independent Casimir invariants as well as the reduction to the Darboux canonical form, can be globally constructed in Ω.

Proof: The proof begins with an auxiliary result.

Lemma 3.3: Let $\Omega \subset \mathbb{R}^4$ be an open set, then every $\mathcal{J} \in \Theta(\Omega)$ is equivalent to a Poisson structure $\mathcal{J}'$ defined in a domain Ω', of rank constant and equal to 2 in Ω' and components of the form

$$J'_{ij}(y) = \sigma_{ij} \eta'(y) \sum_{k,l=1}^{4} \epsilon_{ijkl} \phi'_l(y_l), \quad i,j = 1, \ldots, 4. \tag{16}$$

Moreover, $\mathcal{J}'$ is obtained through the change of variables globally diffeomorphic in Ω,

$$y_i(x_i) = \int \frac{\mathrm{d}x_i}{\psi_i(x_i)}, \quad i = 1, \ldots, 4 \tag{17}$$

and $\Omega' = y(\Omega)$ is the diffeomorphic image of Ω through transformation (17).

Proof of Lemma 3.3: Recall that after a general diffeomorphism $y = y(x)$, a given structure matrix $\mathcal{J}(x)$ is transformed into another one $\mathcal{J}'(y)$ according to the rule

$$J'_{ij}(y) = \sum_{k,l=1}^{n} \frac{\partial y_i}{\partial x_k} J_{kl}(x) \frac{\partial y_j}{\partial x_l}. \tag{18}$$

The use of (18) with transformation (17) on $\mathcal{J}$ leads to (16) with $\eta'(y) = \eta(x(y))$ and $\phi'_i(y) = \phi_i(x(y))$ for $i = 1, \ldots, 4$. The fact that the rank of (16) is constant and of value 2 everywhere in Ω' is a direct consequence of Proposition 2.3 and identity (18). Q.E.D.

The Poisson structure (16) will be the starting point for the rest of the proof. Now two complementary cases are to be distinguished.

Case I: $\sigma_{ij} \neq 0$ for all pairs (i,j), $i \neq j$. The analysis of this case must begin with a definition and some preliminary results.

Definition 3.4: Given an open set $\Omega \subset \mathbb{R}^4$, a Poisson structure belonging to $\Theta(\Omega)$ is said to be σ-positive if all its constants σ_{ij} can be chosen to be positive, where $i,j = 1, \ldots, 4$ and $i \neq j$.

Lemma 3.5: Let $\Omega \subset \mathbb{R}^4$ be an open set, and let $\mathcal{J} \in \Theta(\Omega)$ be a Poisson structure for which $\sigma_{ij} \neq 0$ for every pair $i \neq j$, where $i,j=1,\ldots,4$. Then $\mathcal{J}$ is σ-positive and can be expressed in terms of the set of constants $\tilde{\sigma}_{ij}=|\sigma_{ij}|$.

Proof of Lemma 3.5: From now on, we define $\sigma \equiv \sigma_{12}\sigma_{34}=\sigma_{13}\sigma_{24}=\sigma_{14}\sigma_{23}$ [recall Eq. (6)]. Four main cases can be distinguished.

Case 1: $\sigma_{ij}>0$ for all $i \neq j$. The matrix is already in σ-positive form.

Case 2: $\sigma_{ij}<0$ for all $i \neq j$. This is reduced to Case 1 by redefining $\phi_i(x_i)$ as $\tilde{\phi}_i(x_i)=-\phi_i(x_i)$ for every i.

Case 3: $\sigma>0$ with constants σ_{ij} both positive and negative. There are two subcases.

Case 3.1: There are two negative and four positive constants σ_{ij} with $i<j$.

Case 3.1.1: $\sigma_{12}<0$ and $\sigma_{34}<0$.

Case 3.1.2: $\sigma_{13}<0$ and $\sigma_{24}<0$.

Case 3.1.3: $\sigma_{14}<0$ and $\sigma_{23}<0$.

The three subcases 3.1.x are reduced in two steps.

Step 1: redefine $\phi_i(x_i)$ as $\tilde{\phi}_i(x_i)=-\phi_i(x_i)$ for every i.

Step 2: redefine $\psi_i(x_i)$ as $\tilde{\psi}_i(x_i)=-\psi_i(x_i)$ for $i=3,4$ in subcase 3.1.1, for $i=1,3$ in subcase 3.1.2 and for $i=1,4$ in subcase 3.1.3.

Case 3.2: There are two positive and four negative constants σ_{ij} with $i<j$. These are three possible cases that coincide with the ones appearing after step 1 of items 3.1.1, 3.1.2, and 3.1.3 and therefore their reduction corresponds to the transformations indicated in step 2 of those three subcases.

Case 4: $\sigma<0$. Clearly it can be assumed without loss of generality that $\sigma_{12}<0$. Then there are four possibilities.

Case 4.1: $\sigma_{13}<0$ and $\sigma_{14}<0$. Redefining $\tilde{\psi}_1(x_1)=-\psi_1(x_1)$ it is reduced to Case 1.

Case 4.2: $\sigma_{13}>0$ and $\sigma_{14}>0$. Redefining $\tilde{\psi}_2(x_2)=-\psi_2(x_2)$ it is reduced to Case 1.

Case 4.3: $\sigma_{13}>0$ and $\sigma_{14}<0$. Redefining $\tilde{\psi}_3(x_3)=-\psi_3(x_3)$ it is reduced to Case 2.

Case 4.4: $\sigma_{13}<0$ and $\sigma_{14}>0$. Redefining $\tilde{\psi}_4(x_4)=-\psi_4(x_4)$ it is reduced to Case 2.

This completes the proof of Lemma 3.5. Q.E.D.

A result that complements the last lemma is the next one.

Lemma 3.6: For every set of positive real constants $\{\sigma_{12},\sigma_{13},\sigma_{14},\sigma_{23},\sigma_{24},\sigma_{34}\}$ verifying conditions (6) there exists a unique set of positive real constants $\{\sigma_1,\sigma_2,\sigma_3,\sigma_4\}$ such that the equalities $\sigma_{ij}=\sigma_i\sigma_j$ are satisfied for every pair (i,j), with $i<j$, $1 \leqslant i \leqslant 3$, $2 \leqslant j \leqslant 4$.

Proof of Lemma 3.6: The existence of the constants σ_i can be seen on their explicit expressions

$$\sigma_1=\left(\frac{\sigma_{12}\sigma_{13}\sigma_{14}}{\sigma}\right)^{1/2}, \quad \sigma_2=\left(\frac{\sigma\sigma_{12}}{\sigma_{13}\sigma_{14}}\right)^{1/2}, \quad \sigma_3=\left(\frac{\sigma\sigma_{13}}{\sigma_{12}\sigma_{14}}\right)^{1/2}, \quad \sigma_4=\left(\frac{\sigma\sigma_{14}}{\sigma_{12}\sigma_{13}}\right)^{1/2},$$

where now $\sigma>0$. To prove uniqueness, taking logarithms of equalities $\sigma_{ij}=\sigma_i\sigma_j$ allows reducing the problem to the investigation of the following linear system:

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} \ln \sigma_1 \\ \ln \sigma_2 \\ \ln \sigma_3 \\ \ln \sigma_4 \end{pmatrix} = \begin{pmatrix} \ln \sigma_{12} \\ \ln \sigma_{13} \\ \ln \sigma_{14} \\ \ln \sigma - \ln \sigma_{14} \\ \ln \sigma - \ln \sigma_{13} \\ \ln \sigma - \ln \sigma_{12} \end{pmatrix}. \tag{19}$$

Then the application of the Rouché-Fröbenius theorem shows that system (19) has a unique solution for $\{\sigma_1,\sigma_2,\sigma_3,\sigma_4\}$ and the result is demonstrated. Q.E.D.

Therefore notice that in Case I, Lemma 3.5 can be used to assume that all the $\sigma_{ij}>0$. Moreover, Lemma 3.6 can also be employed to write $\sigma_{ij}=\sigma_i\sigma_j$ in every case. Then from (16) we have the following type of Poisson matrix:

$$J'_{ij}(y)=\sigma_i\sigma_j\eta'(y)\sum_{k,l=1}^{4}\epsilon_{ijkl}\phi'_l(y_l),\quad i,j=1,\ldots,4 \tag{20}$$

with $\sigma_i>0$ for $i=1,\ldots,4$. We can now state.

Lemma 3.7: For an open set $\Omega\subset\mathbb{R}^4$, assume that $\mathcal{J}\in\Theta(\Omega)$ is equivalent after transformation (17) to a Poisson structure $\mathcal{J}'$ of the form (20) defined in $y(\Omega)=\Omega'\subset\mathbb{R}^4$ and such that $\sigma_i>0$ for $i=1,\ldots,4$. Then a complete set of independent Casimir invariants of such Poisson structure $\mathcal{J}'$ which are globally defined in Ω' and $C^2(\Omega')$ is given by

$$C_1(y)=\sigma_2\sigma_3\sigma_4y_1+\sigma_1\sigma_3\sigma_4y_2+\sigma_1\sigma_2\sigma_4y_3+\sigma_1\sigma_2\sigma_3y_4, \tag{21}$$

$$C_2(y)=\sigma_1\sigma_2\sigma_3\sigma_4\sum_{i=1}^{4}\int\frac{\phi_i(y_i)}{\sigma_i}\mathrm{d}y_i. \tag{22}$$

Proof of Lemma 3.7: It is an application of the Pfaffian method.[26] Q.E.D.

We can then proceed to the reduction to the Darboux canonical form in Case I. For this, consider the following change of variables globally diffeomorphic in Ω':

$$\{z_1=y_1,\ z_2=y_2,\ z_3=C_1(y),\ z_4=C_2(y)\}, \tag{23}$$

where $C_1(y)$ and $C_2(y)$ are those in (21) and (22). When the transformation rule (18) is applied for (23) to matrix (20) the result is

$$\mathcal{J}'(z)=\eta''(z)\cdot\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix} \tag{24}$$

which is defined in $\Omega''=z(\Omega')$, and where $\eta''(z)=\sigma_1\sigma_2\eta'(y(z))(\phi'_4(y(z))-\phi'_3(y(z)))$. To conclude, the reduction to the Darboux canonical form is achieved making use of Definition 3.1 to perform a time reparametrization of the form (13), namely $\mathrm{d}\tau=\eta''(z)\mathrm{d}t$, where τ is the new time and $\eta''(z)$ is clearly nonvanishing in Ω'' and $C^1(\Omega'')$. According to (14) and (15) the result is a new Poisson system with Darboux-type structure matrix,

$$\mathcal{J}_D=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}. \tag{25}$$

The reduction is thus globally completed in Case I.

Case II: $\sigma_{ij}=0$ for some pair (i,j), $i\neq j$. Again matrix (16) is our starting point. Now notice that $\sigma=0$ and as a consequence of conditions (6) we actually have $\sigma_{ij}=0$ for at least three of the six pairs (i,j), with $i<j$, $1\leqslant i\leqslant 3$, $2\leqslant j\leqslant 4$. This leads to eight possible subcases,

$$\{(\text{II.A.1:}\quad \sigma_{14}=\sigma_{24}=\sigma_{34}=0),\quad (\text{II.A.2:}\quad \sigma_{12}=\sigma_{13}=\sigma_{14}=0),$$

$$(\text{II.A.3:}\quad \sigma_{12}=\sigma_{23}=\sigma_{24}=0),\quad (\text{II.A.4:}\quad \sigma_{13}=\sigma_{23}=\sigma_{34}=0),$$

$$(\text{II.B.1:}\quad \sigma_{13}=\sigma_{14}=\sigma_{34}=0),\quad (\text{II.B.2:}\quad \sigma_{12}=\sigma_{13}=\sigma_{23}=0),$$

$$(\text{II.B.3:}\quad \sigma_{12}=\sigma_{14}=\sigma_{24}=0),\quad (\text{II.B.4:}\quad \sigma_{23}=\sigma_{24}=\sigma_{34}=0). \tag{26}$$

As it can be seen, these subcases are grouped in two different four-member sets (II.A and II.B). The four members of each set present analogous symplectic structures and similar reduction procedures to Darboux form. Let us start with the II.A possibilities:

Lemma 3.8: For an open set $\Omega\subset\mathbb{R}^4$, assume that $\mathcal{J}\in\Theta(\Omega)$ is equivalent after transformation (17) to a Poisson structure $\mathcal{J}'$ of the form (16) defined in $y(\Omega)=\Omega'\subset\mathbb{R}^4$ and corresponding to one of the subcases II.A.1 to II.A.4 in (26). Then a complete set of independent Casimir invariants of such Poisson structure $\mathcal{J}'$ which are globally defined in Ω' and $C^2(\Omega')$ is, respectively,

$$\text{II.A.1:}\quad C_1(y)=y_4$$

$$C_2(y)=\sigma_{23}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{13}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{12}\int\phi_3(y_3)\mathrm{d}y_3$$

$$-(\sigma_{23}y_1+\sigma_{13}y_2+\sigma_{12}y_3)\phi_4(y_4);$$

$$\text{II.A.2:}\quad C_1(y)=y_1,$$

$$C_2(y)=\sigma_{34}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{24}\int\phi_3(y_3)\mathrm{d}y_3+\sigma_{23}\int\phi_4(y_4)\mathrm{d}y_4$$

$$-(\sigma_{34}y_2+\sigma_{24}y_3+\sigma_{23}y_4)\phi_1(y_1);$$

$$\text{II.A.3:}\quad C_1(y)=y_2,$$

$$C_2(y)=\sigma_{34}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{14}\int\phi_3(y_3)\mathrm{d}y_3+\sigma_{13}\int\phi_4(y_4)\mathrm{d}y_4$$

$$-(\sigma_{34}y_1+\sigma_{14}y_3+\sigma_{13}y_4)\phi_2(y_2);$$

$$\text{II.A.4:}\quad C_1(y)=y_3,$$

$$C_2(y)=\sigma_{24}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{14}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{12}\int\phi_4(y_4)\mathrm{d}y_4$$

$$-(\sigma_{24}y_1+\sigma_{14}y_2+\sigma_{12}y_4)\phi_3(y_3).$$

Proof of Lemma 3.8: It is similar to the one of Lemma 3.7. Q.E.D.

We carry out now the reduction to the Darboux canonical form for subcase II.A. For the sake of conciseness this will be done for the first possibility II.A.1, since the procedure is entirely analogous for the remaining situations II.A.2 to II.A.4. Thus for II.A.1 the following change of variables globally diffeomorphic in Ω' is defined

$$\{v_1=y_1,\ v_2=y_2,\ v_3=C_2(y),\ v_4=C_1(y)\}, \tag{27}$$

where $C_1(y)$ and $C_2(y)$ are those in Lemma 3.8 for subcase II.A.l and according to hypothesis (c) of Theorem 2.1 it is assumed $\sigma_{12}\neq 0$ without loss of generality. Applying (18) and (27) to such structure matrix it is again obtained a Poisson structure of the form $\mathcal{J}''(v)=\eta''(v)$. $\mathcal{J}_D$ defined in $v(\Omega')$, where now $\eta''(v)=\sigma_{12}\eta'(y(v))(\phi_4'(y(v))-\phi_3'(y(v)))$ and $\mathcal{J}_D$ is given in (25). The reduction

is concluded by means of a time reparametrization (13) of the form $\mathrm{d}\tau = \eta''(v)\mathrm{d}t$, where $\eta''(v)$ is nonvanishing in $v(\Omega')$ and $C^1(v(\Omega'))$. The result is thus a Poisson system with structure matrix (25) and the reduction is globally completed.

Consider the next subcases II.B in (26). For each of them both generic and nongeneric possibilities must be distinguished, according to the following definition.

Definition 3.9: Given a Poisson structure of the kind (16) characterized in Lemma 3.3 and corresponding to one of the subcases II.B.l to II.B.4 in (26), such structure will be called generic if only three of the six constants σ_{ij} vanish, for $i<j$, $1\leqslant i\leqslant 3$, $2\leqslant j\leqslant 4$, while if four or five of such constants are zero the same type of structures will be termed nongeneric.

Obviously the case in which all constants σ_{ij} vanish is excluded due to condition (c) of Theorem 2.1. Now the generic II.B subcases will be treated first. For them we have the following result.

Lemma 3.10: For an open set $\Omega\subset\mathbb{R}^4$, assume that $\mathcal{J}\in\Theta(\Omega)$ is equivalent after transformation (17) to a Poisson structure $\mathcal{J}'$ of the form (16) defined in $y(\Omega)=\Omega'\subset\mathbb{R}^4$ and corresponding to one of the generic subcases II.B.l to II.B.4 in (26). Then a complete set of independent Casimir invariants of such Poisson structure $\mathcal{J}'$ which are globally defined in Ω' and $C^2(\Omega')$ is, respectively,

$$\text{II.B.1:}\quad C_1(y)=\sigma_{23}\sigma_{24}y_1+\sigma_{12}\sigma_{24}y_3+\sigma_{12}\sigma_{23}y_4,$$

$$C_2(y)=\sigma_{23}\sigma_{24}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{12}\sigma_{24}\int\phi_3(y_3)\mathrm{d}y_3+\sigma_{12}\sigma_{23}\int\phi_4(y_4)\mathrm{d}y_4;$$

$$\text{II.B.2:}\quad C_1(y)=\sigma_{24}\sigma_{34}y_1+\sigma_{14}\sigma_{34}y_2+\sigma_{14}\sigma_{24}y_3,$$

$$C_2(y)=\sigma_{24}\sigma_{34}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{14}\sigma_{34}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{14}\sigma_{24}\int\phi_3(y_3)\mathrm{d}y_3;$$

$$\text{II.B.3:}\quad C_1(y)=\sigma_{23}\sigma_{34}y_1+\sigma_{13}\sigma_{34}y_2+\sigma_{13}\sigma_{23}y_4,$$

$$C_2(y)=\sigma_{23}\sigma_{34}\int\phi_1(y_1)\mathrm{d}y_1+\sigma_{13}\sigma_{34}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{13}\sigma_{23}\int\phi_4(y_4)\mathrm{d}y_4;$$

$$\text{II.B.4:}\quad C_1(y)=\sigma_{13}\sigma_{14}y_2+\sigma_{12}\sigma_{14}y_3+\sigma_{12}\sigma_{13}y_4,$$

$$C_2(y)=\sigma_{13}\sigma_{14}\int\phi_2(y_2)\mathrm{d}y_2+\sigma_{12}\sigma_{14}\int\phi_3(y_3)\mathrm{d}y_3+\sigma_{12}\sigma_{13}\int\phi_4(y_4)\mathrm{d}y_4.$$

Proof of Lemma 3.10: It is similar to the one of Lemma 3.7. Q.E.D.

Regarding the reduction to the Darboux canonical form for the generic II.B subcases, possibility II.B.1 will be the only one explicitly considered, since again the procedure is completely analogous for the other cases II.B.2 to II.B.4. Then for II.B.1 (generic) the transformation globally diffeomorphic in Ω' to be performed is

$$\{w_1=y_1,\ w_2=y_2,\ w_3=C_1(y),\ w_4=C_2(y)\},\tag{28}$$

where $C_1(y)$ and $C_2(y)$ are those in Lemma 3.10 for II.B.1. Once (28) is defined, the rest of the reduction for the generic II.B.1 case is entirely similar to that of subcase II.A.1.

The only remaining situations are the nongeneric II.B subcases. The results to be presented are completely analogous for the four possibilities II.B.1 to II.B.4, and consequently we shall only deal explicitly with II.B.1 for the sake of brevity. For this, notice that there are two possible nongeneric situations for II.B.1.

II.B.1.a: One of $\{\sigma_{12},\sigma_{23},\sigma_{24}\}$ vanishes. These three subcases are retrieved as particular instances of the II.A cases already analyzed, in such a way that the complete set of independent Casimir invariants and the reduction to the Darboux canonical form are also obtained as particular results of the ones given for II.A. Specifically, we may have

(i) $\sigma_{12}=0$: Such matrix is a particular case of II.A.2 in which $\sigma_{34}=0$.
(ii) $\sigma_{23}=0$: This is a particular case of II.A.4 with $\sigma_{14}=0$.
(iii) $\sigma_{24}=0$: It is a particular case of II.A.1 with $\sigma_{13}=0$.

II.B.1.b: Two of $\{\sigma_{12},\sigma_{23},\sigma_{24}\}$ vanish. Then the Casimir invariants are apparent and only a time reparametrization remains in order to reduce the Poisson system to Darboux form.

The classification is similar for the nongeneric II.B.2 to II.B.4 possibilities. Case II is thus concluded.

The demonstration of Theorem 3.2 is therefore complete. Q.E.D.

Thus not only the Poisson structures considered but also their possible kinds of Casimir invariants and global reductions to the Darboux canonical form are completely characterized after the previous results. Once the main properties have been considered in detail, it is interesting to put in perspective the family just analyzed, as far as it is closely related to other Poisson structures reported in the literature. This is the aim of the next part of the work.

IV. EXAMPLES AND RELATIONSHIP WITH OTHER SOLUTIONS

In this section the relationship of the family of solutions investigated with some other well-known Poisson structures is briefly explored. This is useful not only because the family of form (4) characterized in Theorem 2.1 provides a generalization of other structures or families of structures to be mentioned, but also because pointing up the intersections among different families should be helpful for future investigations regarding the Jacobi equations. Additionally, such illustrations provide interesting examples of the solutions analyzed throughout the paper.

Consider first the particular case of members of $\Theta(\Omega)$ for which functions $\eta(x)$ and $\phi_i(x_i)$ $(i=1,\ldots,4)$ have constant values. The result is always a separable Poisson structure,[31] namely a structure matrix of the form $J_{ij}=a_{ij}\psi_i(x_i)\psi_j(x_j)$, where the a_{ij} are real constants that constitute the entries of a skew-symmetric matrix $A=(a_{ij})$, and the $\psi_i(x_i)$ are nonvanishing $C^1(\Omega)$ functions. Recall that separable matrices are always solutions of the Jacobi equations (2) and (3) independently of the dimension of the Poisson manifold.[31] There are several interesting kinds of Poisson systems for which separable structures are natural in general dimension n, and consequently in the specific case of dimension $n=4$. This is the case of Poisson models arising in the domain of population dynamics (for either Lotka-Volterra[11] or generalized Lotka-Volterra[8] systems), plasma models[19] and systems such as the Toda and relativistic Toda lattices.[15] The interested reader is referred to the primary reference for further examples and the full details regarding issues such as the determination of the Casimir invariants and the reduction to the Darboux canonical form for separable Poisson structures.[31] Note in addition that according to Proposition 2.3 the structures belonging to $\Theta(\Omega)$ have constant rank of value 2 everywhere in Ω, while the rank of a separable matrix is the rank of A. Then it is interesting to remark that the particular case in which η and ϕ_i $(i=1,\ldots,4)$ are constant does not comprise all possible four-dimensional separable matrices but only separable structures of rank two, thus illustrating an intersection between two known families of Poisson structures.

As a second example, consider the limit case in which the functions $\psi_4(x_4)=\phi_4(x_4)=0$ are considered in (12). In the resulting Poisson structure, it is clear that x_4 is a Casimir function. Then if a reduction is carried out to the symplectic leaf $x_4=c$, the outcome is the $3d$ Poisson structure of matrix:

$$\mathcal{J}_{[3d]} = \tilde{\eta} \cdot \begin{pmatrix} 0 & \psi_1\psi_2\tilde{\phi}_3 & -\psi_1\psi_3\tilde{\phi}_2 \\ -\psi_1\psi_2\tilde{\phi}_3 & 0 & \psi_2\psi_3\tilde{\phi}_1 \\ \psi_1\psi_3\tilde{\phi}_2 & -\psi_2\psi_3\tilde{\phi}_1 & 0 \end{pmatrix}, \tag{29}$$

where $\tilde{\eta}(x_1,x_2,x_3)=\eta(x_1,x_2,x_3,c)$ and $\tilde{\phi}_i=\sigma_{jk}\phi_i$ for $i=1,2,3$, where (i,j,k) denotes an arbitrary permutation of $(1,2,3)$. Dropping the tildes for the sake of clarity, the resulting structures can also be expressed as

$$(\mathcal{J}_{[3d]})_{ij}(x_1,x_2,x_3) = \eta(x_1,x_2,x_3)\psi_i(x_i)\psi_j(x_j)\sum_{k=1}^{3}\epsilon_{ijk}\phi_k(x_k), \quad i,j=1,2,3. \tag{30}$$

Poisson structures of the form (29) and (30) have been studied in detail in the literature,[38] and actually they comprise as particular cases very different Poisson matrices employed before in several domains, including the Euler top,[2] the Kermack-McKendrick model,[10,37] certain integrable cases of the Lorenz system,[20] population models such as those of Lotka-Volterra[9,11,37] and generalized Lotka-Volterra[8] types, the Maxwell-Bloch equations,[27] the Rabinovich system,[20] or the RTW interaction equations.[20] A discussion of these particular instances as well as an analysis of structures (29) and (30) including their symplectic structure, Casimir invariants and construction of the Darboux coordinates are present in the aforementioned reference.[38] Such family is also interesting from the point of view of the separable structures considered in the first part of this section, since it is evident that all three-dimensional separable structures are particular cases of (30).

It can be thus appreciated how the identification of the solutions characterized in Theorem 2.1 leads to the establishment of some new links among different families of Poisson structures.

V. FINAL REMARKS

Every new contribution to the study of skew-symmetric solutions of the Jacobi equations tends to provide a more general perspective of the field of finite-dimensional Poisson structures. Typical features of this fact can be appreciated in the previous analysis. Not only the identification of finite-dimensional Poisson structures constitutes in itself a relevant problem from the point of view of mathematical physics, but in addition this knowledge provides a richer framework for the fundamental problem of recasting a given differential flow into a Poisson system, whenever possible. Additionally, it is worth noting that the characterization of a sufficiently general solution family often allows the conceptual and operational unification of diverse Poisson structures and systems previously well-known but unrelated, which can hereafter be regarded from a more general and economic standpoint. Examples of this have been given in Sec. IV. In particular, in such sense it is physically interesting to identify the Casimir invariants and to develop the reduction procedure to the Darboux canonical form for the solution families. These are features of special relevance when they can be globally achieved, thus providing an additional instance of a result that goes beyond the *a priori* scope of Darboux theorem and has been reported only in a limited number of cases. This kind of results suggests that the direct investigation of the Jacobi equations constitutes a fruitful line of research not only for classification purposes but also for the detailed analysis of Poisson structures, not to mention its mathematical interest as an example of nonlinear system of PDEs. Additionally to these considerations, it is worth recalling that dimension three is the simplest nontrivial case for the analysis of the Jacobi equations and has consequently been studied in much more detail than higher dimensions, as discussed in the Introduction. On the other hand, Jacobi equations (3) become increasingly complicated as dimension grows. This explains the relative scarcity of results for dimensions four and higher. Certainly, a complete knowledge of the skew-symmetric solutions of the Jacobi equations is still far, but nevertheless the investigation of the problem seems to be a unavoidable issue for a better understanding of finite-dimensional Poisson structures, and therefore of the scope of Hamiltonian dynamics.

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Generalized nonholonomic mechanics, servomechanisms and related brackets

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It is well known that nonholonomic systems obeying D'Alembert's principle are described on the Hamiltonian side, after using the Legendre transformation, by the so-called almost-Poisson brackets. In this paper we define the Lagrangian and Hamiltonian sides of a class of generalized nonholonomic systems (GNHS), obeying a generalized version of D'Alembert's principle, such as rubber wheels (like some simplified models of pneumatic tires) and certain servomechanisms (like the controlled inverted pendulum), and show that corresponding equations of motion can also be described in terms of a bracket. We present *essentially all* possible brackets in terms of which the mentioned equations can be written down, which include the brackets that appear in the literature, and point out those (if any) that are *naturally* related to each system. In particular, we show there always exists a Leibniz bracket related to a GNHS, and conversely, that every Leibniz system is a GNHS. The control of the inverted pendulum on a cart is studied as an illustrative example. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2165797]

I. INTRODUCTION

In the framework of constrained mechanical systems, recent works[1–3] have pointed out (in a more or less independent way) that, in order to find the trajectories of the system, *kinematic constraints* itself do not provide (in general) all the needed information, but, in addition, the space of possible values of the *constraint forces* (or some equivalent information) must also be specified. The problem has been analyzed from a Hamiltonian point of view in Refs. 1 and 2, and from a Lagrangian one in Ref. 3. The last reference has adopted a variational-like formulation, where such an additional information is given in terms of the space of possible values of variations. The latter is defined, essentially, by a distribution on the configuration space of the system: the so-called *variational constraints*. Possible values of constraint forces correspond to the annihilator of such a distribution, given rise in this way to a generalized version of the *Principle of Virtual Works*.

For systems with linear nonholonomic (and even with affine) constraints in the velocities, the above-mentioned additional data is usually supplied by the *D'Alembert's principle*, which has been the purpose of an extensive research for more than a century.[4–19] In such cases, kinematic constraints are determined by a distribution on the configuration space Q, and D'Alembert's principle says that variational constraints are given precisely by the same distribution. In other words, we can derive variational constrains from the kinematic ones by using this principle. Accordingly, in some sense, no additional information is needed in that situation. For general nonlinear constraints in the velocities,[20] given by submanifolds of TQ, and also for higher order constraints,[21,22] defined by submanifolds of higher order tangent bundles $T^{(k)}Q$,[23,24] the "natural" generalization of D'Alembert's principle is the so-called *Chetaev's rule* or *principle*.[25–27]

Unfortunately, as it has been shown in Marle's work[2] for servomechanisms, and in the work of Cendra *et al.*[3] for some simplified models of pneumatic tires[28–30] (which include, in some cases, higher order constraints), these principles do not always lead us to the correct equations of motion. That is to say, variational constraints derived from kinematic ones by using D'Alembert's or Chetaev's principle (depending on the form of involved kinematic constraints) give rise, in general, to wrong equations. In these cases we say the system does not satisfy D'Alembert's or Chetaev's principle. As a conclusion, kinematic and variational constraints must be taken as independent notions, and one should not attempt to derive, for instance, variational from kinematic constraints by a universal procedure.

It is worth mentioning that applicability of the above principles does not depend on the form of kinematic constraints alone, but on the way they are implemented by the constraint forces in each case: different procedures to realize the same kinematic constraints give rise to different dynamical systems.

One of the aims of the present work is to define and study a subclass of the systems presented in Ref. 3, which we shall call *generalized nonholonomic systems* (GNHS), and propose, by using the Legendre transformation, a Hamiltonian description of them. Such systems are essentially nonholonomic systems that do not necessarily satisfy D'Alembert's or Chetaev's principle. In this way, we compare the Lagrangian approach of Ref. 3 and the Hamiltonian one developed in Ref. 2. All that is contained in Sec. II.

We also start on the Hamiltonian side and define a generalized notion of a constrained Hamiltonian system (which we also call GNHS), following Marle's work, going beyond the case of Hamiltonian systems obtained by a Legendre transformation. We study existence and uniqueness conditions for related equations of motion. We define in this scenario the D'Alembert's and Chetaev's distributions, in order to introduce there the notions of D'Alembert's and Chetaev's principles, respectively. This is done in Sec. III.

In Sec. IV we develop the main aim of the paper: to obtain a bracket description of GNHS. More precisely, we write the equations of motion for such systems in terms of a bracket defined on the constraints submanifold. We present, in essence, *all* possible brackets that can be used to describe dynamic of each GNHS, which includes the brackets that appear in the literature, and point out those that are *naturally* related to such systems. In some cases these brackets turn out to be *Leibniz brackets*[31,32] and even *almost-Poisson brackets*.[2,8,9,33] However, we also consider cases in which the resulting brackets are nonlinear in one of its arguments. We give a local procedure to build up such brackets in the linear and affine cases.

On the other hand, we show that there always exists a Leibniz bracket in terms of which equations of motion can be written down. Conversely, we show that every Leibniz system can be described as the Hamiltonian formulation of a GNHS.

An interesting example from control theory, that we study all along the paper, is the inverted pendulum on a cart. We give the Lagrangian and Hamiltonian formulations, and built up the related bracket, for the control strategies developed in Refs. 2 and 34. In particular, we show how the idea of *virtual constraints*, presented in Ref. 34, can be naturally described in terms of GNHS.

II. GENERALIZED NONHOLONOMIC SYSTEMS

Let Q be an n-dimensional manifold, the *configuration space*. As usual, let us indicate by q^i a local coordinate system of Q, and by $(q^i,\dot{q}^i)$ [or $(q^i,\delta q^i)$] the induced one on TQ. We shall often omit indices.

Let us consider a triple (L,C_K,C_V) with

(i) $L:TQ\to\mathbb{R}$ a function: the *Lagrangian function*.
(ii) $C_K\subset TQ$ a submanifold: the kinematic constraints. We shall often assume that the equality $\tau(C_K)=Q$ holds, being $\tau:TQ\twoheadrightarrow Q$ the canonical projection of the tangent bundle.
(iii) C_V another submanifold: the variational constraints. Its elements will be called variations or virtual displacements. We consider two kinds of C_V:

$$C_V\subset TQ \quad \text{or} \quad C_V\subset C_K\times_Q TQ.$$

In the first case we ask C_V to be a distribution. For the second case we ask, for each $q \in \tau(C_K)$,

(i) the subsets

$$C_V[v] = C_V \cap (\{v\} \times T_qQ)$$

should be nonvoid for all $v \in C_K$ such that $\tau(v)=q$,

(ii) identifying in a natural way $C_V[v]$ with a subset of T_qQ, as we will do from now on, we also ask $C_V[v]$ to be a linear subspace with the same dimension for all $v \in C_K$.

We can think of C_K and C_V, at least locally, as being subsets

$$C_K = \{(q,\dot{q}) : R_K(q,\dot{q}) = 0\}$$

and (sum over repeated indices convention is assumed from now on)

$$C_V = \{(q,\delta q) : R_{V,i}(q)\,\delta q^i = 0\}, \tag{1}$$

or

$$C_V = \{(q,\dot{q},\delta q) : R_K(q,\dot{q}) = 0 \text{ and } R_{V,i}(q,\dot{q})\,\delta q^i = 0\}, \tag{2}$$

being R_K and each $R_{V,i}$ vector valued differentiable functions. If C_K is given by a family R_K^a of real valued functions, the condition $\tau(C_K)=Q$ is equivalent to the condition that the matrix $\partial R_K^a / \partial \dot{q}^j$ has maximal rank.

Definition 1: *We call a triple* (L, C_K, C_V) *a generalized nonholonomic system* (*GNHS*), *and we say that a curve* $q:[t_1,t_2] \to Q$ *is a trajectory of the system if its velocity belongs to* C_K *and if, in addition, it is a critical point of the action, i.e.*,

$$\delta \int_{t_1}^{t_2} L \, \mathrm{d}t = 0,$$

for variations restricted to C_V.

In other words, $q(t)$ is a trajectory of (L, C_K, C_V) if $(q(t), \dot{q}(t)) \in C_K$, and for all variations $\delta q(t)$ such that, depending on the case,

$$(q(t), \delta q(t)) \quad \text{or} \quad (q(t), \dot{q}(t), \delta q(t))$$

belongs to C_V, we have

$$\left(\frac{d}{\mathrm{d}t}\left(\frac{\partial L(q(t),\dot{q}(t))}{\partial \dot{q}^i} \right) - \frac{\partial L(q(t),\dot{q}(t))}{\partial q^i} \right) \delta q^i(t) = 0. \tag{3}$$

In abbreviated form, equations of motions can be written

$$\left(\frac{d}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} \right) \delta q^i = 0, \quad (q,\dot{q}) \in C_K, \quad \begin{cases} (q,\delta q) \in C_V, \\ (q,\dot{q},\delta q) \in C_V. \end{cases} \tag{4}$$

Now it is clear why C_K and C_V are called kinematic and variational constraints, respectively.

Remark 2: *It is easy to prove that, a GNHS* (L, C_K, C_V) *with* $C_V \subset TQ$ *and the related system with triple* $(L, C_K, C_K \times_Q C_V)$ (*corresponding to the second kind*) *are equivalent, in the sense that they have the same set of trajectories. This would enable us to describe all GNHS as belonging to the second kind. However, we prefer to deal with these two kinds of variational constraints separately, in order to appreciate the particular formulas that appears in each situation.*

Remark 3: *We may consider a given* C_V *of the second kind as being a submanifold of the Whitney sum* $TQ \oplus TQ$ *instead of* $C_K \times_Q TQ$. *But, as it can be easily shown, only the part included in* $C_K \times_Q TQ$ *would be relevant to describe the dynamic of the system.*

Constraint forces: Related to C_V we have a submanifold F_V, the *constraint forces space*:

(1) For a constraint $C_V \subset TQ$ of the first kind we define $F_V \subset T^*Q$ as being the codistribution given by the annihilator of C_V, i.e., $F_V = C_V^o$.
(2) For a constraint of the second kind $C_V \subset C_K \times_Q TQ$ we define

$$F_V \subset C_K \times_Q T^*Q$$

such that subsets

$$F_V[v] = F_V \cap (\{v\} \times T_q^*Q)$$

are given by the annihilator of $C_V[v]$ for all $v \in C_K$.

For short, we shall say that F_V is the annihilator of C_V, and write $F_V = C_V^o$ and $F_V^o = C_V$. In local terms [see Eqs. (1) and (2)]

$$F_V = \{(q,f): f_i = \lambda_a R_{V,i}^a(q); \lambda \in \mathbb{R}\}$$

or

$$F_V = \{(q,\dot{q},f): R_K(q,\dot{q}) = 0 \quad and \quad f_i = \lambda_a R_{V,i}^a(q,\dot{q}); \lambda \in \mathbb{R}\}.$$

In order to clarify the meaning of F_V, let us rewrite Eq. (3) as

$$\langle f, \delta q \rangle = f_i \delta q^i = 0 \tag{5}$$

for quantities

$$f_i = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i}.$$

Then, f_i must define a covector f that belongs to the annihilator of C_V, i.e.,

$$(q(t), \dot{q}(t), f(t)) \in C_V^o = F_V.$$

Since in the Lagrangian formalism f represents constraint forces, the meaning of the submanifold F_V is now clear. Going back to Eq. (5), we have a generalized version of the *Principle of Virtual Work: constraint forces f do not realize work along virtual displacements* δq. The generalization here corresponds to the fact that the mentioned virtual displacements have nothing to do, in principle, with kinematic constraints. According to what has been said above, every GNHS can be described in terms of data (L, C_K, C_V) or, alternatively, in terms of its related triple (L, C_K, F_V).

Linear and affine constraints: When C_K is a distribution on Q (respectively, an affine subbundle of TQ) we say the system has *linear* (respectively, *affine*) *kinematic constraints*. In these cases we can write $C_K = C_K^{\text{vec}} + \nu$, being $C_K^{\text{vec}} \subset TQ$ a distribution and $\nu \subset TQ$ a section. Such submanifolds can be locally described by a set of equations for $\dot{q}$,

$$\omega_i^a(q)\dot{q}^i = \gamma^a(q), \quad 1 \leqslant a \leqslant k,$$

for each $q \in Q$. Of course, linear constraints correspond to the $\gamma^a = 0$, or equivalently, to the $\nu = 0$ case. D'Alembert's principle holds when $C_V = C_K^{\text{vec}}$, i.e., when virtual displacements δq satisfy

$$\omega_i^a(q)\delta q^i = 0, \quad 1 \leqslant a \leqslant k,$$

or equivalently, when $F_V = (C_K^{\text{vec}})^o$, which means that constraint forces do not realize work along *standard* virtual displacements: the *standard* Principle of Virtual Works.

Systems with higher order constraints: Systems defined above are a subclass of those presented in Ref. 3. There, a class of dynamical systems with higher order constraints were defined, on a manifold Q, as triples (L, C_K, C_V) with $L \in C^\infty(TQ)$,

$$C_K \subset T^{(k)}Q \quad \textit{and} \quad C_V \subset T^{(l)}Q \times_Q TQ,$$

for some $k,l \geqslant 0$. Symbol $T^{(n)}Q$ denotes the nth order tangent bundle of the manifold Q.[23,24] In particular, $T^{(0)}Q=Q$ and $T^{(1)}Q=TQ$. By definition, a curve $q:[t_1,t_2]\to Q$ is a trajectory of the system if its k-lift

$$[q]^{(k)}(t) \in C_K,$$

and Eq. (3) is fulfilled for all $\delta q(t)$ such that

$$([q]^{(l)}(t), \delta q(t)) \in C_V.$$

It is clear that GNHS correspond to the $k=1$ and $l=0,1$ cases. Note that cases with $k=0$ can be easily included in the class of GNHS. In fact, if we have constraints $C_K \subset Q$, then we can replace them by TC_K, obtaining in this way a system which is equivalent to the original one.

From now on, we shall refer to the cases $C_V \subset TQ$ and $C_V \subset C_K \times_Q TQ$ as the $l=0$ and $l=1$ cases, respectively.

We shall show in a forthcoming paper that any triple (L, C_K, C_V) with higher order constraints is equivalent to a GNHS. This is one of the reasons why we focus on such a subclass.

A. Application to servomechanisms

The inverted pendulum on a cart: In the scenario of automatic control, a widely studied mechanical system is the so-called *inverted pendulum on a cart*. It consists in a straight rod which remains in a vertical plane, such that one of its tips, say O, can move only along a straight horizontal line contained in that plane. The configuration space for this system is $Q=\mathbb{R}\times S^1$. Given $(x,\theta)\in \mathbb{R}\times S^1$, x represents the position of the point O and θ represents the angle of rotation of the rod with respect to the horizontal line, measured in the counter-clockwise sense.

The Lagrangian of the system is (neglecting friction)

$$L(x,\theta,\dot{x},\dot{\theta}) = \tfrac{1}{2}m\dot{x}^2 - ml\dot{\theta}\dot{x}\sin\theta + \tfrac{1}{2}I\dot{\theta}^2 - mgl\sin\theta, \tag{6}$$

where m is the mass of the rod, l is the distance from O to its center of mass, I is its moment of inertia with respect to O, and g is the acceleration of gravity. It is worth remarking that the system has an unstable fixed point at $\theta=\pi/2$.

A classical control problem is to take the rod from any position to the upright position, which should be converted into a stable fixed point. In order to do that, Marle suggest,[2] as a control strategy, to impose a value of $\dot{x}$ as a function of $x,\theta,\dot{\theta}$. In other words, to impose a kinematic constraint $C_K \subset TQ$ of the form

$$C_K = \{(x,\theta,\dot{x},\dot{\theta}) : \dot{x} - f(x,\theta,\dot{\theta}) = 0\}. \tag{7}$$

For instance, one can choose C_K to be an affine subbundle given by

$$\dot{x} - \rho(\theta)\dot{\theta} = \gamma(\theta), \tag{8}$$

with $\rho(\theta)=-b$ and $\gamma(\theta)=a\cos\theta$, taking $a<0$ and $b>I/ml$. This constraint is different from that appearing in Ref. 2, but it has the same effect, i.e., the upright position is effectively converted into a stable point.

Another control problem is the *orbital stabilization*, i.e., to make some periodic orbit of the system asymptotically stable. To this end, in Ref. 34 the method of *virtual constraints* were proposed and applied to the inverted pendulum on a cart. There, in order to make the pendulum oscillate around the upright position on an asymptotically stable orbit, they impose a kinematic constraint as in Eq. (8), with $\rho(\theta)=-L\cos\theta$ and $\gamma(\theta)=0$.

Note this constraint can be integrated to $x+L\sin\theta=c$, for some constant c depending on the initial conditions. This is actually the form in which appears in Ref. 34.

In both cases, constraints are realized by means of a servomechanism, which apply a horizontal force at the point O. (This force is precisely the *control law* that the constraints gives rise.) This means that constraint forces define a codistribution $F_V \subset T^*Q$ with elements of the form $\lambda\, \mathrm{d}x$. Accordingly, variational constraints define a one-dimensional distribution $C_V = F_V^o$ generated by ∂_θ, that is, $\delta x = 0$ and $\delta\theta$ arbitrary. Explicitly,

$$C_V = \{(x, \theta, \delta x, \delta\theta) : \delta x = 0\}. \tag{9}$$

Clearly, D'Alembert's principle is not valid, that is to say $C_V \neq C_K^{\mathrm{vec}}$, unless $\rho(\theta) = \gamma(\theta) = 0$.

Equations of motion of (L, C_K, C_V), given by (6), (7), and (9) are

$$\left(\frac{d}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x}\right)\delta x + \left(\frac{d}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta}\right)\delta\theta = 0,$$

$$\dot{x} = f(x, \theta, \dot{\theta}), \quad \delta x = 0;$$

which, using the explicit form of the Lagrangian, reduce to

$$I\ddot{\theta} - ml\ddot{x}\sin\theta + mgl\cos\theta = 0, \quad \dot{x} = f(x, \theta, \dot{\theta}).$$

Geometric formulation of the method of virtual constraints: We have just seen how the idea of virtual constraints, in the case of the inverted pendulum, fits into the scenario of GNHS. Let us briefly comment how it fits in general (as developed in Ref. 34). Given a Lagrangian system with n degrees of freedom, such a method consists in using $n-1$ independent actuators to implement $n-1$ independent constraints, the virtual constraints themselves, chosen in such a way that the resulting underactuated mechanical system (the so-called *zero dynamics*) has some periodic orbit which is asymptotically stable. The name "virtual" for the involved constraints corresponds to the fact that the actuators, i.e., constraint forces, do not satisfy D'Alembert's principle in general.

Suppose we have a mechanical system defined on an n-dimensional manifold Q and with Lagrangian function L. Following Ref. 34, it can be shown (as we have done for the inverted pendulum) that, by applying the method of virtual constraints, the resulting dynamical system can be described as a GNHS (L, C_K, C_V) with $C_K, C_V \subset TQ$ given by one-dimensional distributions. Note that $F_V \subset T^*Q$ has dimension $n-1$, corresponding to the $n-1$ independent actuators. Thus, C_K represents virtual constraints and C_V the space annihilated by the actuators.

B. Legendre transformation and the Hamiltonian side

As usual, let us denote by (q^i, p_i) the local coordinate system of T^*Q, and by $(q^i, p_i, \dot{q}^i, \dot{p}_i)$ [or $(q^i, p_i, \delta q^i, \delta p_i)$] the one induced by (q^i, p_i) on TT^*Q.

In local terms, the Legendre transformation $\mathbb{F}L : TQ \to T^*Q$ reads

$$\mathbb{F}L(q, \dot{q}) = (q, p), \quad \textit{with } p_i = \frac{\partial L}{\partial \dot{q}^i}(q, \dot{q}).$$

In what follows, we are going to assume that L is hyperregular. The energy function $E : T^*Q \oplus TQ \to \mathbb{R}$ is given by

$$E(\alpha_q, v_q) = \langle \alpha_q, v_q \rangle - L(v_q), \tag{10}$$

or in coordinates,

$$E(q, p, \dot{q}) = \sum_{i=1}^{n} p_i \dot{q}^i - L(q, \dot{q}),$$

and the Hamiltonian $H : T^*Q \to \mathbb{R}$ is given by

$$H(\alpha_q) = E(\alpha_q, \mathbb{F}L^{-1}(\alpha_q)). \tag{11}$$

We will need the function $F: T^*Q \oplus TQ \to \mathbb{R}$, such that

$$F(\alpha_q, v_q) = \langle \alpha_q, v_q \rangle - H(\alpha_q). \tag{12}$$

Now define a submanifold $D \subset T^*Q$ by

$$D = \mathbb{F}L(C_K). \tag{13}$$

The latter represents the phase space constraints associated to the kinematic constraints C_K. Note that, whenever the equality $\tau(C_K) = Q$ holds, we have $\pi(D) = Q$, being $\pi: T^*Q \twoheadrightarrow Q$ the canonical projection of the cotangent bundle.

Associated to C_V we shall define a distribution $\mathcal{V} \subset T_D T^*Q$ along D. In order to do that, denote by $\pi_*: TT^*Q \twoheadrightarrow TQ$ the differential of π, and consider the natural surjection

$$\mathfrak{s}: TT^*Q \twoheadrightarrow T^*Q \oplus TQ: V_{\alpha_q} \mapsto \alpha_q \oplus \pi_*(V_{\alpha_q}).$$

In coordinates, $\mathfrak{s}(q, p, \delta q, \delta p) = (q, p, \delta q)$. Now, we define

$$\begin{aligned} \mathcal{V} &= \mathfrak{s}^{-1}(D \times_Q C_V), \quad l = 0, \\ \mathcal{V} &= \mathfrak{s}^{-1}([\mathbb{F}L \times_Q id_{TQ}](C_V)), \quad l = 1. \end{aligned} \tag{14}$$

Note that for $l = 0$ the distribution $\mathcal{V}$ can be described alternatively as

$$\mathcal{V} = \pi_*^{-1}(C_V)|_D. \tag{15}$$

In fact,

$$\mathcal{V} = \mathfrak{s}^{-1}(D \times_Q C_V) = \pi_*^{-1}(C_V) \cap T_D T^*Q = \pi_*^{-1}(C_V)|_D.$$

Thus, for $l = 0$,

$$\mathcal{V} = \{V_{\alpha_q} \in TT^*Q : \alpha_q \in D, \pi_*(V_{\alpha_q}) \in C_V\},$$

and in coordinates,

$$\mathcal{V} = \{(q, p, \delta q, \delta p) : (q, p) \in D, (q, \delta q) \in C_V\}.$$

For $l = 1$, we can write $\mathcal{V} = \mathfrak{s}^{-1}(\mathcal{V}_1)$, with $\mathcal{V}_1 \subset T^*Q \oplus TQ$ given by

$$\mathcal{V}_1 = \{\alpha_q \oplus v_q \in T^*Q \oplus TQ : \alpha_q \in D, (\mathbb{F}L^{-1}(\alpha_q), v_q) \in C_V\}.$$

In local coordinates, using that the inverse Legendre transformation $\mathbb{F}H = \mathbb{F}L^{-1}$ is given by

$$\mathbb{F}H(q, p) = (q, \dot{q}), \quad \text{with } \dot{q}^i = \frac{\partial H}{\partial p_i}(q, p),$$

we have

$$\mathcal{V}_1 = \left\{ (q, p, \delta q) : (q, p) \in D, \left(q, \frac{\partial H}{\partial p}(q, p), \delta q \right) \in C_V \right\}. \tag{16}$$

Accordingly, for $l = 1$,

$$\mathcal{V} = \{V_{\alpha_q} \in TT^*Q : \alpha_q \in D, \mathfrak{s}(V_{\alpha_q}) = \alpha_q \oplus \pi_*(V_{\alpha_q}) \in \mathcal{V}_1\}$$

or [see (16)]

$$\mathcal{V}=\{(q,p,\delta q,\delta p):(q,p,\delta q)\in\mathcal{V}_1\}.$$

It is worth mentioning that the distributions $\mathcal{V}\subset T_DT^*Q$ above satisfy

$$\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}, \tag{17}$$

what implies that variations δp's are arbitrary. A direct consequence of (17) is that such distributions are coisotropic, i.e., $\mathcal{V}^\perp\subset\mathcal{V}$, where $\perp$ denotes the symplectic orthogonal with respect to the canonical 2-form ω of T^*Q.

Now, in terms of a triple $(H,D,\mathcal{V})$ as given above, we shall derive a set of equations equivalent to those coming from related Lagrangian system. This will enable us to identify the Hamiltonian side of a GNHS.

Proposition 4: *Equations of motion* (4), *defined by* (L,C_K,C_V) *with L hyperregular*, *are equivalent to*

$$\left(\dot{q}^i-\frac{\partial H}{\partial p_i}\right)\delta p_i+\left(\dot{p}_i+\frac{\partial H}{\partial q^i}\right)\delta q^i=0,\quad (q,p,\delta q,\delta p)\in\mathcal{V}, \tag{18}$$

defined by the data $(H,D,\mathcal{V})$ [*see Eqs.* (11), (13), and (14)]. *They can be derived from a variational principle*

$$\delta\int_{t_1}^{t_2}F\,\mathrm{d}t=0,\quad \textit{with variations restricted to } \mathcal{V}.$$

In turn, *Eqs.* (18) *can be intrinsically described by each one of the following equivalent equations for a vector field* $X\in TD$:

$$\omega_D(X,Y)-\mathrm{d}H|_D(Y)=0\quad \textit{for all } Y\in\mathcal{V},$$

$$\omega_D^\flat(X)-\mathrm{d}H|_D\in\mathcal{V}^o,$$

$$X-\omega_D^\sharp(\mathrm{d}H|_D)\in\mathcal{V}^\perp,$$

where ω_D *and* $\mathrm{d}H|_D$ *are the canonical 2-form of* T^*Q *and the differential* $\mathrm{d}H$ *restricted to* $T_DT^*Q\times T_DT^*Q$ *and* T_DT^*Q, *respectively*.

Proof: Equations (4) for $l=0$ are

$$\left(\frac{d}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}^i}\right)-\frac{\partial L}{\partial q^i}\right)\delta q^i=0,\quad (q,\dot{q})\in C_K,\quad (q,\delta q)\in C_V. \tag{19}$$

Having in mind that $p_i=\partial L/\partial\dot{q}^i$ and $\dot{q}^i=\partial H/\partial p_i$, and the fact that

$$\frac{\partial H}{\partial q^j}=-\frac{\partial L}{\partial q^j},$$

Eqs. (19) are equivalent to

$$\dot{q}^i-\partial H/\partial p_i=0,\quad \left(\dot{p}_i+\frac{\partial H}{\partial q^j}\right)\delta q^i=0,\quad (q,p)\in D,\quad (q,\delta q)\in C_V.$$

From definition of $\mathcal{V}$, since δp's are arbitrary, equivalence of the last equations and Eq. (18) follows immediately. For $l=1$ we must proceed similarly. We leave to the reader to show the equivalence with the phase space variational principle.

In order to show that Eq. (18) is equivalent to

$$\omega_D(X,Y) - \mathrm{d}H|_D(Y) = 0 \quad for\ all \quad Y \in \mathcal{V},$$

let us write $X \in TD$ and $Y \in \mathcal{V}$ as $X_{q,p}=(\dot{q},\dot{p})$ and $Y_{q,p}=(\delta q,\delta p)$. Then

$$[\omega_D(X,Y)]_{q,p} = \dot{q}^i \delta p_i - \dot{p}_i \delta q^i, \quad \left[\mathrm{d}H|_D(Y)\right]_{q,p} = \frac{\partial H}{\partial q^i}\delta q^i + \frac{\partial H}{\partial p_i}\delta p_i,$$

and as a consequence

$$\left[\omega_D(X,Y) - \mathrm{d}H|_D(Y)\right]_{q,p} = \left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right)\delta p_i + \left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right)\delta q^i,$$

as we wanted to show. ■

Summing up, related to a triple (L,C_K,C_V) we have defined another one $(H,D,\mathcal{V})$, given by Eqs. (11), (13), and (14), which gives rise to a dynamical system equivalent to the original one. Then, we can talk about (L,C_K,C_V) and $(H,D,\mathcal{V})$ as the *Lagrangian* and *Hamiltonian data*, or *Lagrangian* and *Hamiltonian side*, of a GNHS.

The inverted pendulum revisited: Let us continue with the inverted pendulum on a cart. Consider the case of affine kinematic constraints implemented by constraint forces as described above. Then,

$$C_K = \{(x,\theta,\dot{x},\dot{\theta}) : \dot{x} = \rho(\theta)\dot{\theta} + \gamma(\theta)\}$$

and

$$C_V = \{(x,\theta,\delta x,\delta\theta) : \delta x = 0\}.$$

Applying Legendre transformation, we have

$$p_x = m\dot{x} - v\dot{\theta}, \quad p_\theta = -v\dot{x} + I\dot{\theta},$$

being $v=ml\sin\theta$, and the Hamiltonian function is

$$H(x,\theta,p_x,p_\theta) = \frac{Ip_x^2 + mp_\theta^2 + 2vp_xp_\theta}{2(mI - v^2)} + vg. \tag{20}$$

The submanifold $D=\mathbb{F}L(C_K)$ is given by points of T^*Q with p_x,p_θ obeying

$$\frac{\partial H}{\partial p_x}(x,\theta,p_x,p_\theta) - \rho(\theta)\frac{\partial H}{\partial p_\theta}(x,\theta,p_x,p_\theta) = \gamma(\theta) \tag{21}$$

for all x,θ, or equivalently,

$$p_x - \chi(\theta)p_\theta = \phi(\theta) \tag{22}$$

with

$$\chi(\theta) = \frac{m\rho(\theta) - v}{I - v\rho(\theta)} \quad and \quad \phi(\theta) = \frac{\gamma(\theta)(mI - v^2)}{I - v\rho(\theta)}. \tag{23}$$

On the other hand, the distribution $\mathcal{V}$ can be described as

$$\mathcal{V} = \{(x,\theta,p_x,p_\theta,\delta x,\delta\theta,\delta p_x,\delta p_\theta) : p_x = \chi(\theta)p_\theta + \phi(\theta);\ \delta x = 0\}.$$

Then, using (18) for $\mathcal{V}$ given above, equations of motions are

$$\dot{x} = \frac{Ip_x + vp_\theta}{mI - v^2}, \quad \dot{\theta} = \frac{mp_\theta + vp_x}{mI - v^2},$$

$$\dot{p}_\theta = \frac{wp_x p_\theta}{mI - v^2} + vw\frac{Ip_x^2 + mp_\theta^2 + 2vp_x p_\theta}{(mI - v^2)^2} + wg,$$

$$p_x = \chi(\theta)p_\theta + \phi(\theta),$$

being $w = ml\cos\theta$.

III. CONSTRAINED HAMILTONIAN SYSTEMS

The inverse Legendre transformation: Consider $(H, D, \mathcal{V})$ with

(1) $H \in C^\infty(T^*Q)$,
(2) $D \subset T^*Q$ an embedded submanifold,
(3) and $\mathcal{V} \subset T_D T^*Q$ a distribution such that $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V}) = \mathcal{V}$ [recall Eq. (17)].

Suppose H is hyperregular, i.e., $\mathbb{F}H: T^*Q \to TQ$ is a diffeomorphism. Then,

(i) $L \in C^\infty(TQ)$ such that [see Eq. (12)]

$$L(v_q) = F(\mathbb{F}H^{-1}(v_q), v_q), \tag{24}$$

(ii) $C_K \subset TQ$ the submanifold of TQ defined by

$$C_K = \mathbb{F}H(D), \tag{25}$$

(iii) and C_V given by the distribution

$$C_V = \pi_*(\mathcal{V}) \subset TQ, \tag{26}$$

if for each q we have $(\pi_*)_{\alpha_q}(\mathcal{V}) = (\pi_*)_{\beta_q}(\mathcal{V})$ for all $\alpha_q, \beta_q \in D$, or by

$$C_V = [\mathbb{F}H \times_Q id_{TQ}](\mathfrak{s}(\mathcal{V})) \subset C_K \times_Q TQ, \quad otherwise, \tag{27}$$

defines a GNHS (L, C_K, C_V). Note that (26) and (27) correspond to the $l=0$ and $l=1$ cases, respectively. It can be shown that Eqs. (18) defined by the given triple $(H, D, \mathcal{V})$ (as well as their equivalent forms appearing in the last proposition) are equivalent to Eqs. (4) related to the associated Lagrangian system (L, C_K, C_V). With all that, we conclude that the Hamiltonian side of a GNHS is given by triples $(H, D, \mathcal{V})$ detailed in points (1), (2), (3) above. Nevertheless, we shall consider the following definition, inspired in Marle's work.[2]

Hamiltonian formulation of GNHS:

Definition 5: *We shall also call GNHS a triple* $(H, D, \mathcal{V})$ *with* H *an element of* $C^\infty(T^*Q)$, $D \subset T^*Q$ *a submanifold, and* $\mathcal{V} \subset T_D T^*Q$ *a distribution along* D, *whose equations of motion are*

$$X \in TD, \quad X - \omega_D^\sharp(\mathrm{d}H|_D) \in \mathcal{V}^\perp. \tag{28}$$

Last equations mean that a curve $\gamma: [t_1, t_2] \to T^*Q$ *is a trajectory of the system if its velocity* $\dot{\gamma}$ *satisfies*

$$\dot{\gamma}(t) \in TD, \quad \dot{\gamma}(t) - \omega^\sharp(\mathrm{d}H|_{\gamma(t)}) \in \mathcal{V}^\perp,$$

for all $t \in [t_1, t_2]$.

Remark 6: *We will be mainly interested in the cases in which* D *is a closed embedded submanifold of* T^*Q.

Remark 7: *Note that systems defined above give a generalization of the Hamiltonian side of a triple* (L, C_K, C_V), *since we are not asking for condition*

$$\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V}) = \mathcal{V}.$$

Up to now, regarding the relation between Lagrangian and Hamiltonian formulation of GNHS, we have proved the following results.

Theorem 8: *Every GNHS given by* (L,C_K,C_V), *with L a hyperregular Lagrangian*, *defines*, *through Eqs.* (11), (13), and (14), *a GNHS* $(H,D,\mathcal{V})$.

A GNHS given by $(H,D,\mathcal{V})$, *with H hyperregular Hamiltonian*, *defines*, *through Eqs.* (24) *to* (27), *a GNHS* (L,C_K,C_V) *iff* $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}$.

In both cases, (L,C_K,C_V) *and* $(H,D,\mathcal{V})$ *give rise to equivalent dynamical systems*.

Marle[2] has defined a class of constrained Hamiltonian systems given by multiplets $(P,\Lambda,H,D,\mathcal{W})$, being P a Poisson manifold with Poisson bivector Λ, H a function on P, D a submanifold of P and $\mathcal{W}\subset T_DT^*Q$ a distribution along D that represents the space where constraint forces *live* in Hamiltonian formalism. Of course, we can extend Definition 5 to arbitrary Poisson manifolds, but we shall restrict ourselves only to cotangent bundles, i.e., $P=T^*Q$ and Λ given by the canonical 2-form ω. In these cases the above multiplets can be described simply as triples $(H,D,\mathcal{W})$. Then, it is easy to see that the distribution $\mathcal{W}$ corresponds exactly to $\mathcal{V}^\perp$, in the sense that the dynamical system$(H,D,\mathcal{W})$ defined by Marle and the GNHS $(H,D,\mathcal{V})$ with $\mathcal{V}=\mathcal{W}^\perp$ are equivalent. This enables us to describe a GNHS indistinctly in terms of $\mathcal{V}$ or $\mathcal{W}$. This situation is similar to what we have on the Lagrangian side, where systems can be described by triple (L,C_K,C_V) as well as (L,C_K,F_V).

It is worth mentioning that a particular subclass of equations of the form (28) appears, following Dirac's procedure, in the Hamiltonian description of singular Lagrangian systems.[14] Then, GNHS include singular systems as a special case.

A. Existence and uniqueness conditions

Now, let us study intrinsic conditions for existence and uniqueness of solutions of Eq. (28). In order to do that, let us consider a complement $\mathcal{U}^\perp$ of TD inside T_DT^*Q, i.e., let us write $T_DT^*Q=TD\oplus\mathcal{U}^\perp$ for some appropriate $\mathcal{U}^\perp$ (we take the orthogonal instead of the direct space for later convenience). In other words,

$$\dim TD=\dim\mathcal{U} \quad \textit{and} \quad TD\cap\mathcal{U}^\perp=0.$$

Here 0 means the null section of T_DT^*Q. Let us call $\mathfrak{p}_{\mathcal{U}^\perp}$ the projection with range TD related to the decomposition above. Note the same can be done on an open set of D. The following result is immediate.

Proposition 9: *Equation* (28) *related to data* $(H,D,\mathcal{V})$ *has one and only one solution passing through a point* $x\in D$ *if decomposition* $T_DT^*Q=TD\oplus\mathcal{V}^\perp$ *holds in an open neighborhood U of x. In this case the equation in that neighborhood reduces to the form*

$$X=\mathfrak{p}_{\mathcal{V}^\perp}\omega_D^\sharp(\mathrm{d}H|_D), \tag{29}$$

being $\mathfrak{p}_{\mathcal{V}^\perp}$ *the projection with range* T_UD *related to mentioned decomposition.*

The hypothesis of the preceding proposition has been previously studied in Ref. 2, replacing $\mathcal{V}^\perp$ by $\mathcal{W}$, under the name of *regular systems*; and also in Ref. 14 within the context of singular Lagrangian systems.

Let us translate the above conditions to the Lagrangian side. Observe first that for triples $(H,D,\mathcal{V})$ such that $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}$, in order to have equality $T_DT^*Q=TD\oplus\mathcal{V}^\perp$, which is equivalent to conditions

$$\dim TD=\dim\mathcal{V} \quad \textit{and} \quad TD^\perp\cap\mathcal{V}=0,$$

we can ask that $\pi(D)=Q$. For instance, if $\pi(D)$ is a closed submanifold of Q, it can be shown that $TD^\perp\cap\ker\pi_*\neq 0$, and accordingly, since $\ker\pi_*\subset\mathcal{V}$ for every $\mathcal{V}$ such that $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}$, we have $TD^\perp\cap\mathcal{V}\neq 0$. Thus, on the Lagrangian side, in order to use the result above we shall impose the condition $\tau(C_K)=Q$ [which corresponds to $\pi(D)=Q$ under Legendre transformation].

Proposition 10: *For a GNHS given by* (L, C_K, C_V) *such that* $\tau(C_K)=Q$, *existence and uniqueness of solutions passing through a point* $v \in TQ$ *is ensured by regularity of the Lagrangian at* v *and conditions*

$$\text{for } l=0\text{: } \dim C_K = \dim C_V, \quad C_K^{(0)} \cap C_V = 0,$$

$$\text{for } l=1\text{: } \dim C_K = \tfrac{1}{2}\dim C_V, \quad C_K^{(1)} \cap C_V = 0, \tag{30}$$

in a neighborhood of v, *being*

$$C_K^{(0)} = \pi_*((\mathbb{F}L_* TC_K)^\perp), \quad C_K^{(1)} = [\mathbb{F}L^{-1} \times_Q \mathrm{id}_{TQ}] \circ \mathfrak{s}[(\mathbb{F}L_* TC_K)^\perp].$$

Proof: Consider the $l=0$ case. Everything must be understood locally. For

$$D = \mathbb{F}L(C_K) \quad \textit{and} \quad \mathcal{V} = \pi_*^{-1}(C_V)|_D$$

we have $\dim TD = 2\dim D = 2\dim C_K$ on a neighborhood of v (since L is regular there), and $\dim \mathcal{V} = \dim D + \dim C_V$. Assuming that $\dim C_K = \dim C_V$, the last equations ensure $\dim TD = \dim \mathcal{V}$. Now suppose

$$\pi_*[(\mathbb{F}L_* TC_K)^\perp] \cap C_V = 0.$$

Since

$$\pi_*((\mathbb{F}L_* TC_K)^\perp) = \pi_*(T[\mathbb{F}L(C_K)]^\perp) = \pi_*(TD^\perp)$$

and $C_V = \pi_*(\pi_*^{-1}(C_V))$, then

$$0 = \pi_*(TD^\perp) \cap \pi_*(\pi_*^{-1}(C_V)) \supseteq \pi_*(TD^\perp \cap \pi_*^{-1}(C_V))$$

$$= \pi_*(TD^\perp \cap \pi_*^{-1}(C_V) \cap T_D T^*Q) = \pi_*(TD^\perp \cap \mathcal{V}),$$

and therefore $\pi_*(TD^\perp \cap \mathcal{V}) = 0$. On the other hand, since $\tau(C_K) = Q$, and accordingly $\pi(D) = Q$, we have that $TD^\perp \cap \ker \pi_* = 0$ (see the comments before the proposition). As a direct consequence $TD^\perp \cap \mathcal{V} = 0$, and using equality $\dim TD = \dim \mathcal{V}$ we finally have $T_D T^*Q = TD \oplus \mathcal{V}^\perp$. Thus, our statement follows from previous proposition and Proposition 4. We leave to the reader the $l=1$ case. ■

For completeness, we briefly study what conditions (30) mean in local terms. We focus on the case in which C_K and C_V are distributions on Q, i.e., they are given by points $(q, \dot{q})$ and $(q, \delta q)$ such that

$$\omega_i^a(q)\dot{q}^i = 0 \quad \textit{and} \quad v_i^b(q)\delta q^i = 0, \quad 1 \leqslant a \leqslant k, \quad 1 \leqslant b \leqslant l,$$

respectively. We assume each set of equations is linearly independent. Then, condition $\dim C_K = \dim C_V$ is equivalent to equality $k=l$. Let us build up the distribution $C_K^{(0)}$. First note that $\mathbb{F}L(C_K) = D$ is given by $(q,p) \in T^*Q$ satisfying

$$\omega_i^a(q)\frac{\partial H}{\partial p_i}(q,p) = 0, \quad a = 1, \ldots, k.$$

Accordingly, $\mathbb{F}L_* TC_K = T[\mathbb{F}L(C_K)] = TD$ is defined by points $(q,p,\dot{q},\dot{p})$ obeying for all (q,p) in D,

$$\varpi_{ij}^a(q,p)\dot{q}^j + \omega_i^a(q)\frac{\partial H}{\partial p_i \partial p_j}(q,p)\dot{p}_j = 0, \quad a = 1, \ldots, k,$$

being

$$\varpi_{ij}^{a}(q,p)=\frac{\partial}{\partial q^{j}}\left(\omega_{i}^{a}(q)\frac{\partial H}{\partial p_{i}}\right)(q,p).$$

Its symplectic orthogonal is generated, for each $(q,p)\in D$, by vectors

$$V^{a}=\omega_{i}^{a}(q)\frac{\partial H}{\partial p_{i}\,\partial\, p_{j}}(q,p)\frac{\partial}{\partial q^{j}}-\varpi_{ij}^{a}(q,p)\frac{\partial}{\partial p_{j}}.$$

Applying π_{*}, we see that $C_{K}^{(0)}$ is given by elements $(q,\dot{q})\in TQ$ such that

$$\dot{q}^{j}=c_{a}\omega_{i}^{a}(q)\frac{\partial H}{\partial p_{i}\,\partial\, p_{j}}(q,p),$$

with c_{a} arbitrary and $(q,p)\in D$. Therefore, the condition $C_{K}^{(0)}\cap C_{V}=0$ means that

$$\varphi^{ab}=\omega_{i}^{a}(q)\frac{\partial H}{\partial p_{i}\,\partial\, p_{j}}(q,p)v_{j}^{b}(q) \tag{31}$$

defines a nonsingular matrix for all $(q,p)\in D$. It is easy to see that, on the Hamiltonian side, the last statement about φ^{ab} is equivalent to validity of the decomposition $T_{D}T^{*}Q=TD\oplus\mathcal{V}^{\perp}$.

B. D'Alembert's and Chetaev's distributions

Let us study two particular situations where variational constraints are related to kinematic ones. Consider an arbitrary triple (L,C_{K},C_{V}). Let us define the submanifold

$$\mathcal{K}=\mathfrak{s}^{-1}[\mathbb{F}L\times_{Q}\mathrm{id}_{TQ}](C_{K}\times_{Q}C_{K}), \tag{32}$$

and its *diagonal* part

$$\mathrm{diag}(\mathcal{K})=\mathfrak{s}^{-1}[\mathbb{F}L\times_{Q}\mathrm{id}_{TQ}](\mathrm{diag}(C_{K}\times_{Q}C_{K})). \tag{33}$$

The elements of $\mathrm{diag}(C_{K}\times_{Q}C_{K})$ are of the form (q,v,w) with $v=w\in C_{K}$. Note that $\mathcal{K}$ is a submanifold of $T_{D}T^{*}Q$, with $D=\mathbb{F}L(C_{K})$, and it can also be described as

$$\mathcal{K}=\mathfrak{s}^{-1}(D\times_{Q}C_{K})=\pi_{*}^{-1}(C_{K})|_{D}. \tag{34}$$

If C_{K} is a distribution on Q, then $\mathcal{K}$ is a distribution along D. It is the analogue of $\mathcal{V}$ for $l=0$ [see Eqs. (14) and (15)]. If $C_{K}=C_{K}^{\mathrm{vec}}+v$, i.e., it is an affine subbundle of TQ, we define the distribution

$$\mathcal{K}_{\mathrm{vec}}=\mathfrak{s}^{-1}(D\times_{Q}C_{K}^{\mathrm{vec}})=\pi_{*}^{-1}(C_{K}^{\mathrm{vec}})|_{D}.$$

For C_{K} described by equations

$$\omega_{i}^{a}(q)\dot{q}^{i}=\gamma^{a}(q),\quad 1\leqslant a\leqslant k,\quad q\in Q,$$

the related distribution $\mathcal{K}_{\mathrm{vec}}$ is given by $(q,p,\delta q,\delta p)\in T_{D}T^{*}Q$ such that

$$\omega_{i}^{a}(q)\,\delta q^{i}=0,\quad 1\leqslant a\leqslant k,\quad q\in Q.$$

In these terms, for linear (respectively, affine) constraints, D'Alembert's principle holds if and only if $\mathcal{V}=\mathcal{K}_{\mathrm{vec}}$.

Now, consider a GNHS $(H,D,\mathcal{V})$, and define

$$\mathcal{K}=\mathfrak{s}^{-1}[\mathrm{id}_{T^{*}Q}\times_{Q}\mathbb{F}H](D\times_{Q}D)=\pi_{*}^{-1}(\mathbb{F}H(D))|_{D} \tag{35}$$

and

$$\mathrm{diag}(\mathcal{K}) = \mathfrak{s}^{-1}[\mathrm{id}_{T^*Q} \times_Q \mathbb{F}H](\mathrm{diag}(D \times_Q D)); \tag{36}$$

and for D such that $\mathbb{F}H(D)$ is an affine subbundle, i.e., $\mathbb{F}H(D) = \mathbb{F}H(D)_{\mathrm{vec}} + v$, define

$$\mathcal{K}_{\mathrm{vec}} = \pi_*^{-1}(\mathbb{F}H(D)_{\mathrm{vec}})|_D.$$

Note that the above definitions are given in purely Hamiltonian terms.

Definition 11: *We shall say that D'Alembert's principle holds for* $(H, D, \mathcal{V})$ *if* $\mathbb{F}H(D)$ *is a distribution* (*respectively*, *an affine subbundle*) *and* $\mathcal{V} = \mathcal{K}$ (*respectively*, $\mathcal{K}_{\mathrm{vec}}$). *This is why*, *for linear* (*respectively*, *affine*) *constraints*, *we shall call* $\mathcal{K}$ (*respectively*, $\mathcal{K}_{\mathrm{vec}}$) *the D'Alembert's distribution*.

Let us come back to an arbitrary triple (L, C_K, C_V). When constraints are not linear or affine, the natural generalization of D'Alembert's principle is Chetaev's one, which involves the fiber bundle

$$\widetilde{C}_K = \mathfrak{s}[S^{-1}(TC_K)] \subset C_K \times_Q TQ.$$

Here, S denotes the *canonical endomorphism* $S: TTQ \to TTQ$, which in coordinates reads

$$S(q, \dot{q}, \delta q, \delta \dot{q}) = (q, \dot{q}, 0, \delta q).$$

Chetaev's principle says $C_V = \widetilde{C}_K$. In local coordinates, if C_K is given by

$$\omega^a(q, \dot{q}) = 0, \quad 1 \leqslant a \leqslant k, \quad q \in Q,$$

for certain functions ω^a on TQ, then $\widetilde{C}_K$ is given by points $(q, \dot{q}, \delta q) \in C_K \times_Q TQ$ such that,

$$\frac{\partial \omega^a}{\partial \dot{q}^i}(q, \dot{q})\, \delta q^i = 0, \quad 1 \leqslant a \leqslant k, \quad (q, \dot{q}) \in C_K. \tag{37}$$

When $\omega^a(q, \dot{q}) = \omega_i^a(q)\dot{q}^i - \gamma^a(q)$, i.e., when C_K is an affine subbundle of TQ, we have

$$\widetilde{C}_K = C_K \times_Q C_K^{\mathrm{vec}}.$$

There is a particularly interesting subclass of constraints C_K containing the linear ones, called *homogeneous*, given by functions $\omega^a(q, \dot{q})$ such that

$$\frac{\partial \omega^a}{\partial \dot{q}^i}(q, \dot{q})\, \dot{q}^i = 0, \quad 1 \leqslant a \leqslant k, \quad (q, \dot{q}) \in C_K.$$

They can be characterized by the fact that

$$\mathrm{diag}(C_K \times_Q C_K) \subseteq \widetilde{C}_K.$$

Now, for later convenience, let us define with $\widetilde{C}_K$ a distribution

$$\mathcal{L} = \mathfrak{s}^{-1}[\mathbb{F}L \times_Q \mathrm{id}_{TQ}]\widetilde{C}_K$$

along $D = \mathbb{F}L(C_K)$. Elements of $\mathcal{L}$ are points $(q, p, \delta q, \delta p) \in T_D T^*Q$ such that [see Eq. (37)]

$$\widetilde{\omega}_i^a\left(q, \frac{\partial H}{\partial p}(q,p)\right)\delta q^i = 0, \quad 1 \leqslant a \leqslant k, \quad (q,p) \in D,$$

with $\widetilde{\omega}_i^a = \partial \omega^a / \partial \dot{q}^i$. Note if $\widetilde{C}_K = C_K \times_Q C_K^{\mathrm{vec}}$, then $\mathcal{L} = \mathcal{K}_{\mathrm{vec}}$. Accordingly, for the linear and affine constraints, $\mathcal{L}$ coincide with the related D'Alembert's distribution. On the other hand, homogeneous constraints can be characterized as those such that $\mathrm{diag}(\mathcal{K}) \subseteq \mathcal{L}$.

In Hamiltonian language, for a hyperregular Hamiltonian function H and a submanifold $D \subset T^*Q$, we define

$$\mathcal{L} = \mathfrak{s}^{-1}[\mathbb{F}H^{-1} \times_Q \mathrm{id}_{TQ}]\widetilde{\mathbb{F}H(D)}, \tag{38}$$

with (in the regular situation $\mathcal{L}$ can only be locally defined)

$$\widetilde{\mathbb{F}H(D)} = \mathfrak{s}[S^{-1}(\mathbb{F}H_*(TD))].$$

Definition 12: *We shall say that* $(H, D, \mathcal{V})$ *satisfies Chetaev's principle if* $\mathcal{V} = \mathcal{L}$, *and call* $\mathcal{L}$ *the Chetaev's distribution. Also, we will say that* $(H, D, \mathcal{V})$ *has homogeneous constraints if* $\mathrm{diag}(\mathcal{K}) \subseteq \mathcal{L}$, *where* $\mathrm{diag}(\mathcal{K})$ *and* $\mathcal{L}$ *are given by* (36) and (38), *respectively.*

Note that $\mathcal{K}_{\mathrm{vec}}$ and $\mathcal{L}$ (since δp's are arbitrary) satisfy Eq. (17) and in consequence they are coisotropic.

The following result, which has been previously demonstrated,[35] ensures existence and uniqueness for equations of motion associated to constrained Hamiltonian systems satisfying D'Alembert's or Chetaev's principle. We include a proof here only for completeness.

Proposition 13: *Equation* (28) *related to the data* $(H, D, \mathcal{V})$ *has one and only one solution passing through a point* $x \in D$ *provided* H *is normal at* x (*i.e.*, $\partial^2 H / \partial p_i \partial p_j$ *is a positive or negative defined matrix at* x), $\pi(D) = Q$ *and D'Alembert's or Chetaev's principle is fulfilled in a neighborhood of* x. *In this case, Eq.* (28) *reduces near* x *to the form*

$$X = \mathfrak{p}_{\mathcal{V}^\perp} \omega_D^\sharp(\mathrm{d}H|_D), \quad \textit{with } \mathcal{V} = \mathcal{K}, \quad \mathcal{K}_{\mathrm{vec}} \textit{ or } \mathcal{L}.$$

To prove the last result it is enough to use Proposition 9 and the lemma below.

Remark 14: *Normality of* H *is ensured for Hamiltonian functions of the type* $H = T + V \circ \pi$, *being* $V : Q \to \mathbb{R}$ *the potential energy, and* $T : T^*Q \to \mathbb{R}$ *the kinetic energy, given by one-half of the quadratic form of a Riemannian metric on* Q.

Lemma 15: *Given a submanifold* $D \subset T^*Q$ *such that* $\pi(D) = Q$, *and a normal* (*ipso facto regular*) *Hamiltonian function* $H \in C^\infty(T^*Q)$ *in* $x \in D$, *then* $\mathcal{L}$ *can be defined in a neighborhood of* x *and there we have*

$$T_D T^*Q = TD \oplus \mathcal{L}^\perp = TD^\perp \oplus \mathcal{L}.$$

If $\mathbb{F}H(D)$ *is a linear* (*respectively, affine*) *subbundle of* TQ, *the same decomposition holds for* $\mathcal{K}$ (*respectively,* $\mathcal{K}_{\mathrm{vec}}$).

Proof: Since H is regular in x and $\pi(D) = Q$, submanifold D can be locally described in terms of k equations (being $k \leqslant n$)

$$\omega^a\left(q, \frac{\partial H}{\partial p}(q,p)\right) = 0, \quad 1 \leqslant a \leqslant k,$$

where functions $\omega^a(q, \dot{q})$ are such that matrix

$$\tilde{\omega}_i^a = \partial \omega^a / \partial \dot{q}^i$$

has rank k. It easily follows that TD is given by elements $(q, p, \dot{q}, \dot{p}) \in T_D T^*Q$ obeying, for each $(q, p) \in D$,

$$\varpi_i^a(q,p)\dot{q}^i + \tilde{\omega}_i^a\left(q, \frac{\partial H}{\partial p}(q,p)\right)\frac{\partial^2 H}{\partial p_l \partial p_i}(q,p)\dot{p}_l = 0,$$

with

$$\varpi_i^a(q,p) = \frac{\partial}{\partial q^i}\left(\omega^a\left(q, \frac{\partial H}{\partial p}(q,p)\right)\right).$$

In particular (using regularity of H and the fact that $\tilde{\omega}_i^a$ has rank k), TD has dimension $2n-k$. On the other hand, Chetaev's distribution $\mathcal{L}$ is locally defined and given by $(q,p,\delta q,\delta p) \in T_D T^*Q$ such that

$$\tilde{\omega}_i^a\left(q, \frac{\partial H}{\partial p}(q,p)\right)\delta q^i = 0, \quad 1 \leqslant a \leqslant k.$$

As a consequence, the elements of $\mathcal{L}^\perp$ are generated by vectors with coordinates $\tilde{\omega}_i^a$ (omitting arguments) with respect to $\partial/\partial p_i$, and null coordinates with respect to $\partial/\partial q^i$. This implies $\mathcal{L}^\perp$ has dimension k. To show decomposition in question holds, we must see that $TD \cap \mathcal{L}^\perp = 0$. But, if an element of $\mathcal{L}^\perp$ also belongs to TD, then (omitting arguments of all involved functions)

$$\tilde{\omega}_i^a \frac{\partial^2 H}{\partial p_l \partial p_i}\tilde{\omega}_l^b = 0, \quad \textit{for all } a,b.$$

This is not possible, because H is normal. ■

IV. BRACKETS FOR GNHS

We want to describe the equations of motion for a system $(H,D,\mathcal{V})$ in terms of a bracket on D. In order to do that, it would be desirable to have an expression of X as a function of $H_D := H|_D$, or more precisely, *as a function* of the differential $\mathrm{d}H_D \in T^*D$. In fact, if we could write $X = \Pi^\sharp(\mathrm{d}H_D)$, with $\Pi^\sharp : T^*D \to TD$, then the related map $\Pi : T^*D \times T^*D \to \mathbb{R}$ given by $\Pi(\sigma,\rho) = \langle \sigma, \Pi^\sharp(\rho)\rangle$, would define a bracket

$$\{\cdot,\cdot\} : C^\infty(D) \times C^\infty(D) \to C^\infty(D) : (f,g) \mapsto \{f,g\} = \Pi(\mathrm{d}f, \mathrm{d}g)$$

such that

$$\dot{f} = \{f, H_D\}, \quad \textit{for all } f \in C^\infty(D).$$

The last statement follows from the chain of equalities

$$\dot{f} = X \cdot f = \langle \mathrm{d}f, X\rangle = \langle \mathrm{d}f, \Pi^\sharp(\mathrm{d}H_D)\rangle = \Pi(\mathrm{d}f, \mathrm{d}H_D) = \{f, H_D\}.$$

Note that $\{\cdot,\cdot\}$ is always a derivation, in particular linear, with respect to the first argument. We shall see that nonlinearity with respect to the second argument can naturally appear in the presence of nonlinear kinematic constraints.

A. Intrinsic formulation

Looking at Eq. (29), it is clear that we just need to write $\mathrm{d}H|_D$ as a function of $\mathrm{d}H_D$. Using the embedding $i : D \hookrightarrow T^*Q$, since $H_D = H \circ i$, we have

$$\mathrm{d}H_D = d(H \circ i) = i^*(\mathrm{d}H|_D),$$

being $i^* : T_D^* T^*Q \twoheadrightarrow T^*D$ the pull-back of i. Thus, we essentially need to invert map i^*, in a certain way.

1. Linear and homogeneous constraints

We shall first study the case of linear kinematic constraints. Let us begin with the following general result.

Lemma 16: *Let H be a Hamiltonian function for a manifold Q, and D a submanifold of T^*Q. Then* $\mathrm{d}H|_D \in \mathrm{diag}(\mathcal{K})^\flat$ [*see Eq.* (36)]. *In particular*, $\mathrm{d}H|_D \in \mathcal{K}^\flat$.

Proof: The submanifold $\mathrm{diag}(\mathcal{K}) \subset T_D T^*Q$ is given locally by

$$\mathrm{diag}(\mathcal{K}) = \left\{ \left(q,p,\frac{\partial H}{\partial p}(q,p),\dot{p} \right) : (q,p) \in D \right\}$$

with $\dot{p}$ arbitrary. Accordingly $\mathrm{diag}(\mathcal{K})^\flat$ is given by covectors with arbitrary coordinates with respect to $\mathrm{d}q^i$'s and coordinates $\partial H/\partial p_i$ with respect to $\mathrm{d}p_i$'s. From this we obtain

$$\mathrm{d}H|_x = \left.\frac{\partial H}{\partial q^i}\right|_x \mathrm{d}q^i + \left.\frac{\partial H}{\partial p_i}\right|_x \mathrm{d}p_i \in \mathrm{diag}(\mathcal{K})^\flat, \quad \forall\, x \in D.$$

Finally, since $\mathrm{diag}(\mathcal{K}) \subset \mathcal{K}$, the last statement follows. ■

Recall from the preceding section that when $\mathbb{F}H(D)$ is a distribution on Q, then $\mathcal{K}$ is a distribution too. As we have seen in Lemma 15, the distribution $\mathcal{K}^\perp$ often gives a complement of TD in $T_D T^*Q$. Having this in mind, let us make some observations.

Consider again a complement $\mathcal{U}^\perp$ of TD inside $T_D T^*Q$, and the related projection $\mathfrak{p}_{\mathcal{U}^\perp}$. Associated to $\mathcal{U}^\perp$ we also have a decomposition

$$T^*_D T^*Q = TD^o \oplus \mathcal{U}^\flat.$$

It is clear that $i^*: T^*_D T^*Q \twoheadrightarrow T^*D$, or more precisely the restriction $i^*|_{\mathcal{U}^\flat}$, defines a bijection from $\mathcal{U}^\flat$ to T^*D [note that $\ker(i^*) = TD^o$]. From the latter we have an injective vector bundle morphism

$$\mathfrak{j}_{\mathcal{U}^\flat}: T^*D \hookrightarrow T^*_D T^*Q,$$

with range equal to $\mathcal{U}^\flat$, such that $\mathfrak{j}_{\mathcal{U}^\flat}(x) = (i^*|_{\mathcal{U}^\flat})^{-1}(x)$, for all $x \in T^*D$. Accordingly,

$$i^* \mathfrak{j}_{\mathcal{U}^\flat} = \mathrm{id}_{T^*D} \quad \textit{and} \quad \mathfrak{j}_{\mathcal{U}^\flat} i^*\big|_{\mathcal{U}^\flat} = \mathrm{id}_{\mathcal{U}^\flat}. \tag{39}$$

In addition, we can write $\mathfrak{p}_{\mathcal{U}^\perp} = i_* \mathfrak{j}^*_{\mathcal{U}^\flat}$, being $\mathfrak{j}^*_{\mathcal{U}^\flat}$ the transpose of $\mathfrak{j}_{\mathcal{U}^\flat}$.

Let us assume, from now on, the validity of the decomposition $T_D T^*Q = TD \oplus \mathcal{V}^\perp$. Then, we can set $\mathcal{U} = \mathcal{V}$ in formulas above.

Theorem 17: *Let $(H,D,\mathcal{V})$ be a GNHS such that $\mathbb{F}H(D)$ is a distribution on Q, and $T_D T^*Q = TD \oplus \mathcal{K}^\perp$ is fulfilled. Then, its equations of motion can be written $X = \Pi^\sharp(\mathrm{d}H_D)$, with*

$$\Pi^\sharp: T^*D \to TD \quad \textit{given by } \Pi^\sharp = \mathfrak{j}^*_{\mathcal{V}^\flat} \omega_D^\sharp \mathfrak{j}_{\mathcal{K}^\flat}.$$

As a consequence, related to $(H,D,\mathcal{V})$ we have a bracket on D,

$$\{f,g\} = \Pi(\mathrm{d}f,\mathrm{d}g) = \Lambda_D(\mathfrak{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathfrak{j}_{\mathcal{K}^\flat}(\mathrm{d}g)), \tag{40}$$

where $\Lambda: T^*T^*Q \times T^*T^*Q \to \mathbb{R}$ is the Poisson bivector associated to ω, and Λ_D its restriction to D.

Proof: Consider the decomposition $T_D T^*Q = TD \oplus \mathcal{K}^\perp$ and related injection $\mathfrak{j}_{\mathcal{K}^\flat}: T^*D \hookrightarrow T^*_D T^*Q$. Since $\mathrm{d}H|_D \in \mathcal{K}^\flat$ (by previous lemma), and recalling that $\mathrm{d}H_D = i^*(\mathrm{d}H|_D)$, we have [using Eq. (39) for $\mathcal{U} = \mathcal{K}$], that

$$\mathrm{d}H\big|_D = \left(\mathfrak{j}_{\mathcal{K}^\flat} i^*\big|_{\mathcal{K}^\flat}\right) \mathrm{d}H|_D = \mathfrak{j}_{\mathcal{K}^\flat}[i^*(\mathrm{d}H|_D)] = \mathfrak{j}_{\mathcal{K}^\flat}(\mathrm{d}H_D).$$

Then, from Eq. (29),

$$X = \mathfrak{p}_{\mathcal{V}^\perp} \omega_D^\sharp(\mathrm{d}H|_D) = \mathfrak{p}_{\mathcal{V}^\perp} \omega_D^\sharp(\mathfrak{j}_{\mathcal{K}^\flat}(\mathrm{d}H_D)) = \mathfrak{p}_{\mathcal{V}^\perp} \omega_D^\sharp \mathfrak{j}_{\mathcal{K}^\flat}(\mathrm{d}H_D).$$

Using now that $\mathfrak{p}_{\mathcal{V}^\perp} = i_* \mathfrak{j}^*_{\mathcal{V}^\flat}$, and identifying X and $i_* X$, the first statement of theorem follows. For the second one, we just must define for all $f,g \in C^\infty(D)$ the bilinear $\{f,g\} = \langle \mathrm{d}f, \Pi^\sharp(\mathrm{d}g) \rangle$. Then,

$$\{f,g\} = \langle \mathrm{d}f, \mathrm{j}_{\mathcal{V}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\mathrm{d}g)\rangle = \langle \mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\mathrm{d}g)\rangle$$

$$= \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{K}^\flat}(\mathrm{d}g)),$$

and the theorem is proved. ■

Remark 18: *Note that the bracket given in theorem above is bilinear, and moreover a derivation with respect to both arguments. But it fails to be antisymmetric and Jacobi, in general. The antisymmetry property is explicitly broken by the presence of two different distributions* $\mathcal{V}$ *and* $\mathcal{K}$. *This makes the bracket to have a symmetric part, which implies*

$$\dot{H}_D = \{H_D, H_D\} \neq 0,$$

in general. In other words, the described constrained systems are generically nonconservative, unless $\mathcal{V}=\mathcal{K}$, *which holds in the D'Alembert's case.*

When $\mathcal{V}=\mathcal{K}$, the bracket we have obtained is an almost-Poisson bracket, and coincides exactly with that constructed by van der Schaft and Maschke[9] (as it will become clear later, when the local formulation is analyzed). Also, it gives rise on $\mathcal{H}=\mathcal{K}\cap TD$ to the symplectic fibration defined by Bates and Sniatycki,[8] and to a Poisson bracket on D if and only if $\mathcal{H}$ is involutive, as we show below.

Proposition 19: *Under conditions of the theorem above, suppose* $\mathcal{V}=\mathcal{K}$. *Then* Π *is antisymmetric, and we can write*

$$\Pi(\alpha,\beta) = \tilde{\omega}(\Pi^\sharp(\alpha), \Pi^\sharp(\beta)), \quad \text{for } \alpha,\beta \in T^*D,$$

being $\tilde{\omega}: TD\times TD \to \mathbb{R}$ *the closed 2-form* $\tilde{\omega}=i^*\omega_D$. *Defining* $X_f=\Pi^\sharp(\mathrm{d}f)$, *for every function* $f \in C^\infty(D)$, *the related bracket adopts the form*

$$\{f,g\} = \Pi(\mathrm{d}f, \mathrm{d}g) = \tilde{\omega}(X_f, X_g).$$

In addition, $\{,\}$ *is Jacobi if and only if* $\mathcal{K}\cap TD$ *is involutive.*

Proof: First note that $\Pi^\sharp = \mathrm{j}_{\mathcal{K}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}$, and accordingly

$$\Pi(\alpha,\beta) = \langle \alpha, \mathrm{j}_{\mathcal{K}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\beta)\rangle = \langle \mathrm{j}_{\mathcal{K}^\flat}(\alpha), \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\beta)\rangle$$

$$= \langle \omega_D^\flat \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\alpha), \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\beta)\rangle = \omega_D(\omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\alpha), \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\beta)). \tag{41}$$

On the other hand, since $\mathcal{K}$ is coisotropic (i.e., $\mathcal{K}^\perp \subset \mathcal{K}$), we have

$$\mathcal{K} = \mathcal{K} \cap (TD \oplus \mathcal{K}^\perp) = (\mathcal{K}\cap TD) \oplus \mathcal{K}^\perp,$$

or equivalently, identifying TD and $i_*(TD)$,

$$\mathrm{j}_{\mathcal{K}^\flat}^*(\mathcal{K}) = \mathfrak{p}_{\mathcal{K}^\perp}(\mathcal{K}) = \mathcal{K}\cap TD.$$

Then, given X and Y in $\mathcal{K}$,

$$\omega_D(X,Y) = \omega_D(\mathfrak{p}_{\mathcal{K}^\perp}(X), \mathfrak{p}_{\mathcal{K}^\perp}(Y)) = \omega_D(\mathrm{j}_{\mathcal{K}^\flat}^*(X), \mathrm{j}_{\mathcal{K}^\flat}^*(Y)).$$

Since range of $\omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}$ is $\mathcal{K}$, we can use the last result in Eq. (41), obtaining

$$\Pi(\alpha,\beta) = \omega_D(\mathrm{j}_{\mathcal{K}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\alpha), \mathrm{j}_{\mathcal{K}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(\beta)),$$

from which the first part of the proposition easily follows.

For the second part, suppose $\{,\}$ is Jacobi. Then, the related Hamiltonian vector fields $X_f = \Pi^\sharp(\mathrm{d}f)$ define an involutive distribution. Since

$$\Pi^\sharp(T^*D) = \mathrm{j}^*_{\mathcal{K}^\flat}\omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat}(T^*D) = \mathrm{j}^*_{\mathcal{K}^\flat}(\mathcal{K}) = \mathcal{K} \cap TD = \mathcal{H}, \tag{42}$$

then $\mathcal{H}$ is involutive. On the other hand, if $\mathcal{H}$ is involutive, it can be easily shown that (through usual calculations of symplectic geometry)

$$\tilde{\omega}([X_f, X_g], X_h) = -\tilde{\omega}(X_{\{f,g\}}, X_h)$$

for all functions $f, g, h \in C^\infty(D)$. Using the last equation,

$$\mathrm{d}\tilde{\omega}(X_f, X_g, X_h) = 2[\{f,\{g,h\}\} + \{h,\{f,g\}\} + \{g,\{h,f\}\}],$$

and since $\mathrm{d}\tilde{\omega}=0$, the bracket $\{,\}$ is Jacobi. ■

Remark 20: *If* $(H, D, \mathcal{V})$ *is the Hamiltonian side of a triple* (L, C_K, C_K), *the related bracket* $\{,\}$ *is Jacobi if and only if* C_K *is involutive*, *as it is well known.*

Let us consider general homogeneous constraints. Recall that, given a GNHS $(H, D, \mathcal{V})$ with H hyperregular, we say that D is defined by homogeneous constraints if $\mathrm{diag}(\mathcal{K})$ is contained in $\mathcal{L}$ (the Chetaev's distribution related to the system). From Lemma 16, these systems satisfy $\mathrm{d}H|_D \in \mathcal{L}^\flat$. As a consequence we have the following result, similar to the theorem and proposition above, but changing $\mathcal{K}$ by $\mathcal{L}$.

Theorem 21: *Let* $(H, D, \mathcal{V})$ *be a GNHS with homogeneous constraints*, *i.e.*, $\mathrm{diag}(\mathcal{K}) \subseteq \mathcal{L}$, *and such that* $T_D T^*Q = TD \oplus \mathcal{L}^\perp$. *Then*, *its equations of motion can be written* $X = \Pi^\sharp(\mathrm{d}H_D)$, *with*

$$\Pi^\sharp : T^*D \to TD \quad \textit{given by } \Pi^\sharp = \mathrm{j}^*_{\mathcal{V}^\flat}\omega_D^\sharp \mathrm{j}_{\mathcal{L}^\flat}. \tag{43}$$

Its related bracket reads $\{f, g\} = \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{L}^\flat}(\mathrm{d}g))$. *If in addition* $\mathcal{V} = \mathcal{L}$, *that is to say Chetaev's principle holds*, *then* Π *is antisymmetric and the system is conservative. In such a case* $\{,\}$ *is Jacobi if and only if* $\mathcal{L} \cap TD$ *is involutive.*

Brackets above are examples of the so-called *Leibniz brackets*.[31,32] Given a manifold D, a Leibniz bracket on D is a bilinear map

$$\{,\} : C^\infty(D) \times C^\infty(D) \to C^\infty(D)$$

such that

$$\{f \cdot g, h\} = f \cdot \{g, h\} + \{f, h\} \cdot g \quad \textit{and} \quad \{f, h \cdot g\} = h \cdot \{f, g\} + \{f, h\} \cdot g,$$

i.e., $\{,\}$ is a derivation with respect to both arguments. In such a case we say the pair $(D, \{,\})$ is a Leibniz manifold. Note that giving $\{,\}$ is the same as giving a bilinear $\Pi : T^*D \times T^*D \to \mathbb{R}$, being $\{f, g\} = \Pi(\mathrm{d}f, \mathrm{d}g)$. So, we can see a Leibniz manifold as a couple (D, Π). Given a function $h : D \to \mathbb{R}$, a dynamical system can be defined on D with equation of motion given by a vector field $X = \Pi^\sharp(\mathrm{d}h)$. The triple (h, D, Π) is called a Leibniz system. The following result is immediate.

Proposition 22: *Given a Hamiltonian system* $(H, D, \mathcal{V})$ *as in theorem above* (*in particular*, *with homogeneous constraints*), *the triple* (H_D, D, Π), *with* Π *given by* (43), *is a Leibniz system.*

2. The general case: linear and nonlinear brackets

In the preceding section, in order to build maps Π giving rise to the dynamic of the involved systems, the only properties we needed from D'Alembert's and Chetaev's distributions were that they are submanifolds $\mathcal{N} \subset T_D T^*Q$ such that

(a) $i^*|_{\mathcal{N}^\flat} : \mathcal{N}^\flat \to T^*D$ is a bijection
(b) and $\mathrm{d}H|_D \in \mathcal{N}^\flat$.

In fact, given a triple $(H, D, \mathcal{V})$, and a submanifold $\mathcal{N} \subset T_D T^*Q$ satisfying (a) and (b), that we will call an admissible submanifold, we can define the map $\mathrm{j}_{\mathcal{N}^\flat} = (i^*|_{\mathcal{N}^\flat})^{-1}$ and a bracket

$$\{f,g\} = \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{N}^\flat}(\mathrm{d}g))$$

which reproduces on D equations of motion of the system, i.e., $\dot{f}=\{f,H_D\}$. To prove this we can simply repeat the proof of Theorem 17. Note that if $\mathcal{N}^\flat$ is not a distribution, then the bracket above is not linear, in general, with respect to the second argument. In other words,

$$\Pi^\sharp = \mathrm{j}^*_{\mathcal{V}^\flat}\omega_D^\sharp \mathrm{j}_{\mathcal{N}^\flat} : T^*D \to TD$$

is no longer a vector bundle morphism, and consequently it does not define a Leibniz bracket. Let us investigate how admissible submanifolds can be characterized.

Admissible submanifolds and pairs: Given again a decomposition $T^*_DT^*Q=TD^o\oplus\mathcal{U}^\flat$, the elements of any submanifold $\mathcal{N}^\flat \subset T^*_DT^*Q$ can be written as a sum $x+u$, with $x\in TD^o$ and $u\in\mathcal{U}^\flat$. If $i^*|_{\mathcal{N}^\flat}$ is a surjection, since $i^*(x+u)=i^*(u)$, then given $u\in\mathcal{U}^\flat$ there must exists $x\in TD^o$ such that $u+x\in\mathcal{N}^\flat$. If $i^*|_{\mathcal{N}^\flat}$ is an injection, equality $i^*(x+u)=i^*(x'+u)$ implies $x'=d$. Thus, for each $u\in\mathcal{U}^\flat$ there is only one $x\in TD^o$ such that $x+u\in\mathcal{N}^\flat$. Accordingly, bijectivity of $i^*|_{\mathcal{N}^\flat}$ ensures existence of a function $\Phi:\mathcal{U}^\flat\to T^*_DT^*Q$, with range inside TD^o, given by

$$\Phi(u) = x \quad \text{if } u+x\in\mathcal{N}^\flat.$$

In these terms $\mathcal{N}^\flat$ can be written as $\mathcal{N}^\flat=(\Phi+\mathrm{inc}_{\mathcal{U}^\flat})(\mathcal{U}^\flat)$, being $\mathrm{inc}_{\mathcal{U}^\flat}$ the inclusion of $\mathcal{U}^\flat$ inside $T^*_DT^*Q$, or alternatively,

$$\mathcal{N}^\flat = (\Psi + \mathrm{j}_{\mathcal{U}^\flat})(T^*D), \quad \text{with } \Psi = \Phi \mathrm{j}_{\mathcal{U}^\flat} : T^*D \to T^*_DT^*Q.$$

It is clear that $\mathrm{j}_{\mathcal{N}^\flat}=\Psi+\mathrm{j}_{\mathcal{U}^\flat}$. The other property that $\mathcal{N}^\flat$ must satisfy is $\mathrm{d}H|_D\in\mathcal{N}^\flat$. This is equivalent to the condition

$$\Psi(\mathrm{d}H_D) = \mathrm{d}H|_D - \mathrm{j}_{\mathcal{U}^\flat}(\mathrm{d}H_D). \tag{44}$$

Summing up, related to an admissible submanifold $\mathcal{N}^\flat$ we have

(c) a distribution $\mathcal{U}$, such that $\mathcal{U}^\flat$ is a complement of TD^o,
(d) and a map $\Psi: T^*D\to T^*_DT^*Q$ with range inside TD^o and satisfying (44).

Conversely, let us fix a pair $(\mathcal{U},\Psi)$ satisfying (c) and (d). Then, following the same steps as above, $(\mathcal{U},\Psi)$ gives rise to a submanifold $\mathcal{N}^\flat=(\Psi+\mathrm{j}_{\mathcal{U}^\flat})(T^*D)$ satisfying conditions (a) and (b). We can call such pairs $(\mathcal{U},\Psi)$ admissible pairs related to $(H,D,\mathcal{V})$.

Theorem 23: *The set of admissible pairs associated to an arbitrary system $(H,D,\mathcal{V})$ is never empty, and for each element $(\mathcal{U},\Psi)$ of this set the related bracket*

$$\{f,g\}_\Psi = \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{U}^\flat}(\mathrm{d}g)) + \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \Psi(\mathrm{d}g)) \tag{45}$$

describes the dynamic of the system.

Proof: Given an arbitrary distribution $\mathcal{U}$ as above, we can define Ψ, for each $x\in D$, equal to $\mathrm{d}H|_D-\mathrm{j}_{\mathcal{U}^\flat}(\mathrm{d}H_D)$ for all elements of T^*_xD. ■

If Ψ is a vector bundle morphism, then bracket $\{,\}_\Psi$ is a Leibniz bracket on the manifold D. Moreover,

Theorem 24: *Let $(H,D,\mathcal{V})$ be a GNHS such that $\mathrm{d}H|_x\in T_xD^o$ (or equivalently, $\mathrm{d}H_D|_x=0$) only if $\mathrm{d}H|_x=0$. Then, $(H,D,\mathcal{V})$ defines a Leibniz system on D with bracket $\Pi^\sharp=\mathrm{j}^*_{\mathcal{V}^\flat}\omega_D^\sharp\mathrm{j}_{\mathcal{N}^\flat}$, being $\mathcal{N}$ an admissible distribution.*

Proof: We must prove that for every Hamiltonian function $H\in C^\infty(T^*Q)$, and every submanifold $D\subset T^*Q$, there exists, fixing again a distribution $\mathcal{U}$ as above, a vector bundle morphism $\Psi:T^*D\to T^*_DT^*Q$ with range inside TD^o and satisfying $\Psi(\mathrm{d}H_D)=\mathrm{d}H|_D-\mathrm{j}_{\mathcal{U}^\flat}(\mathrm{d}H_D)$. In this way we are showing that the submanifold $\mathcal{N}^\flat=(\Psi+\mathrm{j}_{\mathcal{U}^\flat})(T^*D)$ is admissible. But this is always possible, in fact, we only need to consider a metric Φ on T^*D, and define Ψ in $\mathrm{d}H_D$ equal to $\mathrm{d}H|_D-\mathrm{j}_{\mathcal{U}^\flat}(\mathrm{d}H_D)$, and equal to zero on the Φ-orthogonal complement of $\mathrm{d}H_D$. The map Ψ is well

defined, since, by hypothesis of the theorem, when $\mathrm{d}H_D|_x=0$ then $\mathrm{d}H|_x=0$. ■

If we choose $\mathcal{U}=\mathcal{V}$ in (45), we have a family of brackets $\Pi_\Psi=\Pi+\pi_\Psi$,

$$\Pi(\alpha,\beta)=\Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\alpha),\mathrm{j}_{\mathcal{V}^\flat}(\beta)),\quad \pi_\Psi(\alpha,\beta)=\Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\alpha),\Psi(\beta)).$$

Note that Π defines an almost-Poisson bracket. Writing $\mathcal{W}=\mathcal{V}^\perp$, and recalling that $\mathfrak{p}_{\mathcal{V}^\perp}=\mathrm{j}^*_{\mathcal{V}^\flat}$, or equivalently $\mathfrak{p}^*_{\mathcal{W}}=\mathrm{j}_{\mathcal{V}^\flat}$, we have

$$\Pi(\alpha,\beta)=\Lambda_D(\mathfrak{p}^*_{\mathcal{W}}(\alpha),\mathfrak{p}^*_{\mathcal{W}}(\beta)).$$

This kind of brackets were first introduced by Marle,[2] and called *pseudo-Poisson* brackets. In Ref. 33 they were denoted $\{,\}_{nh}$. The latter describes dynamic for related systems only if $\mathrm{d}H|_D=\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}H_D)$, as happens for systems with linear constraints and obeying D'Alembert's principle, and for systems with homogeneous constraints and obeying Chetaev's principle (see Theorems 17 and 21). The term we must add to describe the dynamics correctly

$$\pi_\Psi(\mathrm{d}f,\mathrm{d}H_D)=\Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f),\Psi(\mathrm{d}H_D))=\Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f),\mathrm{d}H|_D-\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}H_D)),$$

was called $R_H(f)$ in Ref. 33.

We want to emphasize that, given an arbitrary triple $(H,D,\mathcal{V})$, there is not in general a *naturally* related admissible pair $(\mathcal{U},\Psi)$. Nevertheless, as we have seen in the preceding section, for linear and homogeneous constraints we do have *natural* pairs $(\mathcal{K},0)$ and $(\mathcal{L},0)$, denoting by 0 the null function. In these cases, as we have seen before, such pairs give rise to Leibniz brackets. In the following section we shall see that systems with affine constraints also have a naturally related admissible pair, but the bracket it defines is not a Leibniz one.

Leibniz systems and GNHS: We have seen in the last theorem that (under a technical assumption) every GNHS is a Leibniz system. Now, we shall prove the converse statement.

Theorem 25: *Let* (h,D,Π) *be a Leibniz system. Then*, *there exists a manifold* Q, *an embedding* $i:D\hookrightarrow T^*Q$, *a function* $H\in C^\infty(T^*Q)$ *and a distribution* $\mathcal{V}\subset T_DT^*Q$, *satisfying*

(i) $H\circ i=h$,
(ii) *the decomposition* $T_DT^*Q=TD\oplus\mathcal{V}^\perp$ *holds*,
(iii) *there exists a distribution* $\mathcal{N}$ *along* D *such that*

$$T_DT^*Q=TD\oplus\mathcal{N}^\perp,\quad \mathrm{d}H|_D\in\mathcal{N}^\flat,\quad \textit{and}\quad \Pi^\sharp=\mathrm{j}^*_{\mathcal{V}^\flat}\omega_D^\sharp\mathrm{j}_{\mathcal{N}^\flat}.$$

In other words, *every Leibniz system is defined by a GNHS* $(H,D,\mathcal{V})$ *and a convenient admissible submanifold. Moreover*, H *can be chosen to be hyperregular and* $\mathcal{V}$ *such that* $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}$ [*recall Eq.* (17)]. *Accordingly*, (h,D,Π) *can be derived as being the Hamiltonian side of a triple* (L,C_K,C_V).

Proof: Consider a Leibniz system (h,D,Π). Let us define $Q=D$, and let us see D as the null section $i:D\hookrightarrow T^*Q$ of the cotangent bundle T^*Q. In these terms, D is given in coordinates by points (q,p) such that $p=0$. Define $\mathcal{V}=\ker(\pi_*)|_D$, being $\pi:T^*Q\to Q$ the canonical projection. Note that $TD,\mathcal{V}\subset T^*_DT^*Q$ are Lagrangian distributions along D, with respect to the canonical 2-form ω of T^*Q. In coordinates we have

$$TD=TD^\perp=\{(q,p,\dot q,\dot p):p=0\ \textit{and}\ \dot p=0\},\tag{46}$$

and

$$\mathcal{V}=\mathcal{V}^\perp=\{(q,p,\dot q,\dot p):p=0\ \textit{and}\ \dot q=0\}.\tag{47}$$

It is clear that $T_DT^*Q=TD\oplus\mathcal{V}^\perp$ and also $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V})=\mathcal{V}$.

Now, let us consider the map

$$\Psi = \omega_D^\flat i_* \Pi^\sharp : T^*D \to T^*_D T^*Q,$$

and a related distribution

$$\mathcal{N}^\flat = (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat})(T^*D) \subset T^*_D T^*Q.$$

Note that range of $\omega_D^\flat i_* \Pi^\sharp$ is TD^o, since $TD^\flat = (TD^\perp)^o = TD^o$. Then, $i^*|_{\mathcal{N}^\flat}$ is a bijection between T^*D and its range, in fact

$$i^*\big|_{\mathcal{N}^\flat}(\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat}) = i^* \mathrm{j}_{\mathcal{V}^\flat} = \mathrm{id}_{T^*D},$$

and for all $\nu \in \mathcal{N}^\flat$, since $\nu = (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat})(d)$ for some $d \in T^*D$,

$$(\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat}) i^*\big|_{\mathcal{N}^\flat}(\nu) = (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat}) i^* (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat})(d)$$

$$= (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat})(d) = \nu.$$

As a consequence, decomposition $T_D T^*Q = TD \oplus \mathcal{N}^\perp$ holds, and the related map $\mathrm{j}_{\mathcal{N}^\flat} = (i^*|_{\mathcal{N}^\flat})^{-1}$ is given by

$$\mathrm{j}_{\mathcal{N}^\flat} = \omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat}.$$

Moreover, since range of $\omega_D^\sharp \mathrm{j}_{\mathcal{V}^\flat}$ is $\mathcal{V} = \mathcal{V}^\perp$ (and consequently $\mathrm{j}^*_{\mathcal{V}^\flat} = \mathfrak{p}_{\mathcal{V}^\perp}$ is null there), and $\mathrm{j}^*_{\mathcal{V}^\flat} i_* = \mathfrak{p}_{\mathcal{V}^\perp} i_* = \mathrm{id}_{TD}$, it follows that

$$\mathrm{j}^*_{\mathcal{V}^\flat} \omega_D^\sharp \mathrm{j}_{\mathcal{N}^\flat} = \mathrm{j}^*_{\mathcal{V}^\flat} \omega_D^\sharp (\omega_D^\flat i_* \Pi^\sharp + \mathrm{j}_{\mathcal{V}^\flat}) = \mathrm{j}^*_{\mathcal{V}^\flat} (i_* \Pi^\sharp + \omega_D^\sharp \mathrm{j}_{\mathcal{V}^\flat})$$

$$= \mathrm{j}^*_{\mathcal{V}^\flat} i_* \Pi^\sharp + \mathrm{j}^*_{\mathcal{V}^\flat} \omega_D^\sharp \mathrm{j}_{\mathcal{V}^\flat} = \Pi^\sharp.$$

Let us see that a hyperregular Hamiltonian H such that $H \circ i = h$ and $\mathrm{d}H|_D \in \mathcal{N}^\flat$ can be constructed. Consider a metric Φ on T^*Q, and define the Hamiltonian function

$$H(\alpha_q) = \tfrac{1}{2}\Phi(\alpha_q, \alpha_q) + \Pi(\alpha_q, \mathrm{d}h_q) + h \circ \pi(\alpha_q), \quad \alpha_q \in T^*Q.$$

In coordinates,

$$H(q,p) = \frac{1}{2} p_i \Phi^{ij}(q) p_j + p_i \Pi^{ij}(q) \frac{\partial h}{\partial q^j}(q) + h(q),$$

being $\Phi^{ij}(q)$ and $\Pi^{ij}(q)$ the matrix elements on a point q of the bilinear maps Φ and Π. It is clear that $H \circ i = h$, and it can be shown that

$$\mathrm{d}H|_D = \omega_D^\flat i_* \Pi^\sharp(\mathrm{d}h) + \mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}h) = \mathrm{j}_{\mathcal{N}^\flat}(\mathrm{d}h).$$

This easily follows from Eqs. (46) and (47), and the fact that

$$\frac{\partial H}{\partial q^i}(q,0) = \frac{\partial h}{\partial q^i}(q) \quad \textit{and} \quad \frac{\partial H}{\partial p_i}(q,0) = \Pi^{ij}(q) \frac{\partial h}{\partial q^j}(q).$$

Summing up, from (h, D, Π) we have constructed a GNHS $(H, D, \mathcal{V})$ and a related admissible pair $(\mathcal{V}, \Psi)$, such that $H \circ i = h$ and the derived bracket coincides exactly with Π. The fact that H is hyperregular and $\mathfrak{s}^{-1}\mathfrak{s}(\mathcal{V}) = \mathcal{V}$ ensures that $(H, D, \mathcal{V})$ has a Lagrangian counterpart. ■

B. Local construction for the linear and affine cases

When $\mathbb{F}H(D)$ is an affine subbundle of TQ, then

$$\mathcal{K} = \pi_*^{-1}(\mathbb{F}H(D))\big|_D = \pi_*^{-1}(\mathbb{F}H(D)_{\text{vec}} + \nu)\big|_D = \mathcal{K}_{\text{vec}} + \sigma,$$

with σ a fixed section of $T_D T^*Q$ such that $\pi_*(\sigma) - v \in \mathbb{F}H(D)_{\text{vec}}$. Let us suppose $\mathcal{K}_{\text{vec}}$ is a complement of $TD^\perp$ in $T_D T^*Q$ (e.g., if H is normal, as follows from Lemma 15). Then, there exists a unique section σ inside $TD^\perp$ such that $\mathcal{K} = \mathcal{K}_{\text{vec}} + \sigma$. In what follows, σ will always denote such a section. We know from Lemma 16 that $\mathrm{d}H\big|_D \in \mathcal{K}^\flat$. On the other hand, $\mathcal{K}^\flat = \mathcal{K}_{\text{vec}}^\flat + \sigma^\flat$ with $\sigma^\flat \in TD^o$.Accordingly we can write

$$\mathcal{K}^\flat = \mathrm{j}_{\mathcal{K}^\flat}(T^*D), \quad \mathrm{j}_{\mathcal{K}^\flat} = \Sigma + \mathrm{j}_{\mathcal{K}_{\text{vec}}^\flat},$$

being $\Sigma : T^*D \to T_D^* T^*Q : \alpha \mapsto (\sigma^\flat)_x$ for all $x \in D$ and $\alpha \in T_x^* D$. Thus, $\mathcal{K}$ satisfies admissibility conditions (a) and (b). Note also [from (44)]

$$\sigma = \Sigma(\mathrm{d}H_D) = \omega_D^\sharp(\mathrm{d}H\big|_D - \mathrm{j}_{\mathcal{K}_{\text{vec}}^\flat}(\mathrm{d}H_D)). \tag{48}$$

Using all that, the next result follows straightforwardly.

Proposition 26: *Given a triple* $(H, D, \mathcal{V})$ *such that* $\mathbb{F}H(D)$ *is an affine subbundle of* TQ, *and* $T_D T^*Q = TD \oplus \mathcal{K}_{\text{vec}}^\perp$, *the dynamics of the system is described in terms of the bracket*

$$\{f,g\} = \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{K}^\flat}(\mathrm{d}g))$$

$$= \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \mathrm{j}_{\mathcal{K}_{\text{vec}}^\flat}(\mathrm{d}g)) + \Lambda_D(\mathrm{j}_{\mathcal{V}^\flat}(\mathrm{d}f), \sigma^\flat),$$

or equivalently

$$\{f,g\} = \{f,g\}_{\text{bilin}} + \langle \mathrm{d}f, \mathrm{j}_{\mathcal{V}^\flat}^*(\sigma)\rangle, \quad \{f,g\}_{\text{bilin}} = \langle \mathrm{d}f, \mathrm{j}_{\mathcal{V}^\flat}^* \omega_D^\sharp \mathrm{j}_{\mathcal{K}_{\text{vec}}^\flat}(\mathrm{d}g)\rangle, \tag{49}$$

being σ *the section of* $TD^\perp$ *that enables us to write* $\mathcal{K} = \mathcal{K}_{\text{vec}} + \sigma$.

Remark 27: *Note that*, *if* D *is coisotropic*, *i.e.*, $TD^\perp \subset TD$, *then* $\sigma \in TD$ *and consequently*

$$\{f,g\} = \{f,g\}_{\text{bilin}} + \langle \mathrm{d}f, \sigma\rangle.$$

The bracket above is related to the admissible pair $(\mathcal{K}_{\text{vec}}, \Sigma)$ and, clearly, it is naturally associated to $(H, D, \mathcal{V})$. Of course, we can define a Leibniz bracket to describe the dynamic of these systems, as we have shown in Theorem 25.

Local procedure: In order to give an explicit description of brackets (49), we shall build in local coordinates the maps $\mathfrak{p}_{\mathcal{V}^\perp} = \mathrm{j}_{\mathcal{V}^\flat}^*$ and $\mathrm{j}_{\mathcal{K}_{\text{vec}}^\flat}$. We focus on systems with variational constraints that do not depend on momenta ($l = 0$ case). In the D'Alembert's linear case $\mathcal{V} = \mathcal{K}_{\text{vec}} = \mathcal{K}$, we obtain the bracket of van der Schaft and Maschke.[9] It is worth mentioning that this procedure represents an alternative to that introduced in Ref. 33, to describe equations of motion for systems with affine kinematic constraints.

Let us consider a triple (L, C_K, C_V), such that $C_K = C_K^{\text{vec}} + v$, being v a section, and C_K^{vec} and C_V distributions on Q. We shall assume $\dim C_K = \dim C_V$. Then, in coordinates, C_K and C_V are given by equations of the form

$$w_i^a(q)\dot{q}^i = \gamma^a(q) \quad \text{and} \quad v_i^a(q)\delta q^i = 0, \quad a = 1, \ldots, k,$$

respectively. Of course, C_K^{vec} is given by $w_i^a(q)\dot{q}^i = 0$. On the Hamiltonian side we have the submanifold $D = \mathbb{F}L(C_K)$ given in coordinates by points (q,p) such that

$$w_i^a \frac{\partial H}{\partial p_i}(q,p) = \gamma^a, \quad a = 1, \ldots, k. \tag{50}$$

Related distributions $\mathcal{K}_{\text{vec}}$ and $\mathcal{V}$ read

$$\mathcal{K}_{\text{vec}} = \{(q,p,x,y):(q,p) \in D, w_i^a x^i = 0\} \tag{51}$$

and

$$\mathcal{V} = \{(q,p,x,y):(q,p) \in D, v_i^a x^i = 0\}. \tag{52}$$

We shall assume H is normal and $TD \cap \mathcal{V}^\perp = 0$, or equivalently $C_K^{(0)} \cap C_V = 0$ [recall Eq. (30)]. These facts ensure that there exist

$$v_a^i \quad \text{and} \quad Y_\alpha^i, \quad a = 1, \ldots, k \quad \text{and} \quad \alpha = 1, \ldots, n-k, \tag{53}$$

such that

$$v_i^a v_b^i = \delta_b^a, \quad v_i^a Y_\alpha^i = 0, \quad \text{and} \quad w_i^a v_b^i = \varphi_b^a \text{ is invertible}. \tag{54}$$

The last property is a direct consequence of Eq. (31). Moreover, if we define

$$\widetilde{p}_\alpha = Y_\alpha^i p_i \quad \text{and} \quad \hat{p}_a = v_a^i p_i, \tag{55}$$

then Eqs. (50) can be solved in terms of $\widetilde{p}$'s, i.e., we can write

$$\hat{p}_a = \hat{p}_a(q^i, \widetilde{p}_\alpha), \quad a = 1, \ldots, k.$$

It follows from the last assertion that we can choose local coordinates $(q, \widetilde{p})$ for D such that the embedding $i: D \hookrightarrow T^*Q$ is given by $i(q,\widetilde{p}) = (q, \widetilde{p}, \hat{p}(q,\widetilde{p}))$. Given an arbitrary element

$$X = \mu^i \frac{\partial}{\partial q^i} + \nu_\alpha \frac{\partial}{\partial \widetilde{p}_\alpha} + \varpi_a \frac{\partial}{\partial \hat{p}_a} \tag{56}$$

of $T_D T^*Q$, since elements of $\mathcal{V}^\perp$ are of the form $Y = \varpi_a \partial / \partial \hat{p}_a$, it follows that

$$\mathfrak{p}_{\mathcal{V}^\perp}(X) = \mathfrak{j}^*_{\mathcal{V}^\flat}(X) = \mu^i \frac{\partial}{\partial q^i} + \nu_\alpha \frac{\partial}{\partial \widetilde{p}_\alpha}, \tag{57}$$

seeing $\mathfrak{p}_{\mathcal{V}^\perp}$ as a map onto TD. Then, $\mathfrak{j}^*_{\mathcal{V}^\flat}: T_D T^*Q \to TD$ is locally given by a $(2n-k) \times 2n$ matrix

$$\mathbb{V} = \begin{pmatrix} \mathbb{I}_{2n-k} & \mathbb{O}_{(2n-k)\times k} \end{pmatrix}, \tag{58}$$

where $\mathbb{I}_r$ denotes the $r \times r$ identity matrix, and $\mathbb{O}_{r\times s}$ the $r \times s$ null matrix. On the other hand, in the same coordinates, $\omega^\sharp: T^*T^*Q \to TT^*Q$ is given by the $2n \times 2n$ matrix

$$\mathbb{J} = \begin{pmatrix} \{q,q\}_o & \{q,\widetilde{p}\}_o & \{q,\hat{p}\}_o \\ \{\widetilde{p},q\}_o & \{\widetilde{p},\widetilde{p}\}_o & \{\widetilde{p},\hat{p}\}_o \\ \{\hat{p},q\}_o & \{\hat{p},\widetilde{p}\}_o & \{\hat{p},\hat{p}\}_o \end{pmatrix}, \tag{59}$$

where $\{,\}_o$ denotes the canonical Poisson bracket. Of course, to obtain $\omega_D^\sharp$, we only need to consider the restriction $\mathbb{J}|_D$ of $\mathbb{J}$ to D. Now, let us derive local expressions for $\mathfrak{j}_{\mathcal{K}_{\text{vec}}^\flat}: T^*D \to T_D^* T^*Q$ and the section σ. We can do that simultaneously by using Eq. (48). The idea is to calculate $\mathrm{d}H_D$ in terms of $\mathrm{d}H|_D$, for generic H, and then invert the relation to obtain

$$\mathrm{d}H|_D = \mathfrak{j}_{\mathcal{K}_{\text{vec}}^\flat}(\mathrm{d}H_D) + \sigma^\flat.$$

Writing

$$\widetilde{H}(q,\widetilde{p},\hat{p}) = H(q, p(q,\widetilde{p},\hat{p})),$$

this will give us

$$\left.\begin{pmatrix} \dfrac{\partial \tilde{H}}{\partial q^j} \\ \dfrac{\partial \tilde{H}}{\partial \tilde{p}_\beta} \\ \dfrac{\partial \tilde{H}}{\partial \hat{p}_b} \end{pmatrix}\right|_D = \mathbb{K} \cdot \begin{pmatrix} \dfrac{\partial H_D}{\partial q^j} \\ \dfrac{\partial H_D}{\partial \tilde{p}_\beta} \end{pmatrix} + \begin{pmatrix} s_i \\ s^\alpha \\ s^a \end{pmatrix}, \tag{60}$$

being $\mathbb{K}$ a $2n \times (2n-k)$ rectangular matrix representing $\mathrm{j}_{\mathcal{K}^\flat_{\mathrm{vec}}}$, and s_i, s^α, s^a the coordinates of $\sigma^\flat$ with respect to such coordinates. Accordingly, the section σ can be obtained as

$$\sigma = \begin{pmatrix} \sigma^i \\ \sigma_\alpha \\ \sigma_a \end{pmatrix} = \mathbb{J}\Big|_D \cdot \begin{pmatrix} s_i \\ s^\alpha \\ s^a \end{pmatrix}. \tag{61}$$

Now let us start calculating. First, writing (50) in terms of $\tilde{H}$ we have

$$w_i^a \left(\left.\frac{\partial \tilde{H}}{\partial \tilde{p}_\alpha}\right|_D Y^i_\alpha + \left.\frac{\partial \tilde{H}}{\partial \hat{p}_b}\right|_D v^i_b \right) = \gamma^a. \tag{62}$$

Since $w_i^a v^i_b = \varphi^a_b$ is invertible (by construction), we can write

$$\left.\frac{\partial \tilde{H}}{\partial \hat{p}_a}\right|_D = \gamma^b (\varphi^{-1})^a_b - l^a_\alpha \left.\frac{\partial \tilde{H}}{\partial \tilde{p}_\alpha}\right|_D, \quad \text{being } l^a_\alpha = (\varphi^{-1})^a_b w^b_i Y^i_\alpha. \tag{63}$$

Using that, we have

$$\frac{\partial H_D}{\partial q^i} = \left.\frac{\partial \tilde{H}}{\partial q^i}\right|_D + \left.\frac{\partial \tilde{H}}{\partial \hat{p}_a}\right|_D \frac{\partial \hat{p}_a}{\partial q^i}$$

$$= \left.\frac{\partial \tilde{H}}{\partial q^i}\right|_D - l^a_\alpha \frac{\partial \hat{p}_a}{\partial q^i} \left.\frac{\partial \tilde{H}}{\partial \tilde{p}_\alpha}\right|_D + \gamma^b (\varphi^{-1})^a_b \frac{\partial \hat{p}_a}{\partial q^i}$$

and

$$\frac{\partial H_D}{\partial \tilde{p}_\alpha} = \left.\frac{\partial \tilde{H}}{\partial \tilde{p}_\alpha}\right|_D + \left.\frac{\partial \tilde{H}}{\partial \hat{p}_a}\right|_D \frac{\partial \hat{p}_a}{\partial \tilde{p}_\alpha}$$

$$= \left(\delta^\alpha_\beta - l^a_\beta \frac{\partial \hat{p}_a}{\partial \tilde{p}_\alpha}\right) \left.\frac{\partial \tilde{H}}{\partial \tilde{p}_\beta}\right|_D + \gamma^b (\varphi^{-1})^a_b \frac{\partial \hat{p}_a}{\partial \tilde{p}_\alpha}.$$

Since decomposition $T^*_D T^* Q = TD^o \oplus \mathcal{K}^\flat_{\mathrm{vec}}$ holds (which in the present case follows from normality of H), it can be shown that the matrix

$$\psi^\alpha_\beta = \delta^\alpha_\beta - l^a_\beta \frac{\partial \hat{p}_a}{\partial \tilde{p}_\alpha} \tag{64}$$

is invertible. Then, we can write derivatives of $\widetilde{H}$ restricted to D in terms of those of H_D as (i.e., $\mathrm{d}H|_D$ as a function of $\mathrm{d}H_D$)

$$\left.\frac{\partial \widetilde{H}}{\partial q^i}\right|_D = \frac{\partial H_D}{\partial q^i} + [\Lambda_1]_{i\alpha}\frac{\partial H_D}{\partial \widetilde{p}_\alpha} + s_i,$$

$$\left.\frac{\partial \widetilde{H}}{\partial \widetilde{p}_\alpha}\right|_D = [\Lambda_2]^\alpha_\beta \frac{\partial H_D}{\partial \widetilde{p}_\beta} + s^\alpha,$$

$$\left.\frac{\partial \widetilde{H}}{\partial \hat{p}_a}\right|_D = [\Lambda_3]^a_\alpha \frac{\partial H_D}{\partial \widetilde{p}_\alpha} + s^a,$$

being

$$[\Lambda_1]_{i\alpha} = (\psi^{-1})^\beta_\alpha I^a_\beta \frac{\partial \hat{p}_a}{\partial q^i}, \quad [\Lambda_2]^\alpha_\beta = (\psi^{-1})^\alpha_\beta,$$

$$[\Lambda_3]^a_\alpha = -(\psi^{-1})^\beta_\alpha I^a_\beta, \tag{65}$$

and

$$s_i = -\gamma^b(\varphi^{-1})^a_b\left([\Lambda_1]_{i\alpha}\frac{\partial \hat{p}_a}{\partial \widetilde{p}_\alpha} + \frac{\partial \hat{p}_a}{\partial q^i}\right),$$

$$s^\alpha = -\gamma^b(\varphi^{-1})^a_b[\Lambda_2]^\alpha_\beta \frac{\partial \hat{p}_a}{\partial \widetilde{p}_\beta},$$

$$s^a = -\gamma^b(\varphi^{-1})^c_b\left([\Lambda_3]^a_\alpha \frac{\partial \hat{p}_c}{\partial \widetilde{p}_\alpha} - \delta^a_c\right). \tag{66}$$

Accordingly, having Eq. (60) in mind, the matrix $\mathbb{K}$ is given by

$$\mathbb{K} = \begin{pmatrix} \mathbb{I}_n & \Lambda_1 \\ \mathbb{O}_{(n-k)\times n} & \Lambda_2 \\ \mathbb{O}_{k\times n} & \Lambda_3 \end{pmatrix}, \tag{67}$$

and components $\sigma^i, \sigma_\alpha, \sigma_a$ follows from (61).

With all that, the bilinear part of bracket (49), given by $\mathrm{j}^*_{\mathcal{V}^\flat}\omega_D^\sharp \mathrm{j}_{\mathcal{K}^\flat_{\mathrm{vec}}}$, is

$$\{f,g\}_{\mathrm{bilin}} = \left(\frac{\partial f}{\partial q}\frac{\partial f}{\partial \widetilde{p}}\right)\cdot \mathbb{V}\cdot \mathbb{J}|_D \cdot \mathbb{K}\cdot \begin{pmatrix} \dfrac{\partial g}{\partial q} \\ \dfrac{\partial g}{\partial \widetilde{p}} \end{pmatrix}. \tag{68}$$

In the D'Alembertian case, i.e., when $\mathcal{V}=\mathcal{K}_{\mathrm{vec}}$, or equivalently $C_V = C_K^{\mathrm{vec}}$, since we can take $v_i^a = w_i^a$, we have [recall (54)]

$$\varphi^a_b = \delta^a_b, \quad I^a_\alpha = 0 \text{ and } \psi^\alpha_\beta = \delta^\alpha_\beta.$$

Thus,

$$\mathbb{K}=\begin{pmatrix} \mathbb{I}_n & \mathbb{O}_{n\times(n-k)} \\ \mathbb{O}_{(n-k)\times n} & \mathbb{I}_{n-k} \\ \mathbb{O}_{k\times n} & \mathbb{O}_{k\times(n-k)} \end{pmatrix}=\begin{pmatrix} \mathbb{I}_{2n-k} \\ \mathbb{O}_{k\times(2n-k)} \end{pmatrix}=\mathbb{V}^t,$$

and

$$\mathbb{V}\cdot\mathbb{J}|_D\cdot\mathbb{K}=\mathbb{V}\cdot\mathbb{J}|_D\cdot\mathbb{V}^t$$

gives exactly the antisymmetric matrix appearing in Ref. 9.

Finally, adding the term containing the section σ, since

$$\mathbb{V}^t\cdot\begin{pmatrix} \sigma^i \\ \sigma_\alpha \\ \sigma_a \end{pmatrix}=\begin{pmatrix} \sigma^i \\ \sigma_\alpha \end{pmatrix},$$

the total bracket becomes [see Eq. (49)]

$$\{f,g\}=\{f,g\}_{\text{bilin}}+\left(\frac{\partial f}{\partial q^i}\frac{\partial f}{\partial\tilde{p}_\alpha}\right)\cdot\begin{pmatrix} \sigma^i \\ \sigma_\alpha \end{pmatrix},$$

and equations of motion read

$$\dot{q}^i=\{q^i,H_D\}_{\text{bilin}}+\sigma^i,\quad \dot{\tilde{p}}_\alpha=\{\tilde{p}_\alpha,H_D\}_{\text{bilin}}+\sigma_\alpha.$$

Summing up, given a GNHS $(H,D,\mathcal{V})$ such that H is normal and $T_DT^*Q=TD\oplus\mathcal{V}^\perp$ holds, in order to write down the bracket (49) we must

(1) define v_a^i and Y_α^i obeying (54), and coordinates $(q,\tilde{p},\hat{p})$ given in (55);
(2) construct the function $\hat{p}=\hat{p}(q,\tilde{p})$ [using (62) to set $\hat{p}$ as a function of $q,\tilde{p}$],
(3) calculate matrices $\mathbb{V}$, $\mathbb{J}$ and $\mathbb{J}|_D$ [see (58) and (59)],
(4) calculate matrix $\mathbb{K}$ in terms of φ, l, and ψ [see (54), (63)–(65), and (67)];
(5) construct the section's components σ^i,σ_α from (61) and (66).

Note that all above objects only depend on data w_i^a, γ^a, and v_i^a.

Brackets for the inverted pendulum: Let us come back to the inverted pendulum. Suppose again that we have affine kinematic constraints given by $\dot{x}-\rho(\theta)\dot{\theta}=\gamma(\theta)$, and variational constraints $\delta x=0$. Then, the number of equations is $k=1$, and vectors w_i^a and v_i^a are $w=(1,-\rho)$ and $v=(1,0)$, respectively. From steps (1) and (2) we have

$$\tilde{p}=p_\theta,\quad \hat{p}=p_x,\quad \hat{p}(x,\theta,\tilde{p})=\chi(\theta)\tilde{p}+\phi(\theta)$$

[see (22) and (23)], and matrices $\mathbb{V}$, $\mathbb{J}$, and $\mathbb{J}|_D$ of step (3) are given by

$$\mathbb{V}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}\quad\text{and}\quad \mathbb{J}=\mathbb{J}|_D=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

Since φ, l, and ψ are in this case

$$\varphi=1,\quad l=-\rho,\quad \psi=1+\rho\chi,$$

it follows that

$$[\Lambda_1]_i = -\frac{\rho}{1+\rho\chi}\frac{\partial \hat{p}}{\partial q^i}, \quad \Lambda_2 = \frac{1}{1+\rho\chi}, \quad \Lambda_3 = \frac{\rho}{1+\rho\chi}$$

and accordingly [see step (4)]

$$\mathbb{K} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\dfrac{\rho\Delta}{1+\rho\chi} \\ 0 & 0 & \dfrac{1}{1+\rho\chi} \\ 0 & 0 & \dfrac{\rho}{1+\rho\chi} \end{pmatrix},$$

being

$$\Delta = \tilde{p}\frac{\mathrm{d}\chi}{\mathrm{d}\theta} + \frac{\mathrm{d}\phi}{\mathrm{d}\theta}. \tag{69}$$

Thus,

$$\mathbb{V}\cdot\mathbb{J}|_D\cdot\mathbb{K} = \begin{pmatrix} 0 & 0 & \dfrac{\rho}{1+\rho\chi} \\ 0 & 0 & \dfrac{1}{1+\rho\chi} \\ 0 & -1 & \dfrac{\rho\Delta}{1+\rho\chi} \end{pmatrix}.$$

Now, following step (5), we have

$$s_i = -\frac{\gamma}{1+\rho\chi}\frac{\partial \hat{p}}{\partial q^i}, \quad \tilde{s} = -\frac{\gamma\chi}{1+\rho\chi}, \quad \hat{s} = \frac{\gamma}{1+\rho\chi},$$

and so

$$\sigma = \frac{\gamma}{1+\rho\chi}\begin{pmatrix} 1 \\ -\chi \\ \Delta \end{pmatrix}.$$

In conclusion, the *natural* bracket related to the inverted pendulum with affine constraints is

$$\{f,g\} = \frac{\partial f}{\partial x}\frac{\rho}{1+\rho\chi}\frac{\partial g}{\partial \tilde{p}} + \frac{\partial f}{\partial \theta}\frac{1}{1+\rho\chi}\frac{\partial g}{\partial \tilde{p}} - \frac{\partial f}{\partial \tilde{p}}\left(\frac{\partial g}{\partial \theta} - \frac{\rho\Delta}{1+\rho\chi}\frac{\partial g}{\partial \tilde{p}}\right)$$

$$+ \frac{\gamma}{1+\rho\chi}\left(\frac{\partial f}{\partial x} - \chi\frac{\partial f}{\partial \theta} + \Delta\frac{\partial f}{\partial \tilde{p}}\right).$$

Note that for virtual constraints, where $\rho(\theta) = -L\cos\theta$ and $\gamma(\theta) = 0$, we have a Leibniz bracket. In such a case, it follows from Eq. (23) that

$$\chi(\theta) = \frac{m(l\sin\theta + L\cos\theta)}{mLl\cos\theta\sin\theta - I}, \quad \phi(\theta) = 0,$$

and accordingly [see (69)]

$$\Delta(\theta,\tilde{p}) = \tilde{p}\frac{\chi(\theta-\pi/2)(mLl\cos\theta\sin\theta+I)-\chi(\theta)mLl\cos 2\theta}{mLl\cos\theta\sin\theta-I}.$$

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Geodesics and Killing tensors in mechanics

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Killing tensors give polynomial constants of the geodesic motion. The trajectories of a conservative mechanical system correspond to geodesics when the kinetic energy metric is conformally scaled to the Jacobi metric. Alternatively, the trajectories may be related to geodesics of some higher-dimensional warped product manifold. These two different ways of relating mechanical trajectories to geodesics are reviewed and compared. It is shown how a relation between Killing tensors on configuration space and the potential gives rise to Killing tensors on both the Jacobi and warped product manifolds. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The simplest mechanical system is that of a free point particle. That is, a particle whose motion in a (pseudo)-Riemannian configuration space is determined by the kinetic energy Lagrangian T, which is essentially the metric tensor. The trajectories in configuration space are just geodesics.

More general than the free mechanical systems are the conservative ones, where the kinetic energy Lagrangian is modified by the addition of a potential, $L=T-V$. Whereas the trajectories are clearly not geodesics of the kinetic energy metric, they are geodesics (or more accurately may be reparametrized to be geodesics) of a conformally related metric, the Jacobi metric.[1] The Jacobi metric is obtained by a scaling that not only involves the potential V, but the total energy $E=T+V$, so that the geodesics of a given metric describe only the trajectories of a fixed energy.

There is another, less well known, way of representing the trajectories of a conservative mechanical system as geodesics. The configuration space may be extended in dimension, and the kinetic energy metric and potential used to construct a warped (pseudo)-Riemannian product structure, in such a way that geodesics on this warped product project to trajectories on configuration space. This approach was introduced by Eisenhart[2] who added an extra dimension to configuration space to represent trajectories as geodesics.

There are several reasons why it may be useful to recognize trajectories of a mechanical system as geodesics. One is related to the matter of stability. The behavior of nearby geodesics is governed by the curvature, through the Jacobi equation. Thus the stability of any mechanical system that can be formulated as a geodesic one is amenable to examination by computing the curvature tensor. This has been the motivation of Refs. 3–5. Arnold[6] has shown how one can approach the hydrodynamics of an ideal fluid by recognizing the motion as geodesic for an appropriate metric.

Another reason why it is useful to recognize a mechanical system as a geodesic one is related to Killing tensors. For a geodesic system polynomial constants of the motion are given by Killing tensors. Thus the observation that many mechanical systems can be formulated as geodesic ones gives Killing tensors a wider range of applicability than might be immediately obvious. This

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observation is made in (for example) Ref. 7. One approach then, to finding integrable systems, is to find manifolds admitting nontrivial Killing tensors. This approach has been followed, in two dimensions, by Rosquist and Pucacco.[8]

As well as leading to constants of the geodesic motion, Killing tensors are also related to higher-order symmetries of the Laplacian.[9] In order to have a higher-order symmetry it is certainly necessary to have a Killing tensor, but it is not clear that this is sufficient.[10] To clarify this matter it is useful to look at examples. However, in general, nontrivial Killing tensors are hard to come by. In this regard it is useful to observe that, formulated as geodesic systems, known examples of superintegrable systems provide us with a source of examples of manifolds with nontrivial Killing tensors.

In this paper a condition is established that enables Killing tensors to be constructed on a warped product manifold from Killing tensors on the base. Since geodesics on warped products project to curves on the base that can be interpreted as Newtonian curves, this condition on Killing tensors can be interpreted as a (generalized) Bertrand-Darboux equation relating the Killing tensor to the potential. Recently Jelonek[11] has shown how Killing tensors can arise naturally on Riemannian warped products, and so it is interesting to see how the geometry of warped products provides a link to classical mechanics and integrable systems.

Since Killing tensors are totally symmetric tensors, we begin in Sec. II by introducing necessary notation and conventions for the totally symmetric tensor algebra. In Sec. III we review some properties of Killing tensors that we will need later. Here conformal Killing tensors are also mentioned, anticipating the conformal scaling in mechanics that gives the Jacobi metric. We examine conditions relating Killing tensors and the conformal factor that enable Killing tensors to be constructed on the conformally related manifold.

In Sec. IV we use the preceding formalism to show how Killing tensors on configuration space can give rise to Killing tensors with respect to the Jacobi geometry. The previously established condition for this is, in the mechanical context, a relation between the Killing tensor and the potential that can be recognized as a generalized Bertrand-Darboux equation.

Section V reviews some properties of warped products. In Sec. VI it is shown how Killing tensors on the base can lead to Killing tensors on the warped product. The necessary condition, relating the Killing tensor on the base and the warping function, can be recognized as the generalized Bertrand-Darboux equation if we choose to identify the projection of geodesics onto the base with Newtonian curves. The Eisenhart geometry is just a special case of a warped product with one-dimensional fiber.

Sections V and VI can be read independent of Secs. III and IV: we present some results on Killing tensors on warped products that can be taken without any mention of mechanics. Clearly however, the results presented in Sec. VI parallel those presented for conformally related metrics in Sec. III. In the final section we discuss the exact relation between the results of these different sections.

II. THE TOTALLY SYMMETRIC TENSOR ALGEBRA

We are going to consider Killing tensors, which are totally symmetric tensors. Thus some conventions for the totally symmetric tensor algebra are introduced here first. (It can be noted by anyone more familiar with the exterior algebra that all the conventions and notation here have exterior analogues, only there an extra sign comes from the sign of the permutation.)

The symmetrizing map $\mathcal{S}$ maps any tensor to a totally symmetric one,

$$(\mathcal{S}S)(X_1,X_2,\ldots,X_p)=\frac{1}{p!}\sum_{\sigma} S(X_{\sigma(1)},X_{\sigma(2)},\ldots,X_{\sigma(p)}), \tag{1}$$

where σ is an element of the permutation group. The map $\mathcal{S}$ is a projection operator,

$$\mathcal{S} \circ \mathcal{S} = \mathrm{Id}. \tag{2}$$

We can define a multiplication on symmetric tensors by taking the tensor product and then symmetrizing

$$S \odot T = \mathcal{S}(S \otimes T). \tag{3}$$

This symmetric tensor product makes the totally symmetric tensors into a commutative associative algebra.

If X is some vector field then the contraction map C_X just maps a 1-form A to $A(X)$. The contraction map can be extended to a map on covariant tensors by requiring it to act as a derivation on tensor products. It then follows that $\mathcal{S}C_X = C_X\mathcal{S}$ and so C_X maps totally symmetric tensors to totally symmetric tensors of one lower degree. We have

$$C_X(S \odot T) = C_X S \odot T + S \odot C_X T, \tag{4}$$

$$C_X C_Y = C_Y C_X, \tag{5}$$

$$(C_{X_1} S)(X_2, X_3, \ldots, X_p) = pS(X_1, X_2, \ldots, X_p), \tag{6}$$

$$\theta^a \odot C_{X_a} S = pS, \tag{7}$$

where p is the degree of S, and $\{\theta^a\}$ is dual to $\{X_a\}$.

When we have a metric g (and we always will have when considering Killing tensors) we can define a trace by an invariant double contraction,

$$\mathrm{Tr}\, S = g^{ab} C_{X_a} C_{X_b} S = C_{X^a} C_{X_a} S. \tag{8}$$

The covariant derivative operator, with respect to a vector field X, ∇_X, acts as a derivation on the tensor algebra. Since ∇_X commutes with $\mathcal{S}$ then it is also a derivation on the symmetric tensor algebra. We may define the divergence of a symmetric tensor by following differentiation with contraction:

$$\mathrm{div}\, S = C_{X^a} \nabla_{X_a} S. \tag{9}$$

The covariant derivative of a tensor S, ∇S, is a tensor of one higher covariant degree. The symmetrized covariant derivative of a symmetric tensor may be defined by

$$\nabla \odot S = \mathcal{S}(\nabla S). \tag{10}$$

If $\{\theta^a\}$ is dual to $\{X_a\}$ then

$$\nabla \odot S = \mathcal{S}(\nabla_{X_a} S \otimes \theta^a) = \nabla_{X_a} S \odot \theta^a. \tag{11}$$

It then follows that $\nabla\odot$ acts as a derivation on the symmetric tensor algebra.

III. KILLING TENSORS

Killing vectors generate isometries. So if K is a Killing vector of the metric g then the Lie derivative of g with respect to K must vanish, $\mathcal{L}_K g = 0$. This can be recast as a differential equation for K; Killing's equation,

$$g(\nabla_X K, Y) + g(\nabla_Y K, X) = 0, \tag{12}$$

where ∇ is the (pseudo)-Riemannian connection of g. If $K^\flat$ is the 1-form metrically related to K then Killing's equation requires the symmetrized derivative of $K^\flat$ to vanish,

$$\nabla_X K^\flat(Y) + \nabla_Y K^\flat(X) = 0, \tag{13}$$

$$\text{or } \nabla \odot K^\flat = 0. \tag{13'}$$

A Killing tensor obeys a generalization of Killing's equation. It is a totally symmetric (covariant) tensor whose symmetrized covariant derivative vanishes. That is,

$$\nabla \odot S = 0. \tag{14}$$

In generalizing Killing's equation from an equation for a vector field to one for a tensor, the clear geometrical interpretation is lost. However, one immediate consequence is that Killing tensors give constants of the geodesic motion. If C is geodesic, and S is Killing, then it immediately follows from (14) that $S(\dot{C},\dot{C},\ldots,\dot{C})$ is constant along C,

$$\dot{C}(S(\dot{C},\dot{C},\ldots,\dot{C})) = 0. \tag{15}$$

(It is important to note here that a geodesic is a curve that parallel transports its tangent vector, $\nabla_{\dot{C}}\dot{C}=0$. A curve satisfying $\nabla_{\dot{C}}\dot{C}=f\dot{C}$ for some function f may be reparameterized to become geodesic. Such a curve will be called pregeodesic. Although this terminology is usual it is not universal, with some authors calling geodesic that which is here called pregeodesic.)

The space of Killing tensors is closed under the symmetrized tensor product. Since Killing vectors, and the metric tensor, are certainly Killing tensors, we can always form higher degree Killing tensors from sums of their symmetrized tensor products. Such Killing tensors are called trivial, or reducible. Killing tensors are also closed under a nonassociative product, the Schouten bracket (or symmetric Schouten concomitant), as will be discussed below.

So far we have taken Killing tensors to be covariant, for then it makes sense to symmetrize the covariant derivative. However, since the notion of Killing tensor relies upon the existence of a metric, we can always use that metric to type change tensors. [The connection in Killing's equation is the (pseudo) Riemannian one, and here only torsion-free metric compatible connections will be considered.] The totally symmetric contravariant tensors on M naturally correspond to functions on T^*M that are polynomial in the fiber coordinate. That is, in the context of mechanics, polynomial in the momenta. Thus the symmetric contravariant tensor S corresponds to the function F_S defined by $F_S(\omega)=S(\omega,\omega,\ldots,\omega)$. In local coordinates, $F_S=S^{ab\cdots}p_a p_b\cdots$.

In particular, the kinetic energy Hamiltonian, T, is (up to a factor of 2) the function corresponding to the metric tensor g,

$$T = \tfrac{1}{2} g^{ab} p_a p_b. \tag{16}$$

The associative algebra of symmetric tensors on M, under the symmetrized tensor product, is isomorphic to the algebra of polynomial functions on T^*M under multiplication. The canonical symplectic structure of T^*M defines a Poisson bracket on functions. Functions on T^*M that are polynomial in the momenta are closed under the Poisson bracket. The natural correspondence between polynomial functions and symmetric tensors then enables a bracket to be induced on symmetric tensors. This is the Schouten bracket. That is, the Lie algebra of polynomial functions on T^*M, under the Poisson bracket, is isomorphic to the Lie algebra of symmetric contravariant tensors on M under the Schouten bracket.

The condition that a contravariant tensor S is Killing can be expressed in the following equivalent ways:

$$[S,g] = 0, \tag{17}$$

$$\{F_S,T\} = 0, \tag{18}$$

$$X_T F_S = 0. \tag{19}$$

In (17) [,] denotes the Schouten bracket,[12] with {, } denoting the Poisson bracket in (18). The equivalence of (17) and (18) is just the stated isomorphism between symmetric tensors, under the Schouten bracket, and polynomial functions, under the Poisson bracket. In (19) X_T is the Hamiltonian vector field of the kinetic energy Hamiltonian. Equation (19) gives perhaps the clearest geometrical interpretation of Killing tensors: they are tensors that correspond to polynomial functions that are invariant under the geodesic flow.

A conformal Killing tensor satisfies a conformally covariant generalization of (14). Namely, for a degree-p tensor S,

$$\nabla \odot S = \phi \odot g, \tag{20}$$

where ϕ is some totally symmetric tensor of degree $p-1$. In fact ϕ can be expressed in terms of S and its derivatives by (repeatedly) taking the trace of (20). For example, if S is of degree 2 then we get, in n-dimensions,

$$(n+4)\phi = \nabla \odot \mathrm{Tr}\, S + 2\ \mathrm{div}\, S. \tag{21}$$

For S of degree 3, for example, we arrive at a similar expression by taking another trace of (20).

Sometimes a definition of conformal Killing tensors is taken that further requires them to be trace-free (as discussed in Ref. 13, for example). The reason for this is that (20) is satisfied by any multiple of the metric tensor. In fact if S is any solution to (20) (with the degree of S two or more) then, for an arbitrary symmetric tensor ρ, so is

$$S' = S + \rho \odot g \tag{22}$$

with

$$\phi' = \phi + \nabla \odot \rho. \tag{23}$$

This arbitrariness in solutions to (20) can be removed by requiring the trace to vanish. Here the trace-free requirement will not be imposed on conformal Killing tensors, since it is useful to have the conformal Killing tensors include all the Killing ones (and these are not all trace-free).

It has already been stated that (20) is a conformally covariant generalization of (14). This will now be demonstrated. If $\hat{g}$ is a conformally related to g then the respective Riemannian connections are related by

$$\hat{g} = e^{2\lambda} g, \tag{24}$$

$$\hat{\nabla}_X Y = \nabla_X Y + (X\lambda)Y + (Y\lambda)X - g(X,Y)\mathrm{grad}\,\lambda \tag{25}$$

$$= \nabla_X Y + (X\lambda)Y + (Y\lambda)X - \hat{g}(X,Y)\widehat{\mathrm{grad}}\,\lambda. \tag{25'}$$

Then for ω a 1-form

$$\hat{\nabla} \odot \omega = \nabla \odot \omega + C_{\mathrm{grad}\,\lambda}\omega g - 2\ \mathrm{d}\lambda \odot \omega,$$

from which it follows, from induction, that for S of degree p,

$$\hat{\nabla} \odot S = \nabla \odot S + C_{\mathrm{grad}\,\lambda} S \odot g - 2p\ \mathrm{d}\lambda \odot S. \tag{26}$$

From this it follows that, if the metric is scaled as in (24), and S is of degree p, then (20) is covariant under the following transformations:

$$\hat{S} = e^{2p\lambda} S, \tag{27}$$

$$\hat{\phi} = e^{2(p-1)\lambda}(\phi + C_{\text{grad }\lambda} S). \tag{28}$$

Now if K is a Killing vector of the metric g, then it will also be a Killing vector of a conformally related metric $\hat{g}$ only if the scale function is invariant under K. More generally, if S is any (covariant) Killing tensor of the metric g, then it is also Killing for the metric $\hat{g}=s^{2\lambda}g$ if $C_{\text{grad }\lambda}S=0$. However, there is a more general way in which we can obtain Killing tensors on $(M,\hat{g})$ from those on (M,g).

Proposition 1: Suppose that S is a degree p Killing tensor with respect to g, with $p \geqslant 2$, that additionally satisfies

$$e^{2(p-1)\lambda} C_{\text{grad }\lambda} S = -\hat{\nabla} \odot \Omega \tag{29}$$

for some symmetric tensor Ω. Then $\hat{S}=e^{2p\lambda}S+\Omega\odot\hat{g}$ is a Killing tensor with respect to $\hat{g}=e^{2\lambda}g$.

Proof: Since S is Killing with respect to g it is certainly conformal Killing. Then, from (27) and (28) $e^{2p\lambda}S$ is conformal Killing with respect to $\hat{g}=e^{2\lambda}g$ with $\hat{\phi}=e^{2(p-1)\lambda}C_{\text{grad }\lambda}S$. If we then assume the extra condition (29), then it follows from (22) and (23) that we can add a multiple of the metric to absorb this term. We thus arrive at a conformal Killing tensor with the $(p-1)$-tensor ϕ vanishing; that is, we get a Killing tensor.

The Proposition becomes simpler in the case of $p=2$. The tensor Ω in (29) is then just a function and $\hat{\nabla}\odot\Omega=\nabla\odot\Omega=\mathrm{d}\Omega$. So if S is a degree 2 Killing tensor with respect to g that satisfies

$$C_{\text{grad } e^{2\lambda}} S = -2\, \mathrm{d}\Omega \tag{30}$$

then

$$\hat{S} = e^{4\lambda} S + \Omega \hat{g} \tag{31}$$

is Killing with respect to $\hat{g}=e^{2\lambda}g$. The function Ω in (30) is clearly only defined up to a constant. This arbitrariness results in the Killing tensor $\hat{S}$ only being defined up to the addition of a multiple of the metric.

Now we look at the more general case in which $p>2$. Equation (29) involves a Killing tensor with respect to g, and the connection with respect to $\hat{g}$. We can alternatively express (29) in terms of g and its connection as

$$C_{\text{grad }\lambda}(S + \hat{\Omega}\odot g) = -\nabla\odot\hat{\Omega}, \tag{32}$$

where

$$\hat{\Omega} = e^{-2(p-1)\lambda}\Omega. \tag{33}$$

Rearranging things in terms of the scaling function $e^{2\lambda}$ we get

$$C_{\text{grad } e^{2\lambda}} S = -2\,\nabla\odot(e^{2\lambda}\hat{\Omega}) - C_{\text{grad } e^{2\lambda}}\hat{\Omega}\odot g. \tag{34}$$

Note that whereas (30) only involves the gradient of $e^{2\lambda}$, both $e^{2\lambda}$ and its gradient enter into (34). This will be of significance when we consider the Jacobi geometry, where solutions to (29) will, in general, only give constants of the motion for some fixed energy. To find constants of the motion for arbitrary energy we can restrict the solutions to (29) by imposing a further condition. To see how this can be done we consider the case in which S is of degree four. (It turns out that the results for even and odd degrees are slightly different, and so the case of $p=3$ will be covered afterwards.) Suppose that we have a degree-4 Killing tensor S satisfying (34) for some degree-2 $\hat{\Omega}$. Suppose that in addition we have

$$C_{\text{grad } e^{2\lambda}}\hat{\Omega} = -2\,\mathrm{d}\alpha$$

for some function α. We then have

$$C_{\text{grad } e^{2\lambda}}S = -2\,\nabla \odot (e^{2\lambda}\hat{\Omega} - \alpha g) = -2\,\nabla \odot \omega,$$

where

$$\omega = e^{2\lambda}\hat{\Omega} - \alpha g.$$

Contracting on ω gives

$$C_{\text{grad } e^{2\lambda}}\omega = -2e^{2\lambda}\,\mathrm{d}\alpha - 2\alpha\,\mathrm{d}e^{2\lambda} = -2d(\alpha e^{2\lambda}) = -2\,\mathrm{d}\beta$$

where

$$\beta = \alpha e^{2\lambda}.$$

Since we have assumed a solution to (29) we can construct a Killing tensor with respect to $\hat{g}$. It follows that this can be written in terms of ω and β as

$$\hat{S} = e^{8\lambda}S + e^{6\lambda}\omega \odot g + e^{4\lambda}\beta g \odot g.$$

Now it becomes clear how this result can be generalized to arbitrary even degree.

Proposition 2: If S is a Killing tensor of even degree p, and there exist symmetric tensors $\{\Omega_1, \Omega_2, \ldots, \Omega_{p/2}\}$ such that

$$C_{\text{grad } e^{2\lambda}}S = -2\,\nabla \odot \Omega_1,$$

$$C_{\text{grad } e^{2\lambda}}\Omega_i = -2\,\nabla \odot \Omega_{i+1}, \quad i = 1, \ldots, p/2 - 1$$

then

$$\hat{S} = e^{2p\lambda}S + e^{2(p-1)\lambda}\Omega_1 \odot g + \cdots + e^{p\lambda}\Omega_{p/2}\underbrace{g \odot \ldots \odot g}_{p/2 \text{ times}} \tag{35}$$

is Killing with respect to $\hat{g}$.

The proof follows from (26). Note that the conditions of Proposition 2 are a special case of those of Proposition 1, and that in Proposition 2 only the gradient of the scale function enters.

There is a similar result for Killing tensors of odd degree.

Proposition 3: If S is a Killing tensor of odd degree p, and there exist symmetric tensors $\{\Omega_1, \Omega_2, \ldots, \Omega_{(p-1)/2}\}$ such that

$$C_{\text{grad } e^{2\lambda}}S = -2\,\nabla \odot \Omega_1,$$

$$C_{\text{grad } e^{2\lambda}}\Omega_i = -2\,\nabla \odot \Omega_{i+1}, \quad i = 1, \ldots, (p-3)/2,$$

$$C_{\text{grad } e^{2\lambda}}\Omega_{(p-1)/2} = 0,$$

then

$$\hat{S} = e^{2p\lambda}S + e^{2(p-1)\lambda}\Omega_1 \odot g + \cdots + e^{(p+1)\lambda}\Omega_{(p-1)/2} \odot \underbrace{g \odot \cdots \odot g}_{(p-1)/2 \text{ times}} \tag{36}$$

is Killing with respect to $\hat{g}$.

Note that the last equation, $C_{\text{grad } e^{2\lambda}}\Omega_{(p-1)/2}=\Omega_{(p-1)/2}(\text{grad } e^{2\lambda})=0$, says that the 1-form $\Omega_{(p-1)/2}$ is metrically related to a vector field whose flows leave the conformal factor invariant.

IV. KILLING TENSORS IN THE JACOBI GEOMETRY

Suppose that $C:I\subset R\rightarrow(M,g)$ is some Newtonian curve, satisfying

$$\nabla_{\dot{C}}\dot{C}=-\text{ grad } V \tag{37}$$

for some potential V.

Then the total energy E is a constant of the motion,

$$E=T+V,$$

where $T=\frac{1}{2}g(\dot{C},\dot{C})$. Then the Jacobi metric $\hat{g}$ is obtained by conformally scaling g,

$$\hat{g}=e^{2\lambda}g, \tag{38}$$

where

$$e^{2\lambda}=E-V. \tag{39}$$

(Clearly we could include an overall constant in the scaling and not change the connection.) We then have, from (25),

$$\hat{\nabla}_{\dot{C}}\dot{C}=2\dot{C}\lambda\dot{C}. \tag{40}$$

Thus C is pregeodesic with respect to $\hat{g}$: that is, a reparametrization makes it geodesic. Since geodesics remain geodesic under an affine reparameterization, there is no unique parametrization that makes C geodesic. These affine reparametrizations of C correspond to a change in the strength of the potential in (37). Thus this way (or indeed any other way) of putting Newtonian curves into correspondence with geodesics is insensitive to any coupling constant that scales the strength of the potential.

If we have Killing tensors, with respect to $\hat{g}$, then we have polynomial constants of the motion. The precise relation is as follows.

Proposition 4: If $\hat{S}$ is a degree p Killing tensor with respect to the Jacobi metric $\hat{g}$, then $e^{-2p\lambda}\hat{S}(\dot{C},\ldots,\dot{C})$ is constant along C.

Proof: We have

$$\dot{C}(e^{-2p\lambda}\hat{S}(\dot{C},\ldots,\dot{C}))=-2p\dot{C}\lambda e^{-2p\lambda}\hat{S}(\dot{C},\ldots,\dot{C})+pe^{-2p\lambda}\hat{S}(\hat{\nabla}_{\dot{C}}\dot{C},\ldots,\dot{C})=0 \quad \text{by (40)}.$$

Now we can apply the results of the preceding section to the particular case of the Jacobi metric where we have $\hat{g}=(E-V)g$. A Killing tensor on M that satisfies the conditions of Proposition 1 will give a polynomial constant of the motion. Since the Jacobi metric is obtained by scaling with an energy-dependent conformal factor, this constant will, in general, depend upon the energy. When we have a Killing tensor on M satisfying the more restrictive conditions of Propositions 2 or 3, then we have a Killing tensor for each Jacobi metric, that is, a constant of the motion for any energy. So, for example, taking Propositions 2 and 4 together we see that if S is a Killing tensor on M of even degree p that satisfies

$$\begin{aligned} C_{\text{grad } V}S&=2\,\nabla\odot\Omega_1,\\ C_{\text{grad } V}\Omega_i&=2\,\nabla\odot\Omega_{i+1},\quad i=1,\ldots,p/2-1, \end{aligned} \tag{41}$$

then

$$\rho = S(\dot{C},\dot{C},\ldots,\dot{C}) + 2\Omega_1(\dot{C},\dot{C},\ldots,\dot{C}) + \cdots + 2^{p/2}\Omega_{p/2}. \tag{42}$$

is a constant of the motion. Here we arrived at this expression by examining conformal scaling of Killing tensors. Of course it can be verified directly from (37) and (41) [using (6)] that $\dot{C}\rho=0$.

Unfortunately its not easy to see how to find Killing tensors satisfying (41). There is always one trivial solution. We always have the trivial Killing tensor g, and for any V,

$$C_{\text{grad } V}g = 2\mathrm{d}V, \tag{43}$$

thus for any potential (41) is satisfied by taking $S=g$. In this case the constant of the motion given in (42) is just (twice) the total energy.

Things become a little simpler when $p=2$, for then (41) reduces to

$$C_{\text{grad } V}S = 2\mathrm{d}\Omega \tag{44}$$

which is locally equivalent to

$$d(C_{\text{grad } V}S) = 0, \tag{45}$$

which, for any given S, is a second-order PDE for V. In the case of R^n, with the standard metric, we know what all the Killing tensors look like: they are all trivial, being made from the Killing vectors and the metric. For example, in R^2 the Killing algebra consists of two translations and a rotation. By choosing a suitable basis for this Killing algebra, $\{T_1,T_2,R\}$, any Killing tensor can be written as

$$S = R^\flat \otimes R^\flat + aT_1^\flat \otimes T_1^\flat + bg \tag{46}$$

for constants a and b (where we assume S nonparallel). If we adapt coordinates $\{x,y\}$ such that

$$T_1 = \partial_x, \tag{47}$$

$$T_2 = \partial_y, \tag{48}$$

$$R = x\partial_y - y\partial_x, \tag{49}$$

then (45) becomes

$$3(yV_x - xV_y) + (y^2 - x^2 + a)V_{xy} + xy(V_{xx} - V_{yy}) = 0. \tag{50}$$

This is the Bertrand-Darboux equation.[14] Thus we refer to (41) as the (generalized) Bertrand-Darboux equation.

As an illustration of how (44) relates to known systems admitting quadratic constants of the motion we consider the Kepler problem. The Kepler problem has three nontrivial quadratic constants of the motion, forming the Runge-Lenz vector.[15,16] These constants correspond to three Killing tensors. Consider a Killing tensor such as

$$S_{12} = R_1^\flat \odot T_2^\flat - R_2^\flat \odot T_1^\flat, \tag{51}$$

where R_i generates rotations about the i axis and T_i generates translations along the i axis. Then we look for spherically symmetric solutions to (45),

$$C_{\partial_r}S = r\mathrm{d}x^3 - x^3\mathrm{d}r,$$

and so

$$d(C_{f(r)\partial_r}S) = ((rf)' + f)\mathrm{d}r \wedge \mathrm{d}x^3,$$

and so we have a solution to (45) if $f=Ar^{-2}$ which corresponds to the Kepler potential $V=C/r$.

Note that the first-order constants of the motion correspond to Killing symmetries that leave the potential invariant. That is, we have a vector field K such that

$$\mathcal{L}_K g = KV = 0. \tag{52}$$

Given such a first-order symmetry then for any solution to (44), for some S and Ω, then we have another solution for $\mathcal{L}_K S$ and $\mathcal{L}_K \Omega$. In the case of the Coulomb-Kepler potential, which has spherical symmetry, the three Killing tensors of the form given in (51) are related in this way,

$$\mathcal{L}_{R_1} S_{12} = -S_{13},$$

$$\mathcal{L}_{R_3} S_{12} = 0, \quad \text{etc}.$$

The constants corresponding to these three Killing tensors form the components of the Runge-Lenz vector.

V. GEODESICS AND WARPED PRODUCTS

Eisenhart[2] showed how Newtonian curves on configuration space corresponded to geodesics on a warped product manifold with one more dimension. We here briefly review some properties of warped product geometries. We consider the general case, rather than restricting the fiber to be one dimensional. First, this is no harder; indeed it can be easier to see what is going on by considering the more general setting. Second, it may be useful to regard the phase trajectories as geodesics with respect to some metric. (We will return to this point later.) Finally, Killing tensors on warped products are of interest irrespective of any connection with mechanics. (We refer again to Ref. 11.)

In this section notation and conventions will generally follow O'Neill.[17] Suppose that (B, g_B) and (F, g_F) are pseudo-Riemannian manifolds. Then if f is some function on B the warped product manifold $M = B \times_f F$ is the product manifold endowed with metric

$$G = \pi^* g_B + (f \circ \pi)^2 \sigma^* g_F, \tag{53}$$

where π and σ are the projections,

$$\pi : B \times_f F \to B, \tag{54}$$

$$\sigma : B \times_f F \to F. \tag{55}$$

Let $\mathcal{L}(B)$ denote the space of vector fields lifted from B to M, with $\mathcal{L}(F)$ denoting lifts from F. The connection on M, which will be denoted by D, can be related to those on B and F. If $X, Y \in \mathcal{L}(B)$ and $U, W \in \mathcal{L}(F)$ then

$$D_X Y = \nabla_X Y, \tag{56}$$

$$D_U X = D_X U = X(\ln f) U, \tag{57}$$

$$D_U W = \nabla_U W - \tfrac{1}{2} \operatorname{grad}(f^2) g_F(U, W). \tag{58}$$

[To simplify notation lifts are implied in several places in the above formulas. For example, in (56) we mean of course that the derivative of one lift with respect to another is the lift of the derivative.] Note that a warped product is conformally related to a Riemannian product. Thus one way of obtaining these connection relations is to use connection relations for conformally related metrics given in Eqs. (24) and (25).

Any curve $\Phi : I \to M$ can be decomposed into curves on B and F,

$$\Phi(s) = (\alpha(s), \beta(s)). \tag{59}$$

We can then use (56)–(58) to relate the acceleration of Φ to those of α and β. In particular, Φ is geodesic if

$$\nabla_{\dot\alpha}\dot\alpha - \tfrac{1}{2}\,\mathrm{grad}(f^2) g_F(\dot\beta,\dot\beta) = 0, \tag{60}$$

$$\nabla_{\dot\beta}\dot\beta + 2\dot\alpha(\ln f)\dot\beta = 0. \tag{61}$$

It follows that (again following O'Neill[17])

$$\dot\Phi(f^4 g_F(\dot\beta,\dot\beta)) = 0, \tag{62}$$

so if

$$f^4 g_F(\dot\beta,\dot\beta) = A \tag{63}$$

then A is constant along Φ. (The existence of this quadratic constant of the geodesic motion corresponds to a Killing tensor of course. We will return to this in the following section where Killing tensors in this geometry will be discussed.) So if we set

$$V = \frac{A}{2f^2} \tag{64}$$

then the geodesic equations on M are equivalent to the projected equations

$$\ddot\alpha = -\,\mathrm{grad}\, V, \tag{65}$$

$$\ddot\beta = (\dot\alpha \ln \phi)\dot\beta. \tag{66}$$

That is, the projection onto B corresponds to the motion of a particle moving in a potential, while the projection onto the fiber is a pregeodesic. For geodesic motion we always have the energy constant, and this can be related to the total energy of the curve projected onto the base:

$$G(\dot\Phi,\dot\Phi) = 2E = g_B(\dot\alpha,\dot\alpha) + f^2 g_F(\dot\beta,\dot\beta) = g_B(\dot\alpha,\dot\alpha) + \frac{A}{f^2} = 2(T+V). \tag{67}$$

Note that the potential V occurring in Newton's equations is of course only defined up to a constant. Changing this constant is equivalent to fixing the zero point of the total energy. We can only identify the natural geodesic energy with that of a Newtonian system when the potential is given by (64) (there being no freedom to add an arbitrary constant).

So far we have merely used some mechanical terminology as a convenience in discussing geodesics on warped products. Suppose now that we start with some Newtonian system, and ask to what extent the curves correspond to geodesics of some warped product. First, the potential must be of definite sign. So long as the potential is bounded this can always be achieved by the addition of a suitable constant. If that is the case then a warped product can be constructed, for any choice of fiber. Whatever the fiber all the Newtonian curves will be projections of geodesics. However, whatever the fiber, there will always be geodesics on the warped product that project to geodesics on configuration space. Moreover, whatever the fiber, there will always be infinitely many geodesics that project to the same Newtonian curve: there will always be at least one geodesic that projects to a given Newtonian curve whatever the starting point on the fiber.

The special case of a one-dimensional fiber corresponds to the metric originally considered by Eisenhart.[2] As noted in the preceding paragraph, the correspondence between geodesics and Newtonian curves is not one to one. This is at variance with statements made in Ref. 18.

Suppose that the configuration space has a positive definite metric (the prime example being R^n of course) and that the potential is negative definite (for example, the Newtonian gravitational potential). Then the Eisenhart metric is Lorentzian. The timelike geodesics project to negative energy elliptical orbits, the null geodesics project to parabolic orbits with the spacelike geodesics projecting to hyperbolic scattering orbits. Thus to describe all the Newtonian curves we need to consider timelike geodesics as well as spacelike and null ones, again contrary to what is stated in Ref. 18.

VI. KILLING TENSORS ON WARPED PRODUCTS

When examining the geodesic equations in the preceding section we noted that there was always a quadratic constant of the geodesic motion (in addition to the energy) and hence we always had a nontrivial Killing tensor. This is a special case of the following.

Proposition 5: If R is a degree-p Killing tensor on F then, for any warping function f, $S=(f\circ\pi)^{2p}\sigma^*R$ is a Killing tensor on M.

It follows from the connection relations (56)–(58) that

$$D\odot((f\circ\pi)^{2p}\sigma^*R)=(f\circ\pi)^{2p}\sigma^*\nabla\odot R. \tag{68}$$

The proposition is an immediate consequence.

In particular, since F always has the trivial Killing tensor g_F, we always have the Killing tensor $(f\circ\pi)^4\sigma^*g_F$ on M. We have already essentially noted this when we observed the geodesic constant in (63).

Clearly Killing vectors on B are not necessarily Killing on M. For the lift of a Killing vector K on B to be Killing on M the warping function f must be invariant under the flow of K. More generally, the pullback of a Killing tensor from B to M is not in general Killing, there being an additional requirement relating the Killing tensor to the warping function. However, there is a more general way in which Killing tensors on M can arise from those on B.

Proposition 6: If S is a Killing tensor on B of even degree p, and there exist symmetric tensors $\{\omega_1,\omega_2,\ldots,\omega_{p/2}\}$ such that

$$C_{\mathrm{grad}\,f^{-2}}S=2\nabla\odot\omega_1,$$

$$C_{\mathrm{grad}\,f^{-2}}\omega_i=2\nabla\odot\omega_{i+1},\quad i=1,\ldots,p/2-1,$$

then

$$T=\pi^*S+\pi^*\omega_1\odot(f\circ\pi)^4\sigma^*g_F+\cdots+\pi^*\omega_{p/2}\underbrace{(f\circ\pi)^4\sigma^*g_F\odot\cdots\odot(f\circ\pi)^4\sigma^*g_F}_{p/2\ \text{times}}$$

is a Killing tensor on M.

There is a similar result for Killing tensors of odd degree.

Proposition 7: If S is a Killing tensor on B of odd degree p, and there exist symmetric tensors $\{\omega_1,\omega_2,\ldots,\omega_{(p-1)/2}\}$ such that

$$C_{\mathrm{grad}\,f^{-2}}S=2\nabla\odot\omega_1,$$

$$C_{\mathrm{grad}\,f^{-2}}\omega_i=2\nabla\odot\omega_{i+1},\quad i=1,\ldots,(p-3)/2,$$

$$C_{\mathrm{grad}\,f^{-2}}\omega_{(p-1)/2}=0,$$

then

$$T = \pi^* S + \pi^* \omega_1 \odot (f \circ \pi)^4 \sigma^* g_F + \cdots + \pi^* \omega_{(p-1)/2} \underbrace{\odot (f \circ \pi)^4 \sigma^* g_F \odot \cdots \odot (f \circ \pi)^4 \sigma^* g_F}_{(p-1)/2 \text{ times}}$$

is a Killing tensor on M.

It follows from (56)–(58) that if S is a totally symmetric tensor on B then

$$D \odot \pi^* S = \pi^* \nabla \odot S - \tfrac{1}{2} \pi^* (C_{\text{grad } f^{-2}} S) \odot (f \circ \pi)^4 \sigma^* g_f. \tag{69}$$

Since we have already shown that $(f \circ \pi)^4 \sigma^* g_F$ is Killing, repeated use of (69) establishes the truth of both propositions.

We have seen, from Proposition 5, that the trivial Killing tensor g_F on F always leads to a (nontrivial) Killing tensor on M. In a similar way Proposition 6 shows how g_B always gives a Killing tensor on M. Since

$$C_{\text{grad } f^{-2}} g_B = 2 \mathrm{d} f^{-2}$$

for any warping function f, Proposition 6 enables a Killing tensor on M to be constructed. What we get is nothing other than G, the metric on M.

Any Killing tensor on M constructed from one on B, as in Propositions 6 or 7, gives a polynomial constant of the geodesic motion. This constant can be expressed in terms of the projection of the geodesic onto B, which we know can be interpreted as a Newtonian curve. Thus we arrive at the same constant as we previously obtained via the Jacobi geometry. For example, suppose that S is a Killing tensor of even degree satisfying the conditions of Proposition 6. Then if a geodesic Φ is projected as in (59), then ρ is constant along Φ where

$$\begin{aligned} \rho = T(\dot{\Phi}, \dot{\Phi}, \ldots, \dot{\Phi}) &= S(\dot{\alpha}, \ldots, \dot{\alpha}) + \omega_1(\dot{\alpha}, \ldots, \dot{\alpha})(f \circ \alpha)^4 g_F(\dot{\beta}, \dot{\beta}) + \cdots + \omega_{p/2} \underbrace{(f \circ \alpha)^4 g_F(\dot{\beta}, \dot{\beta}) \cdots}_{p/2 \text{ times}} \\ &= S(\dot{\alpha}, \ldots, \dot{\alpha}) + 2\Omega_1(\dot{\alpha}, \ldots, \dot{\alpha}) + \cdots + 2^{p/2} \Omega_{p/2}, \end{aligned}$$

where

$$\Omega_i = (A/2)^i \omega_i, \tag{70}$$

where A is defined by (63). This is the same expression given in (42). Note that (64) and (70) ensure that the conditions of Proposition 6 can be written as (41).

VII. DISCUSSION AND CONCLUSIONS

Sections V and VI have been written to be largely independent of Secs. III and IV. However, Propositions 6 and 7 are clearly related to Propositions 2 and 3. Since a Killing tensor on the Jacobi manifold, or one on the warped product, gives a polynomial constant of the Newtonian motion, any condition that enables a Killing tensor to be constructed on one space must enable a Killing tensor to be constructed on the other. However, there is a more direct way of seeing why these Propositions are related.

As was noted in Sec. V, a warped product is conformally related to a Riemannian product, and thus we can use the conformal scaling of the connections to establish the connection on a warped product. In a similar way we can use Proposition 2 (for example) to directly prove Proposition 6, as we will now show.

First suppose that we have a Killing tensor S on $\{B, g\}$ satisfying the conditions of Proposition 2, so that we can construct the Killing tensor $\hat{S}$ on $\{B, \hat{g}\}$. Then $\hat{S}$ also satisfies the conditions of Proposition 2 so that we can invert the relation between S and $\hat{S}$. Specifically we have the following:

$$C_{\widehat{\text{grad } e^{-2\lambda}}} \hat{S} = -2 \hat{\nabla} \odot \hat{\Omega}_1,$$

$$C_{\widehat{\text{grad}}\, e^{-2\lambda}\hat{\Omega}_i} = -2\hat{\nabla}\odot\hat{\Omega}_{i+1},$$

where

$$-\hat{\Omega}_1 = e^{(2p-6)\lambda}\left\{\Omega_1 + 2e^{-2\lambda}\Omega_2\odot g + \cdots + \frac{p}{2}e^{-(p-2)\lambda}\Omega_{p/2}\underbrace{g\odot\ldots\odot g}_{p/2-1\ \text{terms}}\right\},$$

$$\hat{\Omega}_2 = e^{2(p-6)\lambda}\{\Omega_2 + \cdots\},$$

and

$$S = e^{-2p\lambda}\hat{S} + e^{-2(p-1)\lambda}\hat{\Omega}_1\odot\hat{g} + e^{-2(p-2)\lambda}\hat{\Omega}_2\odot\hat{g}\odot\hat{g} + \cdots .$$

(Clearly the relation between the $\{\Omega_i\}$ and the $\{\hat{\Omega}_i\}$ is irritatingly complex.)

Second we note that any Killing tensor satisfying the conditions of Proposition 2 may be pulled back to one satisfying the conditions on a Riemannian (unwarped) product manifold. That is, if S is a Killing tensor on $\{B,g\}$ satisfying the conditions of Proposition 2 for some $\{\Omega_i\}$ and some function λ, then π^*S is a Killing tensor on $\{B\times F, \pi^*g+\sigma^*g_F\}$ satisfying the same conditions for $\{\pi^*\Omega_i, \lambda\circ\pi\}$.

Now we can establish Proposition 6 directly from Proposition 2. Suppose that S is a Killing tensor on $\{B,g\}$ satisfying Proposition 2 for some function $e^{2\lambda}=f^{-2}$. Then we can construct $\hat{S}$ that is Killing on $\{B,\hat{g}=f^{-2}g\}$. Then, for any $\{F,g_F\}$ we can pull back to get $\pi^*\hat{S}$ which is Killing on $\{B\times F,\hat{G}=(f\circ\pi)^{-2}\pi^*g+\sigma^*g_F\}$. Finally we may scale with the inverse scaling relations given above to produce a Killing tensor T on the warped product $\{B\times F, G=\pi^*g+(f\circ\pi)^2\sigma^*g_F\}$. What we get is

$$T = \pi^*S - \Omega_1\odot(f\circ\pi)^4\sigma^*g_F + \Omega_2\odot(f\circ\pi)^4\sigma^*g_F\odot(f\circ\pi)^4\sigma^*g_F + \cdots .$$

This is exactly what is given by Proposition 6 when we relate the definition of the $\{\Omega_i\}$ to the $\{\omega_i\}$.

Propositions 2 and 3 (or equivalently 6 and 7) give conditions for Killing tensors (possibly trivial) on one space, to give Killing tensors (not necessarily trivial) on another. However, unfortunately we do not know how to find such Killing tensors. In particular, whereas the propositions refer to Killing tensors of arbitrary degree, the complexity of actually finding such nontrivial tensors increases with the degree. Of course, as can readily be checked, if we have any tensors satisfying these conditions then we can form symmetrized tensor products that also satisfy the conditions.

In our discussions of warped products the details of the fiber have never played a role. The metric originally introduced by Eisenhart takes a one-dimensional fiber which is obviously minimal dimensionally, but in this context dimensions do not cost anything. Clearly the details of the fiber were irrelevant in our construction of Killing tensors from those on the base, in that we only assumed relations between tensors on the base and a function on the base. The recognition that the fiber is arbitrary suggests new possibilities. Perhaps, for a conservative mechanical system, one can construct a metric on phase space in such a way that the phase curves are geodesic. Presumably such a metric would make the phase space (at least locally) a pseudo-Riemannian warped product.

Because we have here looked at constants of the geodesic motion we have considered generalizations of Killing's equation to totally symmetric tensors. The totally antisymmetric generalizations, Killing-Yano tensors, have been much studied. They lead, for example, to symmetry operators for the Dirac equation. Given a Killing-Yano tensor one can construct a (symmetric) Killing tensor. (The Killing tensor of the Kerr geometry is related to a Killing-Yano tensor in this way.) It would be interesting to explore relations between Killing-Yano tensors and Killing tensors in this fruitful arena of warped products.

The main results presented here concern how Killing tensors on one manifold can give rise to Killing tensors on another; either conformally related, or equivalently a warped product. Mechanics need not have been mentioned. However, placing these geometrical constructions in the mechanical context offers the possibility of further symbiotic developments.

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Test particles with acceleration-dependent Lagrangian

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We consider a classical test particle subject to electromagnetic and gravitational fields, described by a Lagrangian depending on the acceleration and on a fundamental length. We associate to the particle a moving local reference frame and we study its trajectory in the principal fiber bundle of all the Lorentz frames. We discuss in this framework the general form of the Lagrange equations and the connection between symmetries and conservation laws (the Noether theorem). We apply these results to a model, already discussed by other authors, which implies an upper bound to the proper acceleration and to another new model in which a similar quantity, called "pseudoacceleration," is bounded. With some simple choices of the fields, we illustrate some other interesting properties of the models and we show that unwanted features may appear, as unstable run-away solutions and unphysical values of the energy momentum or of the velocity. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2170486]

I. INTRODUCTION

At present, the only well established long range relativistic fields, that allow a classical (nonquantum) treatment, are the Maxwell electromagnetic field and the Einstein gravitational field. However, the existence of new long range fields, or of modifications of the above-mentioned ones is often suggested on the basis of theoretical speculations or of not yet well confirmed experimental results. Many crucial problems of present day physics and cosmology can be formulated in terms of long range fields, for instance a possible failure of the Lorentz symmetry can be attributed to a long range nonscalar field.

A long range field can be defined in terms of well chosen test particles. For instance, charged particles are needed to define the electromagnetic field and only spinning particles are affected by a torsion field.[1] We see that the investigations of long range classical fields and of test particles are intimately related. The aim of the present article is to give a contribution to this problem by discussing new kinds of test particles.

By definition, in a test particle model one disregards the influence of the particle on the field, namely several important effects, as the radiated energy, the radiation damping, the electromagnetic contribution to the mass, etc. However, these models are much simpler and permit a better undertanding of some general features of the theory, in particular its symmetry properties.

The test particle models may also suggest a way to introduce in the theory a fundamental length λ of the order of the Planck length with the aim of taking into account approximately some effect of quantum gravity. For instance, as it has been proposed by several authors,[2–10] an effect of quantum gravity should be an upper bound of the order of λ^{-1} to the proper acceleration of particles (we use the convention $c=1$). Note that the gravitational acceleration vanishes in a local inertial frame and a discussion of the maximal acceleration principle requires the presence of an electromagnetic field. More references are given in the report,[11] dedicated to a discussion and a

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comparison of various geometric descriptions of the maximal acceleration principle. Another effect of the fundamental length is the appearance of new degrees of freedom and of excited states of the particle.

In order to study the motion of a test particle, it is useful to associate to every point of its world line, parametrized by the variable τ, a moving local Lorentz frame (a tetrad) $s(\tau)$ and to consider the motion of the point $s(\tau)$ in the principal bundle $\mathcal{S}$ of all the local Lorentz frames. This point of view has been adopted in Refs. 12 and 13 in the framework of presymplectic dynamics[14] and in Refs. 15–17 starting from the balance equations of a field theory and following the ideas of Ref. 18.

The method of moving rest frames has been applied in Refs. 19–22 to Lagrangians depending on the acceleration and also on higher derivatives of the velocity. In the following we develop a more general formalism which is not restricted to rest moving frames.

The geometry based on the space $\mathcal{S}$ of the local Lorentz frames permits a formulation of a wide class of (possibly nonlocal) field theories[23] and particle theories. In the present article we concentrate our attention on the innovative particle models, without a specific consideration of fields different from classical electromagnetism and Einstein's gravitation. The general formalism, however, is ready for the introduction of more general classical fields. It has been remarked[24,25] that this geometry permits an elegant treatment of the upper bounds to the acceleration and the angular velocity of the frames and of the (possibly extended) associated particles.

An important issue is the description of the motion of a maximally accelerated particle in a Lagrangian or Hamiltonian formalism, since it is necessary for the construction of a quantum theory. It has been treated in Refs. 21 and 22 by means of the idea, already mentioned previously, of associating to the particle a moving local Lorentz frame. As it looks natural, rest frames of the particle were chosen, but we shall see in the following that this choice is too restrictive.

The report[26] contains a treatment of various kinds of test particles by means of Lagrangians that depend on the acceleration and on the angular velocity and, for dimensional reasons, must contain a parameter λ that can be interpreted as a fundamental length. This report also contains a treatment of a presymplectic formalism, which is more powerful for the treatment of some models. In the present article we concentrate our attention on Lagrangians not depending on the angular velocity of the moving frame.

In Sec. II we summarize the relevant aspects of the geometry of the fiber bundle $\mathcal{S}$ and of its generalizations. In Sec. III we develop a general Lagrangian dynamics for a point moving in this space. In Sec. IV we introduce the additional assumptions concerning a test particle subject to an Einstein-Maxwell field. In Sec. V we use the Noether theorem to find the conserved quantities corresponding to various kinds of symmetry properties of the system.

In Sec. VI we give a detailed discussion of the relation between the particle and the local reference frames associated to it. We show that, if the Lagrangian depends on the acceleration, the center of mass cannot coincide with the origin of the local frame, where the electric charge is assumed to be concentrated. In this situation, the concept of acceleration is ambiguous and, besides the proper acceleration of the point charge, we define a new different quantity, called pseudoacceleration.

As a first example, in Sec. VII we give two equivalent treatments of the ordinary spinless charged masssive particle. In Sec. VIII we apply the general methods developed in the preceding sections to the model treated in Refs. 21 and 22, based on rest frames. The model has upper bounds to the velocity and to the proper acceleration of the charge, but the energy-momentum four-vector may be spacelike. Moreover, even in the absence of external fields, the solutions present an unstable behavior (run-away solutions) when the initial conditions are slightly modified.

In Sec. IX we introduce a different model based on zero-momentum frames. It has the correct energy-momentum spectrum and an upper bound, which does not concern the acceleration, but the pseudoacceleration, requiring a slight reformulation of the maximal acceleration principle.

In Secs. X and XI we study further this new model by considering a particle in a constant electromagnetic field and we show that the solutions have good stability properties. In some

circumstances, the velocity of the charge may exceed the velocity light, but, since it rotates with a very large frequency, this effect is hardly observable. In Sec. XII we consider a particle in a simple curved space and, even if the curvature is small, we find a serious form of instability.

In Sec. XIII we analyze another model, with a physical energy-momentum spectrum, and the charge moving slower than light. However, the acceleration and the pseudoacceleration have no upper bounds. In Sec. XIV we draw some general conclusions and we suggest some remarks on the quantization.

II. THE BUNDLE OF LORENTZ FRAMES

In the absence of an electromagnetic field, a powerful method to treat the dynamics of a (possibly extended) particle is to consider, for each value of the parameter τ, a local Lorentz frame (tetrad) $s(\tau)$ in such a way that a "distinguished point" of the particle (not necessarily the center of mass) coincides with the origin of the frame (sometimes called a *moving frame*). We indicate by $\mathcal{S}$ the ten-dimensional bundle of the Lorentz frames of the space-time and we describe the motion of the particle by means of the line $\tau \rightarrow s(\tau) \in \mathcal{S}$.

Particle dynamics in this space has been introduced by Künzle[12] (see also Ref. 13) in the framework of the presymplectic formalism.[14] A treatment based on the balance equations for the densities of energy, momentum and relativistic angular momentum, strongly influenced by Dixon's work,[18] is given in Refs. 15–17. In the next section we develop a geometric Lagrangian formalism which avoids the introduction of coordinate systems in the space $\mathcal{S}$. It is more general than the Lagrangian formalism used in Ref. 21, because $s(\tau)$ is not assumed to be a rest frame.

The elements of $\mathcal{S}$ are orthonormal tetrads $\{e_0, \ldots, e_3\}$ of four vectors in the pseudo-Riemannian space-time manifold $\mathcal{M}$. We assume that $\mathcal{M}$ is time oriented and e_0 belongs to the future cone. We consider ten vector fields $A_0, \ldots, A_9$ in the manifold $\mathcal{S}$. The fields $A_0, \ldots, A_3$ generate parallel displacements of the tetrads along the directions of the tetrad vectors, $A_4 = A_{[23]}$, $A_5 = A_{[31]}$, $A_6 = A_{[12]}$ generate rotations around the spatial vectors of the tetrad and $A_7 = A_{[10]}$, $A_8 = A_{[20]}$, $A_9 = A_{[30]}$ generate Lorentz boosts along the same spatial vectors. The latin indices i, k, j, l, m, n take the values 0,…,3 and the greek indices α, β, γ take the values 0,…,9. We assume $A_{[ik]} = A_{[ki]}$ and, when necessary, we use the square brackets to indicate that an antisymmetric pair of Latin indices stands for a greek index.

The vector fields A_α can also be considered as first order differential operators and their commutators (Lie brackets) can be written in the form

$$[A_\alpha, A_\beta] = F^\gamma_{\alpha\beta} A_\gamma. \tag{1}$$

The quantities $F^\gamma_{\alpha\beta} = -F^\gamma_{\beta\alpha}$, are called *structure coefficients* and in the absence of gravitation they are the structure constants of the Poincaré group. In the presence of gravitation, $F^{[jl]}_{ik}$ are the components of the curvature tensor and F^j_{ik} are the components of the torsion tensor, which vanishes in Einstein's theory.

The ten dimensional manifold $\mathcal{S}$ has a structure of principal fiber bundle[27] with base $\mathcal{M}$ and structural group $\mathrm{SO}^\uparrow(1,3)$, but the details of this structure are not needed in the next section. The only relevant feature is that $\mathcal{S}$ is a n-dimensional differentiable manifold in which n differentiable vector fields A_α are defined and that, for each point $s \in \mathcal{S}$, the vectors $A_\alpha(s)$ form a basis of the tangent space $T_s\mathcal{S}$. As a consequence, we can identify all the tangent spaces with a single n-dimensional vector space $\mathcal{T}$, which, in the absence of gravitation and other external fields, is the Lie algebra of the Poincaré group.

In the absence of gravitational field, $\mathcal{S}$ is the bundle of the Lorentz frames of the Minkowski space-time and the orthochronous Poincaré group $\mathcal{P}$ acts freely and transitively on $\mathcal{S}$. We choose a fixed frame $\hat{s}$ and represent univocally all the other frames in the form $s = g\hat{s}$ with $g \in \mathcal{P}$. In this way we may identify $\mathcal{S}$ and $\mathcal{P}$. The vector fields A_α generate the left translations of $\mathcal{P}$.

We shall also use the differential 1-forms ω^β defined by

$$\omega^{\beta}(A_{\alpha}) = \delta^{\beta}_{\alpha}. \tag{2}$$

The vectors $\omega^{\beta}(s)$ provide a basis in the cotangent space $T^{*}_{s}\mathcal{S}$.

More details on this kind of geometry can be found in Ref. 23. In this way we can also treat a large class of external fields, including torsion fields,[1] and, for $n > 10$, gauge fields,[28] including electromagnetic fields,[29] as it is explained in Sec. IV.

III. THE LAGRANGE EQUATIONS

We write the tangent vectors of the curve $\tau \to s(\tau) \in \mathcal{S}$, which describes the motion of the frame, in the form

$$\frac{ds(\tau)}{d\tau} = b^{\alpha}A_{\alpha}(s(\tau)) \in \mathcal{T} \tag{3}$$

and we consider the action principle

$$\delta\int_{\tau_1}^{\tau_2} L(b^{\alpha},s)d\tau = 0, \tag{4}$$

where the Lagrangian L is a homogeneous function of degree one of the "velocities" b^{α}.

In order to derive the dynamical equations, we consider a family, parametrized by ϵ, of varied trajectories $(\epsilon,\tau) \to s(\epsilon,\tau)$ with the usual properties

$$s(0,\tau) = s(\tau), \quad s(\epsilon,\tau_1) = s(\tau_1), \quad s(\epsilon,\tau_2) = s(\tau_2). \tag{5}$$

We put

$$\frac{\partial s(\epsilon,\tau)}{\partial\epsilon} = a^{\alpha}A_{\alpha}. \tag{6}$$

If $\phi(s)$ is a differentiable auxiliary function, we have

$$\frac{\partial\phi(s)}{\partial\epsilon} = a^{\alpha}A_{\alpha}\phi, \quad \frac{\partial\phi(s)}{\partial\tau} = b^{\alpha}A_{\alpha}\phi, \tag{7}$$

$$\frac{\partial^2\phi(s)}{\partial\epsilon\partial\tau} = a^{\alpha}A_{\alpha}(b^{\beta}A_{\beta}\phi) = b^{\alpha}A_{\alpha}(a^{\beta}A_{\beta}\phi). \tag{8}$$

From the last equality we obtain

$$((a^{\alpha}A_{\alpha}b^{\beta})A_{\beta} - (b^{\alpha}A_{\alpha}a^{\beta})A_{\beta} + a^{\alpha}b^{\beta}[A_{\alpha},A_{\beta}])\phi = 0, \tag{9}$$

namely

$$\left(\frac{\partial b^{\gamma}}{\partial\epsilon} - \frac{\partial a^{\gamma}}{\partial\tau} + a^{\alpha}b^{\beta}F^{\gamma}_{\alpha\beta}\right)A_{\gamma}\phi = 0, \tag{10}$$

and, since ϕ is arbitrary,

$$\frac{\partial b^{\gamma}}{\partial\epsilon} = \frac{\partial a^{\gamma}}{\partial\tau} - a^{\alpha}b^{\beta}F^{\gamma}_{\alpha\beta} \tag{11}$$

and finally (disregarding higher order terms in ϵ)

$$\delta b^{\alpha} = \epsilon\left(\frac{\partial b^{\alpha}}{\partial\epsilon}\right)_{\epsilon=0} = \epsilon\left(\frac{da^{\alpha}}{d\tau} - a^{\beta}b^{\gamma}F^{\alpha}_{\beta\gamma}\right)_{\epsilon=0} = \epsilon b^{\gamma}(A_{\gamma}a^{\alpha} - a^{\beta}F^{\alpha}_{\beta\gamma})_{\epsilon=0}. \tag{12}$$

By means of the last formula, one can write, performing a partial integration,

$$\delta\int_{\tau_1}^{\tau_2} L d\tau = \epsilon\int_{\tau_1}^{\tau_2}\left(\frac{\partial L}{\partial b^\alpha}\left(\frac{da^\alpha}{d\tau} - a^\beta b^\gamma F^\alpha_{\beta\gamma}\right) + a^\alpha A_\alpha L\right)d\tau$$

$$= \epsilon\int_{\tau_1}^{\tau_2}\left(-\frac{d}{d\tau}\frac{\partial L}{\partial b^\alpha} - \frac{\partial L}{\partial b^\beta}b^\gamma F^\beta_{\alpha\gamma} + A_\alpha L\right)a^\alpha d\tau + \epsilon\left[\frac{\partial L}{\partial b^\alpha}a^\alpha\right]_{\tau_1}^{\tau_2}. \tag{13}$$

The last term vanishes as a consequence of the conditions (5) and, considering that a^α is an arbitrary function of τ, we obtain the Euler-Lagrange dynamical equations

$$\dot{p}_\alpha = \frac{dp_\alpha}{d\tau} = b^\gamma p_\beta F^\beta_{\gamma\alpha} - A_\alpha L, \tag{14}$$

where

$$p_\alpha = -\frac{\partial L}{\partial b^\alpha}. \tag{15}$$

If we assume that L does not depend directly on s, the last term in Eq. (14) is not present and this equation is exactly the one obtained in Ref. 16 in the pole approximation by integrating the balance equations (the quantities $F^\gamma_{\alpha\beta}$ are defined there with a different sign).

The momenta p_α defined by Eq. (15) are homogeneous functions of degree zero of the velocities b^α, namely they depend only on the ratios $(b^0)^{-1}b^\alpha$ (and possibly on s). It follows that they must satisfy at least a primary constraint.[30] Other primary constraints may exist and we write them in the form

$$\Phi_\rho(p_\alpha, s) = 0, \quad \rho = 0, \ldots, m-1. \tag{16}$$

Since L is a homogeneous function, the Euler theorem gives, taking Eq. (15) into account,

$$L + p_\alpha b^\alpha = 0 \tag{17}$$

and by differentiation we obtain

$$b^\alpha dp_\alpha + (A_\alpha L)\omega^\alpha = 0. \tag{18}$$

The differentials dp_α and the forms ω^α are arbitrary, apart from the constraints

$$\frac{\partial\Phi_\rho}{\partial p_\alpha}dp_\alpha + (A_\alpha\Phi_\rho)\omega^\alpha = 0, \quad \rho = 0, \ldots, m-1 \tag{19}$$

and from Eq. (18) we have

$$b^\alpha = \sum_\rho \alpha^\rho \frac{\partial\Phi_\rho}{\partial p_\alpha}, \tag{20}$$

$$A_\alpha L = \sum_\rho \alpha^\rho A_\alpha \Phi_\rho. \tag{21}$$

Equation (20) inverts, as far as possible, Eq. (15). At this level, the functions $\alpha^\rho(\tau)$ are arbitrary and, if they are not determined by the dynamical equations, they parametrize the gauge transformations of the system. There is at least one kind of gauge transformation, namely a redefinition of the parameter τ.

If, according to the dynamical equations (14), the quantities Φ_ρ are not conserved, the conditions $\dot{\Phi}_\rho = 0$ determine partially the functions α^ρ or give rise to secondary constraints. Some simplification can be obtained from the following consequence of the above-derived equations:

$$\sum_{\rho} \alpha^{\rho}\dot{\Phi}_{\rho} = \sum_{\rho} \alpha^{\rho}\left(\frac{\partial \Phi_{\rho}}{\partial p_{\alpha}}\dot{p}_{\alpha} + A_{\alpha}\Phi_{\rho}b^{\alpha}\right) = b^{\alpha}(\dot{p}_{\alpha} + A_{\alpha}L) = b^{\alpha}b^{\beta}p_{\gamma}F^{\gamma}_{\beta\alpha} = 0. \tag{22}$$

It follows that if $\alpha^0 \neq 0$ and the secondary constraints $\dot{\Phi}_{\rho}=0$ for $\rho=1,\ldots,m-1$ are satisfied, Φ_0 is conserved. In particular, if there is only one primary constraint, it is conserved and there are no secondary constraints.

If one is able to express all the quantities b^{α} and $\dot{p}_{\alpha}$ as smooth functions of s and p_{α} (satisfying some constraints), we say that the equations of motion are in *normal form* and one can apply the theorems on the (local) existence and uniqueness of the solutions. In fact, if one introduces a local system of coordinates q^{α} in the space $\mathcal{S}$, it follows from Eq. (3) that the quantities $\dot{q}^{\alpha}$ are smooth functions of the quantities b^{α}.

IV. EINSTEIN-MAXWELL FIELDS

Now we consider a test particle moving in an Einstein gravitational field and a Maxwell electromagnetic field. In order to describe the electromagnetic field, we adopt the procedure indicated in Refs. 16, 28, and 29, namely we introduce a principal fiber bundle $\mathcal{S}$ with base $\mathcal{M}$ and structural group $\mathrm{SO}^{\uparrow}(1,3)\times\mathrm{U}(1)$ which includes the electromagnetic gauge group. Then the manifold $\mathcal{S}$ has dimension $n=11$ and we have to introduce a new vector field, that we indicate by $A_{\bullet}$ (in order to avoid a two-digit index $\alpha=10$), which generates the global electromagnetic gauge transformations. We use the notation

$$b^{\alpha}A_{\alpha} = b^{i}A_{i} + \tfrac{1}{2}b^{[ik]}A_{[ik]} + b^{\bullet}A_{\bullet}, \quad b^{[ik]} = -b^{[ki]}. \tag{23}$$

The 11-dimensional manifold $\mathcal{S}$ can also be considered as a principal fiber bundle with structural group U(1) and base $\mathcal{S}_0$, the 10-dimensional bundle of the Lorentz frames considered up to now. We shall consider later the projection $\mathcal{S}\to\mathcal{S}_0$ along the fibers generated by the vector field $A_{\bullet}$.

The structure coefficients $F^{\alpha}_{[ik]\beta}$ coincide with the structure constants of the Poincaré algebra. They can be written in the form

$$F^{[mn]}_{[ik][jl]} = \delta^{m}_{i}g_{kj}\delta^{n}_{l} - \delta^{m}_{k}g_{ij}\delta^{n}_{l} - \delta^{m}_{i}g_{kl}\delta^{n}_{j} + \delta^{m}_{k}g_{il}\delta^{n}_{j} - \delta^{n}_{i}g_{kj}\delta^{m}_{l} + \delta^{n}_{k}g_{ij}\delta^{m}_{l} + \delta^{n}_{i}g_{kl}\delta^{m}_{j} - \delta^{n}_{k}g_{il}\delta^{m}_{j}, \tag{24}$$

$$F^{l}_{[ik]j} = \delta^{l}_{i}g_{kj} - \delta^{l}_{k}g_{ij}, \tag{25}$$

$$F^{m}_{[ik][jl]} = 0, \quad F^{[mn]}_{[ik]j} = 0. \tag{26}$$

We also assume that the torsion F^{j}_{ik} vanishes.

The structure coefficients $F^{\bullet}_{ik}=F_{ik}$ represent the electromagnetic field strength and $F^{\beta}_{\alpha\bullet}=F^{\bullet}_{[ik]\alpha}=0$. The electromagnetic interaction Lagrangian is

$$L_I = eb^{\bullet}, \tag{27}$$

where e is the electric charge.

By means of these equations, we can write Eq. (14) in the more explicit form

$$\dot{p}_i = -b_i{}^k p_k + F_i, \quad F_i = b^k G_{ik} - A_i L, \quad G_{ik} = \tfrac{1}{2}p_{[jl]}F^{[jl]}_{ki} + eF_{ik}, \tag{28}$$

$$\dot{p}_{[ik]} = b_i p_k - b_k p_i - b_i{}^j p_{jk} - b_k{}^j p_{ij} - A_{[ik]}L, \tag{29}$$

$$\dot{p}_{\bullet} = 0, \quad p_{\bullet} = -e, \tag{30}$$

where $F_{ki}^{[jl]}$ is the Riemann curvature tensor which describes the gravitational field. As we discuss in the next section, the quantities p^i and $-p_{ik}$ are interpreted as the energy, the momentum and the relativistic angular momentum of the particle, measured in the local reference frame s. The quantity $-p_{\bullet}$ is the conserved electric charge.

It is often convenient to use a three-dimensional vector formalism. We introduce the vectors

$$\mathbf{b} = (b^1, b^2, b^3), \quad \mathbf{b}' = (b^{[23]}, b^{[31]}, b^{[12]}), \quad \mathbf{b}'' = (b^{[10]}, b^{[20]}, b^{[30]}), \tag{31}$$

$$\mathbf{p} = -(p_1, p_2, p_3), \quad \mathbf{p}' = -(p_{[23]}, p_{[31]}, p_{[12]}), \quad \mathbf{p}'' = -(p_{[10]}, p_{[20]}, p_{[30]}), \tag{32}$$

$$\mathbf{f} = -(b^0)^{-1}(F_1, F_2, F_3), \tag{33}$$

$$\mathbf{E} = (F_{01}, F_{02}, F_{03}), \quad \mathbf{B} = (F_{32}, F_{13}, F_{21}), \tag{34}$$

$$\hat{\mathbf{E}} = (G_{01}, G_{02}, G_{03}), \quad \hat{\mathbf{B}} = (G_{32}, G_{13}, G_{21}), \tag{35}$$

and we obtain, if L does not depend on s,

$$\dot{p}_0 = -\mathbf{b}'' \cdot \mathbf{p} + \mathbf{b} \cdot \mathbf{f}, \tag{36}$$

$$\dot{\mathbf{p}} = -\mathbf{b}' \times \mathbf{p} - p_0 \mathbf{b}'' + b^0 \mathbf{f}, \tag{37}$$

$$\dot{\mathbf{p}}' = -\mathbf{b} \times \mathbf{p} - \mathbf{b}' \times \mathbf{p}' - \mathbf{b}'' \times \mathbf{p}'', \tag{38}$$

$$\dot{\mathbf{p}}'' = p_0 \mathbf{b} - b^0 \mathbf{p} - \mathbf{b}' \times \mathbf{p}'' + \mathbf{b}'' \times \mathbf{p}', \tag{39}$$

$$\mathbf{f} = \hat{\mathbf{E}} + (b^0)^{-1} \mathbf{b} \times \hat{\mathbf{B}}. \tag{40}$$

The dimension of the phase space, namely the number of parameters necessary to define the initial conditions, is given by $2n=22$ minus the number of primary and secondary constraints [including the constraint (30)] minus the number of the arbitrary gauge parameters (including the usual electromagnetic gauge transformations).

It is instructive to consider, besides the flat Minkowski space time, the spaces of constant curvature

$$F_{ik}^{[jl]} = \rho(\delta_i^j \delta_k^l - \delta_k^j \delta_i^l). \tag{41}$$

$\mathcal{M}$ is a de Sitter space time if $\rho > 0$, and an anti-de Sitter space time for $\rho < 0$. From Eq. (28) we obtain

$$G_{ik} = -\rho p_{[ik]} + eF_{ik}, \tag{42}$$

or, in the vector notation,

$$\hat{\mathbf{E}} = -\rho \mathbf{p}'' + e\mathbf{E}, \quad \hat{\mathbf{B}} = -\rho \mathbf{p}' + e\mathbf{B}. \tag{43}$$

V. NOETHER'S THEOREM

In order to treat the connection between symmetries and conservation laws (Noether's theorem), we consider a vector field

$$Y(s) = a^{\alpha}(s)A_{\alpha}(s) \tag{44}$$

and the corresponding one-parameter diffeomorphism group $\exp(\epsilon Y)$, which transforms the trajectory $s(\tau)$ into the trajectories $s(\epsilon,\tau)$. If this transformation does not change the action, the expression (13) vanishes and, taking the dynamical equations into account, we obtain the conservation law

$$a^{\alpha}p_{\alpha} = \text{constant}. \tag{45}$$

We assume that L does not depend on s and consider two kinds of applications of this general theorem, which use two different kinds of symmetry properties. In the first case we require

$$[Y,A_{\beta}] = (a^{\alpha}F^{\gamma}_{\alpha\beta} - A_{\beta}a^{\gamma})A_{\gamma} = 0 \tag{46}$$

and from Eq. (12) we see that $\delta b^{\alpha}=0$, and therefore $\delta L=0$. Note that the validity of the conservation law (45) does not depend on the form of the function $L(b^{\alpha})$.

In a second case we assume Eqs. (24)–(26) and consider the infinitesimal Lorentz transformation generated by $A_{[ik]}$. From Eq. (12) we obtain

$$\delta b^{\alpha} = -\epsilon F^{\alpha}_{[ik]\gamma}b^{\gamma}, \tag{47}$$

namely an infinitesimal Lorentz transformation of the quantities b^{α}. If the Lagrangian is invariant under this transformation, the quantity $p_{[ik]}$ is conserved. In particular, if the Lagrangian is a Lorentz scalar function of b^{α} all the six quantities $p_{[ik]}$ are conserved. If the Lagrangian is only a rotational scalar, only the three quantities $p_{[rs]}$ with $r,s=1,2,3$ are conserved. These conservation laws depend on the invariance properties of the Lagrangian and on the form of the structure coefficients $F^{\alpha}_{[ik]\gamma}$. They are also valid in the presence of arbitrary gravitational and electromagnetic fields.

Now we consider the simplest application of the first kind. As we have seen in Sec. II, in the absence of gravitational and electromagnetic fields, $\mathcal{S}$ is the bundle of the Lorentz frames of the Minkowski space time and choosing a fixed frame $\hat{s}$, can be identified with the orthochronous Poincaré group $\mathcal{P}$. The vector fields A_{α} generate the left translations of $\mathcal{P}$, but one can also introduce the vector fields $\hat{A}_{\alpha}$, which generate the right translations, interpreted as Poincaré transformations of the fixed frame $\hat{s}$. They commute with A_{α} and are given by

$$Y = \hat{A}_{\alpha}(g) = D^{\beta}{}_{\alpha}(g)A_{\beta}(g), \tag{48}$$

where $D(g)$ is the adjoint representation of $\mathcal{P}$, which has the property

$$A_{\alpha}D^{\beta}{}_{\gamma}(g) = -F^{\beta}_{\alpha\delta}D^{\delta}{}_{\gamma}(g). \tag{49}$$

It follows from the Noether theorem that the quantities

$$\hat{p}_{\alpha} = D^{\beta}{}_{\alpha}(g(\tau))p_{\beta}(\tau) \tag{50}$$

are conserved. Since they are defined starting from the symmetry under spacetime translations and infinitesimal Lorentz transformations of $\hat{s}$, they have to be interpreted as the components of the energy momentum and the relativistic angular momentum measured in the fixed frame $\hat{s}$.

We indicate an element of $\mathcal{P}$ by $(\Lambda,x)=(\Lambda,0)(1,x)$, where x is the translation four vector and Λ is the Lorentz matrix acting on the contravariant components of the four vectors. If we use the explicit form of the adjoint representation, we obtain the equations

$$\hat{p}_i = \Lambda^k{}_i p_k, \quad \hat{p}_{[ik]} = \Lambda^j{}_i\Lambda^l{}_k p_{[jl]} - x_i\hat{p}_k + x_k\hat{p}_i, \tag{51}$$

which show that the quantities $p_{\beta}(\tau)$ are correctly interpreted as the components of the energy momentum and the relativistic angular momentum measured in the moving frame $s(\tau)$, as we anticipated in the preceding section. The mass μ and the spin σ of the particle are given by the

familiar Poincaré invariant expressions and take the same form when written as functions of $\hat{p}_\beta(\tau)$ or of $p_\beta(\tau)$. In particular we have

$$\mu^2 = p^i p_i, \quad \sigma^2\mu^2 = -S^k S_k, \quad S^k = 2^{-1}\epsilon^{kijl} p_{[ij]} p_l. \tag{52}$$

This interpretation is also valid if an electromagnetic field is present. In fact, from Eqs. (31)–(40) we see that the influence of the electromagnetic field on the derivatives $\dot{p}_\alpha$ is just the one expected for a point charge centered at the origin, if the quantities p_α represent the components of the kinetic energy momentum and relativistic angular momentum. This problem is also discussed in Ref. 20.

The exact definition of the energy momentum and of the relativistic angular momentum of an extended particle in a curved space time is somehow ambiguous[16,18] and in this case the interpretation of p_α can be considered as a definition.

VI. FRAMES AND PARTICLES

In order to interpret the solutions of the dynamical equations, we have to clarify the connection between the Lorentz frames $s(\tau)$ and the physical particle. We indicate by $\pi: \mathcal{S} \to \mathcal{M}$ the projection which associates to the tetrad $s \in \mathcal{S}$ its origin $x = \pi(s) \in \mathcal{M}$. The projection of the curve $\tau \to s(\tau)$ is the world line $\tau \to \pi(s(\tau)) = x(\tau)$ in the space-time manifold $\mathcal{M}$. From Eq. (3), remembering that the vector fields A_i generate the parallel displacements along the four vectors $e_i(\tau)$ of the tetrad $s(\tau)$, we have

$$\dot{x}(\tau) = \frac{dx(\tau)}{d\tau} = b^i(\tau) e_i(\tau). \tag{53}$$

If τ is the proper time, namely if $b_i b^i = 1$, the quantities b^i are the components of the four velocity of the origin of $s(\tau)$, with respect to the same frame.

The tetrad $s(\tau + d\tau)$ differs from the parallel transported tetrad by an infinitesimal Lorentz transformation with parameters $b^{[ik]} d\tau$. This means that the covariant derivatives of the tetrad four vectors are given by

$$\frac{De_i(\tau)}{d\tau} = -b_i^{\ k}(\tau) e_k(\tau), \tag{54}$$

and we obtain the formula

$$a(\tau) = \frac{D\dot{x}(\tau)}{d\tau} = \dot{b}^i e_i - b^i b_i^{\ k} e_k = (\dot{b}^i + b^i_{\ k} b^k) e_i. \tag{55}$$

If τ is the proper time, a is the covariant acceleration four vector and its components in the moving frame $s(\tau)$ are given by

$$a^i = \dot{b}^i + b^i_{\ k} b^k. \tag{56}$$

A *rest frame* is defined by the condition $\mathbf{b} = 0$ and the four velocity of the origin of the frame is equal to the tetrad vector e_0, which is time-like by definition. If τ is the proper time, we also have $b^0 = 1$, and $d\tau$ is a time measured in the rest frame. We have

$$a = \frac{De_0}{d\tau} = b^{[r0]} e_r, \quad a^0 = 0, \quad \mathbf{a} = \mathbf{b}''. \tag{57}$$

The vector $\mathbf{a}$ represents the acceleration of the origin of a rest frame measured in the same frame. If the parameter τ is arbitrary, we can write the more general formula

$$\mathbf{a} = (b^0)^{-1} \mathbf{b}''. \tag{58}$$

We can introduce more specific moving frames by requiring the stronger conditions

$$\mathbf{b}=0, \quad b^{[20]}=b^{[30]}=b^{[31]}=0. \tag{59}$$

In a Lagrangian model they can be imposed by introducing six Lagrangian multipliers. In this case $s(\tau)$ is a Frenet frame and the quantities $k_1=b^{[01]}$, $k_2=b^{[12]}$, $k_3=b^{[23]}$ are the geometric invariants of the world line, which depend on the acceleration and its first and second derivatives.[19,21] The Lagrangian depends on these invariants as in the models considered in Ref. 19.

Now we consider frames defined by nonpurely geometric, but dynamical requirements. The condition $\mathbf{p}=0$ defines a *zero-momentum frame*. It implies that the energy momentum is a timelike four vector. In the case of a free particle, the center of mass is at rest in this frame, but this is not true in general. In a zero-momentum frame $\mathbf{p}'$ represents by definition the spin of the particle. One can still consider the vector (58) but it does not represent the acceleration of the origin $x(\tau)$ and not even the acceleration of the center of mass. We call it the *pseudoacceleration*. From Eq. (37) we have

$$\mathbf{a}=p_0^{-1}\mathbf{f}. \tag{60}$$

Note that p_0 in a zero-momentum frame is the invariant mass and this formula coincides with the Newton formula, valid for a point particle. If the particle is extended, this formula remains valid if we replace the acceleration by the pseudoacceleration. This may be considered as the physical meaning of the pseudoacceleration.

In order to describe the position of the center of mass, we have to introduce for each tetrad a system of coordinates in a suitable open set of $\mathcal{M}$, for instance a system of normal coordinates. In the absence of gravitation, namely in special relativity theory, one can associate to every local frame s a Lorentzian coordinate system in the flat Minkowski spacetime and the space coordinates of the center of mass at zero time in this frame can be written in the form[31]

$$\mathbf{y}=-p_0^{-1}\mathbf{p}''. \tag{61}$$

The condition $\mathbf{p}''=0$ means that the trajectory of the center of mass crosses the origin. A frame with this property is called a *central frame*. This definition can be extended to the case in which gravitation is present. From Eq. (39) we see that, if the spin is zero, a zero-momentum central frame is also a rest frame.

The definition $\mathbf{p}''=0$ is not Lorentz invariant and it is often replaced by the condition

$$p_{[ik]}p^k=0, \tag{62}$$

proposed by Dixon.[18] A frame with this property is called a *Dixon frame*. It can always be obtained from a central zero-momentum frame by means of a Lorentz transformation.

The models treated in the following sections concern extended particles which contain a point charge. In this case, instead of working with central or Dixon frames, it is convenient to assume that the charge lies at the origin of $s(\tau)$. More in general, if the charge is not pointlike, one can require that the electric dipole moment with repect to the frame $s(\tau)$ vanishes.

VII. AN ORDINARY SPINLESS PARTICLE

It is instructive to consider first some Lagrangians that do not contain $\mathbf{b}'$ and $\mathbf{b}''$ and describe a pointlike spinless particle with mass m and charge e. The simplest Lagrangian of this kind is

$$L=-mb^0+eb^\bullet. \tag{63}$$

Since it is linear in the "velocities" b^α, all the momenta p_α are fixed by 11 primary constraints, namely we have $p_0=m$, $p_\bullet=-e$ and the other momenta vanish. As a consequence, the spin vanishes and the center of mass coincides with the charge. From the dynamical equations (36)–(39) we obtain

$$\mathbf{b}=0, \quad m\mathbf{a}=m(b^0)^{-1}\mathbf{b}''=\mathbf{f}=e\mathbf{E}. \tag{64}$$

We see that the frames $s(\tau)$ are zero-momentum rest central frames and that the acceleration is given by the usual formula. The time evolution of the quantities b^0, $\mathbf{b}'$, and $b^\bullet$ is not determined by the dynamical equations, the model has gauge invariances described by five parameters and the phase space has dimension six. If we impose the gauge fixing condition $\mathbf{b}'=0$, the frame is Fermi-Walker transported and if we assume $b^0=1$ the parameter τ is the usual relativistic proper time. If $\mathbf{E}=0$, the frame is parallel transported and the world line of the particle is a geodesic.

In view of the following developments, it is interesting to treat with more detail a charged particle in a constant electromagnetic field in the absence of gravitation. The field is invariant under spacetime translations, but it changes if a Lorentz transformation is applied to the frame. If $b^0=1$, we have

$$\dot{\mathbf{E}}=\mathbf{b}''\times\mathbf{B}-\mathbf{b}'\times\mathbf{E}, \quad \dot{\mathbf{B}}=-\mathbf{b}''\times\mathbf{E}-\mathbf{b}'\times\mathbf{B}. \tag{65}$$

Of course, the Lorentz invariants

$$I=\|\mathbf{E}\|^2-\|\mathbf{B}\|^2, \quad J=\mathbf{E}\cdot\mathbf{B} \tag{66}$$

are constant.

The derivatives (65) vanish if we choose the gauge fixing condition

$$\mathbf{b}'=-em^{-1}\mathbf{B}. \tag{67}$$

The components of the field and all the quantities b^α are constant and we say that this is a "stationary" solution. It follows that the projection of the trajectory on the ten-dimensional space $\mathcal{S}_0$, identified with the Poincaré group $\mathcal{P}$, is given by a one-parameter subgroup, namely

$$g(\tau)=\exp(\tau b^\alpha\widetilde{A}_\alpha)g(0), \tag{68}$$

where $\widetilde{A}_\alpha$ form a basis in the Lie algebra of $\mathcal{P}$ and $\exp(\cdot)$ is the exponential mapping of the group.[32]

We also consider the Lorentz invariant Lagrangian

$$L=-m((b^0)^2-\|\mathbf{b}\|^2)^{1/2}+eb^\bullet. \tag{69}$$

We obtain

$$p_0=mb^0((b^0)^2-\|\mathbf{b}\|^2)^{-1/2}, \quad \mathbf{p}=m((b^0)^2-\|\mathbf{b}\|^2)^{-1/2}\mathbf{b}, \tag{70}$$

$$\mathbf{p}'=\mathbf{p}''=0, \quad p_\bullet=-e \tag{71}$$

and the constraint

$$p_0^2-\|\mathbf{p}\|^2=m^2. \tag{72}$$

It is sufficient to consider the dynamical equations (37), since Eqs. (36), (38), and (39) are consequences of the other equations. We see that the quantities b^0, $\mathbf{b}'$, $\mathbf{b}''$, and $b^\bullet$ are not determined and they are gauge parameters. In particular, the Lorentz transformations assume the character of gauge transformations. We may fix the gauge partially by assuming that $\mathbf{p}=0$ and we obtain exactly the equations of the preceding model. The dynamics of the particle is the same, but in the second model there is more freedom in the choice of the moving frame.

Alternatively, we may require $\mathbf{b}'=\mathbf{b}''=0$, namely that the moving frame is parallel transported, and, also assuming $b^0=1$, Eq. (37) takes the familiar form

$$\dot{\mathbf{p}}=\mathbf{f}. \tag{73}$$

VIII. A MODEL WITH A MAXIMAL ACCELERATION

For dimensional reasons, a Lagrangian which is a homogeneous function of degree one of the velocities b^α and contains a fundamental length λ must contain, besides b^0 and $\mathbf{b}$, some of the quantities $\lambda\mathbf{b}'$ or $\lambda\mathbf{b}''$. In the following we consider Lagrangians that depend on $\mathbf{b}''$, but not on $\mathbf{b}'$, and we treat first a model with a maximal proper acceleration equivalent to the one treated in Ref. 21.

It is easy to obtain an upper limit for the quantity $(b^0)^{-1}\mathbf{b}''$, but, as we have seen in Sec. VI, this quantity coincides with the proper acceleration only if $s(\tau)$ are rest frames, namely if $\mathbf{b}=0$. This constraint is implicit in the formalism of Ref. 21, but in the framework of the preceding sections we have to enforce it by means of the Lagrange multipliers $\boldsymbol{\eta}$. A simple Lagrangian of this kind, that does not contain $\mathbf{b}'$, is given by

$$L = -m((b^0)^2 - \lambda^2\|\mathbf{b}''\|^2)^{1/2} + \boldsymbol{\eta}\cdot\mathbf{b} + eb^\bullet. \tag{74}$$

We obtain the equations

$$\mathbf{b} = 0, \quad \mathbf{p} = \boldsymbol{\eta}, \quad \mathbf{p}' = 0, \quad p_\bullet = -e. \tag{75}$$

The first equality means that we are dealing with rest frames and the second shows that $\mathbf{p}$ can be chosen freely in the initial conditions, even in contrast with the usual requirements on the energy-momentum spectrum. The third formula does not imply that the spin vanishes, because the spin is defined as the angular momentum in a zero-momentum frame, that in general is not a rest frame.

The other momenta are given by

$$\begin{aligned} p_0 &= mb^0((b^0)^2 - \lambda^2\|\mathbf{b}''\|^2)^{-1/2}, \\ \mathbf{p}'' &= m\lambda^2((b^0)^2 - \lambda^2\|\mathbf{b}''\|^2)^{-1/2}\mathbf{b}'' \end{aligned} \tag{76}$$

and satisfy the scalar primary constraint

$$p_0^2 - \lambda^{-2}\|\mathbf{p}''\|^2 = m^2, \tag{77}$$

which, in agreement with Eq. (22), is conserved and does not give rise to secondary constraints. We consider only solutions with $p_0 \geqslant m$ and, as a consequence, $b^0 > 0$. From the preceding formulas one obtains the relations

$$\mathbf{a} = (b^0)^{-1}\mathbf{b}'' = \lambda^{-2}p_0^{-1}\mathbf{p}'' = -\lambda^{-2}\mathbf{y} = \lambda^{-1}(\|\mathbf{p}''\|^2 + \lambda^2 m^2)^{-1/2}\mathbf{p}'', \tag{78}$$

which show that the acceleration $\|\mathbf{a}\|$ has the upper bound λ^{-1} and the distance $\|\mathbf{y}\|$ of the center of mass from the origin has the upper bound λ.

The dynamical equation (36) follows from Eq. (39) and the scalar constraint (77). Equation (38) is automatically satisfied and from Eqs. (37) and (39) we obtain

$$\dot{\mathbf{p}} = -p_0\mathbf{b}'' + b^0\mathbf{f} - \mathbf{b}' \times \mathbf{p}, \quad \dot{\mathbf{p}}'' = -b^0\mathbf{p} - \mathbf{b}' \times \mathbf{p}''. \tag{79}$$

There are no secondary constraints.

As in the simple model considered in the preceding section, the time evolution of the quantities b^0, $\mathbf{b}'$, and $b^\bullet$ is not determined by the dynamical equations and the model has gauge invariances. Since there are five primary constraints and five arbitrary gauge variables, the phase space has dimension twelve. We can impose the gauge fixing conditions $b^0=1$, $\mathbf{b}'=0$ and we get the simpler dynamical equations

$$\dot{\mathbf{p}} = -\lambda^{-2}\mathbf{p}'' + \mathbf{f}, \quad \dot{\mathbf{p}}'' = -\mathbf{p}. \tag{80}$$

This system is in normal form.

We obtain

$$\frac{d}{d\tau}(p_0^2 - \|\mathbf{p}\|^2) = -2\mathbf{f}\cdot\mathbf{p}. \tag{81}$$

Even if initially the four momentum is time-like, by applying a suitable force $\mathbf{f}$, it may become space-like. This means that one cannot simply discard as unphysical the states with space-like four momentum.

We see from Eqs. (28), (35), and (40), that, when the particle is subject to gravitational fields only, if $\mathbf{p}'=\mathbf{p}''=0$ we have $\mathbf{f}=0$. It follows that $\mathbf{p}''=\mathbf{b}''=\mathbf{p}=0$ is a solution which describes an ordinary spinless particle with mass $p_0=m$ moving according to the laws of general relativity. We show in the following that, even in the absence of external fields, there are many other solutions, as it is expected, since the phase space has dimension larger than six.

It is shown in Refs. 21 and 22 that, in space times of constant curvature and in the absence of other external fields, the dynamical equations can be solved exactly. In fact, from Eqs. (43) and (80) we obtain

$$\ddot{\mathbf{p}}'' = (\rho + \lambda^{-2})\mathbf{p}''. \tag{82}$$

For $\rho > -\lambda^{-2}$ it has exponential solutions and for $\rho < -\lambda^{-2}$ it has periodic solutions. Considering with more detail the case $\rho=0$, namely a flat spacetime, the general solution has the form

$$\mathbf{p}'' = \mathbf{u}\exp(\lambda^{-1}\tau) + \mathbf{v}\exp(-\lambda^{-1}\tau). \tag{83}$$

The acceleration $\|\mathbf{a}\|$ and the distance $\|\mathbf{y}\|$ of the center of mass from the origin of the moving frame are given by Eq. (78). For generic initial conditions, they approach their maximum values when time increases or decreases, in particular

$$\lim_{\tau\to\infty} \mathbf{a} = \lambda^{-1}\|\mathbf{u}\|^{-1}\mathbf{u}, \quad \mathbf{u} \neq 0. \tag{84}$$

For $\mathbf{u}=\mathbf{v}=0$, we obtain $\mathbf{p}''=\mathbf{a}=0$, namely the uniform motion that is expected for an ordinary particle in the absence of external forces. This solution, however, is unstable, since small changes of the initial conditions lead to solutions with a large acceleration in the past or in the future. We have

$$p_0^2 - \|\mathbf{p}\|^2 = m^2 + 4\lambda^{-2}\mathbf{u}\cdot\mathbf{v} \tag{85}$$

and we see that for some solutions the energy-momentum four vector is spacelike. The accelerated solutions recall the run-away solutions of the Lorentz-Dirac equation,[33] with the important difference that in our case we are considering test particles and disregarding the radiated energy.

In a flat spacetime one can easily compute the motion of the origin of $s(\tau)$, namely of the point charge associated with the extended particle. In the generic case, it approaches soon the velocity of light with respect to a fixed frame. Of course, the center of mass follows a linear world line and its distance from the charge becomes large in the fixed frame. In the moving frame, however, as an effect of the Lorentz transformation, it remains small.

If, instead of considering a test particle, we take into account effects depending on higher powers of the charge e, it is possible that the radiated energy (bremsstrahlung) prevents the unstable behavior described previously. In the following sections, however, we try a different solution of this problem.

IX. A MODEL WITH A MAXIMAL PSEUDOACCELERATION

In order to avoid the unphysical energy-momentum spectrum and the unstable behavior of the model described in the preceding section, a reasonable attempt is to consider zero-momentum frames instead of rest frames. This can be obtained by dropping the Lagrange multipliers from Eq. (74) namely by assuming

$$L = -m((b^0)^2 - \lambda^2\|\mathbf{b}''\|^2)^{1/2} + eb^\bullet. \tag{86}$$

Besides Eq. (30) we obtain the vector constraints

$$\mathbf{p} = 0, \quad \mathbf{p}' = 0, \tag{87}$$

showing that $s(\tau)$ is a zero-momentum frame and the particle is spinless. It is clear that the four-momentum p is necessarily timelike. Equation (76), the scalar constraint (77) and Eq. (78) of the preceding section are still valid and, in this case too, we consider only solutions with $p_0 \geqslant m$ and, as a consequence, $b^0 > 0$. Equation (78), however, does not give an upper bound to the acceleration, but to the pseudoacceleration **a** defined in Sec. VI.

The relation

$$p_0 = m(1 - \lambda^{-2}\|\mathbf{y}\|^2)^{-1/2} \tag{88}$$

shows that p_0 can be interpreted as a confining potential that binds the charge to the center of mass. When a force is applied to the charge, $\|\mathbf{y}\|$ and p_0 increase and this explains intuitively why the pseudoacceleration remains bounded.

As in the model of the preceding section, the dynamical equation (36) follows from Eq. (39) and the scalar constraint (77), Eq. (38) is automatically satisfied and from Eqs. (37) and (39) we obtain

$$p_0\mathbf{b}'' = b^0\mathbf{f}, \quad \dot{\mathbf{p}}'' = p_0\mathbf{b} - \mathbf{b}' \times \mathbf{p}''. \tag{89}$$

In this case too we have gauge symmetries. If we impose the gauge fixing conditions $b^0 = 1$ and $\mathbf{b}' = 0$, we get the simplified equations

$$\mathbf{p}'' = \lambda^2 p_0\mathbf{b}'' = \lambda^2\mathbf{f} = \lambda^2(\hat{\mathbf{E}} + \mathbf{b} \times \hat{\mathbf{B}}), \tag{90}$$

$$\dot{\mathbf{p}}'' = p_0\mathbf{b}. \tag{91}$$

Note that the four-vector $(b^0, \mathbf{b})$, proportional to the four-velocity of the charge measured in the frame $s(\tau)$, is not necessarily time-like and in Sec. X we find examples in which it is actually space-like. It follows that its time component in some other fixed reference frame $\hat{s}$ may vanish or even become negative. This means that the charge "moves backwards in time," namely, more exactly, the time coordinate with respect to the frame $\hat{s}$ is a decreasing function of the parameter τ. A further discussion will be given in Sec. XIV.

As we have remarked in the preceding section, if there is only a gravitational field, but no other external fields, the equalities $\mathbf{p}' = \mathbf{p}'' = 0$ imply that $\mathbf{f} = 0$. It follows that the equalities $\mathbf{f} = \mathbf{p}'' = \mathbf{b}'' = \mathbf{b}' = \mathbf{b} = 0$ define solutions in which $s(\tau)$ is a parallel transported rest frame. These solutions describe an ordinary spinless particle with mass $p_0 = m$ moving according to the laws of general relativity, but in general there are other different solutions with $\mathbf{p}'' \neq 0$. In a space of constant curvature ρ, as we see from Eq. (43), we have $\mathbf{f} = -\rho\mathbf{p}''$ and if $\rho \neq -\lambda^{-2}$, we have necessarily $\mathbf{f} = \mathbf{p}'' = 0$ and the only solutions are the ones described previously. In this case, the phase space has dimension six.

If $\hat{\mathbf{B}} \neq 0$, from Eq. (90) we obtain the secondary constraint

$$(\hat{\mathbf{E}} - \lambda^{-2}\mathbf{p}'') \cdot \hat{\mathbf{B}} = 0. \tag{92}$$

We have eight primary constraints, one secondary constraint and five arbitrary gauge variables. It follows that, if there are no tertiary constraints, the dimension of the phase space is eight. If $\hat{\mathbf{B}} = 0$ in the whole space $\mathcal{S}$, as in the constant curvature models treated previously, Eq. (90) gives the three secondary constraints

$$\mathbf{p}'' = \lambda^2 \hat{\mathbf{E}} \tag{93}$$

and the phase space has dimension six, as in the free case.

X. A PARTICLE IN A CONSTANT ELECTROMAGNETIC FIELD

It is useful to consider, as in Sec. VII, a particle in a flat space time with a constant electromagnetic field. Some results will be approximately valid for slowly varying fields. We consider first the case in which the invariants (66) have the properties $I \geqslant 0$, $J=0$ and in the frame $s(0)$ we have $\mathbf{B}=0$. If we choose the gauge $\mathbf{b}'=0$, we see from Eqs. (65) and (90) that $\dot{\mathbf{E}}=\dot{\mathbf{B}}=0$. It follows that along the whole trajectory $\mathbf{E}$, $\mathbf{p}''$, and $\mathbf{b}''$ are constant, $\mathbf{B}=0$ and $\mathbf{b}=0$. The frame $s(\tau)$ is a rest frame that moves with a constant acceleration given by

$$\mathbf{b}'' = (m^2 + \lambda^2 \|e\mathbf{E}\|^2)^{-1/2} e\mathbf{E}. \tag{94}$$

We see that, in this case, the singular manifold defined by $\mathbf{B}=0$ is invariant, namely all the trajectories crossing it are completely contained in it. The acceleration remains bounded even if the electric field is very large. As in the case of Sec. VII, $s(0)$ determines the initial conditions completely and the solution is stationary.

If in the frame $s(0)$ we have $\mathbf{B} \neq 0$, we must also specify two components of $\mathbf{p}''$ in order to describe the initial condition completely. We show, however, that there is a finite number of stationary solutions starting from $s(0)$ in which all the components of the field and all the quantities b^α and p_α are constant and $s(\tau)$ is given by the exponential formula (68). The other, nonstationary, solutions will be treated perturbatively in the next section.

We assume first that $\mathbf{E} \times \mathbf{B} \neq 0$, since the case in which this vector vanishes needs a separate treatment. If we require that the derivatives in Eqs. (65) and (89) vanish, we obtain after some calculation,

$$\mathbf{b} = a\mathbf{E} \times \mathbf{B},$$

$$\mathbf{b}' = p_0^{-1} e(-(1 - a\|\mathbf{B}\|^2)\mathbf{B} + a(\mathbf{B} \cdot \mathbf{E})\mathbf{E}),$$

$$\mathbf{b}'' = p_0^{-1} e((1 - a\|\mathbf{B}\|^2)\mathbf{E} + a(\mathbf{B} \cdot \mathbf{E})\mathbf{B}), \tag{95}$$

$$p_0^2 = m^2 + \lambda^2 e^2((1 - a\|\mathbf{B}\|^2)^2 \|\mathbf{E}\|^2 + a(2 - a\|\mathbf{B}\|^2)(\mathbf{E} \cdot \mathbf{B})^2).$$

The second Eq. (89) is satisfied if

$$a p_0^2 = \lambda^2 e^2((1 - a\|\mathbf{B}\|^2)^2 + a^2(\mathbf{B} \cdot \mathbf{E})^2), \tag{96}$$

namely, by substituting the expression for p_0^2,

$$\begin{aligned} f(a) &= (1 - a\|\mathbf{B}\|^2)((1 - a\|\mathbf{B}\|^2)(1 - a\|\mathbf{E}\|^2) - a^2(\mathbf{E} \cdot \mathbf{B})^2) - \lambda^{-2} e^{-2} m^2 a \\ &= (1 - a\|\mathbf{B}\|^2)(1 - a\|\mathbf{B}\|^2 - a\|\mathbf{E}\|^2 + a^2\|\mathbf{E} \times \mathbf{B}\|^2) - \lambda^{-2} e^{-2} m^2 a = 0. \end{aligned} \tag{97}$$

This is, in general, a third degree algebraic equation in the variable a, that has one or three real solutions. The polynomial function $f(a)$ has the following properties:

$$f(a) > 0 \quad \text{for } a \leqslant 0, \quad f(0) = 1,$$

$$f(a) < 0 \quad \text{for } \|\mathbf{E}\|^{-2} \leqslant a \leqslant \|\mathbf{B}\|^{-2},$$

$$f(a) < 0 \quad \text{for } \|\mathbf{B}\|^{-2} \leqslant a \leqslant \|\mathbf{B}\|^{-2}(1 + \lambda^{-2} e^{-2} m^2 (\|\mathbf{E}\|^2 + \|\mathbf{B}\|^2)^{-1}),$$

$$f'(a) < -\lambda^{-2}e^{-2}m^2 \quad \text{for } 0 \leqslant a \leqslant \min(\|\mathbf{E}\|^{-2}, \|\mathbf{B}\|^{-2}). \tag{98}$$

It follows that $f(a)$ has only one zero in the interval

$$0 < a < \min(\lambda^2 e^2 m^{-2}, \|\mathbf{E}\|^{-2}, \|\mathbf{B}\|^{-2}) \tag{99}$$

and, possibly, two zeros in the half line

$$a \geqslant \|\mathbf{B}\|^{-2}(1 + \lambda^{-2}e^{-2}m^2(\|\mathbf{E}\|^2 + \|\mathbf{B}\|^2)^{-1}). \tag{100}$$

If a lies in the interval, (99) we have $\|\mathbf{b}\|^2 < 1$, namely the velocity of the charge is smaller than the velocity of light. We see in the following that, for some values of the fields, if we choose a solution in the half line (100), the charge may move faster than light. Note that if $\|\mathbf{b}\|^2 = \lambda^2\|\mathbf{b}' \times \mathbf{b}''\|^2 > 1$, since $\lambda\|\mathbf{b}''\| < 1$, we have $\lambda\|\mathbf{b}'\| > 1$, namely the frame $s(\tau)$ rotates, with all the dynamical vector variables, with an angular velocity larger than λ^{-1}. If λ is very small, one can only observe an average value of the velocity $\mathbf{b}$, that is negligible, since $\mathbf{b}$ is orthogonal to the angular velocity $\mathbf{b}'$.

Note that the fields $\mathbf{E}$ and $\mathbf{B}$ are measured with respect to the moving frame $s(\tau)$ and if the particle is very fast can be much larger than the fields measured in the laboratory frame. Even if we take this remark into account, if λ is of the order of Planck's length, in all the experimental situations we have

$$\|\mathbf{E}\|, \|\mathbf{B}\| \ll \lambda^{-1}e^{-1}m. \tag{101}$$

Under these conditions, the smallest solution of Eq. (97) is given by the approximate formula

$$a_1 \approx \lambda^2 e^2 m^{-2}. \tag{102}$$

Note that when $\lambda \to 0$, this solution tends to zero and the other two solutions either become complex or tend to infinity. In this limit we obtain, as it is expected, the ordinary model of Sec. VII.

We have to consider the special case in which $\mathbf{B} \neq 0$ and $\mathbf{E} \times \mathbf{B} = 0$, namely $\mathbf{E} = k\mathbf{B}$. We obtain the following conditions for the stationary solutions

$$\mathbf{b} = 0, \quad \mathbf{b}' = h\|\mathbf{B}\|^{-1}\mathbf{B}, \quad p_0\mathbf{b}'' = e\mathbf{E}, \quad p_0^2 = m^2 + \lambda^2\|e\mathbf{E}\|^2, \tag{103}$$

where h is an arbitrary constant that describes just a choice of the rotational gauge. Note that Eq. (94) is also valid in this more general situation.

It is interesting to see if these equations can be obtained as a limit of Eqs. (95) for $\|\mathbf{E} \times \mathbf{B}\| \to 0$. Equation (97) tends to the second degree equation

$$(1 - a\|\mathbf{B}\|^2)(1 - a\|\mathbf{E}\|^2 - a\|\mathbf{B}\|^2) - \lambda^{-2}e^{-2}m^2a = 0 \tag{104}$$

and one of the three solutions of Eq. (97) tends to infinity, more exactly we have

$$a_3 \approx (\|\mathbf{E}\|^2 + \|\mathbf{B}\|^2)\|\mathbf{E} \times \mathbf{B}\|^{-2}. \tag{105}$$

It follows that for this solution we have $\|\mathbf{b}\| \to \infty$, showing that there are stationary solutions with the charge moving faster than light. The other two (necessarily positive) solutions are given by

$$a_{1,2} = (2\|\mathbf{B}\|^2(\|\mathbf{E}\|^2 + \|\mathbf{B}\|^2))^{-1}(\|\mathbf{E}\|^2 + 2\|\mathbf{B}\|^2 + \lambda^{-2}e^{-2}m^2 \pm \Delta^{1/2}), \tag{106}$$

where

$$\Delta = (\|\mathbf{E}\|^2 + \lambda^{-2}e^{-2}m^2)^2 + 4\lambda^{-2}e^{-2}m^2\|\mathbf{B}\|^2 > 0. \tag{107}$$

The corresponding values of the parameter h are

$$h_{1,2} = p_0^{-1} e\|\mathbf{B}\|(a_\pm(\|\mathbf{E}\|^2 + \|\mathbf{B}\|^2) - 1) = e(2p_0\|\mathbf{B}\|)^{-1}(\|\mathbf{E}\|^2 + \lambda^{-2}e^{-2}m^2 \pm \Delta^{1/2}). \tag{108}$$

Only for these values of the gauge parameter h the solutions (103) can be obtained as limits of the solutions (95).

XI. PERTURBATIONS AND STABILITY

The next step is to study perturbatively trajectories slightly different from the stationary ones described previously. Since the infinitesimal perturbations satisfy linear differential equations with constant coefficients, we look for complex exponential solutions, namely we write

$$b^\alpha \to b^\alpha + \Re(\delta b^\alpha \exp(z\tau)), \tag{109}$$

where the constant quantities z and δb^α are complex. A similar notation is used for the other variables. The derivatives with respect to τ can be replaced by the factor z. We are not interested in perturbations with $z=0$, which give other already known stationary solutions. For $z \neq 0$ we obtain new nonstationary solutions, but also stationary solutions, modified by an infinitesimal time-dependent gauge transformation.

From Eq. (65) we obtain

$$\begin{aligned} z\delta\mathbf{E} &= \mathbf{b}'' \times \delta\mathbf{B} - \mathbf{B} \times \delta\mathbf{b}'' - \mathbf{b}' \times \delta\mathbf{E} + \mathbf{E} \times \delta\mathbf{b}', \\ z\delta\mathbf{B} &= -\mathbf{b}'' \times \delta\mathbf{E} + \mathbf{E} \times \delta\mathbf{b}'' - \mathbf{b}' \times \delta\mathbf{B} + \mathbf{B} \times \delta\mathbf{b}'. \end{aligned} \tag{110}$$

Since the invariants (66) are not affected by the perturbation, we also require the relations

$$\mathbf{E} \cdot \delta\mathbf{E} = \mathbf{B} \cdot \delta\mathbf{B}, \quad \mathbf{E} \cdot \delta\mathbf{B} = -\mathbf{B} \cdot \delta\mathbf{E}, \tag{111}$$

which, however, are not independent from Eqs. (110).

From the other dynamical equations we have

$$\begin{aligned} \delta\mathbf{p}'' &= \lambda^2 e(\delta\mathbf{E} + \mathbf{b} \times \delta\mathbf{B} - \mathbf{B} \times \delta\mathbf{b}), \\ z\delta\mathbf{p}'' &= p_0\delta\mathbf{b} + \mathbf{b}\,\delta p_0 - \mathbf{b}' \times \delta\mathbf{p}'' + \mathbf{p}'' \times \delta\mathbf{b}', \\ \delta\mathbf{p}'' &= \lambda^2\mathbf{b}''\delta p_0 + \lambda^2 p_0\delta\mathbf{b}'', \\ \delta p_0 &= \lambda^2 p_0^3 m^{-2}\mathbf{b}'' \cdot \delta\mathbf{b}''. \end{aligned} \tag{112}$$

After the elimination of the variables δp_0, $\delta\mathbf{p}''$, and $\delta\mathbf{b}$, we obtain a system of nine homogeneous linear equations in the twelve unknown variables $\delta\mathbf{E}$, $\delta\mathbf{B}$, $\delta\mathbf{b}''$, and $\delta\mathbf{b}'$.

For all the values of z this system has three linearly independent solutions which represent rotational gauge transformations. They are given by

$$\delta\mathbf{E} = \mathbf{E} \times \mathbf{r}, \quad \delta\mathbf{B} = \mathbf{B} \times \mathbf{r}, \quad \delta\mathbf{b}'' = \mathbf{b}'' \times \mathbf{r}, \quad \delta\mathbf{b}' = \mathbf{b}' \times \mathbf{r} + z\mathbf{r}, \tag{113}$$

where $\mathbf{r}$ is an arbitrary infinitesimal complex vector. Note that unless

$$z^2 = -\|\mathbf{b}'\|^2, \tag{114}$$

the vector $\delta\mathbf{b}'$ can take arbitrary values and when we look for physically relevant perturbations we can choose the gauge $\delta\mathbf{b}'=0$. We obtain in this way a homogeneous linear system of nine equation in nine unknowns, which has nonvanishing solutions only if its determinant $\det M(z)$ vanishes. If z satisfies Eq. (114), there is a pure gauge perturbation with $\delta\mathbf{b}'=0$, and this implies that $\det M(\pm i\|\mathbf{b}'\|)=0$. If we disregard this uninteresting solution, the other nonvanishing solutions of the algebraic equation $\det M(z)=0$ correspond to physically relevant perturbations.

If $\mathbf{E}\times\mathbf{B}\neq 0$, it is convenient to use the projections of all the vectors on the basis formed by the vectors $\mathbf{E}$, $\mathbf{B}$, and $\mathbf{E}\times\mathbf{B}$. Equation (111) permits the elimination of two unknowns and we have to calculate the determinant of a 7×7 matrix. It has almost thousand terms and one has to use a computer algebra program.[34] We find that the determinant $\det M(z)$ contains only the powers z^6, z^4, and z^2, and, since we know that it vanshes for $z^2=-\|\mathbf{b}'\|^2$, we can find the other, physically relevant, solution of the equation $\det M(z)=0$ by means of Ruffini's rule. With an appropriate choice of the variables, the computer calculation gives the unexpectedly simple result

$$-z^2=\omega^2=\lambda^{-4}p_0^2\|e\mathbf{B}\|^{-2}+4\lambda^{-2}m^2p_0^{-2}>0, \tag{115}$$

where p_0^2 is given by Eq. (95). We see that $z=\pm i\omega$ is pure imaginary and this means that the stationary solutions are stable with respect to linear perturbations. The perturbations have a frequency $\omega/2\pi$, that when $\|e\mathbf{B}\|\to 0$, tends to infinity explaining why a degree of freedom disappears for $\|e\mathbf{B}\|=0$. If we use Eq. (101), we see that the frequency $\omega/2\pi$ is much larger than the Planck frequency λ^{-1}.

In order to extend our results to the case in which $\mathbf{E}\times\mathbf{B}=0$ a separate discussion, that does not require computer algebra, is needed. From Eqs. (103), (111), and (112) we find

$$\mathbf{B}\cdot\delta\mathbf{E}=\mathbf{B}\cdot\delta\mathbf{B}=\mathbf{B}\cdot\delta\mathbf{p}''=\mathbf{B}\cdot\delta\mathbf{b}=0,\quad \delta p_0=0. \tag{116}$$

As in the general case, we choose $\delta\mathbf{b}'=0$.

After some calculations we obtain

$$z(\delta\mathbf{B}-\lambda^2kep_0^{-1}\|\mathbf{B}\|^2\delta\mathbf{p}'')=-\mathbf{b}'\times(\delta\mathbf{B}-\lambda^2kep_0^{-1}\|\mathbf{B}\|^2\delta\mathbf{p}'') \tag{117}$$

and if $z^2\neq-\|\mathbf{b}'\|^2$ we have

$$\delta\mathbf{p}''=\lambda^{-2}(ke)^{-1}p_0\|\mathbf{B}\|^{-2}\delta\mathbf{B}. \tag{118}$$

By substituting this formula and Eq. (103) into Eq. (110), we obtain a linear homogeneous system of the form

$$z\begin{pmatrix}\delta\mathbf{E}\\ \delta\mathbf{B}\end{pmatrix}=\|\mathbf{B}\|^{-1}A\begin{pmatrix}\mathbf{B}\times\delta\mathbf{E}\\ \mathbf{B}\times\delta\mathbf{B}\end{pmatrix}, \tag{119}$$

where the matrix A is given by

$$A=\begin{pmatrix}-h & \lambda^{-2}m^2p_0^{-1}\|\mathbf{eE}\|^{-1}\\ -p_0^{-1}\|\mathbf{eE}\| & -h+\lambda^{-2}p_0\|\mathbf{e}B\|^{-1}\end{pmatrix}. \tag{120}$$

Since the vectors $\delta\mathbf{E}$ and $\delta\mathbf{B}$ must be perpendicular to $\mathbf{B}$, by iterating this formula we obtain

$$z^2\begin{pmatrix}\delta\mathbf{E}\\ \delta\mathbf{B}\end{pmatrix}=-A^2\begin{pmatrix}\delta\mathbf{E}\\ \delta\mathbf{B}\end{pmatrix}. \tag{121}$$

One can easily show that this linear system has nonvanishing solutions if

$$z^2=-(h_{1,2}-h)^2, \tag{122}$$

where the quantities $h_{1,2}$ are given by Eq. (108). From the same equation and Eq. (115) we obtain the identity

$$h_2-h_1=\omega. \tag{123}$$

We see that, in this case too, the stationary trajectories are stable, but the frequency of the perturbations depends on the gauge parameter h. There are two independent perturbations with different angular velocities and only their difference is invariant under the rotational gauge and

physically relevant. If we choose $h=h_{1,2}$, in both cases we obtain the solution $z^2=0$ and the solutions given by Eq. (115), namely the limits of the solutions found for $\mathbf{E}\times\mathbf{B}\neq 0$.

XII. A PARTICLE IN A SIMPLE GRAVITATIONAL FIELD

In order to understand the properties of the model in a gravitational field, it is instructive to consider, besides the spacetimes with constant curvature we have already examined in Sec. IX, another simple model, namely the stationary Einstein cosmological model[35] with spatial curvature ρ. The curvature tensor in the frame $s(\tau)$ takes the form

$$F_{ik}^{[jl]}=\rho(\delta_i^j\delta_k^l-\delta_k^j\delta_i^l-\delta_i^j v_k v^l+\delta_k^j v_i v^l+\delta_i^l v_k v^j-\delta_k^l v_i v^j),\quad v_k v^k=1,\quad \rho>0, \tag{124}$$

where, in a cosmological interpretation, $v=(v_0,\mathbf{v})$ is the four velocity with respect to the frame $s\in\mathcal{S}$ of a privileged frame in which the matter and radiation distribution is isotropic.

From Eq. (28) we obtain

$$G_{ik}=-\rho(p_{[ik]}+v^j p_{[ji]}v_k-v^j p_{[jk]}v_i), \tag{125}$$

or, in the vector notation,

$$\hat{\mathbf{E}}=\rho(\|\mathbf{v}\|^2\mathbf{p}''-(\mathbf{v}\cdot\mathbf{p}'')\mathbf{v}),\quad \hat{\mathbf{B}}=\rho v_0\mathbf{v}\times\mathbf{p}''. \tag{126}$$

Equations (90) and (91) give the result

$$(\lambda^{-2}\rho^{-1}-\|\mathbf{v}\|^2)\mathbf{p}''+(\mathbf{v}\cdot\mathbf{p}'')\mathbf{v}=p_0^{-1}v_0\dot{\mathbf{p}}''\times(\mathbf{v}\times\mathbf{p}''), \tag{127}$$

and constraint (92) is identically satisfied. We assume that $\|\mathbf{v}\|^2<\lambda^{-2}\rho^{-1}$. If $\mathbf{v}\times\mathbf{p}''=0$ we must have $\mathbf{p}''=0$, otherwise we obtain

$$\mathbf{v}\cdot\dot{\mathbf{p}}''=-p_0v_0^{-1}(\lambda^{-2}\rho^{-1}-\|\mathbf{v}\|^2),\quad \dot{p}_0=\lambda^{-2}v_0^{-1}(\mathbf{v}\cdot\mathbf{p}''). \tag{128}$$

The component of $\dot{\mathbf{p}}''$ normal to the vectors $\mathbf{v}$ and $\mathbf{p}''$ is not determined by the dynamical equations, namely there is a gauge symmetry. We fix the gauge by means of the condition

$$\dot{\mathbf{p}}''\cdot\mathbf{v}\times\mathbf{p}''=0. \tag{129}$$

One can show that the covariant space-time derivatives $A_i v^k$ vanish and it follows that the derivatives of v^k with respect to the parameter τ are given only by the boost of the Lorentz frame, namely

$$\dot{\mathbf{v}}=-v_0\mathbf{b}''=-\lambda^{-2}p_0^{-1}v_0\mathbf{p}'',\quad \dot{v}_0=-(\mathbf{v}\cdot\mathbf{b}'')=-\lambda^{-2}p_0^{-1}(\mathbf{v}\cdot\mathbf{p}''). \tag{130}$$

From the preceding equations it follows

$$0\leqslant\|\mathbf{v}\times\mathbf{p}''\|^2=\lambda^2(p_0^2-m^2)\|\mathbf{v}\|^2-\lambda^4v_0^2(\dot{p}_0)^2, \tag{131}$$

$$\frac{dw}{d\tau}=0,\quad w=p_0v_0\geqslant m. \tag{132}$$

The conserved quantity w is the energy measured in a privileged frame. We also obtain

$$\frac{d^2}{d\tau^2}\log p_0=-\lambda^{-2}v_0^{-2}(\lambda^{-2}\rho^{-1}+1-w^2m^2p_0^{-4}). \tag{133}$$

If w is not extremely large, the right-hand side is negative, $p_0(\tau)$ has a maximum for $\tau=\tilde{\tau}$ and violates the inequality $p_0\geqslant m$ outside a given interval. A stronger limitation is given by Eq. (131). It is clear that τ cannot vary in the whole real line.

For a detailed discussion, it is convenient to introduce some simplifications. We disregard higher powers of the adimensional quantity $\lambda^2\rho_0$, which is extremely small in all the interesting cases and we also disregard higher powers of $\tau-\tilde{\tau}$. We put $p_0(\tilde{\tau})=\tilde{p}_0$, $v_0(\tilde{\tau})=\tilde{v}_0$, $\mathbf{v}(\tilde{\tau})=\tilde{\mathbf{v}}$ and we obtain the approximate solution

$$p_0(\tau) \approx \tilde{p}_0(1 - 2^{-1}\lambda^{-4}\rho^{-1}\tilde{v}_0^{-2}(\tau-\tilde{\tau})^2), \tag{134}$$

$$\dot{p}_0(\tau) \approx -\tilde{p}_0\lambda^{-4}\rho^{-1}\tilde{v}_0^{-2}(\tau-\tilde{\tau}). \tag{135}$$

From Eq. (131) we see that τ must belong to the interval

$$|\tau-\tilde{\tau}| < 2^{-1}\Delta\tau \approx (1 - m^2\tilde{p}_0^{-2})^{1/2}\lambda^3\rho\tilde{v}_0\|\tilde{\mathbf{v}}\|. \tag{136}$$

This inequality shows that it was consistent to disregard higher powers of $\tau-\tau_0$ together with higher powers of $\lambda^2\rho$. In this interval we have

$$0 \leqslant \tilde{p}_0 - p_0(\tau) \leqslant 2^{-1}\lambda^2\rho\tilde{p}_0(1 - m^2\tilde{p}_0^{-2})\|\tilde{\mathbf{v}}\|^2 \tag{137}$$

and the quantities p_0, $\|\mathbf{p}''\|$, v_0, and $\mathbf{v}$ can be considered as constant.

It follows from Eq. (131) that at the end points of the interval (136) $\mathbf{p}''$ is parallel to $\mathbf{v}$ and by taking Eq. (129) into account, we see that the vector $\mathbf{p}''$ moves approximately on a half circumference in a plane containig the vector $\mathbf{v}$. From Eq. (128) we see that the projection of $\dot{\mathbf{p}}''$ in the direction of $\mathbf{v}$ is constant and it follows that the component of $\dot{\mathbf{p}}''$ normal to $\mathbf{v}$ tends to infinity at the end points.

The connection between τ and the "cosmic" time t, measured in the privileged rest frames defined by $\mathbf{v}=0$, is

$$\frac{dt}{d\tau} = v_i b^i = v_0 - \mathbf{v}\cdot\mathbf{b} = (\lambda^{-2}\rho^{-1} + 1)v_0^{-1} \tag{138}$$

and it follows that the interval (136) measured in terms of the time t is

$$\Delta t \approx 2\lambda(1 - m^2 p_0^{-2})^{1/2}\|\mathbf{v}\|, \tag{139}$$

namely it is, in general, very small. Note that it does not depend on the curvature ρ, but only on the four-vector v that defines the privileged frames.

The singularities at the end points of the interval (136) can be avoided by using, instead of the parameter τ defined by the condition $b^0=1$, another parameter and we can also try to extend the solution outside the interval. This is possible only if, generalizing our Lagrangian formalism, we accept negative values of b^0, namely negative values of the square root in Eq. (76). We do not try to give in this article a physical meaning to this extension, for instance in terms of antiparticles.

In any case, we have shown that, in the presence of an arbitrarily small gravitational field, the geodisic world lines, corresponding to the initial condition $\mathbf{p}''=0$, are badly unstable, since an arbitrarily small change of $\mathbf{p}''$ leads to completely different, physicaly unacceptable, solutions.

XIII. ANOTHER MODEL

In the preceding sections we have examined two models that imply an upper bound to acceleration or to pseudoacceleration. However, these models have unwanted properties, in particular the energy momentum or the four velocity of the charge may become spacelike and unstable solutions may appear. In order to show that it is not easy to avoid all these problems, we consider a model containing a fundamental length, in which both the energy momentum and the four velocity are necessarily timelike, as in the ordinary model of Sec. VII. A simple and natural Lagrangian with these properties is

$$L = -m((b^0)^2 - \|\mathbf{b}\|^2 - \lambda^2\|\mathbf{b}''\|^2)^{1/2} + eb^\bullet. \tag{140}$$

The canonical momenta are given by

$$\mathbf{p}' = 0, \quad p_\bullet = -e, \tag{141}$$

$$p_0 = mb^0((b^0)^2 - \|\mathbf{b}\|^2 - \lambda^2\|\mathbf{b}''\|^2)^{-1/2},$$

$$\mathbf{p} = m((b^0)^2 - \|\mathbf{b}\|^2 - \lambda^2\|\mathbf{b}''\|^2)^{-1/2}\mathbf{b}, \tag{142}$$

$$\mathbf{p}'' = m\lambda^2((b^0)^2 - \|\mathbf{b}\|^2 - \lambda^2\|\mathbf{b}''\|^2)^{-1/2}\mathbf{b}'',$$

and satisfy the scalar primary constraint

$$(p_0)^2 - \|\mathbf{p}\|^2 - \lambda^{-2}\|\mathbf{p}''\|^2 = m^2, \tag{143}$$

which assures that the energy momentum is timelike.

We adopt the gauge fixing conditions $b^0=1$ and $\mathbf{b}'=0$ and we obtain the formulas

$$\mathbf{b} = p_0^{-1}\mathbf{p} = (\lambda^{-2}\|\mathbf{p}''\|^2 + \|\mathbf{p}\|^2 + m^2)^{-1/2}\mathbf{p}, \tag{144}$$

$$\mathbf{b}'' = \lambda^{-2}p_0^{-1}\mathbf{p}'' = \lambda^{-1}(\|\mathbf{p}''\|^2 + \lambda^2\|\mathbf{p}\|^2 + \lambda^2 m^2)^{-1/2}\mathbf{p}'', \tag{145}$$

which assure that $\|\mathbf{b}\|<1$ and $\|\mathbf{b}''\|<\lambda^{-1}$. Note, however, that $s(\tau)$ is neither a rest frame nor a zero-momentum frame and $\mathbf{b}''$ cannot be interpreted as the acceleration or the pseudoacceleration of the particle.

The dynamical equation (36) follows from Eq. (39) and the scalar constraint (143). Equation (38) is automatically satisfied and from Eqs. (37) and (39) we obtain

$$\dot{\mathbf{p}} = -p_0\mathbf{b}'' + \mathbf{f} = -\lambda^{-2}\mathbf{p}'' + \mathbf{f}, \quad \dot{\mathbf{p}}'' = p_0\mathbf{b} - \mathbf{p} = 0. \tag{146}$$

We see that $\mathbf{p}''$ is conserved. If it vanishes, the dynamical equations coincide exactly with the equations of the ordinary model of Sec. VII in its last version and there is no upper bound to the acceleration or to the pseudoacceleration.

XIV. CONCLUSIONS

We have developed a general Lagrangian formalism for the description of test particles in gravitational and electromagnetic fields. It is based on a moving Lorentz frame associated to the particle and it is useful for the introduction of Lagrangians that depend on a fundamental length λ and to discuss a possible upper bound to the proper acceleration. Other interesting effects may be suggested by a detailed discussion of suitable models.

The test particles introduced in this way present some features characteristic of extended objects, in particular, additional degrees of freedom are present, the charge, assumed to be concentrated at the origin of the moving frame, does not necessarily coincide with the center of mass, the energy-momentum four-vector is not necessarily parallel to the four-velocity and the definition of the acceleration is somehow ambiguous.

We have considered with more detail three Lagrangians depending on the acceleration of the frame, but not on its angular velocity, discussing, in particular, the following requirements.

(1) The energy momentum four vector lies in the future cone;
(2) The velocity of the point charge is smaller than the velocity of light, namely the four velocity is time-like;
(3) The solutions have good stability properties; and
(4) There is an upper bound to the acceleration or to some related quantity as the pseudoacceleration defined in Sec. VI.

We have not been able to find a model that satisfies all these requirements and it is reasonable to conjecture that such a model does not exist within the formalism we have considered. Perhaps one should introduce new degrees of freedom that have not a geometric interpretation in terms of a moving frame.

The model described in Sec. VIII, based on rest frames, has an unphysical energy-momentum spectrum and has unstable run-away solutions even in the absence of external fields.

The model introduced in Sec. IX, based on the zero-momentum frames, has unstable solutions when a nonconstant curvature is present and, under some circumstances, the velocity of the charge may become arbitrarily large. Nevertheless, it has some interesting properties. It always has a time-like energy momentum four vector and it has good stability properties if only a slowly varying electromagnetic field is present.

An electric charge faster than light may be embarrassing, but does not seem to contradict the general principles of Maxwell's theory. The charge describes a singular distribution inside the particle of the electric current four vector, that is not required to be time-like. Moreover, in the absence of curvature, the velocity vector rotates very fast and one can only observe its average value.

In a constant electromagnetic field the second model has "stationary" solutions, similar to the trajectories of an ordinary point particle with some small corrections, but, since the model has additional degrees of freedom, more complicated solutions exist, obtained by adding to a stationary solution a periodic perturbation with a frequency $\omega/2\pi$ much larger than λ^{-1}.

In a quantized version of the model, according to Bohr's correspondence principle, this frequency is approximately interpreted as the frequency of the radiation emitted when an excited state of the particle decays. Since the frequency is defined in the zero momentum frame, the energy $\hbar\omega$ has to be interpreted as the additional mass of the excited state. This mass is very large and in ordinary conditions there is not enough energy to excite the periodic degrees of freedom and they are "frozen," as it happens, for instance, to the nuclear degrees of freedom in low-energy atomic physics. These features of the quantized model may provide some very simplified insights into the connection between ordinary and "transplanckian" physics.

The model presented in Sec. XIII has no problem with the properties of the energy momentum and of the four velocity, but the presence of the fundamental length λ in the Lagrangian does not impose any limitation to the acceleration.

Of course, a more precise physical discussion requires a formal quantization procedure of the models, based on Dirac's treatment of constrained systems. In particular, the ground state energy corresponding to the additional (internal) degrees of freedom, which cannot be evaluated by means of the correspondence principle, could give an unacceptably large contribution to the mass. The treatment of many particle states should be given in terms of free quantum fields. For the model of Sec. VIII these problems are treated in Ref. 36 and we shall discuss some other models elsewhere.

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Asymptotic form of the density profile for Gaussian and Laguerre random matrix ensembles with orthogonal and symplectic symmetry

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In a recent study we have obtained correction terms to the large N asymptotic expansions of the eigenvalue density for the Gaussian unitary and Laguerre unitary ensembles of random $N\times N$ matrices, both in the bulk and at the soft edge of the spectrum. In the present study these results are used to similarly analyze the eigenvalue density for Gaussian and Laguerre random matrix ensembles with orthogonal and symplectic symmetry. As in the case of unitary symmetry, a matching is exhibited between the asymptotic expansion of the bulk density, expanded about the edge, and the asymptotic expansion of the edge density, expanded into the bulk. In addition, aspects of the asymptotic expansion of the smoothed density, which involves delta functions at the endpoints of the support, are interpreted microscopically. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2165254]

I. INTRODUCTION

Perhaps the best known result in random matrix theory is the Wigner semicircle law (see e.g., Ref. 17). Consider a real symmetric matrix, with elements on the diagonal i.i.d. random variables having finite variance and similarly the elements above the diagonal. The Wigner semicircle law tells us that after appropriate scaling, the limiting eigenvalue density is given by the semicircle functional form

$$\rho_W(\lambda)=\begin{cases}\dfrac{2}{\pi}(1-\lambda^2)^{1/2}, & |\lambda|<1,\\ 0, & |\lambda|\geqslant 1.\end{cases} \tag{1.1}$$

As a concrete example, the Gaussian orthogonal ensemble (GOE) of real symmetric matrices is specified by its diagonal entries being distributed according to the normal distribution $N[0,1]$ and its upper triangular entries according to $N[0,1/\sqrt{2}]$. Let $\rho^{(N)}(\lambda)$ denote the eigenvalue density for $N\times N$ matrices from the GOE. After the scaling $\sqrt{2N}\rho^{(N)}(\sqrt{2N}\lambda)\mapsto N\rho(\lambda)$ the $N\to\infty$ limiting form of $\rho^{(N)}(\lambda)$ is given by (1.1).

The functional form (1.1) has implications with respect to averaging a so-called linear statistic $A=\Sigma_{j=1}^{N}a(\lambda_j)$ over the spectrum of random real symmetric matrices. Thus, if the $N\to\infty$ scaling is such that $(\alpha_N/N)\rho^{(N)}(\alpha_N\lambda)\to\rho_W(\lambda)$, $a(\alpha_N\lambda)\to\tilde{a}(\lambda)$ for some α_N then

$$\langle A \rangle := \int_{-\infty}^{\infty} \rho^{(N)}(\lambda) a(\lambda)\, d\lambda \sim N \int_{-1}^{1} \rho_W(\lambda) \tilde{a}(\lambda)\, d\lambda. \tag{1.2}$$

The result (1.2) immediately draws attention to corrections to the Wigner semicircle law. Indeed in studies of the full distribution of linear statistics averaged over the GOE and certain of its generalizations, it is necessary to compute the $O(1)$ term in the asymptotic expansion of (1.2).[8] For this one seeks the asymptotic expansion of $\bar{\rho}^{(N)}(\lambda)$, where $\bar{\rho}^{(N)}(\lambda)$ is the signed measure (smoothed density) such that

$$\int_{-\infty}^{\infty} \rho^{(N)}(\lambda) a(\lambda)\, d\lambda = \int_{-\infty}^{\infty} \bar{\rho}^{(N)}(\lambda) a(\lambda)\, d\lambda$$

to all orders in the corresponding asymptotic expansions. In the case of the GOE itself the $O(1)$ term is known,[16,2,8] and one has

$$\frac{\sqrt{2N}}{N} \bar{\rho}^{(N)}(\sqrt{2N}\lambda) \sim \rho_W(\lambda) + \frac{1}{N}\left(\frac{1}{4}\big(\delta(\lambda-1) + \delta(\lambda+1)\big) - \frac{1}{2\pi} \frac{1}{\sqrt{1-\lambda^2}} \chi_{|\lambda|<1} \right) \tag{1.3}$$

where $\chi_T = 1$ if T is true and $\chi_T = 0$ otherwise.

The correction term in (1.3) exhibits a most remarkable feature, namely delta functions at the edge of the support of the spectrum. The appearance of the delta functions at a microscopic level, when one seeks directly the asymptotic expansion of $(\sqrt{2N}/N)\rho^{(N)}(\sqrt{2N}\lambda)$ rather than the asymptotics of the smoothed quantity $\bar{\rho}^{(N)}(\lambda)$ has not, to the best of our knowledge, been previously studied. One of the purposes of this paper is to undertake such a study for the Gaussian and Laguerre ensembles in random matrix theory. Each of the three symmetry classes, orthogonal ($\beta=1$), unitary ($\beta=2$), and symplectic ($\beta=4$) will be considered. For the Gaussian ensemble it is known[8] that (1.3) then generalizes to read

$$\frac{\sqrt{2N}}{N} \bar{\rho}^{(N)}(\sqrt{2N}\lambda) \sim \rho_W(\lambda) + \frac{1}{N}\left(\frac{1}{\beta} - \frac{1}{2} \right)\left(\frac{1}{2}\big(\delta(\lambda-1) + \delta(\lambda+1)\big) - \frac{1}{\pi} \frac{1}{\sqrt{1-\lambda^2}} \chi_{|\lambda|<1} \right). \tag{1.4}$$

Our task is to relate this expansion to the asymptotic expansion of the density itself.

The expansion (1.4) clearly shows both a bulk effect and an edge effect. This is in keeping with there being both a (global) bulk regime, and an edge regime which must be treated separately in the asymptotic analysis. As these expansions relate to the same quantity, one would expect there to be a matching in an appropriate limit. This topic, initiated in Ref. 7 for the GUE and LUE, is another main theme of the present work.

We begin in Sec. II by recalling the results from Ref. 7 relating to the asymptotic expansions of the global bulk density, and the soft edge density, in the GUE and LUE. We then proceed to write down higher order terms in these asymptotic expansions (obtained from the method of Ref. 7). These higher order terms are then used to further investigate the matching phenomenon alluded to above.

In Sec. III formulas required in the study of the asymptotics of the density in the Gaussian and Laguerre ensembles with orthogonal and symplectic symmetry are gathered. These formulas are used in Sec. IV to study the corresponding global density asymptotic expansions, and in Sec. V to study the soft edge density asymptotic expansions. In Sec. VI we use the results of Secs. II, IV and V to study our main topics of interest, namely the matching between the bulk and edge asymptotic expansions, and the microscopic origin of the delta functions in (1.4) and its Laguerre analogue.

II. THE GAUSSIAN AND LAGUERRE ENSEMBLES WITH UNITARY SYMMETRY

A. Definitions and summary of known results

The Gaussian unitary ensemble consists of the set of Hermitian matrices with diagonal entries distributed according to the normal distribution $N[0,1/\sqrt{2}]$ and with upper triangular entries distributed according to $N[0,1/2]+iN[0,1/2]$. The corresponding eigenvalue pdf is given by

$$\frac{1}{C}\prod_{l=1}^{N} e^{-x_l^2} \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^2, \tag{2.1}$$

where here and below C denotes *some* normalization constant.

The Laguerre unitary ensemble can be specified by matrices $X=A^\dagger A$ where A is a $n\times m$ ($n \geqslant m$) complex Gaussian matrix with entries distributed according to $N[0,1/\sqrt{2}]+iN[0,1/\sqrt{2}]$. All the eigenvalues are non-negative and have the joint distribution

$$\frac{1}{C}\prod_{l=1}^{m} x_l^{\alpha} e^{-x_l} \prod_{1\leqslant j<k\leqslant m} (x_k - x_j)^2, \tag{2.2}$$

where $\alpha=n-m$.

The eigenvalue pdf's (2.1) and (2.2) are special cases of the functional form

$$\mathrm{UE}_N(g_2) := \frac{1}{C}\prod_{l=1}^{N} g_2(x_l) \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^2 \tag{2.3}$$

defining a general matrix ensemble with unitary symmetry in terms of its eigenvalue pdf. Thus

$$\mathrm{Ev}(\mathrm{GUE}_N) = \mathrm{UE}_N(e^{-x^2}), \quad \mathrm{Ev}(\mathrm{LUE}_N) = \mathrm{UE}_N(x^{\alpha}e^{-x}),$$

where $\mathrm{Ev}(M)$ denotes the eigenvalue pdf of the matrix ensemble M.

It is a basic result in random matrix theory (see, e.g., Ref. 4) that the eigenvalue density for the ensemble (2.3) can be written in terms of the monic polynomials $\{p_n(x)\}$ orthogonal with respect to the weight $g_2(x)$. Thus with $(p_n,p_n)_2$ denoting the corresponding normalizations we have

$$\rho(x;\mathrm{UE}_N(g_2)) = g_2(x)\sum_{j=0}^{N-1} \frac{(p_j(x))^2}{(p_j,p_j)_2}. \tag{2.4}$$

In a recent study Kalisch and Braak[9] have obtained the leading correction term to the Wigner semicircle law for the asymptotic expansion of (2.4) in the case of the GUE.

Proposition 1: Let $-1<X<1$ *be fixed. One has*

$$\frac{1}{N}\rho(X;\mathrm{UE}_N(e^{-2Nx^2})) \sim \rho_W(X) - \frac{2\cos(2N\pi P_{\mathrm{W}}(X))}{\pi^3\rho_{\mathrm{W}}^2(X)}\frac{1}{N} + \mathrm{O}\left(\frac{1}{N^2}\right), \tag{2.5}$$

where $\rho_W(x)$ *is given by* (1.1) *and*

$$P_W(x) = 1 + \frac{x}{2}\rho_{\mathrm{W}}(x) - \frac{1}{\pi}\mathrm{Arccos}\, x. \tag{2.6}$$

The methods in Ref. 9 are particular to the Gaussian ensembles, relying on an integral formula coming from the supersymmetry method. Subsequently the present authors[7] have introduced a different strategy which reclaims (2.5), and furthermore applies equally well to the Laguerre case, for which the following result was obtained.

Proposition 2: Let $0<X<1$ *be fixed. We have*

$$\frac{1}{N}\rho(X;\mathrm{UE}_N(x^\alpha e^{-4Nx})) \sim \rho_{\mathrm{MP}}(X) - \left(\frac{\cos((2N+\alpha)\pi P_{\mathrm{MP}}(X) - \alpha\pi(1+X\rho_{\mathrm{MP}}(X)))}{\pi^3 X^2 \rho_{\mathrm{MP}}^2(X)} - \frac{\alpha}{\pi^2 X \rho_{\mathrm{MP}}(X)}\right)\frac{1}{N} + O\left(\frac{1}{N^2}\right), \tag{2.7}$$

where

$$\rho_{\mathrm{MP}}(x) := \frac{2}{\pi}\sqrt{\frac{1}{x}-1}, \quad P_{\mathrm{MP}}(x) = 1 + x\rho_{\mathrm{MP}}(x) - \frac{2}{\pi}\mathrm{Arccos}\sqrt{x} \tag{2.8}$$

(*the subscript MP denotes Marčenko-Pastur, who first derived the limit law giving the leading term in this expression*).

The strategy of Ref. 7 was to use integral representations of the product of orthogonal polynomials which result from the Christoffel-Darboux summation of (2.4). In addition to yielding the asymptotics of the global bulk density, it also gave asymptotics of the density at the so-called soft edge. This is the name given to the boundary of the support at leading order, with the feature that the density, appropriately scaled, is nonzero on both sides of this boundary.

Proposition 3: Let ξ be fixed. For the GUE

$$\frac{1}{2N^{2/3}}\rho\left(1 + \frac{\xi}{2N^{2/3}}; \mathrm{UE}_N(e^{-2Nx^2})\right) = [\mathrm{Ai}'(\xi)]^2 - \xi[\mathrm{Ai}(\xi)]^2 - \frac{1}{20}(3\xi^2[\mathrm{Ai}(\xi)]^2 - 2\xi[\mathrm{Ai}'(\xi)]^2 - 3\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi))\frac{1}{N^{2/3}} + O\left(\frac{1}{N}\right), \tag{2.9}$$

while for the LUE

$$\frac{1}{(2N)^{2/3}}\rho\left(1 + \frac{\xi}{(2N)^{2/3}}; \mathrm{UE}_N(x^\alpha e^{-4Nx})\right) = ([\mathrm{Ai}'(\xi)]^2 - \xi[\mathrm{Ai}(\xi)]^2) + \frac{\alpha}{2^{1/3}}[\mathrm{Ai}(\xi)]^2\frac{1}{N^{1/3}} + \frac{2^{1/3}}{10}(3\xi^2[\mathrm{Ai}(\xi)]^2 - 2\xi[\mathrm{Ai}'(\xi)]^2 + (2-5\alpha^2)\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi))\frac{1}{N^{2/3}} + O\left(\frac{1}{N}\right). \tag{2.10}$$

B. Matching of the bulk and edge expansions

We pursue the matching phenomenon observed in Ref. 7 between the asymptotic expansion of the bulk density, expanded about the soft edge, and the asymptotic expansion of the edge density, expanded into the bulk. Explicitly, it was found that setting

$$X = 1 + \xi/2N^{2/3} \quad (\xi < 0) \tag{2.11}$$

in the asymptotic expansion (2.5) multiplied by $N^{2/3}/2$, and then expanding in N, a matching is obtained with the $\xi \to -\infty$ asymptotic expansion on the right-hand side of (2.9). This was checked on terms in ξ in the latter accessible by expanding the former; on this point we note that terms of all orders in inverse powers of N in (2.5), will after substitution of (2.11) contribute to each term in the expansion of (2.9). A similar matching was observed between the bulk LUE density expanded with the substitution (2.11), and the $\xi \to -\infty$ asymptotic expansion of the $O(1)$ and $O(N^{-1/3})$ terms of the edge density (2.10).

Based on this evidence, the hypothesis was put forward in Ref. 7 that the matching persists between all terms in ξ, and at all orders in inverse (fractional) powers of N. Here we probe this

hypothesis further by extending the asymptotic expansions (2.5), (2.7), (2.9), and (2.10). As explained in Ref. 7, the orthogonal polynomial method readily allows for the computation of higher order terms, which we compute to be given as follows.

Proposition 4: The $O(1/N^2)$ *term in* (2.5) *is*

$$\left(\frac{1}{16\pi(1-X^2)^{5/2}}+\frac{X(15+2X^2)\sin[2N\pi P_{\mathrm{W}}(X)]}{48\pi(1-X^2)^{5/2}}\right)\frac{1}{N^2}; \tag{2.12}$$

the $O(1/N^3)$ *term in* (2.5) *is*

$$\frac{180+981X^2+60X^4+4X^6}{2304\pi(1-X^2)^4}\cos[2N\pi P_W(X)]\frac{1}{N^3}; \tag{2.13}$$

the oscillatory $O(1/N^4)$ *term in* (2.5) *is*

$$-X\frac{323\,190+647\,055X^2+20\,358X^4+6084X^6-1112X^8}{829\,440\pi(1-X^2)^{11/2}}\sin[2N\pi P_W(X)]\frac{1}{N^4}; \tag{2.14}$$

the $O(1/N^2)$ *term in* (2.7) *is*

$$\begin{aligned}&\left(\left(\frac{\alpha}{8\pi(1-X)^2}\right)\cos[2N\pi P_{\mathrm{MP}}(X)-2\alpha\,\mathrm{Arccos}\sqrt{X}]\right.\\&+\left(\frac{-3+12X+8X^2+12(-1+X)(-1+2X)\alpha^2}{192\pi(1-X)^{5/2}X^{3/2}}\right)\sin[2N\pi P_{\mathrm{MP}}(X)-2\alpha\,\mathrm{Arccos}\sqrt{X}]\\&\left.+\frac{1+4(-1+X)\alpha^2}{64\pi(1-X)^{5/2}X^{3/2}}\right)\frac{1}{N^2};\end{aligned} \tag{2.15}$$

the $O(1/N)$ *term in* (2.9) *is*

$$\left(\left(-\frac{\xi}{12}+\frac{3\xi^4}{40}+\frac{\xi^7}{48}\right)(\mathrm{Ai}(\xi))^2-\frac{3\xi^2}{40}\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi)+\left(\frac{1}{12}-\frac{\xi^3}{20}-\frac{\xi^6}{48}\right)(\mathrm{Ai}'(\xi))^2\right)\frac{1}{N}; \tag{2.16}$$

the $O(1/N)$ *term in* (2.10) *is*

$$\alpha\left(\left(-\frac{7\xi}{15}+\frac{\alpha^2\xi}{6}\right)(\mathrm{Ai}(\xi))^2-\frac{\xi^2}{5}\mathrm{Ai}(\xi)\mathrm{Ai}'(\xi)+\left(-\frac{1}{6}+\frac{\alpha^2}{6}\right)(\mathrm{Ai}'(\xi))^2\right)\frac{1}{N}. \tag{2.17}$$

Considering first the GUE, we now substitute (2.11) in (2.5) extended by (2.12), (2.13), (2.14). Expanding the asymptotic series (an operation we denote by $\dot{\sim}$) gives the new asymptotic series in N,

$$\begin{aligned}&\frac{1}{N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{UE}_N(e^{-2Nx^2})\right)\\&\quad\dot{\sim}\left(\frac{2\sqrt{|\xi|}}{\pi}+\frac{1}{16\pi|\xi|^{5/2}}+\left(-\frac{1}{2\pi|\xi|}+\frac{1225}{2304\pi\xi^4}\right)\cos(4|\xi|^{3/2}/3)-\frac{17\sin(4|\xi|^{3/2}/3)}{48\pi|\xi|^{5/2}}\right)\\&\qquad+\left(-\frac{|\xi|^{3/2}}{4\pi}+\frac{5}{128\pi|\xi|^{3/2}}+\left(-\frac{43}{480\pi}-\frac{23\,695}{331\,776\pi|\xi|^3}\right)\cos(4|\xi|^{3/2}/3)\right.\\&\qquad\left.+\left(\frac{233}{4608}-\frac{|\xi|^3}{20}\right)\frac{\sin(4|\xi|^{3/2}/3)}{\pi|\xi|^{3/2}}\right)\frac{1}{N^{2/3}}+O\left(\frac{1}{N^{4/3}}\right).\end{aligned} \tag{2.18}$$

On the other hand, making use of the asymptotic series[12]

$$\mathrm{Ai}(-z) \sim \pi^{-1/2} z^{-1/4} \left(\sin(\zeta + \pi/4) \sum_{k=0}^{\infty} (-1)^k c_{2k} \zeta^{-2k} - \cos(\zeta + \pi/4) \sum_{k=0}^{\infty} (-1)^k c_{2k+1} \zeta^{-2k-1} \right), \tag{2.19}$$

where

$$\zeta = \frac{2}{3} z^{3/2}, \quad c_0 = 1, \quad c_k = \frac{(2k+1)(2k+3)\cdots(6k-1)}{(216)^k k!} \quad (k \geqslant 1),$$

the $\xi \to -\infty$ expansion of the $O(1)$ and $O(1/N^{2/3})$ terms in (2.9) can readily be computed. Agreement is found with all terms in (2.18) except the one involving the fraction 23 695/331 776. Thus, even though no terms $O(1/N)$ have yet appeared, whereas (2.16) has a term at this order, the evidence is still in favor of a matching between all terms in ξ, and at all orders in inverse powers of N. However this matching cannot be fully exhibited at any order in N in the expansion of (2.9) without knowledge of all terms in the asymptotic expansion of (2.5).

As already mentioned, a similar matching phenomenon was observed in Ref. 7 in the case of the LUE, and conjectured to hold at general orders as for the GUE. Further evidence for this conjecture can be obtained by substituting (2.11) in (2.7) extended by (2.15), expanding as a series in inverse powers of N, and comparing against the $\xi \to -\infty$ expansion of (2.10). The former operation gives

$$\begin{aligned} &\frac{1}{N^{2/3}} \rho \left(1 + \frac{\xi}{2N^{2/3}}; \mathrm{UE}_N(x^\alpha e^{-4Nx}) \right) \\ &\quad \dot{\sim} \left(\frac{2^{2/3}|\xi|^{1/2}}{\pi} - \frac{\cos(4|\xi|^{3/2}/3)}{2^{4/3}\pi|\xi|} \right) + \frac{\alpha(1 + \sin(4|\xi|^{3/2}/3))}{2^{2/3}\pi|\xi|^{1/2}N^{1/3}} \\ &\qquad + \frac{1}{160\pi|\xi|^{3/2}N^{2/3}} \big(5 - 20\alpha^2 + 80|\xi|^3 + 40(-1 + 2\alpha^2)|\xi|^{3/2} \cos(4|\xi|^{3/2}/3) \\ &\qquad + (5 - 20\alpha^2 + 16|\xi|^3)\sin(4|\xi|^{3/2}/3) \big) + O\left(\frac{1}{N} \right). \end{aligned} \tag{2.20}$$

The latter operation gives agreement with this expansion at $O(1)$, $O(1/N^{1/3})$ and for the terms involving factors of $|\xi|^3$ at $O(1/N^{2/3})$. This is consistent with the matching hypothesis.

III. THE GAUSSIAN AND LAGUERRE ENSEMBLES WITH ORTHOGONAL AND SYMPLECTIC SYMMETRY—GENERAL FORMULAS

The Gaussian orthogonal ensemble has already been defined in the Introduction. At the level of an eigenvalue pdf, the GOE can be defined by the joint distribution

$$\frac{1}{C} \prod_{l=1}^{N} e^{-x_l^2/2} \prod_{1 \leqslant j < k \leqslant N} |x_k - x_j|.$$

Likewise the Gaussian symplectic ensemble, Laguerre orthogonal ensemble and Laguerre symplectic ensemble can be specified either in terms of the distribution of certain classes of random matrices (real symmetric matrices in the cases of orthogonal symmetry, and Hermitian matrices with real quaternion elements in the cases of symplectic symmetry), or in terms of the functional form of the eigenvalue pdf (see, e.g., Ref. 4). Here we will note only the latter, which in the case of the GSE reads

$$\frac{1}{C}\prod_{l=1}^{N} e^{-2x_l^2} \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^4;$$

for the LOE reads

$$\frac{1}{C}\prod_{l=1}^{N} x_l^{\alpha/2} e^{-x_l/2} \prod_{1\leqslant j<k\leqslant N} |x_k - x_j|;$$

and for the LSE reads

$$\frac{1}{C}\prod_{l=1}^{N} x_l^{2\alpha} e^{-2x_l} \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^4.$$

For the Laguerre ensembles one requires the eigenvalues to be positive and thus $x_l > 0$ ($l = 1, \ldots, N$). Thus we see that if we define a matrix ensemble with orthogonal and symplectic symmetry by the eigenvalue pdf's,

$$\mathrm{OE}_N(g_1) := \frac{1}{C}\prod_{l=1}^{N} g_1(x_l) \prod_{1\leqslant j<k\leqslant N} |x_k - x_j|$$

and

$$\mathrm{SE}_N(g_4) := \frac{1}{C}\prod_{l=1}^{N} g_4(x_l) \prod_{1\leqslant j<k\leqslant N} (x_k - x_j)^4,$$

respectively, then we have

$$\mathrm{Ev}(\mathrm{GOE}_N) = \mathrm{OE}_N(e^{-x^2/2}), \quad \mathrm{Ev}(\mathrm{LOE}_N) = \mathrm{OE}_N(x^{\alpha/2} e^{-x/2}),$$

$$\mathrm{Ev}(\mathrm{GSE}_N) = \mathrm{SE}_N(e^{-2x^2}), \quad \mathrm{Ev}(\mathrm{LSE}_N) = \mathrm{SE}_N(x^{2\alpha} e^{-x}). \tag{3.1}$$

In Ref. 1, the eigenvalue densities for the ensembles $\mathrm{OE}(g_1)$ and $\mathrm{SE}(g_4)$ were computed for all the so-called classical weights

$$g_1(x) = \begin{cases} e^{-x^2/2}, & \text{Gaussian}, \\ x^{(\alpha-1)/2} e^{-x/2} \ (x > 0), & \text{Laguerre}, \\ (1-x)^{(a-1)/2}(1+x)^{(b-1)/2} (-1 < x < 1), & \text{Jacobi}, \\ (1+x^2)^{-(\alpha+1)/2}, & \text{Cauchy}, \end{cases} \tag{3.2}$$

$$g_4(x) = \begin{cases} e^{-x^2}, & \text{Hermite}, \\ x^{\alpha+1} e^{-x}, & \text{Laguerre}, \\ (1-x)^{a+1}(1+x)^{b+1}, & \text{Jacobi}, \\ (1+x^2)^{-(\alpha-1)}, & \text{Cauchy} \end{cases} \tag{3.3}$$

in terms of a formula depending on the symmetry class only. Thus for ensembles $\mathrm{OE}_N(g_1)$ with classical weights (3.2) one has

$$\rho(x;\mathrm{OE}_N(g_1(x))) = \rho(x;\mathrm{UE}_{N-1}(g_2(x))) + \frac{c_{N-2}}{(p_{N-2},p_{N-2})_2(p_{N-1},p_{N-1})_2} g_1(x)p_{N-1}(x)\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{sgn}(x-t)p_{N-2}(t)g_1(t)\,\mathrm{d}t, \tag{3.4}$$

while for ensembles $\mathrm{SE}_N(g_4)$ with classical weights (3.3) one has

$$\rho(x;\mathrm{SE}_N(g_4(x))) = \frac{1}{2}\rho(x;\mathrm{UE}_{2N}(g_2)) - g_1(x)\frac{c_{2N-1}p_{2N}(x)}{2(p_{2N},p_{2N})_2(p_{2N-1},p_{2N-1})_2}\int_x^{\infty} g_1(t)p_{2N-1}(t)\,\mathrm{d}t. \tag{3.5}$$

In (3.4) and (3.5),

$$g_2(x) = \begin{cases} e^{-x^2}, & \text{Hermite}, \\ x^{\alpha}e^{-x}, & \text{Laguerre}, \\ (1-x)^a(1+x)^b, & \text{Jacobi}, \\ (1+x^2)^{-\alpha}, & \text{Cauchy} \end{cases} \tag{3.6}$$

while

$$\frac{c_j}{(p_j,p_j)_2} = \begin{cases} 1, & \text{Hermite}, \\ \frac{1}{2}, & \text{Laguerre}. \end{cases} \tag{3.7}$$

The quantities $\{p_n(x)\}$ are the monic classical orthogonal polynomials with respect to the weights (3.6), and $(p_n,p_n)_2$ the corresponding normalizations. Thus in the Gaussian case

$$p_n(x) = 2^{-n}H_n(x), \quad (p_n,p_n)_2 = \pi^{1/2}2^{-n}n! \tag{3.8}$$

while in the Laguerre case

$$p_n(x) = (-1)^n n!\, L_n^{\alpha}(x), \quad (p_n,p_n)_2 = \Gamma(n+1)\Gamma(\alpha+n+1). \tag{3.9}$$

Essential tools in our subsequent analysis of the asymptotic forms of (3.4) and (3.5) are particular asymptotic formulas for the Hermite and Laguerre polynomials. Consider first the bulk region. In the case of the Hermite polynomials, the formula is due to Plancherel and Rotach.[13] It tells us that with

$$x = (2n+1)^{1/2}\cos\phi, \quad \epsilon \leqslant \phi \leqslant \pi - \epsilon,$$

we have

$$e^{-x^2/2}H_n(x) = 2^{n/2+1/4}(n!)^{1/2}(\pi n)^{-1/4}(\sin\phi)^{-1/2}(\sin((n/2+1/4)(\sin 2\phi - 2\phi) + 3\pi/4) + O(n^{-1})).$$

Setting

$$\sqrt{2N}X = (2(N+m)+1)^{1/2}\cos\phi$$

with $-1 < X < 1$ fixed we deduce from this that for m fixed

$$H_{N+m}(\sqrt{2N}X) = \left(\frac{2}{\pi}\right)^{1/4}\frac{2^{m/2+N/2}}{(1-X^2)^{1/4}}N^{m/2-1/4}(N!)^{1/2}e^{NX^2}g_{m,N}^{(H)}(X)\left(1+O\left(\frac{1}{N}\right)\right), \tag{3.10}$$

where

$$g_{m,N}^{(H)}(x) := \cos\left(Nx\sqrt{1-x^2} + (N+1/2)\mathrm{Arcsin}\,x - N\pi/2 - m\,\mathrm{Arccos}\,x\right). \tag{3.11}$$

The Plancherel-Rotach formula (3.10) was extended by Moecklin to the Laguerre polynomials.[10] With

$$x = (4n + 2\alpha + 2)\cos^2 \phi, \quad \epsilon \leqslant \phi \leqslant \pi/2 - \epsilon n^{-1/2}$$

it reads

$$e^{-x/2}L_n^{(\alpha)}(x) = (-1)^n(\pi \sin \phi)^{-1/2}x^{-\alpha/2-1/4}n^{\alpha/2-1/4} \times (\sin((n + (\alpha + 1)/2)(\sin 2\phi - 2\phi) + 3\pi/4) + (nx)^{-1/2}O(1)).$$

Setting

$$4nX = (4(n + m) + 2\alpha + 2)\cos^2 \phi$$

with m fixed and $\epsilon/n < X < 1$ we deduce from this that

$$x^{\alpha/2}e^{-x/2}L_{n+m}^{(\alpha)}(x)|_{x=4nX} = (-1)^{n+m}(2\pi\sqrt{X(1-X)})^{-1/2}n^{\alpha/2-1/2}\left(g_{m,n}^{(L)}(X) + O\left(\frac{1}{n}\right)\right), \tag{3.12}$$

where

$$g_{m,n}^{(L)}(X) := \sin(2n(\sqrt{X(1-X)} - \operatorname{Arccos}\sqrt{X}) - (2m + \alpha + 1)\operatorname{Arccos}\sqrt{X} + 3\pi/4). \tag{3.13}$$

We turn our attention now to the (soft) spectrum edge. In the Hermite case, the formula of Plancherel and Rotach tells us that with

$$x = (2N)^{1/2} + 2^{-1/2}N^{-1/6}t \tag{3.14}$$

we have

$$\exp(-x^2/2)H_N(x) = \pi^{1/4}2^{N/2+1/4}(N!)^{1/2}N^{-1/12}\{\mathrm{Ai}(t) + O(N^{-2/3})\},$$

where $\mathrm{Ai}(t)$ denotes the Airy function. It follows from this that with x again related to t by (3.14),

$$\exp(-x^2/2)H_{N+m}(x) = (2N)^{m/2}\pi^{1/4}2^{N/2+1/4}(N!)^{1/2}N^{-1/12}\left\{\mathrm{Ai}(t) - \frac{m}{N^{1/3}}\mathrm{Ai}'(t) + O(N^{-2/3})\right\}. \tag{3.15}$$

In the Laguerre case, Szegö[15] gives that with

$$x = 4N + 2\alpha + 2 + 2(2N)^{1/3}t \tag{3.16}$$

we have

$$e^{-x/2}L_N^{\alpha}(x) = (-1)^N 2^{-\alpha-1/3}N^{-1/3}(\mathrm{Ai}(t) + O(N^{-2/3})).$$

It then follows that for fixed p,

$$e^{-x/2}L_{N+p}^{\alpha}(x)|_{x=4N+2(2N)^{1/3}\xi} = (-1)^{N+p}2^{-\alpha-1/3}N^{-1/3}\left(\mathrm{Ai}(\xi) - \frac{2p + \alpha + 1}{(2N)^{1/3}}\mathrm{Ai}'(\xi) + O(N^{-2/3})\right). \tag{3.17}$$

IV. ASYMPTOTIC EXPANSIONS IN THE BULK

A. GOE and GSE in the bulk

As with the GUE, the asymptotic expansion of the bulk density for the GOE and GSE has been carried out by Kalisch and Braak.[9] But as their method is particular to the Gaussian case, we give an alternative method which can be extended to the Laguerre case.

Consider first the GOE. Substituting the appropriate formula from (3.7) and (3.8), in (3.4) we see after minor manipulation that

$$\rho(x;\mathrm{OE}_N(e^{-x^2/2})) = \rho(x;\mathrm{UE}_{N-1}(e^{-x^2})) + \frac{e^{-x^2/2}H_{N-1}(x)}{2^{N-1}\pi^{1/2}(N-2)!}\int_0^x e^{-t^2/2}H_{N-2}(t)\,\mathrm{d}t. \tag{4.1}$$

Also, making use of (2.4) shows

$$\rho(x;\mathrm{UE}_{N-1}(e^{-x^2})) = \rho(x;\mathrm{UE}_N(e^{-x^2})) - \frac{2^{-(N-1)}e^{-x^2}}{\pi^{1/2}(N-1)!}(H_{N-1}(x))^2. \tag{4.2}$$

From (4.1) and (4.2) the following asymptotic formula for the bulk eigenvalue density is obtained.

Proposition 5: Let $-1<X<1$ *be fixed. We have*

$$\frac{1}{N}\rho(X;\mathrm{OE}_N(e^{-Nx^2})) \sim \frac{2}{\pi}\sqrt{1-X^2} - \frac{1}{2\pi N\sqrt{1-X^2}} + O\left(\frac{1}{N^2}\right). \tag{4.3}$$

Proof: First we note that

$$\rho(X;\mathrm{OE}_N(e^{-Nx^2})) = \sqrt{2N}\rho(\sqrt{2N}X;\mathrm{OE}_N(e^{-x^2/2})), \tag{4.4}$$

and we proceed to analyze the large N form of the right-hand side using (4.1). In relation to the latter, by a simple change of variables,

$$\int_0^{\sqrt{2N}X} e^{-t^2/2}H_{N-2}(t)\,\mathrm{d}t = \left.\sqrt{2N}\int_0^X e^{-t^2/2}H_{N-2}(t)\right|_{t=\sqrt{2N}T}\mathrm{d}T,$$

while making use of (3.10) shows

$$\sqrt{2N}\int_0^X e^{-t^2/2}H_{N-2}(t)\Big|_{t=\sqrt{2N}T}\mathrm{d}T \sim \sqrt{2N}\left(\frac{2}{\pi}\right)^{1/4}\frac{2^{-1+N/2}}{(1-T^2)^{1/4}}N^{-5/4}(N!)^{1/2}\int_0^X \frac{g^{(H)}_{-2,N}(T)}{(1-T^2)^{1/4}}\mathrm{d}T. \tag{4.5}$$

The leading contribution to the integral for large N comes from the neighborhood of the endpoints $T=0$ and $T=X$. About $T=0$

$$g^{(H)}_{m,N}(T) \sim \cos(2NT - (N+m)\pi/2 + O(T^2)),$$

while about $T=X$,

$$\begin{aligned} g^{(H)}_{m,N}(T) \sim \cos(&NX\sqrt{1-X^2} + (N+1/2)\mathrm{Arcsin}\,X - N\pi/2 - m\,\mathrm{Arccos}\,X \\ &+ 2N\sqrt{1-X^2}(T-X) + O((T-X)^2)). \end{aligned}$$

Thus we have

$$\int_0^X \frac{g^{(H)}_{-2,N}(T)}{(1-T^2)^{1/4}}\mathrm{d}T \sim \frac{1}{2N(1-X^2)^{3/4}}\tilde{g}^{(H)}_{-2,N}(X), \tag{4.6}$$

where

$$\tilde{g}^{(H)}_{m,N}(x) := \sin(Nx\sqrt{1-x^2} + (N+1/2)\mathrm{Arcsin}\,x - N\pi/2 - m\,\mathrm{Arccos}\,x) \tag{4.7}$$

and use has been made of the fact that N is assumed even in (3.4).

We read off from (3.10) that

$$e^{-x^2}H_{N-1}(x)\big|_{x=\sqrt{2N}X} = \left(\frac{2}{\pi}\right)^{1/4}\frac{2^{-1/2+N/2}}{(1-X^2)^{1/4}}N^{-3/4}(N!)^{1/2}g^{(H)}_{-1,N}(X)\left(1+O\left(\frac{1}{N}\right)\right). \tag{4.8}$$

Making use of this together with (4.5), (4.6) and Stirling's formula we deduce

$$\frac{e^{-x^2/2}H_{N-1}(x)}{2^{N-1}\pi^{1/2}(N-2)!}\int_0^{\sqrt{2N}X} e^{-t^2/2}H_{N-2}(t)\mathrm{d}t$$
$$\sim \frac{1}{\pi\sqrt{2N}}\frac{g_{-1,N}^{(H)}(X)\tilde{g}_{-2,N}^{(H)}(X)}{(1-X^2)}\left(1+O\left(\frac{1}{N}\right)\right)$$
$$= \frac{1}{\pi\sqrt{2N}}\frac{g_{-1,N}^{(H)}(X)}{(1-X^2)}\left(X\tilde{g}_{-1,N}^{(H)}(X)+\sqrt{1-X^2}g_{-1,N}^{(H)}(X)\right)\left(1+O\left(\frac{1}{N}\right)\right), \tag{4.9}$$

where the equality follows from simple trigonometric identities.

For the second term in (4.2), use of (4.8) shows

$$-\frac{2^{-(N-1)}e^{-x^2}}{\pi^{1/2}(N-1)!}(H_{N-1}(x))^2\Big|_{x=\sqrt{2N}X} \sim -\frac{1}{\pi}\sqrt{\frac{2}{N}}\frac{(g_{-1,N}^{(H)}(X))^2}{\sqrt{1-X^2}}\left(1+O\left(\frac{1}{N}\right)\right). \tag{4.10}$$

And for the first term in (4.2) we know from (2.5) that

$$\rho(\sqrt{2N}X;\mathrm{UE}_N(e^{-x^2})) \sim \frac{\sqrt{2N}}{\pi}\sqrt{1-X^2}-\sqrt{\frac{2}{N}}\frac{\cos(2NX\sqrt{1-X^2}+2N\,\mathrm{Arcsin}\,X-N\pi)}{2\pi(1-X^2)}+O\left(\frac{1}{N^{3/2}}\right). \tag{4.11}$$

But

$$\cos(2NX\sqrt{1-X^2}+2N\,\mathrm{Arcsin}\,X-N\pi)=\sqrt{1-X^2}(2(\tilde{g}_{-1,N}^{(H)}(X))^2-1)-2X\tilde{g}_{-1,N}^{(H)}(X)g_{-1,N}^{(H)}(X). \tag{4.12}$$

Substituting (4.12) in (4.11), then adding this, (4.9) and (4.10), and recalling (4.4) gives (4.3). □

The result (4.3) agrees with that computed by Kalisch and Braak in Ref. 9 and is also consistent with (1.3). We remark that in Ref. 9 the $O(1/N^2)$ term is also given, being equal to

$$\frac{3+4X^2}{16\pi(1-X^2)^{5/2}N^2}-\frac{\cos((2N-1)\mathrm{Arcsin}\,X+2NX\sqrt{1-X^2})}{8\pi(1-X^2)^{5/2}N^2}. \tag{4.13}$$

In principle the present method offers a systematic approach to all correction terms. For this we need the explicit form of the higher order terms in (3.10), and these can in fact be calculated from the results in Ref. 13. However we have not pursued such calculations. We remark too that a calculation of the nonoscillatory portion of (4.13) is undertaken in Ref. 2; however the result obtained does not agree with (4.13).

We turn our attention now to the GSE. First we note that

$$\rho(X;\mathrm{SE}_N(e^{-4Nx^2}))=2\sqrt{N}\rho(2\sqrt{N}X;\mathrm{SE}_N(e^{-x^2})). \tag{4.14}$$

Regarding the right-hand side, making use of (3.7), (3.8) as well as the integral evaluation (see, e.g., Ref. 1)

$$2^{-N}\int_0^{\infty} e^{-t^2/2}H_N(t)\mathrm{d}t=\sqrt{\frac{\pi}{2}}\frac{N!}{2^N(N/2)!} \tag{4.15}$$

gives

$$\rho(x;\mathrm{SE}_N(e^{-x^2})) = \frac{1}{2}\rho(x;\mathrm{UE}_{2N}(e^{-x^2})) - \frac{e^{-x^2/2}H_{2N}(x)}{4\pi^{1/2}(2N-1)!}\left(\sqrt{\frac{\pi}{2}}\frac{(2N-1)!}{2^{2N-1}(N-1/2)!} - 2^{-(2N-1)}\int_0^x e^{-t^2/2}H_{2N-1}(t)\mathrm{d}t\right). \tag{4.16}$$

The asymptotic form of (4.16) can be calculated according to the strategy of the proof of Proposition 5 to give the following result for the bulk scaled density in the GSE.

Proposition 6: Let $-1<X<1$ *be fixed, and* $g^{(H)}_{0,2N}(X)$ *be given according to* (3.11). *We have*

$$\frac{1}{N}\rho(X;\mathrm{SE}_N(e^{-4Nx^2})) \sim \frac{2}{\pi}\sqrt{1-X^2} - \left(\frac{1}{\sqrt{2\pi N}} + \frac{(-1)^N}{2\pi N}\right)\frac{g^{(H)}_{0,2N}(X)}{(1-X^2)^{1/4}} + \frac{1}{4\pi N}\frac{1}{\sqrt{1-X^2}} + O\left(\frac{1}{N^{3/2}}\right). \tag{4.17}$$

Proof: Analogous to (4.5), it follows from (3.10) that

$$\int_0^{2\sqrt{N}X} e^{-t^2/2}H_{2N-1}(t)\mathrm{d}t \sim 2\sqrt{N}\left(\frac{2^{N-1}}{\pi^{1/4}N^{3/4}}((2N)!)^{1/2}\right)\int_0^X \frac{g^{(H)}_{-1,2N}(t)}{(1-t^2)^{1/4}}\mathrm{d}t,$$

while proceeding as in the derivation of (4.6) shows

$$\int_0^X \frac{g^{(H)}_{-1,2N}(t)}{(1-t^2)^{1/4}}\mathrm{d}t \sim \frac{1}{4N}\frac{1}{(1-X^2)^{3/4}}\tilde{g}^{(H)}_{-1,2N}(X) - \frac{(-1)^N}{4N}.$$

Thus, after making use too of Stirling's formula,

$$\left(\sqrt{\frac{\pi}{2}}\frac{(2N-1)!}{2^{2N-1}(N-1/2)!} - 2^{-(2N-1)}\int_0^{\sqrt{2N}X} e^{-t^2/2}H_{2N-1}(t)\mathrm{d}t\right) \sim (N-1/2)!\left(\frac{1}{\sqrt{2N}} - \frac{2}{\sqrt{\pi}}\left(\frac{1}{4N}\frac{1}{(1-X^2)^{3/4}}\tilde{g}^{(H)}_{-1,2N}(X) - \frac{(-1)^N}{4N}\right)\right).$$

Since (3.10) gives

$$e^{-x^2/2}H_{2N}(x)\big|_{x=2\sqrt{N}X} = \pi^{-1/4}\frac{2^N N^{-1/4}}{(1-X^2)^{1/4}}((2N)!)^{1/2}\left(g^{(H)}_{0,2N}(X) + O\left(\frac{1}{N}\right)\right)$$

we thus have that with $x=2\sqrt{N}X$ the final line in (4.16) has the asymptotic behavior

$$-\frac{1}{4\sqrt{\pi}}\frac{g^{(H)}_{0,2N}(X)}{(1-X^2)^{1/4}}\left(\sqrt{2} - \frac{1}{\sqrt{\pi N}}\left(\frac{1}{(1-X^2)^{3/4}}(X\tilde{g}^{(H)}_{0,2N}(X) + \sqrt{1-X^2}g^{(H)}_{0,2N}(X)) - (-1)^N\right)\right).$$

Further, we see from (2.5) and (3.11) that

$$\frac{1}{2}\rho(2\sqrt{N}X;\mathrm{UE}_{2N}(e^{-x^2})) \sim \frac{\sqrt{N}}{\pi}\sqrt{1-X^2} - \frac{\sqrt{1-X^2}(2(g^{(H)}_{0,2N}(X))^2-1) + 2X\tilde{g}^{(H)}_{0,2N}(X)g^{(H)}_{0,2N}(X)}{8\pi\sqrt{N}(1-X^2)} + O\left(\frac{1}{N^{3/2}}\right).$$

Adding these last two results, and recalling (4.16) and (4.14) gives the stated formula. □

In Ref. 9, at $O(1/N)$ only the nonoscillatory term is reported. We note too that the nonoscillatory term at $O(1/N)$ in (4.17) is consistent with (1.4) in the case $\beta=4$.

B. The LOE and LSE in the bulk

We now apply the same strategy to the Laguerre case. For the LOE, substituting the appropriate formula from (3.7) and (3.9), into (3.4) shows

$$\rho(x;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-x/2})) = \rho(x;\mathrm{UE}_{N-1}(x^\alpha e^{-x})) + \frac{(N-1)!}{4(\alpha+N-2)!}x^{(\alpha-1)/2}e^{-x/2}L_{N-1}^\alpha(x) \times \left(\int_0^\infty L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t - 2\int_0^x L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t\right) \tag{4.18}$$

while

$$\rho(x;\mathrm{UE}_{N-1}(x^\alpha e^{-x})) = \rho(x;\mathrm{UE}_N(x^\alpha e^{-x})) - \frac{(N-1)!}{\Gamma(N+\alpha)}(x^{\alpha/2}e^{-x/2}L_{N-1}^\alpha(x))^2. \tag{4.19}$$

Proposition 7: Let $0<X<1$. *We have*

$$\frac{1}{N}\rho(X;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx})) \sim \rho_{\mathrm{MP}}(X) - \frac{1}{2\pi N}\frac{1-\alpha}{\sqrt{X(1-X)}} + o(N^{-1}). \tag{4.20}$$

Proof: By a change of variables

$$\rho(X;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx})) = 4N\rho(4NX;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-x/2})), \tag{4.21}$$

so the task is to analyze the $N\to\infty$ asymptotics of the right-hand side of (4.18) with x replaced by $4NX$.

We know from Refs. 11 and 1 that

$$\int_0^\infty L_{N-2}^a(t)t^{(a-1)/2}e^{-t/2}\,\mathrm{d}t = \frac{\Gamma((N+1)/2)\Gamma(a+N-1)}{2^{a/2-3/2}\Gamma(N)\Gamma((a+N)/2)} \sim 2N^{(a-1)/2}. \tag{4.22}$$

Regarding the second integral in (4.18), we first write

$$\int_0^{4NX} L_{N-2}^a(t)t^{(a-1)/2}e^{-t/2}\,\mathrm{d}t = \left(\int_0^{4\epsilon} + \int_{4\epsilon}^{4NX}\right)L_{N-2}^a(t)t^{(a-1)/2}e^{-t/2}\,\mathrm{d}t,$$

where $0<\epsilon\ll 1$. In relation to the region $[4\epsilon,4NX]$, (3.12) tells us that for N even

$$L_{N-2}^\alpha(t)t^{a/2}e^{-t/2}\big|_{t\to 4NT} = (2\pi\sqrt{T(1-T)})^{-1/2}N^{(\alpha-1)/2}\left(g_{-2,N}^{(L)}(T) + O\left(\frac{1}{N}\right)\right).$$

Substituting in the integral and changing variables $T=s^2$ shows

$$\int_{4\epsilon}^{4NX} L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t \sim (4N)^{1/2}N^{(\alpha-1)/2}\left(\frac{2}{\pi}\right)^{1/2}\int_{\sqrt{\epsilon/N}}^{\sqrt{X}}\frac{1}{\sqrt{s}(1-s^2)^{1/4}}g_{-2,N}^{(L)}(s^2)\mathrm{d}s. \tag{4.23}$$

In relation to the interval $t\in[0,4\epsilon]$, we know that for $N\to\infty$ (Ref. 15),

$$L_{N-2}^\alpha(t)t^{\alpha/2}e^{-t/2} \sim N^{\alpha/2}J_\alpha(2(Nt)^{1/2}),$$

where $J_n(z)$ denotes the Bessel function, and thus

$$\int_0^{4\epsilon} L_{N-2}^a(t)t^{(a-1)/2}e^{-t/2}\,\mathrm{d}t \sim N^{a/2}\int_0^{4\epsilon} J_\alpha(2(Nt)^{1/2})\frac{\mathrm{d}t}{\sqrt{t}}. \tag{4.24}$$

We expect the leading contributions to come from the neighborhood of the upper terminal $s=\sqrt{X}$ in (4.23), and the lower terminal $t=0$ in (4.24) [the integrands should connect smoothly from the lower terminal of (4.23) to the upper terminal of (4.24)]. Since about $s=\sqrt{X}$,

$$g^{(L)}_{-2,N}(s^2) \sim \sin(2N(\sqrt{X(1-X)} - \mathrm{Arcos}\sqrt{X}) - (\alpha-3)\mathrm{Arcos}\sqrt{X} + 3\pi/4 + 4N\sqrt{1-X}(s-\sqrt{X}))$$

we have

$$\int^{\sqrt{X}} \frac{g^{(L)}_{-2,N}(s^2)}{\sqrt{s}(1-s^2)^{1/4}}\mathrm{d}s \sim -\frac{1}{4N\sqrt{1-X}}\frac{\widetilde{g}^{(L)}_{-2,N}(X)}{X^{1/4}(1-X)^{1/4}},$$

where

$$\widetilde{g}^{(L)}_{m,N}(x) := \cos(2N(\sqrt{x(1-x)} - \mathrm{Arcos}\sqrt{x}) - (\alpha+1+2m)\mathrm{Arcos}\sqrt{x} + 3\pi/4).$$

Also

$$\int_0^\infty J_\alpha(t)\mathrm{d}t = 1,$$

so we have

$$\int_0 J_\alpha(2(Nt)^{1/2})\frac{\mathrm{d}t}{\sqrt{t}} \sim N^{-1/2}.$$

Reading off the asymptotic form of the factor $x^{a/2}e^{-x/2}L^a_{N-1}(x)|_{x=4NX}$ in (4.18) from (3.12) we deduce from this that

$$\rho(4NX;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-x/2})) \sim \rho(4NX;\mathrm{UE}_{N-1}(x^\alpha e^{-x})) - \frac{g^{(L)}_{-1,N}(X)\widetilde{g}^{(L)}_{-2,N}(X)}{8\pi NX(1-X)}.$$

It remains to determine the asymptotic form of (4.19). For this we use the analogue of (4.21) and (3.12), to obtain

$$\rho(4NX;\mathrm{UE}_{N-1}(x^\alpha e^{-x})) \sim \frac{1}{4N}\rho(X;\mathrm{UE}_N(x^\alpha e^{-2Nx})) - \frac{1}{2\pi}\sqrt{\frac{1}{X(1-X)}}(g_{-1,N}(X))^2.$$

Noting from the definitions and by a simple trigonometric identity that

$$\widetilde{g}^{(L)}_{-2,N}(X) = (2X-1)\widetilde{g}^{(L)}_{-1,N}(X) - 2\sqrt{(1-X)X}g^{(L)}_{-1,N}(X),$$

$$\widetilde{g}^{(L)}_{0,N}(X) = (2X-1)\widetilde{g}^{(L)}_{-1,N}(X) + 2\sqrt{(1-X)X}g^{(L)}_{-1,N}(X),$$

we therefore have

$$\rho(4NX;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-x/2})) \sim \frac{1}{4N}\rho(X;\mathrm{UE}_N(x^\alpha e^{-4Nx})) - \frac{1}{8\pi N}\frac{g^{(L)}_{-1,N}(X)\widetilde{g}^{(L)}_{0,N}(X)}{X(1-X)}. \tag{4.25}$$

Now, with

$$A_{N,\alpha}(X) := 2N(\sqrt{X(1-X)} - \mathrm{Arccos}\sqrt{X}) - \alpha\,\mathrm{Arccos}\sqrt{X} \tag{4.26}$$

we have that

$$g^{(L)}_{-1,N}(X) = \sin(A_{N,\alpha}(X) + \mathrm{Arccos}\sqrt{X} + 3\pi/4),$$

$$\tilde{g}^{(L)}_{0,N}(X) = \cos(A_{N,\alpha}(X) - \operatorname{Arccos}\sqrt{X} + 3\pi/4),$$

and thus

$$g^{(L)}_{-1,N}(X)\tilde{g}^{(L)}_{0,N}(X) = \tfrac{1}{2}(-\cos(2A_{N,\alpha}(X)) + 2\sqrt{X(1-X)}). \tag{4.27}$$

Substituting (4.27) in (4.25) and noting from (2.7) that

$$\frac{1}{4N}\rho(X;\mathrm{UE}_N(x^\alpha e^{-4Nx})) \sim \frac{1}{4}\rho_{\mathrm{MP}}(X) - \frac{\cos 2A_{N,\alpha}(X)}{16\pi X(1-X)N} + \frac{\alpha}{8\pi\sqrt{X(1-X)N}} \tag{4.28}$$

we obtain (4.20).

□

Consider now the LSE. Analogous to (4.21), by a change of variables

$$\rho(X;\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})) = 8N\rho(8NX;\mathrm{SE}_N(x^{\alpha+1}e^{-x})),$$

while (3.5) together with the fact[11,1]

$$\int_0^\infty e^{-t/2}t^{(\alpha-1)/2}L^\alpha_{2N-1}(t)\mathrm{d}t = 0 \tag{4.29}$$

shows that

$$\rho(x;\mathrm{SE}_N(x^{\alpha+1}e^{-x})) = \frac{1}{2}\rho(x;\mathrm{UE}_{2N}(x^\alpha e^{-x})) - \frac{\Gamma(1+2N)}{4\Gamma(\alpha+2N)}e^{-x/2}x^{(\alpha-1)/2}L^\alpha_{2N}(x)\int_0^x e^{-t/2}t^{(\alpha-1)/2}L^\alpha_{2N-1}(t)\mathrm{d}t. \tag{4.30}$$

Proposition 8: Let $0<X<1$. *In terms of the notation* (3.13) and (4.26) *we have*

$$\frac{1}{N}\rho(X;\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})) \sim \rho_{\mathrm{MP}}(X) - \frac{1}{2(\pi N)^{1/2}}\frac{g^{(L)}_{0,2N}(X)}{X^{3/4}(1-X)^{1/4}} + \frac{\alpha+1}{4\pi N\sqrt{X(1-X)}} + o(N^{-1}). \tag{4.31}$$

Proof: Following the strategy of the proof of Proposition 7 we find

$$\int_0^{8NX} e^{-t/2}t^{(\alpha-1)/2}L^\alpha_{2N-1}(t)\mathrm{d}t \sim (2N)^{(\alpha-1)/2} + \frac{(2N)^{\alpha/2}}{(2\pi)^{1/2}}\frac{\tilde{g}^{(L)}_{-1,2N}(X)}{2NX^{1/4}(1-X)^{3/4}}.$$

Also, (3.12) and Stirling's formula show

$$\frac{\Gamma(1+2N)}{4\Gamma(\alpha+2N)}e^{-x/2}x^{(\alpha-1)/2}L^\alpha_{2N}(x)\big|_{x=8NX} \sim \frac{1}{16(\pi N)^{1/2}(2N)^{(\alpha-1)/2}}\frac{g^{(L)}_{0,2N}(X)}{X^{3/4}(1-X)^{1/4}}.$$

Substituting in (4.30) gives

$$\rho(8NX;\mathrm{SE}_N(x^{\alpha+1}e^{-x})) \sim \frac{1}{16N}\rho(X;\mathrm{UE}_{2N}(x^\alpha e^{-8Nx})) - \frac{1}{16(\pi N)^{1/2}}\frac{g^{(L)}_{0,2N}(X)}{X^{3/4}(1-X)^{1/4}} - \frac{g^{(L)}_{0,2N}(X)\tilde{g}^{(L)}_{-1,2N}(X)}{32\pi NX(1-X)}. \tag{4.32}$$

Analogous to (4.27) we have

$$g^{(L)}_{0,2N}(X)\tilde{g}^{(L)}_{-1,2N}(X) = -\frac{1}{2}(\cos 2A_{2N,\alpha}(X) + 2\sqrt{X(1-X)}).$$

Substituting this together with (4.28) in (4.32) gives (4.31).

□

V. ASYMPTOTIC EXPANSIONS AT THE EDGE

A. The GOE and GSE

The scaled densities $\rho(X;\mathrm{OE}_N(e^{-NX^2}))$ and $\rho(X;\mathrm{SE}_N(e^{-4NX^2}))$ have to leading order their support on $(-1,1)$. We know from previous studies[5,6] that setting X as specified by (2.11) (with the restriction $\xi<0$ removed) and multiplying by $N^{1/3}$, the limit $N\to\infty$ exists and can be computed explicitly. Here we are interested in computing the first correction, as in the soft edge formula (2.9) for the GUE.

In the case of the GOE, we see from (4.4), (4.1), and (4.2) that in addition to the knowledge of (2.9), an asymptotic formula for $\rho(1+\xi/2N^{2/3};\mathrm{OE}_N(e^{-Nx^2}))$ can be obtained by making use of (3.15).

Proposition 9: We have

$$\frac{1}{2N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{OE}_N(e^{-Nx^2})\right)=(\mathrm{Ai}'(\xi))^2-\xi(\mathrm{Ai}(\xi))^2+\frac{1}{2}\mathrm{Ai}(\xi)\left(1-\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t\right)+\frac{1}{2N^{1/3}}\mathrm{Ai}'(\xi)\times\left(1-\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t\right)+O\left(\frac{1}{N^{2/3}}\right). \tag{5.1}$$

Proof: Consider the integral in (4.1). We know from Ref. 1 that

$$\int_0^x e^{-t^2/2}H_N(t)\mathrm{d}t=\sqrt{\frac{\pi}{2}}\frac{N!}{(N/2)!}-\int_x^\infty e^{-t^2/2}H_N(t)\mathrm{d}t.$$

Replacing N by $N-2$, setting $x=(2N)^{1/2}+2^{-1/2}N^{-1/6}\xi$, making use of (3.15) and simplifying shows that

$$\int_0^{(2N)^{1/2}+2^{-1/2}N^{-1/6}\xi} e^{-t^2/2}H_{N-2}(t)\mathrm{d}t=\sqrt{\frac{\pi}{2}}\frac{(N-2)!}{(N/2-1)!}\left(1-\int_\xi^\infty \mathrm{Ai}(y)\mathrm{d}y+\frac{2}{N^{1/3}}\mathrm{Ai}(\xi)+O\left(\frac{1}{N^{2/3}}\right)\right). \tag{5.2}$$

Now using (3.15) with $m=-1$, and multiplying with the result (5.2) as required by (4.1) we obtain

$$\left(\frac{e^{-x^2/2}H_{N-1}(x)}{2^{N-1}\pi^{1/2}(N-2)!}\int_0^x e^{-t^2/2}H_{N-2}(t)\mathrm{d}t\right)\Bigg|_{x=(2N)^{1/2}+2^{-1/2}N^{-1/6}\xi}\sim\frac{N^{1/6}}{2^{1/2}}\left(\mathrm{Ai}(\xi)+\frac{1}{N^{1/3}}\mathrm{Ai}'(\xi)\right)\left(1-\int_\xi^\infty \mathrm{Ai}(y)\mathrm{d}y+\frac{2}{N^{1/3}}\mathrm{Ai}(\xi)\right).$$

According to (4.2), we also require the asymptotic formula

$$-\frac{2^{-N+1}}{\pi^{1/2}(N-1)!}(e^{-x^2/2}H_{N-1}(x))^2\Bigg|_{x=(2N)^{1/2}+2^{-1/2}N^{-1/6}\xi}\sim-\frac{\sqrt{2}}{N^{1/6}}(\mathrm{Ai}'(\xi))^2,$$

which follows from (3.15). Further

$$\rho((2N)^{1/2}+2^{-1/2}N^{-1/6}\xi;\mathrm{UE}_N(e^{-x^2}))=\frac{1}{(2N)^{1/2}}\rho(1+\xi/2N^{2/3};\mathrm{UE}_N(e^{-2Nx^2}))$$

[cf. (4.4)] so the asymptotic form of the first term on the right-hand side of (4.2) can be read off from (2.9). Doing this, and recalling (4.4), we deduce (5.1).

We turn our attention now to the GSE. We will analyze (4.16) rewritten to read

$$\rho(x;\mathrm{SE}_N(e^{-x^2})) = \frac{1}{2}\rho(x;\mathrm{UE}_{2N}(e^{-x^2})) - \frac{e^{-x^2/2}H_{2N}(x)}{2^{2N+1}\pi^{1/2}(2N-1)!}\int_x^\infty e^{-t^2/2}H_{2N-1}(t)\mathrm{d}t. \tag{5.3}$$

Proposition 10: We have

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{SE}_N(e^{-4Nx^2})\right) \sim (\mathrm{Ai}'(\xi))^2 - \xi(\mathrm{Ai}(\xi))^2 - \frac{1}{2}\mathrm{Ai}(\xi)\left(\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t - \frac{1}{(2N)^{1/3}}\mathrm{Ai}(\xi) + O(N^{-2/3})\right). \tag{5.4}$$

Proof: By a simple change of variables

$$\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{SE}_N(e^{-4Nx^2})\right) = 2\sqrt{N}\rho((4N)^{1/2}+2^{-1/2}(2N)^{-1/6}\xi;\mathrm{SE}_N(e^{-x^2})), \tag{5.5}$$

so we seek the large N asymptotic form of (3.15) with $x\mapsto(4N)^{1/2}+2^{-1/2}(2N)^{-1/6}\xi$. Making use of (3.15) shows

$$\left(\frac{e^{-x^2/2}H_{2N}(x)}{2^{2N+1}\pi^{1/2}(2N-1)!}\int_x^\infty e^{-t^2/2}H_{2N-1}(t)\mathrm{d}t\right)\Bigg|_{x=(4N)^{1/2}+2^{-1/2}(2N)^{-1/6}\xi} \sim \frac{N^{1/6}}{2^{4/3}}\mathrm{Ai}(\xi)\left\{\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t - \frac{1}{(2N)^{1/3}}\mathrm{Ai}(X) + O(N^{-2/3})\right\}, \tag{5.6}$$

while it follows from (2.9) that

$$\frac{1}{2}\rho((4N)^{1/2}+2^{-1/2}(2N)^{-1/6}\xi;\mathrm{UE}_{2N}(e^{-x^2})) \sim \frac{(2N)^{1/6}}{\sqrt{2}}\left((\mathrm{Ai}'(\xi))^2 - \xi(\mathrm{Ai}(\xi))^2 + O\left(\frac{1}{N^{2/3}}\right)\right). \tag{5.7}$$

Substituting (5.7) and (5.6) in (5.3) and recalling (5.5) gives the stated result. □

B. The LOE and LSE

The soft edge scaling variables for the LOE and LSE are the same as those for the LUE, exhibited in (2.10). The leading correction term to the corresponding soft edge densities are given by the following result.

Proposition 11: We have

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{(2N)^{2/3}};\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx})\right) \sim (\mathrm{Ai}'(\xi))^2 - \xi(\mathrm{Ai}(\xi))^2 + \frac{1}{2}\mathrm{Ai}(\xi)\left(1-\int_\xi^\infty \mathrm{Ai}(s)\mathrm{d}s\right) - \frac{(\alpha-1)}{2(2N)^{1/3}}\left[\mathrm{Ai}'(\xi)\left(1-\int_\xi^\infty \mathrm{Ai}(s)\mathrm{d}s\right) - (\mathrm{Ai}(\xi))^2\right] + O(N^{-2/3}) \tag{5.8}$$

and

$$\frac{2}{(4N)^{2/3}}\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})\right)\sim(\mathrm{Ai}'(\xi))^2-\xi(\mathrm{Ai}(\xi))^2-\frac{1}{2}\mathrm{Ai}(\xi)\int_\xi^\infty \mathrm{Ai}(s)\mathrm{d}s$$
$$+\frac{\alpha+1}{2(4N)^{1/3}}\left((\mathrm{Ai}(\xi))^2+\mathrm{Ai}'(\xi)\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t\right)+O(N^{-2/3}). \tag{5.9}$$

Proof: Consider first the LOE. We rewrite (4.18) as

$$\rho(x;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-x/2}))=\rho(x;\mathrm{UE}_{N-1}(x^\alpha e^{-x}))+\frac{(N-1)!}{4(\alpha+N-2)!}x^{(\alpha-1)/2}e^{-x/2}L_{N-1}^\alpha(x)$$
$$\times\left(2\int_x^\infty L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t-\int_0^\infty L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t\right). \tag{5.10}$$

The asymptotic form of the final integral in (5.9) is known from (4.22). According to (4.21), we seek the asymptotic form of the remaining terms with

$$x=4N+2(2N)^{1/3}\xi.$$

For the first integral, use of (3.17) gives

$$\int_{4N+2(2N)^{1/3}\xi}^\infty L_{N-2}^\alpha(t)t^{(\alpha-1)/2}e^{-t/2}\,\mathrm{d}t\sim N^{(\alpha-1)/2}\left(\int_\xi^\infty \mathrm{Ai}(s)\mathrm{d}s-\frac{3-\alpha}{(2N)^{1/3}}\mathrm{Ai}(\xi)+O(N^{-2/3})\right).$$

The asymptotic form of the term outside the parenthetical integrals is given by (3.17) with $p=-1$. For the first term on the right-hand side of (5.10), use of (4.19), the analogue of (4.21), and (2.10) shows

$$\rho(4N+2(2N)^{1/3}\xi;\mathrm{UE}_{N-1}(x^\alpha e^{-x}))\sim\frac{1}{2(2N)^{1/3}}\left((\mathrm{Ai}'(\xi))^2-\xi(\mathrm{Ai}(\xi))^2+\frac{\alpha}{2^{1/3}}(\mathrm{Ai}(\xi))^2\frac{1}{N^{1/3}}\right)$$
$$-2^{-2/3}N^{-2/3}(\mathrm{Ai}(\xi))^2.$$

The asymptotic form of all terms have now been determined, and (5.8) follows.

In relation to the LSE, we use (4.29) to rewrite (4.30) to read

$$\rho(x;\mathrm{SE}_N(x^{\alpha+1}e^{-x}))=\frac{1}{2}\rho(x;\mathrm{UE}_{2N}(x^\alpha e^{-x}))+\frac{\Gamma(1+2N)}{4\Gamma(\alpha+2N)}e^{-x/2}x^{(\alpha-1)/2}L_{2N}^\alpha(x)\int_x^\infty e^{-t/2}t^{(\alpha-1)/2}L_{2N-1}^\alpha(t)\mathrm{d}t. \tag{5.11}$$

A simple change of variables gives

$$\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})\right)=8N\rho(8N+2(4N)^{1/3}\xi;\mathrm{SE}_N(x^{\alpha+1}e^{-x})), \tag{5.12}$$

so we seek the asymptotic form of (5.11) with

$$x=8N+2(4N)^{1/3}\xi.$$

For this, we make use of (3.17) to deduce

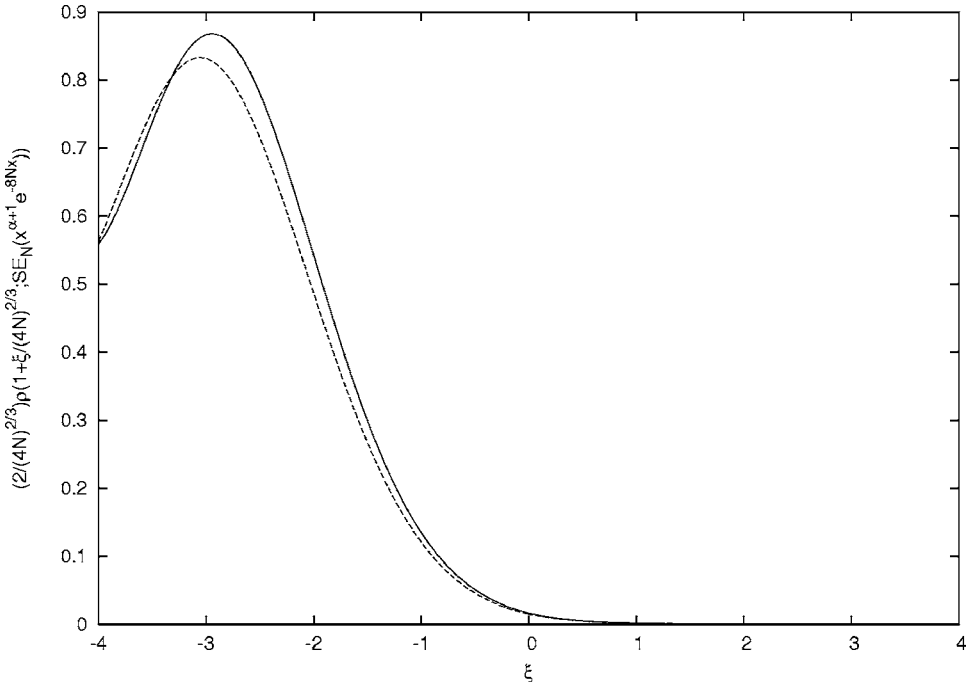

FIG. 1. Numerical comparison of the asymptotic expansion (5.9), shown as the dashed line, and the exact result for the LSE density given by (5.11) and (5.12), shown as the solid line, for the eigenvalue density near the soft edge of the LSE with $N=20$ and $\alpha=1/2$.

$$\frac{\Gamma(1+2N)}{4\Gamma(\alpha+2N)}e^{-x/2}x^{(\alpha-1)/2}L_{2N}^{\alpha}(x)\int_x^{\infty}e^{-t/2}t^{(\alpha-1)/2}L_{2N-1}^{\alpha}(t)\mathrm{d}t \sim -\frac{1}{8}2^{-2/3}N^{-1/3}\left(\mathrm{Ai}(\xi)-\frac{\alpha+1}{(4N)^{1/3}}\mathrm{Ai}'(\xi)\right)$$
$$\times\left(\int_{\xi}^{\infty}\mathrm{Ai}(s)\mathrm{d}s+\frac{\alpha-1}{(4N)^{1/3}}\mathrm{Ai}(\xi)+O(N^{-2/3})\right).$$

Further, making use of the analogue of (5.12) and recalling (2.10) shows

$$\frac{1}{2}\rho(8N+2(4N)^{1/3}\xi;\mathrm{UE}_{2N}(x^{\alpha}e^{-x})) \sim \frac{1}{4(4N)^{1/3}}\left((\mathrm{Ai}'(\xi))^2-\xi(\mathrm{Ai}(\xi))^2+\frac{\alpha}{2^{1/3}(2N)^{1/3}}(\mathrm{Ai}(\xi))^2\right.$$
$$\left.+O(N^{-2/3})\right).$$

The asymptotic form of all terms in (5.11) are now determined. After use of (5.12), (5.9) follows. □

Figure 1 provides a numerical comparison of the asymptotic expansion given by (5.9) with the exact result for the LSE density given by (5.11) and (5.12).

VI. CONSEQUENCES

A. Matching the bulk and edge expansions

1. The GOE and GSE

In Sec. II B the conjectured matching between the bulk asymptotic expansion expanded about the soft edge, and the asymptotic expansion of the edge density expanded into the bulk, for both the GUE and LUE was given further credence by its confirmation on further terms in the

asymptotic expansion. To study the matching in the case of orthogonal and symplectic symmetry, it is therefore convenient to express the corresponding asymptotic expansions in terms of the unitary symmetry expansions. We will consider first the Gaussian cases.

According to (4.3), (4.13), (2.5), (2.12),

$$\frac{1}{N}\rho(X;\mathrm{OE}_N(e^{-Nx^2})) \sim \frac{1}{N}\rho(X;\mathrm{UE}_N(e^{-Nx^2})) + \left(\frac{\cos[2N\pi P_{\mathrm{W}}(X)]}{4\pi(1-X^2)} - \frac{1}{2\pi\sqrt{1-X^2}}\right)\frac{1}{N} + \left(\frac{1+2X^2}{8\pi(1-X^2)^{5/2}} - \frac{X(21+2X^2)\sin[2N\pi P_{\mathrm{W}}(X)]}{48\pi(1-X^2)^{5/2}} - \frac{\cos[2N\pi P_{\mathrm{W}}(X)]}{8\pi(1-X^2)^2}\right)\frac{1}{N^2}; \tag{6.1}$$

according to (5.1) and (2.9)

$$\frac{1}{2N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{OE}_N(e^{-Nx^2})\right) \sim \frac{1}{2N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{UE}_N(e^{-2Nx^2})\right) + \frac{1}{2}\mathrm{Ai}(\xi)\left(1-\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t\right) + \frac{1}{2N^{1/3}}\mathrm{Ai}'(\xi)\left(1-\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t\right) + O\left(\frac{1}{N^{2/3}}\right); \tag{6.2}$$

according to (4.17) and (2.5)

$$\frac{1}{N}\rho(X;\mathrm{SE}_N(e^{-4Nx^2})) \sim \frac{1}{2N}\rho(X;\mathrm{UE}_{2N}(e^{-2Nx^2})) + \frac{\cos[4N\pi P_{\mathrm{W}}(X)]}{8\pi(1-X^2)N} \times \frac{1}{4\pi N\sqrt{1-X^2}} - \left(\frac{1}{\sqrt{2\pi N}} + \frac{1}{2\pi N}\right)\frac{\cos\left[2N\pi P_{\mathrm{W}}(X) + \frac{1}{2}\mathrm{Arcsin}\,X\right]}{(1-X^2)^{1/4}} + O(N^{-3/2}); \tag{6.3}$$

according to (5.4) and (2.9),

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{SE}_N(e^{-4Nx^2})\right) \sim \frac{1}{2(2N)^{2/3}}\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{UE}_{2N}(e^{-4Nx^2})\right) - \frac{1}{2}\mathrm{Ai}(\xi)\int_\xi^\infty \mathrm{Ai}(t)\mathrm{d}t + \frac{(\mathrm{Ai}(\xi))^2}{2(2N)^{1/3}} + O\left(\frac{1}{N^{2/3}}\right); \tag{6.4}$$

substituting (2.11) in (6.1) and (6.3) and expanding as in (2.18) gives

$$\frac{1}{2N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{OE}_N(e^{-Nx^2})\right) \dot{\sim} \frac{1}{2N^{2/3}}\rho\left(1+\frac{\xi}{2N^{2/3}};\mathrm{UE}_N(e^{-2Nx^2})\right) + \frac{3}{16\pi|\xi|^{5/2}} + \frac{23\sin(4|\xi|^{3/2}/3)}{96\pi|\xi|^{5/2}} + \frac{\cos(4|\xi|^{3/2}/3)}{8\pi|\xi|} - \left(\frac{1}{4\pi|\xi|^{1/2}} + \frac{\cos(4|\xi|^{3/2}/3)}{16\pi|\xi|^2}\right)\frac{1}{N^{1/3}} \tag{6.5}$$

and

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{SE}_N(e^{-4Nx^2})\right)\dot{\sim}\frac{1}{2(2N)^{2/3}}\rho\left(1+\frac{\xi}{2(2N)^{2/3}};\mathrm{UE}_{2N}(e^{-4Nx^2})\right)$$
$$-\frac{1}{2}\frac{1}{\sqrt{\pi}}\frac{\sin\left(\frac{2}{3}|\xi|^{3/2}+\pi/4\right)}{|\xi|^{1/4}}+\frac{\cos\left(\frac{4}{3}|\xi|^{3/2}\right)}{8\pi|\xi|}$$
$$+\left(\frac{1}{4\pi|\xi|^{1/2}}+\frac{|\xi|^{1/4}\sin\left(\frac{2}{3}|\xi|^{3/2}-\pi/4\right)}{4\sqrt{\pi}}\right)\frac{1}{(2N)^{1/3}}+O(N^{-1/2}). \tag{6.6}$$

We now compare (6.5) and (6.6) to the $\xi\to-\infty$ expansion of (6.2) and (6.4), respectively. In relation to the latter, a straightforward calculation using the leading two terms of (2.19) shows that for $|\xi|\to\infty$,

$$\int_{|\xi|}^{\infty}\mathrm{Ai}(-t)\mathrm{d}t\sim\frac{1}{\sqrt{\pi}}\left(\frac{1}{|\xi|^{3/4}}\cos\left(\frac{2}{3}|\xi|^{3/2}+\pi/4\right)+\frac{41}{48}\frac{1}{|\xi|^{9/4}}\sin\left(\frac{2}{3}|\xi|^{3/2}+\pi/4\right)\right).$$

Using this, together with (2.19) itself, we find that (6.5) agrees with the $\xi\to-\infty$ expansion of (6.2) for the first two terms of the $O(1)$ part in (6.5), but the rational factor of $\frac{1}{8}$ should be $\frac{1}{4}$ for the third term. At $O(N^{-1/3})$ agreement is obtained with the first term. Similarly, we find that the first term at each order in (6.6) agrees with the $\xi\to-\infty$ expansion of (6.6). These results are all consistent with the matching hypothesis.

2. The LOE and LSE

As in the Gaussian cases, we begin by expressing the densities for the LOE and LSE in terms of the corresponding densities for the LUE.

According to (4.20) and (2.7),

$$\frac{1}{N}\rho(X;\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx}))\sim\frac{1}{N}\rho(X;\mathrm{UE}_N(x^{\alpha}e^{-4Nx}))+\left(\frac{\cos 2A_{N,\alpha}(X)}{4\pi X(1-X)}-\frac{1}{2\pi(X(1-X))^{1/2}}\right)\frac{1}{N}; \tag{6.7}$$

according to (5.8) and (2.10),

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{(2N)^{2/3}};\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx})\right)\sim\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{(2N)^{2/3}};\mathrm{UE}_N(x^{\alpha}e^{-4Nx})\right)$$
$$+\frac{1}{2}\mathrm{Ai}(\xi)\left(1-\int_{\xi}^{\infty}\mathrm{Ai}(s)\mathrm{d}s\right)-\frac{(\alpha-1)}{2(2N)^{1/3}}\mathrm{Ai}'(\xi)\left(1-\int_{\xi}^{\infty}\mathrm{Ai}(s)\mathrm{d}s\right)-\frac{(\alpha+1)}{2(2N)^{1/3}}(\mathrm{Ai}(\xi))^2; \tag{6.8}$$

according to (4.31) and (2.7),

$$\frac{1}{N}\rho(X;\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx}))\sim\frac{1}{2N}\rho(X;\mathrm{UE}_{2N}(x^{\alpha}e^{-8Nx}))-\frac{1}{2(\pi N)^{1/2}}\frac{g^{(L)}_{0,2N}(X)}{X^{3/4}(1-X)^{1/4}}+\frac{\cos 2A_{2N,\alpha}(X)}{8\pi NX(1-X)}$$
$$+\frac{1}{4\pi N\sqrt{X(1-X)}}; \tag{6.9}$$

according to (5.9) and (2.10),

$$\frac{2}{(4N)^{2/3}}\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})\right)\sim\frac{1}{(4N)^{2/3}}\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{UE}_{2N}(x^{\alpha}e^{-8Nx})\right)$$
$$-\frac{1}{2}\mathrm{Ai}(\xi)\int_{\xi}^{\infty}\mathrm{Ai}(s)\mathrm{d}s+\frac{(\alpha+1)}{2(4N)^{1/3}}\mathrm{Ai}'(\xi)\int_{\xi}^{\infty}\mathrm{Ai}(t)\mathrm{d}t$$
$$-\frac{(\alpha-1)}{2(4N)^{1/3}}(\mathrm{Ai}'(\xi))^2. \tag{6.10}$$

Substituting (2.11) in (6.7) and (6.9) and expanding gives

$$\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{(2N)^{2/3}};\mathrm{OE}_N(x^{(\alpha-1)/2}e^{-2Nx})\right)\dot{\sim}\frac{1}{(2N)^{2/3}}\rho\left(1+\frac{\xi}{(2N)^{2/3}};\mathrm{UE}_N(x^{\alpha}e^{-4Nx})\right)+\frac{\cos(4|\xi|^{3/2}/3)}{4\pi|\xi|}$$
$$-\frac{(1+\alpha\sin(4|\xi|^{3/2}/3))}{2\pi\sqrt{|\xi|}}\frac{1}{(2N)^{1/3}} \tag{6.11}$$

and

$$\frac{2}{(4N)^{2/3}}\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{SE}_N(x^{\alpha+1}e^{-8Nx})\right)\dot{\sim}\frac{1}{(4N)^{2/3}}\rho\left(1+\frac{\xi}{(4N)^{2/3}};\mathrm{UE}_{2N}(x^{\alpha}e^{-8Nx})\right)$$
$$+\frac{\sin(2|\xi|^{3/2}/3-3\pi/4)}{2\sqrt{\pi}|\xi|^{1/4}}+\frac{\cos(4|\xi|^{3/2}/3)}{4\pi|\xi|}$$
$$+\frac{1}{2(4N)^{1/3}\pi\sqrt{|\xi|}}\left(1+(1+\alpha)\sqrt{\pi}|\xi|^{3/4}\cos(2|\xi|^{3/2}-3\pi/4)\right.$$
$$\left.-\frac{\alpha}{2^{1/3}}\sin(4|\xi|^{3/2}/3)\right). \tag{6.12}$$

On the other hand, let us expand (6.8) and (6.10) for $\xi\to-\infty$. Doing so we find agreement with the first term at each order in (6.11) and (6.12), respectively, as consistent with the matching hypothesis.

B. Microscopic delta functions

The results of Secs. IV and V tell us the asymptotic expansion of the global density, and the soft edge density. Here we would like to relate these expansions to the result (1.4) and its Laguerre analogue.

Consider first the Gaussian cases. For $|\xi|$ large but otherwise arbitrary, we write

$$\int_{-\infty}^{\infty}\rho(x;\mathrm{ME}_N(e^{-\beta x^2/2}))a(x)\mathrm{d}x=\left(\int_{R_1}+\int_{R_2}\right)\rho(X;\mathrm{ME}_N(e^{-N\beta x^2}))\tilde{a}(X)\mathrm{d}X$$
$$=\int_{R_1}\rho(X;\mathrm{ME}_N(e^{-N\beta x^2}))\tilde{a}(X)\mathrm{d}X$$
$$+\frac{1}{2N^{2/3}}\left(\int_{-|\xi|}^{\infty}\rho(1+y/2N^{2/3};\mathrm{ME}_N(e^{-\beta Nx^2}))\tilde{a}(1+y/2N^{2/3})\mathrm{d}y\right.$$
$$\left.+\int_{-\infty}^{|\xi|}\rho(1-y/2N^{2/3};\mathrm{ME}_N(e^{-\beta Nx^2}))\tilde{a}(-1-y/2N^{2/3})\mathrm{d}y\right), \tag{6.13}$$

where $\mathrm{ME}_N=\mathrm{OE}_N$, UE_N, SE_N, respectively, $R_1=(-1+|\xi|/2N^{2/3},1-|\xi|/2N^{2/3})$ and $R_2=(-\infty,\infty)\backslash R_1$, $\tilde{a}(x)=a(Nx)$ and we have used the fact that ρ is even. Because

$$\rho^{\text{soft}}(y;\text{ME}_N(e^{-\beta N x^2})) := \lim_{N\to\infty} \frac{1}{2N^{2/3}} \rho(1 + y/2N^{2/3};\text{ME}_N(e^{-\beta N x^2})) \tag{6.14}$$

is an $O(1)$ quantity, we see that to leading order the second and third integrals in (6.13) contribute

$$(\widetilde{a}(1) + \widetilde{a}(-1)) \int_{-|\xi|}^{\infty} \rho^{\text{soft}}(y;\text{ME}_N(e^{-\beta N x^2}))\text{d}y. \tag{6.15}$$

However, in relation to the first integral on the right-hand side of (6.13), we know that terms which are different order in N in the asymptotic expansion of $\rho(X;\text{ME}_N(e^{-N\beta x^2}))$ can contribute at the same order upon the substitution (2.11). Unlike the situation at the edge, the asymptotic expansion of this integral does not therefore correspond directly to the asymptotic of the integrand, leaving us without a method of analysis. Nonetheless some insight into the microscopic origin of the delta functions in (1.4) can be obtained as a consequence of the functional form of (6.14) for $\beta=1,4$.

For $\beta=2$ we read off from (2.9),

$$\rho^{\text{soft}}(y;\text{UE}_N(e^{-2Nx^2})) = (\text{Ai}'(y))^2 - y(\text{Ai}(y))^2,$$

while (2.18) tells us that the leading $y\to-\infty$ behavior is $2\sqrt{|y|}/\pi$ so (6.15) diverges for $|\xi|\to\infty$. Because of the result (1.4) it must be that this is exactly canceled by a contribution from the bulk, and thus the edge terms (6.15) cancel.

For $\beta=1$ and 4 we observe from (5.1) and (5.4) that $\rho^{\text{soft}}(y;\text{UE}_N(e^{-2Nx^2}))$ appears as an additive component in the scaled soft edge density, together with a further term in both cases. The further term has the property that it is integrable for $y\to-\infty$. Thinking then of the decomposition (6.13) for $|\xi|$ large, and ignoring the contribution from the nonintegrable additive component, this then suggests that

$$\begin{aligned}\int_{-\infty}^{\infty} \rho(x;\text{OE}_N(e^{-x^2/2}))a(x)\text{d}x &\sim N\int_{-1}^{1} \rho_W(X)\widetilde{a}(X)\text{d}X - \frac{1}{2\pi}\int_{-1}^{1} \frac{\widetilde{a}(X)}{\sqrt{1-X^2}}\text{d}X \\ &+ (\widetilde{a}(1) + \widetilde{a}(-1))\frac{1}{2}\int_{-\infty}^{\infty} \text{Ai}(y)\left(1 - \int_{y}^{\infty} \text{Ai}(t)\text{d}t\right)\text{d}y,\end{aligned} \tag{6.16}$$

$$\begin{aligned}\int_{-\infty}^{\infty} \rho(x;\text{SE}_N(e^{-2x^2}))a(x)\text{d}x &\sim N\int_{-1}^{1} \rho_W(X)\widetilde{a}(X)\text{d}X + \frac{1}{4\pi}\int_{-1}^{1} \frac{\widetilde{a}(X)}{\sqrt{1-X^2}}\text{d}X \\ &- (\widetilde{a}(1) + \widetilde{a}(-1))\frac{1}{4}\int_{-\infty}^{\infty} \text{Ai}(y)\left(\int_{y}^{\infty} \text{Ai}(t)\text{d}t\right)\text{d}y.\end{aligned} \tag{6.17}$$

Here the bulk contributions are the leading two nonoscillatory terms exhibited in (4.3) and (4.17), respectively, and the edge contributions are the leading terms in (5.1) and (5.4), respectively, with the component corresponding to the $\beta=2$ edge deleted. Since

$$\text{Ai}(y)\left(1 - \int_{y}^{\infty} \text{Ai}(t)\text{d}t\right) = \frac{1}{2}\frac{d}{\text{d}y}\left(1 - \int_{y}^{\infty} \text{Ai}(t)\text{d}t\right)^2, \tag{6.18}$$

$$\text{Ai}(y)\int_{y}^{\infty} \text{Ai}(t)\text{d}t = -\frac{1}{2}\frac{d}{\text{d}y}\left(\int_{y}^{\infty} \text{Ai}(t)\text{d}t\right)^2 \tag{6.19}$$

we see from $\int_{-\infty}^{\infty}\text{Ai}(t)\text{d}t=1$ that the final integrals in (6.16) and (6.17) are both equal to $1/2$, thus reclaiming (1.4).

We consider now the Laguerre analogue of (1.4). Let us introduce the so-called chiral matrix ensembles $\mathrm{chME}_N(g(x))$ by the eigenvalue pdf,

$$\frac{1}{C}\prod_{l=1}^{N} g(x_l)x_l^{\beta/2}\prod_{1\leqslant j<k\leqslant N}|x_k^2-x_j^2|^\beta \quad (x_l>0). \tag{6.20}$$

The simple change of variables $x_j^2\mapsto x_j$ shows

$$\tfrac{1}{2}\rho(X;\mathrm{chME}_N(x^{2(a+(2-\beta)/4)}e^{-2N\beta x^2}))=X\rho(X^2;\mathrm{ME}_N(x^a e^{-2N\beta x})), \tag{6.21}$$

and thus that the Laguerre ensembles can be viewed as a Gaussian version of the chiral ensemble, generalized by the factor $x^{2(a+(2-\beta)/4)}$. We see from (6.21), (4.20), (2.7), and (4.31) that

$$\rho(X;\mathrm{chOE}_N(x^{a/2}e^{-2Nx^2}))\sim 2\rho_W(X)+\frac{1}{\pi N}\frac{a-1/2}{\sqrt{1-X^2}},$$

$$\rho(X;\mathrm{chUE}_N(x^a e^{-4Nx^2}))\sim 2\rho_W(X)+\frac{a}{\pi N\sqrt{1-X^2}},$$

$$\rho(X;\mathrm{chSE}_N(x^{2a}e^{-8Nx^2}))\sim 2\rho_W(X)+\frac{a+1/4}{\pi N\sqrt{1-X^2}},$$

where only nonoscillatory terms are included. In the case $a=0$ these expansions are precisely the same as for the corresponding Gaussian ensembles [the leading term in the chiral ensembles is $2\rho_W(X)$ rather than $\rho_W(X)$ because $X\in(0,1)$ rather than $(-1,1)$].

At the soft edge $X=1$ of the chiral ensembles, the fact that the scaled densities are the same as for the Gaussian ensembles tells us that there is a contribution

$$\frac{1}{2N}\left(\frac{1}{\beta}-\frac{1}{2}\right)\delta(X-1)$$

to the smoothed density. And, although not the focus of attention of the present work, for the Laguerre and thus chiral ensembles there is an edge effect at $X=0$ (the so-called hard edge[5]) which one expects to give a microscopic contribution

$$-\frac{a}{2N}\delta^+(X)$$

(see the next section), where $\int_0^\infty f(X)\delta^+(X)\mathrm{d}X=f(0)$. Consequently we expect the Laguerre analogue of (1.4) to be

$$\begin{aligned}\rho(X;\mathrm{chME}_N(x^{\beta a/2}e^{-2\beta Nx^2}))\sim{}& 2\rho_W(X)+\frac{a}{\pi N\sqrt{1-X^2}}-\frac{a}{2N}\delta^+(X)\\ &+\frac{1}{N}\left(\frac{1}{\beta}-\frac{1}{2}\right)\left(\delta(X-1)-\frac{1}{\pi}\frac{1}{\sqrt{1-X^2}}\right).\end{aligned} \tag{6.22}$$

C. Macroscopic balance

In this final section, we will show that the results (1.4), (6.22) are consistent with macroscopic considerations.

In a one-component log-gas, to leading order in N the electrostatic potential created by the particle density $\sigma(x)$ must balance the background potential $u(x)$, and thus the equation

$$u(x) + C = \int_{-c}^{c} \sigma(y) \log|x-y| \mathrm{d}y, \quad x \in (-c,c), \tag{6.23}$$

where C is *some* constant, must hold. This is to be solved subject to the particle conservation constraint

$$\int_{-c}^{c} \sigma(y) \mathrm{d}y = 1. \tag{6.24}$$

For example, with $u(x)=x^2$, (6.23) and (6.24) are satisfied with

$$\sigma(y) = \rho_W(y) \tag{6.25}$$

(see, e.g., Ref. 4). To the next order in N, fluctuations in the particle density create an electric field and thus a force density which must be balanced for the system to be stable. The balancing force is provided by the gradient of the pressure fluctuation, and leads to the refinement of (6.23) (Ref. 3),

$$u(x) + C = \int_{-c}^{c} \sigma(y) \log|x-y| \mathrm{d}y + \frac{1}{N}\left(\frac{1}{2} - \frac{1}{\beta}\right) \log \sigma(x), \quad x \in (-c,c) \tag{6.26}$$

which again is subject to (6.24). With $u(x)=x^2$, setting

$$\sigma(y) = \rho_W(y) + \frac{\mu(y)}{N} \tag{6.27}$$

we see that

$$C = \int_{-c}^{c} \mu(y) \log|x-y| \mathrm{d}y + \left(\frac{1}{2} - \frac{1}{\beta}\right) \log \rho_{\mathrm{W}}(x), \quad x \in (-c,c) \tag{6.28}$$

which must be solved subject to the constraint

$$\int_{-c}^{c} \mu(y) \mathrm{d}y = 0. \tag{6.29}$$

Differentiating (6.28) gives

$$0 = \mathrm{PV} \int_{-1}^{1} \frac{\mu(y)}{x-y} \mathrm{d}y - \left(\frac{1}{2} - \frac{1}{\beta}\right) \frac{x}{1-x^2}, \tag{6.30}$$

where PV denotes the principal value. Making use of the fact that

$$\mathrm{PV} \int_{-1}^{1} \frac{1}{x-y} \frac{1}{\sqrt{1-y^2}} \mathrm{d}y = 0, \quad x \in (-1,1)$$

(see, e.g., Ref. 14), we see that (6.30), (6.29) is solved by

$$\mu(y) = \left(\frac{1}{\beta} - \frac{1}{2}\right)\left(\frac{1}{2}(\delta(y-1) + \delta(y+1)) - \frac{1}{\pi} \frac{1}{\sqrt{1-y^2}}\right)$$

in agreement with (1.4).

The chiral ensemble (6.20) is a log-gas confined to $x>0$ with image charges in $x<0$. At leading order in N balance of the electric field requires

$$u(x) + C = \int_0^c \sigma(y) \log|x^2 - y^2| \mathrm{d}y, \quad x \in (-c, c), \tag{6.31}$$

subject to the constraint

$$\int_0^c \sigma(y) \mathrm{d}y = 0.$$

But (6.31) can be written

$$u(x) + C = \int_{-c}^c \sigma(y) \log|x - y| \mathrm{d}y$$

so we have essentially the previous situation. In particular, with $u(x) = 2x^2$, this shows (6.31) is satisfied with

$$\sigma(y) = 2\rho_W(y). \tag{6.32}$$

To next order in N the chiral ensembles in (6.22) have $u(x) = 2x^2 - (a/2N)\log x$, and the generalization of (6.28) reads

$$-\frac{a}{2}\log x + C = \int_{-1}^1 \mu(y) \log|x - y| \mathrm{d}y + \left(\frac{1}{2} - \frac{1}{\beta}\right) \log \rho_W(x).$$

With $\mu(y) \mapsto \mu(y) - (a/2)\delta(x)$ this is in fact identical to (6.28) and we thus reclaim (6.22).

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Information theoretical properties of Tsallis entropies

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A chain rule and a subadditivity for the entropy of type β, which is one of the nonadditive entropies, were derived by Daróczy. In this paper, we study the further relations among Tsallis type entropies which are typical nonadditive entropies. The chain rule is generalized by showing it for Tsallis relative entropy and the nonadditive entropy. We show some inequalities related to Tsallis entropies, especially the strong subadditivity for Tsallis type entropies and the subadditivity for the nonadditive entropies. The subadditivity and the strong subadditivity naturally lead to define Tsallis mutual entropy and Tsallis conditional mutual entropy, respectively, and then we show again chain rules for Tsallis mutual entropies. We give properties of entropic distances in terms of Tsallis entropies. Finally we show parametrically extended results based on information theory. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2165744]

I. INTRODUCTION

For the probability distribution $p(x) \equiv p(X=x)$ of the random variable X, Tsallis entropy was defined in Ref. 1,

$$S_q(X) \equiv -\sum_x p(x)^q \ln_q p(x) \quad (q \neq 1) \tag{1}$$

with one parameter q as an extension of Shannon entropy, where q-logarithm function is defined by $\ln_q(x) \equiv (x^{1-q}-1)/(1-q)$ for any non-negative real number x and q. Tsallis entropy plays an essential role in nonextensive statistics so that many important results have been presented in mainly statistical physics.[2] In particular, see Refs. 3 and 4 for the recent results on Tsallis entropies. The field of the study on Tsallis entropy and related fields in statistical physics are often called Tsallis statistics or nonextensive statistical physics due to the nonextensivity Eq. (3) below. We easily find that $\lim_{q\to 1} S_q(X) = S_1(X) \equiv -\Sigma_x p(x) \log p(x)$, since q-logarithm converges to natural logarithm as $q \to 1$. After the celebrated discover by Tsallis, it was shown that Tsallis entropy can be uniquely formulated by the generalized Shannon-Khinchin's axioms in Refs. 5–7. The axiomatical characterization of Tsallis entropy was improved and that of Tsallis relative entropy was formulated in Ref. 8. It is a crucial difference of the fundamental property between Shannon entropy and Tsallis entropy that for two independent random variables X and Y, Shannon entropy $S_1(X)$ has an additivity,

$$S_1(X \times Y) = S_1(X) + S_1(Y), \tag{2}$$

however, Tsallis entropy $S_q(X), (q \neq 1)$ has a pseudoadditivity,

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$$S_q(X \times Y) = S_q(X) + S_q(Y) + (1-q)S_q(X)S_q(Y), \tag{3}$$

where $S_q(X \times Y)$ is Tsallis joint entropy, which will be defined below, for the direct product $X \times Y$ of two independent random variables X and Y. The independence between X and Y physically means that there is no interaction between two systems X and Y. This pseudoadditivity of Tsallis entropy in Eq. (3) originally comes from that of q-logarithm function $\ln_q(x)$. We pay attention to whether an additivity [such as Eq. (2)] of entropies for two independent random variables holds or not [such as Eq. (3)]. An entropy is called a nonadditive entropy if it does not satisfy the additivity such as Eq. (2), while an entropy is called an additive entropy if it satisfies the additivity specified in Eq. (2). The entropy of type β introduced by Daróczy in Ref. 9 (also called the structural a-entropy introduced by Havrda and Charvát in Ref. 10),

$$H_\beta(X) \equiv \frac{\sum_x (p(x)^\beta - p(x))}{2^{1-\beta}-1} \quad (\beta > 0, \beta \neq 1)$$

is a nonadditive entropy.

We are now interested in Tsallis entropy which is a typical nonadditive entropy. From Eq. (3), we easily find that we have a subadditivity of Tsallis entropies for two independent random variables X and Y in the case of $q \geqslant 1$ since Tsallis entropy is nonnegative. In the first of the section III, we will review a subadditivity of Tsallis entropies for general random variables X and Y in the case of $q \geqslant 1$.

From the entropy theoretical point of view, for the related entropies such as Tsallis conditional entropy and Tsallis joint entropy were introduced in Refs. 11–13 and then some interesting relations between them were derived. In this paper, in order to derive the relation between them, we adopt the following definition of Tsallis conditional entropy and Tsallis joint entropy.

Definition 1.1: For the conditional probability $p(x|y) \equiv p(X=x|Y=y)$ and the joint probability $p(x,y) \equiv p(X=x, Y=y)$, we define Tsallis conditional entropy and Tsallis joint entropy by

$$S_q(X|Y) \equiv -\sum_{x,y} p(x,y)^q \ln_q p(x|y) \quad (q \neq 1) \tag{4}$$

and

$$S_q(X,Y) \equiv -\sum_{x,y} p(x,y)^q \ln_q p(x,y) \quad (q \neq 1). \tag{5}$$

We note that the above definitions were essentially introduced in Ref. 9 by

$$H_\beta(X,Y) \equiv \frac{\sum_{x,y} (p(x,y)^\beta - p(x,y))}{2^{1-\beta}-1} \quad (\beta > 0,\ \beta \neq 1),$$

$$H_\beta(X|Y) \equiv \sum_y p(y)^\beta H_\beta(X|y) \quad (\beta > 0,\ \beta \neq 1),$$

except for the difference of the multiplicative function. And then a chain rule and a subadditivity,

$$H_\beta(X,Y) = H_\beta(X) + H_\beta(Y|X),$$

$$H_\beta(Y|X) \leqslant H_\beta(Y), \quad \beta > 1,$$

were shown in Theorem 8 of Ref. 9. In this paper, we call the entropy defined by Eq. (1), Eq. (4) or Eq. (5) Tsallis type entropy. It is remarkable that Eq. (4) can be easily deformed by

$$S_q(X|Y) = \sum_y p(y)^q S_q(X|y). \tag{6}$$

Note that for $q \neq 1$ we have $S_q(X|Y) = \Sigma_y p(y)^q S_q(X) \neq S_q(X)$ when X and Y are indepentent each other (i.e., $p(x|y) = p(x)$ for all x and y). Eq. (6) can be further regarded that the following expectation value:

$$E_q(X) \equiv \sum_i p_i^q x_i$$

depending on the parameter q is adopted. Since the expectation value $E_q(X)$ has a crucial lack that it does not hold $E_q(1) = 1$ for $q \neq 1$ in general, a slightly modified definition, the normalized Tsallis entropies such as

$$S_q^{\mathrm{nor}}(X) \equiv \frac{-\sum_x p(x)^q \ln_q p(x)}{\sum_x p(x)^q} \quad (q \neq 1) \tag{7}$$

are sometimes used,[12,13] and then important and meaningful results in physics are derived for the normalized nonadditive conditional entropy defined in Refs. 6 and 12. However, as pointed out in Ref. 14, the normalized Tsallis entropies are not stable, but the original Tsallis entropies are stable as experimental quantities so that it is meaningful to study the original Tsallis entropies from the physical point of view. Inspired by these pioneering works,[6,12,14] we therefore study the information theoretical properties of the original Tsallis type entropies without normalization in this paper. As advantages in information theoretical study, our approach shows chain rules and subadditivities of the Tsallis entropies and then naturally leads to define the Tsallis mutual entropy. Finally the rough meaning of the parameter q of the Tsallis entropy is given from the information theoretical viewpoint. Both entropies defined in Eq. (4) and Eq. (5) recover the usual Shannon entropies as $q \to 1$.

In the past, some parametrically extended entropies were introduced in the mathematical point of view. Especially, the Rényi entropy[15,16] (see also Ref. 17),

$$R_q(X) = \frac{1}{1-q} \log \sum_x p(x)^q \quad (q \neq 1) \tag{8}$$

is famous. For Tsallis entropy and Rényi entropy, we have the following relation:

$$R_q(X) = \frac{1}{1-q} \log\{1 + (1-q) S_q(X)\} \quad (q \neq 1). \tag{9}$$

It is notable that Rényi entropy has an additivity,

$$R_q(X \times Y) = R_q(X) + R_q(Y), \tag{10}$$

for two independent random variables X and Y. Although there exsits a simple transformation between Tsallis entropy and Rényi entropy, they have a different structure in regards to the matter of their additivities.

This paper is organized as follows. In Sec. II, we review a chain rule given in Ref. 9 and give its generalized results. We also give the chain rule for Tsallis relative entropy. In Sec. III, we review a subadditivity given in Ref. 9 and give its generalized results. In addition, we show several inequalities related to Tsallis entropies. In Sec. IV, we introduce Tsallis mutual entropy and then give its fundamental properties. In Sec. V, we discuss entropic distances and correlation coefficients due to Tsallis entropies. In Sec. VI, we give some applications of Tsallis entropies in the context of information theory. Related remarks and discussions are given in Sec. VII.

II. CHAIN RULES FOR TSALLIS ENTROPIES

It is important to study the so-called chain rule which gives the relation between a conditional entropy and a joint entropy in not only information theory[18] but also statistical physics. For these Tsallis entropies, the following chain rule holds as similar as the chain rule holds for the joint entropy of type β and the conditional entropy of type β.

Proposition 2.1 (Ref. 9):

$$S_q(X,Y) = S_q(X) + S_q(Y|X). \tag{11}$$

[Therefore immediately $S_q(X) \leqslant S_q(X,Y)$.]

Proof: From the formulas $\ln_q(xy) = \ln_q x + x^{1-q} \ln_q y$ and $\ln_q(1/x) = -x^{q-1} \ln_q x$, we have

$$\begin{aligned} S_q(X,Y) &= \sum_x \sum_y p(x,y) \ln_q \frac{1}{p(x,y)} = \sum_x \sum_y p(x,y) \ln_q \frac{1}{p(x)p(y|x)} \\ &= \sum_x p(x) \ln_q \frac{1}{p(x)} + \sum_x \sum_y p(x,y) p(x)^{q-1} \ln_q \frac{1}{p(y|x)} \\ &= -\sum_x p(x)^q \ln_q p(x) - \sum_x p(x)^q \sum_y p(y|x)^q \ln_q p(y|x) \\ &= S_q(X) + S_q(Y|X). \end{aligned}$$

■

From the process of the proof of Proposition 2.1, we can easily find that if X and Y are independent [i.e., $p(y|x) = p(y)$ for all x and y], then Eq. (11) recovers the pseudoadditivity Eq. (3),

$$\begin{aligned} S_q(X,Y) &= -\sum_x p(x)^q \ln_q p(x) - \sum_x p(x)^q \sum_y p(y)^q \ln_q p(y) \\ &= S_q(X) + \sum_x p(x)^q S_q(Y) = S_q(X) + S_q(Y) + (1-q) S_q(X) S_q(Y). \end{aligned}$$

As a corollary of the above Proposition 2.1, we have the following lemma.

Lemma 2.2: The following chain rules hold:

(1) $S_q(X,Y,Z) = S_q(X,Y|Z) + S_q(Z)$,
(2) $S_q(X,Y|Z) = S_q(X|Z) + S_q(Y|X,Z)$.

Proof: By using $\ln_q(y/x) = \ln_q y + y^{1-q} \ln_q(1/x)$, we have

$$S_q(X,Y|Z) = S_q(X,Y,Z) - S_q(Z).$$

In the similar way, we have

$$S_q(Y|X,Z) = S_q(X,Y,Z) - S_q(X,Z).$$

Also from the Proposition 2.1, we have

$$S_q(X,Y) = S_q(X) + S_q(Y|X).$$

Therefore we have

$$S_q(Y|X,Z) = S_q(X,Y,Z) - S_q(X,Z) = S_q(X,Y|Z) + S_q(Z) - \{S_q(X|Z) + S_q(Z)\} = S_q(X,Y|Z) - S_q(X|Z).$$

■

From (2) of Lemma 2.2, we have

$$S_q(X|Z) \leqslant S_q(X,Y|Z). \tag{12}$$

Remark 2.3: (2) of Lemma 2.2 can be generalized in the following formula:

$$S_q(X_1, \ldots, X_n|Y) = \sum_{i=1}^{n} S_q(X_i|X_{i-1}, \ldots, X_1, Y). \tag{13}$$

Theorem 2.4: Let $X_1, X_2, \ldots, X_n$ be the random variables obeying the probability distribution $p(x_1, x_2, \ldots, x_n)$. Then we have the following chain rule:

$$S_q(X_1, X_2, \ldots, X_n) = \sum_{i=1}^{n} S_q(X_i|X_{i-1}, \ldots, X_1). \tag{14}$$

Proof: We prove the theorem by induction on n. From Proposition 2.1, we have

$$S_q(X_1, X_2) = S_q(X_1) + S_q(X_2|X_1).$$

Assuming that Eq. (14) holds for some n, from Eq. (11) we have

$$\begin{aligned} S_q(X_1, \ldots, X_{n+1}) &= S_q(X_1, \ldots, X_n) + S_q(X_{n+1}|X_1, \ldots, X_n) \\ &= \sum_{i=1}^{n} S_q(X_i|X_{i-1}, \ldots, X_1) + S_q(X_{n+1}|X_n, \ldots, X_1), \end{aligned}$$

which means Eq. (14) holds for $n+1$. ■

In the rest of this section, we discuss the chain rule for Tsallis relative entropy. To do so, we use Tsallis relative entropy

$$D_q(U|V) \equiv -\sum_x u(x) \ln_q \frac{v(x)}{u(x)}, \tag{15}$$

defined for two probability distributions $u(x)$ and $v(x)$, and $q \geqslant 0$. See Refs. 19–22 for details of Tsallis relative entropy. Equation (15) is equivalent to the following forms:

$$D_q(U|V) = \frac{\sum_x (u(x) - u(x)^q v(x)^{1-q})}{1-q} \tag{16}$$

$$= \sum_x u(x)^q v(x)^{1-q} \ln_q \frac{u(x)}{v(x)}. \tag{17}$$

Along the line of the definition of Tsallis conditional entropy Eq. (4), we naturally define Tsallis conditional relative entropy such as

$$D_q(u(y|x)|v(y|x)) \equiv \sum_{x,y} u(x,y)^q v(x,y)^{1-q} \ln_q \frac{u(y|x)}{v(y|x)} \tag{18}$$

$$= \sum_x u(x)^q v(x)^{1-q} \sum_y u(y|x)^q v(y|x)^{1-q} \ln_q \frac{u(y|x)}{v(y|x)} \tag{19}$$

for two joint probability distributions $u(x,y)$ and $v(x,y)$, and two conditional probability distributions $u(y|x)$ and $v(y|x)$, based on the view of Eq. (17), neither Eq. (15) nor Eq. (16). Taking the limit as $q \to 1$, Eq. (18) recovers the usual conditional relative entropy. Then we have the following chain rule of Tsallis relative entropy for general (possibly *not* independent) case.

Theorem 2.5 (chain rule for Tsallis relative entropy):

$$D_q(u(x,y)|v(x,y)) = D_q(u(x)|v(x)) + D_q(u(y|x)|v(y|x)). \tag{20}$$

Proof: The proof follows by the direct calculations:

$$\begin{aligned}
D_q(u(x,y)|v(x,y)) &= -\sum_{x,y} u(x,y)\ln_q \frac{v(x,y)}{u(x,y)} = -\sum_{x,y} u(x,y)\ln_q \frac{v(x)v(y|x)}{u(x)u(y|x)} \\
&= -\sum_{x,y} u(x,y)\left\{ \ln_q \frac{v(x)}{u(x)} + \ln_q \frac{v(y|x)}{u(y|x)} + (1-q)\ln_q \frac{v(x)}{u(x)} \ln_q \frac{v(y|x)}{u(y|x)} \right\} \\
&= -\sum_{x,y} u(x,y)\left\{ \ln_q \frac{v(x)}{u(x)} + \left\{ \frac{u(x)}{v(x)} \right\}^{q-1} \ln_q \frac{v(y|x)}{u(y|x)} \right\} \\
&= D_q(u(x)|v(x)) - \sum_{x,y} \left\{ \frac{u(x)}{v(x)} \right\}^{q-1} u(x,y)\ln_q \frac{v(y|x)}{u(y|x)}. \\
&= D_q(u(x)|v(x)) + D_q(u(y|x)|v(y|x)).
\end{aligned}$$

■

Taking the limit as $q \to 1$, Theorem 2.5 recovers Theorem 2.5.3 in Ref. 18. It is known that for $u(y|x)=u(y)$ and $v(y|x)=v(y)$, Tsallis relative entropy has a pseudoadditivity,

$$D_q(u(x)u(y)|v(x)v(y)) = D_q(u(x)|v(x)) + D_q(u(y)|v(y)) + (q-1)D_q(u(x)|v(x))D_q(u(y)|v(y)). \tag{21}$$

From the process of the above proof, we find that the chain rule Eq. (20) recovers the pseudoadditivity Eq. (21) when $u(y|x)=u(y)$ and $v(y|x)=v(y)$.

III. SUBADDITIVITIES FOR TSALLIS ENTROPIES

From Eq. (3), for $q \geqslant 1$ and two independent random variables X and Y, the subadditivity holds,

$$S_q(X \times Y) \leqslant S_q(X) + S_q(Y).$$

It is known that the subadditivity for general random variables X and Y holds in the case of $q \geqslant 1$, thanks to the following proposition.

Proposition 3.1 (Ref. 9): The following inequality holds for two random variables X and Y, and $q \geqslant 1$,

$$S_q(X|Y) \leqslant S_q(X), \tag{22}$$

with equality if and only if $q=1$ and $p(x|y)=p(x)$ for all x and y.

Proof: We give the similar proof given in Ref. 9 as a version of Tsallis type entropies for the convenience of the reader. We define the function $\mathrm{Ln}_q(x) \equiv (x^q - x)/(1-q)$ for $q \geqslant 0$, $q \neq 1$, and $x \geqslant 0$. Then the function Ln_q is non-negative for $0 \leqslant x \leqslant 1, q > 1$ and concave in x for $q > 0, q \neq 1$. By the concavity of Ln_q, we have

$$\sum_y p(y)\mathrm{Ln}_q(p(x|y)) \leqslant \mathrm{Ln}_q\left(\sum_y p(y)p(x|y) \right).$$

Taking the summation of both sides on the above inequality on x, we have

$$\sum_y p(y) \sum_x \mathrm{Ln}_q(p(x|y)) \leqslant \sum_x \mathrm{Ln}_q(p(x)). \tag{23}$$

Since $p(y)^q \leqslant p(y)$ for any y and $q > 1$, and $\mathrm{Ln}_q(t) \geqslant 0$ for any $t \geqslant 0$ and $q > 1$, we have

$$p(y)^q \sum_x \mathrm{Ln}_q(p(x|y)) \leqslant p(y) \sum_x \mathrm{Ln}_q(p(x|y)).$$

Taking the summation of both sides on the above inequality on y, we have

$$\sum_y p(y)^q \sum_x \mathrm{Ln}_q(p(x|y)) \leqslant \sum_y p(y) \sum_x \mathrm{Ln}_q(p(x|y)). \tag{24}$$

By Eq. (23) and Eq. (24), we have

$$\sum_y p(y)^q \sum_x \mathrm{Ln}_q(p(x|y)) \leqslant \sum_x \mathrm{Ln}_q(p(x)).$$

Therefore we have $S_q(X|Y) \leqslant S_q(X)$. The equality holds when $q=1$ and $p(x|y)=p(x)$, which means X and Y are independent from each other. Thus the proof of the proposition was completed. ■

Equations (22) and (11) imply the subadditivity of Tsallis entropies.

Theorem 3.2 (Ref. 9): For $q \geqslant 1$, we have

$$S_q(X,Y) \leqslant S_q(X) + S_q(Y). \tag{25}$$

From Eq. (22) and Theorem 2.4, we have the following extended relation which is often called *independence bound on entropy* in information theory.

Theorem 3.3: Let $X_1, X_2, \ldots, X_n$ be the random variables obeying the probability distribution $p(x_1, x_2, \ldots, x_n)$. Then for $q \geqslant 1$, we have

$$S_q(X_1, \ldots, X_n) \leqslant \sum_{i=1}^{n} S_q(X_i) \tag{26}$$

with equality if and only if $q=1$ the random variables are independent from each other.

On the other hand, we easily find that for two independent random variables X and Y, and $0 \leqslant q < 1$, the superadditivity holds,

$$S_q(X \times Y) \geqslant S_q(X) + S_q(Y).$$

However, in general the superadditivity for two correlated random variables X and Y, and $0 \leqslant q < 1$ does not hold. Because we can show many counterexamples. For example, we consider the following joint distribution of X and Y:

$$p(x_1,y_1) = p(1-x), \quad p(x_1,y_2) = (1-p)y, \quad p(x_2,y_1) = px, \quad p(x_2,y_2) = (1-p)(1-y), \tag{27}$$

where $0 \leqslant p, x, y \leqslant 1$. Then each marginal distribution can be computed by

$$p(x_1) = p(1-x) + (1-p)y, \quad p(x_2) = px + (1-p)(1-y), \quad p(y_1) = p, \quad p(y_2) = 1-p. \tag{28}$$

In general, we clearly see X and Y are not independent from each other for the above example. Then the value of $\Delta \equiv S_q(X,Y) - S_q(X) - S_q(Y)$ takes both positive and negative so that there does not exist the complete ordering between $S_q(X,Y)$ and $S_q(X)+S_q(Y)$ for correlated X and Y in the case of $0 \leqslant q < 1$. Indeed, $\Delta = -0.287\,089$ when $q=0.8$, $p=0.6$, $x=0.1$, $y=0.1$, while $\Delta = 0.056\,2961$ when $q=0.8$, $p=0.6$, $x=0.1$, $y=0.9$.

Up to the above discussions, we have the possibility that the strong subadditivity holds in the case of $q \geqslant 1$. Indeed we can prove the following strong subadditivity for Tsallis type entropies.

Theorem 3.4: For $q \geqslant 1$, the strong subadditivity

$$S_q(X,Y,Z) + S_q(Z) \leqslant S_q(X,Z) + S_q(Y,Z) \tag{29}$$

holds with equality if and only if $q=1$ and, random variables X and Y are independent for a given random variable Z.

Proof: Theorem is proven by the similar way of Proposition 3.1. By the concavity of Ln_q, we have

$$\sum_y p(y|z)\mathrm{Ln}_q(p(x|y,z)) \leqslant \mathrm{Ln}_q\left(\sum_y p(y|z)p(x|y,z)\right).$$

Multiplying $p(z)^q$ to the both sides of the above inequality and then taking the summation on z and x, we have

$$\sum_{y,z} p(z)^q p(y|z)\sum_x \mathrm{Ln}_q(p(x|y,z)) \leqslant \sum_z p(z)^q \sum_x \mathrm{Ln}_q(p(x|z)) \tag{30}$$

since $\Sigma_y p(y|z)p(x|y,z)=p(x|z)$.

For any y, z and $q \geqslant 1$, we have $p(y|z)^q \leqslant p(y|z)$. Then by the non-negativity of the function Ln_q, we have

$$p(y|x)^q \sum_x \mathrm{Ln}_q(p(x|y,z)) \leqslant p(y|z)\sum_x \mathrm{Ln}_q(p(x|y,z)).$$

Multiplying $p(z)^q$ to both sides of the above inequality and then taking the summation on y and z, we have

$$\sum_{y,z} p(z)^q p(y|x)^q \sum_x \mathrm{Ln}_q(p(x|y,z)) \leqslant \sum_{y,z} p(z)^q p(y|z)\sum_x \mathrm{Ln}_q(p(x|y,z)). \tag{31}$$

From Eq. (30) and Eq. (31), we have

$$\sum_{y,z} p(y,z)^q \sum_x \mathrm{Ln}_q(p(x|y,z)) \leqslant \sum_z p(z)^q \sum_x \mathrm{Ln}_q(p(x|z)).$$

Thus we have

$$S_q(X|Y,Z) \leqslant S_q(X|Z), \tag{32}$$

which implies

$$S_q(X,Y,Z) - S_q(Y,Z) \leqslant S_q(X,Z) - S_q(Z),$$

by chain rules. The equality holds when $q=1$ and $p(x|y,z)=p(x|z)$, which means X and Y are independent from each other for a given Z. ■

We find that Eq. (29) recovers Eq. (25), by taking the random variable Z as a trivial one. This means that Eq. (29) is a generalization of Eq. (25). We have the further generalized inequality by the similar way of the proof of Theorem 3.4.

Theorem 3.5: Let $X_1, \ldots, X_{n+1}$ be the random variables. For $q>1$, we have

$$S_q(X_{n+1}|X_1, \ldots, X_n) \leqslant S_q(X_{n+1}|X_2, \ldots, X_n). \tag{33}$$

The subadditivity for Tsallis entropies conditioned by Z holds.

Proposition 3.6: For $q \geqslant 1$, we have

$$S_q(X,Y|Z) \leqslant S_q(X|Z) + S_q(Y|Z). \tag{34}$$

Proof: Summing $-2S_q(Z)$ to both sides in Eq. (29), we have

$$S_q(X,Y,Z) - S_q(Z) \leqslant S_q(X,Z) - S_q(Z) + S_q(Y,Z) - S_q(Z).$$

By chain rules, we have the proposition. ■

Proposition 3.6 can be generalized in the following.

Theorem 3.7: For $q \geqslant 1$, we have

$$S_q(X_1, \ldots, X_n|Z) \leqslant S_q(X_1|Z) + \cdots + S_q(X_n|Z). \tag{35}$$

In addition, we have the following propositions.

Proposition 3.8: For $q \geqslant 1$, we have

$$2S_q(X,Y,Z) \leqslant S_q(X,Y) + S_q(Y,Z) + S_q(Z,X).$$

Proof: For Eq. (22) and Eq. (32), we have

$$S_q(X|Y,Z) \leqslant S_q(X),$$

and

$$S_q(Z|X,Y) \leqslant S_q(Z|X).$$

Thus we have

$$S_q(X|Y,Z) + S_q(Z|X,Y) \leqslant S_q(X) + S_q(Z|X).$$

By chain rules, we have

$$S_q(X,Y,Z) - S_q(X,Y) + S_q(X,Y,Z) - S_q(Y,Z) \leqslant S_q(Z,X),$$

which implies the proposition. ■

Proposition 3.9: For $q > 1$, we have

$$S_q(X_n|X_1) \leqslant S_q(X_2|X_1) + \cdots + S_q(X_n|X_{n-1}).$$

Proof: From Eq. (14) and Eq. (32), we have

$$S_q(X_1, \ldots, X_n) \leqslant S_q(X_1) + S_q(X_2|X_1) + \cdots S_q(X_n|X_{n-1}).$$

Therefore we have

$$S_q(X_n|X_1) \leqslant S_q(X_2, \ldots, X_n|X_1) = S_q(X_1, \ldots, X_n) - S_q(X_1) \leqslant S_q(X_2|X_1) + \cdots + S_q(X_n|X_{n-1}),$$

by Eq. (11) and Eq. (12).

IV. TSALLIS MUTUAL ENTROPY

For normalized Tsallis entropies, the mutual information was defined in Ref. 13 with the assumption of its non-negativity. We define the Tsallis mutual entropy in terms of the original (*not* normalized) Tsallis type entropies. The inequality Eq. (22) naturally leads us to define Tsallis mutual entropy without the assumption of its non-negativity.

Definition 4.1: For two random variables X and Y, and $q > 1$, we define the Tsallis mutual entropy as the difference between Tsallis entropy and Tsallis conditional entropy such that

$$I_q(X;Y) \equiv S_q(X) - S_q(X|Y). \tag{36}$$

Note that we never use the term *mutual information* but use mutual entropy through this paper, since a proper evidence of channel coding theorem for information transmission has not ever been shown in the context of Tsallis statistics. From Eq. (11), Eq. (25), and Eq. (22), we easily find that $I_q(X;Y)$ has the following fundamental properties.

Proposition 4.2: (1) $0 \leqslant I_q(X;Y) \leqslant \min\{S_q(X), S_q(Y)\}$.

(2) $I_q(X;Y) = S_q(X) + S_q(Y) - S_q(X,Y) = I_q(Y;X)$.

Note that we have

$$S_q(X) \leqslant S_q(Y) \Leftrightarrow S_q(X|Y) \leqslant S_q(Y|X) \tag{37}$$

from the symmetry of Tsallis mutual entropy. We also define the Tsallis conditional mutual entropy

$$I_q(X;Y|Z) \equiv S_q(X|Z) - S_q(X|Y,Z) \tag{38}$$

for three random variables X, Y, and Z, and $q>1$.

In addition, $I_q(X;Y|Z)$ is non-negative, thanks to Eq. (32). For these quantities, we have the following chain rules.

Theorem 4.3: (1) For three random variables X, Y, and Z, and $q>1$, the chain rule holds,

$$I_q(X;Y,Z) = I_q(X;Z) + I_q(X;Y|Z). \tag{39}$$

(2) For random variables $X_1, \ldots, X_n$ and Y, the chain rule holds,

$$I_q(X_1, \ldots, X_n;Y) = \sum_{i=1}^{n} I_q(X_i;Y|X_1, \ldots, X_{i-1}). \tag{40}$$

Proof: (1) follows from the chain rules of Tsallis entropy,

$$I_q(X;Y|Z) = S_q(X|Z) - S_q(X|Y,Z) = S_q(X|Z) - S_q(X) + S_q(X) - S_q(X|Y,Z) = -I_q(X;Z) + I_q(X;Y,Z).$$

(2) follows from the application of Eq. (14) and Eq. (13),

$$\begin{aligned} I_q(X_1, \ldots, X_n;Y) &= S_q(X_1, \ldots, X_n) - S_q(X_1, \ldots, X_n|Y) \\ &= \sum_{i=1}^{n} S_q(X_i|X_{i-1}, \ldots, X_1) - \sum_{i=1}^{n} S_q(X_i|X_{i-1}, \ldots, X_1, Y) \\ &= \sum_{i=1}^{n} I_q(X_i;Y|X_1, \ldots, X_{i-1}). \end{aligned}$$

■

We have the following inequality for Tsallis mutual entropies by the strong subadditivity.

Proposition 4.4: For $q>1$, we have

$$I_Q(X;Z) \leqslant I_Q(X,Y;Z).$$

V. CORRELATION COEFFICIENTS AND DISTANCES FOR TSALLIS ENTROPIES

We discuss on the entropic distance between X and Y by means of Tsallis conditional entropy $S_q(X|Y)$. If $S_q(X|Y)=0=S_q(Y|X)$, then X and Y are called *equivalence* and denoted by $X \equiv Y$. Defining an entropic distance between X and Y as

$$d_q(X,Y) \equiv S_q(X|Y) + S_q(Y|X), \tag{41}$$

we have the following proposition.

Proposition 5.1: For $q>1$, d_q satisfies

(i) $d_q(X,Y)=0$ if and only if $X \equiv Y$,
(ii) $d_q(X,Y)=d_q(Y,X)$,
(iii) $d_q(X,Z) \leqslant d_q(X,Y)+d_q(Y,Z)$.

Proof: (i) and (ii) are clear from the definition of d_q. In the case of $n=3$ in Proposition 3.9, we have the triangle inequality:

$$S_q(X_3|X_1) \leqslant S_q(X_2|X_1) + S_q(X_3|X_2).$$

Setting $X_1=Z$, $X_2=Y$ and $X_3=X$ in the above inequality, we have

$$S_q(X|Z) \leqslant S_q(Y|Z) + S_q(X|Y). \tag{42}$$

In addition, exchanging X and Z in the above inequality, we have

$$S_q(Z|X) \leqslant S_q(Y|X) + S_q(Z|Y).$$

Summing both sides of the two above inequalities, we have the proposition. ■

$I_q(X;Y)$ represents a kind of correlation between X and Y. Following Ref. 23, we define a parametrically extended correlation coefficient in terms of Tsallis mutual entropy such that

$$\rho_q(X,Y) \equiv \frac{I_q(X;Y)}{S_q(X,Y)} \tag{43}$$

for $S_q(X)>0$, $S_q(Y)>0$, and $q>1$. Then we have the following proposition.

Proposition 5.2: For $q>1$, $S_q(X)>0$, and $S_q(Y)>0$, we have the following properties:

(i) $\rho_q(X,Y)=\rho_q(Y,X)$,
(ii) $0\leqslant\rho_q(X,Y)\leqslant 1$,
(iii) $\rho_q(X,Y)=0$ if and only if X and Y are independent of each other and $q=1$,
(iv) $\rho_q(X,Y)=1$ if and only if $X\equiv Y$.

Proof: (i) is clear from the definition of ρ_q. (ii) follows from $0\leqslant I_q(X;Y)\leqslant S_q(X)\leqslant S_q(X,Y)$. (iii) follows from Proposition 3.1. (iv) follows from $I_q(X;Y)=S_q(X,Y)\Leftrightarrow S_q(X|Y)=S_q(Y|X)=0$. ■

Again, we define an entropic distance between X and Y by

$$\tilde{d}_q(X,Y) \equiv 1 - \rho_q(X,Y). \tag{44}$$

Then we have the following proposition.

Proposition 5.3: For $q>1$, $S_q(X)>0$, $S_q(Y)>0$, and $S_q(Z)>0$, we have the following properties:

(i) $\tilde{d}_q(X,Y)=0$ if and only if $X\equiv Y$,
(ii) $\tilde{d}_q(X,Y)=\tilde{d}_q(Y,X)$,
(iii) $\tilde{d}_q(X,Z)\leqslant\tilde{d}_q(X,Y)+\tilde{d}_q(Y,Z)$.

Proof: (i) and (ii) follows from (iv) and (i) of Proposition 5.2, respectively. From chain rules and Eq. (42), we have

$$\begin{aligned}\frac{S_q(X|Z)}{S_q(X,Z)} &= \frac{S_q(X|Z)}{S_q(X|Z)+S_q(Z)} \leqslant \frac{S_q(X|Y)+S_q(Y|Z)}{S_q(X|Y)+S_q(Y|Z)+S_q(Z)} \\ &= \frac{S_q(X|Y)}{S_q(X|Y)+S_q(Y|Z)+S_q(Z)} + \frac{S_q(Y|Z)}{S_q(X|Y)+S_q(Y|Z)+S_q(Z)} \\ &\leqslant \frac{S_q(X|Y)}{S_q(X|Y)+S_q(Z)} + \frac{S_q(Y|Z)}{S_q(Y|Z)+S_q(Z)} = \frac{S_q(X|Y)}{S_q(X,Y)} + \frac{S_q(Y|Z)}{S_q(Y,Z)}.\end{aligned} \tag{45}$$

Exchanging X and Z, we have

$$\frac{S_q(Z|X)}{S_q(Z,X)} \leqslant \frac{S_q(Z|Y)}{S_q(Z,Y)} + \frac{S_q(Y|X)}{S_q(Y,X)}. \tag{46}$$

Summing both sides of two inequalities Eq. (45) and Eq. (46), we have (iii), since Tsallis joint entropy is symmetry. ■

We also define another correlation coefficient in terms of Tsallis mutual entropy by

$$\hat{\rho}_q(X,Y) \equiv \frac{I_q(X;Y)}{\max\{S_q(X),S_q(Y)\}} \tag{47}$$

for $S_q(X)>0$, $S_q(Y)>0$, and $q>1$. See Ref. 24. Then we have the following proposition.

Proposition 5.4: For $q>1$, $S_q(X)>0$, and $S_q(Y)>0$, we have the following properties:

(i) $\hat{\rho}_q(X,Y)=\hat{\rho}_q(Y,X)$,
(ii) $0\leqslant\hat{\rho}_q(X,Y)\leqslant 1$,
(iii) $\hat{\rho}_q(X,Y)=0$ if and only if X and Y are independent each other and $q=1$,
(iv) $\hat{\rho}_q(X,Y)=1$ if and only if $X\equiv Y$.

Proof: (i)–(iv) follow straightforwardly. ■

We also define an entropic distance between X and Y by

$$\hat{d}_q(X,Y) \equiv 1-\hat{\rho}_q(X,Y). \tag{48}$$

Then we have the following proposition.

Proposition 5.5: For $q>1$, $S_q(X)>0$, $S_q(Y)>0$, and $S_q(Z)>0$, we have the following properties:

(i) $\hat{d}_q(X,Y)=0$ if and only if $X\equiv Y$,
(ii) $\hat{d}_q(X,Y)=\hat{d}_q(Y,X)$,
(iii) $\hat{d}_q(X,Z)\leqslant\hat{d}_q(X,Y)+\hat{d}_q(Y,Z)$.

Proof: (i) and (ii) follows from Proposition 5.4. (iii) is proven by the similar way in Ref. 24. In order to show (iii), we can assume $S_q(Z)\leqslant S_q(X)$ without loss of generality. Then we prove (iii) in the following three cases.

(a) $S_q(Y)\leqslant S_q(Z)\leqslant S_q(X)$: From Eq. (37) and Eq. (42) we have

$$\begin{aligned}\hat{d}_q(X,Z) &= \frac{S_q(X|Z)}{S_q(X)} \leqslant \frac{S_q(X|Y)}{S_q(X)} + \frac{S_q(Y|Z)}{S_q(X)} \leqslant \frac{S_q(X|Y)}{S_q(X)} + \frac{S_q(Y|Z)}{S_q(Z)} \leqslant \frac{S_q(X|Y)}{S_q(X)} + \frac{S_q(Z|Y)}{S_q(Z)} \\ &= \hat{d}_q(X,Y) + \hat{d}_q(Y,Z).\end{aligned}$$

(b) $S_q(Z)\leqslant S_q(X)\leqslant S_q(Y)$: It is shown as similar as (a).
(c) $S_q(Y)\leqslant S_q(Z)\leqslant S_q(X)$: From Eq. (42), we have

$$\begin{aligned}\hat{d}_q(X,Z) &= \frac{S_q(X|Z)}{S_q(X)} = 1-\left(1-\frac{S_q(X|Z)}{S_q(X)}\right) \leqslant 1-\frac{S_q(X)}{S_q(Y)}\left(1-\frac{S_q(X|Z)}{S_q(X)}\right) \\ &= \frac{S_q(Y)-S_q(X)+S_q(X|Z)}{S_q(Y)} \leqslant \frac{S_q(Y)-S_q(X)+S_q(X|Y)+S_q(Y|Z)}{S_q(Y)} \\ &= \hat{d}_q(X,Y)+\hat{d}_q(Y,Z).\end{aligned}$$

■

VI. APPLICATIONS OF TSALLIS ENTROPIES

A. Generalized Fano's inequality

As an application of Tsallis conditional entropy, we give a generalized Fano's inequality.

Theorem 6.1: For $q>1$ and two random variables taking values in the finite (alphabet) set $\mathcal{X}$, the following inequality holds:

$$S_q(X|Y) \leqslant P(X \neq Y)\ln_q(|\mathcal{X}|-1) + s_q(P(X \neq Y)),$$

where s_q represents the Tsallis binary entropy,

$$s_q(p) \equiv -p^q \ln_q p - (1-p)^q \ln_q(1-p).$$

Proof: Define the random variables Z by

$$Z = \begin{cases} 0 & \text{if } X = Y, \\ 1 & \text{if } X \neq Y. \end{cases}$$

By chain rules, $S(Z|X,Y)=0$ and $S_q(Z|Y) \leqslant S_q(Z)=s_q(P(X \neq Y))$, we then have

$$\begin{aligned} S_q(X|Y) &= S_q(X|Y) + S_q(Z|X,Y) = S_q(X,Z|Y) = S_q(X|Y,Z) + S_q(Z|Y) \leqslant S_q(X|Y,Z) + S_q(Z) \\ &= S_q(X|Y=y,Z=0) + S_q(X|Y=y,Z=1) + s_q(P(X \neq Y)) \\ &= S_q(X|Y=y,Z=1) + s_q(P(X \neq Y)) \leqslant \ln_q(X \neq Y) + s_q(P(X \neq Y)), \end{aligned}$$

since the non-negativity of Tsallis relative entropy implies $-\Sigma_{i=1}^{n} p_i^q \ln_q p_i \leqslant \ln_q n$. ■

B. Entropy rate for Tsallis entropy

Moreover, we discuss on the Tsallis entropy rate.

Definition 6.2: The Tsallis entropy rate of a stochastic process $\mathbf{X} \equiv \{X_i\}$ is defined by

$$S_q(\mathbf{X}) \equiv \lim_{n\to\infty} \frac{S_q(X_1, \ldots, X_n)}{n}$$

if the limit exists.

$S_q(\mathbf{X})$ can be considered as Tsallis entropy per a symbol in the limit.

Theorem 6.3: For $q>1$ and a stationary stochastic process, the Tsallis entropy rate exists and is expressed by

$$S_q(\mathbf{X}) = \lim_{n\to\infty} S_q(X_n|X_1, \ldots, X_{n-1}).$$

Proof: By the stationary process and the inequality Eq. (33), we have

$$S_q(X_n|X_1, \ldots, X_{n-1}) = S_q(X_{n+1}|X_2, \ldots, X_n) \geqslant S_q(X_{n+1}|X_1, X_2, \ldots, X_n).$$

Thus $S_q(X_n|X_1, \ldots, X_{n-1})$ converges to a certain value s, since it is a monotone decreasing sequence with respect to n. That is,

$$\lim_{n\to\infty} S_q(X_n|X_1, \ldots, X_{n-1}) = s.$$

Moreover by the chain rule and Cesáro's theorem (e.g., see p. 64 of Ref. 18), we have

$$S_q(\mathbf{X}) \equiv \lim_{n\to\infty} \frac{S_q(X_1, \ldots, X_n)}{n} = \lim_{n\to\infty} \sum_{i=1}^{n} \frac{S_q(X_i|X_1, \ldots, X_{i-1})}{n} = s.$$

■

C. Generalized data processing inequality

Finally we prove the data processing inequality for Tsallis mutual entropy. Let X, Y, and Z be random variables. If the conditional probability distribution of the random variable Z depends only on the random variable Y, namely the random variable Z is independent of the random variable X, then it is called that X, Y, and Z form a simple Markov chain, and denoted by $X \to Y \to Z$.

Theorem 6.4: If $X \to Y \to Z$, then we have the inequality

$$I_q(X;Z) \leqslant I_q(X;Y) \tag{49}$$

for $q>1$, with equality if and only if $X \to Z \to Y$.

Proof: From Eq. (39), $I_q(X;Y,|Z)$ can be expanded in the following two ways:

$$I_q(X;Y) + I_q(X;Z|Y) = I_q(X;Y,Z) = I_q(X;Z) + I_q(X;Y|Z). \tag{50}$$

Since the non-negativity $I_q(X;Y|Z)$ and $I_q(X;Z|Y)=0$ because of the Markovity, we have $I_q(X;Z) \leqslant I_q(X;Y)$. If $I_q(X;Y|Z)=0$, namely $X \to Z \to Y$, then we have $I_q(X;Z)=I_q(X;Y)$. ■

We easily find that the following corollary holds.

Corollary 6.5: (1) If $Z=f(Y)$ with a certain mapping f, then $I_q(X;f(Y)) \leqslant I_q(X;Y)$, with equality if and only if f is a one-to-one mapping. (2) If $X \to Y \to Z$, then $I_q(X;Y|Z) \leqslant I_q(X;Y)$.

VII. REMARKS AND DISCUSSIONS

A. Chain rule and subadditivity for nonadditive entropies

In Ref. 7, the nonadditive entropies including Tsallis entropy and the entropy of type β was axiomatically characterized by the generalized Shannon-Khinchin axiom in the following manner. The function $\widetilde{S}_q(x_1,\ldots,x_n)$ is assumed to be defined for the n-tuple $(x_1,\ldots,x_n)$ belonging to

$$\Delta_n \equiv \left\{ (p_1,\ldots,p_n) | \sum_{i=1}^{n} p_i = 1, p_i \geqslant 0 (i=1,2,\ldots,n) \right\}$$

and to take a value in $R^+ \equiv [0,\infty)$. Then it was shown in Ref. 7 that four conditions *continuity, maximality, generalized Shannon additivity*, and *expandability* in Ref. 7 determine the function $\widetilde{S}_q : \Delta_n \to R^+$ such that

$$\widetilde{S}_q(x_1,\ldots,x_n) = \frac{\sum_{i=1}^{n} (x_i^q - x_i)}{\phi(q)}, \tag{51}$$

where $\phi(q)$ is characterized by the following conditions:

(i) $\phi(q)$ is continuous and $\phi(q)(1-q)>0$ for $q \neq 1$,
(ii) $\lim_{q\to 1} \phi(q)=0$ and $\phi(q) \neq 0$ for $q \neq 1$,
(iii) there exists $(a,b) \subset R^+$ such that $a<1<b$ and $\phi(q)$ is differentiable on $(a,1)$ and $(1,b)$,
(iv) there exists a positive constant number k such that $\lim_{q\to 1}[\mathrm{d}\phi(q)/\mathrm{d}q]=-1/k$.

Simple calculations show the nonextensivity

$$\widetilde{S}_q(X \times Y) = \widetilde{S}_q(X) + \widetilde{S}_q(Y) + \phi(q)\widetilde{S}_q(X)\widetilde{S}_q(Y)$$

for the nonadditive entropy $\widetilde{S}_q$. From the view of the generalization Eq. (51), we have the following chain rule.

Lemma 7.1: For the nonadditive entropy

$$\widetilde{S}_q(X) \equiv \frac{\sum_x (p(x)^q - p(x))}{\phi(q)}$$

and any continuous function $\phi(q)$, we have the chain rule

$$\widetilde{S}_q(X,Y) = \widetilde{S}_q(X) + \widetilde{S}_q(Y|X),$$

where the nonadditive joint entropy and the nonadditive conditional entropy are defined by

$$\widetilde{S}_q(X,Y) \equiv \frac{\sum_{x,y} (p(x,y)^q - p(x,y))}{\phi(q)}$$

and

$$\widetilde{S}_q(X|Y) \equiv \sum_y p(y)^q \widetilde{S}_q(X|y) = \sum_y p(y)^q \left\{ \frac{\sum_x (p(x|y)^q - p(x|y))}{\phi(q)} \right\},$$

respectively.

Proof: It follows immediately,

$$\widetilde{S}_q(Y|X) = \frac{\sum_{y,x} p(x)^q p(y|x)^q - \sum_x p(x)^q}{\phi(q)} = \frac{\sum_{x,y} (p(x,y)^q - p(x,y))}{\phi(q)} - \frac{\sum_x (p(x)^q - p(x))}{\phi(q)}$$
$$= \widetilde{S}_q(X,Y) - \widetilde{S}_q(X).$$

■

From the view of the generalization Eq. (51), Proposition 3.1 also generalized as follows.

Lemma 7.2: For the nonadditive entropy $\widetilde{S}_q(X)$ where $\phi(q)$ is continuous and $\phi(q)(1-q) > 0$ for $q \neq 1$, we have the inequality

$$\widetilde{S}_q(X|Y) \leqslant \widetilde{S}_q(X).$$

Proof: Since the function $\widetilde{\mathrm{Ln}}_q(x) \equiv (x^q - x)/\phi(q)$, $(q \geqslant 0, q \neq 1, x \geqslant 0)$ is non-negative for $0 \leqslant x \leqslant 1, q > 1$ and concave in x for $q > 0, q \neq 1$, the theorem follows as similar as the proof of Proposition 3.1. ■

Form Lemma 7.1 and Lemma 7.2, we have the subadditivity for nonadditive entropy.

Theorem 7.3. (Subadditivity for nonadditive entropy): For the nonadditive entropy $\widetilde{S}_q(X)$ where $\phi(q)$ is continuous and $\phi(q)(1-q) > 0$ for $q \neq 1$, we have the subadditivity

$$\widetilde{S}_q(X,Y) \leqslant \widetilde{S}_q(X) + \widetilde{S}_q(Y).$$

We note that we need the condition that $\phi(q)(1-q) > 0$ for $q \neq 1$ to prove Lemma 7.2, while we do not need any condition to prove Lemma 7.1.

B. Inequalities on pseudoadditivity

The pseudoadditivity Eq. (3) for independent random variables X and Y gives rise to the mathematical interest whether we have the complete ordering between the left-hand side and the right-hand side in Eq. (3) for two general random variables X and Y. Such a kind of problem was taken in the paper[25] for the normalized Tsallis type entropies which are different from the definitions of the Tsallis type entropies in the present paper. However, its inequality appeared in (3.5) of Ref. 25 was not true as we found the counter example in Ref. 26.

Unfortunately, in the present case, we also find the counter example for the inequalities between $S_q(X,Y)$ and $S_q(X) + S_q(Y) + (1-q)S_q(X)S_q(Y)$. In the same setting of Eq. (27) and Eq.

(28), $\delta \equiv S_q(X,Y) - \{S_q(X) + S_q(Y) + (1-q)S_q(X)S_q(Y)\}$ takes both positive and negative values for both cases $0 \leqslant q < 1$ and $q > 1$. Indeed, $\delta = 0.008\,466\,51$ when $q=1.8$, $p=0.1$, $x=0.1$, $y=0.8$, while $\delta = -0.011\,8812$ when $q=1.8$, $p=0.1$, $x=0.8$, $y=0.1$. Also, $\delta = 0.003\,990\,69$ when $q=0.8$, $p=0.1$, $x=0.8$, $y=0.1$, while $\delta = -0.012\,8179$ when $q=0.8$, $p=0.1$, $x=0.1$, $y=0.8$.

Therefore there does not exist the complete ordering between $S_q(X,Y)$ and $S_q(X)+S_q(Y)+(1-q)S_q(X)S_q(Y)$ for both cases $0 \leqslant q < 1$ and $q > 1$.

C. A remarkable inequality derived from subadditivity for Tsallis entropies

From Eq. (25), we have the following inequality:

$$\sum_{i=1}^{n} \left(\sum_{j=1}^{m} p_{ij} \right)^r + \sum_{j=1}^{m} \left(\sum_{i=1}^{n} p_{ij} \right)^r \leqslant \sum_{i=1}^{n} \sum_{j=1}^{m} p_{ij}^r + \left(\sum_{i=1}^{n} \sum_{j=1}^{m} p_{ij} \right)^r \tag{52}$$

for $r \geqslant 1$ and p_{ij} satisfying $0 \leqslant p_{ij} \leqslant 1$ and $\Sigma_{i=1}^{n} \Sigma_{j=1}^{m} p_{ij} = 1$. By setting $p_{ij} = a_{ij} / \Sigma_{i=1}^{n} \Sigma_{j=1}^{m} a_{ij}$ in Eq. (52), we have the following inequality as a corollary of Theorem 3.2.

Corollary 7.4: For $r \geqslant 1$ and $a_{ij} \geqslant 0$,

$$\sum_{i=1}^{n} \left(\sum_{j=1}^{m} a_{ij} \right)^r + \sum_{j=1}^{m} \left(\sum_{i=1}^{n} a_{ij} \right)^r \leqslant \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij}^r + \left(\sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij} \right)^r. \tag{53}$$

It is remarkable that the following inequality holds:[27]

$$\sum_{i=1}^{n} \left(\sum_{j=1}^{m} a_{ij} \right)^r \geqslant \sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij}^r \tag{54}$$

for $r \geqslant 1$ and $a_{ij} \geqslant 0$.

D. Difference between Tsallis entropy and Shannon entropy

We point out the difference between Tsallis entropy and Shannon entropy from the viewpoint of mutual entropy. In the case of $q=1$, the relative entropy between the joint probability $p(x,y)$ and the direct probability $p(x)p(y)$ is equal to the mutual entropy,

$$D_1((X,Y)|X \times Y) = S_1(X) - S_1(X|Y).$$

However, in the general case ($q \neq 1$), there exists the following relation:

$$\begin{aligned} D_q((X,Y)|X \times Y) = S_q(X) - S_q(X|Y) + \sum_{i,j} p(x_i,y_j)\{&p(x_i)^{q-1} \ln_q p(x_i) + p(y_j)^{q-1} \ln_q p(y_j) \\ &- p(x_i,y_j)^{q-1} \ln_q p(x_i)p(y_j)\}, \end{aligned} \tag{55}$$

which gives the crucial difference between the special case ($q=1$) and the general case ($q \neq 1$). The third term on the right-hand side of Eq. (55) vanishes if $q=1$. The existence of the third term of Eq. (55) means that we have two possibilities of the definition of Tsallis mutual entropy, that is, $I_q(X;Y) \equiv S_q(X) - S_q(X|Y)$ or $I_q(X;Y) \equiv D_q((X,Y)|X \times Y)$. We have adopted the former definition in the present paper, along with the definition of the capacity in the origin of information theory by Shannon.[28]

E. Another candidate of Tsallis conditional entropy

It is remarkable that Tsallis entropy $S_q(X)$ can be regarded as the expected value of $\ln_q[1/p(x)]$, that is, since $\ln_q(x) = -x^{1-q} \ln_q(1/x)$, it is expressed by

$$S_q(X) = \sum_x p(x) \ln_q \frac{1}{p(x)} \quad (q \neq 1), \tag{56}$$

where the convention $0 \ln_q(\cdot) = 0$ is set. Along with the view of Eq. (56), we may define Tsallis conditional entropy and Tsallis joint entropy in the following.

Definition 7.5: For the conditional probability $p(x|y)$ and the joint probability $p(x,y)$, we define Tsallis conditional entropy and Tsallis joint entropy by

$$\hat{S}_q(X|Y) \equiv \sum_{x,y} p(x,y) \ln_q \frac{1}{p(x|y)} \quad (q \neq 1) \tag{57}$$

and

$$S_q(X,Y) \equiv \sum_{x,y} p(x,y) \ln_q \frac{1}{p(x,y)} \quad (q \neq 1). \tag{58}$$

We should note that Tsallis conditional entropy defined in Eq. (57) is not equal to that defined in Eq. (4), while Tsallis joint entropy defined in Eq. (58) is equal to that defined in Eq. (5). If we adopt the above definitions Eq. (57) instead of Eq. (4), we have the following inequality.

Proposition 7.6: For $q > 1$, we have

$$S_q(X,Y) \leqslant S_q(X) + \hat{S}_q(Y|X).$$

For $0 \leqslant q < 1$, we have

$$S_q(X,Y) \geqslant S_q(X) + \hat{S}_q(Y|X).$$

Therefore we do not have the chain rule for $\hat{S}_q(Y|X)$ in general, namely we are not able to construct a parametrically extended information theory in this case.

VIII. CONCLUSION

As we have seen, we have found that the chain rules for the Tsallis type entropies hold as similar way of the proofs of the entropy of type β. This result was generalized from a few insights. Also we have proved the strong subadditivity of the Tsallis type entropies for the general two random variables in the case of $q > 1$. Moreover it has been shown that in general the superadditivity of Tsallis entropies does not hold in the case of $0 \leqslant q < 1$. Thus we could give important results for Tsallis entropies in the case of $q > 1$ from the information theoretical point of view. Therefore we have the possibility that the parametrically extended information theory will be constructed by starting from Tsallis entropy for $q > 1$. In other words, there is less possibility of such a construction in the case of $0 \leqslant q < 1$ if our stage is still in the usual probability theory, because the relation which should be satisfied in contrast to the usual information theory does not hold in the case of $0 \leqslant q < 1$. This gives us the rough meaning of the parameter q. That is, we found the crucial different results between $S_q(X)$ for $q > 1$ and $S_q(X)$ for $0 \leqslant q < 1$ from the information theoretical point of view. For $q > 1$, we showed that the Tsallis type entropies have the similar results to Shannon entropies. In other words, it has been shown that the definition of Tsallis conditional entropy Eq. (4) and Tsallis mutual entropy Eq. (36) have a possibility to be a pioneer to construct a nonadditive information theory.

Our results in the present paper are fundamental so that we are convinced that these results will help the progresses of nonextensive statistical physics and information theory. We are now studying the coding problem in nonadditive information theory and searching for the precise meaning of the parameter q.

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Covariant equilibrium statistical mechanics

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A manifest covariant equilibrium statistical mechanics is constructed starting with a $8N$ dimensional extended phase space which is reduced to the $6N$ physical degrees of freedom using the Poincaré-invariant constrained Hamiltonian dynamics describing the microdynamics of the system. The reduction of the extended phase space is initiated forcing the particles on energy shell and fixing their individual time coordinates with help of invariant time constraints. The Liouville equation and the equilibrium condition are formulated in respect to the scalar global evolution parameter which is introduced by the time fixation conditions. The applicability of the developed approach is shown for both, the perfect gas as well as the real gas. As a simple application the canonical partition integral of the monatomic perfect gas is calculated and compared with other approaches. Furthermore, thermodynamical quantities are derived. All considerations are shrinked on the classical Boltzmann gas composed of massive particles and hence quantum effects are discarded.
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I. INTRODUCTION AND MOTIVATION

The motivation to investigate relativistic equilibrium statistical mechanics is given by theoretical reasons as well as by practical reasons. From the theoretical point of view equilibrium statistical mechanics must be brought into accordance with the principles of relativity like all other branches of physics. From the practical point of view there might be important relativistic effects at (very) high temperatures. Those effects may play a major role within cosmological problems. Hence, equilibrium statistical mechanics is also interesting in the framework of general relativity and as a proper base a manifest covariant approach of a special relativistic equilibrium statistical mechanics is demanded.

While the covariant generalization of kinetic equations as a major application of nonequilibrium statistical mechanics can be studied since many years with help of textbooks (see e.g., Ref. 1) the relativistic equilibrium statistical mechanics has not reached such stable states. (The interest on covariant kinetic equations was mainly driven by practical reasons, i.e., by applications in various fields like plasma physics, astrophysics, heavy ion reactions, etc.).

Although Jüttner presented already 1911 relativistic calculations concerning the perfect gas[2] (note, Jüttners calculations are relativistic but not covariant) the manifest covariant description of equilibrium statistical mechanics is still under consideration and a lot of attempts have been performed already to tackle the related problems. An overview about such problems may be studied in older papers and reviews like the ones of Hakim[3] and the one of Havas[4] as well as references therein.

In this paper we mainly focus on the problem that the phase space $\int d\Gamma$ must be conceived in an invariant fashion demanded, e.g., by the invariance of the entropy (i.e., $S=k \ln \Gamma$). ter Haar and Wergeland[5] have summarized very clearly the two possibilities which intuitively offer themselves:

(1) "Either one makes Γ explicitly invariant extending it from $6N$ to $8N$ dimensions. That

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implies a many-time formulation of the underlying dynamics. For equilibrium theory, at any rate, this does not seem to be a suitable approach.

(2) Or, one retains (in the classical limit case) the usual phase space and considers the Lorentz transformations as canonical. This will certainly accomplish the desired invariance, but requires certain auxiliary reinterpretations."

The work of Balescu *et al.*[6] strongly enforces possibility (2) but applying the method on nonequilibrium statistical mechanics only.

The refusing statement of ter Haar and Wergeland concerning possibility (1) was certainly motivated by the fact that any straightforward attempt to formulate classical dynamics in a covariant fashion runs automatically into conflicts defined by the famous no-interaction theorem.[7] This theorem states that only a collection of noninteracting particles can be described within a Poincaré invariant fashion if a straightforward generalization of the usual dynamical description is applied. But the conflicts with the no-interaction theorem can be avoided within the framework of constrained Hamiltonian dynamics. This formalism is based on an algorithm which was introduced by Dirac[8] and Bergmann[9] in order to express a theory based on a singular Lagrangian in a generalized phase space approach with help of constraints. [A general and introductional overview about this formalism can be found in monographs and textbooks (see Ref. 10).] In this context the original $8N$ dimensional extended phase space given by N interacting relativistic particles can be reduced to $6N$ dimensions with the help of $2N$ constraints fixing the energies and the time coordinates of these N particles. Doing this a $6N$ dimensional hypersurface in the original $8N$ dimensional phase space is defined on which the system is allowed to move during its evolution. The evolution of the system is described in respect to a global scalar evolution parameter which is introduced by the time constraints relating the individual time coordinates to this parameter. This formalism is not changing the notion of simultaneity by a change of the frame of reference, means one gets an invariant notion of simultaneity as well as invariant world lines. This method has been successfully applied already in complicated non-equilibrium situations namely, in order to calculate heavy ion reactions at intermediate and high energies (Refs. 11 and 12).

Hence we do not agree that possibility (1) is not a suitable way and we propose in this paper an approach which uses the formalism of constrained Hamiltonian dynamics to describe the microdynamics of the system and which develops on this base an equilibrium statistical mechanics in a manifest covariant fashion.

A similar approach has been presented already by Hsu.[13] But this approach is based on the so-called common relativity (developed by the same author) which is a rather special formulation and interpretation of relativity. In contradiction to the work of Hsu we prefer in this paper to apply the usual framework and interpretion of relativity.

Another interesting approach following possibility (1) is the one of Horwitz *et al.*[14] which is based on the many-body theory of the relativistic mechanics proposed by Stückelberg.[15] The main characteristics of this method are the separation of the center of mass motion in the same way as in the nonrelativistic theory and the allowance of the particles being off-shell resulting finally in a new potential corresponding to the mass degree of freedom of the relativistic system. However, in our opinion, the extended phase space is not reduced in a satisfying way within this approach: phase space integrations are only performed keeping a common time interval Δt because no specific time fixations have been incorporated in this model [see, e.g., Eq. (3.25) in Ref. 14].

Furthermore, we would like to mention the paper of Tretyak.[16] This author used the front form of dynamics to investigate relativistic equilibrium statistical mechanics. But shrinking the phase space *ad hoc* to $6N$ dimensions this approach, although very elegant and useful, cannot be regarded to be manifest covariant.

The presentation of our approach in this paper is organized as follows.

In Sec. II we give a brief overview on the constrained Hamiltonian dynamics in a representation which is suitable for our purpose. In Sec. III we propose the formulation of a covariant equilibrium statistical mechanics using the framework explained in Sec. II. In Sec. IV we apply the developed approach to the canonical ensemble of the monatomic perfect gas. The obtained results are compared with other approaches. Finally, Sec. V contains some concluding remarks.

Some remarks on the used notation are at order.

Throughout the paper relativistic units are used, i.e., $\hbar=c=1$. The diagonal metric tensor has been chosen to be $(1,-1,-1,-1)$. The usual summation convention (i.e., summation of repeated indices in the same expression) is applied in the case with greek indices (representing tensor indices) which are running from 0 to 3. Italic indices indicate the particle index. Capital letters are used for quantities characterizing the complete system while lower case letters are used for quantities related to properties of single particles. The complete set of $8N$ phase space coordinates will be abbreviated by $(q^\mu,p^\mu)=(q_1^\mu,\ldots,q_N^\mu,p_1^\mu,\ldots,p_N^\mu)$. A contravariant 4-vector a^μ is defined as $a^\mu=(a^0,\mathbf{a})$. For the Poisson bracket of two dynamical phase space variables $A(q^\mu,p^\mu)$ and $B(q^\mu,p^\mu)$ the convention

$$\{A,B\}=\sum_i\left(\frac{\partial A}{\partial p_i^\mu}\frac{\partial B}{\partial q_{i\mu}}-\frac{\partial A}{\partial q_i^\mu}\frac{\partial B}{\partial p_{i\mu}}\right) \tag{1}$$

is used. As common within constrained Hamiltonian dynamics we also distinguish between weak equations and strong equations, assigned by $\approx$ and $=$, respectively. While strong equations hold throughout the extended phase space weak equations are demanded to be valid on the submanifold defined by the constraints. Note, weak equations should not be used before all interesting Poisson brackets have been worked out.

II. CONSTRAINED HAMILTONIAN DYNAMICS

The nonrelativistic equilibrium statistical mechanics contains as an essential part the description of the microdynamics using Hamiltonian dynamics, i.e., by classical propagation of particles under mutual interactions "at-a-distance." The generalization of this nonrelativistic particle dynamics to a manifest covariant particle dynamics is not trivial because, one must know how to treat action-at-a-distance in a covariant fashion. The conceptual problems in this field are formulated in the no-interaction theorem,[7] which states that only a collection of free particles can fulfill the following requirements:

(i) The many particle system is described in a Hamiltonian formulation with a canonical representation of the Poincaré group.
(ii) The world lines are invariant (World line condition).
(iii) The physical coordinates are identified with the canonical coordinates.

At least one of these requirements must be violated if one is going to allow an interaction between the particles which depends only on the trajectories of the particles.

In the 1970s three possibilities have been worked out to avoid this negative statement of the no-interaction theorem (an overview about the various attempts are collected in Ref. 17). The predictive relativistic mechanics, the singular Lagrange formalism and the constrained Hamiltonian dynamics. All these formalisms have in common that constraints are used to reduce the original $8N$-dimensional phase space, which is given by the space and time coordinates, the momenta and the energies of the N particles involved. The advantage of the constrained Hamiltonian dynamics is that one can choose these constraints more freely as in the other methods. Furthermore, one can define $2N$ constraints in a way obtaining the usual $6N$ dimensional phase space in the nonrelativistic limit, containing the physical dynamical degrees of freedom. The constrained Hamiltonian dynamics for particles under interaction was developed by Bergmann, Anderson, Goldberg,[9] Todorov,[18] Rohrlich,[19] Komar,[20] Sudarshan, Mokunda, Goldberg,[21] and Samuel.[22] These authors picked up the idea of Dirac[8] who has realized for the first time that constraints are not only reducing the degrees of freedom but can also determine the dynamics.

The model of Samuel contains as an important feature the cluster decomposition in a satisfying way for our purpose. The cluster decomposition, also called cluster separability, makes sure that when a system of interacting particles breaks into dynamical independent clusters, then the set of constraints must break into these dynamical independent clusters as well. The disadvantage of the model of Samuel is that it is not quantizable. But this is playing no role for our purpose

because, shrinking the considerations on the classical Boltzmann gas, we need only a classical Poincaré invariant description of particle dynamics in the framework of an action-at-a-distance theory which respects the cluster separability and the principle of causality.

In the following we demonstrate the concrete usage of this formalism to describe the microdynamics of the perfect gas as well as of the real gas composed of massive particles.

A. Microdynamics of the perfect gas

Modeling the microdynamics of the perfect relativistic gas a system of N noninteracting particles can be considered. The singular Lagrangian of such systems leads directly to N on-shell constraints (see, e.g., Ref. 23)

$$\varphi_i = \frac{1}{2m_i}(p_i^2 - m_i^2) \approx 0, \quad i = 1, \ldots, N, \tag{2}$$

with p_i^μ being the 4-momentum of particle i and m_i being its rest mass. In contradiction to an earlier work[12] and the common usage[10] the mass-shell constraints have been modified by the scalar factor $1/2m_i$. This modification provides several advantages.

First, the transition to the nonrelativistic limit is simplified and needs no further manipulations.

Second, this factor regulates the dimensions of the mass-shell constraints to be the one of an energy instead of an energy squared.

Third, and this is our major motivation, a straightforward performance of phase space integrals is guaranteed by this modification.

Since these primary constraints are first class, i.e., $\{\varphi_i, \varphi_j\} \approx 0$, no secondary constraints exist in this case. Nevertheless, the φ_i must be supplemented by N time fixation conditions which gauge the individual time coordinates parametrizing the world lines. Because noninteracting particles must not be correlated one often uses the simple gauging conditions

$$\chi_i = q_i^0 - \tau \approx 0, \quad i = 1, \ldots, N, \tag{3}$$

which force the time coordinates of the particles to be equal to the global scalar evolution parameter τ in any inertial system. These constraints are obviously not covariant.

But our aim in this paper is a manifest covariant reduction of the extended phase space and hence the constraints (3) are not satisfying in order to treat the relativistic perfect gas. Therefore, we define here another set of time fixations

$$\chi_i = \frac{p_i^\mu q_{i\mu}}{m_i} - \tau \approx 0, \quad i = 1, \ldots, N, \tag{4}$$

which are covariant and also do not create any correlation among the particles under consideration. The acting of these gauging conditions is easily recognized when considering it in the rest frame of a particle i: In this particular frame of reference $p_i^\mu = (m_i, \mathbf{0})$ and χ_i reduces to

$$\chi_i = q_{i0} - \tau \approx 0, \tag{5}$$

i.e., the time coordinates of the particles equal the global evolution parameter τ in their rest frame. In other words, using (4) the proper times of the particles are synchronized to τ within this covariant treatment. Note, both time fixations, (3) and (4) are first class, i.e., $\{\chi_i, \chi_j\} \approx 0$, but the complete set of $2N$ constraints is second class since $\{\varphi_i, \chi_j\} \not\approx 0$.

Because the canonical Hamiltonian derived by a Legendre transformation from the singular Lagrangian of a system of relativistic particles is identical vanishing[23] the Dirac Hamiltonian can be constructed by a linear combination of the τ-independent constraints,

$$H = \sum_{i=1}^{N} \lambda_i \varphi_i. \tag{6}$$

This Hamiltonian generates the equations of motion with respect to τ to be

$$\frac{\mathrm{d}q_i^\mu}{\mathrm{d}\tau} = \{H, q_i^\mu\} \approx \sum_{j=1}^{N} \lambda_j \frac{\partial \varphi_j}{\partial p_{i\mu}}, \tag{7}$$

$$\frac{\mathrm{d}p_i^\mu}{\mathrm{d}\tau} = \{H, p_i^\mu\} \approx -\sum_{j=1}^{N} \lambda_j \frac{\partial \varphi_j}{\partial q_{i\mu}}. \tag{8}$$

The Lagrange multipliers λ_i can be determined with the help of the consistency conditions

$$\frac{\mathrm{d}\psi_j}{\mathrm{d}\tau} = \frac{\partial \psi_j}{\partial \tau} + \{H, \psi_j\} \approx \frac{\partial \psi_j}{\partial \tau} + \sum_{i=1}^{N} \lambda_i \{\varphi_i, \psi_j\} \approx 0, \quad j = 1, \ldots, 2N; \tag{9}$$

which guarantee the validity of the constraints during the complete evolution of the system and which must be valid for the complete set of $2N$ constraints

$$\psi_j = \begin{cases} \varphi_j, & 0 < j \leqslant N, \\ \chi_{j-N}, & N < j \leqslant 2N. \end{cases} \tag{10}$$

Introducing the invertible $N \times N$-matrix C with elements $C_{ij} = \{\varphi_i, \chi_j\}$ the Lagrange multipliers are uniquely determined by

$$\lambda_i \approx -\sum_{j=1}^{N} \frac{\partial \chi_j}{\partial \tau} C_{ij}^{-1} \tag{11}$$

to be $\lambda_i = m_i / p_i^0$ if using (3) and $\lambda_i = m_i^2 / p_i^2$ if using (4).

In the following we will use the term *semicovariant approach* whenever the set of $2N$ constraints is assumed to consist of the N on-shell constraints (2) and the simple time fixations (3) because N covariant constraints are supplemented by N noncovariant constraints. Furthermore, we will use the term *full covariant approach* whenever the on-shell constraints (2) are combined with the covariant time fixations (4) to build the complete set of $2N$ constraints.

Using $p_i^0 = \epsilon_i + m_i$ the on-shell constraints reduce in the nonrelativistic limit ($\epsilon_i \ll m_i$) to

$$\varphi_i = \epsilon_i - \frac{\mathbf{p}_i^2}{2m_i} \approx 0. \tag{12}$$

Furthermore, the covariant time fixations (4) reduce to the simple time fixations (3) in the nonrelativistic limit and the global evolution parameter τ is identified with the absolute time t. Consequently, the usual nonrelativistic Hamiltonian dynamics is obtained as generated by the nonrelativistic Hamiltonian,

$$H^{(nr)} = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i}. \tag{13}$$

B. Microdynamics of the real gas

In contradiction to ideal systems like the perfect gas real systems can only be understood if the intermolecular interactions are taken into account when describing the related microdynamics. Applying the formalism of the constrained Hamiltonian dynamics to the microdynamics of the real gas we therefore must consider a system of N particles in mutual interaction. In this case we prefer

to use a set of constraints quite similar to the constraints which have been successfully applied already within nonequilibrium situations when simulating heavy ion reactions (see Refs. 11 and 12). The first N constraints are chosen as on-shell constraints

$$\varphi_i = \frac{1}{2m_i}(p_i^2 - m_i^2 - \widetilde{V}_i) \approx 0, \quad i = 1, \ldots, N. \tag{14}$$

Note, as already discussed in Sec. II A, the on-shell constraints have been modified by the scalar factor $1/2m_i$. Regarding the potential part $\widetilde{V}_i$ this choice of the constraints requires that $\widetilde{V}_i$ should be a Lorentz scalar and therefore a function of Lorentz scalars. Defining a system with mutual two-body interactions, $\widetilde{V}_i$ should be given by a sum of these two-body interactions

$$\widetilde{V}_i = \sum_{j \neq i} \widetilde{V}_{ij}(q_{Tij}^2). \tag{15}$$

Using Eq. (15) we assume that the two-body interactions depend only on the Lorentz invariant squared transverse distance

$$q_{Tij}^2 = q_{ij}^2 - \frac{(q_{ij}^\mu p_{ij\mu})^2}{p_{ij}^2}, \tag{16}$$

with $q_{ij}^\mu = q_i^\mu - q_j^\mu$ being the four-dimensional distance and $p_{ij}^\mu = p_i^\mu + p_j^\mu$ the sum of the momenta of the two interacting particles i and j. This particular choice has two advantages.

First, in the common CMS of two interacting particles CMS_{ij} q_{Tij}^2 reduces to $-\mathbf{q}_{ij}^2$ which is quite natural since only in the CMS_{ij} particle i and particle j can be treated on the same footing. In addition, in the nonrelativistic limit the potential part $\widetilde{V}_i$ can be connected with the corresponding potential V_i used in the nonrelativistic theory: Using $p_i^0 = \epsilon_i + m_i$ and regarding the nonrelativistic limit ($\epsilon_i \ll m_i$) the on-shell constraints reduce to

$$\varphi_i = \epsilon_i - \frac{\mathbf{p}_i^2}{2m_i} - \frac{\widetilde{V}_i}{2m_i} \approx 0. \tag{17}$$

The comparison of (17) with the usual expression of the nonrelativistic energy suggests

$$\widetilde{V}_i = 2m_i V_i, \tag{18}$$

and the two-body potential acting among two particles i and j felt by particle i reads in the common CMS_{ij},

$$\widetilde{V}_{ij}(-\mathbf{q}_{ij}^2) = 2m_i V_{ij}(-\mathbf{q}_{ij}^2), \tag{19}$$

i.e., a nonrelativistic two-body potential can be generalized to be used in the relativistic theory. For instance, the widely used Lennard-Jones potential can be generalized replacing the squared distance $\mathbf{q}_{ij}^2$ by the Lorentz invariant squared transverse distance q_{Tij}^2 obtaining

$$\widetilde{V}_{ij}^{(\mathrm{LJ})}(q_{Tij}^2) = 2m_i \kappa \left[\left(\frac{\sigma}{\sqrt{q_{Tij}^2}} \right)^{12} - \left(\frac{\sigma}{\sqrt{q_{Tij}^2}} \right)^{6} \right] \tag{20}$$

with the two tuning parameters κ and σ having the dimensions of an energy and a length, respectively. Note, due to the second term on the right-hand side of Eq. (16) this generalized interaction is slightly implicit momentum dependent. Because of this term, which gives the longitudinal squared distance, the interaction depends not only on the distance of the two interacting particles but also on the direction of their center of mass motion in the rest frame of the real gas.

Since the on-shell constraints alone do not specify the world lines one needs additional N constraints which are fixing the relative times of the particles. Like in the model of Samuel[22] this second set of N constraints should fulfill the following conditions:

(1) $N-1$ of them should be Poincaré invariant in order to fulfill the required world line invariance.
(2) Causality must be respected.
(3) One must be consistent with cluster separability.
(4) A global evolution parameter must be defined.

These conditions can be fulfilled by defining the following set of N time fixations:

$$\chi_i = \frac{1}{m_{i\,j(\neq i)}} \sum \omega_{ij} p_{ij}^{\mu} q_{ij\mu} \approx 0, \quad i = 1, \ldots, (N-1), \tag{21}$$

$$\chi_N = P^{\mu} Q_{\mu} - \tau \approx 0 \tag{22}$$

with $P^{\mu} = P^{\mu}/\sqrt{P^2}$, $P^{\mu} = \Sigma_i p_i^{\mu}$, $Q^{\mu} = (1/N)\Sigma_i q_i^{\mu}$ and the dimensionless scalar weighting function

$$\omega_{ij} = \frac{1}{q_{ij}^2/\sigma^2} e^{(q_{ij}^2/\sigma^2)} \tag{23}$$

with σ being a characteristic interaction distance of the modeled interaction. Note, the scalar factor $1/m_i$ regulates the dimension of the time fixations to be the one of a length. The conditions (21) are motivated by studies in the framework of singular Lagrangians.[24] Using this methods one gets up to the weighting functions w_{ij} the same conditions as secondary constraints and the on-shell conditions as primary constraints in a natural way. The important fact for using the expression (23) as weighting function is that this scalar function respects the principle of causality, while the ones used in the singular Lagrangian theories and in the model of Samuel can violate this important physical restriction (see Ref. 11).

The constraints (21) take care that the times of interacting particles are not dispersed to much in their common CMS_{ij}. Furthermore, they specify the dynamics by fixing the times at which the forces must be calculated but they do not specify the global evolution parameter τ. This evolution parameter must be defined to be determined dynamically since the no-interaction theorem can only be avoided in this way and is defined by the gauging condition (22) in a way, that the individual times are increasing with increasing τ.

In the CMS of all particles involved τ is simply given by the average of all time coordinates

$$\tau = P^{\mu} Q_{\mu} \overset{\mathrm{CMS}}{\rightarrow} \frac{1}{N} \sum_{i=1}^{N} q_i^0. \tag{24}$$

This set of $2N$ constraints given by (14), (21), and (22) determines covariant world lines parametrized by the initial data at equal τ.

A linear combination of the $2N-1$ τ-independent constraints

$$\psi_i = \begin{cases} \varphi_i, & 0 < i \leqslant N, \\ \chi_{i-N}, & N < i \leqslant 2N-1 \end{cases} \tag{25}$$

constructs the Dirac Hamiltonian

$$H = \sum_{i=1}^{2N-1} \lambda_i \psi_i \tag{26}$$

which generates the equations of motion with respect to τ to be

$$\frac{\mathrm{d}q_i^\mu}{\mathrm{d}\tau} \approx \sum_{j=1}^{2N-1} \lambda_j \frac{\partial \psi_j}{\partial p_{i\mu}}, \tag{27}$$

$$\frac{\mathrm{d}p_i^\mu}{\mathrm{d}\tau} \approx -\sum_{j=1}^{2N-1} \lambda_j \frac{\partial \psi_j}{\partial q_{i\mu}}. \tag{28}$$

The Lagrange multipliers λ_i can be determined with the help of the consistency conditions

$$\frac{\mathrm{d}\psi_j}{\mathrm{d}\tau} = \frac{\partial \psi_j}{\partial \tau} + \{H, \psi_j\} \approx \frac{\partial \psi_j}{\partial \tau} + \sum_{i=1}^{2N-1} \lambda_i \{\psi_i, \psi_j\} \approx 0, \quad j = 1, \ldots, 2N; \tag{29}$$

and are finally given by

$$\lambda_i \approx -\frac{\partial \chi_N}{\partial \tau} C^{-1}_{i2N} \tag{30}$$

with C being the invertible $2N \times 2N$ matrix with elements $C_{ij} = \{\psi_i, \psi_j\}$.

The whole formalism has a well defined nonrelativistic limit as has been shown by Sorge.[11] In leading order of $1/c$ one gets for the first $2N-1$ constraints

$$\varphi_i = \epsilon_i - \frac{\mathbf{p}_i^2}{2m_i} - \frac{\tilde{V}_i}{2m_i} \approx 0, \quad i = 1, \ldots, N, \tag{31}$$

$$\chi_i = q_i^0 - q_N^0 \approx 0, \quad i = 1, \ldots, N-1 \tag{32}$$

which generate the same dynamics as the nonrelativistic many-body Hamiltonian

$$H^{(nr)} = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m_i} + V_i \right). \tag{33}$$

III. COVARIANT STATISTICAL MECHANICS IN THE FRAMEWORK OF CONSTRAINED HAMILTONIAN DYNAMICS

Regarding the constrained Hamiltonian dynamics as a proper formalism to describe a system of interacting particles in a covariant fashion we are to develop a manifest covariant statistical mechanics on its base. We start this development considering the extended phase space. In case of a system involving N particles this invariant phase space has $8N$ dimensions given by the N 4-momenta p_i^μ and the N 4-position-vectors $q_i^\mu (i = 1, \ldots, N)$.

The phase space distribution function $D(q^\mu, p^\mu, \tau)$ representing the statistical ensemble is assumed to depend on the complete set of $8N$ phase space coordinates and, in general, on the global evolution parameter τ which is introduced by certain time fixation conditions (compare Sec. II). Consequently, the Liouville equation and the equilibrium conditions must be discussed with respect to τ.

The Liouville equation is thus given by

$$\frac{\mathrm{d}D(q^\mu, p^\mu, \tau)}{\mathrm{d}\tau} = 0 \Leftrightarrow \frac{\partial D(q^\mu, p^\mu, \tau)}{\partial \tau} = \{D(q^\mu, p^\mu, \tau), H\}. \tag{34}$$

The microdynamics of the system is generated by the Hamiltonian

$$H = \sum_{i=1}^{M} \lambda_i \psi_i, \tag{35}$$

where $M=N$ in the case of the perfect gas and $M=2N-1$ in the case of the real gas using the constraints as introduced in Sec. II.

Hence we get

$$\frac{\partial D(q^\mu, p^\mu, \tau)}{\partial \tau} \approx \sum_{i=1}^{M} \lambda_i \{D(q^\mu, p^\mu, \tau), \psi_i\}. \tag{36}$$

The reduction of the invariant phase space volume element of the extended phase space

$$\mathrm{d}\Gamma_e = \prod_{i=1}^{N} d^4 q_i d^4 p_i. \tag{37}$$

is performed incorporating all $2N$ constraints by means of δ-functions, i.e.,

$$\mathrm{d}\Gamma = \prod_{i=1}^{N} d^4 q_i d^4 p_i \Theta(p_i^0)\, \delta(\varphi_i)\, \delta(\chi_i). \tag{38}$$

The Heaviside-Θ-function has been added in order to shrink on particles with positive energy which is useful if classical particles are considered only.

Equilibrium distribution functions are τ independent solutions of (34) and hence must fulfill the condition

$$\sum_{i=1}^{M} \lambda_i \{D(q^\mu, p^\mu), \psi_i\} \approx 0. \tag{39}$$

Using (38) the ensemble average (i.e., the classical expectation value) of a measurable quantity $A(p^\mu, q^\mu)$ at equilibrium is given by

$$\langle A \rangle = \frac{\int \prod_{i=1}^{N} d^4 q_i d^4 p_i \Theta(p_i^0)\, \delta(\varphi_i)\, \delta(\chi_i) A(p^\mu, q^\mu) D(q^\mu, p^\mu)}{\int \prod_{i=1}^{N} d^4 q_i d^4 p_i \Theta(p_i^0)\, \delta(\varphi_i)\, \delta(\chi_i) D(q^\mu, p^\mu)}. \tag{40}$$

We mention two simple (and widely used) possibilities to construct solutions of the Liouville equation fulfilling the equilibrium condition:

(i) Constant phase space distributions $D=\text{const}$.
(ii) Phase space distributions depending on quantities X_j which are conserved during the evolution in respect to τ, i.e., $\mathrm{d}X_j/\mathrm{d}\tau=0$.

Assuming $X_j \neq X_j(\tau)$ the condition

$$\sum_{i=1}^{M} \lambda_i \{X_j, \psi_i\} \approx 0 \tag{41}$$

must be valid in the case of such conserved quantities.

Beside the trivial uniform ensemble the microcanonical ensemble can be regarded to be the most typical example for the former case while the canonical as well as the grand canonical ensembles are examples of the latter case.

In the nonrelativistic theory the energy is playing a prominent role as the most important conserved quantity. In a relativistic generalization the energy must be replaced by the

4-momentum P^μ or even by the energy-momentum tensor $T^{\mu\nu}$ of the system. A fruitful alternate is the invariant energy $E=U_\mu P^\mu$ with U_μ being the 4-velocity of the system. In the comoving frame of reference (i.e., the rest frame of the system) we get $E=U_0P^0=P^0$, i.e., the invariant energy is nothing but the total (internal) energy of the system measured in its rest frame. We will use this invariant energy when generalizing the concepts of nonrelativistic statistical mechanics.

In the following we consider briefly the main equilibrium distributions.

(i) *Microcanonical ensemble*: Considering the classical (i.e., nonquantum mechanical) case only and applying our concept of the invariant energy E we can write the distribution function of the microcanonical ensemble using the δ-function (compare, e.g., Ref. 25) as

$$D_M = \frac{1}{Z_M}\delta(E-E_0) \tag{42}$$

with E_0 being the invariant energy of the closed system. The microcanonical partition integral Z_M (which is nothing but the phase space volume Γ) must be determined via

$$Z_M = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \Theta(p_i^0)\delta(\varphi_i)\delta(\chi_i)\delta(E-E_0). \tag{43}$$

The factor $1/N!$ respects the fact that the particles cannot be distinguished.

(ii) *Canonical ensemble*: Considering the canonical ensemble the condition

$$\sum_{i=1}^{M}\lambda_i\{E,\psi_i\} = \sum_{i=1}^{M}\lambda_i\{U_\mu P^\mu,\psi_i\} \approx 0 \tag{44}$$

is to be proved in order to use the ansatz

$$D_C(E) = \frac{1}{Z_C}e^{-\beta U_\mu P^\mu} \tag{45}$$

for the canonical distribution function with the canonical partition integral

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \Theta(p_i^0)\delta(\varphi_i)\delta(\chi_i)e^{-\beta U_\mu P^\mu}. \tag{46}$$

(iii) *Grand canonical ensemble*: The grand canonical ensemble is characterized by another conserved quantity beside the energy namely, the particle number N. Hence, generalizing the canonical ensemble accordingly leads to

$$D_G(E,N) = \frac{1}{Z_G}e^{-\beta U_\mu P^\mu-\alpha N} \tag{47}$$

for the grand canonical distribution function with the grand canonical partition integral

$$Z_G = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \Theta(p_i^0)\delta(\varphi_i)\delta(\chi_i)e^{-\beta U_\mu P^\mu-\alpha N}. \tag{48}$$

(iv) *Related thermodynamics*: Let us briefly discuss the corresponding thermodynamics generated by our approach. Like in the next section, we shrink on the canonical ensemble. The formal properties of the thermodynamics are dominated by the introduction of the invariant energy E. As in the nonrelativistic theory the free energy can be determined with the help of the canonical partition integral Z_C by

$$F = -kT \ln Z_C. \tag{49}$$

Like the invariant energy E the free energy F (as all other thermodynamical potentials) is defined to be a scalar. Furthermore, the temperature T introduced by the parameter $\beta = 1/kT$ (k being the Boltzmann constant) is a scalar quantity and the introduction of a heat vector[26] is superfluous. (Of course, formally we get the same exponential factor [see Eq. (45)] but the 4-velocity of the system U_μ is now defining the invariant energy $E = U_\mu P^\mu$ and not used to define the heat vector $\Theta_\mu = U_\mu / T$ like in other approaches.[26] One can argue about this interpretation but the advantage defining an invariant energy is that this scalar quantity of the exponent can be demanded to be conserved during evolution in respect to τ, i.e., to fulfill Eq. (41).**)** Considering the usual relations defining other macroscopic state variables like the entropy

$$S = k \ln Z_C - \frac{1}{T} \frac{\partial \ln Z_C}{\partial \beta} \tag{50}$$

and the pressure

$$P = -\left(\frac{\partial F}{\partial V} \right)_T \tag{51}$$

we stress that both, the macroscopic state variables as well as the thermodynamical potentials are defined to be scalar quantities in our approach. Hence, an artifical extension of those quantities to higher rank tensors as often done when formulating relativistic thermodynamics (compare, e.g., Ref. 26) is not needed.

The average energy is given by

$$\langle E \rangle = -\frac{\partial \ln Z_C}{\partial \beta}, \tag{52}$$

and the specific heat can be determined with the help of it

$$c_V = \left(\frac{\partial \langle E \rangle}{\partial T} \right)_V. \tag{53}$$

Looking to the grand canonical ensemble we note that the chemical potential M introduced by the parameter $\alpha = \beta M = M/kT$ is a scalar as well in the approach considered.

IV. THE CANONICAL ENSEMBLE OF THE MONATOMIC PERFECT GAS

In this section we want to apply the formalism developed in the preceding sections. Unfortunately, concrete calculations [e.g., determining the canonical partition integral via Eq. (46)] are not easy to be performed due to the structure of the phase space volume element. (Especially, as in the nonrelativistic theory, calculations considering the real gas turn out to be complicated depending on the underlying model of intermolecular interactions.) Hence, as an example, we just apply the formalism to the canonical ensemble of the monatomic perfect gas. In order to determine the canonical partition integral using formula (46) we must prove the validity of condition (44).

By definition, the perfect gas is a system of noninteracting particles and as a consequence the Hamiltonian contains the simple mass shell constraints (2). Hence, the partial derivatives of φ_i with respect to $q_{j\mu}$ are vanishing and condition (44) is fulfilled in the case of the perfect gas.

Unfortunately, no analytical solution of the canonical partition integral (46) can be achieved within the full covariant approach. Hence, numerical solutions have been worked out as will be explained in Sec. IV B.

But before discussing these numerical results let us first present another approach, namely the semicovariant approach which provides analytical results and hence can be easily compared with other approaches known from the literature, e.g., the noncovariant Jüttner approach.[2]

A. Semicovariant approach

In the semicovariant approach the simple time fixation conditions (3) are used and the partition integral reads

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \Theta(p_i^0)\,\delta\left(\frac{1}{2m_i}(p_i^2 - m_i^2)\right)\delta(q_i^0 - \tau)e^{-\beta U_\mu P^\mu}. \tag{54}$$

Using the properties

$$\delta(ax) = \frac{1}{|a|}\delta(x) \tag{55}$$

and

$$\delta(x^2 - a^2) = \frac{1}{2a}[\delta(x-a) - \delta(x+a)] \tag{56}$$

of the δ-function we get

$$Z_C = \frac{!}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \frac{m_i}{p_i^0}\delta(p_i^0 - \sqrt{\mathbf{p}_i^2 + m_i^2})\,\delta(q_i^0 - \tau)e^{-\beta U_\mu P^\mu}. \tag{57}$$

For the further concrete calculation we assume a comoving frame of reference (i.e., the rest frame of the gas). In this frame of reference we get

$$E = U_\mu P^\mu = U_\mu \sum_{i=1}^{N} p_i^\mu = \sum_{i=1}^{N} p_i^0 \tag{58}$$

and integrating the 0-components gives, according to the δ-functions,

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^3q_i d^3p_i \frac{m_i}{\sqrt{\mathbf{p}_i^2 + m_i^2}} e^{-\beta\sqrt{\mathbf{p}_i^2+m_i^2}} = \frac{V^N}{N!}\int \prod_{i=1}^{N} d^3p_i \frac{m_i}{\sqrt{\mathbf{p}_i^2 + m_i^2}} e^{-\beta\sqrt{\mathbf{p}_i^2+m_i^2}}, \tag{59}$$

where V represents the volume measured in the rest frame of the gas. The integral factorizes using spherical coordinates in momentum space and performing the angle integration gives

$$Z_C = \frac{V^N}{N!}\left[4\pi m \int_0^\infty \mathrm{d}\rho \frac{\rho^2}{\sqrt{\rho^2 + m^2}} e^{-\beta\sqrt{\rho^2+m^2}}\right]^N \tag{60}$$

with $\rho = \sqrt{\mathbf{p}^2}$. Note, the particle index becomes superfluous considering a monatomic gas of particles with mass $m_i = m$. The integral in this expression can be solved applying the transformation $\rho = m \sinh \xi$ (see, e.g., Ref. 27),

$$\int_0^\infty \mathrm{d}\rho \frac{\rho^2}{\sqrt{\rho^2 + m^2}} e^{-\beta\sqrt{\rho^2+m^2}} = \int_0^\infty \mathrm{d}\xi\, m^2 \sinh^2 \xi e^{-\beta m \cosh \xi} = \frac{m^2}{\beta m} K_1(\beta m) \tag{61}$$

with K_1 being the modified Bessel function of first order.

Finally, the canonical partition integral within this semicovariant approach is given by

$$Z_C = \frac{V^N}{N!}\left[\frac{4\pi m^3}{\beta m} K_1(\beta m)\right]^N. \tag{62}$$

Now we are able to list the analytical results of three different approaches,

$$Z_C = \begin{cases} \dfrac{V^N}{N!}\left[\dfrac{4\pi m^3}{\beta m}K_1(\beta m)\right]^N, & \text{semicovariant,} \\ \dfrac{V^N}{N!}\left[\dfrac{4\pi m^3}{\beta m}K_2(\beta m)\right]^N, & \text{Jüttner approach,} \\ \dfrac{V^N}{N!}\left[\left(\dfrac{2\pi m^2}{\beta m}\right)^{3/2}\right]^N, & \text{nonrelativistic (see e.g. Ref. 28).} \end{cases} \tag{63}$$

Comparing (62) with the result of Jüttner we realize that the only difference is the order of the modified Bessel function occurring in Z_C: Jüttner's approach contains $K_2(\beta m)$ instead of $K_1(\beta m)$.

We note further that this result is naturally quite similar to the one derived by Horwitz *et al.* [compare Eq. (3.25) in Ref. 14), especially regarding the functional dependence on β. But we stress that the phase space reduction regarding the time constraints in our semicovariant approach is already more satisfying and as a consequence, in contradiction to Ref. 14, no common time interval is remaining in the final result when applying the formalism of constrained Hamiltonian dynamics.

B. Full covariant approach

Evaluating the partition integral within the full covariant approach we apply the covariant time constraints (4) as specified in Sec. II A for a system of noninteracting particles and Eq. (46) reads

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \Theta(p_i^0)\delta\left(\frac{1}{2m_i}(p_i^2 - m_i^2)\right)\delta\left(\frac{1}{m_i}q_i^\mu p_{i\mu} - \tau\right)e^{-\beta U_\mu P^\mu}. \tag{64}$$

Using the properties (55) and (56) of the δ-function we get

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^4q_i d^4p_i \frac{m_i^2}{p_i^{0^2}}\delta(p_i^0 - \sqrt{\mathbf{p}_i^2 + m_i^2})\delta\left(q_i^0 - \frac{1}{p_i^0}(\mathbf{qp} - m\tau)\right)e^{-\beta U_\mu P^\mu}. \tag{65}$$

Until now we have kept strictly the covariant fashion during the calculation. For the further concrete calculation the fixation of a defined frame of reference is demanded. Hence, for simplicity, we choose the rest frame of the gas to determine the invariant energy E as already applied within the semicovariant approach [see Eq. (58)] and get integrating the 0-components according to the δ-functions

$$Z_C = \frac{1}{N!}\int \prod_{i=1}^{N} d^3q_i d^3p_i \frac{m_i^2}{(\mathbf{p}_i^2 + m_i^2)}e^{-\beta\sqrt{\mathbf{p}_i^2+m_i^2}} = \frac{V^N}{N!}\int \prod_{i=1}^{N} d^3p_i \frac{m_i^2}{(\mathbf{p}_i^2 + m_i^2)}e^{-\beta\sqrt{\mathbf{p}_i^2+m_i^2}}. \tag{66}$$

The integral factorizes using spherical coordinates in momentum space and performing the angle integration gives

$$Z_C = \frac{V^N}{N!}\left[4\pi m^2 \int_0^\infty \mathrm{d}\rho \frac{\rho^2}{\rho^2 + m^2}e^{-\beta\sqrt{\rho^2+m^2}}\right]^N \tag{67}$$

with $\rho = \sqrt{\mathbf{p}^2}$. Note, as in Eq. (60), $m_i = m$ has been used again.

Unfortunately, no analytical solution of the integral in Eq. (67) is available. Hence, numerical solutions have been worked out for various monatomic gases.

In order to compare this numerical results obtained by the full covariant approach with the results of other approaches as listed in Eq. (63) we write the canonical partition integral of the monatomic gas in a generic representation:

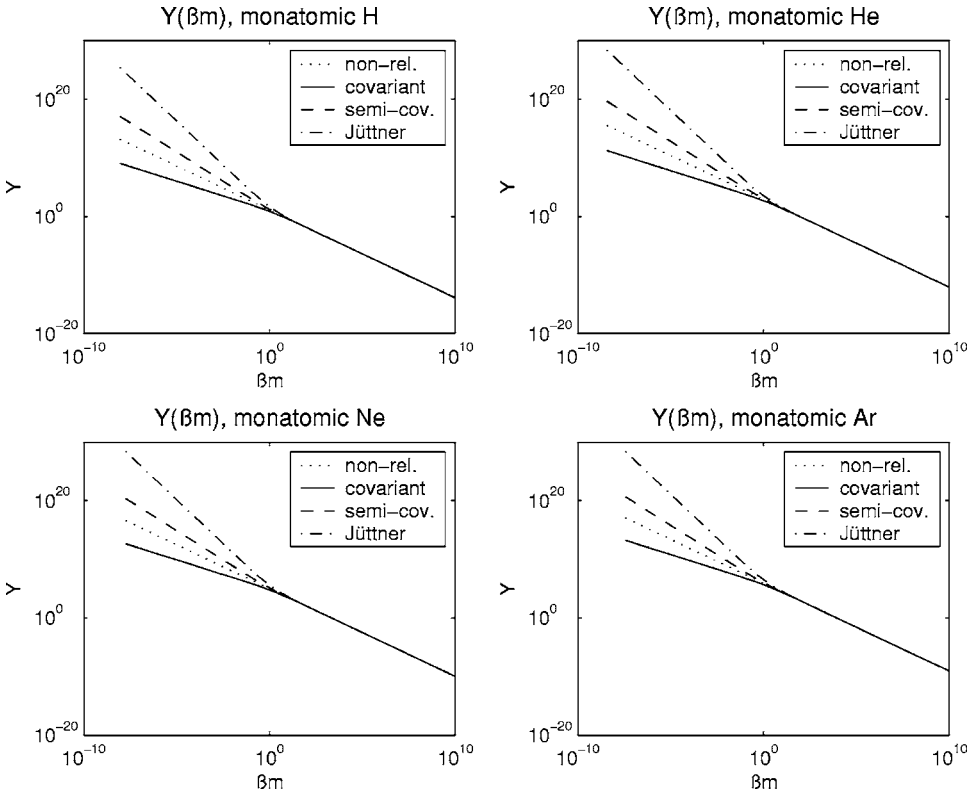

FIG. 1. Quantity Y as a function of βm for various approaches and different monatomic perfect gases.

$$Z_C = \frac{V^N}{N!}(e^{-\beta m}Y)^N. \tag{68}$$

The relativistic renormalization factor $e^{-\beta m}$ has been extracted explicitly in (68) for two reasons:

(1) This factor does not occur in the nonrelativistic partition integral.
(2) The numerical integration is simplified if this factor is extracted explicitly.

The nonanalytical integral occurring in the full covariant approach [see Eq. (67)] has been determined numerically using the Gauss-Laguerre method of 15th order. The results of the two other relativistic approaches (i.e., the Jüttner approach and the semicovariant approach) have been determined using the analytical expressions (i.e., evaluating the related modified Bessel functions K_1 and K_2) as well as using the same numerical integration method in order to justify the accuracy of the applied numerical method.

Figure 1 summarizes the results of calculations for different monatomic perfect gases namely, hydrogen, helium, neon, and argon. The comparison is focused on the quantity Y which determines the canonical partition integral via Eq. (68). As expected, the qualitative behavior is the same for all gases.

At low temperatures (nonrelativistic limit) all approaches give the same result as it should be. Even at higher temperatures ($T \leqslant 10^{12}$ K) (e.g., $T=10^{12}$ K corresponds roughly to $\beta m \simeq 10$ in case of hydrogen) no difference is visible among the various calculations. At extremely high temperatures ($T \geqslant 10^{12}$ K) relativistic effects are dominating the behavior. Compared to the nonrelativistic result the noncovariant Jüttner approach is showing a strong enhancement of the quantity Y in this regime. The semicovariant approach reduces this enhancement and the full covariant approach

turns the enhancement to a reduction even. Therefore, we conclude that a controlled manifest covariant reduction of the extended phase space reduces the value of the quantity Y and hence of the canonical partition integral.

In order to give an overview on the related thermodynamics of the monatomic perfect gas we finally list in dependence of the quantity Y the free energy

$$F = -kT \ln Z_C = -NkT\left(\ln \frac{V}{N} + \ln Y - \beta m + 1 \right), \tag{69}$$

the entropy

$$S = -\left(\frac{\partial F}{\partial T} \right)_V = k \ln Z_C + kT \frac{\partial \ln Z_C}{\partial T} = Nk\left(\ln \frac{V}{N} + \ln Y - \beta \frac{\partial \ln Y}{\partial \beta} + 1 \right), \tag{70}$$

the pressure

$$P = -\left(\frac{\partial F}{\partial V} \right)_T = kT \frac{\partial \ln Z_C}{\partial V} = \frac{NkT}{V}, \tag{71}$$

the average energy

$$\langle E \rangle = N\left(m - \frac{\partial \ln Y}{\partial B} \right), \tag{72}$$

and the specific heat

$$c_V = \left(\frac{\partial \langle E \rangle}{\partial T} \right)_V = \frac{N\beta}{T} \frac{\partial^2 \ln Y}{\partial \beta^2}. \tag{73}$$

Note, since the pressure turns out to be independent of Y all approaches give the same equation of state, namely the one of the nonrelativistic perfect gas,

$$PV = NkT. \tag{74}$$

Since the main differences among the various approaches are showing up at very high temperatures it is very useful to consider explicitly the following.

C. Ultrarelativistic limit

Since in the ultrarelativistic limit the rest mass is neglected in respect to the momentum and in respect to the energy it can be evaluated using $\sqrt{\mathbf{p}_i^2 + m_i^2} \to |\mathbf{p}_i|$ when deriving the integrals in Eqs. (67) and (60). Hence, it is even possible to derive analytical results in case of the full covariant approach since the partition integral simplifies drastically and we get in this limit ($\rho = |\mathbf{p}|$) for the various approaches,

$$Z_C^{(ur)} = \begin{cases} \dfrac{V^N}{N!}\left[4\pi m^2 \displaystyle\int_0^\infty \mathrm{d}\rho\, e^{-\beta\rho} \right]^N, & \text{full covariant,} \\ \dfrac{V^N}{N!}\left[4\pi m \displaystyle\int_0^\infty \mathrm{d}\rho\, \rho e^{-\beta\rho} \right]^N, & \text{semicovariant,} \\ \dfrac{V^N}{N!}\left[4\pi \displaystyle\int_0^\infty \mathrm{d}\rho\, \rho^2 e^{-\beta\rho} \right]^N, & \text{noncovariant (Jüttner).} \end{cases} \tag{75}$$

The integrals in (75) are easily determined with the help of the Γ-function according to

TABLE I. Thermodynamical quantities for the perfect gas in the ultrarelativistic limit.

Thermodynamical quantity	Full covariant	Semicovariant	Noncovariant (Jüttner approach)
$Z_C^{(ur)}$	$\frac{V^N}{N!}\left[\frac{4\pi m^3}{(\beta m)}\right]^N$	$\frac{V^N}{N!}\left[\frac{4\pi m^3}{(\beta m)^2}\right]^N$	$\frac{V^N}{N!}\left[\frac{8\pi m^3}{(\beta m)^3}\right]^N$
$F=-kT\ln Z_C$	$-NkT\left[\ln\frac{V}{N}+\ln(4\pi m^3)-\ln(\beta m)+1\right]$	$-NkT\left[\ln\frac{V}{N}+\ln(4\pi m^3)-2\ln(\beta m)+1\right]$	$-NkT\left[\ln\frac{V}{N}+\ln(8\pi m^3)-3\ln(\beta m)+1\right]$
$S=k\ln Z_C-\frac{1}{T}\partial\ln Z_C/\partial\beta$	$Nk\left[\ln\frac{V}{N}+\ln(4\pi m^3)-\ln(\beta m)+2\right]$	$Nk\left[\ln\frac{V}{N}+\ln(4\pi m^3)-2\ln(\beta m)+3\right]$	$Nk\left[\ln\frac{V}{N}+\ln(8\pi m^3)-3\ln(\beta m)+4\right]$
$\langle E\rangle=-\partial\ln Z_C/\partial\beta$	NkT	$2NkT$	$3NkT$
$c_V=\partial\langle E\rangle/\partial T$	Nk	$2Nk$	$3Nk$
$P=-\partial F/\partial V$	NkT/V	NkT/V	NkT/V

$$\int_0^\infty \mathrm{d}\zeta\,\zeta^n e^{-a\zeta}=\frac{\Gamma(n+1)}{a^{n+1}}. \tag{76}$$

Table I summarizes these results as well as some derived thermodynamical quantities in the case of the ultrarelativistic limit. Progressing from the noncovariant approach towards the full covariant approach via the semicovariant approach at a fixed β the canonical partition integral is decreasing as already mentioned when discussing Fig. 1. This behavior as well as the derivatives in respect to β are fixing the differences in the thermodynamical quantities, e.g., the entropy is reducing when progressing towards the full covariant approach. Especially, we want to focus on the average energy.

While Jüttners noncovariant calculations at the ultrarelativistic limit lead to $3NkT$ the semicovariant approach (as well as the method used in Ref. 14) leads to $2NkT$ and the full covariant treatment gives NkT. Thus, a controlled manifest covariant reduction of the extended phase space by N on-shell constraints reduces the average energy by a factor NkT and the final reduction by N time fixations by another factor NkT. Consequently, the specific heat is showing similar differences. As already mentioned by Horowitz *et al.*[14] no empirical evidence distinguishing between these results is available at the present time.

The following should be noted: Usually the noncovariant Jüttner approach in the ultrarelativistic limit is regarded to represent the classical photon gas. This approximate interpretation is not possible within our approach because the applied classical constrained Hamiltonian dynamics of massive particles cannot be used in the ultrarelativistic limit to approximate massless classical particle dynamics. This fact is showing up in the results and can be recognized inspecting $Z_C^{(ur)}$ (see Table I): In contradiction to the Jüttner approach $Z_C^{(ur)}$ remains mass dependant in the ultrarelativistic limit in case of the semicovariant and the full covariant approach.

D. Nonrelativistic limit

Finally, we examine the nonrelativistic limit of our approach. Since the covariant time fixations (4) reduce to the simple time fixations (3) in this limit the canonical partition integral within both approaches, semicovariant and full covariant, coincide according to Eq. (12) to be

$$Z_C^{(ur)} = \frac{1}{N!} \int \prod_{i=1}^{N} d^4q_i d^4p_i e^{-\beta E} \delta\left(\epsilon_i - \frac{\mathbf{p}_i^2}{2m_i} \right) \delta(q_i^0 - \tau). \tag{77}$$

Special care must be taken regarding the invariant energy E. In order to get a fair comparison in the nonrelativistic limit the rest masses of the particles must be subtracted from their energies getting in the comoving frame of reference

$$E = \sum_i^N (p_i^0 - m_i). \tag{78}$$

Using further $p_i^0 = \epsilon_i + m_i$ Eq. (77) simplifies to

$$Z_C^{(nr)} = \frac{V^N}{N!} \int \prod_{i=1}^{N} d^3p_i e^{-\beta(\mathbf{p}_i^2/2m_i)} = \frac{V^N}{N!} \left[\left(\frac{2\pi m^2}{\beta m} \right)^{3/2} \right]^N, \tag{79}$$

i.e., the nonrelativistic canonical partition integral.

Note, the same result can be achieved starting with the analytical result as obtained by the semicovariant approach. Supplementing Eq. (62) by a factor $e^{\beta N m}$ which covers the effect of the reduction of the energies by the rest masses [compare Eq. (78)], Eq. (62) transforms to

$$Z_C = \frac{V^N}{N!} e^{\beta N m} \left[\frac{4\pi m^3}{\beta m} K_1(\beta m) \right]^N. \tag{80}$$

In the nonrelativistic limit ($m \gg kT$) the asymptotic form of the modified Bessel function ($\beta m \to \infty$)

$$K_n(\beta m) \simeq \sqrt{\frac{\pi}{2\beta m}} e^{-\beta m} \left(1 + \frac{4n^2 - 1}{8\beta m} + \cdots \right) \tag{81}$$

can be applied. Since K_1 and K_2 coincide in the leading order the semicovariant approach and the noncovariant Jüttner approach provide the same result in the nonrelativistic limit namely, the nonrelativistic canonical partition integral (79) within this treatment.

V. SUMMARY AND CONCLUSION

A covariant equilibrium statistical mechanics has been formulated on the base of constrained Hamiltonian dynamics. The usage of this formalism to describe the microdynamics of the ensembles guarantees the manifest covariance of the developed approach.

Unfortunately, concrete calculations are not easily performed within this approach. As a simple application the canonical partition integral of the monatomic perfect gas has been evaluated numerically. Relativistic effects at very high temperatures have been observed.

The comparison of the obtained results with the results of the nonrelativistic theory show a decreasing partition integral at very high temperatures. In contradiction to this findings other relativistic approaches like the noncovariant calculations of Jüttner are showing an increased partition integral at these temperatures. It has been demonstrated that the full covariant treatment of the phase space is responsible for this significant difference. Considering the ultrarelativistic limit the same behavior is visible on a full analytical base. In the nonrelativistic limit the results coincide with the results obtained within the nonrelativistic theory.

As in the nonrelativistic theory the link to thermodynamics has been performed via the free energy. All thermodynamical potentials (like the internal energy, the free energy,…) as well as the thermodynamical state variables (like temperature, entropy, pressure,…) have been defined to be Lorentz scalars. This was achieved introducing the invariant internal energy $E=U_\mu P^\mu$ in the canonical distribution function. Regarding the ultrarelativistic limit the entropy, the average energy, and the specific heat are decreased in comparison to other approaches in this limit.

Unfortunately, the temperature regime which shows significant differences among the various approaches ($T \geqslant 10^{12}$ K) cannot be reached in experiments but may exist in cosmological events. Hence, it may be interesting to use the presented special relativistic approach as a base to develop a general relativistic equilibrium statistical mechanics being manifest covariant from first principle.

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Solvable reaction-diffusion processes without exclusion

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For reaction-diffusion processes without exclusion, in which the particles can exist in the same site of a one-dimensional lattice, we study all the integrable models which can be obtained by imposing a boundary condition on the master equation of the asymmetric diffusion process. The annihilation process is also added. The Bethe ansatz solution and the exact N-particle conditional probabilities are obtained.
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I. INTRODUCTION

There are a variety of phenomena that can be explained by stochastic models, and their nonequilibrium behaviors can be understood by rather simple rules.[1–3] One of the important examples of these models are the reaction-diffusion processes on a one-dimensional lattice for which their dynamics are fully specified by their master equation.[4,5] A simple example of reaction-diffusion process is asymmetric simple exclusion process (ASEP),[2,6,7] which is known to be relevant to various fields of science like the kinetics of biopolymerization,[8,9] traffic models,[10] polymers in random media, dynamical models of interface growth,[11,12] noisy Burgers equation,[13] study of shocks,[14,15] sequence alignment,[16] and molecular motors.[17] For recent reviews, see for instance.[18–20]

The ASEP is a lattice model in which each particle hops to its right (left) nearest-neighboring site with a probability $D_R\,\mathrm{d}t(D_L\,\mathrm{d}t)$ in an infinitesimal interval $\mathrm{d}t$. In addition, particles are subject to hard-core exclusion: each site is either occupied only by one particle or empty. ASEP has been studied in Ref. 21 by introducing a master equation which describes the time evolution of probabilities $P(x_1,\ldots,x_N;t)$, when the particles are not in neighboring sites, and a so-called boundary condition, which specifies the situations in which the probabilities go outside the physical region $x_1<x_2<\cdots<x_N$. These happen when some of the particles are in adjacent sites and the master equation can not be applied to them. It has been shown that the model is integrable in the sense that the N-particle S-matrix is factorized into a product of two-particle S-matrices. The coordinate Bethe ansatz has been used in this proof. Note that the S-matrix can completely determine the dynamics of a Markovian process, i.e., the N-particle probabilities of a model.

By choosing other suitable boundary conditions, without changing the master equation, one may study the more complicated reaction-diffusion processes, even with long-range interaction. In Ref. 22, the so-called drop-push model has been studied by this method. In this model the particle hops to the next right site even if it is occupied. The particle hops to this site by pushing all the neighboring particles to their next right sites, with a rate depending on the number of right neighboring particles. The generalization of this model, by considering both the right and left hopping, has been done in Ref. 23. This method has been also applied to more-than-one-species situations, which become more complicated. The complexity arises from the above-mentioned factorization of N-particle scattering matrix. In these cases, the factorization demands the two-

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particle *S*-matrices to satisfy the spectral Yang-Baxter equation. Various solvable multispecies models have been studied in this way, of which the most recent general cases have been discussed in Refs. 24 and 25.

All of the above studies have been restricted to interactions which include the hard-core exclusion. This made some simplification. In Refs. 26 and 27, an asymmetric diffusion model without exclusion has been shown to be integrable and to have the same *R*-matrix as that of the ASEP. In Ref. 28, it has been shown that the processes

$$mn \to m-l, n+l \quad \text{with rate } \frac{D_R}{[l]},$$

$$mn \to m+l, n-l \quad \text{with rate } \frac{D_R \gamma^l}{[l]}, \tag{1}$$

is integrable, in the sense of the above-mentioned two-particle factorization. The numbers "*m*," "*n*,"… indicate the particle numbers on a site, $\gamma = D_L/D_R$, and

$$[l] = \frac{1-\gamma^l}{1-\gamma}. \tag{2}$$

Note that in Ref. 28, the reaction rates of Eq. (1) are scaled by D_R. These processes are obtained by imposing the boundary condition

$$P_N(\ldots, x_j, x_j - 1, \ldots; t) = D_R P_N(\ldots, x_j - 1, x_j - 1, \ldots; t) + D_L P_N(\ldots, x_j, x_j, \ldots; t) (j = 1, \ldots, N-1), \tag{3}$$

on the master equation of ASEP,

$$\frac{\partial}{\partial t} P(x_1, \ldots, x_j, \ldots, x_N; t) = \sum_{j=1}^{N} D_R P(x_1, \ldots, x_{j-1}, x_j - 1, x_{j+1}, \ldots, x_N; t) + \sum_{j=1}^{N} D_L P(x_1, \ldots, x_{j-1}, x_j + 1, x_{j+1}, \ldots, x_N; t) - N P(x_1, \ldots, x_j, \ldots, x_N; t), \tag{4}$$

in which we have used a time scale so that $D_R + D_L = 1$. In the above equation, $P(x_1, \ldots, x_N; t)$ is the probability for finding at time t the particles at sites $x_1, \ldots, x_N$. We take these functions to define probabilities only in the physical region $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N$. In fact, in the domain $\Omega_N = x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N \subset Z^N$, the function P is the probability defined above, whereas in Z^N/Ω_N it is defined by the master equation (4), but it is not a probability. The master equation (4) is only valid for

$$x_i < x_{i+1}, \tag{5}$$

since for $x_i = x_{i+1}$, there will be terms with $x_i = x_{i+1} + 1$ on the right-hand side of Eq. (4), which is out of the physical region. One can, however, assume that (4) is valid for all physical region $x_i \leqslant x_{i+1}$, and impose a certain boundary condition for $x_i = x_{i+1}$. The boundary condition (3) leads to interactions (1).

In this paper we want to study all possible boundary conditions for single-species systems and derive all the integrable one-dimensional reaction-diffusion processes without exclusion which can be obtained by this method. The scheme of the paper is the following. In Sec. II, we show that there are two types of boundary conditions when $D_R \neq 0$ and $D_L \neq 0$. The first is one considered in Ref. 28, i.e., Eq. (3), which we call the **type 1** model, and the second one is

$$D_R P(x, x-1) + D_L P(x+1, x) = P(x, x). \tag{6}$$

Here we have suppressed all the other coordinates for simplicity. We show that the interactions of this **type 2** model are

$$mn \to m-1,n+1 \quad \text{with rate } D_R,$$

$$mn \to m+1,n-1 \quad \text{with rate } D_L. \tag{7}$$

This is the reactions (1), restricted to $l=1$. In other words, to have an integrable model, it is not necessary to have the simultaneous hoppings of any number of particles from a common site to the neighboring site [as indicated in (1)], but the one particle hoppings can also lead to integrable models. Note that the reactions (7) is not a subset of processes (1).

In the totally asymmetric case with $D_L=0$, we show in Sec. III that there is a new boundary condition which is a linear combination of boundary conditions (3) and (6), i.e.,

$$P(x,x-1)=\lambda P(x,x)+\mu P(x-1,x-1). \tag{8}$$

It is shown that this **type 3** model contains the reactions

$$mn \to m-l,n+l, \tag{9}$$

with rates

$$r_l=\frac{1}{1+\frac{\lambda}{\mu}+\cdots+\left(\frac{\lambda}{\mu}\right)^{l-1}}. \tag{10}$$

This is an interesting one-parameter family of interactions.

In Sec. IV, we generalize the boundary conditions (3), (6), and (8) to include annihilation to the processes (1), (7), and (9), respectively. The resulting models are rather involved. To be specific, we consider $D_L=0$ case of (3), and show that the boundary condition

$$P(x,x-1)=\mu P(x-1,x-1) \quad (\mu<1) \tag{11}$$

describes the reactions

$$mn \to m-l,n+l \quad \text{with rate } \mu^{l-1},$$

$$n \to \begin{cases} n-1 \\ n-2 \\ \cdots \end{cases} \quad \text{with total rates } n-\sum_{l=0}^{n-1}\mu^l. \tag{12}$$

The second reactions are the annihilation processes. We call this model the **type 4** model. It must be mentioned that we cannot extend our investigation to include the creation processes. The main reason is that if we do so, the evolution equation of n-particle sector will not become closed and will depend on the more-than-n-particle configurations.

The Bethe ansatz solution for different models is discussed in Sec. V and the exact N-point conditional probabilities of type 4 model is obtained in Sec. VI. Some interesting physical quantities are also obtained. Finally we discuss the multispecies extension of these processes in the last section and show that this generalization is not possible for the reactions without exclusion.

II. REACTIONS WITH $D_L \neq 0$ AND $D_R \neq 0$

Consider the master equation (4) for the two particle sector, when the particles are at site $x_1=x_2=x$,

$$\dot{P}(x,x)=D_RP(x-1,x)+D_RP(x,x-1)+D_LP(x+1,x)+D_LP(x,x+1)-2P(x,x). \tag{13}$$

The second and third probabilities on the right-hand side of the above equation are out of the physical region, and must be defined through some boundary conditions. There are only two

possibilities which are consistent in more-than-two-particle sectors. The first one is

$$\mu' P(x,x-1) = D_R P(x-1,x-1) + D_L P(x,x), \tag{14}$$

and the second one is

$$D_R P(x,x-1) + D_L P(x+1,x) = \lambda' P(x,x). \tag{15}$$

In the first choice, we take any unphysical terms of Eq. (13) as a linear combination of physical functions, and in the second choice, we take the whole unphysical terms as a linear combination of the physical probabilities. The right-hand sides of Eqs. (14) and (15) are the only allowed combinations which one can write. This was discussed in Ref. 25 for ASEP cases. In fact, one can use any other parameters α and β instead of D_R and D_L in Eq. (14), with condition $\alpha+\beta=1$. Also one can add two other terms $\mu P(x-1,x-1)$ and $\nu P(x+1,x+1)$ to the right-hand side of Eq. (15), but it can be shown that for obtaining a consistent description in more-than-two-particle sectors, one must take $\mu=\nu=0$ (see Sec. III of Ref. 25 for more details in the ASEP case).

To obtain the range of parameters μ' and λ', one can use Eq. (4) to show that

$$\begin{aligned}\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1\leqslant x_2} P(x_1,x_2;t) &= -\sum_x P(x,x;t) + D_R\sum_x P(x,x-1;t) + D_L\sum_x P(x+1,x;t)\\ &= -\sum_x P(x,x;t) + \sum_x P(x,x-1;t).\end{aligned} \tag{16}$$

For boundary condition (14), Eq. (16) results in

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1\leqslant x_2} P(x_1,x_2;t) = \left(\frac{1}{\mu'}-1\right)\sum_x P(x,x;t), \tag{17}$$

and for boundary condition (15), it results in

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1\leqslant x_2} P(x_1,x_2;t) = (\lambda'-1)\sum_x P(x,x;t). \tag{18}$$

In the first step, let us exclude the annihilation processes and therefore it is assumed that the number of particles is constant in time. In this way, the Eqs. (17) and (18) lead to

$$\mu' = 1 \quad [\text{for boundary condition (14)}],$$

$$\lambda' = 1 \quad [\text{for boundary condition (15)}]. \tag{19}$$

Equation (14) exactly becomes the one studied in Ref. 28, i.e., Eq. (3), and it induces the reactions (1), but the second one, Eq. (15), is new. To obtain the reaction introduced by this boundary condition, with $\lambda'=1$, we first consider $\dot{P}(x,x)$ in Eq. (13). Using Eqs. (15) and (19), one finds

$$\dot{P}(x,x) = D_R P(x-1,x) + D_L P(x,x+1) - P(x,x), \tag{20}$$

which is the evolution equation of the following two-particle reactions:

$$10 \to 01 \quad \text{with rate } D_R,$$

$$01 \to 10 \quad \text{with rate } D_L. \tag{21}$$

Remember $D_R+D_L=1$. Generally, for n particles existing at a common site x, one finds from (4),

$$\frac{\partial}{\partial t}P(\underbrace{x,\ldots,x}_{n}) = D_R P(x-1,\underbrace{x,\ldots,x}_{n-1}) + D_L P(\underbrace{x,\ldots,x}_{n-1},x+1)$$
$$+\sum_{j=2}^{n} D_R P(x_1=x,\ldots,x_{j-1}=x,x_j=x-1,x_{j+1}=x,\ldots,x_n=x)$$
$$+\sum_{j=2}^{n} D_L P(x_1=x,\ldots,x_{j-2}=x,x_{j-1}=x+1,x_j=x,\ldots,x_n=x) - nP(\underbrace{x,\ldots,x}_{n})$$
$$= D_R P(x-1,\underbrace{x,\ldots,x}_{n-1}) + D_L P(\underbrace{x,\ldots,x}_{n-1},x+1) - P(\underbrace{x,\ldots,x}_{n}), \tag{22}$$

which is obviously the evolution equation of reactions (7).

III. TOTALLY ASYMMETRIC DIFFUSION WITH $D_L=0$

In $D_L=0$, the boundary condition (3) and (6) becomes

$$P(x,x-1) = P(x-1,x-1),$$

$$P(x,x-1) = P(x,x), \tag{23}$$

respectively, which describe the interactions

$$mn \to m-l,n+l \quad \text{with rate } 1 \tag{24}$$

and

$$mn \to m-1,n+1 \quad \text{with rate } 1, \tag{25}$$

respectively. But as was first noted in Ref. 22 for ASEP, the linear combination of these two boundary conditions may result in a integrable model. So we consider

$$P(x,x-1) = \lambda P(x,x) + \mu P(x-1,x-1), \tag{26}$$

as the boundary condition for the following master equation:

$$\frac{\partial}{\partial t}P(x_1,\ldots,x_N;t) = \sum_{j=1}^{N}[P(x_1,\ldots,x_{j-1},x_j-1,x_{j+1}\ldots,x_N;t) - P(x_1,\ldots,x_N;t)]. \tag{27}$$

First we note that

$$\frac{\partial}{\partial t}\sum_{x_2}\sum_{x_1\leqslant x_2} P(x_1,x_2;t) = (\lambda+\mu-1)\sum_{x} P(x,x;t), \tag{28}$$

from which the conservation of number of particles results

$$\lambda+\mu=1. \tag{29}$$

To obtain the resulting reactions, besides the diffusion $10\to01$ with rate 1, we first consider $\dot{P}(x,x)$. Using (26) and (27), it is found that

$$\dot{P}(x,x) = P(x-1,x) + \mu P(x-1,x-1) - (2-\lambda)P(x,x), \tag{30}$$

which represents the reaction $20\to02$, with rate $\mu=1-\lambda$, as the source and sink of this state. To find the reactions in the general case, we first prove a lemma.

Lemma: Equation (26) implies, for arbitrary n, the following:

$$P(\underbrace{x,\ldots,x}_{n},x-1)=r_{n+1}P(\underbrace{x-1,\ldots,x-1}_{n+1})+(1-r_{n+1})P(\underbrace{x,\ldots,x}_{n+1}), \tag{31}$$

with r_n defined through (10).

Proof: We proceed by induction. For $n=1$, (31) reduces to (26). Assuming (31) is correct for $n-1$, then using (26), we have

$$\begin{aligned}P(\underbrace{x,\ldots,x}_{n},x-1)&=\lambda P(\underbrace{x,\ldots,x}_{n+1})+\mu P(\underbrace{x,\ldots,x}_{n-1},x-1,x-1)\\&=\lambda P(\underbrace{x,\ldots,x}_{n+1})+\mu[r_nP(\underbrace{x-1,\ldots,x-1}_{n+1})\\&\quad+(1-r_n)P(\underbrace{x,\ldots,x}_{n},x-1)],\end{aligned} \tag{32}$$

so

$$P(\underbrace{x,\ldots,x}_{n},x-1)=r_{n+1}P(\underbrace{x-1,\ldots,x-1}_{n+1})+s_{n+1}P(\underbrace{x,\ldots,x}_{n+1}), \tag{33}$$

where

$$r_{n+1}=\frac{\mu r_n}{1-\mu(1-r_n)},\quad s_{n+1}=\frac{\lambda}{1-\mu(1-r_n)}. \tag{34}$$

It is seen that $r_{n+1}+s_{n+1}=1$. The value of r_n can be found by solving the first equation of (34), which can be written as

$$r_{n+1}^{-1}=1+\frac{\lambda}{\mu}r_n^{-1}. \tag{35}$$

Using $r_2^{-1}=(1/\mu)=1+(\lambda/\mu)$, (35) leads to Eq. (10) for r_n's. This proves the lemma. □

We now consider the evolution of $P(\underbrace{x,\ldots,x}_{n})$.
Using (27) and (31), we find

$$\begin{aligned}\frac{\partial}{\partial t}P(\underbrace{x,\ldots,x}_{n})&=\sum_{j=1}^{n}P(x_1=x,\ldots,x_{j-1}=x,x_j=x-1,x_{j+1}=x,\ldots,x_n=x)-nP(\underbrace{x,\ldots,x}_{n})\\&=\sum_{j=1}[r_jP(x_1=x-1,\ldots,x_j=x-1,x_{j+1}=x,\ldots,x_n=x)+(1-r_j)P(\underbrace{x,\ldots,x}_{n})]-nP(\underbrace{x,\ldots,x}_{n})\\&=\sum_{j=1}r_jP(x_1=x-1,\ldots,x_j=x-1,x_{j+1}=x,\ldots,x_n=x)-\left(\sum_{j=1}^{n}r_j\right)P(\underbrace{x,\ldots,x}_{n}).\end{aligned} \tag{36}$$

This equation shows that a collection of j particles hops from site $x-1$ to site x with rate r_j, and this proves that the induced reactions of the boundary condition (8) are those indicated in (9).

At $\lambda=1$ ($\mu=0$), Eq. (10) results in $r_l=\delta_{l1}$. So the reactions are

$$mn\to m-1,n+1,\quad \text{with rate } 1. \tag{37}$$

This is nothing but Eq. (25). At $\lambda=0$ ($\mu=1$), Eq. (10) gives $r_l=1$ for all l's. So the reactions are those shown in (24). In fact, at $\lambda=0$, all the multiparticle hoppings occur with equal rate 1. By increasing λ, the greater number of simultaneous hoppings happen with lower rates, until at $\lambda=1$, in which only the one-particle hopping is allowed.

IV. ANNIHILATION-DIFFUSION PROCESSES

Adding annihilation to the preceding reactions, results in the decreasing of the number of particles with time. Therefore the parameters μ', λ', and (λ,μ) in Eqs. (14), (15), and (26) become

$$\mu' > 1 \quad [\text{for boundary condition (14)}],$$

$$\lambda' < 1 \quad [\text{for boundary condition (15)}],$$

$$\mu + \lambda < 1 \quad [\text{for boundary condition (26)}]. \tag{38}$$

These are obtained from Eqs. (17), (18), and (28), respectively. Note that the annihilation interactions only appear in sink terms of the master equation, since if we consider an initial state with n particles, no annihilation process can lead to a n-particle state at any later time t.

To obtain the corresponding interactions of either of boundary conditions, we begin with (15) with $\lambda' < 1$. Considering $\dot{P}(x,x)$, one finds

$$\dot{P}(x,x) = D_R P(x-1,x) + D_L P(x,x+1) - (2-\lambda')P(x,x), \tag{39}$$

which shows the annihilation rate $1-\lambda'$ for the state of two particle at a common site. In general case, one finds, similar to Eq. (22),

$$\frac{\partial}{\partial t}P(\underbrace{x,\ldots,x}_{n}) = D_R P(x-1,\underbrace{x,\ldots,x}_{n-1}) + D_L P(\underbrace{x,\ldots,x}_{n-1},x+1) - [n-(n-1)\lambda']P(\underbrace{x,\ldots,x}_{n}), \tag{40}$$

which is the evolution equation of the following reactions:

$$mn \to m-1, n+1 \quad \text{with rate } D_R,$$

$$mn \to m+1, n-1 \quad \text{with rate } D_L,$$

$$n \to \begin{cases} n-1 \\ n-2 \\ \cdots \end{cases} \quad \text{with total rates } (n-1)(1-\lambda'). \tag{41}$$

In the case of boundary condition (26) with $\lambda+\mu<1$, it is not easy to obtain a compact form for interaction rates in the general case. For example, in two- and three-particle sectors, considering $\dot{P}(x,x)$ and $\dot{P}(x,x,x)$, one finds

$$mn \to m-1, n+1 \quad \text{with rate } 1,$$

$$mn \to m-2, n+2 \quad \text{with rate } \mu,$$

$$mn \to m-3, n+3 \quad \text{with rate } \frac{\mu^2}{1-\lambda\mu},$$

$$2 \to 1 \quad \text{with rate } \alpha = 1-(\lambda+\mu),$$

$$3 \to \begin{cases} 2 \\ 1 \end{cases} \quad \text{with total rates } \frac{\alpha(\mu^2+\alpha\mu+2)}{1-\lambda\mu}. \tag{42}$$

In this case, we have a two-parameter family of interactions.

When we consider the boundary condition (14) with $\mu' > 1$, again we can not find the compact relations and it is better to restrict ourselves to the subset of totally asymmetric reactions with $D_L = 0$. This means that we take

$$P(x, x-1) = \mu P(x-1, x-1) \quad (\mu < 1) \tag{43}$$

as the boundary condition ($\mu = 1/\mu'$). Considering the general case $P(x, \ldots, x)$, results in

$$\begin{aligned} \frac{\partial}{\partial t} P(\underbrace{x, \ldots, x}_{n}) &= \sum_{j=1}^{n} P(x_1 = x, \ldots, x_{j-1} = x, x_j = x-1, x_{j+1} = x, \ldots, x_n = x) - nP(\underbrace{x, \ldots, x}_{n}) \\ &= \sum_{j=1}^{n} \mu^{j-1} P(x_1 = x-1, \ldots, x_j = x-1, x_{j+1} = x, \ldots, x_n = x) - nP(\underbrace{x, \ldots, x}_{n}). \end{aligned} \tag{44}$$

This equation shows that the sources are the simultaneous hoppings of j particles ($j = 1, \ldots, n$) from the common site $x-1$ to x, with rates μ^{j-1}. So the sinks are also these hoppings and the remaining rate of the sink terms in Eq. (44), i.e., $n - \Sigma_{j=0}^{n-1} \mu^j$, is due to the annihilations of these n particles at site x. So, it is proved that the boundary condition (43) induces the reactions (12).

V. BETHE ANSATZ SOLUTION

Now we try to solve the resulting evolution equations, in all the discussed cases, by the following Bethe ansatz:

$$P(\mathbf{x}; t) = e^{-E_N t} \psi(\mathbf{x}), \tag{45}$$

where $\mathbf{x} = (x_1, \ldots, x_N)$, and

$$\psi(\mathbf{x}) = \sum_{\sigma} A_\sigma e^{i\sigma(\mathbf{p})\cdot\mathbf{x}}. \tag{46}$$

The summation runs over the elements of permutation group of N object. Inserting (46) in master equation (4), results in

$$E_N = \sum_{k=1}^{N} (1 - D_R e^{-ip_k} - D_L e^{ip_k}). \tag{47}$$

To determine A_σ, we must insert the expression (46) in the boundary conditions. For the type 2 model, for instance, we must use Eq. (6), which results in

$$D_R \psi(\ldots, x_i = x, x_{i+1} = x-1, \ldots) + D_L \psi(\ldots, x_i = x+1, x_{i+1} = x, \ldots) = \psi(\ldots, x_i = x, x_{i+1} = x, \ldots), \tag{48}$$

and using (46), gives

$$[D_R e^{-i\sigma(p_{k+1})} + D_L e^{i\sigma(p_k)} - 1] A_\sigma + [D_R e^{-i\sigma(p_k)} + D_L e^{i\sigma(p_{k+1})} - 1] A_{\sigma\sigma_k} = 0. \tag{49}$$

σ_k is an element of permutation group which only interchanges p_k and p_{k+1},

$$\sigma_k : (p_1, \ldots, p_k, p_{k+1}, \ldots, p_N) \to (p_1, \ldots, p_{k+1}, p_k, \ldots, p_N). \tag{50}$$

Equation (49) gives $A_{\sigma\sigma_k}$ in terms of A_σ as follows:

$$A_{\sigma\sigma_k} = S^{(2)}(\sigma(p_k), \sigma(p_{k+1})) A_\sigma, \tag{51}$$

where

$$S^{(2)}(z_1,z_2) = -\frac{D_R z_2 + D_L z_1^{-1} - 1}{D_R z_1 + D_L z_2^{-1} - 1}, \tag{52}$$

where $z_k = e^{-ip_k}$. Equation (51) allows one to compute all A_σ's in terms of A_1, which is set to unity.

The same procedure can be applied to other boundary conditions. For example for type 3 model, boundary condition (8), one finds

$$S^{(3)}(z_1,z_2) = -\frac{\lambda + \mu(z_1+z_2) - z_2}{\lambda + \mu(z_1+z_2) - z_1}, \tag{53}$$

and for boundary condition (15), with $\lambda' < 1$,

$$S(z_1,z_2) = -\frac{D_R z_2 + D_L z_1^{-1} - \lambda'}{D_R z_1 + D_L z_2^{-1} - \lambda'}. \tag{54}$$

These solutions can be used, in principle, to calculate the conditional probabilities $P(x_1,\ldots,x_N;t|y_1,\ldots,y_N;0)$. This is the probability of finding the particles at time t at sites $x_1,\ldots,x_N$, if at $t=0$, they were at sites $y_1,\ldots,y_N$, respectively. But unfortunately, the standard method, used for example, in Refs. 21–25, cannot be used here. This is because the initial condition

$$P(\mathbf{x};0|\mathbf{y};0) = \delta_{\mathbf{x},\mathbf{y}} \tag{55}$$

is satisfied by the standard expression

$$P(\mathbf{x};t|\mathbf{y};0) = \int \frac{d^N p}{(2\pi)^N} e^{-E_N t} e^{-i\mathbf{p}\cdot\mathbf{y}} \psi(\mathbf{x}), \tag{56}$$

only when $y_i < y_{i+1}$ and $x_i < x_{i+1}$. This condition is only satisfied by exclusion processes and for processes without exclusion, we must look for other methods.

VI. *N*-PARTICLE CONDITIONAL PROBABILITIES

In some special cases, it is possible to calculate the conditional probabilities in terms of a specific determinant. This was first proved in Ref. 21, and then used for other cases in Refs. 22 and 23. Now we want to check that this method does work here, and as a specific example, we consider the type 4 model with the boundary condition (11).

We set the following ansatz for N-particle conditional probabilities:

$$P(\mathbf{x};t|\mathbf{y};0) = e^{-Nt} \det[G(\mathbf{x};t|\mathbf{y};0)], \tag{57}$$

where G is a $N\times N$ matrix with elements

$$G_{ij}(\mathbf{x};t|\mathbf{y};0) = g_{i-j}(x_i - y_j;t). \tag{58}$$

Inserting (57) in Eqs. (27) and (11), results in

$$\frac{\partial}{\partial t} G_i(x;t) = G_i(x-1;t),$$

$$G_{i-1}(x;t) = \mu G_{i-1}(x-1;t) + \beta G_i(x-1;t), \tag{59}$$

where G_i denotes the ith row of matrix G, and β is an arbitrary constant. In terms of functions $g_p(n;t)$, (59) becomes

$$\frac{\partial}{\partial t} g_p(n;t) = g_p(n-1;t),$$

$$g_p(n;t) = \mu g_p(n-1;t) + \beta g_{p+1}(n-1;t). \tag{60}$$

Introducing the z-transform

$$\tilde{g}_p(z,t) = \sum_{n=-\infty}^{\infty} z^n g_p(n;t), \tag{61}$$

we find

$$\frac{\partial}{\partial t}\tilde{g}_p(z,t) = z\tilde{g}_p(z,t) \Rightarrow \tilde{g}_p(z,t) = e^{zt}\tilde{g}_p(z,0),$$

$$\tilde{g}_{p+1}(z,t) = \frac{1-\mu z}{\beta z}\tilde{g}_p(z,t). \tag{62}$$

The second equation yields

$$\tilde{g}_p(z,0) = \left(\frac{1-\mu z}{\beta z}\right)^p \tilde{g}_0(z,0). \tag{63}$$

Using $P(x;0|y;0) = g_0(x-y;0) = \delta_{x,y}$, one finds $\tilde{g}_0(z,0) = 1$. Finally

$$\tilde{g}_p(z,t) = e^{zt}\left(\frac{1-\mu z}{z}\right)^p, \tag{64}$$

in which we choose $\beta = 1$. The functions $g_p(n;t)$ can be obtained by expanding the generating functions $\tilde{g}_p(z,t)$. For $p \geqslant 0$, the expansion yields

$$g_p(n;t) = \sum_{m=0}^{p} \binom{p}{m} (-\mu)^m \frac{t^{n+p-m}}{(n+p-m)!}, \tag{65}$$

and for negative p, it yields

$$g_{-|p|}(n;t) = \sum_{m=0}^{n-|p|} \binom{|p|+m-1}{m} \mu^m \frac{t^{n-|p|-m}}{(n-|p|-m)!}. \tag{66}$$

We have thus obtained the explicit relation for conditional probabilities.

It can be checked that the resulting function satisfies the desired initial condition. At $t=0$, where $x_i = y_i$, we have $g_{-|p|}(0;t) = 0$ and $g_0(n;0) = \delta_{n,0}$, which result $P(\mathbf{x};0|\mathbf{x};0) = 1$. Also it may be interesting to obtain the rate of decay of a delta function distribution. Suppose at $t=0$, there are N particles at the same site y. We want to obtain the probability of finding all the particles at their initial positions at later time t, i.e., $P(\mathbf{y};t|\mathbf{y};0)$, where $\mathbf{y} = (y,\ldots,y)$. Using $g_{-|p|}(0;t) = 0$ and $g_0(0;t) = 1$, we obtain

$$P(\mathbf{y};t|\mathbf{y};0) = e^{-Nt}\det[G(\mathbf{y};t|\mathbf{y};0)] = e^{-Nt}, \tag{67}$$

which is independent of μ! It is an interesting result. At $\mu = 1$, where there is no annihilation, the rate of simultaneous hoppings of particles are all 1, irrespective of the number of particles. By decreasing μ, the rates of simultaneous hoppings decrease with increasing the number of particles [see Eq. (12)]. At the same time, the rate of annihilation increases in such a way that the total decaying rate remains constant.

The above determinant method can be applied to any model which its boundary condition equation contains only two terms. Otherwise it does not lead to the consistent relations for matrix elements $g_p(n;t)$'s. So for $D_R = 0$ *or* $D_L = 0$ cases of boundary conditions (3) and (6), and $\lambda = 0$ *or*

$\mu=0$ cases of boundary condition (8), this method leads to explicit expressions for N-particle conditional probabilities.

VII. CONCLUSION

In the preceding sections, we use all the allowed generalizations of the boundary condition in the asymmetric reaction-diffusion processes without exclusion, to obtain several integrable models for one-species cases. The further natural generalization, which has been discussed in many papers for the ASEP case, is the multispecies extensions of these models. In multispecies studies, one considers a p-species system with particles $A_1,\ldots,A_p$. The basic objects are the probabilities $P_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_N;t)$ for finding at time t the particles of type α_1 at x_1, particle of type α_2 at x_2, etc. The master equation, instead of (4), is Ref. 25,

$$\begin{aligned}\frac{\partial}{\partial t}P_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_j,\ldots,x_N;t) &= \sum_{j=1}^{N} D_R P_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_{j-1},x_j-1,x_{j+1},\ldots,x_N;t)\\ &\quad+\sum_{j=1}^{N} D_L P_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_{j-1},x_j+1,x_{j+1},\ldots,x_N;t)\\ &\quad- NP_{\alpha_1\ldots\alpha_N}(x_1,\ldots,x_j,\ldots,x_N;t).\end{aligned} \tag{68}$$

Now if we want to use this equation for reactions without exclusion, the problem will arise when some of the particles are in the same position. Consider, for example, the two-species case $P_{\alpha_1\alpha_2}(x,x)$. It is seen that Eq. (68) has the term $P_{\alpha_1\alpha_2}(x-1,x)$, as the source term of the desired state, but does not contain $P_{\alpha_2\alpha_1}(x-1,x)$, which is as important as the first term. In fact, this is the source of many difficulties that arise in multispecies extension of reaction-diffusion processes which have no exclusion. So it seems that the integrable models discussed in the preceding sections are *all* that one can obtain in this context.

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Separation of noncommutative differential calculus on quantum Minkowski space

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Noncommutative differential calculus on quantum Minkowski space is not separated with respect to the standard generators, in the sense that partial derivatives of functions of a single generator can depend on all other generators. It is shown that this problem can be overcome by a separation of variables. We study the action of the universal L-matrix, appearing in the coproduct of partial derivatives, on generators. Powers of the resulting quantum Minkowski algebra valued matrices are calculated. This leads to a nonlinear coordinate transformation which essentially separates the calculus. A compact formula for general derivatives is obtained in form of a chain rule with partial Jackson derivatives. It is applied to the massive quantum Klein-Gordon equation by reducing it to an ordinary q-difference equation. The rest state solution can be expressed in terms of a product of q-exponential functions in the separated variables. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A. Quantum theory on noncommutative space-time

Much of the development of quantum theories on noncommutative space-times was and still is driven by the question whether noncommutative geometry might lead to an ultraviolet regularization of quantum field theory, as it was suggested by Heisenberg as early as 1938.[1] For the simplest conceivable examples of noncommutative geometries, where the commutator of the coordinates is constant, these hopes for regularization were met with disappointment. Such theories exhibit a mixing of ultraviolet and infrared cutoff scales,[2,3] which has been understood recently on the level of renormalization.[4] For that reason these simple noncommutative spaces, while interesting objects on their own, hardly seem to improve the divergent behavior of quantum field theory at all. The natural next step is to turn again to more complicated noncommutative spaces, such as quantum spaces with Lie type or homogeneous commutation relations.

Quantum Minkowski space is one of the most realistic examples of a quantum deformation of space-time[5] with a rich and fairly well understood mathematical structure: It is four dimensional in the sense that it is generated as algebra by four coordinates such that the ordered monomials are a Poincaré-Birkhoff-Witt basis. The time coordinate is central, which is important for a causal interpretation of quantum theory.[6] By construction, it is a module algebra with respect to the quantum Poincaré algebra,[7] so it has a well-defined quantum symmetry structure.[8] The action of the generators of the inhomogeneous part of the quantum Poincaré algebra, the momenta, on quantum Minkowski space induces a first order covariant differential calculus[9].

With these key mathematical structures present, it was possible to mimic much of the construction of quantum theory on commutative space-time within an algebraic and representation theoretic approach. Sections of noncommutative space-time were studied by spectral theory of

noncommutative coordinates, yielding discrete space-time lattices.[10] Free elementary particles were constructed as irreducible representations of the quantum Poincaré algebra, including Wigner representations of spin.[11] The free particles were shown to obey quantum wave equations which project reducible quantum Lorentz spinor representations on their irreducible subrepresentations.[12] The coupling of free fields to gauge fields was studied systematically within noncommutative gauge theory.[13–17] Quantum statistics of the tensor representation of a second quantized free theory was studied within the framework of braided tensor categories[18] using Drinfeld twists.[19] Only a small selection of the numerous contributions to this program can be cited here. At the time of this writing, many mathematical aspects of free quantum theory on quantum Minkowski space are understood, and the construction of interaction terms on the level of single particle field equations is known. What is not known is how to solve these field equations by noncommutative wave functions, not even for the free case. However, this will be indispensable if free particles are to be coupled by multiplying their noncommutative wave functions within the algebra of quantum space-time, in order to modify the concept of locality on a fundamental level.

We remark, that there are other approaches involving wave equations on noncommutative space-time which are inequivalent to the ones considered here: In Ref. 20 a q-deformed relativistic wave equation was constructed using a q-deformation of the Clifford algebra. This approach yields q-wave equations which are similar to the ones considered here. However, in Ref. 12 it was shown that, from a representation theoretic viewpoint, an additional twisting of the γ-matrices by the universal $\mathcal{R}$-matrix is needed if the q-partial derivatives are to be identified with the q-momenta. In Ref. 21 the construction of deformed wave equations also relied on covariance arguments. But there, a certain deformation of the conformal symmetry algebra was considered which does not contain the standard q-Poincaré algebra as subalgebra. For this reason the wave equations derived in Ref. 21 are different from the ones considered here. In Ref. 22 q-deformed cospinors were used in order to construct q-deformed wave equations. However, these are really cowave equations which are mathematically quite different objects. Finally, a number of authors has used various abstract differential calculi on quantum spaces[23–25] in order to construct q-differential equations. In these cases covariance with respect to the full q-Poincaré algebra, which determined the q-wave equations of Ref. 12 uniquely, was not the guiding principle and is, therefore, not satisfied in general.

B. Noncommutative differential calculus

The free wave equations on quantum Minkowski space can be determined uniquely on a purely representation theoretic level. To give the simplest example, just as in the undeformed case, the momentum square $p_\mu p^\mu$ is central within the quantum Poincaré algebra. Therefore, it must be represented within the irreducible representation corresponding to a free particle by a multiple of the identity operator,

$$p_\mu p^\mu = m^2, \tag{1}$$

m^2 being the square of the particle's mass. This line of reasoning does not depend in any way on how the momenta act on noncommutative wave functions, that is, on elements of quantum Minkowski space.

In order to interpret Eq. (1) as Klein-Gordon equation on noncommutative space-time we must let the momenta act on noncommutative wave functions. Momenta then correspond to partial derivatives, $p^\mu = i\partial^\mu$, defined by the noncommutative first order differential calculus. This yields a wave equation given by a noncommutative partial differential equation,

$$\partial_\mu \partial^\mu \triangleright \psi = -m^2 \psi, \tag{2}$$

where ψ is an element of the algebra of quantum Minkowski space. The triangle notation is used to distinguish the action from the multiplication in the quantum Heisenberg algebra. There is a considerable amount of literature on first order differential calculi on noncommutative algebras, mostly on quantum groups[26] and to some extent on homogeneous quantum spaces.[27,28] Most

mathematical work has concentrated on the construction, structural analysis, and classification of differential calculi. However, hardly any literature on the subject has dealt with concrete calculations within these differential calculi. On quantum Minkowski space a differential calculus has been known for some time, and can be deduced most elegantly from the coproduct of momenta.[9] The coproduct defines the action of partial derivatives on noncommutative functions, recursively. While the recursion relations can be used to expand the derivatives in terms of nested summations and partition functions, as it was carried out in a very detailed manner in Ref. 29, this does not solve the main computational problem which arises with wave equations like Eq. (2).

Trying to solve Eq. (2) by a brute force calculation with a general ansatz for the wave function should work in principle, but turns out to run into considerable computational complexity. Moreover, the solutions thus obtained in terms of recursion relations do not give much structural insight in the solutions which, after all, are the noncommutative counterpart of something as simple and basic as plane waves. Why is this computation so difficult? It can be shown that just as in the commutative case the space of solutions of the massive Klein-Gordon Eq. (2) is generated, as representation of the quantum Poincaré algebra, by a rest state, which satisfies[12]

$$\partial^0 \triangleright \psi = im\psi, \quad \partial^A \triangleright \psi = 0, \tag{3}$$

where A is a three vector index of spatial coordinates. In the commutative case we could now infer that ψ is a function of the time coordinate x_0 alone, thus reducing Eq. (3) to an ordinary differential equation in one coordinate x_0. Not so in the noncommutative case, where the partial derivatives of a function in x_0 depend on all coordinates x_μ, which makes the solution of Eq. (3) so involved. In analogy to partial differential equations in non-Cartesian coordinates we will describe this mixing of dependencies by saying that within the noncommutative calculus the standard variables are not separated.

It is now obvious to ask, whether new variables can be found which separate the differential calculus, such that Eq. (3) becomes easily solvable. The main purpose of this paper is to show that this question has a positive answer.

C. Structure, main results, notation

The paper is organized as follows: In Sec. II the structure of the differential calculus on quantum Minkowski space is reviewed. We recall the commutation relations, general structure of the quantum Lorentz algebra, universal $\mathcal{R}$-matrix, and the definition of the coproduct of momenta in order to make this paper self-contained and fix conventions and notation unambiguously.

Section III contains the bulk of the paper: the computation of derivatives of arbitrary elements in the quantum Minkowski algebra. We first develop a notation and calculus in order to deal with functions of the algebra valued 4×4 matrices which come from the action of the universal L-matrices appearing in the definition of the coproduct of momenta. The computation problem is the calculation of powers of algebra valued matrices, which can then be used to calculate the derivatives of arbitrary functions of the noncommutative coordinates. We do this calculation in two steps: In the first step we deal with polynomials of the noncentral variables. The main result is Proposition 1, Eqs. (69) and can be written in the concise form of a chain rule, where the outer derivatives are partial Jackson derivatives. In the second step we calculate derivatives of functions of the central coordinates, time and four length. The partial derivatives of functions in the time generator are complicated and depend on all other generators. However, we are able to give a noncommutative coordinate transformation such that the derivatives of functions in the central generators are disentangled and take the form of a chain rule, too. This is the main result of the paper, presented in Proposition 3, Eq. (97). The results of these two steps can be combined to yield a compact formula for the derivatives of arbitrary elements of the algebra, given in Eq. (101).

In Sec. IV we apply the formulas for the derivations to the initial problem of finding the momentum eigenstate solutions of the massless and massive quantum Klein-Gordon equation, viewed as differential equations within the noncommutative differential calculus. We show that the separation of variables of the preceding section separates the differential equations completely.

This reduces the partial differential equations to single variable equations involving Jackson derivatives, which are easily solved. The solutions are given in Eqs. (110) and (117) in terms of q-exponential functions.

Following the conlusion in Sec. V, the appendix finally contains a few more technical results which are used in the paper. This makes this paper reasonably self-contained and will be useful for a reader who wishes to reproduce the calculations in detail.

Notation: Throughout the paper q denotes a real positive deformation parameter, such that for $q \to 1$ we retrieve the undeformed, commutative limit. We will often use the abbreviations $\lambda := q - q^{-1}$ and symmetrized and standard quantum numbers,

$$[n] = \frac{q^n - q^{-n}}{q - q^{-1}}, \quad (n)_{q^2} = \frac{q^{2n} - 1}{q^2 - 1}, \tag{4}$$

where n is a natural number. Repeated upper and lower indices are summed over $x_\mu x^\mu \equiv \sum_\mu x_\mu x^\mu$.

II. DIFFERENTIAL CALCULUS ON QUANTUM MINKOWSKI SPACE

A. Quantum Minkowski space

Quantum Minkowski space has first been constructed as braided product of two copies of the quantum plane.[5] We will need the definition in terms of generators which are decomposed into the scalar time coordinate and the three vector of space coordinates.

Definition 1: The algebra generated by the four generators x_0, x_-, x_+, and x_3, divided by the relations

$$x_- x_0 = x_0 x_-, \quad x_+ x_0 = x_0 x_+, \quad x_3 x_0 = x_0 x_3,$$

$$q^{-1} x_- x_3 - q x_3 x_- = -\lambda x_- x_0, \quad q^{-1} x_3 x_+ - q x_+ x_3 = -\lambda x_+ x_0, \tag{5}$$

$$x_- x_+ - x_+ x_- - \lambda x_3 x_3 = -\lambda x_3 x_0,$$

is called the algebra of quantum Minkowski space, denoted by $\mathcal{X}$.

Here, x_0 is the time coordinate, while x_-, x_+, and x_3 are the space coordinates with su_2-weight indices $\{-,3,+\} \equiv \{-1,0,1\}$. The commutation relations (5) can be written in more sophisticated forms, e.g., in terms of q-Clebsch-Gordon coefficients or in terms of an R-matrix as we will recall in the next section.

The center of $\mathcal{X}$ is generated by x_0 and the four-square

$$x^2 := (x_0)^2 + q^{-1} x_- x_+ + q x_+ x_- - (x_3)^2. \tag{6}$$

Since we will not use 2 as index, x^2 cannot be confused with any one of the coordinates. The four-square can also be written as

$$x^2 = x_\mu x_\nu \eta^{\mu\nu} \tag{7}$$

in terms of the q-Minkowski metric defined by

$$\eta^{00} = 1, \quad \eta^{-+} = q^{-1}, \quad \eta^{-+} = q, \quad \eta^{33} = -1, \tag{8}$$

all other components vanishing. The metric defines upper four-vector indices by

$$x^\mu := \eta^{\mu\nu} x_\nu. \tag{9}$$

Note, that $x^2 = x_\mu x^\mu$ but $x^2 \neq x^\mu x_\mu$ because $\eta^{\mu\nu}$ is not symmetric.

B. Quantum Lorentz algebra

By construction $\mathcal{X}$ is a module algebra with respect to the quantum Lorentz algebra $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$. There are several essentially isomorphic forms of $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ in use.[30,9,31,32] In the chiral decomposition form $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ is given, as algebra, by the tensor square of quantum $\mathcal{U}(\mathrm{su}_2)$,

$$\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C})) = \mathcal{U}_q(\mathrm{su}_2) \otimes \mathcal{U}_q(\mathrm{su}_2). \tag{10}$$

The definition of $\mathcal{U}_q(\mathrm{su}_2)$ is recalled in the appendix. The chiral decomposition implies that the irreducible representations of $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ can be labelled by the highest weights of the two tensor factors. For example, the structure morphism of the four-vector representation is given on this chiral form by

$$\rho^{(1/2,1/2)} := \rho^{1/2} \otimes \rho^{1/2}, \tag{11}$$

where $\rho^{1/2}$ is the fundamental representation of $\mathcal{U}_q(\mathrm{su}_2)$ with highest weight or spin $j=\frac{1}{2}$.

The quantum Lorentz algebra is quasitriangular. In the chiral form (10) the universal $\mathcal{R}$-matrix of $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ can be expressed in terms of the well-known universal $\mathcal{R}$-matrix of $\mathcal{U}_q(\mathrm{su}_2)$. There are two inequivalent universal $\mathcal{R}$-matrices,[18]

$$\mathcal{R}_{\mathrm{I}} = \mathcal{R}_{41}^{-1}\mathcal{R}_{31}^{-1}\mathcal{R}_{24}\mathcal{R}_{23}, \quad \mathcal{R}_{\mathrm{II}} = \mathcal{R}_{41}^{-1}\mathcal{R}_{13}\mathcal{R}_{24}\mathcal{R}_{23}, \tag{12}$$

where $\mathcal{R}$ is the universal $\mathcal{R}$-matrix of $\mathcal{U}_q(\mathrm{su}_2)$ given in Eq. (A6), and where we have used the tensor leg notation $\mathcal{R}_{23}=1\otimes\mathcal{R}\otimes 1$, etc. The four-vector representations of the universal $\mathcal{R}$-matrices are denoted by

$$\begin{aligned} R_{\mathrm{I}}{}^{\mu\nu}{}_{\sigma\tau} &:= (\rho^{(1/2,1/2)} \otimes \rho^{(1/2,1/2)})(\mathcal{R}_{\mathrm{I}})^{\mu\nu}{}_{\sigma\tau}, \\ R_{\mathrm{II}}{}^{\mu\nu}{}_{\sigma\tau} &:= (\rho^{(1/2,1/2)} \otimes \rho^{(1/2,1/2)})(\mathcal{R}_{\mathrm{II}})^{\mu\nu}{}_{\sigma\tau}. \end{aligned} \tag{13}$$

With the R-matrices the commutation relations (5) can be written in the compact form

$$x_\sigma x_\tau = x_\mu x_\nu R_{\mathrm{I}}{}^{\mu\nu}{}_{\tau\sigma}. \tag{14}$$

This implies that the $\mathcal{X}$-algebra has the Poincaré-Birkhoff-Witt property, because the R-matrices satisfy the Yang-Baxter equation. From the decomposition of the R-matrices into eigenspaces we can, furthermore, derive the relation

$$(1 + q\hat{R}_{\mathrm{II}})(1 - \hat{R}_{\mathrm{I}}) = 0, \tag{15}$$

where the hat denotes swapping the two upper indices $\hat{R}^{\mu\nu}{}_{\tau\sigma}=R^{\nu\mu}{}_{\tau\sigma}$. We will need this formula later.

The disadvantage of the chiral form (10) is that the inner tensor factors of the coproduct are twisted with the $\mathcal{R}$-matrix of $\mathcal{U}_q(\mathrm{su}_2)$. Since the $\mathcal{R}$-matrix is given by an infinite series, which exists only as formal power series, some of the generators of $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ have a complicated coproduct which then exists only as formal power series, too. Therefore, it is also convenient to use the Drinfeld double form,[33] where $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C}))$ is represented as Drinfeld double of the Hopf-dually paired $\mathcal{U}_q(\mathrm{su}_2)$ and $\mathrm{SU}_q(2)^{\mathrm{op}}$.

C. Noncommutative differential calculus

The generators of q-momenta are required to transform as four-vector with respect to q-Lorentz transformations. The fact that q-momenta transform in the same way as the coordinate generators of q-Minkowski space implies that they must satisfy the same commutation relations as well. This leads to the definition of the q-momentum algebra as the algebra generated by p_0, p_-, p_+, p_3 with commutation relations (5), replacing x with p everywhere.

Noncommutative partial derivatives

$$\partial_\mu := ip_\mu \tag{16}$$

are defined by the action of the momentum generators on the q-Minkowski algebra of space functions. Partial derivatives of the coordinates must be dimensionless numbers from the base field of complex numbers (including the deformation parameter q). Just as in the undeformed case the only tensor in the base field with two four-vector indices is the metric. We conclude that the action of partial derivatives on coordinates is given by

$$\partial_\mu \triangleright x_\nu = \eta_{\mu\nu} \Leftrightarrow \partial^\mu \triangleright x_\nu = \delta^\mu_\nu. \tag{17}$$

This action on the generators extends to the entire algebra of q-Minkowski space by the coproduct of momenta,[9]

$$\Delta(p^\mu) := p^\mu \otimes 1 + (\kappa \otimes 1)\mathcal{R}_{\mathrm{II}}{}^{-1}(1 \otimes p^\mu)\mathcal{R}_{\mathrm{II}} = p^\mu \otimes 1 + \kappa L^\mu{}_\nu \otimes p^\nu. \tag{18}$$

Here $\mathcal{R}_{\mathrm{II}}$ is the second of the universal $\mathcal{R}$-matrices of the q-Lorentz algebra given in Eq. (12). The L-matrix is the four-vector half-representation of this $\mathcal{R}$-matrix

$$L^\mu{}_\nu := \mathcal{R}_{\mathrm{II}[1]}\rho^{(1/2,1/2)}(\mathcal{R}_{\mathrm{II}[2]})^\mu{}_\nu, \tag{19}$$

where we have used a Sweedler-type notation for $\mathcal{R}_{\mathrm{II}} = \mathcal{R}_{\mathrm{II}[1]} \otimes \mathcal{R}_{\mathrm{II}[2]}$. Finally, κ is a grouplike scaling operator,

$$p_\mu \kappa = q\kappa p_\mu, \quad x_\mu \kappa = q^{-1}\kappa x_\mu, \quad \Delta(\kappa) = \kappa \otimes \kappa. \tag{20}$$

The action (17) of partial q-derivatives together with the coproduct (18) defines a q-Lorentz-covariant differential calculus on q-Minkowski space. Letting p^μ act on $x_\nu f$, $f \in \mathcal{X}$, we obtain

$$p^\mu \triangleright (x_\nu f) = -i\delta^\mu_\nu f + qR_{\mathrm{II}}{}^{\nu'\mu}{}_{\nu\mu'} x_{\nu'}(p^{\mu'} \triangleright f), \tag{21}$$

from which we can deduce the q-deformed Heisenberg commutation relations

$$p^\mu x_\nu - qR_{\mathrm{II}}{}^{\nu'\mu}{}_{\nu\mu'} x_{\nu'} p^{\mu'} = -i\delta^\mu_\nu, \tag{22}$$

which are of the type originally introduced by Wess and Zumino.[28]

In order to show that Eqs. (17) and (18) define a differential calculus which is well defined on the algebra $\mathcal{X}$, that is, which does not depend on the ordering of the coordinate generators, we must check if the action of the momenta is consistent with commutation relations (5) defining $\mathcal{X}$. This is best done using the R-matrix form (14),

$$p^\lambda \triangleright (x_\sigma x_\tau - x_\mu x_\nu R_{\mathrm{I}}{}^{\mu\nu}_{\tau\sigma}) = (p^\lambda \triangleright x_\nu x_\mu)(\delta^\nu_\tau \delta^\mu_\sigma - \hat{R}_{\mathrm{I}}{}^{\nu\mu}_{\tau\sigma}) = x_\rho(\delta^\lambda{}_\nu \delta^\rho{}_\mu + q\hat{R}_{\mathrm{II}}{}^{\lambda\rho}{}_{\nu\mu})(\delta^\nu_\tau \delta^\mu_\sigma - \hat{R}_{\mathrm{I}}{}^{\nu\mu}_{\tau\sigma}) = 0, \tag{23}$$

where in the last step we have used Eq. (15).

In principle, the action (17) of the partial derivatives on generators together with the coproduct (18) of momenta defines the action of partial derivatives on arbitrary elements of quantum Minkowski space. Note, however, that this definition is recursive. It does not yield formulas for the partial derivatives of a basis of the noncommutative space algebra, such as the Poincaré-Birkhoff-Witt basis of ordered monomials,

$$\mathcal{B}_{\mathrm{PBW}} := \{(x_0)^{n_0}(x_-)^{n_-}(x_+)^{n_+}(x_3)^{n_3} | n_0, n_-, n_+, n_3 \in \mathbb{N}_0\}. \tag{24}$$

To derive such a formula is one of the goals of the next section.

III. COMPUTATION IN NONCOMMUTATIVE CALCULUS

A. *L*-matrix calculus

Let us first consider the simple case of a power of one single generator, $f=x_\alpha^n$, $\alpha\in\{0,-,+,3\}$, $n\in\mathbb{N}$. Using the coproduct (18) we get by induction

$$\partial^\mu\triangleright x_\alpha^n=\sum_{k=0}^{n-1}q^k(L^\mu{}_\nu\triangleright x_\alpha^k)(\partial^\nu\triangleright x_\alpha)x_\alpha^{n-k-1}, \tag{25}$$

where the factor q^k comes from the action of the scaling operator (20),

$$\kappa\triangleright x_\alpha^k=\kappa_{(1)}x_\alpha^kS(\kappa_{(2)})=\kappa x_\alpha^k\kappa^{-1}=q^kx_\alpha^k. \tag{26}$$

By construction, the L-matrix is a comultiplicative quantum matrix, $\Delta(L^\mu{}_\nu)=L^\mu{}_\sigma\otimes L^\sigma{}_\nu$. So we get for the action of L on a power

$$L^\mu{}_\nu\triangleright x_\alpha^k=(L^\mu{}_{\sigma_1}\triangleright x_\alpha)(L^{\sigma_1}{}_{\sigma_2}\triangleright x_\alpha)\cdots(L^{\sigma_{k-1}}{}_\nu\triangleright x_\alpha). \tag{27}$$

Since each $L^{\sigma_k}{}_{\sigma_{k+1}}\triangleright x_\alpha$ are $\mathcal{X}$-valued 4×4-matrices, the right-hand side is the matrix product of such matrices. This suggests to introduce an index-free notation.

Definition 2: Let $L^\mu{}_\nu$ be the L-matrix defined in Eq. (19), *∂^μ the partial derivatives defined in* (16), *$f\in\mathcal{X}$ an element of the algebra of quantum Minkowski space. Then we denote by L_f the $\mathcal{X}$-valued 4×4-matrix and by ∇f the $\mathcal{X}$-valued four-vector with entries*

$$(L_f)^\mu{}_\nu:=L^\mu{}_\nu\triangleright f\quad\textit{and}\quad(\nabla f)^\mu:=\partial^\mu\triangleright f, \tag{28}$$

respectively.

To illustrate this, we have, for example,

$$(L_f^2\nabla f)^\mu=(L^\mu{}_\nu\triangleright f)(L^\nu{}_\sigma\triangleright f)(\partial^\sigma\triangleright f). \tag{29}$$

In this index-free notation Eq. (27) is written as $L\triangleright x_\alpha^k=L_{x_\alpha}^k$, such that Eq. (25) becomes

$$\nabla x_\alpha^n=\sum_{k=0}^{n-1}q^kL_{x_\alpha}^k(\nabla x_\alpha)x_\alpha^{n-k-1}. \tag{30}$$

We recall that by definition (17) of the action of partial derivatives on the generators we have for the components of the gradient

$$(\nabla x_\alpha)^\mu=\partial^\mu\triangleright x_\alpha=\delta_\alpha^\mu, \tag{31}$$

where $\mu,\alpha\in\{0,-,+,3\}$.

The computationally difficult part of (30) is the evaluation of powers of the algebra-valued matrices L_{x_α}. For example, for $(L_{x_0})^\mu{}_\nu$ we get with respect to four-vector indices $\mu,\nu\in\{0,-,+,3\}$,

$$L_{x_0} = \frac{1}{[2]} \begin{pmatrix} \frac{[4]}{[2]} x_0 & q\lambda x_- & q\lambda x_+ & q\lambda x_3 \\ -\frac{\lambda}{q^2} x_+ & \frac{[4]}{[2]} x_0 - \frac{\lambda^2}{q} x_3 & 0 & \lambda x_+ \\ \lambda x_- & 0 & \frac{[4]}{[2]} x_0 - q\lambda^2 x_3 & -\lambda x_- \\ \frac{\lambda}{q} x_3 & -q\lambda x_- & \frac{\lambda}{q} x_+ & \frac{[4]}{[2]} x_0 - \lambda^2 x_3 \end{pmatrix}. \tag{32}$$

A brute force calculation of the powers $L_{x_0}^n$ of this algebra valued matrix is not feasible as it would require a reordering of an exponentially increasing number of terms to the Poincaré-Birkhoff-Witt basis (or any other ordering). Similar matrices and their eigenvalues have been studied elsewhere[34,35] but it can be seen that L_0 is not of the exact type considered there so the results do not carry over easily.

B. Block decomposition of *L*-matrices

The computational problem of computing the powers of the $\mathcal{X}$-valued L_{x_α}-matrices can be simplified by considering the L-matrix (19) not with respect to four-vector indices running through $\{0, -, +, 3\}$ as in Eq. (32), but with respect to pairs of indices of the two spin-$\frac{1}{2}$ representations of the chiral decomposition $\mathcal{U}_q(\mathrm{sl}_2(\mathbb{C})) = \mathcal{U}_q(\mathrm{su}_2) \otimes \mathcal{U}_q(\mathrm{su}_2)$ of the q-Lorentz algebra, each labelled by the weights $\{-\frac{1}{2}, +\frac{1}{2}\} = \{-, +\}$. We recall that the generators of quantum Minkowski space in this $(\frac{1}{2}, \frac{1}{2})$-spinor basis labelled by indices $\{--, -+, +-, ++\}$ are related to those in the four-vector basis by

$$\begin{aligned} x_{--} &= [2]^{1/2} x_-, \\ x_{-+} &= q^{1/2}(x_3 - x_0), \\ x_{+-} &= q^{-1/2} x_3 + q^{3/2} x_0, \\ x_{++} &= [2]^{1/2} x_+. \end{aligned} \tag{33}$$

Using formula (12) for the universal $\mathcal{R}_{\mathrm{II}}$-matrix in terms of the $\mathcal{R}$-matrix of $\mathcal{U}_q(\mathrm{su}_2)$ and definition (19) of the L-matrix, we calculate the L-matrix with respect to the spinor basis,

$$(L)^{ij}{}_{kl} = (\mathrm{id} \otimes \mathrm{id} \otimes \rho^{1/2} \otimes \rho^{1/2})(\mathcal{R}_{\mathrm{II}})^{ij}{}_{kl} = (L_-^{1/2})^j{}_{j'} (L_+^{1/2})^i{}_{i'} \otimes (L_+^{1/2})^{j'}{}_l (L_+^{1/2})^{i'}{}_k = B^j{}_l (L_+^{1/2})^i{}_k, \tag{34}$$

where all indices run through $\{-\frac{1}{2}, +\frac{1}{2}\} = \{-, +\}$. Here $B = (B^j{}_l)$ is the matrix of "boosts" which generate the $\mathrm{SU}_q(2)^{\mathrm{op}}$ Hopf subalgebra of the Drinfeld double form of the q-Lorentz algebra,[33] and $L_+^{1/2}$ the L_+-matrix[27] of the $\mathcal{U}_q(\mathrm{su}_2)$ subalgebra of rotations,

$$B = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad L_+^{1/2} = \begin{pmatrix} K^{-1/2} & q^{-1/2}\lambda K^{-1/2} E \\ 0 & K^{1/2} \end{pmatrix}, \tag{35}$$

with respect to the $\{-, +\}$ basis. The explicit form of the boosts in the chiral decomposition of the q-Lorentz algebra is given in Eq. (A7).

The decomposition (34) of the L-matrix into boosts and rotations yields a natural block matrix decomposition of the $\mathcal{X}$-valued 4×4-matrices L_{x_α} as defined in Eq. (28). For the four-vector index α it turns out to be convenient to use instead of x_3 the light cone coordinate

$$x_{3\backslash 0} := x_3 - x_0, \tag{36}$$

which is essentially the x_{-+}-coordinate in the spinor basis (33) of quantum Minkowski space. And for the block decomposition it is convenient to define $\mathcal{X}$-valued 2×2-matrices by the action of the boosts

$$(B_f)^i{}_j := B^i{}_j \triangleright f, \quad f \in \mathcal{X}, \tag{37}$$

using the same index-free notation as introduced in Eq. (28). Since $B^i{}_j$ is a comultiplicative quantum matrix, $\Delta(B^i{}_j) = B^i{}_k \otimes B^k{}_j$, the matrices B_{x_α} satisfy the same commutation relations (5) as x_α. Explicitly, the B_{x_α}-matrices can be computed to

$$B_{x_0} = \begin{pmatrix} \dfrac{[4]}{[2]^2}x_0 + \dfrac{\lambda}{q[2]}x_3 & q^{-1/2}\lambda[2]^{-1/2}x_+ \\ -q^{1/2}\lambda[2]^{-1/2}x_- & \dfrac{[4]}{[2]^2}x_0 - \dfrac{q\lambda}{[2]}x_3 \end{pmatrix},$$

$$B_{x_-} = \begin{pmatrix} x_- & q^{-1/2}\lambda[2]^{-1/2}x_{3\backslash 0} \\ 0 & x_- \end{pmatrix},$$

$$B_{x_+} = \begin{pmatrix} x_+ & 0 \\ -q^{1/2}\lambda[2]^{-1/2}x_{3\backslash 0} & x_+ \end{pmatrix}, \tag{38}$$

$$B_{x_{3\backslash 0}} = \begin{pmatrix} q^{-1}x_{3\backslash 0} & 0 \\ 0 & qx_{3\backslash 0} \end{pmatrix},$$

with respect to spin-$\frac{1}{2}$ indices running through $\{-, +\}$. In terms of these matrices the L_{x_α}-matrices can be expressed as

$$L_{x_0} = \begin{pmatrix} B_{x_0} & 0 \\ 0 & B_{x_0} \end{pmatrix},$$

$$L_{x_-} = \begin{pmatrix} qB_{x_-} & q^{-1/2}\lambda[2]^{1/2}B_{x_3} \\ 0 & q^{-1}B_{x_-} \end{pmatrix},$$

$$L_{x_+} = \begin{pmatrix} q^{-1}B_{x_+} & 0 \\ 0 & qB_{x_+} \end{pmatrix}, \tag{39}$$

$$L_{x_{3\backslash 0}} = \begin{pmatrix} B_{x_{3\backslash 0}} & q^{-1/2}\lambda[2]^{1/2}B_{x_+} \\ 0 & B_{x_{3\backslash 0}} \end{pmatrix},$$

with respect to the index structure $(--, -+, +-, ++)$.

C. Calculating powers of *L*-matrices

In the form of Eq. (39) the L_{x_α} matrices are upper block triangular. This makes the computation of their powers a lot easier. L_{x_0} and L_{x_+} are even block diagonal, so we immediately get

$$L^n_{x_0} = \begin{pmatrix} B^n_{x_0} & 0 \\ 0 & B^n_{x_0} \end{pmatrix}, \quad L^n_{x_+} = \begin{pmatrix} q^{-n}B^n_{x_+} & 0 \\ 0 & q^n B^n_{x_+} \end{pmatrix}. \tag{40}$$

For the calculation of $L^n_{x_-}$ and $L^n_{x_{3\backslash 0}}$ we must use the commutation relations (5) for the B_{x_α} matrices. We thus get by induction

$$\begin{aligned} L^n_{x_-} &= \begin{pmatrix} q^n B^n_{x_-} & q^{-1/2}\lambda[2]^{1/2}\left(q^{n-1}\dfrac{[2n]}{[2]}B_{x_{3\backslash 0}} + [n]B_{x_0}\right)B^{n-1}_{x_-} \\ 0 & q^{-n}B^n_{x_-} \end{pmatrix}, \\ L^n_{x_{3\backslash 0}} &= \begin{pmatrix} B^n_{x_{3\backslash 0}} & q^{-1/2}\lambda[2]^{1/2}q^{n-1}[n]B_{x_+}B^{n-1}_{x_{3\backslash 0}} \\ 0 & B^n_{x_{3\backslash 0}} \end{pmatrix}. \end{aligned} \tag{41}$$

Now we have expressed the powers of L_{x_α} matrices in terms of powers of the B_{x_α} matrices. It remains to calculate the powers of the B_{x_α}-matrices. Since $B_{x_{3\backslash 0}}$ is diagonal we immediately get

$$B^n_{x_{3\backslash 0}} = \begin{pmatrix} q^{-n}x^n_{3\backslash 0} & 0 \\ 0 & q^n x^n_{3\backslash 0} \end{pmatrix}. \tag{42}$$

For the powers of the matrices $B_{x_\pm}$, which are block triangular, we use again the commutation relations (5) to obtain by induction

$$\begin{aligned} B^n_{x_-} &= \begin{pmatrix} x^n_- & q^{-1/2}\lambda[2]^{-1/2}q^{n-1}[n]x_{3\backslash 0}x^{n-1}_- \\ 0 & x^n_- \end{pmatrix}, \\ B^n_{x_+} &= \begin{pmatrix} x^n_+ & 0 \\ -q^{1/2}\lambda[2]^{-1/2}q^{1-n}[n]x_{3\backslash 0}x^{n-1}_+ & x^n_+ \end{pmatrix}. \end{aligned} \tag{43}$$

The calculation of the powers of B_{x_0} is more difficult because it is not triangular. Using q-Pauli matrices (A5), B_{x_0} of Eqs. (38) can be written more compactly as

$$B_{x_0} := \frac{[4]}{[2]^2}x_0 - \frac{\lambda}{[2]}\tilde{\sigma}_A x^A, \tag{44}$$

where the index A is summed over $\{-, 3, +\}$. The q-Pauli matrices satisfy the relation

$$\tilde{\sigma}_A\tilde{\sigma}_B = g_{BA} - \tilde{\sigma}_C\varepsilon_B{}^C{}_A, \tag{45}$$

where the quantum metric and epsilon tensor are defined by quantum Clebsch-Gordon coefficients as

$$\begin{aligned} g^{AB} &:= -\sqrt{[3]}C_q(1,1,0;A,B,0), \\ \varepsilon^{AB}{}_C &:= -\sqrt{\frac{[4]}{[2]}}C_q(1,1,1;A,B,C). \end{aligned} \tag{46}$$

Contracting Eq. (45) with $x^A x^B$ and using the commutation relations (5) of the coordinates, which can be written as $x_A x_B \varepsilon^{AB}{}_C = -\lambda x_C x_0$, we derive

$$\tilde{\sigma}_A\tilde{\sigma}_B x^A x^B = (g_{BA} - \tilde{\sigma}_C\varepsilon_B{}^C{}_A)x^A x^B = x_A x^A + \lambda x_0\tilde{\sigma}_A x^A. \tag{47}$$

This can be used to compute the square of Eq. (44),

$$B_{x_0}^2 = \frac{[4]^2}{[2]^2}(x_0)^2 - 2\frac{\lambda[4]}{[2]^3}x_0\tilde{\sigma}_A x^A + \frac{\lambda^2}{[2]^2}\tilde{\sigma}_A\tilde{\sigma}_B x^A x^B$$
$$= \frac{[4]^2}{[2]^4}(x_0)^2 - 2\frac{\lambda[4]}{[2]^3}x_0\tilde{\sigma}_A x^A + \frac{\lambda^2}{[2]^2}(x_A x^A + \lambda x_0\tilde{\sigma}_A x^A) = [2]x_0 B_{x_0} - (x_0)^2 - \frac{\lambda^2}{[2]^2}x^2. \quad (48)$$

Together with Eq. (40) we conclude that L_{x_0} satisfies the polynomial equation

$$0 = L_{x_0}^2 - [2]x_0 L_{x_0} + \left((x_0)^2 + \frac{\lambda^2}{[2]^2}x^2\right) = L_{x_0}^2 - 2bL_{x_0} + c, \quad (49)$$

where we have introduced the abbreviations

$$b := \frac{[2]}{2}x_0, \quad c := (x_0)^2 + \frac{\lambda^2}{[2]^2}x^2, \quad (50)$$

which are both in the center of $\mathcal{X}$. Equation (49) enables us to derive formulas for arbitrary powers of L_{x_0}. This is most elegantly done by considering the generating function of the powers $(1 - L_{x_0}z)^{-1} = 1 + L_{x_0}z + L_{x_0}^2 z^2 + \dots$, where z is a formal parameter. First we rewrite (49) as

$$(1 - L_{x_0}^2 z^2) - 2bz(1 - L_{x_0}z) - (1 - 2bz + cz^2) = 0 \quad (51)$$

and divide it by $(1 - L_{x_0}z)$ and $(1 - 2bz + cz^2)$, yielding

$$\frac{1}{1 - L_{x_0}z} = \frac{1 + (L_{x_0} - 2b)z}{1 - 2bz + cz^2}. \quad (52)$$

The right-hand side can be expanded in powers of z, observing that it contains the generating function for Chebyshev polynomials of the second kind,

$$\frac{1}{1 - 2yt + t^2} = \sum_{n=0}^{\infty} U_n(y)t^n, \quad (53)$$

where we must set $y = b/\sqrt{c}$ and $t = \sqrt{c}z$. We thus obtain

$$L_{x_0}^n = U_n(b/\sqrt{c})c^{n/2} + U_{n-1}(b/\sqrt{c})c^{(n-1)/2}(L_{x_0} - 2b) = -U_{n-2}(b/\sqrt{c})c^{n/2} + U_{n-1}(b/\sqrt{c})c^{(n-1)/2}L_{x_0} \quad (54)$$

for $n \geqslant 2$. The fact that $U_n(y)$ is a polynomial of degree n which contains either only even or only odd powers of y implies that $U_n(1/y)y^n$ is a quadratic polynomial in y. Therefore, the right-hand side of Eq. (54) contains only even positive powers of $\sqrt{c}$, that is, does not contain inverses or square roots of c and, hence, yields well-defined elements of the algebra $\mathcal{X}$. Together with Eqs. (40)–(43) this completes our calculation of powers of the L_{x_α} matrices.

D. Calculating derivatives

1. Choice of basis and partial Jackson derivatives

With the formulas for the powers of the L_α matrices the derivatives of arbitrary elements $f \in \mathcal{X}$ could be computed by calculating the derivatives of the Poincaré-Birkhoff-Witt basis of $\mathcal{X}$. However, it turns out to be more convenient to work in a slightly different basis. Observe that from definition (7) of the q-Lorentz invariant length and the commutation relations (5) we can deduce the relation

$$[2]x_-x_+ = x^2 + q^2(x_{3\backslash 0})^2 + q\lambda x_0 x_{3\backslash 0}. \tag{55}$$

Using this relation, all products of equal powers of x_- and x_+ in the Poincaré-Birkhoff-Witt basis can be substituted by powers of x^2. We thus obtain a basis of ordered monomials which contains powers of x^2 and either powers of x_- or x_+. To be more precise, we have a basis of $\mathcal{X}$,

$$\mathcal{B} = \mathcal{B}_- \cup \mathcal{B}_+, \tag{56}$$

where

$$\begin{aligned} \mathcal{B}_- &:= \{(x_\mu x^\mu)^i (x_0)^j (x_{3\backslash 0})^k (x_-)^l | i,j,k,l \in \mathbb{N}_0\}, \\ \mathcal{B}_+ &:= \{(x_\mu x^\mu)^i (x_0)^j (x_+)^l (x_{3\backslash 0})^k | i,j,k,l \in \mathbb{N}_0\}. \end{aligned} \tag{57}$$

Note, that $\mathcal{B}_-$ and $\mathcal{B}_+$ have a nonempty intersection, the monomials for which $l=0$. But this will not be a problem here. Let us introduce a more suggestive notation for sums of monomials in a particular order.

Definition 3: Let $x_1, \ldots, x_n \in \mathcal{X}$ be *elements of the algebra of quantum Minkowski space. Then we will denote by* $f(x_1, \ldots, x_n)$ *linear combinations of ordered products of monomials in* $x_1, \ldots, x_n \in \mathcal{X}$. *That is*,

$$f(x_1, \ldots, x_n) \in \mathrm{Span}\{(x_1)^{k_1} \cdots (x_n)^{k_n} | k_1, \ldots, k_n \in \mathbb{N}_0\}. \tag{58}$$

With this notation the statement that $\mathcal{B}_- \cup \mathcal{B}_+$ is a basis of quantum Minkowski space can be written as

$$f(x_0, x_+, x_{3\backslash 0}, x_-) = f_-(x^2, x_0, x_{3\backslash 0}, x_-) + f_+(x^2, x_0, x_+, x_{3\backslash 0}), \tag{59}$$

decomposing an arbitrary element of $\mathcal{X}$ into two parts containing powers in either x_- or x_+.

It is important to have a notation which keeps track of the ordering of generators because the formulas for derivatives are most elegantly expressed in terms of partial Jackson derivatives which depend on the ordering. Recall, that the Jackson derivative or q-derivative of a function $f = f(x_\alpha)$ in a single variable x_α is defined as difference quotient,

$$\frac{\partial_{q^2} f}{\partial_{q^2} x_\alpha} := \frac{f(q^2 x_\alpha) - f(x_\alpha)}{q^2 x_\alpha - x_\alpha}. \tag{60}$$

For monomials $f(x_\alpha) = (x_\alpha)^k$, this yields

$$\frac{\partial_{q^2} (x_\alpha)^k}{\partial_{q^2} x_\alpha} = (k)_{q^2} (x_\alpha)^{k-1}, \tag{61}$$

where $(k)_{q^2}$ is the usual q-number defined in Eq. (4). This formula naturally generalizes to a partial Jackson derivative on monomials of several noncommutative variables.

Definition 4: Let $x_1, \ldots, x_n \in \mathcal{X}$ *be elements of the algebra of quantum Minkowski space (or any other algebra). We define the partial Jackson derivative with respect to one of these elements* x_α *on ordered monomials by*

$$\frac{\partial_{q^2}}{\partial_{q^2} x_\alpha} ((x_1)^{k_1} \cdots (x_n)^{k_n}) := (k_\alpha)_{q^2} (x_1)^{k_1} \cdots (x_\alpha)^{k_\alpha - 1} \cdots (x_n)^{k_n}, \tag{62}$$

and extend it linearly to arbitrary linear combinations of such monomials. This defines partial Jackson derivatives on general functions $f = f(x_1, \ldots, x_n)$ *in the sense of Definition 3*.

It must be emphasized that the partial Jackson derivatives depend on the particular order and are not well defined on the algebra. For example, within the algebra we have the commutation relation $x_{3\backslash 0} x_+ - q^2 x_+ x_{3\backslash 0} = 0$, but

$$\frac{\partial_{q^2}}{\partial_{q^2}x_+}(x_{3\backslash 0}x_+ - q^2 x_+ x_{3\backslash 0}) = x_{3\backslash 0} - q^2 x_{3\backslash 0} \neq 0. \tag{63}$$

This is why we have defined the notation $f=f(x_+,x_{3\backslash 0})$ to not just denote elements of the algebra but to denote in addition a specific ordering of the variables. With this notation the action of partial Jackson derivatives is defined unambiguously.

We break up the calculation of derivatives in two steps. First, we calculate the derivatives of noncentral variables, x_-, $x_{3\backslash 0}$, x_+. Working within the basis $\mathcal{B}$ we can limit the considerations in this first step to polynomial functions $f=f(x_{3\backslash 0},x_-)$ and $f=f(x_+,x_{3\backslash 0})$ which depend either on x_- or on x_+. This calculation is rather straightforward. In a second step we consider polynomial functions $f=f(x^2,x_0)$ of the center of $\mathcal{X}$. This calculation is much more involved.

2. Functions of noncentral coordinates

We begin the calculation of the derivatives of the basis $\mathcal{B}$ by reading off Eqs. (38) and (39) that the L_α matrices possess some algebra valued eigenvalues,

$$\begin{aligned} L_{x_A} \nabla x_A &= q x_A \nabla x_A, \\ L_{x_{3\backslash 0}} \nabla x_- &= q^{-1} x_{3\backslash 0} \nabla x_-, \\ L_{x_+} \nabla x_{3\backslash 0} &= q^{-1} x_+ \nabla x_{3\backslash 0}, \end{aligned} \tag{64}$$

for $A \in \{-,+,3\backslash 0\}$ (no summation over A). We recall that ∇x_α is the index free notation for $(\nabla x_\alpha)^\mu = \partial^\mu \triangleright x_\alpha = \delta^\mu_\alpha$.

Inserting the first of these eigenvalue equations into Eq. (30) we obtain for powers of the generators

$$\nabla x_A^n = \sum_{k=0}^{n} q^{2k} x_A^k (\nabla x_A) x_A^{n-k-1} = (n)_{q^2} x_A^{n-1} \nabla x_A, \tag{65}$$

for $A \in \{-,+,3\backslash 0\}$, where $(n)_{q^2}$ denotes the quantum number (4). From Eq. (65) we can deduce that the derivative of any polynomial $f=f(x_A)$ in a single one of the generators x_A can be expressed in terms of the Jackson derivative by

$$\nabla f(x_A) = \frac{\partial_{q^2} f}{\partial_{q^2} x_A} \nabla x_A \Leftrightarrow \partial^\mu \triangleright f(x_A) = \frac{\partial_{q^2} f}{\partial_{q^2} x_A} \delta^\mu_A. \tag{66}$$

Using the second of Eqs. (64) we get

$$\nabla(x_{3\backslash 0}^k x_-^n) = (\nabla x_{3\backslash 0}^k) x_-^n + q^k L_{3\backslash 0}^k (\nabla x_-^n) = (k)_{q^2} x_{3\backslash 0}^{k-1} x_-^n \nabla x_{3\backslash 0} + x_{3\backslash 0}^k (n)_{q^2} x_-^{n-1} \nabla x_-, \tag{67}$$

and analogously for the derivative of $x_+^k x_{3\backslash 0}^n$,

$$\nabla(x_+^k x_{3\backslash 0}^n) = (k)_{q^2} x_+^{k-1} x_{3\backslash 0}^n \nabla x_+ + x_+^k (n)_{q^2} x_{3\backslash 0}^{n-1} \nabla x_{3\backslash 0}. \tag{68}$$

From Eqs. (67) and (68) we can deduce the following result.

Proposition 1: Let $f=f(x_{3\backslash 0},x_-)$ and $f=f(x_+,x_{3\backslash 0})$ be ordered polynomials in the notation of Definition 3. Then their partial derivatives are expressed in terms of partial Jackson derivatives as

$$\nabla f(x_{3\backslash 0},x_-) = \frac{\partial_{q^2} f}{\partial_{q^2} x_{3\backslash 0}} \nabla x_{3\backslash 0} + \frac{\partial_{q^2} f}{\partial_{q^2} x_-} \nabla x_-, \tag{69a}$$

$$\nabla f(x_+, x_{3\backslash 0}) = \frac{\partial_{q^2} f}{\partial_{q^2} x_+} \nabla x_+ + \frac{\partial_{q^2} f}{\partial_{q^2} x_{3\backslash 0}} \nabla x_{3\backslash 0}. \tag{69b}$$

3. Functions of four-length

Next, we calculate the derivative of powers of the coordinate four-square x^2. Since x^2 is a Lorentz scalar the L-matrix acts with the counit ε,

$$L^\mu{}_\nu \triangleright x^2 = \varepsilon(L^\mu{}_\nu) x^2 = \delta^\mu_\nu x^2. \tag{70}$$

By the same reasoning which led to Eq. (30) we obtain for powers of the four-square

$$\nabla (x^2)^n = \sum_{k=0}^{n-1} q^{2k} (x^2)^{n-1} \nabla x^2 = (n)_{q^2} (x^2)^{n-1} \nabla x^2. \tag{71}$$

Again, for a general function $f = f(x^2)$ this can be written in terms of a Jackson derivative by

$$\nabla f(x^2) = \frac{\partial_{q^2} f}{\partial_{q^2}(x^2)} \nabla x^2. \tag{72}$$

It remains to compute the derivative of x^2, which for representation theoretic reasons we expect to be proportional to the coordinate four vector x^μ. After straightforward calculations we, indeed, find

$$(\nabla x^2)^\mu = q^{-1}[2] x^\mu. \tag{73}$$

4. Functions of time

Like the calculation of powers of L_{x_0}, the calculation of derivatives of powers of the time coordinate is more difficult. In order to calculate the derivative of $(x_0)^n$ we first observe that, since x_0 is central in the space algebra we can write Eq. (30) in the form

$$\nabla x_0^n = \frac{(qL_{x_0})^n - (x_0)^n}{qL_{x_0} - x_0} \nabla x_0, \tag{74}$$

which is similar to a q-difference quotient. We can get rid of the matrix in the denominator,

$$\frac{(qL_{x_0})^n - (x_0)^n}{qL_{x_0} - x_0} = \frac{(q^n L_{x_0}^n - x_0^n)(q^{-1} L_{x_0} - x_0)}{(qL_{x_0} - x_0)(q^{-1} L_{x_0} - x_0)} = -\frac{[2](q^{n-1} L_{x_0}^{n+1} - q^n L_{x_0}^n x_0 - q^{-1} L_{x_0} x_0^n - x_0^{n+1})}{\lambda^2 x^2}, \tag{75}$$

where in the second step we have used Eq. (49). The powers of L_{x_0} in the numerator have been calculated in Eq. (54). From explicit expression (32) of L_{x_0} we deduce

$$(L_{x_0} \nabla x_0)^\mu = q x_0 \delta_0^\mu - \frac{\lambda}{q[2]} x^\mu. \tag{76}$$

Putting things together we obtain

$$(\nabla x_0^n)^\mu = \frac{[2]}{\lambda} \left(\frac{U_n c^{n/2} q^{n-2} - U_{n-1} c^{(n-1)/2} q^{n-1} x_0 - x_0^n}{x^2} \right) x^\mu + U_{n-1} c^{(n-1)/2} q^{n-1} \delta_0^\mu, \tag{77}$$

where $U_n = U_n(b/\sqrt{c})$ denotes the Chebyshev polynomials of the second kind with the same argument as in Eq. (54).

In order to generalize the formulas to general functions $f = f(x_0)$ we first note that we can deduce from Eq. (74),

$$\nabla f(x_0) = \frac{f(qL_{x_0}) - f(x_0)}{qL_{x_0} - x_0} \nabla x_0, \tag{78}$$

which could be viewed as matrix valued generalization of the Jackson derivative. In order to compute this expression we need to generalize formula (54) for the powers of L_{x_0} to general functions. The result is given by the following.

Proposition 2: Let L_{x_0} be the $\mathcal{X}$-valued 4×4-matrix given by Eq. (32). Let b and c be defined as in Eq. (50). *Define*

$$\tau_\pm := b \pm \sqrt{b^2 - c} = \frac{1}{2}\left([2]x_0 \pm \lambda \sqrt{(x_0)^2 - \frac{4}{[2]^2}(x^2)}\right), \tag{79}$$

and

$$\Pi_\pm := \frac{1}{2}\left(1 \pm \frac{L_{x_0} - b}{\sqrt{b^2 - c}}\right). \tag{80}$$

Then for any polynomial function f in one variable we have

$$f(L_{x_0}) = f(\tau_+)\Pi_+ + f(\tau_-)\Pi_-. \tag{81}$$

Proof: First, we note that Chebyshev polynomials of the second kind can be written as

$$U_{n-1}(x) = \frac{(x + \sqrt{x^2 - 1})^n - (x - \sqrt{x^2 - 1})^n}{2\sqrt{x^2 - 1}}. \tag{82}$$

For $x = b/\sqrt{c}$ this identity takes the form

$$U_{n-1}(b/\sqrt{c})c^{(n-1)/2} = \frac{\tau_+^n - \tau_-^n}{\tau_+ - \tau_-}, \tag{83}$$

with $\tau_\pm$ defined as in the proposition. Inserting (83) into (54) yields for an arbitrary function

$$f(L_{x_0}) = \frac{f(\tau_+) - f(\tau_-)}{\tau_+ - \tau_-}(L_{x_0} - b) + \frac{1}{2}(f(\tau_+) + f(\tau_-)), \tag{84}$$

which can be written using $\Pi_\pm$ in the form of Eq. (81). □

The $\mathcal{X}$-valued matrices $\Pi_\pm$ arise here naturally because they are orthogonal, complementary idempotents,

$$\Pi_\pm^2 = \Pi_\pm, \quad \Pi_+\Pi_- = 0 = \Pi_-\Pi_+, \quad \Pi_+ + \Pi_- = 1. \tag{85}$$

This property ensures that Eq. (81) is consistent with the algebra structure of functions, because it can be immediately verified that $(fg)(L_{x_0}) = f(L_{x_0})g(L_{x_0})$.

We can now insert Eq. (84) into Eq. (78) to obtain

$$\nabla f(x_0) = \frac{f(q\tau_+) - f(x_0)}{q\tau_+ - x_0}\Pi_+ \nabla x_0 + \frac{f(q\tau_-) - f(x_0)}{q\tau_- - x_0}\Pi_- \nabla x_0 \tag{86}$$

for the derivative of an arbitrary function of the time coordinate. For this formula to be explicit it remains to calculate

$$(\Pi_\pm \nabla x_0)^\mu = \frac{\frac{1}{2}\left(\pm x_0 + \sqrt{(x_0)^2 - \frac{4}{[2]^2}(x^2)}\right)\delta_0^\mu \mp \frac{1}{q[2]}x^\mu}{\sqrt{(x_0)^2 - \frac{4}{[2]^2}(x^2)}}. \tag{87}$$

Finally, we can combine the previous result (72) for the derivative of functions of the four-length $x^2 = x_\mu x^\mu$ and (86) for the derivative of functions of the time coordinate x_0 into a formula for functions $f = f(x^2, x_0)$ of both variables,

$$\begin{aligned}\nabla f(x^2,x_0) = {} & \frac{f(q^2x^2,x_0) - f(x^2,x_0)}{q^2x^2 - x^2}\nabla x^2 + \frac{f(q^2x^2,q\tau_+) - f(q^2x^2,x_0)}{q\tau_+ - x_0}\Pi_+ \nabla x_0 \\ & + \frac{f(q^2x^2,q\tau_-) - f(q^2x^2,x_0)}{q\tau_- - x_0}\Pi_- \nabla x_0.\end{aligned} \tag{88}$$

This formula can be further simplified to

$$\nabla f(x^2,x_0) = \frac{f(q^2x^2,q\tau_+) - f(x^2,x_0)}{q\tau_+ - x_0}\Pi_+ \nabla x_0 + \frac{f(q^2x^2,q\tau_-) - f(x^2,x_0)}{q\tau_- - x_0}\Pi_- \nabla x_0. \tag{89}$$

5. Separation of variables

We have seen that the derivatives of functions of $x_\pm$, $x_{3\backslash 0}$, and x^2 can be written in terms of Jackson q-derivatives. Derivatives of functions of the time coordinate, however, do not have this property but depend on the four-length x^2, as well. In the language of partial differential equations, the partial derivative ∂^μ is not separated with respect to the standard time coordinate of quantum Minkowski space. We will now show that there is a nonlinear transformation of coordinates such that the partial derivatives are separated in the new coordinates.

These new coordinates $\xi_\pm = \xi_\pm(x^2, x_0)$ are given by

$$\xi_\pm = \frac{1}{2}\left(x_0 \pm \sqrt{(x_0)^2 - \frac{4}{[2]^2}(x^2)}\right). \tag{90}$$

In terms of the new variables $\tau_\pm$ is expressed as

$$\begin{aligned}\tau_+ &= q\xi_+ + q^{-1}\xi_-, \\ \tau_- &= q^{-1}\xi_+ + q\xi_-.\end{aligned} \tag{91}$$

The back transform is given by

$$\begin{aligned}x_0 &= \xi_+ + \xi_-, \\ x^2 &= [2]^2\xi_+\xi_-.\end{aligned} \tag{92}$$

A function $f = f(x^2, x_0)$ is expressed in terms of the new variables by the transformed function

$$\tilde{f}(\xi_+,\xi_-) := f(x^2(\xi_+,\xi_-), x_0(\xi_+,\xi_-)) = f([2]^2\xi_+\xi_-, \xi_+ + \xi_-), \tag{93}$$

for which the quotients of Eq. (89) take the form of Jackson derivatives

$$\frac{f(q^2x^2,q\tau_+)-f(x^2,x_0)}{q\tau_+-x_0}=\frac{\tilde{f}(q^2\xi_+,\xi_-)-\tilde{f}(\xi_+,\xi_-)}{q^2\xi_+-\xi_+},$$
$$\frac{f(q^2x^2,q\tau_+)-f(x^2,x_0)}{q\tau_+-x_0}=\frac{\tilde{f}(\xi_+,q^2\xi_-)-\tilde{f}(\xi_+,\xi_-)}{q^2\xi_--\xi_-}. \tag{94}$$

In order to completely rewrite Eq. (89) in q-derivative form we still must rewrite the expressions $\Pi_\pm\nabla x_0$. Towards this end, we must understand on what the projection operators $\Pi_\pm$ actually project.

Key to understanding the operators $\Pi_\pm$ is the calculation of the derivatives of the new coordinates viewed as functions of x^2 and x_0. Inserting these functions $\xi_\pm=\xi_\pm(x^2,x_0)$ into formula (89) and using the formula

$$\sqrt{\tau_\pm^2-\frac{4}{[2]^2}(x^2)}=\frac{1}{2}\left(\pm\lambda x_0+[2]\sqrt{(x_0)^2-\frac{4}{[2]^2}(x^2)}\right), \tag{95}$$

we obtain after long calculations the compact result

$$\nabla\xi_\pm=\Pi_\pm\nabla x_0. \tag{96}$$

In this sense $\Pi_\pm$ can be viewed as generalized Jacobian of the coordinate transformation (90). We thus arrive at the main result of this paper:

Proposition 3: Let $f=f(\xi_+,\xi_-)$ be a general polynomial function in $\xi_\pm$. Then

$$\nabla f(\xi_+,\xi_-)=\frac{\partial_{q^2}f}{\partial_{q^2}\xi_+}\nabla\xi_++\frac{\partial_{q^2}f}{\partial_{q^2}\xi_-}\nabla\xi_-. \tag{97}$$

6. General functions

Finally, we can combine this result with formulas (69) for derivations of functions of the noncentral variables. A general polynomial in $\mathcal{X}$ can be written as a sum of products of functions $g=f(\xi_+,\xi_-)$ and $h=h_+(x_+,x_{3\backslash 0})+h(x_{3\backslash 0},x_-)$. Using the coproduct (18) we obtain for the derivative of the product

$$\nabla(fg)=(\nabla f)g+(\kappa L\triangleright f)\nabla g, \tag{98}$$

where we can derive from Proposition 2 the formula

$$\kappa L\triangleright g(\xi_+,\xi_-)=\Pi_+g(q^2\xi_+,\xi_-)+\Pi_-g(\xi_+,q^2\xi_-). \tag{99}$$

Inserting Eq. (99) into (98) we must observe that $\Pi_\pm$ does not commute with the noncentral observables. In order to write down the end result, we first define for a general linear combination of the basis $\mathcal{B}$ the matrix valued object

$$\delta f:=\Pi_+(f|_{\xi_+\mapsto q^2\xi_+}-f)+\Pi_-(f|_{\xi_-\mapsto q^2\xi_-}-f). \tag{100}$$

This definition does not depend on the ordering because ξ_+ and ξ_- are both central. Putting things together we obtain for a general $f\in\mathrm{Span}\,\mathcal{B}$

$$\begin{aligned}\nabla f=&\frac{\partial_{q^2}f}{\partial_{q^2}\xi_+}\nabla\xi_++\frac{\partial_{q^2}f}{\partial_{q^2}\xi_-}\nabla\xi_-+\frac{\partial_{q^2}f}{\partial_{q^2}x_+}\nabla x_++\frac{\partial_{q^2}f}{\partial_{q^2}x_{3\backslash 0}}\nabla x_{3\backslash 0}+\frac{\partial_{q^2}f}{\partial_{q^2}x_-}\nabla x_-+\frac{\partial_{q^2}(\delta f)}{\partial_{q^2}x_+}\nabla x_+\\&+\frac{\partial_{q^2}(\delta f)}{\partial_{q^2}x_{3\backslash 0}}\nabla x_{3\backslash 0}+\frac{\partial_{q^2}(\delta f)}{\partial_{q^2}x_-}\nabla x_-.\end{aligned} \tag{101}$$

The first two lines look like a generalized chain rule with partial Jackson derivatives as outer

derivatives. The partial Jackson derivatives in the last line are to be understood not to act on the projections $\Pi_\pm$ contained in δf. By definition of δf the last line vanishes for $q \to 1$ and the first two lines reproduce the usual chain rule.

IV. SOLUTIONS OF QUANTUM WAVE EQUATIONS

In order to give an application of the separation of variables and the formulas for derivations, let us now come back to the initial problem of calculating solutions of the quantum Klein-Gordon equation (2). It can be shown that, just as in the commutative case, the space of solutions is generated as representation of the quantum algebra by a momentum eigenstate.[12] However, unlike in the commutative case, there is only a finite number of such momentum eigenstates. In the massless case it is the light cone state, defined by

$$p_0 \triangleright \psi = k\psi, \quad p_3 \triangleright \psi = k\psi, \quad p_\pm \triangleright \psi = 0, \tag{102}$$

where $k \in \mathbb{R}$ is related to helicity. In the massive case it is the rest state

$$p_0 \triangleright \psi = m\psi, \quad p_3 \triangleright \psi = 0, \quad p_\pm \triangleright \psi = 0, \tag{103}$$

where $m \in \mathbb{R}$ is the mass. The difficult part is to calculate these states within the noncommutative differential calculus as solutions of quantum differential equations. All other solutions of the quantum Klein-Gordon equation can then be obtained by quantum Lorentz transformations, which are well known and straightforward to calculate.

A. The massless case

Let us start with the massless case which turns out to be quite simple. As q-differential equation Eq. (102) reads

$$\partial^0 \triangleright \psi = ik\psi, \quad \partial^3 \triangleright \psi = -ik\psi, \quad \partial^\pm \triangleright \psi = 0, \tag{104}$$

where we have raised the indices with the q-Minkowski metric, e.g., $\partial^3 = -\partial_3$. Using the coordinate free notation and the lightcone coordinate $x_{3\backslash 0}$ to be a function of the light cone coordinate $x_{3\backslash 0} = x_3 - x_0$, we can write Eq. (104) as

$$\nabla\psi = -ik\psi \nabla x_{3\backslash 0}. \tag{105}$$

Since $x_{3\backslash 0}$ is one of the variables separating the noncommutative differential calculus, we can conclude that (105) can be solved by a function $\psi = \psi(x_{3\backslash 0})$ of $x_{3\backslash 0}$ alone. Using the formulas (69) for the derivatives we obtain

$$\nabla\psi(x_{3\backslash 0}) = \frac{\partial_{q^2}\psi}{\partial_{q^2} x_{3\backslash 0}} \nabla x_{3\backslash 0} = -ik\psi \nabla x_{3\backslash 0}, \tag{106}$$

which is equivalent to

$$\frac{\partial_{q^2}\psi}{\partial_{q^2} x_{3\backslash 0}} = -ik\psi(x_{3\backslash 0}). \tag{107}$$

This equation is solved by the well-known q-exponential function

$$\exp_q(z) \equiv e_q^z := \sum_{n=1}^{\infty} \frac{z^n}{(n)_{q^2}!}, \tag{108}$$

where the q-factorial is defined in the obvious way as

$$(n)_{q^2}! = (n)_{q^2}(n-1)_{q^2}\cdots(1)_{q^2}. \tag{109}$$

With the q-exponential the general solution of Eq. (107) and, hence, of Eq. (104) can be written as

$$\psi = Ce_q^{-ik(x_3-x_0)}, \tag{110}$$

where C is a normalization constant.

B. The massive case

Let us now turn to the massive case where the calculation of the rest state is more involved. As q-differential function the defining eigenvalue equation (103) reads

$$\partial^0 \triangleright \psi = im\psi, \quad \partial^A \triangleright \psi = 0, \tag{111}$$

where the index runs through $A=-,3,+$. In index free notation we can write this as

$$\nabla\psi = im\psi\nabla x_0. \tag{112}$$

Since the time coordinate x_0 is not one of the variables which separates the noncommutative differential calculus, we cannot conclude that Eq. (112) can be solved by a function in x_0 alone. Since the eigenvalue equation is invariant with respect to quantum rotations we can conclude, though, that ψ must be a function of the scalars with respect to quantum rotations x_0 and x^2. In order to solve Eq. (112) we must separate it with the separating coordinates ξ_- and ξ_+. Using Eq. (97) and $x_0=\xi_-+\xi_-$ we obtain

$$\nabla\psi(\xi_+,\xi_-) = \frac{\partial_{q^2}\psi}{\partial_{q^2}\xi_+}\nabla\xi_+ + \frac{\partial_{q^2}\psi}{\partial_{q^2}\xi_-}\nabla\xi_- = im(\psi\nabla\xi_+ + \psi\nabla\xi_-), \tag{113}$$

which can be rewritten as

$$\left(\frac{\partial_{q^2}\psi}{\partial_{q^2}\xi_+} - im\psi\right)\nabla\xi_+ + \left(\frac{\partial_{q^2}\psi}{\partial_{q^2}\xi_-} - im\psi\right)\nabla\xi_- = 0. \tag{114}$$

The differential equation is now separated so we can make the ansatz

$$\psi(\xi_+,\xi_-) = \psi_+(\xi_+)\psi_-(\xi_-), \tag{115}$$

which solves Eq. (114) if

$$\frac{\partial_{q^2}\psi_+}{\partial_{q^2}\xi_+} = im\psi_+, \quad \frac{\partial_{q^2}\psi_-}{\partial_{q^2}\xi_-} = im\psi_-. \tag{116}$$

We see that the separation of variables of the differential calculus by the new coordinates $\xi_\pm$ leads to a complete separation of the wave equation. Equations (116) are again solved by the q-exponential function (108). As end result we obtain

$$\psi = Ce_q^{im\xi_+}e_q^{im\xi_-} = Ce_q^{(im/2)[x_0+\sqrt{(x_0)^2-(4/[2]^2)(x^2)}]}e_q^{(im/2)[x_0-\sqrt{(x_0)^2-(4/[2]^2)(x^2)}]}, \tag{117}$$

where C is a normalization constant. This rest state is a solution of the massive quantum Klein-Gordon equation (2). All other solutions can be obtained from this one by quantum Lorentz transformations.[36]

V. CONCLUSION

The separation of variables (97) by a nonlinear coordinate transformation (90) seems to be the most intriguing result presented in this paper. We do not yet understand on a fundamental level

what property of quantum Minkowski space is responsible for the existence of such a transformation. Nor do we know if and how this can be generalized to other quantum spaces.

In definition (90) of the separating variables a square root expression appears which, strictly speaking, is not an element of the algebra of Minkowski space proper. In order to make all statements completely rigorous we have to enlarge $\mathcal{X}$ by a central square root element α satisfying

$$\alpha^2 = [2]^2(x_0)^2 - 4(x^2). \tag{118}$$

Alternatively, one could think of the coordinates being represented by operators on a Hilbert space as in Ref. 10. In this case the square root would be defined through functional calculus for normal operators. In the expansion of solution (117) of the quantum Klein-Gordon equation the square root drops out. There, it can be seen as an auxiliary object which makes the notation of a certain generating function more compact. Anyway, it is clear that this mathematical subtlety does not affect the results of this paper.

Finally, we would like to note that expressions for derivatives within the noncommutative calculus can also be derived in a straightforward manner using the recursion relations defined by the commutation relations of momenta and coordinates. While this approach circumvents to some degree the mathematical machinery we have introduced here, it produces lengthy formulas which do not give the structural insight desirable for solving noncommutative differential equations. Even when free field equation can be solved by brute force, using computer algebra, for example, the results turn to be quite complicated. But if already something as basic as the wave function of a free particle were described by complicated expressions, some fundamental questions of quantum field theory, such as independence of in and out states, would become very hard to tackle. In this respect we believe results of the type presented here to be not just a matter of computational convenience but an indispensable requirement for the further development of quantum theory on quantum Minkowski space.

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APPENDIX

Definition 5: The Hopf $*$-algebra generated by E, F, K, and K^{-1} *with relations*

$$KK^{-1} = 1 = K^{-1}K, \quad KEK^{-1} = q^2E,$$
$$KFK^{-1} = q^{-2}F, \quad [E,F] = \lambda^{-1}(K - K^{-1}), \tag{A1}$$

Hopf structure

$$\Delta(E) = E \otimes K + 1 \otimes E, \quad \Delta(F) = F \otimes 1 + K^{-1} \otimes F,$$
$$\Delta(K) = K \otimes K, \quad \varepsilon(E) = 0 = \varepsilon(F), \quad \varepsilon(K) = 1, \tag{A2}$$
$$S(E) = -EK^{-1}, \quad S(F) = -KF, \quad S(K) = K^{-1},$$

and $*$-structure

$$E^* = FK, \quad F^* = K^{-1}E, \quad K^* = K \tag{A3}$$

is called $\mathcal{U}_q(\mathrm{su}_2)$, the q-deformation of the enveloping algebra $\mathcal{U}(\mathrm{su}_2)$.[37,38]

Another useful set of generators is given by angular momentum three-vector $\{J_A\} = \{J_-, J_3, J_+\}$ which is a vector operator with respect to the Hopf adjoint action of $\mathcal{U}(\mathrm{su}_2)$ on itself,[12]

$$J_- := q[2]^{-1/2}KF,$$

$$J_3 := [2]^{-1}(q^{-1}EF - qFE), \tag{A4}$$

$$J_+ := -[2]^{-1/2}E.$$

The spin-$\frac{1}{2}$ representation of the antipode of this vector operator yields by $\tilde{\sigma}_A := -[2]\rho^{\frac{1}{2}}(SJ_A)$ a variant of the q-Pauli matrices which we will need here. Explicitly, we obtain

$$\tilde{\sigma}_- = [2]^{1/2}\begin{pmatrix} 0 & q^{1/2} \\ 0 & 0 \end{pmatrix}, \quad \tilde{\sigma}_+ = [2]^{1/2}\begin{pmatrix} 0 & 0 \\ -q^{-1/2} & 0 \end{pmatrix}, \quad \tilde{\sigma}_3 = \begin{pmatrix} -q^{-1} & 0 \\ 0 & q \end{pmatrix} \tag{A5}$$

with respect to the $\{-, +\}$ basis. $\mathcal{U}_q(\mathrm{su}_2)$ is quasitriangular with universal $\mathcal{R}$-matrix[39]

$$\mathcal{R} = e^{\hbar(H\otimes H)/2}\sum_{n=0}^{\infty} e^{\hbar n(n-1)/2}\frac{(e^{\hbar} - e^{-\hbar})^n}{[n]!}(E^n \otimes F^n), \tag{A6}$$

where $\hbar := \ln q$. The quantum Lorentz algebra contains a $\mathrm{SU}_q(2)^{\mathrm{op}}$ Hopf subalgebra,[33] the generators of which are given explicitly by

$$a := K^{1/2} \otimes K^{-1/2},$$

$$b := q^{-1/2}\lambda K^{1/2} \otimes K^{-1/2}E,$$

$$c := -q^{1/2}\lambda FK^{1/2} \otimes K^{-1/2}, \tag{A7}$$

$$d := K^{-1/2} \otimes K^{1/2} - \lambda^2 FK^{1/2} \otimes K^{-1/2}E.$$

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Generalized quantum entropy

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The generalized quantum entropies are introduced in this paper. Some important properties such as nonnegativity, continuity, and concavity are proved. But different from the Von Neumann entropy, the subadditivity and additivity fail for the quantum unified (r,s)-entropy in general. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The successful application of Shannon's information quantities in information theory and coding theory has stimulated the investigation of more information measures. People have made much efforts in applying information theory to other fields and further extended Shannon's information measures in variable senses. There are various generalizations of Shannon's entropy.

For a discrete probability distribution $P=(p_1,p_2,\ldots,p_d)$ with $0\leqslant p_j\leqslant 1$ and $\Sigma_{j=1}^{d}p_j=1$. Let us consider the following generalized entropies:

Rényi entropy of order r,[1]

$$H_r(P)=(1-r)^{-1}\log\left(\sum_{j=1}^{d}p_j^r\right),\quad r>0,\quad r\neq 1. \tag{1}$$

Entropy of degree r (Tsallis entropy),[2]

$$H^r(P)=(1-r)^{-1}\left(\sum_{j=1}^{d}p_j^r-1\right),\quad r>0,\quad r\neq 1. \tag{2}$$

Entropy of type r,[3]

$${}_rH(P)=(r-1)^{-1}\left[\left(\sum_{j=1}^{d}p_j^{1/r}\right)^r-1\right],\quad r>0,\quad r\neq 1. \tag{3}$$

It is easy to verify that

$$\lim_{r\to 1}H_r(P)=\lim_{r\to 1}H^r(P)=\lim_{r\to 1}{}_rH(P)=H(P),$$

where

$$H(P)=-\sum_{j=1}^{d}p_j\log p_j \tag{4}$$

is the well-known Shannon entropy.

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Among multitude of information entropies, Shannon entropy, Rényi entropy and Tsallis entropy have found utility in a wide range of physical problems. Shannon entropy is well known to be successfully applied to modern information theory, and is frequently used in such areas as economics, geophysics, biology, medical diagnosis, and astronomy;[4] Rényi entropy is routinely measured in numerous situations ranging from coding theory and cryptography;[5] a possible generalization of Boltzmann-Gibbs statistical mechanics was proposed on the basis of Tsallis entropy, and Tsallis nonextensive formalism of statistical mechanics has been designed to treat those systems which cannot be treated within Boltzmann-Gibbs formalism owing to the presence of long-range interactions, spatio-temporal complexity, fractal dynamics and so on.[6]

However the above four entropies can be obtained easily as limiting or particular cases from the following entropy which is called (r,s)-entropy[7,8] involving two real parameters r and s:

$$H_r^s(P) = [(1-r)s]^{-1}\left[\left(\sum_{j=1}^{d} p_j^r\right)^s - 1\right], \quad r>0, \quad r\neq 1, \quad s\neq 0. \tag{5}$$

When $r=\alpha$, $s=(\beta-1)/(\alpha-1)$, $\alpha>0$, $\beta>0$, $\alpha\neq 1$, $\beta\neq 1$, then this reduces to Sharma and Mittal's entropy of order α and degree β.[9] The (r,s)-entropy (5) includes the entropies (1) and (4) as limiting cases. The entropies (2) and (3) are particular cases of (5). This can be written in composite form with the entropy of order r as follows:

$$H_r^s(P) = [(1-r)s]^{-1}[e^{(1-r)s\cdot H_r(P)} - 1], \quad r>0, \quad r\neq 1, \quad s\neq 0. \tag{6}$$

Let us write the continuous version of the above five entropies with respect to the parameters r,s as follows:

$$E_r^s(P) = \begin{cases} H_r^s(P) & \text{if } r\neq 1, \quad s\neq 0, \\ H_r(P) & \text{if } r\neq 1, \quad s=0, \\ H^r(P) & \text{if } r\neq 1, \quad s=1, \\ {}_rH(P) & \text{if } r\neq 1, \quad s=1/r, \\ H(P) & \text{if } r=1. \end{cases} \tag{7}$$

for all $r>0$ and for any s. $E_r^s(P)$is called the unified (r,s)-entropy.[7,8]

The Von Neumann entropy is the quantum version of the Shannon entropy. In Sec. II we review the definition of the Von Neumann entropy and define its various generalizations. The main results of this paper are presented in Sec. III. Some important properties of quantum unified (r,s)-entropy are proved.

II. QUANTUM ENTROPY

Von Neumann defined the entropy of a quantum state ρ by the formula[10,11]

$$S(\rho) = -\operatorname{tr}(\rho\log\rho), \tag{8}$$

where ρ is any density operator, i.e., positive operator on a complex separable Hilbert space $\mathcal{H}$ having a unit trace. The generalized entropies also have their quantum versions as follows.

Quantum Rényi entropy of order r,

$$S_r(\rho) = (1-r)^{-1}\log[\operatorname{tr}(\rho^r)], \quad r>0, \quad r\neq 1. \tag{9}$$

Quantum entropy of degree r (quantum Tsallis entropy),

$$S^r(\rho) = (1-r)^{-1}[\operatorname{tr}(\rho^r) - 1], \quad r>0, \quad r\neq 1. \tag{10}$$

Quantum entropy of type r,

$${}_rS(\rho) = (r-1)^{-1}\{[\operatorname{tr}(\rho^{1/r})]^r - 1\}, \quad r>0, \quad r\neq 1. \tag{11}$$

Quantum (r,s)-entropy,

$$S_r^s(\rho) = [(1-r)s]^{-1}\{[\mathrm{tr}(\rho^r)]^s - 1\}, \quad r > 0, \quad r \neq 1. \tag{12}$$

Quantum unified (r,s)-entropy,

$$E_r^s(\rho) = \begin{cases} S_r^s(\rho) & \text{if } r \neq 1, \quad s \neq 0, \\ S_r(\rho) & \text{if } r \neq 1, \quad s = 0, \\ S^r(\rho) & \text{if } r \neq 1, \quad s = 1, \\ {}_rS(\rho) & \text{if } r \neq 1, \quad s = 1/r, \\ S(\rho) & \text{if } r = 1. \end{cases} \tag{13}$$

for all $r>0$ and for any s.

Using the spectral decomposition theorem and noting $\mathrm{tr}(U\rho U^\dagger)=tr(\rho)$, where U is unitary, we can easily verify that

$$\lim_{r\to 1} S_r(\rho) = \lim_{r\to 1} S^r(\rho) = \lim_{r\to 1} {}_rS(P) = S(\rho).$$

III. PROPERTIES OF THE QUANTUM UNIFIED (r,s)-ENTROPY

Proposition 1: The quantum unified (r,s)-entropy is non-negative, i.e., $E_r^s(\rho)\geqslant 0$, where ρ is any density operator. The equality holds if and only if the state is pure.

Proof: The Von Neumann entropy $S(\rho)\geqslant 0$ (Refs. 10 and 11) and the quantum Rényi entropy $S_r(\rho)\geqslant 0$ (Ref. 12) are well known. Now we prove $S_r^s(\rho)\geqslant 0$. One has $x^r \leqslant (\text{resp.}\geqslant)x$ for $x \in [0,1]$ with equality iff $x=0$ or $x=1$ when $r>1$(resp.$0<r<1$). Since the eigenvalues p_j of ρ lie in $[0,1]$, we conclude the operator inequality $\rho^r \leqslant (\text{resp.}\geqslant)\rho$, where equality holds iff ρ is pure, i.e., a one-dimensional projection. It then follows that $\mathrm{tr}(\rho^r)\leqslant(\text{resp.}\geqslant)1$ with equality iff ρ is pure. Noting the sign of $(1-r)s$ in different cases, we complete the proof.

Proposition 2: In a finite dimension d, $E_r^s(\rho)$ is bounded, i.e.,

$$E_r^s(\rho) \leqslant \begin{cases} \log(\mathrm{rank}\,\rho) & \text{if } r = 1, \\ (1-r)^{-1}\log(\mathrm{rank}\,\rho) & \text{if } r \neq 1, \quad s = 0, \\ [(1-r)s]^{-1}[(\mathrm{rank}\,\rho)^{(1-r)s} - 1] & \text{if } r \neq 1, \quad s \neq 0. \end{cases} \tag{14}$$

Equality holds in the inequality if and only if ρ is an equidistribution of order rank ρ.

Proof: To prove the upper bounds of (14) we use Hölder's inequality. For $0<r<1$,

$$\mathrm{tr}(\rho^r) = \sum_{j=1}^{\mathrm{rank}\,\rho} p_j^r \leqslant \left(\sum_{j=1}^{\mathrm{rank}\,\rho} (p_j^r)^{1/r}\right)^r \left(\sum_{j=1}^{\mathrm{rank}\,\rho} 1^{1/(1-r)}\right)^{1-r} = (\mathrm{rank}\,\rho)^{1-r}, \tag{15}$$

where p_j is the eigenvalue of ρ, Equality holds iff p_j is constant for $j=1,2,\ldots,\mathrm{rank}\,\rho$, i.e., $p_j = (\mathrm{rank}\,\rho)^{-1}$. When $s>0$ or $s<0$, we have the same result as follows:

$$S_r^s(\rho) \leqslant [(1-r)s]^{-1}[(\mathrm{rank}\,\rho)^{(1-r)s} - 1], \tag{16}$$

which is the third inequality in (14). For $r>1$, the inequality in (15) is reversed but the conditions for equality are the same. When $s\neq 0$, the proof is similar. From (6) and (16), we have $S_r(\rho) = [(1-r)s]^{-1}\log[(1-r)s\cdot S_r^s(\rho)+1]$ and thus $S_r(\rho)\leqslant\log(\mathrm{rank}\,\rho)$. For $r=1$, Von Neumann entropy is at most $\log(\mathrm{rank}\,\rho)$.[10,11] This completes the proof.

Noting that $\mathrm{rank}(\rho)\leqslant d$ and letting $d\to\infty$, we have the following conclusions.

Corollary 1: In an infinite dimension

(i) for $0<r<1, s<0$ or $r>1, s>0$, $0\leqslant E_r^s(\rho)<[(r-1)s]^{-1}$;
(ii) for $0<r<1, s>0$ or $r>1, s<0$, $0\leqslant E_r^s(\rho)\leqslant\infty$.

Concavity is another important property of $E_r^s(\rho)$ similar to the Von Neumann entropy. To prove this property, we have the following lemma.

Lemma 1: Let $G_r^s(\rho)=[\mathrm{tr}(\rho^r)]^s$, $r>0, s\neq 0$, then

(i) $G_r^s(\rho)$ is a concave function of the density operator ρ for $0<r<1$, $s>0$, $rs\leqslant 1$;
(ii) $G_r^s(\rho)$ is a convex function of the density operator ρ for $r\geqslant 1$, $rs\geqslant 1$ or $0<r<1, s<0$.

Proof: We apply Minkowski's inequality to positive operators: Let ρ,σ be positive operators, and $1<r<\infty$, then

$$[\mathrm{tr}(\rho+\sigma)^r]^{1/r}\leqslant [tr(\rho)^r]^{1/r}+[\mathrm{tr}(\sigma)^r]^{1/r}. \tag{17}$$

Case 1: when $r\geqslant 1$, from (17), we have

$$[\mathrm{tr}(\lambda\rho+\mu\sigma)^r]^{1/r}\leqslant \lambda[\mathrm{tr}(\rho)^r]^{1/r}+\mu[\mathrm{tr}(\sigma)^r]^{1/r},$$

where $\lambda\geqslant 0$, $\mu\geqslant 0$, $\lambda+\mu=1$. If $rs>1$, we have

$$[\mathrm{tr}(\lambda\rho+\mu\sigma)^r]^s\leqslant [\lambda(\mathrm{tr}(\rho)^r)^{1/r}+\mu(\mathrm{tr}(\sigma)^r)^{1/r}]^{rs}\leqslant \lambda[\mathrm{tr}(\rho)^r]^s+\mu[\mathrm{tr}(\sigma)^r]^s. \tag{18}$$

Equation (18) is obtained from the convexity of the function $y=x^{rs}$, $rs\geqslant 1$. Therefore $G_r^s(\rho)$ is a convex function for $r>1$ with $rs\geqslant 1$.

Case 2: when $0<r<1$, the inequality in (17) is reversed,

$$[\mathrm{tr}(\rho+\sigma)^r]^{1/r}\geqslant [\mathrm{tr}(\rho)^r]^{1/r}+[\mathrm{tr}(\sigma)^r]^{1/r},$$

where $\lambda\geqslant 0, \mu\geqslant 0, \lambda+\mu=1$. We consider the following two cases:

(a) when $0<rs<1$, we have

$$[\mathrm{tr}(\lambda\rho+\mu\sigma)^r]^s\geqslant [\lambda(\mathrm{tr}(\rho)^r)^{1/r}+\mu(\mathrm{tr}(\sigma)^r)^{1/r}]^{rs}\geqslant \lambda[\mathrm{tr}(\rho)^r]^s+\mu[\mathrm{tr}(\sigma)^r]^s.$$

So $G_r^s(\rho)$ is a concave function for $0<r<1$, $0<rs<1$.

(b) When $rs<0$, i.e., $s<0$, (18) is also true. Therefore $G_r^s(\rho)$ is a convex function for $0<r<1$ with $rs<0$. This complete the proof.

Concavity of $E_r^s(\rho)$ follows from Lemma 1 and the sign of $(1-r)s$.

Proposition 3: Suppose ρ and σ are density operators and $0\leqslant\lambda\leqslant 1$. Then

$$E_r^s(\lambda\rho+(1-\lambda)\sigma)\geqslant \lambda E_r^s(\rho)+(1-\lambda)E_r^s(\sigma), \tag{19}$$

for all r and s satisfying either $0<r\leqslant 1, rs\leqslant 1$ or $r\geqslant 1, rs\geqslant 1$.

Remarks:

(i) For $r=1$, the Von Neumann entropy is a concave function.[10]
(ii) For $r>0, r\neq 1, s=0$, the quantum Rényi entropy fails for concavity.[12]
(iii) For $r>0, r\neq 1, s=1$, the quantum Tsallis entropy is a concave function.[13]

There is an upper bound for the convex combination.

Proposition 4: Setting $F_r^s(\lambda)=[(1-r)s]^{-1}[\lambda^{rs}+(1-\lambda)^{rs}-1]$, $0\leqslant\lambda\leqslant 1$, we have the following:

(i) For $r>1$, $s\geqslant 1$ or $0<r<1$, $0<s<1$ or $r>1$, $s<0$,

$$E_r^s(\lambda\rho+(1-\lambda)\sigma)\leqslant \lambda^{rs}E_r^s(\rho)+(1-\lambda)^{rs}E_r^s(\sigma)+F_r^s(\lambda). \tag{20}$$

(ii) In particular, for $r>1$, $s\geqslant 1$,

$$E_r^s(\lambda\rho+(1-\lambda)\sigma)\leqslant \lambda E_r^s(\rho)+(1-\lambda)E_r^s(\sigma)+F_r^s(\lambda). \tag{21}$$

Proof: It is clear that for positive numbers a and b,

$$(a+b)^s \geqslant a^s + b^s \quad \text{if } s \geqslant 1, \quad (a+b)^s \leqslant a^s + b^s \quad \text{if } 0 < s < 1 \quad \text{or } s < 0.$$

By using the trace inequalities:[14] for positive operators ρ and σ,

$$\mathrm{tr}((\rho+\sigma)^r) \geqslant [\text{resp. } \leqslant]\mathrm{tr}(\rho^r) + \mathrm{tr}(\sigma^r), \quad \text{for } r \geqslant 1[\text{resp.} 0 < r < 1].$$

Noting the sign of $(1-r)s$, we can complete the proof.

Remarks: From Corollary 1, some properties of $F_r^s(\lambda)$ follow:

(i) $(\lambda-\lambda^{rs})E_r^s(\rho)+[(1-\lambda)-(1-\lambda)^{rs}]E_r^s(\sigma) < F_r^s(\lambda)$ for $r>1$, $s>1$,
(ii) $(\lambda-\lambda^{rs})E_r^s(\rho)+[(1-\lambda)-(1-\lambda)^{rs}]E_r^s(\sigma) > F_r^s(\lambda)$ for $0<r<1$, $s<0$,

where ρ and σ are arbitrary density operators.

Using the method of mathematical induction, we obtain the following.

Corollary 2: Suppose $\rho=\Sigma_{i=1}^n p_i\rho_i$, where $\{p_i, 1 \leqslant i \leqslant n\}$ is a probability distribution, and ρ_i are density operators. If $r \geqslant 1$, $s \geqslant 1$ then

$$\sum_{i=1}^n p_i E_r^s(\rho_i) \leqslant E_r^s(\rho) \leqslant \sum_{i=1}^n p_i E_r^s(\rho_i) + F_r^s(p_1, p_2, \ldots, p_n), \tag{22}$$

where $F_r^s(p_1, p_2, \ldots, p_n)=[(1-r)s]^{-1}(p_1^{rs}+p_2^{rs}+\cdots+p_n^{rs}-1)$.

We can define the generalized Holevo bound denoted by χ and

$$\chi = E_r^s\left(\sum_{i=1}^n p_i\rho_i\right) - \sum_{i=1}^n p_i E_r^s(\rho_i). \tag{23}$$

The Holevo χ quantity is very useful in quantum information.[10]

Let ρ and σ be density operators, we say ρ majorizes σ and write it as $\rho \succ \sigma$ which means that the spectrum of the operator ρ majorizes the spectrum of the operator σ. That is, if ρ and σ have eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_d$ and $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_d$, respectively, then $\Sigma_{j=1}^l \lambda_j \geqslant \Sigma_{j=1}^l \mu_j$ for all $1 \leqslant l \leqslant d$. If $\rho \succ \sigma$ then $E_r^s(\rho) \leqslant E_r^s(\sigma)$ which is called Schur concavity.

Proposition 5: The quantum unified (r,s)-entropy does not satisfy Schur concavity, moreover, if ρ majorizes σ, i.e., $\rho \succ \sigma$ then $E_r^s(\rho) \geqslant E_r^s(\sigma)$.

To prove this proposition, we need a lemma.

Lemma 2: If $\lambda_i \geqslant \mu_i \geqslant 0$, $i=1,2,\ldots,d$, then for $r>1$ or $r<0$,

$$\left(\sum_{i=1}^d \lambda_i\right)^r - \sum_{i=1}^d \lambda_i^r \geqslant \left(\sum_{i=1}^d \mu_i\right)^r - \sum_{i=1}^d \mu_i^r. \tag{24}$$

For $0<r<1$, the inequality in (24) is reversed.

Proof: See Ref. 8.

Proof of Proposition 5: If λ_i and μ_i are eigenvalues of density operators ρ and σ, respectively, then by Lemma 2 we obtain that if $\rho \succ \sigma$ then $\mathrm{tr}(\rho^r) \leqslant \mathrm{tr}(\sigma^r)$ for $r>1$ and $\mathrm{tr}(\rho^r) \geqslant \mathrm{tr}(\sigma^r)$ for $0<r<1$. For quantum (r,s)-entropy$(r>0, r\neq 1, s\neq 1)$, it is easy to verify $S_r^s(\rho) \geqslant S_r^s(\sigma)$. For the quantum Rényi entropy, the quantum Tsallis entropy and the quantum entropy of type r, the proof is similar by Lemma 2. For the Von Neumann entropy, Wehrl[11] gave the proof. This completes the proof of Proposition 5.

Suppose we vary the density operator ρ by a small amount. How much does $E_r^s(\rho)$ change? We know the Von Neumann entropy satisfies Fannes's inequality.[15] With respect to the trace distance $\|\rho-\sigma\| = \frac{1}{2}\mathrm{tr}|\rho-\sigma|$, $E_r^s(\cdot)$ is Lipschitz under certain conditions.

Proposition 6 (*Lipschitz continuity*): For $r>1$ and $s \geqslant 1$

$$|E_r^s(\rho) - E_r^s(\sigma)| \leqslant r(r-1)^{-1}\|\rho-\sigma\|. \tag{25}$$

Proof: Applying the generalized Klein's inequality,[16] we obtain, for $\rho \leqslant \sigma$,

$$\mathrm{tr}[(\rho-\sigma)f'(\sigma)] \leqslant \mathrm{tr}[f(\rho)-f(\sigma)] \leqslant \mathrm{tr}[(\rho-\sigma)f'(\rho)],$$

where $f(x)=x^r$, $r>1$, $x\in(0,1]$ is a convex function. So

$$|\mathrm{tr}(\rho^r)-\mathrm{tr}(\sigma^r)| \leqslant r\cdot\max\{|\mathrm{tr}[(\rho-\sigma)\rho^{r-1}|,|\mathrm{tr}[(\rho-\sigma)\sigma^{r-1}|\}.$$

By the spectral decomposition, we may decompose $\rho-\sigma=Q-R$, where Q and R are positive operators with orthogonal support, $\|\rho-\sigma\|=\mathrm{tr}(Q)+\mathrm{tr}(R)$, so

$$|\mathrm{tr}[(\rho-\sigma)\rho^{r-1}| = |\mathrm{tr}[(Q-R)\rho^{r-1}| \leqslant \mathrm{tr}(Q\rho^{r-1})+\mathrm{tr}(R\rho^{r-1}) \leqslant \mathrm{tr}(Q+R) = \|\rho-\sigma\|.$$

By symmetry between density operators ρ and σ, we also have $|\mathrm{tr}[(\rho-\sigma)\sigma^{r-1}| \leqslant \|\rho-\sigma\|$.

Therefore

$$|\mathrm{tr}(\rho^r)-\mathrm{tr}(\sigma^r)| \leqslant r\cdot\|\rho-\sigma\| \quad (r>1).$$

The derivative sx^{s-1} of the map $x\to x^s$ is bounded on $[0,1]$, so that this map is Lipschitz with constant $s\geqslant 1$. Hence

$$|[\mathrm{tr}(\rho^r)]^s-[\mathrm{tr}(\sigma^r)]^s| \leqslant s\cdot|\mathrm{tr}(\rho^r)-\mathrm{tr}(\sigma^r)| \leqslant sr\cdot\|\rho-\sigma\|.$$

The Lipschitz continuity of $E_r^s(\rho)$ follows from the above inequalities.

We now turn to properties of the quantum unified (r,s)-entropy for composite system. We recall that the familiar Von Neumann entropy $S(\rho)$ satisfies (see, e.g., Refs. 10 and 11),

$$S(\rho_{AB}) \leqslant S(\rho_A\otimes\rho_B) = S(\rho_A)+S(\rho_B), \tag{26}$$

for any state ρ_{AB} on $\mathcal{H}_A\otimes\mathcal{H}_B$, where $\rho_A=\mathrm{tr}_B(\rho_{AB})$ and $\rho_B=\mathrm{tr}_A(\rho_{AB})$.

The inequality in (26) is known as the subadditivity property of entropy; it is customarily paraphrased by saying that since all correlations between the subsystems present in ρ_{AB} are lost in the state $\rho_A\otimes\rho_B$ (when ρ_{AB} is not a product state) the entropy should increase. The equality holds iff $\rho_{AB}=\rho_A\otimes\rho_B$. Unfortunately, subadditivity of the form $S(\rho_{AB})\leqslant S(\rho_A)+S(\rho_B)$ and additivity of the form $S(\rho_{AB})=S(\rho_A)+S(\rho_B)$ fail for quantum unified (r,s)-entropy in general.

Proposition 7: Suppose ρ and σ are density operators, and $\rho\otimes\sigma$ is a product state, then

$$E_r^s(\rho\otimes\sigma) = E_r^s(\rho)+E_r^s(\sigma)+(1-r)sE_r^s(\rho)E_r^s(\sigma), \tag{27}$$

$$E_r^s(\rho\otimes\sigma) \leqslant E_r^s(\rho)+E_r^s(\sigma), \quad 0<r<1, \quad s<0 \text{ or } r\geqslant 1, \quad s\geqslant 0, \tag{28}$$

$$E_r^s(\rho\otimes\sigma) \geqslant E_r^s(\rho)+E_r^s(\sigma), \quad r>1, \quad s<0 \text{ or } 0<r<1, \quad s>0. \tag{29}$$

With equalities if and only if either of the states ρ,σ is pure.

Proof: When $r\neq 1$, $s\neq 0$, Direct computation gives (27)

$$S_r^s(\rho\otimes\sigma)-S_r^s(\rho)-S_r^s(\sigma) = [(1-r)s]^{-1}\{[\mathrm{tr}(\rho\otimes\sigma)^r]^s-[\mathrm{tr}(\rho)^r]^s-[\mathrm{tr}(\sigma)^r]^s+1\}$$

$$=[(1-r)s]^{-1}[(\mathrm{tr}(\rho^r))^s-1][(\mathrm{tr}(\sigma^r))^s-1]$$

$$=(1-r)s\cdot S_r^s(\rho)S_r^s(\sigma),$$

When $r\neq 1$, $s=0$ and $r=1$, the quantum Rényi entropy and the Von Neumann entropy, respectively, satisfy the additivity property.[10–12] The inequalities in (28) and (29) are clear. This completes the proof.

Due to (27), one has in general $E_r^s(\rho_{AB})\neq E_r^s(\rho_A)+E_r^s(\rho_B)$, moreover subadditivity of the form $E_r^s(\rho_{AB})\leqslant E_r^s(\rho_A)+E_r^s(\rho_B)$ fails due to (29). However under certain conditions, the subadditivity

inequality is true. For example, for $r>1$, the quantum Tsallis entropy satisfies the subadditivity property.[13] Because of the generality of quantum unified (r,s)-entropy, it is hard to obtain the subadditivity property.[17–19]

Proposition 8: If a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$ is in a pure state ρ_{AB}, then

$$E_r^s(\rho_A) = E_r^s(\rho_B). \tag{30}$$

Proof: From the Schmidt decomposition we know that eigenvalues of density operators of systems $\mathcal{H}_A$ and $\mathcal{H}_B$ are the same. The entropy is determined by the eigenvalues, so $E_r^s(\rho_A) = E_r^s(\rho_B)$.

It is clear in this case, $0 = E_r^s(\rho_{AB}) \leqslant E_r^s(\rho_A) + E_r^s(\rho_B)$.

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Hyperbolic geometrical optics: Hyperbolic glass

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We study the geometrical optics generated by a refractive index of the form $n(x,y)=1/y$ $(y>0)$, where y is the coordinate of the vertical axis in an orthogonal reference frame in $\mathbb{R}^2$. We thus obtain what we call "hyperbolic geometrical optics" since the ray trajectories are geodesics in the Poincaré-Lobachevsky half-plane $\mathbb{H}^2$. Then we prove that the constant phase surface are horocycles and obtain the *horocyclic waves*, which are closely related to the classical Poisson kernel and are the analogs of the Euclidean plane waves. By studying the transport equation in the Beltrami pseudosphere, we prove (i) the conservation of the flow in the entire strip $0<y\leqslant 1$ in $\mathbb{H}^2$, which is the limited region of physical interest where the ray trajectories lie; (ii) the nonuniform distribution of the density of trajectories: the rays are indeed focused toward the horizontal x axis, which is the boundary of $\mathbb{H}^2$. Finally the process of ray focusing and defocusing is analyzed in detail by means of the sine-Gordon equation. © *2006 American Institute of Physics.*
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I. INTRODUCTION

It is well known that the geometrical optics approximation of the wave equation is related to the asymptotic form of the integral representation of the field (if such exists), which is an exact solution of the wave problem. Suppose, for instance, that the field in a uniform medium can be written as an expansion in plane waves; the evaluation of this integral by the stationary phase method yields an asymptotic series. Then the leading term of this asymptotic expansion, which is composed by an amplitude and a phase, can be extracted to yield the approximation. The ray trajectories are the lines orthogonal to the constant phase surface and are described by the eikonal equation; the amplitude satisfies the transport equation, whose physical meaning is related to the conservation of the flow. In the simplest case of uniform medium, whose refractive index n is a real constant, the rays are straight lines which are characterized by the following properties:

(i) They are geodesics of the Euclidean space.
(ii) Phase and amplitude are real-valued functions.
(iii) They can be derived by the Fermat's principle.

Constrained by these properties the methods of geometrical optics are rather limited and fail to explain several phenomena as, for instance, the diffraction by a compact and opaque obstacle, that is the existence of non-null field in the geometrical shadow which, for this reason, is usually referred to as the classically (or geometrically) forbidden region.

In the decade 1950–1960 Keller[1–3] wrote several papers where he introduced the so-called geometrical theory of diffraction (GTD). The latter can be regarded as an extension of geometrical optics, which accounts for diffraction by introducing the diffracted rays in addition to the usual

rays of geometrical optics. After these seminal works there has been a steady flow of papers addressing various aspects of the theory. On the one hand papers oriented to pure and applied electromagnetic theory, like radiation and scattering of waves, antenna design, waveguide theory and so on;[3] on the other hand, a highly theoretical and mathematically sophisticated theory of propagation of singularities and diffraction of waves on manifolds.[4] In spite of these efforts and a wide literature on these topics, not all the cases of interest have been studied. An example is what we could call the "hyperbolic geometrical optics," that is the geometrical optics generated by the rays in the specific case of a refractive index of the form $n(x,y)=1/y$ $(y>0)$, where y denotes a spatial coordinate, say vertical, in an appropriate orthogonal reference frame in $\mathbb{R}^2$. As far as we know, this problem has never been treated, except for some very marginal remarks (see, for instance, Ref. 5), in spite of its intrinsic geometrical interest and some possible applications to the physics of nonuniform optical fibers. It is precisely the main purpose of the present paper to fill this gap.

Let us return to the Keller's program of widening, from a geometrical viewpoint, the arena of Euclidean geometrical optics. With this in mind we adopt, first of all, the Jacobi's form of the principle of least action (instead of Fermat's), which concerns with the path of the system point rather than with its time evolution.[6] More precisely, the Jacobi's principle (generally applied in mechanics) can be formulated as follows: If there are no forces acting on the body, then the system travels along the shortest path length in the configuration space. Here we assume a wide extension of the Jacobi's principle, which can be formulated as follows: the geodesics associated with the Riemannian metric $n(x,y)\sqrt{\mathrm{d}x^2+\mathrm{d}y^2}$, i.e., the paths making the functional $\int n(x,y)\sqrt{\mathrm{d}x^2+\mathrm{d}y^2}$ stationary, are nicknamed rays. In other words, in place of Fermat's principle which reads $\delta\int_{P_0}^{P_1}\mathrm{d}t=0$, where $\mathrm{d}t$ is the travel time measure, and P_0 and P_1 are prescribed starting and end points of the path, we write

$$\delta\int_{P_0}^{P_1} n(x,y)\sqrt{\mathrm{d}x^2+\mathrm{d}y^2}=0, \tag{1}$$

or, equivalently,

$$\delta\int_{x_0}^{x_1} F(x,y,y')\mathrm{d}x=0, \quad (F(x,y,y')=n(x,y)\sqrt{1+y'^2}), \tag{2}$$

where $y'=\tan\alpha$, α being the angle that the tangent to the curve $y=y(x)$ forms with the x axis.

The simplest realization of this Jacobi's principle consists in identifying n^2 with the Riemann metric tensor g_{ij}, *whenever this identification is admissible*. This identification requires great caution, indeed; the form $g_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j$ must be symmetric and positive definite, and this poses a strict restriction. For instance, consider a refractive index (or, in mechanics, a potential) of the following form: $n^2=1-V/E$, where E is the energy of the incoming particle and V is the height of the potential, with $V>E$ as in the case of the tunnel effect. In this situation the geometric interpretation of the trajectory as a real-valued geodesic in a Riemannian manifold is no longer possible. The only chance remains to extend the admissible values of the phase to imaginary and/or complex values and, consequently, to speak of complex rays in the sense of Landau.[7]

But let us return to the cases where this identification is admissible. As we already mentioned, it is obviously possible in the case of a uniform nonabsorbing medium: in this case we simply obtain a physical realization of Euclidean geometry. But it is also certainly admissible when the refractive index is of the form introduced above, i.e., $n(x,y)=1/y$ $(y>0)$, where y denotes the coordinate of the vertical axis in an orthogonal reference frame in $\mathbb{R}^2$. In this case we are led to the Lobachevskian metric: $\mathrm{d}s^2=(\mathrm{d}x^2+\mathrm{d}y^2)/y^2$. Then the rays are geodesics in the hyperbolic half-plane (Poincaré half-plane), i.e., Euclidean half-circles with centers on the x axis (horizontal axis), or Euclidean straight lines normal to the x axis. Let us recall that the refractive index n is defined as $n=c/v_{\mathrm{ph}}$, where c is the light speed in vacuum, and v_{ph} is the phase velocity of radiation of a specific frequency in a specific material. Therefore $n\geqslant 1$, and in the case $n(x,y)=1/y$ only the

strip $0<y\leqslant 1$ has physical interest; hence the actual rays will lie necessarily in this band. Accordingly, hereafter, the only optical paths considered will be the Euclidean half-circles with centers on the x axis and radius R bounded by $0<R\leqslant 1$.

The subsequent step in developing an optical geometry consists in finding the constant phase surfaces and, accordingly, describing the analog of the Euclidean plane wave. This problem will be solved in Sec. II, studying some geometrical properties of horocycles and introducing what we call *horocyclic waves*, which play in hyperbolic geometrical optics the same role as the plane waves do in the Euclidean one. At this point we have the main ingredients needed for writing the geometrical approximation of the wave function; what it is still missing is an analysis of the amplitude and of the related flux density. This latter problem can be analyzed at two different levels. First we prove that the flow of rays is conserved: once a pointlike source is fixed, no ray will be absorbed or created. This result will be proved in Sec. II. A more subtle question is the following: Is the flow of the ray trajectories homogeneous or do the rays focus? This issue, besides its intrinsic geometrical interest, could in our opinion be of some interest in possible applications to the propagation in optical fibers with nonuniform refractive index.[8] This problem will be analyzed in detail in Sec. III. First we study the transport equation in the Beltrami pseudosphere, and prove that the flow of ray trajectories is not homogeneous, but there is a focusing of rays on the horizontal x axis. Glancing to possible applications to propagation in optical fibers this result suggests a conjecture indicating a strong ray focusing along the fiber axis, when the refractive index profile in the fiber is of hyperbolic type, instead of paraboliclike, as is customary. Next, this problem will be reconsidered by studying the variation of the angle that the tangent to the meridian of the Beltrami pseudosphere makes with the rotation axis of this surface, which can be indeed represented as a surface of revolution generated by a curve in $\mathbb{R}^3$. This leads to the sine-Gordon equation and provides a more precise description of the ray focusing and defocusing processes. This analysis is necessarily local, since the problem is worked out inside each horocycle; at the end of Sec. III, we show how to pass from a local description of the flow inside each horocycle to a global one.

Finally, in the Appendix , the geometric and algebraic ingredients which occur in Secs. II and III will be given. This appendix is split in three parts: the first part is devoted to the various models of hyperbolic geometry and to the conformal maps which allows the transformation between them; in the second part we study the group $\mathrm{SU}(1,1)$, which acts transitively on the non-Euclidean disk, and prove some relationships connecting the spherical functions to the horocyclic waves; the last part is devoted to the Beltrami pseudosphere.

II. THE FLOW IN THE STRIP $0<y\leqslant 1$

A. Variational minimization of the Jacobi's functional and the rays in hyperbolic geometrical optics

Let us consider the upper half-plane model of the hyperbolic two-dimensional space $\mathbb{H}^2$: i.e., $U=\{z=x+iy: y>0\}$ equipped with the metric d derived from the differential $\mathrm{d}s=|\mathrm{d}z|/\mathrm{Im}\, z$ (see the Appendix). Then we apply the typical methods of variational calculus to the Jacobi functional

$$J=\int_{P_0}^{P_1}\frac{\sqrt{(\mathrm{d}x)^2+(\mathrm{d}y)^2}}{y}$$

or, equivalently,

$$J=\int_{x_0}^{x_1}\frac{\sqrt{1+(y')^2}}{y}\mathrm{d}x$$

(P_0 and P_1 denote two points of the ambient space where light propagates). First we prove the following proposition, which refers to the whole upper half plane U.

Proposition 1: (*i*) *Let J be the following functional*:

$$J = \int_{x_0}^{x_1} \frac{\sqrt{1 + (y')^2}}{y} \mathrm{d}x, \tag{3}$$

and let F denote the integrand of (3). *The Euler-Lagrange equation for this functional reads*

$$yy'' + y'^2 + 1 = 0. \tag{4}$$

(*ii*) *The extremals of functional* (3) *are Euclidean half-circles with centers on the x axis, or Euclidean straight lines normal to the x axis lying in the half plane* $y>0$. *These are the geodesics in the hyperbolic geometry realized in the half plane* $y>0$.

(*iii*) *The Weierstrass condition for the functional* (3) *reads*

$$F_{y'y'} = \frac{1}{y(1 + y'^2)^{3/2}} > 0 \quad (y > 0), \tag{5}$$

and it is satisfied for any y'.

(*iv*) *There exists a field of extremals of functional* (3), *and the transversality condition becomes an orthogonality condition of these extremals to the curve* $\Phi(x,y)=const$ (*constant phase curve*), *which satisfies the following equation* (*eikonal equation*):

$$g^{ij} \frac{\partial \Phi}{\partial x_i} \frac{\partial \Phi}{\partial x_j} = 1, \tag{6}$$

where $x_1=x$, $x_2=y$, *and* g_{ij} *is the metric tensor.*

Proof: The proof makes use of standard procedures and can be found, for instance, in Ref. 5.□

Remark: Let us recall once again that the domain of physical interest where the optical paths necessarily lie (in view of the fact that $n \geqslant 1$) is the strip $0<y\leqslant 1$; therefore we shall consider only a subclass of the extremals of functional (3): i.e., the half-circles with centers on the x axis and radius bounded by $0<R\leqslant 1$.

B. Poisson kernel and horocyclic waves

Let us now give a more precise formulation of the physical problem. Suppose that a pointlike source of light is pushed to $-\infty$ on the (x,y) plane. For the sake of simplicity, here we limit ourselves to the scalar representation of light, and phenomena associated with polarization will not be considered. From Proposition 1 it follows that light rays are half-circles with centers on the x axis. For several reasons which will appear clear in what follows, it is convenient to map conformally the half-plane $y>0$ into the unit disk $|\zeta|<1$, which amounts to pass from the Poincaré half-plane model U to the Poincaré disk model D (see the Appendix and Fig. 1). The appropriate conformal mapping is given by $\zeta=i(z-i)/(z+i)$ ($z=x+iy$; $\zeta=\xi+i\eta$).

In the unit disk the light source will be located at $\zeta=i$. The band $y>1$ will be mapped, in the ζ-plane, into the disk tangent to the boundary B of D in i with Euclidean radius $\frac{1}{2}$, and represents the *forbidden region* for the light rays. The circular arcs lying in the half-plane $y>0$ and normal to the x axis will be mapped, in the unit disk, into circular arcs perpendicular to the boundary $|\zeta|=1$, which are precisely the geodesics of the hyperbolic geometry in the unit disk model.

From the transversality condition [see statement (iv) of Proposition 1], it follows that the constant phase curve is the curve that intersects orthogonally the extremals of functional (3): i.e., the geodesics. In the unit disk, parallel geodesics are geodesics corresponding to the same point $b=e^{i\phi}$ on the boundary B of D. Therefore, in the physical problem being treated, the circles tangent to the unit circle at the point b, which intersects orthogonally the pencil of *parallel straight lines* (i.e., arcs of circle orthogonal to B) are the constant phase curves, they are a family of *horocycles*, and are denoted by H_b.

We can now state the following proposition.

Proposition 2: (*i*) *The Poisson kernel*

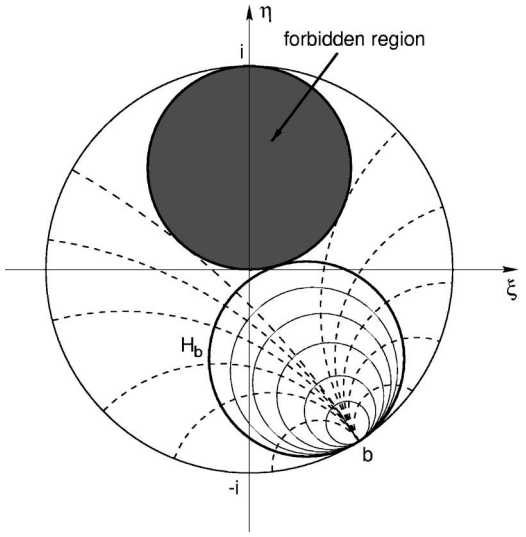

FIG. 1. Horocyclic flow outside the forbidden region in the Poincaré disk D.

$$P(\zeta,b)=\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|\cos(\theta-\phi)} \quad (\zeta=|\zeta|e^{i\theta};b=e^{i\phi}), \tag{7}$$

is constant on each horocycle H_b with normal b.

(*ii*) *The function*

$$[P(\zeta,b)]^{\nu}=\left[\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|\cos(\theta-\phi)}\right]^{\nu} \quad (\nu\in\mathbb{C}), \tag{8}$$

is an eigenfunction of the Laplace-Beltrami operator on the hyperbolic disk D corresponding to the eigenvalue $\nu(\nu-1)$.

(*iii*) *The hyperbolic waves* (*horocyclic waves*) *are represented by the following expression*:

$$e^{\nu\langle\zeta,b\rangle}=\left[\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|\cos(\theta-\phi)}\right]^{\nu} \quad (\nu\in\mathbb{C}), \tag{9}$$

where $\langle\zeta,b\rangle$ is the hyperbolic distance between the origin of D and the horocycle of normal b passing through $\zeta\in D$.

(*iv*) *The conical functions $\mathcal{P}_{-1/2+i\lambda}(\cosh r)$* (*i.e., the first kind Legendre functions of index $\left(-\frac{1}{2}+i\lambda\right)$ $(\lambda\in\mathbb{R})$*) *can be represented by*

$$\mathcal{P}_{-\frac{1}{2}+i\lambda}(\cosh r)=\int_B e^{\left(\frac{1}{2}-i\lambda\right)\langle\zeta,b\rangle}\,db \quad (\lambda\in\mathbb{R},B=\{\zeta:|\zeta|=1\}), \tag{10}$$

and correspond to the fundamental series of the irreducible unitary representation of the group SU(1,1), *which acts transitively on the hyperbolic disk D.*

(*v*) *The following equality holds*:

$$\mathcal{P}_{-\frac{1}{2}+i\lambda}(\cosh r)=\mathcal{P}_{-\frac{1}{2}-i\lambda}(\cosh r) \quad (\lambda\in\mathbb{R}). \tag{11}$$

Proof: (i) The level lines of the Poisson kernel $P(\zeta,b)$ are the circles tangent to the unit circle at the point $b=e^{i\phi}$: i.e., the images of the horocycles H_b with normal b (see Ref. 9).

(ii) The Laplace-Beltrami operator Δ_D on the hyperbolic unit disk D is given by[10]

$$\Delta_D = \frac{1}{4}\left[1-(\xi^2+\eta^2)\right]^2\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right). \tag{12}$$

If $\nu\in\mathbb{C}$ is any complex number, a direct computation gives[10]

$$\Delta_D P^\nu(\zeta,b) = \nu(\nu-1)P^\nu(\zeta,b). \tag{13}$$

(iii) In the Euclidean case the function $\mathbf{x}\to e^{ik(\mathbf{x},\boldsymbol{\omega})}$, where $k\in\mathbb{R}$, $\boldsymbol{\omega}\in\mathbb{S}^{(n-1)}$, $\mathbf{x}\in\mathbb{R}^n$, represents a plane wave with normal $\boldsymbol{\omega}$. It is indeed constant on each hyperplane perpendicular to $\boldsymbol{\omega}$, and furthermore is an eigenfunction of the Laplacian on $\mathbb{R}^n$. The geometric analog of the plane wave in the case of the hyperbolic disk D is the function represented by the equality (9) (see Ref. 11). In fact, it is an eigenfunction of the Laplace-Beltrami operator on D, as proved by statement (ii) [see Eq. (13)]. Further, setting $\theta=\phi$ in formulas (7) and (8), we have

$$\ln\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|} = \ln\frac{1+|\zeta|}{1-|\zeta|} = d(0,\zeta) = \langle|\zeta|e^{i\phi},e^{i\phi}\rangle = \langle\zeta,b\rangle, \tag{14}$$

where $d(0,\zeta)=\ln[(1+|\zeta|)/(1-|\zeta|)]$ is the hyperbolic distance between the origin and the point $\zeta\in D$ (see the Appendix). Therefore, $\langle\zeta,b\rangle$ is the hyperbolic analog of $(\mathbf{x},\boldsymbol{\omega})$. In fact, in view of statement (i), $\langle\zeta,b\rangle$ is the distance between the origin and the horocycle of normal b passing through $\zeta\in D$, assuming that the origin falls outside the horocycle; $\langle\zeta,b\rangle$ is positive if the origin is external to the horocycle, while it is negative ($\langle\zeta,b\rangle=\ln[(1-|\zeta|)/(1+|\zeta|)]$) if the origin is internal to the horocycle.

(iv) If we set $\xi=\tanh(r/2)\cos\theta$, $\eta=\tanh(r/2)\sin\theta$, then $|\zeta|=\tanh(r/2)$. The Riemannian metric $\mathrm{d}s^2=4(\mathrm{d}\xi^2+\mathrm{d}\eta^2)/(1-\xi^2-\eta^2)^2$ becomes $\mathrm{d}s^2=\mathrm{d}r^2+\sinh^2 r\,\mathrm{d}\theta^2$. By the use of this substitution in the expression of the Poisson kernel (7) or (8), we have

$$\left[\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|\cos(\theta-\phi)}\right]^\nu = \frac{1}{[\cosh r-\sinh r\cos(\theta-\phi)]^\nu} \quad (\nu\in\mathbb{C}), \tag{15}$$

and the integral sum of *horocyclic waves* [see statement (iii)] gives (see Ref. 11 and Proposition 6 in the Appendix):

$$\int_B e^{\nu\langle\zeta,b\rangle}\,\mathrm{d}b = \frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1}{\cosh r+\sinh r\cos\phi}\right)^\nu \mathrm{d}\phi = \mathcal{P}_{-\nu}(\cosh r) \quad (\nu\in\mathbb{C}), \tag{16}$$

where B is the boundary of the hyperbolic disk D, and $\mathcal{P}_{-\nu}(\cosh r)$ are the first kind Legendre functions.[12] Finally, setting $\nu=\frac{1}{2}-i\lambda$ ($\lambda\in\mathbb{R}$) we obtain the conical functions $\mathcal{P}_{-1/2+i\lambda}(\cosh r)$, which correspond to the fundamental series of the irreducible unitary representation of the group SU(1,1): i.e., the group of the matrices of the form[13] $\begin{pmatrix} a & c \\ \bar{c} & \bar{a}\end{pmatrix}$, $|a|^2-|c|^2=1$; $a,c\in\mathbb{C}$, which acts as a group of isometries of the hyperbolic disk D by means of the map

$$g(\zeta) = \frac{a\zeta+c}{\bar{c}\zeta+\bar{a}} \quad (\zeta\in D). \tag{17}$$

(v) Equality (11) is proved in the Appendix (see Proposition 6). □

Remark: It is well known that the classical Fourier transform refers to the decomposition of a function, belonging to an appropriate space, into exponentials of the form e^{ikx} (k real), which can also be viewed as the irreducible unitary representation of the additive group of real numbers. Analogously, the exponentials $e^{i(\mathbf{k},\mathbf{x})}$ are characters of the group $\mathbb{R}^2$. But the hyperbolic disk is not a group. Therefore a straightforward generalization of the exponential for D is not possible. Nevertheless, in view of the fact that the function $\mathcal{P}_{-\nu}(\cosh r)$ corresponds to the fundamental series of the irreducible unitary representation of the group SU(1,1) for $\nu=\frac{1}{2}-i\lambda$, the exponential

$e^{(1/2-i\lambda)\langle\zeta,b\rangle}$ $(\lambda \in \mathbb{R})$ represents the analog of the Euclidean exponential, and plays the same role in the hyperbolic Fourier analysis.[11]

C. Conservation of the flow

As already said in the Introduction, the ray trajectories are the lines orthogonal to the constant phase surface, and are described by the eikonal equation; moreover, $\langle\zeta,b\rangle$ is the hyperbolic distance between the origin and the horocycle H_b of normal b passing through ζ. Therefore, in close analogy with the Euclidean optical geometry, and recalling that $\mathcal{P}_{-1/2+i\lambda}(\cosh r) = \mathcal{P}_{-1/2-i\lambda}(\cosh r)$ $(\lambda \in \mathbb{R})$ [see statement (v) of Proposition 2], the expression of the analog of the Euclidean plane wave e^{ikx} $(k \in \mathbb{R})$ can be written as follows: $e^{(1/2-i\lambda)\langle\zeta,b\rangle}$ $(\lambda \in \mathbb{R})$. Thus the geometrical approximation of the wave function ψ can be obtained by multiplying $e^{(1/2-i\lambda)\langle\zeta,b\rangle}$times a function which represents the amplitude. Then we can state the following proposition.

Proposition 3: *The geometrical approximation of the wave function* ψ *reads*:

$$\psi(\zeta,\lambda,b) = A(\lambda)e^{\left(\frac{1}{2}-i\lambda\right)\langle\zeta,b\rangle} \quad (\lambda \in \mathbb{R}, \zeta \in D, b \in B), \tag{18}$$

and the flow in the entire strip $0 < y \leqslant 1$ *is conserved*.

Proof: Let σ be the conformal map

$$z = \sigma(\zeta) = -i\frac{\zeta+i}{\zeta-i}, \tag{19}$$

defined in the Appendix, that transfers the geometry of D into U. Since $\sigma(0)=i$ and $\sigma(i)=\infty$, then the image by σ of the horocycle H_i passing through $\zeta=0$ is the horizontal line $\widetilde{H}_\infty=\{x+iy : y=1\}$ in U (the horocycles in the Poincaré half-plane will be hereafter denoted by $\widetilde{H}_b$). The image by σ of the horocycle $H_{\sigma^{-1}(b)}$ tangent to H_i in D is the horocycle $\widetilde{H}_b$ of radius $1/2$ through $b \in \mathbb{R}$ and tangent to the horizontal line $\widetilde{H}_\infty$ (in order to avoid proliferation of notations, we denote by the same letter b both the points on the boundary B of D and the corresponding points belonging to the boundary of $\mathbb{H}^2$, i.e., belonging to $\mathbb{R}$).

We already saw that the horocycle $\widetilde{H}_b$ of normal b is perpendicular to each geodesic starting from b. To calculate the amplitude of the wave function, we must see how many geodesics perpendicular to $\widetilde{H}_b$ intersect $\widetilde{H}_b$, with the additional condition that these geodesics belong to the band $0 < y \leqslant 1$. This corresponds to find the amount of normal vectors at $\widetilde{H}_b$, with unit norm, that are tangent vectors of geodesics in the band $0 < y \leqslant 1$.

In general, if b is a point in $\mathbb{R}\cup\{\infty\}$ and T_1U is the unit tangent bundle of U, then the horocycle flow $h_{j,b}: T_1U \to T_1U$ is the flow which slides the inward normal vectors to each $\widetilde{H}_b$ to the right along $\widetilde{H}_b$ at unit speed. To find the equation of the flow $h_{j,b}$, first we consider the flow $h_{j,\infty}$ of geodesics perpendicular to the horocycle $\widetilde{H}_\infty$ of normal ∞. Then we choose a transformation M_b which maps the horocycle $\widetilde{H}_\infty$ into the horocycle $\widetilde{H}_b$. In particular, the map M_b transfers the flow $h_{j,\infty}$ into the flow $h_{j,b}$.

From the definition,

$$h_{j,\infty}(v_i) = \begin{pmatrix} 1 & j \\ 0 & 1 \end{pmatrix} v_i, \tag{20}$$

where v_i denotes the unit vector vertically upwards based at $i \in U$. This is because in the simplest case of horocycle flow $h_{j,\infty}$, the geodesics perpendicular to $\widetilde{H}_\infty$ are vertical lines and the isometry sending one vertical line into another vertical line is the horizontal translation. Therefore, the horocycle flow along $\widetilde{H}_\infty$ is simply the horizontal translation.

Let us now consider the transformation M_b such that $M_b(\infty)=b$. Then, the horocycle flow $h_{j,b}$ along $\widetilde{H}_b$ is the image of $h_{j,\infty}$ by M_b, hence

$$h_{j,b}(v) = M_b \begin{pmatrix} 1 & j \\ 0 & 1 \end{pmatrix} v. \tag{21}$$

It is clear from the definition that the amount of geodesics in the flow $h_{j,b}$ does not depend on the radius of the horocycle. Given two different points b_1 and b_2 in the boundary of the hyperbolic plane, then the composition of M_{b_1} and $M_{b_2}^{-1}$ sends the point b_2 in b_1. Moreover, $M_{b_1} \circ M_{b_2}^{-1}$ sends the horocycle flow h_{j,b_2} into the horocycle flow h_{j,b_1}. This proves that the amplitude of the wave does not depend on b and ζ.

Using Proposition 2, we obtain that there exists a function $A(\lambda)$ independent of ζ and b such that Eq. (18) is satisfied, and the conservation of the flow along the entire strip $0 < y \leqslant 1$ is proved. □

Remark: It is interesting to compare the propagation of light in vacuum with that within the strip $0 < y \leqslant 1$ belonging to $\mathbb{H}^2$. In vacuum each ray cuts orthogonally all the constant phase planes: i.e., each ray emerging from a plane cuts orthogonally all the other parallel planes. In $\mathbb{H}^2$ propagation proceeds in a completely different form. Take two horocycles lying in the strip $0 < y \leqslant 1$, and tangent at the point $z=(1+i)/2$: the first horocycle, denoted by $\widetilde{H}_0$, has normal $b_0 = 0$; the second one, denoted by $\widetilde{H}_1$, has normal $b_1 = 1$. Only one geodesic, denoted γ_t, lying in $\widetilde{H}_0$, cuts orthogonally $\widetilde{H}_1$; it emerges from $b_0=0$ and ends at $b_1=1$. All the geodesics $\gamma_>$, emerging from $b_0=0$ and lying in $\widetilde{H}_0$ above γ_t, cut orthogonally horocycles $\widetilde{H}_b$ with $b>1$; the geodesics $\gamma_<$, emerging from $b_0=0$ and lying in $\widetilde{H}_0$ below γ_t, cut orthogonally horocycles $\widetilde{H}_b$ with $b<1$. However, the density of the flow of geodesics entering orthogonally each horocycle equals the density of the flow of geodesics exiting orthogonally the same horocycle.

III. TRANSPORT EQUATION AND DISTRIBUTION OF THE DENSITY OF TRAJECTORIES

A. Transport equation in the Beltrami pseudosphere

Working out the problem in the space $\mathbb{H}^2$ allows us to describe each trajectory as a geodesic in the Poincaré plane (or disk), but this setting is not appropriate for describing the evolution of a bunch of trajectories. Hereafter we will switch to a representation more suitable for an effective characterization of the amplitude factor in the geometrical approximation of the field. To this aim, let us first recall the following well-known negative result due to Hilbert: there is no regular smooth isometric immersion $X: \mathbb{H}^2 \to \mathbb{R}^3$. However, one can look for a local immersion $X: \mathcal{U} \to \mathbb{R}^3$, where X is a continuous differentiable function, and $\mathcal{U} \subset \mathbb{H}^2$ is an open subset. We keep for $\mathcal{U}$ an open horocycle based at b. This local immersion can be realized by means of the Beltrami pseudosphere, denoted hereafter by P_b (see the Appendix and Fig. 2). In fact, let us consider in the hyperbolic disk D an infinite strip lying between two parallel straight lines emerging from the source point located on the absolute at $\zeta=-i$. Then we take on these parallel geodesics a pair of points A_0 and B_0, lying on a horocycle of normal $b_0=e^{-i\pi/2}=-i$ and cutting orthogonally these straight lines; A_0 and B_0 are spaced at distance of 2π. One is then led to consider the domain $(-i, A_0, B_0)$. The Beltrami surface cut along any of its generators can be isometrically mapped into the domain $(-i, A_0, B_0)$ (see Ref. 14). On a Lobachevskian plane there always exists reflection (i.e., a hyperbolic isometry) about an arbitrary straight line; in particular, reflecting the strip $(-i, A_0, B_0)$ about the straight line $(-i, A_0)$ we obtain a new strip isometric to the initial one and realized as a cut of the Beltrami surface in $\mathbb{R}^3$. Reflecting then this new strip $(-i, A_1, A_0)$ (the segment A_1A_0 has length 2π) about the straight line $(-i, A_1)$ we obtain the strip $(-i, A_2, A_1)$ with the same properties. Exactly the same procedure can be repeated on the other side of $(-i, A_0, B_0)$, leading to $(-i, B_2, B_1)$. We thus obtain strips of the form $(-i, A_k, A_{k-1})$ and $(-i, B_k, B_{k-1})$ $(1 \leqslant k < \infty)$; all segments (A_k, A_{k-1}) and (B_k, B_{k-1}) have the same length 2π. Working with the same procedure we can now construct the map of the open horocycle H_{b_0}, tangent at the boundary to the forbidden region (this latter represented by the horocycle H_i of normal i and passing through the origin), into a Beltrami funnel, such that each strip of the type $(-i, A_k, A_{k-1})$, $(-i, A_0, B_0)$, and $(-i, B_k, B_{k-1})$, $(1 \leqslant k < \infty)$ (referred, now, to the horocycle H_{b_0}), is mapped iso-

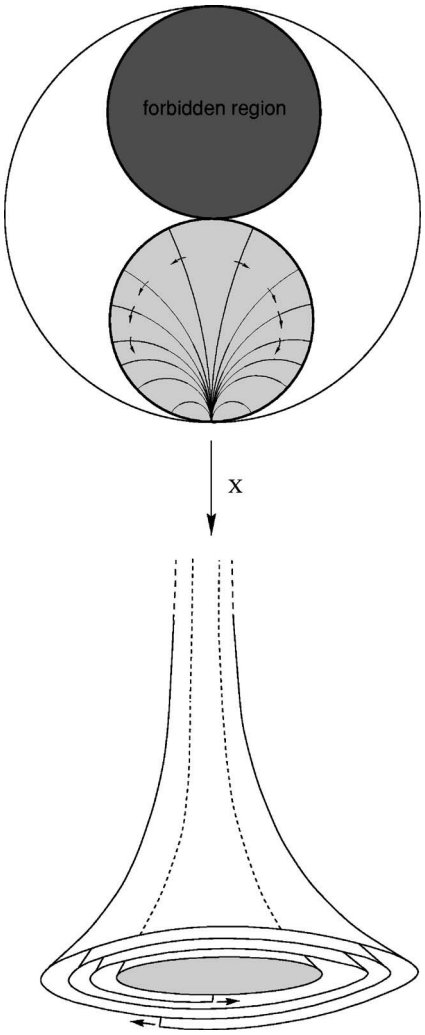

FIG. 2. Mapping of a horocycle in the disk D into a Beltrami pseudosphere.

metrically into the Beltrami surface, the horocycle H_{b_0} being wound infinitely many times into the Beltrami surface[14] (see Fig. 2). We can repeat the same procedure for each point $b \in B$, since there is a rotation (i.e., a hyperbolic isometry) sending each $b \in B$ onto b_0.

For an explicit equation of the immersion X, the reader is referred to Ref. 15.

In general, the Laplace-Beltrami operator Δ_M on a two-dimensional Riemannian manifold M with metric tensor g_{ij} ($g=|\det(g_{ij})|$, $g^{ij}=g_{ij}^{-1}$) is defined as follows:

$$\Delta_M = \frac{1}{\sqrt{g}}\left[\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(\sum_{j=1}^{2} g^{ij}\sqrt{g}\frac{\partial}{\partial x_j}\right)\right]. \tag{22}$$

In the specific case of the hyperbolic metric associated with the refractive index $n(y)=1/y$ (see the Appendix), the Laplace-Beltrami operator reads

$$\Delta_{\mathrm{H}} = \frac{1}{n^2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) = y^2\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right). \tag{23}$$

We then have the following proposition.

Proposition 4: (*i*) *The Helmholtz equation reads*

$$\Delta_{\mathbb{H}}\psi + k_{\mathbb{H}}^2\psi = 0, \tag{24}$$

where $k_{\mathbb{H}}^2 = \lambda^2 + \frac{1}{4}$ $(\lambda \in \mathbb{R})$.

(*ii*) *The geometrical approximation of the wave function* ψ (*for* $|\lambda| \to \infty$), *written in terms of the Beltrami coordinates* (*see the Appendix*), *reads*

$$\psi_{\pm}(\lambda, u) = C(\lambda) e^{u/2}\, e^{\mp i\lambda u} \quad (\lambda \in \mathbb{R}; u \geqslant 0). \tag{25}$$

Proof: (i) Let us consider the *horocyclic waves* which generate the conical functions $\mathcal{P}_{-1/2\pm i\lambda}(\cosh r)$, corresponding to the irreducible unitary representation of the SU(1,1) group, which acts transitively on the hyperbolic disk D. This amounts to put in the exponent $\nu \in \mathbb{C}$ of the Poisson kernel, $\nu = \frac{1}{2} \pm i\lambda$ $(\lambda \in \mathbb{R})$. Accordingly, the *horocyclic waves* read $e^{(1/2 \pm i\lambda)\langle \zeta, b\rangle}$ [see statements (iv) and (v) of Proposition 2]. From statement (ii) of Proposition 2 and Eq. (13) we get

$$\Delta_{\mathbb{H}} e^{\left(\frac{1}{2} \pm i\lambda\right)\langle \zeta, b\rangle} = -\left(\lambda^2 + \frac{1}{4}\right) e^{\left(\frac{1}{2} \pm i\lambda\right)\langle \zeta, b\rangle} = -k_{\mathbb{H}}^2 e^{\left(\frac{1}{2} \pm i\lambda\right)\langle \zeta, b\rangle}, \tag{26}$$

where $k_{\mathbb{H}}^2 = \lambda^2 + \frac{1}{4}$ $(\lambda \in \mathbb{R})$. Next, proceeding in close analogy with the Euclidean case, where the Euclidean plane wave plays the role of the *horocyclic wave*, we obtain Eq. (24).

(ii) Let us now go back to the mapping of the horocycle into the Beltrami funnel (without a cut) in $\mathbb{R}^3$, illustrated above. Next, we apply the Laplace-Beltrami operator to the wave function ψ, supposed to belong to $C^{\infty}(\mathcal{B})$ ($\mathcal{B}$ denoting the Beltrami pseudosphere); in (22) x_i $(i = 1, 2)$ stand for the Beltrami coordinates u, v. Recall that the first fundamental form in Beltrami coordinates reads [see part (C) of the Appendix]:

$$I = \mathrm{d}u^2 + e^{-2u}\, \mathrm{d}v^2 \quad (u \geqslant 0). \tag{27}$$

Accordingly, we have $g_{11} = 1$, $g_{22} = e^{-2u}$, $g_{12} = g_{21} = 0$, $g = |\det(g_{ij})| = e^{-2u}$, $g^{ij} = g_{ij}^{-1}$. Thus, we are led to the following equation:

$$\Delta_{\mathcal{B}}\psi + k_{\mathbb{H}}^2\psi = 0, \tag{28}$$

where $\Delta_{\mathcal{B}}$ is the Laplace-Beltrami operator, referred to the Beltrami pseudosphere. In this equation, we pass from the coordinates (ξ, η) of the hyperbolic disk D to the Beltrami coordinates (u, v) of the Beltrami pseudosphere. We illustrate with more details this passage. First we embed an open horocycle H_b of normal b and tangent to the *forbidden region* (represented by the horocycle H_i passing through the origin of D and with normal i; see Fig. 1) into a Beltrami pseudosphere. Notice that in the present analysis, as well as in Proposition 3, and in strict analogy with the classical Euclidean procedure, we consider the distance from the origin of the hyperbolic disk D (rather than from the point source located at $\zeta = i$) to the horocycle $H_{\zeta,b}$ (inside H_b) of normal b passing through a point ζ. Thus we have

$$\langle \zeta, b\rangle = d(0, H_b) + d(H_b, H_{\zeta,b}) := d_b + d(H_b, H_{\zeta,b}). \tag{29}$$

When we embed H_b into a Beltrami pseudosphere, the distance $d(H_b, H_{\zeta,b})$ between horocycles corresponds to the distance between different parallels $u = \text{const}$ inside the pseudosphere. Since H_b is fixed, then d_b is fixed too. Then, following the standard method of stationary phase, we look now for a solution of Eq. (28), of the following form:

$$\begin{aligned}\psi(\lambda, \mathbf{x}) &= \int A(\mathbf{x}, \ell\,) e^{\left(\frac{1}{2} - i\lambda\right)\langle \zeta, b\rangle}\, \mathrm{d}\ell\, = e^{\left(\frac{1}{2} - i\lambda\right)d_b} \int A(\mathbf{x}, \ell\,) e^{\left(\frac{1}{2} - i\lambda\right)d(H_b, H_{\zeta,b})}\, \mathrm{d}\ell \\ &= C(\lambda) \int A(\mathbf{x}, \ell\,) e^{\left(\frac{1}{2} - i\lambda\right)\Phi(\mathbf{x}, \ell)}\, \mathrm{d}\ell\,,\end{aligned} \tag{30}$$

where $\mathbf{x} = (x_1, x_2)$, $x_1 = u$, $x_2 = v$; ℓ is the pathlength inside the pseudosphere to the point of coordinate $\mathbf{x}$, $\Phi(\mathbf{x}, \ell\,)$ denotes the phase (recall the statements of Proposition 2).

The right-hand side (rhs) of equality (30) is an integral of oscillating type. The principal contribution to $\psi(\lambda,\mathbf{x})$, as $|\lambda|\to+\infty$, corresponds to the stationary point of Φ, in the neighborhood of which the exponential ceases to oscillate rapidly. These stationary points can be obtained from the equation $\partial\Phi/\partial\ell=0$ (provided that $\partial^2\Phi/\partial\ell^2\neq 0$). If the condition $\partial\Phi/\partial\ell=0$ is satisfied by a unique value ℓ_0 of ℓ, corresponding to the unique ray trajectory (geodesic) passing across the point of coordinates (u,v), we say that Φ has a critical nondegenerate point at $\ell=\ell_0$. Moreover, recalling that the manifolds with nonpositive curvature do not have conjugate points, we can state that all the critical points of Φ are nondegenerate. Then, by applying the Morse lemma on the representation of the functions all of whose critical points are nondegenerate, we obtain the following asymptotic evaluation of integral (30):

$$\psi(\lambda,\mathbf{x})=C(\lambda)e^{\frac{1}{2}\Phi(\mathbf{x},\ell_0)}e^{-i\lambda\Phi(\mathbf{x},\ell_0)}\sum_{m=0}^{\infty}\frac{A_m(\mathbf{x})}{(i\lambda)^m}. \tag{31}$$

The leading term of expansion (31) reads

$$\psi(\lambda,\mathbf{x})=C(\lambda)A_0(\mathbf{x})e^{\frac{1}{2}\Phi(\mathbf{x},\ell_0)}e^{-i\lambda\Phi(\mathbf{x},\ell_0)}, \tag{32}$$

where

$$A_0(\mathbf{x})=A(\mathbf{x},\ell_0)\left(\left|\frac{\partial^2\Phi}{\partial\ell^2}\right|^{-1/2}\right)_{\ell=\ell_0}\exp\left[i\,\frac{\pi}{4}\,\mathrm{sgn}\left(\frac{\partial^2\Phi}{\partial\ell^2}\right)\right]_{\ell=\ell_0}. \tag{33}$$

For simplicity, in the following we shall write the leading term of expansion (31) as $C(\lambda)A(\mathbf{x})e^{(1/2-i\lambda)\Phi(\mathbf{x})}$, dropping the zero subscripts. Substituting this expression into Eq. (28), collecting powers of $(i\lambda)$ and, finally, equating to zero their coefficients, two equations are obtained: the eikonal (or Hamilton-Jacobi) equation

$$g^{ij}\frac{\partial\Phi}{\partial x_i}\frac{\partial\Phi}{\partial x_j}=1, \tag{34}$$

and the transport equation

$$\frac{1}{\sqrt{g}}\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left[\sqrt{g}A^2e^{\Phi}\sum_{j=1}^{2}g^{ij}\frac{\partial\Phi}{\partial x_j}\right]=0. \tag{35}$$

Let us note that in the present problem the wave functions are radial, in view of the fact that we are considering a family of horocycles having all the same normal b. Therefore, $\psi(\lambda,\mathbf{x})$ [where $\mathbf{x}\equiv(u,v)$, u,v being the Beltrami coordinates, see the Appendix] does not depend on v. Then, Eq. (34) becomes

$$\left(\frac{\mathrm{d}\Phi}{\mathrm{d}u}\right)^2=1, \tag{36}$$

which gives the following expression of the phase: $\Phi^{(\pm)}=\pm u+c$ ($c=$const). Proceeding analogously with Eq. (35), we have

$$\frac{\mathrm{d}}{\mathrm{d}u}\left(A^2e^{\pm u}e^{-u}\frac{\mathrm{d}\Phi^{(\pm)}}{\mathrm{d}u}\right)=0. \tag{37}$$

Substituting in the leading term (32) the expressions of Φ and A, which derive from (36) and (37), the rhs of (25) follows. □

B. Sine-Gordon equation and the flow of trajectories

The analysis of propagation in the Beltrami pseudosphere has allowed us to study the distribution of the density of trajectories and, accordingly, the ray focusing along the horizontal axis. Another parameter, related once again to the Beltrami pseudosphere, and whose characterization is relevant in our description of the flow of trajectories, is the angle φ that the tangent to the meridian (in the Beltrami pseudosphere) makes with the z axis [see section (C) of the Appendix].

In the Appendix, the Beltrami pseudosphere is described in terms of the Beltrami coordinates u and v. Here we choose another parametrization (p,q) by setting

$$\mathrm{d}p = -\csc\varphi\,\mathrm{d}\varphi, \tag{38a}$$

$$\mathrm{d}q = -\mathrm{d}v. \tag{38b}$$

Integrating (38a), we obtain

$$\varphi = 2\tan^{-1}(e^{-p}), \tag{39}$$

and

$$\frac{\mathrm{d}\varphi}{\mathrm{d}p} = -\sin\varphi = \frac{1}{\cosh p}. \tag{40}$$

Next, substituting in formula (A31) of the Appendix (with $\rho=-1$) φ and v in terms of the parameters p and q, the position vector $\mathbf{r}$ of the pseudosphere can be rewritten as follows:

$$\mathbf{r}(p,q) = \begin{pmatrix} -\dfrac{1}{\cosh p}\cos q \\ \dfrac{1}{\cosh p}\sin q \\ p - \tanh p \end{pmatrix}, \tag{41}$$

where the downward vertex of the pseudosphere corresponds to $p\to-\infty$, while the rim corresponds to $p=0$. The parameters (p,q) can be related to the arc lengths (α,β) along asymptotic lines as follows:

$$p = \alpha + \beta,$$

$$q = \alpha - \beta. \tag{42}$$

Setting $\omega=2\varphi$, the first fundamental form reads

$$I = \mathrm{d}\alpha^2 + 2\cos\omega\,\mathrm{d}\alpha\,\mathrm{d}\beta + \mathrm{d}\beta^2, \tag{43}$$

which can be easily derived from the expression (A32) of the Appendix through the formulas (38a) and (42) (recalling that $\rho^2=1$). Moreover, from Gauss' and Weingarten's equations, it follows that ω, which is the angle between the asymptotic lines, satisfies the *classical* sine-Gordon equation, which reads

$$\frac{\partial^2\omega}{\partial\alpha\,\partial\beta} = \sin\omega. \tag{44}$$

This latter equation rewritten in terms of the coordinates p,q becomes

$$\frac{\partial^2\varphi}{\partial p^2} - \frac{\partial^2\varphi}{\partial q^2} = \sin\varphi\cos\varphi. \tag{45}$$

We can finally state the following proposition.

Proposition 5: (*i*) *The angle* φ, *that the tangent to the meridian of the pseudosphere makes with the z axis* (*i.e.*, *the rotation axis*), *is represented by the following formula*:

$$\varphi = 2\tan^{-1}(e^{-p}), \tag{46}$$

which is the so-called "*one-soliton*" *solution of the sine-Gordon equation* (45).

(*ii*) *The angle* φ *varies from* $\varphi=\pi/2$ *to* $\varphi=\pi$ *in the process of focusing*, *and from* $\varphi=\pi$ *to* $\varphi=\pi/2$ *in the process of defocusing*.

Proof: (i) The proof of this statement follows easily by direct calculation.

(ii) The downward vertical z axis of the pseudosphere we are considering is negatively oriented; then varying p from 0 to $-\infty$ [in Eq. (46)], φ varies from $\varphi=\pi/2$ to $\varphi=\pi$ (focusing). Next varying p from $-\infty$ to 0, φ varies from $\varphi=\pi$ to $\varphi=\pi/2$ (defocusing). □

So far in this section we have considered a local description of the flow in order to show that the density of the flow is not homogeneously distributed. We now want to recover a global description in the entire strip $0<y\leqslant 1$. But we have already remarked that the map of a horocycle into a pseudosphere excludes the boundary of the horocycle. Therefore this global description cannot be reached by considering only horocycles lying in the strip $0<y\leqslant 1$ and tangent to the line $y=1$. Recall, however, that while the *physical* geodesics, which lie within the strip $0<y\leqslant 1$ in $\mathbb{H}^2$, cannot enter the forbidden region $y>1$, this is not the case for horocycles, provided we limit ourselves to consider in these horocycles (i.e., those entering the forbidden region) those segments of geodesics which lie in the strip $0<y\leqslant 1$. In view of these considerations it is sufficient to consider horocycles $\widetilde{H}'_b \supset \widetilde{H}_b$ ($\widetilde{H}'_b$ entering the forbidden region), and, accordingly, the maps X'_b embedding $\widetilde{H}'_b$ into a Beltrami pseudosphere P'_b. We can thus obtain a sequence of Beltrami pseudospheres P'_b which, by varying b, allows us to connect in $\mathbb{R}^3$ the geodesics lying in the strip $0<y\leqslant 1$. We thus pass from a local to a global description.

IV. CONCLUSIONS AND DISCUSSION

In this paper we have presented the geometrical optics generated by a refractive index of hyperbolic type. The ray trajectories are geodesics in the Poincaré-Lobachevsky half-plane, and the horocyclic waves, which are related to the Poisson kernel, represent the analogs of the Euclidean plane waves. We thus obtain two main results.

(a) The flow in the entire strip $0<y\leqslant 1$ is conserved (see Proposition 3);
(b) inside each horocycle (by embedding horocycles in Beltrami pseudospheres) the ray focusing on each point b of the horizontal x axis: i.e., toward the boundary of $\mathbb{H}^2$, is shown.

The connection between hyperbolic geometry and optics of spatially nonuniform media can be made even tighter. In fact, it can be shown that the transfer matrix associated with lossless layered optical media is an element of the group SU(1,1), no matter how complicated the stepwise profile of the refractive index might be.[16–18] Therefore, the action of any lossless optical multilayer can be regarded as a Möbius transformation on the unit disk,[16] and therefore the natural geometric environment for these physical systems is the hyperbolic one. From this point of view, the geometrical optics description of light propagation in the "hyperbolic glass" discussed so far can be regarded as the study (in a spatially continuum setting) of the particular case of special interest, in which only motions along hyperbolic geodesics are allowed.

APPENDIX

(A) Let us consider the upper half-plane model of the hyperbolic two-dimensional space $U=\{z=x+iy : y>0\}$. Then the boundary ∂U of U is the real axis and infinity. On U we can define a

metric d derived from the differential $ds=|dz|/\Im z$ where dz is the standard Euclidean metric. The geodesics of U are vertical half-lines and Euclidean semicircles with center on the real axis. The group of the orientation preserving isometries of (U,d) is the Möbius group $\mathrm{PSL}_2(\mathbb{R})$, that is the group of the 2×2 matrices of real coefficients with determinant 1. The action on $U\cup\partial U$ is defined as $\gamma(z)=(az+b)/(cz+d)$, where $\begin{pmatrix} a & b \\ c & d \end{pmatrix}\in \mathrm{PSL}_2(\mathbb{R})$.

Another model of the hyperbolic two-dimensional space is the Poincaré disk $D=\{\zeta=\xi+i\eta:\xi^2+\eta^2<1\}$. The map

$$\zeta = i\frac{z-i}{z+i} \tag{A1}$$

{with inverse $z=-i[(\zeta+i)/(\zeta-i)]$} transfers the geometry of U into the geometry of D. In particular, the metric on D is given by the differential

$$d\zeta = \frac{2}{1-|\zeta|^2}d_E\zeta, \tag{A2}$$

where d_E is the standard Euclidean metric. In this model, the geodesics are circular arcs perpendicular to the boundary $|\zeta|=1$. Moreover, the group of the orientation preserving isometries of the Poincaré disk D is the group $\mathrm{SU}(1,1)$ of the maps of the following form:

$$\left\{\frac{a\zeta+\bar{c}}{c\zeta+\bar{a}}:|a|^2-|c|^2=1\right\}. \tag{A3}$$

(B) The group $G=\mathrm{SU}(1,1)$ admits two subgroups relevant for our analysis:

(1) The subgroup K of rotations

$$k_\theta=\begin{pmatrix} e^{i\frac{\theta}{2}} & 0 \\ 0 & e^{-i\frac{\theta}{2}} \end{pmatrix},$$

with $0\leqslant\theta<4\pi$.

(2) The subgroup A of matrices

$$a_r=\begin{pmatrix} \cosh\frac{r}{2} & \sinh\frac{r}{2} \\ \sinh\frac{r}{2} & \cosh\frac{r}{2} \end{pmatrix},$$

with $r\in\mathbb{R}$.

Let A^+ denote the set a_r with $r\geqslant 0$. Then the following decomposition holds.

Cartan decomposition:[10] Any element $g\in G$ can be decomposed as follows:

$$g=k_\theta a_r k_\phi \quad (r\geqslant 0, 0\leqslant\theta<4\pi, 0\leqslant\phi<2\pi), \tag{A4}$$

i.e., $G=KA^+K$. The decomposition is unique if $g\notin K$.

We now introduce the so-called *spherical functions* $\Phi_\nu(g)$ on G/K $[g\in G=\mathrm{SU}(1,1), \nu\in\mathbb{C}]$, which are defined as follows.[19]

Definition 1: *The spherical functions on* G/K $[G=\mathrm{SU}(1,1), K=\mathrm{SO}(2)]$ *are defined as follows*:

$$\Phi_\nu(g)=\int_B \left|\frac{d(g^{-1}\cdot b)}{db}\right|^\nu db \quad [g\in \mathrm{SU}(1,1), \nu\in\mathbb{C}], \tag{A5}$$

where B *is the boundary of the hyperbolic disk* D (*i.e.*, $B=\{\zeta:|\zeta|=1\}$).

We can then prove the following proposition.

Proposition 6: *The functions* $\Phi_\nu(g)$ *satisfy the following properties*:

(i)

$$\Phi_\nu(g) = \mathcal{P}_{-\nu}(\cosh r), \quad [g \in \mathrm{SU}(1,1), \nu \in \mathbb{C}], \tag{A6}$$

where $\mathcal{P}_{-\nu}(\cdot)$ *are the first kind Legendre functions*.

(ii)

$$\Delta_D \Phi_\nu(g) = \nu(\nu-1)\Phi_\nu(g), \quad [g \in \mathrm{SU}(1,1), \nu \in \mathbb{C}], \tag{A7}$$

where Δ_D *is the hyperbolic Laplace-Beltrami operator*.

(iii)

$$\mathcal{P}_{-\frac{1}{2}+i\lambda}(\cosh r) = \mathcal{P}_{-\frac{1}{2}-i\lambda}(\cosh r) \quad (\lambda \in \mathbb{R}). \tag{A8}$$

Proof: Let us consider the following integral $(1/2\pi)\int_0^{2\pi} f(e^{i\phi})\mathrm{d}\phi$ $[f \in L^1(B)]$, and evaluate how the Lebesgue measure $(1/2\pi)\mathrm{d}\phi$ changes when an element $g \in \mathrm{SU}(1,1)$ acts on B (boundary of D). Recalling that the action of g is $g\cdot\zeta = (a\zeta + c)/(\bar{c}\zeta + \bar{a})$ $(\zeta \in D)$ (see Proposition 2), we have $g \cdot e^{i\phi} = e^{i\chi} = (ae^{i\phi} + c)/(\bar{c}e^{i\phi} + \bar{a})$. We thus have[19]

$$\left|\frac{\mathrm{d}\phi}{\mathrm{d}\chi}\right| = |\bar{c}e^{i\chi} - a|^{-2} = |a|^{-2}\left|\frac{\bar{c}}{a}e^{i\chi} - 1\right|^{-2} = \left(1 - \frac{|c|^2}{|a|^2}\right)\left|\frac{\bar{c}}{a}e^{i\chi} - 1\right|^{-2}, \tag{A9}$$

since $|a|^2 - |c|^2 = 1$. Let us now note that $g\cdot 0 = c/\bar{a}$; on the other hand, in view of the Cartan decomposition, we have

$$g \cdot 0 = k_\theta a_r \cdot 0 = e^{i\theta}\tanh\left(\frac{r}{2}\right) = |\zeta| e^{i\theta}. \tag{A10}$$

Therefore $(1 - |c|^2/|a|^2) = 1 - |\zeta|^2$, and

$$\left|\frac{\bar{c}}{a}e^{i\chi} - 1\right|^{-2} = \frac{1}{|1 - |\zeta| e^{i(\chi-\theta)}|^2} = \frac{1}{1 + |\zeta|^2 - 2|\zeta|\cos(\chi - \theta)}. \tag{A11}$$

We thus have

$$\frac{1}{2\pi}\int_0^{2\pi} f(g \cdot e^{i\phi})\mathrm{d}\phi = \frac{1}{2\pi}\int_0^{2\pi} f(e^{i\chi})\left|\frac{\mathrm{d}\phi}{\mathrm{d}\chi}\right|\mathrm{d}\chi, \tag{A12}$$

and, in view of formulas (A9), (A10), (A11), (A12), we get

$$P(g\cdot 0, b) = \frac{1 - |\zeta|^2}{1 + |\zeta|^2 - 2|\zeta|\cos(\chi - \theta)} = \left|\frac{\mathrm{d}(g^{-1}\cdot b)}{\mathrm{d}b}\right|. \tag{A13}$$

Recalling Definition 1 we can write

$$\Phi_\nu(g) = \int_B \left|\frac{\mathrm{d}(g^{-1}\cdot b)}{\mathrm{d}b}\right|^\nu \mathrm{d}b = \frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1 - |\zeta|^2}{1 + |\zeta|^2 - 2|\zeta|\cos\phi}\right)^\nu \mathrm{d}\phi. \tag{A14}$$

Finally, writing $\tanh(r/2)$ in place of $|\zeta|$ [see formula (A10)], we obtain

$$\Phi_\nu(g) = \frac{1}{2\pi}\int_0^{2\pi}\frac{1}{(\cosh r + \sinh r\cos\phi)^\nu}\mathrm{d}\phi = \mathcal{P}_{-\nu}(\cosh r), \tag{A15}$$

where the last equality follows from the integral representation of the first kind Legendre functions.[12] Formula (A15) proves statement (i).

From formula (A15) it follows that the spherical functions $\Phi_\nu(g)$ are bi-k-invariant; indeed, using the Cartan decomposition, we have

$$\Phi_\nu(g) = \Phi_\nu(k_\theta a_r k_\phi) = \Phi_\nu(a_r) = \mathcal{P}_{-\nu}(\cosh r). \tag{A16}$$

Furthermore, we can prove that [see formulas (A13) and (A14)]

$$\Phi_\nu(E) = \int_B [P(E\cdot 0,b)]^\nu \, \mathrm{d}b = 1 = \mathcal{P}_{-\nu}(1). \tag{A17}$$

Let us now return to statement (ii) of Proposition 2, and recall that $P^\nu(\zeta,b)$ is an eigenfunction of the hyperbolic Laplace-Beltrami operator with eigenvalue $\nu(\nu-1)$. We then consider an integral of the following form:

$$\int_B [P(g\cdot 0,b)]^\nu \, \mathrm{d}b = \Phi_\nu(g). \tag{A18}$$

It can be proved that this integral superposition is still an eigenfunction of the hyperbolic Laplace-Beltrami operator Δ_D, having $\nu(\nu-1)$ as eigenvalue.[19] In particular, it follows that $\Phi_\nu(g)$ and $\Phi_{1-\nu}(g)$ $[g \in \mathrm{SU}(1,1)]$ are both eigenfunctions of Δ_D with the same eigenvalue, and therefore they coincide. We can thus state that $\mathcal{P}_{-1/2+i\lambda}(\cosh r) = \mathcal{P}_{-1/2-i\lambda}(\cosh r)$; statements (ii) and (iii) are thus proved.

Finally, from the representation of the Poisson kernel in terms of *horocyclic waves*, we have

$$\begin{aligned}\mathcal{P}_{-\frac{1}{2}+i\lambda}(\cosh r) &= \frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1}{\cosh r + \sinh r\cos\phi}\right)^{1/2-i\lambda}\mathrm{d}\phi \\ &= \frac{1}{2\pi}\int_0^{2\pi}\left(\frac{1-|\zeta|^2}{1+|\zeta|^2-2|\zeta|\cos\phi}\right)^{1/2-i\lambda}\mathrm{d}\phi = \int_B e^{\left(\frac{1}{2}-i\lambda\right)\langle\zeta,b\rangle}\,\mathrm{d}b \quad (\lambda\in\mathbb{R},\zeta\in D).\end{aligned} \tag{A19}$$

□

(C) In Sec. III, we have seen that it is possible to have a local isometric immersion from an horocycle to $\mathbb{R}^3$. The image of this immersion is a Beltrami pseudosphere. Now, we describe in more details the equation of the pseudosphere and its coordinates.

First, we want to recover the pseudosphere as a surface of revolution of a curve in $\mathbb{R}^3$. Let us recall that, in general, the position vector $\mathbf{r}$ of the surface of revolution generated by the rotation of a plane curve $z=\Phi(r)$ about the z axis is given by

$$\mathbf{r} = \begin{pmatrix} r\cos v \\ r\sin v \\ \Phi(r)\end{pmatrix}, \tag{A20}$$

where v varies between 0 and 2π. Here the circles $r=$const are the parallels and the curves $v=$const are the meridians. The first fundamental form associated with the surface (A20) is given by

$$I = \{1+[\Phi'(r)]^2\}\mathrm{d}r^2 + r^2\,\mathrm{d}v^2. \tag{A21}$$

We now rewrite the form (A21) as follows:

$$I = \mathrm{d}u^2 + r^2\,\mathrm{d}v^2, \tag{A22}$$

where

$$du = \sqrt{1 + [\Phi'(r)]^2}\,dr, \quad r = r(u). \tag{A23}$$

From the general Gauss' theory of surfaces, we have that the total curvature is given by[20]

$$K = -\frac{1}{r}\frac{d^2 r}{du^2}, \tag{A24}$$

whence the general pseudospherical surface of revolution with $K=-1/\rho^2$ adopts the form[20]

$$r(u) = c_1 \cosh\frac{u}{\rho} + c_2 \sinh\frac{u}{\rho}. \tag{A25}$$

In the case $c_1=c_2=c$, which corresponds to a parabolic pseudospherical surface of revolution, the meridians are given by

$$r(u) = ce^{u/\rho}, \tag{A26}$$

while

$$z = \Phi(r) = \int \sqrt{1 - \left(\frac{c}{\rho}\right)^2 e^{2u/\rho}}\,du. \tag{A27}$$

Then, the first fundamental form, with $c=1$, has the following expression:

$$I = du^2 + e^{2u/\rho}\,dv^2. \tag{A28}$$

The coordinates u,v are called *Beltrami coordinates*.

The substitution

$$\sin\varphi = \frac{c}{\rho}e^{u/\rho} \tag{A29}$$

in (A27) yields

$$z = \rho\left(\cos\varphi + \ln\left|\tan\frac{\varphi}{2}\right|\right). \tag{A30}$$

From formulas (A20), (A26), (A29), and (A30) we obtain

$$\mathbf{r} = \begin{pmatrix} \rho\sin\varphi\cos v \\ \rho\sin\varphi\sin v \\ \rho\left(\cos\varphi + \ln\left|\tan\frac{\varphi}{2}\right|\right) \end{pmatrix}, \tag{A31}$$

and the first fundamental form (in terms of φ and v) is

$$I = \rho^2\cot^2\varphi\,d\varphi^2 + \rho^2\sin^2\varphi\,dv^2. \tag{A32}$$

Equation (A31) is the parametric form of the parabolic pseudosphere, seen as surface of revolution about the z axis of the curve called *tractrix*, which satisfies the following property: the length of the tangent from the point where it touches the curve to the point where it intersects the z axis is constant and equal to $|\rho|$; φ is the angle that the tangent to the meridian makes with the z axis. The angle φ varies between 0 and π so that, keeping $\rho=1$, the related parabolic pseudosphere has vertices at $z=+\infty$ (corresponding to $\varphi=\pi$) and at $z=-\infty$ (corresponding to $\varphi=0$) and rim at $z=0$ (corresponding to $\varphi=\pi/2$). The curve is continuous and regular except at the point $z=0$, which is a cusp point. Choosing $\rho=-1$ and varying φ from 0 to π, we shall have the upward vertical z axis positively oriented (φ varying from 0 to $\pi/2$), and the downward vertical z axis negatively oriented (φ varying from $\pi/2$ to π). In accordance with the Hilbert's theorem, for

which it is impossible to embed the entire hyperbolic disk onto $\mathbb{R}^3$, and since we want the immersion from the horocycle to the pseudosphere to be regular, then the image must be contained either in the downward component or in the upward component of the pseudosphere; thus it does not contain the cuspidal rim. Accordingly, taking $\rho=-1$ once and for all, the first form, written in Beltrami coordinates, reads

$$I = \mathrm{d}u^2 + (e^{-u}\,\mathrm{d}v)^2 \quad (u \geqslant 0), \tag{A33}$$

and the tractrix is

$$\begin{aligned} x &= -\sin\varphi, \\ z &= -\left(\cos\varphi + \ln\left|\tan\frac{\varphi}{2}\right|\right). \end{aligned} \tag{A34}$$

Then, in Sec. III A we use the form (A33) with $u \geqslant 0$, varying φ from $\pi/2$ to 0 and, accordingly, $z \geqslant 0$ (see Fig. 2). In Sec. III B, where the coordinate u does not enter the game and we have chosen the coordinates p and q, it is convenient to vary φ from $\pi/2$ to π and, in accordance, taking the downward vertical axis negatively oriented, i.e., $z \leqslant 0$.

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Schouten tensor and bi-Hamiltonian systems of hydrodynamic type

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The necessary conditions are derived for existence of a bi-Hamiltonian structure for a given hydrodynamic type system. One of the conditions is the vanishing of its Haantjes tensor. A theorem is proved on the canonical forms of the generic bi-Hamiltonian systems. The Schouten (2,1)-tensor S_i^{jk} is connected with any Hamiltonian system of hydrodynamic type. The complete symmetry of the (3,0)-tensor S^{ijk} is demonstrated. The necessary conditions for existence of a single nondegenerate Hamiltonian structure are obtained in terms of the special differential k-forms $\Omega_{p_1\cdots p_k}(u_1,\ldots,u_k)$. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We present new applications of the Schouten (2,1)-tensor S_i^{jk} (Ref. 1) that exists for any (2,0)-tensor g^{ij} and any (1,1)-tensor A_k^j satisfying the equation

$$g^{i\alpha}A_\alpha^j = A_\alpha^i g^{\alpha j}. \tag{1.1}$$

Equation (1.1) naturally arises in the theory of bi-Hamiltonian dynamical systems[2–8]

$$\dot{x}^i = P_1^{i\alpha}\frac{\partial H_1(x)}{\partial x^\alpha} = P_2^{i\alpha}\frac{\partial H_2(x)}{\partial x^\alpha} \tag{1.2}$$

and in the theory of Hamiltonian systems of hydrodynamic type[9–11]

$$\frac{\partial u^i}{\partial t} = \sum_{j=1}^{n} A_j^i(u^1,\ldots,u^n)\frac{\partial u^j}{\partial x}. \tag{1.3}$$

For systems (1.3), $u^i = u^i(t,x)$ are unknown functions and $A_j^i(u)$ form a (1,1)-tensor on a manifold M^n with charts of local coordinates $u^1,\ldots,u^n$.

For a bi-Hamiltonian dynamical system (1.2), the (2,0)-tensor g^{ij} is one of the Poisson structures P_1^{ij} or P_2^{ij} and the (1,1)-tensor A_k^j is the recursion operator $A_k^j = P_1^{j\alpha}(P_2^{-1})_{\alpha k}$ provided that the Poisson structure P_2^{ij} is nondegenerate.

For the Hamiltonian systems (1.3) with a local or nonlocal structure of Poisson brackets, the (1,1)-tensor $A_j^i(u)$ is given by the formula

$$A_j^i(u) = g^{i\alpha}(u)\frac{\partial^2 f(u)}{\partial u^\alpha\,\partial u^j} + b_j^{i\alpha}(u)\frac{\partial f(u)}{\partial u^\alpha} + Kf(u)\delta^i_j, \tag{1.4}$$

where symmetric (2,0)-tensor $g^{ij}(u)$ and coefficients $b_j^{ik}(u)$ are connected by certain nonlinear equations that follow from the Jacobi identity;[9–11] $f(u)$ is the density of the Hamiltonian functional. Equation (1.1) holds for all Hamiltonian system (1.3) and (1.4) and thus allows to relate with them the Schouten (2,1)-tensor S_i^{jk}.[12]

In the paper, we show that for any Hamiltonian system (1.3) and (1.4) the corresponding Schouten (3,0)-tensor $S^{ijk}=g^{i\alpha}S^{jk}_{\alpha}$ is completely symmetric, even when the (2,0)-tensor g^{jk} is degenerate and the Hamiltonian structure is nonlocal, $K\neq 0$. In Ref. 12, we proved the symmetry of S^{ijk} for some special cases. The symmetry implies certain algebraic identities for the Nijenhuis and Haantjes tensors of the (1,1)-tensor $A^i_j(u)$.

We derive necessary conditions for existence of bi-Hamiltonian structures (1.4) having two different (2,0)-tensors g_1^{jk} and g_2^{jk}. Since the tensors $g_1^{ij}(u)$ and $g_2^{ij}(u)$ are not given *a priori*, the necessary conditions are formulated for the (1,1)-tensor $A^i_j(u)$ only, namely in terms of its Nijenhuis and Haantjes tensors[13,14] and in terms of the special differential k-forms $\Omega_{p_1\cdots p_k}(u_1,\ldots,u_k)$ introduced in this paper.

For the bi-Hamiltonian systems (1.3) and (1.4) with nondegenerate (2,0)-tensor g_2^{jk} and the (1,1)-tensor $B^i_j=g_1^{i\alpha}(g_2^{-1})_{\alpha j}$ having distinct eigenvalues we prove that the Haantjes (1,2)-tensor H^i_{jk} necessarily vanishes. For hyperbolic systems (1.3) with real and distinct eigenvalues of the (1,1)-tensor $A^i_j(u)$, this implies the existence of Riemann invariants for the system (1.3) and (1.4) and hence its integrability by the generalized hodograph transform.[15] For the generic bi-Hamiltonian systems with complex eigenvalues of $A^i_j(u)$, we prove a theorem on their canonical forms.

II. SCHOUTEN TENSORS FOR BI-HAMILTONIAN SYSTEMS

For any (1,1)-tensor A^i_k and the (2,0)-tensor g^{jk} on the manifold M^n satisfying Eq. (1.1), Schouten introduced the (2,1)-tensor,

$$S^{jk}_i=A^{\alpha}_i\frac{\partial g^{jk}}{\partial x^{\alpha}}-g^{j\alpha}\frac{\partial A^k_i}{\partial x^{\alpha}}-g^{\alpha k}\frac{\partial A^j_i}{\partial x^{\alpha}}+g^{j\alpha}\frac{\partial A^k_{\alpha}}{\partial x^i}-A^j_{\alpha}\frac{\partial g^{\alpha k}}{\partial x^i}. \tag{2.1}$$

In Ref. 12, we show that the Schouten tensor has the following invariant meaning: for any vector field $u(x)=u^i(x)$ on the manifold M^n the (2,0)-tensor $(S_u)^{jk}=S^{jk}_i u^i$ has the form

$$S_u=L_{Au}g-AL_ug+gL_uA, \tag{2.2}$$

where L_u is the Lie derivative operator with respect to the vector field $u(x)$.

Suppose a system (1.3) has two Hamiltonian structures (1.4) with two different (2,0)-tensors g_1^{jk} and g_2^{jk}. Then two equations (1.1) hold,

$$g_1^{i\alpha}A^j_{\alpha}=A^i_{\alpha}g_1^{\alpha j},\quad g_2^{i\alpha}A^j_{\alpha}=A^i_{\alpha}g_2^{\alpha j}. \tag{2.3}$$

Hence for any parameter λ we have

$$g_{\lambda}^{i\alpha}A^j_{\alpha}=A^i_{\alpha}g_{\lambda}^{\alpha j}, \tag{2.4}$$

where $g_{\lambda}=\lambda g_1+g_2$. Suppose that for some λ the (2,0)-tensor g_{λ} is nondegenerate and define the (1,1)-tensor $B^i_{\lambda j}=g_1^{i\alpha}(g_{\lambda}^{-1})_{\alpha j}$. As is known, Eqs. (2.3) and (2.4) imply that the operators A^i_j and $B^j_{\lambda k}$ commute,

$$AB_{\lambda}=B_{\lambda}A. \tag{2.5}$$

Evidently we have $g_1=B_{\lambda}g_{\lambda}$. Hence for the corresponding Schouten tensor S_{1u} (2.2) we get

$$S_{1u}=L_{Au}(B_{\lambda}g_{\lambda})-AL_u(B_{\lambda}g_{\lambda})+B_{\lambda}g_{\lambda}L_uA.$$

Applying the Leibniz formula and Eq. (2.5), we find

$$S_{1u}=B_{\lambda}(L_{Au}g_{\lambda}-AL_ug_{\lambda}+g_{\lambda}L_uA)+(L_{Au}B_{\lambda}-AL_uB_{\lambda})g_{\lambda}. \tag{2.6}$$

The first parentheses here evidently is the Schouten tensor

$$S_{\lambda u} = L_{Au} g_\lambda - A L_u g_\lambda + g_\lambda L_u A = \lambda S_{1u} + S_{2u}.$$

The second parentheses for the two commuting operators A and B_λ is the Nijenhuis tensor.[13] Indeed, for any two vector fields U and V and (1,1)-tensor A we have $(L_U A)V = [U, AV] - A[U, V]$. Hence we have

$$(L_{Au} B_\lambda - A L_u B_\lambda)v = [Au, B_\lambda v] - B_\lambda [Au, v] - A[u, B_\lambda v] + A B_\lambda [u, v], \tag{2.7}$$

$$(L_{B_\lambda v} A - B_\lambda L_v A)u = [B_\lambda v, Au] - A[B_\lambda v, u] - B_\lambda [v, Au] + B_\lambda A[v, u]. \tag{2.8}$$

Formula (2.7) does not depend on a smooth continuation of vector v, and formula (2.8) does not depend on a continuation of vector u. Since $AB_\lambda = B_\lambda A$, these formulas differ only by sign. Therefore $\widetilde{N}_{\lambda u} = L_{Au} B_\lambda - A L_u B_\lambda$ is a tensor; its components are

$$\widetilde{N}^i_{\lambda jk} = A^\alpha_j \frac{\partial B^i_{\lambda k}}{\partial x^\alpha} - B^\alpha_{\lambda k} \frac{\partial A^i_j}{\partial x^\alpha} + B^i_{\lambda \alpha} \frac{\partial A^\alpha_j}{\partial x^k} - A^i_\alpha \frac{\partial B^\alpha_{\lambda k}}{\partial x^j}. \tag{2.9}$$

Thus Eq. (2.6) has the form

$$S^{jk}_{1i} = B^j_{\lambda \alpha} S^{\alpha k}_{\lambda i} + \widetilde{N}^j_{\lambda i \alpha} g^{\alpha k}_\lambda,$$

that gives the following relation between the two Schouten tensors:

$$S^{jk}_{1i} = B^j_{\lambda \alpha} (\lambda S^{\alpha k}_{1i} + S^{\alpha k}_{2i}) + \widetilde{N}^j_{\lambda i \alpha} (\lambda g^{\alpha k}_1 + g^{\alpha k}_2). \tag{2.10}$$

Equation (2.10) depends on an arbitrary parameter λ.

III. SHOUTEN TENSOR S^{ijk} FOR ANY HAMILTONIAN SYSTEM (1.3) IS COMPLETELY SYMMETRIC

(i) It is evident that the Schouten tensor (2.1) has also the form

$$S^{jk}_i = A^\alpha_i \frac{\partial g^{jk}}{\partial x^\alpha} - \frac{\partial (A^k_\alpha g^{j\alpha})}{\partial x^i} + g^{j\alpha} \left(\frac{\partial A^k_\alpha}{\partial x^i} - \frac{\partial A^k_i}{\partial x^\alpha} \right) + \left(\frac{\partial A^j_\alpha}{\partial x^i} - \frac{\partial A^j_i}{\partial x^\alpha} \right) g^{\alpha k}. \tag{3.1}$$

Therefore for any symmetric (2,0)-tensor g^{ij} the Schouten tensor (3.1) has the following symmetry:

$$S^{jk}_i = S^{kj}_i. \tag{3.2}$$

Hence the Schouten (3,0)-tensor $S^{ijk} = g^{i\alpha} S^{jk}_\alpha$ possesses the partial symmetry, $S^{ijk} = S^{ikj}$.

Let us consider a nonlinear system of hydrodynamic type

$$u^i_t = \sum_{j=1}^n A^i_j (u^1, \ldots, u^n) u^j_x, \tag{3.3}$$

where $u^i(t,x)$ are unknown functions. Note that for the systems of hydrodynamic type (3.3) the variables $u^1, \ldots, u^n$ play the role of the coordinates $x^1, \ldots, x^n$ of Sec. II.

The Poisson brackets structure for the Hamiltonian systems (3.3) is defined by the operator $I^{ij}(u)$ for the local[9] and nonlocal case $K \neq 0$,[10,11]

$$I^{ij}(u) = g^{ij}(u) \frac{\partial}{\partial x} + b^{ij}_k(u) u^k_x + K u^i_x \left(\frac{\partial}{\partial x} \right)^{-1} u^j_x. \tag{3.4}$$

The corresponding Hamiltonian systems (3.3) have the form

$$u_t^i = I^{i\alpha}(u)\frac{\partial f(u)}{\partial u^\alpha} = A_j^i(u^1, \ldots, u^n)u_x^j, \tag{3.5}$$

with the following (1,1)-tensors $A_j^i(u)$:

$$A_j^i(u) = g^{i\alpha}(u)\frac{\partial^2 f(u)}{\partial u^\alpha\, \partial\, u^j} + b_j^{i\alpha}(u)\frac{\partial f(u)}{\partial u^\alpha} + Kf(u)\delta^i_j, \tag{3.6}$$

where $f(u)$ is the density of the Hamiltonian functional.

(ii) First we study the Hamiltonian systems (3.5) and (3.6) with the nondegenerate (2,0)-tensor g^{jk}. As is known,[9–11] such (2,0)-tensor $g^{ij}(u)$ corresponds to a metric $g_{ij}(u)$ of constant curvature K. The corresponding (1,1)-tensor $A_j^i(u)$ (3.6) has the invariant form

$$A_j^i(u) = g^{i\alpha}f(u)_{;\alpha;j} + Kf(u)\delta^i_j, \tag{3.7}$$

where $(;\alpha)$ means the g_{ij}-covariant derivative with respect to variable u^α.

Proposition 1: For the (1,1)*-tensor* A_j^i (3.7) *and nondegenerate* (2,0)*-tensor* g^{ij}, *the Schouten* (3,0)*-tensor* S^{ijk} *is completely symmetric.*

Proof: For $K=0$, the metric $g_{ij}(u)$ is flat and hence is constant and diagonal in some coordinates $v^1, \ldots, v^n$, $g^{ij}(v)=q^i\delta^i_j$. The corresponding (1,1)-tensor (3.7) takes the form[9]

$$A_j^i(v) = q^i\frac{\partial^2 f(v)}{\partial v^i\, \partial\, v^j}. \tag{3.8}$$

Hence the definition (2.1) yields the following formula for the Schouten (3,0)-tensor:

$$S^{ijk} = -\,q^iq^jq^k\frac{\partial^3 f(v)}{\partial v^i\, \partial\, v^j\, \partial\, v^k}. \tag{3.9}$$

Tensor (3.9) is evidently symmetric in the coordinates $v^1, \ldots, v^n$, hence it is completely symmetric in any coordinates $u^1, \ldots, u^n$.

For $K \neq 0$, the proof is presented in paper.[12] □

Remark 1: Formulas (3.8) and (3.9) yield that if the Schouten (2,1)-tensor S_i^{jk} is zero for a nondegenerate Hamiltonian system (1.3) and (1.4) with $K=0$ then the system is linearizable in some coordinates $v^1, \ldots, v^n$.

Remark 2: Let us consider the invariant function $h(u)=A_j^i(u)A_i^j(u)=\mathrm{Tr}\,A^2(u)$. Formula (3.8) implies

$$h(v) = \sum_{i,j} q^iq^j\left(\frac{\partial^2 f(v)}{\partial v^i\, \partial\, v^j}\right)^2. \tag{3.10}$$

Hence if a system (1.3) has a Hamiltonian structure (1.4) with positive (or negative) definite metric g^{jk} and $K=0$ then necessarily $h(u)\geqslant 0$. Thus if $h(u)\leqslant 0$ then the metric g^{jk} must be indefinite.

(iii) The operator $I^{ij}(u)$ (3.4) defines a structure of Poisson brackets

$$\{\hat{F}_1(u), \hat{F}_2(u)\} = \int_{-\infty}^{\infty}\frac{\delta F_1(u)}{\delta u^i(x)}I^{ij}(u)\frac{\delta F_2(u)}{\delta u^j(x)}\mathrm{d}x \tag{3.11}$$

for the local functionals

$$\hat{F}_\gamma = \int_{-\infty}^{\infty} F_\gamma(u, u_x, u_{xx}, \dots)\mathrm{d}x.$$

The coefficients $g^{ij}(u)$ and $b_k^{ij}(u)$ (3.4) satisfy certain equations[9,11] that follow from the conditions that the Poisson brackets (3.11) are skew and the Jacobi identity holds. The skew-symmetricity condition for the Poisson brackets (3.11) is equivalent to the equations

$$g^{ij} = g^{ji}, \tag{3.12}$$

$$\frac{\partial g^{ij}}{\partial u^k} = b_k^{ij} + b_k^{ji}. \tag{3.13}$$

The Jacobi identity for the Poisson brackets (3.11) is equivalent to the relations[11]

$$b_\alpha^{ik} g^{\alpha j} = b_\alpha^{jk} g^{\alpha i}, \tag{3.14}$$

$$\left(\frac{\partial b_\alpha^{jr}}{\partial u^k} - \frac{\partial b_k^{jr}}{\partial u^\alpha}\right) g^{\alpha i} + b_\alpha^{ij} b_k^{\alpha r} - b_\alpha^{ir} b_k^{\alpha j} + K(g^{ij}\delta^r_k - g^{ir}\delta^j_k) = 0, \tag{3.15}$$

$$\sum_{\sigma,\tau}\left(\frac{\partial b_{\tau(k)}^{\sigma(i)\sigma(j)}}{\partial u^\alpha} - \frac{\partial b_\alpha^{\sigma(i)\sigma(j)}}{\partial u^{\tau(k)}}\right) b_{\tau(s)}^{\alpha\sigma(m)} + K(b_{\tau(k)}^{\sigma(m)\sigma(i)} - b_{\tau(k)}^{\sigma(i)\sigma(m)})\delta_{\tau(s)}^{\sigma(j)} = 0. \tag{3.16}$$

Here summation is taken with respect to index α and in (3.16) with respect to the three cyclic permutations σ of indices i, j, m and two transpositions τ of indices k and s.

For the (1,1)-tensor $A_j^i(u)$ (3.6), we have

$$A_\alpha^i g^{\alpha j} - g^{i\alpha} A_\alpha^j = (g^{i\beta} g^{j\alpha} - g^{i\alpha} g^{j\beta}) \frac{\partial^2 f(u)}{\partial u^\alpha \partial u^\beta} + (b_\alpha^{i\beta} g^{\alpha j} - b_\alpha^{j\beta} g^{\alpha i}) \frac{\partial f(u)}{\partial u^\beta}.$$

This expression is zero in view of Eqs. (3.12) and (3.14). Hence the (1,1)-tensor $A_j^i(u)$ (3.6) satisfies the equation[9] $g^{i\alpha} A_\alpha^j = A_\alpha^i g^{\alpha j}$ (1.1) and therefore the corresponding Schouten (2,1)-tensor S_i^{jk} (3.1) does exist and satisfies Eq. (3.2), $S_i^{jk} = S_i^{kj}$.

Theorem 1: *For any Hamiltonian system of hydrodynamic type* (3.5) and (3.6), *the Schouten (3,0)-tensor S^{ijk} is completely symmetric*.

Proof: In view of Eq. (1.1), formula (3.1) implies

$$S^{ijk} = g^{i\beta} S_\beta^{jk} = A_\alpha^i \frac{\partial g^{jk}}{\partial u^\beta} g^{\beta\alpha} + A_\alpha^j \left(\frac{\partial g^{i\alpha}}{\partial u^\beta} g^{\beta k} - \frac{\partial g^{\alpha k}}{\partial u^\beta} g^{\beta i}\right) + \left(\frac{\partial A_\alpha^k}{\partial u^\beta} - \frac{\partial A_\beta^k}{\partial u^\alpha}\right) g^{\alpha j} g^{\beta i} - \frac{\partial (g^{i\beta} A_\beta^j)}{\partial u^\alpha} g^{\alpha k}. \tag{3.17}$$

In view of (1.1), the last term in (3.17) is symmetric with respect to the indices i, j. Hence formula (3.17) yields

$$\begin{aligned} S^{ijk} - S^{jik} = {} & A_\alpha^i \left(\frac{\partial g^{jk}}{\partial u^\beta} g^{\beta\alpha} - \frac{\partial g^{j\alpha}}{\partial u^\beta} g^{\beta k} + \frac{\partial g^{\alpha k}}{\partial u^\beta} g^{\beta j}\right) - A_\alpha^j \left(\frac{\partial g^{ik}}{\partial u^\beta} g^{\beta\alpha} - \frac{\partial g^{i\alpha}}{\partial u^\beta} g^{\beta k} + \frac{\partial g^{\alpha k}}{\partial u^\beta} g^{\beta i}\right) \\ & + 2\left(\frac{\partial A_\alpha^k}{\partial u^\beta} - \frac{\partial A_\beta^k}{\partial u^\alpha}\right) g^{\alpha j} g^{\beta i}. \end{aligned} \tag{3.18}$$

Let us prove that the expression (3.18) vanishes. Using formulas (3.13) and (3.14), we find

$$\frac{\partial g^{jk}}{\partial u^\beta} g^{\beta\alpha} - \frac{\partial g^{j\alpha}}{\partial u^\beta} g^{\beta k} + \frac{\partial g^{\alpha k}}{\partial u^\beta} g^{\beta j} = 2b_\beta^{jk} g^{\beta\alpha}. \tag{3.19}$$

The formulas (3.6) and (3.13) imply

$$\frac{\partial A_\beta^k}{\partial u^\alpha} = g^{k\gamma} \frac{\partial^3 f(u)}{\partial u^\gamma \partial u^\beta \partial u^\alpha} + b_\beta^{k\gamma} \frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\alpha} + b_\alpha^{k\gamma} \frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\beta} + b_\alpha^{\gamma k} \frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\beta} + \frac{\partial b_\beta^{k\gamma}}{\partial u^\alpha} \frac{\partial f(u)}{\partial u^\gamma} + K \frac{\partial f(u)}{\partial u^\alpha} \delta_\beta^k. \tag{3.20}$$

Here the sum of the first three terms is evidently symmetric with respect to the indices α, β; hence these summands can be cancelled in the last term of (3.18). Substituting the formulas (3.19) and (3.20) into (3.18), we find

$$S^{ijk} - S^{jik} = 2(A_\alpha^i b_\beta^{jk} - A_\alpha^j b_\beta^{ik}) g^{\beta\alpha} + 2\left(\frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\alpha} b_\beta^{\gamma k} - \frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\beta} b_\alpha^{\gamma k} \right) g^{\alpha j} g^{\beta i}$$
$$+ 2 \frac{\partial f(u)}{\partial u^\gamma} \left(\frac{\partial b_\alpha^{k\gamma}}{\partial u^\beta} - \frac{\partial b_\beta^{k\gamma}}{\partial u^\alpha} \right) g^{\alpha j} g^{\beta i} + 2K \left(\frac{\partial f(u)}{\partial u^\beta} \delta_\alpha^k - \frac{\partial f(u)}{\partial u^\alpha} \delta_\beta^k \right) g^{\alpha j} g^{\beta i}.$$

Substituting here expressions (3.6) and using Eqs. (3.14), we obtain

$$S^{ijk} - S^{jik} = 2 \frac{\partial^2 f(u)}{\partial u^\gamma \partial u^\alpha} [(g^{i\gamma} b_\beta^{\alpha k} - g^{i\alpha} b_\beta^{\gamma k}) g^{\beta j} + (g^{j\alpha} b_\beta^{\gamma k} - g^{j\gamma} b_\beta^{\alpha k}) g^{\beta i}] + 2 \frac{\partial f(u)}{\partial u^\gamma} g^{i\beta} \Bigg[\left(\frac{\partial b_\alpha^{k\gamma}}{\partial u^\beta} - \frac{\partial b_\beta^{k\gamma}}{\partial u^\alpha} \right) g^{\alpha j}$$
$$+ b_\alpha^{jk} b_\beta^{\alpha\gamma} - b_\alpha^{j\gamma} b_\beta^{\alpha k} + K(g^{kj} \delta_\beta^\gamma - g^{\gamma j} \delta_\beta^k) \Bigg] + 2Kf(u)(b_\beta^{jk} g^{\beta i} - b_\beta^{ik} g^{\beta j}). \tag{3.21}$$

The first square brackets in (3.21) vanishes in view of the equality of the mixed derivatives, $f_{,\gamma,\alpha} = f_{,\alpha,\gamma}$. The second square bracket is zero because it coincides with Eq. (3.15) after changing the indices k, γ, β, j into j, r, k, i, respectively. Finally the last bracket is zero in view of Eq. (3.14). Thus the equality $S^{ijk} = S^{jik}$ is proven. Together with the equality (3.2) this implies that the Schouten (3,0)-tensor S^{ijk} is completely symmetric. □

IV. TENSOR M^j_{ik} AND DIFFERENTIAL k-FORMS $\Omega_{p_1 \dots p_k}$

(i) The Haantjes (1,2)-tensor[14] is defined by the formula

$$H(u,v) = A^2 N(u,v) + N(Au,Av) - AN(Au,v) - AN(u,Av). \tag{4.1}$$

Here $N(u,v)$ is the Nijenhuis (1,2)-tensor[13]

$$N(u,v) = A^2[u,v] + [Au,Av] - A[Au,v] - A[u,Av], \tag{4.2}$$

where $[u,v]$ is the commutator of any two vector fields that continually extend the given tangent vectors. The Nijenhuis tensor (4.2) has the following components:

$$N_{jk}^i = A_j^\alpha \frac{\partial A_k^i}{\partial x^\alpha} - A_k^\alpha \frac{\partial A_j^i}{\partial x^\alpha} + A_\alpha^i \frac{\partial A_j^\alpha}{\partial x^k} - A_\alpha^i \frac{\partial A_k^\alpha}{\partial x^j}. \tag{4.3}$$

The components of the Haantjes tensor are

$$H_{jk}^i = A_\alpha^i A_\beta^\alpha N_{jk}^\beta + N_{\alpha\beta}^i A_j^\alpha A_k^\beta - A_\alpha^i N_{\beta k}^\alpha A_j^\beta - A_\alpha^i N_{j\beta}^\alpha A_k^\beta. \tag{4.4}$$

The skew-symmetricity of the Nijenhuis (1,2)-tensor, $N_{jk}^i = -N_{kj}^i$, evidently yields $H_{jk}^i = -H_{kj}^i$. Raising up indices j and k in (4.4) by contractions with the (2,0)-tensor $g^{\alpha\beta}$ and using Eq. (1.1), we obtain for the Haantjes (3,0)-tensor $H^{ijk} = H_{\alpha\beta}^i g^{\alpha j} g^{\beta k}$,

$$H^{ijk} = A_\alpha^i A_\beta^\alpha N^{\beta jk} + N^{i\alpha\beta} A_\alpha^j A_\beta^k - A_\alpha^i N^{\alpha\beta k} A_\beta^j - A_\alpha^i N^{\alpha j\beta} A_\beta^k.$$

(ii) Let us consider the (1,2)-tensor[16]

$$M(u,v) = N(Au,v) - AN(u,v), \tag{4.5}$$

that has the following components:

$$M^j_{ik} = N^j_{\alpha k}A^\alpha_i - A^j_\alpha N^\alpha_{ik}. \tag{4.6}$$

Contracting (4.6) with any tangent vector $V^i \in T_x(M^n)$, we obtain the operator

$$M_V = N_{AV} - AN_V. \tag{4.7}$$

For the operator H_V corresponding to the Haantjes tensor (4.1), (4.4), we find

$$H_V = N_{AV}A - AN_VA - AN_{AV} + A^2N_V = M_VA - AM_V. \tag{4.8}$$

Definition 1: For any two non-negative integers p and q, we define the differential 2-form

$$\Omega_{pq}(u,v) = \mathrm{Tr}(M_uA^pM_vA^q - M_vA^pM_uA^q), \tag{4.9}$$

where u,v are tangent vectors $u,v \in T_x(M^n)$. For any non-negative integers $p_1,\dots,p_k$ and tangent vectors $u_1,\dots,u_k$, we introduce the differential k-form

$$\Omega_{p_1\dots p_k}(u_1,\dots,u_k) = \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_1)}A^{p_1},\dots,M_{\tau(u_k)}A^{p_k}), \tag{4.10}$$

where summation is taken over all permutations τ of k symbols.

It is evident that the forms (4.9) and (4.10) are skew-symmetric.

Definition 2: For any non-negative integer p we introduce a (1,3)-tensor L_p that defines for any three vectors v^j, w^k, u^m a vector

$$\begin{aligned} L_p(v,w,u) &= M(v,A^pM(w,u)) - M(w,A^pM(v,u)) \\ &= N(Av,A^pN(Aw,u)) - N(Aw,A^pN(Av,u)) + N(Aw,A^{p+1}N(v,u)) \\ &\quad - N(Av,A^{p+1}N(w,u)) + AN(w,A^pN(Av,u)) - AN(v,A^pN(Aw,u)) \\ &\quad + AN(v,A^{p+1}N(w,u)) - AN(w,A^{p+1}N(v,u)). \end{aligned} \tag{4.11}$$

It is evident that

$$L_p(v,w,u) = (M_vA^pM_w - M_wA^pM_v)u. \tag{4.12}$$

(iii) The (1,2)-tensor M^j_{ik} (4.6) leads to the following (3,0)-tensor

$$M^{jik} = M^j_{\beta\gamma}g^{\beta i}g^{\gamma k} = N^j_{\alpha\gamma}A^\alpha_\beta g^{\beta i}g^{\gamma k} - A^j_\alpha N^\alpha_{\beta\gamma}g^{\beta i}g^{\gamma k},$$

that in view of Eq. (1.1) has the form

$$M^{jik} = N^{j\beta k}A^i_\beta - A^j_\beta N^{\beta ik}, \tag{4.13}$$

where $N^{ijk}=N^i_{\alpha\beta}g^{\alpha j}g^{\beta k}$. The skew-symmetricity of the Nijenhuis (1,2)-tensor N^i_{jk} yields $N^{ijk} = -N^{ikj}$.

Lemma 1: The (3,0)*-tensor* M^{jik} *possesses the partial symmetry*,

$$M^{jik} = M^{kij}, \tag{4.14}$$

provided that the Schouten (3,0)*-tensor* S^{ijk} *is completely symmetric.*

Proof: In Ref. 12, we prove that the Schouten (2,1)-tensor S^{jk}_i (3.1) and the Nijenhuis (1,2)-tensor N^j_{ik} (4.3) satisfy the identity

$$S_u A - A S_u = N_u g - g N_u,$$

that has the following form in the components:

$$S_i^{j\alpha} A_\alpha^k - A_\alpha^j S_i^{\alpha k} = N_{i\alpha}^j g^{\alpha k} - g^{j\alpha} N_{i\alpha}^k. \tag{4.15}$$

As is shown in Ref. 12, for the completely symmetric Schouten tensor S^{ijk} identity (4.15) implies

$$N^{ijk} = S^{ij\alpha} A_\alpha^k - S^{ik\alpha} A_\alpha^j. \tag{4.16}$$

Equations (4.13) and (4.16) yield

$$M^{jik} = A_\beta^i (S^{j\beta\alpha} A_\alpha^k + S^{\alpha k\beta} A_\alpha^j) - S^{jk\alpha} A_\beta^i A_\alpha^\beta - S^{\alpha i\beta} A_\alpha^j A_\beta^k.$$

This expression obviously possesses symmetry (4.14). □

Remark 3: It is evident that Eq. (4.14) has the form

$$(M_{\alpha\beta}^j g^{\beta k} - M_{\alpha\beta}^k g^{\beta j}) g^{\alpha i} = 0.$$

Hence for any tangent vector V of the form $V^\alpha = g^{\alpha i}\omega_i$ we find for the operator M_V (4.7), $M_{V\beta}^j g^{\beta k} = M_{V\beta}^k g^{\beta j}$. This equality has the following matrix form:

$$M_V g = g M_V^t. \tag{4.17}$$

We denote L_{kx} a linear subspace $L_{kx} \subset T_x(M^n)$ consisting of all vectors $V^i = g_k^{i\alpha}\omega_\alpha$ where ω_α are arbitrary covectors, and $k = 1,2$.

Lemma 2: Suppose that a hydrodynamic type system (1.3) *is bi-Hamiltonian, so it has two Hamiltonian forms* (1.4) *with two* (2,0)*-tensors* g_1^{jk} *and* g_2^{jk}. *Assume that tensor* $g_\lambda^{jk} = \lambda g_1^{jk} + g_2^{jk}$ *is nondegenerate. Then the* (1,1)*-tensor* $B_{\lambda k}^j = g_1^{j\alpha}(g_\lambda^{-1})_{\alpha k}$ *commutes with all* (1,1)*-tensors* M_V *and A where* $V \in L_{1x} \cap L_{2x}$, *or* $V^i = g_1^{i\alpha}\omega_\alpha = g_2^{i\alpha}\eta_\alpha$.

Proof: For the two Hamiltonian structures (1.4), the commutativity equation (2.5) holds. For the two (2,0)-tensors g_1 and g_2 equations (4.17) yield

$$g_1 M_V^t = M_V g_1, \quad g_2 M_V^t = M_V g_2,$$

for vectors $V \in L_{1x} \cap L_{2x}$. Hence we find $g_\lambda M_V^t = M_V g_\lambda$ and the commutativity equation

$$B_\lambda M_V = M_V B_\lambda \tag{4.18}$$

follows. □

V. NECESSARY CONDITIONS FOR EXISTENCE OF A NONDEGENERATE HAMILTONIAN STRUCTURE

Theorem 2: *For existence of a nondegenerate Hamiltonian structure* (1.3) and (1.4) *the following necessary conditions must hold:*

- *(a) the differential 2-forms* $\Omega_{pq}(u,v)$ *(4.9) vanish for all p and q;*
- *(b) the differential k-forms* $\Omega_{p_1 \cdots p_k}(u_1, \ldots, u_k)$ *(4.10) vanish if (1)* $p_i = p_{k-i}$ *for* $k = 4m+2$, *and* $k = 4m+3$ *or if (2)* $p_i = p_{k-i+1}$ *for* $k = 4m$, *and* $k = 4m+3$.

Proof: (a) If a Hamiltonian structure (1.3) and (1.4) exists and has a nondegenerate (2,0)-tensor g^{jk}, then Eq. (4.17) holds for all vectors $V \in T_x(M^n)$. Hence for any two tangent vectors u and v we have

$$M_u^t = g^{-1} M_u g, \quad M_v^t = g^{-1} M_v g, \quad A^t = g^{-1} A g. \tag{5.1}$$

Using these equalities, we obtain for the 2-form $\Omega_{pq}(u,v)$ (4.9),

$$\begin{aligned}\Omega_{pq}(u,v) &= \mathrm{Tr}(M_u A^p M_v A^q - M_v A^p M_u A^q)^t \\ &= \mathrm{Tr}(A^{qt} M_v^t A^{pt} M_u^t - A^{qt} M_u^t A^{pt} M_v^t) \\ &= \mathrm{Tr}(g^{-1}(A^q M_v A^p M_u - A^q M_u A^p M_v) g) = \Omega_{pq}(v,u) = -\Omega_{pq}(u,v). \end{aligned} \tag{5.2}$$

Hence $\Omega_{pq}(u,v) \equiv 0$.

(b) At the same assumptions, applying equalities (5.1) we find for the k-form (4.10),

$$\begin{aligned}\Omega_{p_1 \dots p_k}(u_1, \dots, u_k) &= \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_1)} A^{p_1} \cdots M_{\tau(u_k)} A^{p_k})^t \\ &= \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(A^{p_k t} M^t_{\tau(u_k)} \cdots A^{p_1 t} M^t_{\tau(u_1)}) \\ &= \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(g^{-1}(A^{p_k} M_{\tau(u_k)} \cdots A^{p_1} M_{\tau(u_1)}) g) \\ &= \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_k)} A^{p_{k-1}} \cdots A^{p_1} M_{\tau(u_1)} A^{p_k}) \\ &= \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_1)} A^{p_k} M_{\tau(u_k)} \cdots M_{\tau(u_2)} A^{p_1}). \end{aligned} \tag{5.3}$$

(1) Suppose that $p_i = p_{k-i}$. Then we get from (5.3),

$$\Omega_{p_1 \dots p_k}(u_1, \dots, u_k) = \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_k)} A^{p_{k-1}} \cdots A^{p_1} M_{\tau(u_1)} A^{p_k}) = \mathrm{sign}(\sigma_1)\Omega_{p_1 \dots p_k}(u_1, \dots, u_k), \tag{5.4}$$

where σ_1 is the permutation $\sigma_1(j) = p - j + 1$. It is evident that $\mathrm{sign}(\sigma_1) = (-1)^{k(k-1)/2}$. Hence for $k = 4m+2$ and $k = 4m+3$ we have $\mathrm{sign}(\sigma_1) = -1$ and the equality (5.4) yields $\Omega_{p_1 \dots p_k}(u_1, \dots, u_k) \equiv 0$. This case is realized for the 2-forms $\Omega_{pq}(u,v)$ above.

(2) Suppose that $p_i = p_{k-i+1}$. Then we get from the last equality (5.3),

$$\Omega_{p_1 \dots p_k}(u_1, \dots, u_k) = \sum_\tau \mathrm{sign}(\tau)\mathrm{Tr}(M_{\tau(u_1)} A^{p_k} M_{\tau(u_k)} \cdots M_{\tau(u_2)} A^{p_1}) = \mathrm{sign}(\sigma_2)\Omega_{p_1 \dots p_k}(u_1, \dots, u_k), \tag{5.5}$$

where σ_2 is the permutation $\sigma_2(1) = 1$, $\sigma_2(j) = k - j + 2$. Hence $\mathrm{sign}(\sigma_2) = (-1)^{(k-1)(k-2)/2}$ and for $k = 4m$ and $k = 4m+3$ we get $\mathrm{sign}(\sigma_2) = -1$ and the equality (5.5) implies $\Omega_{p_1 \dots p_k}(u_1, \dots, u_k) \equiv 0$. □

VI. NECESSARY CONDITIONS FOR EXISTENCE OF BI-HAMILTONIAN STRUCTURES

Theorem 3: *Suppose that for a bi-Hamiltonian system* (1.3) and (1.4) *the* (2,0)*-tensor* $g_\lambda = \lambda g_1 + g_2$ *is nondegenerate for some* λ, *and the* (1,1)*-tensor* $B^i_{\lambda k}(u) = g_1^{j\alpha}(g_\lambda^{-1})_{\alpha k}$ *has distinct eigenvalues. Then the following necessary conditions hold:*

- *(a) the Haantjes tensor* $H(V,W)$ *(4.1), (4.4) vanishes for all tangent vectors* $V \in L_x = L_{1x} \cap L_{2x}$;
- *(b) the (1,3)-tensors* $L_p(v,w,u)$ *(4.11) vanish for all vectors* $v, w \in L_x$;
- *(c) the differential k-forms* $\Omega_{p_1 \dots p_k}(u_1, \dots, u_k)$ *(4.9), (4.10) vanish for all* $k \geqslant 2$ *and all tangent vectors* $u_1, \dots, u_k \in L_x$ *and all non-negative integers* $p_1, \dots, p_k$;
- *(d) If in addition* rank $g_2 = n$ *then* $H(U,W) = 0$ *for all* $U, W \in T_x(M^n)$. *If the eigenvalues of the (1,1)-tensor* $A^i_j(u)$ *are real and distinct, then the system (1.3) possesses Riemann invariants: there exist local coordinates* $v^1, \dots, v^n$ *where tensor* $A^i_j(v)$ *is diagonal* $A^i_j(v) = A^i(v)\delta^i_j$ *and the system has the form*

$$v^i_t = A^i(v^1, \dots, v^n) v^i_x. \tag{6.1}$$

In these local coordinates both (2,0)*-tensors* $g_1^{ij}(v)$ *and* $g_2^{ij}(v)$ *are diagonal.*

Proof: (a) Since the (1,1)-tensor $B^j_{\lambda k}$ has distinct eigenvalues, it can have only one zero eigenvalue. Hence the (2,0)-tensor g_1^{jk} has rank $\geqslant n-1$. Equations (2.5) and (4.18) imply that the operators A and M_V are diagonal in the basis of eigenvectors of the operators $B^j_{\lambda k}$. Hence operator A and all operators M_{V_1}, M_{V_2} commute with each other for $V_1, V_2 \in L_x$. Hence the commutators $H_V = M_V A - A M_V$ vanish for all vectors $V \in L_x$ and the Haantjes tensor $H(V,U)=0$ for all $V \in L_x$.

(b),(c) The commutativity of the operators A, M_v, M_w for $v, w \in L_x$ implies that the (1,3)-tensors $L_p(v,w,u)$ (4.11) and (4.12) vanish for $v, w \in L_x$. Analogously, all operators in the definitions of the k-forms (4.9), (4.10) commute, hence due to their skew-symmetricity the forms vanish for all $p_1, \ldots, p_k$.

(d) If rank $g_2 = n$, then $L_x = L_{1x}$. Since the Haantjes (1,2)-tensor $H(U,W)$ is skew and $\dim(L_{1x}) \geqslant n-1$, we obtain that the Haantjes (1,2)-tensor $H(U,W)$ vanishes. If the (1,1)-tensor $A^i_k(u)$ has real and distinct eigenvalues then the Nijenhuis-Haantjes theorem[13,14] for $H(U,W)=0$ yields that there are some local coordinates $v^1, \ldots, v^n$ where the (1,1)-tensor $A^i_j(v)$ is diagonal. In these coordinates the system (1.3) has diagonal form (6.1) with Riemann invariants $A^i(v^1, \ldots, v^n)$. In the coordinates $v^1, \ldots, v^n$, Eqs. (2.3) imply that both (2,0)-tensors $g_1^{jk}(v)$ and $g_2^{jk}(v)$are diagonal. □

Proposition 2: For the existence of two Hamiltonian structures (1.3) and (1.4) *with two degenerate* (2,0)*-tensors* g_1^{jk}, rank $g_1 = m_1$, *and* g_2^{jk}, rank $g_2 = m_2$, *provided that for some* λ *the tensor* $g_\lambda = \lambda g_1 + g_2$ *is nondegenerate, the following necessary condition must hold for tangent vectors* $u_1, \ldots, u_k$ *of some subspace* $L_x \subset T_x(M^n)$ *of dimension* $m_1 + m_2 - n$:

The differential k-forms $\Omega_{p_1,\ldots,p_k}(u_1, \ldots, u_k)$ (4.10) *vanish if* (1) $p_i = p_{k-i}$ *for* $k = 4m+2$, *and* $k = 4m+3$ *or if (2)* $p_i = p_{k-i+1}$ *for* $k = 4m$, *and* $k = 4m+3$.

Proof: Applying Lemma 2 of Sec. IV, we find that equations

$$M_V^t = g_\lambda^{-1} M_V g_\lambda, \quad A^t = g_\lambda^{-1} A g_\lambda$$

hold for all tangent vectors $V \in L_x = L_{1x} \cap L_{2x}$. It is evident that $\dim L_x \geqslant \dim L_{1x} + \dim L_{2x} - n = m_1 + m_2 - n$. Hence the same proof as in Theorem 2 gives the necessary condition for $u_1, \ldots, u_k \in L_x$. □

Remark 4: Theorem 3 implies that the necessary condition for the existence of two Hamiltonian structures in general position [when tensor $B(u) = g_1(u) g_2^{-1}(u)$ has n distinct eigenvalues] for a system (1.3) is the vanishing of the Haantjes (1,2)-tensor $H(U,W)$ for the (1,1)-tensor $A^i_j(u)$. Another necessary condition is the vanishing of the (1,3)-tensor $L(V,W,U)$ (4.11) and the skew-symmetric k-forms $\Omega_{p_1 \ldots p_k}(u_1, \ldots, u_k)$ (4.9), (4.10) for any non-negative integers $p_1, \ldots, p_k$.

VII. CANONICAL FORMS OF THE GENERIC BI-HAMILTONIAN SYSTEMS

Let $A^i_j(u)$ be a smooth real (1,1)-tensor on a smooth real manifold M^n.

Theorem 4: *Assume that for the* (1,1)*-tensor* $A^i_j(u)$ *its Haantjes* (1,2)*-tensor* (4.4) *vanishes. Then if the eigenvalues of the operators* $A^i_j(u)$ *are all distinct in some open domain* $\mathcal{D}^n \subset M^n$ *then there exist local coordinates* $x^1, \ldots, x^n$ *in* $\mathcal{D}^n$ *in which the tensor* $A^i_j(u)$ *has block-diagonal form with k nonzero* 2×2 *blocks and* $n-2k$ *nonzero* 1×1 *blocks, where* $2k$ *is the number of complex eigenvalues and* $n-2k$ *is the number of real eigenvalues of operator* $A^i_j(u)$.

Proof: Let $\lambda_1(u), \ldots, \lambda_{2k}(u)$ be the complex eigenvalues of $A^i_j(u)$ and $\lambda_{2k+1}(u), \ldots, \lambda_n(u)$ be the real ones. Since complex eigenvalues appear in conjugate pairs, we reorder them so that $\lambda_{2m}(u) = \overline{\lambda_{2m-1}(u)}$ for $m = 1, \ldots, k$. Let $e_{2m-1}(u)$ and $e_{2m}(u)$ be the corresponding smooth complex-valued eigenvector fields. The vectors $e_{2m-1}(u)$ and $e_{2m}(u)$ belong to the complexification of the tangent spaces $T_u(\mathcal{D}^n)$. It is evident that we can assume that they also are complex conjugates, $e_{2m}(u) = \overline{e_{2m-1}(u)}$. Let

$$e_{2m-1}(u) = v_m(u) + i w_m(u), \tag{7.1}$$

where $v_m(u), w_m(u) \in T_u(\mathcal{D}^n)$ are real-valued tangent vector fields. Then

$$e_{2m}(u) = \overline{e_{2m-1}(u)} = v_m(u) - iw_m(u). \tag{7.2}$$

For $\lambda_{2m-1}(u) = \alpha_m(u) + i\beta_m(u)$, the two complex equations $A(e_{2m-1}) = \lambda_{2m-1}e_{2m-1}$ and $A(e_{2m}) = \overline{\lambda}_{2m-1}e_{2m}$ are equivalent to the two real equations

$$A(v_m) = \alpha_m v_m - \beta_m w_m, \quad A(w_m) = \beta_m v_m + \alpha_m w_m. \tag{7.3}$$

For the $n-2k$ real eigenvalues $\lambda_j(u)$ we define smooth real eigenvector fields $e_j(u)$ where $j = 2k+1, \ldots, n$. It is evident that the vectors $v_m(u), w_m(u), e_j(u)$ form a basis in each tangent space $T_u(\mathcal{D}^n)$. Here $m = 1, \ldots, k$ and $j = 2k+1, \ldots, n$.

For any two eigenvector fields $e_p(u)$, $e_q(u)$, complex or real, Eqs. (4.1), (4.2) lead to the following formula:[16]

$$H(e_p, e_q) = (A - \lambda_p)^2 (A - \lambda_q)^2 [e_p, e_q], \tag{7.4}$$

where $[e_p, e_q]$ is the commutator of the vector fields and $p, q = 1, \ldots, n$. For the vanishing Haantjes tensor, the equations

$$(A - \lambda_p)^2 (A - \lambda_q)^2 [e_p, e_q] = 0 \tag{7.5}$$

hold for all pairs of eigenvector fields $e_p(u)$, $e_q(u)$. For the real ones, equation $H(e_p, e_q) = 0$ implies[13,14]

$$[e_j(u), e_\ell(u)] = a_{j\ell}(u) e_j(u) + b_{j\ell}(u) e_\ell(u), \tag{7.6}$$

with some real-valued functions $a_{j\ell}(u)$ and $b_{j\ell}(u)$. Hence the two-dimensional distribution generated by vector fields $e_j(u)$, $e_\ell(u)$ is involutive.[17]

For the generic case of distinct complex eigenvalues, Eq. (7.5) evidently yields

$$[e_p(u), e_q(u)] = g_{pq}(u) e_p(u) + h_{pq}(u) e_q(u), \tag{7.7}$$

where $g_{pq}(u)$ and $h_{pq}(u)$ are some smooth complex-valued functions. Let us consider three different cases.

(1) Two complex conjugate eigenvalues $\lambda_{2m-1}(u)$, $\lambda_{2m}(u)$. For the corresponding eigenvector fields (7.1) and (7.2), we find

$$[e_{2m-1}(u),\, e_{2m}(u)] = -2i[v_m(u),\, w_m(u)]. \tag{7.8}$$

Hence applying Eq. (7.7), we obtain

$$[v_m(u), w_m(u)] = a_m(u) v_m(u) + b_m(u) w_m(u), \tag{7.9}$$

with some real-valued functions $a_m(u)$ and $b_m(u)$. Hence the two-dimensional distribution in $T_u(\mathcal{D}^n)$ generated by the tangent vector fields $v_m(u)$ and $w_m(u)$ is involutive.

(2) One real, $\lambda_j(u)$, and one complex, $\lambda_{2m-1}(u)$ or $\lambda_{2m}(u)$, eigenvalues. Equation (7.7) together with Eq. (7.9) imply that the three-dimensional distribution in $T_u(\mathcal{D}^n)$ generated by $e_j(u)$, $v_m(u)$, and $w_m(u)$ is involutive.

(3) Two pairs of complex conjugate eigenvalues, $\lambda_{2m-1}(u)$, $\lambda_{2m}(u)$, and $\lambda_{2s-1}(u)$ or $\lambda_{2s}(u)$. Equations (7.7) along with two equations (7.9) for the indices m and s yield that the four-dimensional distribution in $T_u(\mathcal{D}^n)$ generated by the tangent vector fields $v_m(u)$, $w_m(u)$, $v_s(u)$, and $w_s(u)$ is involutive.

For every real eigenvalue $\lambda_j(u)$, $j = 2k+1, \ldots, n$, we consider the $(n-1)$-dimensional distribution in $T_u(\mathcal{D}^n)$ generated by the vector fields $e_\ell(u)$ and $v_m(u)$, $w_m(u)$ corresponding to all other eigenvalues $\lambda_p(u) \neq \lambda_j(u)$. The above results (1)–(3) show that the distribution is involutive. Applying Frobenius theorem,[17] we obtain that the distribution is integrable and hence there exists a smooth nondegenerate function $x^j(u)$ that is constant on the $(n-1)$-dimensional integral submanifolds of the distribution. Hence we get

$$\mathrm{d}x^j(e_p(u)) = f_j(u)\,\delta^j_p, \quad f_j(u) \neq 0, \tag{7.10}$$

where $f_j(u)$ is some nonzero smooth function. Therefore the $(n-1)$-dimensional linear subspace in $T_u(\mathcal{D}^n)$ defined by

$$\mathrm{d}x^j(V) = 0, \quad V \in T_u(\mathcal{D}^n) \tag{7.11}$$

is generated by the tangent vectors $e_\ell(u)$, $\ell \neq j$, and $v_m(u)$, $w_m(u)$. Hence the subspaces $\mathrm{d}x^j(V) = 0$ are invariant under the operators $A^i_j(u)$, in view of $A(e_\ell) = \lambda_\ell e_\ell$ and Eqs. (7.3).

For any pair of complex conjugate eigenvalues $\lambda_{2m}(u) = \overline{\lambda_{2m-1}(u)}$, we consider the $(n-2)$-dimensional distribution in $T_u(\mathcal{D}^n)$ generated by the tangent vectors $v_s(u)$, $w_s(u)$, $s \neq m$, and $e_j(u)$ corresponding to all other eigenvalues. The above results (1)–(3) prove that this distribution is involutive. Hence by Frobenius theorem it is integrable and there exist two smooth functionally independent functions $x^{2m-1}(u)$ and $x^{2m}(u)$ that are constant on the integral submanifolds for this distribution. Hence we have

$$\mathrm{d}x^{2m-1}(v_s(u)) = a_m(u)\,\delta^m_s, \quad \mathrm{d}x^{2m-1}(w_s(u)) = b_m(u)\,\delta^m_s,$$

$$\mathrm{d}x^{2m}(v_s(u)) = c_m(u)\,\delta^m_s, \quad \mathrm{d}x^{2m}(w_s(u)) = d_m(u)\,\delta^m_s, \tag{7.12}$$

$$\mathrm{d}x^{2m-1}(e_j(u)) = 0, \quad \mathrm{d}x^{2m}(e_j(u)) = 0,$$

where $a_m(u)$, $b_m(u)$, $c_m(u)$, $d_m(u)$ are some smooth functions and the corresponding 2×2 matrix is nondegenerate,

$$a_m(u)d_m(u) - b_m(u)c_m(u) \neq 0. \tag{7.13}$$

Equations (7.12) imply that the $(n-2)$-dimensional linear subspaces defined by the two equations

$$\mathrm{d}x^{2m-1}(V) = 0, \quad \mathrm{d}x^{2m}(V) = 0, \quad V \in T_u(\mathcal{D}^n) \tag{7.14}$$

are invariant under the linear operators $A^i_j(u)$.

Thus we have constructed n smooth functions $x^1, \ldots, x^n$ on the domain $\mathcal{D}^n$. Equations (7.10), (7.12), and (7.13) prove that the functions are functionally independent and hence can be considered as a system of local coordinates in $\mathcal{D}^n$. In the coordinates $x^1, \ldots, x^n$, we define the unit tangent vector fields $\mathbf{e}_1, \ldots, \mathbf{e}_n$: $\mathrm{d}x^p(\mathbf{e}_q) = \delta^p_q$.

For $\ell = 2k+1, \ldots, n$, the vector $\mathbf{e}_\ell$ generates the subspace $C\mathbf{e}_\ell$ that is the intersection of the linear subspaces $\mathrm{d}x^j(V) = 0$ (7.10), $\mathrm{d}x^{2m-1}(V) = 0$, $\mathrm{d}x^{2m}(V) = 0$ (7.14), for all $j \neq \ell$ and $m = 1, \ldots, k$. Each of these subspaces is invariant under the operator $A^i_j(u)$. Hence their intersection that is the one-dimensional subspace $C\mathbf{e}_\ell$ is also invariant. Hence the $\mathbf{e}_\ell$ is an eigenvector of the operator $A^i_j(u)$ and defines an invariant diagonal 1×1 block of $A^i_j(u)$. Formulas (7.10) imply that the corresponding eigenvalue is $\lambda_\ell(x)$.

For $s = 1, \ldots, k$, the two tangent vectors $\mathbf{e}_{2s-1}$ and $\mathbf{e}_{2s}$ generate the space $C_1\mathbf{e}_{2s-1} + C_2\mathbf{e}_{2s}$ that is the intersection of the linear subspaces $\mathrm{d}x^j(V) = 0$ (7.10), $\mathrm{d}x^{2m-1}(V) = 0$, $\mathrm{d}x^{2m}(V) = 0$ (7.14), for all $j = 2k+1, \ldots, n$ and $m \neq s$. Since each of these subspaces is invariant under $A^i_j(u)$, their intersection also is invariant. Hence the subspace $C_1\mathbf{e}_{2s-1} + C_2\mathbf{e}_{2s}$ defines an invariant diagonal 2×2 block of the operator $A^i_j(u)$ in the coordinates $x^1, \ldots, x^n$. Formula (7.12) yields that the invariant subspace $C_1\mathbf{e}_{2s-1} + C_2\mathbf{e}_{2s}$ corresponds to the pair of complex eigenvalues $\lambda_{2s-1}(x)$ and $\lambda_{2s}(x) = \overline{\lambda_{2s-1}(x)}$.

Hence the (1,1)-tensor $A^i_j(u)$ in the local coordinates $x^1, \ldots, x^n$ has canonical block-diagonal form with k 2×2 blocks in the subspaces $C_1\mathbf{e}_{2s-1} + C_2\mathbf{e}_{2s}$ and $n-2k$ 1×1 blocks in the subspaces $C\mathbf{e}_\ell$. □

Theorem 5: *A generic bi-Hamiltonian system* (1.3) *with nondegenerate* (2,0)*-tensor* g_2^{jk} *and operators* $B^i_k(u) = g_1^{j\alpha}(g_2^{-1})_{\alpha k}$ *and* $A^i_k(u)$ *having distinct eigenvalues, complex or real, has canonical block diagonal form in some coordinates* $v^1, \ldots, v^n$ *with* k *nonzero* 2×2 *blocks and* $n-2k$ *nonzero* 1×1 *blocks where* $2k$ *is the number of complex eigenvalues of the* (1,1)*-tensor* $A^j_k(u)$.

Theorem 5 follows from Theorems 3 and 4. Indeed, since operators $B^i_k(u)$ have distinct eigenvalues, Theorem 3 implies that the Haantjes tensor H^i_{jk} vanishes. Applying Theorem 4 to the (1,1)-tensor $A^i_j(u)$ with distinct eigenvalues and $H^i_{jk}=0$, we obtain that tensor $A^i_j(v)$ has the block diagonal form in some coordinates $v^1,\dots,v^n$ (denoted above as $x^1,\dots,x^n$). Hence the bi-Hamiltonian system (1.3) has the canonical block diagonal form in the coordinates $v^1,\dots,v^n$.

Remark 5: Theorem 4 contains as a special case (for $k=0$) the classical Nijenhuis–Haantjes theorem that was proved in Refs. 13 and 14 for the case of real and distinct eigenvalues of $A^i_j(u)$. Nijenhuis and Haantjes did not study the generic case of complex eigenvalues because they were concerned with a pure geometric problem on "X_{n-1}*-forming sets of eigenvectors*." For the bi-Hamiltonian systems (1.3), the generic case of complex eigenvalues of $A^i_j(u)$ is as important as the real case.

VIII. ALGEBRAIC IDENTITIES FOR THE BI-HAMILTONIAN SYSTEMS (1.3)

In Ref. 12, we prove that if the Schouten (3,0)-tensor S^{ijk} is completely symmetric, then the Nijenhuis (3,0)-tensor N^{ijk} satisfies the identities

$$N^{ikj}+N^{kji}+N^{jik}=0, \tag{8.1}$$

$$A^i_\alpha N^{\alpha jk}+A^j_\alpha N^{\alpha ki}+A^k_\alpha N^{\alpha ij}=0. \tag{8.2}$$

The corresponding Haantjes (3,0)-tensor H^{ijk} obeys the identity

$$H^{ijk}=A^i_\beta A^\beta_\alpha N^{\alpha jk}+A^j_\beta A^\beta_\alpha N^{\alpha ki}+A^k_\beta A^\beta_\alpha N^{\alpha ij} \tag{8.3}$$

and is completely skew-symmetric.

In Sec. III, we have shown that the Schouten (3,0)-tensor S^{ijk} is completely symmetric for all Hamiltonian systems of hydrodynamic type (1.3) and (1.4). Therefore the identities (8.1)–(8.3) hold for an arbitrary Hamiltonian system of hydrodynamics type with degenerate or nondegenerate symmetric (2,0)-tensor g^{ij}.

For a bi-Hamiltonian system (1.3) and (1.4), there are two sets of identities (8.1)–(8.3) for the two tensors $N^{ijk}_1=N^i_{\alpha\beta}g_1^{\alpha j}g_1^{\beta k}$ and $N^{ijk}_2=N^i_{\alpha\beta}g_2^{\alpha j}g_2^{\beta k}$. Suppose the (2,0)-tensor g_2^{jk} is nondegenerate and define $B^i_j=g_1^{i\alpha}(g_2^{-1})_{\alpha j}$.

Proposition 3: For the bi-Hamiltonian system (1.3) and (1.4)*, tensor* N^{ijk}_1 *satisfies the additional identities*

$$B^i_\gamma N_1^{\gamma kj}+B^k_\gamma N_1^{\gamma ji}+B^j_\gamma N_1^{\gamma ik}=0, \tag{8.4}$$

$$B^i_\gamma A^\gamma_\alpha N_1^{\alpha jk}+B^j_\gamma A^\gamma_\alpha N_1^{\alpha ki}+B^k_\gamma A^\gamma_\alpha N_1^{\alpha ij}=0, \tag{8.5}$$

$$B^i_\gamma H_1^{\gamma jk}=B^i_\gamma A^\gamma_\beta A^\beta_\alpha N_1^{\alpha jk}+B^j_\gamma A^\gamma_\beta A^\beta_\alpha N_1^{\alpha ki}+B^k_\gamma A^\gamma_\beta A^\beta_\alpha N_1^{\alpha ij}. \tag{8.6}$$

Proof: Let us contract the identity (8.1),

$$N_2^{ikj}+N_2^{kji}+N_2^{jik}=0,$$

for the tensor N_2^{ijk} with the tensor $(g_2^{-1})_{\alpha i}(g_2^{-1})_{\beta k}(g_2^{-1})_{\gamma j}$. After changing the indices we get the identity for the Nijenhuis tensor N^i_{jk},

$$(g_2^{-1})_{i\gamma}N^\gamma_{kj}+(g_2^{-1})_{k\gamma}N^\gamma_{ji}+(g_2^{-1})_{j\gamma}N^\gamma_{ik}=0. \tag{8.7}$$

Contracting this identity with the tensor $g_1^{\alpha i}g_1^{\beta k}g_1^{\delta j}$ and again changing notations, we arrive at the identity (8.4). The identities (8.5) and (8.6) follow in an analogous way. □

Identity (8.6) implies that along with the (3,0)-tensors H_1^{ijk} and H_2^{ijk} also the (3,0)-tensor $B^i_\gamma H_1^{\gamma jk}$ is completely skew-symmetric.

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A realization of the Lie algebra associated to a Kantor triple system

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We present a nonlinear realization of the 5-graded Lie algebra associated to a Kantor triple system. Any simple Lie algebra can be realized in this way, starting from an arbitrary 5-grading. In particular, we get a unified realization of the exceptional Lie algebras $\mathfrak{f}_4, \mathfrak{e}_6, \mathfrak{e}_7, \mathfrak{e}_8$, in which they are respectively related to the division algebras $\mathbb{R}, \mathbb{C}, \mathbb{H}, \mathbb{O}$. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The product in an associative but noncommutative algebra can be decomposed into one symmetric part, leading to a *Jordan algebra*, and one antisymmetric part, leading to a *Lie algebra*. A deeper relationship between these two important kinds of algebras is suggested by the Kantor-Koecher-Tits construction,[1–3] which associates a Lie algebra to any Jordan algebra, and it becomes more evident when generalizing Jordan algebras to *Jordan triple systems* (JTS). These can further be generalized to *Kantor triple systems* (KTS).

The Lie algebra associated to a Jordan algebra or a JTS is 3-graded, written $\mathfrak{g}_{-1}+\mathfrak{g}_0+\mathfrak{g}_1$ as a direct sum of subspaces, while the Lie algebra associated to a KTS is 5-graded, written $\mathfrak{g}_{-2}+\mathfrak{g}_{-1}+\mathfrak{g}_0+\mathfrak{g}_1+\mathfrak{g}_2$. We will discuss graded Lie algebras more in the following section. In Sec. III we will describe how triple systems may be obtained from graded Lie algebras and conversely construct the graded Lie algebras associated to these triple systems. Under certain conditions, we get back the original algebra, together with a nonlinear realization.

In Sec. III A we will consider Jordan triple systems and the associated 3-graded Lie algebras. In this case, the realization of the Lie algebra is said to be *conformal*. The operators act on $\mathfrak{g}_{-1}$ and are each either constant, linear or quadratic, according to the 3-grading. In the case of $\mathfrak{so}(2,d)$ we get the well-known realization of the conformal algebra in d dimensions, where the elements in the algebra are regarded as generators of translations (constant), Lorentz transformations together with dilatations (linear) and special conformal transformations (quadratic).

The main result of this paper, to be presented in Sec. III B, is a corresponding realization of the 5-graded Lie algebra associated to a Kantor triple system. This Lie algebra has earlier been defined as a special case of a *Kantor algebra*,[4] using a functor that associates a Lie algebra to any generalized Jordan triple system.[5] It has also been defined in a simpler but rather abstract way, as a direct sum of vector spaces together with the appropriate commutation relations.[6]

In our construction, the Lie algebra associated to a KTS consists of nonlinear operators acting on an extension of the KTS. The bracket arises naturally when we regard the operators as vector fields, which we will explain in Sec. II B. To our knowledge, such a construction has not appeared before. However, the concomitant realization of any simple 5-graded Lie algebra on its subspace $\mathfrak{g}_{-2}+\mathfrak{g}_{-1}$ has been obtained in Ref. 7, using a general formula for the Lie algebra of a homogeneous space.

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The corresponding realization of the Lie algebra associated to a *Freudenthal triple system* (FTS) was given in Ref. 8, called *quasiconformal*, and led us to the present work. The difference is that our realization is based on an arbitrary 5-grading, while in Ref. 8 the subspaces $\mathfrak{g}_{\pm 2}$ must be one dimensional. The connection between these two realizations will be clarified in Sec. III C. As an example of interesting cases where the subspaces $\mathfrak{g}_{\pm 2}$ are not one dimensional, we will in Sec. IV show how the exceptional Lie algebras $\mathfrak{f}_4, \mathfrak{e}_6, \mathfrak{e}_7, \mathfrak{e}_8$ can be given 5-gradings related to the division algebras $\mathbb{R}, \mathbb{C}, \mathbb{H}, \mathbb{O}$, respectively. This construction, given in Ref. 6, together with our main result, leads to a unified realization of these exceptional Lie algebras.

II. GRADED LIE ALGEBRAS

We start with some definitions concerning graded Lie algebras in general, after which we will consider the cases of semisimple and simple algebras.

A Lie algebra $\mathfrak{g}$ is *graded* if it is the direct sum of subspaces $\mathfrak{g}_k \subset \mathfrak{g}$ for all integers k, such that

$$[\mathfrak{g}_i, \mathfrak{g}_j] \subseteq \mathfrak{g}_{i+j}$$

for all integers i, j. It is $(2\nu+1)$-graded for some integer $\nu \geqslant 1$ if $\mathfrak{g}_{\pm\nu} \neq 0$ and

$$|k| > \nu \Rightarrow \mathfrak{g}_k = 0.$$

(If $\mathfrak{g}_k = 0$ for all $k \neq 0$, then $\mathfrak{g}$ will not be regarded as a graded Lie algebra.) The grade k of an element $x \in \mathfrak{g}_k$ may be measured by a *characteristic element* $Z \in \mathfrak{g}$, satisfying

$$x \in \mathfrak{g}_k \Rightarrow [Z, x] = kx$$

for all integers k. A *graded involution* τ on $\mathfrak{g}$ is an automorphism of $\mathfrak{g}$ such that $\tau(\tau(x)) = x$ for all $x \in \mathfrak{g}$ and $\tau(\mathfrak{g}_k) = \mathfrak{g}_{-k}$ for all integers k. If we instead of the last condition have $\tau(\mathfrak{g}_k) = (-1)^k \mathfrak{g}_{-k}$, then τ will be called a *graded pseudoinvolution*.

A. Semisimple algebras

Let the graded Lie algebra $\mathfrak{g}$ be semisimple, complex, and finite dimensional. Then $\mathfrak{g}$ has a unique characteristic element Z that belongs to a Cartan subalgebra of $\mathfrak{g}$ contained in $\mathfrak{g}_0$. With respect to this Cartan subalgebra, the subspaces $\mathfrak{g}_k$ with $k \neq 0$ are spanned by step operators E^α corresponding to roots α such that

$$E^\alpha \in \mathfrak{g}_k \Leftrightarrow E^{-\alpha} \in \mathfrak{g}_{-k},$$

while $\mathfrak{g}_0$ is spanned by the Cartan elements H^i and the remaining step operators. It follows that $\mathfrak{g}$ is $(2\nu+1)$-graded for some integer $\nu \geqslant 1$ and the *Chevalley involution*

$$E^{\pm\alpha} \mapsto -E^{\mp\alpha}, \quad H^i \mapsto -H^i$$

is a graded involution on $\mathfrak{g}$. Not all real forms of $\mathfrak{g}$ inherit the grading, since these are spanned by complex linear combinations of the step operators and the Cartan elements. In particular, the compact form of $\mathfrak{g}$ cannot be graded.

If we expand a root β in the basis of simple roots α_j as $\beta = \beta^j \alpha_j$, then any set of simple roots $\alpha_{i_1}, \alpha_{i_2}, \ldots, \alpha_{i_n}$ generates a grading of $\mathfrak{g}$ where $\mathfrak{g}_k$ is spanned by all step operators E^β such that $\beta^{i_1} + \beta^{i_2} + \cdots + \beta^{i_n} = k$ and, if $k = 0$, the Cartan elements. Any 3-grading or 5-grading of a simple Lie algebra can be obtained in this way (possibly after an automorphism). If $\mathfrak{g}$ is simple and 3-graded or 5-graded, we also have $[\mathfrak{g}_i, \mathfrak{g}_j] = \mathfrak{g}_{i+j}$ for $i, j = \pm 1$ and (up to an automorphism) there is a unique 5-grading with one dimensional subspaces $\mathfrak{g}_{\pm 2}$, except for $\mathfrak{g} = \mathfrak{a}_1$. On the other hand, $\mathfrak{e}_8, \mathfrak{f}_4, \mathfrak{g}_2$ cannot be 3-graded. A table of all simple 3-graded and 5-graded Lie algebras can be found in Ref. 9.

B. Algebras of operators

We will now describe how any vector space U or pair of vector spaces V,W gives rise to an infinite dimensional graded Lie algebra $T(U)$ or $T(V,W)$ consisting of operators acting on U or $V\oplus W$.

With an operator f on a vector space U we mean a map $U\to U$. It is of order $p\geqslant 1$ if there is a symmetric p-linear map $F:U^p\to U$ such that

$$f(u)=F(u,\ldots,u)$$

for all $u\in U$, and of order 0 if there is a vector $v\in U$ such that $f(u)=v$ for all $u\in U$. We define the composition of f and another operator g on U by

$$(f\circ g)(u)=pF(g(u),u,\ldots,u)$$

or $f\circ g=0$ if f is of order 0.

For any integer $k\geqslant -1$, let $T_k(U)$ be the vector space consisting of all operators on U of order $k+1$. Furthermore, set $T_k(U)=0$ for all integers $k\leqslant -2$ and let $T(U)$ be the direct sum of all these vector spaces. Now $T(U)$, together with the bracket

$$[f,g]=f\circ g-g\circ f,$$

is a graded Lie algebra, isomorphic to the algebra of all vector fields $f^i\partial_i$ on U such that $f\in T(U)$. The isomorphism is given by $f\mapsto -f^i\partial_i$.

Similarly, for any pair of vector spaces V,W, we can define a graded Lie algebra $T(V,W)$ of operators on $V\oplus W$, isomorphic to the algebra of all vector fields $f^i\partial_i$ on $V\oplus W$ such that $f\in T(V,W)$. As a graded Lie algebra, $T(V,W)$ is the direct sum of subspaces $T_k(V,W)$ for all integers k, where $T_k(V,W)=0$ for $k\leqslant -3$.

With a *realization* of a Lie algebra $\mathfrak{g}$ on U or $V\oplus W$ we mean a homomorphism from $\mathfrak{g}$ to $T(U)$ or $T(V,W)$. If all elements are mapped on linear operators, it reduces to a linear *representation*. In the following section, we will see that any simple 3-graded or 5-graded Lie algebra $\mathfrak{g}$ can be described as a subalgebra of $T(\mathfrak{g}_{-1})$ or $T(\mathfrak{g}_{-1},\mathfrak{g}_{-2})$ and this description will thus give us a realization of the algebra.

III. TRIPLE SYSTEMS

In this section, we will clarify the connection between graded Lie algebras and triple systems. Jordan triple systems and Kantor triple systems correspond to general 3-graded and 5-graded algebras, respectively, while Freudenthal triple systems correspond to 5-graded algebras with one dimensional subspaces $\mathfrak{g}_{\pm 2}$.

A *triple system* (or *ternary algebra*) is a vector space U together with a linear map

$$U\times U\times U\to U,\quad (x,y,z)\mapsto (xyz)$$

called *triple product*. For any two elements u,v in a triple system U, we define the linear operator $\langle u,v\rangle$ on U by

$$\langle u,v\rangle(z)=(uzv)-(vzu).$$

Let $\mathfrak{g}$ be a graded Lie algebra with a graded involution τ. Then the vector space $\mathfrak{g}_{-1}$ together with the triple product

$$(xyz)=[[x,\tau(y)],z]$$

is a triple system, which will be called the triple system *derived* from $\mathfrak{g}$. We have the identity

$$(uv(xyz))-(xy(uvz))=((uvx)yz)-(x(vuy)z) \tag{3.1}$$

from the fact that τ is an involution and from the Jacobi identity, which also gives us

$$\langle u,v\rangle(z) = [[u,v],\tau(z)]$$

for all $u,v,z \in \mathfrak{g}_{-1}$.

A. Jordan triple systems

Let $\mathfrak{g}$ be a 3-graded Lie algebra with a graded involution. Since $[u,v]=0$ for any $u,v \in \mathfrak{g}_{-1}$ we have

$$\langle u,v\rangle(z) = 0 \tag{3.2}$$

in the triple system derived from $\mathfrak{g}$, which means that the triple product (uzv) is symmetric in u and v.

We define a *Jordan triple system* (JTS)[10] as a triple system where the identities (3.1) and (3.2) hold. Thus the triple system derived from a 3-graded Lie algebra with a graded involution is a JTS. Conversely, any Jordan triple system J gives rise to a 3-graded subalgebra of $T(J)$, spanned by the operators

$$u_a(x) = a,$$

$$s_{ab}(x) = (abx),$$

$$\tilde{u}_a(x) = -\tfrac{1}{2}(xax),$$

where $a,b,x \in J$. This is the Lie algebra $L(J)$ *associated* to the Jordan triple system J. From (3.1) and (3.2) we get the commutation relations

$$[s_{ab},s_{cd}] = s_{(abc)d} - s_{c(bad)}, \quad [s_{ab},u_c] = u_{(abc)},$$

$$[s_{ab},\tilde{u}_c] = -\tilde{u}_{(bac)}, \quad [u_a,\tilde{u}_b] = s_{ab},$$

and $[\tilde{u}_a,\tilde{u}_b]=0$. [We also have $[u_a,u_b]=0$ already from the definition of $T(J)$.] It follows that if J is derived from a simple 3-graded Lie algebra $\mathfrak{g}$ with a graded involution τ, then $\mathfrak{g}$ is isomorphic to $L(J)$ with the isomorphism

$$\begin{array}{r|ccc} +1 & \tau(a) & \mapsto & \tilde{u}_a \\ 0 & [a,\tau(b)] & \mapsto & [u_a,\tilde{u}_b] \\ -1 & a & \mapsto & u_a \end{array} \tag{3.3}$$

where $a,b \in \mathfrak{g}_{-1}$. This is the *conformal realization* of $\mathfrak{g}$ on $\mathfrak{g}_{-1}$.

B. Kantor triple systems

If $\mathfrak{g}$ is a 5-graded Lie algebra with a graded involution, then the identity

$$(uv(xyz)) - (xy(uvz)) = ((uvx)yz) - (x(vuy)z) \tag{3.4}$$

still holds in the triple system derived from $\mathfrak{g}$ but instead of $\langle u,v\rangle=0$ we now have the identity

$$\langle\langle u,v\rangle(x),y\rangle = \langle(yxu),v\rangle - \langle(yxv),u\rangle. \tag{3.5}$$

We define a *Kantor triple system* (KTS),[11] or a JTS *of second order*[5] as a triple system such that (3.4) and (3.5) hold. Thus the triple system derived from a 5-graded Lie algebra with a graded involution is a KTS, and so is any JTS.

Let K be a KTS and let L be the vector space spanned by all linear operators $\langle u,v\rangle$ on K, where $u,v \in K$. If K is derived from a simple 5-graded Lie algebra $\mathfrak{g}$ with a graded involution τ,

then we can identify not only K with $\mathfrak{g}_{-1}$, but also L with $\mathfrak{g}_{-2}$ by $\langle u,v\rangle=[u,v]$. In analogy with the construction of $L(J)$ in the preceding section we can now construct a 5-graded subalgebra of $T(K,L)$ spanned by the operators

$$K_{ab}(z+Z)=2\langle a,b\rangle,$$

$$U_a(z+Z)=a+\langle a,z\rangle,$$

$$S_{ab}(z+Z)=(abz)-\langle a,Z(b)\rangle,$$

$$\tilde{U}_a(z+Z)=-\tfrac{1}{2}(zaz)-\tfrac{1}{2}Z(a)+\tfrac{1}{6}\langle(zaz),z\rangle-\tfrac{1}{2}\langle Z(a),z\rangle,$$

$$\tilde{K}_{ab}(z+Z)=-\tfrac{1}{6}(z\langle a,b\rangle(z)z)-\tfrac{1}{2}Z(\langle a,b\rangle(z))+\tfrac{1}{12}\langle(z\langle a,b\rangle(z)z),z\rangle+\tfrac{1}{2}\langle Z(a),Z(b)\rangle, \tag{3.6}$$

where $a,b,z\in K$ and $Z\in L$. This is the Lie algebra $L(K)$ *associated* to the Kantor triple system K. We get the commutation relations

$$[S_{ab},S_{cd}]=S_{(abc)d}-S_{c(bad)},\quad [S_{ab},U_c]=U_{(abc)},$$

$$[S_{ab},K_{cd}]=K_{\langle c,d\rangle(b)a},\quad [U_a,U_b]=K_{ab},$$

$$[S_{ab},\tilde{U}_c]=-\tilde{U}_{(bac)},\quad [S_{ab},\tilde{K}_{cd}]=-\tilde{K}_{\langle c,d\rangle(a)b},$$

$$[U_a,\tilde{U}_b]=S_{ab},\quad [U_a,\tilde{K}_{cd}]=-\tilde{U}_{\langle c,d\rangle(a)},$$

$$[K_{ab},\tilde{U}_c]=U_{\langle a,b\rangle(c)},\quad [K_{ab},\tilde{K}_{cd}]=S_{\langle a,b\rangle(c)d}-S_{\langle a,b\rangle(d)c},$$

$$[\tilde{U}_a,\tilde{U}_b]=\tilde{K}_{ab},\quad [\tilde{K}_{ab},\tilde{K}_{cd}]=[\tilde{K}_{ab},\tilde{U}_c]=0.$$

It follows that if K is derived from a simple 5-graded Lie algebra $\mathfrak{g}$ with a graded involution τ, then $\mathfrak{g}$ is isomorphic to $L(K)$ with the isomorphism

$$\begin{array}{r|ccccc}
+2 & [\tau(a),\tau(b)] & \mapsto & [\tilde{U}_a,\tilde{U}_b] & = & \tilde{K}_{ab} \\
+1 & \tau(a) & \mapsto & \tilde{U}_a & & \\
0 & [a,\tau(b)] & \mapsto & [U_a,\tilde{U}_b] & = & S_{ab} \\
-1 & a & \mapsto & U_a & & \\
-2 & [a,b] & \mapsto & [U_a,U_b] & = & K_{ab}
\end{array} \tag{3.7}$$

where $a,b\in\mathfrak{g}_{-1}$. Then this isomorphism will be a realization of $\mathfrak{g}$ on its subspace $\mathfrak{g}_{-2}+\mathfrak{g}_{-1}$. The Lie algebra associated to a Kantor triple system can also be *defined* by the commutation relations above, and this is partly the definition given in Refs. 6 and 12, but it does not directly lead to a realization like (3.6). On the other hand, with our construction, we have to *derive* the commutation relations from the definition of the operators and the defining properties of a Kantor triple system. This requires long calculations and we will only give a few of them here. The full expressions are written out in Ref. 13. As an example, we have

$$
\begin{aligned}
[U_a,\tilde{U}_b](z+Z) &= \left\langle a,-\tfrac{1}{2}(zbz)-\tfrac{1}{2}Z(b)\right\rangle \\
&\quad +\tfrac{1}{2}(abz)+\tfrac{1}{2}(zba)+\tfrac{1}{2}\langle a,z\rangle(b) \\
&\quad -\tfrac{1}{6}\langle(abz),z\rangle-\tfrac{1}{6}\langle(zba),z\rangle-\tfrac{1}{6}\langle(zbz),a\rangle \\
&\quad +\tfrac{1}{2}\langle\langle a,z\rangle(b),z\rangle+\tfrac{1}{2}\langle Z(b),a\rangle \\
&=(abz)+\langle Z(b),a\rangle+\tfrac{3}{6}\langle\langle a,z\rangle(b),z\rangle \\
&\quad -\tfrac{1}{6}\langle(zba),z\rangle-\tfrac{1}{6}\langle(abz),z\rangle+\tfrac{2}{6}\langle(zbz),a\rangle \\
&=(abz)+\langle Z(b),a\rangle=S_{ab}(z+Z),
\end{aligned}
$$

where we have used

$$
\begin{aligned}
3\langle\langle a,z\rangle(b),z\rangle &= 2\langle\langle a,z\rangle(b),z\rangle+\langle\langle a,z\rangle(b),z\rangle \\
&=2(\langle(zba),z\rangle-2\langle(zbz),a\rangle) \\
&\quad +\langle(abz),z\rangle-\langle(zba),z\rangle \\
&=\langle(zba),z\rangle+\langle(abz),z\rangle-2\langle(zbz),a\rangle.
\end{aligned}
$$

Among the other commutators, $[U_a,U_b]$ and $[S_{ab},U_c]$ are easy to calculate, while $[\tilde{U}_a,\tilde{U}_b]$ and $[S_{ab},\tilde{U}_c]$ are much harder. It is convenient to first verify the identities

$$
\{((zbz)az)+2(za(zbz))\}_{ab}=(z\langle b,a\rangle(z)z), \tag{3.8}
$$

$$
\{(\langle x,y\rangle(b)az)\}_{ab}=(x\langle a,b\rangle(y)z)-(y\langle a,b\rangle(x)z), \tag{3.9}
$$

where we denote antisymmetrization by curly brackets, $\{f(a,b)\}_{ab}=f(a,b)-f(b,a)$ for any function f. We can also use (3.9) to rewrite the last term in $\tilde{K}_{ab}(z+Z)$ and show that the map (3.7) is well defined in the sense that $\tilde{K}_{ab}=\tilde{K}_{cd}$ if $[a,b]=[c,d]$. It turns out that

$$
\begin{aligned}
2\langle\langle u,v\rangle(a),\langle x,y\rangle(b)\rangle &= \langle(x\langle a,b\rangle(y)u),v\rangle-\langle(y\langle a,b\rangle(x)u),v\rangle \\
&\quad +\langle(y\langle a,b\rangle(x)v),u\rangle-\langle(x\langle a,b\rangle(y)v),u\rangle.
\end{aligned}
$$

The remaining nonzero commutation relations follow from the Jacobi identity. Finally, we can show that

$$
[[\tilde{K}_{ab},\tilde{U}_c],K_{xy}]=[[\tilde{K}_{ab},\tilde{U}_c],U_z]=0
$$

which gives us

$$
[\tilde{K}_{ab},\tilde{U}_c]=[\tilde{K}_{ab},\tilde{K}_{cd}]=0.
$$

C. Freudenthal triple systems

Let $\mathfrak{g}$ be a 5-graded Lie algebra and let T be an element in $\mathfrak{g}_2$. Then $\mathfrak{g}_{-1}$ together with the triple product

$$
(xyz)=[[x,[T,y]],z]
$$

is a triple system satisfying

$$
\langle x,y\rangle(z)=(yxz)-(xyz). \tag{3.10}
$$

Suppose now that the subspaces $\mathfrak{g}_{\pm 2}$ are one dimensional. If we extend the map

$$\mathfrak{g}_{-1} \to \mathfrak{g}_1, \quad x \mapsto [T,x]$$

to a graded pseudoinvolution τ on $\mathfrak{g}$, then for any $x,y \in \mathfrak{g}_{-1}$ there is a scalar α such that $\langle x,y\rangle \times(z)=\alpha z$. Thus we can identify the vector space spanned by all operators $\langle x,y\rangle$ where $x,y \in \mathfrak{g}_{-1}$ with the field over which the Lie algebra is defined, writing

$$\langle x,y\rangle(z) = \langle x,y\rangle z \tag{3.11}$$

and we can regard $\langle x,y\rangle$ as an antisymmetric bilinear form on the triple system rather than an operator. Since τ is not an involution but a pseudoinvolution, we now have the identity

$$(uv(xyz)) - (xy(uvz)) = ((uvx)yz) + (x(vuy)z) \tag{3.12}$$

with a changed sign of the last term, in comparison to (3.4). However, (3.5) still holds. We define a *Freudenthal triple system* (FTS) as a triple system with an antisymmetric bilinear form satisfying (3.5), (3.10), and (3.12). To sum up, we have

$$(uv(xyz)) = ((uvx)yz) + (x(vuy)z) + (xy(uvz)), \tag{3.13}$$

$$\langle x,y\rangle z = (xzy) - (yzx) = (yxz) - (xyz), \tag{3.14}$$

$$\langle u,v\rangle\langle x,y\rangle = \langle (yxu),v\rangle - \langle (yxv),u\rangle. \tag{3.15}$$

We note that (3.13) cannot be replaced by (3.4) or, in other words, that a KTS cannot satisfy (3.14) and (3.15) for some antisymmetric bilinear form (unless this is identically equal to zero, in which case the KTS reduces to a JTS).

Let F be a FTS and let L be the vector space spanned by all operators $\langle u,v\rangle$ on F where $u,v \in F$. If we change some of the signs in the definition of $\widetilde{K}_{ab}$ in (3.6), keep the definitions of all the other operators and simplify the expressions by (3.10)–(3.12), then we get

$$K_{ab}(z+\zeta) = 2\langle a,b\rangle,$$

$$U_a(z+\zeta) = a + \langle a,z\rangle,$$

$$S_{ab}(z+\zeta) = (abz) - \zeta\langle a,b\rangle, \tag{3.16}$$

$$\widetilde{U}_a(z+\zeta) = -\tfrac{1}{2}(zaz) - \tfrac{1}{2}\zeta a + \tfrac{1}{6}\langle (zzz),a\rangle - \tfrac{1}{2}\zeta\langle a,z\rangle,$$

$$\widetilde{K}_{ab}(z+\zeta) = \tfrac{1}{6}\langle a,b\rangle(zzz) + \tfrac{1}{2}\zeta\langle a,b\rangle z - \tfrac{1}{12}\langle a,b\rangle\langle (zzz),z\rangle + \tfrac{1}{2}\zeta^2\langle a,b\rangle,$$

where $a,b,z \in F$ and $\zeta \in L$. These operators span a subalgebra of $T(F,L)$ with the commutation relations

$$[S_{ab},S_{cd}] = S_{(abc)d} + S_{c(bad)}, \quad [S_{ab},U_c] = U_{(abc)},$$

$$[S_{ab},K_{cd}] = \langle c,d\rangle K_{ba}, \quad [U_a,U_b] = K_{ab},$$

$$[S_{ab},\widetilde{U}_c] = \widetilde{U}_{(bac)}, \quad [S_{ab},\widetilde{K}_{cd}] = \langle c,d\rangle\widetilde{K}_{ab},$$

$$[U_a,\widetilde{U}_b] = S_{ab}, \quad [U_a,\widetilde{K}_{cd}] = \langle c,d\rangle\widetilde{U}_a,$$

$$[K_{ab},\tilde{U}_c]=\langle a,b\rangle U_c,\quad [K_{ab},\tilde{K}_{cd}]=\langle a,b\rangle(S_{cd}-S_{dc}),$$

$$[\tilde{U}_a,\tilde{U}_b]=\tilde{K}_{ab},\quad [\tilde{K}_{ab},\tilde{K}_{cd}]=[\tilde{K}_{ab},\tilde{U}_c]=0.$$

It follows that if F is derived from a simple 5-graded Lie algebra $\mathfrak{g}$ with one dimensional subspaces $\mathfrak{g}_{\pm 2}$ and a graded pseudoinvolution as described above, then the map (3.7) is again an isomorphism. This is the *quasiconformal realization* of $\mathfrak{g}$ on $\mathfrak{g}_{-2}+\mathfrak{g}_{-1}$, given in Ref. 8 [where the factor of -2 in (17) and the opposite sign of the bracket lead to different coefficients in (29)].

Freudenthal triple systems where the antisymmetric bilinear form is nondegenerate are in a one-to-one correspondence to simple, complex, and finite-dimensional Lie algebras.[14] Since such a Lie algebra is also associated to a KTS, it follows that any nondegenerate FTS can be obtained from a KTS. Although Freudenthal triple systems are sufficient to obtain all simple finite-dimensional Lie algebras, the result in the following section shows that also Kantor triple systems may be useful.

IV. EXCEPTIONAL LIE ALGEBRAS

We end this paper with some comments on the exceptional Lie algebras $\mathfrak{f}_4,\mathfrak{e}_6,\mathfrak{e}_7,\mathfrak{e}_8$. These are associated to Kantor triple systems which in turn can be defined using the division algebras $\mathbb{R},\mathbb{C},\mathbb{H},\mathbb{O}$. We will briefly describe this construction, given in Ref. 6 and extended in Ref. 12.

Let $\mathbb{K}$ be one of the division algebras $\mathbb{R},\mathbb{C},\mathbb{H},\mathbb{O}$, consisting of real and complex numbers, quaternions and octonions,[15] respectively. Then the tensor product algebra $\mathbb{K}\otimes\mathbb{O}$ is a KTS with the triple product

$$(xyz)=x(y^*z)+z(y^*x)-y(x^*z),$$

where the conjugation in $\mathbb{K}\otimes\mathbb{O}$ is given from the conjugations in $\mathbb{K}$ and $\mathbb{O}$ simply by

$$(a,b)^*=(a^*,b^*).$$

The complex Lie algebras $L(\mathbb{K}\otimes\mathbb{O})$ associated to these triple systems are

$$L(\mathbb{R}\otimes\mathbb{O})=\mathfrak{f}_4,$$

$$L(\mathbb{C}\otimes\mathbb{O})=\mathfrak{e}_6,$$

$$L(\mathbb{H}\otimes\mathbb{O})=\mathfrak{e}_7,$$

$$L(\mathbb{O}\otimes\mathbb{O})=\mathfrak{e}_8.$$

Thus we obtain 5-gradings of these algebras, but the subspaces $\mathfrak{g}_{\pm 2}$ are not one dimensional. If we include also the *split forms* of $\mathbb{C},\mathbb{H},\mathbb{O}$ in a similar way and consider the real Lie algebras, we get all noncompact forms of $\mathfrak{f}_4,\mathfrak{e}_6,\mathfrak{e}_7,\mathfrak{e}_8$.[12]

The construction (3.6) of $L(K)$ for any Kantor triple system K now leads to a unified realization of the exceptional Lie algebras $\mathfrak{f}_4,\mathfrak{e}_6,\mathfrak{e}_7,\mathfrak{e}_8$. This would be an interesting subject of further studies.

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Open-closed homotopy algebra in mathematical physics

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In this paper we discuss various aspects of open-closed homotopy algebras (OCHAs) presented in our previous paper, inspired by Zwiebach's open-closed string field theory, but that first paper concentrated on the mathematical aspects. Here we show how an OCHA is obtained by extracting the tree part of Zwiebach's quantum open-closed string field theory. We clarify the explicit relation of an OCHA with Kontsevich's deformation quantization and with the B-models of homological mirror symmetry. An explicit form of the minimal model for an OCHA is given as well as its relation to the perturbative expansion of open-closed string field theory. We show that our open-closed homotopy algebra gives us a general scheme for deformation of open string structures (A_∞ algebras) by closed strings (L_∞ algebras). © *2006 American Institute of Physics.* [DOI: 10.1063/1.2171524]

I. INTRODUCTION

In this paper we discuss various aspects of open-closed homotopy algebras (OCHAs) defined in our previous paper.[35] They are a kind of homotopy algebra inspired by Zwiebach's classical open-closed string field theory[74] and also related to the deformation quantization setup by Kontsevich.[40] In Ref. 35 we showed that an OCHA actually defines a homotopy invariant algebraic structure and also it gives us a general scheme for deformation of open string structures (A_∞ algebras) by closed strings (L_∞ algebras).

As tree closed strings and open strings are related to the conformal plane $\mathbb{C}$ with punctures and the upper half plane H with punctures on the boundary, respectively, tree open-closed strings are related to the upper half plane H with punctures both in the bulk and on the boundary, which appears recently in the context of deformation quantization.[40] In operad theory (see Ref. 53), the relevance of the little disk operad to closed string theory is known. The little interval operad and associahedra are relevant to open string theory. The Swiss-cheese operad,[69] that combines the little disk operad with the little interval operad, also is inspired by Kontsevich's approach to deformation quantization. Our OCHA should be homotopy equivalent to a part of an algebra over the Swiss-cheese operad. It should be very interesting to investigate the remaining structures (see Ref. 23, which is related to this direction).

We first present the definition of OCHAs together with recalling two typical homotopy algebras, A_∞ algebras and L_∞ algebras, in Sec. II.

In Sec. III, we give an alternate interpretation in terms of odd formal vector fields (often called homological vector fields) on a supermanifold, which we believe is a more acceptable description for physicists.

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The connection to classical open-closed string field theory by Zwiebach[74] is given in Sec. IV. It is known that classical closed string field theory has an L_∞ structure,[73,66,38] and classical open string field theory has an A_∞ structure.[11,74,55,31] We show that an OCHA is obtained by extracting the tree part of Zwiebach's quantum open-closed string field theory. Since in general homotopy algebras are something whose structures are governed by the underlying tree graph (operad) structure, the structures of quantum string field theories are something beyond the ordinary homotopy algebra (see loop homotopy algebras[50] for quantum closed string field theories). Thus, we can say that OCHAs are the maximal homotopy algebraic structures which string field theories should have. Namely,

$$\text{Quantum open-closed SFT} \supset \text{OCHA} \supset L_\infty \oplus A_\infty.$$

One of the key theorems in homotopy algebra is the minimal model theorem which was proven for A_∞ algebras by Kadeishvili.[30] It holds true also for L_∞ algebras in a similar way, and in our previous paper[35] we stated the minimal model theorem holds for OCHAs, too. In Sec. V we present an explicit way of constructing a minimal model for an OCHA, and explain its relation to the perturbative expansion of classical open-closed string field theory.

Section VI is devoted to explaining some deformation theory aspect of OCHAs. An open-closed homotopy algebra consists of a direct sum of graded vector spaces $\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o$. It has an L_∞ structure on $\mathcal{H}_c$ and reduces to an A_∞ algebra if we set $\mathcal{H}_c=0$. From such a viewpoint, an open-closed homotopy algebra gives a general scheme of deformation of the A_∞ algebra by $\mathcal{H}_c$, where the deformation space is parametrized by a moduli space of the L_∞ algebra on $\mathcal{H}_c$.[35] In Sec. VI A we recall this fact in a more explicit way than Ref. 35. After that, we explain the relation of this viewpoint to various aspects of string theory; Kontsevich's deformation quantization[40] in Sec. VI B, and open-closed B-models (cf. Ref. 26) in Sec. VI C.

II. OPEN-CLOSED HOMOTOPY ALGEBRA

An open-closed homotopy algebra, as we proposed in our previous paper,[35] is a homotopy algebra which combines two typical homotopy algebras, an A_∞ algebra and an L_∞ algebra. There are various equivalent ways of defining and/or describing strong homotopy algebras. In this paper, we shall present them in terms of multivariable operations in this section, and in Sec. III we shall reinterpret them in terms of the supermanifold description. For the equivalent coalgebra description and tree graph description, see Ref. 35. Here we recall just enough so that this paper can be read without having to read Ref. 35. The reader familiar with A_∞ algebras and L_∞ algebras can go directly to Definition 2.8.

We first begin with recalling A_∞ algebras and L_∞ algebras in Sec. II A. The definition of open-closed homotopy algebras are given in Sec. II B. In Sec. II C we define cyclic structures in open-closed homotopy algebras together with explaining some background of such structures.

We restrict our arguments to the case that the characteristic of the field k is zero. We further let $k=\mathbb{C}$ for simplicity.

A. A_∞ algebras and L_∞ algebras

Definition 2.1 [A_∞ *algebra* (*strong homotopy associative algebra*)[64]]: Let $\mathcal{H}_o$ be a $\mathbb{Z}$-graded vector space $\mathcal{H}_o=\oplus_{r\in\mathbb{Z}}\mathcal{H}_o^r$ and suppose that there exists a collection of degree one multilinear maps

$$\mathfrak{m} := \{m_k:(\mathcal{H}_o)^{\otimes k}\to\mathcal{H}_o\}_{k\geqslant 1}.$$

$(\mathcal{H}_o,\mathfrak{m})$ is called an A_∞ *algebra* when the multilinear maps m_k satisfy the following relations:

$$\sum_{k+l=n+1}\sum_{j=0}^{k-1}(-1)^{o_1+\cdots+o_j}m_k(o_1,\ldots,o_j,m_l(o_{j+1},\ldots,o_{j+l}),o_{j+l+1},\ldots,o_n)=0 \tag{2.1}$$

for $n\geqslant 1$, where o_i on (-1) denotes the degree of o_i. A *weak* A_∞ *algebra* $(\mathcal{H}_o,\mathfrak{m})$ consists of a

collection of degree one multilinear maps $\mathfrak{m} := \{m_k : (\mathcal{H}_o)^{\otimes k} \to \mathcal{H}_o\}_{k\geqslant 0}$ satisfying the corresponding relations

$$\sum_{k+l=n+1} \sum_{j=0}^{k-1} (-1)^{o_1+\cdots+o_j} m_k(o_1, \ldots, o_j, m_l(o_{j+1}, \ldots, o_{j+l}), o_{j+l+1}, \ldots, o_n) = 0$$

for $n \geqslant 0$.

Remark 2.2: The definition above is different from the original one[64] in the definition of the degree of the multilinear maps m_k. Both are in fact equivalent and related by *suspension*.[15,53] In Ref. 64, the m_k are multilinear maps on $\downarrow\mathcal{H}_o$ where $(\downarrow\mathcal{H}_o)^{r+1} = \mathcal{H}_o^r$; in algebraic topology the desuspension is denoted by $\downarrow$, which is equivalent to $[-1]$ in the algebraic geometry tradition: $\downarrow\mathcal{H}_o = \mathcal{H}_o[-1]$. Since it might be more familiar also in mathematical physics as in Sec. VI, in this paper we denote the suspension and desuspension by $[1]$ and $[-1]$, respectively.

For an A_∞ algebra $(\mathcal{H}_o, \mathfrak{m})$ (in the case $m_0 = 0$), the first three relations of the A_∞ condition (2.1) are

$$0 = m_1^2,$$

$$0 = m_1(m_2(o_1, o_2)) + m_2(m_1(o_1), o_2) + (-1)^{o_1} m_2(o_1, m_1(o_2)),$$

$$0 = m_1(m_3(o_1, o_2, o_3)) + m_3(m_1(o_1), o_2, o_3) + (-1)^{o_1} m_3(o_1, m_1(o_2), o_3) + (-1)^{o_1+o_2} m_3(o_1, o_2, m_1(o_3))$$

$$+ m_2(m_2(o_1, o_2), o_3) + (-1)^{o_1} m_2(o_1, m_2(o_2, o_3)).$$

The first equation, in the physics terminology, says m_1 is nilpotent; $(\mathcal{H}_o, m_1)$ defines a complex on the $\mathbb{Z}$-graded vector space $\mathcal{H}_o$. The second equation says the differential m_1 satisfies the Leibniz rule for the product m_2. The third equation means the product m_2 is associative up to the term including m_3. Thus, a differential graded algebra (DGA) is described as an A_∞ algebra on $\downarrow\mathcal{H}_o = \mathcal{H}_o[-1]$ with a differential m_1, a product m_2, and $m_3 = m_4 = \cdots = 0$.

Definition 2.3 (A_∞ *morphism*): For two A_∞ algebras $(\mathcal{H}_o, \mathfrak{m})$ and $(\mathcal{H}'_o, \mathfrak{m}')$, suppose that there exists a collection of degree zero (degree preserving) multilinear maps

$$f_k : \mathcal{H}_o^{\otimes k} \to \mathcal{H}'_o, \quad k \geqslant 1.$$

The collection $\{f_k\}_{k\geqslant 1} : (\mathcal{H}_o, \mathfrak{m}) \to (\mathcal{H}'_o, \mathfrak{m}')$ is called an A_∞ *morphism* iff it satisfies the following relations:

$$\sum_{1\leqslant k_1 < k_2 \ldots < k_i = n} m'_i(f_{k_1}(o_1, \ldots, o_{k_1}), f_{k_2-k_1}(o_{k_1+1}, \ldots, o_{k_2}) \cdots f_{n-k_{i-1}}(o_{k_{i-1}+1}, \ldots, o_n))$$
$$= \sum_{k+l=n+1} \sum_{j=0}^{k-1} (-1)^{o_1+\cdots+o_j} f_k(o_1, \ldots, o_j, m_l(o_{j+1}, \ldots, o_{j+l}), o_{j+l+1}, \ldots, o_n) \tag{2.2}$$

for $n \geqslant 1$. If $(\mathcal{H}_o, \mathfrak{m})$ and $(\mathcal{H}'_o, \mathfrak{m}')$ are *weak* A_∞ algebras, then a *weak* A_∞ morphism consists of multilinear maps $\{f_k\}_{k\geqslant 0}$, where $f_0 : \mathbb{C} \to A'$, satisfying the above conditions and in addition

$$f_1 \circ m_0 = \sum m'_k(f_0, \ldots, f_0).$$

As an A_∞ algebra can be thought of as a generalization of a differential graded algebra (DGA), an L_∞ algebra is a generalization of a differential graded Lie algebra (DGLA). As ordinary associative and Lie algebras are related by skew-symmetrization and the universal enveloping construction, there are corresponding relations for A_∞ algebras and L_∞ algebras.[42]

Definition 2.4 (*graded symmetry*): A *graded symmetric multilinear map* of a graded vector

space V to itself is a linear map $f: V^{\otimes n} \to V$ such that, for any $c_i \in V$ $1 \leqslant i \leqslant n$ and any $\sigma \in \mathfrak{S}_n$ (the permutation group of n elements), the relation

$$f(c_1, \ldots, c_n) = (-1)^{\epsilon(\sigma)} f(c_{\sigma(1)}, \ldots, c_{\sigma(n)}) \tag{2.3}$$

holds, where the sign $(-1)^{\epsilon(\sigma)}$ is the Koszul sign of the permutation σ.

Also we adopt the convention that tensor products of functions or operators have the signs built in; e.g., $(f \otimes g)(x \otimes y) = (-1)^{g \cdot x} f(x) \otimes g(y)$.

Definition 2.5 [L_∞ *algebra* (*strong homotopy Lie algebra*)[43]]: Let $\mathcal{H}_c$ be a graded vector space and suppose that a collection of degree one graded symmetric multilinear maps $\mathfrak{l} := \{l_k : \mathcal{H}_c^{\otimes k} \to \mathcal{H}_c\}_{l \geqslant 0}$ is given. $(\mathcal{H}_c, \mathfrak{l})$ is called a *weak* L_∞ *algebra* iff the multilinear maps satisfy the following relations:

$$\sum_{k+l=n+1} \sum_{\sigma \in \mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{l\,!\,(n-l)!} l_k(l_l(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), c_{\sigma(l+1)}, \ldots, c_{\sigma(n)}) = 0 \tag{2.4}$$

for $n \geqslant 0$. If the relation is satisfied for $n \geqslant 1$ without the additional map $l_0 : \mathbb{C} \to \mathcal{H}_c^1 \subset \mathcal{H}_c$, then $(\mathcal{H}_c, \mathfrak{l})$ is called an L_∞ *algebra*.

Remark 2.6: L_∞ algebras are usually defined in a similar but different fashion, where the summation for the permutation $\mathfrak{S}_n$ in Eq. (2.4) is replaced by the summation over the unshuffle permutations (2.3). This unshuffled description would enable us to drop all the symmetrization factors in this paper. However, we take the one with all the permutations since it fits the dual description in the next section.

For an L_∞ algebra $(\mathcal{H}_c, \mathfrak{l})$, the first three relations of the L_∞ condition (2.4) are

$$0 = (l_1)^2,$$

$$0 = l_1(l_2(c_1, c_2)) + l_2(l_1(c_1), c_2) + (-1)^{c_1} l_2(c_1, l_1(c_2)),$$

$$0 = l_1(l_3(c_1, c_2, c_3)) + l_3(l_1(c_1), c_2, c_3) + (-1)^{c_1} l_3(c_1, l_1(c_2), c_3) + (-1)^{c_1 + c_2} l_3(c_1, c_2, l_1(c_3))$$

$$+ l_2(l_2(c_1, c_2), c_3) + (-1)^{c_1(c_2+c_3)} l_2(l_2(c_2, c_3), c_1) + (-1)^{c_3(c_1+c_2)} l_2(l_2(c_3, c_1), c_2).$$

As in the case of an A_∞ algebra, the first equation indicates that $(\mathcal{H}_c, l_1)$ defines a complex, while, after a shift in grading, the second equation implies the differential l_1 satisfies a Leibniz rule with respect to the Lie bracket l_2, and the third equation means the bracket l_2 satisfies the Jacobi identity up to the terms including l_3. Thus, a differential graded Lie algebra is described as an L_∞ algebra on $\downarrow \mathcal{H}_c = \mathcal{H}_c[-1]$ with a differential l_1, a Lie bracket l_2, and $l_3 = l_4 = \cdots = 0$.

Definition 2.7 (L_∞ *morphism*): For two weak L_∞ algebras $(\mathcal{H}_c, \mathfrak{l})$ and $(\mathcal{H}'_c, \mathfrak{l}')$, suppose that there exists a collection of degree zero (degree preserving) graded symmetric multilinear maps

$$f_k : \mathcal{H}_c^{\otimes k} \to \mathcal{H}'_c, \quad l \geqslant 0.$$

Here f_0 is a map from $\mathbb{C}$ to a degree zero subvector space of $\mathcal{H}_c$. The collection $\{f_k\}_{k \geqslant 0} : (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$ is called a *weak* L_∞ *morphism* iff it satisfies the following relations:

$$\sum_{k+l=n+1} \sum_{\sigma \in \mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{l\,!\,(n-l)!} f_k(l_l \otimes \mathbf{1}_c^{\otimes n-l})(c_{\sigma(1)}, \ldots, c_{\sigma(n)}) = \sum_{k_1 + \cdots k_j = n} \sum_{\sigma \in \mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{k_1\,!\,k_2\,!\,\cdots k_j\,!\,\cdot j!} l'_j(f_{k_1} \otimes f_{k_2}$$
$$\otimes \cdots \otimes f_{k_j})(c_{\sigma(1)}, \ldots, c_{\sigma(n)}) \tag{2.5}$$

for $n \geqslant 0$. In particular, when $(\mathcal{H}_c, \mathfrak{l})$ and $(\mathcal{H}'_c, \mathfrak{l}')$ are L_∞ algebras, a weak L_∞ morphism $\{f_k\}_{k \geqslant 0} : (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$ is called an L_∞ *morphism* if in addition $f_0 = 0$.

B. Open-closed homotopy algebra

Definition 2.8 (*open-closed homotopy algebra*[35]): Let $\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o$ be a graded vector space and $(\mathcal{H}_c,\mathfrak{l})$ be a weak L_∞ algebra. Consider a collection of multilinear maps

$$\mathfrak{n} := \{n_{k,l}:(\mathcal{H}_c)^{\otimes k}\otimes(\mathcal{H}_o)^{\otimes l}\to\mathcal{H}_o\}_{k,l\geqslant 0}$$

each of which is graded symmetric on $(\mathcal{H}_c)^{\otimes l}$. We call $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ a *weak open-closed homotopy algebra* (*weak OCHA*) when $\mathfrak{n}$ satisfies the following relations:

$$\begin{aligned}0=&\sum_{p+r=n}\sum_{\sigma\in\mathfrak{S}_n}\frac{(-1)^{\epsilon(\sigma)}}{p!\,r!}n_{1+r,m}(l_p(c_{\sigma(1)},\ldots,c_{\sigma(p)}),c_{\sigma(p+1)},\ldots,c_{\sigma(n)};o_1,\ldots,o_m)\\&+\sum_{p+r=n}\sum_{i+s+j=m}\sum_{\sigma\in\mathfrak{S}_n}\frac{(-1)^{\mu_{p,i}(\sigma)}}{p!\,r!}\\&\times n_{p,i+1+j}(c_{\sigma(1)},\ldots,c_{\sigma(p)};o_1,\ldots,o_i,n_{r,s}(c_{\sigma(p+1)},\ldots,c_{\sigma(n)};o_{i+1},\ldots,o_{i+s}),o_{i+s+1},\ldots,o_m).\end{aligned}\tag{2.6}$$

Here the sign exponent $\mu_{p,i}(\sigma)$ is given explicitly by

$$\mu_{p,i}(\sigma)=\epsilon(\sigma)+(c_{\sigma(1)}+\cdots+c_{\sigma(p)})+(o_1+\cdots+o_i)+(o_1+\cdots+o_i)(c_{\sigma(p+1)}+\cdots+c_{\sigma(n)}),\tag{2.7}$$

corresponding to the signs effected by the interchanges. In particular, if $l_0=n_{0,0}=0$, we call $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ an *open-closed homotopy algebra*. We can also write the defining equation (2.6) in the following shorthand expression:

$$\begin{aligned}0=&\sum_{p+r=n}\sum_{\sigma\in\mathfrak{S}_n}\frac{(-1)^{\epsilon(\sigma)}}{p!\,r!}(-1)^{\epsilon(\sigma)}n_{1+r,m}((l_p\otimes\mathbf{1}_c^{\otimes r}\otimes\mathbf{1}_o^{\otimes m})(c_{\sigma(1)},\ldots,c_{\sigma(n)};o_1,\ldots,o_m))\\&+\sum_{p+r=n}\sum_{i+s+j=m}\sum_{\sigma\in\mathfrak{S}_n}\frac{(-1)^{\epsilon(\sigma)}}{p!\,r!}n_{p,i+1+j}((\mathbf{1}_c^{\otimes p}\otimes\mathbf{1}_o^{\otimes i}\otimes n_{r,s}\otimes\mathbf{1}_o^{\otimes j})(c_{\sigma(1)},\ldots,c_{\sigma(n)};o_1,\ldots,o_m)),\end{aligned}$$

where the complicated sign is absorbed into this expression.

Remark 2.9: For an OCHA $(\mathcal{H},\mathfrak{l},\mathfrak{n})$, the substructure $(\mathcal{H}_c,\mathfrak{l})$ is by definition an L_∞ algebra and $(\mathcal{H}_o,\{n_{0,k}\})$ forms an A_∞ algebra. Furthermore, the substructure $(\mathcal{H},\{n_{1,q}\}_{q\geqslant 0})$ forms an A_∞ module over the A_∞ algebra $(\mathcal{H}_o,\mathfrak{m})$ in the sense of Refs. 49 and 67. Also, if $n_{p,0}=0$ for all $p\geqslant 1$, the substructure $(\mathcal{H},\{n_{p,1}\})$ makes $\mathcal{H}_o$ an L_∞ module over $(\mathcal{H}_c,\mathfrak{l})$.[42]

Now, let us denote $l_1=d_c$ and $n_{0,1}=d_o$. The first few relations which do not appear as A_∞ or L_∞ conditions are

$$0=d_on_{1,0}+n_{1,0}d_c,\tag{2.8}$$

$$0=d_on_{1,1}(c;o)+n_{1,1}(c;d_o(o))+n_{1,1}(d_c(c);o)+n_{0,2}(n_{1,0}(c),o)+(-1)^{c(o+1)}n_{0,2}(o,n_{1,0}(c)),\tag{2.9}$$

$$\begin{aligned}0=&d_on_{2,0}(c_1,c_2)+n_{2,0}(d_c(c_1),c_2)+(-1)^{c_1c_2}n_{2,0}(d_c(c_2),c_1)+n_{1,0}l_2(c_1,c_2)+(-1)^{c_1}n_{1,1}(c_1,n_{1,0}(c_2))\\&+(-1)^{c_2(1+c_1)}n_{1,1}(c_2,n_{1,0}(c_1)),\end{aligned}\tag{2.10}$$

$$0 = d_o n_{1,2}(c;o_1,o_2) + n_{1,2}(d_c(c);o_1,o_2) + (-1)^c n_{1,2}(c;d_o(o_1),o_2) + (-1)^{c+o_1} n_{1,2}(c;o_1,d_o(o_2))$$
$$+ n_{1,1}(c,n_{0,2}(o_1,o_2)) + n_{0,2}(n_{1,1}(c;o_1),o_2) + (-1)^{o_1(1+c)} n_{0,2}(o_1,n_{1,1}(c,o_2)) + n_{0,3}(n_{1,0}(c),o_1,o_2)$$
$$+ (-1)^{o_1(1+c)} n_{0,3}(o_1,n_{1,0}(c),o_2) + (-1)^{(o_1+o_2)(1+c)} n_{0,3}(o_1,o_2,n_{1,0}(c)), \tag{2.11}$$

$$0 = d_o n_{2,1}(c_1,c_2;o) + n_{2,1}(d_c(c_1),c_2;o) + (-1)^{c_1} n_{2,1}(c_1,d_c(c_2);o) + (-1)^{c_1+c_2} n_{2,1}(c_1,c_2;d_o(o))$$
$$+ n_{1,1}(l_2(c_1,c_2);o) + + (-1)^{c_1} n_{1,1}(c_1;n_{1,1}(c_2;o)) + (-1)^{c_2(c_1+1)} n_{1,1}(c_2;n_{1,1}(c_1;o))$$
$$+ n_{0,2}(n_{2,0}(c_1,c_2),o) + (-1)^{o(1+c_1+c_2)} n_{0,2}(o,n_{2,0}(c_1,c_2)) + (-1)^{c_2(1+c_1)} n_{1,2}(c_2;n_{1,0}(c_1),o)$$
$$+ (-1)^{(c_2+o)(1+c_1)} n_{1,2}(c_2;o,n_{1,0}(c_1)) + (-1)^{c_1} n_{1,2}(c_1;n_{1,0}(c_2),o)$$
$$+ (-1)^{c_1+o(1+c_2)} n_{1,2}(c_1;o,n_{1,0}(c_2)), \quad \dots . \tag{2.12}$$

Equation (2.8) implies $n_{1,0}$ is a chain map by an appropriate relative shift of the grading. On the other hand, in the case $n_{0,1}=0$, Eq. (2.9) is an extended Leibniz rule. Suppose that we have an OCHA with only nonzero structures $d_c, d_o, l_2, n_{1,1}, m_2 := n_{0,2}$. In Eq. (2.11) only the second line survives, which means that $\mathcal{H}_c$ acts on an algebra $(\mathcal{H}_o, m_2)$ by $n_{1,1}$ as derivations. Furthermore, in Eq. (2.12) only the second line survives, which implies that $\mathcal{H}_o$ represents a Lie algebra $(\mathcal{H}_c, l_2)$. Then $(\mathcal{H}, d_c, d_o, l_2, n_{1,1}, m_2)$ forms what is called a $\mathfrak{g}$ algebra or Leibniz pair (see Ref. 35 and references there).

Definition 2.10 (*open-closed homotopy algebra morphism*): For two weak OCHAs $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$ and $(\mathcal{H}', \mathfrak{l}', \mathfrak{n}')$, consider a collection $\mathfrak{f}$ of degree zero (degree preserving) multilinear maps

$$f_k : (\mathcal{H}_c)^{\otimes k} \to \mathcal{H}'_c \quad \text{for } k \geqslant 0,$$

$$f_{k,l} : (\mathcal{H}_c)^{\otimes k} \otimes (\mathcal{H}_o)^{\otimes l} \to \mathcal{H}'_o \quad \text{for } k,l \geqslant 0,$$

where f_k and $f_{k,l}$ are graded symmetric with respect to $(\mathcal{H}_c)^{\otimes k}$. We call $\mathfrak{f} : (\mathcal{H}, \mathfrak{l}, \mathfrak{n}) \to (\mathcal{H}', \mathfrak{l}', \mathfrak{n}')$ a *weak OCHA morphism* when $\{f_k\}_{k\geqslant 0} : (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$ is a weak L_∞ morphism and $\{f_{k,l}\}_{k,l\geqslant 0}$ further satisfies the following relations:

$$\sum_{p+r=n} \sum_{\sigma\in\mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{p!\,r!} f_{1+r,m}((l_p \otimes \mathbf{1}_c^{\otimes r} \otimes \mathbf{1}_o^{\otimes m})(c_{\sigma(1)}, \dots, c_{\sigma(n)}; o_1, \dots, o_m))$$
$$+ \sum_{p+r=n} \sum_{i+s+j=m} \sum_{\sigma\in\mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{p!\,r!} f_{p,i+1+j}((\mathbf{1}_c^{\otimes p} \otimes \mathbf{1}_o^{\otimes i} \otimes n_{r,s} \otimes \mathbf{1}_o^{\otimes j})(c_{\sigma(1)}, \dots, c_{\sigma(n)}; o_1, \dots, o_m))$$
$$= \sum_{\substack{(r_1+\cdots+r_i)+(p_1+\cdots+p_j)=n \\ (q_1+\cdots+q_j)=m}} \sum_{\sigma\in\mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{i!\,(r_1!\cdots r_i!)(p_1!\cdots p_j!)} n'_{i,j}((f_{r_1} \otimes \cdots \otimes f_{r_i} \otimes f_{p_1,q_1}$$
$$\otimes \cdots \otimes f_{p_j,q_j})(c_{\sigma(1)}, \dots, c_{\sigma(n)}; o_1, \dots, o_m)). \tag{2.13}$$

The right-hand side is written explicitly as

$$n'_{i,j}((f_{r_1} \otimes \cdots \otimes f_{r_i} \otimes f_{p_1,q_1} \otimes \cdots \otimes f_{p_j,q_j})(c_{\sigma(1)}, \dots, c_{\sigma(n)}; o_1, \dots, o_m))$$
$$= (-1)^{\tau_{\vec{p},\vec{q}}(\sigma)} n'_{i,j}(f_{r_1}(c_{\sigma(1)}, \dots, c_{\sigma(r_1)}), \dots, f_{r_i}(c_{\sigma(\bar{r}_{i-1}+1)}, \dots, c_{\sigma(\bar{r}_i)});$$
$$\times f_{p_1,q_1}(c_{\sigma(\bar{r}_i+1)}, \dots, c_{\sigma(\bar{p}_1)}; o_1, \dots, o_{q_1}), \dots, f_{p_j,q_j}(c_{\sigma(\bar{p}_{j-1}+1)}, \dots, c_{\sigma(\bar{p}_j)}; o_{\bar{q}_{j-1}+1}, \dots, o_{\bar{q}_j})),$$

where $\bar{r}_k := r_1 + \cdots + r_k$, $\bar{p}_k := \bar{r}_i + p_1 + \cdots + p_k$, $\bar{q}_k := q_1 + \cdots + q_k$ and $\tau_{\vec{p},\vec{q}}(\sigma)$ is given by

$$\tau_{\vec{p},\vec{q}}(\sigma) = \sum_{k=1}^{j-1} (c_{\sigma(\bar{p}_k+1)} + \cdots + c_{\sigma(\bar{p}_{k+1})})(o_1 + \cdots + o_{\bar{q}_k}).$$

In particular, if $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ and $(\mathcal{H}',\mathfrak{l}',\mathfrak{n}')$ are OCHAs and if $f_0=f_{0,0}=0$, we call it an *OCHA morphism*.

Definition 2.11 (*quasi-isomorphism*): Suppose that two OCHAs $(\mathcal{H},\mathfrak{l},\mathfrak{n})$, $(\mathcal{H}',\mathfrak{l}',\mathfrak{n}')$ and an OCHA morphism $\mathfrak{f}:(\mathcal{H},\mathfrak{l},\mathfrak{n})\to(\mathcal{H}',\mathfrak{l}',\mathfrak{n}')$ are given. $\mathfrak{f}$ is called an *open-closed homotopy algebra quasi-isomorphism* if $f_1:\mathcal{H}_c\to\mathcal{H}_c'$ induces an isomorphism between the cohomology spaces of the complexes $(\mathcal{H}_c,l_1)$ and $(\mathcal{H}_c',l_1')$, and further $f_{0,1}:\mathcal{H}_o\to\mathcal{H}_o'$ induces an isomorphism between the cohomology spaces of the complexes $(\mathcal{H}_o,n_{0,1})$ and $(\mathcal{H}_o',n_{0,1}')$. In particular, if $f_1$and $f_{0,1}$ are isomorphisms, we call $\mathfrak{f}$ an open-closed homotopy algebra isomorphism.

C. Cyclic structures in OCHAs

Now we consider an additional structure, cyclicity, (cf. Ref. 16) on open-closed homotopy algebras. It is defined in terms of constant symplectic inner products. The string theory motivation for this additional structure is that punctures on the boundary of the disk inherit a cyclic order from the orientation of the disk and the operations are to respect this cyclic structure, just as the L_∞ structure reflects the symmetry of the punctures in the interior of the disk or on the sphere. Alternatively, a typical Lagrangian of a (quantum) field theory originally has such structure and in particular in the Batalin-Vilkovisky (BV) formalism,[3,4] such structure is defined in terms of an odd (degree minus one) symplectic structure on the corresponding supermanifold.[3,62,1,33] Both pictures are then combined with each other in string field theory as discussed in Sec. IV.

From such background, in Ref. 33 a "cyclicity" is defined for A_∞ algebras in terms of a degree minus one constant symplectic inner product, and it is shown that homotopy invariant properties of A_∞ algebras hold true also in the category of cyclic A_∞ algebras. However, in string theory or in particular topological string theory, there often exist cyclic structures defined by inner products having some different degree. For the arguments on homotopy invariant properties in Ref. 33, the degree of the inner product is not essential. Thus, we define cyclic structures with constant symplectic inner products of arbitrary fixed integer degrees.

Definition 2.12 (*constant symplectic structure*): Bilinear maps, $\omega_c:\mathcal{H}_c\otimes\mathcal{H}_c\to\mathbb{C}$ and $\omega_o:\mathcal{H}_o\otimes\mathcal{H}_o\to\mathbb{C}$, are called *constant symplectic structures* when they have fixed integer degrees $|\omega_c|,|\omega_o|\in\mathbb{Z}$ and are nondegenerate and skew-symmetric. Here skew-symmetric indicates that

$$\omega_c(c_2,c_1)=-(-1)^{c_1c_2}\omega_c(c_1,c_2),\quad \omega_o(o_2,o_1)=-(-1)^{o_1o_2}\omega_o(o_1,o_2)$$

for any $c_1,c_2\in\mathcal{H}_c$, $o_1,o_2\in\mathcal{H}_o$, and the degree of ω_c,ω_o implies that $\omega_c(c_1,c_2)=0$ except for $\deg(c_1)+\deg(c_2)+|\omega_c|=0$ and $\omega_o(o_1,o_2)=0$ except for $\deg(o_1)+\deg(o_2)+|\omega_o|=0$. We further denote the constant symplectic structure on $\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o$ by $\omega:=\omega_c\oplus\omega_o$.

Suppose that an open-closed homotopy algebra $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ is equipped with constant symplectic structures $\omega_c:\mathcal{H}_c\otimes\mathcal{H}_c\to\mathbb{C}$ and $\omega_o:\mathcal{H}_o\otimes\mathcal{H}_o\to\mathbb{C}$ as in Definition 2.12.

For $\{l_k\}_{k\geqslant 1}$ and $\{n_{p,q}\}_{p+q\geqslant 1}$, let us define two kinds of multilinear maps by

$$\mathcal{V}_{k+1}=\omega_c(l_k\otimes\mathbf{1}_c):(\mathcal{H}_c)^{\otimes(k+1)}\to\mathbb{C},\quad \mathcal{V}_{p,q+1}=\omega_o(n_{p,q}\otimes\mathbf{1}_o):(\mathcal{H}_c)^{\otimes p}\otimes(\mathcal{H}_o)^{\otimes(q+1)}\to\mathbb{C}$$

or more explicitly

$$\mathcal{V}_{k+1}(c_1,\ldots,c_{k+1})=\omega_c(l_k(c_1,\ldots,c_k),c_{k+1})$$

and

$$\mathcal{V}_{p,q+1}(c_1,\ldots,c_p;o_1,\ldots,o_{q+1})=\omega_o(n_{p,q}(c_1,\ldots,c_p;o_1,\ldots,o_q),o_{q+1}).$$

The degree of $\mathcal{V}_{k+1}$ and $\mathcal{V}_{p,q+1}$ are $|\omega_c|+1$ and $|\omega_o|+1$. Note that the degrees of $\mathcal{V}_{k+1}$ and $\mathcal{V}_{p,q+1}$ are zero when they come from odd constant symplectic structures $|\omega_c|=|\omega_o|=-1$.

Definition 2.13 (*cyclic open-closed homotopy algebra*): An open-closed homotopy algebra $(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$ is called a *cyclic open-closed homotopy algebra* (COCHA) when $\mathcal{V}_{k+1}$ is graded symmetric with respect to any permutation of $(\mathcal{H}_c)^{\otimes(k+1)}$ and $\mathcal{V}_{p,q+1}$ has cyclic symmetry with respect to cyclic permutations of $(\mathcal{H}_o)^{\otimes(q+1)}$, that is, if

$$\mathcal{V}_{k+1}(c_1,\ldots,c_{k+1}) = (-1)^{\epsilon(\sigma)}\mathcal{V}_{k+1}(c_{\sigma(1)},\ldots,c_{\sigma(k+1)}), \quad \sigma \in \mathfrak{S}_{k+1}$$

and

$$\mathcal{V}_{p,q+1}(c_1,\ldots,c_p;o_1,\ldots,o_{q+1}) = (-1)^{o_1(o_2+\cdots+o_{q+1})}\mathcal{V}_{k+1,l}(c_1,\ldots,c_p;o_2,\ldots,o_{q+1},o_1).$$

The graded commutativity of $\mathcal{V}_{p,q+1}$ with respect to permutations of $(\mathcal{H}_c)^{\otimes p}$, that is,

$$\mathcal{V}_{p,q+1}(c_1,\ldots,c_p;o_1,\ldots,o_{q+1}) = (-1)^{\epsilon(\sigma)}\mathcal{V}_{p,q+1}(c_{\sigma(1)},\ldots,c_{\sigma(p)};o_1,\ldots,o_{q+1}), \quad \sigma \in \mathfrak{S}_p$$

automatically holds by the definition of $\mathfrak{n}$.

Note also that there are many situations where the inner products exist only for open strings. This is the case for the topological string situation in the B-model we will discuss later in Sec. VI C. For instance, on the topological open string side, there often exists a natural inner product coming essentially from an integral (trace) of products of two differential forms. The inner products of this kind in fact turn out to be skew-symmetric (symplectic) in our suspended notation (see Ref. 34). See also Ref. 57 for more general cyclic structures including nonskew inner products.

On the other hand, if we have ω_c and ω_o, nondegenerate inner products in both open and closed string sides, we can identify $\mathcal{H}$ with its linear dual, then reverse the process and define further maps

$$r_{p-1,q+1}:(\mathcal{H}_c)^{\otimes(p-1)} \otimes (\mathcal{H}_o)^{\otimes(q+1)} \to \mathcal{H}_c$$

with relations amongst themselves and with the operations already defined, which can easily be deduced from their definition. In particular, for $n_{1,0}:\mathcal{H}_c \to \mathcal{H}_o$ we have $r_{0,1}:\mathcal{H}_o \to \mathcal{H}_c$. Namely, for the cyclic case the fundamental object is the multilinear map $\mathcal{V}_{p,q+1}$ where $n_{p,q}$ and $r_{p-1,q+1}$ are equivalent under the relation above.

Physically, the multilinear map $\mathcal{V}_{p,q+1}$ is related to the (scattering) amplitudes of a disk with p closed strings and $(q+1)$ open strings insertions. Choosing an open string state as a root edge instead of a closed string state, that is, taking $n_{p,q}$ instead of $r_{p-1,q+1}$, for defining an OCHA is related to a standard compactification of the moduli spaces of the corresponding Riemann surface [a disk with p points interior and $(q+1)$ points on the boundary]. Also, in the next section we shall see that, due to this choice of the root edge, the OCHA structure $(\mathfrak{l},\mathfrak{n})$ can be singled out to be an odd vector field on the appropriate supermanifold.

Remark 2.14(*Category version*): As an A_∞ category is defined as a straightforward extension of an A_∞ algebra,[9] one can extend our open-closed homotopy algebra to its category version by replacing $\mathcal{H}_o$ by the space of morphisms of a category. This category extension corresponds to considering many D-branes on which open strings end. This is important for applying OCHAs to topological string theory, see Sec. VI C.

III. THE DUAL SUPERMANIFOLD DESCRIPTION

A. OCHAs and odd formal vector fields

For a graded vector space $\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o$, denote by $\{\mathbf{e}_{c,i}\}$ a basis of $\mathcal{H}_c$ and by $\{\mathbf{e}_{o,i}\}$ a basis of $\mathcal{H}_o$. For each $\mathbf{e}_{c,i}\in\mathcal{H}_c$ represent the dual base as ψ^i and similarly the dual base of $\mathbf{e}_{o,i}\in\mathcal{H}_o$ as ϕ^i. We set the degree of the dual basis by $\deg(\psi^i)=-\deg(\mathbf{e}_{c,i})$ and $\deg(\phi^i)=-\deg(\mathbf{e}_{o,i})$. We consider the formal power series ring in the variables $\{\phi^i\}$, $\{\psi^i\}$, and $\{\phi^i\}\sqcup\{\psi^i\}$, and denote them by $C(\phi)$, $C(\psi)$, and $C(\psi,\phi)$, respectively. We define $\{\psi^i\}$ to be associative and graded commutative and $\{\phi^i\}$ to be associative but noncommutative. More precisely, in the space of the formal power series of associative fields $\{\phi^i\}\sqcup\{\psi^i\}$, an element in $\{\psi^i\}$ is graded commutative with respect to all elements. Therefore, any element in $C(\psi,\phi)$ is represented as

$$a(\psi,\phi) = \sum_{k,l} a_{i_1\cdots i_k;j_1\cdots j_l}(\phi^{j_l}\cdots\phi^{j_1})(\psi^{i_k}\cdots\psi^{i_1}), \tag{3.1}$$

where the coefficient $a_{i_1\cdots i_k;j_1\cdots j_l}\in\mathbb{C}$ is graded symmetric with respect to $i_1\cdots i_k$. We can call

$(\mathcal{H}, C(\phi,\psi))$ the *formal supermanifold*[1,40] corresponding to an OCHA $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$. Though usually the term super indicates $\mathbb{Z}_2$ graded, we use it for $\mathbb{Z}$ graded objects. On the other hand, an A_∞ algebra is described on a formal noncommutative supermanifold $(\mathcal{H}_o, C(\phi))$,[31,33] and an L_∞ algebra is described on a formal graded commutative supermanifold $(\mathcal{H}_c, C(\psi))$.

For a weak OCHA $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$, express the collection of multilinear maps

$$l_k : (\mathcal{H}_c)^{\otimes k} \to \mathcal{H}_c, \quad n_{k,l} : (\mathcal{H}_c)^{\otimes k} \otimes (\mathcal{H}_o)^{\otimes l} \to \mathcal{H}_o,$$

in terms of the bases,

$$l_k(\mathbf{e}_{c,i_1}, \ldots, \mathbf{e}_{c,i_k}) = \mathbf{e}_{c,j} c^j_{i_1 \cdots i_k}, \quad c^j_{i_1 \cdots i_k} \in \mathbb{C},$$

$$n_{k,l}(\mathbf{e}_{c,i_1}, \ldots, \mathbf{e}_{c,i_k}; \mathbf{e}_{o,j_1}, \ldots, \mathbf{e}_{o,j_l}) = \mathbf{e}_{o,j} c^j_{i_1 \cdots i_k; j_1 \cdots j_l}, \quad c^j_{i_1 \cdots i_k; j_1 \cdots j_l} \in \mathbb{C}.$$

Correspondingly, let us define an odd formal vector field $\delta := \delta_S + \delta_D : C(\phi,\psi) \to C(\phi,\psi)$, where

$$\delta_S = \frac{\overleftarrow{\partial}}{\partial \psi^j} c^j(\psi) = \sum_{k \geqslant 0} \frac{1}{k!} \frac{\overleftarrow{\partial}}{\partial \psi^j} c^j_{i_1 \cdots i_k} \psi^{j_k} \cdots \psi^{j_1}, \quad c^j(\psi) \in C(\psi),$$

$$\delta_D = \frac{\overleftarrow{\partial}}{\partial \phi^j} c^j(\phi,\psi) = \sum_{k+l \geqslant 0} \frac{1}{k!} \frac{\overleftarrow{\partial}}{\partial \phi^j} c^j_{i_1 \cdots i_k; j_1 \cdots j_l} (\phi^{j_l} \cdots \phi^{j_1})(\psi^{j_k} \cdots \psi^{j_1}), \quad c^j(\phi,\psi) \in C(\phi,\psi). \tag{3.2}$$

We use right derivatives just for the sign problem; it is easy to relate this dual supermanifold description to the convention in the preceding section. Since $\mathfrak{l}$ and $\mathfrak{n}$ have degree one, δ also has degree one.

It acts on $C(\phi,\psi)$ as follows:

$$\begin{aligned} \delta(a(\phi,\psi)) = & \sum_{k,l} a_{i_1 \cdots i_k; j_1 \cdots j_l} \sum_{s=1}^{k} (-1)^{\beta_S(s-1)} (\phi^{j_l} \cdots \phi^{j_1})(\psi^{j_k} \cdots \delta_S(\psi^{j_s}) \cdots \psi^{j_1}) \\ & + \sum_{k,l} a_{i_1 \cdots i_k; j_1 \cdots j_l} \sum_{t=1}^{l} (-1)^{\beta_D(t-1)} (\phi^{j_l} \cdots \delta_D(\phi^{j_t}) \cdots \phi^{j_1})(\psi^{j_k} \cdots \psi^{j_1}), \end{aligned} \tag{3.3}$$

where $\delta_D(\phi^{j_t}) = c^{j_t}(\phi,\psi)$ and $\delta_S(\psi^{j_s}) = c^{i_s}(\psi)$. Then, $\beta_S(s-1)$ (respectively, $\beta_D(t-1)$) is the sign arising when δ_S (respectively, δ_D) acts from the right and passes the corresponding superfields and is given explicitly by

$$\beta_S(s-1) = \mathbf{e}_{c,i_1} + \cdots + \mathbf{e}_{c,i_{s-1}}, \quad \beta_D(t-1) = (\mathbf{e}_{c,i_1} + \cdots + \mathbf{e}_{c,i_k}) + \mathbf{e}_{o,j_1} + \cdots + \mathbf{e}_{o,j_{t-1}}.$$

The above $\delta(a(\phi,\psi))$ is further rewritten; in the first line ψ's in $\delta_D(\phi^{j_t})$ are brought to the right of ϕ's, and ψ's on each line of Eq. (3.3) are treated as graded symmetric. The $\delta(a(\phi,\psi))$ is expressed in the form in Eq. (3.1) again but with a different coefficient. In the supermanifold language, δ is called an (odd) *formal vector field* on the formal supermanifold. A formal manifold with such a δ is called a *Q-manifold* in Ref. 1 if $Q = \delta$ with $Q^2 = 0$.

Lemma 3.1: *The condition that* $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$ *is a weak OCHA is equivalent to*

$$(\delta)^2 = 0. \tag{3.4}$$

In particular, δ *defines an OCHA if the* $k=0$ *part of* δ_S *and* $k=l=0$ *part of* δ_D *in Eq.* (3.2) *are absent or zero.*

The equation above can be expanded as $(\delta_S)^2+[\delta_S,\delta_D]+(\delta_D)^2=0$, where $[\delta_S,\delta_D]=\delta_S(\delta_D)+\delta_D(\delta_S)$, $\delta_S(\delta_D)=(\overleftarrow{\partial}/\partial\phi^j)(\delta_S(c^j(\phi,\psi)))$. Note that $\delta_D(\delta_S)$ vanishes since δ_S does not include ϕ. Furthermore, one can see that

$$(\delta_S)^2=0, \quad \delta_S(\delta_D)+(\delta_D)^2=0$$

hold independently. The first one is just the dual of the L_∞ condition (2.4), and the second one is the dual description of the OCHA condition (2.6). The pair of the equations above can also be thought of as a deformation of δ_S by $\delta_S+\delta_D$, though we do not discuss this type of deformation in this paper.

A (weak) OCHA morphism in Definition 2.10 can also be rewritten in the same way. For the collection $\mathfrak{f}$ of degree zero multilinear maps,

$$f_l:(\mathcal{H}_c)^{\otimes l}\to\mathcal{H}'_c, \quad f_{k,l}:(\mathcal{H}_c)^{\otimes k}\otimes(\mathcal{H}_o)^{\otimes l}\to\mathcal{H}'_o,$$

let us now express f_k and $f_{k,l}$ as

$$f_k(\mathbf{e}_{c,i_1},\ldots,\mathbf{e}_{c,i_k})=\mathbf{e}_{c,j'}f^{j'}_{i_1\cdots i_k}, \quad f^{j'}_{i_1\cdots i_k}\in\mathbb{C},$$

$$f_{k,l}(\mathbf{e}_{c,i_1},\ldots,\mathbf{e}_{c,i_k};\mathbf{e}_{o,j_1},\ldots,\mathbf{e}_{o,j_l})=\mathbf{e}_{o,j'}f^{j'}_{i_1\cdots i_k;j_1\cdots j_l}, \quad f^{j'}_{i_1\cdots i_k;j_1\cdots j_l}\in\mathbb{C}. \tag{3.5}$$

They define the following coordinate transformation between the two supermanifolds $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ and $(\mathcal{H}',\mathfrak{l}',\mathfrak{n}')$:

$$\psi^{j'}=\mathfrak{f}^{j'}_*(\psi)=f^{j'}+f^{j'}_i\psi^i+f^{j'}_{i_1i_2}\psi^{i_2}\psi^{i_1}+\cdots+f^{j'}_{i_1\cdots i_n}\psi^{i_n}\cdots\psi^{i_1}+\cdots,$$

$$\phi^{j'}=\mathfrak{f}^{j'}_*(\phi,\psi)=\sum_{k,l\geqslant 0}f^{j'}_{i_1\cdots i_k;j_1\cdots j_l}(\phi^{j_l}\cdots\phi^{j_1})(\psi^{j_k}\cdots\psi^{j_1}). \tag{3.6}$$

This induces a pullback from $C(\phi',\psi')$ to $C(\phi,\psi)$,

$$\mathfrak{f}^*(a(\phi',\psi'))=a(\mathfrak{f}_*(\phi,\psi),\mathfrak{f}_*(\psi)),$$

where $\{\phi^i\}$ and $\{\phi^{i'}\}$ are the coordinates on $\mathcal{H}$ and $\mathcal{H}'$, respectively.

Lemma 3.2: *The condition that this* $\mathfrak{f}$ *is a weak OCHA morphism is then that the map between two formal supermanifolds* $\mathfrak{f}_*$ *is compatible with the actions of* δ *and* δ' *on both sides, that is,*

$$\mathfrak{f}^*\delta'(a(\phi',\psi'))=\delta\mathfrak{f}^*a(\phi',\psi') \tag{3.7}$$

holds for any $a(\phi',\psi')\in C(\phi',\psi')$. *In other words,* $\mathfrak{f}_*$ *is a morphism between Q manifolds. If in addition* $f^{j'}=f^{j'}_{\emptyset;\emptyset}=0$, $\mathfrak{f}_*$ *preserves the origin of the formal supermanifolds.* $\mathfrak{f}_*$ *is then an OCHA morphism in the situation that both* δ *and* δ' *define OCHAs.*

All these structures in the supermanifold description are dual to the coalgebra description explained in Ref. 35 in the following sense (see Ref. 33 for the A_∞ case). Let us introduce natural pairings

$$\langle\psi^i|\mathbf{e}_{c,j}\rangle=\delta^i_j, \quad \langle\phi^i|\mathbf{e}_{o,j}\rangle=\delta^i_j$$

and also the extended pairings

$$\langle(\phi^{j_l}\cdots\phi^{j_1})(\psi^{j_k}\cdots\psi^{j_1})|(\mathbf{e}_{c,i'_1}\cdots\mathbf{e}_{c,i'_k})\otimes(\mathbf{e}_{o,j'_1}\cdots\mathbf{e}_{o,j'_l})\rangle=\epsilon^{i_1\cdots i_k}_{i'_1\cdots i'_k}\delta^{j_1}_{j'_1}\cdots\delta^{j_k}_{j'_k}$$

for $k+l>1$, where $\epsilon^{i_1\cdots i_k}_{i'_1\cdots i'_k}:=\Sigma_{\sigma\in\mathfrak{S}_k}\epsilon(\sigma)\delta^{i_{\sigma(1)}}_{i'_1}\cdots\delta^{i_{\sigma(k)}}_{i'_k}$. We set the pairing to be zero if the number of elements ψ/ϕ and $\mathbf{e}_c/\mathbf{e}_o$ does not coincide. The space spanned by $(\mathbf{e}_{c,i_1}\cdots\mathbf{e}_{c,i_k})\otimes(\mathbf{e}_{o,j_1}\cdots\mathbf{e}_{o,j_l})$, $k+l\geqslant 1$, is what is denoted $C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)$ in Ref. 35. As the adjoint of the product on $C(\psi,\phi)$, a

coproduct $\Delta: C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)\to (C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o))\otimes (C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o))$ is defined; for $a,b \in C(\psi,\phi)$ and $x\in C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)$,

$$\langle b\cdot a|x\rangle = \sum_i \langle a|x_i^+\rangle\cdot\langle b|x_i^-\rangle, \quad \Delta := \sum_i (x_i^+\otimes x_i^-).$$

Thus, $C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)$ forms a coalgebra. Then, a codifferential $\mathfrak{l}+\mathfrak{n}: C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)\to C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)$ is given as the adjoint of $\delta=\delta_S+\delta_D$,

$$\langle a|(\mathfrak{l}+\mathfrak{n})(x)\rangle := \langle \delta(a)|x\rangle.$$

In a similar way, a coalgebra homomorphism $\mathfrak{f}: C(\mathcal{H}_c)\otimes T^c(\mathcal{H}_o)\to C(\mathcal{H}_c')\otimes T^c(\mathcal{H}_o')$ is obtained as the adjoint of the pullback $\mathfrak{f}^*: C(\phi',\psi')\to C(\phi,\psi)$. Thus, the coalgebra description given in Ref. 35 is obtained as the dual of the algebra description in terms of formal power series on supermanifolds.

B. Cyclicity and constant symplectic and/or Poisson structures

Next, we discuss the cyclicity (Definition 2.13). If cyclicity is imposed on the ϕ^i's, we indicate that by $C(\phi)_{\mathrm{cyc}}$ or $C(\phi,\psi)_{\mathrm{cyc}}$. Any element of $C(\phi,\psi)_{\mathrm{cyc}}\subset C(\phi,\psi)$ is represented in the form in Eq. (3.1) but the coefficient $a_{i_1\cdots i_k;j_1\cdots j_l}$ is in addition graded cyclic symmetric with respect to the indices $j_1\cdots j_l$. On this algebra, a constant Poisson structure is introduced naturally by dualizing the constant symplectic structures in Definition 2.12.

Definition 3.3 (*constant Poisson structure*): Suppose $\mathcal{H}_c$ and $\mathcal{H}_o$ have constant symplectic structures $\omega_c:\mathcal{H}_c\otimes\mathcal{H}_c\to\mathbb{C}$ and $\omega_o:\mathcal{H}_o\otimes\mathcal{H}_o\to\mathbb{C}$ (Definition 2.12). The corresponding Poisson brackets are denoted by

$$(\ ,\ )_c = \frac{\overleftarrow{\partial}}{\partial\phi^i}\omega_c^{ij}\frac{\overrightarrow{\partial}}{\partial\phi^j}, \quad (\ ,\ )_o = \frac{\overleftarrow{\partial}}{\partial\phi^i}\omega_o^{ij}\frac{\overrightarrow{\partial}}{\partial\phi^j}.$$

Here $\omega_c^{ij}\in\mathbb{C}$ and $\omega_o^{ij}\in\mathbb{C}$ are the inverse matrices of $\omega_{c,ij}:=\omega_c(\mathbf{e}_{c,i},\mathbf{e}_{c,j})$ and $\omega_{o,ij}:=\omega_o(\mathbf{e}_{o,i},\mathbf{e}_{o,j})$. That is, $\omega_{c,ij}\omega_c^{jk}=\omega_c^{kj}\omega_{c,ji}=\delta_i^k$ and $\omega_{o,ij}\omega_o^{jk}=\omega_o^{kj}\omega_{o,ji}=\delta_i^k$ hold. Thus $(\ ,\ )_c$ is a graded Poisson bracket for a graded commutative algebra and $(\ ,\ )_o$ is a Poisson bracket for the cyclic algebra as in Ref. 31. $C(\psi)_{\mathrm{cyc}}$ and $C(\phi)_{\mathrm{cyc}}$ form graded Poisson algebras with Poisson brackets $(\ ,\ )_c$ and $(\ ,\ )_o$, respectively. Furthermore, these two Poisson brackets can be combined naturally and extended to one on $C(\phi,\psi)_{\mathrm{cyc}}$.

A COCHA (Definition 2.13) is dualized as follows. For the collection of multilinear maps $\mathcal{V}_k$ and $\mathcal{V}_{k,l}$, let us define their coefficients by

$$\mathcal{V}_k(\mathbf{e}_{c,i_1},\ldots,\mathbf{e}_{c,i_k}) := \mathcal{V}_{i_1\cdots i_k}\in\mathbb{C}, \quad \mathcal{V}_{k,l}(\mathbf{e}_{c,i_1},\ldots,\mathbf{e}_{c,i_k};\mathbf{e}_{o,j_1},\ldots,\mathbf{e}_{o,j_l}) := \mathcal{V}_{i_1\cdots i_k;j_1\cdots j_l}\in\mathbb{C}.$$

Note that they are graded symmetric with respect to the indices $i_1\cdots i_k$ and cyclic with respect to the indices $j_1\cdots j_l$. Consider further a formal sum of polynomial functions S,

$$S(\phi,\psi)=S_S(\psi)+S_D(\phi,\psi), \quad S_S(\psi)\in C(\psi), \quad S_D(\phi,\psi)\in C(\phi,\psi)_{\mathrm{cyc}}, \tag{3.8}$$

where S_S and S_D are defined by

$$S_S(\psi)=\sum_{l\geqslant 2}\frac{1}{l!}\mathcal{V}_{i_1\cdots i_l}\psi^{i_l}\cdots\psi^{i_1}, \quad \mathcal{V}_{i_1\cdots i_l}\in\mathbb{C},$$

$$S_D(\phi,\psi)=\sum_{k\geqslant 0,l\geqslant 1,k+l\geqslant 2}\frac{1}{k!\,l}\mathcal{V}_{i_1\cdots i_k;j_1\cdots j_l}(\phi^{j_l}\cdots\phi^{j_1})(\psi^{i_k}\cdots\psi^{i_1}), \quad \mathcal{V}_{i_1\cdots i_k;j_1\cdots j_l}\in\mathbb{C}. \tag{3.9}$$

Then one can define the formal vector field δ acting on $C(\phi,\psi)_{\mathrm{cyc}}$ as follows:

$$\delta := \delta_S + \delta_D, \quad \delta_S = (\ ,S_S)_c, \quad \delta_D = (\ ,S_D)_o. \tag{3.10}$$

The condition $(\delta)^2=0$ coincides with the condition that $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ is a COCHA.

IV. ZWIEBACH'S OPEN-CLOSED STRING FIELD THEORY

String field theory is defined on a fixed conformal background of a space-time (target space) M to which world sheets of strings (Riemann surfaces) are mapped, where the conformal background is a background (metric, etc., of M) in which string world sheet theory has conformal symmetry. There exist several classes of string field theories corresponding to the classes of Riemann surfaces. The most general one is quantum open-closed string field theory,[74] which is associated to the most general class of Riemann surfaces: Riemann surfaces of arbitrary genus, possibly with boundaries and punctures.

It includes various substring field theories: classical open string field theories—associated to disks (one boundary and zero genus) with punctures only on the boundary, classical closed string field theories—associated to spheres (no boundary and genus zero) with punctures, quantum closed string field theories—associated to Riemann surfaces with punctures (and various genera) and without boundary, and so on. Genera and multiboundaries relate to closed and open string loops (in the sense of Feynman diagrams), respectively. We use the term classical (respectively, quantum) for theory without loops (respectively, with loops). In this section we shall explain that, extracting the tree open-closed part from Zwiebach's quantum open-closed string field theory,[74] one obtains an OCHA. Namely, an OCHA is a general homotopy algebraic structure for tree open-closed string field theory as L_∞ algebras (respectively, A_∞ algebras) are for tree closed (respectively, open) string field theories.

The quantum open-closed string field theory discussed by Zwiebach[74] is defined by all possible open-closed interaction vertices together with closed and open string kinetic terms satisfying the quantum BV master equation. The interaction term is expressed formally in the following form [Eq. (5.7) of Ref. 74]:

$$f(\mathcal{V}^{g,n}_{b,m}) = \left[\frac{1}{n!}\frac{1}{b!}\prod_{k=1}^{b}\frac{1}{m_k}\right]\int_{\mathcal{V}^{g,n}_{b,n}} \langle\Omega|\underbrace{|\Psi\rangle\cdots|\Psi\rangle}_{n}\prod_{k=1}^{b}\underbrace{|\Phi\rangle\cdots|\Phi\rangle}_{m_k}. \tag{4.1}$$

Here the kets $|\Psi\rangle\in\mathcal{H}_c$ and $|\Phi\rangle\in\mathcal{H}_o$ are the *closed string fields* and the *open string fields*, respectively. $\mathcal{V}^{g,n}_{b,m}\subset\bar{\mathcal{M}}^{g,n}_{b,m}$ is the appropriate subspace of the compactified moduli space of Riemann surfaces with genus g, n-interior punctures and b boundaries S^1 having $m_1,\ldots,m_b$ punctures on them. Equivalently, it has n-closed string punctures and m_i-open string insertions on the corresponding boundary S^1. The bra $\langle\Omega|$ denotes a differential form on $\bar{\mathcal{M}}^{g,n}_{b,m}$ which takes its value in $(\mathcal{H}^*_c)^{\otimes n}\otimes(\mathcal{H}^*_o)^{\otimes m_1}\otimes\cdots\otimes(\mathcal{H}^*_o)^{\otimes m_b}$. This data is determined by the conformal field theory for a fixed conformal background. Then, the combination $\int_{\mathcal{V}^{g,n}_{b,m}}\langle\Omega|$ defines a map

$$\int_{\mathcal{V}^{g,n}_{b,m}}\langle\Omega|:(\mathcal{H}_c)^{\otimes n}\otimes(\mathcal{H}_o)^{\otimes m_1}\otimes\cdots\otimes(\mathcal{H}_o)^{\otimes m_b}\to\mathbb{C}. \tag{4.2}$$

In terms of bases $\mathbf{e}_{c,i}$ and $\mathbf{e}_{o,j}$ of the *spaces of states* $\mathcal{H}_c$ and $\mathcal{H}_o$, the kets can be expressed as $|\Psi\rangle := \Sigma_i\mathbf{e}_{c,i}\psi^i$ and $|\Phi\rangle := \Sigma_j\mathbf{e}_{o,j}\phi^j$, and the coordinates ψ^i and ϕ^j play the role of fields. The degree of each basis element $\mathbf{e}_{c,i}$ or $\mathbf{e}_{o,j}$ is determined by the corresponding conformal field theory on the string world sheet and is related to the degree of field ψ^i or ϕ^j through the relations $\deg(\psi^i) = -\deg(\mathbf{e}_{c,i})$ and $\deg(\phi^i)=-\deg(\mathbf{e}_{o,i})$. The degrees $\deg(\psi^i)$ and $\deg(\phi^i)$ in turn denote the ghost numbers in the sense of the BV-formalism for the target space field theory. The map (4.2) is defined to be of degree zero because of a ghost number preserving condition on the string world sheets, naturally extended to the polynomials of ψ^i and ϕ^j. Then $f(\mathcal{V}^{g,n}_{b,m})$ in Eq. (4.1), which is the image of $|\Psi\rangle^{\otimes n}\otimes\Pi_{k=1}^{b}|\Phi\rangle^{\otimes m_k}$ by the map (4.2), belongs to a subspace of $C(\psi,\phi)$ whose elements are expressed in general in the form

$$a(\phi,\psi)=\sum_{k,l}\frac{1}{k!\,l!\,|J_1|\cdots|J_l|}a_{i_1\cdots i_k;J_1,\ldots,J_l}(\phi^{J_l}\cdots\phi^{J_1})(\psi^{j_k}\cdots\psi^{j_1}).$$

For the interaction terms, $|J_i|=m_i$ in the notation in Eq. (4.1). Here $J=(j_1,\ldots,j_{|J|})$ is the multi-index, $\phi^J=\phi^{j_{|J|}}\cdots\phi^{j_1}$. The coefficient $a_{i_1\cdots i_k;J_1,\ldots,J_l}\in\mathbb{C}$ is then graded symmetric with respect to the cyclic permutations of each multi-index $J=(j_1,\ldots,j_{|J|})$, all the permutations of $i_1\cdots i_k$, and those of $J_1,\ldots,J_l$. We denote the corresponding subspace by $C(\phi,\psi)_{\mathrm{qoc}}:=C_{\mathrm{sym}}(\psi)\otimes C_{\mathrm{sym}}(C(\phi)_{\mathrm{cyc}})\subset C(\phi,\psi)$, where qoc indicates quantum open-closed. Note that, by construction, the degree of $f(\mathcal{V}^{g,n}_{b,m})$ is zero. The closed string kinetic term and the open string kinetic term are expressed as follows:

$$\tfrac{1}{2}\langle\Psi,Q_c\Psi\rangle_c,\quad \tfrac{1}{2}\langle\Phi,Q_o\Phi\rangle_o \tag{4.3}$$

which also belong to $C(\phi,\psi)_{\mathrm{qoc}}$ and have degree zero. In our notation, $Q_c=l_1:\mathcal{H}_c\to\mathcal{H}_c$ and $Q_o=n_{0,1}:\mathcal{H}_o\to\mathcal{H}_o$. Physically, Q_c (respectively, Q_o) is called the *BRST operator* for closed (respectively, open) strings, where BRST is taken in the sense of the conformal field theory on the string world sheet. Their cohomologies then define the physical state spaces of strings. Also, the brackets are just the constant symplectic structures in Definition 2.12,

$$\langle\ ,\ \rangle_c=\omega_c:\mathcal{H}_c\otimes\mathcal{H}_c\to\mathbb{C},\quad \langle\ ,\ \rangle_o=\omega_o:\mathcal{H}_o\otimes\mathcal{H}_o\to\mathbb{C}.$$

Since these constant symplectic structures come from the BV formalism[3,4] in which string field theories are described, the degrees of ω_c and ω_o are set to be minus one. In such a superfield description of the BV formalism, they are called *odd symplectic structures*[62,1] since degree minus one implies *odd* in $\mathbb{Z}_2$ grading. The corresponding odd Poisson brackets

$$(\ ,\ )=(\ ,\ )_c+(\ ,\ )_o,\quad (\ ,\ )_c=\frac{\overleftarrow{\partial}}{\partial\psi^j}\omega_c^{ij}\frac{\overrightarrow{\partial}}{\partial\psi^j},\quad (\ ,\ )_o=\frac{\overleftarrow{\partial}}{\partial\phi^i}\omega_o^{ij}\frac{\overrightarrow{\partial}}{\partial\phi^j}$$

are what are called the *BV brackets*. Since they have degree one, $(\psi^j,\psi^j)_c=\omega_c^{ij}\neq 0$ only when the sum of the degree of ψ^j and the degree of ψ^j is equal to minus one. In the BV formalism,[3,4] two fields ψ^j and ψ^j having nonzero ω_c^{ij} make a pair of a *field* and an *antifield*. Of course these facts hold true similarly for open string fields (see Refs. 31 and 33). Both Poisson brackets are naturally combined and extended to $(\ ,\ )$ on $C(\phi,\psi)_{\mathrm{qoc}}$. Also, define second order operators as

$$\Delta=\Delta_c+\Delta_o,\quad \Delta_c=\frac{1}{2}(-1)^{\mathbf{e}_{c,i}}\omega_c^{ij}\frac{\overrightarrow{\partial}}{\partial\psi^j}\frac{\overrightarrow{\partial}}{\partial\psi^j},\quad \Delta_o=\frac{1}{2}(-1)^{\mathbf{e}_{o,i}}\omega_o^{ij}\frac{\overrightarrow{\partial}}{\partial\phi^i}\frac{\overrightarrow{\partial}}{\partial\phi^j}. \tag{4.4}$$

Since the BV brackets have degree one, we have $\deg(\Delta)=1$, while $(C(\psi),\Delta_c,\bullet,(\ ,\ )_c)$ and $(C(\phi)_{\mathrm{cyc}},\Delta_o,\bullet,(\ ,\ )_o)$ form BV algebras (see Refs. 3, 4, and 14).

Further $(C(\psi,\phi)_{\mathrm{qoc}},\Delta,\bullet,(\ ,\ ))$ forms a BV algebra, where $\bullet:C(\psi,\phi)_{\mathrm{qoc}}\otimes C(\psi,\phi)_{\mathrm{qoc}}\to C(\psi,\phi)_{\mathrm{qoc}}$ is the associative product, symmetric in the ψ's. We shall soon reduce them to the tree open-closed structures, so do not stress to explain the detail of the structure on the whole $C(\psi,\phi)_{\mathrm{qoc}}$ in this paper.

The action of quantum open-closed string field theory is then given by summing up the kinetic terms (4.3) and all the interaction terms (vertices) in Eq. (4.1),

$$S_{\mathrm{qoc}}(\phi,\psi)=\sum_{g,b,n}\frac{1}{n!\,b!\,|J_1|\cdots|J_b|}\mathcal{V}^g_{i_1\cdots i_n;J_1,\ldots,J_b}(\phi^{J_b}\cdots\phi^{J_1})(\psi^{j_n}\cdots\psi^{j_1}),$$

$$\mathcal{V}^{g}_{i_1\cdots i_n;J_1,\ldots,J_b} := \int_{\mathcal{V}^{g,n}_{b,m}} \langle\Omega|(\mathbf{e}_{c,i_1},\ldots,\mathbf{e}_{c,i_n};\mathbf{e}_{o,J_1},\ldots,\mathbf{e}_{o,J_b}), \tag{4.5}$$

where $\mathbf{e}_{o,J}=\mathbf{e}_{o,j_1}\cdots\mathbf{e}_{o,j_{|J|}}$ for $J=(j_1,\ldots,j_{|J|})$, and the summation $\Sigma_{g,b,n}$ is taken for all $g\geqslant 0$, $b\geqslant 0$ and $n\geqslant 0$ except for the cases $(g,b)=(0,0), n\leqslant 1$, $(g,n,b)=(0,0,1), |J_1|\leqslant 1$ and $(g,n,b)=(1,0,0)$. In particular, the terms with $(g,n,b)=(0,2,0)$ and $(g,n,b)=(0,0,1)$ with $|J_1|=2$ are the kinetic terms of closed strings and open strings, respectively.

A quantum open-closed string field theory $S_{\mathrm{qoc}}(\phi,\psi)$ is defined so that it satisfies the *quantum master equation*

$$\tfrac{1}{2}(S_{\mathrm{qoc}},S_{\mathrm{qoc}}) + \Delta S_{\mathrm{qoc}} = 0. \tag{4.6}$$

Note that ΔS_{qoc} is the term peculiar to the *quantum* string field theory. Δ_c increases g by one and Δ_o increases b by one for $b>0$. The quantum master equation splits into separate equations for each genus g and number of boundaries b. When we concentrate on the equations for $g=0$ and $b=0$ or 1, we get

$$(g,b)=(0,0), \quad 0=(S_S,S_S)_c, \tag{4.7}$$

$$(g,b)=(0,1), \quad 0=(\widetilde{S}_D,S_S)_c+\tfrac{1}{2}(\widetilde{S}_D,\widetilde{S}_D)_o, \tag{4.8}$$

where S_S and $\widetilde{S}_D$ consist of the corresponding terms in S_{qoc} in Eq. (4.5); explicitly, S_S is of the same form as S_S in Eq. (3.9) and $\widetilde{S}_D$ consists of S_D in Eq. (3.9) with additional terms corresponding to $(k,l)=(k,0)$ below,

$$S_S(\psi)=\sum_{l\geqslant 2}\frac{1}{l!}\mathcal{V}_{i_1\cdots i_l}\psi^{j_l}\cdots\psi^{j_1}\in C(\psi),$$

$$\widetilde{S}_D(\phi,\psi)=\sum_{k\geqslant 0,l\geqslant 0,2k+l\geqslant 2}\frac{1}{k!\;l}\mathcal{V}_{i_1\cdots i_k;j_1\cdots j_l}(\phi^{j_l}\cdots\phi^{j_1})(\psi^{j_k}\cdots\psi^{j_1})\in C(\phi,\psi)_{\mathrm{cyc}}. \tag{4.9}$$

Here we dropped the index g used in Eq. (4.5) since $g=0$. Namely, we denote

$$\mathcal{V}^{g=0}_{i_1\cdots i_l;\varnothing}=:\mathcal{V}_{i_1\cdots i_l}, \quad \mathcal{V}^{g=0}_{i_1\cdots i_l;J=(j_1,\ldots,j_l)}=:\mathcal{V}_{i_1\cdots i_l;j_1\cdots j_l}.$$

The action S_S corresponds to punctured spheres [since the corresponding Riemann surfaces have no boundary $(\varnothing)$], whereas $\widetilde{S}_D$ corresponds to disks with punctures both in the disks and on the boundary of the disks. Equation (4.8) is often called a *Maurer-Cartan equation*.

A classical (tree) open-closed string field theory[74] is then given by the action $S_{\mathrm{toc}}(\phi,\psi)=S_S(\psi)+\widetilde{S}_D(\phi,\psi)$ satisfying Eqs. (4.7) and (4.8), the Batalin-Vilkovisky[3,4] classical open-closed master equations. The identity (4.7) implies that S_S is just the action of the classical closed string field theory.[73] Namely, S_S has a cyclic L_∞ structure. For the operadic construction of the classical closed string field theory, see Ref. 38. The relevant operad is the L_∞ operad of nonplanar trees, where the composition of the trees corresponds to the *twist-sewing* of two S^1's parametrizing two closed strings and/or boundaries in a Riemann surface picture.[73,38]

Just in the same way as for Eq. (3.10), one can define the following formal vector fields acting on $C(\phi,\psi)_{\mathrm{cyc}}$:

$$\delta := \delta_S+\delta_D, \quad \delta_S=(\ ,S_S)_c, \quad \delta_D=(\ ,\widetilde{S}_D)_o. \tag{4.10}$$

The condition $(\delta)^2=0$ that $(\mathcal{H},\mathfrak{l},\mathfrak{n})$ is a cyclic OCHA is equivalent to the derivatives of the master equations (4.7) and (4.8),

$$0 = (\ ,(S_S,S_S)_c)_c,$$

$$0 = \left(\ ,(\widetilde{S}_D,S_S)_c + \tfrac{1}{2}(\widetilde{S}_D,\widetilde{S}_D)_o\right)_o.$$

Here note that, as has been explained in Eq. (4.9), $\widetilde{S}_D$ consists of S_D with the following additional terms:

$$\frac{1}{l!}\mathcal{V}_{j_1\cdots j_l;J=\emptyset}(\psi^{j_l}\cdots\psi^{j_1}) \tag{4.11}$$

each of which corresponds to a disk with punctures only in the bulk (the interior of the disk) and no punctures $J=\emptyset$ on the boundary. However, one can see that these terms drop out in Eq. (4.10): $(\ ,\widetilde{S}_D)_o=(\ ,S_D)_o$, since no open string field ϕ^i is included in Eq. (4.11). This is why we do not include the corresponding terms in the definition of (cyclic) OCHAs. Thus, a classical open-closed string field theory is a cyclic OCHA with the additional terms (4.11).

Of course, there exist situations in which these terms (4.11) are also important physically. For example, the terms (4.11) contribute to a constant term for open string field theory in discussing its deformation as in Sec. VI, and the constant term is relevant to D-brane mass, since the value of the action is believed to correspond to D-brane mass in open string field theory. But, it is enough to consider a cyclic OCHA structure in a classical open-closed string field theory at present if we examine its homotopy algebraic structures in the sense of the next section.

V. MAURER-CARTAN EQUATION, MINIMAL MODEL, AND TREE OPEN-CLOSED STRING AMPLITUDES

Homotopy algebras should have some homotopical properties.[7,51] One of the key theorems in homotopy algebra is the minimal model theorem. The minimal model theorem for A_∞ algebras was proved by Kadeishvili.[30] For the construction of minimal models of A_∞ structures, homological perturbation theory was developed by Refs. 17, 28, 18, 21, 19, and 20, for instance, and the form of a minimal model is then given explicitly in Refs. 54 and 41. Also, the existence of a stronger theorem, called the decomposition theorem in Refs. 33 and 36, is mentioned in Ref. 40 and proven by employing a kind of homological perturbation theory in Refs. 33 and 36 (see also Ref. 47). It is clear that the same arguments hold true for L_∞ algebras, and in our previous paper[35] we stated that they hold also for OCHAs.

In this section, we present the explicit form of a minimal model for an OCHA, which in the cyclic case can be thought of as the perturbative expansion of a classical open-closed string field theory.

Definition 5.1 (*minimal open-closed homotopy algebra*): An OCHA $(\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o,\mathfrak{l},\mathfrak{n})$ is called minimal if $l_1=0$ on $\mathcal{H}_c$ and $n_{0,1}=0$ on $\mathcal{H}_o$.

Theorem 5.2 (**Minimal model theorem for open-closed homotopy algebras**[35]): *For any OCHA, there exists a minimal OCHA and an OCHA quasi-isomorphism from the minimal OCHA to the original OCHA.*

The minimal model theorem holds also for COCHAs. Namely, for any COCHA, there exists a minimal COCHA and a COCHA quasi-isomorphism from the minimal COCHA to the original COCHA. This fact also follows from the explicit minimal model we shall construct here.

First of all, we fix a Hodge decomposition of the complex $(\mathcal{H},d=l_1+n_{0,1})$. Namely, for $d_c=l_1$ and $d_o=n_{0,1}$, we give Hodge decompositions of the complexes $(\mathcal{H}_c,d_c)$ and $(\mathcal{H}_o,d_o)$ separately, by fixing degree minus one (homotopy) operators $h_c:\mathcal{H}_c\to\mathcal{H}_c$ and $h_o:\mathcal{H}_o\to\mathcal{H}_o$,

$$d_ch_c+h_cd_c+\iota_c\circ\pi_c=\mathbf{1}_c,\quad d_oh_o+h_od_o+\iota_o\circ\pi_o=\mathbf{1}_o. \tag{5.1}$$

Here, π and ι indicate the projection to and the inclusion into the corresponding cohomologies. Thus, these data give a contraction (deformation retract) of $\mathcal{H}=\mathcal{H}_c\oplus\mathcal{H}_o$ as a graded vector space (see Ref. 35),

$$(H(\mathcal{H}) \underset{\pi}{\overset{\iota}{\rightleftarrows}} \mathcal{H}, h), \tag{5.2}$$

where $\iota := \iota_c + \iota_o$, $\pi := \pi_c + \pi_o$ and $h = h_c + h_o$.

We would like to follow the arguments in Refs. 31 and 33, where a minimal model is obtained by a process of solving the Maurer-Cartan equation for an A_∞ algebra. For OCHAs, the Maurer-Cartan equations are defined as follows.[35]

Definition 5.3 (*Maurer-Cartan equation*): For an OCHA $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$ and degree zero elements $\bar{c} \in \mathcal{H}_c$ and $\bar{o} \in \mathcal{H}_o$, we call the following pair of equations

$$0 = \sum_k \frac{1}{k!} l_k(\bar{c}, \ldots, \bar{c}), \quad 0 = \sum_{k,l} \frac{1}{k!} n_{k,l}(\bar{c}, \ldots, \bar{c}; \bar{o}, \ldots, \bar{o}) \tag{5.3}$$

the *Maurer-Cartan equations* for the OCHA $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$.

Remark 5.4: Recall that, for the cyclic A_∞ or L_∞ case, the Maurer-Cartan equations are just the equations of motions for the action (of the corresponding string field theory).[31,33] In field theory, the equations of motions are defined by the derivatives of the action with respect to the fields. For instance, for classical closed string field theory with the action S_S, the equations of motions are $0 = (\vec{\partial}/\partial\psi^i) S_S$ for each i. Here, since the BV bracket $(\ ,\ )_c := (\overleftarrow{\partial}/\partial\psi^i)\omega_c^{ij}(\vec{\partial}/\partial\psi^j)$ is nondegenerate, the equations of motions are equivalent to $0 = (\ , S_S)$ $(= \delta_S)$. Usually, we set degree nonzero fields to be zero and concentrate on the solutions for the fields of degree zero. Then, further identifying $\vec{\partial}/\partial\psi^i$ with $\mathbf{e}_c^i$ in $0 = \delta_S$, one obtains the Maurer-Cartan equations for the L_∞ algebra, which is the first equation in Eq. (5.3). However, note that, for a COCHA $(\mathcal{H}, \omega, \mathfrak{l}, \mathfrak{n})$, the zeroes of the corresponding odd formal vector field $\delta = \delta_S + \delta_D$ are not the same as solutions to the equations of motions $0 = (\ , S) = (\ , S)_c + (\ , S)_o$, or separately

$$0 = \frac{\overleftarrow{\partial}}{\partial\psi^i}\omega_c^{ij}\frac{\vec{\partial}}{\partial\psi^j}(S_S + S_D) = 0, \quad 0 = \frac{\overleftarrow{\partial}}{\partial\phi^i}\omega_o^{ij}\frac{\vec{\partial}}{\partial\phi^j}S_D = 0,$$

for the COCHA. Namely, the first equation above includes the term $(\ , S_D)_c$, the corresponding term of which is absent in the Maurer-Cartan equations (5.3) for the COCHA.

One can see that, if one solves the equations of motions, instead of solving the Maurer-Cartan equations, the resulting structure includes terms corresponding to $b > 1$.

If we apply the arguments in Refs. 31 and 33 to an OCHA, the Maurer-Cartan equations for an OCHA should be considered formally for the pair of string fields $(\Psi, \Phi) \in (\mathcal{H}_c \otimes \mathcal{H}_c^*, \mathcal{H}_o \otimes \mathcal{H}_o^*)$ instead of their degree zero parts $(\bar{c}, \bar{o}) \in (\mathcal{H}_c^0, \mathcal{H}_o^0)$.

Then, for instance for the L_∞ part, solving the Maurer-Cartan equation recursively one gets first an L_∞ quasi-isomorphism $\{f_k\}_{k\geqslant 1} : (H(\mathcal{H}_c))^{\otimes k} \to \mathcal{H}_c$. This somewhat physical procedure is closely related to the homological perturbation theory developed earlier, and in particular, $\mathfrak{f} := \oplus_k f_k \in \oplus_k \mathrm{Hom}((H(\mathcal{H}_c))^{\otimes k}, \mathcal{H}_c)$ is just what is called a *twisting cochain* τ (see Ref. 29 for the DGLA case). Then, substituting $\mathfrak{f}$ instead of Ψ into the initial Maurer-Cartan equation, one obtains an equation on $H(\mathcal{H}_c)$, which is in fact the Maurer-Cartan equation for the corresponding minimal L_∞ algebra, so one can read the minimal L_∞ structure from the Maurer-Cartan equation. For the case of an OCHA, its minimal model is obtained by first considering the Maurer-Cartan equation for the L_∞ algebra as above and, after that, considering the Maurer-Cartan equation for $\mathfrak{n}$.

For an L_∞ algebra $(\mathcal{H}_c, \mathfrak{l})$, a minimal L_∞ algebra and an L_∞ quasi-isomorphism $\{f_l\}_{l\geqslant 1} : (H(\mathcal{H}_c), \mathfrak{l}') \to (\mathcal{H}_c, \mathfrak{l})$ are constructed as follows.

We set $f_1 = \iota_c : H(\mathcal{H}_c) \to \mathcal{H}_c$, and assume that we have $\{f_l : (H(\mathcal{H}_c))^{\otimes l} \to \mathcal{H}_c\}_{l\geqslant 1}$ for $l \leqslant n-1$. Then, for $c_1', \ldots, c_n' \in H(\mathcal{H}_c)$, f_n is defined by

$$f_n(c_1', \ldots, c_n') = -h_c \sum_{k_1+\cdots+k_j=n} \sum_{\sigma\in\mathfrak{S}_n} \frac{(-1)^{\epsilon(\sigma)}}{k_1!\,k_2!\cdots k_j!\cdot j!} l_j(f_{k_1} \otimes f_{k_2} \otimes \cdots \otimes f_{k_j})(c'_{\sigma(1)}, \ldots, c'_{\sigma(n)}).$$

The minimal L_∞ structure is then determined by

$$l'_n(c'_1,\ldots,c'_n)=\pi_c\sum_{k_1+\cdots+k_j=n}\sum_{\sigma\in\mathfrak{S}_n}\frac{(-1)^{\epsilon(\sigma)}}{k_1!\,k_2!\cdots k_j!\cdot j!}l_j(f_{k_1}\otimes f_{k_2}\otimes\cdots\otimes f_{k_j})(c'_{\sigma(1)},\ldots,c'_{\sigma(n)}),$$

in particular, for $l=2$ one gets $l'_2=H(l_2):=\pi_c\circ l_2\circ(\iota_c)^{\otimes 2}$.

Once the L_∞ quasi-isomorphism $\{f_l\}_{l\geqslant 1}$ is given, we have an OCHA $(H(\mathcal{H}_c)\oplus\mathcal{H}_o,\mathfrak{l}',\mathfrak{n}'')$ for some $\mathfrak{n}''$. Next we should construct $\{f_{k,l}:(H(\mathcal{H}_c))^{\otimes k}\otimes(H(\mathcal{H}_o))^{\otimes l}\to H(\mathcal{H}_o)\}_{k+l\geqslant 1}$ and $\mathfrak{n}'=\{n'_{k,l}:(H(\mathcal{H}_c))^{\otimes k}\otimes(H(\mathcal{H}_o))^{\otimes l}\to H(\mathcal{H}_o)\}_{2k+l\geqslant 2}$; these are obtained in a similar way as follows. $f_{0,1}$ is given as inclusion $f_{0,1}=\iota_o:H(\mathcal{H}_o)\to\mathcal{H}_o$. $f_{r,s}$ and $f_{p,q}$ are ordered as $f_{r,s}<f_{p,q}$ if $r+s<p+q$ or $r<p$ for $r+s=p+q$. Then, a similar recursive procedure as above can be carried out also here. For $c'_1,\ldots,c'_n\in H(\mathcal{H}_c)$ and $o'_1,\ldots,o'_m\in H(\mathcal{H}_o)$, $f_{n,m}$ is determined by

$$\begin{aligned}&f_{n,m}(c'_1,\ldots,c'_n;o'_1,\ldots,o'_m)\\&\quad=-h_o\sum\frac{(-1)^{\epsilon(\sigma)}}{i!\,(r_1!\cdots r_i!)(p_1!\cdots p_j!)}n_{i,j}(f_{r_1}\otimes\cdots\otimes f_{r_i}\otimes f_{p_1,q_1}\otimes\cdots\otimes f_{p_j,q_j})\\&\qquad(c'_{\sigma(1)},\ldots,c'_{\sigma(n)};o'_1,\ldots,o'_m),\end{aligned}$$

where the summation Σ runs over all $r_1,\ldots,r_i,p_1,\ldots,p_j,q_1,\ldots,q_j$ such that $(r_1+\cdots+r_i)+(p_1+\cdots+p_j)=n$, $(q_1+\cdots+q_j)=m$, and also all $\sigma\in\mathfrak{S}_n$.

Then $\mathfrak{n}'=\{n'_{k,l}\}_{2k+l\geqslant 2}$ is obtained by replacing $-h_o$ above with π_o,

$$\begin{aligned}&n'_{n,m}(c'_1,\ldots,c'_n;o'_1,\ldots,o'_m)\\&\quad=\pi_o\sum\frac{(-1)^{\epsilon(\sigma)}}{i!\,(r_1!\cdots r_i!)(p_1!\cdots p_j!)}n_{i,j}(f_{r_1}\otimes\cdots\otimes f_{r_i}\otimes f_{p_1,q_1}\otimes\cdots\otimes f_{p_j,q_j})\\&\qquad(c'_{\sigma(1)},\ldots,c'_{\sigma(n)};o'_1,\ldots,o'_m),\end{aligned}$$

where the summation Σ stands for the same one as above. In particular, for $2k+l=2$ one gets $n'_{0,2}=H(n_{0,2}):=\pi_o\circ n_{0,2}\circ(\iota_o)^{\otimes 2}$ and $n'_{1,0}=H(n_{1,0}):=\pi_o\circ n_{1,0}\circ\iota_c$. In the equation above, we used the convention presented in Definition 2.10.

For a COCHA $(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$, we do this construction by starting with an *orthogonal* Hodge decomposition with respect to the symplectic form ω. Namely, we give a decomposition

$$(H(\mathcal{H})\underset{\pi}{\overset{\iota}{\rightleftarrows}}\mathcal{H},h)$$

of $\mathcal{H}$ in Eq. (5.2) with a homotopy $h:\mathcal{H}\to\mathcal{H}$ satisfying $\omega(\mathbf{1}\otimes h)=\omega(h\otimes\mathbf{1})$, where $\mathbf{1}:=\mathbf{1}_c\oplus\mathbf{1}_o$. The existence of such a homotopy h follows from the nondegeneracy of ω and the cyclicity for the terms $\omega_c(l_1\otimes\mathbf{1}_c)$ and $\omega_o(n_{0,1}\otimes\mathbf{1}_o)$, and then $\omega(\mathbf{1}\otimes(\iota\circ\pi))=\omega((\iota\circ\pi)\otimes\mathbf{1})$ also holds. Then, for the COCHA $(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$, forgetting the cyclic structure ω having already used it to fix the contraction (5.2), one can obtain a minimal model $(H(\mathcal{H}),\mathfrak{l}',\mathfrak{n}')$ as an OCHA by the construction we have seen above. The resulting minimal OCHA $(H(\mathcal{H}),\mathfrak{l}',\mathfrak{n}')$ is in fact cyclic with respect to the induced inner product $\omega':=\omega(\iota\otimes\iota)$ and the OCHA quasi-isomorphism a COCHA quasi-isomorphism.

To summarize we give the following.

Theorem 5.5: *$(H(\mathcal{H}),\mathfrak{l}',\mathfrak{n}')$ forms a minimal OCHA and $\mathfrak{f}:=\{\{f_l\}_{l\geqslant 1},\{f_{k,l}\}_{k+l\geqslant 1}\}$ is an OCHA quasi-isomorphism $\mathfrak{f}:(H(\mathcal{H}),\mathfrak{l}',\mathfrak{n}')\to(\mathcal{H},\mathfrak{l},\mathfrak{n})$.*

Theorem 5.6: *For a COCHA $(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$ and an orthogonal Hodge decomposition with respect to ω, $(H(\mathcal{H}),\omega',\mathfrak{l}',\mathfrak{n}')$ forms a minimal COCHA and $\mathfrak{f}:=\{\{f_l\}_{l\geqslant 1},\{f_{k,l}\}_{k+l\geqslant 1}\}$ is a COCHA quasi-isomorphism $\mathfrak{f}:(H(\mathcal{H}),\omega',\mathfrak{l}',\mathfrak{n}')\to(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$.*

Since the explicit forms are given, one can check the cyclicity directly in a similar way to that in the A_∞ case (see Ref. 33).

Remark 5.7 (*rooted planar tree graphs*): One can also present an alternate description of this

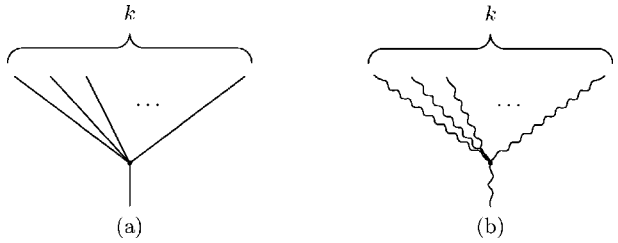

FIG. 1. (a) The k-corolla, the planar tree corresponding to the A_∞ structure $m_k=n_{0,k}$. (b) The k-corolla, the nonplanar tree corresponding to the L_∞ structure l_k.

minimal model in terms of rooted planar trees in a similar way as for A_∞ algebras (see Refs. 41, 31, 33, 52, 7, 11, 15, 16, 27, 36, 47, 51, and 60, etc.). This is related to Feynman graphs in field theory. For an A_∞ algebra $(\mathcal{H}_o,\{n_{0,k}\})$, it is convenient to associate $n_{0,k}$ to the k-corolla of planar rooted trees. An L_∞ algebra also has such a description, where the L_∞ structure l_k is associated with the k-corolla of nonplanar rooted trees (Fig. 1). In our OCHA, we need to introduce also $n_{k,l}$, to which we associate a mixed corolla as in Fig. 2. As stated previously, from a string theory viewpoint, l_k corresponds to the sphere with $(k+1)$-(closed string) punctures and $n_{k,l}$ corresponds to the disk with $(k+1)$-(open string) punctures on the boundary and l-(closed string) punctures in the bulk (interior) of the disk. In fact, one may think of the tubular neighborhood of these tree graphs as the corresponding world sheet, where we take strips and cylinders for the neighborhood of the straight lines and meandering lines, respectively. The minimal OCHA structure l'_k and $n'_{k,l}$ are then obtained by grafting corollas in all possible ways such that straight lines are grafted to straight and wiggly to wiggly (Fig. 3), where we assign to corollas the corresponding multilinear maps $l_k,n_{p,q}$, and to internal edges h_c, h_o, and so on. Physically, h_c and h_o are the propagators for closed string and open string, respectively.

Remark 5.8 (*string amplitude*): For a classical open-closed string field theory $S=S_S+S_D$, the string amplitudes are obtained as follows. Let $(\mathcal{H},\omega,\mathfrak{l},\mathfrak{n})$ be the corresponding COCHA, and suppose that its minimal COCHA $(H(\mathcal{H}),\omega',\mathfrak{l}',\mathfrak{n}')$ is constructed as above.

By definition, string field theory is constructed so that its perturbative expansion reproduces the corresponding world sheet string amplitudes. Thus,

$$\mathcal{V}'_{k+1} := \omega'_c(l'_k \otimes \mathbf{1}_c), \quad \mathcal{V}'_{k,l+1} = \omega'_o(n'_{k,l} \otimes \mathbf{1}_o) \tag{5.4}$$

just define the on-shell $(k+1)$-closed strings sphere amplitudes and k-closed $(l+1)$-open string disk amplitudes, respectively. Moreover, the n-closed string disk amplitude, which we denote $\mathcal{V}'_{n,0}$, is given by composing the L_∞ quasi-isomorphism with $\mathcal{V}_{k,0}$ as follows:

$$\mathcal{V}'_{n,0} = \sum_{i=1}^{n} \sum_{k_1+\cdots+k_i=n} \frac{1}{k_1!\cdots k_i!} \mathcal{V}_{i,0}(f_{k_1} \otimes \cdots \otimes f_{k_i})$$

for $\mathfrak{f}=\{f_k\}_{k\geqslant 1}$, the L_∞ quasi-isomorphism.

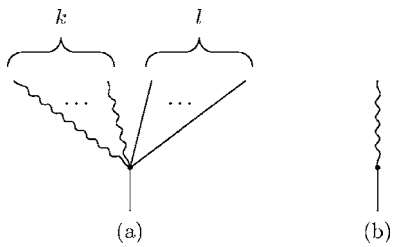

FIG. 2. (a) The (k,l)-corolla corresponding to $n_{k,l}$. (b) For the open-closed case, the (k,l)-corollas include the $(1,0)$-corolla corresponding to $n_{1,0}$.

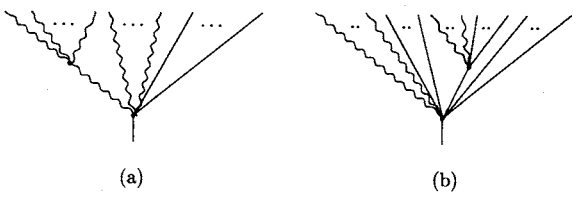

FIG. 3. Grafting of corollas. (a) Wiggly to wiggly. (b) Straight to straight.

Note also that we can prove the decomposition theorem for a (cyclic) OCHA,[35] which implies that all classical open-closed string field theories constructed on a fixed *conformal background* (the data of the conformal field theory on the Riemann surfaces) are isomorphic. From the field theory viewpoint, an OCHA morphism is a field transformation and in particular an OCHA isomorphism is a field redefinition. Since field theory actions related by a field redefinition are physically equivalent, one can say the decomposition theorem can prove the equivalence of all classical open-closed string field theories constructed on a fixed conformal background. (See Ref. 33 for the A_∞ case.)

VI. DEFORMATION OF A_∞ STRUCTURES AND THE FORMALITY THEOREM

For an L_∞ algebra $(\mathcal{H}_c,\mathfrak{l})$ and an A_∞ algebra $(\mathcal{H}_o,\mathfrak{m})$, if there exists an OCHA $(\mathcal{H}=\mathcal{H}_c \oplus \mathcal{H}_o,\mathfrak{l},\mathfrak{n})$ whose subalgebra $(\mathcal{H}_o,\{n_{0,k}\}_{k\geqslant 1})$ coincides with $(\mathcal{H}_o,\{m_k\}_{k\geqslant 1})$, one obtains deformations of the A_∞ algebra $(\mathcal{H}_o,\{m_k\}_{k\geqslant 1})$ parametrized by the L_∞ algebra $(\mathcal{H}_c,\mathfrak{l})$. On the other hand, the whole deformation space of the A_∞ algebra is also described by a moduli space of the L_∞ algebra(Coder$(T^c\mathcal{H}_o),\mathfrak{m},[\ ,\ ]))$, which we denote by $(\mathcal{H}_c',\mathfrak{l}')$. The maps $\{n_{k,l}\}$ for $k\geqslant 1$ define an L_∞ morphism from $(\mathcal{H}_c,\mathfrak{l})$ to $(\mathcal{H}_c',\mathfrak{l}')$. The defining equation for an OCHA (2.6) just converts to the defining equation for an L_∞ morphism (2.5).[35] In Sec. VI A we reexplain this in a more explicit way. Such structure appears in various aspects of mathematical physics; the relation to deformation quantization by Kontsevich[40] is explained in Sec. VI B, and the application to the open-closed topological B-model[26] from the viewpoint of the homological mirror symmetry setup[39] is discussed in Sec. VI C. Note also that, in string field theory, this picture is related to the arguments in Sec. 8 of Ref. 74.

A. Deformations of A_∞ structures from open-closed homotopy algebras

Definition 6.1 [(graded) Gerstenhaber bracket[12]]: For $\mathcal{H}_o$ a $\mathbb{Z}$-graded vector space, let $\mathrm{Hom}_k^r := \mathrm{Hom}^r(\mathcal{H}_o^{\otimes k},\mathcal{H}_o)$ be the space of degree r k-linear maps, and

$$\mathrm{Hom} := \oplus_r \mathrm{Hom}^r, \quad \mathrm{Hom}^r := \oplus_{k\geqslant 0} \mathrm{Hom}_k^r.$$

It is known that Hom is in one-to-one correspondence with the space of coderivations on $T^c(\mathcal{H}_o)$, Coder$(T^c(\mathcal{H}_o))$.[65] For two elements in Coder$(T^c(\mathcal{H}_o))$, the commutator of any two elements in fact belongs to Coder$(T^c(\mathcal{H}_o))$, and further satisfies the Jacobi identity. After a shift in degree, this induces a graded Lie bracket on Hom, which is the *Gerstenhaber bracket*. For $m\in\mathrm{Hom}_k^r$, $m'\in\mathrm{Hom}_{k'}^{r'}$ and $o_1,\ldots,o_{k+k'-1}\in\mathcal{H}_o$, the graded Lie bracket $[m,m']\in\mathrm{Hom}_{k+k'-1}^{r+r'}$ is defined by

$$[m,m'] = m\circ m' - (-1)^{r\cdot r'} m'\circ m,$$

$$m\circ m'(o_1,\ldots,o_{k+k'-1}) = \sum_{i=0}^{k-1} (-1)^{l'(o_1+\cdots+o_i)} m(o_1,\ldots,o_i,m'(o_{i+1},\ldots,o_{i+k'}),o_{i+k'+1},\ldots,o_{k+k'-1}).$$

Thus, (Hom,[,]) forms a *graded Lie algebra*.[12,65]

In the supermanifold description in Sec. III, this Gerstenhaber bracket corresponds to the graded Lie bracket of formal vector fields on the corresponding formal supermanifold.

Furthermore, let us denote by $\bar{m} \in \mathrm{Hom}^1$ the degree one element corresponding to a degree one coderivation in $(\mathcal{H}'_c, \mathfrak{l}') = \mathrm{Coder}(T(\mathcal{H}_o))$, that is, an A_∞ structure on $\mathcal{H}_o$. Then, it is clear that $[\bar{m}, \bar{m}] = 0$ holds and $(\mathrm{Hom}, d, [\ ,\ ])$ forms a DGLA with $d = [\bar{m},\ ]$.

Remark 6.2 (*suspension*): A DGLA is described as an L_∞ algebra through the suspension s. For the DGLA $(\mathrm{Hom}, d, [\ ,\ ])$, the suspension is a degree shifting operator

$$s : \mathrm{Hom} \to \mathrm{Hom}[1] =: \mathcal{H}'_c.$$

By this, a degree r element $m \in \mathrm{Hom}^r$ is mapped to be a degree $(r-1)$ element $s(m) \in \mathrm{Hom}[1]^{r-1} = \mathcal{H}'^{r-1}_c$. This actually converts the degree preserving bracket $[\ ,\ ] : \mathrm{Hom} \otimes \mathrm{Hom} \to \mathrm{Hom}$ into a degree one bilinear map $l'_2 : \mathcal{H}'_c \otimes \mathcal{H}'_c \to \mathcal{H}'_c$ defined by

$$l'_2(s(m), s(m')) := s((-1)^r [m, m']), \quad m \in \mathrm{Hom}^r, \quad m' \in \mathrm{Hom}^{r'}.$$

One can see that the graded anticommutativity $[m', m] = -(-1)^{rr'}[m, m']$ is in fact replaced by the graded commutativity in Eq. (2.3), $l'_2(s(m'), s(m)) = (-1)^{(r-1)(r'-1)} l'_2(s(m), s(m'))$, where l'_1 is given simply by $l'_1 = s\, \mathrm{d} s^{-1} = d$. Then $(\mathcal{H}'_c, \mathfrak{l}' = \{l'_1, l'_2, l'_3 = l'_4 = \cdots = 0\})$ forms an L_∞ algebra.

Now, let us express the open-closed multilinear maps as

$$n_{k,l}(c_1, \ldots, c_k; o_1, \ldots, o_l) =: (n^*_l(c_1, \ldots, c_k))(o_1, \ldots, o_l),$$

where $n^*_l(c_1, \ldots, c_k)$ belongs to $\mathrm{Hom}_k^{\deg(c_1)+\cdots+\deg(c_k)+1}$. By this, the second term of the OCHA relation (2.6) can be rewritten as

$$-(-1)^{(c_{\sigma(1)}+\cdots+c_{\sigma(l)}+1)} \frac{1}{2} [n^*_{m+1-k}(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), n^*_k(c_{\sigma(l+1)}, \ldots, c_{\sigma(n)})](o_1, \ldots, o_m),$$

which, acting further with the suspension s on the equation above, yields

$$-\tfrac{1}{2} l'_2(s(n^*_{m+1-k})(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), s(n^*_k)(c_{\sigma(l+1)}, \ldots, c_{\sigma(n)}))(o_1, \ldots, o_m).$$

Thus, one obtains

$$\sum_{k,l \geqslant 0} \sum_{p=0}^{m-k} \sum_{\sigma \in \mathfrak{S}_n} \frac{1}{2} \frac{(-1)^{\epsilon(\sigma)}}{l!\,(n-l)!} l'_2(s(n^*_{m+1-k})(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), s(n^*_k)(c_{\sigma(l+1)}, \ldots, c_{\sigma(n)}))$$

$$= \sum_{\sigma \in \mathfrak{S}_n} \sum_{l=1}^{n} \frac{(-1)^{\epsilon(\sigma)}}{l!\,(n-l)!} s(n^*_m)(l_l(c_{\sigma(1)}, \ldots, c_{\sigma(l)}), c_{\sigma(l+1)} \ldots, c_{\sigma(n)}). \tag{6.1}$$

These are just the defining equations for an L_∞ morphism (2.5). By treating the $l=0$ and $l=n$ cases separately in the first line of the equation above, it becomes just the condition that the collection of multilinear maps $s(n^*_k) : (\mathcal{H}_c)^{\otimes^*} \to \mathrm{Hom}_k[1]$ forms an L_∞ morphism from $(\mathcal{H}_c, \mathfrak{l})$ to $(\mathcal{H}'_c, \mathfrak{l}')$. Here, note that $l'_1 = [\bar{m},\ ]$ and $\bar{m} = \Sigma_{l \geqslant 0} m_k$, the A_∞ structure included in $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$ as $m_l := n_{0,l}$. From these arguments, it is clear that the converse also holds.

Theorem 6.3 (**Ref.** 35)**:** *For an OCHA* $(\mathcal{H}, \mathfrak{l}, \mathfrak{n})$, *let* $(\mathcal{H}'_c, \mathfrak{l}')$ *denote the DGLA* $\mathrm{Coder}(T^c \mathcal{H}_o)$. *The OCHA structure gives an* L_∞ *morphism from* $(\mathcal{H}_c, \mathfrak{l})$ *to* $(\mathcal{H}'_c, \mathfrak{l}')$. *Conversely, if there exists an* L_∞ *algebra* $(\mathcal{H}_c, \mathfrak{l})$ *and an* L_∞ *morphism from it to the DGLA* $(\mathcal{H}'_c, \mathfrak{l}')$ *of an* A_∞ *algebra* $(\mathcal{H}_o, \mathfrak{m})$, *then one obtains an OCHA.*

For an L_∞ algebra $(\mathcal{H}_c, \mathfrak{l})$, let us denote by $\mathcal{MC}(\mathcal{H}_c, \mathfrak{l})$ the *solution space* of the Maurer-Cartan equation

$$\mathcal{MC}(\mathcal{H}_c, \mathfrak{l}) = \left\{ \bar{c} \in \mathcal{H}^0_c \,\middle|\, 0 = \sum_{k \geqslant 1} \frac{1}{k!} l_k(\bar{c}, \ldots, \bar{c}) \right\},$$

where $\mathcal{H}^0_c$ is the degree zero subvector space of $\mathcal{H}_c$. In addition, we have an equivalence relation $\sim$ called *gauge equivalence* between the solutions of the Maurer-Cartan equation. The moduli

space of the solution space of the Maurer-Cartan equation for $(\mathcal{H}_c, \mathfrak{l})$ is defined by

$$\mathcal{M}(\mathcal{H}_c, \mathfrak{l}) = \mathcal{MC}(\mathcal{H}_c, \mathfrak{l})/\sim . \tag{6.2}$$

Suppose that we have an L_∞ morphism $\mathfrak{f}: (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$ between two L_∞ algebras. Then it is known that the L_∞ morphism $\mathfrak{f}$ induces a map $\mathfrak{f}: \mathcal{M}(\mathcal{H}_c, \mathfrak{l}) \to \mathcal{M}(\mathcal{H}'_c, \mathfrak{l}')$, and furthermore it is an isomorphism if $\mathfrak{f}$ is an L_∞ quasi-isomorphism (cf. Ref. 40). Similar facts hold also for A_∞ algebras and also for OCHAs,[35] but what is relevant here is just the L_∞ case.

Note that, for an L_∞ algebra (DGLA) $(\mathcal{H}'_c, \mathfrak{l}') = \mathrm{Coder}(T^c \mathcal{H}_o)$ as above, its moduli space $\mathcal{M}(\mathcal{H}'_c, \mathfrak{l}')$ is the moduli space of deformations of the A_∞ algebra in the space of weak A_∞ algebras. Thus, we have the following.

Corollary 6.4 (A_∞ *structure parameterized by the moduli space of* L_∞ *structures*[35]): *For an* L_∞ *algebra* $(\mathcal{H}_c, \mathfrak{l})$ *and an* A_∞ *algebra* $(\mathcal{H}_o, \mathfrak{m})$, *suppose there exists an OCHA* $(\mathcal{H} = \mathcal{H}_c \oplus \mathcal{H}_o, \mathfrak{l}, \mathfrak{n})$ *such that* $(\mathcal{H}_o, \{n_{0,k}\}) = (\mathcal{H}_o, \mathfrak{m})$. *Then, for each element* $c \in \mathcal{M}(\mathcal{H}_c, \mathfrak{l})$, *we have a weak* A_∞ *algebra which is a deformation of the original* A_∞ *algebra* $(\mathcal{H}_o, \mathfrak{m})$. *If* $\{n_{1,k}\}_{k \geqslant 0}: \mathcal{H}_c \to \mathcal{H}'_c$ *gives a quasi-isomorphism of complexes* $(\mathcal{H}_c, l_1) \to (\mathcal{H}'_c, l'_1)$, *then all the equivalence classes of deformations of* $(\mathcal{H}, \mathfrak{m})$ *as weak* A_∞ *algebras, described by* $\mathcal{M}(\mathcal{H}'_c, l'_1)$, *are in one-to-one correspondence with the space* $\mathcal{M}(\mathcal{H}_c, \mathfrak{l})$.

B. The construction of deformation quantization by Kontsevich

The deformation quantization problem is to construct a star product corresponding to the Poisson algebra on a manifold M. Namely, for a formal (deformation) parameter ν and a given Poisson algebra $(\mathcal{A} = C^\infty(M), \cdot, \{\ ,\ \})$, a bilinear, bidifferential ν-linear map $*: \mathcal{A}[[\nu]] \otimes \mathcal{A}[[\nu]] \to \mathcal{A}[[\nu]]$,

$$f * g = \sum_{r=0}^{\infty} m_r(f,g) \nu^r, \quad f, g \in \mathcal{A}[[\nu]] \tag{6.3}$$

is called a *deformation quantization* of M if $m_0(f,g) = f \cdot g$, the usual commutative product on $C^\infty(M)$, $m_1(f,g) = \frac{1}{2}\{f,g\}$ and the *star product* $*$ is associative.[5] (Notice here m_r is still a function of two variables and should not be confused with the m_l of an A_∞ algebra.) In Ref. 40, Kontsevich reformulated this problem in a homotopy algebraic setup. For any associative algebra $\mathcal{A}$, deformations as associative multiplications are controlled by the Hochschild complex, which is essentially $\mathrm{Coder}(T^c \mathcal{A})$ and hence a DGLA.[12] In fact, control is equally well exercised by any quasi-isomorphic DGLA or even L_∞ algebra.[60] The obstructions to existence and to equivalence are identified by the quasi-isomorphism. For the special case of $\mathcal{A} = C^\infty(M)$, the deformations relevant to deformation quantization are controlled by the subcomplex of multidifferential Hochschild cochains, which we denote $D_{\mathrm{poly}}(M)$ (Definition 6.5) and which is quasi-isomorphic to the full Hochschild complex. The smooth analog of the Hochschild-Kostant-Rosenberg theorem.[25] (an explicit proof can be found in Ref. 22) equates the Hochschild cohomology with $T_{\mathrm{poly}}(M)$, the space of polyvector fields, which possesses a DGLA structures with $d = 0$ and the Schouten-Nijenhuis bracket.

Kontsevich treated these DGLAs as L_∞ algebras and obtained the existence and the classification of deformation quantizations by constructing an L_∞ morphism between $T_{\mathrm{poly}}(M)$ and $D_{\mathrm{poly}}(M)$, which is in a sense a nonlinear generalization of a DGLA map. Moreover, the specific L_∞ morphism provides a specific star product. In this setting, the space of Poisson structures and the space of star products given by bidifferential operators are then described by the Maurer-Cartan equations of the corresponding DGLAs.

In this section, we shall first present these tools and then relate them to an OCHA.

Definition 6.5 [*DGLA of multidifferential operators for* $C^\infty(M)$]: For $\mathcal{A} = C^\infty(M)$, denote by $D^k_{\mathrm{poly}}(M)$ the space of multilinear maps from $\mathcal{A}^{\otimes(k+1)}$ to $\mathcal{A}$ of multidifferential operators. Then define $D_{\mathrm{poly}} = \oplus_{k \in \mathbb{Z}} D^k_{\mathrm{poly}}$ by

$$D^k_{\mathrm{poly}} = D^k_{\mathrm{poly}}(M)(k \geqslant -1), \quad D^k_{\mathrm{poly}} = 0(k < -1).$$

For d, we take the Hochschild coboundary operator. Namely, for any $C \in D^k_{\mathrm{poly}}$, d is given by

$$(\mathrm{d}C)(g_0, \ldots, g_{k+1}) = g_0 C(g_1, \ldots, g_{k+1}) - \sum_{r=0}^{k} (-1)^r C(g_0, \ldots, g_r g_{r+1}, \ldots, g_{k+1})$$

$$+ (-1)^k C(g_0, \ldots, g_k) g_{k+1}.$$

We take for $[\ ,\ ]$ the Gerstenhaber bracket.[12] Namely, for $C \in D^k_{\mathrm{poly}}$, $C' \in D^{k'}_{\mathrm{poly}}$, it is defined by

$$[C, C'] = C \circ C' - (-1)^{kk'} C' \circ C,$$

$$C \circ C'(g_0, \ldots, g_{k+k'}) = \sum_{r=0}^{k} (-1)^{rk'} C(g_0, \ldots, g_{r-1}, C'(g_r, \ldots, g_{r+k'}), g_{r+k'+1}, \ldots, g_{k+k'}).$$

Then $(D_{\mathrm{poly}}, [\ ,\ ], d)$ forms a DGLA.

One can see that d can be written as

$$(-1)^k (dC)(g_0, \ldots, g_{k+1}) = [\bar{m}, C], \quad C \in D^k_{\mathrm{poly}},$$

where $\bar{m}$ is the usual commutative product of functions $\bar{m}(f,g) = f \cdot g$. Though the operation $[\bar{m},\ ]$ is different in sign from the original d, $[\bar{m},\ ]$ also forms a DGLA on D_{poly} with $[\ ,\ ]$. So, we take this as d. This DGLA is described as a sub-DGLA of $(\mathrm{Hom}, d, [\ ,\ ])$. First, set $\mathcal{H}^{-1}_o = \mathcal{A}$ and $\mathcal{H}^k_o = 0$ otherwise. Then $C: \mathcal{A}^{\otimes(k+1)} \to \mathcal{A}$ has degree k as defined above. Namely, $D_{\mathrm{poly}}(M)$ is included in the restricted subvector space $\mathrm{Hom}_{\mathrm{sub}} = \oplus_k \mathrm{Hom}^{k-1}_k$ of Hom.

Let us state the necessary condition for the existence of a deformation quantization in the language of DGLAs here. If we write the star product (6.3) as $f * g = m(f,g)$, $m \in \mathrm{Hom}^1_2$, the associativity condition $(f*g)*h = f*(g*h)$ is expressed algebraically as $[m,m] = 0$. This just indicates that m defines a codifferential on $T^c(\mathcal{A})$ as previously or, equivalently, that m is associative. Since m should be obtained as a deformation of $\bar{m}$, writing $m = \bar{m} + \theta$, $\theta \in \nu D_{\mathrm{poly}}[[\nu]]$, one gets a Maurer-Cartan equation in the DGLA $(\nu D_{\mathrm{poly}}[[\nu]], d, [\ ,\ ])$,

$$\mathrm{d}\theta + \tfrac{1}{2}[\theta, \theta] = 0. \tag{6.4}$$

Definition 6.6 (DGLA of polyvector fields): For $k \geqslant -1$, set $T^k_{\mathrm{poly}}(M) := \Gamma(M, \wedge^{k+1} TM)$, and define $T_{\mathrm{poly}} = \oplus_k T^k_{\mathrm{poly}}$ by

$$T^k_{\mathrm{poly}} = T^k_{\mathrm{poly}}(M)(k \geqslant -1), \quad T^k_{\mathrm{poly}} = 0(k < -1).$$

Here, when $k = -1$ we set $T^{-1}_{\mathrm{poly}} = T^{-1}_{\mathrm{poly}}(M) = C^\infty(M)$. The differential d is defined by $d = 0$. Therefore, the cohomology of the complex of T^n_{poly} with respect to d coincides with T^n_{poly} itself. $[\ ,\ ]$ is taken to be the *Schouten-Nijenhuis bracket*.[61,56] For $\xi_s, \eta_t \in T^0_{\mathrm{poly}} = \Gamma(M, TM)$, the bracket of $\xi_0 \wedge \cdots \wedge \xi_k, \in T^k_{\mathrm{poly}}$ with $\eta_0 \wedge \cdots \wedge \eta_l \in T^l_{\mathrm{poly}}$, $k, l \geqslant 0$, is defined by

$$[\xi_0 \wedge \cdots \wedge \xi_k, \eta_0 \wedge \cdots \wedge \eta_l]$$
$$= \sum_{i=0}^{k} \sum_{j=0}^{l} (-1)^{s+t} [\xi_s, \eta_t] \wedge \xi_0 \wedge \cdots \wedge \xi_{s-1} \wedge \xi_{s+1} \wedge \cdots \wedge \xi_k \wedge \eta_0 \wedge \cdots \wedge \eta_{t-1} \wedge \eta_{t+1} \wedge \cdots \wedge \eta_l,$$

and for $k \geqslant 0$, $h \in T^{-1}_{\mathrm{poly}} = C^\infty(M)$, the bracket is

$$[\xi_0 \wedge \cdots \wedge \xi_k, h] = \sum_{r=0}^{k} (-1)^r \xi_r(h)(\xi_0 \wedge \cdots \wedge \xi_{r-1} \wedge \xi_{r+1} \wedge \cdots \wedge \xi_k).$$

We can define $\mathcal{H}_c^{k-1} := T^k_{\text{poly}}$ with this Schouten-Nijenhuis bracket.

Now, a bivector $\alpha = \Sigma_{i,j} \alpha^{ij} (\partial/\partial x_i) \wedge (\partial/\partial x_j) \in T^1_{\text{poly}}$ in the local expression represents the Poisson bracket by $\{f,g\} = \Sigma_{i,j} \alpha^{ij} (\partial f/\partial x_i)(\partial g/\partial x_j)$, where $(x_1, \ldots, x_n)$ are local coordinates of M. This bracket by definition satisfies all the axioms of a Poisson algebra except the Jacobi identity. The Jacobi identity is then described by

$$[\alpha, \alpha] = 0. \tag{6.5}$$

Since $d=0$, Eq. (6.5) is also the Maurer-Cartan equation. A bivector satisfying (6.5) is called a Poisson bivector. Similarly, a quantum deformation of the Poisson bivector is defined by $\alpha_{[\nu]} \in \nu T^1_{\text{poly}}[[\nu]]$ satisfying

$$[\alpha_{[\nu]}, \alpha_{[\nu]}] = 0. \tag{6.6}$$

In the expansion $\alpha_{[\nu]} = \nu\alpha_1 + \nu^2\alpha_2 + \cdots$, the original classical Poisson bivector α is α_1. In fact, expanding (6.6) in terms of powers of ν, one can see that the lowest identity reads $[\alpha_1, \alpha_1] = 0$.

Thus, the conditions that an element in $\nu T^1_{\text{poly}}[[\nu]]$ is a Poisson bracket and that an associative product on $C^\infty(M)[[\nu]]$ as an element in $\nu D^1_{\text{poly}}[[\nu]]$ are both described by Maurer-Cartan equations for DGLAs. Let us set two L_∞ algebras $(\mathcal{H}_c, \mathfrak{l})$ and $(\mathcal{H}'_c, \mathfrak{l}')$ as the suspension of DGLAs T_{poly} and D_{poly}, respectively. Namely, we have $\mathcal{H}_c^k = T^{k+1}_{\text{poly}}$ and $\mathcal{H}_c'^k = D^{k+1}_{\text{poly}}$. The Maurer-Cartan equations for DGLAs (6.6), (6.4) are of course rewritten as the Maurer-Cartan equations for L_∞ algebras through the suspension in Remark 6.2.

The existence and the classification of the deformation quantization follows from the formality theorem,[40] which claims the existence of an L_∞ quasi-isomorphism $\mathfrak{f}: (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$. Note that this fact implies that the DGLA of Hochschild cochains is (homotopically) formal; in particular, the higher L_∞ structures vanish on its cohomologies. In order that $\mathfrak{f}$ is an L_∞ quasi-isomorphism, the chain map $f_1: (\mathcal{H}_c, d_c = 0) \to (\mathcal{H}'_c, d'_c)$ must be a quasi-isomorphism, that is, f_1 must induce an isomorphism on cohomologies. One may set

$$(f_1(\xi_{i_1} \wedge \cdots \wedge \xi_{i_k}))(g_1, \ldots, g_k) = \frac{1}{k!} \sum_{\sigma \in \mathfrak{S}} (-1)^{\epsilon(\sigma)} (\xi_{i_{\sigma(1)}} g_1) \cdots (\xi_{i_{\sigma(k)}} g_k).$$

Kontsevich constructs all the higher multilinear maps f_k explicitly as local expressions on $M = \mathbb{R}^n$ in terms of Feynman graphs, which are just those derived from a certain topological open-closed string theory as revealed explicitly by Cattaneo-Felder[8] (see for review Ref. 48).

When an L_∞ quasi-isomorphism $\mathfrak{f} = \{f_1, f_2, \ldots\}$ is given, it preserves the Maurer-Cartan equations, and the deformed Poisson bivector is given by the following nonlinear map:

$$\theta = \sum_{k=1}^{\infty} \frac{1}{k!} f_k(\alpha_{[\nu]}, \ldots, \alpha_{[\nu]}), \tag{6.7}$$

for $\alpha_{[\nu]} \in \mathcal{M}(\mathcal{H}_c, \mathfrak{l})$ and $\theta \in \mathcal{M}(\mathcal{H}'_c, \mathfrak{l}')$. Here the L_∞ quasi-isomorphism $\mathfrak{f}: (\mathcal{H}_c, \mathfrak{l}) \to (\mathcal{H}'_c, \mathfrak{l}')$ has been extended by tensoring with the formal power series $\nu\mathbb{C}[[\nu]]$. If we expand the deformation $m = \bar{m} + \theta, \theta \in \nu D_{poly}[[\nu]]$ as in Eq. (6.3):

$$m = \bar{m} + \nu m_1 + \nu^2 m_2 + \cdots$$

with $m_1 = (1/2)\alpha_1$, Kontsevich's quasi-isomorphism of L_∞ algebras then provides a choice for m_2 and in fact for all the m_i.

Now, let us summarize Kontsevich's deformation quantization in terms of OCHAs. First, we set $\mathcal{H}_c^{r-2} := \Gamma(M, \wedge^r TM)$. It forms a formal L_∞ algebra with l_2 the Schouten-Nijenhuis bracket, and $l_1 = l_3 = \cdots = 0$. For $\mathcal{H}_o$, we take $\mathcal{H}_o^{-1} := C^\infty(M)$ and $\mathcal{H}_o^k = 0$ for $k \neq -1$. The A_∞ structure is $n_{0,2} = \bar{m}$,

the usual commutative product of functions $C^\infty(M)$, and $n_{0,l}=0$ except for $l=2$. The multilinear maps of the L_∞ quasi-isomorphism are then identified as the adjoints$\{n_{k,l}:(\mathcal{H}_c)^{\otimes k}\otimes(\mathcal{H}_o)^{\otimes l}\to\mathcal{H}_o\}$ with $k\geqslant 1$. In particular, $n_{1,2}(\alpha_{[\nu]};f,g)=(1/2)\{f,g\}$, and $n_{1,k}(\xi_{i_1}\wedge\cdots\wedge\xi_{i_k};g_1,\ldots,g_k)=(1/k!)\Sigma_{\sigma\in\mathfrak{S}}(-1)^{\epsilon(\sigma)}(\xi_{i_{\sigma(1)}}g_1)\cdots(\xi_{i_{\sigma(k)}}g_k)$. These structures form a minimal OCHA on cohomology. Corollary 6.4 then implies that, for a fixed element of $\mathcal{MC}(\mathcal{H}_c,\mathfrak{l})$, an A_∞ structure is obtained. However, in this situation, since Hom is restricted to $\mathrm{Hom}_{\mathrm{sub}}=\oplus\,\mathrm{Hom}_r^{r-1}$ and the elements of Maurer-Cartan equations, especially $\mathcal{M}(\mathcal{H}_c',\mathfrak{l}')$are degree zero, the deformed A_∞ structure also has $m_2\in(\mathrm{Hom}_2[1])^0$ only, i.e., m_1 and higher product $m_3,m_4,\ldots$ are absent. Equivalently, when $\mathcal{H}_c$ is restricted to its degree zero part $\mathcal{H}_c^0$, $n_{k,l}$ vanishes except for $(k,l)=(k,2)$. This m_2 is just the star product, an associative but noncommutative product $C^\infty(M)\otimes C^\infty(M)\to C^\infty(M)$ of a deformation quantization. The next example below is a natural extension of this situation, but in the case that Hom is not restricted to $\mathrm{Hom}_{\mathrm{sub}}$.

C. Open-closed B-model

A natural extension of Kontsevich's deformation quantization setup is to the B-model side of homological mirror symmetry.[39]

The mirror symmetry, a symmetry between Calabi-Yau manifolds, can be interpreted as topological closed string physics. There are two types of topological string theories whose target spaces are Calabi-Yau manifolds. One is called the A-model, which depends only on the complexified symplectic structure and is independent of the complex structure of the Calabi-Yau manifold. Another one, the B-model in contrast depends only on the complex structure. For a given Calabi-Yau manifold M, the mirror symmetry conjecture is the existence of a mirror Calabi-Yau manifold $\hat{M}$ such that the A-model closed string on $\hat{M}$ is equivalent to the B-model closed string on M and vice versa.[71] Homological mirror symmetry is thought of as an open string version[72] of the mirror symmetry conjecture. open string theory in general includes some kind of D-branes, which form a D-brane category (see Ref. 45); the D-branes and open strings are identified with objects and morphisms between the objects. For the tree open string A-model, the corresponding category is Fukaya's A_∞ category,[9] which depends only on the complexified symplectic structure. On the other hand, what is constructed on the B-model side is a category of holomorphic vector bundles or coherent sheaves more generally. The homological mirror symmetry conjecture[39] then states that the Fukaya category on a Calabi-Yau manifold M is in some sense equivalent to the category of coherent sheaves on the mirror dual Calabi-Yau manifold $\hat{M}$. Now, the conjecture is checked successfully in the case M is an elliptic curve,[39,59,57] an Abelian variety,[10,41] a quartic surface,[63] and so on. For noncommutative two-tori, see Refs. 32, 37, and 34 and a related work.[58]

One of the original motivations to argue for this homological mirror symmetry conjecture[39] is that it might explain the (tree closed string parts of) mirror symmetry: the family (deformations) of tree open string A- (respectively, B-) models should be in one-to-one correspondence with that of tree closed string A-(respectively, B-) model, and the tree closed string structure should follow from the corresponding family of the tree open string structures. These concepts have their background in the open-closed string physics in our sense. Since the A side and B side should be mirror dual, they should have isomorphic structures in some sense. However, that which is directly related to us is the B-model side, since there the classical solution of string world sheet theory is only a constant map (no world sheet instanton) and the corresponding moduli spaces are just the usual ones of Riemann surfaces with boundaries and punctures.[71]

One can see that the tree open-closed B-model is just a particular example of the arguments in Sec. VI A, and gives a natural extension of that in the preceding section. However, the mathematical formulation of the tree open-closed B-model is not yet established completely, nor is there known the explicit formula as in the case of deformation quantization in the preceding section.

An interesting attempt and a partial result can be found in Hofman's work.[26] We can identify some set of multilinear maps $\{l_k,n_{p,q}\}$ on open and closed string observables for this situation. Of course we could have an infinite number of homotopy equivalent open-closed homotopy struc-

tures. For instance, for the tree closed string part, the world sheet action of the B-twisted topological string theory as given in Ref. 71 has the space of observables which is identified with the cohomology of $\oplus_{p,q}\Gamma(M,\wedge^p TM\otimes\wedge^q\overline{T^*M})$ with respect to the Dolbeault operator $\bar{\partial}$ and hence, in principle, one can compute closed string $(k+1)$-point functions (=scattering amplitudes) related to l_k. However, in general this is complicated; it is better if one can find a corresponding string field theory in a simple form. Such a string field theory is given by Ref. 6, where the B-twisted topological closed string field theory action consists of the kinetic term and a three point vertex only, and so a DGLA structure is associated to it. Note that the equations of motions are just the Maurer-Cartan equations defining deformations of the complex structures, with additional extended directions mentioned below. The string field theory gives, at least for tree level (genus zero), a simple way of calculating $(k+1)$-point functions in terms of Feynman rules, and this procedure just coincides with taking a minimal model of the DGLA from a homotopy algebraic point of view. (However, for the action given in Ref. 6, they use an inner product which is not nondegenerate in our sense. In particular, it vanishes on the cohomology. Together with an additional structure called a differential Gerstenhaber structure, the pull-back of this action with respect to the L_∞ quasi-isomorphism, or equivalently the superpotential or the collection of tree closed string amplitudes, has a Frobenius structure,[6,2] even though the minimal L_∞ structure is trivial, all $l_k=0$. We do not deal with this Frobenius structure in this paper.)

In a similar way, one can also consider open strings in the B-twisted topological string theory, and, in a similar spirit, one can construct a particular open string topological string field theory action,[72,6] called a holomorphic Chern-Simons action, a holomorphic version of the usual Chern-Simons action or Witten's bosonic open string field theory.[70] Thus, it has a structure of a differential graded associative algebra (DGA) with cyclicity, a cyclic A_∞ structure. Again, tree open string world sheet scattering amplitudes are obtained by taking the minimal model of the DGA.

Although the B-twisted topological string is controlled by such a simple DGLA or DGA for the closed or open string case, respectively, it is known that the same story does not hold for tree open-closed string in general.[74] Therefore, we consider here a minimal OCHA structure whose purely closed string part $\{l_k\}$ and purely open string part $\{m_k=n_{0,k}\}$ are given by taking the minimal models of the DGLA and DGA, respectively. For the closed string side, the corresponding DGLA structure is $(\Gamma(M,\wedge^\star TM\otimes\wedge^\star\overline{T^*M}),\bar{\partial},[\ ,\ ])$, where $[\ ,\ ]$ is the Schouten-Nijenhuis bracket, the one in Definition 6.6 extended to $\overline{T^*M}$ naturally. However, for closed strings, the $\partial\bar{\partial}$ lemma and the Tian-Todorovs lemma lead to the corresponding minimal L_∞ structure, given by the procedure in Sec. V, being trivial (see Refs. 6 and 2). Thus, we have $l_k=0$ for$k\geqslant 1$ for $\mathcal{H}_c^k=\oplus_{p+q-2=k}H^q(\wedge^p TM)$, and the corresponding moduli space is itself,

$$\mathcal{M}(\mathcal{H}_c,\mathfrak{l})=\mathcal{H}_c^0.$$

Here, we restrict $\mathcal{H}_c$ to its degree zero part only. It might be reasonable to think that one can deform in these $\mathcal{H}_c^0$ directions finitely in principle and that the other $\mathcal{H}_c^k$ directions provide fibers of an infinitesimal neighborhood. In fact, the whole deformation space $\mathcal{H}_c$ is called the extended moduli space in Barannikov-Kontsevich.[2] Note that $H^1(\wedge^1 TM)\in\mathcal{H}_c^0$ describes the complex structure deformations. This is the original deformation theory of complex structures, and the Barannikov-Kontsevich's setup can be thought of as an extension of it.

Next, for pure open string structure, we should stress what is taken for $\mathcal{H}_o$. The open string theory forms a D-brane category, which should be treated as an A_∞ category in our context. The objects, B-type D-branes, are the coherent sheaves on M. Thus, $\mathcal{H}_o$ is identified with the space of morphisms between them. A general construction of a minimal model in this situation is found in Refs. 44, 46, 68, and 45, and See Ref. 34 for an explicit construction in the noncommutative two-tori case. However, for simplicity, here we consider the case that the object is only the structure sheaf $\mathcal{O}(M)$. One can see that this simplified situation is enough for our purpose here under some appropriate assumptions. The differential is then simply $\bar{\partial}$, and one obtains a minimal model of DGA $(\mathcal{O}^{0,*}(M),\bar{\partial},\wedge)$, which we denote by $(\mathcal{H}_o,\bar{m}=\{n_{0,k}\}_{k\geqslant 2})$, where $\mathcal{H}_o^{k-1}=H^k(\mathcal{O}^{0,*}(M))$.

For this particular choice of $\mathcal{H}_o$, let us consider the space of multilinear maps $\mathrm{Hom} := \oplus \mathrm{Hom}_k^r$,

$$\mathrm{Hom}_k^r = \mathrm{Hom}^r(\mathcal{H}_o^{\otimes k}, \mathcal{H}_o).$$

Again, the result of Gerstenhaber-Schack,[13] in a similar way as the Hochschild-Konstant-Rosenberg theorem does in the preceding section, implies that the cohomology of $\mathrm{Hom} = \oplus_{k,r} \mathrm{Hom}_k^r$ coincides with $\mathcal{H}_c$ itself (see Ref. 39).

Alternatively, the existence of an L_∞ quasi-isomorphism from $(\mathcal{H}_c, \mathfrak{l})$ to $(\mathcal{H}_c', \mathfrak{l}')$ is guaranteed at least physically, since $\{n_{k,l}\}$ can be constructed as open-closed disk amplitudes of the open-closed B-model, where the string world sheet action is of the same form as the one for pure closed strings, and the space of observables are just those used in separate open-closed B-model. An open-closed disk amplitude is then obtained by the integral of a disk correlation function, calculated in the usual way in physics, over the moduli space of the corresponding disk with punctures, both in the interior and on the boundary.

Moreover, it was checked in Ref. 26 that $n_{1,q}$ given by this physical argument in fact gives the linear part of the L_∞ quasi-isomorphism f_1,

$$n_{1,k}(\xi_{i_1} \wedge \cdots \wedge \xi_{i_k}, f_1, \ldots, f_k) = \frac{1}{k!} \sum_{\sigma \in \mathfrak{S}} (-1)^{\epsilon(\sigma)} (\xi_{i_{\sigma(1)}} f_1) \cdots (\xi_{i_{\sigma(k)}} f_k),$$

where $\xi_i \in TM$ acts on $f_i \in \mathcal{H}_o$ as the Lie derivative. Also, in the spirit of homological mirror symmetry, since the collection $\{n_{k,l}\}$ gives an L_∞ quasi-isomorphism even with the restriction to the category of coherent sheaves to $\mathcal{O}(M)$, it does also in case the full category would be treated for the open string side.

To summarize, we set $\mathcal{H}_c^k = \oplus_{p+q-2=k} H^q(\wedge^p TM)$, $\mathcal{H}_o^{k-1} = H^k(\mathcal{O}^{0,*}(M))$, and $\mathrm{Hom}_k^r = \mathrm{Hom}^r(\mathcal{H}_o^{\otimes k}, \mathcal{H}_o)$. Then we have $l_k = 0$ on $\mathcal{H}_c$ and $n_{0,q}$ is the minimal A_∞ structure of DGA $(\mathcal{O}^{0,*}(M), \bar{\partial}, \wedge)$. The operation l' is defined as in Sec. VI A, that is, $l_1' = [\bar{m}, \ ]$ with $\bar{m} = \Sigma_{0,q} n_{0,q}$ and $\mathfrak{l}_2'$ is related to the commutator $[\ ,\ ]$ through the suspension.

The corresponding OCHA structure in this case reduces to the generalized WDVV relation discussed in Ref. 24. Namely, it corresponds to a minimal OCHA with trivial L_∞ structure. At present, the explicit form of multilinear maps $n_{p,q}$ of $p \geqslant 2$ and $q \geqslant 0$ are not known in general, though physically existence is guaranteed by the open-closed scattering amplitudes of disks in B-twisted topological string theory. There is an interesting restriction where we can understand the form of $n_{k,l}$. Hofman discussed in Ref. 26 that if we restrict $\mathcal{H}_c$ to $\wedge^p TM$, the situation reduces to a complex version of Kontsevich's deformation quantization and hence $n_{p,q}$ are obtained in a similar way.

An interesting difference from the deformation quantization setup in the preceding section is that, since $\mathrm{Hom} = \oplus \mathrm{Hom}_k^r$ is not restricted to $\mathrm{Hom}_{\mathrm{sub}}$, even if $r = 1$ we can have nontrivial deformed m_k. In particular, we could in general obtain a deformation of the A_∞ structure $\bar{m}$ to a weak A_∞ structure, which should be one of the interesting future directions to be investigated.

In this case, for the closed string part, the L_∞ structure is trivial, including the bracket, and hence the obstructions vanish. In a more general model, however, it should not be trivial, as discussed by Huebschmann-Stasheff.[29] It should be interesting to find such models which can be calculated explicitly.

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Vector coherent state theory of the generic representations of $\mathfrak{so}(5)$ in an $\mathfrak{so}(3)$ basis

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For applications of group theory in quantum mechanics, one generally needs explicit matrix representations of the spectrum generating algebras that arise in bases that reduce the symmetry group of some Hamiltonian of interest. Here we use vector coherent state techniques to develop an algorithm for constructing the matrices for arbitrary finite-dimensional irreps of the SO(5) Lie algebra in an SO(3) basis. The SO(3) subgroup of SO(5) is defined by regarding SO(5) as linear transformations of the five-dimensional space of an SO(3) irrep of angular momentum two. A need for such irreps arises in the nuclear collective model of quadrupole vibrations and rotations. The algorithm has been implemented in MAPLE, and some tables of results are presented. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A vector coherent state (VCS) representation is a representation of a group (or Lie algebra) on a space of vector-valued functions. It is a representation induced from a multidimensional representation of a subgroup. Such representations have been used widely in the construction of explicit representations of Lie algebras and Lie groups,[1–6] in the construction of shift tensors,[7] and for the computation of Clebsch–Gordan coefficients for reducing tensor product representations.[8,9]

The VCS construction for a representation of a group G involves two subgroups that play quite different roles. A so-called "intrinsic" subgroup (sometimes called the "core" subgroup) acts in a known way on a subspace of the representation of interest. A second "orbiter" subgroup acts upon this subspace to generate the larger representation of the group G. A prototypical example of the construction is that for the dynamical group of the rigid rotor given by the semidirect product $G=\mathbb{R}^5 \ltimes \mathrm{SO}(3)$ of an intrinsic $\mathbb{R}^5$ subgroup, which describes the quadrupole moments (hence the shape) of an object, and an orbiter group SO(3), corresponding to physical rotations of the object, which describes its possible orientations. The quantum mechanics of such a rotor are then described by the unitary irreducible representations (irreps) of G.[10]

The key requirement is that the Lie algebras of the intrinsic and orbiter groups, together with those elements of the complexified Lie algebra $\mathfrak{g}_{\mathbb{C}}$ of G that leave the intrinsic space invariant, span the complex extension of the Lie algebra. Finding such groups is often easier in the complex extension of G. In many cases there are then mathematically naturally choices of intrinsic and orbiter subgroups for which the VCS construction of an induced representation is straightforward. Unfortunately a mathematically natural choice often produces a representation in a basis that is not adapted to the symmetries of a physical problem. A goal of this paper is to show how to construct representations of $\mathfrak{so}(5)$ in a basis that reduces a physically relevant $\mathfrak{so}(3) \subset \mathfrak{so}(5)$ subalgebra.

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The group SO(5) and its Lie algebra $\mathfrak{so}(5)$ arise in many physical contexts. For example, they are needed for the classification of states in the Bohr–Mottelson model[11] and Interacting Boson model[12] of nuclear collective states. They arise in a charge-independent pairing theory and in the use of isospin for the classification of nuclear shell model basis states.[13,14] They have also been used for the study of algebraic many-body equations of motion methods[15] and high-temperature superconductivity.[16] Depending on the context, $\mathfrak{so}(5)$ irreps may be required in an $\mathfrak{su}(2)$ (e.g., isospin) or an $\mathfrak{so}(3)$ (angular momentum) basis. The isospin $\mathfrak{su}(2)$ algebra is embedded in $\mathfrak{so}(5)$ as a subalgebra $\mathfrak{su}(2)\subset\mathfrak{su}(2)\times\mathfrak{su}(2)\cong\mathfrak{so}(4)\subset\mathfrak{so}(5)$. Thus, the required $\mathfrak{so}(5)\supset\mathfrak{su}(2)$ irreps are given in a basis that reduces the Gel'fand chain $\mathrm{SO}(5)\supset\mathrm{SO}(4)\supset\mathrm{SO}(3)\supset\mathrm{SO}(2)$.[17] Such irreps were constructed years ago[14,18] and reconstructed more simply by VCS methods in Refs. 3 and 19. Note, however, that the $\mathfrak{so}(3)\subset\mathfrak{so}(4)$ subalgebra of the SO(3) group in the Gel'fand chain is not the same as the above-mentioned angular momentum algebra that generates a "geometrical" $\mathrm{SO}(3)\subset\mathrm{SO}(5)$ subgroup of rotations of an associated three-dimensional space; as a result the construction of $\mathfrak{so}(5)$ irreps in an angular-momentum basis is more challenging.

The so-called one-rowed representations that occur in the decomposition of the Hilbert space of the five-dimensional harmonic oscillator can be inferred in an $\mathfrak{so}(3)$ basis from the results of Chaćon, Moshinsky, and others[20–22] or from the SO(5) hyperspherical harmonics and Clebsch–Gordan coefficients given in Ref. 21. An explicit VCS (vector coherent state) construction of irreps with highest weights of the type $(v,0)$ and $(0,f)$ (this notation is explained below) was given by Rowe and Hecht.[22]

In this paper we give a systematic construction of the generic (v,f) irreps in an $\mathfrak{so}(3)$ basis. In addition to its obvious relevance to the representation theory of $\mathfrak{so}(5)$, the construction is a prototype for a relatively sophisticated application of VCS theory.

II. VECTOR COHERENT STATE REPRESENTATIONS

Vector coherent state (VCS) theory is a generalization of standard (scalar) coherent state theory.[23] It was introduced[1] for the purpose of providing an explicit systematic construction of the irreducible unitary representations of the compact and noncompact symplectic Lie algebras. Simplicity and efficiency were achieved in the construction by making use of the already well-known representation theory of the unitary subalgebras. Important aspects of the theory were also introduced independently by Deenen and Quesne in their *partial coherent state representations*.[24] Subsequently, VCS has been used to construct representations of a large number of Lie algebras, groups, and superalgebras (cf. Ref. 6 for a review). Early applications of VCS theory gave realizations of the so-called *holomorphic representations* (reviewed by Hecht[25]). A more general class of VCS representations was later used in the construction of $\mathfrak{su}(3)$ irreps in an $\mathfrak{so}(3)$ basis.[26] It has also been shown that VCS theory is compatible with the theory of induced representations[6] and the theory of geometric quantization.[27] A more general perspective on the theory was given in Ref. 28.

The construction of the finite-dimensional irreps of $\mathfrak{so}(5)$ in an $\mathfrak{so}(3)$ basis has much in common with the construction of irreps of $\mathfrak{su}(3)$ in an $\mathfrak{so}(3)$ basis. The $\mathfrak{su}(3)$ Lie algebra is spanned by the components of $\mathfrak{so}(3)$ tensors of angular momentum $L=1$ and $L=2$, while the $\mathfrak{so}(5)$ Lie algebra is spanned by $\mathfrak{so}(3)$ tensors of angular momentum $L=1$ and $L=3$. However, whereas for $\mathfrak{su}(3)$ it was possible to use scalar coherent state wave functions, a special case of VCS functions, it proves to be essential to use vector-valued wave functions for $\mathfrak{so}(5)$.

The VCS theory of $\mathfrak{su}(3)$ relies on the fact that the carrier space for an $\mathfrak{su}(3)$ irrep is spanned by the set of states generated by SO(3) rotations of a highest weight state. The carrier space for a generic irrep of $\mathfrak{so}(5)$ is generated by SO(3) rotations of a set of highest *grade* states.

A. Highest grade states for an $\mathfrak{so}(5)$ irrep

The $\mathfrak{so}(5)$ Lie algebra is semisimple, of rank 2, and has the root diagram shown in Fig. 1. It is conventional to separate the roots of a semisimple Lie algebra into positive and negative roots and to regard the corresponding root vectors as raising and lowering operators, respectively. Every irrep is then characterized by a highest weight state.

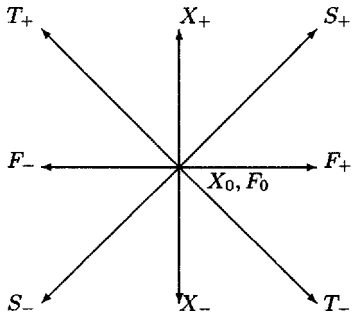

FIG. 1. Root diagram for the $\mathfrak{so}(5)$ Lie algebra.

Let α_1 be the root corresponding to the vector T_+ and α_2 be that corresponding to F_+. Then in the standard labeling scheme, the highest weight Λ for an irrep is given by two integers λ_1 and λ_2 such that $\Lambda=(\lambda_1+\frac{1}{2}\lambda_2)\alpha_1+(\lambda_1+\lambda_2)\alpha_2$. In keeping with the nuclear structure notation, we use the label $v=\lambda_1$ (the "seniority"), and find it convenient to introduce the half-integer $f=\frac{1}{2}\lambda_2$ since it also labels a $\mathfrak{u}(2)$ irrep, as is shown below. Thus, we label an $\mathfrak{so}(5)$ irrep (vf); the highest weight is then given by $\Lambda=(v+f)(\alpha_1+\alpha_2)+f\alpha_2$.

For present purposes, we separate the root vectors into grade raising, grade conserving, and grade lowering operators, as shown in Fig. 2. The horizontal grade-conserving root vectors $\{F_\pm, F_0, X_0\}$ then define what we shall refer to as an *intrinsic* or *core* $\mathfrak{u}(2)$ subalgebra. This grading of the $\mathfrak{so}(5)$ Lie algebra generates a grading of any irrep. Each irrep has a set of highest grade states $\{|(vf)m\rangle\}$ that are annihilated by the grade-raising operators $\hat{T}_+$, $\hat{X}_+$, and $\hat{S}_+$, and carry an irrep of the above-mentioned intrinsic $\mathfrak{u}(2)$ algebra; the highest grade states satisfy the equations

$$\hat{S}_+|(vf)m\rangle = \hat{X}_+|(vf)m\rangle = \hat{T}_+|(vf)m\rangle = 0, \tag{1}$$

$$\hat{X}_0|(vf)m\rangle = (v+f)|(vf)m\rangle, \quad \hat{F}_0|(vf)m\rangle = m|(vf)m\rangle, \tag{2}$$

$$\hat{F}_\pm|(vf)m\rangle = \sqrt{(f\mp m)(f\pm m+1)}|(vf)m\pm 1\rangle. \tag{3}$$

The weights for the highest grade states of a generic irrep of $\mathfrak{so}(5)$ are as illustrated in Fig. 2. A set of wave functions $\{\xi_m^{(vf)}; m=-f,\ldots,f\}$ for these highest grade states are regarded as *intrinsic* wave functions in the VCS construction—it is in the Hilbert space of these intrinsic functions that the VCS wave functions take their *vector* values.

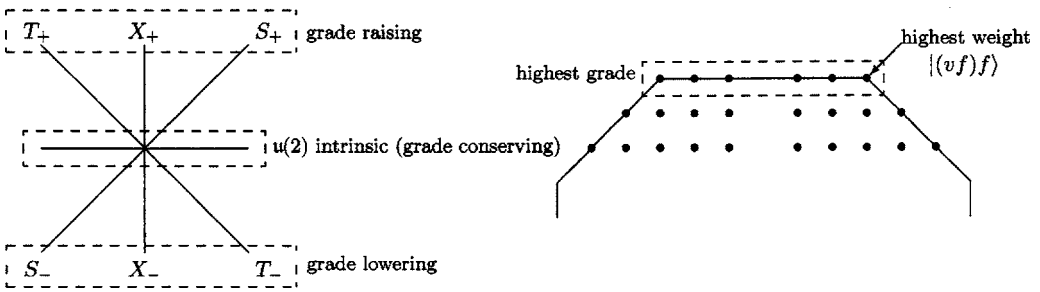

FIG. 2. The $\mathfrak{u}(2)$ intrinsic subalgebra and grade raising/lowering operators. The highest grade and highest weight of a generic $\mathfrak{so}(5)$ irrep are shown in the second digram.

B. Holomorphic VCS wave representations

Let $|\psi\rangle$ be a state in the carrier space of an $\mathfrak{so}(5)$ irrep (vf). Then a holomorphic VCS wave function is defined for this state by

$$\Psi(z) = \sum_m \xi_m^{(vf)} \langle (vf)m | e^{\hat{z}} | \psi \rangle, \tag{4}$$

where

$$\hat{z} = z_1 \hat{S}_+ + z_2 \hat{X}_+ + z_3 \hat{T}_+ \tag{5}$$

and $z=(z_1,z_2,z_3)$ is a set of complex numbers. The corresponding VCS representation Γ of the $\mathfrak{so}(5)$ Lie algebra is defined by

$$[\Gamma(X)\Psi](z) = \sum_m \xi_m^{(vf)} \langle (vf)m | e^{\hat{z}} \hat{X} | \psi \rangle, \quad X \in \mathfrak{so}(5). \tag{6}$$

Such holomorphic representations are natural generalizations of the familiar Bargmann–Segal representations[29] of the Heisenberg–Weyl algebras. They were the first to be considered in the formulation of VCS theory.[1] However, in practical applications they are not always the most useful. In particular, they do not reduce the $\mathfrak{so}(3) \subset \mathfrak{so}(5)$ angular momentum subalgebra.

C. VCS wave functions in an SO(3)-coupled basis

The group SO(3) can be embedded as a subgroup in SO(5) in many ways. We consider the SO(3) subgroup defined up to conjugation by regarding SO(5) as a group of orthogonal transformations of the five-dimensional carrier space for an $L=2$ irrep of SO(3). This embedding is motivated by the rotational properties of the five quadrupole degrees of freedom in the nuclear collective model. The construction of an SO(3)-coupled basis for a VCS irrep of $\mathfrak{so}(5)$ then parallels a similar construction of an SO(3)-coupled basis for a VCS irrep of $\mathfrak{su}(3)$.[26] The $\mathfrak{so}(5)$ construction makes use of the following theorem, which constrains the choice of the SO(3) subgroup.

Theorem 1: Provided no $\mathfrak{so}(3)$ angular momentum operator lies within the $\mathfrak{u}(2)$ intrinsic subalgebra, the set of states $\{\hat{R}(\Omega)|(vf)m\rangle; m=-f,\ldots,f; \Omega \in \mathrm{SO}(3)\}$ obtained by all SO(3) rotations of an orthonormal basis for the highest grade subspace spans the Hilbert space for the $\mathfrak{so}(5)$ irrep (vf).

Proof: The set of states generated by repeated application of the lowering operators $\{\hat{S}_-,\hat{X}_-,\hat{T}_-\}$ to the highest grade states spans the Hilbert space of the irrep. Now, if $\{\hat{L}_i; i=1,2,3\}$ is a Hermitian basis for the $\mathfrak{so}(3) \subset \mathfrak{so}(5)$ subalgebra, then each $\hat{L}_i$ can be expanded $\hat{L}_i = \hat{L}_i^- + \hat{L}_i^0 + \hat{L}_i^+$, where $\hat{L}_i^-$ is a grade lowering operator, $\hat{L}_i^0$ is of grade zero, and $\hat{L}_i^+$is a grade raising operator. By hermiticity, if $\hat{L}_i$ has a nonzero component $\hat{L}_i^+$, it must also have a nonzero $\hat{L}_i^-$ component. Thus, if no $\hat{L}_i$ lies in the zero grade $\mathfrak{u}(2)$ subalgebra, then each $\hat{L}_i$ must have a nonzero $\hat{L}_i^-$ component. By linear independence, it must be that the span of $\{\hat{L}_i^-\}$ equals the span of $\{\hat{S}_-,\hat{X}_-,\hat{T}_-\}$. **QED**

This theorem means that an arbitrary state $|\psi\rangle$ in an irrep (vf) is defined by the set of overlaps $\{\langle (vf)m|\hat{R}(\Omega)|\psi\rangle; m=-f,\ldots,+f; \Omega \in \mathrm{SO}(3)\}$, provided that the SO(3) subgroup is chosen as required by the theorem, which we assume from now on. It also means that, if $\{|(vf)\tau LM\rangle\}$ is an SO(3)-coupled basis for an $\mathfrak{so}(5)$ irrep and $\{|(vf)m\rangle\}$, with wave functions $\{\xi_m^{(vf)}\}$, is an orthonormal $\mathfrak{u}(2)$ basis of highest grade states for this irrep, then the basis states $\{|(vf)\tau LM\rangle\}$ have VCS wave functions given as vector-valued functions over SO(3) by

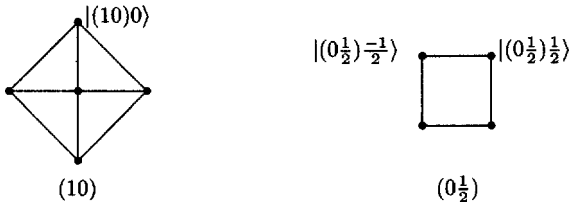

FIG. 3. The weight diagrams for the fundamental irreps (10) and $(0\frac{1}{2})$ with highest grade states labeled $|(vf)m\rangle$

$$\Phi^{(vf)}_{\tau LM}(\Omega) = \sum_m \xi^{(vf)}_m \langle (vf)m|\hat{R}(\Omega)|(vf)\tau LM\rangle. \tag{7}$$

These wave functions are very much like rotor-model wave functions.[11] Indeed, with basis states chosen to have good SO(3) transformation properties, they can be expanded

$$\Phi^{(vf)}_{\tau LM}(\Omega) = \sum_{mK} \xi^{(vf)}_m \langle (vf)m|(vf)\tau LK\rangle \mathcal{D}^L_{KM}(\Omega), \tag{8}$$

where $\mathcal{D}^L(\Omega)$ is a Wigner rotation matrix. It follows that a basis state $|(vf)\tau LM\rangle$ is characterized by the set of expansion coefficients,

$$b^{(vf)}_{mK}(\tau L) = \langle (vf)m|(vf)\tau LK\rangle. \tag{9}$$

The following gives a systematic procedure for determining these coefficients and for deriving the transformations of these coefficients by elements of the $\mathfrak{so}(5)$ Lie algebra as defined by the VCS representation

$$[\Gamma(X)\Phi^{(vf)}_{\tau LM}](\Omega) = \sum_m \xi^{(vf)}_m \langle (vf)m|\hat{R}(\Omega)\hat{X}|(vf)\tau LM\rangle, \quad X \in \mathfrak{so}(5). \tag{10}$$

III. REPRESENTATION SPACES FOR $\mathfrak{so}(5)$

A. A subspace of harmonic oscillator states

Irreps of $\mathfrak{so}(5)$ can be built up from its two fundamental irreps with highest weights (10) and $(0\frac{1}{2})$. The former is the fundamental five-dimensional irrep; the latter is the fundamental four-dimensional irrep. Both weight diagrams are shown in Fig. 3. These fundamental irreps are carried by the spaces generated by the raising operators $\{\eta^\dagger_\nu; \nu = 0, \pm 1, \pm 2\}$ of a five-dimensional harmonic oscillator with symmetry group U(5) and by the raising operators $\{\zeta^\dagger_m; m = \pm\frac{1}{2}, \pm\frac{3}{2}\}$ of a four-dimensional harmonic oscillator with symmetry group U(4), respectively. The operators $\{\eta^\dagger_\nu\}$ and $\{\zeta^\dagger_m\}$, together with the corresponding lowering operators, satisfy the usual boson commutation relations,

$$[\eta^\mu, \eta^\dagger_\nu] = \delta_{\mu\nu}\hat{I}, \quad [\eta^\mu, \eta^\nu] = [\eta^\dagger_\mu, \eta^\dagger_\nu] = 0, \tag{11}$$

$$[\zeta^m, \zeta^\dagger_n] = \delta_{mn}\hat{I}, \quad [\zeta^m, \zeta^n] = [\zeta^\dagger_m, \zeta^\dagger_n] = 0, \tag{12}$$

where we use the notation $\eta^\nu = (\eta^\dagger_\nu)^\dagger$ and $\zeta^m = (\zeta^\dagger_m)^\dagger$.

The invariants of U(5) and U(4) are given by their respective number operators,

$$\hat{n}_\eta = \eta^\dagger \cdot \eta = \sum_\nu \eta^\dagger_\nu \eta^\nu, \quad \hat{n}_\zeta = \zeta^\dagger \cdot \zeta = \sum_m \zeta^\dagger_m \zeta^m. \tag{13}$$

For the natural SO(3) embedding (defined to within conjugation), we can regard these number operators as coupled products, e.g.,

$$\hat{n}_\zeta = 2\sum_m \left(\tfrac{3}{2}, -m, \tfrac{3}{2}, m|0,0\right)\zeta_m^\dagger \zeta_{-m} = \sum_m (-1)^{3/2+m}\zeta_m^\dagger \zeta_{-m}, \tag{14}$$

where

$$\zeta_{-m} = (-1)^{3/2+m}\zeta^m.$$

Similarly, we can define

$$\eta_{-\nu} = (-1)^\nu \eta^\nu. \tag{15}$$

The fundamental five-dimensional irrep of the group SO(5) can be realized as the group of special orthogonal transformations of the creation operators $\{\eta_\nu^\dagger; \nu = 0, \pm 1, \pm 2\}$ that leave invariant the quantity $\eta^\dagger \cdot \eta^\dagger = \Sigma_\nu (-1)^\nu \eta_\nu^\dagger \eta_{-\nu}^\dagger$. This realization exhibits SO(5) as a subgroup of U(5). The four-dimensional fundamental irrep is a spinor irrep of SO(5). It can be realized as the group of special orthogonal transformations of the (boson) creation operators $\{\zeta_m^\dagger; m = \pm\frac{1}{2}, \pm\frac{3}{2}\}$ that leave invariant the quantity $\zeta^\dagger \cdot \zeta^\dagger = \Sigma_m (-1)^{3/2+m}\zeta_m^\dagger \zeta_{-m}^\dagger$. This realization exhibits USp(4), the two-fold cover of SO(5), as a subgroup of U(4). Because every irrep of a group is contained in a tensor product of copies of its fundamental irreps, it follows that every irrep of $\mathfrak{so}(5)$ can be realized on a subspace of the tensor product $\mathbb{H} = \mathbb{H}^{(5)} \otimes \mathbb{H}^{(4)}$, where $\mathbb{H}^{(n)}$ is the Hilbert space of an n-dimensional harmonic oscillator. Highest grade states for an $\mathfrak{so}(5)$ irrep in $\mathbb{H}$ are given by

$$|(vf)m\rangle = \frac{(\zeta_{3/2}^\dagger)^{f+m}(\zeta_{1/2}^\dagger)^{f-m}(\eta_2^\dagger)^v}{\sqrt{(f+m)!\,(f-m)!\,v!}}|0\rangle, \quad m = -f, \ldots, f. \tag{16}$$

B. A model space of VCS wave functions

A model space for a compact Lie group G is a representation of G that is a direct sum of irreps comprising precisely one copy from each equivalence class of irreps.[30] As emphasized by Biedenharn and Flath,[31] a model space provides a valuable framework for a realization of the tensor algebra of the group. We now show that a Hilbert space of VCS wave functions for the states of $\mathbb{H}$ provides a model space with very useful properties.

It follows from Eq. (7) that, provided the conditions of Theorem 1 are satisfied, any state $|\psi\rangle$ in $\mathbb{H}$ has VCS wave function Ψ given by

$$\Psi(\Omega) = \sum_{vfm} \xi_m^{(vf)} \langle (vf)m|\hat{R}(\Omega)|\psi\rangle. \tag{17}$$

Now observe that, if the wave functions $\{\xi_m^{(vf)}\}$ of the highest grade states are expressed in Bargmann form as the holomorphic functions,

$$\xi_m^{(vf)}(x,y) = \frac{x_1^{f+m}x_2^{f-m}y^v}{\sqrt{(f+m)!\,(f-m)!\,v!}}, \tag{18}$$

then, using Eq. (16), the $\mathfrak{u}(2)$-intertwining operator $\Sigma_{vfm}\xi_m^{(vf)}\langle (vf)m|$ can be expressed as

$$\sum_{vfm} \xi_m^{(vf)}\langle (vf)m| = \langle 0|e^{\hat{\mathfrak{X}}}, \tag{19}$$

where

$$\hat{\mathfrak{X}} = x_1\zeta^{3/2} + x_2\zeta^{1/2} + y\,\eta^2. \tag{20}$$

Thus, any state $|\psi\rangle$ in $\mathbb{H}$ has VCS wave function defined by

$$\Psi(\Omega) = \langle 0|e^{\hat{\mathfrak{X}}}\hat{R}(\Omega)|\psi\rangle. \tag{21}$$

Let $\mathcal{F}^{(vf)}$ denote the Hilbert space of VCS wave functions for an $\mathfrak{so}(5)$ irrep of highest weight (vf), relative to the inner product inherited from that of $\mathbb{H}$. The space of all VCS wave functions for states in $\mathbb{H}$ is then the direct sum

$$\mathcal{F} = \bigoplus_{(vf)} \mathcal{F}^{(vf)}, \tag{22}$$

of all such Hilbert spaces. Hence, by construction, it is a model space for $\mathfrak{so}(5)$. The following theorem, which generalizes a theorem of Rowe and Hecht,[22] shows that $\mathcal{F}$ is also a ring and that it can be generated from the VCS wave functions of the fundamental irreps (1,0) and $(0,\frac{1}{2})$.

Theorem 2: If $\Phi = \Phi_1 \odot \Phi_2$ is the *model product* of VCS wave functions defined by

$$\Phi(x,y,\Omega) = \Phi_1(x,y,\Omega)\Phi_2(x,y,\Omega), \tag{23}$$

then, if Φ_1 is in $\mathcal{F}^{(v_1f_1)}$ and Φ_2 is in $\mathcal{F}^{(v_2f_2)}$, the product Φ is in $\mathcal{F}^{(v_1+v_2,f_1+f_2)}$. Moreover, if $\mathcal{F}^{(v_1f_1)} \odot \mathcal{F}^{(v_2f_2)}$ denotes the linear span of model products of the functions of $\mathcal{F}^{(v_1f_1)}$ with the functions of $\mathcal{F}^{(v_2f_2)}$, then

$$\mathcal{F}^{(v_1f_1)} \odot \mathcal{F}^{(v_2f_2)} = \mathcal{F}^{(v_1+v_2,f_1+f_2)}. \tag{24}$$

Proof: Let $\hat{Z}_1^{(v_1f_1)}$ be a homogeneous polynomial of degree v_1 in the $\{\eta_\nu^\dagger\}$ raising operators and degree $2f_1$ in the $\{\zeta_m^\dagger\}$ raising operators, which creates a state with a VCS wave function,

$$\Phi^{(v_1f_1)}(\Omega) = \langle 0|e^{\hat{\mathfrak{X}}}\hat{R}(\Omega)\hat{Z}_1^{(v_1f_1)}|0\rangle. \tag{25}$$

Let

$$\hat{Z}_1^{(v_1f_1)}(\Omega) = \hat{R}(\Omega)\hat{Z}_1^{(v_1f_1)}\hat{R}(\Omega^{-1}) \tag{26}$$

denote the corresponding rotated operator. Then

$$\begin{aligned}\Phi^{(v_1f_1)}(\Omega) &= \langle 0|e^{\hat{\mathfrak{X}}}\hat{Z}_1^{(v_1f_1)}(\Omega)e^{-\hat{\mathfrak{X}}}|0\rangle \\ &= \langle 0|\left(\hat{Z}_1^{(v_1f_1)}(\Omega) + [\hat{\mathfrak{X}},\hat{Z}_1^{(v_1f_1)}(\Omega)] + \frac{1}{2!}[\hat{\mathfrak{X}},[\hat{\mathfrak{X}},\hat{Z}_1^{(v_1f_1)}(\Omega)]] + \cdots\right)|0\rangle.\end{aligned} \tag{27}$$

The successive terms in the sequence of multiple commutators inside the brackets are homogenous polynomials of decreasing degree in the raising operators. This sequence terminates with a polynomial of degree zero (a number) at the (v_1+2f_1)th term. Moreover, this last term is the only term in the sequence with a nonvanishing vacuum expectation value. It follows that

$$\Phi^{(v_1f_1)}(\Omega) = \frac{1}{(v_1+2f_1)!}[\underbrace{\hat{\mathfrak{X}},[\hat{\mathfrak{X}},[\cdots\hat{Z}_1^{(v_1f_1)}(\Omega)]]\cdots}_{v_1+2f_1 \text{ commutators}}]. \tag{28}$$

If $Z_2^{(v_2f_2)}$ is similarly defined for the wave function $\Phi_2^{(v_2f_2)}$, then the wave function $\Phi = \Phi_1^{(v_1f_1)} \odot \Phi_2^{(v_2f_2)}$ has values given by

$$\Phi(\Omega) = \langle 0|(e^{\hat{\mathfrak{X}}}\hat{Z}_1^{(v_1f_1)}(\Omega)e^{-\hat{\mathfrak{X}}})(e^{\hat{\mathfrak{X}}}\hat{Z}_2^{(v_2f_2)}(\Omega)e^{-\hat{\mathfrak{X}}})|0\rangle = \langle 0|e^{\hat{\mathfrak{X}}}\hat{R}(\Omega)\hat{Z}_1^{(v_1f_1)}\hat{Z}_2^{(v_2f_2)}|0\rangle. \tag{29}$$

The state $\hat{Z}_1^{(v_1f_1)}\hat{Z}_2^{(v_2f_2)}|0\rangle$ does not necessarily belong to an irreducible $\mathfrak{so}(5)$ subspace. However, it is of degree (v_1+v_2) and $2(f_1+f_2)$ in the $\{\eta_\nu^\dagger\}$ and $\{\zeta_m^\dagger\}$ operators, respectively, and, therefore, only the component of the state $\hat{Z}_1^{(v_1f_1)}\hat{Z}_2^{(v_2f_2)}|0\rangle$ that does lie within the irreducible SO(5) subspace of highest weight (v_1+v_2,f_1+f_2) will have nonzero overlap with $\langle 0|e^{\hat{\mathfrak{X}}}\hat{R}(\Omega)$.Thus, Φ is a VCS wave function for a state belonging to an SO(5) irrep of highest weight (v_1+v_2,f_1+f_2), as claimed by the theorem. The second part of the theorem follows from the observation that, if $\{\hat{Z}_\alpha^{(vf)}\}$ is a

basis for the linear space $P^{(vf)}$ of homogeneous polynomials of degree v in $\{\eta_\nu^\dagger\}$ and degree $2f$ in $\{\zeta_m^\dagger\}$, then the space $P^{(v_1+v_2,f_1+f_2)}$ is spanned by the products $\{\hat{Z}_{\alpha_1}^{(v_1f_1)}\hat{Z}_{\alpha_2}^{(v_2f_2)}\}$. **QED**

The theorem shows that $\mathcal{F}$ can be constructed from the two fundamental irreps, and that this process will generate all the irreps of $\mathfrak{so}(5)$. The importance of a model space is that, since it is multiplicity free, calculations performed in $\mathcal{F}$ are not complicated by any need to keep track of equivalent copies of the same $\mathfrak{so}(5)$ irreps.

IV. BASES FOR THE $\mathfrak{so}(5)$ LIE ALGEBRA

The VCS representations of $\mathfrak{so}(5)$ in an SO(3)-coupled basis make use of two bases for the $\mathfrak{so}(5)$ Lie algebra: a Cartan basis of root vectors and a basis of components of SO(3) tensors.

A. A Cartan basis

Starting from two copies of the (10) irrep, one spanned by the creation operators $\{\eta_\nu^\dagger\}$ and one spanned by the annihilation operators $\{\eta_\nu\}$, one can construct a realization of the $\mathfrak{so}(5)$ Lie algebra, which carries a (01) irrep, by taking an antisymmetric tensor product of the two. This gives the $\mathfrak{so}(5)$ root vectors of Fig. 1 as a subset of $\mathfrak{u}(5)$ operators,

$$\hat{S}_+ = \eta_1^\dagger\eta_2 - \eta_2^\dagger\eta_1 = \eta_1^\dagger\eta^{-2} + \eta_2^\dagger\eta^{-1}, \tag{30}$$

$$\hat{T}_+ = \eta_{-1}^\dagger\eta_2 - \eta_2^\dagger\eta_{-1} = \eta_{-1}^\dagger\eta^{-2} + \eta_2^\dagger\eta^{1}, \tag{31}$$

$$\hat{X}_+ = \sqrt{2}(\eta_2^\dagger\eta_0 - \eta_0^\dagger\eta_2) = \sqrt{2}(\eta_2^\dagger\eta^{0} - \eta_0^\dagger\eta^{-2}), \tag{32}$$

$$\hat{F}_+ = \sqrt{2}(\eta_1^\dagger\eta_0 - \eta_0^\dagger\eta_1) = \sqrt{2}(\eta_1^\dagger\eta^{0} + \eta_0^\dagger\eta^{-1}), \tag{33}$$

$$\hat{S}_- = (\hat{S}_+)^\dagger, \quad \hat{T}_- = (\hat{T}_+)^\dagger, \tag{34}$$

$$\hat{X}_- = (\hat{X}_+)^\dagger, \quad \hat{F}_- = (\hat{F}_+)^\dagger. \tag{35}$$

A basis for the Cartan subalgebra is given by

$$\hat{X}_0 = \tfrac{1}{2}[\hat{X}_+,\hat{X}_-] = \eta_2^\dagger\eta^2 - \eta_{-2}^\dagger\eta^{-2}, \tag{36}$$

$$\hat{F}_0 = \tfrac{1}{2}[\hat{F}_+,\hat{F}_-] = \eta_1^\dagger\eta^1 - \eta_{-1}^\dagger\eta^{-1}. \tag{37}$$

A realization of the $\mathfrak{so}(5)$ algebra as a subalgebra of $\mathfrak{u}(4)$ is similarly obtained from the symmetric tensor product of two copies of the $\left(0,\frac{1}{2}\right)$ irrep:

$$\hat{S}_+ = -\zeta_{3/2}^\dagger\zeta^{-3/2}, \quad \hat{T}_+ = \zeta_{1/2}^\dagger\zeta^{-1/2}, \tag{38}$$

$$\hat{X}_+ = \zeta_{1/2}^\dagger\zeta^{-3/2} - \zeta_{3/2}^\dagger\zeta^{-1/2}, \tag{39}$$

$$\hat{F}_+ = \zeta_{3/2}^\dagger\zeta^{1/2} + \zeta_{-1/2}^\dagger\zeta^{-3/2}, \tag{40}$$

$$\hat{X}_0 = \tfrac{1}{2}(\zeta_{3/2}^\dagger\zeta^{3/2} + \zeta_{1/2}^\dagger\zeta^{1/2} - \zeta_{-1/2}^\dagger\zeta^{-1/2} - \zeta_{-3/2}^\dagger\zeta^{-3/2}), \tag{41}$$

$$\hat{F}_0 = \tfrac{1}{2}(\zeta^\dagger_{3/2}\zeta^{3/2} - \zeta^\dagger_{1/2}\zeta^{1/2} + \zeta^\dagger_{-1/2}\zeta^{-1/2} - \zeta^\dagger_{-3/2}\zeta^{-3/2}). \tag{42}$$

B. An SO(3) tensor basis

Let $\{\hat{L}_k\}$ denote a set of angular momentum operators for the $\mathfrak{so}(3)$ subalgebra of $\mathfrak{so}(5)$ and let $\{d^\dagger_M; M=0,\pm1,\pm2\}$ and $\{p^\dagger_M; M=\pm\frac{1}{2},\pm\frac{3}{2}\}$ denote linear combinations of the $\{\eta^\dagger_\nu\}$ and $\{\zeta^\dagger_m\}$ operators, respectively, which satisfy the commutation relations

$$[\hat{L}_0, d^\dagger_M] = M d^\dagger_M, \quad [\hat{L}_\pm, d^\dagger_M] = \sqrt{(2 \mp M)(3 \pm M)}\, d^\dagger_{M\pm1}, \tag{43}$$

$$[\hat{L}_0, p^\dagger_M] = M p^\dagger_M, \quad [\hat{L}_\pm, p^\dagger_M] = \sqrt{\left(\tfrac{3}{2} \mp M\right)\left(\tfrac{5}{2} \pm M\right)}\, p^\dagger_{M\pm1}. \tag{44}$$

A basis for a realization of the $\mathfrak{so}(5)$ Lie algebra on the combined (tensor product) Hilbert spaces of the four- and five-dimensional harmonic oscillators is then provided by the $(L=1)$- and $(L=3)$-coupled operators,

$$\hat{L}_k = -\sqrt{10}[d^\dagger \otimes d]_{1k} - \sqrt{5}[p^\dagger \otimes p]_{1k}, \tag{45}$$

$$\hat{O}_\nu = -\sqrt{10}[d^\dagger \otimes d]_{3\nu} + \sqrt{5}[p^\dagger \otimes p]_{3\nu}, \tag{46}$$

where $[d^\dagger \otimes d]_{1k}$ signifies the SU(2)-coupled product,

$$[d^\dagger \otimes d]_{1k} = \sum_{mn} (2,n,2,m|1,k) d^\dagger_m d_n. \tag{47}$$

These operators satisfy the commutation relations

$$[\hat{L}_k, \hat{L}_l] = \sqrt{2}(1l,1k|1k+l)\hat{L}_{k+l}, \tag{48}$$

$$[\hat{L}_k, \hat{O}_\nu] = 2\sqrt{3}(3\nu,1k|3k+\nu)\hat{O}_{k+\nu}, \tag{49}$$

$$[\hat{O}_\mu, \hat{O}_\nu] = 2\sqrt{7}(3\nu,3\mu|1\mu+\nu)\hat{L}_{\mu+\nu} - \sqrt{6}(3\nu,3\mu|3\mu+\nu)\hat{O}_{\mu+\nu}. \tag{50}$$

Specification of the $\{d^\dagger_M\}$ and $\{p^\dagger_M\}$ operators in terms of the $\{\eta^\dagger_\nu\}$ and $\{\zeta^\dagger_m\}$ operators then defines the embedding of $\mathrm{SO}(3) \subset \mathrm{SO}(5)$ as the subgroup with Lie algebra $\mathfrak{so}(3)$ spanned by the $\{\hat{L}_k\}$ angular momentum operators. From now on, all references to SO(3) or $\mathfrak{so}(3)$ will mean this subgroup or its Lie algebra.

C. Relationships between the two bases

Many choices of relationship are possible. However, the simple relationship defined by $d^\dagger_M = \eta^\dagger_M$ and $p^\dagger_M = \zeta^\dagger_M$ is unsatisfactory because, for this choice, it is found that $\hat{L}_0 = 2\hat{X}_0 + \hat{F}_0$; this means that $\hat{L}_0$ lies in the intrinsic $\mathfrak{u}(2)$ subalgebra and the conditions for Theorem 1 are violated. A satisfactory relationship is given by setting

$$d^\dagger_M = e^{(\pi/4)(\hat{S}_+ - \hat{S}_-)} \eta^\dagger_M e^{-(\pi/4)(\hat{S}_+ - \hat{S}_-)}, \tag{51}$$

$$p^\dagger_M = e^{(\pi/4)(\hat{S}_+ - \hat{S}_-)} \zeta^\dagger_M e^{-(\pi/4)(\hat{S}_+ - \hat{S}_-)}. \tag{52}$$

This relationship gives

$$\eta^\dagger_2 = \sqrt{\tfrac{1}{2}}(d^\dagger_2 + d^\dagger_{-1}), \quad \eta^\dagger_{-2} = \sqrt{\tfrac{1}{2}}(d^\dagger_{-2} - d^\dagger_1), \tag{53}$$

$$\eta_0^\dagger = d_0^\dagger, \tag{54}$$

$$\eta_1^\dagger = \sqrt{\tfrac{1}{2}}(d_1^\dagger + d_{-2}^\dagger), \quad \eta_{-1}^\dagger = \sqrt{\frac{1}{2}}(d_{-1}^\dagger - d_2^\dagger), \tag{55}$$

and

$$\zeta_{\frac{3}{2}}^\dagger = \sqrt{\tfrac{1}{2}}(p_{3/2}^\dagger - p_{-3/2}^\dagger), \quad \zeta_{-3/2}^\dagger = \sqrt{\tfrac{1}{2}}(p_{-3/2}^\dagger + p_{3/2}^\dagger), \tag{56}$$

$$\zeta_{1/2}^\dagger = p_{1/2}^\dagger, \quad \zeta_{-1/2}^\dagger = p_{-1/2}^\dagger. \tag{57}$$

The relationship between the two bases for $\mathfrak{so}(5)$ is then given by

$$\hat{L}_0 = \tfrac{1}{2}(\hat{X}_0 - \hat{F}_0) - \tfrac{3}{2}(\hat{S}_+ + \hat{S}_-), \tag{58}$$

$$\hat{L}_\pm = 2\hat{T}_\pm + \sqrt{\tfrac{3}{2}}(\hat{F}_\pm + \hat{X}_\mp), \tag{59}$$

$$\hat{O}_0 = \tfrac{3}{2}(\hat{X}_0 - \hat{F}_0) + \tfrac{1}{2}(\hat{S}_+ + \hat{S}_-), \tag{60}$$

$$\hat{O}_{\pm 1} = \mp \sqrt{3}\hat{T}_\pm \pm \sqrt{\tfrac{1}{2}}(\hat{F}_\pm + \hat{X}_\mp), \tag{61}$$

$$\hat{O}_{\pm 2} = \tfrac{\sqrt{5}}{2}(\hat{X}_\pm - \hat{F}_\mp), \tag{62}$$

$$\hat{O}_{\pm 3} = \tfrac{\sqrt{5}}{2}(\mp \hat{X}_0 \mp \hat{F}_0 - \hat{S}_+ + \hat{S}_-), \tag{63}$$

where $\hat{L}_\pm = \mp \sqrt{2}\hat{L}_{\pm 1}$.

V. CONSTRUCTION OF VCS BASIS WAVE FUNCTIONS

Orthonormal basis states $\{|(vf)\tau LM\rangle\}$ for the (10) and $(0\frac{1}{2})$ irreps, for which the multiplicity index τ is redundant, are given by

$$|(10)2M\rangle = d_M^\dagger|0\rangle, \quad M = 0, \pm 1, \pm 2, \tag{64}$$

$$\left|\left(0\tfrac{1}{2}\right)\tfrac{3}{2}M\right\rangle = p_M^\dagger|0\rangle, \quad M = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}. \tag{65}$$

Thus, from the definitions (18)–(21), the corresponding VCS wave functions are given by

$$\Psi_{2M}^{(10)}(\Omega) = \xi_0^{(10)}\langle 0|\eta^2\hat{R}(\Omega)d_M^\dagger|0\rangle = \sum_K \xi_0^{(10)}\langle 0|\eta^2 d_K^\dagger|0\rangle \mathcal{D}_{KM}^2(\Omega) = \tfrac{1}{\sqrt{2}}\xi_0^{(10)}[\mathcal{D}_{2M}^2(\Omega) + \mathcal{D}_{-1,M}^2(\Omega)], \tag{66}$$

and

$$\begin{aligned}\Psi_{\frac{3}{2}M}^{\left(0\frac{1}{2}\right)}(\Omega) &= \xi_{\frac{1}{2}}^{\left(0\frac{1}{2}\right)}\langle 0|\zeta^{3/2}\hat{R}(\Omega)p_M^\dagger|0\rangle + \xi_{-1/2}^{(01/2)}\langle 0|\zeta^{1/2}\hat{R}(\Omega)p_M^\dagger|0\rangle \\ &= \tfrac{1}{\sqrt{2}}\xi_{1/2}^{(01/2)}[\mathcal{D}_{3/2M}^{3/2}(\Omega) - \mathcal{D}_{-3/2,M}^{3/2}(\Omega)] + \xi_{-1/2}^{(01/2)}\mathcal{D}_{1/2M}^{3/2}(\Omega).\end{aligned} \tag{67}$$

From Eq. (18), it follows that

$$\xi_{m_1}^{(v_1 f_1)} \odot \xi_{m_2}^{(v_2 f_2)} = \sqrt{\frac{(f+m)!\,(f-m)!\,v!}{(f_1+m_1)!\,(f_1-m_1)!\,(f_2+m_2)!\,(f_2-m_2)!\,v_1!\,v_2!}}\,\xi_m^{(vf)}, \tag{68}$$

where

$$v = v_1 + v_2, \quad f = f_1 + f_2, \quad m = m_1 + m_2. \tag{69}$$

From the properties of the Wigner rotation matrices, it also follows that

$$\mathcal{D}_{K_1 M_1}^{L_1} \odot \mathcal{D}_{K_2 M_2}^{L_2} = \sum_{L=|L_1-L_2|}^{L_1+L_2} (L_2 M_2, L_1 M_1 | L M)(L_2 K_2, L_1 K_1 | L K)\mathcal{D}_{KM}^{L}, \tag{70}$$

where

$$K = K_1 + K_2, \quad M = M_1 + M_2. \tag{71}$$

Thus, Theorem 2 and these expressions lead naturally to an algorithm for constructing (nonorthonormal) basis wave functions for an arbitrary $\mathfrak{so}(5)$ irrep.

It is convenient to start by constructing a nonorthonormal basis of VCS wave functions of the form

$$\Phi_{\tau LM}^{(vf)} = \sum_{mK} \xi_m^{(vf)} b_{mK}^{(vf)}(\tau L)\mathcal{D}_{KM}^{L}, \tag{72}$$

with $b_{mK}^{(vf)}(\tau L)$ coefficients conveniently chosen to be real and normalized such that

$$\sum_{mK} b_{mK}^{(vf)}(\tau L) b_{mK}^{(vf)}(\sigma L) = \delta_{\tau\sigma}. \tag{73}$$

The functions Φ so normalized will be related to the orthonormal $\mathfrak{so}(5)$ functions Ψ in Sec. VII.

In order to carry out this basis construction efficiently, it is useful to know the values of the angular momentum and the multiplicity of their occurrence in any given irrep. In other words, we need to know the $\mathfrak{so}(5)\downarrow\mathfrak{so}(3)$ branching rules that give the $\mathfrak{so}(3)$ irreps contained in any given $\mathfrak{so}(5)$ irrep. The $\mathfrak{so}(5)\downarrow\mathfrak{so}(3)$ branching rules for irreps of the type $(v0)$ were conveniently summarized by Williams and Pursey[32] in the form

$$L = 2K,\ 2K-2,\ 2K-3,\ \ldots,K$$

$$K = v,\ v-3,\ v-6,\ \ldots,K_{\min}, \tag{74}$$

where $K_{\min}=0$, 1, or 2. The branching rules for the irreps of type $(0f)$ are given[33] by

$$L = 3K,\ 3K-2,\ 3K-3,\ \ldots,K$$

$$K = f,\ f-2,\ f-4,\ \ldots,K_{\min}, \tag{75}$$

where $K_{\min}=0$ or 1. The branching rules for a generic irrep can be inferred by use of character theory[34] or by a simple "peeling-off" program[35] that uses knowledge of the number of eigenvalues of the $\hat{L}_0$ operator. The $\mathfrak{so}(3)$ content of some low-dimensional $\mathfrak{so}(5)$ irreps is given in Table I.

A basis for any irrep of highest weight (vf) can now be built up by taking coupled products of the above basic wave functions. For example, for the (20) irrep,

$$\Phi_{LM}^{(20)} \propto [\Psi_2^{(10)} \odot \Psi_2^{(10)}]_{LM}, \quad L = 2,4, \tag{76}$$

gives

TABLE I. The $\mathfrak{so}(3)$ content of some low-dimensional $\mathfrak{so}(5)$ irreps; note that the spinor irreps are labeled in the table by $2L$ for convenience.

Genuine irreps		Spinor irreps	
(v,f)	L	(v,f)	$2L$
(1,0)	2	(0,1/2)	3
(0,1)	1,3	(1,1/2)	1,5,7
(2,0)	2,4	(0,3/2)	3,5,9
(1,1)	1,2,3,4,5	(1,3/2)	1,3,5,7,7,9,11,13
(0,2)	0,2,3,4,6	(2,1/2)	3,5,7,9,11
(3,0)	0,3,4,6	(0,5/2)	3,5,7,9,11,15
(2,1)	1,2,3,3,4,5,5,6,7	(1,5/2)	1,3,5,5,7,7,9,9,11,11,13,13,15,17,19
(1,2)	1,2,2,3,4,4,5,5,6,7,8	(2,3/2)	1,3,5,5,7,7,9,9,11,11,13,13,15,17
(0,3)	1,3,3,4,5,6,7,9	(3,1/2)	3,5,7,9,9,11,13,15
(4,0)	2,4,5,6,8	(0,7/2)	3,5,7,9,9,11,13,15,17,21

$$\Phi^{(20)}_{LM} \propto \xi^{(20)}_0 \sum_{K_1K_2} b^{(10)}_{0K_1}(2) b^{(10)}_{0K_2}(2)(2K_1,2K_2|L,K_1+K_2)\mathcal{D}^L_{K_1+K_2,M}$$
$$\propto \xi^{(20)}_0[(22,22|L4)\mathcal{D}^L_{4M} + 2(22,2,-1|L1)\mathcal{D}^L_{1M} + (2,-1,2,-1|L,-2)\mathcal{D}^L_{-2,M}]. \quad (77)$$

Thus, we obtain the results shown in Table II. Similarly, we have for the (01) irrep

$$\Phi^{(01)}_{LM} \propto \xi^{(01)}_1 \sum_{K_1K_2} b^{(01/2)}_{1/2K_1}\left(\tfrac{3}{2}\right) b^{(01/2)}_{1/2K_2}\left(\tfrac{3}{2}\right)\left(\tfrac{3}{2}K_1,\tfrac{3}{2}K_2|L,K_1+K_2\right)\mathcal{D}^L_{K_1+K_2,M}$$
$$+ \sqrt{2}\,\xi^{(01)}_0 \sum_{K_1K_2} b^{(01/2)}_{-1/2K_1}\left(\tfrac{3}{2}\right) b^{(01/2)}_{1/2K_2}\left(\tfrac{3}{2}\right)\left(\tfrac{3}{2}K_1,\tfrac{3}{2}K_2|L,K_1+K_2\right)\mathcal{D}^L_{K_1+K_2,M}$$
$$+ \xi^{(01)}_{-1} \sum_{K_1K_2} b^{(01/2)}_{-1/2K_1}\left(\tfrac{3}{2}\right) b^{(01/2)}_{-1/2K_2}\left(\tfrac{3}{2}\right)\left(\tfrac{3}{2}K_1,\tfrac{3}{2}K_2|L,K_1+K_2\right)\mathcal{D}^L_{K_1+K_2,M}, \quad (78)$$

which leads to a set of coefficients given in Table III.

TABLE II. The $b^{(v0)}_{0K}(\tau L)$ coefficients for some irreps of type $(v0)$. Note that here and in the following tables the coefficients are normalized according to Eq. (73) and their phases are chosen so that the leading nonzero coefficient for each (L,τ) is positive.

$(vf) = (10)$

	K	
L	2	−1
2	$1/\sqrt{2}$	$1/\sqrt{2}$

$(vf) = (20)$

	K		
L	4	1	−2
2	0	$2/\sqrt{5}$	$-1/\sqrt{5}$
4	$\sqrt{7/13}$	$\sqrt{2/13}$	$2/\sqrt{13}$

$(vf) = (30)$

	K			
L	6	3	0	−3
0	0	0	1	0
3	0	$\sqrt{2/5}$	$-\sqrt{1/2}$	$-\sqrt{1/10}$
4	0	$2\sqrt{5/32}$	$\sqrt{7/32}$	$-\sqrt{5/32}$
6	$\sqrt{77/124}$	$3\sqrt{7/620}$	$\sqrt{3/31}$	$2\sqrt{7/155}$

TABLE III. The $b^{(0f)}_{mK}(\tau L)$ coefficients for some irreps of type $(0f)$. Note that for an $\mathfrak{so}(5)$ irrep (vf) the coefficients among different $\mathfrak{so}(3)$ irreps can all be indexed by the same values of $K-m$, hence, this is used to label columns.

$(vf)=(0\frac{1}{2})$

		$K-m$	
L	m	1	-2
$\frac{3}{2}$	$+\frac{1}{2}$	$1/2$	$-1/2$
	$-\frac{1}{2}$	$1/\sqrt{2}$	

$(vf)=(01)$

		$K-m$		
L	m	2	-1	-4
1	$+1$	0	$3/\sqrt{23}$	0
	0	0	$\sqrt{6/23}$	
	-1	$2\sqrt{2/23}$		
3	$+1$	$\sqrt{5/37}$	$-1/\sqrt{37}$	$\sqrt{5/37}$
	0	$\sqrt{10/37}$	$-2/\sqrt{37}$	
	-1	$2\sqrt{3/37}$		

$(vf)=(0\frac{3}{2})$

		$K-m$			
L	m	3	0	-3	-6
$\frac{3}{2}$	$+\frac{3}{2}$	0	$\sqrt{27/152}$	$\sqrt{27/152}$	0
	$+\frac{1}{2}$	0	$3\sqrt{2/152}$	0	
	$-\frac{1}{2}$	0	$4\sqrt{3/152}$		
	$-\frac{3}{2}$	$-4\sqrt{2/152}$			
$\frac{5}{2}$	$+\frac{3}{2}$	0	$\sqrt{27/232}$	$-\sqrt{27/232}$	0
	$+\frac{1}{2}$	0	$4\sqrt{3/232}$	$-\sqrt{30/232}$	
	$-\frac{1}{2}$	$2\sqrt{5/232}$	$2\sqrt{2/232}$		
	$-\frac{3}{2}$	$6\sqrt{2/232}$			
$\frac{9}{2}$	$+\frac{3}{2}$	$2\sqrt{7/328}$	$-\sqrt{3/328}$	$\sqrt{3/328}$	$-2\sqrt{7/328}$
	$+\frac{1}{2}$	$2\sqrt{14/328}$	$-4\sqrt{1/328}$	$\sqrt{14/328}$	
	$-\frac{1}{2}$	$2\sqrt{21/328}$	$-2\sqrt{6/328}$		
	$-\frac{3}{2}$	$6\sqrt{2/328}$			

In general, we can form basis states for an irrep (vf) from the coupled products

$$[\Phi^{(v0)}_{\tau_2 L_2}\odot\Phi^{(0f)}_{\tau_1 L_1}]_{LM}=\sum_m \xi^{(v0)}_0\odot\xi^{(f0)}_m\sum_{K_1K_2} b^{(v0)}_{0K_2}(\tau_2L_2)b^{(0f)}_{mK_1}(\tau_1L_1)(L_1K_1,L_2K_2|L,K_1+K_2)\mathcal{D}^L_{K_1+K_2,M}. \tag{79}$$

Some examples are given in Table IV.

It is important to recognize that the basis $\{\Phi^{(vf)}_{\tau LM}\}$ is not orthonormal relative to the appropriate inner product for VCS wave functions. An orthonormal basis is one relative to which the VCS representations are unitary; i.e., for which the elements of the $\mathfrak{so}(5)$ Lie algebra are represented by Hermitian operators.

VI. VCS REPRESENTATION OF THE $\mathfrak{so}(5)$ ALGEBRA

According to Eq. (10), the action of the angular momentum operators on any SO(3)-coupled VCS wave functions of the form

TABLE IV. The $b^{(vf)}_{mK}(\tau L)$ coefficients for some generic irreps.

$(vf) = (1\frac{1}{2})$

		$K-m$		
L	m	3	0	-3
$\frac{1}{2}$	$+\frac{1}{2}$	0	$\sqrt{3/5}$	0
	$-\frac{1}{2}$	0	$-\sqrt{2/5}$	
$\frac{5}{2}$	$+\frac{1}{2}$	0	$\sqrt{15/47}$	$\sqrt{6/47}$
	$-\frac{1}{2}$	$-4/\sqrt{47}$	$\sqrt{10/47}$	
$\frac{7}{2}$	$+\frac{1}{2}$	$\sqrt{7/22}$	$1/\sqrt{110}$	$-\sqrt{2/11}$
	$-\frac{1}{2}$	$\sqrt{2/11}$	$\sqrt{6/55}$	

$(vf) = (11)$

		$K-m$			
L	m	4	1	-2	-5
1	$+1$	0	0	$3/\sqrt{29}$	0
	0	0	$-2\sqrt{3/29}$	0	
	-1	0	$-2\sqrt{2/29}$		
2	$+1$	0	$2\sqrt{3/31}$	$-\sqrt{3/31}$	0
	0	0	$2/\sqrt{31}$	$2/\sqrt{31}$	
	-1	0	$-2\sqrt{2/31}$		
3	$+1$	0	$\sqrt{15/109}$	$2\sqrt{6/109}$	0
	0	0	$\sqrt{2/109}$	$2\sqrt{5/109}$	
	-1	$2\sqrt{10/109}$	$2\sqrt{2/109}$		
4	$+1$	0	$5\sqrt{3/829}$	$-2\sqrt{6/829}$	$-2\sqrt{21/829}$
	0	$-4\sqrt{7/829}$	$11\sqrt{2/829}$	$-2/\sqrt{829}$	
	-1	$-2\sqrt{42/829}$	$2\sqrt{30/829}$		
5	$+1$	$\sqrt{70/313}$	0	$-\sqrt{3/313}$	$2\sqrt{7/313}$
	0	$2\sqrt{21/313}$	$2/\sqrt{313}$	$-2\sqrt{7/313}$	
	-1	$2\sqrt{14/313}$	$2\sqrt{10/313}$		

$$\Phi^{(vf)}_{\tau LM}(\Omega) = \sum_{mK} \xi^{(vf)}_m \langle (vf)m|(vf)\tau LK\rangle \mathcal{D}^L_{KM}(\Omega) = \sum_{mK} \xi^{(vf)}_m b^{(vf)}_{mK}(\tau L)\mathcal{D}^L_{KM}(\Omega) \tag{80}$$

is given by the standard action

$$[\Gamma(L_0)\Phi^{(vf)}_{\tau LM}](\Omega) = M\Phi^{(vf)}_{\tau LM}(\Omega), \tag{81}$$

$$[\Gamma(L_\pm)\Phi^{(vf)}_{\tau LM}](\Omega) = \sqrt{(L \mp M)(L \pm M + 1)}\,\Phi^{(vf)}_{\tau L,M\pm 1}(\Omega). \tag{82}$$

The action of the octupole operators is given by

$$[\Gamma(O_\nu)\Phi^{(vf)}_{\tau LM}](\Omega) = \sum_{mK\mu} \xi^{(vf)}_m \langle (vf)m|\hat{O}_\mu|(vf)\tau LK\rangle \mathcal{D}^3_{\mu\nu}(\Omega)\mathcal{D}^L_{KM}(\Omega), \tag{83}$$

or, in coupled form,

$$[\Gamma(O)\otimes \Phi^{(vf)}_{\tau L}]_{L'M} = \sum_{mK\mu} \xi^{(vf)}_m \langle (vf)m|\hat{O}_\mu|(vf)\tau LK\rangle (LK,3\mu|L',K+\mu)\mathcal{D}^{L'}_{K+\mu,M}. \tag{84}$$

Thus, it remains to determine the matrix elements $\{\langle (vf)m|\hat{O}_\mu|(vf)\tau LK\rangle\}$ to define an $\mathfrak{so}(5)$ irrep (vf). From the definition of the states $\{|(vf)m\rangle\}$ as highest grade states, cf. Eqs. (1)–(3), we have the identities

$$\langle (vf)m|\hat{S}_-|(vf)\tau LK\rangle = \langle (vf)m|\hat{X}_-|(vf)\tau LK\rangle = \langle (vf)m|\hat{T}_-|(vf)\tau LK\rangle = 0, \tag{85}$$

$$\langle (vf)m|\hat{X}_0|(vf)\tau LK\rangle = (v+f)\langle (vf)m|(vf)\tau LK\rangle, \quad \langle (vf)m|\hat{F}_0|(vf)\tau LK\rangle = m\langle vfm|(vf)\tau LK\rangle, \tag{86}$$

$$\langle (vf)m|\hat{F}_{\pm}|(vf)\tau LK\rangle = \sqrt{(f\pm m)(f\mp m+1)}\langle (vf)m\mp 1|(vf)\tau LK\rangle, \tag{87}$$

and from the standard action of the angular momentum operators on the states $\{|(vf)\tau LK\rangle\}$, we have

$$\langle (vf)m|\hat{L}_0|(vf)\tau LK\rangle = K\langle (vf)m|(vf)\tau LK\rangle, \tag{88}$$

$$\langle (vf)m|\hat{L}_{\pm}|(vf)\tau LK\rangle = \sqrt{(L\mp K)(L\pm K+1)}\langle (vf)m|(vf)\tau L,K\pm 1\rangle. \tag{89}$$

Equations (58) and (59) give the relationships

$$\hat{S}_+ = \frac{1}{3}(\hat{X}_0 - \hat{F}_0) - \hat{S}_- - \frac{2}{3}\hat{L}_0, \tag{90}$$

$$\hat{X}_+ = \sqrt{\frac{2}{3}}\hat{L}_- - 2\sqrt{\frac{2}{3}}\hat{T}_- - \hat{F}_-, \tag{91}$$

$$\hat{T}_+ = \frac{1}{2}\hat{L}_+ - \frac{1}{2}\sqrt{\frac{3}{2}}(\hat{F}_+ + \hat{X}_-), \tag{92}$$

which makes it possible to rewrite Eqs. (60)–(63) in the form

$$\hat{O}_0 = \frac{5}{3}(\hat{X}_0 - \hat{F}_0) - \frac{1}{3}\hat{L}_0, \tag{93}$$

$$\hat{O}_1 = -\frac{\sqrt{3}}{2}\hat{L}_+ + \frac{5}{2\sqrt{2}}(\hat{F}_+ + \hat{X}_-), \tag{94}$$

$$\hat{O}_{-1} = -\frac{1}{\sqrt{3}}\hat{L}_- + \frac{5}{\sqrt{3}}\hat{T}_-, \tag{95}$$

$$\hat{O}_2 = \sqrt{\frac{5}{6}}\hat{L}_- - \sqrt{\frac{10}{3}}\hat{T}_- - \sqrt{5}\hat{F}_-, \tag{96}$$

$$O_{-2} = \frac{\sqrt{5}}{2}\hat{X}_- - \frac{\sqrt{5}}{2}\hat{F}_+, \tag{97}$$

$$O_3 = -\frac{2\sqrt{5}}{3}\hat{X}_0 - \frac{\sqrt{5}}{3}\hat{F}_0 + \sqrt{5}\hat{S}_- + \frac{\sqrt{5}}{3}\hat{L}_0, \tag{98}$$

$$O_{-3} = \frac{\sqrt{5}}{3}\hat{X}_0 + \frac{2\sqrt{5}}{3}\hat{F}_0 + \sqrt{5}\hat{S}_- + \frac{\sqrt{5}}{3}\hat{L}_0. \tag{99}$$

We now have all of the $\mathfrak{so}(5)$ operators in terms of the basis operators $\{S_-, T_-, X_-, X_0, F_0, F_\pm, L_0, L_\pm\}$ with known algebraic actions on either the highest grade states or on

the $\mathfrak{so}(3)$-coupled states. Note that Theorem 1 ensures that this set is linearly independent and spans $\mathfrak{so}(5)$. This is a general feature of a useful VCS construction.

We obtain

$$\langle (vf)m|\hat{O}_0|(vf)\tau LK\rangle = \frac{1}{3}(5v+5f-5m-K)b^{(vf)}_{mK}(\tau L), \tag{100}$$

$$\langle (vf)m|\hat{O}_1|(vf)\tau LK\rangle = \tfrac{5}{2}\sqrt{\tfrac{1}{2}(f+m)(f-m+1)}\,b^{(vf)}_{m-1,K}(\tau L) - \tfrac{1}{2}\sqrt{3(L-K)(L+K+1)}\,b^{(vf)}_{m,K+1}(\tau L), \tag{101}$$

$$\langle (vf)m|\hat{O}_{-1}|(vf)\tau LK\rangle = -\sqrt{\tfrac{1}{3}(L+K)(L-K+1)}\,b^{(vf)}_{m,K-1}(\tau L), \tag{102}$$

$$\langle (vf)m|\hat{O}_2|(vf)\tau LK\rangle = \sqrt{\tfrac{5}{6}(L+K)(L-K+1)}\,b^{(vf)}_{m,K-1}(\tau L) - \sqrt{5(f-m)(f+m+1)}\,b^{(vf)}_{m+1,K}(\tau L), \tag{103}$$

$$\langle (vf)m|\hat{O}_{-2}|(vf)\tau LK\rangle = -\tfrac{1}{2}\sqrt{5(f+m)(f-m+1)}\,b^{(vf)}_{m-1,K}(\tau L), \tag{104}$$

$$\langle (vf)m|\hat{O}_3|(vf)\tau LK\rangle = -\tfrac{\sqrt{5}}{3}(2v+2f+m-K)b^{(vf)}_{mK}(\tau L), \tag{105}$$

$$\langle (vf)m|\hat{O}_{-3}|(vf)\tau LK\rangle = \tfrac{\sqrt{5}}{3}(v+f+2m+K)b^{(vf)}_{mK}(\tau L). \tag{106}$$

It follows that Eq. (84) has the explicit expansion given by

$$[\Gamma(O)\otimes\Phi^{(vf)}_{\tau L}]_{L'M} = \sum_{mKm'K'} b^{(vf)}_{mK}(\tau L)M^{(vf)}_{mKL,m'K'L'}\xi^{(vf)}_{m'}\mathcal{D}^{L'}_{K'M}, \tag{107}$$

where $M^{(vf)}$ is a matrix with nonzero entries,

$$\begin{aligned}
M^{(vf)}_{mKL,mKL'} &= \tfrac{1}{3}(5v+5f-5m-K)(LK,\,30|L'K) - \tfrac{1}{2}\sqrt{3(L+K)(L-K+1)}\,(LK-1,3\;1|L'K)\\
&\quad - \sqrt{\tfrac{1}{3}(L-K)(L+K+1)}\,(LK+1,3\;-1|L'K),\\
M^{(vf)}_{mKL,m+1K+1L'} &= \tfrac{5}{2}\sqrt{\tfrac{1}{2}(f-m)(f+m+1)}\,(LK,3\;1|L'K+1),\\
M^{(vf)}_{mKL,m-1K+2L'} &= -\sqrt{5(f+m)(f-m+1)}\,(LK,3\;2|L'K+2),\\
M^{(vf)}_{mKL,mK+3L'} &= \sqrt{\tfrac{5}{6}(L-K)(L+K+1)}\,(LK+1,3\;2|L'K+3) - \frac{\sqrt{5}}{3}(2v+2f+m-K)(LK,3\;3|L'K+3),\\
M^{(vf)}_{mKL,m+1K-2L'} &= -\tfrac{1}{2}\sqrt{5(f-m)(f+m+1)}\,(LK,3\;-2|L'K-2),\\
M^{(vf)}_{mKL,mK-3L'} &= \tfrac{\sqrt{5}}{3}(v+f+2m+K)(LK,3\;-3|L'K-3).
\end{aligned} \tag{108}$$

Now, if the basis wave functions $\{\Phi^{(vf)}_{\tau LM}\}$ are chosen, as defined in Sec. V, with $\{b^{(vf)}_{mK}(\tau L)\}$ coefficients that are real and satisfy Eq. (73), it follows that Eq. (107) can be expressed as

$$[\Gamma(O)\otimes\Phi^{(vf)}_{\tau L}]_{L'M}=\sum_{\sigma}\Phi^{(vf)}_{\sigma L'M}\mathcal{O}^{(vf)}_{\sigma L',\tau L}, \tag{109}$$

where

$$\mathcal{O}^{(vf)}_{\sigma L',\tau L}=\sum_{mKm'K'}b^{(vf)}_{mK}(\tau L)M^{(vf)}_{mKL,m'K'L'}b^{(vf)}_{m'K'}(\sigma L'). \tag{110}$$

Thus, together with Eqs. (81) and (82), these equations give the explicit transformations of the $\{\Phi^{(vf)}_{\tau LM}\}$ basis wave functions for any $\mathfrak{so}(5)$ irrep.

Unfortunately, these matrices do not satisfy the hermiticity conditions required of a unitary representation. This is because the $\{\Phi^{(vf)}_{\tau LM}\}$ basis is not orthonormal relative to the appropriate VCS inner product.

VII. THE MATRICES OF UNITARY IRREPS

We now suppose that $\{|(vf)\alpha LM\rangle\}$ is an orthonormal basis for an irrep (vf) and that the corresponding VCS wave functions have expansions

$$\Psi^{(vf)}_{\alpha LM}=\sum_{mK}\xi^{(vf)}_{m}\langle(vf)m|(vf)\alpha LK\rangle\mathcal{D}^{L}_{KM}=\sum_{mK}\xi^{(vf)}_{m}a^{(vf)}_{mK}(\alpha L)\mathcal{D}^{L}_{KM}. \tag{111}$$

Note that for an orthonormal basis we have called the expansion coefficients of the VCS wave functions $a^{(vf)}_{mK}$ in order to distinguish them from the $b^{(vf)}_{mK}$ coefficients of the nonorthonormal $\Phi^{(vf)}_{\sigma LM}$ basis. The Wigner–Eckart theorem for matrix elements in an orthonormal basis,

$$\langle(vf)\beta L'M'|\hat{O}_{\nu}|(vf)\alpha LM\rangle=\frac{1}{\sqrt{2L'+1}}(LM,3\nu|L'M')\langle(vf)\beta L'\|\hat{O}\|(vf)\alpha L\rangle \tag{112}$$

then implies that

$$[\Gamma(O)\otimes\Psi^{(vf)}_{\alpha L}]_{L'M'}=\frac{1}{\sqrt{2L'+1}}\sum_{\beta}\Psi^{(vf)}_{\beta L'}\langle(vf)\beta L'\|\hat{O}\|(vf)\alpha L\rangle. \tag{113}$$

It follows from Eq. (110) that if the orthornormal basis wave functions are expanded as

$$\Psi^{(vf)}_{\alpha LM}=\sum_{\sigma}\Phi^{(vf)}_{\sigma LM}K^{(vf)}_{\sigma\alpha}(L); \tag{114}$$

then the desired reduced matrix elements, relative to the orthonormal basis, are given by

$$\langle(vf)\beta L'\|\hat{O}\|(vf)\alpha L\rangle=\sqrt{2L'+1}\sum_{\sigma\tau}\overline{K}^{(vf)}_{\beta\tau}\mathcal{O}^{(vf)}_{\tau L',\sigma L}K^{(vf)}_{\sigma\alpha}, \tag{115}$$

where $\overline{K}^{(vf)}$ is the inverse of the matrix $K^{(vf)}$, i.e., it is defined such that

$$\sum_{\sigma}\overline{K}^{(vf)}_{\beta\sigma}K^{(vf)}_{\sigma\alpha}=\delta_{\alpha\beta}. \tag{116}$$

The $K^{(vf)}(L)$ matrices are chosen in VCS theory[1] such that the reduced matrix elements satisfy the hermiticity condition

$$\langle(vf)\alpha L'\|\hat{O}\|(vf)\beta L\rangle^{*}=(-1)^{L-L'}\langle(vf)\beta L\|\hat{O}\|(vf)\alpha L'\rangle, \tag{117}$$

required of a unitary representation. Such a transformation is found in two steps.[36]

First observe that the submatrices $\mathcal{O}(L)$ with elements

$$\mathcal{O}_{\sigma\tau}(L) = \mathcal{O}^{(vf)}_{\sigma L,\tau L} \tag{118}$$

are real and symmetric. Thus, we first make an orthogonal transformation

$$\tilde{\Phi}^{(vf)}_{\alpha LM} = \sum_{\sigma} \Phi^{(vf)}_{\sigma LM} \mathcal{K}^{(vf)}_{\sigma\alpha}(L), \tag{119}$$

which diagonalizes the $\mathcal{O}(L)$ matrices. The transformed matrix,

$$\tilde{\mathcal{O}}^{(vf)}_{\beta L',\alpha L} = \sum_{\sigma\tau} \mathcal{K}^{(vf)}_{\tau\beta}(L') \mathcal{O}^{(vf)}_{\tau L',\sigma L} \mathcal{K}^{(vf)}_{\sigma\alpha}(L), \tag{120}$$

then satisfies the equality

$$\tilde{\mathcal{O}}^{(vf)}_{\beta L,\alpha L} = \delta_{\alpha\beta} \mathcal{O}^{(vf)}_{\beta L,\beta L}. \tag{121}$$

Before proceeding, it is important to note that states of different L and M are automatically orthogonal by virtue of their transformation properties under $SO(3)$. Moreover, if the reduced matrices for $L=L'$ are diagonal, this subset of matrices automatically satisfies the hermiticity condition (117).

Thus, in general, it only remains to apply suitable scale factors to the basis vectors $\{\tilde{\Phi}^{(vf)}_{\alpha LM}\}$ to obtain an orthonormal basis. The required scale factors $\{k^{(vf)}_{\alpha L}\}$ must be such that

$$(k^{(vf)}_{\alpha L})^{-1} \tilde{\mathcal{O}}^{(vf)}_{\alpha L,\beta L'} k^{(vf)}_{\beta L'} = (-1)^{L-L'} (k^{(vf)}_{\beta L'})^{-1} \tilde{\mathcal{O}}^{(vf)}_{\beta L',\alpha L} k^{(vf)}_{\alpha L}. \tag{122}$$

The desired $K^{(vf)}$ matrices are then given by

$$K^{(vf)}_{\tau\alpha}(L) = \mathcal{K}^{(vf)}_{\tau\alpha}(L) k^{(vf)}_{\alpha L}, \tag{123}$$

with

$$\left| \frac{k^{(vf)}_{\alpha L}}{k^{(vf)}_{\beta L'}} \right|^2 = (-1)^{L-L'} \frac{\tilde{\mathcal{O}}^{(vf)}_{\alpha L,\beta L'}}{\tilde{\mathcal{O}}^{(vf)}_{\beta L',\alpha L}}. \tag{124}$$

Special consideration must be given to the relatively few irreps for which there is a multiplicity of states of $L=0$, $\frac{1}{2}$, or 1. This is because the $\mathcal{O}(L)$ matrices are identically zero for these L values. However, to ensure the orthogonality and correct normalization of, for example, the $L=0$ states it is sufficient to determine linear combinations of these states that satisfy the equations

$$\langle (vf)\alpha 0 \| \hat{O} \| (vf)\beta L \rangle = (-1)^L \langle (vf)\beta L \| \hat{O} \| (vf)\alpha 0 \rangle, \tag{125}$$

where $\{|(vf)\beta LM\rangle\}$ is a small subset of states that have already been orthonormalized.

VIII. SAMPLE RESULTS

In this section we tabulate the a coefficients $a^{(vf)}_{mK}(\tau L)$ of the unitary basis wave functions and the unitary SO(3)-reduced $\mathfrak{so}(5)$ matrix elements of the $\hat{O}$ operator for the simplest generic $\mathfrak{so}(5)$ irreps as well as the table for the first irrep with a multiplicity, namely $(1\frac{3}{2})$ [we index the multiple $\mathfrak{so}(3)$ irreps as L_τ]. Because of the SO(3) reduction, we need only provide values between states of different L, since the Wigner–Ekart theorem provides the rest. Note that the matrix elements of the $\hat{L}$ operator are easily computed using Eqs. (81) and (82), and so they are not included in the tables. Since the diagonalization of Eq. (119) must be done numerically, the values are given in floating point form. (See Tables V–VIII.)

TABLE V. Expansion coefficients and reduced matrix elements for $\mathfrak{so}(5)$ irrep $(1,\frac{1}{2})$.

	a coefficients $K-m$				Reduced $\hat{O}$ matrix elements		
m	3	0	−3	L	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{7}{2}$
$\frac{1}{2}$	0	0.474 341	0	$\frac{1}{2}$	0	6.123 724	5.999 999
$-\frac{1}{2}$	0	−0.387 298	0				
$\frac{1}{2}$	0	0.517 549	0.327 326	$\frac{5}{2}$	6.123 724	2.535 462	11.338 934
$-\frac{1}{2}$	−0.534 522	0.422 577	0				
$\frac{1}{2}$	0.499 999	0.084 515	−0.377 964	$\frac{7}{2}$	−5.999 999	−11.338 934	3.070 597
$-\frac{1}{2}$	0.462 910	0.414 039	0				

IX. CONCLUDING REMARKS

As mentioned in the Introduction, the group SO(5) and its Lie algebra $\mathfrak{so}(5)$ arise in many physical contexts and, depending on the situation, their irreps are needed in different bases. In particular, they are needed in bases that reduce one of the following: (i) the U(2) subgroup whose Lie algebra is the grade-conserving intrinsic subalgebra shown in Fig. 2; (ii) the SO(4) subgroup generated by the S and T root vectors shown in Fig. 2; and (iii) the geometric SO(3) subgroup considered in this paper. VCS theory[1] has now been used in systematic ways to construct SO(5) irreps in all of these bases.

VCS theory was originally formulated to construct the holomorphic representations of the compact and noncompact discrete-series representations of the symplectic algebras. A first application constructed the irreps of the noncompact $\mathfrak{sp}(6,\mathbb{R})$ algebra [also called $\mathfrak{sp}(3,\mathbb{R})$] in a U(3) coupled basis. A next application, by Hecht and Elliott,[19] derived similar results for the compact $\mathfrak{sp}(4)$ algebra [isomorphic to $\mathfrak{so}(5)$] in a U(2)-coupled basis.

The common feature of the holomorphic VCS representations, which makes them particularly simple,[25] is their use of Abelian orbiter groups with Lie algebras spanned by commuting sets of grade-lowering (or grade-raising) operators to complement the grade-conserving intrinsic subgroups that generate highest- (or lowest-) grade intrinsic vectors for a VCS representation. A problem is that Abelian orbiter groups cannot be found in many important situations. For example, in constructing irreps of $\mathfrak{so}(5)$ in an $\mathfrak{so}(4)$-coupled basis, it is natural to use SO(4) as the intrinsic subgroup. However, the complementary $\mathfrak{so}(5)$ lowering operators (i.e., the operators F_- and X_- of Fig. 2) do not then commute. Fortunately, it was possible to extend the VCS construction[37] to accommodate this situation. It was also discovered[26] that VCS theory could be extended to give the much needed irreps of, for example, $\mathfrak{su}(3)$ in an $\mathfrak{so}(3)$ basis by using SO(3) itself as an orbiter group to complement an intrinsic U(2) group. This method was subsequently used[22] to construct the so-called one-rowed irreps of $\mathfrak{so}(5)$ [the irreps of type $(v,0)$ in the notation of this paper] for which only scalar-valued VCS wave functions are needed. The techniques have been further developed in this paper to give the generic $\mathfrak{so}(5)$ irreps in what is the most sophisticated explicit VCS construction of irreps to date.

Some novel features that considerably simplify the construction of VCS representations were introduced in Ref. 22 and further developed here. In particular, we have found that the Hilbert space $\mathcal{H}$ of all SO(5) VCS wave functions is a model space for SO(5), in the sense that it contains precisely one copy of every irrep. A particularly valuable feature of this model space is that it is a ring in as much as the product of any two VCS wave functions is another VCS wave function in $\mathcal{H}$. This observation greatly facilitates the construction of an $\mathrm{SO}(5)\supset\mathrm{SO}(3)$-coupled basis for $\mathcal{H}$; one has simply to construct multiple SO(3)-coupled products of the generating functions given by the VCS wave functions for the fundamental $(1,0)$ and $(0,\frac{1}{2})$ irreps. As a result, it is very easy to construct (nonorthonormal) basis wave functions for any $\mathfrak{so}(5)$ irrep. It is also shown that, once a basis has been determined, the matrices of the $\mathfrak{so}(5)$ Lie algebra in this basis can be determined

TABLE VI. Expansion coefficients and reduced matrix elements for $\mathfrak{so}(5)$ irrep $(2, \frac{1}{2})$.

	a coefficients					Reduced $\hat{O}$ matrix elements				
	$K-m$									
m	5	2	−1	−4	L	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$
$\frac{1}{2}$	0	0	0.439 155	0	$\frac{3}{2}$	4.225 771	9.486 832	10.954 451	−6.866 065	0
$-\frac{1}{2}$	0	0.414 039	0.207 019	0						
$\frac{1}{2}$	0	0.365 148	−0.204 124	0.241 522	$\frac{5}{2}$	−9.486 832	11.409 582	−1.380 131	8.391 463	9.486 832
$-\frac{1}{2}$	0	−0.158 113	−0.316 227	0						
$\frac{1}{2}$	0	0.365 148	−0.204 124	0.241 522	$\frac{7}{2}$	10.954 451	1.380 131	−11.258 858	−8.164 965	11.775 681
$-\frac{1}{2}$	0	0.516 397	−0.129 099	0						
$\frac{1}{2}$	0	0.217 597	0.255 883	0.174 077	$\frac{9}{2}$	6.866 065	8.391 463	8.164 965	12.465 753	11.742 179
$-\frac{1}{2}$	−0.426 401	0.023 262	0.232 621	0						
$\frac{1}{2}$	0.353 553	0.082 572	0	−0.190 692	$\frac{11}{2}$	0	−9.486 832	11.775 681	−11.742 179	8.628 704
$-\frac{1}{2}$	0.261 116	0.190 692	0.190 692	0						

TABLE VII. Expansion coefficients and reduced matrix elements for so(5) irrep (1,1).

		a coefficients $K-m$				Reduced $\hat{O}$ matrix elements				
m	4	1	−2	−5	L	1	2	3	4	5
1	0	0	0.380 319	0	1	0	9.258 201	−1.224 744	9.315 885	0
0	0	−0.439 155	0	0						
−1	0	−0.358 568	0	0						
1	0	0.462 910	−0.231 455	0	2	−9.258 201	−3.585 685	−8.660 254	1.463 850	9.710 083
0	0	0.267 261	0.267 261	0						
−1	0	−0.377 964	0	0						
1	0	0.306 186	0.387 298	0	3	−1.224 744	8.660 254	9.721 111	9.082 951	9.082 951
0		0.111 803	0.353 553	0						
0										
−1	0.499 999	0.223 606	0	0						
1	0	0.258 774	−0.146 385	−0.273 861	4	−9.315 885	1.463 850	−9.082 951	−5.946 187	12.377 975
0	−0.316 227	0.464 834	−0.059 761	0						
−1	−0.387 298	0.327 326	0	0						
1	0.353 553	0	−0.073 192	−0.223 606	5	0	−9.710 083	9.082 951	−12.377 975	0
0	0.387 298	0.084 515	−0.223 606	0						
−1	0.316 227	0.267 261	0	0						

TABLE VIII. Expansion coefficients and reduced matrix elements for $\mathfrak{so}(5)$ irrep $(1,\frac{3}{2})$.

	a coefficients						Reduced $\hat{O}$ matrix elements							
m	$K-m$ 5	2	-1	-4	-7	L	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}_1$	$\frac{7}{2}_2$	$\frac{9}{2}$	$\frac{11}{2}$	$\frac{13}{2}$
$\frac{3}{2}$	0	0	0.396 130	0	0	$\frac{1}{2}$	0	0	−8.964 214	−7.598 895	−5.949 760	0	0	0
$\frac{1}{2}$	0	0	0.560 213	0	0									
$-\frac{1}{2}$	0	0	0	0	0									
$-\frac{3}{2}$	0	0.431 252	0	0	0									
$\frac{3}{2}$	0	0	0.662 853	0	0	$\frac{3}{2}$	0	−4.225 771	9.486 832	−12.794 126	4.038 603	6.866 065	0	0
$\frac{1}{2}$	0	0	0	0	0									
$-\frac{1}{2}$	0	0.441 902	−0.441 902	0	0									
$-\frac{3}{2}$	0	−0.360 811	0	0	0									
$\frac{3}{2}$	0	0	0.177 154	−0.560 213	0	$\frac{5}{2}$	−8.964 214	−9.486 832	−7.606 388	−6.510 670	−2.843 828	−5.163 977	12.928 374	0
$\frac{1}{2}$	0	−0.528 173	0.417 558	0	0									
$-\frac{1}{2}$	0	−0.771 447	0.192 861	0	0									
$-\frac{3}{2}$	0	−0.578 585	0	0	0									
$\frac{3}{2}$	0	−0.666 136	0.063 536	−0.324 072	0	$\frac{7}{2}_1$	7.598 895	−12.794 126	6.510 670	−0.634 212	−10.096 484	3.705 020	−1.797 956	−13.815 832
$\frac{1}{2}$	0	−0.525 280	0.059 902	0.223 850	0									
$-\frac{1}{2}$	0	−0.216 048	−0.432 096	0	0									
$-\frac{3}{2}$	0.208 236	0.463 617	0	0	0									
$\frac{3}{2}$	0	0.008 606	0.559 438	0.254 742	0	$\frac{7}{2}_2$	5.949 760	4.038 603	2.843 828	−10.096 484	6.403 215	17.274 085	8.534 437	0.178 497
$\frac{1}{2}$	0	−0.229 439	0.527 444	0.309 605	0									
$-\frac{1}{2}$	0	0.169 828	0.339 656	0	0									
$-\frac{3}{2}$	−0.724 373	0.298 976	0	0	0									
$\frac{3}{2}$	0	0.394 124	0.105 334	−0.394 124	0	$\frac{9}{2}$	0	−6.866 065	−5.163 977	−3.705 020	−17.274 085	0.530 457	8.616 404	12.924 606
$\frac{1}{2}$	0	0.371 584	0.347 585	−0.371 584	0									
$-\frac{1}{2}$	0.455 096	0.198 620	0.198 620	0	0									
$-\frac{3}{2}$	0.643 602	0.344 020	0	0	0									
$\frac{3}{2}$	0	0.226 294	−0.140 542	−0.078 390	0.335 648	$\frac{11}{2}$	0	0	−12.928 374	−1.797 956	8.534 437	−8.616 404	−11.283 690	13.274 930
$\frac{1}{2}$	−0.316 452	0.480 398	−0.265 008	−0.021 335	0									
$-\frac{1}{2}$	−0.467 431	0.618 721	−0.149 346	0	0									
$-\frac{3}{2}$	−0.443 444	0.382 507	0	0	0									
$\frac{3}{2}$	0.403 399	−0.023 853	−0.029 214	0.075 431	−0.223 765	$\frac{13}{2}$	0	0	0	13.815 832	−0.178 497	12.924 606	−13.274 930	−2.884 731
$\frac{1}{2}$	0.474 678	0	−0.123 946	0.202 403	0									
$-\frac{1}{2}$	0.474 678	0.116 857	−0.233 715	0	0									
$-\frac{3}{2}$	0.350 573	0.286 242	0	0	0									

algebraically; cf. Eqs. (107) and (108). These results are remarkable in view of the fact that there is generally a multiplicity in the $SO(5) \supset SO(3)$ reduction of the representation space.

An important component of VCS theory is its incorporation of algorithms that go under the name of *K*-matrix theory,[36] whose purpose is to determine the inner product of a Hilbert space, transform a nonorthonormal basis into an orthonormal basis, and a nonunitary VCS irrep into a unitary representation whenever it is equivalent to a unitary irrep (or more generally to an isometric irrep when it is equivalent to an isometric irrep). For the irreps considered in this paper, a particularly simple version of the *K*-matrix transformation is given[36] by first finding an orthogonal basis in which off-diagonal matrix elements of the SO(5) octupole operator are zero between states of the same SO(3) angular momentum. This is simply achieved by diagonalization of subblocks of the octupole matrices. The renormalization factors needed to give an orthonormal basis can then be read off, as shown in Sec. VII. Unfortunately, this simple method does not work for states of angular momentum $L=0, \frac{1}{2}$, or 1, when there are multiple states of these L values. One must then resort to less simple *K*-matrix methods.

To summarize, the construction of the SO(3)-reduced matrices of the octupole operators in a generic $\mathfrak{so}(5)$ irrep is achieved in three simple steps: (i) the construction of basis wave functions with good SO(3) angular momentum quantum numbers; (ii) a calculation of the reduced matrix elements of the $\mathfrak{so}(5)$ octupole operators in this basis; and (iii) transforming these matrices to those of a unitary representation in an orthonormal basis.

Step (i) is simply achieved for a (vf) irrep by first computing the basis wave functions for the $(v0)$ and $(0f)$ irreps and then taking their SO(3)-coupled products, as indicated in Sec. V. Step (ii) is achieved by use of the analytical expressions given in Sec. VI in terms of SU(2) Clebsch–Gordan coefficients and the coefficients of the wave functions of step (i). Finally, step (iii) is achieved by the unitarization process described above and in Sec. VII. The routine has been coded in MAPLE, which is amenable to both algebraic and numeric computations. Steps (i) and (ii) are carried out algebraically; thus, the results in Tables II–IV are given in exact arithmetic. Step (iii), in which diagonalizations are used to orthogonalize states of a common angular momentum, is done numerically; thus the results given in Sec. VIII are floating point numbers. The current code has not been designed to handle large-dimensional irreps. However, should large irreps be of interest, the routine could be coded entirely in a numerical language such as FORTRAN, MATLAB, or C^{++}.

The representations of $\mathfrak{so}(5)$ in an SO(3)-coupled basis are of interest for several reasons. The so-called one-row irreps of type $(v0)$ feature in the Bohr–Mottelson and IBM-1 collective models and, consequently, have received much attention.[20–22] The generic irreps, constructed in this paper, show up in these collective models whenever the neutron and proton degrees of freedom are considered independently. They could also prove useful in the classification of shell-model states of fermions in an angular momentum $l=2$ orbital. Generic $\mathfrak{so}(5)$ irreps also show up in supersymmetric boson–fermion models.[38,39] For example, the irreps of the orthosymplectic $\mathfrak{osp}(5/4)$ superalgebra of Iachello's model contain irreps of the $\overline{\mathfrak{so}}(5)$ subalgebra in the chain:

$$\mathfrak{osp}(5/4) \supset \mathfrak{so}(5) \oplus \mathfrak{sp}(4) \supset \overline{\mathfrak{sp}}(4) \simeq \overline{\mathfrak{so}}(5), \tag{126}$$

where $\overline{\mathfrak{so}}(5)$ here signifies the subalgebra of $\mathfrak{so}(5) \oplus \mathfrak{sp}(4)$ obtained by adding the corresponding infinitesimal generators of the isomorphic $\mathfrak{so}(5)$ and $\mathfrak{sp}(4)$ algebras. The construction of VCS representations of orthosymplectic superalgebras was considered by LeBlanc and Rowe[40] in a natural extension of the holomorphic representations to include representations over Grassmann as well as complex variables. Thus, it would be useful for the development of supersymmetric models of coupled boson–fermion systems to extend the construction given in this paper for $\mathfrak{so}(5) \simeq \mathfrak{usp}(4)$ irreps in an SO(3) basis to the irreps of the orthosymplectic algebras.

It is interesting to note that, in the present construction of $\mathfrak{so}(5)$ irreps, the $\mathfrak{so}(5)$ algebra has been realized as a combination of $L=2$ and $L=3/2$ boson operators. The use of bosons of half-odd integer angular momentum is admittedly unusual in physics. But, in spite of the spin-statistics theorem, there is no algebraic reason forbidding their use in this way. The fact is that bilinear products of either boson or fermion operators of any given angular momentum obey

precisely the same commutation relations. However, the number of $\mathfrak{so}(5)$ irreps that can be built up with fermions is severely limited by the Pauli principle whereas with bosons there is no such limitation.

A major motivation for the present study was that the methods developed for $\mathfrak{so}(5)$ would serve as prototype examples of what can be done in more general situations. Constructing the irreps of a Lie algebra (or a Lie group) in a basis that reduces a noncanonical subgroup chain is generally much more challenging than in a basis that reduces a canonical subgroup chain. Thus, it is an order of magnitude simpler to construct $\mathfrak{so}(5)$ irreps in a canonical $\mathrm{SO}(5)\supset\mathrm{SO}(4)\supset\mathrm{SO}(3)$ basis than in the geometrical SO(3) basis considered in this paper. For example, analytical expressions are readily derived for the irreps of $\mathfrak{su}(3)$ in the canonical $\mathrm{SU}(3)\supset\mathrm{SU}(2)$ basis. But, prior to the development of apposite VCS techniques,[26] special *ad hoc* methods were needed to obtain these irreps in $\mathrm{SU}(3)\supset\mathrm{SO}(3)$ bases. A possible application of the methods developed in this paper might be to construct irreps of the exceptional Lie algebra $\mathfrak{g}_2$ in an $\mathrm{SU}(3)\supset\mathrm{SO}(3)$-coupled basis. This would appear to be possible by choosing intrinsic states that carry an irrep of a $\mathfrak{u}(2)$ subalgebra, corresponding to a pair of short $\mathfrak{g}_2$ roots, and employing SU(3) as the orbiter group. The construction of such irreps of $\mathfrak{g}_2$ is of physical interest as a step toward the construction of $\mathfrak{so}(7)$ irreps in a $G_2\supset\mathrm{SO}(3)$-coupled basis. The need for such irreps would surface if it were considered desirable to formulate a collective model of octupole dynamics analogous to Bohr's quadrupole model or to classify shell-model states of fermions in an angular momentum $l=3$ orbital.

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A simple and unified approach to identify integrable nonlinear oscillators and systems

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In this paper, we consider a generalized second-order nonlinear ordinary differential equation (ODE) of the form $\ddot{x}+(k_1x^q+k_2)\dot{x}+k_3x^{2q+1}+k_4x^{q+1}+\lambda_1x=0$, where k_i's, $i=1,2,3,4$, λ_1, and q are arbitrary parameters, which includes several physically important nonlinear oscillators such as the simple harmonic oscillator, anharmonic oscillator, force-free Helmholtz oscillator, force-free Duffing and Duffing–van der Pol oscillators, modified Emden-type equation and its hierarchy, generalized Duffing–van der Pol oscillator equation hierarchy, and so on, and investigate the integrability properties of this rather general equation. We identify several new integrable cases for arbitrary value of the exponent $q, q \in R$. The $q=1$ and $q=2$ cases are analyzed in detail and the results are generalized to arbitrary q. Our results show that many classical integrable nonlinear oscillators can be derived as subcases of our results and significantly enlarge the list of integrable equations that exists in the contemporary literature. To explore the above underlying results we use the recently introduced generalized extended Prelle-Singer procedure applicable to second-order ODEs. As an added advantage of the method, we not only identify integrable regimes but also construct integrating factors, integrals of motion, and general solutions for the integrable cases, wherever possible, and bring out the mathematical structures associated with each of the integrable cases.
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I. INTRODUCTION

A. Overview of the problem

In a recent paper[1] we have shown that the force-free Duffing–van der Pol (DVP) oscillator,

$$\ddot{x} + (\alpha + \beta x^2)\dot{x} - \gamma x + x^3 = 0, \tag{1}$$

is integrable for the parametric restriction $\alpha=4/\beta$ and $\gamma=-3/\beta^2$. In Eq. (1) the overdot denotes differentiation with respect to t and α, β and γ are arbitrary parameters. Under the transformation

$$w = -xe^{(1/\beta)t}, \quad z = e^{-(2/\beta)t}, \tag{2}$$

Eq. (1) with restriction $\alpha=4/\beta$ and $\gamma=-3/\beta^2$ was shown to be transformable to the form

$$w'' - \frac{\beta^2}{2} w^2 w' = 0, \tag{3}$$

which can then be integrated.[1]

In a parallel direction, while performing the invariance analysis of a similar kind of problem, we find that not only the Eq. (1) but also its generalized version,

$$\ddot{x} + \left(\frac{4}{\beta} + \beta x^2\right)\dot{x} + \frac{3}{\beta^2} x + x^3 + \delta x^5 = 0, \quad \delta = \text{arbitrary parameter}, \tag{4}$$

is invariant under the same set of Lie point symmetries.[2] As a consequence one can use the same transformation (2) to integrate Eq. (4). The transformation (2) modifies Eq. (4) to the form

$$w'' - \frac{\beta^2}{2} w^2 w' + \delta w^5 = 0, \tag{5}$$

which is not so simple to integrate straightforwardly. However, we observe that this equation coincides with the second equation in the so-called modified Emden equation (MEE) hierarchy, investigated by Feix *et al.*,[3]

$$\ddot{x} + x^l \dot{x} + g x^{2l+1} = 0, \quad l = 1, 2, \ldots, n, \tag{6}$$

where g is an arbitrary parameter.

In fact, Feix *et al.*[3] have shown that through a direct transformation to a third-order equation the above Eq. (6) can be integrated to obtain the general solution for the specific choice of the parameter g, namely, for $g = 1/(l+2)^2$. For this choice of g, the general solution of (6) can be written as

$$x(t) = \left(\frac{(2 + 3l + l^2)(t + I_1)^l}{l(t + I_1)^{l+1} + (2 + 3l + l^2) I_2}\right)^{1/l}, \quad I_1, I_2 = \text{arbitrary constants}. \tag{7}$$

Consequently, Eq. (4) can be integrated under the specific parametric choice $\delta = 1/16$, and it belongs to the $l = 2$ case of the MEE hierarchy (6) with $g = 1/16$. Now the question arises as to whether there exist other new integrable second-order nonlinear differential equations which are linear in $\dot{x}$ and contain fifth and other powers of nonlinearity. As far as our knowledge goes, only few equations in this class have been shown to be integrable. For example, Smith had investigated a class of nonlinear equations coming under the category

$$\ddot{x} + f(x)\dot{x} + g(x) = 0, \tag{8}$$

with $f(x) = (n+2) b x^n - 2a$ and $g(x) = x(c + (b x^n - a)^2)$, where a, b, c, and n are arbitrary parameters. He had shown that Eq. (8) with this specific form of f and g admits explicit oscillatory solutions. However, one can also expect that there should be a number of integrable equations which also admit solutions which are both oscillatory and nonoscillatory types in the class

$$\ddot{x} + (k_1 x^q + k_2)\dot{x} + k_3 x^{2q+1} + k_4 x^{q+1} + \lambda_1 x = 0, \quad q \in R, \tag{9}$$

where k_i's, $i = 1, 2, 3, 4$, and λ_1 are arbitrary parameters. When $q = 1$, Eq. (9) becomes the generalized MEE

$$\ddot{x} + (k_1 x + k_2)\dot{x} + k_3 x^3 + k_4 x^2 + \lambda_1 x = 0, \tag{10}$$

and for $q = 2$ it becomes

$$\ddot{x} + (k_1 x^2 + k_2)\dot{x} + k_3 x^5 + k_4 x^3 + \lambda_1 x = 0. \tag{11}$$

We note that Eq. (4) is a special case of (11).

Needless to say, Eq. (9) is a unified model for several ground-breaking physical systems which includes simple harmonic oscillator, anharmonic oscillator, force-free Helmholtz oscillator, force-free Duffing oscillator, MEE hierarchy, generalized DVP hierarchy, and so on.

As noted earlier, there exists no rigorous mathematical analysis in the literature for the second-order nonlinear differential equations which contain fifth or higher degree nonlinearity in x and linearity in $\dot{x}$, and the results are very scarce on integrability or exact solutions. Our motivation to analyze this problem is not only to explore new integrable cases/systems of Eq. (9) but also to synthesize all earlier results under one approach.

Having described the problem and motivation, now we can start analyzing the integrability properties of Eq. (9). To identify the integrable regimes we employ the recently introduced extended Prelle-Singer procedure applicable to second-order ordinary differential equations (ODEs).[5–11] Through this method we not only identify integrable regimes but also construct integrating factors, integrals of motion, and general solution for the integrable cases, wherever possible.

B. Results

We unearth several new integrable equations for any real value of the exponent q in Eq. (9). In the following we summarize the results for the case $q=$*arbitrary* only and discuss in detail the $q=1$, $q=2$, and $q=$*arbitrary* cases separately in the following sections.

For the choice $q=$*arbitrary* we find that the following equations are completely integrable (after suitable reparametrizations), all of which appear to be new to the literature:

$$\ddot{x}+(k_1x^q+(q+2)k_2)\dot{x}+k_1k_2x^{q+1}+(q+1)k_2^2x=0, \tag{12}$$

$$\ddot{x}+((q+2)k_1x^q+k_2)\dot{x}+k_1^2x^{2q+1}+k_1k_2x^{q+1}+\lambda_1x=0, \tag{13}$$

$$\ddot{x}+(q+4)k_2\dot{x}+k_4x^{q+1}+2(q+2)k_2^2x=0, \tag{14}$$

$$\ddot{x}+((q+1)k_1x^q+k_2)\dot{x}+\frac{(r-1)}{r^2}[(q+1)k_1^2x^{2q+1}+(q+2)k_1k_2x^{q+1}+k_2^2x]=0, \quad r\neq 0, \tag{15}$$

$$\ddot{x}+((q+1)k_1x^q+(q+2)k_2)\dot{x}+(q+1)\left[\frac{(r-1)}{r^2}k_1^2x^{2q+1}+k_1k_2x^{q+1}+k_2^2x\right]=0, \quad r\neq 0, \tag{16}$$

where k_1, k_2, k_4, λ_1, and r are arbitrary parameters. We stress that the above results are true for any arbitrary values of q. We discuss the special cases, namely, $q=1$ and $q=2$ separately in detail in Secs. III and IV in order to put the results of q arbitrary case in proper perspective.

We show that the Eq. (12) is nothing but a generalization of the Duffing–van der Pol oscillator Eq. (1). In a recent work[1,9] three of the present authors have established the integrability of Eq. (12) with $q=2$. However, in this work we show that the generalized Eq. (12) itself is integrable. Equation (13) is nothing but the generalized MEE among which the hierarchy of Eq. (6), studied by Feix *et al.*,[3] can be identified as a subcase. In fact, the general solution constructed by Feix *et al.*, Eq. (7), can be derived straightforwardly as a subcase. Equation (13) also contains the family of equations studied by Smith.[4] In particular, the latter author has derived a general solution for the case $k_2^2<4\lambda_1$, which turns out to be an oscillatory one. However, in this work, we show that even for arbitrary values of k_2 and λ_1 one can construct the general solution. Interestingly, the system (14) generalizes several physically important nonlinear oscillators. For example, in the case $q=1$ and 2, Eq. (14) provides us the force-free Helmholtz and Duffing oscillators, respectively, whose nonlinear dynamics is well documented in the literature.[12–17] Here, we present certain integrable generalizations of these nonlinear oscillators. Equation (15) admits a conservative Hamiltonian for all values of the parameters r, k_1, and k_2 and any integer value of q. We also provide the explicit form of the Hamiltonian for all values of q. As a result we conclude that it is

a Liouville integrable system. As far as Eq. (16) is concerned we construct a time-dependent integral of motion and transform the latter to a time-independent Hamiltonian one, thereby ensuring its Liouville integrability.

The plan of the paper is as follows. In the following section we briefly describe the extended Prelle-Singer procedure applicable to second-order ODEs. In Sec. III, we consider the case $q=1$ in (9) and identify the integrable parametric choices of this equation through the extended PS procedure. To do so, first we identify the integrable cases where the system admits time-independent integrals and construct explicit conservative Hamiltonians for the respective parametric choices. We then identify the cases which admit explicit time-dependent integrals of motion. To establish the complete integrability of these cases we use our own procedure and transform the time-dependent integrals of motion into time-independent integrals of motion and integrate the latter and derive the general solution. In Sec. IV, we repeat the procedure for the case $q=2$ in Eq. (9) and identify the integrable systems. In Sec. V, we consider the case $q=$arbitrary in (9) and unearth several new integrable equations and their associated mathematical structures. Finally, we present our conclusions in Sec. VI.

II. GENERALIZED EXTENDED PRELLE-SINGER (PS) PROCEDURE

In this section we briefly recall the generalized extended or modified PS procedure before applying it to the specific problem in hand. Some time ago, Prelle and Singer[5] proposed a procedure for solving first-order ODEs that admits solutions in terms of elementary functions if such solutions exist. The attractiveness of the PS method is that if the given system of first-order ODEs has a solution in terms of elementary functions, then the method guarantees that this solution will be found. Very recently Duarte *et al.*[7,8] modified the technique developed by Prelle and Singer[5,6] and applied it to second-order ODEs. Their approach was based on the conjecture that if an elementary solution exists for the given second-order ODE then there exists at least one elementary first integral $I(t,x,\dot{x})$ whose derivatives are all rational functions of t, x, and $\dot{x}$. For a class of systems these authors have deduced first integrals and in some cases for the first time through their procedure.[7] Recently the present authors generalized the theory of Duarte *et al.*[7] in different directions and showed that for the second-order ODEs one can isolate even two independent integrals of motion[9–11] and obtain general solutions explicitly without any integration. This theory has also been illustrated for a class of problems.[1,9–11] The authors have also generalized the theory successfully to higher order ODEs.[10,18] For example, in the case of third-order ODEs the theory has been appropriately generalized to yield three independent integrals of motion unambiguously so that the general solution follows immediately from these integrals of motion.[18]

We stress that the PS procedure has many advantages over other methods. To name a few, we cite: (1) For a given problem if the solution exists it has been conjectured that the PS method guarantees to provide first integrals. (2) The PS method not only gives the first integrals but also the underlying integrating factors, that is, multiplying the equation with these functions we can rewrite the equation as a perfect differentiable function which upon integration gives the first integrals directly. (3) The PS method can be used to solve nonlinear as well as linear second-order ODEs. (4) As the PS method is based on the equations of motion rather than on Lagrangian or Hamiltonian description, the analysis is applicable to deal with both Hamiltonian and non-Hamiltonian systems.

A. PS method

Let us rewrite Eq. (9) in the form

$$\ddot{x} = -\left((k_1 x^q + k_2)\dot{x} + k_3 x^{2q+1} + k_4 x^{q+1} + \lambda_1 x\right) \equiv \phi(x,\dot{x}). \tag{17}$$

(In fact the method is applicable to a general situation where ϕ can be a rational function of the variables x, $\dot{x}$, and t; for details see for example Ref. 9 and for a related approach see Ref. 15.) Further, we assume that the ODE (17) admits a first integral $I(t,x,\dot{x})=C$, with C constant on the solutions, so that the total differential becomes

$$dI = I_t\,dt + I_x\,dx + I_{\dot{x}}\,d\dot{x} = 0, \tag{18}$$

where each subscript denotes partial differentiation with respect to that variable. Rewriting Eq. (17) in the form $\phi dt - d\dot{x} = 0$ and adding a null term $S(t,x,\dot{x})\dot{x}dt - S(t,x,\dot{x})dx$ to the latter, we obtain that on the solutions the 1-form

$$(\phi + S\dot{x})dt - S\,dx - d\dot{x} = 0. \tag{19}$$

Hence, on the solutions, the 1-forms (18) and (19) must be proportional. Multiplying (19) by the factor $R(t,x,\dot{x})$ which acts as the integrating factors for (19), we have on the solutions that

$$dI = R(\phi + S\dot{x})dt - RS\,dx - R\,d\dot{x} = 0. \tag{20}$$

Comparing Eq. (18) with (20) we have, on the solutions, the relations

$$I_t = R(\phi + \dot{x}S), \quad I_x = -RS, \quad I_{\dot{x}} = -R. \tag{21}$$

Then, the compatibility conditions, $I_{tx} = I_{xt}$, $I_{t\dot{x}} = I_{\dot{x}t}$, $I_{x\dot{x}} = I_{\dot{x}x}$, between Eqs. (21) provide us

$$S_t + \dot{x}S_x + \phi S_{\dot{x}} = -\phi_x + \phi_{\dot{x}}S + S^2, \tag{22}$$

$$R_t + \dot{x}R_x + \phi R_{\dot{x}} = -(\phi_{\dot{x}} + S)R, \tag{23}$$

$$R_x - SR_{\dot{x}} - RS_{\dot{x}} = 0. \tag{24}$$

Solving Eqs. (22)–(24), one can obtain expressions for S and R. It may be noted that any set of special solutions (S,R) is sufficient for our purpose. Once these forms are determined the integral of motion $I(t,x,\dot{x})$ can be deduced from the relation

$$I = r_1 - r_2 - \int \left[R + \frac{d}{d\dot{x}}(r_1 - r_2) \right] d\dot{x}, \tag{25}$$

where

$$r_1 = \int R(\phi + \dot{x}S)dt, \quad r_2 = \int \left(RS + \frac{d}{dx}r_1 \right) dx.$$

Equation (25) can be derived straightforwardly by integrating the Eq. (21).

The crux of the problem lies in finding the explicit solutions satisfying all three determining equations (22)–(24), since once a particular solution is known the integral of motion can be readily constructed. The difficulties in constructing admissible set of solutions (S,R) satisfying all three equations (22)–(24) and possible ways of obtaining the solutions have been discussed in detail in Ref. 9. In this context we wish to point out that our above method of finding solutions using Eqs. (22)–(25) is closely related to the integrating factor/first integral method of Bluman and Anco.[15] In fact in Refs. 15 and 16 effective Ansätze for solving the integrating factor determining equations are treated and the present method can also be considered as a generalization of the method developed in Refs. 15 and 16.

III. APPLICATION OF PS PROCEDURE TO EQ. (10)

Let us first consider the case $q=1$ in Eq. (9) or equivalently (10),

$$\ddot{x} + (k_1 x + k_2)\dot{x} + k_3 x^3 + k_4 x^2 + \lambda_1 x = 0. \quad \text{[Eq. (10)]}$$

Equation (10) itself includes several physically important models. For example, choosing $k_i = 0$, $i = 1, \ldots, 4$, we get the simple harmonic oscillator equation and the choice k_1, $k_2 = 0$ gives us the anharmonic oscillator equation. When k_1, $k_4 = 0$ Eq. (10) becomes the force-free Duffing oscillator

equation.[12] The choice k_2, k_4, $\lambda_1=0$ provides us the MEE.[19] In the limit $k_3=k_1^2/9$, $k_4=k_1k_2/3$, Eq. (10) becomes MEE with linear term which is another linearizable equation which we have studied extensively in Refs. 9 and 20. The restriction k_1, $k_3=0$ leads us to the force-free Helmhotz oscillator.[12,13] In the following we investigate whether the system (10) admits any other integrable case besides the above.

We solve Eq. (10) through the extended PS procedure in the following way. For a given second-order equation (10), the first integral I should be either a time-independent or time-dependent one. In the former case, it is a conservative system and we have $I_t=0$ and in the latter case we have $I_t\neq 0$. So, let us first consider the case $I_t=0$ and determine the null forms and the corresponding integrating factors, and from these we construct the integrals of motion and then we do extend the analysis for the case $I_t\neq 0$.

A. The case $I_t=0$

1. Null forms

In this case one can easily fix the null form S from the first equation in (21) as

$$S=\frac{-\phi}{\dot{x}}=-\frac{((k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1x)}{\dot{x}}. \tag{26}$$

2. Integrating factors

Substituting this form of S, given in (26), into (23), we get

$$\dot{x}R_x-((k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1x)R_{\dot{x}}=\left((k_1x+k_2)+\frac{((k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1x)}{\dot{x}}\right)R. \tag{27}$$

Equation (27) is a first-order linear partial differential equation with variable coefficients. As we noted earlier any particular solution is sufficient to construct an integral of motion (along with the function S). To seek a particular solution for R one can make a suitable Ansatz instead of looking for the general solution. We assume R to be of the form

$$R=\frac{\dot{x}}{(A(x)+B(x)\dot{x})^r}, \tag{28}$$

where A and B are functions of their arguments, and r is a constant which are all to be determined. We demand the above form of Ansatz (28), due to the following reason. To deduce the first integral I we assume a rational form for I, that is, $I=[f(x,\dot{x})]/[g(x,\dot{x})]$, where f and g are arbitrary functions of x and $\dot{x}$ and are independent of t. Since we already assumed that I is independent of t, we have $I_x=(f_xg-fg_x)/g^2$ and $I_{\dot{x}}=(f_{\dot{x}}g-fg_{\dot{x}})/g^2$. From (21) one can see that $R=I_{\dot{x}}=(f_{\dot{x}}g-fg_{\dot{x}})/g^2$, $S=I_x/I_{\dot{x}}=(f_xg-fg_x)/(f_{\dot{x}}g-fg_{\dot{x}})$, and $RS=I_x$, so that the denominator of the function S should be the numerator of the function R. Since the denominater of S is $\dot{x}$ [*vide* Eq. (26)] we fixed the numerator of R as $\dot{x}$. To seek a suitable function in the denominator initially one can consider an arbitrary form $R=\dot{x}/[h(x,\dot{x})]$. However, it is difficult to proceed with this choice of h. So, let us assume that $h(x,\dot{x})$ is a function which is polynomial in $\dot{x}$. To begin with let us consider the case where h is linear in $\dot{x}$, that is, $h=A(x)+B(x)\dot{x}$. Since R is in rational form while taking differentiation or integration the form of the denominator remains the same but the power of the denominator decreases or increases by a unit order from that of the initial one. So, instead of considering h to be of the form $h=A(x)+B(x)\dot{x}$, one may consider a more general form $h=(A(x)+B(x)\dot{x})^r$, where r is a constant to be determined. Such a generalized form of h and so R leads to several new integrable cases as we see below.

Substituting (28) into (27) and solving the resultant equations, we arrive at the relation

$$r(\dot{x}(A_x + B_x\dot{x}) + \phi B) = (A + B\dot{x})\phi_{\dot{x}}. \tag{29}$$

Solving Eq. (29) with $\phi = -((k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1 x)$, we find nontrivial forms for the functions A and B for two choices, namely (i) k_1, k_2 arbitrary and (ii) k_1=arbitrary, $k_2=0$ with restrictions on other parameters as given below. The respective forms of the functions and the restriction on the parameters are

(i) k_1, k_2: arbitrary

$$A(x) = \frac{(r-1)b_0}{r}\left(\frac{k_1}{2}x^2 + k_2x\right), \quad B(x) = b_0 = \text{constant}, \quad r = \text{constant},$$

$$k_3 = \frac{b_0(r-1)}{2r^2}k_1^2, \quad k_4 = \frac{3b_0(r-1)}{2r^2}k_1k_2, \quad \lambda_1 = \frac{b_0(r-1)k_2^2}{r^2}, \tag{30a}$$

(ii) k_1=arbitrary, $k_2=0$

$$A(x) = \frac{(r-1)b_0}{2r}k_1x^2 + \frac{r\lambda_1}{k_1}, \quad B(x) = b_0,$$

$$k_3 = \frac{b_0(r-1)}{2r^2}k_1^2, \quad k_4 = 0, \quad \lambda_1 = \text{arbitrary parameter (here)}. \tag{30b}$$

We note that the case (ii) cannot be derived from case (i) by taking $k_2=0$. For example, choosing $k_2=0$ in (30a) we get not only $k_4=0$ but also $\lambda_1=0$, whereas in the case (ii) we have the freedom λ_1=arbitrary, so the cases (30a) and (30b) are to be treated as separate. Making use of the forms of A and B from Eqs. (30a) and (30b) into (28), the integrating factor, "R," for the two cases can be obtained as

(i) k_1, k_2: arbitrary

$$R = \frac{\dot{x}}{\left[\frac{(r-1)}{r}\left(\frac{k_1}{2}x^2 + k_2x\right) + \dot{x}\right]^r}, \quad r \neq 0 \tag{31a}$$

(ii) k_1=arbitrary, $k_2=0$

$$R = \frac{\dot{x}}{\left[\frac{(r-1)}{2r}k_1x^2 + \frac{r\lambda_1}{k_1} + \dot{x}\right]^r}, \quad r \neq 0. \tag{31b}$$

We note that b_0 is a common parameter in the above and it is absorbed in the definition of R; see Eqs. (23) and (24). While deriving the above forms of R [Eqs. (31a) and (31b)] we assumed that $r \neq 0$ and for the choice $r=0$ we obtain a consistent solution only if both the parameters k_1 and k_2 become zero. Of course, this subcase can be treated as a trivial one since when $k_1, k_2=0$ the damping term in Eq. (10) vanishes and the system becomes an integrable anharmonic oscillator. In this trivial case we have the integrating factor of the form

(iii) k_1, $k_2=0$

$$R = \dot{x}, \quad r = 0. \tag{31c}$$

Finally, one has to check the compatibility of forms S and R with the third Eq. (24). We indeed verified that the sets

$$\text{(i)} \quad S = -\frac{\left((k_1x+k_2)\dot{x} + \frac{(r-1)}{r^2}\left(\frac{k_1^3}{2}x^2 + \frac{3k_1k_2}{2}x^2 + k_2^2x\right)\right)}{\dot{x}},$$

$$R = \frac{\dot{x}}{\left(\frac{(r-1)}{r}\left(\frac{k_1}{2}x^2 + k_2x\right) + \dot{x}\right)^r}, \quad k_1,k_2 = \text{arbitrary}, \quad r \neq 0 \tag{32a}$$

$$\text{(ii)} \quad S = -\frac{\left(k_1x\dot{x} + \frac{(r-1)}{2r^2}k_1^2x^3 + \lambda_1x\right)}{\dot{x}},$$

$$R = \frac{\dot{x}}{\left(\frac{(r-1)}{2r}k_1x^2 + \frac{r\lambda_1}{k_1} + \dot{x}\right)^r}, \quad k_1 = \text{arbitrary}, \quad k_2 = 0, \quad r \neq 0 \tag{32b}$$

and

$$\text{(iii)} \quad S = -\frac{(k_3x^3 + k_4x^2 + \lambda_1x)}{\dot{x}}, \quad R = \dot{x}, \quad k_1,k_2 = 0, \tag{32c}$$

satisfy Eq. (24) individually. As a consequence all three pairs form compatible sets of solution for the equations (22)–(24).

3. Integrals of motion

Having determined the explicit forms of S and R, one can proceed to construct integrals of motion using the expressions (25). The parametric restrictions (30a) and (30b) fix the equation of motion (10) to the following specific forms:

$$\text{(i)} \quad \ddot{x} + (k_1x+k_2)\dot{x} + \frac{(r-1)}{2r^2}(k_1^2x^3 + 3k_1k_2x^2 + 2k_2^2x) = 0, \quad r \neq 0, \tag{33a}$$

$$\text{(ii)} \quad \ddot{x} + k_1x\dot{x} + \frac{(r-1)k_1^2}{2r^2}x^3 + \lambda_1x = 0, \quad r \neq 0, \tag{33b}$$

$$\text{(iii)} \quad \ddot{x} + k_3x^3 + k_4x^2 + \lambda_1x = 0, \quad r = 0. \tag{33c}$$

In the above k_1, k_2, k_3, k_4, λ_1, and r are arbitrary parameters.

We note that the transformation $x = y - k_2/k_1$ transforms Eq. (33a) to the form

$$\ddot{y} + k_1y\dot{y} + \frac{(r-1)k_1^2}{2r^2}y^3 - \frac{(r-1)k_2^2}{2r^2}y = 0, \quad r \neq 0. \tag{34}$$

Equation (34) is obtained from Eq. (33b) by fixing $\lambda_1 = -[(r-1)k_2^2]/2r^2$. So, hereafter, we consider Eq. (33a) as a special case of Eq. (33b) and so discuss only Eq. (33b) as the general one. It may be noted that Eq. (33b) includes several known integrable cases. For example, the choice $r=3$ and $\lambda_1=0$ in Eq. (33b) yields the MEE.[19] On the other hand the choice $r=-1$ leads us to the equation $\ddot{x}+k_1x\dot{x}-k_1^2x^3+\lambda_1x=0$, which can be solved in terms of Weierstrass elliptic function.[21] *The other choices of r lead to new integrable cases* as we see below.

Substituting the forms of S and R [vide Eqs. (32b) and (32c)] into the general form of the integral of motion (25) and evaluating the resultant integrals, we obtain the following time independent first integrals for the cases (33b) and (33c):

$$\text{(iia)}\quad I_1=\left(\dot{x}+\frac{(r-1)}{2r}k_1x^2+\frac{r\lambda_1}{k_1}\right)^{-r}\left[\dot{x}\left(\dot{x}+\frac{k_1}{2}x^2+\frac{r^2\lambda_1}{(r-1)k_1}\right)+\frac{(r-1)}{r^2}\left(\frac{k_1}{2}x^2+\frac{r^2\lambda_1}{(r-1)k_1}\right)^2\right],\quad r\neq 0,1,2, \tag{35a}$$

$$\text{(iib)}\quad I_1=\frac{4k_1\dot{x}}{k_1^2x^2+4k_1\dot{x}+8\lambda_1}-\log(k_1^2x^2+4k_1\dot{x}+8\lambda_1),\quad r=2, \tag{35b}$$

$$\text{(iic)}\quad I_1=\dot{x}+\frac{k_1}{2}x^2-\frac{\lambda_1}{k_1}\log(k_1\dot{x}+\lambda_1),\quad r=1, \tag{35c}$$

$$\text{(iii)}\quad I_1=\frac{\dot{x}^2}{2}+\frac{k_3}{4}x^4+\frac{k_4}{3}x^3+\frac{\lambda_1}{2}x^2,\quad r=0. \tag{35d}$$

Note that in Eq. (35a), r can take any real value, except 0, 1, 2. In the above integrals I_1 given by Eqs. (35a)–(35c) correspond to the ODE (33b), while (35d) corresponds to Eq. (33c).

Due to the fact that the integrals of motion (35) are time independent, one can look for a Hamiltonian description for the respective equations of motion. In fact, we obtain the explicit Hamiltonian forms for all the above cases.

4. Hamiltonian description of (35)

Assuming the existence of a Hamiltonian

$$I(x,\dot{x})=H(x,p)=p\dot{x}-L(x,\dot{x}), \tag{36}$$

where $L(x,\dot{x})$ is the Lagrangian and p is the canonically conjugate momentum, we have

$$\frac{\partial I}{\partial\dot{x}}=\frac{\partial H}{\partial\dot{x}}=\frac{\partial p}{\partial\dot{x}}\dot{x}+p-\frac{\partial L}{\partial\dot{x}}=\frac{\partial p}{\partial\dot{x}}\dot{x},$$

$$\frac{\partial I}{\partial x}=\frac{\partial H}{\partial x}=\frac{\partial p}{\partial x}\dot{x}-\frac{\partial L}{\partial x}. \tag{37}$$

From (37) we identify

$$p=\int\frac{I_{\dot{x}}}{\dot{x}}\mathrm{d}\dot{x},$$

$$L=\int(p_x\dot{x}-I_x)\mathrm{d}x+\int\left[p-\frac{\mathrm{d}}{\mathrm{d}\dot{x}}\int(p_x\dot{x}-I_x)\mathrm{d}x\right]\mathrm{d}\dot{x}. \tag{38}$$

Plugging the expressions (36) into (38), one can evaluate the canonically conjugate momentum and the associated Lagrangian as well as the Hamiltonian. They read as follows:

(a) The canonical momenta:

$$\text{(iia,b)}\quad p=\frac{1}{r-1}\left(\dot{x}+\frac{(r-1)}{r}\frac{k_1}{2}x^2+\frac{r\lambda_1}{k_1}\right)^{1-r},\quad r\neq 0,1 \tag{39a}$$

$$\text{(iic)} \quad p = \log(k_1\dot{x} + \lambda_1), \quad r = 1 \tag{39b}$$

$$\text{(iii)} \quad p = \dot{x}, \quad r = 0. \tag{39c}$$

[Note in the above $r=2$ is included in Eq. (39a) itself.]

(b) The Lagrangian:

$$\text{(iia)} \quad L = \frac{1}{(2-r)(r-1)}\left(\dot{x} + \frac{(r-1)}{r}\frac{k_1x^2}{2} + \frac{r\lambda_1}{k_1}\right)^{2-r}, \quad r \neq 0,1,2 \tag{40a}$$

$$\text{(iib)} \quad L = \log(4k_1\dot{x} + 8\lambda_1 + k_1^2x^2), \quad r = 2 \tag{40b}$$

$$\text{(iic)} \quad L = \frac{\lambda_1}{k_1}\log(k_1\dot{x} + \lambda_1) + \dot{x}(\log(k_1\dot{x} + \lambda_1) - 1) - \frac{1}{2}k_1x^2, \quad r = 1 \tag{40c}$$

$$\text{(iii)} \quad L = \frac{\dot{x}^2}{2} - \frac{k_3}{4}x^4 - \frac{k_4}{3}x^3 - \frac{\lambda_1}{2}x^2, \quad r = 0. \tag{40d}$$

(c) The Hamiltonian:

$$\text{(iia)} \quad H = \left[\frac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)} - p\left(\frac{(r-1)}{2r}k_1x^2 + \frac{r\lambda_1}{k_1}\right)\right], \quad r \neq 0,1,2 \tag{41a}$$

$$\text{(iib)} \quad H = \frac{2\lambda_1}{k_1}p + \frac{k_1}{4}x^2p + \log\left(\frac{4k_1}{p}\right), \quad r = 2 \tag{41b}$$

$$\text{(iic)} \quad H = \frac{1}{k_1}\left(e^p - \lambda_1 p + \frac{k_1^2}{2}x^2 - \lambda_1\right), \quad r = 1 \tag{41c}$$

$$\text{(iii)} \quad H = \frac{p^2}{2} + \frac{k_3}{4}x^4 + \frac{k_4}{3}x^3 + \frac{\lambda_1}{2}x^2, \quad r = 0. \tag{41d}$$

One can check that the Hamilton's equations of motion are indeed equivalent to the appropriate equation (10).

Since Eqs. (33b) and (33c) admit time-independent Hamiltonians, they can be classified as Liouville integrable systems. *The important fact we want to stress here is that for arbitrary values of r, including fractional values, Eq. (33b) is integrable*.

5. Canonical transformation for the Hamiltonian Eqs. (41)

Interestingly, we also identified suitable canonical transformation to standard particle in a potential description for the Hamiltonians (41). Now, introducing the canonical transformations

$$x = \frac{2rP}{k_1U}, \quad p = -\frac{k_1U^2}{4r}, \quad r \neq 0,1, \tag{42}$$

$$x = \frac{P}{k_1}, \quad p = -k_1U, \quad r = 1 \tag{43}$$

the Hamiltonian H in Eq. (41) can be recast in the standard form (after rescaling)

$$H=\begin{cases}\dfrac{1}{2}P^2+\dfrac{(1-r)}{(r-2)}\left(\dfrac{(r-1)k_1U^2}{4r}\right)^{(r-2)/(r-1)}+\dfrac{(r-1)\lambda_1}{4}U^2, & r\neq 0,1,2\\ \dfrac{1}{2}P^2+\dfrac{\lambda_1}{4}U^2+\log\left(\dfrac{32}{U^2}\right), & r=2\\ \dfrac{1}{2}P^2+e^{-k_1U}+\lambda_1k_1U, & r=1\\ \dfrac{1}{2}P^2+\dfrac{k_3}{4}U^4+\dfrac{\lambda_1}{2}U^2, & r=0.\end{cases} \tag{44}$$

It is straightforward to check that when U and P are canonical so are x and p (and vice versa), and the corresponding equations of motion turn out to be

$$\ddot{U}-2\left(\frac{(r-1)k_1}{4r}\right)^{(2-r)/(1-r)}U^{(3-r)/(1-r)}+\frac{(r-1)\lambda_1}{2}U=0,\quad r\neq 0,1 \tag{45a}$$

$$\ddot{U}-k_1e^{-U}+k_1\lambda_1=0,\quad r=1 \tag{45b}$$

$$\ddot{U}+k_3U^3+\lambda_1U=0,\quad r=0. \tag{45c}$$

One may note that the equations of motion now become standard-type anharmonic oscillator equations.

B. The case $I_t\neq 0$

In the previous subsection we considered the case $I_t=0$. As a consequence S turns out to be $-\phi/\dot{x}$. However, in the case $I_t=0$, the function S has to be determined from Eq. (22), that is,

$$S_t+\dot{x}S_x-((k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1x)S_{\dot{x}}=(k_1\dot{x}+3k_3x^2+2k_4x+\lambda_1)-(k_1x+k_2)S+S^2. \tag{46}$$

Since it is too difficult to solve Eq. (46) for its general solution, we seek a particular solution for S, which is sufficient for our purpose. In particular, we seek a simple rational expression for S in the form

$$S=\frac{a(t,x)+b(t,x)\dot{x}}{c(t,x)+d(t,x)\dot{x}}, \tag{47}$$

where a, b, c, and d are arbitrary functions of t and x which are to be determined. Of course, the analysis of this form alone does not exhaust all possible cases of interest. We hope to make a more exhaustive study of Eq. (46) separately. Substituting (47) into (46) and equating the coefficients of different powers of $\dot{x}$ to zero, we get

$$db_x-bd_x-k_1d^2=0,$$

$$db_t-bd_t+cb_x-bc_x+a_xd-ad_x-2k_1cd-(3k_3x^2+2k_4x+\lambda_1)d^2+(k_1x+k_2)bd-b^2=0,$$

$$cb_t-bc_t+da_t-ad_t+ca_x-ac_x-k_1c^2-2(3k_3x^2+2k_4x+\lambda_1)cd+2(k_1x+k_2)ad-2ab=0,$$

$$ca_t - ac_t - (k_3x^3 + k_4x^2 + \lambda_1 x)(bc - ad) - (3k_3x^2 + 2k_4x + \lambda_1)c^2 + (k_1x + k_2)ac - a^2 = 0. \tag{48}$$

The determining equation for the functions a, b, c, and d have now turn out to be nonlinear. To solve these equations we further assume that the functions a, b, c, and d are polynomials in x with coefficients which are arbitrary functions in t. Substituting these forms into Eqs. (48) we obtain another enlarged set of determining equations for the unknowns and solving the latter consistently we obtain nontrivial solutions for the functions a, b, c, and d for four sets of parametric choices. We present the explicit forms of the associated null function S given by (47) and the parametric restrictions in Table I.

Now substituting the forms of S into Eq. (23) and solving the resultant equation, we obtain the corresponding forms of R. To solve the determining equation for R we again seek the same form of Ansatz (28) but with explicit t dependence on the coefficient functions, that is, $R = S_d/[(A(t,x)+B(t,x)\dot{x})^r]$, where S_d is the denominator of S. We report the resultant forms of R in Table I. Once S and R are determined then one has to verify the compatibility of this set (S,R) with the extra constraint Eq. (24). We find that the forms S and R given in Table I do satisfy the extra constraint equation and form a compatible solution. Now substituting S_i's and R_i's into Eq. (25) one can construct the associated integrals of motion. We report the integrals of motion (I) in Table I along with the forms S and R.

At this stage, we note that the first integral for the case (i) with $k_2, \lambda_1 = 0$ has been derived in Ref. 19 through Lie symmetry analysis. However, recently, we have derived[9] the first integral for arbitrary values of k_2 and λ_1. Case (ii) is new to the literature. The first integral for case (iii) was reported recently in Refs. 9, 12, and 13. The first integral for the case (iva) is new to the literature. The *case* $r=0$ discussed as (ivb) is nothing but the force-free Duffing oscillator whose integrability has been discussed in Refs. 12 and 14.

Since we obtained only one integral in each case [except case (i), where we have found a second explicit time-dependent integral; see Ref. 9], which are also time-dependent ones, we need to integrate them further to obtain the second integration constant and prove the complete integrability of the respective systems, which is indeed a difficult task.

In this connection we have introduced a new method[1,9] which can be effectively used to transform the time-dependent integral into a time-independent one, for a class of problems, so that the latter can be integrated easily. We invoke this procedure here in order to integrate the time-dependent first integrals and obtain the general solution for all the cases in Table I [except case (iv), see below]. For case (iv), we prove the Liouville integrability of it.

C. Method of transforming time-dependent first integral to time-independent one

Let us assume that there exists a first integral for Eq. (10) of the form

$$I = F_1(t,x,\dot{x}) + F_2(t,x). \tag{49}$$

Now let us split the function F_1 further in terms of two functions such that F_1 itself is a function of the product of the two functions, say, a perfect differentiable function $(\mathrm{d}/\mathrm{d}t)G_1(t,x)$ and another function $G_2(t,x,\dot{x})$, that is,

$$I = F_1\left(\frac{1}{G_2(t,x,\dot{x})}\frac{\mathrm{d}}{\mathrm{d}t}G_1(t,x)\right) + F_2(G_1(t,x)), \tag{50}$$

where F_1 is a function which involves the variables t, x, and $\dot{x}$, whereas F_2 should involve only the variable t and x. We note that while rewriting Eq. (49) in the form (50), we demand the function $F_2(t,x)$ in (49) automatically to be a function of $G_1(t,x)$. Now identifying the function G_1 as the new dependent variable and the integral of G_2 over time as the new independent variable, that is,

TABLE I. Parametric restrictions, null forms (S), integrating factors (R) and time dependent integrals of motion (I) of $\ddot{x}+(k_1x+k_2)\dot{x}+k_3x^3+k_4x^2+\lambda_1x=0$ (identified with the assumed Ansatz form of S and R).

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(i)	$k_3=\frac{k_1^2}{9}, \quad k_4=\frac{k_1k_2}{3}$ (k_1,k_2,λ_1: arbitrary)	$\frac{\left(\frac{k_1}{3}x^2-\dot{x}\right)}{x}$	$\frac{xe^{\mp\omega t}}{\left(\dot{x}-\frac{(k_2\pm\omega)}{2}x+\frac{k_1}{3}x^2\right)^2}$	(a) $I=e^{\mp\omega t}\left(\frac{3\dot{x}-\frac{3(-k_2\mp\omega)}{2}x+k_1x^2}{3\dot{x}-\frac{3(-k_2\pm\omega)}{2}x+k_1x^2}\right)$, $k_2,\lambda_1\neq 0, \quad \omega=(k_2^2-4\lambda_1)^{1/2}$ (b) $I=-t+\frac{x}{\left(\frac{k_2}{2}x+\frac{k_1}{3}x^2+\dot{x}\right)}, \quad k_2^2=4\lambda_1$
(ii)	$k_3=0, k_4=\frac{k_1}{4}(k_2\pm\omega)$, ($k_1,k_2,\lambda_1$: arbitrary)	$\frac{1}{2}(k_2\mp\omega)+k_1x$,	$e^{[(k_2\pm\omega)/2]t}$	$I=\left(\dot{x}+\frac{k_2\mp\omega}{2}x+\frac{k_1}{2}x^2\right)e^{[(k_2\pm\omega)/2]t}$, $\omega=(k_2^2-4\lambda_1)^{1/2}$
(iii)	$k_1,k_3=0, \quad \lambda_1=\frac{6k_2^2}{25}$ (k_2,k_4: arbitrary)	$\frac{\left(\frac{2k_2\dot{x}}{5}+\frac{4k_2^2x}{25}+k_4x^2\right)}{\left(\dot{x}+\frac{2k_2}{5}x\right)}$	$\left(\dot{x}+\frac{2k_2}{5}x\right)e^{(6/5)k_2t}$	$I=e^{(6/5)k_2t}\left(\frac{\dot{x}^2}{2}+\frac{2k_2}{5}x\dot{x}+\frac{2k_2^2}{25}x^2+\frac{k_4}{3}x^3\right)$

TABLE I. (*Continued.*)

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(iva)	$k_3=\frac{(r-1)k_1^2}{2r^2}, \quad k_4=\frac{k_1k_2}{3},$ $\lambda_1=\frac{2k_2^2}{9}, \quad r\neq 0$ (k_1,k_2,r: arbitrary)	$\frac{k_2}{3}+k_1x+\frac{3k_3x^3}{(3\dot{x}+k_2x)}$	$\frac{(k_2x+3\dot{x})e^{[2(2-r)k_2/3]t}}{\left(\frac{k_2}{3}x+rk_3x^2+\dot{x}\right)^r}$	$I=\left(\frac{k_3}{2}x^4+\left(\dot{x}+\frac{k_2}{3}x\right)\left(\dot{x}+\frac{k_2}{3}x+\frac{k_1}{2}x^2\right)\right)$ $\times\left(\dot{x}+\frac{k_2}{3}x+rk_3x^2\right)^{-r}e^{[(2(2-r))/3]k_2t}, \quad r\neq 2$
				$I=\frac{2}{3}k_2t+\log(4k_2x+3k_1x^2+12\dot{x})$ $-\frac{4(k_2x+3\dot{x})}{(4k_2x+3k_1x^2+12\dot{x})}, \quad r=2$
(ivb)	$k_1=0, \quad k_4=0,$ $\lambda_1=\frac{2k_2^2}{9}, \quad r=0$ (k_2,k_3: arbitrary)	$\frac{\left(\frac{k_2}{3}\dot{x}+\frac{k_2^2}{9}x+k_3x^3\right)}{\left(\dot{x}+\frac{k_2x}{3}\right)}$	$e^{(4/3)k_2t}\left(\dot{x}+\frac{k_2x}{3}\right)$	$I=e^{(4/3)k_2t}\left[\frac{\dot{x}^2}{2}+\frac{k_2}{3}x\dot{x}+\frac{k_2^2}{18}x^2+\frac{k_3}{4}x^4\right]$

$$w = G_1(t,x), \quad z = \int_o^t G_2(t',x,\dot{x})\mathrm{d}t', \tag{51}$$

one indeed obtains an explicit transformation to remove the time-dependent part in the first integral. We note here that the integration on the right-hand side of (51) leading to z can be performed provided the function G_2 is an exact derivative of t, that is, $G_2=(\mathrm{d}/\mathrm{d}t)z(t,x)=\dot{x}z_x+z_t$, so that z turns out to be a function t and x alone. In terms of the new variables, Eq. (50) can be modified to the form

$$I = F_1\left(\frac{\mathrm{d}w}{\mathrm{d}z}\right) + F_2(w). \tag{52}$$

In other words,

$$F_1\left(\frac{\mathrm{d}w}{\mathrm{d}z}\right) = I - F_2(w). \tag{53}$$

Now rewriting Eq. (52), one obtains a separable equation

$$\frac{\mathrm{d}w}{\mathrm{d}z} = f(w), \tag{54}$$

which can lead to the solution after an integration. Now rewriting the solution in terms of the original variables one obtains a general solution for the given equation.

In the following, using the above idea we integrate the first integrals given in Table I and deduce the second integration constant and general solution.

D. Application

Case (ia): $k_3=k_1^2/9$, $k_4=k_1k_2/3$, k_1, k_2 and λ_1: arbitrary.

The parametric restrictions given above fix the equation of motion (10) in the form

$$\ddot{x} + (k_1x + k_2)\dot{x} + \frac{k_1^2}{9}x^3 + \frac{k_1k_2}{3}x^2 + \lambda_1 x = 0. \tag{55}$$

Let us rewrite the first integral associated for this case [*vide* case (i) in Table I] in the form

$$I_1 = -\frac{k_1 e^{[(k_2\mp\omega)/2]t}x^2}{(3\dot{x} - [(-k_2\pm\omega)/2]3x + k_1x^2)}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\left(\frac{-3}{k_1x} + \frac{-k_2\pm\omega}{2\lambda_1}\right)e^{[(-k_2\mp\omega)/2]t}\right)\right], \tag{56}$$

where $\omega=\sqrt{k_2^2-4\lambda_1}$. Comparing this with Eq. (50), and using (51), we obtain

$$w = \left(\frac{-3}{k_1x} + \frac{-k_2\pm\omega}{2\lambda_1}\right)e^{[(-k_2\mp\alpha)/2]t}, \quad z = \left(\frac{-3}{k_1x} + \frac{-k_2\mp\omega}{2\lambda_1}\right)e^{[(-k_2\pm\omega)/2]t}. \tag{57}$$

Substituting (57) into Eq. (55), the latter becomes the free particle equation, namely, $\mathrm{d}^2w/\mathrm{d}z^2=0$, whose general solution is $w=I_1z+I_2$, where I_1 and I_2 are integration constants. Rewriting w and z in terms of x and t, one gets

$$x(t) = \left(\frac{6\lambda_1(1-I_1e^{\omega t})}{k_1\omega(1+I_1e^{\omega t}) - (k_2\pm\omega)I_2e^{[(k_2\pm\omega)/2]t} - k_1k_2(1-I_1e^{\omega t})}\right), \tag{58}$$

where $\omega=\sqrt{k_2^2-4\lambda_1}$.

Interestingly one can consider several subcases. In the following we discuss some important ones which are being widely discussed in the current literature. In particular, the difference in

dynamics arises mainly depending on the sign of the parameter α $(=\sqrt{k_2^2-4\lambda_1})$. We consider the cases (i) $k_2^2<4\lambda_1$; (ii) $k_2^2>4\lambda_1$; and (iii) $k_2^2=4\lambda_1$ separately. The restriction $k_2^2<4\lambda_1$ reduces the solution (58) to the form[4]

$$x(t)=\frac{A\cos(\omega_0 t+\delta)}{\left(e^{(k_2/2)t}+\frac{2k_1A}{3(k_2^2+4\omega_0^2)}(2\omega_0\sin(\omega_0 t+\delta)-k_2\cos(\omega_0 t+\delta))\right)}, \tag{59}$$

where $\omega_0=\sqrt{4\lambda_1-k_2^2}/2$ and δ, A are arbitrary constants. A further restriction $k_2=0$ gives us the purely sinusoidally oscillating solution[20]

$$x(t)=\frac{A\sin(\omega_0 t+\delta)}{1-\left(\frac{k}{3\omega_0}\right)A\cos(\omega_0 t+\delta)}, \quad 0\leqslant A<\frac{3\omega_0}{k}, \quad \omega_0=\sqrt{\lambda_1}, \tag{60}$$

where A and δ are arbitrary constants. The associated equation of motion, namely $\ddot{x}+k_1x\dot{x}+(k_1^2/9)x^3+\lambda_1x=0$, admits very interesting nonlinear dynamics; see for example in Ref. 20.

On the other hand, in the limit $k_2^2>4\lambda_1$ the solution looks like a dissipative/frontlike one.[19] A further restriction $\lambda_1=0$ takes us to the solution of the form[11]

$$x(t)=\left(\frac{3k_2(I_1e^{k_2t}-1)}{k_1+k_2(3I_2+k_1I_1t)e^{k_2t}}\right). \tag{61}$$

Case (ib): $k_3=k_1^2/9$, $k_4=k_1k_2/3$, $k_2^2=4\lambda_1$, k_1 and k_2: arbitrary.

The third choice $k_2^2=4\lambda_1$ in (58) leads us to the solution

$$x(t)=\left(\frac{3(I_1+t)}{3I_2e^{(k_2/2)t}-\frac{2k_1}{k_2^2}(2+I_1k_2+k_2t)}\right). \tag{62}$$

Further parametric restriction k_2, $\lambda_1=0$ provides us the general solution of the form

$$x(t)=\left(\frac{6(I_1+t)}{k_1(I_1+t)^2+6I_2}\right). \tag{63}$$

The underlying equation, that is, $\ddot{x}+k_1x\dot{x}+(k_1^2/9)x^3=0$, is the $l=1$ integrable case of Eq. (6) with the solution (7) (see for example in Refs. 19 and 20).

Case (ii): $k_3=0$, $k_4=(k_1/4)(k_2\pm\sqrt{k_2^2-4\lambda_1})$, k_1, k_2, and λ_1: arbitrary.

In this case we have the equation of the form

$$\ddot{x}+(k_1x+k_2)\dot{x}+\frac{k_1}{4}(k_2\pm\sqrt{k_2^2-4\lambda_1})x^2+\lambda_1x=0. \tag{64}$$

The associated first integral reads [*vide* case (ii) in Table I]

$$I=\left(\dot{x}+\frac{k_2\mp\sqrt{k_2^2-4\lambda_1}}{2}x+\frac{k_1}{2}x^2\right)e^{[(k_2\pm\sqrt{k_2^2-4\lambda_1})/2]t}. \tag{65}$$

Note that Eq. (65) can be rewritten as a Riccati equation of the form[22]

$$\dot{x}=Ie^{[(-k_2\mp\sqrt{k_2^2-4\lambda_1})/2]t}-\left(\frac{k_2\mp\sqrt{k_2^2-4\lambda_1}}{2}\right)x-\frac{k_1}{2}x^2. \tag{66}$$

The general solution of the Riccati equation is known to be free from movable critical points and satisfies the Painlevé property. In this sense Eq. (64) can be considered as integrable in the Painlevé criteria sense. However, in the general case (66), it is not clear whether it can be

explicitly integrated further. However, for the special case $\lambda_1=2k_2^2/9$ it can be integrated as follows.

The restriction $\lambda_1=2k_2^2/9$ fixes the equation of motion (64) and the first integral (65) in the forms

$$\ddot{x}+(k_1x+k_2)\dot{x}+\frac{k_1k_2}{3}x^2+\frac{2k_2^2}{9}x=0, \tag{67}$$

and

$$I=\left(\dot{x}+\frac{k_2}{3}x+\frac{k_1}{2}x^2\right)e^{(2k_2/3)t}, \tag{68}$$

respectively. Now rewriting (68) in the form (50), we get

$$I=e^{(k_2/3)t}\left(\frac{d}{dt}(xe^{(k_2/3t)})\right)+\frac{k_1}{2}(xe^{(k_2/3)t})^2. \tag{69}$$

Identifying the dependent and independent variables from (69) and using the identities (51), we obtain the transformation

$$w=xe^{(k_2/3)t}, \quad z=-\frac{3}{k_2}e^{-(k_2/3)t}. \tag{70}$$

Using the transformation (70), the first integral (68) can be rewritten in the form

$$\hat{I}=w'+\frac{k_1}{2}w^2, \tag{71}$$

which in turn leads to the solution by an integration, that is,

$$w(z)=\sqrt{\frac{2I}{k_1}}\tanh\left[\sqrt{\frac{k_1I}{2}}(z-z_0)\right], \tag{72}$$

where z_0 is arbitrary constant. Rewriting (72) in terms of old variables we get

$$x(t)=\sqrt{\frac{2I}{k_1}}e^{-(k_2/3)t}\tanh\left[\frac{3}{k_2}\left(\sqrt{\frac{k_1I}{2}}\right)(e^{-(k_2/3)t_0}-e^{-(k_2/3)t})\right], \tag{73}$$

where t_0 is the second integration constant.

Case (iii): k_1, $k_3=0$, $\lambda_1=6k_2^2/25$, k_2 and k_4: arbitrary.

The corresponding equation of motion is

$$\ddot{x}+k_2\dot{x}+k_4x^2+\frac{6k_2^2}{25}x=0. \tag{74}$$

Rewriting the associated first integral I_1, given in case (iii) in Table I, in the form (49), we get

$$I=\frac{1}{2}\left(\dot{x}+\frac{2k_2}{5}x\right)^2e^{(6/5)k_2t}+\frac{k_4}{3}x^3e^{(6/5)k_2t}. \tag{75}$$

Now splitting the first term in Eq. (75) further in the form (50), we obtain

$$I = e^{2k_2t/5}\left(\frac{d}{dt}\left(\frac{1}{\sqrt{2}}xe^{2k_2t/5}\right)\right)^2 + \frac{k_4}{3}(xe^{(2/5)k_2t})^3. \tag{76}$$

Identifying the dependent and independent variables from (76) and using the relations (51), we obtain the transformation

$$w = \frac{1}{\sqrt{2}}xe^{2k_2t/5}, \quad z = -\frac{5}{k_2}e^{-(k_2t/5)}. \tag{77}$$

Using this transformation (77), the first integral (75) can be rewritten in the form

$$\hat{I} = w'^2 + \frac{\hat{k}_4}{3}w^3, \tag{78}$$

where $\hat{k}_4 = 2\sqrt{2}k_4$, which in turn leads to

$$w'^2 = 4w^3 - g_3, \tag{79}$$

where $z = 2\sqrt{3/\hat{k}_4}\hat{z}$ and $g_3 = -12I_1/\hat{k}_4$. The solution of this differential equation can be represented in terms of the Weierstrass function[12,13] $\varrho(\hat{z};0,g_3)$.

Case (iv): $k_3 = [(r-1)/2r^2]k_1^2$, $k_4 = k_1k_2/3$, $\lambda_1 = 2k_2^2/9$, k_1, k_2, and r: arbitrary (but not zero).

The above parameters fix the equation of motion (10) in the form

$$\ddot{x} + (k_1x + k_2)\dot{x} + \frac{(r-1)k_1^2}{2r^2}x^3 + \frac{k_1k_2}{3}x^2 + \frac{2k_2^2}{9}x = 0, \quad r \neq 0. \tag{80}$$

The associated first integral reads [*vide* case (iva) in Table I]

$$I = \begin{cases} \left(\frac{(r-1)}{4r^2}k_1^2x^4 + \left(\dot{x} + \frac{k_2}{3}x\right)\left(\dot{x} + \frac{k_2}{3}x + \frac{k_1}{2}x^2\right)\right)\left(\dot{x} + \frac{k_2}{3}x + \frac{(r-1)}{2r}k_1x^2\right)^{-r} e^{[2(2-r)/3]k_2t}, & r \neq 0,2 \\ \frac{2}{3}k_2t + \log(4k_2x + 3k_1x^2 + 12\dot{x}) - \frac{4(k_2x + 3\dot{x})}{(4k_2x + 3k_1x^2 + 12\dot{x})}, & r = 2. \end{cases} \tag{81}$$

Rewriting Eq. (81) in the form (50), we get

$$I = \begin{cases} \left(\frac{(r-1)k_1^2}{4r^2}(xe^{(k_2/3)t})^4 + \frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})\left(\frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})e^{(k_2/3)t} + \frac{k_1}{2}(xe^{(k_2/3)t})^2\right)e^{(k_2/3)t}\right) \\ \quad \times \left(\frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})e^{(k_2/3)t} + \frac{k_1(r-1)}{2r}(xe^{(k_2/3)t})^2\right)^{-r}, & r \neq 0,2 \\ \frac{4\frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})e^{(k_2/3)t}}{k_1(xe^{(k_2/3)t})^2 + 4\frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})e^{(k_2/3)t}} - \log\left(k_1(xe^{(k_2/3)t})^2 + 4\frac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/3)t})e^{(k_2/3)t}\right), & r = 2. \end{cases} \tag{82}$$

Identifying the dependent and independent variables from (82) and the relations (51), we obtain the transformation

$$w = xe^{(k_2/3)t}, \quad z = -\frac{3}{k_2}e^{-(k_2/3)t}. \tag{83}$$

In terms of the new variables (83), the first integral I given above (82), can be written as

$$I = \begin{cases} \left(w' + \dfrac{(r-1)}{2r}k_1w^2\right)^{-r}\left[\dfrac{(r-1)}{4r^2}k_1^2w^4 + w'\left(w' + \dfrac{k_1}{2}w^2\right)\right], & r \neq 0,2 \\ \dfrac{4w'}{k_1w^2 + 4w'} - \log(k_1w^2 + 4w'), & r = 2. \end{cases} \tag{84}$$

On the other hand the transformation (83) modifies the equation (80) to the form

$$w'' + k_1ww' + \frac{(r-1)k_1^2}{2r^2}w^3 = 0, \quad r \neq 0, \quad \text{and } ' = \frac{\mathrm{d}}{\mathrm{d}z}. \tag{85}$$

Finally, for the case $r=0$, we have an equation of the form [*vide* case (ivb) in Table I], $\ddot{x} + k_2\dot{x} + k_3x^3 + (2/9)k_2^2x = 0$, which is nothing but the force-free Duffing oscillator equation. Again using the transformation (83), the associated time-dependent integral given in Table I can be rewritten as

$$I = \frac{w'^2}{2} + \frac{k_3}{4}w^4, \quad r = 0. \tag{86}$$

Though it is difficult to integrate the above time-independent first integrals (84), as they are in complicated forms, one can easily check that Eq. (86) ($r=0$) can be integrated in terms of Jacobian elliptic function[14] and the case $r=1$ is already discussed as case (ii) in this section. For the other cases one can give a Hamiltonian formulation as in Sec. III A 4 and write the corresponding Hamiltonian as

$$H = \begin{cases} \left[\dfrac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)} - p\left(\dfrac{(r-1)}{2r}k_1w^2\right)\right], & r \neq 0,1,2 \\ \dfrac{k_1}{4}w^2p + \log\left(\dfrac{4k_1}{p}\right), & r = 2 \\ e^p + \dfrac{k_1}{2}w^2, & r = 1 \\ \dfrac{p^2}{2} + \dfrac{k_3}{4}w^4, & r = 0, \end{cases} \tag{87}$$

where

$$p = \begin{cases} \dfrac{1}{r-1}\left(\dfrac{(r-1)}{2r}k_1w^2 + w'\right)^{1-r}, & r \neq 0,1 \\ \log(w'), & r = 1 \\ w', & r = 0. \end{cases} \tag{88}$$

Thus one is ensured of Liouville integrability of system (85) and so (80) for all values of r. Further, following the analysis in the above Sec. III A 5, one can make a canonical transformation [*vide* Eqs. (42)–(44)] to standard nonlinear oscillator equations.

E. Summary of results for the $q=1$ case

To summarize the results obtained in this section, we have identified six integrable cases in Eq. (10), among which four of them were already known in the literature and the remaining two are new. In the following, we tabulate all of them for convenience.

1. Integrable equations already known in the literature

(1) $\ddot{x}+(k_1x+k_2)\dot{x}+\frac{k_1^2}{9}x^3+\frac{k_1k_2}{3}x^2+\lambda_1x=0$ [Eq. (55)],

(2) $\ddot{x}+(k_1x+k_2)\dot{x}+\frac{k_1k_2}{3}x^3+\frac{2k_2^2}{9}x=0$ [Eq. (67)],

(3) $\ddot{x}+k_2\dot{x}+k_4x^2+\frac{6k_2^2}{25}x=0$ [Eq. (74)],

(4) $\ddot{x}+k_3x^3+k_4x^2+\lambda_1x=0$ [Eq. (33c)],

We note that the dynamics and certain transformation properties of Eq. (55) have been studied in detail recently by three of the present authors in Refs. 9 and 11. In particular, we have shown that this equation admits certain unusual nonlinear dynamics.[20] The dynamics of Eqs. (67), (74), and (33c) can be found in Ref. 12.

2. New integrable equations

(1) $\ddot{x}+k_1x\dot{x}+k_3x^3+\lambda_1x=0$ [Eq. (33b)],

(2) $\ddot{x}+(k_1x+k_2)\dot{x}+k_3x^3+\frac{k_1k_2}{3}x^2+\frac{2k_2^2}{9}x=0$ [Eq. (80)],

where $r^2k_3=[(r-1)k_1^2]/2$ and k_1, k_2, λ_1, and r are arbitrary parameters. We note that (33b) includes the first equation of MEE hierarchy (6) as a subcase. Importantly, we showed that (33b) is a Hamiltonian system [see Eq. (41)] and so it is Liouville integrable. Equation (80) can be transformed to the integrable Eq. (85). Explicit general solution of certain special cases, namely, $r=3$ or $\frac{3}{2}$ and $r=-1$ or $\frac{1}{2}$ are reported in Ref. 21.

IV. GENERALIZED FORCE FREE DVP FORM OF EQUATIONS

Let us now consider the case $q=2$ in Eq. (9) or equivalently (11), that is,

$$\ddot{x}=-((k_1x^2+k_2)\dot{x}+k_3x^5+k_4x^3+\lambda_1x)\equiv\phi(x,\dot{x})\ \text{[Eq. (11)]}.$$

Interestingly, Eq. (11) includes another class of physically important nonlinear oscillators. For example, choosing $k_3=0$ one can get the force-free Duffing-van der Pol oscillator equation. With the choice k_2, k_4, $\lambda_1=0$, it coincides with the second equation in the MEE hierarchy equation. Equation (11) with the restriction $k_3=k_1^2/16$, $k_4=k_1k_2/4$, and $\lambda_1=[\omega_0^2+(k_2^2/4)]$, has been investigated in a different perspective in Ref. 4. However, the general equation of the form (11) has never been considered for an integrability test and so we perform the same here.

To identify integrals of motion and the general solution of Eq. (11) we again seek the PS procedure. As the calculations are similar to the $q=1$ case of Eq. (9) which was carried out in the previous section, in the following we give only the important steps.

A. The case $I_t=0$

By considering the same arguments given in Sec. III A 1, the null form S can be fixed easily in the form

$$S = -\frac{((k_1x^2+k_2)\dot{x}+k_3x^5+k_4x^3+\lambda_1 x)}{\dot{x}}. \tag{89}$$

The respective R equation becomes

$$\dot{x}R_x - ((k_1x^2+k_2)\dot{x}+k_3x^5+k_4x^3+\lambda_1 x)R_{\dot{x}} = \left((k_1x^2+k_2)+\frac{((k_1x^2+k_2)\dot{x}+k_3x^5+k_4x^3+\lambda_1 x)}{\dot{x}}\right)R. \tag{90}$$

To seek a particular form for R one may seek a suitable Ansatz. We assume R to be of the form (28) and investigate the system (90) as before. Following a similar procedure we find that a nontrivial particular solution for (90) exists in the form

$$R = \frac{\dot{x}}{\left(\frac{(r-1)}{r}\left(\frac{k_1}{3}x^3+k_2x\right)+\dot{x}\right)^r}, \tag{91}$$

where r, k_1, and k_2 are arbitrary parameters and the remaining parameters, k_3, k_4, and λ_1, are fixed by the relations

$$k_3 = \frac{(r-1)}{3r^2}k_1^2, \quad k_4 = \frac{4(r-1)}{3r^2}k_1k_2, \quad \lambda_1 = \frac{(r-1)}{r^2}k_2^2. \tag{92}$$

Further, we confirmed the compatibility of the functions S and R with the extra constraint (24) also. We note that, unlike the earlier case, $q=1$, we do not get a nontrivial solution for the parametric restriction k_2, $k_4=0$. The above restrictions fix Eq. (11) to the following specific forms:

$$\text{(ia)} \quad \ddot{x}+(k_1x^2+k_2)\dot{x}+\frac{(r-1)}{3r^2}k_1^2x^5+\frac{4(r-1)k_1k_2}{3r^2}x^3+\frac{(r-1)k_2^2}{r^2}x=0, \quad r\neq 0 \tag{93a}$$

$$\text{(ib)} \quad \ddot{x}+k_3x^5+k_4x^3+\lambda_1 x=0, \quad r=0. \tag{93b}$$

Now substituting (89) and (91) into (25) and evaluating the integrals, we obtain the first integrals in the form

$$\text{(ia)} \quad I_1 = \left(\dot{x}+\frac{(r-1)}{r}\left(\frac{k_1}{3}x^3+k_2x\right)\right)^{-r}\left[\dot{x}\left(\dot{x}+\frac{k_1}{3}x^3+k_2x\right)+\frac{(r-1)}{r^2}\left(\frac{k_1}{3}x^3+k_2x\right)^2\right], \quad r\neq 0,2, \tag{94a}$$

$$\text{(ib)} \quad I_1 = \frac{6\dot{x}}{(6\dot{x}+3k_2x+k_1x^3)}-\log(6\dot{x}+3k_2x+k_1x^3), \quad r=2, \tag{94b}$$

$$\text{(ii)} \quad I_1 = \frac{\dot{x}^2}{2}+\frac{k_3}{6}x^6+\frac{k_4}{4}x^4+\frac{\lambda_1}{2}x^2, \quad r=0. \tag{94c}$$

Further, as in the $q=1$ case in Sec. III A 4, the integrals (94) can be recast into the Hamiltonian form

$$\text{(ia)} \quad H = \left[\frac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)}-\frac{(r-1)}{r}p\left(\frac{k_1}{3}x^3+k_2x\right)\right], \quad r\neq 0,1,2, \tag{95a}$$

$$\text{(ib)} \quad H = \frac{k_2}{2}xp + \frac{k_1}{6}x^3p + \log\left(\frac{6}{p}\right), \quad r = 2, \tag{95b}$$

$$\text{(ic)} \quad H = e^p + \frac{k_1}{3}x^3 + k_2x, \quad r = 1, \tag{95c}$$

$$\text{(ii)} \quad H = \frac{p^2}{2} + \frac{k_3}{6}x^6 + \frac{k_4}{4}x^4 + \frac{\lambda_1}{2}x^2, \quad r = 0, \tag{95d}$$

where the corresponding canonical momenta, respectively, are

$$\text{(ia,b)} \quad p = \frac{1}{(r-1)}\left(\dot{x} + \frac{(r-1)}{r}\left(\frac{k_1}{3}x^3 + k_2x\right)\right)^{(1-r)}, \quad r \neq 0,1, \tag{96a}$$

$$\text{(ic)} \quad p = \log \dot{x}, \quad r = 1, \tag{96b}$$

$$\text{(ii)} \quad p = \dot{x}, \quad r = 0. \tag{96c}$$

Note that in the above the parameters r, k_1, k_2, k_3, and λ_1 are all arbitrary. We also note here that unlike the $q=1$ case discussed in Sec. III, so far we have been unable to find suitable canonical transformations for the above Hamiltonian systems so that the standard "potential" equation results. The problem is being further investigated.

B. The case $I_t \neq 0$

Now let us study the case $I_t \neq 0$. In this case S has to be determined from Eq. (22), that is,

$$S_t + \dot{x}S_x - ((k_1x^2 + k_2)\dot{x} + k_3x^5 + k_4x^3 + \lambda_1x)S_{\dot{x}} = (2k_1x\dot{x} + 5k_3x^4 + 3k_4x^2 + \lambda_1) - (k_1x^2 + k_2)S + S^2. \tag{97}$$

As we did in the $q=1$ case of Eq. (9) we proceed to solve Eq. (97) with the same form of Ansatz (47). Doing so we find that Eq. (97) admits nontrivial forms of solutions for certain specific parametric restrictions. We report both the parametric values and their respective forms of S in Table II.

Now substituting the forms of S into Eq. (23) and solving the resultant equation we obtain the corresponding forms of R. Once S and R are determined then one has to verify the compatibility of this solution with the extra constraint (24). Then, one can substitute the null forms and integrating factors into (25) and construct the associated integrals of motion. We report the integrating factors (R) and time-dependent integrals of motion (I) in Table II.

The remaining task is to derive the general solution and establish the complete integrability of Eq. (11) for each parametric restriction. We again adopt the procedure given in Sec. III C and transform the time-dependent integrals into time-independent ones and integrate the latter and deduce the general solution. As the procedure is exactly the same we provide only the results in the following.

Case (ia): $k_3 = k_1^2/16$, $k_4 = k_1k_2/4$, k_1, k_2, and λ_1: arbitrary.

Substituting the parametric restrictions given above in Eq. (11), we get

$$\ddot{x} + (k_1x^2 + k_2)\dot{x} + \frac{k_1^2}{16}x^5 + \frac{k_1k_2}{4}x^3 + \lambda_1x = 0. \tag{98}$$

We observed that the first integral of this case (i) (see Table II), when rewritten, is nothing but the Bernoulli equation which can be integrated strightforwardly[22] and leads to the general solution of the form

TABLE II. Parametric restrictions, null forms (S), integrating factors (R), and time-dependent integrals of motion (I) of $\ddot{x}+(k_1x^2+k_2)\dot{x}+k_3x^5+k_4x^3+\lambda_1x=0$ (identified with the assumed Ansatz form of S and R).

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(i)	$k_3=\frac{k_1^2}{16}, \quad k_4=\frac{k_1k_2}{4}$ (k_1, k_2, λ_1: arbitrary)	$\frac{\frac{k_1}{2}x^3-\dot{x}}{x}$	$\frac{xe^{\mp\omega t}}{\left(\dot{x}-\frac{(k_2\pm\omega)}{2}x+\frac{k_1}{4}x^3\right)^2}$	(a) $I=e^{\mp\omega t}\left(\frac{4\dot{x}+2(k_2\pm\omega)x+k_1x^3}{4\dot{x}+2(k_2\mp\omega)x+k_1x^3}\right)$, $k_2,\lambda_1\neq 0, \quad \omega=(k_2^2-4\lambda_1)^{1/2}$ (b) $I=-t+\frac{x}{\left(\frac{k_2}{2}x+\frac{k_1x^3}{4}+\dot{x}\right)}, \quad k_2^2=4\lambda_1$
(ii)	$k_3=0, \quad k_4=\frac{k_1}{6}(k_2\pm\omega)$, ($k_1$, k_2, λ_1: arbitrary)	$\frac{1}{2}(k_2\mp\omega)+k_1x^2$	$e^{[(k_2\pm\omega)/2]t}$	$I=\left(\dot{x}+\frac{k_2\mp\omega}{2}x+\frac{k_1}{3}x^3\right)e^{[(k_2\pm\omega)/2]t}$, $\omega=(k_2^2-4\lambda_1)^{1/2}$
(iii)	$k_1, \quad k_3=0, \quad \lambda_1=\frac{2k_2^2}{9}$ (k_2, k_4: arbitrary)	$\left(\frac{\frac{k_2}{3}\dot{x}+\frac{k_2^2}{9}x+k_4x^3}{\dot{x}+\frac{k_2}{3}x}\right)$	$\left(\dot{x}+\frac{k_2}{3}x\right)e^{(4/3)k_2t}$	$I=e^{(4/3)k_2t}\left[\frac{\dot{x}^2}{2}+\frac{k_2}{3}x\dot{x}+\frac{k_2^2}{18}x^2+\frac{k_4}{4}x^4\right]$

TABLE II. (*Continued.*)

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(iva)	$k_3=\frac{(r-1)k_1^2}{3r^2}, \quad k_4=\frac{k_1k_2}{4},$ $\lambda_1=\frac{3k_2^2}{16}, \quad r\neq 0$ (k_1, k_2, r: arbitrary)	$\frac{k_2}{4}+k_1x^2+\frac{4k_3x^5}{(4\dot{x}+k_2x)}$	$\frac{(k_2x+4\dot{x})e^{\{[3(2-r)]/4\}k_2t}}{\left(\frac{k_2}{4}x+rk_3x^3+\dot{x}\right)^r}$	$I=\left(\frac{k_3}{3}x^6+\left(\dot{x}+\frac{k_2}{4}x\right)\left(\dot{x}+\frac{k_2}{4}x+\frac{k_1}{3}x^3\right)\right)$ $\times\left(\dot{x}+\frac{k_2}{4}x+rk_3x^3\right)^{-r}e^{\{[3(2-r)]/4\}k_2t}, \quad r\neq 2$ $I=\frac{3}{4}k_2t+\log(6k_2x+4k_1x^3+24\dot{x})$ $-\frac{6(k_2x+4\dot{x})}{(6k_2x+4k_1x^3+24\dot{x})}, \quad r=2$
(ivb)	$k_1=0, \quad k_4=0,$ $\lambda_1=\frac{3k_2^2}{16}, \quad r=0$ (k_2, k_3: arbitrary)	$\left(\frac{\frac{k_2}{4}\dot{x}+\frac{k_2^2}{16}x+k_3x^5}{\dot{x}+\frac{k_2}{4}x}\right)$	$e^{(3k_2/2)t}\left(\dot{x}+\frac{k_2}{4}x\right)$	$I=e^{(3k_2/2)t}\left(\frac{\dot{x}^2}{2}+\frac{k_2}{4}x\dot{x}+\frac{k_2^2}{32}x^2+\frac{k_3}{6}x^6\right)$

$$x(t)=\left(\frac{8k_2\lambda_1(e^{\omega t}-I_1)^2}{I_1^2k_1k_2(-k_2+\omega)-e^{2\omega t}k_1k_2(k_2+\omega)+8I_2k_2\lambda_1e^{(k_2+\omega)t}+8I_1k_1\lambda_1e^{\omega t}}\right)^{1/2}, \tag{99}$$

where $\omega=\sqrt{k_2^2-4\lambda_1}$. A subcase of Eq. (98), namely, $k_2^2<4\lambda_1$ has been studied by Smith[4,23] who showed that the corresponding equation of motion admits a damped oscillatory form of solution, namely,

$$x(t)=\frac{A\cos(\omega_0t+\delta)}{\left(e^{k_2t}-\frac{k_1A}{4k_2}+\frac{k_1A}{4(k_2^2+4\omega_0^2)}(2\omega_0\sin 2(\omega_0t+\delta)-k_2\cos 2(\omega_0t+\delta))\right)^{1/2}}, \tag{100}$$

where $\omega_0=\frac{1}{2}\sqrt{4\lambda_1+k_2^2}$ and δ, A are arbitrary constants.

On the other hand for $k_2^2>4\lambda_1$, the solution (99) becomes of dissipative type, having a frontlike structure. In particular, for $\lambda_1=0$ we get a solution of the form

$$x(t)=\left(\frac{2\sqrt{k_2}(I_1e^{k_2t}-1)}{(-k_1+2k_1I_1e^{k_2t}(2+k_2I_1te^{k_2t})+4k_2I_2e^{2k_2t})^{1/2}}\right). \tag{101}$$

Case (ib): $k_3=k_1^2/16$, $k_4=k_1k_2/4$, $k_2^2=4\lambda_1$, k_1 and k_2: arbitrary.

In this case we get the general solution of the form from (101) as

$$x(t)=\left(\frac{2(I_1+t)^2}{2e^{k_2t}I_2-\frac{k_1}{k_2^3}(2+I_1^2k_2^2+2k_2t+k_2^2t^2+2I_1k_2(1+k_2t))}\right)^{1/2}. \tag{102}$$

One may note that a subcase of this equation, namely, $k_2=\lambda_1=0$, leads us to the second equation in the MEE hierarchy (6) and the corresponding solution follows from Eq. (102) as

$$x(t)=\sqrt{6}\left(\frac{(I_1+t)^2}{6I_2+k_1t(3I_1^2+3I_1t+t^2)}\right)^{1/2}. \tag{103}$$

This form exactly coincides with the solution (7) for $l=2$.

Case (ii): $k_3=0$, $k_4=(k_1/6)(k_2\pm\sqrt{k_2^2-4\lambda_1})$, k_1, k_2 and λ_1: arbitrary.

The repective equation of motion and the first integral are (see Table II)

$$\ddot{x}+(k_1x^2+k_2)\dot{x}+\frac{k_1}{6}(k_2\pm\sqrt{k_2^2-4\lambda_1})x^3+\lambda_1x=0, \tag{104}$$

and

$$I=\left(\dot{x}+\frac{k_2\mp\sqrt{k_2^2-4\lambda_1}}{2}x+\frac{k_1}{3}x^3\right)e^{[(k_2\pm\sqrt{k_2^2-4\lambda_1})/2]t}. \tag{105}$$

Equation (105) can be rewritten as an Abel's equation in the form

$$\dot{x}=Ie^{[(-k_2\mp\sqrt{k_2^2-4\lambda_1})/2]t}-\left(\frac{k_2\mp\sqrt{k_2^2-4\lambda_1}}{2}\right)x-\frac{k_1}{3}x^3. \tag{106}$$

It is not clear whether Eq. (106) can be explicitly integrated in general. However, for the special case $\lambda_1=\frac{3}{16}k_2^2$ it can be integrated as follows.

The restriction $\lambda_1=\frac{3}{16}k_2^2$ fixes the equation of motion (104) and the first integral (105) in the forms

$$\ddot{x} + (k_1 x^2 + k_2)\dot{x} + \frac{k_1 k_2}{4} x^3 + \frac{3k_2^2}{16} x = 0, \tag{107}$$

and

$$I = \left(\dot{x} + \frac{k_2}{4} x + \frac{k_1}{3} x^3 \right) e^{(3k_2/4)t}, \tag{108}$$

respectively.

Now following our procedure given in Sec. III C one arrives at the general solution[1] as

$$z + z_0 = -\frac{a}{3I} \left[\frac{1}{2} \log\left(\frac{(w-a)^2}{w^2 + aw + a^2} \right) + \sqrt{3} \arctan\left(\frac{-w\sqrt{3}}{2a + w} \right) \right], \tag{109}$$

with $w = xe^{(k_2/4)t}$, $z = -(2/k_2)e^{-k_2/2t}$, and $a = \sqrt[3]{3I/k_1}$ and z_0 is the second integration constant. Rewriting w and z in terms of old variables one can get the explicit solution.

Case (iii): k_1, $k_3 = 0$, $\lambda_1 = 2k_2^2/9$, k_2 and k_4: arbitrary.

The parametric restrictions given above fix the equation of motion (11) to the force-free Duffing oscillator, namely, $\ddot{x} + k_2\dot{x} + k_4 x^3 + (2k_2^2/9)x = 0$. We have already discussed the general solution of this equation in Sec. III [*vide* case (iv)].

Case (iv): $k_3 = [(r-1)k_1^2]/3r^3$, $k_4 = k_1 k_2/4$, $\lambda_1 = 3k_2^2/16$, k_1, k_2, and r: arbitrary.

The equation of motion turns out to be

$$\ddot{x} + (k_1 x^2 + k_2)\dot{x} + \frac{(r-1)k_1^2}{3r^2} x^5 + \frac{k_1 k_2}{4} x^3 + \frac{3k_2^2}{16} x = 0, \quad r \neq 0. \tag{110}$$

Rewriting the associated first integral I, given in case (iv) in Table II, in the form (50), we get

$$I = \begin{cases} \left(\dfrac{(r-1)k_1^2}{9r^2} (xe^{(k_2/4)t})^6 + \dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) \left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) e^{(k_2/2)t} + \dfrac{k_1}{3}(xe^{(k_2/4)t})^3 \right) e^{(k_2/2)t} \right) \\ \quad \times \left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) e^{(k_2/2)t} + \dfrac{k_1(r-1)}{3r}(xe^{(k_2/4)t})^3 \right)^{-r}, \quad r \neq 0, 2, \\ \dfrac{6\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) e^{(k_2/2)t}}{k_1(xe^{(k_2/4)t})^3 + 6\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) e^{(k_2/2)t}} - \log\left(k_1(xe^{(k_2/4)t})^3 + 6\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) e^{(k_2/2)t} \right), \quad r = 2 \\ \dfrac{1}{2}\left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{(k_2/4)t}) \right)^2 e^{k_2 t} + \dfrac{k_3}{6}(xe^{(k_2/4)t})^6, \quad r = 0 \end{cases} \tag{111}$$

and identifying the dependent and independent variables from (111) and the relations (51), we obtain the transformation

$$w = xe^{(k_2/4)t}, \quad z = -\frac{2}{k_2} e^{-(k_2/2)t}. \tag{112}$$

In terms of the new variables (112) the first integral I given above (111), can be written as

$$I=\begin{cases}\left(w'+\dfrac{(r-1)}{3r}k_1w^3\right)^{-r}\left[w'\left(w'+\dfrac{k_1}{3}w^3\right)+\dfrac{(r-1)}{9r^2}k_1^2w^6\right], & r\neq 0,2\\ \dfrac{6w'}{k_1w^3+6w'}-\log(k_1w^3+6w'), & r=2,\\ \dfrac{w'^2}{2}+\dfrac{k_3}{6}w^6, & r=0.\end{cases}\tag{113}$$

On the other hand substituting the transformation (112) into the equation of motion (110), we get

$$w''+k_1w^2w'+\frac{(r-1)k_1^2}{3r^2}w^5=0,\quad r\neq 0,\quad '=\frac{\mathrm{d}}{\mathrm{d}z}.\tag{114}$$

In the case $r=0$, we have an equation of the form [*vide* case (ivb) in Table II]

$$\ddot{x}+k_2\dot{x}+k_3x^5+\frac{3k_2^2}{16}x=0.\tag{115}$$

We note that Eq. (114) is the $l=2$ case of Eq. (6). As we mentioned in the Introduction, the general solution of this equation can be obtained only for certain specific choices, namely, $[(r-1)k_1^2]/3r^2=1/16$. This in turn gives $r=4k_1$ or $\frac{4}{3}k_1$. The respective solutions for these values of r of Eq. (114) can be fixed from Eq. (7) with $l=2$. The other cases do not seem to be amenable to explicit integration. However, all of them can be recast in the Hamiltonian form as we see below.

As the first integrals (113) are now "time" independent ones, one can give a Hamiltonian formalism for all the integrals (113) by following the ideas given in Sec. III A 4. Doing so we obtain

$$H=\begin{cases}\left[\dfrac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)}-\dfrac{(r-1)}{3r}k_1w^3p\right], & r\neq 0,1,2,\\ \dfrac{k_1}{6}w^3p+\log\left(\dfrac{6}{p}\right), & r=2\\ e^p+\dfrac{k_1}{3}w^3, & r=1\\ \dfrac{p^2}{2}+\dfrac{k_3}{6}w^6, & r=0\end{cases}\tag{116}$$

where

$$p=\begin{cases}\dfrac{1}{(r-1)}\left(w'+\dfrac{(r-1)}{3r}k_1w^3\right)^{(1-r)}, & r\neq 0,1\\ \log w', & r=1\\ \dfrac{p^2}{2}+\dfrac{k_3}{6}w^6, & r=0.\end{cases}\tag{117}$$

In this sense these cases may be considered as Liouville integrable systems. Finally, the $r=0$ case in Eq. (113) can be integrated in terms of Jacobian elliptic function (see for example in Ref. 24). Again, here, we have not been able to identify canonical transformations which can lead to the identification of suitable potential equations.

C. Summary of results in $q=2$ case

To summarize the results obtained for the $q=2$ case, we have identified six integrable cases in Eq. (11), among which three of them were already known in the literature and the remaining three are new. In the following, we tabulate both of them.

1. Integrable equations already known in the literature

$$(1)\ \ddot{x}+(k_1x^2+k_2)\dot{x}+\frac{k_1k_2}{4}x^3+\frac{3k_2^2}{16}x=0\ [\text{Eq. (107)}],$$

$$(2)\ \ddot{x}+k_2\dot{x}+k_3x^3+\frac{2k_2^2}{9}x=0, \tag{118}$$

$$(3)\ \ddot{x}+k_3x^5+k_4x^3+\lambda_1x=0\ [\text{Eq. (93b)}].$$

We mention that Eq. (107) is nothing but the force-free DVP whose integrability is established in Ref. 1 and Eq. (118) is nothing but the force-free Duffing oscillator.[12,14]

2. New integrable equations

$$(1)\ \ddot{x}+(k_1x^2+k_2)\dot{x}+k_3x^5+\frac{4(r-1)k_1k_2}{3r^2}x^3+\frac{(r-1)k_2^2}{r^2}x=0,\quad r\neq 0\ [\text{Eq. (93a)}],$$

$$(2)\ \ddot{x}+(k_1x^2+k_2)\dot{x}+\frac{k_1^2}{16}x^5+\frac{k_1k_2}{4}x^3+\lambda_1x=0\ [\text{Eq. (98)}],$$

$$(3)\ \ddot{x}+(k_1x^2+k_2)\dot{x}+k_3x^5+\frac{k_1k_2}{4}x^3+\frac{3k_2^2}{16}x=0\ [\text{Eq. (110)}],$$

where $r^2k_3=[(r-1)k_1^2]/3$ and k_1, k_2, λ_1, and r are arbitrary parameters. We proved that Eq. (93a) is a Liouville integrable one. As far as Eq. (98) is concerned we derived the general solution for arbitrary values of k_1, k_2, and λ_1. Finally, for Eq. (110), though we identified only one time-dependent integral, we have demonstrated that it can be transformed into a time-independent Hamiltonian, thereby ensuring its Liouville integrability.

V. EXTENDED PRELLE-SINGER METHOD TO GENERALIZED EQ. (9)

One can investigate the integrability properties of Eq. (9) by considering the cases $q=3,4,5,\ldots$, one by one and classifying the integrable equations. Since the procedure and the mathematical techniques in exploring the integrating factors (R), null forms (S), first integrals (I), and general solution are the same in each case we do not consider each case in detail. We straightaway move to the case $q=$*arbitrary*, that is, $q\in R$ and not necessarily an integer, and present the outcome of our investigations.

As we did earlier, we consider the cases $I_t=0$ and $I_t\neq 0$ separately for the choice $q=$*arbitrary* also. First let us consider the case $I_t=0$.

A. The case $I_t=0$

By considering the same arguments given in Sec. III A 1, the null form S and the integrating factor R can be fixed easily in the form

$$S=-\frac{((k_1x^q+k_2)\dot{x}+k_3x^{2q+1}+k_4x^{1+q}+\lambda_1x)}{\dot{x}},$$

$$R=\frac{\dot{x}}{\left(\frac{(r-1)}{r}\left(\frac{k_1}{(q+1)}x^{q+1}+k_2x\right)+\dot{x}\right)^r}, \tag{119}$$

where k_1 and k_2 are arbitrary and the remaining parameters, k_3, k_4, and λ_1, are related to the parameters k_1 and k_2 through the relations

$$k_3=\frac{(r-1)}{r^2}(q+1)\hat{k}_1^2,\quad k_4=\frac{(r-1)}{r^2}(q+2)\hat{k}_1k_2,\quad \lambda_1=\frac{(r-1)}{r^2}k_2^2, \tag{120}$$

where $\hat{k}_1=k_1/(q+1)$. The above restrictions fix Eq. (9) to the following specific forms:

$$\text{(ia)}\quad \ddot{x}+((q+1)\hat{k}_1x^q+k_2)\dot{x}+\frac{(r-1)}{r^2}[(q+1)\hat{k}_1^2x^{2q+1}$$
$$+(q+2)\hat{k}_1k_2x^{q+1}+k_2^2x]=0,\quad r\neq 0\ [\text{Eq. (15)}],$$
$$\text{(ib)}\quad \ddot{x}+k_3x^{2q+1}+k_4x^{q+1}+\lambda_1x=0,\quad r=0. \tag{121}$$

Now substituting (119) into (25) and evaluating the integrals, we obtain the first integrals of the form

$$\text{(ia)}\ I_1=\left(\dot{x}+\frac{(r-1)}{r}(\hat{k}_1x^{q+1}+k_2x)\right)^{-r}\left[\dot{x}(\dot{x}+\hat{k}_1x^{q+1}+k_2x)+\frac{(r-1)}{r^2}(\hat{k}_1x^{q+1}+k_2x)^2\right],\quad r\neq 0,2, \tag{122a}$$

$$\text{(ib)}\quad I_1=\frac{\dot{x}}{\left(\dot{x}+\frac{k_2}{2}x+\frac{\hat{k}_1}{2}x^{q+1}\right)}-\log\left(\dot{x}+\frac{k_2}{2}x+\frac{\hat{k}_1}{2}x^{q+1}\right),\quad r=2, \tag{122b}$$

$$\text{(ii)}\quad I_1=\frac{\dot{x}^2}{2}+\frac{k_3}{2(q+1)}x^{2(q+1)}+\frac{k_4}{(q+2)}x^{q+2}+\frac{\lambda_1}{2}x^2,\quad r=0. \tag{122c}$$

Further, using the above forms of the first integrals, one can show that the equation of motion (9), with the parametric restrictions (120), can also be derived from the Hamiltonians

$$\text{(ia)}\ H=\left[\frac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)}-\frac{(r-1)}{r}p(\hat{k}_1x^{q+1}+k_2x)\right],\quad r\neq 0,1,2, \tag{123a}$$

$$\text{(ib)}\ H=\frac{k_2}{2}xp+\frac{\hat{k}_1}{2}x^{q+1}p+\log\left(\frac{2(q+1)}{p}\right),\quad r=2 \tag{123b}$$

$$\text{(ic)}\ H=e^p+\hat{k}_1x^{q+1}+k_2x,\quad r=1, \tag{123c}$$

$$\text{(ii)}\ H=\frac{p^2}{2}+\frac{k_3}{2(q+1)}x^{2(q+1)}+\frac{k_4}{(q+1)}x^{q+1}+\frac{\lambda_1}{2}x^2,\quad r=0, \tag{123d}$$

where the corresponding canonical momenta, respectively, are

$$\text{(ia,b)}\ p=\frac{1}{(r-1)}\left(\dot{x}+\frac{(r-1)}{r}(\hat{k}_1x^{q+1}+k_2x)\right)^{(1-r)},\quad r\neq 0,1, \tag{124a}$$

$$\text{(ic) } p = \log \dot{x}, \quad r = 1, \tag{124b}$$

$$\text{(ii) } p = \dot{x}, \; r = 0. \tag{124c}$$

With the above Hamiltonian formulation, for the parametric set (120), the integrability of the associated equation of motion is assured for these parametric cases through Liouville theorem.

B. The case $I_t \neq 0$

We use the same Ansatz and ideas which we followed for the $q=1$ and $q=2$ cases to determine the forms of S and R. As the procedure is exactly the same as in the earlier cases, we present the parametric restrictions and the respective form of expressions of the integrating factors, null forms, and integrals of motions in Table III without further discussion.

Since we derived only one integral, which is also a time-dependent one for each parametric restriction, we need to integrate each one of them further and obtain the second integration constant in order to prove the complete integrability of each of the cases reported in Table III. In the following we deduce the second integral and general solution by utilizing the procedure given in Sec. III C.

Case (ia): $k_3=k_1^2/(q+2)^2$, $k_4=k_1k_2/(q+2)$, k_1, k_2, and λ_1: arbitrary.

We have an equation of the form

$$\ddot{x} + ((q+2)\hat{k}_1 x^q + k_2)\dot{x} + \hat{k}_1^2 x^{2q+1} + \hat{k}_1 k_2 x^{q+1} + \lambda_1 x = 0 \text{ [Eq. (13)]},$$

where $k_1=(q+2)\hat{k}_1$. The corresponding first integral given in Table III is nothing but the Bernoulli equation which can be solved using the standard method.[22] The general solution turns out to be

$$x(t) = (e^{\omega t} - I_1)\left(e^{(q/2)(k_2+\omega)t}\left(I_2 + \hat{k}_1 q \int \left(\frac{e^{\omega t} - I_1}{e^{(1/2)(k_2+\omega)t}} \right)^q \mathrm{d}t \right) \right)^{-1/q}, \tag{125}$$

where $\omega=\sqrt{k_2^2-4\lambda_1}$. We note here that a subcase of the above, namely, $k_2^2<4\lambda_1$, has been studied by Smith,[4] who had shown that the corresponding system admits the general solution of the form

$$x(t) = A\cos(\omega_0 t + \delta)e^{-(k_2/2)t}\left(1 + q\hat{k}_1 A \int e^{(-qk_2/2)t}\cos^q(\omega_0 t + \delta)\mathrm{d}t \right)^{-1/q}, \tag{126}$$

where $\omega_0=\frac{1}{2}\sqrt{4\lambda_1+k_2^2}$ and δ, A are arbitrary constants. For $k_2^2>4\lambda_1$, the solution become a dissipative type/frontlike structure. In particular, for $\lambda_1=0$ the general solution takes the form

$$x(t) = (e^{k_2 t}I_1 - 1)\left[e^{qk_2 t}\left(I_2 + \hat{k}_1 q \int (I_1 - e^{-k_2 t})^q \mathrm{d}t \right) \right]^{-1/q}. \tag{127}$$

Case (ib): $k_3=k_1^2/16$, $k_4=k_1k_2/4$, $k_2=4\lambda_1$, k_1 and k_2: arbitrary.

A general solution for this case can be fixed from (127) as

$$x(t) = (I_1 + t)e^{-(k_2/2)t}\left(I_2 + q\hat{k}_1 \int e^{-(qk_2/2)t}(I_1 + t)^q \mathrm{d}t \right)^{-1/q}. \tag{128}$$

On the other hand the general solution for the parametric choice k_2, $\lambda_1=0$ turns out to be

$$x(t) = \left(\frac{(q+1)(I_1+t)^q}{\hat{k}_1 q(I_1+t)^{q+1} + (q+1)I_2} \right)^{1/q}, \tag{129}$$

which exactly coincides with the result (7) obtained by Feix *et al.*[3] for integer $q(=l)$ values.

Case (ii): $k_3=0$, $k_4=\{k_1/[2(q+1)]\}(k_2\pm\sqrt{k_2^2-4\lambda_1})$, k_1, k_2 and λ_1: arbitrary.

The associated equation of motion and the first integral are (see Table III)

TABLE III. Parametric restrictions, null forms (S), integrating factors (R), and time-dependent integrals of motion (I) of $\ddot{x}+(k_1x^q+k_2)\dot{x}+k_3x^{2q+1}+k_4x^{q+1}+\lambda_1x=0$ (identified with the assumed Ansatz form of S and R).

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(i)	$k_3=\dfrac{k_1^2}{(q+2)^2}$, $\quad k_4=\dfrac{k_1k_2}{(q+2)}$ (k_1, k_2, λ_1: arbitrary)	$\dfrac{\left(\dfrac{qk_1}{(q+2)}x^{q+1}-\dot{x}\right)}{x}$	$\dfrac{xe^{\mp\omega t}}{\left(\dot{x}-\dfrac{(k_2\pm\omega)}{2}x+\dfrac{k_1}{(q+2)}x^{q+1}\right)^2}$	(a) $I=e^{\mp\omega t}\left(\dfrac{\dot{x}-\dfrac{(-k_2\mp\omega)}{2}x+\dfrac{k_1}{q+2}x^{q+1}}{\dot{x}-\dfrac{(-k_2\pm\omega)}{2}x+\dfrac{k_1}{q+2}x^{q+1}}\right)$ $k_2,\lambda_1\neq0$, $\quad\omega=(k_2^2-4\lambda_1)^{1/2}$ (b) $I=-t+\dfrac{x}{\left(\dfrac{k_2}{2}x+\dfrac{k_1x^{q+1}}{q+2}+\dot{x}\right)}$, $\quad k_2^2=4\lambda_1$
(ii)	$k_4=\dfrac{k_1(k_2\pm\omega)}{2(q+1)}$, $\quad k_3=0$, (k_1, k_2, λ_1: arbitrary)	$\dfrac{1}{2}(k_2\mp\omega)+k_1x^q$,	$e^{[(k_2\pm\omega)/2]t}$	$I=\left(\dot{x}+\dfrac{k_2\mp\omega}{2}x+\dfrac{k_1}{(q+1)}x^{q+1}\right)e^{[(k_2\pm\omega)/2]t}$, $\omega=(k_2^2-4\lambda_1)^{1/2}$
(iii)	$k_1,k_3=0$, $\quad\lambda_1=\dfrac{2(q+2)k_2^2}{(q+4)^2}$ (k_2, k_4: arbitrary)	$\dfrac{\dfrac{2k_2\dot{x}}{(q+4)}+\dfrac{4k_2^2x}{(q+4)^2}+k_4x^{q+1}}{\left(\dot{x}+\dfrac{2k_2x}{(q+4)}\right)}$	$\left(\dot{x}+\dfrac{2k_2x}{(q+4)}\right)e^{\{[2(q+2)]/[(q+4)]\}k_2t}$	$I=e^{\{[2(q+2)]/[(q+4)]\}k_2t}\left[\dfrac{\dot{x}^2}{2}+\dfrac{2k_2x\dot{x}}{(q+4)}+\dfrac{2k_2^2x^2}{(q+4)^2}+\dfrac{k_4x^{q+2}}{(q+2)}\right]$

TABLE III. (*Continued.*)

Cases	Parametric restrictions	Null form (S)	Integrating factor (R)	Integrals of motion (I)
(iv)a	$k_3=\dfrac{(r-1)k_1^2}{(q+1)r^2}$, $k_4=\dfrac{k_1k_2}{(q+2)}$, $\lambda_1=\dfrac{(q+1)k_2^2}{(q+2)^2}$, $r\neq 0$ (k_1, k_2, r: arbitrary)	$\dfrac{k_2}{(q+2)}+k_1x^q+\dfrac{k_3x^{2q+1}}{\left(\dot{x}+\dfrac{k_2}{(q+2)}x\right)}$	$\dfrac{(k_2x+(q+2)\dot{x})e^{\{[(q+1)(2-r)]/[(q+2)]\}k_2t}}{\left(\dfrac{k_2}{(q+2)}x+rk_3x^{q+1}+\dot{x}\right)^r}$	$I=\left(\dfrac{k_3x^{2(q+1)}}{(q+1)}+\left(\dot{x}+\dfrac{k_2x}{q+2}\right)\left(\dot{x}+\dfrac{k_2x}{q+2}+\dfrac{k_1x^{q+1}}{q+1}\right)\right)\times\left(\dfrac{k_2}{(q+2)}x+rk_3x^{q+1}+\dot{x}\right)^{-r}e^{\{[(q+1)(2-r)]/[(q+2)]\}k_2t}$, $r\neq 2$ $I=\dfrac{q+1}{q+2}k_2t+\log\left(k_1x^{q+1}+2(q+1)\left(\dot{x}+\dfrac{k_2}{q+2}x\right)\right)-\left(\dfrac{2(q+1)\left(\dot{x}+\dfrac{k_2}{q+2}x\right)}{k_1x^{q+1}+2(q+1)\left(\dot{x}+\dfrac{k_2}{q+2}x\right)}\right)$, $r=2$
(iv)b	$k_1=0$, $k_4=0$, $\lambda_1=\dfrac{(q+1)k_2^2}{(q+2)^2}$, $r=0$ (k_2, k_3: arbitrary)	$\dfrac{k_2}{(q+2)}+\dfrac{k_3x^{2q+1}}{\left(\dot{x}+\dfrac{k_2}{(q+2)}x\right)}$	$e^{\{[(2q+2)k_2]/[(q+2)]\}t}\left(\dot{x}+\dfrac{k_2}{(q+2)}x\right)$	$I=\left(\dfrac{\dot{x}^2}{2}+\dfrac{k_2x\dot{x}}{(q+2)}+\dfrac{k_2^2x^2}{2(q+2)^2}+\dfrac{k_3x^{2q+2}}{(2q+2)}\right)e^{\{[(2q+2)k_2]/(q+2)\}t}$

$$\ddot{x} + ((q+1)\hat{k}_1 x^q + k_2)\dot{x} + \frac{\hat{k}_1}{2}(k_2 \pm \sqrt{k_2^2 - 4\lambda_1})x^{q+1} + \lambda_1 x = 0, \tag{130}$$

and

$$I = \left(\dot{x} + \frac{k_2 \mp \sqrt{k_2^2 - 4\lambda_1}}{2}x + \hat{k}_1 x^{q+1}\right)e^{[(k_2 \pm \sqrt{k_2^2 - 4\lambda_1})/2]t}, \tag{131}$$

where $k_1=(q+1)\hat{k}_1$. As in the earlier cases, that is, $q=1$ and $q=2$, we are able to integrate the first integral (131) explicitly only for a specific parametric restriction, namely, $\lambda_1=(q+1)\hat{k}_2^2$, where $k_2=(q+2)\hat{k}_2$. In this case the equation of motion (130) and the first integral, Eq. (131), can be recast in the form

$$\ddot{x} + (k_1 x^q + (q+2)\hat{k}_2)\dot{x} + k_1\hat{k}_2 x^{q+1} + (q+1)\hat{k}_2^2 x = 0 \text{ [Eq.(12)]},$$

and

$$I = \left(\dot{x} + \hat{k}_2 x + \hat{k}_1 x^{q+1}\right)e^{(q+1)\hat{k}_2 t}, \tag{132}$$

respectively. Now comparing (132) with (50), we get

$$I = e^{q\hat{k}_2 t}\left(\frac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2 t})\right) + \hat{k}_1(xe^{\hat{k}_2 t})^{(q+1)}. \tag{133}$$

Next, identifying the dependent and independent variables from (133) using the relations (51), we obtain the transformation

$$w = xe^{\hat{k}_2 t}, \quad z = -\frac{1}{q\hat{k}_2}e^{-q\hat{k}_2 t}. \tag{134}$$

Using the transformation (134), the first integral (133) can be rewritten in the form

$$I = w' + \hat{k}_1 w^{(q+1)}, \tag{135}$$

which in turn leads to the solution by an integration, that is,

$$z - z_0 = \int \frac{\mathrm{d}w}{I - \hat{k}_1 w^{(q+1)}}, \tag{136}$$

where z_0 is an arbitrary constant. Solving Eq. (136), we get[25]

$$z - z_0 = \frac{1}{Ig^{1/(q+1)}}\begin{cases} -\dfrac{2}{q+1}\displaystyle\sum_{i=0}^{(q-1)/2} P_i \cos\frac{2i}{q+1}\pi + \frac{2}{q+1}\sum_{i=0}^{(q-1)/2} Q_i \sin\frac{2i}{q+1}\pi \\ \qquad + \dfrac{1}{q+1}\ln\dfrac{(1+w)}{(1-w)}, q\text{-a positive odd number}, \\ -\dfrac{2}{q+1}\displaystyle\sum_{i=0}^{(q-2)/2} R_i \cos\frac{2i+1}{q+1}\pi + \frac{2}{q+1}\sum_{i=0}^{\frac{q-2}{2}} T_i \sin\frac{2i+1}{q+1}\pi \\ \qquad + \dfrac{1}{q+1}\ln(1+w), \quad q\text{-a positive even number}, \end{cases} \tag{137}$$

where $g=\hat{k}_1/I$ and

$$P_i = \frac{1}{2}\ln\left(w^2 - 2w\cos\frac{2i}{q+1}\pi + 1\right), \quad Q_i = \arctan\left[\frac{w - \cos\frac{2i}{q+1}\pi}{\sin\frac{2i}{q+1}\pi}\right],$$

$$R_i = \frac{1}{2}\ln\left(w^2 + 2w\cos\frac{2i+1}{q+1}\pi + 1\right), \quad T_i = \arctan\left[\frac{w + \cos\frac{2i+1}{q+1}\pi}{\sin\frac{2i+1}{q+1}\pi}\right].$$

Rewriting w and z in terms of old variables, one can get the explicit solution.

Case (iii): k_1, $k_3=0$, $\lambda_1=[2(q+2)k_2^2]/[(q+4)^2]$, k_2 and k_4: arbitrary.

The parametric choice given above fixes the equation of motion of the form

$$\ddot{x} + (q+4)\hat{k}_2\dot{x} + k_4 x^{(q+1)} + 2(q+2)\hat{k}_2^2 x = 0 \text{ [Eq.(14)]},$$

where $k_2=(q+4)\hat{k}_2$. Rewriting the first integral I given in case (iii) in Table III, in the form (49), we get

$$I = \frac{1}{2}(\dot{x} + 2\hat{k}_2 x)^2 e^{2(q+2)\hat{k}_2 t} + \frac{k_4 x^{(q+2)}}{(q+2)} e^{2(q+2)\hat{k}_2 t}. \tag{138}$$

Now splitting the first term in Eq. (138) further in the form of (50),

$$I = \left[e^{q\hat{k}_2 t}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{x}{\sqrt{2}}e^{2\hat{k}_2 t}\right)\right]^2 + \frac{2^{((q+2)/2)}k_4}{(q+2)}\left(\frac{x}{\sqrt{2}}e^{2\hat{k}_2 t}\right)^{(q+2)}, \tag{139}$$

and identifying the dependent and independent variables from (139) using the relations (51), we obtain the transformation

$$w = \frac{x}{\sqrt{2}}e^{2\hat{k}_2 t}, \quad z = -\frac{1}{q\hat{k}_2}e^{-q\hat{k}_2 t}. \tag{140}$$

Using the transformation (140), the first integral (138) can be brought to the form

$$I = w'^2 + \frac{2^{((q+2)/2)}k_4}{(q+2)}w^{(q+2)}. \tag{141}$$

Separating the dependent and independent variables and integrating the resultant equation we get

$$z - z_0 = \int \frac{\mathrm{d}w}{\sqrt{I - \hat{k}_4 w^{(q+2)}}}, \tag{142}$$

where $\hat{k}_4=\{[2^{(q+2)/2}]/[(q+2)]\}k_4$ and z_0 is an arbitrary constant.

Case (iv): $k_3=[(r-1)k_1^2]/[(q+1)r^2]$, $k_4=k_1k_2/(q+2)$, $\lambda_1=[(q+1)k_2^2]/[(q+2)^2]$, k_1, k_2, and r: arbitrary.

The equation of motion in this case turns out to be

$$\ddot{x} + ((q+1)\hat{k}_1 x^q + (q+2)\hat{k}_2)\dot{x} + (q+1)\left(\frac{(r-1)}{r^2}\hat{k}_1^2 x^{2q} + \hat{k}_1\hat{k}_2 x^q + \hat{k}_2^2\right)x = 0, \quad r \neq 0 \text{ [Eq. (16)]},$$

where $k_1=(q+1)\hat{k}_1$, $k_2=(q+2)\hat{k}_2$. Rewriting the associated first integral I, given in case (iv) in Table III, in the form (50), we get

$$I=\begin{cases}\left(\dfrac{(r-1)\hat{k}_1^2}{r^2}(xe^{\hat{k}_2t})^{2(q+1)}+\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})\left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})e^{q\hat{k}_2t}+\hat{k}_1(xe^{\hat{k}_2t})^{q+1}\right)e^{q\hat{k}_2t}\right), & \\ \qquad\times\left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})e^{q\hat{k}_2t}+\dfrac{\hat{k}_1(r-1)}{r}(xe^{\hat{k}_2t})^{q+1}\right)^{-r}, & r\neq 0,2\\ \dfrac{\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})e^{q\hat{k}_2t}}{\dfrac{\hat{k}_1}{2}(xe^{\hat{k}_2t})^{q+1}+\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})e^{q\hat{k}_2t}}-\log\left(\dfrac{\hat{k}_1}{2}(xe^{\hat{k}_2t})^{q+1}+\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})e^{q\hat{k}_2t}\right), & r=2\\ \dfrac{1}{2}\left(\dfrac{\mathrm{d}}{\mathrm{d}t}(xe^{\hat{k}_2t})\right)^2e^{2qk_2t}+\dfrac{k_3}{2(q+1)}(xe^{\hat{k}_2t})^{2(q+1)}, & r=0.\end{cases} \tag{143}$$

Identifying the dependent and independent variables from (143) and the relations (51), we obtain the transformation

$$w=xe^{\hat{k}_2t},\quad z=-\frac{1}{q\hat{k}_2}e^{-q\hat{k}_2t}. \tag{144}$$

Subsituting the transformation (144) into (16), one obtains

$$w''+(q+1)\hat{k}_1w^qw'+(q+1)\frac{(r-1)}{r^2}\hat{k}_1^2w^{2q+1}=0,\quad r\neq 0,\quad {}'=\frac{\mathrm{d}}{\mathrm{d}z}. \tag{145}$$

In terms of the new variables (144), the time-dependent first integral (143) can be transformed into time-independent ones of the form

$$I=\begin{cases}\left(w'+\dfrac{(r-1)}{r}\hat{k}_1w^{q+1}\right)^{-r}\left[w'(w'+\hat{k}_1w^{q+1})+\dfrac{(r-1)}{r^2}\hat{k}_1^2w^{2(q+1)}\right], & r\neq 0,2,\\ \dfrac{w'}{w'+\dfrac{\hat{k}_1}{2}w^{q+1}}-\log\left(w'+\dfrac{\hat{k}_1}{2}w^{q+1}\right), & r=2,\\ \dfrac{w'^2}{2}+\dfrac{k_3}{2(q+1)}w^{2(q+1)}, & r=0.\end{cases} \tag{146}$$

Once again one can deduce the Hamiltonians in the form

$$H=\begin{cases}\left[\dfrac{((r-1)p)^{(r-2)/(r-1)}}{(r-2)}-\dfrac{(r-1)}{r}\hat{k}_1w^{q+1}p\right], & r\neq 0,1,2,\\ \dfrac{1}{2}\hat{k}_1w^{q+1}p+\log\left(\dfrac{2(q+1)}{p}\right), & r=2,\\ e^p+\hat{k}_1w^{q+1}, & r=1,\\ \dfrac{p^2}{2}+\dfrac{k_3}{2(q+1)}w^{2(q+1)}, & r=0,\end{cases} \tag{147}$$

with

$$p = \begin{cases} \dfrac{1}{(r-1)}\left(w' + \dfrac{(r-1)}{r}\hat{k}_1 w^{q+1}\right)^{(1-r)}, & r \neq 0,1 \\ \log(w'), & r = 1 \\ w', & r = 0, \end{cases} \tag{148}$$

thereby ensuring Liouville integrability of Eq. (16).

C. Summary of results in *q=arbitrary* case

To conclude the integrability of Eq. (9), we have established the fact that the following equations are integrable:

(1) $\ddot{x} + (k_1 x^q + (q+2)k_2)\dot{x} + k_1 k_2 x^{q+1} + (q+1)k_2^2 x = 0$ [Eq. (12)],

(2) $\ddot{x} + ((q+2)k_1 x^q + k_2)\dot{x} + k_1^2 x^{2q+1} + k_1 k_2 x^{q+1} + \lambda_1 x = 0$ [Eq. (13)],

(3) $\ddot{x} + (q+4)k_2\dot{x} + k_4 x^{q+1} + 2(q+2)k_2^2 x = 0$ [Eq. (14)],

(4) $\ddot{x} + ((q+1)k_1 x^q + k_2)\dot{x} + \dfrac{(r-1)}{r^2}((q+1)k_1^2 x^{2q} + (q+2)k_1 k_2 x^q + k_2^2)x = 0,$

$r \neq 0$ [Eq. (15)],

(5) $\ddot{x} + ((q+1)k_1 x^q + (q+2)k_2)\dot{x} + (q+1)(k_3 x^{2q} + k_1 k_2 x^q + k_2^2)x = 0$ [Eq. (16)],

where $r^2 k_3 = (r-1)k_1^2$ and k_1, k_2, k_4, λ_1, and r are arbitrary parameters [for simplicity we have removed the hats in the k_i's, $i=1,2$, in Eqs. (12)–(16)]. The significance and newness of Eqs. (12)–(16) were already pointed out in Sec. I B.

VI. DISCUSSION AND CONCLUSIONS

In this paper, we have investigated the integrability properties of Eq. (9) and shown that it admits a large class of integrable nonlinear systems. In fact, many classical integrable nonlinear oscillators can be derived as subcases of our results. One of the important outcomes of our investigation is that the entire class of Eq. (6) can be derived from a conservative Hamiltonian [*vide* Eq. (123)], even though the system deceptively looks like a dissipative equation.

From our detailed analysis we have shown that Eq. (9) admits both conservative Hamiltonian systems and dissipative systems, depending on the choice of parameters. As far as the former is concerned we have deduced the explicit forms of the Hamiltonians for the respective equations. In fact, for the case $q=1$, we have constructed suitable canonical transformations and transformed the equations into conservative nonlinear oscillator equations. However, the canonical transformations for the conservative Hamiltonian systems for the cases $q=2,\ldots$, arbitrary, if they exist at all, still remain to be obtained. Exploring the classical dynamics underlying these conservative Hamiltonian systems is also of considerable interest for further study. As far as dissipative systems are concerned we have not only shown that Eq. (9) contains the well-known force-free Helmholtz, Duffing, and Duffing–van der Pol oscillators but also have several integrable generalizations which are another important outcome of our investigations. The study of chaotic dynamics of these nonlinear oscillators under further perturbations is one of the current topics[23] in the contemporary literature in nonlinear dynamics. In principle one can extend such analysis to the above-generalized equations as well.

In this paper, we also have not touched the question of linearizability of the integrable cases of Eq. (9). In our earlier work, we have shown that Eq. (55) is linearizable to the free particle

equation, $d^2w/dz^2=0$. Of course one can show that this is the only linearizable equation in (9) through invertible point transformation.[9,11,19] However, linearizablity of other integrable cases through more general transformations still remains to be explored.

In addition to the above, we have also carried out the Painlevé singularity structure analysis of Eq. (9) and compared the results obtained through both the methods. The details of this will be published elsewhere.

As we mentioned at the end of Sec. II, the crux of the PS procedure lies in finding the explicit solutions satisfying all three determining equations (22)–(24). In this paper we have considered only certain specific Ansatz forms to determine the null forms S, and integrating factors R. As a consequence only a specific class of integrable equations have been derived. It is not clear whether the Ansatz forms used in this paper exhaust all possible integrable cases of Eq. (9). One needs to consider more generalized Ansatz forms, and if possible to solve Eqs. (22)–(24) for the most general forms of R and S, and try to identify all possible integrable cases underlying Eq. (9). This is being explored further.

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On Shannon entropies in μ-deformed Segal-Bargmann analysis

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We consider a μ-deformation of the Segal-Bargmann transform, which is a unitary map from a μ-deformed quantum configuration space onto a μ-deformed quantum phase space (the μ-deformed Segal-Bargmann space). Both of these Hilbert spaces have canonical orthonormal bases. We obtain explicit formulas for the Shannon entropy of some of the elements of these bases. We also consider two reverse log-Sobolev inequalities in the μ-deformed Segal-Bargmann space, which have been proved in a previous work, and show that a certain known coefficient in them is the best possible. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this paper we will study a certain entropy in the context of a deformation of quantum mechanics called μ-deformed Segal-Bargmann analysis. This latter we will describe further on. So to start we would like to discuss the role of entropy in quantum mechanics in order to place this work in a broader context. (The text by Ohya and Petz[23] is a good general reference for this.) First of all, the concept of entropy comes from thermodynamics as developed in the 19th century. Entropy was later interpreted in terms of the classical statistical mechanics of the constituent entities (molecules) of matter. This led to the idea that entropy measures the uncertainty (meaning a lack of complete knowledge or information) on a microscopic scale of a macroscopic thermodynamic state. After quantum mechanics was formulated as a physical theory by Schrödinger and Heisenberg, the concept of entropy was soon introduced into this new theory in Ref. 37 by von Neumann, who took thermodynamics as a source of intuition.

The point was to define an entropy of a quantum mechanical state which von Neumann had defined as a positive (and so self-adjoint) trace class operator ρ with $\mathrm{Tr}\,\rho=1$. This operator could in turn be expanded by the spectral theorem in terms of an orthonormal basis $\{\phi_k\}$, depending on ρ, of the underlying Hilbert space of the quantum system under consideration as $\rho=\Sigma_k\lambda_k|\phi_k\rangle\langle\phi_k|$, where $\{\lambda_k\}$ is the set of eigenvalues of ρ and $|\phi_k\rangle\langle\phi_k|$ is the Dirac notation for the orthogonal projection whose range in the one-dimensional subspace spanned by the normalized eigenvector ϕ_k of ρ. The hypotheses on ρ imply that $\lambda_k\geqslant 0$ and $\Sigma_k\lambda_k=1$.

The *pure states* in quantum mechanics are usually thought of as the vectors ψ in the Hilbert space with $\|\psi\|=1$, modulo the equivalence relation $\psi_1\sim\psi_2$ provided that $\psi_1=e^{i\alpha}\psi_2$ for some real number α. In the present context, this is the same as taking the pure states to be the orthogonal projections $|\psi\rangle\langle\psi|$ with ψ satisfying $\|\psi\|=1$. Physical intuition says that any two pure states should have the same entropy, and since entropy in thermodynamics is only defined up to an overall additive constant (as is voltage in electrostatics), one can take the entropy of the pure states to be zero. These considerations, among others, led von Neumann to define the entropy of a general

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state ρ (also called a *density matrix* or a *mixed state*) as $-\Sigma_k \lambda_k \log \lambda_k$, using the above notation. (We set $0 \log 0 = 0$ by convention.)

Some years later while developing a mathematical theory of communication Shannon (in Ref. 31) introduced a similar definition for the entropy of a probability distribution. Specifically, for a discrete probability space S with probability p_k for each $k \in S$ (so that $p_k \geqslant 0$ and $\Sigma_{k \in S} p_k = 1$), the entropy defined by Shannon is $-\Sigma_{k \in S} p_k \log p_k$, the same formula as used by von Neumann but in another context (and with another notation). These two entropies, as well as natural adaptations of them to more general situations, have been used in many applications in physics, mathematics, computer science and so on. Note that our Definition 2.5 is one such adaptation. (We dropped the minus sign in Definition 2.5 to obtain a positive quantity, so that technically speaking what we then have is an "information" rather than an "uncertainty" or "entropy.")

However, there also arise situations in quantum mechanics where one is led to nontrivial entropies of pure states. To our knowledge the first instance of this in the literature occurs in an article (Ref. 14) by Hirschman in 1957, where the interest is in understanding the relation between a function f and its Fourier transform $\mathcal{F}f$ in terms of an "information" content. Under some hypotheses on $f \in L^2(\mathbf{R})$, Hirschman shows that

$$E_{\mathrm{Sh}}(|f|^2) + E_{\mathrm{Sh}}(|\mathcal{F}f|^2) \leqslant 0,$$

where $E_{\mathrm{Sh}}(g) = \int_{\mathbf{R}} \mathrm{d}x\, g(x) \log g(x)$ is the appropriate Shannon entropy of a function $g \geqslant 0$ in this context and $\mathcal{F}f(k) = \int_{\mathbf{R}} \mathrm{d}x\, e^{-2\pi i k x} f(x)$ is the Fourier transform of f. Moreover, Hirschman conjectured (and many years later in 1975 Beckner[5] proved) that

$$E_{\mathrm{Sh}}(|f|^2) + E_{\mathrm{Sh}}(|\mathcal{F}f|^2) \leqslant \log 2 - 1,$$

where the constant on the right-hand side is now optimal. From this second stronger version Hirschman proved the Heisenberg uncertainty principle in the usual form (due actually to Kennard in Ref. 15) that says that the product of the variances of $|f|^2$ and $|\mathcal{F}f|^2$ has a positive lower bound, or explicitly that

$$\mathrm{Var}(|f|^2)\mathrm{Var}(|\mathcal{F}f|^2) \geqslant \frac{1}{16\pi^2}$$

for our definition of the Fourier transform and with $\|f\|_{L^2} = 1$. Consequently, entropy-entropy inequalities of the sort proved by Hirschman and Beckner are often called entropic uncertainty relations. (See Chap. 16 in Ref. 23.)

Later in 1975, Gross[10] studied log-Sobolev inequalities, which are a type of energy-entropy inequality, again involving a Shannon entropy of a pure state as in Definition 2.5. These inequalities arose in the mathematical study of quantum field theory (see Ref. 8) and have found many applications in quantum theory, statistical mechanics, analysis, probability, etc. A recent survey with many references to the literature in statistical mechanics and probability is Ref. 11. It turns out that log-Sobolev inequalities are related to hypercontractivity, with this relation going back to Federbush's work[8] in 1969. For a rather comprehensive review of the literature on hypercontractivity up to the time of its publication in 1992, see Ref. 7.

Using the article[14] of Hirschman in Fourier analysis as an inspiration, but also keeping in mind the ground-breaking article (Ref. 10), Sontz in Ref. 33 began a study of Segal-Bargmann analysis, and in particular the Segal-Bargmann transform, in terms of a Shannon entropy that arises naturally in that context. This led to new Hirschman-type inequalities (that is, entropic uncertainty relations) and log-Sobolev inequalities, but also rather surprisingly to a reverse log-Sobolev inequality, where the Shannon entropy times a positive constant (together with a norm term) dominates the energy. (In a log-Sobolev inequality, the Shannon entropy is bounded above by a positive constant times the energy.) For a review of these results plus a number of open problems and more references, see Ref. 35.

More recently, Sontz and collaborators (in Refs. 2, 3, and 24) have established similar inequalities in μ-deformed Segal-Bargmann analysis, where the entropy is again an adaptation of

Shannon entropy to the theory. The present paper is a continuation of those works. We would like to understand better these inequalities and, in particular, their optimal constants. The results of Sec. VI are one step in that direction. In this paper we propose to study the entropies of the canonical basis elements of the μ-deformed Hilbert spaces. While it remains an open problem whether these functions are those that give us the optimal constants of the various inequalities that we have proved in our previous works, it is an interesting problem in its own right to evaluate these entropies since they are natural quantities in the theory. A minor surprise is that Euler's constant appears, though this constant has a way of "spontaneously" arising in many situations in analysis. This extends earlier work by Sontz in Ref. 34 to the context of another quantization scheme of classical mechanics, which we will call μ-deformed quantum mechanics and which we will explain shortly.

As a final comment about entropy in quantum mechanics, let us note that the Shannon entropy we are using is closely related to the Wehrl entropy, as introduced in Ref. 39. The idea of Wehrl in our terminology is to take first the Segal-Bargmann transform (described below) of a pure state ψ and then to calculate the Shannon entropy of the resulting state ϕ in the Segal-Bargmann space. (However, his formula is different since he uses a related coherent state transform.) This is then called the *classical entropy* of the state ψ. (This can also be done for mixed states.) We prefer however to refer to this as the Shannon entropy of ϕ, since ψ has its own Shannon entropy, which is not in general equal to the Shannon entropy of ϕ. (See Ref. 33.) We note that Lieb in Ref. 18 proves a reasonable conjecture of Wehrl concerning an inequality for the Wehrl entropy (see Ref. 39), and that he also makes a conjecture about a similar sort of inequality for a finite-dimensional situation involving the Bloch coherent states for spin. Also this conjectured inequality involves a Wehrl entropy, so that it should be amenable to our point of view. However, despite some recent partial results (Refs. 6 and 28), this tantalizing conjecture remains unsolved. And this even though Lieb proved in Ref. 18 the supposedly harder conjecture of Wehrl (in an infinite-dimensional context) almost 30 years ago.

We now review some structures in usual quantum mechanics as preparation for discussing a deformation of it. Two of the basic operators in quantum mechanics for a single one-dimensional particle are the position operator Q and the momentum operator P, which can be represented as $Q\psi(x)=x\psi(x)$ and $P\psi(x)=-i(d/dx)\psi(x)$, acting on complex-valued functions ψ belonging to (a dense subspace of) the Hilbert space $L^2(\mathbb{R},\mathrm{d}x)$. (This space is commonly thought of as a quantum configuration space.) It turns out that P and Q are self-adjoint operators in $L^2(\mathbb{R},\mathrm{d}x)$ and that they satisfy the commutation relation $[P,Q]=-iI$, called the *canonical commutation relation* (CCR). In terms of Q and P we can define the operators $a=2^{-1/2}(Q+iP)$ (annihilation) and $a^*=2^{-1/2}(Q-iP)$ (creation), which are each adjoint to the other and satisfy the CCR $[a,a^*]=I$. In 1932 Fock[9] realized that the relation $[a,a^*]=I$ is also satisfied by the operators $a\varphi(z)=(d/dz)\varphi(z)$ and $a^*\varphi(z)=z\varphi(z)$ acting on the space of all holomorphic functions φ. This interesting observation opened a critical mathematical question: does there exist a Hilbert space of holomorphic functions where the operators described above are each adjoint to the other? In 1961 Bargmann[4] answered this question giving the mathematical foundations for Fock's observation. He defined a Gaussian measure $\mathrm{d}\nu_{\mathrm{Gauss}}$ and considered the holomorphic subspace $\mathcal{B}^2$ of the Hilbert space $L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})$, and showed that in $\mathcal{B}^2$ the creation and annihilation operators are adjoints of each other. [It turns out that $\mathcal{B}^2$ is closed in $L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})$, and then is itself a Hilbert space.] Because of this and similar work by Segal,[29,30] the space $\mathcal{B}^2$ is known as the *Segal-Bargmann space*, and this space is commonly thought of as a quantum phase space.

So we have two Hilbert spaces, $L^2(\mathbb{R},\mathrm{d}x)$ and $\mathcal{B}^2$, in both of which are defined two unbounded operators a and a^*, each adjoint to the other and satisfying the CCR $[a,a^*]=I$. One refers to this fact by saying that the spaces $L^2(\mathbb{R},\mathrm{d}x)$ and $\mathcal{B}^2$ carry representations of the Lie group generated by the exponentiated form of the CCR. It turns out that these representations are irreducible. The so-called Bargmann transform $\tilde{B}:L^2(\mathbb{R},\mathrm{d}x)\to\mathcal{B}^2$ (also described in Ref. 4) is an isomorphism, that is a unitary onto map, between these two quantum spaces which also intertwines the actions of a and a^*. It is possible to replace the quantum configuration space $L^2(\mathbb{R},\mathrm{d}x)$ by another unitarily equivalent space, namely $L^2(\mathbb{R},\mathrm{d}g)$, called the *ground state representation*, where $\mathrm{d}g$ is another

Gaussian measure. In this case, the resulting transform B that maps the ground state representation unitarily onto the Segal-Bargmann space is called the *Segal-Bargmann transform*. What we call *Segal-Bargmann analysis* has to do mainly with the study of operators related to B and spaces of holomorphic functions related to $\mathcal{B}^2$. The present work is a part of Segal-Bargmann analysis. For other related works in the theory of white noise see Kuo's book[16] (where the S-transform is essentially the Segal-Bargmann transform), in microlocal analysis see the works of Martinez[22] and of Sjöstrand[32] (where the FBI transform is closely related though not identical to the Segal-Bargmann transform), in heat kernel analysis (since the kernel function of the Segal-Bargmann transform is related to the heat kernel) see the review article of Hall,[13] in coherent state theory see the book by Ali, Antoine, and Gazeau[1] (since the Segal-Bargmann transform is an example of a coherent state transform), and in all the references therein.

It is easy to see that the CCR implies the *equations of motion* $i[P,H]=Q$ and $i[Q,H]=-P$, where $H:=2^{-1}(P^2+Q^2)$ is the Hamiltonian of the harmonic oscillator. In 1950, Wigner[40] proved that the converse implication is false by exhibiting unbounded operators P_μ and Q_μ, labeled by a parameter $\mu>-1/2$, that satisfy the equations of motion, where $H_\mu:=2^{-1}(P_\mu^2+Q_\mu^2)$ replaces H, but do not satisfy the CCR. We consider this μ-deformation of quantum mechanics to be interesting since it gives a mathematically consistent way of effecting a quantization of classical mechanics. It is well known that at a mathematical level quantization is not unique. However in physics we see that nature manifests just one of these possibilities. (Nelson refers to this as "a mystery" in an oft-cited quotation. See Ref. 25, p. 207.) We hope that further mathematical studies will be able to elucidate the mathematical properties characteristic of nature's choice. As a further comment, we should note that experiment can set a limit on the absolute value of the parameter μ, but cannot definitively prove that it is equal to zero.

Later, Rosenblum and Marron (in Refs. 26, 27, and 21) realized these operators P_μ and Q_μ explicitly acting in a μ-quantum configuration space $L^2(\mathbb{R},|x|^{2\mu}\mathrm{d}x)$ and in a μ-Segal-Bargmann space $\mathcal{B}_\mu^2$. They also defined a μ-Bargmann transform $\widetilde{B}_\mu$, which is a unitary onto transformation mapping the former Hilbert space to the latter Hilbert space. This theory can be understood as a μ-deformation of standard Segal-Bargmann analysis with the property that if one sets $\mu=0$ the standard theory is recovered (see Ref. 36). So we will refer to $L^2(\mathbb{R},|x|^{2\mu}\mathrm{d}x)$ and $\mathcal{B}_\mu^2$, as the "μ-deformed quantum configuration space" and the "μ-deformed Segal-Bargmann space," respectively, and to $\widetilde{B}_\mu$ as the "μ-deformed Bargmann transform." It is also straightforward to obtain explicitly the "μ-deformed ground state representation" $L^2(\mathbb{R},\mathrm{d}g_\mu)$ and the "μ-deformed Segal-Bargmann transform" B_μ, which is a unitary map from $L^2(\mathbb{R},\mathrm{d}g_\mu)$ onto $\mathcal{B}_\mu^2$.

In Ref. 34, Sontz obtained explicit formulas for the entropy of relevant elements of the Hilbert spaces $L^2(\mathbb{R},\mathrm{d}g)$ and $\mathcal{B}^2$, namely, elements of the corresponding canonical (orthonormal) basis of these spaces. By denoting by ζ_n, $n=0,1,\ldots$ the functions of the canonical basis $\{\zeta_n\}_{n=0}^\infty$ of the ground state representation $L^2(\mathbb{R},\mathrm{d}g)$, and by ξ_n, $n=0,1,\ldots$ the functions of the canonical basis $\{\xi_n\}_{n=0}^\infty$ of the Segal-Bargmann space $\mathcal{B}^2$, Sontz proved in Ref. 34 that for $n=0,1,\ldots$ one has that

$$S_{L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})}(\xi_n)=n\left(-\gamma+1+\frac{1}{2}+\cdots+\frac{1}{n}\right)-\log n!, \tag{1.1}$$

$$S_{L^2(\mathbb{R},\mathrm{d}g)}(\zeta_1)=2-\log 2-\gamma, \tag{1.2}$$

where γ is Euler's constant.

In this work we will obtain for the μ-deformed theory results similar to (1.1) and (1.2). More precisely, in Theorem 4.3 we will show that for any $\mu>-1/2$, the entropy $S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(\xi_n^\mu)$ of the nth μ-deformed element ξ_n^μ, $n=0,1,\ldots$, of the μ-deformed canonical basis $\{\xi_n^\mu\}_{n=0}^\infty$ of the μ-deformed Segal-Bargmann space $\mathcal{B}_\mu^2$ is given by

$$S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(\xi_n^\mu)=\frac{n}{2}\left(\psi\left(\mu+\frac{n+\theta(n)+1}{2}\right)+\psi\left(\frac{n+\theta(n+1)+1}{2}\right)\right)-\log\frac{\gamma_\mu(n)}{2^n},\qquad(1.3)$$

where ψ is the logarithmic derivative of the gamma function, θ is the characteristic function of the odd positive integers, and γ_μ is a μ-deformation of the factorial function (defined in Sec. II). We will show that in the case $\mu=0$ this formula reduces to (1.1), so (1.3) is a generalization of (1.1) for the μ-deformed theory. Also, in Sec. IV we will show that the entropy $S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu)$ of the μ-deformed element ζ_1^μ of the μ-deformed canonical basis $\{\zeta_n^\mu\}_{n=0}^\infty$ of the μ-deformed ground state representation $L^2(\mathbb{R},\mathrm{d}g_\mu)$ is given by

$$S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu)=\psi\left(\mu+\tfrac{3}{2}\right)-\log\left(\mu+\tfrac{1}{2}\right),\qquad(1.4)$$

and when $\mu=0$ this formula reduces to (1.2), so (1.4) generalizes (1.2).

In this paper we want to emphasize the importance of an idea that has not played a role in our previous research in Segal-Bargmann analysis. This is the idea of an extensive quantity, which meant originally in the context of thermodynamics a quantity proportional to the size of a physical system. In the context of this paper the size is the index n (or *quantum number*) of the states forming the canonical orthonormal bases of the Hilbert spaces under study. So we say that a number depending on the nth basis element is an *extensive quantity* if it is asymptotically proportional to n. For example, the energy levels of the harmonic oscillator are extensive in this sense of the word. So our main results in Sec. IV concerning the entropies of the basis elements ξ_n^μ show these entropies to be extensive quantities. At one and the same time this shows that entropy is a useful concept from a physical point of view as well as that the μ-deformation of quantum mechanics under study here has this desirable property. Even though being an extensive quantity according to our definition is an asymptotic property, we realize this result by an actual explicit computation of the entropies and only later by doing the asymptotic analysis. In Sec. V we do a similar analysis of the entropies of the monomials t^n in $L^2(\mathbb{R},\mathrm{d}g_\mu)$, basically because we have the mathematical tools for doing this. But it turns out that these entropies are not extensive quantities. This is not surprising since these monomials, while mathematically simple, are not the eigenfunctions of a physically interesting self-adjoint operator. In Sec. VI, we study a μ-deformed energy (defined there) and, among other things, show that it is an extensive quantity.

We now outline in detail the content of the work. In Sec. II we give, on the one hand, the definitions and notation of the μ-deformed objects that will be used throughout the work [here we introduce the μ-deformed Hilbert spaces $L^2(\mathbb{R},\mathrm{d}g_\mu)$ and $\mathcal{B}_\mu^2$, and their canonical bases as well]. On the other hand, we give the definition of the Shannon entropy of a function f in a complex Hilbert space $L^2(\Omega,\mathrm{d}\nu)$ where $(\Omega,\mathrm{d}\nu)$ is a finite measure space. All the material in Sec. II is previously known and is included here only for the clarity of the exposition. In Sec. III we prove some results about the behavior of the μ-deformed factorial function γ_μ and of the logarithmic derivative ψ of the gamma function [both involved in formula (1.3)], that will help us to obtain some properties of the sequence of entropies of the functions ξ_n^μ, $n=0,1,\ldots$. In particular, these entropies are extensive quantities. These properties are not explicitly given (in the case $\mu=0$) in Ref. 34, but we give them as a proposition at the end of Sec. III. Lemma 3.1 in Sec. III is new for us, but we can hardly claim originality for a result about the well-studied special function ψ. However, Lemma 3.2 and the rest of the results of this article (except as noted in Sec. VI) are new. In Sec. IV, besides the discussion that led us to formula (1.3) which generalizes (1.1), we also obtain a generalization of the proposition at the end of Sec. III about some properties of the sequence of entropies. Again, these entropies are extensive quantities. In Sec. V we consider the μ-deformed ground state representation and we obtain explicit formulas for the entropies of the monomials $t^n \in L^2(\mathbb{R},\mathrm{d}g_\mu)$, $n=0,1,\ldots$ and these turn out not to be extensive quantities. Unfortunately the technique we use here to obtain these formulas (and those of Sec. IV) does not work to obtain the entropies of the elements ζ_n^μ of the canonical basis of $L^2(\mathbb{R},\mathrm{d}g_\mu)$, for $n\geqslant 2$. It turns out that our method for calculating the entropy of a function f works only in the case of f being a monomial, and the elements ζ_n^μ are monomials only for $n=0,1$. Also, by means of a concrete example, in Sec. V we show that the μ-deformed Segal-Bargmann transform B_μ does not preserve entropy. In Sec.

VI we consider two reverse log-Sobolev inequalities proved in Ref. 3, in which the condition $c>1$ of a certain parameter c appears as a sufficient condition. In this section we show that this condition is also necessary, or in other words, that the condition $c>1$ is the best possible. Finally, in Sec. VII we make some comments about what we left unfinished in this paper and what is possible to do beyond the results presented here.

We would also like to note that our results can be generalized to the case of $\mathbb{R}^n$ and $\mathbb{C}^n$ (in place of $\mathbb{R}$ and $\mathbb{C}$) for any integer $n>1$. This works out because the functions (of n variables) of the canonical bases can be factored as products of functions (of one variable), which are precisely the basis elements considered here in the one-dimensional case. Since all the relevant measures also factorize in terms of the measures used here, we can immediately calculate all the entropies of the basis functions in dimension n in terms of the entropies studied here in the one-dimensional case. (See Lemma 2.1 in Ref. 34.)

II. DEFINITIONS AND NOTATION

In this section we give the definitions and the notation that we will use throughout the work. First, we take $\mu>-\frac{1}{2}$ to be a fixed parameter (unless otherwise stated). The (Coxeter) group $\mathbb{Z}_2$ is the multiplicative group $\{-1,1\}$, and log is the natural logarithm (base e). We use the convention $0\log 0=0$ [which makes the function $\phi:[0,\infty)\to\mathbb{R}$, $\phi(x)=x\log x$ continuous]. We also use the convention that C denotes a constant (a quantity that does not depend on the variables of interest in the context), which may change its value every time it appears. We denote by $\mathcal{H}(\mathbb{C})$ the space of holomorphic functions $f:\mathbb{C}\to\mathbb{C}$ with the topology of uniform convergence on compact sets.

We begin by defining the μ-deformations of the factorial function and of the exponential function. Let $\mathbb{N}$ denote the set of positive integers.

Definition 2.1: The μ-deformed factorial function $\gamma_\mu:\mathbb{N}\cup\{0\}\to\mathbb{R}$ is defined by $\gamma_\mu(0)=1$ and

$$\gamma_\mu(n) := (n+2\mu\theta(n))\gamma_\mu(n-1),$$

where $n\in\mathbb{N}$ and $\theta:\mathbb{N}\to\{0,1\}$ is the characteristic function of the odd positive integers. The μ-deformed exponential function $\mathbf{e}_\mu:\mathbb{C}\to\mathbb{C}$, is defined by the power series

$$\mathbf{e}_\mu(z) := \sum_{n=0}^{\infty}\frac{z^n}{\gamma_\mu(n)}.$$

We note that $\gamma_0(n)=n!$ (the usual factorial function) and so $\mathbf{e}_0(z)=\exp(z)$ (the usual complex exponential function). It is clear that the power series in the definition of $\mathbf{e}_\mu(z)$ is absolutely convergent for all $z\in\mathbb{C}$. So the μ-deformed exponential $\mathbf{e}_\mu$ is an entire function.

We will use the following explicit formulas for $\gamma_\mu(2n)$ and $\gamma_\mu(2n+1)$, $n=0,1,2,\ldots$ (see Ref. 26, p. 371):

$$\gamma_\mu(2n)=\frac{2^{2n}\Gamma(n+1)\Gamma\left(\mu+n+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}=\frac{(2n)!\Gamma\left(\frac{1}{2}\right)\Gamma\left(\mu+n+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)\Gamma\left(n+\frac{1}{2}\right)}, \tag{2.1}$$

$$\gamma_\mu(2n+1)=\frac{2^{2n+1}\Gamma(n+1)\Gamma\left(\mu+n+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}=\frac{(2n+1)!\Gamma\left(\frac{1}{2}\right)\Gamma\left(\mu+n+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)\Gamma\left(n+\frac{3}{2}\right)}. \tag{2.2}$$

The following definition (from Ref. 26) gives us a μ-deformation of the classical Hermite polynomials.

Definition 2.2: For $n=0,1,\ldots$ *we define the* nth μ*-deformed Hermite polynomial* $H_n^\mu(t)$ *by the generating function*

$$\exp(-z^2)\mathbf{e}_\mu(2tz)=\sum_{n=0}^{\infty}H_n^\mu(t)\frac{z^n}{n!}.$$

It is easy to check that $H_n^\mu(t)$ is in fact a polynomial of degree n in the real variable t. For example, we have that $H_0^\mu(t)=1$, $H_1^\mu(t)=[2/(1+2\mu)]t$, $H_2^\mu(t)=[4/(1+2\mu)]t^2-2$, and so on.

The normalized μ-deformed Hermite polynomials $\zeta_n^\mu(t)$, $n=0,1,\ldots$ defined by

$$\zeta_n^\mu(t):=2^{-n/2}(n!)^{-1}(\gamma_\mu(n))^{1/2}H_n^\mu(t), \tag{2.3}$$

form an orthonormal basis of the μ-deformed ground state representation $L^2(\mathbb{R},\mathrm{d}g_\mu)$, where $\mathrm{d}g_\mu$ is the μ*-deformed Gaussian measure* defined by

$$\mathrm{d}g_\mu(t):=\left(\Gamma\left(\mu+\frac{1}{2}\right)\right)^{-1}\exp(-t^2)|t|^{2\mu}\,\mathrm{d}t. \tag{2.4}$$

The basis $\{\zeta_n^\mu\}_{n=0}^\infty$ is called *the canonical basis of* $L^2(\mathbb{R},\mathrm{d}g_\mu)$. (See Refs. 26 and 24.)

The case $\mu=0$ recovers the well-known fact that for $n=0,1,\ldots$, the normalized polynomials $\zeta_n(t)=2^{-n/2}(n!)^{-1/2}H_n(t)$, where $H_n(t)$ denotes the nth Hermite polynomial, form the canonical orthonormal basis of the ground state representation $L^2(\mathbb{R},\mathrm{d}g)$, where $\mathrm{d}g$ is the Gaussian probability measure $\mathrm{d}g(t)=\pi^{-1/2}\exp(-t^2)\mathrm{d}t$. (See Ref. 12.)

Definition 2.3: We define the measure $\mathrm{d}\nu_\mu$ *on the space* $\mathbb{C}\times\mathbb{Z}_2$ *by*

$$\mathrm{d}\nu_\mu(z,1):=\frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)}K_{\mu-1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y, \tag{2.5}$$

$$\mathrm{d}\nu_\mu(z,-1):=\frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)}K_{\mu+1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y, \tag{2.6}$$

where Γ *is the Euler gamma function,* K_α *is the Macdonald function of order* α *(both defined in Ref. 17), and* $\mathrm{d}x\,\mathrm{d}y$ *is Lebesgue measure on* $\mathbb{C}$.

By using that $\mathbb{C}\cong\mathbb{C}\times\{1\}\cong\mathbb{C}\times\{-1\}$, we will identify the restrictions (2.5) and (2.6) as measures on $\mathbb{C}$.

The Macdonald function K_α is the modified Bessel function of the third kind (with purely imaginary argument, as described in Ref. 38, p. 78), which is known to be a holomorphic function on $\mathbb{C}\backslash(-\infty,0]$ and is entire with respect to the parameter α. Nevertheless, our interest will be only in the values and behavior of this function for $x\in\mathbb{R}^+$ and $\alpha\in\mathbb{R}$. For $z\in\mathbb{C}$, $|\arg z|<\pi$ and $\alpha\notin\mathbb{Z}$, the Macdonald function can be defined as

$$K_\alpha(z)=\frac{\pi}{2}\frac{I_{-\alpha}(z)-I_\alpha(z)}{\sin(\alpha\pi)}$$

(see Ref. 17, p. 108), where $I_\alpha(z)$ is the modified Bessel function of the first kind. For $\alpha\in\mathbb{Z}$, we define $K_\alpha(z)=\lim_{\beta\to\alpha}K_\beta(z)$. This expression shows that $K_a(z)$ is an even function of the parameter α. In particular, since $I_{1/2}(z)=(2/\pi z)^{1/2}\sinh z$ and $I_{-1/2}(z)=(2/\pi z)^{1/2}\cosh z$ (see Ref. 17, p. 112), we have that

$$K_{\pm 1/2}(z) = \left(\frac{\pi}{2z}\right)^{1/2} \exp(-z),$$

which shows that for $\mu=0$ the measures defined on $\mathbb{C}$ by (2.5) and (2.6) are the same Gaussian measure,

$$\mathrm{d}\nu_0(z,1) = \mathrm{d}\nu_0(z,-1) = \pi^{-1} \exp(-|z|^2)\mathrm{d}x\,\mathrm{d}y,$$

which is the Gaussian measure $\mathrm{d}\nu_{\mathrm{Gauss}}$ of the Segal-Bargmann space $\mathcal{B}^2=\mathcal{H}(\mathbb{C})\cap L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})$.

By using the formula

$$\int_0^\infty K_\alpha(s)s^{\beta-1}\,\mathrm{d}s = 2^{\beta-2}\Gamma\left(\frac{\beta-\alpha}{2}\right)\Gamma\left(\frac{\beta+\alpha}{2}\right), \tag{2.7}$$

which holds if $\mathrm{Re}\,\beta>|\mathrm{Re}\,\alpha|$ (see Ref. 38, p. 388), we can see that (2.5) and (2.6) are finite measures on $\mathbb{C}$, and moreover that the former is a probability measure. (See Ref. 24.)

The integral representation

$$K_\alpha(z) = \int_0^\infty \exp(-z\cosh u)\cosh(\alpha u)\mathrm{d}u, \quad \mathrm{Re}\,z>0 \tag{2.8}$$

(see Ref. 17, p. 119) gives us at once two important properties of the Macdonald function. The first is that $K_\alpha(x)>0$ for all $x\in\mathbb{R}^+$, and the second is that K_α is a monotone decreasing function for $x\in\mathbb{R}^+$.

We will work with the Hilbert space $L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)$. The norm of a vector $f\in$ will be denoted by $\|f\|_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}$. Let us consider the space

$$\mathfrak{H}_{2,\mu} = \{f:\mathbb{C}\to\mathbb{C} | f_e \in L^2(\mathbb{C},\,\mathrm{d}\nu_\mu|_{\mathbb{C}\times\{1\}}) \text{ and } f_o \in L^2(\mathbb{C},\,\mathrm{d}\nu_\mu|_{\mathbb{C}\times\{-1\}})\},$$

where $f=f_e+f_o$ is the decomposition of f into its even and odd parts. (We will use this decomposition and its notation without further comment.) Observe that when $\mu=0$ we have $\mathfrak{H}_{2,0}=L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})$.

For $f\in\mathfrak{H}_{2,\mu}$ we define

$$\|f\|^2_{\mathfrak{H}_{2,\mu}} := \|f_e\|^2_{L^2(\mathbb{C},\,\mathrm{d}\nu_\mu|_{\mathbb{C}\times\{1\}})} + \|f_o\|^2_{L^2(\mathbb{C},\,\mathrm{d}\nu_\mu|_{\mathbb{C}\times\{-1\}})}.$$

The linear map $\Phi:\mathfrak{H}_{2,\mu}\to L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)$ defined as $(\Phi f)(z,1)=f_e(z)$ and $(\Phi f)(z,-1)=f_o(z)$ is injective and has the property that

$$\|f\|_{\mathfrak{H}_{2,\mu}} = \|\Phi f\|_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)} \tag{2.9}$$

for all $f\in\mathfrak{H}_{2,\mu}$. Therefore $\|\cdot\|_{\mathfrak{H}_{2,\mu}}$ is a norm on $\mathfrak{H}_{2,\mu}$. It is not hard to show that the range of Φ is a closed subspace of $L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)$. Therefore $\mathfrak{H}_{2,\mu}$ is a Hilbert space, since we have identified it with a closed subspace of the Hilbert space $L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)$. For a function $f\in\mathfrak{H}_{2,\mu}$ we will sometimes write its norm as $\|f\|_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}$, meaning that we are using (2.9) and identifying f with Φf.

We will use the notations $\mathrm{d}\nu_{e,\mu}$ and $\mathrm{d}\nu_{o,\mu}$ for the restrictions $\mathrm{d}\nu_\mu|_{\mathbb{C}\times\{1\}}$ and $d\nu_\mu|_{\mathbb{C}\times\{-1\}}$, respectively. So for $f\in\mathfrak{H}_{2,\mu}$ we have

$$\|f\|^2_{\mathfrak{H}_{2,\mu}} = \|f_e\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})} + \|f_o\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})} = \|f_e\|^2_{\mathfrak{H}_{2,\mu}} + \|f_o\|^2_{\mathfrak{H}_{2,\mu}}.$$

Definition 2.4: The μ-deformed Segal-Bargmann space, denoted by $\mathcal{B}^2_\mu$, is defined as

$$\mathcal{B}^2_\mu := \mathcal{H}(\mathbb{C}) \cap \mathfrak{H}_{2,\mu}. \tag{2.10}$$

That is, $\mathcal{B}^2_\mu$ is the holomorphic subspace of $\mathfrak{H}_{2,\mu}$. It turns out that $\mathcal{B}^2_\mu$ is closed in $\mathfrak{H}_{2,\mu}$, and then it is also closed in $L^2(\mathbb{C}\times\mathbb{Z}_2, d\nu_\mu)$, so $\mathcal{B}^2_\mu$ is itself a Hilbert space. (The proof of this fact does not depend on μ; see Theorem 2.2 in Ref. 12 for the case $\mu=0$.) Observe that when $\mu=0$ we have $\mathcal{B}^2_0=\mathcal{H}(\mathbb{C})\cap\mathfrak{H}_{2,0}=\mathcal{H}(\mathbb{C})\cap L^2(\mathbb{C}, d\nu_{\text{Gauss}})=\mathcal{B}^2$.

If we decompose the space $\mathcal{H}(\mathbb{C})$ of holomorphic functions $f:\mathbb{C}\to\mathbb{C}$ as $\mathcal{H}(\mathbb{C})=\mathcal{H}_e(\mathbb{C})\oplus\mathcal{H}_o(\mathbb{C})$, where

$$\mathcal{H}_e(\mathbb{C}) := \{f \in \mathcal{H}(\mathbb{C}): f = f_e\}$$

and

$$\mathcal{H}_o(\mathbb{C}) := \{f \in \mathcal{H}(\mathbb{C}): f = f_o\}$$

are the subspaces of the even and odd functions of $\mathcal{H}(\mathbb{C})$, respectively, then by writing $\mathcal{H}(\mathbb{C}) \ni f=f_e+f_o$, the space $\mathcal{B}^2_\mu$ is just the space of holomorphic functions $f:\mathbb{C}\to\mathbb{C}$ such that the even part f_e (the odd part f_o) of f is square integrable with respect to the measure $d\nu_{e,\mu}$ (with respect to the measure $d\nu_{o,\mu}$, respectively). That is,

$$\mathcal{B}^2_\mu = \{f \in \mathcal{H}(\mathbb{C}): f_e \in L^2(\mathbb{C}, d\nu_{e,\mu}) \text{ and } f_o \in L^2(\mathbb{C}, d\nu_{o,\mu})\}.$$

Yet another way to think of $\mathcal{B}^2_\mu$ is as

$$\mathcal{B}^2_\mu = \mathcal{B}^2_{e,\mu} \oplus \mathcal{B}^2_{o,\mu}, \tag{2.11}$$

where

$$\mathcal{B}^2_{e,\mu} = \mathcal{H}_e(\mathbb{C}) \cap \mathfrak{H}_{2,\mu}$$

and

$$\mathcal{B}^2_{o,\mu} = \mathcal{H}_o(\mathbb{C}) \cap \mathfrak{H}_{2,\mu}$$

are the even and odd subspaces of $\mathcal{B}^2_\mu$.

Observe that the inner product of the Hilbert space $\mathcal{B}^2_\mu$ (from which the norm on $\mathcal{B}^2_\mu$ defined above comes) is

$$\langle f, g\rangle_{\mathcal{B}^2_\mu} = \langle f_e, g_e\rangle_{L^2(\mathbb{C}, d\nu_{e,\mu})} + \langle f_o, g_o\rangle_{L^2(\mathbb{C}, d\nu_{o,\mu})}. \tag{2.12}$$

We then have that $\mathcal{B}^2_{e,\mu}$ and $\mathcal{B}^2_{o,\mu}$ are orthogonal subspaces of $\mathcal{B}^2_\mu$, and that (2.11) holds as Hilbert spaces.

The monomials $\xi^\mu_n(z)$, $n=0,1,\ldots$ defined for $z\in\mathbb{C}$ by

$$\xi^\mu_n(z) := (\gamma_\mu(n))^{-1/2} z^n, \tag{2.13}$$

form an orthonormal basis of the μ-deformed Segal-Bargmann space $\mathcal{B}^2_\mu$. The basis $\{\xi^\mu_n\}_{n=0}^\infty$ is called the *canonical basis of* $\mathcal{B}^2_\mu$. When $\mu=0$ we obtain the monomials $\xi_n(z)=(n!)^{-1/2}z^n$, $n=0,1,\ldots$ which are known to form the canonical basis of the Segal-Bargmann space $\mathcal{B}^2$. (See Ref. 12.)

The μ-deformed Segal-Bargmann transform $B_\mu: L^2(\mathbb{R}, dg_\mu)\to\mathcal{B}^2_\mu$ can be defined as $B_\mu(\zeta^\mu_n)=\xi^\mu_n$, $n=0,1,\ldots$. It is clear that B_μ so defined is a unitary map. An explicit formula for B_μ is

$$(B_\mu f)(z) = \int_{\mathbb{R}} \exp\left(-\frac{z^2}{2}\right) \mathbf{e}_\mu(2^{1/2}tz) f(t) \mathrm{d}g_\mu(t). \tag{2.14}$$

(See Ref. 24.) When $\mu=0$ this formula becomes

$$(B_0 f)(z) = \int_{\mathbb{R}} \exp\left(-\frac{z^2}{2} + 2^{1/2}tz\right) f(t) \mathrm{d}g(t),$$

which is the undeformed Segal-Bargmann transform studied, for example, in Ref. 12, where it is shown that it is a unitary map from the quantum configuration space $L^2(\mathbb{R}, \mathrm{d}g)$ onto the quantum phase space $\mathcal{B}^2$.

Definition 2.5: Let $(\Omega, \mathrm{d}\nu)$ *be a finite measure space, that is,* $0 < \nu(\Omega) < \infty$. *For* $f \in L^2(\Omega, \mathrm{d}\nu)$, *the Shannon entropy* $S_{L^2(\Omega,\mathrm{d}\nu)}(f)$ *is defined by*

$$S_{L^2(\Omega,\mathrm{d}\nu)}(f) := \int_\Omega |f(\omega)|^2 \log |f(\omega)|^2 \, \mathrm{d}\nu(\omega) - \|f\|^2_{L^2(\Omega,\mathrm{d}\nu)} \log \|f\|^2_{L^2(\Omega,\mathrm{d}\nu)}. \tag{2.15}$$

By considering the convex function $\phi:[0,\infty) \to \mathbb{R}$, $\phi(x) = x \log x$, and the probability measure space $(\Omega, \mathrm{d}\nu')$, where $\mathrm{d}\nu' = W^{-1}\mathrm{d}\nu$, $W = \nu(\Omega)$, we have by Jensen's inequality (see Ref. 19, p. 38) that

$$\left(\int_\Omega |f(\omega)|^2 \, \mathrm{d}\nu(\omega)\right) \log\left(\frac{1}{W}\int_\Omega |f(\omega)|^2 \, \mathrm{d}\nu(\omega)\right) \leqslant \int_\Omega |f(\omega)|^2 \log |f(\omega)|^2 \, \mathrm{d}\nu(\omega)$$

or

$$(-\log W)\|f\|^2_{L^2(\Omega,\mathrm{d}\nu)} \leqslant S_{L^2(\Omega,\mathrm{d}\nu)}(f),$$

which shows that $S_{L^2(\Omega,\mathrm{d}\nu)}(f) \neq -\infty$, though $S_{L^2(\Omega,\mathrm{d}\nu)}(f) = +\infty$ can happen. In particular, this entropy is well defined for every element of $L^2(\Omega, \mathrm{d}\nu)$ since $\nu(\Omega)$ is finite. This is not so if $\nu(\Omega) = \infty$. For example, see Ref. 14 for the case of Lebesgue measure. Also observe that $S_{L^2(\Omega,\mathrm{d}\nu')}(f) \geqslant 0$, though $S_{L^2(\Omega,\mathrm{d}\nu)}(f)$ can be negative. Finally, note that $S_{L^2(\Omega,\mathrm{d}\nu)}(f)$ is homogeneous of degree 2.

Observe that for $f \in \mathcal{B}^2_\mu$, $f \neq 0$, the entropy $S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(f)$ is *not in general* equal to $S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(f_e) + S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(f_o)$. What we really have is

$$S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(f) = S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(f_e) + S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(f_o) + \|f_e\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})} \log \frac{\|f_e\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}}{\|f\|^2_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}}$$

$$+ \|f_o\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})} \log \frac{\|f_o\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}}{\|f\|^2_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}}. \tag{2.16}$$

Nevertheless, observe that if f is an even (odd) function, its entropy is given by $S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(f)$ [$S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(f)$, respectively]. Then, for the functions ξ^μ_n of the canonical basis of $\mathcal{B}^2_\mu$ we have $S^\mu_n = S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(\xi^\mu_n)$ when n is even, and $S^\mu_n = S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(\xi^\mu_n)$ when n is odd, where $S^\mu_n := S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(\xi^\mu_n)$, $n = 0, 1, 2, \ldots$.

III. PRELIMINARY RESULTS

In the calculations we will do in the Secs. IV and V, the derivative of the gamma function will arise naturally. Recall that the *logarithmic derivative* of $z \mapsto \Gamma(z)$, also called the *digamma function* and denoted by $\psi(z)$, is defined by

$$\psi(z) := \frac{\Gamma'(z)}{\Gamma(z)}$$

for all $z \neq 0, -1, -2, \ldots$. (See Ref. 17, p. 5.) We will be interested only in the values and behavior of $\psi(x)$ with $x \in \mathbb{R}^+$.

From the basic property of the gamma function $\Gamma(x+1)=x\Gamma(x)$ one obtains the formula

$$\psi(x+1) = \frac{1}{x} + \psi(x),$$

from which one gets by induction that

$$\psi(x+n) = \sum_{k=0}^{n-1} \frac{1}{x+k} + \psi(x)$$

for $n \in \mathbb{N}$. Using the identities $\psi(1)=-\gamma$ and $\psi(\frac{1}{2})=-\gamma-2\log 2$ (see Ref. 17, p. 6), the previous formula implies (by taking $x=1$ and $x=\frac{1}{2}$) that

$$\psi(n+1) = -\gamma + \sum_{k=1}^{n} \frac{1}{k}$$

and

$$\psi\left(n+\frac{1}{2}\right) = -\gamma - 2\log 2 + 2\sum_{k=1}^{n} \frac{1}{2k-1}.$$

When necessary we will use these formulas without further comment.

In this section we will state and prove two lemmas that we will be using in Secs. IV and V.

Lemma 3.1: (a) The inequality $0 < \psi(x+m) - \log x < (2m-1)(2x)^{-1}$ *holds for all* $x \in \mathbb{R}^+$ *and* $m \in \mathbb{N}$. *In particular, we have that for any* $m \in \mathbb{N}$

$$\lim_{x\to+\infty} (\psi(x+m) - \log x) = 0.$$

(b) For $y > 0$ *fixed we have that*

$$\lim_{x\to+\infty} (\psi(x+y) - \log x) = 0.$$

(c) The inequality $-x^{-1} < \psi(x) - \log x < -(2x)^{-1}$ *holds for all* $x \in \mathbb{R}^+$. *In particular, we have that*

$$\lim_{x\to+\infty} (\psi(x) - \log x) = 0.$$

Proof: From the integral representation of $\psi(z)$,

$$\psi(z) = \int_0^\infty \left(\frac{e^{-t}}{t} - \frac{e^{-tz}}{1-e^{-t}}\right) \mathrm{d}t,$$

and the integral representation of $\log(z)$,

$$\log(z) = \int_0^\infty \frac{e^{-t} - e^{-tz}}{t} \mathrm{d}t,$$

both valid for $\mathrm{Re}\, z > 0$ (see Ref. 17, pp. 6 and 7), one obtains for all $x > 0$ and $m > 0$ that

$$\psi(x+m)-\log x=\int_0^\infty\left(\frac{1}{t}-\frac{e^{-tm}}{1-e^{-t}}\right)e^{-tx}\,dt. \tag{3.1}$$

For $m\in\mathbb{N}$, let us consider the function $h_m:\mathbb{R}\to\mathbb{R}$,

$$h_m(t)=\frac{1}{t}-\frac{e^{-tm}}{1-e^{-t}},$$

where we define $h_m(0)=\lim_{t\to 0}h_m(t)=(2m-1)/2>0$. So h_m is continuous. For all $t>0$ we will prove by induction that $0<h_m(t)<(2m-1)/2$ holds for all $m\in\mathbb{N}$. Observe that $e^t>1+t$ for $t>0$ implies $h_1(t)>0$ for $t>0$. Also observe that $\beta(t)=\tanh(t/2)-(t/2)$ is a decreasing function in $\mathbb{R}^+$, so that $\tanh(t/2)<(t/2)$ for $t>0$, which implies that $h_1(t)<\frac{1}{2}$ for $t>0$. This proves the inequality $0<h_m(t)<(2m-1)/2$ for $m=1$. Suppose now that the inequality holds for a given $m\in\mathbb{N}$. The hypothesis $h_m(t)>0$ gives us

$$h_{m+1}(t)=\frac{1}{t}-\frac{e^{-tm}}{1-e^{-t}}e^{-t}=\left(\frac{1}{t}-\frac{e^{-tm}}{1-e^{-t}}\right)e^{-t}+\frac{1-e^{-t}}{t}>0$$

for $t>0$. Also, the case $m=1$ gives us that $(1/t)<\frac{1}{2}+[e^{-t}/(1-e^{-t})]$, which together with the hypothesis $h_m(t)<(2m-1)/2$ gives us (for $t>0$) that

$$\begin{aligned}h_{m+1}(t)&=\left(\frac{1}{t}-\frac{e^{-tm}}{1-e^{-t}}\right)e^{-t}+\frac{1-e^{-t}}{t}<\frac{2m-1}{2}e^{-t}+(1-e^{-t})\left(\frac{1}{2}+\frac{e^{-t}}{1-e^{-t}}\right)=\frac{2m-1}{2}e^{-t}+\frac{1+e^{-t}}{2}\\&=me^{-t}+\frac{1}{2}<\frac{2m+1}{2},\end{aligned}$$

as wanted. Then (3.1) and the inequality $0<h_m(t)<(2m-1)/2$ we just proved above gives us that

$$0<\psi(x+m)-\log x<\frac{2m-1}{2}\int_0^\infty e^{-tx}\,dt=(2m-1)(2x)^{-1},$$

which proves (a).

For $x\in\mathbb{R}^+$ we have that

$$\psi(x)-\log(x)=\psi(x+1)-\log(x)-x^{-1}.$$

So, by using (a) with $m=1$ we have that

$$-x^{-1}<\psi(x)-\log(x)<(2x)^{-1}-x^{-1}=-(2x)^{-1},$$

which proves (c).

Now we prove (b). (We need to prove the result for $y\notin\mathbb{N}$.) Observe that it is sufficient to demonstrate the result for $y\in(0,1)$, since given that for any fixed noninteger $Y>0$ we can write $Y=\lfloor Y\rfloor+y$, where $\lfloor Y\rfloor$ is the floor function of Y and $y\in(0,1)$. Then, by defining $X:=x+\lfloor Y\rfloor$ we have that

$$\begin{aligned}\lim_{x\to+\infty}(\psi(x+Y)-\log x)&=\lim_{X\to+\infty}(\psi(X+y)-\log(X-\lfloor Y\rfloor))=\lim_{X\to+\infty}\left(\psi(X+y)-\log X-\log\frac{X-\lfloor Y\rfloor}{X}\right)\\&=\lim_{X\to+\infty}(\psi(X+y)-\log X)=0.\end{aligned}$$

We consider the continuous function $h_y:\mathbb{R}\to\mathbb{R}$, $h_y(t)=(1/t)-[e^{-ty}/(1-e^{-t})]$, where $h_y(0)=\lim_{t\to 0}h_y(t)=(2y-1)/2$, and $0<y<1$ is fixed. According to (3.1), with $m=y\in(0,1)$, it is sufficient to prove that h_y is bounded in $[0,\infty)$, since if $|h_y(t)|\leqslant C$ for all $t\geqslant 0$, then

$$|\psi(x+y)-\log x| = \left|\int_0^\infty h_y(t)e^{-tx}\,dt\right| \leqslant C\int_0^\infty e^{-tx}\,dt = \frac{C}{x},$$

and thus $\psi(x+y)-\log x \to 0$ as $x \to +\infty$. But observe that $\lim_{t\to+\infty} h_y(t)=0$ and that h_y is continuous, which shows that h_y is bounded on $[0,\infty)$. Q.E.D.

Lemma 3.2: Let $\mu > -\frac{1}{2}$ be fixed. Then

$$\lim_{n\to\infty} \frac{(\gamma_\mu(n))^{1/n}}{n} = e^{-1}.$$

(Note that this limit does not depend on μ.)

Proof: It is sufficient to prove that

$$\lim_{n\to\infty} \frac{(\gamma_\mu(2n))^{1/2n}}{2n} = \lim_{n\to\infty} \frac{(\gamma_\mu(2n+1))^{1/(2n+1)}}{2n+1} = e^{-1}.$$

Let us consider the even case. We can write by using formula (2.1) that

$$\frac{(\gamma_\mu(2n))^{1/2n}}{2n} = \frac{((2n)!)^{1/2n}}{2n}\left(\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\right)^{1/2n}\left(\frac{\Gamma\left(\mu+n+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}\right)^{1/2n}.$$

We have that $\lim_{n\to\infty}[((2n)!)^{1/2n}/2n]=e^{-1}$ and $\lim_{n\to\infty}(\Gamma(\frac{1}{2})/\Gamma(\mu+\frac{1}{2}))^{1/2n}=1$. So it remains to prove that the limit of the third factor in the left-hand side is 1. By using Stirling's formula we have that

$$\lim_{n\to\infty}\left(\frac{\Gamma\left(\mu+n+\frac{1}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}\right)^{1/2n} = \lim_{n\to\infty}\left(\frac{\sqrt{2\pi}\left(\mu+n+\frac{1}{2}\right)^{\mu+n}e^{-(\mu+n+1/2)}}{\sqrt{2\pi}\left(n+\frac{1}{2}\right)^{n}e^{-(n+1/2)}}\right)^{1/2n}$$

$$= \lim_{n\to\infty}\left(\left(\mu+n+\frac{1}{2}\right)^{\mu/2n}e^{-\mu/2n}\left(\frac{\mu+n+\frac{1}{2}}{n+\frac{1}{2}}\right)^{1/2}\right) = 1.$$

For the odd case, by using (2.2) we have that

$$\frac{(\gamma_\mu(2n+1))^{1/(2n+1)}}{2n+1} = \frac{((2n+1)!)^{1/(2n+1)}}{2n+1}\left(\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\right)^{1/(2n+1)}\left(\frac{\Gamma\left(\mu+n+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)}\right)^{1/(2n+1)}.$$

We have that

$$\lim_{n\to\infty}\frac{((2n+1)!)^{1/(2n+1)}}{2n+1} = e^{-1} \text{ and } \lim_{n\to\infty}\left(\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\right)^{1/(2n+1)} = 1.$$

So the proof ends by showing that the limit of the third factor in the left-hand side is 1. By using Stirling's formula we have that

$$\lim_{n\to\infty}\left(\frac{\Gamma\left(\mu+n+\frac{3}{2}\right)}{\Gamma\left(n+\frac{3}{2}\right)}\right)^{1/(2n+1)} = \lim_{n\to\infty}\left(\frac{\sqrt{2\pi}\left(\mu+n+\frac{3}{2}\right)^{\mu+n+1}e^{-(\mu+n+3/2)}}{\sqrt{2\pi}\left(n+\frac{3}{2}\right)^{n+1}e^{-(n+3/2)}}\right)^{1/(2n+1)}$$

$$= \lim_{n\to\infty}\left(\left(\mu+n+\frac{3}{2}\right)^{\mu/(2n+1)}e^{-\mu/(2n+1)}\left(\frac{\mu+n+\frac{3}{2}}{n+\frac{3}{2}}\right)^{(n+1)/(2n+1)}\right)=1.$$

Q.E.D.

Observe that formula (1.1), which gives us the entropy of the elements of the canonical basis $\{\xi_n\}$ of $\mathcal{B}^2$, can be written as

$$S_{L^2(\mathbb{C},d\nu_{\text{Gauss}})}(\xi_n) = n\psi(n+1) - \log n!. \tag{3.2}$$

In the case $n=0$ we have $\xi_0(z)=1$ and then from (2.15) we have that $S_{L^2(\mathbb{C},d\nu_{\text{Gauss}})}(1)=0$. [Note that this case is also included in (3.2).]

We can use Lemmas 3.1 and 3.2 to prove some properties of the sequence of entropies $\{S_n\}_{n=0}^{\infty}$, where $S_n := S_{L^2(\mathbb{C},d\nu_{\text{Gauss}})}(\xi_n)$. First, we note that

$$S_{n+1} = (n+1)\psi(n+2) - \log(n+1)! = (n+1)\left(\frac{1}{n+1}+\psi(n+1)\right) - \log n! - \log(n+1)$$

$$= S_n + 1 + \psi(n+1) - \log(n+1) > S_n + 1 - \frac{1}{n+1},$$

where we used Lemma (3.1) (c). Thus, for $n=0$ we have that $S_1>0$, and for $n\in\mathbb{N}$ we have $S_{n+1}>S_n$. That is, the sequence $\{S_n\}_{n=0}^{\infty}$ is increasing. Moreover, $\{S_n\}_{n=0}^{\infty}$ is a sequence of nonnegative terms. [This conclusion also comes from the fact that $(\mathbb{C},d\nu_{\text{Gauss}})$ is a probability measure space.]

Next, by using the equality $S_{n+1}-S_n=1+\psi(n+1)-\log(n+1)$ of the previous argument and Lemma 3.1 (c) we have that

$$\lim_{n\to\infty}(S_{n+1}-S_n)=1,$$

which proves that the sequence $\{S_n\}_{n=1}^{\infty}$ is unbounded and, moreover, implies that

$$\lim_{n\to\infty}\frac{S_n}{n}=1.$$

Proof: $\lim_{n\to\infty}(S_{n+1}-S_n)=1 \Rightarrow \lim_{n\to\infty}(1/n)\sum_{k=0}^{n-1}(S_{k+1}-S_k)=1 \Rightarrow$

$$\lim_{n\to\infty}[(S_n-S_0)/n]=1 \Rightarrow \lim_{n\to\infty}(S_n/n)=1.$$

This limit can also be proved directly by noting that

$$\frac{S_n}{n} = \psi(n+1) - \frac{1}{n}\log n! = \psi(n+1) - \log n - \log\frac{(n!)^{1/n}}{n},$$

and thus, by using that $\psi(n+1)-\log n\to 0$ as $n\to\infty$ [Lemma 3.1 (a)] and that $\log[(n!)^{1/n}/n] \to e^{-1}$ as $n\to\infty$, we obtain the desired result $\lim_{n\to\infty}(S_n/n)=1$.

In conclusion, we have proved the following.

Proposition 3.1 The sequence $\{S_n\}_{n=0}^{\infty}$, *where* $S_n = S_{L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})}(\xi_n)$ *is the entropy of the n*th *canonical basis element in* $L^2(\mathbb{C},\mathrm{d}\nu_{\mathrm{Gauss}})$ *is an unbounded increasing sequence of non-negative terms, with the property* $\lim_{n\to\infty}(S_{n+1}-S_n)=1$. *In particular,* S_n *is an extensive quantity.*

IV. ENTROPIES IN $\mathcal{B}_\mu^2$

As noted in Sec. II, for calculating the entropies $S_n^\mu = S_{L^2(\mathbb{C}\times\mathbb{Z}_2,\mathrm{d}\nu_\mu)}(\xi_n^\mu)$ of the elements of the canonical basis $\{\xi_n^\mu\}_{n=0}^{\infty}$ of the μ-deformed Segal-Bargmann space $\mathcal{B}_\mu^2$, we need to consider the cases when n is even [in which case we have that $S_n^\mu = S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(\xi_n)$] and when n is odd [in which case we have that $S_n^\mu = S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(\xi_n)$]. We begin by considering the even case. For $n=0$ we have $\xi_0^\mu(z)=1$ and then $S_0^\mu=0$. So we are interested in calculating S_{2n}^μ for $n\geqslant 1$. Formula (2.15) tells us that

$$S_{2n}^\mu = \int_{\mathbb{C}} |\xi_{2n}(z)|^2 \log|\xi_{2n}(z)|^2 \,\mathrm{d}\nu_{e,\mu}(z) - \|\xi_{2n}\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})} \log\|\xi_{2n}\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}$$
$$= \frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)} \int_{\mathbb{C}} \left|\frac{z^{2n}}{(\gamma_\mu(2n))^{1/2}}\right|^2 \log\left|\frac{z^{2n}}{(\gamma_\mu(2n))^{1/2}}\right|^2 K_{\mu-1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y.$$

Since the log term in the integral of the right-hand side is $\log|z^{2n}|^2 - \log\gamma_\mu(2n)$, we can write S_{2n}^μ as a difference of two integrals, $I_1 - I_2$ say, in which $I_2 = \log\gamma_\mu(2n)\|\xi_{2n}\|^2_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})} = \log\gamma_\mu(2n)$. In I_1 we change (x,y) to polar coordinates (r,θ), and then let $s=r^2$ to obtain

$$S_{2n}^\mu = \frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)} \int_{\mathbb{C}} \left|\frac{z^{2n}}{(\gamma_\mu(2n))^{1/2}}\right|^2 \log|z^{2n}|^2 K_{\mu-1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y - \log\gamma_\mu(2n)$$
$$= \frac{2^{1/2-\mu}2}{\gamma_\mu(2n)\Gamma\left(\mu+\frac{1}{2}\right)} \int_0^\infty r^{4n}(\log r^{4n}) K_{\mu-1/2}(r^2) r^{2\mu+2}\,\mathrm{d}r - \log\gamma_\mu(2n)$$
$$= \frac{2^{1/2-\mu}}{\gamma_\mu(2n)\Gamma\left(\mu+\frac{1}{2}\right)} \int_0^\infty s^{2n}(\log s^{2n}) K_{\mu-1/2}(s) s^{\mu+1/2}\,\mathrm{d}s - \log\gamma_\mu(2n).$$

For calculating the integral $\int_0^\infty (\log s^{2n}) K_{\mu-1/2}(s) s^{\mu+2n+1/2}\,\mathrm{d}s$, we define the function φ in a neighborhood of $\alpha=1$ as

$$\varphi(\alpha) = \int_0^\infty s^{2n\alpha} K_{\mu-1/2}(s) s^{\mu+1/2}\,\mathrm{d}s.$$

Observe that for $\mu > -\frac{1}{2}$, $n\in\mathbb{N}$ and α in a neighborhood of 1, one has that $2n\alpha+\mu+\frac{3}{2} > |\mu-\frac{1}{2}|$, so we can use formula (2.7) to write

$$\varphi(\alpha) = 2^{2n\alpha+\mu-1/2}\Gamma(n\alpha+1)\Gamma\left(\mu+n\alpha+\tfrac{1}{2}\right).$$

The derivative φ' is on the one hand

$$\varphi'(\alpha) = \int_0^\infty s^{2n\alpha}(\log s^{2n}) K_{\mu-1/2}(s) s^{\mu+1/2}\,\mathrm{d}s,$$

and on the other hand,

$$\varphi'(\alpha) = 2^{2n\alpha+\mu-1/2}\Gamma(n\alpha+1)n\Gamma'\left(\mu+n\alpha+\frac{1}{2}\right) + 2^{2n\alpha+\mu-1/2}n\Gamma'(n\alpha+1)\Gamma\left(\mu+n\alpha+\frac{1}{2}\right)$$
$$+ 2^{2n\alpha+\mu-1/2}2n(\log 2)\Gamma(n\alpha+1)\Gamma\left(\mu+n\alpha+\frac{1}{2}\right)$$
$$= 2^{2n\alpha+\mu-1/2}\Gamma(n\alpha+1)\Gamma\left(\mu+n\alpha+\frac{1}{2}\right)\left(n\psi\left(\mu+n\alpha+\frac{1}{2}\right)+n\psi(n\alpha+1)+2n\log 2\right).$$

Then

$$\varphi'(1) = \int_0^\infty s^{2n}(\log s^{2n})K_{\mu-1/2}(s)s^{\mu+1/2}\,\mathrm{d}s = 2^{2n+\mu-1/2}\Gamma(n+1)\Gamma\left(\mu+n+\frac{1}{2}\right)\begin{pmatrix} n\psi\left(\mu+n+\frac{1}{2}\right) \\ +n\psi(n+1) \\ +2n\log 2 \end{pmatrix}.$$

Thus we have that

$$S_{2n}^{\mu} = \frac{\Gamma(n+1)\Gamma\left(\mu+n+\frac{1}{2}\right)2^{2n}}{\gamma_\mu(2n)\Gamma\left(\mu+\frac{1}{2}\right)}\left(n\psi\left(\mu+n+\frac{1}{2}\right)+n\psi(n+1)+\log 2^{2n}\right)-\log\,\gamma_\mu(2n).$$

By using formula (2.1) for $\gamma_\mu(2n)$ we have that the entropy of the even elements ξ_{2n} is

$$S_{2n}^{\mu} = n\left(\psi\left(\mu+n+\frac{1}{2}\right)+\psi(n+1)\right)-\log\frac{\gamma_\mu(2n)}{2^{2n}}. \tag{4.1}$$

Note that this formula makes sense for $n=0$, obtaining the known result $S_0^\mu=0$.
In the case $\mu=0$, formula (4.1) becomes

$$S_{2n}^{0} = n\left(\psi\left(n+\frac{1}{2}\right)+\psi(n+1)\right)-\log\frac{(2n)!}{2^{2n}}$$
$$= n\left(-\gamma-2\log 2+2\sum_{k=1}^{n}\frac{1}{2k-1}-\gamma+\sum_{k=1}^{n}\frac{1}{k}\right)-\log(2n)!+2n\log 2$$
$$= 2n\left(-\gamma+\sum_{k=1}^{n}\frac{1}{2k-1}+\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k}\right)-\log(2n)! = 2n\left(-\gamma+\sum_{k=1}^{2n}\frac{1}{k}\right)-\log(2n)!,$$

which is (1.1) for even positive integers, as expected.

Since $(\mathbb{C},\mathrm{d}\nu_{e,\mu})$ is a probability measure space, we have that $S_{2n}^{\mu}\geqslant 0$ for all $n=0,1,2,\ldots$. But we can arrive at this conclusion directly from the formula obtained for S_{2n}^{μ} as follows. Observe that for $n\in\mathbb{N}$ we can write formula (2.1) as

$$\frac{\gamma_\mu(2n)}{2^{2n}} = n!\prod_{k=1}^{n}\left(\mu+k-\frac{1}{2}\right). \tag{4.2}$$

Then

$$S_{2n}^{\mu} = n\psi\left(\mu+n+\frac{1}{2}\right) + n\psi(n+1) - \log\left(n!\prod_{k=1}^{n}\left(\mu+k-\frac{1}{2}\right)\right)$$

$$= \sum_{k=1}^{n}\left(\psi\left(\mu+n+\frac{1}{2}\right) - \log\left(\mu+k-\frac{1}{2}\right) + \psi(n+1) - \log(k)\right).$$

Lemma 3.1(a) gives us that $\psi\left(\mu+n+\frac{1}{2}\right)-\log\left(\mu+k-\frac{1}{2}\right)>0$ and that $\psi(n+1)-\log(k)>0$ for all $k=1,\ldots,n$. So we conclude that $S_{2n}^{\mu}>0$, as wanted. Moreover, observe that for fixed $n\in\mathbb{N}$, we have that [again by Lemma 3.1(a)] $\psi\left(\mu+n+\frac{1}{2}\right)-\log\left(\mu+k-\frac{1}{2}\right)\to 0$ as $\mu\to+\infty$, and so

$$\lim_{\mu\to+\infty} S_{2n}^{\mu} = \sum_{k=1}^{n}(\psi(n+1)-\log(k)) = n\psi(n+1) - \log n!\ .$$

That is, for $n\in\mathbb{N}$ fixed we have that

$$\lim_{\mu\to+\infty} S_{2n}^{\mu} = S_n.$$

Let us consider the particular case when $\mu=\frac{1}{2}+m$, $m=0,1,2,\ldots$. Formula (4.2) becomes in this case

$$\frac{\gamma_{1/2+m}(2n)}{2^{2n}} = n!\prod_{k=1}^{n}(k+m) = \frac{n!(m+n)!}{m!},$$

and then formula (4.1) gives us

$$S_{2n}^{1/2+m} = n(\psi(n+m+1)+\psi(n+1)) - \log\frac{n!(m+n)!}{m!}$$

$$= (n+m)\psi(n+m+1) - \log(m+n)! + n\psi(n+1) - \log n! - m\psi(n+m+1) + \log m!$$

$$= S_{n+m} + S_n - m\left(\sum_{k=0}^{n-1}\frac{1}{m+k+1} + \psi(m+1)\right) + \log m! = S_{n+m} + S_n - S_m - \sum_{k=1}^{n}\frac{m}{m+k}.$$

That is, for $n,m=0,1,2,\ldots$, we have the formula

$$S_{n+m} + S_n - S_m = S_{2n}^{1/2+m} + \sum_{k=1}^{n}\frac{m}{m+k},$$

which shows that the values of the entropies S_{n+m}, S_n, and S_m (of the undeformed case) are related by means of the entropy $S_{2n}^{1/2+m}$ corresponding to the $\left(m+\frac{1}{2}\right)$-deformed case.

We claim that $\{S_{2n}^{\mu}\}_{n=0}^{\infty}$ is an increasing sequence for fixed $\mu>-\frac{1}{2}$. In fact, we have that

$$S_{2n+2}^{\mu} = (n+1)\psi\left(\mu+n+\frac{3}{2}\right) + (n+1)\psi(n+2) - \log\frac{\gamma_{\mu}(2n+2)}{2^{2n+2}}$$

$$= n\left(\frac{1}{\mu+n+\frac{1}{2}} + \psi\left(\mu+n+\frac{1}{2}\right)\right) + \psi\left(\mu+n+\frac{3}{2}\right) + n\left(\frac{1}{n+1}+\psi(n+1)\right) + \psi(n+2)$$

$$- \log\frac{(2n+2)(2n+1+2\mu)\gamma_{\mu}(2n)}{2^2 2^{2n}}$$

$$= S_{2n}^{\mu} + \psi\left(\mu + n + \frac{3}{2}\right) - \log\left(\mu + n + \frac{1}{2}\right) + \psi(n+2) - \log(n+1) + \frac{n}{\mu + n + \frac{1}{2}} + \frac{n}{n+1}.$$

Lemma 3.1(a) gives us $\psi(\mu+n+\frac{3}{2})-\log(\mu+n+\frac{1}{2})>0$ and $\psi(n+2)-\log(n+1)>0$. Thus we have that $S_{2n+2}^{\mu}-S_{2n}^{\mu}>0$, as wanted. Lemma 3.1(a) also tells us that $\psi(\mu+n+\frac{3}{2})-\log(\mu+n+\frac{1}{2}) \to 0$ and $\psi(n+2)-\log(n+1)\to 0$ as $n\to\infty$. Thus, for fixed $\mu>-\frac{1}{2}$, we have by the expression above that $\lim_{n\to\infty}(S_{2n+2}^{\mu}-S_{2n}^{\mu})=2$. In particular we see that the sequence $\{S_{2n}^{\mu}\}_{n=0}^{\infty}$ is unbounded. This limit implies that $\lim_{n\to\infty}(S_{2n}/2n)=1$, but we can give a direct proof of this last result by noting that

$$\begin{aligned}\frac{S_{2n}^{\mu}}{2n} &= \frac{1}{2}\left(\psi\left(\mu + n + \frac{1}{2}\right) + \psi(n+1)\right) - \frac{1}{2n}\log\frac{\gamma_{\mu}(2n)}{2^{2n}} \\ &= \frac{1}{2}\left(\psi\left(\mu + n + \frac{1}{2}\right) + \psi(n+1)\right) - \log\frac{(\gamma_{\mu}(2n))^{1/2n}}{2n} - \log n \\ &= \frac{1}{2}\left(\psi\left(\mu + n + \frac{1}{2}\right) - \log n + \psi(n+1) - \log n\right) - \log\frac{(\gamma_{\mu}(2n))^{1/2n}}{2n}.\end{aligned}$$

Lemma 3.1(b) tells us that $\psi(\mu+n+\frac{1}{2})-\log n\to 0$ and $\psi(n+1)-\log n\to 0$ as $n\to\infty$. Lemma 3.2 tells us that $\log[(\gamma_{\mu}(2n))^{1/2n}/2n]\to -1$ as $n\to\infty$. Then we have that $\lim_{n\to\infty}(S_{2n}/2n)\to 1$, as wanted.

In conclusion, we have proved the following theorem.

Theorem 4.1: *The entropy of ξ_{2n}^{μ} is given by*

$$S_{2n}^{\mu} = n\left(\psi\left(\mu + n + \frac{1}{2}\right) + \psi(n+1)\right) - \log\frac{\gamma_{\mu}(2n)}{2^{2n}},$$

where $\mu>-\frac{1}{2}$ and $n=0,1,\ldots$. For fixed $\mu>-\frac{1}{2}$, the sequence $\{S_{2n}^{\mu}\}_{n=1}^{\infty}$ is an unbounded increasing sequence of positive terms such that

$$\lim_{n\to\infty}(S_{2n+2}^{\mu} - S_{2n}^{\mu}) = 2,$$

which implies that

$$\lim_{n\to\infty}\frac{S_{2n}^{\mu}}{2n} = 1.$$

For fixed $n\in\mathbb{N}$, we have that

$$\lim_{\mu\to+\infty} S_{2n}^{\mu} = S_n,$$

where $S_n=S_n^0$.

For $n,m=0,1,2,\ldots$, we have that

$$S_{n+m} + S_n - S_m = S_{2n}^{1/2+m} + \sum_{k=0}^{n-1}\frac{m}{m+k+1}.$$

We now calculate the entropies of the odd functions ξ_{2n+1}, $n=0,1,2,\ldots$. The steps we will follow in the calculations are analogues of the even case. Since $S_{2n+1}^{\mu}=S_{L^2(\mathbb{C},d\nu_{o,\mu})}(\xi_{2n+1})$ we have that

$$S^{\mu}_{2n+1} = \frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)}\int_{\mathbb{C}}\left|\frac{z^{2n+1}}{(\gamma_\mu(2n+1))^{1/2}}\right|^2\log\left|\frac{z^{2n+1}}{(\gamma_\mu(2n+1))^{1/2}}\right|^2 K_{\mu+1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y$$

$$= \frac{2^{1/2-\mu}2}{\gamma_\mu(2n+1)\Gamma\left(\mu+\frac{1}{2}\right)}\int_0^\infty r^{4n+2}(\log r^{4n+2})K_{\mu+1/2}(r^2)r^{2\mu+2}\,\mathrm{d}r - \log\,\gamma_\mu(2n+1)$$

$$= \frac{2^{1/2-\mu}}{\gamma_\mu(2n+1)\Gamma\left(\mu+\frac{1}{2}\right)}\int_0^\infty s^{2n+1}(\log s^{2n+1})K_{\mu+1/2}(s)s^{\mu+1/2}\,\mathrm{d}s - \log\,\gamma_\mu(2n+1).$$

We define

$$\phi(\alpha) = \int_0^\infty s^{(2n+1)\alpha}K_{\mu+1/2}(s)s^{\mu+1/2}\,\mathrm{d}s.$$

Since for $\mu > -\frac{1}{2}$, $n \in \mathbb{N}\cup\{0\}$ and α in a neighborhood of 1, one has that $(2n+1)\alpha+\mu+\frac{3}{2} > |\mu+\frac{1}{2}|$, we can use formula (2.7) to write

$$\phi(\alpha) = 2^{(2n+1)\alpha+\mu-1/2}\Gamma\left(\left(n+\tfrac{1}{2}\right)\alpha+\tfrac{1}{2}\right)\Gamma\left(\left(n+\tfrac{1}{2}\right)\alpha+\mu+1\right).$$

By calculating the derivative $\phi'(1)$ in two different ways as we did in the even case, we get

$$\phi'(1) = \int_0^\infty s^{2n+1}\log s^{2n+1}K_{\mu+1/2}(s)s^{\mu+1/2}\,\mathrm{d}s$$

$$= 2^{2n+\mu+1/2}\Gamma(n+1)\Gamma\left(\mu+n+\frac{3}{2}\right)\left(\begin{array}{c}\frac{2n+1}{2}\psi\left(\mu+n+\frac{3}{2}\right)\\ +\frac{2n+1}{2}\psi(n+1)\\ +(2n+1)\log 2\end{array}\right).$$

Thus, by using formula (2.2) for $\gamma_\mu(2n+1)$ we find that the entropy of ξ_{2n+1} is

$$S^{\mu}_{2n+1} = \left(n+\frac{1}{2}\right)\left(\psi\left(\mu+n+\frac{3}{2}\right)+\psi(n+1)\right) - \log\frac{\gamma_\mu(2n+1)}{2^{2n+1}}. \tag{4.3}$$

In the case $\mu=0$ this formula becomes

$$S^{0}_{2n+1} = \left(n+\frac{1}{2}\right)\left(\psi\left(n+\frac{3}{2}\right)+\psi(n+1)\right) - \log\frac{(2n+1)!}{2^{2n+1}}$$

$$= \left(n+\frac{1}{2}\right)\left(\frac{1}{n+\frac{1}{2}}+\psi\left(n+\frac{1}{2}\right)+\psi(n+1)\right) - \log(2n+1)! + (2n+1)\log 2$$

$$= (2n+1)\left(-\gamma+\frac{1}{2n+1}+\sum_{k=1}^{n}\frac{1}{2k-1}+\frac{1}{2}\sum_{k=1}^{n}\frac{1}{k}\right) - \log(2n+1)!$$

$$= (2n+1)\left(-\gamma+\sum_{k=1}^{2n+1}\frac{1}{k}\right) - \log(2n+1)!\,,$$

which is (1.1) for odd positive integers.

Observe that for $n \in N$ we can write formula (2.2) as

$$\frac{\gamma_\mu(2n+1)}{2^{2n+1}} = n! \prod_{k=1}^{n+1} \left(\mu + k - \frac{1}{2} \right).$$

Thus (4.3) can be written as

$$S^\mu_{2n+1} = \sum_{k=1}^{n} \left(\psi\left(\mu + n + \frac{3}{2} \right) - \log\left(\mu + k - \frac{1}{2} \right) \right) + \frac{1}{2}\left(\psi\left(\mu + n + \frac{3}{2} \right) - \log\left(\mu + n + \frac{1}{2} \right) \right)$$
$$+ \left(n + \frac{1}{2} \right) \psi(n+1) - \log n! - \frac{1}{2} \log\left(\mu + n + \frac{1}{2} \right). \tag{4.4}$$

For fixed $n=0,1,2,\ldots$, we have by Lemma 3.1(a) that $\psi\left(\mu+n+\frac{3}{2}\right)-\log\left(\mu+k-\frac{1}{2}\right)\to 0$ and $\psi\left(\mu+n+\frac{3}{2}\right)-\log\left(\mu+n+\frac{1}{2}\right)\to 0$ as $\mu\to+\infty$. Thus, because of the last term of the right-hand side in (4.4), we have that $\lim_{\mu\to+\infty} S^\mu_{2n+1}=-\infty$. That is, negative entropies do occur in the odd case. [Recall that $(\mathbb{C}, \mathrm{d}\nu_{o,\mu})$ *is not* a probability measure space for $\mu \neq 0$.] Nevertheless we will see now that for fixed $\mu > -\frac{1}{2}$ the sequence $\{S^\mu_{2n+1}\}_{n=0}^\infty$ is increasing and unbounded, and so it is eventually positive. We have that

$$S^\mu_{2n+3} = \left(n + \frac{1}{2} \right)\left(\psi\left(\mu + n + \frac{3}{2} \right) + \psi(n+1) \right) - \log \frac{\gamma_\mu(2n+1)}{2^{2n+1}} + \left(n + \frac{3}{2} \right)\left(\frac{1}{\mu + n + \frac{3}{2}} + \frac{1}{n+1} \right)$$
$$+ \psi\left(\mu + n + \frac{3}{2} \right) + \psi(n+1) - \log\left((n+1)\left(\mu + n + \frac{3}{2} \right) \right)$$
$$= S^\mu_{2n+1} + \left(n + \frac{3}{2} \right)\left(\frac{1}{\mu + n + \frac{3}{2}} + \frac{1}{n+1} \right) + \psi\left(\mu + n + \frac{3}{2} \right) - \log\left(\mu + n + \frac{3}{2} \right) + \psi(n+1)$$
$$- \log(n+1) > S^\mu_{2n+1} + \left(n + \frac{3}{2} \right)\left(\frac{1}{\mu + n + \frac{3}{2}} + \frac{1}{n+1} \right) - \frac{1}{\mu + n + \frac{3}{2}} - \frac{1}{n+1}$$
$$= S^\mu_{2n+1} + \left(n + \frac{1}{2} \right)\left(\frac{1}{\mu + n + \frac{3}{2}} + \frac{1}{n+1} \right) > S^\mu_{2n+1},$$

where we used Lemma 3.1(c). This proves that the sequence $\{S^\mu_{2n+1}\}_{n=0}^\infty$ is increasing. Moreover, since

$$S^\mu_{2n+3} - S^\mu_{2n+1} = \left(n + \frac{3}{2} \right)\left(\frac{1}{\mu + n + \frac{3}{2}} + \frac{1}{n+1} \right) + \psi\left(\mu + n + \frac{3}{2} \right) - \log\left(\mu + n + \frac{3}{2} \right) + \psi(n+1)$$
$$- \log(n+1)$$

and by Lemma 3.1(c) we have that $\psi\left(\mu+n+\frac{3}{2}\right)-\log\left(\mu+n+\frac{3}{2}\right)\to 0$ and also that $\psi(n+1)-\log(n+1)\to 0$ as $n\to\infty$, then we conclude that $\lim_{n\to\infty}(S^\mu_{2n+3}-S^\mu_{2n+1})=2$, which implies the unboundedness of the sequence $\{S^\mu_{2n+1}\}_{n=0}^\infty$. This limit implies that $\lim_{n\to\infty}[S^\mu_{2n+1}/(2n+1)]=1$, but a direct proof of this is as follows. Note that

$$\frac{S^{\mu}_{2n+1}}{2n+1} = \frac{1}{2}\left(\psi\left(\mu+n+\frac{3}{2}\right)+\psi(n+1)\right) - \log\frac{(\gamma_{\mu}(2n+1))^{1/(2n+1)}}{2n+1} - \log\left(n+\frac{1}{2}\right)$$
$$= \frac{1}{2}\left(\psi\left(\mu+n+\frac{3}{2}\right) - \log\left(n+\frac{1}{2}\right) + \psi(n+1) - \log\left(n+\frac{1}{2}\right)\right) - \log\frac{(\gamma_{\mu}(2n+1))^{1/(2n+1)}}{2n+1}.$$

Note that Lemmas 3.1(b) and 3.2 give us that $\psi\left(\mu+n+\frac{3}{2}\right)-\log\left(n+\frac{1}{2}\right)\to 0$, $\psi(n+1)-\log\left(n+\frac{1}{2}\right)\to 0$ and $\log[(\gamma_{\mu}(2n+1))^{1/(2n+1)}/(2n+1)]\to -1$ as $n\to\infty$. Then we have that $[S^{\mu}_{2n+1}/(2n+1)]\to 1$ as $n\to\infty$.

Thus, we have proved the following theorem.

Theorem 4.2: *The entropy of ξ^{μ}_{2n+1} is given by*

$$S^{\mu}_{2n+1} = \left(n+\frac{1}{2}\right)\left(\psi\left(\mu+n+\frac{3}{2}\right)+\psi(n+1)\right) - \log\frac{\gamma_{\mu}(2n+1)}{2^{2n+1}},$$

where $\mu>-\frac{1}{2}$ and $n=0,1,2,\ldots$. For fixed $\mu>-\frac{1}{2}$, the sequence $\{S^{\mu}_{2n+1}\}_{n=0}^{\infty}$ is an unbounded increasing sequence such that

$$\lim_{n\to\infty}(S^{\mu}_{2n+3} - S^{\mu}_{2n+1}) = 2,$$

which implies that

$$\lim_{n\to\infty}\frac{S^{\mu}_{2n+1}}{2n+1} = 1.$$

For fixed $n=0,1,2,\ldots$, we have that

$$\lim_{\mu\to+\infty} S^{\mu}_{2n+1} = -\infty.$$

We can relate the entropies S^{μ}_{2n+1} with the entropies S^{μ}_{2n} as follows. We note that

$$S^{\mu}_{2n+1} = \frac{2n+1}{2}\left(\psi\left(\mu+n+\frac{3}{2}\right)+\psi(n+1)\right) - \log\frac{\gamma_{\mu}(2n+1)}{2^{2n+1}}$$
$$= \left(n+\frac{1}{2}\right)\left(\frac{1}{\mu+n+\frac{1}{2}} + \psi\left(\mu+n+\frac{1}{2}\right)+\psi(n+1)\right) - \log\frac{\gamma_{\mu}(2n+1)}{2^{2n+1}}$$
$$= \left(1+\frac{1}{2n}\right)\left(S^{\mu}_{2n} + \log\frac{\gamma_{\mu}(2n)}{2^{2n}}\right) + \frac{n+\frac{1}{2}}{\mu+n+\frac{1}{2}} - \log\frac{\gamma_{\mu}(2n+1)}{2^{2n+1}}$$
$$= \left(1+\frac{1}{2n}\right)S^{\mu}_{2n} + \frac{n+\frac{1}{2}}{\mu+n+\frac{1}{2}} + \log\frac{(\gamma_{\mu}(2n))^{1/2n}}{2\left(\mu+n+\frac{1}{2}\right)}.$$

So we have that

$$S^{\mu}_{2n+1} - S^{\mu}_{2n} = \frac{S^{\mu}_{2n}}{2n} + \frac{n+\frac{1}{2}}{\mu+n+\frac{1}{2}} + \log\frac{(\gamma_{\mu}(2n))^{1/2n}}{2\left(\mu+n+\frac{1}{2}\right)}.$$

By using Lemma 3.2 and Theorem 4.1 we obtain

$$\lim_{n\to\infty}(S^{\mu}_{2n+1}-S^{\mu}_{2n})=1.$$

Similarly one has that

$$S^{\mu}_{2n}-S^{\mu}_{2n-1}=\frac{S^{\mu}_{2n-1}}{2n-1}+1+\log\frac{\gamma_{\mu}(2n-1)^{1/(2n-1)}}{2n}.$$

Lemma 3.2 and Theorem 4.2 allow us to conclude

$$\lim_{n\to\infty}(S^{\mu}_{2n}-S^{\mu}_{2n-1})=1.$$

Finally, observe that we can express the formulas (4.1) and (4.3) in terms of the characteristic function θ of the odd positive integers as

$$S^{\mu}_{n}=\frac{n}{2}\left(\psi\left(\mu+\frac{n+\theta(n)+1}{2}\right)+\psi\left(\frac{n+\theta(n+1)+1}{2}\right)\right)-\log\frac{\gamma_{\mu}(n)}{2^{n}}.$$

From this formula one can obtain at once the case $\mu=0$ [formula (1.1)] by using the identity

$$\psi\left(\frac{n+1}{2}\right)+\psi\left(\frac{n+2}{2}\right)=2\psi(n+1)-2\log 2,$$

whose proof is an easy exercise by induction.

Combining Theorems 4.1 and 4.2 with the previous results, we have the following.

Theorem 4.3: *Let $\mu>-\frac{1}{2}$ be fixed. The entropy S^{μ}_{n} is given by*

$$S^{\mu}_{n}=\frac{n}{2}\left(\psi\left(\mu+\frac{n+\theta(n)+1}{2}\right)+\psi\left(\frac{n+\theta(n+1)+1}{2}\right)\right)-\log\frac{\gamma_{\mu}(n)}{2^{n}}.$$

The sequence $\{S^{\mu}_{n}\}_{n=0}^{\infty}$ of entropies is such that the subsequences of even terms $\{S^{\mu}_{2n}\}_{n=1}^{\infty}$ and of odd terms $\{S^{\mu}_{2n+1}\}_{n=0}^{\infty}$ are increasing, the former being positive and the latter being eventually positive. Moreover, we have that

$$\lim_{n\to\infty}(S^{\mu}_{n+1}-S^{\mu}_{n})=1,$$

which shows that the sequence $\{S^{\mu}_{n}\}_{n=0}^{\infty}$ is unbounded and implies that

$$\lim_{n\to\infty}\frac{S^{\mu}_{n}}{n}=1.$$

So we have that S^{μ}_{n} is an extensive quantity in n. Note that this assertion is independent of μ.

V. ENTROPIES IN $L^2(\mathbb{R},\mathrm{d}g_{\mu})$

Following the same sort of ideas we used in the preceding section, we will calculate in this section the entropies of the monomials $t^n\in L^2(\mathbb{R},\mathrm{d}g_{\mu})$, $n=1,2,\ldots$. [In the case $n=0$ we obtain from the definition that $S_{L^2(\mathbb{R},\mathrm{d}g_{\mu})}(1)=0$.] That is, for $n=1,2,\ldots$ we will calculate explicitly

$$S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t^n) = \frac{1}{\Gamma\left(\mu+\frac{1}{2}\right)}\int_{\mathbb{R}} |t^n|^2 \log|t^n|^2 \exp(-t^2)|t|^{2\mu}\,\mathrm{d}t - \|t^n\|^2_{L^2(\mathbb{R},\mathrm{d}g_\mu)} \log\|t^n\|^2_{L^2(\mathbb{R},\mathrm{d}g_\mu)}$$

$$= \frac{1}{\Gamma\left(\mu+\frac{1}{2}\right)}\int_0^\infty u^n(\log u^n)\exp(-u)u^{\mu-1/2}\,\mathrm{d}u - \|t^n\|^2_{L^2(\mathbb{R},\mathrm{d}g_\mu)} \log\|t^n\|^2_{L^2(\mathbb{R},\mathrm{d}g_\mu)}.$$

A direct calculation gives us

$$\|t^n\|^2_{L^2(\mathbb{R},\mathrm{d}g_\mu)} = \frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}.$$

Next, define the function

$$\eta(\alpha) = \int_0^\infty u^{n\alpha}\exp(-u)u^{\mu-1/2}\,\mathrm{d}s = \Gamma\left(n\alpha+\mu+\frac{1}{2}\right)$$

in a neighborhood of $\alpha=1$. By calculating the derivative $\eta'(1)$ in two different ways (using the technique from the preceding section) we find that

$$\int_0^\infty u^n(\log u^n)\exp(-u)u^{\mu-1/2}\,\mathrm{d}u = n\psi\left(n+\mu+\frac{1}{2}\right)\Gamma\left(n+\mu+\frac{1}{2}\right).$$

Then the entropy $S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t^n)$ is

$$S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t^n) = \frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\left(n\psi\left(n+\mu+\frac{1}{2}\right) - \log\frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\right). \tag{5.1}$$

When $n=1$ formula (5.1) becomes

$$S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t) = \frac{\Gamma\left(\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\left(\psi\left(\mu+\frac{3}{2}\right) - \log\frac{\Gamma\left(\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\right) = \left(\mu+\frac{1}{2}\right)\left(\psi\left(\mu+\frac{3}{2}\right) - \log\left(\mu+\frac{1}{2}\right)\right).$$

By using that $S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t)$ is homogeneous of degree 2 we can calculate the entropy of the monomial $\zeta_1^\mu(t)=(2/(1+2\mu))^{1/2}t$, which is the second element of the canonical basis $\{\zeta_n^\mu\}_{n=0}^\infty$ of $L^2(\mathbb{R},\mathrm{d}g_\mu)$. In fact, we have that $S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu)=[2/(1+2\mu)]S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t)$, and then

$$S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu) = \psi\left(\mu+\tfrac{3}{2}\right) - \log\left(\mu+\tfrac{1}{2}\right). \tag{5.2}$$

When $\mu=0$ this formula becomes

$$S_{L^2(\mathbb{R},\mathrm{d}g)}(\zeta_1^0) = \psi\left(\frac{3}{2}\right) - \log\left(\frac{1}{2}\right) = 2 - \log 2 - \gamma,$$

using $\psi\left(\frac{3}{2}\right)=2-2\log 2-\gamma$, which is (1.2) as expected.

Unfortunately we cannot continue the previous procedure in order to obtain explicit formulas for the entropies of $\zeta_n^\mu \in L^2(\mathbb{R},\mathrm{d}g_\mu)$ with $n\geqslant 2$, since for those values of n the polynomials ζ_n^μ are

no longer monomials, and then (5.1) is not useful. Nevertheless we will study some properties of the sequence $\{s_n^\mu\}_{n=0}^\infty$, where $s_n^\mu := S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(t^n)$, and compare them with the results obtained in Sec. IV.

Before that, recall that the μ-deformed Segal-Bargmann transform $B_\mu: L^2(\mathbb{R},\mathrm{d}g_\mu) \to \mathcal{B}_\mu^2$ is such that $B_\mu(\zeta_n^\mu) = \xi_n^\mu$, $n=0,1,\ldots$. When $n=0$ we have $\zeta_0^\mu(t)=1$, $\xi_0^\mu(z)=1$, and $S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(1) = S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(1)=0$. So in this case we see that B_μ preserves entropy. Let us consider the case $n=1$. Formula (4.3) gives us

$$S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(B_\mu(\zeta_1^\mu)) = \tfrac{1}{2}\left(\psi\left(\mu+\tfrac{3}{2}\right)+\psi(1)\right) - \log\left(\mu+\tfrac{1}{2}\right).$$

This formula, $\psi(1)=-\gamma$, and (5.2) give us that

$$S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(B_\mu(\zeta_1^\mu)) - S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu) = -\tfrac{1}{2}\left(\psi\left(\mu+\tfrac{3}{2}\right)+\gamma\right). \tag{5.3}$$

Observe that $\lim_{\mu\to-\frac{1}{2}+}\left(\psi\left(\mu+\frac{3}{2}\right)+\gamma\right) = \psi(1)+\gamma = 0$, and that $\mu \mapsto \psi\left(\mu+\frac{3}{2}\right)+\gamma$ is an increasing function since we have that $\psi'(x)>0$ for $x>0$ (see Ref. 20, p. 14). Then $\psi\left(\mu+\frac{3}{2}\right)+\gamma>0$ for $\mu>-\frac{1}{2}$, and thus formula (5.3) tells us that $S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(B_\mu(\zeta_1^\mu)) < S_{L^2(\mathbb{R},\mathrm{d}g_\mu)}(\zeta_1^\mu)$. That is, the μ-deformed Segal-Bargmann transform B_μ decreases the entropy of ζ_1^μ. We have already noted that B_μ preserves the entropy of ζ_0^μ. It seems reasonable to conjecture that B_μ increases the entropy of other functions in $L^2(\mathbb{R},\mathrm{d}g_\mu)$. (This is known to be true in the case $\mu=0$. See Ref. 33.)

As happens in the case of the sequence of entropies $\{S_n^\mu\}_{n=0}^\infty$ in the preceding section, the sequence of entropies $\{s_n^\mu\}_{n=0}^\infty$ is unbounded as we will prove now. By using the asymptotics

$$\psi(z) = \log z + O(z^{-1}), \tag{5.4}$$

valid for $|\arg z|<\pi$ and $z\to\infty$ (see Ref. 20, p. 18), and Stirling's formula

$$\log\Gamma(z) = \left(z-\tfrac{1}{2}\right)\log z - z + O(1), \tag{5.5}$$

also valid for $|\arg z|<\pi$ and $z\to\infty$ (see Ref. 20, p. 12), we see that for large n the term in parentheses on the right-hand side of (5.1) behaves like

$$\begin{aligned} &n\left(\log\left(n+\mu+\tfrac{1}{2}\right)+O(n^{-1})\right) - (n+\mu)\log\left(n+\mu+\tfrac{1}{2}\right) + \left(n+\mu+\tfrac{1}{2}\right) + O(1) \\ &\quad = n - \mu\log\left(n+\mu+\tfrac{1}{2}\right) + O(1), \end{aligned}$$

which is unbounded. In turn this implies that the sequence of entropies $\{s_n^\mu\}_{n=0}^\infty$ is unbounded, as wanted.

Now let us see that the sequence $\{s_n^\mu\}_{n=0}^\infty$ is increasing (as the sequence $\{S_n^\mu\}_{n=0}^\infty$ is). First note that Lemma (3.1) (a) gives us

$$s_1^\mu = \left(\mu+\tfrac{1}{2}\right)\left(\psi\left(\mu+\tfrac{3}{2}\right) - \log\left(\mu+\tfrac{1}{2}\right)\right) > 0 = s_0^\mu,$$

so let us prove that $s_{n+1}^\mu > s_n^\mu$ for $n \geqslant 1$. Observe that

$$\frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)} = \prod_{k=1}^{n}\left(k+\mu-\frac{1}{2}\right).$$

So we can write (5.1) as

$$s_n^\mu = \frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\left(n\psi\left(n+\mu+\frac{1}{2}\right) - \log\prod_{k=1}^{n}\left(k+\mu-\frac{1}{2}\right)\right)$$

$$= \frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\sum_{k=1}^{n}\left(\psi\left(n+\mu+\frac{1}{2}\right) - \log\left(k+\mu-\frac{1}{2}\right)\right).$$

Then, by using Lemma (3.1) (a) we get

$$s_{n+1}^\mu = \frac{\Gamma\left(n+\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\sum_{k=1}^{n+1}\left(\psi\left(n+\mu+\frac{3}{2}\right) - \log\left(k+\mu-\frac{1}{2}\right)\right)$$

$$= \frac{\Gamma\left(n+\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\sum_{k=1}^{n}\left(\frac{1}{n+\mu+\frac{1}{2}} + \psi\left(n+\mu+\frac{1}{2}\right) - \log\left(k+\mu-\frac{1}{2}\right)\right)$$

$$+ \frac{\Gamma\left(n+\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\left(\psi\left(n+\mu+\frac{3}{2}\right) - \log\left(n+\mu+\frac{1}{2}\right)\right)$$

$$= \frac{n\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)} + \left(n+\mu+\frac{1}{2}\right)s_n^\mu + \frac{\Gamma\left(n+\mu+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\left(\psi\left(n+\mu+\frac{3}{2}\right) - \log\left(n+\mu+\frac{1}{2}\right)\right) > s_n^\mu,$$

which proves that $\{s_n^\mu\}_{n=0}^\infty$ is increasing, as wanted. In particular we have that the sequence $\{s_n^\mu\}_{n=1}^\infty$ is positive. [Recall that since $L^2(\mathbb{R}, \mathrm{d}g_\mu)$ is a probability measure space, we have that $s_n^\mu \geqslant 0$ for all $n=0,1,\ldots$.]

Finally, observe that from formulas (2.1), (3.2), and (4.1) we see that (5.1) can be written as

$$s_n^\mu = \frac{\Gamma\left(n+\mu+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}(S_{2n}^\mu - S_n).$$

We know that $\lim_{n\to\infty}(S_{2n}^\mu/2n)=1$ (Theorem 4.1) and $\lim_{n\to\infty}(S_n/n)=1$ (Proposition 3.1). Then we have that

$$\lim_{n\to+\infty}\frac{s_n^\mu}{n\Gamma\left(n+\mu+\frac{1}{2}\right)} = \left(\Gamma\left(\mu+\frac{1}{2}\right)\right)^{-1}.$$

So the sequence $\{s_n^\mu\}_{n=0}^\infty$ diverges to infinity much faster than the sequence $\{S_n^\mu\}_{n=0}^\infty$ does. In particular, s_n^μ is not asymptotic to n, namely it is not extensive in n. Using the log-Sobolev

inequalities proved in Ref. 24, one can show that the entropies of the basis elements ζ_n^μ are comparable, modulo terms linear in n, with the entropies S_n^μ studied in the preceding section. This implies that the entropies of the ζ_n^μ are extensive quantities in n.

VI. μ-DEFORMED ENERGIES

In this section we study two entropy-energy inequalities, known as *reverse log-Sobolev inequalities* (in the μ-deformed Segal-Bargmann space $\mathcal{B}_\mu^2$) that are proved in Ref. 2. We first quote the appropriate definition of energy from Ref. 2 and then calculate it for the functions in the canonical basis of $\mathcal{B}_\mu^2$. Since we already have calculated the entropies for these functions, we can then proceed to the analysis of the two reverse log-Sobolev inequalities.

Definition 6.1: For $f \in \mathcal{B}_{e,\mu}^2$ we define its μ-deformed energy $E_{e,\mu}(f)$ as

$$E_{e,\mu}(f) = \int_{\mathbb{C}} |f(z)|^2 |z|^2 \, \mathrm{d}\nu_{e,\mu}(z).$$

For $f \in \mathcal{B}_{o,\mu}^2$ we define its μ-deformed energy $E_{o,\mu}(f)$ as

$$E_{o,\mu}(f) = \int_{\mathbb{C}} |f(z)|^2 |z|^2 \, \mathrm{d}\nu_{o,\mu}(z).$$

In general, for $f \in \mathcal{B}_\mu^2$ we define its μ-deformed energy $E_\mu(f)$ as $E_\mu(f) = E_{e,\mu}(f_e) + E_{o,\mu}(f_o)$.

We will denote by E_n^μ to the μ-deformed energy $E_\mu(\xi_n^\mu)$, so we have $E_{2n}^\mu = E_{e,\mu}(\xi_{2n}^\mu)$ and $E_{2n+1}^\mu = E_{o,\mu}(\xi_{2n+1}^\mu)$. We have that

$$E_{2n}^\mu = \frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)} \int_{\mathbb{C}} \left| \frac{z^{2n}}{(\gamma_\mu(2n))^{1/2}} \right|^2 |z|^2 K_{\mu-1/2}(|z|^2) |z|^{2\mu+1} \, \mathrm{d}x \, \mathrm{d}y$$

$$= \frac{2^{1/2-\mu} 2}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n)} \int_0^\infty K_{\mu-1/2}(r^2) r^{2(2n+\mu+2)} \, \mathrm{d}r = \frac{2^{1/2-\mu}}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n)} \int_0^\infty K_{\mu-1/2}(s) s^{2n+\mu+3/2} \, \mathrm{d}s.$$

Since $2n+\mu+\frac{5}{2} > |\mu-\frac{1}{2}|$ we can use formula (2.7) to write

$$E_{2n}^\mu = \frac{2^{1/2-\mu}}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n)} 2^{2n+\mu+1/2} \Gamma\left(n+\frac{3}{2}\right)\Gamma(n+\mu+1),$$

which simplifies [by using (2.1)] to

$$E_{2n}^\mu = \frac{2\Gamma\left(n+\frac{3}{2}\right)\Gamma(n+\mu+1)}{\Gamma(n+1)\Gamma\left(n+\mu+\frac{1}{2}\right)}. \tag{6.1}$$

Similarly we have that

$$E_{2n+1}^{\mu} = \frac{2^{1/2-\mu}}{\pi\Gamma\left(\mu+\frac{1}{2}\right)}\int_{\mathbb{C}}\left|\frac{z^{2n+1}}{(\gamma_\mu(2n+1))^{1/2}}\right|^2 |z|^2 K_{\mu+1/2}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y$$

$$= \frac{2^{1/2-\mu}2}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n+1)}\int_0^\infty K_{\mu+1/2}(r^2)r^{2(2n+\mu+3)}\,\mathrm{d}r$$

$$= \frac{2^{1/2-\mu}}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n+1)}\int_0^\infty K_{\mu+1/2}(s)s^{2n+\mu+5/2}\,\mathrm{d}s.$$

Since $2n+\mu+\frac{7}{2} > |\mu+\frac{1}{2}|$ we can use formula (2.7) to write

$$E_{2n+1}^{\mu} = \frac{2^{1/2-\mu}}{\Gamma\left(\mu+\frac{1}{2}\right)\gamma_\mu(2n+1)}2^{2n+\mu+3/2}\Gamma\left(n+\frac{3}{2}\right)\Gamma(n+\mu+2),$$

which simplifies [by using (2.2)] to

$$E_{2n+1}^{\mu} = \frac{2\Gamma\left(n+\frac{3}{2}\right)\Gamma(n+\mu+2)}{\Gamma(n+1)\Gamma\left(n+\mu+\frac{3}{2}\right)}. \tag{6.2}$$

When $\mu=0$ formulas (6.1) and (6.2) become

$$E_{2n}^{0} = 2n+1 \quad \text{and } E_{2n+1}^{0} = 2n+2,$$

which agrees with the known result that the (undeformed) energy E_n of the function ξ_n is $n+1$ (see Ref. 33).

In Ref. 2 the following two reverse log-Sobolev inequalities are proved in the context of μ-deformed Segal-Bargmann analysis (Theorems 5.1 and 5.2).

Theorem 6.1: *For all $c>1$ there exists a real number $P_e(c,\mu)$ such that for $f \in \mathcal{B}_{e,\mu}^2$ we have*

$$E_{e,\mu}(f) \leqslant cS_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(f) + P_e(c,\mu)\|f\|_{\mathcal{B}_{e,\mu}^2}.$$

Theorem 6.2: *For all $c>1$ there exists a real number $P_o(c,\mu)$ such that for $f \in \mathcal{B}_{o,\mu}^2$ we have*

$$E_{o,\mu}(f) \leqslant cS_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(f) + P_o(c,\mu)\|f\|_{\mathcal{B}_{o,\mu}^2}.$$

A direct consequence of these results is the following reverse log-Sobolev inequality in the μ-deformed Segal-Bargmann space $\mathcal{B}_\mu^2$ (Theorem 5.3 in Ref. 2).

Theorem 6.3: *For all $c>1$ there exists a real number $P(c,\mu)$ such that for $f \in \mathcal{B}_\mu^2$ we have*

$$E_\mu(f) \leqslant c(S_{L^2(\mathbb{C},\mathrm{d}\nu_{e,\mu})}(f_e) + S_{L^2(\mathbb{C},\mathrm{d}\nu_{o,\mu})}(f_o)) + P(c,\mu)\|f\|_{\mathcal{B}_\mu^2}.$$

In particular, if we consider the elements ξ_n^μ, $n=0,1,\ldots$ of the canonical basis of $\mathcal{B}_\mu^2$, Theorem 6.1 tells us that for all $c>1$ there exists a constant $P_e(c,\mu)$ such that for all $n=0,1,\ldots$ we have that

$$E_{2n}^{\mu} \leqslant cS_{2n}^{\mu} + P_e(c,\mu), \tag{6.3}$$

and Theorem 6.2 tells us that for all $c>1$ there exists a constant $P_o(c,\mu)$ such that for all $n=0,1,\ldots$. we have that

$$E_{2n+1}^{\mu} \leqslant cS_{2n+1}^{\mu} + P_o(c,\mu). \tag{6.4}$$

Remark: By using Stirling's formula it is easy to see from (6.1) and (6.2) that for fixed $n=0,1,\ldots$, we have that $E_n^{\mu} \to +\infty$ as $\mu \to +\infty$. We already know that $S_{2n+1}^{\mu} \to -\infty$ as $\mu \to +\infty$ (see Theorem 4.2). Then (6.4) tells us that for any $c>1$ and any $n=0,1,\ldots$ we have that $P_o(c,\mu) \geqslant E_{2n+1}^{\mu} - cS_{2n+1}^{\mu} \to +\infty$ as $\mu \to +\infty$. That is, the values of the constant $P_o(c,\mu)$ in Theorem 6.2 will be as large as we want, by taking $\mu>0$ large enough.

So Theorem 6.1 tells us that $c>1$ is a sufficient condition to conclude the existence of the constant $P_e(c,\mu)$ such that the inequality (6.3) holds for all $n=0,1,\ldots$. We will prove now that this condition is also necessary, by showing that for fixed $\mu > -\frac{1}{2}$, the sequence $\{E_{2n}^{\mu} - cS_{2n}^{\mu}\}_{n=0}^{\infty}$ is bounded above if and only if $c>1$.

By using the formula

$$\frac{\Gamma(z+\alpha)}{\Gamma(z+\beta)} = z^{\alpha-\beta}(1+O(z^{-1})), \tag{6.5}$$

valid for $|\arg z| < \pi$ and $z \to \infty$ (see Ref. 20, p. 12) we can write the following asymptotics for E_{2n}^{μ}:

$$E_{2n}^{\mu} = 2\frac{\Gamma\left(n+\frac{3}{2}\right)}{\Gamma(n+1)}\frac{\Gamma(n+\mu+1)}{\Gamma\left(n+\mu+\frac{1}{2}\right)} = 2n^{1/2}(1+O(n^{-1}))n^{1/2}(1+O(n^{-1})) = 2n+O(1).$$

Also, by using (2.1), (5.4), and (5.5) and formula (4.1) for S_{2n}^{μ}, we can write

$$\begin{aligned} S_{2n}^{\mu} &= n\left(\psi\left(\mu+n+\frac{1}{2}\right)+\psi(n+1)\right) - \log\frac{\Gamma(n+1)\Gamma\left(\mu+n+\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)} \\ &= n\left(\log\left(\mu+n+\frac{1}{2}\right)+\log(n+1)+O(n^{-1})\right) \\ &\quad -\left(n+\frac{1}{2}\right)\log(n+1)+n+1-(\mu+n)\log\left(\mu+n+\frac{1}{2}\right)+\mu+n+\frac{1}{2}+O(1) \\ &= -\frac{1}{2}\log(n+1)-\mu\log\left(\mu+n+\frac{1}{2}\right)+2n+O(1). \end{aligned}$$

Then we have that

$$\begin{aligned} E_{2n}^{\mu} - cS_{2n}^{\mu} &= 2n+O(1)-c\left(-\tfrac{1}{2}\log(n+1)-\mu\log\left(\mu+n+\tfrac{1}{2}\right)+2n+O(1)\right) \\ &= (1-c)2n+\frac{c}{2}\log(n+1)+c\mu\log\left(\mu+n+\frac{1}{2}\right)+O(1) \\ &= (1-c)2n+\frac{c}{2}\log\frac{n+1}{\mu+n+\frac{1}{2}}+c\left(\mu+\frac{1}{2}\right)\log\left(\mu+n+\frac{1}{2}\right)+O(1) \\ &= (1-c)2n+c\left(\mu+\frac{1}{2}\right)\log\left(\mu+n+\frac{1}{2}\right)+O(1). \end{aligned}$$

Clearly, the sequence $\{E_{2n}^{\mu} - cS_{2n}^{\mu}\}_{n=0}^{\infty}$ is bounded above if and only if $c>1$. This shows that the condition $c>1$ is the best possible in the reverse log-Sobolev inequality in Theorem 6.1, namely that this inequality does not hold for $c \leqslant 1$.

Now let us consider Theorem 6.2. We know that $c>1$ is a sufficient condition to conclude the existence of the constant $P_o(c,\mu)$ such that the inequality (6.4) holds for all $n=0,1,\ldots$. We will see now that this condition is also necessary, by showing that for fixed $\mu>-\frac{1}{2}$, the sequence $\{E^{\mu}_{2n+1}-cS^{\mu}_{2n+1}\}_{n=0}^{\infty}$ is bounded above if and only if $c>1$.

By using (6.5) we can write the following asymptotics for E^{μ}_{2n+1}:

$$E^{\mu}_{2n+1}=\frac{2\Gamma\left(n+\frac{3}{2}\right)\Gamma(n+\mu+2)}{\Gamma(n+1)\Gamma\left(n+\mu+\frac{3}{2}\right)}=2n^{1/2}(1+O(n^{-1}))n^{1/2}(1+O(n^{-1}))=2n+O(1).$$

By using (2.2), (5.4), and (5.5) and formula (4.3) for S^{μ}_{2n+1}, we can write

$$\begin{aligned}S^{\mu}_{2n+1}&=\left(n+\frac{1}{2}\right)\left(\psi\left(\mu+n+\frac{3}{2}\right)+\psi(n+1)\right)-\log\frac{\Gamma(n+1)\Gamma\left(\mu+n+\frac{3}{2}\right)}{\Gamma\left(\mu+\frac{1}{2}\right)}\\&=\left(n+\frac{1}{2}\right)\left(\log\left(\mu+n+\frac{3}{2}\right)+\log(n+1)+O(n^{-1})\right)\\&\quad-\left(n+\frac{1}{2}\right)\log(n+1)+n+1-(\mu+n+1)\log\left(\mu+n+\frac{3}{2}\right)+\mu+n+\frac{3}{2}+O(1)\\&=-\left(\mu+\frac{1}{2}\right)\log\left(\mu+n+\frac{3}{2}\right)+2n+O(1).\end{aligned}$$

Then we have that

$$\begin{aligned}E^{\mu}_{2n+1}-cS^{\mu}_{2n+1}&=2n+O(1)-c\left(-\left(\mu+\frac{1}{2}\right)\log\left(\mu+n+\frac{3}{2}\right)+2n+O(1)\right)\\&=(1-c)2n+c\left(\mu+\frac{1}{2}\right)\log\left(\mu+n+\frac{3}{2}\right)+O(1).\end{aligned}$$

As in the case of Theorem 6.1 considered above, we see now that the sequence $\{E^{\mu}_{2n+1}-cS^{\mu}_{2n+1}\}_{n=0}^{\infty}$ is bounded above if and only if $c>1$, which shows that the condition $c>1$ is the best possible in the reverse log-Sobolev inequality in Theorem 6.2.

Either one of the two cases considered in this section shows that the condition $c>1$ in Theorem 6.3 is also the best possible. Note that the asymptotics that we have proved for E^{μ}_{n} show that it is extensive in n.

VII. FINAL REMARKS

In conclusion, we have just a few comments.

First, it would be interesting to evaluate in closed form the entropies of the elements ζ^{μ}_{n} for $n\geqslant 2$ of the canonical basis of $L^2(\mathbb{R},\mathrm{d}g_{\mu})$. This has not even been done yet in the case $\mu=0$.

Second, we would like to repeat the conjecture that the μ-deformed Segal-Bargmann transform increases the entropy of some functions. And again, this is plausible since it is known to be true when $\mu=0$. (See Ref. 33.)

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The quantum fidelity for the time-periodic singular harmonic oscillator

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In this paper we perform an exact study of "quantum fidelity" (also called Loschmidt echo) for the time-periodic quantum harmonic oscillator of the following Hamiltonian: $\hat{H}_g(t) := (P^2/2) + f(t)(Q^2/2) + (g^2/Q^2)$, when compared with the quantum evolution induced by $\hat{H}_0(t)$ $(g=0)$, in the case where f is a T-periodic function and g a real constant. The reference (initial) state is taken to be an arbitrary "generalized coherent state" in the sense of Perelomov. We show that, starting with a quadratic decrease in time in the neighborhood of $t=0$, this quantum fidelity may recur to its initial value 1 at an infinite sequence of times t_k. We discuss the result when the classical motion induced by Hamiltonian $\hat{H}_0(t)$ is assumed to be stable versus unstable. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178153]

I. INTRODUCTION

A growing interest has been devoted recently on the study of the so-called "quantum fidelity"

$$F_g(t) := \langle U_0(t,0)\psi, U_g(t,0)\psi \rangle \tag{1}$$

for some reference state ψ that we take as initial wave packet, $U_0(t,0)$ being the quantum unitary evolution operator induced by some Hamiltonian, and $U_g(t,0)$ the quantum evolution for a perturbation of it, g being the size of the perturbation. The long-time behavior of $F_g(t)$ is of particular interest, and it has been studied for a large class of (time independent) Hamiltonians in a more or less heuristic way, and this long-time behavior has been suggested to depend sensitively on the regular versus chaotic motion of the underlying classical motion (see the reference section).

The first occurrence of this notion in the literature is due to Peres.[22] Recently a large amount of work has been presented on this topic (see Refs. 1–6, 9–19, and 23–44). In most of these works, it is claimed that the quantum fidelity decays very fast to zero as time grows, when the underlying classical (unperturbed) dynamics is generically chaotic.

Although the short time decay of the fidelity is rather well understood,[42] some of the arguments put forward in the above cited works are not entirely convincing, since they are either purely numerical, or extrapolate the "short time" behavior to guess the (Gaussian or exponential) decay at infinity. However there are few (semiclassical and/or perturbative) approaches which explain quantitatively behaviors in different time regimes. In particular there is a semiclassical dephasing approximation put forward by Vanicek,[32] and perturbative semiclassical calculations of Prosen and Znidaric[27] which are valid in the regime of integrable, chaotic, and mixed dynamics regimes. Finally let us mention exact perturbative calculations of fidelity decay via random-matrix description by Gorin *et al.*,[16] and an exact nonperturbative supersymmetric random-matrix de-

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scription by Stoeckmann *et al.*[31] Thus it is a field of very rich and promising insight for the study of stability under perturbations of the quantum dynamics when the underlying classical motion displays chaotic behavior.

In other approaches,[18,41] the case of integrable or regular systems is considered as well, and seems to indicate the occurrence of an anomalous power law decay. Moreover, in a case of nearly integrable system a recurrence of fidelity has been exhibited;[28] in this case the quantum fidelity manifests recurrences very close to the initial value 1 as time evolves.

Thus it is a very intriguing subject of high interest to know more about the complete time behavior of the quantum fidelity when the underlying dynamics is chaotic versus regular. To our knowledge, no completely rigorous approach of this topic has been attempted yet. It would be highly desirable to have a mathematically explicit description of the long-time behavior of the quantum fidelity, although it is a very difficult task.

This paper is a first attempt towards this rigorous understanding. It relies on a rather simplistic class of Hamiltonians for which the perturbed as well as unperturbed quantum dynamics can be explicitly solved in terms of the classical dynamics. Moreover the reference quantum states are taken in a suitable large class of quantum states known as "generalized coherent states" in the sense of Perelomov. The results are rather surprising:

(i) for a large class of reference states, the quantum fidelity never decreases to 0, but instead remains bounded from below by some constant;
(ii) in the unstable case, the quantum fidelity either decays exponentially fast to some nonzero constant, as $t \to \infty$, or manifests strong recurrences to 1;
(iii) in the stable case the quantum fidelity always manifests strong recurrences to 1 as time evolves.

These facts are strongly related to the underlying SU (1, 1) structure underlying the corresponding Hamiltonians, as can be seen from the work of Perelomov.[21]

We also are able to show a strong relationship between "quantum and classical fidelity" for this specific situation.[8]

To complete this Introduction, let us notice that a notion of classical fidelity that "mimics" the quantum fidelity has been proposed in the literature,[27,12,2,36] where decay properties similar to those of the quantum fidelity appear. Thus it would be desirable to understand more deeply the relationships between the classical and quantum fidelity on a firm mathematical basis. We shall pursue this investigation in future presentations, notably in the semiclassical limit (see Refs. 8 and 7).

II. CALCULUS OF THE QUANTUM FIDELITY

Let us consider the following operators in $\mathcal{H}=L^2(\mathbb{R})$ with suitable domains (see Ref. 21):

$$K_0 = \frac{Q^2+P^2}{4} + \frac{g^2}{2Q^2}, \tag{2}$$

$$K_\pm = \frac{Q^2-P^2}{4} \mp i\frac{QP+PQ}{4} - \frac{g^2}{2Q^2}, \tag{3}$$

where Q is the usual multiplication operator by x and

$$P := -i\frac{d}{dx},$$

K_0 and $K_\pm$ satisfy the usual commutation rules of SU (1, 1) algebra, namely

$$[K_0, K_\pm] = \pm K_\pm, \tag{4}$$

$$[K_-, K_+] = 2K_0. \tag{5}$$

We define the "generalized coherent states" (squeezed states) as follows: given any $\beta \in \mathbb{C}$,

$$S_\beta = \exp(\beta K_+ - \bar{\beta} K_-), \tag{6}$$

$$\psi_\beta = S(\beta)\psi, \tag{7}$$

ψ being a normalized state in $\mathcal{H}$ such that

$$K_-\psi = 0, \tag{8}$$

$$2K_0\psi = \left(\alpha + \tfrac{1}{2}\right)\psi, \tag{9}$$

with

$$\alpha := \tfrac{1}{2} + \sqrt{\tfrac{1}{4} + 2g^2}. \tag{10}$$

We shall focus on the following cases $g=1$, $g=\sqrt{3}$, where ψ has the following form:

$$\varphi(x) = c_1 x^2 e^{-x^2/2}, \tag{11}$$

$$\chi(x) = c_2 x^3 e^{-x^2/2} \tag{12}$$

with

$$c_1 = \sqrt{\tfrac{4}{3}}, \tag{13}$$

$$c_2 = \sqrt{\tfrac{8}{15}} \tag{14}$$

(omitting the factors in π).

This makes φ and χ to be (normalized to 1) finite linear combinations of Hermite functions. It has been shown (see Ref. 21) that for $\psi=\varphi$, ψ_β has the following form:

$$\psi_\beta = c_1 x^2 e^{-2(u-\epsilon)} \exp\left(-\frac{5i\theta}{2} + i\frac{\dot{u}x^2}{2} - \frac{1}{2}(u-\epsilon) - \frac{1}{2}(xe^{-(u-\epsilon)})^2\right), \tag{15}$$

where the constants $u, \dot{u}, \theta, \epsilon$ are suitably determined from $\beta \in \mathbb{C}$, whereas for $\psi=\chi$, ψ_β is

$$\psi_\beta = c_2 x^3 e^{-3(u-\epsilon)} \exp\left(-\frac{7i\theta}{2} + i\frac{\dot{u}x^2}{2} - \frac{1}{2}(u-\epsilon) - \frac{1}{2}(xe^{-(u-\epsilon)})^2\right). \tag{16}$$

Now the evolutions of ψ_β with respect to $U_1(t,0)$ and $U_{\sqrt{3}}(t,0)$, respectively, together with $U_0(t,0)$ are completely explicit.

Consider a complex solution of the classical equations of motion induced by Hamiltonian $\hat{H}_0(t)$,

$$\ddot{x} + fx = 0 \tag{17}$$

and look for it in the form

$$x = e^{u+i\theta}, \tag{18}$$

where the functions $t \mapsto u$ and $t \mapsto \theta$ are real.

We assume for $u(t)$ and $\theta(t)$ the following initial data:

$$u(0) = u_0,$$

$$\dot{u}(0) = \dot{u}_0,$$

$$\theta(0) = \theta_0,$$

$$\dot{\theta}(0) = e^{-2(u_0-\epsilon)}.$$

Since f is real, the Wronskian of x and $\bar{x}$ is constant and equals

$$2ie^{2\epsilon} = 2i\dot{\theta}(t)e^{2u(t)}. \tag{19}$$

This yields

$$\ddot{x} = [\ddot{u} + i\ddot{\theta} + (\dot{u} + i\dot{\theta})^2]x = [\ddot{u} + \dot{u}^2 - e^{-4(u-\epsilon)}]x = -fx \tag{20}$$

and therefore u obeys the following differential equation:

$$\ddot{u} + \dot{u}^2 - e^{-4(u-\epsilon)} + f = 0. \tag{21}$$

We have the following result.

Lemma 2.1: Let $\hat{H}_g = (P^2+Q^2)/2 + g^2/Q^2$. *Then the quantum propagator for* $\hat{H}_g(t)$ *is of the following form:*

$$U_g(t,0) = e^{i\dot{u}Q^2/2}e^{-i(u-\epsilon)(QP+PQ)/2}e^{-i(\theta-\theta_0)\hat{H}_g}e^{i(u_0-\epsilon)(QP+PQ)/2}e^{-i\dot{u}_0Q^2/2}. \tag{22}$$

The same formula holds for the propagator $U_0(t,0)$ *of* $\hat{H}_0(t)$ *with* $\hat{H}_g$ *replaced by* $\hat{H}_0$.

Proof: Let us denote

$$V(t) := e^{i\dot{u}Q^2/2}e^{-i(u-\epsilon)(QP+PQ)/2}e^{-i\theta\hat{H}_g}. \tag{23}$$

We have

$$i\frac{d}{dt}V(t) = \left(-\ddot{u}\frac{Q^2}{2} + \frac{\dot{u}}{2}e^{i\dot{u}Q^2/2}(QP+PQ)e^{-i\dot{u}Q^2/2}\right)V(t)$$
$$+ (\dot{\theta}e^{i\dot{u}Q^2/2}e^{i(u-\epsilon)(QP+PQ)/2}\hat{H}_g e^{-i(u-\epsilon)(QP+PQ)/2}e^{-i\dot{u}Q^2/2})V(t) \tag{24}$$

and since

$$e^{i\dot{u}Q^2/2}Pe^{-i\dot{u}Q^2/2} = P - \dot{u}Q \tag{25}$$

we have

$$e^{i\dot{u}Q^2/2}(PQ+QP)e^{-i\dot{u}Q^2/2} = PQ + QP - 2i\dot{u}Q^2. \tag{26}$$

Therefore the first line on the right-hand side (RHS) of (24) is

$$\left(\left(-\frac{\ddot{u}}{2} - \dot{u}^2\right)Q^2 + \frac{\dot{u}}{2}(QP+PQ)\right)V(t). \tag{27}$$

Furthermore

$$e^{-i(u-\epsilon)(QP+PQ)/2}\hat{H}_g e^{-i(u-\epsilon)(PQ+QP)/2} = \left(\frac{P^2}{2} + \frac{g^2}{Q^2}\right)e^{2(u-\epsilon)} + \frac{Q^2}{2}e^{-2(u-\epsilon)} \tag{28}$$

which implies that the second line on the RHS of (24) is

$$\left(\frac{1}{2}(P-\dot{u}Q)^2+\frac{g^2}{Q^2}+\frac{Q^2}{2}e^{-4(u-\epsilon)}\right)V(t), \tag{29}$$

where we have used that

$$\dot{\theta}=e^{-2(u-\epsilon)}.$$

Collecting the different terms, we get

$$i\frac{d}{dt}V(t)=\left(\frac{P^2}{2}+\frac{g^2}{Q^2}+\frac{Q^2}{2}(-\ddot{u}-\dot{u}^2+e^{-4(u-\epsilon)})\right)V(t)=\left(\frac{P^2}{2}+\frac{g^2}{Q^2}+f(t)\frac{Q^2}{2}\right)V(t) \tag{30}$$

using (21). □

We shall now consider the "quantum fidelity" in two particular cases $g=1$ and $g=\sqrt{3}$, starting, respectively, with the initial states $\psi_{\beta,1}=S(\beta)\varphi$, and $\psi_{\beta,2}=S(\beta)\chi$,

$$F_1(t)=\langle U_0(t,0)\psi_{\beta,1},U_g(t,0)\psi_{\beta,1}\rangle, \tag{31}$$

and similarly for $F_2(t)$ with $\psi_{\beta,1}$ replaced by $\psi_{\beta,2}$.

Theorem 2.2: *(i) Let $g=1$ and $\psi_{\beta,1}=S(\beta)\varphi$. Then we have*

$$F_1(t)=\tfrac{2}{3}+\tfrac{1}{3}e^{-2i(\theta(t)-\theta(0))}. \tag{32}$$

(ii) Let $g=\sqrt{3}$ and $\psi_{\beta,2}=S(\beta)\chi$. Then we have

$$F_2(t)=\tfrac{2}{5}+\tfrac{3}{5}e^{-3i(\theta(t)-\theta(0))}. \tag{33}$$

Proof: Since x^2 is expanded as

$$x^2=\tfrac{1}{4}H_2(x)+\tfrac{1}{2}H_0(x)$$

it is clear that

$$U_0(t,0)\psi_{\beta,1}=c_1\exp\left(\frac{i}{2}\dot{u}(t)x^2-\frac{1}{2}(u(t)-\epsilon)\right)\left\{\frac{1}{4}e^{-5i\theta(t)/2}H_2(xe^{-(u(t)-\epsilon)})+\frac{1}{2}e^{-i\theta(t)/2-2i\theta(0)}\right\}$$
$$\times\exp\left(-\frac{1}{2}x^2e^{-2(u(t)-\epsilon)}\right) \tag{34}$$

and

$$U_g(t)\psi_{\beta,1}=V(t)\varphi=c_1\exp\left(-\frac{5}{2}i\theta(t)+\frac{i}{2}\dot{u}(t)x^2-\frac{1}{2}(xe^{-(u(t)-\epsilon)})^2\right) \tag{35}$$

from which we deduce that

$$F_1(t)=c_1^2\int\left[x^2\left(x^2-\frac{1}{2}\right)+\frac{e^{-2i(\theta(t)-\theta(0))}}{2}x^2\right]e^{-x^2}\,dx=\frac{4}{3}\left(\frac{1}{2}+\frac{1}{4}e^{-2i(\theta(t)-\theta(0))}\right)=\frac{2}{3}+\frac{1}{3}e^{-2i(\theta(t)-\theta(0))}, \tag{36}$$

(ii) follows from a very similar calculation using that

$$H_3(x)=8x^3-12x.$$

□

Let us now assume that g has an arbitrary real value [not specifically of the form $g=\sqrt{k(k+1)/2}$ for $k\in\mathbb{N}$ which gives rise to integer values of $\alpha=\frac{1}{2}+\sqrt{\frac{1}{4}+2g^2}$]. Then the state $\psi:=cx^{\alpha}e^{-x^2/2}$ is no longer a finite linear combination of Hermite functions. It has nevertheless an infinite expansion on the basis of Hermite functions φ_n,

$$\psi=\sum_{n=0}^{\infty}\lambda_n\varphi_n$$

and one can establish the following general result about the corresponding "quantum fidelity."

Theorem 2.3:

$$F_g(t)=\exp(-i\alpha(\theta(t)-\theta(0)))\sum_{n=0}^{\infty}|\lambda_n|^2\exp(in(\theta(t)-\theta(0)))$$

which, since $\Sigma_{n=0}^{\infty}|\lambda_n|^2=1$, *returns in absolute value to 1 as long as* $\theta(t)-\theta(0)=0(mod\,2\pi)$. *If* $\alpha=p/q$ *is rational, then the quantum fidelity recurs exactly to 1 (not only in absolute value) provided that* $\theta(t)-\theta(0)=0(mod\,2q\pi)$.

Proof: Again according to Ref. 21, we have

$$\psi_\beta:=S(\beta)\psi=e^{-i(\alpha+1/2)\theta_0}D(u_0)\psi,$$

where by $D(u)$ we denote the following unitary operator:

$$D(u):=e^{iuQ^2/2}e^{-i(u-\epsilon)(QP+PQ)/2}.$$

Then

$$U_0(t,0)\psi_\beta=D(u_t)e^{-i(\theta_t-\theta_0)\hat{H}_0}\sum_{n=0}^{\infty}\lambda_n e^{-i\theta_0(\alpha+1/2)}\varphi_n=D(u_t)\sum_{n=0}^{\infty}\lambda_n e^{-i\theta_t(n+1/2)+i\theta_0(n-\alpha)}\varphi_n,$$

whereas

$$U_g(t,0)\psi_\beta=e^{-i\theta_t(\alpha+1/2)}D(u_t)\psi,$$

so that

$$\langle U_0(t,0)\psi_\beta,U_g(t,0)\psi_\beta\psi_\beta\rangle=\sum_{n,m}\bar{\lambda}_n\lambda_m e^{i\theta_t(n+1/2)-i\theta_0(n-\alpha)-i\theta_t(\alpha+1/2)}\langle\varphi_n,\varphi_m\rangle=\sum_{n=0}^{\infty}|\lambda_n|^2e^{i(\theta_t-\theta_0)(n-\alpha)}.$$

□

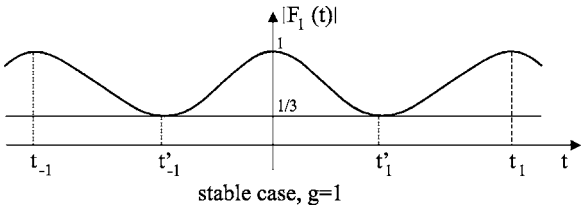
III. DISCUSSION OF THE RESULT

Since f is a T-periodic function, Floquet analysis applies to Eq. (17) which is nothing but the well-known Hill's equation. Depending to the parameters characterizing the function f [as, for example, γ and δ in the case of Mathieu equation where $f(t)=\gamma+\delta\cos\omega t$], the solutions can be either stable or unstable. In all cases the quantum fidelity $F_1(t)$ and $F_2(t)$ are bounded from below by some positive constant in absolute value, and therefore never decrease to zero.

The phase $\theta(t)$ is determined by

$$\theta(t)-\theta(0)=e^{2\epsilon}\int_0^t e^{-2u(s)}\,ds. \tag{37}$$

In the stable case, the function $t \mapsto u(t)$ is T-periodic. Therefore $\theta(t)$ grows from $-\infty$ to $+\infty$ as time evolves from $-\infty$ to $+\infty$. It follows that there exists an infinite sequence of times $\{t_k\}$ where $F_1(t)$ recurs to its initial value 1, and an infinite squence $\{t'_k\}$ where $|F_1(t)|$ attains its minimum $1/3$. The same statement holds for $F_2(t)$ where $1/3$ is replaced by $1/5$.



In the unstable case there is some positive Lyapunov exponent λ and some real solution of Hill's equation such that

$$x(T) = e^{\lambda T} x(0),$$

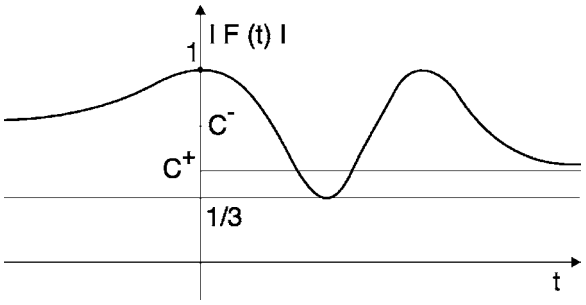
$$\dot{x}(T) = e^{\lambda T} \dot{x}(0).$$

Here, since we deal with complex solutions $x(t)$ such that the Wronskian of x and $\bar{x}$ is nonzero, we deduce that $|x(t)| > 0$. Moreover, depending on the instability zone, $|x(t)|^{-2} = e^{-2u(t)}$ can be integrable near $\pm\infty$, or diverge at $\pm\infty$. These topics are clearly detailed in Ref. 20. In the first case the conclusion is that there exists two constants $\theta_{\pm}$ such that

$$\theta(t) \to \theta_{\pm} \quad \text{as } t \to \pm\infty. \tag{38}$$

This is the case for the inverted harmonic oscillator $(f=-1)$ that we describe in the preceding section.

Therefore the quantum fidelity in this case behaves generically as described in the following picture:



If the instability zone in which the solution $x(t)$ lies is such that $|x(t)|^{-2}$ is not integrable near $\pm\infty$, then the diagram is typically similar to that of the stable case, which shows infinite recurrences to 1 of the quantum fidelity.

IV. LINK WITH THE "CLASSICAL INFIDELITY"

We can call "classical infidelity" the discrepancy between two classical trajectories, along their evolution, when they merge from the same initial phase-space point at $t=0$. The possible crossing of the two trajectories governed by $H_0(t)$ and $H_g(t)$, in phase space, as time evolves, could then be a signature of the "classical fidelity" as defined in the literature.

From now on we assume that ϵ of Sec. II is determined by $(g>0)$,

$$e^{2\epsilon} = g\sqrt{2}. \tag{39}$$

Proposition 1: Let $x(t)$ *be a* real *trajectory for the time-periodic Hamiltonian* $H_0(t)$, *and* $y(t)$

a real *trajectory for Hamiltonian* $H_g(t)$. *Assume in addition that they satisfy* $x(0)=y(0)\in\mathbb{R}$, $\dot{x}(0)=\dot{y}(0)\in\mathbb{R}$. *Then we have*

$$|x(t)-y(t)| = |y(t)|(1-\cos\tilde{\theta}(t)), \tag{40}$$

where $\tilde{\theta}(t)$ *is defined as follows:*

$$\tilde{\theta}(t) := g\sqrt{2}\int_0^t y(s)^{-2}\,\mathrm{d}s \equiv \theta(t)-\theta(0). \tag{41}$$

Proof: Let $z(t)$ be a complex solution of the equation

$$\ddot{z}+fz=0. \tag{42}$$

It can be written as $z(t)=e^{u+i\tilde{\theta}}$ as above, where $t\mapsto u$ and $t\mapsto\tilde{\theta}$ are real functions. Assume that $x(t)$ is such that $x(0)>0$. Then it is easy to see that $x(t)=\Re z(t)=e^{u(t)}\cos\tilde{\theta}(t)$ is a solution of Eq. (42), and that the positive function $y(t):=e^{u(t)}$ is a solution of

$$\ddot{y}+fy-\frac{2g^2}{y^3}=0 \tag{43}$$

which means that it defines a classical trajectory for $H_g(t)$.

Namely we get from Eq. (41) that

$$\frac{d}{\mathrm{d}t}\tilde{\theta}(t)=g\sqrt{2}e^{-2u(t)} \tag{44}$$

and therefore

$$\ddot{x}=(\ddot{u}+\dot{u}^2-2g^2e^{-4u})x=-fx, \tag{45}$$

so that

$$(\ddot{u}+\dot{u}^2-2g^2e^{-4u}+f)e^u=0 \tag{46}$$

which is nothing but Eq. (43) noting that

$$\ddot{y}=(\ddot{u}+\dot{u}^2)y. \tag{47}$$

Moreover, they satisfy $x(0)=y(0)$, $\dot{x}(0)=\dot{y}(0)$, and

$$|x(t)-y(t)| = y(t)(1-\cos\tilde{\theta}(t)).$$

In the case where $x(0)<0$, we just take $x(t)=-\Re z(t)$ and $y(t)=-e^{u(t)}$, which completes the result. □

Conclusion: The classical infidelity vanishes for $\tilde{\theta}(t)=2k\pi$ ($k\in\mathbb{Z}$), which precisely gives rise to recurrences to 1 of the "quantum fidelity" (Theorem 2.3). We expect this remarkable property to be true in more general situations, in particular in the semiclassical regime (see Ref. 8).

By "vanishing of the classical infidelity" we mean that given any solution of the unperturbed dynamics, there exists a solution of the perturbed one that coincides with it at the origin, and at any values of time solving the equation

$$g\sqrt{2}\int_0^t \mathrm{d}s\; y(s)^{-2}=0 \pmod{2\pi}.$$

One may ask whether this holds true for general solution $x(t)$, $y(t)$ of Eqs. (42) and (43). This is answered in the following particular cases below.

(i) *Particular case* $f=1$ (the case $f=\omega^2$ could be treated as well): When we apply the result above, we find that solutions $x(t)=A\cos t$ and $y=A$ coincide for $t=2k\pi$, $k\in\mathbb{Z}$, and that y obeys Eq. (43) provided $A=(2g^2)^{1/4}$. One shows that a more general result holds, involving general solutions of the equations under consideration.

The general solution of Eq. (43) is of the form (apart from the sign before the square root)

$$y(t)=\sqrt{\alpha+\beta\cos 2t+\gamma\sin 2t} \tag{48}$$

with α,β,γ related to each other by the relation

$$\alpha^2-(\beta^2+\gamma^2)=2g^2. \tag{49}$$

It obeys the initial data

$$y(0)=\sqrt{\alpha+\beta},$$

$$\dot{y}(0)=\frac{\gamma}{\sqrt{\alpha+\beta}},$$

and the conserved energy is simply α.

We take as real solution of Eq. (43) (harmonic oscillator),

$$x(t)=\sqrt{\alpha+\beta}\cos t+\frac{\gamma}{\sqrt{\alpha+\beta}}\sin t, \tag{50}$$

which has the same initial data as $y(t)$. Both functions being 2π-periodic, the generic "classical infidelity" vanishes when $t=2k\pi$, $k\in\mathbb{Z}$.

(ii) Particular case $f=-1$ (the case $f=-\omega^2$ could be treated as well): Any complex solution of the differential equation (inverted harmonic oscillator)

$$\ddot{z}-z=0 \tag{51}$$

can be written in the form

$$z(t)=(a+ib)e^t+(c+id)e^{-t}, \tag{52}$$

where a,b,c,d are real constants. We define

$$Z(t):=|z(t)|^2.$$

One can prove that $y(t)=\sqrt{Z(t)}$ obeys the differential equation

$$\ddot{y}-y-\frac{2g^2}{y^3}=0 \tag{53}$$

with

$$g^2=2(ad-bc)^2>0 \tag{54}$$

It is important to note that this implies $Z(t)>0$, $\forall t$.

Define $x(t):=y(t)\cos\theta(t)$, with $\theta(0)=0$. Then, clearly

$$x(0)=y(0),$$

$$\dot{x}(0)=\dot{y}(0).$$

We want $x(t)$ to be a real solution of Eq. (53). Since

$$\ddot{x} - x = \frac{1}{\sqrt{Z}}\left(\frac{\ddot{Z}}{2} - \frac{\dot{Z}^2}{4Z} - Z - \dot{\theta}^2 Z\right)\cos\,\theta - \left(\frac{\dot{\theta}\dot{Z}}{\sqrt{Z}} + \ddot{\theta}\sqrt{Z}\right)\sin\,\theta \tag{55}$$

and since Z obeys

$$\frac{\ddot{Z}}{2} - \frac{\dot{Z}^2}{4Z} - Z - \frac{2g^2}{Z} = 0 \tag{56}$$

the RHS of Eq. (55) vanishes provided

$$\dot{\theta}^2 = 2g^2 Z^{-2}. \tag{57}$$

Then $x(t)$ and $y(t)$ are two trajectories for Hamiltonians $(P^2-Q^2)/2$ and $(P^2-Q^2)/2 + (g^2/Q^2)$ respectively, with the same initial data, and we have

$$|x(t) - y(t)| = y(t)(1 - \cos\,\theta(t)). \tag{58}$$

Using the particular solution of Eq. (51)

$$z(t) = \frac{1+i}{2}e^{t} + \frac{1-i}{2}e^{-t}$$

that can be rewritten as

$$z(t) = \sqrt{\cosh 2t}\,\exp\left(\frac{i}{2}\,\text{arcsin tanh}\,2t\right),$$

i.e., with $u(t)=\frac{1}{2}\ln\cosh 2t$ [which satisfies $u(0)=\dot{u}(0)=0$], the formula (22) can be rewritten in the simple form

$$U_g(t,0) = \exp\left(\frac{i}{2}Q^2\tanh 2t\right)\exp\left(\frac{i}{4}(QP+PQ)\ln\cosh 2t\right)\exp\left(-\frac{i}{2}\hat{H}_g\,\text{arcsin tanh}\,2t\right) \tag{59}$$

which holds true for $g=0$, and $g=1/\sqrt{2}$. For $g=0$, this is nothing but the well-known Mehler's formula.

(iii) Study of $\theta(t)$: Recall that the fidelity $F_g(t)$ strongly depends on the reference state via the constants a,b,c,d,

$$\theta(t) = g\sqrt{2}\int_0^t \frac{\mathrm{d}s}{(a^2+b^2)e^{2s} + (c^2+d^2)e^{-2s} + 2(ac+bd)} = \left(\arctan\left(\frac{ac+bd+(a^2+b^2)e^{2t}}{|ad-bc|}\right)\right.$$
$$\left. - \arctan\left(\frac{ac+bd+(a^2+b^2)}{|ad-bc|}\right)\right). \tag{60}$$

This implies that $\theta(t)\to\theta_{\pm}$ as $t\to\pm\infty$ exponentially fast in the future and in the past. The calculus is especially simple in the particular case where we choose $a=d=g/\sqrt{2}$, $c=b=0$,

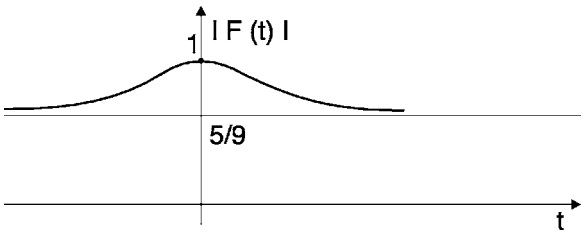
$$\theta(t) = \arctan(e^{2t}) - \frac{\pi}{4}. \tag{61}$$

No crossing of the classical trajectories happens in this case between the perturbed and unperturbed dynamics, and the square of the quantum fidelity in the case $g=1$ is nothing but

$$|F_1(t)|^2 = \frac{5}{9} + \frac{8}{9(e^{2t}+e^{-2t})} \sim \frac{5}{9} + \frac{4}{9}e^{-2|t|} \tag{62}$$

as $t\to\pm\infty$.

Here the symmetry is perfect between the future and the past, and the quantum fidelity has no recurrences to 1, but instead decays exponentially fast to 5/9.



V. CONCLUSION

It has been suggested in many recent works that the type of decay of the quantum fidelity may help to discriminate between chaotic or regular underlying classical motion; in other words the hypersensitivity of quantum dynamics under small perturbations, as measured by the type of decrease of the quantum fidelity, could be a signature of what is often called (rather improperly) "quantum chaos."

Thus it is highly desirable to have a better understanding of how this function of time [represented by Eq. (1) for suitable class of reference quantum states ψ] behaves at infinity in general as well in particular systems. In this paper we have been able to describe the full time behavior of the quantum fidelity for a rather specific class of systems, and for reference states in a suitable class of "generalized coherent states". The underlying SU(1,1) structure possessed by these systems allows us to perform an exact calculus of the quantum fidelity, and to compare it with the "classical infidelity" of the corresponding classical motion. This classical motion can be either stable, or unstable with positive Lyapunov exponent. The quantum fidelity has the following remarkable properties:

(i) either it decays to a (generally nonzero) limit in the past and in the future,
(ii) or it manifests an infinite sequence of recurrences to 1 as time evolves.

This sheds a new light on this question which has been addressed in a great variety of cases in the physics literature, and where the quantum fidelity is generally claimed to decay very rapidly to zero. Thus the first mathematical study presented here on the long-time behavior of the quantum fidelity could allow in the future a better understanding of these features in more general situations on a rigorous level.

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Effective Hamiltonians for atoms in very strong magnetic fields

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We propose three effective Hamiltonians which approximate atoms in very strong homogeneous magnetic fields B modelled by the Pauli Hamiltonian, with fixed total angular momentum with respect to magnetic field axis. All three Hamiltonians describe N electrons and a fixed nucleus where the Coulomb interaction has been replaced by B-dependent one-dimensional effective (vector valued) potentials but without magnetic field. Two of them are solvable in at least the one electron case. We briefly sketch how these Hamiltonians can be used to analyze the bottom of the spectrum of such atoms. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Pauli Hamiltonian of a nonrelativistic atom with an infinitely heavy nucleus and electrons with spin in a constant magnetic field $\mathbb{B}$ of strength B is given by

$$H^B(Z,N)=\sum_{j=1}^{N}\left(\frac{1}{2}\left(\frac{1}{i}\nabla_j-\frac{1}{2}\mathbb{B}\wedge r_j\right)^2+\vec{\sigma}_j\cdot\mathbb{B}-\frac{Z}{|r_j|}\right)+\sum_{1\leqslant j<k\leqslant N}\frac{1}{|r_j-r_k|},\tag{1}$$

where $r_j=(x_j,y_j,z_j)\in\mathbb{R}^3$ are the coordinates of the jth electron, $\vec{\sigma}_j$ is its spin, and ∇_j is the gradient with respect to r_j. Note that we have made the choice of $\frac{1}{2}\mathbb{B}\wedge r$ for the vector potential of $\mathbb{B}$, and that we are working in atomic units.

We fix the direction of $\mathbb{B}$ to be the z direction: $\mathbb{B}=B(0,0,1)$ with $B\geqslant 0$ without loss of generality. Recall that the z-component of $\vec{\sigma}_j$ is given, in the Pauli representation, by

$$I\otimes\cdots\sigma_{z_j}\cdots\otimes I,\quad \sigma_{z_j}=\frac{1}{2}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},$$

acting on the N-fold tensor product $\mathbb{C}^2\otimes\cdots\otimes\mathbb{C}^2$. It is known (see Ref. 13) that $H^B:=H^B(Z,N)$ defines an essentially self-adjoint operator on

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$$\mathcal{H} = \bigotimes_{j=1}^{N} L^2(\mathbb{R}^2) \otimes \mathbb{C}^2, \tag{2}$$

the Hilbert space of distinguishable electrons or "boltzons" (meaning particles satisfying the Boltzman statistics: we thank Beth Ruskai for introducing us to this expression). Physical atoms are of course modeled by H^B restricted to the fermionic subspace

$$\mathcal{H}_{\mathrm{f}} = \bigwedge_{j=1}^{N} L^2(\mathbb{R}^3) \otimes \mathbb{C}^2, \tag{3}$$

of totally antisymmetric wave functions in $\mathcal{H}$, where $\wedge$ stands for exterior product. A useful alternative description of $\mathcal{H}$, used in atomic physics, is given by the unitary map

$$\mathcal{H} \to L^2((\mathbb{R}^3 \times \{\pm 1\})^N), \quad \psi \to U(\psi)(r_1, s_1; \ldots; r_N, s_N),$$

the isometry being defined by taking the components of $\psi(r_1, \ldots, r_N)$ with respect to the natural basis of $\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$ consisting of the products $\otimes_j e_{s_j}$ of the normalized eigenvectors $e_\pm$ of σ_{z_j}, e_- corresponding to "spin down" and e_+ to "spin up." In this new representation, σ_{z_j} acts as the multiplication operator by $s_j/2$, and the fermionic subspace $\mathcal{H}_f$ of (2) is simply obtained by antisymmetrizing with respect to the 4-tuples of variables $(r_1, s_1), \ldots, (r_N, s_N)$.

The main results of this paper can be summarized in the following five theorems below. It is worthwhile to observe that H^B commutes with each individual spin operator σ_{z_j} and therefore decomposes in a direct sum which is unitarily equivalent to

$$\bigoplus_{s_{z_j} \in \{\pm 1\}} H^{B, \mathbb{S}_z = -(NB/2)} + \sum_{j=1}^{N} (1 + s_{z_j}) \frac{B}{2},$$

where $\mathbb{S}_z := \sum_{j=1}^{N} \sigma_{z_j}$ denotes the z component of the total spin operator. So from now on we will consider only $H^{B, S_z = -(NB/2)}$ and denote it again by H^B. Notice that this operator simply acts in $\otimes_{j=1}^{N} L^2(\mathbb{R}^3)$. Since the Hamiltonian H^B also commutes with the total angular momentum operator in the field direction, which we will call $\mathbb{L}_z$, we can fix a value $\mathbb{M} \geqslant 0$ of the latter. Our results will imply that the bottom of the spectrum of H^B will necessarily occur for a non-negative value of $\mathbb{M}$, and we will therefore restrict ourselves to $\mathbb{M} \geqslant 0$. Let $H^{B,\mathbb{M}}$ be the restriction of H^B to the $\mathbb{M}$th angular momentum channel (in the field direction), and let $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ be the orthogonal projection onto the lowest Landau states with z-angular momentum $\mathbb{M}$ [cf. (31) for the precise definition]. We define the *effective* Hamiltonian $h_{\mathrm{eff}} = h_{\mathrm{eff}}^{B,\mathbb{M}}$ by

$$h_{\mathrm{eff}}^{B,\mathbb{M}} = \Pi_{\mathrm{eff}}^{B,\mathbb{M}} H^{B,\mathbb{M}} \Pi_{\mathrm{eff}}^{B,\mathbb{M}}, \tag{4}$$

and let

$$\Pi_{\perp}^{B,\mathbb{M}} = I - \Pi_{\mathrm{eff}}^{B,\mathbb{M}}$$

be the projection onto the orthogonal complement (always restricting ourselves to the $\mathbb{M}$th z-angular momentum channel). The operator $h_{\mathrm{eff}}^{B,\mathbb{M}}$ is the first, and most encompassing, of three "effective Hamiltonians" we will consider in this paper. The two other ones, called $h_C^{B,\mathbb{M}}$ and h_δ^B, will be defined below. It will be convenient to complete $h_{\mathrm{eff}}^{B,\mathbb{M}}$ as follows:

$$H_{\mathrm{eff}}^{B,\mathbb{M}} := h_{\mathrm{eff}}^{B,\mathbb{M}} \oplus H_{\perp}^{B,\mathbb{M}}, \quad \text{with } H_{\perp}^{B,\mathbb{M}} := \Pi_{\perp}^{B,\mathbb{M}} H^{B,\mathbb{M}} \Pi_{\perp}^{B,\mathbb{M}}. \tag{5}$$

For any self-adjoint operator A, we let $\sigma(A)$ denote the spectrum of A and $\rho(A)$ its resolvent set. Our first main result is the following.

Theorem 1.1: Let $\alpha = \alpha(B)$ be the unique positive solution of the equation

$$\alpha + \log \alpha = \tfrac{1}{2} \log B, \tag{6}$$

and let $d_{\mathrm{eff}}(\xi)=\mathrm{dist}(\xi,\sigma(h_{\mathrm{eff}}^{B,\mathbb{M}}))$. *There exist positive constants* B_{eff}, c_{eff}, *and* C_{eff}, *which only depend on* Z, N, *and* $\mathbb{M}$, *such that for all* $B\geqslant B_{\mathrm{eff}}$, *and all real* ξ *satisfying*

$$c_{\mathrm{eff}}\frac{\alpha}{\sqrt{B}}\leqslant d_{\mathrm{eff}}(\xi)\leqslant\frac{1}{2}\alpha^2$$

we have that $\xi\in\rho(H^{B,\mathbb{M}})$, *and*

$$\|(H^{B,\mathbb{M}}-\xi)^{-1}-(H_{\mathrm{eff}}^{B,\mathbb{M}}-\xi)^{-1}\|\leqslant C_{\mathrm{eff}}\frac{\alpha(B)^2}{d_{\mathrm{eff}}(\xi)^2\sqrt{B}}. \tag{7}$$

Remarks 1.2: (i) We shall see in Theorem 3.1 that $\sigma(H_{\perp}^{B,\mathbb{M}})\subset\mathbb{R}_+$ for $B\geqslant B_{(36)}$, where the latter is defined by formula (36) (see our convention on constants at the end of this introduction). Since $B_{\mathrm{eff}}\geqslant B_{(36)}$ by (106), and since one can see from (9) and (10) below that $\mathbb{R}_+\subset\sigma(h_{\mathrm{eff}}^{B,\mathbb{M}})$, it follows that $\sigma(h_{\mathrm{eff}}^{B,\mathbb{M}})=\sigma(H_{\mathrm{eff}}^{B,\mathbb{M}})$ when $B\geqslant B_{\mathrm{eff}}$.

(ii) The equation for $\alpha(B)$ is equivalent to $\alpha e^{\alpha}=\sqrt{B}$, and can therefore be written as

$$\alpha(B)=W(\sqrt{B}),$$

where W is the principal branch of the Lambert W function, see, e.g., Ref. 8. Using known properties of the Lambert W function, or by elementary arguments, one shows that

$$\alpha(B)=\frac{1}{2}\log B-\log^{(2)}B+\log 2+O\left(\frac{\log^{(2)}B}{\log B}\right),\quad B\to\infty, \tag{8}$$

where $\log^{(2)}(x):=\log(\log x)$, for $x>1$. In particular, $\alpha(B)\simeq\log(\sqrt{B})$, as $B\to\infty$.

(iii) Our proof yields explicit constants B_{eff}, c_{eff}, and C_{eff}, for given N, $\mathbb{M}$, and Z. This is also true for the constants in Theorems 1.3 and 1.5 below.

(iv) The upper bound $\alpha^2/2$ on $d_{\mathrm{eff}}(\xi)$ is only there to allow a simple expression for the upper bound in (7), and is by no means essential. The same remark applies to Theorems 1.3, 1.5, and 1.6 below.

Some applications of Theorem 1.1, as well as of Theorems 1.3, 1.5, 1.6, and 1.8 below, to the study of spectral properties of $H^{B,\mathbb{M}}$ are given in the concluding remarks section.

The operator $h_{\mathrm{eff}}^{B,\mathbb{M}}$ has the structure of a multiparticle Schrödinger operator on the real line, $\mathbb{R}$,

$$h_{\mathrm{eff}}^{B,\mathbb{M}}=-\frac{1}{2}\Delta-Z\sum_j V_j^{B,\mathbb{M}}(z_j)+\sum_{j<k}V_{jk}^{B,\mathbb{M}}(z_j-z_k), \tag{9}$$

with operator-valued potentials acting pointwise on a certain finite-dimensional Hilbert space $F_{\mathbb{M}}^B$, defined in (32) below. Essentially, $F_{\mathbb{M}}^B$ is the vector space spanned by the lowest Landau states with angular momentum $\mathbb{L}_z=\mathbb{M}$. As we will see, $\mathrm{Ran}\,\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ is canonically isomorphic to the space $L^2(\mathbb{R}^N,F_{\mathbb{M}}^B)$ of vector-valued L^2-functions, and the potentials in (9) are simply obtained by projecting the respective Coulomb terms in (1) along $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$,

$$V_j^{B,\mathbb{M}}(z_j):=\Pi_{\mathrm{eff}}^{B,\mathbb{M}}\frac{1}{|r_j|}\Pi_{\mathrm{eff}}^{B,\mathbb{M}},\quad V_{jk}^{B,\mathbb{M}}(z_j-z_k):=\Pi_{\mathrm{eff}}^{B,\mathbb{M}}\frac{1}{|r_j-r_k|}\Pi_{\mathrm{eff}}^{B,\mathbb{M}}. \tag{10}$$

We will show that the potentials (10) can be approximated by certain simpler ones, which will give rise to our two other effective Hamiltonians. Define the tempered distribution q^B on $\mathbb{R}$ by

$$q^B(z)=\log B\,\delta(z)+\mathrm{Pf}\left(\frac{1}{|z|}\right), \tag{11}$$

where

$$\mathrm{Pf}\left(\frac{1}{|z|}\right) := \frac{\mathrm{d}}{\mathrm{d}x}(\mathrm{sgn}(z)\log|z|),$$

(with distributional derivative) is the finite part (in the sense of Hadamard) of the singular function $1/|z|$; $\mathrm{Pf}(|z|^{-1})$ should be interpreted as a regularization of the (three-dimensional) Coulomb potential restricted to the line. Also introduce (constant) finite-dimensional operators $C_j^{n,B,\mathbb{M}}$ and $C_{jk}^{e,B,\mathbb{M}}$, acting on the vector space $F_{\mathbb{M}}^B$ introduced above, defined by

$$C_j^{n,B,\mathbb{M}} := -\Pi_{\mathrm{eff}}^{B,\mathbb{M}} \log\left(\frac{B}{4}(x_j^2+y_j^2)\right)\Pi_{\mathrm{eff}}^{B,\mathbb{M}} \tag{12}$$

and

$$C_{jk}^{e,B,\mathbb{M}} := -\Pi_{\mathrm{eff}}^{B,\mathbb{M}} \log\left(\frac{B}{4}((x_j-x_k)^2+(y_j-y_k)^2)\right)\Pi_{\mathrm{eff}}^{B,\mathbb{M}}. \tag{13}$$

The superscripts "n" and "e" stand for "nucleus" and "electron," respectively, as a reminder that (12) is a vestige of the interaction between the jth electron and the nucleus, while (13) originates in the electron-electron interaction between electrons j and k. Finally, define an operator $h_C^{B,\mathbb{M}}$ on $L^2(\mathbb{R},F_{\mathbb{M}}^B)$ (the C standing for Coulomb) by

$$h_C^{B,\mathbb{M}} = -\frac{1}{2}\Delta - Z\sum_j (q^B(z_j)+C_j^{n,B,\mathbb{M}}\delta(z_j)) + \sum_{j<k}(q^B(z_j-z_k)+C_{jk}^{e,B,\mathbb{M}}\delta(z_j-z_k)). \tag{14}$$

As we will see in Sec. IV, the right-hand side of (14) defines a self-adjoint operator $h_C^{B,\mathbb{M}}$ on $L^2(\mathbb{R}^N)$, despite the distributional potentials. This will be a consequence of the Kato-Lax-Lions-Milgram-Nelson theorem. The form domain of $h_C^{B,\mathbb{M}}$ is simply the vector-valued first Sobolev space $H^1(\mathbb{R}^N;F_{\mathbb{M}})$, while its operator domain will be characterized in the Appendix. As in (5) we introduce

$$H_C^{B,\mathbb{M}} := h_C^{B,\mathbb{M}} \oplus H_\perp^{B,\mathbb{M}}.$$

Our second main theorem then is the following.

Theorem 1.3: *Let $\alpha=\alpha(B)$ be as in Theorem 1.1, and set $d_C(\xi) := \mathrm{dist}(\xi,\sigma(h_C^{B,\mathbb{M}}))$. There exists positive constants B_C, c_C, and C_C which depend only on Z, N, and $\mathbb{M}$, such that for all $B \geqslant B_C$ and all real ξ satisfying*

$$c_C\frac{\alpha^{3/2}}{B^{1/4}} \leqslant d_C(\xi) \leqslant \frac{1}{4}\alpha^2$$

we have that $\xi \in \rho(H^{B,\mathbb{M}})$, and

$$\|(H^{B,\mathbb{M}}-\xi)^{-1}-(H_C^{B,\mathbb{M}}-\xi)^{-1}\| \leqslant \frac{C_C\alpha^{3/2}}{B^{1/4}d_C(\xi)^2}. \tag{15}$$

Remark 1.4: In top order in B, all that remains of the electrostatic potentials in $H^{B,\mathbb{M}}$ are the extremely short-range δ-potentials. In next order, the long-range character of the original Coulomb potentials reasserts itself in two ways: in the magnetic field direction, through the $\mathrm{Pf}(|\cdot|^{-1})$-terms in $h_C^{B,\mathbb{M}}$, and in the transversal directions, through the $C_j^{n,B,\mathbb{M}}$ and $C_{jk}^{e,B,\mathbb{M}}$ terms. The latter are in fact simply the quantum mechanical mean, with respect to the projection onto the lowest Landau band states of total angular momentum $\mathbb{M}$ (in the field direction), of a two-dimensional logarithmic potential, minus a B-dependent constant. This logarithmic potential is the natural electrostatic potential for the plane. Physically, this can be understood as follows: under the influence of the strong magnetic field the electrons will spiral closely around the field lines, along circles of radius $O(B^{-1/2})$ in the plane transversal to the field, while occupying an interval of size $O((\log B)^{-1})$ in the field direction itself, as a consequence of the nuclear attraction. For big B, and at different

locations in the (x,y)-plane, they will see each other and the nucleus as so many infinitely long charged wires, and, as is known from classical electrostatics, such wires interact via a logarithmic potential.

A simpler effective Hamiltonian, our third and last one, and historically the first to be proposed (cf. Refs. 14, 4, and 6), is roughly speaking obtained by only keeping the leading term in the potential of $h_C^{B,\mathbb{M}}$. More precisely, we set

$$h_\delta^B = -\tfrac{1}{2}\Delta_z + 2\alpha(B)v_\delta, \tag{16}$$

where

$$v_\delta(z) = -Z\sum_{j=1}^{N}\delta(z_j) + \sum_{j<k}\delta(z_j - z_k). \tag{17}$$

Looking back at (11) it would seem natural to take as potential $\log B v_\delta$, but it turns out that $2\alpha(B)v_\delta$ leads to smaller error estimates; notice that in view of (8), $2\alpha v_\delta$ is also a $O(\log B)$ part of the potential in h_C^B. Furthermore, with this choice the coupling constant $2\alpha(B)$ is positive for all $B>0$ which is not the case for $\log B$. Contrary to our previous two effective Hamiltonians, h_δ^B does not explicitly depend on $\mathbb{M}$ anymore, but it will operate on an $\mathbb{M}$ and B-dependent Hilbert space, namely $L^2(\mathbb{R}^N, F_{\mathbb{M}}^B) \simeq L^2(\mathbb{R}^N)\otimes F_{\mathbb{M}}^B$ (which in fact are canonically isomorphic for different B). Considering (16) as acting on scalar $L^2(\mathbb{R}^N)$, we define the δ-model as being the operator

$$h_\delta^{B,\mathbb{M}} := h_\delta^B \otimes I_{F_{\mathbb{M}}^B}, \quad I_{F_{\mathbb{M}}^B} \text{ being the identity operator.} \tag{18}$$

We will often simply write h_δ^B, except when we want to stress the vector-valued nature of the L^2-functions in the domain. Again as in (5) we introduce

$$H_\delta^{B,\mathbb{M}} := h_\delta^{B,\mathbb{M}} \oplus H_\perp^{B,\mathbb{M}}.$$

Our third approximation theorem is the following.

Theorem 1.5: *Let $\alpha := \alpha(B)$ be as in Theorem 1.1, and set $d_\delta(\xi) := \operatorname{dist}(\xi, \sigma(h_\delta^{B,\mathbb{M}}))$. There exist positive constants B_δ, c_δ, and C_δ, depending on N, Z, and $\mathbb{M}$, such that for all $B \geqslant B_\delta$ and real ξ satisfying*

$$c_\delta\alpha \leqslant d_\delta(\xi) \leqslant \tfrac{1}{4}\alpha^2, \tag{19}$$

we have that $\xi \in \rho(H^{B,\mathbb{M}})$, and

$$\left\|(H^{B,\mathbb{M}} - \xi)^{-1} - (H_\delta^{B,\mathbb{M}} - \xi)^{-1}\right\| \leqslant \frac{C_\delta\alpha}{d_\delta(\xi)^2}. \tag{20}$$

See Ref. 6 for weaker versions of this theorem. We also mention Ref. 4, which established the convergence of the ground state energy of fermionic H^B (see below) to that of bosonic (scalar) h_δ^B on $L^2(\mathbb{R}^N)$, using variational arguments: these authors did not fix $\mathbb{M}$, but they only proved convergence of the ground state energy, while we can conclude much more from the norm resolvent convergence to the effective Hamiltonians; see Sec. IX for a list of applications of the results of the present paper. (Reference 4, following Ref. 14, first did a rescaling of H^B's ground state energy which allowed them to compare with h_δ^B for a fixed B [e.g., fixing $2\alpha(B)=1$]. Since this homogeneity property is not valid anymore for our other two effective Hamiltonians, we prefer not to do this here (contrary to our earlier papers[6]), in order to have a coherent presentation.) Earlier, Ref. 14 had shown that the ground state of the Hartree mean-field model associated to (16) approximates the quantum mechanical ground state energy in the so-called hyperstrong limit Z, $B/Z^3 \to \infty$, assuming N/Z uniformly bounded. The idea that a model such as the δ-model could be relevant in the context of strong magnetic fields is not new in the physics literature, see, e.g., Ref. 19.

We next turn to the effects of particle symmetry. Electrons in physical atoms are fermions, and we now consider the analogues of Theorems 1.1, 1.3, and 1.5 for H^B restricted to the fermionic subspace $\mathcal{H}_\mathrm{f}=P^{AS}(\mathcal{H})$, where P^{AS} is the orthogonal projection onto the subspace of antisymmetric symmetric wave functions defined by

$$P^{\mathrm{AS}}\psi(r_1,s_1;\ldots;r_N,s_N) := \frac{1}{N!}\sum_{\sigma\in S_N}(-1)^\sigma\psi(r_{\sigma(1)},s_{\sigma(1)};\ldots;r_{\sigma(N)},s_{\sigma(N)}),$$

with $(-1)^\sigma := (-1)^{\mathrm{sgn}(\sigma)}$. The projection P^{AS} commutes with H^B, $\mathbb{L}_z$, $\mathbb{S}_z$ and with the N-particle Landau Hamiltonian H_0^B defined in (24) below, and therefore also with $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ (see Sec. II). Recalling that we have fixed our spins to $\mathbb{S}_z=-NB/2$, P^{AS} for us will only act in the spatial variables $(r_1,\ldots,r_N)$. Let $H_\mathrm{f}^{B,\mathbb{M}} := P^{\mathrm{AS}}H^{B,\mathbb{M}}P^{\mathrm{AS}}=H^{B,\mathbb{M}}P^{\mathrm{AS}}$ the fermionic Pauli operator with z-angular momentum $\mathbb{M}$. Similarly, introduce fermionized versions of the other operators: $\Pi_{\mathrm{eff,f}}^{B,\mathbb{M}} := P^{\mathrm{AS}}\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$, $\Pi_{\perp,\mathrm{f}}^{B,\mathbb{M}} := P^{\mathrm{AS}}\Pi_{\perp}^{B,\mathbb{M}}$, $H_{\mathrm{eff,f}}^{B,\mathbb{M}} := P^{AS}H_{\mathrm{eff}}^{B,\mathbb{M}}=P^{AS}h_{\mathrm{eff}}^{B,\mathbb{M}}\oplus H_{\perp,\mathrm{f}}^{B,\mathbb{M}} := h_{\mathrm{eff,f}}^{B,\mathbb{M}}\oplus H_{\perp,\mathrm{f}}^{B,\mathbb{M}}$, $h_{C,\mathrm{f}}^{B,\mathbb{M}}=P^{AS}h_C^{B,\mathbb{M}}$, $h_{\delta,\mathrm{f}}^{B} := P^{AS}h_\delta^B$, $H_{C,\mathrm{f}}^{B,\mathbb{M}}=P^{AS}H_C^{B,\mathbb{M}}$ and finally $H_{\delta,\mathrm{f}}^{B,\mathbb{M}} := P^{AS}H_\delta^{B,\mathbb{M}}$. A careful examination of the proofs of Theorems 1.1, 1.3, and 1.5 will show the following.

Theorem 1.6: *Theorems 1.1, 1.3, and 1.5 also hold true for the fermionized operators. For example, if ξ satisfies the conditions of Theorem 1.1 with $d_{\mathrm{eff}}(\xi)$ replaced by $d_{\mathrm{eff,f}}(\xi) := \mathrm{dist}(\xi,\sigma(h_{\mathrm{eff,f}}^{B,\mathbb{M}}))$, then*

$$\|(H_\mathrm{f}^{B,\mathbb{M}}-\xi)^{-1}-(H_{\mathrm{eff,f}}^{B,\mathbb{M}}-\xi)^{-1}\| \leqslant C_{\mathrm{eff}}\frac{\alpha(B)^2}{d_{\mathrm{eff,f}}(\xi)^2\sqrt{B}}, \tag{21}$$

with the same constants as before. Similarly for $H_{C,\mathrm{f}}^{B,\mathbb{M}}$, $H_{\delta,\mathrm{f}}^{B,\mathbb{M}}$.

Remark 1.7: Theorem 1.6 is not simply obtained by "sandwiching" Theorems 1.1, 1.3, and 1.5 between P^{AS}, since the statements thus obtained would not involve the distances to the spectra of the fermionized operators. Also, we established the fermionic versions with the same constants as for the boltzonic ones, but it is conceivable that one could have smaller constants in the fermionic case.

The operators $h_{\mathrm{eff,f}}^{B,\mathbb{M}}$ and $h_{C,\mathrm{f}}^{B,\mathbb{M}}$ are easily described

$$h_{\mathrm{eff,f}}^{B,\mathbb{M}} = -\frac{1}{2}\Delta - Z\sum_{j=1}^{N}V_{\mathrm{av};1}^{B,\mathbb{M}}(z_j)+\sum_{j<k}V_{\mathrm{av}:2}^{B,\mathbb{M}}(z_j-z_k), \tag{22}$$

where, using the notation of (10),

$$V_{\mathrm{av}:1}^{B,\mathbb{M}}(z) := \frac{1}{N}\sum_j V_j^{B,\mathbb{M}}(z),$$

and

$$V_{\mathrm{av}:2}^{B,\mathbb{M}}(z) := \binom{N}{2}^{-1}\sum_{j<k}V_{jk}^{B,\mathbb{M}}(z),$$

the average one-, respectively, two-particle potentials. Similarly, $h_{C,\mathrm{f}}^{B,\mathbb{M}}$ equals

$$h_{C,\mathrm{f}}^{B,\mathbb{M}} = -\frac{1}{2}\Delta - Z\sum_{j=1}^{N}(q^B(z_j)+C_{\mathrm{av}:1}^{b,B,\mathbb{M}}\delta(z_j))+\sum_{j<k}(q^B(z_j-z_k)+C_{\mathrm{av}:2}^{e,B,\mathbb{M}}\delta(z_j-z_k)), \tag{23}$$

with

$$C^{n,B,\mathbb{M}}_{\mathrm{av:1}} := \frac{1}{N}\sum_{j=1}^{N} C^{n,B,\mathbb{M}}_{j}$$

and

$$C^{e,B,\mathbb{M}}_{\mathrm{av:2}} := \binom{N}{2}^{-1} \sum_{j<k} C^{e,B,\mathbb{M}}_{jk},$$

while $h^{B,\mathbb{M}}_{\delta,\mathrm{f}}$ is given by the same expression as h^{B}_{δ}, except of course that its domain changes.

To complete the picture, we finish with an explicit description of $\mathrm{Ran}(\Pi^{B,\mathbb{M}}_{\mathrm{eff,f}})$, which is equal to $P^{\mathrm{AS}}(\mathrm{Ran}\,\Pi^{B,\mathbb{M}}_{\mathrm{eff}}) = P^{AS}(L^2(\mathbb{R}^N)\otimes F^{B}_{\mathbb{M}})$. Fix $\mathbb{M}\geqslant 0$, and let

$$\Sigma(\mathbb{M}) = \{m \in \mathbb{N}^N : |m| = \mathbb{M}\},$$

the set of partitions of $\mathbb{M}$, where, as usual, $|m| = m_1 + \ldots + m_N$ if $m = (m_1, \ldots, m_N)$. The vector space $F^{B}_{\mathbb{M}}$ is spanned by the lowest Landau (generalized) eigenstates indexed by $m \in \Sigma(\mathbb{M})$, cf. Sec. II below. The symmetric group S_N acts on $\Sigma(\mathbb{M})$ in the natural way, by permuting the indices of an element $m = (m_1, \ldots, m_N)$ of $\Sigma(\mathbb{M})$. Under this action, $\Sigma(\mathbb{M})$ will decompose as a finite union of disjoint orbits,

$$\Sigma(\mathbb{M}) = \bigcup_{\bar{m}\in\mathcal{M}} S_N \cdot \bar{m},$$

$\mathcal{M}$ being a set of representatives of the orbits. If $G_{\bar{m}}$ denotes the stabilizer of $\bar{m} \in \mathcal{M}$, then we write $\mathcal{M}$ as a disjoint union $\mathcal{M} = \mathcal{M}_1 \cup \mathcal{M}_2$, with $\mathcal{M}_1$ the subset of those $\bar{m} \in \mathcal{M}$ such that $G_{\bar{m}} = \{e\}$, and $\mathcal{M}_2 = \mathcal{M}\setminus\mathcal{M}_1$, its complement. In other words, $\bar{m} \in \mathcal{M}_1$ iff no two components of $\bar{m}$ are the same, and $\bar{m} \in \mathcal{M}_2$ iff at least two of its components are identical. Let $L^2_{\mathrm{AS}}(\mathbb{R}^N)$ be the space of anitsymmetrical wave functions in $L^2(\mathbb{R}^N)$. We then will prove, in Sec. VIII, the following.

Theorem 1.8: *There is a natural unitary isomorphism*

$$U^{B}_{\mathbb{M}} : \mathrm{Ran}(\Pi^{B,\mathbb{M}}_{\mathrm{eff,f}}) \to \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_1}} L^2(\mathbb{R}^N) \oplus \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_2}} L^2_{AS}(\mathbb{R}^N)$$

and

$$U^{B}_{\mathbb{M}} h^{B,\mathbb{M}}_{\delta,\mathrm{f}} U^{B*}_{\mathbb{M}} = \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_1}} h^{B}_{\delta}|_{L^2(\mathbb{R}^N)} \oplus \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_2}} h^{B}_{\delta}|_{L^2_{AS}(\mathbb{R}^N)}.$$

Remark 1.9: The operators $U^{B}_{\mathbb{M}} h^{B,\mathbb{M}}_{C,\mathrm{f}} U^{B*}_{\mathbb{M}}$ and $U^{B}_{\mathbb{M}} h^{B,\mathbb{M}}_{\mathrm{eff,f}} U^{B*}_{\mathbb{M}}$ can mix different components of $\mathrm{Ran}(U^{B}_{\mathbb{M}})$, as we will see at the end of Sec. VIII, and will therefore have a more complicated structure.

The paper is organized as follows. Section II contains the precise definition of our effective projector $\Pi^{B,\mathbb{M}}_{\mathrm{eff}}$. In Sec. III we establish, with the help of the Feshbach decomposition, a first approximation theorem, comparing $H^{B,\mathbb{M}}$'s resolvent at ξ with that of $H^{B,\mathbb{M}}_{\mathrm{eff}} + \mathcal{W}^{B,\mathbb{M}}(\xi)$, where the last term is an auxiliary potential which itself depends on the spectral parameters ξ. Section IV analyzes the large-B behavior of the potential of $H^{B,\mathbb{M}}_{\mathrm{eff}}$, as well as that of $\mathcal{W}^{B,\mathbb{M}}$. Sections V–VII are devoted to the proofs of, respectively, Theorems 1.1, 1.3, and 1.5. In Sec. VIII we prove Theorems 1.6 and 1.8. Section IX, finally, concludes with some applications to the spectral theory of $H^{B,\mathbb{M}}$, and some general observations.

Convention on constants: In the course of this work, we have had to introduce a large number of constants. To keep track of them, we will use the convention that whenever the subscript of a constant is a number, the number refers to the formula where the constant in question was first introduced. That is, $C_{(x)} :=$ constant defined in formula (x).

II. NONINTERACTING ELECTRONS AND THE LOWEST LANDAU BAND

We begin by reviewing the spectral decomposition of

$$H_0^B := H_0^B(N) := \sum_{j=1}^{N} \frac{1}{2}\left(\left(\frac{1}{i}\nabla_{r_j} - \frac{1}{2}\mathbb{B}\wedge r_j\right)^2 - NB\right), \tag{24}$$

the "free" Hamiltonian of N independent electrons interacting only with the field $\mathbb{B}$. Recall that we have fixed all electron spins in their $s_{z_j}=-1$ state. The operator H_0^B is just a direct sum of N one-particle operators $\frac{1}{2}\left((i^{-1}\nabla_r - \frac{1}{2}\mathbb{B}\wedge r)^2 - B\right)$, whose spectral decomposition is explicitly known,

$$\oplus_{m\in\mathbb{Z},n\in\mathbb{N}}\left(\frac{1}{2}p_z^2 + \frac{B}{2}(2n+|m|-m)\right)\Pi_{m,n}^B.$$

Here, p_z is the momentum in the field direction, and $\Pi_{m,n}^B$ is the projection, in the x,y variables, onto the normalized eigenfunctions $\chi_{m,n}^B=\chi_{m,n}^B(x,y)\in L^2(\mathbb{R}^2)$ of the operator

$$-\frac{1}{2}\Delta_{x,y} + \frac{B^2}{8}(x^2+y^2) - \frac{B}{2},$$

restricted to the m-eigenspace of $L_z=xp_y-yp_x$, the angular momentum in the field direction. These eigenfunctions are explicitly known in terms of Laguerre functions, see, e.g., Ref. 10, but for our purposes we will only need those with $n=0$, $m\geqslant 0$. These have a particularly simple expression: if (ρ,φ) are polar coordinates in the x,y plane, then

$$\chi_m^B := \chi_{m,0}^B:(x,y) \to \left(\frac{B^{m+1}}{2\pi 2^m m!}\right)^{1/2}\rho^m e^{+im\varphi}e^{-B\rho^2/4}. \tag{25}$$

The spectral decomposition of H_0^B is simply the sum of the one-particle decompositions, and the projections onto its eigenstates will be indexed by N-tuples $m=(m_1,\ldots,m_N)\in\mathbb{Z}^N$, $n=(n_1,\ldots n_N)\in\mathbb{N}^N$. If we let

$$\Pi_{m,n}^B := \Pi_{m_1,n_1}^B \otimes \cdots \otimes \Pi_{m_N,n_N},$$

then

$$H_0^B = \oplus_{m,n}\left(\sum_{j=1}^{N}\frac{1}{2}p_{z_j}^2 + \frac{B}{2}(2n_j+|m_j|-m_j)\right)\Pi_{m,n}^B. \tag{26}$$

The lowest Landau band of H_0^B is defined as

$$\mathcal{L}_0^B = \oplus_{m\in\mathbb{Z}_+^N}\mathrm{Ran}\,\Pi_{m,0}^B, \tag{27}$$

where $\mathbf{0}:=(0,\ldots,0)$, and if we set

$$X_m^B(x,y) := \prod_{j=1}^{N}\chi_{m_j}^B(x_j,y_j), \quad m_1,\ldots,m_N\geqslant 0, \tag{28}$$

then $\mathcal{L}_0$ will be spanned by the tensor products $X_m^B\otimes u$, with $u=u(z)\in L^2(\mathbb{R}^N)$. We will call the X_m^B the lowest Landau band states (these are not eigenvectors of H_0^B, but $X_m^B\otimes 1$ would be generalized eigenvectors with eigenvalue 0). The operator H_0^B restricted to $\mathcal{L}_0^B$ simply is the free Laplacian in the field direction,

$$\frac{1}{2}\sum_j p_{z_j}^2 = -\frac{1}{2}\Delta_z,$$

where $z=(z_1,\ldots,z_N)$.

We next reduce the Hamiltonian H^B and H_0^B to their angular momentum sectors with respect to the field direction. The total orbital angular momentum in the direction of $\mathbb{B}=(0,0,B)$,

$$\mathbb{L}_z = \sum_j (x_j p_{y_j} - y_j p_{x_j}), \quad (p_x,p_y,p_z) = \frac{1}{i}\nabla_r,$$

commutes with H^B and H_0^B, and is therefore a constant of motion for both Hamiltonians. If $P^{\mathbb{M}}$ is the orthogonal projection onto the $\mathbb{M}$th eigenspace of $\mathbb{L}_z$, then we let

$$H^{B,\mathbb{M}} := H^B P^{\mathbb{M}}, \quad H_0^{B,\mathbb{M}} := H_0^B P^{\mathbb{M}} \tag{29}$$

acting on $\mathcal{H} := L^2(\mathbb{R}^{3N}) \otimes \mathbb{C}^{2N}$. Since we are primarily interested in the spectral behavior of H^B near the bottom of its spectrum, we will restrict $\mathbb{M}$ to $\mathbb{Z}_+$, for $\mathcal{L}_0^B \cap \mathrm{Ran}\, P^{\mathbb{M}} \neq \{0\} \Leftrightarrow \mathbb{M} \geqslant 0$. Indeed, notice that since $H^{B,-\mathbb{M}}$ is unitarily equivalent to $H^{B,\mathbb{M}} + \mathbb{M}B$, one has $\inf \sigma(H^B|_{\mathbb{M}\geqslant 0}) < \inf \sigma(H^B|_{\mathbb{M}<0})$ as soon as $B>0$.

We next let

$$\Sigma(\mathbb{M}) = \{m=(m_1,\ldots,m_N) \in \mathbb{Z}^N : m_j \geqslant 0,\ m_1+\cdots+m_N = \mathbb{M}\}, \tag{30}$$

the set of partitions of $\mathbb{M}$, and define the *effective projection* $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ by

$$\Pi_{\mathrm{eff}}^{B,\mathbb{M}} := \sum_{m\in\Sigma(\mathbb{M})} \Pi_{m,0}^B. \tag{31}$$

This is simply the orthogonal projection onto $\mathcal{L}_0 \cap (\mathbb{L}_z = \mathbb{M}\}$. We also let $\Pi_\perp^{B,\mathbb{M}}$ be the orthogonal projection onto the orthogonal complement of $\mathrm{Ran}(\Pi_{\mathrm{eff}}^{B,\mathbb{M}})$ in $\mathrm{Ran}(P^{\mathbb{M}})$. Observe that

$$\Pi_\perp^{B,\mathbb{M}} = \bigoplus_{\substack{m_1+\cdots+m_N=\mathbb{M},\\ \Sigma_j 2n_j+|m_j|-m_j\geqslant 2}} \Pi_{m,n}.$$

If we let $F_{\mathbb{M}}^B$ be the finite-dimensional vector space spanned by the lowest Landau states with total angular momentum $\mathbb{M}$,

$$F_{\mathbb{M}}^B := \mathrm{Span}\{X_m^B : m \in \Sigma(\mathbb{M})\}, \tag{32}$$

then we can identify the range of $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ with the space $L^2(\mathbb{R}^N, F_{\mathbb{M}}^B)$ of $F_{\mathbb{M}}^B$-valued L^2-functions, as we will do without further comment.

To lighten the notations, we will often suppress one or both upper indices B or $\mathbb{M}$, unless where this would cause confusion. This will always be clearly indicated, usually at the beginning of a section.

III. ESTIMATES FOR FESHBACH DECOMPOSITIONS

We fix a non-negative integer $\mathbb{M} \geqslant 0$. In this section we will drop all upper-indices B, $\mathbb{M}$, and simply write H for $H^{B,\mathbb{M}}$, H_0 for $H_0^{B,\mathbb{M}}$ and Π_{eff}, respectively, $\Pi_\perp$ for $\Pi_{\mathrm{eff}}^{B,\mathbb{M}}$ and $\Pi_\perp^{B,\mathbb{M}}$. We write our atomic Hamiltonian $H^{B,\mathbb{M}}$ as

$$H = H_0 + \mathcal{V},$$

where

$$\mathcal{V} := -\sum_j \frac{Z}{|r_j|} + \sum_{j<k} \frac{1}{|r_j - r_k|}, \tag{33}$$

is the electrostatic potential, and introduce the operators

$$\mathcal{V}_{\text{eff}} := \Pi_{\text{eff}} \mathcal{V} \Pi_{\text{eff}}, \quad \mathcal{V}_\perp := \Pi_\perp \mathcal{V} \Pi_\perp, \quad \mathcal{V}_{\perp,\text{eff}} := \Pi_\perp \mathcal{V} \Pi_{\text{eff}},$$

and its adjoint, $\mathcal{V}_{\text{eff},\perp} = \Pi_{\text{eff}} \mathcal{V} \Pi_\perp$. These are to be considered as operators on Ran Π_{eff}, Ran $\Pi_\perp$, and between these two Hilbert spaces, respectively. We furthermore set

$$h_{\text{eff}} := \Pi_{\text{eff}} H \Pi_{\text{eff}}, \quad H_\perp := \Pi_\perp H \Pi_\perp, \quad H_{\perp,\text{eff}} := \Pi_\perp H \Pi_{\text{eff}} = H^*_{\text{eff},\perp},$$

and for $\xi \in \mathbb{C}$ introduce the resolvents (wherever defined)

$$R := R(\xi) := (H_\perp - \xi)^{-1}, \quad R^{\mathcal{W}}_{\text{eff}} := R^{\mathcal{W}}_{\text{eff}}(\xi) := (h_{\text{eff}} + \mathcal{W}(\xi) - \xi)^{-1},$$

where

$$\mathcal{W} := \mathcal{W}(\xi) = -\mathcal{V}_{\text{eff},\perp} R(\xi) \mathcal{V}_{\perp,\text{eff}}.$$

Strictly speaking $R^{\mathcal{W}}_{\text{eff}}$ is not a resolvent since the potential $\mathcal{W}(\xi)$ depends on the spectral parameter ξ. The operators R and $R^{\mathcal{W}}_{\text{eff}}$ act on, respectively, the ranges of $\Pi_\perp$ and of Π_{eff}. Finally, let

$$T := H_0 P^{\mathbb{M}}, \quad T_{\text{eff}} := \Pi_{\text{eff}} T \Pi_{\text{eff}}, \quad T_\perp := \Pi_\perp T \Pi_\perp;$$

T commutes with Π_{eff} and $\Pi_\perp$, and $\Pi_\perp T \Pi_{\text{eff}} = 0$. Note that

$$T_\perp \geqslant B \Pi_\perp,$$

on the range of $P^{\mathbb{M}}$.

Using matrix notation associated to the decomposition $P^{\mathbb{M}}\mathcal{H} = \text{Ran}\, \Pi_{\text{eff}} \oplus \text{Ran}\, \Pi_\perp$, we decompose H as

$$H = \begin{pmatrix} h_{\text{eff}} & H_{\text{eff},\perp} \\ H_{\perp,\text{eff}} & H_\perp \end{pmatrix} = \begin{pmatrix} T_{\text{eff}} + \mathcal{V}_{\text{eff}} & \mathcal{V}_{\text{eff},\perp} \\ \mathcal{V}_{\perp,\text{eff}} & T^{\mathcal{B}}_\perp + \mathcal{V}_\perp \end{pmatrix}. \tag{34}$$

By the classical Feshbach formula, we then have

$$(H - \xi)^{-1} = \begin{pmatrix} R^{\mathcal{W}}_{\text{eff}} & -R^{\mathcal{W}}_{\text{eff}} \mathcal{V}_{\text{eff},\perp} R \\ -R \mathcal{V}_{\perp,\text{eff}} R^{\mathcal{W}}_{\text{eff}} & R + R \mathcal{V}_{\perp,\text{eff}} R^{\mathcal{W}}_{\text{eff}} \mathcal{V}_{\text{eff},\perp} R \end{pmatrix}, \tag{35}$$

for those $\xi \in \mathbb{C}$ for which the right-hand side makes sense. The following theorem is the main result of this section: recall that $\rho(A)$ denotes the resolvent set of an operator A, and $\sigma(A)$ its spectrum.

Theorem 3.1: *Let*

$$B_{(36)} := 16 Z^2 N (\mathbb{M} + N + 2) \tag{36}$$

and

$$C_{(37)} := c_0 + \frac{c_0^2}{\sqrt{B_{(36)}}}, \quad c_0^2 = (32 Z^2 N + 8 N (N-1)^2)(\mathbb{M} + N + 2). \tag{37}$$

If $\xi \leqslant 0$ *and if the field strength* $B \geqslant B_{(36)}$, *then* $\xi \in \rho(H_\perp)$. *If, moreover,* $\xi \notin \sigma(H_{\text{eff}} + \mathcal{W})$, *then* $\xi \in \rho(H)$, *and*

$$\left\| (H - \xi)^{-1} - (h_{\text{eff}} + \mathcal{W} - \xi)^{-1} \oplus R(\xi) \right\| \leqslant \frac{C_{(37)}}{d^{\mathcal{W}}_{\text{eff}}(\xi) \sqrt{B}}, \tag{38}$$

where $d_{\mathrm{eff}}^{\mathcal{W}}(\xi)$ *is the distance of* ξ *to* $\sigma(h_{\mathrm{eff}}+\mathcal{W})$.

Proof of Theorem 3.1: The proof consists of estimating the relevant matrix elements in the Feshbach formula. This will be done in several steps. Let

$$R_0 = (T_\perp - \xi)^{-1},$$

the resolvent of $T_\perp$ on $\mathrm{Ran}\,\Pi_\perp$.

Bound on R_0: Since $T_\perp \geqslant B$ on $\mathrm{Ran}\,\Pi_\perp$ and since $\xi \leqslant 0$, it immediately follows that $\|R_0\| \leqslant B^{-1}$. Write $\mathcal{V}$ as

$$\mathcal{V} = \mathcal{V}_n + \mathcal{V}_e, \quad \text{where } \mathcal{V}_n := -\sum_j \frac{Z}{|r_j|}, \quad \text{and } \mathcal{V}_e := \sum_{j<k} \frac{1}{|r_j - r_k|}, \tag{39}$$

the sum of electron-nucleus and the electron-electron interactions.

A remark on notation: we will often leave the projection $\Pi_\perp$ understood when multiplying operators on the left and/or right by R_0 or R, and for example, simply write $R_0^{1/2}\mathcal{V}_n R_0^{1/2}$ instead of the more explicit $R_0^{1/2}\Pi_\perp \mathcal{V}_n \Pi_\perp R_0^{1/2}$.

Bound on $R_0^{1/2}\mathcal{V}_n R_0^{1/2}$. First, since $R_0 \leqslant B^{-1}$ on the range of $\Pi_\perp$,

$$0 \leqslant (\sqrt{R_0}\mathcal{V}_n\sqrt{R_0})^2 \leqslant B^{-1}\sqrt{R_0}\mathcal{V}_n^2\sqrt{R_0}.$$

By Cauchy-Schwarz,

$$\sqrt{R_0}\mathcal{V}_n^2\sqrt{R_0} \leqslant Z^2 N \sqrt{R_0}\sum_j |r_j|^{-2}\sqrt{R_0}.$$

Next, using Hardy's inequality on $\mathbb{R}^3$: $|r_j|^{-2} \leqslant -4\Delta_j$, and the fact that

$$H_0^B = \sum_j -\frac{1}{2}\Delta_j + \frac{1}{8}|\mathbb{B}\wedge r_j|^2 - \frac{B}{2}(\mathbb{L}_z + N),$$

we find that

$$\sqrt{R_0}\left(\sum_j |r_j|^{-2}\right)\sqrt{R_0} \leqslant 8\sqrt{R_0}\sum_j\left(-\frac{\Delta_j}{2} + \frac{|\mathbb{B}\wedge r_j|^2}{8}\right)\sqrt{R_0} = 8\sqrt{R_0}\left(T_\perp + \frac{B}{2}(\mathbb{M}+N)\right)\sqrt{R_0} = 8\Pi_\perp + 8\xi R_0$$
$$+ 4(\mathbb{M}+N)BR_0 \leqslant (8 + 4(\mathbb{M}+N))\Pi_\perp,$$

since $\xi \leqslant 0$. It follows from these estimates that

$$\|R_0^{1/2}\mathcal{V}_n R_0^{1/2}\| \leqslant 2ZB^{-1/2}\sqrt{N(\mathbb{M}+N+2)}.$$

We note, as a consequence, that if $b_0 = 4Z^2N(\mathbb{M}+N+2)$, then $\|R_0^{1/2}\mathcal{V}_n R_0^{1/2}\| \leqslant (b_0 B^{-1})^{1/2} < 1$ if $B > b_0$. For later reference we also note the following.

Bound on $R_0^{1/2}\mathcal{V}_n^2 R_0^{1/2}$: the estimates above immediately imply that this positive operator is bounded from above by $4Z^2N(\mathbb{M}+N+2)$.

Existence of and bound on R: Since the electron-electron repulsion $\mathcal{V}_e \geqslant 0$, it follows that $R \leqslant R_{\mathrm{NI}}$, where $R_{\mathrm{NI}} = (T_\perp + \mathcal{V}_{n,\perp} - \xi)^{-1}$, the resolvent of an atom with noninteracting electrons. Using the symmetrized resolvent formula,

$$R_{\mathrm{NI}} = \sqrt{R_0}(1 + \sqrt{R_0}\mathcal{V}_n\sqrt{R_0})^{-1}\sqrt{R_0}, \tag{40}$$

we see that R_{NI} exists and is positive if $B > b_0$ and $\xi \leqslant 0$. Hence $T_\perp + \mathcal{V}_{n,\perp} - \xi \geqslant 0$ and therefore also $H_\perp - \xi$ and R. Moreover, if $B > 4b_0 = 16Z^2N(\mathbb{M}+N+2) = B_{(36)}$, then every $\xi \leqslant 0$ belongs to $\rho(H_\perp)$ and

$$0 \leqslant R \leqslant \frac{\|R_0\|}{1-\|R_0^{1/2}\mathcal{V}_n R_0^{1/2}\|} \leqslant B^{-1}\left(\frac{1}{1-(b_0 B^{-1})^{1/2}}\right) \leqslant 2B^{-1}.$$

Bound on $R_0^{1/2}\mathcal{V}_e^2 R_0^{1/2}$: The following elementary operator inequality is very useful to estimate the electron-electron interactions.

Lemma 3.2:

$$\frac{1}{|r_j - r_k|^2} \leqslant 2(-\Delta_j - \Delta_k). \tag{41}$$

Proof: The unitary transformation induced by the following orthogonal transformation of $\mathbb{R}^3 \times \mathbb{R}^3$:

$$s := \frac{r_1 - r_2}{\sqrt{2}}, \quad t := \frac{r_1 + r_2}{\sqrt{2}} \tag{42}$$

commutes with the Laplacian, and transforms $|r_j - r_k|^{-2}$ into $2^{-1}|s|^{-2}$. By Hardy's inequality,

$$\frac{1}{2|s|^2} \leqslant -2\Delta_s \leqslant -2(\Delta_s + \Delta_t),$$

and transforming back to the (r_j, r_k)-coordinates yields (41). Q.E.D.

We can then estimate

$$\mathcal{V}_e^2 = \left(\sum_{i<j}\frac{1}{|r_i - r_j|}\right)^2 \leqslant \frac{N(N-1)}{2}\sum_{i<j}\frac{1}{|r_i - r_j|^2} \leqslant N(N-1)\sum_{i<j}(-\Delta_i - \Delta_j) = N(N-1)^2\sum_i(-\Delta_i)$$
$$\leqslant 2N(N-1)^2\sum_i\left(-\frac{\Delta_i}{2} + \frac{|\mathbb{B}\wedge r_j|^2}{8}\right),$$

and therefore, by similar arguments as before,

$$\sqrt{R_0}\mathcal{V}_e^2\sqrt{R_0} \leqslant 2N(N-1)^2\sqrt{R_0}\left(T_\perp + \frac{B}{2}(\mathbb{M}+N)\right)\sqrt{R_0} \leqslant N(N-1)^2(\mathbb{M}+N+2),$$

on $\mathrm{Ran}(\Pi_\perp)$.

Bound on $\mathcal{V}R_0^{1/2}$: By the general identity $\|AA^*\| = \|A\|^2$, we have

$$\|\mathcal{V}R_0^{1/2}\|^2 = \|R_0^{1/2}\mathcal{V}^2 R_0^{1/2}\| \leqslant 2(\|R_0^{1/2}\mathcal{V}_n^2 R_0^{1/2}\| + \|R_0^{1/2}\mathcal{V}_e^2 R_0^{1/2}\|) \leqslant (8Z^2N + 2N(N-1)^2)(\mathbb{M}+N+2).$$

Bound on $\mathcal{V}_{\mathrm{eff},\perp}R^{1/2}$: (Remember that we have shown that $R \geqslant 0$, so its square root is well-defined.) We first estimate $\|\mathcal{V}R\mathcal{V}\|$, as follows. Recalling the noninteracting resolvent R_{NI} introduced above, we have that

$$0 \leqslant \mathcal{V}R\mathcal{V} \leqslant \mathcal{V}R_{\mathrm{NI}}\mathcal{V} = \mathcal{V}R_0^{1/2}(1 + R_0^{1/2}\mathcal{V}_n R_0^{1/2})^{-1}R_0^{1/2}\mathcal{V}.$$

Hence its norm can be estimated by

$$\|\mathcal{V}R\mathcal{V}\| \leqslant \frac{\|\mathcal{V}R_0^{1/2}\|^2}{1-\|R_0^{1/2}\mathcal{V}_n R_0^{1/2}\|},$$

from which we obtain an estimate for $\|\mathcal{V}R^{1/2}\|$ by taking square roots. Therefore, if $B \geqslant B_{(36)} = 4b_0$ as above,

$$\|\mathcal{V}_{\mathrm{eff},\perp}R^{1/2}\| \leqslant \|\mathcal{V}R^{1/2}\| \leqslant \sqrt{(16Z^2N + 4N(N-1)^2)(\mathbb{M}+N+2)}.$$

We now come to the proof of (38). By Feshbach's formula, we have

$$\|(H-\xi)^{-1}-R_{\mathrm{eff}}^{\mathcal{W}}\oplus R(\xi)\| = \left\| \begin{pmatrix} 0 & -R_{\mathrm{eff}}^{\mathcal{W}}\mathcal{V}_{\mathrm{eff},\perp}R \\ -R\mathcal{V}_{\perp,\mathrm{eff}}R_{\mathrm{eff}}^{\mathcal{W}} & R\mathcal{V}_{\perp,\mathrm{eff}}R_{\mathrm{eff}}^{\mathcal{W}}\mathcal{V}_{\mathrm{eff},\perp}R \end{pmatrix} \right\| \leqslant \|R_{\mathrm{eff}}^{\mathcal{W}}\mathcal{V}_{\mathrm{eff},\perp}R\| + \|R\mathcal{V}_{\perp,\mathrm{eff}}R_{\mathrm{eff}}^{\mathcal{W}}\mathcal{V}_{\mathrm{eff},\perp}R\| \leqslant \|R_{\mathrm{eff}}^{\mathcal{W}}\|\|\mathcal{V}_{\mathrm{eff},\perp}R^{1/2}\|\|R^{1/2}\| + \|R_{\mathrm{eff}}^{\mathcal{W}}\| \times \|\mathcal{V}_{\mathrm{eff},\perp}R^{1/2}\|^2\|R^{1/2}\|^2, \tag{43}$$

where we have used the following elementary estimate for the norm of matrices of operators:

$$\left\| \begin{pmatrix} 0 & A \\ A^* & B \end{pmatrix} \right\| \leqslant \|A\| + \|B\|.$$

Hence if $B > B_{(36)}$ and if $\xi \notin \sigma(R_{\mathrm{eff}}^{\mathcal{W}})$, we obtain

$$\|(H-\xi)^{-1}-R_{\mathrm{eff}}^{\mathcal{W}}\oplus R(\xi)\| \leqslant \frac{1}{d_{\mathrm{eff}}^{\mathcal{W}}(\xi)}\left(\frac{\sqrt{2}\|\mathcal{V}R^{1/2}\|}{\sqrt{B}} + \frac{2\|\mathcal{V}R^{1/2}\|^2}{B}\right) \leqslant \frac{1}{d_{\mathrm{eff}}^{\mathcal{W}}(\xi)B^{1/2}}\left(c_0 + \frac{c_0^2}{\sqrt{B_{(36)}}}\right),$$

with $c_0^2=(32Z^2N+8N(N-1)^2)(\mathbb{M}+N+2)$. Q.E.D.

Corollary 3.3 (of the proof): Theorem 3.1 also holds, if we replace H and $h_{\mathrm{eff}}+\mathcal{W}$ *by their fermionized versions* H_f, $h_{\mathrm{eff},f}+\mathcal{W}_f$, *and* $d_{\mathrm{eff}}^{\mathcal{W}}(\xi)$ *by the distance of* ξ *to the spectrum of* $h_{\mathrm{eff},f}+\mathcal{W}_f$.

Proof: Simply write down the Feshbach's formula (35) for H_f with respect to the decomposition $I=\Pi_{\mathrm{eff},f}+\Pi_{\perp,f}$ of $\mathcal{H}_f$, and estimate as in (43), where all operators will now have a subindex f. Next use that P^{AS} commutes with everything, and trivially estimate $\|A_f\|=\|P^{AS}A\|\leqslant\|A\|$, for $A=R$, $R^{1/2}$ and $\mathcal{V}_{\mathrm{eff},\perp}R^{1/2}$, except for $\|R_{\mathrm{eff},f}^{\mathcal{W}}\|$, which will be estimated by 1 over the distance of ξ to the spectrum of $H_{\mathrm{eff},f}+\mathcal{W}_f$. Q.E.D.

The proof shows that in the fermionic case, Theorem 3.1 will at least be true with the same constants as for the boltzonic case. The optimal constants for fermions might be smaller, though.

Remark 3.4: In the proof of Theorem 3.1 we systematically used Hardy's inequality. Alternatively, one can use, at least when $N=1$, the bounds on the matrix elements of the Coulomb potential with respect to the Landau levels which were derived in Ref. 10.

IV. EFFECTIVE POTENTIALS FOR LARGE FIELDS

The operator $h_{\mathrm{eff}}+\mathcal{W}=h_{\mathrm{eff}}^{B,\mathbb{M}}+\mathcal{W}^{B,\mathbb{M}}$ of Theorem 3.1 acts on $\mathrm{Ran}(\Pi_{\mathrm{eff}}^{B,\mathbb{M}})=\Pi_{\mathrm{eff}}^{B,\mathbb{M}}(\mathcal{H})$, a Hilbert space which depends on both B and $\mathbb{M}$, and which is canonically isomorphic to the space of $F_{\mathbb{M}}^B$-valued L^2-functions on $\mathbb{R}^N$,

$$\mathrm{Ran}(\Pi_{\mathrm{eff}}^{B,\mathbb{M}}) = L^2(\mathbb{R}^N, F_{\mathbb{M}}^B). \tag{44}$$

(Recall that $F_{\mathbb{M}}^B=\mathrm{Span}\ \{X_m^B : m\in\Sigma(\mathbb{M})\}$.) We will mostly suppress the $\mathbb{M}$-dependence from our notations, $\mathbb{M}$ being fixed in our analysis. The potential term of h_{eff}^B,

$$\mathcal{V}_{\mathrm{eff}}^B = \Pi_{\mathrm{eff}}^B\mathcal{V}\Pi_{\mathrm{eff}}^B, \tag{45}$$

can be interpreted as an operator valued function of $z=(z_1,\ldots,z_N)\in\mathbb{R}^N$, with values in the space of linear operators on $F_{\mathbb{M}}^B$ and acting in the natural way on $L^2(\mathbb{R}_z^N;F_{\mathbb{M}}^B)$. To get rid of the B-dependence of our Hilbert spaces we do a unitary rescaling. Let us pose $x=(x_1,\ldots,x_N)\in\mathbb{R}^N$ and similarly for y and z. Define a unitary operator U_{xy}^B on $\mathcal{H}$ by

$$U_{xy}^B\psi(x,y,z) = B^{N/2}\psi(\sqrt{B}x,\sqrt{B}y,z). \tag{46}$$

Since $X_m^B(x,y)=B^{N/2}X_m^1(\sqrt{B}x,\sqrt{B}y)$, it follows that

$$U_{xy}^{B*}\Pi_{\mathrm{eff}}^B U_{xy}^B = \Pi_{\mathrm{eff}}^1.$$

Let us write $\mathcal{V}_{\mathrm{eff}}^B$ in multiparticle form,

$$\mathcal{V}^B_{\text{eff}} = -\sum_j ZV^B_j + \sum_{j<k} V^B_{jk}, \tag{47}$$

with V^B_j and V^B_{jk} defined by (10). Then $U^{B*}_{xy}V^B_j U^B_{xy} = \Pi^1_{\text{eff}} U^{B*}_{xy} |r_j|^{-1} U^B_{xy} \Pi^1_{\text{eff}} = \sqrt{B} V^1_j(\sqrt{B}z_j)$, with

$$V^1_j(z) = \Pi^1_{\text{eff}} \frac{1}{\sqrt{x_j^2 + y_j^2 + z^2}} \Pi^1_{\text{eff}}, \tag{48}$$

and likewise for V^B_{jk}: $U^{B*}_{xy}V^B_{jk}U^B_{xy}(z) = \sqrt{B}V^1_{jk}(\sqrt{B}(z_j - z_k))$, with

$$V^1_{jk}(z) = \Pi^1_{\text{eff}} \frac{1}{\sqrt{(x_j - x_k)^2 + (y_j - y_k)^2 + z^2}} \Pi^1_{\text{eff}}. \tag{49}$$

The operator

$$\hat{h}^B_{\text{eff}} := U^{B*}_{xy} H^{\text{B}}_{\text{eff}} U^B_{xy}, \tag{50}$$

will now act on the fixed, B-independent, Hilbert space, $L^2(\mathbb{R}^N, F^1_{\mathbb{M}})$, and

$$\hat{h}^B_{\text{eff}} = -\frac{1}{2}\Delta_z - \sum_j Z\sqrt{B}V^1_j(\sqrt{B}z_j) + \sum_{j<k} \sqrt{B}V^1_{jk}(\sqrt{B}(z_j - z_k)) = -\frac{1}{2}\Delta_z + \sqrt{B}\mathcal{V}^1_{\text{eff}}(\sqrt{B}z).$$

The next step will be to examine the asymptotic behavior of $\sqrt{B}\mathcal{V}^1_{\text{eff}}(\sqrt{B}z)$ as $B \to \infty$. The main idea is contained in Lemma 4.1 below. We introduce the free Laplacian on $\mathbb{R}^N$,

$$h_{00} = -\tfrac{1}{2}\Delta_z, \tag{51}$$

and its resolvent

$$R_{00}(-\alpha^2) = (h_{00} + \alpha^2)^{-1}. \tag{52}$$

We will need this resolvent both in dimension N and dimension 1. To distinguish between these two cases we will, in the one-dimensional case, systematically use β^2 as spectral parameter instead of α^2, reserving the latter for the multidimensional case.

If u is a function or tempered distribution on $\mathbb{R}^N$, with values in some auxiliary Hilbert space F, then $\|R_{00}(-\alpha^2)^{-s/2}u\|_{L^2(\mathbb{R}^N;F)}$ is a norm on the sth Sobolev space $H^s(\mathbb{R}^N;F)$. A linear operator A sends $H^s(\mathbb{R}^N;F)$ continuously into $H^{-s}(\mathbb{R}^N;F)$ iff the L^2-operator norm $\|R_{00}(-\alpha^2)^{s/2}AR_{00}(-\alpha^2)^{s/2}\|$ is finite. The case of interest for us will be $s=1$. We will also need the Fourier transform $\mathcal{F}$, but only in dimension 1, for which we normalize as follows:

$$\mathcal{F}(u)(\zeta) = \int_{\mathbb{R}} u(z)e^{-iz\zeta}\,\mathrm{d}z.$$

There will consequently be a factor of $(2\pi)^{-1}$ in the inversion formula.

Recall that

$$\text{Pf}\left(\frac{1}{|x|}\right) = \frac{\mathrm{d}}{\mathrm{d}x}(\text{sgn}(x)\log|x|),$$

with the derivative in distribution sense. Let F be a finite-dimensional complex Hilbert space, and $L(F)$ the space of linear operators on F.

Lemma 4.1: Let $\mathfrak{v}$ *be an* $L(F)$*-valued tempered distribution on* $\mathbb{R}$*, such that its Fourier transform can be identified with a locally integrable function* $\mathcal{F}\mathfrak{v} = \mathcal{F}\mathfrak{v}(\zeta)$*. Assume also the following:*

(i) *There exist* C_0, $C_1 \in L(F)$ *and* $a > 1/2$*, such that*

$$\mathcal{F}\mathfrak{v}(\zeta) = -C_0 \log|\zeta| + C_1 + O(|\zeta|^a), \quad \zeta \to 0. \tag{53}$$

(ii) *If*

$$\mathfrak{e}(\zeta) := \mathcal{F}\mathfrak{v}(\zeta) + C_0 \log|\zeta| - C_1,$$

denotes the error in the approximation (53), then

$$C_{\mathfrak{v}}^2 := \int_{\mathbb{R}} \frac{\|\mathfrak{e}(\zeta)\|^2}{|\zeta|^2} \mathrm{d}\zeta < \infty. \tag{54}$$

For each $\lambda > 0$ *let*

$$\mathfrak{v}_{\infty,\lambda} := C_0 \log \lambda \cdot \delta + \frac{1}{2} C_0 \cdot \mathrm{Pf}\left(\frac{1}{|x|}\right) + (\gamma C_0 + C_1) \cdot \delta, \tag{55}$$

where δ *is Dirac's delta distribution in 0, and* $\gamma = \Gamma'(1)$ *is the Euler constant. If* $R_{00}(-\beta^2)$ *denotes the free resolvent in dimension 1 and* $\beta > 0$, *then*

$$\|R_{00}(-\beta^2)^{1/2}(\lambda \mathfrak{v}(\lambda \cdot) - \mathfrak{v}_{\infty,\lambda})R_{00}(-\beta^2)^{1/2}\| \leqslant \frac{2^{1/4} C_{\mathfrak{v}}}{\sqrt{\beta \lambda \pi}}. \tag{56}$$

Remark: Observe that the integral (54) converges in 0, since we assumed that $a > 1/2$ in (53).
Proof: It is known that

$$\mathcal{F}^{-1}(\log|\zeta|) = -\frac{1}{2}\mathrm{Pf}\left(\frac{1}{|x|}\right) - \gamma\delta_0, \tag{57}$$

where γ is Euler's constant, cf., e.g., Ref. 17. [Equation (57) can also easily be shown directly, using the observation that $\mathrm{Pf}(1/|x|)$ and $-2\mathcal{F}^{-1}(\log|\zeta|)$ are both solutions of the distributional equation $x\Lambda = -\operatorname{sgn} x$ and therefore only differ by a multiple of δ, which can then be computed to be -2γ.] Therefore

$$\mathfrak{v}_{\infty,\lambda} = C_0(\log\lambda)\delta - C_0\mathcal{F}^{-1}(\log|\zeta|) + C_1\delta = \mathcal{F}^{-1}(-C_0 \log(|\zeta|/\lambda) + C_1),$$

and

$$\mathcal{F}(R_{00}(-\beta^2)^{1/2}(\lambda \mathfrak{v}(\lambda \cdot) - \mathfrak{v}_{\infty,\lambda})R_{00}(-\beta^2)^{1/2})\mathcal{F}^{-1}$$

is an integral operator with kernel

$$\frac{1}{2\pi}\frac{1}{(\zeta^2/2 + \beta^2)^{1/2}}\mathfrak{e}\left(\frac{\zeta - \zeta'}{\lambda}\right)\frac{1}{(\zeta'^2/2 + \beta^2)^{1/2}}, \tag{58}$$

since multiplication by a distribution $a(x)$ becomes an integral operator with kernel $(2\pi)^{-1}\mathcal{F}a(\zeta - \zeta')$ after conjugation by $\mathcal{F}$. Since conjugation by the Fourier transform does not change the operator norm, it follows that the norm in (56) can be bounded by the Hilbert-Schmidt norm of (58), whose square equals

$$\frac{1}{\pi^2}\int_{\mathbb{R}}\left(\int_{\mathbb{R}}\frac{1}{((\zeta-\eta)^2 + 2\beta^2)(\zeta^2 + 2\beta^2)}\mathrm{d}\zeta\right)\left|\mathfrak{e}\left(\frac{\eta}{\lambda}\right)\right|^2 \mathrm{d}\eta = \frac{\sqrt{2}}{\pi\beta}\int_{\mathbb{R}}\frac{|\mathfrak{e}(\eta/\lambda)|^2}{\eta^2 + 8\beta^2}\mathrm{d}\eta$$
$$= \frac{\sqrt{2}}{\pi\beta\lambda}\int_{\mathbb{R}}\frac{|\mathfrak{e}(\eta)|^2}{\eta^2 + (\beta^2/8\lambda^2)}\mathrm{d}\eta \leqslant \frac{C_{\mathfrak{v}}^2\sqrt{2}}{\pi\beta\lambda}.$$

Here we have used the elementary integral identity:

$$\int_{\mathbb{R}} \frac{1}{(a\zeta^2+b)(a(\zeta-\eta)^2+b)}\mathrm{d}\zeta = \frac{2\pi}{\sqrt{ab}}\frac{1}{a\eta^2+4b}, \tag{59}$$

where $a,b>0$. This finishes the proof of Lemma 4.1. Q.E.D.

We will apply the previous lemma to our potentials (10), but before doing so we first state and prove a weaker variant, which will be used to prove Theorem 1.1. Let us introduce the (numerical) constant,

$$C_{(60)} := \left(\frac{1}{4\pi}\int_{\mathbb{R}} \frac{(|\log|\eta|+2)^2}{\eta^2+4}\mathrm{d}\eta\right)^{1/2}. \tag{60}$$

Numerical evaluation of the integral (using either Mathematica or Maple 8) gives $C_{(60)}^2 \simeq 1.53$.

Lemma 4.2: Let $\mathfrak{v}=\mathfrak{v}(z)$ *be an* $L(F)$*-valued tempered distribution on* $\mathbb{R}$ *such that*

$$C_{\mathfrak{v}} := \sup_{\zeta\in\mathbb{R}} \|(|\log|\zeta|+1)^{-1}\mathcal{F}\mathfrak{v}(\zeta)\| < \infty. \tag{61}$$

Then for all $\lambda \geqslant e$ *and all* $\varepsilon>0$,

$$\left\|(-\varepsilon\Delta+\varepsilon^{-1})^{-1/2}\left(\frac{\lambda}{\log\lambda}\mathfrak{v}(\lambda z)\right)(-\varepsilon\Delta+\varepsilon^{-1})^{-1/2}\right\| \leqslant C_{(60)}C_{\mathfrak{v}}(|\log\varepsilon|+2). \tag{62}$$

Proof: Conjugating as before by the Fourier transform, and estimating the operator norm by the Hilbert-Schmidt one, we find that the left-hand side of (62) is bounded, by the square root of

$$(2\pi)^{-2}\int_{\mathbb{R}}\left(\int_{\mathbb{R}}\frac{1}{(\varepsilon\zeta^2+\varepsilon^{-1})(\varepsilon(\zeta-\eta)^2+\varepsilon^{-1})}\mathrm{d}\zeta\right)\frac{1}{(\log\lambda)^2}\left\|\mathcal{F}\mathfrak{v}\left(\frac{\eta}{\lambda}\right)\right\|^2\mathrm{d}\eta.$$

By (61) we can bound

$$\frac{1}{(\log\lambda)^2}\|\mathcal{F}\mathfrak{v}(\eta/\lambda)\|^2 \leqslant C_{\mathfrak{v}}^2\left(\frac{|\log|\eta||}{\log\lambda}+1+\frac{1}{\log\lambda}\right)^2 \leqslant C_{\mathfrak{v}}^2(|\log|\eta||+2)^2,$$

since we suppose that $\lambda\geqslant e$. Hence, using (59) again, we find that our norm is bounded by the square root of

$$\frac{C_{\mathfrak{v}}^2}{2\pi}\int_{\mathbb{R}}\frac{(|\log|\eta||+2)^2}{\varepsilon\eta^2+4\varepsilon^{-1}}\mathrm{d}\eta \leqslant \frac{C_{\mathfrak{v}}^2}{2\pi}\int_{\mathbb{R}}\frac{(|\log|\eta||+|\log\varepsilon|+2)^2}{\eta^2+4}\mathrm{d}\eta \leqslant \frac{C_{\mathfrak{v}}^2}{\pi}(\log\varepsilon)^2\int_{\mathbb{R}}\frac{\mathrm{d}\eta}{\eta^2+4}$$
$$+\frac{C_{\mathfrak{v}}^2}{\pi}\int_{\mathbb{R}}\frac{(|\log|\eta||+2)^2}{\eta^2+4}\mathrm{d}\eta = C_{\mathfrak{v}}^2\left(\frac{(\log\varepsilon)^2}{2}+4C_{(60)}^2\right),$$

by (60). Since $C_{(60)}^2\geqslant 1/2$, we see that (62) will be bounded by $C_{(60)}C_{\mathfrak{v}}(|\log\varepsilon|+2)$, as claimed. Q.E.D.

The next step will be to apply Lemma 4.1 to the potentials V_j^1 and V_{jk}^1, with $\lambda=\sqrt{B}$. We introduce the B-dependent tempered distribution $q=q^B$, and linear operators C_j^n, $C_{jk}^e \in L(F_{\mathbb{M}}^1)$ by

$$q^B(z) = \log B\,\delta(z) + \mathrm{Pf}\left(\frac{1}{|z|}\right), \tag{63}$$

$$C_j^n := C_j^{n,\mathbb{M}} := -\Pi^1_{\text{eff}} \log\left(\tfrac{1}{4}(x_j^2+y_j^2)\right)\Pi^1_{\text{eff}}, \tag{64}$$

$$C_{jk}^e := C_{jk}^{e,\mathbb{M}} := -\Pi^1_{\text{eff}} \log\left(\tfrac{1}{4}((x_j-x_k)^2+(y_j-y_k)^2)\right)\Pi^1_{\text{eff}}. \tag{65}$$

Observe that (64) and (65) are related to (12) and (13) by conjugation by U^B_{xy}. See also Remark 1.4 for a physical interpretation of these three terms.

Lemma 4.3: Let $R_{00}(-\beta^2)=\left(-\frac{1}{2}\Delta_z+\beta^2\right)^{-1}$, $\beta>0$ *be the free resolvent in dimension 1. There exists a positive constant* $C_{(66)}:=C_{(66)}(\mathbb{M})>0$ *only depending on* $\mathbb{M}$, *such that for all* $B,\beta>0$,

$$\|R_{00}(-\beta^2)^{1/2}(\sqrt{B}V_j^1(\sqrt{B}z)-(q^B(z)+C_j^n\delta(z)))R_{00}(-\beta^2)^{1/2}\| \leqslant \frac{C_{(66)}}{\sqrt{\beta}B^{1/4}} \tag{66}$$

and

$$\|R_{00}(-\beta^2)^{1/2}(\sqrt{B}V_{jk}^1(\sqrt{B}z)-(q^B(z)+C_{jk}^e\delta(z)))R_{00}(-\beta^2)^{1/2}\| \leqslant \frac{C_{(66)}}{\sqrt{\beta}B^{1/4}}, \tag{67}$$

the norm being the operator norm on $L^2(\mathbb{R},F^1_{\mathbb{M}})$.

To simplify future estimates, we have taken the same constant in both inequalities.

Proof: Recall the formulas (48) and (49) for $V_j^1(z)$ and $V_{jk}^1(z)$. We need the asymptotics of their Fourier transforms at 0. By Ref. 1, 9.6.21, the Fourier transform of $(1+z^2)^{-1/2}$ equals

$$\mathcal{F}((1+z^2)^{-1/2})(\zeta)=2K_0(|\zeta|),$$

where K_0 is the Macdonald function. Since the projector Π^1_{eff} effectively only acts in the x and y variables, it follows that

$$\mathcal{F}V_j^1(\zeta)=\Pi^1_{\text{eff}}\mathcal{F}_{z\to\zeta}((x_j^2+y_j^2)^{-1/2}(1+((x_j^2+y_j^2)^{-1/2}z)^2)^{-1/2})\Pi^1_{\text{eff}}=2\Pi^1_{\text{eff}}K_0(\sqrt{x_j^2+y_j^2}\cdot\zeta)\Pi^1_{\text{eff}},$$

with a similar formula for $\mathcal{F}V_{jk}^1$.

Now it is known that

$$K_0(|\zeta|)=-\log|\zeta|+\log 2-\gamma+O(||\zeta^2\log|\zeta||), \quad |\zeta|\to 0,$$

and that $K_0(|\zeta|)$ is bounded on $|\zeta|\geqslant 1$ (even exponentially decreasing there): see, e.g., [Ref. 1 9.6.13]. It then easily follows that, as $\zeta\to 0$ and as operators on $\operatorname{Ran}\Pi^1_{\text{eff}}$,

$$\mathcal{F}V_j^1(\zeta)\simeq -2\log|\zeta|-2\gamma+C_j^n,$$

$$\mathcal{F}V_{jk}^1(\zeta)\simeq -2\log|\zeta|-2\gamma+C_{jk}^e, \tag{68}$$

with an error of $O(|\zeta^2\log|\zeta||)$. An appeal to Lemma 4.1, with $\lambda=\sqrt{B}$ and with $C_0=2$ and $C_1=-2\gamma+C_j^n$, respectively, $C_1=-2\gamma+C_{jk}^e$, then finishes the proof. Q.E.D.

Remark 4.4: An explicit computation of the matrices of C_j^n and C_{jk}^e with respect to the natural basis $X_m^1, m\in\Sigma(\mathbb{M})$ shows that C_j^n and C_{jk}^e do depend on their indices j and j, k, respectively.

We will likewise need Lemma 4.2 for $\mathfrak{v}=V_j^1$. We can without loss of generality assume that $j=1$, by permutational symmetry of $\Sigma(\mathbb{M})$. As we have seen above, $\mathcal{F}V_1^1(\zeta)=2\Pi^1_{\text{eff}}K_0(|\zeta|\sqrt{x_1^2+y_1^2})\Pi^1_{\text{eff}}$. It can easily be verified that $\|(|\log'|\zeta||+1)^{-1}K_0(\zeta)\|_\infty=1$, so that, for example,

$$C_{V_1^1}\leqslant C_{(69)}:=2+2\|\Pi^1_{\text{eff}}|\log\sqrt{x_1^2+y_1^2}|\Pi^1_{\text{eff}}\|. \tag{69}$$

The operator norm on the right-hand side can be evaluated explicitly, and behaves asymptotically for large positive $\mathbb{M}$ as $2\log(\mathbb{M})$.

We next extend Lemma 4.3 to multiparticle potentials. Let us define the multiparticle potential v_C by

$$v_C(z) = v_C^B(z) = -Z\sum_j (q^B(z_j) + C_j^n \delta(z_j)) + \sum_{j<k} (q^B(z_j - z_k) + C_{jk}^e \delta(z_j - z_k)). \tag{70}$$

Lemma 4.5: Let $R_{00}(-\alpha^2) = \left(-\frac{1}{2}\Delta_z + \alpha^2\right)^{-1}$, $\alpha > 0$, *be the resolvent of the free Hamiltonian in* $\mathbb{R}^N$. *Then*

$$\|R_{00}(-\alpha^2)^{1/2}(\sqrt{B}\mathcal{V}_{\text{eff}}^1(\sqrt{B}z) - v_C(z))R_{00}(-\alpha^2)^{1/2}\| \leqslant \frac{C_{(72)}}{\sqrt{\alpha}B^{1/4}}, \tag{71}$$

where

$$C_{(72)} := C_{(72)}(N,Z,\mathbb{M}) := C_{(66)}N^{1/4}\left(Z + \tfrac{1}{2}(N-1)\right). \tag{72}$$

Proof: We split both potentials into their electron-nucleus and electron-electron parts,

$$\mathcal{V}_{\text{eff}}^1 = \mathcal{V}_{\text{eff},n}^1 + \mathcal{V}_{\text{eff},e}^1,$$

and similarly for v_C: $v_C = v_{C,n} + v_{C,e} = v_{C,n}^B + v_{C,e}^B$. Writing $\mathcal{V}_{s,\nu}^B(z)$ for $\sqrt{B}\mathcal{V}_{s,\nu}^1(\sqrt{B}z)$ (with a mild abuse of notation), where $\nu = n$ or e, we bound the left-hand side of (71) by

$$\|R_{00}(-\alpha^2)^{1/2}(\mathcal{V}_{\text{eff},n}^B - v_{C,n})R_{00}(-\alpha^2)^{1/2}\| + \|R_{00}(-\alpha^2)^{1/2}(\mathcal{V}_{\text{eff},e}^B - v_{C,e})R_{00}(-\alpha^2)^{1/2}\|, \tag{73}$$

and estimate the two terms separately. Let $R_{00,j}(-\beta^2)$ be the one-dimensional resolvent in the variable z_j, with a β which will be picked below. We will simply write R_{00} for $R_{00}(-\alpha^2)$ and $R_{00,j}$ for $R_{00,j}(-\beta^2)$. If we set

$$\Delta V_j := V_j^B(z_j) - q^B(z_j) - C_j^n \delta(z_j)$$

and

$$\Delta\mathcal{V}_n := Z\sum_j \Delta V_j = \mathcal{V}_{\text{eff},n}^B - v_{C,n},$$

then, by (66),

$$\begin{aligned} R_{00}^{1/2}\Delta\mathcal{V}_n R_{00}^{1/2} &= Z\sum_j (R_{00}^{1/2}R_{00,j}^{-1/2})(R_{00,j}^{1/2}\Delta V_j R_{00,j}^{1/2})(R_{00,j}^{-1/2}R_{00}^{1/2}) \leqslant \frac{C_{(66)}Z}{\sqrt{\beta}B^{1/4}}\sum_j R_{00}^{1/2}R_{00,j}^{-1}R_{00}^{1/2} \\ &= \frac{C_{(66)}Z}{\sqrt{\beta}B^{1/4}}R_{00}(-\alpha)^2\left(-\frac{1}{2}\Delta_z + N\beta^2\right) \leqslant \frac{C_{(66)}Z}{\sqrt{\beta}B^{1/4}}\max_{\xi\in\mathbb{R}^N}\frac{|\xi|^2/2 + N\beta^2}{|\xi|^2/2 + \alpha^2} \\ &= \frac{C_{(66)}Z\max(1, N\beta^2/\alpha^2)}{\sqrt{\beta}B^{1/4}} = \frac{C_{(66)}ZN^{1/4}}{\sqrt{\alpha}B^{1/4}} \end{aligned}$$

if we pick $\beta = \alpha/\sqrt{N}$; this choice actually minimizes $\beta^{-1/2}\max(1, N\beta^2/\alpha^2)$ as a function of $\beta \geqslant 0$, as is easily checked. Similar estimates show that $-R_{00}^{1/2}\Delta\mathcal{V}_n R_{00}^{1/2}$ is bounded from above, in operator sense, by the same number, and we therefore conclude that the first norm in (73) is bounded by $C_{(66)}ZN^{1/4}/\sqrt{\alpha}B^{1/4}$.

To estimate the second term of (73), we will use the following lemma, which is analogous to Lemma 3.2 from Sec. II. Let $\Delta_j = -d^2/\mathrm{d}z_j^2$, $\Delta_k = -d^2/\mathrm{d}z_k^2$.

Lemma 4.6: Let $\mathfrak{v} = \mathfrak{v}(z)$ *be an* $L(F)$*-valued distribution on* $\mathbb{R}$ *(F a finite-dimensional Hilbert space), such that* $R_{00}(-\beta^2)^{1/2}\mathfrak{v}R_{00}(-\beta^2)^{1/2}$ *is self-adjoint, for* $\beta > 0$. *Then for all* $\mu > 0$,

$$\left\| \left(-\frac{1}{2}\Delta_j - \frac{1}{2}\Delta_k + \mu^2 \right)^{-1/2} \mathfrak{v}(z_j - z_k) \left(-\frac{1}{2}\Delta_j - \frac{1}{2}\Delta_k + \mu^2 \right)^{-1/2} \right\|$$
$$\leqslant \frac{1}{2} \left\| \left(-\frac{1}{2}\Delta_s + \frac{\mu^2}{2} \right)^{-1/2} \mathfrak{v}(s) \left(-\frac{1}{2}\Delta_s + \frac{\mu^2}{2} \right)^{-1/2} \right\|. \tag{74}$$

Proof: We use a similar change of variables as in the proof of Lemma 3.2: $s=(z_j-z_k)/\sqrt{2}$, $t=(z_j+z_k)/\sqrt{2}$. Then, with $\simeq$ denoting unitary equivalence,

$$\left(-\frac{1}{2}\Delta_j - \frac{1}{2}\Delta_k + \mu^2 \right)^{1/2} \mathfrak{v}(z_j - z_k) \left(-\frac{1}{2}\Delta_j - \frac{1}{2}\Delta_k + \mu^2 \right)^{-1/2}$$
$$\simeq \left(-\frac{1}{2}\Delta_s - \frac{1}{2}\Delta_t + \mu^2 \right)^{-1/2} \mathfrak{v}(\sqrt{2}s) \left(-\frac{1}{2}\Delta_s - \frac{1}{2}\Delta_t + \mu^2 \right)^{-1/2}$$
$$\simeq \frac{1}{2} \left(-\frac{1}{2}\Delta_s - \frac{1}{2}\Delta_t + \frac{\mu^2}{2} \right)^{-1/2} \mathfrak{v}(s) \left(-\frac{1}{2}\Delta_s - \frac{1}{2}\Delta_t + \frac{\mu^2}{2} \right)^{-1/2}.$$

Observing that

$$\left\| \left(-\frac{1}{2}\Delta_s + \frac{\mu^2}{2} \right)^{1/2} \left(-\frac{1}{2}\Delta_s - \frac{1}{2}\Delta_t + \frac{\mu^2}{2} \right)^{-1/2} \right\| \leqslant 1$$

on $L^2(\mathbb{R}^2)$, the lemma follows. Q.E.D.

Let us write

$$R_{00,jk} = R_{00,jk}(-\mu^2) = \left(-\tfrac{1}{2}(\Delta_j + \Delta_k) + \mu^2 \right)^{-1/2}, \tag{75}$$

the two-dimensional free resolvent, where μ will be optimized at the end of the proof. Recall that $R_{00}=R_{00}(-\alpha^2)$, and set

$$\Delta V_{jk} = V^B_{jk}(z_j - z_k) - q^B(z_j - z_k) - C^e_{jk}\delta(z_j - z_k).$$

Then, using Lemmas 4.6 and 4.3, $R_{00}^{1/2}(\mathcal{V}^B_{\mathrm{eff},e} - v^B_{C,e})R_{00}^{1/2}$ can be estimated from above as follows:

$$R_{00}^{1/2} \sum_{j<k} \Delta V_{jk} R_{00}^{1/2} = \sum_{j<k} (R_{00}^{1/2} R_{00,jk}^{-1/2})(R_{00,jk}^{-1} \Delta V_{jk} R_{00,jk}^{1/2})(R_{00,jk}^{-1/2} R_{00}^{1/2}) \leqslant \frac{C_{(66)}}{2^{3/4}\sqrt{\mu} B^{1/4}} \sum_{j<k} R_{00}^{1/2} R_{00,jk}^{-1} R_{00}^{1/2}$$
$$= \frac{C_{(66)}}{2^{3/4}\sqrt{\mu} B^{1/4}} R_{00}(-\alpha^2) \left(\sum_{j<k} \left(-\frac{1}{2}(\Delta_j + \Delta_k) + \mu^2 \right) \right)$$
$$= \frac{C_{(66)}(N-1)}{2^{3/4}\sqrt{\mu} B^{1/4}} R_{00}(-\alpha^2) \left(-\frac{1}{2}\Delta_z + \frac{N\mu^2}{2} \right)$$
$$\leqslant \frac{C_{(66)}(N-1)}{2^{3/4} B^{1/4}} \frac{1}{\sqrt{\mu}} \max\left(1, \frac{N\mu^2}{2\alpha^2} \right) \leqslant \frac{C_{(66)}(N-1)N^{1/4}}{2\sqrt{\alpha} B^{1/4}},$$

where we minimized the right-hand side over μ by choosing $\mu=\alpha\sqrt{2/N}$. The similar upper bound for $-R^{1/2}(\mathcal{V}_e - v^B_{C,e})R_{00}^{1/2}$ gives the desired estimate for the second norm in (73), and combining the two estimates, we have proved Lemma 4.5. Q.E.D.

We now derive a similar estimate for $\mathcal{W}^B$ as $B\to\infty$.

Lemma 4.7: Let $R_{00}(-\alpha^2)$ be the free resolvent in dimension N, and let $U=U^B_{xy}$ be the unitary transformation defined by (46). Then, if, $\xi\leqslant 0$,

$$\| R_{00}(-\alpha^2)^{1/2} U^* \mathcal{W}^B U R_{00}(-\alpha^2)^{1/2} \| \leqslant \frac{C_{(77)}}{\alpha\sqrt{B}}, \tag{76}$$

with

$$C_{(77)} := C_{(77)}(N,Z) := 2\pi^{3/2}N^{3/2}\left(Z^2 + \frac{(N-1)^2}{4}\right). \tag{77}$$

Proof: Recall that $\mathcal{W}^B = -\mathcal{V}_{\mathrm{eff},\perp} R \mathcal{V}_{\perp,\mathrm{eff}}$, where $R = R(\xi) = (H_\perp - \xi)^{-1}$ on $\mathrm{Ran}\,\Pi_\perp^B$. Hence

$$U^* \mathcal{W}^B U = -B\mathcal{V}^1_{\mathrm{eff},\perp}(\sqrt{B}z) U^* R U \mathcal{V}^1_{\perp,\mathrm{eff}}(\sqrt{B}z),$$

where $\mathcal{V}^1_{\mathrm{eff},\perp} = \Pi^1_{\mathrm{eff}} \mathcal{V} \Pi^1_\perp$, and similarly for $\mathcal{V}^1_{\perp,\mathrm{eff}}$. Since for $\xi \leqslant 0$, $0 \leqslant R \leqslant 2/B$ (see Sec. III), we have that, letting $\mathcal{V}(\cdot,z)$ be the function $(x,y) \to \mathcal{V}(x,y,z)$,

$$\begin{aligned} 0 \leqslant -U^* \mathcal{W}^B U &\leqslant 2\Pi^1_{\mathrm{eff}} \mathcal{V}(\cdot,\sqrt{B}z) \Pi_\perp \mathcal{V}(\cdot,\sqrt{B}z) \Pi^1_{\mathrm{eff}} \leqslant 2\Pi^1_{\mathrm{eff}} \mathcal{V}(\cdot,\sqrt{B}z)^2 \Pi^1_{\mathrm{eff}} \leqslant 4(\Pi^1_{\mathrm{eff}} \mathcal{V}_n(\cdot,\sqrt{B}z)^2 \Pi^1_{\mathrm{eff}} \\ &+ \Pi^1_{\mathrm{eff}} \mathcal{V}_e(\cdot,\sqrt{B}z)^2 \Pi^1_{\mathrm{eff}}). \end{aligned} \tag{78}$$

As in the previous lemma, we treat the two terms separately. By Cauchy-Schwarz,

$$\mathcal{V}_n(x,y,\sqrt{B}z)^2 \leqslant Z^2 N \sum_{j=1}^N \frac{1}{\rho_j^2 + Bz_j^2},$$

where $\rho_j^2 = x_j^2 + y_j^2$. As before, let $R_{00,j}(-\beta^2)$ be the resolvent of $h_{00,j} = -(1/2)d^2/\mathrm{d}z_j^2$ on $\mathbb{R}$. We first estimate the L^2-norm of each

$$R_{00,j}(-\beta^2)^{1/2} \Pi^1_{\mathrm{eff}} (\rho_j^2 + Bz_j^2)^{-1} \Pi^1_{\mathrm{eff}} R_{00,j}(-\beta^2)^{1/2}, \tag{79}$$

by conjugating with the Fourier transform $\mathcal{F}$. Since $\mathcal{F}((1+z^2)^{-1})(\zeta) = \pi e^{-|\zeta|}$, (79) then becomes an integral operator with kernel

$$\frac{1}{2} B^{-1/2} \left(\frac{\zeta_j^2}{2} + \beta^2\right)^{-1/2} (\Pi^1_{\mathrm{eff}} \rho_j^{-1} e^{-\rho_j B^{-1/2} |\zeta_j - \eta_j|} \Pi^1_{\mathrm{eff}}) \left(\frac{\eta_j^2}{2} + \beta^2\right)^{-1/2}. \tag{80}$$

The norm of (80) can be estimated by its Hilbert-Schmidt norm, whose square can be bounded by

$$\frac{1}{4B} \left\| \Pi^1_{\mathrm{eff}} \frac{1}{\rho_j} \Pi^1_{\mathrm{eff}} \right\|^2 \left(\int_{\mathbb{R}} \left(\frac{\xi^2}{2} + \beta^2 \right)^{-1} \mathrm{d}\xi \right)^2 = \frac{\pi^2 C_{(81)}^2}{2\beta^2 B},$$

where we have set

$$C_{(81)} := \| \Pi^1_{\mathrm{eff}} \rho_j^{-1} \Pi^1_{\mathrm{eff}} \|. \tag{81}$$

Note that $C_{(81)}$ is independent of j, because of the permutational symmetry of $\Sigma(\mathbb{M})$. It follows that

$$R_{00,j}(-\beta^2)^{1/2} \Pi^1_{\mathrm{eff}} (\rho_j^2 + Bz_j^2)^{-1} \Pi^1_{\mathrm{eff}} R_{00,j}(-\beta^2)^{1/2} \leqslant \frac{\pi C_{(81)}}{\sqrt{2}\beta\sqrt{B}}, \tag{82}$$

and therefore

$$\begin{aligned} 0 &\leqslant R_{00}(-\alpha^2)^{1/2} \Pi^1_{\mathrm{eff}} \mathcal{V}_n(\cdot,\sqrt{B})^2 \Pi^1_{\mathrm{eff}} R_{00}(-\alpha^2)^{1/2} \leqslant \frac{\pi C_{(81)} Z^2 N}{\sqrt{2}\beta B^{1/2}} R_{00}(-\alpha^2) \sum_j (h_{00,j} + \beta^2) \\ &= \frac{\pi C_{(81)} Z^2 N}{\sqrt{2}\beta B^{1/2}} R_{00}(-\alpha^2)(h_{00} + N\beta^2) \leqslant \frac{\pi C_{(81)} Z^2 N^{3/2}}{\sqrt{2}\alpha B^{1/2}}, \end{aligned}$$

if we choose $\beta = \alpha/\sqrt{N}$. The same inequality then holds for the norm, since the operator we estimate is positive.

We next treat the interaction term $R_{00}(\alpha^2)^{1/2}\mathcal{V}_e(\cdot,\sqrt{B}z)^2R_{00}(\alpha^2)^{1/2}$ in a similar way as in the proof of Lemma 4.5. First, by Cauchy-Schwarz again,

$$\mathcal{V}_e(\cdot,\sqrt{B}z)^2 \leqslant \frac{N(N-1)}{2}\sum_{j<k}\frac{1}{\rho_{jk}^2+B(z_j-z_k)^2},$$

where we have set $\rho_{jk}^2=(x_j-x_k)^2+(y_j-y_k)^2$. Since the rotation $(r_j,r_k)\to(2^{-1/2}(r_j-r_k),2^{-1/2}(r_j+r_k))$ commutes with Π_{eff}^1 (since it commutes with H_0^1 and with $\mathbb{L}_z$), we find, after a unitary transformation, that

$$\begin{aligned}&\|R_{00,jk}(-\mu^2)^{1/2}\Pi_{\mathrm{eff}}^1(\rho_{jk}^2+B(z_j-z_k)^2)^{-1}\Pi_{\mathrm{eff}}^1R_{00,jk}(-\mu^2)^{1/2}\|\\&\quad\leqslant\left\|\frac{1}{2}R_{00,j}\left(-\frac{\mu^2}{2}\right)^{1/2}\Pi_{\mathrm{eff}}^1(\rho_j^2+Bz_j^2)^{-1}\Pi_{\mathrm{eff}}^1R_{00,j}\left(-\frac{\mu^2}{2}\right)^{1/2}\right\|\leqslant\frac{\pi C_{(81)}}{2\mu\sqrt{B}};\end{aligned}$$

compare the proof of Lemma 4.6. Hence, using similar arguments as before,

$$\begin{aligned}R_{00}(-\alpha^2)^{1/2}\Pi_{\mathrm{eff}}^1\mathcal{V}_e(\cdot,\sqrt{B})^2\Pi_{\mathrm{eff}}^1R_{00}(-\alpha^2)^{1/2}&\leqslant\frac{\pi C_{(81)}N(N-1)}{4\mu\sqrt{B}}R_{00}(-\alpha^2)\sum_{j<k}(h_{00,jk}+\mu^2)\\&\leqslant\frac{\pi C_{(81)}N(N-1)^2}{4\mu\sqrt{B}}R_{00}(-\alpha^2)\left(h_{00}+\frac{N\mu^2}{2}\right)\\&\leqslant\frac{\pi C_{(81)}N^{3/2}(N-1)^2}{4\sqrt{2}\alpha\sqrt{B}},\end{aligned}$$

if we choose $\mu=\alpha\sqrt{2/N}$. Adding this estimate to the one for $\mathcal{V}_n^2$, and remembering the factor 4 from (78), we have proved (76) with the constant $C_{(77)}=2^{3/2}\pi C_{(81)}N^{3/2}(Z^2+[(N-1)^2/4])$. *A priori*, $C_{(81)}$ might still depend on $\mathbb{M}$, but it in fact does not, as we will finally show. We compute $C_{(81)}$ in the Landau basis (28) of $F_{\mathbb{M}}^1$, with respect to which $\Pi_{\mathrm{eff}}^1\rho_1^{-1}\Pi_{\mathrm{eff}}^1$ diagonalizes,

$$C_{(81)}=\max_{0\leqslant m\leqslant\mathbb{M}}\frac{1}{2^m m!}\int_0^\infty\rho_1^{2m}e^{-\rho_1^2/2}\,\mathrm{d}\rho_1=\max_{0\leqslant m\leqslant\mathbb{M}}\frac{1}{m!\sqrt{2}}\int_0^\infty s^{m-1/2}e^{-s}\,\mathrm{d}s=\max_{0\leqslant m\leqslant\mathbb{M}}\frac{\Gamma\left(m+\frac{1}{2}\right)}{\sqrt{2}\Gamma(m+1)}.$$

It is known that

$$\Gamma\left(m+\frac{1}{2}\right)=\frac{1\times3\times5\times\cdots\times(2m-1)}{2^m}\Gamma\left(\frac{1}{2}\right),$$

cf. e.g., Ref. 1, formula 6.1.12, p. 255. Using this, one easily finds that

$$C_{(81)}=\frac{1}{\sqrt{2}}\Gamma\left(\frac{1}{2}\right)=\sqrt{\frac{\pi}{2}},$$

which completes the proof of the lemma. Q.E.D.

To prove Theorem 1.5 we will need to control the Sobolev norm of $V_1^B-v_\delta^B$. This is done in the following lemma, which we formulate in slightly greater generality than needed, with an eye to future applications.

Lemma 4.8: Let $V_1^B:=V_1^{B,\mathbb{M}}$ be defined as in (10), $c>0$ and let $\alpha_c=\alpha_c(B)$ be the unique positive solution of

$$\alpha_c=\frac{2}{c}\log\left(\frac{\sqrt{B}}{\alpha_c}\right). \tag{83}$$

Then the constant

$$C_{(84)} := \left(\pi^2 + 9\log^2(2) + \frac{64\sqrt{2}}{\pi} + \sup_{|\zeta|\leqslant 1} |\mathcal{F}V_1^1(\zeta) + 2\log(|\zeta|)|^2 + \frac{8\sqrt{2}}{\pi} \sup_{|\zeta|\geqslant 1} |\mathcal{F}V_1^1(\zeta)|^2 \right)^{1/2} \tag{84}$$

is finite and depends only on $\mathbb{M}$. *Moreover for all* $c>0$ *and all* $B>0$

$$\|R_{00}(-\alpha_c^2)^{1/2}(V_1^B - c\alpha_c(B)\delta)R_{00}(-\alpha_c^2)^{1/2}\| \leqslant \frac{C_{(84)}}{\alpha_c(B)}. \tag{85}$$

Observe that if $c=2$, then $\alpha_c(B)$ is the $\alpha(B)$ from Theorem 1.1: cf. (6). Also note that the constant $C_{(84)}$ is independent of $c>0$.

Proof: The first statement follows at once using the explicit knowledge of $\mathcal{F}V_1^1$ obtained in the proof of Lemma 4.3. To prove the estimate (85) we introduce the auxiliary function X by

$$\mathcal{F}V_1^B(\zeta) - c\alpha_c\mathcal{F}\delta(\zeta) = \mathcal{F}V_1^1\left(\frac{\zeta}{\sqrt{B}}\right) + 2\log\frac{|\zeta|}{\sqrt{B}} - 2\log\frac{|\zeta|}{\alpha_c} =: X\left(\frac{\zeta}{\sqrt{B}}\right) - 2\log\frac{|\zeta|}{\alpha_c},$$

where in the first line we used Eq. (83). The Fourier transform of $V_1^B - c\alpha_c(B)\delta$ acts as convolution by a function, and we estimate the norm of $Y := R_{00}(-\alpha_c^2)^{1/2}(V_1^B - c\alpha_c\delta)R_{00}(-\alpha_c^2)^{1/2}$ by its Hilbert-Schmidt norm, as in the proofs of Lemmas 4.1 and 4.2. It follows that

$$\|Y\|^2 \leqslant \frac{\sqrt{2}}{\pi\alpha_c}\int_{\mathbb{R}} \frac{|\mathcal{F}V_1^B(\zeta) - c\alpha_c\mathcal{F}\delta(\zeta)|^2}{8\alpha_c^2+\zeta^2}\mathrm{d}\zeta \leqslant \frac{2\sqrt{2}}{\pi\alpha_c}\int_{\mathbb{R}} \frac{\left|X\left(\frac{\zeta}{\sqrt{B}}\right)\right|^2 + \left|2\log\frac{|\zeta|}{\alpha_c}\right|^2}{8\alpha_c^2+\zeta^2}\mathrm{d}\zeta.$$

First,

$$\frac{1}{\alpha_c}\int_{\mathbb{R}} \frac{4}{8\alpha_c^2+\zeta^2}\left|\log\frac{|\zeta|}{\alpha_c}\right|^2 \mathrm{d}\zeta = \frac{\pi}{2\sqrt{2}\alpha_c^2}(\pi^2 + 9\log^2(2)).$$

We next look at the contribution of X, which we split in two parts,

$$\int_{\sqrt{B}}^{\infty} \frac{\left|X\left(\frac{\zeta}{\sqrt{B}}\right)\right|^2 \mathrm{d}\zeta}{8\alpha_c^2+\zeta^2} = \frac{1}{\sqrt{B}}\int_1^{\infty} \frac{|X(\zeta)|^2\,\mathrm{d}\zeta}{8B^{-1}\alpha_c^2+\zeta^2} \leqslant \frac{2}{\sqrt{B}}\int_1^{\infty} \frac{|\mathcal{F}V(\zeta)|^2 + 4(\log|\zeta|)^2}{\zeta^2}\mathrm{d}\zeta$$

$$\leqslant \frac{2}{\sqrt{B}}\left(\sup_{|\zeta|\geqslant 1}|\mathcal{F}V(\zeta)|^2 + 8\right),$$

since

$$\int_1^{\infty} \frac{(\log|\zeta|)^2}{|\zeta|^2}\mathrm{d}\zeta = 2$$

and

$$\int_0^{\sqrt{B}} \frac{\left|X\left(\frac{\zeta}{\sqrt{B}}\right)\right|^2 \mathrm{d}\zeta}{8\alpha_c^2+\zeta^2} \leqslant \sup_{|\zeta|\leqslant 1}|X(\zeta)|^2 \int_0^{\sqrt{B}} \frac{\mathrm{d}\zeta}{8\alpha_c^2+\zeta^2} \leqslant \frac{\pi}{4\sqrt{2}\alpha_c}\sup_{|\zeta|\leqslant 1}|X(\zeta)|^2.$$

The rest is now elementary. Notice in particular that $\sup_{B>0}\alpha_c(B)/\sqrt{B}=1$. Q.E.D.

The limit potential (70) suggests defining an effective Hamiltonian $h_C = h_C^B$ by

$$h_C := h_{00} + v_C. \tag{86}$$

As it stands, this is just a formal expression, and our first task is to give a meaning to h_C as a self-adjoint operator on $L^2(\mathbb{R}^N; F^1_{\mathbb{M}})$. We do this by showing that v_C is form-bounded with respect h_{00}, with zero relative form-bound. Let $\langle \cdot, \cdot \rangle$ denote the duality between distributions and test functions.

Lemma 4.9: The quadratic forms $u \to \langle \delta, |u|^2 \rangle = |u(0)|^2$ *and* $u \to \langle \mathrm{Pf}(1/|z|), |u|^2 \rangle$ *are well defined on* $H^1(\mathbb{R})$, *and form-bounded with respect to* h_{00}, *with relative bound zero. More precisely, we have for all* $\varepsilon > 0$ *that*

$$\delta \leqslant \tfrac{1}{2}(-\varepsilon\Delta_z + \varepsilon^{-1}), \tag{87}$$

and

$$\mathrm{Pf}(|z|^{-1}) \leqslant C_{(89)}(|\log \varepsilon| + 1)(-\varepsilon\Delta_z + \varepsilon^{-1}), \tag{88}$$

where

$$C_{(89)} := \sqrt{\frac{\pi^2}{2} + 2(\log 2)^2} + \gamma. \tag{89}$$

Proof: This is well known for δ. For $\mathrm{Pf}(|z|^{-1})$ we first note that, since $\mathrm{Pf}(|z|^{-1}) = -2\mathcal{F}^{-1}(\log|\zeta|) - 2\gamma\delta_0$, it suffices to prove the form-boundedness of $\mathcal{F}^{-1}(\log|\zeta|)$. The latter will follow from

$$\|(-\varepsilon\Delta + \varepsilon^{-1})^{-1/2}\mathcal{F}^{-1}(\log|\zeta|)(-\varepsilon\Delta + \varepsilon^{-1})^{-1/2}\|^2 \leqslant \frac{1}{2}(\log \varepsilon)^2 + \frac{\pi^2 + 4(\log 2)^2}{8}, \tag{90}$$

for all $\varepsilon > 0$. To prove (90), observe that after conjugation by the Fourier transform $\mathcal{F}$, and estimating the operator norm by the Hilbert-Schmidt norm, the square of (90) can be bounded by

$$\frac{1}{(2\pi)^2}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{(\log|\zeta - \eta|)^2}{(\varepsilon\zeta^2 + \varepsilon^{-1})(\varepsilon\eta^2 + \varepsilon^{-1})} \mathrm{d}\zeta\, \mathrm{d}\eta. \tag{91}$$

Changing variables and using (59), we find that (91) can be bounded by

$$\frac{1}{2\pi}\int_{\mathbb{R}} \frac{(\log|\zeta|)^2}{\varepsilon\zeta^2 + 4\varepsilon^{-1}} d\zeta = \frac{1}{2\pi}\int_{\mathbb{R}} \frac{(\log|\zeta/\varepsilon|)^2}{\zeta^2 + 4} \mathrm{d}\zeta \leqslant \frac{1}{\pi}(\log \varepsilon)^2 \int_{\mathbb{R}} \frac{\mathrm{d}\zeta}{\zeta^2 + 4} + \frac{1}{\pi}\int_{\mathbb{R}} \frac{(\log \zeta)^2}{\zeta^2 + 4} \mathrm{d}\zeta$$
$$= \frac{1}{2}(\log \varepsilon)^2 + \frac{\pi^2 + 4(\log 2)^2}{8}.$$

Hence, using (87),

$$|\langle \mathrm{Pf}(|x|^{-1}), |u|^2 \rangle| = 2 \cdot |\langle \mathcal{F}^{-1}(\log|\xi|), |u|^2 \rangle + \gamma \langle \delta, |u|^2 \rangle| \leqslant \left\{ \left(2(\log \varepsilon)^2 + \frac{\pi^2}{2} + 2(\log 2)^2 \right)^{1/2} + \gamma \right\}$$
$$\times \{-\varepsilon(\Delta u, u) + \varepsilon^{-1}\|u\|^2\} = (\sqrt{2}|\log \varepsilon| + C_{(89)})\{-\varepsilon(\Delta u, u) + \varepsilon^{-1}\|u\|^2\},$$

which implies (88) since $\sqrt{2}/C_{(89)} < 1$. Q.E.D.

Because of the terms $C^n_j \delta(z_j)$ and $C^e_{jk}\delta(z_j - z_k)$ we must extend the first part of Lemma 4.9 to the vector-valued case, but this is immediate: we just note that if C a linear operator on $F^1_{\mathbb{M}}$ (or any finite-dimensional vector space, for that matter), then the right interpretation of $C\delta$ as quadratic form on $H^1(\mathbb{R}, F^1_{\mathbb{M}})$ is given by $\langle \delta(z), (Cu(z), u(z)) \rangle$, where $(\cdot, \cdot)$ is the inner product on $F^1_{\mathbb{M}}$.

Finally, we lift Lemma 4.9 to $\mathbb{R}^N$. Recall that if $L: \mathbb{R}^N \to \mathbb{R}$ is a linear map, then the pull-back $L^*\Lambda$ of a distribution Λ on $\mathbb{R}$ is well defined, and can be computed by going to linear coordinates

z' with respect to which $L(z')=z'_1$. It then immediately follows from Lemma 4.9 that $L^*\delta$ and L^*q^B will be form-bounded with respect to h_{00} on $\mathbb{R}^N$, with relative bound 0. Taking $L(z)=L_j(z)=z_j$ and $L(z)=L_{jk}(z)=z_j-z_k$, we see that the sequilinear form $t_C^B(u)$ given by

$$t_C^B(u)=\frac{1}{2}\|\nabla u\|^2-Z\sum_j\langle L_j^*q^B,|u|^2\rangle+\langle(L_j^*\delta,(C_j^nu,u)\ \rangle+\sum_{j<k}\langle L_{jk}^*q^B,|u|^2\rangle+\langle L_{jk}^*\delta,(C_{jk}^eu,u)\rangle, \tag{92}$$

is well defined on $H^1(\mathbb{R}^N,F_{\mathbb{M}}^1)$, and bounded from below by $-C\|u\|^2$, for some constant C, depending on B, Z, N, and $\mathbb{M}$. By the Kato-Lax-Lions-Milgram-Nelson theorem (cf., e.g., Ref. 15, Theorem X.17), t_C^B defines a unique self-adjoint operator, which we will call $h_C=h_C^{B,\mathbb{M}}$, and informally write as (86). In the Appendix we will give a characterization of the operator domain of h_C^B. Similar arguments will define h_δ^B as a self-adjoint operator, cf. Ref. 6.

V. PROOF OF THEOREM 1.1

We will first compare the resolvents of $h_{\text{eff}}:=h_{\text{eff}}^{B,\mathbb{M}}$ and of $h_{\text{eff}}+\mathcal{W}$, where $\mathcal{W}:=\mathcal{W}^{B,\mathbb{M}}(\xi)$ was defined at the beginning of Sec. III. Set

$$r_{\text{eff}}:=r_{\text{eff}}(\xi):=(h_{\text{eff}}-\xi)^{-1},\quad R_{\text{eff}}^{\mathcal{W}}:=R_{\text{eff}}^{\mathcal{W}}(\xi):=(h_{\text{eff}}+\mathcal{W}-\xi)^{-1},$$

and let

$$B_{(93)}:=\frac{4C_{(77)}^2}{\alpha(C_{(77)})^2}, \tag{93}$$

where $\alpha=\alpha(B)$ is the function defined by (6), and

$$c_{\text{eff}}:=2\left(\frac{N}{2\varepsilon_{\text{eff}}^2}+1\right)C_{(77)}, \tag{94}$$

with $\varepsilon_{\text{eff}}=\varepsilon_{\text{eff}}(Z,\mathbb{M})$ the unique positive solution of

$$ZC_{(60)}C_{V_1^1}\varepsilon(|\log\varepsilon|+2)=\tfrac{1}{4}, \tag{95}$$

where $C_{V_1^1}$ is defined by (61) with $\mathfrak{v}=V_1^1$ [see (69) for an upper bound]. Note that both constants only depend on N, Z, and $\mathbb{M}$, and this in a controlled way.

We then have the following.

Theorem 5.1: *If* $B\geqslant B_{(93)}$, $\xi\leqslant 0$ *and*

$$c_{\text{eff}}\frac{\alpha}{\sqrt{B}}\leqslant d_{\text{eff}}(\xi)\leqslant\frac{1}{2}\alpha^2, \tag{96}$$

with $\alpha=\alpha(B)$ *is as in Theorem 1.1, then* $\xi\in\rho(h_{\text{eff}}+\mathcal{W})$, *and* $\|R_{\text{eff}}^{\mathcal{W}}(\xi)\|\leqslant 2\|r_{\text{eff}}(\xi)\|$. *Furthermore*,

$$\|R_{\text{eff}}^{\mathcal{W}}(\xi)-r_{\text{eff}}(\xi)\|\leqslant c_{\text{eff}}\frac{\alpha}{d_{\text{eff}}(\xi)^2\sqrt{B}}. \tag{97}$$

Proof of Theorem 5.1: It clearly suffices to establish Theorem 5.1 after conjugation by U_{xy}^B, defined by (46). To simplify notations, we will simply denote the conjugated operators by the same letters as the original ones. Using the symmetrized resolvent formula we estimate

$$\|R_{\text{eff}}^{\mathcal{W}}(\xi)-r_{\text{eff}}(\xi)\|\leqslant\frac{1}{d_{\text{eff}}(\xi)}\left(\frac{\|K_{\text{eff}}(\xi)\|}{1-\|K_{\text{eff}}(\xi)\|}\right), \tag{98}$$

where

$$K_{\mathrm{eff}}(\xi) := |r_{\mathrm{eff}}(\xi)|^{1/2}\mathcal{W}(\xi)r_{\mathrm{eff}}(\xi)^{1/2}, \tag{99}$$

with the convention that $A^{1/2} := \mathrm{sgn}(A)|A|^{1/2}$, if A is a self-adjoint operator. [Note that since ξ is not necessarily below the infimum of the spectrum, $r_{\mathrm{eff}}(\xi)$ is not necessarily positive, and we use the symmetrized resolvent formula in the following form: $R^{\mathcal{W}}_{\mathrm{eff}} = r^{1/2}_{\mathrm{eff}}(1+|r_{\mathrm{eff}}|^{1/2}\mathcal{W}r^{1/2}_{\mathrm{eff}})^{-1}|r_{\mathrm{eff}}|^{1/2}$.] Now let $\mu < \inf\sigma(h_{\mathrm{eff}})$, to be specified later. The following elementary lemma will allow us to replace ξ by μ in (99).

Lemma 5.2: If $\mu < \inf\sigma(h_{\mathrm{eff}})$, then for all real ξ in the resolvent set $\rho(h_{\mathrm{eff}})$,

$$\|r_{\mathrm{eff}}(\xi)(h_{\mathrm{eff}}-\mu)\| \leqslant \max\left(\frac{|\mu|}{d_{\mathrm{eff}}(\xi)}, 1\right). \tag{100}$$

Proof: We distinguish two cases: $\inf\sigma(h_{\mathrm{eff}}) < \xi < 0$ and $\xi < \inf\sigma(h_{\mathrm{eff}})$. [Observe that $\inf\sigma(h_{\mathrm{eff}}) < 0$, by the HVZ theorem, since this is already the case for $N=1$.] In the first case, let (ξ_-, ξ_+) be the largest open interval in $\rho(h_{\mathrm{eff}})$ which contains ξ. Since $[0,\infty)$ is in the spectrum (it is already in the essential spectrum), $\xi_+ \leqslant 0$. It is easy to see that the function $x \to |x-\mu|/|x-\xi|$ is increasing on $(-\infty, \xi_-) \cap \sigma(h_{\mathrm{eff}})$ and decreasing on $(\xi_+, \infty) \cap \sigma(h_{\mathrm{eff}})$. It follows that

$$\|r_{\mathrm{eff}}(\xi)(h_{\mathrm{eff}}-\mu)\| \sup_{x\in\sigma(h_{\mathrm{eff}})} \frac{|x-\mu|}{|x-\xi|} = \max\left(\frac{|\xi_- - \mu|}{|\xi_- - \xi|}, \frac{|\xi_+ - \mu|}{|\xi_+ - \xi|}\right) \leqslant \frac{|\mu|}{d_{\mathrm{eff}}(\xi)},$$

as was to be shown. One shows in a similarly way that (100) equals $[\inf\sigma(h_{\mathrm{eff}}) - \mu]/(\inf\sigma(h_{\mathrm{eff}}) - \xi) \leqslant |\mu|/d_{\mathrm{eff}}(\xi)$, if $\mu < \xi < \inf\sigma(h_{\mathrm{eff}})$, and is equal to 1 if $\xi < \mu$. Q.E.D.

Substituting $\mathrm{Id} = r_{\mathrm{eff}}(\mu)^{1/2}(h_{\mathrm{eff}}-\mu)^{1/2} = (h_{\mathrm{eff}}-\mu)^{1/2}r_{\mathrm{eff}}(\mu)^{1/2}$ at the appropriate places in formula (99), we see that if $\xi \leqslant 0$,

$$\|K_{\mathrm{eff}}(\xi)\| \leqslant \max\left(\frac{|\mu|}{d_{\mathrm{eff}}(\xi)}, 1\right)\|K_{\mathrm{eff}}(\mu;\xi)\|, \tag{101}$$

with

$$K_{\mathrm{eff}}(\mu;\xi) := r_{\mathrm{eff}}(\mu)^{1/2}\mathcal{W}(\xi)r_{\mathrm{eff}}(\mu)^{1/2}.$$

Repeating the same argument for $K_{\mathrm{eff}}(\mu;\xi)$ using $\mathrm{Id} = (h_{00}+\alpha^2)^{1/2}R_{00}(-\alpha^2)^{1/2}$, we obtain from Lemma 4.7 that

$$\|K_{\mathrm{eff}}(\mu;\xi)\| \leqslant \frac{C_{(77)}}{\alpha\sqrt{B}}\|r_{\mathrm{eff}}(\mu)^{1/2}(h_{00}+\alpha^2)^{1/2}\|^2. \tag{102}$$

We will now estimate the norm on the right-hand side, for suitably chosen μ.

Lemma 5.3: Assume $B \geqslant e^2$. Define

$$\mu_{\mathrm{eff}} = \mu_{\mathrm{eff}}(N,Z,\mathbb{M}) := -\frac{\alpha^2}{2}\left(\frac{N}{2\varepsilon^2_{\mathrm{eff}}} + 1\right), \tag{103}$$

where α is as in Theorem 1.1, and where $\varepsilon = \varepsilon_{\mathrm{eff}}$ is the unique positive solution to the equation (95). Then $\mu_{\mathrm{eff}} < \inf\sigma(h_{\mathrm{eff}})$, and

$$\|r_{\mathrm{eff}}(\mu_{\mathrm{eff}})^{1/2}(h_{00}+\alpha^2)^{1/2}\| \leqslant \sqrt{2}. \tag{104}$$

Assuming the lemma for the moment, we continue with the proof of Theorem 5.1: we have, by (101), (102), and (104), that if $d_{\mathrm{eff}}(\xi) \geqslant c_{\#}\alpha/\sqrt{B}$, then

$$\|K_{\mathrm{eff}}(\xi)\| \leqslant 2\max\left\{\frac{\alpha^2}{2}\left(\frac{N}{2\varepsilon^2_{\mathrm{eff}}}+1\right)\frac{1}{d_{\mathrm{eff}}(\xi)}, 1\right\}\frac{C_{(77)}}{\alpha\sqrt{B}} \leqslant \frac{1}{2},$$

provided that $c_{\#}$ satisfies

$$c_{\#} \geqslant 2\left(\frac{N}{2\varepsilon_{\text{eff}}^2}+1\right)C_{(77)} \quad \text{and} \quad \frac{C_{(77)}}{\alpha\sqrt{B}} \leqslant \frac{1}{4}.$$

Since $\alpha(B)\sqrt{B}$ is increasing, and since $\alpha(B)\sqrt{B}=x$ iff $B=x^2/(4\alpha(x/4)^2)$, the last inequality is implied by $B \geqslant B_{(93)}$. Choosing $c_{\#}=c_{\text{eff}}$ defined by (94), we conclude that if ξ is such that $d_{\text{eff}}(\xi) \geqslant c_{\text{eff}}\alpha/\sqrt{B}$, then by (98), (101) and (102) and our choice of $\mu=\mu_{\text{eff}}$,

$$\|R_{\text{eff}}^{\mathcal{W}} - r_{\text{eff}}(\xi)\| \leqslant \frac{4}{d_{\text{eff}}(\xi)} \max\left\{\frac{\alpha^2}{2}\left(\frac{N^2}{2\varepsilon_{\text{eff}}}+1\right)\frac{1}{d_{\text{eff}}(\xi)}, 1\right\}\frac{C_{(77)}}{\alpha\sqrt{B}} \leqslant 2C_{(77)}\left(\frac{N}{2\varepsilon_{\text{eff}}^2}+1\right)\frac{\alpha}{d_{\text{eff}}(\xi)^2\sqrt{B}},$$

provided that $d_{\text{eff}}(\xi) \leqslant \alpha^2/2$. This proves Theorem 5.1, modulo that of Lemma 5.3. Q.E.D.

Proof of Lemma 5.3: We will use a scaling argument. If we let $\simeq$ denote the unitary equivalence induced by the change of variables $z \to z/\alpha$, where $\alpha>0$ is for the moment a free parameter, and if we write $\mathcal{V}_{\text{eff}}^{B}$ for $\sqrt{B}\mathcal{V}_{\text{eff}}^{1}(\sqrt{B}\cdot)$, then if $\mu < \inf\sigma(h_{\text{eff}})$,

$$\begin{aligned} 0 &\leqslant (h_{00}+\alpha^2)^{1/2} r_{\text{eff}}(\mu)(h_{00}+\alpha^2)^{1/2} \simeq (h_{00}+1)^{1/2}\left(-\frac{1}{2}\Delta_z + \alpha^{-2}\mathcal{V}_{\text{eff}}^{B}\left(\frac{\cdot}{\alpha}\right) - \alpha^{-2}\mu\right)^{-1}(h_{00}+1)^{1/2} \\ &\leqslant (h_{00}+1)^{1/2}\left(-\frac{1}{2}\Delta_z + \alpha^{-2}\mathcal{V}_{\text{eff},n}^{B}\left(\frac{\cdot}{\alpha}\right) - \alpha^{-2}\mu\right)^{-1}(h_{00}+1)^{1/2}, \end{aligned} \tag{105}$$

$\mathcal{V}_{\text{eff},n}^{1}$ being the attractive part of $\mathcal{V}_{\text{eff}}$. We now choose $\alpha=\log(\sqrt{B}/\alpha)$, as in (6), and set $\lambda := \sqrt{B}/\alpha$. Notice that $B \geqslant e^2$ implies that $\lambda \geqslant e$. Then, by Lemma 4.2,

$$\begin{aligned} \frac{\sqrt{B}}{\alpha^2}\mathcal{V}_{\text{eff},n}^{1}\left(\frac{\sqrt{B}}{\alpha}z\right) &= -Z\sum_{j=1}^{N}\frac{\lambda}{\log\lambda}V_j^1(\lambda z_j) \geqslant -2C_{(60)}ZC_{V_1^1}\varepsilon(|\log\varepsilon|+2)\left(-\frac{1}{2}\Delta_z + \frac{N}{2\varepsilon^2}\right), \quad \varepsilon>0 \\ &= -\frac{1}{2}h_{00} - \frac{N}{4\varepsilon_{\text{eff}}^2}, \end{aligned}$$

uniformly in λ, if we choose $\varepsilon := \varepsilon_{\text{eff}} = \varepsilon_{\text{eff}}(Z,\mathbb{M})$ such that (95) holds. We now take

$$\mu = \mu_{\text{eff}} = -\frac{\alpha^2}{2}\left(\frac{N}{2\varepsilon_{\text{eff}}^2}+1\right).$$

Then it follows that $\mu_{\text{eff}} < \inf\sigma(h_{\text{eff}})$, since $h_{\text{eff}} - \mu_{\text{eff}} \geqslant \frac{1}{2}(h_{00}+1) \geqslant \frac{1}{2}$. Furthermore, (105) can be estimated by

$$(h_{00}+1)^{1/2}\left(\frac{1}{2}h_{00} - \left(\frac{N}{4\varepsilon_{\text{eff}}^2} + \frac{\mu_{\text{eff}}}{\alpha^2}\right)\right)^{-1}(h_{00}+1)^{1/2} = 2,$$

which implies (104).

Proof of Theorem 1.1: It now suffices to combine Theorem 3.1 and Theorem 5.1, while carefully keeping track of the constants. First of all, (96), implies that $\|R_{\text{eff}}^{\mathcal{W}}\| \leqslant 2\|r_{\text{eff}}(\xi)\|$, and therefore $d_{\text{eff}}^{\mathcal{W}}(\xi) \geqslant d_{\text{eff}}(\xi)/2$. Furthermore, $\xi<0$ if $d_{\text{eff}}(\xi)>0$, and if

$$B \geqslant B_{\text{eff}} := \max\{B_{(36)}, B_{(93)}, e^2\}, \tag{106}$$

then

$$\begin{aligned}\|(H-\xi)^{-1}-(h_{\mathrm{eff}}-\xi)^{-1}\oplus(H_\perp-\xi)^{-1}\| &\leqslant \|(H-\xi)^{-1}-R^{\mathcal{W}}_{\mathrm{eff}}(\xi)\oplus(H_\perp-\xi)^{-1}\|+\|R^{\mathcal{W}}_{\mathrm{eff}}(\xi)-r_{\mathrm{eff}}(\xi)\| \\ &\leqslant \frac{C_{(37)}}{\sqrt{B}}\frac{1}{d^{\mathcal{W}}_{\mathrm{eff}}(\xi)}+c_{\mathrm{eff}}\frac{\alpha}{d_{\mathrm{eff}}(\xi)^2\sqrt{B}}\leqslant\left(2C_{(37)}+c_{\mathrm{eff}}\frac{\alpha}{d_{\mathrm{eff}}(\xi)}\right) \\ &\quad\times\frac{1}{d_{\mathrm{eff}}(\xi)\sqrt{B}}\ [\text{using } d_{\mathrm{eff}}(\xi)/2\leqslant d^{\mathcal{W}}_{\mathrm{eff}}(\xi)] \\ &\leqslant\left(C_{(37)}+\frac{c_{\mathrm{eff}}}{\alpha}\right)\frac{\alpha^2}{d_{\mathrm{eff}}(\xi)^2\sqrt{B}}\ [\text{using } d_{\mathrm{eff}}(\xi)\leqslant\alpha^2/2 \text{ again}] \\ &\leqslant\left(C_{(37)}+\frac{c_{\mathrm{eff}}}{\alpha(B_{\mathrm{eff}})}\right)\frac{\alpha^2}{d_{\mathrm{eff}}(\xi)^2\sqrt{B}},\end{aligned}$$

since $\alpha(B)^{-1}$ is a decreasing function of B. This proves Theorem 1.1 with a constant C_{eff} which is equal to

$$C_{\mathrm{eff}}:=C_{(37)}+\frac{c_{\mathrm{eff}}}{\alpha(B_{\mathrm{eff}})}.$$

Q.E.D.

VI. PROOF OF THEOREM 1.3

As a first step, we will compare the resolvents $r_{\mathrm{eff}}(\xi)$ of h_{eff} and $r_C(\xi):=(h_C-\xi)^{-1}$ of $h_C:=h_C^B$. Recall, that $d_C(\xi):=\mathrm{dist}(\xi,\sigma(h_C))$.

Theorem 6.1: *Let $\alpha=\alpha(B)$ be defined by (6). There exist (computable) constants $B'_C, C'_C\geqslant 0$, only depending on Z, N, and $\mathbb{M}$, such that for all $B\geqslant B'_C$ and all real $\xi\leqslant 0$ satisfying*

$$d_C(\xi)\geqslant C'_C\alpha^{3/2}B^{-1/4}, \tag{107}$$

then $\xi\in\rho(H_{\mathrm{eff}})$, with $\|r_{\mathrm{eff}}(\xi)\|\leqslant 2\|r_C(\xi)\|$. In addition, letting [with $\varepsilon_{\mathrm{eff}}$ defined in (95)]

$$C''_C=\max\left\{C'_C,4C_{(72)}\left(\frac{N}{2\varepsilon^2_{\mathrm{eff}}}+1\right)\right\}\geqslant C'_C,$$

then if

$$d_C(\xi)\geqslant C''_C\alpha^{3/2}B^{-1/4}, \tag{108}$$

we also have that $\|r_C(\xi)\|\leqslant 2\|r_{\mathrm{eff}}(\xi)\|$.

Finally, if

$$C'_C\alpha^{3/2}B^{-1/4}\leqslant d_C(\xi)\leqslant\tfrac{1}{2}\alpha^2, \tag{109}$$

then

$$\|r_{\mathrm{eff}}(\xi)-r_C(\xi)\|\leqslant C'_C\frac{\alpha^{3/2}}{d_C(\xi)^2B^{1/4}}. \tag{110}$$

Proof: The proof is similar to the proof of Theorem 5.1, with however some technical changes, due to the fact that v_C is not homogeneous of degree -1, and that its electron-electron part is not positive anymore. As before, we conjugate all operators by U^B_{xy}, keeping the same letters for the conjugated operators.

Arguing as in the proof of Theorem 5.1, one shows that

$$\|r_{\text{eff}}(\xi) - r_C(\xi)\| \leqslant \frac{1}{d_C(\xi)} \frac{\|K_C(\xi)\|}{1 - \|K_C(\xi)\|},$$

where $K_C := |r_C(\xi)|^{1/2}(h_{\text{eff}} - h_C) r_C(\xi)^{1/2}$. Using Lemma 4.5, we find that, for any $\mu < \inf \sigma(h_C)$,

$$\|K_C(\xi)\| \leqslant \frac{C_{(72)}}{B^{1/4}\sqrt{\alpha}} \max\left\{ \frac{|\mu|}{d_C(\xi)}, 1 \right\} \|r_C(\mu)^{1/2}(h_{00} + \alpha^2)^{1/2}\|^2. \tag{111}$$

We then use the following analogue of Lemma 5.3, of which we only state a qualitative version.

Lemma 6.2: There exists a constant $\nu_C = \nu_C(Z,N,\mathbb{M}) \geqslant 1/2$ *such that if* $B \geqslant e$, *and if* $\mu_C := -\nu_C \alpha^2$, α *defined by (6), then* $\mu_C < \inf \sigma(h_C)$, *and*

$$\|r_C(\mu_C)^{1/2}(h_{00} + \alpha^2)^{1/2}\|^2 \leqslant 2. \tag{112}$$

Proof: As before, we will use scaling. However, contrary to $\delta(z)$, the distribution $\text{Pf}(1/|z|)$ is not homogeneous of degree -1 on $\mathbb{R}$. In fact, if ρ_α is the dilation $\rho_\alpha(z) = \alpha^{-1} z$ on $\mathbb{R}$, $\alpha > 0$ arbitrary, then the pullback of $\text{Pf}\,(1/|\cdot|)$ by ρ_α equals

$$\rho_\alpha^* \text{Pf}\left(\frac{1}{|\cdot|}\right) = \alpha \text{Pf}\left(\frac{1}{|\cdot|}\right) - 2\alpha \log \alpha \delta. \tag{113}$$

Let us split the potential $v_C := v_C^B$ of h_C as

$$v_C = \log B v_\delta + v_Q,$$

where v_δ is defined in (17) and

$$v_Q = -Z \sum_j \left(\text{Pf} \frac{1}{|z_j|} + C_j^n \delta(z_j) \right) + \sum_{j<k} \left(\text{Pf} \frac{1}{|z_j - z_k|} + C_{jk}^e \delta(z_j - z_k) \right),$$

the (pseudo-) Coulombic part. If $\simeq$ denotes unitary equivalence with respect to the dilation ρ_α (on $\mathbb{R}^N$), then in view of our choice of α

$$\begin{aligned} h_C - \mu &\simeq \alpha^2 \left(h_{00} + \frac{\log B - 2 \log \alpha}{\alpha} v_\delta + \frac{1}{\alpha} v_Q - \alpha^{-2} \mu \right) = \alpha^2 \left(h_{00} + 2 v_\delta + \frac{1}{\alpha} v_Q - \alpha^{-2} \mu \right) \\ &\geqslant \alpha^2 \left(\frac{1}{2} h_{00} - b - \alpha^{-2} \mu \right) \end{aligned}$$

form some $b > 0$ depending only on Z, N, and $\mathbb{M}$, since by Lemma 4.9 we know that $2v_\delta + (1/\alpha) v_Q$ is h_{00} form bounded with relative bound 0. Recall that $B \geqslant e$ implies $\alpha \geqslant 1$. Choosing $\mu = \mu_C := -\alpha^2(\frac{1}{2} + b) =: -\alpha^2 \nu_c$ will insure that $(h_{00} + \alpha^2) r_C(\mu)(h_{00} + \alpha^2)^{1/2} \leqslant 2$ which is what we want to prove. A more careful argument, which we will skip, will yield an explicit b. Q.E.D.

We continue with the proof of Theorem 6.1. By (112) and (111) with $\mu = \mu_C$, we find that

$$\|K_C(\xi)\| \leqslant \frac{2C_{(72)}}{B^{1/4}\sqrt{\alpha}} \max\left\{ \frac{\nu_C \alpha^2}{d_C(\xi)}, 1 \right\} \leqslant \frac{1}{2},$$

if both

$$d_C(\xi) \geqslant 4 C_{(72)} \nu_C \frac{\alpha^{3/2}}{B^{1/4}} =: C'_C \frac{\alpha^{3/2}}{B^{1/4}},$$

and $\alpha^{1/2} B^{1/4} \geqslant 4 C_{(72)}$ which, since $B \mapsto \alpha(B)^2 B$ is increasing, is equivalent to $B \geqslant 4^3 C_{(72)}^4 \alpha (4 C_{(72)}^2)^{-2}$. Since we also need $B \geqslant e$ we set

$$B'_C := \max\left\{\frac{4^3 C_{(72)}^4}{4\alpha(C_{(72)}^2)^2}, e\right\}.$$

This fixes our constants C'_C and B'_C, and also implies that $\|r_{\text{eff}}(\xi)\| \leqslant 2\|r_C(\xi)\|$, by the resolvent formula.

To show that (108) implies that $\|r_C(\xi)\| \leqslant 2\|r_{\text{eff}}(\xi)\|$, we repeat the argument with r_C and r_{eff} interchanged: by the resolvent formula,

$$r_C(\xi) = r_{\text{eff}}(\xi)^{1/2}(1 + \widetilde{K}_C(\xi))^{-1}|r_{\text{eff}}(\xi)|^{1/2},$$

with

$$\widetilde{K}_C(\xi) := |r_{\text{eff}}(\xi)|^{1/2}(h_C - h_{\text{eff}})r_{\text{eff}}(\xi)^{1/2},$$

so that, using Lemmas 4.5, 5.2, and 5.3, we arrive at

$$\|\widetilde{K}_C(\xi)\| \leqslant \frac{2C_{(72)}}{B^{1/4}\sqrt{\alpha}} \max\left\{\frac{|\mu_{\text{eff}}|}{d_{\text{eff}}(\xi)}, 1\right\} \leqslant \frac{2C_{(72)}}{B^{1/4}\sqrt{\alpha}} \max\left\{\frac{2|\mu_{\text{eff}}|}{d_C(\xi)}, 1\right\},$$

if $d_C(\xi) \geqslant C'_C\alpha^{3/2}B^{-1/4}$, by the first part. We therefore conclude that $\|\widetilde{K}_C(\xi)\| \leqslant 1/2$, and hence $\|r_C(\xi)\| \leqslant 2\|r_{\text{eff}}(\xi)\|$, if both $\sqrt{\alpha}B^{1/4} \geqslant 4C_{(72)}$, which will be satisfied if $B \geqslant B'_C$ defined above, and if

$$\frac{4|\mu_{\text{eff}}|C_{(72)}}{\sqrt{\alpha}B^{1/4}d_C(\xi)} \leqslant \frac{1}{2}.$$

The latter inequality is equivalent to

$$d_C(\xi) \geqslant 4\left(\frac{N}{2\varepsilon_{\text{eff}}^2} + 1\right)C_{(72)}\frac{\alpha^{3/2}}{B^{1/4}},$$

which yields condition (108).

Finally, if ξ satisfies (109), then

$$\|r_{\text{eff}}(\xi) - r_C(\xi)\| \leqslant \frac{4C_{(72)}}{\alpha^{1/2}B^{1/4}d_C(\xi)} \max\left\{\frac{\nu_C\alpha^2}{d_C(\xi)}, 1\right\} \leqslant 4\nu_C C_{(72)}\frac{\alpha^{3/2}}{d_C(\xi)^2B^{1/4}} = C'_C\frac{\alpha^{3/2}}{d_C(\xi)^2B^{1/4}},$$

where we used that $d_C(\xi) \leqslant \alpha^2/2 \leqslant \nu_C\alpha^2$. This finishes the proof of Theorem 6.1. Q.E.D.

Proof of Theorem 1.3: We define

$$B_C := \max\{B_{\text{eff}}, B'_C\} \tag{114}$$

and

$$c_C := \max\{C''_c, 2c_{\text{eff}}\alpha(B_C)^{-1/2}B_C^{-1/4}\}. \tag{115}$$

Suppose that $B \geqslant B_C$, and that

$$c_C\alpha^{3/2}B^{-1/4} \leqslant d_C(\xi) \leqslant \tfrac{1}{4}\alpha^2.$$

By Theorem 6.1, $d_{\text{eff}}(\xi) \leqslant 2d_C(\xi) \leqslant \alpha^2/2$. By the same theorem, and by (115),

$$d_{\text{eff}}(\xi) \geqslant \tfrac{1}{2}d_C(\xi) \geqslant c_{\text{eff}}\alpha(B_C)^{-1/2}B_C^{-1/4}\alpha^{3/2}B^{-1/4} \geqslant c_{\text{eff}}\alpha(B)B^{-1/2},$$

since $\alpha(B)/\sqrt{B}$ is a decreasing function of $B > 0$. The conditions of Theorem 1.1 are therefore met. Since the condition (109) of Theorem 6.1 is clearly also satisfied, we conclude that the difference of the resolvents (15) can be estimated by

$$C_{\text{eff}}\frac{\alpha^2}{d_{\text{eff}}(\xi)^2\sqrt{B}}+C'_C\frac{\alpha^{3/2}}{d_C(\xi)^2B^{1/4}}\leqslant C_c\frac{\alpha^{3/2}}{d_C(\xi)^2B^{1/4}},$$

for $B\geqslant B_C$, with

$$C_C:=4C_{\text{eff}}\frac{\sqrt{\alpha(B_C)}}{B_C^{1/4}}+C'_C, \tag{116}$$

where we used that $\alpha(B)/\sqrt{B}$ is decreasing. Q.E.D.

VII. PROOF OF THEOREM 1.5

This will be done by closely following the strategy of Sec. VI. First, we compare the resolvents $r_{\text{eff}}(\xi)$ of h_{eff} and $r_\delta(\xi):=(h_\delta-\xi)^{-1}$ of $h_\delta:=h_\delta^{B,\mathbb{M}}$. Recall, that $d_\delta(\xi):=\text{dist}(\xi,\sigma(h_\delta))$.

Theorem 7.1: *Let $\alpha=\alpha(B)$ be defined by (6). There exist (computable) constants B'_δ, $C'_\delta\geqslant 0$, only depending on Z, N, and $\mathbb{M}$, such that for all $B\geqslant B'_\delta$ and all real ξ satisfying*

$$d_\delta(\xi)\geqslant C'_\delta\alpha, \tag{117}$$

we have that $\xi\in\rho(h_{\text{eff}})$, with $\|r_{\text{eff}}(\xi)\|\leqslant 2\|r_\delta(\xi)\|$. In addition, letting

$$C''_\delta=\max\left\{C'_\delta,4C_{(118)}\left(\frac{N}{2\varepsilon_{\text{eff}}^2}+1\right)\right\}\quad\text{with } C_{(118)}:=\left(NZ+\frac{N(N-1)}{2}\right)C_{(84)}, \tag{118}$$

and ε_{eff} given by (95), then if

$$d_\delta(\xi)\geqslant C''_\delta\alpha, \tag{119}$$

we also have that $\|r_\delta(\xi)\|\leqslant 2\|r_{\text{eff}}(\xi)\|$. Finally, if

$$C'_\delta\alpha\leqslant d_\delta(\xi)\leqslant\tfrac{1}{2}\alpha^2, \tag{120}$$

then

$$\|r_{\text{eff}}(\xi)-r_\delta(\xi)\|\leqslant C'_\delta\frac{\alpha}{d_\delta(\xi)^2}. \tag{121}$$

Proof: As in the proof of Theorem 5.1, Theorem 6.1 shows that

$$\|r_{\text{eff}}(\xi)-r_\delta(\xi)\|\leqslant\frac{1}{d_\delta(\xi)}\frac{\|K_\delta(\xi)\|}{1-\|K_\delta(\xi)\|},$$

where $K_\delta:=|r_\delta(\xi)|^{1/2}(h_{\text{eff}}-h_\delta)r_\delta(\xi)^{1/2}$. Using Lemma 4.8 with $c=2$, Lemma 4.6, the triangle inequality, and similar comparison arguments as in the proofs of Theorems 5.1 and 6.1, we easily find that, for any $\mu<\inf\sigma(h_\delta)$,

$$\|K_\delta(\xi)\|\leqslant\frac{C_{(118)}}{\alpha}\max\left\{\frac{|\mu|}{d_\delta(\xi)},1\right\}\|r_\delta(\mu)^{1/2}(h_{00}+\alpha^2)^{1/2}\|^2, \tag{122}$$

where $C_{(118)}$ was defined above. We then use the following analogue of Lemmas 5.3 and 6.2.

Lemma 7.2: Let $\nu_\delta=1/2+4NZ^2$, $\mu_\delta:=-\nu_\delta\alpha^2$ and let α be defined by (6). Then $\mu_\delta<\inf\sigma(h_\delta)$, and

$$\|r_\delta(\mu_\delta)^{1/2}(h_{00}+\alpha^2)^{1/2}\|^2\leqslant 2. \tag{123}$$

Proof: We will use, as before, the scaling $z\mapsto z/\alpha$. We get, with the help of Lemma 4.9,

$$h_\delta - \mu \simeq \alpha^2(h_{00} + 2v_\delta - \alpha^{-2}\mu) \geqslant \alpha^2\left(h_{00} - 2Z\sum_{j=1}^{N}\delta(z_j) - \alpha^{-2}\mu\right)$$

$$\geqslant \alpha^2(h_{00}(1-2Z\varepsilon) - N\varepsilon^{-1}Z - \alpha^{-2}\mu) \quad (\varepsilon > 0) = \frac{1}{2}\alpha^2(h_{00}+1),$$

if we choose $\varepsilon = \varepsilon_\delta := 1/(4Z)$ and $\mu = \mu_\delta := -\alpha^2(\frac{1}{2} + 4NZ^2)$. Q.E.D.

We continue with the proof of Theorem 7.1. By (122) and (123) with $\mu = \mu_\delta$, we find that

$$\|K_\delta(\xi)\| \leqslant \frac{2C_{(118)}}{\alpha}\max\left\{\frac{\nu_\delta\alpha^2}{d_\delta(\xi)}, 1\right\} \leqslant \frac{1}{2},$$

if both

$$d_\delta(\xi) \geqslant 4C_{(118)}\nu_\delta\alpha =: C'_\delta\alpha,$$

and $\alpha \geqslant 4C_{(118)}$ which, since $B \mapsto \alpha(B)$ is increasing, is equivalent to

$$B \geqslant B'_\delta := 16C^2_{(118)}e^{8C_{(118)}}.$$

This fixes our constants C'_δ and B'_δ, and also implies that $\|r_{\text{eff}}(\xi)\| \leqslant 2\|r_\delta(\xi)\|$, by the resolvent formula. To show that (119) implies that $\|r_\delta(\xi)\| \leqslant 2\|r_{\text{eff}}(\xi)\|$, we repeat the argument with r_δ and r_{eff} interchanged: by the resolvent formula,

$$r_\delta(\xi) = r_{\text{eff}}(\xi)^{1/2}(1 + \widetilde{K}_\delta(\xi))^{-1}|r_{\text{eff}}(\xi)|^{1/2},$$

with

$$\widetilde{K}_\delta(\xi) := |r_{\text{eff}}(\xi)|^{1/2}(h_\delta - h_{\text{eff}})r_{\text{eff}}(\xi)^{1/2},$$

so that, using Lemmas 4.8, 5.2, and 5.3, we arrive at

$$\|\widetilde{K}_\delta(\xi)\| \leqslant 2\max\left\{\frac{|\mu_{\text{eff}}|}{d_{\text{eff}}(\xi)}, 1\right\}\frac{C_{(118)}}{\alpha} \leqslant 2\max\left\{\frac{2|\mu_{\text{eff}}|}{d_\delta(\xi)}, 1\right\}\frac{C_{(118)}}{\alpha},$$

if $d_\delta(\xi) \geqslant C'_\delta\alpha$, by the first part. We therefore conclude that $\|\widetilde{K}_\delta(\xi)\| \leqslant 1/2$ if both $\alpha \geqslant 4C_{(118)}$, which is satisfied since $B \geqslant B'_\delta$ defined above, and if

$$\frac{4|\mu_{\text{eff}}|C_{(118)}}{\alpha d_\delta(\xi)} \leqslant \frac{1}{2}.$$

The latter inequality is equivalent to

$$d_\delta(\xi) \geqslant 4\left(\frac{N}{2\varepsilon^2_{\text{eff}}} + 1\right)C_{(118)}\alpha,$$

which yields condition (119). Finally, if ξ satisfies (120), then

$$\|r_{\text{eff}}(\xi) - r_\delta(\xi)\| \leqslant \frac{4C_{(118)}}{\alpha d_\delta(\xi)}\max\left\{\frac{\nu_\delta\alpha^2}{d_\delta(\xi)}, 1\right\} = 4\nu_\delta C_{(118)}\frac{\alpha}{d_\delta(\xi)^2} = C'_\delta\frac{\alpha}{d_\delta(\xi)^2},$$

where we used that $d_\delta(\xi) \leqslant \alpha^2/2 \leqslant \nu_\delta\alpha^2$. This finishes the proof of Theorem 7.1. Q.E.D.

Proof of Theorem 1.5: We want to realize the assumptions of Theorems 1.1 and 7.1 with conditions on B and d_δ. We define

$$B_\delta := \max\{B_{\text{eff}}, B'_\delta\}$$

and

$$c_\delta =: \max\{C''_\delta, 2c_{\text{eff}}B_\delta^{-1/2}\}. \tag{124}$$

Clearly $B \geqslant B_\delta$ and $c_\delta \alpha \leqslant d_\delta(\xi) \leqslant \alpha^2/4$ will do, for under these conditions, using Theorems 1.1 and 7.1, the left-hand side of (20) can be estimated by

$$\frac{C_{\text{eff}}\alpha^2}{d_{\text{eff}}^2(\xi)\sqrt{B}} + \frac{C'_\delta \alpha}{d_\delta^2(\xi)} \leqslant \left(\frac{4C_{\text{eff}}\alpha(B_\delta)}{\sqrt{B_\delta}} + C'_\delta\right)\frac{\alpha}{d_\delta(\xi)^2} =: C_\delta \frac{\alpha}{d_\delta(\xi)^2}$$

since we know that both $2d_{\text{eff}}(\xi) \geqslant d_\delta(\xi)$ and $2d_\delta(\xi) \geqslant d_{\text{eff}}(\xi)$, by Theorem 7.1, and since $\alpha(B)/\sqrt{B}$ is a decreasing function of $B > 0$. Q.E.D.

VIII. THE FERMIONIC CASE

We first prove Theorem 1.6. This is simply done by repeating the proofs of Theorems 1.1, 1.3, and 1.5 for the fermionized operators, that is, for the operators sandwiched between P^{AS}. We must check that the main ingredients of these proofs remain valid. First of all, Corollary 3.3 is used to compare the resolvents of $H_f^{B,\mathbb{M}}$ and $H_{\text{eff},f}^{B,\mathbb{M}} + \mathcal{W}_f$. Next, Lemma 4.7 remains valid for $\mathcal{W}_f := P^{AS}\mathcal{W}P^{AS}$, with the operator norm being the one on $P^{AS}(\text{Ran}\,\Pi_{\text{eff}}^{B,\mathbb{M}})$, since P^{AS} commutes with h_{00} on $\text{Ran}\,\Pi_{\text{eff}}^{B,\mathbb{M}} = L^2(\mathbb{R}^N, F_{\mathbb{M}}^B)$ (as we will explicitly see below, P^{AS} not only mixes the coordinates of $\mathbb{R}^N$, but also the different components with respect to the natural basis of $F_{\mathbb{M}}^B$; however, h_{00} acts in a scalar way). We then repeat the proof of Theorem 1.1 in Sec. V, replacing d_{eff} everywhere by $d_{\text{eff},f}$. Similar remarks apply to the proofs of Theorems 1.3 and 1.5. Q.E.D.

We next turn to Theorem 1.8. The parameter B here plays a nonessential role, and we will simply drop it, writing X_m, χ_m, $F_{\mathbb{M}}$ for X_m^B, χ_m^B, $F_{\mathbb{M}}^B$, etc. We start by analyzing the subspace of antisymmetric wave functions in the range of $\Pi_{\text{eff}} := \Pi_{\text{eff}}^B$. Recall that

$$\Sigma(\mathbb{M}) = \{m = (m_1, \ldots, m_N) : m_j \geqslant 0, m_1 + \cdots + m_N = \mathbb{M}\}.$$

The permutation group S_N acts on $\Sigma(\mathbb{M})$ by $\sigma \cdot (m_1, \ldots, m_N) = (m_{\sigma(1)}, \ldots, m_{\sigma(N)})$ and $\Sigma(\mathbb{M})$ can therefore be written as a disjoint union of orbits of S_N,

$$\Sigma(\mathbb{M}) = \bigcup_{\bar{m} \in \mathcal{M}} S_N \cdot \bar{m},$$

$\mathcal{M} \subset \Sigma(\mathbb{M})$ being a set of representatives of $S_N \backslash \Sigma(\mathbb{M})$. If we let

$$V_{\bar{m}} = \text{Span}\{X_{\sigma \cdot \bar{m}} : \sigma \in S_N\}, \tag{125}$$

then, recalling that $F_{\mathbb{M}} = \text{Span}\,\{X_m : m \in \Sigma(\mathbb{M})\}$, we have the orthogonal decomposition

$$F_{\mathbb{M}} = \bigoplus_{\bar{m} \in \mathcal{M}} F_{\bar{m}}.$$

From this it follows that

$$\Pi_{\text{eff}}^{1,\mathbb{M}}(L^2(\mathbb{R}^{3N}) \otimes \mathbb{C}^{2N}) = L^2(\mathbb{R}^N) \otimes F_{\mathbb{M}} = \bigoplus_{\bar{m} \in \mathcal{M}} L^2(\mathbb{R}^N) \otimes F_{\bar{m}}.$$

Since P^{AS} leaves each $L^2(\mathbb{R}^N) \otimes F_{\bar{m}}$ invariant, it suffices to analyze the subspace of antisymmetric wave functions in each of the latter. We therefore fix an $\bar{m} \in \mathcal{M}$ and let

$$G_{\bar{m}} = \{\sigma \in S_N : \sigma \cdot \bar{m} = \bar{m}\}, \tag{126}$$

the stabilizer of $\bar{m}$. Choose representatives $\sigma_1, \ldots, \sigma_K$, $K = K(\bar{m})$, for the right equivalence classes of $G_{\bar{m}}$ in S_N: $S_N / G_{\bar{m}} = \{\sigma_1 G_{\bar{m}}, \ldots, \sigma_K G_{\bar{m}}\}$ with $\sigma_i G_{\bar{m}} \cap \sigma_j G_{\bar{m}} = \emptyset$ if $i \neq j$. Then $X_{\sigma_1 \cdot \bar{m}}, \ldots, X_{\sigma_K \cdot \bar{m}}$ con-

stitutes an orthonormal basis for $F_{\bar{m}}$, and each element $\psi=\psi(x,y,z)$ of $L^2(\mathbb{R}^N)\otimes F_{\bar{m}}$ can be uniquely written as

$$\psi=\sum_{j=1}^{K} a_j X_{\sigma_j\cdot\bar{m}}=\sum_{j=1}^{K} a_j(z)X_{\sigma_j\cdot\bar{m}}(x,y), \tag{127}$$

for suitable $a_j=a_j(z)\in L^2(\mathbb{R}^N)$. For any such ψ and $r=(x,y,z)\in\mathbb{R}^{3N}=(\mathbb{R}^N)^3$,

$$\psi(\tau\cdot r)=\sum_j a_j(\tau\cdot z)X_{\sigma_j\cdot\bar{m}}(\tau\cdot x,\tau\cdot y)=\sum_j a_j(\tau\cdot z)X_{(\tau^{-1}\cdot\sigma_j)\cdot\bar{m}}(x,y),$$

where $\tau\cdot r=(r_{\tau(1)},\ldots,r_{\tau(N)})$, and similarly for $\tau\cdot x$, $\tau\cdot y$, and $\tau\cdot z$, and where we used that

$$X_m(\tau\cdot x,\tau\cdot y)=\prod_j \chi_{m_j}(x_{\tau(j)},y_{\tau(j)})=X_{\tau^{-1}\cdot m}(x,y).$$

It follows that $\psi\in L^2(\mathbb{R}^N)\otimes F_{\bar{m}}$ is antisymmetric iff, for any $\tau\in S_N$,

$$\sum_j a_j(\tau\cdot z)X_{(\tau^{-1}\sigma_j)\cdot\bar{m}}=(-1)^\tau\sum_j a_j(z)X_{\sigma_j\cdot\bar{m}}.$$

This is equivalent to the statement that ψ is antisymmetric iff,

$$\sum_j a_j(\tau\cdot z)X_{(\tau\sigma_j)\cdot\bar{m}}=(-1)^\tau\sum_j a_j(z)X_{\sigma_j\cdot\bar{m}}, \tag{128}$$

since the two statements are equivalent when τ is a transposition, and these generate S_N. The version (128), with no τ^{-1}, will be more convenient to work with. We next observe that the map $\sigma_j\to\tau\sigma_j$ gives rise to a permutation $\rho(\tau)$ of S_K.

Lemma 8.1: For any $\bar{m}\in\mathcal{M}$ the map $\rho=\rho_{\bar{m}}:S_N\to S_K$, $K=K(\bar{m})$, such that

$$\rho(\tau)(i)=j\Leftrightarrow\tau\sigma_i\in\sigma_j G_{\bar{m}}$$

is a well-defined homomorphism. Q.E.D.

In other words, $\rho(\tau)$ is characterized by

$$\tau\sigma_i\in\sigma_{\rho(\tau)(i)}G_{\bar{m}}.$$

One easily verifies that $\rho(\tau)$ is indeed a permutation of $\{1,\ldots,K\}$, and that ρ is an homomorphism of S_N into S_K.

With this notation, the left-hand side of (128) reads

$$\sum_j a_j(\tau\cdot z)X_{\sigma_{\rho(\tau)(j)}\cdot\bar{m}},$$

and on replacing j by $\rho(\tau)^{-1}(j)$ and using the fact that the $X_{\sigma_j\cdot\bar{m}}$ form a basis of $F_{\bar{m}}$, we find that ψ is antisymmetric iff, for all j and all $\tau\in S_N$,

$$a_j(z)=(-1)^\tau a_{\rho(\tau^{-1})(j)}(\tau\cdot z). \tag{129}$$

If we successively replace τ by τ^{-1} and z by $\tau\cdot z$, this becomes

$$a_j(\tau\cdot z)=(-1)^\tau a_{\rho(\tau)(j)}(z), \tag{130}$$

which implies that all a_j are uniquely determined by any one of them, a_1, say, which we let, by definition, correspond to $\sigma_1=e$, the unity element of S_N. More explicitly, since $\rho(\sigma_j)(1)=j$ (for $\sigma_j\sigma_1=\sigma_j\in\sigma_j G_{\bar{m}}=G_{\rho(\sigma_j)(1)\cdot\bar{m}}$, by definition of ρ), Eq. (129) with $\tau=\sigma_j$ implies the important relation

$$a_j(z) = (-1)^{\sigma_j} a_1(\sigma_j \cdot z). \tag{131}$$

In particular, $P^{AS}(L^2(\mathbb{R}^N) \otimes F_{\bar{m}})$ can be identified with a subspace of $L^2(\mathbb{R}^N)$, by sending ψ to a_1 [see (132)]. We now analyze the symmetry properties of a_1 imposed by the antisymmetry of ψ.

Lemma 8.2: Let H be the subgroup of S_N generated by the set $\{\tau\sigma_{\rho(\tau)(1)}^{-1}: \tau \in S_N\}$. Then, for all $\sigma \in H$, $a_1(\sigma\cdot z)=(-1)^{\sigma}a_1(z)$, and these are the only symmetry-conditions which the anti-symmetry of ψ imposes on a_1.

Proof: Let $\tau \in S_N$ be arbitrary. Then by (130), $a_1(\tau\cdot z)=(-1)^{\tau}a_{\rho(\tau)(1)}(z)$ which, by (131), equals $(-1)^{\tau}(-1)^{\sigma_{\rho(\tau)(1)}}a_1(\sigma_{\rho(\tau)(1)}\cdot z)$. Therefore

$$a_1(\tau\sigma_{\rho(\tau)(1)}^{-1} \cdot z) = (-1)^{\tau\sigma_{\rho(\tau)(1)}^{-1}} a_1(z),$$

whence the lemma. Q.E.D.

Lemma 8.3: The group H of Lemma 8.2 is generated by the union of all stabilizers $G_{\sigma_j\cdot\bar{m}}$ of $\sigma_j\cdot\bar{m}$, $1 \leqslant j \leqslant K$.

Proof: Let $\tau \in S_N$. Then $\tau \in \sigma_j G_{\bar{m}}$, for some j. Since $\tau\sigma_1 = \tau e \in \sigma_j G_{\bar{m}}$, we have that $\rho(\tau)(1) = j$, and therefore $\tau\sigma_{\rho(\tau)(1)}^{-1} \in \sigma_j G_{\bar{m}}\sigma_j^{-1} = G_{\sigma_j\cdot\bar{m}}$.

Conversely, if $\sigma \in G_{\sigma_j\cdot\bar{m}}$, then $\sigma = \sigma_j\sigma'\sigma_j^{-1}$, for some $\sigma' \in G_{\bar{m}}$. Set $\tau = \sigma_j\sigma'$. Then $\rho(\tau)(1)=j$, since $\sigma_j\sigma'\sigma_1 \in \sigma_j G_{\bar{m}}$, and therefore $\sigma = \tau\sigma_j^{-1} = \tau\sigma_{\rho(\tau)(1)}^{-1}$ is a generator of H. We conclude that the set of generators of H equals $\cup_j G_{\sigma_j\cdot\bar{m}}$, which proves the lemma. Q.E.D.

Lemma 8.4: Let H be the subgroup from Lemma 8.2. If $G_{\bar{m}}=\{e\}$, then $H=\{e\}$, while if $G_{\bar{m}} \neq \{e\}$, then $H=S_N$.

Proof: It is obvious, from Lemma 8.3, that if $G_{\bar{m}}=\{e\}$, then $H=\{e\}$, and a_1 does not have to satisfy any symmetry conditions with respect to the action of S_N, by Lemma 8.2.

Now suppose that $G_{\bar{m}}$ is nontrivial. Then there exist two indices i and j such that $\bar{m}_i = \bar{m}_j$. We can suppose, without loss of generality, that $i=1$ and $j=2$. In that case, the transposition (12) is in $G_{\bar{m}}$, and therefore $(\sigma(1),\sigma(2)) = \sigma(12)\sigma^{-1} \in H$, for all $\sigma \in S_N$, by Lemma 8.3 again. But then all transpositions will be in H, which clearly implies that $H=S_N$. Q.E.D.

Define a linear mapping

$$U_{\bar{m}}: P^{AS}(L^2(\mathbb{R}^N) \otimes F_{\bar{m}}) \to L^2(\mathbb{R}^N), \tag{132}$$

by

$$U_{\bar{m}}(\psi)(z) = \sqrt{K}(\psi(\cdot,z), X_{\bar{m}})_{L^2(\mathbb{R}^{2N})},$$

where we recall that $K=K(\bar{m})=\#(S_N/G_{\bar{m}})$. If ψ is given by (127), then $U_{\bar{m}}(\psi)(z)=\sqrt{K}a_1(z)$. By (130), $\|U_{\bar{m}}\psi\|^2 = \|\psi\|^2$, so that $U_{\bar{m}}$ is unitary and therefore injective. If $G_{\bar{m}}$ is nontrivial, then $H = S_N$, and the image of $U_{\bar{m}}$ is contained in the space $L^2_{AS}(\mathbb{R}^N)$ of antisymmetric wave functions on $\mathbb{R}^N$, by Lemmas 8.2 and 8.4. Since the only symmetries of a_1 are those imposed by H, it follows that $U_{\bar{m}}$ is surjective onto $L^2_{AS}(\mathbb{R}^N)$. Similarly, if $G_{\bar{m}}=\{e\}$, then $H=\{e\}$, and the image of $U_{\bar{m}}$ is $L^2(\mathbb{R}^N)$: indeed, if $a_1 = a_1(z)$ is arbitrary, then

$$\psi_{a_1} := \sum_{\sigma \in S_N} a_1(\sigma \cdot z) X_{\sigma\cdot\bar{m}}(y,z)$$

is an antisymmetric element of $L^2(\mathbb{R}^N) \otimes F_{\mathbb{M}}$ such that $U_{\bar{m}}(\psi_{a_1}) = a_1$.

Proof of Theorem 1.8: Recall that

$$\mathcal{M}_1 = \{\bar{m} \in \mathcal{M}: G_{\bar{m}} = \{e\}\}, \quad \mathcal{M}_2 = \{\bar{m} \in \mathcal{M}: G_{\bar{m}} \neq \{e\}\},$$

and define

$$U_{\mathbb{M}} =: U_{\mathbb{M}}^{B}:P^{AS}(L^2(\mathbb{R}^N \otimes F_{\mathbb{M}})) \to \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_1}} L^2(\mathbb{R}^N) \oplus \overset{\oplus}{\sum_{\bar{m}\in\mathcal{M}_2}} L^2_{AS}(\mathbb{R}^N), \tag{133}$$

by $U_{\mathbb{M}} := \oplus_{\bar{m}\in\mathcal{M}} U_{\bar{m}}$. Then we have shown that $U_{\mathbb{M}}$ is a surjective isometry. The intertwining formula of $h^{\mathbb{M}}_{\delta,f}$ with $U_{\mathbb{M}}$ being obvious, this proves Theorem 1.8. Q.E.D.

Contrary to $h^{\mathbb{M}}_{\delta,f}$, the operator $U_{\mathbb{M}} h^{\mathbb{M}}_{C,f} U^*_{\mathbb{M}}$ will in general not act diagonally anymore on the range of $U_{\mathbb{M}}$, but will contain terms which couple antisymmetric and boltzonic components in (133), that is, components in $L^2_{AS}(\mathbb{R}^N)$ and $L^2(\mathbb{R}^N)$. The potentially problematic terms in $h^{\mathbb{M}}_{C,f}$ are $U_{\mathbb{M}} C^{n,\mathbb{M}}_{\mathrm{av}:1} U^*_{\mathbb{M}}$ and $U_{\mathbb{M}} C^{e,\mathbb{M}}_{\mathrm{av}:2} U^*_{\mathbb{M}}$ (still dropping the B from our notations). The first one is easily seen to act diagonally on the right-hand side of (133): recall that

$$C^{n,\mathbb{M}}_{\mathrm{av}:1} = -\Pi^1_{\mathrm{eff}} \left(\frac{1}{N} \sum_{j=1}^{N} \log\left(\frac{1}{4}\rho_j^2 \right) \right) \Pi^1_{\mathrm{eff}},$$

and identify this with a Hermitian operator on $F_{\mathbb{M}} = \mathrm{Span}\,\{X_m : m \in \Sigma(\mathbb{M})\}$ [it acts as a multiplication operator on $L^2(\mathbb{R}^N, F_{\mathbb{M}})$]. The matrix of $C^{n,\mathbb{M}}_{\mathrm{av}:1}$ in the basis X_m, $m \in \Sigma(\mathbb{M})$, is easily seen to be diagonal. Moreover,

$$\langle X_{\sigma\cdot m} | C^{n,\mathbb{M}}_{\mathrm{av}:1} | X_{\sigma\cdot m} \rangle = -\int_{\mathbb{R}^{2N}} |X_m(\sigma^{-1}\cdot(x,y))|^2 \log \frac{1}{4} (\Pi_{j=1}^N \rho_j^2)^{1/N} \, \mathrm{d}x \, \mathrm{d}y = \langle X_m | C^{n,\mathbb{M}}_{\mathrm{av}:1} | X_m \rangle.$$

Hence, taking $B=1$, for simplicity, $C^{n,\mathbb{M}}_{\mathrm{av}:1}$ will act on $F_{\bar{m}}$ as scalar multiplication by

$$\begin{aligned}\langle X_{\bar{m}} C^{n,\mathbb{M}}_{\mathrm{av}:1} | X_{\bar{m}} \rangle &= -\frac{1}{N}\sum_{j=1}^{N} \int_{\mathbb{R}^{2N}} \left(\log \frac{\rho_j^2}{4} \right) \Pi_{\nu=1}^N |\chi^1_{\bar{m}_\nu}|^2(\rho_\nu) \mathrm{d}x_\nu \, \mathrm{d}y_\nu = -\frac{1}{N}\sum_{j=1}^{N} \int_{\mathbb{R}^2} \left(\log \frac{\rho^2}{4} \right) |\chi^1_{\bar{m}_j}|^2(\rho) \mathrm{d}x \, \mathrm{d}y \\ &= -\frac{1}{N}\sum_{j=1}^{N} (2^{\bar{m}_j} \bar{m}_j!)^{-1} \int_0^\infty \rho^{2\bar{m}_j+1} \log \frac{\rho^2}{4} e^{-\rho^2/2} \, \mathrm{d}\rho = \log 2 - \frac{1}{N}\left(\sum_{j=1}^{N} \psi(\bar{m}_j + 1) \right),\end{aligned}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$, the logarithmic derivative of the Γ-function. Hence $U_{\mathbb{M}} C^{n,\mathbb{M}}_{\mathrm{av}:1} U^*_{\mathbb{M}}$ simply acts diagonally on the right-hand side of (133), and more precisely, by scalar multiplication in each component.

The operator $U_{\mathbb{M}} C^{e,\mathbb{M}}_{\mathrm{av}:2} U^*_{\mathbb{M}}$ is more complicated: it is not going to be diagonal in the natural basis and it will in general mix the different components Ran $U_{\mathbb{M}}$, even those with index in $\mathcal{M}_1$ and $\mathcal{M}_2$. This is already the case in the simplest case in which both $\mathcal{M}_1$ and $\mathcal{M}_2$ are nonempty, namely that of two electrons, $N=2$, and a total angular momentum of $\mathbb{M}=2$. In that case $\Sigma(\mathbb{M})$ is the union of two orbits under S_2, namely $\{(0,2), (2,0)\}$, and $\{(1,1)\}$ the first having as stabilizer the identity, and the second having as stabilizer the full group S_2. We can therefore take $\mathcal{M}_1 = \{(0,2)\}$ and $\mathcal{M}_1 = \{(1,1)\}$. We will now compute the matrix element

$$\langle X^1_{(0,2)} | C^{e,2}_{\mathrm{av}:2} | X^1_{(1,1)} \rangle, \tag{134}$$

and simply observe that the result is nonzero. For this computation it is convenient to use complex notation for the lowest Landau functions (25): if we let $\zeta = x + iy$, then (taking $B=1$ again)

$$\chi^1_m = c_m \zeta^m e^{-|\zeta|^2/4},$$

where $c_m = (2\pi 2^m m!)^{-1/2}$. We then find that (134) equals

$$-c_0 c_2 c_1^2 \int_{\mathbb{C}} \int_{\mathbb{C}} \zeta_1 \zeta_2 \bar{\zeta}_2^2 \log\left(\frac{|\zeta_1 - \zeta_2|^2}{4} \right) e^{-(|\zeta_1|^2 + |\zeta_2|^2)/2} \, \mathrm{d}\zeta_1 \, \mathrm{d}\zeta_2.$$

Making the (by now familiar) change of variables $u = (\zeta_1 + \zeta_2)/\sqrt{2}$, $v = (\zeta_1 - \zeta_2)/\sqrt{2}$, this integral becomes

$$-\frac{c_0c_2c_1^2}{4}\int_{\mathbb{C}}\int_{\mathbb{C}}(u^2-v^2)(\bar{u}-\bar{v})^2\log(|v|^2/8)e^{-(|u|^2+|v|^2)/2}\,\mathrm{d}u\,\mathrm{d}v.$$

Since $(u^2-v^2)(\bar{u}^2-2\overline{uv}+\bar{v}^2)=|u|^4-|v|^4+2i\,\mathrm{Im}\,u^2\bar{v}^2+2\overline{uv}(v^2-u^2)$, and since, in general,

$$\int_{\mathbb{C}}\int_{\mathbb{C}}u^\sigma\bar{u}^\beta v^\nu\bar{v}^\kappa g(|u|^2,|v|^2)\mathrm{d}u\,\mathrm{d}v=0,$$

unless $\alpha=\beta$ and $\nu=\kappa$, we obtain that (134) equals

$$\begin{aligned}&-\frac{c_0c_2c_1^2}{4}\int_{\mathbb{C}}\int_{\mathbb{C}}(|u|^4-|v|^4)\log(|v|^2/8)e^{(|u|^2+|v|^2)/4}\,\mathrm{d}u\,\mathrm{d}v\\&=-\frac{c_0c_2c_1^2}{4}\left\{\int_{\mathbb{C}}|u|^4e^{-|u|^2/2}\,\mathrm{d}u\int_{\mathbb{C}}\log(|v|^2/8)e^{-|v|^2/2}\,\mathrm{d}v\right.\\&\left.-\int_{\mathbb{C}}e^{-|u|^2/2}\,\mathrm{d}u\int_{\mathbb{C}}|v|^4\log(|v|^2/8)e^{-|v|^2/2}\,\mathrm{d}v\right\}=\frac{3}{16\sqrt{2}},\end{aligned}$$

as can be shown using the Γ-function and its derivative. So (134) is nonzero, and $U_{\mathbb{M}}h^{\mathbb{M}}_{C,f}U^*_{\mathbb{M}}$ mixes the two sectors.

IX. CONCLUDING REMARKS

We finally want to give an idea what these effective Hamiltonians might be good for. Our original motivation for introducing them was for studying the structure of the bottom of spectrum of $H^{B,\mathbb{M}}$, in connection with the maximum ionization problem for atoms in strong magnetic fields; see below. To illustrate how this works, we first consider the comparison with $H^{B,\mathbb{M}}_\delta=h^{B,\mathbb{M}}_\delta\oplus H^{B,\mathbb{M}}_\perp$; cf. Theorem 1.5. Since, by construction, $B_\delta>B_{(36)}$, we know from Theorem 3.1 that $\sigma(H^{B,\mathbb{M}}_\perp)\subset(0,\infty)$ if $B>B_\delta$. Let $E_\delta:=\inf h^B_\delta$, then clearly $E_\delta<0$.

Since h^B_δ is unitarily equivalent to $\alpha^2\left(-\frac{1}{2}\Delta_z+2v_\delta\right)$ we conclude that whenever E_δ is an isolated eigenvalue, its position as well as its isolation distance is proportional to α^2. That E_δ is an eigenvalue is true for Z large enough when N is fixed; to determine how big Z must be exactly, relative to N, for this to happen is an open problem (see below). Let us assume henceforth that E_δ is an eigenvalue, which then necessarily is simple. Consequently E_δ is an eigenvalue of $H^{B,\mathbb{M}}_\delta$ with multiplicity $\dim F^B_{\mathbb{M}}$, see (18). Choose two points $\xi_\pm:=E_\delta\pm C\alpha^2$ in $\rho(H^{B,\mathbb{M}}_\delta)\cap\rho(H^{B,\mathbb{M}})$, which satisfy (19). This is possible when $B>B_\delta$, see Theorem 1.5. Let Γ be the circle in the complex plane centered at E_δ with radius $C\alpha^2$ and define P and P_δ as the eigenprojections associated to $H^{B,\mathbb{M}}$ and $h^{B,\mathbb{M}}_\delta$, respectively, onto their spectrum inside Γ. To estimate $P-P_\delta$ we need a bound on $R(\xi)-R_\delta(\xi):=(H^{B,\mathbb{M}}-\xi)^{-1}-(H^{B,\mathbb{M}}_\delta-\xi)^{-1}$ for all $\xi\in\Gamma$. We know already that $\|R(\xi_\pm)-R_\delta(\xi_\pm)\|\leqslant C_\delta\alpha/d_\delta(\xi_\pm)^2=C_\delta C^{-2}\alpha^{-3}$ by Theorem 1.5. To propagate this estimate on all of Γ we use the convenient formula [see Ref. 12, Sec. IV, (3.10)]

$$\|R(\xi)-R_\delta(\xi)\|\leqslant\frac{\left\|\frac{H^{B,M}_\delta-\xi_\pm}{H^{B,M}_\delta-\xi}\right\|^2\|R(\xi_\pm)-R_\delta(\xi_\pm)\|}{1-|\xi-\xi_\pm|\left\|\frac{H^{B,M}_\delta-\xi_\pm}{H^{B,M}_\delta-\xi}\right\|\|R(\xi_\pm)-R_\delta(\xi_\pm)\|}\leqslant\frac{C_\delta C^{-2}\alpha^{-3}}{1-\sqrt{2}C_\delta C^{-1}\alpha^{-1}}.$$

Then integrating over the contour Γ finally gives $\|P-P_\delta\|=\mathcal{O}(\alpha^{-1})$ as B tends to infinity. This shows that for B large enough these two projections have the same dimension and since they are continuous with respect to B we finally get that for all $B>B_\delta$, $\dim P=\dim P_\delta=\dim F^B_{\mathbb{M}}$.

Our conclusion is therefore that, for sufficiently large B, $H^{B,\mathbb{M}}$ will have a cluster of eigenvalues in the interval $(E_\delta - c_\delta\alpha^2, E_\delta + c_\delta\alpha^2)$ with total multiplicity of $\dim F^B_{\mathbb{M}}$, and apart from this no eigenvalues at a distance $C\alpha^2$ from E_δ (the allowed B's will depend on C), so that the cluster is separated from the rest of the spectrum by a distance proportional to α^2. In the particular case when $\dim F^B_{\mathbb{M}}=1$, i.e., $\mathbb{M}=0$ or $N=1$, we get an estimate on the difference of the eigenvectors $\Phi - \Phi_\delta = \mathcal{O}(\alpha^{-1})$ as $B\to\infty$ (in the L^2 norm). Here Φ denotes the eigenvector of $H^{B,\mathbb{M}}$ and $\Phi_\delta(x,y,z) := \varphi^B_\delta(z)X^B_{m=0}(x,y)$ if $\mathbb{M}=0$, where φ^B_δ is the ground state of h^B_δ. In the case $N=1$ one has $\varphi^B_\delta(z) = \sqrt{2\alpha Z}e^{-2\alpha Z|z|}$.

Consider now the comparison with $h^{B,\mathbb{M}}_C$. The difficulty here is to find the necessary *a priori* information on the structure of $\sigma(h^{B,\mathbb{M}}_C)$. In the case of $N=1$, using the invariance of $\sigma(h^{B,\mathbb{M}}_C)$ under the reflection $z\mapsto -z$, and the characterization of the domain of $\sigma(h^{B,\mathbb{M}}_C)$ in the Appendix, one sees that the odd spectrum (that is, the spectrum of h_C restricted to the odd wave functions) is B-independent and coincides with the spectrum of the hydrogen in the s sector of symmetry. Since the even spectrum intertwines with the odd spectrum and since it is monotonically decreasing with respect to B, cf. (11), it is easy to realize that $\sigma(h^{B,\mathbb{M}}_C)\cap\mathbb{R}_-$, apart from the ground state energy, is made up of clusters of two eigenvalues, the clusters being separated by a distance of order 1 as $B\to\infty$. Thus by using Theorem 1.3 and following a similar strategy as above one can conclude that for $N=1$, and arbitrarily small ε, $\sigma(H^{B,\mathbb{M}})\cap(-\infty,-\varepsilon]$ has the same cluster structure for $B > B_\varepsilon$ sufficiently large. Moreover this spectrum deviates from the one of the Coulomb model by at most $c_C\alpha(B)^{3/2}B^{-1/4}$ as $B\to\infty$.

The model operator $h^{B,\mathbb{M}}_{\text{eff}}$ is for the moment of mainly theoretical interest since it does not seem to be solvable even in the one electron case. Notice however that one could solve $h^{B,\mathbb{M}}_{\text{eff}}$ numerically, at least for few electrons and small $\mathbb{M}$, and subsequently use Theorem 1.1 to approximate the true spectrum of $H^{B,\mathbb{M}}$ for large B. Given the nontrivial dimension reduction achieved by Theorem 1.1 (from wave functions of $3N$ variables to ones of N variables, albeit vector-valued) such a procedure would, from a numerical point of view, seem preferable to attacking $H^{B,\mathbb{M}}$ directly.

Whether the simpler models, i.e., the delta and the Coulomb model, are solvable in the N-electron case, $N\geqslant 2$, is a challenging question in view of applications. We are thinking in particular of the problem of *determining the maximum number N_c of electrons which a clamped nucleus with charge Z can bind when an intense homogeneous magnetic field is applied*. Reference 14 has shown that $\liminf N_c/Z \geqslant 2$ as Z, $B/Z^3\to\infty$. Very little precise is known for fixed Z and high B. It is conjectured that there should be a B-independent absolute (that is, nonasymptotic) upper bound of the form $N_c \leqslant aZ+b$, similar to Lieb's bound $N_c \leqslant 2Z+1$ valid when $B=0$, but this is as yet unproved. Some weaker results are known, of which the best to date is the one of Ref. 18; see also Ref. 7 for work on heuristic models related to our $h^{B,\mathbb{M}}_{\text{eff}}$. It is natural to first try to solve the maximal binding question for h^B_δ, or any of our other effective Hamiltonian, and use the approximation theorems of this paper to draw conclusions for $H^{B,\mathbb{M}}$ itself. Some modest progress is possible in this way. It is, for example, known that the delta model with two electrons is at least numerically solvable, see Ref. 16, and that this model possesses a unique bound state at the bottom of its spectrum as long as $Z>0.375$. Therefore using Theorem 1.5 we see that for all $Z>0.375$ there exists $B_Z\geqslant 0$ such that for all $B\geqslant B_Z$ one nucleus with such a charge can bind two electrons. As a consequence, Lieb's bound of $N_c\leqslant 2Z+1$ is no longer valid in strong magnetic fields. For general Z, no maximum ionization bound for the δ-model is known as yet.

Let us now briefly turn to the effect of particle symmetry. It follows from Theorems 1.6 and 1.8 that $H^{B,\mathbb{M}}_f$ can be approximated by a direct sum of copies of h^B_δ acting on antisymmetric $L^2(\mathbb{R}^N)$ plus a direct sum of copies of h^B_δ acting on $L^2(\mathbb{R}^N)$ *without any symmetry condition*. The latter will occur iff $\mathcal{M}_1\neq\emptyset$, which is the case iff $\mathbb{M}\geqslant 0+1+\cdots+(N-1)=\frac{1}{2}N(N-1)$. For such $\mathbb{M}$, the ground state energy will be approximately that of boltzonic h^B_δ, which is also the ground state energy of the bosonic h^B_δ, and the same can be shown to be the case for the ground state wave function (assuming there is one), by standard permutation arguments. In fact, Theorem 1.6 plus Theorem 1.8 predict the existence of a cluster of $\#\mathcal{M}_1$ eigenvalues at the bottom of the spectrum of $H^{B,\mathbb{M}}_f$, at a distance of order $\alpha(B)^2$ from the origin as $B\to\infty$.

A further interesting corollary to Theorem 1.8 can be obtained by considering $\mathbb{M}$ as a free parameter. If h_δ^B possesses a ground state, whose energy is isolated in its spectrum, then for sufficiently large B, $H_f^B := P^{\mathrm{AS}} H^B$ will assume its ground state for an $\mathbb{M} \geqslant \frac{1}{2}N(N-1)$. Stated otherwise, assuming there is a mechanism for transfer of the angular momentum (e.g., emission and absorption of photons), atoms in strong magnetic fields will have an orbital angular momentum in the field direction of at least $\frac{1}{2}N(N-1)$. A natural conjecture is that we have equality here. Notice that this conjecture was shown to be true in the case of $N=1$ in Ref. 2, see also Ref. 3.

We mention one further application of these effective Hamiltonians. After the location of the spectrum to leading order one can now use regular perturbation theory to compute lower order corrections. We have shown how this can be done in Ref. 5. This seems definitely more convenient than variational techniques and more familiar than the Birman-Schwinger method used in Ref. 2 for the one electron case. Continuing, for example, the above comparison of $H^{B,\mathbb{M}}$ with $h_\delta^{B,\mathbb{M}}$, it is immediate to realize that adding the first order perturbative correction will give an error of order 1. In case $N=1$ we get that the ground state energy of $H^{B,\mathbb{M}}$ is equal to $\langle h_{\mathrm{eff}}^{B,\mathbb{M}} \Phi_\delta, \Phi_\delta \rangle + \mathcal{O}(1)$ with $\Phi_\delta(x,y,z) = \sqrt{2\alpha Z} e^{-2\alpha Z|z|} \chi_{\mathbb{M}}^B(x,y)$. This should be compared to Theorem 2.5 of Ref. 2. In fact, one can write the ground state energy as a convergent power series, each term of which being of order α^{-k} for k running from -2 to infinity. However, as pointed out in Ref. 2, in view of the $\log(B)$ behavior of α this series is of limited value. The situation will be much better with the Coulomb model $h_C^{B,\mathbb{M}}$ since the perturbation series will converge much faster because of the $\alpha^{3/2}B^{-1/4}$ behavior of the rhs of (15). We hope to tackle this program soon.

The above remarks concentrated on applications of our effective Hamiltonians to the ground state energy of $H^{B,\mathbb{M}}$, but their potential interest is not limited to that. As the example of h_C shows, other parts of the discrete spectrum of $H^{B,\mathbb{M}}$ will also become amenable to analysis, if this is the case for the effective operator. On a conceptual level, Theorem 1.1 gives a precise mathematical sense to, and justification of, the physicist's attractive heuristic picture of an atom in a strong homogeneous magnetic field as consisting of electrons in their lowest Landau band states interacting through a kind of "residual" electrostatic interaction. Finally let us note that the techniques developed in this paper are expected to work in other contexts. An interesting example is that of two-dimensional electronic systems on a cylinder which describe excitons in carbon nanotubes; cf. Ref. 9.

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APPENDIX: A CHARACTERIZATION OF THE OPERATOR DOMAIN OF h_C

In this appendix we will characterize the operator domain of $h_C = h_C^B$. It will in fact be convenient to consider a slightly more general situation. Let $\mathcal{L} = \{L_\nu, 1 \leqslant \nu \leqslant K\}$, be a finite collection of hyperplanes in $\mathbb{R}^N$ (we might more generally consider nonsingular C^1 hypersurfaces). Let F be a finite-dimensional complex vector space, with Hermitian inner product $(\cdot,\cdot)$ and let A_ν, B_ν be Hermitian operators on F. Let $H^k(\mathbb{R}^N, F)$ be the kth Sobolev space on $\mathbb{R}^N$, with values in F. Then the following sesquilinear form is well defined on $H^1(\mathbb{R}^N, F)$ and bounded from below:

$$t_{\mathcal{L}}(u,v) = \frac{1}{2}(\nabla u, \nabla v) + \sum_\nu \langle L_\nu^* \mathrm{Pf}(|\cdot|^{-1}), (A_\nu u, v) \rangle + \langle L_\nu^* \delta, (B_\nu u, v) \rangle, \tag{A1}$$

$\langle \cdot,\cdot \rangle$ denoting the duality between distributions and test functions. We let

$$h_{\mathcal{L}} = -\frac{1}{2}\Delta_z + \sum_\nu A_\nu \mathrm{Pf}\left(\frac{1}{L(z)}\right) + B_\nu \delta(L_\nu(z)).$$

be the associated self-adjoint operator, whose existence is guaranteed by the KL^{2}MN-theorem. Let $\mathcal{R}$ be the set of connected components of $\mathbb{R}^N \backslash \cup_\nu \mathrm{Ker}\, L_\nu$, so that $\mathbb{R}^N \backslash \cup_\nu \mathrm{Ker}\, L_\nu = \cup_{R\in\mathcal{R}} R$ and $R \cap R' = \emptyset$, if R, $R' \in \mathcal{R}$, $R \neq R'$. Note that, on any of these components R, $L_j^* \mathrm{Pf}(1/|\cdot|)$ simply equals the function $1/|L_j(z)|$. We will identify L_j with an element of $\mathbb{R}^N$, using the Euclidean inner product on $\mathbb{R}^N$; the latter will be denoted by a dot: $z \cdot w$, to distinguish it from the Hermitian inner product (v,w) on F. If we let $H^2(R,F)$ be the F-valued Sobolev space of order 2 on the open subset $R \subset \mathbb{R}^N$, then the domain of $h_{\mathcal{L}}$ can be characterized as follows.

Theorem A.1: *Let $u \in L^2(\mathbb{R}^N, F)$. Then $u \in \mathrm{Dom}(h_{\mathcal{L}})$ iff the following three conditions hold*:

(i) $u \in H^1(\mathbb{R}^N, F)$.

(ii) *For each $R \in \mathcal{R}$,*

$$-\frac{1}{2}\Delta u + \sum_\nu \frac{1}{|L_\nu(z)|} A_\nu u \in H^2(R,F).$$

(iii) *For each j and for each $x \in \{L_j = 0\} \backslash \cup_{k\neq j}\{L_k = 0\}$:*

$$L_j \cdot \nabla u\left(x + \varepsilon \frac{L_j}{\|L_j\|}\right) - L_j \cdot \nabla u\left(x - \varepsilon \frac{L_j}{\|L_j\|}\right) \simeq 4 \log \varepsilon A_j u(x) + 2B_j u(x) + o(1),$$

as $\varepsilon \to 0$.

Proof: We will use the following characterization (see Ref. 12) of $\mathrm{Dom}(h_{\mathcal{L}})$:

$$u \in \mathrm{Dom}(h_{\mathcal{L}}) \Leftrightarrow \begin{cases} u \in \mathrm{Dom}(t_{\mathcal{L}}) = H^1(\mathbb{R}^N, F), \\ \text{and} \\ |t_{\mathcal{L}}(u,v)| \leq C_u \|v\|^2, \qquad \forall v \in \mathrm{Dom}(t_{\mathcal{L}}) = H^1(\mathbb{R}^N, F), \end{cases} \tag{A2}$$

the norm on the right-hand side being the L^2-norm. Here we may, and will, suppose without loss of generality that $v \in C_c^1(\mathbb{R}^N, F)$, the space of compactly supported F-valued C^1-functions.

To analyze (A2), we will first establish a convenient integral expression for the pull-backs of δ and of Pf $(1/|\cdot|)$ under a linear map $L: \mathbb{R}^N \to \mathbb{R}$. Using the Euclidean inner product, we can identify L with an element of $\mathbb{R}^N$, which we also denote by L. Using the definition of pull-back (cf. Hörmander,[11] Chap. 6), one easily shows that if $\mathrm{d}\sigma_L$ denotes the Euclidean surface measure on $\mathrm{Ker}(L)$, and $\|L\|$ is the Euclidean norm of L, then

$$\langle L^* \delta, \varphi \rangle = \int_{\{L=0\}} \frac{\varphi}{\|L\|} \mathrm{d}\sigma_L, \tag{A3}$$

and

$$\langle L^* \mathrm{Pf}(1/|\cdot|), \varphi \rangle = -\int_{\mathbb{R}^N} \frac{\mathrm{sgn}(L(z)) \log |L(z)|}{\|L\|^2} L \cdot \nabla u(z) \mathrm{d}z. \tag{A4}$$

In fact, since taking pull-backs is coordinate invariant, it suffices to verify these formulas in an orthogonal coordinate system in which $L = (\|L\|, 0, \ldots, 0)$.

We next observe that, for each $R \in \mathcal{R}$, there exists a (unique) function $s_R: \{1, \ldots, K\} \to \{0,1\}$, such that

$$R = \{z \in \mathbb{R}^N : (-1)^{s_R(j)} L_j(z) \geqslant 0, j = 1, \ldots, K\},$$

and if $\varepsilon > 0$, we define R_ε by

$$R_\varepsilon = \{z \in \mathbb{R}^N : (-1)^{s_R(j)} L_j(z) \geqslant \varepsilon, j = 1, \ldots, K\}.$$

Observe that the boundary of R_ε, as well as that of R, are polyhedrae, each of whose faces are contained in one of the hypersurfaces $\{(-1)^{s_R(j)} L_j = \varepsilon\}$ and $\{L_j = 0\}$, respectively. On such face, the outward-pointing normal $n_{R,\varepsilon}$ can be identified with the vector $-(-1)^{s_R(j)} L_j / \|L_j\|$ (translated to the relevant base point on the face, to be precise). Note, that $n_{R,\varepsilon}$ is only defined almost everywhere on the boundary (with respect to the surface measure). This will not cause difficulties, though.

Suppose now that $u \in \mathrm{Dom}(h_{\mathcal{L}})$ and in particular satisfies the conditions (A2). We then have, for any $v \in C_c^1(\mathbb{R}^N, F)$,

$$t_{\mathcal{L}}(u,v) = \lim_{\varepsilon \to 0} \left\{ \frac{1}{2} \sum_{R \in \mathcal{R}} \int_{R_\varepsilon} (\nabla u, \nabla v) \mathrm{d}z - \sum_\nu \sum_R \int_{R_\varepsilon} \frac{\mathrm{sgn}(L_\nu) \log |L_\nu|}{\|L_\nu\|^2} (L_\nu \cdot \nabla)(A_\nu u, v) \mathrm{d}z \right.$$
$$\left. + \sum_\nu \int_{\{L_\nu = 0\}} \frac{(B_\nu u, v)}{\|L_\nu\|} \mathrm{d}\sigma_{L_\nu} \right\}. \tag{A5}$$

We want to apply Gauss' divergence theorem to each of the integrals over R_ε: this is allowed since if $u \in H^1(\mathbb{R}^N, F)$ satisfies (A2), then by choosing v compactly supported in R, we see that

$$-\frac{1}{2} \Delta_z u + \sum_\nu A_\nu \left(\frac{1}{L(z)} \right) u \in L^2_{\mathrm{loc}}(R, F),$$

which obviously implies that $\Delta u \in L^2_{\mathrm{loc}}(R, F)$ (since we are staying away from the singularities on the hyperplanes), and hence $u \in H^2_{\mathrm{loc}}(R, F)$. Now

$$\int_{R_\varepsilon} (\nabla u, \nabla v) \mathrm{d}z = \int_{R_\varepsilon} (-\Delta u, v) \mathrm{d}z + \int_{\partial R_\varepsilon} (n_{R,\varepsilon} \cdot \nabla u, v) \mathrm{d}\sigma_{R,\varepsilon}, \tag{A6}$$

$\mathrm{d}\sigma_{R,\varepsilon}$ being the Euclidean surface measure on the boundary. Furthermore,

$$-\|L_\nu\|^{-2} \int_{R_\varepsilon} \mathrm{sgn}(L_\nu) \log |L_\nu| (L_\nu \cdot \nabla)[(A_\nu u, v)] \mathrm{d}z = \int_{R_\varepsilon} \frac{(A_\nu u, v)}{|L_\nu(z)|} \mathrm{d}z - \|L_\nu\|^{-2} \int_{\partial R_\varepsilon} \mathrm{sgn}(L_\nu) \log |L_\nu|$$
$$\times (A_\nu u, v)(L_\nu \cdot n_{R,\varepsilon}) \mathrm{d}\sigma_{R,\varepsilon}.$$

Using this, the second term in (A5) can, after rearranging, be written as

$$\sum_{R \in \mathcal{R}} \int_{R_\epsilon} \left(\sum_j \frac{(A_j u, v)}{|L_j(z)|} \right) \mathrm{d}z + \sum_j \sum_{\pm} \pm \|L_j\|^{-1} \int_{\substack{L_j = \pm\varepsilon, \\ |L_\nu| > \varepsilon \text{ if } \nu \neq j}} \mathrm{sgn}(L_j(z)) \log |L_j(z)| (A_j u, v)$$
$$+ \sum_{j,k: j \neq k} \sum_{\pm} \pm \|L_k\|^{-1} \|L_j\|^{-2} L_k \cdot L_j \int_{\substack{L_k = \pm\varepsilon, \\ |L_\nu| > \varepsilon \text{ if } \nu \neq k}} \mathrm{sgn}(L_j(z)) \log |L_j(z)| (A_j u, v),$$

the surface integrals being with respect to the natural surface measures. Since v is compactly supported, the third sum will vanish, in the limit of $\varepsilon \to 0$. This follows from the local integrability of $u \cdot \log |L_j|$ on $\{L_k = 0\}$ (if $j \neq k$), which can be seen as follows. Since $u \in H^1$, its restriction $u|_{\{L_k = 0\}}$ is in (vector-valued) L^2. On the other hand, $\log |L_j|$, restricted to $\{L_k = 0\}$ is in $L^2_{\mathrm{loc}}(\mathbb{R}^{N-1})$, and therefore $u \log |L_j|$, restricted to $\{L_k = 0\}$ is locally integrable. Rearranging also the sum over $\mathcal{R}$ of the boundary terms in (A6) as a sum of integrals over the various hypersurfaces $\{L_j = \pm\varepsilon\}$, we conclude that for $v \in C_c^1(\mathbb{R}^N, F)$,

$$t_{\mathcal{L}(u,v)} = \lim_{\varepsilon\to 0} \int_{R_\varepsilon} \left(-\frac{1}{2}\Delta u + \sum_\nu \frac{A_\nu u}{|L_\nu(z)|}, v \right) \mathrm{d}z + \sum_j \sum_\pm \mp \frac{1}{2} \int_{L_j=\pm\varepsilon, |L_\nu|>\varepsilon(\nu\neq j)} \frac{(L_j\cdot\nabla u, v)}{\|L_j\|} \mathrm{d}\sigma_{\{L_j=\pm\varepsilon\}}$$
$$+ \sum_j 2\log\varepsilon \sum_\pm \int_{L_j=\pm\varepsilon, |L_\nu|>\varepsilon(\nu\neq j)} \frac{(A_j u, v)}{\|L_j\|} \mathrm{d}\sigma_{\{L_j=\pm\varepsilon\}} + \int_{\{L_j=0\}} \frac{(B_j u, v)}{\|L_j\|} \mathrm{d}\sigma_{\{L_j=0\}}.$$

Since $u \in H^1$ implies that $\|u(\cdot+\varepsilon L_j/\|L_j\|) - u(\cdot)\|_{L^2(\{L_j=0\})} = O(\sqrt{\varepsilon})$, and since $(u,v) \in L^1(\{L_j=0\})$, we can replace the next to last term by

$$2\log\varepsilon \|L_j\|^{-1} \int_{\{L_j=0\}} (A_j u, v) \mathrm{d}\sigma_{\{L_j=0\}} + o(1), \quad \varepsilon \to 0.$$

We can, for the same reason, replace v in the second integral by its restriction to $\{L_j=0\}$. Letting $\varepsilon \to 0$, it follows that if u satisfies (A2), then it satisfies (i), (ii), and (iii).

Conversely, suppose that u satisfies conditions (i), (ii), and (iii) of the theorem. Then running the argument backwards shows that $|t_{\mathcal{L}}(u,v)| \leqslant C_u \|v\|^2$, first for all compactly supported v and thence for all $v \in H^1(\mathbb{R}^N, F)$. Hence $u \in \mathrm{Dom}(\mathrm{h}_{\mathcal{L}})$, by (A2).

Q.E.D.

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Reflection symmetries for multiqubit density operators

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For multiqubit density operators in a suitable tensorial basis, we show that a number of nonunitary operations used in the detection and synthesis of entanglement are classifiable as reflection symmetries, i.e., orientation changing rotations. While one-qubit reflections correspond to antiunitary symmetries, as is known, for example, from the partial transposition criterion, reflections on the joint density of two or more qubits are not accounted for by the Wigner theorem and are well-posed only for sufficiently mixed states. One example of such nonlocal reflections is the unconditional NOT operation on a multiparty density, i.e., an operation yeilding another density and such that the sum of the two is the identity operator. This nonphysical operation is admissible only for sufficiently mixed states. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2181827]

I. INTRODUCTION

The Wigner theorem asserts that unitary and antiunitary operations exhaust all possible symmetric transformations applicable to the wave function of a quantum mechanical system. The unitary transformations are physically associated with forward-in-time evolution, and antiunitary with backward-in-time evolution (see, for example, Ref. 1). The characteristic feature of this last class is the presence of a conjugation operation on a wave function or a transposition operation on a density operator. It is known[2] that the geometric interpretation of the time reversing operation for a density operator in a two-dimensional Hilbert space (also known as "qubit") is a *reflection*, i.e., an orientation-changing rotation in $\mathrm{O}^{-}(3)=\mathrm{O}(3)\backslash\mathrm{SO}(3)$ of the corresponding Bloch vector.

A closely related operation, variously known as a spin flip,[3] (unconditional) NOT operation, or universal inverter,[4] changes the sign of the entire Bloch vector. In this sense it corresponds geometrically to inversion in the origin, which is widely known as the parity operation.[5] For a single isolated qubit these operations are indistinguishable from equivalent orientation preserving operations, since O(3) and SO(3) both act transitively on the Bloch sphere, but for multiqubit systems they correspond to partially antiunitary transformations such as the "partial transposition," which can be used to detect bipartite entanglement.[6] This highlights the intrinsically "discrete" nature of such tests and their invariance under LOCC (local operations and classical communication).

In this paper we introduce a more general class of involutory "symmetry" operations, and argue that these are likewise useful in studying the multiparty nonseparability of density operators. These operations are most easily described in terms of the Stokes tensor[7–9] and its "unfolding" to the so-called real density matrix,[10] both of which are equivalent, as carrier spaces, to the coherence vector.[11,12] All these representations parametrize the real linear space of multiqubit density operators by the expectation values of all possible tensor products of the Pauli operators, differing only in their notations and indexing systems. The Stokes tensor indexing has the advantage of making the "affine" structure of the set of n-qubit density operators $\mathcal{D}_n$ explicit, whereas the real density

matrix has the advantages that both the matrix itself, as well as any operations on it which are diagonal with respect to the Stokes tensor, can be displayed as a compact two-dimensional (2D) table on a printed page (see below for examples).

As is well known, unitary operations on the usual Hermitian density operator induces orientation-preserving rotations of the coherence vector, and thereby also norm-preserving linear group actions on the Stokes tensor and/or real density matrix [*loc. cit.*]. In the following, we shall frequently use the term "density," without further qualification, to indicate an equivalence class of probability distributions over an ensemble of multiqubit systems which all give rise to the same density operator, irrespective of how this is represented (as a Hermitian matrix, or a Stokes tensor, etc.).

We now distinguish the following two types of nonunitary but norm-preserving operations on a multiqubit Stokes tensor:

(i) local reflections applied simultaneously to two or more qubits;
(ii) "nonlocal" reflections, i.e., reflections applied to the *joint* density of two or more qubits.

The two cases are *qualitatively different*: while (i) is equivalent, up to local unitary operations, to multiqubit partial transposition, (ii) is a genuinely new operation and does not correspond to any local operation on two or more qubits. In particular, the total reflection of all components of the Stokes tensor other than the expectation value of the identity does *not* correspond to time-reversal (i.e., to the total transpose of the density matrix) but rather to a multiparty NOT operation.

Reflections on more than one qubit are nonunitary operations that do not necessarily yield valid (positive semidefinite) density operators. However, it can be shown that any mixed state with eigenvalues "small enough" is still a density operator when it is totally reflected. In other words, total reflection is a nonunitary involution which preserves such sufficiently mixed sets of density operators. On this set, total reflection behaves like a antiunitary operation in the sense that it preserves the Hermitian structure, the trace and the (Hilbert-Schmidt) inner product. This tells us that for general mixed states there are more symmetries to be exploited than those of Wigner theorem.

For three qubits, the set of density operators admitting a total reflection includes, for example, the unextendible product basis (UPB) states used in Ref. 13 to generate a bound entangled density operator with all positive partial transpositions (PPT). The "complement" operation that turns a separable density into the bound entangled UPB state is in fact a total reflection of the type (ii) above. The various entanglement measures (the concurrence, the negativity and the tangle among them) that rely on the use of spin-flip operations are also examples of application of multiple one-qubit reflections of the type (i). In between local and total reflections lies a class of "nonlocal yet partial" reflections which also belong to the class (ii) above. These maps resemble very closely those used in the so-called reduction criterion.[14,15]

Besides their unifying mathematical (group theoretic) character, we see reflections as a new tool to "probe" the structure of the set of multiparticle density operators, in particular its nonseparable regions, by means of operations analogous, but inequivalent, to partial transposition. Hopefully this will eventually lead to a better understanding of bound entanglement in multipartite systems.

II. ONE QUBIT: TRANSPOSITION AND TIME-REVERSAL

For a single qubit with density operator $\rho \in \mathcal{D}_1 \subset \mathbb{C}^{2\times 2}$, the Stokes tensor is the affine 3-vector $[\varrho^0\ \vec{\varrho}^T]^T$, where $\varrho^0=\mathrm{tr}(\rho)/\sqrt{2}=1/\sqrt{2}$ and $\vec{\varrho}=[\varrho^1\ \varrho^2\ \varrho^3]^T$ is the Bloch vector of the qubit times $\sqrt{2}$. Thus (summing over repeated indices) we have $\rho=\varrho^j\lambda_j$ where $\lambda_j=\sigma_j/\sqrt{2}$ are the rescaled Pauli matrices ($j=1,2,3$), $\lambda_0=\mathbb{1}_2/\sqrt{2}$, and $\varrho^j=\mathrm{tr}(\rho\lambda_j)$. In this notation, the real density matrix is given by

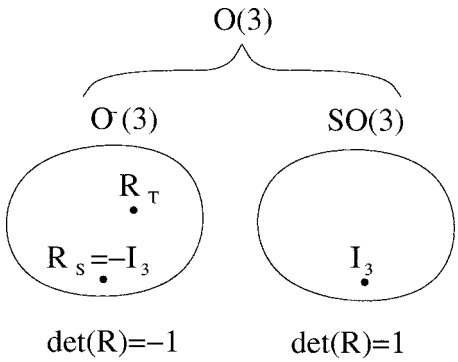

FIG. 1. Topological structure of the rotation group O(3).

$$\sigma = \sigma(\rho) \equiv \sqrt{2}\begin{bmatrix} \varrho^0 & \varrho^2 \\ \varrho^1 & \varrho^3 \end{bmatrix}. \tag{1}$$

The Stokes tensor is readily recovered from this by applying the "col"[16] (or reshaping[17]) operator to it and dividing by $\sqrt{2}$. As is well known, unitary transformations of ρ by $U \in \mathrm{SU}(2)$, namely $U\rho U^\dagger$, induce rotations of the corresponding Bloch vector. This geometric interpretation will now be extended to antiunitary transformations.[18,19]

Any antiunitary operation can be written as the product of a unitary operation and complex conjugation K. Given a pure state with wave vector $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$ $(c_0, c_1 \in \mathbb{C})$, let $|\tilde{\psi}\rangle$ be the wave vector obtained by means of K alone: $|\tilde{\psi}\rangle = K|\psi\rangle = c_0^*|0\rangle + c_1^*|1\rangle$. The corresponding density matrix is $\rho = |\psi\rangle\langle\psi| = \Sigma_{j,k=0}^{1,1} c_j c_k^* |j\rangle\langle k|$, so that $|\tilde{\psi}\rangle\langle\tilde{\psi}| = \Sigma_{j,k=0}^{1,1} c_j^* c_k |j\rangle\langle k| = (|\psi\rangle\langle\psi|)^T$. Since any density matrix is a convex combination of pure state density matrices, the effect of K on a general ρ is to transpose it, i.e., $\rho^T = K\rho K^\dagger = \varrho^0\lambda_0 + \varrho^1\lambda_1 - \varrho^2\lambda_2 + \varrho^3\lambda_3$. As indicated, this is simply a change in the sign of the λ_2 component of the Bloch vector, i.e., $[\varrho^1 \ -\varrho^2 \ \varrho^3]^T$.

The rotation group O(3), of course, has two connected components, one of which preserves the orientation of a frame [namely SO(3), which contains the identity operator $\mathbb{1}_3$], and one of which changes its orientation [denoted here by $\mathrm{O}^-(3)$, to which $-\mathbb{1}_3$ belongs]. This topological structure is illustrated in Fig. 1. A *reflection* is a rotation which does not preserve orientation. The canonical example is *spatial inversion*, which is defined as multiplication by $R_S \equiv -\mathbb{1}_3$. Any reflection $R \in \mathrm{O}^-(3)$ is obtained by multiplying R_S with a rotation in SO(3). For example, the reflection used in the transpose, $R_T = \mathrm{diag}(1, -1, 1)$, can be written as the product of a spatial inversion with a rotation by π about the y axis.

For any vector $\vec{\varrho}$, spatial inversion maps $\vec{\varrho}$ to its antipode $-\vec{\varrho} = R_S(\vec{\varrho})$ on a sphere of radius $\|\vec{\varrho}\| = \sqrt{(\varrho^1)^2 + (\varrho^2)^2 + (\varrho^3)^2}$. It follows from this together with the above that, for density matrices, $\rho^S \equiv UK\rho K^\dagger U^\dagger = \varrho^0\lambda_0 - \varrho^1\lambda_1 - \varrho^2\lambda_2 - \varrho^3\lambda_3$ where $U = i\lambda_2 \in \mathrm{SU}(2)$ rotates the Bloch vector by π about the y axis. In addition, it is easily shown that the eigenvalues of ρ are given by

$$\mathrm{eig}(\rho) = \left\{ \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}} \pm \|\vec{\varrho}\| \right) \right\}. \tag{2}$$

Since reflections, like rotations in SO(3), are length preserving actions on the Bloch sphere, we see that the eigenvalues are preserved under reflections: $\mathrm{eig}(\rho^S) = \mathrm{eig}(\rho^T) = \mathrm{eig}(\rho)$. For pure states, an important difference between R_S and R_T is that R_S maps any ket $|\psi\rangle$ to an orthogonal one, whereas R_T does not. In other words, spatial inversion corresponds exactly to the spin-flip operation.[3,20]

Both the transposition and the spin-flip can also be defined in terms of the real density matrix, using the componentwise (also known as Hadamard, or sometimes Schur) matrix product "$\odot$." In the case of the transpose, this is simply

$$\sigma(\rho^T) = \sqrt{2}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \odot \begin{bmatrix} \varrho^0 & \varrho^2 \\ \varrho^1 & \varrho^3 \end{bmatrix}. \tag{3}$$

As shown in Ref. 16, an operator sum representation is obtained from the singular value decomposition of the sign matrix (left-hand factor), leading to

$$\sigma(\rho^T) = \sigma(\rho)|0\rangle\langle 0| - \sqrt{2}\lambda_3\sigma(\rho)|1\rangle\langle 1|. \tag{4}$$

For the spin-flip, on the other hand, it is easily seen that

$$\sigma(\rho^S) = \sqrt{2}\begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} \odot \begin{bmatrix} \varrho^0 & \varrho^2 \\ \varrho^1 & \varrho^3 \end{bmatrix} = 2|0\rangle\langle 0| - \sigma(\rho). \tag{5}$$

These alternative representations of transposition and spin-flip will be useful in studying multiqubit reflections below.

For a single qubit the notion of reflection admits a further interpretation in terms of "co-completely positive" (co-CP) maps. From the Størmer-Woronowicz theorem, any positive 2×2 map Φ is decomposable as

$$\Phi = c\Phi_1 + (1-c)\Phi_2 \circ T \quad (0 \leqslant c \leqslant 1), \tag{6}$$

where Φ_1, Φ_2 are completely positive (CP) maps and T is transposition. The composition $\Phi_2 \circ T$ is called a *co-CP map*. For the Bloch vector, the CP maps form a semigroup in the group of orientation-preserving affine maps $\mathrm{GL}^+(3,\mathbb{R})\textcircled{S}\mathbb{R}^3$, where $\mathrm{GL}^+(3,\mathbb{R}) = \{g \in \mathrm{GL}(3,\mathbb{R}^3) \,|\, \det(g) > 0\}$ and "Ⓢ" denotes its semidirect product with the translation group $\mathbb{R}^3$.[17,21,22] Unital CP maps live in the $\mathrm{GL}^+(3,\mathbb{R})$ component, while unital co-CP maps live in the other component, $\mathrm{GL}^-(3,\mathbb{R}) \equiv \{g \in \mathrm{GL}(3,\mathbb{R}^3) \,|\, \det(g) < 0\}$. Restricting further to symmetries (i.e., trace- and norm-preserving maps), one gets rotations and reflections as above.

III. TWO QUBITS: PARTIAL TRANSPOSITION, PARTIAL TIME REVERSAL, MULTIPLE LOCAL REFLECTIONS AND TOTAL REFLECTIONS

For two qubits, a complete basis for the space of density matrices $\mathcal{D}_2 \subset \mathbb{C}^{4\times 4}$ is given by $\Lambda_{jk} = \lambda_j \otimes \lambda_k$ $(j,k \in \{0,1,2,3\})$. This basis is also orthonormal relative to the Hilbert-Schmidt inner product, i.e., $\mathrm{tr}(\Lambda_{jk}\Lambda_{lm}) = \delta_{jl}\delta_{km}$ for all $j,k,l,m \in \{0,1,2,3\}$. For a given density matrix ρ, the Λ-basis defines a real, rank 2 tensor ϱ^{jk} which gives a contravariant representation of the same density, $\rho = \varrho^{jk}\Lambda_{jk}$. Viewed as a 16-vector, ϱ^{jk} is affine, i.e., $\varrho^{00} = \mathrm{tr}(\rho\Lambda_{00}) = 1/2$, and it is bounded by the 15-dimensional sphere in $\mathbb{R}^{16}$ of radius 1,

$$\mathrm{tr}(\rho^2) = \mathrm{tr}((\varrho^{jk}\Lambda_{jk})^2) = \sum_{j,k=0}^{3,3} (\varrho^{jk})^2 \leqslant 1, \tag{7}$$

with equality if and only if the state is pure.

A two-qubit density matrix ρ is said to be *separable* if it can be written as a convex combination $\rho = \sum_{r=1}^{s} w^r \rho_{A,r} \otimes \rho_{B,r}$ for some set of real numbers $w^r \geqslant 0$ such that $\sum_{r=0}^{s} w^r = 1$, where $\rho_{A,r}$, $\rho_{B,r}$ are all single-qubit density matrices. A necessary and sufficient condition for the separability of a two-qubit density is provided by the positive partial transpose (PPT) criterion of Peres[6] and Horodecki.[23] The partial transpose of a two-qubit density matrix ρ with respect to the first (left) subsystem A is defined as $\rho^{T_A} \equiv (K \otimes \mathbb{1}_2)\rho(K \otimes \mathbb{1}_2)^\dagger$, and similarly $\rho^{T_B} \equiv (\mathbb{1}_2 \otimes K)\rho(\mathbb{1}_2 \otimes K)^\dagger$. Each partial transpose is still a well-defined (i.e., positive semidefinite) density operator if and only if ρ is separable. The PPT criterion may be viewed as a check on the feasibility of the "partial time reverse" operation:[18,19] changing the time arrow of one of the subsystems alone.

In terms of the Stokes tensor ϱ^{jk}, the description of partial transposition is very intuitive and relies on the observation that $\lambda_2 = -\lambda_2^T$ is the only Pauli matrix with imaginary elements.

Proposition 1: *For two qubits, the partial transpose operations on the density matrix* ρ^{T_A} *and*

TABLE I. Action (sign changes) of the rotations and reflections involving $\bar{R}_T$, $\bar{R}_S$, and $\bar{R}_{S,16}$ on the components of the 2-qubit Stokes tensor ϱ^{jk}.

ϱ^{jk}	$\bar{R}_T\otimes\mathbb{1}_4$	$\mathbb{1}_4\otimes\bar{R}_T$	$\bar{R}_T\otimes\bar{R}_T$	$\bar{R}_S\otimes\mathbb{1}_4$	$\mathbb{1}_4\otimes\bar{R}_S$	$\bar{R}_S\otimes\bar{R}_S$	$\bar{R}_{S,16}$
ϱ^{00}	+	+	+	+	+	+	+
ϱ^{01}	+	+	+	+	−	−	−
ϱ^{02}	+	−	−	+	−	−	−
ϱ^{03}	+	+	+	+	−	−	−
ϱ^{10}	+	+	+	−	+	−	−
ϱ^{11}	+	+	+	−	−	+	−
ϱ^{12}	+	−	−	−	−	+	−
ϱ^{13}	+	+	+	−	−	+	−
ϱ^{20}	−	+	−	−	+	−	−
ϱ^{21}	−	+	−	−	−	+	−
ϱ^{22}	−	−	+	−	−	+	−
ϱ^{23}	−	+	−	−	−	+	−
ϱ^{30}	+	+	+	−	+	−	−
ϱ^{31}	+	+	+	−	−	+	−
ϱ^{32}	+	−	−	−	−	+	−
ϱ^{33}	+	+	+	−	−	+	−
# sign changes	4	4	6	12	12	6	15

ρ^{T_B} act on the Stokes tensor ϱ^{jk} by changing the sign of all elements bearing the index "2" *in the corresponding subsystem*:

$$\rho^{T_A} = \varrho^{0k}\Lambda_{0k} + \varrho^{1k}\Lambda_{1k} - \varrho^{2k}\Lambda_{2k} + \varrho^{3k}\Lambda_{3k}, \tag{8a}$$

$$\rho^{T_B} = \varrho^{j0}\Lambda_{j0} + \varrho^{j1}\Lambda_{j1} - \varrho^{j2}\Lambda_{j2} + \varrho^{j3}\Lambda_{j3}. \tag{8b}$$

The verification is just a straightforward calculation, which may be found in Table I. Note also that for the "total" transpose ρ^T $(=(\rho^{T_A})^{T_B})$ we have instead

$$\Lambda_{jk}^T = \Lambda_{jk} \quad \text{if } j,k \neq 2 \quad \text{or } j=k=2, \tag{9a}$$

$$\Lambda_{jk}^T = -\Lambda_{jk} \quad \text{if } j=2 \quad \text{or } k=2, \quad j \neq k, \tag{9b}$$

showing that Λ_{22} behaves differently under partial or total transposition.

The PPT separability test of Peres-Horodecki relies essentially on the decomposability property (6): any 1-qubit positive but not CP map, when applied to a 2-qubit density, returns a density if and only if the original density is separable. Restricting from positive maps to symmetry operations is the same as restricting to local reflections. In fact, the map (8a) can be thought of as the linear transformation $\bar{R}_T\otimes\mathbb{1}_4$, where $\bar{R}_T$ is the following affine orientation-changing three-dimensional rotation: $\bar{R}_T=\mathrm{diag}(1,R_T)=\mathrm{diag}(1,1,-1,1)$. Since all single qubit reflections are unitarily equivalent, any matrix $R\in\mathrm{O}^-(3)$ can be used in place of R_T. Indeed, if $\bar{R}=\mathrm{diag}(1,R)$, then local operations from the same connected component of O(3) satisfy

$$\mathrm{eig}((\bar{R}\otimes\mathbb{1}_4)(\rho)) = \mathrm{eig}((\bar{R}_T\otimes\mathbb{1}_4)(\rho)), \tag{10}$$

where the notation must be interpreted as follows: the matrix $\bar{R}\otimes\mathbb{1}_4$ acts on the 16-vector ϱ^{jk} and the resulting 16-vector provides the coefficients in the sum over the basis elements Λ_{jk}, i.e., $(\bar{R}\otimes\mathbb{1}_4)(\rho)=((\bar{R}\otimes\mathbb{1}_4)^{lm}_{jk}\varrho^{jk})\Lambda_{lm}$.

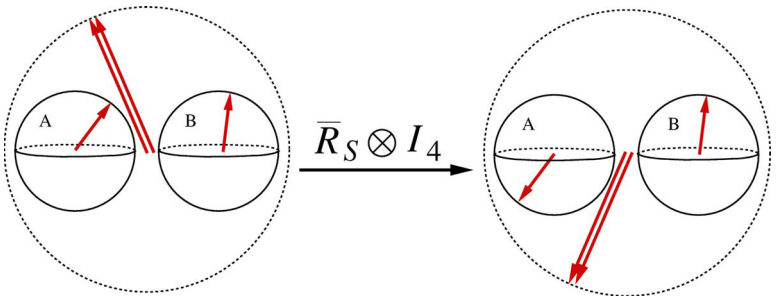

FIG. 2. (Color online) Reflections on a 2-qubit density matrix: the single qubit reflection $\bar{R}_S \otimes \mathbb{1}_4$ (PPT test).

Equation (10) shows that all reflections are positive but not completely positive. Thus we can reformulate the PPT criterion for the separability of two qubits as follows:

Theorem 1: *A two-qubit density matrix ρ is separable if and only if $(\bar{R} \otimes \mathbb{1}_4)(\rho)$ is a density matrix for any $R \in \mathrm{O}^-(3)$.*

A particularly simple such map is $\bar{R}_S = \mathrm{diag}(1, R_S)$, where R_S is the spin-flip operation from the preceding section. It is easily seen that $(\bar{R}_S \otimes \mathbb{1}_4)(\rho) = 2\varrho^{0k}\Lambda_{0k} - \rho$, so that the sign is changed in all elements ϱ^{jk} except those appearing in the reduced density matrix of the second qubit (i.e., the ϱ^{0k}).

The (total) transpose ρ^T of ρ corresponds to the matrix $\bar{R}_{T,16} = \bar{R}_T \otimes \bar{R}_T = \mathrm{diag}(1, R_{T,15})$ with $R_{T,15} = \mathrm{diag}(1,-1,1,1,1,-1,1,-1,-1,1,-1,1,1,-1,1) \in \mathrm{SO}(15)$, where the minus signs correspond to the six basis elements obeying (9b). Since the determinant of this matrix is positive, for two qubits the transpose is an orientation-preserving operation. Up to local operations $\bar{R}_T \otimes \bar{R}_T$ is equivalent to the "double local reflection" (or double spin-flip) map $\bar{R}_S \otimes \bar{R}_S$. The difference between $\bar{R}_S \otimes \mathbb{1}_4$ and $\bar{R}_S \otimes \bar{R}_S$ is easily understood by looking at Figs. 2 and 3. [In Figs. 2–4, the two vectors contained in the smaller spheres correspond to the Bloch vectors ϱ^{j0} and ϱ^{0k} of the two reduced density matrices, the third vector (double arrow) to the two-body correlation part of the Stokes tensor ϱ^{jk}, $j,k \neq 0$.] While $\bar{R}_S \otimes \mathbb{1}_4$ leaves the reduced density of the second qubit unchanged (Fig. 2), the correlation part remains unchanged under the action of $\bar{R}_S \otimes \bar{R}_S$ because its sign is flipped twice (Fig. 3). It may be shown, however, that both are positive but not-completely-positive maps.

All the "local" maps in O(3) mentioned so far are orientation-preserving when acting on two qubits, even though they all have at least one factor that is orientation-changing when acting on a single, isolated qubit: $\det(\bar{R}_T \otimes \mathbb{1}_4) = \det(\bar{R}_T \otimes \bar{R}_T) = \det(\bar{R}_S \otimes \mathbb{1}_4) = \det(\bar{R}_S \otimes \bar{R}_S) = 1$. The recovery of "parity" whenever an orientation-changing map is applied to two or more qubits is due to the

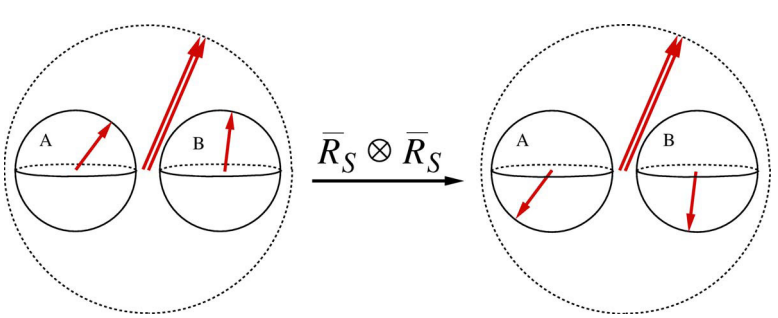

FIG. 3. (Color online) Reflections on a 2-qubit density matrix: the double local reflection $\bar{R}_S \otimes \bar{R}_S$ (which is equivalent to the total transpose under LOCC).

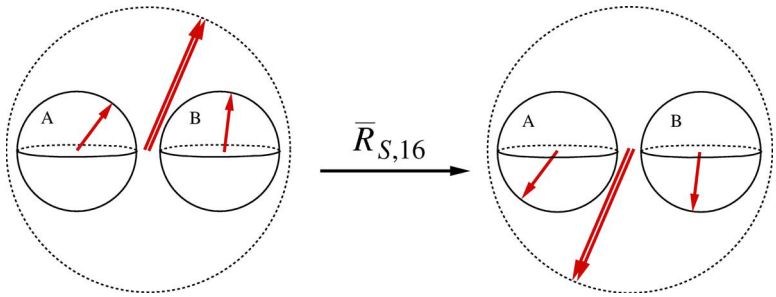

FIG. 4. (Color online) Reflections on a 2-qubit density matrix: the total reflection $\bar{R}_{S,16}$ (a nonlocal operation).

affine structure of the Hilbert space of a qubit (resulting in a *affine Bloch vector*), itself a consequence of the trace-preserving condition,

$$\begin{bmatrix} 1 & \\ & \mathrm{O}(3) \end{bmatrix} \otimes \begin{bmatrix} 1 & \\ & \mathrm{O}(3) \end{bmatrix} \subset \begin{bmatrix} 1 & \\ & \mathrm{SO}(15) \end{bmatrix}.$$

Hence the question arises: do there exist any orientation-changing symmetric operations on two qubits? One such map is the 2-qubit total reflection $\bar{R}_{S,16}=\mathrm{diag}(1,-\mathbb{1}_{15})$, $-\mathbb{1}_{15}\in O(15)\backslash\mathrm{SO}(15)=\mathrm{O}^{-}(15)$. Its action (see Fig. 4) corresponds to changing the sign of the entire tensor ϱ^{jk} except for affine component $\varrho^{00}=1/2$, thus the name *total reflection*. This nonlocal operation is genuinely new and inequivalent to any composition of local symmetric operations.

The most significant difference between total transpose and total reflection is that whereas the former map preserves the eigenvalues of the density matrix, the latter does not. Indeed, the total reflection is not even a positive map, since it converts the density matrix of any pure state to one with eigenvalues $[1,1,1,-1]/2$. This fact is readily established by writing the total reflection directly in terms of the Hermitian density matrix as

$$\bar{R}_{S,16}(\rho)=\tfrac{1}{2}\mathbb{1}_4-\rho, \tag{11}$$

which makes it clear that it holds for the density matrices of the basis states $|00\rangle\langle 00|$, $|01\rangle\langle 01|$, $|10\rangle\langle 10|$, and $|11\rangle\langle 11|$, and that the total reflection commutes with arbitrary two-sided unitary transformations of ρ.

The changes in the signs of the elements of the Stokes tensor are summarized in Table I for all the discrete symmetric operations mentioned in this section. It may be observed that $\bar{R}_S\otimes\bar{R}_S$ and $\bar{R}_{T,16}=\bar{R}_T\otimes\bar{R}_T$ both have an even number of "–" signs (6), whereas $\bar{R}_{S,16}$ has an odd number (namely 15), thus confirming that a total reflection on a two-qubit joint density is inequivalent to such operations.

In terms of density matrices, the positive-but-not-completely-positive operation $\bar{R}_S\otimes\bar{R}_S$ corresponds to

$$\bar{R}_S\otimes\bar{R}_S(\rho)=(\sigma_2\otimes\sigma_2)\rho^*(\sigma_2\otimes\sigma_2)=4\Lambda_{22}\rho^*\Lambda_{22}. \tag{12}$$

The transformed density matrix $\rho'\equiv\bar{R}_S\otimes\bar{R}_S(\rho)$ is frequently found in entanglement measures, including the concurrence $C(\rho)=\max\{0,\nu_1-\nu_2-\nu_3-\nu_4\}$ [where $\nu_j\in\mathrm{eig}(\rho\rho')$ (Ref. 24)] and the Lorentzian metric $\mathrm{tr}(\rho\rho')=(\varrho^{00})^2-\Sigma_{j=1}^3((\varrho^{0j})^2+(\varrho^{j0})^2)+\Sigma_{j,k=1}^3(\varrho^{jk})^2$.[9]

IV. TWO QUBITS: MATRIX STRUCTURES AND THE COMPUTABLE CROSS-NORM

In this section, we show how the foregoing nonunitary symmetry operations on a two-qubit density matrix can be expressed compactly using the Hadamard product of matrices[25] together with either the Stokes tensor or the real density matrix. We will also show that a non-separability

criterion called the computable cross-norm[26] (or the matrix realignment method[27]), which is inequivalent to the PPT criterion, can be computed directly from the Stokes tensor without having to convert back to the traditional Hermitian representation. For two qubits, the Stokes tensor can also be viewed as a square array of real numbers, which is related to the real density matrix as follows:

$$2\begin{bmatrix} \varrho^{00} & \varrho^{01} & \varrho^{02} & \varrho^{03} \\ \varrho^{10} & \varrho^{11} & \varrho^{12} & \varrho^{13} \\ \varrho^{20} & \varrho^{21} & \varrho^{22} & \varrho^{23} \\ \varrho^{30} & \varrho^{31} & \varrho^{32} & \varrho^{33} \end{bmatrix} \leftrightarrow \begin{bmatrix} \varrho^{00} & \varrho^{20} & \varrho^{02} & \varrho^{22} \\ \varrho^{10} & \varrho^{30} & \varrho^{12} & \varrho^{32} \\ \varrho^{01} & \varrho^{21} & \varrho^{03} & \varrho^{23} \\ \varrho^{11} & \varrho^{31} & \varrho^{13} & \varrho^{33} \end{bmatrix}. \tag{13}$$

The rearrangement of the elements seen here corresponds to the Choi[16] (also known as reshuffling[17]) map for $n=2$ qubits, but for $n>2$ the Stokes tensor-to-real density matrix map is not the same as the Choi map; indeed, then the order of the Stokes tensor is greater than 2, so it can no longer be identified so simply with a matrix.

The real density matrix has the useful feature of preserving the tensor product structure of the corresponding Hermitian density matrix, i.e., for two qubits: $\sigma(\rho\otimes\rho')=\sigma(\rho)\otimes\sigma(\rho')\equiv\sigma\otimes\sigma'$. It follows immediately that a 2-qubit real density matrix can be written as a convex combination of 1-qubit real density matrices if and only if the 2-qubit density is separable. A 2×2 real matrix, on the other hand, is a real density matrix if and only if its upper-left element is unity and the length of the Bloch vector determined by the remaining elements does not exceed unity [cf. Eq. (2)]. It should also be noted that, with either the real density matrix or the Stokes tensor, the partial trace operation involves only discarding elements involving the qubit traced over: no additional operations are needed as in the Hermitian representation.

As shown previously for the 1-qubit case, we can express involutory symmetry operations by means of Hadamard products of the real density matrix with matrices the elements of which are all ± 1. Moreover, these matrices will be tensor products if and only if the operations that define them are. This may be seen in the following list of sign matrices for all the operations given in Table I:

$$\bar{R}_T\otimes \mathbb{1}_4 \leftrightarrow \begin{bmatrix} +1 & -1 \\ +1 & +1 \end{bmatrix} \otimes \begin{bmatrix} +1 & +1 \\ +1 & +1 \end{bmatrix}, \tag{14a}$$

$$\mathbb{1}_4\otimes \bar{R}_T \leftrightarrow \begin{bmatrix} +1 & +1 \\ +1 & +1 \end{bmatrix} \otimes \begin{bmatrix} +1 & -1 \\ +1 & +1 \end{bmatrix}, \tag{14b}$$

$$\bar{R}_T\otimes \bar{R}_T \leftrightarrow \begin{bmatrix} +1 & -1 \\ +1 & +1 \end{bmatrix} \otimes \begin{bmatrix} +1 & -1 \\ +1 & +1 \end{bmatrix}, \tag{14c}$$

$$\bar{R}_S\otimes \mathbb{1}_4 \leftrightarrow \begin{bmatrix} +1 & -1 \\ -1 & -1 \end{bmatrix} \otimes \begin{bmatrix} +1 & +1 \\ +1 & +1 \end{bmatrix}, \tag{14d}$$

$$\mathbb{1}_4\otimes \bar{R}_S \leftrightarrow \begin{bmatrix} +1 & +1 \\ +1 & +1 \end{bmatrix} \otimes \begin{bmatrix} +1 & -1 \\ -1 & -1 \end{bmatrix}, \tag{14e}$$

$$\bar{R}_S\otimes \bar{R}_S \leftrightarrow \begin{bmatrix} +1 & -1 \\ -1 & -1 \end{bmatrix} \otimes \begin{bmatrix} +1 & -1 \\ -1 & -1 \end{bmatrix}, \tag{14f}$$

$$\bar{R}_{S,16} \leftrightarrow \begin{bmatrix} +1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \end{bmatrix}. \tag{14g}$$

Note that $\bar{R}_{S,16}$ is distinguished from the other operations not only by the fact that it is not orientation-preserving, but also by the fact that it is nonlocal and hence does not preserve the tensor product structure in the space of (real or Hermitian) density matrices. It is easily seen that the involutory mapping induced by any tensor product of sign matrices as above must preserve orientation, but there are many orientation-preserving mappings that are not tensor products, including the pair given below:

$$\begin{bmatrix} +1 & +1 & +1 & +1 \\ +1 & -1 & -1 & +1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & +1 & +1 \end{bmatrix} \leftrightarrow \begin{bmatrix} +1 & +1 & +1 & -1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & +1 & +1 \\ -1 & +1 & +1 & +1 \end{bmatrix}. \tag{15}$$

As indicated by the double arrow, these two are related by the Choi map, i.e., taking the Hadamard product of one with the real density matrix is the same as taking the Hadamard product of the other with the Stokes tensor [cf. Eq. (13)]. Tests with randomly generated pure states quickly show that neither of these maps is positive, let alone completely positive.

Similarly, one can easily construct many other discrete reflection symmetries which are neither locally nor unitarily equivalent to the total reflection, simply by composing the latter with any other nonlocal and nonunitary rotation symmetry. One interesting example is obtained by composing the local reflections $\bar{R}_S \otimes \bar{R}_S$ with the total reflection $\bar{R}_{S,16}$ on two qubits, obtaining

$$(\bar{R}_S \otimes \bar{R}_S)\bar{R}_{S,16} \leftrightarrow C \equiv \begin{bmatrix} +1 & +1 & +1 & -1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ -1 & -1 & -1 & -1 \end{bmatrix}. \tag{16}$$

The Hadamard product with C changes the sign of the bilinear (two-body) part of the Stokes tensor. It is, of course, a nonpositive map which takes the Hermitian density matrix of any pure state to one with eigenvalues $[1,1,1,-1]/2$. This map may also be written quite simply as an operator sum, as follows:

$$\sigma^{-1}(C \odot \sigma(\rho)) = \sum_{k=1}^{3} (\Lambda^{k0}\rho\Lambda^{k0} + \Lambda^{0k}\rho\Lambda^{0k}) - \frac{1}{2}\mathbb{1}_4. \tag{17}$$

Finally, we show how a separability test based on the so-called computable cross-norm (CCN), denoted in what follows by "ξ," can be performed directly using the Stokes tensor. The CCN is a lower bound on the cross-norm entanglement measure in a bipartite system, denoted by "Ξ," which satisfies $\Xi(\rho)=1$ if ρ is separable and $\Xi(\rho)>1$ if it is not.[26] Consequently, $\xi(\rho)>1$ implies ρ is nonseparable, though not vice versa; this condition is neither weaker nor stronger than the PPT criterion, but inequivalent to it. The CCN ξ is not itself an entanglement measure, since it may increase under the partial trace operation, but it has the advantage that it is readily computed as the sum of the singular values (also known as trace class norm) of the reshuffled density matrix Choi(ρ). For two qubits it can also be computed directly from the Stokes tensor, as shown by the following:

Proposition 2: *For two qubits, the singular values of the Stokes tensor* $\varrho^{k\ell}$, *regarded as a matrix as in Eq.* (13), *are twice those of the reshuffled density matrix* Choi(ρ).

Proof: The reshuffling operation is defined to satisfy $\mathrm{Choi}(\rho_1^T \otimes \rho_2) = |\rho_2\rangle\langle\rho_1^T|$, where $|\rho_2\rangle$ denotes the result of applying the reshaping operator to ρ_2, and $\langle\rho_1^T| = |\rho_1\rangle^T$. The one nonzero singular value of this matrix is simply the product of the Hilbert-Schmidt norms of its factors $\|\rho_1\|\|\rho_2\|$. Recall now that ρ is factorizable if and only if the corresponding real density matrix $\sigma(\rho)$ is and that the linear mapping $\sigma/2^{n/2}$ preserves the Hilbert-Schmidt norm (where n is the number of qubits). Hence $|\sigma(\rho_2)\rangle\langle\sigma(\rho_1^T)|/2$ is the singular value decomposition of the corresponding reshuffled real density matrix $\mathrm{Choi}(\sigma(\rho_1^T \otimes \rho_2))/2$, and its nonzero singular value is $\|\sigma(\rho_1)\|\|\sigma(\rho_2)\|/2 = \|\rho_1\|\|\rho_2\|$. Together with the fact that for two qubits the Stokes tensor and the real density matrix are related by the Choi map, this establishes the result for factorizable states.

To prove the general case, we recall that the reshaping map Choi is self-inverse. Thus the singular value decomposition of a general matrix $\mathrm{Choi}(\rho) = \Sigma_k \xi_k r_k s_k^T$ provides a canonical decomposition of ρ into a sum of tensor products $\Sigma_k p_k \rho_{1k}^T \otimes \rho_{2k}$, where $p_k = \xi_k r_k^T|\mathbb{1}_2\rangle s_k^T|\mathbb{1}_2\rangle$. Although p_k may be negative and the factors ρ_{1k}^T, ρ_{2k} of each term in this sum are not necessarily states (i.e., non-negative definite), we are free to apply the composition $\mathrm{Choi} \circ \sigma$ to each term $\rho_{1k}^T \otimes \rho_{2k}$ thereby obtained. Then noting that σ also preserves orthogonality and invoking the uniqueness of singular value decompositions completes the proof. □

The claim that ρ is separable implies $\xi(\rho) \leqslant 1$ can now be established directly, since $\xi(\rho_1 \otimes \rho_2) = \|\rho_1\|\|\rho_2\| \leqslant 1$ and ξ satisfies the triangle inequality just like any norm, so that for any $p_k \geqslant 0$ summing to unity we have $\xi(\Sigma_k p_k \rho_{1k} \otimes \rho_{2k}) \leqslant \Sigma_k p_k = 1$. The singular value decomposition of these matrices can be regarded as an extension of the Schmidt composition for pure states to mixed states. Indeed it can be shown that for pure states $\mathrm{Choi}(\rho)$ has a degenerate pair of singular values which are equal to twice the product of the corresponding Schmidt coefficients.

V. REFLECTIONS ON THREE OR MORE QUBITS

The situation is similar for three (or more) qubits, since the adjoint action (conjugation) still corresponds to a real "one-sided" rotation of the Stokes tensor, and the rotation group in all dimensions splits into orientation preserving and changing connected components. The main difference is that the number of inequivalent kinds of rotations and reflections goes us rapidly with the number of qubits. It is possible, however, to identify some particularly significant involutions. In the case of three qubits $\rho = \varrho^{jkl}\Lambda_{jkl}$, the following are some of the new possibilities:

(ia) the two-qubit partial transposition $\bar{R}_{T,16} \otimes \mathbb{1}_4$ (and the two others obtained by qubit permutation);

(ib) the total transposition $\bar{R}_{T,64} = \mathrm{diag}(1, R_{T,63})$ [where $R_{T,63} \in \mathrm{SO}(63)$ is diagonal with 28 −1's and 35 +1's in it], which changes the sign of just those elements ϱ^{jkl} with an odd number of indices equal "2";

(iia) the two-qubit "reflection" $\bar{R}_{S,16} \otimes \mathbb{1}_4$ (and the two others obtained by qubit permutation)—which is however an orientation-preserving rotation on three qubits;

(iib) the total (three-qubit) reflection $\bar{R}_{S,64} = \mathrm{diag}(1, -\mathbb{1}_{63})$.

The effect of $\bar{R}_{S,64}$ on ϱ^{jkl} is to change the sign of the entire tensor except for its constant component $\varrho^{000} = 1/(2\sqrt{2})$, showing that it may be expressed as

$$\bar{R}_{S,64}(\rho) = 2\varrho^{000}\Lambda_{000} - \rho = \tfrac{1}{4}\mathbb{1}_8 - \rho. \tag{18}$$

This is again a nonlocal operation which admits no factorization into independent one-qubit operations. Similarly, the action of $\bar{R}_{S,16} \otimes \mathbb{1}_4$ on $\varrho^{jk\ell}$ is to change the sign of the entire tensor except for the Bloch vector of the 1-qubit reduced density $\varrho^{00\ell}$. Items (ia) and (ib) above are fundamentally different from (iia) and (iib). The first two produce a Hermitian matrix with negative eigenvalues whenever the density has bipartite entanglement through the cut, whereas the latter two instead may map even separable densities to Hermitian matrices with negative eigenvalues. This can be seen looking at the components of the UPB state. If $\bar{R}_{S,64}$ is applied to the

(separable) density $\rho_{\mathrm{UPB-sep}}=\frac{1}{4}\Sigma_{j=1}^{4}|\psi_j\rangle\langle\psi_j|$ with $|\psi_j\rangle=|01+\rangle,|1+0\rangle,|+01\rangle,|---\rangle$ and $|\pm\rangle=1/\sqrt{2}(|0\rangle\pm|1\rangle)$, one gets the bound entangled state ρ_{UPB} used in Ref. 13. So in this case a separable state is reflected into an entangled state. However, no one of the four components $|\psi_j\rangle\langle\psi_j|$ taken alone (each is obviously separable) is a density when reflected. Obviously (ib) only reverses the time arrow on any 3-qubit density.

In similar fashion, for any number $n>1$ of qubits one can define an *m-qubit* $(1<m\leqslant n)$ *nonlocal* "reflection" $\bar{R}_{S,4^m}\otimes\mathbb{1}_{4^{n-m}}$, which is only a true (i.e., orientation-changing) reflection when the reflection is total $(m=n)$. Assuming the reflection acts on the first m qubits of an n-qubit density operator ρ, this may be written as

$$\bar{R}_{S,4^m}\otimes\mathbb{1}_{4^{n-m}}(\rho)=2\varrho^{0\cdots0j_{m+1}\cdots j_n}\Lambda_{0\cdots0j_{m+1}\cdots j_n}-\rho. \tag{19}$$

These operations leave the norm of the n-qubit tensor $\varrho^{j_1\cdots j_n}$ [i.e., $\mathrm{tr}(\rho^2)$] invariant, but need not preserve the spectrum nor even leave it nonnegative, as we saw above. Hence it is a "generically" ill-defined operation on the set of density operators of composite systems $\mathcal{D}_n$.

These observations are summarized in the following:

Proposition 3: *In* $\mathcal{D}_n$, *the linear map* $\bar{R}_{S,4^n}$ $(1<n)$:

(i) *preserves the trace and Hermiticity*;
(ii) *preserves the Hilbert-Schmidt inner product*;
(iii) *is neither unitary nor antiunitary*;
(iv) *is not* $\mathcal{D}_n$*-invariant*.

Properties (i) and (ii) together say that $\bar{R}_{S,4^n}$ is neither a contraction nor a dilation map, whereas (iv) affirms that $\bar{R}_{S,4^n}$ is not a positive map.

Nevertheless, it is possible to specify a simple spectral condition on the density matrix that guarantees that its total reflection is still non-negative definite.

Theorem 2: *Given* $\rho=\varrho^{0\ldots0}\Lambda_{0\ldots0}+\chi\in\mathcal{D}_n$ (*where* χ *is the associated homogeneous tensor*), *a sufficient condition for* $\tilde{\rho}=\bar{R}_{S,4^n}(\rho)=\varrho^{0\ldots0}\Lambda_{0\ldots0}-\chi\in\mathcal{D}_n$ *is that the set of eigenvalues satisfies* $\mathrm{eig}(\rho)\subset[0,2^{1-n}]$.

Proof: The proof is based on the well-known fact[25] that adding a multiple of the identity $c\mathbb{1}_m$ onto an $m\times m$ Hermitian matrix A shifts its eigenvalues by c, i.e., $\mathrm{eig}(A+c\mathbb{1}_m)=\mathrm{eig}(A)+c$. Since the eigenvalues of the random state's density matrix $\mathrm{eig}(\varrho^{0\ldots0}\Lambda_{0\ldots0})=\{2^{-n}\}$ (with multiplicity 2^n), we see that $\mathrm{eig}(\rho)\in[0,2^{1-n}]$ implies both $\mathrm{eig}(\chi)\in[-2^{-n},2^{-n}]$ and $\mathrm{eig}(-\chi)\in[-2^{-n},2^{-n}]$, so that $\mathrm{eig}(\tilde{\rho})\in[0,2^{1-n}]$, as well. □

Hence the linear map $\bar{R}_{S,4^n}$ is well-defined (positive) in the subset of densities with eigenvalues in the interval $[0,2^{1-n}]$.

Corollary 1: *A necessary but not sufficient condition for Theorem 2 to hold is that* $\mathrm{tr}(\rho^2)\leqslant 2^{1-n}$.

Proof: If $\mu_{\chi_1},\ldots,\mu_{\chi_{2^n}}$ are the eigenvalues of χ, when Theorem 2 holds it must be $r^2=\mu_{\chi_1}^2+\cdots+\mu_{\chi_{2^n}}^2\leqslant 1/2^n$. Hence $r\leqslant 1/2^{n/2}$ and $\mathrm{tr}(\rho^2)=(\varrho^{0\cdots0})^2+r^2\leqslant 1/2^{n-1}$. □

Corollary 2: *A necessary but not sufficient condition for* $\tilde{\rho}$ *to be a density is that* $\mathrm{rank}(\rho)\geqslant 2^{n-1}$.

In fact, only when ρ is a mixture of at least 2^{n-1} pure states one can achieve $\mathrm{eig}(\rho)\in[0,1/2^{n-1}]$.

On a 3-qubit density, the action of $\bar{R}_{S,16}\otimes\mathbb{1}_4$ is depicted in Fig. 5. Essentially the entire Stokes tensor changes sign, except for the reduced density $\mathrm{tr}_{AB}(\rho)$. Its action closely resembles the reduction criterion of Refs. 14 and 15. That criterion also makes implicit use of nonlocal reflections, but it is formulated based on a positive map, hence it is well-posed on all of $\mathcal{D}_n$. For a 3-qubit density it affirms that a necessary condition for separability is $\mathbb{1}_2\otimes\mathbb{1}_2\otimes\mathrm{tr}_{AB}(\rho)-\rho\geqslant 0$ as well as $\mathbb{1}_2\otimes\mathrm{tr}_A(\rho)\geqslant 0$ (and likewise for the other indexes). Since $\mathrm{tr}(\mathbb{1}_2\otimes\mathbb{1}_2\otimes\mathrm{tr}_{AB}(\rho)-\rho)=3$, one difference between our partial reflection and the reduction criterion is that the latter is not a trace preserving

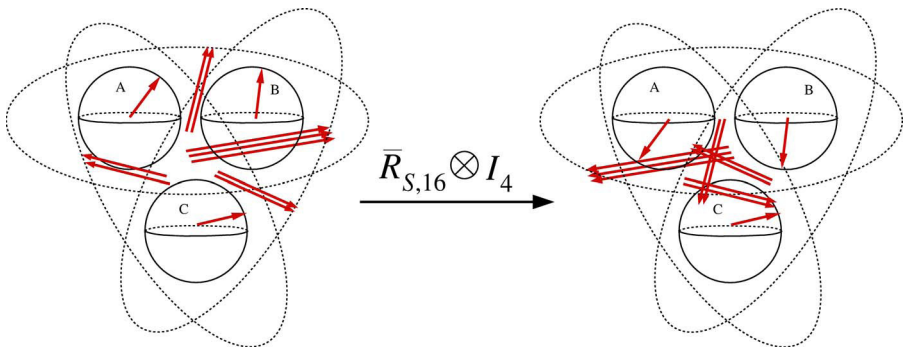

FIG. 5. (Color online) Schematic illustration of the action of a two-qubit reflection $\bar{R}_{S,16}\otimes\mathbb{1}_4(\rho)$ on three qubits. One-body (ϱ^{j00}, ϱ^{0k0} and $\varrho^{00\ell}$), two-body (ϱ^{jk0}, $\varrho^{j0\ell}$ and $\varrho^{0k\ell}$), and three-body ($\varrho^{jk\ell}$) correlation terms are indicated by single, double, and triple arrows. All the signs are changed except for those of $\varrho^{00\ell}$.

map. Thus it is not a symmetry in the sense used in the paper. Nonetheless, the reduction criterion utilizes a positive map which can be used to test separability. In our case $\bar{R}_{S,16}\otimes\mathbb{1}_4$ is not a positive map even when restricted to separable states with eigenvalues in $[0,1/4]$, in which the 3-qubit total reflection $\bar{R}_{S,64}$ is always well-posed.

We can, however, convert our 2-qubit total reflection $\bar{R}_{S,16}$ into a "relaxed" total reflection, namely

$$\bar{R}^{\mathrm{rel}}_{S,16}(\rho)=\tfrac{1}{3}(\mathbb{1}_4-\rho), \tag{20}$$

which is the same as $\bar{R}_{S,16}$ applied to the "remixed" density matrix $(\mathbb{1}_4/2+\rho)/3$. Since the remixed density matrix now has eigenvalues in $[0,1/2]$, the relaxed reflection is a positive map by Theorem 2. It is also easily shown that $\bar{R}^{\mathrm{rel}}_{S,16}$ is not completely positive, and hence provides a necessary condition for the separability of an arbitrary $2^n\times 2^n$, $n>2$, density matrix. It should be possible to relax all the reflections described in this paper to positive maps by a similar strategy.

Concerning a total reflection, all pairs ρ and $\tilde{\rho}=\bar{R}_{S,4^n}(\rho)$ satisfying Theorem 2 are complementary in the sense that their mixture is the random state:

$$\frac{1}{2}(\rho+\tilde{\rho})=\frac{1}{2^n}\mathbb{1}_{2^n}. \tag{21}$$

Equation (21) implies that $\bar{R}_{S,4^n}$ corresponds to a multiparty NOT operation. In fact, also in the single qubit case, the NOT operation corresponds to a change of sign to the homogeneous part (i.e., the Bloch vector) but it is not modifying the sign of the trace part and hence a qubit and its reflection obey to (21). Such operation is used for example to map a density operator belonging to a subset of the Hilbert space $\mathcal{D}_n$ to its complement in $\mathcal{D}_n$, for example in the UPB construction mentioned above.[13,28]

VI. CONCLUDING REMARKS

Reflections are a natural discrete class of transformations relative to the Stokes tensor and/or real density matrix parametrization. Their meaning and relation to LOCC is interesting and calls for natural generalizations to nonlocal operations in the way explained above. The nonlocal reflections, in fact, originate from the nonconnectedness of the group of rotations acting on the Stokes tensor parametrization. In terms of density matrices, this interpretation is not as sharp. As a matter of fact, operations reducible to reflections appear in the PPT test and in the various measures of entanglement relying upon "spin-flip" operations (like concurrence, negativity and tangle) for what concerns (multiple) 1-qubit reflections. Also nonlocal reflections are used: for

example a total reflection corresponds to what is normally referred to as "taking the complement of a density," used for example, in the construction of unextendible product basis states.[13] Likewise, the reduction criterion makes use of a positive map closely related to our nonlocal reflections.

For the purposes of further understanding the structure of composite quantum systems, we find it useful to have a unifying perspective on these nonunitary yet symmetric (in the sense of Wigner theorem) transformations.

It is worth pointing out that reflections can be defined in the same terms also for SLOOC (stochastic LOCC).[9,29,30] For the Stokes tensor, in fact, this class of operations relaxes the group of admissible local transformations from affine rotations to proper orthochronous local Lorentz transformations $\mathrm{SO}(1,3)$. The reflected action in $\mathrm{O}^{-}(3)$ then corresponds to choosing the other connected component of $\mathrm{O}(1,3)$ with the same time direction as $\mathrm{SO}(1,3)$ (i.e., with positive "timelike" metric element). Also nonlocal reflections fit in with the group structure of nonlocal filtering operations. For example, total reflections belong to $\mathrm{O}(1,4^n-1)\backslash\mathrm{SO}(1,4^n-1)$. Note further that the idea of restricting the set of density operators in order to have a larger set of symmetries is "dual" to the idea of using group actions that are contractions.[31,32]

The idea of using reflections does not extend in a straightforward manner to qutrids (nor to higher dimension quantum systems), as in this case the admissible parameters live on a rather complicated subset of the seven-dimensional sphere[33,34] for which the rotation representing transposition is always admissible but spatial inversion may not be. However, the various UPB constructions on 3×3 systems of Ref. 13 correspond to well-defined reflections.

Finally notice that there are many isometries of the Stokes tensor that do not correspond to reflections relative to any basis; those that do are of course involutions, and it would be interesting to show that any Stokes tensor isometry which is an involution (and hence is described by a symmetric orthogonal matrix) is a reflection relative to some basis.

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Finite quantum kinematics of the harmonic oscillator[a)]

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Arbitrarily small changes in the commutation relations suffice to transform the usual singular quantum theories into regular quantum theories. This process is an extension of canonical quantization that we call general quantization. Here we apply general quantization to the time-independent linear harmonic oscillator. The unstable Heisenberg group becomes the stable group SO(3). This freezes out the zero-point energy of very soft or very hard oscillators, like those responsible for the infrared or ultraviolet divergencies of usual field theories, without much changing the medium oscillators. It produces pronounced violations of equipartition and of the usual uncertainty relations for soft or hard oscillators, and interactions between the previously uncoupled excitation quanta of the oscillator, weakly attractive for medium quanta, strongly repulsive for soft or hard quanta. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2070088]

I. MAKE IT SIMPLE

The three main evolutions of physics in the twentieth century have a suggestive family resemblance. Each introduces a new kind of noncommutativity. The new noncommutativity in special relativity was that of boosts, in general relativity and the standard model gauge theories that of infinitesimal translations, and in quantum theory that of filter operations. The seminal work of Segal,[17] which stimulated the present work, pointed out that further changes of this kind are necessary for stability and suggested one. Our main goal is finiteness, not stability, but the stabilizing changes Segal suggested lead ultimately to a finite quantum theory, including one of space-time. Such a theory has been sought by physicists since the formulation of quantum theory.

By gently modifying the commutation relations of an existing quantum theory one produces a simpler theory with the existing quantum theory as a suitable limiting case, and with nearly the same continuous symmetries. A special form of Segal's general concept was applied retroactively to the relation between special relativity and Galileo relativity.[13,12] More proactively, Snyder's space-time quantization[19] was an attempted regularization and moved unwittingly toward simplicity but did not simplify the momentum algebra. Vilela made the first efforts to find a new particle theory on a simple algebra.[21] Something like the regularization of the harmonic oscillator proposed by Segal is now under study by several groups from several points of view.[6,1,14,15,20]

For example, 'tHooft[20] studies the classical particles on a circle and shows that under certain conditions, this system is equivalent to a quantum harmonic oscillator. The work of Vilela Mendes differs from others in presenting the quantum harmonic oscillator as a limit case of a "more quantum" oscillator that has a more stable algebra in the sense of Segal. We follow that line here.[18]

Naturally one discards the unregularized theory in favor of the regularized one. This last step is overlooked in some older studies.

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General quantization changes the quantization rules. It replaces the usual quantization prescription by the following one:

Make the commutator algebra of the generators a simple Lie algebra.

Briefly put: If the algebra is simple, keep it simple. If it is not simple, make it simple by the least change possible.

We apply this strategy to all the algebras postulated in a physical theory, on the grounds that they must all depend continuously on experimental data that are subject to error. An algebra that is not stable is not empirical but is at least partly based on ideology. It is not possible to eliminate all such ideology-based hypotheses from physics. But it is possible to reduce their number systematically.

This implies that canonical quantization and special and general relativization are relatively small parts of a vast unifying drift toward simplicity and unity of the groups beneath our physical theories. General quantization is an attempt to take part in that drift.

In the case of the algebra of variables, semisimplicity is as good as simplicity, since it implies a direct sum that we can reduce to a simple term forever by a single measurement of the superselection variable that distinguishes these terms.

Canonical quantization introduced one quantum constant and stabilized the atom. General quantization introduces as many quantum constants as necessary to stabilize the group of the theory.

General quantization has no effect on (say) the rotator quantum algebra with given angular momentum l [$\mathbf{L}\times\mathbf{L}=\mathbf{L}$, $\mathbf{L}\cdot\mathbf{L}=l(l+1)$], whose group is already simple. But it changes the quantum dynamics of a free particle deeply, revising the theories of both space and time.

We test general quantization here on the kinematics of the linear harmonic oscillator, a ubiquitous constituent of all present field theories, and compare the finite quantum oscillators with the usual quantum oscillators, which are singular in several senses. The differences have profound consequences for extreme energy physics: the physics of both very high and very low energies.

Planck's quantum constant h froze out the very stiff oscillators responsible for the infinite heat capacity of cavity radiation in Maxwell's theory, but the zero-point energy of the resulting quantum theory of electromagnetism still diverged, however, unless one arbitrarily replaced the local Lagrangian and Hamiltonian of Maxwell by nonlocal ones tailored to have some finite zero-point energy, usually set to 0 on grounds of Lorentz invariance. Indeed, the quantum theory of the harmonic oscillator carries the germs of all the main divergences of quantum field theory. Its basic operators of position q, momentum p, and Hamiltonian $H\sim\frac{1}{2}(p^2+q^2)$ are undefined on almost every vector ψ in its Hilbert space, $q\psi=p\psi=H\psi=\infty$. Such divergences occur in a quantum theory if and only if its Hilbert space is infinite dimensional.

The usual quantum oscillator theory is also unstable in the Segal sense detailed below. It is not as unstable as the classical theory, which has the operators q and p commute, and we have become accustomed to its foibles, but it is still not operational, in that its basic operations usually cannot be carried out. General quantization makes its Hilbert space finite dimensional. The result is a finite quantum theory whose operations can in principle be carried out, with two Segal quantum constants h',h'' besides the usual Planck constant.

We find that introducing these constants freezes out even the offending zero-point oscillations of extremely hard or soft oscillators without greatly changing the zero-point energies of medium ones. The frozen oscillators have infinitesimal zero-point energies compared to the usual quantum values. They also grossly violate the usual equipartition and uncertainty relations.

This toy model illustrates how a finite quantum theory of the cavity might produce a finite zero-point energy without conflicting with the many finite predictions and symmetries of the usual quantum theory. We propose that the linear harmonic field oscillators considered fundamental in present quantum physics—those of supposedly fundamental fields, not those of elastic solids, say—are actually finite quantum oscillators near the bottoms of their energy spectra. The unobserved oscillators responsible for the infrared and ultraviolet divergencies of present quantum theories are frozen by finite quantum effects described here and contribute negligibly to the zero-point energy.

The change we carry out here is not enough to make quantum field theory finite. For that we must also simplify the Heisenberg algebra of the space-time operators x^μ and ∂_μ. This replaces the manifold theory of space-time, which assumes an infinity of events, by a simple quantum theory, with only a finite number of disjoint events, though the number may be arbitrarily large. Field theory has compound algebra on two levels, that of the underlying space-time and that of the overlying canonical commutation relations. In this paper we change only one level.

II. ALGEBRA FLEXING AND FLATTENING

A *semisimple* group is a Lie group whose Lie algebra has no invariant solvable subalgebras; a Lie algebra A being solvable if for some integer $n \geqslant 0$, $A^n = \{0\}$. Then its Lie algebra has no radical. A group that is not semisimple we call *compound*. General quantization reduces the radical and ultimately eliminates it.

Lie products $\times$ on a given vector space A, also called structure tensors, form a submanifold $\{\times\}$ of the tensor space $A \otimes A\dagger \otimes A\dagger$. A *regular* (stable, robust) algebra is one that is unchanged up to isomorphism by all sufficiently small changes in its structure tensor (Lie product) within the manifold $\{\times\}$. For example, the Lorentz algebra is stable against corrections to the speed of light. By algebra *flexing* we mean a homotopy of the structure tensor of a compound algebra that makes it semisimple. Algebra *flattening* is the inverse process. The well-known contraction process of Inönü and Wigner[13] is a special case of flattening accomplished by a one-parameter group of dilations of a coordinate system of the Lie algebra in a fixed direction. The inverse to group contraction is *group expansion*[11] and is a special case of flexing.

Several regularization processes have been used to remove unwanted infinities from physics. Unphysical regularizations cope with the divergencies of a theory without changing the finite results. They are regarded as giving the theory meaning rather than changing the theory. These include Pauli-Villars regularization,[16] lattice regularization (lattice gauge theory)[22] and dimensional regularization.[4,5,20] They contain regularization parameters that go to singular limits, like the lattice spacing going to 0. Physical regularizations, on the contrary, change the finite predictions as well as making the infinite ones finite, and are intended as distinct physical theories in their own right. Their regularization parameters do not go to a singular limit but must be determined by experiment. The most famous example is Planck's, which ultimately led to quantum theory. This was a simplification in that the associative algebra generated by the position and momentum variables has a Lie algebra with an infinite-dimensional radical for $h=0$ but only a one-dimensional radical for $h>0$.

Physical regularizations are subtler than unphysical ones but their consequences for human thought have been more dramatic. General quantization is proposed as a physical regularization.

Compound algebras are *unstable* with respect to a small change in their structures.[17] Flexing stabilizes them.

Conversely, flattening destabilizes. Approximating a circle by a tangent line or a sphere by a tangent plane are well-known flattenings. The circle and sphere are finite and their flattened form is infinite. Finite dimensional representations of the group of the sphere—such as spherical harmonic polynomials—form a complete set on the sphere, and all the operators of an irreducible representation have finite bounded spectra. On the other hand, the tangent plane is not compact and requires infinite-dimensional representations of the translation group for a complete set, and its algebra generators have unbounded spectra.

III. SIMPLIFYING THE HEISENBERG ALGEBRA

The Heisenberg Lie algebra $\mathbf{H}(1)$ is defined by the commutation relations:

$$[p,x] = -i\hbar,$$

$$[i,x] = 0, \tag{1}$$

$$[x,i] = 0.$$

It is compound and the imaginary unit i generates its radical. Segal proposed to simplify H1 by introducing two more quantum constants, which we designate here by $\hbar'$ and $\hbar''$. His expanded commutation relations are, except for notation,

$$[p,x] = -\hbar i,$$

$$[i,p] = -\hbar' x, \tag{2}$$

$$[x,i] = \hbar'' p.$$

(Refs. 6, 21, and 17). The irreducible unitary representations of this group are infinite dimensional. To avoid possible divergences and other problems, we instead use the SO(3) regularization[3,2,9,10]

$$[p,x] = -i\hbar,$$

$$[i,p] = -x\hbar', \tag{3}$$

$$[x,i] = -p\hbar''.$$

Ultimately we will need an indefinite metric for physical reasons, but not for the time-independent harmonic oscillator.

Regularizing the Heisenberg algebra means changing the role of i in the theory from constant central element to quantum variable operator on the same footing as p and q. We call this i-activation. The new variable that it introduces is called a regulator. A previous exploration in quaternion quantum theory activated an i that served as the electromagnetic axis $\eta(x)$ that resolves the electroweak gauge boson into electromagnetic and weak bosons,[8] and gives mass to the charged partner of the photon through the Stückelberg-Higgs effect. This led to a natural SU(2) that was interpreted as isospin. That theory was dropped because it did not leave room for color SU(3). Here we activate i on more principled grounds, namely the principle of simplicity. There is now plenty of room for internal groups like color SU(3), though they do not arise for the harmonic oscillator.

General quantization leads to the same kind of factor-ordering problems as the special case of canonical quantization. To reduce these we regularize not Hermitian observables directly but skew-Hermition generators

$$\hat{q} = iq, \quad \hat{p} = -ip. \tag{4}$$

The usual quantum commutation relations are then

$$[\hat{q},\hat{p}] = \hbar i,$$

$$[i,\hat{q}] = 0, \tag{5}$$

$$[\hat{p},i] = 0,$$

$$\breve{\imath}^2 = -1.$$

The regularized generators $\breve{q},\breve{p},\breve{\imath}$ obey

$$[\breve{q},\breve{p}] = \hbar\breve{\imath},$$

$$[\breve{\imath},\breve{q}] = \hbar'\breve{p}, \tag{6}$$

$$[\breve{p},\breve{\imath}] = \hbar''\breve{q},$$

We suppose $\hbar,\hbar',\hbar''>0$ so the orthogonal group is SO(3). The quantities with a breve "" are the new expanded quantum operators. In this way the simplification process introduces a new dynamically variable generator $\breve{\imath}$, somewhat as general-relativization introduced the new dynamical variable $g_{\mu\nu}$ the gravitational metric tensor field. The most primitive theory with a dynamical variable like $\breve{\imath}$ is quaternion quantum field theory.[8] There $\breve{\imath}$ generates rotations about the electric (or electromagnetic) axis in isospin space, defining a natural Higgs field. We suppose that the present generator $\breve{\imath}$ is also a Higgs field.

When general quantization introduces new group generators in this way for simplification, we call these regularization operators or "regulators." The physical constants to which regulators reduce in the singular theory we call regularization constants or "regulants." Examples of a regulator in present physics are the Riemann curvature of space-time (as the commutator of covariant transports) and the gravitational field itself (as the anticommutator of unit Clifford vectors). Examples of regulants are $\hbar$ and c.

Except for scale factors the simplified commutation relations are those of an SU(3) quantum skew-angular-momentum operator-valued vector $\breve{\mathbf{L}}=\breve{\mathbf{L}}\times\breve{\mathbf{L}}$ for a dipole rotator in three dimensions. We assume an irreducible representation with

$$\breve{\mathbf{L}}^2 = -l(l+1), \tag{7}$$

where l can have any non-negative half-integer eigenvalue. In the present work it suffices to consider only integer values of l. Then the $\breve{L}_x,\breve{L}_y,\breve{L}_z$ are represented by $(2l+1)\times(2l+1)$ matrices obeying

$$[\breve{L}_1,\breve{L}_2] = \breve{L}_3,$$

$$[\breve{L}_2,\breve{L}_3] = \breve{L}_1, \tag{8}$$

$$[\breve{L}_3,\breve{L}_1] = \breve{L}_2,$$

$$(\breve{L}_1)^2 + (\breve{L}_2)^2 + (\breve{L}_3)^2 = -l(l+1).$$

We fix the scale factors with

$$\breve{q} = Q\breve{L}_1,$$

$$\breve{p} = P\breve{L}_2, \tag{9}$$

$$\breve{\imath} = J\breve{L}_3.$$

By (6),

$$J = \sqrt{\hbar' \hbar''} = 1/l,$$

$$Q = \sqrt{\hbar \hbar'}, \tag{10}$$

$$P = \sqrt{\hbar \hbar''}.$$

The commutation relations (8) and the angular momentum quantum number l determine a simple (associative) enveloping algebra $\mathrm{Alg}(\mathbf{L}, l)$. The spectral spacing of the $\check{L}_3$ is 1, so the finite quantum constants Q, P, J serve as quanta of position, momentum and $\check{\imath}$. Since q, p are supposed to have continuous spectra in quantum theory, the constants Q, P must be very small on the ordinary quantum scale. It follows that $J = QP/\hbar$ is also very small on that scale and $l \gg 1$.

For $l \gg \sqrt{l} \gg 1$, variations $\delta(\check{\imath}^2) \leqslant O(l^{-1/2}) \ll 1$ about $(\check{\imath})^2 = -1$ can be negligible at the same time as the spectral intervals $\delta p \leqslant P\sqrt{l}$ and $\delta q \leqslant Q\sqrt{l}$ for quasicontinuous $p, q \approx 0$. This simulates the usual oscillator.

IV. FINITE LINEAR HARMONIC OSCILLATOR

Now we specialize to the oscillator by fixing a Hamiltonian. For given finite-quantum constants P, Q the finite harmonic oscillator has a Hamiltonian of the form

$$H = \frac{P^2 L_x^2}{2m} + \frac{kQ^2 L_y^2}{2} := \frac{K}{2}(L_x{}^2 + \kappa^2 L_y{}^2), \tag{11}$$

where

$$K = \frac{P^2}{m}, \quad \kappa^2 = \frac{\hbar' mk}{\hbar''}. \tag{12}$$

For fixed $\hbar, \hbar', \hbar''$, all finite oscillators are divided into three kinds with ill-defined boundaries: *medium*, where kinetic and potential terms in H are of comparable size ($\kappa \sim 1$); *soft*, when the potential energy term is dominant ($\kappa \to 0$); and hard, when the kinetic energy term is dominant ($\kappa \to \infty$). Examination of the Hamiltonian of a spin-zero scalar field (Klein-Gordon field) in quantum field theory shows that the possibilities $\kappa \ll 1$ and $\kappa \gg 1$ are also important. The oscillators that give rise to infrared divergencies of the quantum field theory correspond to soft oscillators of the finite quantum theory. Those that feed ultraviolet divergencies correspond to hard oscillators.

V. MEDIUM OSCILLATORS

The case $\kappa = 1$ is symmetric under rotations about the z axis, and so is especially simple.[20] Since

$$(\check{L}_1)^2 + (\check{L}_2)^2 + (\check{L}_3)^2 = (\check{L}^2), \tag{13}$$

$$\check{H} = \frac{K}{2}(l(l+1) + (\check{L}_3)^2). \tag{14}$$

The oscillator quantum number n that labels the energy level is now

$$n = l + m. \tag{15}$$

The expanded energy spectrum is

$$E_n = \frac{K}{2}(l(l+1) - (n-l)^2) = lK\left(n + \frac{1}{2} - \frac{n^2}{2l}\right). \tag{16}$$

For $n \ll \sqrt{l} \ll l$ this reproduces the usual uniformly spaced oscillator energy spectrum as closely as desired, but with multiplicity 2 for each level instead of 1.

The ground-state energy for this oscillator is

$$E_0 = \tfrac{1}{2}Kl = \tfrac{1}{2}1/2\hbar\omega, \tag{17}$$

exactly the usual oscillator ground energy, since $Kl = \hbar\omega$.

The main new feature is that this finite oscillator has an upper energy limit

$$E_{\max} = \tfrac{1}{2}Kl(l+1) \tag{18}$$

as required by a finite quantum theory.

In the general case of $\kappa \sim 1$ we obtain an upper bound for the ground energy by a variational approximation with the trial function $|L_z = \pm l\rangle$. This reproduces our previous result (17), now as an upper bound for the ground energy of a medium FLHO,

$$E_0 \leqslant \tfrac{1}{2}Kl. \tag{19}$$

Medium oscillators have many states with m-value close to its extremum value $m = \pm l$. The usual Heisenberg uncertainty principle

$$(\Delta p)^2(\Delta q)^2 \geqslant \frac{1}{4}\langle i[p,q]\rangle^2 = \frac{\hbar^2}{4} \tag{20}$$

becomes

$$(\Delta L_x)^2(\Delta L_y)^2 \geqslant \frac{\hbar^2}{4}\langle L_z\rangle^2_{|L_z \approx \pm l\rangle} \tag{21}$$

for a low-lying energy level of a medium oscillator. By (9) and (10),

$$(\Delta p)^2(\Delta y)^2 \geqslant \frac{\hbar^2}{4} \tag{22}$$

for large l. So medium oscillator states in low-lying energy levels have uncertainties at or above the lower limit set by the Heisenberg uncertainty principle.

VI. SOFT OSCILLATORS

Recall our finite quantum oscillator Hamiltonian

$$\check{H} = \frac{K}{2}(\check{L}_x^2 + \kappa^2 \check{L}_y^2). \tag{23}$$

When $\kappa \ll 1$ we can estimate the spectrum of $\check{H}$ using perturbation theory. The unperturbed Hamiltonian for our problem is the kinetic energy

$$H_0 = \frac{K}{2}L_x^2 \tag{24}$$

and the unperturbed eigenvectors are $|L_x = m\rangle$ so the unperturbed energy levels are

$$E_m(0) = \frac{K}{2}m^2. \tag{25}$$

The first-order shifts are

$$\delta E_m = \frac{K}{2}\langle L_x = m|L_y^2|L_x = m\rangle. \tag{26}$$

Due to the axial symmetry of $|L_x=m\rangle$,

$$\langle L_x = m|L_y^2|L_x = m\rangle = \langle L_x = m|L_z^2|L_x = m\rangle. \tag{27}$$

Therefore the energy shift is, to lowest order in κ^2,

$$\begin{aligned}\frac{K}{2}\langle L_x = m|\kappa^2 L_y^2|L_x = m\rangle &= \frac{K}{4}\kappa^2\langle m|L_x^2 + L_y^2|m\rangle \\ &= \frac{K}{4}\kappa^2\langle m|L^2 - L_z^2|m\rangle \\ &= \frac{K}{4}\kappa^2 l(l+1) - m^2.\end{aligned} \tag{28}$$

The new energy spectrum is then

$$E_m \approx \frac{K}{2}m^2 + \Delta E_m = \frac{K}{2}m^2 + \frac{1}{4}K\kappa^2[l(l+1) - m^2]. \tag{29}$$

The estimated upper bound for the energy is

$$E_{\max} \approx \frac{1}{2}Kl^2\left(1 + \frac{\kappa^2}{2l}\right). \tag{30}$$

For $\kappa \to 0$ this reproduces the upper bound for the unperturbed Hamiltonian L_z^2, as it should. The zero-point energy E_0 of first-order perturbation theory is

$$E_0 \approx \tfrac{1}{4}\kappa^2 Kl(l+1). \tag{31}$$

For $\kappa \to 0$ this is infinitesimal compared to the usual QLHO.

A soft oscillator shows no resemblance to the usual quantum oscillator. Its energy levels do not have uniform spacing. Its kinetic energy dwarfs its potential energy, so equipartition is grossly violated. The low energy states are near $|L_x=0\rangle$ instead of $|L_z=\pm l\rangle$. Its p degree of freedom is frozen out. It is "too soft to oscillate:" There is not enough energy in the q degree of freedom, even at its maximum excitation, to produce one quantum of p. The uncertainty relation reads

$$(\Delta L_x)^2(\Delta L_y)^2 \geqslant \frac{\hbar^2}{4}\langle L_z\rangle^2_{|L_x\approx 0\rangle} \approx 0. \tag{32}$$

Therefore

$$\Delta p \Delta q \ll \frac{\hbar}{2}, \tag{33}$$

which violates the Heisenberg uncertainty principle grossly.

VII. HARD OSCILLATORS

The story is just reversed for hard oscillators but the gross violations of usual quantum principles remain the same. A hard oscillator has much greater potential than kinetic energy. Its low energy states are now near $|L_y=0\rangle$ instead of $|L_z=\pm l\rangle$ (the medium case) or $|L_x=0\rangle$ (the soft case). Its q degree of freedom is frozen out. It is "too hard to oscillate." There is not enough energy in the p degree of freedom, even at maximum excitation, to arouse one quantum of q.

A hard oscillator can also be treated by perturbation theory. The kinetic energy is the perturbation. We may carry all of the main results in the preceding section for soft FLHO oscillators to the hard ones simply by replacing κ with $1/\kappa$ and K with $K\kappa^2$. A hard FLHO shows no resemblance to the usual QLHO. Its zero-point energy E_0 is now

$$E_0 \approx \frac{K}{4} l(l+1). \tag{34}$$

For $\kappa \to \infty$ this is infinitesimal compared to the usual quantum oscillator zero-point energy. Its energy levels of a hard oscillator are not uniformly spaced. Its uncertainty relation reads

$$(\Delta L_x)^2 (\Delta L_y)^2 \geqslant \frac{\hbar^2}{4} \langle L_z \rangle^2_{|L_y \approx 0\rangle} \approx 0. \tag{35}$$

Therefore

$$\Delta p \Delta q \ll \frac{\hbar}{2}, \tag{36}$$

which seriously violates the Heisenberg uncertainty principle again.

VIII. UNITARY REPRESENTATIONS

Variables p and q do not have finite-dimensional unitary representations in classical and quantum physics. They are continuous variables and generate unbounded translations of each other. But since in the finite quantum theory, all operators become finite and quantized, we expect all translations to become rotations with simple finite-dimensional unitary representations.

The canonical group of a classical oscillator becomes the unitary group of an infinite-dimensional Hilbert space for a quantum oscillator, and the unitary group of a $2l+1$ dimensional Hilbert space for the finite oscillator.

The Lie algebra generated by momentum and position as infinitesimal symmetry generators is $\mathbf{H}(1)$ for the classical and quantum oscillator and the $\mathbf{SO}(3)$ angular momentum algebra for the finite oscillator. The corresponding Lie groups are the Heisenberg group $\mathbf{H}(1)$ and $\mathbf{SO}(3)$.

Unitarily inequivalent unitary representations of the canonical commutation relations are forbidden in quantum mechanics but are present and important in quantum field theory, but general quantization eliminates them. After general quantization the commutation relations become those of a large simple group, and we presently explore the orthogonal groups. Once its invariants are fixed, as by measurement, the finite-dimensional unitary representations of this group are uniquely determined up to unitary equivalence. Yet the general quantized theory approaches the usual singular theory in an appropriate limit, where the dimension of the representations grow without bound and the group becomes compound. The inequivalent representations of quantum field theory must return in that singular limit. More than that we cannot say at this stage in the development.

IX. CONCLUSION

We suggest that algebra flattening causes the infinities of present physics. Since quantum theory began as a regularization procedure of Planck, it is rather widely accepted that further regularization of present quantum physics calls for further quantization, but what to quantize and

how to quantize it remains at least a bit unclear. If we regard quantization as another step in group regularization, the rest of the path becomes clear. It is blazed with radicals ripe for relativization. General quantization of the linear harmonic oscillator results in a finite quantum theory with three quantum constants $\hbar, \hbar', \hbar''$ instead of the usual one. The finite quantum oscillator is isomorphic to a dipole rotator with $N=l(l+1)\sim 1/(\hbar'\hbar'')\gg 1$ states and bounded Hamiltonian $H=A(L_x)^2+B(L_y)^2$. Its position and momentum variables are quantized with uniformly spaced bounded finite spectra and supposedly universal quanta of position and momentum. For fixed quantum constants and large $N\gg 1$ there are three broad classes of finite oscillator, soft, medium, and hard. The field oscillators responsible for infrared and ultraviolet divergences are soft and hard, respectively. Medium oscillators have $\sim\sqrt{N}$ low-lying states having nearly the same zero-point energy and level spacing as the quantum oscillator and nearly obeying the Heisenberg uncertainty principle and the equipartition principle. The corresponding rotators are nearly polarized along the z axis with $L_z \sim \pm l$.

The soft and hard oscillators have infinitesimal 0-point energy, and grossly violate both equipartition and the Heisenberg uncertainty relation. They do not resemble the quantum oscillator at all. Their low-lying energy states correspond to rotators with $L_x\sim 0$ or $L_y\sim 0$ instead of $L_z\sim \pm l$. Soft oscillators have frozen momentum $p\approx 0$ because their maximum potential energy is too small to produce one quantum of momentum. Hard oscillators have frozen position $q\approx 0$ because their maximum kinetic energy is too small to produce one quantum of position.

The zero-point energy of a physical oscillator likely contributes to its gravitational field. It will be interesting to estimate its contribution to astronomical gravitational fields. For a consistent estimate we should regularize the quantum field theory, not just one of its oscillators. This changes not only the structure of the individual oscillators, as considered here, but also the number and distribution of the oscillators. We leave this study for later, but it is already easy to say how it will proceed, and what form it will take.

Field theory has compound algebras on two levels, that of the underlying space-time and that of the overlying canonical commutation relations regularization. In this paper we change only the top level, but to simplify field theory we must also simplify the Heisenberg algebra of the lower-level space-time operators x^μ and ∂_μ. This replaces the manifold theory of space-time, which assumes an infinity of events, by a simple quantum space-time theory, with only a finite number of disjoint events, though that number may be arbitrarily large.

We must then combine two finite-dimensional algebras, that of the local field variables and that of the space-time-energy-momentum variables, to make the finite-dimensional algebra of the field theory. In c discrete theories, the combination process is exponentiation S^T where S is the local field-variable state-set and T is the space-time set. In the q/c theories that work best today, where the numerator q indicates that S is quantum and the denominator c indicates that T is still classical, an exponential still exists and is used. General quantization leads to q/q theories. In that case the usual exponential S^T becomes basis dependent, and the most economical invariant construct that includes all the special cases is the exterior algebra over $S\otimes T$, but this is still finite dimensional. Since general quantization gives time too a beginning and an end, the time development is certainly not unitary. As a result the problem of reconciling unitarity, causality, and Lorentz invariance[7] is eliminated. On the other hand, since the Lorentz group is already simple, Lorentz invariance is unaffected by general quantization.

General quantization modifies low- and high-energy physics. Because the low-lying energy levels of medium oscillators have nearly uniform spacing, the energy of two excitations is but slightly less than the sum of their separate energies. The corresponding quanta nearly do not interact, and the small interaction that they have is attractive. For soft or hard oscillators, the energy level varies quadratically with the energy quantum number. The energy of two quanta of oscillation is twice the sum of their separate energies, for example. The corresponding quanta have a repulsive interaction of great strength; the interaction energy is equal to the total energy of the separate quanta. Thus the simplest regularization leads to interactions between the previously uncoupled excitation quanta of the oscillator, weakly attractive for medium quanta, strongly repulsive for soft or hard quanta.

Like Dirac's theory of the "anomalous" magnetic moment of the relativistic electron, these extreme-energy effects depend on factor ordering. They can be adjusted to fit the data by reordering factors and so are not crucial tests of the theory. A group regularization of a time-dependent free Dirac equation has been carried out[10] and the extension to interactions is under study.

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Exact supersymmetry in the relativistic hydrogen atom in general dimensions—supercharge and the generalized Johnson-Lippmann operator

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A Dirac particle in general dimensions moving in a $1/r$ potential is shown to have an exact supersymmetry, for which the two supercharge operators are obtained in terms of (a D-dimensional generalization of) the Johnson-Lippmann operator, an extension of the Runge-Lenz-Pauli vector that relativistically incorporates spin degrees of freedom. So the extra symmetry (S(2)) in the quantum Kepler problem, which determines the degeneracy of the levels, is so robust as to accommodate the relativistic case in arbitrary dimensions. © *2006 American Institute of Physics.*
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INTRODUCTION

There is an increasing amount of fascination with supersymmetry (SUSY) in various fields of physics.[1,2] In a broad context SUSY is a kind of (graded) Lie algebra that closes under a combination of commutation and anticommutation.[3] One of the simplest realizations of such a symmetry may be found in one of the oldest problems in physics—motion of an electron in a hydrogen atom, or, classically, Kepler's problem. It has long been known that there is a hidden symmetry (a dynamical symmetry) in the problem, which is related to an extra conservation (the Runge-Lenz vector). So the symmetry of the problem is higher (SO(4)) than the trivial SO(3), which is the cause of the "accidental" degeneracy (i.e., the energy level independent of l) in the spectrum of the hydrogen in nonrelativistic quantum mechanics. If we move on to the Dirac electron in hydrogen in the relativistic quantum mechanics, the accidental degeneracy is lifted (since the Runge-Lenz vector, which designates the direction of the perihelion, is no longer conserved). However, the degeneracy is lifted only incompletely, and twofold degeneracies [for the Dirac-operator quantum number $\kappa \equiv -(2\mathbf{S}\cdot\mathbf{L}+1) = \pm(j+1/2)$ with j being the total angular momentum] remain, which was puzzling.

In 1985 Sukumar made an interesting suggestion that the strange degeneracy may be explained as a supersymmetry in the problem.[4] Subsequently however, Tangerman and Tjon[5] who have pointed out that there is indeed an exact supersymmetry for the nonrelativistic hydrogen atom, criticized that Sukumar's work has not actually constructed supercharges for the relativistic hydrogen atom. On the other hand, analytic studies for the relativistic hydrogen in general spatial dimensions have been developed, and analytic solutions are now obtained.[6,7]

Given this background, the purpose of the present paper is to show that an exact supersymmetry for the relativistic Dirac particle in a $1/r$ potential in fact exists in general D spatial dimensions. In doing so we have actually constructed the supercharges $Q_{\pm}$ (i.e., mutually anticommuting operators that commute with the Hamiltonian) for the Dirac Hamiltonian in $(D+1)$ dimensions. The symmetry enables us to obtain the lowest eigenenergy and its wave function for each sector of (the D-dimensional generalization of) $|\kappa|$ in a simple and transparent manner, so the problem indeed turns out to be algebraically solvable.

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One interesting point is whether the supersymmetry in the hydrogen problem is related to the Runge-Lenz vector that describes the hidden conservation law on the nonrelativistic level. Dahl and Jorgensen[8] have shown, for the relativistic hydrogen in $(3+1)$ dimensions, that the Runge-Lenz-Pauli vector (that necessarily involves spin degrees of freedom for the Dirac particle, and is called Johnson-Lippmann operator[9]) may be indeed used to construct supercharges describing the supersymmetry. So the question we address here amounts to whether this extends to general dimensions. We first construct the Johnson-Lippmann operator generalized to the relativistic hydrogen in $(D+1)$ dimensions, and then show that the generalized operator may actually be used to construct the supercharges. The supercharges are in fact shown to reduce to (the $(D+1)$ dimensional generalization of) Runge-Lenz-Pauli vector in the nonrelativistic limit. While the Runge-Lenz-Pauli vector in general dimensions has been discussed in Refs. 10 and 11 for the nonrelativistic case, the relativistic one is obtained for the first time. So we shall conclude that the supersymmetry is unexpectedly robust enough to be extended to the most general case, i.e., relativistic case in general dimensions. We can summarize the situation as

	$D=3$	General D
Nonrelativistic	SUSY (Ref. 5)	energy levels (Ref. 12)
Relativistic	SUSY (Ref. 8)	SUSY (present work)

DIRAC'S EQUATION

Dirac's equation for the relativistic hydrogen atom in $(D+1)$ dimensions is written, in natural units (where $c=\hbar=1$), as

$$\{\gamma^0(p_0 - eA_0) + \gamma^j p_i - m\}\Psi(x) = 0 \tag{1}$$

in standard notations, where γ's satisfy $\{\gamma^\mu, \gamma^\nu\}=g^{\mu\nu}=\mathrm{diag}(1,-1,-1,\ldots)$, $p_\mu = i\partial_\mu$, $x=(x^0,x^1,\ldots,x^D)$, and summations over repeated indices are implied. We assume a $1/r$ potential, so we have $eA_0=-Z\alpha/r$, where $\alpha=e^2/(\hbar c)$ is the fine-structure constant and Z the atomic number. When the lines of electric force are allowed to spread in the D spatial dimensions the Coulomb potential becomes $1/r^{D-2}$, but we focus on the $1/r$ potential for general dimensions to retain the atomic stability.[13] We come back to this point later. If the time derivative is explicitly written, we have

$$\begin{aligned} i\frac{\partial}{\partial x^0}\Psi(x^0,x^1,\ldots,x^D) &= H\Psi(x^0,x^1,\ldots,x^D), \\ H &= \gamma^0 m + \gamma^0\gamma^j p^i - \frac{Z\alpha}{r}(i=1,2,\ldots,D), \end{aligned} \tag{2}$$

where H is the Hamiltonian and summations are implied for repeated spatial superscripts.

The operators that commute with the Hamiltonian are the total angular momentum (in D spatial dimensions),

$$\begin{aligned} J_{ab} &= L_{ab} + \frac{i}{2}\gamma^a\gamma^b, \\ L_{ab} &= ix_a\partial_b - ix_b\partial_a, \end{aligned} \tag{3}$$

and the Dirac operator (in D dimensions),

$$K \equiv \gamma^0 \left\{ \frac{i}{2} \sum_{a \neq b} \gamma^a \gamma^b L_{ab} + \frac{1}{2}(D-1) \right\} = \gamma^0 \left\{ \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 + \frac{1}{2}(D-1) \right\}, \tag{4}$$

that is related to the spin-orbit interaction.

GENERALIZED JOHNSON-LIPPMANN OPERATOR

While $\mathbf{J}$ and K are (usually the only) constants of motion for arbitrary central fields, it is known, for the ordinary $D=3$, that there is an extra operator, a relativistic analogue of the Runge-Lenz-Pauli vector, that commutes with the Hamiltonian, as first constructed by Johnson and Lippmann.[9] We now generalize the Johnson-Lippmann operator to $(D+1)$ dimensions to define a generalized Johnson-Lippmann operator,

$$A \equiv \gamma^{D+1} \gamma^0 \gamma^j \frac{x^i}{r} - \frac{i}{Zm\alpha} K \gamma^{D+1} (H - \gamma^0 m). \tag{5}$$

Here we have defined γ^{D+1}, a pseudoscalar, which is a generalization of γ^5 in $(3+1)$ dimensions, and which satisfies $(\gamma^{D+1})^\dagger = \gamma^{D+1}, (\gamma^{D+1})^2 = 1$, $\{\gamma^{D+1}, \gamma^\mu\} = 0$. γ^{D+1} is constructed from $\{\gamma^0, \gamma^1, \ldots, \gamma^D\}$, but its actual form depends on whether the spatial dimension is even or odd.

From the (anti)commutation relations above, we can show, after a rather tedious manipulation, that we have indeed $[H,A]=0$ with a notable relation between H and A,

$$A^2 = 1 + \left(\frac{K}{Z\alpha} \right)^2 \left(\frac{H^2}{m^2} - 1 \right). \tag{6}$$

The expression reduces to the $D=3$ counterpart obtained in Refs. 8 and 14.

For K and A, on the other hand, we can show that

$$\{A,K\} = 0,$$

i.e., we end up with mutually anticommuting operators, K,A, that commute with H.

CONSTRUCTION OF THE SUPERCHARGE OPERATORS

We are now in position to construct the generators of the supersymmetry, which was left undone in Ref. 8 and stated in Ref. 5 as an operator interesting to find. We can do so by going back to a supersymmetric quantum mechanical model originally conceived by Witten,[3,15] to which the present Hamiltonian is shown to be formally equivalent. Due to the relation (6), we can take $\mathcal{H} \equiv A^2$ as a Hamiltonian of the present problem. We can construct two operators Q_1, Q_2 that commute with $\mathcal{H}$,

$$Q_1 = A, \quad Q_2 = i \frac{AK}{|\kappa|}, \tag{7}$$

where κ is the eigenvalue of K. We have then

$$\begin{aligned} \mathcal{H} &= Q_1^2 = Q_2^2, \\ \{Q_1, Q_2\} &= 0. \end{aligned} \tag{8}$$

If we further define

$$Q_\pm \equiv \frac{1}{2}(Q_1 \pm iQ_2) = \frac{1}{2}\left(1 \pm \frac{K}{|\kappa|}\right)A = \frac{1}{2}A(1 \mp \mathcal{P}_\kappa) \tag{9}$$

with $\mathcal{P}_\kappa \equiv K/|\kappa|$, we have

$$\begin{aligned} Q_+^2 = Q_-^2 = 0, \\ \mathcal{H} = \{Q_+, Q_-\}. \end{aligned} \tag{10}$$

This establishes an equivalence to Witten's model.

So we can take the eigenvectors $|n, \pm\rangle$ that satisfy

$$\begin{aligned} \mathcal{H}|n, \pm\rangle = E_n^{(\pm)}|n, \pm\rangle, \\ \mathcal{P}_\kappa|n, \pm\rangle = \pm|n, \pm\rangle, \end{aligned} \tag{11}$$

since $\mathcal{H}=A^2$ commutes with K, and we can talk about the simultaneous eigenvectors.

$\mathcal{P}_\kappa$ does not commute with $Q_\pm$, for which we have $Q_\pm|n, \pm\rangle = 0$. On the other hand, $[\mathcal{H}, Q_\mp] = 0$ implies that $|n, \pm\rangle$ and $Q_\mp|n, \pm\rangle$ have a degenerate eigenvalue of $\mathcal{H}$ with different eigenvalues of $\mathcal{P}_\kappa$. From the relation (6) a zero eigenstate of $\mathcal{H}=A^2$ is the ground state of the original H (or, more precisely, the lowest-energy state for each value of κ). Since $\langle n, \sigma|\mathcal{H}|n, \sigma\rangle = \langle n, \sigma|\{Q_+, Q_-\}|n, \sigma\rangle = |Q_+|n, \sigma\rangle|^2 + |Q_-|n, \sigma\rangle|^2 \geqslant 0$ (for $\sigma = \pm$), a state is the ground state of H if the equality holds in the above inequality. The equality occurs when $Q_+|0, -\rangle = 0$ or $Q_-|0, +\rangle = 0$. If we go back to the definition of $Q_\pm$ [Eq. (9)], the zero-eigenvalue state $|0\rangle$ should satisfy

$$A|0\rangle = 0,$$

since $(1 \mp \mathcal{P}_\kappa)|n, \mp\rangle \neq 0$.

KERNEL OF *A*

One way to establish the existence of such a state is an analytic method. Following Ref. 6, we write the wave function for odd spatial dimensions $D=2N+1$ as

$$\psi_\kappa(x^1, x^2, \ldots, x^D) = r^{-N}\begin{pmatrix} F(r)\phi_\kappa(\Omega) \\ iG(r)\phi_{-\kappa}(\Omega) \end{pmatrix}, \tag{12}$$

where $F(G)$ is the "large (small)" components, ϕ_κ is the angular part with angular coordinates Ω, and $K\psi_\kappa = \kappa\psi_\kappa$ holds. If we plug this into $A\psi_\kappa = 0$, we have, after some manipulation,

$$\begin{aligned} \left[\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{sign}(\kappa)x\right)^2 - s^2\right]\begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = 0, \\ s \equiv \sqrt{\kappa^2 - (Z\alpha)^2}, \end{aligned} \tag{13}$$

where we have defined $F(r) \equiv f(x)$, $G(r) \equiv g(x)$ in terms of a dimensionless $x \equiv (Z\alpha m/|\kappa|)r = (Z/|\kappa|a_0)r$ with a_0 being the Bohr radius.

For this differential equation of second order, there are two independent solutions, $f(x) \propto x^{-s}e^{-\mathrm{sign}(\kappa)x}$ or $x^s e^{-\mathrm{sign}(\kappa)x}$ with

$$\kappa = \pm\left[l + \tfrac{1}{2}(D-1)\right],$$

where $l(=0, 1, \ldots)$ is the orbital angular momentum, but the only normalizable one is the latter with $\kappa > 0$. With a similar argument for $g(x)$, we arrive at the kernel of A,

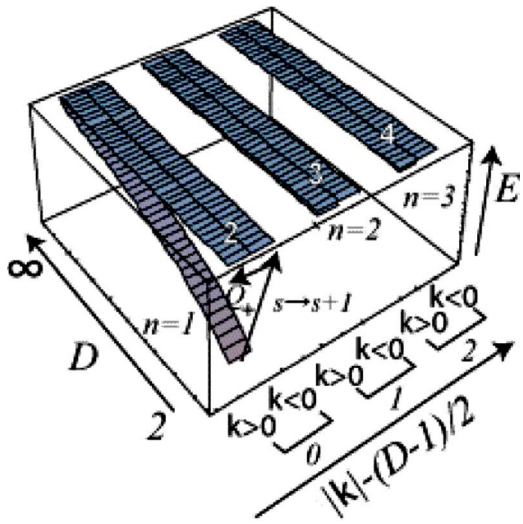

FIG. 1. (Color online) Energy level scheme for the relativistic hydrogen in D spatial dimensions. The lowest few levels are plotted against the Dirac quantum number κ and $\tanh D$, where the energy is plotted on a logarithmic scale to make the level splittings clearer. How the S(2) ladder is obtained with a shift in s and the supercharge operation Q_+ is indicated by arrows with the sign of κ and the principal quantum number n (solid and open numbers) indicated.

$$\psi_\kappa \propto x^{s-N}e^{-x}\begin{pmatrix} \phi_\kappa(\Omega) \\ i\dfrac{\kappa - s}{Z\alpha}\phi_{-\kappa}(\Omega) \end{pmatrix} \tag{14}$$

as the nondegenerate lowest state (the unpaired levels in Fig. 1).

For even $D=2N$ we can perform a similar procedure, again following Ref. 6. This time we can set $\psi_\kappa = r^{-N+1/2}[F(r)\phi_\kappa(\Omega) + iG(r)\phi_{-\kappa}(\Omega)]$, for which the same differential equation results for $F(r), G(r)$, so we have a nondegenerate ground state, $\psi_\kappa \propto x^{s-N+1/2}e^{-x}\{\phi_\kappa(\Omega) + i[(\kappa - s)/Z\alpha]\phi_{-\kappa}(\Omega)\}$.

EIGENENERGIES AND THE GROUP THEORY

Eigenenergies may readily be obtained algebraically: As used above, Eq. (6) dictates that each of the zero eigenstates of the supersymmetric Hamiltonian $\mathcal{H}=A^2$ is the lowest-energy state (for each sector of K) of the original H. This immediately implies that E, the lowest-lying (within each sector of K) eigenvalue of H, is

$$E/m = \sqrt{1 - \left(\frac{Z\alpha}{\kappa}\right)^2} = \left[1 + \left(\frac{Z\alpha}{s}\right)^2\right]^{-1/2}, \tag{15}$$

in agreement with the analytical result in Ref. 6. We can go up the ladder (where the leg corresponds to $\kappa = \pm|\kappa|$ while the rung spanned by a quantum number we call n') by making $s \equiv \sqrt{\kappa^2 - (Z\alpha)^2} \to s+1$.

So we end up with

$$E/m = \left[1 + \frac{(Z\alpha)^2}{\left(n - |\kappa| + \dfrac{D-3}{2} + \sqrt{\kappa^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2},$$

where we assume $Z\alpha < (D-1)/2$ for the atomic stability. Here the principal quantum number is given as

$$n = l + 1 + n'$$

with $n' = 0, 1, \ldots$, where each level is doubly degenerated [corresponding to $\kappa = \pm(l + (D-1)/2)$ and related by Q_+], except at the bottom of each ladder at $n' = 0$ (i.e., $n = l + 1$) for which only $\kappa > 0$ should be taken (Fig. 1). We can also see that the interdimensional degeneracy, which exists between the levels $(l, D) \to (l \pm 1, D \mp 2)$ noted for the nonrelativistic case,[12] persists for the relativistic case, and the supersymmetric ladders live on such a spectrum.

Group theoretically the present result implies the following. The nonrelativistic hydrogen atom in D spatial dimensions has a hidden symmetry (with the Runge-Lenz vector conserved), and the symmetry of the problem is higher (SO($D+1$)) than the symmetry (SO(D)) of the space. If we go to the relativistic case the symmetry is degraded, but only partially degraded into SO(D) $\otimes$ S(2) due to the supersymmetry. So the conjecture, stated in Ref. 5, is established here for general dimensions.

RELATION WITH THE RUNGE-LENZ-PAULI VECTOR

Related to the above, we can note a certain relation between the generalized Johnson-Lippmann operator (A) and the Runge-Lenz-Pauli vector as follows. Since A is Hermitian, we have

$$A = \frac{1}{2}(A + A^\dagger) = -\gamma^{D+1}\gamma^0\gamma^j\left[\frac{1}{2Zm\alpha}\gamma^0(p^j L_{ij} - L_{ji}p^j) - \frac{x^i}{r}\right] + \frac{i}{m}K\gamma^{D+1}\frac{1}{r}. \tag{16}$$

This expression reduces, in the nonrelativistic limit, to

$$A \to -\sigma^i M^i,$$

where

$$M^i = \frac{1}{2mZ\alpha}(p^j L_{ij} - L_{ji}p^j) - \frac{x^i}{r}$$

is the nonrelativistic Runge-Lenz-Pauli vector in D spatial dimensions[10,11] and $\sigma^i = \gamma^{D+1}\gamma^0\gamma^i$ the spin operator in D dimensions. Namely, the operator in this limit is the inner product of the Runge-Lenz-Pauli vector ($\mathbf{M}$) and the spin ($\boldsymbol{\sigma}$) in D dimensions.[16]

SUMMARY AND DISCUSSIONS

So the higher symmetry for the $1/r$ potential in general dimensions is revealed to be surprisingly robust against the relativistic generalization and is retained as a supersymmetry. The supercharge is indeed related to (a D-dimensional generalization of) the Johnson-Lippmann operator.

Given the formula for the general D, we are tempted to ask what happens in the $D \to \infty$ limit. In the nonrelativistic case the kinetic energy ($\sim(1/D) \times$ potential energy) is dominated by the potential energy, so the system reduces to a set of harmonic oscillations around the classical potential minima as stressed in Ref. 12. In the relativistic case, however, we see that we cannot eliminate the small component (G) in the $D \to \infty$ limit, since the coupling between F and G does not vanish in this limit. This implies that we cannot trivially relate the supersymmetry with a set of oscillators even asymptotically.

Another basic question is whether the supersymmetry is just accidental to the $1/r$ potential. As mentioned above, electromagnetically there is a problem of how we can conceive the $1/r$ potential as the Coulomb potential in general dimensions. We should have $1/r^{D-2}$ potential from Gauss's law if the lines of electromagnetic force extend over the D spatial dimensions, but there is a well-known Ehrenfest's 1920 result that the atom becomes unstable for this potential. Some authors argue that we should in fact stick to $1/r$ in general dimensions.[17] Experimentally, a low-dimensional ($D=2$) case may be interesting as an accessible one.

In a broader context, a supercharge is a kind of generalization of the Dirac operator, so it could be that supersymmetry is shared by a wide class of Dirac-type equations. Recently, Leviatan[18] has explicitly constructed the supercharges of the Dirac equation in $(3+1)$ dimensions for more general potentials which include the case of the $1/r$ potential. Furthermore, some authors[19] have discussed generalization of the Runge-Lenz-Pauli vector, such as the case of a particle around a magnetic monopole with a vector potential around it. So the exploration of supersymmetry in wider gauge-field models will be an interesting future problem.

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Bose-Einstein condensate and spontaneous breaking of conformal symmetry on Killing horizons II

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In the paper cited in the title [J. Math. Phys. **46**, 062303 (2005)] local scalar QFT (in Weyl algebraic approach) has been constructed on degenerate semi-Riemannian manifolds $\mathbb{S}^1\times\Sigma$ corresponding to the extension of Killing horizons by adding points at infinity to the null geodesic forming the horizon. It has been proved that the theory admits a natural representation of $\mathrm{PSL}(2,\mathbb{R})$ in terms of *-automorphisms and this representation is unitarily implementable if referring to a certain invariant state λ. Among other results it has been proved that the theory admits a class of inequivalent algebraic (coherent) states $\{\lambda_\zeta\}$, with $\zeta\in L^2(\Sigma)$, which break part of the symmetry, in the sense that each of them is not invariant under the full group $\mathrm{PSL}(2,\mathbb{R})$ and so there is no unitary representation of whole group $\mathrm{PSL}(2,\mathbb{R})$ which leaves fixed the cyclic GNS vector. These states, if restricted to suitable portions of $\mathbb{M}$ are invariant and extremal KMS states with respect to a surviving one-parameter group symmetry. In this paper we clarify the nature of symmetry breakdown. We show that, in fact, *spontaneous* symmetry breaking occurs in the natural sense of algebraic quantum field theory: if $\zeta\neq 0$, there is no unitary representation of whole group $\mathrm{PSL}(2,\mathbb{R})$ which implements the *-automorphism representation of $\mathrm{PSL}(2,\mathbb{R})$ itself in the GNS representation of λ_ζ (leaving fixed or not the state). © *2006 American Institute of Physics.*
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I. SUMMARY OF SOME ACHIEVED RESULTS

In Ref. 1 local scalar QFT (in Weyl algebraic approach) is constructed on degenerate semi-Riemannian manifolds $\mathbb{M}=\mathbb{S}^1\times\Sigma$ corresponding to the extension of future Killing horizons by adding points at infinity to the null geodesic forming the horizon. Above the transverse manifold Σ has a Riemannian metric inducing the volume form ω_Σ, whereas $\mathbb{S}^1$ is equipped with the null metric. To go on, fix a standard frame (see Sec. II A of Ref. 1) $\theta\in(-\pi,\pi]$ on $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$ – so that $\mathbb{S}^1$ is realized as $(-\pi,\pi]$ with the endpoints identified—and consider the C^*-algebra of Weyl $\mathcal{W}(\mathbb{M})$ generated by nonvanishing elements $V(\omega)$ in Eq. 12 in Sec. II E in Ref. 1, the smooth forms ω of the space $\mathcal{D}(\mathbb{M})$ being the space of forms ϵ_ψ defined in Eq. 1 in Sec. 2.1 in Ref. 1. We shall exploit the group of *-automorphisms α defined in Eq. 19 in Ref. 1 representing the Möbius group $\mathrm{PSL}(2,\mathbb{R})$ viewed as a subgroup of diffeomorphisms of $\mathbb{S}^1$ and thus of $\mathbb{M}$ (see Sec. III A of Ref. 1):

$$\alpha_g(V(\omega))=V(\omega^{(g^{-1})}), \tag{1}$$

$\omega^{(g)}:=g^*\omega$ being the natural pullback action of $g\in\mathrm{PSL}(2,\mathbb{R})$ on forms. In the following $\{\alpha_t^{(\mathcal{X})}\}_{t\in\mathbb{R}}$ indicates the one-parameter subgroup associated with the vector field $\mathcal{X}$ on $\mathbb{M}$ corresponding to an element of the Lie algebra of $\mathrm{PSL}(2,\mathbb{R})$. In particular the vector field on $\mathbb{M}$, $\mathcal{D}$, generating a

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one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$, is that defined in Eq. 16 in Ref. 1. If $\zeta \in L^2(\Sigma, \omega_\Sigma)$ and λ_ζ is the coherent state on $\mathcal{W}(\mathbb{M})$ defined by means of 33 of Sec. IV B in Ref. 1, we indicate its GNS triple by $(\mathfrak{H}_\zeta, \Pi_\zeta, \Psi_\zeta)$.States λ_ζ are constructed as follows with respect to $\lambda := \lambda_0$. The map $V(\omega) \mapsto V(\omega) e^{i \int_{\mathbb{M}} \Gamma(\zeta \omega_+ + \overline{\zeta \omega_+})}$, $\omega \in \mathcal{D}(\mathbb{M})$, uniquely extends to a *-automorphism γ_ζ on $\mathcal{W}(\mathbb{M})$ such that $\gamma_\zeta \circ \alpha_t^{(\mathcal{D})} = \alpha_t^{(\mathcal{D})} \circ \gamma_\zeta$ for all $t \in \mathbb{R}$. The function $\Gamma := \ln|\tan(\theta/2)|$ and the $\mathcal{D}$-positive-frequency part of ω, ω_+, are, respectively, defined and discussed in Sec. IV B [Eq. 32] and in Lemma 3.1 of Sec. III B of Ref. 1.

$$\lambda_\zeta(w) := \lambda(\gamma_\zeta w) \quad \text{for all } w \in \mathcal{W}(\mathbb{M}). \tag{2}$$

The state λ was defined in Eq. 13 in Ref. 1 and it is pure in accordance with Lemma A.2 in Ref. 2, because the real linear map $K: \mathcal{S}(\mathbb{M}) \ni \psi \mapsto \psi_+$ has dense range in the one-particle space $\mathcal{H}$ by construction. It is clear that the GNS representation generated by λ_ζ is irreducible if that of λ is irreducible. As a consequence every λ_ζ is pure.

Among other results it has been proved that (Theorems 4.1, 4.2, and 5.1) the pure states λ_ζ are inequivalent states and, the restrictions to the algebra localized at the "half circle times Σ," give rise to different extremal KMS states at rationalized Hawking temperature $T = 1/2\pi$ with respect to $\{\alpha_t^{(\mathcal{D})}\}_{t \in \mathbb{R}}$. If one is dealing with a bifurcate Killing horizon of a black hole the "half circle times Σ" is nothing but $\mathbb{F}_+$, the future right branch of the Killing horizon (see Sec. I and figure in Ref. 1). In this case $-\zeta^{-1}\mathcal{D}$, with $\zeta^{-1} = \kappa$ being the surface gravity of the examined black hole, can be recognized as the restriction to the horizon to the Killing vector field defining Schwarzschild time, kT becomes proper Hawking's temperature and the order parameter associated with the breakdown of symmetry can be related with properties of the black hole.

II. SPONTANEOUS BREAKING OF PSL(2,*R*) SYMMETRY

As illustrated in further details below, a remarkable property of states λ_ζ is that, for $\zeta \neq 0$, they break part of the symmetry, in the sense that each of them is not invariant under the full group $\mathrm{PSL}(2,\mathbb{R})$ and so there is no unitary representation of whole group $\mathrm{PSL}(2,\mathbb{R})$ which leaves fixed the cyclic GNS vector. We want here to clarify the nature of this breakdown of $\mathrm{PSL}(2,\mathbb{R})$ symmetry, proving that, actually there is no unitary representation of $\mathrm{PSL}(2,\mathbb{R})$ which implements the full group action of $\mathrm{PSL}(2,\mathbb{R})$ no matter the issue of the invariance of λ_ζ under $\mathrm{PSL}(2,\mathbb{R})$. This leads to *spontaneous* breaking of $\mathrm{PSL}(2,\mathbb{R})$ symmetry.

Let us focus on this issue from a general point of view. In the physical literature there are several, also strongly inequivalent, definitions of *spontaneous* breaking of symmetry related to different approaches to quantum theories. We adopt the following elementary definition which is quite natural in algebraic QFT and is equivalent to the definition given on p.119 of the recent review[3] on breaking symmetry theory (see the end of the paper for further comments).

Definition 1: Referring to a C^*-algebra $\mathcal{A}$, one says that

(a) *A Lie group $\mathcal{G}$ is a* group of symmetries *for $\mathcal{A}$ if there is a representation β of $\mathcal{G}$ made of *-automorphisms of $\mathcal{A}$. If some notion of time evolution is provided, it is required that it corresponds to a one parameter subgroup of $\mathcal{G}$.* [If this subgroup does not belong to the center of $\mathcal{G}$, *the self-adjoint generators of unitary representations of $\mathcal{G}$ implementing β, if any, give rise to constants of motion which may depend parametrically on time. It happens, for instance, for Poincaré-invariant systems, where the conserved self-adjoint operator $K^i(t)$ associated with boost invariance along the i*th *axis depend parametrically on time. Indeed, on the appropriate domain, $K^i(t) = K^i(0) - tP^i$ and it is conserved under Heisenberg evolution $U_t K^i(t) U_t^\dagger = K^i(0)$.*]

(b) *Assuming that* (a) *is valid*, spontaneous breaking of $\mathcal{G}$ symmetry *occurs with respect to an algebraic state μ on $\mathcal{A}$ and β, if there are elements $g \in \mathcal{G}$ such that β_g are not implementable unitarily in the GNS representation $(\mathfrak{H}_\mu, \Pi_\mu, \Psi_\mu)$ of μ, i.e. for those elements there is no unitary operator U_g on $\mathfrak{H}_\omega$ with $U_g \Pi_\mu(a) U_g^\dagger = \Pi_\mu(\beta_g(a))$ for all $a \in \mathcal{A}$.*

Considering the inequivalent GNS triples $(\mathfrak{H}_\zeta, \Pi_\zeta, \Psi_\zeta)$, Theorems 3.2 and 3.3 in Ref. 1 show that, if $\zeta=0$ the group of automorphisms α representing $\mathrm{PSL}(2,\mathbb{R})$ can be unitarily implemented in the space $\mathfrak{H}=\mathfrak{H}_0$ and the cyclic vector $\Psi:=\Psi_0$ of the GNS representation is invariant under that (strongly continuous) unitary representation of $\mathrm{PSL}(2,\mathbb{R})$. [In the proof theorem 3.2 in all occurrences of the symbol $\widetilde{\mathrm{PSL}(2,\mathbb{R})}$ before the statement "…is in fact a representation of $\mathrm{PSL}(2,\mathbb{R})$." It must be replaced by $\widetilde{\mathrm{PSL}(2,\mathbb{R})}$, it denoting the universal covering of $\mathrm{PSL}(2,\mathbb{R})$.] Conversely, if $\zeta\neq 0$, $\mathrm{PSL}(2,\mathbb{R})$ symmetry turns out to be broken. Indeed, Theorem 4.1 states that each state λ_ζ with $\zeta\neq 0$ is invariant under $\{\alpha_t^{(\mathcal{D})}\}_{t\in\mathbb{R}}$, but it is not under any other one-parameter subgroup of α (barring those associated with $c\mathcal{D}$ for $c\in\mathbb{R}$ constant). In the general case this is not enough to assure occurrence of *spontaneous* breaking of $\mathrm{PSL}(2,\mathbb{R})$ symmetry as defined in Definition 1.

In a different context, it is possible to show that—see Sec. III.3.2 of Ref. 4—if $\mathcal{G}$ is Poincaré group or an internal symmetry group for a special relativistic system and the reference state μ is a primary vacuum state over the net of algebras of observables, then non-$\mathcal{G}$ invariance of the vacuum state implies—and in fact is equivalent to—spontaneous breaking of $\mathcal{G}$ symmetry. Our considered case is far from that extent and thus there is no *a priori* guarantee for the occurrence of spontaneous breaking of $\mathrm{PSL}(2,\mathbb{R})$ symmetry for states λ_ζ with $\zeta\neq 0$ and the issue deserves further investigation. The following theorem gives an answer to the issue.

Theorem 1: *If* $L^2(\Sigma,\omega_\Sigma)\ni\zeta\neq 0$, *spontaneous breaking of* $PSL(2,\mathbb{R})$*-symmetry occurs with respect to* λ_ζ *and the representation* α. [*In particular, there is no unitary implementation of the nontrivial elements of the subgroup of* $PSL(2,\mathbb{R})$ *generated from the vector field* $\partial/\partial\theta$.]

Proof: Referring to the GNS triple of λ_ζ define $\hat{V}_\zeta(\omega):=\Pi_\zeta(V(\omega))$. The existence of a unitary implementation, $L_g:\mathfrak{H}_\zeta\to\mathfrak{H}_\zeta$, of α in the GNS triple $(\mathfrak{H}_\zeta,\Pi_\zeta,\Psi_\zeta)$ implies, in particular, that

$$L_g\hat{V}_\zeta(\omega)L_g^\dagger=\Pi_\zeta(\alpha_g(V_\zeta(\omega))),\quad \text{for all } \omega\in\mathcal{D}(\mathbb{M}) \quad\text{and}\quad \text{every } g\in\mathrm{PSL}(2,\mathbb{R}). \tag{3}$$

By construction, $(\mathfrak{H}_\zeta,\Pi,\Psi_\zeta)$ (notice that we wrote Π instead of Π_ζ) is a GNS triple of λ (notice that we wrote λ instead of λ_ζ) if

$$\Pi:V(\omega)\mapsto\hat{V}(\omega):=\hat{V}_\zeta(\omega)e^{-i\int_{\mathbb{M}}\Gamma(\zeta\omega_+ +\overline{\zeta\omega_+})}. \tag{4}$$

In this realization α can be unitarily implemented (Theorem 3.2 in Ref. 1): There is a (strongly continuous) unitary representation U of $\mathrm{PSL}(2,\mathbb{R})$ such that

$$U_g\hat{V}(\omega)U_g^\dagger=\Pi(\alpha_g(V(\omega))),\quad \text{for all } \omega\in\mathcal{D}(\mathbb{M}) \text{ and every } g\in\mathrm{PSL}(2,\mathbb{R}). \tag{5}$$

Suppose that α can be implemented also in $(\mathfrak{H}_\zeta,\Pi_\zeta,\Psi_\zeta)$, where now $\Pi_\zeta:V(\omega)\mapsto\hat{V}_\zeta(\omega)$, and let L be the corresponding unitary representation of $\mathrm{PSL}(2,\mathbb{R})$ satisfying (3). That equation together with (4) entail that the unitary operator $S_g:=U_g^\dagger L_g$ satisfies

$$\begin{gathered} S_gV(\omega)S_g^\dagger=e^{ic_{g,\omega}}V(\omega),\\ c_{g,\omega}:=\int_{\mathbb{M}}(\zeta(\omega^{(g^{-1})})_+ +\overline{\zeta(\omega^{(g^{-1})})_+}-\zeta\omega_+-\overline{\zeta\omega_+})\Gamma. \end{gathered} \tag{6}$$

Now, dealing with exactly as in the proof of (ii) of (b) of Theorem 4.1 [where the role of our S_g was played by the operator U and the role of $c_{g,\omega}$ was played by the simpler phase $\int_{\mathbb{M}}(\zeta\omega_+ +\overline{\zeta\omega_+})\Gamma$] one finds that (6) entails that $\langle\Psi_\zeta,S_g\Psi_\zeta\rangle\neq 0$ and

$$\|S_g\Psi_\zeta\|^2=|\langle\Psi_\zeta,S_g\Psi_\zeta\rangle|^2e^{\sum_{n,j}^{\infty}|\eta_{n,j}|^2},$$

$$\eta_{n,j} := -2i\int_{\mathbb{M}} \Gamma(\theta)\overline{\zeta(s)}u_j(s)\frac{\partial}{\partial\theta}\frac{e^{i\theta_g}-e^{i\theta}}{\sqrt{4\pi n}}\mathrm{d}\theta\,\mathrm{d}\omega_\Sigma(s). \tag{7}$$

Above the real compactly supported functions u_j defines a Hilbert base in $L^2(\Sigma,\omega_\Sigma)$, and $(\theta_g,s_g):=g(\theta,s)\in\mathbb{M}$ is obtained by the action of $g\in\mathrm{PSL}(2,\mathbb{R})$ on $(\theta,s)\in\mathbb{M}$ [obviously $s_g=s$ since $\mathrm{PSL}(2,\mathbb{R})$ acts on the factor $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$]. Now take $g\in\{\alpha_t^{(\mathcal{K})}\}_{t\in\mathbb{R}}$, the one-parameter subgroup of $\mathrm{PSL}(2,\mathbb{R})$ generated by the vector field $\mathcal{K}:=\partial/\partial\theta$, and realize the factor $\mathbb{S}^1$ of $\mathbb{M}=\mathbb{S}^1\times\Sigma$ as $[-\pi,\pi)$ with the identification of its endpoints. In this case, obviously, $\theta_g=\theta+t$. A direct computation shows that, for some j_0 with $\int_\Sigma u_j(s)\overline{\zeta(s)}\omega_\Sigma(s)=0$ (which does exist otherwise $\zeta=0$ almost everywhere)

$$|\eta_{2n+1,j_0}|^2 = C\left[\frac{1}{2n+1}-\frac{\cos((2n+1)t)}{2n+1}\right]$$

for some constant $C>0$ independent form n. The series of elements $-\cos((2n+1)t)/(2n+1)$ converges for $t\neq 0,\pm\pi$ (it diverges to $+\infty$ for $t=\pm\pi$), whereas that of elements $1/(2n+1)$ diverges to $+\infty$. Thus the exponent in (7) and L_g cannot exist, if $g=\alpha_t^{(\mathcal{K})}$ with $t\neq 0$ □

Remark: The automorphism γ_ζ is a symmetry of the system because it commutes with time evolution α_t. (It is worth noticing that, if restricting to real functions ζ, $\zeta\mapsto\gamma_\zeta$ defines a group of automorphisms.) Since $\lambda_\zeta\restriction_{\mathcal{W}(\mathbb{F}_+)}\neq\lambda_{\zeta'}\restriction_{\mathcal{W}(\mathbb{F}_+)}$ for $\zeta\neq\zeta'$, and all these states are extremal $\alpha^{(\mathcal{D})}$-KMS states at the same temperature, following Haag (Sec. V.I.5 in Ref. 4), we can say that *spontaneous symmetry breaking* with respect to γ_ζ occurs in the context of extremal KMS states theory.

III. FINAL COMMENTS ON INEQUIVALENT APPROACHES CONCERNING SYMMETRY BREAKDOWN

If μ is a state on the C^*-algebra $\mathcal{A}$, its *Gelfand ideal*, $\mathcal{I}_\mu$, consists of the elements $a\in\mathcal{A}$ such that $\mu(a^*a)=0$. $\mathcal{I}_\mu$ plays a central role in GNS reconstruction procedure. Breakdown of symmetry could be investigated from another point of view—relying upon the invariance properties of Gelfand ideal—with some overlap with our approach. It is based on the following proposition.

*Proposition 1: Let β be a faithful *-automorphism representation of the group $\mathcal{G}$ on the C^*-algebra $\mathcal{A}$ with unit $\mathbb{I}$ and let $\mu:\mathcal{A}\to\mathbb{C}$ be a state with GNS triple $(\mathfrak{H}_\mu,\Pi_\mu,\Psi_\mu)$.*

The Gelfand ideal $\mathcal{I}_\mu$ is invariant under β if and only if there is a $\mathcal{G}$-representation made of densely defined operators $U_g:\Pi_\mu(\mathcal{A})\to\Pi_\mu(\mathcal{A})$ which implements β leaving fixed Ψ_μ, i.e.,

$$\text{(i) } U_g\Pi_\mu(a)U_g^{-1}=\Pi_\mu(\beta_g(a)) \text{ for all } a\in\mathcal{A}, g\in\mathcal{G} \quad \text{and (ii) } U_g\Psi_\mu=\Psi_\mu \text{ for all } g\in\mathcal{G}. \tag{8}$$

If a representation $\mathcal{G}\ni g\mapsto U_g$ satisfying (8) *exists the following holds.*

(a) *It is unique and the operators U_g are completely determined by*

$$U_g\Pi_\mu(a)\Psi_\mu=\Pi_\mu(\beta_g a)\Psi_\mu \quad \text{for all} \quad a\in\mathcal{A} \text{ and } g\in\mathcal{G}. \tag{9}$$

(b) *Operators U_g are* [*restrictions to the dense domain $\Pi_\mu(\mathcal{A})$ of uniquely determined*] *unitary operators on $\mathfrak{H}_\mu$, if and only if μ is invariant under β.*

Sketch of proof: From GNS theorem $\mathcal{I}_\mu=\{a\in\mathcal{A}\,|\,\Pi_\mu(a)\Psi_\mu=0\}$. From it one easily proves that if $\mathcal{I}_\mu$ is β-invariant (9) define a well-posed representation of $\mathcal{G}$ satisfying (8) [notice that, $\beta_g(\mathbb{I})=\mathbb{I}$ and $\Pi_\mu(\mathbb{I})=I$ so that (ii) in (8) holds true from (9)]. Since (i) and (ii) in (8) entails (9), $\mathcal{I}_\mu=\{a\in\mathcal{A}\,|\,\Pi_\mu(a)\Psi_\mu=0\}$ proves that the existence of a representation satisfying (8) implies β-invariance of $\mathcal{I}_\mu$and (a) is valid as well. Proofs of (b) are based on the identities (from GNS theorem) $\|U_g\Pi_\mu(a)\Psi_\mu\|^2=\mu(\beta_g(a^*a))$ and $\mu(a^*a)=\|\Pi_\mu(a)\Psi_\mu\|^2$. □

In view of that result, by a pure mathematical point of view, a strategy to distinguish several degrees of $\mathcal{G}$-symmetry breakdowns for a state $\mu:\mathcal{A}\to\mathbb{C}$ when $\mathcal{G}$ is represented, at algebraic level, by the *-automorphism representation β, could be the following.

(1) (*No symmetry breaking*) Gelfand ideal is invariant under β_g—i.e., (i) and (ii) in (8) are valid for an operator representation of $\mathcal{G}$.

(2) Gelfand ideal is invariant under β—so that both (i) and (ii) in (8) hold true—but the induced action of β in the GNS representation of μ is *not* unitarily implementable.

(3) Gelfand ideal is *not* invariant under β_g—so that at least one of (i) and (ii) in (8) is not valid for any operator representation of $\mathcal{G}$ on the relevant domain.

In this paper we, instead, have adopted quite a different point of view (sharing however some overlap with the point of view illustrated above) entirely based on the definition of spontaneous breaking of symmetry defined on p. 119 of Ref. 3. We considered only the problem of *unitary* (non)implementability of $(\mathrm{PSL}(2,\mathbb{R}))$ symmetry. This is in accordance with the well-known general Wigner-Kadison notion of *quantum symmetry* described in terms of appropriate (projective) unitary or antiunitary operators.[5] The three degree of symmetry breakdown one may consider in this context are the following, referring to $\mu,\mathcal{G},\beta$ as before.

(U1) (*No symmetry breaking*) Algebraic symmetry β is implementable for μ by means of unitary operators *and* the state μ is invariant under the action β of the full group $\mathcal{G}$—(i), and (ii) in (8) are valid for a unitary representation of $\mathcal{G}$.

(U2) (*Symmetry breaking due to the cyclic vector*) Algebraic symmetry β is implementable for μ by means of unitary operators *and* the state μ is *not* invariant under the action β of the full group $\mathcal{G}$—(i), but not (ii) in (8), is valid for a unitary representation of $\mathcal{G}$.

(U3) (*Spontaneous symmetry breaking*) Algebraic symmetry β is not implementable for μ by means of unitary operators—(i) in (8) does not hold for any unitary representation of $\mathcal{G}$.

In Ref. 1 we established, for states λ_ζ with $\zeta\neq 0$ the validity of either degree (U2) or (U3) concerning $\mathcal{G}=\mathrm{PSL}(2,\mathbb{R})$ symmetry breaking. This paper shows that, actually, the strongest degree (U3) takes place.

A priori this extent may be compatible with either (2) or (3) of the other scheme. A closed scrutiny would be necessary to examine this issue but it is far from the goal of this paper where only Wigner-Kadison unitary symmetries are considered since they are the only way to preserve quantum probabilities and have direct physical meaning.

To conclude we notice that an example of the intermediate case (U2) is realized in the framework of Ref. 1 with respect to the Weyl algebra $\mathcal{W}(\mathbb{M})$, with $\mathbb{M}=\mathbb{S}^1$, and for the fully $\mathrm{PSL}(2,\mathbb{R})$-symmetric state $\lambda_{\zeta=0}$. Breaking of symmetry at level (U2) occurs when extending the symmetry group from $\mathrm{PSL}(2,\mathbb{R})$ to the infinite dimensional one $\mathcal{G}:=\mathrm{Diff}^+(\mathbb{S}^1)$.

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Non-Abelian gauge field theory in scale relativity

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Gauge field theory is developed in the framework of scale relativity. In this theory, space-time is described as a nondifferentiable continuum, which implies it is fractal, i.e., explicitly dependent on internal scale variables. Owing to the principle of relativity that has been extended to scales, these scale variables can themselves become functions of the space-time coordinates. Therefore, a coupling is expected between displacements in the fractal space-time and the transformations of these scale variables. In previous works, an Abelian gauge theory (electromagnetism) has been derived as a consequence of this coupling for global dilations and/or contractions. We consider here more general transformations of the scale variables by taking into account separate dilations for each of them, which yield non-Abelian gauge theories. We identify these transformations with the usual gauge transformations. The gauge fields naturally appear as a new geometric contribution to the total variation of the action involving these scale variables, while the gauge charges emerge as the generators of the scale transformation group. A generalized action is identified with the scale-relativistic invariant. The gauge charges are the conservative quantities, conjugates of the scale variables through the action, which find their origin in the symmetries of the "scale-space." We thus found in a geometric way and recover the expression for the covariant derivative of gauge theory. Adding the requirement that under the scale transformations the fermion multiplets and the boson fields transform such that the derived Lagrangian remains invariant, we obtain gauge theories as a consequence of scale symmetries issued from a geometric space-time description. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In standard gauge field theory, the nature of the gauge transformations, of the gauge fields and of the conserved charges are postulated and designed from experimental considerations. The group of gauge transformations does not act upon the space-time coordinates, as does, for example, the SU(2) spin rotation group or the Lorentz group, but in an "internal space" whose physical meaning is not understood from first principles. For a general gauge group G, the particle wave functions that are multiplets of Dirac bi-spinors form a n-component vector in the internal space, and the gauge potentials A_μ (more generally W_μ^α) are fields in standard space-time defined only up to a gauge transformation.

There is indeed a fundamental difference between the situation of transformations in the standard gauge theories and of, e.g., Lorentz transformations. Thanks to the fact that space-time coordinates are directly observable, we know from the very beginning what Lorentz transformations are, namely, space-time rotations of the coordinates, $dx' = \Lambda_\beta^\alpha dx^\beta$. They write in the case of an infinitesimal transformation, (i) $dx'^\alpha = (\delta_\beta^\alpha + \omega_\beta^\alpha) dx^\beta$, where the ω^{ij} (i and $j = 1$ to 3) represent the

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infinitesimal angles of rotation in space and the $\omega^{0i}=v^i/c$ ($v^i \ll c$) are the infinitesimal Lorentz boosts. Then, once this basic definition is given, one can consider the effect of these transformations on various physical quantities defined in space-time, e.g., the wave function ψ. This involves representations of the Lorentz group adapted to the nature of the physical object under consideration, i.e., (ii) $\psi' = \left(1+\frac{1}{2}\omega^{\alpha\beta}\sigma_{\alpha\beta}\right)\psi$ (see, e.g., Ref. 1).

In contradistinction with this situation, in standard gauge theories the gauge functions, being arbitrary, are considered to be devoid of physical meaning. As a consequence, there is up to now no equivalent of the basic defining transformation (i). Therefore, in the standard framework, the gauge group is indirectly defined through its action on the various physical objects according to its representations, in similarity with relation (ii), but the physical meaning of the gauge space itself is lacking.

In the present paper, we place ourselves in the framework of the scale relativity theory, in which the description of the space-time geometry is generalized to continuous but nondifferentiable manifolds. In this theory, one attempts to recover the quantum behavior as a manifestation of the nondifferentiability, then the gauge fields themselves as a manifestation of the nondifferentiable and fractal geometry (in analogy with gravitation interpreted as a manifestation of the non-Euclidean curved geometry in general relativity).

In this framework, we give a geometric meaning to the gauge space, then we can rebuild the gauge transformations of the various physical quantities (namely, the various quantum fields) as consequences of the fundamental transformations of the variables which define this gauge space. In other words, it is precisely an equivalent for gauge theories of the defining transformation (i) that can be proposed in scale relativity. The specifically new results given in the present paper consist of extending to non-Abelian gauge theory the results of previous works[2–4] devoted to the understanding of the simpler gauge invariant theory of electromagnetism.

The paper is organized as follows. After a summarized review (Sec. II) of the main steps of the construction of the scale relativity theory, including the exposition of the salient features that have led to the demonstration of the Dirac equation[5,6] from the scale relativistic first principles, we give a brief reminder of the results previously obtained for electromagnetism (Sec. III). Then we give, in Sec. IV, an extension of the concepts and methods thus obtained, and we apply them to a general development of the non-Abelian gauge formalism. Section V is devoted to the conclusion.

II. SCALE RELATIVITY AND QUANTUM MECHANICS: SUMMARY

A. Foundations of scale relativity

The theory of scale relativity is based on the giving up of the hypothesis of manifold differentiability which is a key assumption of Einstein's general relativity. In the new theory, the coordinate transformations are continuous but can be differentiable (and therefore it includes general relativity) or non-differentiable. The giving up of the assumption of differentiability implies several consequences,[7] leading to the successive steps of the construction of the theory:

(1) It has been proved[7,3,8] that a continuous and nondifferentiable curve is fractal in a general meaning, namely, its length is explicitly scale dependent and goes to infinity when the scale interval ε goes to zero, i.e., $\mathcal{L}=\mathcal{L}(\varepsilon)\to\infty$ when $\varepsilon\to 0$. This result can be readily extended to a continuous and nondifferentiable manifold.

(2) The fractality of space-time[9,10] involves the scale dependence of the reference frames. We therefore add to the usual variables defining the reference frames (position, orientation, motion), new variables ε characterizing their state of scale. In particular, the coordinates themselves become functions of these scale variables, i.e., $X=X(\varepsilon)$ (in the simplified case of only one variable). In an experimental situation, these scale variables are identified with the resolution scale of the measurement apparatus. In the case of a theoretical physics description, they are identified with the differential elements themselves, of which the coordinates become explicit functions, i.e., $X=X(\mathrm{d}X)$.

(3) The scale variables ε can never be defined in an absolute way, but only in a relative way. Namely, only their ratio $\rho=\varepsilon'/\varepsilon$ does have a physical meaning. This universal behavior leads to

extend to scales the principle of relativity,[11,12,7] in order to include in the possible changes of reference frames the new ones which are described by the transformations of these scale variables.

(4) Though the nondifferentiability manifests itself at the limit $\varepsilon \to 0$, the use of differential equations is made possible by representing physical quantities f by fractal functions $f[X(\varepsilon),\varepsilon]$.[7] Even if the function $f(X,0)$ is nondifferentiable with respect to the variable X, the fractal function $f(X,\varepsilon)$ is differentiable for any $\varepsilon \neq 0$ with respect to both X and ε. This allows us to complete the differential equations of standard physics by new differential equations of scale, which are constrained by the principle of scale relativity. The study of the scale laws derived from these differential equations has been developed according to various levels of relativistic transformations.[12,3,13] In what follows, we consider only the simplest case, namely Galilean-type scale transformations (i.e., characterized by a constant fractal dimension).

(5) The simplest possible scale differential equation is a first order equation, $\partial X/\partial \ln \varepsilon = \beta(X)$, which can be simplified again by Taylor expanding the unknown function β, so that it reads $\partial X/\partial \ln \varepsilon = a + bX + \cdots$. The solution of this equation is made of two terms, a scale-independent, differentiable, classical part and a power-law, nondifferentiable fractal part, which read

$$X = x + \zeta\left(\frac{\lambda}{\varepsilon}\right)^{-b}, \tag{1}$$

where $x = -a/b$. When the coefficient b is constant, the second term is the standard expression for the length of a fractal curve of dimension $D_F = 1 - b$.[14] Moreover, the transformation law of this power-law term under a scale transformation $\ln(\lambda/\varepsilon) \to \ln(\lambda/\varepsilon')$ takes the mathematical form of the Galileo group, and it therefore comes under the principle of relativity,[12] as initially required.

B. Metric of a fractal space-time

In Eq. (1), the scale variable ε is a space resolution, e.g., $\varepsilon = \delta X$. The next step consists of considering its four-dimensional differential counterpart and to express it in terms of intervals of the invariant length (proper time) $\mathrm{d}s$, by using the standard relation between the resolution interval of projected coordinates and the resolution interval of the invariant length on a fractal, $(\delta X^\mu)^{D_F} \sim \delta s$,

$$\mathrm{d}X^\mu = \mathrm{d}x^\mu + \mathrm{d}\xi^\mu = v^\mu\,\mathrm{d}s + \zeta^\mu \times (\lambda_c)^{1-1/D_F} \times \mathrm{d}s^{1/D_F}, \tag{2}$$

where ζ^μ is dimensionless, λ_c is a length scale which must be introduced for dimensional reasons and D_F is a fractal (covering) dimension. In the case where this description holds for a quantum particle of mass m, λ_c will be identified with its Compton length $\hbar/mc$. The elementary displacement on a fractal space-time is therefore the sum of a classical, standard differentiable element, which is leading at large scales, and of a fractal, nonstandard fluctuation which is leading at small scales.

In what follows, we simplify again the description by considering only the case $D_F = 2$. For this, we base ourselves on Feynman's result[15,16] according to which the typical paths of quantum particles (those which contribute mainly to the path integral) are nondifferentiable and (in modern words) fractal of dimension $D_F = 2$. The case $D_F \neq 2$ has also been studied in detail: it has been shown that $D_F = 2$ is a critical dimension for which the explicit scale dependence disappears in the final equations (see Ref. 3 and references therein).

Let us now show how Eq. (2) can be used to give an explicit form to the metric of a fractal space-time (disregarding at this step of the construction other consequences of nondifferentiability such as the multivaluedness of derivatives, see next sections). The fractal fluctuations (here in four dimensions) write for fractal dimension 2,

$$\mathrm{d}\xi^\mu = \zeta^\mu \sqrt{\lambda_c\,\mathrm{d}s}, \tag{3}$$

where the ζ^μ are dimensionless highly fluctuating functions.

In what follows, we replace them (in a provisional way) by stochastic variables such that $\langle\zeta^\mu\rangle=0$, $\langle(\zeta^0)^2\rangle=-1$, and $\langle(\zeta^k)^2\rangle=1$ ($k=1$ to 3). We recover here a description which is familiar in usual stochastic processes, which can also be separated in a regular part and a stochastic part, but here this is done at the level of the metric. As we shall see, we do not have to be more specific about the probability distribution of these stochastic variables. Their zero mean and unit variance is the only information needed in the subsequent calculations, which are therefore valid whatever this distribution.

Now we can write the fractal fluctuations in terms of the coordinate differentials instead of the invariant length differential,

$$\mathrm{d}\xi^\mu = \zeta^\mu\sqrt{\lambda^\mu\,\mathrm{d}x^\mu}. \tag{4}$$

The identification of Eqs. (3) and (4) leads very simply to the establishment of the expressions for the de Broglie-Einstein length and time scales from the Compton one, i.e., for two variables,

$$\lambda_x = \frac{\lambda_c}{\mathrm{d}x/\mathrm{d}s} = \frac{\hbar}{p_x}, \quad \tau = \frac{\lambda_c}{\mathrm{d}t/\mathrm{d}s} = \frac{\hbar}{E}. \tag{5}$$

The de Broglie scale (and the Compton scale in rest frame) therefore plays an essential role in the properties of the scale variables (identified here with the differential elements). It stands out as a natural reference scale for them, since it plays the role of a fractal to nonfractal transition (that should not be understood as a transition acting in position space but instead in scale space). Indeed we see from the relation $\langle\mathrm{d}\xi_x^2\rangle=\lambda_x\,\mathrm{d}x$ (and similar relations for the other variables) that when $|\mathrm{d}x|\ll\lambda_x$, the fractal fluctuation becomes $|\mathrm{d}\xi_x|\gg|\mathrm{d}x|$ and therefore it dominates the classical (differentiable) contribution. On the contrary, when $|\mathrm{d}x|\gg\lambda_x$, the fractal fluctuation $|\mathrm{d}\xi_x|\ll|\mathrm{d}x|$ becomes negligible and only the classical term remains. The subsequent developments of the theory, which lead to construct a wave function and to derive Schrödinger and Dirac equations (see Sec. II D), finally allow one to identify this transition with a quantum to classical transition.[7]

Let us now assume that the large scale (classical) behavior is given by Riemannian metric potentials $g_{\mu\nu}(x,y,z,t)$. The invariant proper time $\mathrm{d}S$ along a geodesic (which is therefore subjected to curvature at large scale and fractality at small scales) writes in terms of the complete differential elements $\mathrm{d}X^\mu=\mathrm{d}x^\mu+\mathrm{d}\xi^\mu$,

$$\mathrm{d}S^2 = g_{\mu\nu}\,\mathrm{d}X^\mu\,\mathrm{d}X^\nu = g_{\mu\nu}(\mathrm{d}x^\mu+\mathrm{d}\xi^\mu)(\mathrm{d}x^\nu+\mathrm{d}\xi^\nu). \tag{6}$$

Now replacing the $\mathrm{d}\xi$'s by their expression [Eq. (4)], we obtain a fractal metric. Assuming for simplicity (1+1) dimensions, a diagonal classical part of the metric and a fractal dimension $D_F=2$, it reads

$$\mathrm{d}S^2 = g_{00}\left(1+\zeta_0\sqrt{\frac{\tau}{\mathrm{d}t}}\right)^2 c^2\,\mathrm{d}t^2 - g_{11}\left(1+\zeta_1\sqrt{\frac{\lambda_x}{\mathrm{d}x}}\right)^2\mathrm{d}x^2. \tag{7}$$

We therefore obtain generalized fractal metric potentials which are explicitly dependent on the coordinate differential elements, in agreement with the program of Refs. 11 and 7. More generally the metric potentials can be written in their turn as the sum of the standard metric potentials (which describe curvature) and of divergent, highly fluctuating terms (which describe fractality), e.g., for the g_{00} component,

$$\tilde{g}_{00}(x,t;\mathrm{d}t) = g_{00}(x,t) + \gamma_{00}(x,t)\left(\frac{\tau}{\mathrm{d}t}\right), \tag{8}$$

where we have kept only the leading term, owing to the fact that $\langle\zeta^\mu\rangle=0$. The $\gamma_{\mu\nu}(x,t)$ can be described at a first approximation in terms of stochastic variables. We recover here our result[7] according to which, in the limit $(\mathrm{d}x,\mathrm{d}t\to0)$, the metric is divergent (singular) at each of its points and instants, which is the very intrinsic expression of the fractality of space-time. As a consequence, the curvature is also explicitly scale-dependent and divergent when the scale intervals tend

to zero. This property ensures the fundamentally non-Riemannian character of a fractal space-time as well as the ability to characterize it in an intrinsic way.

Note that all the above developments have been made in the framework of Galilean scale relativity, in which the fractal dimension is assumed to be constant (we call it Galilean because its laws of scale transformation are similar to inertial laws of motion). However it is worth briefly recalling here that a special scale relativity theory has been proposed,[7,12] in which the transformation laws of the scale variables $\ln \rho$ take the form of a Lorentz group, so that the fractal dimension becomes itself a variable. In this framework, the differential elements $\mathrm{d}X$ can no longer tend to zero since they are limited at small scales by a minimal length scale, invariant under dilations, that we have identified with the Planck length $\lambda_{\mathrm{P}}=\sqrt{\hbar G/c^3}$. It has a status similar to that of c in motion special relativity, i.e., of an unreachable and impassable horizon rather than of a cutoff or a barrier: namely, it replaces the zero point since an infinite contraction would be needed to obtain it from another scale. Combined with the role of scale transition played by the Compton length (in rest frame), this interpretation of the Planck scale leads to introduce a set of fundamental constants $\mathbb{C}=\ln(\lambda_c/\lambda_{\mathrm{P}})=\ln(m_{\mathrm{P}}/m)$ which are characteristic of elementary particles of mass m and Compton length $\lambda_c=\hbar/mc$. These constants play an essential role in structuring the geometry of the geodesics families of the fractal space-time[3] (to which we identify the particles, see next Sec. II C), in particular when accounting for the coupling between scale and motion that leads to the emergence of gauge fields, which is the main subject of the present paper.

C. Geodesics of a fractal space-time

1. Infinity of geodesics

The next step in such a geometric approach consists of writing the geodesics equation. We make the conjecture that the description of quantum particles can be reduced to that of these geodesics. Then their internal properties are the geometrical properties of the geodesics bundle corresponding to their state, according to the various conservative quantities (prime integrals) that define them.

Any measurement performed on the "particle" is interpreted as a selection of the geodesics bundle linked to the interaction with the measurement apparatus (that depends on its resolution) and/or to the information known about it (for example, the which-way-information in a two-slit experiment[3]).

Generalizing to space-times the definition of fractal functions, we have defined a fractal space-time as the equivalence class of a family of Riemannian manifolds, explicitly depending on the scale variables. In such space-times, the geodesics equations are also scale dependent and the number of geodesics that relate any two events (or starts from any event) is infinite. We are therefore led to adopt a generalized statistical fluidlike description where the deterministic velocity $V^\mu(s)$ is replaced by a scale-dependent, fractal velocity field $V^\mu[X^\mu(s,\mathrm{d}s),s,\mathrm{d}s]$.

2. Discrete symmetry breaking

Another consequence of nondifferentiability is the breaking of the invariance by reflexion of the differential element $\mathrm{d}s$. Indeed, for fractal functions $f(s,\mathrm{d}s)$, two generalized derivatives are defined instead of one,

$$f'_+(s,\mathrm{d}s)=\frac{f(s+\mathrm{d}s,\mathrm{d}s)-f(s,\mathrm{d}s)}{\mathrm{d}s},\quad f'_-(s,\mathrm{d}s)=\frac{f(s,\mathrm{d}s)-f(s-\mathrm{d}s,\mathrm{d}s)}{\mathrm{d}s},\tag{9}$$

that are transformed one into the other by the reflexion $\mathrm{d}s\leftrightarrow-\mathrm{d}s$. Applied to the space-time coordinates, these two derivatives give two divergent velocity fields, $V^\mu_+[x(s,\mathrm{d}s),s,\mathrm{d}s]$ and $V^\mu_-[x(s,\mathrm{d}s),s,\mathrm{d}s]$. Each of them can be in turn decomposed in terms of classical parts v_+ and v_-, and of fractal parts w_+ and w_-.

Then we define two "classical" derivatives $d_+/\mathrm{d}s$ and $d_-/\mathrm{d}s$, which, when they are applied to x^μ, yield the "classical" velocity fields

$$\frac{d_+}{ds}x^\mu(s) = v_+^\mu, \quad \frac{d_-}{ds}x^\mu(s) = v_-^\mu. \tag{10}$$

Since there is no reason to privilegize one process rather than the other, we consider both (+) and (−) processes on the same footing, and we combine them in a unique twin process in terms of which the microscopic reversibility is recovered.[7] A simple and natural way to account for this doubling is to use complex numbers and the complex product.[6] In the scale relativity framework, this fundamental two-valuedness implied by nondifferentiability can be shown to be the origin of the complex nature of the wave function of quantum mechanics.

3. Quantum-covariant derivative

The next step of the scale-relativity program amounts to include in the construction of a complex derivative operator the various effects (described above) of nondifferentiability and fractality,[7]

$$\frac{\bar{d}}{ds} = \frac{1}{2}\left(\frac{d_+}{ds} + \frac{d_-}{ds}\right) - \frac{i}{2}\left(\frac{d_+}{ds} - \frac{d_-}{ds}\right). \tag{11}$$

Such an operator will play the role of a covariant derivative (in Einstein's general meaning given to this word, i.e., as a tool of implementation of the principle of covariance, according to which the fundamental equations of physics should keep their form under transformations of the reference system). It can be used to define a complex four-velocity field,

$$\mathcal{V}^\mu = \frac{\bar{d}}{ds}x^\mu = V^\mu - iU^\mu = \frac{v_+^\mu + v_-^\mu}{2} - i\frac{v_+^\mu - v_-^\mu}{2}. \tag{12}$$

The total derivative of a fractal function contains finite terms up to highest orders. For a constant fractal dimension $D_F=2$, a finite contribution only proceeds from terms up to second order. Since only stationary functions which do not depend explicitly on s are considered, one can show that the complex covariant derivative operator reads in the relativistic case[2,6]

$$\frac{\bar{d}}{ds} = \left(\mathcal{V}^\mu + i\frac{\lambda_c}{2}\partial^\mu\right)\partial_\mu. \tag{13}$$

Finally, using the strong covariance principle (extended to scales), we are led to write a geodesics equation by using this covariant derivative in terms of a freelike equation of motion,

$$\frac{\bar{d}}{ds}\mathcal{V}^\mu = 0. \tag{14}$$

At this stage, the wave function $\psi = e^{iS/m\lambda_c}$ is defined as a mere re-expression of the complex action S. By introducing it in the above geodesics equation thanks to its relation to the velocity field $\mathcal{V}_\mu = i\lambda\partial_\mu \ln\psi$, it gives after integration the complex (standard) free Klein-Gordon equation, $\lambda_c^2\partial^\mu\partial_\mu\psi + \psi = 0$.[2,3]

Note that we consider in this paper only the full relativistic case in which both space and time are fractal (which corresponds to energies larger than mc^2, i.e., to scales smaller than the Compton scale). However it is worth briefly recalling that nonrelativistic quantum mechanics (which usually applies at intermediate scales) is recovered in our framework in terms of a three-dimensional fractal space, with no fractal time. In this case a generalized Schrödinger equation for a complex wave function is derived.[7,3,6,17–19] The reason for such an asymmetry between space and time in the scale-relativity description (and in quantum mechanics) is to be found in the quantum-classical transition, identified with the fractal-nonfractal transition (see Sec. II B). Indeed, for a free particle it is given by the Einstein-de Broglie scale $\lambda_\mu = \hbar/p^\mu$, whose time scale $\tau = \hbar/E$ is always smaller than its corresponding space-scales $\lambda = \hbar/p$, because of the relation $E^2 = p^2 + m^2$ (and therefore

finally because of the existence of mass). This implies a first transition from standard space-time to fractal space, then at smaller scales a second transition to fractal space-time.[7] These three regimes manisfest themselves successively as classical, quantum nonrelativistic then quantum relativistic mechanics.

D. The Dirac equation as a geodesics equation in a fractal space-time

As recalled hereabove, the Klein-Gordon equation is obtained as a result of the $\mathrm{d}s \leftrightarrow -\mathrm{d}s$ symmetry breaking. The consideration of a more general case where we add the breaking of the symmetries $dx^\mu \leftrightarrow -dx^\mu$ and $x^\mu \leftrightarrow -x^\mu$ leads to the appearance of bispinors which are solutions of the Dirac equation.[6]

Following the method described in Sec. II C 3, these additional discrete symmetry breakings lead to two new doublings of the velocity field and of the classical derivative. The four-velocity field has now eight components, which are used to construct a biquaternionic (complex-quaternionic) velocity field. Then a biquaternionic covariant derivative operator may be built, which keeps once again the same form [Eq. (13)] as in the complex case,[6] even though the velocity field is now a biquaternion instead of a complex number.

The biquaternionic geodesics equation reads

$$\frac{\bar{d}}{\mathrm{d}s}\mathcal{V}_\alpha = \left(\mathcal{V}^\mu + i\frac{\lambda_c}{2}\partial^\mu\right)\partial_\mu \mathcal{V}_\alpha = 0. \tag{15}$$

A biquaternionic action is defined according to

$$\delta\mathcal{S} = \partial_\mu \mathcal{S}\,\mathrm{d}x^\mu = -mc\mathcal{V}_\mu \delta x^\mu. \tag{16}$$

The biquaternionic four-momentum can therefore be written $\mathcal{P}_\mu = mc\mathcal{V}_\mu = -\partial_\mu \mathcal{S}$. Then we introduce a biquaternionic wave function, which is once again a mere reexpression of the action, as

$$\psi^{-1}\partial_\mu \psi = \frac{i}{cS_0}\partial_\mu \mathcal{S}, \tag{17}$$

which yields for the biquaternionic four-velocity the expression

$$\mathcal{V}_\mu = i\lambda_c \psi^{-1}\partial_\mu \psi. \tag{18}$$

This relation is destined to play an essential role in the subsequent construction of the non-Abelian gauge theory. Indeed, its specific form $(\psi^{-1}\partial_\mu\psi)$, which is linked to the noncommutativity of biquaternions, will allow a proper generalization to multiplets which permits in its turn a geometric construction of the non-Abelian charges in accordance with the standard Yang-Mills theory (Sec. IV).

Then we replace in Eq. (15) the velocity field $\mathcal{V}_\alpha$ by its expression [Eq. (18)]. We obtain the motion equation as a third-order differential equation, which becomes after some calculations $\partial_\mu[(\partial^\nu\partial_\nu\psi)\psi^{-1}]=0$ and may therefore be integrated. This yields the Klein-Gordon equation for a free particle, $\lambda_c^2\partial^\mu\partial_\mu\psi+\psi=0$, but now generalized to complex quaternions.[5,6]

Long-known properties of the quaternionic formalism (see, e.g., Refs. 20 and 21) can finally be used to readily obtain the Dirac equation for a free particle, namely,

$$\frac{1}{c}\frac{\partial\psi}{\partial t} = -\alpha^k\frac{\partial\psi}{\partial x^k} - i\frac{mc}{\hbar}\beta\psi, \tag{19}$$

as a mere square root of the Klein-Gordon operator,[5,6] which was itself derived from the geodesics equation (15). Then the isomorphism which can be established between the quaternionic and spinorial algebrae[22] allows us to identify the wave-function ψ to a Dirac spinor. In a Lagrangian formalism, the Dirac equation proceeds from the Lagrangian density,

$$\mathcal{L} = \bar{\psi}(i\gamma^{\mu}\partial_{\mu} - m)\psi, \tag{20}$$

which therefore becomes a direct consequence of the scale relativity principles.[6] It is also easy to derive the Pauli equation, since it is known that it can be obtained as a non-(motion)-relativistic approximation of the Dirac equation, while, in this approximation, Dirac bi-spinors become Pauli spinors.

Let us conclude this section by a final remark: one of the consequences of this theory is that it provides a physical picture of the nature of spin. In the scale-relativistic framework, the complex nature of the wave function and the existence of spin have both a common origin, namely, the fundamental two valuedness of the derivative (in its generalized definition) coming from nondifferentiability. These two successive doublings are naturally accounted for in terms of algebra doublings (see Appendix of Ref. 6), i.e., of a description tool that jumps from real numbers $\mathbb{R}$ to complex numbers $\mathbb{C}=\mathbb{R}^2$, then to quaternions $\mathbb{H}=\mathbb{C}^2$. However, while the origin of the complex nature of the wave function is linked to the total derivative (and therefore to proper time) through the doubling $d/\mathrm{d}s \rightarrow (d_+/\mathrm{d}s, d_-/\mathrm{d}s)$, the origin of spin is linked to the partial derivative with respect to the coordinates through the doubling $\partial/\partial x^{\mu} \rightarrow (\partial_+/\partial x^{\mu}, \partial_-/\partial x^{\mu})$, which finally leads to the two valuedness of the wave function itself $\psi \rightarrow (\psi_1, \psi_2)$, characterizing a (Pauli) spinor.

Such a physical effect has naturally a consequence on the angular momentum $(x^{\mu}\partial/\partial x^{\nu} - x^{\nu}\partial/\partial x^{\mu})$, leading to the two directions in which spin can become locked. Moreover, numerical simulations of the fractal geodesical curves (work in preparation) which are solutions of Eq. (15) allow us to obtain a more specific picture of the spin as an internal angular momentum of these geodesics. Indeed, these solutions are characterized by spiral structures at all scales, in agreement with Ord's reformulation of the Feynman relativistic chessboard model in terms of spiral paths.[23] They also support our early models of emergence of a spinlike internal angular momentum in fractal spiral curves of fractal dimension 2.[7,11] We here recall briefly the argument: the angular momentum $L_z = mr^2\dot{\varphi}$ should classically vanish for $r \rightarrow 0$. But in the fractal spiral model, $\dot{\varphi} \rightarrow \infty$ when $r \rightarrow 0$ in such a way that $r^2\dot{\varphi}$ remains finite when $D_F = 2$ (while it is vanishing for $D_F < 2$ and divergent for $D_F > 2$). This result solves the problem of the apparent impossibility to define a spin in a classical way both for an extended object and for a pointlike object, and provides another proof of the critical character of the value $D_F = 2$ for the fractal dimension of quantum particle paths (which can be derived from the Heisenberg relations).

III. SCALE-RELATIVISTIC THEORY OF ELECTROMAGNETISM: SUMMARY

A. Electromagnetic field and electric charges

Let us now briefly recall the results previously obtained in the case of a U(1) field.[2–4]

We consider here a special situation in which the set of the scale variables comes down to only one element, $\varrho = \varepsilon/\lambda$. This amounts to limit ourselves to the study of global scale transformations (contractions/dilations) in "scale-space."

Because, according to the principle of scale relativity, this "scale-space" is fundamentally nonabsolute, the scale of a structure (internal to the fractal geodesics which are identified with a "particle") is expected to change during a displacement in space-time. In other words, we now consider scale variables which become explicit functions of the coordinates, i.e., $\varrho = \varrho(x, y, z, t)$.

This is analogous to the situation encountered in general relativity (GR) for a curved space-time: namely, in a parallel displacement, a vector V^{μ} is subjected to an increase $\delta V^{\mu} = -\Gamma^{\mu}_{\nu\rho} V^{\nu}\,\mathrm{d}x^{\rho}$ (where the $\Gamma^{\mu}_{\nu\rho}$ are the Christoffel symbols, i.e., the gravitational field), due to the geometric effects of curvature. Then, if one subtracts this geometric increase from its total variation $\mathrm{d}V^{\mu}$, one recovers the inertial part of the variation (see, e.g., Ref. 24). This allows one to define the GR covariant derivative D as $DV^{\mu} = \mathrm{d}V^{\mu} - \delta V^{\mu} = \mathrm{d}V^{\mu} + \Gamma^{\mu}_{\nu\rho} V^{\nu}\,\mathrm{d}x^{\rho}$.

The same kind of behavior is true in the scale relativity framework, but with an essential difference: while the effects of curvature affect vectors, tensors, etc., but not scalars, the effects of fractality begin already at the level of scalars, among which the "invariant" of length $\mathrm{d}s^2$ itself.

Therefore, we expect in a displacement the appearance of a resolution change due to the fractal geometry, that reads

$$\delta\varepsilon = -\frac{1}{q}A_\mu \varepsilon \, \mathrm{d}x^\mu, \tag{21}$$

i.e., in terms of the scale ratio,

$$\delta \ln \varrho = \frac{1}{q}A_\mu \, \mathrm{d}x^\mu. \tag{22}$$

The introduction of the $(1/q)$ term in this definition is an important point for the electromagnetic case and also for its non-Abelian generalizations. Indeed, as we shall see in what follows, the "field" A_μ will be identified with an electromagnetic potential. Since $\ln \varrho$ is dimensionless, we are led to divide the potential term by the "active" electric charge q, leaving a charge-independent purely geometric contribution.

This leads to the appearance of a dilation field, according to the construction of a scale-covariant derivative,

$$D\chi = \mathrm{d}\chi - \delta\chi = \mathrm{d}\chi - A_\mu \, \mathrm{d}x^\mu, \tag{23}$$

where we have set $\chi = q \ln \varrho$. We finally obtain the partial derivative as the sum of the inertial and of the geometric terms as

$$\partial_\mu \chi = D_\mu \chi + A_\mu. \tag{24}$$

Let us now consider the action S for, e.g., an electron. In the framework of a space-time theory based on a relativity principle, which is here the case, its variation should be given directly by the space-time invariant $\mathrm{d}s$, i.e., $\delta \int \mathrm{d}S = 0$ becomes identical with a geodesics (Fermat) principle $\delta \int \mathrm{d}s = 0$. But now the fractality of the geodesical curves to which the electron wave field is identified means that their proper length becomes a function of the scale variable, so that $S = S(\chi)$.

Therefore the differential of the action reads

$$\mathrm{d}S = \frac{\partial S}{\partial \chi}\mathrm{d}\chi = \frac{\partial S}{\partial \chi}(D\chi + A_\mu \, \mathrm{d}x^\mu), \tag{25}$$

so that we obtain

$$\partial_\mu S = D_\mu S + \frac{\partial S}{\partial \chi}A_\mu. \tag{26}$$

This result provides us with a definition for the "passive" charge (on which the electromagnetic field acts) as[2,3]

$$\frac{e}{c} = -\frac{\partial S}{\partial \chi}. \tag{27}$$

This is a second important point worth to be emphasized, since it will play an important role for the generalization to non-Abelian gauge theories. In the standard theory, the charge is set from experiment, then it is shown to be related to gauge transformations, while the gauge functions are considered to be arbitrary and devoid of physical meaning. In the scale relativity approach, the charges are built from the symmetries of the "scale-space." One indeed recognizes in Eq. (27) the standard expression that relates a conservative quantity to the symmetry of a fundamental variable (here, the relative resolution), according to Noether's theorem.

Note that, at this level of the construction of the theory, the charge is defined as a large scale prime integral (conservative quantity). But, once this result is obtained, a second step consists of

studying in detail the internal structures of the fractal geodesics (that are identified with the charged particle).[3,7] These internal structures can afterwards be interpreted (at time scales smaller than $\tau=\hbar/E$), in terms of virtual particle-antiparticle pairs, then of radiative corrections and of the scale variation of the charge toward small scales, as described by the renormalization group equations.

It is also remarkable that, in such a relativistic foundation of electromagnetism, we are led to introduce in a separate way an active and a passive charge. This is also analogous to the introduction in GR of an active gravitational mass and of a passive mass which are equal according to the GR strong principle of equivalence. As a consequence, a scale-relativistic principle of equivalence of these charges can be set (in order to account for the action-reaction principle in Coulomb's law). Under this principle, $e=q$ and Eq. (27) becomes $e^2/c=-\partial S/\partial \ln \varrho$.

We have therefore established from first principles the form of the action in the classical electromagnetic theory, in particular the form of the particle-field coupling term (which was postulated in the standard theory), as (see, e.g., Ref. 24)

$$\mathrm{d}S=-mc\,\mathrm{d}s-\frac{e}{c}A_\mu\,\mathrm{d}x^\mu. \tag{28}$$

But this form has also a new geometrical interpretation. It means that, in this framework, an increase of the length can come from two contributions: the first is the usual variation due to the motion of the particle, while the second new contribution, which is of geometric nature, is a length dilation of the internal fractal structures.

We are now able to write a geodesics equation minimizing the length invariant (i.e., the proper time), which coincides with the least-action principle $\delta\int \mathrm{d}S=0$ (see Ref. 24). The variation of the above action yields the Lorentz equation of electrodynamics,

$$mc\frac{\mathrm{d}u_\alpha}{\mathrm{d}s}=\frac{e}{c}F_{\alpha\mu}u^\mu, \tag{29}$$

where $F_{\alpha\mu}=\partial_\alpha A_\mu-\partial_\mu A_\alpha$ is the electromagnetic tensor field. We also recover the standard form for the differential of the action as a function of the coordinates, namely,

$$\mathrm{d}S=-\left(mcu_\mu+\frac{e}{c}A_\mu\right)\mathrm{d}x^\mu. \tag{30}$$

B. Quantum electrodynamics

Let us proceed with a brief account of the generalization of this approach to quantum electrodynamics. As recalled in Sec. II, in the scale relativistic approach to the quantum theory,[3,7] the four-velocity $\mathcal{V}^\mu$ that describes a scalar particle is complex, so that its action is also a complex number and it now writes $S=S(x^\mu,\mathcal{V}^\mu,\chi)$. The wave function is defined from this action as $\psi=\exp(iS/\hbar)$.

Therefore Eq. (30) now takes the form

$$\mathrm{d}S=-mc\mathcal{V}_\mu\,\mathrm{d}x^\mu-\frac{e}{c}A_\mu\,\mathrm{d}x^\mu. \tag{31}$$

The new relation between the wave function and the velocity reads

$$mc\mathcal{V}_\mu=i\hbar\,D_\mu\ln\psi=i\hbar\,\partial_\mu\ln\psi-\frac{e}{c}A_\mu, \tag{32}$$

so that we recover the standard QED covariant derivative as being nothing but the scale-covariant derivative previously introduced, but now acting on the wave function,

$$D_\mu = \partial_\mu + i\frac{e}{\hbar c}A_\mu. \tag{33}$$

C. Gauge invariance

Let us now consider a second internal structure of the fractal geodesics, that lies at a relative scale $\varepsilon' = \rho'\lambda$. Equation (22) becomes

$$\delta \ln \rho' = \frac{1}{q}A'_\mu \, \mathrm{d}x^\mu. \tag{34}$$

Let φ be the ratio between the scales ε' and ε. In the framework of Galilean scale relativity (where the product of two successive dilations ρ and ρ' is $\rho'' = \rho \times \rho'$), this ratio is simply $\varphi = \rho'/\rho$. One therefore finds

$$A'_\mu = A_\mu + q\partial_\mu \ln \varphi, \tag{35}$$

which is the standard gauge invariance relation for the potential. But here a gauge transformation, instead of being arbitrary, is identified with a scale transformation of the resolution variable in scale space. Under such a transformation, the wave function of the particle becomes

$$\psi' = \psi \exp\left(-i\frac{eq}{\hbar c}\ln \varphi\right). \tag{36}$$

As a consequence, the Lagrangian given by Eq. (31), that includes the particle and field-particle coupling terms, remains globally invariant under a gauge transformation.

When $q = e$ (the electron charge), we have $e^2 = 4\pi\alpha\hbar c$, where α is the "fine structure constant," i.e., the electromagnetic coupling constant. The previous expression becomes in this case $\psi' = \psi \exp(-i4\pi\alpha \ln \varphi)$. In the framework of the special scale-relativity theory[12] in which possible scale ratios become limited $[\ln \varphi < \ln(m_\mathrm{P}/m_e)]$ because of the identification of the Planck length scale with a lowest (invariant under dilations) scale, this expression has been used to suggest the existence of a relation between the mass and the charge of the electron.[2–4]

Let us conclude this review part by stressing that the scale-relativity theory of electromagnetism shares some features with the Weyl-Dirac theory,[25,26] but that it has new and essential differences. Namely, the Weyl theory considers scale transformations of the line element, $\mathrm{d}s \rightarrow \mathrm{d}s' = \rho\, \mathrm{d}s$, but without specifying any fundamental cause for this dilation. The variation of $\mathrm{d}s$ should therefore exist at all scales, in contradiction with the observed invariance of the Compton length of the electron (i.e., of its mass).

In the scale-relativity proposal, the change of the line element comes from the fractal geometry of space-time, and it is therefore a consequence of the dilation of the scale variables ("resolutions"). Moreover, the explicit effects of the dependence on resolutions is observable only below the transition between scale dependence and scale independence, which is identified with the Compton scale of the particle in its rest frame. This ensures the invariance, in this theory, of the observed electron mass.

IV. NON-ABELIAN GAUGE FIELDS

A. Scale-relativistic description

1. Introduction

We now generalize the electromagnetic description to a geometric foundation of non-Abelian gauge theories, based upon the scale-relativity first principles. We consider that the internal fractal structures of the "particle" (i.e., of the family of geodesics of a nondifferentiable space-time) are now described in terms of several scale variables $\eta_{\alpha\beta\ldots}(x,y,z,t)$, that generalize the single reso-

lution variable ε. We write them for simplicity in units of λ, and we assume that the various indices can be gathered into one common index: we therefore write the scale variables under the simplified form η_α ($\alpha=0$ to N).

In the simplest case, $\eta_\alpha=\varepsilon_\alpha$, where ε_α correspond to the resolutions of the space-time coordinates X_α ($\alpha=1-4$). However, other situations can be considered, since their true nature is tensorial rather than vectorial, and since, in analogy with GR, general transformations can be applied to these variables, for example, the transformation $\varepsilon_\alpha \to \ln \varepsilon_\alpha$ may be particularly relevant for such scale variables. In this paper, we shall not be more specific about the choice of the scale variables, in order to keep generality. Moreover, our aim here is mainly to relate in a general way the scale-relativistic tools to the standard description of current gauge theories, so that we shall present only a general description of the scale transformations obtained, leaving to future works a more specific establishment of the final gauge group. However, even at this preliminary stage of the analysis, we can show that in any case it contains at least an SU(2) subgroup, e.g., the three-dimensional rotations in scale-space which can be identified with the isospin transformation group (see Sec. IV A 4 below).

2. General scale transformations

Let us consider infinitesimal scale transformations. The transformation law on the η_α can be written in a linear way as

$$\eta'_\alpha = \eta_\alpha + \delta\eta_\alpha = (\delta_{\alpha\beta} + \delta\theta_{\alpha\beta})\eta^\beta, \tag{37}$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol, or equivalently,

$$\delta\eta_\alpha = \delta\theta_{\alpha\beta}\eta^\beta. \tag{38}$$

Let us now assume that the η_α's are functions of the standard space-time coordinates. This leads us to generalize the scale-covariant derivative previously defined in the electromagnetic case as follows: the total variation of the resolution variables becomes the sum of the inertial one, described by the covariant derivative, and of the new geometric contribution, namely,

$$\mathrm{d}\eta_\alpha = D\eta_\alpha - \eta^\beta\delta\theta_{\alpha\beta} = D\eta_\alpha - \eta^\beta W^\mu_{\alpha\beta}\,\mathrm{d}x_\mu. \tag{39}$$

Note that, here, this covariant derivative is similar to that of GR, i.e., it amounts to subtract the new geometric part in order to keep only the inertial part (for which the motion equation will therefore take a geodesical, freelike form). This is different from the case of the quantum-covariant derivative [Eq. (13)], which includes the effects of nondifferentiability by adding new terms in the total derivative.

Recall that in the Abelian case, which corresponds to a unique global dilation, this expression can be simplified since $\mathrm{d}\eta/\eta=\mathrm{d}\ln\eta=\mathrm{d}\chi$. We want also to note here that we have chosen to write the new geometric contribution $-\eta^\beta\delta\theta_{\alpha\beta}$, i.e., with a minus sign, in order to recover the covariant derivative of gauge theories in its standard form (this is actually an inessential sign ambiguity).

In this new situation we are led to introduce "gauge field potentials" $W^\mu_{\alpha\beta}$ that enter naturally in the geometrical frame of Eq. (39). These potentials are linked to the scale transformations as follows:

$$\delta\theta_{\alpha\beta} = W^\mu_{\alpha\beta}\,\mathrm{d}x_\mu. \tag{40}$$

One should remain cautious about this expression and keep in mind that these potentials find their origin in a covariant derivative process and are therefore not gradients (this is expressed by the use of a difference sign $\delta\theta_{\alpha\beta}$ instead of $\mathrm{d}\theta_{\alpha\beta}$). They formalize the coupling between displacements in space-time and transformations of the scale variables and play in Eq. (39) a role analogous to the one played in general relativity by the Christoffel symbols. It is also important to notice that the $W^\mu_{\alpha\beta}$ introduced at this level of the analysis do not include charges. They are functions of the space and time coordinates only. This is a necessary choice because our method generates, as we shall

see, not only the fields but also the charges from, respectively, the scale transformations and the scale symmetries of the dynamical fractal space-time.

3. Multiplets

After having written the transformation law of the basic variables (the η_α's), we are now led to describe how various physical quantities transform under these η_α transformations. These new transformation laws are expected to depend on the nature of the objects to transform (e.g., vectors, tensors, spinors, etc.), which implies to jump to group representations.

In the case where the particle is a spin-1/2 fermion, it has been recalled in Eq. (18) that the relation between the velocity and the spinor fields reads

$$\mathcal{V}_\mu = i\lambda\psi^{-1}\partial_\mu\psi, \tag{41}$$

where $\mathcal{V}_\mu$ and ψ are complex quaternions and the constant $\lambda = \hbar/mc$ is the Compton length of the particle.

However, bispinors are not a general enough description for fermions subjected to a general gauge field. Indeed, we consider here a generalized group of transformations which therefore involves generalized charges. As a consequence of these new charges (whose existence will be fully justified below and their form specified), the very nature of the fermions is expected to become more complicated. Experiments have indeed shown that new degrees of freedom must be added in order to represent the weak isospin, hypercharge and color. In order to account in a general way for this more complicated description, we shall simply introduce multiplets ψ_k, where each component is a Dirac bispinor. Therefore, as already remarked in previous presentations,[3] when the scale variables become multiplets, the same is true of the charges. As we shall see in what follows, in the present approach it is at the level of the construction of the charges that the set generators enter.

In this case the multivalued velocity becomes a biquaternionic matrix,

$$\mathcal{V}^\mu_{jk} = i\lambda\psi_j^{-1}\partial^\mu\psi_k. \tag{42}$$

The biquaternionic (therefore noncommutative) nature of the wave function (which is equivalent to Dirac bispinors) plays here an essential role, as previously announced. Indeed, it leads to write the velocity field as $\psi^{-1}\partial^\mu\psi$ instead of $\partial^\mu \ln\psi$ in the complex case, so that its generalization to multiplets involves two indices instead of one. As we shall see in what follows, the general structure of Yang-Mills theories and the correct construction of non-Abelian charges will be obtained thanks to this result.

Therefore the action becomes also a tensorial two-index quantity,

$$\mathrm{d}S_{jk} = \mathrm{d}S_{jk}(x^\mu, \mathcal{V}^\mu_{jk}, \eta_\alpha). \tag{43}$$

In the absence of a field, it is linked to the generalized velocity (and therefore to the spinor multiplet) by the relation

$$\partial^\mu S_{jk} = -mc\mathcal{V}^\mu_{jk} = -i\hbar\,\psi_j^{-1}\partial^\mu\psi_k. \tag{44}$$

Now, in the presence of a field [i.e., when the second-order effects of the fractal geometry appearing in the right-hand side of Eq. (39) are included], using the complete expression for $\partial^\mu\eta_\alpha$,

$$\partial^\mu\eta_\alpha = D^\mu\eta_\alpha - W^\mu_{\alpha\beta}\eta^\beta, \tag{45}$$

we are led to write a relation that generalizes Eq. (25) to the non-Abelian case,

$$\partial^\mu S_{jk} = \frac{\partial S_{jk}}{\partial\eta_\alpha}\partial^\mu\eta_\alpha = \frac{\partial S_{jk}}{\partial\eta_\alpha}(D^\mu\eta_\alpha - W^\mu_{\alpha\beta}\eta^\beta). \tag{46}$$

Thus we obtain

$$\partial^{\mu} S_{jk} = D^{\mu} S_{jk} - \eta^{\beta} \frac{\partial S_{jk}}{\partial \eta_{\alpha}} W^{\mu}_{\alpha\beta}. \tag{47}$$

We are finally led to define a general group of scale transformations whose generators are

$$T^{\alpha\beta} = \eta^{\beta} \partial^{\alpha} \tag{48}$$

(where we use the compact notation $\partial^{\alpha} = \partial / \partial \eta_{\alpha}$), yielding the generalized charges,

$$\frac{\tilde{g}}{c} t^{\alpha\beta}_{jk} = \eta^{\beta} \frac{\partial S_{jk}}{\partial \eta_{\alpha}}. \tag{49}$$

This group is submitted to a unitarity condition, since, when it is applied to the wave functions, $\psi\psi^{\dagger}$ must be conserved.

4. Rotations in "scale-space"

In order to enlight the meaning of the new definition we have obtained for the charges, we consider in the present section a subsample of the possible scale transformations on intrinsic scale variables: namely, those which are built from the antisymmetric part of the gauge set (that can therefore be identified as rotations in the scale space). In this case the infinitesimal transformation is such that

$$\delta\theta_{\alpha\beta} = -\delta\theta_{\beta\alpha} \Rightarrow W^{\mu}_{\alpha\beta} = -W^{\mu}_{\beta\alpha}. \tag{50}$$

Therefore, reversing the indices in Eq. (47), we may write

$$\partial_{\mu} S_{jk} = D_{\mu} S_{jk} - \eta^{\alpha} \frac{\partial S_{jk}}{\partial \eta_{\beta}} W^{\mu}_{\beta\alpha}. \tag{51}$$

Taking the half-sum of Eqs. (47) and (51) we finally obtain

$$\partial_{\mu} S_{jk} = D_{\mu} S_{jk} - \frac{1}{2} \left(\eta^{\beta} \frac{\partial S_{jk}}{\partial \eta_{\alpha}} - \eta^{\alpha} \frac{\partial S_{jk}}{\partial \eta_{\beta}} \right) W^{\mu}_{\alpha\beta}. \tag{52}$$

This leads to define the new charges,

$$\frac{\tilde{g}}{c} t^{\alpha\beta}_{jk} = \frac{\partial S_{jk}}{\partial \theta_{\alpha\beta}} = \frac{1}{2} \left(\eta^{\beta} \frac{\partial S_{jk}}{\partial \eta_{\alpha}} - \eta^{\alpha} \frac{\partial S_{jk}}{\partial \eta_{\beta}} \right). \tag{53}$$

We recognize here a definition similar to that of the angular momentum, i.e., of the conservative quantity that finds its origin in the isotropy of space; but the space under consideration is here the "scale-space," i.e., the space of the scale variables that must be added for a proper description of a fractal geometry of space-time. Therefore the charges of the gauge fields are identified, in this interpretation, with "scale-angular momenta."

The subgroup of transformations corresponding to these generalized charges is, in three dimensions, a SO(3) group related to a SU(2) group by the homomorphism which associates to two distinct 2×2 unitary matrices of opposite sign the same rotation. We are therefore naturally led to define a "scale-spin," which we propose to identify to the simplest non-Abelian charge in the current standard model: the weak isospin.

Coupling this SU(2) representation of the rotations in a three-dimensional sub-"scale-space" to the U(1) representation of the global scale dilations (that describes the electromagnetism process) analyzed in Sec. III, we are therefore able to give a physical geometric meaning to the transformation group corresponding to the $U(1) \times SU(2)$ representation of the standard electroweak theory.[27,28]

It is worth stressing here that the group of three-dimensional rotations in "scale-space" is only a subgroup of an at least four-dimensional rotation group (one scale variable for each space-time coordinate), and therefore at least SO(4), and, more precisely, its universal covering group $\mathrm{SU}(2)\times\mathrm{SU}(2)$.

B. Yang-Mills theory with the scale-relativity tools

1. Simplified notation

For the subsequent developments, we shall simplify the notations and use only one index $a=(\alpha,\beta)$ for the scale transformations: this index runs on the gauge group parameters, now written θ_a. For example, in three dimensions, this means that we replace the three rotations $\theta_{23},\theta_{31},\theta_{12}$, respectively, by $\theta_1,\theta_2,\theta_3$. We obtain the following more compact form for the complete action:

$$\mathrm{d}S_{jk}=\left(D_\mu S_{jk}-\frac{\widetilde{g}}{c}t^a_{jk}W_{a\mu}\right)\mathrm{d}x^\mu, \tag{54}$$

and therefore

$$D^\mu S_{jk}=-i\hbar\,\psi_j^{-1}D^\mu\psi_k=-i\hbar\,\psi_j^{-1}\partial^\mu\psi_k+\frac{\widetilde{g}}{c}t^a_{jk}W^\mu_a. \tag{55}$$

2. Scale relativistic tools for Yang-Mills theory

The previous equations have used new concepts that are specific of the scale-relativity approach, namely (i) the scale variables η_α, (ii) the biquaternionic velocity matrix $\mathcal{V}^\mu_{jk}$, and (iii) its associated action S_{jk}. The standard concepts of quantum field theories, namely the fermionic field ψ, the bosonic field W^μ_a, the charges g, the gauge group generators t^a_{jk} and the gauge-covariant derivative D_μ are here all of them derived from these new tools.

Let us show that we are thus able to recover the basic relations of standard non-Abelian gauge theories (see, e.g., Ref. 29). From Eq. (55), we first obtain the standard form for the covariant partial derivative, now acting on the wave-function multiplets,

$$D^\mu\psi_k=\partial^\mu\psi_k+i\frac{\widetilde{g}}{\hbar c}t^{ja}_k W^\mu_a\psi_j. \tag{56}$$

The ψ_k's do not commute together since they are biquaternionic quantities, but this is the case neither of t^{ja}_k nor of W^μ_a, so that ψ_j can be set to the right as in the standard way of writing; from the multiplet point of view (index j), we simply exchange the lines and columns.

Now introducing a dimensionless coupling constant α_g and a dimensionless charge g, such that

$$g^2=4\pi\alpha_g=\frac{\widetilde{g}^2}{\hbar c}, \tag{57}$$

and redefining the dimensionality of the gauge field (namely, we replace $W^\mu_a/\sqrt{\hbar c}$ by W^μ_a), the covariant derivative may be more simply written under its standard form,

$$D^\mu\psi_k=\partial^\mu\psi_k+igt^{ja}_k W^\mu_a\psi_j, \tag{58}$$

where all of the three new contributions, g, t^{ja}_k, and W^μ_a have been constructed from the origin by the theory and given a geometric meaning.

In the simplified case of a fermion singlet, it reads

$$D^{\mu} = \partial^{\mu} + igt^{a}W_{a}^{\mu}. \tag{59}$$

Let us now derive the laws of gauge transformation for the fermion field. Consider a transformation θ_a of the scale variables. As we shall now see, the θ_a can be identified with the standard parameters of a non-Abelian gauge transformation. Indeed, using the above remark about the exchange of lines and columns, Eq. (44) becomes

$$-i\hbar\,\partial^{\mu}\psi_{k} = \partial^{\mu}S_{k}^{j}\psi_{j} \tag{60}$$

and allows us to recover by a different way Eq. (58), from which we obtain the standard form for the transformed fermion multiplet in the case of an infinitesimal gauge transformation $\delta\theta_a$,

$$\psi_{k}' = (\delta_{k}^{j} - igt_{k}^{ja}\delta\theta_{a})\psi_{j}. \tag{61}$$

3. Yang-Mills theory

We have now at our disposal all the tools of quantum gauge theories. The subsequent developments are standard ones in terms of these tools. Namely, one introduces the commutator of the matrices t_a (which have *a priori* no reason to commute), under the form

$$t_{a}t_{b} - t_{b}t_{a} = if_{ab}^{c}t_{c}. \tag{62}$$

Therefore the t_a's are identified with the generators of the gauge group and the if_{ab}^{c}'s with the structure constants of its associated Lie algebra. The noncommutativity of the generators and the requirement of the full Lagrangian invariance under the scale transformations finally imply the appearance of an additional term in the gauge transformation law of the boson fields. We obtain this additional term by the standard method recalled below.

We replace into the Lagrangian of the fermionic field given by Eq. (20) the partial derivative ∂_μ by its covariant counterpart D_μ of Eq. (59). The development of the covariant derivative leads to the appearance of two terms, a free particle one and a fermion-boson coupling term,

$$\mathcal{L} = \bar{\psi}(i\gamma^{\mu}\partial_{\mu} - m)\psi - g\bar{\psi}\gamma^{\mu}t_{a}W_{\mu}^{a}\psi. \tag{63}$$

Let us now consider an infinitesimal scale transformation of the fermion field,

$$\psi \to \psi e^{-ig\,\delta\theta^{b}t_{b}}. \tag{64}$$

The requirement of the full Lagrangian invariance under this transformation involves also the coupling term. Let us consider the transformation of this term, except for the W_μ contribution,

$$\bar{\psi}\gamma^{\mu}t_{a}\psi \to \bar{\psi}e^{ig\,\delta\theta^{b}t_{b}}\gamma^{\mu}t_{a}\psi e^{-ig\,\delta\theta^{b}t_{b}}. \tag{65}$$

Accounting for the fact that this is an infinitesimal transformation, it becomes

$$\bar{\psi}(1 + ig\,\delta\theta^{b}t_{b})\gamma^{\mu}t_{a}\psi(1 - ig\,\delta\theta^{b}t_{b}) = \bar{\psi}\gamma^{\mu}t_{a}\psi + ig\bar{\psi}\gamma^{\mu}\delta\theta^{b}(t_{b}t_{a} - t_{a}t_{b})\psi. \tag{66}$$

We replace the commutator $t_bt_a - t_at_b$ by its expression in Eq. (62), and we obtain

$$\bar{\psi}\gamma^{\mu}t_{a}\psi \to \bar{\psi}\gamma^{\mu}t_{a}\psi - g\bar{\psi}\gamma^{\mu}\delta\theta^{b}f_{ba}^{c}t_{c}\psi. \tag{67}$$

Then the requirement of invariance could be fulfilled only provided the transformation of the field W_μ^a itself involves a new term (in addition to the Abelian term $\partial_\mu\delta\theta^a$), i.e.,

$$W_{\mu}^{a} \to W_{\mu}^{a} + \delta W_{\mu}^{a}. \tag{68}$$

The transformation of the full coupling term now reads

$$\bar{\psi}\gamma^{\mu}t_a W_{\mu}^{a}\psi \to [(\bar{\psi}\gamma^{\mu}t_a\psi) - g f_{ba}^{c}\delta\theta^{b}(\bar{\psi}\gamma^{\mu}t_c\psi)][W_{\mu}^{a} + \delta W_{\mu}^{a}]. \tag{69}$$

Neglecting the second order term in the elementary variations and using the fact that we can interchange the running indices, we see that this expression is invariant provided

$$\bar{\psi}\gamma^{\mu}\{t_a[\delta W_{\mu}^{a} - g f_{bc}^{a}\delta\theta^{b}W_{\mu}^{c}]\}\psi = 0. \tag{70}$$

One general solution, independent of the t_a's, to the requirement of the Lagrangian invariance in the non-Abelian case is therefore

$$\delta W_{\mu}^{a} = g f_{bc}^{a}\delta\theta^{b}W_{\mu}^{c}. \tag{71}$$

Finally, under an infinitesimal scale transformation $\delta\theta^{b}$, the non-Abelian gauge boson field W_{μ}^{a} transforms as

$$W_{\mu}^{a} \to W'^{a}_{\mu} = W_{\mu}^{a} + \partial_{\mu}\delta\theta^{a} + g f_{bc}^{a}\delta\theta^{b}W_{\mu}^{c}. \tag{72}$$

We recognize here once again a standard transformation of non-Abelian gauge theories, which is now derived from the basic transformations on the η_a's of Eq. (39).

We can finish as usual the development of standard Yang-Mills theory. The gauge field self-coupling term, $-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$, is retained as the simplest invariant scalar that can be added to the Lagrangian. It is defined as follows.

First, one defines the Yang-Mills field,

$$A_{\mu} \equiv t_a W_{\mu}^{a}, \tag{73}$$

which yields the covariant derivative of Eq. (59) under the standard form,

$$D_{\mu} = \partial_{\mu} + igA_{\mu}. \tag{74}$$

Then, one establishes the analogue of the Faraday tensor of electromagnetism, by defining

$$F_{\mu\nu}^{a} \equiv \partial_{\mu}W_{\nu}^{a} - \partial_{\nu}W_{\mu}^{a} - g f_{bc}^{a}W_{\mu}^{b}W_{\nu}^{c} \tag{75}$$

and

$$F_{\mu\nu} \equiv t_a F_{\mu\nu}^{a}, \tag{76}$$

which gives

$$F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} + ig[A_{\mu},A_{\nu}]. \tag{77}$$

One adds to the Lagrangian density $\mathcal{L}$ a kinetic term for the free Yang-Mills gauge field,

$$\mathcal{L}_A = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}. \tag{78}$$

This form is justified by the same reasons as in the standard theory (namely, it must be a scalar and constructed from the fields and not from the potentials, which are gauge dependent). The Euler-Lagrange equations therefore read

$$\partial_{\mu}F^{\mu\nu} + ig[A_{\mu},F^{\mu\nu}] = 0. \tag{79}$$

Introducing the Yang-Mills derivative operator,

$$\nabla_{\mu} = \partial_{\mu} + ig[A_{\mu}, \ ], \tag{80}$$

one finally obtains the standard Yang-Mills equations which generalize to the non-Abelian case the source-free Maxwell equation,

$$\nabla_\mu F^{\mu\nu} = 0. \tag{81}$$

We are therefore provided with a fully consistent gauge theory obtained as a consequence of scale symmetries issued from a geometric space-time description.

V. CONCLUSION

In the present paper our purpose has been to give a physical meaning to the various items entering the gauge field theories in the framework of scale relativity, extending to the non-Abelian case the results of previous works devoted to the understanding of the Abelian gauge-invariant theory of electromagnetism.

We have so far reached an understanding of the nature of gauge transformations, in terms of a geometric space-time description. We decompose, for simplification purpose, the dynamics emerging from displacements in the fractal space-time of scale relativity into (i) transformations occuring on the scale variables in the framework of a nondirectly observable local "scale-space" coupled to (ii) displacements in space-time. The scale variables become thus functions of the space-time coordinates.

The gauge charges appear as the generators of the set of scale transformations applied to a generalized action, therefore emerging from the scale symmetries of the dynamical fractal space-time. Considering the transformation laws verified by the scale variables, we are able to establish how the various physical quantities transform under these laws and to recover the standard gauge theory form of these transformations.

We are now provided with a theory where the gauge group is no more defined through its only action on the physical objects, as in the standard framework, but as the transformation group of the scale variables, and where the boson fields and the charges are given a physical meaning. We have established the following correspondences between the standard gauge theory items and the scale-relativistic tools:

(i) gauge transformations $\leftrightarrow$ scale transformations in scale-space,
(ii) internal gauge space $\leftrightarrow$ local "scale-space,"
(iii) gauge fields $\leftrightarrow$ manifestations of the fractal and scale-relativistic geometry of space-time (analogues of the Christoffel symbols issuing from the curvature of space-time in general relativity),
(iv) gauge charges $\leftrightarrow$ conservative quantities, conjugate to the scale variables, originating from the symmetries of the "scale space" and generators of the scale transformation group.

Since, in the present study, our aim was to recover the standard description of current gauge theory, we have, in the main part of the work, retained a general form for the scale variables. However we have shown that, whatever will be their more specific form, the gauge set will contain in any case the $U(1) \times SU(2)$ electroweak theory group as subset.

In future works, we shall study other sets of transformations that can be derived from the present study, where the scale variables will be given new precise definitions and which hopefully could yield hypercharge, color and maybe new developments in gauge field theory. We shall also consider in more details the issues of the fermion sectors, of the mass and charge renormalization and of the Higgs field.

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The generalized Ricci flow for three-dimensional manifolds with one Killing vector

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We consider three-dimensional (3D) flow equations inspired by the renormalization group (RG) equations of string theory with a three-dimensional target space. By modifying the flow equations to include a U(1) gauge field, and adding carefully chosen De Turck terms, we are able to extend recent two-dimensional results of Bakas to the case of a 3D Riemannian metric with one Killing vector. In particular, we show that the RG flow with De Turck terms can be reduced to two equations: the continual Toda flow solved by Bakas, plus its linearizaton. We find exact solutions which flow to homogeneous but not always isotropic geometries. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178585]

I. INTRODUCTION

The Ricci flow of d-dimensional manifolds is interesting because of its relationship to the renormalization group (RG) equations of generalized two-dimensional (2D) sigma models with d-dimensional target space. In two space-time dimensions, Ricci flow also provides a proof[1] of the uniformization theorem,[2] which states that every closed orientable two-dimensional manifold with handle number 0,1, or >1 admits *uniquely* the constant curvature geometry with positive, zero, or negative curvatures, respectively. Bakas[3] has shown that the 2D Ricci flow equations in conformal gauge provide a continual analogue of the Toda field equations. Using this algebraic approach he was able to write down the general solution.

The potential importance of a three-dimensional (3D) uniformization theorem is evident particularly in the context of (super) membrane physics and three-dimensional quantum gravity where one should be able to perform path-integral quantization via a similar procedure to that in two dimensions. Unfortunately, there is no uniformization theorem in three dimensions, only a conjecture due to Thurston[4,5].

Recently there has been speculation that Perelman[6] has overcome some roadblocks in Hamilton's program to prove the conjecture using the Ricci flow.[7,8] It is therefore important to understand in detail the properties of this flow.

In the following, we follow up on a suggestion by Bakas to use his 2D results in order to analyze the flow equations for 3D manifolds with a single Killing vector. This provides a tractable midisuperspace approach which can be systematically studied in the context of the stringy flow first considered in Ref. 9. We will show that this flow reduces to the infinite dimensional generalization of the Toda equation for the conformal factor of the invariant 2D submanifold plus a linear equation for the scale factor of the extra dimension. Note that since the latter scale factor depends on the coordinates of the invariant subspace, our manifolds are not simple direct products. In addition, we will analyze two exact analytic solutions in detail and show that they have the expected behavior.

The paper is organized as follows. Section II reviews 2D flow equations and Bakas' results, Sec. III reviews the stringy flow of Ref. 9, but with the De Turck modification.[10] The De Turck

modification contains a vector field ξ_i, and we show that if we choose this vector field as a linear combination of two vector fields, one of which is proportional to the gradient of the dilaton field, then the dilaton can be decoupled from the flow of the remaining fields. In Sec. IV we discuss the flow for a metric ansatz where one of the coordinates is in the direction of a Killing vector field, and the remaining part of the metric is in the form of a conformal 2D metric. We use the second part of the De Turck vector field to preserve this form of the metric throughout the flow. In order that the flow is self-consistent, the U(1) vector field in the stringy flow must be fixed in terms of the functions that occur in the metric tensor. The flow then reduces to two equations for the two metric degrees of freedom. One of these is the continual Toda equation[3] for the conformal factor of the 2D geometry orthogonal to the Killing vector field, and the other, for the component of the metric in the direction of the Killing vector field, is the linearization of the continual Toda equation. Section V presents specific solutions and Sec. VI ends with conclusions and prospects for future work.

II. THE 2D CASE

We now summarize the methodology and results of Bakas[3] since they play a crucial role in the following. The Ricci flow equations, for arbirary 2-metric g_{AB} are

$$\frac{\partial g_{ij}}{\partial t} = -R_{ij} + \nabla_i \xi_j + \nabla_j \xi_i. \tag{1}$$

The last two terms (the so-called "De Turck" terms) incorporate the effects of all possible diffeomorphisms and can be chosen arbitrarily in order to simplify the equations and/or optimize convergence. The original reason for the inclusion of these terms was to show that the bare Ricci flow—without the Lie derivative term—satisfied short term existence. To do this, one had to break the diffeomorphism invariance and this was accomplished by introducing a background symmetric connection $\bar{\Gamma}^i_{jk}$, and the vector field $\xi^i := g^{jk}(\Gamma^i_{jk} - \bar{\Gamma}^i_{jk})$, where the last term is the Christoffel connection with respect to the metric g_{ij}. It was shown[10] that the resulting flow was strongly parabolic and short time existence could be proved. It was also shown that any solution of the bare Ricci flow was also a solution of the De Turck modified flow.

Bakas chose to work in the conformal gauge,

$$ds^2 = g_{ij}\, dx^i\, dx^j = \tfrac{1}{2} \exp(\Phi)(dx^2 + dy^2). \tag{2}$$

In this gauge there is no need to add De Turck terms and the flow takes the form of a nonlinear "heat equation:"

$$\frac{\partial}{\partial t} e^{\Phi} = \nabla^2 \Phi. \tag{3}$$

The Toda equations describe the integrable interactions of a collection of two-dimensional fields $\Phi_i(x,y)$ coupled via the Cartan matrix K_{ij},

$$\sum_j K_{ij} e^{\Phi_j(x,y)} = \nabla^2 \Phi_i(x,y). \tag{4}$$

Bakas argues that Eq. (3) is a continual analogue of the above, with the Cartan matrix replaced by the kernel,

$$K_{ij} \to K(t,t') = \frac{\partial}{\partial t} \delta(t,t'). \tag{5}$$

This leads to a general solution to (3) in terms of a power series around the free field expanded in path ordered exponentials. Each term in the perturbation series is itself a solution of the Ricci flow. Although the resulting expression is difficult to work with explicitly, it does provide a formal

complete solution to the 2D flow equations. Bakas showed that several solutions of the flow found by other means can be written as continual Toda flows, and this provides some confidence in the convergence of the latter. One of these solutions is the so-called sausage model, and this 2D flow will appear in the 3D case discussed below. Furthermore, Bakas indicates that the continual Toda flow, though formally a solution of the RG flow in 2D only to lowest order in the coupling constant, may be lifted at least in some cases to a solution of the flow with higher order terms.[3] Finally, it is clear that the solution will provide some insight into how uniformization works that cannot be easily seen via the more conventional discussion of the heat equation.

In the next sections we will show that a similar formal solution can also be found for three-dimensional metrics with at least one Killing field.

III. 3D FLOW EQUATIONS

We consider here a generalization of the Ricci flow, in which, besides the metric g_{ij}, there are additional fields which flow, consisting of a dilaton ϕ, a gauge two-form potential B_{ij} with field strength H_{ijk} and finally, a U(1) gauge field with potential 1-form A_i and corrresponding field strength F_{ij} which couples as a Maxwell-Chern-Simons theory. Including De Turck terms plus gauge terms for the flow of the nonmetric fields, the flow is

$$\dot{g}_{ij} = -2\left(R_{ij} + 2\phi_{|ij} - \left(\epsilon_F F_i{}^k F_{jk} + \frac{\epsilon_H}{4} H_{ikl} H_j{}^{kl}\right)\right) + L_\xi g_{ij}, \tag{6}$$

$$\dot{A}_i = -\left(e^{2\phi}\nabla_j(e^{-2\phi}F_i{}^j) + \frac{e\epsilon_F}{2}\eta_i{}^{jk}F_{jk}\right) + L_\xi A_i + \partial_i\Lambda, \tag{7}$$

$$\dot{B}_{ij} = e^{2\phi}\nabla_k(e^{-2\phi}H^k{}_{ij}) + L_\xi B_{ij} + \partial_i\Lambda_j - \partial_j\Lambda_i, \tag{8}$$

$$\dot{\phi} = -\chi + \Delta\phi - |\nabla\phi|^2 + \frac{\epsilon_F}{2}F^2 + \frac{\epsilon_H}{12}H^2 + L_\xi\phi. \tag{9}$$

In the above, the terms in the Lie derivatives L_ξ are the De Turck terms. The terms containing Λ and Λ_i appear for similar reasons to the De Turck terms: that is, they correspond to arbitrary gauge transformations on the gauge fields with potentials A_i and B_{ij}. By choosing the gauge and coordinate transformation terms judiciously, we are able to simplify the equations considerably.

This flow is motivated by two considerations. First, as shown in Ref. 9, all of the Thurston geometries are solutions of the equations of motion of this theory for various values of the parameters χ, ϵ_H, ϵ_F, e, as well as the other fields. In particular, the addition of the Maxwell term alone ($e=0$) yields $S^2\times E^1$, $H^2\times E^1$ and Sol as solutions. Moreover, there exists a generalized Birkhoff theorem which guarantees that these are the only solutions when $\phi=$constant and $A\neq 0$. With $e\neq 0$, one finds that the remaining Thurston geometries Nil and $\mathrm{SL}(2,R)$ are also solutions. As argued in Ref. 9 it seems plausible that these are the only solutions, but to date no rigorous proof exists.

The second motivation comes from string theory. In particular, the RG flow for a nonlinear sigma model with a four-dimensional (4D) Kaluza-Klein target space resembles the flow above, with the A_i potential originating as the twist potential of the 4D Kaluza-Klein metric. That is, the idea is to introduce an extra fourth dimension y, with the g_{yi} components of the metric and the B_{iy} components of the antisymmetric tensor field proportional to each other. The g_{yy} component of the metric is a constant, and all the remaining components of the various fields are independent of the y coordinate. The Chern-Simons term arises from the presence of such a term in the definition of the field strength H_{ijk} in terms of the B_{ij} and B_{yj} potentials. The details of this are being investigated elsewhere.[11]

We choose $\xi_i = k_i + 2\nabla_i\phi$ and let $\Lambda = -2A_j\phi^{|j}$ and $\Lambda_i = 2B_{ji}\phi^{|j}$, where k_i is as yet arbitrary. With these choices the dilaton is completely eliminated from the flow equations for the metric and gauge fields,

$$\dot{g}_{ij} = -2\left(R_{ij} - \left(\epsilon_F F_i{}^k F_{jk} + \frac{\epsilon_H}{4} H_{ikl} H_j{}^{kl}\right)\right) + L_k g_{ij}, \tag{10}$$

$$\dot{A}_i = -\left(\nabla_j F_i{}^j + \frac{e\epsilon_F}{2}\eta_i{}^{jk} F_{jk}\right) + L_k A_i + \partial_i \lambda, \tag{11}$$

$$\dot{B}_{ij} = \nabla_k H^k{}_{ij} + L_k B_{ij} + \partial_i \lambda_j - \partial_j \lambda_i, \tag{12}$$

$$\dot{\phi} = -\chi + \Delta\phi - 2|\nabla\phi|^2 + \frac{\epsilon_F}{2}F^2 + \frac{\epsilon_H}{6}H^2 + L_k\phi. \tag{13}$$

The arbitrary vector k^i and gauge parameters λ, λ_i indicate that we are still free to add further De Turck and gauge terms to the equations. We will use this freedom later to simplify the equations that result from a particular *ansatz*.

IV. A PARTICULAR CASE WITH ONE KILLING VECTOR FIELD

Henceforth we set B_{ij} identically equal to 0, which is consistent with the flow equations. We also consider the case $e=0$ (no Chern-Simons term). We assume the metric to have a single Killing vector and to be manifestly hypersurface orthogonal (i.e., diagonal),

$$ds^2 = e^{\Phi}(dx^2 + dy^2) + e^{\sigma} dw^2. \tag{14}$$

We also choose the following *ansatz* for the vector potential:

$$A_i = [e^{\sigma/2}, 0, 0]. \tag{15}$$

Consistency of the above *ansatz* requires that the flow equations preserve the diagonal nature of the metric. It turns out that this can be accomplished by choosing the vector field k_i as

$$k_i = -\tfrac{1}{2}\partial_i\sigma, \tag{16}$$

With these choices the flow equations simplify to

$$\dot{g}_{xx} = e^{\Phi}\dot{\Phi} = \nabla^2\Phi + \tfrac{1}{2}(1+\epsilon_F)(\partial_x\sigma)^2,$$

$$\dot{g}_{yy} = e^{\Phi}\dot{\Phi} = \nabla^2\Phi + \tfrac{1}{2}(1+\epsilon_F)(\partial_y\sigma)^2,$$

$$\dot{g}_{xy} = 0 = \tfrac{1}{2}(1+\epsilon_F)\partial_x\sigma\partial_y\sigma, \tag{17}$$

$$\dot{A}_x = \dot{A}_y = 0,$$

$$\dot{A}_w = \epsilon_f\nabla^2 e^{\sigma/2} + (1+\epsilon_F)(\partial\sigma)^2. \tag{18}$$

In the above, ∇^2 denotes the flat space Laplacian.

We now fix $\epsilon_F = -1$, in which case the flow boils down to two simple partial differential equations. The first is

$$\partial_t e^{\Phi} = \nabla^2 \Phi, \tag{19}$$

which is the "continual Toda eqn" from Ref. 3. The other flow is the linearization of the continual Toda flow,

$$e^{\Phi} \partial_t e^{-\sigma/2} = -\nabla^2 e^{-\sigma/2}. \tag{20}$$

To the best of our knowledge, there is no simpler flow constructed from the Ricci-De Turck flow alone, without other fields, which can self-consistently flow the metric preserving the manifestly static form. Note that for any given solution Φ of (19), there exists a corresponding solution for σ,

$$e^{-\sigma/2} = \Phi(x,y,-t) + \chi(x,y), \tag{21}$$

where $\chi(x,y)$ is any harmonic function on the x,y subspace, i.e., satisfying, $\nabla^2 \chi = 0$.

V. EXACT SOLUTIONS OF THE FLOW

We first examine a nontrivial flow, namely the sausage solution of Bakas[3] (also called the Rossineau flow in the mathematical literature[8]). This is an exact solution of the continual Toda equation of the form

$$e^{\Phi} = \frac{2 \sinh[2\gamma t]}{\gamma(\cosh[2\gamma t] + \cosh(2y))}. \tag{22}$$

In this case,

$$e^{-\sigma/2} = \ln \left| \frac{2 \sinh[2\gamma t]}{\gamma(\cosh[2\gamma t] + \cosh(2y))} \right|, \tag{23}$$

where we have eliminated an imaginary term from $e^{-\sigma/2}$ by using the freedom to shift by a harmonic function.

In the limit as $t \to \infty$, $e^{\Phi} \to 2/\gamma$, and $e^{\sigma} \to \ln|2/\gamma|^{-2}$, so that the Ricci tensor goes to zero and in this limit, the geometry is flat. On the other hand, in the limit $t \to 0^+$, $e^{\Phi} \to 2t/\cosh^2 y$. In this limit, we find that the Ricci scalar $R \sim 1/t$. So, if we flow the highly curved nonhomogeneous metric with initial value at $t = \epsilon > 0$,

$$ds^2 = \left(\ln \frac{2\epsilon}{\cosh^2 y} \right)^{-2} dw^2 + \frac{2\epsilon}{\cosh^2(y)} (dx^2 + dy^2), \tag{24}$$

we end up at $t \to \infty$ with the flat metric. This is consistent with Thurston's conjecture.

The second type of solution is of the Liouville type. We set

$$e^{\Phi(x,y;t)} = T(t) e^{\psi(x,y)}. \tag{25}$$

Now for $t \geqslant 0$, we find that

$$\begin{aligned} T(t) &= \beta t, \\ \nabla^2 \psi - \beta e^{\psi} &= 0, \end{aligned} \tag{26}$$

where β is a separation constant. The second of the above equations is the Liouville equation, so the two-dimensional part of the metric, $e^{\Phi}(dx^2 + dy^2)$, has constant negative curvature (for $t \geqslant 0$).

Again we choose $e^{-\sigma/2} = \Phi$, so that

$$e^{\sigma} = [\ln \beta t + \psi(x,y)]^{-2}. \tag{27}$$

The separation constant $\ln \beta$ can be absorbed into ψ without loss of generality.

Hence the metric is

$$ds^2 = [\ln t + \psi(x,y)]^{-2}\, dw^2 + \beta t e^{\psi(x,y)}(dx^2 + dy^2). \tag{28}$$

The quantity $\psi(x,y)$ is a solution of the Liouville equation.

If $t \geqslant 0$, then the flow starts from some highly curved nonhomogeneous metric near $t=0$. As $t \to \infty$, we have

$$R_{AB} \sim -\frac{1}{2t} g_{AB},$$
$$R_{ww} \sim 0, \tag{29}$$

with $A, B, \cdots = x, y$. Hence, the geometry is asymptotically that of the homogeneous, but anisotropic geometry $H^2 \times E^1$.

Thus the flow is consistent with the Thurston conjecture.

VI. CONCLUSIONS

We have shown that the modified Ricci flow equations (9) for 3D metrics with at least one Killing vector can be integrated in precisely the same manner as the 2D equations, at least for the special case $\epsilon_F = -1$. In addition to extending this analysis to other values of the parameters in the action, and hence to other topologies, it is interesting to speculate whether these techniques could work for more general 3D metrics.

Consider, without loss of generality, a diagonal metric

$$ds^2 = e^{\Phi_1(x;t)}(dx^1)^2 + e^{\Phi_2(x;t)}(dx^2)^2 + e^{\Phi_3(x;t)}(dx^3)^2, \tag{30}$$

where the functions $\Phi_i(x;t)$ depend on all three coordinates x^i. The resulting bare Ricci flow is again not manifestly elliptic, and the equations have non-trivial off-diagonal terms on the right-hand side that make direct integration difficult. Since in three dimensions any metric can be made diagonal with a suitable coordinate transformation, it is reasonable to assume that there exists a modified flow that ensures that diagonal metrics evolve into diagonal metrics. We have as yet not succeeded in constructing this modified flow, but if it did exist, it is possible that the resulting three flow equations for each of the three scale factors would take a form similar to what we have found above, albeit with nontrivial coupling. It may therefore provide a basis for solving the 3D flow equations in a more general setting.

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Casimir effect in a two-dimensional signature changing space-time

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We study the Casimir effect for free massless scalar fields propagating on a two-dimensional cylinder with a metric that admits a change of signature from Lorentzian to Euclidean. We obtain a nonzero pressure, on the hypersurfaces of signature change, which destabilizes the signature changing region and so alters the energy spectrum of scalar fields. The modified region and spectrum, themselves, back react on the pressure. Moreover, the central term of diffeomorphism algebra of corresponding infinite conserved charges changes correspondingly. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2174291]

I. INTRODUCTION

The Casimir effect is usually regarded as the most well-known manifestation of vacuum fluctuations in quantum field theory. In this effect, the presence of reflecting boundaries in the quantum vacuum alters the zero-point modes of the quantized fields, and results in the shifts of the vacuum expectation values of quantities such as energy densities and stresses. These shifts lead to vacuum forces which act on the reflecting boundaries. The particular features of these forces depend on the nature of the quantum field, the type of space-time manifold and its dimensionality, the boundary geometries and the specific boundary conditions imposed on the field. Since the original work by Casimir in 1948[1] many theoretical and experimental works have been done on this problem.[2–11] In general, there are several approaches to calculate the Casimir energy: mode summation,[2] Green's function method,[4] heat kernel method,[8] along with appropriate regularization schemes such as point separation,[12,13] dimensional regularization,[14] and zeta function regularization.[15–19] Recently, general new methods have been obtained to compute the renormalized one-loop quantum energies and energy densities.[20,21]

On the other hand, signature changing space-times have recently been of particular importance as the specific geometries with interesting physical effects. The original idea of signature change was due to Hartle, Hawking, and Sakharov.[22] This interesting idea would make it possible to have both Euclidean and Lorentzian metrics in path integral approach to quantum gravity. Later, it was shown that the signature change may happen in classical general relativity, as well.[23] There are two different approaches, continuous and discontinuous, to study the signature change in classical general relativity.[23,24] In the continuous approach, the signature of metric changes continuously in passing from Euclidean to Lorentzian region. Hence, the metric becomes degenerate at the border of these regions. In the discontinuous approach, however, the metric becomes nondegenerate everywhere and is discontinuous at the border of Euclidean and Lorentzian regions.

The issue of propagation of quantum fields on signature-changing space-times has also been of some interest.[24] For example, Dray *et al.* have shown that the phenomenon of particle production may happen for scalar particles propagating in a space-time with heterotic signature. They

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have also obtained a rule for propagation of massless scalar fields on a two-dimensional space-time with signature change. Dynamical determination of the metric signature in space-time of nontrivial topology is another interesting issue which has been studied in Ref. 25

To the authors knowledge, no attempt has been done to study the Casimir effect within the geometries with signature change. A relevant work to the present paper is Ref. 26. In this work, a model of free massless scalar fields on a two-dimensional cylinder with a signature-changing strip has been studied and shown that the energy spectrum depends on the strip's width and differs from the ordinary bosonic spectrum, for low energies. Moreover, It was shown that the diffeomorphism algebra of the corresponding infinite conserved charges is different from "Virasoro" algebra and approaches it at higher energies.

In this paper, we study the Casimir effect for the free massless scalar field propagating on the above two-dimensional signature-changing cylinder. We will obtain a nonzero pressure on the hypersurfaces of signature change which leads to instability in the signature-changing region. Therefore, depending on situation, Euclidean or Lorentzian region will grow or shrink, and this will alter the energy spectrum and the diffeomorphism algebra discussed above.

Meanwhile, a lot of topics related to the Casimir effect have been explored in the context of string theory.[10,27] The above two-dimensional signature-changing cylinder is topologically similar to a closed string, with two Euclidean and Lorentzian parts, propagating in a distributional way in the two-dimensional target space, and the discontinuous nature of the model in classifying Euclidean and Lorentzian solutions with discrete symmetry motivates one to study it in the context of *orbifolds*.[26,28] On the other hand, a closed string with two Euclidean and Lorentzian parts may be of some importance in the context of *D*-branes and related conformal field theories. Therefore, taking into account this similarity, the study of Casimir effect in our model may have nontrivial impacts on closed strings or *D*-branes.

In general, we believe the idea of Casimir effect in signature-changing space-times is novel and interesting. In the present paper this effect is inevitably limited to two-dimensional space-time, which may be relevant to the study of closed bosonic strings with Euclidean and Lorentzian parts. But, further study of Casimir effect in $3+1$ dimensional signature changing space-times may have more important physical implications, especially at early universe.[29]

II. CASIMIR STRESS TENSOR IN SIGNATURE CHANGING SPACE-TIME

We consider a free massless scalar field ϕ which propagates on a two-dimensional manifold $M=R\times S^1$ (the circle S^1 represents *space* and the real line R represents *time*) with the following metric:

$$\mathrm{d}s^2 = -\,\mathrm{d}\tau^2 + g(\sigma)\mathrm{d}\sigma^2, \tag{1}$$

where τ is timelike coordinate and σ is a periodic spacelike coordinate with the period L (we assume L is the circumference of the circle with radius r), and $g(\sigma)$ is a periodic function of σ, which takes $+1$ for Lorentzian and -1 for Euclidean regions [notice that in this region the metric will be $g_{\alpha\beta}=\mathrm{diag}(-1,-1)$]

$$g(\sigma) = \begin{cases} -1 & 0 < \sigma < \sigma_0 + \mathrm{mod}\, L, \\ +1 & \sigma_0 < \sigma < L + \mathrm{mod}\, L, \end{cases} \tag{2}$$

where $\sigma=0$, L, and $\sigma=\sigma_0$ are the hypersurfaces of signature change. We assume the scalar field to satisfy specific junction conditions at these hypersurfaces. In the literature of signature change there are two kinds of junction conditions:

(i) ϕ and its derivatives are continuous across $\sigma=\sigma_0$, (Dray *et al.*),[24]
(ii) ϕ is continuous but its derivatives vanish across $\sigma=\sigma_0$, (Hayward).[23]

In this paper, we assume the first junction conditions as the appropriate boundary conditions at each region. We assume the continuity of ϕ as well as its derivatives at all times τ as

$$\phi^E|_{\Sigma,\Sigma'} = \phi^L|_{\Sigma,\Sigma'},$$
$$\partial_\sigma \phi^E|_{\Sigma,\Sigma'} = -\epsilon \partial_\sigma \phi^L|_{\Sigma,\Sigma'}, \tag{3}$$

where Σ, Σ' are the hypersurfaces of signature change, and $\epsilon = \epsilon^+/\epsilon^-$ takes the values ± 1 according to the orientation of the coordinates τ and σ in both regions of different signatures. Assuming $\epsilon^+ = +1$ and $\epsilon^- = +1$ for Euclidean and Lorentzian regions, respectively, the junction conditions (3) are written as[26]

$$\phi^E|_0 = \phi^L|_L, \quad \phi^E|_{\sigma_0} = \phi^L|_{\sigma_0},$$
$$\partial_\sigma \phi^E|_0 = -\partial_\sigma \phi^L|_L, \quad \partial_\sigma \phi^E|_{\sigma_0} = -\partial_\sigma \phi^L|_{\sigma_0}. \tag{4}$$

By solving the wave equations,

$$(\partial_\tau{}^2 + \partial_\sigma{}^2)\phi^E(\sigma,\tau) = 0,$$
$$(\partial_\tau{}^2 - \partial_\sigma{}^2)\phi^L(\sigma,\tau) = 0, \tag{5}$$

in both Euclidean and Lorentzian regions and imposing the junction conditions (4), we obtain nontrivial solutions for ϕ_ω, provided the continuous spectrum ω satisfies the following "quantization condition"[26]

$$\cosh \omega\sigma_0 \cos \omega(\sigma_0 - L) = 1. \tag{6}$$

[The spectrum ω in this model is obtained by solving the quantization condition which leads to real and σ_0-dependent values. It differs from ordinary spectrum (with pure Lorentzian signature) at low energies and coincides with the integer roots of $\cos \omega(L-\sigma_0)$, at high energies. Therefore, "sum over energies" approaches "sum over integers" at higher energies.[26]] It is shown in Ref. 26, that due to the same *time evolution* of the functions Φ^E_ω and Φ^L_ω one can construct a set of real *distributional* orthogonal and complete solutions on the arbitrary τ=const hypersurface as

$$\Phi_\omega(\sigma,\tau) = \Theta^+\Phi^E_\omega(\sigma,\tau) + \Theta^-\Phi^L_\omega(\sigma,\tau), \tag{7}$$

where $\Phi^E_\omega = (\phi^E_\omega + \phi^E_{-\omega})$, $\Phi^L_\omega = (\phi^L_\omega + \phi^L_{-\omega})$, and Θ^+, Θ^- are Heaviside distributions with support in Euclidean and Lorentzian regions, respectively. (Heaviside distributions have the property $d\Theta^\pm = \pm\delta$, where δ is the hypersurface Dirac distribution with support on the hypersurfaces of signature change.) The solutions Φ_ω are then expanded as normal mode expansions.[26]

One can also obtain the following expressions for the components of energy-momentum tensors associated with the scalar field $\Phi(\sigma,\tau)$ in both Euclidean and Lorentzian regions[26]

$$T^E_{00} = [(\partial_\tau \Phi^E)^2 - (\partial_\sigma \Phi^E)^2], \quad T^E_{01} = 2\partial_\tau \Phi^E \partial_\sigma \Phi^E,$$
$$T^L_{00} = [(\partial_\tau \Phi^L)^2 + (\partial_\sigma \Phi^L)^2], \quad T^L_{01} = 2\partial_\tau \Phi^L \partial_\sigma \Phi^L. \tag{8}$$

By introducing new coordinates σ^E_+, σ^E_- in the Euclidean region, and σ^L_+, σ^L_- in the Lorentzian one as

$$\sigma^E_+ = \tau + i\sigma, \quad \sigma^L_+ = \tau + \sigma,$$
$$\sigma^E_- = \tau - i\sigma, \quad \sigma^L_- = \tau - \sigma, \tag{9}$$

we obtain

$$T^E_{++} = (T^E_{00} - iT^E_{01})/2, \quad T^L_{++} = (T^L_{00} + T^L_{01})/2,$$

$$T^E_{--} = (T^E_{00} + iT^E_{01})/2, \quad T^L_{--} = (T^L_{00} - T^L_{01})/2, \tag{10}$$

$$T^E_{+-} = T^E_{-+} = 0, \quad T^L_{+-} = T^L_{-+} = 0.$$

Then by substituting the normal mode expansions of the solutions Φ_ω we obtain[26]

$$T^E_{++} = \tfrac{1}{2}[(\partial_\tau\Phi - i\partial_\sigma\Phi)]^2 = 2\sum_{\omega\omega'} \tilde{f}^E_\omega(+)\tilde{f}^E_{\omega'}(+)\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'},$$

$$T^E_{--} = \tfrac{1}{2}[(\partial_\tau\Phi + i\partial_\sigma\Phi)]^2 = 2\sum_{\omega\omega'} \tilde{f}^E_{-\omega}(-)\tilde{f}^E_{-\omega'}(-)\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'},$$

$$T^L_{++} = \tfrac{1}{2}[(\partial_\tau\Phi + \partial_\sigma\Phi)]^2 = 2\sum_{\omega\omega'} \tilde{f}^L_\omega(+)\tilde{f}^L_{\omega'}(+)\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'}, \tag{11}$$

$$T^L_{--} = \tfrac{1}{2}[(\partial_\tau\Phi - \partial_\sigma\Phi)]^2 = 2\sum_{\omega\omega'} \tilde{f}^L_{-\omega}(-)\tilde{f}^L_{-\omega'}(-)\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'},$$

where $\tilde{\alpha}^\dagger$ and $\tilde{\alpha}$ are the creation and annihilation operators, respectively, and (the scalar product $\langle\Phi_\omega, \Phi_\omega\rangle$ has been defined in Ref. 26)

$$\tilde{f}^E_\omega(\pm) = [(a/b)_\omega + 1]\exp(-i\omega\sigma^E_\pm)/\sqrt{4\pi\langle\Phi_\omega, \Phi_\omega\rangle},$$

$$\tilde{f}^L_\omega(\pm) = [(c/b)_\omega + (1/b)_{-\omega}]\exp(-i\omega\sigma^L_\pm)/\sqrt{4\pi\langle\Phi_\omega, \Phi_\omega\rangle}, \tag{12}$$

with $(a/b)_\omega$, $(c/b)_\omega$, $(1/b)_\omega$ given by[26]

$$(a/b)_\omega = \frac{\sin\omega(\sigma_0 - L)}{\cosh\omega\sigma_0 + \sinh\omega\sigma_0 - \cos\omega(\sigma_0 - L)},$$

$$(c/b)_\omega = \frac{(1+i)\exp(2\pi i\omega)(\sinh\omega\sigma_0 + \cosh\omega\sigma_0 - \exp(i\omega(\sigma_0 - L)))}{2(\cosh\omega\sigma_0 + \sinh\omega\sigma_0 - \cos\omega(\sigma_0 - L))}, \tag{13}$$

$$(1/b)_\omega = \frac{(1-i)\exp(-2\pi i\omega)(\sinh\omega\sigma_0 + \cosh\omega\sigma_0 - \exp(-i\omega(\sigma_0 - L)))}{2(\cosh\omega\sigma_0 + \sinh\omega\sigma_0 - \cos\omega(\sigma_0 - L))}.$$

Notice that in obtaining these results we have imposed the quantization condition (6).

Now, substituting the normal mode expansions (11) into Eqs. (10) leads to

$$T^E_{01} = i(T^E_{++} - T^E_{--}) = 2i\sum_{\omega\omega'} (\tilde{f}^E_\omega(+)\tilde{f}^E_{\omega'}(+) - \tilde{f}^E_{-\omega}(-)\tilde{f}^E_{-\omega'}(-))\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'},$$

$$T^L_{00} = T^L_{++} + T^L_{--} = 2\sum_{\omega\omega'} (\tilde{f}^L_\omega(+)\tilde{f}^L_{\omega'}(+) + \tilde{f}^L_{-\omega}(-)\tilde{f}^L_{-\omega'}(-))\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'}, \tag{14}$$

$$T^L_{01} = T^L_{++} - T^L_{--} = 2\sum_{\omega\omega'} (\tilde{f}^L_\omega(+)\tilde{f}^L_{\omega'}(+) - \tilde{f}^L_{-\omega}(-)\tilde{f}^L_{-\omega'}(-))\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'}.$$

III. VEV OF CASIMIR STRESS TENSOR

The poisson bracket structure for Φ and its conjugate momentum Π is given by equal time relations

$$\{\Phi(\sigma),\Pi(\sigma')\} = \delta(\sigma-\sigma'),$$
$$\{\Phi(\sigma),\Phi(\sigma')\} = \{\Pi(\sigma),\Pi(\sigma')\} = 0. \tag{15}$$

By substituting the normal mode expansions of Φ and Π together with the expansion of $\delta(\sigma-\sigma')$ we obtain[26]

$$[\tilde{\alpha}_\omega, \tilde{\alpha}^\dagger_{\omega'}] = \omega\delta_{\omega+\omega',0}. \tag{16}$$

If we assume $|0_L\rangle$ to be the vacuum state for the signature changing cylinder $R\times S^1$ with circumference L, then

$$\tilde{\alpha}_\omega|0_L\rangle = 0,$$
$$\langle 0_L|\tilde{\alpha}^\dagger_\omega = 0, \tag{17}$$
$$\langle 0_L|\tilde{\alpha}_\omega\tilde{\alpha}^\dagger_{\omega'}|0_L\rangle = \omega\delta_{\omega+\omega',0}$$

and we obtain the following vacuum expectation values for the components of energy momentum tensors:

$$\langle 0_L|T^E_{00}|0_L\rangle = 2\sum_{\omega\omega'}(\tilde{f}^E_\omega(+)\tilde{f}^E_{\omega'}(+)+\tilde{f}^E_{-\omega}(-)\tilde{f}^E_{-\omega'}(-))\omega\delta_{\omega+\omega',0},$$
$$\langle 0_L|T^E_{01}|0_L\rangle = 2i\sum_{\omega\omega'}(\tilde{f}^E_\omega(+)\tilde{f}^E_{\omega'}(+)-\tilde{f}^E_{-\omega}(-)\tilde{f}^E_{-\omega'}(-))\omega\delta_{\omega+\omega',0},$$
$$\langle 0_L|T^L_{00}|0_L\rangle = 2\sum_{\omega\omega'}(\tilde{f}^L_\omega(+)\tilde{f}^L_{\omega'}(+)+\tilde{f}^L_{-\omega}(-)\tilde{f}^L_{-\omega'}(-))\omega\delta_{\omega+\omega',0}, \tag{16}$$
$$\langle 0_L|T^L_{01}|0_L\rangle = 2\sum_{\omega\omega'}(\tilde{f}^L_\omega(+)\tilde{f}^L_{\omega'}(+)-\tilde{f}^L_{-\omega}(-)\tilde{f}^L_{-\omega'}(-))\omega\delta_{\omega+\omega',0},$$
$$\langle 0_L|T^E_{11}|0_L\rangle = -\langle 0_L|T^E_{00}|0_L\rangle,$$
$$\langle 0_L|T^L_{11}|0_L\rangle = \langle 0_L|T^L_{00}|0_L\rangle.$$

Now, by the following normalization,

$$4\pi\langle\Phi_\omega,\Phi_\omega\rangle = \tfrac{1}{2}(L-\sigma_0), \tag{19}$$

and inserting it into Eqs. (12) and then applying the delta function $\delta_{\omega+\omega',0}$ we obtain

$$\langle 0_L|T^E_{00}|0_L\rangle = \frac{2}{L-\sigma_0}\sum_{\omega=0}^{\infty}\left[\left(\frac{a}{b}\right)_\omega+1\right]\left[\left(\frac{a}{b}\right)_{-\omega}+1\right]\omega,$$
$$\langle 0_L|T^E_{01}|0_L\rangle = \langle 0_L|T^E_{10}|0_L\rangle = 0,$$

$$\langle 0_L|T^E_{11}|0_L\rangle = -\langle 0_L|T^E_{00}|0_L\rangle,$$
$$\langle 0_L|T^L_{00}|0_L\rangle = \frac{2}{L-\sigma_0}\sum_{\omega=0}^{\infty}\left[\left(\frac{c}{b}\right)_{\omega}+\left(\frac{1}{b}\right)_{-\omega}\right]\left[\left(\frac{c}{b}\right)_{\omega}+\left(\frac{1}{b}\right)_{-\omega}\right]^{*}\omega, \tag{20}$$
$$\langle 0_L|T^L_{01}|0_L\rangle = \langle 0_L|T^L_{10}|0_L\rangle = 0,$$
$$\langle 0_L|T^L_{11}|0_L\rangle = \langle 0_L|T^L_{00}|0_L\rangle.$$

By using the Heaviside distribution Θ^+, Θ^- we may write

$$\langle 0_L|T_{00}|0_L\rangle = \Theta^+\langle 0_L|T^E_{00}|0_L\rangle + \Theta^-\langle 0_L|T^L_{00}|0_L\rangle,$$
$$\langle 0_L|T_{11}|0_L\rangle = \Theta^+\langle 0_L|T^E_{11}|0_L\rangle + \Theta^-\langle 0_L|T^L_{11}|0_L\rangle. \tag{21}$$

The normal ordered expressions are then as follows:

$$\langle 0_L|:T_{00}:|0_L\rangle = \Theta^+\langle 0_L|:T^E_{00}:|0_L\rangle + \Theta^-\langle 0_L|:T^L_{00}:|0_L\rangle,$$
$$\langle 0_L|:T_{11}:|0_L\rangle = \Theta^+\langle 0_L|:T^E_{11}:|0_L\rangle + \Theta^-\langle 0_L|:T^L_{11}:|0_L\rangle, \tag{22}$$

such that

$$\langle 0_L|:T^E_{00}:|0_L\rangle = \langle 0_L|T^E_{00}|0_L\rangle - \lim_{L'\to\infty}\langle 0_{L'}|T^E_{00}|0_{L'}\rangle,$$
$$\langle 0_L|:T^L_{00}:|0_L\rangle = \langle 0_L|T^L_{00}|0_L\rangle - \lim_{L'\to\infty}\langle 0_{L'}|T^L_{00}|0_{L'}\rangle,$$
$$\langle 0_L|:T^E_{11}:|0_L\rangle = \langle 0_L|T^E_{11}|0_L\rangle - \lim_{L'\to\infty}\langle 0_{L'}|T^E_{11}|0_{L'}\rangle, \tag{23}$$
$$\langle 0_L|:T^L_{11}:|0_L\rangle = \langle 0_L|T^L_{11}|0_L\rangle - \lim_{L'\to\infty}\langle 0_{L'}|T^L_{11}|0_{L'}\rangle,$$

where the second terms are introduced to remove the ultraviolet divergences in the first terms.[2] Since we have Euclidean and Lorentzian quantities in the second terms, then the state $|0_{L'}\rangle$ should have the property: $|0_{L'}\rangle \to |0\rangle$ as $L' \to \infty$, such that $|0\rangle$ is the vacuum state of an $R\times R$ signature changing space-time. The Casimir energy is measured with respect to this state.

IV. REGULARIZATION OF VEV OF CASIMIR STRESS TENSOR

Because both terms on the right-hand side (rhs) of the above equations are individually divergent they must be subtracted by careful analysis. By introducing the cutoff to the sums in 00 components we obtain

$$\langle 0_L|T^E_{00}|0_L\rangle_{\text{cutoff}} = \frac{2}{L-\sigma_0}\sum_{\omega=0}^{\infty}\left[\left(\frac{a}{b}\right)_{\omega}+1\right]\left[\left(\frac{a}{b}\right)_{-\omega}+1\right]\omega e^{-\alpha\omega},$$
$$\langle 0_L|T^L_{00}|0_L\rangle_{\text{cutoff}} = \frac{2}{L-\sigma_0}\sum_{\omega=0}^{\infty}\left[\left(\frac{c}{b}\right)_{\omega}+\left(\frac{1}{b}\right)_{-\omega}\right]\left[\left(\frac{c}{b}\right)_{\omega}+\left(\frac{1}{b}\right)_{-\omega}\right]^{*}\omega e^{-\alpha\omega}. \tag{24}$$

The 11 components will be easily obtained in terms of 00 components through Eqs. (20). We now break down each sum into two separate sums,

$$\langle 0_L|T_{00}^E|0_L\rangle_{\text{cutoff}} = \frac{2}{L-\sigma_0}\sum_{\omega<N}\left[\left(\frac{a}{b}\right)_\omega + 1\right]\left[\left(\frac{a}{b}\right)_{-\omega} + 1\right]\omega e^{-\alpha\omega} + \frac{2}{L-\sigma_0}\sum_{\omega=N}^{\infty}\left[\left(\frac{a}{b}\right)_\omega + 1\right]\left[\left(\frac{a}{b}\right)_{-\omega} + 1\right]\omega e^{-\alpha\omega},$$

$$\langle 0_L|T_{00}^L|0_L\rangle_{\text{cutoff}} = \frac{2}{L-\sigma_0}\sum_{\omega<N}\left[\left(\frac{c}{b}\right)_\omega + \left(\frac{1}{b}\right)_{-\omega}\right]\left[\left(\frac{c}{b}\right)_\omega + \left(\frac{1}{b}\right)_{-\omega}\right]^*\omega e^{-\alpha\omega} + \frac{2}{L-\sigma_0}\sum_{\omega=N}^{\infty}\left[\left(\frac{c}{b}\right)_\omega + \left(\frac{1}{b}\right)_{-\omega}\right]\left[\left(\frac{c}{b}\right)_\omega + \left(\frac{1}{b}\right)_{-\omega}\right]^*\omega e^{-\alpha\omega}, \tag{25}$$

where N is the root of quantization condition so that for any $\omega \geqslant N$ the spectrum almost coincides with integer values. As is shown in Fig. 2 in Ref. 26, it is easily seen from quantization condition that whatever can σ_0 be, the real spectrum of ω approaches the integer one, generally at higher values of N. Hence, we assume N to be sufficiently large so that the first sums over $\omega<N$ be (finite) *sums over real values* and the second sums over $\omega \geqslant N$ be almost (infinite) *sums over integer values*. Thus, we may discard the cutoff $e^{-\alpha\omega}$ from the finite sums and keep them just for infinite sums.

Now, we consider the second sum in $\langle 0_L|T_{00}^E|0_L\rangle_{\text{cutoff}}$. Since each of the terms $[(a/b)_\omega+1]$ and $[(a/b)_{-\omega}+1]$ approaches 1 for large ω [because $(a/b)_{\pm\omega}$ almost vanish for large ω] then this sum goes like

$$\frac{2}{L-\sigma_0}\sum_{\omega=N}^{\infty}\omega e^{-\alpha\omega}. \tag{26}$$

In the same way for $\langle 0_L|T_{00}^L|0_L\rangle_{\text{cutoff}}$, it is easily shown that each of the terms $[(c/b)_\omega+(1/b)_{-\omega}]$ and $[(c/b)_\omega+(1/b)_{-\omega}]^*$ approaches 1 for large integerlike values $\omega \geqslant N$, and the second sum goes like

$$\frac{2}{L-\sigma_0}\sum_{\omega=N}^{\infty}\omega e^{-\alpha\omega}, \tag{27}$$

as well. Therefore, we calculate this sum for both regions. We know that $\omega \geqslant N$ denotes for integers, hence we redefine $\omega=N$ to (integer) $\Omega=0$. To this end, we note that $\omega \geqslant N$ indicates, by definition, the integer roots of $\cos\omega(L-\sigma_0)=0$ in the quantization condition, from which we obtain $\omega \geqslant (n+1/2)/(L-\sigma_0)\pi$ and $N=(n+1/2)/(L-\sigma_0)\pi$. This is equal to $n=[N(L-\sigma_0)/\pi]-\frac{1}{2}$ with integer n. Therefore, we may define $\Omega=n-[N(L-\sigma_0)/\pi]+\frac{1}{2}$, with $\Omega=0,1,2,\ldots$. We also obtain ω in terms of Ω as $\omega=N+[\pi\Omega/(L-\sigma_0)]$.

Therefore, the sum (26) or (27) in Euclidean and Lorentzian regions is written as

$$\frac{2}{L-\sigma_0}\sum_{\Omega=0}^{\infty}\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}},$$

which, after some calculations, leads to [we have used $\Sigma_{n=0}^{\infty} n e^{-2\pi\alpha n/L}=e^{2\pi\alpha/L}(e^{2\pi\alpha/L}-1)^{-2}$ (Ref. 2)]

$$\frac{2}{L-\sigma_0}\sum_{\Omega=0}^{\infty}\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}=\frac{2}{L-\sigma_0}e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}. \tag{28}$$

First, we focus on the Euclidean calculations. By using Eqs. (22) and (23) for the Euclidean region we find

$$\begin{aligned}\Theta^+\langle 0_L|:T^E_{00}:|0_L\rangle=\Theta^+\Bigg\{&\frac{2}{L-\sigma_0}\Bigg[\sum_{\omega=0}^{N-1}\left[\left(\frac{a}{b}\right)_{\omega}+1\right]\left[\left(\frac{a}{b}\right)_{-\omega}+1\right]\omega\\&+e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\Bigg]\\&-\frac{2}{L-\sigma_0}\Bigg[\sum_{\omega=0}^{N-1}\omega+\lim_{L\to\infty}e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\Bigg]\Bigg\},\end{aligned} \tag{29}$$

or

$$\begin{aligned}\Theta^+\Bigg\{&\frac{2}{L-\sigma_0}\Bigg[\sum_{\omega=0}^{N-1}\left[\left[\left(\frac{a}{b}\right)_{\omega}+1\right]\left[\left(\frac{a}{b}\right)_{-\omega}+1\right]-1\right]\omega\Bigg]\\&+\frac{2}{L-\sigma_0}\Bigg[e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\\&-\lim_{L\to\infty}e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\Bigg]\Bigg\},\end{aligned} \tag{30}$$

where the finite sum has appeared without cutoff. In obtaining $\Sigma_{\omega=0}^{N-1}\omega$ in the second line of (29), we have used $\lim_{L\to\infty}(a/b)_{\pm\omega}\equiv\lim_{\sigma_0\to\infty}(a/b)_{\pm\omega}=0$ in the finite sum. We now expand the

$$e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha(N+\pi\Omega/L-\sigma_0)}-1)^2}$$

terms in the second bracket of (30) about $\alpha=0$. After some calculation we obtain

$$\begin{aligned}&\frac{2}{L-\sigma_0}\left[e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\right]\\&\quad=\frac{2}{\alpha^2\pi}-\left(\frac{\alpha^2N^2}{2}-\alpha N+1\right)\left[\frac{\pi}{6(L-\sigma_0)^2}+\frac{13}{6(L-\sigma_0)}N\right]-\frac{N^2}{\pi}(1-\alpha N).\end{aligned}$$

Substituting this result into the above bracket and taking $\alpha\to 0$ leads to

$$\frac{2}{L-\sigma_0}\left[e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}-\lim_{L\to\infty}e^{-\alpha N}\frac{\left(N+\frac{\pi\Omega}{L-\sigma_0}\right)e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-N}{(e^{-\alpha\{N+[\pi\Omega/(L-\sigma_0)]\}}-1)^2}\right]$$
$$=-\frac{\pi}{6(L-\sigma_0)^2}-\frac{13}{6(L-\sigma_0)}N.$$

Finally, we have the following expression for the Euclidean region:

$$\langle 0_L|:T^E_{00}:|0_L\rangle=\left\{\frac{2}{L-\sigma_0}\sum_{\omega=0}^{N-1}\left[\left[\left[\left(\frac{a}{b}\right)_\omega+1\right]\left[\left(\frac{a}{b}\right)_{-\omega}+1\right]-1\right]\omega-\frac{\pi}{6(L-\sigma_0)^2}-\frac{13}{6(L-\sigma_0)}N\right\}.\right. \tag{31}$$

In the same way, the calculations for the Lorentzian region lead to

$$\langle 0_L|:T^L_{00}:|0_L\rangle=\left\{\frac{2}{L-\sigma_0}\sum_{\omega=0}^{N-1}\left[\left[\left[\left(\frac{c}{b}\right)_\omega+\left(\frac{1}{b}\right)_{-\omega}\right]\left[\left(\frac{c}{b}\right)_\omega+\left(\frac{1}{b}\right)_{-\omega}\right]^*-1\right]\omega-\frac{\pi}{6(L-\sigma_0)^2}\right.\right.$$
$$\left.\left.-\frac{13}{6(L-\sigma_0)}N\right\}.\right. \tag{32}$$

Note that, since N is not uniquely determined, then the expectation values (31) and (32) are evaluated approximately. Therefore, for a given σ_0, replacing N by $N+1$ or $N-1$ leads to better or worse approximation, respectively. This is because, as we go to higher values of N the real spectrum coincides with integer one with better approximation.

V. FINITE ENERGY DENSITY AND PRESSURE IN EUCLIDEAN AND LORENTZIAN REGIONS

By using Eqs. (20) for the 11 components we have

$$\langle 0_L|:T^E_{11}:|0_L\rangle=-\langle 0_L|:T^E_{00}:|0_L\rangle,$$
$$\langle 0_L|:T^L_{11}:|0_L\rangle=\langle 0_L|:T^L_{00}:|0_L\rangle. \tag{33}$$

Therefore, the state $|0_L\rangle$ contains the finite energy density and pressure in the Euclidean and Lorentzian regions as follows:

$$\rho^E=\langle 0_L|:T^E_{00}:|0_L\rangle,$$
$$\rho^L=\langle 0_L|:T^L_{00}:|0_L\rangle, \tag{34}$$

$$p^E=\langle 0_L|:T^E_{11}:|0_L\rangle=-\rho^E,$$
$$p^L=\langle 0_L|:T^L_{11}:|0_L\rangle=\rho^L. \tag{35}$$

We then find that the total pressure acting on the signature-changing hypersurfaces $\sigma=0,L$ and $\sigma=\sigma_0$ is given by

$$p^T=p^L-p^E=\rho^L+\rho^E, \tag{36}$$

which is generally nonzero according to Eqs. (31), (32), and (34). This nonzero pressure causes instability in the location of σ_0 relative to $\sigma=0$. Depending on the initial location of σ_0, the corresponding value and sign of the pressure may lead one of the regions (L or E) to grow or shrink. It is very hard to judge about the exact behavior of the pressure from Eqs. (31) and (32),

because it depends on N, the location of σ_0, and the complicated functions $(a/b)_\omega$, $(c/b)_\omega$, $(1/b)_\omega$ in which the energy spectrum ω, itself, depends on σ_0 through the quantization condition (6).

Nevertheless, one may evaluate the situation in the two limits of σ_0. In the limit $\sigma_0 \to 0$, the term $\pi/6(L-\sigma_0)^2$ may be neglected in comparison with two other terms. Therefore, there is a competition between the first sums and third terms in Eqs. (31) and (32). And, upon this competition the pressure may cause the Euclidean region to grow or shrink. On the other hand, in the limit $\sigma_0 \to L$, the term $\pi/6(L-\sigma_0)^2$ may dominate the other two terms and the pressure $p^T=\rho^L+\rho^E$ becomes negative, $p^L<p^E$, which means the Euclidean region is growing (with increasing pressure) toward $\sigma_0=L$. Fortunately, in this case, there is no divergency problem at $\sigma_0=L$. This is because, once the circle is completely covered by Euclidean metric, the quantization condition and all subsequent calculations break down.

The nonzero pressure obtained above and the consequent change in the signature changing region will certainly change the energy spectrum of the scalar fields through the quantization condition

$$\cosh \omega\sigma_0 \cos \omega(\sigma_0 - L) = 1 .$$

The modified signature-changing region σ_0 and energy spectrum ω back react on the pressure through Eqs. (31) and (32). The central term of the algebra corresponding to infinite conserved charges[26]

$$[L_\omega, L_{\omega'}] = (\omega - \omega')L_{\omega+\omega'} + C(\omega, \omega')$$

is correspondingly changed through

$$C(\omega,\omega') = \delta_{\omega+\omega',0} f(\omega,\omega',\sigma_0) - 4 \sum_{\omega_1,\omega_2>0}^{N} {\omega_1}^2 {\omega_2}^2 C^{-\omega'}_{\omega_1,\omega_2} C^{\omega}_{\omega_1,\omega_2} + \sum_{\omega_1>0}^{N} {\omega_1}^2 (\omega-\omega_1)^2 C^{-\omega'}_{\omega_1,\omega-\omega_1},$$

where

$$f(\omega,\omega',\sigma_0) = 3 \sum_{l=-n}^{0} [-2(l+k)a - \omega - \omega'][2(l+k)a+\omega]^2 [|(2(l+k)a+\omega+\omega')(2(l+k)a)|]^{1/2}$$

and

$$N = (2k-1)a, \quad \omega = (2n-1)a, \quad a = \frac{\pi}{2(2\pi - \sigma_0)}$$

with k and n as integers.

It is seen that in the special case $N=0$ the first sums and the last terms vanish in (31) and (32) and these lead to the standard result $-\pi/6L^2$ for the pure Lorentzian metric $\sigma_0=0$ on the cylinder.[2] In fact, $N=0$ corresponds to $\omega=N=0$ which means ω is an integer starting from zero; a case which occurs only in the pure Lorentzian region.

VI. CONCLUSION

We have studied a two-dimensional model in which the space-time is a cylinder (circle $\times$ real number) with the circle representing *space* and the real line representing *time*. Moreover, we have assumed that this manifold admits a signature change of the type which had already been reported in Ref. 26.

We were interested in studying the Casimir effect for the real massless scalar fields propagating over this manifold. To this end, we have considered the expressions for the components of energy-momentum tensors associated with the real scalar field and calculated the corresponding vacuum expectation values. These expressions are found to be infinite, hence a regularization scheme is used to make them finite. By introducing a convenient cutoff and a regularization scheme, we obtain the finite expressions for the vacuum expectation values of the energy momen-

tum tensors. These provide us with the finite energy densities and pressures in both Euclidean and Lorentzian regions so that the net pressure on the signature changing hypersurfaces is obtained. This pressure causes instability in the signature changing region σ_0 and this instability alters the energy spectrum through the quantization condition. The modified σ_0 and spectrum ω themselves back react on the pressure through Eqs. (31) and (32). Moreover, the central term of diffeomorphism algebra of real massless scalar fields obtained in Ref. 26 is altered due to modifications in σ_0 and spectrum ω.

The action for free massless scalar field propagating on the signature-changing background

$$S=\frac{1}{2}\int \mathrm{d}t\int_{\text{Lorentzian}} \mathrm{d}\sigma\sqrt{|g|}g_L^{\mu\nu}\partial_\mu\phi_\omega^L\partial_\nu\phi_\omega^L+\frac{1}{2}\int \mathrm{d}t\int_{\text{Euclidean}} \mathrm{d}\sigma\sqrt{|g|}g_E^{\mu\nu}\partial_\mu\phi_\omega^E\partial_\nu\phi_\omega^E$$

may be rewritten in the form of string action

$$S\sim\frac{1}{2}\int \mathrm{d}t\int \mathrm{d}\sigma\sqrt{|g|}g^{\mu\nu}\partial_\mu\phi_\omega^a\partial_\nu\phi_\omega^b\eta_{ab}$$

with the distribution $g_{\mu\nu}=\Theta^+g_{\mu\nu}^E+\Theta^-g_{\mu\nu}^L$ and $\phi_\omega^a=(\phi_\omega^E,\phi_\omega^L)$ with $\eta_{ab}=\mathrm{diag}(\Theta^+,\Theta^-)$. In this way it looks like we have a closed string with Euclidean and Lorentzian parts propagating in a distributional way in the two-dimensional target space $(\phi_\omega^E,\phi_\omega^L)$.[26] The discontinuous nature of the model in classifying Euclidean and Lorentzian solutions $\Phi_\omega^E,\Phi_\omega^L$ with discrete symmetry under $\omega\leftrightarrow-\omega$ in each class motivates one to study it in the context of *orbifolds*. For example, if we suppose the target space M to be $\phi_\omega^a=(\phi_\omega^E,\phi_{-\omega}^E,\phi_\omega^L,\phi_{-\omega}^L)$ and assume a permutation of it $\pi=(\phi_\omega^E\phi_{-\omega}^E)\times(\phi_\omega^L\phi_{-\omega}^L)$, then regarding the definition of an orbifold as the object one obtains by dividing a manifold by the action of a discrete group, it seems to be possible to define an orbifold M/π which results in $\phi_\omega^a=(\phi_\omega^E,\phi_\omega^L)$. In this way, perhaps at a formal level, we may have *a string on an orbifold*.[26]

Therefore, the study of Casimir effect in the present model may provide important results relevant to the study of closed bosonic strings. It is also appealing to proceed with the idea of Casimir effect in different 3+1 dimensional signature-changing space-times to investigate what secondary effects may be produced by the Casimir effect.[29]

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Nonintegrability of density perturbations in the Friedmann-Robertson-Walker universe

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We investigate the evolution equation of linear density perturbations in the Friedmann-Robertson-Walker universe with matter, radiation, and the cosmological constant. The concept of solvability by quadratures is defined and used to prove that there are no "closed form" solutions except for the known Chernin, Heath, Meszaros and simple degenerate ones. The analysis is performed applying Kovacic's algorithm. The possibility of the existence of other, more general solutions involving special functions is also investigated. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178584]

I. INTRODUCTION

This paper is an attempt to apply the methods of differential algebra, and the differential Galois theory in particular, to a problem of cosmology. Although the considerations are mostly mathematical, the problem itself, and its solutions, are of rather practical interest. Linear perturbations of the Einstein equations in many forms are investigated due to their direct relation to such practical questions as the formation of galaxies or the CMB inhomogeneities. We, however, enter the physical domain only as the source of a theoretical problem, on which we concentrate.

The result itself is of negative nature, or, in other words, it makes any further investigation of this kind unnecessary. All the known solutions are given, together with the conditions for their validity. As no new ones can exist, this closes and completes the analysis of the given equation.

Of course, that is not to say that apart from those special cases nothing can be said about the behavior of the solution. It is only to some extent that differential algebra can make exact the intuitive concepts of "being possible to solve" or "expressible in a closed form." The definition of nonintegrability employed here is but one of many which were born as classical mechanics evolved. The Liouville's theorem implies that enough first integrals might yield a complete solution of a dynamical system, and accordingly many criteria regarding the existence of certain classes of first integrals were developed. The first achievements were those of Kovalevskaya and Lyapunov, greatly improved only recently by Ziglin, Morales, and Ramis. The Galois theory used here, can also be applied to prove nonexistence of meromorphic first integrals in more complex systems. Paradoxically here, we are presented with an equation simple enough not to allow for the application of those advanced methods. Thus, only a small part of the theory is put into practice and explained here. For a complete bibliography and exposition see, for example, Ref. 1.

The paper is organized as follows. In Sec. II we derive the equation in question in a nonstandard but intuitively clear way. The next two sections describe the concept of Liouvillian

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solutions, integrability and give the basic criteria, which we proceed to use in Sec. V. We also investigate the possibility of solving the problem by a combination of some special and Liouvillian functions, and give the theorem which is the main result in Sec. VI. Finally, conclusions and finishing remarks are given in Sec. VII.

II. DENSITY PERTURBATION EQUATION

We will be considering the Friedmann-Robertson-Walker universe given by the metric

$$\mathrm{d}s^2 = c^2\,\mathrm{d}t^2 - a(t)^2\left[\frac{\mathrm{d}r^2}{1-Kr^2} + r^2\,\mathrm{d}\Omega^2\right], \tag{1}$$

where K is the curvature index, $\mathrm{d}\Omega^2$ is the distance element on a two-sphere. The universe will be filled with radiation and baryonic matter characterized by their pressures and densities p and ρ. A nonzero cosmological constant's effect will also be considered.

The Einstein equations for this model give

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi \boldsymbol{G}}{3}\rho + \frac{\Lambda}{3} - \frac{K}{a^2},$$
$$\frac{\ddot{a}}{a} = -\frac{4\pi \boldsymbol{G}}{3}(3p+\rho) + \frac{\Lambda}{3}, \tag{2}$$

where $\boldsymbol{G}$, and Λ are the gravitational and cosmological constants, respectively. The conservation equation reduces to

$$c^2\dot{\rho} = -3H(p+\rho c^2), \tag{3}$$

with the dot representing the time derivative. This can be expressed as the following transformation laws for matter and radiation, respectively:

$$p_m = 0 \Rightarrow \frac{\rho_m}{\rho_{m0}} = \left(\frac{a_0}{a}\right)^3,$$
$$p_r = \frac{1}{3}\rho_r \Rightarrow \frac{\rho_r}{\rho_{r0}} = \left(\frac{a_0}{a}\right)^4. \tag{4}$$

ρ_{m0} and ρ_{r0} are the values of the densities for the moment when $a=a_0$, which can be chosen as the present day.

The fluctuation is introduced by the means of the scale factor

$$a = \tilde{a}(1+y), \tag{5}$$

and $\tilde{a}$ is the solution of the original equations (2). As it is a matter perturbation only, we have

$$\rho_r = \tilde{\rho}_r,$$

$$\rho_m = \tilde{\rho}_m\left(\frac{a}{\tilde{a}}\right)^{-3} = \tilde{\rho}_m(1+y)^{-3} = \tilde{\rho}_m(1-3y),$$

where we use the scaling law (4) and linearize the problem. Substituting this into the second of Eqs. (2), we obtain

$$\ddot{\tilde{a}}(1+y)+2\dot{\tilde{a}}\dot{y}=-\frac{8\pi G}{3}\tilde{a}(1+y)\rho_r-\frac{4\pi G}{3}\tilde{a}(1+y)\tilde{\rho}_m(1-3y)+\frac{1}{3}\Lambda\tilde{a}(1+y), \tag{6}$$

which, after substituting the equation satisfied by the unperturbed $\tilde{a}$, simplifies to

$$\ddot{y}+2H\dot{y}-4\pi G\tilde{\rho}_m y=0, \tag{7}$$

with the Hubble "constant"

$$H:=\frac{\dot{\tilde{a}}}{\tilde{a}}. \tag{8}$$

This kind of perturbation is of the scalar type, i.e., constructed from a single function y. Here, we take it to depend on time only, although in general it could also involve spatial variables. This case could then be thought of as the zeroth order coefficient in the expansion of $y(t,r,\theta,\varphi)$ in terms of eigenfunctions of the spatial Laplace operator. Another generalization would be to consider the vector and tensor type perturbations (see Ref. 2 for details of the decomposition). As it turns out, vector perturbations also admit quite general exact solutions.[3]

In order to simplify Eq. (7) fully, that is, bring it to the linear form with rational coefficients, we choose new variables,

$$x:=\frac{\tilde{a}}{\tilde{a}_0},\quad u:=H_0 t, \tag{9}$$

and constant density parameters,

$$\Omega_{r0}:=\frac{8\pi G\rho_{r0}}{3H_0^2},\quad \Omega_{m0}:=\frac{8\pi G\rho_{m0}}{3H_0^2}, \tag{10}$$

$$\Omega_{K0}:=-\frac{c^2K}{\tilde{a}_0^2H_0^2},\quad \Omega_{\Lambda0}:=\frac{c^2\Lambda}{3H_0^2} \tag{11}$$

which allow us to rewrite the main equation as

$$\left(\frac{\mathrm{d}x}{\mathrm{d}u}\right)^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+\left[\frac{\mathrm{d}^2x}{\mathrm{d}u^2}+\frac{2}{x}\left(\frac{\mathrm{d}x}{\mathrm{d}u}\right)^2\right]\frac{\mathrm{d}y}{\mathrm{d}x}-\frac{3}{2}\Omega_{m0}\frac{1}{x^3}y=0, \tag{12}$$

where the perturbation y is now considered as a function of x. Finally, using the first of Eqs. (2), which in the new variables reads

$$x^2\left(\frac{\mathrm{d}x}{\mathrm{d}u}\right)^2=\Omega_{\Lambda0}x^4+\Omega_{K0}x^2+\Omega_{m0}x+\Omega_{r0}=:W(x), \tag{13}$$

we can eliminate the derivatives with respect to u, and denoting the differentiation with respect to x with a prime, we get

$$x(\Omega_{\Lambda0}x^4+\Omega_{K0}x^2+\Omega_{m0}x+\Omega_{r0})y''+\left(3\Omega_{\Lambda0}x^4+2\Omega_{K0}x^2+\tfrac{3}{2}\Omega_{m0}x+\Omega_{r0}\right)y'-\tfrac{3}{2}\Omega_{m0}y=0. \tag{14}$$

As follows from the definitions, Ω_{K0} and $\Omega_{\Lambda0}$ are of arbitrary signs, while Ω_{r0} and Ω_{m0} are non-negative. We take Ω_{m0} to be strictly positive, though, because of the nature of the examined perturbations.

We also introduce the functions $p(x)$ and $q(x)$ related to the above equation in the following form:

$$y''(x) + p(x)y'(x) + q(x)y(x) = 0. \tag{15}$$

They are

$$p(x) = \frac{6\Omega_{\Lambda 0}x^4 + 4\Omega_{K0}x^2 + 3\Omega_{m0}x + 2\Omega_{r0}}{2x(\Omega_{\Lambda 0}x^4 + \Omega_{K0}x^2 + \Omega_{m0}x + \Omega_{r0})} \quad \text{and } q(x) = \frac{-3\Omega_{m0}}{2x(\Omega_{\Lambda 0}x^4 + \Omega_{K0}x^2 + \Omega_{m0}x + \Omega_{r0})}. \tag{16}$$

Having obtained the solutions as functions of x it is straightforward to express them as functions of the cosmological or conformal time, since $x(u)$ satisfies Eq. (13), and is therefore expressible in terms of the elliptic functions. The exact formulas can be found, for example, in Ref. 4.

III. LIOUVILLIAN SOLUTIONS

Equation (14) is, in general, a Fuchsian one, and the solutions can be found by means of series. In particular, in vicinities of the singular points

$$y_{\pm}(x) = (x - x_0)^{\alpha_{\pm}}\left(1 + \sum_{n=1}^{\infty} c_n(x - x_0)^n\right), \tag{17}$$

where $\alpha_{\pm}$ are the characteristic exponents at the point x_0. Such solutions are local, and the area of convergence around a given point is restricted by the remaining singular points. However, there are some special cases in which the solutions can be expressed by means of known special functions, and become global. It is then much easier to investigate and understand their behavior. Thus, we are lead to the natural question of existence of such "simple" solutions. In this section we give a short description of a class of functions, which could here be called closed-form solutions.

It is natural to start seeking for the solutions in a class of functions to which the given equation's coefficients belong, but such a set proves to be insufficient in most cases. As we are dealing with an equation whose coefficients are rational functions, the first choice is the field $\mathbb{C}(x)$—rational functions with complex numbers as the field of constants. Or, in the language of differential algebra, $(\mathbb{C}(x), \partial)$—the above field equipped with a suitable derivation operation, which, in this case, coincides with the usual, complex one, and will be denoted by a prime throughout this section.

This field is much too small, of course, and we are soon forced to extend it, introducing new elements. Just, as $\mathbb{C}(x)$ is an extension of $\mathbb{C}$ obtained by adjoining an indeterminate variable x, our new fields will be $\mathbb{C}(x)$ to which new functions are added. Naturally, the derivation on the extended field must coincide with the subfield's derivation when restricted to it (that is essentially what a differential extension is).

To keep the new functions relatively simple, so that the usual notion of "solvability by quadratures" could still be applied, the new elements are restricted to three classes.

Definition 1: For a differential field extension $F \subset G$, an element $a \in F$ is

primitive *over G if $a' \in G$,*

exponential *over G if $a'/a \in G$, or*

algebraic *over G if $P(a) = 0$ for some $P(x) \in G[x]$ — the ring of polynomials with coefficients in G.*

Definition 2: A field extension is called Liouvillian if it is a result of a finite number of extensions, each the adjunction of an algebraic, exponential, or primitive element.

Some examples of "new" functions appearing in this process are radicals (for algebraic elements), logarithms and inverse circular function (for primitives), and trigonometric functions (for exponentials). In short, the new elements are expressible as combinations of exponentials, integrals, and algebraic and elementary functions.

Finally, we are able to formulate what we mean by integrability.

Definition 3: A linear differential equation with coefficients in $\mathbb{C}(x)$ *is said to possess Liouvillian solutions, or be solvable by quadratures, if its solutions belong to a Liouvillian extension of* $\mathbb{C}(x)$.

IV. MONODROMY AND GALOIS GROUPS

In order to characterize a differential equation we can introduce two groups whose invariant properties are closely connected with those of the first integrals of the given equation.

The first, called the monodromy group $\mathcal{M}$ is associated with the continuation of the local solutions of a linear differential equation, along closed paths in the domain where the equation is defined. The group itself is an image of the fundamental group of that domain, and a subgroup of $\mathrm{GL}(n,\mathbb{C})$ for n the order of the equation. The only other fact, concerning $\mathcal{M}$, that we will need here is that $\mathcal{M}\subset\mathcal{G}$—the differential Galois group, which we proceed to describe.

$\mathcal{G}$ is directly connected with the extension of the base field $\mathbb{C}(x)$ to a bigger field F, which contains the solutions of the considered equation. $\mathcal{G}$ is defined as the group of automorphisms of F that leave $\mathbb{C}(x)$ elementwise fixed. Carrying this information regarding the equation, the Galois group enables to test for particular forms of solutions. One of the fundamental properties is as follows.

Lemma 1: Let $\mathcal{G}$ *be the differential Galois group of a linear differential equation* $w''(x)=r(x)w(x)$, $r(x)\in\mathbb{C}(x)$. *Then it is an algebraic subgroup of* $SL(2,\mathbb{C})$, *and one of the following cases can occur.*

(1) $\mathcal{G}$ *is triangulizable. There is a solution of the form* $\exp\int\omega$, *where* $\omega\in\mathbb{C}(x)$.

(2) $\mathcal{G}$ *is conjugate to a subgroup of*

$$D^{\dagger}=\left\{\begin{pmatrix}c_1 & 0\\ 0 & c_1^{-1}\end{pmatrix}\middle| c_1\in\mathbb{C}^*\right\}\cup\left\{\begin{pmatrix}0 & c_2\\ -c_2^{-1} & 0\end{pmatrix}\middle| c_2\in\mathbb{C}^*\right\},$$

where $\mathbb{C}^*=\mathbb{C}\backslash\{0\}$. *There is a solution of the form* $\exp\int\omega$, *with* ω *algebraic over* $\mathbb{C}(x)$ *of degree 2.*

(3) $\mathcal{G}$ *is finite. All the solutions are algebraic.*

(4) $\mathcal{G}=SL(2,\mathbb{C})$. *The equation has no Liouvillian solutions.*

V. NONINTEGRABILITY OF THE EQUATIONS

We now proceed to the direct analysis of the integrability of Eq. (14), based mainly on the Kovacic's algorithm.[5] First we consider the equation with $\Omega_{\Lambda 0}=0$, for which the calculation is not too cumbersome, and next, we outline the reasoning for the general case.

A. Models without the cosmological constant

In order to apply the algorithm, Eq. (15) is cast into a reduced form

$$v''(x)=r(x)v(x), \tag{18}$$

with

$$r(x)=-\frac{1}{4x^2}-\frac{3(2\kappa x+1)^2}{(\kappa x^2+x+\varrho)^2}+\frac{4\kappa x+7}{x(\kappa x^2+x+\varrho)}, \tag{19}$$

where we have introduced new parameters

$$\kappa := \frac{\Omega_{K0}}{\Omega_{m0}}, \quad \varrho := \frac{\Omega_{r0}}{\Omega_{m0}}.$$

The reduction itself is performed by means of the following change in the dependent variable:

$$y(x) = v(x)\exp\left[-\frac{1}{2}\int_{x_0}^{x} p(s)\mathrm{d}s\right], \tag{20}$$

where the constant x_0 is arbitrary. This transformation does not change the class of solutions we are interested in, as it uses the "admissible" operations only.

In the general case, there are two distinct roots of the polynomial $W(x)$ in Eq. (14) and they are both nonzero. The degenerate cases will be treated separately.

Looking for the local solutions around $x=0$, which is a regular singular point of the equation with both characteristic exponents equal to $\frac{1}{2}$, we find

$$\begin{aligned} v_1(x) &= x^{1/2}w_1(x), \\ v_2(x) &= \ln(x)v_1(x) + x^{1/2}w_2(x), \end{aligned} \tag{21}$$

and w_1 and w_2 are holomorphic at $x=0$. Using these, it is now possible to obtain an element of the monodromy group, by continuation of the fundamental solution matrix along a small closed path around $x=0$,

$$\begin{pmatrix} v_1 & v_2 \\ v_1' & v_2' \end{pmatrix} \to \begin{pmatrix} -1 & -2\pi i \\ 0 & -1 \end{pmatrix}\begin{pmatrix} v_1 & v_2 \\ v_1' & v_2' \end{pmatrix}. \tag{22}$$

Since $\mathcal{M} \subset \mathcal{G}$, the Galois group cannot be $D^{\dagger}$, as that group does not contain nondiagonalizable matrices. Also, a triangular, nondiagonal matrix cannot generate a finite group, so that $\mathcal{G}$ itself cannot be finite. We have thus excluded cases 2 and 3 of Lemma 1.

Case 1 can also be easily excluded applying the aforementioned algorithm. In order for the solution to be of the form

$$P(x)\exp\left[\int \omega(x)\mathrm{d}x\right], \tag{23}$$

with a monic $P(x) \in \mathbb{C}[x]$, and $\omega(x) \in \mathbb{C}(x)$, the following equation must be satisfied:

$$P''(x) + 2\omega(x)P'(x) + [\omega'(x) + \omega(x)^2 - r(x)]P(x) \equiv 0, \tag{24}$$

for $P(x)$ and $\omega(x)$ found according to the algorithm, as follows. First, we define a set of auxiliary quantities,

$$\alpha_c^{\pm} = \tfrac{1}{2} \pm \tfrac{1}{2}\sqrt{1+4b}, \tag{25}$$

where $c \in \Gamma \cup \{\infty\}$—the set of all the finite poles of $r(x)$ including infinity, and b is the coefficient of $(x-c)^{-2}$ in the Laurent expansion of $r(x)$ around a given point $x=c$. Next, for all possible combinations of signs $s(\infty), s(c)$ we compute the possible degrees of $P(x)$ as

$$d = \alpha_{\infty}^{s(\infty)} - \sum_{c\in\Gamma} \alpha_c^{s(c)}, \tag{26}$$

and, for the same combinations of signs $s(c)$, the respective possible ω

$$\omega(x) = \sum_{c \in \Gamma} \frac{\alpha_c^{s(c)}}{x - c}. \tag{27}$$

Inserting the functions just obtained into Eq. (24) we are left with a system of linear equations determining the unknown coefficients of $P(x)$. In this particular case, the only non-negative value of d is 0, so that $P(x)=1$, and the system is reduced to

$$\frac{3}{2x(\kappa x^2 + x + \varrho)} \equiv 0, \tag{28}$$

which cannot hold. The first case of Lemma 1 is also excluded, which means that $\mathcal{G}$ is $\mathrm{SL}(2,\mathbb{C})$, and the equation has no Liouvillian solutions in the general case.

When we admit a double nonzero root of $W(x)$, or in other words, when

$$\Omega_{m0} = 2\sqrt{\Omega_{r0}}(1 - \sqrt{\Omega_{r0}}), \tag{29}$$

we have the well-known Chernin solution[6]

$$y(x) = {}_2F_1\left(-i\sqrt{3}, i\sqrt{3}, 1; \frac{x}{x + 2\Omega_{r0}}\right). \tag{30}$$

where ${}_2F_1$ is the Gauss hypergeometric function.

In the current notation it means that $4\varrho\kappa=1$, and that the root itself is $x_0=-2\varrho$. As Eq. (15) now has three regular singular points: 0, x_0, and ∞, it becomes a Riemann P-equation. The complete set of solutions is denoted by

$$y(x) = P\left\{\begin{matrix} 0 & -2\varrho & \infty & \\ 0 & -i\sqrt{3} & 0 & x \\ 0 & i\sqrt{3} & 1 & \end{matrix}\right\}. \tag{31}$$

Such a P-function is not Liouvillian either, as can be immediately checked using Kimura's theorem.[7]

Another degenerate subcase occurs when $\varrho=0$, and $\kappa\neq 0$, so that 0 becomes a root of $W(x)$ and there is another nonzero root $x=-1/\kappa$. Like before the solution is a P-function,

$$y(x) = P\left\{\begin{matrix} 0 & -\frac{1}{\kappa} & \infty & \\ -\frac{3}{2} & 0 & 0 & x \\ 1 & \frac{1}{2} & 1 & \end{matrix}\right\}. \tag{32}$$

This time however, it is a Liouvillian solution because we can express the above symbol as two base solutions,

$$\begin{aligned} y_1(x) &= x^{-3/2}\sqrt{\Omega_{m0} + \Omega_{K0}x}, \\ y_2(x) &= x\,{}_2F_1\left(1, 2, \frac{7}{2}; -\frac{\Omega_{K0}}{\Omega_{m0}}x\right), \end{aligned} \tag{33}$$

The next subcase is $\kappa=0$ and only two simple roots remain, 0 and $-\varrho$. We accordingly get

$$y(x) = P\begin{Bmatrix} 0 & -\varrho & \infty & \\ 0 & 0 & -1 & x \\ 0 & \frac{1}{2} & \frac{3}{2} & \end{Bmatrix}. \tag{34}$$

As before, this is a Liouvillian function, according to Kimura's theorem, and it can be rewritten as the following two independent solutions:

$$\begin{aligned} y_1(x) &= 1 + \frac{3\Omega_{m0}}{2\Omega_{r0}}x, \\ y_2(x) &= \sqrt{\Omega_{r0} + \Omega_{m0}}x_2F_1\left(2, -\frac{1}{2}, \frac{3}{2}; 1 + \frac{\Omega_{m0}}{\Omega_{r0}}x\right), \end{aligned} \tag{35}$$

which are the solutions discovered by Meszaros.[8]

The last possibility is that $\varrho=\kappa=0$ which implies $\Omega_{m0}=1$, and we simply obtain

$$\begin{aligned} y_1(x) &= x, \\ y_2(x) &= x^{3/2}. \end{aligned} \tag{36}$$

Taking into account that condition (29) makes it impossible for the physical cases ($\Omega_{m0}>0$) to have zero as a triple root, we conclude that the only Liouvillian solutions of Eq. (14) for $\Omega_{\Lambda 0}=0$, appear when at least one of the parameters Ω_{r0} or Ω_{K0} is equal to zero.

B. Models with the cosmological constant

The reasoning for $\Omega_{\Lambda 0}\neq 0$ is the same as in the preceding section, but since the leading coefficient now contains a polynomial of the fourth degree, the calculations are somewhat more laborious.

In general, when $W(x)$ has only simple roots, and they are all nonzero (which means $\Omega_{r0}\neq 0$), we obtain, as before, a triangular element of the monodromy group $\mathcal{M}$. This leaves us with only the first case of the Kovacic's algorithm to check, and the physical requirement of $\Omega_{m0}>0$ causes the equation to be nonintegrable.

In fact, even if the roots become multiple, but still nonzero, the local solutions in the vicinity of $x=0$ do not change and, again, we only need to consider the first case of the algorithm. We introduce the roots by the following formula:

$$W(x) = \Omega_{\Lambda 0}(x-e_1)(x-e_2)(x-e_3)(x-e_4).$$

Taking $e_2=e_4$, we could rewrite the polynomial as $W(x)=\Omega_{\Lambda 0}(x-e_1)(x+e1+2e_2)(x-e_2)^2$, because we must have $e_1+e_2+e_3+e_4=0$.

This time, the coefficients b, as defined in the preceding section, is not numeric, but depends on the roots. We now have

$$\alpha_{e_2}^{\pm} = \frac{1}{2} \pm \frac{1}{2}\sqrt{1 + 4\left(\frac{3}{4} + \frac{3e_1}{e_2 - e_1} - \frac{e_1}{e_1 + 3e_2}\right)} =: \frac{1 \pm n}{2}. \tag{37}$$

We see that n must be at least a positive integer, and that initially there are countably many possibilities to check. Since the relation between the roots and the densities Ω is known, we might obtain an important restriction of the form

$$\frac{\Omega_{r0}}{\Omega_{\Lambda 0}} = -\frac{3(n^2-4)}{n^2+12}e_2^4, \tag{38}$$

which means that $\Omega_{\Lambda 0}$ must be negative if $n>2$. One can readily check that $n=1,2$ give no solution. Further calculations with these restrictions on $\Omega_{\Lambda 0}$ and n, determining the coefficients of

the appropriate polynomial $P(x)$ require us to solve a system of n homogeneous, linear equations. Unfortunately we have been unable to do that for general n, but it is easy to check for the first 50 values that the determinant of the system is not zero, with its modulus monotonically increasing with n. Thus we conjecture that there are no values of n for which a solution exists.

When the double root becomes triple, it also becomes a pole of the third order of the function $r(x)$. This means that only the second case of Kovacic's algorithm needs to be considered, but it yields no Liouvillian solutions.

It is impossible for $W(x)$ to have two double roots or a quadruple root, because as we noted the sum of all roots must be zero, and that would lead to $\Omega_{m0}=0$.

Letting $\Omega_{r0}=0$ changes the multiplicity of $x=0$ as a singular point, and the monodromy argument no longer holds. We note also that no further increase in the multiplicity of that point is possible as $\Omega_{m0}\neq 0$.

Assuming first that there are no multiple roots of $W(x)$, the algorithm immediately yields the following fundamental solutions:

$$y_1(x) = x^{-3/2}\sqrt{\Omega_{\Lambda 0}x^3 + \Omega_{K0}x + \Omega_{m0}},$$
$$y_2(x) = y_1(x)\int \left(\frac{x}{\Omega_{\Lambda 0}x^3 + \Omega_{K0}x + \Omega_{m0}}\right)^{3/2} \mathrm{d}x, \tag{39}$$

which holds even if one of the roots becomes double. This solution is also known, and was found by Heath.[9]

As above, a triple root would mean $\Omega_{m0}=0$ and is thus not physical.

VI. ON MORE GENERAL SOLUTIONS

Although the concept of Liouvillian solutions gives us a simple and applicable formulation of solvability by quadratures, it is easily seen to be insufficient on itself as a mean to discard an equation as insolvable in general. The fact that the Bessel or hypergeometric functions (except for some special cases) are not Liouvillian is the best example of that.

Of course, there are no algorithms for finding more complex solutions, but it is possible to extend the considered class somewhat. Following the paper of Bronstein,[10] we try to find solutions in the form

$$y_1(x) = m(x)F_1[\xi(x)],$$
$$y_2(x) = m(x)F_2[\xi(x)], \tag{40}$$

where $F_1(\xi)$ and $F_2(\xi)$ are fundamental solutions of a given target equation

$$y''(\xi) = u(\xi)y(\xi), \tag{41}$$

and $m(x)$ and $\xi(x)$ are Liouvillian over $\mathbb{C}(x)$. The quoted paper presents an algorithmic approach for target equations which have an irregular singularity at infinity, and $\xi(x)\in\mathbb{C}(x)$. It also offers a check for a certain class of algebraic $\xi(x)$.

Upon substituting the form of solutions (40) into Eq. (18), and using the target equation (41), we are left with an expression containing only $F(\xi)$ and $F'(\xi)$. Making the coefficients equal to zero gives the fundamental equations to be solved

$$3\xi''(x)^2 - 2\xi'''(x)\xi'(x) + 4u[\xi(x)]\xi'(x)^4 - 4r(x)\xi'(x)^2 = 0, \tag{42}$$

$$m(x) = \frac{1}{\sqrt{\xi'(x)}}. \tag{43}$$

The main theorem of Ref. 10 makes it possible to find all rational solutions of Eq. (42), by bounding the degrees of the polynomials involved.

Theorem 1: *Let* $\Pi_i Q_i^i$ *be the square-free decomposition of the denominator of* $r \in \mathbb{C}(x)$. *If the order of* $u(x)$ *at infinity* $\nu_\infty(u) < 2$, *then any solution* $\xi \in \mathbb{C}(x)$ *of (42) can be written as* $\xi = P/Q$ *where*

$$Q = \prod_i Q^i_{(2-\nu_\infty(u))i+2} \in \mathbb{C}[x], \tag{44}$$

and $P \in C[x]$ *is such that either* $\deg(P) \leqslant \deg(Q)+1$ *or*

$$\deg(P) = \deg(Q) + \frac{2-\nu_\infty(r)}{2-\nu_\infty(u)}. \tag{45}$$

For the algebraic case, they also provide a possible (but not exhaustive) ansatz of the form

$$\xi(x) = P(x^{1/(2-\nu_\infty(u))}) \prod_{i>2} Q_i^{(i-2)(2-\nu_\infty(u))}, \tag{46}$$

and a bound for $\deg(P)$ of either

$$\deg(P) < (2-\nu_\infty(u))(\deg(Q)+2)$$

or

$$\deg(P) = (2-\nu_\infty(u))\deg(Q) + 2 - \nu_\infty(r).$$

Here, we choose to investigate the Bessel and Kummer functions, as the solutions of the target equation. The other classical classes of ${}_0F_1$ and ${}_1F_1$ functions, to which Theorem 1 is applicable, are equivalent to these two classes, rationally or algebraically.

In the general case of $\Omega_{\Lambda 0} \neq 0$, and no multiple roots of $W(x)$, the denominator of $r(x)$ is $16x^2W(x)^2$, and hence its square-free decomposition has only one term $Q_2 = xW(x)$. We take first the Bessel equation,

$$F''(\xi) = \left(\frac{4n^2-1}{4\xi^2} - \epsilon\right) F(\xi), \tag{47}$$

where ϵ is 1 for the Bessel and -1 for modified Bessel functions. We have $\nu_\infty(u) = 0$, and $\nu_\infty(r) = 2$, so

$$Q = \prod_i Q^i_{2i+2} = 1, \tag{48}$$

and $\deg(P) \leqslant 1$. Finally, substituting $\xi(x) = c_1 x + c_0$ into Eq. (42) yields no nonconstant solutions.

Proceeding in the same way, for Kummer functions, algebraic forms of $\xi(x)$, and possible cases of the roots of $W(x)$, we found no new solutions of this more general class.

Thus, we can finally formulate the main results as the following theorem.

Theorem 2: *If* $\Omega_{m0} > 0$, $\Omega_{r0} \geqslant 0$, $\Omega_{K0} \in \mathbb{R}$, *and* $\Omega_{\Lambda 0} \in \mathbb{R}$ [*unless* $W(x)$ *admits a double root, which requires the assumption of* $\Omega_{\Lambda 0} \geqslant 0$], *then the matter density perturbation equation (14) does not possess any solutions Liouvillian over* $\mathbb{C}(x)$, *or, in other words, is not solvable by quadratures, except for the following three cases*:

(1) *Heath's solution* ($\Omega_{r0} = 0$). *It is given by (39), for* $\Omega_{\Lambda 0} \neq 0$, *and by (33), when* $\Omega_{\Lambda 0} = 0$.
(2) *Meszaros's solution* ($\Omega_{K0} = 0$, $\Omega_{\Lambda 0} = 0$). *Given by (35).*
(3) *Matter only* ($\Omega_{\Lambda 0} = \Omega_{r0} = \Omega_{K0} = 0, \Omega_{m0} = 1$). *Given by (36).*

Moreover, there exist no solutions of the class $m(x)F[\xi(x)]$, *where* $F(\xi)$ *is a classical special function of the type* ${}_0F_1$ *or* ${}_1F_1$, $m(x)$ *is Liouvillian over* $\mathbb{C}(x)$, *and* $\xi(x) \in C(x)$ *or is algebraic of the form (46).*

However, when $\Omega_{\Lambda 0}=0$ *and* $W(x)$ *admits a double root, the non-Liouvillian solution of Chernin's, given by (30), applies.*

VII. CONCLUSIONS

The problem studied in this paper is a good example of a possible application of the differential Galois theory in practice. The known solution of the perturbation equation were originally discovered in different contexts and over the span of a few years, whereas here, one theory allows for full analysis.

Furthermore, the existence of other closed-form solutions has been ruled out. The one exception is the case of a double root of $W(x)$, when the cosmological constant is negative. Although Λ is usually assumed to be positive now, it still remains a viable mathematical possibility. However, we expect that case will not yield any new solutions, as the "manual" check for the first, simplest candidates failed.

Despite the fact that the analysis of perturbations can be performed numerically, without the need of explicit solutions, we feel that a more exact approach is always valuable—providing a better understanding of the complexity of the problem, revealing hidden, special solutions, or simply providing a more exact formula for numerical work. It also reflects, in some sense, the fact that general relativity, as the next step in the theory of gravitation, introduces nonintegrability into the basic equations. This can be seen clearly in a more advanced employment of the Galois theory applied to cosmological models themselves, for example, Refs. 1 and 11.

From the physical point of view, this model is a relatively simple one, and it is already known that the solutions found are not on themselves strong enough to explain the density fluctuations levels today. The main problem is the fact that they would need to be exponential, whereas they grow at most like a fixed power of the scale factor, and there is not enough time for the initial perturbations to increase sufficiently. One must also be aware that linear instability might be dumped when considered in the quadratic regime, so the least to be required of the linear equation's solutions is appropriate amplification. Nevertheless, these basic effects, being the first approximation, have physical meaning and should be taken into account when constructing more complicated models or explaining observational data.

We hope to investigate this field further in the future, as it does not limit the results to negative statements on integrability only, as we tried to demonstrate in this paper.

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Analytical integrability and physical solutions of *d*-KdV equation

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A new idea of electron inertia-induced ion sound wave excitation for *transonic plasma* equilibrium has already been reported. In such unstable plasma equilibrium, a linear source driven Korteweg-de Vries (*d*-KdV) equation describes the nonlinear ion sound wave propagation behavior. By numerical techniques, two distinct classes of solution (*soliton* and *oscillatory shocklike* structures) are obtained. Present contribution deals with the systematic methodological efforts to find out its (*d*-KdV) analytical solutions. As a first step, we apply the Painleve method to test whether the derived *d*-KdV equation is analytically integrable or not. We find that the derived *d*-KdV equation is indeed analytically integrable since it satisfies Painleve property. Hirota's bilinearization method and the modified *sine-Gordon* method (also termed as *sine-cosine* method) are used to derive the analytical results. Perturbative technique is also applied to find out quasistationary solutions. A few graphical plots are provided to offer a glimpse of the structural profiles obtained by different methods applied. It is conjectured that these solutions may open a new scope of *acoustic spectroscopy* in plasma hydrodynamics. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2173087]

I. INTRODUCTION

Recently, we have discovered an interesting property of a theoretically defined *transonic plasma* system, assumed to have hydrodynamic equilibrium configuration of physical interest.[1–3] Local normal mode theory defines the desired length of the theoretical transonic plasma system. The ion flow gradient is assumed to be weak enough so as to justify the uniform ion flow motion over the defined transonic plasma length. Of course, the equilibrium charge neutrality condition limits the range of allowed Mach number domain of plasma flows in transonic equilibrium. Self-similar plasma expansion[4] into vacuum may be a good example of transonic plasma flow under plasma approximation. Likewise, the solar wind plasmas are also of the category of self-similar plasma flow motion. The transonic plasma layer, in laboratory plasmas, exists near the Debye sheath edge created by plasma-boundary wall interaction processes. This is supposed to patch the Debye sheath layer on one end and the presheath layer on the other end.

According to our own proposed inertia-induced ion acoustic excitation theory, we argue that the large-scale plasma flow motion feeds the energy to the short scale fluctuations near the pre-sheath termination at sonic point. This is a kind of energy transfer process from large-scale flow energy to wave energy through short scale instability. In order to maintain the turbulence equilibrium there must be some source to feed large-scale flow and sink to arrest the infinite growth of the excited short waves. The growing wave energy could be used to remodify the global transonic equilibrium such that the transonic transition becomes a natural equilibrium with smooth change in flow motion from subsonic to supersonic. Of course, this is a quite involved problem to

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handle the self-consistent turbulence theory of transonic plasma in terms of anomalous transport. Now the question arises, how to produce such boundary layer with sufficient size of the transonic plasma layer for laboratory experimentations?

This is an experimental challenge to design such experiments to produce extended length of the transonic zone to sufficient extent to resolve the desired unstable wave spectral components. Creation of a thick boundary layer of transonic flow dynamics is, no doubt, an important task. This zone lies between subsonic and supersonic domains and is bounded by low supersonic and high subsonic speeds. Mind it, here the sonic velocity corresponds to the phase velocity of the bulk plasma mode of the dispersionless ion acoustic wave. In case of sheath edge boundary, transonic layer could be probed by high-resolving diagnosis of the Debye length order. The desired experiments of spectral analysis of the unstable ion acoustic waves in *transonic plasma condition* may be quite useful to resolve the mystery of sheath edge singularity. Using *de-Lavel nozzle mechanism* of hydrodynamic flow motion, experiments could be designed to produce transonic transition layer of desired length.

Study of the ambient acoustic spectrum associated with plasma flow motion can be termed as the *acoustic spectroscopy* of equilibrium plasma flows. This may be useful for expanding background plasmas,[4] solar wind plasmas[5] and also in space plasmas through which the space vehicles' motion and aerodynamic motion[5] occur. Basic principles of the acoustic spectroscopy have concern to the linear and nonlinear ion acoustic wave turbulence theory and properties of the transonic plasma equilibrium.[4,6] These properties may be used to develop the required diagnostic tools to study and describe the hydrodynamic equilibrium states of plasma flows by suitable observations and analysis of the waves and instabilities they exhibit. In fact, the ambient turbulence-driven plasma flow is quite natural to occur in toroidal and poloidal directions of the magnetic confinement of tokamak device. Similar physical mechanism is supposed to be operative in the transonic transition behavior of equilibrium plasma flow motion. Thorough investigations of acoustic wave turbulence theory in transonic plasma condition will be needed.

Recently, there has been an outburst of interest in plasma states where the assumption of static equilibrium practically is violated. Great deals of research activities are now going on in transonic and supersonic magnetohydrodynamic flows in laboratory and astrophysical plasmas.[5] Similar activities are also important for understanding the designing of supersonic aerodynamics[7] having relevance in spacecraft-based laboratory experimentations of space plasma research as well. It is also argued that future tokamak reactors need the consideration of rotation of fusion plasma with high speeds that do not permit the assumption of static equilibrium to hold good. This may be brought about due to neutral beam heating and pumped divertor action for the extraction of heat and exhaust.

In astrophysics, the primary importance of plasma flows is revealed in such diverse situations as coronal flux tubes, stellar winds, rotating accretion disks, and jets emitted from radio galaxies. The main point is to argue that the basic understanding of the acoustic wave dynamics in transonic plasma system constitutes an important subject of future interdisciplinary research. This may be useful for development of the appropriate diagnostics for acoustic spectroscopy to measure and characterize the hydrodynamic equilibrium of transonic plasmas.

Consideration of the Boltzmannian electrons for ion acoustic wave description is no more practical in such plasma equilibrium. For example, it hides the unstable behavior of the ion acoustic wave fluctuations in transonic plasma equilibrium. For simple monoenergetic but uniform ion flow dynamics, it is predicted that the ion acoustic wave remains no more stable in transonic plasma condition. It suffers linear resonant growth[1] of explosive type due to linear process of resonance mode-mode coupling of positive and negative energy waves.[2] It is thus natural to argue that the acoustic wave turbulence should constitute the unique property of the transonic plasma system in the absence of magnetic and gravitational force fields. It is further argued that the conventional idea of Bohm condition for stable sheath formation requires a fresh review. Similar outlook is needed to understand the formation of other nonlinear localized structures of low frequency acoustic waves like solitons, double layers, etc.

The lowest order nonlinear wave theory of the ion acoustic wave dynamics predicts that the

usual KdV equation is not suitable to describe the kinetics of the nonlinear traveling ion acoustic waves in transonic plasma condition.[3] The *d*-KdV equation is prescribed as a more suitable nonlinear differential equation to describe the nonlinear traveling ion acoustic wave dynamics in transonic plasma condition. By mathematical structure of the derived *d*-KdV equation, it looks analytically nonintegrable and physically nonconservative dynamical system. Due to the linear source term, an additional class of nonlinear traveling wave solution of oscillatory shocklike nature is obtained. This is more prominent in the shorter scale domain of the unstable ion acoustic wave spectrum but within the validity limit of weak nonlinearity and weak dispersion. Researchers having interest in the subject are advised to read our earlier presentations for details.[1–3]

In this contribution, we make specific methodological attempts to analytically solve the *d*-KdV equation to reproduce our own predicted numerical results. We first apply the well-known Painleve method[8–14] of mathematical calculations to check the mathematical possibility of finding its analytical solutions. We find that it is indeed analytically integrable. In the process, Hirota's bilinear transformation[14,15] is obtained for analytical solutions. We then proceed further and apply the mathematical technique of *sine-cosine* method (also known as *modified sine-Gordon method*)[16,17] to derive the desired analytical solutions. Solution obtained by this method is akin to the linear superposition of two distinct nonlinear stationary waves. In the asymptotic limit of long wavelength of the driving source term, usual KdV soliton solution is recovered. For shorter wavelengths of the linear driving source, shock-dominated solution is found without any oscillatory character. But, due to limitations of the available mathematical tools, only approximate results are possible.

Quasistationary solutions with the well-known *perturbative technique*[18,19] are also derived. Physical significance of *quasistationarity* means that the amplitudes of the solutions are slowly varying and they are free from any secular terms in the asymptotic expansion of dynamical variables. In fact, as per required relative accuracy, the analytical results obtained by all these different mathematical methods are graphically compared. In all the cases a linear superposition of shock and soliton is obtained. Thus the numerical solutions[2] are partially verified with the help of obtained analytical findings. Absence of the oscillations in graphical representation of the shock-dominated solution may be attributed to the limitations of the applied mathematical tools. This provides further scope for suitable improvement of existing mathematical methods to produce the oscillatory shocklike solutions that comprise of oscillatory peaks in the shock-dominated solution. That means the well-defined (explicit) functional form of oscillatory shocklike solution is still unknown. This forms a good mathematical problem for future research work.

Contents of this research paper are organized as follows. Section II includes general physical discussions on integrability of the *d*-KdV equation. Section III highlights the methodology of analytical integration and derivation of the exact analytical (traveling wave) solutions. Section IV includes the results and discussions obtained thereof. Last, Sec. V contains a compact summary of the conclusions drawn from this present contribution.

II. INTEGRABILITY TEST OF *d*-KdV EQUATION

Actually, the concept of integrability is not well defined in mathematical sense. However, the question of integrable nonlinear dynamical equations could be associated with the following conceptual view of the unknown solutions. It is basically a mathematical property of the function of the unknown solutions of the given nonlinear dynamical equation. It is used to enhance the predictive ability of the given nonlinear equation to provide more and more quantitative and qualitative informations regarding the governing dynamical physical systems. There are two well-known broad notions as defined and discussed in mathematical literature.[8–14] We have used the notion of integrability in the complex time plane, which is now called the Painleve property. Fixed singularities occur at points where the coefficients of the equation are singular.[8–14] The ordinary differential system is said to possess the Painleve property when all the movable singularities are single valued (simple poles).

More briefly, a dynamical evolution equation is said to satisfy the Painleve property[9] when the solutions of the equation are single valued about the movable singularity manifold and the singu-

larity manifold is noncharacteristic. Theoretically speaking, a given dynamical evolution equation is said to have analytical integrability if it can have the reduced structures like mathematical forms of the Painleve transcendents[11] after proper mathematical transformations. The next section deals with the mathematical derivations of the Painleve property to predict integrable and conservative dynamical behavior of the *d*-KdV equation having self-consistent linear driving source term. This is to point out that this equation is an outcome of our own theoretical derivations[2,3] while describing the nonlinear ion acoustic wave dynamics in transonic plasma system.

A. Basic governing equations

For the sake of instant reference for readers of this paper, the self-consistently closed set of basic governing equations for fluid description of transonic plasma system in normalized form is given as follows.

Electron continuity equation

$$\frac{\partial \phi}{\partial t} + v_e \cdot \frac{\partial \phi}{\partial x} + \frac{\partial v_e}{\partial x} = 0. \tag{1}$$

Electron momentum equation

$$\frac{m_e}{m_i}\left(\frac{\partial v_e}{\partial t} + v_e \cdot \frac{\partial v_e}{\partial x}\right) = \frac{\partial \phi}{\partial x} - \frac{1}{n_e}\frac{\partial n_e}{\partial x}. \tag{2}$$

This is to remind the readers that this equation is obtained by substituting zero-order solution of Boltzmann electron density distribution into the normal electron continuity equation. In fact, in the asymptotic limit of $m_e/m_i \to 0$, electron continuity equation as such is redundant because the left-hand side (electron inertial effect) of (2) is ignorable. Equation (1) basically offers a scope to introduce the weak but finite role of electron to ion inertial mass ratio on the normal mode behavior of the ion acoustic wave.

Ion continuity equation

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial x}(n_i v_i) = 0. \tag{3}$$

Ion momentum equation

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = -\frac{\partial \phi}{\partial x}. \tag{4}$$

Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} = n_e - n_i. \tag{5}$$

Our previous theoretical calculations of linear ion acoustic wave analysis[1,2] provide a clear-cut idea of the possible existence of linear ion acoustic wave turbulence in transonic zone of plasma flows within fluid model approach. The following form of the derived *d*-KdV equation[3] obtained by reductive perturbation method then describes the nonlinear ion acoustic wave dynamics under transient limit:

$$K_0 \frac{\partial \phi}{\partial t} + M_0 \phi \frac{\partial \phi}{\partial x} + \frac{1}{2}\frac{\partial^3 \phi}{\partial x^3} = \gamma K_0 \phi. \tag{6}$$

Here the notations K_0 and M_0 termed as *complex response coefficients*[3] and the linear resonant growth rate (γ) of the ion acoustic wave appearing in Eq. (6) are defined as follows:

$$K_0 = [A^2 + B^2]^{1/2},$$

where

$$A = \left(\frac{M_r}{\varepsilon_m} + \frac{M_{Dr}^3 - 3M_{Dr}M_i^2}{(M_{Dr}^2 + M_i^2)^3} \right)$$

and

$$B = \left(\frac{M_i}{\varepsilon_m} + \frac{M_i^3 - 3M_{Dr}^2 M_i}{(M_{Dr}^2 + M_i^2)^3} \right),$$

$$M_0 = [C^2 + D^2]^{1/2},$$

where

$$C = \frac{1}{2}\left[\frac{3\{(M_{Dr}^2 - M_i^2)^2 - 4M_{Dr}^2 M_i^2\}}{(M_{Dr}^2 + M_i^2)^4} - \frac{(M_r^2 - M_i^2)^2 - 4M_r^2 M_i^2}{\varepsilon_m^2} - 1 \right]$$

and

$$D = -\frac{1}{2}\left\{ \frac{12(M_{Dr}^2 - M_i^2)M_{Dr}M_i}{(M_{Dr}^2 + M_i^2)^4} + \frac{4(M_r^2 - M_i^2)M_r M_i}{\varepsilon_m^2} \right\},$$

$$\gamma = \sqrt{2\left(\frac{m_i}{m_e}\right)} k\lambda_{De} |(1 - v_{i0})^{1/2}|.$$

Here the notation M_{Dr} represents for the real part of Doppler shifted ion sound wave Mach number and M_i represents for the imaginary part of the same and is correlated to the linear growth rate as discussed earlier.[3] The other notations like $k\lambda_{De}$ and v_{io} represent for the normalized acoustic wave number and equilibrium ion fluid flow velocity of the transonic plasma, respectively. Likewise, the notation defined as $\varepsilon_m = m_i/m_e$ denotes for the ion to electron mass ratio. Here it will be pertinent to comment that in our defined plasma system, the plasma ions are self-consistently drifting or streaming through a negative neutralizing background of hot electrons having relatively zero inertia. As such the time response of the electron fluid for ion sound wave description is normally ignored. As a result, the unique role of finite but weak electron inertia having an ability to destabilize the ion sound wave in transonic plasma equilibrium even within fluid model approach of normal mode description is masked.

Physical description of our proposed excitation theory of ion sound wave in transonic plasma equilibrium differs from those of the others (Refs. 20–24) to drive the same ion acoustic wave instability. Driving physics suggests that even a slight temporal delay of thermal electrons that offer instantaneous response to the ion sound wave potential fluctuations may cause a resonant explosive growth[1,2] if the ion flow velocity falls within the transonic domain of quasineutral plasma flow motion. In fact, an appropriate phase difference between the ion density and electron density perturbations are introduced so as to yield the growth. Contributions of other sources of ion sound wave instability driving may, however, be evaluated by the relative comparison of the growth rates and ion sound excitation thresholds.

B. Comments on derivation of *d*-KdV equation

In our earlier presentation,[3] the invariance property of stretched coordinates is assumed to hold good during transient time effect of the instability. This results into Eq. (6) with the stretched coordinate system defined by $\xi = \varepsilon^{1/2}(x - Mt)$ and $\tau = \varepsilon^{3/2}t$ where x and t are normalized forms. This can be justified as follows. Due to linear instability, Mach number M that defines the ratio of nonlinear phase velocity and ion sound speed becomes complex, i.e., $M = M_r + iM_i$. As a result,

$\xi_r=\varepsilon^{1/2}(x-M_r t)$ and $\xi_i=-\varepsilon^{1/2}M_i t$, where $\varepsilon=k^2\lambda_{De}^2$. If we define the transient time as $t=t_t\sim\varepsilon^{-1/2}\sim 1/k\lambda_{De}\sim X_\omega$, then $\xi_i=-M_i$ and the corresponding differential operators (under Galilean transformations) are transformed as follows: $\partial/\partial x\equiv\varepsilon^{1/2}\partial/\partial\xi_r$ and $\partial/\partial t\equiv -M_r\varepsilon^{1/2}\partial/\partial\xi_r+\varepsilon^{3/2}\partial/\partial\tau$. This implies that the differential operators remain invariant during transient effect of the instability on global structure of the nonlinear traveling wave solution.

Let us now consider the cyclic behavior of the space coordinate in Galilean frame of solitary wave and assume circular geometry to define $\xi=\xi_0 e^{i\alpha(t)}$ in time domain. Now for $M_i<1$, $\alpha(t)=\tan^{-1}(\xi_i/\xi_r)\sim(-M_i/X_\omega)=-M_i$ for $X_\omega\sim 1$, where $\varepsilon^{1/2}(x-M_r t)\sim X_\omega$ is the rescaled width of the solitary wave. The radius of the considered circular geometry is given by

$$\xi_0=\xi_r(1+\xi_i^2/\xi_r^2)^{1/2}\sim\varepsilon^{1/2}(x-M_r t)(1+\alpha^2)^{1/2}\sim\xi_r \quad \text{for } |\alpha|<1.$$

Thus under the defined circular geometry under the conditions $M_i<1$ and, one gets the following values of the phase angles β for K_0 and γ for M_0 as follows:

$$\beta=\tan^{-1}(B/A)=\tan^{-1}(-3M_i/1)\sim -3M_i,$$

$$\gamma=\tan^{-1}(D/C)=\tan^{-1}(-6M_i/1)\sim -6M_i.$$

These estimations of α, β, and γ are made for resonant conditions $M_{Dr}\sim 1$ for ion acoustic wave excitation. It is notable that $\alpha\sim\beta\sim\gamma<1$ within an order of magnitude. It is thus found that in the above limiting cases of the global phase transformation method (GPTM),[3] the compact form of the linear source driven KdV (d-KdV) equation is well verified and justified.

C. Painleve test of *d*-KdV equation

Now let us look into the details of the methodological description of the Painleve property of the derived d-KdV equation from these basic equations. Following the prescribed mathematical procedure, we will now prove that the d-KdV equation satisfies the Painleve property. The assumed Laurent's series expansion of the unknown solution of Eq. (6) around singularity (near singularity and not at singularity) as a function of singularity manifold $f(x,t)\neq 0$ is given as follows:

$$\phi=\sum_{j=0}^{\infty}\phi_j f^{j+\alpha}. \tag{7}$$

After substituting this expression into Eq. (6) and following the basic principle of homogeneity of leading order analysis (balancing the highest order contributions from the linear and nonlinear terms of the d-KdV equation), we get $\alpha=-2$ under the soliton formation condition of nonlinearity balanced by dispersion.

Now substituting the various differential terms obtained from (7) into Eq. (6) and collecting the coefficients of the power of f^{j-5} from each term, we get what is known as the *recurrence relation* (RR) and can be set in the more compact form as follows:

$$\begin{aligned}K_0\{\phi_{j-3,t}+\phi_{j-2}(j-4)f_t\}+M_0\left[\sum_{k=0}^{j}\phi_{j-k}\{f_{k-1,x}+(k-2)\phi_k f_x\}\right]+\frac{1}{2}[\phi_{j-3,xxx}+3\phi_{j-2,xx}(j-4)f_x\\ +3\phi_{j-1,x}(j-3)(j-4)f_x^2+3\phi_{j-2,x}(j-4)f_{xx}+3\phi_{j-1}(j-3)(j-4)f_x f_{xx}\\ +\phi_j(j-2)(j-3)(j-4)f_x^3+\phi_{j-2}(j-4)f_{xxx}]=\gamma K_0\phi_{j-3}.\end{aligned} \tag{8}$$

From this recurrence relation of general nature, one can generate order-by-order equations for different cases of j values.

Case (1): For $j=0$, we get from (8),

$$\phi_0 = -\left(\frac{6}{M_0}\right) f_x^2. \tag{9}$$

Case (2): For $j=1$, we get from (8),

$$\phi_1 = \left(\frac{6}{M_0}\right) \phi_{xx}. \tag{10}$$

Case (3): For $j=2$, we get from (8),

$$\frac{K_0}{M_0}(f_x f_t) + \frac{2}{M_0}(f_x f_{xxx}) - \frac{3}{2M_0} f_{xx}^2 + \phi_2 f_x^2 = 0. \tag{11}$$

Case (4): For $j=3$, we get from (8),

$$f_{xt} - \frac{M_0}{K_0}\phi_3 f_x^2 + \frac{1}{2K_0} f_{xxxx} + \frac{M_0}{K_0}\phi_2 f_{xx} = \gamma f_x. \tag{12}$$

Case 5: For $j=4$, we get from (8),

$$\frac{\partial}{\partial x}\left[f_{xt} - \frac{M_0}{K_0}\phi_3 f_x^2 + \frac{1}{2K_0} f_{xxxx} + \frac{M_0}{K_0}\phi_2 f_{xx} - \gamma f_x \right] = 0. \tag{13}$$

The arbitrary function is chosen such that $\phi_j = 0 \forall j \geqslant 3$ (closure property depending on the highest order of differentiation $j=3$ for d-KdV equation). It is noteworthy that the equation (13) with the help of condition (12) is known as the *compatibility condition* for d-KdV equation (6). This is also noted from the transcendental equations (11) and (12) that the recurrence relations for $j \geqslant 3$ are modified by an additional term proportional to linear growth rate (γ) of the ion acoustic wave instability in transonic plasma system.

Now collecting all the terms involving ϕ_j from (8), we determine the locations of the resonant terms (termed as the *resonances*) as follows:

$$M_0\phi_0\phi_j(j-4)f_x + \tfrac{1}{2}\{\phi_j(j-2)(j-3)(j-4)f_x^3\} = 0 \Rightarrow \tfrac{1}{2}(j+1)(j-4)(j-6)\phi_j f_x^3 = 0$$

$$\Rightarrow j = -1, 4, 6 (\text{resonances}). \tag{14}$$

This is to note that the resonances[8–14] at $j=-1,4,6$ are obtained by substituting the value of ϕ_0 in the above identity of Eq. (14). At these values of j the function ϕ_j is allowed to have arbitrary values. Now the solution can be shown to allow the Bäcklund transformation as given below,

$$\phi = \sum_{j=0}^{2} \phi_j f^{j-2} = \phi_0 f^{-2} + \phi_1 f^{-1} + \phi_2,$$

$$\phi = -\left(\frac{6}{M_0}\right)\frac{f_x^2}{f^2} + \frac{\phi_1}{f} + \phi_2,$$

$$\phi = \left(\frac{6}{M_0}\right)\frac{\partial^2}{\partial x^2}[(\ln(f))] + \phi_2. \tag{15}$$

It is now methodologically proved that the derived d-KdV equation of our concern satisfies the Painleve properties. That means that the assumed solutions are free from movable singularity and hence the d-KdV equation is, indeed, analytically integrable and solvable. Thus the equation (15) represents a form of analytical solution in terms of assumed singularity manifold. However, the

exact nature of the singularity manifold has been neither identified nor characterized analytically for explicit solutions.

D. Properties of *d*-KdV equation

One can now show that the deduced *d*-KdV equation derived for physical situation of *transonic plasma* system possesses the properties of integrable dynamical systems with sufficient number of conserved quantities.[14] The sufficiency of conserved quantities, however, depends on the order of the dynamical evolution equation describing the system. This is to remind the readers that for simplicity, the transonic plasma of infinite extension is assumed. Of course, realistic situation of laboratory produced transonic plasma will require nonlocal theory within fluid and Vlasov models. Moreover, detailed study will be required to develop an appropriate theory of saturation mechanism through turbulence production or otherwise. Other complexities like presence of external forces and collisions, etc., may be included to provide a wide range scanning of plasma and flow parameter domains to test the effect on the proposed excitation theory of ion sound wave.

1. Bäcklund transformations

A Bäcklund transformation (BT) is defined as a mathematical transformation that connects the same or distinct analytical solutions of two differential equations. If the transformation, however, connects two distinct solutions of the same differential equation, it is termed as the auto-Bäcklund transformation (*a*-BT). A BT[13] for the *d*-KdV equation (6) is obtained from the equation (15) with $\phi_2 \neq 0$ ($\phi_2=0$ for Hirota's bilinear transformation) as follows:

$$\phi = -\left(\frac{6}{M_0}\right)\frac{f_x^2}{f^2} + \frac{\phi_1}{f} + \phi_2. \tag{16}$$

It gives a mathematical idea of how the arbitrary function (f) enters the assumed solution of Eq. (6).

2. Lax pair

Now for our *d*-KdV equation (6), we can construct two canonically conjugate operators corresponding to the *invariance property* of usual KdV equation in absence of any driving source under Galilean transformations. These two operators (designated as L and B as given below) together form what is known as Lax pair and the connecting mathematical equation is termed as Lax equation of the *d*-KdV equation,

$$L = \frac{1}{2K_0}\frac{\partial^2}{\partial x^2} + \left(\frac{M_0}{K_0}\right)\phi I, \tag{17}$$

$$B = -\frac{2}{K_0}\frac{\partial^3}{\partial x^3} - \frac{M_0}{2K_0}\left(\phi\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\phi\right), \tag{18}$$

$$\frac{\partial L}{\partial t} = [L,B]. \tag{19}$$

This equation (19) is known as the Lax equation[11,14] in terms of the Lax pair (Lax operators) L and B, which can be termed as the Lax equivalence of the derived *d*-KdV equation with I as an identity operator. In mathematical language, the existence of Lax pair is a decisive criterion for integrable systems. If L is time independent, one gets a commutator $[L,B]=0$ signifying a conservative and integrable dynamical system.

III. ANALYTICAL SOLUTIONS OF *d*-KdV EQUATION

Now it is clear that the *d*-KdV equation is integrable and hence one can, in principle, find out its analytical solutions. Analytical solution of a given dynamical equation means to derive the well-defined (explicit) functional form of the solution that satisfies the given equation. It is indeed difficult to analytically solve it in space and time domain as two-dimensional (2D) problem. To simplify the situation, we look for the steady state solution. For this we apply Galilean transformation to reduce 2D form of the nonlinear differential *d*-KdV equation into one-dimensional (1D) form of nonlinear differential equation. After that, we apply the sine-cosine method as discussed earlier[16,17] to derive analytical solutions of the steady state *d*-KdV.

A. Application of Hirota bilinear transformation method

The analytical transformation depicted by the equation (15) under the arbitrary condition of $\phi_2=0$ is known as Hirota's bilinear transformation.[14,15] The mathematical significance of bilinear is that the sum of the various powers of f in each term of the transformed differential equation (as follows) is equal to 2. After replacing the various differential terms of the equation (6) with the help of (15), we get the following transformed equation:

$$K_0\left[\frac{f_{xxt}}{f}-\frac{f_{xx}f_t}{f^2}-2\frac{f_xf_{xt}}{f^2}+2\frac{f_x^2f_t}{f^2}\right]+\frac{f_{xx}f_{xxx}}{f^2}-3\frac{f_xf_{xx}^2}{f^3}+4\frac{f_x^2f_{xxx}}{f^3}+\frac{1}{2}\frac{f_{xxxxx}}{f}-\frac{5}{2}\frac{f_xf_{xxxx}}{f^2}-48\frac{f_x^3f_{xx}}{f^4}$$
$$=\gamma K_0\frac{f_{xx}}{f}-\gamma K_0\frac{f_x^2}{f^2}. \tag{20}$$

Now, let us apply the reductive (nonlinear) perturbation technique about the vacuum in the form of harmonics in $\varepsilon(\ll 1)$ known as the dispersion strength representing the balancing between weak dispersion and weak nonlinearity, to expand the arbitrarily chosen singularity manifold function ϕ as $f=1+\varepsilon f^{(1)}+\varepsilon^2 f^{(2)}+\cdots$. By the first order analysis (with respect to ε) in the above mathematical method, we get the solution of the *d*-KdV equation (6) for one soliton system as follows:

$$\phi(x,t)=1.5\left(\frac{k^2}{M_0}\right)\sec h^2\left\{\frac{1}{2}(\eta_r+i\eta_i)\right\}. \tag{21}$$

Equation (21) represents analytical (traveling wave) solution of *d*-KdV equation propagating under transonic conditions, ignores to produce the analytical form of oscillatory shocklike structures. From a physical point of view, one may give a conclusion hereof that the argument $(\eta/2)$ of the soliton solution is getting self-consistently transformed into a complex one owing to the complex nature of the ion acoustic propagation vector (k) while passing through the unstable conditions of transonic plasmas. Complex nature of the argument in presence of a linear free energy source in transonic condition is itself a physical signature of the said instability. The real as well as imaginary parts of the complex argument of the KdV soliton are given as follows:

$$\eta_r=kx+\tfrac{1}{2}k^3t,$$

$$\eta_i=-\gamma K_0t.$$

Again, expanding Hirota solution as given by Eq. (21) by well-known expansion formulas of

circular and hyperbolic functions, this solution can be written in the following expanded form:

$$\phi(\eta_r,\eta_i)=1.5\left(\frac{k^2}{M_0}\right)\sec h^2\left\{\frac{1}{2}(\eta_r)\right\}\left[\frac{\cos(\eta_i)+\sin^2\left(\frac{1}{2}\eta_i\right)\sec h^2\left(\frac{1}{2}\eta_r\right)}{1-\sec h^2\left(\frac{1}{2}\eta_r\right)\sin^2\left(\frac{1}{2}\eta_i\right)}\right]-i1.5\left(\frac{k^2}{M_0}\right)\tanh\left\{\frac{1}{2}(\eta_r)\right\}$$
$$\times\left[\frac{\sin(\eta_i)\sec h^2\left(\frac{1}{2}\eta_r\right)}{1-\sec h^2\left(\frac{1}{2}\eta_r\right)\sin^2\left(\frac{1}{2}\eta_i\right)}\right]. \tag{22}$$

Now solution (22) can be simplified in the transient limit of $\eta_i<1$ into the following form:

$$\phi_r(\eta_r,\eta_i)=1.5\left(\frac{k^2}{M_0}\right)\sec h^2\left\{\frac{1}{2}(\eta_r)\right\}, \tag{23}$$

$$\phi_i(\eta_r,\eta_i)=1.5\left(\frac{k^2}{2M_0}\right)\eta_i\sinh(\eta_r)\sec h^4\left\{\frac{1}{2}\eta_r\right\}. \tag{24}$$

It is, however, noticed that the asymmetric structures represented by Eq. (24) fail to produce the expected nature of shocklike solutions. But, of course, the average qualitative features in transonic domains are reflected. And hence, it paves the way for further application of improved mathematical tools for more accurate results.

B. Application of sine-cosine method

Yan[15] developed *sine-cosine* method directly from the modified transformation of famous *sine-Gordon* equation. A new form of nonlinear mathematical transformation is obtained by suitable mathematical tailoring of the sine-Gordon equation. This was applied to solve the usual KdV equation and a new class of solutions was predicted for the usual KdV equation. The same is supposed to be true for other well studied nonlinear dynamical equations too. We apply this method to solve the *d*-KdV equation derived to describe the structural behaviors of nonlinear traveling ion acoustic wave in unique equilibrium condition of transonic plasma system.

This effort is primarily motivated by our own numerical results of the same *d*-KdV equation that predicts the possibility of oscillatory shocklike solution in addition to usual soliton solution. The main issue is to find out the explicit form of analytical solution for the oscillatory shocklike profile. As we will see later that even this method is incapable to yield the desired result. However, an explicit term of shock profile is analytically deduced. As per the mathematical procedure laid down for *sine-cosine* method to solve the usual KdV equation, we express the traveling wave solution of *d*-KdV equation as follows:

$$\phi(\eta)=A_0+\sum_{j=1}^{n}\tanh^{j-1}(\eta)[A_j\tanh(\eta)+B_j\sec h(\eta)], \tag{25}$$

where $\eta=x-t$ and the same is used to numerically solve the *d*-KdV equation to find out the steady state solution in our earlier work.[3] Accordingly, the nonlinear transformation derived from improved sine-Gordon equation (*sine-cosine* method) is given below,

$$\frac{d\omega}{d\eta}=\sin\omega. \tag{26}$$

After integration of Eq. (26), we arrive at the following transformations ($\omega\Leftrightarrow\eta$):

$$\sin(\omega) = \sec h(\eta),$$

$$\cos(\omega) = \tanh(\eta).$$

Now, the principle of homogeneous balancing used for evaluation of the upper limit of summation after equalizing the highest order contributions from the linear as well as nonlinear terms, yields $n=2$ for the equation (6). After using these transformations, the assumed solution (25) can be expressed in a new form as functions of the intermediate variable ω,

$$\phi(\omega) = A_0 + \sum_{j=1}^{n} \cos^{j-1}(\omega)[A_j \cos(\omega) + B_j \sin(\omega)]. \tag{27}$$

Substitution of this solution into the Galilean transformed form of Eq. (6) through the relation $\eta=x-t$ results into a trigonometric identity of algebraic shape. After collecting common terms, the coefficient of each term in the trigonometric identity must vanish. As a result, the following forms of algebraical relationships among the various unknown coefficients appearing in the transformed form of the d-KdV equation are derived by homogeneous equalization of various powers of $\sin^m \omega \cos^n \omega$ from both sides. It will be definitely noticed that there will be existence of some more terms with respect to the usual KdV equation because of the presence of an additional self-consistent source term involving γ in the d-KdV equation.

Constant:

$$A_1\left(1 - \frac{M_0}{K_0}A_0\right) + \frac{A_1}{K_0} - \gamma A_0 = 0.$$

$\sin \omega$:

$$B_2\left(1 - \frac{M_0}{K_0}A_0\right) - \frac{M_0}{K_0}A_1B_1 + \frac{5B_2}{2K_0} - \gamma B_1 = 0.$$

$\cos \omega$:

$$2A_2\left(1 - \frac{M_0}{K_0}A_0\right) - \frac{M_0}{K_0}(A_1^2 - B_1^2 + B_2^2) + \frac{8A_2}{K_0} - \gamma A_1 = 0.$$

$\cos^2 \omega$:

$$-A_1\left(1 - \frac{M_0}{K_0}A_0\right) - 3\frac{M_0}{K_0}\left(A_1A_2 - \frac{4}{3}B_1B_2\right) - \frac{4A_1}{K_0} - \gamma A_2 = 0.$$

$\cos^3 \omega$:

$$-2A_2\left(1 - \frac{M_0}{K_0}A_0\right) + \frac{M_0}{K_0}(A_1^2 - 2A_1^2 - B_1^2 + 3B_2^2) - \frac{20A_2}{K_0} = 0.$$

$\cos^4 \omega$:

$$A_1A_2 - B_1B_2 + \frac{A_1}{M_0} = 0.$$

$\cos^5$:

$$A_2^2 - B_2^2 + \frac{6A_2}{M_0} = 0.$$

$\sin \omega \cos \omega$:

$$-B_1\left(1-\frac{M_0}{K_0}A_0\right)-2\frac{M_0}{K_0}(A_1B_2+A_2B_1)-\frac{5}{2K_0}B_1-\gamma B_2=0.$$

$\sin\omega\cos^2\omega$:

$$-2B_2\left(1-\frac{M_0}{K_0}A_0\right)+\frac{M_0}{K_0}(2A_1B_1-3A_2B_2)-\frac{14}{K_0}B_2=0.$$

$\sin\omega\cos^3\omega$:

$$A_1B_2+A_2B_1+\frac{B_1}{M_0}=0.$$

$\sin\omega\cos^4\omega$:

$$A_2B_2+\frac{3}{M_0}B_2=0.$$

This is to note that a few additional terms in the above recursion equations are appearing due to linear resonant growth effect (γ) of the ion acoustic wave in transonic plasma equilibrium. Solving all these equations for an arbitrary choice of $B_1=0$ and $B_2=0$, we arrive at the following approximate values of the unknown coefficients:

$$A_0=\frac{K_0}{M_0}+\frac{4}{M_0},$$

$$A_1=-\frac{\gamma K_0}{M_0},$$

$$A_2=-\frac{6}{M_0}.$$

The above values of coefficients are calculated under weak dispersion and weak nonlinearity under ignorable resonant growth rate such that $\gamma\neq 0$ and $\gamma^p=0\,\forall\, p>1$. And, otherwise, all the recurrence relations could not be satisfied simultaneously. Last, the exact traveling wave analytical solutions of the *d*-KdV equation as an intermixed superposition of two distinct classes (shock and soliton) can be written as

$$\phi(\eta)=\left(\frac{K_0}{M_0}+\frac{4}{M_0}\right)+\left(-\frac{\gamma K_0}{M_0}\right)\tanh(\eta)+\left(-\frac{6}{M_0}\right)\tanh^2(\eta), \tag{28}$$

$$\phi(x-t)=\left(\frac{K_0}{M_0}-\frac{2}{M_0}\right)+\left[-\frac{\gamma K_0}{M_0}\tanh(x-t)+\frac{6}{M_0}\sec h^2(x-t)\right]. \tag{29}$$

After rescalings with $\phi\rightarrow(K_0/2)\phi$ and $\eta\rightarrow(K_0/2)^{-1/2}\eta$, the solution (29) can be written in the scaled out form as follows:

$$\phi_{SC}(\eta)=a_0\sec h^2\left(\sqrt{\frac{1}{2}K_0}\eta\right)+\left[a_2+a_3\tanh\left(\sqrt{\frac{1}{2}K_0}\eta\right)\right], \tag{30}$$

where $a_0=3K_0/M_0$, $a_1=K_0/2(K_0/M_0-2/M_0)$, and $a_2=-\gamma K_0^2/M_0$.

It is obviously clear from Eq. (30) that there is a linear superposition of both shock (tanh)-like and soliton (sech^2)-ic solutions over some dc background formed by the coherent self-coupling of identical spectral components of ion acoustic wave fluctuations in transonic plasma.

C. Application of perturbative method

New physical but analytically quasistationary solutions have already been obtained by perturbations over usual KdV solitons and solitary waves in a new frame of reference described by a set of fast and slow variables by Kodama *et al.*[18] We apply the same method to find out analytical solutions of the *d*-KdV equation of our concern. This method is actually believed to be motivated for newer and more satisfactory analytical results for a driven KdV system over others.

To apply the perturbative technique,[18,19] first of all, new transformations in terms of fast coordinate (η); and slow coordinates (τ) and (χ) are introduced for quasistationary solutions as follows: $\eta=x-t$, $\tau=\varepsilon t$, and $\chi=\varepsilon x$. These give $\partial\eta/\partial x=1$, $\partial\eta/\partial t=-1$, $\partial\tau/\partial t=\varepsilon$, and $\partial\chi/\partial x=\varepsilon$. Now, for quasistationary character, we assume that the usual potential function is of the form, $\phi=f(\eta,\tau,\varepsilon)=\phi_0+\varepsilon\phi_1+\cdots$, where ϕ_0 is the leading order solution (usual soliton) of the *d*-KdV in absence of the linear growth term, that is treated as perturbation. Then, these results on being substituted on the *d*-KdV equation, order-by-order analyses are performed and integrated to have the desired analytical results.

Now, as already reported in our earlier work,[3] $\varepsilon(\ll 1)$ is a smallness parameter specifying the strength of balancing between nonlinearity and dispersion of the plasma medium, we take $\gamma\equiv\varepsilon$ for the calculations by perturbative technique and substitute $\varepsilon\equiv\gamma$ back finally to get the desired analytical results. This is, of course, not going to change the physical properties of the plasma medium under the approximation of weak nonlinearity and weak dispersion during the lowest order nonlinear expansion of relevant physical variables with respect to leading order ones. With this background, our *d*-KdV equation (6) can now be written as

$$-\frac{\partial}{\partial\eta}(\phi_0+\varepsilon\phi_1+\cdots)+\frac{M_0}{K_0}(\phi_0+\varepsilon\phi_1+\cdots)\frac{\partial}{\partial\eta}(\phi_0+\varepsilon\phi_1+\cdots)+\frac{1}{2K_0}\frac{\partial^3}{\partial\eta^3}(\phi_0+\varepsilon\phi_1+\cdots)$$
$$=\varepsilon(\phi_0+\varepsilon\phi_1+\cdots)-\varepsilon\frac{\partial}{\partial\tau}(\phi_0+\varepsilon\phi_1+\cdots). \tag{31}$$

Now equating the coefficients of $\varepsilon^0,\varepsilon^1$, etc., to zero from both sides of Eq. (31), respectively, we get the following equations:

$$-\frac{\partial\phi_0}{\partial\eta}+\frac{M_0}{K_0}\phi_0\frac{\partial\phi_0}{\partial\eta}+\frac{1}{2K_0}\frac{\partial^3\phi_0}{\partial\eta^3}=0, \tag{32}$$

$$-\frac{\partial\phi_1}{\partial\eta}+\frac{M_0}{K_0}\left(\phi_0\frac{\partial}{\partial\eta}+\frac{\partial}{\partial\eta}\phi_0\right)\phi_1+\frac{1}{2K_0}\frac{\partial^3\phi_1}{\partial\eta^3}=\phi_0-\phi_{0\tau}. \tag{33}$$

The solution of Eq. (32) is the leading order unperturbed solution of Eq. (6), which is a usual soliton having amplitude-width relationship as $A\times w^2=6/M_0$. It is given by

$$\phi_0=3\left(\frac{K_0}{M_0}\right)\sec h^2\left(\sqrt{\frac{1}{2}K_0}\eta\right). \tag{34}$$

Now since we are interested in quasistationary solutions, a new slow variable $a=f(\tau)$ has been introduced for the description of slow amplitude variation such that $3K_0/M_0=4a^2$, that is, $a=\sqrt{3K_0/4M_0}$. Then from the equation (34), one gets

$$\phi_{0\tau}=\frac{a_\tau}{a}[2u_0+\eta u_{0\eta}]. \tag{35}$$

Under the assumption that equation (33) should be free from secular terms and for solutions quasistationary in nature, we equate the integration results of the right-hand side to zero to yield $a(\tau)=a_0\exp(2/3\tau)$. Now, in order to solve, the equation (33) on being substituted with $y=\tanh(a\eta)$ becomes

$$(1-y^2)\frac{d^2\phi_1}{dy^2}-2y\frac{d\phi_1}{dy}+\left[3(3+1)-\frac{4}{1-y^2}\right]\phi_1=\frac{2}{3}\sqrt{\frac{4M_0}{3K_0}}\frac{1}{1+y}+\frac{2}{3}\sqrt{\frac{4M_0}{3K_0}}\ln\left(\frac{1+y}{1-y}\right). \tag{36}$$

Applying the well-known *method of separation of variables*,[18,19] the solution of the equation (36) as a perturbation over usual soliton can be written as

$$\phi_1(\eta)=-\frac{1}{3}\sqrt{\frac{M_0}{3K_0}}[-1+\tanh\,\eta+2(1-\eta\tanh\,\eta)\sec h^2\eta+\eta(2-\eta\tanh\,\eta)\sec h^2\eta]. \tag{37}$$

Thus the total solution $\phi(\eta)=\phi_0(\eta)+\gamma\phi_1(\eta)+\cdots$ of the equation (6) as a superposition of the leading order solution and the perturbation over it obtained by perturbative technique as discussed above, can be written as

$$\phi(\eta)=3\left(\frac{K_0}{M_0}\right)\sec h^2\left(\sqrt{\frac{1}{2}K_0}\eta\right)-\frac{\gamma}{3}\sqrt{\frac{M_0}{3K_0}}[-1+\tanh\,\eta+2(1-\eta\tanh\,\eta)\sec h^2\eta+\eta(2-\eta\tanh\,\eta)\sec h^2\eta]. \tag{38}$$

The solution (38) can be set into a compact expression as follows:

$$\phi_{PT}(\eta)=a_0\sec h^2\left(\sqrt{\frac{1}{2}K_0}\eta\right)+[A(\eta)\sec h^2(\eta)+b_0(1-\tanh(\eta))], \tag{39}$$

where $a_0=3K_0/M_0$, $A(\eta)=-2b_0\{1+\eta(1-1.5\tanh\,\eta)\}$, $b_0=\gamma/3\sqrt{a_0}$.

It is again obvious from the equation (39), in conformity with the equation (30), that there is a linear superposition of both shock (tanh)-like and soliton (sech^2)-ic solutions over some preexisting dc background formed by the self-interaction of identical spectral components of ion acoustic wave fluctuations in transonic plasma. However, under the no-growth limit ($\gamma=0$), only solitonic structures exist and no shock at all. The analytically derived solutions represented by the equations (30) and (39) both, therefore, physically suffice to exhibit analogous characteristics.

IV. RESULTS AND DISCUSSIONS

Our mathematical calculations clearly demonstrate that the derived *d*-KdV is really analytically integrable. Solving it analytically, a solution as a linear superposition of two distinct modes of nonlinear traveling waves is generated. In mutual isolation, one corresponds to the usual *soliton* solution and the other corresponds to the *shock* solution. Of course, the oscillatory part with sinusoidal or nonsinusoidal peaks as depicted in numerically obtained profiles of the oscillatory shocklike solutions[3] does not appear there in our analytical solution. Furthermore, the depression and amplifications of solitons are feeble. This could be attributed to the limitation of the used mathematical techniques that seems to be blind to these oscillations. These two possible modes of nonlinear traveling ion acoustic wave should be observable in transonic plasma system if one allows the ion acoustic wave to propagate through it.

Required study of magnetohydrodynamic waves and instabilities of both laboratory and space plasmas has been carried out for many years under the assumption of static equilibrium. However, there are many practical situations as mentioned in the introduction where plasma flows are significantly large to violate the condition of static equilibrium. There are several efforts to conduct experiments in transonic and supersonic wind tunnels. Certain experimental facility like high frequency plasmatron is demonstrated to behave as ideal facility for MHD phenomena under real flight conditions of aircraft.

In the moving frame of space vehicles, which carry the payloads for exploring the properties of space plasma environment, background plasmas are always in motion. Its velocity can be approximately taken equal to the velocity of the vehicle itself but in opposite direction. The space

laboratory frame observations of the low frequency range in acoustic domain must have some signature of our results provided that the space vehicle is moving with near sonic or near supersonic speeds. We are not aware of any such particular observations of ion acoustic wave fluctuations in transonic condition of plasma flows.

Most of the plasma devices of industrial applications like dense plasma focus machine, plasma torches, etc., depend on the plasma flows that violate the static equilibrium.[4–6] In fusion plasmas of future generations too, the static approximation of the equilibrium plasma description may not be suitable to describe the wave behavior. In future course of fusion research, rotational motions of fusion plasmas in poloidal and toroidal directions may decide the equilibrium. This is important to state that in toroidal plasmas, the geodesic acoustic mode[20] becomes of fundamental importance in comparison to the ordinary sound modes. This may be more important when these rotational motions are in the defined range of the transonic limit. Simplicity is correlated to the local mode approximation of the acoustic wave description in the transonic limit of uniform and unidirectional plasma flow motion without magnetic field.

There are some indications that the magnetized plasma flow systems may emit nonlinear standing MHD waves. In plasmas only nonlinear wave modes like soliton, shock, etc., in general, can travel for long before suffering major modifications. Transonic plasma zone seems to act as an interesting site for rich varieties of linear and nonlinear ion acoustic wave activities. Like MHD spectroscopy, the coining of the idea of *acoustic spectroscopy*[5] in unmagnetized plasma flow motions may have far reaching impact to study the unique property of the transonic plasmas of laboratory or space productions for basic and applied research. The real key to open the mystery of the sheath edge singularity lies in thorough investigations of wave turbulence physics in transonic boundary layer, which is assumed to have diffuse nature of near quasineutral plasma potential distribution over a finite extension.

One can then speculate that the wave induced diffusion and transport phenomena may have gone into the evolutionary processes of the equilibrium formation of transonic plasma flows, wherever it exists. Logically speaking the residues of participating waves, even if a little, must have left behind a signature of turbulent state of transonic plasma in a self-consistent nonlinear hydrodynamic equilibrium. This can be verified if and only if one can observe and analyze the wide range acoustic spectrum, especially shorter scales, in defined transonic plasma zone. This is the logical basis to put forth our own hypothesis that the transonic plasma equilibrium should, in principle, look like a turbulent plasma medium maintained by anomalous diffusion processes. Here we expect that the collective scale energy exchange processes in between the ion acoustic wave energy and the ion flow energy occur predominantly in an adiabatic manner so that there is no violation of the law of conservation of energy. This, in fact, is the distinctive characteristic of any conservative dynamical system.

The driving source of energy transfers part of its amount to amplify the spectral components of the usual ion acoustic soliton. As a result, the usual global balancing between the nonlinearity and dispersion strength will be disturbed. If the dispersion strength of the source wavelength remains negligibly weaker to compete with soliton dispersion strength, the phase coordination among the spectral components of the soliton remains intact and only amplification or suppression of the soliton amplitude occurs. However, when the source dispersion strength becomes significant, the space-symmetry of the soliton potential distribution breaks down and a new steady state solution of oscillatory shocklike structure is obtained. Adiabatic process is supposed to govern the energy exchange process among different spectral acoustic components.

The nonlinear traveling wave solutions of the d-KdV equation as derived from Hirota's method, sine-cosine method as well as perturbative technique are graphically depicted in Figs. 1 and 2 for the characterization of the ion acoustic wave motion through transonic zone for some typical values[3] of resonance excitation threshold as deviation from sonic point $\delta=1-M_r$ and scale length $k\lambda_{De}$ of source perturbation. The graphical depictions are, however, in partial agreement with the predicted numerical results[3] in terms of average properties.

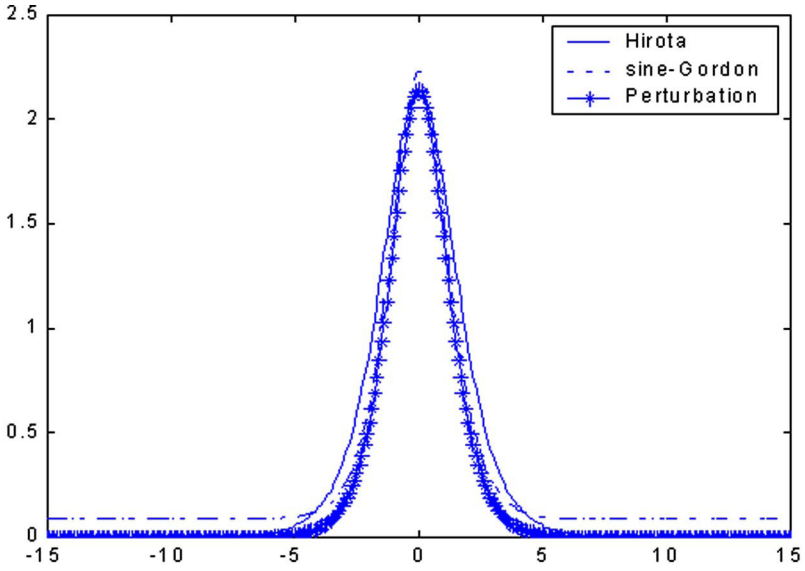

FIG. 1. (Color online) Solitonic symmetric structures obtained by Hirota, sine-Gordon, and perturbative techniques for $\delta=1.5\times10^{-8}$ and $k\lambda_{De}=1.5\times10^{-6}$.

V. CONCLUSIONS

In brief, we conclude that the present mathematical study of *d*-KdV equation offers a significant contribution of analytical supports to our numerical prediction of structural transformation of the traveling nonlinear ion acoustic waves in transonic plasma equilibrium of desired quality. It clearly shows that the actual solution of *d*-KdV equation is a resultant of linear mixing (superposition) of soliton and shock both.

Dominating features of the individual nonlinear modes is decided by an appropriate choice of the specific values of unstable wave number (or wavelength) for a given value of the ion flow Mach number. It is obvious to note that in zero growth limit of *d*-KdV equation, the shock-term disappears and only soliton remains. This limit is correlated with dc range of the chosen unstable wave number of quite weaker dispersion strength. As the dispersion strength becomes significant

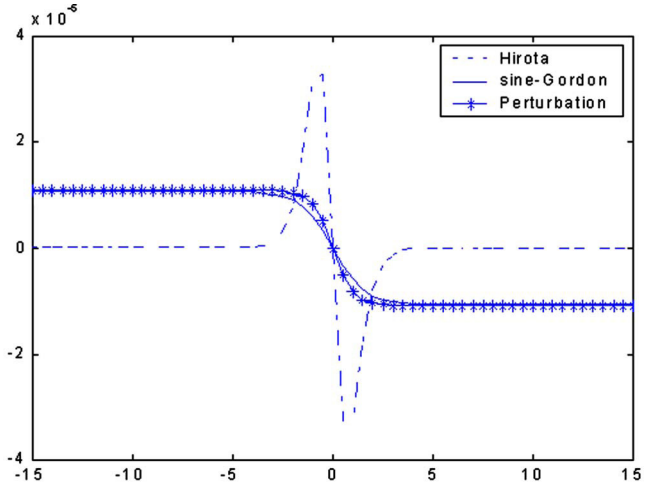

FIG. 2. (Color online) Shocklike asymmetric structures obtained by Hirota, sine-Gordon, and perturbative techniques for $\delta=2.5\times10^{-6}$ and $k\lambda_{De}=1.0\times10^{-4}$.

to influence the original soliton strength of weak nonlinearity and weak dispersion in the defined transonic plasma of finite extension, structural modification of the usual KdV soliton profile occurs.

We further argue that the linear and nonlinear normal mode behaviors of the ion acoustic waves in transonic plasma condition differ qualitatively from those derived for static and dynamic equilibriums without electron inertial correction. The finite but weak hydrodynamic tailoring of the electron fluid motion on ion acoustic space and time scales brings about this difference. It is then argued that the plasma flows in transonic equilibrium should exhibit rich spectrum of linear and nonlinear ion acoustic waves and oscillations. Of course, under Vlasov model the hot electrons with streaming velocity comparable to the phase speed of the ion sound wave may destabilize the ion sound mode through wave-particle resonance effect[21] too. However, our excitation mechanism of ion sound wave differs from the other known mechanisms[22–24] to excite the same ion sound wave on many grounds.[24]

This kind of theoretical scenario of *transonic plasmas* offers a unique scope of *acoustic spectroscopy* to describe the internal state of transonic equilibrium of plasma flows, if it exists at all. These calculations may have potential applications in thorough study of the ion acoustic wave turbulence related with aerodynamics, solar wind, and space plasmas, fusion plasmas of future generation, industrial plasmas, and plasma flows in astrophysical context, etc.

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On Burnett coefficients in periodic media

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The aim of this work is to demonstrate a curious property of general periodic structures. It is well known that the corresponding homogenized matrix is positive definite. We calculate here the next order Burnett coefficients associated with such structures. We prove that these coefficients form a tensor which is negative semidefinite. We also provide some examples showing degeneracy in multidimension. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2179048]

I. INTRODUCTION

The aim of this paper is to demonstrate a curious property of general periodic structures. Let us consider acoustic wave propagation in a periodic medium with a small period denoted by ε. To first order, we can approximate this medium by the associated homogenized medium. It is well known that the acoustic wave propagation in the homogenized medium provides good approximation to the propagation of sufficiently long waves in the original periodic medium (Refs. 1 and 9).

Here, we are interested in higher order approximation. From our previous work,[2] it is known that the homogenized medium is described by the second order derivatives of the first Bloch eigenvalue $\lambda_1(\eta)$ at $\eta=0$ and the next order approximation to the periodic medium is provided by a fourth order tensor, namely the fourth derivatives of $\lambda_1(\eta)$ at $\eta=0$. In the physics literature such higher order derivatives are known as *Burnett coefficients* and they are of great interest (Refs. 14 and 8). It is known that the homogenized matrix is positive definite.[1] This work is devoted to the study of the next order approximation.

The approximation of the periodic medium comes about from the asymptotic expansion of $\lambda_1(\eta)$ near $\eta=0$,

$$\lambda_1(\eta) = \frac{1}{2!}\lambda_1''(0)\,\eta^2 + \frac{1}{4!}\lambda_1^{(4)}(0)\,\eta^4 + \cdots .$$

Substituting $\eta=\varepsilon\xi$, we get the asymptotic expansion of the first eigenvalue associated to the ε-periodic operator A^ε near $\eta=0$,

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$$\lambda_1^\varepsilon(\xi) = \varepsilon^{-2}\lambda_1(\varepsilon\xi) = \frac{1}{2!}\lambda_1''(0)\xi^2 + \frac{1}{4!}\varepsilon^2\lambda_1^{(4)}(0)\xi^4 + \cdots.$$

It is already established that the Hessian matrix $\lambda_1''(0)/2$ coincides with the homogenized matrix denoted by $(q_{k\ell})$ (defined for instance in Ref. 1) and hence is positive definite. In this write-up, we show that

$$\frac{1}{4!}\lambda_1^{(4)}(0)\,\eta^4 \leqslant 0 \quad \forall\ \eta \in \mathbb{R}^N.$$

Further, we show that there can be directions $\eta \neq 0$ such that

$$\frac{1}{4!}\lambda_1^{(4)}(0)\,\eta^4 = 0.$$

However, in one dimension, as we show below, such a degeneracy cannot happen unless the medium is homogeneous.

Before starting our computations, let us interpret the above result in terms of acoustic wave propagation in the original ε-periodic medium. From the above expansion, it is clear that

$$\lambda_1^\varepsilon(\xi) \approx \frac{1}{2!}\lambda_1''(0)\xi^2 \quad \text{if } \varepsilon^2|\xi|^4 \text{ is small.}$$

This shows that the usual homogenized medium, as remarked above, provides a good description provided the waves are long. However, for short waves the above approximation is poor. Indeed if $\varepsilon^2|\xi|^4 = O(1)$ and $\varepsilon^4|\xi|^6 = o(1)$ then we have

$$\lambda_1^\varepsilon(\xi) \approx \frac{1}{2!}\lambda_1''(0)\xi^2 + \frac{1}{4!}\varepsilon^2\lambda_1^{(4)}(0)\xi^4.$$

The above picture shows that long waves experience hyperbolic effects while short waves in question undergo some dispersion too. This dispersive nature medium is described by the fourth order tensor $\lambda_1^{(4)}(0)$. However, the dispersion is not classical. It has a negative sign and we may then call it *negative dispersion*. Strictly speaking, the corresponding initial value problem modeling the propagation of such short waves is not well posed. We would like to bring to the attention of homogenization community that some curious materials (with negative refraction, negative reflection coefficients) are being conceived and produced (see Refs. 5, 10, 11, and 13). Viewed in this light, our result says that a fine periodic structure provides one such curious material as far as short wave propagation is concerned. At this point, we would like to emphasize other features of our result. It came as a surprise to us to see a definite sign for the fourth order derivative, as it was not expected. Though our computations follow a general pattern, it is not clear to us whether higher order derivatives too have a definite sign. The next remark is concerned with the level of generality at which we are working: we have no restriction whatsoever on the original periodic medium except the classical ones. In other words, the material components used in mixing are arbitrary, their proportions are arbitrary and the microgeometry of mixing is also arbitrary. This contrasts sharply with the current efforts in producing curious or smart materials using particular components and following a particular design, for example, photonic crystals (see Refs. 7, 6, and 12).

II. PRELIMINARIES

Let us now introduce the problem to be studied in this work. First, we remark that the summation with respect to the repeated indices is understood throughout this paper. We consider the operator

$$A \overset{\text{def}}{=} -\frac{\partial}{\partial y_k}\left(a_{k\ell}(y)\frac{\partial}{\partial y_\ell}\right), \quad y \in \mathbb{R}^N, \tag{2.1}$$

where the coefficients satisfy

$$\begin{aligned} &a_{k\ell} \in L^\infty_{\#}(Y) \quad \text{where } Y =]0,2\pi[^N, \text{ i.e., each } a_{k\ell} \text{ is a} \\ &Y\text{-periodic bounded measurable function defined on } \mathbb{R}^N, \text{ and} \\ &\exists\, \alpha > 0 \quad \text{such that } a_{k\ell}(y)\eta_k\eta_\ell \geqslant \alpha|\eta|^2 \quad \forall\, \eta \in \mathbb{R}^N, \quad y \in Y \text{ a.e.}, \\ &a_{k\ell} = a_{\ell k} \quad \forall\, k, \ell = 1, \ldots, N. \end{aligned} \tag{2.2}$$

For each $\varepsilon > 0$, we consider also the ε-periodic operator A^ε where

$$A^\varepsilon \overset{\text{def}}{=} -\frac{\partial}{\partial x_k}\left(a^\varepsilon_{k\ell}(x)\frac{\partial}{\partial x_\ell}\right) \quad \text{with } a^\varepsilon_{k\ell}(x) \overset{\text{def}}{=} a_{k\ell}\left(\frac{x}{\varepsilon}\right), \quad x \in \mathbb{R}^N. \tag{2.3}$$

In homogenization theory, it is usual to refer to x and y as the slow and the fast variables, respectively. They are related by $y = x/\varepsilon$.

Our results are based on Bloch waves ψ associated with the operator A which we define now. Let us consider the following spectral problem parametrized by $\eta \in \mathbb{R}^N$: find $\lambda = \lambda(\eta) \in \mathbb{R}$ and $\psi = \psi(y;\eta)$ (not zero) such that

$$\begin{aligned} &A\psi(\cdot;\eta) = \lambda(\eta)\psi(\cdot;\eta) \quad \text{in } \mathbb{R}^N, \quad \psi(\cdot;\eta) \text{ is } (\eta;Y)\text{-periodic, i.e.,} \\ &\psi(y + 2\pi m;\eta) = e^{2\pi i m\cdot\eta}\psi(y;\eta) \quad \forall\, m \in \mathbb{Z}^N, \quad y \in \mathbb{R}^N. \end{aligned} \tag{2.4}$$

Next, by the Floquet theory, we define $\phi(y;\eta) = e^{-iy\cdot\eta}\psi(y;\eta)$ and (2.4) can be rewritten in terms of ϕ as follows:

$$A(\eta)\phi = \lambda\phi \quad \text{in } \mathbb{R}^N, \quad \phi \quad \text{is} \quad Y\text{-periodic}. \tag{2.5}$$

Here, the operator $A(\eta)$ is called the translated operator and is defined by

$$A(\eta) = e^{-iy\cdot\eta}Ae^{iy\cdot\eta}.$$

It is well known (see Refs. 1 and 3) that for each $\eta \in Y' = [-1/2, 1/2[^N$, the above spectral problem (2.5) admits a discrete sequence of eigenvalues and their eigenfunctions (referred to as *Bloch waves*) introduced above enable us to describe the spectral resolution of A [an unbounded self-adjoint operator in $L^2(\mathbb{R}^N)$] in the orthogonal basis $\{e^{iy\cdot\eta}\phi_m(y;\eta)\,|\,m \geqslant 1, \eta \in Y'\}$.

To obtain the spectral resolution of A^ε, let us introduce Bloch waves at the ε-scale,

$$\lambda^\varepsilon_m(\xi) = \varepsilon^{-2}\lambda_m(\eta), \quad \phi^\varepsilon_m(x;\xi) = \phi_m(y;\eta), \quad \psi^\varepsilon_m(x;\xi) = \psi_m(y;\eta),$$

where the variables (x,ξ) and (y,η) are related by $y = x/\varepsilon$ and $\eta = \varepsilon\xi$. Observe that $\phi^\varepsilon_m(x;\xi)$ is εY-periodic (in x) and $\varepsilon^{-1}Y'$ periodic with respect to ξ. In the same manner, $\psi^\varepsilon_m(\cdot;\xi)$ is $(\varepsilon\xi;\varepsilon Y)$ periodic because of the relation $\psi^\varepsilon_m(x;\xi) = e^{ix\cdot\xi}\phi^\varepsilon_m(x;\xi)$. Note that the dual cell at ε-scale is $\varepsilon^{-1}Y'$ and hence we take ξ to vary in $\varepsilon^{-1}Y'$ in the sequel. With these notations, we have (see Ref. 1) the following.

Theorem 2.1: *Let $g \in L^2(\mathbb{R}^N)$. The m*th *Bloch coefficient of g at the ε-scale is defined as follows:*

$$(B^\varepsilon_m g)(\xi) = \int_{\mathbb{R}^N} g(x)e^{-ix\cdot\xi}\overline{\phi}^\varepsilon_m(x;\xi)\mathrm{d}x \quad \forall\, m \geqslant 1, \quad \xi \in \varepsilon^{-1}Y'.$$

Then the following inverse formula and Parseval's identity hold:

$$g(x) = \int_{\varepsilon^{-1}Y'} \sum_{m=1}^{\infty} (B_{m\delta}^{\varepsilon} g)(\xi) e^{ix\cdot\xi} \phi_m^{\varepsilon}(x;\xi) \mathrm{d}\xi,$$

$$\int_{\mathbb{R}^N} |g(x)|^2 \, \mathrm{d}x = \int_{\varepsilon^{-1}Y'} \sum_{m=1}^{\infty} |(B_m^{\varepsilon} g)(\xi)|^2 \, \mathrm{d}\xi.$$

Finally, for all g in the domain of A^{ε}, *we get*

$$A^{\varepsilon} g(x) = \int_{\varepsilon^{-1}Y'} \sum_{m=1}^{\infty} \lambda_m^{\varepsilon}(\xi)(B_{m\delta}^{\varepsilon} g)(\xi) e^{ix\cdot\xi} \phi_m^{\varepsilon}(x;\xi) \mathrm{d}\xi.$$

■

In the homogenization process, one can neglect all the modes for $m \geqslant 2$ (see Refs. 4 and 2). To this end, we consider a sequence of solutions u^{ε} of the equation

$$A^{\varepsilon} u^{\varepsilon} = f \quad \text{in } \mathbb{R}^N. \tag{2.6}$$

We can show that the component of u^{ε} in the higher Bloch modes are not significant. More precisely, let us consider v^{ε} defined by

$$v^{\varepsilon}(x) = \int_{\varepsilon^{-1}Y'} \sum_{m=2}^{\infty} (B_m^{\varepsilon} u^{\varepsilon})(\xi) e^{ix\cdot\xi} \phi_m^{\varepsilon}(x;\xi) \mathrm{d}\xi. \tag{2.7}$$

which is nothing but the projection of u^{ε} corresponding to all higher Bloch modes. Then the following estimates on v^{ε} are derived in Ref. 2.

Proposition 2.2: *Depending on the regularity of the source term f in* (2.6), *we have*

(i) *If* $f \in H^{-1}(\mathbb{R}^N)$: $\|v^{\varepsilon}\|_{L^2(\mathbb{R}^N)} \leqslant c\varepsilon \|f\|_{H^{-1}(\mathbb{R}^N)}$.
(ii) *If* $f \in L^2(\mathbb{R}^N)$: $\|v^{\varepsilon}\|_{L^2(\mathbb{R}^N)} \leqslant c\varepsilon^2 \|f\|_{L^2(\mathbb{R}^N)}$.
(iii) *If* $f \in L^2(\mathbb{R}^N)$: $|v^{\varepsilon}|_{H^1(\mathbb{R}^N)} \leqslant c\varepsilon \|f\|_{L^2(\mathbb{R}^N)}$.
(iv) *If* $f \in H^1(\mathbb{R}^N)$: $\|v^{\varepsilon}\|_{L^2(\mathbb{R}^N)} \leqslant c\varepsilon^3 |f|_{H^1(\mathbb{R}^N)}$.
(v) *If* $f \in H^1(\mathbb{R}^N)$: $|v^{\varepsilon}|_{H^1(\mathbb{R}^N)} \leqslant c\varepsilon^2 |f|_{H^1(\mathbb{R}^N)}$.

Here, we denote by $|\cdot|_{H^1(\mathbb{R}^N)}$ *the seminorm of* $H^1(\mathbb{R}^N)$. ■

The above result is at the basis of neglecting higher order Bloch eigenvalues $\{\lambda_m^{\varepsilon}(\xi)\}_{m\geqslant 2}$ in the context of our discussion in the Introduction.

III. FOURTH ORDER TENSOR $\lambda_1^{(4)}(0)$

In this section, we present the expression for the fourth order tensor $\lambda_1^{(4)}(0)$ and show that it is negative semidefinite. Recall that $\lambda_1(\eta)$ and $\phi_1(\cdot;\eta)$ depend analytically on η in a small neighborhood B_δ of $\eta=0$ (see Ref. 4).

A. Derivatives of the first Bloch eigenvalue and eigenvector

The purpose of this section is to present expressions for derivatives of the first Bloch eigenvalue $\lambda_1(\eta)$ and the first Bloch eigenvector $\phi_1(\cdot;\eta)$ at $\eta=0$ and indicate a systematic method to compute them. For details of these computations, the reader is referred to Ref. 2. Our approach exploits the connection between the Bloch space computation with the multiscale computation.

The derivatives of the first eigenvalue and eigenfunction in $\eta=0$ exist thanks to the regularity property established in Ref. 4. In fact, we know that there exists $\delta>0$ such that the first eigenvalue $\lambda_1(\eta)$ is an analytic function on $B_\delta=\{\eta \,|\, |\eta|<\delta\}$, and there is a choice of the first eigenvector $\phi_1(y;\eta)$ satisfying

$$\eta \to \phi_1(\cdot;\eta) \in H^1_{\#}(Y) \text{ is analytic on } B_\delta, \quad \phi_1(y;0) = |Y|^{-1/2} = \frac{1}{(2\pi)^{N/2}}.$$

Apart from the above result of regularity on the Bloch spectrum, the following proposition was also proved in Ref. 2.

Proposition 3.1: *We have the relations*

$$\lambda_1(0) = 0, \quad D_k\lambda_1(0) = \frac{\partial \lambda_1}{\partial \eta_k}(0) = 0 \quad \forall\, k = 1, \ldots, N,$$

$$\frac{1}{2} D^2_{k\ell}\lambda_1(0) = \frac{1}{2}\frac{\partial^2 \lambda_1}{\partial \eta_k\, \partial\, \eta_\ell}(0) = q_{k\ell} \quad \forall\, k, \ell = 1, \ldots, N,$$

where $q_{k\ell}$ *are the homogenized coefficients defined by*

$$q_{k\ell} = \mathcal{M}_Y\left(a_{k\ell} + a_{km}\frac{\partial \chi_\ell}{\partial y_m}\right) \overset{\text{def}}{=} \frac{1}{|Y|}\int_Y \left(a_{k\ell} + a_{km}\frac{\partial \chi_\ell}{\partial y_m}\right) \mathrm{d}y \quad \forall\, k, \ell = 1, \ldots, N, \tag{3.1}$$

with test function χ_k *defined by the following cell problem*:

$$A\chi_k = \frac{\partial a_{k\ell}}{\partial y_\ell} \quad \text{in } \mathbb{R}^N,$$

$$\chi_k \in H^1_{\#}(Y), \quad \mathcal{M}_Y(\chi_k) = 0. \tag{3.2}$$

Moreover, all odd order derivatives of λ_1 *at* $\eta = 0$ *vanish, i.e.*,

$$D^\beta \lambda_1(0) = 0 \quad \forall\, \beta \in \mathbb{Z}^N_+, \quad |\beta| \text{ odd}.$$

All even order derivatives of λ_1 *at* $\eta = 0$ *can be calculated in a systematic fashion. For instance, the fourth order derivatives have the following expressions: for all* $k, \ell, m, n = 1, \ldots, N$,

$$\begin{aligned}\frac{1}{4!} D^4_{k\ell mn}\lambda_1(0) = {} & \frac{1}{4}\frac{1}{|Y|}\int_Y \{C_n\chi_{k\ell m} + C_k\chi_{\ell mn} + C_\ell\chi_{mnk} + C_m\chi_{nk\ell}\}\mathrm{d}y \\ & - \frac{1}{3!}\frac{1}{|Y|}\int_Y \{(a_{k\ell} - q_{k\ell})\chi_{mn} + (a_{\ell m} - q_{\ell m})\chi_{nk} + (a_{mn} - q_{mn})\chi_{k\ell} \\ & + (a_{nk} - q_{nk})\chi_{\ell m} + (a_{km} - q_{km})\chi_{\ell n} + (a_{\ell n} - q_{\ell n})\chi_{km}\}\mathrm{d}y.\end{aligned}$$

Here, the operator C_k *is defined by*

$$C_k\phi \overset{\text{def}}{=} -a_{kj}(y)\frac{\partial \phi}{\partial y_j} - \frac{\partial}{\partial y_j}(a_{kj}(y)\phi) \tag{3.3}$$

(*is skew-adjoint*, $C^*_k = -C_k$), *and* $\chi_{k\ell}$, $\chi_{k\ell m}$ *are the test functions defined by the following cell problems*:

$$A\chi_{k\ell} = (a_{k\ell} - q_{k\ell}) - \tfrac{1}{2}(C_k\chi_\ell + C_\ell\chi_k) \quad \text{in } \mathbb{R}^N,$$

$$\chi_{k\ell} \in H^1_{\#}(Y), \quad \mathcal{M}_Y(\chi_{k\ell}) = 0, \tag{3.4}$$

$$A\chi_{k\ell m} = \tfrac{1}{3}[(a_{k\ell} - q_{k\ell})\chi_m + (a_{\ell m} - q_{\ell m})\chi_k + (a_{mk} - q_{mk})\chi_\ell]$$

$$- \tfrac{1}{3}[C_k\chi_{\ell m} + C_\ell\chi_{mk} + C_m\chi_{k\ell}] \quad \text{in } \mathbb{R}^N, \tag{3.5}$$

$$\chi_{k\ell m} \in H^1_{\#}(Y), \quad \mathcal{M}_Y(\chi_{k\ell m}) = 0.$$

■

The above expressions are obtained by differentiating the eigenvalue problem,

$$(A(\eta) - \lambda_1(\eta))\phi_1(\cdot\,;\eta) = 0,$$

and using that the branch $\eta \mapsto \phi_1(\cdot\,;\eta)$ can be so chosen that the following conditions are satisfied simultaneously:

$$\eta \in B_\delta \mapsto \phi_1(\cdot\,;\eta) \in H^1_{\#}(Y) \quad \text{is analytic},$$

$$\|\phi_1(\cdot\,;\eta)\|_{L^2(Y)} = 1 \quad \forall\ \eta \in B_\delta,$$

$$\mathrm{Im}\int_Y \phi_1(y;\eta)\mathrm{d}y = 0 \quad \forall\ \eta \in B_\delta.$$

B. $D^4\lambda_1(0)$ is negative semidefinite

First, we denote the fourth derivatives as

$$B_{k\ell mn} = \frac{1}{4!}D^4_{k\ell mn}\lambda_1(0).$$

Thus, by the Proposition 3.1, for any $\eta \in \mathbb{R}^N$ we get

$$\begin{aligned}
B_{k\ell mn}\eta_k\eta_\ell\eta_n\eta_m = {} & \frac{1}{4}\frac{1}{|Y|}\int_Y [(C_n\eta_n)(\chi_{k\ell m}\eta_k\eta_\ell\eta_m) + (C_k\eta_k)(\chi_{\ell mn}\eta_\ell\eta_m\eta_n)]\mathrm{d}y \\
& + \frac{1}{4}\frac{1}{|Y|}\int_Y [(C_\ell\eta_\ell)(\chi_{mnk}\eta_m\eta_n\eta_k) + (C_m\eta_m)(\chi_{nk\ell}\eta_k\eta_\ell\eta_n)]\mathrm{d}y \\
& - \frac{1}{3!}\frac{1}{|Y|}\int_Y [\eta_k\eta_\ell(a_{k\ell} - q_{k\ell})(\chi_{mn}\eta_m\eta_n) + \eta_\ell\eta_m(a_{\ell m} - q_{\ell m})(\chi_{nk}\eta_k\eta_n)]\mathrm{d}y \\
& - \frac{1}{3!}\frac{1}{|Y|}\int_Y [\eta_m\eta_n(a_{mn} - q_{mn})(\chi_{k\ell}\eta_k\eta_\ell) + \eta_k\eta_n(a_{nk} - q_{nk})(\chi_{\ell m}\eta_m\eta_\ell)]\mathrm{d}y \\
& - \frac{1}{3!}\frac{1}{|Y|}\int_Y [\eta_m\eta_k(a_{km} - q_{km})(\chi_{\ell n}\eta_\ell\eta_n) + \eta_\ell\eta_m(a_{\ell n} - q_{\ell n})(\chi_{km}\eta_m\eta_k)]\mathrm{d}y.
\end{aligned}$$

Now, we introduce the following notations:

$$C = \eta_n C_n, \quad \chi^{(1)} = \eta_k\chi_k, \quad \chi^{(2)} = \eta_k\eta_\ell\chi_{k\ell}, \quad \chi^{(3)} = \eta_k\eta_\ell\eta_m\chi_{k\ell m},$$

$$a = \eta_k\eta_m a_{km}, \quad q = \eta_k\eta_m q_{km}. \tag{3.6}$$

Then, by the summation, the above expression is simplified to the following:

$$B_{k\ell mn}\eta_k\eta_\ell\eta_m\eta_n = \frac{1}{|Y|}\int_Y C\chi^{(3)}\,\mathrm{d}y - \frac{1}{|Y|}\int_Y (a-q)\chi^{(2)}\,\mathrm{d}y. \tag{3.7}$$

Since the test function χ_k satisfies the cell problem (3.2), we have by the notations (3.6),

$$A\chi^{(1)} = \eta_k\frac{\partial a_{k\ell}}{\partial y_\ell}. \tag{3.8}$$

Analogously, by the cell problems (3.4) and (3.5), we have the following Y-periodic problems:

$$A\chi^{(2)} = (a-q) - C\chi^{(1)}, \tag{3.9}$$

$$A\chi^{(3)} = (a-q)\chi^{(1)} - C\chi^{(2)}. \tag{3.10}$$

By the notation (3.6), since C_k is defined in (3.3), we get

$$\frac{1}{|Y|}\int_Y C\chi^{(3)}\,\mathrm{d}y = -\frac{1}{|Y|}\int_Y \eta_k a_{k\ell}\frac{\partial\chi^{(3)}}{\partial y_\ell}\mathrm{d}y.$$

Using (3.8) and integrating by parts, we have

$$\frac{1}{|Y|}\int_Y C\chi^{(3)}\,\mathrm{d}y = \frac{1}{|Y|}\int_Y A\chi^{(1)}\chi^{(3)}\,\mathrm{d}y = \frac{1}{|Y|}\int_Y \chi^{(1)}A\chi^{(3)}\,\mathrm{d}y = \frac{1}{|Y|}\int_Y [(a-q)(\chi^{(1)})^2 - \chi^{(1)}C\chi^{(2)}]\mathrm{d}y,$$

by (3.10). Therefore, from (3.7), we obtain

$$B_{k\ell mn}\eta_k\eta_\ell\eta_m\eta_n = \frac{1}{|Y|}\int_Y (a-q)(\chi^{(1)})^2\,\mathrm{d}y - \frac{1}{|Y|}\int_Y \chi^{(1)}C\chi^{(2)}\,\mathrm{d}y - \frac{1}{|Y|}\int_Y (a-q)\chi^{(2)}\,\mathrm{d}y.$$

Again, by definition of C, we have $C^*=-C$ and hence

$$B_{k\ell mn}\eta_k\eta_\ell\eta_m\eta_n = \frac{1}{|Y|}\int_Y (a-q)(\chi^{(1)})^2\,\mathrm{d}y - \frac{1}{|Y|}\int_Y [(a-q) - C\chi^{(1)}]\chi^{(2)}\,\mathrm{d}y.$$

Using now (3.9), we get

$$B_{k\ell mn}\eta_k\eta_\ell\eta_n\eta_m = \frac{1}{|Y|}\int_Y (a-q)(\chi^{(1)})^2\,\mathrm{d}y - \frac{1}{|Y|}\int_Y A\chi^{(2)}\chi^{(2)}\,\mathrm{d}y.$$

Substituting,

$$a-q = A\chi^{(2)} + C\chi^{(1)},$$

we can rewrite the above expression as follows:

$$B_{k\ell mn}\eta_k\eta_\ell\eta_m\eta_n = -\frac{1}{|Y|}\int_Y A\left[\chi^{(2)} - \frac{1}{2}(\chi^{(1)})^2\right]\cdot\left[\chi^{(2)} - \frac{1}{2}(\chi^{(1)})^2\right]\mathrm{d}y + \frac{1}{4}\frac{1}{|Y|}\int_Y A(\chi^{(1)})^2\cdot(\chi^{(1)})^2\,\mathrm{d}y$$
$$+ \frac{1}{|Y|}\int_Y C\chi^{(1)}\cdot(\chi^{(1)})^2\,\mathrm{d}y. \tag{3.11}$$

We show now that the last two terms of the above expression add up to zero. More precisely, we prove

$$\frac{1}{4}\frac{1}{|Y|}\int_Y A(\chi^{(1)})^2\cdot(\chi^{(1)})^2\,dy+\frac{1}{|Y|}\int_Y C\chi^{(1)}\cdot(\chi^{(1)})^2\,dy=0. \tag{3.12}$$

To this end, let us first consider the last term. By definition of C,

$$\int_Y C\chi^{(1)}\cdot(\chi^{(1)})^2\,dy=-2\eta_k\int_Y a_{k\ell}\frac{\partial}{\partial y_\ell}\left(\frac{1}{3}(\chi^{(1)})^3\right)dy-\eta_k\int_Y\frac{\partial a_{k\ell}}{\partial y_\ell}(\chi^{(1)})^3\,dy.$$

Via a simple integration by parts, we obtain

$$\int_Y C\chi^{(1)}\cdot(\chi^{(1)})^2\,dy=-\frac{1}{3}\int_Y A\chi^{(1)}\cdot(\chi^{(1)})^3\,dy. \tag{3.13}$$

On the other hand, regarding the first term in (3.12), we can establish a more general relation,

$$\frac{1}{(p+1)^2}\int_Y A(\chi^{(1)})^{p+1}\cdot(\chi^{(1)})^{p+1}\,dy=\frac{1}{2p+1}\int_Y A\chi^{(1)}\cdot(\chi^{(1)})^{2p+1}\,dy\quad\forall\,p\in\mathbb{N}. \tag{3.14}$$

This proof is simply obtained by writing the expression

$$a_{k\ell}\frac{\partial\chi^{(1)}}{\partial y_\ell}\frac{\partial\chi^{(1)}}{\partial y_k}(\chi^{(1)})^{2p}$$

in two different ways, namely

$$a_{k\ell}\frac{\partial\chi^{(1)}}{\partial y_\ell}\frac{\partial}{\partial y_k}\left(\frac{1}{2p+1}(\chi^{(1)})^{2p+1}\right)\quad\text{and}\quad a_{k\ell}\frac{\partial}{\partial y_\ell}\left(\frac{1}{p+1}(\chi^{(1)})^{p+1}\right)\frac{\partial}{\partial y_k}\left(\frac{1}{p+1}(\chi^{(1)})^{p+1}\right).$$

A simple integration of these expressions leads us to the above relation (3.14). Finally, taking $p=1$ in (3.14) and using (3.13), we get (3.12). Thus, we conclude the proof of the following result.

Proposition 3.2: *The tensor of fourth derivatives of* λ_1 *in* 0 *is negative semidefinite. More precisely, for any* $\eta\in\mathbb{R}^N$, *we get*

$$\frac{1}{4!}D^4_{k\ell mn}\lambda_1(0)\,\eta_k\eta_\ell\eta_m\eta_n=-\frac{1}{|Y|}\int_Y A\left[\chi^{(2)}-\frac{1}{2}(\chi^{(1)})^2\right]\cdot\left[\chi^{(2)}-\frac{1}{2}(\chi^{(1)})^2\right]dy\leqslant 0. \tag{3.15}$$

■

C. One-dimensional case

In this case, we get a more simple formula for the form associated with the fourth order derivatives of λ_1. More exactly, we show that, for any $\eta\in\mathbb{R}$, we have

$$\frac{1}{4!}D^4\lambda_1(0)\,\eta^4=-\frac{q}{2\pi}\int_0^{2\pi}(\chi^{(1)})^2\,dy\leqslant 0. \tag{3.16}$$

Indeed, by (3.7) we know that

$$\frac{1}{4!}D^4\lambda_1(0)\,\eta^4=\frac{1}{2\pi}\int_0^{2\pi}(C\chi^{(3)}-(a-q)\chi^{(2)})dy.$$

Then, we prove (3.16) by showing that

$$\int_0^{2\pi}C\chi^{(3)}\,dy=\int_0^{2\pi}(-q(\chi^{(1)})^2+(a-q)\chi^{(2)})dy. \tag{3.17}$$

To prove the above result, we first establish some formulas where we use one-dimensional nature of the problem. Considering (3.8) and integrating, we get

$$a\frac{\mathrm{d}\chi^{(1)}}{\mathrm{d}y} = (q-a)\,\eta. \tag{3.18}$$

Now, considering (3.9) and integrating, we get

$$a\frac{\mathrm{d}\chi^{(2)}}{\mathrm{d}y} = -a\chi^{(1)}\eta + c,$$

where c is some constant. Dividing the above relation by a and integrating it over Y, we get $c=0$ and then the following relation results:

$$\frac{\mathrm{d}\chi^{(2)}}{\mathrm{d}y} = -\chi^{(1)}\eta. \tag{3.19}$$

Because of the above relations (3.18) and (3.19), there are simplifications in one dimension which can be exploited to establish (3.17). To this end, it is enough to use the equations satisfied by $\chi^{(1)}$ and $\chi^{(3)}$ and integration by parts.

Remark 3.3: An immediate consequence of (3.16) is

$$D^4\lambda_1(0) = 0 \;\Leftrightarrow\; a(y) \quad \textit{is constant}. \tag{3.20}$$

Indeed, if $D^4\lambda_1(0)=0$ *then* $\chi^{(1)}=0$ *and by (3.18), the coefficient* $a(y)$ *is constant.* ■

IV. DEGENERATE CASES

Unfortunately, in several space dimensions (3.20) need not be true. It can happen that the coefficients $\{a_{k\ell}\}$ are not constants and yet

$$D^4_{k\ell mn}\lambda_1(0)\,\eta_k\eta_\ell\eta_m\eta_n = 0 \quad \text{for some } \eta \neq 0. \tag{4.1}$$

In this section, we show some examples of such degenerates cases.

First, we propose to prove two equivalent expressions for (4.1).

Proposition 4.1: Let us pose

$$\beta^{(2)} = \beta^{(2)}_{k\ell}\eta_k\eta_\ell,$$

where the constants $\beta^{(2)}_{k\ell}$ *are defined by*

$$\beta^{(2)}_{k\ell} = \frac{1}{2!}\frac{1}{|Y|}\int_Y \chi_\ell\chi_k\,\mathrm{d}y. \tag{4.2}$$

Then, if there exists $\eta\in\mathbb{R}^N-\{0\}$ *satisfying (4.1), we get*

$$\chi^{(2)} = \tfrac{1}{2}(\chi^{(1)})^2 - \beta^{(2)}. \tag{4.3}$$

Also (4.1), is equivalent to the following Hamilton-Jacobi type equation for $\chi^{(1)}$*:*

$$a - q + 2\eta_k a_{k\ell}\frac{\partial\chi^{(1)}}{\partial y_\ell} + a_{k\ell}\frac{\partial\chi^{(1)}}{\partial y_k}\frac{\partial\chi^{(1)}}{\partial y_\ell} = 0. \tag{4.4}$$

■

Proof: From (3.15) and (4.1), we have immediately that $\chi^{(2)}-\frac{1}{2}(\chi^{(1)})^2=C$, for some constant C. Integrating this relation and using the definition of $\chi^{(1)}$ and $\chi^{(2)}$, we get

$$C|Y| = -\frac{1}{2}\eta_k \eta_\ell \int_Y \chi_k \chi_\ell \, \mathrm{d}y,$$

and by definition (4.2) of $\beta_{k\ell}^{(2)}$, we obtain (4.3).

Applying the operator A on the relation (4.3), we get

$$A\chi^{(2)} = A\left[\tfrac{1}{2}(\chi^{(1)})^2\right].$$

Since $\chi^{(1)}$ and $\chi^{(2)}$ are solutions of (3.8) and (3.9), respectively, we have

$$A\chi^{(2)} = a - q + 2\,\eta_k a_{k\ell} \frac{\partial \chi^{(1)}}{\partial y_\ell} + A\chi^{(1)} \cdot \chi^{(1)}$$

and

$$A\left[\frac{1}{2}(\chi^{(1)})^2\right] = A\chi^{(1)} \cdot \chi^{(1)} - a_{k\ell} \frac{\partial \chi^{(1)}}{\partial y_\ell} \frac{\partial \chi^{(1)}}{\partial y_k}.$$

We subtract the last two expressions and arrive at (4.4). Conversely, we can start from (4.4) and deduce (4.3). This completes the proof. ■

Next, we present some examples of degenerate cases in several space dimensions.

Case of laminates: We place ourselves in two dimensions. Consider the matrix of coefficients $(a_{k\ell}(y))$,

$$\begin{pmatrix} a_{11}(y_1) & 0 \\ 0 & a_{22} \end{pmatrix},$$

with a_{22} being a constant. Taking $\eta=(0,1)$, the following can be easily checked:

$$\chi_2 \equiv 0, \quad \chi^{(1)} \equiv 0, \quad q_{22} = a_{22}, \quad a = q = a_{22}.$$

[Recall that χ_2 is the solution of (3.2)]. Thus, the equation (4.4) and hence the property (4.1) are easily satisfied but $(a_{k\ell}(y))$ is not a constant matrix.

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Real irreducible sesquilinear-quadratic tensor concomitants of complex bivectors

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Irreducible tensor concomitants of an arbitrary complex antisymmetric second rank tensor, or bivector, in a Minkowski space-time are presented. These tensors are quadratic in the complex bivector and invariant under an overall multiplicative phase change of the bivector; in other words, they are sesquilinear-quadratic tensor concomitants of the complex bivector. The tensors are real and irreducible under the full real Lorentz group. Particular consideration is given to when the complex bivector is the electromagnetic field strength tensor (complex description is appropriate for radiation), and it is found that some of these irreducible tensors are novel electromagnetic observables not previously mentioned in the literature. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2173176]

I. INTRODUCTION

Quadratic concomitants of bivectors[12,8] (antisymmetric second rank tensors) are of fundamental importance in physics in general and in electromagnetism in particular. In electromagnetism, see Ref. 4, the electromagnetic field strength can be described by the real bivector

$$F^{\alpha\beta}=\begin{pmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & -B_3 & B_2 \\ E_2 & B_3 & 0 & -B_1 \\ E_3 & -B_2 & B_1 & 0 \end{pmatrix}, \quad \alpha,\beta=0,1,2,3, \tag{1}$$

where (E_1,E_2,E_3) is the electric field and (B_1,B_2,B_3) is the magnetic field (Greek indices run over 0,1,2,3 where 0 is associated with a timelike coordinate and 1,2,3 with spacelike coordinates). $F^{\alpha\beta}$ has the following well-known bilinear concomitants: the two scalars.

$$C_+^{(r)}=\tfrac{1}{4}F^{\mu\nu}F_{\nu\mu}, \tag{2}$$

$$C_-^{(r)}=\tfrac{1}{8}F^{\mu\nu}F^{\alpha\beta}\epsilon_{\nu\mu\alpha\beta}, \tag{3}$$

where $\epsilon^{\alpha\beta\gamma\delta}$ is the Levi-Civita tensor in four dimensions (with $\epsilon^{0123}=-1$), and the second rank tensor

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$$T^{\alpha\beta}_{(r)} = F^{\alpha\mu}F_{\mu}{}^{\beta} - \tfrac{1}{4}C^{(r)}_{+}\eta^{\alpha\beta}, \tag{4}$$

where $\eta^{\alpha\beta}$ is the metric tensor of Minkowski space. $C^{(r)}_{+}$ is the Lagrangian density of the free electromagnetic field, $C^{(r)}_{-}$ is the electromagnetic pseudoscalar, and $T^{\alpha\beta}_{(r)}$ is the electromagnetic energy-momentum density tensor.

However, there are cases when we need to consider bivectors that are complex. For electromagnetic radiation, for instance, it is more convenient to use complex rather than real field quantities. From quantum theory of light it is known that the observables of an electromagnetic field are ultimately constructed from a complex field strength $F^{\alpha\beta}$, see Refs. 2 and 11. Of these observables, the simplest are sesquilinear-quadratic in $F^{\alpha\beta}$, that is, they are functions of the components of $F^{\alpha\beta}\bar{F}^{\gamma\delta}$, where $\bar{F}^{\gamma\delta}$ is the complex conjugate of $F^{\alpha\beta}$, see Ref. 5.

A question that has not yet been addressed fully, however, is which tensor valued observables can be constructed from an arbitrary complex $F^{\alpha\beta}$. At first glance this question seems pointless since one quickly realizes that an infinite number of sesquilinear-quadratic tensor concomitants of $F^{\alpha\beta}$ are possible. However, we will show that all sesquilinear-quadradric tensor concomitants of a complex $F^{\alpha\beta}$ can be constructed from a unique (up to duality transform) set of tensors. This is the set of tensor concomitants that are real irreducible under the full Lorentz group.[10]

The main objective of this paper is therefore to introduce this set of real irreducible tensors which are sesquilinear-quadratic concomitants of an arbitrary complex bivector. Although the results are of particular interest when the complex bivector is the electromagnetic field, we will keep the treatment general so it applies to any complex bivector. In Sec. II we provide the relevant definitions and criteria for the unique sesquilinear-quadratic concomitant which are then presented in Sec. III where we also show that any sesquilinear-quadratic concomitant of a complex bivector can be completely decomposed in terms of these tensors. Finally, we write these tensors explicitly in terms of electric and magnetic 3-vectors and find that some of them have not been previously discussed in the literature.

This work is related to Olofsson[7] which attempts to decompose rank-4 bilinear concomitants of complex bivectors. A paper using a spinor algebra approach, as opposed to the tensor algebra approach used here, is in preparation.[9]

II. CRITERIA FOR THE SESQUILINEAR-QUADRATIC TENSOR CONCOMITANTS

In what follows, we will be concerned with 4-tensors in a complex Minkowski space-time with the real metric tensor $g^{\alpha\beta}=\eta^{\alpha\beta}=\mathrm{diag}(+1,-1,-1,-1)$. Consider an arbitrary (in general not self-dual) complex bivector $F^{\alpha\beta}$. By definition it fulfills

$$F^{\alpha\beta} = -F^{\beta\alpha}, \quad \text{where } F^{\alpha\beta} \in \mathbb{C} \tag{5}$$

for all α,β. We will be interested in the tensor concomitants which are sesquilinear-quadratic in $F^{\alpha\beta}$. These are defined as follows.

Definition: A *sesquilinear-quadratic tensor concomitant* $H^{\mu_1\cdots\mu_m}_{\nu_1\cdots\nu_n}$ of a complex bivector $F^{\alpha\beta}$ is a tensor valued function $H^{\mu_1\cdots\mu_m}_{\nu_1\cdots\nu_n}(F^{\alpha\beta})$ of even rank $m+n$ that scales as $H^{\mu_1\cdots\mu_m}_{\nu_1\cdots\nu_n} \to |\lambda|^2 H^{\mu_1\cdots\mu_m}_{\nu_1\cdots\nu_n}$ under the change $F^{\alpha\beta}\to\lambda F^{\alpha\beta}$ where λ is an arbitrary complex scalar.

In practice, to construct sesquilinear-quadratic concomitants of a complex $F^{\alpha\beta}$, it is necessary to use the complex conjugate of the bivector which we denote $\bar{F}^{\alpha\beta}$ and define as

$$\bar{F}^{\alpha\beta} := \Re\{F^{\alpha\beta}\} - \mathrm{i}\Im\{F^{\alpha\beta}\}, \tag{6}$$

where $\Re\{\cdot\}$ and $\Im\{\cdot\}$ denote the real part and imaginary part, respectively, of its argument.

To be clear then, a sesquilinear-quadratic tensor concomitant of $F^{\alpha\beta}$ is any tensor constructed from the set $\{\bar{F}^{\alpha\beta}F^{\gamma\delta}, \eta^{\alpha\beta}, \epsilon^{\alpha\beta\gamma\delta}\}$, and their related covariant and mixed tensors, using the usual rules and operations of tensor algebra. Some examples of sesquilinear-quadratic tensor concomitants of $F^{\alpha\beta}$ are $\bar{F}_{\alpha\beta}F^{\gamma\mu}\epsilon_{\mu\delta\kappa\nu} - \bar{F}_{\alpha\mu}F^{\gamma\mu}\eta_{\beta\delta}\eta_{\kappa\nu}$ and $3\bar{F}_{\alpha\beta}F_{\mu\nu}\epsilon^{\mu\nu\gamma\delta}$.

We will show that out of the infinite number of possible sesquilinear-quadratic tensor concomitants of a complex bivector, there exists a unique (up to duality transform) finite set from which any sesquilinear-quadratic tensor concomitant can be constructed. The tensors in this set are the real irreducible tensors under the full real Lorentz group, $\mathcal{L}$. By real irreducible tensor under $\mathcal{L}$, we mean that the tensor cannot be written as a sum of tensors which transform independently of each other under a general transformation in $\mathcal{L}$, see Refs. 1 and 10.

Let us now stipulate some explicit criteria that the sesquilinear-quadratic tensor concomitants of a complex bivector should fulfill to be real irreducible under $\mathcal{L}$, and which we have used to find these tensors. Tensors of all ranks should be decomposed into proper tensors and pseudotensors; this because $\mathcal{L}$ includes improper transformations. Tensors of second rank should be traceless, that is, they should vanish when fully contracted with the metric tensor,

$$T_{\mu}{}^{\mu} = 0, \tag{7}$$

and they should be decomposed into symmetric and antisymmetric parts. Tensors of fourth rank should be traceless over all pairs of indices and in addition vanish when contracted over three or four indices of the Levi-Civita tensor; that is, for a fourth rank tensor concomitant $W^{\alpha\beta\gamma\delta}$ to be irreducible it must satisfy all of the following conditions:

$$W_{\mu}{}^{\mu\alpha\beta} = W_{\mu}{}^{\alpha\mu\beta} = W^{\alpha}{}_{\mu}{}^{\mu\beta} = W^{\alpha}{}_{\mu}{}^{\beta\mu} = W^{\alpha\beta}{}_{\mu}{}^{\mu} = W_{\mu}{}^{\alpha\beta\mu} = 0, \tag{8}$$

$$\epsilon_{\mu\nu\alpha\beta} W^{\mu\nu\alpha\beta} = 0, \tag{9}$$

$$\epsilon_{\alpha\mu\nu\gamma} W^{\beta\mu\nu\gamma} = \epsilon_{\alpha\mu\nu\gamma} W^{\mu\beta\nu\gamma} = \epsilon_{\alpha\mu\nu\gamma} W^{\mu\nu\beta\gamma} = \epsilon_{\alpha\mu\nu\gamma} W^{\mu\nu\gamma\beta} = 0. \tag{10}$$

These conditions ensure that a fourth rank tensor cannot be decomposed, for example, as $W^{\alpha\beta\gamma\delta} = X^{\alpha\beta\gamma\delta} + Y^{\alpha\delta}\eta^{\beta\gamma}$ or $W^{\alpha\beta\gamma\delta} = X^{\alpha\beta\gamma\delta} + c\epsilon^{\alpha\beta\gamma\delta}$ or $W^{\alpha\beta\gamma\delta} = X^{\alpha\beta\gamma\delta} + Y^{\alpha}{}_{\mu}\epsilon^{\mu\beta\gamma\delta}$, for some fourth rank tensor $X^{\alpha\beta\gamma\delta}$, second rank tensor $Y^{\alpha\delta}$, and scalar c. Tensors of ranks higher than four need not be considered as they can be constructed from the tensors of rank 0, 2, and 4 through multiplication with $\eta^{\alpha\beta}$ or $\epsilon^{\alpha\beta\gamma\delta}$. Finally, to be real[13] irreducible tensors we require that all the tensors be real (imaginary part is zero) for real representations of $\mathcal{L}$.

In conclusion the tensors in the irreducible tensorial set we wish to introduce must be

(1) Sesquilinear-quadratic concomitants of complex $F^{\alpha\beta}$,
(2) (all ranks) either proper tensors or pseudotensors,
(3) (second rank) symmetric or antisymmetric, and fulfill (7),
(4) (fourth rank) fulfill (8)–(10).

III. THE IRREDUCIBLE TENSORIAL SET

The irreducible tensorial set which fulfills the criteria enumerated in Sec. II are the six tensors

$$\mathcal{H} := \{C_+, C_-, Q^{\alpha\beta}, T^{\alpha\beta}, U^{\alpha\beta}, W^{\alpha\beta\gamma\delta}\} \tag{11}$$

defined as follows. The two scalars are the proper scalar

$$C_+ := (\bar{F}_{\mu\nu} F^{\nu\mu} - {}^*\bar{F}_{\mu\nu}{}^* F^{\nu\mu})/8 \tag{12}$$

and the pseudoscalar

$$C_- := (\bar{F}_{\mu\nu}{}^* F^{\nu\mu} + {}^*\bar{F}_{\mu\nu} F^{\nu\mu})/8, \tag{13}$$

where we have used the dual of $F^{\alpha\beta}$ defined as

$$^{*}F^{\alpha\beta} := \tfrac{1}{2}\epsilon^{\alpha\beta\mu\nu}F_{\mu\nu} = \tfrac{1}{2}\epsilon^{\alpha\beta}{}_{\mu\nu}F^{\mu\nu}. \tag{14}$$

The three second rank tensors are the antisymmetric pseudotensor

$$Q^{\alpha\beta} := \mathrm{i}(\bar{F}^{\alpha}{}_{\mu}F^{\mu\beta} - {}^{*}\bar{F}^{\alpha}{}_{\mu}{}^{*}F^{\mu\beta} - 2C_{+}\eta^{\alpha\beta})/2, \tag{15}$$

the symmetric proper tensor

$$T^{\alpha\beta} := (\bar{F}^{\alpha}{}_{\mu}F^{\mu\beta} + {}^{*}\bar{F}^{\alpha}{}_{\mu}{}^{*}F^{\mu\beta})/2, \tag{16}$$

and the symmetric pseudotensor

$$U^{\alpha\beta} := \mathrm{i}(\bar{F}^{\alpha}{}_{\mu}{}^{*}F^{\mu\beta} - {}^{*}\bar{F}^{\alpha}{}_{\mu}F^{\mu\beta})/2. \tag{17}$$

The fourth rank tensor is the proper tensor

$$W^{\alpha\beta\gamma\delta} := (\bar{F}^{\alpha\beta}F^{\gamma\delta} - {}^{*}\bar{F}^{\alpha\beta *}F^{\gamma\delta})/2 + 2\mathrm{i}Q^{[\alpha[\delta}\eta^{\gamma]\beta]} - \tfrac{2}{3}C_{+}\eta^{\alpha[\delta}\eta^{\gamma]\beta} - \tfrac{1}{3}C_{-}\epsilon^{\alpha\beta\gamma\delta}, \tag{18}$$

where the square brackets denotes antisymmetrization over the enclosed indices, e.g., $T^{\alpha[\delta}g^{\gamma]\beta} = \frac{1}{2}(T^{\alpha\delta}g^{\gamma\beta} - T^{\alpha\gamma}g^{\delta\beta})$, and nested brackets are not operated on by enclosing brackets, e.g., $T^{[\alpha[\delta}g^{\gamma]\beta]} = \frac{1}{4}(T^{\alpha\delta}g^{\gamma\beta} - T^{\alpha\gamma}g^{\delta\beta} - T^{\beta\delta}g^{\gamma\alpha} + T^{\beta\gamma}g^{\delta\alpha})$. It fulfills the symmetries $W^{\alpha\beta\gamma\delta} = -W^{\beta\alpha\gamma\delta} = -W^{\alpha\beta\delta\gamma} = W^{\gamma\delta\alpha\beta}$ and $W^{\alpha[\beta\gamma\delta]} = 0$.

Note that all the tensors in the set are either self-dual or anti-self-dual with respect to the duality transform: $F^{\alpha\beta} \mapsto {}^{*}F^{\alpha\beta}$ and ${}^{*}F^{\alpha\beta} \mapsto -F^{\alpha\beta}$ jointly. Note also that if $F^{\alpha\beta}$ is purely real, then $Q^{\alpha\beta}$ and $U^{\alpha\beta}$ vanish.

The importance of $\mathcal{H}$ is brought out in the following theorem.

Theorem: *Any sesquilinear-quadratic concomitant of a complex antisymmetric 4-tensor $F^{\mu\nu}$ can be completely decomposed in terms of the tensors in the set $\mathcal{H}$.*

Proof: As mentioned previously, any sesquilinear-quadratic tensor concomitant of $F^{\mu\nu}$ can be written exclusively as linear combinations of tensor terms of the form $\bar{F}^{\alpha\beta}F^{\gamma\delta}$ (possibly) multiplied and contracted over any of its indices by the tensors $\eta^{\mu\nu}$ and $\epsilon^{\mu\nu\iota\kappa}$.

Therefore it suffices to show that $\bar{F}^{\alpha\beta}F^{\gamma\delta}$ can be decomposed into the tensors in $\mathcal{H}$. Using straightforward tensor algebra, it is possible to show that

$$\begin{aligned}\bar{F}^{\alpha\beta}F^{\gamma\delta} = {} & T^{[\alpha[\delta}\eta^{\gamma]\beta]} - \tfrac{1}{8}\mathrm{i}(U^{\alpha\mu}\epsilon_{\mu}{}^{\beta\gamma\delta} - U^{\beta\mu}\epsilon_{\mu}{}^{\gamma\delta\alpha} - U^{\gamma\mu}\epsilon_{\mu}{}^{\delta\alpha\beta} + U^{\delta\mu}\epsilon_{\mu}{}^{\alpha\beta\gamma}) + W^{\alpha\beta\gamma\delta} \\ & - 2\mathrm{i}Q^{[\alpha[\delta}\eta^{\gamma]\beta]} + \tfrac{2}{3}C_{+}\eta^{\alpha[\delta}\eta^{\gamma]\beta} + \tfrac{1}{3}C_{-}\epsilon^{\alpha\beta\gamma\delta} + \tfrac{1}{2}\mathrm{i}\epsilon^{\gamma\delta}{}_{\mu\nu}U^{[\alpha[\nu}\eta^{\mu]\beta]} \\ & + \tfrac{1}{16}\epsilon^{\gamma\delta}{}_{\mu\nu}(T^{\alpha\kappa}\epsilon_{\kappa}{}^{\beta\mu\nu} - T^{\beta\kappa}\epsilon_{\kappa}{}^{\mu\nu\alpha} - T^{\mu\kappa}\epsilon_{\kappa}{}^{\nu\alpha\beta} + T^{\nu\kappa}\epsilon_{\kappa}{}^{\alpha\beta\mu}).\end{aligned}$$

It is clear from inspection of this expansion that the sesquilinear-quadratic dependency on F is completely contained in the six irreducible tensors: C_{+}, C_{-}, $Q^{\alpha\beta}$, $T^{\alpha\beta}$, $U^{\alpha\beta}$, and $W^{\alpha\beta\gamma\delta}$. ■

A further check of the above theorem is gained from the dimensionality of the space of sesquilinear-quadratic concomitants of a complex bivector. $F^{\alpha\beta}$ has 12 degrees of freedom counting both real and imaginary parts while $\bar{F}^{\alpha\beta}F^{\gamma\delta}$ has 36 degrees of freedom. The set $\mathcal{H}$ has, respectively, {1, 1, 6, 9, 9, 10} degrees of freedom, which in total gives 36 degrees of freedom. Thus, dimensionally $[\bar{6}]\otimes[6] = [1]\oplus[1]\oplus[6]\oplus[9]\oplus[9]\oplus[10]$, where a sesquilinear-quadratic product on a complex space is assumed on the left-hand side.

The set $\mathcal{H}$ is unique under the conditions enumerated in Sec. II up to a duality transform of either $Q^{\alpha\beta}$ or $W^{\alpha\beta\gamma\delta}$; that is,

$$^{*}Q^{\alpha\beta}, \tag{19}$$

$$^{*}W^{\alpha\beta\gamma\delta} := \tfrac{1}{2}\epsilon^{\alpha\beta}{}_{\mu\nu}W^{\mu\nu\gamma\delta} \tag{20}$$

are alternatives to either $Q^{\alpha\beta}$ or $W^{\alpha\beta\gamma\delta}$, respectively, as elements in the minimal set of real irreducible tensors.

IV. ELECTROMAGNETIC COMPONENTS OF THE IRREDUCIBLE TENSORS AND THEIR ASSOCIATION WITH KNOWN QUANTITIES

It is instructive to write out the components of the irreducible tensorial set, $\mathcal{H}$, in terms of complex electric and magnetic field 3-vectors. Any complex electromagnetic field strength 4-tensor can be written

$$F^{\alpha\beta} = \begin{pmatrix} 0 & -\mathbf{E}^{\mathsf{T}} \\ \mathbf{E} & \mathbf{B}\times \end{pmatrix}, \tag{21}$$

where

$$\mathbf{E} = (E_1, E_2, E_3)^{\mathsf{T}} \in \mathbb{C}^3, \tag{22}$$

$$\mathbf{B} = (B_1, B_2, B_3)^{\mathsf{T}} \in \mathbb{C}^3, \tag{23}$$

are the electric 3-vector and the magnetic 3-vector, respectively. Here T denotes the transpose operator, and the $\mathbf{B}\times := \epsilon_{ijk}B_j$ where ϵ_{ijk} is the Levi-Civita tensor in three dimensions (lower case italic letters $i,j,k=1,2,3$ represent Cartesian components in 3-space).

In terms of the **E** and **B** 3-vectors, the components of the irreducible tensors are as follows: The two scalars are

$$C_+ = (|\mathbf{E}|^2 - |\mathbf{B}|^2)/2, \tag{24}$$

$$C_- = -\Re\{\bar{\mathbf{E}}\cdot\mathbf{B}\}. \tag{25}$$

The three second rank tensors consists of the antisymmetric pseudotensor

$$Q^{00} = 0, \tag{26}$$

$$Q^{i0} = \Im\{\bar{\mathbf{E}}\times\mathbf{B}\}, \tag{27}$$

$$Q^{ij} = \Im\{\bar{\mathbf{E}}\otimes\mathbf{E} - \bar{\mathbf{B}}\otimes\mathbf{B}\} = \frac{\mathrm{i}}{2}(\bar{\mathbf{E}}\times\mathbf{E} - \bar{\mathbf{B}}\times\mathbf{B})\times, \tag{28}$$

$$Q^{ji} = -Q^{ij}, \tag{29}$$

and the symmetric proper tensor

$$T^{00} = (|\mathbf{E}|^2 + |\mathbf{B}|^2)/2, \tag{30}$$

$$T^{i0} = \Re\{\bar{\mathbf{E}}\times\mathbf{B}\}, \tag{31}$$

$$T^{ij} = -\Re\{\bar{\mathbf{E}}\otimes\mathbf{E} + \bar{\mathbf{B}}\otimes\mathbf{B}\} + T^{00}\mathbf{1}_3, \tag{32}$$

$$T^{ji} = T^{ij} \tag{33}$$

and the symmetric pseudotensor

$$U^{00} = \Im\{\bar{\mathbf{E}} \cdot \mathbf{B}\}, \tag{34}$$

$$U^{i0} = \frac{\mathrm{i}}{2}(\bar{\mathbf{E}} \times \mathbf{E} + \bar{\mathbf{B}} \times \mathbf{B}), \tag{35}$$

$$U^{ij} = -\Im\{\bar{\mathbf{E}} \otimes \mathbf{B} - \bar{\mathbf{B}} \otimes \mathbf{E}\} + U^{00}\mathbf{1}_3, \tag{36}$$

$$U^{ji} = U^{ij}, \tag{37}$$

where $\mathbf{1}_3$ is the identity matrix in three dimensions.

As for the last tensor in the set, the fourth rank proper tensor $W^{\alpha\beta\gamma\delta}$, it is more efficient to write its components out using a bivector indexing scheme, see Ref. 3. We will denote a bivector index with upper case italic letters, such as A or B, and let it run through the integers 1 through 6. F^A is used to represent the tensor component $F^{\alpha\beta}$ of an antisymmetric tensor according to the index mapping: $A \leftrightarrow [\alpha\beta]$, where $1 \leftrightarrow [10]$, $2 \leftrightarrow [20]$, $3 \leftrightarrow [30]$, $4 \leftrightarrow [32]$, $5 \leftrightarrow [13]$, $6 \leftrightarrow [21]$. Based on this scheme, the second rank antisymmetric tensor (21) can be written in terms of the 3-vectors $\mathbf{E}$ and $\mathbf{B}$ as

$$F^{\alpha\beta} = \begin{pmatrix} 0 & -\mathbf{E}^{\mathsf{T}} \\ \mathbf{E} & \mathbf{B}\times \end{pmatrix} \leftrightarrow \begin{pmatrix} \mathbf{E} \\ \mathbf{B} \end{pmatrix} = F^A \tag{38}$$

where the six-component vector on the right-hand side, F^A, is known as a sixtor, see Ref. 10. A fourth rank tensor can be written out in terms of its components using two bivector indices: the first and second 4-tensor indices map to the first bivector index, and the third and fourth 4-tensor indices map to the second bivector index. With this scheme we can write down the components of $W^{\alpha\beta\gamma\delta}$ accordingly

$$W^{\alpha\beta\gamma\delta} \leftrightarrow W^{AB} = \frac{1}{2}\begin{pmatrix} \Re\{\bar{\mathbf{E}} \otimes \mathbf{E} - \bar{\mathbf{B}} \otimes \mathbf{B}\} - \frac{2}{3}C_+\mathbf{1}_3 & \Re\{\bar{\mathbf{E}} \otimes \mathbf{B} + \bar{\mathbf{B}} \otimes \mathbf{E}\} - \frac{2}{3}C_-\mathbf{1}_3 \\ \Re\{\bar{\mathbf{E}} \otimes \mathbf{B} + \bar{\mathbf{B}} \otimes \mathbf{E}\} - \frac{2}{3}C_-\mathbf{1}_3 & -\Re\{\bar{\mathbf{E}} \otimes \mathbf{E} - \bar{\mathbf{B}} \otimes \mathbf{B}\} + \frac{2}{3}C_+\mathbf{1}_3 \end{pmatrix}. \tag{39}$$

From the above expressions of the irreducible tensors explicitly in terms of the complex electric and magnetic field components, it is possible to identify some quantities from electromagnetic theory. The tensors C_+, C_-, and $T^{\alpha\beta}$ are sesquilinear-quadratic generalizations of the well-known electromagnetic scalar-invariants and energy-momentum density tensor, respectively. Tensors closely related to $T^{\alpha\beta}$ and $U^{\alpha\beta}$ were introduced by Ref. 5. Also some of the 3-vectors are already known: Q^{i0} in Eq. (27) is the imaginary part of the complex Poynting vector, see Ref. 4, and the 3-vector U^{i0} in Eq. (35) is mentioned in Ref. 6. As far as the authors are aware the rest of the quantities, specifically the 4-tensors $Q^{\alpha\beta}$ and $W^{\alpha\beta\gamma\delta}$, are novel in the theory of electromagnetism.

V. CONCLUSION

We have shown that any sesquilinear-quadratic concomitant of a complex bivector can be completely decomposed into tensors in the set $\mathcal{H}$ as defined in Sec. III and summarized in Table I. The tensors in $\mathcal{H}$ are either proper tensors or pseudotensors and are real irreducible under the full real Lorentz group. This tensorial set is unique up to a duality transform of $Q^{\alpha\beta}$ or $W^{\alpha\beta\gamma\delta}$.

Of the tensors in set $\mathcal{H}$, the electromagnetic quantities related to C_+, C_-, and $T^{\alpha\beta}$ are all sesquilinear-quadratic generalizations of previously known quadratic tensor concomitants of real (electromagnetic) bivector fields; while Kujawski[5] introduced quantities closely related to $T^{\alpha\beta}$ and $U^{\alpha\beta}$. As far as the authors are aware the other tensors, $Q^{\alpha\beta}$ and $W^{\alpha\beta\gamma\delta}$, have not been previously considered in the literature.

TABLE I. Summary of the complete tensorial set $\mathcal{H}$. The + and − signs in column "Proper/Pseudo" correspond to whether the concomitant is a proper tensor or a pseudotensor, respectively. The heading "# comp" stands for "number of independent components." For the second rank the "*A*" and the "*S*" in the "Rank" column denote whether the tensor is antisymmetric or symmetric, respectively. $W^{\alpha\beta\gamma\delta}$ fulfills the same index symmetries as the Weyl tensor.

Concomitant	Rank	Proper/Pseudo	# comp
C_+	0	+	1
C_-	0	−	1
$Q^{\alpha\beta}$	2 (*A*)	−	6
$T^{\alpha\beta}$	2 (*S*)	+	9
$U^{\alpha\beta}$	2 (*S*)	−	9
$W^{\alpha\beta\gamma\delta}$	4	+	10

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[12] By concomitant we mean here a 4-tensor constructed from the bivector, the metric tensor, and the Levi-Civita tensor using the laws of tensor algebra; see Ref. 8. By quadratic concomitant we mean that the concomitant is second order in the bivector, that is, it exclusively contains terms involving the bivector multiplied with itself.
[13] In this paper we choose to study real irreducible tensors as opposed to complex irreducible tensors because they correspond more closely to the well-known quadratic tensors of real bivectors in electromagnetism.

From Stäckel systems to integrable hierarchies of PDE's: Benenti class of separation relations

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We propose a general scheme of constructing of soliton hierarchies from finite dimensional Stäckel systems and related separation relations. In particular, we concentrate on the simplest class of separation relations, called Benenti class, i.e., certain Stäckel systems with quadratic in momenta integrals of motion. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2176908]

I. INTRODUCTION

The theory of integrable nonlinear evolution equations has a long history as a part of many branches of theoretical physics and applied mathematics. Generally it can be divided in two parts: the theory of integrable nonlinear ordinary differential equations (ODE's) and the theory of integrable nonlinear partial differential equations (PDE's). Within the first class of equations (ODE's) we will consider finite dimensional Hamiltonian systems, integrable by the Hamilton-Jacobi method, called *Stäckel systems*, while within the second class (PDE's) we will consider $(1+1)$-dimensional field systems, having infinite hierarchy of commuting symmetries and called further for simplicity *soliton systems*. The solvability by quadratures of some class of finite dimensional systems by the Hamilton-Jacobi method, laid in the 19th century one of the fundaments of analytical mechanics of integrable systems, while the solvability by quadratures of some class of infinite dimensional field systems by the inverse scattering method, laid in the second half of the 20th century, one of the fundaments of the so-called soliton theory.

During the last few decades both theories have been developed very intensively using many common modern mathematical tools like Lax representation, r-matrix theory, multi-Hamiltonian theory, etc. In that time some links between both theories were investigated. It was found (Refs. 1–4, see also references in Ref. 5) that finite dimensional restrictions, invariant with respect to the action of a given soliton system, like stationary flows, restricted flows or constrained flows of Lax representation, are Liouville integrable Hamiltonian systems of Stäckel type. Moreover, analytical solutions of an appropriate finite dimensional systems are closely related to a special class of solutions of related soliton systems, like for example, so-called finite-gap solutions.[6,7]

In the present paper we are interested in passing in the opposite direction—building integrable hierarchies of PDE's from Stäckel systems.[8] In that sense we would like to initiate a unified approach to Stäckel ODE's and soliton PDE's. Our claim is the following: *both a wide class of Stäckel systems and a wide class of soliton systems can be constructed form common fundamental objects known as separation relations (or from separation curves).*

The paper is organized as follows. Section II is devoted to general description of the concept of separation relations. Section III explains the main ideas of relating soliton systems with separation curves that are quadratic in momenta. The idea is to apply to a set of Killing vector fields

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a set of invariants generated by Euler-Lagrange equations associated with appropriately chosen Lagrangian densities. This allows for elimination of some variables in our Killing systems which leads to dispersive soliton hierarchies. Section IV is a brief introduction to what can be called Benenti class of Stäckel systems. In Sec. V we describe the structure of our systems in Viète coordinates. In Sec. VI we explain the details of our elimination procedure which allows, in a systematic way, to construct soliton hierarchies. It is divided into two sections as the elimination procedure differs in case of "positive" and "negative" (see below) separable potentials. Section VII concludes the article with several examples.

II. SEPARATION RELATIONS

Let us consider a $2n$-dimensional manifold M equipped with a Poisson operator Π with some canonical (Darboux) coordinates labelled as $M \ni u=(\mu,\lambda)$, with $\mu=(\mu_1,\ldots,\mu_n)$ and $\lambda=(\lambda_1,\ldots,\lambda_n)$. The following definition introduces the basic object of our considerations.[9]

Definition 1: A set of n relations of the form

$$\varphi_i(\lambda_i,\mu_i,a_1,\ldots,a_n)=0, \quad i=1,\ldots,n, \quad a_i\in\mathbf{R} \tag{1}$$

(each involving only one pair λ_i,μ_i of canonical coordinates) are called separation relations provided that the dependence of φ on a is essential, i.e., that $\det(\partial\varphi_i/\partial a_j)\neq 0$.

The condition in (1) means that we can resolve the equations (1) with respect to a_i obtaining $a_i=H_i(\lambda,\mu)$, $i=1,\ldots,n$. This defines some new functions $H_i(\lambda,\mu)$ that in turn define the following Hamiltonian systems (evolutionary vector fields) on M,

$$u_{t_i}=\Pi\,\mathrm{d}H_i=X_{H_i}, \quad i=1,\ldots,n. \tag{2}$$

If the functions $W_i(\lambda_i,a)$ are solutions of a system of n decoupled ODE's obtained from (1) by substituting $\mu_i=\partial W_i(\lambda_i,a)/\partial\lambda_i$

$$\varphi_i\left(\lambda_i,\mu_i=\frac{\partial W_i(\lambda_i,a)}{\partial\lambda_i},a_1,\ldots,a_n\right)=0, \quad i=1,\ldots,n, \tag{3}$$

then the function $W(\lambda,a)=\sum_{i=1}^n W_i(\lambda_i,a)$ is an additively separable solution of *all* the equations (3) and *simultaneously* it is a solution of all Hamilton-Jacobi equations

$$a_i=H_i\left(\lambda,\mu=\frac{\partial W(\lambda,a)}{\partial\lambda}\right), \quad i=1,\ldots,n \tag{4}$$

related with the Hamiltonians H_i—simply because solving (1) to the form $a_i=H_i(\lambda,\mu)$ is a purely algebraic operation. Assume now that $\det(\partial^2 W/\partial\lambda_i\partial a_j)=\det(\partial^2 W_i/\partial\lambda_i\partial a_j)\neq 0$. Then the Hamiltonians H_i Poisson-commute since the constructed function $W(\lambda,a)$ is a generating function for the canonical transformation $(\lambda,\mu)\to(b,a)$ where

$$b_i=\frac{\partial W(\lambda,\alpha)}{\partial a_i}=t_i+\mathrm{const}_i, \quad i=1,\ldots,n. \tag{5}$$

Equations (5) are implicit solutions of (2) known as the *inversion Jacobi problem.* Thus, starting from a set of n separation relations we can create an n-dimensional separable Liouville system. All systems separable in the sense of Hamilton-Jacobi theory can be obtained in this way.

In an important case, when the functions φ_i in (1) do not depend on the index i, the separation relations (1) can be generated by taking n copies of a curve in λ-μ plane:

$$\varphi(\lambda,\mu,a_1,\ldots,a_n)=0, \quad a_i\in\mathbf{R} \tag{6}$$

called *separation curve*.

Restricting our considerations to a subclass of (1), when all separation relations are affine in $a_i=H_i$ with coefficients being monomials in λ and μ, we obtain

$$\sum_{k=1}^{n} H_k \mu_i^{\alpha_k} \lambda_i^{\beta_k} = \psi_i(\lambda_i, \mu_i), \quad i = 1, \ldots, n, \quad \alpha_k, \beta_k \in \mathbf{N}, \tag{7}$$

where ψ_i are arbitrary smooth functions of two arguments. Equations (7) are called generalized *Stäckel separation relations* and the related dynamic systems, generated by Hamiltonian functions H_i, are called the *Stäckel separable* ones. To recover explicit Stäckel form of Hamiltonians it is sufficient to solve the linear system (7) with respect to H_i. If additionally $\psi_i(\lambda_i, \mu_i) = \psi(\lambda_i, \mu_i)$ then the above separation conditions can be represented by n copies of the following separation curve:

$$\sum_{k=1}^{n} H_k \mu^{\alpha_k} \lambda^{\beta_k} = \psi(\lambda, \mu). \tag{8}$$

The separable systems that were most intensively studied in the last century were one-particle dynamical systems on Riemannian manifolds with flat or constant curvature metrics. All these systems can be obtained by choosing $\alpha_i = 0, \beta_i = n - i$, $i = 1, \ldots, n$ with ψ quadratic in momenta

$$\psi(\lambda, \mu) = \tfrac{1}{2} f(\lambda) \mu^2 + \gamma(\lambda). \tag{9}$$

This case will be considered in the next sections of this paper.

We can now shortly present—by a simple example—the possibility of passing from a separation curve to soliton systems.[10] Let us consider the separation curve (8) with $n = 2, \alpha_1 = \alpha_2 = 0, \beta_1 = 1, \beta_2 = 0$ and with ψ in the form of (9),

$$H_1 \lambda + H_2 = \tfrac{1}{2} \lambda \mu^2 + \lambda^4. \tag{10}$$

The related separation conditions (7) are

$$\begin{aligned} H_1 \lambda_1 + H_2 &= \tfrac{1}{2} \lambda_1 \mu_1^2 + \lambda_1^4, \\ H_1 \lambda_2 + H_2 &= \tfrac{1}{2} \lambda_2 \mu_2^2 + \lambda_2^4. \end{aligned} \tag{11}$$

Solving this linear system with respect to H_1 and H_2 one gets the Liouville integrable system (2) on four-dimensional phase space, written in separation coordinates (λ, μ). The explicit form of Hamiltonians H_i is

$$H_1 = \frac{1}{2} \frac{\lambda_1 \mu_1^2 - \lambda_2 \mu_2^2 + 2\lambda_1^4 - 2\lambda_2^4}{\lambda_1 - \lambda_2}, \quad H_2 = \frac{1}{2} \frac{\lambda_1 \lambda_2 (\mu_1^2 - \mu_2^2 + 2\lambda_1^3 - 2\lambda_2^3)}{\lambda_2 - \lambda_1}.$$

The canonical transformation of the form

$$q_1 = \lambda_1 + \lambda_2, \quad \tfrac{1}{4} q_2^2 = -\lambda_1 \lambda_2,$$

$$p_1 = \frac{\lambda_1 \mu_1}{\lambda_1 - \lambda_2} + \frac{\lambda_2 \mu_2}{\lambda_2 - \lambda_1}, \quad p_2 = \sqrt{-\lambda_1 \lambda_2} \left(\frac{\mu_1}{\lambda_1 - \lambda_2} + \frac{\mu_2}{\lambda_2 - \lambda_1} \right)$$

transforms the system to new coordinates (q, p), with

$$H_1 = \tfrac{1}{2} p_1^2 + \tfrac{1}{2} p_2^2 + q_1^3 + \tfrac{1}{2} q_1 q_2^2, \quad H_2 = \tfrac{1}{2} q_2 p_1 p_2 - \tfrac{1}{2} q_1 p_2^2 + \tfrac{1}{16} q_2^4 + \tfrac{1}{4} q_1^2 q_2^2.$$

The function $H_1(q, p)$ turns out to be the Hamiltonian function of the integrable case of the Henon-Heiles system, while $H_2(q, p)$ is the additional involutive first integral of this system. Let us now denote the evolution parameters t_1 and t_2 of the system by x and t, respectively. Then we obtain

$$q_{1,x} = \frac{\partial H_1}{\partial p_1} = p_1, \quad q_{2,x} = \frac{\partial H_1}{\partial p_2} = p_2,$$

$$q_{1,t} = \frac{\partial H_2}{\partial p_1} = \frac{1}{2} q_2 p_2, \quad q_{2,t} = \frac{\partial H_2}{\partial p_2} = \frac{1}{2} q_2 p_1 - q_1 p_2,$$

from which eliminating p_1 and p_2 we obtain a system of first order PDE's for $q_1(x,t)$ and $q_2(x,t)$,

$$q_{1,t} = \tfrac{1}{2} q_2 q_{2,x} = \tfrac{1}{4}(q_2^2)_x, \quad q_{2,t} = \tfrac{1}{2} q_2 q_{1,x} - q_1 q_{2,x}. \tag{12}$$

Finally, we can eliminate q_2 through

$$q_{1,xx} = p_{1,x} = -\frac{\partial H_1}{\partial q_1} = -3q_1^2 - \frac{1}{2} q_2^2$$

which yields $q_2^2 = -6q_1^2 - 2q_{1,xx}$ and then generate a higher order (in x-derivatives) PDE. The first equation in (12) turns then into the famous KdV soliton system

$$q_{1,t} + \tfrac{1}{2} q_{1,xxx} + 3q_1 q_{1,x} = 0, \tag{13}$$

while the second equation in (12) turns into a differential consequence of the first one. Obviously, just from the presented construction, there is no guarantee that Eq. (13) is integrable. We can only say that $q_1(x,t)$ calculated from the corresponding inversion Jacobi problem is a nontrivial particular solution (one-gap solution) for the field system (13). To prove the integrability of (13) one must construct some related infinite hierarchy of symmetries using some more regular procedure.

III. FROM SEPARATION CURVES TO CONSTRAINED DISPERSIONLESS SYSTEMS

In this paper we will concentrate on a special but important class of separation curves with the function $\psi(\lambda,\mu)$ in (8) being quadratic in momenta μ [more precisely, of the form (9)] and with multipliers of Hamiltonian functions being monomials with respect to λ,

$$H_1 \lambda^{\beta_1} + \cdots + H_n \lambda^{\beta_n} = \tfrac{1}{2} \lambda^m \mu^2 + \lambda^k, \tag{14}$$

where $\beta_1 > \cdots > \beta_{n-1} > \beta_n = 0$, $\beta_i \in \mathbf{N}, m, k \in \mathbf{Z}$ and $n \in \mathbf{N}$. Separable systems from this class describe one-particle dynamics on Riemannian manifolds and belong to classical Stäckel systems. Each class of these systems is labelled by a decreasing sequence $(\beta_1, \ldots, \beta_n)$ while members of a given class are numbered by pairs $(m,k) \in \mathbf{Z}^2$. Taking n copies of the curve (14) with variables (λ,μ) labelled within each copy as (λ_i, μ_i), we obtain a system of n separation relations in the form of n equations linear in the coefficients H_i. Solving it we obtain n functions $H_r^{(m,k)} = H_r^{(m,k)}(\lambda,\mu)$ of the form

$$H_r^{(m,k)} = \tfrac{1}{2} \mu^T K_r G^{(m)} \mu + V_r^{(k)}, \quad r = 1, \ldots, n, \quad m,k \in \mathbf{Z}, \tag{15}$$

where we denote $\lambda = (\lambda_1, \ldots, \lambda_n)^T$ and $\mu = (\mu_1, \ldots, \mu_n)^T$. The functions (15) can be interpreted as n Hamiltonians on the phase space $T^*\mathcal{Q}$ cotangent to a Riemannian manifold $\mathcal{Q}$ equipped with the contravariant metric tensor $G^{(m)}$. These Hamiltonians are in involution with respect to the canonical Poisson bracket on $T^*\mathcal{Q}$. Moreover, they are separable in the sense of Hamilton-Jacobi theory since they by the very definition satisfy Stäckel relations (14). The objects K_r in (15) can be interpreted as (1, 1)-type Killing tensors on $\mathcal{Q}$. The scalar functions $V_r^{(k)}$ are separable potentials. Further, all the metric tensors $G^{(m)}$ and all the Killing tensors K_r are diagonal in λ-variables so that

$$K_r = \operatorname{diag}(v_r^1, \ldots, v_r^n), \tag{16}$$

where v_r^i are eigenvalues of K_r. We will constantly assume that these eigenvalues are single.

The set (15) of n Hamiltonian functions leads to n Hamiltonian systems on $T^*\mathcal{Q}$ of the form

$$\lambda_{t_r} = \frac{\partial H_r^{(k,m)}}{\partial \mu}, \quad \mu_{t_r} = -\frac{\partial H_r^{(k,m)}}{\partial \lambda}, \quad r = 1, \ldots, n. \tag{17}$$

Let us now call the variable t_1 as x; $t_1 \equiv x$. Since all the Hamiltonians $H_r^{(k,m)}$ (for fixed k and m) commute, the equations (17) have a common set of solutions depending on all the evolution parameters t_i

$$\lambda_i = \lambda_i(t_1 = x, t_2, \ldots, t_n), \quad \mu_i = \mu_i(t_1 = x, t_2, \ldots, t_n).$$

We have, due to (17), that

$$\lambda_x \equiv \lambda_{t_1} = \frac{\partial H_1^{(k,m)}}{\partial \mu} = G^{(m)}\mu \quad \text{so that } \mu = g^{(m)}\lambda_x,$$

where the inverse of $G^{(m)}$ (i.e., respective covariant metric tensors) is denoted as $g^{(m)}$. Observe that the above relation does not depend on k. Using this to eliminate μ from the first part of (17) we obtain

$$\lambda_{t_r} = \frac{\partial H_r^{(k,m)}}{\partial \mu} = K_r G^{(m)}\mu,$$

or, according to the above

$$\lambda_{t_r} = K_r \lambda_x \equiv Z_r^n(\lambda, \lambda_x), \quad r = 1, \ldots, n. \tag{18}$$

This is a set of n autonomous systems of n coupled first order PDE's of evolutionary type, with the right-hand sides depending linearly on the derivatives λ_x.[11] More precisely, it is a set of n integrable dispersionless equations, belonging to the class of so-called weakly nonlinear semi-Hamiltonian systems,[12,13] where the variables λ_i are the Riemann invariants for (18). We will call them *Killing dispersionless system* as they are constructed directly from Killing tensors.

We will interpret the right-hand sides of (18) as vector fields on an infinite dimensional manifold $\mathcal{M}$ the points of which are vector functions of x of the form $u = (\lambda_1(x), \ldots, \lambda_n(x))$, where we assume that the functions $\lambda_i(x)$ are either periodic in x or they vanish together with all their derivatives when $x \to \pm\infty$. A vector field X is at a point $u \in \mathcal{M}$ given by an n-tuple of the form $X(u) = (f_1[\lambda], \ldots, f_n[\lambda])$ where $f_i[\lambda] = f_i(\lambda_1, \lambda_{1,x}, \ldots, \lambda_2, \lambda_{2,x}, \ldots, \lambda_n, \lambda_{n,x}, \ldots)$ are differential functions of λ. Similarly, a covector field α on $\mathcal{M}$ is in a point $u = (\lambda_1(x), \ldots, \lambda_n(x))$ given by $\alpha(u) = (g_1[\lambda], \ldots, g_n[\lambda])$. The dual map between $T_u\mathcal{M}$ and $T_u^*\mathcal{M}$ is given by

$$\langle \alpha, X \rangle(u) = \int_x \sum_{i=1}^{n} f_i[\lambda] g_i[\lambda] \mathrm{d}x.$$

Here and below the integration is performed over one period (in case of periodic boundary conditions) or over $\mathbf{R}$ in case of functions vanishing at $\pm\infty$. All functions and expressions are always assumed to be integrable. For any two given vector fields X and Y on $\mathcal{M}$ their commutator is defined in a usual way as $[X, Y] = X'[Y] - Y'[X]$ where $X'[Y]$ denotes the directional derivative of X in the direction of Y.

As was shown in Ref. 14, the vector fields Z_i^n pairwise commute,

$$[Z_i^n, Z_j^n] = 0, \quad i, j = 1, \ldots, n,$$

thus, (18) is a set of n commuting evolutionary dynamic systems (vector fields) on $\mathcal{M}$. We will need the superscript n to indicate the number of components (dimension) of these systems. Below we will introduce invariants on (18) that eventually turn these systems into hierarchies of soliton systems with lower number of fields. This is the main idea of this paper.

We begin by defining the following differential functions (currents, Lagrangians):

$$\mathcal{L}_r^{(n,m,k)} \overset{\text{def}}{=} \tfrac{1}{2}\lambda_x^T g^{(m)} K_r \lambda_x - V_r^{(k)}, \quad r=1,\dots,n. \tag{19}$$

In our further considerations we will especially need the first current $\mathcal{L}_1^{(n,m,k)}$, so we will denote it simply by $\mathcal{L}^{(n,m,k)}$,

$$\mathcal{L}^{(n,m,k)} \overset{\text{def}}{=} \mathcal{L}_1^{(n,m,k)}.$$

This current is a Legendre transform of $H_1^{(n,m,k)}$ (this is not true for $H_r^{(n,m,k)}$ with $r>1$). These differential functions yield the following functionals on $\mathcal{M}$:

$$I_r^{(n,m,k)}(u) \overset{\text{def}}{=} \int_x \mathcal{L}_r^{(n,m,k)}[\lambda]\mathrm{d}x,$$

where, as usual, $u=(\lambda_1(x),\dots,\lambda_n(x))$. We have, of course,

$$\frac{\mathrm{d}I_r^{(n,m,k)}}{\mathrm{d}t_s} = \left\langle \frac{\delta I_r^{(n,m,k)}}{\delta\lambda}, Z_s^n[\lambda] \right\rangle = \langle E(\mathcal{L}_r^{(n,m,k)}), Z_s^n[\lambda]\rangle,$$

where $E=(E_1,\dots,E_n)=(\delta/\delta\lambda_1,\dots,\delta/\delta\lambda_n)$ is the Euler-Lagrange operator on $\mathcal{M}$.

Lemma 2: In the notation as above,

$$\frac{\mathrm{d}I_1^{(n,m,k)}}{\mathrm{d}t_r} = 0, \quad r=1,\dots,n.$$

Proof: It suffices to prove that

$$\sum_{i=1}^n E_i(\mathcal{L}^{(n,m,k)})\lambda_{i,t_r} = \sum_{i=1}^n E_i(\mathcal{L}_r^{(n,m,k)})\lambda_{i,x} \tag{20}$$

since integrating of (20) yields,

$$\frac{\mathrm{d}I_1^{(n,m,k)}}{\mathrm{d}t_r} = \frac{\mathrm{d}I_r^{(n,m,k)}}{\mathrm{d}t_1}, \quad r=1,\dots,n$$

while

$$\frac{\mathrm{d}I_r^{(n,m,k)}}{\mathrm{d}t_1} = \int_x \sum_{i=1}^n E_i(\mathcal{L}_r^{(n,m,k)})\lambda_{i,x}\,\mathrm{d}x = \int_x \frac{d}{\mathrm{d}x}(\mathcal{L}_r^{(n,m,k)})\mathrm{d}x = 0$$

due to the appropriately chosen boundary conditions. The proof of (20) can be found in Appendix A. ■

Corollary 3: Lemma 2, due to theorem of Ref. 15 (see also Ref. 16) implies that the $2n$*-dimensional set* $\mathcal{E}\subset\mathcal{M}$ *defined as*

$$\mathcal{E} = \{u : E_i(\mathcal{L}^{(n,m,k)}) = 0 \text{ for all } i=1,\dots,n\}$$

is Z_r^n*-invariant for all* $r=1,\dots,n$.

Thus, if $u_0\in\mathcal{E}$ then the integral (Fröbenius) n-dimensional submanifold $\mathcal{S}_{u_0}$ of $\mathcal{M}$ spanned by the commuting vector fields Z_r^n and containing u_0 is a subset of $\mathcal{E}$. This means that the solution $\lambda(x,t_r)$ of the rth Killing system in (18) that starts at a point $u_0\in\mathcal{E}$, i.e., initially satisfying the set of Euler-Lagrange equations

$$E_i(\mathcal{L}^{(n,m,k)}) = 0, \quad i = 1, \ldots, n \tag{21}$$

remains in $\mathcal{E}$, i.e., always satisfy (21). This further means that we can use the set of equations (21) to eliminate some of the variables λ_i in (18). Such an operation does not alter (18), but reparametrizes it, leading to fewer equations of higher order, and the dispersion will occur. As we will see below, this operation of elimination of variables from (18) through the use of (21) will lead both to known and new soliton hierarchies in (1+1) dimensions.

IV. BENENTI CLASS OF STÄCKEL SYSTEMS

In the rest of this paper we consider the simplest class of separation curves (14) in the form

$$H_1\lambda^{n-1} + H_2\lambda^{n-2} + \cdots + H_n = \tfrac{1}{2}\lambda^m\mu^2 + \lambda^k \tag{22}$$

($\lambda, \mu \in \mathbf{R}$ for a moment), where $n \in \mathbf{N}$ while $m, k \in \mathbf{Z}$. This object contains a complete information about the so-called Benenti systems.[17–19] Hamiltonian functions calculated from the related system of separation relations take the form (15).[20] Due to a special form of (22) it turns out that the metric tensors $G^{(m)}$ are now

$$G^{(m)} = L^m G^{(0)}, \quad \text{with } G^{(0)} = \operatorname{diag}\left(\frac{1}{\Delta_1}, \ldots, \frac{1}{\Delta_n}\right), \quad m \in \mathbf{Z},$$

where $\Delta_i = \prod_{j\neq i}(\lambda_i - \lambda_j)$ and where $L = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ is a (1, 1)-tensor on $\mathcal{Q}$ (it is a conformal Killing tensor with respect to all the metrics $G^{(m)}$). Moreover, Killing tensors K_r can now be obtained by the following recursion relation:

$$K_{r+1} = LK_r + q_r I, \quad K_1 = I, \quad K_{n+1} = 0, \quad r = 1, \ldots, n, \tag{23}$$

so that indeed they are diagonal (in λ-coordinates) in accordance with (16): $K_r = \operatorname{diag}(v_r^1, \ldots, v_r^n)$. The functions $q_r = q_r(\lambda)$ are coefficients of the characteristic polynomial of the tensor L, i.e., they are defined by

$$\det(\lambda I - L) = \sum_{i=0}^{n} q_i \lambda^{n-i}, \tag{24}$$

so that $q_0 = 1, q_1 = -\Sigma_{i=1}^n \lambda_i, \ldots, q_n = (-1)^n \Pi_{i=1}^n \lambda_i$ (q_i are Viète polynomials in the variables λ). Moreover, the potentials $V_r^{(k)}$ in Hamiltonians (15) can now be obtained from the following recursion relation:[20]

$$V_r^{(k)} = V_{r+1}^{(k-1)} - q_r V_1^{(k-1)}, \quad k \in \mathbf{Z} \tag{25}$$

(with the convention that $V_r^{(k)} \equiv 0$ for $r < 1$ or $r > n$) with the initial condition

$$V_r^{(0)} = \delta_{r,n}, \quad r = 1, \ldots, n. \tag{26}$$

This recursion can be reversed. The inverse recursion is given by

$$V_r^{(k)} = V_{r-1}^{(k+1)} - \frac{q_{r-1}}{q_n} V_n^{(k+1)}, \quad k \in \mathbf{Z}, \quad r = 1, \ldots, n. \tag{27}$$

The first potentials are rather trivial,

$$V_r^{(k)} = \delta_{r,n-k} \quad \text{for } k = 0, 1, \ldots, n-1, \quad V_r^{(n)} = -q_r, \quad V_r^{(-1)} = -\frac{q_{r-1}}{q_n}, \tag{28}$$

but for $r < -1$ or for $r > n$ the potentials become complicated polynomial (for $r > n$) or rational (for $r < -1$) functions of q.

From (25) we get

$$V_n^{(k)} = -q_n V_1^{(k-1)}, \quad k \in \mathbf{Z} \tag{29}$$

and

$$V_r^{(k)} = -q_r V_1^{(k-1)} - q_{r+1} V_1^{(k-2)} - \cdots - q_n V_1^{(k-n+r-1)}, \quad k \in \mathbf{Z} \tag{30}$$

while iteration of (27) leads to

$$V_r^{(k)} = -\frac{1}{q_n}(q_{r-1} V_n^{(k+1)} + \cdots + q_1 V_n^{(k+r-1)} + V_n^{(k+r)}) = q_{r-1} V_1^{(k)} + \cdots + q_1 V_1^{(k+r-2)} + V_1^{(k+r-1)}, \quad k \in \mathbf{Z}. \tag{31}$$

V. KILLING SYSTEMS AND RELATED INVARIANTS FOR THE BENENTI CLASS IN VIÈTE COORDINATES

The functions $q_r(\lambda)$ defined in (24) can serve as a new set of variables on $\mathcal{Q}$ (we will call them Viète coordinates). It turns out that these coordinates [that also reparametrize the infinite-dimensional manifold $\mathcal{M}$ so that $\mathcal{M} \ni u=(q_1(x), \ldots, q_n(x))$ now] are much more convenient for our further purposes. The above considerations, in particular Lemma 2 and the corollary that follows, remain true independently of coordinate system since the Euler-Lagrange equations are invariant with respect to point transformations. In this section we sort out the structure of (18) and (21) for the Benenti class in Viète coordinates as well as we prove many other important relations.

The tensors L, L^{-1}, $G^{(0)}$ and $g^{(0)}=(G^{(0)})^{-1}$ have in Viète coordinates (24) the form

$$L = \begin{pmatrix} -q_1 & 1 & & 0 \\ -q_2 & 0 & \ddots & \\ \vdots & & & 1 \\ -q_n & 0 & \cdots & 0 \end{pmatrix}, \quad L^{-1} = \begin{pmatrix} 0 & \cdots & 0 & -\dfrac{1}{q_n} \\ 1 & 0 & 0 & -\dfrac{q_1}{q_n} \\ & \ddots & 0 & \vdots \\ 0 & & 1 & -\dfrac{q_{n-1}}{q_n} \end{pmatrix}, \tag{32}$$

$$G^{(0)} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & \cdots & \cdots & q_1 \\ 0 & 1 & \cdots & \vdots \\ 1 & q_1 & \cdots & q_{n-1} \end{pmatrix}, \quad g^{(0)} = \begin{pmatrix} V_1^{(2n-2)} & \cdots & -q_1 & 1 \\ \cdots & \cdots & \cdots & 0 \\ -q_1 & 1 & \cdots & \\ 1 & 0 & & 0 \end{pmatrix}, \tag{33}$$

so that $L_j^i = V_i^{(n-j+1)}$ and $g_{ij}^{(0)} = V_1^{(2n-i-j)}$. Moreover, for the Benenti class, the system (18) attains in Viète coordinates (24) the form $q_{t_r} = K_r(q) q_x$ or, explicitly

$$\frac{d}{dt_r} q_j = (q_{j+r-1})_x + \sum_{k=1}^{j-1} (q_k (q_{j+r-k-1})_x - q_{j+r-k-1}(q_k)_x) \equiv (Z_r^n[q])^j, \quad r,j = 1, \ldots, n, \tag{34}$$

where $q_\alpha = 0$ as soon as $\alpha > n$ and $(Z_r^n[q])^j$ denotes the jth component of the vector field $Z_r^n[q]$. One proves (34) by a direct calculation, using (32) and (23). Observe, that the following symmetry relation takes place: $(Z_i^n[q])^j = (Z_j^n[q])^i$, $i,j = 1, \ldots, n$.

We can, in accordance with the above, also define the *infinite Killing hierarchy* for the Benenti class

$$\frac{d}{dt_r}q_j = (q_{j+r-1})_x + \sum_{k=1}^{j-1}(q_k(q_{j+r-k-1})_x - q_{j+r-k-1}(q_k)_x) \equiv (Z_r^\infty[q])^j, \quad r,j = 1, \ldots, \infty \tag{35}$$

that is formally given by the same expression as (34) but where we now do not impose the restriction $q_\alpha = 0$ for $\alpha > n$. By comparing (34) and (35) one sees directly that for the nth Killing vector field $Z_r^n[q]$ from (34) its first $n+1-r$ components coincide with the corresponding components of the infinite vector field $Z_r^\infty[q]$,

$$(Z_r^n[q])^j = (Z_r^\infty[q])^j \quad \text{for } j + r - 1 \leqslant n. \tag{36}$$

Lemma 4: The infinite-component vector fields $Z_r^\infty[q]$ in (35) mutually commute:

$$[Z_i^\infty[q], Z_j^\infty[q]] = 0 \quad \textit{for all } i,j = 1, \ldots \infty.$$

Proof: This can be proved by using $[Z_i^n[q], Z_j^n[q]] = 0$ for all $i,j = 1, \ldots, n$ and (36). Indeed, from (36) and the relation

$$(Z_i^\infty[q])^j = (Z_i^\infty)^j[q_1, \ldots, q_{i+j-1}]$$

one finds that

$$([Z_i^\infty[q], Z_j^\infty[q]])^l = ([Z_i^{3(n-1)}[q], Z_j^{3(n-1)}[q]])^l, \quad i,j,l = 1, \ldots, n$$

for arbitrary $n \in \mathbf{N}$. ■

Let us point out that the infinite Killing hierarchy (35) is exactly the so-called universal hierarchy considered recently in Refs. 21 and 22 from the point of view of Lax representation.

Lemma 5: In Viète coordinates the following relations hold:

(1)

$$\frac{\partial V_1^{(k)}}{\partial q_i} = \frac{\partial V_1^{(k+\alpha)}}{\partial q_{i+\alpha}} \quad \text{for } i = 1, \ldots, n-\alpha, k \in \mathbf{Z}, \tag{37}$$

(2)

$$(L^k)_j^i = V_i^{(n+k-j)}, \quad k \in \mathbf{Z}, \tag{38}$$

(3)

$$g_{ij}^{(m)} = V_1^{(2n-m-i-j)}, \quad m \in \mathbf{Z}. \tag{39}$$

Proof: For relation (37) the proof is inductive with the help of formula (30). For relation (38) the proof is by induction with respect to k. By (32), $L_j^i = V_i^{(n-j+1)}$. By the induction assumption and due to the recursion (25),

$$(L^{k+1})_j^i = \sum_{r=1}^{n} L_r^i (L^k)_j^r = -q_i V_1^{(n+k-j)} + V_{i+1}^{(n+k-j)} = V_i^{(n+k-j+1)},$$

which concludes the inductive step up. Similarly, due to the recursion (27),

$$(L^{k-1})_j^i = \sum_{r=1}^{n} (L^{-1})_r^i (L^k)_j^r = V_{i-1}^{(n+k-j)} - \frac{q_{i-1}}{q_n} V_n^{(n+k-j)} = V_i^{(n+k-j-1)},$$

which concludes the inductive step down. Finally, for relation (39), according to (33), we have $g_{ij}^{(0)} = V_1^{(2n-i-j)}$. By induction

$$g_{ij}^{(m+1)} = \sum_{k=1}^{n} V_1^{(2n-m-i-k)} (L^{-1})_j^k.$$

Thus, due to (32) we have for $j<n$,

$$g_{ij}^{(m+1)} = g_{i,j+1}^{(m)} = V_1^{(2n-m-i-j-1)}$$

while for $j=n$ we have

$$g_{in}^{(m+1)} = -\frac{1}{q_n}(q_{n-1}V_1^{(n-m-i)} + \ldots + q_1 V_1^{(2n-m-2-i)} + V_1^{(2n-m-1-i)}) = -\frac{1}{q_n}V_n^{(n-m-i)} = V_1^{(n-m-i-1)},$$

which follows from (29) and (31). This concludes the inductive step up. The induction down (for $m<0$) is proved in a similar way. ■

The next theorem describes symmetry properties of functions (19). Observe that due to (28) the functions (19) are in the Benenti case geodesic (without the potential part) for $k=0,\ldots,n-1$.

Theorem 6: *For the Lagrangian densities*

$$\mathcal{L}^{n,m,k} = \frac{1}{2}\sum_{i,j=1}^{n} q_{i,x} g_{ij}^{(m)}(q) q_{j,x} - V_1^{(k)} = \frac{1}{2}\sum_{i,j=1}^{n} q_{i,x} V_1^{(2n-m-i-j)} q_{j,x} - V_1^{(k)}$$

the following relations hold:

(1) for $\alpha=1,\ldots,n-1$

$$E_i(\mathcal{L}^{n,m,k}) = E_{i-\alpha}(\mathcal{L}^{n,m+\alpha,k-\alpha}), \quad i=\alpha+1,\ldots,n, \tag{40}$$

that can also be written as

$$E_i(\mathcal{L}^{n,m,k}) = E_{i+\alpha}(\mathcal{L}^{n,m-\alpha,k+\alpha}), \quad i=1,\ldots,n-\alpha. \tag{41}$$

(2)

$$E_l(\mathcal{L}^{n,0,2n+\sigma}) = E_{l+1}(\mathcal{L}^{n+1,0,2n+\sigma+2}), \quad \sigma=1,\ldots,n-1, \quad l=\sigma+1,\ldots,n. \tag{42}$$

(3)

$$E_l(\mathcal{L}^{n,n-\sigma,0}) = E_l(\mathcal{L}^{n+1,n+1-\sigma,0}), \quad \sigma=1,\ldots,n-1, \quad l=1,\ldots,\sigma \tag{43}$$

$$E_{\sigma+l}(\mathcal{L}^{n,n-\sigma,-n})_{|q_j\to q_{j+1}} = E_l(\mathcal{L}^{n+1,n+1-\sigma,-n-1}), \quad l=1,\ldots,n-\sigma, \quad j=1,\ldots,n. \tag{44}$$

The proof of this theorem can be found in Appendix B. As it will be shown in the next section, Theorem 6 guarantees that the form of invariants survives the passage from n-component to $(n+1)$-component Killing system and hence it will be crucial for the construction of soliton hierarchies. The index σ will be related with the number of components of the obtained soliton systems.

VI. ELIMINATION PROCEDURE

Using the results of the preceding section we will now construct in a systematic way soliton hierarchies related to Benenti class of separation relations. These hierarchies will be generated by a procedure of elimination of variables in the set of dispersionless systems (34) with the help of Euler-Lagrange equations (21) (with suitable chosen parameters n, m, and k determining the metric tensor $g^{(m)}$ and the separable potential $V_1^{(k)}$). Actually, we present two separate elimination procedures, one for positive potentials (i.e., with $k>n$) and one for negative potentials (i.e., those with $k<0$), leading to different soliton hierarchies.

As we pointed out, the set $\mathcal{E}\subset\mathcal{M}$ of solutions of Euler-Lagrange equations (21) is invariant with respect to all the vector fields Z_r of Killing systems (18). The same must be true even in Viète coordinates: (21) written in Viète coordinates is also invariant with respect to (34). This means that we can use the set of equations (21) to eliminate some of the variables q_i in (34), since along the solutions of systems from (34) they are all the time mutually related by the relations (21).

A. Elimination for positive potentials

First, let us concentrate on the case with positive (polynomial) separable potentials. Our aim is to produce s ($s\in\mathbf{N}$) commuting σ-component ($\sigma\in\mathbf{N}$) vector fields (evolutionary systems) from (34) and (21). In order to do this we choose n as $n=s+\sigma-1$ and consider the set of systems (34) with this chosen n,

$$q_{t_r}=Z_r^{s+\sigma-1}[q_1,\ldots,q_{s+\sigma-1}],\quad r=1,\ldots,n=s+\sigma-1. \tag{45}$$

Notice that r can reach $r=s+\sigma-1$ but only up to $r=s$ the first σ components of (45) are complete in the sense of the infinite Killing hierarchy (35), i.e., coincide with the corresponding components of this hierarchy [see (36)]. We will now use (21) generated by $\mathcal{L}^{n,0,2n+\sigma}$ in order to perform the elimination. The structure of these equations is described in the lemma below.

Lemma 7: The last $n-\sigma$ invariant equations in (21) for $\mathcal{L}^{n,0,2n+\sigma}$, with $n=s+\sigma-1$ (so that $m=0$ and $k=2n+\sigma=2s+3\sigma-2$) have the form

$$\begin{aligned} w_{\sigma+1}^{(n,\sigma)}&\equiv -2q_n+\varphi_{\sigma+1}^{(n,\sigma)}[q_1,\ldots,q_{n-1}]=0,\\ &\cdots,\\ w_n^{(n,\sigma)}&\equiv -2q_{\sigma+1}+\varphi_n^{(n,\sigma)}[q_1,\ldots,q_\sigma]=0, \end{aligned} \tag{46}$$

where we denoted, to shorten the notation, $E_i(\mathcal{L}^{n,0,2n+\sigma})$ as $w_i^{(n,\sigma)}$.

Proof: From the recursion (25) it follows that

$$V_1^{(n+j)}=V_1^{(n+j)}(q_1,\ldots,q_{j+1}),\quad j=0,\ldots,n-1 \tag{47}$$

so that, again by (37) and (30),

$$\frac{\partial V_1^{(2n+\sigma)}}{\partial q_{n+1-j+\sigma}}=\frac{\partial V_1^{(n+j)}}{\partial q_1}=2q_j+f_j(q_1,\ldots,q_{j-1}),\quad j=2,\ldots,n,\quad \sigma=1,\ldots,n-1 \tag{48}$$

(for $j=1$ we would have $f_1\equiv 0$) where the first equality follows by inserting $i=1$, $k=n+j$ and $\alpha=n-j+\sigma$ in (37) and the second one from the fact that according to (28) and (30) $V_1^{(n+j)}=-q_{j+1}+2q_1q_j+\varphi_j(q_1,\ldots,q_{j-1})$ for $j=2,\ldots,n$. On the other hand, for the geodesic Lagrangian density

$$\mathcal{L}^{n,0,0}=\frac{1}{2}\sum_{i,j=1}^{n}V_1^{(2n-i-j)}q_{i,x}q_{j,x}$$

from (B2), as $V_1^{(k)}\neq 0$ for $k\geqslant n-1$ and $\partial V_1^{(k)}/\partial q_1\neq 0$ for $k\geqslant n$, we find that

$$E_l(\mathcal{L}^{n,0,0})=F_l[q_1,\ldots,q_{n-l+1}],\quad l=1,\ldots,n.$$

Since $\mathcal{L}_1^{n,0,2n+\sigma}=\mathcal{L}_1^{n,0,0}-V_1^{(2n+\sigma)}$, we obtain [setting $j=n+1-i+\sigma$ in (48)]

$$E_i(\mathcal{L}^{n,0,2n+\sigma})=-2q_{\sigma+n-i+1}+\varphi_i^{(n,\sigma)}[q_1,\ldots,q_{\sigma+n-i}],\quad i=1,\ldots,n,$$

(where as usual we denote $q_\alpha=0$ for $\alpha>n$) where

$$\varphi_i^{(n,\sigma)}[q_1,\ldots,q_{\sigma+n-i}] = F_i[q_1,\ldots,q_{n-i+1}] + f_{\sigma+n-i+1}(q_1,\ldots,q_{\sigma+n-i}).$$

■

Due to their structure, Eqs. (46) make it possible to successively express (eliminate) the variables $q_{\sigma+1},\ldots,q_{s+\sigma-1}\equiv q_n$ as differential functions of $q_1,\ldots,q_\sigma$,

$$\begin{aligned} q_{\sigma+1} &= f^n_{\sigma+1}[q_1,\ldots,q_\sigma],\\ q_{\sigma+2} &= f^n_{\sigma+2}[q_1,\ldots,q_\sigma],\\ &\cdots,\\ q_n &= f^n_n[q_1,\ldots,q_\sigma]. \end{aligned} \tag{49}$$

Let us first observe that performing the elimination (49) in the systems (45) must lead to σ-component systems of the form $\bar{q}_{t_r}=\bar{Z}^\sigma_r[q_1,\ldots,q_\sigma]$, while for each system in (45) the last $s-1$ components turn into some system of differential consequences of $w_1^{(n,\sigma)},\ldots,w_\sigma^{(n,\sigma)}$ (and are zero on $\mathcal{S}_{u_0}$, i.e., they are satisfied along any solutions of $\bar{q}_{t_r}=\bar{Z}^\sigma_r$). Therefore, after this elimination we obtain

$$\begin{aligned} \bar{q}_{t_r} &= \bar{Z}^\sigma_r[q_1,\ldots,q_\sigma], \quad r=1,\ldots,n,\\ 0 &= \varphi^i_r[w_1,\ldots,w_\sigma], \quad i=\sigma+1,\ldots,n, \end{aligned} \tag{50}$$

with $\bar{q}=(q_1,\ldots,q_\sigma)^T$ and $\varphi^i_r\equiv q_{i,t_r}-(Z^n_r)^i$.

Lemma 8: The first s vector fields $\bar{Z}^\sigma_r$ in (50) commute:

$$[\bar{Z}^\sigma_i,\bar{Z}^\sigma_j]=0, \quad i,j=1,\ldots,s.$$

Proof: Obviously, in general, for $i,j=1,\ldots,n$,

$$[\bar{Z}^\sigma_i,\bar{Z}^\sigma_j] = V_{ij}[w_1^{(n,\sigma)},\ldots,w_\sigma^{(n,\sigma)}]$$

for some vector fields V_{ij} that vanish on $\mathcal{E}\subset\mathcal{M}$ only. Assume for a moment that for $n=s+\sigma-1$ and for some $i,j\leqslant s$ we have $V_{ij}[w_1^{(n,\sigma)},\ldots,w_\sigma^{(n,\sigma)}]\neq 0$. As the vector fields $\bar{Z}^\sigma_i,\bar{Z}^\sigma_j$ were obtained by the reduction of the complete (in the sense of the infinite hierarchy) components of Z^n_i,Z^n_j, thus by increasing $n\to n+\beta$, we do not change the form of V_{ij}, which now must be expressed by a higher dimension invariants $w_j^{(n+\beta,\sigma)}$: $V_{ij}=V_{ij}[w_1^{(n+\beta,\sigma)},\ldots,w_\sigma^{(n+\beta,\sigma)}]$. But $w_j^{(n+\beta,\sigma)}=w_j^{(n+\beta,\sigma)}[q_1,\ldots,q_{n+\beta}]$ and lower dimensional invariants $w_j^{(n,\sigma)}$ are nonexpressible by the higher dimensional invariants $w_i^{(n+\beta,\sigma)}$, so we get a contradiction. ■

We will now show that this procedure leads in fact to an infinite hierarchy of commuting flows. In order to do this, we will for a moment introduce a new index so that the vector fields in (50) will be denoted $\bar{Z}^{n,\sigma}_r$ as being obtained by reducing the n-component Killing systems (45).

Lemma 9: In the above notation

$$\bar{Z}^{n+1,\sigma}_r = \bar{Z}^{n,\sigma}_r \quad \text{for } r=1,\ldots,s.$$

Proof: According to (42) we have

$$w^{(n+1,\sigma)}_{\sigma+i+1} = w^{(n,\sigma)}_{\sigma+i} \quad \text{for } i=1,\ldots,n-\sigma.$$

Thus, increasing s to $s+1$ and keeping σ unaltered (so that n changes to $n+1$) the $n-\sigma$ equations (49) change to $n-\sigma+1$ equations

$$q_{\sigma+i} = f^{n+1}_{\sigma+i}[q_1, \ldots, q_\sigma] = f^{n}_{\sigma+i}[q_1, \ldots, q_\sigma], \quad i = 1, \ldots, n-\sigma,$$

$$q_{n+1} = f^{n+1}_{n+1}[q_1, \ldots, q_\sigma],$$

so that the variables $q_{\sigma+1}, \ldots, q_n$ are expressed by the same functions of $q_1, \ldots, q_\sigma$ and a new elimination equation for q_{n+1} appears. Moreover, $(Z^{n+1}_r[q])^j = (Z^n_r[q])^j$ for $j = 1, \ldots, \sigma$ and $r = 1, \ldots, s$. Thus, replacing $q_{\sigma+i}$ by $f^n_{\sigma+i}[q_1, \ldots, q_\sigma]$ in $(Z^{n+1}_r[q])^j$ and in $(Z^n_r[q])^j$ yields for $j = 1, \ldots, \sigma$ and $r = 1, \ldots, s$ the same expression. But the first operation leads to the reduced vector field $\bar{Z}^{n+1,\sigma}_r$ while the second to $\bar{Z}^{n,\sigma}_r$. ■

Let us now take $s+1$ instead of s (so that $n \to n+1$) in (45) and (49) and perform the reduction. According to the above lemma we obtain the following sequence of $s+1$ reduced systems:

$$\bar{q}_{t_r} = \bar{Z}^{n+1,\sigma}_r = \bar{Z}^{n,\sigma}_r \quad \text{for } r = 1, \ldots, s \text{ and } \bar{q}_{t_{n+1}} = \bar{Z}^{n+1,\sigma}_{n+1},$$

i.e., we obtain the same sequence of s systems as before plus an additional system at the end of the sequence. Therefore, we see that this procedure leads to infinite hierarchies of commuting systems, since we can always increase n as much as we please without altering the already obtained systems generated in previous steps.

The procedure described above can be generalized by using only some part of the equations in (46) in order to perform the elimination, since all of these equations are invariant along the flows of our Killing systems. Namely, we can skip the last α (with $0 \leqslant \alpha \leqslant n-\sigma-1 = s-2$) equations in (46) and use only the remaining equations (i.e., $w^{(n,\sigma)}_{\sigma+1} = 0, w^{(n,\sigma)}_{\sigma+2} = 0, \ldots, w^{(n,\sigma)}_{n-\alpha} = 0$) to eliminate $q_{\sigma+\alpha+1}, \ldots, q_n$ in the Killing systems with $n = s+\sigma+\alpha-1$,

$$q_{t_r} = Z^{s+\sigma+\alpha-1}_r[q_1, \ldots, q_{s+\sigma+\alpha-1}], \quad r = 1, \ldots, n = s+\sigma+\alpha-1. \tag{51}$$

Thus, the index α indicates how many of the last equations in (46) we "forget" about. It turns out that the elimination that follows leads also to hierarchies of commuting equations. To see that, let us first observe, that this elimination can formally be obtained by performing the above described procedure with the help of the Lagrangian density $\mathcal{L}^{n,-\alpha,2n+\sigma+\alpha}$, since according to Theorem 6 we have

$$E_i(\mathcal{L}^{n,-\alpha,2n+\sigma+\alpha}) = E_{i-\alpha}(\mathcal{L}^{n,0,2n+\sigma}) \equiv w^{(n,\sigma)}_{i-\alpha} \quad \text{for } i = \alpha+1, \ldots, n. \tag{52}$$

Denoting $E_i(\mathcal{L}^{n,m,2n+k})$ as $w^{(n,m,k)}_i$, where now $w^{(n,0,k)}_i \equiv w^{(n,k)}_i$ [in the notation of (46)], the last $n-\sigma-\alpha$ Euler-Lagrange equations (invariants), associated with $\mathcal{L}^{n,-\alpha,2n+\sigma+\alpha}_1$, have therefore the form

$$\begin{gathered} w^{(n,-\alpha,\sigma+\alpha)}_{\sigma+\alpha} = w^{(n,\sigma)}_{\sigma} = w^{(n,\sigma)}_{\sigma}[q_1, \ldots, q_n] = 0, \\ w^{(n,-\alpha,\sigma+\alpha)}_{\sigma+1+\alpha} = w^{(n,\sigma)}_{\sigma+1} = -2q_n + \varphi^{(n,\sigma)}_{\sigma+1}[q_1, \ldots, q_{n-1}] = 0, \\ \cdots, \\ w^{(n,-\alpha,\sigma+\alpha)}_{n} = w^{(n,\sigma)}_{n-\alpha} = -2q_{\sigma+\alpha+1} + \varphi^{(n,\sigma)}_{n-\alpha}[q_1, \ldots, q_{\sigma+\alpha}] = 0. \end{gathered} \tag{53}$$

These equations make it possible to successively express (eliminate) the variables $q_{\sigma+\alpha+1}, \ldots, q_n$ as differential functions of $q_1, \ldots, q_{\sigma+\alpha}$, which yields

$$q_{\sigma+\alpha+1} = q_{\sigma+\alpha+1}[q_1, \dots, q_{\sigma+\alpha}],$$

$$\cdots, \tag{54}$$

$$q_n = q_n[q_1, \dots, q_{\sigma+\alpha}].$$

Therefore, after this elimination the Killing equations (51) take the form

$$\begin{gathered} \bar{q}_{t_r} = \bar{Z}_r^{\sigma+\alpha}[\bar{q}], \\ 0 = \varphi_r^i[w_1^{(n,-\alpha,\sigma+\alpha)}, \dots, w_{\sigma+\alpha}^{(n,-\alpha,\sigma+\alpha)}], \quad i = \sigma+\alpha+1, \dots, n \end{gathered} \tag{55}$$

for $r=1,\dots,n=s+\sigma+\alpha-1$ and with $\bar{q}=(q_1,\dots,q_{\sigma+\alpha})^T$ and $\varphi_r^i \equiv q_{i,t_r} - (Z_r^n)^i$ (so that the reduced systems will have $N=\sigma+\alpha$ components). Similarly as before, in Killing equations (51), only up to $r=s$ the first $\sigma+\alpha$ components are complete in the sense of the infinite Killing hierarchy (35). As before, it stems from the fact that the first s vector fields $\bar{Z}_r^{\sigma+\alpha}$ commute to zero,

$$[\bar{Z}_i^{\sigma+\alpha}, \bar{Z}_j^{\sigma+\alpha}] = 0, \quad i,j = 1, \dots, s,$$

the proof of which is analogous as in the case $\alpha=0$ but now we must take $n=s+\sigma+\alpha-1$. As previously, we can repeat the elimination procedure taking $s+1$ instead of s [so that n increases to $n+1$ and $k=2n+\sigma+\alpha$ increases to $2(n+1)+\sigma+\alpha=k+2$ while σ and α are kept unaltered]. By the same argument as before, this new procedure (with $n+1$ instead of n) will lead to a sequence of $s+1$ autonomous $(\sigma+\alpha)$-component systems in which the first s systems will coincide with the corresponding systems obtained from the original procedure (with n). Thus, again we will obtain infinite hierarchies of soliton systems.

B. Elimination for negative potentials

We now present the second possibility of elimination—with the use of negative (rational) separable potentials. Again, our aim is to produce s ($s \in \mathbf{N}$) commuting σ-component ($\sigma \in \mathbf{N}$) vector fields (evolutionary systems) from (34) and (21). This time however we have to choose $n=s+2\sigma-1$ and the Lagrangian density $\mathcal{L}^{n,n-\sigma,-n}$ in order to create an infinite hierarchy of commuting flows.

Lemma 10: The first $n-\sigma$ invariant equations (21) with $\mathcal{L}^{n,n-\sigma,-n}$, i.e., with $m=n-\sigma$ and $k=-n$, have the form

$$\begin{gathered} v_1^{(n,\sigma)} \equiv -\frac{1}{q_n^2} + \gamma_1^{(n,\sigma)}[q_1, \dots, q_\sigma] = 0, \\ v_i^{(n,\sigma)} \equiv \frac{2q_{n-i+1}}{q_n^3} + \gamma_i^{(n,\sigma)}[q_1, \dots, q_{\sigma-i+1}, q_{n-i+2}, \dots, q_n] = 0, \quad i = 2, \dots, n-\sigma, \end{gathered} \tag{56}$$

where we denote, to shorten the notation, $E_i(\mathcal{L}^{n,n-\sigma,-n})$ as $v_i^{(n,\sigma)}$ and $q_\alpha=0$ when $\alpha<1$.

Proof: From the recursion (27) it follows that

$$V_1^{(-j)} = V_1^{(-j)}(q_{n-j+1}, \dots, q_n), \quad j = 1 \dots, n. \tag{57}$$

From this and from (B5), (47), and (B7), we have

$$E_i(\mathcal{L}^{n,n-\sigma,0}) = G_i[q_1, \ldots, q_{\sigma-i+1}], \quad i = 1, \ldots, \sigma,$$
$$E_i(\mathcal{L}^{n,n-\sigma,0}) = G_i[q_{n-i+1+\sigma}, \ldots, q_n], \quad i = \sigma+1, \ldots, n-\sigma. \tag{58}$$

Moreover, by using Lemma 5 we find

$$\frac{\partial V_1^{(-n+1-i)}}{\partial q_1} = -\frac{2q_{n-i+1}}{q_n^3} + g_i(q_{n-i+2}, \ldots, q_n), \quad i = 2, \ldots, n-\sigma$$

and

$$\frac{\partial V_1^{(-n+\sigma)}}{\partial q_{\sigma+1}} = \frac{\partial V_1^{(-n)}}{\partial q_1} = \frac{1}{q_n^2}.$$

Plugging all this into $E_i(\mathcal{L}^{n,n-\sigma,-n}), i=1,\ldots,n-\sigma$, we obtain (56) where $\gamma_i^{(n,\sigma)}[q]=G_i[q]-g_i(q)$. ■

Let us now consider the following Killing systems:

$$q_{t_r} = Z_r^n[q], \quad r = \sigma+1, \ldots, \sigma+s, \quad \text{with } n = s+2\sigma-1. \tag{59}$$

We can use the $n-\sigma$ equations (56) to successively express (eliminate) the variables $q_{\sigma+1}, \ldots, q_n$ as differential functions of $q_1, \ldots, q_\sigma$. This leads to the elimination relations of the form

$$q_{\sigma+i} = f_{\sigma+i}^n[q_1, \ldots, q_\sigma], \quad i = 1, \ldots, n-\sigma. \tag{60}$$

Performing the elimination (60) in (59) we obtain an autonomous sequence of s evolution equations

$$\bar{q}_{t_r} = \bar{Z}_r^\sigma[q_1, \ldots, q_\sigma], \quad r = \sigma+1, \ldots, \sigma+s \tag{61}$$

such that the vector fields $\bar{Z}_r^\sigma$ mutually commute to zero. One proves this by the same arguments as in the positive case, since the first σ components of all the vector fields in (59) are complete in the sense of infinite hierarchy (35).

Analogously to the positive case, we will now show that this procedure leads to an infinite hierarchy. As in the positive case, we will for a moment introduce a new index so that the vector fields in (61) will be denoted $\bar{Z}_r^{n,\sigma}$ as being obtained by reducing the n-component Killing systems (59).

Lemma 11: In the notation as above

$$\bar{Z}_{r+1}^{n+1,\sigma} = \bar{Z}_r^{n,\sigma} \quad \textit{for } r = \sigma+1, \ldots, \sigma+s.$$

Proof: Let us observe that, according to results (41), (43), (44), and (B9),

$$v_i^{(n+1,\sigma)} = v_i^{(n,\sigma)}\big|_{q_j \to q_{j+1}, j=n-i+1,\ldots,n} \quad \text{for } i = 1, \ldots, n-\sigma. \tag{62}$$

Thus, increasing s to $s+1$ and keeping σ unaltered (so that n changes to $n+1$) the $n-\sigma$ equations (60) change to $n-\sigma+1$ equations

$$q_{\sigma+1} = f_{\sigma+1}^{n+1}[q_1, \ldots, q_\sigma], \quad q_{\sigma+i+1} = f_{\sigma+i+1}^{n+1}[q_1, \ldots, q_\sigma] = f_{\sigma+i}^n[q_1, \ldots, q_\sigma], \quad i = 1, \ldots, n-\sigma. \tag{63}$$

Observe that the last $n-\sigma$ equations (60) express now $q_{\sigma+i+1}$ (instead of $q_{\sigma+i}$) as $f_{\sigma+i}^n[q_1, \ldots, q_\sigma]$. On the other hand, due to (34), by changing $q_i \to q_{i+1}$ for all $i > \sigma$ in the sequence $q_{t_r} = Z_r^{n+1}[q]$ we transform it so that $(Z_r^{n+1}[q])^j \to (Z_{r+1}^{n+1}[q])^j$ for $j = 1, \ldots, \sigma$ and $r = \sigma+1, \ldots, \sigma+s$. Thus, inserting

$f^n_{\sigma+i}[q_1,\dots,q_\sigma]$ instead of $q_{\sigma+i+1}$ in $(Z^{n+1}_{r+1}[q])^j$ (for $j=1,\dots,\sigma$ and $r=\sigma+1,\dots,\sigma+s$) yields the same expression as inserting the same function $f^n_{\sigma+i}[q_1,\dots,q_\sigma]$ instead of $q_{\sigma+i}$ in $(Z^{n+1}_r[q])^j$. But the first operation leads to the reduced vector field $\bar{Z}^{n+1,\sigma}_{r+1}$ while the second—to $\bar{Z}^{n,\sigma}_r$. ■

Let us now take $s+1$ instead of s (so that $n\to n+1$) in (59) and (60) and perform the reduction. According to Lemma 11 we obtain the following sequence of $s+1$ reduced systems:

$$\bar{q}_{t_{\sigma+1}}=\bar{Z}^{n+1,\sigma}_{\sigma+1},\quad \bar{q}_{t_{r+1}}=\bar{Z}^{n+1,\sigma}_{r+1}=\bar{Z}^{n,\sigma}_r \quad \text{for } r=\sigma+1,\dots,\sigma+s,$$

i.e., we obtain the same sequence of s systems as before but shifted and an additional system in the beginning of the sequence. This first system can therefore be treated as a next system in some infinite, commuting hierarchy of vector fields.

Let us also observe that we could use (60) to eliminate variables in Killing systems of the form (45) and this would lead to a system of s commuting evolutionary systems. However, this choice does not lead to any hierarchy: by increasing s to $s+1$ we obtain a different sequence of systems.

As before, this procedure can be generalized: we can use the first $n-\sigma-\alpha$ equations ($0\leqslant\alpha<n-\sigma-1$) in (56) to eliminate $q_{\sigma+\alpha+1},\dots,q_n$ from the following sequence of s Killing systems:

$$q_{t_r}=Z^n_r[q],\quad r=\sigma+\alpha+1,\dots,\sigma+\alpha+s \text{ with } n=s+2(\sigma+\alpha)-1. \tag{64}$$

This elimination leads—similarly as above—to s commuting to zero $N=\sigma+\alpha$-component systems $\bar{q}_{t_r}=\bar{Z}^{\sigma+\alpha}_r[q_1,\dots,q_{\sigma+\alpha}]$ and by increasing s by 1 we always obtain a new system of the hierarchy at the beginning of the sequence.

Next section contains some examples of the above described elimination procedures.

VII. EXAMPLES

A. Elimination with positive potentials

Below we will present some examples performed with the help of the (generalized) procedure described in the preceding section. Soliton hierarchies are now classified by pairs (σ,α), $\sigma=1,2,\dots,\alpha=0,1,\dots$, where $N=\sigma+\alpha$ is a number of components in the systems of a given hierarchy. Assume we would like to construct first s members of the hierarchy. We have then to fix $n=s+\sigma+\alpha-1$ and take first s Killing equations in (51). Then, we have to eliminate coordinates $q_{\sigma+\alpha+1},\dots,q_{\sigma+\alpha+s-1}=q_n$ using invariants $w^{(n,\sigma)}_{\sigma+1}=0,\dots,w^{(n,\sigma)}_{n-\alpha}=0$. According to (52), these invariants can be generated, for example, from $\mathcal{L}^{n,0,2n+\sigma}$ by taking the equations $E_i(\mathcal{L}^{n,0,2n+\sigma})=0$, $i=\sigma+1,\dots,n-\alpha$. After the elimination procedure, soliton equations are represented by first $N=\sigma+\alpha$ components of first s reduced Killing equations. Observe, that in this procedure the first soliton equation has always the trivial form $\bar{q}_{t_1}=\bar{q}_x$, $\bar{q}=(q_1,\dots,q_{\sigma+\alpha})^T$.

Let us start with a one-field hierarchy: $N=\sigma+\alpha=1$. There is only one possibility here: $\sigma=1$, $\alpha=0$. We present how to produce first $s=3$ flows which will be recognized as the first members of the KdV hierarchy. We have therefore to take $n=3$ and $k=7$. Killing systems (34) have the form

$$\frac{d}{dt_1}\begin{pmatrix}q_1\\q_2\\q_3\end{pmatrix}=\begin{pmatrix}q_{1,x}\\q_{2,x}\\q_{3,x}\end{pmatrix}=Z^3_1,$$

$$\frac{d}{dt_2}\begin{pmatrix}q_1\\q_2\\q_3\end{pmatrix}=\begin{pmatrix}q_{2,x}\\q_{3,x}+q_1q_{2,x}-q_2q_{1,x}\\q_1q_{3,x}-q_3q_{1,x}\end{pmatrix}=Z^3_2,$$

$$\frac{d}{\mathrm{d}t_3}\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} q_{3,x} \\ q_1 q_{3,x} - q_3 q_{1,x} \\ q_2 q_{3,x} - q_3 q_{2,x} \end{pmatrix} = Z_3^3 \tag{65}$$

while the Lagrangian $\mathcal{L}^{3,0,7}$ is

$$\mathcal{L}^{3,0,7} = \tfrac{1}{2}q_1^2 q_{1,x}^2 - \tfrac{1}{2}q_2 q_{1,x}^2 - q_1 q_{1,x} q_{2x} + q_{1,x} q_{3,x} + \tfrac{1}{2}q_{2,x}^2 - 2q_2 q_3 + 3q_1^2 q_3 + 3q_1 q_2^2 - 4q_1^3 q_2 + q_1^5$$

and the Euler-Lagrange equations (46) for the above Lagrangian attain the form

$$w_2^{(3,1)} \equiv -2q_3 + 6q_1 q_2 - 4q_1^3 + \tfrac{1}{2}q_{1,x}^2 + q_1 q_{1,xx} - q_{2,xx} = 0,$$

$$w_3^{(3,1)} \equiv -2q_2 + 3q_1^2 - q_{1,xx} = 0.$$

These equations can be solved with respect to q_2, q_3 yielding (49) of the form

$$q_2 = -\tfrac{1}{2}q_{1,xx} + \tfrac{3}{2}q_1^2, \quad q_3 = \tfrac{1}{4}q_{1,xxxx} - \tfrac{5}{2}q_1 q_{1,xx} - \tfrac{5}{4}q_{1,x}^2 + \tfrac{5}{2}q_1^3. \tag{66}$$

Substituting it to the above Killing systems gives (50) that read now explicitly as

$$\begin{cases} q_{1,t_1} = q_{1,x} = \bar{Z}_1^1, \\ 0 = 0, \\ 0 = 0, \end{cases}$$

$$\begin{cases} q_{1,t_2} = -\tfrac{1}{2}q_{1,xxx} + 3q_1 q_{1,x} = \bar{Z}_2^1, \\ 0 = 0, \\ 0 = \tfrac{1}{2}w_{1,x}, \end{cases}$$

$$\begin{cases} q_{1,t_3} = \tfrac{1}{4}q_{1,xxxxx} - 5q_{1,x}q_{1,xx} - \tfrac{5}{2}q_1 q_{1,xxx} + \tfrac{15}{2}q_1^2 q_{1,x} = \bar{Z}_3^1, \\ 0 = \tfrac{1}{2}w_{1,x}, \\ 0 = -\tfrac{1}{4}w_{1,xxx} + \tfrac{3}{2}q_1 w_{1,x} \end{cases}$$

so that the first components $q_{1,t_i} = \bar{Z}_i^1[q_1]$ are the first three flows of the KdV hierarchy while the remaining equations are just differential consequences of w_1, which of course vanish on any $\mathcal{S}_{u_0}$. By taking larger s we can produce an arbitrary number of flows from the KdV hierarchy.

Next, let us consider two-field systems: $N=\sigma+\alpha=2$. There are two possibilities: $(\sigma,\alpha)=(2,0)$ and $(\sigma,\alpha)=(1,1)$. Therefore, as a second example we consider the case $(\sigma,\alpha)=(2,0)$, and $s=3$. We have now to take $n=s+\sigma+\alpha-1=4$ and $k=2n+\sigma=10$. The Euler-Lagrange equations $E_4(\mathcal{L}^{4,0,10})=w_4^{(4,2)}=0$ and $E_3(\mathcal{L}^{4,0,10})=w_3^{(4,2)}=0$ can be solved with respect to q_3, q_4 yielding (49) of the form

$$q_3 = -\tfrac{1}{2}q_{1,xx} + 3q_1 q_2 - 2q_1^3,$$

$$q_4 = \tfrac{1}{4}q_{1,x}^2 - \tfrac{1}{2}q_{2,xx} - q_1 q_{1,xx} - \tfrac{7}{2}q_1^4 + 3q_1^2 q_2 + \tfrac{3}{2}q_2^2.$$

Substituting it to two first components of Killing equations $Z_2^4[q]$, $Z_3^4[q]$ yields two first nontrivial members of another two-field soliton hierarchy,

$$q_{1,t_2} = q_{2,x},$$
$$q_{2,t_2} = -\tfrac{1}{2}q_{1,xxx} + 4q_1q_{2,x} + 2q_2q_{1,x} - 6q_1^2q_{1,x}, \tag{67}$$

and

$$q_{1,t_3} = -\tfrac{1}{2}q_{1,xxx} + 3q_1q_{2,x} + 3q_2q_{1,x} - 6q_1^2q_{1,x},$$

$$q_{2,t_3} = -\tfrac{1}{2}q_{2,xxx} - \tfrac{3}{2}q_1q_{1,xxx} + 3q_2q_{2,x} + 6q_1q_2q_{1,x} + 6q_1^2q_{2,x} - 18q_1^3q_{1,x}.$$

In the second two-field case $(\sigma,\alpha)=(1,1)$, if we keep $s=3$ unchanged, we have to take $n=s+\sigma+\alpha-1=4$ and $k=2n+\sigma=9$. From the Euler-Lagrange equations (46) for $\mathcal{L}^{4,0,9}$,

$$E_3(\mathcal{L}^{4,0,9}) = w_3^{(4,1)} = 0, \quad E_2(\mathcal{L}^{4,0,9}) = w_2^{(4,1)} = 0$$

we can eliminate q_3 and q_4, which yields (54). Explicitly, we obtain

$$q_3 = \tfrac{1}{4}q_{1,xxxx} - \tfrac{5}{2}q_1q_{1,xx} - \tfrac{5}{4}q_{1,x}^2 + \tfrac{5}{2}q_1^3,$$

$$q_4 = \tfrac{1}{4}q_{2,xxxx} - \tfrac{1}{4}q_1q_{1,xxxx} - \tfrac{3}{4}q_{1,x}q_{1,xxx} - \tfrac{1}{2}q_{1,xx}^2 - q_2q_{1,xx} - \tfrac{5}{2}q_{1,x}q_{2,x} + 4q_1^2q_{1,xx} - \tfrac{5}{2}q_1q_{2,xx} + \tfrac{25}{4}q_1q_{1,x}^2 + 3q_1^2q_2 - \tfrac{7}{2}q_1^4 + \tfrac{3}{2}q_2^2.$$

Then, two first components of the Killing equations $q_{t_2}=Z_2^4[q]$, $q_{t_3}=Z_3^4[q]$ turn into

$$q_{1,t_2} = q_{2,x},$$

$$q_{2,t_2} = -\tfrac{1}{2}q_{2,xxx} + \tfrac{1}{2}q_1q_{1,xxx} + q_{1,x}q_{1,xx} + 4q_1q_{2,x} + 2q_2q_{1,x} - 6q_1^2q_{1,x},$$

and

$$q_{1,t_3} = -\tfrac{1}{2}q_{2,xxx} + \tfrac{1}{2}q_1q_{1,xxx} + q_{1,x}q_{1,xx} + 3q_1q_{2,x} + 3q_2q_{1,x} - 6q_1^2q_{1,x},$$

$$q_{2,t_3} = \tfrac{1}{4}q_{2,xxxxx} - \tfrac{1}{4}q_1q_{1,xxxxx} - q_{1,x}q_{1,xxxx} - \tfrac{7}{4}q_{1,xx}q_{1,xxx} - q_2q_{1,xxx} - \tfrac{7}{2}q_{2,x}q_{1,xx} + \tfrac{9}{2}q_1^2q_{1,xxx} - 3q_1q_{2,xxx} - \tfrac{9}{2}q_{1,x}q_{2,xx} + 21q_1q_{1,x}q_{1,xx} + 6q_1q_2q_{1,x} + 3q_2q_{2,x} + 6q_1^2q_{2,x} + 6q_{1,x}^2 - 18q_1^3q_{1,x}.$$

Finally, we shortly mention the three-field case: $N=\sigma+\alpha=3$. There are three different hierarchies with the following first nontrivial member of each hierarchy: for $(\sigma,\alpha)=(3,0)$,

$$q_{1,t_2} = q_{2,x},$$

$$q_{2,t_2} = q_{3,x} + q_1q_{2,x} - q_2q_{1,x},$$

$$q_{3,t_2} = -\tfrac{1}{2}q_{2,xxx} - 12q_1q_2q_{1,x} - 6q_1^2q_{2,x} + 3q_2q_{2,x} + 2q_3q_{1,x} + 4q_1q_{3,x} + 10q_1^3q_{1,x};$$

for $(\sigma,\alpha)=(2,1)$,

$$q_{1,t_2} = q_{2,x},$$

$$q_{2,t_2} = q_{3,x} + q_1q_{2,x} - q_2q_{1,x},$$

$$q_{3,t_2} = -\tfrac{1}{2}q_{2,xxx} + \tfrac{1}{2}q_1 q_{1,xxx} + q_{1,x}q_{1,xx} - 12q_1 q_2 q_{1,x} - 6q_1^2 q_{2,x} + 3q_2 q_{2,x} + 2q_3 q_{1,x} + 4q_1 q_{3,x} + 10q_1^3 q_{1,x};$$

and for $(\sigma,\alpha)=(1,2)$,

$$q_{1,t_2} = q_{2,x},$$

$$q_{2,t_2} = q_{3,x} + q_1 q_{2,x} - q_2 q_{1,x},$$

$$q_{3,t_2} = -\tfrac{1}{2}q_{3,xxx} + \tfrac{1}{2}q_1 q_{2,xxx} + \tfrac{1}{2}q_2 q_{1,xxx} - \tfrac{1}{2}q_1^2 q_{1,xxx} - 2q_1 q_{1,x} q_{1,xx} + q_{1,x}q_{2,xx} + q_{2,x}q_{1,xx} - \tfrac{1}{2}q_{1,x}^3 + 2q_3 q_{1,x} + 4q_1 q_{3,x} - 12q_1 q_2 q_{1,x} - 6q_1^2 q_{2,x} + 3q_2 q_{2,x} + 10q_1^3 q_{1,x}.$$

In general, for a fixed $N=\sigma+\alpha$, this procedure leads to N different N-component hierarchies of soliton systems. As the field representation of constructed hierarchies is nonstandard, it is not easy to recognize which hierarchies are known and which are new. We immediately recognized the KdV hierarchy. We also found that two-field hierarchy starting from (67) turns after the transformation

$$u_1 = -3q_1^2 + 2q_2, \quad u_2 = 2q_1, \quad x \to \sqrt{2}ix, \quad t \to \sqrt{2}it$$

into the 2-component coupled KdV hierarchy in the representation of Fordy and Antonowicz.[23] For example, the first flow of this hierarchy (67) turns into

$$u_{1,t_1} = \tfrac{1}{4}u_{2,xxx} + \tfrac{1}{2}u_2 u_{1,x} + u_1 u_{2,x},$$

$$u_{2,t_1} = u_{1,x} + \tfrac{3}{2}u_2 u_{2,x}$$

[yielding (3.18) in Ref. 23].

B. Elimination with negative potentials

We start by presenting the first two ($s=2$) flows of the only $N=1$-component hierarchy that can be obtained within our scheme by using the negative separable potentials. Since $N=1=\alpha+\sigma$, the only choice is to set $\sigma=1$, $\alpha=0$, which yields $n=s+2(\sigma+\alpha)-1=3$. The Euler-Lagrange equations (56) for

$$\mathcal{L}^{n,n-\sigma,-n} = \mathcal{L}^{3,2,-3} = \frac{1}{2}q_{1,x}^2 - \frac{q_{2,x}q_{3,x}}{q_3} + \frac{q_{3,x}^2 q_2}{2q_3} - \frac{q_1}{q_3^2} + \frac{q_2^2}{q_3^3}$$

attain the form

$$-1 - q_3^2 q_{1,xx} = 0, \quad 4q_2 + 2q_3^2 q_{3,xx} - q_3 q_{3,x}^2 = 0 \tag{68}$$

which allows for expressing q_2 and q_3 as differential functions of q_1,

$$q_3 = q_3[q_1] = (-q_{1,xx})^{-1/2},$$

$$q_2 = q_2[q_1] = -\tfrac{1}{16}(5q_{1,xxx}^2 - 4q_{1,xx}q_{1,xxxx})(-q_{1,xx})^{-7/2}$$

(here and in what follows we only consider the positive solution for q_n, otherwise we can change $t \to -t$). Substituting these expressions to the Killing systems (64) and performing the necessary derivations we obtain the following two commuting flows:

$$q_{1,t_2} = (q_2[q_1])_x, \quad q_{1,t_3} = (q_3[q_1])_x$$

with the differential functions $q_2[q_1]$ and $q_3[q_1]$ given as above. After substitution $u=-q_{1,xx}$ the second equation turns into the well known Harry Dym equation while the first one becomes the second member of the hierarchy. If we want to produce a next member of this hierarchy we have to take $s=3$. According to the general remarks in the previous section this new system will appear as the first system in our sequence of systems.

Let us now consider two-field systems: $N=\sigma+\alpha=2$. As before, we have now two choices: $(\sigma,\alpha)=(1,1)$ and $(\sigma,\alpha)=(2,0)$. We start with $(\sigma,\alpha)=(2,0)$. We have now $n=s+2\sigma-1=5$ and thus we consider the Lagrangian $\mathcal{L}^{n,n-\sigma,-n}=\mathcal{L}^{5,3,-5}$. The associated Euler-Lagrange equations (56) can be written as

$$q_5^2(q_{1,x}^2 + 2q_{1,xx}q_1 - 2q_{2,xx}) - 2 = 0, \quad 2q_4 - q_5^3 q_{1,xx} = 0,$$

$$4q_3q_5 - q_{5,x}^2 q_5^2 - 6q_4^2 + 2q_5^3 q_{5,xx} = 0$$

and they can be solved to

$$q_5 = f_5^5[q_1,q_2] = 2w^{-1/2},$$

$$q_4 = f_4^5[q_1,q_2] = 4q_{1,xx}w^{-3/2},$$

$$q_3 = f_3^5[q_1,q_2] = \left(-\tfrac{5}{2}w_x^2 + 12q_{1,xx}^2 w + 2ww_{xx}\right)w^{-7/2},$$

where $w=2q_{1,x}^2+4q_{1,xx}q_1-4q_{2,xx}$. Substituting it into (64) we arrive at the following two commuting two-component systems:

$$q_{1,t_3} = (f_3^5[q_1,q_2])_x,$$

$$q_{2,t_3} = q_1(f_3^5[q_1,q_2])_x - (f_3^5[q_1,q_2])q_{1,x} + (f_4^5[q_1,q_2])_x$$

and

$$\begin{aligned} q_{1,t_4} &= (f_4^5[q_1,q_2])_x, \\ q_{2,t_4} &= q_1(f_4^5[q_1,q_2])_x - (f_4^5[q_1,q_2])q_{1,x} + (f_5^5[q_1,q_2])_x. \end{aligned} \tag{69}$$

The system (69) can be written more explicitly as

$$q_{1,t_4} = 2(2q_{1,xxx}w - 3q_{1,xx}w_x)w^{-5/2},$$

$$q_{2,t_4} = (4q_1q_{1,xxx}w - 6q_1q_{1,xx}w_x - 4q_{1,x}q_{1,xx}w - ww_x)w^{-5/2}.$$

Finally, let us consider the case $(\sigma,\alpha)=(1,1)$. Again, we have $n=5$, but this time we consider the Lagrangian $\mathcal{L}^{n,n-\sigma-\alpha,-n+\alpha}=\mathcal{L}^{5,3,-4}$. Its first $n-\sigma-\alpha=3$ Euler-Lagrange equations

$$0 = -q_5^2 q_{1,xx} - 1,$$

$$0 = 4q_4 + 2q_5^2 q_{5,xx} - q_5 q_{5,x}^2,$$

$$0 = 2q_3q_5 - q_5^2 q_{4,x}q_{5,x} + q_4q_5q_{5,x}^2 - 3q_4^2 + q_5^3 q_{4,xx} - q_5^2 q_4 q_{5,xx}$$

yield the following elimination equations:

$$q_5 = f_5^5[q_1] = (-q_{1,xx})^{-1/2},$$

$$q_4 = f_4^5[q_1] = -\frac{1}{2^4}(5q_{1,xxx}^2 - 4q_{1,xx}q_{1,xxxx})(-q_{1,xx})^{-7/2}, \tag{70}$$

$$q_3 = f_3^5[q_1] = \frac{1}{2^9}P[q_1](-q_{1,xx})^{-13/2},$$

where $P[q_1]$ is some complicated differential polynomial of q_1 (homogeneous of degree 4 and of order 6) with integer coefficients. Substituting (70) into the Killing systems (64) we arrive at the following two commuting two-component flows:

$$q_{1,t_3} = (f_3^5[q_1])_x,$$

$$q_{2,t_3} = q_1(f_3^5[q_1])_x - f_3^5[q_1]q_{1,x} + (f_4^5[q_1])_x$$

and

$$q_{1,t_4} = (f_4^5[q_1])_x,$$

$$q_{2,t_4} = q_1(f_4^5[q_1])_x - f_4^5[q_1]q_{1,x} + (f_5^5[q_1])_x.$$

The last vector field can be written more explicitly as

$$q_{1,t_4} = \frac{1}{2^5}(-40ww_xw_{xx} + 35w_x^3 + 8w^2w_{xxx})w^{-9/2},$$

$$q_{2,t_4} = \frac{1}{2^5}(10q_{1,x}ww_x^2 - 8q_{1,x}w^2w_{xx} - 40q_1ww_xw_{xx} + 35q_1w_x^3 + 8q_1w^2w_{xxx})w^{-9/2},$$

where $w=-q_{1,xx}$. Let us notice that in this case we obtain a hierarchy of systems such that every system is driven by its first equation which is a consecutive equation of Harry Dym hierarchy. One can see that, contrary to the positive case, if $\alpha>0$ the obtained systems are always driven by its first σ components that coincide with the corresponding systems from $\alpha=0$ hierarchy.

VIII. CONCLUSIONS

In this paper we developed a method of unified constructing of Stäckel systems and soliton hierarchies from the same common denominator in the form of separation relations (7). We developed our theory starting from separation relations generated by separation curves of the form

$$H_1\lambda^{\beta_1} + \ldots + H_n\lambda^{\beta_n} = \tfrac{1}{2}\lambda^m\mu^2 + \lambda^k, \quad \beta_i, n \in \mathbf{N}, \quad m,k \in \mathbf{Z}. \tag{71}$$

We performed a detailed, systematic construction of soliton hierarchies for the Benenti class of separation relations, given by the particular form of (71), namely

$$H_1\lambda^{n-1} + H_2\lambda^{n-2} + \cdots + H_n = \tfrac{1}{2}\lambda^m\mu^2 + \lambda^k.$$

The results we obtained are hopefully only a first step of a new research program. The next step of this program would be finding out a way for systematic constructing of other soliton hierarchies from different classes of separation curves (71), when the sequence $(\beta_1,\ldots,\beta_n)$ differs from $(n-1,\ldots,0)$. The next-nontrivial-step would be to extend the theory to the case of polynomial separation curves (8) with $(\alpha_1,\ldots,\alpha_n)\neq(0,\ldots,0)$. We expect by presented procedure to generate not only the majority of known soliton systems but also to construct in a systematic way a vast

number of new integrable hierarchies. One should also investigate the possibility of "prolongation" of standard integrable structures of separable systems (such as integrals of motion, bi-Hamiltonian structure) onto the corresponding evolutionary hierarchies of PDE's.

APPENDIX A

The involutivity of $H_1^{(m,k)}$ and $H_r^{(m,k)}$ (15) leads to the following relations imposed on $g_{kk}^{(m)}(\lambda), v_r^k(\lambda), V_1^{(k)}(\lambda)$ and $V_r^{(k)}(\lambda)$:[14]

$$\frac{\partial v_r^i}{\partial \lambda_i} = 0, \quad i = 1, \ldots, n, \tag{A1}$$

$$\frac{\partial}{\partial \lambda_i} \ln g_{kk}^{(m)} = \frac{\dfrac{\partial v_r^k}{\partial \lambda_i}}{v_r^k - v_r^i}, \quad i \neq k, \quad \text{all } m, r \tag{A2}$$

$$\frac{\partial V_r^{(k)}}{\partial \lambda_i} = v_r^i \frac{\partial V_1^{(k)}}{\partial \lambda_i} \quad \text{for all } i, r, \text{ and } k. \tag{A3}$$

We will prove here the relation (20), i.e.,

$$\sum_{i=1}^{n} E_i(\mathcal{L}^{(n,m,k)})\lambda_{i,t_r} - \sum_{i=1}^{n} E_i(\mathcal{L}_r^{(n,m,k)})\lambda_{i,x} = 0. \tag{A4}$$

First, let us consider the geodesic case. Due to (18) we have $\lambda_{i,t_r} = v_r^i \lambda_{i,x}$ where v_r^i are eigenvalues of K_r [see (16)]. For the geodesic Hamiltonians,

$$\mathcal{L}^{(n,m,0)} = \frac{1}{2}\sum_{i=1}^{n} g_{ii}^{(m)} \lambda_{i,x}^2 \quad \text{and} \quad \mathcal{L}_r^{(n,m,0)} = \frac{1}{2}\sum_{i=1}^{n} g_{ii}^{(m)} v_r^i \lambda_{i,x}^2$$

so that in this case the left-hand side of (A4) attains the form

$$\begin{aligned}
&\sum_{i=1}^{n} E_i(\mathcal{L}^{(n,m,0)})\lambda_{i,t_r} - \sum_{i=1}^{n} E_i(\mathcal{L}_r^{(n,m,0)})\lambda_{i,x} \\
&\quad = \left(\frac{1}{2}\sum_{i,k=1}^{n} \frac{\partial g_{kk}^{(m)}}{\partial \lambda_i} (\lambda_{k,x})^2 v_r^i \lambda_{i,x} - \sum_{i=1}^{n} \frac{d}{dx}(g_{ii}^{(m)} \lambda_{i,x}) v_r^i \lambda_i^x \right) \\
&\qquad - \left(\frac{1}{2}\sum_{i,k=1}^{n} \frac{\partial g_{kk}^{(m)}}{\partial \lambda_i} (\lambda_{k,x})^2 v_r^k \lambda_{i,x} + \frac{1}{2}\sum_{i,k=1}^{n} g_{kk}^{(m)} \frac{\partial v_r^k}{\partial \lambda_i} (\lambda_{k,x})^2 \lambda_{i,x} \right. \\
&\qquad \left. - \sum_{i=1}^{n} \frac{d}{dx}(g_{ii}^{(m)} \lambda_{i,x}) v_r^i \lambda_{i.x} - \sum_{i=1}^{n} g_{ii}^{(m)} \lambda_{i,x}^2 \frac{dv_r^i}{dx} \right) \\
&\quad = \frac{1}{2}\sum_{i,k=1}^{n} \frac{\partial g_{kk}^{(m)}}{\partial \lambda_i} (\lambda_{k,x})^2 (v_r^i - v_r^k) \lambda_{i,x} - \left(\frac{1}{2}\sum_{i,k=1}^{n} g_{kk}^{(m)} \frac{\partial v_r^k}{\partial \lambda_i} (\lambda_{k,x})^2 \lambda_{i,x} - \sum_{i=1}^{n} g_{ii}^{(m)} \lambda_{i,x}^2 \frac{dv_r^i}{dx} \right) = 0
\end{aligned}$$

since the expression in the last parentheses equals to

$$\frac{1}{2}\sum_{i,k=1}^{n} g_{kk}^{(m)}\frac{\partial v_r^k}{\partial \lambda_i}(\lambda_{k,x})^2\lambda_{i,x} - \sum_{i,k=1}^{n} g_{ii}^{(m)}\lambda_{i,x}^2\frac{\partial v_r^i}{\partial \lambda_k}\lambda_{k,x} = -\frac{1}{2}\sum_{i,k=1}^{n} g_{kk}^{(m)}\frac{\partial v_r^k}{\partial \lambda_i}(\lambda_{k,x})^2\lambda_{i,x}$$

$$= +\frac{1}{2}\sum_{i,k=1}^{n}\frac{\partial g_{kk}^{(m)}}{\partial \lambda_i}(\lambda_{k,x})^2(v_r^i - v_r^k)\lambda_{i,x},$$

where the last equality follows from formula (A2) which can be written in equivalent form

$$g_{kk}^{(m)}\frac{\partial v_r^k}{\partial \lambda_i} = \frac{\partial g_{kk}^{(m)}}{\partial \lambda_i}(v_r^k - v_r^i)$$

(that is in fact also valid for $k=i$). Thus, the statement has been proved for geodesic densities. For the potential parts,

$$\sum_{i=1}^{n} E_i(V_1^{(k)})\lambda_{i,t_r} - \sum_{i=1}^{n} E_i(V_r^{(k)})\lambda_{i,x} = \sum_{i=1}^{n}\left(\frac{\partial V_1^{(k)}}{\partial \lambda_i}v_r^i - \frac{\partial V_r^{(k)}}{\partial \lambda_i}\right)\lambda_{i,x} = 0$$

due to (A3). This concludes the proof.

APPENDIX B

We will prove here Theorem 6. The relation (40) is a consequence of (37) and (39) of Lemma 5. Indeed, by (39),

$$E_l(\mathcal{L}^{n,m,k}) = \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial V_1^{(2n-m-i-j)}}{\partial q_l}(q_i)_x(q_j)_x - \frac{\partial V_1^{(k)}}{\partial q_l} - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{(2n-m-i-l)}(q_i)_x\right),$$

and

$$E_{l-\alpha}(\mathcal{L}^{n,m+\alpha,k-\alpha}) = \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial V_1^{(2n-m-\alpha-i-j)}}{\partial q_{l-\alpha}}(q_i)_x(q_j)_x - \frac{\partial V_1^{(k-\alpha)}}{\partial q_{l-\alpha}} - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{(2n-m-\alpha-i-l+\alpha)}(q_i)_x\right)$$

$$\overset{\text{lemma 5}}{=} E_l(\mathcal{L}^{n,m,k}).$$

The relation (41) is just a rewritten form of (40).

Since in what follows we will compare separable potentials with different n, in the rest of the proof we will use temporary extended notation for potentials in the form $V_1^{n,(k)}$. From (28) and (47) it follows that

$$V_1^{n,(n+k)} = V_1^{n+1,(n+1+k)}, \quad k = -n, \ldots, n-1. \tag{B1}$$

We prove now (42). Using the relation (37) for $r=1$ we obtain

$$E_l(\mathcal{L}^{n,0,0}) = \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial V_1^{n,(2n-i-j)}}{\partial q_l}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{n,(2n-i-l)}(q_i)_x\right)$$

$$= \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial V_1^{n,(2n-i-j-l+1)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{n,(2n-i-l)}(q_i)_x\right). \tag{B2}$$

and in a similar way we have

$$E_{l+1}(\mathcal{L}^{n+1,0,0}) = \frac{1}{2}\sum_{i,j=1}^{n+1} \frac{\partial V_1^{n+1,(2n+2-i-j-l)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{\mathrm{d}x}\left(\sum_{i=1}^{n+1} V_1^{n+1,(2n-i-l+1)}(q_i)_x\right)$$
$$\overset{(*)}{=} \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n+1,(2n-i-j-l+2)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{\mathrm{d}x}\left(\sum_{i=1}^{n} V_1^{n+1,(2n-i-l+1)}(q_i)_x\right)$$
$$\overset{(B1)}{=} \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(2n-i-j-l+1)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{\mathrm{d}x}\left(\sum_{i=1}^{n} V_1^{n,(2n-i-l)}(q_i)_x\right).$$

The equality $(*)$ is due to the fact that $V_1^{n+1,(2n-i-l+1)}=0$ for $i=n+1$ and similarly $V_1^{n+1,(2n-i-j-l+2)}$ does not depend on q_1 for $i=n+1$ or $j=n+1$ [this follows from (42) and (57)]. Thus

$$E_l(\mathcal{L}^{n,0,0}) = E_{l+1}(\mathcal{L}^{n+1,0,0}), \quad l=1,\ldots,n. \tag{B3}$$

Moreover, from (30) it follows that

$$V_1^{n,(2n+\sigma)} = -q_1 V_1^{n,(2n+\sigma-1)} - \cdots - q_n V_1^{n,(n+\sigma)},$$

hence, for $l>\sigma$

$$\frac{\partial V_1^{n,(2n+\sigma)}}{\partial q_l} = -q_1\frac{\partial V_1^{n,(2n+\sigma-1)}}{\partial q_l} - \cdots - q_n\frac{\partial V_1^{n,(n+\sigma)}}{\partial q_l} - V_1^{n,(2n+\sigma-l)}$$
$$= -q_1\frac{\partial V_1^{n,(2n+\sigma-l)}}{\partial q_1} - \cdots - q_n\frac{\partial V_1^{n,(n+\sigma-l+1)}}{\partial q_1} - V_1^{n,(2n+\sigma-l)}.$$

On the other hand, we have

$$V_1^{n+1,(2n+\sigma+2)} = -q_1 V_1^{n+1,(2n+\sigma+1)} - \cdots - q_n V_1^{n+1,(n+\sigma+2)} - q_{n+1} V_1^{n+1,(n+\sigma+1)},$$

hence, for $l>\sigma$ and according to (B1) and (47)

$$\frac{\partial V_1^{n+1,(2n+\sigma+2)}}{\partial q_{l+1}} = -q_1\frac{\partial V_1^{n+1,(2n+\sigma+1)}}{\partial q_{l+1}} - \cdots - q_n\frac{\partial V_1^{n+1,(n+\sigma+2)}}{\partial q_{l+1}} - V_1^{n+1,(2n+\sigma-l+1)}$$
$$= -q_1\frac{\partial V_1^{n+1,(2n+\sigma+1-l)}}{\partial q_1} - \cdots - q_n\frac{\partial V_1^{n+1,(n+\sigma+2-l)}}{\partial q_1} - V_1^{n+1,(2n+\sigma-l+1)}$$
$$= -q_1\frac{\partial V_1^{n,(2n+\sigma-l)}}{\partial q_1} - \cdots - q_n\frac{\partial V_1^{n,(n+\sigma+1-l)}}{\partial q_1} - V_1^{n,(2n+\sigma-l)} = \frac{\partial V_1^{n,(2n+\sigma)}}{\partial q_l}, \tag{B4}$$

and from (37) it follows that

$$\frac{\partial V_1^{n,(n+s)}}{\partial q_l} = \frac{\partial V_1^{n+1,(n+s+2)}}{\partial q_{l+1}}, \quad 0 \leqslant s-l+1 \leqslant n.$$

So, from (B3) and (B4) for $\sigma<l\leqslant n$ equation (42) is fulfilled.

Now, we pass to the proof of relations (43). First, we have

$$E_l(\mathcal{L}^{n,n-\sigma,0}) = \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(n+\sigma-i-j)}}{\partial q_l}(q_i)_x(q_j)_x - \frac{d}{\mathrm{d}x}\left(\sum_{i=1}^{n} V_1^{n,(n+\sigma-i-l)}(q_i)_x\right)$$
$$= \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(n+\sigma-i-j-l+1)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{\mathrm{d}x}\left(\sum_{i=1}^{n} V_1^{n,(n+\sigma-i-l)}(q_i)_x\right). \tag{B5}$$

On the other hand,

$$E_l(\mathcal{L}^{n+1,n+1-\sigma,0}) = \frac{1}{2}\sum_{i,j=1}^{n+1} \frac{\partial V_1^{n+1,(n+\sigma-i-j-l+2)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n+1} V_1^{n+1,(n+\sigma-i-l+1)}(q_i)_x\right).$$

By (42) and (57), for $l \leqslant \sigma$ the last term in both sums does not contribute. Moreover, according to (B1) and the fact that $V_1^{n,(2n)} - q_{n+1} = V_1^{n+1,(2n+1)}$, we have

$$\frac{\partial V_1^{n,(n+k)}}{\partial q_1} = \frac{\partial V_1^{n+1,(n+k+1)}}{\partial q_1}, \quad k = -n, \ldots, n,$$

hence

$$E_l(\mathcal{L}^{n+1,n+1-\sigma,0}) = \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(n+\sigma-i-j-l+1)}}{\partial q_1}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{n,(n+\sigma-i-l)}(q_i)_x\right) = E_l(\mathcal{L}^{n,n-\sigma,0}).$$

Finally, we prove the relation (44). From the negative recursion (27), we have

$$V_1^{n,(-k)}(q_{n-k+1}, \ldots, q_n)\big|_{q_i \to q_{i+1}, i=n-k+1,\ldots,n} = V_1^{n+1,(-k)}(q_{n-k+2}, \ldots, q_{n+1}), \quad k = 1, \ldots, n. \tag{B6}$$

Then

$$\begin{aligned} E_{\sigma+l}(\mathcal{L}^{n,n-\sigma,0}) &= \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(n-i-j+1-\sigma)}}{\partial q_{l+\sigma}}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{n,(n-i-l)}(q_i)_x\right) \\ &= \frac{1}{2}\sum_{i,j=1}^{n} \frac{\partial V_1^{n,(2n-i-j-l+1)}}{\partial q_n}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n} V_1^{n,(n-i-l)}(q_i)_x\right) \end{aligned} \tag{B7}$$

and

$$E_{\sigma+l}(\mathcal{L}^{n+1,n+1-\sigma,0}) = \frac{1}{2}\sum_{i,j=1}^{n+1} \frac{\partial V_1^{n+1,(n-i-j+2-\sigma)}}{\partial q_{l+\sigma}}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n+1} V_1^{n+1,(n-i-l+1)}(q_i)_x\right)$$

$$\frac{1}{2}\sum_{i,j=1}^{n+1} \frac{\partial V_1^{n+1,(2n-i-j-l+3)}}{\partial q_{n+1}}(q_i)_x(q_j)_x - \frac{d}{dx}\left(\sum_{i=1}^{n+1} V_1^{n+1,(n-i-l+1)}(q_i)_x\right)$$

$$\frac{1}{2}\sum_{i,j=0}^{n} \frac{\partial V_1^{n+1,(2n-i-j-l+1)}}{\partial q_{n+1}}(q_{i+1})_x(q_{j+1})_x - \frac{d}{dx}\left(\sum_{i=0}^{n} V_1^{n+1,(n-i-l)}(q_{i+1})_x\right).$$

As for $i,j=0$ there is no contribution to the sum, so according to (B6) we have

$$E_{\sigma+l}(\mathcal{L}^{n,n-\sigma,0})_{|q_j \to q_{j+1}} = E_{\sigma+l}(\mathcal{L}^{n+1,n+1-\sigma,0}), \quad l = 1, \ldots, n-\sigma, \quad j = 1, \ldots, n. \tag{B8}$$

From (37) and (B6) we have

$$\left.\frac{\partial V_1^{n,(-n)}}{\partial q_i}\right|_{q_j \to q_{j+1}, j=1,\ldots,n} = \frac{\partial V_1^{n+1,(-n)}}{\partial q_{i+1}} = \frac{\partial V_1^{n+1,(-n-1)}}{\partial q_i}, \quad i = 1, \ldots, n \tag{B9}$$

that together with (B8) proves the relation (44).

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Extended Klein-Gordon action, gravity and nonrelativistic fluid

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We consider a scalar field action for which the Lagrangian density is a power of the massless Klein-Gordon Lagrangian. The coupling of gravity to this matter action is considered. In this case, we show the existence of nontrivial scalar field configurations with vanishing energy-momentum tensor on any static, spherically symmetric vacuum solutions of the Einstein equations. These configurations in spite of being coupled to gravity do not affect the curvature of space-time. The properties of this particular matter action are also analyzed. For a particular value of the exponent, the extended Klein-Gordon action is shown to exhibit a conformal invariance without requiring the introduction of a nonminimal coupling. We also establish a correspondence between this action and a nonrelativistic isentropic fluid in one fewer dimension. This fluid can be identified with the (generalized) Chaplygin gas for a particular value of the power. It is also shown that the nonrelativistic fluid admits, apart from the Galileo symmetry, an additional symmetry whose action is a rescaling of the time. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The fundamental tenet of general relativity is the manifestation of the curvature of space-time produced by the presence of matter. This phenomena is encoded through the Einstein equations that relate the Einstein tensor (with or without a cosmological constant) to the energy-momentum tensor of the matter,

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \kappa T_{\mu\nu}. \tag{1}$$

Since the energy-momentum tensor depends explicitly on the metric, both sides of the equations must be solved simultaneously.

In the first part of this paper, we address the following question: for a fixed geometry solving the vacuum Einstein equations, is it possible to find a matter source coupled to this space-time without affecting it. Concretely, this problem consists of examining a particular solution of the Einstein equations (1) for which both sides of the equations vanish, i.e.,

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = 0 = \kappa T_{\mu\nu}. \tag{2}$$

In three dimensions, such gravitationally undetectable solutions have been obtained in the context of scalar fields nonminimally coupled to gravity with a negative cosmological constant.[1] Recently, the same problem has been considered in higher dimensions but with a flat geometry.[2]

In our case, we show that for any static, spherically symmetric vacuum solutions of the Einstein equations (eventually with a cosmological constant), a particular matter source action can

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be coupled to this geometry yielding to nontrivial solutions of the equations (2). This matter source is described in $(D,1)$ dimensions by an extended Klein-Gordon action,

$$S_\alpha = \int d^D\vec{x}\, dt \sqrt{-g}(g^{\mu\nu}\nabla_\mu\theta\nabla_\nu\theta)^\alpha, \tag{3}$$

where θ is the dynamical field and α is a real parameter whose range will be fixed later. For $\alpha=1$, this action reduces to the well-known massless Klein-Gordon action.

The derivation of solutions of the equations (2) is shown to be equivalent of finding a null vector field k^μ (for the vacuum metric $g_{\mu\nu}$) which derives from the scalar field θ. For a static, spherically symmetric space-time, the derivation of vector fields satisfying these conditions is always possible. In this case, the potential θ can be expressed as a general smooth function that depends only on a null coordinate.

The existence of these gravitationally undetectable solutions is essentially due to the particular form of the matter action (3). For this reason, we investigate some properties of this matter action in the second part of this paper. In particular, the symmetries of the extended Klein-Gordon action (3) are analyzed. It is shown that for the particular value $\alpha=(D+1)/2$, this action exhibits a conformal invariance for which the conformal weight of the scalar field θ is zero. In contrast with the massless Klein-Gordon action, this conformal symmetry is achieved without requiring the introduction of a nonminimal coupling. Finally, we establish a correspondence between the relativistic action (3) and a nonrelativistic isentropic fluid defined in one fewer dimension. The clue of this correspondence lies in the fact that the nonrelativistic space-time can be viewed as the quotient of a higher-dimensional Lorentz manifold by the integral curves of a covariantly, lightlike vector field.[3] For $\alpha=1/2$, this nonrelativistic fluid is identified with the Chaplygin gas while for $0<\alpha<1/2$, the model corresponds to the generalized Chaplygin gas. Note that the Chaplygin cosmology provides an interesting setup to explain that the expansion of the universe is accelerating.[4–6] The Chaplygin gas has also raised a growing attention because of its connection with the Nambu-Goto action,[7] its rich symmetrical structure[8] and its supersymmetric extension.[9] For a general review on this topics see Ref. 10 and works on supersymmetric fluid models are reported in Ref. 11. The features of the Chaplygin gas can also be understood in a Kaluza-Klein-type framework.[12] The symmetries of the nonrelativistic fluid are also investigated and it is shown the existence, apart from the Galileo symmetry, of an additional symmetry whose action is a time rescaling.

The paper is organized as follows. We first derive solutions of the equations (2) for the energy-momentum tensor associated to the extended Klein-Gordon action (3). In the remaining sections, we discuss some general features of the matter action. In particular, we explain the origin of the conformal invariance of the extended Klein-Gordon action for the particular value $\alpha=(D+1)/2$. The last part of the paper is devoted to the correspondence between the relativistic matter action and a nonrelativistic isentropic and polytropic fluid in one fewer dimension. The symmetries of this nonrelativistic fluid are also analyzed.

II. STEALTH SOLUTIONS

We consider the action of $(D+1)$-dimensional gravity coupled to a scalar field θ with dynamics described by the extended Klein-Gordon action (3),

$$I = \int d^D\vec{x}\, \mathrm{d}t \sqrt{-g}\left[\frac{1}{2\kappa}(R-2\Lambda) - \frac{1}{2}(g^{\mu\nu}\nabla_\mu\theta\nabla_\nu\theta)^\alpha\right], \tag{4}$$

where R is the scalar curvature and κ is the gravitational constant. The field equations obtained by varying the metric and the scalar field read, respectively,

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \kappa T_{\mu\nu}, \tag{5a}$$

$$\nabla_\mu(\sqrt{-g}g^{\mu\nu}\nabla_\nu\theta(\nabla_\sigma\theta\nabla^\sigma\theta)^{\alpha-1}) = 0, \tag{5b}$$

where the energy-momentum tensor is given by

$$T_{\mu\nu} = 2\alpha\nabla_\mu\theta\nabla_\nu\theta(\nabla_\sigma\theta\nabla^\sigma\theta)^{\alpha-1} - g_{\mu\nu}(\nabla_\sigma\theta\nabla^\sigma\theta)^\alpha. \tag{6}$$

We look for a particular solution of the Einstein equations (5a) for which both sides of the equations vanish (2). We first show that the equation $T_{\mu\nu}=0$ implies some restrictions on the scalar field θ and on the real parameter α. Indeed, independently of the background metric, the vanishing of the energy-momentum tensor is possible only if the scalar field satisfies $\nabla_\sigma\theta\nabla^\sigma\theta=0$, otherwise the metric would be proportional to

$$g_{\mu\nu} \propto \frac{\nabla_\mu\theta\nabla_\nu\theta}{\nabla_\sigma\theta\nabla^\sigma\theta},$$

and, hence its determinant would vanish. Consequently, the condition $T_{\mu\nu}=0$ can be consistently achieved only for a scalar field satisfying $\nabla_\sigma\theta\nabla^\sigma\theta=0$ and for $\alpha>1$ because of the form of the energy-momentum tensor (6). It is interesting to note that under these conditions, the extended Klein-Gordon equation (5b) is automatically satisfied.

In sum, the system described by the particular Einstein equations (2) together with the extended wave equation (5b) is equivalent of finding a vacuum metric and a null vector field that derives from θ,

$$g_{\mu\nu}k^\mu k^\nu = 0, \quad k_\mu = \partial_\mu\theta. \tag{7}$$

We now show that a static and spherically symmetric space-time geometry always admits such vector field (7). Indeed, let us consider such geometry which in addition is supposed to solve the vacuum Einstein equations. The line element is given by

$$\mathrm{d}s^2 = -f(r)h(r)\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{f(r)} + r^2\,\mathrm{d}\Sigma_{D-1}^2, \tag{8}$$

where $\mathrm{d}\Sigma_{D-1}^2$ is the line element of the $(D-1)$-dimensional sphere. It is simple to see that the vector field defined by

$$k^\mu = \mp\frac{1}{\sqrt{h(r)}}\delta_r^\mu - \frac{1}{f(r)h(r)}\delta_t^\mu \tag{9}$$

is null and derived from the potential

$$t \mp \int^r \frac{\mathrm{d}\tilde{r}}{f(\tilde{r})\sqrt{h(\tilde{r})}}. \tag{10}$$

Hence, any smooth function of this potential (10)

$$\theta = F\left(t \mp \int^r \frac{\mathrm{d}\tilde{r}}{f(\tilde{r})\sqrt{h(\tilde{r})}}\right), \tag{11}$$

is a solution on the vacuum space-time metric of the constraint

$$g^{\mu\nu}\nabla_\mu\theta\nabla_\nu\theta = 0. \tag{12}$$

This result is not surprising and can be explained as follows. The null coordinates u and v associated to the space-time (8) can be defined as

$$u = t - \int^{r} \frac{\mathrm{d}\tilde{r}}{f(\tilde{r})\sqrt{h(\tilde{r})}}, \tag{13a}$$

$$v = t + \int^{r} \frac{\mathrm{d}\tilde{r}}{f(\tilde{r})\sqrt{h(\tilde{r})}}, \tag{13b}$$

and, in these coordinates, the metric (8) takes the following form:

$$\mathrm{d}s^2 = -f(r)h(r)\mathrm{d}u\,\mathrm{d}v + r^2\,\mathrm{d}\Sigma_{D-1}^2. \tag{14}$$

Consequently, any smooth function F of one of the null coordinate, i.e., $F(u)$ or $F(v)$, will provide a nontrivial solution to the equation (12). In the original coordinates (8), this solution becomes precisely (11).

Thus, we have shown that the curvature of vacuum space-time (8) may not react to the presence of matter source described by the action (3) provided the scalar field is given by the expression (11). The existence of such configurations is a direct consequence of the particular form of the matter action. In what follows, we analyze some properties of this action.

III. PROPERTIES OF THE EXTENDED KLEIN-GORDON ACTION

We first show that the matter action (3) can be derived from the action of a massive complex scalar field with Lagrangian given by

$$\mathcal{L} = \tfrac{1}{2}g^{\mu\nu}(\partial_\mu\Phi)(\partial_\nu\Phi^\star) + V(|\Phi|^2), \tag{15}$$

where V denotes a potential that depends only on the module of the scalar field. Decomposing the scalar field as

$$\Phi = \frac{f}{m}e^{-im\theta}, \tag{16}$$

where m represents the mass of the complex scalar field, the Lagrangian density (15) becomes

$$\mathcal{L} = \frac{1}{2m^2}g^{\mu\nu}\partial_\mu f\partial_\nu f + \frac{1}{2}f^2 g^{\mu\nu}\partial_\mu\theta\partial_\nu\theta + V(f^2/m^2). \tag{17}$$

As shown below, this expression reduces to the extended Klein-Gordon Lagrangian (3) provided the first term in (17) is neglected or eliminated and also for a particular election of the potential. One possibility to eliminate the first term is to consider an effective potential that depends also on the derivatives of the scalar field,

$$V_{\mathrm{eff}}(|\Phi|,\partial_\mu|\Phi|) = V(|\Phi|) - \tfrac{1}{2}g^{\mu\nu}(\partial_\mu|\Phi|)(\partial_\nu|\Phi|).$$

In this case the starting Lagrangian (15) with this potential reduces to

$$\mathcal{L} = \tfrac{1}{2}f^2 g^{\mu\nu}\partial_\mu\theta\partial_\nu\theta + V(f^2/m^2). \tag{18}$$

One can also reach this expression (18) by neglecting the first term of (17) by considering the scale of the inhomogeneities as corresponding to the space-time variations of f on scales greater than m^{-1}, i.e., $\partial_\mu f \ll mf$. This has been considered in the context of cosmology to show that the generalized Chaplygin gas can be described by a generalized Born-Infeld Lagrangian.[5]

The field equations resulting from the variation of the Lagrangian (18) read

$$\tfrac{1}{2}g^{\mu\nu}(\partial_\mu\theta)(\partial_\nu\theta) = -V'(f^2), \tag{19a}$$

$$\nabla_\mu(f\sqrt{-g}g^{\mu\nu}\nabla_\nu\theta)=0. \tag{19b}$$

where we have set the mass to unity for simplicity. We consider a self-interacting potential V given by

$$V(|\Phi|)=\lambda(\Phi\Phi^\star)^{\alpha/(\alpha-1)}, \tag{20}$$

where λ is a constant. In this case, the action (18) becomes

$$S=\int_M d^D\vec{x}\,\mathrm{d}t\sqrt{-g}\left[\frac{1}{2}f^2(\partial_\mu\theta)(\partial^\mu\theta)+\lambda f^{2\alpha/(\alpha-1)}\right], \tag{21}$$

and the function f can be eliminated in favor of the phase θ through the equation of motion (19a),

$$f^2\propto(\partial_\sigma\theta\partial_\sigma\theta)^{\alpha-1}.$$

Finally, the substitution of this last expression into the Lagrangian (21) yields the extended Klein-Gordon action (3).

A. Conformal symmetry

In $(D+1)$ dimensions, the extended Klein-Gordon action (3) possesses the conformal invariance for a value of the parameter α given by

$$\alpha=\frac{D+1}{2}. \tag{22}$$

Indeed, it is simple to see that the trace of the energy-momentum tensor (6) vanishes for this value,

$$g^{\mu\nu}T_{\mu\nu}=[2\alpha-(D+1)](\partial_\sigma\theta\partial^\sigma\theta)^\alpha.$$

The implementation of this symmetry on the scalar field θ is with a zero conformal weight,

$$g_{\mu\nu}\to\Omega^2 g_{\mu\nu},\quad \theta\to\theta. \tag{23}$$

Various comments can be made with respect to this conformal symmetry. First, in contrast with the standard Klein-Gordon action this conformal symmetry is achieved without the introduction of the nonminimal coupling. Moreover, it is interesting to note that the scalar field action (3) remains unchanged against the transformations (23), i.e.,

$$S_{(D+1)/2}(\Omega^2 g_{\mu\nu},\theta)=S_{(D+1)/2}(g_{\mu\nu},\theta).$$

Finally, the origin of this conformal invariance can be explained as follows. It is well known that in $(D+1)$ dimension with $D>1$, the following generalized Klein-Gordon Lagrangian density:

$$\mathcal{L}_{(D,1)}=\frac{1}{2}g^{\mu\nu}(\partial_\mu\Phi)(\partial_\nu\Phi^\star)+\frac{(D-1)}{8D}R\Phi\Phi^\star+\lambda(\Phi\Phi^\star)^{(D+1)/(D-1)} \tag{24}$$

is conformally invariant. Here R represents the scalar curvature of the metric and the last term in (24) is the unique potential that preserves the conformal invariance. For convenience, we rewrite this action in terms of the module and the phase, $\Phi=fe^{i\theta}$,

$$\mathcal{L}_{(D,1)}=\frac{1}{2}\partial_\mu f\partial^\mu f+\frac{1}{2}f^2\partial_\mu\theta\partial^\mu\theta+\frac{(D-1)}{8D}Rf^2+\lambda f^{2(D+1)/(D-1)}, \tag{25}$$

and the implementation of the conformal symmetry on the dynamical fields is given by

$$g_{\mu\nu} \to \Omega^2 g_{\mu\nu}, \quad f \to \Omega^{(1-D)/2} f, \quad \theta \to \theta. \tag{26}$$

A simple but tedious computation shows that the term proportional to Rf^2 is precisely introduced to cancel the variation of the term $\partial_\mu f \partial^\mu f$ under the conformal transformation (26). Consequently, if one drops this kinetic term (as we did in the previous derivation), the following Lagrangian

$$\mathcal{L}_{(D,1)} = \frac{1}{2} f^2 g^{\mu\nu} \partial_\mu \theta \partial_\nu \theta + \lambda f^{2(D+1)/(D-1)} \tag{27}$$

also exhibits the conformal invariance. This expression corresponds precisely to the Lagrangian (21) for the conformal value of the parameter α given by (22).

B. Nonrelativistic fluid

We now establish a correspondence between the relativistic action (3) defined in $(D,1)$ dimensions and a nonrelativistic fluid in $(D-1,1)$ dimensions through a Kaluza-Klein-type framework. The clue of this correspondence lies in the fact that the quotient of a Lorentz $(D,1)$ manifold by the integral curves of a covariantly constant and lightlike vector field ξ is a $(D-1,1)$ manifold which carries the geometric structure of nonrelativistic space-time.[3]

We first illustrate this framework with a simple example. On the Lorentz manifold we consider a coordinate system given by $(t,\vec{x},z)$ where $(t,\vec{x})$ are the coordinates on the nonrelativistic space-time and z represents the additional coordinate. Let Φ be a complex scalar field satisfying the wave equation in $(D,1)$ dimensions together with an equivariance condition

$$\Box \Phi = 0, \tag{28a}$$

$$\xi^\mu \partial_\mu \Phi = i\Phi. \tag{28b}$$

This system of equations (28) has been shown to be strictly equivalent to the free Schrödinger equation in $(D-1,1)$ dimensions on a general Newton-Cartan space-time.[3]

In our case, we consider the action defined in (21) which has been shown to be equivalent to the extended Klein-Gordon action (3). The field equations associated to (21) read

$$\frac{1}{2} g^{\mu\nu} (\partial_\mu \theta)(\partial_\nu \theta) = -\frac{\lambda \alpha}{\alpha - 1} \rho^{1/(\alpha-1)}, \tag{29a}$$

$$\partial_\mu (\rho \sqrt{-g} g^{\mu\nu} \partial_\nu \theta) = 0, \tag{29b}$$

where for convenience we have substituted f^2 by ρ. In order to fix the set up of the Kaluza-Klein-type framework, we consider the Minkowski metric written in the light-cone coordinates

$$\mathrm{d}s^2 = 2\, \mathrm{d}t\, \mathrm{d}z + \mathrm{d}\vec{x}^2, \tag{30}$$

for which the lightlike vector field ξ can be chosen to be $\xi^\mu \partial_\mu = \partial_z$. Since ρ is the module and θ the phase of the complex scalar field (16), the analogue of the equivariance condition (28) is given by

$$\xi^\mu \partial_\mu \rho = 0 \Rightarrow \rho = \rho(t,\vec{x}), \tag{31a}$$

$$\xi^\mu \partial_\mu \theta = 1 \Rightarrow \theta(t,\vec{x},z) = \Theta(t,\vec{x}) + z. \tag{31b}$$

It is easy to see that on the flat background (30) and for fields ρ and θ satisfying the conditions (31), the relativistic field equations (29) project onto the following $(D-1,1)$-dimensional nonrelativistic equations:

$$\partial_t \rho + \vec{\nabla} \cdot (\rho \vec{\nabla} \Theta) = 0, \tag{32a}$$

$$\partial_t\Theta + \frac{1}{2}|\vec{\nabla}\Theta|^2 = -\frac{\lambda\alpha}{\alpha-1}\rho^{1/(\alpha-1)}. \tag{32b}$$

These equations turn out to be the nonrelativistic equations of an isentropic, irrotational and polytropic fluid. Indeed, identifying Θ as the potential velocity, i.e., $\vec{v}=\vec{\nabla}\Theta$ and ρ as the density, the first equation (32a) is a continuity relation while the gradient of the second equation (32b) yields a Euler equation of an isentropic fluid with pressure given by

$$p = \frac{\lambda}{\alpha-1}\rho^{\alpha/(\alpha-1)}. \tag{33}$$

For a potential strength $\lambda>0$ and for $\alpha=1/2$ (respectively, for $0<\alpha<1/2$), the relation (33) represents the state equation of the Chaplygin gas (respectively, the generalized Chaplygin gas). Finally, we remark that the field equations (32) can be derived from the following action principle:

$$S(\rho,\Theta) = \int d^{D-1}\vec{x}\,\mathrm{d}t\left[\rho\left(\partial_t\Theta + \frac{1}{2}|\vec{\nabla}\Theta|^2\right) + \lambda\rho^{\alpha/(\alpha-1)}\right]. \tag{34}$$

In what follows, we study the symmetries of the nonrelativistic fluid model whose dynamics is described by the equations (32).

Nonrelativistic symmetries: We analyze the dynamical symmetries of the nonrelativistic isentropic fluid described by the equations (32). This model being nonrelativistic possesses the appropriate symmetry, namely the Galileo symmetry. The action of this symmetry on the coordinates is given by

$$t \to T = t + \epsilon,$$

$$\vec{x} \to \vec{X} = \mathcal{R}\vec{x} + \vec{\delta} - \vec{\beta}t,$$

where $\mathcal{R}\in \mathrm{SO}(D-1)$, ϵ, $\vec{\delta}$, and $\vec{\beta}$ are the parameters associated to the rotations, the time translations, the space translations and the Galileo boosts, respectively. The implementation of the Galileo symmetry on the dynamical fields reads

$$\rho \to \tilde{\rho}(t,\vec{x}) = \rho(T,\vec{X})$$

and

$$\Theta \to \tilde{\Theta}(t,\vec{x}) = \Theta(T,\vec{X}) + \vec{\beta}\cdot\vec{x} - \tfrac{1}{2}|\vec{\beta}|^2 t.$$

The application of the Noether theorem yields to the following constants of motion:

$$H = \int d^{D-1}\vec{x}\mathcal{H} = \int\left[\frac{1}{2}\rho|\vec{\nabla}\Theta|^2 + \lambda\rho^{\alpha/(\alpha-1)}\right] \tag{35a}$$

$$\vec{P} = \int d^{D-1}\vec{x}\vec{\mathcal{P}} = \int d^{D-1}\vec{x}(\rho\vec{\nabla}\Theta), \tag{35b}$$

$$M_{ij} = \int d^{D-1}\vec{x}(x_i\mathcal{P}_j - x_j\mathcal{P}_i), \tag{35c}$$

$$\vec{G} = t\vec{P} - \int d^{D-1}\vec{x}(\vec{x}\rho), \tag{35d}$$

which corresponds to the energy ϵ, the momentum $\vec{\delta}$, the rotations $\mathcal{R}$ and the Galileo boosts $\vec{\beta}$, respectively. The equations are also invariant under a shift of the velocity potential by constant, $\Theta \to \Theta + \text{constant}$, and the associated conserved charge is given by

$$N = \int d^{D-1}\vec{x}\rho. \tag{36}$$

The corresponding Lie algebra generated by H, $\vec{P}$, M_{ij}, $\vec{G}$, and N is the Galileo algebra with a central extension given by (36) and corresponds to the Galileo 2-cocycle.

(i) For a generic value of the parameter α, there exists an additional symmetry which does not belong to the Galileo group. This symmetry acts on the coordinates by rescaling only the time

$$t \to T = e^{\omega}t,$$

$$\vec{x} \to \vec{X} = \vec{x}, \tag{37}$$

while its action on the dynamical fields is given by

$$\rho \to \tilde{\rho}(t,\vec{x}) = e^{2(\alpha-1)\omega}\rho(T,\vec{X}),$$

$$\Theta \to \tilde{\Theta}(t,\vec{x}) = e^{\omega}\Theta(T,\vec{X}), \tag{38}$$

or infinitesimally

$$\delta\rho = 2(\alpha-1)\rho(t,\vec{x}) + t\partial_t\rho(t,\vec{x}),$$

$$\delta\Theta = \Theta(t,\vec{x}) + t\partial_t\Theta(t,\vec{x}). \tag{39}$$

The associated conserved quantity reads

$$B_\alpha = tH - \frac{(3-2\alpha)}{2\alpha+1}\int d^{D-1}\vec{x}(\rho\Theta) - \frac{(2\alpha-1)}{2\alpha+1}\int d^{D-1}\vec{x}(\vec{x}\cdot\vec{\nabla}\Theta)\rho. \tag{40}$$

This expression is clearly not defined for $\alpha=-1/2$ in spite of the fact that this value is not singular at the level of the transformations (37) and (38). In fact, a careful application of the Noether procedure shows that for $\alpha=-1/2$ the associated conserved quantity does not involve the energy density and instead is given by

$$B_{-1/2} = \int d^{D-1}\vec{x}\left[\rho\Theta - \frac{1}{2}(\vec{x}\cdot\vec{\nabla}\Theta)\rho\right]. \tag{41}$$

In the case of the Chaplygin gas, $\alpha=1/2$, the last piece of the expression (40) vanishes and the Noether charge corresponds to the one derived in Ref. 8. Interestingly, for $\alpha \neq 1/2$, the two conserved charges (40) and (41) involve a piece proportional to the space coordinate $\vec{x}$. This fact is intriguing since the transformations (37) only affect the time and not the space coordinate. This can be explained by the fact that, under the infinitesimal changes of the dynamical fields (39), the variation of the action (34) becomes

$$\Delta S = S(\rho + \delta\rho, \Theta + \delta\Theta) - S(\rho, \Theta) = (2\alpha - 1)S(\rho, \Theta) + \int \partial_t[\rho\partial_t(t\Theta) - \rho\Theta + t\mathcal{H}], \tag{42}$$

where $\mathcal{H}$ represents the density energy (35a). For $\alpha = 1/2$, this variation (42) reduces to a surface term and, hence a direct application of the Noether theorem yields to the conserved charge (40). For $\alpha \neq 1/2$, the reason for which the transformation (37) still acts as a symmetry is due to the fact that the original action can also be written as a surface term. Indeed, using the equations of motion (32), the action (34) can be expressed on-shell as

$$S(\rho, \Theta) = \frac{1}{2\alpha + 1} \int d^{D-1}\vec{x}\, \mathrm{d}t\, \partial_t(2\rho\Theta - \rho\vec{x} \cdot \vec{\nabla}\Theta). \tag{43}$$

As a consequence, for $\alpha \neq 1/2$, the variation ΔS of the action (42) under the time dilatation transformation (37) is also a surface term. This proves that these transformations act as a symmetry for the action and also the reason for which the conserved quantities (40) and (41) involve the space coordinate $\vec{x}$.

For a generic value of the parameter α, the group structure of the symmetries is given by the semidirect sum of the Galileo group with central extension $\mathcal{G}$ with the generator associated to this extra symmetry (40),

$$G = \mathcal{G} \times \mathcal{B}. \tag{44}$$

There exist two particular values of the parameter α for which the symmetry group can be larger than the one discussed before (44).

(ii) For the value $\alpha = 1/2$, which corresponds to the Chaplygin gas, it has been shown that, apart from the time dilation (37), there exists an extra symmetry whose action is field dependent, i.e.,

$$t \to T = t + \tfrac{1}{2}\vec{\omega} \cdot (\vec{x} + \vec{X}),$$

$$\vec{x} \to \vec{X} = \vec{x} + \vec{\omega}\Theta(T, \vec{X}), \tag{45}$$

and

$$\rho \to \tilde{\rho}(t, \vec{x}) = \rho(T, \vec{X})\frac{1}{|J|},$$

$$\Theta \to \tilde{\Theta}(t, \vec{x}) = \Theta(T, \vec{X}), \tag{46}$$

where $|J|$ is the Jacobian of the transformation, $J = \det(\partial X^\mu / \partial x^\sigma)$.[8] The Noether conserved quantity is given by

$$\vec{D} = \int d^{D-1}\vec{x}\, \mathrm{d}t(\vec{x}\mathcal{H} - \Theta\vec{\mathcal{P}}), \tag{47}$$

and the group structure generated by the quantities (35), (40), and (47) is the Poincaré group in one higher dimension, namely in $(D, 1)$ dimensions. The existence of this symmetry is due to the fact that for $\alpha = 1/2$, the action expressed in terms of Θ can be written as a square root,

$$S = \int d^{D-1}\vec{x}\, \mathrm{d}t \sqrt{\partial_t\Theta + \frac{1}{2}|\vec{\nabla}\Theta|^2},$$

and this later can be seen to descend from a Nambu-Goto action in one higher dimension in the light cone parametrization.[7] This explains the arising of the Poincaré symmetry only for $\alpha = 1/2$

since for the other values of α, the action is not a square root and hence it is not longer parametrization invariant.

(iii) In $(D-1,1)$ dimensions and for a value of α given by $(D+1)/2$, the polytropic fluid exhibits a Schrödinger symmetry for which the group structure is the semidirect sum of the static Galileo group with $\mathrm{SL}(2,\mathbb{R})$, (see Refs. 13 and 14 and for an extension to discontinuous flows see Ref. 15). The arising of this symmetry is a consequence of the conformal symmetry of the relativistic model in one higher dimension.

IV. DISCUSSION

Here, we have considered the Einstein equations with a matter source scalar field. The dynamics of the scalar field is described by an extended Klein-Gordon action that depends on a real parameter α. We have restricted ourselves to a particular class of solutions for which both sides of the Einstein equations vanish. In this case, we have shown that for any static, spherically symmetric vacuum solutions of the Einstein equations, a nontrivial scalar field with zero energy-momentum on-shell can be derived. This means that this matter source in spite of being coupled to gravity does not affect the curvature of the space-time. An interesting work will consist to see whether scalar field with a nonzero energy momentum tensor can be coupled to black hole geometry. The existence of these undetectable solutions is essentially due to the form of the matter action. For this reason, some properties of this action have been analyzed. In particular, we have shown that the extended Klein-Gordon action possesses a conformal invariance for a particular value of the exponent α. This invariance does not require the introduction of the nonminimal coupling as it is the case for the standard Klein-Gordon action. We have also established a correspondence between this extended Klein-Gordon dynamics and a nonrelativistic isentropic fluid in one fewer dimension. This gas can be identified with the (generalized) Chaplygin gas for specific values of the parameter α. The nonrelativistic model corresponds to an irrotational, isentropic, and polytropic fluid. This fluid admits, apart from the Galileo symmetry, an additional symmetry. The action of this extra symmetry on the coordinate consists of a rescaling of the time only. An interesting work will consist of finding solutions of this nonrelativistic fluid and to make use of this extra symmetry to generate nontrivial solutions.

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Sojourn time for rank one perturbations

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We consider a self-adjoint, purely absolutely continuous operator M. Let P be a rank one operator $Pu=\langle\varphi,u\rangle\varphi$ such that for β_0 $H_{\beta_0}:=M+\beta_0 P$ has a simple eigenvalue E_0 embedded in its absolutely continuous spectrum, with corresponding eigenvector ψ. Let H_ω be a rank one perturbation of the operator H_{β_0}, namely, $H_\omega=M+(\beta_0+\omega)P$. Under suitable conditions, the operator H_ω has no point spectrum in a neighborhood of E_0, for ω small. Here, we study the evolution of the state ψ under the Hamiltonian H_ω, in particular, we obtain explicit estimates for its sojourn time $\tau_\omega(\psi)=\int_{-\infty}^{\infty}|\langle\psi,e^{-iH_\omega t}\psi\rangle|^2\,dt$. By perturbation theory, we prove that $\tau_\omega(\psi)$ is finite for $\omega\neq 0$, and that for ω small it is of order ω^{-2}. Finally, by using an analytic deformation technique, we estimate the sojourn time for the Friedrichs model in $\mathbb{R}^n$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2174236]

I. INTRODUCTION

A rank one perturbation of an operator H_0 may drastically change the nature of its spectrum. See for instance Refs. 2 and 16. Here we study a class of perturbations for a self-adjoint operator H_0 having a simple eigenvalue E_0 embedded in its absolutely continuous spectrum. We impose general conditions on the rank one perturbation P, $Pu=\langle\varphi,u\rangle\varphi$, which guarantee that the operator $H_\omega=H_0+\omega P$ is purely absolutely continuous. Moreover if H_0 has a normalized eigenvector ψ_0 with corresponding eigenvalue E_0 then we explicitly estimate the sojourn time $\tau_\omega(\psi_0)$, precisely,

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$$\tau_\omega(\psi_0) \sim \frac{1}{\pi}\frac{1}{\omega^2}\frac{1}{|\langle P\psi_0,\psi_0\rangle|^2\mu'_{\psi_0}(E_0)}$$

under conditions which guarantee in particular suitable regularity of the spectral measure μ_{ψ_0} of M.

In the case where M is the multiplication operator by x and φ is analytic (in the sense of Sec. V) we can use the analytic translation technique to prove that

$$\tau_\omega(\psi_0) = \frac{1}{2|\Gamma|} + O\left(\frac{1}{|\omega|}\right),$$

where $1/2\Gamma$ is the Fermi golden rule term,

$$\frac{1}{2}\Gamma = \omega^2 \operatorname{Im}\langle P\psi_0, S(E_0+i0)P\psi_0\rangle.$$

Here, $S(E_0+i0)$ is the reduced resolvent of H_{β_0} at E_0 (Ref. 8, Chap. III, Sec. 6.5, for the definition of the reduced resolvent).

There are numerous works which describe resonances by analyzing the behavior of the survival amplitude, i.e., the function $\mathbb{R} \ni t \mapsto \langle e^{-itH}\psi_0, \psi_0\rangle$, which, in many cases, include explicit exponential decay laws for this quantity. We mention, Refs. 1, 3, 4, 6, 10, 11, 17, 19, 18, and 20, for example. On the other hand, as it was suggested in Ref. 10, the study of the sojourn time seems to be an approach to resonances more general than analytic continuation techniques. (See Refs. 7, 13, and 15.)

The present work is also an attempt to give a dynamical characterization of quantum resonances, by estimating directly the sojourn time, that is, the L^2 norm of this survival amplitude, which measures the total amount of time that well chosen states remain on itself. We expect that this direct approach of the sojourn time will allow less regular Hamiltonian than the ones considered with the survival amplitude method. For example, in the concrete Friedrichs model, see Sec. IV A, we need only that our perturbation P is twice differentiable with respect to the x variable, which seems to be a rather weak condition in view of the above quoted papers. This hope must be tested with a genuine potential perturbation. Also, contrary to what is usually done, we have not localized ψ_0 within an ad hoc spectral subspace of H_ω, i.e., $g(H_\omega)\psi_0$, where g is a function localized around the embedded eigenvalue E_0; this is mainly because our assumptions on M do not allow neither thresholds nor other eigenvalues than E_0.

This paper has the following structure: in the first two sections we establish some technical facts. The following section contains our main result, the asymptotics of the sojourn time. In the last section we use the analytic translation technique to establish the connection with resonance theory.

II. RANK ONE PERTURBATIONS OF SELF-ADJOINT OPERATORS

Although the content of this section is classical, we include it for the reader's convenience. Let M be a self-adjoint operator on a Hilbert space $\mathcal{H}$. We consider rank one perturbations of M,

$$H_\beta = M + \beta P, \tag{2.1}$$

where $\beta \in \mathbb{R}$ and $P = |\varphi\rangle\langle\varphi|$ denotes the orthogonal projection $Pu = \langle\varphi, u\rangle\varphi$ and $\|\varphi\| = 1$.

Let E_x^M be the resolution of the identity associated to M, that is $M = \int_{-\infty}^{\infty} x\, \mathrm{d}E_x^M$ and let $\mu_\varphi(x) := \langle\varphi, E_x^M\varphi\rangle$. For $z \in \mathbb{C}$ with $\operatorname{Im} z > 0$ we consider the Borel transform of the measure μ_φ, that is

$$F_\varphi(z) = \langle\varphi, (M-z)^{-1}\varphi\rangle. \tag{2.2}$$

Lemma 2.1: Assume E_0 is not an eigenvalue of M. Given $\beta \neq 0$, the real number E_0 is an eigenvalue of H_β if and only if $\lim_{\epsilon\to 0}(M - E_0 - i\epsilon)^{-1}\varphi$ exists in $\mathcal{H}$ and $F_\varphi(E_0+i0) = -1/\beta$.

Proof: If $H_\beta\psi_0=E_0\psi_0$, ψ_0 normalized, then,

$$M\psi_0+\beta\langle\varphi,\psi_0\rangle\varphi=E_0\psi_0. \tag{2.3}$$

Since E_0 is not an eigenvalue of M, we have that $\langle\psi_0,\varphi\rangle\neq 0$ and φ belongs to the range of $M-E_0$.

On the other hand,

$$(M-E_0)(M-E_0-i\epsilon)^{-1}\psi_0=-\beta\langle\varphi,\psi_0\rangle(M-E_0-i\epsilon)^{-1}\varphi.$$

But $(M-E_0)(M-E_0-i\epsilon)^{-1}$ is a bounded operator which is strongly convergent to the identity as ϵ approaches 0. By computing such limit we have that $\psi:=\lim_{\epsilon\to 0}(M-E_0-i\epsilon)^{-1}\varphi$ exists and it satisfies $\psi_0+\beta\langle\varphi,\psi_0\rangle\psi=0$. It follows that,

$$F_\varphi(E_0+i0)=\langle\varphi,\psi\rangle=-\frac{1}{\beta}.$$

Conversely, if both conditions hold, then $\psi:=\lim_{\epsilon\to 0}(M-E_0-i\epsilon)^{-1}\varphi$ satisfies $\langle\varphi,\psi\rangle=-1/\beta$. Consider $\psi(\epsilon)=(M-E_0-i\epsilon)^{-1}\varphi$. Then,

$$(M-E_0)\psi(\epsilon)=(M-E_0)(M-E_0-i\epsilon)^{-1}\varphi,$$

converges to φ, when ϵ approaches 0. Since M is a closed operator, we obtain that ψ belongs to the domain of M and $(M-E_0)\psi=\varphi$.

Hence, $M\psi-\varphi=E_0\psi$. The eigenvalue equation (2.3) follows from the identity $-1=\beta\langle\varphi,\psi\rangle$.

□

Corollary 2.1: Let E_0 be an eigenvalue of H_β. Then E_0 is simple with eigenvector $\psi=\lim_{\epsilon\to 0}(M-E_0-i\epsilon)^{-1}\varphi$. Also,

$$\|\psi\|^2=\int_{-\infty}^{\infty}\frac{d\mu_\varphi}{(x-E_0)^2}\quad \textit{and}\ \langle\psi,\varphi\rangle=\int_{-\infty}^{\infty}\frac{d\mu_\varphi}{x-E_0}. \tag{2.4}$$

Proof: The first part of the corollary follows from the proof of the Lemma 2.1. To prove formula (2.4), we note that since $\|\psi\|^2=\lim_{\epsilon\to 0}\|(M-E_0-i\epsilon)^{-1}\varphi\|^2$ exists, by the monotone convergence theorem,

$$\int_{\mathbb{R}}\frac{d\mu_\varphi}{(x-E_0)^2}=\lim_{\epsilon\to 0}\int_{\mathbb{R}}\frac{d\mu_\varphi}{(x-E_0)^2+\epsilon^2}=\|\psi\|^2.$$

So the integrals $\int_{\mathbb{R}}[d\mu_\varphi/(x-E_0)^2]$ and $\int_{\mathbb{R}}(d\mu_\varphi/|x-E_0|)$ are finite. The Lebesgue theorem then implies

$$\langle\psi,\varphi\rangle=\lim_{\epsilon\to 0}\int_{\mathbb{R}}\frac{d\mu_\varphi}{(x-E_0)+i\epsilon}+\int_{\mathbb{R}}\frac{d\mu_\varphi}{x-E_0}.$$

□

We now consider a family of rank one perturbations of the operator $H_{\beta_0}=M+\beta_0 P$ on $\mathcal{H}$, explicitly,

$$H_\beta=M+\beta|\varphi\rangle\langle\varphi|, \tag{2.5}$$

where $\varphi\in\mathcal{H}$ is a fixed unit vector. We are mainly interested on studying the time behavior of possible bound states of H_{β_0}, under the Hamiltonian H_β, for β near β_0.

Let us assume that $H_{\beta_0}=M+\beta_0|\varphi\rangle\langle\varphi|$ has an eigenvalue E_0 with corresponding eigenvector ψ. Because of Lemma 2.1 and Corollary 2.1, this means that $1+\beta_0\lim_{\epsilon\to 0}F_\varphi(E_0+i\epsilon)=0$ and

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\mu_\varphi}{(x-E_0)^2} < \infty.$$

Our goal is to study the time evolution of ψ under the perturbed Hamiltonian H_β for the parameter ω close to zero.

For this purpose, we study the function

$$\mathbb{R} \ni t \mapsto |\langle \psi, e^{-iH\beta t}\psi\rangle|^2$$

which represents the probability of finding at time t the system in its initial state ψ, and

$$\tau_\omega(\psi) = \int_{-\infty}^{\infty} |\langle \psi, e^{-iH\beta t}\psi\rangle|^2 \,\mathrm{d}t, \quad \omega = \beta - \beta_0 \tag{2.6}$$

which measures the total amount of time the state remains in its initial subspace $\{s\psi : s \in \mathbb{C}\}$. We observe that $|\langle \psi, e^{-iH_{\beta_0}t}\psi\rangle|^2 = 1$ for all t and so $\tau_0(\psi)$ is infinite.

We shall prove that for $\omega \neq 0$ and small, the sojourn time $\tau_\omega(\psi)$ is finite and of order ω^{-2}, when the operator H_β has no bound states [see assumption (H3)].

III. FINITENESS OF THE SOJOURN TIME OF ψ

Let H be a self-adjoint operator on a complex Hilbert space $\mathcal{H}$. For any vector ϕ in the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(H)$ associated to H, we know that

$$\langle \phi, e^{-iHt}\phi\rangle = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} e^{-i\lambda t}\, \mathrm{Im}\langle \phi, (H - \lambda - i0)^{-1}\phi\rangle \mathrm{d}\lambda.$$

This allows us to express the sojourn time in terms of resolvent operators, explicitly,

$$\tau(\psi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\mathrm{Im}\langle \psi, (H - \lambda - i0)^{-1}\psi\rangle|^2 \,\mathrm{d}\lambda. \tag{3.1}$$

It is known that (2.6) and (3.1) are both valid expressions for the sojourn time, as soon as the survival amplitude $\mathbb{R} \ni t \mapsto (e^{-itH}\varphi, \varphi)$ is in $L^2(\mathbb{R})$, see Ref. 12.

In all what follows, we assume the following hypothesis.

(H0): *M is a purely absolutely continuous operator acting on the Hilbert space $\mathcal{H}$, $\varphi \neq 0$ a normalized element of $\mathcal{H}$, $P := |\varphi\rangle\langle\varphi|$ and $H_\beta := M + \beta P$.*

(H1): *There exists $\beta_0 \neq 0$, such that H_{β_0} has a unique eigenvalue E_0, $H_{\beta_0}\psi = E_0\psi$.* Notice that, by Lemma 2.1, this implies in particular that $\psi := (M - E_0 \pm i0)^{-1}\varphi$ exists in $\mathcal{H}$ and $\langle \varphi, \varphi\rangle = -\beta_0^{-1}$.

(H2): *The function $\lambda \in \mathbb{R} \mapsto \langle \varphi, (M - \lambda - i0)^{-1}\varphi\rangle \in \mathbb{C}$ is continuous. We assume moreover that*

$$\lim_{|\lambda| \to \infty} \langle \varphi, (M - \lambda - i0)^{-1}\varphi\rangle = 0.$$

Notice that, by the first resolvent equation, this implies in particular that

$$\mathbb{R} \setminus \{E_0\} \ni \lambda \mapsto \langle \psi, (M - \lambda - i0)^{-1}\psi\rangle \in \mathbb{C}$$

exists as a continuous function.

(H3): *There exists $\omega_0 > 0$ such that for all $0 < |\omega| \leqslant \omega_0$, the function*

$$D(\lambda, \omega) := 1 + (\beta_0 + \omega)\langle \varphi, (M - \lambda - i0)^{-1}\varphi\rangle$$

does not vanish, for any $\lambda \in \sigma(M)$. Clearly, for such ω, the operator $H_{\beta_{0+\omega}}$ has no eigenvalues.

(H4): *The function $\lambda \mapsto \langle \psi, (M - \lambda - i0)^{-1}\psi\rangle \in \mathbb{C}$ is of class C^1 in a neighborhood of E_0, that is,*

$$g(\lambda) := \mathrm{Re}\langle \psi, (M - \lambda - i0)^{-1}\psi\rangle,$$

$$\mu'_\varphi(\lambda) := \frac{1}{\pi}\,\mathrm{Im}\langle\psi,(M-\lambda-i0)^{-1}\psi\rangle$$

exist and they are C^1 *functions in a neighborhood of* E_0.
(H5): *The function* μ'_ψ *belongs to* $L^2(\mathbb{R})$.
(H6): $\mu'_\psi(E_0)>0$.
Concerning the resolvent operators, we use the following notation:

$$R_\omega(z)=(H_\beta-z)^{-1},\quad R_0(z)=(H_{\beta_0}-z)^{-1},\quad R(z)=(M-z)^{-1},$$

where $\omega=\beta-\beta_0$. The Aronszjan-Krein formula[9,16] expresses the resolvent $R_\omega(z)$ in terms of $R_0(z)$ for any $z=\lambda+i\epsilon\in\mathbb{C}$, with $\epsilon\neq 0$. This formula gives

$$R_\omega = R_0 - \frac{\omega}{1+\omega\langle\varphi,R_0\varphi\rangle}R_0PR_0. \tag{3.2}$$

Similarly,

$$R_0 = R - \frac{\beta_0}{1+\beta_0\langle\varphi,R\varphi\rangle}RPR. \tag{3.3}$$

Again, we use the Borel transform $F_\varphi(z)=\langle\varphi,(M-z)^{-1}\varphi\rangle$, which, because of (3.3) gives

$$\langle\varphi,R_0(z)\varphi\rangle=\frac{F_\varphi(z)}{1+\beta_0F_\varphi(z)}.$$

Thus, by replacing in (3.2),

$$R_\omega = R_0 - \omega\frac{1+\beta_0F_\varphi}{1+(\beta_0+\omega)F_\varphi}R_0|\varphi\rangle\langle\varphi|R_0. \tag{3.4}$$

Since, $\mu_\varphi(\lambda)=\langle\varphi,E^M_\lambda\varphi\rangle$, for any positive ϵ we have that

$$F_\varphi(z)=\int_{-\infty}^{\infty}\frac{x-\lambda}{(x-\lambda)^2+\varepsilon^2}\mathrm{d}\mu_\varphi(x)+i\int_{-\infty}^{\infty}\frac{\varepsilon}{(x-\lambda)^2+\varepsilon^2}\mathrm{d}\mu_\varphi(x). \tag{3.5}$$

By our hypothesis, we have that $\mathrm{d}\mu_\varphi(\lambda)=\mu'_\varphi(\lambda)\mathrm{d}\lambda=(1/\pi)\mathrm{Im}\,F_\varphi(\lambda+i0)\mathrm{d}\lambda$, where μ'_φ denotes the Radon-Nikodym derivative of the measure μ_φ relative to the Lebesgue measure. So the limit when $\varepsilon\to 0$ in (3.5) exists thanks to (H6) and gives

$$F_\varphi(\lambda+i0)=PV\int_{-\infty}^{\infty}\frac{\mu'_\varphi(x)}{x-\lambda}\mathrm{d}x+i\pi\mu'_\varphi(\lambda), \tag{3.6}$$

where the first term on the right-hand side of (3.6) is the Cauchy principal value.

Lemma 3.1: Suppose that (H0), (H1), (H2), (H3), and (H5) hold. Then, for all $0<|\omega|\leqslant\omega_0$ *is finite and*

$$\tau_\omega(\psi)=\frac{2\pi\omega^4}{\beta_0^4}\int_{\mathbb{R}}\frac{|\mu'_\psi(\lambda)|^2}{|D(\omega,\lambda)|^4}\mathrm{d}\lambda, \tag{3.7}$$

where

$$D(\lambda,\omega):=1+(\beta_0+\omega)F_\varphi(\lambda+i0). \tag{3.8}$$

Proof: From the formula (3.1), we only need to compute $\mathrm{Im}\langle\psi,R_\omega(\lambda+i0)\psi\rangle$ for $\lambda\neq E_0$.

Since $H_{\beta_0}\psi=E_0\psi$ and $\psi=(M-E_0-i0)^{-1}\varphi$, we have that $\beta_0\langle\psi,\varphi\rangle=-1$. Hence, the identity (3.4) gives

$$\langle \psi, R_\omega(z)\psi\rangle = \frac{1}{E_0 - z}\|\psi\|^2 - \omega\frac{1+\beta_0 F_\varphi(z)}{1+(\beta_0+\omega)F_\varphi(z)}\frac{1}{\beta_0^2(E_0-z)^2}.$$

Consider $z=\lambda+i\epsilon$ with $\epsilon>0$. Hypothesis (H2) allows us to compute the limit as $\varepsilon\to 0$ to obtain that

$$\langle \psi, R_\omega(\lambda+i0)\psi\rangle = \frac{1}{(E_0-\lambda)}\|\psi\|^2 - \frac{\omega}{\beta_0^2(E_0-\lambda)^2}\lim_{\varepsilon\to 0}\frac{1+\beta_0 F_\varphi(\lambda+i\epsilon)}{1+(\beta_0+\omega)F_\varphi(\lambda+i\epsilon)}.$$

By taking the imaginary part, it follows immediately that

$$\mathrm{Im}\langle \psi, R_\omega(\lambda+i0)\psi\rangle = -\frac{\omega}{\beta_0^2(E_0-\lambda)^2}\lim_{\varepsilon\to 0}\mathrm{Im}\frac{1+\beta_0 F_\varphi(z)}{1+(\beta_0+\omega)F_\varphi(z)}.$$

Now,

$$\mathrm{Im}\frac{1+\beta_0 F_\varphi(z)}{1+(\beta_0+\omega)F_\varphi(z)} = \frac{\omega\,\mathrm{Im}\,\overline{F_\varphi}(z)}{|1+(\beta_0+\omega)F_\varphi(z)|^2}.$$

Hence, by using that $[1/(E_0-\lambda)^2]\mu_\varphi'(\lambda)=\mu_\psi'(\lambda)$ we conclude that

$$\mathrm{Im}\langle \psi, R_\omega(\lambda+i0)\psi\rangle = -\frac{\omega^2}{\beta_0^2(E_0-\lambda)^2}\lim_{\varepsilon\to 0}\frac{\mathrm{Im}\,\overline{F_\varphi}(\lambda+i\epsilon)}{|1+(\beta_0+\omega)F_\varphi(\lambda+i\epsilon)|^2} = \frac{\omega^2}{\beta_0^2}\frac{\pi\mu_\psi'(\lambda)}{|D(\lambda,\omega)|^2}$$

for any $\lambda\neq E_0$, thus ending the proof. The integral of (3.7) makes sense, i.e., is finite, thanks to (H2), (H3), and (H5). □

IV. EXACT ASYMPTOTICS FOR τ_ω

In this section we prove the explicit asymptotics for the sojourn time in a general context and we will apply it to some concrete examples.

Theorem 4.1: *Assume that* (H0)–(H6) *holds. Then the sojourn time* $\tau_\omega(\psi)$ *has the following behavior:*

$$\lim_{\omega\to 0}\omega^2\tau_\omega(\psi) = \frac{1}{\pi}\frac{\beta_0^2\|\psi\|^{10}}{\mu_\varphi'(E_0)}.$$

Proof: By using the first resolvent equation and (H1), we can rewrite $D(\lambda,\omega)$ as

$$D(\lambda,\omega) = 1+\beta\langle\varphi, R(\lambda+i0)\varphi\rangle = 1-\frac{\beta}{\beta_0}+\beta(\lambda-E_0)\langle\psi, R(\lambda+i0)\varphi\rangle.$$

By (H4) and applying the resolvent equation twice, we obtain that

$$D(\lambda,\omega) = -\frac{\omega}{\beta_0}+\beta(\lambda-E_0)q(\lambda)+i\pi\beta(\lambda-E_0)^2\mu_\psi'(\lambda)$$

with

$$q(\lambda) := \|\psi\|^2+(\lambda-E_0)g(\lambda).$$

By Lemma 3.1 we known that $\tau_\omega(\psi)$ is finite and it is represented by (3.7).

Consider the interval $I_\delta := \{\lambda\in\mathbb{R}, |\lambda-E_0|\leq\delta\}$ for some $\delta>0$. Let us split the integral in two parts,

$$A_\delta := \frac{2\pi\omega^6}{\beta_0^4}\int_{I_\delta}\frac{|\mu_\psi'(\lambda)|^2}{|D(\lambda,\omega)|^4}\mathrm{d}\lambda, \quad B_\delta := \frac{2\pi\omega^6}{\beta_0^4}\int_{\mathbb{R}\setminus I_\delta}\frac{|\mu_\psi'(\lambda)|^2}{|D(\lambda,\omega)|^4}\mathrm{d}\lambda.$$

We will prove first that $B_\delta \to 0$ as $\omega \to 0$ and second that A_δ tends to the desired limit using the Lebesgue dominated convergence theorem.

We get at once that $B_\delta = \mathcal{O}(\omega^6)$ since $|D(\lambda,\omega)| \geqslant c_\delta > 0$ on $\mathbb{R}\setminus I_\delta$, and μ_ψ' belongs to $L^2(\mathbb{R})$ by assumption (H5).

For $\omega \neq 0$ one defines

$$s_\omega(\lambda) := \omega^{-2}(-\omega\beta_0^{-1} + \beta(\lambda - E_0)q(\lambda)).$$

Thanks to (H4) we know that $g(\lambda)$ is a C^1 function in a neighborhood I_{δ_g} of E_0. Then s is a C^1 function with derivative

$$s_\omega'(\lambda) = \frac{\beta(q(\lambda) + (\lambda - E_0)q'(\lambda))}{\omega^2}$$

in I_{δ_g} and $s_\omega'(E_0) = \omega^{-2}\beta\|\psi\|^2$.

We choose $\omega_0 \leqslant |\beta_0|/2$ so that β does not vanish and therefore E_0 is not a critical point of s_ω. By the inverse mapping theorem we know that s_ω is locally in E_0 a C^1 diffeomorphism, i.e., we can choose $\delta_s > 0$ small enough so that the restriction of s_ω to I_{δ_s} is such a C^1-diffeomorphism. In view of the explicit dependence of s_ω with respect to ω one can choose this δ_s independently of ω. We continue to denote δ_s by δ. We note that

$$s \in \widetilde{I}_\delta \Leftrightarrow \left| s + \frac{1}{\omega\beta_0}\right| < \delta\frac{|\beta q(\lambda(s))|}{\omega^2}.$$

Let $\widetilde{I}_\delta \ni s \mapsto \lambda_\omega(s) \in I_\delta$ be the inverse of the previous change of variable. The quantities D and A_δ can now be written as

$$D(\lambda_\omega(s),\omega) = \omega^2 s + \frac{i\pi}{\beta}\left(\frac{\omega^2 s + \omega\beta_0^{-1}}{q(\lambda_\omega(s))}\right)^2 \mu_\psi'(\lambda_\omega(s)) =: \omega^2\widetilde{D}(s,\omega)$$

with

$$\widetilde{D}(s,\omega) = s + \frac{i\pi}{\beta}\left(\frac{\omega s + \beta_0^{-1}}{q(\lambda_\omega(s))}\right)^2 \mu_\psi'(\lambda_\omega(s))$$

and

$$\begin{aligned} A_\delta &= \frac{2\pi\omega^6}{\beta_0^4}\int_{\widetilde{I}_\delta}\frac{|\mu_\psi'(\lambda_\omega(s))|^2}{\omega^8|\widetilde{D}(s,\omega)|^4}\frac{\omega^2}{\beta(q(\lambda_\omega(s)) + (\lambda_\omega(s) - E_0)q'(\lambda_\omega(s)))}\mathrm{d}s \\ &= \frac{2\pi}{\beta\beta_0^4}\int_{\mathbb{R}} 1_{\widetilde{I}_\delta}\frac{|\mu_\psi'(\lambda_\omega(s))|^2}{|\widetilde{D}(s,\omega)|^4}\frac{1}{q(\lambda_\omega(s)) + (\lambda_\omega(s) - E_0)q'(\lambda_\omega(s))}\mathrm{d}s, \end{aligned}$$

where $1_{\widetilde{I}_\delta}$ denotes the characteristic function of I_δ.

We know that $q(\lambda) = \|\psi\|^2 + (\lambda - E_0)g(\lambda)$ and g is assumed to be C^1 on I_{δ_g} so g is bounded there. Therefore we can choose $0 < \delta_q < \min\{\delta_g, \delta_s\}$ small enough such that $q(\lambda) \geqslant \frac{1}{2}\|\psi\|^2$ on I_{δ_q}. In view of

$$\forall s \in I_{\delta_s}, \quad \omega^2 s + \omega\beta_0^{-1} = \beta(\lambda(s) - E_0)q(\lambda(s))$$

we see at once that $\lim_{\omega\to 0}\lambda_\omega(s) = E_0$. Then, by assumption (H4),

$$\lim_{\omega\to 0}\mu'_\psi(s)=\mu'_\psi(E_0),\quad \lim_{\omega\to 0}\tilde{D}(s,\omega)=s+\frac{i\pi}{\beta_0^3\|\psi\|^4}\mu'_\psi(E_0)$$

and

$$\lim_{\omega\to 0}\frac{1}{(q(\lambda_\omega(s))+(\lambda_\omega(s)-E_0)q'(\lambda_\omega(s)))}=\frac{1}{\|\psi\|^2}.$$

Therefore,

$$\lim_{\omega\to 0}(\text{integrand})=\frac{2\pi}{\beta_0^5}\frac{|\mu'_\psi(E_0)|^2}{\left|s^2+\frac{\pi^2|\mu'_\psi(E_0)|^2}{\beta_0^6\|\psi\|^8}\right|^2}=\frac{1}{\|\psi\|^2}.$$

By formal integration one arrives at

$$\frac{2\pi}{\beta_0^5}\frac{|\mu'_\psi(E_0)|^2}{\|\psi\|^2}\int_{\mathbb{R}}\frac{1}{\left|s^2+\frac{|\pi\mu'_\psi(E_0)|^2}{\beta_0^6\|\psi\|^8}\right|^2}\mathrm{d}s=\frac{2\pi}{\beta_0^5}\frac{|\mu'_\psi(E_0)|^2}{\|\psi\|^2}\frac{\pi}{2\left(\frac{\pi|\mu'_\psi(E_0)|}{\beta_0^3\|\psi\|^4}\right)^3}=\frac{\beta_0^4}{\pi}\frac{\|\psi\|^{10}}{|\mu'_\psi(E_0)|}.$$

Then, it remains to justify the interchange of the limit with the integral.

First we have

$$|\tilde{D}(s,\omega)|^2=s^2+\frac{\pi^2}{\beta^2}\left(\frac{\omega s+\beta_0^{-1}}{q(\lambda_\omega(s))}\right)^4(\mu'_\psi(\lambda_\omega(s)))^2.$$

Due to assumptions (H4), (H6) we know that there exists a neighborhood of E_0 on which $\mu'_\psi>0$. Let K be a compact interval which contains 0 in its interior, the image of K in the λ variable is a compact interval which contains E_0 and shrinks as $\omega\to 0$. So for $|\omega|$ small enough we are sure that $\mu'_\psi(\lambda_\omega(s))^2\geqslant c>0$ with c independent of ω. Since we can also easily make that the quantity $(1/\beta^2)(\omega s+\beta_0^{-1}/q(\lambda_\omega(s)))^4$ is also bounded below uniformly with respect to ω we get that

$$\exists\,\omega_0>0,\quad \forall\, s\in K,\quad \forall\,|\omega|\leqslant\omega_0,\quad |\tilde{D}(s,\omega)|^2\geqslant c>0.$$

It follows that

$$\forall\, s\in\tilde{I}_\delta,\quad |\tilde{D}(s,\omega)|^2\geqslant\max\{s^2,c\}.$$

Then since g is C^1 on I_{δ_g} one has that $\lambda\mapsto q(\lambda)-(\lambda-E_0)q'(\lambda)$ is C^0 on I_{δ_g} and since $q(E_0)=\|\psi\|^2>0$ one can choose $\delta:=\delta_g$ small enough so that

$$\forall\, s\in\tilde{I}_\delta,\quad q(\lambda_\omega(s))+(\lambda_\omega(s)-E_0)q'(\lambda_\omega(s))\geqslant c>0.$$

Finally thanks to (H4) we can choose δ small enough so that $|\mu'_\psi|\leqslant c_1$ on I_δ. In conclusion we have obtained

$$\exists\,\delta>0,\quad \exists\,\omega_0>0,\quad \forall\, s\in\tilde{I}_\delta,\quad \forall\,|\omega|\leqslant\omega_0,\quad 0\leqslant\text{integrand}\leqslant\frac{4\pi}{\beta_0^5}\frac{c_1^2}{\max\{s^4,c^2\}c}$$

and since outside $\tilde{I}_\delta$ the integrand vanishes this bound is valid on $\mathbb{R}$. □

A. The Friedrichs model

The Friedrichs model corresponds to a very simple choice of the operator M, namely, the multiplication operator $M\varphi(x)=x\varphi(x)$ acting in $\mathcal{H}:=L^2(\mathbb{R})$. The operator M with domain $D(M)=\{\varphi: x\varphi\in L^2(\mathbb{R})\}$ is purely absolutely continuous with spectrum $\sigma(M)=\mathbb{R}$. Moreover, its spectral measure is given by $\mu'_\varphi(x)=\langle\varphi, E_x^M\varphi\rangle=|\varphi(x)|^2$.

We consider the rank one perturbation $H_\beta=M+\beta|\varphi\rangle\langle\varphi|$. In order to verify our hypothesis, we impose on the vector φ the following conditions.

(F0): φ is normalized in $\mathcal{H}$.

(F1): φ belongs to the Sobolev space $\mathcal{H}^2(\mathbb{R})$.

(F2): φ has a unique zero at $x=E_0$.

(F3): $\beta_0\neq 0$ and φ satisfy the relation

$$1+\beta_0\int_{-\infty}^{\infty}\frac{|\varphi(x)|^2}{x-E_0}\mathrm{d}x=0.$$

(F4): $\varphi'(E_0)\neq 0$, and $\varphi\in C^2$ in a neighborhood of E_0.

Clearly (H0) holds. On the other hand, conditions (F1)–(F3) imply hypothesis (H1)–H(5). Also, (F4) guarantees condition (H6). By Theorem 4.1 we deduce the following result.

Theorem 4.2 (Friedrichs model): *Assume that* (F1)–(F4) *holds. Then the sojourn time* $\tau_\omega(\psi)$ *has the following behavior:*

$$\lim_{\omega\to 0}\omega^2\tau_\omega(\psi)=\frac{1}{\pi}\frac{\beta_0^4\|\psi\|^{10}}{|\psi(E_0)|^2},$$

or else if $\psi_0:=\psi\|\psi\|^{-1}$ *denotes the normalized eigenvector then*

$$\tau_\omega(\psi_0)\overset{\omega\to 0}{\sim}\frac{1}{\pi}\frac{1}{\omega^2}\frac{1}{|\langle P\psi_0,\psi_0\rangle\psi_0(E_0)|^2}.$$

Actually conditions (F1)–(F4) can be relaxed by asking local properties, around E_0, for the vector φ.

B. Model $M=X^2$

Another choice of the operator M is the multiplication by x^2 in $\mathcal{H}:=L^2(\mathbb{R})$, which it is purely absolutely continuous with spectrum $\sigma(M)=[0,\infty)$. Its spectral measure is just

$$\mu'_\phi(\lambda)=\begin{cases}0 & \text{if } \lambda<0,\\ \dfrac{|\phi(\sqrt{\lambda})|^2+|\phi(-\sqrt{\lambda})|^2)}{2\sqrt{\lambda}} & \text{if } \lambda>0.\end{cases}$$

Again, we consider rank one perturbations $H_\beta=M+\beta|\varphi\rangle\langle\varphi|$. As we mentioned in the Introduction, in order to apply our results we must choose φ as $g(M)$ times an adequate function, where g is a suitable cutoff function. It is easy to verify that if we just take $g(x)=x^2$ and φ_0 satisfies

(1) φ_0 is in the Schwartz' class and $\varphi_0(x)>0$, for all $x\in\mathbb{R}$,
(2) $\int_{-\infty}^{\infty}(x^2-E_0)x^4|\varphi_0|^2=-1/\beta_0$,
(3) $\int_{-\infty}^{\infty}(x^2-E_0)x^4|\varphi_0|^2\neq\int_{-\infty}^{\infty}(x^2-E_0)^2x^2|\varphi_0|^2$, and
(4) $\int_{-\infty}^{\infty}(x^2-E_0)^2x^4|\varphi_0|^2=1$.

then, with E_0 positive and $\varphi(x)=g(M)(x^2-E_0)\varphi_0(x)=x^2(x^2-E_0)\varphi_0(x)$ all the hypothesis (H0)–(H6) are satisfied.

V. SOJOURN TIME AND RESONANCES DEFINED BY ANALYTIC TRANSLATION

This section is concerned with the connection between the sojourn time and the resonance width which can be shown for the Friedrichs model in $L^2(\mathbb{R}^n)$, $n \geqslant 1$. We first recall its definition.

Let $\mathbf{e}=(e_1,e_2,\ldots,e_n)$ be a unit vector in $\mathbb{R}^n$ and consider the multiplication operator by the function $\mathbf{e}\cdot x=\sum_{i=1}^n e_i x_i$, i.e., the operator

$$(M\phi)(x) = \mathbf{e}\cdot x\phi(x). \tag{5.1}$$

We denote by $\mathcal{D}$ its natural domain. Let now $\varphi \in L^2(\mathbb{R}^n)$, $\|\varphi\|=1$ and denote by P the projector on the vector φ. Then the Friedrichs operators,

$$H(\beta) = M + \beta P, \quad \beta \in \mathbb{R} \tag{5.2}$$

with domain $\mathcal{D}$ are well defined in $L^2(\mathbb{R}^n)$ as self-adjoint operators. We are interested in the study of the sojourn time associated to the dynamics defined from the family of Hamiltonians $\{H_\beta, \beta \in \mathbb{R}\}$ for a dense subset of vectors of $L^2(\mathbb{R}^n)$ (Ref. 12, p. 88). We shall estimate the time evolution under $H(\beta)$ and the sojourn time, following a method developed by Herbst in the context of Stark effect see, e.g., Refs. 3 and 4. From now we use the notation $H := H(\beta)$.

For $\theta \in \mathbb{R}$, define the following family of unitary transformations:

$$\forall\, \phi \in L^2(\mathbb{R}^n), \quad (U_\theta\phi)(x) := \phi(x - \theta\mathbf{e}). \tag{5.3}$$

Then, U_θ; $\theta \in \mathbb{R}$ is a strongly continuous one-parameter unitary group and

$$H_\theta := U_\theta H U_\theta^{-1} = M_\theta + \beta P_\theta, \quad M_\theta = \mathbf{e}\cdot x - \theta, \tag{5.4}$$

where P_θ is the projector on the span generated by the vector $\varphi_\theta := U_\theta\varphi$.

Our general assumption is the following.

(HA): There exists some $a>0$ such that the vector valued function, $\mathbb{R} \ni \theta \to \varphi_\theta \in L^2(\mathbb{R}^n)$ has an analytic extension in the strip $\mathcal{S}_a := \{z \in \mathbb{C}, |\mathrm{Im}\, z| < a\}$.

We denote by $\mathcal{D}_a$ the set of vectors satisfying the assumption (HA). This set is a dense subset of $L^2(\mathbb{R}^n)$.[5]

We extend P_θ, for $\theta \in S_a$ by

$$\forall\, \phi \in L^2(\mathbb{R}^n), \quad P_\theta\phi := \langle \varphi_{\bar\theta}, \phi\rangle \varphi_\theta$$

which is an analytic family of rank one operators. Then $\{H_\theta; \theta \in \mathcal{S}_a\}$ is a self-adjoint analytic family of type A operators.[8] Moreover, due to the Weyl theorem,[14] we have that $\sigma_{\mathrm{ess}}(H_\theta) = \sigma_{\mathrm{ess}}(H_{0,\theta}) = \mathbb{R} - i\,\mathrm{Im}\,\theta$. Our first technical result is the following.

Lemma 5.1: Suppose that (HA) *is satisfied. Then for* $a > \mathrm{Im}\,\theta > 0$ *and* $0 < \epsilon \leqslant 1$, *there exists a positive energy e such that*

$$\sup\{\|(H_\theta - z)^{-1}\|;\ z \in \mathbb{C},\ |\mathrm{Re}\, z| \geqslant e,\ \mathrm{Im}\, z \geqslant -\mathrm{Im}\,\theta(1-\epsilon)\} < \infty. \tag{5.5}$$

Lemma 5.1, together with the discreteness of the spectrum in $\{z \in \mathbb{C}, \mathrm{Im}\, z > -\mathrm{Im}\,\theta\}$ imply that for $a > \mathrm{Im}\,\theta \geqslant 0$, the operators H_θ have only a finite number of eigenvalues localized in the compact set $\{z \in \mathbb{C}, 0 \geqslant \mathrm{Im}\, z \geqslant -\mathrm{Im}\,\theta(1-\epsilon), |\mathrm{Re}\, z| \leqslant e\}$, $0 < \epsilon \leqslant 1$. Some of them can be real, in that case they correspond to embedded eigenvalues for the self-adjoint operator H while the nonreal eigenvalues correspond to resonances for the pair (M,H) (see, e.g., Refs. 14 and 4). Notice that the upper bound on the number of eigenvalues given by the proof below diverges when a tends to 0.

Proof: Because of the unitary property for real θ, it is sufficient to choose $\theta = i\eta$, $a > \eta > 0$. Then for $z \in \mathbb{C}$, $\mathrm{Im}\, z > -\eta$ we have

$$\|(M_{i\eta} - z)^{-1}\| \leqslant (\eta + \mathrm{Im}\, z)^{-1}. \tag{5.6}$$

Recall that by the Aronszjan-Krein formula we get

$$(H_{i\eta}-z)^{-1}=(M_{i\eta}-z)^{-1}-\beta\frac{(M_{i\eta}-z)^{-1}P_{i\eta}(M_{i\eta}-z)^{-1}}{1+\beta\langle\varphi_{-i\eta},(M_{i\eta}-z)^{-1}\varphi_{i\eta}\rangle}. \tag{5.7}$$

Hence the lemma is proven if we show that the denominator on the right-handside (rhs) of (5.7) is uniformly bounded below by a strictly positive constant. Then consider the following integral:

$$I=\int_{\mathbb{R}^n}\mathrm{d}x\frac{|\varphi_{i\eta}(x)|^2}{(|\mathbf{e}\cdot x-\mathrm{Re}\,z|^2+|\eta+\mathrm{Im}\,z|^2)^{1/2}}. \tag{5.8}$$

For $\delta>0$ let $\Omega_\delta:=\{x\in\mathbb{R}^n,|\mathbf{e}\cdot x-\mathrm{Re}\,z|\geqslant\delta\}$ and Ω_δ^c its complement, accordingly let

$$I_\delta=\int_{\Omega_\delta}\mathrm{d}x\frac{|\varphi_{i\eta}(x)|^2}{(|\mathbf{e}\cdot x-\mathrm{Re}\,z|^2+|\eta+\mathrm{Im}\,z|^2)^{1/2}}$$

and $I_\delta^c=I-I_\delta$. Since obviously

$$I_\delta\leqslant\frac{\|\varphi_{i\eta}\|^2}{\delta}$$

we can choose $\delta>0$ such that $I_\delta\leqslant 1/4$. On the other hand,

$$I_\delta^c\leqslant\frac{1}{|\eta+\mathrm{Im}\,z|}\int_{\Omega_\delta^c}|\varphi_{i\eta}(x)|^2\,\mathrm{d}x$$

but the rhs of this last inequality goes to zero as $|\mathrm{Re}\,z|$ goes to infinity, uniformly in $\mathrm{Im}\,z\geqslant-\eta(1-\epsilon)$. Hence there exists a positive energy e such that for $z\in\mathbb{C}$, $|\mathrm{Re}\,z|\geqslant e$, $\mathrm{Im}\,z\geqslant-\eta(1-\epsilon)$, $I_\delta^c\leqslant 1/4$ and then $1+|\langle\varphi_{-i\eta},(M_{i\eta}-z)^{-1}\varphi_{i\eta}\rangle|\geqslant 1/2$ which finishes to prove the lemma. □

We turn now on the dynamics defined by the operators (5.2). Let $\{E_j\}_{j=1,\ldots,N}$ be the real eigenvalues of H and $\{\Pi_j\}_{j=1,\ldots,N}$ the associated orthogonal eigenprojectors. We know from Refs. 14 and 4 that for $j=1,\ldots,N$, $\{\Pi_j(\theta),\theta\in\mathcal{S}_a\}$ are analytic families of projectors and that for $\mathrm{Im}\,\theta\neq 0$ they coincide with

$$\Pi_j(\theta)=-\frac{1}{2\pi i}\int_{|z-E_j|=\rho}(H_\theta-z)^{-1}\,\mathrm{d}z,\quad \rho>0 \text{ and small enough}. \tag{5.9}$$

Fix $\mathrm{Re}\,\theta=0$, $\mathrm{Im}\,\theta=\eta$, $0<\eta<a$ and denote by $\{Z_j\}_{j=1,\ldots,M}$ the set of complex eigenvalues of $H_{i\eta}$ and by $\{\tilde{\Pi}_j(i\eta)\}_{j=1,\ldots,M}$, the associated eigenprojectors defined through the Cauchy integral formula as in (5.9). We have the following.

Theorem 5.1: *Assume* (HA). *Let* $0<\eta<a$ *as above and* $\phi\in\mathcal{D}_a$, *then there exist* $0<\epsilon<1$ *such that for all* $t\geqslant 0$,

$$\langle\phi,e^{-itH}\phi\rangle\overset{t\to\infty}{=}\sum_{j=1..N}e^{-itE_j}\langle\phi,\Pi_j\phi\rangle+\sum_{j=1..M}e^{-itZ_j}\langle\tilde{\phi}_{-i\eta},\tilde{\Pi}_j(i\eta)\tilde{\phi}_{i\eta}\rangle+O_{\phi,\eta}(e^{-(\eta(1-\epsilon))t}). \tag{5.10}$$

Here $\tilde{\phi}_{\pm i\eta}:=(1-\Pi(i\eta))\phi_{\pm i\eta}$ *and* $\Pi:=\Sigma_{j=1\ldots N}\Pi_j$. *If* H *has no eigenvalue take* $\Pi=0$ *on the rhs of (5.10) and similarly for the complex eigenvalues* Z_j *of* $H_{i\eta}$.

It is worth to notice, in particular to well understand (5.18), that due to the analyticity and unitary properties, the coefficients $\{\langle\tilde{\phi}_{-i\eta},\tilde{\Pi}_j(i\eta)\tilde{\phi}_{i\eta}\rangle\}_{j=1,\ldots,M}$ are η independent.

Proof: By using the spectral theorem and since H has no singular continuous spectrum (H is a rank one perturbation of the purely ac operator M, see Ref. 8), for every $\phi\in\mathcal{D}_a$, we have

$$\langle \phi, e^{-itH}\phi\rangle = \sum_{j=1..N} e^{-itE_j}\langle \phi, \Pi_j \phi\rangle + \int_{\mathbb{R}} \mathrm{d}\lambda\, Q_\phi(\lambda) e^{-it\lambda}. \tag{5.11}$$

Here

$$Q_\phi(\lambda) = \frac{1}{2i\pi}(G_{\tilde{\phi}}(\lambda + i0) - G_{\tilde{\phi}}(\lambda - i0)), \tag{5.12}$$

where

$$G_\phi(z) := \langle \phi, (H-z)^{-1}\phi\rangle. \tag{5.13}$$

From our previous discussion, it is clear that $\{G_{\tilde{\phi}}(z), \mathrm{Im}\, z > 0\}$ has a meromorphic extension in $\{\mathrm{Im}\, z > -\eta\}$ given by

$$G_{\tilde{\phi}}(z) = \langle \tilde{\phi}_{-i\eta}, (H_{i\eta} - z)^{-1}\tilde{\phi}_{i\eta}\rangle.$$

Similarly $\{G_{\tilde{\phi}}(z), \mathrm{Im}\, z < 0\}$ has a meromorphic extension in $\mathrm{Im}\, z < \eta$ with the expression

$$G_{\tilde{\phi}}(z) = \langle \tilde{\phi}_{i\eta}, (H_{-i\eta} - z)^{-1}\tilde{\phi}_{-i\eta}\rangle.$$

Moreover by using the formula

$$(H-z)^{-1} = -\frac{1}{z} - \frac{1}{z^2}H + \frac{1}{z^2}H(H-z)^{-1}H$$

and the analyticity properties evoked above, we have for $0 > \mathrm{Im}\, z > -\eta$, $|\mathrm{Re}\, z| \geqslant e$,

$$Q_\phi(z) = \frac{1}{2i\pi z^2}(\langle H_{-i\eta}\tilde{\phi}_{-i\eta}, (H_{i\eta} - z)^{-1}H_{i\eta}\tilde{\phi}_{i\eta}\rangle - \langle H\tilde{\phi}, (H-z)^{-1}H\tilde{\phi}\rangle) \tag{5.14}$$

which together with Lemma 5.1 immediately implies

$$|Q_\phi(z)| = Q_{\phi,\eta}\left(\frac{1}{|z|^2}\right) \tag{5.15}$$

if $0 > \mathrm{Im}\, z > -\eta(1-\epsilon)$, $0 < \epsilon \leqslant 1$, and $|\mathrm{Re}\, z|$ large enough. Then the integral on the rhs of (5.11) can be computed by using the Cauchy theorem,

$$\int_{\mathbb{R}} \mathrm{d}\lambda\, Q_\phi(\lambda) e^{-it\lambda} = \sum_{j=1..M} e^{-itZ_j}\, \mathrm{Res}\, G_{\tilde{\phi}}(z)\big|_{z=Z_j} + e^{-(\eta(1-\epsilon))t}\int_{\mathbb{R}} \mathrm{d}\lambda\, Q_\phi(\lambda - i(\eta(1-\epsilon))\; e^{-it\lambda}. \tag{5.16}$$

The parameter ϵ, $0 < \epsilon < 1$ is chosen such that the operator $H_{i\eta}$ has no complex eigenvalues on the line $\{\lambda - i(\eta - \epsilon); \lambda \in \mathbb{R}\}$. Standard arguments show that the first term of the rhs of (5.16) gives the second term of the rhs of (5.10). By using the estimate (5.15) we get that the second term of the rhs of (5.16) is $O_{\phi,\eta}(e^{-\eta(1-\epsilon)t})$ so that (5.16) implies the theorem. □

Theorem 5.1 provides a general framework to study sojourn times associated to the family of operators $\{H(\beta), \beta > 0\}$ given in (5.2), for the dense set of analytic vectors associated to the one parameter unitary group $\{U_\theta, \theta \in \mathbb{R}\}$.

According to the general context of this paper we consider the following situation. Suppose that $H(\beta_0)$ has only one real eigenvalue E_0 for some β_0. Lemma 2.1 gives a necessary and sufficient condition for this property to take place and Corollary 2.1 asserts that E_0 is simple. Let $\Pi := |\psi_0\rangle\langle\psi_0|$ be the orthogonal projector onto the corresponding eigenvector. We know that E_0 remains a simple eigenvalue of $H_{i\eta}(\beta_0)$ for $a > \eta > 0$. Denote by $\{Z_j\}_{j=1,\ldots,M}$ the (eventual) complex eigenvalues of $H_{i\eta}(\beta_0)$.

We also assume that, for β near β_0 and $\beta \neq \beta_0$, the operator $H(\beta)$ has only continuous spectrum. Then, $H_{i\eta}(\beta)$ has no real eigenvalues and therefore, by the usual perturbation theory, the operator $H_{i\eta}(\beta)$ has an eigenvalue $E(\beta)$ near E_0 with $\operatorname{Im} E(\beta) \neq 0$ and eigenvalues $\{Z_j(\beta)\}_{j=1,\ldots,M}$ near $\{Z_j\}_{j=1,\ldots,M}$.

Using the classical formulas of regular perturbation theory, see Ref. 8, Chap. 2, one gets with $\omega := \beta - \beta_0$,

$$E(\beta) \overset{\omega\to 0}{=} E_0 + \omega\langle \psi_{0,-i\eta}, P_{i\eta}\psi_{0,i\eta}\rangle - \omega^2\langle \psi_{0,-i\eta}, P_{i\eta}S_{i\eta}(E_0)P_{i\eta}\psi_{0,i\eta}\rangle + \mathcal{O}_\eta(\omega^3)$$
$$\overset{\omega\to 0}{=} E_0 + \omega\langle \psi_0, P\psi_0\rangle - \omega^2\langle P\psi_0, S(E_0+i0)P\psi_0\rangle + \mathcal{O}_\eta(\omega^3),$$

where $S_{i\eta}(E_0)$ denotes the reduced resolvent of $H_{i\eta}(\beta_0)$ at E_0, see Ref. 8, Chap. III, Sec. 6.5 for the definition of the reduced resolvent. Let

$$\Gamma := 2\omega^2 \operatorname{Im}\langle P\psi_0, S(E_0+i0)P\psi_0\rangle, \tag{5.17}$$

be the resonance width of $E(\beta)$; one has $\operatorname{Im} E(\beta) = -\frac{1}{2}\Gamma + \mathcal{O}(\omega^3)$. One also obtains that $|Z_j(\beta) - Z_j| = \mathcal{O}(\omega)$ and therefore $|\operatorname{Im} Z_j(\beta)|$ remains uniformly away from zero for ω small enough. Finally the perturbation theory gives the expansion of the eigenprojector associated to $E(\beta)$,

$$\Pi(i\eta,\beta) \overset{\omega\to 0}{=} \Pi(i\eta,\beta_0) + \mathcal{O}_\eta(\omega) \quad \text{with } \Pi(i\eta,\beta_0) = |\psi_{0,i\eta}\rangle\langle\psi_{0,-i\eta}|.$$

Define now $\tau_\omega^\pm$ (the sojourn time in the future, respectively, in the past)

$$\tau_\omega^\pm(\phi) := \int_{\mathbb{R}_\pm} |\langle \phi, e^{-itH(\beta_0+\omega)}\phi\rangle|^2 \, \mathrm{d}t.$$

By using Theorem 5.1 one gets integrating (5.10) over $\mathbb{R}_+$ (notice that here $\tilde{\phi} = \phi$),

$$\tau_\omega^+(\phi) \overset{\omega\to 0}{=} \frac{|\langle \phi_{-\eta}, \Pi(i\eta,\beta)\phi_{i\eta}\rangle|^2}{-2\operatorname{Im} E(\beta)} + \mathcal{O}_{\phi,\eta}(1) \overset{\omega\to 0}{=} \frac{|\langle \phi, \psi_0\rangle|^4}{\Gamma} + \mathcal{O}_{\phi,\eta}(\omega^{-1}).$$

Since clearly $\tau_\omega^- = \tau_\omega^+$ we have proven the following.

Theorem 5.2: *In the conditions stated above let $\phi \in \mathcal{D}_a$ and assume in addition that Γ defined in (5.17) does not vanish. Then for $\beta = \beta_0 + \omega$,*

$$\tau_\omega(\phi) \overset{\omega\to 0}{=} \frac{|\langle \phi_{-i\eta}, \Pi(i\eta,\beta)\phi_{i\eta}\rangle|^2}{-\operatorname{Im} E(\beta)} + \mathcal{O}_{\phi,\eta}(1) \tag{5.18}$$

$$= 2\frac{|\langle \phi, \psi_0\rangle|^4}{\Gamma} + \mathcal{O}_\phi(\omega^{-1}), \tag{5.19}$$

where ψ_0 denotes the normalized eigenvector associated to the eigenvalue E_0 of $H(\beta_0)$.

Remark 5.1: (a) Let us illustrate this result in the one dimensional case. Again with the Aronszjan-Krein formula

$$S(E_0+i0) = R_0(E_0+i0) + (R_0(E_0+i0)\psi_0,\psi_0)\Pi - (R_0(E_0+i0)\Pi + \Pi R_0(E_0+i0))$$

so that

$$\frac{1}{2}\Gamma = \omega^2 \operatorname{Im}\langle P\psi_0, S(E_0+i0)P\psi_0\rangle = \omega^2|(\varphi,\psi_0)|^4 \operatorname{Im}(R(E_0+i0)\psi_0,\psi_0) = \pi\omega^2|\langle\psi_0, P\psi_0\rangle|^2|\psi_0(E_0)|^2$$
$$= \frac{\pi\omega^2|\psi(E_0)|^2}{\beta_0^4\|\psi\|^6} = \frac{\pi\omega^2|\varphi'(E_0)|^2}{\beta_0^4\|\psi\|^6}.$$

First we see that the assumption $\varphi'(E_0) \neq 0$ *guarantees that* $\Gamma \neq 0$. *Then* $\omega^2 \tau_\omega(\psi_0) = \langle \psi_0, P\psi_0 \rangle|^{-2} |\psi_0(E_0)|^{-2} + \mathcal{O}(\omega)$ *which indeed is what we found in Theorem 4.1 with a more precise estimate here on the rate of decay of the remainder.*

(b) Instead of requiring that $H(\beta)$ *has no real eigenvalue for* β *near* β_0 *we could equivalently demand that the resonance width* Γ *is not zero since as we have seen above* $E(\beta_0 + \omega) = E_0 + \omega \langle \psi_0, P\psi_0 \rangle - \frac{1}{2}\Gamma + \mathcal{O}(\omega^3)$.

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Exact and quasiexact solvability of second-order superintegrable quantum systems: I. Euclidean space preliminaries

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We show that second-order superintegrable systems in two-dimensional and three-dimensional Euclidean space generate both exactly solvable (ES) and quasiexactly solvable (QES) problems in quantum mechanics via separation of variables, and demonstrate the increased insight into the structure of such problems provided by superintegrability. A principal advantage of our analysis using nondegenerate superintegrable systems is that they are multiseparable. Most past separation of variables treatments of QES problems via partial differential equations have only incorporated separability, not multiseparability. Also, we propose another definition of ES and QES. The quantum mechanical problem is called ES if the solution of Schrödinger equation can be expressed in terms of hypergeometric functions ${}_mF_n$ and is QES if the Schrödinger equation admits polynomial solutions with coefficients necessarily satisfying a three-term or higher order of recurrence relations. In three dimensions we give an example of a system that is QES in one set of separable coordinates, but is not ES in any other separable coordinates. This example encompasses Ushveridze's tenth-order polynomial QES problem in one set of separable coordinates and also leads to a fourth-order polynomial QES problem in another separable coordinate set. © *2006 American Institute of Physics.*
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I. INTRODUCTION

It is well known that N-dimensional nonrelativistic quantum systems described by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + V(x_1, x_2, \ldots, x_N) \tag{1}$$

are integrable if there exist N linearly independent and global differential operators $\mathcal{I}_\ell$, $\ell = 0, 1, \ldots, N-1$ and $\mathcal{I}_0 = \mathcal{H}$, commuting with the Hamiltonian (1) and with each other

$$[\mathcal{I}_\ell, \mathcal{H}] = 0, \quad [\mathcal{I}_\ell, \mathcal{I}_j] = 0, \quad \ell, j = 1, 2, \ldots, N-1. \tag{2}$$

This particular class of integrable systems is called (maximally) superintegrable (this term was introduced first by Rauch-Wojciechowski in Ref. 1) if it is integrable and, also, possesses $2N-1$

functionally independent differential operators (integrals of motion). The additional $N-1$ integrals $\mathcal{L}_k$, commute with the Hamiltonian

$$[\mathcal{L}_k,\mathcal{H}]=0, \quad k=1,2,\ldots,N-1, \tag{3}$$

but not necessarily with each other. (These definitions have obvious classical analogs for the classical Hamiltonian.) Three examples of this kind have been well known for a long time, viz. the Kepler-Coulomb problem, the isotropic harmonic oscillator, and the nonisotropic oscillator with commensurable frequencies.

The existence of additional quantum integrals of motion for these systems leads to many interesting properties not shared by integrable systems. In classical mechanics the corresponding additional integrals of motion have the consequence that in the case of superintegrable systems in two dimensions and maximally superintegrable systems in three dimensions all finite trajectories are found to be periodic.

One of the most important properties for many superintegrable systems (particularly second-order systems where there are $2N-1$ functionally independent quadratic constants of the motion) is multiseparability, i.e., the separation of variables for the Hamilton-Jacobi and Schrödinger equations in more than one orthogonal coordinate system.[2–8] (Each separable coordinate system is associated with N commuting second-order constants of the motion.) For instance, the isotropic harmonic oscillator in three dimensions is separable in eight coordinate systems, namely in Cartesian, spherical, circular polar, circular elliptic, conical, oblate spheroidal, prolate spheroidal, and ellipsoidal coordinates. The Kepler-Coulomb potential is separable in four coordinate systems, namely in conical, spherical parabolic, and prolate spheroidal coordinates.

A systematic search for such systems in two- and three-dimensional Euclidean space was started in the pioneering work of Smorodinsky and Winternitz with collaborators in Refs. 9–11 and was continued in Ref. 12. Particularly, in Ref. 10 it was shown that in two-dimensional real Euclidean space there exist four superintegrable potentials, three of which could be considered as the singular generalization of Kepler-Coulomb, circular oscillator and anisotropic oscillator systems. These results were extended for two- and three-dimensional spaces with constant curvature (both positive and negative),[13] and on the complex two-dimensional sphere and Euclidean space.[14–18] The program is continuing for various conformally flat space spaces.[19–30,5–7]

In the last 15 years superintegrable systems have become a subject of investigation from many points of view: in Refs. 13, 18, 31, and 32 via the path integral approach, in Refs. 19, 21, and 22 by solving the Schrödinger equation with the help of the Niven ansatz,[33] in Refs. 34–39 from the purely algebraic approach, and generally in Ref. 40. As has been shown by a number of authors, many superintegrable systems generate an algebraic structure which may be considered as a nonlinear extension of the Lie algebra (in classical mechanics Poisson algebras), namely a quadratic algebra. The general form of quadratic algebras, which are encountered in the case of two-dimensional quantum superintegrable systems has been investigated.[39,5,6]

Particularly useful is the exact solvability of many superintegrable systems. Essentially, this means that after any separation of variables each of the separated ordinary differential equations admits an exact solution. However, the term exact solvability is defined differently by different authors. In Refs. 41 and 42 [see also the recent paper (Ref. 43)] we read that "an exactly solvable quantum mechanical system can be characterized by the fact that in its solution space one can indicate explicitly an infinite flag of functional linear spaces, which is preserved by the Hamiltonian" or the "Hamiltonian is exactly solvable if its spectrum can be calculated algebraically." Indeed, in spite of an "intuitive" understanding of the term exactly solvable, no universal definition exists up to now.

On the other hand, there are limiting cases of well-known one-dimensional exactly solvable systems, namely the harmonic oscillator and Coulomb problems with γ/x^2 $(\gamma>-1/4)$ interaction, Morse potential, trigonometric and modified Pöschl-Teller potentials, trigonometric and hyperbolic Manning-Rosen potentials,[44,45] and the Natanson potential.[46] All these potentials have the general property that the Schrödinger spectral problem has an explicit formula for the *whole* energy spectrum including the continuous spectrum, and the eigenfunctions (up to the asymptotic

ansatz or gauge transformations[41,42]) are of hypergeometric type ${}_1F_1$, ${}_2F_1$. For the bound states we have solutions in terms of classical polynomials[47] whereas for continuous states just infinite series. Moreover, hypergeometric functions describe both the continuous quantum systems as well as the finite systems and appear also as solutions of related difference equations, for instance, the finite one- and two-dimensional oscillator expressed in terms of discrete variables polynomials, Krawchuk, Meixner, and Hahn.[48] The standard definitions of exact solvability do not include many of these systems.

Thus, we propose another definition of exact solvability: a *quantum mechanical system is called exactly solvable if the solutions of the Schrödinger equation can be expressed in terms of hypergeometric functions* ${}_mF_n$. (Basically, we are requiring that the coefficients in power series expansions of the solutions satisfy two-term recurrence relations, rather than recurrence relations of higher order.) It is obvious that an N-dimensional Schrödinger equation is exactly solvable if it is separable in some coordinate systems and each of the separated equations is exactly solvable. Further, *we say that a superintegrable system is exactly solvable if it is exactly solvable in at least one system of coordinates*.

At first sight, such a definition of exactly solvable problems may seem too narrow, but it leads us to distinguish two kinds of models: (1) those which it is possible to study analytically and (2) those which can be solved numerically via the solution of algebraic equations.

The process of separation of variables in the N-dimensional Schrödinger equation leads to ordinary differential equations having as solutions many of the special functions of mathematical physics. A complication of the separated equations involves the N separation constants. In general we have a multiparameter eigenvalue problem.[49] It is possible to distinguish three different cases, namely when there is complete, partial or nonseparability of the separation constants. It is obvious that in the case of complete separability (of separation constants) the initial N-dimensional Schrödinger equation splits into N independent second-order differential equations, each involving a single separation parameter. This situation occurs, for instance, in the case of separation of variables in the Helmholtz (free Schrödinger equation, which is also superintegrable) or the Schrödinger equation for the harmonic oscillator in Cartesian coordinates. The second "extremal" case, when complete nonseparability exists, is realized, in separation of variables for the same problems but in ellipsoidal coordinates. In the last case each separated second-order differential equation contains simultaneously all separation constants (usually depending on dimensional or nondimensional parameters),[3,4] for which the simultaneous quantization becomes nontrivial.

The standard method of solution of a second-order ordinary differential equation, obtained after separation of variables in N-dimensional Schrödinger equations, involves (after taking into account the asymptotic ansatz) expansions around one of the singular points of the differential equation (the standard power series method,[50] or the so-called Hill-determinant method[51]). The problem reduces to the solution of the recurrence relations for the expansion coefficients. If one can express the equation in a form such that the coefficients obey a two-term recurrence relation, then the corresponding solution can be written in closed or analytic form or in terms of hypergeometric functions and we have an exactly solvable problem. Such situations occur when separation of variables for superintegrable systems is possible in subgroup type coordinate (spherical, cylindrical, and Cartesian)[52] and often in parabolic type coordinates. This method is also powerful when separation of variables is possible in nonsubgroup systems of coordinates such as spheroidal or elliptic types. In this case we arrive at high-order recurrence relations, the subsequent analysis of which allows us to investigate the behavior of the solution and to determine if polynomial solutions exist.

There is another general approach for solving the Schrödinger equation by exploring the Niven-type ansatz,[33] based on the existence of polynomial solutions. According to this method the complete solution can be constructed without direct separation of variables and computed in terms of the zeros of the corresponding polynomial. This method has been used in Refs. 19, 21, and 22 for the investigation of two- and three-dimensional superintegrable systems in Euclidean and curved spaces. We illustrate the difference between systems that are merely separable and those

that are superintegrable. Consider the problem of motion in the plane for a charged particle with two fixed Coulomb centers with coordinates $(\pm D/2,0)$ (the so-called plane two center problem)

$$V(x,y) = -\frac{\alpha_1}{\sqrt{y^2+(x+D/2)^2}} - \frac{\alpha_2}{\sqrt{y^2+(x-D/2)^2}}. \tag{4}$$

This system is not superintegrable and separation of variables is possible only in two-dimensional elliptic coordinates [see Eq. (70)]. Upon the substitution $\psi(\nu,\mu;D^2)=X(\nu;D^2)Y(\mu;D^2)$ and the separation constant $A(D)$, the Schrödinger equation splits into a system of two ordinary differential equations

$$\frac{d^2X}{d\nu^2} + \left[\frac{D^2E}{2}\cosh^2\nu + D(\alpha_1+\alpha_2)\cosh\nu + A(D)\right]X = 0, \tag{5}$$

$$\frac{d^2Y}{d\mu^2} - \left[\frac{D^2E}{2}\cos^2\mu + D(\alpha_1-\alpha_2)\cos\mu + A(D)\right]Y = 0. \tag{6}$$

Both Eqs. (5) and (6) belong to the class of nonexactly solvable problems. In general polynomial solutions do not exist even for the case of discrete spectrum $E<0$ (to be completely correct let us note that polynomial solutions exist only for special values of parameters α_1,α_2, and R), and each of the wave functions $X(\nu;D^2)$ and $Y(\mu;D^2)$ is expressed as an infinite series with a three-term recurrence relation.

Let us now set $\alpha_2=0$. Then the potential (4) transforms to the ordinary two-dimensional (2D) hydrogen atom problem, which is well known as a superintegrable system[53–55] with dynamical symmetry group SO(3), and admits separation of variables in three systems of coordinates: polar, parabolic, and elliptic. In this case we can see that the separation equations (5) and (6), namely

$$\frac{d^2X}{d\nu^2} + \left[\frac{D^2E}{2}\cosh^2\nu + D\alpha_1\cosh\nu + A(D)\right]X = 0, \tag{7}$$

$$\frac{d^2Y}{d\mu^2} - \left[\frac{D^2E}{2}\cos^2\mu + D\alpha_1\cos\mu + A(D)\right]Y = 0 \tag{8}$$

transform into each other by the change $\mu\leftrightarrow i\nu$. Thus separation of variables in elliptic coordinates for the 2D hydrogen atom gives two functionally identical one-dimensional Schrödinger type equations with two parameters: coupling constant E and energy $A(D)$ (correspondingly energy and separation constant for 2D), but one defined on the real and the other on the imaginary axis. In other words, instead of the systems of differential equations (7) and (8), the problem reduces to solving only one of the equations (7) or (8) for which the "domain of definition" is the complex plane. The requirement of finiteness for the wave functions in the complex plane permits only polynomial solutions (see for details Ref. 56). As a result we obtain *simultaneous* quantization of the energy spectrum

$$E_n = -\frac{\alpha_1^2}{2(n+1/2)^2}, \quad n=0,1,2,\ldots \tag{9}$$

and the elliptic separation constant $A_s(D)$ where $s=0,1,2,\ldots,n$ (as a solution of an nth-degree algebraic equation). The polynomial solution is defined by a finite series with three-term recurrence relations for the coefficients. They cannot be considered as exactly solvable and can be investigated only numerically. A similar situation occurs, for instance, in the case of the two-center problem in three-dimensional Euclidean space (the so-called prolate spheroidal radial and angular Coulomb wave functions)[57] and three-dimensional sphere (Heun wave functions),[58] where after eliminating one of the Coulomb centers the problems reduce to superintegrable systems admitting only polynomial solutions. These (and many other) examples suggest a deep connection of the

notion of superintegrability and existence of polynomial solutions of the corresponding Schrödinger equation.

We note that each of equations (7) or (8) has the form of a one-dimensional Schrödinger equation with the parameter E and eigenvalue $A(D)$, and could be separately considered in the regions $\mu \in [0, 2\pi]$ or $\nu \in [0, \infty)$, correspondingly. Then for arbitrary values of constant E [for example when $E_n = 0$ $(n \to \infty)$ the equations (7) and (8) transform to periodic and modified Mathieu equations, which are nonexactly solvable] the solutions of Eqs. (7) or (8) expressed via infinite series and only on the "energy surface" of the 2D hydrogen atom (9), split into polynomial and nonpolynomial sectors (each of these sectors is noncomplete) and for fixed number n, only *some* of the eigenvalues $A_s(D)$ $(s = 0, 1, 2, \ldots, n)$ can be calculated from an nth-degree algebraic equation. We can say that Eqs. (7) and (8) "remember" their polynomial solutions. It is obvious that the spectrum of $A_s(D)$, $(s = 0, 1, 2 \ldots, n)$ and occurrence of polynomial solutions of each of the equations (7) and (8) coincides with the eigenvalues of separation constants and the wave function after the reduction to one of the regions $\mu \in [0, 2\pi]$ or $\nu \in [0, \infty)]$ for the 2D hydrogen atom.

These phenomena have been intensively discussed in the literature in the late 1980s and called *quasiexact solvability* (this term was first introduced by Turbiner and Ushveridze in Ref. 59) and models of this type called *quasiexactly solvable* systems[60–62] (see also Ref. 63 and references therein). The crucial example that stimulated the investigation of quasiexactly solvable systems is the Hamiltonian (1) with anharmonic potential

$$V(x) = \frac{1}{2}\omega^2 x^6 + 2\beta\omega^2 x^4 + (2\beta^2\omega^2 - 2\delta\omega - \lambda)x^2 + 2\frac{\left(\delta - \frac{1}{4}\right)\left(\delta - \frac{3}{4}\right)}{x^2}, \tag{10}$$

where ω, β, $\delta > 1/2$ and λ are constants. As noticed by many authors,[64–66] this system admits polynomial solutions only for special values of constant $\lambda = \omega(2n+1)$ $(n = 0, 1, 2 \ldots)$

$$\Psi(x) \approx x^{2\delta - 1/2} e^{-(\omega/4)x^4 - \beta\omega x^2} P_n(x^2). \tag{11}$$

There are different approaches to the investigation of quasiexactly solvable systems. In the algebraic approach formulated by Turbiner in Ref. 60 quasiexact solvability is explained in terms of a "hidden symmetry algebra" $\mathrm{sl}(2, R)$. [This is not a hidden dynamical symmetry in the usual sense because the Hamiltonian (12) belongs to the enveloping algebra but is not a Casimir operator.] More precisely this means the following: The one-dimensional Hamiltonian (1) after suitable changes of variable $z = \xi(x)$ and "gauge transformation" $H = e^{-\alpha(z)}\mathcal{H}e^{\alpha(z)}$ can be written in the form

$$H = \sum_{a,b=0,\pm} C_{ab} J_a J_b + \sum_{a=0,\pm} C_a J_a, \tag{12}$$

where the first-order differential operators $\{J_\pm, J_0\}$ satisfy the commutation relations for $\mathrm{sl}(2, R)$.[60]

The above mentioned analysis for the 2D hydrogen atom shows that, despite the elegance of the algebraic approach, the phenomena of quasiexactly solvability has deeper roots than can be explained via the "one-dimensional" model (12). Other examples are the hydrogen atom and oscillator problems on two- and three-dimensional spheres[19,67] and two-dimensional hyperboloids,[22] which generate not only hyperbolic and trigonometric but elliptic quasiexactly solvable systems (see also Refs. 68, 56, 69, and 70). We should also mention Lamé polynomials. They come from separation of variables for the Helmholtz (also superintegrable!) or Schrödinger equation in elliptic coordinates on the two-dimensional sphere. As also determined in Ref. 37 (without showing the mechanism of this phenomena) some of the quasiexactly solvable systems can be obtained through dimensional reduction from two- and three-dimensional superintegrable models with quadratic invariants (second-order superintegrability).

A second approach, known as analytic, was formulated by Ushveridze (see, for example, Refs. 61–63) and represents a one-dimensional reduction of the Niven-Stieltjes method for solving multiparameter spectral problems such as the generalized Lamé equation (or ellipsoidal equation).[33] The solution in this method is determined by the zeros of polynomials $P_n(x^2)$. Then the wave function (11) can be rewritten in the form

$$\Psi(x) \approx x^{2\delta-1/2} e^{-(\omega/4)x^4-\beta\omega x^2} \prod_{i=0}^{n} (x^2 - \xi_i), \tag{13}$$

where the numbers $(\xi_1, \xi_2, \ldots, \xi_n)$ satisfy a system of n algebraic equations (see Sec. II C). According to the oscillation theorem, the number of zeros in the physical interval $\xi_i \in [0, \infty)$ enumerates the ground state and first n excitations, described in terms of all zeros (complete solutions of the systems of algebraic equations and including nonphysical section $\xi_i \in (-\infty, 0]$) as

$$E = 4\delta \left[\beta\omega + \sum_{i=1}^{n} \frac{1}{\xi_i} \right]. \tag{14}$$

Two natural questions occur in this approach: what is the physical meaning of the negative zeros ξ_i, and why in the correct formula for the energy spectrum (14) do n zeros of the polynomial $P_n(x^2)$ appear?

With this paper we begin an investigation of second-order superintegrable systems on constant curvature spaces (Euclidean, sphere, hyperboloid and pseudo-Euclidean) based on the superintegrability and direct solutions of the Schrödinger equation. We pay special attention to nonsubgroup type coordinates and prove the existence of polynomial solutions for several of these systems. We demonstrate that quasiexact solvability is directly related with multiseparability of second-order superintegrable systems, on one hand, and with the presence of polynomial solutions for these systems on the other.

The first part of this paper is devoted to two (singular anisotropic and singular circular oscillators) from the four possible superintegrable systems in two-dimensional real Euclidean space (see, for example, Ref. 19). The other two systems may be transformed (only for the discrete spectrum) to the singular circular oscillator (for V_3) or ordinary shifted oscillator (for V_4) systems by the help of the Levi-Civita mapping,[71] so are less fundamental for our purposes. In the second part of the paper we give some examples of superintegrable systems in three dimensions that reinforce our definitions of exact and quasiexact solvability. In particular we exhibit a quasiexactly solvable superintegrable system which is not at the same time exactly solvable in any separable set of coordinates. In one set of separable coordinates this provides deeper insight into an example of Ushveridze,[63] p. 155 (the tenth-order polynomial QES problem) and also leads to a fourth-order polynomial QES problem in another separable coordinate set. In addition we indicate precisely how the eigenvalues of the symmetry operators which describe separation can be calculated from a determinant condition. For these examples we will work with complex superintegrable systems and not address the relatively simple issue of determining the distinct real restrictions of the complex spaces. These examples greatly clarify the concepts and show how the extension to N dimensions can be achieved.

II. THE SINGULAR ANISOTROPIC OSCILLATOR

Let us first consider the potential $(k_2 > 0)$

$$V_1(x,y) = \frac{1}{2}\omega^2(4x^2 + y^2) + k_1 x + \frac{k_2^2 - \frac{1}{4}}{2y^2} \tag{15}$$

the *singular anisotropic oscillator*. The Schrödinger equation has the form

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)\Psi + \left[2E - \omega^2(4x^2 + y^2) - 2k_1 x - \frac{k_2^2 - \frac{1}{4}}{y^2} \right]\Psi = 0. \tag{16}$$

For $k_2 > 1/2$ the singular term at $y=0$ is repulsive and the motion takes place only on one of the half planes $(-\infty < x < \infty, y > 0)$ or $(-\infty < x < \infty, y < 0)$, whereas for $0 < k_2 < 1/2$ in whole plane (x,y). The Schrödinger equation separates in two systems: *Cartesian and parabolic coordinates.*

A. Cartesian bases

Separation of variables for Eq. (16) in Cartesian coordinates leads to the two *independent* one-dimensional Schrödinger equations

$$\frac{d^2\psi_1}{dx^2} + (2\lambda_1 - 4\omega^2 x^2 - 2k_1 x)\psi_1 = 0, \tag{17}$$

$$\frac{d^2\psi_2}{dy^2} + \left(2\lambda_2 - \omega^2 y^2 - \frac{k_2^2 - \frac{1}{4}}{y^2}\right)\psi_2 = 0, \tag{18}$$

where

$$\Psi(x,y;k_1, \pm k_2) = \psi_1(x;k_1)\psi_2(y; \pm k_2) \tag{19}$$

and λ_1, λ_2 are *Cartesian separation constants* with $\lambda_1+\lambda_2=E$.

Equation (18) represents the well-known linear singular oscillator system (see for instance Refs. 72 and 73 and Refs. 10, 20, and 74). It is an exactly solvable problem and has been used in many applications, for example, as a model in N-body problems,[75] or fractional statistics and anyons.[76,77] The complete set of orthonormalized eigenfunctions, (on $1/2$) in the interval $0<y<\infty$ of Eq. (18), can be expressed in terms of finite confluent hypergeometric series or Laguerre polynomials

$$\psi_{n_2}(y; \pm k_2) = \sqrt{\frac{2\omega^{(1\pm k_2)} n_2!}{\Gamma(n_2 \pm k_2 + 1)}} y^{1/2\pm k_2} e^{-1/2\omega y^2} L_{n_2}^{\pm k_2}(\omega y^2), \tag{20}$$

where $\lambda_2=\omega(2n_2+1\pm k_2)$. We assume that the positive sign at the k_2 must be taken if $k_2>\frac{1}{2}$ and both the positive and the negative sign must be taken if $0<k_2<\frac{1}{2}$, so that the polynomials have finite norm. Let us also note that unlike the potential (15) the wave function is not invariant under the replacement $k_2\rightarrow -k_2$ and splits into two families of solutions that transform to one another under this change.

The second equation (17) easily transforms to the ordinary one-dimensional oscillator problem. In terms of Hermite polynomials the orthonormal solutions (in region $-\infty<x<\infty$) are

$$\psi_{n_1}(x;k_1) = \left(\frac{2\omega}{\pi}\right)^{1/4} \frac{e^{-\omega z^2}}{\sqrt{2^{n_1} n_1!}} H_{n_1}(\sqrt{2\omega} z), \quad z = x + \frac{k_1}{4\omega^2}, \tag{21}$$

where $\lambda_1=\omega(2n_1+1)-(k_1^2/8\omega^2)$. Thus the complete energy spectrum is

$$E = \lambda_1 + \lambda_2 = \omega[2n + 2 \pm k_2] - \frac{k_1^2}{8\omega^2}, \quad n = n_1 + n_2 = 0,1,2,\ldots \tag{22}$$

and the degree of degeneracy for fixed principal quantum number n is $(n+1)$. Finally note that the separation of variables in Cartesian coordinates leads to two exactly solvable one-dimensional Schrödinger equations and the complete wave function may be constructed with the help of formulas (20), (21), and (19).

B. Parabolic bases

1. Separation of variables

Parabolic coordinates ξ and η are connected with the Cartesian x and y by

$$x = \tfrac{1}{2}(\xi^2 - \eta^2), \quad y = \xi\eta, \quad \xi \in \mathbf{R}, \quad \eta > 0. \tag{23}$$

The Laplacian and the two-dimensional volume element are given by

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{\xi^2 + \eta^2}\left(\frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2}\right), \quad \mathrm{d}v = \mathrm{d}x\,\mathrm{d}y = (\xi^2 + \eta^2)\mathrm{d}\xi\,\mathrm{d}\eta. \tag{24}$$

The Schrödinger equation in parabolic coordinates (23) is

$$\frac{1}{\xi^2 + \eta^2}\left(\frac{\partial^2 \Psi}{\partial \xi^2} + \frac{\partial^2 \Psi}{\partial \eta^2}\right) + \left[2E - \omega^2(\xi^4 - \xi^2\eta^2 + \eta^4) - k_1(\xi^2 - \eta^2) - \frac{k_2^2 - \frac{1}{4}}{\xi^2 \eta^2}\right]\Psi = 0. \tag{25}$$

Upon substituting

$$\Psi(\xi, \eta) = X(\xi)Y(\eta)$$

and introducing the parabolic separation constant λ, the equation (25) splits into two ordinary differential equations,

$$\frac{d^2X}{\mathrm{d}\xi^2} + \left(2E\xi^2 - \omega^2\xi^6 - k_1\xi^4 - \frac{k_2^2 - \frac{1}{4}}{\xi^2}\right)X = -\lambda X, \tag{26}$$

$$\frac{d^2Y}{\mathrm{d}\eta^2} + \left(2E\eta^2 - \omega^2\eta^6 + k_1\eta^4 - \frac{k_2^2 - \frac{1}{4}}{\eta^2}\right)Y = +\lambda Y. \tag{27}$$

Equations (26) and (27) are transformed into one another by change $\xi \leftrightarrow i\eta$. We have

$$\Psi(\xi, \eta; E, \lambda) = C(E, \lambda)Z(\xi; E, \lambda)Z(i\eta; E, \lambda), \tag{28}$$

where $C(E, \lambda)$ is the normalization constant determined by the condition

$$\int_0^\infty \mathrm{d}\eta \int_{-\infty}^{\infty} \mathrm{d}\xi(\xi^2 + \eta^2)|\Psi(\xi, \eta; E, \lambda)|^2 = 1 \tag{29}$$

and the function $Z(\mu; E, \lambda)$ is a solution of the equation

$$\left[-\frac{d^2}{\mathrm{d}\mu^2} + \left(\omega^2\mu^6 + k_1\mu^4 - 2E\mu^2 + \frac{k_2^2 - \frac{1}{4}}{\mu^2}\right)\right]Z(\mu; E, \lambda) = \lambda Z(\mu; E, \lambda). \tag{30}$$

Thus, at $\mu \in (-\infty, \infty)$ we have Eq. (26) and at $\mu \in [0, i\infty)$—Eq. (27). Note that in the complex μ domain the "physical" region is just the two lines Im $\mu = 0$ and Re $\mu = 0$, Im $\mu > 0$. Our task is to find the solutions of Eq. (30) that are regular and decreasing as $\mu \to \pm\infty$ and $\mu \to i\infty$.

2. Recurrence relations

Consider now the equation (30). To solve it we make the substitution

$$Z(\mu; E, \lambda) = \exp\left(-\frac{\omega}{4}\mu^4 - \frac{k_1}{4\omega}\mu^2\right)\mu^{\frac{1}{2} \pm k_2}\psi(\mu; E, \lambda), \tag{31}$$

and obtain the differential equation

$$\frac{d^2\psi}{\mathrm{d}\mu^2} + \left[\frac{2\left(\frac{1}{2} \pm k_2\right)}{\mu} - 2\omega\mu\left(\mu^2 + \frac{k_1}{2\omega^2}\right)\right]\frac{\mathrm{d}\psi}{\mathrm{d}\mu} + [2\tilde{E}\mu^2 + \tilde{\lambda}]\psi = 0, \tag{32}$$

where

$$\tilde{E} = E + \frac{k_1^2}{8\omega^2} - \omega(2 \pm k_2), \quad \tilde{\lambda} = \lambda - \frac{k_1}{\omega}(1 \pm k_2). \tag{33}$$

Passing to a new variable $z = \mu^2$ in Eq. (32), we have

$$z\frac{d^2\psi}{dz^2}+\left[(1\pm k_2)-\omega z\left(z+\frac{k_1}{2\omega^2}\right)\right]\frac{d\psi}{dz}+\left[\frac{1}{2}\tilde{E}z+\frac{1}{4}\tilde{\lambda}\right]\psi=0. \tag{34}$$

We express the wave function $\psi(z)$ in the form

$$\psi(z;E,\lambda)=\sum_{s=0}^{\infty}A_s(E,\lambda)z^s. \tag{35}$$

The substitution (35) in Eq. (34) leads to the following three-term recurrence relation for the expansion coefficients $A_s\equiv A_s(E,\lambda)$,

$$(s+1)(s+1\pm k_2)A_{s+1}+\frac{1}{4}\left[\lambda-\frac{k_1}{\omega}(2s+1\pm k_2)\right]A_s+\frac{1}{2}\left[E+\frac{k_1}{8\omega^2}-\omega(2s\pm k_2)\right]A_{s-1}=0, \tag{36}$$

with the initial conditions $A_{-1}=0$ and $A_0=1$.

As shown in the Appendix, the asymptotic behavior of the expansion coefficients $A_s\equiv A_s(E,\lambda)$ for large s is $A_s\sim\sqrt{\xi_\pm}\sqrt{\omega^s/s!}$, depending on whether s is even or odd, and

$$\psi(z)\sim\sum\frac{\sqrt{\xi_\pm}(\sqrt{\omega}z)^s}{\sqrt{s!}}. \tag{37}$$

Then we have for $z>0$ [the case of Eq. (26)],

$$\sum\frac{\sqrt{\xi_\pm}(\sqrt{\omega}z)^s}{\sqrt{s!}}>\sqrt{\sum\frac{\xi_\pm(\omega z^2)^s}{s!}}=\xi_\pm\cosh\left(\frac{\omega}{2}z^2\right)+\xi_\mp\sinh\left(\frac{\omega}{2}z^2\right). \tag{38}$$

This function does not belong to the Hilbert space. If $k_1>0$ then we must make the replacements $b_s\to -b_s$ and $\xi_s\to-\xi_s$. This has the effect of replacing z by $-z$ in (37). Now the asymptotic solution is oscillatory. However, for $z<0$ [the case of Eq. (27)] the solution does not belong to the Hilbert space. The solution we have found is the minimal solution of the three-term recurrence relations. There is a linearly independent solution, but the coefficients grow more rapidly than the minimal solution coefficients.

3. Energy spectrum and separation constant

The function $Z(\mu)$ cannot converge simultaneously at large μ for real and imaginary μ and therefore the series (35) should be truncated in order to obtain convergence. The condition for series (35) to be truncated results in the energy spectrum (22) where now the coefficients $A_s\equiv A_s^{nq}(k_1,\pm k_2)$ satisfy the relation

$$(s+1)(s+1\pm k_2)A_{s+1}+\beta_sA_s+\omega(n+1-s)A_{s-1}=0,\quad \beta_s=\frac{\lambda}{4}-\frac{k_1}{4\omega}(2s+1\pm k_2). \tag{39}$$

The three-term recurrence relations (39) represent a homogeneous system of $n+1$ algebraic equations for $n+1$ coefficients $\{A_0,A_1,A_2,\ldots,A_n\}$. The requirement for the existence of a nontrivial solution leads to a vanishing of the determinant

$$D_n(\lambda)=\begin{vmatrix}\beta_0 & 1\pm k_2 & & & \\ \omega n & \beta_1 & 2(2\pm k_2) & & \\ & & & & \\ & & & 2\omega & \beta_{n-1} & n(n\pm k_2)\\ & & & & \omega & \beta_n\end{vmatrix}=0. \tag{40}$$

The roots of the corresponding algebraic equation give us the $(n+1)$ eigenvalues of the parabolic separation constant $\lambda_n(k_1,\pm k_2)$. It is known that all roots for such determinants are real and

distinct.[78] Thus all values of the separation constant are real and can be enumerated with the help of the integer q, namely the values are $\lambda_n(k_1,\pm k_2)\to\lambda_{nq}(k_1,\pm k_2)$, where $0\leqslant q\leqslant n$. The degeneracy for the n-energy state, as in the Cartesian case, equals $n+1$.

Note that Eq. (40) is invariant under the simultaneous transformation $k_1\to -k_1$ and $\lambda\to-\lambda$. Thus if one of the $\lambda=\lambda_n(k_1,\pm k_2)$ is a root of Eq. (40), then $\lambda=-\lambda_n(-k_1,\pm k_2)$ is also a root of the same equation. We see that for the odd energy state (n-odd) the range of $\lambda_{nq}(k_1,\pm k_2)$ splits into two subsets $\lambda_{nq}^{(1)}$ and $\lambda_{nq}^{(2)}$ connected by the relation $\lambda_{nq}^{(1)}(k_1,\pm k_2)\leftrightarrow-\lambda_{nq'}^{(2)}(-k_1,\pm k_2)$. For n-even, there exists the additional root $\lambda_{nq}(k_1,\pm k_2)=-\lambda_{nq}(-k_1,\pm k_2)$, which equals zero when $k_1=0$.

4. Wave functions

We will term the polynomial solutions of Eq. (34), or Eq. (32), as $Mk_{nq}(z;k_1,\pm k_2)$, and the function (31) as $Ta_{nq}(z;k_1,\pm k_2)$. [The notation Ta is in memory of Professor V. Ter-Antonyan (1942–2003).] Then the physical admissible solutions of Eq. (34) have the form

$$Mk_{nq}(z;k_1,\pm k_2)\equiv\psi(z;E,\lambda)=\sum_{s=0}^{n}A_s^{nq}(k_1,\pm k_2)z^s, \tag{41}$$

and the corresponding solution of Eq. (31) is

$$Ta_{nq}(\mu;k_1,\pm k_2)=\exp\left(-\frac{\omega}{4}\mu^4-\frac{k_1}{4\omega}\mu^2\right)\mu^{\frac{1}{2}\pm k_2}Mk_{nq}(\mu^2;k_1,\pm k_2). \tag{42}$$

Observe that parabolic wave functions (and also Cartesian wave functions) split into two classes and transform to each other via $k_2\to-k_2$. In the case $k_2=0$ (when the centrifugal term disappears), the solution (42) becomes an even and odd parity wave function under the exchange $\mu\to-\mu$.

It is known that there exists a direct connection between the quantum numbers q and numbers of zeros of the polynomial (41) and, therefore, the eigenvalues of the separation constant $\lambda_{nq}(k_1,\pm k_2)$ may be ordered by the numbers of nodes of the wave function $Ta_{nq}(\mu;k_1,\pm k_2)$. Indeed we will see that these are orthogonal polynomials, hence,[50] all the n zeros of the $Mk_{nq}(z;k_1,\pm k_2)$ are situated on the real axis $-\infty<z<\infty$, and all zeros have multiplicity one. Assume that the separation constants $\lambda_{nq}(k_1,\pm k_2)$ are enumerated in ascending order, i.e.,

$$\lambda_{n0}(k_1,\pm k_2)<\lambda_{n1}(k_1,\pm k_2)<\cdots<\lambda_{n,n-1}(k_1,\pm k_2)<\lambda_{n,n}(k_1,\pm k_2). \tag{43}$$

Then according to the oscillation theorem,[79] the quantum number q also enumerates the zeros of polynomials $Mk_{nq}(z;k_1,\pm k_2)$ in the region $z>0$, or the real axis of μ. Let us now introduce two quantum numbers q_1 and q_2, which determine the zeros of polynomials $Mk_{nq}(z;k_1,\pm k_2)$ for $z>0$ and $z<0$, correspondingly. Then $q_1+q_2=n$, and

$$\lambda_{nq_1}(k_1,\pm k_2)=-\lambda_{nq_2}(-k_1,\pm k_2). \tag{44}$$

For $\mu=\xi$ the function (42) gives the solution of Eq. (26), and for $\mu=i\eta$ the solution of Eq. (27). Thus the parabolic wave function (28) can be written in the following way:

$$\Psi_{nq_1q_2}(\xi,\eta;k_1,\pm k_2)=C_{nq_1q_2}(k_1,\pm k_2)Ta_{nq_1}(\xi;k_1,\pm k_2)Ta_{nq_2}(i\eta;k_1,\pm k_2). \tag{45}$$

5. Orthogonality relations and normalization constant

The wave functions (45) as eigenfunctions of Hamiltonians are orthogonal for quantum number n, or for $n\neq n'$,

$$\int_0^\infty d\eta \int_{-\infty}^\infty d\xi(\xi^2+\eta^2)\Psi^*_{n'q_1q_2}(\xi,\eta;k_1,\pm k_2)\Psi^*_{nq_1q_2}(\xi,\eta;k_1,\pm k_2)=0. \tag{46}$$

Because the energy spectrum is degenerate there exist additional orthogonality relations for quantum number q. Using the equations (26) and (27) it is easy to prove that for $q_1 \neq q_1'$ and $q_2 \neq q_2'$,

$$\int_{-\infty}^\infty d\xi\, Ta^*_{nq_1'}(\xi;k_1,\pm k_2)Ta_{nq_1}(\xi;k_1,\pm k_2)=\int_0^\infty d\eta\, Ta^*_{nq_2'}(i\eta;k_1,\pm k_2)Ta_{nq_2}(i\eta;k_1,\pm k_2)=0. \tag{47}$$

Thus we have for $q \neq q'$,

$$\int_0^\infty d\eta \int_{-\infty}^\infty d\xi(\xi^2+\eta^2)\Psi^*_{nq_1'q_2'}(\xi,\eta;k_1,\pm k_2)\Psi_{nq_1q_2}(\xi,\eta;k_1,\pm k_2)=0. \tag{48}$$

Let us now calculate the normalization constant $C_{nq_1q_2}(k_1,\pm k_2)$. From the explicit form of the wave function $\Psi^*_{nq_1q_2}(\xi,\eta;k_1,\pm k_2)$ and the normalization condition (29), it follows that

$$\frac{1}{8}|C_{nq_1q_2}(k_1,\pm k_2)|^2 \sum_{s,s',t,t'=0}^{n}(-1)^{t+t'}A^n_s(k_1,\pm k_2)A^n_{s'}(k_1,\pm k_2)A^n_t(k_1,\pm k_2)A^n_{t'}(k_1,\pm k_2)\{F^{-1/4}_{t,t'}F^{+1/4}_{s,s'} + F^{+1/4}_{t,t'}F^{-1/4}_{s,s'}\}=1, \tag{49}$$

where

$$F^{\pm 1/4}_{t,t'}=\sum_{m=0}^{\infty}\frac{\Gamma\left(\frac{m+t+t'\pm k_2+1}{2}+\frac{1}{4}\pm\frac{1}{4}\right)}{m!}\left(\frac{k_1}{2\omega}\right)^m. \tag{50}$$

C. Niven approach

Let us express solutions of the Schrödinger equation (16) in the following form:[19]

$$\Psi(x,y)=e^{-\omega[x+(k_1/4\omega^2)]^2-\frac{1}{2}\omega y^2}y^{\frac{1}{2}\pm k_2}\Phi(x,y). \tag{51}$$

From Eqs. (20), (21), and (31) follows that the function $\Phi(x,y)$ is a polynomial (product of two polynomials) in terms of the variables (x,y^2) in Cartesian coordinates and (ξ^2,η^2) for parabolic ones. It satisfies the equation

$$\mathcal{R}\Phi(x,y)=-2E\Phi(x,y), \tag{52}$$

where the operator $\mathcal{R}$ is

$$\mathcal{R}=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\left[\frac{(1\pm 2k_2)}{y}-2\omega y\right]\frac{\partial}{\partial y}-4\omega\left[x+\frac{k_1}{4\omega^2}\right]\frac{\partial}{\partial x}-\omega(2\pm k_2)+\frac{k_1^2}{8\omega^2}. \tag{53}$$

Taking into account that

$$Mk_{nq}(z;k_1,\pm k_2)=\sum_{s=0}^{n}A^{nq}_s(k_1,\pm k_2)z^s=\Pi^n_{\ell=1}(z-\alpha_\ell), \tag{54}$$

where α_ℓ, $\ell=1,2,\ldots,n$ are zeros of polynomials $Mk_{nq}(z)$ on the real axis $-\infty<z<\infty$, and that in parabolic coordinates

$$\frac{y^2}{\alpha}+2x-\alpha=\frac{(\xi^2-\alpha)(\eta^2+\alpha)}{\alpha}, \tag{55}$$

we can choose a solution of Eq. (52) in the form

$$\Phi(x,y)=Mk_{nq_1}(\xi^2;k_1,\pm k_2)Mk_{nq_2}(-\eta^2;k_1,\pm k_2)\cong\Pi_{\ell=1}^{n}\left(\frac{y^2}{\alpha_\ell}+2x-\alpha_\ell\right). \tag{56}$$

Then from (52) it follows that the zeros α_ℓ must satisfy the systems of n algebraic equations

$$\sum_{m\neq\ell}^{n}\frac{2}{\alpha_\ell-\alpha_m}+\frac{(1\pm k_2)}{\alpha_\ell}-\omega\alpha_\ell=\frac{k_1}{2\omega},\quad \ell=1,2,\ldots,n, \tag{57}$$

and for the energy spectrum we again have a formula (22). The system of algebraic equations (57) contains n sets of solutions (zeros) $(\alpha_1^{(q)},\alpha_2^{(q)},\ldots,\alpha_n^{(q)})$, $q=1,2,\ldots,n$ and all zeros are real. The positive zeros $\alpha_\ell>0$ define the nodes of wave functions for Eq. (26), whereas negative zeros $\alpha_\ell<0$ define the nodes of wave functions for Eq. (27).

The eigenvalues of the parabolic separation constant can be calculated in the same way via the operator equation $\Lambda\Phi(x,y)=\lambda\Phi(x,y)$ (see for details Ref. 19). A more elegant way is to use directly the differential equation (34).[63] We first rewrite Eq. (34) in the form

$$\left\{4z\frac{d^2}{dz^2}+4\left[(1\pm k_2)-\omega z\left(z+\frac{k_1}{2\omega^2}\right)\right]\frac{d}{dz}+\left[4n\omega z-\frac{k_1}{\omega}(1\pm k_2)\right]\right\}Mk_{nq}(z;k_1,\pm k_2)$$
$$=\lambda Mk_{nq}(z;k_1,\pm k_2). \tag{58}$$

Setting the wave function $Mk_{nq}(z;k_1,\pm k_2)$ in the form of (54), we arrive at the following result:

$$\lambda_{nq}(k_1,\pm k_2)=4(1\pm k_2)\left[\frac{k_1}{4\omega}+\sum_{\ell=1}^{n}\frac{1}{\alpha_\ell^{(q)}}\right], \tag{59}$$

(in case of $n=0$ the sum must be eliminated) where the quantum number $q=1,2,\ldots,n$ labels the eigenvalue of the parabolic separation constant.

III. THE SINGULAR CIRCULAR OSCILLATOR

The potential of the singular circular oscillator is $(k_1,k_2>0)$

$$V_2(x,y)=\frac{1}{2}\omega^2(x^2+y^2)+\frac{1}{2}\left(\frac{k_1^2-\frac{1}{4}}{x^2}+\frac{k_2^2-\frac{1}{4}}{y^2}\right). \tag{60}$$

The corresponding Schrödinger equation separates in three different orthogonal coordinate systems: **Cartesian, polar, and elliptical coordinates**.

A. Cartesian bases

From the asymptotic ansatz,

$$\Psi(x,y)=x^{\frac{1}{2}\pm k_1}y^{\frac{1}{2}\pm k_2}\exp[-\omega(x^2+y^2)]X(x)X(y) \tag{61}$$

we obtain two independent and identical separation equations

$$\left[\frac{\partial^2}{\partial z_i^2}+\left(-2\omega+\frac{1\pm 2k_i}{x_i^2}\right)x\frac{\partial}{\partial x_i}-(1\pm 2k_i)\omega\right]X(x_i)=2\lambda_i X(x_i),\quad i=1,2, \tag{62}$$

where $x_1=x$, $x_2=y$, and $\lambda_1+\lambda_2=-E$. As in the case of the singular anisotropic oscillator we assume that the positive sign of k_i must be taken if $k_i>\frac{1}{2}$ and both the positive and the negative sign must be taken if $0<k_i<\frac{1}{2}$.

The last equation is just that for confluent hypergeometric functions. The quantization rule gives

$$\lambda_i=-\omega(2n_i\pm k_i+1),\quad n_i=0,1,2,\ldots \tag{63}$$

and the solution of Eq. (62) in terms of Laguerre polynomials is $X(x_i)=L_{n_i}^{\pm k_i}(\omega x_i^2)$. Thus the corresponding set of orthonormal eigenfunctions which are normalized in quadrant $x>0, y>0$ (on 1/4) is

$$\Psi_{n_1,n_2}^{(\pm k_1,\pm k_2)}(x,y)=C_{n_1,n_2}^{(\pm k_1,\pm k_2)}(x)^{\frac{1}{2}\pm k_1}(y)^{\frac{1}{2}\pm k_2}e^{-(\omega/2)(x^2+y^2)}L_{n_1}^{\pm k_1}(\omega x^2)L_{n_2}^{\pm k_2}(\omega y^2), \tag{64}$$

where

$$C_{n_1,n_2}^{(\pm k_1,\pm k_2)}=\sqrt{\frac{\omega^{2\pm k_1\pm k_2}n_1!\,n_2!}{\Gamma(n_1\pm k_1+1)\Gamma(n_2\pm k_2+1)}}. \tag{65}$$

From (63) we have

$$E_n=\omega(2n+2\pm k_1\pm k_2), \tag{66}$$

where $n=n_1+n_2=0,1,2,\ldots$ is the principal quantum number and the degree of degeneracy is $n+1$.

B. Polar bases

Separation of variables in the Schrödinger equation for the potential (61) in polar coordinates

$$x=r\cos\phi,\quad y=r\sin\phi,\quad 0\leqslant r<\infty,\quad 0\leqslant\phi<2\pi \tag{67}$$

gives us the orthonormal solution in polynomial form

$$\Psi_{n_r,m}^{(\pm k_1,\pm k_2)}(r,\phi)=\sqrt{\frac{2\omega n_r!}{\Gamma(n_r+2m\pm k_1\pm k_2+2)}}(\sqrt{\omega}r)^{(2m\pm k_1\pm k_2+1)}e^{-\omega r^2/2}L_{n_r}^{2q\pm k_1\pm k_2+1}(\omega r^2)\Phi_m^{(\pm k_1,\pm k_2)}(\phi),$$
$$n_r,m=0,1,2,\ldots, \tag{68}$$

$$\Phi_m^{(\pm k_1,\pm k_2)}(\phi)=\sqrt{\frac{(2m\pm k_1\pm k_2+1)q!\,\Gamma(q\pm k_1\pm k_2+1)}{2\Gamma(m\pm k_2+1)\Gamma(m\pm k_1+1)}}(\cos\phi)^{1/2\pm k_1}(\sin\phi)^{1/2\pm k_2}P_m^{(\pm k_2,\pm k_1)}$$
$$\times(\cos 2\phi), \tag{69}$$

where $P_m^{(\alpha,\beta)}(x)$ is a Jacobi polynomial and $E=\omega(2n\pm k_1\pm k_2+2)$, with $n=n_r+m$ and with the same degree of degeneracy $(n+1)$.

Thus the quantum system (60) is exactly solvable in the Cartesian and polar systems of coordinates.

C. Elliptic bases

1. Separation of variables

Elliptic coordinates (ν,μ) connect with Cartesian ones by $(0\leqslant\nu<\infty, 0\leqslant\mu<2\pi)$

$$x = \frac{D}{2}\cosh\nu\cos\mu, \quad y = \frac{D}{2}\sinh\nu\sin\mu, \tag{70}$$

where D is the interfocal distance. The Laplacian and volume element are

$$\Delta = \frac{8}{D^2(\cosh 2\nu - \cos 2\mu)}\left(\frac{\partial^2}{\partial\nu^2} + \frac{\partial^2}{\partial\mu^2}\right), \quad \mathrm{d}V = \frac{D^2}{8}(\cosh 2\nu - \cos 2\mu)\mathrm{d}\nu\,\mathrm{d}\mu. \tag{71}$$

The Schrödinger equation with (60) can be rewritten as

$$\frac{\partial^2\psi}{\partial\nu^2} + \frac{\partial^2\psi}{\partial\mu^2} + \left\{\frac{D^2E}{4}(\cosh 2\nu - \cos 2\mu) - \frac{D^4\omega^2}{64}(\cosh^2 2\nu - \cos^2 2\mu) - \left[\frac{\left(k_1^2 - \frac{1}{4}\right)}{\cos^2\mu} + \frac{\left(k_2^2 - \frac{1}{4}\right)}{\sin^2\mu}\right] - \left[\frac{\left(k_1^2 - \frac{1}{4}\right)}{\sinh^2\nu} - \frac{\left(k_2^2 - \frac{1}{4}\right)}{\cosh^2\nu}\right]\right\}\psi = 0, \tag{72}$$

and after the separation ansatz

$$\psi(\nu,\mu;D^2) = X(\nu;D^2)Y(\mu;D^2) \tag{73}$$

transforms to two ordinary differential equations

$$\frac{d^2X}{\mathrm{d}\nu^2} + \left[\frac{D^2E}{4}\cosh 2\nu - \frac{D^4\omega^2}{64}\cosh^2 2\nu - \frac{k_2^2 - \frac{1}{4}}{\sinh^2\nu} + \frac{k_1^2 - \frac{1}{4}}{\cosh^2\nu}\right]X = -\lambda(D^2)X, \tag{74}$$

$$\frac{d^2Y}{\mathrm{d}\mu^2} - \left[\frac{D^2E}{4}\cos 2\mu - \frac{D^4\omega^2}{64}\cos^2 2\mu + \frac{k_1^2 - \frac{1}{4}}{\cos^2\mu} + \frac{k_2^2 - \frac{1}{4}}{\sin^2\mu}\right]Y = +\lambda(D^2)Y, \tag{75}$$

where λ is the elliptic separation constant. These equations can be written in the unit form

$$\frac{d^2Z(\zeta)}{\mathrm{d}\zeta^2} + \left[\frac{D^4\omega^2}{64}\cos^2 2\zeta - \frac{D^2E}{4}\cos 2\zeta - \frac{k_1^2 - \frac{1}{4}}{\cos^2\zeta} - \frac{k_2^2 - \frac{1}{4}}{\sin^2\zeta}\right]Z(\zeta) = \lambda(D^2)Z(\zeta), \tag{76}$$

where at $\zeta \in [0, 2\pi]$ we have the equation (75) but at $\zeta \in [0, i\infty)$—Eq. (74). In other words, in the complex ζ plane the "physical regions" are only the shaded domains on the two lines Im $\zeta = 0$ and Re $\zeta = 0$.

For $k_{1,2} > \frac{1}{2}$ the centrifugal barrier is repulsive and motion takes place in only one of the quadrants, as $\zeta \in [0, \pi/2]$, whereas for $0 < k_{1,2} < \frac{1}{2}$ it takes place in the whole region $\zeta \in [0, 2\pi]$. For the particular case $k_1 = k_2 = \frac{1}{2}$ the equation (76) transforms to the problem of the ordinary two-dimensional oscillator and has been investigated in detail in Ref. 69. In this paper we have shown that the solution of Eq. (76) (for $k_1 = k_2 = 1/2$) is described by Ince polynomials.[80]

In the case where k_1 and k_2 are integers, Eqs. (74) and (75) coincide with those that have been found via separation of variables in the Schrödinger equation for the four-dimensional isotropic oscillator in spheroidal coordinates.[70]

2. Recurrence relations

Let us now consider the equation (76). First, introducing the function $W(\zeta;D^2)$ according to

$$Z(\zeta;D^2) = \exp\left[-\frac{D^2\omega}{16}\cos 2\zeta\right]W(\zeta;D^2), \tag{77}$$

we have the equation

$$\frac{d^2W}{d\zeta^2}+\frac{D^2\omega}{4}\sin 2\zeta\frac{dW}{d\zeta}+\left[\frac{D^2\omega}{4}\cos 2\zeta-\frac{D^2E}{2}\cos^2\zeta-\frac{k_1^2-\frac{1}{4}}{\cos^2\zeta}-\frac{k_2^2-\frac{1}{4}}{\sin^2\zeta}-\lambda\right]W=0. \tag{78}$$

For $k_1=k_2=1/2$ this is the Ince equation.[50]

Next the substitution

$$W(\zeta;D^2)=(\sin\zeta)^{\frac{1}{2}\pm k_2}(\cos\zeta)^{\frac{1}{2}\pm k_1}U(\zeta;D^2) \tag{79}$$

yields the equation

$$\frac{d^2U}{d\zeta^2}+\left[(1\pm 2k_2)\cot\zeta-(1\pm 2k_1)\tan\zeta+\frac{D^2\omega}{4}\sin 2\zeta\right]\frac{dU}{d\zeta}+[p\cos^2\zeta-\tilde{\lambda}]U=0, \tag{80}$$

where

$$p=\frac{D^2}{2}[\omega(2\pm k_1\pm k_2)-E],\quad \tilde{\lambda}=\lambda+\frac{D^2\omega}{2}(1\pm k_1)+(1\pm k_1\pm k_2)^2-\frac{D^2E}{4}-\frac{D^4\omega^2}{64}. \tag{81}$$

Passing to a new variable $t=\cos^2\zeta$ we find

$$t(1-t)\frac{d^2U}{dt^2}+\left\{(1\pm k_1)(1-t)-(1\pm k_2)t+\frac{D^2\omega}{4}t(t-1)\right\}\frac{dU}{dt}+\frac{1}{4}[pt-\tilde{\lambda}]U=0. \tag{82}$$

Finally, looking for the solution of the last equation in the form

$$U(t;D^2)=\sum_{s=0}^{\infty}A_s(D^2)t^s, \tag{83}$$

for coefficients $A_s(D^2)$ we have the three-term recurrence relation

$$(s+1)(s+1\pm k_1)A_{s+1}-\left[s(s+1\pm k_1\pm k_2)+\frac{D^2\omega}{4}s+\frac{\tilde{\lambda}}{4}\right]A_s+\frac{1}{4}[p+D^2\omega(s-1)]A_{s-1}=0, \tag{84}$$

with $A_{-1}=0$ and initial condition $A_0=1$.

3. Energy spectrum and separation constant

In analogy with our asymptotic solution of the recurrence relation for the singular anisotropic operator in the parabolic basis we use continued fractions. For the minimal solution of the recurrence relations we find for $s^{-1}\ll 1$,

$$\frac{A_{s+1}}{A_s}\sim\frac{D^2\omega}{4s}\left(1+O\left(\frac{1}{\sqrt{s}}\right)\right). \tag{85}$$

Thus we have

$$A_s\sim\frac{\left(\frac{D^2\omega}{4}\right)^s}{s!},$$

and

$$U(\cos\zeta) \sim \sum \frac{\left(\frac{D^2\omega}{4}\right)^k}{k!} \cos^{2k}\zeta \sim \exp\left(\frac{D^2\omega}{8}\cos 2\zeta\right). \tag{86}$$

Therefore we see that for this case the function $Z(\cos\zeta;D^2)$ as $\zeta\to i\infty$ is not normalizable. There is a linearly independent solution of the recurrence relations, but the coefficients grow even faster. Hence it follows that the series (83) should be truncated. The condition that the series (83) be truncated gives us well-known formulas for the energy spectrum (66) and reduces the solution to polynomials,

$$U_n^{(\pm k_1,\pm k_2)}(t;D^2) = \sum_{s=0}^{n} A_s^{(\pm k_1,\pm k_2)}(D^2)t^s, \tag{87}$$

where now the coefficients $A_s \equiv A_s^{(\pm k_1,\pm k_2)}(D^2)$ satisfy the following three-term recurrent relations:

$$(s+1)(s+1\pm k_1)A_{s+1} + \beta_s A_s - \frac{D^2\omega}{4}(n-s+1)A_{s-1} = 0, \quad s = 0,1,\ldots,n \tag{88}$$

with

$$\beta_s = -\frac{1}{4}\left[(2s+1\pm k_1\pm k_2)^2 + \frac{D^2\omega}{2}(2s-n+4\pm 4k_1) - \frac{D^2\omega}{4}(2\pm k_1\pm k_2) - \frac{D^4\omega^2}{64} + \lambda(D^2)\right] \tag{89}$$

and $A_{-1}=A_{n+1}=0$.

The recurrence relations (88) become a system of $(n+1)$ linear homogeneous equations for the coefficients A_s. Equating the corresponding determinant to zero,

$$D_n(\lambda) = \begin{vmatrix} \beta_0 & (1\pm k_1) & & & \\ -\frac{D^2\omega}{4}n & \beta_1 & 2(2\pm k_1) & & \\ & & & -\frac{D^2\omega}{2} & \beta_{n-1} \quad n(n\pm k_1) \\ & & & & -\frac{D^2\omega}{4} \quad \beta_n \end{vmatrix} = 0 \tag{90}$$

leads to the algebraic equation of degree $(n+1)$ which determines the eigenvalues of the elliptic separation constant $\lambda_{nq}^{(\pm k_1,\pm k_2)}(D^2)$. The quantum number $q=0,1,2,\ldots,n$ labels the $(n+1)$ roots of Eq. (90) and therefore the degree of degeneracy, as in the polar and Cartesian cases, for the nth energy state is $n+1$. It is also known that the corresponding enumeration of the quantum number q defines the numbers of zeros of the polynomial (87), which has exactly n zeros situated in the open interval $0<t<\infty$, and therefore, the elliptic separation constant $\lambda_{nq}^{(\pm k_1,\pm k_2)}(D^2)$ may be ordered also by the numbers of the nodes of the eigenfunction of Eq. (76).

4. Wave functions

The condition of finiteness of the solution of Eq. (78) allows the following polynomials:

$$\mathcal{I}_{nq}^{(\pm k_1,\pm k_2)}(\zeta;D^2) = (\sin\zeta)^{\frac{1}{2}\pm k_2}(\cos\zeta)^{\frac{1}{2}\pm k_1}\sum_{s=0}^{n} A_s^{(\pm k_1,\pm k_2)}(D^2)(\cos\zeta)^{2s}, \tag{91}$$

while the corresponding solution of Eq. (76) is

$$\mathcal{Z}_{nq}^{(\pm k_1,\pm k_2)}(\zeta;D^2) = e^{-(D^2\omega/16)\cos 2\zeta}\mathcal{I}_{nq}^{(\pm k_1,\pm k_2)}(\zeta;D^2). \tag{92}$$

We will denote the polynomials $\mathcal{I}_{nq}^{(\pm k_1,\pm k_2)}(\zeta;D^2)$ as *associated Ince polynomials*. In the case of $k_1=k_2=1/2$ these polynomials transform to the four types of ordinary *Ince polynomials*, which are even or odd with respect to the changes $\zeta\to-\zeta$ and $\zeta\to\zeta+\pi$.[80,69]

At $\zeta=\mu$ the wave functions (92) give us the solution of the angular equation (75), and for $\zeta=i\nu$ the solution of the radial equation (74). For each of the wave functions, radial or angular, there corresponds a definite number of zeros which can be represented by two quantum numbers q_1 and q_2, obeying the condition $q_1+q_2=n$. Then the complete elliptic wave function (73) may be written as

$$\Psi_{nq_1q_2}^{(\pm k_1,\pm k_2)}(\nu,\mu;D^2)=C_{nq_1q_2}(\pm k_1,\pm k_2;D^2)\mathcal{Z}_{nq_1}^{(\pm k_1,\pm k_2)}(\mu;D^2)\mathcal{Z}_{nq_2}^{(\pm k_1,\pm k_2)}(i\nu;D^2), \tag{93}$$

where $C_{nq_1q_2}(\pm k_1,\pm k_2;D^2)$ is the normalization constant. It could be calculated from the condition

$$\frac{D^2}{4}\int_0^\infty \mathrm{d}\nu\int_0^{\pi/2}\mathrm{d}\mu(\cosh^2\nu-\cos^2\mu)\Psi_{nq_1q_2}^{(\pm k_1,\pm k_2)*}(\nu,\mu;D^2)\Psi_{nq_1q_2}^{(\pm k_1,\pm k_2)}(\nu,\mu;D^2)=\frac{1}{4}. \tag{94}$$

5. Orthogonality relations

The wave functions (93) as eigenfunctions of the Hamiltonians are orthogonal $n\neq n'$,

$$\int_0^\infty\int_0^{\pi/2}\Psi_{n'q_1q_2}^{(\pm k_1,\pm k_2)*}(\nu,\mu;D^2)\Psi_{nq_1q_2}^{(\pm k_1,\pm k_2)}(\nu,\mu;D^2)\mathrm{d}V=0. \tag{95}$$

Equations (74) and (75) enable one to prove the property of *double orthogonality* for wave functions $\mathcal{Z}_{nq}^{(\pm k_1,\pm k_2)}(\zeta;D^2)$, namely

$$\int_0^\infty \mathcal{Z}_{nq_2'}^{(\pm k_1,\pm k_2)*}(i\nu;D^2)\mathcal{Z}_{nq_2}^{(\pm k_1,\pm k_2)}(i\nu;D^2)\mathrm{d}\nu=0, \tag{96}$$

$$\int_0^{\pi/2}\mathcal{Z}_{nq_1'}^{(\pm k_1,\pm k_2)*}(\mu;D^2)\mathcal{Z}_{nq_1}^{(\pm k_1,\pm k_2)}(\mu;D^2)\mathrm{d}\mu=0 \tag{97}$$

for $q_1\neq q_1'$ and $q_2\neq q_2'$, and therefore when $q\neq q'$,

$$\int_0^\infty \mathrm{d}\nu\int_0^{\pi/2}\mathrm{d}\mu(\cosh^2\nu-\cos^2\mu)\Psi_{nq_1'q_2'}^{(\pm k_1,\pm k_2)*}(\nu,\mu;D^2)\Psi_{nq_1q_2}^{(\pm k_1,\pm k_2)}(\nu,\mu;D^2)=0. \tag{98}$$

IV. THREE-DIMENSIONAL SPACE

So far we have considered only superintegrable systems in two dimensions. To make clearer our approach and how it extends to all dimensions, we consider some three-dimensional (3D) examples.

A. The harmonic oscillator

As is very well known, the Schrödinger equation for the 3D harmonic oscillator (a superintegrable system) is exactly solvable in Cartesian coordinates. We consider it in elliptic coordinates where the separation equations are QES. We will show explicitly that the polynomial solutions of the uncoupled 3D problem can be found directly and that the results greatly simplify the determination of the polynomial solutions of the separated QES equations. In elliptic coordinates the Schrödinger equation has the form

$$H=\frac{1}{(u-v)(u-w)}\left[4\sqrt{P(u)}\frac{\partial}{\partial u}\left(\sqrt{P(u)}\frac{\partial}{\partial u}\right)-\omega^2(u^3-E_1u^2)\right]$$
$$+\frac{1}{(v-u)(v-w)}\left[4\sqrt{P(v)}\frac{\partial}{\partial v}\left(\sqrt{P(v)}\frac{\partial}{\partial v}\right)-\omega^2(v^3-E_1v^2)\right]$$
$$+\frac{1}{(v-w)(v-u)}\left[4\sqrt{P(w)}\frac{\partial}{\partial w}\left(\sqrt{P(w)}\frac{\partial}{\partial w}\right)-\omega^2(w^3-E_1w^2)\right],$$

where

$$E_1=e_1+e_2+e_3,\quad P(\lambda)=(\lambda-e_1)(\lambda-e_2)(\lambda-e_3).$$

Here the elliptic coordinates are given by

$$x^2=\frac{(u-e_1)(v-e_1)(w-e_1)}{(e_1-e_2)(e_1-e_3)},\quad y^2=\frac{(u-e_2)(v-e_2)(w-e_2)}{(e_2-e_1)(e_2-e_3)},$$

$$z^2=\frac{(u-e_3)(v-e_3)(w-e_3)}{(e_3-e_2)(e_3-e_1)}.$$

The separation equations that describe the solutions of $H\Psi=E\Psi$ are

$$\left[4\sqrt{P(\lambda)}\frac{\partial}{\partial\lambda}\left(\sqrt{P(\lambda)}\frac{\partial}{\partial\lambda}\right)-\omega^2(\lambda^3+(-E_1+E)\lambda^2)+L_1\lambda-L_2\right]\Lambda(\lambda)=0$$

for $\lambda=u,v,w$. The operators that describe the separation constants are

$$L_1=\frac{vw}{(u-v)(u-w)}\left[4\sqrt{P(u)}\frac{\partial}{\partial u}\left(\sqrt{P(u)}\frac{\partial}{\partial u}\right)-\omega^2(u^3-E_1u^2)\right]$$
$$+\frac{uw}{(v-u)(v-w)}\left[4\sqrt{P(v)}\frac{\partial}{\partial v}\left(\sqrt{P(v)}\frac{\partial}{\partial v}\right)-\omega^2(v^3-E_1v^2)\right]$$
$$+\frac{uv}{(w-u)(w-v)}\left[4\sqrt{P(w)}\frac{\partial}{\partial w}\left(\sqrt{P(w)}\frac{\partial}{\partial w}\right)-\omega^2(w^3-E_1w^2)\right],$$

and

$$L_2=\frac{v+w}{(u-v)(u-w)}\left[4\sqrt{P(u)}\frac{\partial}{\partial u}\left(\sqrt{P(u)}\frac{\partial}{\partial u}\right)-\omega^2(u^3-E_1u^2)\right]$$
$$+\frac{u+w}{(v-u)(v-w)}\left[4\sqrt{P(v)}\frac{\partial}{\partial v}\left(\sqrt{P(v)}\frac{\partial}{\partial v}\right)-\omega^2(v^3-E_1v^2)\right]$$
$$+\frac{u+v}{(w-u)(w-v)}\left[4\sqrt{P(w)}\frac{\partial}{\partial w}\left(\sqrt{P(w)}\frac{\partial}{\partial w}\right)-\omega^2(w^3-E_1w^2)\right].$$

In order to find square integrable solutions to this problem it is natural to remove an exponential factor according to

$$\Psi(u,v,w)=\exp\left(-\frac{\omega}{2}(u+v+w)\right)\Phi(u,v,w).$$

Then there are polynomial solutions for $\Phi(u,v,w)$ of the form

$$\Phi(u,v,w) = \prod_{j=1}^{r}(u-\theta_j)(v-\theta_j)(w-\theta_j).$$

The zeros of the polynomials satisfy the relations

$$-4\omega + \sum_{i\neq j}\frac{4}{\theta_i-\theta_j} + \sum_{s=1}^{3}\frac{1}{\theta_j-e_s} = 0.$$

It follows that the eigenvalues E and ℓ_1, ℓ_2 of the operators L_1 and L_2 can be expressed in the form

$$\ell_1 = -4r^2E_1 + 2(3+4r)\sum_{j=1}^{r}\theta_j + \left[-(1+4r)E_2 + 4E_1\sum_{j=1}^{r}\theta_j - \sum_{j=1}^{r}\theta_j^2\right]\omega - E_3\omega^2,$$

$$\ell_2 = -2r(2r+1) - 2(2r+1)E_1\omega + 4\omega\sum_{j=1}^{r}\theta_i - E_2\omega^2,$$

where $E_2=e_1e_2+e_2e_3+e_1e_3$ and $E_3=e_1e_2e_3$. Because of the relations among the zeros θ_j there are also alternative expressions available for these eigenvalues. We now turn our attention to calculating the eigenvalues. Let us first consider the special case $r=1$. If we choose a basis of functions of u, v, and w $F_0=1, F_1=u+v+w, F_2=uv+uw+vw$, and $F_3=uvw$ then we can find solutions

$$\Phi(u,v,w) = a_0F_0 + a_1F_1 + a_2F_2 + a_3F_3.$$

If we look for eigenfunctions for the operator L_1 that correspond to this form we obtain the conditions

$$(2E_3\omega^2 + 5E_2\omega + 4E_1 + \ell_1)a_3 + (4E_1\omega + 6)a_2 + 4\omega a_1 = 0,$$

$$(-2E_2 - 4E_3\omega)a_3 + (\ell_1 + \omega E_2 + \omega^2E_3)a_2 = 0,$$

$$(-2E_2 - 4E_3\omega)a_2 + (\ell_1 + \omega E_2 + \omega^2E_3)a_1 = 0, \quad (-2E_2 - 4E_3\omega)a_1 + (\ell_1 + \omega E_2 + \omega^2E_3)a_0 = 0.$$

For these equations to have a nontrivial solution the corresponding determanental condition must hold viz.

$$\begin{aligned}(\ell_1 + \omega E_2 + \omega^2E_3)(\ell_1^3 + (4E_1 + 7E_2\omega + 3E_3\omega^2)\ell_1^2 + (14E_3E_2\omega^3 + (24E_1E_3 + 11E_2^2)\omega^2 \\ + (16E_1E_2 + 24E_3)\omega + 12E_2)\ell_1 + E_3(20E_1E_3 + 11E_2^2)\omega^4 + (5E_2^3 + 188E_3^2 + 32E_1E_2E_3)\omega^3 \\ + 4E_2(6E_1E_2 - 14E_3)\omega^2 + 28E_2\omega) = 0.\end{aligned}$$

For the operator L_2 the corresponding relations among the a_i are

$$(6 + \ell_2 + E_2\omega^2 + 6\omega E_1)a_3 + 4\omega a_2 = 0, \quad (6 + \ell_2 + E_1\omega + E_2\omega^2)a_2 + 4\omega a_3 = 0,$$

$$-(2E_2 - 4E_3\omega)a_3 + (-4E_2\omega + 4E_1)a_2 + (E_2\omega^2 + 2\omega E_1 + \ell_2)a_1 = 0,$$

$$-(2E_2 - 4E_3\omega)a_2 + (-4E_1 + 4E_2\omega)a_1 + (\ell_2 + 2E_1\omega + E_2\omega^2)a_0 = 0,$$

with the determinant condition

$$(\ell_2 + 2\omega E_1 + \omega^2 E_2)(\ell_2^3 + (14\omega E_1 + 3\omega^2 E_2)\ell_2^2 + (3\omega^4 E_2^2 + 28\omega^3 E_1 E_2 + \omega^2(60E_1^2 + 40E_2) + 112\omega E_1 + 36)\ell_2 + \omega^6 E_2^3 + 14\omega^5 E_1 E_2^2 + 4\omega^4 E_2(15E_1^2 + 7E_2) + \omega^3(72E_1^3 + 208E_1 E_2 - 343E_3) + \omega^2(240E_1^2 + 100E_2) + 168\omega E_1) = 0.$$

This illustrates clearly that our method gives the eigenvalues of L_1 and L_2 as solutions of polynomial equations. If we substitute in this way into the Schrödinger equation itself then we obtain the conditions

$$(E + 7\omega)a_j = 0, \quad j = 1,2,3,$$

$$(2E_2 + 4E_3\omega)a_3 + 4(E_1 + \omega E_2)a_2 + 2(3 + 2\omega E_1)a_1 - (E + 3\omega)a_0 = 0$$

yielding the two eigenvalues -7ω *and* -3ω for E. This method has obvious extensions to $r = 2, \ldots$.

Note that if we look for polynomial solution of the separation equations then we obtain different equations. In particular if we look for solutions of the form $\Lambda(\lambda) = \exp[-(\omega/2)\lambda](\lambda - c)$ in the separation equation

$$\sqrt{P(\lambda)}\frac{\partial}{\partial\lambda}\left(\sqrt{P(\lambda)}\frac{\partial}{\partial\lambda}\Lambda(\lambda)\right) + (\omega^2(-\lambda^3 + (E_1 - E)\lambda^2) + \ell_2\lambda - \ell_1)\Lambda(\lambda) = 0$$

we obtain the relations

$$\ell_2^2 + \ell_2(6 + 8\omega E_1 + 2\omega^2 E_2) + 4\omega\ell_1 + \omega^4 E_2^2 + \omega^3(8E_1 E_2 + 4E_3) + \omega^2(12E_1^2 + 26E_2) + 28\omega = 0,$$

$$\ell_1\ell_2 + \omega(E_2 + E_3\omega)\ell_2 + \omega(6E_1 + \omega E_2)\ell_1 + E_2 E_3\omega^4 + \omega^3(6E_1 E_3 + E_2^2) + \omega^2(6E_1 E_2 + 22E_3) + 14E_2\omega = 0,$$

where

$$c = ((12 + 2\ell_2) + 6\omega E_1 + \omega^2 E_2)/4\omega.$$

If we were to pursue this approach further then we would obtain more complicated relations among the ℓ_1 and ℓ_2 which could be uncoupled to produce the individual equations for ℓ_1 and ℓ_2, respectively. This example shows clearly how study of the full 3D superintegrable system yields results for solutions of the separation equations that could not easily be obtained from a direct study of the separation equations themselves.

B. Ushveridze's separation of variables example

A critical further example is that studied by Ushveridze on p. 115 of Ref. 63. He takes two copies of an ordinary differential QES problem (polynomial potential of order 10) and combines them to form a single 2D partial differential equation from which the original ordinary differential equations can be obtained by separation of variables. However, the partial differential equation that he obtains is merely separable, not multiseparable. In particular it is not superintegrable. Here we show the increased insight and greater simplicity obtained by using three copies of the QES problem to form a 3D superintegrable system. We proceed as follows. Consider the Schrödinger equation $H\Psi = E\Psi$ where

$$H = \frac{1}{(u^2-v^2)(u^2-w^2)}\left[\frac{\partial^2}{\partial u^2} - 36k_1^2u^{10} - 48k_1k_2u^8 - 8(2k_2^2+3k_1k_3)u^6 + \frac{p(1-p)}{u^2}\right]$$
$$+ \frac{1}{(v^2-u^2)(v^2-w^2)}\left[\frac{\partial^2}{\partial v^2} - 36k_1^2v^{10} - 48k_1k_2v^8 - 8(2k_2^2+3k_1k_3)v^6 + \frac{p(1-p)}{v^2}\right]$$
$$+ \frac{1}{(w^2-v^2)(w^2-u^2)}\left[\frac{\partial^2}{\partial w^2} - 36k_1^2w^{10} - 48k_1k_2w^8 - 8(2k_2^2+3k_1k_3)w^6 + \frac{p(1-p)}{w^2}\right].$$

This equation is clearly separable in the u,v,w coordinates. Passing to Cartesian coordinates $z = iuvw$ and

$$x+iy = \tfrac{1}{2}(u^2v^2+u^2w^2+v^2w^2) - \tfrac{1}{4}(u^4+v^4+w^4), \quad x-iy = \tfrac{1}{2}(u^2+v^2+w^2),$$

we can recognize the Hamiltonian operator in the form

$$H = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + 36k_1^2(2(x-iy)^3 - 4(x^2+y^2) - z^2) + 48k_1k_2(3(x-iy)^2 - (x+iy))$$
$$- 16(2k_2^2+3k_1k_3)(x+iy) - \frac{p(p-1)}{z^2}. \tag{99}$$

This in turn can be recognized as essentially the complex Euclidean space superintegrable system with nondegenerate potential

$$V = \alpha(z^2 - 2(x-iy)^3 + 4(x^2+y^2)) + \beta(2(x+iy) - 3(x-iy)^2 2) + \gamma(x+iy) + \frac{\delta}{z^2}, \tag{100}$$

in which the six basis second-order symmetry operators can be taken in the form

$$H = \partial_x^2 + \partial_y^2 + \partial_z^2 + V,$$

$$S_1 = (\partial_x - i\partial_y)2 + f_1, \quad S_2 = \partial_z^2 + f_2, \quad S_3 = \{\partial_z, J_2 + iJ_1\} + f_3, \tag{101}$$

$$S_4 = \frac{1}{2}\{J_3, \partial_x - i\partial_y\} - \frac{i}{4}(\partial_x + i\partial_y)^2 + f_4, \quad S_5 = (J_2+iJ_1)^2 + 2i\{\partial_z, J_1\} + f_5,$$

where $\{A,B\}=AB+BA$, the J_i are the angular momentum operators, e.g., $J_3=x\partial_y - y\partial_x$, and the f_i are appropriate functions. There is a quadratic algebra generated by these symmetries. This is a direct consequence of the observation that this potential is an example of a nondegenerate potential in three dimensions.[7,8]

The separation equations for the Schrödinger equation have the form

$$\left[\frac{\partial^2}{\partial \lambda^2} - 36k_1^2\lambda^{10} - 48k_1k_2\lambda^8 - 8(2k_2^2+3k_1k_3)\lambda^6 + \frac{p(1-p)}{\lambda^2} + E\lambda^4 + \ell_2\lambda^2 + \ell_3\right]\Lambda(\lambda) = 0,$$

essentially, Ushveridze's 1D QES problem. The operators with the separation constants as eigenvalues are

$$L_2 = \frac{v^2+w^2}{(u^2-v^2)(u^2-w^2)}\left[\frac{\partial^2}{\partial u^2} - 36k_1^2u^{10} - 48k_1k_2u^8 - 8(2k_2^2+3k_1k_3)u^6 + \frac{p(1-p)}{u^2}\right]$$
$$+ \frac{u^2+w^2}{(v^2-u^2)(v^2-w^2)}\left[\frac{\partial^2}{\partial v^2} - 36k_1^2v^{10} - 48k_1k_2v^8 - 8(2k_2^2+3k_1k_3)v^6 + \frac{p(1-p)}{v^2}\right]$$
$$+ \frac{u^2+v^2}{(w^2-v^2)(w^2-u^2)}\left[\frac{\partial^2}{\partial w^2} - 36k_1^2w^{10} - 48k_1k_2w^8 - 8(2k_2^2+3k_1k_3)w^6 + \frac{p(1-p)}{w^2}\right] \tag{102}$$

and

$$L_3 = \frac{v^2w^2}{(u^2-v^2)(u^2-w^2)}\left[\frac{\partial^2}{\partial u^2} - 36k_1^2u^{10} - 48k_1k_2u^8 - 8(2k_2^2+3k_1k_3)u^6 + \frac{p(1-p)}{u^2}\right]$$
$$+ \frac{u^2w^2}{(v^2-u^2)(v^2-w^2)}\left[\frac{\partial^2}{\partial v^2} - 36k_1^2v^{10} - 48k_1k_2v^8 - 8(2k_2^2+3k_1k_3)v^6 + \frac{p(1-p)}{v^2}\right]$$
$$+ \frac{u^2v^2}{(w^2-v^2)(w^2-u^2)}\left[\frac{\partial^2}{\partial w^2} - 36k_1^2w^{10} - 48k_1k_2w^8 - 8(2k_2^2+3k_1k_3)w^6 + \frac{p(1-p)}{w^2}\right]. \tag{103}$$

In searching for finite solutions of $H\Psi = E\Psi$ we write

$$\Psi(u,v,w) = \exp(k_1(u^6+v^6+w^6) + k_2(u^4+v^4+w^4) + k_3(u^2+v^2+w^2))(uvw)^p\Phi(u,v,w),$$

where

$$\Phi(u,v,w) = \prod_{j=1}^{r}(u^2-\theta_j)(v^2-\theta_j)(w^2-\theta_j).$$

The zeros of the polynomials satisfy the relations

$$\frac{2r+1}{2\theta_i} - 12k_1\theta_i^2 - 4k_2\theta_i - k_3 + \sum_{j\neq i}\frac{1}{\theta_i-\theta_j} = 0.$$

Solving these equations we see that the eigenvalues of the operators H, L_2, and L_3 have the form

$$E = -(30+24r+12p)k_1 - 16k_2k_3, \quad \ell_2 = -4k_3^2 - (12+16r)k_2 - 24k_1\sum_{j=1}^{r}\theta_j,$$

$$\ell_3 = -(2+8r+4p)k_3 - 16k_2\sum_{j=1}^{r}\theta_j - 24k_1\sum_{j=1}^{r}\theta_j^2.$$

Because of the relations among the zeros there are many other expressions for these eigenvalues. If we look for solutions of the form

$$\Phi(u,v,w) = a_0G_0 + a_1G_1 + a_2G_2 + a_3G_3,$$

where $G_0=1$, $G_1=u^2+v^2+w^2$, $G_2=u^2v^2+u^2w^2+v^2w^2$, and $G_3=u^2v^2w^2$, i.e., second-order polynomial solutions, and substitute this expression into the eigenvalue equations, we obtain the following polynomial equations for the eigenvalues:

$$(E+k_1(54+12p))^3(E+k_1(30+12p)) = 0,$$

$$(\ell_2 + 2k_2(4p+1) + 4k_3^2)(\ell_2^3 + (12k_3^2 + (68+24p)k_2)\ell_2^2$$

$$+ (192k_1k_3 + 16(2p+7)(6p+13)k_2^2 + 32k_3^2k_2(6p+17) + 48k_3^4)\ell_2$$

$$+ 64(17+6p)k_2k_3^4 + 768k_1k_3^3 + 64(2p+7)(6p+13)k_2^2k_3^2 + 768(2p+7)k_1k_2k_3$$

$$+ 64(2p+3)(2p+7)^2k_3^2 - 1152(2p+1)k_1^2 = 0,$$

$$(\ell_3 + 2k_3(p+1))(\ell_3^3 + 2(6p+7)k_3\ell_3^2 + 4(6p+11)(1+2p)k_3^2\ell_3 + 8(1+2p)^2(12k_1 + 2pk_3^2 + 5k_3^3)) = 0.$$

On the other hand, if we study the separation equations individually and look for a solution of the form

$$\Lambda(\lambda) = \exp(k_1\lambda^6 + k_2\lambda^4 + k_3\lambda^2)\lambda^p(\lambda - c)$$

in the above separation equation then we obtain different relations

$$\ell_2^2 + (4k_2(10+4p) + 8k_3^2)\ell_2 + 24k_1\ell_3 + 16k_3^4 + 8(4k_2k_3^2 + 6k_1k_3)(5+2p) + 16k_2^2(2p+7)(2p+3) = 0,$$

$$\ell_2\ell_3 + 2(2p+1)\ell_2 + (4k_2(2p+7) + 4k_3^2)\ell_3 + 48k_1(1+2p) + 8k_2k_3(2p+7)(2p+1) + 8(1+2p)k_3^3 = 0,$$

where

$$c = -\frac{1}{24k_1}(4k_2(p+7) + 4k_3^3 + \ell_2).$$

The above computation extends in an obvious manner to the computation of polynomial solutions of any order. There is a clear relationship with Ushveridze's equation on p. 115 of Ref. 63 through the correspondence $a=6k_1$, $b=4k_2$, $c=2k_3$, and $s=(2p+1)/4$.

We now look for solutions determined by other second-order constants of the motion and corresponding (possibly separable) coordinate systems. First consider our basic equation $H\Psi = E\Psi$ written in terms of different coordinates $\xi=x+iy$, $\eta=x-iy$, z. We can find nonseparable solutions in these coordinates of the form

$$\Psi = \exp\Bigg(2\sqrt{[\lambda + (k_2+3k_1\xi)^2]}\,\eta \times \int\left[-\frac{3k_1(k_2+3k_1\xi)}{[\lambda+(k_2+3k_1\xi)^2]} + \frac{\xi(-9k_1^2\xi^2 + 9k_1k_2\xi + 6k_1k_2 + 4k_2^2) + E}{\sqrt{(\lambda+(k_2+3k_1\xi)^2)}}\right]d\xi\Bigg) \times \exp(-3k_1z^2)z^pL_n^{p+\frac{1}{2}}(6k_1z^2),$$

where

$$E = E - 6k_1(4n+2p+1)$$

and $L_m^{\alpha}(t)$ is a Laguerre polynomial. It is clear that the above ξ integral can be calculated in terms of elementary functions but we prefer the form given as it is more compact. This possibility for an explicit solution comes about from the existence of a symmetry of the form $p_\eta^2 + f$.

If we choose new separable coordinates u, v, z defined by

$$x+iy=-\tfrac{1}{2}(u-v)^2,\quad x-iy=u+v$$

then the Schrödinger equation has the separable form

$$H\Psi=\left[\frac{1}{u-v}\left[\left(\frac{\partial}{\partial u^2}-144k_1^2u^4-96k_1k_2u^3+16(2k_2^2+3k_1k_3)u^2\right)\right.\right.$$
$$\left.\left.-\left(\frac{\partial}{\partial v^2}-144k_1^2v^4-96k_1k_2v^3+16(2k_2^2+3k_1k_3)v^2\right)\right]+\frac{\partial^2}{\partial z^2}-36k_1^2z^2+\frac{p(1-p)}{z^2}\right]\Psi=E\Psi. \tag{104}$$

The symmetry operator L associated with separation in these coordinates is of the form

$$L\Psi=\left[\frac{1}{u-v}\left[v\left(\frac{\partial}{\partial u^2}-144k_1^2u^4-96k_1k_2u^3+16(2k_2^2+3k_1k_3)u^2\right)\right.\right.$$
$$\left.\left.-u\left(\frac{\partial}{\partial v^2}-144k_1^2v^4-96k_1k_2v^3+16(2k_2^2+3k_1k_3)v^2\right)\right]\Psi.$$

Searching for finite solutions using these coordinates, we see that they can be taken in the form

$$\Psi=\exp\left(4k_1(u^3+v^3)+2k_2(u^2+v^2)-2\left(\frac{k_2^2}{k_1}+k_3\right)(u+v)\right)\Pi_{i=0}^{r}[(u-\theta_i)(v-\theta_i)]$$
$$\times\exp(-3k_1z^2)z^pL_n^{p+\frac{1}{2}}(6k_1z^2).$$

For solutions of this kind these zeros satisfy

$$-2k_1k_3-2k_2^2+4k_1k_2\sum_{i=1}^{r}\theta_i+12k_1^2\sum_{i=1}^{r}\theta_i^2+\sum_{j\neq i}\frac{k_1}{\theta_i-\theta_j}=0.$$

The eigenvalues of L and H' have the form

$$\lambda_r=-4\frac{k_2^4}{k_1^2}-8\frac{k_2^2k_3}{k_1}-4k_3^2-4(1+2r)k_2-24\sum_{i=1}^{r}\theta_i,\quad E_r=16k_2k_3+16\frac{k_2^3}{k_1}-24(r+1)k_1,$$

and $E=E_r+6k_1(4n+2p+1)$.

It is clear that we can find solutions of the form given above but with a choice of polynomial, say $c_1uv+c_2(u+v)+c_3$ for illustration. The resulting polynomial equation for the eigenvalues of L is

$$(\lambda k_1^2+4k_1^2k_3^2+4k_2k_1^2+4k_2^4+8k_1k_3k_2^2)(k_1^4\lambda^2+8k_1^2(2k_2k_1^2+k_3^2k_1^2+2k_1k_3k_1^2+k_2^4)\lambda)$$

$$-96k_3k_1^5-48k_2^2k_1^4+64k_3^2k_1^4k_2+16k_3^4k_1^4+128k_2^3k_3k_1^3+64k_3^3k_1^3k_2^2+64k_2^5k_1^2+96k_1^2k_2^4k_3^2$$

$$+64k_2^6k_1k_3+16k_2^8=0.$$

These are finite solutions, clearly different from those given previously. The above analysis can be extended in an obvious manner to yield polynomial solutions of any order.

Note that for this last coordinate system we have given an example of a QES problem with a quartic potential, something hitherto not known to be possible (as mentioned in Ushveridze's book). Indeed the separation equations have the form

$$\left(\frac{\partial^2}{\partial \ell^2} - 144k_1^2\ell^4 - 96k_1k_2\ell^3 + 16(2k_2^2 + 3k_1k_3)\right)\ell^2$$
$$-\left\{16k_2k_3 + 16\frac{k_3^2}{k_1} + 6k_1(4n - 4r + 2p - 3)\ \ell\ + \lambda_r\right\}\Lambda(\ell) = 0,$$

where $\Lambda = U, V$ and $\ell = u, v$. There are typically $r+1$ solutions

$$\Lambda(\ell) = \exp\left(4k_1\ell^3 + 2k_2\ell^2 - 2\left(\frac{k_2^2}{k_1} + k_3\right)\ \ell\ \right)\Pi_{i=0}^{r}(\ell - \theta_i)$$

of this equation, with corresponding eigenvalues $\lambda_r^{(s)}, s = 1, \ldots, r+1$. It is clear from our definition of QES that if we look for series solutions then the recurrence relations involved will contain more than three terms. The analysis then proceeds in analogy with what has been demonstrated for the case of three terms and the requirement of polynomial solutions (to within a factor) is a consequence of the solutions generated in this manner being well behaved at the regular singular points.

It is clear that in higher dimensions there are many examples which generalize the examples occurring in Ref. 63. The utility of the use of partial differential operators, rather than ordinary differential operators, is evident. Finally, we note in the superintegrable example presented here, though our system is multiseparable there are no separable coordinates in which the separated equations are each exactly solvable.

V. CONCLUSIONS AND SUMMARY

We have demonstrated that solutions of the Schrödinger equation for the potential V_1 may be constructed via separation of variables in two different ways. Using Cartesian coordinates we arrive at two independent exactly solvable equations (17) and (18), each of them representing a one-dimensional *nonparametric* spectral problem where the Cartesian separation constants λ_i play the role of energy. To obtain solutions in the form of Laguerre and Hermite polynomials, both separation constants are quantized and as a result the energy spectrum for the two-dimensional Schrödinger equation is obtained. For the second separable system which uses parabolic coordinates the solution method is more complex. We have shown that the separation procedure reduces to an ordinary differential equation for real and imaginary variables. It has been proven that the requirement of convergence for solutions of Eq. (30) at the singular points $\mu = \pm\infty$ and $\mu = i\infty$ leads to only polynomial solutions (42) with the restriction for the energy spectrum E in the form (22) and for a fixed energy (or quantum number n) gives the spectrum of the separation constant as the root of an nth-degree polynomial equation. In contrast to the solution in Cartesian coordinates the coefficients of the polynomial solutions satisfy three-term recurrence relations and cannot be written in explicit form in general. For this reason we refer to the equation (30) as quasiexactly solvable.

On the other hand, the substitution of the formula for the energy spectrum into Eq. (30) gives rise to the equation

$$\left[-\frac{d^2}{d\mu^2} + \left(\omega^2\mu^6 + k_1\mu^4 + \left[\frac{k_1^2}{4\omega^2} - \omega(4n + 4 \pm 2k_2)\right]\mu^2 + \frac{k_2^2 - \frac{1}{4}}{\mu^2}\right)\right]Z_n(\mu) = \lambda Z_n(\mu), \tag{105}$$

which on the real axis completely coincides for $k_1 = 4\beta\omega^2$ and $1 \pm k_2 = 2\delta$, with the one-dimensional spectral problem (10), and is called a quasiexactly solvable problem. Now it is easy to understand the origins of the occurrence of quasiexactly solvable systems. The requirement of convergence just in real space (which is possible to determine following Ref. 37 as the dimensional reduction) in the vicinity of singular points $\mu = \pm\infty$ requires that there are polynomial solutions of the form (41). We also can shed light on the mystery of the zeros of the polynomial $P_n(x^2)$. Indeed, the substitution of the wave function (11) into the Schrödinger equation with potential (10) leads to

the differential equation for polynomial $P_n(x^2)$ in the same form as Eq. (58) (in variable $x^2=z$), but with the difference that the physical region of Eq. (58) is the whole real axis $z \in (-\infty, \infty)$, and therefore all zeros (for positive and negative x^2) of $P_n(x^2)$ correspond to the zeros of two-dimensional eigenfunction of singular anisotropic oscillator in parabolic coordinates.

The situation is repeated in the case of the second potential (60). We have determined that the separation of variables in two-dimensional elliptic coordinates leads to a Schrödinger type equation (76) in the complex plane and the requirement of convergence at the point $\zeta=0,2\pi$ and $\zeta=i\infty$ requires polynomial solutions and defines the energy spectrum (66). As a consequence trigonometric and hyperbolic quasiexactly solvable systems (see potentials 5 and 8 in Ref. 61) are generated in the form

$$\frac{d^2X}{d\nu^2} + \left[\left(\frac{\alpha^2}{4} + \alpha(2n+2\pm k_1 \pm k_2)\right)\cosh^2\nu - \frac{\alpha^2}{4}\cosh^4\nu - \frac{k_1^2-\frac{1}{4}}{\sinh^2\nu} + \frac{k_2^2-\frac{1}{4}}{\cosh^2\nu} + \lambda\right]X = 0,$$

$$\frac{d^2Y}{d\mu^2} - \left[\left(\frac{\alpha^2}{4} + \alpha(2n+2\pm k_1 \pm k_2)\right)\cos^2\mu - \frac{\alpha^2}{4}\cos^4\mu + \frac{k_1^2-\frac{1}{4}}{\cos^2\mu} + \frac{k_2^2-\frac{1}{4}}{\sin^2\mu} + \lambda\right]Y = 0,$$

where $\alpha=D^2\omega/2$. Thus we have established that an integral part of the notion of quasiexact solvability is the reduction of superintegrable systems to one-dimensional problems.

Indeed, we can express our observation in the form of the following hypothesis: All quantum-mechanical problems which are expressible as one-dimensional quasiexactly solvable systems can be determined via separation of variables in an N-dimensional Schrödinger equation for superintegrable systems.

This analogy prompts us to use the term quasiexact solvability for the equations of type (30) or (76), defined in the complex plane and which are not exactly solvable but which admit polynomial solutions. Thus we suggest calling quantum mechanical systems first-order quasiexactly solvable if the polynomial solution of the one-parametric differential equation of the kind of Schrödinger equation or N-dimensional equation after separation of variables is defined through recurrence relations which must always contain three terms or more and the discrete eigenvalues can be calculated as the solutions of algebraic equations. According to this definition systems (30) and (76) are first order quasiexactly solvable.

In three dimensions we have provided even more striking examples of 1D QES problems obtained as restrictions from superintegrable systems. We exhibited a quasiexactly solvable superintegrable system which is not at the same time exactly solvable in any separable set of coordinates. In one set of separable coordinates we obtain Ushveridze's tenth-order polynomial QES problem and in another set a fourth-order polynomial QES problem. We have shown how the eigenvalues of the symmetry operators which describe separation can be calculated from a determinant condition. These examples, and more to come on other manifolds and in higher dimensional spaces, indicate that our modified definition of QES systems can be extended to N-dimensional spaces and fine tuned to distinguish between the number of parameters in the systems. These matters will be taken up in other papers in this series.

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APPENDIX: ASYMPTOTIC BEHAVIOR OF COEFFICIENTS

To understand the behavior of the solutions of relations (36) for large s we use continued fractions theory.[81] Setting

$$\frac{A_s}{A_{s-1}} = \xi_s f(s),$$
$$f(s) = \sqrt{\frac{\omega}{2}} \frac{\Gamma\left(\frac{s}{2}+\frac{1}{2}\right)\Gamma\left(\pm\frac{k_2}{2}+\frac{s}{2}+\frac{1}{2}\right)\Gamma\left(\frac{\alpha}{2\omega}\pm\frac{k_2}{2}+\frac{s}{2}+1\right)}{\Gamma\left(\frac{s}{2}+1\right)\Gamma\left(\pm\frac{k_2}{2}+\frac{s}{2}+1\right)\Gamma\left(\frac{\alpha}{2\omega}\pm\frac{k_2}{2}+\frac{s}{2}+\frac{1}{2}\right)}, \tag{A1}$$

where $\Gamma(z)$ is the gamma function, we can write the recurrence relation (36) in the standard form

$$\xi_s = \frac{1}{b_s + \xi_{s+1}},$$
$$b_s = \sqrt{\frac{2}{\omega}} \frac{\Gamma\left(\frac{s}{2}+\frac{1}{2}\right)\Gamma\left(\pm\frac{k_2}{2}+\frac{s}{2}+\frac{1}{2}\right)\Gamma\left(\frac{\alpha}{2\omega}\pm\frac{k_2}{2}+\frac{s}{2}+1\right)\left[-\lambda+\frac{k_1}{\omega}(2s+1\pm k_2)\right]}{\Gamma\left(\frac{s}{2}+1\right)\Gamma\left(\pm\frac{k_2}{2}+\frac{s}{2}+1\right)\Gamma\left(\frac{\alpha}{2\omega}\pm\frac{k_2}{2}+\frac{s}{2}+\frac{3}{2}\right)2^3}, \tag{A2}$$

where $\alpha=-(E+k_1/(8\omega^2))/2$. Note that

$$f(s+1)f(s) = \omega \frac{\left(\frac{\alpha}{\omega}\pm k_2+s+1\right)}{(s+1)(\pm k_2+s+1)}.$$

Stirling's formula for the gamma function $\Gamma(z)=z^{z-1/2}e^{-z}\sqrt{2\pi}(1+O(1/z))$ as $|z|\to\infty$ with $|\arg z|<\pi$, gives $f(s)=-\sqrt{\omega}/s(1+O(1/s))$ and $b_s=\pm(k_2/2\omega\sqrt{s\omega})(1+O(1/s))$. In the following we take $k_1\leqslant 0$, k_2,λ,E real and $\omega>0$. Without loss of generality we can assume b_s is positive for sufficiently large s since, otherwise, we could make the replacements $b_s\to -b_s$, $\xi_s\to-\xi_s$.

Since $\Sigma b_s=\infty$, it is a consequence of the Seidel-Stern theorem that the formal continued fraction expressions for the ξ_s converge,

$$\xi_s = \frac{1}{b_s} + \frac{1}{b_{s+1}} + \cdots + \frac{1}{b_{s+k}} + \cdots .$$

Moreover, standard continued fraction theory tells us that

$$\xi_s = \lim_{n\to\infty} \frac{A_n^{(s)}}{B_n^{(s)}}, \tag{A3}$$

where

$$\begin{pmatrix} A_{-1}^{(s)} \\ B_{-1}^{(s)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} A_0^{(s)} \\ B_0^{(s)} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{A4}$$

and

$$\begin{pmatrix} A_n^{(s)} \\ B_n^{(s)} \end{pmatrix} = b_{n+s}\begin{pmatrix} A_{n-1}^{(s)} \\ B_{n-1}^{(s)} \end{pmatrix} + \begin{pmatrix} A_{n-2}^{(s)} \\ B_{n-2}^{(s)} \end{pmatrix}, \quad n \geqslant 1.$$

Furthermore the relation $A_n^{(s)}B_{n-1}^{(s)}-A_{n-1}^{(s)}B_n^{(s)}=(-1)^{n-1}$ holds for all $n\geqslant 0$, which implies

$$\frac{A_n^{(s)}}{B_n^{(s)}} - \frac{A_{n-1}^{(s)}}{B_{n-1}^{(s)}} = \frac{(-1)^{n-1}}{B_{n-1}^{(s)} B_n^{(s)}}.$$

This result in turn implies that the sequence $A_{2n}^{(s)}/B_{2n}^{(s)}$ is, for large s and n, monotone increasing in n and goes to ξ_s in the limit, whereas $A_{2n+1}^{(s)}/B_{2n+1}^{(s)}$ is monotone decreasing in n and goes to ξ_s in the limit. For example,

$$\frac{A_{2n+2}^{(s)}}{B_{2n+2}^{(s)}} - \frac{A_{2n}^{(s)}}{B_{2n}^{(s)}} = \frac{b_{2n+2+s}}{B_{2n}^{(s)} B_{2n+2}^{(s)}}. \tag{A5}$$

It follows from (A3), (A5) that

$$\xi_s = \frac{A_0^{(s)}}{B_0^{(s)}} + \sum_{n=1}^{\infty} \frac{b_{2n+2+s}}{B_{2n}^{(s)} B_{2n+2}^{(s)}}. \tag{A6}$$

Simple estimates using the recurrence relations (A4) give

$$B_{2n}^{(s)} > 1 + b_{s+1} \sum_{m=1}^{n} b_{2m+s}, \quad B_{2n+1}^{(s)} > \sum_{m=0}^{n} b_{2m+1+s}.$$

Substituting these results into the identities

$$B_{2n}^{(s)} = \sum_{m=1}^{n} b_{2m+s} B_{2m-1}^{(s)}, \quad B_{2n+1}^{(s)} = \sum_{m=0}^{n} b_{2m+s+1} B_{2m}^{(s)}$$

we get refined upper bounds for $B_{2n}^{(s)}, B_{2n+2}^{(s)}$. We can approximate the sum $\Sigma_{m=s}^{n} 1/\sqrt{m}$ by the integral $\int_s^n (1/\sqrt{x})\mathrm{d}x$ and use similar approximations to get an upper bound for the series (A6),

$$|\xi_s| < \kappa_1 \int_0^{\infty} \frac{\mathrm{d}y}{\sqrt{y+s}(y^2+1)} + \kappa_2$$

for positive constants κ_j independent of s. This shows that $|\xi_s|$ is uniformly bounded in s. Since $\xi_{s+1} = -b_s + 1/\xi_s$ and $b_s \to 0$ as $s \to \infty$ it is also true that $|1/\xi_s|$ is uniformly bounded in s.

It follows from (A2) that

$$\xi_{s+1} - \xi_{s-1} = \frac{\xi_{s-1} - (b_s + \xi_{s-1})(1 - b_{s-1}\xi_{s-1})}{1 - b_{s-1}\xi_{s-1}}.$$

Now choose s_0 so large that $b_{s+1} < b_s$ and $b_s \xi_s < 1$ for all $s \geqslant s_0$. Note from this identity that if $\xi_{s_1-1} > 1$ for some $s_1 > s_0$ then $\xi_{s_1+1} > \xi_{s_1-1} > 1$. Thus the sequence ξ_{s_1+2k-1} is monotonically increasing for all $k \geqslant 0$. Since $|\xi_s|$ is bounded, it follows that in this case $\lim_{k\to\infty} \xi_{s_1+2k-1} = \xi_+$ exists, and $\xi_+ > 1$. Since $\xi_{s+1} = -b_s + 1/\xi_s$, $b_s \to 0$ as $s \to \infty$ and $|1/\xi_s|$ is uniformly bounded in s, then the sequence ξ_{s_1+2k} is also convergent, $\lim_{k\to\infty} \xi_{s_1+2k} = \xi_-$ where $0 < \xi_- < 1$.

The other possibility is that $\xi \leqslant 1$ for all $s \geqslant s_0$. Since $1/\xi_s - \xi_{s+1} = b_s \to 0$ as $s \to \infty$, and $1/\xi_s \geqslant 1$, $\xi_{s+1} \leqslant 1$ for all $s \geqslant s_0$ it follows that $\lim_{k\to\infty} \xi_k = \xi_+ = \xi_- = 1$. Thus in all cases the sequences ξ_{2k} and ξ_{2k+1} converge.

We conclude that

$$\frac{A_{s+1}}{A_s} = f(s+1)\xi_s = \sqrt{\frac{\omega \xi_\pm}{s}}(1 + O(1/s)), \quad \xi_+ \xi_- = 1,$$

depending on whether s is even or odd.

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Intrinsic spectral geometry of the Kerr-Newman event horizon

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We uniquely and explicitly reconstruct the instantaneous intrinsic metric of the Kerr-Newman event horizon from the spectrum of its Laplacian. In the process we find that the angular momentum parameter, radius, area; and in the uncharged case, mass, can be written in terms of these eigenvalues. In the uncharged case this immediately leads to the unique and explicit determination of the Kerr metric in terms of the spectrum of the event horizon. Robinson's "no hair" theorem now yields the corollary: One can "hear the shape" of noncharged stationary axially symmetric black hole space-times by listening to the vibrational frequencies of its event horizon only. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Although in general the spectrum of the Laplacian on a manifold determines, via the heat kernel, a sequence of invariants which restrict the geometry, it is a rare occasion indeed that the metric is uniquely determined by the eigenvalues (see, for example, Ref. 6). In fact one of the few uniqueness results of this kind was proved by Brüning and Heintze:[1] An S^1 invariant two-dimensional surface diffeomorphic to the sphere, which has, in addition, a mirror symmetry about its equator is uniquely determined by its spectrum. This has been generalized by Zelditch,[16] but the Brüning and Heintze result is the appropriate setting for our purposes since this is exactly the class of metrics which include Kerr-Newman event horizons.

In 1973 Smarr[11] studied the metric of the horizon in terms of a scale parameter and a distortion parameter and in a particularly convenient coordinate system for calculating, for example, the curvature. More recently, the first author of the present paper has used a similar coordinate system to study the spectrum of S^1 invariant surfaces. As it turns out, Smarr's form of the horizon metric is a scaled version of a special case of our form of the metric.

S^1 invariant metrics on S^2 can be described in terms of a single function $f(x)$. One can show that the sum of the reciprocals of the nonzero, S^1 invariant eigenvalues (i.e., the trace of the S^1 invariant Greens operator) is given by an integral involving the function $f(x)$. The key to the results we obtain here is that, in the case of the Kerr-Newman event horizon, the function $f(x)$ is a simple rational function and the above-mentioned integral can be calculated explicitly. Together with a similar equivariant trace formula, one can now write Smarr's parameters in terms of these traces and hence explictly display the metric in terms of it's spectrum. As far as we know, this is the only nontrivial example of this phenomonen (the Brüning and Heintze result is not constructive in this sense).

An interesting byproduct of our results (in the uncharged case), together with Robinson's uniqueness theorem, is the unique reconstruction of space-time in terms of these eigenvalues. We conclude the paper with a discussion of possible physical interpretations of these results.

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II. SMARR'S FORM OF THE METRIC

The *Kerr-Newman metric* describing the geometry of a rotating charged black hole written in Kerr ingoing coordinates (v,r,θ,ϕ) is

$$ds^2 = -\left(1-\frac{2mr-e^2}{\Sigma}\right)dv^2 + 2\,dr\,dv - \frac{(2mr-e^2)2a\sin^2\theta}{\Sigma}dv\,d\phi - 2a\sin^2\theta\,dr\,d\phi + \Sigma\,d\theta^2 + \left(\frac{(r^2+a^2)^2-\delta a^2\sin^2\theta}{\Sigma}\right)\sin^2\theta\,d\phi^2, \tag{1}$$

in which (m,a,e) represent, respectively, the total mass, angular momentum per unit mass, and the charge. Also $\Sigma=r^2+a^2\cos^2\theta$ and $\delta=r^2-2mr+a^2+e^2$ (we use the lower case letter here, instead of the traditional upper case, to avoid confusion with the equally traditional use of Δ for the Laplacian). The uncharged $(e=0)$ case is the *Kerr metric*.

This family of metrics is quite general. To quote Wald[15] "… the Kerr-Newman family of solutions completely describes all the stationary black holes which can possibly occur in general relativity." This fact is due to the famous uniquess theorems of Israel,[7] Carter and Robinson,[10] and Mazur,[8] for example.

For the Kerr-Newman metric the surface of the event horizon can be thought of as a spacelike slice through the null hypersurface defined by the largest root, r_+, of $\delta=0$, i.e., $r_+=m+\sqrt{m^2-a^2-e^2}$. The intrinsic instantaneous metric on the event horizon is obtained by setting $r=r_+$, so that $dr=0$, and also setting $dv=0$ to get

$$ds^2_{eh} = (r_+^2+a^2\cos^2\theta)d\theta^2 + \left(\frac{(r_+^2+a^2)^2}{r_+^2+a^2\cos^2\theta}\right)\sin^2\theta\,d\phi^2. \tag{2}$$

In Ref. 11, Smarr defines *the scale parameter* by $\eta=\sqrt{r_+^2+a^2}$ and *the distortion parameter* by $\beta=a/\sqrt{r_+^2+a^2}$ and introducing a new variable $x=\cos\theta$ one finds that the event horizon metric is

$$ds^2_{eh} = \eta^2\left(\frac{1}{f(x)}dx^2 + f(x)d\phi^2\right), \tag{3}$$

where $(x,\phi)\in(-1,1)\times[0,2\pi)$ and

$$f(x) = \frac{1-x^2}{1-\beta^2(1-x^2)}. \tag{4}$$

It is well known that the Gauss curvature of a metric in this form is simply $K(x)=-1/(2\eta^2)f''(x)$ so that in this case

$$K(x) = \frac{1}{\eta^2}\left(\frac{1-\beta^2(1+3x^2)}{(1-\beta^2(1-x^2))^3}\right), \tag{5}$$

and the surface area of the metric is $A=4\pi\eta^2$. We point out that in case $a=0$ $(\beta=0)$, $e=0$ (1) gives the Schwarzschild black hole and (3) is the metric of the constant Gauss curvature$=1/\eta^2$ metric on S^2.

III. SPECTRUM OF S^1 INVARIANT METRICS

For any Riemannian manifold with metric g_{ij} *the Laplacian* is given by

$$\Delta_g = -\frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\left(\sqrt{g}g^{ij}\frac{\partial}{\partial x^j}\right).$$

This is the Riemannian version of the *Klein-Gordon*, or *D'Alembertian*, or *wave* operator usually denoted by $\Box$.

In this section we outline some previous work on the spectrum of the Laplacian on S^1 invariant metrics on S^2. The interested reader may consult Refs. 2–4 for further details.

To simplify the discussion the area of the metric is normalized to $A=4\pi$ for this section only. The metrics we study have the form

$$\mathrm{d}l^2 = \frac{1}{f(x)}\mathrm{d}x^2 + f(x)\mathrm{d}\phi^2, \tag{6}$$

where $(x,\phi)\in(-1,1)\times[0,2\pi)$ and $f(x)$ satisfies $f(-1)=0=f(1)$ and $f'(-1)=2=-f'(1)$. In this form, it is easy to see that the Gauss curvature of this metric is given by $K(x)=(-1/2)f''(x)$. The canonical (i.e., constant curvature) metric is obtained by taking $f(x)=1-x^2$ and the metric (3) is a homothety (scaling) of a particular example of the general form (6).

The Laplacian for the metric (6) is

$$\Delta_{\mathrm{d}l^2} = -\frac{\partial}{\partial x}\left(f(x)\frac{\partial}{\partial x}\right) - \frac{1}{f(x)}\frac{\partial^2}{\partial\phi^2}.$$

Let λ be any eigenvalue of $-\Delta$. We will use the symbols E_λ and $\dim E_\lambda$ to denote the eigenspace for λ and it's multiplicity (degeneracy), respectively. In this paper the symbol λ_m will always mean the mth *distinct* eigenvalue. We adopt the convention $\lambda_0=0$. Since S^1 (parametrized here by $0\leqslant\phi<2\pi$) acts on (M,g) by isometries we can separate variables and because $\dim E_{\lambda_m}\leqslant 2m+1$ (see Ref. 4 for the proof), the orthogonal decomposition of E_{λ_m} has the special form

$$E_{\lambda_m} = \bigoplus_{k=-m}^{k=m} e^{ik\theta}W_k$$

in which $W_k(=W_{-k})$ is the "eigenspace" (it might contain only 0) of the ordinary differential operator

$$L_k = -\frac{\mathrm{d}}{\mathrm{d}x}\left(f(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \frac{k^2}{f(x)}$$

with suitable boundary conditions. It should be observed that $\dim W_k\leqslant 1$, a value of zero for this dimension occurring when λ_m is not in the spectrum of L_k.

The set of positive eigenvalues is given by $\mathrm{Spec}(\mathrm{d}l^2)=\cup_{k\in Z}\mathrm{Spec}\,L_k$ and consequently the nonzero part of the spectrum of $-\Delta$ can be studied via the spectra $\mathrm{Spec}\,L_k=\{0<\lambda_k^1<\lambda_k^2<\cdots<\lambda_k^j<\cdots\}\,\forall\,k\in\mathbb{Z}$. The eigenvalues λ_0^j in the case $k=0$ above are called the S^1 *invariant eigenvalues* since their eigenfunctions are invariant under the action of the S^1 isometry group. If $k\neq 0$ the eigenvalues are called k *equivariant* or simply *of type* $k\neq 0$. Each L_k has a Green's operator, $\Gamma_k:(H^0(M))^\perp\to L^2(M)$, whose spectrum is $\{1/\lambda_k^j\}_{j=1}^\infty$, and whose trace is defined by

$$\gamma_k \equiv \sum_{j=1}^{\infty}\frac{1}{\lambda_k^j}. \tag{7}$$

The formulas of present interest were derived in Refs. 2 and 3 and are given by

$$\gamma_0 = \frac{1}{2}\int_{-1}^{1}\frac{1-x^2}{f(x)}\mathrm{d}x \tag{8}$$

and

$$\gamma_k = \frac{1}{|k|} \quad \text{if } k\neq 0. \tag{9}$$

Remark: One must be careful with the definition of γ_0 since $\lambda_0^0=0$ is an S^1 invariant eigen-

value of $-\Delta$. To avoid this difficulty we studied the S^1 invariant spectrum of the Laplacian on 1-forms in Ref. 3 and then observed that the nonzero eigenvalues are the same for functions and 1-forms.

IV. SPECTRAL DETERMINATION OF THE EVENT HORIZON

In case $f(x)$ is given by (4) the metric (3) is related to (6) via the homothety $ds^2_{eh}=\eta^2\, dl^2$, and it is well known that

$$\lambda \in \mathrm{Spec}(dl^2) \quad \text{if and only if } \frac{\lambda}{\eta^2} \in \mathrm{Spec}(\eta^2\, dl^2)$$

so that, after an elementary integration, the trace formulas for the event horizon are

$$\gamma_0 = \eta^2\left(1-\frac{2\beta^2}{3}\right) \tag{10}$$

and

$$\gamma_k = \frac{\eta^2}{|k|} \quad \forall\, k \neq 0. \tag{11}$$

For the $k=1$ case, for example, one can invert the resulting pair of equations to get

$$\beta^2 = \frac{3}{2}\left(1-\frac{\gamma_0}{\gamma_1}\right) \tag{12}$$

and

$$\eta^2 = \gamma_1, \tag{13}$$

and thereby write the event horizon metric explicitly and uniquely in terms of the spectrum as follows.

Proposition: With γ_0 *and* γ_1 *defined as in* (7) *the instantaneous intrinsic metric of the Kerr-Newman event horizon is given by*

$$ds^2_{eh} = \gamma_1\left(\frac{1-\frac{3}{2}\left(1-\frac{\gamma_0}{\gamma_1}\right)(1-x^2)}{1-x^2}dx^2 + \frac{1-x^2}{1-\frac{3}{2}\left(1-\frac{\gamma_0}{\gamma_1}\right)(1-x^2)}d\phi^2\right). \tag{14}$$

An immediate consequence of (11) is that the area of the metric has a representation for each $k \in \mathbb{N}$ given by

$$A = 4\pi k \gamma_k. \tag{15}$$

Remarks: (i) One might view Eqs. (10) and (11) as nothing more than definitions of new parameters in terms of the old. On the other hand, the quantities γ_k are fundamental and naturally defined quantities coming from the discrete set of vibrational wave frequencies on the surface. Alternatively, one can think of each trace, γ_k as the sum of the squares of all wavelengths of given quantum number k.

(ii) One can use γ_0 together with γ_k for any k to reconstruct the metric. In some sense one can "construct the metric in $\aleph_0$ ways."

(iii) Brüning and Heintze proved that for S^1 invariant metrics symmetric about the equator the S^1 invariant spectrum determines the metric. Their result requires the prescription of all of the eigenvalues of the $k=0$ spectrum to uniquely determine the surface of revolution. In the example of the present paper the metric is, therefore, uniquely determined once we have knowledge of the

entire list of S^1 invariant eigenvalues. For the explicit construction one exchanges complete knowledge of the $k=0$ spectrum for partial spectral data, namely the traces of the Greens operators for $k=0$ and any $k\neq 0$.

All the physical parameters can also be written in terms of the spectra as follows:

$$a^2 = \tfrac{3}{2}(\gamma_1 - \gamma_0), \tag{16}$$

$$r_+^2 = \frac{3\gamma_0 - \gamma_1}{2}, \tag{17}$$

$$m^2 = \frac{(\gamma_1 + e^2)^2}{6\gamma_0 - 2\gamma_1}, \tag{18}$$

as well as the angular velocity and surface gravity. We observe, however, that the mass depends on the charge e as well as the spectrum so that the mass is uniquely determined by the spectrum only in the Kerr ($e=0$) case.

We set together Remark (iii) with (16) and (18) (with $e=0$), (1), and Robinson's uniqueness theorem[10] to observe.

Theorem: *A noncharged stationary axially symmetric asymptotically flat vacuum space-time with a regular event-horizon is uniquely determined by the S^1 invariant spectrum of the intrinsically defined Laplacian on its event horizon. The space-time is explicitly constructed from the S^1 invariant trace together with any $k\neq 0$ trace of the associated Green's operator on the event horizon.*

V. DISCUSSION

It is well known (see Refs. 5, 13, and 9, among many others) that the quasinormal mode frequencies for scalar, electromagnetic, and gravitational radiation of black holes are related to the separation constants arising from separating variables in the Teukolsky master equation. These "characteristic sounds" of the black hole are considered to be observable in an astrophysical sense. The angular operator (and, respectively, its separation constants) coming from the separation of variables is closely related to the Laplacian (and, respectively, its eigenvalues) on the event horizon in the sense that, for scalar fields, they both reduce to the Laplacian (and corresponding eigenvalues) on the constant curvature S^2 for the Schwarzschild ($a=0$) case. There is also some evidence (this is a work in progress) that the $a>0$ Teukolsky angular equation can be viewed, after a change of variables, as a Laplace eigenvalue equation for a fourth order Taylor polynomial approximation of the horizon metric function. We hope to pursue these matters in our future work.

On a more philosophical note, the reader may have noticed that the main result of this paper is consistent with the holographic principle (Refs. 12 and 14) in as much as the structure of the (3+1 dimensional) Kerr-Newman space-time is encoded in the intrinsic spectral data of the (two-dimensional) event horizon surface.

These phenomena suggest that the spectrum of the Laplacian on event horizons is playing an important, if rather subtle and not well understood, role in the physics of the space-time manifold.

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Flow equations for uplifting half-flat to Spin(7) manifolds

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In this supplement to the paper by Franzen *et al.* [Fortschr. Phys. (to be published)], we discuss the uplift of half-flat sixfolds to Spin(7) eightfolds by fibration of the former over a product of two intervals. We show that the same can be done in two ways—one, such that the required Spin(7) eightfold is a double G_2 sevenfold fibration over an interval, the G_2 sevenfold itself being the half-flat sixfold fibered over the other interval, and second, by simply considering the fibration of the half-flat sixfold over a product of two intervals. The flow equations one gets are an obvious generalization of the Hitchin's flow equations [to obtain sevenfolds of G_2 holonomy from half-flat sixfolds [Hitchin (2001)]]. We explicitly show the uplift of the Iwasawa using both methods, thereby proposing the form of new Spin(7) metrics. We give a plausibility argument ruling out the uplift of the Iwasawa manifold to a Spin(7) eightfold at the "edge," using the second method. For Spin(7) eightfolds of the type $X_7 \times S^1$, X_7 being a sevenfold of SU(3) structure, we motivate the possibility of including elliptic functions into the "shape deformation" functions of sevenfolds of SU(3) structure of Franzen *et al.* via some connections between elliptic functions, the Heisenberg group, theta functions, the already known $D7$-brane metric [Greene *et al.*, Nucl. Phys. B 337, 1 (1990)], and hyper-Kähler metrics obtained in twistor spaces by deformations of Atiyah-Hitchin manifolds by a Legendre transform [Chalmers, Phys. Rev. D 58, 125011 (1998)]. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178156]

INTRODUCTION

It is known that manifolds with G_2 and Spin(7) holonomies, are very useful in getting minimal amount of supersymmetry after compactification of seven and eight dimensions, respectively, in string/M-theory.[1] In the past few years, half-flat manifolds have been shown to be relevant to flux compactifications in string theory (see Refs. 2 and 3 and references therein). In Ref. 4, using the results of Ref. 5, we explicitly showed how to uplift the Iwasawa manifold, an example of a half-flat manifold, to sevenfolds of either G_2-holonomy or SU(3) structure. In this short note, we show how to uplift half-flat manifolds to Spin(7) eightfolds. We will be following the notations of Ref. 4. We also give plausibility arguments in favor of inclusion of the Weierstrass elliptic function in Spin(7)-metrics of the type $X_7 \times S^1$, X_7 being sevenfolds of SU(3) structure.

Spin(7) folds are characterized by a self-dual closed (and hence co-closed) Cayley four-form (with the additional constraint that the $\hat{A}$-genus of the eightfold equals unity[6]). We will begin with the construction of a Spin(7) eightfold as a double G_2-fibration over an interval. We then go on to constructing a Spin(7) eightfold as a fibration of a half-flat over the product of two intervals.

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SPIN(7) AS A DOUBLE G_2-FIBRATION OVER AN INTERVAL

Let us begin with the following construction of a Spin(7) eightfold $X_8^{\mathrm{Spin}(7)}$ (see diagram 1 below):

$$
\begin{array}{ccccc}
I_{t_1} & & & & \\
\uparrow & & & & \\
| & X_7^{G_2}(t_2) & \longrightarrow & I_{t_2} & \\
| & & & M_6 & \\
| & & & & \\
X_8^{\mathrm{Spin}(7)} & \longrightarrow & I_{t_2} & & \\
 & & X_7^{G_2}(t_1) & & \\
 & & | & & \\
 & & \downarrow M_6 & & \\
 & & I_{t_1} & &
\end{array}
$$

In other words, one has a "double" G_2-fibration structure in the sense that the Spin(7) eightfold is a fibration of a $G_2(t_1)$-manifold over an interval $I(t_2)$ *as well as* a $G_2(t_2)$-manifold over an interval $I(t_1)$, where the $G_2(t_i)$-manifold is itself a fibration of a half-flat sixfold over an interval $I(t_i)$ (via the Hitchin's construction[7]). Given a half-flat manifold $M_6(\Omega, J)$, the Hitchin's construction involves (with respect to seven dimensions) a closed and co-closed three-form $\phi_3 = J \wedge \mathrm{d}t + \Omega_+(t)$, $\Omega_+ \equiv \mathrm{Re}(\Omega)$, one can write down the following Cayley four-form ϕ_4:

$$\phi_4 = \alpha_1 * {}_7\phi_3^1 + \alpha_2 * {}_7\phi_3^2 + \tilde{\alpha}_1 \phi^1 \wedge \mathrm{d}t_2 + \tilde{\alpha}_2 \phi_3^2 \wedge \mathrm{d}t_1$$

$$+ \beta_1 \Omega_+ \wedge \mathrm{d}t_1 + \beta_2 \Omega_+ \wedge \mathrm{d}t_2 + \gamma_1 \Omega_- \wedge \mathrm{d}t_1 + \gamma_2 \Omega_- \wedge \mathrm{d}t_2 + \delta J \wedge J + \epsilon J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2. \tag{1}$$

The self-duality condition would thus imply

$$\alpha_1 (J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2 + \Omega_+ \wedge \mathrm{d}t_2) + \alpha_2 (J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2 - \Omega_+ \wedge \mathrm{d}t_1)$$

$$+ \tilde{\alpha}_1 \left(\frac{1}{2} J \wedge J + \Omega_- \wedge \mathrm{d}t_1 \right) + \tilde{\alpha}_2 \left(- \frac{1}{2} J \wedge J - \Omega_- \wedge \mathrm{d}t_2 \right)$$

$$- \beta_1 \Omega_- \wedge \mathrm{d}t_2 + \beta_2 \Omega_- \wedge \mathrm{d}t_1 + \gamma_1 \Omega_+ \wedge \mathrm{d}t_2 - \gamma_2 \Omega_+ \wedge \mathrm{d}t_1$$

$$+ 2\delta J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2 + \frac{\epsilon}{2} J \wedge J$$

$$= \alpha_1 \left(\frac{1}{2} J \wedge J + \Omega_- \wedge \mathrm{d}t_1 \right) + \alpha_2 \left(\frac{1}{2} J \wedge J + \Omega_- \wedge \mathrm{d}t_2 \right)$$

$$+ \tilde{\alpha}_1 (J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2 + \Omega_+ \wedge \mathrm{d}t_2) + \tilde{\alpha}_2 (- J \wedge \mathrm{d}t_1 \wedge \mathrm{d}t_2 + \Omega_+ \wedge \mathrm{d}t_1)$$

$$+\beta_1\Omega_+\wedge \mathrm{d}t_1+\beta_2\Omega_+\wedge \mathrm{d}t_2+\gamma_1\Omega_-\wedge \mathrm{d}t_1+\gamma_2\Omega_-\wedge \mathrm{d}t_2$$

$$\delta J\wedge J+\epsilon J\wedge \mathrm{d}t_1\wedge \mathrm{d}t_2, \tag{2}$$

implying

$$\alpha_1+\alpha_2+2\delta=\tilde{\alpha}_1-\tilde{\alpha}_2+\epsilon,$$

$$\alpha_1+\gamma_1=\tilde{\alpha}_1+\beta_2,\quad -\alpha_2-\gamma_2=\tilde{\alpha}_2+\beta_1. \tag{3}$$

Hence, the following is the form of the self-dual four-form:

$$\begin{aligned}\phi_4=\alpha_1 *_7\phi_3^1+\alpha_2 *_7\phi_3^2+\tilde{\alpha}_1\phi^1\wedge \mathrm{d}t_2+\tilde{\alpha}_2\phi_3^2\wedge \mathrm{d}t_1+\beta_1\Omega_+\wedge \mathrm{d}t_1+\beta_2\Omega_+\wedge \mathrm{d}t_2+(\tilde{\alpha}_1+\beta_2\\ -\alpha_1)\Omega_-\wedge \mathrm{d}t_1-(\alpha 2+\tilde{\alpha}_2+\beta_1)\Omega_-\wedge \mathrm{d}t_2+\delta J\wedge J+(\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1)J\wedge \mathrm{d}t_1\wedge \mathrm{d}t_2.\end{aligned} \tag{4}$$

For (4) to be a Cayley four-form, it must satisfy the condition that it is closed, which on using

$$d *_7\phi_3^1=\left(\hat{d}+\mathrm{d}t_1\wedge\frac{\partial}{\partial t_1}+\mathrm{d}t_2\wedge\frac{\partial}{\partial t_2}\right)*_7\phi_3^1=\mathrm{d}t_2\wedge\frac{\partial *_7\phi_3^1}{\partial t_2},$$

$$d *_7\phi_3^2=\left(\hat{d}+\mathrm{d}t_1\wedge\frac{\partial}{\partial t_1}+\mathrm{d}t_2\wedge\frac{\partial}{\partial t_2}\right)*_7\phi_3^2=\mathrm{d}t_1\wedge\frac{\partial *_7\phi_3^2}{\partial t_2},$$

$$\mathrm{d}\phi_3^1=\mathrm{d}t_2\wedge\frac{\partial\phi_3^1}{\partial t_2},\quad \mathrm{d}\phi_3^2=\mathrm{d}t_2\wedge\frac{\partial\phi_3^2}{\partial t_1}, \tag{5}$$

implies

$$\begin{aligned}\mathrm{d}\phi_4\Big|_{\hat{\mathrm{d}}J\wedge J=\hat{\mathrm{d}}\Omega_+=0}=\alpha_1\left(\mathrm{d}t_2\wedge\frac{\partial J}{\partial t_2}\wedge J+\mathrm{d}t_2\wedge\frac{\partial\Omega_-}{\partial t_2}\wedge \mathrm{d}t_1\right)+\alpha_2\left(\mathrm{d}t_1\wedge\frac{\partial J}{\partial t_1}\wedge J+\mathrm{d}t_1\wedge\frac{\partial\Omega_-}{\partial t_1}\wedge \mathrm{d}t_1\right)\\ +\beta_1\left(\mathrm{d}t_2\wedge\frac{\partial\Omega_+}{\partial t_2}\wedge \mathrm{d}t_1\right)+\beta_2\left(\mathrm{d}t_1\wedge\frac{\partial\Omega_+}{\partial t_1}\wedge \mathrm{d}t_2\right)+(\tilde{\alpha}_1+\beta_2-\alpha_1)\left(\hat{\mathrm{d}}\Omega_1\wedge \mathrm{d}t_1\right.\\ \left.+\mathrm{d}t_2\wedge\frac{\partial\Omega_-}{\partial t_2}\wedge \mathrm{d}t_1\right)-(\alpha_2+\tilde{\alpha}_2+\beta_1)\left(\hat{\mathrm{d}}\Omega_1\wedge \mathrm{d}t_2+\mathrm{d}t_1\wedge\frac{\partial\Omega_-}{\partial t_1}\wedge \mathrm{d}t_2\right)\\ +2\delta\left(\mathrm{d}t_1\wedge\frac{\partial J}{\partial t_1}\wedge J+\mathrm{d}t_2\wedge\frac{\partial J}{\partial t_2}\wedge J\right)+(\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1)\hat{\mathrm{d}}J\wedge \mathrm{d}t_1\wedge \mathrm{d}t_2=0.\end{aligned} \tag{6}$$

One thus gets the following flow equations:

$$(\alpha_1+2\delta)\frac{\partial J}{\partial t_2}\wedge J=(\alpha_2+\tilde{\alpha}_2+\beta_1)\hat{\mathrm{d}}\Omega_-,$$

$$(2\delta+\alpha_2)\frac{\partial J}{\partial t_1}\wedge J=(\alpha_1-\beta_2+\tilde{\alpha}_1)\hat{\mathrm{d}}\Omega_-,$$

$$(\tilde{\alpha}_1+\tilde{\beta}_2)\frac{\partial\Omega_-}{\partial t_2}+(\tilde{\alpha}_2+\beta_1)\frac{\partial\Omega_-}{\partial t_1}+\beta_1\frac{\partial\Omega_+}{\partial t_2}-\beta_2\frac{\partial\Omega_+}{\partial t_1}+(\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1)\hat{\mathrm{d}}J=0. \tag{7}$$

Let us use the flow equations of (7) to explicitly uplift the Iwasawa manifold to a Spin(7) eightfold, working with the standard complex structure limit of the Iwasawa, and consider its deformation of the type

$$J(t_1,t_2)=e^{a(t_1,t_2)}e^{12}+e^{b(t_1,t_2)}e^{34}+e^{c(t_1,t_2)}e^{56} \tag{8}$$

and

$$\Omega(t_1,t_2)=e^{(a+b+c)(t_1,t_2)/2}(e^1+ie^2)\wedge(e^3+ie^4)\wedge(e^5+ie^6). \tag{9}$$

Then the flow equations (7) imply

$$\frac{\partial a}{\partial t_1}=\frac{\partial b}{\partial t_1}=-\frac{\partial c}{\partial t_1},\quad 2\frac{\partial a}{\partial t_1}e^{a+b}=4\xi_1 e^{(a+b+c)/2}, \tag{10}$$

where $\xi_1\equiv(\alpha_1-\beta_2+\tilde{\alpha}_1)/(2\delta+\alpha_2)$, which could be satisfied by equality of $a,b,-c$, and

$$a(t_1,t_2)=\frac{2}{3}\ln(3\xi_1 e^{\lambda_1}t_1+f_2(t_2)), \tag{11}$$

λ_1 being a linear combination of the integration constants that would appear in the integration of the first set of equations in (10); similarly,

$$a(t_1,t_2)=\tfrac{2}{3}\ln(3\xi_2 e^{\lambda_1}t_2+f_1(t_1)), \tag{12}$$

where $\xi_2\equiv(\alpha_2+\tilde{\alpha}_2+\beta_1)/(\alpha_1+2\delta)$,

$$\frac{(\tilde{\alpha}_1+\beta_2)}{2}\frac{\partial a}{\partial t_2}+\frac{(\tilde{\alpha}_2+\beta_1)}{2}\frac{\partial a}{\partial t_1}=0,$$

$$\Leftrightarrow(\tilde{\alpha}_1+\beta)\xi_2+(\tilde{\alpha}_2+\beta_1)\xi_1=0,$$

$$e^{(a+b+c)/2}\left(\frac{\beta_1}{2}\frac{\partial a}{\partial t_2}-\frac{\beta_2}{2}\frac{\partial a}{\partial t_1}\right)=(\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1)e^c, \tag{13}$$

$$\Leftrightarrow(\beta_1\xi_2-\beta_2\xi_1)e^{-(3a/2)+\lambda_1}=(\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1)e^{-a+\lambda_3},$$

$$\Rightarrow\beta_1\xi_2-\beta_2\xi_1=\alpha_1+\alpha_2+2\delta+\tilde{\alpha}_2-\tilde{\alpha}_1.$$

Hence, the metric corresponding to the Spin(7) eightfold obtained by uplifting the Iwasawa manifold via the flow equations of (7) such that the eightfold is a double G_2-fibration over an interval, is given by the following solutions to (10)–(13):

$$ds_8^2 = ds_{I\times I}^2(t_1,t_2) + (1+\xi_1 t_1 + \xi_2 t_2)^{\frac{2}{3}}(|dz|^2 + |dv|^2) + \frac{1}{d(1+\xi_2 t_1 + \xi_2 t_2)^{\frac{2}{3}}}|du - z dv|^2, \quad (14)$$

with the constraints

$$\beta_1\xi_2 - \beta_2\xi_1 = \alpha_1 + \alpha_2 + 2\delta + \tilde{\alpha}_2 - \tilde{\alpha}_1,$$

$$\frac{\xi_1}{\xi_2} = -\frac{\tilde{\alpha}_1 + \beta_2}{\tilde{\alpha}_2 + \beta_1}, \quad \text{or } \tilde{\alpha}_1 = -\beta_2,\ \tilde{\alpha}_2 = -\beta_1. \quad (15)$$

Notice that (14) has the required double G_2-fibration structure of diagram 1 by noting that (14) is made up of

$$ds_7^2(t_1, \text{given } t_2) = dt_1^2 + (\xi_1' + \xi_1 t_1)^{\frac{2}{3}}(|dz|^2 + |dv|^2) + \frac{1}{(\xi_1' + \xi_1 t_1)^{\frac{2}{3}}}|du - z\, dv|^2 \quad (16)$$

and

$$ds_7^2(t_2, \text{given } t_1) = dt_2^2 + (\xi_2' + \xi_2 t_2)^{\frac{2}{3}}(|dz|^2 + |dv|^2) + \frac{1}{(\xi_2' + \xi_2 t_2)^{\frac{2}{3}}}|du - z\, dv|^2, \quad (17)$$

which are the two-parameter G_2-metrics of Ref. 4. (In Ref. 4, however, one had set $\xi_i' = 1$.) The metric of (14) also thus has G_2-holonomy. (The authors thank J. Maldacena for pointing this out.)

SPIN(7) AS A FIBRATION OF A HALF-FLAT OVER $I\times I$

Let us now consider the following fibration structure:

$$\begin{array}{ccc} X_8^{\text{Spin(7)}} & \longrightarrow & I_{t_1} \times I_{t_2} \\ & & M_6 \end{array} \quad (18)$$

Let us assume that the Cayley four-form is given by

$$\phi_4 = a_1\Omega_- \wedge dt_1 + a_2\Omega_- \wedge dt_2 + b_1\Omega_+ \wedge dt_1 + b_2\Omega_+ \wedge dt_2 + cJ \wedge J + fJ \wedge dt_1 \wedge dt_2. \quad (19)$$

One then gets

$$*_8\phi_4 = a_1\Omega_+ \wedge dt_2 - a_2\Omega_+ \wedge dt_1 - b_1\Omega_- \wedge dt_2 + b_2\Omega_- \wedge dt_1 + 2cJ \wedge dt_1 \wedge dt_2 + \frac{f}{2}J \wedge J, \quad (20)$$

implying that for $\phi_4 = *_8\phi_4$,

$$a_1 = b_1, \quad a_2 = -b_1, \quad c = \frac{d}{2}. \quad (21)$$

The required Cayley four-form is

$$\phi_4 = a_1\Omega_- \wedge dt_1 + a_2\Omega_- \wedge dt_2 - a_2\Omega_+ \wedge dt_1 + a_1\Omega_+ \wedge dt_2 + \frac{f}{2}J \wedge J + fJ \wedge dt_1 \wedge dt_2. \quad (22)$$

Finally, the condition that ϕ_4 of (22) is closed gives

$$
\begin{aligned}
\mathrm{d}\phi_4 = a_1\left(\hat{\mathrm{d}}\Omega_- \wedge \mathrm{d}t_1 + \mathrm{d}t_2 \wedge \frac{\partial \Omega_-}{\partial t_2} \wedge \mathrm{d}t_1\right) + a_2\left(\hat{\mathrm{d}}\Omega_- \wedge \mathrm{d}t_2 + \mathrm{d}t_1 \wedge \frac{\partial \Omega_-}{\partial t_1} \wedge \mathrm{d}t_2\right) \\
+ a_1\left(\hat{\mathrm{d}}\Omega_+ \wedge \mathrm{d}t_2 + \mathrm{d}t_1 \wedge \frac{\partial \Omega_+}{\partial t_1} \wedge \mathrm{d}t_2\right) - a_2\left(\hat{\mathrm{d}}\Omega_+ \wedge \mathrm{d}t_1 + \mathrm{d}t_2 \wedge \frac{\partial \Omega_-}{\partial t_2} \wedge \mathrm{d}t_1\right) \\
+ f\left(\hat{\mathrm{d}}J \wedge J + \mathrm{d}t_1 \wedge \frac{\partial J}{\partial t_1} \wedge J + \mathrm{d}t_2 \wedge \frac{\partial J}{\partial t_2} \wedge J\right) = 0. \qquad (23)
\end{aligned}
$$

Using that for half-flat manifolds, $\hat{\mathrm{d}}J \wedge J = \hat{\mathrm{d}}\Omega_+ = 0$, one thus gets the following flow equations:

$$
a_1\,\hat{\mathrm{d}}\Omega_- = -f\frac{\partial J}{\partial t_1} \wedge J,
$$

$$
a_2\,\hat{\mathrm{d}}\Omega_- = -f\frac{\partial J}{\partial t_2} \wedge J,
$$

$$
-a_1\frac{\partial \Omega_+}{\partial t_2} + a_2\frac{\partial \Omega_-}{\partial t_1} + a_2\frac{\partial \Omega_+}{\partial t_2} + a_1\frac{\partial \Omega_+}{\partial t_2} = f\,\hat{\mathrm{d}}J. \qquad (24)
$$

One can again show that one can explicitly uplift the Iwasawa manifold to a Spin(7) eightfold at standard complex structure limit of the Iwasawa and consider its deformation of the type as given in (8) and (9). The set of equations that one gets from (24), are

$$
\frac{\partial a}{\partial t_i} = \frac{\partial b}{\partial t_i} = -\frac{\partial c}{\partial t_i},
$$

$$
\frac{\partial a}{\partial t_1} = -\frac{2a_1}{f}e^{-(3a/2)+\lambda_1}, \quad \frac{\partial a}{\partial t_2} = -\frac{2a_2}{f}e^{-(3a/2)+\lambda_1}, \qquad (25)
$$

$$
\left(\frac{a_1}{2}\frac{\partial a}{\partial t_2} - a_2\frac{\partial a}{\partial t_1}\right)e^{(a+b+c)/2} = 0, \quad \left(-\frac{a_2}{2}\frac{\partial a}{\partial t_2} - \frac{a_1}{2}\frac{\partial a}{\partial t_1}\right)e^{(a+b+c)/2} = fe^c,
$$

which are satisfied by

$$
a(t_1,t_2) = \frac{2}{3}\ln\left(1 + 3\frac{a_1e^{\lambda_1}}{f}t_1 + 3\frac{a_2e^{\lambda_2}}{f}t_2\right),
$$

$$
\text{with } a_1^2 + a_2^2 = f^2. \qquad (26)
$$

Thus, the metric for the Spin(7) eightfold is

$$
\begin{aligned}
\mathrm{d}s_8^2 = \mathrm{d}s_{I\times I}^2(t_1,t_2) + \left(1 + \frac{a_1}{\sqrt{a_1^2+a_2^2}}t_1 + \frac{a_2}{\sqrt{a_1^2+a_2^2}}t_2\right)^{\frac{2}{3}}(|\mathrm{d}z|^2 + |\mathrm{d}v|^2) \\
+ \left(1 + \frac{a_1}{\sqrt{a_1^2+a_2^2}}t_1 + \frac{a_2}{\sqrt{a_1^2+a_2^2}}t_2\right)^{-\frac{2}{3}}|\mathrm{d}u - z\,\mathrm{d}v|^2. \qquad (27)
\end{aligned}
$$

Again, the metric also has G_2-holonomy.

However, it is unlikely to be able to uplift the Iwasawa to a Spin(7) eightfold at the "edge." One notes that at the edge (see Ref. 2 and references therein), the one-forms, incorporating $t_{1,2}$-dependent deformations, are $\alpha = -e^{\mathcal{A}(t_1,t_2)}f^1$, $\beta = e^{\mathcal{B}(t_1,t_2)}(f^3 + if^4)$, $\gamma = e^{\mathcal{C}(t_1,t_2)}(e^5 + ie^6)$, and J

$=(i/2)$ $(\alpha\wedge\overline{\alpha}+\beta\wedge\overline{\beta}+\gamma\wedge\overline{\gamma}$and $\Omega=\alpha\wedge\beta\wedge\gamma)$. The one-forms $f^i, i=1,\ldots,4$ are defined via $f^i=P^i_j e^j$, where $P\in \mathrm{SO}(4)$ matrix, and one writes it as$\left(\begin{smallmatrix} X & 0 \\ 0 & Y \end{smallmatrix}\right)$, where $X,Y\in \mathrm{SU}(2)$, i.e.,

$$\begin{pmatrix} P^1_1 & P^1_2 & 0 & 0 \\ P^2_1 & P^2_2 & 0 & 0 \\ 0 & 0 & P^3_3 & P^3_4 \\ 0 & 0 & P^4_3 & P^4_4 \end{pmatrix},$$

where $P^1_1P^2_2-P^1_2P^2_1=P^3_3P^4_4-P^3_4P^4_3=1$. The flow equations $\hat{\mathrm{d}}\Omega_-=-\partial J/\partial t_1\wedge J=-\partial J/\partial t_2\wedge J$ implies $\mathcal{A}$ gives the same result after differentiation with respect to t_1 or t_2. Unlike the standard complex structure limit, there are common components to Ω_+ and Ω_- in the edge. One can show that the other flow equation

$$a_1\frac{\partial\Omega_-}{\partial t_2}-a_2\frac{\partial\Omega_-}{\partial t_1}-a_2\frac{\partial\Omega_+}{\partial t_2}-a_1\frac{\partial\Omega_+}{\partial t_1}+f\hat{\mathrm{d}}J=0$$

becomes

$$\begin{aligned} e^{\mathcal{A}+\mathcal{B}+\mathcal{C}}\Big[&\big(\mathcal{D}_-(P^1_1P^3_3+P^2_1P^4_3)-\mathcal{D}_+(P^2_1P^3_3-P^1_1P^4_3)\big)e^{136}+\big(\mathcal{D}_-(P^1_1P^3_4+P^2_1P^4_4)-\mathcal{D}_+(P^2_1P^3_4-P^1_1P^4_4)\big)e^{146}\\ &+\big(\mathcal{D}_-(P^1_2P^3_3+P^2_2P^4_3)-\mathcal{D}_+(P^2_2P^3_3-P^1_2P^4_3)\big)e^{236}\\ &+\big(\mathcal{D}_-(P^1_2P^3_4+P^2_2P^4_4)-\mathcal{D}_+(P^2_2P^3_4-P^1_2P^4_4)\big)e^{246}\\ &+\big(\mathcal{D}_-(-P^1_1P^4_3+P^2_1P^3_3)-\mathcal{D}_+(-P^1_1P^3_3-P^2_1P^4_3)\big)e^{135}\\ &+\big(\mathcal{D}_-(-P^1_1P^4_4+P^2_1P^3_4)-\mathcal{D}_+(-P^1_1P^3_4-P^2_1P^4_4)\big)e^{145}\\ &+\big(\mathcal{D}_-(-P^1_2P^4_3+P62_2P^3_3)-\mathcal{D}_+(-P^1_2P^3_3-P^2_2P^4_3)\big)e^{235}\\ &+\big(\mathcal{D}_-(-P^1_2P^4_4+P^2_2P^3_4)-\mathcal{D}_+(-P^1_2P^3_4-P^2_2P^4_4)\big)e^{246}\\ &=-e^{2\mathcal{C}}(e^{135}+e^{425}-e^{614}-e^{623}), \end{aligned} \tag{28}$$

(where $\mathcal{D}_+\equiv[a_2(\partial/\partial t_2)+a_1(\partial/\partial t_1)]\,\mathcal{ABC}$ and $\mathcal{D}_-\equiv[a_1(\partial/\partial t_2)-a_2(\partial/\partial t_1)]\mathcal{ABC}$), which implies that one will overconstrain the matrix P [from the first set of flow equations, one sees that $\mathcal{D}_-=0$, and hence one gets from (28), eight equations in the six parameters P^i_j]. Hence, the uplift of the edge to a Spin(7) is quite likely to be impossible.

POSSIBILITY OF INTRODUCING WEIERSTRASS ELLIPTIC FUNCTIONS IN SPIN(7) EIGHTFOLDS INCLUDING AN S^1

We now give some very compelling evidence in support of the possibility of inclusion of Weierstrass elliptic functions in those Spin(7) eightfolds which are of the type $X_7\times S^1$, X_7 being a sevenfold of SU(3) structure.

Seven-dimensional manifolds of G_2-holonomy or SU(3) structure are required for getting $\mathcal{N}=1$ supersymmetry in four dimensions from the 11-dimensional M-theory. Similarly, Spin(7) eightfolds are required for getting $\mathcal{N}=1$ supersymmetry in three dimensions from (the 11 dimensional) M-theory. One could explore the option of getting compact Spin(7) uplifts using S^1's instead of intervals by using the same flow equations as derived in this paper, but further demanding periodicity with respect to t_1 and t_2, of the solutions.

Assuming the existence of Spin(7) eightfolds of the type $X_7 \times S^1$, one could first argue the existence of a G_2-structure by noting the existence of a singlet in the decomposition under $G_2 \subset \mathrm{Spin}(7)$ of the **8** in the fundamental spinorial representation ($\mathbf{8} \to \mathbf{7}+\mathbf{1}$). Further, assuming that Majorana-Weyl spinors ($\xi = \xi^+ \oplus \xi^-$, the $\pm$ signs referring to the chiralities) on the Spin(7) eightfold are nowhere vanishing, there is a further reduction of the structure group to $G_{2+} \cap G_{2-} = \mathrm{SU}(3)$, the two G_2's corresponding to the two chiralities of $\xi^{\pm}$.

Having established the connection between (the use of) Spin(7) eightfolds and sevenfolds with SU(3)-structure, let us now move to the main theme of this section—the possibility of inclusion of Weierstrass elliptic functions in sevenfolds with SU(3) structure and thereby Spin(7) eightfolds of the type $X_7 \times S^1$.

Using the results of Ref. 5, explicit metrics for sevenfolds with SU(3) structure were obtained. The "shape" deformation functions "$A(z, \overline{z}; v, \overline{v})$" and "$B(z, \overline{z}; v, \overline{v})$," as indicated in Ref. 4, could also be related to elliptic functions—the seven-dimensional SU(3) structure does not impose too many constraints if one allows wrapped $M5$-branes in the analysis. The following are some interesting connections between some concepts, thereby motivating further the idea of having singular uplifts to seven dimensions of the Iwasawa manifold, involving elliptic functions.

(i) The $D7$-brane metric (relevant to "cosmic strings" in Ref. 8) is given by

$$\mathrm{d}s_{10}^2 = \mathrm{d}s_8^2 + \tau_2(z)\,|\eta(\tau(z))|^4 |z|^{-N/6} |\mathrm{d}z|^2, \tag{29}$$

where $\tau_2 \equiv \mathrm{Im}\,\tau$, $\tau = a + ie^{-\phi}$, $a \equiv$ axion and $\phi \equiv$ dilaton, $\eta \equiv$ Dedekind eta function (see below), $N \equiv$ the number of $D7$-branes, and z is the complex coordinate transverse to the $D7$-brane. Hence, one has one explicit example of a metric involving η, which is related to theta functions, as indicated below.

(ii) The Jacobi theta function[9] defined for two complex variables z and τ where $\mathrm{Im}\,\tau > 0$, $\vartheta(z:\tau) = \Sigma_{-\infty}^{\infty} e^{i\pi n^2 \tau + 2\pi i n z}$. The theta function is related to the Dedekind eta function via $\vartheta(0;\tau) = \eta^2[(\tau+1)/2]/\eta(\tau+1)$.

(iii) The Weierstrass elliptic function[9] is a doubly periodic function with periods $2\omega_1$ and $2\omega_2$ such that $\omega_1 \omega_2$ is not real,

$$\mathcal{P}(z;\omega_1,\omega_2) = \frac{1}{z^2} + \sum_{m,n \in \mathbf{Z}\setminus(0,0)} \left(\frac{1}{(z - 2m\omega_1 - 2n\omega_2)^2} - \frac{1}{(2m\omega_1 + 2n\omega_2)^2} \right).$$

$\mathcal{P}$ satisfies the following cubic equation:

$$\left(\frac{\mathrm{d}\mathcal{P}(z;\tau)}{\mathrm{d}z} \right)^2 = \mathcal{P}^3(z;\tau) - g_2 \mathcal{P} - g_3,$$

where $g_2 = 60\Sigma_{m,n \in \mathbf{Z}\setminus(0,0)}[1/(2m\omega_1 + 2n\omega_2)^4]$, $g_3 = 140\Sigma_{m,n \in \mathbf{Z}\setminus(0,0)}[1/(2m\omega_1 + 2n\omega_2)^6]$. This is an equation of a torus, which could be related to the Riemann surface that is referred to in Ref. 5. The torus degenerates, i.e., becomes singular along the discriminant locus given by $\Delta = g_2^3 - 27 g_3^2 = 0$. There is the following relation between the discriminant locus and the Dedekind eta function: $\Delta = (2\pi)^{12} \eta^{24}$. The following relations are true: $\mathcal{P}(z;\omega_1 = 1, \omega_2 = \tau) = -(d^2/\mathrm{d}z^2)\vartheta_{11}(z;\tau) + \text{constant} = \pi^2 \vartheta^2(0;\tau)\vartheta_{10}^2(0;\tau)[\vartheta_{10}^2(z;\tau)/\vartheta_{11}^2(z;\tau)] + e_2(\tau)$, where e_2 is one of the three roots $e_{i=1,2,3}$, of the cubic equation $4t^3 - g_2 t - g_3 = 0$, and $\mathcal{P}(\omega_1) = e_1$, $\mathcal{P}(\omega_2) = e_2$, $\mathcal{P}(-\omega_1 - \omega_2) = e_3$. [The e_i's are given by $e_1(\tau) = (\pi^2/3)(\vartheta^4(0;\tau) + \vartheta_{01}^4(0;\tau))$, $e_2(\tau) = -(\pi^2/3) \times (\vartheta^4(0;\tau) + \vartheta^4(0;\tau))$ $e_3(\tau) = (\pi^2/3)(\vartheta_{10}^4(0;\tau) - \vartheta^4(0;\tau))$, where the three other theta functions are defined as $\vartheta_{01}(z;\tau) = \vartheta\left(z + \frac{1}{2};\tau\right)$ $\vartheta_{10}(z;\tau) = e^{i(\pi/4) + i\pi z}\vartheta(z + (\tau/2);\tau)$ $\vartheta_{11}(z;\tau) = e^{i(\pi/4) + i\pi\left(z + \frac{1}{2}\right)}\vartheta(z + [(\tau+1)/2];\tau)$.]

(iv) Consider a holomorphic function $f(z)$ and $a, b \in \mathbf{R}$. Define two operators S_a and T_b as follows: $(S_a f)(z) = f(z+a)$, $(T_b f)(z) = e^{i\pi b^2 \tau + 2i\pi b z} f(z + b\tau)$. Then S, T and a phase factor form the generators of the nilpotent Heisenberg group central to the group-theoretic way of understanding the Iwasawa manifold. If $U(\lambda \in \mathbf{C}, a, b) \in H \equiv$ Heisenberg group, then

$$U(\lambda,a,b)f(z)=\lambda(S_a\circ T_b f)(z)=\lambda e^{i\pi b^2\tau+2i\pi bz}f(z+b\tau+a),$$

and U is referred to as the theta representation of the Heisenberg group.[10]

(v) (Inverse) Elliptic functions, as shown in Ref. 11, naturally figure in the hyper-Kähler metrics in twistor spaces obtained by deformations of Atiyah-Hitchin spaces and Legendre transform. Lets elaborate upon this a little.

Deformations of Atiyah-Hitchin manifolds (written as hypersurface in $\mathbf{C}^3$: $x^2+y^2z=1$) of the type $x^2z+(yz+a)^2=z^2+a^2$ have been considered. The twistor threefolds are obtained as holomorphic sections $\Gamma(\mathcal{O}_{\mathbf{CP}^1}(4))$ with the following similar equation: $x^2(\zeta)\eta(\zeta)+(y(\zeta)\eta(\zeta)+p(\zeta))^2=\eta(\zeta)+p^2(\zeta)$, where η is $\Gamma(\mathcal{O}_{\mathbf{CP}^1}(4))$ and the deformation p is $\Gamma(\mathcal{O}_{\mathbf{CP}^1}(2))$, and ζ is a $\mathbf{CP}^1$-valued coordinate. The reality involution: $\overline{\eta^{(2m)}}(\zeta)=(-)^m(\overline{\zeta})^{(2m)}(-1/\overline{\zeta})$,where $\eta^{(2m)}(\zeta)$ is $\Gamma(\mathcal{O}_{\mathbf{CP}^1}(2m))$, implies that $\eta(\zeta)$ has five independent parameters, i.e., $\eta(\zeta)=z+v\zeta+w\zeta^2-\overline{v}\overline{\zeta}^3+\overline{z}\overline{\zeta}^4$ $(z,v\in\mathbf{C}$ and $w\in\mathbf{R})$ and the deformation $p(\zeta)=a+b\zeta-\overline{a}\overline{\zeta}^2, a\in\mathbf{C}, b\in\mathbf{R}$. An $\mathrm{SL}(2,\mathbf{C})$ transformation: $\zeta\rightarrow(a\zeta+b)/(-b\zeta+\overline{a})$, $|a|^2+|b|^2=1$ can be used to restrict $p(\zeta)=\tilde{b}\zeta$. For genericvalues of the five real parameters in $\eta(\zeta)$, one gets eight points on an elliptic curve, $\gamma^2=\eta(z\zeta)$, corresponding to the roots of $\eta(\zeta)+p^2(\zeta)=0$—the divisor for four of these eight should correspond to $\Gamma(L^m)$, where L^m are holomorphic line bundles over $T\mathbf{CP}^1$ with $e^{-m\xi/\zeta}$ (ξ being a fiber coordinate) the transition functions. The splitting of the eight roots into two groups of four each is determined by the following condition: $(\int_\alpha^\infty+\int_\beta^\infty-\int_{-1/\overline{\alpha}}^\infty-\int_{-1/\overline{\beta}}^\infty)[\mathrm{d}\zeta/\sqrt{\eta(\zeta)}]=2$; the roots of $\eta(\zeta)+p^2(\zeta)=0$ are $\alpha,\beta,-1/\overline{\alpha},-1/\overline{\beta}$.Now, if x_1,x_2 are roots of $\eta(\zeta)+\tilde{b}\zeta=0$ *after* the $\mathrm{SL}(2,\mathbf{C})$ transformation,

$$\begin{pmatrix}\eta(\zeta)\\ p(\zeta)\end{pmatrix}\overset{\zeta\rightarrow\frac{a\zeta+b}{-b\zeta+a}}{\rightarrow}\begin{pmatrix}\dfrac{r_1\zeta^3-r_2\zeta^2-r_1\zeta}{(-\overline{b}\zeta+\overline{a})^4}\\ \dfrac{\tilde{b}(a\zeta+b)}{(-\overline{b}\zeta+\overline{a})}\end{pmatrix},$$

$r_1,r_2\in\mathbf{R}$, then the aforementioned constraint can be rewritten in terms of inverse elliptic functions,

$$\mathcal{P}^{-1}\left(x_1-\frac{r_2}{3r_1}\right)+\mathcal{P}^{-1}\left(x_2-\frac{r_2}{3r_1}\right)-\mathcal{P}^{-1}\left(-\frac{1}{\overline{x_1}}-\frac{r_2}{3r_1}\right)-\mathcal{P}^{-1}\left(-\frac{1}{\overline{x_2}}-\frac{r_2}{3r_1}\right)=\frac{m\sqrt{r_1}}{2},$$

where the inverse elliptic function $\mathcal{P}^{-1}(z)\equiv\int_\infty^z(\mathrm{d}\zeta/\sqrt{4\zeta^3-g_2\zeta-g_3})$. The constraint is also equivalent to $\partial F/\partial w=0$ for a suitable constraint function F defined in terms of appropriate contour integrals. The Kähler potential is then given in terms of the Legendre transform of $F:K(z,\overline{z};\partial F/\partial v,\partial\overline{F}/\partial\overline{v})=F(z,\overline{z};v,\overline{v};w)-v(\partial F/\partial v)-\overline{v}(\partial\overline{F}/\partial\overline{v})$ evaluated at the constraint, $\partial F/\partial w=0$.

Thus, one sees the existence of (inverse) elliptic functions in the hyper-Kähler metrics in twistor spaces obtained using deformations of Atiyah-Hitchin spaces and Legendre transforms.

To summarize, we have obtained the relevant flow equations for uplifting half-flat manifolds to Spin(7) eightfolds by two methods—first, by considering a double G_2 (constructed from the half-flat) fibration over an interval, and the second, by considering a fibration of the half-flat over the product of two intervals. We were able to explicitly uplift the Iwasawa at the standard complex structure limit in the moduli space of almost complex structures on the Iwasawa. We gave a plausibility argument against the same for the second method, at the "edge." We also gave motivating reasons for considering singular uplifts involving doubly periodic functions—the physical interpretation of the same is not yet clear.

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A note on the Zassenhaus product formula

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We provide a simple method for the calculation of the terms c_n in the Zassenhaus product $e^{a+b}=e^a\cdot e^b\cdot\Pi_{n=2}^{\infty}e^{c_n}$ for noncommuting a and b. This method has been implemented in a computer program. Furthermore, we formulate a conjecture on how to translate these results into nested commutators. This conjecture was checked up to order $n=17$ using a computer. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178586]

I. INTRODUCTION

The product of the exponentials of two noncommuting variables x and y may be expressed in terms of the Baker-Campbell-Hausdorff (BCH) series

$$e^x e^y = e^{x+y+\Sigma_{n=2}^{\infty} z_n}. \tag{1}$$

The terms z_n of the sum may be written as linear combinations of words W of length n consisting of letters x and y,

$$z_n = \sum_{W(s_1,\ldots,s_n)} z(W) W(s_1,\ldots,s_n), \tag{2}$$

where each word $W(s_1,\ldots,s_n)$ is a product of n factors $s_i=x$ or $s_i=y$. The sum in Eq. (2) is over all possible different words, i.e., the sum over W has in principle 2^n terms. Some of these terms vanish, because the corresponding coefficient $z(W)$ equals zero. The coefficients $z(W)$ may be determined in various ways. A simple method to determine these coefficients has been suggested recently by Reinsch.[1] His method is easily implemented in a computer program.[1,2] Another method was presented by Goldberg,[3] and his method was implemented in a program by Newman and Thompson.[4]

The terms z_n of the BCH series may be expressed as linear combinations of nested commutators of x and y. This was originally shown by Baker, Campbell, and Hausdorff.[5] However, explicit determination of the coefficients was difficult for general n. Dynkin[6,7] showed that the coefficients are in fact easily obtained, so that the z_n can be represented as

$$z_n = \frac{1}{n} \sum_{W(s_1,\ldots,s_n)} z(W)[[\cdots[[s_1,s_2],s_3],\ldots],s_n], \tag{3}$$

where $[[\cdots[[s_1,s_2],s_3],\ldots],s_n]$ is a direct translation of the word W into a left normal nested commutator, i.e., the order of the letters in the commutator and the word are the same. The representation of the z_n in terms of commutators is not unique due to the Jacobi identity

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$[[x,y],z]+[[y,z],x]+[[z,x],y]=0$ and similar identities for higher order commutators. Some of them are discussed by Oteo.[8] Oteo also formulates a conjecture concerning another translation of the BCH terms into a linear combination of commutators. This translation consists of fewer terms than Dynkin's translation, but a general proof of its validity is not known to us. We have checked the validity of Oteo's conjecture up to order $n=17$ on a computer.

It was first shown by Zassenhaus[9] that there exists a formula analogous to the BCH formula for the exponential of the sum of two noncommuting variables a and b,

$$\mathrm{e}^{a+b} = \mathrm{e}^{a} \cdot \mathrm{e}^{b} \cdot \prod_{n=2}^{\infty} \mathrm{e}^{c_n}, \tag{4}$$

which is known as the Zassenhaus product formula. The individual terms c_n will be called the Zassenhaus exponents in the following. They may also be written in terms of words of length n consisting of the letters a and b, i.e.,

$$c_n = \sum_{W(t_1,\ldots,t_n)} c(W) W(t_1, \ldots, t_n) \tag{5}$$

with $t_i=a$ or $t_i=b$. It is the goal of this paper to provide a simple method for the calculation of the coefficients $c(W)$ as well as to propose a suitable computer implementation. Our method has been developed in analogy to the procedure proposed by Reinsch[1] for the BCH terms.

The Zassenhaus exponents may also be obtained in terms of nested commutators as shown, e.g., in Refs. 9 and 10. Dynkin's theorem[6] provides a (generally valid) translation of words into nested commutators, if such a translation exists. Therefore, it is possible to directly translate the expressions for the Zassenhaus exponents (5) into a linear combination of left normal nested commutators as in Eq. (3). In analogy to the conjecture by Oteo[8] for the BCH terms, we formulate here a conjecture concerning another translation of words into left normal nested commutators for the Zassenhaus exponents involving fewer terms than Dynkin's translation. Using a computer, we found this conjecture to be valid for the Zassenhaus exponents up to order $n=17$, but at this time we cannot provide a general proof.

II. THE ZASSENHAUS EXPONENTS

In this section we state a corollary which allows a recursive determination of the Zassenhaus exponents.

Let $\tau_1, \ldots, \tau_n$ be commuting variables. In terms of these variables we define three upper triangular $(n+1)\times(n+1)$ matrices H, K, and L with matrix elements given by

$$H_{ij} = \frac{1}{(j-i)!} \cdot \prod_{k=i}^{j-1} (1+\tau_k), \quad K_{ij} = \frac{(-1)^{i+j}}{(j-i)!}, \tag{6}$$

$$L_{ij} = \frac{(-1)^{i+j}}{(j-i)!} \cdot \prod_{k=i}^{j-1} \tau_k, \tag{7}$$

for $1 \leqslant i \leqslant j \leqslant n+1$ and zero otherwise. These matrices may be expressed as exponentials of the $(n+1)\times(n+1)$ matrices P and Q defined by

$$P_{ij} = \delta_{i+1,j}, \quad Q_{ij} = \delta_{i+1,j}\tau_i, \tag{8}$$

where δ_{ij} is the Kronecker symbol,

$$H = \exp(P+Q), \quad K = \exp(-P), \quad L = \exp(-Q). \tag{9}$$

Furthermore, we define an operator U which operates on products p of the variables τ_i,

$$p = \tau_1^{\mu_1}\tau_2^{\mu_2}\tau_3^{\mu_3}\cdots\tau_n^{\mu_n}$$

with $\mu_i \in \{0,1\}$ for $i=1,\ldots,n$. The operator U "translates" such a product p into a word consisting of letters a and b according to the following rule: If $\mu_i=0$, $\tau_i^{\mu_i}$ is replaced by an a, and if $\mu_i=1$, $\tau_i^{\mu_i}$ is replaced by a b. The index i determines the position of the letter in the word. For example, for $n=6$ the product $p=\tau_1^1\tau_2^0\tau_3^1\tau_4^1\tau_5^0\tau_6^0=\tau_1\tau_3\tau_4$ is translated as follows:

$$U(p) = U(\tau_1^1\tau_2^0\tau_3^1\tau_4^1\tau_5^0\tau_6^0) = U(\tau_1\tau_3 u_4) = babbaa.$$

The operator U is a vector-space isomorphism mapping the space of polynomials in the τ variables (with $\mu_i=0$ or $\mu_i=1$) into the space of words of length n.

Corollary 1: The Zassenhaus exponent c_2 defined in Eq. (4) is obtained in terms of the 3×3 *matrices L, K, H as $c_2=U(L\cdot K\cdot H)_{1,3}$. For $n>2$, the Zassenhaus exponents c_n are given in terms of the corresponding $(n+1)\times(n+1)$ matrices as*

$$c_n = U((\mathrm{e}^{-\mathcal{C}_{n-1}}\cdot\ \cdots\ \cdot\mathrm{e}^{-\mathcal{C}_2}\cdot L\cdot K\cdot H)_{1,n+1}). \tag{10}$$

Here, $\mathcal{C}_m$ $(1<m<n)$ are the Zassenhaus exponents written in terms of the $(n+1)\times(n+1)$ matrices P and Q, and the index $1,n+1$ indicates the upper right element of a matrix.

This corollary permits a recursive determination of the Zassenhaus exponents. In fact, due to the special structure of the matrices P and Q all exponentials in Eq. (10) are obtained as finite sums, and the whole calculation can be done in a finite amount of steps either by hand or on a computer. A suitable computer implementation will be presented in Sec. IV.

Examples: Before proving Corollary 1 we work out a number of examples.

For $n=2$ we need to use the 3×3 matrices given by

$$L=\begin{pmatrix} 1 & -\tau_1 & \frac{1}{2}\tau_1\tau_2 \\ 0 & 1 & -\tau_2 \\ 0 & 0 & 1 \end{pmatrix}, \quad K=\begin{pmatrix} 1 & -1 & \frac{1}{2} \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix},$$

$$H=\begin{pmatrix} 1 & (1+\tau_1) & \frac{1}{2}(1+\tau_1)(1+\tau_2) \\ 0 & 1 & (1+\tau_2) \\ 0 & 0 & 1 \end{pmatrix}.$$

Then,

$$L\cdot K\cdot H=\begin{pmatrix} 1 & 0 & \frac{1}{2}\tau_1-\frac{1}{2}\tau_2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

and the second Zassenhaus exponent takes the form

$$c_2 = U(L\cdot K\cdot H)_{1,n+1} = U\left(\tfrac{1}{2}\tau_1-\tfrac{1}{2}\tau_2\right) = \tfrac{1}{2}U(\tau_1^1\tau_2^0-\tau_1^0\tau_2^1) = \tfrac{1}{2}(ba-ab). \tag{11}$$

For $n=3$ we need to use the 4×4 matrices,

$$L=\begin{pmatrix} 1 & -\tau_1 & \frac{1}{2}\tau_1\tau_2 & -\frac{1}{6}\tau_1\tau_2\tau_3 \\ 0 & 1 & -\tau_2 & \frac{1}{2}\tau_2\tau_3 \\ 0 & 0 & 1 & -\tau_3 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$K=\begin{pmatrix} 1 & -1 & \frac{1}{2} & -\frac{1}{6} \\ 0 & 1 & -1 & \frac{1}{2} \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$H=\begin{pmatrix} 1 & (1+\tau_1) & \frac{1}{2}(1+\tau_1)(1+\tau_2) & \frac{1}{6}\sum_{i=1}^{3}(1+\tau_i) \\ 0 & 1 & (1+\tau_2) & \frac{1}{2}\sum_{i=2}^{3}(1+\tau_i) \\ 0 & 0 & 1 & (1+\tau_3) \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

and the matrices P and Q defined in Eq. (8),

$$P=\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and } Q=\begin{pmatrix} 0 & \tau_1 & 0 & 0 \\ 0 & 0 & \tau_2 & 0 \\ 0 & 0 & 0 & \tau_3 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

It follows from Eq. (11) that

$$e^{-C_2}=\exp\left(-\frac{1}{2}(Q\cdot P-P\cdot Q)\right)=\begin{pmatrix} 1 & 0 & \frac{1}{2}(\tau_2-\tau_1) & 0 \\ 0 & 1 & 0 & \frac{1}{2}(\tau_3-\tau_2) \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Therefore, the third Zassenhaus exponent takes the form

$$\begin{aligned} c_3 &= U(e^{-C_2}\cdot L\cdot K\cdot H)_{1,n+1} \\ &= U\left(\tfrac{2}{3}\tau_1\tau_3-\tfrac{1}{3}\tau_2-\tfrac{1}{3}\tau_2\tau_3-\tfrac{1}{3}\tau_1\tau_2+\tfrac{1}{6}\tau_1+\tfrac{1}{6}\tau_3\right) \\ &= \tfrac{2}{3}bab-\tfrac{1}{3}aba-\tfrac{1}{3}abb-\tfrac{1}{3}bba+\tfrac{1}{6}baa+\tfrac{1}{6}aab. \end{aligned}$$

In an analogous way one obtains for c_4,

$$\begin{aligned} c_4 = &-\tfrac{1}{24}aaab+\tfrac{1}{8}aaba+\tfrac{1}{8}aabb-\tfrac{1}{8}abaa-\tfrac{1}{4}abab-\tfrac{1}{8}abbb+\tfrac{1}{24}baaa+\tfrac{1}{4}baba+\tfrac{3}{8}babb-\tfrac{1}{8}bbaa \\ &-\tfrac{3}{8}bbab+\tfrac{1}{8}bbba. \end{aligned}$$

These results all agree with the standard results given in the literature, see, e.g., Ref. 11.

III. PROOF OF COROLLARY 1

The $(n+1)\times(n+1)$ matrices P and Q have nonzero elements only in their first superdiagonal. A product of m factors P or Q is a $(n+1)\times(n+1)$ matrix which contains nonzero elements only in the mth superdiagonal. In particular, a product of n factors P or Q has only one nonzero element in its upper right corner. A product of k factors P or Q with $k>n$ is a null matrix.

Each Zassenhaus exponent c_n is a linear combination of words of length n. As a consequence, $\mathcal{C}_n$ is a $(n+1)\times(n+1)$ matrix, which has a nonzero entry only in its upper right-hand corner, and for each $n\in\mathbb{N}$,

$$e^{P+Q} = e^{P} \cdot e^{Q} \cdot \prod_{i=1}^{n} e^{\mathcal{C}_i} \tag{12}$$

is obtained in terms of a finite product with n factors. Therefore, one obtains

$$e^{\mathcal{C}_n} = e^{-\mathcal{C}_{n-1}} \cdot \cdots \cdot e^{-\mathcal{C}_2} \cdot e^{-Q} \cdot e^{-P} \cdot e^{P+Q}. \tag{13}$$

The exponentials can be calculated from a finite sum.

Since $\mathcal{C}_n$ only has one nonzero element in its upper right-hand corner, it holds that $\mathbf{e}^{\mathcal{C}_n} = I + \mathcal{C}_n$, and we find

$$(\mathcal{C}_n)_{1,n+1} = \left(\sum c(A_1 \cdots A_n) A_1 \cdots A_n\right)_{1,n+1} = (e^{\mathcal{C}_n})_{1,n+1} = (e^{-\mathcal{C}_{n-1}} \cdot \cdots \cdot e^{-\mathcal{C}_2} \cdot e^{-Q} \cdot e^{-P} \cdot e^{P+Q})_{1,n+1}, \tag{14}$$

where $A_i = P$ or $A_i = Q$, and the sum runs over all different matrix products $A_1 \cdots A_n$. The next step is to show that the upper-right element of a product matrix $A_1 \cdots A_n$ is given by a product of τ_i, and that the indices on the τ_i variables determine the positions of the Q's in the matrix product $A_1 \cdots A_n$. This has been shown in Ref. 1 and is not repeated here. Applying the operator U on this product of τ_i then transforms the result Eq. (14) into a linear combination of words in terms of the letters a and b. This proves Corollary 1.

IV. COMPUTER IMPLEMENTATION

The following *Mathematica* program implements Corollary 1. Calling it will return the Zassenhaus exponent c_n in terms of the variables a and b.

The program consists of three parts: First the matrices L, K, H, P, and Q are defined. Then the product of exponentials as required by Corollary 1 is calculated (starting from $n=2$), and finally the translation U is implemented. The program works with strings in order to prevent *Mathematica* from sorting the words alphabetically.

```
ZH[n_,a_,b_]:=Module[{C,L,K,H,P,Q,m,t,r,i,j,k,u,z},
C[2]=(t[1]^2 t[2])/2-(t[1] t[2]^2)/2;
For [m=2, m<=n, m++,
L=Table[(-1)^(i+j)/(j-i)! Product[t[k],{k,i,j-1}], {i,m+1},
  {j,m+1}];
K=Table[(-1)^(i+j)/(j-i)!, {i,m+1}, {j,m+1}];
H=Table[1/(j-i)! Product[(1+t[k]), {k,i,j-1}], {i,m+1}, {j,m+1}];
P=Table[KroneckerDelta [i+1,j], {i,m+1}, {j,m+1}];
Q=Table[KroneckerDelta [i+1,j] t[i], {i,m+1}, {j,m+1}];
C[m]=Expand[
     ((Dot @@ Table[MatrixExp[-Sum[
     r=(List @@ C[m-u][[z]]) /. {t[i_]→P, t[i_]^2→Q};
     r[[1]] (Dot @@ Take [r,-Length[r]+1]),
     {z,Length[C[m-u]]}]],
     {u,1,m-2}]) .L.K.H) [[1, m+1]] Product [t[j], {j,m}]]];
Sum[r=(List @@ C[n][[k]])
    /. {t[i_]→ToString[a], t[i_]^2 → ToString[b]};
    r[[1]] (StringJoin @@ Take [r,-n]), {k, Length [C[n]]}]];
```

More elegant but less readable *Mathematica* implementations than the one given above are possible, e.g., using NestList instead of a For loop. Since the Zassenhaus exponents for larger n are rather lengthy expressions, the computer needs a significant amount of memory for this calculation. On a standard personal computer with 2 GB of memory we could obtain the Zassenhaus exponents up to $n=17$ within about one hour of computer time.

V. EXPRESSION IN TERMS OF COMMUTATORS

In the introduction we briefly discussed Dynkin's translation[6,7] of words into commutators, which is applicable, whenever such a translation exists. Since it is known that a representation in terms of commutators exists for the Zassenhaus exponents,[9,10] we may directly use Dynkin's prescription in order to obtain an explicit representation of the Zassenhaus exponents in terms of commutators. We checked the validity of this procedure using a computer up to order $n=17$. A translation for the BCH terms into commutators involving fewer terms than Dynkin's prescription was proposed by Oteo.[8] To our knowledge the validity of this translation has never been proved in general. Oteo showed it to be valid up to order $n=10$, and we checked this conjecture up to order $n=17$ on a computer.

In analogy to Oteo's prescription for the BCH terms, we now write down an expression for the Zassenhaus exponents

$$c_n = \sum_{W(t_1,\ldots,t_n)} c(W) W(t_1,\ldots,t_n) \tag{15}$$

in terms of commutators. The words W consist of letters a and b; $n_a(W)$ counts the number of a's in that word. Analogously, $n_b(W)=n-n_a(W)$ counts the number of b's in the word W. We conjecture that the Zassenhaus exponent c_n may be expressed in terms of the left normal commutator as follows:

$$c_n = \sum_{\substack{W(t_1,\ldots,t_n)\\ t_1=b,t_2=a}} \frac{c(W)}{n_b(W)} [[\cdots[[t_1,t_2],t_3],\ldots],t_n]. \tag{16}$$

Here we only sum over words starting with the letters ba. Similarly, one may write

$$c_n = \sum_{\substack{W(t_1,\ldots,t_n)\\ t_1=a,t_2=b}} \frac{c(W)}{n_a(W)} [[\cdots[[t_1,t_2],t_3],\ldots],t_n] \tag{17}$$

and only sum over words starting with the letters ab.

We checked this conjecture up to order $n=17$ using *Mathematica* and compared results up to order $n=6$ with expressions given in the literature, e.g., in Ref. 11.

Example: For $n=4$ one finds the following representation of the Zassenhaus exponent in terms of words

$$c_4 = -\tfrac{1}{24}aaab + \tfrac{1}{8}aaba + \tfrac{1}{8}aabb - \tfrac{1}{8}abaa - \tfrac{1}{4}abab - \tfrac{1}{8}abbb + \tfrac{1}{24}baaa + \tfrac{1}{4}baba + \tfrac{3}{8}babb - \tfrac{1}{8}bbaa - \tfrac{3}{8}bbab + \tfrac{1}{8}bbba.$$

According to our conjecture this may be translated into nested commutators as

$$\begin{aligned} c_4 &= \tfrac{1}{24}[[[b,a],a],a] + \tfrac{1}{8}[[[b,a],b],a] + \tfrac{1}{8}[[[b,a],b],b] \\ &= -\tfrac{1}{24}[[[a,b],a],a] - \tfrac{1}{8}[[[a,b],a],b] - \tfrac{1}{8}[[[a,b],b],b]. \end{aligned}$$

This result agrees with results given in the literature (e.g., in Ref. 10).

VI. CONCLUSION

We developed a method for the calculation of the Zassenhaus exponents c_n in the Zassenhaus product formula $e^{a+b}=e^a\cdot e^b\cdot\prod_{n=2}^{\infty}e^{c_n}$ for noncommuting a and b. The method is given in Corollary 1, from which we obtain the Zassenhaus exponents in terms of words. It appears that our method is simpler and faster than previous methods (see, e.g., Ref. 10). We provide a suitable computer implementation.

We would like to mention that the method presented here can be easily generalized to the Zassenhaus product formula for q-deformed exponentials. (The Zassenhaus formula for q-deformed exponentials is discussed, e.g., in Ref. 11 and references therein.)

Furthermore, we formulated a conjecture on how to translate the Zassenhaus exponents given in terms of words into a form in terms of left normal nested commutators. This representation involves fewer terms than a translation based on Dynkin's theorem[7] and has been found to be valid for Zassenhaus exponents up to order $n=17$ using a computer. We expect a proof of our conjecture to be possible along the lines of Dynkin's proof for his representation of the BCH formula in terms of commutators. This proof shows essentially by direct calculation that the conjectured commutator representation is equivalent to the representation in terms of words. We will address this issue in a forthcoming paper.

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On the Birman-Schwinger principle applied to $\sqrt{-\Delta+m^2}-m$

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The condition for $E=0$ to be an eigenvalue of the operator $\sqrt{-\Delta+m^2}-m+\lambda V$ is obtained through the use of the Birman-Schwinger principle (Theorem 3.2). By setting $E=-\alpha^2$ and using the analyticity of the corresponding Birman-Schwinger kernel (Theorem 3.1), the series development of λ^{-1} is obtained up to second order on α (Theorem 4.1). © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Birman-Schwinger principle[2,24] has been extensively used in several branches of physics and mathematics. The original motivation for its implementation was the possibility of having eigenvalue counting functions for the Schrödinger equation. In this approach, the potential term is taken to be of the form λV with λ being a constant and V a potential satisfying a certain number of properties (e. g., V is nonpositive). The eigenvalue counting functions thus obtained will depend on λ, and in general, for a given operator $\mathcal{O}$, they can be defined by the following expression:

$$N(\lambda)=\{\text{number of } \mu_j \in \text{Spec}(\mathcal{O}), \mu_j < \lambda\}.$$

Research on this class of functions was actually initiated by Weyl for the Laplace operator Δ,[27,28] with an emphasis in the following years on the asymptotic expression for $N(\lambda)$ when $\lambda \to \infty$.[5,20,26] More recently, the use of microlocal analysis has indeed allowed a more detailed study of asymptotics with some proposals to replace eigenvalue counting functions by spectral shift functions.[10]

Generalizations of the method itself have also been proposed to deal with certain physical situations arising in quantum mechanics[6] and modified versions have been formulated, for example, in phonon physics where perturbations on acoustic and electromagnetic waves can be described through the presence of exponentially localized eigenmodes of their corresponding operators,[8,9] and where an analogy with the appearance of bound states for the Schrödinger equation can also be established.

In Ref. 15 the eigenvalue equation

$$(-\Delta+\lambda V)\psi=E\psi \tag{1}$$

was studied through the use of the Birman-Schwinger principle and some conditions expressing the fact that the solutions to the Schrödinger equation are in $\mathcal{L}^2(\mathbb{R}^3)$ were obtained. A related study was also done for the Dirac operator in Ref. 14. In both cases the potential V were assumed to satisfy a certain set of properties. In this work we shall apply the same techniques to the case of the pseudodifferential operator $\sqrt{-\Delta+m^2}-m$, which was studied by Herbst in the presence of a Coulomb potential.[12] This operator had also been used in other contexts such as hadronic physics.[25,7,18] For a discussion of several aspects of this relativistic operator and its relation to the Dirac operator we refer to Refs. 16, 11, 18, and 17.

In the next section we mention some basic facts regarding the Birman-Schwinger principle. Section III deals with the analyticity of the Birman-Schwinger kernel for $\sqrt{\Delta+m^2}-m$ (Theorem 3.1). In this section we also state a theorem (Theorem 3.2) providing the condition under which $E=0$ is an eigenvalue of $\sqrt{\Delta+m^2}-m+\lambda V$, with V a nonpositive potential with compact support. The series expansion of λ^{-1} up to second order on α is discussed in Sec. IV and the corresponding

expressions for the coefficients are given (Theorem 4.1). Several expressions used in the main text are derived in Appendix A and Appendix B. Appendix C contains a simple estimate on $|(\sqrt{-\Delta+m^2}-E)^{-1}(x)|$.

II. THE BIRMAN-SCHWINGER PRINCIPLE

For convenience we recall the steps leading to the Birman-Schwinger principle and how it can be used in order to extract some information about eigenvalues. One begins from a general eigenvalue equation of the form

$$H\psi=(H_0+\lambda V)\psi=E\psi \tag{2}$$

with H_0 an operator representing the kinetic energy. We shall suppose in the following that the potential $V\in C_0^\infty(\mathbb{R}^3)$ and takes negative values. The above equation then can be recast in the form

$$\psi=\lambda(H_0-E)^{-1}|V|\psi.$$

By multiplying this equation by $|V|^{1/2}$ and defining $\phi:=|V|^{1/2}\psi$ one obtains

$$\lambda K\phi=\phi,\quad K=|V|^{1/2}(H_0-E)^{-1}|V|^{1/2}. \tag{3}$$

The physical meaning behind this rewriting is that the operator K has an eigenvalue λ_0^{-1} if and only if H has an eigenvalue $E=E_0$ for $\lambda=\lambda_0$, the multiplicity in both cases being the same. One can think of this in some sense as transformation which preserves the multiplicity among the eigenvalues of these two different operators.

It is clear that the main feature of the method is to interchange the role played by the constant λ and the energy E: the usual approach in quantum mechanics when dealing with an equation as Eq. (1) is to consider the potential term as being a perturbation and under suitable assumptions, the techniques of perturbation theory can then be employed to obtain a (convergent) solution for the eigenfunctions ψ and the eigenvalues E in terms of the perturbation parameter λ. The Birman-Schwinger principle on the other hand allows one to consider the energy E as a free parameter on which a series expansion for λ can be obtained. In fact, for most practical reasons it is useful to set $E=-\alpha^2$ and consider a series development on powers of the parameter α (which is identified with the fine structure constant) as

$$(\lambda(\alpha))^{-1}=\lambda_0^{-1}+a\alpha+b\alpha^2+\cdots. \tag{4}$$

After this is done, the question is to know if one can solve the above relation for α in terms of λ and if the resulting series obtained in this way is analytic. As outlined in Ref. 15, most of the steps leading to Eq. (4) pose no difficulties on this regard but a careful analysis must be done for the second part.

III. KERNEL IN COORDINATE SPACE

In this section we study some properties of the Birman-Schwinger kernel for the operator $\sqrt{-\Delta+m^2}-m$. The integral kernel is given by Eqs. (1) and (2) in Appendix A, namely

$$K(x,y)=|V(x)|^{1/2}\frac{m}{4\pi|x-y|}\left[\left(1-\frac{\mu^2}{m^2}\right)^{1/2}e^{-\mu|x-y|}+\frac{2}{\pi}F(m|x-y|;\mu)\right]|V(y)|^{1/2}. \tag{5}$$

The potential V is assumed to be nonpositive and with compact support Ω. The parameter μ is determined from $\mu^2=m^2-(m+E)^2=-2mE-E^2$. By setting $E=-\alpha^2$, one has $\mu^2=2m\alpha^2-\alpha^4$; this parametrization will be used at the end of this section and in Sec. IV.

In order to use perturbation theory on this operator, it is necessary to prove that it depends analytically on the parameter μ. For convenience we shall set $m=1$ in the following. First, if one considers the case of real μ, it is more or less clear that Eq. (5) makes only sense as long as $0<\mu<1$, and thus one can try to look for analyticity inside the disc $|\mu|<1$ in the complex plane

(we shall see that this is not an arbitrary choice for the problem). Let us then consider (f,Kg) for $f,g\in\mathcal{L}^2$. There are four different integrals over $\mathbb{R}^3\times\mathbb{R}^3$ to be considered:

$$\text{(i)}\quad (1-\mu^2)^{1/2}\left(f,|V|^{1/2}\frac{e^{-\mu|\cdot|}}{|\cdot|}|V|^{1/2}g\right),$$

$$\text{(ii)}\quad \left(f,|V|^{1/2}\frac{K_1(|\cdot|)}{|\cdot|}|V|^{1/2}g\right),$$

$$\text{(iii)}\quad (1-\mu^2)\left(f,|V|^{1/2}e^{-\mu|\cdot|}\int_0^{|\cdot|}\cosh(\mu z)K_0(z)\mathrm{d}z\ \ V|^{1/2}g\right),$$

$$\text{(iv)}\quad (1-\mu^2)\left(f,|V|^{1/2}\sinh(\mu|\cdot|)\int_{|\cdot|}^{\infty}e^{-\mu z}K_0(z)\mathrm{d}z|V|^{1/2}g\right).$$

To deal with them we shall argue in the same way as in Ref. 14 for the Dirac operator. The argument is based on writing (f,Kg) as a sum of integrals of the form

$$c(\mu)\int\int f(x)\frac{h(x,y)}{|x-y|^2}e^{-\mu|x-y|}g(y)d^3xd^3y$$

with $h(x,y)$ a function in $\mathcal{L}^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ having compact support and $c(\mu)$ an analytic function of μ. By using Sobolev's inequality one then finds that $f(x)[h(x,y)/|x-y|^2]g(y)\in\mathcal{L}^1(\mathbb{R}^3\times\mathbb{R}^3)$. The fact that K as an operator can be bounded by operators with compact support in $\mathcal{L}^2$ means that one is dealing with a meaningful object. In this way the whole problem of an analytic extension on μ is contained in the expression of the coefficients $c(\mu)$ and the exponential $e^{-\mu|x|}$.

For the first integral one immediately has $c(\mu)=(1-\mu^2)^{1/2}$ and $h(x,y)=|V(x)|^{1/2}|x-y||V(y)|^{1/2}$. In the second case obviously there is no dependence on μ and it suffices to note that with the function $h(x,y)=|V(x)|^{1/2}|x-y|K_1(|x-y|)|V(y)|^{1/2}$, which has compact support and is in $\mathcal{L}^\infty(\mathbb{R}^3\times\mathbb{R}^3)$, one has $f(x)[h(x,y)/|x-y|^2]g(y)\in\mathcal{L}^1(\mathbb{R}^3\times\mathbb{R}^3)$.

The third and fourth integral require more care: first, for the third integral one must consider $c(\mu)=(1-\mu^2)$, which is analytical on μ, and a function

$$h_\mu(x,y)=|V(x)|^{1/2}|x-y|\int_0^{|x-y|}\cosh(\mu z)K_0(z)\mathrm{d}z|V(y)|^{1/2}.$$

However, it is clear that $h_\mu(x,y)<F_1(\mu)|V(x)|^{1/2}|x-y||V(y)|^{1/2}$ where

$$F_1(\mu)=\int_0^\infty\cosh(\mu z)K_0(z)\mathrm{d}z=\frac{\pi}{2\sqrt{1-\mu^2}}$$

as an elementary calculation shows. This also points to the necessity of considering $|\mu|\neq 1$. One can now apply Sobolev inequality to the product $|V(x)|^{1/2}|x-y||V(y)|^{1/2}$, obtaining thus that $f(x)[h_\mu(x,y)/|x-y|^2]g(y)\in\mathcal{L}^1(\mathbb{R}^3\times\mathbb{R}^3)$. Furthermore, by writing $\cosh(\mu z)$ in terms of exponentials functions, it is clear that $h_\mu(x,y)$ is analytical on μ.

Consider now the fourth integral: one has as before $c(\mu)=(1-\mu^2)$ and

$$h_\mu(x,y)=|V(x)|^{1/2}|x-y|\sinh(\mu|x-y|)\int_{|x-y|}^\infty e^{-\mu z}K_0(z)\mathrm{d}z|V(y)|^{1/2}.$$

One can now see that $h_\mu(x,y)<\frac{1}{2}c|V(x)|^{1/2}|x-y||V(y)|^{1/2}$, where $c=\int_0^\infty K_0(z)\mathrm{d}z=\pi/2$, using the fact that $e^{-\mu z}\leqslant e^{-\mu a}$ for $z\in[a,\infty)$ and that $\int_a^\infty K_0(z)\mathrm{d}z\leqslant\int_0^\infty K_0(z)\mathrm{d}z$ for $a\geqslant 0$. Sobolev's inequality then

leads as in the previous case to $f(x)[h_\mu(x,y)/|x-y|^2]g(y) \in \mathcal{L}^1(\mathbb{R}^3 \times \mathbb{R}^3)$. As before, the function h_μ is analytical on μ since it involves in a simple way analytical functions of μ in its definition.

From the previous considerations we have the following.

Theorem 3.1: *Let $f,g \in \mathcal{L}^2(\mathbb{R}^3)$ then (f,Kg) where the kernel $K(x,y)$ is given by Eq. (5) is analytical in the sense of norm.*

Proof: Since we already know that (f,Kg) is analytical on μ, Theorem 3.12 in Ref. 13 can be used to deduce that K is indeed analytic in the sense of norm. □

One should notice that the fact that one is considering a potential V with compact support Ω is fundamental for this argument to work. Let us now proceed to finding under which conditions is 0 an eigenvalue of Eq. (2). On general grounds one can argue in the following way: given an operator $\mathcal{O}$ with inverse $\mathcal{O}^{-1}$, consider a function ϕ solution to the equation

$$l_0\phi = \mu_0\phi, \tag{6}$$

where $l_0 = |V|^{1/2}\mathcal{O}^{-1}|V|^{1/2}$. This equation is similar in structure to Eq. (3). Let us now define a function u through the relation

$$u = \mathcal{O}^{-1}|V|^{1/2}\phi.$$

This function satisfies the integral equation

$$u = \mathcal{O}^{-1}|V|^{1/2}\phi = \mu_0^{-1}\mathcal{O}^{-1}|V|^{1/2}|V|^{1/2}\mathcal{O}^{-1}|V|^{1/2}\phi = \mu_0^{-1}\mathcal{O}^{-1}|V|u,$$

namely

$$u(x) = \mu_0^{-1}\int_{\text{supp } V} \mathcal{O}^{-1}(x,y)|V(y)|u(y)d^3y. \tag{7}$$

In the case of a potential V with compact support, let us say Ω, one obtains a development in series for large $|x|$ of the previous expression as

$$u(x) = \mu_0^{-1}|x|^{-1}\int_\Omega c_1(y)|V(y)|u(y)d^3y + \mu_0^{-1}|x|^{-2}\int_\Omega c_2(y)|V(y)|u(y)d^3y + \cdots \tag{8}$$

and therefore

$$\int_\Omega c_1(y)|V(y)|u(y)d^3y = \mu_0\int_\Omega c_1(y)|V(y)|^{1/2}\phi(y)d^3y = 0 \tag{9}$$

must be imposed in order to have $u \in \mathcal{L}^2(\mathbb{R}^3)$. In the above the functions $c_1(y)$ and $c_2(y)$ are determined from the series development of $\mathcal{O}^{-1}(x,y)$ in powers of $1/|x|$ for large $|x|$. We have assumed that the negative powers of $|x|$ appearing in this series development are integers, which is clearly seen from Eq. (8). This might be not necessarily the most general scenario, but as long as the first term has a factor $|x|^{-\gamma}$ with $\gamma \leqslant 3/2$, as in the case we are considering, Eq. (9) will be obtained.

Along the precedent lines we can state the following theorem.

Theorem 3.2: *Let V be a nonpositive potential with compact support $\Omega \in \mathbb{R}^3$. Then $E=0$ is an eigenvalue of $\sqrt{-\Delta+m^2}-m+\lambda V$ if and only if $\int_\Omega |V(y)|u(y)d^3y = 0$, where u is the corresponding eigenfunction assumed to be in $\mathcal{L}^2(\mathbb{R}^3)$.*

Proof: According to the previous discussion, let us consider $\mathcal{O} = \sqrt{-\Delta+m^2}-m$. We have then that the operator $l_0 = |V|^{1/2}\mathcal{O}^{-1}|V|^{1/2}$ is given by

$$l_0 = |V(x)|^{1/2}\frac{m}{4\pi|x-y|}\left[1 + \frac{2}{\pi}K_1(m|x-y|) + \frac{2}{\pi}\int_0^{m|x-y|} K_0(y)\mathrm{d}y\right]|V(y)|^{1/2}$$

and that u defined as $u = \mathcal{O}^{-1}|V|^{1/2}\phi$, with $l_0\phi = \mu_0\phi$, satisfies

$$u(x)=\mu_0^{-1}(\mathcal{O}^{-1}|V|u)(x)=\frac{m}{4\pi\mu_0}\int_\Omega\frac{1}{|x-y|}\left[1+\frac{2}{\pi}K_1(m|x-y|)+\frac{2}{\pi}\int_0^{m|x-y|}K_0(y)\mathrm{d}y\right]u(y)d^3y. \tag{10}$$

Using this expression one obtains for large values of $|x|$,

$$u(x)=\frac{m}{2\pi\mu_0}\frac{1}{|x|}\int_\Omega|V(y)|u(y)d^3y+\cdots, \tag{11}$$

since $\int_0^\infty K_0(y)\mathrm{d}y=\pi/2$ and $K_1(z)\sim\sqrt{\pi/2z}e^{-z}$ for large z. It is clear that Eq. (11) corresponds to having $c_1(y)=m/2\pi$ in Eq. (8). It is then clear that if $u\in\mathcal{L}^2(\mathbb{R}^3)$ then the coefficient of $|x|^{-1}$ in Eq. (11) should vanish, leading to the condition $\int_\Omega|V(y)|u(y)d^3y=0$. On the other hand, from the Birman-Schwinger principle one knows that $u=\mu_0^{-1}\mathcal{O}^{-1}|V|u$ iff $(\mathcal{O}+\mu_0^{-1}V)u=0$, this last equation being understood in the sense of distributions. Therefore, the constraint $\int_\Omega|V(y)|u(y)d^3y=0$ is a necessary and sufficient condition for $E=0$ to be an eigenvalue of $\sqrt{-\Delta+m^2}-m+\mu_0^{-1}V$. □

One should notice that a similar condition exists for the Schrödinger operator. This can be understood on the grounds of the nonlocal behavior associated to $\sqrt{-\Delta+m^2}-m$: nonlocality is contained in the Bessel function $K_1(z)$ appearing in the function $F(m|x|;\mu=0)$ in Eq. (6) and for large distances (at least greater than m^{-1}) it becomes highly suppressed. In this situation the main contribution arises from a Schrödinger-type term [first term in Eq. (5)].

One can also try to see what happens for small values of $|x|$. In this case there are two terms to lowest order to be considered,

$$A_1=\int_\Omega\frac{1}{|y|}|V(y)|u(y)d^3y \tag{12}$$

and

$$A_2=\int_\Omega\frac{1}{|y|}|V(y)|u(y)\int_{|y|}^\infty\frac{K_1(z)}{z}\mathrm{d}z\,d^3y. \tag{13}$$

Both terms are constants, independent of $|x|$. If supp $V=\Omega$ contains the origin, then for a nondivergent value of $u(|x|=0)$ to exist, these constants should have finite values. The constant A_1 also appears when one considers a similar situation for the kernel of the Schrödinger operator. If the product $|V(y)|u(y)$ behaves like $y^{-\beta}$ with $\beta\leqslant 2$ near 0 then it is well defined (strict inequality means $A_1=0$). On the other hand, A_2 is more singular due to the presence of the integral involving the Bessel function K_1. The first integral (from $|y|$ to infinity) diverges as $1/y$ near the origin. This means that finite values are possible in this case when the product $|V(y)|u(y)$ behaves like $y^{-\beta}$ with $\beta\leqslant 1$ (again, strict inequality means a vanishing value for A_2).

IV. PERTURBATION THEORY AND FOURIER TRANSFORM

In what follows we shall consider perturbation theory for Eq. (5). From this kernel we can immediately write for α small the series development $K=L_0+(2m)^{1/2}\alpha A+2m\alpha^2B+\cdots$ where

$$L_0(x,y)=|V(x)|^{1/2}\frac{m}{4\pi|x-y}\left[2+\frac{2}{\pi}\int_{m|x-y|}^\infty\frac{K_1(z)}{z}\mathrm{d}z\right]|V(y)|^{1/2}, \tag{14}$$

$$A(x,y)=-\frac{m}{2\pi}|V(x)|^{1/2}|V(y)|^{1/2}, \tag{15}$$

and

$$B(x,y)=|V(x)|^{1/2}\frac{1}{|x-y|}\left\{\frac{1}{2}\left(|x-y|^2-\frac{1}{m^2}\right)+\frac{1}{\pi}\left(|x-y|^2-\frac{2}{m^2}\right)\int_0^{m|x-y|}K_0(z)\mathrm{d}z\right.$$
$$\left.+\frac{2|x-y|}{\pi m}\int_{m|x-y|}^{\infty}K_0(z)z\,\mathrm{d}z+\frac{1}{\pi m^2}\int_0^{m|x-y|}K_0(z)z^2\,\mathrm{d}z\right\}|V(y)|^{1/2}. \tag{16}$$

As mentioned before, the presence of the second term inside the brackets in Eq. (14) is an indication of the nonlocality of the Herbst operator. Furthermore, by going into Fourier space, one can see that the kernel of L_0 is not positive definite, and for large values of k it can take arbitrary positive and negatives values. This is due to the strong divergence produced by the integral of the quotient $K_1(z)/z$, which when coupled with the factor $1/|x-y|$ is of order 3.

Let us now find an expression for $\lambda^{-1}=(\phi,K\phi)$ [see Eq. (3)] where ϕ satisfies $L_0\phi=\mu_0\phi$ and $\|\phi\|_2=1$. We have

$$(\lambda(\alpha))^{-1}=(\phi,L_0\phi)+(2m)^{1/2}\alpha(\phi,A\phi)+2m\alpha^2(\phi,B\phi)+\cdots$$
$$=\mu_0-\frac{\alpha m^{3/2}}{\sqrt{2}\pi}\left(\int_\Omega|V(y)|^{1/2}\phi(y)d^3y\right)^2+b\alpha^2+\cdots. \tag{17}$$

The expression for the coefficient b is rather cumbersome as can be deduced from Eq. (16) and no definite statement on the sign of this coefficient can readily be established. But before with the analysis of it, let us review the general procedure used to write the energy E as a function of the parameter λ. Assuming $\mu_0\neq 0$, one deduces from the expression

$$(\lambda(\alpha))^{-1}=\mu_0+a\alpha+b\alpha^2+\cdots$$

the relation

$$\lambda_0^{-1}\lambda(\alpha)=1-\lambda_0 a\alpha+\lambda_0(\lambda_0 a^2-b)\alpha^2+\cdots,\quad \lambda_0:=\mu_0^{-1},$$

for α small. The next step is to invert this relation and to find α as a function of λ; it is here where care should be taken. If a does not vanish then one has

$$\alpha(\lambda)=-\frac{1}{\lambda_0^2 a}(\lambda-\lambda_0)+\frac{\lambda_0 a^2-b}{\lambda_0^4 a^3}(\lambda-\lambda_0)^2+\cdots$$

and therefore

$$E(\lambda)=-\alpha(\lambda)^2=-\frac{1}{(\lambda_0^2 a)^2}(\lambda-\lambda_0)^2+\cdots.$$

On the other hand, if a vanishes then

$$\lambda_0^{-1}\lambda(\alpha)=1-\lambda_0 b\alpha^2+c\alpha^3+\cdots$$

and it follows that there are two different expressions for α,

$$\alpha_\pm(\lambda)=\tilde{n}\left[\frac{1}{\lambda_0^2(-b)}(\lambda-\lambda_0)-\frac{c}{\lambda_0^3(-b)^{3/2}}(\lambda-\lambda_0)^{3/2}+\cdots\right]^{1/2}.$$

One obtains then

$$E_\pm(\lambda)=-\alpha_\pm(\lambda)^2=-\frac{1}{\lambda_0^2(-b)}(\lambda-\lambda_0)+\cdots$$

and moreover, the series development is done in powers of $(\lambda-\lambda_0)^{1/2}$. For $\mathcal{O}=\sqrt{-\Delta+m^2}-m$, the coefficient a is proportional to $(\int_\Omega|V(y)|^{1/2}\phi(y)d^3y)^2$ according to Eq. (17) and then it suffices to

recall the discussion leading to Eq. (11) to conclude that the (first) second series development corresponds to $E=0$ (not) being an eigenvalue. For the first series, when $a\neq 0$, it is possible to appeal to the implicit theorem function to deduce analyticity of $\alpha(\lambda)$ at the point λ_0 and thus of $E(\lambda)$. When $a=0$, analyticity does not hold in the Schrödinger case[15] because of an argument making use of the fact that $-\Delta+\lambda V$ only admits nonpositive eigenvalues for all $\lambda>0$ [Theorem XIII.11 in Ref. 21 applied to $V\in\mathcal{C}_0^\infty(\mathbb{R}^3)$]. Unfortunately we have not been able to find a similar result for the Herbst operator in the three-dimensional case.

We also remark that in the case when $a=0$, if λ approaches λ_0 from above by real values then b should necessarily be negative for $\alpha_\pm(\lambda)$ to be well defined. In the case of the Schrödinger equation it is known through an argument involving Fourier transform that b takes negative values when a vanishes,[15] in consequence the energy approaches a value $E_0=0$ from below as $\lambda\to\lambda_0^+$. For the Herbst operator one can proceed in the same way, i.e., one can write

$$B(x,y)=|V(x)|^{1/2}\mathcal{B}(x,y)|V(y)|^{1/2}$$

and therefore

$$b=2m^2(\phi,B\phi)=2m^2(\phi,|V|^{1/2}\mathcal{B}|V|^{1/2}\phi)=2m^2(f,\mathcal{B}f)=2m^2\int\hat{\mathcal{B}}(k)|\hat{f}(k)|^2d^3k \tag{18}$$

with $f=|V|^{1/2}\phi$. The sign of b is then related to the behavior of the Fourier transform $\hat{\mathcal{B}}$. We should also note that the fact that $a=0$ guarantees that the expression in momentum space on the right-hand side of Eq. (18) is defined as $k\to 0$.

As seen from Eq. (16) not all functions appearing in that expression have norm in $\mathcal{L}^2(\mathbb{R}^3)$, and it is then necessary to use Fourier transform in the sense of distributions to find the Fourier transform $\hat{\mathcal{B}}(k)$. The details of this are given in Appendix B, here we only write the final result of the calculations which reads as

$$\begin{aligned}b&=2m^2\int\hat{\mathcal{B}}(k)|\hat{f}(k)|^2d^3k=2m\int(m^4\hat{\mathcal{B}}(m\sigma))|\hat{f}(m\sigma)|^2d^3\sigma\\&=2m\int\left[-\frac{1}{2\pi\sigma^2}-\frac{1}{4\pi^3\sigma^4}-\frac{1}{\pi}\left[\frac{1}{8\pi^2\sigma^4}\frac{6w^4+5w^2+2}{(1+w^2)^{5/2}}+\frac{1}{\sigma^2}\frac{1}{(1+w^2)^{1/2}}\right]\right.\\&\quad\left.+\frac{3}{2\pi^2\sigma^3}\frac{w^3}{(1+w^2)^{5/2}}-\frac{1}{2\pi\sigma^2}\frac{2w^2-1}{(1+w^2)^{5/2}}\right]|\hat{f}(m\sigma)|^2d^3\sigma,\end{aligned} \tag{19}$$

where $\vec{\sigma}=\vec{k}/m$, $\sigma=|\vec{\sigma}|\in[0,\infty)$, and $w=2\pi\sigma$. Even though a positive term is present in this expression, its contribution is dominated by similar negative terms as one can easily verify from Eq. (19). Therefore one concludes that b is (conditionally) negative and that $E\to 0^-$ when $\lambda\to\lambda_0^+$. Moreover, it also follows from this expression that in the nonrelativistic case ($k=m\sigma\to 0$) the leading order contribution is given by $-\pi^{-1}\sigma^{-2}-(2\pi^3)^{-1}\sigma^{-4}$, an analogous result to the Schrödinger case.

We can resume the previous calculations in the following theorem.

Theorem 4.1: *Consider the series development of* $\lambda^{-1}=(\phi,K\phi)=\lambda_0^{-1}+a\alpha+b\alpha^2+\cdots$ *in powers of* α, *then*

(i) $a=-(m^{3/2}/\sqrt{2}\pi)(\int_\Omega|V(y)|^{1/2}\phi(y)d^3y)^2$,

(ii) *if* $a=0$ *then* $b=2m^2(f,\mathcal{B}f)$ *with* $f=|V|^{1/2}\phi$, *is conditionally negative and the Fourier transform* $\hat{\mathcal{B}}(k)$ *of the kernel* $\mathcal{B}(x,y)$ *can be read out from Eq. (19).*

V. CONCLUSIONS

It has been shown that having wave functions of the operator $\sqrt{-\Delta+m^2}-m$ in $\mathcal{L}^2(\mathbb{R}^3)$ is closely related to the vanishing of the first order coefficient a in the series development given by

Eq. (4), perturbation theory being permitted due to the analyticity of the corresponding Birman-Schwinger kernel (Theorem 3.1). The coefficient a has the same form as in the Schödinger case as seen from Eq. (17) and its vanishing can be recast as a statement on the fact that $E=0$ is an eigenvalue of the equation $(\sqrt{-\Delta+m^2}-m+\lambda V)\phi=E\phi$ (Theorem 3.2). Moreover, the second order coefficient b in Eq. (4) can be shown to consist of a Schrödinger-type part and more involved contributions due to the nonlocal nature of the operator under study. Fourier analysis however can be used to show that b is conditionally negative (Theorem 4.1). The physical consequence of these facts is similar to the Schrödinger case, namely, the phenomenon of "coupling constant threshold."

When considering the Schrödinger operator with a spherically symmetric potential V, the above characterization can be explicitly formulated as a condition for the presence of s-waves as solutions of the equation $(-\Delta+V)\Psi=0$ and indeed, it is only the behavior of Ψ at infinity, where the potential V vanishes, which should be considered to obtain this result.[15]

In the case of the Herbst operator a similar criteria should be also possible, however there is a simple feature that is present in one case and not in the other: the answer for the Schrödinger operator can readily be given because one knows precisely the expression for the operator Δ in spherical coordinates meanwhile for the Herbst operator one should study instead an integral equation. The following auxiliary problem then arises: is it possible to write an appropriate integral equation for $\Delta\Psi=0$ from which one can recover the well known radial dependence r^l and r^{-l-1}, $l=0,1,\ldots$, of the spherically symmetric solutions? The answer is yes. The next natural step is to see if the same process can be applied to the integral equation obtained from $(\sqrt{-\Delta+m^2}-m)\Psi=0$. This is a subject that we hope to discuss in a future work.

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APPENDIX A: INVERSE FOURIER TRANSFORM

In this section we would like to derive the expression for $(\sqrt{-\Delta+m^2}-E)^{-1}$ in coordinate space. Since one is lead to deal with tempered function, the Fourier transform in the generalized sense should be considered. Several ways exist to calculate the Fourier transform of tempered functions, such as the ϵ-prescription, where it is customary to consider after the calculations only those terms with no dependence on ϵ in the limit $\epsilon\to 0$. This method was widely used in the evaluation of propagators in the early days of QED. The Hankel transform[3] is the other method introduced to deal with tempered functions. It is known that the ϵ-prescription, the same being the case with the Hankel transform, is related to the notion of finite part, *Pf.* of a distributional pseudofunction (Ref. 22, pp. 20) acting on Schwartz's space $\mathcal{S}$ of infinitely differentiable and rapidly vanishing functions, together with its derivatives, at infinity. We shall also use the fact that for a distribution f, the relations $\langle\mathcal{F}(f),\phi\rangle=\langle f,\mathcal{F}(\phi)\rangle$ and $\langle\mathcal{F}^{-1}(f),\phi\rangle=\langle f,\mathcal{F}^{-1}(\phi)\rangle$ where $\phi\in\mathcal{S}$ hold.[4]

Accordingly one can write

$$\int_{\mathbb{R}^3}\frac{1}{\sqrt{4\pi^2p^2+m^2}-E}\phi(p)d^3p=E\int_{\mathbb{R}^3}\frac{1}{4\pi^2p^2+m^2-E^2}\phi(p)d^3p+\int_{\mathbb{R}^3}\frac{\sqrt{4\pi^2p^2+m^2}}{4\pi^2p^2+m^2-E^2}\phi(p)d^3p$$

$$=E\int_{\mathbb{R}^3}\frac{1}{4\pi^2p^2+m^2-E^2}\phi(p)d^3p$$

$$+(-\Delta+m^2)\int_{\mathbb{R}^3}\frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\phi(p)d^3p$$

$$= E\int_{\mathbb{R}^3} \frac{1}{4\pi^2p^2+\mu^2}\phi(p)d^3p$$
$$+ (-\Delta+\mu^2)\int_{\mathbb{R}^3} \frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\phi(p)d^3p$$
$$+ (m^2-\mu^2)\int_{\mathbb{R}^3} \frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\phi(p)d^3p,$$

where we have set $\mu^2=m^2-E^2$. Therefore, from $<\mathcal{F}(f),\phi>=<f,\mathcal{F}(\phi)>=<\mathcal{F}^{-1}(\mathcal{F}(f)),\phi>$, one has in the sense of distributions acting on $\mathcal{S}$,

$$\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}-E}\right](x) = E\mathcal{F}^{-1}\left[\frac{1}{4\pi^2p^2+\mu^2}\right](x)$$
$$+ (-\Delta+\mu^2)\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\right](x)$$
$$+ (m^2-\mu^2)\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\right](x).$$

The first term is a standard example in textbooks on Fourier transforms or potential theory and can be easily found:

$$\int_{\mathbb{R}^3}\frac{1}{4\pi^2p^2+\mu^2}\phi(p)d^3p = \int_{\mathbb{R}^3}\int_0^\infty e^{-(4\pi^2p^2+\mu^2)t}\,\mathrm{d}t\;\phi(p)d^3p$$
$$= \int_{\mathbb{R}^3}\int_0^\infty\int_{\mathbb{R}^3} e^{-4\pi^2p^2t+2\pi p\cdot x}d^3p e^{-\mu^2t}\mathcal{F}(\phi)(x)d^3x$$
$$= \int_{\mathbb{R}^3}\int_0^\infty \frac{1}{(4\pi t)^{3/2}}\exp[-|x|^2/4t-\mu^2t]dt\mathcal{F}(\phi)(x)d^3x$$
$$= \frac{\mu}{(4\pi)^{3/2}}2\sqrt{\frac{2}{\mu|x|}}\int_{\mathbb{R}^3}K_{1/2}(m|x|)\mathcal{F}(\phi)(x)d^3x = \int_{\mathbb{R}^3}\frac{e^{-\mu|x|}}{4\pi|x|}\mathcal{F}(\phi)(x)d^3x$$

with $\phi\in\mathcal{S}$. In the above we have use Fubini's theorem and an integral representation of the Bessel functions $K_\nu(z)$. For the second and third term one should calculate the inverse Fourier transform

$$\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}[4\pi^2p^2+\mu^2]}\right](x).$$

Using the fact that the usual properties of convolution of the (inverse) Fourier transform remain valid for distributions,[4] then the problem reduces to the convolution of $\mathcal{F}^{-1}[1/(4\pi^2p^2+\mu^2)](x)$ with $\mathcal{F}^{-1}[1/\sqrt{4\pi^2p^2+m^2}](x)$. This latter inverse Fourier transform can be found in the same way as done before with the result

$$\int_{\mathbb{R}^3}\frac{1}{\sqrt{4\pi^2p^2+m^2}}\phi(p)d^3p = \frac{m}{2\pi^2}\int_{\mathbb{R}^3}\frac{K_1(m|x|)}{|x|}\mathcal{F}(\phi)(x)d^3x.$$

Therefore, in distributional sense, one has the following expression:

$$\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}-E}\right](x)=\frac{E}{4\pi|x|}e^{-\mu|x|}+(-\Delta+\mu^2)\left[\frac{e^{-\mu|\cdot|}}{4\pi|\cdot|}*\frac{m}{2\pi^2}\frac{K_1(m|\cdot|)}{|\cdot|}\right](x)$$
$$+\frac{m(m^2-\mu^2)}{8\pi^3}\left[\frac{e^{-\mu|\cdot|}}{|\cdot|}*\frac{K_1(m|\cdot|)}{|\cdot|}\right](x)$$
$$=\frac{E}{4\pi|x|}e^{-\mu|x|}+\frac{m}{2\pi^2}\frac{K_1(m|x|)}{|x|}+\frac{m(m^2-\mu^2)}{8\pi^3}\left[\frac{e^{-\mu|\cdot|}}{|\cdot|}*\frac{K_1(m|\cdot|)}{|\cdot|}\right](x).$$

It is clear from the above that this expression might be treated indeed as an ordinary function if the convolution in the last line makes sense. In fact, using the expansion[1]

$$\frac{e^{-\lambda R}}{\lambda R}=\frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\left[\sqrt{\frac{\pi}{2\lambda r_1}}I_{l+1/2}(\lambda r_1)\right]\left[\sqrt{\frac{\pi}{2\lambda r_2}}K_{l+1/2}(\lambda r_2)\right]P_l(\cos\gamma),$$

where $R=[r^2+\rho^2-2r\rho\cos(\gamma)]^{1/2}, r_1=\min(r,\rho), r_2=\max(r,\rho)$, only the term with $l=0$ is seen to give a nonvanishing contribution for the convolution after performing the integral over the angular variables. Therefore, one obtains

$$\left[\frac{e^{-\mu|\cdot|}}{|\cdot|}*\frac{K_1(m|\cdot|)}{|\cdot|}\right](x)=\frac{4\pi}{m^2}\frac{2\mu}{\pi}\sqrt{\frac{\pi}{2\mu|x|}}K_{1/2}(\mu|x|)\int_0^{m|x|}\sqrt{\frac{m\pi}{2\mu y}}I_{1/2}\left(\frac{\mu y}{m}\right)K_1(y)y\,dy$$
$$+\frac{4\pi}{m^2}\frac{2\mu}{\pi}\sqrt{\frac{\pi}{2\mu|x|}}I_{1/2}(\mu|x|)\int_{m|x|}^{\infty}\sqrt{\frac{m\pi}{2\mu y}}K_{1/2}\left(\frac{\mu y}{m}\right)K_1(y)y\,dy$$
$$=\frac{4\pi}{m^2|x|}e^{-\mu|x|}\int_0^{m|x|}\frac{m}{\mu y}\sinh\left(\frac{\mu y}{m}\right)K_1(y)y\,dy$$
$$+\frac{4\pi}{m}\frac{\sinh(\mu|x|)}{\mu|x|}\int_{m|x|}^{\infty}e^{-\mu y/m}K_1(y)dy.$$

The explicit expressions of the Bessel functions $I_{1/2}(x)$ and $K_{1/2}(x)$ have been used in order to write the above relation. The final outcome of the previous calculations is then

$$\mathcal{F}^{-1}\left[\frac{1}{\sqrt{4\pi^2p^2+m^2}-E}\right](x)=\frac{m}{4\pi|x|}\left[\frac{E}{m}e^{-\mu|x|}+\frac{2}{\pi}F(m|x|;\mu)\right]$$
$$=\frac{m}{4\pi|x|}\left[\left(1-\frac{\mu^2}{m^2}\right)^{1/2}e^{-\mu|x|}+\frac{2}{\pi}F(m|x|;\mu)\right] \tag{A1}$$

with

$$F(m|x|;\mu)=K_1(m|x|)+\frac{m^2-\mu^2}{4\pi}|x|\left[\frac{e^{-\mu|\cdot|}}{|\cdot|}*\frac{K_1(m|\cdot|)}{|\cdot|}\right](x)=K_1(m|x|)+\left(1-\frac{\mu^2}{m^2}\right)$$
$$\times\left[e^{-\mu|x|}\int_0^{m|x|}\left[\frac{m}{\mu y}\right]\sinh\left(\frac{\mu y}{m}\right)K_1(y)y\,dy+\frac{m}{\mu}\sinh(\mu|x|)\int_{m|x|}^{\infty}e^{-\mu y/m}K_1(y)dy\right]$$
$$=K_1(m|x|)+\left(1-\frac{\mu^2}{m^2}\right)\left[e^{-\mu|x|}\int_0^{m|x|}\cosh\left(\frac{\mu y}{m}\right)K_0(y)dy-\sinh(\mu|x|)\int_{m|x|}^{\infty}e^{-\mu y/m}K_0(y)dy\right]. \tag{A2}$$

In the above we have used some relations among integrals involving Bessel and exponentials functions[19,1] in order to write the last expression.

APPENDIX B: FOURIER TRANSFORM OF $\mathcal{B}(x,y)$

For convenience we present here the calculations leading to Eq. (19) in the text. In the expression for $\mathcal{B}$, several tempered functions in the sense of distributions appear and their Fourier transforms, which will be also tempered functions, can be found in this context.

In the following we shall apply the Hankel transform to a well-behaved function suited to the problem (strictly speaking the Hankel transform refers to the one-dimensional case) and then argue its validity for more general cases.

To begin with we shall use the formula (Ref. 3, Sec. 43)

$$\mathcal{F}(f,k)=\frac{2\pi}{k^{(n-2)/2}}\int_0^{+\infty}\mathrm{d}r\, f(r)r^{n/2}J_{(n-2)/2}(2\pi kr).$$

Here n is the dimension of the space under consideration. Let us apply this to the function $f(x)=|x|^{-\alpha}\int_0^{m|x|}g(z)\mathrm{d}z$ with $0<\alpha$, we have

$$\begin{aligned}\mathcal{F}(f,r)&=\frac{2\pi}{r^{(n-2)/2}}\int_0^{\infty}\mathrm{d}r\, r^{-\alpha}\int_0^{mr}\mathrm{d}z\, g(z)r^{n/2}J_{(n-2)/2}(2\pi kr)\\&=\frac{2\pi}{r^{(n-2)/2}}\int_0^{\infty}\mathrm{d}r\, r^{n/2-\alpha}J_{(n-2)/2}(2\pi kr)\int_0^{mr}\mathrm{d}z\, g(z)\\&=\frac{2\pi}{k^{(n-2)/2}}\frac{1}{(2\pi k)^{n/2-\alpha+1}}\int_0^{\infty}\mathrm{d}z\, g(z)\int_{z/m}^{\infty}\mathrm{d}u\, u^{n/2-\alpha}J_{(n-2)/2}(u)\\&=\frac{1}{(2\pi)^{n/2-\alpha}}\frac{1}{k^{n-\alpha}}\left[\int_0^{\infty}\mathrm{d}z\, g(z)\int_0^{\infty}\mathrm{d}u\, u^{n/2-\alpha}J_{(n-2)/2}(u)-\int_0^{\infty}\mathrm{d}z\, g(z)\int_0^{wz}\mathrm{d}u\, u^{n/2-\alpha}J_{(n-2)/2}(u)\right].\end{aligned}$$

In the above we have defined a dimensionless parameter $w=2\pi k/m$ and assumed that the function $g(z)$ is well behaved so that Fubini's theorem can be used. For our function $g(z)$ we shall take indeed $g(z)=z^{\beta}K_0(z), 0\leqslant\beta$. The previous expression is justified as long as $n/2<\alpha<n$ since the integrals involving the Bessel function $J_\nu(u)$ are then well defined. After using the relations

$$\int_0^{\infty}s^{\mu}J_{\nu}(s)\mathrm{d}s=2^{\mu}\Gamma\left(\frac{\nu+\mu+1}{2}\right)\Big/\Gamma\left(\frac{\nu-\mu+1}{2}\right),$$

$$\int_0^{\infty}s^{\mu}K_{\nu}(s)\mathrm{d}s=2^{\mu-1}\Gamma\left(\frac{\mu+\nu+1}{2}\right)\Gamma\left(\frac{\mu-\nu+1}{2}\right),$$

and

$$\int_0^{x}s^{\mu}J_{\nu}(s)\mathrm{d}s=x^{\mu+1}\sum_{k=0}^{\infty}\frac{(-1)^k(x/2)^{\nu+2k}}{k!(\mu+\nu+2k+1)\Gamma(\nu+k+1)},$$

one arrives to

$$\mathcal{F}(f,r)=\frac{1}{(2\pi)^{n/2-\alpha}}\frac{1}{k^{n-\alpha}}\left[2^{\beta+n/2-\alpha-1}\Gamma\left(\frac{\beta+1}{2}\right)^2\frac{\Gamma\left(\frac{n-\alpha}{2}\right)}{\Gamma\left(\frac{\alpha}{2}\right)}\right.$$
$$\left.-w^{n-\alpha}2^{\beta+n/2-\alpha-1}\sum_{m=0}^{\infty}\frac{(-w^2)^m}{m!\left(m+\frac{n-\alpha}{2}\right)}\frac{\Gamma\left(m+\frac{\beta+n-\alpha+1}{2}\right)^2}{\Gamma\left(m+\frac{n}{2}\right)}\right].$$

The sum inside the brackets is just a hypergeometric function; the final result then reads as

$$\mathcal{F}(f,r)=\frac{1}{(2\pi)^{n/2-\alpha}}\frac{1}{k^{n-\alpha}}\left[2^{\beta+n/2-\alpha-1}\Gamma\left(\frac{\beta+1}{2}\right)^2\frac{\Gamma\left(\frac{n-\alpha}{2}\right)}{\Gamma\left(\frac{\alpha}{2}\right)}-w^{n-\alpha}2^{\beta+n/2-\alpha}\frac{\Gamma\left(\frac{\beta+n-\alpha+1}{2}\right)^2}{(n-\alpha)\Gamma\left(\frac{n}{2}\right)}\right.$$
$$\left.\times\,{}_3F_2\left(\frac{n-\alpha}{2},\frac{\beta+n-\alpha+1}{2},\frac{\beta+n-\alpha+1}{2};\frac{n}{2},1+\frac{n-\alpha}{2};-w^2\right)\right]. \tag{B1}$$

Using a reasoning due to Schwartz (Ref. 23, p. 113), this expression can be seen to hold also for other values of α, in particular for $\alpha<0$, if one keeps in mind that the function f should be then understood as a tempered function as well as its Fourier transform. More care should be taken when $n-\alpha=-2h$, $\alpha=-2h$, or $\beta+n-\alpha+1=-2h$, h being a positive integer, where poles appear in the Γ function, but the appropriate modification to be used for those cases has also been pointed out by Schwartz. This modification will not concern us however because of the values of α (±1 or 0) appearing in Eq. (16) and of the dimension $n=3$. As a particular case then one can consider $\alpha=1,\beta=0,n=3$,

$$\mathcal{F}(f,r)=\frac{1}{(2\pi)^{1/2}}\frac{1}{k^2}\left[\frac{\pi^{1/2}}{2^{1/2}}-\frac{w^2}{2^{1/2}}\Gamma(3/2)\,{}_3F_2(1,3/2,3/2;3/2,2;-w^2)\right]=\frac{1}{2k^2}\frac{1}{(1+w^2)^{1/2}}.$$

This corresponds, taking into account a factor $-2/(\pi m^2)$ and replacement $k=m\sigma$, to the second term inside the brackets in Eq. (19).

It is also straightforward from the previous computation to identify the Fourier transform of $f(x)=|x|^{-\alpha}\int_{m|x|}^{\infty}g(z)\mathrm{d}z, 0<\alpha$, this is given by the second term in Eq. (B1), namely

$$\mathcal{F}(f,r)=\frac{1}{(2\pi)^{n/2-\alpha}}\frac{1}{k^{n-\alpha}}w^{n-\alpha}2^{\beta+n/2-\alpha}\frac{\Gamma\left(\frac{\beta+n-\alpha+1}{2}\right)^2}{(n-\alpha)\Gamma\left(\frac{n}{2}\right)}$$
$$\left.\times\,{}_3F_2\left(\frac{n-\alpha}{2},\frac{\beta+n-\alpha+1}{2},\frac{\beta+n-\alpha+1}{2};\frac{n}{2},1+\frac{n-\alpha}{2};-w^2\right)\right]. \tag{B2}$$

This formula can also be generalized to other values of α than those in the interval $(n/2,n)$, with care needed only to be taken in more detail at the points mentioned in a previous paragraph. Taking this into account, if we now calculate the case $\alpha=0,\beta=1,n=3$, the following expression is obtained:

$$\mathcal{F}(f,r)=\frac{1}{(2\pi)^{3/2}}\frac{1}{k^3}w^3 2^{5/2}\frac{\Gamma(5/2)^2}{3\Gamma(3/2)}{}_3F_2(3/2,5/2,5/2;3/2,5/2;-w^2)=\frac{3}{4\pi}\frac{1}{k^3}w^3 2^{3/2}\frac{1}{(1+w^2)^{5/2}}$$

corresponding, times a factor $2/(\pi m)$ and replacement $k=m\sigma$, to the positive term in Eq. (19).

APPENDIX C: AN ESTIMATE

We rewrite Eq. (1) as

$$(\sqrt{-\Delta+m^2}-E)^{-1}(|x|)=\frac{m}{4\pi|x|^2}\left[\left(1-\frac{\mu^2}{m^2}\right)^{1/2}|x|e^{-\mu|x|}+\frac{2}{\pi}|x|F(m|x|;\mu)\right].$$

We would like to show that for a fixed value of μ, each term inside the brackets is bounded as function of $|x|$. This is obviously true for $h_0(|x|)=|x|e^{-\mu|x|}(\leqslant\mu^{-1})$ and also for the first term coming from the product $|x|F(m|x|;\mu)$, namely $h_1(|x|)=|x|K_1(m|x|)(\leqslant 1)$. The next two terms to consider are

$$h_2(|x|)=|x|e^{-\mu|x|}\int_0^{m|x|}\cosh\left(\frac{\mu y}{m}\right)K_0(y)\mathrm{d}y$$

and

$$h_3(|x|)=|x|\sinh(\mu|x|)\int_{m|x|}^{\infty}e^{-\mu y/m}K_0(y)\mathrm{d}y.$$

h_2 can be seen to be bounded as follows:

$$\begin{aligned}h_2(|x|)&\leqslant\mu^{-1}\int_0^{\infty}\cosh\left(\frac{\mu y}{m}\right)K_0(y)\mathrm{d}y=\frac{1}{2\mu}\int_0^{\infty}\cosh\left(\frac{\mu y}{m}\right)\int_0^{\infty}\exp\left[-\frac{1}{u}-\frac{uy^2}{4}\right]\frac{\mathrm{d}u}{u}\mathrm{d}y\\&=\frac{1}{4\mu}\int_0^{\infty}\int_{-\infty}^{\infty}\exp\left[-\frac{uy^2}{4}+\frac{\mu y}{m}\right]\mathrm{d}y\,e^{-1/u}\frac{\mathrm{d}u}{u}=\frac{\pi^{1/2}}{2\mu}\int_0^{\infty}\exp\left[-\frac{1}{u}\left(1-\frac{\mu^2}{m^2}\right)\right]\frac{\mathrm{d}u}{u^{3/2}}\\&=\frac{\pi}{2\mu}\left(1-\frac{\mu^2}{m^2}\right)^{-1/2}.\end{aligned}$$

Let us turn now to h_3, one has

$$h_3(|x|)\leqslant|x|e^{\mu|x|}\int_{m|x|}^{\infty}K_0(y)e^{-\mu y/m}\,\mathrm{d}y\leqslant|x|\int_{m|x|}^{\infty}K_0(y)\mathrm{d}y\leqslant m|x_0|^2K_0(m|x_0|),$$

where $m|x_0|$ satisfies the transcendental equation $\int_z^{\infty}K_0(y)\mathrm{d}y=zK_0(z)$ with solution $z=0.745\,1315$. From this follows also that $m|x_0|K_0(m|x_0|)<\pi/2$ and hence

$$h_3(|x|)<\pi|x_0|/2\leqslant c\pi/2m,\quad c\in[0.745\,1315,\infty).$$

Collecting all the previous results we have the following estimate:

$$\begin{aligned}|(\sqrt{-\Delta+m^2}-E)^{-1}(|x|)|&\leqslant\frac{m}{4\pi|x|^2}\left[\left(1-\frac{\mu^2}{m^2}\right)^{1/2}\frac{1}{\mu}+\frac{2}{\pi}\left[1+\left(1-\frac{\mu^2}{m^2}\right)\left[\frac{\pi}{2\mu}\left(1-\frac{\mu^2}{m^2}\right)^{-1/2}+\frac{c\pi}{2m}\right]\right]\right]\\&\leqslant\frac{m}{4\pi|x|^2}\left[1+\frac{2}{\mu}+\frac{c}{m}\right].\end{aligned}\tag{C1}$$

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The multitime correlation functions, free white noise, and the generalized Poisson statistics in the low density limit

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In the present paper the low density limit of the nonchronological multitime correlation functions of boson number type operators is investigated. We prove that the limiting truncated nonchronological correlation functions can be computed using only a subclass of diagrams associated to noncrossing pair partitions and thus coincide with nontruncated correlation functions of suitable free number operators. The independent in the limit subalgebras are found and the limiting statistics is investigated. In particular, it is found that the cumulants of certain elements coincide in the limit with the cumulants of the Poisson distribution. An explicit representation of the limiting correlation functions and thus of the limiting algebra is constructed in a special case through suitably defined quantum white noise operators. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2178154]

I. INTRODUCTION

The reduced dynamics of a quantum open system interacting with a reservoir in certain physical regimes is approximated by Markovian master equations. These regimes include the weak system-reservoir interactions and dilute reservoirs and in the theoretical framework they are described by certain limits. For a weakly interacting system one considers the limit as the coupling constant goes to zero (weak coupling limit, WCL) whereas for a dilute reservoir one considers the limit as the density of the reservoir goes to zero (low density limit, LDL) and an appropriate time rescaling should be performed in order to get a nontrivial limit. The Markovian reduced dynamics in these limits is considered in the review papers by Spohn and Lebowitz.[1,2] The reduced dynamics in the LDL was considered in details later by Dümcke[3] using the method based on the quantum Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy.

The total dynamics in these limits is governed by various quantum stochastic equations. There is a unique up to now approach, called the *stochastic limit method*, which allows an efficient derivation of the stochastic equations in the WCL. This approach is based on the quantum white noise technique and was developed by Accardi, Lu, and Volovich.[4]

The convergence of the evolution operator of the total system in the LDL to a solution of a quantum stochastic equation was proved by Accardi and Lu[5] and by Rudnicki, Alicki, and Sadowski.[6] Recently the low density limit was investigated with the quantum white noise technique.[7,8] This technique, well developed for the WCL, was nontrivially modified to include the LDL and for this case was called *the stochastic golden rule for the low density limit*. This technique was applied to the derivation of the quantum stochastic equations in the LDL. An advantage of the obtained equations is that they, in contrast with the exact Schrödinger equation, are explicitly solvable. At the same time they provide a good approximation of the exact dynamics.

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The approach of Refs. 7 and 8 uses the so-called Fock–anti-Fock representation for the canonical commutation relations (CCR) algebra (this representation is unitary equivalent to the Gel'fand-Naimark-Segal representation). The difficulty with this approach is that the creation and annihilation operators in the Fock–anti-Fock Hilbert space do not describe creation and annihilation of physical particles and thus do not have direct physical meaning. To avoid this difficulty the investigation of the LDL directly in terms of the physical fields was performed.[9] Using this approach the chronological correlation functions in the LDL were found and the corresponding stochastic equations derived.

In the present paper we investigate the low density limit of the nonchronologically ordered correlation functions of boson number type operators. The investigation is related with *ab initio* derivations of quantum stochastic equations describing quantum dynamics of a test particle interacting with a dilute gas. We find the limiting truncated correlation functions of the number type operators and show that they can be computed by representing the number operators through creation and annihilation operators and then considering only a subclass of diagrams associated to noncrossing pair partitions. This fact allows to represent the limiting truncated correlation functions as the nontruncated correlation functions of number operators of a free quantum white noise thus making a connection with the Voiculescu free probability theory. We find the limiting statistics and show that the cumulants of certain elements coincide in the limit with the cumulants of the Poisson distribution.

The free probability theory was developed by Voiculescu around 1985 as a way to deal with von Neumann algebras of free groups. Then the theory was separated from this special context and began to develop as an independent field. In particular, applications of the free independence theory to random matrices were found. The details of free probability theory and its applications to random matrices could be found, for example, in Refs. 10 and 11.

Expectations of free random variables are characterized by diagrams associated to noncrossing pair partitions. The vanishing of crossing diagrams in the stochastic weak coupling limit for nonrelativistic QED and for the Anderson model was found in Refs. 4 and 12, respectively, thus making a connection between the WCL and free probability. The WCL is typically described by the quantum Boltzmann statistics.[4] In Ref. 13 a generalized version of Boltzmann commutation relations, the so-called entangled commutation relations, was found in the weak coupling limit for nonlinear interactions and possible applications to photon splitting cascades were discussed.

The investigation of the multitime nonchronologically ordered correlation functions could have a connection with the behavior of fluctuations in certain asymptotic regimes. The latter is described in the review paper by Andries, Benatti, De Cock, and Fannes.[14] In that approach the limiting statistics is defined in terms of ground state distribution determined by nontrivial pair partitions. The authors conjecture the appearance of exotic statistics in certain asymptotic regimes. The asymptotic fluctuations are the limiting correlation functions of appropriate centered elements and thus the results of the present paper could be applied to study the fluctuations in the low density limit.

In Sec. II the truncated nonchronologically ordered correlation functions are defined and their low density limit is established (Theorem 1). In Sec. III the irreducible diagrams (pair partitions) which contribute to the limiting correlation functions are found (Theorem 2). In Sec. IV the limiting truncated correlation functions are represented as correlation functions of a suitable free white noise. In Sec. V we identify the independent in the limit subalgebras (Theorem 4) and calculate the limiting cumulants which for some elements coincide with the cumulants of the Poisson distribution (Theorem 5). In Sec. VI an explicit representation of the limiting correlation functions and thus of the limiting algebra is constructed for a special case by using suitable quantum white noise operators.

II. THE CORRELATION FUNCTIONS IN THE LDL

We begin this section with construction of a general class of noncommutative probability spaces relevant for the investigation of the low density limit. The framework of a *-probability space is used. A relation between the objects defined in this section and the model of a test particle interacting with a dilute gas is given in Appendix A.

Definition 1: A *-probability space *is a pair* $(\mathcal{A},\omega)$, *where* $\mathcal{A}$ *is a unital* *-*algebra over* $\mathbb{C}$ *and* $\omega:\mathcal{A}\to\mathbb{C}$ *is a state, i.e., a linear normalized,* $\omega(1_{\mathcal{A}})=1$, *and strictly positive functional.*

Let $\mathcal{H}$ be a Hilbert space with inner product denoted by $\langle\cdot,\cdot\rangle$ (called as one particle Hilbert space), $\{S_t\}_{t\in\mathbb{R}}$ a one parameter unitary group in $\mathcal{H}$ (a one particle free evolution), $\hat{n}$ a bounded positive operator in $\mathcal{H}$ (density operator) such that $\forall t\in\mathbb{R}, S_{-t}\hat{n}S_t=\hat{n}$, and B a countable set of real numbers.

Let $\Gamma(\mathcal{H})$ be the symmetric Fock space over $\mathcal{H}$. For any trace class self-adjoint operator T acting in $\mathcal{H}$ we denote by $N(T)\equiv \mathrm{d}\Gamma(T)$ its second quantization operator in $\Gamma(\mathcal{H})$ and extend this definition by complex linearity to the set of all trace class operators $\mathcal{T}(\mathcal{H})$. For any $T\in\mathcal{T}(\mathcal{H}), \omega\in B$, and a positive number $\epsilon>0$ we define the following operator in $\Gamma(\mathcal{H})$:

$$N_{T,\omega,\epsilon}(t) := \frac{e^{-it\omega/\epsilon}}{\epsilon} N(S_{t/\epsilon}TS_{-t/\epsilon}). \tag{1}$$

Let $L(\mathbb{R})=\cap_{p\in\mathbb{N}}L^p(\mathbb{R})$, where $L^p(\mathbb{R})$ is the space of p-power integrable functions over $\mathbb{R}$. For any open subset $\Lambda\subseteq\mathbb{R}$ let $L(\Lambda)$ be the set of functions from $L(\mathbb{R})$ with support in Λ. We denote by $\mathcal{A}_{\Lambda,\epsilon}$ the *-algebra generated by operators $N_{T,\omega,\epsilon}(\varphi) := \int \mathrm{d}t\, \varphi(t)N_{T,\omega,\epsilon}(t)$ with $T\in\mathcal{T}(\mathcal{H})$, $\omega\in B$, $\varphi\in L(\Lambda)$ and denote $\mathcal{A}_{\epsilon} := \mathcal{A}_{\mathbb{R},\epsilon}$.

Let $A^{\pm}(g)$, $g\in\mathcal{H}$ be the creation and annihilation operators in $\Gamma(\mathcal{H})$ [we denote in the sequel $A^{-}(g)\equiv A(g)$] with the canonical commutation relations $[A(f),A^{+}(g)]=\langle f,g\rangle$ and let $\mathcal{A}_{\mathrm{CCR}}$ be the algebra of polynomials in $A^{\pm}(\cdot)$. Any operator $N(T)$ can be represented in terms of the creation and annihilation operators. For example, if $T=|f\rangle\langle g|$, where we use Dirac's notations for elements $f,g\in\mathcal{H}$, then $N(T)=A^{+}(f)A(g)$. An arbitrary operator $N(T)$ can be expressed in terms of $A^{\pm}$ using the fact that any trace class operator T is a limit of finite rank operators. Thus the algebra $\mathcal{A}_{\epsilon}$ is a subalgebra of $\mathcal{A}_{\mathrm{CCR}}$.

Let $\omega_{\hat{n}}$ be a Gaussian gauge-invariant mean-zero state on $\mathcal{A}_{\mathrm{CCR}}$ with the two point correlation function $\omega_{\hat{n}}(A^{+}(f)A(g)) := \langle g,\hat{n}f\rangle$ [thus $\omega_{\hat{n}}(N(T))=\mathrm{Tr}(\hat{n}T)$ and here we use the assumption for T being trace class]. Denoting by the same symbol its restriction to $\mathcal{A}_{\Lambda,\epsilon}$, we finally have for any $\epsilon>0$ and for any open subset $\Lambda\subseteq\mathbb{R}$ the *-probability space $(\mathcal{A}_{\Lambda,\epsilon},\omega_{\epsilon\hat{n}})$.

Remark 1: The condition $\forall t: S_{-t}\hat{n}S_t=\hat{n}$ *leads to the invariance of the state* $\omega_{\hat{n}}$ *under the free evolution generated by* S_t.

With the notations above we define the nonchronologically ordered multitime correlation functions as

$$W_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(t_1,\ldots,t_n) := \omega_{\epsilon\hat{n}}(N_{T_1,\omega_1,\epsilon}(t_1)\cdots N_{T_n,\omega_n,\epsilon}(t_n)), \tag{2}$$

$$W_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(\varphi_1,\ldots,\varphi_n) := \omega_{\epsilon\hat{n}}(N_{T_1,\omega_1,\epsilon}(\varphi_1)\cdots N_{T_n,\omega_n,\epsilon}(\varphi_n)). \tag{3}$$

We will use for the correlation functions (2) and (3) also the shorter notations $W_{\epsilon}(t_1,\ldots,t_n)$ and $W_{\epsilon}(\varphi_1,\ldots,\varphi_n)$. The reason for introducing the averaged operators $N_{T,\omega,\epsilon}(\varphi)$ and the averaged correlation functions (3) is that, as we will show below, the nonaveraged operators $N_{T,\omega,\epsilon}(t)$ and the correlation functions (2) in the limit as $\epsilon\to 0$ become singular distributions. Clearly, one has the relation

$$W_{\epsilon}(\varphi_1,\ldots,\varphi_n)=\int \mathrm{d}t_1\cdots\mathrm{d}t_n\, W_{\epsilon}(t_1,\ldots,t_n)\varphi_1(t_1)\cdots\varphi_n(t_n).$$

Definition 2: The truncated correlation functions $W^{\mathrm{T}}_{\epsilon}(t_1,\ldots,t_n)$ *are defined for* $n=1$ *by*

$W^{\mathrm{T}}_{\epsilon}(t_1) := W_{\epsilon}(t_1)$ *and for* $n>1$ *by induction through the relation:*

$$W_{\epsilon}(t_1,\ldots,t_n) = W^{\mathrm{T}}_{\epsilon}(t_1,\ldots,t_n) + \sum_{l=2}^{n}\sum_{n}{}' W^{\mathrm{T}}_{\epsilon}(t_{i_1},\ldots,t_{i_{k_1}}) \times W^{\mathrm{T}}_{\epsilon}(t_{i_{k_1+1}},\ldots,t_{i_{k_2}})\cdots W^{\mathrm{T}}_{\epsilon}(t_{i_{k_l}},\ldots,t_{i_n}),$$

where Σ'_n *is the sum over* $i_1<i_2<\cdots i_{k_1}$, $i_{k_1+1}<\cdots<i_{k_2},\ldots,<i_{k_l+1}<\cdots<i_n$.

The truncated correlation functions are often used in quantum field theory and in quantum kinetic theory.[15] They entirely determine the corresponding nonchronological correlation functions. Thus the investigation of the limit of the nonchronological correlation functions can be reduced to the investigation of the limit of the truncated correlation functions.

We define the "projection" $P_E := (2\pi)^{-1}\int \mathrm{d}t\, S_t e^{-itE}$ [it has the property $P_E P_{E'} = \delta(E-E')P_E$] and for any $k=1,2,\ldots,n$ denote $\tilde{\omega}_k = \omega_n+\cdots+\omega_k$. The following theorem states the low density limit of the truncated correlation functions.

Theorem 1: One has the limit in the sense of distributions in variables $t_1,\ldots,t_n$,

$$\lim_{\epsilon\to 0} W^{\mathrm{T}}_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(t_1,\ldots,t_n) = (2\pi)^{n-1}\delta(t_2-t_1)\cdots\delta(t_n-t_{n-1}) \times \delta_{\tilde{\omega}_1,0}\int \mathrm{d}E\,\mathrm{Tr}[\hat{n}P_{E+\tilde{\omega}_1}T_1 P_{E+\tilde{\omega}_2}T_2\cdots P_{E+\tilde{\omega}_n}T_n], \tag{4}$$

where Tr *denotes trace and* $\delta_{\tilde{\omega}_1,0}$ *is the Kronecker delta symbol.*

The theorem is a corollary of Theorem 2 from Sec. III.

III. THE NONTRIVIAL DIAGRAMS

In the present section we investigate the low density limit of the nonchronologically ordered correlation functions for the particular case of operators of the form $T_l = |f_l\rangle\langle g_l|$ and find the diagrams which are nontrivial in the low density limit.

In order to simplify the notations we will use the following energy representation for the creation and annihilation operators:

$$A^+_l := \frac{e^{-it_l E_l/\epsilon}}{\sqrt{\epsilon}} A^+(P_{E_l} f_l), \quad A_l := \frac{1}{\sqrt{\epsilon}} A(S_{t_l/\epsilon} g_l)$$

(a slightly different version of the energy representation was introduced in Ref. 7). One has $N_{T_l,\omega_l,\epsilon}(t_l) = e^{-it_l\omega_l/\epsilon}\int \mathrm{d}E_l\, A^+_l A_l$. Notice that the operator A^+_l is not the adjoint of A_l. The symbols A_l, A^+_l are used only to simplify the notations below.

A multitime correlation function can be expressed using Gaussianity of the state $\omega_{\hat{n}}$ and the energy representation for the creation and annihilation operators as

$$W_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(t_1,\ldots,t_n) = \exp\left(-i\sum_{l=1}^{n}\omega_l t_l/\epsilon\right)\sum{}' \int \mathrm{d}E_1\cdots\mathrm{d}E_n\, \omega_{\epsilon\hat{n}}(A^+_{i_1}A_{j_1})\cdots \times \omega_{\epsilon\hat{n}}(A^+_{i_k}A_{j_k})\omega_{\epsilon\hat{n}}(A_{j_{k+1}}A^+_{i_{k+1}})\cdots\omega_{\epsilon\hat{n}}(A_{j_n}A^+_{i_n}), \tag{5}$$

where Σ' is the sum over $k=1,\ldots,n$, $1=i_1<i_2<\cdots<i_k, j_{k+1}<\cdots<j_n$, $i_l \leqslant j_l$ for $l=1,\ldots,k$ and $j_l<i_l$ for $l=k+1,\ldots,n$. The sum contains terms of the form

$$\omega_{\epsilon\hat{n}}(A^+_{i_1}A_{j_1})\cdots\omega_{\epsilon\hat{n}}(A^+_{i_k}A_{j_k})\omega_{\epsilon\hat{n}}(A_{j_{k+1}}A^+_{i_{k+1}})\cdots\omega_{\epsilon\hat{n}}(A_{j_n}A^+_{i_n}). \tag{6}$$

To each such term we associate a diagram by pairing in the string $A^+_1A_1A^+_2A_2\cdots A^+_nA_n$ the operators $A^+_{i_l}$ and A_{j_l} for $l=1,2,\ldots,n$.

Definition 3: We say that the expression (6) *corresponds to a reducible diagram if there exists*

a nonempty subset $I \subset \{1,\ldots,n\}$ *(strict inclusion) such that* $i_l \in I \Leftrightarrow j_l \in I$. *Otherwise we say that the expression* (6) *corresponds to an irreducible diagram.*

An important property of the truncated correlation functions (Definition 2) is that they keep only all irreducible diagrams. The following are the examples of irreducible (first) and reducible (second) diagrams for $n=2$:

$$A_1^+ A_1 A_2^+ A_2 \qquad\qquad A_1^+ A_1 A_2^+ A_2 \tag{7}$$

Given a reducible diagram, one can represent the set $\{1,\ldots,n\}$ as a union of several disjoint subsets $I_1,\ldots,I_l$ such that the diagram contains only pairings between operators with indices from the same subsets. In this sense a general reducible diagram can be represented as a union of mutually disjoint irreducible diagrams. Examples of the truncated correlation functions, the corresponding irreducible diagrams, and their limits as $\epsilon \to 0$ for $n=1,2,3$ are given below.

Example 1: $n=1$. The invariance of the state under the free evolution leads to the identity $W_\epsilon^{\mathrm{T}}(t) = W_\epsilon(t) = W_\epsilon(0) = \langle g_1, \hat{n} f_1 \rangle$.

Example 2: $n=2$. One has

$$W_\epsilon^{\mathrm{T}}(t_1,t_2) = W_\epsilon(t_1,t_2) - W_\epsilon(t_1)W_\epsilon(t_2) = \int \mathrm{d}E_1\, \mathrm{d}E_2\, \omega_{\epsilon\hat{n}}(A_1^+ A_2)\omega_{\epsilon\hat{n}}(A_1 A_2^+)$$

$$= \int \mathrm{d}E_1\, \mathrm{d}E_2 \frac{e^{i(t_2-t_1)(E_2-E_1)/\epsilon}}{\epsilon} \langle g_2, P_{E_2}\hat{n} f_1\rangle \langle g_1, (1+\epsilon\hat{n}) P_{E_2} f_2\rangle. \tag{8}$$

This expression corresponds to the first (irreducible) diagram in (7) which is nonzero in the limit. Application of Lemma 1 (see Appendix B) to the right-hand side (rhs) of (8) gives

$$\lim_{\epsilon\to 0} W_\epsilon^{\mathrm{T}}(t_1,t_2) = 2\pi\delta(t_2-t_1) \int \mathrm{d}E \langle g_2, P_E \hat{n} f_1\rangle \langle g_1, P_E f_2\rangle.$$

Example 3: $n=3$. One has

$$W_\epsilon^{\mathrm{T}}(t_1,t_2,t_3) = \int \mathrm{d}E_1\, \mathrm{d}E_2\, \mathrm{d}E_3 [\omega_{\epsilon\hat{n}}(A_1^+ A_3)\omega_{\epsilon\hat{n}}(A_1 A_2^+)\omega_{\epsilon\hat{n}}(A_2 A_3^+) + \omega_{\epsilon\hat{n}}(A_1^+ A_2)\omega_{\epsilon\hat{n}}(A_1 A_3^+)\omega_{\epsilon\hat{n}}(A_2^+ A_3)].$$

This expression corresponds to the sum of the two irreducible diagrams:

$$A_1^+ A_1 A_2^+ A_2 A_3^+ A_3 + A_1^+ A_1 A_2^+ A_2 A_3^+ A_3$$

In this case only the first diagram is non-zero in the limit and Lemma 1 gives

$$\lim_{\epsilon\to 0} W_\epsilon^{\mathrm{T}}(t_1,t_2,t_3) = (2\pi)^2 \delta(t_3-t_2)\delta(t_2-t_1) \int \mathrm{d}E \langle g_3, P_E \hat{n} f_1\rangle \langle g_1, P_E f_2\rangle \langle g_2, P_E f_3\rangle.$$

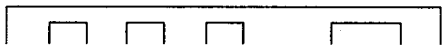
The case of arbitrary n is described by the following theorem.

Theorem 2: Let $T_l = |f_l\rangle\langle g_l|$, *where* $f_l, g_l \in \mathcal{H}$ *for* $l=1,2,\ldots,n$. *One has the limit in the sense of distributions in variables* $t_1,\ldots,t_n$,

$$\lim_{\epsilon\to 0} W^{\mathrm{T}}_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(t_1,\ldots,t_n) = (2\pi)^{n-1}\delta(t_2-t_1)\cdots\delta(t_n-t_{n-1})\delta_{\tilde{\omega}_1,0} \int \mathrm{d}E \langle g_n, P_E \hat{n} f_1\rangle$$

$$\times \langle g_1, P_{E+\tilde{\omega}_2} f_2\rangle \cdots \langle g_{n-1}, P_{E+\tilde{\omega}_n} f_n\rangle. \tag{9}$$

For each n only the following irreducible diagram is non zero as $\epsilon \to 0$:



$$A_1^+ A_1 A_2^+ A_2 A_3^+ A_3 A_4^+ \ldots A_{n-1} A_n^+ A_n \tag{10}$$

Proof: Case (a): $\omega_1 = \omega_2 = \cdots = \omega_n = 0$. Using the correlation functions

$$\omega_{\epsilon\hat{n}}(A_{i_\alpha}^+ A_{j_\alpha}) = e^{i(t_{i\alpha} - t_{j_\alpha})E_{i_\alpha}/\epsilon} \langle g_{j_\alpha}, \hat{n} f_{i_\alpha} \rangle,$$

$$\omega_{\epsilon\hat{n}}(A_{j_\beta} A_{i_\beta}^+) = \frac{e^{i(t_{i\beta} - t_{j_\beta})E_{i_\beta}/\epsilon}}{\epsilon} \langle g_{j_\beta}, (1 + \epsilon\hat{n}) f_{i_\beta} \rangle,$$

one can write (6) as

$$\frac{1}{\epsilon^n} \exp\{i[(t_1 - t_{j_1})E_1 + \cdots + (t_{i_n} - t_{j_n})E_{i_n}]/\epsilon\}(\epsilon^k F(E) + O(\epsilon^{k+1})), \tag{11}$$

where

$$F(E) = \prod_{l=1}^{k} \langle g_{j_l}, P_{E_l} \hat{n} f_{i_l} \rangle \prod_{l=k+1}^{n} \langle g_{j_l}, P_{E_{il}} f_{i_l} \rangle.$$

Define the permutations p_i and p_j of the set $(1, \ldots, n)$ by $p_i(l) = i_l$ and $p_j(l) = j_l$ for $l = 1, \ldots, n$ and let $p_\alpha = p_i p_j^{-1}$. Consider the expression in the square brackets in the exponent in (11). The term proportional to t_l in this expression has the form $t_l(E_l - E_{\alpha_l})$, where $\alpha_l = p_\alpha(l)$. Thus (11) can be written as

$$\frac{1}{\epsilon^n} \exp\{i[t_n(E_n - E_{\alpha_n}) + \cdots + t_1(E_1 - E_{\alpha_1})]/\epsilon\}(\epsilon^k F(E) + O(\epsilon^{k+1}))$$

and with the notations $\Omega_l(E) = E_n + \cdots + E_l - E_{\alpha_n} - \cdots - E_{\alpha_l}$ for $l = 2, \ldots, n$ as

$$\frac{e^{i(t_n - t_{n-1})\Omega_n(E)/\epsilon}}{\epsilon} \cdots \frac{e^{i(t_2 - t_1)\Omega_2(E)/\epsilon}}{\epsilon} (\epsilon^{k-1} F(E) + O(\epsilon^k)). \tag{12}$$

If the expression (6) corresponds to an irreducible diagram then the functions $\Omega_l(E)$ are linearly independent and, since they are linear in their arguments, the convolution $\delta(\Omega_2(E)) \cdots \delta(\Omega_n(E))$ is well defined.

In the case $k > 1$, since for any $l = 2, \ldots, n$ (see Lemma 1),

$$\lim_{\epsilon \to 0} \frac{e^{i(t_l - t_{l-1})\Omega_l(E)/\epsilon}}{\epsilon} = 2\pi \delta(t_l - t_{l-1}) \delta(\Omega_l(E)) \tag{13}$$

and $k - 1 > 0$, the limit of (12) equals zero.

In the case $k = 1$ the expression (6) corresponds to the diagram (10) and one has

$$\omega_{\epsilon\hat{n}}(A_1^+ A_n) \omega_{\epsilon\hat{n}}(A_1 A_2^+) \cdots \omega_{\epsilon\hat{n}}(A_{n-1} A_n^+)$$

$$= \frac{e^{i(t_n - t_{n-1})\Omega_n(E)/\epsilon}}{\epsilon} \cdots \frac{e^{i(t_2 - t_1)\Omega_2(E)/\epsilon}}{\epsilon} (F(E) + O(\epsilon)), \tag{14}$$

where $\Omega_l(E) = E_l - E_1$. Using (13) one finds that the limit of the rhs of (14) is

$$(2\pi)^{n-1} \delta(t_2 - t_1) \cdots \delta(t_n - t_{n-1}) \delta(E_2 - E_1) \cdots \delta(E_n - E_1)$$

$$\times\langle g_n, P_{E_1}\hat{n}f_1\rangle\langle g_1, P_{E_2}f_2\rangle\cdots\langle g_{n-1}, P_{E_n}f_n\rangle.$$

Integration over $E_1\cdots E_n$ gives the equality (9) in the case (a).

Case (b): arbitrary $\omega_1,\ldots,\omega_n$. In this case the expression (14) in the decomposition (5) is multiplied by the factor $\exp(-i\Sigma_l\omega_l t_l/\epsilon)$. The product can be written as

$$\frac{e^{i(t_n-t_{n-1})(\Omega_n(E)-\tilde{\omega}_n)/\epsilon}}{\epsilon}\cdots\frac{e^{i(t_2-t_1)(\Omega_2(E)-\tilde{\omega}_2)/\epsilon}}{\epsilon}e^{-it_1\tilde{\omega}_1/\epsilon}(F(E)+O(\epsilon)).$$

If $\tilde{\omega}_1=0$ then the statement of the theorem follows by the same arguments as in the case (a). If $\tilde{\omega}_1\neq 0$ then the limit of this term equals to zero by Riemann-Lebesgue lemma due to the presence of the rapidly oscillating factor $\exp(-it_1\tilde{\omega}_1/\epsilon)$. □

IV. THE FREE WHITE NOISE NUMBER OPERATORS

In the present section we show that the limiting truncated correlation functions coincide with the complete (i.e., nontruncated) correlation functions of the free white noise number operators.

Definition 4: Free white noise operators $N_T(t)$ *are the operators satisfying the multiplication rule*

$$N_T(t)N_{T'}(t') = \delta(t-t')N_{T*T'}(t), \tag{15}$$

*where the *-product of operators T and T' is defined by* $T*T' := 2\pi\int \mathrm{d}E\, P_E T P_E T'$.

Remark 2: *We call the operators $N_T(t)$ as* free (or Boltzmann) number operators *since they can be constructed using the creation and annihilation operators $B_f^{\pm}(t)$ satisfying the free relations $B_f^-(t)B_g^+(t')=2\pi\delta(t-t')\langle f,g\rangle$. In fact, define $N_{|f\rangle\langle g|}(t) := \int \mathrm{d}E\, B^+_{P_{Ef}}(t)B^-_{P_{Eg}}(t)$ and extend this definition by linearity to any T. Then such defined operators satisfy the relation* (15).

Let $\mathcal{A}$ be the algebra generated by the free white noise operators $N_T(t)$ and let $\phi_{\hat{n}}$ be the state on $\mathcal{A}$ characterized by $\phi_{\hat{n}}(N_T(t))=Tr(\hat{n}T)$.

Theorem 3: *One has the equality*

$$\lim_{\epsilon\to 0} W^{\mathrm{T}}_{\epsilon,\hat{n},T_1,0,\ldots,T_n,0}(t_1,\ldots,t_n) = \phi_{\hat{n}}(N_{T_1}(t_1)\cdots N_{T_n}(t_n)). \tag{16}$$

Proof: By direct calculations using the Eq. (4) and the relation (15).

The existence of the representation of the limiting truncated correlation functions by the free white noise number operators is related to the fact that only a subclass of the noncrossing irreducible diagrams survives in the low density limit. We emphasize however, that the left-hand side (lhs) of Eq. (16) is the limit of a truncated correlation function whereas the rhs contains the complete correlation function.

V. INDEPENDENCE AND THE GENERALIZED POISSON STATISTICS IN THE LDL

The fact that the limiting truncated correlation functions are the distributions in variables $t_1,\ldots,t_n$ with support at $t_1=\cdots=t_n$ leads to the appearance of independent subalgebras in the low density limit. In the beginning of this section we remind the basic notions of independent subalgebras and of cumulants. Then we find the asymptotically independent subalgebras of $\mathcal{A}_\epsilon$ and discuss the limiting statistics. We show that the cumulants and the moments of certain elements in the algebra $\mathcal{A}_\epsilon$ in the low density limit coincide with the cumulants and the moments of the Poisson distribution.

Definition 5: *Let $(\mathcal{A},\omega)$ be a *-probability space. A family of unital *-subalgebras $\{\mathcal{A}_i\}_{i\in I}$, $\mathcal{A}_i\subset\mathcal{A}$, is called* independent *if $\omega(a_1\cdots a_n)=0$ whenever $a_l\in\mathcal{A}_{i_l}, \omega(a_l)=0$, and $k\neq l$ implies $i_k\neq i_l$.*

Definition 6: *Let $(\mathcal{A},\omega)$ be a *-probability space*. Cumulants *of the space $(\mathcal{A},\omega)$ are the multilinear functionals $\kappa_n:\mathcal{A}^n\to\mathbb{C}, n\geq 1$, uniquely determined by $\kappa_1(a):=\omega(a), a\in\mathcal{A}$, and for $n>1$ by induction through the relation*

$$\omega(a_1 \cdots a_n) = \sum_{\pi,\pi=:\{A_1,\ldots,A_k\}} \kappa_{|A_j|}((a_1,\ldots,a_n)|A_j),$$

where the sum is over all partitions π *of the set* $\{1,\ldots,n\}$ *and* "$(a_1,\ldots,a_n)|A$" *designates the set of* a_i *with* $i \in A$.

Remark 3: The cumulants $\kappa_n^{(\epsilon)}$ *for a *-probability space* $(\mathcal{A}_\epsilon, \omega_{\epsilon\hat{n}})$ *are directly related to the truncated correlation functions. Namely, if* $a_1 = N_{T_1,\omega_1,\epsilon}(\varphi_1), \ldots, a_n = N_{T_n,\omega_n,\epsilon}(\varphi_n)$, *then* $\kappa_n^{\epsilon}(a_1,\ldots,a_n) = W^{\mathrm{T}}_{\epsilon,\hat{n},T_1,\omega_1,\ldots,T_n,\omega_n}(\varphi_1,\ldots,\varphi_n)$.

For the analysis of independence in the low density limit we introduce the notion of asymptotically independent subalgebras for a *-probability space $(\mathcal{A}_\epsilon, \omega_{\epsilon\hat{n}})$.

Definition 7: Let $(\mathcal{A}_\epsilon, \omega_{\epsilon\hat{n}})$ *be a *-probability space for the LDL. We say that a family of subalgebras* $\mathcal{A}_{1,\epsilon},\ldots,\mathcal{A}_{l,\epsilon}$ *of* $\mathcal{A}_\epsilon$ *is* asymptotically independent *if*

$$\lim_{\epsilon\to 0} \omega_{\epsilon\hat{n}}(a_1,\ldots,a_n) = 0$$

whenever $a_l \in \mathcal{A}_{i_l,\epsilon}, \omega_{\epsilon\hat{n}}(a_l) = 0$, *and* $k \neq l$ *implies* $i_k \neq i_l$.

The next theorem identifies asymptotically independent subalgebras of $\mathcal{A}_\epsilon$.

Theorem 4: *Let* $\Lambda_1,\ldots,\Lambda_l$ *be a family of disjoint open subsets in* $\mathbb{R}$. *Then the family of subalgebras* $\mathcal{A}_{\Lambda_1,\epsilon},\ldots,\mathcal{A}_{\Lambda_l,\epsilon}$ *is asymptotically independent*.

The proof follows from the fact that the truncated correlation functions become in the limit as $\epsilon \to 0$ distributions in variables $t_1,\ldots,t_n$ with support at $t_1 = t_2 = \cdots = t_n$. □

Now let us analyze the statistics which appears in the low density limit. From Theorem 1 and the relation between the cumulants and the truncated correlation functions it follows that lth cumulant for the element $a = N_{T,\omega,\epsilon}(\varphi)$ in the limit has the form

$$\kappa_l(a,\ldots,a) := \lim_{\epsilon\to 0} W^{\mathrm{T}}_{\epsilon,\hat{n},T,\omega,\ldots,T,\omega}(\varphi,\ldots,\varphi) = \frac{1}{2\pi}\delta_{\omega,0}\int \mathrm{d}t\,\mathrm{d}E\,\mathrm{Tr}\,\hat{n}[2\pi\varphi(t)P_E T]^l. \tag{17}$$

We specify the further consideration to the case $\mathcal{H} = L^2(\mathbb{R}^3)$. Consider $\hat{n} = 1$ (identity operator) and $S_t = e^{itH_1}$ where H_1 is the multiplication operator by the function $\omega(\mathbf{k}) = |\mathbf{k}|^2$, $\mathbf{k} \in \mathbb{R}^3$. Let T_λ be the integral operator in $\mathcal{H}$ with the kernel $T_\lambda(\mathbf{k},\mathbf{k}') = (2\pi\sqrt{|\mathbf{k}||\mathbf{k}'|})^{-1}\chi_{[0,\sqrt{\lambda}]}(|\mathbf{k}|)\chi_{[0,\sqrt{\lambda}]}(|\mathbf{k}'|)$, where λ is a positive number and $\chi_{[0,\sqrt{\lambda}]}$ is the characteristic function of the interval $[0,\sqrt{\lambda}]$. Let $\varphi_0(t) = (2\pi)^{-1}\chi_{[0,2\pi]}(t)$.

Theorem 5: *Let* $a_\lambda = N_{T_\lambda,\omega,\epsilon}(\varphi_0)$, *where* T_λ *and* φ_0 *are defined as above. Then for any* $l \in \mathbb{N}$ *one has*

$$\kappa_l(a_\lambda,\ldots,a_\lambda) = \lambda\,\delta_{\omega,0}.$$

Thus, the cumulants of the element a_λ *in the case* $\omega = 0$ *coincide in the low density limit with the cumulants of the Poisson distribution with expectation equal to* λ.

Proof: The proof of the theorem is based on the direct calculation of the cumulants using Eq. (17). One has

$$\frac{1}{2\pi}\int \mathrm{d}t[2\pi\varphi_0(t)]^l = 1.$$

One also has

$$\int \mathrm{d}E\,\mathrm{Tr}\,\hat{n}[P_E T_\lambda]^l = \int \mathrm{d}E \int \mathrm{d}\mathbf{k}_1\cdots\mathrm{d}\mathbf{k}_l\,\delta(|\mathbf{k}_1|^2 - E)T_\lambda(\mathbf{k}_1,\mathbf{k}_2)$$

$$\times\,\delta(|\mathbf{k}_2|^2 - E)T_\lambda(\mathbf{k}_2,\mathbf{k}_3)\cdots\delta(|\mathbf{k}_l|^2 - E)T_\lambda(\mathbf{k}_l,\mathbf{k}_1)$$

$$= \int \mathrm{d}E \left[T_\lambda(\sqrt{E}, \sqrt{E}) \int \mathrm{d}\mathbf{k}\ \delta(|\mathbf{k}|^2 - E) \right]^l = \int \mathrm{d}E\ \chi_{[0,\sqrt{\lambda}]}(\sqrt{E}) = \lambda .$$

Thus the rhs of Eq. (17) equals $\lambda \delta_{\omega,0}$. This proves the theorem. □

Moments of the element a_λ in the case $\omega=0$ in the low density limit are equal to the sum over all partitions of the limiting cumulants and given by Touchard polynomials,

$$\lim_{\epsilon \to 0} \omega_{\epsilon \hat{n}}(a_\lambda^n) = \sum_{k=1}^{n} S(n,k) \lambda^k,$$

where $S(n,k)$ is a Stirling number of the second kind, i.e., the number of partitions of a set of size n into k disjoint nonempty subsets. The limiting moments coincide with the moments of the Poisson distribution with expectation equal to λ. For a_1 one has

$$\lim_{\epsilon \to 0} \omega_{\epsilon \hat{n}}(a_1^n) = B_n,$$

where B_n is the nth Bell number, i.e., the number of partitions of a set of size n. The Bell numbers are the moments of the Poisson distribution with expectation equal to 1.

VI. AN OPERATOR REPRESENTATION OF THE LIMITING CORRELATION FUNCTIONS

In the present section we explicitly realize the limiting correlation functions as correlation functions of certain operators acting in a suitable Hilbert space. Presence of delta functions in the limiting correlation functions suggests that they can be represented as correlation functions of certain white noise operators. Here such a representation is constructed in the special case using the results of Ref. 7.

Let $g_0, g_1 \in \mathcal{H}$ satisfy the condition $\langle g_0, S_t g_1 \rangle = 0$ for any $t \in \mathbb{R}$. Define for $n,m=0,1$ the Hilbert space $\mathcal{K}_{nm} := L^2(\mathrm{Spec}\, H_1, \mathrm{d}\mu_{nm})$, where $\mathrm{Spec}\, H_1 \subset \mathbb{R}$ is the spectrum of H_1 and $\mathrm{d}\mu_{nm} := \langle g_n, P_E g_n \rangle \langle g_m, P_E \hat{n} g_m \rangle \mathrm{d}E$. Let $\mathcal{K} := \oplus_{n,m=0,1} \mathcal{K}_{nm}$ and let $\mathcal{H}_{\mathrm{WN}} := \Gamma(L^2(\mathbb{R}, \mathcal{K}))$ be the symmetric Fock space over the Hilbert space of square integrable $\mathcal{K}$-valued functions on $\mathbb{R}$ (abbreviation WN here stands for white noise). Using the natural decomposition $\mathcal{H}_{\mathrm{WN}} = \oplus_{n,m=0,1} \Gamma(L^2(\mathbb{R}, \mathcal{K}_{nm}))$ one can define the creation and annihilation operator valued distributions $B^{\pm}_{m,n}(E,t)$ acting in $\mathcal{H}_{\mathrm{WN}}$ and satisfying the canonical commutation relations

$$[B^-_{m,n}(E,t), B^+_{m',n'}(E',t')] = 2\pi \delta(t'-t) \delta(E'-E) \langle g_m, P_E g_{m'} \rangle \langle g_{n'}, P_E \hat{n} g_n \rangle. \tag{18}$$

The operator valued distributions $B^{\pm}_{m,n}(E,t)$ are called time-energy quantum white noise due to the presence of $\delta(t'-t)\delta(E-E')$ in (18). Let us define the number operators,

$$\tilde{N}_{m,n}(E,t) := \sum_{n'=0,1} \frac{1}{\langle g_{n'}, P_E \hat{n} g_{n'} \rangle} B^+_{m,n'}(E,t) B^-_{n,n'}(E,t)$$

and denote $N_{g_m, g_n}(t) := \int \mathrm{d}E [\tilde{N}_{m,n}(E,t) + B^-_{n,m}(E,t) + B^+_{m,n}(E,t)]$. Let $\Omega \in \mathcal{H}_{\mathrm{WN}}$ be the vacuum vector.

Theorem 6: *Let* $T_1 = |g_{m_1}\rangle\langle g_{n_1}|, \ldots, T_k = |g_{m_k}\rangle\langle g_{n_k}|$, *where* $m_1, n_1, \ldots, m_k, n_k \in \{0,1\}$. *One has the equality*

$$\lim_{\epsilon \to 0} W_{\epsilon, \hat{n}, T_1, 0, \ldots, T_k, 0}(t_1, \ldots, t_k) = \langle \Omega, N_{g_{m_1}, g_{n_1}}(t_1) \cdots N_{g_{m_k}, g_{n_k}}(t_k) \Omega \rangle. \tag{19}$$

Proof. The right-hand side of (19) has the form

$$\langle \Omega, N_{g_{m_1},g_{n_1}}(t_1)\cdots N_{g_{m_k},g_{n_k}}(t_k)\Omega\rangle = \int \mathrm{d}E_1\cdots \mathrm{d}E_k \langle \Omega, [\tilde{N}_{m_1,n_1}(E_1,t_1) + B^-_{m_1,n_1}(E_1,t_1) + B^+_{m_1,n_1}(E_1,t_1)]\cdots [\tilde{N}_{m_k,n_k}(E_k,t_k) + B^-_{n_k,m_k}(E_k,t_k) + B^+_{m_k,n_k}(E_k,t_k)]\Omega\rangle$$

Let us denote $\tilde{N}_{m,n}(t) := \int \mathrm{d}E\, \tilde{N}_{m,n}(E,t)$. The truncated correlation function corresponds to the term

$$\int \mathrm{d}E\, \mathrm{d}E' \langle \Omega, B^-_{n_1,m_1}(E,t_1)\tilde{N}_{m_2,n_2}(t_2)\tilde{N}_{m_3,n_3}(t_3)\cdots \tilde{N}_{m_{k-1},n_{k-1}}(t_{k-1})B^+_{m_k,n_k}(E',t_k)\Omega\rangle. \tag{20}$$

Notice that $\tilde{N}_{m,n}(t)\Omega = 0$. Therefore (20) equals

$$\int \mathrm{d}E\, \mathrm{d}E' \langle \Omega, [\cdots [[B^-_{n_1,m_1}(E,t_1), \tilde{N}_{m_2,n_2}(t_2)], \tilde{N}_{m_3,n_3}(t_3)]\cdots \tilde{N}_{m_{k-1},n_{k-1}}(t_{k-1})]B^+_{m_k,n_k}(E',t_k)\Omega\rangle.$$

The commutators can be calculated by induction using the canonical commutation relations (18). The result is

$$(2\pi)^{k-2}\delta(t_2-t_1)\cdots\delta(t_{k-1}-t_{k-2})\int \mathrm{d}E\, \mathrm{d}E' \langle g_{n_1}, P_E g_{m_2}\rangle\cdots\langle g_{n_{k-2}}, P_E g_{m_{k-1}}\rangle \times \langle \Omega, B^-_{n_{k-1},m_1}(E,t_{k-1})B^+_{m_k,n_k}(E',t_k)\Omega\rangle. \tag{21}$$

The last two-point correlation function can be calculated using the commutation relations (18). This gives for (21) the expression

$$(2\pi)^{k-1}\delta(t_2-t_1)\cdots\delta(t_k-t_{k-1})\int \mathrm{d}E \langle g_{n_1}, P_E g_{m_2}\rangle\cdots\langle g_{n_{k-1}}, P_E g_{m_1}\rangle\langle g_{n_k}, P_E \hat{n} g_{m_1}\rangle$$

which coincides with the rhs of (9) in the case $\omega_1 = \cdots = \omega_k = 0$.

Remark 4: The limiting correlation functions could be represented as expectations of certain quantum white noise operators in the general case if one could construct a Hilbert space $\mathcal{H}_{\mathrm{WN}}$, *a vector* $\Omega \in \mathcal{H}_{\mathrm{WN}}$, *and operator valued distributions* $B^{\pm}_{f,g}(E,t)$ *and* $\tilde{N}_{f,g}(E,t)$ *in* $\mathcal{H}_{\mathrm{WN}}$ *with the property* $B^-_{f,g}(E,t)\Omega = \tilde{N}_{f,g}(E,t)\Omega = 0$ *and satisfying the commutation relations*

$$[B^-_{f,g}(E,t), B^+_{f',g'}(E',t')] = 2\pi\delta(t'-t)\delta(E'-E)\langle f, P_E f'\rangle\langle g', P_E \hat{n} g\rangle, \tag{22}$$

$$[B^-_{f,g}(E,t), \tilde{N}_{f',g'}(E',t')] = 2\pi\delta(t'-t)\delta(E-E')\langle f, P_E f'\rangle B^-_{g',g}(E,t), \tag{23}$$

$$[\tilde{N}_{f,g}(E,t), \tilde{N}_{f',g'}(E',t')] = 2\pi\delta(t'-t)\delta(E'-E)[\langle g, P_E f'\rangle N_{f,g'}(E,t) - \langle g', P_E f\rangle N_{f',g}(E,t)]. \tag{24}$$

Suppose there exist such operators. Define $N_{f,g}(t) := \int \mathrm{d}E[\tilde{N}_{f,g}(E,t) + B^-_{g,f}(E,t) + B^+_{f,g}(E,t)]$. *Then one can prove exactly in the same way as in Theorem 6 that*

$$\lim_{\epsilon\to 0} W_{\epsilon,\hat{n}|f_1\rangle\langle g_1|,0,\ldots,|f_n\rangle\langle g_n|,0}(t_1,\ldots,t_n) = \langle \Omega, N_{f_1,g_1}(t_1)\cdots N_{f_n,g_n}(t_n)\Omega\rangle.$$

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APPENDIX A

Here we make a connection between the objects defined in Sec. II and the model of a test particle interacting with a dilute Bose gas (see Ref. 9 for details).

The one particle Hilbert space for this model has the form $\mathcal{H}\equiv L^2(\mathbb{R}^3)$, where $\mathbb{R}^3$ is the three-dimensional coordinate or momentum space. The one particle free evolution is a unitary group $S_t\equiv e^{itH_1}$ whose generator H_1 in the momentum representation is the multiplication operator by the function $\omega(\mathbf{k})=|\mathbf{k}|^2/2m$, where m is the mass of a gas particle. The test particle is characterized by its Hilbert space $\mathcal{H}_S$ and its free Hamiltonian H_S acting in $\mathcal{H}_S$ which is assumed to have a discrete spectrum. The discrete set B is the set of all transition frequencies of the test particle, or equivalently, the spectrum of its free Liouvillean $-i[H_S,\cdot]$.

The dynamics of a test particle interacting with a gas is described by an evolution operator $U(t)$ acting in $\mathcal{H}_S\otimes\Gamma(\mathcal{H})$ and satisfying in the interaction picture, after the time rescaling $t\rightarrow t/\epsilon$, the following Schrödinger equation:

$$\frac{\mathrm{d}U(t/\epsilon)}{\mathrm{d}t}=-i\left[\sum_{l,\omega}Q_{l,\omega}\otimes N_{T_l,\omega,\epsilon}(t)\right]U(t/\epsilon). \tag{A1}$$

Here $Q_{l,\omega}$ are certain operators in $\mathcal{H}_S$ such that $[H_S,Q_{l,\omega}]=-\omega Q_{l,\omega}$ and T_l are certain operators in $\mathcal{H}$. The explicit form of these operators is determined by the details of the microscopic interaction between the test particle and particles of the gas. Equation (A1) is the place where the operators $N_{T,\omega,\epsilon}(t)$ appear.

The condition $S_{-t}\hat{n}S_t=\hat{n}$ and positivity of $\hat{n}$ imply that for this model $\hat{n}$ is a multiplication operator by a function $n:\mathbb{R}^3\rightarrow[0,\infty)$. The value $n(\mathbf{k})$ has the meaning of the density of gas particles at momentum $\mathbf{k}$. If the state of the gas is $\omega_{\epsilon\hat{n}}$ then the density of gas particles and the rate of collisions between the test particle and the gas are of order ϵ. Thus the limit $\epsilon\rightarrow 0$ is the low density limit. The limit is nontrivial since the dynamics is studied on the kinetic time scale of order $1/\epsilon$.

APPENDIX B

Let $S(\mathbb{R})$ be the Schwartz space over $\mathbb{R}$ and let $S'(\mathbb{R})$ be the dual space of distributions. We reproduce the following lemma from Ref. 4.

Lemma 1: One has the limit in $S'(\mathbb{R})\times S'(\mathbb{R})$,

$$\lim_{\epsilon\rightarrow 0}\frac{e^{itx/\epsilon}}{\epsilon}=2\pi\delta(t)\delta(x),$$

Proof: Let $f,\phi\in S(\mathbb{R})$ and let $\tilde{f}$ be Fourier transform of f, $\tilde{f}(\tau)=\int\mathrm{d}x\,e^{i\tau x}f(x)$. One has the identifies

$$I:=\lim_{\epsilon\rightarrow 0}\int\mathrm{d}t\,\mathrm{d}x\frac{e^{itx/\epsilon}}{\epsilon}f(x)\phi(t)=\lim_{\epsilon\rightarrow 0}\int\mathrm{d}\tau\,\phi(\epsilon\tau)\int\mathrm{d}x\,e^{i\tau x}f(x)=\lim_{\epsilon\rightarrow 0}\int\mathrm{d}\tau\,\phi(\epsilon\tau)\tilde{f}(\tau).$$

Since $\tilde{f}\in S(\mathbb{R})$, the function $\phi(\epsilon\tau)\tilde{f}(\tau)$ satisfies the conditions of the Lebesgue lemma which allows to exchange the limit and integration in the last expression. Thus

$$I=\phi(0)\int\mathrm{d}\tau\,\tilde{f}(\tau)=2\pi\phi(0)f(0).$$

□

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Anyons, group theory and planar physics

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Relativistic and nonrelativistic anyons are described in a unified formalism by means of the coadjoint orbits of the symmetry groups in the free case as well as when there is an interaction with a constant electromagnetic field. To deal with interactions we introduce the extended Poincaré and Galilei Maxwell groups.
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I. INTRODUCTION

The first works, of a rather theoretical character, devoted to particles with an arbitrary spin and statistics in (2+1) dimensions go back to 1977,[1] but the real interest in physics behind the anyons started some years later when the fractional quantum Hall effect was explained just in terms of anyons.[2]

In the last years some works analyzing the role of the Galilei and Poincaré groups in (2+1) dimensions in the theory of anyons have appeared in the literature.[3–10] Although the usual group theoretical considerations fit well when the anyons are free, this is not the case when the action of an external electromagnetic field is considered.[11] However, recently[12,13] we have introduced two noncentral extensions of the Poincaré and Galilei groups by homogeneous and constant electromagnetic fields, called Maxwell groups[14,15] that seem to provide an appropriate group theoretical framework for anyons in the presence of constant fields. Our intention here is to adopt this viewpoint to present a unified approach for these kinds of interacting systems in 2-space +1-time dimensions which can also involve noncommuting coordinates. In this context we mention a recent work[16] where the authors also obtain, in a different way, the extended Galilei-Maxwell group (called by them "enlarged Galilei group").

The paper has been organized as follows. In the first two sections we revise the Poincaré and Galilei groups to recover the main features of the free relativistic and nonrelativistic anyons and fix the notation. As in all the cases presented along this paper, we have made a systematic use of the coadjoint orbit method that supply us with a canonical setup of classical systems bearing enough symmetry in terms of the corresponding symmetry group; in particular, for the Galilei group we have taken into account its double central extension. In the next two sections we deal with interacting anyons and constant electromagnetic fields. First, in Sec. IV within a relativistic frame, while the nonrelativistic situation is considered in the following section, where we also discuss how to perform the nonrelativistic limit. As we mentioned before the groups involved in our analysis are certain noncentral extensions of the Galilei and Poincaré groups where the key point is that electromagnetic fields take part as dynamical objects. Some conclusions and comments on the main differences with other approaches end the paper.

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We have also added two Appendixes for the sake of completness. In the first Appendix we give a brief review about the symplectic structures associated to a Lie group. In the second Appendix we supply a classification of orbits for the space $\mathcal{GM}^*(2+1)$ dual to the Lie algebra of the Galilei-Maxwell group.

II. ANYONS AND THE POINCARÉ GROUP

The Poincaré group $P(2+1)$, is a six-dimensional (6D) Lie group of transformations of the $(2+1)$-D Minkowski space-time provided with the metric tensor $g_{ij}=\mathrm{diag}(1,-1,-1)$. Two spatial Cartesian axes will be denoted by X_1 and X_2.

Our $(2+1)$-D system may be seen as embedded in the $(3+1)$-D Minkowski space-time equipped with the metric tensor $g_{ij}=\mathrm{diag}(1,-1,-1,-1)$. Then, the third spatial axis perpendicular to the X_1X_2 plane will be denoted by X_3. We will make use of this embedding; for example, a rotation on the plane X_1X_2 may be considered as the rotation around X_3. In that case vectors on the spatial plane are thought to be three-dimensional (3D) objects.

Each element of $P(2+1)$ is parametrized by a pair (a,Λ), where $a=(b,a_1,a_2)$ represents a time (b) and space (a_1,a_2) translation, and Λ a Lorentz transformation. The element Λ can be factorized as $\Lambda=\Lambda(\chi,\vec{n})\Lambda(R_\phi)$, with $\Lambda(\chi,\vec{n})$ being a boost of rapidity χ in the direction of the unit planar vector $\vec{n}$ and $\Lambda(R_\phi)$ denoting a rotation of angle ϕ around the axis X_3.

The Lie algebra $\mathcal{P}(2+1)$ of the Poincaré group $P(2+1)$ is spanned by the basis $\{P_0\equiv H,P_1,P_2,K_1,K_2,J\}$, which are the infinitesimal generators of time and space translations, boosts transformations along axes X_1, X_2, and X_3 rotations, respectively. The nonvanishing commutators are

$$[H,K_i]=-P_i,\quad [P_i,K_i]=-H,\quad [P_i,J]=-\varepsilon_{ij}P_j,$$

$$[K_i,K_j]=-\varepsilon_{ij}J,\quad [K_i,J]=-\varepsilon_{ij}K_j,\quad i,j=1,2, \tag{2.1}$$

where ε_{ij} denotes the 2D completely skew-symmetric tensor.

A. Coadjoint orbits

Let (h,p_1,p_2,k_1,k_2,j) be the coordinates of an arbitrary point of $\mathcal{P}^*(2+1)$, the dual space of $\mathcal{P}(2+1)$, in a basis dual to $\{H,P_1,P_2,K_1,K_2,J\}$. The coadjoint action of $P(2+1)$ on $\mathcal{P}^*(2+1)$ is given by[17]

$$g:(h,p_1,p_2,k_1,k_2,j)\to(h',p_1',p_2',k_1',k_2',j'),\quad g=(b,a_1,a_2,\Lambda(\chi,\vec{n}),\Lambda(R_\phi)),$$

$$h'=\cosh\chi h-\sinh\chi\vec{n}\cdot\vec{p}^{\,\phi},$$

$$\vec{p}\,'=\vec{p}^{\,\phi}-\sinh\chi h\vec{n}+(\cosh\chi-1)(\vec{n}\cdot\vec{p}^{\,\phi})\vec{n},$$

$$\begin{aligned}\vec{k}'=&\vec{k}^{\,\phi}+\sinh\chi\vec{j}\times\vec{n}^{\pi/2}-(\cosh\chi-1)(\vec{n}^{\pi/2}\cdot\vec{k}^{\,\phi})\vec{n}^{\pi/2}\\&+b[\vec{p}^{\,\phi}-\sinh\chi h\vec{n}+(\cosh\chi-1)(\vec{n}\cdot\vec{p}^{\,\phi})\vec{n}]+\vec{a}[\cosh\chi h-\sinh\chi\vec{n}\cdot\vec{p}^{\,\phi}],\end{aligned}$$

$$\vec{j}\,'=\cosh\chi\vec{j}+\sinh\chi\vec{n}\times\vec{k}^{\,\phi}+\vec{a}\times[\vec{p}^{\,\phi}-\sinh\chi h\vec{n}+(\cosh\chi-1)(\vec{n}\cdot\vec{p}^{\,\phi})\vec{n}], \tag{2.2}$$

where we have used the following notation:

$$\vec{n}=(n_1,n_2,0),\quad \vec{p}=(p_1,p_2,0),\quad \vec{k}=(k_1,k_2,0),\quad \vec{a}=(a_1,a_2,0),\quad \vec{j}=(0,0,j), \tag{2.3}$$

and $\vec{x}^{\,\phi}$ stands for the rotation of a vector $\vec{x}$ around the axis X_3 by an angle ϕ.

The invariants of the coadjoint action (2.2) are

$$C_1 = \rho^2 = g^{\mu\nu}\rho_\mu\rho_\nu = h^2 - p_1^2 - p_2^2, \quad C_2 = h\vec{j} + \vec{p} \times \vec{k}, \tag{2.4}$$

where $\rho=(h,p_1,p_2)$ and $g_{\mu\nu}=\mathrm{diag}(1,-1,-1)$.

The invariant C_2 is in fact a 3D vector, but its only nonzero component is the third one, equal to $hj+p_1k_2-k_1p_2$. It is a lower dimensional version of the Pauli-Lubanski four-vector. Recall that in (3+1)-D Minkowski space-time the Pauli-Lubanski vector w takes the form

$$w = (w^0, \mathbf{w}) = (\mathbf{j}\cdot\mathbf{p}, h\mathbf{j} + \mathbf{p}\times\mathbf{k}), \tag{2.5}$$

where now the involved vectors are generic 3D. The scalar w^2 is invariant under the (3+1)-Poincaré group action. In (2+1) dimensions the Pauli-Lubanski vector reduces to the expression (2.4) of C_2.

The classification of the coadjoint orbits was published in Refs. 17 and 18. There are orbits of dimension 4, 2, and 0 (points). The four-dimensional (4D) orbits are divided in three classes,

(i) $C_1>0$ relativistic particles of a mass $\sqrt{C_1}$,
(ii) $C_1<0$ tachyons,
(iii) $C_1=0$, $\vec{p}\neq 0$ massless particles.

We will consider the strata of orbits with $C_1>0$. Rewriting $C_1=m^2$, where m is the rest mass of the particle, the invariant C_1 leads to the equation of a hyperboloid of two sheets $h^2-p_1^2-p_2^2-m^2=0$. We will restrict to that one of positive energy $h>0$, denoted H_m^+, as usual. For the second invariant, we rewrite $C_2=m\vec{s}$, where

$$\vec{s} = \frac{h\vec{j} + \vec{p}\times\vec{k}}{\sqrt{h^2 - p_1^2 - p_2^2}}. \tag{2.6}$$

The nontrivial component of $\vec{s}$ is the spin s of the system.

B. Symplectic structure

The two independent invariants m and s fix, in the way presented above, a coadjoint orbit $\mathcal{O}_{m,s}^+$ that constitutes a 4D differentiable submanifold of $\mathcal{P}^*(2+1)$. Moreover, we can cover $\mathcal{O}_{m,s}^+$ with one chart $(\mathcal{O}_{m,s}^+,\varphi)$ using as coordinates (p_1,p_2,k_1,k_2). Indeed, the Jacobian of the transformation

$$(h,p_1,p_2,k_1,k_2,j) \to (C_1,C_2,p_1,p_2,k_1,k_2)$$

being $(2h^2)^{-1}$, it is always positive on the sheet H_m^+. On the orbits $\mathcal{O}_{m,s}^+$ there is a natural Poisson structure (A5)—see Appendix A—given by

$$\Lambda = h\frac{\partial}{\partial k_i} \wedge \frac{\partial}{\partial p_i} - j\frac{\partial}{\partial k_1} \wedge \frac{\partial}{\partial k_2}. \tag{2.7}$$

The symplectic form related with the tensor Λ is

$$\omega = -\frac{1}{h}\mathrm{d}k_i \wedge \mathrm{d}p_i - \frac{j}{h^2}\mathrm{d}k_1 \wedge \mathrm{d}k_2, \tag{2.8}$$

where, according to (2.4),

$$h = +\sqrt{\vec{p}^2 + m^2}, \quad j = \frac{ms - p_1k_2 + p_2k_1}{\sqrt{\vec{p}^2 + m^2}}. \tag{2.9}$$

The coordinates, p_i, k_i, $i=1,2$ are not canonical since their Poisson brackets are

$$\{k_1,k_2\}=-j,\quad \{p_1,p_2\}=0,\quad \{k_i,p_j\}=h\delta_{ij}. \tag{2.10}$$

The equations of the time evolution obtained from the law of motion (A6) with the Hamiltonian (2.9) are

$$\dot{p}_i=0,\quad \dot{k}_i=p_i,\quad i=1,2. \tag{2.11}$$

They look like the equations of motion of a nonrelativistic free particle.

We find a set of canonical coordinates $\{\vec{p},\vec{q}\}$, where

$$\vec{q}=\frac{\vec{k}}{h}-\frac{\vec{p}\times\vec{s}}{h(m+h)} \tag{2.12}$$

and the expression for the angular momentum becomes

$$j=\frac{ms}{h}+\vec{q}\times\vec{p}+\frac{ms}{h(m+h)}\vec{p}^2. \tag{2.13}$$

Now, if we identify q_i as position coordinates, the equations of motion are the well-known relations

$$\dot{p}_i=0,\quad \dot{q}_i=\frac{p_i}{h},\quad i=1,2. \tag{2.14}$$

A detailed analysis of the different coordinate systems for anyons can be found in Ref. 19.

C. Irreducible unitary representations

In quantum mechanics the coadjoint orbits of a Lie group allow us to define the irreducible unitary representations (IUR) associated to quantum elementary physical systems having such a symmetry group. Thus, the IUR's of $P(2+1)$ associated to the stratum of orbits $\mathcal{O}^+_{m,s}$ are

$$[U_{m,s}(a,\Lambda)]\psi(p)=e^{ip\cdot a}e^{is\theta(p,\Lambda)}\psi(\Lambda^{-1}p), \tag{2.15}$$

where s is the quantum number labelling a representation of SO(2) and $\theta(p,\Lambda)$ is the Wigner angle, which is determined by the little group of a point of the orbit. More explicitly, choosing the point $p_m=(m,0,0)$, whose isotropy group is SO(2), and the boost elements $\Lambda_{p\to p'}\in \mathrm{SO}(2,1)$ transforming the point p into p', then

$$\theta(p,\Lambda)=\Lambda^{-1}_{p_m\to\Lambda(p)}\Lambda\Lambda_{p_m\to p}. \tag{2.16}$$

The functions $\psi(p)$ belong to the Hilbert space $\mathcal{H}=\mathcal{L}^2(H^+_m,\mathrm{d}\mu(p))$, being $\mathrm{d}\mu(p)$ the SO(2,1)-invariant measure in H^+_m.

The differential realization of the generators for this representation is

$$\hat{H}=h,\quad \hat{P}_i=p_i,\quad \hat{K}_j=i(h\partial_{p_j}+p_j\partial_h)+\frac{\varepsilon^{jk}p_k}{2m}s,\quad \hat{J}=i(p_2\partial_{p_1}-p_1\partial_{p_2})+\frac{h}{m}s. \tag{2.17}$$

The two Casimirs corresponding to the invariants (2.4), $C_1=\hat{P}^2$ and $C_2=\hat{H}\cdot\hat{J}+\hat{\vec{P}}\times\hat{\vec{K}}$, give the following equations:

$$(p^2-m^2)\psi(p)=0,\quad (h\hat{J}+\hat{\vec{P}}\times\hat{\vec{K}}-ms)\psi(p)=0. \tag{2.18}$$

The first one corresponds to the mass shell condition which gives rise to the Klein-Gordon equation. The second one is the Pauli-Lubanski equation describing the spin of the particle. In two dimensions the unitarity of the realizations does not impose restrictions on the values of s, thus allowing for the existence of anyons. In this way we easily recover results of Ref. 4.

III. NONRELATIVISTIC ANYONS AND THE GALILEI GROUP

In the nonrelativistic case we must deal with the Galilei group $G(2+1)$ in $(2+1)$-D, which can be seen as a contraction of the Poincaré group $P(2+1)$. The commutation rules of its Lie algebra $\mathcal{G}(2+1)$ are those of Poincaré (2.1) except that now

$$[K_1,K_2]=0, \quad [K_i,P_j]=0, \quad i,j=1,2. \tag{3.1}$$

The algebra $\mathcal{G}(2+1)$ admits a 2D central extension $\bar{\mathcal{G}}(2+1)$ characterized by the new commutators[20,21]

$$[P_i,K_j]=-\delta_{ij}M, \quad [K_1,K_2]=\mathcal{K}, \tag{3.2}$$

where M and $\mathcal{K}$ are central generators, i.e., $[M,\cdot]=[\mathcal{K},\cdot]=0$ for any element of $\mathcal{G}(2+1)$.

Both extensions can also be obtained by a contraction from the Poincaré group.[21,22] It is enough to consider the direct product $\tilde{P}(2+1)=\mathbb{R}^2\otimes P(2+1)$. Obviously, at the level of the Lie algebra we have $\tilde{\mathcal{P}}(2+1)=\mathbb{R}^2\oplus\mathcal{P}(2+1)$. Hence, a basis is constituted by the generators of $\mathbb{R}^2$ $(M,\mathcal{K})$ plus the known generators of the Poincaré algebra (H,P_1,P_2,K_1,K_2,J). Let us consider a new basis given by

$$M'=M, \quad \mathcal{K}'=\mathcal{K}, \quad H'=H-M, \quad P_i'=P_i, \quad K_i'=K_i, \quad J'=J+\mathcal{K}, \quad i=1,2. \tag{3.3}$$

The nonvanishing commutators of $\tilde{\mathcal{P}}(2+1)$ in this new basis are

$$[H',K_i']=-P_i', \quad [P_i',K_i']=-H'-M', \quad [P_i',J']=-\varepsilon_{ij}P_j',$$

$$[K_i',K_j']=-\varepsilon_{ij}(J'-\mathcal{K}'), \quad [K_i',J']=-\varepsilon_{ij}K_j', \quad i,j=1,2. \tag{3.4}$$

Now in order to perform the contraction we define an appropriate rescaled basis

$$M''=\epsilon^2M', \quad \mathcal{K}''=\epsilon^2\mathcal{K}', \quad H''=H', \quad P_i''=\epsilon P_i', \quad K_i''=\epsilon K_i', \quad J''=J', \tag{3.5}$$

where ϵ is a fixed real positive number. The nonvanishing Lie commutators are now

$$[H'',K_i'']=-P_i'', \quad [P_i',K_i']=-\epsilon^2\left(H''+\frac{1}{\epsilon^2}M''\right), \quad [P_i'',J'']=-\varepsilon_{ij}P_j'',$$

$$[K_i'',K_j'']=-\varepsilon_{ij}\epsilon^2\left(J''-\frac{1}{\epsilon^2}\mathcal{K}''\right), \quad [K_i'',J'']=-\varepsilon_{ij}K_j'', \quad i,j=1,2.$$

In the limit $\epsilon\to 0$ we recover the Lie commutators of the extended algebra $\bar{\mathcal{G}}(2+1)$.

To give a physical interpretation of the contraction procedure we identify the contraction parameter ϵ with the inverse of the light speed $(\epsilon=1/c)$. From a cohomological point of view a change of the basis defined by relations (3.3)–(3.5) corresponds to introducing a trivial two-cocycle on the Poincaré group. After the contraction $\epsilon\to 0$ this trivial two-cocyle becomes a nontrivial one of the Galilei group.[23]

A. Coadjoint orbits

By $\bar{\mathcal{G}}^*(2+1)$ we will denote the space dual to the algebra $\bar{\mathcal{G}}(2+1)$. Each vector belonging to $\bar{\mathcal{G}}^*(2+1)$ is characterized by eight components $(m,\kappa,h,p_1,p_2,k_1,k_2,j)$ in the basis dual to $(M,\mathcal{K},H,P_1,P_2,K_1,K_2,J)$ of $\bar{\mathcal{G}}(2+1)$.

Let us denote by $g=(\theta,\eta,b,\vec{a},\vec{v},R_\phi)$ the elements of $\bar{G}(2+1)$, with a convention similar to that of Poincaré $\mathcal{P}(2+1)$ except that $\vec{v}$ stands for the Galilean boosts, and (θ,η) parametrize the group elements generated by $(M,\mathcal{K})$. The coadjoint action of $g\in\bar{G}(2+1)$ on the dual space $\bar{\mathcal{G}}^*(2+1)$ is given by[21]

$$m'=m,$$

$$\kappa'=\kappa,$$

$$h'=h-\vec{v}\cdot\vec{p}^{\phi}+\tfrac{1}{2}m\vec{v}^2,$$

$$\vec{p}'=\vec{p}^{\phi}-m\vec{v},$$

$$\vec{k}'=\vec{k}^{\phi}+b\vec{p}^{\phi}+m(\vec{a}-b\vec{v})+\vec{v}\times\vec{\kappa},$$

$$\vec{j}'=\vec{j}+\vec{a}\times\vec{p}^{\phi}+\vec{v}\times\vec{k}^{\phi}-\tfrac{1}{2}\kappa\vec{v}^2-m\vec{a}\times\vec{v}, \tag{3.6}$$

where we have also used the notation

$$\vec{p}=(p_1,p_2,0),\quad \vec{v}=(v_1,v_2,0),\quad \vec{k}=(k_1,k_2,0),\quad \vec{a}=(a_1,a_2,0),\quad \vec{\kappa}=(0,0,\kappa),\quad \vec{j}=(0,0,j).$$

The invariants of the coadjoint action (3.6), besides m and κ, are

$$C_1=\vec{p}^2-2mh,\quad C_2=m\vec{j}-\vec{\kappa}h+\vec{p}\times\vec{k}. \tag{3.7}$$

Note that the first one can be written as $U=-C_1/2m$ and is interpreted as the internal energy of the physical system. As in the relativistic case we denote $C_2=m\vec{s}$, but now

$$\vec{s}=\vec{j}-\frac{\vec{\kappa}h}{m}+\frac{\vec{p}\times\vec{k}}{m}. \tag{3.8}$$

It is easy to derive the expressions (3.7) from their relativistic counterparts (2.4) following the contraction procedure outlined above (see also Ref. 22). Obviously, expression (3.8) is the nonrelativistic limit of (2.6).

The classification of the coadjoint orbits (4D, 2D, and 0D) was presented in Ref. 21. The relevant 4D orbits characterized by the values $\{m\neq 0,\kappa,U,s\}$ are denoted by $\mathcal{O}^{\kappa,U}_{m,s}$. In the following we will assume $\kappa\neq 0$, since the results for $\kappa=0$ can be obtained directly.

B. Symplectic structure

A set of coordinates adapted to the orbit $\mathcal{O}^{\kappa,U}_{m,s}$ are $(m,\kappa,U,s,p_1,p_2,x_1,x_2)$, where $x_i=k_i/m$. Since the transformation

$$(m,\kappa,h,p_1,p_2,k_1,k_2,j)\rightarrow(m,\kappa,U,s,p_1,p_2,x_1=k_1/m,x_2=k_2/m)$$

has a nonzero Jacobian (as long as $m\neq 0$!), we can cover the whole orbit $\mathcal{O}^{\kappa,U}_{m,s}$ with one chart $(\mathcal{O}^{\kappa,U}_{m,s},\varphi)$ using coordinates (p_1,p_2,x_1,x_2). The induced Poisson tensor Λ on the orbit $\mathcal{O}^{\kappa,U}_{m,s}$ takes the form

$$\Lambda=\frac{\partial}{\partial x_i}\wedge\frac{\partial}{\partial p_i}+\frac{\kappa}{m^2}\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2},\quad i=1,2. \tag{3.9}$$

The inverse of Λ gives the symplectic form ω on $\mathcal{O}^{\kappa,U}_{m,s}$,

$$\omega = \mathrm{d}x_i \wedge \mathrm{d}p_i + \frac{\kappa}{m^2}\mathrm{d}x_1 \wedge \mathrm{d}x_2, \quad i = 1,2. \tag{3.10}$$

The coordinates $(\vec{p},\vec{x})$ are not canonical since their Poisson brackets are

$$\{x_1,x_2\} = \frac{\kappa}{m^2}, \quad \{p_1,p_2\} = 0, \quad \{x_i,p_j\} = \delta_{ij}. \tag{3.11}$$

Nevertheless, the Hamiltonian

$$h = \frac{\vec{p}^2}{2m} + U \tag{3.12}$$

has the usual form of a free nonrelativistic particle, leading to the motion equations

$$\dot{\vec{p}} = 0, \quad \dot{\vec{x}} = \frac{\vec{p}}{m}. \tag{3.13}$$

We see that the dynamics of the particle is independent of the parameter κ because the Hamiltonian function (3.12) does not contain any function of $\vec{x}$. Equations (3.13) are consistent with (3.6) if we assume that the parameter b represents the time and the coadjoint action gives the relation between the coordinates in two different inertial frames. Indeed, let the laboratory frame Σ' and the (instantaneous) rest frame Σ of the particle be related by the element $g=(t,\vec{a},-\vec{v},0) \in G(2+1)$. Then, Eqs. (3.6) can be read as

$$\vec{p}_{\Sigma'} = m\vec{v}, \quad \vec{x}_{\Sigma'} = t\frac{\vec{p}_{\Sigma'}}{m} - \frac{\vec{p}_{\Sigma'}}{m^2} \times \vec{\kappa} + \vec{a}. \tag{3.14}$$

The angular momentum is given by

$$j = \vec{x} \times \vec{p} + \frac{\vec{\kappa}}{m}\left(\frac{\vec{p}^2}{2m} + U\right) + s \tag{3.15}$$

which is the nonrelativistic limit of (2.13).

A set of canonical coordinates $(\vec{p},\vec{q})$ can be straightforwardly obtained from $(\vec{p},\vec{k})$ by

$$q_i = x_i + \frac{\varepsilon_{ij}\kappa p_j}{2m^2}. \tag{3.16}$$

It is worth to consider (3.16) as the nonrelativistic limit of the corresponding ones (2.12) for Poincaré. The coadjoint action of the Galilei group $G(2+1)$ in these coordinates is expressed by formulas

$$\vec{p}\,' = \vec{p}^{\,\phi} - m\vec{v},$$

$$\vec{q}\,' = \vec{q}^{\,\phi} + \frac{b}{m}\vec{p}^{\,\phi} + (\vec{a} - b\vec{v}) + \frac{1}{2m}\vec{v} \times \vec{\kappa}. \tag{3.17}$$

Although κ does not affect the dynamics, it gives the contribution $(1/2m)\vec{v}\times\vec{\kappa}$ to $\vec{q}$. The time evolution of canonical variables is given by [cf. (3.13)]

$$\dot{p}_i = 0, \quad \dot{q}_i = p_i, \quad i = 1,2. \tag{3.18}$$

Note that in the coordinates $(\vec{p},\vec{q})$ the angular momentum takes the form

$$\vec{j} = \vec{q} \times \vec{p} + \frac{\vec{\kappa} U}{m} + s, \tag{3.19}$$

where κ gives rise to an extra term. Similarly to (3.14) equations (3.17) give now

$$\vec{p} = m\vec{v}, \quad \vec{q} = t\frac{\vec{p}}{m} - \frac{\vec{p}}{2m^2} \times \vec{\kappa} + a. \tag{3.20}$$

The κ term is the only one that remains without a clear physical interpretation in the free case.[21,24]

C. Irreducible unitary representations

The IUR of $G(2+1)$ associated to this stratum of orbits are[21]

$$[U^{\kappa,U}_{m,s}(g)]\psi(\vec{p}) = e^{i([(1/2m)\vec{p}^2+U]b-\vec{p}\cdot\vec{a})} e^{i\kappa[(1//2m)\vec{v}\times\vec{p}]} e^{i[s+\kappa(U/m)]\phi} \psi(R^{-1}(\phi)(\vec{p}-m\vec{v})), \tag{3.21}$$

where $R(\phi)$ is a rotation of angle ϕ. The carrier space of the representation is the Hilbert space $\mathcal{H}=\mathcal{L}^2(\mathbb{R}^2)$. Note that the differential realization of the generators in this representation is

$$\hat{P}_j = p_j, \quad \hat{K}_j = im\partial_{p_j} - \frac{\kappa}{2m}\varepsilon^{jk}p_k, \quad \hat{H} = \frac{1}{2m}\vec{p}^2 + U, \quad \hat{J} = i(p_2\partial_{p_1} - p_1\partial_{p_2}) + s + \kappa U. \tag{3.22}$$

After a global change of phase, $U'(g)=\lambda(g)U(g)$, the IUR $U^{\kappa,U}_{m,s}$ is shown to be equivalent to $U^{\kappa,0}_{m,0}$.

It is worth mentioning that we can consider massless particles in the Galilean framework. In this case their 4D coadjoint orbits are characterized by $(m=0, \kappa\neq 0)$ and the invariants $C_1=\vec{p}^2 \neq 0$ and $C_2=\vec{p}\times\vec{k}-\kappa h$. If we compare C_2 with the relativistic Pauli-Lubanski operator for $m=0$ in (2.18), $(h\hat{J}+\hat{\vec{P}}\times\hat{\vec{K}}-C_2)\psi(p)=0$, we see that C_2 gives the helicity of our system, while J is now replaced by κ. We remark that this case is not equivalent to that of the orbit $(m=0, \kappa=0)$, and that in the present context the Hamiltonian becomes linear in $\vec{p}$. However, one must be careful about the interpretation since the coordinates $(\vec{k},\vec{p})$ are not canonical (see also Ref. 4).

The IUR associated to the null-mass orbits are

$$[U^{\kappa}_{C_1,C_2}(g)]\psi(\vec{w},\theta) = e^{i\kappa\left(\frac{1}{2}\vec{w}\times\vec{y}\right)} e^{i\vec{p}\cdot(\vec{a}-b\vec{y})} e^{-i(C_2/2\kappa)b} \psi(\vec{y}-\vec{w},\theta-\phi), \tag{3.23}$$

where $\vec{p}=\sqrt{C_1}(\cos\theta,\sin\theta)$ and $\psi\in\mathcal{L}^2(\mathbb{R}^2\times S^1)$.

IV. RELATIVISTIC ANYONS IN AN EXTERNAL ELECTROMAGNETIC FIELD

Once revisited the description of free anyons, in the next sections we will analyze the more interesting case when charged particles move in a constant electromagnetic field. The presence of external forces modifies the symmetry group of the system. This is the reason why instead of the Poincaré $P(2+1)$ and Galilei $G(2+1)$ groups, we will consider the so-called Poincaré-Maxwell PM$(2+1)$ and Galilei-Maxwell GM$(2+1)$ groups.[14,15]

Let us start with the relativistic case. The Poincaré-Maxwell group PM$(2+1)$ is a nine-dimensional (9D) Lie group with six infinitesimal generators $\{H,P_1,P_2,K_1,K_2,J\}$, corresponding to $P(2+1)$, plus three new elements $\{B,E_1,E_2\}$ related to the electromagnetic field.[14] It can be considered as a 3D noncentral extension of the Poincaré group. The nonvanishing commutators for its Lie algebra, $\mathcal{PM}(2+1)$, are

$$[B,K_i]=\varepsilon_{ij}E_j, \quad [E_i,K_j]=-\varepsilon_{ij}B, \quad [E_i,J]=-\varepsilon_{ij}E_j,$$

$$[H,P_i]=E_i,\quad [H,K_i]=-P_i,\quad [P_i,P_j]=-\varepsilon_{ij}B,$$

$$[P_i,K_j]=-\delta_{ij}H,\quad [P_i,J]=-\varepsilon_{ij}P_j,\quad [K_i,K_j]=-\varepsilon_{ij}J,$$

$$[K_i,J]=-\varepsilon_{ij}K_j,\quad i,j=1,2. \tag{4.1}$$

A. Coadjoint orbits

We will denote by $(\beta,\epsilon_1,\epsilon_2,h,p_1,p_2,k_1,k_2,j)$ the coordinates fixing a point on $\mathcal{PM}^*(2+1)$ by means of the dual basis of $(B,E_1,E_2,H,P_1,P_2,K_1,K_2,J)$. The general formula expressing the coadjoint action of a group element $g=(c,\vec{d},b,\vec{a},\Lambda(\chi,\vec{n})\Lambda(R_\phi))\in PM(2+1)$ on $\mathcal{PM}^*(2+1)$ is given by

$$\vec{\beta}'=(\cosh\chi)\vec{\beta}+(\sinh\chi)(\vec{n}\cdot\vec{\epsilon}^{\phi})\vec{n}^{\pi/2},$$

$$\vec{\epsilon}'=\vec{\epsilon}-(\sinh\chi)(\vec{\beta}\times\vec{n}^{\pi/2})+(\cosh\chi-1)(\vec{n}^{\pi/2}\cdot\vec{\epsilon}^{\phi})\vec{n}^{\pi/2},$$

$$h'=(\cosh\chi)h-(\sinh\chi)(\vec{n}\cdot\vec{p}^{\phi})-\vec{a}\cdot\vec{\epsilon}',$$

$$\vec{p}'=\vec{p}^{\phi}-(\sinh\chi)h\vec{n}+(\cosh\chi-1)(\vec{n}\cdot\vec{p}^{\phi})\vec{n}+b\vec{\epsilon}'-\vec{\beta}'\times\vec{a},$$

$$\vec{k}'=\vec{k}^{\phi}-(\sinh\chi)\vec{j}\times\vec{n}^{\pi/2}+(\cosh\chi-1)(\vec{n}^{\pi/2}\times\vec{k}^{\phi})\vec{n}^{\pi/2}$$
$$+b\vec{p}'-\tfrac{1}{2}b^2\vec{\epsilon}'+h'\vec{a}+\tfrac{1}{2}\vec{a}^2\vec{\epsilon}'-\vec{\beta}'\times\vec{d}-\vec{c}\times\vec{\epsilon}',$$

$$\vec{j}'=(\cosh\chi)\vec{j}+(\sinh\chi)(\vec{n}\times\vec{k}^{\phi})+\vec{a}\times\vec{p}'+\tfrac{1}{2}\vec{a}^2\vec{\beta}'+\vec{d}\times\vec{\epsilon}', \tag{4.2}$$

where the notation used is the same as in (2.3) with the additional vectors

$$\vec{\beta}=(0,0,\beta),\quad \vec{\epsilon}=(\epsilon_1,\epsilon_2,0),\quad \vec{c}=(0,0,c),\quad \vec{d}=(d_1,d_2,0).$$

The parameters c, d_1, and d_2 describe the group elements generated by B, E_1, and E_2, respectively. Notice that (h,p_1,p_2) represents the 3D energy-momentum vector covariant under (2+1) Lorentz transformations.

The invariants under the coadjoint action (4.2) are

$$C_0=\vec{\epsilon}^2-\vec{\beta}^2,$$

$$C_1=h^2-\vec{p}^2-2(\vec{k}\cdot\vec{\epsilon}-\vec{j}\cdot\vec{\beta}),$$

$$C_2=h\vec{\beta}+\vec{p}\times\vec{\epsilon}. \tag{4.3}$$

The first one is, of course, the invariant of the electromagnetic field under Lorentz transformations, $C_0=-F_{\mu\nu}F^{\mu\nu}$, where $F_{0i}=\epsilon_i$ and $F_{12}=\beta$. If $C_0>0$, $C_0<0$ or $C_0=0$ we say that the electromagnetic field (or the orbit) is of electric, magnetic, or perpendicular type, respectively.

The second invariant C_1 describes the interaction: it includes the electric coupling term $\vec{k}\cdot\vec{\epsilon}$, and the coupling of angular momentum and magnetic field, $\vec{j}\cdot\vec{\beta}$. The last invariant C_2 from (4.3) admits a covariant expression $C_2=-\varepsilon^{\mu\nu\sigma}p_\mu F_{\nu\sigma}$. It has no immediate interpretation, but its appearance is a consequence of the symmetries of the system.

Since we have three independent invariants the maximal dimension of the coadjoint orbits is six. In this work we will be concerned only with this kind of orbits, henceforth denoted $\mathcal{O}^{C_0}_{C_1C_2}$.

B. Symplectic structure

A suitable chart of coordinates for the points of the 9D differentiable manifold $\mathcal{PM}^*(2+1)$ is given by $(C_0,C_1,C_2,\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)$. Each 6D orbit $\mathcal{O}^{C_0}_{C_1C_2}$ can be covered with just one chart $(\mathcal{O}^{C_0}_{C_1C_2},\varphi)$ with coordinates $(\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)$. Indeed, from (4.3) we find that the Jacobian of the transformation

$$(\beta,h,j,\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)\to(C_0,C_1,C_2,\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)$$

equals $4\beta^3$. A singularity appears if $\beta=0$, but we shall deal here only with orbits of magnetic type $(\beta\neq 0)$.

In the chart $(\mathcal{O}^{C_0}_{C_1C_2},\varphi)$ the Poisson tensor Λ takes the form

$$\Lambda=-\beta\frac{\partial}{\partial\epsilon_1}\wedge\frac{\partial}{\partial k_2}+\beta\frac{\partial}{\partial\epsilon_2}\wedge\frac{\partial}{\partial k_1}-\beta\frac{\partial}{\partial p_1}\wedge\frac{\partial}{\partial p_2}-h\frac{\partial}{\partial p_1}\wedge\frac{\partial}{\partial k_1}-h\frac{\partial}{\partial p_2}\wedge\frac{\partial}{\partial k_2}-j\frac{\partial}{\partial k_1}\wedge\frac{\partial}{\partial k_2},\tag{4.4}$$

where β,h,j are functions of the coordinates obtained from relations (4.3). To make easy further comparisons with the nonrelativistic case we will represent it as a matrix (using the previous order of the coordinates)

$$\Lambda^{ij}=\begin{pmatrix}0&0&0&0&0&-\beta\\0&0&0&0&\beta&0\\0&0&0&-\beta&-h&0\\0&0&\beta&0&0&-h\\0&-\beta&h&0&0&-j\\\beta&0&0&h&j&0\end{pmatrix}\tag{4.5}$$

whose determinant is β^6. The symplectic two-form is

$$\omega=\frac{h^2-j\beta}{\beta^3}\mathrm{d}\epsilon_1\wedge\mathrm{d}\epsilon_2+\frac{h}{\beta^2}\mathrm{d}\epsilon_1\wedge\mathrm{d}p_1+\frac{1}{\beta}\mathrm{d}\epsilon_1\wedge\mathrm{d}k_2\frac{h}{\beta^2}\mathrm{d}\epsilon_2\wedge\mathrm{d}p_2-\frac{1}{\beta}\mathrm{d}\epsilon_2\wedge\mathrm{d}k_1+\frac{1}{\beta}\mathrm{d}p_1\wedge\mathrm{d}p_2.\tag{4.6}$$

Such a symplectic form is not canonical: the nonvanishing Poisson brackets are

$$\{\epsilon_i,k_l\}=-\varepsilon_{il}\beta,\quad\{p_i,p_l\}=\varepsilon_{il}\beta,\quad\{p_i,k_l\}=-\delta_{il}h,\quad\{k_i,k_l\}=-\varepsilon_{il}j,\quad i,l=1,2.\tag{4.7}$$

In order to find the equations of motion we need to know the Hamiltonian of the system. From the invariant C_2 [see (4.3)] we get

$$h=\frac{C_2}{\beta}+\frac{\vec{\epsilon}\times\vec{p}}{\beta},\tag{4.8}$$

where from (4.3) we can write $\beta=\sqrt{\vec{\epsilon}^2-C_0}$. Thus, we obtain

$$\dot{\epsilon}_i=0,\quad\dot{p}_i=-\epsilon_i,\quad\dot{k}_i=p_i,\quad i=1,2.\tag{4.9}$$

Equations (4.9) are extremely simple. The first one says that the fields are constant. The others look like the equations of motion for a nonrelativistic particle with a unit negative charge inside an electric field. Comparing the time evolution from these formulas with the transformation rules

(4.2) we can identify the time t with the parameter b. This is natural because b is associated to the Hamiltonian generator H.

Let us remark that the above relations are quite different from the usual ones derived from the standard Hamiltonian formalism. In that approach the Hamilton function is

$$H=\sqrt{m^2+\left(\vec{\pi}+\tfrac{1}{2}\vec{\beta}\times\vec{r}\right)^2}-\vec{\epsilon}\cdot\vec{r}, \tag{4.10}$$

where m denotes the mass of the particle and $\vec{r}$ its vector of position, being $(\vec{\pi},\vec{r})$ canonically conjugated variables. Then, the equations of motion are

$$\dot{\vec{\pi}}=\vec{\epsilon}-\frac{1}{2}\dot{\vec{r}}\times\vec{\beta},\quad \dot{\vec{r}}=\frac{1}{\mathcal{E}}\left(\vec{\pi}+\frac{1}{2}\vec{\beta}\times\vec{r}\right), \tag{4.11}$$

with $\mathcal{E}=H+\vec{\epsilon}\cdot\vec{r}$ the energy of the system. But, the "group" coordinates $\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2$ have not a simple interpretation in terms of $\vec{\pi}$ and $\vec{r}$ (4.11). In fact, there is not a punctual transformation relating both pictures. We shall comment on this problem more carefully in the last section.

V. NONRELATIVISTIC ANYONS IN AN EXTERNAL ELECTROMAGNETIC FIELD

The magnetic limit[25] of the Poincaré-Maxwell group, that we call Galilei-Maxwell group,[15] is the most suitable to describe nonrelativistic anyons in the presence of external covariant fields.

The Galilei-Maxwell group is a 10-dimensional (10D) Lie group, whose infinitesimal generators are those of $G(2+1)$, $\{H,P_1,P_2,K_1,K_2,J\}$, together with $\{E_1,E_2,B,M\}$. However, here, we will take into account also the central extension characterized by the nonvanishing commutator $[K_1,K_2]=\mathcal{K}$, leading to a group denoted simply GM(2+1). The nonvanishing commutators of its Lie algebra, $\mathcal{GM}(2+1)$, are

$$[E_i,K_j]=-\varepsilon_{ij}B,\quad [E_i,J]=-\varepsilon_{ij}E_j,$$

$$[H,P_i]=E_i,\quad [H,K_i]=-P_i,\quad [P_i,P_j]=-\varepsilon_{ij}B,$$

$$[P_i,K_j]=-\delta_{ij}M,\quad [P_i,J]=-\varepsilon_{ij}P_j,\quad [K_i,K_j]=\varepsilon_{ij}\mathcal{K},$$

$$[K_i,J]=-\varepsilon_{ij}K_j,K_j,\quad i,j=1,2. \tag{5.1}$$

It is interesting to point out that in a frame where the electric field $\vec{E}$ vanishes we recover the commutators corresponding to a pure magnetic Landau system.[15,26]

On the other hand, it is worthy to note that in order to relate the extended and nonextended GM algebras, we can redefine the basis generators inside the enveloping algebra taking into account the central character of M, $\mathcal{K}$, and B. So, we can write

$$K_i'=K_i+\lambda\varepsilon_{ij}P_j,\quad P_i'=P_i+\frac{M}{B}\varepsilon_{ij}E_j, \tag{5.2}$$

where $\lambda=(-M+\sqrt{M^2+\kappa B})/B$, and $M_e=\sqrt{M^2+\kappa B}$ is a kind of effective mass.[7] Then, the new commutators entering K_i',P_i' are the same as above except that

$$[K_i',K_j']=0. \tag{5.3}$$

A. Coadjoint orbits

Let us denote by $(m,\kappa,\beta,\epsilon_1,\epsilon_2,h,p_1,p_2,k_1,k_2,j)$ the coordinates of an arbitrary point of $\mathcal{G}^*(2+1)$ in a basis dual to $(M,\mathcal{K},B,E_1,E_2,H,P_1,P_2,K_1,K_2,J)$. The coadjoint action of an element $g=(\theta,\eta,c,\vec{d},b,\vec{a},v,\phi)\in\mathrm{GM}(2+1)$ on the dual space $\mathcal{GM}^*(2+1)$ is given by

$$m' = m,$$

$$\vec{\kappa}' = \vec{\kappa},$$

$$\vec{\beta}' = \vec{\beta},$$

$$\vec{\epsilon}' = \vec{\epsilon}^{\phi} - \vec{v} \times \vec{\beta},$$

$$h' = h - \vec{v} \cdot \vec{p}^{\phi} + \tfrac{1}{2} m \vec{v}^2 - \vec{a} \cdot (\vec{\epsilon}^{\phi} - \vec{v} \times \vec{\beta}),$$

$$\vec{p}' = \vec{p}^{\phi} - m\vec{v} - b(\vec{\epsilon}^{\phi} - \vec{v} \times \vec{\beta}) - \vec{\beta} \times \vec{a},$$

$$\vec{k}' = \vec{k}^{\phi} + m\vec{a} + b\vec{p}^{\phi} - \tfrac{1}{2} b^2 \vec{\epsilon}' + \vec{v} \times \vec{\kappa} - \vec{\beta} \times \vec{d} + \tfrac{1}{2} \vec{a} \times \vec{\beta},$$

$$\vec{j}' = \vec{j} - \vec{a} \times \vec{p}^{\phi} - \vec{v} \times \vec{k}^{\phi} + \tfrac{1}{2} \vec{\kappa} \cdot \vec{v}^2 + m\vec{a} \times \vec{v} + \tfrac{1}{2} \vec{\beta} \cdot \vec{a}^2 - \vec{d} \times \vec{\epsilon}^{\phi} + \tfrac{1}{2} b \vec{\epsilon}' \times \vec{a} - \vec{\beta}(\vec{d} \cdot \vec{v}). \tag{5.4}$$

Besides m, κ, and $C_0 \equiv \beta$ we have the following invariants of the coadjoint action:

$$C_1 = \vec{\beta}\vec{p}^2 - 2mh\vec{\beta} + 2\vec{\beta}(\vec{\epsilon} \cdot \vec{k}) - 2\beta^2 \vec{j} + \vec{\kappa}\vec{\epsilon}^2, \quad C_2 = 2\vec{\beta}^2 h + 2\vec{\beta} \cdot (\vec{p} \times \vec{\epsilon}) + m\vec{\epsilon}^2. \tag{5.5}$$

These invariants are the nonrelativistic version of (4.3). The invariance of the magnetic field $\vec{\beta}$ may be seen as the consequence of the invariance of the Lorentz force $\vec{F} = \vec{\epsilon} + \vec{v} \times \vec{\beta}$ under (homogeneous) Galilei transformations. A charged particle moving slowly can see mainly the magnetic field in our magnetic limit,[25]

$$\frac{\sqrt{\vec{\epsilon}^2}}{\beta} \ll 1. \tag{5.6}$$

Let us consider the relativistic invariant $C_0 = \vec{\epsilon}^2 - \beta^2$ from (4.3). Using (5.6) in the 0-term approximation term we obtain the nonrelativistic invariant

$$C_0 = -\beta_0^2.$$

We can omit the vector symbol because the magnetic field has only one component, so that

$$\beta = \sqrt{\beta_0^2 + \vec{\epsilon}^2} \overset{(5.6)}{\approx} \beta_0 + \frac{1}{2} \frac{\vec{\epsilon}^2}{\beta_0}. \tag{5.7}$$

By substituting

$$h \to m\left(1 + \frac{h}{m}\right), \quad j \to -\kappa\left(1 - \frac{j}{\kappa}\right), \quad \beta \to \beta\left(1 + \frac{1}{2}\frac{\vec{\epsilon}^2}{\beta^2}\right)$$

in the other invariants C_1 and C_2 of (4.3), and omitting terms of higher order in h/m, j/κ, and $\vec{\epsilon}^2/\beta^2$, we obtain their nonrelativistic counterparts of (5.5), respectively.

The classification of the coadjoint orbits is displayed in Appendix B. There are orbits of dimension 6 and 4, but the most important for us are the 6D orbits denoted $\mathcal{O}^{C_1 C_2}_{m\kappa\beta}$ with $\beta \neq 0$.

B. Symplectic structure

Each 6D orbit $\mathcal{O}^{C_1C_2}_{m\kappa\beta}$ can be covered with one chart $(\mathcal{O}^{C_1C_2}_{m\kappa\beta},\varphi)$. As coordinates we can choose $(\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)$ since the Jacobian of the transformation

$$(m,\kappa,\beta,\epsilon_1,\epsilon_2,h,p_1,p_2,k_1,k_2,j)\to(m,\kappa,\beta,C_1,C_2,\epsilon_1,\epsilon_2,p_1,p_2,k_1,k_2)$$

equals $4\beta^4$ $(\neq 0)$. The Poisson tensor Λ on the orbit $\mathcal{O}^{C_1C_2}_{m\kappa\beta}$ is

$$\Lambda = m\frac{\partial}{\partial k_i}\wedge\frac{\partial}{\partial p_i}+\kappa\frac{\partial}{\partial k_1}\wedge\frac{\partial}{\partial k_2}-\beta\frac{\partial}{\partial p_1}\wedge\frac{\partial}{\partial p_2}-\beta\varepsilon^{ij}\frac{\partial}{\partial k_i}\wedge\frac{\partial}{\partial\epsilon_j}. \tag{5.8}$$

The components of Λ, written in matrix form, are

$$\Lambda^{ij}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\beta \\ 0 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & -\beta & -m & 0 \\ 0 & 0 & \beta & 0 & 0 & -m \\ 0 & -\beta & m & 0 & 0 & \kappa \\ \beta & 0 & 0 & m & -\kappa & 0 \end{pmatrix}, \tag{5.9}$$

The determinant of Λ is β^6 $(\neq 0$, for our orbits). The natural symplectic form on $\mathcal{O}^{C_1C_2}_{m\kappa\beta}$ is

$$\omega=\frac{\beta\kappa+m^2}{\beta^3}\mathrm{d}\epsilon_1\wedge\mathrm{d}\epsilon_2+\frac{m}{\beta^2}\mathrm{d}\epsilon_i\wedge\mathrm{d}p_i+\frac{1}{\beta}\varepsilon_{ij}\mathrm{d}k_i\wedge\mathrm{d}\epsilon_j+\frac{1}{\beta}\mathrm{d}p_1\wedge\mathrm{d}p_2. \tag{5.10}$$

Therefore the coordinates $(\epsilon_i,p_i,k_i;\ i=1,2)$ are not canonical since the nonvanishing Poisson brackets are

$$\{\epsilon_i,k_j\}=-\varepsilon_{ij}\beta,\quad \{p_1,p_2\}=-\beta,\quad \{p_i,k_j\}=-\delta_{ij}m,\quad \{k_1,k_2\}=\kappa. \tag{5.11}$$

Notice in particular that even the coordinates k_1,k_2 do not commute.

On the other hand, observe that the above tensor (5.9) coincides with (4.5) if we simply substitute h by m and j by $-\kappa$. The root of the proposed substitution is the fact that the Galilei-Maxwell group GM(2+1) is the nonrelativistic limit of the Poincaré-Maxwell group PM(2+1). We can look at κ as a nonrelativistic track of the angular momentum j (see also in this respect the arguments supplied in Ref. 4).

Using the invariant C_2 from (5.5) we get a Hamiltonian linear in momenta $\vec{p}$ [which is the nonrelativistic version of (4.8)],

$$h=-\frac{\vec{p}\times\vec{\epsilon}}{\beta}-\frac{m}{2\beta^2}\vec{\epsilon}^{\,2}+\frac{C_2}{2\beta^2}. \tag{5.12}$$

Observe that by a naive limit $\beta\to 0$ we do not recuperate the free Hamiltonian (3.12); in fact $\lim_{\beta\to 0}h$ is not defined, and the same happens with the Poisson tensor.

After simple calculations we obtain the equations of motion

$$\dot{\vec{\epsilon}}_i=0,\quad \dot{p}_i=-\epsilon_i,\quad \dot{k}_i=p_i,\quad i=1,2. \tag{5.13}$$

Of course, our system includes constant homogeneous fields $\vec{\epsilon},\vec{\beta}$ perpendicular to each other as we already knew from the coadjoint action. We can also see that β does not take part in any of the formulas (5.13), so, surprisingly, the equations of motion are not affected by the magnetic field. Comparing formulas (5.13) with transformation rules (5.4) we conclude that these two sets of equations are compatible if we identify the parameter b with time. Moreover, the equations of motion are also independent of the parameter κ.

It would be interesting to compare our results with those obtained in a more standard way following the minimal coupling recipe. For simplicity we will assume here that the exotic extension κ vanishes. Let us consider a nonrelativistic particle with a unit negative electric charge moving on a plane in a constant homogeneous electric $\vec{\epsilon}=(\epsilon_1,\epsilon_2,0)$ and magnetic $\vec{\beta}=(0,0,\beta)$ fields. A phase space for this system is a 4D symplectic manifold $(M,\tilde{\omega})$, where the differentiable manifold M is diffeomorphic to $\mathbb{R}^4$ with canonical coordinates denoted by π_1,π_2,r_1,r_2. The first pair $\vec{\pi}=(\pi_1,\pi_2,0)$ is interpreted as the generalized momentum and the second $\vec{r}=(r_1,r_2,0)$ is for the vector of position. The symplectic form is

$$\tilde{\omega}=\mathrm{d}\pi_1\wedge\mathrm{d}r_1+\mathrm{d}\pi_2\wedge\mathrm{d}r_2. \tag{5.14}$$

The Poisson tensor $\tilde{\Lambda}$ in coordinates (π_1,π_2,r_1,r_2) takes the natural form

$$\tilde{\Lambda}^{ij}=\begin{pmatrix}0&0&-1&0\\0&0&0&-1\\1&0&0&0\\0&1&0&0\end{pmatrix}. \tag{5.15}$$

Finally, the Hamiltonian is represented by the minimal coupling expression

$$H=\frac{1}{2m}\left(\vec{\pi}+\frac{1}{2}\vec{\beta}\times\vec{r}\right)^2+\vec{\epsilon}\cdot\vec{r}, \tag{5.16}$$

leading to the motion equations

$$\dot{\vec{\pi}}=-\vec{\epsilon}+\frac{1}{2}\vec{\beta}\times\dot{\vec{r}},\quad \dot{\vec{r}}=\frac{1}{m}\left(\vec{\pi}+\frac{1}{2}\vec{\beta}\times\vec{r}\right). \tag{5.17}$$

Integrals of the motion equations (5.17) are the Hamiltonian (5.16) and

$$C_1=\vec{\epsilon}\times\left(\vec{\pi}-\tfrac{1}{2}\vec{\beta}\times\vec{r}\right), \tag{5.18}$$

$$C_2=\left[\vec{\epsilon}\cdot\left(\vec{\pi}+\tfrac{1}{2}\vec{\beta}\times\vec{r}\right)\right]^2-2(\vec{\epsilon}\cdot\vec{r})[\vec{\beta}\cdot(\vec{\pi}\times\vec{\epsilon})-m\vec{\epsilon}^2]. \tag{5.19}$$

We can get canonical coordinates from the group coordinates $(\vec{p},\vec{k})$, but unfortunately, there is no point transformation connecting these two nonrelativistic interacting pictures.

VI. CONCLUDING REMARKS

The symmetry group of a system plus the formalism (Hamiltonian mechanics on a symplectic manifold) restrict the equations of motion, allow to define elementary systems, and may lead to interacting systems compatible with the symmetries. The natural framework to display such symmetries is the method of coadjoint orbits. In this way we get a manifold, the invariant symplectic form, and the Hamiltonian.

This situation is quite different for the Hamilton formulation of mechanics in the phase space. In this frame the same symplectic manifold (M,ω) may be used to describe physical systems with different Hamiltonians. In order to build a Hamiltonian for interactions, one is guided by other principles such as the minimal coupling rule. However, there is not a canonical way to display the symmetries in this context.

These two approaches have significative differences that could be appreciated along the examples worked in this paper. For instance, in our coadjoint orbit scheme, the Hamiltonians obtained for the interacting cases are linear in $\vec{p}$, the equations of motion depend on the electric field $\vec{\epsilon}$, while the magnetic field $\vec{\beta}$ takes part only in the symplectic two-form. These features are in sharp contrast to the usual interacting Hamiltonian in phase space.

Another difference is with respect to the role played by the fields. They are an integral part of the system in the group approach, while in the phase space they are treated as external parameters. The reason is that in our procedure we have considered the fields on the same foot as coordinates and momenta. In other words, the fields have been treated as dynamical fields instead of external fields, as usual. If we want to set a complete theory for the whole interacting system (particle +fields) it is expected that both components should take part of the system at the same level.

The group approach also enlightens us on how to go from a relativistic to a nonrelativistic description of the system in a very simple and natural way. So, manifolds, symplectic forms, Hamiltonians, invariants, and equations of motion are related through a contraction procedure.

The price for the simplicity of the group approach is the fact that we must use noncanonical and noncommuting coordinates which obscure the physical interpretation. (However this is usual in the new formulations of planar physics, see for instance, Refs. 16 and 27–30).

To show the explicit relation between the group approach and the formulation in phase space is an open problem. This situation of having different descriptions for the same system (one more appropriate to handle symmetries, the other adapted for an easier interpretation) happens also in quantum mechanics. In this framework symmetries can be described by unitary irreducible representations of symmetry groups in a representation space related to the coadjoint orbits as has been shown in Secs. III C and IV C. On the other side, quantum mechanical systems are usually described by means of wave functions of the configuration space. The connection between these two pictures sometimes is easy (the free case), but when interactions are included it is more involved.

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APPENDIX A: *G*-INVARIANT SYMPLECTIC STRUCTURES

This Appendix contains some basic information about Poisson structures on a space $\mathcal{G}^*$ dual to a Lie algebra $\mathcal{G}$. We start from the definition of the Poisson bracket on some real n-dimensional manifold M, then we concentrate on the case when the manifold M is an orbit $\mathcal{O}^*$ of the coadjoint action. We prove that $\mathcal{O}^*$ is endowed in a canonical way with a symplectic structure.

Let M be a real n-dimensional differentiable manifold. The set of smooth real-valued functions $C^\infty(M)$ with a commutative multiplication constitutes a ring.

The Poisson bracket, $\{\cdot,\cdot\}: C^\infty(M)\times C^\infty(M)\to C^\infty(M)$, on the manifold M is a bilinear relation satisfying the following conditions:

(1) antisymmetry $\{f_1,f_2\}=-\{f_2,f_1\}$,
(2) Jacobi's identity $\{f_1,\{f_2,f_3\}\}+\{f_2,\{f_3,f_1\}\}+\{f_3,\{f_1,f_2\}\}=0$,
(3) derivation rule $\{f_1,f_2f_3\}=f_2\{f_1,f_3\}+f_3\{f_1,f_2\}$,

for every $f_1,f_2,f_3\in C^\infty(M)$.

The first two properties equip $C^\infty(M)$ with the structure of a real Lie algebra. The derivation rule (known also as the Leibniz identity) and the bilinearity of the Poisson bracket say that for every $f\in C^\infty(M)$ there exists a vector field X_f such that

$$X_f g=\{f,g\},\quad \forall\, g\in C^\infty(M).$$

Let us cover some open subset $U\subset M$ by a chart (U,φ), such that $(x_1,\ldots,x_n)$ denotes the coordinates of $x\in U$ in this chart. In a natural basis $\partial/\partial x_i\equiv\partial_{x_i}$ $(i=1,\ldots,n)$ induced by the chart we have $X_f=(X_f)^i\partial_{x_i}$, where Einstein's sum convention is used. It is easy to check that

$$(X_f)^i = X_f(x_i) = \{f, x_i\}. \tag{A1}$$

Using (A1) we find that the Poisson bracket

$$\{f, g\} = X_f g = (X_f)^i \partial_{x_i} g = \{f, x_i\} \frac{\partial g}{\partial x_i}. \tag{A2}$$

On the other hand,

$$\{f, x_i\} = -\{x_i, f\} = -X_{x_i}(f) = -\{x_i, x_j\} \frac{\partial f}{\partial x_j} = \{x_j, x_i\} \frac{\partial f}{\partial x_j}. \tag{A3}$$

Setting (A3) into (A2) we finally have

$$\{f, g\} = \frac{\partial f}{\partial x_j} \frac{\partial g}{\partial x_i} \{x_j, x_i\}. \tag{A4}$$

Hence, it is enough to know the Poisson brackets of the coordinate functions $\{x_j, x_i\}$, $i, j = 1, \ldots, n$, to compute the Poisson bracket of any pair of functions. The expression (A4) defines a two-contravariant skew-symmetric tensor Λ by

$$\Lambda(\mathrm{d}f, \mathrm{d}g) = \{f, g\}. \tag{A5}$$

So, we conclude that the correspondence $f \to X_f$ defines a map $\pi(x): T_x^* M \to T_x M$ in every point $x \in M$. The rank of $\pi(x)$ is called the rank of the Poisson structure in x.

The differential equations that determine the integral curves of X_f in M are

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \{f, x_i\}, \quad i = 1, \ldots, n. \tag{A6}$$

They look like Hamilton equations being $-f$ the Hamiltonian function. For this reason the vector fields X_f are called Hamiltonian vector fields and f is called the Hamiltonian of X_f.

Let us consider now the problem of defining a Poisson structure on the space $\mathcal{G}^*$, dual to a Lie algebra $\mathcal{G}$. For every smooth function $f \in \mathcal{C}^\infty(\mathcal{G}^*)$ its (total) differential $(\mathrm{d}f)_x$ at $x \in \mathcal{G}^*$ is a linear mapping $(\mathrm{d}f)_x: T_x\mathcal{G}^* \to \mathbb{R}$, where $T_x\mathcal{G}^*$ denotes the tangent space of $\mathcal{G}^*$ at the point x. The dual space $\mathcal{G}^*$ is a vector space and it can be identified with $T_x\mathcal{G}^*$. The differential $(Df)_x$ is the functional over the tangent space $T_x\mathcal{G}^*$ and, hence, also over $\mathcal{G}^*$. It means that $(Df)_x \in (\mathcal{G}^*)^*$ which is isomorphic to $\mathcal{G}$. Thus, to any function $f \in \mathcal{C}^\infty(\mathcal{G}^*)$ we assign $\delta_x f \in \mathcal{G}$, in such a way that for every $y \in \mathcal{G}^*$,

$$\langle y, \delta_x f \rangle = (\mathrm{d}f)_x(y) = \frac{d}{\mathrm{d}t} f(x + ty)|_{t=0}. \tag{A7}$$

The formula (A7) allows us to define the Poisson structure on $\mathcal{G}^*$ by

$$\{g, f\}(x) = \langle x, [\delta_x g, \delta_x f] \rangle. \tag{A8}$$

Defining the functions $\xi_a \in \mathcal{C}^\infty(\mathcal{G}^*)$, with $a \in \mathcal{G}$, by $\xi_a(x) = \langle x, a \rangle$ we obtain from (A7) that $\delta_x \xi_a = a$. Hence

$$\{\xi_a, \xi_b\}(x) = \langle x, [a, b] \rangle = \xi_{[a,b]}(x). \tag{A9}$$

If $\{a_1, \ldots, a_n\}$ is a basis of $\mathcal{G}$ then $\xi_i \equiv \xi_{a_i}$, $i = 1, \ldots, n$, can be chosen as a set of coordinate functions on $\mathcal{G}^*$. From (A4) and (A7) we obtain that the Poisson structure on $\mathcal{G}^*$ takes the form

$$\{f,g\}(x) = \frac{\partial f}{\partial \xi_i}\frac{\partial g}{\partial \xi_j}\{\xi_i,\xi_j\} = \frac{\partial f}{\partial \xi_i}\frac{\partial g}{\partial \xi_j}c_{ij}^k\xi_k, \tag{A10}$$

with c_{ij}^k being the structure constants of $\mathcal{G}$ relative to its basis $\{a_1,\ldots,a_n\}$. Thus, for a set of coordinate functions ξ_i, $i=1,\ldots,n$, on $\mathcal{G}^*$ we have

$$\{\xi_i,\xi_j\} = c_{ij}^k\xi_k, \tag{A11}$$

so that the Poisson bracket of $\{\xi_i,\xi_j\}$ is a linear function of ξ_k.

A special case of manifold with a Poisson structure is the symplectic manifold. A pair (M,ω) is called a symplectic manifold if M is a finite-dimensional differentiable manifold and ω a nondegenerate two-form satisfying the condition $\mathrm{d}\omega=0$. The nondegeneracy condition of ω is equivalent to the requirement that the rank of $\hat{\omega}: T_x(M)\to T_x^*(M)$, defined by

$$\langle\hat{\omega}(v),v'\rangle = \omega(v,v'),$$

is maximal at each point $x\in M$. The map $\hat{\omega}$ allows us to define a skew-symmetric contravariant tensor field Λ on M by

$$\Lambda(\alpha,\beta) = \omega(\hat{\omega}^{-1}(\alpha),\hat{\omega}^{-1}(\beta)), \quad \alpha,\beta\in T^*M. \tag{A12}$$

The tensor Λ constitutes the Poisson structure on M. Thus, when $\alpha=\mathrm{d}g$ and $\beta=\mathrm{d}f$ we obtain that

$$\{g,f\} = \Lambda(\mathrm{d}g,\mathrm{d}f) = \omega(\hat{\omega}^{-1}(\mathrm{d}g),\hat{\omega}^{-1}(\mathrm{d}f)). \tag{A13}$$

Let G be a Lie group and $\mathcal{G}$ its Lie algebra. For every element $g\in G$ the inner automorphism $i_g: G\to G$ defined as

$$i_g(g') = gg'g^{-1}$$

induces a Lie algebra automorphism $i_{g^*}:\mathcal{G}\to\mathcal{G}$ which gives rise to the adjoint representation of G on $\mathcal{G}$ by $\mathrm{Ad}_g=\exp i_{g^*}$. The coadjoint representation of G on $\mathcal{G}^*$ is now given by

$$\langle\mathrm{CoAd}_g(u),a\rangle = \langle u,\mathrm{Ad}_{g^{-1}}(a)\rangle, \quad u\in\mathcal{G}^*, \quad a\in\mathcal{G}. \tag{A14}$$

Each orbit $\mathcal{O}^*$ of the coadjoint action is a symplectic submanifold of the Poisson manifold $\mathcal{G}^*$, and it is endowed in a canonical way with a symplectic structure characterized by the two-form (Kirillov-Kostant-Souriau theorem)

$$\omega(X_a,X_b) = \langle u,[a,b]\rangle, \quad u\in\mathcal{O}^*, \quad a,b\in\mathcal{G}, \tag{A15}$$

where X_a is the fundamental vector field associated with the coadjoint action

$$(X_af)(u) = \frac{d}{\mathrm{d}t}f(\mathrm{CoAd}_{e^{-ta}u})\big|_{t=0}. \tag{A16}$$

The Poisson structure on $\mathcal{O}^*$, as a submanifold of $\mathcal{G}^*$, defined through the symplectic two-form ω (A15) coincides with that induced by the Poisson structure (A10) on $\mathcal{G}^*$.

APPENDIX B

We have the following Table I.

TABLE I. Coadjoint orbits classification for $\mathcal{GM}^*(2+1)$.

Constraints	Dimension	Invariants
$\beta\neq 0,\ m\neq 0,\ \kappa\neq 0$	6	$C_1=\frac{1}{2}\vec{\varepsilon}^2\cdot\vec{\kappa}+(\vec{\varepsilon}\cdot\vec{k})\cdot\vec{\beta}+\frac{1}{2}\vec{p}^2\cdot\vec{\beta}-mh\vec{\beta}-(\vec{j}\cdot\vec{\beta})\cdot\vec{\beta}$ $C_2=\vec{\beta}^2h+(\vec{p}\times\vec{\varepsilon})\cdot\vec{\beta}+\frac{m}{2}\vec{\varepsilon}^2$
$\beta=0,\ m\neq 0,\ \kappa\neq 0$	6	$C_1=-m/2\vec{p}^2+m^2h-m\vec{\varepsilon}\cdot\vec{k}+(\vec{p}\times\vec{\varepsilon})\cdot\vec{k}$ $C_2=\vec{\varepsilon}^2$
$m=0,\ \beta\neq 0,\ \kappa\neq 0$	6	$C_1=\frac{1}{2}\vec{\varepsilon}^2\cdot\vec{\kappa}+(\vec{\varepsilon}\cdot\vec{k})\cdot\vec{\beta}+\frac{1}{2}\vec{p}^2\cdot\vec{\beta}-(\vec{j}\cdot\vec{\beta})\cdot\vec{\beta}$ $C_2=h\cdot\vec{\beta}+(\vec{p}\times\vec{\varepsilon})$
$\kappa=0,\ \beta\neq 0,\ m\neq 0$	6	$C_1=(\vec{\varepsilon}\cdot\vec{k})\cdot\vec{\beta}+\frac{1}{2}\vec{p}^2\cdot\vec{\beta}-mh\cdot\vec{\beta}-(\vec{j}\cdot\vec{\beta})\cdot\vec{\beta}$ $C_2=\vec{\beta}^2h+(\vec{p}\times\vec{\varepsilon})\cdot\vec{\beta}+\frac{m}{2}\vec{\varepsilon}^2$
$\beta=m=0,\ \kappa\neq 0$	6	$C_1=\vec{p}\times\vec{\varepsilon}$ $C_2=\vec{\varepsilon}^2$
$\beta=\kappa=0,\ m\neq 0$	6	$C_1=-\frac{1}{2}\vec{p}^2+mh-\vec{\varepsilon}\cdot\vec{k}$ $C_2=\vec{\varepsilon}^2$
$m=\kappa=0,\ \beta\neq 0$	6	$C_1=-\frac{1}{2}\vec{p}^2-\vec{\varepsilon}\cdot\vec{k}+\vec{\beta}\cdot\vec{j}$ $C_2=h\cdot\vec{\beta}+\vec{p}\times\vec{\varepsilon}$
$\beta=m=\kappa=0$	4	$C_1=\frac{1}{2}\vec{p}^2+\vec{\varepsilon}\cdot\vec{k}$ $C_2=\vec{p}\times\vec{\varepsilon}$ $C_3=\vec{\varepsilon}^2$ $C_4=(\vec{p}\cdot\vec{\varepsilon})\cdot(\vec{p}\times\vec{\varepsilon})+\vec{\varepsilon}^2\cdot(\vec{k}\times\vec{\varepsilon})$

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Certain hidden symmetries of crystals

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Recently, among schemes for crystals classification, the arithmetic criterion has been introduced in solid-mechanics literature devoted to solid-to-solid phase transitions. Its main feature is to detect subtle symmetries ignored by standard classification schemes, e.g., space-group type classification. Using the arithmetic criterion, certain phase transitions can be identified by symmetry change, even when occurring between isosymmetric allotropes. Unfortunately, its original formulation is somewhat involved and not completely general. We give a general coordinate-free definition for it and prove that such a classification scheme has intrinsic character. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2121147]

I. INTRODUCTION

This is the first of a series of papers devoted to the systematic investigation of the arithmetic scheme for crystal structures classification. By crystal structures we mean point sets in the Euclidean space, possibly admitting a group of translational symmetries, each point of which carries a color. These are geometric models for aggregates of points, each point giving for example the (average) position of an atom or cluster of atoms, such as in crystalline solids, each color identifying, for instance, different types of atoms. These objects have varying nomenclature in the literature, such as *lattices with a basis*,[2,20] *ideal crystals*,[6] *multiregular point systems*,[5] *multilattices*.[24,25]

A basic way of describing their symmetries of crystal structures use their space groups. This leads to the well-known 219 types in three dimensions (230 types when orientation is taken into account).[15] One difficulty with this approach is that it only captures the intrinsic space geometries of the crystals, i.e., the orbifolds they generate,[26,21] ignoring the arrangement of the atoms with respect to these landscapes. As a consequence, crystals with reasonably different symmetry properties cannot be distinguished. Concretely this happens with isosymmetric solid-to-solid phase transformations, i.e., crystalline substances which exhibit distinct allotropes with the same space-group type[16,24,4] (see Fig. 4 for a simple theoretical example).

In this case, the existence of different symmetries for the two phases involved is confirmed by the presence of a phase transition. This raises the problem of how to define a good way of classifying structures so as to be able to distinguish between them even in the above-mentioned critical situation. While there exist well-known empirical lists of classes of structures such as Strukturberichte,[1] the literature does not currently show general, sufficiently subtle, accepted criteria for the classification of all the (possibly colored) crystal structures. This is evident in the comprehensive crystal structure database at http://cst-www.nrl.navy.mil/lattice/.

The arithmetic criterion has been recently developed in the context of solid mechanics and martensitic transformations, see Refs. 24, 25, and 3, following earlier works,[7,22,23] as a classification scheme for (colored) crystals based on symmetry. It extends to general structures the classical arithmetic method used in crystallography to classify simple lattices (i.e., crystals with one atom per primitive translational cell) into Bravais types,[6] obtaining, for instance, the well-known 14 Bravais types in three dimensions.

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TABLE I. Some results on arithmetic equivalence.

dim. Euclid. space=2		dim. Euclid. space=3	
Archit type	No. arithm equiv classes	Archit type	No. arithm equiv classes
{1}	5	{1}	14
{2}	5	{2}	29
{1,1}	10	{1,1}	51

The classification into Bravais types considers the equivalence classes of natural representations of the point group on the translation group. The arithmetic method instead, involves the equivalence classes of natural representations of the point group on a particular group obtained combining the translation group with the group of permutations of the (colored) set of the translation-group orbits. It has been shown[24] that this actually produces a finer classification of crystals than that based on the space-group type (and even that by Pearson Symbol); see also Sec. V C.

Furthermore it produces symmetry hierarchies among crystals that are more general than the standard ones.[17] In Refs. 8, 11, 10, and 9 (see Table I for a summary of the corresponding results) the systematic enumeration of the classes of structures generated by the arithmetic criterion were worked out in the simplest cases, while in Ref. 10 the symmetry hierarchies among crystals were shown, again in the simplest cases.

Unfortunately the original definition of the arithmetic criterion is involved, and not directly expressed in a coordinate-free way, nor completely general for certain aspects. We think this is what has prevented its diffusion from solid mechanics and crystallography. In fact, it has natural applications in other fields, such as solid state physics and chemistry, in the investigation of diffusionless solid-to-solid phase transitions and *ab initio* computations of materials. Theoretical crystallographers and solid-mechanics researchers may also find the perspective presented here interesting. The only requirements for reading this paper are an understanding of basic crystallography and some familiarity with group theory.

Our main objective is to give a simpler and coordinate-free formulation of the arithmetic criterion, making it available to a wider spectrum of scientists. In doing this, we have developed a unified treatment for structures of any dimension, such as bulk crystalline materials, slabs, linear polymers and molecules, embedded in a Euclidean space of arbitrary dimension, possibly different from that of the structure considered. This lays the foundation for further generalization to modulated crystals and quasicrystals.

The classification according to the arithmetic criterion belongs, together with Bravais and space-group type schemes, to the family of classification criteria based on global symmetry, i.e., the space group of structures. There are other schemes based on different ideas, such as the topological and combinatorial properties of structures.[13] Notice that the structures we consider are modeled by points, maybe of different colors; no other information is encoded. In particular, we do not consider relations among points like chemical bonds, such as in Ref. 14, though a generalization aimed to include these features is straightforward.

The basic expected requirements for symmetry-based criteria are: to coincide with the Bravais classification scheme whenever applied to simple lattices; to have intrinsic character (in the sense that it is possible to formulate them directly in a coordinate-free way); and, possibly, to produce a finite number of equivalence classes once the number of (colored) atoms per (primitive translational) cell has been fixed. The criteria producing the classification into Bravais types, lattice complexes, or space-group types, all satisfy these properties. We show this is true for the arithmetic criterion too, though the finiteness property will be proved in a separate paper.

This paper is structured as follows. In Sec. II we give the basic definitions of (crystal) structures in a Euclidean space, while in Sec. III we state the minimal properties expected from any (symmetry-based) criterion classifying structures. In Sec. IV we review the standard space-

group type scheme, reformulated in such a way that the arithmetic principle can be introduced as an extension of it. In Sec. V we state, in a coordinate-free form, the generalized form of the arithmetic classification principle, and in Sec. VI we give some results pertaining to the arithmetic scheme and we conclude with some examples showing how sensitive this criterion is. In the Appendix we provide some background material used throughout the paper.

Notations and conventions. Our notation is close to Ref. 19, which can be consulted for a more detailed exposition of the mathematics summarized in the Appendix.

(1) We write maps à la Hormander: $f: X \ni x \mapsto y \in Y$.
(2) For A, B, C objects in a category, the symbol $\mathrm{Iso}(A,B)$ denotes the set of isomorphisms in that category from A to B; $\mathrm{Iso}(C)$ means $\mathrm{Iso}(C,C)$ and id_C refers to the identity morphism of C.
(3) When an equivalence relation is clear from the context, we denote by $[x]$ the equivalence class of the element x; sometimes, however, we omit the square brackets.
(4) A morphism is often depicted as an arrow between two objects. All diagram of objects and morphisms are understood to be commutative, i.e. one gets the same results whatever way one performs composition of morphisms between the same two objects.
(5) We omit zero submatrices and write $\left(\begin{array}{c|c} a & b \\ \hline & c \end{array}\right)$ for $\left(\begin{array}{c|c} a & b \\ \hline 0 & c \end{array}\right)$.
(6) The symbol $\square$ denotes the end of a proof.

II. PRELIMINARIES AND DEFINITION OF STRUCTURES

We first restate some basic notions regarding the symmetry of Euclidean spaces and structures, presented in a way suitable for later developments. (One can choose to operate within either the *oriented* or *nonoriented* context. In the former case one works with oriented Euclidean spaces and uses orientation-preserving affinities, isometries and their linear parts.)

A. Euclidean spaces and their space groups

Definition 2.1: Let $\mathbb{E}$ be a Euclidean space; the *space group* $G(\mathbb{E})$ of $\mathbb{E}$ is the group of all the isometries of $\mathbb{E}$. Other key concepts are:

(1) $L(\mathbb{E})$, the *translation group* of $\mathbb{E}$, is the (additive) group underlying $\mathbb{E}$;
(2) $P(\mathbb{E})$, the *point group* of $\mathbb{E}$, is the group of orthogonal linear maps of the vector space $L(\mathbb{E})$;
(3) $\eta: P(\mathbb{E}) \to \mathrm{Iso}(L(\mathbb{E}))$, the *action* of $P(\mathbb{E})$ on $L(\mathbb{E})$, is the natural action $q.t := qt$.

We write $\mathcal{I}: L(\mathbb{E}) \to G(\mathbb{E})$ for the map taking a vector to the translation by that vector; for clarity vectors will sometimes be written in bold. Choosing an origin O for $\mathbb{E}$ defines in a natural way a (*Group*-)morphism $\sigma: P(\mathbb{E}) \to G(\mathbb{E})$ called a *splitting* (*morphism*) of $\mathbb{E}$. The origin is the only point fixed by all the elements of the image of $\sigma: \sigma(q).O = O \; \forall\, q \in P(\mathbb{E})$.

B. Structures and their space groups

Next, we give the definition of structures. We make no *a priori* hypotheses on the (dimensions of the) Euclidean spaces involved. Hence the host Euclidean space, though sometimes omitted for brevity, is part of the data needed to specify a structure. In view of this generality, structures need not "fill" the underlying space. We say that a structure is *full* when it "fills" such a space, i.e., with notation introduced just below in the text, when $\dim_{\mathbb{R}} L(\mathbb{S}) = \dim_{\mathbb{R}} L(\mathbb{E})$. Full structures are those of Examples 2.4, 2.5, 5.8, 5.9, but not that of Example 5.10, for which $\dim_{\mathbb{R}} L(\mathbb{S}) = 0 < 3 = \dim_{\mathbb{R}} L(\mathbb{E})$. For a $\mathbb{Z}$-submodule N of an $\mathbb{R}$-module M, we write $\dim_{\mathbb{R}} N$ for $\dim_{\mathbb{R}} \mathbb{R}N$, where $\mathbb{R}N$ is the $\mathbb{R}$-span of N in M.

Definition 2.2: For a set of colors $\mathfrak{C}$, a $\mathfrak{C}$-*structure* embedded into the Euclidean space $\mathbb{E}$, which we write as $\mathbb{S} \hookrightarrow \mathbb{E}$, is a $\mathfrak{C}$-set $c(\mathbb{S}): S(\mathbb{S}) \to \mathfrak{C}$ with $S(\mathbb{S})$ a subset of $\mathbb{E}$. The concept of $\mathfrak{C}$-set is recalled in the Appendix. When $\mathfrak{C}$ is a made up of one only element we refer to the *noncolored*

case, colors playing no role at all. We will often speak of structures rather than $\mathfrak{C}$-structures when $\mathfrak{C}$ is clear from the context.

Definition 2.3: $G(\mathrm{S}) := \{g \in G(\mathbb{E}) \text{ such that } g.\mathrm{S}=\mathrm{S}\}$ is the *space group* of S. (In other words, the space group is made up of all the isometries mapping the set $S(\mathrm{S})$ in itself and respecting the colors of its points.) In this context (compare with Definition 2.1):

(1) $L(\mathrm{S}) := \mathcal{I}^{-1}(G(\mathrm{S}) \cap \mathcal{I}(L(\mathbb{E})))$ is the *translation group* (also known as *skeletal lattice*[24,25]) of S;
(2) $P(\mathrm{S}) := G(\mathrm{S})/\mathcal{I}(L(\mathrm{S}))$ is the *point group* of S;
(3) $\eta: P(\mathrm{S}) \to \mathrm{Iso}(L(\mathbb{E})_{L(\mathrm{S})})$ induced by $\eta: P(\mathbb{E}) \to \mathrm{Iso}(L(\mathbb{E}))$ is the *arithmetic point group* of S.

Notice that we do not restrict our attention only to structures S with a discrete translation group, i.e., with $\dim_{\mathbb{R}} L(\mathrm{S}) = \dim_{\mathbb{Z}} L(\mathrm{S})$.

C. Examples of structures

For a Euclidean space $\mathbb{E}$ choose an origin O and an orthonormal basis $(\mathbf{e}_i)_{i\in 1}$ for $L(\mathbb{E})$.

Example 2.4: The crystal of cesium chloride (CsCl).
$S(\mathrm{S}) := S_1 \amalg S_2$, where, for $L := \mathbb{Z}\mathbf{e}_1 + \mathbb{Z}\mathbf{e}_2 + \mathbb{Z}\mathbf{e}_3$,

$$S_1 := O + \mathbf{0} + L,$$

$$S_2 := O + \tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3) + L;$$

$c(\mathrm{S}) := (S_1 \to \{\mathrm{Cs}\}) \amalg (S_2 \to \{\mathrm{Cl}\})$.

Example 2.5: The crystal of C-diamond (C).
$S(\mathrm{S}) := S_1 \amalg S_2$, where, for $L := \mathbb{Z}\frac{1}{2}(\mathbf{e}_1+\mathbf{e}_2) + \mathbb{Z}\frac{1}{2}(\mathbf{e}_2+\mathbf{e}_3) + \mathbb{Z}\frac{1}{2}(\mathbf{e}_3+\mathbf{e}_1)$,

$$S_1 := O + \mathbf{0} + L,$$

$$S_2 := O + \tfrac{1}{4}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3) + L;$$

$c(\mathrm{S}) := (S_1 \amalg S_2 \to \{\mathrm{C}\})$.

Example 2.6: The crystal of sodium (Na).
$S(\mathrm{S}) := \hat{S}_1 \amalg \hat{S}_2$, where, for $\hat{L} := \mathbb{Z}\mathbf{e}_1 + \mathbb{Z}\mathbf{e}_2 + \mathbb{Z}\mathbf{e}_3$,

$$\hat{S}_1 := O + \mathbf{0} + \hat{L},$$

$$\hat{S}_2 := O + \tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3) + \hat{L};$$

$c(\mathrm{S}) := (\hat{S}_1 \amalg \hat{S}_2 \to \{\mathrm{Na}\})$.

Equivalently, putting in evidence the entire translation group, we have: $S(\mathrm{S}) := S_1$, where, for $L := \mathbb{Z}\frac{1}{2}(-\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3) + \mathbb{Z}\frac{1}{2}(+\mathbf{e}_1-\mathbf{e}_2+\mathbf{e}_3) + \mathbb{Z}\frac{1}{2}(+\mathbf{e}_1+\mathbf{e}_2-\mathbf{e}_3)$,

$$S_1 := O + \mathbf{0} + L;$$

$c(\mathrm{S}) := (S_1 \to \{\mathrm{Na}\})$.

III. GENERALITIES ON SCHEMES FOR CRYSTALS CLASSIFICATION

For a classification scheme written in terms of crystal bases (a crystal basis for E_L is an $\mathbb{R}$-basis of E which by restriction induces a $\mathbb{Z}$-basis of L) the restriction of having intrinsic character is usually stated by requiring its independence from the crystal bases chosen. We avoid the use of such bases, in which case such a property is expressed as follows (Fig. 1):

Definition 3.1: Let $\sim$ be an equivalence relation among structures. The equivalence $\sim$ has *intrinsic character* if for every couple $\mathrm{S}' \hookrightarrow \mathbb{E}'$, $\mathrm{S}'' \hookrightarrow \mathbb{E}''$ and every $\phi \in \mathrm{Aff}(\mathbb{E}', \mathbb{E}'')$ such that

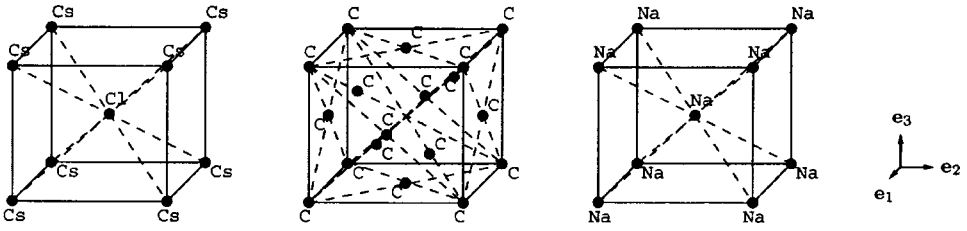

FIG. 1. From left of right: CsCl, C-Diamond, and Na crystals. Primitive (left) and conventional (middle and right) translational cells are shown.

$\mathbb{S}' \overset{\phi}{\to} \mathbb{S}''$ is a ($\mathfrak{C}$-*Set*-)isomorphism and $G(\mathbb{S}') \overset{\mathcal{C}_\phi}{\to} G(\mathbb{S}'')$ is a (*Group*-) isomorphism, we have $\mathbb{S}' \sim \mathbb{S}''$.

IV. CLASSIFYING STRUCTURES: SPACE-GROUP TYPE APPROACH REVISED

The arithmetic equivalence is formulated in terms of lattice groups of structures with respect to given essential arithmetic descriptors, while the space-group type equivalence is formulated in terms of space groups of structures. In some sense lattice groups generalize space groups and the arithmetic equivalence generalizes the space-group type equivalence. We reformulate the concepts of the space group of a structure and the space-group type equivalence in order to make this fact more evident, shortening the abstraction necessary to grasp the arithmetic criterion. To this purpose we rewrite space groups as objects encoding the absolute translational motion of primitive translational cells for each element of the point group. (A primitive translational cell is a fundamental domain for the action $\mathcal{I}L(\mathbb{S}) \to Iso(\mathbb{E})$.) Formally, we interpret them as representations of the point group on the translation group of the entire Euclidean space $L(\mathbb{E})$.

Fix a splitting $\sigma: P(\mathbb{E}) \to G(\mathbb{E})$. (Actually, in this context, a splitting should be thought as modulo $L(\mathbb{S})$, where the action of $L(\mathbb{S})$ on the set of splittings of $\mathbb{E}$ is $l.\sigma := \mathcal{C}_{\mathcal{I}(l)} \circ \sigma$.) Since $G(\mathbb{E}) = \mathcal{I}L(\mathbb{E}) \rtimes_\zeta \sigma P(\mathbb{E})$, where $\zeta: \sigma P(\mathbb{E}) \to \mathrm{Iso}(\mathcal{I}L(\mathbb{E}))$ is given by conjugation in $G(\mathbb{E})$, i.e., $\sigma(q).\mathcal{I}l := \mathcal{C}_{\sigma(q)}\mathcal{I}l$,[6] the following construction makes sense. For $t \in L(\mathbb{E})$ and $q \in P(\mathbb{E})$ write $t *_\sigma q$ for $\mathcal{I}(t) \circ \sigma(q)$. (The element $t *_\sigma \mathrm{id}$ is the same for every splitting σ and it will be denoted simply by $t * \mathrm{id}$.) Consider the (*Group*-)monomorphism (notice that $\eta: P(\mathbb{S}) \to \mathrm{Iso}(L(\mathbb{E})_{L(\mathbb{S})})$ is faithful, since $\eta: P(\mathbb{E}) \to \mathrm{Iso}(L(\mathbb{E}))$ is so):

$$G(\mathbb{S}) \hookrightarrow L(\mathbb{E}) \rtimes_\eta P(\mathbb{S}),$$

$$t *_\sigma q \mapsto \left(\begin{array}{c|c} \eta(q) & t \\ \hline & 1 \end{array} \right),$$

by restriction we get:

$$j: \mathcal{I}L(\mathbb{S}) \hookrightarrow j(\mathcal{I}L(\mathbb{S})),$$

$$\mathcal{I}(l) \mapsto \left(\begin{array}{c|c} \eta(\mathrm{id}) & l \\ \hline & 1 \end{array} \right).$$

The following (*Group*-)monomorphism is then naturally induced:

$$G(\mathbb{S})/\mathcal{I}L(\mathbb{S}) \hookrightarrow (L(\mathbb{E})/L(\mathbb{S})) \rtimes_\eta P(\mathbb{S}),$$

$$[t *_\sigma q] \mapsto \left(\begin{array}{c|c} \eta(q) & [t] \\ \hline & 1 \end{array} \right),$$

i.e.,

TABLE II. Some results on space-group type equivalence.

dim. transl. group	dim. Euclid. space	No. space-group types	Nomenclature
2	2	17	plane groups
2	3	80	layer groups
3	3	230	(3–) space groups

$$\mathfrak{G}_\sigma(\mathbb{S}):P(\mathbb{S}) \hookrightarrow (L(\mathbb{E})/L(\mathbb{S}))\rtimes_\eta P(\mathbb{S})$$

$$q \mapsto \left(\begin{array}{c|c} \eta(q) & [t] \\ \hline & 1 \end{array}\right). \tag{4.1}$$

Writing space groups explicitly, we omit the square brackets in the last expression and identify elements of $L(\mathbb{E})$ when they differ by an element of $L(\mathbb{S})$.

Remark 4.1: For a structure $\mathbb{S}$, we indicate by $\mathfrak{G}_\sigma(\mathbb{S})$ the image of the (*Group*-)morphism in (4.1) and we call it the *compact representation* of the space group of $\mathbb{S}$ relative to the splitting σ. This representation of the space group gets rid of the trivial part $L(\mathbb{S})$ pertaining to the translation group $L(\mathbb{E})$. Unlike $G(\mathbb{S})$, $\mathfrak{G}_\sigma(\mathbb{S})$ is always a finite group, and still keeps all the information of $G(\mathbb{S})$. In fact, there is a bijective correspondence between space groups and their compact representations:

$$\mathfrak{G}_\sigma(\mathbb{S}) = \left\{ \left(\begin{array}{c|c} \eta(q) & [t] \\ \hline & 1 \end{array}\right) \text{ such that } \left(\begin{array}{c|c} \eta(q) & t \\ \hline & 1 \end{array}\right) \in G(\mathbb{S}) \right\}$$

and

$$G(\mathbb{S}) = \left\{ \left(\begin{array}{c|c} \eta(q) & t \\ \hline & 1 \end{array}\right) \text{ such that } \left(\begin{array}{c|c} \eta(q) & [\tau] \\ \hline & 1 \end{array}\right) \in \mathfrak{G}(\mathbb{S})_\sigma, \text{ with } \mathcal{I}L(\mathbb{S}) \,.\, t = [\tau] \right\}.$$

Definition 4.2: Two structures $\mathbb{S}' \hookrightarrow \mathbb{E}', \mathbb{S}'' \hookrightarrow \mathbb{E}''$ are space-group type equivalent if there exists $\phi \in \mathrm{Aff}(\mathbb{E}', \mathbb{E}'')$ such that $\mathcal{C}_\phi: G(\mathbb{S}') \to G(\mathbb{S}'')$ is a (*Group*-)isomorphism.

In terms of compact representations of space groups, denoting by $\xi: Iso(E_L) \to Iso(E/L)$ the action induced by $E_L \ni t \mapsto [t] \in E/L$, we have:

Remark 4.3: Two structures $\mathbb{S}' \hookrightarrow \mathbb{E}', \mathbb{S}'' \hookrightarrow \mathbb{E}''$ are space-group type equivalent if and only if

1. $L(\mathbb{E}')_{L(\mathbb{S}')} = L(\mathbb{E}'')_{L(\mathbb{S}'')}$ (call them E_L),
2. there exists $([T], A) \in (E/L) \rtimes_\xi \mathrm{Iso}(E_L)$ such that $\mathcal{C}_{\left(\begin{array}{c|c} A & [T] \\ \hline & 1 \end{array}\right)}: \mathfrak{G}_{\sigma'}(\mathbb{S}') \to \mathfrak{G}_{\sigma''}(\mathbb{S}'')$ is a (*Group*-)isomorphism.

Again, performing explicit computation, we omit the square brackets in the last expression and identify elements of $L(\mathbb{E})$ differing by an element of $L(\mathbb{S})$.

Notice that in Remark 4.3, the structures enter only through their compact representations; the chosen splittings are not directly involved. In fact, we know that the concept of space-group type equivalence does not depend on the splittings chosen.

Some know results on space-group type quivalence

Table II shows some known results[15] which refer to the space-group type classification for structures with a discrete translation group. (In the nonoriented case, the "230" in such a table should be replaced by "219.")

V. CLASSIFYING STRUCTURES: THE ARITHMETIC APPROACH

A. Arithmetic description of structures

One way to look at crystal structures is as multilattices, i.e., unions of simple lattices[24,25] all with the same skeletal lattice. The most natural choice for it is the whole translation group of the structure they belong to. In this context, the orbit space $\mathbb{S}\backslash\mathcal{I}L(\mathbb{S})$ consists of one (colored) point for each of these simple lattices. The multiset (see the Appendix) associated to such an orbit space gives the number of such simple lattices, together with their color distribution, i.e., the number of "atoms," for each different species, in a primitive translational cell. We name these two concepts as follows:

Definition 5.1: For a structure $\mathbb{S}$, we call the $\mathfrak{C}$-set $\mathbb{S}\backslash\mathcal{I}L(\mathbb{S})$ the *arithmetic architecture* of $\mathbb{S}$, and the multiset associated to it, $|\mathbb{S}\backslash\mathcal{I}L(\mathbb{S})|$, the *arithmetic architecture type* of $\mathbb{S}$. For instance, simple lattices are those structures whose arithmetic architecture type is $\{1\}$, while structures with arithmetic architecture type $\{1, 2\}$ are those made up of $1+2=3$ translation-group orbits, two of them with the same color and the third one with a different color.

Example 5.2: Cesium chloride crystal CsCl (Example 2.4). The arithmetic description is

$$\mathbb{S}\backslash\mathcal{I}L(\mathbb{S}) = \{\underbrace{(S_1 \mapsto \{\mathrm{Cs}\})}_{1}, \underbrace{(S_2 \mapsto \{\mathrm{Cl}\})}_{1}\},$$

hence its arithmetic architecture type is $\{1, 1\}$.

Example 5.3: Diamond C (Example 1.5). The arithmetic description is

$$\mathbb{S}\backslash\mathcal{I}L(\mathbb{S}) = \{(\underbrace{S_1 \amalg S_2 \mapsto \{\mathrm{C}\}}_{2})\},$$

hence its arithmetic architecture type is $\{2\}$.

Example 5.4: Sodium crystal Na (Example 2.6). The arithmetic description is

$$\mathbb{S}\backslash\mathcal{I}L(\mathbb{S}) = \{\underbrace{(S_1 \mapsto \{\mathrm{Na}\})}_{1}\},$$

hence its arithmetic architecture type is $\{1\}$. Notice that we have to use the description in terms of the *whole* translation group; equivalently we have to refer to a *primitive* translational cell. For instance the arithmetic description:

$$\mathbb{S}\backslash\mathcal{I}L(\mathbb{S}) \overset{\text{(false)}}{=} \{\underbrace{(\hat{S}_1 \amalg \hat{S}_2 \mapsto \{\mathrm{Na}\})}_{2}\},$$

would wrongly lead us to conclude that the arithmetic architecture type is $\{2\}$.

B. Essential arithmetic descriptors of structures

We now introduce the concept of essential arithmetic descriptors for structures. This concept is close to the notion of bases relative to a primitive translational cell,[2,18] though its elements need not be confined to the closure of such a cell. A structure can be reconstructed from one of its essential arithmetic descriptors; in fact, an essential arithmetic descriptor is a minimal colored set generating the structure once the elements of its translation group are applied to such a set. Formally:

Definition 5.5: For a structure $\mathbb{S}$ and $\mathcal{A}$ a $\mathfrak{C}$-set isomorphic to the arithmetic architecture of $\mathbb{S}$, an *essential arithmetic descriptor* for $\mathbb{S}$ is a sub-$\mathfrak{C}$-set of the $\mathfrak{C}$-set $\mathbb{S}$, $(P_\alpha)_{\alpha\in\mathcal{A}}$, such that

$$\mathbb{S} = \amalg_{\alpha\in\mathcal{A}} P_\alpha + L(\mathbb{S}).$$

Actually an essential arithmetic descriptor should be thought of modulo $L(\mathbb{S})$ (the same transition for all of its points), i.e., as an element of $\mathbb{E}^{\mathcal{A}}\backslash L(\mathbb{S})$ rather than $\mathbb{E}^{\mathcal{A}}$, the action $L(\mathbb{S})\to \mathrm{Iso}(\mathbb{E}^{\mathcal{A}})$ being $l.(Q_\alpha)_{\alpha\in\mathcal{A}} := (Q_\alpha + l)_{\alpha\in\mathcal{A}}$.

Example 5.6: For the structure of C-Diamond in Example 2.5; the following is a 1-1 parametrization of the set of all its essential arithmetic descriptors:

$$c:\left(\left\{O + \mathbf{0} + \mathbf{1}_{(a,b,c)}, O + \tfrac{1}{4}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3) + \mathbf{1}_{(d,e,f)}\right\} \mapsto \{\mathrm{C}\}\right),$$

with $\mathbf{1}_{(x,y,z)} := x\frac{1}{2}(\mathbf{e}_1+\mathbf{e}_2) + y\frac{1}{2}(\mathbf{e}_2+\mathbf{e}_3) + z\frac{1}{2}(\mathbf{e}_3+\mathbf{e}_1)$ and each of a,b,c,d,e,f ranging in the integers. In other words, every essential arithmetic descriptor appears for a unique value of $((a,b,c),(d,e,f))$. Notice that each essential arithmetic descriptor is a $\mathfrak{C}$-set.

For an essential arithmetic descriptor $(P_\alpha)_{\alpha\in\mathcal{A}}$ of $\mathbb{S}$ one has the ($\mathfrak{C}$-*Set*-)isomorphism $\Upsilon_{(P_\alpha)_{\alpha\in\mathcal{A}}}: \mathcal{A} \ni \alpha \mapsto \mathcal{I}L(\mathbb{S}).P_\alpha \in \mathbb{S}\backslash\mathcal{I}L(\mathbb{S})$. This simply describes the labeling in terms of the elements of $\mathcal{A}$, induced by the chosen essential arithmetic descriptor, for the simple lattices forming $\mathbb{S}$.

C. The lattice group of a structure

Lattice groups encode the relative (translational) motion of the "atoms" inside primitive translational cells for each element of the point group. These are representations of the point group on the group $W_{\mathcal{A}}(\mathbb{S}) := L(\mathbb{S})\chi\mathrm{Iso}(\mathcal{A})$ obtained by intertwining the translation group and the group of permutations of its arithmetic architecture.

Definition 5.7: Let $\mathbb{S}$ be a structure and $(P_\alpha)_{\alpha\in\mathcal{A}}$ an arithmetic descriptor for it. We will make use of the following group: $W_{\mathcal{A}}(\mathbb{S}) \rtimes_{\eta_{\mathcal{A}}} P(\mathbb{S})$, where $\eta_{\mathcal{A}}: P(\mathbb{S}) \to \mathrm{Iso}(W_{\mathcal{A}}(\mathbb{S}))$ is $q.((\omega_\alpha)_{\alpha\in\mathcal{A}}, \delta) := ((q.\omega_\alpha)_{\alpha\in\mathcal{A}}, \delta))$. Consider the (*Group*-)monomorphism:

$$G(\mathbb{S}) \to W_{\mathcal{A}}(\mathbb{S}) \rtimes_{\eta_{\mathcal{A}}} P(\mathbb{S}),$$

$$t*_\sigma q \mapsto \left(\begin{array}{c|c} \eta(q) & \omega(q) \\ \hline & \tilde{\delta}(q) \end{array}\right),$$

where, for $t*_\sigma q \in G(\mathbb{S})$, $(\omega(q), \delta(q)) \in W_{\mathcal{A}}(\mathbb{S})$ is uniquely determined by

$$(t*_\sigma q) \,.\, P_\alpha = (\omega(q)_\alpha * \mathrm{id}) \,.\, P_{\delta(q)(\alpha)} \;\forall\; \alpha \in \mathcal{A};$$

by restriction we get

$$j:\mathcal{I}L(\mathbb{S}) \hookrightarrow j\mathcal{I}L(\mathbb{S}),$$

$$\mathcal{I}(l) \mapsto \left(\begin{array}{c|c} \eta(\mathrm{id}) & (l)_{\alpha\in\mathcal{A}} \\ \hline & \mathrm{id} \end{array}\right).$$

Hence the following (*Group*-)monomorphism is induced:

$$G(\mathbb{S})/\mathcal{I}L(\mathbb{S}) \hookrightarrow (W_{\mathcal{A}}(\mathbb{S})/L(\mathbb{S})) \rtimes_{\eta_{\mathcal{A}}} P(\mathbb{S}),$$

$$[t*_\sigma q] \mapsto \left(\begin{array}{c|c} \eta(q) & [\omega(q)] \\ \hline & \tilde{\delta}(q) \end{array}\right).$$

i.e.,

$$\Lambda(\mathbb{S})_{(P_\alpha)_{\alpha\in\mathcal{A}}}: P(\mathbb{S}) \hookrightarrow (W_{\mathcal{A}}(\mathbb{S})/L(\mathbb{S})) \rtimes_{\eta_{\mathcal{A}}} P(\mathbb{S})$$

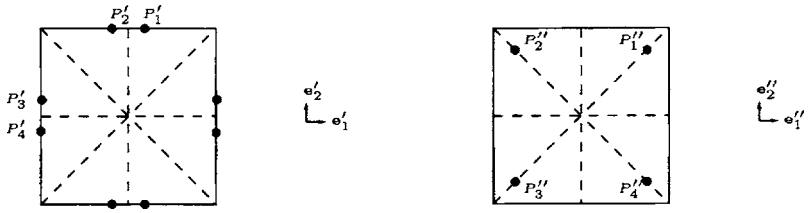

FIG. 2. The plane regular point systems *p*4*mm e* (left), and *p*4*mm f* (right) (basis vectors not in scale; primitive translational cells shown).

$$q \mapsto \left(\begin{array}{c|c} \eta(q) & [\omega(q)] \\ \hline & \widetilde{\delta}(q) \end{array} \right) \tag{5.1}$$

Although to obtain (5.1) we used a splitting for $\mathbb{E}$, this formula does not depend upon such a choice. We omitted the diagonal inclusion $j: L(\mathbb{S}) \ni l \mapsto ((l)_{\alpha\in\mathcal{A}}, \mathrm{id}) \in W_{\mathcal{A}}(\mathbb{S})$ (all columns, indexed by α, equal l). Similarly to what we did with the elements of compact representations of space groups, for the elements of lattice groups we omit square brackets and identify the top right submatrices differing by a matrix with all equal columns.

The group image $\Lambda(\mathbb{S})_{(P_\alpha)_{\alpha\in\mathcal{A}}}$ of $P(\mathbb{S})$ via (5.1) is called the *lattice group* of the structure $\mathbb{S}$ with respect to the essential arithmetic descriptor $(P_\alpha)_{\alpha\in\mathcal{A}}$.

Notice that, choosing a crystal basis for the structure $\mathbb{S} \hookrightarrow \mathbb{E}$, any element $\left(\begin{array}{c|c} \eta(q) & [\omega] \\ \hline & \widetilde{\delta} \end{array} \right)$ of its lattice group can be written referring to such a basis; in this case both $\eta(q)$ and ω are represented by matrices with integer coefficients.[24,25]

D. Examples of explicit computations of space groups and lattice groups of structures

Example 5.8: Consider the (full noncolored) structure $\mathbb{S}'$ sketched in Fig. 2—the plane regular point system *p*4*mm*#*d*.[15] Its arithmetic point group is $\eta'(P(\mathbb{S}')) = \langle 4^+(0,0), m(0,y)\rangle$. [Notations here are as in Ref. 15: $4^+(0,0)$ is the counterclock wise rotation by $+2\pi/4$ around the axis perpendicular to the page passing through the origin and pointing toward the reader, while $m(0,y)$ is the mirror reflection across the plane with axis $\mathbf{e}_2$ and passing through the origin.]

Referring to the figure, we choose the center of the square sketched as origin O' of the Euclidean space $\mathbb{E}'$, the points P'_1, P'_2, P'_3, P'_4 as essential arithmetic descriptor and the vectors $\mathbf{e}'_1, \mathbf{e}'_2$ shown as crystal basis.

The action of the point group on the origin O' is

$$\eta'^{-1} \,.\, 4^+(0,0) \mapsto (O' \mapsto O' + \mathbf{0}),$$

$$\eta'^{-1} \,.\, m(0,y) \mapsto (O' \mapsto O' + \mathbf{0}).$$

The action of the point group on the essential arithmetic descriptor P'_1, P'_2, P'_3, P'_4 is

$$\eta'^{-1} \,.\, 4^+(0,0) \mapsto \begin{pmatrix} P'_1 & \mapsto & P'_3 + \mathbf{0} \\ P'_2 & \mapsto & P'_4 + \mathbf{0} \\ P'_3 & \mapsto & P'_2 - \mathbf{e}'_2 \\ P'_4 & \mapsto & P'_1 - \mathbf{e}'_2 \end{pmatrix},$$

$$\eta'^{-1}\,.\,m(0,y)\mapsto\begin{pmatrix} P'_1 & \mapsto & P'_2+\mathbf{0}\\ P'_2 & \mapsto & P'_1+\mathbf{0}\\ P'_3 & \mapsto & P'_3+\mathbf{e}'_1\\ P'_4 & \mapsto & P'_4+\mathbf{e}'_1 \end{pmatrix}.$$

So the compact representation of the space group of $\mathbb{S}'$ written with respect to the origin O' and with coordinates relative to the basis $\mathbf{e}'_1,\mathbf{e}'_2$ is

$$\left\langle\left(\left(\begin{array}{cc|c} 0 & -1 & 0\\ 1 & 0 & 0\\ \hline & & 1 \end{array}\right),\left(\begin{array}{cc|c} -1 & 0 & 0\\ 0 & 1 & 0\\ \hline & & 1 \end{array}\right)\right)\right\rangle, \tag{g'}$$

while the lattice group of $\mathbb{S}'$ written with respect to the essential arithmetic descriptor P'_1,P'_2,P'_3,P'_4 and with coordinates relative to the basis $\mathbf{e}'_1,\mathbf{e}'_2$ is

$$\left\langle\left(\left(\begin{array}{cc|cccc} 0 & -1 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & -1 & -1\\ \hline & & 0 & 0 & 0 & 1\\ & & 0 & 0 & 1 & 0\\ & & 1 & 0 & 0 & 0\\ & & 0 & 1 & 0 & 0 \end{array}\right),\left(\begin{array}{cc|cccc} -1 & 0 & 0 & 0 & 1 & 1\\ 0 & 1 & 0 & 0 & 0 & 0\\ \hline & & 0 & 1 & 0 & 0\\ & & 1 & 0 & 0 & 0\\ & & 0 & 0 & 1 & 0\\ & & 0 & 0 & 0 & 1 \end{array}\right)\right)\right\rangle. \tag{λ'}$$

Incidentally, the action $\delta':P(\mathbb{S}')\to\mathrm{Iso}(\mathcal{A})$ in this case is

$$\eta''^{-1}\,.\,4^+(0,0)\mapsto(1,3,2,4),$$

$$\eta''^{-1}\,.\,m(0,y)\mapsto(1,2)(3)(4).$$

Example 5.9: Consider the (full noncolored) structure $\mathbb{S}''$ sketched in Fig. 2—the plane regular point system *p4mm#f*.[15] Its arithmetic point group is $\eta''(P(\mathbb{S}''))=\langle 4^+(0,0),m(0,y)\rangle$. (This is the same arithmetic point group as in the previous example, once we have identified the Euclidean spaces $\mathbb{E}',\mathbb{E}''$ via the affinity defined by $O'\mapsto O''$ and $\mathbf{e}'_i\mapsto\mathbf{e}''_i$. In addition, with this identification, the space groups of these two structures coincide.)

Referring to the figure, we choose the center of the square sketched as origin O'' of the Euclidean space $\mathbb{E}''$, the points P''_1,P''_2,P''_3,P''_4 as essential arithmetic descriptor and the vectors $\mathbf{e}''_1,\mathbf{e}''_2$ shown as crystal basis, the same as the one in the previous example identifying in an obvious way the two underlying Euclidean spaces. The action of the point group on the chosen origin for $\mathbb{E}''$ is

$$\eta''^{-1}\,.\,4^+(0,0)\mapsto(O''\mapsto O''+\mathbf{0}),$$

$$\eta''^{-1}\,.\,m(0,y)\mapsto(O''\mapsto O''+\mathbf{0}),$$

while the action of the point group on the chosen essential arithmetic descriptor is

$$\eta''^{-1}\,.\,4^+(0,0)\mapsto\begin{pmatrix} P''_1 & \mapsto & P''_2+\mathbf{0}\\ P''_2 & \mapsto & P''_3+\mathbf{0}\\ P''_3 & \mapsto & P''_4+\mathbf{0}\\ P''_4 & \mapsto & P''_1+\mathbf{0} \end{pmatrix},$$

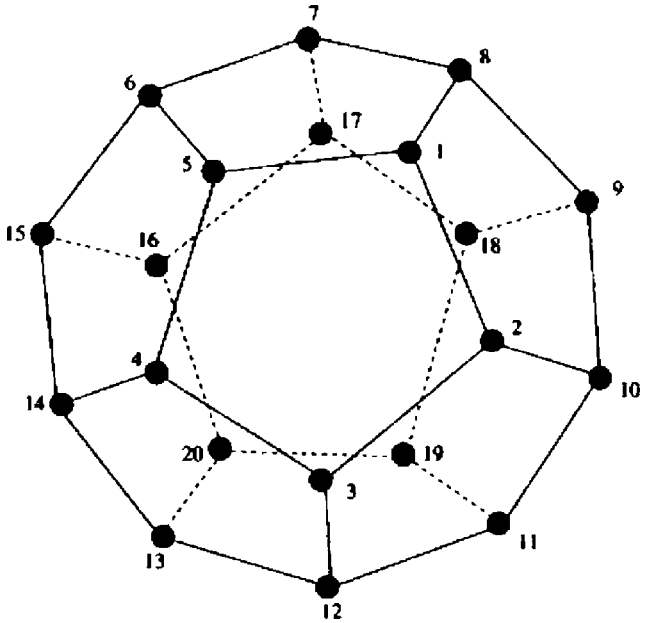

FIG. 3. The fullerene C_{20} molecule. Numbering according to IUPAC Recommendations 2004; see Ref. 12, Ref. No. 20:1, CAS Reg. No. 104375-45-3.

$$\eta''^{-1}\,.\,m(0,y)\mapsto\begin{pmatrix} P_1'' & \mapsto & P_2''+\mathbf{0} \\ P_2'' & \mapsto & P_1''+\mathbf{0} \\ P_3'' & \mapsto & P_4''+\mathbf{0} \\ P_4'' & \mapsto & P_3''+\mathbf{0} \end{pmatrix}.$$

Hence the compact representation of the space group of $\mathbb{S}''$ written with respect to the origin O'' of $\mathbb{E}''$ and with coordinates relative to the basis $\mathbf{e}_1'', \mathbf{e}_2''$ is

$$\left\langle\left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline & & 1 \end{array}\right),\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline & & 1 \end{array}\right)\right\rangle, \qquad (g'')$$

while the lattice group of $\mathbb{S}''$ written with respect to the above essential arithmetic descriptor and with coordinates relative to the chosen crystal basis is

$$\left\langle\left(\begin{array}{cc|cccc} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -1 & -1 \\ \hline & & 0 & 0 & 0 & 1 \\ & & 0 & 0 & 1 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & 0 & 1 & 0 & 0 \end{array}\right),\left(\begin{array}{cc|cccc} -1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \hline & & 0 & 1 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & 0 & 0 & 1 & 0 \\ & & 0 & 0 & 0 & 1 \end{array}\right)\right\rangle. \qquad (\lambda'')$$

The action $\delta'': P(\mathbb{S}'') \to \mathrm{Iso}(\mathcal{A})$ is

$$\eta''^{-1}\,.\,4^{+}(0,0)\mapsto(1,2,3,4),$$

$$\eta''^{-1}\,.\,m(0,y)\mapsto(1,2)(3,4).$$

Example 5.10: Consider the {C}-structure $\mathbb{S}$ sketched in Fig. 3, modeling C_{20} fullerene mol-

ecule. Its arithmetic point group is $\eta(P(\mathbb{S}))=\langle 5_a^+, 5_b^+, m\rangle$. [We use the following (nonstandard) notation: 5_a^+ (respectively, 5_b^+) denotes the counterclock wise rotation by $+2\pi/5$ around the axis perpendicular to the two faces with vertices 5, 4, 3, 2, 1 (respectively, 1, 8, 7, 6, 5) and 20, 19, 18, 17, 16 (respectively, 20, 13, 12, 11, 19), pointing from the latter to the former and passing through the origin; m denotes the mirror reflection across the plane passing through vertices 3, 7, 12, 17.]

Referring to the figure, we choose the center of the square sketched as origin O of the Euclidean space $\mathbb{E}$, the points $P_1,\ldots,P_{20}$ as essential arithmetic descriptor (denoted simply by 1,…,20 in the figure).

The action of the point group on the chosen origin for $\mathbb{E}$ is

$$\eta^{-1}\,.\,5_a^+ \mapsto (O \mapsto O+\mathbf{0}),$$

$$\eta^{-1}\,.\,5_b^+ \mapsto (O \mapsto O+\mathbf{0}),$$

$$\eta^{-1}\,.\,m \mapsto (O \mapsto O+\mathbf{0}),$$

while the action of the point group on the chosen essential arithmetic descriptor is

$$\eta^{-1}\,.\,5_a^+ \mapsto \begin{pmatrix} P_1 & \mapsto & P_{\delta(\eta^{-1}.5_a^+)(1)}+\mathbf{0} \\ & \cdots & \\ P_{20} & \mapsto & P_{\delta(\eta^{-1}.5_a^+)(20)}+\mathbf{0} \end{pmatrix},$$

$$\eta^{-1}\,.\,5_b^+ \mapsto \begin{pmatrix} P_1 & \mapsto & P_{\delta(\eta^{-1}.5_b^+)(1)}+\mathbf{0} \\ & \cdots & \\ P_{20} & \mapsto & P_{\delta(\eta^{-1}.5_b^+)(20)}+\mathbf{0} \end{pmatrix},$$

$$\eta^{-1}\,.\,m \mapsto \begin{pmatrix} P_1 & \mapsto & P_{\delta(\eta^{-1}.m)(1)}+\mathbf{0} \\ & \cdots & \\ P_{20} & \mapsto & P_{\delta(\eta^{-1}.m)(20)}+\mathbf{0} \end{pmatrix},$$

where the action $\delta: P(\mathbb{S}) \to \mathrm{Iso}(\mathcal{A})$ is

$$\eta^{-1}\,.\,5_a^+ \mapsto (5,4,3,2,1)(14,12,10,8,6)(15,13,11,9,7)(20,19,18,17,16),$$

$$\eta^{-1}\,.\,5_b^+ \mapsto (1,8,7,6,5)(2,9,17,15,4)(3,10,18,16,14)(11,19,20,13,12),$$

$$\eta^{-1}\,.\,m \mapsto (1,5)(2,4)(3)(6,8)(7)(9,15)(10,14)(11,13)(12)(16,18)(17)(19,20).$$

From this, the lattice group of $\mathbb{S}$ written with respect to the above essential arithmetic descriptor can be immediately written, though the matrix notation is awkward. Notice that in the definition of wreath product we used matrix notation just to avoid being too abstract. The drawback of this choice is a cumbersome notation in a case like the above where the arithmetic architecture is large. In such a case one should switch to cycles' notation; the modifications are straightforward.

E. Relationship between space groups and lattice groups

As we said, while space groups keep track of the absolute translational motion of primitive translational cells, lattice groups record the relative (translational) motion of the "atoms" inside such cells. Hence there seems to be no correlation between space groups and lattice groups, but

actually the latter can be recovered from the former (but not vice-versa;[24,25] see also Examples 6.4, 6.5). The reason is that the baricenter of the "atoms" inside a primitive translational cell, being rigidly attached to it, determines its position. Formally:

Remark 5.11: The following is a (*Group*-)isomorphism:

$$\Lambda(\mathbb{S})_{(P_\alpha)_{\alpha\in\mathcal{A}}} \ni \left(\begin{array}{c|c} \eta(q) & [\omega(q)] \\ \hline & \widetilde{\delta}(q) \end{array}\right) \mapsto \left(\begin{array}{c|c} \eta(q) & [\overline{\omega(q)} + (\mathrm{id} - q)\,.\,(\bar{P} - O)] \\ \hline & 1 \end{array}\right) \in \mathfrak{G}_\sigma(\mathbb{S}),$$

fitting the diagram:

$$\begin{array}{ccc} \Lambda(\mathbb{S})_{(P_\alpha)_{\alpha\in\mathcal{A}}} & \longrightarrow & P(\mathbb{S}) \\ \downarrow & & \downarrow \mathrm{id} \\ \mathfrak{G}_\sigma(\mathbb{S}) & \longrightarrow & P(\mathbb{S}) \end{array},$$

where, for $[(\omega_\alpha)_{\alpha\in\mathcal{A}}] \in L(\mathbb{S})^{\mathcal{A}}/L(\mathbb{S})$, $[\bar{\omega}] \in L(\mathbb{E})/L(\mathbb{S})$ is well defined as [average of $(\omega_\alpha)_{\alpha\in\mathcal{A}}$]. Hence the lattice group retains (strictly) more information than the space group.

Example 5.12: We apply this remark to obtain the space group from the lattice group in some explicit cases.

1. Example 4.8. $\overline{P'} = O' - \frac{1}{4}\mathbf{e}_1' + \frac{1}{4}\mathbf{e}_2'$; from (λ') we get $\overline{\omega'(\eta''^{-1}.4^+(0,0))} = -\frac{1}{2}\mathbf{e}_2'$, $\omega'(\eta''^{-1}.m(0,y)) = \frac{1}{2}\mathbf{e}_1'$ and, by Remark 5.11, we get (g').

2. Example 4.9. $P'' = O'' + \mathbf{0}$; (λ'') gives $\overline{\omega''(\eta''^{-1}.4^+(0,0))} = \mathbf{0}$, $\overline{\omega''(\eta''^{-1}.m(0,y))} = \mathbf{0}$; by Remark 5.11 we get (g'').

F. The arithmetic classification principle

We are now ready to give an intrinsic definition of the arithmetic equivalence for structures. Write $\eta_{\mathcal{A}}: E_L \to Iso\,(W_{\mathcal{A}})$ for $A.((\omega_\alpha)_{\alpha\in\mathcal{A}}, \delta) := ((A.\omega_\alpha)_{\alpha\in\mathcal{A}}, \delta)$.

Definition 5.13: Two structures with the same arithmetic architecture $\mathcal{A}$, $\mathbb{S}' \hookrightarrow \mathbb{E}'$ and $\mathbb{S}'' \hookrightarrow \mathbb{E}''$, are *arithmetically equivalent* if

1. $L(\mathbb{E}')_{L(\mathbb{S}')} = L(\mathbb{E}'')_{L(\mathbb{S}'')}$ (call them E_L), and hence $W_{\mathcal{A}}(\mathbb{S}') = W_{\mathcal{A}}(\mathbb{S}'')$ (call them $W_{\mathcal{A}}$),

2. for $(P'_\alpha)_{\alpha\in\mathcal{A}}$, $(P''_\alpha)_{\alpha\in\mathcal{A}}$ essential arithmetic descriptors for $\mathbb{S}'$, $\mathbb{S}''$, respectively, there exist $(([\Omega], \Delta), A) \in (W_{\mathcal{A}}/L) \rtimes_{\eta_{\mathcal{A}}} Iso(E_L)$ such that

$$\mathcal{C}\left(\begin{array}{c|c} A & [\Omega] \\ \hline & \widetilde{\Delta} \end{array}\right) : \Lambda(\mathbb{S}')_{(P'_\alpha)_{\alpha\in\mathcal{A}}} \to \Lambda(\mathbb{S}'')_{(P''_\alpha)_{\alpha\in\mathcal{A}}} \text{ is a (Group-)isomorphism.} \tag{5.2}$$

Explicitly, the conjugation in (5.2) is:

$$\mathcal{C}\left(\begin{array}{c|c} A & [\Omega] \\ \hline & \widetilde{\Delta} \end{array}\right)\left(\begin{array}{c|c} \eta'(q') & [\omega'] \\ \hline & \widetilde{\delta'} \end{array}\right) = \left(\begin{array}{c|c} \eta''(\eta''^{-1}\mathcal{C}_A\eta'(q')) & [A\,.\,\omega'\widetilde{\Delta}^{-1} + (\Omega\widetilde{\Delta}^{-1}.\widetilde{C_\Delta(\delta')} - \eta''^{-1}\mathcal{C}_A\eta'(q')\,.\,\Omega\widetilde{\Delta}^{-1})] \\ \hline & \widetilde{C_\Delta(\delta')} \end{array}\right),$$

where the symbol "$\widetilde{\ }$" refers to the standard permutation representation (see the Appendix). This definition should be compared with that of Ref. 24. Although slightly different, they are equivalent; the main differences are: (a) the use of a different representation, where we use the standard one, for the colored permutations; (b) the use, in $W_{\mathcal{A}}$, of the quotient with respect to the first component $((1,0,\ldots,0)L(\mathbb{S}), \mathrm{id})$, where we use that with respect to the diagonal $((1,\ldots,1)L(\mathbb{S}), \mathrm{id})$.

Remark 5.15: By proceeding in a more involved way, one can avoid, in Definition 5.13, to assume *a priori* that the two structures share the same arithmetic architecture, and show this is a necessary consequence of their arthmetic equivalence.

In Definition 5.13, the structures are involved only through their lattice groups; the chosen essential arithmetic descriptors are not directly involved. Actually:

Remark 5.15: Definition 5.13 does not depend on the essential arithmetic descriptors chosen.

Proof: Let $(P'_\alpha)_{\alpha\in\mathcal{A}}$, $(P''_\alpha)_{\alpha\in\mathcal{A}}$, be two essential arithmetic descriptors for a structure $\mathbb{S}$. By definition there exists $t\in L(\mathbb{E})/L(\mathbb{S})$ and $(\Omega,\Delta)\in W_{\mathcal{A}}(\mathbb{S})/L(\mathbb{S})$ such that

$$(t*_\sigma \mathrm{id})\,.\,P'_\alpha=(\Omega_\alpha*\mathrm{id})\,.\,P''_{\Delta(\alpha)}\ \forall\ \alpha\in\mathcal{A}.$$

It is straightforward to see that $\mathcal{C}_{\left(\begin{array}{c|c}\eta(\mathrm{id}) & [\Omega]\\ \hline & \tilde{\Delta}\end{array}\right)}:\Lambda(\mathbb{S})_{(P'_\alpha)_{\alpha\in\mathcal{A}}}\to\Lambda(\mathbb{S})_{(P''_\alpha)_{\alpha\in\mathcal{A}}}$ is a (*Group*-) isomorphism satisfying condition (5.2). □

VI. SOME RESULTS ON THE ARITHMETIC CLASSIFICATION SCHEME

A. Basic features of the arithmetic criterion

We now show that the arithmetic criterion satisfies the basic requirements for any symmetry-based classification schemes mentioned in Sec. I.

Remark 6.1: The arithmetic criterion coincides with the Bravais classification scheme when restricted to simple lattices.

Proof: When $|\mathcal{A}|$ is made up of one only element, $W_{\mathcal{A}}$ is the trivial group; the conclusion is now straightforward from the definitions. □

Remark 6.2: The arithmetic criterion has intrinsic character.

Proof: Let $\mathbb{S}'\hookrightarrow\mathbb{E}'$, $\mathbb{S}''\hookrightarrow\mathbb{E}''$ be two structures, $\phi\in\mathrm{Aff}(\mathbb{E}',\mathbb{E}'')$ with $\mathbb{S}'\overset{\phi}{\to}\mathbb{S}''$ ($\mathfrak{C}$-*Set*-)isomorphism and $G(\mathbb{S}')\overset{C_\phi}{\to}G(\mathbb{S}'')$ (*Group*-)isomorphism. We must prove that $\mathbb{S}'$ and $\mathbb{S}''$ are arithmetically equivalent. To do so, let $(P'_\alpha)_{\alpha\in\mathcal{A}}$ be an essential arithmetic descriptor for $\mathbb{S}'$ and $(P''_\alpha)_{\alpha\in\mathcal{A}}:=\phi(P'_\alpha)_{\alpha\in\mathcal{A}}$, with $c(P''_\alpha)_{\alpha\in\mathcal{A}}:=c(P'_\alpha)_{\alpha\in\mathcal{A}}$. It is easily seen that $(P''_\alpha)_{\alpha\in\mathcal{A}}$ is an essential arithmetic descriptor for $\mathbb{S}''$. We prove that:

$$\mathcal{C}_{\left(\begin{array}{c|c}A & [0]\\ \hline & \tilde{\mathrm{id}}\end{array}\right)}:\Lambda(\mathbb{S}')_{(P'_\alpha)_{\alpha\in\mathcal{A}}}\to\Lambda(\mathbb{S}'')_{(P''_\alpha)_{\alpha\in\mathcal{A}}}\ \text{is a (}\textit{Group}\text{-)isomorphism,}$$

where $A:=\mathcal{I}''^{-1}\circ\phi\circ\mathcal{I}'$. We establish $\mathcal{C}_{\left(\begin{array}{c|c}A & [0]\\ \hline & \tilde{\mathrm{id}}\end{array}\right)}:\Lambda(\mathbb{S}')_{(P'_\alpha)_{\alpha\in\mathcal{A}}}\hookrightarrow\Lambda(\mathbb{S}'')_{(P''_\alpha)_{\alpha\in\mathcal{A}}}$, the other inclusion being shown in an analogous way. Take $\left(\begin{array}{c|c}\eta'(q') & [\omega']\\ \hline & \tilde{\delta}'\end{array}\right)\in\Lambda(\mathbb{S}')_{(P'_\alpha)_{\alpha\in\mathcal{A}}}$; hence:

$(([\omega'],\delta'),q')\in(W_{\mathcal{A}}/L)\rtimes_{\eta_{\mathcal{A}}}P$ and there exists a unique $[t']\in E/L$ such that

$$(t'*_{\sigma'}q')\,.\,P'_\alpha=(\omega'_\alpha*\mathrm{id})\,.\,P'_{\delta'(\alpha)}\ \forall\ \alpha\in\mathcal{A}.$$

By inserting the identity $\phi^{-1}\circ\phi=\mathrm{id}$ into the left-hand side, pre-composing both sides by ϕ and defining $A:=\mathcal{I}''^{-1}\circ\phi\circ\mathcal{I}'$, we have:

$$\mathcal{C}_\phi(t'*_{\sigma'}q')\phi\,.\,P'_\alpha=(A\,.\,\omega'_\alpha*\mathrm{id})\,.\,\phi P'_{\delta'(\alpha)}\ \forall\ \alpha\in\mathcal{A}.$$

By construction $(P''_\alpha)_{\alpha\in\mathcal{A}}=\phi(P'_\alpha)_{\alpha\in\mathcal{A}}$; hence we have:

$$\mathcal{C}_\phi(t'*_{\sigma'}q')\,.\,P''_\alpha=(A\,.\,\omega'_\alpha*\mathrm{id})\,.\,P''_{\delta'(\alpha)}\ \forall\ \alpha\in\mathcal{A}.$$

Defining $[T]\in E/L$ by $\phi=:T*_{\sigma''}A$ (it depends on the splittings σ',σ''):

$$((At' *_{\sigma''}(\mathrm{id} - \eta''^{-1}(\mathcal{C}_A(\eta'(q')))) \,.\, T) *_{\sigma''} \mathcal{C}_A(\eta'(q'))) \,.\, P''_\alpha = (A \,.\, \omega'_\alpha * \mathrm{id}) \,.\, P''_{\delta'(\alpha)} \;\forall\; \alpha \in \mathcal{A}.$$

For $[t''] := A[t'] *_{\sigma''} (\mathrm{id} - \eta''^{-1}\mathcal{C}_A\eta'(q')) \,.\, [T]$, we have:

$$(([A \,.\, \omega'], \delta'), \eta''^{-1}\mathcal{C}_A\eta'(q')) \in (W_{\mathcal{A}}/L) \times_{\eta_{\mathcal{A}}} P$$

and

$$(t'' *_{\sigma''} \eta''^{-1}\mathcal{C}_A\eta'(q')) \,.\, P''_\alpha = (A \,.\, \omega'_\alpha * \mathrm{id}) \,.\, P''_{\delta'(\alpha)} \;\forall\; \alpha \in \mathcal{A}.$$

Therefore, by the explicit formula for conjugation in (5.2), we get:

$$\left(\begin{array}{c|c} \eta''(\eta''^{-1}\mathcal{C}_A\eta'(q')) & [A \,.\, \omega'] \\ \hline & \widetilde{\delta}' \end{array}\right) \in \Lambda(\mathbb{S}'')_{(P''_\alpha)_{\alpha\in\mathcal{A}}},$$

i.e.,

$$\mathcal{C}_{\left(\begin{array}{c|c} A & [0] \\ \hline & \widetilde{\mathrm{id}} \end{array}\right)} \left(\begin{array}{c|c} \eta'(q') & [\omega'] \\ \hline & \widetilde{\delta}' \end{array}\right) \in \Lambda(\mathbb{S}'')_{(P''_\alpha)_{\alpha\in\mathcal{A}}},$$

and we are finished. □

In view of the intrinsic character of the arithmetic principle, its finiteness property can be formulated as follows:

Remark 6.3: There exists only a finite number of arithmetic nonequivalent classes of structures with given finite arithmetic architecture type and given space-group type.

B. Some known results on arithmetic classification

We summarize in Table I some known results[6,8,9,15,25,11] which refer to the arithmetic classification of full structures in dimensions 2 and 3.

C. Examples of arithmetically nonequivalent isosymmetric structures

We conclude with two examples of structures which are space-group type, but not arithmetically, equivalent. These show once more that the arithmetic scheme is finer than classification by space-group type.

Example 6.4: The two structures described in Examples 5.8, 5.9 have the same space-group type *p*4*mm* (actually the same space group once their Euclidean spaces are identified as we did earlier), same arithmetic architecture type {4}, and same geometric architecture type {1}. (The geometric architecture type describes the number of space-group orbits forming a structure and their colors, much the same way the arithmetic architecture type describes the number of translation-group orbits forming a structure and their colors. In other words, the crystallographic architecture type gives the number of "atoms," of each different species, that are present in a asymmetric cell.[15]) Notice anyway that the two structures are space-group orbits of different lattice complexes, *p*4*mm#d* and *p*4*mm#f*, respectively.[15,6].

Example 6.5: The following, taken from Ref. 24, is a subtler example. Figure 4 shows two structures with the same space-group type *Pmmm* (even the same space group if their Euclidean spaces are identified in the obvious way), same arithmetic architecture type {3} (the space-group type together with the arithmetic architecture type amounts to giving the colored version of the Pearson symbol[15]), same geometric architecture type {3}, whose space-group orbits all belong to the same lattice complex *Pmmm#a*. These two structures have *symmetry* properties whose differences are detected by the arithmetic scheme (Ref. 24) but not by any of the established criteria currently used in crystallography or physics.

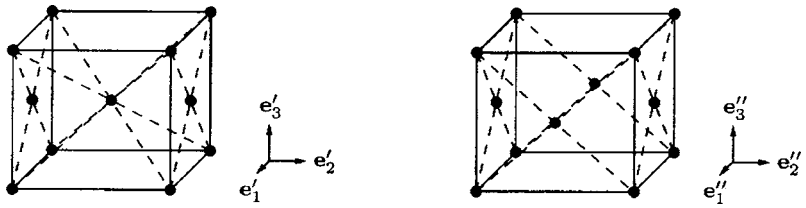

FIG. 4. Example of isosymmetric structures (Ref. 24). All the faces are rectangles (primitive translational cells shown).

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APPENDIX

We briefly recall the essential mathematics we need; see Ref. 19 for more details.

1. Set theory

a. For a family of sets $(X_\alpha)_{\alpha\in\mathcal{A}}$ (respectively, maps $(X_\alpha \overset{f_\alpha}{\to} Y_\alpha)_{\alpha\in\mathcal{A}}$), $\amalg_{\alpha\in\mathcal{A}}(X_\alpha)$ (respectively, $\amalg_{\alpha\in\mathcal{A}}(X_\alpha \overset{f_\alpha}{\to} Y_\alpha)$) denotes their *disjoint union*. For an indexing set $\mathcal{A}$ and a set X (respectively, a map $X \overset{f}{\to} Y$), $X^{\mathcal{A}}$ (respectively, $f^{\mathcal{A}}$) denotes the *direct product* of copies of the set X (respectively, the map $X \overset{f}{\to} Y$), one copy for each element of $\mathcal{A}$.

b. For any given set $\mathfrak{C}$, to be interpreted as a set of colors, we define the $\mathfrak{C}$-*Set* category as follows: an object is a (*Set*-)morphism $c: S \to \mathfrak{C}$ (S is a set S and c specifies how S is colored); a morphism between the objects $c': S' \to \mathfrak{C}$ and $c'': S'' \to \mathfrak{C}$ is a (*Set*-)morphism $f: S' \to S''$ preserving colors, i.e., such that

$$\begin{array}{ccc} S' & \xrightarrow{c'} & \mathfrak{C} \\ f\downarrow & & \downarrow \mathrm{id}\,. \\ S'' & \xrightarrow{c''} & \mathfrak{C} \end{array}$$

Clearly in the noncolored case, i.e., when $\mathfrak{C}$ is made up of one only element, the $\mathfrak{C}$-*Set* category and the *Set* category are equivalent; in this case $c: S \to \mathfrak{C}$ is trivially determined by S only.

c. For a $\mathfrak{C}$-set $\mathbb{X}$, we write $|\mathbb{X}|$ for its associated *multiset*. This is the nonordered family of natural numbers (repetitions are allowed) counting the elements of $\mathbb{X}$ for each of its colors. For example, for $\mathbb{X} = (\{a,b\} \mapsto \alpha) \amalg (\{c\} \mapsto \beta) \amalg (\{d,e\} \mapsto \gamma)$, we have $|\mathbb{X}| = \{1,2,2\}$.

2. Group theory

a. For a group G and $g \in G$, $\mathcal{C}_g$: $G \ni h \mapsto ghg^{-1} \in G$ denotes the *conjugation* by g. $\langle (g_k)_{k\in K} \rangle$ denotes the subgroup of G generated by $(g_k)_{k\in K}$.

The next two definitions give the construction of certain groups. Instead of using the more compact description, we represent them more concretely via suitable matrix groups; although this is somewhat awkward, it avoids excessive formal style.

b. Given two groups X, Z and an action $\eta: Z \to \mathrm{Iso}(X)$, the *semi-direct product* $X \rtimes_\eta Z$ can be described, when η is faithful, by the group of matrices of the form:

$$\left(\begin{array}{c|c} \eta(z) & x \\ \hline & \mathrm{id} \end{array}\right),$$

with $z \in Z$ and $x \in X$. Performing the matrix product, one formally proceeds by paying attention to the order of the operations involved; the product operation must be replaced by the action of $\mathrm{Iso}(X)$ on X, while the sum operation by $\cdot_{X^{\mathrm{op}}}$; X^{op} is the opposite group of X. In this paper X can be non-Abelian, so strictly speaking, the common matrix notation is slightly out of place. The matrix shown above is denoted by (x,z). Explicitly:

$$\left(\begin{array}{c|c} \eta(z') & x' \\ \hline & \mathrm{id} \end{array}\right) \cdot_{X \rtimes_\eta Z} \left(\begin{array}{c|c} \eta(z'') & x'' \\ \hline & \mathrm{id} \end{array}\right) = \left(\begin{array}{c|c} \eta(z' \cdot_Z z'') & x' \cdot_X (\eta(z') \,.\, x'') \\ \hline & \mathrm{id} \end{array}\right).$$

c. For H a group, I a $\mathfrak{C}$-set and S a subgroup of $\mathrm{Iso}(I)$, the *wreath product* $H \chi S$ can be described by the group of matrices of the form:

$$\left(\begin{array}{c|c} \mathrm{id} & \omega \\ \hline & \widetilde{\delta} \end{array}\right).$$

The right part of the matrix has columns indexed by the elements of I, $\omega = (\omega_i)_{i \in I} \in H^I$ and $\widetilde{\delta}$ is the standard representation of $\delta \in Iso(I)$ on the set I. The matrix shown above is denoted by (ω, δ). Explicitly:

$$\left(\begin{array}{c|c} \mathrm{id} & \omega' \\ \hline & \widetilde{\delta'} \end{array}\right) \cdot_{H \chi S} \left(\begin{array}{c|c} \mathrm{id} & \omega'' \\ \hline & \widetilde{\delta''} \end{array}\right) = \left(\begin{array}{c|c} \mathrm{id} & \omega'' \cdot_H (\omega' \,.\, \widetilde{\delta''}) \\ \hline & \widetilde{\delta' \cdot_S \delta''} \end{array}\right).$$

d. For G a group and H a subgroup of it, G_H denotes them when considered simultaneously. In particular, $\mathrm{Iso}(G_H)$ is the subset of $\mathrm{Iso}(G)$ whose elements induce morphisms in $\mathrm{Iso}(H)$.

3. Group actions

a. Given an action $\delta: G \to \mathrm{Iso}(X)$, $X \backslash G$ denotes the *G-orbit space* of X relative to δ; the points of $X \backslash G$ are called the orbits of G acting on X via δ. The natural projection is $X \ni x \mapsto [x] \in X \backslash G$. An action $\eta: G \to \mathrm{Iso}(X)$ is *faithful* if $\eta: G \to \mathrm{Iso}(X)$ is injective.

b. A (*Group*-)morphism $\delta: G \to \mathrm{Iso}(X)$ with G group and X $\mathfrak{C}$-set is called a *permutation representation* of the group G on the $\mathfrak{C}$-set X. We write the elements of $\mathrm{Iso}(X)$ via cycles' notation[19] or via the standard linear permutation representation. The latter is constructed as follows: for a set $\mathcal{A}$, consider the abstract vector space with $(\alpha)_{\alpha \in \mathcal{A}}$ as basis, then the standard linear permutation representation of $\delta \in \mathrm{Iso}(\mathcal{A})$ is the (*Vectorspace*-)morphism sending the vector α to the vector $\delta(\alpha)$. For example, let $\mathcal{A} = \{a,b,c\}$; representing the permutation via cycles' notation we have (we write the elements of the basis $\mathcal{A}$ from left to right in the order a,b,c):

$$(a)(b)(c) \rightsquigarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (a,b)(c) \rightsquigarrow \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (a,b,c) \rightsquigarrow \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

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Markov property and strong additivity of von Neumann entropy for graded quantum systems

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The quantum Markov property is equivalent to the strong additivity of von Neumann entropy for graded quantum systems. The additivity of von Neumann entropy for bipartite graded systems implies the statistical independence of states. However, the structure of Markov states for graded systems is different from that for tensor-product systems which have trivial grading. For three-composed graded systems we have U(1)-gauge invariant Markov states whose restriction to the marginal pair of subsystems is nonseparable. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We are interested in characterization of state correlations for general composite systems which do not necessarily satisfy the local commutativity. Here we specifically consider finite-dimensional quantum systems with graded commutation relations. For such systems as well, we can divide the total system into the subsystem on a specified region and that on its complement region and discuss the nature of state correlations between them as in the tensor-product systems.

We have pointed out that known criterions of separability for tensor-product systems should be altered for lattice fermion systems[11] when fermion hopping terms are present. (Note that purely fermionic correlation due to fermion hopping terms cannot be distilled to use.)

We are going to discuss quantum Markov property,[1] a quantum version of Markov property invented by Accardi. This is given by means of quasiconditional expectations and has played various roles, see, e.g., Ref. 2. We can view the Markov property as a kind of characterization of state correlation for composite systems. A pivotal example of quantum composite systems is tensor product of Hilbert spaces for which lots of works, prominently those on Markov chains for one-dimensional quantum spin lattice systems have been done.

We note that the definition of Markov property has been given under a very general setting that is not limited to the most familiar case of tensor-product systems. That is, it does not require in principle any specific *algebraic location* among subsystems imbedded in the total system.[3] Its detailed analysis for the setting of nonindependent systems, however, has started only recently. Reference 4 investigates Markov chains for one-dimensional (spinless) fermion lattice systems. It has been clarified there that the notion of Markov property and of the Markov chain is well applicable to fermion lattice systems. [More precisely, the above Markov chain refers to (d)-Markovian chain,[1] see also Ref. 13 on the generalized Markov chain.] Furthermore, a class of U(1)-gauge invariant Markov chains with fermionic hopping correlations is given.[4]

It has been shown that the Markov property is tightly related to the sufficiency of conditional expectations through the strong subadditivity of von Neumann entropy: A state of a three-composed tensor-product system is Markovian if and only if it takes the equality for the strong subadditivity inequality of entropy, which will be referred to as "the strong additivity of entropy."[16,6,12,7]

We show that a similar equivalence relation of the Markov property and the strong additivity of entropy is valid for graded quantum systems. Its proof proceeds in much the same way as that

for the tensor-product case following Ref. 15 (whose methods and results can be used in the present nonindependent situation) with some simple modifications due to the grading.

We now introduce the graded systems under our consideration. Let $\mathfrak{F}$ be a lattice and $\{\mathcal{A}_{\mathbf{I}};\mathbf{I}\in\mathfrak{F}\}$ be a family of $*$-algebras that have a common unital element denoted $\mathbf{1}$. If $\mathbf{I}\subset\mathbf{J}$, then $\mathcal{A}_{\mathbf{I}}\subset\mathcal{A}_{\mathbf{J}}$, and if $\mathbf{I}\cap\mathbf{J}=\emptyset$, then $\mathcal{A}_{\mathbf{I}}\cap\mathcal{A}_{\mathbf{J}}=\mathbb{C}\mathbf{1}$. Let Θ be an involutive $*$-automorphism of $\mathcal{A}$ that determines the grading as

$$\mathcal{A}^e := \{A\in\mathcal{A}\,|\,\Theta(A)=A\},\quad \mathcal{A}^o := \{A\in\mathcal{A}\,|\,\Theta(A)=-A\}. \tag{1}$$

We assume that our grading transformation Θ is nontrivial. The above $\mathcal{A}^e$ and $\mathcal{A}^o$ (which is not empty) are called the even and odd parts of $\mathcal{A}$. For $\mathbf{I}\in\mathfrak{F}$

$$\mathcal{A}^e_{\mathbf{I}} := \mathcal{A}^e\cap\mathcal{A}_{\mathbf{I}},\quad \mathcal{A}^o_{\mathbf{I}} := \mathcal{A}^o\cap\mathcal{A}_{\mathbf{I}}. \tag{2}$$

For $A\in\mathcal{A}(\mathcal{A}_{\mathbf{I}})$ we have the even-odd decomposition:

$$A=A_+ + A_-,\quad A_+ := \tfrac{1}{2}(A+\Theta(A))\in\mathcal{A}^e(\mathcal{A}^e_{\mathbf{I}}),\quad A_- := \tfrac{1}{2}(A-\Theta(A))\in\mathcal{A}^o(\mathcal{A}^o_{\mathbf{I}}). \tag{3}$$

We introduce U(1) gauge transformation:

$$\gamma_\theta(a_i^*)=e^{i\theta}a_i^*,\quad \gamma_\theta(a_i)=e^{-i\theta}a_i \tag{4}$$

for $\theta\in\mathbb{C}^1$. A state invariant under Θ is called even, and that invariant under γ_θ for any $\theta\in\mathbb{C}^1$ is called U(1)-gauge invariant.

If a pair of subsets $\mathbf{I}$ and $\mathbf{J}$ of $\mathfrak{F}$ are disjoint, then the following graded commutation relations hold:

$$[\mathcal{A}^e_{\mathbf{I}},\mathcal{A}^e_{\mathbf{J}}]=0,\quad [\mathcal{A}^e_{\mathbf{I}},\mathcal{A}^o_{\mathbf{J}}]=0,\quad [\mathcal{A}^o_{\mathbf{I}},\mathcal{A}^e_{\mathbf{J}}]=0,\quad \{\mathcal{A}^o_{\mathbf{I}},\mathcal{A}^o_{\mathbf{J}}\}=0, \tag{5}$$

where $[A,B]=AB-BA$ denotes the commutator and $\{A,B\}=AB+BA$ the anticommutator.

We assume that $\mathcal{A}_{\mathbf{I}}$ is isomorphic to a finite-dimensional type-I factor (a full matrix algebra) for any $\mathbf{I}\in\mathfrak{F}$. Under this assumption, there is a unitary $v_{\mathbf{I}}$ in $\mathcal{A}_{\mathbf{I}}$ that implements Θ on $\mathcal{A}_{\mathbf{I}}$ as

$$v_{\mathbf{I}}^*(A)v_{\mathbf{I}}=\Theta(A),\quad A\in\mathcal{A}_{\mathbf{I}}. \tag{6}$$

This $v_{\mathbf{I}}$ is even, since $\Theta(v_{\mathbf{I}})=v_{\mathbf{I}}^*(v_{\mathbf{I}})v_{\mathbf{I}}=(v_{\mathbf{I}}^*v_{\mathbf{I}})v_{\mathbf{I}}=v_{\mathbf{I}}$. For disjoint $\mathbf{I}$ and $\mathbf{J}$, the unitary $v_{\mathbf{I}\cup\mathbf{J}}$ of (6) for $\mathcal{A}_{\mathbf{I}\cup\mathbf{J}}$ is given by $v_{\mathbf{I}}v_{\mathbf{J}}$.

The lattice fermion system is a typical example of the graded quantum systems. Let a_i^* and a_i be creation and annihilation operators on the specified site i in a lattice. For each finite subset $\mathbf{I}$, the subsystem $\mathcal{A}_{\mathbf{I}}$ are generated by a_i^* and a_i in $\mathbf{I}$. The even-odd grading transformation is given by

$$\Theta(a_i^*)=-a_i^*,\quad \Theta(a_i)=-a_i.$$

The unitary $v_{\mathbf{I}}$ is given by $v_{\mathbf{I}}:=\Pi_{i\in\mathbf{I}}v_i$, $v_i:=a_i^*a_i-a_ia_i^*$.

We shall provide the plan of this paper. In Sec. II we introduce a formula of strong subadditivity of entropy (SSA)[8] in terms of the densities with respect to the tracial state for general composite systems made of finite-dimensional type-I factors. For the graded systems, it becomes the familiar formula of SSA in terms of the density matrices with respect to the matrix trace.

In Sec. III, the equivalence of the Markov property and the strong additivity of entropy for even states of the graded systems is shown. For noneven states, we have a weak result.

In Sec. IV, we consider restrictions of Markov states onto the marginal subsystems that are separated from each other. It was shown in Refs. 6 and 12 that a Markov state of a three-composed tensor-product system is separable (classically correlated) with respect to the marginal pair of subsystems. We show that this statement is invalid for the graded systems; there are U(1)-gauge invariant (hence obviously even) Markov states that are nonseparable for the marginal pair. Intuitively speaking, such Markov states have fermion hopping correlations between the marginal subsystems.

In Sec. V, we show that a state of a graded bipartite system satisfies the additivity of von Neumann entropy if and only if it is a product state. This is almost obvious if the state under consideration is assumed to be even. The point is that the evenness (at least on one of the pair of subsystems) follows from the additivity of entropy.

II. STRONG SUBADDITIVITY OF ENTROPY

We provide the strong subadditivity of entropy for a general setting that encompasses non-independent systems. Let $\mathcal{A}$ be a finite-dimensional type-I factor. Let τ denote the tracial state on $\mathcal{A}$. If an element $d \in \mathcal{A}$ is positive and normalized as $\tau(d)=1$, then it is called a density. For any state φ of $\mathcal{A}$, there exists a unique density $\rho_\varphi \in \mathcal{A}$ called the density of φ satisfying that

$$\varphi(a) = \tau(\rho_\varphi a), \quad a \in \mathcal{A}.$$

For the tracial state τ, its density is obviously $\mathbf{1}$, the unity of $\mathcal{A}$.

Let ρ_1 and ρ_2 be a pair of densities of $\mathcal{A}$. The relative entropy for them is defined by

$$H(\rho_1,\rho_2) := \tau(\rho_1(\ln \rho_1 - \ln \rho_2)) \tag{7}$$

if the support of ρ_1 is contained in ρ_2. Otherwise, we set it $+\infty$. For a pair of two states φ and ψ on $\mathcal{A}$, their relative entropy is

$$H(\varphi,\psi) := H(\rho_\varphi,\rho_\psi). \tag{8}$$

We define the entropy for a given state φ as

$$\hat{S}(\varphi) := -\varphi(\ln \rho_\varphi). \tag{9}$$

We see

$$\hat{S}(\varphi) = -H(\varphi,\tau).$$

Probably the following is a more frequently used definition of entropy:

$$S(\varphi) := -\mathbf{Tr}(D_\varphi \ln D_\varphi) = -\varphi(\ln D_\varphi),$$

where $\mathbf{Tr}$ is the matrix trace that takes 1 for each one-dimensional projection, and D_φ denotes the density matrix of φ with respect to $\mathbf{Tr}$. We see

$$\hat{S}(\varphi) = S(\varphi) - S(\tau) = S(\varphi) - \ln \mathbf{Tr}(\mathbf{1}) \tag{10}$$

for any state φ. Hence if $\mathcal{A}$ is a n by n full matrix algebra, $n \in \mathbb{N}$, then the difference $S(\varphi) - \hat{S}(\varphi)$ is constantly $\ln n$.

Let $\mathcal{B}$ be a subalgebra of $\mathcal{A}$. We denote the (uniquely determined) conditional expectation from $\mathcal{A}$ onto $\mathcal{B}$ with respect to the tracial state by $E_{\mathcal{B}}^{\mathcal{A}}$. Here, the upper-right subscript of E indicates the domain and the lower-right the range. Let $\varphi_{\mathcal{B}}$ denote the restriction of φ to $\mathcal{B}$. Then the density of $\varphi_{\mathcal{B}}$ is given by that of φ as

$$\rho_{\varphi_{\mathcal{B}}} = E_{\mathcal{B}}^{\mathcal{A}}(\rho_\varphi). \tag{11}$$

We have

$$\hat{S}(\varphi_{\mathcal{B}}) - \hat{S}(\varphi) = H(\rho_\varphi,\rho_{\varphi_{\mathcal{B}}}) = H\left(\varphi,\varphi_{\mathcal{B}} \otimes \mathrm{tr}\big|_{\mathcal{A}\cap\mathcal{B}'}\right) = H(\varphi,\varphi\circ E_{\mathcal{B}}^{\mathcal{A}}). \tag{12}$$

As a special case of (12),

$$\hat{S}(\varphi_{\mathcal{B}}) = \hat{S}(\varphi\circ E_{\mathcal{B}}^{\mathcal{A}}). \tag{13}$$

In fact, we have so far assumed that φ is a faithful state, but (12) is valid when φ is nonfaithful. To see this, we take $\varepsilon\cdot\tau+(1-\varepsilon)\varphi$ where ε is a positive small number and then take the limit $\varepsilon\to 0$.

Let us take three disjoint subsets A, B, and C. Let $\mathcal{A}_{ABC}$, $\mathcal{A}_{AB}$, $\mathcal{A}_{BC}$, and $\mathcal{A}_B$ denote finite-dimensional quantum systems corresponding to the indexes. Let $E_{A,B}^{A,B,C}$ and $E_A^{A,B}$ denote the trace preserving conditional expectation from $\mathcal{A}_{ABC}$ onto $\mathcal{A}_{AB}$ and that from $\mathcal{A}_{AB}$ onto $\mathcal{A}_A$, respectively. We use similar notations for other indexes. If the domain is the total system $\mathcal{A}_{ABC}$, then we simply write, e.g., $E_{A,B}$ instead of $E_{A,B}^{A,B,C}$ when there is no fear of confusion.

The following five conditions, called the commuting square condition, are all equivalent to each other:

(1) $E_{A,B}|\mathcal{A}_{BC}=E_B^{B,C}$,
(2) $E_{B,C}|\mathcal{A}_{AB}=E_B^{A,B}$,
(3) $\mathcal{A}_B=\mathcal{A}_{AB}\cap\mathcal{A}_{BC}$ and $E_{A,B}E_{B,C}=E_{B,C}E_{A,B}$,
(4) $E_{A,B}E_{B,C}=E_B$,
(5) $E_{B,C}E_{A,B}=E_B$.

If our three-composed system $\mathcal{A}_{ABC}$ satisfies this commuting square condition, then the strong subadditivity of entropy $\hat{S}(\psi)$ for any state ψ follows. The proof is standard and easy, but we recapture it for completeness.

Proposition 1: Let $\mathcal{A}_{ABC}$, $\mathcal{A}_{AB}$, $\mathcal{A}_{BC}$, and $\mathcal{A}_B$ be finite-dimensional factors satisfying the commuting square condition, and let ψ_{ABC} be an arbitrary state on $\mathcal{A}_{ABC}$. Then

$$\hat{S}(\psi_{ABC})-\hat{S}(\psi_{AB})-\hat{S}(\psi_{BC})+\hat{S}(\psi_B)\leqslant 0. \tag{14}$$

Furthermore, if the system satisfies the graded commutation relations (5), then

$$S(\psi_{ABC})-S(\psi_{AB})-S(\psi_{BC})+S(\psi_B)\leqslant 0. \tag{15}$$

Proof: By (12) and (13), and the relation $E_{B,C}E_{A,B}=E_{A,B}E_{B,C}=E_B$, we obtain

$$\begin{aligned}\hat{S}(\psi_{BC})-\hat{S}(\psi_{ABC}) &= H(\psi_{ABC},\psi_{ABC}\circ E_{B,C})\geqslant H(\psi_{ABC}\circ E_{A,B},\psi_{ABC}\circ E_{B,C}\circ E_{A,B})\\ &= H(\psi_{ABC}\circ E_{A,B},\psi_{ABC}\circ E_{A,B}\circ E_{B,C})=H(\psi_{ABC}\circ E_{A,B},\psi_{ABC}\circ E_B)\\ &= \hat{S}(\psi_{ABC}\circ E_B)-\hat{S}(\psi_{ABC}\circ E_{A,B})=\hat{S}(\psi_B)-\hat{S}(\psi_{AB}),\end{aligned} \tag{16}$$

where the inequality is due to the monotonicity of relative entropy under the action of completely positive maps.

Let us turn to the graded systems of finite-dimensional factors, which satisfy the commuting square condition.[5] Suppose that $\mathbf{I}$ and $\mathbf{J}$ are disjoint subsets. Then the matrix trace on $\mathcal{A}_{\mathbf{I}\cup\mathbf{J}}$ denoted $\mathbf{Tr}_{\mathbf{I}\cup\mathbf{J}}$ is given by the product extension of those in $\mathcal{A}_{\mathbf{I}}$ and in $\mathcal{A}_{\mathbf{J}}$ denoted $\mathbf{Tr}_{\mathbf{I}}$ and $\mathbf{Tr}_{\mathbf{J}}$, respectively. Thus we have $\mathbf{Tr}_{\mathbf{I}\cup\mathbf{J}}(\mathbf{1})=\mathbf{Tr}_{\mathbf{I}}(\mathbf{1})\times\mathbf{Tr}(\mathbf{1})$. Now (14) and (10) imply (15). ■

As this proposition indicates, the strong additivity of entropy is satisfied irrespective of whether states are even or not. In Refs. 9 and 10 we have shown that noneven states may induce pathological state correlations and some entropy inequalities known for tensor-product systems do not hold in general for the graded systems.

III. MARKOV PROPERTY AND STRONG ADDITIVITY

It is obvious that the equality of (14) and of (15) is equivalent to that of (16), i.e.,

$$H(\psi_{ABC},\psi_{ABC}\circ E_{B,C})=H(\psi_{ABC}\circ E_{A,B},\psi_{ABC}\circ E_B), \tag{17}$$

equivalently,

$$H(\rho_{\psi_{ABC}},\rho_{\psi_{BC}})=H(\rho_{\psi_{AB}},\rho_{\psi_B}). \tag{18}$$

By a general result of the sufficiency given in Ref. 15, (17) implies that the conditional expectation $E_{A,B}$ is sufficient for $\psi_{ABC}\circ E_{B,C}$ and ψ_{ABC}, that is, there exists a completely positive map that recovers $\psi_{ABC}\circ E_{B,C}$ and ψ_{ABC} from $\psi_{ABC}\circ E_{B,C}\circ E_{A,B}$ and $\psi_{ABC}\circ E_{A,B}$, respectively. The canonical form of such maps is given as follows.[12]

Let α denote the completely positive map on $\mathcal{A}$ defined by

$$\alpha(X) := \rho_{\psi_B}{}^{-1/2} E_{A,B}(\rho_{\psi_{BC}}{}^{1/2} X \rho_{\psi_{BC}}{}^{1/2}) \rho_{\psi_B}{}^{-1/2}, \quad X \in \mathcal{A}_{ABC}. \tag{19}$$

Let $T^\sharp$ denote the dual of α with respect to the tracial stare, which is written as

$$T^\sharp(X) := \rho_{\psi_{BC}}{}^{1/2} \rho_{\psi_B}{}^{-1/2} X \rho_{\psi_B}{}^{-1/2} \rho_{\psi_{BC}}{}^{1/2}, \quad X \in \alpha(\mathcal{A}_{ABC}). \tag{20}$$

It is easy to see $T^\sharp(\rho_{\psi_B}) = \rho_{\psi_{BC}}$. Also $T^\sharp(\rho_{\psi_{AB}}) = \rho_{\psi_{ABC}}$ is satisfied if and only if $E_{A,B}$ is sufficient for the given pair of states ψ_{ABC} and $\psi_{ABC}\circ E_{B,C}$, equivalently, (17) holds.

The following is a more or less summary of the contents stated above. It corresponds to Theorem 5.2 of Ref. 16 and also Sec. V of Ref. 12 where the statement is for the tensor-product systems.

Proposition 2: Let $\mathcal{A}_{ABC}$, $\mathcal{A}_{AB}$, $\mathcal{A}_{BC}$, and $\mathcal{A}_B$ be finite-dimensional factors satisfying the commuting square condition. Let ψ_{ABC} be an arbitrary faithful state on $\mathcal{A}_{ABC}$. The strong additivity of von Neumann entropy, i.e.,

$$S(\psi_{ABC}) - S(\psi_{AB}) - S(\psi_{BC}) + S(\psi_B) = 0 \tag{21}$$

is satisfied if and only if $E_{A,B}$ is sufficient for the pair of states ψ_{ABC} and $\psi_{ABC}\circ E_{B,C}$. Let α denote the ψ_{ABC}-preserving (and $\psi_{ABC}\circ E_{B,C}$-preserving) conditional expectation from $\mathcal{A}_{ABC}$ to $\mathcal{A}_{AB}$ given as (19). Let $T^\sharp$ denote the dual of this α with respect to the tracial state whose concrete formula is given as (20). This $T^\sharp$ gives the canonical left inverse of $E_{A,B}$ for the densities of ψ_{ABC} and $\psi_{ABC}\circ E_{B,C}$, that is,

$$T^\sharp(\rho_{\psi_B}) = \rho_{\psi_{BC}} \tag{22}$$

and

$$T^\sharp(\rho_{\psi_{AB}}) = \rho_{\psi_{ABC}}. \tag{23}$$

The set of fixed points of α contains $\mathcal{A}_A^e$. If the state ψ_{ABC} is even, then the set of fixed points of α contains $\mathcal{A}_A$ and accordingly the Markov property of ψ_{ABC} with respect to a triplet $(\mathcal{A}_A, \mathcal{A}_B, \mathcal{A}_C)$ is satisfied.

Proof: We shall confirm the part about the fixed point elements of α. Take $X \in \mathcal{A}_A^e$, which is in the commutant of $\mathcal{A}_{BC}$. We have

$$\begin{aligned}\alpha(X) &= \rho_{\psi_B}^{-1/2} E_{A,B}(\rho_{\psi_{BC}}^{1/2} X \rho_{\psi_{BC}}^{1/2}) \rho_{\psi_B}^{-1/2} = \rho_{\psi_B}^{-1/2} E_{A,B}(X \rho_{\psi_{BC}}) \rho_{\psi_B}^{-1/2} = \rho_{\psi_B}^{-1/2} X E_{A,B}(\rho_{\psi_{BC}}) \rho_{\psi_B}^{-1/2} \\ &= \rho_{\psi_B}^{-1/2} X E_{A,B}(E_{B,C}(\rho_{\psi_{BC}})) \rho_{\psi_B}^{-1/2} = \rho_{\psi_B}^{-1/2} X E_B(\rho_{\psi_{BC}}) \rho_{\psi_B}^{-1/2} = \rho_{\psi_B}^{-1/2} X \rho_{\psi_B} \rho_{\psi_B}^{-1/2} = X \rho_{\psi_B}^{-1/2} \rho_{\psi_B} \rho_{\psi_B}^{-1/2} = X.\end{aligned} \tag{24}$$

Suppose now that ψ_{ABC} is even. Then $\rho_{\psi_{BC}} \in \mathcal{A}_{BC}^e$ and also $\rho_{\psi_B} \in \mathcal{A}_B^e$ commute with any $X \in \mathcal{A}_A$. Hence we see that the above set of equalities (24) holds for this case. ■

From this result, if an even state satisfies the strong additivity of entropy, then the Markov property with respect to a triplet $(\mathcal{A}_A, \mathcal{A}_B, \mathcal{A}_C)$ in the sense of Ref. 1 (cf. Lemma 11.3 of Ref. 14) is satisfied. This in fact precisely specifies what we mean by the Markov property.

IV. MARKOV STATES ON THE MARGINAL SUBSYSTEMS

The definition of separable states (i.e., classically correlated states) for nonindependent systems is much the same as that for the tensor-product systems.[11] That is, if a state is written as a convex sum of some product states, then it is called a separable state. Let A and C be a pair of disjoint subsets, and ω be a state on $\mathcal{A}_{AC}$. If

$$\omega(XY) = \omega(X)\omega(Y) \tag{25}$$

for all $X \in \mathcal{A}_A$ and $Y \in \mathcal{A}_C$, then ω is called a product state with respect to the pair $(\mathcal{A}_A, \mathcal{A}_C)$. It is easy to see that the product property in the converse order,

$$\omega(YX) = \omega(Y)\omega(X) = \omega(XY) \tag{26}$$

follows from (25) and the graded commutation relations.

We discuss the property of Markov states with respect to $(\mathcal{A}_A, \mathcal{A}_B, \mathcal{A}_C)$ for the marginal subsystem $\mathcal{A}_{AC}$. As we announced in the introduction, Corollary 7 of Ref. 6 is invalid for the graded systems.

Proposition 3: For a three-composed graded system $(\mathcal{A}_A, \mathcal{A}_B, \mathcal{A}_C)$, *there exist U(1)-gauge invariant states that satisfy the Markov property for* $(\mathcal{A}_A, \mathcal{A}_B, \mathcal{A}_C)$ but are nonseparable for $(\mathcal{A}_A, \mathcal{A}_C)$.

We shall construct such Markov states. Using the Jordan-Wigner transformation, we set a three-composed tensor-product system in the following way. Let υ_A, υ_B, and $\upsilon_{A,B}$ denote the unitaries implementing Θ on the specified subsystems. Let $\mathcal{A}^s_A := \mathcal{A}_A$, $\mathcal{A}^s_{AB} := \mathcal{A}_{AB}$, $\mathcal{A}^s_{ABC} := \mathcal{A}_{ABC}$, $\mathcal{A}^s_B := \{\mathcal{A}^e_B, \upsilon_A \mathcal{A}^o_B\}$, $\mathcal{A}^s_C := \{\mathcal{A}^e_C, \upsilon_{A,B}\mathcal{A}^o_C\}$, and $\mathcal{A}^s_{BC} := \{\mathcal{A}^e_{BC}, \upsilon_A \mathcal{A}^o_{BC}\}$ where the notation $\{,\}$ denotes the algebra generated by the arguments. They induce a tensor-product system $\mathcal{A}^s_{ABC} = \mathcal{A}^s_A \otimes \mathcal{A}^s_B \otimes \mathcal{A}^s_C$. We assign finite-dimensional Hilbert spaces $\mathcal{H}_{\bar{A}}$, $\mathcal{H}_{\bar{B}}$ and $\mathcal{H}_{\bar{C}}$ to $\mathcal{A}^s_A$, $\mathcal{A}^s_B$ and $\mathcal{A}^s_C$, respectively. We will use the next lemma later. Its proof is obvious.

Lemma 4: Let ψ_{ABC} *be an arbitrary even state on* $\mathcal{A}_{ABC}$. *It satisfies*

$$S(\psi_{ABC}) - S(\psi_{AB}) - S(\psi_{BC}) + S(\psi_B) = 0, \tag{27}$$

if and only if

$$S(\psi_{ABC}) - S(\psi|_{\mathcal{A}^s_{AB}}) - S(\psi|_{\mathcal{A}^s_{BC}}) + S(\psi|_{\mathcal{A}^s_B}) = 0. \tag{28}$$

For a while we will focus on the two composed system, $\mathcal{A}_{AC}$. In Ref. 11 we have discussed how the state correlation (separability, nonseparability) will remain or change under the Jordan-Wigner transformation which maps the CAR pair $(\mathcal{A}_A, \mathcal{A}_C)$ to $(\mathcal{A}_A, \mathcal{A}^{\tilde{s}}_C)$, where $\mathcal{A}^{\tilde{s}}_C$ denotes the commutant of $\mathcal{A}_A$ in $\mathcal{A}_{AC}$ and is explicitly given as $\{\mathcal{A}^e_C, \upsilon_A \mathcal{A}^o_C\}$. (Note that $\mathcal{A}^{\tilde{s}}_C$ is different from previously introduced $\mathcal{A}^s_C$.) It has been shown that the set of all separable states for the CAR pair is strictly smaller than that for the tensor-product pair. That is, if ω_{AC} is a separable state for the pair $(\mathcal{A}_A, \mathcal{A}_C)$, then so it is for $(\mathcal{A}_A, \mathcal{A}^{\tilde{s}}_C)$. However, there exist U(1)-invariant states that are separable for the latter but nonseparable for the former. We introduce an example of such states from Ref. 11.

Let k_A and k_C be some nonzero odd elements in $\mathcal{A}_A$ and in $\mathcal{A}_C$, e.g., field operators on specified regions. Let $K := 1/2(k^*_A k_C - k_A k^*_C)$ which is self-adjoint and denotes fermion-hopping interaction between $\mathcal{A}_A$ and $\mathcal{A}_C$. Suppose that $\|k_A\| \leqslant 1 \|k_C\| \leqslant 1$, then $\|K\| \leqslant 1$. For $\lambda \in \mathbb{R}$, $|\lambda| \leqslant 1$, $\rho_{AC,\lambda} := 1 + \lambda K$ gives a density operator. For $0 < |\lambda| \leqslant 1$, the state on $\mathcal{A}_{AC}$ with its density $\rho_{AC,\lambda}$ gives a state satisfying all the desired conditions.

Now take such a U(1)-gauge invariant state ω_{AC} on $\mathcal{A}_{AC}$. It has a state decomposition $\omega_{AC} = \sum^n_{i=1} \lambda_i \omega_{AC,i}$, $0 < \lambda_i < 1$, $\Sigma \lambda_i = 1$, such that each $\omega_{AC,i}$ is a product state for $(\mathcal{A}_A, \mathcal{A}^{\tilde{s}}_C)$, but has no product-state decomposition for $(\mathcal{A}_A, \mathcal{A}_C)$. From this, we are going to construct a state on $\mathcal{A}_{ABC}$ that proves Proposition 3.

Let us assume that the dimension of $\mathcal{H}_{\bar{B}}$ is equal or more than n. Then we have a set of n non-zero even orthogonal projections $p_i \in \mathcal{A}^e_B$, $1 \leqslant i \leqslant n$. Let $\omega_{B,i}(X) := \tau(p_i X)/\tau(p_i)$, for $X \in \mathcal{A}_B$.

Those are all even states of $\mathcal{A}_B$. Let $\omega_{ABC} := \Sigma_{i=1}^{n} \lambda_i \omega_{AC,i} \circ \omega_{B,i}$, where $\omega_{AC,i} \circ \omega_{B,i}$ denotes the (uniquely determined) product state extension of $\omega_{AC,i}$ on $\mathcal{A}_{AC}$ and $\omega_{B,i}$ on $\mathcal{A}_B$, see Ref. 5.

We will see that $\omega_{AC,i} \circ \omega_{B,i}$ gives a product state for $(\mathcal{A}_A, \mathcal{A}_C^s)$ when restricted to $\mathcal{A}_A \otimes \mathcal{A}_C^s$. We must check this for the product element ac_+ such that $a \in \mathcal{A}_A$ and $c_+ \in \mathcal{A}_C^e$, and for $a(v_A v_B c_-)$ such that $a \in \mathcal{A}_A$ and $c_- \in \mathcal{A}_C^o$. We have

$$\omega_{AC,i} \circ \omega_{B,i}(ac_+) = \omega_{AC,i}(ac_+) = \omega_{AC,i}(a)\omega_{AC,i}(c_+) = \omega_{AC,i} \circ \omega_{B,i}(a)\omega_{AC,i} \circ \omega_{B,i}(c_+), \tag{29}$$

and using the product property of $\omega_{AC,i}$ for $(\mathcal{A}_A, \mathcal{A}_C^{\tilde{s}})$,

$$\begin{aligned}\omega_{AC,i} \circ \omega_{B,i}(av_A v_B c_-) &= \omega_{AC,i} \circ \omega_{B,i}(av_A c_- v_B) = \omega_{AC,i}(av_A c_-)\omega_{B,i}(v_B) = \omega_{AC,i}(a)\omega_{AC,i}(v_A c_-)\omega_{B,i}(v_B) \\ &= \omega_{AC,i}(a)\omega_{AC,i} \circ \omega_{B,i}(v_A c_- v_B) = \omega_{AC,i} \circ \omega_{B,i}(a)\omega_{AC,i} \circ \omega_{B,i}(v_A v_B c_-). \end{aligned} \tag{30}$$

Hence, $\omega_{AC,i} \circ \omega_{B,i}$ has a product state restriction, and accordingly ω_{ABC} has a separable state restriction for $(\mathcal{A}_A, \mathcal{A}_C^s)$. We conclude that our ω_{ABC} has the structure as in Theorem 6 of Ref. 6 or as the formula (14) of Ref. 12 with respect to $(\mathcal{H}_A^-, \mathcal{H}_B^-, \mathcal{H}_C^-)$. Hence, it satisfies the Markov property with respect to $(\mathcal{A}_A^s, \mathcal{A}_B^s, \mathcal{A}_C^s)$.

From the equivalence of the Markov property and the strong additivity of entropy for three-composed tensor-product systems, which has been shown in the above references, (28) is satisfied for ω_{ABC}. Since it is even, it satisfies (27) as well and, hence, is Markovian with respect to $(\mathcal{A}_A^s, \mathcal{A}_B^s, \mathcal{A}_C^s)$ by Proposition 2. As $\omega_{AC}|_{\mathcal{A}_{AC}} = \omega_{AC}$ is obviously nonseparable for $(\mathcal{A}_A, \mathcal{A}_C)$ by definition, ω_{ABC} gives a state showing Proposition 3.

V. ADDITIVITY OF VON NEUMANN ENTROPY AND THE PRODUCT PROPERTY

In this section, we consider a two-composed graded system $\mathcal{A}_{AC}$ generated by $\mathcal{A}_A$ and $\mathcal{A}_C$. Namely, we treat the case where the intersection region B is trivial. Then the strong subadditivity of entropy (15) becomes

$$S(\psi_{AC}) - S(\psi_A) - S(\psi_C) \leqslant 0, \tag{31}$$

which is called the subadditivity of entropy. We discuss characterization of additivity of entropy, i.e., the condition of equality of this inequality.

The answer is very simple for tensor-product systems: a state satisfies the additivity of entropy if and only if it is a product state. For the graded system, we can show a similar result easily under the assumption that the marginal states ψ_A and ψ_C are not both noneven. Let $\psi_A \circ \psi_C$ denote the product state of $\mathcal{A}_{AC}$ whose restrictions to $\mathcal{A}_A$ and $\mathcal{A}_C$ are ψ_A and ψ_C. Its existence is guaranteed if ψ_A and/or ψ_C is even. Then we have

$$S(\psi_{AC}) - S(\psi_A) - S(\psi_C) = -H(\psi_{AC}, \psi_A \circ \psi_C) \leqslant 0. \tag{32}$$

By the strict positivity of relative entropy, it is 0 if and only if $\psi_{AC} = \psi_A \circ \psi_C$.

Now we drop the evenness assumption on the states. If ψ_A and ψ_C are both noneven, then there is no product state extension for them.[5] Hence, the above argument using the strict positivity of relative entropy does not work for the general case.

Using Ref 12 we obtain the following result.

Proposition 5: Let ψ_{AC} be a state of the two-composed graded system $\mathcal{A}_{AC}$. It satisfies the additivity of entropy

$$S(\psi_{AC}) - S(\psi_A) - S(\psi_C) = 0, \tag{33}$$

if and only if it is a product state for $(\mathcal{A}_A, \mathcal{A}_C)$. If it is the case, at least one of ψ_A and ψ_C is even.

Proof: The equivalence of (33) and (18) when the middle part B is empty implies that (33) is equivalent to

$$H(\rho_{\psi_{AC}},\rho_{\psi_C}) = H(\rho_{\psi_A},\mathbf{1}). \tag{34}$$

This is equivalent to say that E_A is sufficient for $\rho_{\psi_{AC}}$ and ρ_{ψ_C}. Now from (20) the canonical left inverse of E_A for those densities is given by

$$T^\sharp(X) := \rho_{\psi_C}^{1/2} X \rho_{\psi_C}^{1/2}, \quad X \in \mathcal{A}_A. \tag{35}$$

Hence we have

$$\rho_{\psi_{AC}} = T^\sharp(\rho_{\psi_A}) = \rho_{\psi_C}^{1/2} \rho_{\psi_A} \rho_{\psi_C}^{1/2}. \tag{36}$$

Exchanging A and C and repeating the same argument as above, we have also

$$\rho_{\psi_{AC}} = \rho_{\psi_A}^{1/2} \rho_{\psi_C} \rho_{\psi_A}^{1/2}. \tag{37}$$

Let us take the decomposition of ρ_{ψ_A} into its even-odd parts and that of ρ_{ψ_C} as in (3),

$$\rho_{\psi_A} = \rho_{\psi_{A^+}} + \rho_{\psi_{A^-}}, \quad \rho_{\psi_{A^+}} \in \mathcal{A}_A^e, \quad \rho_{\psi_{A^-}} \in \mathcal{A}_A^o,$$

$$\rho_{\psi_C} = \rho_{\psi_{C^+}} + \rho_{\psi_{C^-}}, \quad \rho_{\psi_{C^+}} \in \mathcal{A}_C^e, \quad \rho_{\psi_{C^-}} \in \mathcal{A}_C^o. \tag{38}$$

Similarly take the even-odd decomposition of $\rho_{\psi_A}^{1/2}$ and that of $\rho_{\psi_C}^{1/2}$ in the following:

$$\rho_{\psi_A}^{1/2} = a_+ + a_-, \quad a_+ \in \mathcal{A}_A^e, \quad a_- \in \mathcal{A}_A^o,$$

$$\rho_{\psi_C}^{1/2} = c_+ + c_-, \quad c_+ \in \mathcal{A}_C^e, \quad c_- \in \mathcal{A}_C^o. \tag{39}$$

Since the densities are positive hence self-adjoint, each of a_+, a_-, c_+, and c_- is self-adjoint. We have

$$\rho_{\psi_A} = (\rho_{\psi_A}^{1/2})^2 = a_+^2 + a_-^2 + a_+a_- + a_-a_+,$$

$$\rho_{\psi_{A^+}} = a_+^2 + a_-^2,$$

$$\rho_{\psi_{A^-}} = a_+a_- + a_-a_+, \tag{40}$$

and

$$\rho_{\psi_C} = c_+^2 + c_-^2 + c_+c_- + c_-c_+,$$

$$\rho_{\psi_{A^+}} = c_+^2 + c_-^2,$$

$$\rho_{\psi_{A^-}} = c_+c_- + c_-c_+. \tag{41}$$

Now we shall express the equality $\rho_{\psi_C}^{1/2}\rho_{\psi_A}\rho_{\psi_C}^{1/2} = \rho_{\psi_A}^{1/2}\rho_{\psi_C}\rho_{\psi_A}^{1/2} = \rho_{\psi_{AC}}$ in terms of a_+, a_-, c_+, and c_-. We compute

$$\begin{aligned}
\rho_{\psi_C}^{1/2}\rho_{\psi_A}\rho_{\psi_C}^{1/2} &= \rho_{\psi_C}^{1/2}(\rho_{\psi_{A^+}} + \rho_{\psi_{A^-}})\rho_{\psi_C}^{1/2} = (\rho_{\psi_{A^+}}\rho_{\psi_C}^{1/2} + \rho_{\psi_{A^-}}\Theta(\rho_{\psi_C}^{1/2}))\rho_{\psi_C}^{1/2} = \rho_{\psi_{A^+}}\rho_{\psi_C} + \rho_{\psi_{A^-}}\Theta(\rho_{\psi_C}^{1/2})\rho_{\psi_C}^{1/2} \\
&= (a_+^2 + a_-^2)(c_+^2 + c_-^2 + c_+c_- + c_-c_+) + (a_+a_- + a_-a_+)(c_+ - c_-)(c_+ + c_-) \\
&= a_+^2(c_+^2 + c_-^2 + c_+c_- + c_-c_+) + a_-^2(c_+^2 + c_-^2 + c_+c_- + c_-c_+) + a_+a_-(c_+^2 - c_-^2 - c_-c_+ + c_+c_-)
\end{aligned}$$

$$+ a_-a_+(c_+^2 - c_-^2 - c_-c_+ + c_+c_-). \tag{42}$$

Also,

$$\begin{aligned}\rho_{\psi_A}^{1/2}\rho_{\psi_C}\rho_{\psi_A}^{1/2} &= \rho_{\psi_A}^{1/2}(\rho_{\psi_{C^+}} + \rho_{\psi_{C^-}})\rho_{\psi_A}^{1/2} = \rho_{\psi_A}\rho_{\psi_{C^+}} + \rho_{\psi_A}^{1/2}\Theta(\rho_{\psi_A}^{1/2})\rho_{\psi_{C^-}} \\ &= (a_+^2 + a_-^2 + a_+a_- + a_-a_+)(c_+^2 + c_-^2) + (a_+^2 - a_-^2 - a_+a_- + a_-a_+)(c_+c_- + c_-c_+) \\ &= a_+^2(c_+^2 + c_-^2 + c_+c_- + c_-c_+) + a_-^2(c_+^2 + c_-^2 - c_+c_- - c_-c_+) + a_+a_-(c_+^2 + c_-^2 - c_+c_- - c_-c_+) \\ &\quad + a_-a_+(c_+^2 + c_-^2 + c_+c_- + c_-c_+). \end{aligned} \tag{43}$$

Equating (42) and (43), we have

$$a_-^2(c_+c_- + c_-c_+) + a_+a_-(-c_-^2 + c_+c_-) + a_-a_+(-c_-^2 - c_-c_+) = 0. \tag{44}$$

Taking the even and odd parts of this, we have

$$a_+a_-c_+c_- - a_-a_+c_-c_+ = 0, \tag{45}$$

$$a_-^2(c_+c_- + c_-c_+) - (a_+a_- + a_-a_+)c_-^2 = 0. \tag{46}$$

By acting the unitary transformation $\mathrm{Ad}(v_A)$ on both sides of (46) where v_A in $\mathcal{A}_A^e$ gives the implementation of Θ on $\mathcal{A}_A$ as (6), we have

$$a_-^2(c_+c_- + c_-c_+) + (a_+a_- + a_-a_+)c_-^2 = 0.$$

By averaging this and (46), we have

$$a_-^2(c_+c_- + c_-c_+) = 0. \tag{47}$$

Similarly, we have

$$(a_+a_- + a_-a_+)c_-^2 = 0. \tag{48}$$

We will see that from (45), (47), and (48), our assertion, i.e., the evenness of ρ_{ψ_A} or (and) ρ_{ψ_C} follows. For (47) to be satisfied,

$$a_-^2 = 0 \quad \text{or/and } (c_+c_- + c_-c_+) = 0, \tag{49}$$

as $a_-^2 \in \mathcal{A}_A^e$ and hence $a_-^2(c_+c_- + c_-c_+) = a_-^2 \otimes (c_+c_- + c_-c_+) = 0$. In the same way,

$$c_-^2 = 0 \quad \text{or/and } (a_+a_- + a_-a_+) = 0. \tag{50}$$

If $a_-^2 = 0$, then $a_- = 0$ since a_- is self-adjoint. Therefore, $\rho_{\psi_A}^{1/2}$ is even and so ρ_{ψ_A} is. If $c_-^2 = 0$, then ρ_{ψ_C} is even. We now consider the remaining possibility, i.e., the case where $a_+a_- + a_-a_+ = c_+c_- + c_-c_+ = 0$. This implies that $\rho_{\psi_{A^-}} = \rho_{\psi_{C^-}} = 0$, namely both of ρ_{ψ_A} and ρ_{ψ_C} are even. In conclusion, at least one of the marginal states ρ_{ψ_A} and ρ_{ψ_C} should be even.

Now we know that the product state $\psi_A \circ \psi_C$ exists and can use the argument in (32) that leads to our desired assertion. ■

We shall go back to three-composed systems and comment on the condition of the strong additivity of entropy. For now, we are only able to produce the desiarble form of Markov property for even states. We guess that the assumed strong additivity of entropy may control in a certain sense *nonevenness* of the states satisfying this as for the case of two-composed systems above. Without the evenness assumption, we need more involved analysis to understand the structure of those states satisfying the strong additivity of entropy.

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Generalized quantum Gaudin spin chains, involutive automorphisms and "twisted" classical *r*-matrices

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Using automorphisms σ of finite-dimensional Lie algebras and classical skew-symmetric *r*-matrices we construct "twisted" nonskew symmetric *r*-matrices with the spectral parameters. Using them and results of our previous papers we construct new quantum spin chains that generalize famous Gaudin spin chains. We consider several examples of the twisted nonskew symmetric *r*-matrices and the corresponding Gaudin-type systems. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Gaudin models[1] are one of the most celebrated integrable models of mathematical physics. They were shown to be connected with the conformal field theory via solutions of the Knizhnik-Zamolodchikov equations,[2,3] and with the BCS model in one dimension.[4,5] These facts give a special importance to their investigation. Standard Gaudin spin chains,[1,6,7] are connected with the skew-symmetric classical *r*-matrices introduced in Ref. 8, i.e., with the skew symmetric solutions of the classical Yang-Baxter equations, which were investigated and classified in Ref. 9.

In the papers[10] we have constructed new integrable classical spin chains starting from the general non-skew symmetric solutions of the "generalized" classical Yang-Baxter equations (a dualized form of the modified Yang-Baxter equations[11–13]) with values in a semisimple (reductive) Lie algebras $\mathfrak{g}$. In particular we have constructed the second order in spin variables Hamiltonians of these systems and showed that they are direct analogs of the famous Gaudin Hamiltonians. We have called our systems "generalized Gaudin systems." In our previous paper[14] we have considered a problem of the quantization of the generalized Gaudin systems. The quantization of the basic (spin) variables is achieved by the standard procedure of substitution of the Lie-Poisson bracket on $\mathfrak{g}^{\oplus N}$ by commutator, or by other words in passing from $(S(\mathfrak{g}^{\oplus N}),\{\ ,\ \})$ to $(\mathfrak{A}(\mathfrak{g}^{\oplus N}),[\ ,\ ])$ or some of its representations in the Hilbert space $\mathcal{H}$. Nevertheless, due to the problem of ordering, such a simple recipe does not solve the problem of commutativity of the classically Poisson-commutative integrals which are nonlinear in basic variables. At the present moment no general approach to a proof of the quantum integrability of such the classical integrable systems is known. That is why we have dealt with this problem in the case of the our systems directly. In Ref. 14 we have given a direct proof that after symmetrization in spin variables generalized Gaudin Hamiltonians stay commutative also in the quantum case. We have also considered a class of examples of nonskew *r*-matrices with spectral parameters connected with some special infinite-dimensional Lie algebras of Ref. 15 and associated quantum Gaudin Hamiltonians.

In the present paper we consider other important class of examples of nonskew *r*-matrices and associated Gaudin-type systems. We show that for each classical skew-symmetric *r*-matrix $r(u-v)$, which is *anti-invariant* with respect to some automorphism σ of the second order of the Lie algebra $\mathfrak{g}$, prolonged to the algebra of functions, it is possible to define "twisted" nonskew *r*-matrix $r^{\sigma}_{12}(u,v)$ given by the following formula:

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$$r_{12}^{\sigma}(u,v) = r_{12}(u-v) - r_{12}^{\sigma_2}(u+v), \quad \text{where } r_{12}^{\sigma_2}(u+v) = (1 \otimes \sigma) r_{12}(u+v). \tag{1}$$

We consider examples of the r-matrices (1) associated with the rational r-matrix of Yang and elliptic r-matrix of Belavin[16] in details.

With the help of the r-matrices (1) we construct new quantum-commuting Gaudin-type Hamiltonians. They have the following form:

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} \sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} (r^{\alpha\beta}(u_k - u_l) - (r^{\sigma_2})^{\alpha\beta}(u_k + u_l)) \hat{S}_{\alpha}^{k} \hat{S}_{\beta}^{l} - \sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} (r^{\sigma_2})^{\alpha\beta}(2u_l) \hat{S}_{\alpha}^{l} \hat{S}_{\beta}^{l}, \tag{2}$$

where N is a number of sites, $\hat{S}_{\alpha}^{l}$, $\hat{S}_{\beta}^{k}$ are components of the generalized spin operators in the site l and k, correspondingly, that obey the commutation relations of $\mathfrak{g}^{\oplus N}$, $r^{\alpha\beta}(u_k - u_l)$ are the matrix elements of the $\mathfrak{g} \otimes \mathfrak{g}$-valued skew symmetric classical r matrix and u_k, $k \in 1, N$ are nonzero complex numbers such that $u_k \neq \pm u_l$.

We consider examples of such Hamiltonians, in particular, those connected with the "twisted" Belavin sl(n) elliptic r-matrix. In the most physically important case of $\mathrm{sl}(2) \simeq \mathrm{so}(3)$ we obtain the following quantum spin chain Hamiltonians:

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} \sum_{i=1}^{3} (w_i(u_k - u_l) - w_i(u_k + u_l)) \hat{S}_{i}^{k} \hat{S}_{i}^{l} - \sum_{i=1}^{3} w_i(2u_l) \hat{S}_{i}^{l} \hat{S}_{i}^{l}, \tag{3}$$

where $\hat{S}_{i}^{k}$ are the components of the usual spin operators and $w_i(u_k)$ are expressed via the elliptic Jacobi functions.[8]

The structure of the present paper is the following: in the second section we introduce the main definitions and notations and formulate the theorem concerning the commutativity of the generalized Gaudin Hamiltonians associated with the nonskew symmetric r-matrices. In the third section we consider the construction of the nonskew symmetric classical r-matrices with the spectral parameter using automorphism of $\mathfrak{g}$ of the second order and skew symmetric classical r-matrices. In the fourth section we consider the generalized Gaudin Hamiltonians (10) associated with the constructed in the preceding section "twisted" classical r-matrices. In the appendix we give the direct proof of the commutativity of such Hamiltonians.

II. INTEGRABLE SPIN CHAINS AND CLASSICAL *r*-MATRICES

Let $\mathfrak{g}$ be a simple (reductive) Lie algebra. Let $X_{\alpha}, \alpha = 1, \dim \mathfrak{g}$ be some basis in $\mathfrak{g}$ with the commutation relations

$$[X_{\alpha}, X_{\beta}] = \sum_{\gamma=1}^{\dim \mathfrak{g}} C_{\alpha\beta}^{\gamma} X_{\gamma}. \tag{4}$$

Let $\hat{S}_{\alpha}^{i}, \alpha = 1, \dim \mathfrak{g}$, $i = 1, N$ be linear operators in some Hilbert space that constitute Lie algebra isomorphic to $\mathfrak{g}^{\oplus N}$ with the commutation relations

$$[\hat{S}_{\alpha}^{i}, \hat{S}_{\beta}^{j}] = \delta^{ij} \sum_{\gamma=1}^{\dim \mathfrak{g}} C_{\alpha\beta}^{\gamma} \hat{S}_{\gamma}^{j}. \tag{5}$$

We will consider operators $\hat{S}_{\alpha}$ to be α component of the "generalized spin operator." Then operators $\hat{S}_{\alpha}^{i}$ could be interpreted as the α component of the generalized spin operator living at the i-cite of the generalized spin chain.

Remark 1: In the case $\mathfrak{g} = \mathrm{so}(3)$ operators $\hat{S}_{a}, \alpha = 1, 3$ are components of the usual spin and operator and $\hat{S}_{\alpha}^{i}$ have the usual $\mathrm{so}(3)^{\oplus N}$ commutation relations,

$$[\hat{S}^i_\alpha, \hat{S}^j_\beta] = \delta^{ij} \sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma} \hat{S}^j_\gamma. \tag{6}$$

We will be interested in a construction of a family of the second order in "spin" variable $\hat{S}^i_\alpha$ mutually commuting operators $\hat{H}^j, j=1,N$ that generalize standard Gaudin Hamiltonians.

We will need the following definition.

Definition 1: A function of two complex variables $r(u_1,u_2)$ with values in the tensor square of the algebra $\mathfrak{g}$ is called a classical r-matrix if it satisfies the following "general" or "generalized" classsical Yang-Baxter equation:

$$[r_{12}(u_1,u_2), r_{13}(u_1,u_3)] = [r_{23}(u_2,u_3), r_{12}(u_1,u_2)] - [r_{32}(u_3,u_2), r_{13}(u_1,u_3)], \tag{7}$$

where $r_{12}(u_1,u_2) \equiv \Sigma_{\alpha,\beta=1}^{\dim \mathfrak{g}} r^{\alpha\beta}(u_1,u_2) X_\alpha \otimes X_\beta \otimes 1$, etc. (This equation first appeared in somewhat different form in Refs. 11 and 13. In the present form it appeared later in Ref. 17.)

Remark 2: If the matrix $r(u_1,u_2)$ is "skew," i.e., $r_{12}(u_1,u_2) = -r_{21}(u_2,u_1)$ Eq. (7) passes into the usual classical Yang-Baxter equation

$$[r_{12}(u_1,u_2), r_{13}(u_1,u_3)] = [r_{23}(u_2,u_3), r_{12}(u_1,u_2) + r_{13}(u_1,u_3)]. \tag{8}$$

Due to the fact that all solutions of the equations (8) are skew[18] each solution of (8) is also a solution of (7).

Remark 3: Note, that by reparametrizations and gauge transformations each solution of the equation (8) could be transformed to the form $r_{12}(u_1,u_2) \equiv r_{12}(u_1-u_2)$.[18] This statement is not true for general nonskew solutions of the equation (7).

Let us fix N distinct points $\{u_k\}$ on the complex plane such that in the neighborhood of these points $r(u,v)$ possesses the following decomposition:

$$r(u,v) = \frac{\hat{c}}{(u-v)} + r_0(u,v), \tag{9}$$

where $r_0(u,v)$ is a regular in the neighborhood of $u=u_k$, $v=u_m$, $k,m \in 1,N$ $\mathfrak{g} \otimes \mathfrak{g}$-valued function, $\hat{c} \in \mathfrak{g} \otimes \mathfrak{g}$ is the tensor Casimir, $\hat{c} = \Sigma_{\alpha,\beta} g^{\alpha\beta} X_\alpha \otimes X_\beta$, $g^{\alpha\beta}$ is the nondegenerate invariant metric on $\mathfrak{g}$.

The following theorem holds true.[14]

Theorem 2.1: *Let $r(u_i,u_j) \equiv \Sigma_{\alpha,\beta=1}^{\dim \mathfrak{g}} r^{\alpha\beta}(u_i,u_j) X_\alpha \otimes X_\beta$ be the classical r-matrix and $r_0(u_i,u_j)$ its regular part. Then the second order in spin variables operators $\hat{H}^l, l=1,N$ of the type*

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} \sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} r^{\alpha\beta}(u_k,u_l) \hat{S}^k_\alpha \hat{S}^l_\beta + \frac{1}{2} \sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} r_0^{\alpha\beta}(u_l,u_l) (\hat{S}^l_\alpha \hat{S}^l_\beta + \hat{S}^l_\beta \hat{S}^l_\alpha) \tag{10}$$

form commutative family in the universal enveloping algebra $\mathfrak{A}(\mathfrak{g}^{\oplus N})$ and its representations.

Remark 4: In the case of the skew symmetric r-matrices we have that $r_0^{\alpha,\beta}(u_l,u_l) = -r_0^{\beta,\alpha}(u_l,u_l)$ and, hence, additional term in the corresponding Hamiltonian $\hat{H}^l$ turns zero and $\hat{H}^l$ coincides with the standard Gaudin Hamiltonian.

Remark 5: Theorem 2.1 implies also commutativity of the corresponding classical Hamiltonians with respect to the natural Lie-Poisson bracket. Their classical commutativity was shown by an other method in Ref. 10. For the case of a $\mathfrak{g}$ of a higher rank these Hamiltonians do not form complete family of the commuting integrals and should be completed by the "higher" integrals.[10] Proof of their quantum commutativity is a separate complicated problem even in the case of the standard skew symmetric r-matrices. This problem for the case of the general skew symmetric r-matrices was approached in Ref. 19 and solved for the case of the simplest rational r-matrix in Ref. 20.

III. AUTOMORPHISMS OF THE SECOND ORDER AND "TWISTED" NONSKEW *r*-MATRICES

In this section we construct nonskew symmetric classical r-matrices with spectral parameters starting from the standard skew symmetric classical r-matrices with spectral parameters.

Let σ be involutive automorphism of $\mathfrak{g}$, i.e., $\sigma^2=1$ and $\sigma([X,Y])=[\sigma(X),\sigma(Y)]$, $\forall X,Y\in\mathfrak{g}$. We will use the following notations: $\sigma_1=\sigma\otimes 1$, $\sigma_2=1\otimes\sigma$, etc. Let $\widetilde{\sigma}$ be a lift of σ onto the algebra of $\mathfrak{g}$-valued functions given by the formula $\widetilde{\sigma}X(u)=\sigma X(-u)$, and on the level of their tensor product by the formula $(\widetilde{\sigma}_1\widetilde{\sigma}_2)r_{12}(u,v)=(\sigma_1\sigma_2)r_{12}(-u,-v)$, etc.

The following theorem holds true.

Theorem 3.1: *Let $r_{12}(u-v)$ be skew symmetric r-matrix, i.e., a solution of the equation (8) which is anti-invariant with respect to the action of the automorphism $\widetilde{\sigma}$,*

$$\widetilde{(\sigma_1\sigma_2)}r_{12}(u-v)=-r_{12}(u-v). \tag{11}$$

Then (i) the function $r_{12}^{\sigma_2}(u+v)\equiv\sigma_2 r_{12}(u+v)$ is symmetric,

$$r_{12}^{\sigma_2}(u+v)=r_{21}^{\sigma_1}(u+v)=-r_{12}^{\sigma_1}(-u-v), \tag{12}$$

(ii) the function

$$r_{12}^{\sigma}(u,v)=r_{12}(u-v)-r_{12}^{\sigma_2}(u+v)=r_{12}(u-v)+r_{12}^{\sigma_1}(-u-v), \tag{13}$$

is a nonskew symmetric solution of the equation (7).

Remark 6: Note, that formula (13) differs from the one that can be extracted from Ref. 13. Indeed, in Ref. 13 it is imposed the condition of invariance of the r-matrix $r(u-v)$ under the action of $\widetilde{\sigma}$, $\widetilde{(\sigma_1\sigma_2)}r_{12}(u-v)=r_{12}(u-v)$ instead of the anti-invariance condition (11). Using formula of Ref. 13 for the case $\sigma^2=1$ one obtains the different formula, $r_{12}^{\sigma}(u,v)=r_{12}(u-v)+r_{12}^{\sigma_2}(u+v)$, which is not true for anti-invariant r-matrices $r_{12}(u-v)$.

Remark 7: The construction of the theorem holds also in the case of the trivial involutive automorphism $\sigma\equiv 1$. In this case $\widetilde{\sigma}(X(u))=X(-u)$ and anti-invariance condition for $r_{12}(u-v)$ is equivalent to the condition $r_{12}(u-v)=-r_{12}(v-u)$, or taking into account skew symmetry of $r(u-v)$ to the following symmetry condition: $r_{12}(u-v)=r_{21}(u-v)$.

Proof: Let us at first prove item (i). At first let us note that using skew symmetry, $r_{12}(u+v)=-r_{21}(-v-u)$ condition (11) is easily shown to be equivalent to the condition $(\sigma_1\sigma_2)r_{12}(u+v)=r_{21}(u+v)$. Now it is easy to see that due to the equality $\sigma_1^2=1$ this implies identity $r_{12}^{\sigma_2}(u+v)=r_{21}^{\sigma_1}(u+v)$. Using the skew symmetry condition for $r(u+v)$ again we obtain $r_{21}^{\sigma_1}(u+v)=-r_{12}^{\sigma_1}(-u-v)$. This proves item (i).

Let us now prove item (ii). For this purpose we must show that generalized classical Yang-Baxter equation (7) for the r-matrix $r^{\sigma}(u,v)$ given by the formula (13) follows from the usual classical Yang-Baxter equation (8) for the r-matrix $r_{12}(u-v)$. We must prove that

$$\begin{aligned}[r_{12}(u_1-u_2)+r_{12}^{\sigma_1}(-u_1-u_2),r_{13}(u_1-u_3)+r_{13}^{\sigma_1}(-u_1-u_3)]=[r_{23}(u_2-u_3)+r_{23}^{\sigma_2}(-u_2-u_3),r_{12}(u_1-u_2)+r_{12}^{\sigma_1}(-u_1-u_2)]\\-[r_{32}(u_3-u_2)+r_{32}^{\sigma_3}(-u_3-u_2),r_{13}(u_1-u_3)+r_{13}^{\sigma_1}(-u_1-u_3)].\end{aligned}$$

This equation is equivalent to the following four equations:

$$[r_{12}(u_1-u_2),r_{13}(u_1-u_3)]=[r_{23}(u_2-u_3),r_{12}(u_1-u_2)+r_{13}(u_1-u_3)], \tag{14a}$$

$$[r_{12}^{\sigma_1}(-u_1-u_2),r_{13}^{\sigma_1}(-u_1-u_3)]=[r_{23}(u_2-u_3),r_{12}^{\sigma_1}(-u_1-u_2)+r_{13}^{\sigma_1}(-u_1-u_3)], \tag{14b}$$

$$[r_{12}(u_1-u_2),r_{13}^{\sigma_1}(-u_1-u_3)]=[r_{23}^{\sigma_2}(-u_2-u_3),r_{12}(u_1-u_2)]-[r_{32}^{\sigma_3}(-u_2-u_3),r_{13}^{\sigma_1}(-u_1-u_3)], \tag{14c}$$

$$[r_{12}^{\sigma_1}(-u_1-u_2),r_{13}(u_1-u_3)]=[r_{23}^{\sigma_2}(-u_2-u_3),r_{12}^{\sigma_1}(-u_1-u_2)]-[r_{32}^{\sigma_3}(-u_2-u_3),r_{13}(u_1-u_3)]. \tag{14d}$$

Equation (14a) is the standard Yang-Baxter equation which is satisfied by $r(u_1-u_2)$ by the conditions of the theorem. Equation (14b) passes to the equation (14a) after the change of variable $u_1\to -u_1$ and action on both sides of the automorphism σ_1.

Changing the sign of the variable u_3 in the equation (14c) and taking into account that $r_{13}^{\sigma_1}(-u_1+u_3)=-r_{31}^{\sigma_1}(u_1-u_3)=-r_{13}^{\sigma_3}(u_1-u_3)$ and $r_{23}^{\sigma_2}(-u_2+u_3)=-r_{23}^{\sigma_3}(u_2-u_3)$, we see that Eq. (14c) is equivalent to the following equation:

$$[r_{12}(u_1-u_2),r_{13}^{\sigma_3}(u_1-u_3)]=[r_{23}^{\sigma_3}(u_2-u_3),r_{12}(u_1-u_2)]-[r_{32}^{\sigma_3}(u_3-u_2),r_{13}^{\sigma_3}(u_1-u_3)].$$

Acting on both sides of this equation by the automorphism σ_3 we obtain that Eq. (14c) is also equivalent to Eq. (14a). At last Eq. (14d) is equivalent to (14c). To see this it is enough to change indices $2\leftrightarrow 3$ in Eq. (14d).

Theorem is proved.

Let us consider several examples of this construction.

Example 1: Let $\mathfrak{g}=\mathrm{gl}(n)$ and $r(u-v)=(u-v)^{-1}\Sigma_{i,j=1}^{n}X_{ij}\otimes X_{ji}$, is r-matrix of Yang. Here $(X_{ij})_{\alpha\beta}=\delta_{i\alpha}\delta_{j\beta}$ is the standard matrix basis of $\mathrm{gl}(n)$. Let us consider automorphism $\widetilde{\sigma}$ of $\mathrm{gl}(n)$ given on the basis elements by the formula $\sigma(X_{ij})=-X_{ji}$. It is easy to show, that $\widetilde{\sigma_1\sigma_2}(r(u-v))=-r(u-v)$. Hence by the virtue of Theorem 3.1 we obtain that the following $\mathrm{gl}(n)\otimes\mathrm{gl}(n)$-valued function

$$r^{\sigma}(u,v)=(u-v)^{-1}\sum_{i,j=1}^{n}X_{ij}\otimes X_{ji}+(u+v)^{-1}\sum_{i,j=1}^{n}X_{ij}\otimes X_{ij} \tag{15}$$

satisfies the generalized classical Yang-Baxter equation (7). This r-matrix coincides with the classical r-matrix found previously in Ref. 21.

Example 2: Let us consider the case $\mathfrak{g}=\mathrm{sl}(n)$ and the classical elliptic r-matrix of Ref. 16,

$$r(u-v)=\sum_{a\in Z_n^2\setminus\{0\}}\epsilon(a)w_a(u-v)X_{\alpha}\otimes X_{-\alpha}, \tag{16}$$

where $a=(a_1,a_2)$, $\epsilon(a)=e^{(2\pi i a_1 a_2)/n}$, $Z_n^2=Z_n\times Z_n$ and $Z_n=\mathbb{Z}/n\mathbb{Z}$, $w_a(u)$ is expressed via the θ-functions with characteristic:

$$w_a(u)=\frac{\theta_{(a_2/n+1/2,a_1/n+1/2)}(u)\,\theta'_{1/2,1/2}(0)}{\theta_{1/2,1/2}(u)\,\theta_{a_2/n+1/2,a_1/n+1/2}(0)}, \tag{17}$$

and basic elements X_{α} satisfy the following commutation relations:[22]

$$[X_a,X_b]=\alpha_{a,b}X_{a+b}, \tag{18}$$

where $\alpha_{a,b}=e^{(2\pi i a_2 b_1)/n}-e^{(2\pi i a_1 b_2)/n}$. Using the fact that $\alpha_{-a,-b}=\alpha_{a,b}$ it is easy to see, that the map $\sigma(X_a)=X_{-a}$ is the automorphism of $\mathrm{sl}(n)$. Moreover, from the skew symmetry of $r(u-v)$ it follows that $w_a(u-v)=-w_{-a}(v-u)$ and $\epsilon(a)=\epsilon(-a)$, and it is straightforward to show that $(\widetilde{\sigma_1\sigma_2})r_{12}(u-v)=-r_{12}(u-v)$. Hence we can use the formula (13) and obtain the following "twisted" elliptic r-matrix:

$$r^{\sigma}(u,v)=\sum_{a\in Z_n^2\setminus\{0\}}\epsilon(a)(w_a(u-v)X_{\alpha}\otimes X_{-\alpha}-w_a(u+v)X_{\alpha}\otimes X_{\alpha}). \tag{19}$$

Example 3: Let us consider in details the previous example but in the special case $\mathfrak{g}=\mathrm{sl}(2)$. Introducing new generators $X_1=i/2X_{(1,1)}$, $X_2=i/2X_{(0,1)}$, $X_3=1/2X_{(1,0)}$ we obtain the following commutation relations: $[X_i,X_j]=\epsilon_{ijk}X_k$, which reflect isomorphism $\mathrm{sl}(2,\mathbb{C})\simeq\mathrm{so}(3,\mathbb{C})$. Taking into account that in the group Z_2^2 we have that $a=-a$ and, hence, we obtain that formula (16) (up to a coefficient) acquires the form of Sklyanin,[8]

$$r(u-v)=\sum_{k=1}^{3} w_k(u-v)X_k\otimes X_k, \tag{20}$$

where $w_k(u)$ are expressed via Jacobi functions, $w_1(u)=1/\mathrm{sn}(u)$, $w_2(u)=\mathrm{dn}(u)/\mathrm{sn}(u)$, $w_3(u)=\mathrm{cn}(u)/\mathrm{sn}(u)$.

It is easy to see that in this case $\sigma=1$ and $r_{12}(u-v)=-r_{12}(v-u)$ due to the fact that functions $w_k(u)$ are odd. Hence the condition of Theorem 3.1 is true and we obtain the following nonskew symmetric so (3) elliptic r-matrix:[10]

$$r^{\sigma}(u,v)=\sum_{k=1}^{3}(w_k(u-v)-w_k(u+v))X_\kappa\otimes X_\kappa. \tag{21}$$

This r-matrix could also be obtained using the results of Refs. 23 or 24.

IV. INTEGRABLE SPIN CHAINS ASSOCIATED WITH $r^{\sigma}(u,v)$

In this section using classical r-matrices constructed in the preceding section will explicitly obtain Hamiltonians of the new integrable quantum spin chains (10).

The following theorem holds true.

Theorem 4.1: *Let $r(u-v)$ be the classical skew symmetric r-matrix satisfying equation (8). Let $u_k, k\in 1,N$ be some fixed nonzero complex numbers such that $u_k\neq\pm u_l$. Then the second order in spin variables $\hat{S}^k_\alpha$ operators $\hat{H}^l, l=1,N$ of the type*

$$\hat{H}^l=\sum_{k=1,k\neq l}^{N}\sum_{\alpha,\beta=1}^{\dim\mathfrak{g}}(r^{\alpha\beta}(u_k-u_l)-(r^{\sigma_2})^{\alpha\beta}(u_k+u_l))\hat{S}^k_\alpha\hat{S}^l_\beta-\sum_{\alpha,\beta=1}^{\dim\mathfrak{g}}(r^{\sigma_2})^{\alpha\beta}(2u_l)\hat{S}^l_\alpha\hat{S}^l_\beta \tag{22}$$

form commutative family in the universal enveloping algebra $\mathfrak{A}(\mathfrak{g}^{\oplus N})$ and its representations.

Proof: Proof of this theorem follows from the Theorems 2.1 and 3.1. It is necessary only to find out the explicit form of the tensor $r^{\sigma}_0(u,u)$. By the direct calculation we obtain that

$$r^{\sigma}_0(u,u)=\lim_{v\to u}(r(u-v)-r^{\sigma_2}(u+v)-(u-v)^{-1}\hat{c})=r^0-r^{\sigma_2}(2u), \tag{23}$$

where we have used that $r(u-v)=(u-v)^{-1}\hat{c}+r^0+\Sigma_{k=1}^{\infty}r^k(u-v)^k$.

Now, substituting the explicit expression for the "twisted" classical r-matrix (13) and its regular part (23) into the formula (10) and taking into account skew symmetry of the tensor r^0 and symmetry of the tensor $r^{\sigma_2}_{12}(2u)$ we obtain the formula (22).

Theorem is proved.

Remark 8: Note that due to the symmetry of the tensor $r^{\sigma_2}_{12}(2u)$ no additional symmetrization of the operators $\hat{S}^l_\alpha,\hat{S}^l_\beta$ as in formula (10) is needed in the formula (22).

Remark 9: Theorem 4.1 could be also proved directly without appealing to the more general Theorem 2.1. Moreover, proof of this theorem in such a case is much simpler and we expose it for the sake of completeness in the Appendix.

Let us consider concrete examples of the formula (22) for the concrete r-matrices.

Example 4: Let us consider the case $\mathfrak{g}=\mathrm{gl}(n)$ and r-matrix $r^{\sigma}(u,v)$ from the Example 1. In this case the spin operators are labeled by two matrix indices, i.e., $\hat{S}^k_\alpha\equiv\hat{S}^k_{ij}$ and we obtain the following explicit formula for the commuting Gaudin-type Hamiltonians $\hat{H}^l, l\in 1,N$:

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} (u_k - u_l)^{-1} \sum_{i,j=1}^{n} \hat{S}_{ij}^k \hat{S}_{ji}^l + \sum_{k=1,k\neq l}^{N} (u_k + u_l)^{-1} \sum_{i,j=1}^{n} \hat{S}_{ij}^k \hat{S}_{ij}^l + (2u_l)^{-1} \sum_{i,j=1}^{n} \hat{S}_{ij}^l \hat{S}_{ij}^l, \tag{24}$$

where commutation relations among the generalized spin operators are

$$[\hat{S}_{ij}^m, \hat{S}_{kl}^n] = \delta^{mn}(\delta_{kj}\hat{S}_{il}^n - \delta_{il}\hat{S}_{kj}^n).$$

Example 5: Let us consider the case $\mathfrak{g}=\mathrm{sl}(n)$ and nonskew symmetric elliptic r matrix $r^{\sigma}(u,v)$ from the Example 2. This example yields the following commuting generalized Gaudin-type Hamiltonians $\hat{H}^l, l \in 1,N$:

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} \left(\sum_{a\in Z_n^2\setminus 0} \epsilon(a) w_a(u_k - u_l) \hat{S}_a^k \hat{S}_{-a}^l - \sum_{a\in Z_n^2\setminus 0} \epsilon(a) w_a(u_k + u_l) \hat{S}_a^k \hat{S}_a^l \right) - \sum_{a,b\in Z_n^2\setminus 0} \epsilon(a) w_a(2u_l) \hat{S}_a^l \hat{S}_a^l. \tag{25}$$

Commutation relations among the generalized spin operators are

$$[\hat{S}_a^n, \hat{S}_b^m] = \delta^{nm} \alpha_{a,b} \hat{S}_{a+b}^m. \tag{26}$$

Example 6: Let us consider the case $\mathfrak{g}=\mathrm{sl}(2)\simeq \mathrm{so}(3)$ and nonskew symmetric elliptic r matrix $r^{\sigma}(u,v)$ from the Example 3. This example yields the following commuting Gaudin-type Hamiltonians $\hat{H}^l, l \in 1,N$,

$$\hat{H}^l = \sum_{k=1,k\neq l}^{N} \sum_{i=1}^{3} (w_i(u_k - u_l) - w_i(u_k + u_l)) \hat{S}_i^k \hat{S}_i^l - \sum_{i=1}^{3} w_i(2u_l) \hat{S}_i^l \hat{S}_i^l. \tag{27}$$

Commutation relations among the usual spin operators are standard,

$$[\hat{S}_i^n, \hat{S}_j^m] = \delta^{nm} \epsilon_{ijk} \hat{S}_k^m. \tag{28}$$

Hamiltonian (27) is a quantum version of classical Hamiltonian obtained by us in Ref. 10.

Example 7: Finally, let us consider the previous example in the special cases $N=1$ and $N=2$ in order to show that our quantum spin systems is a generalization of the well known ones. Indeed, in the case $N=1$ our construction yields the following Hamiltonian:

$$\hat{H}^1 = -\sum_{i=1}^{3} w_i(2u_1) \hat{S}_i^1 \hat{S}_i^1.$$

Setting $w_k(2u_1) = -J_k$ we obtain quantum Hamiltonian of the anisotropic Euler top,

$$\hat{H}^1 = \sum_{k=1}^{3} J_k \hat{S}_k^1 \hat{S}_k^1.$$

In the case $N=2$ we have two spin operators and two commuting Gaudin-type Hamiltonians,

$$\hat{H}^1 = \sum_{i=1}^{3} (w_i(u_2 - u_1) - w_i(u_1 + u_2)) \hat{S}_i^2 \hat{S}_i^1 - \sum_{i=1}^{3} w_i(2u_1) \hat{S}_i^1 \hat{S}_i^1,$$

$$\hat{H}^2 = \sum_{i=1}^{3} (w_i(u_1 - u_2) - w_i(u_1 + u_2)) \hat{S}_i^1 \hat{S}_i^2 - \sum_{i=1}^{3} w_i(2u_2) \hat{S}_i^2 \hat{S}_i^2.$$

These Hamiltonians are exactly quantized Hamiltonians of the classical Steklov system on $\mathrm{so}(3)+\mathrm{so}(3)$ in the form proposed in Ref. 22.

V. CONCLUSION AND DISCUSSION

In the present paper using automorphisms of the second order of semisimple Lie algebras $\mathfrak{g}$ and standard skew symmetric $\mathfrak{g}\otimes\mathfrak{g}$-valued r-matrices we have constructed new nonskew symmetric classical r-matrices with the spectral parameters. Using them we have explicitly constructed new integrable quantum Gaudin-type spin chains. We have considered several examples of our nonskew symmetric r-matrices and the corresponding commuting quantum Hamiltonians.

An interesting and important mathematical problem is a diagonalization of these Hamiltonians, i.e., an explicit construction of their eigenvectors and eigenvalues. It would be also interesting to find direct physical applications for the constructed integrable spin systems. One of the possible applications of our models are integrable fermionic systems with BCS-type Hamiltonians.[4,5] We hope, that using our results it will be possible to obtain an exactly solvable generalization of the one-dimensional BCS Hamiltonian. The work over these problems is now in progress and we will return to them in our future presentations.

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APPENDIX: DIRECT PROOF OF THE THEOREM 4.1

We will prove the theorem directly showing that $[\hat{H}^k,\hat{H}^l]=0\,\forall\, k,l,k\neq l$. The first stage of the proof is independent of the choice of the concrete r-matrix $r^{\alpha\beta}(u_k,u_l)$ and repeats the part of the proof of the Theorem 2.1 in details exposed in Ref. 14.

Let us represent our Hamiltonians as follows: $\hat{H}^k=\hat{H}^k_0+\hat{H}^k_1$, $\hat{H}^l=\hat{H}^l_0+\hat{H}^l_1$, where

$$\hat{H}^l_0=\sum_{\alpha,\beta=1}^{\dim\mathfrak{g}}\sum_{k\neq l}^{N} r^{\alpha\beta}(u_k,u_l)\hat{S}^k_\alpha\hat{S}^l_\beta,\hat{H}^l_1=1/2\sum_{\alpha,\beta=1}^{\dim\mathfrak{g}} r_0^{\alpha\beta}(u_l,u_l)(\hat{S}^l_\alpha\hat{S}^l_\beta+\hat{S}^l_\beta\hat{S}^l_\alpha).$$

Here we use the notation of the Sec. I. It is easy to see that $[\hat{H}^k_1,\hat{H}^l_1]=0$, and hence,

$$[\hat{H}^k,\hat{H}^l]=[\hat{H}^k_0,\hat{H}^l_0]+[\hat{H}^k_0,\hat{H}^l_1]+[\hat{H}^k_1,\hat{H}^l_0]. \tag{A1}$$

Let us calculate each of this summands separately,

$$\begin{aligned}
[\hat{H}^k_0,\hat{H}^l_0]&=\sum_{m\neq k}\sum_{n\neq l}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_m,u_k)r^{\gamma,\delta}(u_n,u_l)[\hat{S}^m_\alpha\hat{S}^k_\beta,\hat{S}^n_\gamma\hat{S}^l_\delta]\\
&=\sum_{m,n\neq k,l}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_m,u_k)r^{\gamma,\delta}(u_n,u_l)[\hat{S}^m_\alpha\hat{S}^k_\beta,\hat{S}^n_\gamma\hat{S}^l_\delta]\\
&\quad+\sum_{n\neq l,k}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_l,u_k)r^{\gamma,\delta}(u_n,u_l)[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^n_\gamma\hat{S}^l_\delta]+\sum_{m\neq k,l}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_m,u_k)r^{\gamma,\delta}(u_k,u_l)\\
&\quad\times[\hat{S}^m_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta]+\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_l,u_k)r^{\gamma,\delta}(u_k,u_l)[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta]\\
&=\sum_{m\neq k,l} r^{\alpha,\beta}(u_m,u_k)r^{\gamma,\delta}(u_m,u_l)C^\kappa_{\alpha\gamma}\hat{S}^m_\kappa\hat{S}^k_\beta\hat{S}^l_\delta+\sum_{m\neq l,k}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_l,u_k)r^{\gamma,\delta}(u_m,u_l)C^\kappa_{\alpha\delta}\hat{S}^l_\kappa\hat{S}^k_\beta\hat{S}^m_\gamma\\
&\quad+\sum_{m\neq k,l}\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_m,u_k)r^{\gamma,\delta}(u_k,u_l)C^\kappa_{\beta\gamma}\hat{S}^m_\alpha\hat{S}^k_\kappa\hat{S}^l_\delta+\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_l,u_k)r^{\gamma,\delta}(u_k,u_l)[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta].
\end{aligned}$$

Note that in the first three summands of the final expression on the right-hand side of this equality indices m,k,l are all different and the order of the operators, $\hat{S}^m_\kappa$, $\hat{S}^k_\beta$, $\hat{S}^l_\delta$, is not important. Let us consider these summands in more details. Taking into account that $r_{12}(u_m,u_k)=\sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} r^{\alpha\beta}(u_m,u_k)X_\alpha\otimes X_\beta\otimes 1$, $r_{13}(u_m,u_l)=\sum_{\gamma,\delta=1}^{\dim \mathfrak{g}} r^{\gamma\delta}(u_m,u_l)X_\gamma\otimes 1\otimes X_\delta$, $r_{23}(u_k,u_l)=\sum_{\gamma,\delta=1}^{\dim \mathfrak{g}} r^{\gamma\delta}(u_k,u_l)1\otimes X_\gamma\otimes X_\delta$, $r_{32}(u_l,u_k)=\sum_{\alpha,\beta=1}^{\dim \mathfrak{g}} r^{\alpha\beta}(u_k,u_l)1\otimes X_\beta\otimes X_\alpha$ we obtain that they can be rewritten in the following way:

$$\langle [r_{12}(u_m,u_k),r_{13}(u_m,u_l)]+[r_{12}(u_m,u_k),r_{23}(u_k,u_l)]+[r_{32}(u_l,u_k),r_{13}(u_m,u_l)],\hat{S}^m_1\hat{S}^k_2\hat{S}^l_3\rangle,$$

where we have used the following notations:

$$\hat{S}^m_1=\sum_{\alpha=1}^{\dim \mathfrak{g}}\hat{S}^m_\alpha X^\alpha\otimes 1\otimes 1,\quad \hat{S}^k_2=\sum_{\beta=1}^{\dim \mathfrak{g}} 1\otimes \hat{S}^m_\beta X^\beta\otimes 1,\quad \hat{S}^l_3=\sum_{\delta=1}^{\dim \mathfrak{g}} 1\otimes 1\otimes \hat{S}^m_\delta X^\delta,$$

and $\langle,\rangle$ is a scalar product on $\mathfrak{g}\otimes\mathfrak{g}\otimes\mathfrak{g}$ extended in a natural way from the scalar product on $\mathfrak{g}$ and $\langle X_\alpha,X^\beta\rangle=\delta^\beta_\alpha$. By the virtue of the generalized Yang-Baxter equation these summands cancel. Hence, we obtain

$$[\hat{H}^k_0,\hat{H}^l_0]=\sum_{\alpha,\beta,\gamma,\delta} r^{\alpha,\beta}(u_l,u_k)r^{\gamma,\delta}(u_k,u_l)[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta]. \tag{A2}$$

This expression could be rewritten as $[\hat{H}^k_0,\hat{H}^l_0]=[\hat{H}^{k,l},\hat{H}^{l,k}]$, where

$$\hat{H}^{k,l}=\sum_{\alpha,\beta} r^{\alpha,\beta}(u_l,u_k)\hat{S}^l_\alpha\hat{S}^k_\beta,\quad \hat{H}^{l,k}=\sum_{\beta,\alpha} r^{\beta,\alpha}(u_k,u_l)\hat{S}^k_\beta\hat{S}^l_\alpha.$$

Let us now use the explicit form of our twisted r-matrices,

$$r^{\alpha,\beta}(u_l,u_k)=r^{\alpha,\beta}(u_l-u_k)-(r^{\sigma_2})^{\alpha,\beta}(u_l+u_k),$$

$$r^{\beta,\alpha}(u_k,u_l)=r^{\beta,\alpha}(u_k-u_l)-(r^{\sigma_2})^{\beta,\alpha}(u_l+u_k).$$

Using the skew symmetry of $r(u_l-u_k)$: $r^{\alpha,\beta}(u_l-u_k)=-r^{\beta,\alpha}(u_k-u_l)$ and symmetry of $r^{\sigma_2}(u_l+u_k)$: $(r^{\sigma_2})^{\alpha,\beta}(u_l+u_k)=(r^{\sigma_2})^{\beta,\alpha}(u_l+u_k)$ we obtain that in our case $\hat{H}^{k,l}$ and $\hat{H}^{k,l}$ can be rewritten as follows:

$$\hat{H}^{k,l}=-\hat{h}^{kl}_--\hat{h}^{kl}_+,\hat{H}^{l,k}=\hat{h}^{kl}_--\hat{h}^{kl}_+, \tag{A3}$$

where $\hat{h}^{k,l}_-=\sum_{\alpha,\beta}r^{\beta,\alpha}(u_k-u_l)\hat{S}^l_\alpha\hat{S}^k_\beta$, $\hat{h}^{k,l}_+=\sum_{\alpha,\beta}(r^{\sigma_2})^{\alpha,\beta}(u_k+u_l)\hat{S}^l_\alpha\hat{S}^k_\beta$. Hence we obtain

$$[\hat{H}^k_0,\hat{H}^l_0]=2[\hat{h}^{kl}_-,\hat{h}^{kl}_+]=2\sum_{\alpha,\beta,\gamma,\delta} r^{\beta,\alpha}(u_k-u_l)(r^{\sigma_2})^{\gamma,\delta}(u_k+u_l)[\hat{S}^k_\beta\hat{S}^l_\alpha,\hat{S}^k_\gamma\hat{S}^l_\delta]. \tag{A4}$$

Let us consider in details the expression $[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta]=\hat{S}^l_\alpha\hat{S}^l_\delta[\hat{S}^k_\beta,\hat{S}^k_\gamma]+[\hat{S}^l_\alpha,\hat{S}^l_\delta]\hat{S}^k_\gamma\hat{S}^k_\beta$. Let us show that this expression is symmetric with respect to the permutation of the operators with the same upper indices. We have

$$\begin{aligned}[\hat{S}^l_\alpha\hat{S}^k_\beta,\hat{S}^k_\gamma\hat{S}^l_\delta]&=\tfrac{1}{2}(\hat{S}^l_\alpha\hat{S}^l_\delta+\hat{S}^l_\delta\hat{S}^l_\alpha)[\hat{S}^k_\beta,\hat{S}^k_\gamma]+\tfrac{1}{2}[\hat{S}^l_\alpha,\hat{S}^l_\delta](\hat{S}^k_\gamma\hat{S}^k_\beta+\hat{S}^k_\beta\hat{S}^k_\gamma)+\tfrac{1}{2}([\hat{S}^l_\alpha,\hat{S}^l_\delta][\hat{S}^k_\beta,\hat{S}^k_\gamma]+[\hat{S}^l_\alpha,\hat{S}^l_\delta][\hat{S}^k_\gamma,\hat{S}^k_\beta])\\&=\tfrac{1}{2}C^\kappa_{\beta\gamma}(\hat{S}^l_\alpha\hat{S}^l_\delta+\hat{S}^l_\delta\hat{S}^l_\alpha)\hat{S}^k_\kappa+\tfrac{1}{2}C^\kappa_{\alpha\delta}\hat{S}^l_\kappa(\hat{S}^k_\gamma\hat{S}^k_\beta+\hat{S}^k_\beta\hat{S}^k_\gamma),\end{aligned}$$

We obtain that formula (A2) can be rewritten in the symmetrized tensor form,

$$[\hat{H}_0^k,\hat{H}_0^l]=\langle[r_{12}(u_k-u_l),r_{13}^{\sigma_3}(u_k+u_l)],\hat{S}_1^k((\hat{S}_2^l\hat{S}_3^l))\rangle-\langle[r_{23}^{\sigma_3}(u_l+u_k),r_{13}(u_k-u_l)],((\hat{S}_1^k\hat{S}_2^k))\hat{S}_3^l\rangle, \tag{A5}$$

where $((\hat{S}_2^l\hat{S}_3^l))\equiv\Sigma_{\alpha\beta}(\hat{S}_\alpha^l\hat{S}_\beta^l+\hat{S}_\beta^l\hat{S}_\alpha^l)1\otimes X_\alpha\otimes X_\beta$, $((\hat{S}_1^k\hat{S}_2^k))\equiv\Sigma_{\alpha\beta}(\hat{S}_\alpha^k\hat{S}_\beta^k+\hat{S}_\beta^k\hat{S}_\alpha^k)X_\alpha\otimes X_\beta\otimes 1$ and we have used the symmetry of the tensors $r_{23}^{\sigma_3}(u_l+u_k)$ and $r_{13}^{\sigma_3}(u_k+u_l)$.

Let us now explicitly calculate expression $[\hat{H}_1^k,\hat{H}_0^l]$,

$$\begin{aligned}
[\hat{H}_1^k,\hat{H}_0^l]&=\frac{1}{2}\sum_{m\neq k}\sum_{\alpha,\beta,\gamma,\delta}r^{\alpha,\beta}(u_m,u_k)r_0^{\gamma,\delta}(u_l,u_l)[\hat{S}_\alpha^m\hat{S}_\beta^k,(\hat{S}_\gamma^l\hat{S}_\delta^l+\hat{S}_\delta^l\hat{S}_\gamma^l)]\\
&=\frac{1}{2}\sum_{m\neq k}\sum_{\alpha,\beta,\gamma,\delta}(r^{\beta,\alpha}(u_k-u_m)+(r^{\sigma_2})^{\alpha,\beta}(u_m+u_k))(r^{\sigma_2})^{\gamma,\delta}(2u_l)[\hat{S}_\alpha^m\hat{S}_\beta^k,(\hat{S}_\gamma^l\hat{S}_\delta^l+\hat{S}_\delta^l\hat{S}_\gamma^l)]\\
&=\frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta}(r^{\beta,\alpha}(u_k-u_l)+(r^{\sigma_2})^{\alpha,\beta}(u_l+u_k))(r^{\sigma_2})^{\gamma,\delta}(2u_l)[\hat{S}_\alpha^l\hat{S}_\beta^k,(\hat{S}_\gamma^l\hat{S}_\delta^l+\hat{S}_\delta^l\hat{S}_\gamma^l)]\\
&=\frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta,\kappa}(r^{\beta,\alpha}(u_k-u_l)+(r^{\sigma_2})^{\alpha,\beta}(u_l+u_k))(r^{\sigma_2})^{\gamma,\delta}(2u_l)\hat{S}_\beta^k(C_{\alpha\delta}^\kappa(\hat{S}_\kappa^l\hat{S}_\gamma^l+\hat{S}_\kappa^l\hat{S}_\gamma^l)\\
&\quad+C_{\alpha\gamma}^\kappa(\hat{S}_\kappa^l\hat{S}_\delta^l+\hat{S}_\kappa^l\hat{S}_\delta^l))=\langle[r_{12}(u_k-u_l)+r_{13}^{\sigma_3}(u_l+u_k),r_{23}^{\sigma_3}(2u_l)],\hat{S}_1^k((\hat{S}_2^l\hat{S}_3^l))\rangle,
\end{aligned} \tag{A6}$$

where we have used symmetry of the tensors $(r^{\sigma_3})_{13}(u_l+u_k)$ and $(r^{\sigma_3})_{23}(2u_l)$.

In analogous way we obtain

$$[\hat{H}_0^k,\hat{H}_1^l]=-\langle[r_{12}^{\sigma_2}(2u_k),r_{13}(u_k-u_l)-r_{23}^{\sigma_3}(u_k+u_l)],((\hat{S}_1^k\hat{S}_2^k))\hat{S}_3^l\rangle. \tag{A7}$$

On the other hand, using identities (14b) and (14d) and condition (12) it is easy to show that

$$[r_{12}(u_k-u_l),r_{13}^{\sigma_3}(u_k+u_l)]=-([r_{12}(u_k-u_l)+r_{13}^{\sigma_3}(u_k+u_l),r_{23}^{\sigma_3}(2u_l)]), \tag{A8}$$

$$[r_{13}(u_k-u_l),r_{23}^{\sigma_3}(u_k+u_l)]=[r_{12}^{\sigma_2}(2u_k),r_{13}(u_k-u_l)-r_{23}^{\sigma_3}(u_k+u_l)]. \tag{A9}$$

Substituting equalities (A8) and (A9) into expression (A5) and then substituting (A5) together with the expressions (A6) and (A7) into the equation (A1) we obtain that $[\hat{H}^k,\hat{H}^l]=0$.

Theorem is proved.

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Symmetries on the discrete Heisenberg group C^*-algebra

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We consider symmetries on the C^*-algebra of the discrete Heisenberg group and their generalization to the generalized discrete Heisenberg groups, and study the structure of the crossed products by the symmetries and their fixed point algebras, and also compute the stable rank of the crossed products and their fixed point algebras. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2180625]

INTRODUCTION

The group C^*-algebras of either Lie, discrete, or locally compact groups have been very interesting objects in the theory of C^*-algebras (cf. Dixmier[8] and Pedersen[17]). Among many things, their (algebraic) structure is well studied to some great extent. For this subject, see Green[12] or Poguntke.[19] In particular, it is shown by Ref. 19, Theorem 2, that the group C^*-algebra of a connected Lie group has only either the C^*-algebra of compact operators on a (finite or infinite dimensional) Hilbert space, noncommutative tori or their tensor products as simple quotients. On the other hand, symmetries on C^*-algebras regarded as as noncommutative spaces have been of much interest and studied well. See Ref. 2 for symmetries of the CAR algebras, and see Bratteli, Elliott, Evans, and Kishimoto (Refs. 4–6) for symmetries on the irrational or rational rotation C^*-algebras, and see also Ref. 3 for symmetries on certain noncommutative tori. Recently, the ultimate result for symmetries on noncommutative tori has been obtained by Phillips.[18]

Our first interest is to study the structure of the group C^*-algebras of discrete solvable groups and to compute their stable rank since little is known about this case in the literature. As the first step toward this program, we consider symmetries on the group C^*-algebra of the discrete Heisenberg group and their generalization to the generalized discrete Heisenberg groups. After we obtained the structure of the crossed products of those group C^*-algebras by the symmetries, we find as a corollary that group C^*-algebras of solvable discrete groups may have certain simple AF algebras as quotients. Compared with the result of Ref. 19 mentioned above, this consequence as a point of view seems to be interesting. We also obtain that group C^*-algebras of disconnected Lie groups may have certain AH algebras (in fact AT algebras) as simple quotients. The estimates of the stable rank of the crossed products by the symmetries and their fixed point algebras should be also interesting. Indeed, we show that the estimates of the stable rank for the group C^*-algebras of solvable discrete groups are different from those for nilpotent discrete groups obtained in Ref. 14 in the sense that the stable rank of the group C^*-algebras is determined by the spaces of all two-dimensional irreducible representations of the groups, and however, the stable rank of their fixed point algebras is estimated by the spaces of all one-dimensional representations of them. See Ref. 20 for the stable rank of C^*-algebras, and see also Refs. 15, 21, and 24 for some results on the stable rank.

The contents of this paper are as follows: Section I, the symmetries; Sec. II, the structure; Sec. III, the stable rank, and Sec. IV, applications to Lie group C^*-algebras. In Sec. I we construct the symmetries mentioned above by a simple procedure. This construction method to obtain symmetries and to derive solvable discrete groups from nilpotent ones could prove useful in other

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situations. In Sec. II we consider the structure of the crossed products of the group C^*-algebras of the generalized discrete Heisenberg groups by the symmetries and their fixed point algebras. For the proofs, we use some results of Bratteli, Elliott, Evans, and Kishimoto (Refs. 4–6) about noncommutative spheres, which are crossed products of rotation algebras by the flips and their fixed point algebras. In fact, the crossed products by some (canonical ones) of our symmetries and their fixed point algebras are continuous field C^*-algebras with fibers given by noncommutative spheres in the sense above, but not always as shown below. In Sec. III we estimate the stable rank of the crossed products by our symmetries and their fixed point algebras using the structure of Sec. II, some basic results on the stable rank and an estimate for the stable rank of continuous field C^*-algebras (Ref. 13). In Sec. IV we apply the methods above to the group C^*-algebras of the Mautner groups and Dixmier groups and their generalizations. See also Refs. 27, 32, and 30 and Refs. 33 and 34 for the structure and stable rank of the group C^*-algebras of certain connected solvable Lie groups and see Refs. 28, 29, and 31 for the cases of certain disconnected solvable Lie groups.

I. THE SYMMETRIES

Notation: Let $C^*(G)$ be the (full) group C^*-algebra of a locally compact group G (cf. Refs. 8 and 17). Let $\mathfrak{A}\rtimes_\alpha G$ be the (full) crossed product of a C^*-algebra $\mathfrak{A}$ by a locally compact group G with α an action by automorphisms of $\mathfrak{A}$.[17]

Recall that the discrete Heisenberg group of rank 3 is

$$H_3^{\mathbb{Z}}=\left\{g=(c,b,a)=\begin{pmatrix}1 & a & c\\ 0 & 1 & b\\ 0 & 0 & 1\end{pmatrix}\middle| a,b,c\in\mathbb{Z}\right\}.$$

Define the semidirect product $H_3^{\mathbb{Z}}\rtimes_{\beta^{(1)}}\mathbb{Z}_2$ to be the group generated by $H_3^{\mathbb{Z}}$ and the diagonal matrix $d_1=-1\oplus 1\oplus 1$ (the diagonal sum), where the action $\beta^{(1)}$ of $\mathbb{Z}_2$ is defined by $\beta^{(1)}_{-1}(c,b,a)=d_1gd_1^{-1}=(-c,b,-a)\in H_3^{\mathbb{Z}}$.

Similarly, we define the semidirect product $H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ generated by $H_3^{\mathbb{Z}}$ and the diagonal matrix $d_2=1\oplus -1\oplus 1$, where the action $\beta^{(2)}$ of $\mathbb{Z}_2$ is defined by $\beta^{(2)}_{-1}(c,b,a)=d_2gd_2^{-1}=(c,-b,-a)\in H_3^{\mathbb{Z}}$. Moreover, define the semidirect product $H_3^{\mathbb{Z}}\rtimes_{\beta^{(3)}}\mathbb{Z}_2$ generated by $H_3^{\mathbb{Z}}$ and the diagonal matrix $d_3=1\oplus 1\oplus -1$, where the action $\beta^{(3)}$ of $\mathbb{Z}_2$ is defined by $\beta^{(3)}_{-1}(c,b,a)=d_3gd_3^{-1}=(-c,-b,a)\in H_3^{\mathbb{Z}}$.

Furthermore, we may take the following diagonal matrices: $d_{1,2}=-1\oplus -1\oplus 1$, $d_{1,3}=-1\oplus 1\oplus -1$, and $d_{2,3}=1\oplus -1\oplus -1$ to define the semidirect products with the, respectively, corresponding actions $\beta^{(1,2)}$, $\beta^{(1,3)}$, and $\beta^{(2,3)}$. But it follows from direct computation that $\beta^{(1,2)}=\beta^{(3)}$, $\beta^{(1,3)}=\beta^{(2)}$, and $\beta^{(2,3)}=\beta^{(1)}$.

Let $C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(j)}}\mathbb{Z}_2)$ be the group C^*-algebra of $H_3^{\mathbb{Z}}\rtimes_{\beta^{(j)}}\mathbb{Z}_2$ for $1\leqslant j\leqslant 3$. Then $C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(j)}}\mathbb{Z}_2)$ is isomorphic to the crossed product $C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(j)}}\mathbb{Z}_2$ of the group C^*-algebra $C^*(H_3^{\mathbb{Z}})$ by the action $\beta^{(j)}$ of $\mathbb{Z}_2$. Let U,V,W be the unitaries generating $C^*(H_3^{\mathbb{Z}})$, respectively, corresponding to the following matrices: (0,0,1), (0,1,0), and $(1,0,0)\in H_3^{\mathbb{Z}}$. By definition of the actions $\beta^{(j)}$ of $\mathbb{Z}_2$ (called symmetries), we obtain

Proposition 1.1: There exist symmetries $\beta^{(j)}(1\leqslant j\leqslant 3)$ on the group C^*-algebra $C^*(H_3^{\mathbb{Z}})$ with U, V, W the canonical generators such that

$$\beta^{(1)}(U)=U^*,\quad \beta^{(1)}(V)=V,\quad \beta^{(1)}(W)=W^*,$$

$$\beta^{(2)}(U)=U^*,\quad \beta^{(2)}(V)=V^*,\quad \beta^{(2)}(W)=W,$$

$$\beta^{(3)}(U)=U,\quad \beta^{(3)}(V)=V^*,\quad \beta^{(3)}(W)=W^*.$$

Recall that the discrete Heisenberg group of rank $2n+1$ is

$$H_{2n+1}^{\mathbb{Z}} = \left\{ g = (c,b,a) = \begin{pmatrix} 1 & a & c \\ 0_n^t & 1_n & b^t \\ 0 & 0_n & 1 \end{pmatrix} | a,b \in \mathbb{Z}^n, c \in \mathbb{Z} \right\},$$

where 1_n is the $n \times n$ identity matrix, $0_n = (0) \in \mathbb{Z}^n$, and b^t, 0_n^t are the transposes of b, 0_n, respectively. Define the semidirect product $H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(1)}} \mathbb{Z}_2$ to be the group generated by $H_{2n+1}^{\mathbb{Z}}$ and the diagonal matrix $d_1 = -1 \oplus 1_n \oplus 1$, where the action $\beta^{(1)}$ of $\mathbb{Z}_2$ is defined by $\beta_{-1}^{(1)}(c,b,a) = d_1 g d_1^{-1} = (-c,b,-a) \in H_{2n+1}^{\mathbb{Z}}$, where $-a = (-a_j) \in \mathbb{Z}^n$.

Similarly, define the semidirect product $H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(n+2)}} \mathbb{Z}_2$ to be the group generated by $H_{2n+1}^{\mathbb{Z}}$ and the diagonal matrix $d_{n+2} = 1 \oplus 1_n \oplus -1$, where the action $\beta^{(n+2)}$ of $\mathbb{Z}_2$ is defined by $\beta_{-1}^{(n+2)}(c,b,a) = d_{n+2} g d_{n+2}^{-1} = (-c,-b,a) \in H_{2n+1}^{\mathbb{Z}}$, where $-b = (-b_j) \in \mathbb{Z}^n$.

Furthermore, for $2 \leqslant j \leqslant n+1$ we define the semidirect product $H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(j)}} \mathbb{Z}_2$ generated by $H_3^{\mathbb{Z}}$ and the diagonal matrix $d_j = 1_{j-1} \oplus -1 \oplus 1_{n+2-j}$, where the action $\beta^{(j)}$ of $\mathbb{Z}_2$ is defined by

$$\beta_{-1}^{(j)}(c,b,a) = d_j g d_j^{-1} = (c, b - 2\tilde{b_j}, a - 2\tilde{a_j}),$$

where $\tilde{b_j} = (0,\ldots,0,b_j,0,\ldots,0)$ and $\tilde{a_j} = (0,\ldots,0,a_j,0,\ldots,0)$ (b_j, a_j are jth components).

Let $C^*(H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(j)}} \mathbb{Z}_2)$ be the group C^*-algebra of $H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(j)}} \mathbb{Z}_2$ for $1 \leqslant j \leqslant n+2$. Then $C^*(H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta^{(j)}} \mathbb{Z}_2)$ is isomorphic to the crossed product $C^*(H_{2n+1}^{\mathbb{Z}}) \rtimes_{\beta^{(j)}} \mathbb{Z}_2$ of the group C^*-algebra $C^*(H_{2n+1}^{\mathbb{Z}})$ by the symmetry $\beta^{(j)}$. Let U_j, V_j, W ($1 \leqslant j \leqslant n$) be the unitaries generating $C^*(H_{2n+1}^{\mathbb{Z}})$, respectively, corresponding to the following diagonal matrices: $(0,0_n,\tilde{1_j})$, $(0,\tilde{1_j},0_n)$, and $(1,0_n,0_n)$, where $\tilde{1_j} = \tilde{a_j}$ with $a_j = 1$. By definition of the actions $\beta^{(j)}$ of $\mathbb{Z}_2$ (called symmetries), we obtain the following.

Proposition 1.2: There exist symmetries $\beta^{(j)}$ ($1 \leqslant j \leqslant n+2$) on the group C^*-algebra $C^*(H_{2n+1}^{\mathbb{Z}})$ with U_j, V_j, W ($1 \leqslant j \leqslant n$) the generators such that

$$\beta^{(1)}(U_j) = U_j^*, \quad \beta^{(1)}(V_j) = V_j \quad (1 \leqslant j \leqslant n), \quad \beta^{(1)}(W) = W^*,$$

$$\beta^{(n+2)}(U_j) = U_j, \quad \beta^{(n+2)}(V_j) = V_j^* \quad (1 \leqslant j \leqslant n), \quad \beta^{(n+2)}(W) = W^*,$$

and for $2 \leqslant j \leqslant n+1$,

$$\beta^{(j)}(U_j) = U_j^*, \quad \beta^{(j)}(V_j) = V_j^*, \quad \beta^{(j)}(W) = W,$$

$$\beta^{(j)}(U_k) = U_k \quad (k \neq j), \quad \beta^{(j)}(V_k) = V_k \quad (k \neq j).$$

Moreover, define the semidirect product $H_{2n+1}^{\mathbb{Z}} \rtimes_{\gamma} \mathbb{Z}_2$ to be the group generated by $H_{2n+1}^{\mathbb{Z}}$ and the diagonal matrix $d_{1_n} = 1 \oplus -1_n \oplus 1$, where the action γ of $\mathbb{Z}_2$ is defined by $\gamma_{-1}(c,b,a) = d_{1_n} g d_{1_n}^{-1} = (c,-b,-a) \in H_{2n+1}^{\mathbb{Z}}$.

Definition: We say that an action β of $\mathbb{Z}_2$ on the group C^*-algebra $C^*(H_{2n+1}^{\mathbb{Z}})$ is a canonical symmetry if it is induced from a semidirect product $H_{2n+1}^{\mathbb{Z}} \rtimes_{\beta} \mathbb{Z}_2$ generated by $H_{2n+1}^{\mathbb{Z}}$ and an $(n+2) \times (n+2)$ diagonal matrix with 1 or -1 on the diagonal, where β is the adjoint action by the diagonal matrix.

Proposition 1.3: There exist $2^{n+1} - 1$ nontrivial canonical symmetries on the group C^*-algebra $C^*(H_{2n+1}^{\mathbb{Z}})$. In particular, if one of the symmetries is γ defined above, then

$$\gamma(U_j) = U_j^*, \quad \gamma(V_j) = V_j^* \quad (1 \leqslant j \leqslant n), \quad \gamma(W) = W,$$

where U_j, V_j, W are generating unitaries of $C^*(H_{2n+1}^{\mathbb{Z}})$.

Proof: Let d be the diagonal matrix associated with a canonical symmetry. Note that $dgd^{-1} = dgd = (-d)g(-d)^{-1}$ for $g \in H_{2n+1}^{\mathbb{Z}}$. Thus, the number of choosing diagonal matrices with 1 or -1 on the diagonal is reduced to $2^{n+2}/2 = 2^{n+1}$. Since $1_{n+2} g 1_{n+2} = (-1_{n+2}) g (-1_{n+2}) = g$ for $g \in H_{2n+1}^{\mathbb{Z}}$, there are $2^{n+1} - 1$ nontrivial canonical symmetries. □

II. THE STRUCTURE

Notation: We identify elements z of $\mathbb{T}$ with $\theta \in \mathbb{R}(\mathrm{mod}\ 1)$ via $z=e^{2\pi i\theta}$, and write $\theta \in \mathbb{T}$. Let $C(X)$ be the C^*-algebra of continuous complex-valued functions on a compact Hausdorff space X. For a C^*-algebra $\mathfrak{A}$, let $C(X,\mathfrak{A})$ be the C^*-algebra of continuous $\mathfrak{A}$-valued functions on X. Let $\Gamma(X,\{\mathfrak{A}_t\}_{t\in X})$ be the continuous field C^*-algebra of continuous operator fields on X with fibers $\mathfrak{A}_t$ for $t \in X$ C^*-algebras (Ref. 8). An AF algebra is an inductive limit of finite-dimensional C^*-algebras, and an AT algebra is an inductive limit of matrix algebras over $C(\mathbb{T})$, and an AH algebra is an inductive limit of homogeneous C^*-algebras (cf. Ref. 23).

Theorem 2.1: *The crossed product $C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ is isomorphic to the continuous field C^*-algebra $\Gamma(\mathbb{T},\{\mathfrak{A}_\theta\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})$, where $\mathfrak{A}_\theta$ are rotation algebras for $\theta\in\mathbb{R}(mod\ 1)$.*

Proof: Since $H_3^{\mathbb{Z}}$ is isomorphic to the semidirect product $\mathbb{Z}^2\rtimes\mathbb{Z}$ through the identification between $g\in H_3^{\mathbb{Z}}$ and (c,b,a) for $c,b,a\in\mathbb{Z}$, $C^*(H_3^{\mathbb{Z}})$ is isomorphic to $C^*(\mathbb{Z}^2)\rtimes\mathbb{Z}$. By the Fourier transform, $C^*(\mathbb{Z}^2)\rtimes\mathbb{Z}\cong C(\mathbb{T}^2)\rtimes\mathbb{Z}$. Furthermore, we have

$$C(\mathbb{T}^2)\rtimes\mathbb{Z}\cong\Gamma(\mathbb{T},\{C(\mathbb{T})\rtimes_\theta\mathbb{Z}\}_{\theta\in\mathbb{T}})$$

and $C(\mathbb{T})\rtimes_\theta\mathbb{Z}=\mathfrak{A}_\theta$ (cf. Ref. 1). Therefore, we obtain

$$C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(2)}}\mathbb{Z}_2\cong\Gamma(\mathbb{T},\{\mathfrak{A}_\theta\}_{\theta\in\mathbb{T}})\rtimes\mathbb{Z}_2\cong\Gamma(\mathbb{T},\{\mathfrak{A}_\theta\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})$$

since $\mathfrak{A}_\theta$ generated by U,V are invariant under $\mathbb{Z}_2$, and note also that $C(\mathbb{T})$ generated by W is the center of $C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ since W is fixed by $\beta^{(2)}$ (see Proposition 1.1) (cf. Ref. 16 Theorem 1.2 and see also Ref. 22). □

Remark: Since the action of $\mathbb{Z}_2$ on $\mathfrak{A}_\theta$ is the flip, the crossed product $\mathfrak{A}_\theta\rtimes\mathbb{Z}_2$ for θ irrational is a simple C^*-algebra with a unique tracial state by Ref. 4 and is AF by Ref. 6, Theorem 1.1. In fact, the crossed products $\mathfrak{A}_\theta\rtimes\mathbb{Z}_2$ are inductive limits of finite direct sums of the building blocks $C_{n,k}$ defined by $C_{n,k}=M_n(\mathbb{C})\otimes C_k$ for $n\geqslant 1$ and $k=-1,0,1,2$, where $C_{-1}=\mathbb{C}$, $C_0=C([-1,1])$, $C_1=\{f\in C([0,1],M_2(\mathbb{C}))\,|\,f(0)\in\mathbb{C}\oplus\mathbb{C}\}$, and

$$C_2=\{f\in C([-1,1],M_2(\mathbb{C}))\,|\,f(-1)\in\mathbb{C}^2,f(1)\in\mathbb{C}^2\}$$

(see Ref. 6, Corollary 7.4). Then it follows that the crossed products are AF since they are simple with unique tracial states (Ref. 6, Theorem 8.1 and see Ref. 25). If $\theta=p/q$ with p, q mutually prime positive integers, the crossed products $\mathfrak{A}_\theta\rtimes\mathbb{Z}_2$ are regarded as certain subalgebras of $C(S^2,M_{2q}(\mathbb{C}))$ (Ref. 5, Theorem 1.3).

Moreover, we have the following.

Theorem 2.2: *The crossed product $C^*(H_{2n+1}^{\mathbb{Z}})\rtimes_\gamma\mathbb{Z}_2$ is isomorphic to the continuous field C^*-algebra $\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})$, where $\mathfrak{A}_\theta$ are rotation algebras for $\theta\in\mathbb{R}(mod\ 1)$.*

Proof: Since $H_{2n+1}^{\mathbb{Z}}$ is isomorphic to the semidirect product $\mathbb{Z}^{n+1}\rtimes\mathbb{Z}^n$ through the identification between $g\in H_{2n+1}^{\mathbb{Z}}$ and (c,b,a) for $c\in\mathbb{Z}$, b, $a\in\mathbb{Z}^n$, $C^*(H_{2n+1}^{\mathbb{Z}})$ is isomorphic to $C^*(\mathbb{Z}^{n+1})\rtimes\mathbb{Z}^n$. By the Fourier transform, $C^*(\mathbb{Z}^{n+1})\rtimes\mathbb{Z}^n\cong C(\mathbb{T}^{n+1})\rtimes\mathbb{Z}^n$. Furthermore, we have

$$C(\mathbb{T}^{n+1})\rtimes\mathbb{Z}^n\cong\Gamma(\mathbb{T},\{C(\mathbb{T}^n)\rtimes_\theta\mathbb{Z}^n\}_{\theta\in\mathbb{T}})$$

and $C(\mathbb{T}^n)\rtimes_\theta\mathbb{Z}^n=\otimes^n\mathfrak{A}_\theta$. Therefore, we obtain

$$C^*(H_{2n+1}^{\mathbb{Z}})\rtimes_\gamma\mathbb{Z}_2\cong\Gamma(\mathbb{T},\{\otimes^n\mathfrak{A}_\theta\}_{\theta\in T})\rtimes\mathbb{Z}_2\cong\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})$$

since $\otimes^n\mathfrak{A}_\theta$ generated by U_j, $V_j(1\leqslant j\leqslant n)$ are invariant under $\mathbb{Z}_2$, and note also that $C(\mathbb{T})$ generated by W is the center of $C^*(H_{2n+1}^{\mathbb{Z}})\rtimes_\gamma\mathbb{Z}_2$ since W is fixed by γ (see Proposition 1.3) (cf. Ref. 16, Theorem 1.2 and see also Ref. 22). □

Remark: Since the action of $\mathbb{Z}_2$ on $\otimes^n\mathfrak{A}_\theta$ is the flip, the crossed product $(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2$ for θ irrational is a simple AF algebra by Refs. 4 and 6 (or Ref. 18, Theorem 10.11).

Corollary 2.3: The group C^*-algebras of solvable discrete groups may have certain AF algebras as simple quotients.

Proof: For instance, we take $H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ as a solvable discrete group. □

Corollary 2.4: The group C^*-algebras of solvable discrete groups may have certain AT algebras as simple quotients.

Proof: For instance, we take $H^{\mathbb{Z}}_{2n+1} \rtimes_{\beta^{(2)}} \mathbb{Z}_2$ as a solvable discrete group. In this case, we have

$$C^*(H^{\mathbb{Z}}_{2n+1}) \rtimes_{\beta^{(2)}} \mathbb{Z}_2 \cong \Gamma(\mathbb{T}, \{(\otimes^n \mathfrak{A}_\theta) \rtimes \mathbb{Z}_2\}_{\theta \in \mathbb{T}})$$

and $(\otimes^n \mathfrak{A}_\theta) \rtimes \mathbb{Z}_2 \cong (\mathfrak{A}_\theta \rtimes \mathbb{Z}_2) \otimes (\otimes^{n-1} \mathfrak{A}_\theta)$ since U_1, V_1 are invariant under $\mathbb{Z}_2$ and the action of $\mathbb{Z}_2$ is trivial elsewhere. If θ is irrational, $\mathfrak{A}_\theta \rtimes \mathbb{Z}_2$ is a simple AF algebra by Refs. 4 and 6, and $\mathfrak{A}_\theta$ is a simple AT algebra by Ref. 10, where an AT algebra is an inductive limit of direct sums of matrix algebras over $C(\mathbb{T})$. Therefore, $(\otimes^n \mathfrak{A}_\theta) \rtimes \mathbb{Z}_2$ with the tensor product decomposition is a simple AH algebra. Furthermore, since $\mathfrak{A}_\theta$ has real rank zero by Choi-Elliott[7] we have that the tensor product $\otimes^{n-1} \mathfrak{A}_\theta$ is in fact an AT algebra by Elliott-Gong (Ref. 11, Theorems 3.11 and 3.19). Hence $(\otimes^n \mathfrak{A}_\theta) \rtimes \mathbb{Z}_2$ is an AT algebra. □

Theorem 2.5: *The fixed point algebra $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}$ associated with the crossed product $C^*(H^{\mathbb{Z}}_3) \rtimes_{\beta^{(2)}} \mathbb{Z}_2$ is isomorphic to $\Gamma(\mathbb{T}, \{\mathfrak{A}_\theta^{\beta^{(2)}}\}_{\theta \in \mathbb{T}})$ the associated continuous field C^*-algebra, where $\mathfrak{A}_\theta^{\beta^{(2)}}$ are the fixed point algebras of the rotation algebras $\mathfrak{A}_\theta$ for $\theta \in \mathbb{R}(mod\ 1)$.*

Proof: Note that $C(\mathbb{T})$ generated by W is contained in $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}$ and is the center. Thus, $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}$ is written as the C^*-algebra of a continuous field on $\mathbb{T}$ with fibers contained in $\mathfrak{A}_\theta \rtimes \mathbb{Z}_2$. In fact, the fibers are given by $\mathfrak{A}_\theta^{\beta^{(2)}}$. □

Remark: The fixed point algebra $\mathfrak{A}_\theta^{\beta^{(2)}}$ for θ irrational is a simple AF algebra. Indeed, the fixed point algebras $\mathfrak{A}_\theta^{\beta^{(2)}}$ for θ irrational are corners of $\mathfrak{A}_\theta \rtimes_{\beta^{(2)}} \mathbb{Z}_2$. Hence they are AF. If $\theta = p/q$ with p, q mutually prime positive integers, the fixed point algebras $\mathfrak{A}_\theta^{\beta^{(2)}}$ are regarded as certain subalgebras of $C(S^2, M_q(\mathbb{C}))$ (Ref. 5, Theorem 1.2). If $q \geqslant 3$, then $\mathfrak{A}_\theta^{\beta^{(2)}}$ and $\mathfrak{A}_\theta \rtimes_{\beta^{(2)}} \mathbb{Z}_2$ are Morita equivalent, but not for $q=1$ or $q=2$.

Furthermore, we have the following.

Theorem 2.6: *The fixed point algebra $C^*(H^{\mathbb{Z}}_{2n+1})^\gamma$ associated with the crossed product $C^*(H^{\mathbb{Z}}_{2n+1}) \rtimes_\gamma \mathbb{Z}_2$ is isomorphic to $\Gamma(\mathbb{T}, \{(\otimes^n \mathfrak{A}_\theta)^\gamma\}_{\theta \in \mathbb{T}})$ the associated continuous field C^*-algebra, where $(\otimes^n \mathfrak{A}_\theta)^\gamma$ are the fixed point algebras of the noncommutative tori $\otimes^n \mathfrak{A}_\theta$ for $\theta \in \mathbb{R}(mod\ 1)$.*

Proof: Note that $C(\mathbb{T})$ generated by W is contained in $C^*(H^{\mathbb{Z}}_{2n+1})^\gamma$ and is the center. Thus, $C^*(H^{\mathbb{Z}}_{2n+1})^\gamma$ is written as the C^*-algebra of a continuous field on $\mathbb{T}$ with fibers contained in $(\otimes^n \mathfrak{A}_\theta) \rtimes \mathbb{Z}_2$. In fact, the fibers are given by $(\otimes^n \mathfrak{A}_\theta)^\gamma$. □

Remark: The fixed point algebra $(\otimes^n \mathfrak{A}_\theta)^\gamma$ for θ irrational is a simple AF algebra. Indeed, the fixed point algebras $(\otimes^n \mathfrak{A}_\theta)^\gamma$ for θ irrational are corners of $(\otimes^n \mathfrak{A}_\theta) \rtimes_\gamma \mathbb{Z}_2$. Hence they are AF. See also Ref. 3 Theorem 3.1.

We next consider the case of symmetries $\beta^{(1)}, \beta^{(3)}$ in Proposition 1.1.

Theorem 2.7: *The crossed products $C^*(H^{\mathbb{Z}}_3) \rtimes_{\beta^{(j)}} \mathbb{Z}_2$ $(j=1,3)$ are isomorphic to $C(\mathbb{T}^2) \rtimes (\mathbb{Z}_2 \times \mathbb{Z})$ which has the decomposition into the following exact sequence:*

$$0 \to \Gamma_0((0,\pi), \{C((\{z\} \times \mathbb{T}) \sqcup (\{\bar{z}\} \times \mathbb{T})) \rtimes (\mathbb{Z}_2 \times \mathbb{Z})\}_{z \in (0,\pi)})$$
$$\to C(\mathbb{T}^2) \rtimes (\mathbb{Z}_2 \times \mathbb{Z}) \to C^*(\mathbb{Z}_2) \otimes (C(\mathbb{T}) \rtimes \mathbb{Z} \oplus C(\mathbb{T}) \rtimes_{-1} \mathbb{Z}) \to 0,$$

where the closed ideal is the C^*-algebra of continuous operator fields on $(0,\pi)$ vanishing at infinity with fibers double rotation C^*-algebras on the disjoint union $\mathbb{T} \sqcup \mathbb{T}$ that we call, and the actions of two crossed products in the quotient are the flip and the minus flip on $\mathbb{T}$, respectively. Moreover, the double rotation C^*-algebras for irrational $z \in (0,\pi)$ are isomorphic to $(\mathfrak{A}_z \oplus \mathfrak{A}_{\bar{z}}) \rtimes \mathbb{Z}_2$ and are simple AF algebras.

Proof: As in the proof of Theorem 2.1, we have $C^*(H^{\mathbb{Z}}_3) \cong C(\mathbb{T}^2) \rtimes \mathbb{Z}$. Furthermore, note that

$$(C(\mathbb{T}^2) \rtimes \mathbb{Z}) \rtimes_{\beta^{(3)}} \mathbb{Z}_2 \cong C(\mathbb{T}^2) \rtimes (\mathbb{Z}_2 \times \mathbb{Z})$$

since $\beta^{(3)}(U) = U$ so that the actions of $\mathbb{Z}$ and $\mathbb{Z}_2$ commute. For $j=1$, we replace the role of U with that of V via $(W,V,U) \leftrightarrow (W,U,V)$ exchanging the order in $C(\mathbb{T}^2) \rtimes \mathbb{Z}$. Since $\beta^{(1)}(V) = V$, we can

replace $\beta^{(3)}$ with $\beta^{(1)}$ in the isomorphism above. Set $\beta=\beta^{(j)}$ for $j=1,3$. The action β on $\mathbb{T}$ is given by

$$\beta_{(-1,1)}(z,w)=\beta_{(1,1)}\beta_{(-1,0)}(z,w)=\beta_{(1,1)}(\bar{z},\bar{w})=(\bar{z},\bar{z}\bar{w})\in\mathbb{T}^2$$

for $(-1,1)\in\mathbb{Z}_2\times\mathbb{Z}$. It follows that the closed subspaces $\{\pm1\}\times\mathbb{T}$ of $\mathbb{T}^2$ are invariant under β, and $\mathbb{Z}_2$ acts trivially on the subspace. Since $\beta_{(-1,1)}(1,w)=(1,\bar{w})$ and $\beta_{(-1,1)}(-1,w)=(-1,-\bar{w})$, the actions on $\{1\}\times\mathbb{T}$ and $\{-1\}\times\mathbb{T}$ are the flip and the minus flip, respectively. Therefore, we obtain

$$C(\mathbb{T}^2)\rtimes(\mathbb{Z}_2\times\mathbb{Z})\to C(\{\pm1\}\times\mathbb{T})\rtimes(\mathbb{Z}_2\times\mathbb{Z})\cong C^*(\mathbb{Z}_2)\otimes(C(\mathbb{T})\rtimes\mathbb{Z}\oplus C(\mathbb{T})\rtimes_{-1}\mathbb{Z})\to 0.$$

Furthermore, note that the disjoint unions $(\{z\}\times\mathbb{Z})\sqcup(\bar{z}\times\mathbb{T})$ in $\mathbb{T}^2$ for $z\neq\pm1$ are invariant under β. Thus the kernel of the onto homomorphism above is given by

$$\Gamma_0((0,\pi),\{C((\{z\}\times\mathbb{T})\sqcup(\{\bar{z}\}\times\mathbb{T}))\rtimes(\mathbb{Z}_2\times\mathbb{Z})\}_{z\in(0,\pi)}),$$

where we identify the quotient space $(\mathbb{T}\backslash\{\pm1\})/\mathbb{Z}_2$ with $(0,\pi)$. Simplicity of the fibers for irrational $z\in(0,\pi)$ follows from minimality of the action β on $(\{z\}\times\mathbb{T})\sqcup(\{\bar{z}\}\times\mathbb{T})$, that is, any orbit under β in this disjoint union is dense in it. Note that $\beta_{(1,n)}(z,w)=(z,z^nw)\in\{z\}\times\mathbb{T}$ and $\beta_{(1,n)}\times(\bar{z},w)=(\bar{z},(\bar{z})^nw)\in\{\bar{z}\}\times\mathbb{T}$. Moreover, we note that

$$C((\{z\}\times\mathbb{T})\sqcup(\{\bar{z}\}\times\mathbb{T}))\rtimes(\mathbb{Z}_2\times\mathbb{Z})\cong C((\{z\}\times\mathbb{T})\sqcup(\{\bar{z}\}\times\mathbb{T}))\rtimes\mathbb{Z}\rtimes\mathbb{Z}_2\cong(\mathfrak{A}_z\oplus\mathfrak{A}_{\bar{z}})\rtimes\mathbb{Z}_2.$$

Also observe that the crossed products $\mathfrak{A}_z\rtimes\mathbb{Z}_2$ and $\mathfrak{A}_{\bar{z}}\rtimes\mathbb{Z}_2$ are C^*-subalgebras of $(\mathfrak{A}_z\oplus\mathfrak{A}_{\bar{z}})\rtimes\mathbb{Z}_2$, and their union is equal to it. Since the crossed products $\mathfrak{A}_z\rtimes\mathbb{Z}_2$ and $\mathfrak{A}_{\bar{z}}\rtimes\mathbb{Z}_2$ for irrational z are AF algebras with building blocks invariant under the flip, it follows that $(\mathfrak{A}_z\oplus\mathfrak{A}_{\bar{z}})\rtimes\mathbb{Z}_2$ is also AF. □

Theorem 2.8: *The fixed point algebras $C^*(H_3^{\mathbb{Z}})^{\beta^{(j)}}$ associated with the crossed products $C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(j)}}\mathbb{Z}_2$ $(j=1,3)$ are isomorphic to $C(\mathbb{T}^2)^{\beta^{(j)}}\rtimes\mathbb{Z}$ which are isomorphic to*

$$C(S^2/\mathbb{T}\times\mathbb{T})\rtimes\mathbb{Z}\cong\Gamma([0,\pi],\{C(\mathbb{T}\cup_1\mathbb{T})\rtimes_\theta\mathbb{Z}\}_{\theta\in(0,\pi)}\cup\{C([\pi,2\pi])\rtimes_\theta\mathbb{Z}\}_{\theta=0}\cup\{C(\mathbb{T})\rtimes_\theta\mathbb{Z}\}_{\theta=\pi}),$$

the continuous field C^*-algebra on $[0,\pi]$ with fibers the double rotation algebras $C(\mathbb{T}\cup_1\mathbb{T})\rtimes_\theta\mathbb{Z}$ on the space $\mathbb{T}\cup_1\mathbb{T}$ attached at $1\in\mathbb{T}$ for $\theta\in(0,\pi]$ and $C([\pi,2\pi])\rtimes_0\mathbb{Z}=C([\pi,2\pi]\times\mathbb{T})$, and $S^2/\mathbb{T}\times\mathbb{T}$ is obtained from S^2 identifying four edges in S^2 to make two circles $\mathbb{T}$.

Proof: As in the proof of Theorem 2.7, we have that for $\beta=\beta^{(j)}$ $(j=1,3)$,

$$C^*(H_3^{\mathbb{Z}})\rtimes_{\beta^{(j)}}\mathbb{Z}_2\cong C(\mathbb{T}^2)\rtimes_\beta\mathbb{Z}_2\rtimes\mathbb{Z}.$$

Since $C(\mathbb{T}^2)^\beta=C(S^2)$ (Ref. 5), we have $C^*(H_3^{\mathbb{Z}})^\beta=C(S^2)\rtimes\mathbb{Z}$. We may view S^2 as follows. Consider the space obtained from $\{(s,t)\in[0,2\pi]\times[0,2\pi]\,|\,s\leqslant t\}$ by identifying the points $(s,0)$ with $(2\pi-s,0)$ for $0\leqslant s\leqslant\pi$, $(2\pi,t)$ with $(2\pi,2\pi-t)$ for $0\leqslant t\leqslant\pi$, and (0,0) with both $(0,2\pi)$ and $(2\pi,2\pi)$, and consider the space obtained from $\{(s,t)\in[0,2\pi]\times[0,2\pi]\,|\,s\geqslant t\}$ by identifying the points $(0,t)$ with $(0,2\pi-t)$ for $0\leqslant t\leqslant\pi$, $(s,2\pi)$ with $(2\pi-s,2\pi)$ for $0\leqslant s\leqslant\pi$, and (0,0) with both $(2\pi,0)$ and $(2\pi,2\pi)$. Then we attach the spaces along with the line $\{(s,s)\,|\,0\leqslant s\leqslant2\pi\}$ and obtain the attached space that is homeomorphic to S^2. Moreover, we need to identify the edges (circles) $\{(s,t)\,|\,0\leqslant s\leqslant\pi\}$ for $t=0,1$ and $\{(s,t)\,|\,0\leqslant t\leqslant\pi\}$ for $s=0,1$ in S^2 to make two circles $\mathbb{T}$. Thus, we need to replace S^2 with $S^2/\mathbb{T}\times\mathbb{T}$.

Since the subspaces $\{(s,0)\,|\,0\leqslant s\leqslant\pi\}$, $\{(s,t)\,|\,0\leqslant s\leqslant2\pi,t=s,t=2\pi-s\}$ for $s\in(0,\pi)$, and $\{(s,t)\,|\,0\leqslant s\leqslant2\pi,t=\pi\}$ are invariant under the action of $\mathbb{Z}$, we obtain the decomposition as in the claim. □

III. THE STABLE RANK

Notation and facts: For a unital C^*-algebra $\mathfrak{A}$, its stable rank $\mathrm{sr}(\mathfrak{A})$ is defined to be the smallest integer $n\geqslant1$ such that any element (a_j) of $\mathfrak{A}^n$ is approximated by elements (b_j) of $\mathfrak{A}^n$

such that $\Sigma_{j=1}^{n} b_j^* b_j$ are invertible in $\mathfrak{A}$. For a nonunital C^*-algebra $\mathfrak{A}$, its stable rank is defined to be that of the unitization $\mathfrak{A}^+$ by $\mathbb{C}$ (see Ref. 20). For x a real number, by $[x]$ we mean the maximum integer $\leqslant x$, and by $\{x\}$ we mean the least integer $\geqslant x$ in what follows. In particular, recall that

$$\mathrm{sr}(C_0(X)) = [\dim X^+/2] + 1, \quad \mathrm{sr}(M_n(\mathfrak{A})) = \{(\mathrm{sr}(\mathfrak{A}) - 1)/2\} + 1$$

for X a locally compact Hausdorff space, X^+ its one point compactification, and $C_0(X)$ the C^*-algebra of continuous functions on X vanishing at infinity, and $M_n(\mathfrak{A})$ the $n \times n$ matrix algebra over $\mathfrak{A}$ a C^*-algebra (see Ref. 20, Proposition 1.7 and Theorem 6.1). Note that $C_0(X)^+ \cong C(X^+)$. For a (unital) C^*-algebra $\mathfrak{A}$, its connected stable rank $\mathrm{csr}(\mathfrak{A})$ is defined to be the smallest integer $n \geqslant 1$ such that the set of all (b_j) of $\mathfrak{A}^n$ with $\Sigma_{j=1}^{n} b_j^* b_j$ invertible in $\mathfrak{A}$ is connected (see Ref. 20). Recall that

$$\max\{\mathrm{sr}(\mathfrak{I}), \mathrm{sr}(\mathfrak{A}/\mathfrak{I})\} \leqslant \mathrm{sr}(\mathfrak{A}) \leqslant \max\{\mathrm{sr}(\mathfrak{I}), \mathrm{sr}(\mathfrak{A}/\mathfrak{I}), \mathrm{csr}(\mathfrak{A}/\mathfrak{I})\}$$

for a short exact sequence: $0 \to \mathfrak{I} \to \mathfrak{A} \to \mathfrak{A}/\mathfrak{I} \to 0$ of C^*-algebras (Ref. 20, Theorems 4.3, 4.4, and 4.11). Also recall that

$$\mathrm{csr}(M_n(\mathfrak{A})) \leqslant \{(\mathrm{csr}(\mathfrak{A}) - 1)/n\} + 1, \quad \mathrm{csr}(C_0(X)) \leqslant [(\dim X^+ + 1)/2] + 1$$

for $\mathfrak{A}$ a C^*-algebra and X a locally compact Hausdorff space (Ref. 21, Theorem 4.7 and Ref. 15, Corollary 2.5). Moreover,

$$\mathrm{sr}(\Gamma(X, \{\mathfrak{A}_t\}_{t \in X})) \leqslant \sup_{t \in X} \mathrm{sr}(C([0,1]^k) \otimes \mathfrak{A}_t)$$

for $\Gamma(X, \{\mathfrak{A}_t\}_{t \in X})$ a continuous field C^*-algebra on a σ-compact, locally compact k-dimensional metric space X with fibers $\mathfrak{A}_t$ unital C^*-algebras by Ref. 14 (see also Ref. 13 for the case where $X = [0,1]$ the interval or $\mathbb{T}$ the torus) and see Ref. 8, Chap. 10 for continuous field C^*-algebras.

Lemma 3.1: The crossed product $C(\mathbb{T}^2) \rtimes \mathbb{Z}_2$ by the flip has a composition series such that

$$0 \to \mathfrak{I} \to C(\mathbb{T}^2) \rtimes \mathbb{Z}_2 \to \oplus^4 \mathbb{C}^2 \to 0,$$

$$0 \to C_0(\mathbb{R}^2) \otimes M_2(\mathbb{C}) \to \mathfrak{I} \to \oplus^4 C_0(\mathbb{R}) \otimes M_2(\mathbb{C}) \to 0.$$

Proof: Note that the flip on $\mathbb{T}^2$ is given by $(z, w) \mapsto (\bar{z}, \bar{w}) \in \mathbb{T}^2$. Since the four points $(\pm 1, \pm 1) \in \mathbb{T}^2$ are fixed under the flip, we have the following exact sequence:

$$0 \to C_0(\mathbb{T}^2 \setminus \{(\pm 1, \pm 1)\}) \rtimes \mathbb{Z}_2 \to C(\mathbb{T}^2) \rtimes \mathbb{Z}_2 \to \mathbb{C}^4 \rtimes \mathbb{Z}_2 \to 0$$

and $\mathbb{C}^4 \rtimes \mathbb{Z}_2 \cong \oplus^4 C^*(\mathbb{Z}_2) \cong \oplus^4 \mathbb{C}^2$, where $C_0(\mathbb{T}^2 \setminus \{(\pm 1, \pm 1)\})$ is the C^*-algebra of continuous functions on $\mathbb{T}^2 \setminus \{(\pm 1, \pm 1)\}$ vanishing at infinity. Since the subspaces $\{\pm 1\} \times (\mathbb{T} \setminus \{\pm 1\})$ and $(\mathbb{T} \setminus \{\pm 1\}) \times \{\pm 1\}$ are disjoint and closed in $\mathbb{T}^2 \setminus \{(\pm 1, \pm 1)\}$, we have

$$\begin{aligned} 0 \to C_0((\mathbb{T} \setminus \{\pm 1\}) \times (\mathbb{T} \setminus \{\pm 1\})) \rtimes \mathbb{Z}_2 \to C_0(\mathbb{T}^2 \setminus \{(\pm 1, \pm 1)\}) \rtimes \mathbb{Z}_2 \\ \to C_0(\{\pm 1\} \times (\mathbb{T} \setminus \{\pm 1\})) \rtimes \mathbb{Z}_2 \otimes C_0\left((\mathbb{T} \setminus \{\pm 1\}) \times \{\pm 1\})\right) \rtimes \mathbb{Z}_2 \to 0. \end{aligned}$$

In addition, we have

$$C_0(\{(\pm 1\} \times (\mathbb{T} \setminus \{\pm 1\})) \rtimes \mathbb{Z}_2 \cong \oplus^2 C_0(\mathbb{T} \setminus \{\pm 1\}) \rtimes \mathbb{Z}_2,$$

$$C_0((\mathbb{T} \setminus \{\pm 1\}) \times \{\pm 1\}) \rtimes \mathbb{Z}_2 \cong \oplus^2 (\mathbb{T} \setminus \{\pm 1\}) \rtimes \mathbb{Z}_2.$$

Moreover, we obtain

$$C_0(\mathbb{T} \setminus \{\pm 1\}) \rtimes \mathbb{Z}_2 \cong C_0((0, \pi)) \otimes \mathbb{C}^2 \rtimes \mathbb{Z}_2 \cong C_0(\mathbb{R}) \otimes M_2(\mathbb{C}),$$

$$C_0((\mathbb{T}\setminus\{\pm 1\})^2)\rtimes \mathbb{Z}_2 \cong C_0((0,\pi)^2)\otimes \mathbb{C}^2 \rtimes \mathbb{Z}_2 \cong C_0(\mathbb{R}^2)\otimes M_2(\mathbb{C})$$

since the flip on $\mathbb{T}\setminus\{\pm 1\}$ is the reflection on it. □

Remark: Compare this result with Eilers-Loring-Pedersen (Ref. 9, 4.3) using the different methodology.

Theorem 3.2: *The C^*-algebra $C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)$ of the discrete solvable group $H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ has stable rank* 2. *In the process we obtain*

$$\mathrm{sr}(C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)) = 2 = \mathrm{sr}(C(\mathbb{T}^2)\rtimes \mathbb{Z}_2)$$

and

$$\mathrm{sr}(C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)) = [\dim(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)_2^{\wedge}/2]+1 = \mathrm{sr}(C_0(\mathbb{R}^2)\otimes M_2(\mathbb{C})) = \{[2/2]/2\}+1 = \{1/2\}+1 = 2,$$

and

$$\mathrm{sr}(C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)) \neq [\dim(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)_1^{\wedge}/2]+1 = [0/2]+1 = 1,$$

where $(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)_1^{\wedge}$, $(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)_2^{\wedge}$ are the spaces of all 1,2*-dimensional irreducible representations of $H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2$, respectively.*

Proof: Using Theorem 2.1 and Ref. 13 we obtain

$$\mathrm{sr}(C^*(H_3^{\mathbb{Z}}\rtimes_{\beta^{(2)}}\mathbb{Z}_2)) = \mathrm{sr}(\Gamma(\mathbb{T},\{\mathfrak{A}_\theta\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})) \leqslant \sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta\rtimes\mathbb{Z}_2)).$$

Since $\mathfrak{A}_\theta\rtimes\mathbb{Z}_2$ for θ irrational are AF, the fibers $C(\mathbb{T},\mathfrak{A}_\theta\rtimes\mathbb{Z}_2)$ for θ irrational are AT algebras. Hence we have $\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta\rtimes\mathbb{Z}_2))=1$.

When $\theta=0$, using Lemma 3.1 we have

$$0\to C(\mathbb{T},\mathfrak{I})\to C(\mathbb{T},C(\mathbb{T}^2)\rtimes\mathbb{Z}_2)\to C(\mathbb{T},\oplus^4\mathbb{C}^2)\to 0,$$

$$0\to C_0(\mathbb{T}\times\mathbb{R}^2)\otimes M_2(\mathbb{C})\to C(\mathbb{T},\mathfrak{I})\to \oplus^4 C_0(\mathbb{T}\times\mathbb{R})\otimes M_2(\mathbb{C})\to 0,$$

and $C(\mathbb{T},\oplus^4\mathbb{C}^2)\cong\oplus^8 C(\mathbb{T})$. By Ref. 20, Proposition 1.7 and Theorem 6.1,

$$\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}^2)\otimes M_2(\mathbb{C})) = \{(\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}^2))-1)/2\}+1 = \{[3/2]/2\}+1 = 2,$$

$$\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R})\otimes M_2(\mathbb{C})) = \{(\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}))-1)/2\}+1 = \{[2/2]/2\}+1 = 2.$$

By Ref. 21, Theorem 4.7 and Ref. 15, Corollary 2.5 we have

$$\mathrm{csr}(C_0(\mathbb{T}\times\mathbb{R})\otimes M_2(\mathbb{C})) \leqslant \{(\mathrm{csr}(C_0(\mathbb{T}\times\mathbb{R}))-1)/2\}+1 \leqslant \{[3/2]/2\}+1 = 2.$$

Therefore, using Ref. 20, Theorems 4.3, 4.4, and 4.11 we obtain $\mathrm{sr}(C(\mathbb{T},\mathfrak{I}))=2$. Since $\mathrm{sr}(C(\mathbb{T}))=1$ and $\mathrm{csr}(C(\mathbb{T}))=2$ (Ref. 24, p. 381), we obtain $\mathrm{sr}(C(\mathbb{T},C(\mathbb{T}^2)\rtimes\mathbb{Z}_2))=2$ by Ref. 20, Theorems 4.3, 4.4, and 4.11. Similarly, using Lemma 3.1 and the argument above for computing stable rank we also have $\mathrm{sr}(C(\mathbb{T}^2)\rtimes\mathbb{Z}_2)=2$.

For $\theta=p/q$ nonzero rationals for mutually prime positive integers p,q, it is shown by Ref. 5, Theorem 1.3 that

$$\mathfrak{A}_\theta\rtimes\mathbb{Z}_2 \cong \Gamma(S^2,\{M_{2q}(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}),$$

the continuous field C^*-algebra on the two-dimensional sphere S^2 with fibers $M_{2q}(\mathbb{C})$ for $t\in S^2\setminus\cup_{j=0}^3\{p_j\}$ and $\mathfrak{M}_{p_j}$ at certain points p_j of S^2 for $0\leqslant j\leqslant 3$, where $\mathfrak{M}_{p_j}$ are subalgebras of $M_{2q}(\mathbb{C})$ that are the sums of certain two matrix algebras over $\mathbb{C}$. Hence, by Ref. 13 we obtain

$$\begin{aligned}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta \rtimes \mathbb{Z}_2)) &= \mathrm{sr}(\Gamma(\mathbb{T}\times S^2,\{M_{2q}(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}))\\ &\leqslant \max\{\mathrm{sr}(C(\mathbb{T}\times S^2,M_{2q}(\mathbb{C}))),\max_{0\leqslant j\leqslant 3}\{\mathrm{sr}(C(\mathbb{T}\times S^2,\mathfrak{M}_{p_j}))\}\}\\ &\leqslant \max\{\{[3/2]/2q\}+1,\max_{0\leqslant j\leqslant 3}\{\{3/2]/q_j\}+1\}\}\leqslant 2,\end{aligned}$$

where $\mathfrak{M}_{p_j}=M_{q_j}(\mathbb{C})\oplus M_{q_j'}(\mathbb{C})$ for $1\leqslant q_j\leqslant q_j'$.

Therefore, we obtain

$$2=\mathrm{sr}(C(\mathbb{T}^2)\rtimes\mathbb{Z}_2)\leqslant \mathrm{sr}(\Gamma(\mathbb{T},\{\mathfrak{A}_\theta\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}}))\leqslant \sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta\rtimes\mathbb{Z}_2))=2.$$

Furthermore, using Lemma 3.1 and from the discussions above we conclude that the dimension of the space $(H_3^{\mathbb{Z}}\rtimes_\gamma\mathbb{Z}_2)_2^\wedge$ is equal to the dimension of $\mathbb{R}^2$, and the dimension of the space $(H_3^{\mathbb{Z}}\rtimes_\gamma\mathbb{Z}_2)_1^\wedge$ is equal to zero since it corresponds to $\oplus^4\mathbb{C}^2$. □

Lemma 3.3: The crossed product $C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2$ by the flip has a composition series $\{\mathfrak{J}_j\}_{j=0}^{2n+1}$ such that $\mathfrak{J}_0=\{0\}$, $\mathfrak{J}_{2n+1}=C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2$ and

$$0\to\mathfrak{J}_{2n}\to C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2\to\oplus^{2^{2n}}\mathbb{C}^2\to 0,$$

$$\mathfrak{J}_{2n-k+1}/\mathfrak{J}_{2n-k}\cong\oplus^{\binom{2n}{k}}\oplus^2 C_0(\mathbb{R}^k)\otimes M_2(\mathbb{C})\quad(1\leqslant k\leqslant 2n).$$

Proof: Note that the flip on $\mathbb{T}^{2n}$ is given by $(z_j,w_j)_{j=1}^n\mapsto(\bar z_j,\bar w_j)_{j=1}^n\in\mathbb{T}^{2n}=\Pi^n\mathbb{T}^2$. Since the 2^{2n} points $(\pm1,\pm1)_{j=1}^n\in\mathbb{T}^{2n}$ are fixed under the flip, we have the following exact sequence:

$$0\to C_0(\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\})\rtimes\mathbb{Z}_2\to C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2\to\mathbb{C}^{2^{2n}}\rtimes\mathbb{Z}_2\to 0$$

and $\mathbb{C}^{2^{2n}}\rtimes\mathbb{Z}_2\cong\oplus^{2^{2n}}C^*(\mathbb{Z}_2)\cong\oplus^{2^{2n}}\mathbb{C}^2$, where $C_0(\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\})$ is the C^*-algebra of continuous functions on $\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\}$ vanishing at infinity. Since the $2n$ subspaces

$$((\mathbb{T}\setminus\{\pm1\})\times\{\pm1\})\times(\pm1,\pm1)\times\cdots\times(\pm1,\pm1),$$

$$(\{\pm1\}\times(\mathbb{T}\setminus\{\pm1\}))\times(\pm1,\pm1)\times\cdots\times(\pm1,\pm1),$$

$$(\pm1,\pm1)\times((\mathbb{T}\setminus\{\pm1\})\times\{\pm1\})\times(\pm1,\pm1)\times\cdots\times(\pm1,\pm1),\cdots,$$

$$(\pm1,\pm1)\times\cdots\times(\pm1,\pm1)\times(\{\pm1\}\times(\mathbb{T}\setminus\{\pm1\}))\subset\Pi^n\mathbb{T}^2$$

are disjoint and closed in $\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\}$, we have

$$0\to C_0(X_{2n-1})\rtimes\mathbb{Z}_2\to C_0(\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\})\rtimes\mathbb{Z}_2\to\oplus^{2n}\oplus^2 C_0(\mathbb{T}\setminus\{\pm1\})\rtimes\mathbb{Z}_2\to 0,$$

where X_{2n-1} is the complement of the union of the $4n$ closed subspaces homeomorphic to $\mathbb{T}\setminus\{\pm1\}$ in $\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\}$. Inductively, we have the following exact sequences for $1\leqslant k\leqslant 2n-1$:

$$0\to C_0(X_{2n-k})\rtimes\mathbb{Z}_2\to C_0(X_{2n-k+1})\rtimes\mathbb{Z}_2\to\oplus^{\binom{2n}{k}}\oplus^2 C_0((\mathbb{T}\setminus\{\pm1\})^k)\rtimes\mathbb{Z}_0\to 0,$$

where the combination $\binom{2n}{k}$ corresponds to choosing k copies of the subspace $\mathbb{T}\setminus\{\pm1\}$ of $\mathbb{T}$ in $\mathbb{T}^{2n}$, and $X_{2n}=\mathbb{T}^{2n}\setminus\{(\pm1,\pm1)_{j=1}^n\}$ and $X_1=(\mathbb{T}\setminus\{\pm1\})^{2n}$. Moreover, we obtain

$$C_0((\mathbb{T}\setminus\{\pm1\})^k)\rtimes\mathbb{Z}_2\cong C_0((0,\pi)^k)\otimes\mathbb{C}^2\rtimes\mathbb{Z}_2\cong C_0(\mathbb{R}^k)\otimes M_2(\mathbb{C})$$

since the flip on $(\mathbb{T}\setminus\{\pm1\})^k$ is the reflection on it. □

Theorem 3.4: *The C^*-algebra $C^*(H_{2n+1}^{\mathbb{Z}}\rtimes_\gamma\mathbb{Z}_2)$ of the discrete solvable group $H_{2n+1}^{\mathbb{Z}}\rtimes_\gamma\mathbb{Z}_2$ has stable rank $\{n/2\}+1$. In the process we obtain*

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2))=\{n/2\}+1=\mathrm{sr}(C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)$$

and

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2))=[\dim(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2)^\wedge_2/2]+1=\mathrm{sr}(C_0(\mathbb{R}^{2n})\otimes M_2(\mathbb{C}))=\{[2n/2]/2\}+1=\{n/2\}+1,$$

and

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2))\neq[\dim(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_1)^\wedge_1/2]+1=[0/2]+1=0,$$

where $(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2)^\wedge_1$, $(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2)^\wedge_2$ *are the spaces of all* 1,2*-dimensional irreducible representations of* $H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2$, *respectively*.

Proof: Using Theorem 2.2 and Ref. 13 we obtain

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2))=\mathrm{sr}(\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})\leqslant\sup_{\theta\in T}\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2)).$$

Since $(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2$ for θ irrational are AF, the fibers $C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2)$ for θ irrational are AT algebras. Hence we have $\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2))=1$.

When $\theta=0$, by using Lemma 3.3, $C(\mathbb{T},C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)$ has a composition series $\{\mathfrak{K}_j\}_{j=0}^{2n+1}$ such that $\mathfrak{K}_0=\{0\}$, $\mathfrak{K}_{2n+1}=C(\mathbb{T},C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)$ and

$$0\to\mathfrak{K}_{2n}\to C(\mathbb{T},C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)\to\oplus^{2^{2n}}\oplus^2C(\mathbb{T})\to 0,$$

$$\mathfrak{K}_{2n-k+1}/\mathfrak{K}_{2n-k}\cong\oplus^{\binom{2n}{k}}\oplus^2C_0(\mathbb{T}\times\mathbb{R}^k)\otimes M_2(\mathbb{C})$$

for $1\leqslant k\leqslant 2n$. By Ref. 20, Proposition 1.7 and Theorem 6.1,

$$\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}^k)\otimes M_2(\mathbb{C}))=\{(\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}^k))-1)/2\}+1=\{[(k+1)/2]/2\}+1.$$

In particular, if $k=2n$, then $\mathrm{sr}(C_0(\mathbb{T}\times\mathbb{R}^{2n})\otimes M_2(\mathbb{C}))=\{n/2\}+1$. By Ref. 21, Theorem 4.7 and Ref. 15, Corollary 2.5 we have

$$\mathrm{csr}(C_0(\mathbb{T}\times\mathbb{R}^k)\otimes M_2(\mathbb{C}))\leqslant\{(\mathrm{csr}(C_0(\mathbb{T}\times\mathbb{R}^k))-1)/2\}+1\leqslant\{[(2+k)/2]/2\}+1.$$

In particular, if $k=2n-1$, then $\mathrm{csr}(C_0(\mathbb{T}\times\mathbb{R}^{2n-1})\otimes M_2(\mathbb{C}))\leqslant\{n/2\}+1$. Therefore, inductively using Ref. 20, Theorems 4.3, 4.4, and 4.11 to the finite composition series of $C(\mathbb{T},C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)$ we obtain

$$\mathrm{sr}(C(\mathbb{T},C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2))=\{n/2\}+1.$$

Similarly, using Lemma 3.3 and the argument above for computing the stable rank we also have $\mathrm{sr}(C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)=\{n/2\}+1$.

For $\theta=p/q$ nonzero rationals for mutually prime positive integers p,q, it follows from Ref. 5, Theorem 1.3 that

$$\otimes^n(\mathfrak{A}_\theta\rtimes\mathbb{Z}_2)\cong\otimes^n\Gamma(S^2,\{M_{2q}(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}),$$

which is viewed as the continuous field C^*-algebra on the product space Π^nS^2 with fibers $\otimes^2M_{2q}(\mathbb{C})\cong M_{2^nq^n}(\mathbb{C})$ for $t\in\Pi^n(S^2\setminus\cup_{j=0}^3\{p_j\})$ and n-fold tensor products of some copies of $M_{2q}(\mathbb{C})$ and $\mathfrak{M}_{p_j}$ for other points of Π^nS^2. Since $(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2$ is a canonical subalgebra of $\otimes^n(\mathfrak{A}_\theta\rtimes\mathbb{Z}_2)$, it can also be viewed as the continuous field on Π^nS^2 with fibers $M_{2q^n}(\mathbb{C})$ for $t\in\Pi^n(S^2\setminus\cup_{j=0}^3\{p_j\})$ and n-fold tensor products of some copies of $M_q(\mathbb{C})$ and $\mathfrak{M}_{p_j}$ and one copy of $M_{2q}(\mathbb{C})$ for other points of Π^nS^2. Let $\mathfrak{B}_t$ for $t\in\Pi^nS^2$ be those fibers and let $M_{l_t}=\mathfrak{B}_t$ or M_{l_t} be the direct factor of $\mathfrak{B}_t$ with the size l_t smallest among direct factors of $\mathfrak{B}_t$. By Ref. 13 we obtain

$$\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2))=\mathrm{sr}(\Gamma(\Pi^nS^2,\{C(\mathbb{T},\mathfrak{B}_t)\}_{t\in\Pi^nS^2})$$
$$\leqslant\sup_{t\in\Pi^nS^2}\mathrm{sr}(C(\mathbb{T}\times\Pi^nS^2,M_{l_t}(\mathbb{C})))=\sup_{t\in\Pi^nS^2}\{[(1+2n)/2]/l_t\}+1\leqslant\{n/2\}+1.$$

Therefore, we obtain

$$\{n/2\}+1=\mathrm{sr}(C(\mathbb{T}^{2n})\rtimes\mathbb{Z}_2)\leqslant\mathrm{sr}(\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2\}_{\theta\in\mathbb{T}})$$
$$\leqslant\sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)\rtimes\mathbb{Z}_2))=\{n/2\}+1.$$

Furthermore, using Lemma 3.3 and from the discussions above we conclude that the dimension of the space $(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2)^\wedge_2$ is equal to the dimension of $\mathbb{R}^{2n}$, and the dimension of the space $(H^{\mathbb{Z}}_{2n+1}\rtimes_\gamma\mathbb{Z}_2)^\wedge_1$ is equal to zero since it corresponds to $\oplus^{2^{2n}}\mathbb{C}^2$. □

Remark: Reference 14 shows that for Γ a finitely generated, torsion free, two-step nilpotent (discrete) group and $C^*(\Gamma)$ its group C^*-algebra,

$$\mathrm{sr}(C^*(\Gamma))=\mathrm{sr}(C(\Gamma^\wedge_1))=[\dim\Gamma^\wedge_1/2]+1,$$

where $\Gamma^\wedge_1$ is the space of one-dimensional representations of Γ. See also the same equality for Γ a nilpotent Lie group[33] (for the simply connected case) and Ref. 26 (for the connected case). Furthermore, by Ref. 34, for G a simply connected solvable Lie group,

$$\mathrm{sr}(C^*(G))=\min\{\dim G,\max\{2,\mathrm{sr}(C_0(G^\wedge_1))\}\}.$$

Our theorem above says that this formula for a discrete solvable group Γ is not valid even if replacing $\dim G$ with the rank of Γ.

Theorem 3.5: *The fixed point algebra $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}$ associated with the crossed product $C^*(H^{\mathbb{Z}}_3)\rtimes_{\beta^{(2)}}\mathbb{Z}_2$ has stable rank* 2. *In the process we obtain*

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}})=2=\mathrm{sr}(C(\mathbb{T}^2)^{\beta^{(2)}})$$

and

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}})=\mathrm{sr}(C((C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}})^\wedge_1))=\mathrm{sr}(C(S^2))=[\dim S^2/2]+1=2,$$

where $(C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}})^\wedge_1$ means the space of all one-dimensional representations of $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}$.

Proof: By Theorem 2.5 we have $C^*(H^{\mathbb{Z}}_3)^{\beta^{(2)}}\cong\Gamma(\mathbb{T},\{\mathfrak{A}_\theta^{\beta^{(2)}}\}_{\theta\in\mathbb{T}})$, where $\mathfrak{A}_\theta^{\beta^{(2)}}$ are the fixed point algebras of the rotation algebras $\mathfrak{A}_\theta$ for $\theta\in\mathbb{R}(\mathrm{mod}\,1)$. By Ref. 13 we obtain

$$\mathrm{sr}(\Gamma(\mathbb{T},\{\mathfrak{A}_\theta^{\beta^{(2)}}\}_{\theta\in\mathbb{T}}))\leqslant\sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta^{\beta^{(2)}})).$$

If θ is irrational, then $\mathfrak{A}_\theta^{\beta^{(2)}}$ is an AF algebra. Hence $C(\mathbb{T},\mathfrak{A}_\theta^{\beta^{(2)}})$ is an AT algebra. Therefore, we have $\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta^{\beta^{(2)}}))=1$.

If $\theta=0$, then $\mathfrak{A}_0^{\beta^{(2)}}=C(S^2)$ (Ref. 5, a remark after Theorem 1.2). Since $C(\mathbb{T},C(S^2))\cong C(\mathbb{T}\times S^2)$, we have $\mathrm{sr}(C(\mathbb{T},C(S^2)))=[3/2]+1=2$.

For $\theta=p/q$ nonzero rationals for mutually prime positive integers p,q, it is shown by Ref. 5, Theorem 1.2 that

$$\mathfrak{A}_\theta^{\beta^{(2)}}\cong\Gamma(S^2,\{M_q(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}),$$

the continuous field C^*-algebra on S^2 with fibers $M_q(\mathbb{C})$ for $t\in S^2\setminus\cup_{j=0}^3\{p_j\}$ and $\mathfrak{M}_{p_j}$ at certain points p_j of S^2 for $0\leqslant j\leqslant 3$, where $\mathfrak{M}_{p_j}$ are subalgebras of $M_q(\mathbb{C})$ that are the sums of certain two matrix algebras over $\mathbb{C}$. Hence, by Ref. 13 we obtain

$$\begin{aligned}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta^{\beta^{(2)}})) &= \mathrm{sr}(\Gamma(\mathbb{T}\times S^2,\{M_q(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}))\\ &\leqslant \max\{\mathrm{sr}(C(\mathbb{T}\times S^2,M_q(\mathbb{C}))),\max_{0\leqslant j\leqslant 3}\{\mathrm{sr}(C(\mathbb{T}\times S^2,\mathfrak{M}_{p_j}))\}\}\\ &\leqslant \max\{\{[3/2]/q\}+1,\max_{0\leqslant j\leqslant 3}\{\{[3/2]/q_j\}+1\}\}\leqslant 2,\end{aligned}$$

where $\mathfrak{M}_{p_j}=M_{q_j}(\mathbb{C})\oplus M_{q_j'}(\mathbb{C})$ with $1\leqslant q_j\leqslant q_j'$.

Therefore, we obtain

$$2=\mathrm{sr}(C(\mathbb{T}^2)^{\beta^{(2)}})\leqslant \mathrm{sr}(\Gamma(\mathbb{T},\{\mathfrak{A}_\theta^{\beta^{(2)}}\}_{\theta\in\mathbb{T}}))\leqslant \sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},\mathfrak{A}_\theta^{\beta^{(2)}}))=2.$$

□

Theorem 3.6: *The fixed point algebra $C^*(H_{2n+1}^{\mathbb{Z}})^\gamma$ associated with the crossed product $C^*(H_{2n+1}^{\mathbb{Z}})\rtimes_\gamma\mathbb{Z}_2$ has stable rank $n+1$. In the process we obtain*

$$\mathrm{sr}(C^*(H_{2n+1}^{\mathbb{Z}})^\gamma)=n+1=\mathrm{sr}(C(\Pi^n\mathbb{T}^2)^\gamma)$$

and

$$\mathrm{sr}(C^*(H_{2n+1}^{\mathbb{Z}})^\gamma)=\mathrm{sr}(C((C^*(H_{2n+1}^{\mathbb{Z}})^\gamma)_1^\wedge))=\mathrm{sr}(C(\Pi^nS^2))=[2n/2]+1=n+1,$$

where $(C^*(H_{2n+1}^{\mathbb{Z}})^\gamma)_1^\wedge$ means the space of all one-dimensional representations of $C^*(H_{2n+1}^{\mathbb{Z}})^\gamma$.

Proof: By Theorem 2.6 we have

$$C^*(H_{2n+1}^{\mathbb{Z}})^\gamma\cong\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)^\gamma\}_{\theta\in\mathbb{T}}),$$

where $(\otimes^n\mathfrak{A}_\theta)^\gamma$ are the fixed point algebras of the noncommutative tori $(\otimes^n\mathfrak{A}_\theta)$ for $\theta\in\mathbb{R}(\mathrm{mod}\,1)$. By Ref. 13 we obtain

$$\mathrm{sr}(\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)^\gamma\}_{\theta\in\mathbb{T}}))\leqslant\sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)^\gamma)).$$

If θ is irrational, then $(\otimes^n\mathfrak{A}_\theta)^\gamma$ is an AF algebra. Hence $C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)^\gamma)$ is an AT algebra. Therefore, we have $\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)^\gamma))=1$.

If $\theta=0$, then $(\otimes^n\mathfrak{A}_0)^\gamma=C(\Pi^nS^2)$. Since $C(\mathbb{T},C(\Pi^nS^2))\cong C(\mathbb{T}\times\Pi^nS^2)$, we have $\mathrm{sr}(C(\mathbb{T},C(\Pi^nS^2)))=[(2n+1)/2]+1=n+1$.

For $\theta=p/q$ nonzero rationals for mutually prime positive integers p,q, it follows from Ref. 5, Theorem 1.2 that

$$(\otimes^n\mathfrak{A}_\theta)^\gamma\cong\otimes^n\Gamma(S^2,\{M_q(\mathbb{C})\}_{t\in S^2\setminus\cup_{j=0}^3\{p_j\}}\cup\{\mathfrak{M}_{p_j}\}_{0\leqslant j\leqslant 3}),$$

which is viewed as the continuous field C^*-algebra on Π^nS^2 with fibers $\otimes^nM_q(\mathbb{C})\cong M_{q^n}(\mathbb{C})$ for $t\in\Pi^n(S^2\setminus\cup_{j=0}^3\{p_j\})$ and n-fold tensor products of some copies of $M_q(\mathbb{C})$ and $\mathfrak{M}_{p_j}(0\leqslant j\leqslant 3)$ at other points of Π^nS^2, where $\mathfrak{M}_{p_j}$ are subalgebras of $M_q(\mathbb{C})$ that are the sums of certain two matrix algebras over $\mathbb{C}$. Let $\mathfrak{B}_t$ for $t\in\Pi^nS^2$ be those fibers and let $M_{l_t}(\mathbb{C})=M_{q^n}(\mathbb{C})$ or $M_{l_t}(\mathbb{C})$ be the direct factor with the size l_t smallest among direct factors of $\mathfrak{B}_t$. Hence, by Ref. 13 we obtain

$$\begin{aligned}\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)^\gamma)) &= \mathrm{sr}(\Gamma(\mathbb{T}\times\Pi^nS^2,\{\mathfrak{B}_t\}_{t\in\Pi^nS^2}))\\ &\leqslant \sup_{t\in\Pi^nS^2}\mathrm{sr}(C(\mathbb{T}\times\Pi^nS^2,M_{l_t}(\mathbb{C})))\leqslant\{[(2n+1)/2]/l_t\}+1\leqslant\{n/2\}+1.\end{aligned}$$

Therefore, we obtain

$$n+1=\mathrm{sr}(C(\Pi^n\mathbb{T}^2)^\gamma)\leqslant\mathrm{sr}(\Gamma(\mathbb{T},\{(\otimes^n\mathfrak{A}_\theta)^\gamma\}_{\theta\in\mathbb{T}}))\leqslant\sup_{\theta\in\mathbb{T}}\mathrm{sr}(C(\mathbb{T},(\otimes^n\mathfrak{A}_\theta)^\gamma))=n+1.$$

□

Corollary 3.7: We obtain

$$\mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1})\rtimes_\gamma \mathbb{Z}_2) = \{n/2\} + 1 \leqslant n + 1 = \mathrm{sr}(C^*(H^{\mathbb{Z}}_{2n+1})^\gamma)$$

for $n \geqslant 1$, *where* $\gamma = \beta^{(2)}$ *when* $n = 1$.

Theorem 3.8: *The crossed products* $C^*(H^{\mathbb{Z}}_3)\rtimes_{\beta(j)}\mathbb{Z}_2$ $(j=1,3)$ *have stable rank* 2. *Furthermore, we obtain* $\mathrm{sr}(C^*(H^{\mathbb{Z}}_3)^{\beta^{(j)}}) = 2$.

Proof: By Theorem 2.7, we may view $C^*(H^{\mathbb{Z}}_3)\rtimes_{\beta(j)}\mathbb{Z}_2$ as the continuous field C^*-algebra on $[0,\pi]$ with fibers simple AF algebras $(\mathfrak{A}_z \oplus \mathfrak{A}_{\bar{z}})\rtimes\mathbb{Z}_2$ for $z \in (0,\pi)$, $C^*(\mathbb{Z}_2)\otimes(C(\mathbb{T})\rtimes\mathbb{Z})$ at 0, and $C^*(\mathbb{Z}_2)\otimes(C(\mathbb{T})\rtimes_{-1}\mathbb{Z})$ at π. Using Lemma 3.1 and the methods of Theorem 3.2 similarly, one can obtain the conclusion. Using Theorem 2.8 we obtain the claim for the fixed point algebras $C^*(H^{\mathbb{Z}}_3)^{\beta^{(j)}}$ $(j=1,3)$. □

IV. APPLICATIONS TO LIE GROUP C^*-ALGEBRAS

Using the methods of Sec. I one can construct symmetries on the C^*-algebras of Lie groups such as the Mautner group M_5 (a real five-dimensional solvable Lie group $\mathbb{C}^2\rtimes_\alpha\mathbb{R}$ with α the action defined by $\alpha_t(z,u) = (e^{2\pi i t}z, e^{2\pi i\theta t}w)$ for $z, w \in \mathbb{C}$ and θ an irrational) and the Dixmier group D_7 (a real seven-dimensional solvable Lie group $\mathbb{C}^2\rtimes_\alpha H^{\mathbb{R}}_3$ a semidirect product by the real three-dimensional Heisenberg Lie group with α the action defined by $\alpha_g(z,w) = (e^{ia}z, e^{ib}w)$ for z, $w \in \mathbb{C}$ and $g = (c,b,a) \in H^{\mathbb{R}}_3$) (cf. Refs. 27 and 32). Indeed, the symmetries on $C^*(M_5)$ and $C^*(D_7)$ are induced from the flip on $\mathbb{C}^2$ in $\mathbb{C}^2\rtimes_\alpha\mathbb{R}$ and $\mathbb{C}^2\rtimes H^{\mathbb{R}}_3$, respectively. Moreover, the structure of $C^*(M_5)$ as a continuous field C^*-algebra is given by

$$C^*(M_5) \cong \Gamma_0([0,\infty)^2, \{C(\mathbb{T}^2)\rtimes_\theta\mathbb{R}\}_{t\in(0,\infty)^2} \cup \{C(\mathbb{T})\rtimes\mathbb{R}\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})} \cup \{C^*(\mathbb{R})\}_{t=(0,0)}),$$

where $C(\mathbb{T}^2)\rtimes_\theta\mathbb{R} \cong \mathbb{K}\otimes\mathfrak{A}_\theta$ with $\mathfrak{A}_\theta$ the irrational rotation algebra with θ and $\mathbb{K}$ the C^*-algebra of compact operators, and $C(\mathbb{T})\rtimes\mathbb{R} \cong \mathbb{K}\otimes C(\mathbb{T})$ (cf. Ref. 27). On the other hand, the structure of $C^*(D_7)$ as a continuous field C^*-algebra is given by

$$C^*(D_7) \cong \Gamma_0([0,\infty)^2, \{C(\mathbb{T}^2)\rtimes H^{\mathbb{R}}_3\}_{t\in(0,\infty)^2} \cup \{C(\mathbb{T})\rtimes H^{\mathbb{R}}_3\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})} \cup \{C^*(H^{\mathbb{R}}_3)\}_{t=(0,0)}),$$

where the fibers are decomposed into the following (cf. Ref. 32):

$$C(\mathbb{T}^2)\rtimes H^{\mathbb{R}}_3 \cong \Gamma_0(\mathbb{R}, \{\mathfrak{A}_\theta\otimes\mathbb{K}\}_{\theta\in\mathbb{R}}),$$

$$C(\mathbb{T})\rtimes H^{\mathbb{R}}_3 \cong \Gamma_0(\mathbb{R}, \{C(\mathbb{T})\otimes\mathbb{K}\}_{\theta\in\mathbb{R}\setminus\{0\}} \cup \{C_0(\mathbb{R}\times\mathbb{T})\otimes\mathbb{K}\}_{\theta=0}),$$

$$C^*(H^{\mathbb{R}}_3) \cong \Gamma_0(\mathbb{R}, \{\mathbb{K}\}_{\theta\in\mathbb{R}\setminus\{0\}} \cup \{C_0(\mathbb{R}^2)\}_{\theta=0}).$$

Note that the centers of the left-hand sides are given by the center of $C^*(H^{\mathbb{R}}_3)$ that is isomorphic to $C^*(\mathbb{R}) \cong C_0(\mathbb{R})$.

From the above and further analysis we have the following.

Theorem 4.1: *There exist symmetries on the group* C^**-algebras* $C^*(M_5)$ *and* $C^*(D_7)$ *of* $M_5 = \mathbb{C}^2\rtimes\mathbb{R}$ *and* $D_7 = \mathbb{C}^2\rtimes H^{\mathbb{R}}_3$ *induced from the flip on* $\mathbb{C}^2$. *Moreover, the structures of* $C^*(M_5)\rtimes\mathbb{Z}_2$ *and* $C^*(D_7)\rtimes\mathbb{Z}_2$ *by the symmetries are given by*

$$C^*(M_5)\rtimes\mathbb{Z}_2 \cong \Gamma_0([0,\infty)^2, \{\mathbb{K}\otimes\mathfrak{A}_\theta\rtimes\mathbb{Z}_2\}_{t\in(0,\infty)^2} \cup \{\mathbb{K}\otimes C(\mathbb{T})\rtimes\mathbb{Z}_2\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})} \cup \{C^*(\mathbb{R}\times\mathbb{Z}_2)\}_{t=(0,0)})$$

and

$$C^*(D_7)\rtimes\mathbb{Z}_2 \cong \Gamma_0([0,\infty)^2, \{C(\mathbb{T}^2)\rtimes H^{\mathbb{R}}_3\rtimes\mathbb{Z}_2\}_{t\in(0,\infty)^2} \cup \{C(\mathbb{T})\rtimes H^{\mathbb{R}}_3\rtimes\mathbb{Z}_2\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})} \cup \{C^*(H^{\mathbb{R}}_3\times\mathbb{Z}_2)\}_{t=(0,0)}),$$

where the fibers are decomposed into the following:

$$C(\mathbb{T}^2) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2 \cong \Gamma_0(\mathbb{R}, \{\mathfrak{A}_\theta \otimes \mathbb{K} \rtimes \mathbb{Z}_2\}_{\theta \in \mathbb{R}\setminus\{0\}} \cup \{\mathbb{K} \otimes C(\mathbb{T}^2) \rtimes \mathbb{Z}_2\}_{\theta=0}),$$

$$C(\mathbb{T}) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2 \cong \Gamma_0(\mathbb{R}, \{C(\mathbb{T}) \otimes \mathbb{K} \rtimes \mathbb{Z}_2\}_{\theta \in \mathbb{R}\setminus\{0\}} \cup \{C_0(\mathbb{R} \times \mathbb{T}) \otimes \mathbb{K} \rtimes \mathbb{Z}_2\}_{\theta=0}).$$

Remark: Note that the fibers $\mathbb{K} \otimes \mathfrak{A}_\theta \rtimes \mathbb{Z}_2$ for θ irrational involved in the decompositions above are simple AF algebras.

Corollary 4.2: The group C^*-algebras of disconnected solvable Lie groups may have certain AF algebras as simple quotients.

Proof: For instance, we take $M_5 \rtimes \mathbb{Z}_2$ or $D_7 \rtimes \mathbb{Z}_2$ considered above as a disconnected solvable Lie group. □

Corollary 4.3: The group C^*-algebras of disconnected solvable Lie groups may have certain AT algebras as simple quotients.

Proof: For instance, for the generalized Dixmier group D_{6n+1} considered in Ref. 32 we define a disconnected solvable Lie group $D_{6n+1} \rtimes \mathbb{Z}_2$ similarly and extensively. See Ref. 32 for the structure of $C^*(D_{6n+1})$. Using this we obtain the similar result as Theorem 4.1. In particular, $C^*(D_{6n+1} \rtimes \mathbb{Z}_2)$ has a simple AH algebra $(\otimes \mathfrak{A}_\theta) \otimes \mathbb{K} \rtimes \mathbb{Z}_2$ as a quotient, and this AH algebra is in fact an AT algebra by the same reason as given in the proof of Corollary 2.4. □

Theorem 4.4: *The crossed product $C^*(M_5) \rtimes \mathbb{Z}_2$ has stable rank* 2, *and for the crossed product $C^*(D_7) \rtimes \mathbb{Z}_2$, we have $2 \leqslant \mathrm{sr}(C^*(D_7) \rtimes \mathbb{Z}_2) \leqslant 3$. Furthermore, we obtain*

$$\mathrm{sr}(C^*(M_5) \rtimes \mathbb{Z}_2) = 2 = \mathrm{sr}(\mathbb{K} \otimes C([1,2]^2) \otimes M_2(\mathbb{C})),$$

where $\mathbb{K} \otimes C([1,2]^2) \otimes M_2(\mathbb{C})$ is a certain quotient of $C^*(M_5) \rtimes \mathbb{Z}_2$, and

$$\mathrm{sr}(C^*(M_5) \rtimes \mathbb{Z}_2) \neq [\dim(C^*(M_5) \rtimes \mathbb{Z}_2)_1^\wedge/2] + 1 = [1/2] + 1 = 1,$$

while $(C^*(D_7) \rtimes \mathbb{Z}_2)_1^\wedge$ is $\mathbb{R}^2$, where $(C^*(M_5) \rtimes \mathbb{Z}_2)_1^\wedge$, $(C^*(D_7) \rtimes \mathbb{Z}_2)_1^\wedge$ are the spaces of all one-dimensional representations of $C^*(M_5) \rtimes \mathbb{Z}_2$, $C^*(D_7) \rtimes \mathbb{Z}_2$, respectively.

Proof: We use the structures of $C^*(M_5) \rtimes \mathbb{Z}_2$ and $C^*(D_7) \rtimes \mathbb{Z}_2$ in Theorem 4.1. By Ref. 13 and Ref. 20, Proposition 1.7 and Theorems 3.6 and 6.4, we obtain

$$\begin{aligned}\mathrm{sr}(C^*(M_5) \rtimes \mathbb{Z}_2) \leqslant \max\{&\mathrm{sr}(C_0([0,\infty)^2) \otimes \mathbb{K} \otimes \mathfrak{A}_\theta \rtimes \mathbb{Z}_2),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes \mathbb{K} \otimes C(\mathbb{T}) \rtimes \mathbb{Z}_2),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes C_0(\mathbb{K} \times \mathbb{Z}_2))\} = \max\{2,2,2\} = 2\end{aligned}$$

and

$$\begin{aligned}\mathrm{sr}(C^*(D_7) \rtimes \mathbb{Z}_2) \leqslant \max\{&\mathrm{sr}(C_0([0,\infty)^2) \otimes C(\mathbb{T}^2) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes C(\mathbb{T}) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes C^*(H_3^{\mathbb{R}} \times \mathbb{Z}_2))\}.\end{aligned}$$

Furthermore, we obtain

$$\mathrm{sr}(C_0([0,\infty)^2) \otimes C(\mathbb{T}^2) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2) \leqslant \sup_{\theta \in \mathbb{R}} \mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes \mathbb{K} \otimes \mathfrak{A}_\theta \rtimes \mathbb{Z}_2) = 2,$$

$$\mathrm{sr}(C_0([0,\infty)^2) \otimes C(\mathbb{T}) \rtimes H_3^{\mathbb{R}} \rtimes \mathbb{Z}_2) \leqslant \sup_{\theta \in \mathbb{R}} \mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes \mathbb{K} \otimes C(\mathbb{T}) \rtimes \mathbb{Z}_2) = 2,$$

$$\mathrm{sr}(C_0([0,\infty)^2)\otimes C^*(H_3^{\mathbb{R}}\times\mathbb{Z}_2)) \leqslant \max\{\mathrm{sr}(C_0(\mathbb{R}\times[0,\infty)^2)\otimes\mathbb{K}\otimes C(\mathbb{Z}_2)),\ \mathrm{sr}(C_0(\mathbb{R}\times[0,\infty)^2)\otimes C_0(\mathbb{R}^2\times\mathbb{Z}_2))\} = \max\{2,3\} = 3.$$

On the other hand, we have

$$\mathrm{sr}(C^*(M_5)\rtimes\mathbb{Z}_2) \geqslant \mathrm{sr}(\mathbb{K}\otimes C([1,2]^2)\otimes M_2(\mathbb{C})) = 2$$

since $C_0(\mathbb{T}\backslash\{\pm1\})\rtimes\mathbb{Z}_2\cong C_0(\mathbb{R})\otimes M_2(\mathbb{C})$ and $\mathbb{K}\otimes C([1,2])\otimes M_2(\mathbb{C})\otimes C([1,2])$ is a quotient of $C^*(M_5)\rtimes\mathbb{Z}_2$, where the first interval $[1,2]$ corresponds to the closed subset of $\mathbb{R}$ of $C_0(\mathbb{R})$, and the second interval $[0,1]$ corresponds to the closed subset of the subspace $\{0\}\times(0,\infty)$ in the base space $[0,\infty)^2$.

Furthermore, it follows from Theorem 4.1 that the space $(C^*(M_5)\rtimes\mathbb{Z}_2)_1^\wedge$ is given by $\mathbb{R}\times\mathbb{Z}_2$. Hence its dimension is one. Also, we have $(C^*(D_7)\rtimes\mathbb{Z}_2)_1^\wedge$ is $\mathbb{R}^2\times\mathbb{Z}_2$ from Theorem 4.1 and the decompositions of $C^*(D_7)$ and $C^*(H_3^{\mathbb{R}})$ given before Theorem 4.1. □

Theorem 4.5: *The structures of the fixed point algebras $C^*(M_5)^\gamma$, $C^*(D_7)^\gamma$ associated with the crossed products $C^*(M_5)\rtimes_\gamma\mathbb{Z}_2$, $C^*(D_7)\rtimes_\gamma\mathbb{Z}_2$ are given by*

$$C^*(M_5)^\gamma \cong \Gamma_0([0,\infty)^2,\{\mathbb{K}\otimes\mathfrak{A}_\theta^\gamma\}_{t\in(0,\infty)^2}\cup\{\mathbb{K}\otimes C(\mathbb{T})^\gamma\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})}\cup\{C^*(\mathbb{R}\times\mathbb{Z}_2)\}_{t=(0,0)}),$$

and

$$C^*(D_7)^\gamma \cong \Gamma_0([0,\infty)^2,\{(C(\mathbb{T}^2)\rtimes H_3^{\mathbb{R}})^\gamma\}_{t\in(0,\infty)^2} \cup\{(C(\mathbb{T})\rtimes H_3^{\mathbb{R}})^\gamma\}_{t\in(\{0\}\times(0,\infty))\cup((0,\infty)\times\{0\})}\cup\{C^*(H_3^{\mathbb{R}}\times\mathbb{Z}_2)\}_{t=(0,0)}),$$

where the fibers are decomposed into the following:

$$(C(\mathbb{T}^2)\rtimes H_3^{\mathbb{R}})^\gamma \cong \Gamma_0(\mathbb{R},\{\mathbb{K}\otimes\mathfrak{A}_\theta^\gamma\}_{\theta\in\mathbb{R}}),$$

$$(C(\mathbb{T})\rtimes H_3^{\mathbb{R}})^\gamma \cong \Gamma_0(\mathbb{R},\{\mathbb{K}\otimes C(\mathbb{T})^\gamma\}_{\theta\in\mathbb{R}\backslash\{0\}}\cup\{\mathbb{K}\otimes C_0(\mathbb{R}\times\mathbb{T})^\gamma\}_{\theta=0}).$$

Remark: Note that the fibers $\mathbb{K}\otimes\mathfrak{A}_\theta^\gamma$ for θ irrational involved in the decompositions above are simple AF algebras.

Theorem 4.6: *For the fixed point algebras $C^*(M_5)^\gamma$ and $C^*(D_7)^\gamma$, we have*

$$1 \leqslant \mathrm{sr}(C^*(M_5)^\gamma) \leqslant 2, \quad 2 \leqslant \mathrm{sr}(C^*(D_7)^\gamma) \leqslant 3.$$

Furthermore, we have

$$[\dim(C^*(M_5)^\gamma)_1^\wedge/2]+1 = [1/2]+1 = 1, \quad [\dim(C^*(D_7)^\gamma)_1^\wedge/2]+1 = [2/2]+1 = 2,$$

where $(C^*(M_5)^\gamma)_1^\wedge$, $(C^*(D_7)^\gamma)_1^\wedge$ are the spaces of all one-dimensional representations of $C^*(M_5)^\gamma$, $C^*(D_7)^\gamma$, respectively.

Proof: We use the structures of $C^*(M_5)^\gamma$ and $C^*(D_7)^\gamma$ given in Theorem 4.5. By Ref. 13 and Ref. 20, Proposition 1.7 and Theorems 3.6 and 6.4,

$$\mathrm{sr}(C^*(M_5)^\gamma) \leqslant \max\{\mathrm{sr}(C_0([0,\infty)^2)\otimes\mathbb{K}\otimes\mathfrak{A}_\theta^\gamma), \mathrm{sr}(C_0([0,\infty)^2)\otimes\mathbb{K}\otimes C(\mathbb{T})^\gamma), \mathrm{sr}(C_0([0,\infty)^2)\otimes\mathbb{K}\otimes C_0(\mathbb{R}\times\mathbb{Z}_2))\} = \max\{2,2,2\} = 2$$

and

$$\begin{aligned}\mathrm{sr}(C^*(D_7)^\gamma) \leqslant \max\{&\mathrm{sr}(C_0([0,\infty)^2) \otimes (C(\mathbb{T}^2) \rtimes H_3^{\mathbb{R}})^\gamma),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes (C(\mathbb{T}) \rtimes H_3^{\mathbb{R}})^\gamma),\\ &\mathrm{sr}(C_0([0,\infty)^2) \otimes C^*(H_3^{\mathbb{R}} \times \mathbb{Z}_2))\}.\end{aligned}$$

Furthermore, we obtain

$$\mathrm{sr}(C_0([0,\infty)^2) \otimes (C(\mathbb{T}^2) \rtimes H_3^{\mathbb{R}})^\gamma) \leqslant \sup_{\theta\in\mathbb{R}} \mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes \mathbb{K} \otimes \mathfrak{A}_\theta^\gamma) = 2,$$

$$\mathrm{sr}(C_0([0,\infty)^2) \otimes (C(\mathbb{T}) \rtimes H_3^{\mathbb{R}})^\gamma) \leqslant \sup_{\theta\in\mathbb{R}} \mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes \mathbb{K} \otimes C(\mathbb{T})^\gamma) = 2,$$

$$\begin{aligned}\mathrm{sr}(C_0([0,\infty)^2) \otimes C^*(H_3^{\mathbb{R}} \times \mathbb{Z}_2)) \leqslant \max\{&\mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes \mathbb{K} \otimes \mathbb{C}^2), \mathrm{sr}(C_0(\mathbb{R} \times [0,\infty)^2) \otimes C_0(\mathbb{R}^2)\\ &\otimes \mathbb{C}^2)\} = \max\{2,3\} = 3.\end{aligned}$$

Furthermore, it follows from Theorem 4.5 that the space $(C^*(M_5)^\gamma)_1^\wedge$ is given by $\mathbb{R}\times\mathbb{Z}_2$, and the space $(C^*(D_7)^\gamma)_1^\wedge$ is given by $\mathbb{R}^2\times\mathbb{Z}_2$.

Furthermore, we can define symmetries on the generalized Mautner groups M_{2n+m} (the semidirect products $\mathbb{C}^n\rtimes_\alpha\mathbb{R}^m$ with α multirotations on $\mathbb{C}^n$)[30] and the generalized Dixmier groups D_{6n+1} (the semidirect product $\mathbb{C}^{2n}\rtimes_\alpha H_{2n+1}^{\mathbb{R}}$ by the generalized Heisenberg groups $H_{2n+1}^{\mathbb{R}}$ with α multirotations on $\mathbb{C}^{2n}$)[32] induced from the flips on $\mathbb{C}^n$ and $\mathbb{C}^{2n}$, respectively.

Theorem 4.7: *There exist symmetries on the group C^*-algebras $C^*(M_{2n+m})$ and $C^*(D_{6n+1})$ of the generalized Mautner groups $M_{2n+m}=\mathbb{C}^n\rtimes\mathbb{R}^m$ and the generalized Dixmier groups $D_{6n+1}=\mathbb{C}^{2n}\rtimes H_{2n+1}^{\mathbb{R}}$ induced from the flip on $\mathbb{C}^n$ and $\mathbb{C}^{2n}$, respectively. Moreover, the structures of $C^*(M_{2n+m})\rtimes\mathbb{Z}_2$ and $C^*(D_{6n+1})\rtimes\mathbb{Z}_2$ by the symmetries are given by*

$$\begin{aligned}C^*(M_{2n+m}) \rtimes \mathbb{Z}_2 \cong \Gamma_0([0,\infty)^n, &\{C(\mathbb{T}^n) \rtimes \mathbb{R}^m \rtimes \mathbb{Z}_2\}_{t\in(0,\infty)^n}\\ &\cup \cup_{k=1}^{n-1}\{C(\mathbb{T}^k) \rtimes \mathbb{R}^m \rtimes \mathbb{Z}_2\}_{t\in\sqcup\binom{n}{k}(0,\infty)^k} \cup \{C^*(\mathbb{R}^m \times \mathbb{Z}_2)\}_{t=(0,\ldots,0)\in\mathbb{C}^n}),\end{aligned}$$

where the fibers $C(\mathbb{T}^k)\rtimes\mathbb{R}^m\rtimes\mathbb{Z}_2$ $(1\leqslant k\leqslant n)$ are given by

$$\mathbb{K} \otimes C_0(\mathbb{T}^{k-l} \times \mathbb{R}^s) \rtimes \mathbb{Z}_2,$$

$$\mathbb{K} \otimes C_0(\mathbb{T}^{k-l} \times \mathbb{R}^s) \otimes \mathfrak{A}_\Theta \rtimes \mathbb{Z}_2$$

for certain $0\leqslant l\leqslant k$ and $0\leqslant s\leqslant m-1$ and $\mathfrak{A}_\Theta$ a certain noncommutative torus, and

$$\begin{aligned}C^*(D_{6n+1}) \rtimes \mathbb{Z}_2 \cong \Gamma_0([0,\infty)^{2n}, &\{C(\mathbb{T}^{2n}) \rtimes H_{2n+1}^{\mathbb{R}} \rtimes \mathbb{Z}_2\}_{t\in(0,\infty)^{2n}}\\ &\cup \cup_{k=1}^{n-1}\{C(\mathbb{T}^k) \rtimes H_{2n+1}^{\mathbb{R}} \rtimes \mathbb{Z}_2\}_{t\in\sqcup\binom{2n}{k}(0,\infty)^k} \cup \{C^*(H_{2n+1}^{\mathbb{R}} \times \mathbb{Z}_2)\}_{t=(0,\ldots,0)\in\mathbb{C}^{2n}}),\end{aligned}$$

where the fibers $C(\mathbb{T}^k)\rtimes H_{2n+1}^{\mathbb{R}}\rtimes\mathbb{Z}_2$ $(1\leqslant k\leqslant 2n)$ are given by

$$C(\mathbb{T}^k) \rtimes H_{2n+1}^{\mathbb{R}} \rtimes \mathbb{Z}_2 \cong \Gamma_0(\mathbb{R}, \{\mathbb{K} \otimes (\otimes^s\mathfrak{A}_\theta) \otimes C(\mathbb{T}^l) \rtimes \mathbb{Z}_2\}_{\theta\in\mathbb{R}\setminus\{0\}} \cup \{\mathbb{K} \otimes C_0(\mathbb{R}^{2n-k} \times \mathbb{T}^k) \rtimes \mathbb{Z}_2\}_{\theta=0})$$

for certain $2s+l=k$ with s, $l\geqslant 0$.

Moreover, the structures of the fixed point algebras $C^*(M_{2n+m})^\gamma$, $C^*(D_{6n+1})^\gamma$ by the symmetries are given by replacing the above fibers $C(\mathbb{T}^k)\rtimes\mathbb{R}^m\rtimes\mathbb{Z}_2$ with $(C(\mathbb{T}^k)\rtimes\mathbb{R}^m)^\gamma$ and the above fibers $C(\mathbb{T}^k)\rtimes H_{2n+1}^{\mathbb{R}}\rtimes\mathbb{Z}_2$ with $(C(\mathbb{T}^k)\rtimes H_{2n+1}^{\mathbb{R}})^\gamma$, respectively, and the replaced fibers are, respectively, isomorphic to

$$\mathbb{K} \otimes C_0(\mathbb{T}^{k-l} \times \mathbb{R}^s)^\gamma \quad or \quad \mathbb{K} \otimes (C_0(\mathbb{T}^{k-l} \times \mathbb{R}^s) \otimes \mathfrak{A}_\Theta)^\gamma,$$

$$\Gamma_0(\mathbb{R},\{\mathbb{K}\otimes((\otimes^s\mathfrak{A}_\theta)\otimes C(\mathbb{T}^l))^\gamma\}_{\theta\in\mathbb{R}\setminus\{0\}}\cup\{\mathbb{K}\otimes C_0(\mathbb{R}^{2n-k}\times\mathbb{T}^k)^\gamma\}_{\theta=0}).$$

Theorem 4.8: *For the crossed products* $C^*(M_{2n+m})\rtimes\mathbb{Z}_2$ *and* $C^*(D_{6n+1})\rtimes\mathbb{Z}_2$, *we have*

$$[m/2]+1\leqslant \mathrm{sr}(C^*(M_{2n+m})\rtimes\mathbb{Z}_2)\leqslant[(n+m)/2]+1,$$

$$n+1\leqslant \mathrm{sr}(C^*(D_{6n+1})\rtimes\mathbb{Z}_2)\leqslant 2n+1.$$

For the their fixed point algebras $C^*(M_{2n+m})^\gamma$, $C^*(D_{6n+1})^\gamma$,

$$[m/2]+1\leqslant \mathrm{sr}(C^*(M_{2n+m})^\gamma)\leqslant[(n+m)/2]+1,$$

$$n+1\leqslant \mathrm{sr}(C^*(D_{6n+1})^\gamma)\leqslant 2n+1.$$

Furthermore, we have

$$[\dim(C^*(M_{2n+m})\rtimes\mathbb{Z}_2)^\wedge_1/2]+1=[m/2]+1=[\dim(C^*(M_{2n+m})^\gamma)^\wedge_1/2]+1,$$

$$[\dim(C^*(D_{6n+1})\rtimes\mathbb{Z}_2)^\wedge_1/2]+1=n+1=[\dim(C^*(D_{6n+1})^\gamma)^\wedge_1/2]+1,$$

where for $G=C^*(M_{2n+m})\rtimes\mathbb{Z}_2$, $C^*(M_{2n+m})^\gamma$, $C^*(D_{6n+1})\rtimes\mathbb{Z}_2$, *or* $C^*(D_{6n+1})^\gamma$, $G^\wedge_1$ *is the space of all one-dimensional representations of* G.

Proof: We use the structures of the crossed products and the fixed point algebras in the statement given in Theorem 4.7, and estimate their stable rank as given in the proofs of Theorems 4.4 and 4.6. In particular, note that

$$\mathrm{sr}(C_0([0,\infty)^n\times\mathbb{R}^m))=[(n+m)/2]+1,\quad \mathrm{sr}(C^*(\mathbb{R}^m))=[m/2]+1$$

for the stable rank of $C^*(M_{2n+m})\rtimes\mathbb{Z}_2$ and $C^*(M_{2n+m})^\gamma$, and

$$\mathrm{sr}(C_0([0,\infty)^{2n}\times\mathbb{R}^{2n}))=2n+1,\quad \mathrm{sr}(C_0(\mathbb{R}^{2n}))=n+1$$

for the stable rank of $C^*(D_{6n+1}))\rtimes\mathbb{Z}_2$ and $C^*(D_{6n+1}))^\gamma$.

Furthermore, note that the spaces $(C^*(M_{2n+m})\rtimes\mathbb{Z}_2)^\wedge_1$, $(C^*(M_{2n+m})^\gamma)^\wedge_1$ are given by $\mathbb{R}^m\times\mathbb{Z}_2$, and the spaces $(C^*(D_{6n+1})\rtimes\mathbb{Z}_2)^\wedge_1$, $(C^*(D_{6n+1})^\gamma)^\wedge_1$ are given by $\mathbb{R}^{2n}\times\mathbb{Z}_2$. □

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$SO_0(1,d+1)$ Racah coefficients: Type I representations

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We use AdS/CFT inspired methods to study the Racah coefficients for type I representations of the Lorentz group $SO_0(1,d+1)$ with $d>1$. For such representations (a multiple of) the Racah coefficient can be represented as an integral of a product of six bulk-to-bulk propagators over four copies of the hyperbolic space H_{d+1}. To compute the integrals we represent the bulk-to-bulk propagators in terms of bulk-to-boundary ones. The bulk integrals can be computed explicitly, and the boundary integrations are carried out by introducing Feynman parameters. The final result is an integral representation of the Racah coefficient given by four Barnes-Mellin type integrals. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2180626]

I. INTRODUCTION AND THE MAIN RESULT

Racah or Racah-Wigner (RW) coefficients or, as they are often called, $6j$-symbols are important objects in group representation theory. They depend on six irreducible representations of the group and are obtained by multiplying four Clebsch-Gordan coefficients and summing over the basis labels. Explicit formulas for RW coefficients are available for the case of group SU(2). They are given by a (finite) generalized hypergeometric series ${}_4F_3(1)$ of unit argument.[1] RW coefficients for other compact groups, especially the unitary group $U(n)$ and the rotation group $SO(n)$ have also been computed. For noncompact groups these coefficients have received much less attention. This has to do with the envisaged physical application of the RW coefficients: they figure prominently in the lattice approach to QCD. As QCD concerns itself with compact gauge groups such as $SU(n)$ there is no field theoretic motivation to compute the noncompact RW coefficients. This situation changed with the introduction of the spin foam models of quantum gravity.[2] Here of physical interest are exactly models with noncompact groups such as the Lorentz group. These models use RW and other similar coefficients in an essential way.[3] It thus became of importance to study and derive explicit expressions for the noncompact RW coefficients. Of particular interest are the Lorentz group RW coefficients. This is the problem that is considered in the present paper. Another obvious complication that arises in the noncompact case is that the unitary representations are infinite dimensional. Sums of the compact case get replaced by integrals; the problem requires a more careful analytical treatment, including a careful analysis of the convergence of all the expressions. This paper gives such a treatment for $SO_0(1,d+1)$ RW coefficients for type I representations, for $d>1$. Here $SO_0(1,d+1)$ denotes the connected component of $SO(1,d+1)$. We shall assume $d>1$ throughout the paper when not explicitly mentioned otherwise.

Motivations for considering the RW coefficients for type I representations are twofold: (i) these are the representations that are of importance for quantum gravity applications;[3,4] (ii) RW

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coefficients for type I representations can be obtained from a certain integral over several copies of the hyperbolic space. As we show in this paper, these integrals and thus the RW coefficients can be given in terms of four Barnes-Mellin-type integrals. One may be able to use this integral representation for an analytic continuation, and in this way obtain RW coefficients for other representations.

We recall here some basic facts about $SO_0(1,d+1)$ representation theory.[5] Representations of type I form the most degenerate series of representations. At the same time they are the simplest and the most studied ones. These irreducible unitary representations appear in the decomposition of the space $L^2(H_{d+1})$ of square integrable functions on the hyperbolic space H_{d+1} into irreducible representations. Thus, type I representations can be realized in the space of $L^2(H_{d+1})$ functions. It is this realization that will be the starting point for our analysis.

These representations can also be realized in the space of homogeneous functions on the light cone in Minkowski space $M^{1,d+1}$. We shall refer to minus degree of homogeneity by the conformal dimension Δ of the representation. For representations of type I,

$$\Delta = d/2 + i\rho, \quad \rho \in \mathbb{R}. \tag{1.1}$$

There is another important series of unitary representations with real integral Δ. We shall not consider them here. We shall also require a notion of the dual representation. Its conformal dimension $\bar{\Delta}$ is such that

$$\Delta + \bar{\Delta} = d. \tag{1.2}$$

The dual representation is an equivalent representation.

A brief description of the logic of the paper is as follows. We represent the RW coefficient as an integral over four copies of the hyperbolic space of a product of six "propagators," the corresponding expression to be given in the main text. This way of representing the $6j$-symbols was proposed in Ref. 4 and later explored in papers by many authors, in particular Refs. 3 and 6. In Ref. 3 the bulk-to-bulk propagator was represented as a composition of two "bulk-to-boundary" ones. This representation will be of central importance for us in this paper. The terminology "bulk-to-boundary" and "bulk-to-bulk" is that used in the AdS/CFT context.[7]

Replacing each bulk-to-bulk propagator by a composition of two bulk-to-boundary ones and using the usual field theoretic trick of Feynman parameters, all the integrals over the hyperbolic space as well as over the boundary can be taken. Moreover, as we shall see, all the integrals over the Feynman parameters can be taken as well, at the expense of introducing four Barnes-Mellin-type integrals. The expression we end up with has these four integrals remaining. Our final result for the RW coefficient is

$$\begin{aligned}(6\Delta) = {} & K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6} K_{\Delta_4,\bar{\Delta}_2,\bar{\Delta}_3,\bar{\Delta}_5,\Delta_6} \int \frac{d\lambda\, ds}{(2\pi i)^2} \int \frac{d\lambda'\, ds'}{(2\pi i)^2} \Gamma(-s)\Gamma(-\lambda)\Gamma(-s')\Gamma(-\lambda') \\ & \times \Gamma(\gamma - s)\Gamma(\delta - \lambda)\Gamma(\alpha + s + \lambda)\Gamma(\beta + s + \lambda)\Gamma(\gamma' - s')\Gamma(\delta' - \lambda')\Gamma(\alpha' + s' + \lambda') \\ & \times \Gamma(\beta' + s' + \lambda')\pi^{d/2} \frac{\Upsilon_d(\lambda - s' - \lambda' - A)\Upsilon_d(\lambda' - s - \lambda + A)}{\Upsilon_d(-s - s')},\end{aligned} \tag{1.3}$$

where

$$\Upsilon_d(x) = \frac{\Gamma(x)}{\Gamma(d/2 - x)}. \tag{1.4}$$

The integration contour in each of the four variables is parallel to the imaginary axis at $\mathrm{Re}(z) = r$, where the parameter r can be chosen freely in the interval $-d/8 < r < 0$. Various quantities that appear in (1.3) are defined as follows:

$$\alpha = \frac{\overline{\Delta_1} + \Delta_3 - \Delta_2}{2}, \quad \alpha' = \frac{\overline{\Delta_4} + \overline{\Delta_6} - \overline{\Delta_2}}{2},$$

$$\beta = \frac{\overline{\Delta_1} + \Delta_6 - \Delta_5}{2}, \quad \beta' = \frac{\overline{\Delta_4} + \overline{\Delta_3} - \overline{\Delta_5}}{2},$$

$$\gamma = \frac{\Delta_2 - \Delta_3 + \Delta_5 - \Delta_6}{2}, \quad \gamma' = \frac{\overline{\Delta_2} - \overline{\Delta_3} + \overline{\Delta_5} - \overline{\Delta_6}}{2}, \tag{1.5}$$

$$\delta = \frac{\Delta_1 - \overline{\Delta_1}}{2}, \quad \delta' = \frac{\Delta_4 - \overline{\Delta_4}}{2},$$

$$A = \frac{\Delta_1 - \Delta_4 + \Delta_2 + \Delta_5 - d}{2},$$

$$K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6} = \frac{\pi^{3d/2}\Gamma\left(\frac{\Delta_1+\Delta_2+\Delta_3-d}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_5+\Delta_6-d}{2}\right)\Gamma\left(\frac{\Delta_2+\Delta_3-\Delta_1}{2}\right)\Gamma\left(\frac{\Delta_5+\Delta_6-\Delta_1}{2}\right)}{4\Gamma^2(\Delta_1)\Gamma(\Delta_2)\Gamma(\Delta_3)\Gamma(\Delta_5)\Gamma(\Delta_6)}.$$

As is shown in the main text, for type I representations the Barnes-Mellin integrals in (1.3) converge in absolute value, so that this formula gives a well-defined representation of the RW coefficient. The expression (1.3) can potentially be used for numerical study of the $6j$-symbol as well as for the study of the asymptotics. We do not consider these problems in the present paper.

Given the answer (1.3) for the RW coefficient one may ask if it is "as expected" from general considerations. For instance, it can be expected that the noncompact case answer can be obtained by some "analytic continuation" from the one of the compact case. By "analytic continuation" one could mean some procedure of rather free manipulation with the compact answer by replacing the finite sums with integrals and continuing the representation labels to complex values. For example, the answer for the SU(2) RW coefficient is given by a single finite sum. Should one expect the $SO_0(1,2)$, and more generally $SO_0(1,d+1)$, RW coefficient to be given by a single integral? Here we would like to argue against this expectation.

As is clear from the computation of the $6j$-symbol given in Ref. 1, the fact that representations of SU(2) are highest weight is used in an essential way. The idea of the computation is as follows. Consider a product of three Clebsch-Gordan coefficients contracted to form a "star-triangle." When the Clebsch-Gordan coefficients are appropriately normalized, this star-triangle is proportional to a single Clebsch-Gordan coefficient with the proportionality coefficient being the $6j$-symbol,

$$\sum_{m_{ij}} C^{l_1 l_{12} l_{13}}_{m_1 m_{12} m_{13}} C^{l_2 l_{23} l_{12}}_{m_2 m_{23} m_{12}} C^{l_3 l_{13} l_{23}}_{m_3 m_{13} m_{23}} = (6j) C^{l_1 l_2 l_3}_{m_1 m_2 m_3}. \tag{1.6}$$

Here the m-labels should satisfy a conservation law for each Clebsch-Gordan coefficient,

$$m_1 = m_{12} + m_{13}, \quad m_2 = m_{23} + m_{12}, \quad m_3 = m_{23} - m_{13}, \quad m_2 = m_1 + m_3. \tag{1.7}$$

Thus, there is only a single loop "momentum" to be summed over. Each Clebsch-Gordan coefficient is also given by a finite sum, see Ref. 1. Therefore, we have four sums on the left-hand side and one sum times the $6j$-symbol on the right-hand side. What simplifies the computation considerably is that one can set the basis labels m_1, m_2 to be highest weight. For such values of m the

sum that gives the Clebsch-Gordan coefficient reduces to a single term. Thus, if we set two of the external states to be highest weight, we get only two sums remaining on the left-hand side and no sum times the $6j$ on the right. One of the summations on the left-hand side can be carried out explicitly using Gauss's sum. One gets an expression for the $6j$ given by a single sum.

Let us now return to the noncompact case. Going to a "momentum" basis, analogous to the m-basis of SU(2), one can have momentum conserved at each vertex. One analogously will have to do only a single integral over the loop momentum. However, in the momentum basis the Clebsch-Gordan coefficients are no longer as simple as in (4.13). One should expect an integral representation with at least one integral. Now, the type I representations are not highest or lowest weight. Thus, there is no simplification of the momentum basis Clebsch-Gordan coefficients that can be used in the computation of the $6j$-symbol. The total number of integrals remains at least four on the left-hand side and at least one on the right-hand side. Thus, at the very best one expects the noncompact $6j$-symbol for type I representations to be given by three integrals. We have tried to further simplify our answer (1.3) in line with this this expectation. Unfortunately, no summation theorems for the generalized hypergeometric series seem to be applicable, and we were not able to simplify the result further. It thus remains an interesting open problem to find a simpler representation for the RW coefficient than the one given by (1.3).

This paper is organized as follows. We start in Sec. II by reviewing the bulk-to-bulk and bulk-to-boundary propagators. Section III gives a formula for the RW coefficients in terms of bulk-to-bulk propagators, as well as another convenient representation in terms of a boundary 4-point function. In Sec. IV we compute the 3-point function, and in Sec. V we discuss its normalization. An important regularization procedure is introduced here. In Sec. VI we compute the 4-point function. Finally, in Sec. VII we compute the remaining sphere integrals. Certain technical results are given in two appendixes.

II. BULK-TO-BULK AND BULK-TO-BOUNDARY PROPAGATORS

In this section we allow d to be any positive integer.

We consider the d-dimensional conformal group $\mathrm{SO}_0(1,d+1)$. One of the associated homogeneous spaces is the hyperbolic space $H_{d+1}=\mathrm{SO}_0(1,d+1)/\mathrm{SO}(d+1)$. The space $L^2(H_{d+1})$ of square integrable functions on H_{d+1} decomposes into irreducible representations of the so-called type I series. More generally, the most degenerate series of representations of the conformal group is that in the space of homogeneous functions on the light cone in Minkowski space $M^{1,d+1}$. Functions of degree of homogeneity $-\Delta$ form an irreducible representation of "conformal dimension" Δ. Not all of these representations are unitary. For unitary representations of type I the conformal dimension is given by (1.1).

Thoughout the paper, we label the representations by their conformal dimension Δ. While the final results will be justified only for the type I values (1.1), several intermediate results remain valid for more general values, and we present the intermediate results in this form in view of potential extensions beyond type I representations.

To proceed, we need the notions of bulk-to-bulk and bulk-to-boundary propagators.[7] We use the upper half-space model of H_{d+1}. Let the coordinates in the upper half-space be $(\xi_0>0,\xi_i)$, $i=1,\ldots,d$. The metric is then

$$\mathrm{d}s^2=\frac{1}{\xi_0^2}\left(\mathrm{d}\xi_0^2+\sum_i \mathrm{d}\xi_i^2\right). \tag{2.1}$$

The boundary of H_{d+1} is the set of points with $\xi_0=0$ and the point at infinity. When referring to points of the boundary we shall use a different letter $x:x_i=\xi_i$.

Following Ref. 7, we introduce the following function of a point on the boundary x and a bulk point ξ in H_{d+1}:

$$K_\Delta(\xi,x)=\frac{\xi_0^\Delta}{(\xi_0^2+|\xi-x|^2)^\Delta}. \tag{2.2}$$

We refer to this function as the bulk-to-boundary propagator. Another, more familiar from mathematics literature, expression for this object is given by

$$K_\Delta(\hat{\xi},\hat{x})=(\hat{\xi}\cdot\hat{x})^{-\Delta}, \tag{2.3}$$

where the vectors $\hat{\xi}$ and $\hat{x}$ in Minkowski space $M^{1,d+1}$ are the representatives of, respectively, ξ and x in the hyperboloid model of H_{d+1} and the dot product is the Minkowski pairing. $\hat{\xi}$ is unit timelike and $\hat{x}$ is null.

The bulk-to-bulk propagator is obtained by taking a product of two propagators (2.2), one for representation Δ, another for the dual representation $\bar{\Delta}$, and integrating over the point on the boundary:

$$K_\Delta(\xi_1,\xi_2)=\int_{S^d} d^dx K_\Delta(\xi_1,x)K_{\bar{\Delta}}(\xi_2,x). \tag{2.4}$$

We have denoted the integration domain, $x\in\mathbb{R}^d$, by S^d as a reminder of the boundary topology in the Poincare ball model of H_{d+1}. As the integrand is asymptotic to a constant times $|x|^{-2d}$ at $|x|\to\infty$, the integral converges for all $\Delta\in\mathbb{C}$.

The bulk-to-bulk propagator (2.4) can be computed explicitly. To begin, assume $\mathrm{Re}(\Delta)>0$ and $\mathrm{Re}(\bar{\Delta})>0$. Using the Feynman representation reviewed in Appendix A, we obtain

$$K_\Delta(\xi_1,\xi_2)=\frac{(\xi_1^0)^\Delta(\xi_2^0)^{\bar{\Delta}}}{\Gamma(\Delta)\Gamma(\bar{\Delta})}\int_{S^d} d^dx\int \mathrm{d}t\,\mathrm{d}u\, t^{\Delta-1}u^{\bar{\Delta}-1}\times e^{-t(\xi_1^0)^2-u(\xi_2^0)^2-t|\xi_1-x|^2-u|\xi_2-x|^2}. \tag{2.5}$$

Taking the integral over x yields

$$K_\Delta(\xi_1,\xi_2)=\frac{(\xi_1^0)^\Delta(\xi_2^0)^{\bar{\Delta}}}{\Gamma(\Delta)\Gamma(\bar{\Delta})}\int \mathrm{d}t\,\mathrm{d}u\, t^{\Delta-1}u^{\bar{\Delta}-1}e^{-t(\xi_1^0)^2-u(\xi_2^0)^2}\frac{\pi^{d/2}}{(t+u)^{d/2}}e^{-[tu/(t+u)]|\xi_1-\xi_2|^2}.$$

By construction, $K_\Delta(\xi_1,\xi_2)$ is invariant under the action of the Lorentz group and hence depends on ξ_1 and ξ_2 only through their hyperbolic distance l. Using this invariance, we can choose $\xi_1=(\xi_1^0,0)$ and $\xi_2=(\xi_2^0,0)$, in which case

$$l=\ln(\xi_1^0/\xi_2^0). \tag{2.6}$$

Writing $\mu=e^l$ and rescaling the integration variables, we obtain

$$K_\Delta(\xi_1,\xi_2)=\frac{\pi^{d/2}\mu^\Delta}{\Gamma(\Delta)\Gamma(\bar{\Delta})}\int\frac{\mathrm{d}t\,\mathrm{d}u}{(t+u)^{d/2}}t^{\Delta-1}u^{\bar{\Delta}-1}e^{-t\mu^2-u}. \tag{2.7}$$

The integrals over t and u can now be taken with the change of variables

$$\lambda=\frac{t}{t+u},\quad \mathrm{d}t\,\mathrm{d}u=\frac{u\,\mathrm{d}\lambda\,\mathrm{d}u}{(1-\lambda)^2}, \tag{2.8}$$

where $0<\lambda<1$. We get

$$K_\Delta(\xi_1,\xi_2)=\frac{\pi^{d/2}\mu^\Delta}{\Gamma(\Delta)\Gamma(\bar{\Delta})}\int_0^1\frac{\mathrm{d}\lambda}{(1-\lambda)^{2-d/2}}\int_0^\infty\frac{\mathrm{d}u}{u^{d/2-1}}\left(\frac{\lambda u}{1-\lambda}\right)^{\Delta-1}u^{\bar{\Delta}-1}e^{-u\{[\lambda\mu^2/(1-\lambda)]+1\}}. \tag{2.9}$$

The integral over u gives

$$K_\Delta(\xi_1,\xi_2)=\frac{\pi^{d/2}\mu^\Delta\Gamma(d/2)}{\Gamma(\Delta)\Gamma(\overline{\Delta})}\int_0^1 \mathrm{d}\lambda\,\lambda^{\Delta-1}(1-\lambda)^{d-\Delta-1}(1-\lambda(1-\mu^2))^{-d/2}. \tag{2.10}$$

Using the integral representation of the hypergeometric function,

$$F(a,b,c;z)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 \mathrm{d}t\,t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}, \tag{2.11}$$

we finally obtain

$$K_\Delta(\xi_1,\xi_2)=\frac{\pi^{d/2}\mu^\Delta\Gamma(d/2)}{\Gamma(d)}F(d/2,\Delta,d,1-\mu^2). \tag{2.12}$$

By analytic continuation, the result (2.12) holds for all $\Delta\in\mathbb{C}$. Note that there is no singularity when Δ is a nonpositive integer; the hypergeometric series just terminates then. We also note that, in view of the identity

$$F(c-a,c-b,c;z)=(1-z)^{a+b-c}F(a,b,c;z) \tag{2.13}$$

we have $K_\Delta(\xi_1,\xi_2)=K_{\overline{\Delta}}(\xi_1,\xi_2)$. Thus, the bulk-to-bulk propagator is a nonoriented one. Indeed, the change of orientation is equivalent to the replacement $\Delta\to\overline{\Delta}$, but this does not change the propagator.

The result (2.12) can be expressed in terms of a Legendre function.[8] For $d=1$, the formula was given in Ref. 6. For $d=2$, the result can be given in terms of an elementary function as

$$K_\Delta(\xi_1,\xi_2)=\frac{\pi}{\Delta-1}\frac{\sinh(\Delta-1)l}{\sinh l}. \tag{2.14}$$

For type I representations this reduces to

$$K_\rho(\xi_1,\xi_2)=\frac{\pi}{\rho}\frac{\sin\rho l}{\sinh l}. \tag{2.15}$$

III. RACAH-WIGNER COEFFICIENTS

We shall compute the RW coefficients through an object called the (6Δ) symbol, given by an integral over four copies of H_{d+1} of a product of six bulk-to-bulk propagators:

$$(6\Delta)=\int_{H_{d+1}}\mathrm{d}\xi_1\cdots\mathrm{d}\xi_4\prod_{i<j}K_{\Delta_{ij}}(\xi_i,\xi_j). \tag{3.1}$$

Here $i,j=1,\ldots,4$ enumerate the points integrated over and Δ_{ij} are the six representations that the (6Δ) symbols depend upon. We begin formally with general $\Delta_{ij}\in\mathbb{C}$ but will eventually specialize to the type I values (1.1). Since the non-type-I representations are not realizable in $L^2(H_{d+1})$, we do not expect that the integral (3.1) can be made convergent for them even after eliminating the infinite volume factor by the procedure of Sec. V.

The relation between the (6Δ) symbol (3.1) and the RW coefficients has been discussed in Ref. 4. To make the present paper self-contained, we shall briefly recall the relation here.

By definition, the representations of type I (with respect to a subgroup H) are those which contain a vector invariant under H. When $G=\mathrm{SO}_0(1,d+1)$, the subgroup H is taken to be the maximal compact subgroup $H=\mathrm{SO}(d+1)$. Let π^ρ be a type I representation, labelled by the index ρ, and let ω be an H-invariant vector. We define on G the function ϕ^ρ as the $\omega\omega$ matrix element of π^ρ,

$$\phi^{\rho}(g) := t^{\rho}_{\omega\omega}(g) := \langle \omega | \pi^{\rho}(g) | \omega \rangle. \tag{3.2}$$

ϕ^{ρ} is called a *spherical* function. Given ϕ^{ρ}, we define the kernel

$$K_{\rho}(g_1, g_2) := \phi^{\rho}(g_1^{-1} g_2). \tag{3.3}$$

As ω is invariant under H, (3.2) shows that ϕ^{ρ} projects into a function on the double coset $H\backslash G/H$, and (3.3) then shows that the kernel projects into a function on two copies of the homogeneous space G/H. In the case of $G=\mathrm{SO}_0(1,d+1)$ and $H=\mathrm{SO}(d+1)$, this homogeneous space is the hyperbolic space H^{d+1}, and from the explicit evaluation of the spherical function in Sec. 9.3.1 of Ref. 5 it is seen that the kernel (3.3) concides (up to a multiple that depends on the normalization of ω) with the bulk-to-bulk propagator (2.12).

Next, we recall the definition of the Clebsch-Gordon coefficients. Given two (irreducible) representations V^{ρ_1}, V^{ρ_2} of G, one can decompose the tensor product representation $V^{\rho_1} \otimes V^{\rho_2}$ into irreducible representations V^{ρ} as

$$V^{\rho_1} \otimes V^{\rho_2} = \oplus_{\rho_3} n(\rho_3) V^{\rho_3}, \tag{3.4}$$

where $n(\rho)$ are multiplicities. The Clebsch-Gordan coefficients are the matrix elements of the intertwining map defined by this decomposition. Explicitly, if i_1 and i_2 are vectors in, respectively, V^{ρ_1} and V^{ρ_2}, we have

$$|i_1\rangle \otimes |i_2\rangle = \sum_{\alpha \rho_3 i_3} {}^{\alpha}C^{\rho_3 i_3}_{\rho_1 i_1 \rho_2 i_2} |i_3\rangle, \tag{3.5}$$

where $\{i_3\}$ is a (generalized) basis in V^{ρ_3}, the sum on the right-hand side includes a sum over the multiplicity label $\alpha=1,\ldots,n(\rho_3)$, and the sum over the other labels is understood in the sense of a sum or an integral depending on whether the labels are discrete or continuous. The C's on the right-hand side are then the Clebsch-Gordan coefficients in the respective bases.

We will further need the orthogonality relation for the matrix elements $t^{\rho}_{i_1 i_2}(g) := \langle i_1 | \pi^{\rho}(g) | i_2 \rangle$. This relation reads

$$\int \mathrm{d}g \, t^{\rho_1}_{i_1 j_1}(g) t^{\rho_2}_{i_2 j_2}(g) = \delta^{\rho_1 \rho_2} \delta_{i_1 i_2} \delta_{j_1 j_2}, \tag{3.6}$$

where we have used the reality of the matrix elements for $G=\mathrm{SO}_0(1,d+1)$, and the δ's on the right-hand side are understood as Kronecker or Dirac deltas as appropriate. For a compact group, whose representations are finite dimensional, the right-hand side of (3.6) would usually be normalized to include the factor $1/\dim(j_1)$, but in our case of a noncompact group the representations are infinite dimensional and such a normalization is not an option. Using (3.5) and (3.6), it is then possible to compute the integral of the product of three matrix elements, with the result

$$\int \mathrm{d}g \, t^{\rho_1}_{i_1 j_1}(g) t^{\rho_2}_{i_2 j_2}(g) t^{\rho_3}_{i_3 j_3}(g) = \sum_{\alpha} {}^{\alpha}C^{\rho_3 i_3}_{\rho_1 i_1 \rho_2 i_2} \, {}^{\alpha}C^{\rho_3 j_3}_{\rho_1 j_1 \rho_2 j_2}. \tag{3.7}$$

Now, when the multiplicity of type I representations in the tensor product (3.4) of two such representations is equal to 1, the multiplicity label on the type I Clebsch-Gordan coefficients becomes redundant, and it can be shown from (3.7) that the (6Δ) symbol (3.1) equals the usual type I RW coefficient, constructed from the Clebsch-Gordan coefficients, multiplied by four factors of the form $C^{\rho_3 \omega}_{\rho_1 \omega \rho_2 \omega}$, one such factor coming from each ξ in (3.1). In this case one can therefore regard the (6Δ) symbol (3.1) as the type I RW coefficient up to a certain normalization factor. When the multiplicity of type I representations in the tensor product of two such representations is not equal to 1, on the other hand, the multiplicity label on the type I Clebsch-Gordan coefficients cannot be dropped. The (6Δ) symbol (3.1) involves then factors of the form ${}^{\alpha}C^{\rho_3 \omega}_{\rho_1 \omega \rho_2 \omega}$

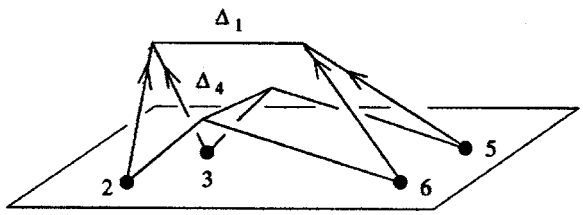

FIG. 1. Expression for the Racah-Wigner coefficient in terms of the 4-point functions.

for each ξ, and there is a sum over the four independent multiplicity labels. As the type I RW coefficients then have a multiplicity label corresponding to each ξ, the (6Δ) symbol (3.1) is no longer a simple multiple of the type I RW coefficients.

Thus, to establish the relation of the (6Δ) symbol (3.1) to the usual RW coefficients it remains to find the multiplicity of type I representations in the tensor product (3.4) of two such representations. For $SO_0(1,2)$ this multiplicity is known to be 2.[9] The $SO_0(1,2)$ (6Δ) symbol (3.1) is therefore not a simple multiple of (any of the) RW coefficients. The $SO_0(1,2)$ (6Δ) symbol (3.1) can still be computed and used as a basis of a state sum model,[6] but its group theoretic interpretation does not appear straightforward.

For $SO_0(1,d+1)$ with $d>1$, the multiplicity of type I representations in the tensor product (3.4) of two such representations is one. To see this, we recall that the principal series representations can be obtained as the induced representations of the parabolic subgroup MAN, where N is the d-dimensional Abelian group of null rotations, A is the one-dimensional group of dilatations and $M=SO(d)$, and in particular the type I representations are induced from the *trivial* representation of M.[10] The claim then follows from Theorem 16 of Ref. 11 and the discussion of $SO_0(1,d+1)$ on pages 182–183 therein. This establishes the relation of our (6Δ) symbol (3.1) to the usual RW coefficients for $SO_0(1,d+1)$ with $d>1$.

To proceed with the analysis of the (6Δ) symbol, we represent four of the six bulk-to-bulk propagators in (3.1) as in (2.4), while leaving the two bulk-to-bulk propagators corresponding to the opposite edges of the tetrahedron in their original form. By doing this one achieves the representation as is shown in Fig. 1.

Thus, let us introduce the following object:

$$D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)=\int_{H_{d+1}} \mathrm{d}\xi\,\mathrm{d}\eta\,K_{\Delta_2}(\xi,x_2)K_{\Delta_3}(\xi,x_3)K_{\Delta_1}(\xi,\eta)K_{\Delta_5}(\eta,x_5)K_{\Delta_6}(\eta,x_6). \tag{3.8}$$

This quantity is a particular 4-point function on the boundary. With the help of this 4-point function, the RW coefficient can be written as

$$(6\Delta)=\int_{S^d} d^dx_2 d^dx_3 d^dx_5 d^dx_6 D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)D_{\Delta_4,\bar{\Delta}_2,\bar{\Delta}_6,\bar{\Delta}_5,\bar{\Delta}_3}(x_2,x_6,x_5,x_3). \tag{3.9}$$

This representation is much more convenient than the one given by (3.1), since the 4-point function $D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)$ can be computed explicitly. Computing the RW coefficient then reduces to the computation of the S^d integrals in (3.9). As we shall see in Sec. V, after a certain gauge fixing that is necessary to render the results finite, what one has is actually not four integrals but a single integral over the sphere. This makes the representation (3.9) very convenient for practical applications. We note that this representation is only available in the context of noncompact conformal groups, when there is a boundary and the associated representation (2.4). For compact groups like $SO(n)$ one can also compute the RW coefficients for type I representations by integrating over the appropriate homogeneous manifold. However, there is no analog of the representation (3.9).

Thus, we would like to compute the 4-point function given by (3.8). In order to do this, we use the representation (2.4) for the remaining bulk propagator. Thus, we represent the 4-point function as

$$D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)=\int d^dx_1 C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)C^{-}_{\Delta_1,\Delta_5,\Delta_6}(x_1,x_5,x_6), \tag{3.10}$$

where we have defined the 3-point function

$$C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=\int_{H_{d+1}} \mathrm{d}\xi\, K_{\Delta_1}(\xi,x_1)K_{\Delta_2}(\xi,x_2)K_{\Delta_3}(\xi,x_3). \tag{3.11}$$

We need to find this 3-point function.

IV. 3-POINT FUNCTION

We note in passing that the 3-point function (3.11) is the Clebsch-Gordan coefficient when the representations are realized in the space of functions on the boundary. Since $d>1$ by assumption, these Clebsch-Gordon coefficients have no multiplicity indices.

The conditions for the integral in (3.11) to converge are

$$\mathrm{Re}\left(\sum_i \Delta_i\right)>d \tag{4.1}$$

and

$$\mathrm{Re}(\Delta_1+\Delta_2-\Delta_3)>0,\quad \mathrm{Re}(\Delta_2+\Delta_3-\Delta_1)>0,\quad \mathrm{Re}(\Delta_1+\Delta_3-\Delta_2)>0. \tag{4.2}$$

These conditions can be conveniently obtained by transforming to the Poincare ball model of H_{d+1}: (4.2) comes from neighborhoods of the three boundary points x_i, and (4.1) comes from the remaining part of the boundary. Note that (4.2) implies $\mathrm{Re}(\Delta_i)>0$ for all i. Note also that the convergence holds for type I representations.

In order to compute the bulk integral we use the Feynman parametrization (A1) for each of the bulk-to-boundary propagators. We get

$$\begin{aligned}C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=&\frac{1}{\Gamma(\Delta_1)}\frac{1}{\Gamma(\Delta_2)}\frac{1}{\Gamma(\Delta_3)}\int_0^\infty \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\, t_1^{\Delta_1-1}t_2^{\Delta_2-1}t_3^{\Delta_3-1}\\&\times\int_0^\infty\frac{\mathrm{d}\xi_0}{\xi_0^{d+1}}\xi_0^{\Sigma_i\Delta_i}\int_{S^d}d^d\xi e^{-t_1(\xi_0^2+|\xi-x_1|^2)-t_2(\xi_0^2+|\xi-x_2|^2)-t_3(\xi_0^2+|\xi-x_3|^2)}.\end{aligned} \tag{4.3}$$

We now use the formulas (A2) and (A3) of Appendix A to get

$$\begin{aligned}C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=&\frac{\pi^{d/2}\Gamma\left(\frac{\Sigma_i\Delta_i-d}{2}\right)}{2\Gamma(\Delta_1)\Gamma(\Delta_2)\Gamma(\Delta_3)}\int_0^\infty \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\, t_1^{\Delta_1-1}t_2^{\Delta_2-1}t_3^{\Delta_3-1}\\&\times(S_t)^{-(\Sigma_i\Delta_i)/2}e^{-(1/S_t)(\Sigma_{i<j}t_it_j|x_i-x_j|^2)}.\end{aligned} \tag{4.4}$$

We now make a series of changes of variables of integration. The first change is

$$t_i=(S_t)^{1/2}t_i'=\left(\sum_j t_j'\right)t_i',\quad \det\left(\frac{\partial t_i}{\partial t_j'}\right)=2(S_t)^{3/2}. \tag{4.5}$$

Removing the primes, we get

$$C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=\frac{\pi^{d/2}\Gamma\left(\frac{\Sigma_i\Delta_i-d}{2}\right)}{\Gamma(\Delta_1)\Gamma(\Delta_2)\Gamma(\Delta_3)}\int_0^\infty \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,t_1^{\Delta_1-1}t_2^{\Delta_2-1}t_3^{\Delta_3-1}e^{-\Sigma_{i<j}t_it_jx_{ij}^2}. \tag{4.6}$$

Here we have introduced

$$x_{ij}=|x_i-x_j|. \tag{4.7}$$

The second change of variables is

$$t_1t_2\to\frac{t_1t_2}{x_{12}^2},\quad t_1t_3\to\frac{t_1t_3}{x_{13}^2},\quad t_2t_3\to\frac{t_2t_3}{x_{23}^2}. \tag{4.8}$$

The integral reduces to

$$\begin{aligned}C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=&\frac{1}{(x_{12})^{\Delta_1+\Delta_2-\Delta_3}(x_{13})^{\Delta_1+\Delta_3-\Delta_2}(x_{23})^{\Delta_2+\Delta_3-\Delta_1}}\\&\times\frac{\pi^{d/2}\Gamma\left(\frac{\Sigma_i\Delta_i-d}{2}\right)}{\Gamma(\Delta_1)\Gamma(\Delta_2)\Gamma(\Delta_3)}\int_0^\infty \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,t_1^{\Delta_1-1}t_2^{\Delta_2-1}t_3^{\Delta_3-1}e^{-\Sigma_{i<j}t_it_j}.\end{aligned} \tag{4.9}$$

It is now possible to take the remaining integral in Feynman parameters by the following change of variables:

$$t_1t_2=u_3,\quad t_1t_3=u_2,\quad t_2t_3=u_1, \tag{4.10}$$

so that

$$t_1^2=\frac{u_2u_3}{u_1},\quad t_2^2=\frac{u_1u_3}{u_2},\quad t_3^2=\frac{u_1u_2}{u_3},\quad \det\left(\frac{\partial t_i}{\partial u_j}\right)=\frac{1}{2\sqrt{u_1u_2u_3}}. \tag{4.11}$$

The integral over t_i thus reduces to

$$\begin{aligned}&\frac{1}{2}\int_0^\infty \mathrm{d}u_1\,\mathrm{d}u_2\,\mathrm{d}u_3\,u_1^{(\Delta_2+\Delta_3-\Delta_1-2)/2}u_2^{(\Delta_1+\Delta_3-\Delta_2-2)/2}u_3^{(\Delta_1+\Delta_2-\Delta_3-2)/2}e^{-u_1-u_2-u_3}\\&\quad=\frac{1}{2}\Gamma\left(\frac{\Delta_2+\Delta_3-\Delta_1}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_3-\Delta_2}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_2-\Delta_3}{2}\right).\end{aligned} \tag{4.12}$$

Thus, we get for the Clebsch-Gordan coefficients,

$$C_{\Delta_1,\Delta_2,\Delta_3}(x_1,x_2,x_3)=\frac{C(\Delta_1,\Delta_2,\Delta_3)}{(x_{12})^{\Delta_1+\Delta_2-\Delta_3}(x_{13})^{\Delta_1+\Delta_3-\Delta_2}(x_{23})^{\Delta_2+\Delta_3-\Delta_1}}, \tag{4.13}$$

where

$$C(\Delta_1,\Delta_2,\Delta_3)=\frac{\pi^{d/2}\Gamma\left(\frac{\Delta_1+\Delta_2+\Delta_3-d}{2}\right)\Gamma\left(\frac{\Delta_2+\Delta_3-\Delta_1}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_3-\Delta_2}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_2-\Delta_3}{2}\right)}{2\Gamma(\Delta_1)\Gamma(\Delta_2)\Gamma(\Delta_3)}. \tag{4.14}$$

V. NORMALIZATION OF THE CLEBSCH-GORDAN COEFFICIENTS: GAUGE FIXING PROCEDURE

In this section we introduce a certain gauge fixing procedure that is necessary to render the integrals defining the RW coefficient finite. We do this considering as an example the question of normalization of the Clebsch-Gordan coefficient. To this end, let us compute the so-called theta symbol given by

$$\theta(\Delta_1,\Delta_2,\Delta_3)=\int_{H_{d+1}} \mathrm{d}\xi_1\,\mathrm{d}\xi_2\,K_{\Delta_1}(\xi_1,\xi_2)K_{\Delta_2}(\xi_1,\xi_2)K_{\Delta_3}(\xi_1,\xi_2). \tag{5.1}$$

Using the expression for the $3j$-symbol that we have just computed, this becomes

$$\theta(\Delta_1,\Delta_2,\Delta_3)=C(\Delta_1,\Delta_2,\Delta_3)C(\overline{\Delta}_1,\overline{\Delta}_2,\overline{\Delta}_3)\int_{S^d} d^dx_1d^dx_2d^dx_3\frac{1}{d_{12}^dx_{13}^dx_{23}^d}. \tag{5.2}$$

The integral over x_1,x_2,x_3 in (5.2) is divergent. This divergence is a manifestation of the obvious divergence in integrating over H_{d+1} a function that is invariant under the isometries: The integral is proportional to the infinite volume of H_{d+1}. As the volume of H_{d+1} is related to the volume of the Lorentz group, the divergence ultimately comes from the fact that the Lorentz group is noncompact.

In (5.1), the divergence can be removed by fixing one of the integration points and only integrating over the remaining one. To remove the divergence in (5.2), and in similar integrals with more integration points, we can use the action of the conformal group on the sphere to put three of the integration points to specific locations. For $d=2$ this procedure completely fixes the $\mathrm{SO}_0(1,d+1)$ invariance and hence eliminates the divergence.[12] For $d>2$ this procedure fixes the $\mathrm{SO}_0(1,d+1)$ invariance up to the $\mathrm{SO}(d-1)$ subgroup that leaves the three prescribed points invariant, but as this subgroup is compact, the divergence has again been eliminated.

To implement this procedure, one needs to find the Faddeev-Popov determinant that makes the result independent of the locations to which the three integration points are fixed. We shall do this in Appendix B by decomposing the Haar measure on $\mathrm{SO}_0(1,d+1)$ in terms of the locations of the three fixed points and the invariantly normalized volume of the compact subgroup $\mathrm{SO}(d-1)$ (which is trivial for $d=2$). The result is the replacement

$$\prod_i d^dx_i \to |x_A-x_B|^d|x_A-x_C|^d|x_B-x_C|^d\times\delta^d(x_A-x_A^0)\delta^d(x_B-x_B^0)\delta^d(x_C-x_C^0)\prod_i d^dx_i, \tag{5.3}$$

where x_A, x_B, and x_C are the three integration points that are fixed, respectively, to the locations x_A^0, x_B^0, and x_C^0. For $d=2$, formula (5.3) reduces to that found in Ref. 12.

In the divergent integral (5.2), the gauge fixing (5.3) simply removes the integral. This gives for the normalization of the Clebsch-Gordan coefficients the formula

$$\theta(\Delta_1,\Delta_2,\Delta_3)=C(\Delta_1,\Delta_2,\Delta_3)C(\overline{\Delta}_1,\overline{\Delta}_2,\overline{\Delta}_3). \tag{5.4}$$

VI. COMPUTATION OF THE 4-POINT FUNCTION

Using the expression (4.13) for the 3-point function, the 4-point function becomes

$$D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6) = C_{\Delta_1,\Delta_2,\Delta_3} C^{-}_{\Delta_1,\Delta_5,\Delta_6} \int_{S^d} d^d x_1 \frac{1}{(x_{12})^{\Delta_1+\Delta_2-\Delta_3}(x_{13})^{\Delta_1+\Delta_3-\Delta_2}(x_{23})^{\Delta_2+\Delta_3-\Delta_1}} \times \frac{1}{(x_{15})^{\bar{\Delta}_1+\Delta_5-\Delta_6}(x_{16})^{\bar{\Delta}_1+\Delta_6-\Delta_5}(x_{56})^{\Delta_5+\Delta_6-\bar{\Delta}_1}}. \tag{6.1}$$

In addition to the convergence conditions of Sec. IV for each of the 3-point functions, the conditions for the integral in (6.1) to converge are

$$\mathrm{Re}(\Delta_1+\Delta_2-\Delta_3) < d, \quad \mathrm{Re}(\Delta_1+\Delta_3-\Delta_2) < d,$$

$$\mathrm{Re}(\bar{\Delta}_1+\Delta_5-\Delta_6) < d, \quad \mathrm{Re}(\bar{\Delta}_1+\Delta_6-\Delta_5) < d. \tag{6.2}$$

Note that these conditions are satisfied for the type I representations.

We see that only four of the quantities in the denominator involve x_1. In order to take the integral, let us use the Feynman representation for them. In other words, let us consider

$$I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6) = \int_0^\infty \mathrm{d}t_{12}\,\mathrm{d}t_{13}\,\mathrm{d}t_{15}\,\mathrm{d}t_{16} \times t_{12}^{[(\Delta_1+\Delta_2-\Delta_3)/2]-1} t_{13}^{[(\Delta_1+\Delta_3-\Delta_2)/2]-1} t_{15}^{[(\bar{\Delta}_1+\Delta_5-\Delta_6)/2]-1} t_{16}^{[(\bar{\Delta}_1+\Delta_6-\Delta_5)/2]-1} \times \int_{S^d} d^d x_1 e^{-t_{12}x_{12}^2 - t_{13}x_{13}^2 - t_{15}x_{15}^2 - t_{16}x_{16}^2}. \tag{6.3}$$

In terms of this function

$$D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6) = \frac{I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)}{(x_{23})^{\Delta_2+\Delta_3-\Delta_1}(x_{56})^{\Delta_5+\Delta_6-\bar{\Delta}_1}} \times \frac{C_{\Delta_1,\Delta_2,\Delta_3} C^{-}_{\Delta_1,\Delta_5,\Delta_6}}{\Gamma\left(\frac{\Delta_1+\Delta_2-\Delta_3}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_3-\Delta_2}{2}\right)\Gamma\left(\frac{\bar{\Delta}_1+\Delta_5-\Delta_6}{2}\right)\Gamma\left(\frac{\bar{\Delta}_1+\Delta_6-\Delta_5}{2}\right)}. \tag{6.4}$$

Let us now evaluate the function (6.3). The integral over x_1 is taken using (A3)

$$\int_{S^d} d^d x_1 e^{-t_{12}x_{12}^2 - t_{13}x_{13}^2 - t_{15}x_{15}^2 - t_{16}x_{16}^2} = \frac{\pi^{d/2}}{(S_t^1)^{d/2}} e^{-(t_{12}t_{13}x_{23}^2 + t_{12}t_{15}x_{25}^2 + t_{12}t_{16}x_{26}^2 + t_{13}t_{15}x_{35}^2 + t_{13}t_{16}x_{36}^2 + t_{15}t_{16}x_{56}^2)/S_t^1}, \tag{6.5}$$

where

$$S_t^1 = t_{12} + t_{13} + t_{15} + t_{16}. \tag{6.6}$$

Let us now make a series of changes of variables. First, let us choose

$$t_{1i} = (S_t^1)^{1/2} t'_{1i}, \quad \det\left(\frac{\partial t_{1i}}{\partial t'_{1i}}\right) = 2(S_t^1)^2. \tag{6.7}$$

After this change of variables we get

$$I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6) = 2\pi^{d/2}\int_0^\infty \mathrm{d}t_{12}\,\mathrm{d}t_{13}\,\mathrm{d}t_{15}\,\mathrm{d}t_{16}$$
$$\times t_{12}^{[(\Delta_1+\Delta_2-\Delta_3)/2]-1} t_{13}^{[(\Delta_1+\Delta_3-\Delta_2)/2]-1} t_{15}^{[(\bar{\Delta}_1+\Delta_5-\Delta_6)/2]-1} t_{16}^{[(\bar{\Delta}_1+\Delta_6-\Delta_5)/2]-1}$$
$$\times e^{-t_{12}t_{13}x_{23}^2-t_{12}t_{15}x_{25}^2-t_{12}t_{16}x_{26}^2-t_{13}t_{15}x_{35}^2-t_{13}t_{16}x_{36}^2-t_{15}t_{16}x_{56}^2}. \tag{6.8}$$

The second change of variables is

$$t_{12}t_{13}\to\frac{t_{12}t_{13}}{x_{23}^2},\quad t_{12}t_{15}\to\frac{t_{12}t_{15}}{x_{25}^2},\quad t_{12}t_{16}\to\frac{t_{12}t_{16}}{x_{26}^2},\quad t_{13}t_{15}\to\frac{t_{13}t_{15}}{x_{35}^2}. \tag{6.9}$$

As a consequence we get

$$t_{13}t_{16}=\frac{t_{13}t_{15}t_{12}t_{16}}{t_{12}t_{15}}\to\frac{x_{25}^2}{x_{35}^2x_{26}^2}t_{13}t_{16},\quad t_{15}t_{16}=\frac{t_{13}t_{15}t_{12}t_{16}}{t_{12}t_{13}}\to\frac{x_{23}^2}{x_{35}^2x_{26}^2}t_{15}t_{16}. \tag{6.10}$$

Or, equivalently,

$$t_{12}\to t_{12}\frac{x_{35}}{x_{23}x_{25}},\quad t_{13}\to t_{13}\frac{x_{25}}{x_{23}x_{35}},\quad t_{15}\to t_{15}\frac{x_{23}}{x_{25}x_{35}},\quad t_{16}\to t_{16}\frac{x_{25}x_{23}}{x_{26}^2x_{35}}. \tag{6.11}$$

As the result of this transformation we get

$$I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)=\frac{2\pi^{d/2}}{(x_{23})^{\Delta_1-\bar{\Delta}_1}(x_{25})^{\Delta_2-\Delta_3+\Delta_5-\Delta_6}(x_{26})^{\bar{\Delta}_1+\Delta_6-\Delta_5}(x_{35})^{\bar{\Delta}_1+\Delta_3-\Delta_2}}$$
$$\times\int_0^\infty \mathrm{d}t_{12}\,\mathrm{d}t_{13}\,\mathrm{d}t_{15}\,\mathrm{d}t_{16}\,e^{-t_{12}t_{13}-t_{12}t_{15}-t_{12}t_{16}-t_{13}t_{15}-t_{13}t_{16}u-t_{15}t_{16}v}$$
$$\times t_{12}^{[(\Delta_1+\Delta_2-\Delta_3)/2]-1} t_{13}^{[(\Delta_1+\Delta_3-\Delta_2)/2]-1} t_{15}^{[(\bar{\Delta}_1+\Delta_5-\Delta_6)/2]-1} t_{16}^{[(\bar{\Delta}_1+\Delta_6-\Delta_5)/2]-1}. \tag{6.12}$$

Here we have introduced the cross ratios,

$$u=\frac{x_{25}^2x_{36}^2}{x_{26}^2x_{35}^2},\quad v=\frac{x_{23}^2x_{56}^2}{x_{26}^2x_{35}^2}. \tag{6.13}$$

The two cross ratios are related for $d=2$ but independent for $d>2$.

We now specialize to the type I representations.

To compute the integrals over the Feynman parameters we, following an analogous computation in Ref. 13, use the Mellin-Barnes integral representation:

$$e^{-z}=\frac{1}{2\pi i}\int_{r-i\infty}^{r+i\infty}\mathrm{d}s\,\Gamma(-s)z^s,\quad r<0,\quad |\arg z|<\frac{\pi}{2}. \tag{6.14}$$

Thus, the integral over Feynman parameters becomes

$$\frac{1}{2}I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v) := \int\frac{\mathrm{d}\lambda\,\mathrm{d}s}{(2\pi i)^2}\Gamma(-\lambda)\Gamma(-s)u^sv^\lambda\int_0^\infty \mathrm{d}t_{12}\,\mathrm{d}t_{13}\,\mathrm{d}t_{15}\,\mathrm{d}t_{16}\,e^{-t_{12}t_{13}-t_{12}t_{15}-t_{12}t_{16}-t_{13}t_{15}}$$
$$\times t_{12}^{[(\Delta_1+\Delta_2-\Delta_3)/2]-1} t_{13}^{[(\Delta_1+\Delta_3-\Delta_2)/2]+s-1} t_{15}^{[(\bar{\Delta}_1+\Delta_5-\Delta_6)/2]+\lambda-1} t_{16}^{[(\bar{\Delta}_1+\Delta_6-\Delta_5)/2]+s+\lambda-1}. \tag{6.15}$$

To justify the interchange of integrals that has led to (6.15), we assume that the parameter r in the

two Mellin-Barnes contours is the same and satisfies $-d/8<r<0$. This guarantees that the exponent of each t_{ij} in (6.15) has real part greater than -1.

In the Feynman parameter integrals, we change variables by

$$t_{12}t_{13}=u_1, \quad t_{12}t_{15}=u_2, \quad t_{12}t_{16}=u_3, \quad t_{13}t_{15}=u_4, \tag{6.16}$$

or, equivalently,

$$t_{12}^2=\frac{u_1u_2}{u_4}, \quad t_{13}^2=\frac{u_1u_4}{u_2}, \quad t_{15}^2=\frac{u_2u_4}{u_1}, \quad t_{16}^2=u_3^2\frac{u_4}{u_1u_2}. \tag{6.17}$$

The Jacobian of this transformation is

$$\det\left(\frac{\partial t_{1i}}{\partial u_j}\right)=\frac{1}{2u_1u_2}. \tag{6.18}$$

Therefore, we get

$$I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v)=\int\frac{\mathrm{d}\lambda\,\mathrm{d}s}{(2\pi i)^2}\Gamma(-\lambda)\Gamma(-s)u^sv^\lambda\Gamma(\alpha+s+\lambda)\Gamma(\beta+s+\lambda)\Gamma(\gamma-s)\Gamma(\delta-\lambda), \tag{6.19}$$

where we have introduced the following quantities:

$$\begin{aligned}\alpha&=\frac{\overline{\Delta_1}+\Delta_3-\Delta_2}{2},\\ \beta&=\frac{\overline{\Delta_1}+\Delta_6-\Delta_5}{2},\\ \gamma&=\frac{\Delta_2-\Delta_3+\Delta_5-\Delta_6}{2},\\ \delta&=\frac{\Delta_1-\overline{\Delta_1}}{2}.\end{aligned} \tag{6.20}$$

Combining this, and the expressions (6.12) and (6.4), we have for the 4-point function,

$$\begin{aligned}D_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(x_2,x_3,x_5,x_6)&=K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}\frac{I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v)}{(x_{25})^{\Delta_2-\Delta_3+\Delta_5-\Delta_6}}\\ &\times\frac{1}{(x_{23})^{\Delta_2+\Delta_3-\overline{\Delta_1}}(x_{26})^{\overline{\Delta_1}+\Delta_6-\Delta_5}(x_{35})^{\overline{\Delta_1}+\Delta_3-\Delta_2}(x_{56})^{\Delta_5+\Delta_6-\overline{\Delta_1}}},\end{aligned} \tag{6.21}$$

where we have introduced

$$K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}=\frac{\pi^{d/2}C_{\Delta_1,\Delta_2,\Delta_3}C_{\bar{\Delta}_1,\Delta_5,\Delta_6}}{\Gamma\left(\frac{\Delta_1+\Delta_2-\Delta_3}{2}\right)\Gamma\left(\frac{\Delta_1+\Delta_3-\Delta_2}{2}\right)\Gamma\left(\frac{\bar{\Delta}_1+\Delta_5-\Delta_6}{2}\right)\Gamma\left(\frac{\bar{\Delta}_1+\Delta_6-\Delta_5}{2}\right)}. \tag{6.22}$$

Thus, essentially all nontriviality of the 4-point function is in the dependence of the function $I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v)$ given by (6.19) on the two cross ratios u,v. The integral representation (6.19) that we have obtained may be used to derive power series expansions of $I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v)$ in u and v.[13]

VII. COMPUTATION OF THE RACAH-WIGNER COEFFICIENTS

Having obtained the 4-point function we can use this result to compute the RW coefficients. Recalling (3.9), we get

$$\begin{aligned}(6\Delta)=&K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}K_{\Delta_4,\bar{\Delta}_2,\bar{\Delta}_3,\bar{\Delta}_5,\bar{\Delta}_6}\int_{S^d}\frac{d^dx_2d^dx_3d^dx_5d^dx_6}{x_{23}^dx_{26}^dx_{35}^dx_{56}^d}\\&\times\left(\frac{1}{v}\right)^{(\Delta_1-\Delta_4+\Delta_2+\Delta_5-d)/2}I_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6}(u,v)I_{\Delta_4,\bar{\Delta}_2,\bar{\Delta}_6,\bar{\Delta}_5,\bar{\Delta}_3}(u/v,1/v).\end{aligned} \tag{7.1}$$

Here we have used the fact that under the exchange of x_3, x_6 we have $v\to 1/v$, $u\to u/v$. We have also used the relation (1.2) between the conformal dimension and its dual and combined all powers of x_{ij}. Note that the integration measure in (7.1) is exactly right to give an invariant expression, as this measure can be verified to be invariant under conformal transformations of the x_i.

What remains is to compute the sphere integrals in (7.1). This integral is

$$I_d(a,b)=\int_{S^d}\frac{\mathrm{d}x_2\,\mathrm{d}x_3\,\mathrm{d}x_5\,\mathrm{d}x_6}{x_{23}^dx_{56}^dx_{26}^dx_{35}^d}\left(\frac{x_{23}x_{56}}{x_{26}x_{35}}\right)^{2a}\left(\frac{x_{25}x_{36}}{x_{26}x_{35}}\right)^{2b}, \tag{7.2}$$

where

$$a=-A+\lambda-s'-\lambda',\quad b=s+s',\quad A=\frac{\Delta_1-\Delta_4+\Delta_2+\Delta_5-d}{2}. \tag{7.3}$$

As it stands, the integral (7.2) still diverges because of the volume of the gauge group. We eliminate this divergence by the replacement (5.3), leaving x_2 to be integrated over but fixing the locations of the other three points. The integral becomes

$$I_d(a,b)=|x_3^0-x_6^0|^d\left|\frac{x_5^0-x_6^0}{x_3^0-x_5^0}\right|^{2a}\left|\frac{x_3^0-x_6^0}{x_3^0-x_5^0}\right|^{2b}\widetilde{I}_d(a,b), \tag{7.4}$$

where

$$\widetilde{I}_d(a,b)=\int_{S^d}\mathrm{d}x_2\frac{|x_2-x_3^0|^{2a-d}|x_2-x_5^0|^{2b}}{|x_2-x_6^0|^{2a+2b+d}}. \tag{7.5}$$

The convergence conditions in (7.5) are

$$\mathrm{Re}(a)>0,\quad \mathrm{Re}(b+d/2)>0,\quad \mathrm{Re}(a+b)<0, \tag{7.6}$$

and they are satisfied for our Mellin-Barnes contour choice, $-d/8<r<0$.

To compute the integral over x_2 we use the Feynman parametrization. We have

$$\widetilde{I}_d(a,b) = \frac{1}{\Gamma(d/2-a)\Gamma(-b)\Gamma(a+b+d/2)} \int_{S^d} dx_2 t_3^{d/2-a-1} t_5^{-b-1} t_6^{a+b+d/2-1} \times e^{-t_3|x_2-x_3^0|^2 - t_5|x_2-x_5^0|^2 - t_6|x_2-x_6^0|^2}. \tag{7.7}$$

We have already dealt with essentially the same integral in Sec. IV, formula (4.3). Thus, we shall be sketchy here. One first takes the x_2 integral using (A3). One then makes a series of rescalings of Feynman parameters t_i. The powers of these parameters in (7.7) are such that the rescaling (4.5) completely removes the quantity S_t from the integral. Rescaling (4.8) takes the differences $|x_i^0 - x_j^0|$ out of the integral, and their resulting powers are exactly such that they cancel the similar quantities in (7.4). The last change of variables (4.10) reduces all the integrals to those giving Γ-functions. The final result is

$$I_d(a,b) = \frac{\pi^{d/2}\Gamma(a)\Gamma(d/2+b)\Gamma(-a-b)}{\Gamma(d/2-a)\Gamma(-b)\Gamma(a+b+d/2)} = \frac{\pi^{d/2}\Upsilon_d(a)\Upsilon_d(-a-b)}{\Upsilon_d(-b)}, \tag{7.8}$$

where we have introduced a dimension-dependent Υ-function given by

$$\Upsilon_d(x) = \frac{\Gamma(x)}{\Gamma(d/2-x)}. \tag{7.9}$$

Substituting the values (7.3) of the parameters a and b, our final result for the (6Δ) symbol is

$$\begin{aligned}(6\Delta) = K_{\Delta_1,\Delta_2,\Delta_3,\Delta_5,\Delta_6} K_{\Delta_4,\bar{\Delta}_2,\bar{\Delta}_3,\bar{\Delta}_5,\bar{\Delta}_6} \times \pi^{d/2} \int \frac{\mathrm{d}\lambda\, \mathrm{d}s}{(2\pi i)^2} \int \frac{\mathrm{d}\lambda'\, \mathrm{d}s'}{(2\pi i)^2} \Gamma(-s)\Gamma(-\lambda)\Gamma(-s')\Gamma(-\lambda') \\ \times \Gamma(\gamma-s)\Gamma(\delta-\lambda)\Gamma(\alpha+s+\lambda)\Gamma(\beta+s+\lambda)\Gamma(\gamma'-s')\Gamma(\delta'-\lambda')\Gamma(\alpha'+s'+\lambda') \\ \times \Gamma(\beta'+s'+\lambda') \frac{\Upsilon_d(\lambda-s'-\lambda'-A)\Upsilon_d(\lambda'-s-\lambda+A)}{\Upsilon_d(-s-s')}.\end{aligned} \tag{7.10}$$

Using Stirling's formula and the assumption $-d/8 < r < 0$ for the Mellin-Barnes contours, it can be verified that the quadruple integral in (7.10) is convergent in absolute value. Equation (7.10) therefore gives a manifestly well-defined expression for the (6Δ) symbol.

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APPENDIX A: INTEGRALS

In this appendix we give the formulas that are central to the methods of integration that we use. The same method was exploited in the context of AdS/CFT correspondence, see e.g., Ref. 13. The standard Feynman parameter method is based on the following representation:

$$\frac{1}{z^\lambda} = \frac{1}{\Gamma(\lambda)} \int_0^\infty \mathrm{d}t\, t^{\lambda-1} e^{-tz}. \tag{A1}$$

We shall also need the following two integrals:

$$\int_0^\infty \frac{\mathrm{d}\xi_0}{\xi_0^{d+1}} \xi_0^{\Sigma_i \Delta_i} e^{-\Sigma_i t_i \xi_0^2} = \frac{1}{2} (S_t)^{(d-\Sigma_i\Delta_i)/2} \Gamma\left(\frac{\sum_i \Delta_i - d}{2}\right) \tag{A2}$$

and

$$\int_{S^d} d^d x e^{-\Sigma_i t_i |x - x_i|^2} = \frac{\pi^{d/2}}{S_t^{d/2}} e^{-(1/S_t)(\Sigma_{i<j} t_i t_j |x_i - x_j|^2)}. \tag{A3}$$

In both of these formulas,

$$S_t = \sum_i t_i. \tag{A4}$$

APPENDIX B: GAUGE-FIXED INTEGRATION MEASURE

In this appendix we verify that the gauge-fixing procedure (5.3) results from decomposing the Haar measure on $\mathrm{SO}_0(1,d+1)$ as stated in Sec. V. We assume $d>1$ as in the main text.

1. Notation

We first recall some basic properties of the conformal group.[10]

We view $\mathrm{SO}_0(1,d+1)$ as the matrix group in its defining representation, acting on $\mathbb{R}^{1,d+1}$ by matrix multiplication of a column vector. We write the points in $\mathbb{R}^{1,d+1}$ as $(t,y,z^1,\ldots,z^d) =: (t,y,z)$, where z is in $\mathbb{R}^d$.

The action of $\mathrm{SO}_0(1,d+1)$ as the conformal group on $\mathbb{R}^d \cup \{\infty\}$ is obtained from that on the future null cone in $\mathbb{R}^{1,d+1}$, $t=\sqrt{y^2+z^2}$, by parameterizing the cone as $(t,y,z)=s\left(\frac{1}{2}(1+x^2), \frac{1}{2}(1-x^2), x\right)$, where $s \geqslant 0$ and $x \in \mathbb{R}^d \cup \{\infty\}$. The point $x=\infty$ corresponds to the null ray $t+y=0=z$.

If $q \in \mathbb{R}^d$ and $\lambda > 0$, we define the $\mathrm{SO}_0(1,d+1)$ matrices

$$N_+(q) := \begin{pmatrix} 1+\frac{1}{2}q^2 & \frac{1}{2}q^2 & q^T \\ -\frac{1}{2}q^2 & 1-\frac{1}{2}q^2 & -q^T \\ q & q & \mathbb{I}_d \end{pmatrix}, \tag{B1}$$

$$N_-(q) := \begin{pmatrix} 1+\frac{1}{2}q^2 & -\frac{1}{2}q^2 & q^T \\ \frac{1}{2}q^2 & 1-\frac{1}{2}q^2 & q^T \\ q & -q & \mathbb{I}_d \end{pmatrix}, \tag{B2}$$

$$A(\lambda) := \begin{pmatrix} \frac{1}{2}(\lambda^{-1}+\lambda) & \frac{1}{2}(\lambda^{-1}-\lambda) & 0 \\ \frac{1}{2}(\lambda^{-1}-\lambda) & \frac{1}{2}(\lambda^{-1}+\lambda) & 0 \\ 0 & 0 & \mathbb{I}_d \end{pmatrix}, \tag{B3}$$

where q is viewed as a column vector and $\mathbb{I}_d$ is the $d \times d$ unit matrix. In terms of the action on $\mathbb{R}^{1,d+1}$, $N_\pm(q)$ are null rotations and $A(\lambda)$ is a boost. The conformal action of $N_+(q)$ on $\mathbb{R}^d$ is the translation $x \mapsto x+q$, the action of $N_-(q)$ is the proper conformal transformation $x/(x^2) \mapsto x/(x^2)+q$, and the action of $A(\lambda)$ is the dilatation $x \mapsto \lambda x$.

Finally, if u and v are two unit vectors in $\mathbb{R}^d$, $u \neq -v$, we define the $\mathrm{SO}(d)$ matrix

$$\widetilde{S}(v,u) := \mathbb{I}_d + 2v \otimes u^T - \frac{(u+v) \otimes (u+v)^T}{1+u \cdot v}. \tag{B4}$$

$\widetilde{S}(v,u)$ is a rotation in the plane of u and v and takes u to v, reducing to $\mathbb{I}_d$ when $u=v$. Given $\widetilde{S}(v,u)$, we define the corresponding block-diagonal $\mathrm{SO}_0(1,d+1)$ matrix by $S(v,u) := \mathrm{diag}(\mathbb{I}_2, \widetilde{S}(v,u))$.

2. Parametrization

Let x_A, x_B, and x_C be three distinct points in $\mathbb{R}^d$. We set

$$x_D := \frac{x_{AB}^2 x_{AC}^2}{x_{BC}^2}\left(\frac{x_B - x_A}{x_{AB}^2} - \frac{x_C - x_A}{x_{AC}^2}\right), \tag{B5}$$

where $x_{ij} := |x_i - x_j|$ as in the main text. As $|x_D| = x_{AB} x_{AC} x_{BC}^{-1}$, it follows that $x_D \neq 0$.

Let v be a unit vector in $\mathbb{R}^d$. When $x_D/|x_D| \neq -v$, we define

$$h(x_A,x_B,x_C) := S(v, x_D/|x_D|) A(1/|x_D|) N_-(b) N_+(a), \tag{B6}$$

where $a := -x_A$ and $b := x_{AC}^{-2}(x_A - x_C)$. A direct computation shows that the conformal action of h takes the triple (x_A,x_B,x_C) to the triple $(0,v,\infty)$. Each $\mathrm{SO}_0(1,d+1)$ matrix g whose conformal action takes (x_A,x_B,x_C) to $(0,v,\infty)$ can therefore be uniquely written as

$$g = Rh, \tag{B7}$$

where $R = \mathrm{diag}(\mathbb{I}_2, \widetilde{R})$ and $\widetilde{R}$ is an $\mathrm{SO}(d)$ matrix in the $\mathrm{SO}(d-1)$ subgroup that fixes v. Note that this subgroup is trivial for $d=2$ but nontrivial for $d>2$.

If v is considered fixed, the above discussion shows that formulas (B6) and (B7) give a unique parameterization of an open subset in $\mathrm{SO}_0(1,d+1)$ by the triple (x_A,x_B,x_C) and a group isomorphic to $\mathrm{SO}(d-1)$. This parametrization does not cover all of $\mathrm{SO}_0(1,d+1)$, but the missing subset is of measure zero and can be recovered by choosing a different v and by limits in which one of x_A, x_B, and x_C is taken to infinity.

Now, the right action of $\mathrm{SO}_0(1,d+1)$ on (B7) induces on the triple (x_A,x_B,x_C) the conformal $\mathrm{SO}_0(1,d+1)$ action of the main text. To eliminate the volume divergence of the main text, we therefore need to write the Haar measure on $\mathrm{SO}_0(1,d+1)$ in the decomposition (B7) and identify the part of the measure that is associated with the noncompact factor h. If this measure is $\mu(x_A,x_B,x_C)\, d^d x_A d^d x_B d^d x_C$, the divergence will be eliminated by the replacement

$$d^d x_A d^d x_B d^d x_C \to \frac{\delta^d(x_A - x_A^0)\,\delta^d(x_B - x_B^0)\,\delta^d(x_C - x_C^0)}{\mu(x_A,x_B,x_C)} d^d x_A d^d x_B d^d x_C, \tag{B8}$$

where the distinct points x_A^0, x_B^0, and x_C^0 can be chosen arbitrarily.

3. Measure computation

From (B6) and (B7) we find

$$(AR)^{-1}(\mathrm{d}g\, g^{-1})(AR) = R^{-1}\,\mathrm{d}R + \mathrm{d}S\, S^{-1} + SQS^{-1}, \tag{B9}$$

where

$$
\begin{aligned}
Q = (|x_D|^{-1} d(|x_D|) + 2b \cdot \mathrm{d}a) &\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&+ \begin{pmatrix} 0 & 0 & (1+b^2)\mathrm{d}a^T - 2(b\cdot \mathrm{d}a)b^T + \mathrm{d}b^T \\ 0 & 0 & 0 \\ (1+b^2)\mathrm{d}a - 2(b\cdot \mathrm{d}a)b + \mathrm{d}b & 0 & 0 \end{pmatrix} \\
&+ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & (1-b^2)\mathrm{d}a^T + 2(b\cdot \mathrm{d}a)b^T - \mathrm{d}b^T \\ 0 & (1-b^2)\mathrm{d}a + 2(b\cdot \mathrm{d}a)b - \mathrm{d}b & 0 \end{pmatrix} \\
&+ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2(b\otimes \mathrm{d}a^T - \mathrm{d}a \otimes b^T) \end{pmatrix}. \qquad \text{(B10)}
\end{aligned}
$$

The explicit form of the term $\mathrm{d}S\, S^{-1}$ can be found from (B4).

To find the part of the Haar measure that corresponds to the noncompact factor h, we project the right-hand side of (B9) to the subspace orthogonal (with respect to the Killing form) to the subspace generated by $R^{-1}\,\mathrm{d}R$. Choosing v for concreteness to be (1,0,0,…), this amounts to setting the lower-right $(d-1)\times(d-1)$ block to zero but leaving the other components unchanged. From the coefficients of the remaining $3d$ Lie algebra elements we can then identify the $3d \times 3d$ determinant that gives the desired measure. Evaluating the determinant by elementary matrix algebra techniques, we find that this measure is

$$
\frac{d^d x_A d^d x_B d^d x_C}{|x_A - x_B|^d |x_B - x_C|^d |x_C - x_A|^d}. \qquad \text{(B11)}
$$

Hence the gauge fixing procedure (5.3) follows.

As a check, it can be directly verified that the measure (B11) is invariant under the conformal action of $\mathrm{SO}_0(1,d+1)$.

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Soliton solutions of the Kadomtsev-Petviashvili II equation

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We study a general class of line-soliton solutions of the Kadomtsev-Petviashvili II (KPII) equation by investigating the Wronskian form of its tau-function. We show that, in addition to the previously known line soliton solutions of KPII, this class also contains a large variety of multisoliton solutions, many of which exhibit nontrivial spatial interaction patterns. We also show that, in general, such solutions consist of unequal numbers of incoming and outgoing line solitons. From the asymptotic analysis of the tau function, we explicitly characterize the incoming and outgoing line solitons of this class of solutions. We illustrate these results by discussing several examples. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Kadomtsev-Petviashvili (KP) equation

$$\frac{\partial}{\partial x}\left(-4\frac{\partial u}{\partial t}+\frac{\partial^3 u}{\partial x^3}+6u\frac{\partial u}{\partial x}\right)+3\sigma^2\frac{\partial^2 u}{\partial y^2}=0, \tag{1.1}$$

where $u=u(x,y,t)$ and $\sigma^2=\pm 1$, is one of the prototypical $(2+1)$-dimensional integrable nonlinear partial differential equations. The case $\sigma^2=-1$ is known as the KPI equation, and $\sigma^2=1$ as the KPII equation. Originally derived[11] as a model for small-amplitude, long-wavelength, weakly two-dimensional (y-variation much slower than the x-variation) solitary waves in a weakly dispersive medium, the KP equation arises in disparate physical settings including water waves and plasmas, astrophysics, cosmology, optics, magnetics, anisotropic two-dimensional lattices, and Bose-Einstein condensation. The remarkably rich mathematical structure underlying the KP equation, its integrability and large classes of exact solutions have been studied extensively for the past 30 years, and are documented in several monographs.[1,3,8,15,18,21]

In this paper we study a large class of solitary wave solutions of the KPII equation. It is well known (e.g., see Refs. 5 and 15) that solutions of the KPII equation can be expressed as

$$u(x,y,t)=2\frac{\partial^2}{\partial x^2}\ln\tau(x,y,t), \tag{1.2}$$

where the tau function $\tau(x,y,t)$ is given in terms of the Wronskian determinant[7,15]

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$$\tau(x,y,t) = \mathrm{Wr}(f_1, \ldots, f_N) = \det\begin{pmatrix} f_1 & f_2 & \cdots & f_N \\ f_1' & f_2' & \cdots & f_N' \\ \vdots & \vdots & & \vdots \\ f_1^{(N-1)} & f_2^{(N-1)} & \cdots & f_N^{(N-1)} \end{pmatrix}. \tag{1.3}$$

with $f^{(i)} = \partial^i f / \partial x^i$, and where the functions $f_1, \ldots, f_N$ are a set of linearly independent solutions of the linear system

$$\frac{\partial f}{\partial y} = \frac{\partial^2 f}{\partial x^2}, \quad \frac{\partial f}{\partial t} = \frac{\partial^3 f}{\partial x^3}. \tag{1.4}$$

Equations (1.2) and (1.3) can also be obtained as the N-fold Darboux transformation for KPII (Ref. 15) starting from a seed solution $u=0$. In fact, the functions $f_1, \ldots, f_N$ in Eqs. (1.3) are precisely N independent solutions of the KPII Lax pair: $\partial_y f - \partial_x^2 f + uf = 0$ and $\partial_t f - \partial_x^3 f + 6u(\partial_x u)f + 3(\partial_x^{-1}\partial_y u)f = 0$, with $u=0$. A one-soliton solution of the KPII equation is obtained by choosing $N=1$ and $f(x,y,t) = e^{\theta_1} + e^{\theta_2}$, where

$$\theta_m(x,y,t) = k_m x + k_m^2 y + k_m^3 t + \theta_{m,0} \tag{1.5}$$

with $k_m, \theta_{m,0} \in \mathbb{R}$, $m=1,2$ and with $k_1 \neq k_2$ for nontrivial solutions. Without loss of generality, one can order the parameters as $k_1 < k_2$. The above choice yields the following traveling-wave solution:

$$u(x,y,t) = \tfrac{1}{2}(k_2 - k_1)^2 \operatorname{sech}^2 \tfrac{1}{2}(\theta_2 - \theta_1) = \Phi(\mathbf{k}\cdot\mathbf{x} + \omega t), \tag{1.6}$$

where $\mathbf{x} = (x,y)$. The wave-vector $\mathbf{k} = (l_x, l_y)$ and the frequency ω are given by

$$\mathbf{k} = (k_1 - k_2, k_1^2 - k_2^2), \quad \omega = k_1^3 - k_2^3, \tag{1.7}$$

and they satisfy the nonlinear dispersion relation

$$-4\omega l_x + l_x^4 + 3l_y^2 = 0. \tag{1.8}$$

The solution in Eq. (1.6) is localized along points satisfying $\theta_1 = \theta_2$, which defines a line in the xy plane, for fixed t. Such solitary wave solutions of the KPII equation are thus called *line solitons*. They are stable with respect to transverse perturbations unlike the KPI [Eq. (1.1) with $\sigma^2 = -1$] line-soliton solutions which are not stable with respect to small transverse perturbations. Equation (1.6) also implies that, apart from the constant $\theta_{1,0} - \theta_{2,0}$ corresponding to an overall translation of the solution, a line soliton of KPII is characterized by either the phase parameters k_1, k_2, or the physical parameters, namely, the *soliton amplitude* a and the *soliton direction* c, defined, respectively, as

$$a = k_2 - k_1, \quad c = k_1 + k_2. \tag{1.9}$$

Note that $c = \tan\alpha$, where α is the angle, measured counterclockwise, between the line soliton and the positive y axis. Hence, the soliton direction c can also be viewed as the "velocity" of the soliton in the xy plane, $c = -\mathrm{d}x/\mathrm{d}y = l_y/l_x$. For any given choice of amplitude and direction of the soliton, one obtains the phase parameters $k_{1,2}$ uniquely as $k_1 = \frac{1}{2}(c-a)$ and $k_2 = \frac{1}{2}(c+a)$.

When $c=0$ (equivalently, $k_1 = -k_2$), the solution in Eq. (1.6) becomes y-independent and reduces to the one-soliton solution of the Korteweg-de Vries (KdV) equation. Similar to KdV, it is also possible to obtain multisoliton solutions of the KPII equation. Each of the multisoliton solutions decay exponentially in the xy plane, except along a number of rays or line solitons as $y \to \pm\infty$. These line solitons are sorted according to their directions, with increasing values of c from left to right as $y \to -\infty$ and increasing values of c from right to left as $y \to \infty$. However, the multisoliton solution space of the KPII equation turns out to be much richer than that of the $(1+1)$-dimensional KdV equation due to the dependence of the KPII solutions on the additional

spatial variable y. It is possible to construct a general family of multisoliton solutions via the Wronskian of Eq. (1.3) by choosing M phases $\theta_1,\ldots,\theta_M$ defined as in Eq. (1.5) with distinct real *phase parameters* $k_1<k_2<\cdots<k_M$ and then defining the functions $f_1,\ldots,f_N$ in Eq. (1.3) by

$$f_n(x,y,t)=\sum_{m=1}^{M} a_{n,m}e^{\theta_m},\quad n=1,2,\ldots,N. \tag{1.10}$$

The constant coefficients $a_{n,m}$ define the $N\times M$ *coefficient matrix* $A:=(a_{n,m})$, which is required to be of full rank [i.e., rank$(A)=N$] and all of whose nonzero $N\times N$ minors must be sign definite. The full rank condition is necessary and sufficient for the functions f_n in Eq. (1.10) to be linearly independent. The sign definiteness of the nonzero minors is sufficient to ensure that the tau function $\tau(x,y,t)$ has no zeros in the xy plane for all t, so that the KPII solution $u(x,y,t)$ resulting from Eq. (1.2) is nonsingular.

One of the main results of this work (cf. Theorem 3.6) is to show that, when the coefficient matrix A satisfies certain conditions (cf. Definition 2.2), Eq. (1.10) leads to a multisoliton configuration with N_- asymptotic line solitons as $y\to-\infty$ and N_+ asymptotic line solitons as $y\to\infty$, where $N_-=M-N$ and $N_+=N$. Furthermore, each of the asymptotic line solitons has the form of a plane wave similar to the one-soliton solution in Eq. (1.6). We refer to these multisoliton configurations the (N_-,N_+)-*soliton solutions* of KPII, and call the asymptotic line solitons as $y\to-\infty$ and as $y\to\infty$ the *incoming* and *outgoing* line solitons, respectively. The amplitudes, directions and even the number of incoming solitons are in general different from those of the outgoing ones, depending on the values of M,N, the phase parameters $k_1,\ldots,k_M$ and the coefficient matrix A. We note that a special family of KPII (N_-,N_+)-soliton solutions which also satisfy the finite Toda lattice hierarchy, was found earlier in Ref. 2. In this paper, we generalize the results of Ref. 2 to the entire class of (N_-,N_+)-soliton solutions of KPII generated by arbitrary coefficient matrices A. These solutions exhibit a variety of spatial interaction patterns which include the formation of intermediate line solitons and web structures in the xy plane.[2,12,16,23] In contrast, the line solitons for the previously known[5,15,24] *ordinary* soliton solutions of KPII (cf. Sec. IV) and the KdV solitons experience only a phase shift after collision. The existence of these nontrivial spatial features was found to be related to the presence of *resonant* soliton interactions in some earlier studies.[4,17,19,22] Several examples of these (N_-,N_+)-soliton solutions of KPII are discussed throughout this work (e.g., see Figs. 1–4). If $M=2N$, it follows from Theorem 3.6 that $N_-=N_+=N$, i.e., the numbers incoming and outgoing asymptotic line solitons are the same. We call the resulting solutions the *N-soliton solutions* of KPII. Among these, there is an important subclass called the *elastic N*-soliton solutions, for which the amplitudes and directions of the out-going line solitons coincide with those of the incoming line solitons. Elastic N-soliton solutions possess a number of interesting features, some of which have been studied in Ref. 12. A detailed study of the specific properties of the elastic N-solutions will be reported in a future presentation.

We note that multisoliton solutions exhibiting nontrivial spatial structures and interaction patterns were also recently found in other $(2+1)$-dimensional integrable equations. For example, solutions with soliton resonance and web structure were presented in Refs. 9 and 10 for a coupled KP system, and similar solutions were also found in Ref. 14 in discrete soliton systems such as the two-dimensional Toda lattice, together with its fully discrete and ultradiscrete analogues. From these works, the existence of these solutions appears to be a rather common feature of $(2+1)$-dimensional integrable systems. Thus, we expect that the scope of the results described in this paper will not be limited to the KP equation alone, but will also be applicable to a variety of other $(2+1)$-dimensional integrable systems.

II. THE TAU FUNCTION AND THE ASYMPTOTIC LINE SOLITONS

In this section we investigate the properties of the tau function given by Eq. (1.3) when the N functions $f_1,\ldots,f_N$ are chosen according to Eq. (1.10) as linear combinations of M exponentials $e^{\theta_1},\ldots,e^{\theta_M}$. We should emphasize that Eq. (1.10) represents the most general form for the functions involving linear combinations of exponential phases. Since the elements of the $N\times M$ coef-

ficient matrix $A=(a_{n,m})$ are the linear combination coefficients of the functions $f_1,\dots,f_N$, one can naturally identify each f_n with one of the rows of A and each phase θ_m with one of the columns of A, and vice versa. Next, we examine the asymptotic behavior of the tau function in the xy plane as $y\to\pm\infty$. It is clear that, with the above choice of functions, the tau function is a linear combination of exponentials. Consequently, the leading order behavior of the tau function as $y\to\pm\infty$ in a given asymptotic sector of the xy plane is governed by those exponential terms which are dominant in that sector. A systematic analysis of the dominant exponential phases allows us to characterize the incoming and outgoing line solitons of (N_-,N_+)-soliton solutions of KPII.

A. Basic properties of the tau function

We present here some general properties of the tau function. Without loss of generality, throughout this work we choose the phase parameters k_m to be distinct and well ordered as $k_1<k_2<\cdots<k_M$.

Lemma 2.1: Suppose $\tau_{N,M}=\mathrm{Wr}(f_1,\dots,f_N)$ *as in Eq.* (1.3) *with the functions* $f_1,\dots,f_N$ *given by Eq.* (1.10). *Then*

$$\tau_{N,M}(x,y,t)=\det(A\Theta K^T), \tag{2.1}$$

where $A=(a_{n,m})$ *is the* $N\times M$ *coefficient matrix,* $\Theta=\mathrm{diag}(e^{\theta_1},\dots,e^{\theta_M})$, *and the* $N\times M$ *matrix* K *is given by*

$$K=\begin{pmatrix} 1 & 1 & \cdots & 1 \\ k_1 & k_2 & \cdots & k_M \\ \vdots & \vdots & & \vdots \\ k_1^{N-1} & k_2^{N-1} & \cdots & k_M^{N-1} \end{pmatrix},$$

where the superscript T *denotes matrix transpose. Moreover,* $\tau_{N,M}$ *can be expressed as*

$$\tau_{N,M}(x,y,t)=\sum_{1\leqslant m_1<m_2<\cdots<m_N\leqslant M} V(m_1,\dots,m_N)A(m_1,\dots,m_N)\exp[\theta_{m_1,\dots,m_N}], \tag{2.2}$$

where $\theta_{m_1,\dots,m_N}$ *denotes the phase combination*

$$\theta_{m_1,\dots,m_N}(x,y,t)=\theta_{m_1}(x,y,t)+\cdots+\theta_{m_N}(x,y,t), \tag{2.3}$$

$A(m_1,\dots,m_N)$ *denotes the* $N\times N$ *minor of* A *obtained by selecting columns* $m_1,\dots,m_N$, *and* $V(m_1,\dots,m_N)$ *denotes the Van der Monde determinant*

$$V(m_1,\dots,m_N)=\prod_{1\leqslant s_1\leqslant s_2\leqslant N}(k_{m_{s_2}}-k_{m_{s_1}}). \tag{2.4}$$

Proof: Equation (2.1) follows by direct computation of the Wronskian determinant (1.3). Next, to prove Eq. (2.2) apply the Binet-Cauchy theorem to expand the determinant in Eq. (2.1) and note that the $N\times N$ minor of K obtained by selecting columns $1\leqslant m_1<\cdots<m_N\leqslant M$ is given by the Van der Monde determinant $V(m_1,\dots,m_N)$. □

From Lemma 2.1 we have the following basic properties of the tau function:

(i) The spatiotemporal dependence of the tau function in Eq. (2.2) is confined to a sum of exponential phase combinations $\theta_{m_1,\dots,m_N}$ which according to Eq. (2.3) are linear in x,y,t. Moreover, all the Van der Monde determinants $V(m_1,\dots,m_N)$ are positive, as the phase parameters $k_1,\dots,k_M$ are well ordered. A sufficient condition for the tau function in Eq. (2.2) to generate a nonsingular solution of KPII is that it is sign-definite for all $(x,y,t)\in\mathbb{R}^3$. In turn, a sufficient condition for the sign-definiteness of the tau-function is that the minors of the coefficient matrix A are either all non-negative or all nonpositive. However,

it is not clear at present whether these conditions are also necessary. If the tau function in Eq. (2.2) is taken as a sum of exponential phase combinations with non-negative coefficients, the solution $u(x,y,t)$ in Eq. (1.2) can be expressed as a ratio of two sums, each containing the *same* set of exponential terms, and with non-negative coefficients. Consequently, the resulting solution of KPII is bounded and positive definite for all $(x,y,t) \in \mathbb{R}^3$.

(ii) Each exponential term in the tau function of Eq. (2.2) contains combinations of N *distinct* phases $\theta_{m_1},\ldots,\theta_{m_N}$ identified by integers $m_1,\ldots,m_N$ chosen from $\{1,\ldots,M\}$. Thus, the maximum number of terms in the tau function is given by the binomial coefficient $\binom{M}{N}$. However, a given phase combination $\theta_{m_1,\ldots,m_N}$ is actually *present* in the tau function if and only if the corresponding minor $A(m_1,\ldots,m_N)$ is nonzero.

(iii) If $M<N$ the functions $f_1,\ldots,f_N$ are linearly dependent; in this case there are no terms in the summation in Eq. (2.2), and therefore the tau function $\tau_{N,M}(x,y,t)$ is identically zero. Also, if $M=N$, there is only one term in the summation corresponding to the determinant of A; then $\tau_{N,M}(x,y,t)$ depends linearly on x and therefore it generates the trivial solution $u(x,y,t)=0$. Finally, if $\text{rank}(A)<N$, all $N\times N$ minors of A vanish identically, leading once again to $\tau_{N,M}(x,y,t)=0$. Therefore, for nontrivial solutions one needs $M>N$ and $\text{rank}(A)=N$.

(iv) The transformation $A\to A'=GA$ with $G\in \text{GL}(N,\mathbb{R})$ (corresponding to elementary row operations on A) amounts to an overall rescaling $\tau(x,y,t)\to\tau'(x,y,t)=\det(G)\tau(x,y,t)$ of the tau function (2.1). Such rescaling leaves the solution $u(x,y,t)$ in Eq. (1.2) invariant. This reflects the fact that N independent linear combinations of the functions $f_1,\ldots,f_N$ in Eq. (1.10) generate equivalent tau functions. This $\text{GL}(N,\mathbb{R})$ gauge freedom can be exploited to choose the coefficient matrix A in Eq. (2.1) to be in reduced row-echelon form (RREF). The $\text{GL}(N,\mathbb{R})$ invariance means that the tau function (2.1) represents a point in the real Grassmannian $\text{Gr}(N,M)$.[12]

(v) Suppose that one of the functions in Eq. (1.10) contains only one exponential term, and is given by $f_p=a_{p,q}e^{\theta_q}$ with $a_{p,m}=0\ \forall m\neq q$. Then, the minors $A(m_1,\ldots,m_N)=0$ whenever $q\notin\{m_1,\ldots,m_N\}$. As a result, the tau function in Eq. (2.2) can be expressed as $\tau_{N,M}(x,y,t)=e^{\theta_q}\tau'(x,y,t)$, and $\tau'(x,y,t)$ is a sum of exponential phase combinations, where each combination consists of $N-1$ distinct phases chosen from all M phases except θ_q. From Eq. (1.2) it is evident that $\tau_{N,M}(x,y,t)$ and $\tau'(x,y,t)$ generate the same solution of KPII. Moreover, the function $\tau'(x,y,t)$ is effectively equivalent to a tau function $\tau_{N-1,M-1}(x,y,t)$ with a coefficient matrix obtained by deleting the pth row and qth column of A. Hence in this case the tau function $\tau_{N,M}(x,y,t)$ is reducible to another tau function $\tau_{N-1,M-1}(x,y,t)$ obtained from a Wronskian of $N-1$ functions with $M-1$ distinct phases.

In accordance with the above remarks, throughout this work we consider the coefficient matrix A to be in RREF. Also, to avoid trivial and singular cases, from now on we assume that $M>N$ and $\text{rank}(A)=N$, and that all nonzero $N\times N$ minors of A are positive. Finally, we assume that A satisfies the following irreducibility conditions.

Definition 2.2 (Irreducibility): A matrix A of rank N is said to be irreducible if, in RREF:

(i) *Each column of A contains at least one nonzero element.*

(ii) *Each row of A contains at least one nonzero element in addition to the pivot.*

Condition (i) in Definition 2.2 requires that each exponential phase appear in at least one of the functions $f_1,\ldots,f_N$. If a particular phase is absent, then the corresponding tau function $\tau_{N,M}$ can be reexpressed in terms of a reduced tau function $\tau_{N,M-1}$. Condition (ii) requires that each function contains at least two exponential phases in order to avoid reducible situations like those in part (v) of the above remarks. Note also that if an $N\times M$ matrix A is irreducible, then $M>N$.

B. Dominant phase combinations and index pairs

We now study the asymptotic behavior of the tau function in the xy-plane for large values of $|y|$ and finite values of t. Let Θ denote the set of all phase combinations $\theta_{m_1,\ldots,m_N}$ such that $A(m_1,\ldots,m_N)\neq 0$, that is, the set of phase combinations that are actually present in the tau function $\tau(x,y,t)$.

Definition 2.3 (Dominant phase): A given phase combination $\theta_{m_1,\ldots,m_N}\in\Theta$ is said to be dominant for the tau function $\tau(x,y,t)$ of Eq. (2.2) *in a region $R\in\mathbb{R}^3$ if $\theta_{m'_1,\ldots,m'_N}(x,y,t)\leqslant\theta_{m_1,\ldots,m_N}(x,y,t)$ for all $\theta_{m'_1,\ldots,m'_N}\in\Theta$ and for all $(x,y,t)\in R$. The region R is called the dominant region of $\theta_{m_1,\ldots,m_N}$.*

The phase combinations $\theta_{m_1,\ldots,m_N}(x,y,t)$ are linear functions of x, y, and t. So, each of the inequalities in Definition 2.3 defines a convex subset of $\mathbb{R}^3$. The dominant region R associated with each phase combination is also convex because it is defined by the intersection of finitely many convex subsets. Furthermore, since the phase combinations are defined globally on $\mathbb{R}^3$, each point $(x,y,t)\in\mathbb{R}^3$ belongs to some dominant region R. As a result, we obtain a partition of the entire $\mathbb{R}^3$ into a finite number of convex dominant regions, intersecting only at points on the boundaries of each region. It is important to note that such boundaries always exist whenever there is more than one phase combination in the tau function, because then there are more than one dominant region in $\mathbb{R}^3$. The significant of the dominant regions lies in the following:

Lemma 2.4: The solution $u(x,y,t)$ of the KPII equation generated by the tau function (2.2) *is exponentially small at all points in the interior of any dominant region. Thus, the solution is localized only at the boundaries of the dominant regions, where a balance exists between two or more dominant phase combinations in the tau function of Eq.* (2.2).

Proof: Let R be the dominant region of $\theta_{m_1,\ldots,m_N}$, which is therefore the *only* dominant phase in the interior of R. Then from Eq. (2.2), $\tau_{N,M}(x,y,t)\sim O(e^{\theta_{m_1,\ldots,m_N}})$ in the interior of R. As a result, $\ln\tau_{N,M}(x,y,t)$ locally becomes a linear function of x apart from exponentially small terms. Hence, it follows from Eq. (1.2) that the solution $u(x,y,t)$ of KPII is exponentially small at all such interior points of R. □

The boundary between any two adjacent dominant regions is the set of points across which *a transition* from one dominant phase combination $\theta_{m_1,\ldots,m_N}$ to another dominant phase combination $\theta_{m'_1,\ldots,m'_N}$ takes place. Such boundary is therefore identified by the equation $\theta_{m_1,\ldots,m_N}=\theta_{m'_1,\ldots,m'_N}$, which defines a line in the xy plane for fixed values of t. The simplest instance of a transition between dominant phase combinations arises for the one-soliton solution (1.6), which is localized along the line $\theta_1=\theta_2$ defining the boundary of the two regions of the xy plane where θ_1 and θ_2 dominate. In the one-soliton case, these two regions are simply half-planes. But in the general case the dominant regions are more complicated, although the solution $u(x,y,t)$ is still localized along the boundaries of these regions, corresponding to similar phase transitions. For example, Fig. 1(a) illustrates a (2,1)-soliton known as a *Miles resonance*[17] (also called a Y junction), generated by the tau function $\tau_{1,2}=e^{\theta_1}+e^{\theta_2}+e^{\theta_3}$. In this case, the xy plane is partitioned into three dominant regions corresponding to each of the dominant phases θ_1, θ_2, and θ_3. Once again, the solution $u(x,y,t)$ is exponentially small in the interior of each dominant regions, and is localized along the phase transition boundaries: here, $\theta_1=\theta_2$, $\theta_1=\theta_3$, and $\theta_2=\theta_3$. It should also be noted that some of these regions have infinite extension in the xy plane, while others are bounded, as in the case of resonant soliton solutions, described in Sec. IV and Ref. 2. Each phase transition which occurs asymptotically as $y\to\pm\infty$ defines an *asymptotic line soliton*, which is infinitely extended in the xy plane.

When studying the asymptotics of the tau function for large $|y|$ it is useful to consider the limit $y\to\pm\infty$ along the straight lines

$$L_c: x+cy=\xi, \tag{2.5}$$

parametrized by the direction c. Note that c increases counterclockwise, namely from the positive x axis to the negative x axis for $y>0$ and from the negative x axis to the positive x axis for y

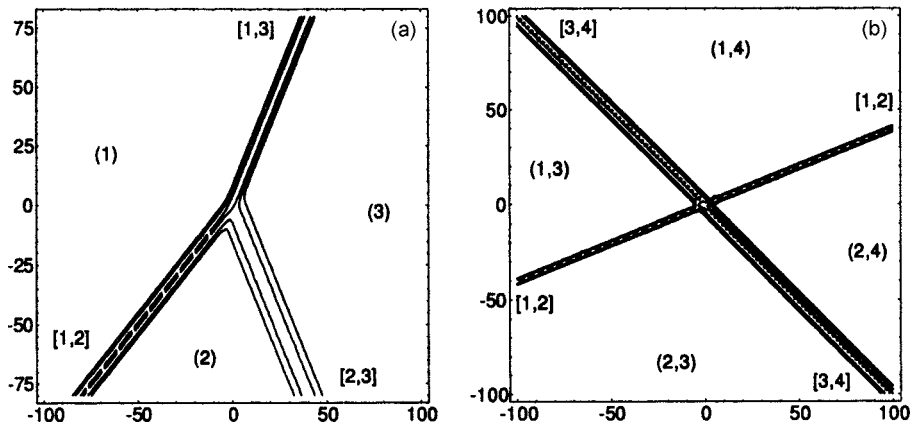

FIG. 1. Dominant phase combinations in the different regions of the xy plane (labeled by the indices in parentheses) and the asymptotic line solitons (labeled by the indices in square braces) for two different line soliton solutions: (a) a fundamental Miles resonance (Y junction) produced by the tau function with $N=1$, $M=3$ and $(k_1,k_2,k_3)=(-1,0,\frac{1}{2})$ at $t=0$; (b) an ordinary two-soliton solution, produced by the coefficient matrix in Example 2.7 with $(k_1,\ldots,k_4)=(-\frac{3}{2},-\frac{1}{2},0,1)$ at $t=0$ (see text for details). Here and in all of the following figures, the horizontal and vertical axes are, respectively, x and y, and the graphs show contour lines of $\ln u(x,y,t)$ at a fixed value of t.

<0. From Eqs. (1.5) and (2.5), each exponential phases along L_c is $\theta_m=k_m(k_m-c)y+k_m\xi+k_m^3t+\theta_{m,0}$. The difference between two such phases along L_c then becomes

$$\theta_m-\theta_{m'}=(k_m-k_{m'})(k_m+k_{m'}-c)y+(k_m-k_{m'})\xi+(k_m^3-k_{m'}^3)t+\theta_{m,0}-\theta_{m',0}, \tag{2.6a}$$

and the difference between any two phase combinations along L_c is given by

$$\theta_{m_1,\ldots,m_N}-\theta_{m'_1,\ldots,m'_N}=\left(\sum_{j=1}^{N}(k_{mj}-k_{m'_j})(k_{m_j}+k_{m'_j}-c)\right)y+\delta(\xi,t), \tag{2.6b}$$

where $\delta(\xi,t)=\Sigma_{j=1}^{N}[(k_{m_j}-k_{m'_j})\xi+(k_{m_j}^3-k_{m'_j}^3)t+\theta_{m_j,0}-\theta_{m'_j,0}]$. In particular, the *single-phase-transition* line $L_{m,m'}:\theta_m=\theta_{m'}$ given by Eq. (2.5) with $c_{m,m'}=k_m+k_{m'}$, will play an important role below.

It is also convenient at this point to introduce the following notations which will be employed throughout this paper. We denote by $A[m]\in\mathbb{R}^N$ the mth column of a matrix A, and we denote by $A[m_1,\ldots,m_r]$ the $N\times r$ submatrix obtained by selecting the r columns $A[m_1],\ldots,A[m_r]$. We also label the N pivot columns of an irreducible, $N\times M$ matrix A by $A[e_1],\ldots,A[e_N]$, with $1=e_1<e_2<\cdots<e_N<M$, and we label the $M-N$ nonpivot columns by $A[g_1],\ldots,A[g_{M-N}]$, where $1<g_1<g_2<\cdots<g_{M-N}=M$. Note that A has N pivot columns because it is rank N; also, $e_1=1$ since A is in RREF, and $e_N<M$ since it is irreducible. We now establish a result that will be useful in order to characterize the asymptotics of the tau function.

Theorem 2.5: *(Single-phase transition) Asymptotically as $y\to\pm\infty$, and for generic values of the phase parameters $k_1,\ldots,k_M$, the dominant phase combinations in the tau function* (2.2) *exhibit the following behaviors in the xy plane.*

(i) *For finite values of t, the set of dominant phase combinations remains invariant in time.*
(ii) *The dominant phase combinations in any two adjacent dominant regions contain $N-1$ common phases.*

We discuss below several consequences of Theorem 2.5 which is proved in the Appendix.

Consider the single-phase transition as $y\to\pm\infty$ in which a phase θ_i from the dominant phase combination in one region is replaced by another phase θ_j to produce the dominant phase combination in the adjacent region. We refer to this transition as an $i\to j$ transition, which takes place along the line $L_{ij}:\theta_i=\theta_j$ whose direction in the xy plane is given by $c_{ij}=k_i+k_j$. As $y\to\infty$, it is clear

from Eq. (2.6a) that, if $k_i < k_j$, the transition $i \to j$ takes place from the left of the line $L_{i,j}$ to its right, while if $k_i > k_j$ the transition $i \to j$ takes place from the right of the line $L_{i,j}$ to its left. Thus, as $y \to \infty$, each dominant phase region R is bounded on the left by the transition line $L_{i,j}$ given by the *minimum* value of $c_{i,j}$ that corresponds to an allowed transition and, on the right by the transition line $L_{i,j}$ given by the *maximum* value of $c_{i,j}$ that corresponds to an allowed transition. Here, an *allowed* transition from one dominant phase combination to another means that the minors associated with those phase combinations in the tau function of Eq. (2.2), are both nonzero. In turn, these nonvanishing minors determine the values of c_{ij} corresponding to the allowed single-phase transitions. A similar statement can be made for transitions occurring as $y \to -\infty$. So, each dominant phase region R as $y \to \pm\infty$ has boundaries defined by a counterclockwise and a clockwise single-phase transitions which can be determined in the following way.

Corollary 2.6: Suppose that $\theta_{m_1,\dots,m_N}$ is the dominant phase combination on a region R asymptotically as $y \to \pm\infty$. Let J be the complement of the set of indices $\{m_1, m_2, \dots, m_N\}$ in $\{1, 2, \dots, M\}$. For each $j \in J$, define $I_j \subseteq \{m_1, m_2, \dots, m_N\}$ as the set of all indices $m_r \in \{m_1, m_2, \dots, m_N\}$ such that the minor $A(m_1, \dots, m_{r-1}, j, m_{r+1}, \dots, m_N) \neq 0$. Then, the following hold.

(i) *As $y \to \infty$, the directions of the counterclockwise and clockwise transition boundaries of R are, respectively, given by*

$$c_+ = \min_{i \in I_j, j \in J} [c_{i,j}] \quad \text{with } k_i > k_j, \quad c_- = \max_{i \in I_j, j \in J} [c_{i,j}] \quad \text{with } k_i < k_j. \tag{2.7a}$$

(ii) *As $y \to -\infty$, the directions of the counterclockwise and clockwise transition boundaries of R are, respectively, given by*

$$c_+ = \min_{i \in I_j, j \in J} [c_{i,j}] \quad \text{with } k_i > k_j, \quad c_- = \max_{i \in I_j, j \in J} [c_{i,j}] \quad \text{with } k_i > k_j. \tag{2.7b}$$

The results of Theorem 2.5 and Corollary 2.6 can be used to determine the asymptotic behavior of the tau function, thereby obtaining an important characterization of the asymptotic line solitons corresponding to (N_-, N_+)-soliton solutions of the KPII equation. Namely, for the tau function $\tau_{N,M}(x, y, t)$ of Eq. (2.2) with generic values of the phase parameters $k_1, \dots, k_M$ we have the following:

(i) As $y \to \pm\infty$, the dominant phase combinations of the tau function in adjacent regions of the xy plane contain $N-1$ common phases and differ by only a single phase. The transition between any two such dominant phase combinations $\theta_{i,m_2,\dots,m_N}$ and $\theta_{j,m_2,\dots,m_N}$ occurs along the line $L_{i,j}: \theta_i = \theta_j$, where a single phase θ_i in the dominant phase combination is replaced by a phase θ_j. Moreover, if the dominant phase combination $\theta_{i,m_2,\dots,m_N}$ in a given region is known, the transition line $L_{i,j}$ and the dominant phase combination $\theta_{j,m_2,\dots,m_N}$ are determined via Corollary 2.6. In particular, Eqs. (2.7) for $c_\pm$ determine explicitly the pair of phase parameters k_i and k_j corresponding to the single-phase transition $i \to j$ across each boundary $L_{i,j}$ of a given dominant phase region.

(ii) As $y \to \pm\infty$ along the line $L_{i,j}$, the asymptotic behavior of the tau function is determined by the balance between the two dominant phase combinations $\theta_{i,m_2,\dots,m_N}$ and $\theta_{j,m_2,\dots,m_N}$, and is given by

$$\tau_{N,M}(x,y,t) \sim V_i A(i, m_2, \dots, m_N) e^{\theta_{i,m_2,\dots,m_N}} + V_j A(j, m_2, \dots, m_N) e^{\theta_{j,m_2,\dots,m_N}},$$

where $V_i := V(i, m_2, \dots, m_N)$ and $V_j := V(j, m_2, \dots, m_N)$ are Van der Monde determinants defined in Eq. (2.4), and where the minors $A(i, m_2, \dots, m_N)$ and $A(j, m_2, \dots, m_N)$ of the coefficient matrix A are both nonzero. The solution $u(x, y, t)$ of the KPII equation in a neighborhood of such a single-phase transition is then obtained from Eq. (1.2) as

$$u(x,y,t) \sim \tfrac{1}{2}(k_i - k_j)^2 \operatorname{sech}^2\left[\tfrac{1}{2}(\theta_i - \theta_j)\right]. \tag{2.8}$$

Moreover, Lemma 2.4 and Theorem 2.5 together imply that the solution of the KPII equation is exponentially small everywhere in the xy-plane except at the locations of such single-phase transitions. Equation (2.8), which is a traveling wave solution satisfying the dispersion relation in Eq. (1.8), coincides with the one-soliton solution in Eq. (1.6). Thus, it defines an asymptotic line soliton associated with the single-phase transition $i \to j$. The phase parameters k_i and k_j associated with the single-phase transition $i \to j$ are determined by Eqs. (2.7). Then, the soliton amplitude is given by $a_{i,j} = |k_i - k_j|$, and the soliton direction is given by the direction of $L_{i,j}$, which is $c_{i,j} = k_i + k_j$.

(iii) All of the asymptotic line solitons resulting from the single-phase transitions described above are invariant in time, in the sense that their number, amplitudes, and directions are constants.

Motivated by these results, *we label each asymptotic line soliton by the index pair* $[i,j]$ *which uniquely identifies the phase parameters* k_i *and* k_j *in the ordered set* $\{k_1, \ldots, k_M\}$. The results summarized in the above remarks can be applied to explicitly delineate the dominant phase combinations and the asymptotic line solitons associated with the tau function of a given (N_-, N_+)-soliton solution of the KPII equation, as illustrated by the following example.

Example 2.7: When $N=2$ and $M=4$, Lemma 2.1 implies that the tau function $\tau(x,y,t)$ is given by

$$\tau(x,y,t) = \operatorname{Wr}(f_1, f_2) = \sum_{1 \leqslant m < m' \leqslant 4} (k_{m'} - k_m) A(m,m') e^{\theta_m + \theta_{m'}}, \tag{2.9}$$

where the phases are given by $\theta_m = k_m x + k_m^2 y + k_m^3 t + \theta_{m,0}$ for $m = 1, \ldots, 4$, as in Eq. (1.5), and where the phase parameters are ordered as $k_1 < \cdots < k_4$. We consider the line-soliton solution constructed from the functions $f_1 = e^{\theta_1} + e^{\theta_2}$ and $f_2 = e^{\theta_3} + e^{\theta_4}$, so that the associated 2×4 coefficient matrix is

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \tag{2.10}$$

Then $A(1,2) = A(3,4) = 0$, and the remaining four minors are all equal to 1. We apply Corollary 2.6 to determine the asymptotic line solitons associated with the tau function in Eq. (2.9). First note from the expression $\theta_{m,m'} = (k_m + k_{m'})x + (k_m^2 + k_{m'}^2)y + (k_m + k_{m'}^3)t + (\theta_{m,0} + \theta_{m',0})$ that for every finite value of y the dominant phase combination as $x \to -\infty$ is given by $\theta_{1,3}$, which corresponds to the *minimum* value of $k_m + k_{m'}$ such that $A(m,m') \neq 0$ (cf. Definition 2.3). We denote by $R_{1,3}$ the region of the xy plane where $\theta_{1,3}$ is the dominant phase. The transition boundaries of $R_{1,3}$ are determined by applying Corollary 2.6 as follows: The complement of the index set $\{1,3\}$ is $J = \{2,4\}$. When $j = 2 \in J$, we have $A(1,2) = 0$ but $A(2,3) \neq 0$; hence $I_2 = \{1\}$. Similarly, when $j = 4$ we have $I_4 = \{3\}$ because $A(1,4) \neq 0$ but $A(4,3) = 0$. Thus the possible transitions $i \to j$ from $R_{1,3}$ are $1 \to 2$ and $3 \to 4$. As $y \to \infty$, the second of Eqs. (2.7a) implies that the clockwise transition boundary of $R_{1,3}$ is given by the transition line $L_{3,4}$, whose direction $c_{3,4} = k_3 + k_4$ is greater than the direction $c_{1,2} = k_1 + k_2$ of the line $L_{1,2}$. Across the transition line $L_{3,4}$, the dominant phase combination switches from $\theta_{1,3}$ to $\theta_{1,4}$, onto the corresponding dominant region $R_{1,4}$. Similarly, as $y \to -\infty$, the first of Eqs. (2.7b) implies that the counterclockwise transition boundary of $R_{1,3}$ is given by the transition line $L_{1,2}$, whose direction $c_{1,2}$ is less than the direction $c_{3,4}$ of the line $L_{3,4}$. This implies that the dominant phase combination and dominant region change to $\theta_{2,3}$ and $R_{2,3}$, respectively. Applying Corollary 2.6 again to the region $R_{2,3}$ as $y \to -\infty$, one finds $J = \{1,4\}$ with $I_1 = \{2\}$ and $I_4 = \{3\}$, so the possible transitions from $R_{2,3}$ are $2 \to 1$ and $3 \to 4$. The $2 \to 1$ transition corresponds to a clockwise transition from $R_{2,3}$ back to $R_{1,3}$, whereas the $3 \to 4$ transition corresponds to a counterclockwise transition from $R_{2,3}$ to the region $R_{2,4}$, where $\theta_{2,4}$ is the dominant phase combination. Continuing counterclockwise from $R_{1,3}$ we finally obtain the following dominant phase regions asymptotically as $y \to \pm\infty$, together with the associated single-phase transitions:

$$R_{1,3} \xrightarrow{1\to 2} R_{2,3} \xrightarrow{3\to 4} R_{3,4} \xrightarrow{2\to 1} R_{1,4} \xrightarrow{4\to 3} R_{1,3}. \tag{2.11}$$

It is then clear that there are two asymptotic line solitons as $y\to-\infty$ as well as $y\to\infty$, and in both cases they correspond to the lines $\theta_1=\theta_2$ and $\theta_3=\theta_4$. The dominant phase regions, denoted by indices (m,m'), and the asymptotic line solitons, identified by the index pairs $[i,j]$, are illustrated in Fig. 1(b). The corresponding solution is called an ordinary 2-soliton solution. The ordinary N-soliton solutions are described in Sec. IV.

In the following section we obtain several results that will allow us to identify more precisely the index pairs corresponding to each asymptotic line soliton. In addition, we will prove a general result concerning the numbers of asymptotic line solitons present in an (N_-,N_+)-soliton solution corresponding to the tau function of Eq. (2.2).

III. ASYMPTOTIC LINE SOLITONS AND THE COEFFICIENT MATRIX

In this section we continue our investigation of the tau function in the general setting introduced in Sec. II. We have seen in the preceding section that an asymptotic line soliton corresponds to a dominant balance between two phase combinations in the tau function. But we still need to identify which phase combinations in a given tau function are indeed dominant as $y\to\pm\infty$. This requires a detailed study of the structure of the $N\times M$ coefficient matrix A associated with the tau function. In this section we carry out this analysis, which enables us to explicitly identify all the asymptotic line solitons of a given tau function in an algorithmic fashion. One of our main results of this section will be to establish that, for arbitrary values of N and M, and for irreducible coefficient matrices (cf. Definition 2.2) with non-negative $N\times N$ minors, the tau function (2.2) produces an (N_-,N_+)-soliton solution with $N_-=M-N$ and $N_+=N$, i.e., a solution in which there are $N_-=M-N$ asymptotic line solitons as $y\to-\infty$ and $N_+=N$ asymptotic line solitons as $y\to\infty$.

A. Dominant phases and the structure of the coefficient matrix

We begin by presenting a simple yet useful result (see also Ref. 2, Lemma 2.4) that will be frequently used to determine the dominant phase combinations in the tau function as $y\to\pm\infty$.

Lemma 3.1 (Dominant phase conditions): As $y\to\pm\infty$ along the line $L_{i,j}$: $\theta_i=\theta_j$ with $i<j$, the exponential phases $\theta_1,\dots,\theta_M$ satisfy the following relations.

(i) *As* $y\to\infty$, $\theta_m<\theta_*$, $\forall m\in\{i+1,\dots,j-1\}$, *and* $\theta_m>\theta_*$, $\forall m\in\{1,\dots,i-1,j+1,\dots,M\}$, *where* $\theta_*:=\theta_i=\theta_j$.

(ii) *As* $y\to-\infty$, $\theta_m>\theta_*$, $\forall m\in\{i+1,\dots,j-1\}$, *while* $\theta_m<\theta_*$, $\forall m\in\{1,\dots,i-1,j+1,\dots,M\}$.

Proof: It follows from Eq. (2.6a) that, along the line $L_{i,j}$ whose direction is $c_{i,j}=k_i+k_j$, the difference between any two exponential phases θ_m and $\theta_{m'}$ is given by

$$\theta_m-\theta_{m'}=(k_m-k_{m'})[(k_m+k_{m'})-(k_i+k_j)]y+\delta'(\xi,t), \tag{3.1}$$

where $\delta'(\xi,t)$ is a linear function of ξ and t and which also depends on the constants $\theta_{m,0}$, $\theta_{m',0}$, $\theta_{i,0}$, and $\theta_{j,0}$. It is clear that the sign of $\theta_m-\theta_{m'}$ as $y\to\pm\infty$ and for finite values of ξ and t is determined by the coefficient of y on the right-hand side of Eq. (3.1). Then, setting $m'=i$ (or $m'=j$) in Eq. (3.1) one obtains the desired inequalities. □

Lemma 3.1, which is illustrated in Fig. 2, will be used to obtain a set of conditions that are necessary for a given pair of phase combinations in the tau-function to be dominant. These conditions are given in terms of the vanishing of certain $N\times N$ minors of the coefficient matrix A, and they determine which phase combinations are present (or absent) in the tau function of Eq. (1.3). In order to derive these conditions, it is convenient to introduce two submatrices $P_{i,j}$ and $Q_{i,j}$ associated with any index pair $[i,j]$ with $1\leqslant i<j\leqslant M$, and given by

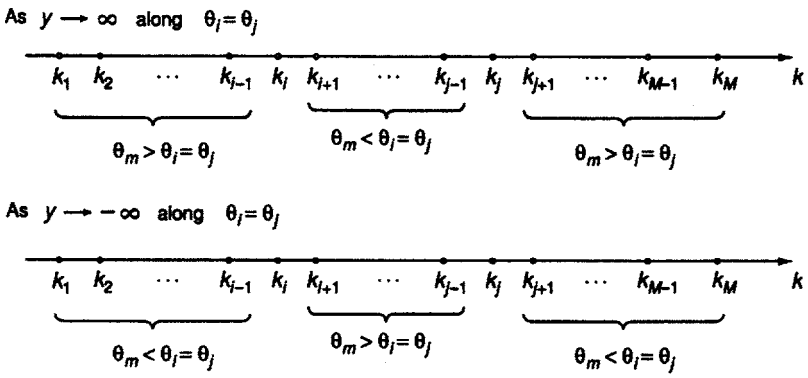

FIG. 2. Relations among the exponential phases as $y \to \pm\infty$ along the direction $L_{i,j}$: $\theta_i = \theta_j$.

$$P_{i,j} = A[1,2,\ldots,i-1,j+1,\ldots,M], \quad Q_{i,j} = A[i+1,\ldots,j-1]. \tag{3.2}$$

The matrix $P_{i,j}$ is formed by the consecutive columns of A to the left of column $A[i]$ and those to the right of column $A[j]$, while $Q_{i,j}$ is formed by the consecutive columns of A between columns $A[i]$ and $A[j]$. Using the matrices $P_{i,j}$ and $Q_{i,j}$ and the dominant phase conditions in Lemma 3.1 we then have the following.

Lemma 3.2 (Vanishing minor conditions): Suppose that the index pair $[i,j]$ *identifies an asymptotic line soliton. Let the two dominant phase combinations along the line* $L_{i,j}$: $\theta_i = \theta_j$ *be given by* $\theta_{i,p_1,\ldots,p_r,q_1,\ldots,q_s}$ *and* $\theta_{j,p_1,\ldots,p_r,q_1,\ldots,q_s}$, *and let* $A(i,p_1,\ldots,p_r,q_1,\ldots,q_s)$, $A(j,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *be the corresponding nonzero minors where* $A[p_1],\ldots,A[p_r] \in P_{i,j}$ *and* $A[q_1],\ldots,A[q_s] \in Q_{i,j}$.

(i) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y \to \infty$, *then*

(a) *all* $N \times N$ *minors obtained by replacing one of the columns* $A[i],A[j],A[q_1],\ldots,A[q_s]$ *from either* $A(i,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *or* $A(j,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *with any column* $A[p] \in P_{i,j}$, *are zero*;

(b) *all* $N \times N$ *minors obtained by replacing one of the columns* $A[q_1],\ldots,A[q_s]$ *from either* $A(i,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *or* $A(j,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *with either* $A[i]$ *or* $A[j]$, *are zero.*

(ii) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y \to -\infty$, *then*

(a) *all* $N \times N$ *minors obtained by replacing one of the columns* $A[i],A[j],A[p_1],\ldots,A[p_r]$ *from either* $A(i,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *or* $A(j,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *with any column* $A[q] \in Q_{i,j}$, *are zero;*

(b) *all* $N \times N$ *minors obtained by replacing one of the columns* $A[p_1],\ldots,A[p_r]$ *from either* $A(i,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *or* $A(j,p_1,\ldots,p_r,q_1,\ldots,q_s)$ *with either* $A[i]$ *or* $A[j]$, *are zero.*

Proof: All of the above conditions follow from the repeated use of the dominant phase conditions in Lemma 3.1. For example, as $y \to \infty$ along the line $L_{i,j}$, Lemma 3.1 implies $\theta_p > \theta_m$ for all $p \in \{1,\ldots,i-1,j+1,\ldots,M\}$ and for all $m \in \{i,j,q_1,\ldots,q_s\}$. Consequently, if condition (b) in part (i) of the Lemma does not hold, each of the phase combinations obtained by replacing θ_m with θ_p in either $\theta_{i,p_1,\ldots,p_r,q_1,\ldots,q_s}$ or $\theta_{j,p_1,\ldots,p_r,q_1,\ldots,q_s}$ will be greater than both $\theta_{i,p_1,\ldots,p_r,q_1,\ldots,q_s}$ and $\theta_{j,p_1,\ldots,p_r,q_1,\ldots,q_s}$. But this contradicts the hypothesis that $\theta_{i,p_1,\ldots,p_r,q_1,\ldots,q_s}$ and $\theta_{j,p_1,\ldots,p_r,q_1,\ldots,q_s}$ are the dominant phase combinations as $y \to \infty$ along $L_{i,j}$. The other conditions follow in a similar fashion. □

We should emphasize that in general, the asymptotic solitons and the index pairs labeling them as $y \to \infty$ are different from those as $y \to -\infty$. Lemma 3.2 allows us to determine the ranks of the submatrices P_{ij} and Q_{ij} associated with each asymptotic line soliton $[i,j]$. This information

will be exploited later in Theorem 3.6 to identify explicitly the asymptotic line solitons produced by any given tau function. The next two results are direct consequences of the conditions specified in Lemma 3.2.

Lemma 3.3 (Span): Let $A[p_1],\dots,A[p_r]\in P_{i,j}$ *and* $A[q_1],\dots,A[q_s]\in Q_{i,j}$ *be the columns in the minors associated with the dominant pair of phase combinations of Lemma 3.2.*

(i) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y\to\infty$, *the columns* $A[p_1],\dots,A[p_r]$ *form a basis for the column space of the matrix* $P_{i,j}$.
(ii) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y\to-\infty$, *the columns* $A[q_1],\dots,A[q_s]$ *form a basis for the column space of the matrix* $Q_{i,j}$.

Proof: We prove part (i). Since $A(i,p_1,\dots,p_r,q_1,\dots,q_s)\neq 0$ by Lemma 3.2, the set of columns $\mathcal{A}=\{A[i],A[p_1],\dots,A[p_r],A[q_1],\dots,A[q_s]\}$ is a basis for $\mathbb{R}^N$. Hence the set $\{A[p_1],\dots,A[p_r]\}\subset\mathcal{A}$ is linearly independent. Moreover, any $A[p]\in P_{i,j}$ can be expanded with respect to the basis $\mathcal{A}$ as

$$A[p]=aA[i]+\sum_{m=1}^{r}b_mA[p_m]+\sum_{m=1}^{s}c_mA[q_m]. \tag{3.3}$$

Replacing one of the columns $A[i],A[q_1],\dots,A[q_s]$ in $A(i,p_1,\dots,p_r,q_1,\dots,q_s)$ with $A[p]\in P_{ij}$, we have from Lemma 3.2(i)(a) that

$$A(p,p_1,\dots,p_r,q_1,\dots,q_s)=0,\quad A(i,p_1,\dots,p_r,q_1,\dots q_{m-1},p,q_{m+1},\dots q_s)=0.$$

Hence in Eq. (3.3) we have $a=0$ and $c_m=0\,\forall\, m=1,\dots,s$. Therefore $A[p]\in\operatorname{span}(\{A[p_1,\dots,A[p_r]\})$ for all $A[p]\in P_{i,j}$. Similarly, part (ii) follows from the conditions in Lemma 3.2(ii)(a). □

Lemma 3.4 (Rank conditions): Let r *be the number of columns from* $P_{i,j}$ *and let* s *be the number of columns from* $Q_{i,j}$ *in the minors associated with the dominant pair of phase combinations of Lemma 3.2.*

(i) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y\to\infty$, *then* $\operatorname{rank}(P_{i,j})=r\leqslant N-1$ *and* $\operatorname{rank}(P_{i,j}|A[i])=\operatorname{rank}(P_{i,j}|A[j])=\operatorname{rank}(P_{i,j}|A[i,j])=r+1$.
(ii) *If* $[i,j]$ *identifies an asymptotic line soliton as* $y\to-\infty$, *then* $\operatorname{rank}(Q_{i,j})=s\leqslant N-1$ *and* $\operatorname{rank}(Q_{i,j}|A[i])=\operatorname{rank}(Q_{i,j}|A[j])=\operatorname{rank}(Q_{i,j}|A[i,j])=s+1$.

Above and hereafter, $(A|B)$ *denotes the matrix* A *augmented by the matrix* B.

Proof: Let us prove part (i). Since the columns $A[p_1],\dots,A[p_r]$ form a basis for the column space of $P_{i,j}$, from Lemma 3.3(i) we immediately have $\operatorname{rank}(P_{i,j})=r$. Moreover, since $\mathcal{A}=\{A[i],A[p_1],\dots,A[p_r],A[q_1],\dots,A[q_s]\}$ is a basis for $\mathbb{R}^N$, the vectors $A[i],A[p_1],\dots,A[p_r]$ are linearly independent, and therefore $\operatorname{rank}(P_{i,j}|A[i])=r+1$. Similarly, replacing $A[i]$ with $A[j]$ in the previous statement we have $\operatorname{rank}(P_{i,j}|A[j])=r+1$. It remains to prove that $\operatorname{rank}(P_{i,j}|A[i,j])=r+1$. Expanding the jth column of A in terms of $\mathcal{A}$ as in Lemma 3.3 we have

$$A[j]=aA[i]+\sum_{m=1}^{r}b_mA[p_m]+\sum_{m=1}^{s}c_mA[q_m]. \tag{3.4}$$

By replacing one of the columns $A[q_1],\dots,A[q_s]$ in $A(i,p_1,\dots,p_r,q_1,\dots,q_s)$ with $A[j]$, we have from Lemma 3.2(i)(b) that $A(i,p_1,\dots,p_r,q_1,\dots,q_{m-1},j,q_{m+1},\dots,q_s)=0$. Therefore $c_m=0$ for all $m=1,\dots,s$. Consequently we have $A[j]\in\operatorname{span}(\{A[i],A[p_1],\dots,A[p_r]\})$, which implies that $\operatorname{rank}(P_{i,j}|A[i,j])=r+1$. Similarly, using Lemma 3.2(ii)(b) one can establish the corresponding results in part (ii) for the asymptotic line solitons as $y\to-\infty$. □

It is important to note that, even though Lemmas 3.3–3.4 were proved by using the vanishing minor conditions in Lemma 3.2, they provide additional information on the structure of the coefficient matrix A. For example, when $r<N-1$ for an asymptotic line soliton as $y\to\infty$, Lemma

3.4 yields $\text{rank}(P_{i,j}|A[i,j]) < N$, and when $s < N-1$ for an asymptotic line soliton as $y \to -\infty$, Lemma 3.4 yields $\text{rank}(Q_{i,j}|A[i,j]) < N$. As a consequence, we immediately have the following additional vanishing minor conditions:

(i) If $[i,j]$ identifies an asymptotic line soliton as $y \to \infty$, then

$$A(i,j,p_1,\ldots,p_r,m_1,\ldots,m_{N-r-2}) = 0 \quad \forall \{m_1,\ldots,m_{N-r-2}\} \subset \{1,\ldots,M\}. \tag{3.5a}$$

(ii) If $[i,j]$ identifies an asymptotic line soliton as $y \to -\infty$, then

$$A(i,j,q_1,\ldots,q_s,m_1,\ldots,m_{N-s-2}) = 0 \quad \forall \{m_1,\ldots,m_{N-s-2}\} \subset \{1,\ldots,M\}. \tag{3.5b}$$

We remark that conditions (3.5) were also introduced (without proof) in Ref. 12 (cf. Definition 4.2) in order to characterize the tau functions of the elastic N-soliton solutions which correspond to the special case $M=2N$. It should also be noted that, when $[i,j]$ identifies an asymptotic line soliton as $y \to \infty$, Lemma 3.4(i) only provides information on $P_{i,j}$, and the only condition on $Q_{i,j}$ is that $\text{rank}(Q_{i,j}) \geqslant s$. Similarly, when $[i,j]$ identifies an asymptotic line soliton as $y \to -\infty$, all is known about $P_{i,j}$ is that $\text{rank}(P_{i,j}) \geqslant r$.

B. Characterization of the asymptotic line solitons from the coefficient matrix

In the preceding section we derived several conditions that an index pair $[i,j]$ must satisfy in order to identify an asymptotic line soliton. Those results are now applied to obtain a complete characterization of the incoming and outgoing asymptotic line solitons of a generic line-soliton solution of the KPII equation.

Lemma 3.5 (Pivots and nonpivots): Consider an index pair $[i,j]$ with $1 \leqslant i < j \leqslant M$.

(i) *If $[i,j]$ identifies an asymptotic line soliton as $y \to \infty$, the index i labels a pivot column of the coefficient matrix A. That is, $A[i]=A[e_n]$ with $1 \leqslant n \leqslant N$.*

(ii) *If $[i,j]$ identifies an asymptotic line soliton as $y \to -\infty$, the index j labels a nonpivot column of the coefficient matrix A. That is, $A[j]=A[g_n]$ with $1 \leqslant n \leqslant M-N$.*

Proof: We first prove part (i). Suppose that $\theta_{i,m_2,\ldots,m_N}$ is one of the dominant phase combinations corresponding to the asymptotic line soliton $[i,j]$ as $y \to \infty$. The corresponding minor $A(i,m_2,\ldots,m_N)$ is nonzero. Since A is in RREF, we have $A[i]=\sum_{r=1}^{n} c_r A[e_r]$ for some $n \leqslant N$, where $e_1 < \cdots < e_n \leqslant i$. Therefore $A(i,m_2,\ldots,m_N)=\sum_{r=1}^{n} c_r A(e_r,m_2,\ldots,m_N)$. If $e_n < i$, we have $A[e_1],\ldots,A[e_n] \in P_{i,j}$, where $P_{i,j}$ is the submatrix of A defined in Eq. (3.2). Then from condition (a) in Lemma 3.2(i) we have $A(e_r,m_2,\ldots,m_N)=0 \; \forall r=1,\ldots,n$, implying that $A(i,m_2,\ldots,m_N)=0$. But this is impossible, since $\theta_{i,m_2,\ldots,m_N}$ is a dominant phase combination. Therefore we must have $i=e_n$, meaning that $A[i]$ is a pivot column.

Part (ii) follows from the rank conditions in Lemma 3.4(ii). In particular, $\text{rank}(Q_{i,j}|A[i]) = \text{rank}(Q_{i,j}|A[i,j]) = s+1$ implies that $A[j] \in \text{span}(\{A[i],\ldots,A[j-1]\})$. Since A is in RREF, none of its pivot column can be spanned by the preceding columns. Hence $A[j]$ is not a pivot column. □

Lemma 3.5 identifies outgoing and incoming asymptotic line solitons, respectively, with the pivot and the nonpivot columns of A. It is then natural to ask if in fact each of the N pivot columns and each of the $M-N$ nonpivot columns identifies an outgoing or incoming line soliton, and whether such identification is unique. Both of these questions can be answered affirmatively by the following theorem which constitutes one of the main results of this work, and is proved in the Appendix.

Theorem 3.6: *(Asymptotic line solitons) Let $\tau_{N,M}(x,y,t)$ be the tau function in Eq. (2.1) associated with a rank N, irreducible coefficient matrix A with non-negative minors.*

(i) *For each pivot index e_n there exists a unique asymptotic line soliton as $y \to \infty$, identified by an index pair $[e_n,j_n]$ with $n=1,\ldots,N$ and $1 \leqslant e_n < j_n \leqslant M$.*

(ii) *For each nonpivot index g_n there exists a unique asymptotic line soliton as $y \to -\infty$, identified by an index pair $[i_n,g_n]$ with $n=1,\ldots,M-N$ and $1 \leqslant i_n < g_n \leqslant M$.*

Thus, the solution of KPII generated by the coefficient matrix A via Eq. (2.1) *has exactly* $N_+=N$ *asymptotic line solitons as* $y\to\infty$ *and* $N_-=M-N$ *asymptotic line solitons as* $y\to-\infty$.

Part (i) of Theorem 3.6 uniquely identifies the asymptotic line solitons as $y\to\infty$ by the index pairs $[e_n,j_n]$ where $e_n<j_n$. The indices $e_1,\dots,e_N$ label the N pivot columns of A, however, the j_n's may correspond to either pivot or nonpivot columns, and indeed both cases appear in examples. Moreover, when the pivot indices are sorted in increasing order $1=e_1<e_2<\cdots<e_N<M$, the indices $j_1,\dots,j_N$ in general *are not sorted* in any specific order. For example, the line solitons as $y\to\infty$ generated by the matrix A in Eq. (4.5) of Sec. IV have $j_1<j_3<j_2$. In fact, the indices $j_1,\dots,j_N$ need not necessarily even be distinct. Similarly, part (ii) of Theorem 3.6 uniquely identifies the asymptotic line solitons as $y\to-\infty$ by index pairs $[i_n,g_n]$, where $i_n<g_n$. In this case, the indices $g_1,\dots,g_{M-N}$ label the $M-N$ nonpivot columns of A, but the i_n's may correspond to either pivot or nonpivot columns. Moreover, when the nonpivot indices are sorted in increasing order $1<g_1<\cdots<g_{M-N}=M$, the indices $i_1,\dots,i_{M-N}$ are not in general sorted, and need not be distinct. Theorem 3.6 yields an important characterization of the solution via the associated coefficient matrix A, and it provides a concrete method to identify the asymptotic line solitons as $y\to\pm\infty$, as illustrated with the examples below. Further examples are discussed in Sec. IV.

Example 3.7: Consider the tau function $\tau_{N,M}$ with $N=2$ and $M=5$ generated by the coefficient matrix

$$A=\begin{pmatrix}1&1&0&-1&-2\\0&0&1&1&1\end{pmatrix}. \tag{3.6}$$

The pivot columns of A are labeled by the indices $\{e_1,e_2\}=\{1,3\}$, and the nonpivot columns by the indices $\{g_1,g_2,g_3\}=\{2,4,5\}$. It follows from Theorem 3.6 that there will be $N_+=N=2$ asymptotic line solitons as $y\to\infty$, identified by the index pairs $[1,j_1]$ and $[3,j_2]$ for some $j_1>1$ and $j_2>3$, and that there will be $N_-=M-N=3$ asymptotic line solitons as $y\to-\infty$, identified by the index pairs $[i_1,2]$, $[i_2,4]$, and $[i_3,5]$, for some $i_1<2$, $i_2<4$, and $i_3<5$. We first determine the asymptotic line solitons as $y\to\infty$ using part (i) of Theorem 3.6 together with the rank conditions in Lemma 3.4(i). The we find the asymptotic line solitons as $y\to-\infty$ using part (ii) of Theorem 3.6 and the rank conditions in Lemma 3.4(ii).

For the first pivot column, $e_1=1$, we start with $j=2$ and consider the submatrix $P_{1,2}=\left(\begin{smallmatrix}0&-1&-2\\1&1&1\end{smallmatrix}\right)$. Since $\operatorname{rank}(P_{1,2})=2>1=N-1$, from Lemma 3.4(i) we conclude that the pair [1,2] cannot identify an asymptotic line soliton as $y\to\infty$. Incrementing j to $j=3,4,5$ and checking the rank of each submatrix $P_{1,j}$ we find that the rank conditions in Lemma 3.4(i) are satisfied when $j=4$, and $P_{1,4}=\left(\begin{smallmatrix}-2\\1\end{smallmatrix}\right)=A[5]$. So, $\operatorname{rank}(P_{1,4})=1$ and $\operatorname{rank}(P_{1,4}|A[1])=\operatorname{rank}(P_{1,4}|A[4])=2$. The condition $\operatorname{rank}(P_{1,4}|A[1,4])=2$ is trivial here, since any three columns are linearly dependent. Thus, the first asymptotic line soliton as $y\to\infty$ is identified by the index pair [1,4]. For the second pivot, $e_2=3$, proceeding in a similar manner we find that $j=4$ does not satisfy the rank conditions because $P_{3,4}$ has rank 2. But $j=5$ satisfies Lemma 3.4(i), since $P_{3,5}=\left(\begin{smallmatrix}1&1\\0&0\end{smallmatrix}\right)$, which yields $\operatorname{rank}(P_{3,5})=1$ and $\operatorname{rank}(P_{3,5}|A[3])=\operatorname{rank}(P_{3,5}|A[5])=2$. Again, $\operatorname{rank}(P_{3,5}|A[3,5])=2$ is trivially satisfied here. So the asymptotic line solitons as $y\to\infty$ are given by the index pairs [1,4] and [3,5], and the associated phase transition diagram (cf. Corollary 2.6) is given by

$$R_{1,3}\xrightarrow{3\to5}R_{1,5}\xrightarrow{1\to4}R_{4,5}.$$

We now consider the asymptotics for $y\to-\infty$. Starting with the nonpivot column $g_1=2$, the only column to its left is $i=1$. We have $Q_{1,2}=\emptyset$, and $\operatorname{rank}(Q_{1,2}|A[1])=\operatorname{rank}(Q_{1,2}|A[2])=\operatorname{rank}(Q_{1,2}|A[1,2])=1$. Consequently, the pair [1,2] identifies an asymptotic line soliton as $y\to-\infty$. For $g_2=4$ we consider $i=1,2,3$ and find that the rank conditions in Lemma 3.4(ii) are satisfied only for $i=2$. In this case, $Q_{2,4}=\left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)=A[3]$, so $\operatorname{rank}(Q_{2,4})=1=N-1$ and $\operatorname{rank}(Q_{2,4}|A[2])=\operatorname{rank}(Q_{2,4}|A[4])=2$, while $\operatorname{rank}(Q_{2,4}|A[2,4])=2$ is trivially satisfied. Hence [2,4] is the unique

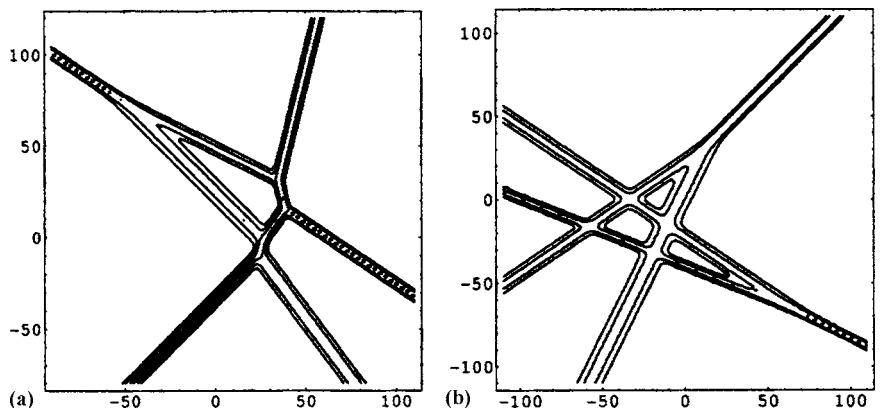

FIG. 3. Line soliton solutions of KPII: (a) the (3,2)-soliton solution generated by the coefficient matrix A in Example 3.7 with $(k_1,\ldots,k_5)=(-1,0,\frac{1}{4},\frac{3}{4},\frac{5}{4})$ at $t=-32$; (b) the inelastic 3-soliton solution generated by the coefficient matrix A in Example 3.8 with $(k_1,\ldots,k_6)=(-1,-\frac{1}{2},0,\frac{1}{2},1,\frac{3}{2})$ at $t=20$ (see text for details).

asymptotic line soliton as $y\to-\infty$ associated to the nonpivot column $g_2=4$. In a similar way we can uniquely identify the last asymptotic line soliton as $y\to-\infty$ as given by the indices [3,5]. The phase transition diagram for $y\to-\infty$ is thus given by

$$R_{1,3}\xrightarrow{1\to2}R_{2,3}\xrightarrow{2\to4}R_{3,4}\xrightarrow{3\to5}R_{4,5}.$$

To summarize, there are $N_+=2$ outgoing line solitons, each associated with one of the pivot columns $e_1=1$ and $e_2=3$, given by the index pairs [1,4] and [3,5], and there are $N_-=3$ incoming line solitons, each associated with one of the nonpivot columns $g_1=2$, $g_2=4$, and $g_3=5$, given by the index pairs [1,2], [2,4], and [3,5]. A snapshot of the solution at $t=-32$ is shown in Fig. 3(a).

Example 3.8: Consider the tau function with $N=3$ and $M=6$ generated by the coefficient matrix in RREF,

$$A=\begin{pmatrix}1&1&1&0&0&0\\0&0&0&1&0&-1\\0&0&0&0&1&2\end{pmatrix}. \tag{3.7}$$

Again, we first determine the asymptotic line solitons as $y\to\infty$, and then the asymptotic line solitons as $y\to-\infty$.

The pivot columns of A are labeled by the indices $e_1=1$, $e_2=4$, and $e_3=5$. Thus, we know that the asymptotic line solitons as $y\to\infty$ will be given by the index pairs $[1,j_1]$, $[4,j_2]$, and $[5,j_3]$ for some $j_1>1$, $j_2>4$, and $j_3>5$. Starting with the first pivot, $e_1=1$, we take $j=2,3,\ldots$ and check the rank of the submatrix $P_{i,j}$ in each case. When $j=2$ we have $P_{1,2}=\begin{pmatrix}1&0&0&0\\0&1&0&-1\\0&0&1&2\end{pmatrix}$, and $\mathrm{rank}(P_{1,2})=3>N-1$. So, by Lemma 3.4(i), the index pair [1,2] does not correspond to an asymptotic line soliton as $y\to\infty$. In fact, using Lemma 3.1 it can be verified that $\theta_{3,5,6}$ is the only dominant phase combination along the line $\theta_1=\theta_2$ as $y\to\infty$. Next, we consider $j=3$. In this case we have $P_{1,3}=\begin{pmatrix}0&0&0\\1&0&-1\\0&1&2\end{pmatrix}$, with $\mathrm{rank}(P_{1,3})=2=:r$ and $\mathrm{rank}(P_{1,3}|A[1])=\mathrm{rank}(P_{1,3}|A[3])=\mathrm{rank}(P_{1,3}|A[1,3])=3=r+1$. So the rank conditions in Lemma 3.4(i) are satisfied. Therefore the index pair [1,3] corresponds to an asymptotic line soliton as $y\to\infty$. Moreover, by considering $j=4,5,6$ one can easily check that the rank conditions are no longer satisfied. Thus [1,3] is the *unique* asymptotic line soliton associated with the pivot index $e_1=1$ as $y\to\infty$, in agreement with Theorem 3.6. Let us now

consider the second pivot column, $e_2=4$. In this case we find that the rank conditions are only satisfied when $j=5$, since $P_{4,5}=\begin{pmatrix}1&1&1&0\\0&0&0&-1\\0&0&0&2\end{pmatrix}$, with $\mathrm{rank}(P_{4,5})=2=:r$ and $\mathrm{rank}(P_{4,5}|A[4])=\mathrm{rank}(P_{4,5}|A[5])=\mathrm{rank}(P_{4,5}|A[4,5])=3=r+1$. Therefore, the index pair [4,5] corresponds to an asymptotic line soliton as $y\to\infty$. Finally, for $e_3=5$, since we know from Theorem 3.6 that $j>e_3$, we immediately find that the third asymptotic line soliton as $y\to\infty$ is given by the index pair [5,6]. From Corollary 2.6, the phase transition diagram as $y\to\infty$ is given by

$$R_{1,4,5}\xrightarrow{5\to6}R_{1,4,6}\xrightarrow{4\to5}R_{1,5,6}\xrightarrow{1\to3}R_{3,5,6}.$$

The nonpivot columns of the coefficient matrix A are labeled by the indices $g_1=2$, $g_2=3$, and $g_3=6$. For $g_1=2$, the only possible value of $i<j$ is $i=1$. In this case $Q_{1,2}=\emptyset$, so $\mathrm{rank}(Q_{1,2})=0$ and $\mathrm{rank}(Q_{1,2}|A[1])=\mathrm{rank}(Q_{1,2}|A[2])=\mathrm{rank}(Q_{1,2}|A[1,2])=1$. Thus the pair [1,2] identifies an asymptotic line soliton as $y\to-\infty$. For $g_2=3$ we consider $i=2,1$. When $i=2$, the rank conditions in Lemma 3.4(ii) are satisfied, leading to the asymptotic line soliton [2,3] as $y\to-\infty$. We can check that the soliton associated with the nonpivot column $g_2=3$ is unique by considering $i=1$ and verifying that the rank conditions are not satisfied. Similarly, it is easy to verify that for $g_3=6$ the index pair [4,6] uniquely identifies the asymptotic line soliton as $y\to-\infty$. The phase transition diagram as $y\to-\infty$ reads as follows:

$$R_{1,4,5}\xrightarrow{1\to2}R_{2,4,5}\xrightarrow{2\to3}R_{3,4,5}\xrightarrow{4\to6}R_{3,5,6}.$$

Summarizing, there are $N_+=3$ asymptotic line solitons as $y\to\infty$ identified by the index pairs [1,3], [4,5], and [5,6], and there are $N_-=3$ asymptotic line solitons as $y\to-\infty$ identified by the index pairs [1,2], [2,3], and [4,6]. A snapshot of the solution at $t=-20$ is shown in Fig. 3(b).

Examples 3.7 and 3.8 illustrate the fact that, starting from any given coefficient matrix A in RREF, the asymptotic line solitons as $y\to\pm\infty$ can be identified in an algorithmic way by applying Theorem 3.6 together with the rank conditions in Lemma 3.4.

IV. FURTHER EXAMPLES

In this section we present a variety of line-soliton solutions of KPII generated by the tau function (2.2) with different choices of coefficient matrices.

Ordinary N-soliton solutions: These are constructed by taking $M=2N$ and choosing the functions $\{f_n\}_{n=1}^N$ in Eq. (1.10) as (e.g., see Refs. 5 and 15)

$$f_n(x,y,t)=e^{\theta_{2n-1}}+e^{\theta_{2n}},\quad n=1,\dots,N. \tag{4.1}$$

The corresponding coefficient matrix is thus given by

$$A=\begin{pmatrix}1&1&0&0&\cdots&0&0\\0&0&1&1&\cdots&0&0\\\vdots&\vdots&\vdots&\vdots&\vdots&\vdots&\vdots\\0&0&0&0&\cdots&1&1\end{pmatrix},$$

with N pairs of identical columns at positions $\{2n-1,2n\}$, $n=1,\dots,N$. There are only 2^N nonzero minors of A, which are given by $A(m_1,m_2,\dots,m_N)=1$ where, for each $n=1,\dots,N$, either $m_n=2n-1$ or $m_n=2n$. The asymptotic analysis of the preceding section implies that the nth asymptotic line soliton as $y\to\pm\infty$ is identified by the index pair $[2n-1,2n]$ for $n=1,\dots,N$, where $i_n=2n-1$ and $j_n=2n$ label, respectively, the pivot and nonpivot columns of A. Therefore the amplitude and direction are given by $a_n=k_{2n}-k_{2n-1}$ and $c_n=k_{2n-1}+k_{2n}$. Moreover, the dominant pair of phase combinations for the nth soliton as $y\to\infty$ is given by $\theta_{1,3,\dots,2n-1,2n+2,2n+4,\dots,2N}$ and $\theta_{1,3,\dots,2n-3,2n,2n+2,\dots,2N}$, while the dominant phase combinations for the same soliton as $y\to-\infty$ by

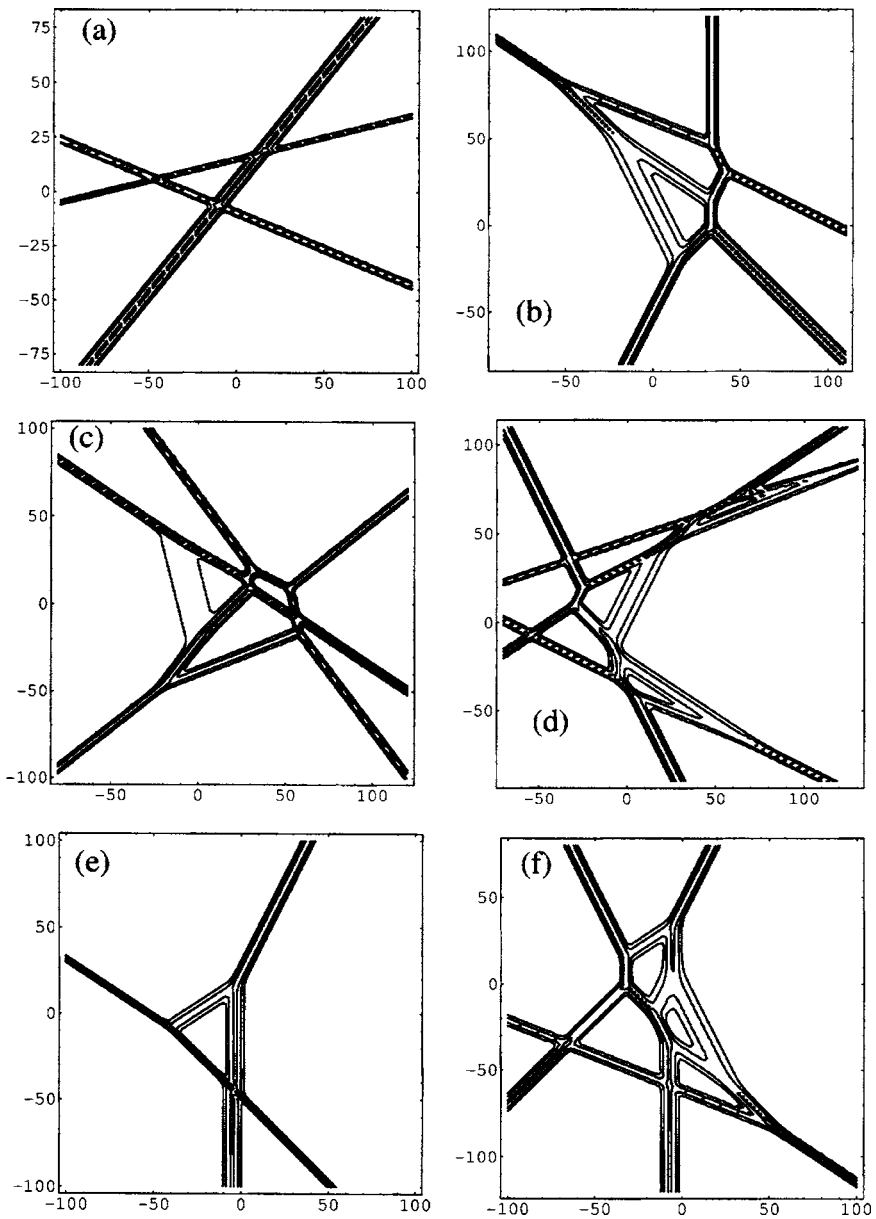

FIG. 4. Line-soliton solutions of KPII: (a) an ordinary 3-soliton solution with $(k_1,\ldots,k_6)=(-3,-2,0,1,\frac{3}{2},2)$ at $t=4$; (b) a fully resonant (3,2)-soliton solution with $(k_1,\ldots,k_5)=(-1,0,\frac{1}{2},1,\frac{3}{2})$ at $t=-32$; (c) an elastic, partially resonant 3-soliton solution with A given by Eq. (4.5) and $(k_1,\ldots,k_6)=(-\frac{3}{2},-1,0,\frac{1}{4},\frac{3}{2},\frac{7}{4})$ at $t=-20$; (d) an elastic, partially resonant 4-soliton solution with A given by Eq. (4.6) and $(k_1,\ldots,k_8)=(-2,-\frac{3}{2},-1,-\frac{1}{2},0,\frac{1}{2},1,\frac{3}{2})$ at $t=20$; (e) an inelastic 2-soliton solution with A given by Eq. (4.7) and $(k_1,\ldots,k_4)=(-1,-\frac{1}{2},\frac{1}{2},2)$ at $t=16$; (f) an inelastic 3-soliton solution with A given by Eq. (4.8) and $(k_1,\ldots,k_6)=(-1,-\frac{1}{2},0,\frac{1}{2},1,\frac{3}{2})$ at $t=32$.

$\theta_{2,4,\ldots,2n,2n+1,2n+3,\ldots,2N-1}$ and $\theta_{2,4,\ldots,2n-2,2n-1,2n+1,\ldots,2N-1}$. Apart from the phase shift of each line soliton, the interaction gives rise to a pattern of N intersecting lines in the xy plane, as shown in Fig. 4(a).

Solutions of KPII which also satisfy the finite Toda lattice hierarchy: Another class of (N_-,N_+)-soliton solutions of KPII is given by the following choice of functions $\{f_n\}_{n=1}^N$ in Eq. (1.10):

$$f_n = f^{(n-1)}, \quad n = 1, \ldots, N. \tag{4.2}$$

In addition to generating solutions of KPII, the set of tau functions $\tau_{N,M}$ for $N=1,\ldots,M$ also satisfy the Plücker relations for the finite Toda lattice hierarchy.[2] Choosing $f(x,y,t)=\sum_{m=1}^{M} e^{\theta_m}$ yields the following coefficient matrix:

$$A = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ k_1 & k_2 & \cdots & k_M \\ \vdots & \vdots & \ddots & \vdots \\ k_1^{N-1} & k_2^{N-1} & \cdots & k_M^{N-1} \end{pmatrix}. \tag{4.3}$$

Note that A in Eq. (4.3) is not in RREF, and coincides with the matrix K in Lemma 2.1. The pivot columns of A are labeled by indices $1,\ldots,N$. Furthermore, all the $N\times N$ minors of A are nonzero, and coincide with the Van der Monde determinants in Eq. (2.4). The corresponding class of KPII solutions was studied in Ref. 2, where it was shown that the N asymptotic line solitons as $y\to\infty$ are identified by the index pairs $[n,n+M-N]$ for $n=1,\ldots,N$, while the $M-N$ asymptotic line solitons as $y\to-\infty$ are identified by the index pairs $[n,n+N]$ for $n=1,\ldots,M-N$. These pairings can also be easily verified using Theorem 3.6. The dominant pair of phase combinations for the nth soliton as $y\to\infty$ is given by $\theta_{1,\ldots,n,M-N+n+1,\ldots,M}$ and $\theta_{1,\ldots,n-1,M-N+n,\ldots,M}$, while the dominant pair of phase combinations for the nth soliton as $y\to-\infty$ by $\theta_{n,\ldots,N+n-1}$ and $\theta_{n+1,\ldots,N+n}$. The solution displays phenomena of soliton resonance and web structure [e.g., see Fig. 4(b)]. More precisely, the interaction of the asymptotic line solitons results in a pattern with $(2N_- -1)N_+$ interaction vertices, $(3N_- -2)N_+$ intermediate interaction segments and $(N_- -1)(N_+ -1)$ "holes" in the xy plane. Each of the intermediate interaction segments can be effectively regarded as a line soliton since it satisfies the dispersion relation (1.8). Furthermore, all of the asymptotic and intermediate line solitons interact via a collection of *fundamental resonances*. A fundamental resonance, also called a Y junction, describes an interaction of three line solitons whose wave numbers $\mathbf{k}_a$ and frequencies ω_a $(a=1,2,3)$ satisfy the three-wave resonance conditions[17,19]

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3, \quad \omega_1 + \omega_2 = \omega_3. \tag{4.4}$$

Such a solution is shown in Fig. 1(a).

Elastic N-soliton solutions: As mentioned in Sec. I and in the Appendix, the elastic N-soliton solutions are those for which the sets of incoming and outgoing asymptotic line solitons are the same. In this case we necessarily have $M=2N$. Ordinary N-soliton solutions and solutions of KPII which also satisfy the finite Toda lattice hierarchy with $M=2N$ are two special classes of elastic N-soliton solutions. However, a large variety of other elastic N-soliton solutions do also exist, and were recently investigated in Ref. 12. For example, Fig. 4(c) shows an elastic 3-soliton solution generated by the coefficient matrix,

$$A = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & -2 & -2 & -1 \\ 0 & 0 & 1 & 2 & 1 & 0 \end{pmatrix}. \tag{4.5}$$

In this case the pivot columns are labeled by indices 1, 2, and 3. So, from Lemma 3.5 we know that the asymptotic line solitons as $y\to\infty$ will be identified by index pairs $[1,j_1]$, $[2,j_2]$, and $[3,j_3]$, while those as $y\to-\infty$ by index pairs $[i_1,4]$, $[i_2,5]$, and $[i_3,6]$, for certain values of $i_1,\ldots,i_3$ and $j_1,\ldots,j_3$. Indeed, from the results developed in Sec. III one can verify that both the incoming and the outgoing asymptotic line solitons are given by the *same* index pairs [1,4], [2,6], and [3,5]. The soliton interactions in this case are *partially resonant*, in the sense that the pairwise interaction among solitons [1,4] and [2,6] and that among solitons [1,4] and [3,5] are both resonant, but the pairwise interaction among solitons [2,6] and [3,5] is nonresonant. Similarly, Fig. 4(d) shows an elastic, partially resonant 4-soliton solution generated by the coefficient matrix

$$A = \begin{pmatrix} 1 & 0 & -1 & 0 & 1 & 0 & -1 & -2 \\ 0 & 1 & 2 & 0 & -1 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 & 2 & 0 & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \end{pmatrix}. \tag{4.6}$$

In this case the pivot columns are labeled by the indices 1, 2, 4, and 6 and the nonpivot columns by the indices 3, 5, 7, and 8. The asymptotic line solitons as $y \to \pm\infty$ are identified by the index pairs [1,3], [2,5], [4,7], and [6,8]. As can be seen from Fig. 4(f), the pairwise interaction of solitons [1,3] and [2,5], solitons [2,5] and [4,7], and [4,7] and [6,8] are resonant, but the remaining pairwise interactions between solitons [1,3] and [4,7], [1,3] and [6,8], [2,5] and [6,8], are nonresonant. It should be clear from these examples that a large variety of elastic N-soliton solutions with resonant, partially resonant and nonresonant interactions is possible.

Inelastic N-soliton solutions: There also exist a large class of N-soliton solutions that are not elastic. We have already seen such solutions in Examples 3.7 and 3.8 [cf. Figs. 3(a) and 3(b)] of Sec. III. As a further example, Fig. 4(e) shows an inelastic 2-soliton solution generated by the coefficient matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 1 \end{pmatrix}. \tag{4.7}$$

In this case the pivot columns are labeled by indices 1 and 2. The asymptotic line solitons as $y \to -\infty$ are identified by the index pairs [1,4] and [2,3], while those as $y \to \infty$ by the index pairs [1,3] and [2,4]. Notice that the outgoing solitons interact resonantly via two Y junctions, while the incoming soliton pair interact nonresonantly. This is in contrast with an elastic 2-soliton solution, where both incoming and outgoing pairs of solitons exhibit the same kind of interaction. Similarly, Fig. 4(f) shows inelastic 3-soliton solution generated by the coefficient matrix

$$A = \begin{pmatrix} 1 & 0 & -1 & -1 & 0 & 2 \\ 0 & 1 & 2 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}. \tag{4.8}$$

Here the pivot columns are labeled by indices 1, 2, and 5. The asymptotic line solitons as $y \to \infty$ are identified by the index pairs [1,3], [2,5], and [5,6], while those as $y \to -\infty$ by the index pairs [1,3], [2,4], and [3,6].

Finally, we remark that in the generic case $M \neq 2N$, the numbers of asymptotic line solitons as $y \to \pm\infty$ are different, as in the solutions shown in Figs. 3(a) and 4(b). Also, note that the one-soliton solutions, the ordinary two-soliton solutions and the Y junction solutions have the property that their time evolution is just an overall translation of a fixed spatial pattern. However, for all other solutions discussed above, the interaction patterns formed by the asymptotic line solitons, and the relative positions of the interaction vertices in the xy plane are in general time dependent.

V. CONCLUSIONS

In this paper we have studied a class of line-soliton solutions of the Kadomtsev-Petviashvili II equation by expressing the tau function as the Wronskian of N linearly independent combinations of M exponentials. From the asymptotics of the tau function as $y \to \pm\infty$ we showed that each of these solutions of KPII is composed of asymptotic line solitons which are defined by the transition between two dominant phase combinations with $N-1$ common phases. Moreover, the number, amplitudes and directions of the asymptotic line solitons are invariant in time. We also derived an algorithmic method to identify these asymptotic line solitons in a given solution by examining the $N \times M$ coefficient matrix A associated with the corresponding tau function. In particular, we proved that every $N \times M$, irreducible coefficient matrix A produces an (N_-, N_+)-soliton solution of KPII in which there are $N_+ = N$ asymptotic line solitons as $y \to \infty$, labeled by the pivot columns of A, and $N_- = M - N$ asymptotic line solitons as $y \to -\infty$, labeled by the nonpivot columns of A. Such

solutions exhibit a rich variety of time-dependent spatial patterns which include resonant soliton interactions and web structure. Finally, we discussed a number of examples of such (N_-,N_+)-soliton solutions in order to illustrate the above results.

It is remarkable that the KPII equation possesses such a rich structure of line-soliton solutions generated by a simple form of the tau function. In this work we have primarily focused on the asymptotic behavior of the solutions as $y\to\pm\infty$, but not on their interactions in the xy plane. A full characterization of the interaction patterns of the general (N_-,N_+)-soliton solutions is an important open problem, which is left for further study. Nonetheless, we believe that our results will provide a key step toward that endeavor. We point out that resonant interaction described by the line solitons of KPII is a physical phenomenon that has been observed experimentally in ion-acoustic waves (see e.g., Refs. 20 and 13). Hence, we expect that the resonant solutions considered in this work are likely to be stable with respect to small perturbations and physically relevant. However, a formal stability analysis of these $(2+1)$-dimensional solutions is a highly nontrivial task, and has not yet been carried out to the best of our knowledge. Finally, we note that soliton solutions exhibiting phenomena of soliton resonance and web structure have been found for several other $(2+1)$-dimensional integrable systems, and those solutions can also be described by direct algebraic methods similar to the ones used here. Therefore we expect that the results presented in this work will also be useful to study solitonic solutions in a variety of other $(2+1)$-dimensional integrable systems.

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APPENDIX A: PROOF OF THEOREM 2.5

To prove part (i) of Theorem 2.5, it is sufficient to show that, along each line L_c, the sign of the inequalities among the phase combinations in Definition 2.3 remain unchanged in time as $y\to\pm\infty$. For this purpose, note that the sign of $\theta_{m_1,\ldots,m_N}-\theta_{m_1',\ldots,m_N'}$ in Eq. (2.6b) is determined by the coefficient of y on the right-hand side as $y\to\pm\infty$ and for finite ξ and t, if this coefficient is nonzero. For generic values of the phase parameters $k_1,\ldots,k_M$ this coefficient is indeed nonvanishing, and its sign depends only on the direction c of the line L_c. Consequently, the dominant phase combinations asymptotically as $y\to\pm\infty$ are determined only by the constant c for finite time.

Part (ii) of the theorem is proved by showing that the only possible phase transitions are those in which a single phase, say θ_m changes to $\theta_{m'}$ between the two dominant phase combinations across adjacent regions, and that no other type of transitions can occur. We first prove that single-phase transitions are allowed; then we show that no other type of transitions are allowed. In the following, we will assume t to be finite so that the dominant phase combinations remain invariant, according to part (i). Suppose that $\theta_{m_1,\ldots,m_N}$ is the dominant phase combination in a region R asymptotically for large values of $|y|$. Since R is a proper subset of $\mathbb{R}^3$, it *must* have a boundary, across which a transition will take place from $\theta_{m_1,\ldots,m_N}$ to some other dominant phase combination. Since $\theta_{m_1,\ldots,m_N}$ is dominant, $A(m_1,\ldots,m_N)\neq 0$ according to Definition 2.3. Therefore, the columns $A[m_1],\ldots,A[m_N]$ of the coefficient matrix form a basis of $\mathbb{R}^N$, and for all $j\notin\{m_1,\ldots,m_N\}$ we have that $A[j]$ is in the span of $A[m_1],\ldots,A[m_N]$. Thus there exists at least one column $A[m_s]$ such that the coefficient of $A[m_s]$ in the expansion of $A[j]$ is nonzero. We then have $A(m_1,\ldots,m_{s-1},j,m_{s+1},\ldots,m_N)\neq 0$, implying that the phase combination $\theta_{m_1,\ldots,m_{s-1},j,m_{s+1},\ldots,m_N}$ is actually present in the tau function. Then, for *any* $j\notin\{m_1,\ldots,m_N\}$ it is possible to have a single-phase transition from R to the adjacent region R' across the line $\theta_{m_s}=\theta_j$, since the sign of $\theta_{m_s}-\theta_j$ changes across this line, implying that $\theta_{m_1,\ldots,m_{s-1},j,m_{s+1},\ldots,m_N}$ is larger than $\theta_{m_1,\ldots,m_N}$ in R'.

We next show that no *other* type of transitions can occur apart from single-phase transitions; we do so by *reduction ad absurdum*. Suppose that at least two phases $\theta_{m_1}, \theta_{m_2}$ from the dominant phase combination $\theta_{m_1,\ldots,m_N}$ in a region R are replaced with phases $\theta_{m_1'}, \theta_{m_2'}$ during the transition from R to an adjacent region R'. This transition occurs along the common boundary of R and R', which is given by line $L:(\theta_{m_1}+\theta_{m_2})-(\theta_{m_1'}+\theta_{m_2'})=0$. Thus, along L, the differences $\theta_{m_1}-\theta_{m_1'}$ and $\theta_{m_2}-\theta_{m_2'}$ (or, equivalently, the differences $\theta_{m_1}-\theta_{m_2'}$ and $\theta_{m_2}-\theta_{m_1'}$) must have opposite signs or be both zero.

If both differences are zero along L, the lines $\theta_{m_1}=\theta_{m_1'}$ and $\theta_{m_2}=\theta_{m_2'}$ (or, equivalently, the lines $\theta_{m_1}=\theta_{m_2'}$ and $\theta_{m_1'}=\theta_{m_2}$) must both coincide with the line L in the xy plane. This is possible only at a given instant of time *and* if the directions of the two lines are the same, i.e., if $k_{m_1}+k_{m_1'}=k_{m_2}+k_{m_2'}$ (or, equivalently, $k_{m_1}+k_{m_2'}=k_{m_1'}+k_{m_2}$). So for generic values of the phase parameters, or for generic values of time, this exceptional case can be excluded. Hence, we assume that $\theta_{m_1}-\theta_{m_1'}$ and $\theta_{m_2}-\theta_{m_2'}$ are of opposite signs.

Note that $\theta_{m_1}-\theta_{m_1'}=\theta_{m_1,\ldots,m_N}-\theta_{m_1',m_2,\ldots,m_N}$ and $\theta_{m_2}-\theta_{m_2'}=\theta_{m_1,\ldots,m_N}-\theta_{m_1,m_2',m_3\ldots,m_N}$. Moreover, since $\theta_{m_1,\ldots,m_N}$ is the dominant phase in R, both of these phase differences must be *positive* in the interior of R if the minors $A(m_1',m_2,\ldots,m_N)$ and $A(m_1,m_2',m_3\ldots,m_N)$ are nonzero. Hence, we must conclude that $\theta_{m_1}-\theta_{m_1'}$ and $\theta_{m_2}-\theta_{m_2'}$ cannot have opposite signs unless one or both of the phase combinations $\theta_{m_1',m_2,\ldots,m_N}$ and $\theta_{m_1,m_2',m_3,\ldots,m_N}$ is absent from the tau function. This requires that either $A(m_1',m_2,\ldots,m_N)$ or $A(m_1,m_2',m_3\ldots,m_N)$ must be zero. A similar argument applied to the phase differences $\theta_{m_1}-\theta_{m_2'}$ and $\theta_{m_2}-\theta_{m_1'}$ leads to the conclusion that one or both of the minors $A(m_2',m_2,\ldots,m_N)$ and $A(m_1,m_1',m_3\ldots,m_N)$ must vanish. However, from the Plücker relations among the $N\times N$ minors of A we have

$$A(m_1,m_2\ldots,m_N)A(m_1',m_2',\ldots m_N)=A(m_1,m_2',m_3,\ldots m_N)A(m_1',m_2,\ldots,m_N)-A(m_1,m_1',m_3\ldots,m_N)A(m_2',m_2,\ldots,m_N).$$

It follows from above that either $A(m_1,\ldots,m_N)=0$ or $A(m_1',m_2',m_3,\ldots,m_N)=0$. But this is impossible since by assumption both minors on the left-hand-side are associated with dominant phase combinations. Thus, they are both nonzero. Hence we have reached a contradiction which implies that as $y\to\pm\infty$, phase transitions where more than one phase changes simultaneously across adjacent dominant phase regions, are impossible.

APPENDIX B: PROOF OF THEOREM 3.6

First we need to establish the following Lemma that will be useful in proving the theorem.

Lemma B.1: If P_{ij} is the submatrix defined in Eq. (3.2) *and e_n labels the nth pivot column of an irreducible coefficient matrix A, then $N-1\leqslant \mathrm{rank}(P_{e_n e_n+1})\leqslant N$, $\forall n=1,\ldots,N$.*

Proof: Recall that the pivot indices are ordered as $1=e_1<e_2<\cdots<e_N<M$ for an irreducible matrix A. Then it follows from Definition 2.2(ii) that, corresponding to each pivot column $A[e_n]$ of an irreducible matrix A, there exists at least one nonpivot column $A[j_*]$, with $j_*>e_n$, that has a nonzero entry in its nth row. Hence we have $A(e_1,\ldots,e_{n-1},j_*,e_{n+1},\ldots,e_N)\neq 0$. This implies that the matrix $A[1,\ldots,e_n-1,e_n+1,\ldots,M]=(P_{e_n e_n+1}|A[e_n+1])$ which contains the columns $A[e_1],\ldots,A[e_{n-1}],A[j_*],A[e_{n+1}],\ldots,A[e_N]$, has rank N. Thus, the rank of $P_{e_n e_n+1}$ is *at least* $N-1$, and this yields the desired result. □

We are now ready to prove Theorem 3.6. We prove part (i) here; the proof of part (ii) follows similar steps. The proof of part (i) is divided in two parts. First we show that for each pivot index e_n, $n=1,\ldots,N$, there exists an index $j_n>e_n$ with the necessary and sufficient properties for $[e_n,j_n]$ to identify an asymptotic line soliton as $y\to\infty$; then we prove that such a j_n is unique.

Existence: The proof is constructive. For each pivot index e_n, and for any $j>e_n$, we consider the rank of the matrix $P_{e_n,j}=A[1,2,\ldots,e_n-1,j+1,\ldots,M]$ starting from $j=e_n+1$. When $j=e_n+1$ we have $P_{e_n,j}=P_{e_n,e_n+1}$, and therefore $N-1\leqslant\mathrm{rank}(P_{e_n,e_n+1})\leqslant N$ from Lemma B.1. If $\mathrm{rank}(P_{e_n,e_n+1})=N$, then Lemma 3.4(i) implies that the pair $[e_n,e_n+1]$ *does not* identify an

asymptotic line soliton as $y\to\infty$. In this case, we increment the value of j successively from e_n+1, until $\operatorname{rank}(P_{e_n,j})$ decreases from N to $N-1$. Note that a value of j such that $\operatorname{rank}(P_{e_n,j})=N-1$ always exists because if $j=M$, then $\operatorname{rank}(P_{e_n,M})=\operatorname{rank}(A[1,\dots,e_n-1])=n-1\leqslant N-1$, since A is in RREF. Suppose $j=j_*$ is the smallest index such that $\operatorname{rank}(P_{e_n,j_*})=N-1$ and $\operatorname{rank}(P_{e_n,j_*}|A[j_*])=N$. We next check the rank of $\operatorname{rank}(P_{e_n,j_*}|A[e_n])$. Since $\operatorname{rank}(P_{e_n,j_*})=N-1$, two cases are possible: either (a) $\operatorname{rank}(P_{e_n,j_*}|A[e_n])=N$ or (b) $\operatorname{rank}(P_{e_n,j_*}|A[e_n])=N-1$. We discuss these two cases separately.

(a) Suppose that $\operatorname{rank}(P_{e_n,j_*}|A[e_n])=N$. By construction we have $\operatorname{rank}(P_{e_n,j_*}|A[j_*])=N$, and since $N=\operatorname{rank}(A)$ one also has $\operatorname{rank}(P_{i_n,j_*}|A[e_n,j_*])=N$. In this case we set $j_*=j_n$. It follows from Lemma 3.4 that the pair $[e_n,j_n]$ satisfies the necessary rank conditions to identify an asymptotic line soliton as $y\to\infty$. Next we show that these rank conditions are also *sufficient* in order to determine a pair of dominant phase combinations in the tau function corresponding to the single-phase transition $e_n\to j_n$. Since $\operatorname{rank}(P_{e_n,j_n})=N-1$, it is possible to choose $N-1$ linearly independent columns $A[p_1],\dots,A[p_{N-1}]$ from the matrix P_{e_n,j_n} so that for all choices of linearly independent columns $A[l_1],\dots,A[l_{N-1}]\in P_{e_n,j_n}$ one has $\theta_{p_1,\dots,p_{N-1}}\geqslant\theta_{l_1,\dots,l_{N-1}}$ as $y\to\infty$ along the transition line L_{e_n,j_n}. The existence of such a set is guaranteed because part (i) of the dominant phase condition 3.1 implies that, as $y\to\infty$ in the $[e_n,j_n]$ direction, the phases corresponding to the index set P_{e_n,j_n} are ordered as $\theta_1>\theta_2>\cdots>\theta_{e_n-1}$ and $\theta_{j_n+1}<\theta_{j_n+2}<\cdots<\theta_M$. Therefore, it is possible to select the top $N-1$ phases from the above two lists so that the corresponding columns are linearly independent. Furthermore, the conditions $\operatorname{rank}(P_{e_n,j_n}|A[e_n])=\operatorname{rank}(P_{e_n,j_n}|A[j_n])=N$ imply that the minors $A(e_n,p_1,\dots,p_{N-1})$ and $A(j_n,p_1,\dots,p_{N-1})$ are both nonzero, and thus $\theta_{e_n,p_1,\dots,p_{N-1}}$ and $\theta_{j_n,p_1,\dots,p_{N-1}}$ form a dominant pair of phase combinations as $y\to\infty$ along the direction of L_{e_n,j_n}.

(b) Suppose that $\operatorname{rank}(P_{e_n,j_*}|A[e_n])=N-1$. Note that this is possible only for $n<N$, because when $n=N$ the submatrix $P_{e_N,j}$ for any $j>e_N$ contains the pivot columns $A[e_1],\dots,A[e_{N-1}]$. Hence, $\operatorname{rank}(P_{e_N,j})=N-1$ and $\operatorname{rank}(P_{e_N,j}|A[e_N])=N$. Consequently, $n=N$ always belongs to case (a) above and not to case (b). So we consider only the case $n<N$ below.

Since $\operatorname{rank}(P_{e_n,j_*})=\operatorname{rank}(P_{e_n,j_*}|A[e_n])=N-1$, this means that $A[e_n]\in\operatorname{span}(P_{e_n,j_*})$. However, since $A[e_n]$ is a pivot column, it cannot be spanned only by its preceding columns $A[1],\dots,A[e_n-1]$. Hence the spanning set of $A[e_n]$ from P_{e_n,j_*} must contain at least one column from $A[j_*+1],\dots,A[M]$. In this case we continue incrementing the value of j starting from j_* until the pivot column $A[e_n]$ is no longer in the span of the columns of the resulting submatrix $P_{e_n,j}$. Let j_n be the smallest index such that $A[e_n]$ is spanned by the columns of the submatrix $P_{e_n,j_n}|A[j_n]$ but *not* by those of P_{e_n,j_n}. Then, by construction we have $\operatorname{rank}(P_{e_n,j_n})=:r<N-1$, and $\operatorname{rank}(P_{e_n,j_n}|A[e_n])=\operatorname{rank}(P_{e_n,j_n}|A[j_n])=\operatorname{rank}(P_{e_n,j_n}|A[e_n,j_n])=r+1$. The rank conditions in Lemma 3.4(i) are once again satisfied for the index pair $[e_n,j_n]$ thus found. The sufficiency of these conditions can then be established by following similar steps as in case (a). Namely, it is possible to choose a set of linearly independent vectors $A[l_1],\dots,A[l_r]\in P_{e_n,j_n}$ and extend this set to a basis of $\mathbb{R}^N$ as follows: $\{A[e_n],A[l_1],\dots,A[l_r],A[m_1],\dots,A[m_s]\}$, where $A[m_1],\dots,A[m_s]\in Q_{e_n,j_n}$ and $r+s=N-1$. We then have $A(e_n,l_1,\dots,l_r,m_1,\dots,m_s)\neq 0$, which also implies $A(j_n,l_1,\dots,l_r,m_1,\dots,m_s)\neq 0$ since $A[e_n]\in\operatorname{span}(P_{e_n,j_n}|A[j_n])$. As in case (a), we can now maximize the phase combinations over all such sets $\{l_1,\dots,l_r,m_1,\dots,m_s\}$, and find a set of indices $\{p_1,\dots,p_r,q_1,\dots,q_s\}$ such that $\theta_{e_n,p_1,\dots,p_r,q_1,\dots,q_s}$ and $\theta_{j_n,p_1,\dots,p_r,q_1,\dots,q_s}$ form a dominant pair of phase combinations as $y\to\infty$ along the direction of L_{e_n,j_n}. Summarizing, we have shown that for each pivot index $e_n,n=1,2,\dots,N$, there exists at least one asymptotic line soliton $[e_n,j_n]$ with $j_n>e_n$ as $y\to\infty$. Next we prove uniqueness.

Uniqueness: Suppose that $[e_n,j_n]$ and $[e_n,j_n']$ are two asymptotic line solitons identified by the same pivot index e_n as $y\to\infty$. Without loss of generality, assume that $j_n'>j_n$, and consider the line soliton $[e_n,j_n']$. Lemma 3.4(i) implies that $\operatorname{rank}(P_{e_n,j_n'}|A[j_n'])=\operatorname{rank}(P_{e_n,j_n}|A[e_n,j_n'])$. Hence the pivot column $A[e_n]$ is spanned by the columns of the submatrix $(P_{e_n,j_n'}|A[j_n'])$. But by assumption we have $(P_{e_n,j_n'}|A[j_n'])\subseteq P_{e_n,j_n}$, since $j_n'>j_n$. Hence $A[e_n]$ is also spanned by the columns of P_{e_n,j_n}. This however implies that $\operatorname{rank}(P_{e_n,j_n}|A[e_n])=\operatorname{rank}(P_{e_n,j_n})$, which contradicts the necessary rank

conditions in Lemma 3.4(i) for $[e_n, j_n]$ to identify an asymptotic line soliton as $y \to \infty$. Therefore we must have $j_n = j_{n'}$. Thus, it is not possible to have two distinct asymptotic line solitons as $y \to \infty$ associated with the same pivot index e_n. Part (i) of Theorem 3.6 is now proved.

APPENDIX C: EQUIVALENCE CLASSES AND DUALITY OF SOLUTIONS

In this appendix, we investigate the relationship between two classes of KPII multisoliton solutions with complementary sets of asymptotic line solitons. Note that the KPII equation (1.1) is invariant under the inversion symmetry $(x,y,t) \to (-x,-y,-t)$. As a result, if $u(x,y,t)$ is an $(M-N,N)$-soliton solution of KPII with $M-N$ incoming and N outgoing line solitons, then $u(-x,-y,-t)$ is a $(N,M-N)$-soliton solution of KPII where the numbers of incoming and outgoing line solitons are reversed. It follows from Theorem 3.6 that the solution $u(-x,-y,-t)$ should correspond to *some* tau function $\tau_{M-N,M}(x,y,t)$ associated with an $M-N \times M$ coefficient matrix whose pivot and nonpivot columns uniquely identify the asymptotic line solitons of $u(-x,-y,-t)$.

Before proceeding further, we introduce the notion of an equivalence class which plays an important role in subsequent discussions. Let Θ as in Definition 2.3 denote the set of all phase combinations $\theta_{m_1,\ldots,m_N}$ which appear with nonvanishing coefficients in the tau function $\tau(x,y,t)$ of Eq. (2.2).

Definition C.2 (Equivalence class): Two tau functions are defined to be in the same equivalence class if (up to an overall exponential phase factor) the set Θ *is the same for both. The set of* (N_-,N_+)*-soliton solutions of KPII generated by an equivalence class of tau functions defines an equivalence class of solutions.*

It is clear from the above definition that tau functions in a given equivalence class can be viewed as positive-definite sums of the *same* exponential phase combinations but with different sets of coefficients. They are parametrized by the same set of phase parameters $k_1, \ldots, k_M$, but the constants θ_{m0} in the phase θ_m are different. Moreover, the irreducible coefficient matrices associated with the tau functions have exactly the same sets of vanishing and nonvanishing minors, but the magnitudes of the nonvanishing minors are different for different matrices. Thus, it is evident from the remarks following Corollary 2.6 in Sec. II that the asymptotic line solitons of each solution in an equivalence class arise from the *same* $i \to j$ single phase transition, and are therefore labeled by the same index pair $[i,j]$. Theorem 3.6 then implies that the coefficient matrices associated with the tau functions in the same equivalence class have identical sets of pivot and nonpivot indices labeling the asymptotic line solitons as $y \to \infty$ and as $y \to -\infty$, respectively. Thus, solutions in the same equivalence class can differ only in the position of each asymptotic line solitons and in the location of each interaction vertex. As a result, any (N_-,N_+)-soliton solution of KPII can be transformed into any other solution in the same equivalence class by spatio-temporal translations of the individual asymptotic line solitons. We refer to the two tau functions $\tau_{N,M}(x,y,t)$ and $\tau_{M-N,M}(x,y,t)$ as *dual* to each other if the solution $u(-x,-y,-t)$ obtained from the function $\tau_{N,M}(-x,-y,-t)$ and the solution generated by $\tau_{M-N,M}(x,y,t)$ are in the same equivalence class. Note that $\tau_{N,M}(-x,-y,-t)$ is not exactly a tau function according to Eq. (2.2), but it is possible to construct from it a dual tau function $\tau_{M-N,M}(x,y,t)$ whose coefficient matrix B can be derived from the coefficient matrix A associated with the tau function $\tau_{N,M}(x,y,t)$. We describe this construction below.

Since A is of rank N and in RRFF, it can be expressed as $A=[I_N,G]P$, where I_N is the $N \times N$ identify matrix of pivot columns, G is the $N \times (M-N)$ matrix of nonpivot columns, and P denotes the $M \times M$ permutation matrix of M columns of A. We augment A with $M-N$ additional rows to form the invertible $M \times M$ matrix,

$$S = \begin{pmatrix} I_N & G \\ O & I_{M-N} \end{pmatrix} P, \tag{C1}$$

where O is the $(M-N) \times N$ zero matrix and I_{M-N} is the $(M-N) \times (M-N)$ identify matrix. Let A' be the $(M-N) \times M$ matrix obtained by selecting the last $M-N$ rows of $(S^{-1})^T$. The rank of A' is $M-N$, and the following complementarity relation holds between A and A'.

Lemma C.3: The pivot columns of A' are labeled by exactly the same set of indices which label the nonpivot columns of A, and vice versa. Moreover, if A is irreducible then A' is also irreducible.

Proof: From Eq. (C1) and the fact that $P^{-1}=P^T$ for a permutation matrix, we obtain

$$(S^{-1})^T=\begin{pmatrix} I_N & O^T \\ -G^T & I_{M-N} \end{pmatrix}P, \tag{C2}$$

which implies that $A'=[-G^T,I_{M-N}]P$. Then (by performing row reduction in *reverse* order), the pivot columns of $A'P^{-1}$ can be identified with its last $M-N$ columns which correspond to the nonpivot columns of $AP^{-1}=[I_N,G]$, and vice versa. The same correspondence between pivot and nonpivot columns also holds for A and A' because the columns of both matrices are permuted by the same matrix P^{-1}. This proves the first part of the lemma.

To establish that A' is irreducible, note first from Definition 2.2 that the permutation of columns preserves irreducibility of a matrix. Since A is irreducible, Definition 2.2 implies that all rows or columns of G and G^T are nonzero. Therefore the matrix $A'P^{-1}=[-G^T,I_{M-N}]$, and hence A', are both irreducible. □

Note that A' is *not* in the canonical RREF, but can be set in RREF by a GL $(N,\mathbb{R})$ transformation. Next, we define the matrix B which is also of rank $M-N$ and irreducible like A', and whose columns are obtained from A' as

$$B[m]=(-1)^m A'[m], \quad m=1,\ldots,M. \tag{C3}$$

Then using Eqs. (C2) and (C3), the minors of A can be expressed in terms of the complementary minors of B via (see, e.g., Ref. 6, p. 21)

$$A(l_1,\ldots,l_N)=(-1)^\sigma \det(P)B(m_1,\ldots,m_{M-N}), \tag{C4}$$

where $\sigma=M(M+1)/2+N(N+1)/2$, and where the indices $m_1\leqslant m_2\leqslant\cdots\leqslant m_{M-N}$ are the complement of $1\leqslant l_1\leqslant l_2\leqslant\cdots l_N$ in $\{1,2,\ldots,M\}$. The matrix B plays the role of a coefficient matrix for the dual tau function as given by the following lemma.

Lemma C.4 (Duality): If $\tau_{N,M}(x,y,t)$ is the tau function associated with an irreducible $N\times M$ coefficient matrix A, then the matrix B defined via Eq. (C3) *generates a tau function $\tau_{M-N,M}(x,y,t)$ that is dual to $\tau_{N,M}(x,y,t)$.*

Proof: Without loss of generality we choose the tau function $\tau_{N,M}(x,y,t)$ associated with the given equivalence class of solutions such that $\theta_{m,0}=0$ for all $m=1,\ldots,M$ in Eq. (2.2). Then, using Eq. (C4) we can express the tau function as

$$\tau_{N,M}(-x,-y,-t)=(-1)^\sigma \det(P)e^{-\theta_{1,\ldots,M}}\tau'(x,y,t), \tag{C5a}$$

where

$$\tau'(x,y,t)=\sum_{1\leqslant m_1<m_2<\cdots<m_{M-N}\leqslant M} V(l_1,\ldots,l_N)B(m_1,\ldots,m_{M-N})e^{\theta_{m_1,\ldots,m_{M-N}}}, \tag{C5b}$$

with $V(l_1,\ldots,l_N)$ denoting the Van der Monde determinant as in Eq. (2.2) and where the sum is now taken over the complementary indices $m_1,\ldots,m_{M-N}$ instead of $l_1,\ldots,l_N$. [The number of terms in the sum remains the same since $\binom{M}{N}=\binom{M}{M-N}$.] It is clear from Eq. (1.2) that both $\tau_{N,M}(-x,-y,-t)$ and $\tau'(x,y,t)$ in Eq. (C5a) generate the same solution $u(x,y,t)$ of KPII although $\tau'(x,y,t)$ itself is *not* a tau function. Note that all the nonzero minors of B have the same sign, which is determined by the sign of $(-1)^\sigma \det(P)>0$. Thus, by replacing each Van der Monde coefficient $V(l_1,\ldots,l_N)$ by $V(m_1,\ldots,m_{M-N})$ in Eq. (C5b), it is possible to obtain from $\tau'(x,y,t)$, a new tau function $\tau_{M-N,M}(x,y,t)$ associated with the irreducible coefficient matrix B. Since both $\tau'(x,y,t)$ and $\tau_{M-N,M}(x,y,t)$ are sign-definite sums of the *same* exponential phase combinations, they generate solutions that are in the same equivalence class. Therefore, the tau function $\tau_{M-N,M}(x,y,t)$ constructed via the above prescription is dual to the tau function $\tau_{N,M}(x,y,t)$. This

yields the desired result. □

By applying Lemma C.4, it is easy to show that part (i) of Theorem 3.6 implies part (ii) and vice versa. For example, by applying part (i) of Theorem 3.6 to the tau function $\tau_{M-N,M}(x,y,t)$ in Lemma C.4 one can conclude that as $y\to\infty$, $\tau_{M-N,M}(x,y,t)$ generate a solution with exactly $M-N$ line solitons, identified by the *pivot* indices $g_1,\ldots,g_{M-N}$ of the associated coefficient matrix B. One should however note that since the ordering of the pivot and nonpivot columns of B is reversed with respect to that of A, if $[i,j]$ with $i<j$ labels an asymptotic line soliton generated by $\tau_{M-N,M}(x,y,t)$ as $y\to\infty$, then j is the pivot index, not i. The solution generated by $\tau_{M-N,M}(x,y,t)$ is in the same equivalence class as $u(-x,-y,-t)$ because $\tau_{M-N,M}(x,y,t)$ is dual to $\tau_{M,N}(x,y,t)$. Consequently, as $y\to\infty$, $u(-x,-y,-t)$ has $M-N$ asymptotic line solitons labeled by exactly the same indices $g_1,\ldots,g_{M-N}$. Then as $y\to-\infty$, it follows that the solution $u(x,y,t)$ generated by $\tau_{N,M}(x,y,t)$ also has $M-N$ asymptotic line solitons. Furthermore, these line solitons are labeled by the same indices $g_1,\ldots,g_{M-N}$ which are the nonpivot indices of the coefficient matrix A of the tau function $\tau_{N,M}(x,y,t)$. This proves part (ii) of Theorem 3.6. Similarly, one could also prove part (i) of the Theorem using part (ii) and Lemma C.4.

Another consequence of Lemma C.4 is that the dominant pairs of phase combinations for the asymptotic line solitons of $\tau_{M-N,N}(x,y,t)$ as $y\to\infty$ are the complement of those for the asymptotic line solitons of the dual tau function $\tau_{N,M}(x,y,t)$ as $y\to-\infty$. Thus, if the dominant pair of phase combinations for $\tau_{M-N,M}(x,y,t)$ as $y\to\infty$ along the line $L_{i,j}$ is given by $\theta_{i,m_2,\ldots,m_{M-N}}$ and $\theta_{j,m_2,\ldots,m_{M-N}}$, the dominant phase combinations for $\tau_{N,M}(x,y,t)$ as $y\to-\infty$ along $L_{i,j}$ are $\theta_{i,l_2,\ldots,l_N}$ and $\theta_{j,l_2,\ldots,l_N}$, where the index set $\{l_2,\ldots,l_N\}$ is the complement of $\{i,j,m_2,\ldots,m_{M-N}\}$ in $\{1,\ldots,M\}$.

A particularly interesting subclass of (N_-,N_+)-soliton solutions is obtained by requiring the solutions $u(x,y,t)$ and $u(-x,-y,-t)$ to be in the same equivalence class. Thus, this class of solutions is generated tau functions which can be regarded as "self-dual." The corresponding solutions are the elastic N-soliton solutions of KPII, for which the amplitudes and directions of the N incoming line solitons coincide with those of the N outgoing line solitons. Hence, the set of incoming line solitons and the set of outgoing line solitons are both labeled by the same index pairs $\{[i_n,j_n]\}_{n=1}^N$. Clearly, in this case we have $N_+=N_-=N$ and $M=2N$. Some properties of the elastic N-soliton solution have been studied in Ref. 12, and we will discuss several other properties in a future presentation. Here we only mention one result which is a direct consequence of Theorem 3.6 and the above discussions:

Corollary C.5: A necessary condition for a set of index pairs $\{[i_n,j_n]\}_{n=1}^N$ *to describe an elastic N-soliton solution is that the indices* $i_1,\ldots,i_N$ *and* $j_1,\ldots,j_N$ *form a disjoint partition of the integers* $1,\ldots,2N$.

Proof: From part (i) of Theorem 3.6, the indices $i_1,\ldots,i_N$ for the N asymptotic line solitons as $y\to\infty$ label the pivot columns of A, and from part (ii) of Theorem 3.6, the indices $j_1,\ldots,j_N$ for the N asymptotic line solitons as $y\to-\infty$ label the nonpivot columns of A. In order for the N asymptotic line solitons as $y\to-\infty$ to be the same as those as $y\to\infty$, however, the index pairs $[i_n,j_n]$ must obviously be the same as $y\to\pm\infty$ for all $n=1,\ldots,N$. But the sets of pivot and nonpivot indices of any matrix are of course disjoint; hence the desired result. □

Note however that the condition in Corollary C.5 is necessary but *not* sufficient to describe an elastic N-soliton solution. It is indeed possible to have N-soliton solutions where the index pairs labeling the asymptotic line solitons as $y\to\infty$ and as $y\to-\infty$ form two different disjoint partition of integers $\{1,2,\ldots,2N\}$. Such N-soliton solutions are *not* elastic. See, for example, the 2-soliton solution in Fig. 4(e).

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Comment on "Exact analytic solutions of nonlinear boundary value problems in fluid mechanics (Blasius equations)" [J. Math. Phys. 46, 033101 (2005)].

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A simple procedure is given to transform the Blasius equation into an Abel equation of the second kind. © *2006 American Institute of Physics.*
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In this Comment, we focus on the nonlinear ode

$$y''' + \alpha y y'' - \beta y'^2 = 0, \tag{1}$$

where the prime denotes derivation with respect to the independent variable x, and α, β are arbitrary constants. This equation describes similarity solutions of the Navier-Stokes equations, corresponding to (axisymmetric) flows caused by the stretching of a flat boundary.[1] For $\beta=0$, it reduces to the Blasius equation.[2]

Equation (1) has been investigated analytically in a recent work by Panayotounakos *et al.*,[3] to which we refer for further details, such as the specification of the boundary conditions. The main results of Ref. 3 are (i) the transformation of (1) into an Abel equation of the second kind; (ii) the definition of a methodology for the construction of exact solutions to the Abel equation, and consequently, of exact solutions to (1). Here we concentrate on the result at point (i). This result involves an elaborate procedure, that relies on first reducing (1), through a sequence of admissible functional transformations, to a generalized Emden-Fowler equation, and then transforming the latter equation into an Abel equation of the second kind. The authors note that this procedure is in fact quite general, and could also be applied to other important equations of mathematical physics, such as those for the Duffing and the Van der Pol nonlinear oscillators, the Kidder equation, etc.

A general approach is always commendable, but sometimes, when dealing with specific problems, simpler ad hoc approaches may be devised. The purpose of this Comment is to provide such an approach for the problem at hand. We first notice that the substitution

$$y' = \frac{\mathrm{d}f(y)}{\mathrm{d}y}, \tag{2}$$

reduces (1) to

$$\frac{\mathrm{d}}{\mathrm{d}y}(\dddot{f}\ddot{f}) + \alpha y \ddot{f} - \beta \dot{f} = 0, \tag{3}$$

with the overdot denoting derivation with respect to y. After a simple manipulation of the middle term on the left-hand side, (3) can be integrated once, yielding

$$\dddot{f}\ddot{f} + \alpha y \dot{f} - (\alpha + \beta) f = C, \tag{4}$$

with C an arbitrary constant. Note that in the special case $\alpha+\beta=0$, (4) already has the form of an Abel equation of the second kind, in the variable $\dot{f}$.

In the general case $\alpha+\beta\neq 0$, a further step is needed to complete the reduction. In this case, we may take $C=0$ in (4) (the addition of a constant to f would not modify y), and set

$$z = y\frac{\dot{f}}{f}, \quad w = A\frac{y^3}{f}, \tag{5}$$

with A an arbitrary constant, to transform (4) into the Abel equation of the second kind

$$[(\alpha+\beta-\alpha z)w - Az^2(z-1)]\frac{\mathrm{d}w}{\mathrm{d}z} = Az(3-z)w. \tag{6}$$

Given a solution $w(z)$ of the Abel equation (6), one may solve (5) to get $f(y)$, and then (2) to obtain $y(x)$. However, finding exact solutions of (5) is likely to be difficult in practical cases, and it is more convenient to construct a parametric representation of the solution, in analogy to what is done in Ref. 3 [see Sec. 3, equations from (3.33) to (3.38)]. It readily follows from (5), (6), and (2) that

$$y = y(z) = \left(\frac{wf}{A}\right)^{1/3}, \tag{7}$$

$$x = x(z) = C_1 + \frac{1}{A^{2/3}}\int \mathrm{d}z \frac{w^{2/3}}{z^2 f^{4/3}}\frac{\mathrm{d}f}{\mathrm{d}z}, \tag{8}$$

with $f(z)$ given by

$$f(z) = \exp\left(C_2 + A\int \frac{z^2\mathrm{d}z}{(\alpha+\beta-\alpha z)w - Az^2(z-1)}\right), \tag{9}$$

and C_1, C_2 integration constants.

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The Wigner-Weyl transformation and the quantum path integral

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We show that the space of quantum states for a spinless particle possesses a (trivial) fiber bundle structure $\mathcal{B}\times\mathcal{F}$ where $\mathcal{B}$ is the classical phase space. This geometric point of view allows us to define a "quantum path integral" that connects quantum observables with their classical counterparts. We show that this path integral reduces in fact to the Wigner-Weyl transformation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2184768]

I. INTRODUCTION

Among the different methods that have been developed to link classical and quantum formalisms, one of the most famous is the Wigner-Weyl transformation. This operation defines a one-to-one correspondence between quantum operators $\mathbf{A}$ and functions in phase space $a(p,q)$ in such a way that the quantum evolution of $a(p,q)$ reduces to the classical one when $\hbar$ vanishes.[1,2] In this framework quantization is mathematically a deformation of the Abelian algebra of functions in phase space into a noncommutative algebra.[3]

In this paper we bring to the fore a geometric property of the quantum Hilbert space that allows us to identify a part of the quantum space with the classical phase space. In fact we prove that the quantum space possesses a trivial fiber bundle structure $\mathcal{B}\times\mathcal{F}$. The basis $\mathcal{B}$ is the classical phase space, while the fiber $\mathcal{F}$ contains the quantum effects. The group of translation along the basis $\mathcal{B}$ is the Weyl group: two fibers $\mathcal{F}_\alpha$ and $\mathcal{F}_\beta$ (corresponding to projections α and β on the basis) are linked by a Weyl transformation. Following this picture, we define the classical observable $a(\alpha)$ corresponding to a quantum operator $\mathbf{A}$ as being some "averaged value" of $\mathbf{A}$ over the fiber $\mathcal{F}_\alpha$. To represent this "averaged value," we introduce a "quantum path integral" over the fibers, specifying the rules of calculation. We show that this intuitive definition leads us to the Wigner-Weyl transformation.

The paper is organized as follows:

(i) The first section is devoted to the fiber bundle structure and related questions.
(ii) Then we introduce the "quantum path integral," the rules of calculation and the first consequences.
(iii) We show how this quantum path integral and the Wigner-Weyl transformation are linked and we investigate some consequences.
(iv) Finally we conclude our paper.

Remark: In the following we restrict ourselves to the one dimension case. Moreover bold letters stand for operators.

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II. FIBER BUNDLE STRUCTURE

A. Definition

To be able to identify some classical structure into the "quantum world" $\mathcal{H}=L^2(\mathbb{R})$, we need to specify how the basic quantum quantities (observables $\mathbf{Q}$ and $\mathbf{P}=-i\hbar\partial_q$) are connected with classical ones. Since quantum mechanics introduces intrinsic uncertainties, while classical mechanics ignore them, we can say that the classical equivalent of a (normalized) state $|\dot{\psi}\rangle$ is the point of phase space (p,q) with $p=\langle\psi|\mathbf{P}|\psi\rangle$ and $q=\langle\psi|\mathbf{Q}|\psi\rangle$. Of course these quantities do not exist for any square integrable function $\psi\in L^2(\mathbb{R})$, so we restrict the space of functions to $\mathcal{S}$, where $\mathcal{S}$ is the set of C^∞ functions with rapid decrease. Moreover we see that the space of interest is not really the Hilbert space, but rather the set of projectors $\boldsymbol{\pi}_\psi=(1/\|\dot{\psi}\|^2)|\psi\rangle\langle\psi|$. So we define $\mathcal{P}=\{\boldsymbol{\pi}_\psi/\dot{\psi}\in\mathcal{S}\}$. We define the projection Π as

$$\forall\,\pi_\psi\in\mathcal{P},\quad \Pi(\boldsymbol{\pi}_\psi)=(\mathrm{Tr}(\boldsymbol{\pi}_\psi\mathbf{P}),\mathrm{Tr}(\boldsymbol{\pi}_{\dot{\psi}}\mathbf{Q})). \tag{1}$$

So Π is the projection from $\mathcal{P}$ onto the basis $\mathcal{B}$ which is in fact the classical phase space.

Now we define the fiber $\mathcal{F}_0$ as $\mathcal{F}_0=\Pi^{-1}[\{(0,0)\}]$ and more generally $\mathcal{F}_{p,q}=\Pi^{-1}[\{(p,q)\}]$. If we call $\{\mathbf{W}_{p,q}\}$ the Weyl group of unitary transformations

$$\mathbf{W}_{p,q}=\exp[(i/\hbar)(\mathbf{P}q-\mathbf{Q}p)]. \tag{2}$$

We know that

$$\mathbf{W}_{p,q}^\dagger\mathbf{P}\mathbf{W}_{p,q}=\mathbf{P}-p\quad\text{and}\quad\mathbf{W}_{p,q}^\dagger\mathbf{Q}\mathbf{W}_{p,q}=\mathbf{Q}-p. \tag{3}$$

This implies

$$\mathcal{F}_{p,q}=\mathbf{W}_{p,q}^\dagger\mathcal{F}_0\mathbf{W}_{p,q}. \tag{4}$$

We deduce that for any $\boldsymbol{\pi}\in\mathcal{P},\mathbf{W}_{\Pi(\pi)}\boldsymbol{\pi}\mathbf{W}_{\Pi(\pi)}^\dagger\in\mathcal{F}_0$. Then any element $\boldsymbol{\pi}\in\mathcal{P}$ is specified by the pair $(b,\boldsymbol{\pi}_0)$ where $b=(p,q)\in\mathcal{B}$ and $\boldsymbol{\pi}_0\in\mathcal{F}_0$. Then $\mathcal{P}$ is homeomorphic to the Cartesian product $\mathcal{B}\times\mathcal{F}_0$.

B. Remark

This representation of $\mathcal{P}$ is instructive for the study of time evolution. Generally we have a pair $(b(t),\boldsymbol{\pi}_0(t))$, but special cases are interesting.

For example, if the Hamiltonian is $\mathbf{H}=\mathbf{P}^2/2m+V(\mathbf{Q})$ where the potential $V(\mathbf{Q})$ is at the most quadratic, then the equations of motion for the observables $\mathbf{P}(t)$ and $\mathbf{Q}(t)$ are linear. So the expressions of $\mathbf{P}(t)$ and $\mathbf{Q}(t)$ are the classical ones (linear in $\mathbf{P}$ and $\mathbf{Q}$) and the point $(p(t),q(t))$ follows a classical trajectory, while the projector $\boldsymbol{\pi}_0(t)$ evolves as $\boldsymbol{\pi}_0(t)=\mathbf{U}^\dagger(t)\boldsymbol{\pi}_0\mathbf{U}(t)$. Then the evolution of classical quantities (expectation values of $\mathbf{P}$ and $\mathbf{Q}$) does not depend on the evolution of quantum effects represented by $\boldsymbol{\pi}_0(t)$. But if the potential $V(\mathbf{Q})$ is more than quadratic, modifications on the classical behavior of $(p(t),q(t))$ appear due to quantum effects.

Another example is the case of eigenstates. If we start with a bound eigenstate of $\mathbf{H}$ then $(p(t),q(t))=(0,q_0)$ and $\boldsymbol{\pi}_0(t)=\boldsymbol{\pi}_0$. So a bound eigenstate looks like a classical equilibrium point.

III. CLASSICAL OBSERVABLES AND THE QUANTUM PATH INTEGRAL

A. Definition

If $\mathbf{A}$ is a quantum observable and if $\boldsymbol{\pi}_\psi\in\mathcal{P}$ is the state, since classical mechanics ignore quantum uncertainties, we should say that $\mathrm{Tr}(\boldsymbol{\pi}_\psi\mathbf{A})$ is the corresponding classical value of $\mathbf{A}$. But since classical mechanics is only sensitive to the values of p and q, it does not distinguish the states $\boldsymbol{\pi}_\psi\in\mathcal{F}_{p,q}$. So we have in fact an infinity of values for $\mathrm{Tr}(\boldsymbol{\pi}_\psi\mathbf{A})$ corresponding to a unique classical point. So we can think that the true classical value is some "averaged value" of $\mathrm{Tr}(\boldsymbol{\pi}_\psi\mathbf{A})$

over $\mathcal{F}_{p,q}$. To implement this idea we introduce a *symbolic* "quantum path integral" over $\mathcal{P}$ with the notation $\int \mathcal{D}\{\boldsymbol{\pi}\}$ and we give the following axioms:

(i) The classical expression $\mathcal{C}(\mathbf{A})(p,q)=\widetilde{\mathbf{A}}(p,q)$ of the observable $\mathbf{A}$ is given by

$$\widetilde{A}(P,q) = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(P-\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{A}\rangle_{\boldsymbol{\pi}}, \tag{5}$$

where $\langle \mathbf{O}\rangle_{\boldsymbol{\pi}}=\mathrm{Tr}(\boldsymbol{\pi}\mathbf{O})$. The distributions δ specify the "integration" over $\mathcal{F}_{p,q}$.

(ii) We assume that the "measure" $\mathcal{D}\{\boldsymbol{\pi}\}$ is real (but not necessarily positive) in order to transform self-adjoint operators into real functions, then $\mathcal{C}(\mathbf{A}^{\dagger})(p,q)=\mathcal{C}(\mathbf{A})(p,q)^{*}$.

(iii) Since the group of symmetry in the quantum space is the unitary group, we assume that the "measure" $\mathcal{D}\{\boldsymbol{\pi}\}$ is invariant under these transformations,

$$\mathcal{D}\{\mathbf{U}^{\dagger}\boldsymbol{\pi}\mathbf{U}\} = \mathcal{D}\{\boldsymbol{\pi}\} \quad \text{if } \mathbf{U}^{\dagger}\mathbf{U} = \mathbf{U}\mathbf{U}^{\dagger} = \mathbf{1}_{\mathcal{H}}. \tag{6}$$

(iv) The condition of "normalization,"

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}}) = 1, \tag{7}$$

stipulates that the "integral" over the fiber $\mathcal{F}_0$ is equal to 1.

Remarks: Following our definition, the path integral over $\mathcal{P}$ is limited to projectors $\boldsymbol{\pi}_{\psi}$ with $\psi\in\mathcal{S}$. So the invariance of the "measure" under unitary transformations must be limited to transformations that leave $\mathcal{S}$ invariant.

Furthermore, in this paper we do not assume that the path integral is really an integral in the mathematical meaning of the word. We think that the symbol $\int \mathcal{D}\{\boldsymbol{\pi}\}$ rather corresponds to a bra-ket of duality as for $\langle \delta,\varphi\rangle=\int \mathrm{d}x\ \delta(x)\varphi(x)$. But this is not a real problem if we understand the symbol $\int \mathcal{D}\{\boldsymbol{\pi}\}$ as a convenient notation and if the axioms are sufficient to give effective rules of calculation (with no contradiction). A rigorous mathematical approach probably involves some generalization of Gleason theorem.[4]

Last, our definition of classical counterparts for quantum observables seems to introduce losses of information since we perform some "average." As we will see later this is not true.

B. Consequences

1. First relations

Introducing the invariance of the "measure" for Weyl transformations ($\mathbf{W}_{p,q}$) into the expression of $\widetilde{A}(p,q)$, and taking into account Eq. (3), we find

$$\widetilde{A}(p,q) = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p+p_0-\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q+q_0-\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{W}^{\dagger}_{p_0,q_0}\mathbf{A}\mathbf{W}_{p_0,q_0}\rangle_{\boldsymbol{\pi}}. \tag{8}$$

We deduce

$$\widetilde{A}(p-p_0,q-q_0) = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{W}^{\dagger}_{p_0,q_0}\mathbf{A}\mathbf{W}_{p_0,q_0}\rangle_{\boldsymbol{\pi}}. \tag{9}$$

We recover that the translation of quantum observables by the Weyl group corresponds to a classical translation in phase space,

$$\mathcal{C}(\mathbf{W}^{\dagger}_{p_0,q_0}\mathbf{A}\mathbf{W}_{p_0,q_0})(p,q) = \mathcal{C}(\mathbf{A})(p-p_0,q-q_0). \tag{10}$$

The same calculation with the parity $\mathbf{K}_P$ gives

$$\widetilde{A}(-p,-q)=\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{K}_P^{\dagger}\mathbf{A}\mathbf{K}_P\rangle_{\boldsymbol{\pi}}. \tag{11}$$

So,

$$\mathcal{C}(\mathbf{K}_P^{\dagger}\mathbf{A}\mathbf{K}_P)(p,q)=\mathcal{C}(\mathbf{A})(-p,-q). \tag{12}$$

For the unitary group of rescaling $\mathbf{R}_\alpha=\exp[(i\alpha/2\hbar)(\mathbf{PQ}+\mathbf{QP})]$ we obtain

$$\mathcal{C}(\mathbf{R}_\alpha^{\dagger}\mathbf{A}\mathbf{R}_\alpha)(p,q)=\mathcal{C}(\mathbf{A})(e^{\alpha}p,e^{-\alpha}q), \tag{13}$$

since $\mathbf{R}_\alpha^{\dagger}\mathbf{P}\mathbf{R}_\alpha=e^{\alpha}\mathbf{P}$ and $\mathbf{R}_\alpha^{\dagger}\mathbf{Q}\mathbf{R}_\alpha=e^{-\alpha}\mathbf{Q}$.

The invariance for Weyl transformations applied to the condition of normalization gives

$$1=\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}}). \tag{14}$$

On the one hand, this equation says that the "integral" over each fiber $\mathcal{F}_{p,q}$ is equal to 1, on the other hand, if we notice that $\mathrm{Tr}(\boldsymbol{\pi}\mathbf{1}_{\mathcal{H}})=1$, this equation means that the classical representation of the identity operator $\mathbf{1}_{\mathcal{H}}$ is 1,

$$\mathcal{C}(\mathbf{1}_{\mathcal{H}})(p,q)=1. \tag{15}$$

Now if we replace the general observable $\mathbf{A}$ by $\mathbf{P}$ or $\mathbf{Q}$ and we take into account the δ in the integral, we find

$$\begin{aligned}&\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{P}\rangle_{\boldsymbol{\pi}}=p,\\ &\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}}=q.\end{aligned} \tag{16}$$

Then the classical representation of $\mathbf{P}$ is p and the classical representation of $\mathbf{Q}$ is q,

$$\mathcal{C}(\mathbf{P})(p,q)=p \quad \text{and } \mathcal{C}(\mathbf{Q})(p,q)=q. \tag{17}$$

Let us prove that these relations can be extended to more complicated functions of $\mathbf{P}$ or $\mathbf{Q}$.

We define the function $f_\alpha(p,q)=\mathcal{C}(e^{i\alpha\mathbf{P}})(p,q)$. Thanks to Eqs. (3) and (10) we obtain

$$f_\alpha(p-p_0,q-q_0)=e^{-i\alpha p_0}f_\alpha(p,q). \tag{18}$$

The case $p_0=0$ tells us that $f_\alpha(p,q-q_0)=f_\alpha(p,q)$, then f_α is in fact independent of q. So $f_\alpha(p,q)=g_\alpha(p)$ and g_α verifies $g_\alpha(p-p_0)=e^{-i\alpha p_0}g_\alpha(p)$. We deduce that $g_\alpha(p)=C(\alpha)e^{i\alpha p}$, so

$$\mathcal{C}(e^{i\alpha\mathbf{P}})(p,q)=C(\alpha)e^{i\alpha p}. \tag{19}$$

Moreover the rescaling operators $\mathbf{R}_\xi$ give $\mathcal{C}(\mathbf{R}_\xi^{\dagger}e^{i\alpha\mathbf{P}}\mathbf{R}_\xi)=\mathcal{C}(\exp[i\alpha e^{\xi}\mathbf{P}])$, then using Eq. (13), we find that $\mathcal{C}(\alpha)=C(\alpha e^{\xi})$. We deduce $C(\alpha)=\lim_{\xi\to-\infty}C(\alpha e^{\xi})=C(0)$. But $C(0)=1$ because $\mathcal{C}(\mathbf{1}_{\mathcal{H}})=1$ and we obtain

$$\mathcal{C}(e^{i\alpha\mathbf{P}})(p,q)=e^{i\alpha p}. \tag{20}$$

By Fourier transform we can extend this result to any operator $f(\mathbf{P})$,

$$\mathcal{C}[f(\mathbf{P})](p,q)=f(p). \tag{21}$$

The same reasoning is possible for operators $f(\mathbf{Q})$ and

$$\mathcal{C}[f(\mathbf{Q})](p,q)=f(q). \tag{22}$$

Finally, we introduce the self-adjoint operator $\boldsymbol{\rho}$ by the formula

$$\boldsymbol{\rho} = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\boldsymbol{\pi}, \tag{23}$$

and we define $\boldsymbol{\rho}_{p,q}=\mathbf{W}_{p,q}^{\dagger}\boldsymbol{\rho}\mathbf{W}_{p,q}$. The invariance of the measure $\mathcal{D}\{\boldsymbol{\pi}\}$ under Weyl translations shows that

$$\boldsymbol{\rho}_{p,q} = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle \mathbf{P}\rangle_{\boldsymbol{\pi}})\delta(q-\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\boldsymbol{\pi}. \tag{24}$$

Then the path integral expression $\mathcal{C}(\mathbf{A})(p,q)$ reduces to

$$\mathcal{C}(\mathbf{A})(p,q) = \mathrm{Tr}(\boldsymbol{\rho}_{p,q}\mathbf{A}). \tag{25}$$

Remark: We notice that the operator $\boldsymbol{\rho}$ must be bounded if we want that $\langle\varphi|\boldsymbol{\rho}|\varphi\rangle=\mathrm{Tr}(\boldsymbol{\rho}|\varphi\rangle\times\langle\varphi|)$ exists for any $\varphi\in\mathcal{H}$.

Furthermore, the invariance of $\mathcal{D}\{\boldsymbol{\pi}\}$ under unitary transformations gives

$$\mathbf{U}^{\dagger}\boldsymbol{\rho}\mathbf{U} = \int \mathcal{D}\{\boldsymbol{\pi}\}\delta(\langle \mathbf{U}^{\dagger}\mathbf{P}\mathbf{U}\rangle_{\boldsymbol{\pi}})\delta(\langle \mathbf{U}^{\dagger}\mathbf{Q}\mathbf{U}\rangle_{\boldsymbol{\pi}})\boldsymbol{\pi}. \tag{26}$$

This implies that $\boldsymbol{\rho}$ must be invariant under different transformations because of the δ distributions. Under parity we have $\mathbf{K}_P^{\dagger}\mathbf{P}\mathbf{K}_P=-\mathbf{P}$ and $\mathbf{K}_P^{\dagger}\mathbf{Q}\mathbf{K}_P=-\mathbf{Q}$, then $\mathbf{K}_P^{\dagger}\boldsymbol{\rho}\mathbf{K}_P=\boldsymbol{\rho}$. Under rescaling we have $\mathbf{R}_{\alpha}^{\dagger}\mathbf{P}\mathbf{R}_{\alpha}=e^{\alpha}\mathbf{P}$, and $\mathbf{R}_{\alpha}^{\dagger}\mathbf{Q}\mathbf{R}_{\alpha}=e^{-\alpha}\mathbf{Q}$ then $\mathbf{R}_{\alpha}^{\dagger}\boldsymbol{\rho}\mathbf{R}_{\alpha}=\boldsymbol{\rho}$ again. Finally under the operators $\mathbf{U}_t=\exp[(-(i\hbar t/2m)\mathbf{P}^2]$ of free evolution, we have $\mathbf{U}_t^{\dagger}\mathbf{P}\mathbf{U}_t=\mathbf{P}$ and $\mathbf{U}_t^{\dagger}\mathbf{Q}\mathbf{U}_t=\mathbf{Q}+\mathbf{P}t/m$, so $\mathbf{U}_t^{\dagger}\boldsymbol{\rho}\mathbf{U}_t=\boldsymbol{\rho}$.

We conclude that $\boldsymbol{\rho}$ must be invariant (at least) under the following family of unitary transformations $\{\mathbf{K}_P,\mathbf{R}_{\alpha},\mathbf{U}_t\}$.

2. Relations with integrals on phase space

If we multiply Eq. (14) by $a(p,q)$ and we perform integration on p and q we obtain

$$\int \mathcal{D}\{\boldsymbol{\pi}\}a(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}}) = \int \mathrm{d}p\,\mathrm{d}q\,a(p,q). \tag{27}$$

Moreover if we have two operators $\mathbf{A}$, $\mathbf{B}$ with their classical counterparts $\widetilde{A}(p,q),\widetilde{B}(p,q)$, and if we multiply the expression of $\widetilde{A}(p,q)$ by the function $\widetilde{B}(p,q)$, after an integration on p and q we obtain

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{B}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{A}\rangle_{\boldsymbol{\pi}} = \int \mathrm{d}p\,\mathrm{d}q\,\widetilde{B}(p,q)\widetilde{A}(p,q). \tag{28}$$

Since this expression is invariant by the exchange of $\widetilde{A}$ and $\widetilde{B}$, we deduce

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{B}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{A}\rangle_{\boldsymbol{\pi}} = \int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{A}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{B}\rangle_{\boldsymbol{\pi}}. \tag{29}$$

To go further, we must be able to specify the operator $\boldsymbol{\rho}$.

IV. THE QUANTUM PATH INTEGRAL AND THE WIGNER-WEYL TRANSFORMATION

A. The Wigner-Weyl transformation revisited

From the symmetry properties already analyzed, we know that the bounded self-adjoint operator $\boldsymbol{\rho}$ is invariant under the family of unitary transformations $\{\mathbf{K}_P,\mathbf{R}_{\alpha},\mathbf{U}_t\}$. So what are the possible $\boldsymbol{\rho}$? In fact the solution is

$$\boldsymbol{\rho} = Z_1 \mathbf{1}_{\mathcal{H}} + 2Z_2 \mathbf{K}_P, \tag{30}$$

where Z_1 and Z_2 are real numbers. We differ the proof to the appendix since it is rather technical.

The constant Z_1 leads to a constant contribution to $\boldsymbol{\rho}_{p,q}$ that can be eliminated, then we choose $Z_1=0$.

Let us define $\boldsymbol{\Omega}=2\mathbf{K}_P$ and $\boldsymbol{\Omega}_{p,q}=\mathbf{W}_{p,q}^{\dagger}\boldsymbol{\Omega}\mathbf{W}_{p,q}$, then $\boldsymbol{\rho}_{p,q}=Z_2\boldsymbol{\Omega}_{p,q}$. A direct calculation shows that

$$\mathrm{Tr}(\boldsymbol{\Omega}_{p',q'}^{\dagger}\boldsymbol{\Omega}_{p,q}) = \mathrm{Tr}(\boldsymbol{\Omega}_{p',q'}\boldsymbol{\Omega}_{p,q}) = 2\pi\hbar\ \delta(p'-p)\,\delta(q'-q). \tag{31}$$

Moreover for any operator $\mathbf{A}$,

$$\mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A}) = \int \mathrm{d}x\, e^{-(i/\hbar)px}\left\langle q+\frac{x}{2}\middle|\,\mathbf{A}\,\middle|q-\frac{x}{2}\right\rangle. \tag{32}$$

Then $\mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A})$ corresponds to the Wigner-Weyl transformation.

Furthermore our classical mapping $\mathbf{A}\to\mathcal{C}(\mathbf{A})$ verifies $\mathcal{C}(\mathbf{A})(p,q)=\mathrm{Tr}(\boldsymbol{\rho}_{p,q}\mathbf{A})$, then $\mathcal{C}(\mathbf{A})(p,q)=Z_2\,\mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A})$. But we know that $\mathcal{C}(\mathbf{1}_{\mathcal{H}})=1$, so $Z_2^{-1}=\mathrm{Tr}(\boldsymbol{\Omega}_{p,q})$ and we deduce that $Z_2=1$ from $\mathrm{Tr}(\boldsymbol{\Omega}_{p,q})=1$. We conclude that $\boldsymbol{\rho}_{p,q}=\boldsymbol{\Omega}_{p,q}$ and the classical mapping $\mathbf{A}\to\mathcal{C}(\mathbf{A})$ is exactly the Wigner-Weyl transformation.

So our axioms for the path integral uniquely define the symbol $\int\mathcal{D}\{\boldsymbol{\pi}\}$ for "integrals" involving functions $\boldsymbol{\pi}\to b(\langle\mathbf{P}\rangle_{\boldsymbol{\pi}},\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{A}\rangle_{\boldsymbol{\pi}}$.

Moreover, Eq. (24) implies

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\,\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\,\boldsymbol{\pi} = \boldsymbol{\Omega}_{p,q}. \tag{33}$$

Furthermore, we have the following expression of the path integral:

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\delta(p-\langle\mathbf{P}\rangle_{\boldsymbol{\pi}})\,\delta(q-\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{A}\rangle_{\boldsymbol{\pi}} = \mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A}). \tag{34}$$

In turn these relations induce new properties for the path integral.

B. Consequences for the path integral

Taking into account Eq. (33) we find

$$\mathbf{A} = \frac{1}{2\pi\hbar}\int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{A}(\langle\mathbf{P}\rangle_{\boldsymbol{\pi}},\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\,\boldsymbol{\pi} \quad \text{with } \widetilde{A}(p,q)=\mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A}). \tag{35}$$

Multiplying Eq. (34) by $\widetilde{B}(p,q)$ associated with the quantum observable $\mathbf{B}$, we find after integration

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{B}(\langle\mathbf{P}\rangle_{\pi},\langle\mathbf{Q}\rangle_{\pi})\langle\mathbf{A}\rangle_{\pi} = 2\pi\hbar\ \mathrm{Tr}[\mathbf{BA}]. \tag{36}$$

We can exchange $\mathbf{A}$ and $\mathbf{B}$ so

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\widetilde{A}(\langle\mathbf{P}\rangle\boldsymbol{\pi},\langle\mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle\mathbf{B}\rangle_{\boldsymbol{\pi}} = 2\pi\hbar\ \mathrm{Tr}[\mathbf{BA}]. \tag{37}$$

Specially if $\mathbf{B}$ is the identity, then $b=1$, so

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\langle \mathbf{A}\rangle_{\boldsymbol{\pi}} = \int \mathcal{D}\{\boldsymbol{\pi}\}\tilde{A}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}}) = 2\pi\hbar\ \mathrm{Tr}[\mathbf{A}]. \tag{38}$$

This implies

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\langle [\mathbf{A},\mathbf{B}]\rangle_{\boldsymbol{\pi}} = 0. \tag{39}$$

Using Eqs. (27) and (28) and Eqs. (36) and (38) we recover the well-known relations

$$\int \frac{\mathrm{d}p\ \mathrm{d}q}{2\pi\hbar}\tilde{A}(p,q) = \mathrm{Tr}\,\mathbf{A} \quad \text{and} \quad \int \frac{\mathrm{d}p\ \mathrm{d}q}{2\pi\hbar}\tilde{A}(p,q)\tilde{B}(p,q) = \mathrm{Tr}(\mathbf{AB}). \tag{40}$$

Always from Eqs. (29), (36), and (38), we have

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\langle \mathbf{AB}\rangle_{\boldsymbol{\pi}} = \int \mathcal{D}\{\boldsymbol{\pi}\}\tilde{A}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{B}\rangle_{\boldsymbol{\pi}} \tag{41}$$

or

$$\int \mathcal{D}\{\boldsymbol{\pi}\}\langle \mathbf{AB}\rangle_{\boldsymbol{\pi}} = \int \mathcal{D}\{\boldsymbol{\pi}\}\langle \mathbf{A}\rangle_{\boldsymbol{\pi}}\tilde{B}(\langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}}). \tag{42}$$

Finally Eq. (36) presents a special interest when we are looking for expectation values. If we assume that $\mathbf{D}$ is a density operator with a classical counterpart $\tilde{D}(p,q)$ then

$$\mathrm{Tr}(\mathbf{DA}) = \frac{1}{2\pi\hbar}\int \mathcal{D}\{\boldsymbol{\pi}\}\tilde{D}(\ \langle \mathbf{P}\rangle_{\boldsymbol{\pi}},\langle \mathbf{Q}\rangle_{\boldsymbol{\pi}})\langle \mathbf{A}\rangle_{\boldsymbol{\pi}}. \tag{43}$$

The probability law appears thanks to the classical function $\tilde{D}(p,q)$, while the observable is represented by the quantum quantity $\langle \mathbf{A}\rangle_{\boldsymbol{\pi}}$. This expression is very close to a classical formula of expectation value, but with an "integral" over quantum space.

V. CONCLUSION

Thanks to the structure of the fiber bundle, we have introduced an intuitive definition for the classical counterparts of quantum observables, using a "quantum path integral." The path integral formulation reveals hidden properties of the Wigner-Weyl transformation that in turn gives special relations for the path integral. Moreover we remark that while the Feymann path integral allows us to calculate quantum amplitudes by integration over classical trajectories, this new path integral allows us to define classical quantities by integration over quantum states. Of course the mathematical nature of the notation $\int \mathcal{D}\{\boldsymbol{\pi}\}$ remains unspecified and this needs a special study.

APPENDIX

In this appendix we will prove the uniqueness of $\boldsymbol{\rho}$ verifying the conditions: $\boldsymbol{\rho}$ is a bounded self-adjoint operator invariant under $\{\mathbf{K}_P,\mathbf{R}_\alpha,\mathbf{U}_t\}$. To investigate the solutions, we use the Wigner-Weyl transformation (with the notations previously introduced).

Let us assume that $\mathbf{A}$ is a bounded self-adjoint operator invariant under $\mathbf{K}_P$ and $\mathbf{R}_\alpha$ with a classical counterpart $a(p,q)=\mathrm{Tr}(\boldsymbol{\Omega}_{p,q}\mathbf{A})$.

We know that $a(p,q)$ can be a distribution, but since distributions are limits of functions we first investigate the case where $a(p,q)$ is a function. The hypothesis for $\mathbf{A}$ are translated into the following properties of a:

$$a(p,q) \text{ is real and even}, \quad a(e^{\alpha}p,e^{-\alpha}q) = a(p,q). \tag{A1}$$

This implies that

$$a(p,q) = F(pq) \quad \text{with } F \text{ real}. \tag{A2}$$

For convenience, let us write F as a Fourier transform,

$$a_f(p,q) = \int \frac{\mathrm{d}\alpha}{|\alpha|} f(\alpha) \exp\left(-2i\frac{pq}{\alpha\hbar}\right), \tag{A3}$$

with $f(-\alpha)^* = f(\alpha)$.

The corresponding operator $\mathbf{A}_f$ is obtained with the formula due to the Wigner-Weyl transformation

$$\int \frac{\mathrm{d}p\,\mathrm{d}q}{2\pi\hbar} a_f(p,q)\mathbf{\Omega}_{p,q}. \tag{A4}$$

This relation gives

$$\mathbf{A}_f = \int \mathrm{d}\alpha\, f(\alpha) \int \frac{\mathrm{d}k}{2\pi} |(\alpha-1)k\rangle\langle(\alpha+1)k|, \tag{A5}$$

where the kets $|k\rangle$ verify $\mathbf{P}|k\rangle = \hbar k|k\rangle$ and $\langle k|k'\rangle = 2\pi\delta(k-k')$.

Let us introduce the operators $\mathbf{\Delta}_\alpha$ defined as

$$\mathbf{\Delta}_\alpha = \int \frac{\mathrm{d}k}{2\pi} |(1-\alpha)k\rangle\langle(\alpha+1)k|, \tag{A6}$$

we notice that $\mathbf{\Delta}_{1/\alpha} = |\alpha|\mathbf{K}_p\mathbf{\Delta}_\alpha$.

If we divide the α domain into $|\alpha| \leqslant 1$ and $|\alpha| \geqslant 1$ in Eq. (A5) we obtain

$$\mathbf{A}_f = \mathbf{K}_P \int_{|\alpha|\leqslant 1} \mathrm{d}\alpha\, f(\alpha)\mathbf{\Delta}_\alpha + \int_{|\alpha|\geqslant 1} \frac{\mathrm{d}\alpha}{|\alpha|} f(\alpha)\mathbf{\Delta}_{1/\alpha}. \tag{A7}$$

Then if we define the independent functions f_1 and f_2 by $f_1(\alpha) = f(\alpha)$ for $|\alpha| \leqslant 1$ and $f_2(1/\alpha) = |\alpha| f(\alpha)$ for $|\alpha| \geqslant 1$ we obtain

$$\mathbf{A}_f = \mathbf{K}_P \int_{|\alpha|\leqslant 1} \mathrm{d}\alpha\, f_1(\alpha)\mathbf{\Delta}_\alpha + \int_{|\alpha|\leqslant 1} \mathrm{d}\alpha\, f_2(\alpha)\mathbf{\Delta}_\alpha. \tag{A8}$$

Moreover we want $\mathbf{A}_f$ to be invariant under $\mathbf{U}_t = \exp[-(i\hbar t/2m)\mathbf{P}^2]$. This is equivalent to the condition $[\mathbf{P}^2, \mathbf{A}_f] = 0$. But from the previous expression of $\mathbf{\Delta}_\alpha$ we deduce

$$[\mathbf{P}^2, \mathbf{\Delta}_\alpha] = -4\alpha \int \frac{\mathrm{d}k}{2\pi} (\hbar k)^2 |(1-\alpha)k\rangle\langle(\alpha+1)k|. \tag{A9}$$

So the condition $[\mathbf{P}^2, \mathbf{A}_f] = 0$ is equivalent to $\alpha f_1(\alpha) = \alpha f_2(\alpha) = 0$ and then $f_1(\alpha) = C_1\delta(\alpha)$ and $f_2(\alpha) = C_2\delta(\alpha)$. Replacing f_1 and f_2 into the expression of $\mathbf{A}_f$, we find $\mathbf{A}_f = C_1\mathbf{K}_P + C_2\mathbf{1}_\mathcal{H}$ since $\mathbf{\Delta}_0 = \mathbf{1}_\mathcal{H}$. Finally since $\mathbf{A}_f$ is self-adjoint C_1 and C_2 must be real.

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Reduced Gutzwiller formula with symmetry: Case of a finite group

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We consider a classical Hamiltonian H on $\mathbb{R}^{2d}$, invariant by a finite group of symmetry G, whose Weyl quantization $\hat{H}$ is a self-adjoint operator on $L^2(\mathbb{R}^d)$. If χ is an irreducible character of G, we investigate the spectrum of its restriction $\hat{H}_\chi$ to the symmetry subspace $L^2_\chi(\mathbb{R}^d)$ of $L^2(\mathbb{R}^d)$ coming from the decomposition of Peter-Weyl. We give reduced semiclassical asymptotics of a regularized spectral density describing the spectrum of $\hat{H}_\chi$ near a noncritical energy $E \in \mathbb{R}$. If $\Sigma_E := \{H=E\}$ is compact, assuming that periodic orbits are nondegenerate in Σ_E/G, we get a reduced Gutzwiller trace formula which makes periodic orbits of the reduced space Σ_E/G appear. The method is based upon the use of coherent states, whose propagation was given in the work of Combescure and Robert. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2184890]

I. INTRODUCTION

The purpose of this work is to give a Gutzwiller trace formula for a reduced quantum Hamiltonian in the framework of symmetries given by a finite group G of linear applications of the configuration space $\mathbb{R}^d$. This semiclassical trace formula will link the reduced spectral density to periodic orbits of the dynamical system in the classical reduced space, i.e., the space of G-orbits. [Results of this paper were presented without proof in a Note aux Comptes Rendus (see Ref. 3).]

The role that symmetry plays in quantum dynamics appeared since the beginning of the theory, and was emphasized by Hermann Weyl in the book. "The theory of groups and quantum mechanics" (Ref. 28). Pioneering physical results were given for models having a lot of symmetries. In the mathematical domain, first systematical investigations were done in 1978–1979, mainly for the eigenvalues counting function of the Laplacian on a Riemannian compact manifold simultaneously by Donnelly and Brüning and Heintze (see Refs. 2 and 7). Later, Guillemin and Uribe described the relation with closed trajectories in Refs. 12 and 13. In $\mathbb{R}^d$, a general study was done in the early 1980s for globally elliptic pseudodifferential operators, both in cases of compact finite and Lie groups, by Helffer and Robert (see Refs. 15 and 16) for high energy asymptotics, and later by El Houakmi and Helffer in the semiclassical setting (see Refs. 9 and 10). Main results were then given in terms of reduced asymptotics of Weyl type for a counting function of eigenvalues of the operator. Here, in a semiclassical study with a finite group of symmetry, we want to go one step beyond Weyl formulas, investigating oscillations of the spectral density, and establishing a Gutzwiller formula for the *reduced* quantum Hamiltonian. The case of a compact Lie group will be carried out in another paper (see Ref. 4).

Without symmetry, in 1971, Gutzwiller published for the first time his trace formula linking semiclassically the spectrum of a quantum Hamiltonian $\hat{H}$ near an energy E, to periodic orbits of the classical Hamiltonian system of H on $\mathbb{R}^{2d}$, lying in the energy shell $\Sigma_E := \{H=E\}$. This was one of the strongest illustrations of the so-called correspondence principle. Later, mathematical proofs

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were given (see, for example, Refs. 20, 21, 19, and 8), using various techniques like wave equation, heat equation, microlocal analysis, and more recently wave packets (see Ref. 5).

Coming back to classical dynamics, let $H:\mathbb{R}^{2d}\to\mathbb{R}$ be a smooth Hamiltonian with a finite group of symmetry G, such that H is G-invariant, i.e., suppose that there is an action M from G into $\mathrm{Sp}(d,\mathbb{R})$, the group of symplectic matrices of $\mathbb{R}^{2d}$, such that

$$H(M(g)z)=H(z),\quad \forall\, g\in G,\quad \forall\, z\in\mathbb{R}^{2d}. \tag{1.1}$$

The Hamiltonian system associated to H is

$$\dot{z}_t=J\nabla H(z_t),\quad \text{where } J=\begin{pmatrix}0 & I_d\\ -I_d & 0\end{pmatrix}. \tag{1.2}$$

In the framework of symmetry, specialists in classical dynamics are used to investigate this system in the space of G-orbits: $\mathbb{R}^{2d}/G$, also called the *reduced space*.

Here, for a quantum study with symmetry, it is therefore natural to expect a reduced Gutzwiller formula, linking semiclassically the spectrum of the *reduced* quantum Hamiltonian near the energy E to periodic orbits of the *reduced* classical dynamical system on Σ_E/G.

We now briefly describe our main result. First, we introduce our quantum reduction. We follow the same setting as in papers by Helffer and Robert:[15,16] let $H:\mathbb{R}^{2d}\to\mathbb{R}$ be a smooth Hamiltonian and G a finite subgroup of the linear group $\mathrm{Gl}(d,\mathbb{R})$. If $g\in G$, we set

$$M(g)(x,\xi):=({}^{t}g^{-1}x,{}^{t}g^{-1}\xi) \tag{1.3}$$

and we assume that H is G-invariant as in (1.1). As usual, we make suitable assumptions—see (3.5)—to have nice properties for the Weyl quantization of H (as functional calculus), which is defined as follows: for $u\in\mathcal{S}(\mathbb{R}^d)$,

$$\mathrm{Op}_h^w(H)u(x)=(2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}e^{(i/h)(x-y)\xi}H\left(\frac{x+y}{2},\xi\right)u(y)\mathrm{d}y\,\mathrm{d}\xi. \tag{1.4}$$

In particular, $\mathrm{Op}_h^w(H)$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d)$ and we denote by $D(\hat{H})$, $\hat{H}$ its self-adjoint extension.

G acts on the quantum space $L^2(\mathbb{R}^d)$ by $\tilde{M}$ defined for $g\in G$ by

$$\tilde{M}(g)(f)(x)=f(g^{-1}x),\quad \forall\, f\in L^2(\mathbb{R}^d),\quad \forall\, x\in\mathbb{R}^d. \tag{1.5}$$

If χ is an irreducible character of G, we set $d_\chi:=\chi(Id)$. Then, we define the symmetry subspace $L^2_\chi(\mathbb{R}^d)$ associated to χ, by the image of $L^2(\mathbb{R}^d)$ by the projector

$$P_\chi:=\frac{d_\chi}{|G|}\sum_{g\in G}\overline{\chi(g)}\tilde{M}(g), \tag{1.6}$$

$L^2(\mathbb{R}^d)$ splits into a Hilbertian sum of $L^2_\chi(\mathbb{R}^d)$'s (Peter-Weyl decomposition), and the property (1.1) implies that each $L^2_\chi(\mathbb{R}^d)$ is stable by $\hat{H}$. Our goal is to give semiclassical trace formulas for the restriction $\hat{H}_\chi$ of $\hat{H}$ to $L^2_\chi(\mathbb{R}^d)$, which will be called the *reduced quantum Hamiltonian*. We define the following *reduced regularized spectral density*:

$$\mathcal{G}_\chi(h):=\mathrm{Tr}\left(\psi(\hat{H}_\chi)f\left(\frac{E-\hat{H}_\chi}{h}\right)\right), \tag{1.7}$$

where ψ is smooth, compactly supported in a neighborhood $]E-\delta E,E+\delta E[$ of $E\in\mathbb{R}(\delta E>0)$ such that $H^{-1}([E-\delta E,E+\delta E])$ is compact [$\psi(\hat{H}_\chi)$ is an energy cutoff which is trace class], f is smooth and $\hat{f}$ (the Fourier transform of f) is compactly supported in $\mathbb{R}$. The case where $\mathrm{Supp}(\hat{f})$ is localized near zero is the one that leads to the Weyl formulas, and gives an asymptotic expansion

of the counting function of $\hat{H}_\chi$ (see Theorem 4.5, Corollary 4.7). Here we want to focus on the oscillating part of $\mathcal{G}_\chi(h)$. Thus we suppose that $0 \notin \mathrm{Supp}(\hat{f})$.

In order to state the theorem in terms of the reduced space, we need a smooth structure on Σ_E/G, and thus we suppose that the group acts freely on Σ_E, so that dynamics of H on Σ_E would descend to the quotient. Note that this is not an essential assumption, since we have proved the asymptotic without this hypothesis (see Theorem 4.8). The following result involves the quantity $\chi(g_{\bar{\gamma}})$, defined as follows.

If π denotes the projection on the quotient and $\bar{\gamma}$ is a periodic orbit in Σ_E/G if $\pi(\gamma)=\bar{\gamma}$, then, there is only one g_γ in G such that, $\forall z \in \gamma$, $M(g_\gamma)\Phi_{T^*_{\bar{\gamma}}}(z)=z$, where $T^*_{\bar{\gamma}}$ is the primitive period of $\bar{\gamma}$. If $\pi(\gamma_1)=\pi(\gamma_2)$ then $g_{\gamma 1}$ and $g_{\gamma 2}$ are conjugate elements of G, and we denote by $\chi(g_{\bar{\gamma}})$ the quantity $\chi(g_{\gamma 1})=\chi(g_{\gamma 2})$.

In order to have a finite number of periodic orbits of the reduced space involved in the trace formula, we will suppose that periodic orbits of Σ_E/G are *non-degenerate*, in the following sense: If $\bar{\gamma}$ is a periodic orbit of Σ_E/G, with primitive period $T^*_{\bar{\gamma}}$, and if $n \in \mathbb{Z}^*$ is such that $nT_{\bar{\gamma}^*} \in \mathrm{Supp}(\hat{f})$, then 1 is not an eigenvalue of the differential of the Poincaré map $P_{\bar{\gamma}}$ of $\bar{\gamma}$ in Σ_E/G at $nT_{\bar{\gamma}^*}$: $\ker[(\mathrm{d}P_{\bar{\gamma}})^n - Id]=\{0\}$. Then we have the following result.

Theorem 1.1: *Under previous assumptions, suppose that the group G acts freely on* Σ_E *and that periodic orbits of* Σ_E/G *are non–degenerate in the sense given above. We then have a complete asymptotic expansion of* $\mathcal{G}_\chi(h)$ *in powers of h, modulo an oscillating factor of the form* $e^{i(\alpha/h)}$ *as* $h \to 0^+$ *(see Theorem 4.8 for details). The first term is given by*

$$\mathcal{G}_\chi(h) = d_\chi \psi(E) \sum_{\substack{\bar{\gamma} \text{ periodic} \\ \text{orbit of } \Sigma_E/G}} \sum_{\substack{n \in \mathbb{Z}^* s.t. \\ nT^*_{\bar{\gamma}} \in \mathrm{Supp} f}} \hat{f}(nT^*_{\bar{\gamma}}) \overline{\chi(g^n_{\bar{\gamma}})} e^{(i/h) n S_{\bar{\gamma}}} \frac{T^*_{\bar{\gamma}} e^{i(\pi/2)\sigma_{\bar{\gamma},n}}}{2\pi \left|\det(\mathrm{d}P_{\bar{\gamma}})^n - Id\right|^{1/2}} + O(h),$$

where $S_{\bar{\gamma}} := \int_0^{T^*_{\bar{\gamma}}} p_s \dot{q}_s \mathrm{d}s$, $P_{\bar{\gamma}}$ *is the Poincaré map of* $\bar{\gamma}$ *in* Σ_E/G, *and* $\sigma_{\bar{\gamma},n} \in \mathbb{Z}$. *Other terms in* $O(h)$ *are distributions at* $\hat{f}$, *with support in the set of periods of orbits in* Σ_E/G.

Remark 1: The case with $0 \in \mathrm{Supp}(\hat{f})$ could have been included in the preceding theorem, and we would get a Weyl term in addition to this oscillating part. This term was already described by El Houakmi (see Ref. 9) for the leading contribution. See also Theorem 4.5, where we obtain slightly more detailed asymptotics for this Weyl part, by calculating the contribution of each g in G.

Remark 2: One could also consider a symmetry directly given in phase space $\mathbb{R}^d \times \mathbb{R}^d$, and set G as a finite subgroup of $\mathrm{Sp}(d,\mathbb{R})$. Then we would have to suppose that there exists a unitary action $\tilde{M}: G \to \mathcal{L}(L^2(\mathbb{R}^d))$ which is metaplectic, i.e., satisfies

$$\tilde{M}(g)^{-1}\, \mathrm{Op}^w_h(H)\tilde{M}(g) = \mathrm{Op}^w_h(H \circ g), \quad \text{for all } g \text{ in } G. \tag{1.8}$$

For a fixed g, there is always some $\tilde{M}(g)$ satisfying (1.8), but it is not unique [multiply $\tilde{M}(g)$ by a complex of modulus 1]. The difficulty is to find a $\tilde{M}$ that is also a group homomorphism.

The method used is close to the one of Ref. 5: unlike papers previously quoted, which used an approximation of the propagator $\exp[-i(t/h)H]$ by some FIO following the WKB method, we will use here the work of Combescure and Robert on the propagation of coherent states. This method avoids problems of caustics and looks simpler to us. Moreover, the symmetry behaves well with coherent states, and we get very pleasant formulas [see (3.10)]. Thanks to these wave packets, we first reduce the problem to an application of the generalized stationary phase theorem (Sec. III). Then we find minimal hypotheses for the critical set to be a smooth manifold, and to ensure that the transverse Hessian of the phase is nondegenerate. These hypotheses will be called G-clean flow conditions, and we get a theoretical asymptotic expansion of $\mathcal{G}_\chi(h)$ under these assumptions

(Theorem 4.4). Finally, as in the particular cases, we will show that these conditions are fulfilled on the one hand when $\hat{f}$ is supported near zero (Weyl term Theorem 4.5), and on the other hand when periodic orbits are nondegenerate (oscillating term, Theorem 4.8). In both cases, we calculate geometrically first terms of the asymptotic expansion, to make quantities of the reduced classical dynamics appear, as the energy level, periodic orbits and the Poincaré map. The symmetry of periodic orbits plays an important part in the result.

We found strong motivation in the work of physicists Lauritzen, Robbins, and Whelan.[17,18,23]

II. QUANTUM REDUCTION

A. Symmetry subspaces

We recall some basic facts on representations (see Refs. 26 and 27 or 22). A representation $\rho: G \to \mathrm{Gl}(E)$ of the group G on a finite dimensional complex vector space E is said to be irreducible if there is no nontrivial subspace of E stable by $\rho(g)$, for all g in G. The character $\chi_\rho: G \to \mathbb{C}$ of a representation is defined by $\chi_\rho(g) := \mathrm{Tr}(\rho(g))$, for $g \in G$. The degree of the representation ρ is denoted by d_{χ_ρ} and is the dimension of E. Two such representations are isomorphic if and only if they have the same character. We will denote by $\hat{G}$ the set of all irreducible characters, that is the set of characters of irreducible representations. Moreover, G finite implies $\hat{G}$ finite.

A representation $\widetilde{M}$ of G on a Hilbert space is said to be unitary if each $\widetilde{M}(g)$ is a unitary operator. This is the case of our representation $\widetilde{M}$ on the Hilbert space $L^2(\mathbb{R}^d)$ defined by (1.5) since $|\det(g)| = 1$. One can easily check that $\widetilde{M}$ is strongly continuous. Then, the Peter-Weyl theorem (see Refs. 27 or 22) says that if one set $L^2_\chi(\mathbb{R}^d) := P_\chi(L^2(\mathbb{R}^d))$, where P_χ is defined by (1.6), then the P_χ's are orthogonal projectors of sum identity, and we have the Hilbertian decomposition,

$$L^2(\mathbb{R}^d) = \overset{\perp}{\underset{\chi \in \hat{G}}{\oplus}} L^2_\chi(\mathbb{R}^d). \tag{2.1}$$

Furthermore, if $\chi \in \widetilde{G}$, then any irreducible subrepresentation of $\widetilde{M}$ in $L^2_\chi(\mathbb{R}^d)$ is of character χ, and a decomposition having such a property is unique. These $L^2_\chi(\mathbb{R}^d)$'s will be called here the *symmetry subspaces*.

One must think of them as a certain class of functions of $L^2(\mathbb{R}^d)$ having a certain symmetry linked to G and χ. For example, if $G = \{\pm Id_{\mathbb{R}^d}\}$, then we have two irreducible characters χ_+ and χ_- such that $L^2_{\chi_+}(\mathbb{R}^d)$ is the set of even functions of $L^2(\mathbb{R}^d)$, and $L^2_{\chi_-}(\mathbb{R}^d)$ is the set of odd functions. More generally, if χ is a character of degree 1, then χ is multiplicative, and we have

$$L^2_\chi(\mathbb{R}^d) = \{f \in L^2(\mathbb{R}^d) : \forall\, g \in G, \widetilde{M}(g)f = \chi(g)f\}.$$

This is in particular the case for Abelian groups. If $G \simeq \sigma_d$ is the symmetric group of permutation matrices acting on $\mathbb{R}^d$, then there is at least two characters of degree 1: χ_0, the trivial character (always equal to 1), and the signature ε. Thus we get

$$L^2_{\chi_0}(\mathbb{R}^d) = \{f \in L^2(\mathbb{R}^d) : \forall\, \sigma \in G,\ f(x_{\sigma(1)}, \ldots, x_{\sigma(d)}) = f(x_1, \ldots, x_d)\},$$

$$L^2_\varepsilon(\mathbb{R}^d) = \{f \in L^2(\mathbb{R}^d) : \forall\, \sigma \in G,\ f(x_{\sigma(1)}, \ldots, x_{\sigma(d)}) = \varepsilon(\sigma) f(x_1, \ldots, x_d)\}.$$

B. Reduced Hamiltonians

It is easy to check on the formula (1.4) that we have on $\mathcal{S}(\mathbb{R}^d)$,

$$\widetilde{M}(g)^{-1}\,\mathrm{Op}_h^w(H)\widetilde{M}(g)=\mathrm{Op}_h^w(H\circ M(g)),\quad \forall\, g\in G. \tag{2.2}$$

Thus we see that the property of G-invariance (1.1) is equivalent to the commutation of $\hat{H}$ with all $\widetilde{M}(g)$. In particular, it implies that $\hat{H}$ commutes with all P_χ's, and thus, $L^2_\chi(\mathbb{R}^d)$ is stable by $\hat{H}$. We can then define the operator that we plan to study: if $\chi\in\hat{G}$, set

$$D(\hat{H}_\chi):=L^2_\chi(\mathbb{R}^d)\cap D(\hat{H}).$$

The restriction $\hat{H}_\chi$ of $\hat{H}$ to $L^2_\chi(\mathbb{R}^d)$ is called the *reduced quantum Hamiltonian*, and is a self-adjoint operator on the Hilbert space $L^2_\chi(\mathbb{R}^d)$. If $f:\mathbb{R}\to\mathbb{C}$ is Borelian, then we have

$$[f(\hat{H}),P_\chi]=0,\quad D(f(\hat{H}_\chi))=D(f(\hat{H}))\cap L^2_\chi(\mathbb{R}^d),\quad f(\hat{H})=\sum_{\chi\in\hat{G}} f(\hat{H}_\chi)P_\chi,$$

$f(\hat{H}_\chi)$ is the restriction of $f(\hat{H})$ to $L^2_\chi(\mathbb{R}^d)$. Last, if $\sigma(A)$ denotes the spectrum of a self-adjoint operator A, then we have $\sigma(\hat{H})=\cup_{\chi\in\hat{G}}\sigma(\hat{H}_\chi)$. Moreover, the following trace formula will be essential for the rest of this paper.

If $f:\mathbb{R}\to\mathbb{R}$ is Borelian, and if $f(\hat{H})$ is trace class on $L^2(\mathbb{R}^d)$, then, for all $\chi\in\hat{G}$, $f(\hat{H}_\chi)$ is trace class on $L^2_\chi(\mathbb{R}^d)$ and

$$\mathrm{Tr}(f(\hat{H}_\chi))=\mathrm{Tr}(f(\hat{H})P_\chi). \tag{2.3}$$

Indeed, by completing a Hilbertian basis of $L^2_\chi(\mathbb{R}^d)$ into one of $L^2(\mathbb{R}^d)$, we have that $|f(\hat{H}_\chi)|^{1/2}$ is Hilbert-Schmidt, i.e., $f(\hat{H}_\chi)$ is trace class. Moreover the equality of traces is easily obtained by noting that if $\lambda\neq 0$, then $\mathrm{Ker}(f(\hat{H})\circ P_\chi-\lambda)=\mathrm{Ker}(f(\hat{H}_\chi)-\lambda)$.

C. Interpretation of the symmetry

The investigation of $\hat{H}_\chi$ provides informations on the spectrum of $\hat{H}$.

Lemma 2.1: If $\chi\in\hat{G}$ then eigenvalues of $\hat{H}_\chi$ have a multiplicity proportional to d_χ.

Indeed, if $F\subset L^2_\chi(\mathbb{R}^d)$ is an eigenspace of $\hat{H}_\chi$, then it is $\widetilde{M}$-invariant. One can decompose it into irreducible representations By the Peter-Weyl theorem, the only irreducible representation appearing is the one of character χ, and thus is of dimension d_χ. In particular, the operator $\hat{H}_\chi$ provides a lower bound for the multiplicity of some eigenvalues of $\hat{H}$.

Another remark: by splitting an eigenfunction of $\hat{H}$ on the symmetry subspaces, we get at least an eigenvector in one $L^2_\chi(\mathbb{R}^d)$. This means that each eigenspace of $\hat{H}$ contains an eigenfunction having a certain symmetry. As it is well known for the double-well potential ($G=\{\pm Id\}$), where eigenspaces are of dimension 1, this leads to an alternance of even/odd eigenspaces related to tunneling effect.

If $N_\chi(I)$ denotes the number of eigenvalues of $\hat{H}_\chi$ (with multiplicity) in an interval I of $\mathbb{R}$, and $N(I)$ the one of $\hat{H}$, then the quantity $N_\chi(I)/N(I)$ can be thought as the proportion of eigenfunctions of symmetry χ among those corresponding to eigenvalues of $\hat{H}$.

D. Examples

We give a few examples of Schrödinger Hamiltonians with a finite group of symmetry:

$$H(x,\xi):=|\xi|^2+V(x).$$

(1) $G=\{\pm Id\}$: Double well $V(x)=(x^2-1)^2$, harmonic or quadratic oscillator $V(x)=x^2$ or x^4, the well on the island $V(x)=(x^2+a)e^{-x^2}$ $(a>0)$. For the two first examples, $V(x)\to_{+\infty}+\infty$, so $\hat{H}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R})$ and with compact resolvent.
(2) $G\simeq\sigma_2$, $d=2$. Any potential satisfying $V(x,y)=V(y,x)$.
(3) Group of isometries of the triangle, $d=2$: $V(x,y)=\frac{1}{2}\ (x^2+y^2)^2-xy^2+\frac{1}{3}x^3$, which in polar coordinates is $\widetilde{V}(r,\theta)=V(r\cos\theta,r\sin\theta)=\frac{1}{2}r^2+\frac{1}{3}r^3\cos(3\theta)$ [see also the Hénon-Heiles potential: $V(x,y)=\frac{1}{2}(x^2+y^2)-xy^2+\frac{1}{3}x^3$, but one must look for the self-adjointness of this operator].
(4) Group of isometries of the square, $d=2$: $V(x,y)=\frac{1}{2}x^2y^2$.
(5) $G\simeq(\mathbb{Z}/2\mathbb{Z})^d$: harmonic oscillator with distinct frequencies: $V(x)=\langle Sx,x\rangle_{\mathbb{R}^d}$, with S symmetric positive definite matrix with eigenvalues pairwise distincts. In this case, $\hat{H}$ is still essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d)$ and with compact resolvent. This is one of the few cases where we can calculate periodic orbits of the dynamical system.

III. REDUCTION OF THE PROOF BY COHERENT STATES

We adapt here the method of Ref. 5. The essential tool is the use of coherent states. We refer to the Appendix where we recall basic things about it (see also Refs. 5 and 6). Note that, by an averaging argument (see Lemma 4.6), we could suppose that the group G is composed of *isometries*. For the moment, we still use the general expression of (1.3), to keep in mind the symplectic form of $M(g)$. We suppose that ψ and f are in $\mathcal{S}(\mathbb{R})$ such that $\mathrm{Supp}(\psi)\subset\,]E-\delta E,E+\delta E[$ and the Fourier transform $\hat{f}$ of f is with compact support. We know from Refs. 14 and 24, that, under hypothesis (3.5), $\psi(\hat{H})$ is trace class for small h, and, by formula (2.3), we have

$$\mathcal{G}_\chi(h)=\mathrm{Tr}\left(\psi(\hat{H}_\chi)f\left(\frac{E-\hat{H}_\chi}{h}\right)\right)=\frac{d_\chi}{|G|}\sum_{g\in G}\overline{\chi(g)}I_g(h),$$

where

$$I_g(h):=\mathrm{Tr}\left(\psi(\hat{H})f\left(\frac{E-\hat{H}}{h}\right)\widetilde{M}(g)\right).\tag{3.1}$$

Then, by Fourier inversion, we make the h-unitary quantum propagator $U_h(t):=e^{-i(t/h)\hat{H}}$ appear, and write

$$I_g(h)=\frac{1}{2\pi}\int_{\mathbb{R}}e^{i(tE/h)}\hat{f}(t)\mathrm{Tr}(\psi(\hat{H})U_h(t)\widetilde{M}(g))\mathrm{d}t.\tag{3.2}$$

Then we use the trace formula with coherent states—see (5.5)—to write

$$I_g(h)=\frac{(2\pi h)^{-d}}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}_a}e^{i(tE/h)}\hat{f}(t)m_h(\alpha,t,g)\mathrm{d}\alpha\,\mathrm{d}t,\tag{3.3}$$

where

$$m_h(\alpha,t,g):=\langle U_h(t)\varphi_\alpha;\widetilde{M}(g)^{-1}\psi(\hat{H})\varphi_\alpha\rangle_{L^2(\mathbb{R}^d)}.\tag{3.4}$$

Using an expansion of the type (3.6), with the same proof as in Ref. 5, we get the following lemma.

Lemma 3.1: There exists a compact set K in $\mathbb{R}^{2d}$ *such that*

$$\int_{\mathbb{R}^{2d}\setminus K} |m_h(\alpha,t,g)|\mathrm{d}\alpha = O(h^{+\infty})$$

uniformly with respect to $g \in G$ *and* $t \in \mathbb{R}$.

We can then suppose that $\Sigma_E := \{H=E\}$ is included in K, and choose a real cutoff function χ_1, compactly supported in $\mathbb{R}^{2d}$ and equal to 1 on K. Then, we classically write $1=\chi_1+(1-\chi_1)$ in (3.3), and settle problems at infinity in α. Besides, we want to use the functional calculus of Helffer and Robert[14,24] for the description of $\psi(\hat{H})$. Thus we make the following hypothesis: $\exists C>0$, $\exists C_\alpha>0$, $\exists m>0$ such that

$$\langle H(z)\rangle \leqslant C\langle H(z')\rangle\langle z-z'\rangle^m, \quad \forall\, z,z' \in \mathbb{R}^{2d},$$

$$\left|\partial_z^\alpha H(z)\right| \leqslant C_\alpha\langle H(z)\rangle, \quad \forall\, z \in \mathbb{R}^{2d}, \quad \forall\, \alpha \in \mathbb{N}^{2d}, \tag{3.5}$$

$$H \text{ has a lower bound on } \mathbb{R}^{2d}.$$

Then, we can write for $N_0 \in \mathbb{N}$,

$$\psi(\hat{H}) = \sum_{j=0}^{N_0} h^j \operatorname{Op}_h^w(a_j) + h^{N_0+1}R_{N_0+1}(h), \tag{3.6}$$

where $\mathrm{Supp}(a_j) \subset H^{-1}(]E-\delta E, E+\delta E[)$, $a_0(z)=\psi(H(z))$, with $\|R_{N_{0+1}}(h)\|\mathrm{Tr} \leqslant Ch^{-d}$.

We obtain

$$I_g(h) = \sum_{j=0}^{N_0} h^j I_g^j(h) + O(h^{-d}h^{N_0+1}). \tag{3.7}$$

Now, we are led to give a complete asymptotic expansion for a fixed j_0 in $\mathbb{N}$ of the quantity

$$I_g^{j_0}(h) = \frac{(2\pi h)^{-d}}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}_\alpha} e^{i(tE/h)}\cdot \hat{f}(t)\chi_1(\alpha)m_h^{j_0}(\alpha,t,g)\mathrm{d}\alpha\,\mathrm{d}t, \tag{3.8}$$

with

$$m_h^{j_0}(\alpha,t,g) := \langle U_h(t)\varphi_\alpha; \widetilde{M}(g)^{-1}\operatorname{Op}_h^w(a_{j_0})\varphi_\alpha\rangle_{L^2(\mathbb{R}^d)}. \tag{3.9}$$

For the right-hand term of the brackets in (3.9), we expand $\operatorname{Op}_h^w(a_{j0})\varphi_\alpha$ in powers of h, by Lemma 3.1 of Ref. 5. Namely, if $N \in \mathbb{N}^*$, then it exists $C_{d,N}>0$, such that for all $\alpha \in \mathbb{R}^{2d}$,

$$\left\| \operatorname{Op}_h^w(a_{j_0})\varphi_\alpha - \sum_{k=0}^{N} h^{h/2} \sum_{\gamma\in\mathbb{N}^{2d},|\gamma|=k} \frac{\partial^\gamma a_{j_0}(\alpha)}{\gamma!}\mathcal{T}_h(\alpha)\Lambda_h \operatorname{Op}_1^w(z^\gamma)\widetilde{\psi}_0 \right\|_{L^2(\mathbb{R}^d)} \leqslant C_{d,N}\cdot h^{(N+1)/2}.$$

Thanks to (2.2), using the definition (5.1) of $\mathcal{T}_h(\alpha)$, we have

$$\widetilde{M}(g)^{-1}\mathcal{T}_h(\alpha) = \mathcal{T}_h(M(g^{-1})\alpha)\widetilde{M}(g)^{-1}. \tag{3.10}$$

For the left-hand term of the brackets in (3.9), we use the theorem of propagation of coherent states given by Combescure and Robert (Refs. 5 and 6 or 25). If $M \in \mathbb{N}$, then we have

$$\left\| U_h(t)\varphi_\alpha - e^{i[\delta(t,\alpha)/h]}\mathcal{T}_h(\alpha_t)\Lambda_h\left[\sum_{j=0}^{M} h^{i/2}b_j(t,\alpha)(x)\cdot e^{(i/2)\langle M_0 x,x\rangle}\right]\right\|_{L^2(\mathbb{R}^d)} \leqslant C_{M,T}(\alpha)\cdot h^{(M+1)/2},$$

where $\alpha_t=\Phi_t(\alpha)$ is the solution of the system (1.2) with initial condition α (see the Appendix for other notations). After all, since there is no problem of control for α at infinity, we get

$$m_h^{j_0}(\alpha,t,g)=\sum_{k=0}^{2N}\sum_{j=0}^{2N-k} h^{j/2}h^{h/2}\sum_{|\gamma|=k}\frac{\partial^\gamma a_{j_0}(\alpha)}{\gamma!}e^{i[\delta(t,\alpha)/h]}\Upsilon_{j,\gamma}(\alpha,t,g,h)+O(h^{-d}h^{N+(1/2)}), \tag{3.11}$$

with

$$\Upsilon_{j,\gamma}(\alpha,t,g,h):=\langle \mathcal{T}_h(\alpha_t)\Lambda_h b_j(t,\alpha)e^{(i/2)\langle M_0 x,x\rangle};\mathcal{T}_h(M(g^{-1})\alpha)\Lambda_h\tilde{M}(g)^{-1}Q_\gamma\tilde{\psi}_0\rangle,$$

where Q_γ is the polynomial in d variables such that

$$\mathrm{Op}_1^w(z^\gamma)\tilde{\psi}_0=Q_\gamma.\,\tilde{\psi}_0. \tag{3.12}$$

In view of the Appendix, we have

$$\Lambda_h^*\mathcal{T}_h(-M(g^{-1})\alpha)\mathcal{T}_h(\alpha_t)\Lambda_h=e^{(i/2h)\langle M(g^{-1})\alpha,J\alpha_t\rangle}\mathcal{T}_1\left(\frac{\alpha_t-M(g^{-1})\alpha}{\sqrt{h}}\right).$$

Thus

$$\Upsilon_{j,\gamma}(\alpha,t,g,h)=e^{(i/2h)\langle M(g^{-1})\alpha,J\alpha_t\rangle}\left\langle \mathcal{T}_1\left(\frac{\alpha_t-M(g^{-1})\alpha}{\sqrt{h}}\right)b_j(t,\alpha)e^{(i/2)\langle M_0 x,x\rangle};\tilde{M}(g)^{-1}Q_\gamma\tilde{\psi}_0\right\rangle_{L^2}.$$

We will use the notation

$$\alpha=(q,p)\in\mathbb{R}^d\times\mathbb{R}^d \quad \text{and } (q_t,p_t):=\alpha_t=\Phi_t(\alpha).$$

Make the change of variable $g^{-1}y:=x-(q_t-g^{-1}q)/\sqrt{h}$ in the previous $\langle;\rangle_{L^2}$. Since G is compact, $|\det(g)|=1$, and we obtain after calculation:

$$\Upsilon_{j,\gamma}(\alpha,t,g,h)=\pi^{-d/4}e^{(i/h)\{[(qp+q_tp_t)/2]-{}^tgpq_t\}+(i/2)|gq_t-q|^2}\int_{\mathbb{R}^d}e^{-(1/2)\langle Ay,y\rangle+By}Q_\gamma\left(y+\frac{gq_t-q}{\sqrt{h}}\right)b_j(\alpha,t)(y)\mathrm{d}y,$$

where

$$A:=I-{}^tg^{-1}M_0g^{-1} \quad \text{and } \beta:=\frac{i}{\sqrt{h}}[(q-gq_t)+i({}^tg^{-1}p_t-p)]. \tag{3.13}$$

Then we set

$$Q_\gamma(x)=:\sum_{|\mu|\leqslant|\gamma|}\kappa_{\mu,\gamma}x^\mu \quad \text{and } b_j(t,\alpha)(x)=:\sum_{|\nu|\leqslant 3j}c_{\nu,j}(t,\alpha)x^\nu$$

(where $c_{\nu,j}$ is smooth in t, α). For the same reasons as in Ref. 5 [parity of Q_γ and $b_j(t,\alpha)$], only integer powers of h have nonzero coefficients. Then, we can expend Q_γ and $b_j(t,\alpha)$ and use the following calculus of the integral of a Gaussian.

Lemma 3.2: Let $A\in M_d(\mathbb{C})$ such that ${}^tA=A$, and that $\Re A$ is a positive definite matrix, $\beta\in\mathbb{C}^d$ and $\alpha\in\mathbb{N}^d$. Then A is invertible and

$$\int_{\mathbb{R}_x^d}e^{-(1/2)\langle Ax,x\rangle+\beta x}x^\alpha\,\mathrm{d}x=(2\pi)^{1/2}\det{}^{-1/2}(A)e^{(1/2)\langle A^{-1}\beta,\beta\rangle}\sum_{\eta\leqslant\alpha}(A^{-1}\beta)^\eta P_\eta(A),$$

where $P_\eta(A)$ *does not depend on* β, *and* $P_0(A)=1$ *(*$det_*^{-1/2}$ *is defined in* Ref. 5, *Theorem 3.3).*

We get

$$e^{i(t/i)E}e^{(i/h)\delta(t,\alpha)}\Upsilon_{j,\gamma}(\alpha,t,g,h)=\sum_{|\nu|\leqslant 3j}\sum_{|\mu|\leqslant|\gamma|}\kappa_{\mu,\gamma}c_{\nu,j}(t,\alpha)\sum_{\eta\leqslant\mu}\binom{\mu}{\nu}(2\pi)^{d/2}$$
$$\times\det{}_*^{-1/2}(I-i^tg^{-1}M_0g^{-1})\sum_{\sigma\leqslant\mu-\eta+\nu}(gq_t-q)^\eta[(I-i^tg^{-1}M_0g^{-1})^{-1}$$
$$\times(\beta_0)]^\sigma P_\sigma(A)h^{-(1/2)(|\sigma|+|\eta|)}\exp\left(\frac{i}{h}\varphi_E(t,\alpha,g)\right),$$

where $\beta_0:=\sqrt{h}\beta$, and

$$\varphi_E(t,\alpha,g)=tE+S(t,\alpha)+qp-{}^tgpq_t+\frac{i}{2}|gq_t-q|^2-\frac{i}{2}\langle A^{-1}\beta_0,\beta_0\rangle. \tag{3.14}$$

Thus, (3.8) and (3.9) give

$$I_g^{j_0}(h)=\frac{(2\pi h)^{-d}}{2\pi}\sum_{k=0}^{2N}\sum_{j=0}^{2N-k}h^{(i+h)/2}\sum_{|\gamma|=k}\sum_{|\nu|\leqslant 3j}\sum_{|\mu|\leqslant|\gamma|}\frac{\kappa_{\mu,\gamma}}{\pi^{d/2}\gamma!}(2\pi)^{d/2}\sum_{\eta\leqslant\mu}\binom{\mu}{\nu}L_{\eta,\nu,\mu,\gamma,j}(h)+O(h^{N+(1/2)-d}),$$

with

$$L_{\eta,\nu,\mu,\gamma,j}(h):=\sum_{\sigma\leqslant\mu-\eta+\nu}h^{-(1/2)(|\sigma|+|\eta|)}$$
$$\times\int_{\mathbb{R}_t}\int_{\mathbb{R}_a^{2d}}\exp\left(\frac{i}{h}\varphi_E(t,\alpha,g)\right)\hat{f}(t)\partial^\gamma a_{j_0}(\alpha)\chi_1(\alpha)D_{\sigma,\eta,\nu,j}(t,\alpha,g)\mathrm{d}\alpha\,\mathrm{d}t, \tag{3.15}$$

where

$$D_{\sigma,\eta,\nu,j}(t,\alpha,g):=c_{\nu,j}(t,\alpha)\det{}_*^{-1/2}(I-i^tg^{-1}M_0g^{-1})P_\sigma(A)[A^{-1}[(q-gq_t)+i({}^tg^{-1}p_t-p)]]^\sigma(gq_t-q)^\eta. \tag{3.16}$$

A tiresome but straightforward computation gives from (3.14) and (3.13),

$$\varphi_E=\varphi_1+i\varphi_2,$$

$$\varphi_1(t,\alpha,g):=(E-H(\alpha))t+\frac{1}{2}<M(g)^{-1}\alpha,J,\alpha>-\frac{1}{2}\int_0^t(\alpha_t-M(g^{-1})\alpha)J\dot{\alpha}_s\,\mathrm{d}s, \tag{3.17}$$

$$\varphi_2(t,\alpha,g):=\frac{i}{4}\langle(I-\hat{W}_t)(M(g)\alpha_t-\alpha);(M(g)\alpha_t-\alpha)\rangle,$$

where $\hat{W}_t:=\begin{pmatrix}W_t & -iW_t\\ -iW_t & -W_t\end{pmatrix}$ with $\frac{1}{2}(I+W_t):=(I-i^tg^{-1}M_0g^{-1})^{-1}$.

Lemma 3.3: We have $\|W_t\|_{\mathcal{L}(\mathbb{C}^d)}<1$.

Proof: We introduce the Siegel half-plane,

$$\Sigma_d:=\{Z\in M_d(\mathbb{C}):{}^tZ=Z,\text{ and }\Im Z\text{ is positive definite}\}.$$

We know from Ref. 11, pp. 202 and 203 that if $Z\in\Sigma_d$, then $\|(I-iZ)^{-1}(I+iZ)\|_{\mathcal{L}(\mathbb{C}^d)}<1$. Now, we can take $Z={}^tg^{-1}M_0g^{-1}$. Indeed M_0 is symmetric, and, since $F_\alpha(t)$ is symplectic, we have

$$\forall X \in \mathbb{R}^d, \quad \Im({}^tX \cdot M_0 X) = |(A+iB)^{-1}X|^2_{\mathbb{C}^d}.$$

Thus $Z \in \Sigma_d$. The proof is clear if we note that $(I - i^t g^{-1} M_0 g^{-1})^{-1}(I + i^t g^{-1} M_0 g^{-1}) = W_t$. □

We are led to use a stationary phase theorem to get an expansion of each $L_{\eta,\nu,\mu,\gamma,j}(h)$ in powers of h. Note that the term $D_{\sigma,\eta,\nu,j}$ in (3.16) and its derivatives are vanishing on the critical set of the phase for derivatives up to $|\sigma|+|\eta|$ [see (4.1)]. Therefore, when applying the stationary phase theorem to $L_{\eta,\nu,\mu,\gamma,j}(h)$, the first terms of the asymptotic will vanish up to $h^{(1/2)(|\sigma|+|\eta|)}$. This fact compensates for the term in $h^{-(1/2)(|\sigma|+|\eta|)}$, at the beginning of the expression of $L_{\eta,\nu,\mu,\gamma,j}(h)$ in (3.15).

IV. THE STATIONARY PHASE PROBLEM

Now, we fix g in G and we want to find the conditions under which we will be able to apply the stationary phase theorem under the form of Ref. 5 (Theorem 3.3) on $L_{\eta,\nu,\mu,\gamma,j}(h)$. A necessary and sufficient condition will be called g-clean flow. Then we will give particular cases for which this criterium is satisfied (see Secs. IV A and IV B). Our method will first consist of calculating the critical set of the phase φ_E and its Hessian. Then we will calculate the kernel of this Hessian, and, under assumption of smoothness of the critical set, we will describe the conditions for this kernel to be equal to the tangent space of the critical set. In this section, since g is fixed in G, we will denote $\varphi_E(t,z,g)$ by $\varphi_{E,g}(t,z)$, for $z \in \mathbb{R}^{2d}$ and $t \in \mathbb{R}$.

A. Computations and *g*-clean flow

Computation of the critical set:

$$\text{Let } \mathcal{C}_{E,g} := \{a \in \mathbb{R} \times \mathbb{R}^{2d} : \Im(\varphi_{E,g}(a)) = 0, \nabla\varphi_{E,g}(a) = 0\}.$$

Proposition 4.1: The critical set is

$$\mathcal{C}_{E,g} = \{(t,z) \in \mathbb{R} \times \mathbb{R}^{2d} : z \in \Sigma_E, M(g)\Phi_t(z) = z\}, \tag{4.1}$$

where $(t,z) \mapsto \Phi_t(z)$ *is the flow of the system (1.2).*

Proof:

$$\Im\varphi_E(t,z,g) = \Re\varphi_2(t,z,g) = 1/4|z_t - M(g^{-1})z|^2 - \tfrac{1}{4}\Re\langle \hat{W}_t(M(g)z_t - z); M(g)z_t - z\rangle_{\mathbb{R}^{2d}}.$$

We note that, if a and b are in $\mathbb{R}^d$, then

$$\langle \hat{W}_t(a,b);(a,b)\rangle_{\mathbb{R}^{2d}} = \langle W_t(a-ib);(a-ib)\rangle_{\mathbb{R}^d}.$$

Thus,

$$\Im\varphi_E(t,z,g) = 0 \Leftrightarrow |z_t - M(g^{-1})z|^2 = \Re\langle W_t\beta,\beta\rangle_{\mathbb{R}^d} = \Re\langle W_t\beta,\bar{\beta}\rangle_{\mathbb{C}^d},$$

where

$$\beta := (gq_t - q) - i({}^tg^{-1}p_t - p).$$

Therefore, by Lemma 3.3, we have $\Im\varphi_E(t,z,g) = 0 \Leftrightarrow \Phi_t(z) = M(g^{-1})z$.

Computation of the gradient of φ_1:

$$\partial_t\varphi_1(t,z,g) = E - H(z) - \tfrac{1}{2}\langle (z_t - M(g^{-1})z); J\dot{z}_t\rangle,$$

$$\nabla_z\varphi_1(t,z,g) = \tfrac{1}{2}({}^tM(g^{-1}) + {}^tF_z(t))J(z_t - M(g^{-1})z).$$

Computation of the gradient of φ_2:

$$4\partial_t\varphi_2(t,z,g) = 2\langle (I-\hat{W}_t)(M(g)z_t - z); M(g)\dot{z}_t\rangle - \langle \partial_t(\hat{W}_t)(M(g)z_t - z); (M(g)z_t - z)\rangle,$$

$$4\nabla_z\varphi_2(t,z,g) = 2({}^tF_z(t){}^tM(g) - I)(I-\hat{W}_t)(M(g)z_t - z) - {}^t[\partial_z(\hat{W}_t)(M(g)z_t - z)](M(g)z_t - z).$$

Thus, we see that $(t,z,g) \in \mathcal{C}_{E,g}$ if and only if $\Phi_t(z) = M(g^{-1})z$ and $H(z) = E$. □

Computation of Hess $\varphi_{E,g}(t,z)$: We first need some formulas coming from the symmetry that will be helpful for the computation. We recall that $F_z(t) = \partial_z(\Phi_t(z))$. By differentiating formula (1.1), we get

$$\nabla H(M(g)z) = {}^tM(g^{-1})\,\nabla H(z), \quad \forall\, z \in \mathbb{R}^{2d}, \quad \forall\, g \in G. \tag{4.2}$$

This formula implies that we have also

$$\Phi_t(M(g)z) = M(g)\Phi_t(z), \quad \forall\, z \in \mathbb{R}^{2d}, \quad \forall\, g \in G, \quad \forall\, t \in \mathbb{R} \text{ such that } \Phi_t(z) \text{ exists}. \tag{4.3}$$

Moreover we recall that, since $M(g)$ is symplectic, we have

$$JM(g) = {}^tM(g^{-1})J \quad \text{and } M(g)J = J{}^tM(g^{-1}). \tag{4.4}$$

Finally, if t and z are such that $M(g)\Phi_t(z) = z$, then we have

$$(M(g)F_z(t) - I)J\nabla H(z) = 0 \quad \text{and } ({}^tF_z(t){}^tM(g) - I)\,\nabla H(z) = 0. \tag{4.5}$$

The second identity comes from the first since $M(g)F_z(t)$ is symplectic. For this first relation, one can differentiate at $s = t$ the equation:

$$\Phi_t(M(g)\Phi_s(z)) = \Phi_s(z).$$

With these formulas, it is easy to find the following.

Proposition 4.2:

$$\text{Hess } \varphi_{E,g}(t,z) = \begin{pmatrix} \frac{i}{2}\langle l(I-\hat{W}_t)J\nabla H(z); J\nabla H(z)\rangle & -{}^t\nabla H(z) + \frac{i}{2}{}^t[({}^tF_z(t){}^tM(g) - I)(I-\hat{W}_t)J\nabla H(z)] \\ -\nabla H(z) + \frac{i}{2}({}^tF_z(t){}^tM(g) - I)(I-\hat{W}_t)J\nabla H(z) & \frac{1}{2}[JM(g)F_z(t) - {}^t(M(g)F_z(t))J] + \frac{i}{2}({}^tF_z(t){}^tM(g) - I)(I-\hat{W}_t)(M(g)F_z(t) - I) \end{pmatrix}.$$

Computation of the real kernel of the Hessian: If $A \in M_n(\mathbb{C})$, then we define $\ker_{\mathbb{R}}(A) := \{x \in \mathbb{R}^n : A(x) = 0\} = \ker(\Re(A)) \cap \ker(\Im(A))$.

Proposition 4.3: Let $(t,z) \in \mathcal{C}_{E,g}$. *Then the real kernel of the Hessian is*

$$\ker_{\mathbb{R}} \text{Hess } \varphi_{E,g}(t,z) = \{(\tau,\alpha) \in \mathbb{R} \times (\mathbb{R}\,\nabla H(z))^{\perp} : \tau J\nabla H(z) + (M(g)F_z(t) - Id)\alpha = 0\}. \tag{4.6}$$

Proof: Let $\tau \in \mathbb{R}$ and $\alpha \in \mathbb{R}^{2d}$. We set

$$x := \tau J\nabla H(z) + (M(g)F_z(t) - I)\alpha.$$

Let us denote by $\hat{W}_1$ and $\hat{W}_2$ the real and imaginary part of $\hat{W}_t$. Then, $(\tau,\alpha) \in \ker_{\mathbb{R}} \text{Hess } \varphi_{E,g}(t,z)$ if and only if

$$\langle \hat{W}_2 J\nabla H(z); x\rangle = 2\langle \nabla H(z); \alpha\rangle, \tag{4.7}$$

$$\langle (I-\hat{W}_1)J\nabla H(z); x\rangle = 0, \tag{4.8}$$

$$({}^tF_z(t){}^tM(g)-I)(I-\hat{W}_1)x=0, \tag{4.9}$$

and

$$-2\tau\nabla H(z)+[JM(g)F_z(t)-{}^t(M(g)F_z(t))J]\alpha+({}^tF_z(t){}^tM(g)-I)\hat{W}_2x=0.$$

We multiply this last identity by $(M(g)F_z(t))J$, we note that $\hat{W}_2=J\hat{W}_1$ and recall that $M(g)F_z(t)$ is symplectic to obtain the equivalent identity,

$$(M(g)F_z(t)-I)(\hat{W}_1-I)x=2x. \tag{4.10}$$

Now, if $(\tau,\alpha)\in\ker_{\mathbb{R}}$ Hess $\varphi_{E,g}(t,z)$, then, by (4.10) and (4.9), we have

$$\langle x,(I-\hat{W}_1)x\rangle=0, \quad \text{i.e., } |x|^2=\langle\hat{W}_1x,x\rangle.$$

By Lemma 3.3, $\|\hat{W}_1\|_{\mathcal{L}(\mathbb{R}^{2d})}<1$, thus $x=0$, and by (4.7), $\nabla H(z)\perp\alpha$.

Conversely, if $x=0$ and $\nabla H(z)\perp\alpha$, then, we have (4.7)–(4.10). Thus $(\tau,\alpha)\in\ker_{\mathbb{R}}$ Hess $\varphi_{E,g}(t,z)$. □

We are now able to describe the conditions under which we can apply the generalized stationary phase theorem on $L_{\eta,\nu,\mu,\gamma,j}(h)$: we easily check the positivity of the imaginary part of the phase $\varphi_{E,g}$ by Lemma 3.3. Moreover, if $\mathcal{C}_{E,g}$ is a union of smooth submanifolds of $\mathbb{R}\times\mathbb{R}^{2d}$, if $X\in\mathcal{C}_{E,g}$, then the Hessian of $\varphi_{E,g}(X)$ is nondegenerate on the normal space $N_X\mathcal{C}_{E,g}$ if and only if $\ker_{\mathbb{R}}$ Hess $\varphi_{E,g}(X)\subset T_X\mathcal{C}_{E,g}$, the tangent space of $\mathcal{C}_{E,g}$ at X. Besides, note that, by the nonstationary phase theorem, we can restrict this hypothesis to points X in $\mathrm{Supp}(\hat{f})\times\mathrm{Supp}(a_{j_0})$.

Definition: Let $g\in G$, $T>0$, such that $\mathrm{Supp}(\hat{f})\subset]-T,T[$, and

$$\Psi_g:=\begin{cases}\,]-T;T[\times\Sigma_E\to\mathbb{R}^{2d}\ ,\\ (t,z)\mapsto M(g)\Phi_t(z)-z.\end{cases}$$

We say that the flow is g-clean on $]-T,T[\times\Sigma_E$ if zero is a weakly regular value of Ψ, i.e.,

$$\Psi_g^{-1}(\{0\})=:\mathcal{C}_{E,g} \text{ is a finite union of smooth submanifolds of } \mathbb{R}\times\mathbb{R}^{2d},$$

$$\forall(t,z)\in\mathcal{C}_{E,g},\quad T_{(t,z)}\mathcal{C}_{E,g}=\ker d_{(t,z)}\Psi_g.$$

We say that the flow is G-clean on $]-T,T[\times\Sigma_E$ if it is g-clean for all g in G.

By Proposition 4.3, we see that if $(t,z)\in\mathcal{C}_{E,g}$, then $\ker d_{(t,z)}\Psi_g=\ker_{\mathbb{R}}$ Hess $\varphi_{E,g}(t,z)$. Thus, if we only know that the support of $\hat{f}$ is in $]-T,T[$, then the g-clean flow condition is the minimal hypothesis under which we can apply the stationary phase theorem to $L_{\eta,\nu,\mu,\gamma,j}(h)$. Therefore, we can state the theorem.

Theorem 4.4: Reduced trace formula with G-clean flow.

Let G be a finite subgroup of $\mathrm{Gl}(\mathbb{R},d)$ *and* $H:\mathbb{R}^{2d}\to\mathbb{R}$ *a smooth Hamiltonian G-invariant. Suppose that $E\in\mathbb{R}$ is such that there exists $\delta E>0$ such that $H^{-1}([E-\delta E,E+\delta E])$ is compact, and $\Sigma_E=\{H=E\}$ has no critical points. Make hypothesis (3.5). Let f* and *ψ be real functions in $\mathcal{S}(\mathbb{R})$ such that $\mathrm{Supp}(\psi)\subset]E-\delta E,E+\delta E[$ and f is compactly supported in $]-T,T[$, where $T>0$. Suppose that the flow is G-clean on $]-T,T[\times\Sigma_E$. Then the spectral density*

$$\mathcal{G}_\chi(h)=\frac{d_\chi}{|G|}\sum_{g\in G}\overline{\chi(g)}I_g(h)$$

has a complete asymptotic expansion as $h\to0^+$ [where the definition of $I_g(h)$ is given by (3.1)]. Moreover, if $g\in G$, and, if $[\mathcal{C}_{E,g}]$ denotes the set of connected components of $\mathcal{C}_{E,g}$, then the quantity $\int_0^t p_sq_s\,\mathrm{d}s$ is constant on each element Y of $[\mathcal{C}_{E,g}]$, denoted by $S_{Y,g}$, and we have the following expansion:

$$I_g(h)\sum_{Y\in[\mathcal{C}_{E,g}]}(2\pi h)^{(1-\dim Y)/2}e^{(i/h)S_{Y,g}}\frac{1}{2\pi}\left(\int_Y \hat{f}(t)\psi(E)d_g(t,z)\mathrm{d}\sigma_Y(t,z)+\sum_{j\geqslant 1}h^j a_{j,Y}\right)+O(h^{+\infty}),$$

where $a_{j,Y}$ *are distributions in* $\hat{f}\otimes(\psi\circ H)$ *with support in* Y, *and the density* $d_g(t,z)$ *is defined by*

$$d_g(t,z):=\det{}_*^{-1/2}\left(\frac{\varphi''_{E,g}(t,z)_{|\mathcal{N}_{(t,z)}Y}}{i}\right)\det{}_*^{-1/2}\left(\frac{A+iB-i(C+iD)}{2}\right). \tag{4.11}$$

$\varphi_{E,g}$ *is given by (3.17) and* A,B,C,D *are the* $d\times d$ *blocks of the matrix* $F_z(t):=\partial_z(\Phi_t(z))$ [*see (A8)*].

Remark: Without symmetry, this theorem can be compared to papers by Paul and Uribe (cf. Refs. 20 and 21) or to the Gutzwiller formula in the Ph.D. thesis of Dozias,[8] see also Ref. 19. A notion of clean flow is also present in Ref. 5. The density $d_g(t,z)$ is difficult to compute in general, even without symmetry. The purpose of the next sections is to calculate it in two special cases: when $\hat{f}$ is supported near zero (Weyl part), and under an assumption of nondegenerate periodic orbits of the classical flow in Σ_E (oscillating part).

Proof: As we have seen before, we can apply the stationary phase theorem on each $L_{\eta,\nu,\mu,\gamma,j}(h)$, which gives an expansion of each $I_g^{j_0}(h)$ and each $I_g(h)$. The first term is given by

$$I_g(h)\underset{h\to 0^+}{\sim}\frac{(2\pi h)^{-d}}{2\pi}\int_{\mathbb{R}_t}\int_{\mathbb{R}^{2d}_\alpha}\chi_2(\alpha)\hat{f}(t)\psi(H(\alpha))\det{}_*^{-1/2}\left(\frac{A+iB-i(C+iD)}{2}\right)e^{(i/h)\varphi_{E,g}(t,\alpha)}\,\mathrm{d}t\,\mathrm{d}\alpha.$$

By definition of $\mathcal{C}_{E,g}$, $\varphi_{E,g}$ is constant on each connected component of $\mathcal{C}_{E,g}$, and equal to

$$\varphi_{E,g}(t,\alpha)=S(\alpha,t)+Et=\int_0^t p_s\dot{q}_s\,\mathrm{d}s,\quad \text{where } (q_s,p_s)=\Phi_s(\alpha).$$

This ends the proof of Theorem 4.4. □

B. The Weyl part

We now deal with one case which leads to an asymptotic expansion at the first order of the counting function of $\hat{H}_\chi$ in an interval of $\mathbb{R}$. Fix g in G and define

$$\mathcal{L}_{E,g}:=\{t\in\mathbb{R}:\exists\, z\in\Sigma_E: M(g)\Phi_t(z)=z\}. \tag{4.12}$$

Theorem 4.5: *Let* G *be a finite subgroup of* $\mathrm{Gl}(\mathbb{R},d)$ *and* $H:\mathbb{R}^{2d}\to\mathbb{R}$ *a smooth* G*-invariant Hamiltonian. Let* $E\in\mathbb{R}$ *be such that* $H^{-1}([E-\delta E,E+\delta E])$ *is compact for some* $\delta E>0$, *and that* $\Sigma_E=\{H=E\}$ *has no critical points. Make hypothesis (3.5). Let* f *and* ψ *be real functions in* $\mathcal{S}(\mathbb{R})$ *with* $\mathrm{Supp}(\psi)\subset]E-\delta E,E+\delta E[$ *and* $\hat{f}$ *compactly supported. For* g *in* G, *we set*

$$\nu_g:=\dim\ker(g-Id_{\mathbb{R}^d}),\quad F_g:=\ker(M(g)-Id_{\mathbb{R}^{2d}})\quad \text{and } \widetilde{F}_g:=\ker(g-Id_{\mathbb{R}^d}).$$

Set

$$I_{g,E}(h):=Tr\left(\psi(\hat{H})f\left(\frac{E-\hat{H}}{h}\right)\widetilde{M}(g)\right).$$

Then, under previous assumptions, we have the following:

IF $\mathrm{Supp}\,\hat{f}\cap\mathcal{L}_{E,g}=\emptyset$, *then* $I_{g,E}(h)=O(h^{+\infty})$.

If $\mathrm{Supp}\,\hat{f}\cap\mathcal{L}_{E,g}=\{0\}$ *then we have the following expansion modulo* $O(h^{+\infty})$:

$$I_{g,\lambda}(h)\asymp h^{1-\nu_g}\sum_{k\geqslant 0}c_k(\hat{f},g)h^k,\quad \text{as } h\to 0^+ \tag{4.13}$$

uniformly in λ *in a small neighborhood of* E, *where* $\hat{f}\mapsto c_k(\hat{f},g)$ *is a distribution in* $\hat{f}$ *with support in* $\{0\}$, *and, if* $d(\Sigma_\lambda\cap F_g)$ *denotes the Euclidian measure on* $\Sigma_\lambda\cap F_g$, *then we have*

$$c_0(\hat{f},g)=\psi(\lambda)\hat{f}(0)\frac{(2\pi)^{-\nu_g}}{\det(\ (Id_{\mathbb{R}^d}-g)|_{\widetilde{F}_g^{\perp}})}\int_{\Sigma_\lambda\cap F_g}\frac{d(\Sigma_\lambda\cap F_g)(z)}{|\nabla H(z)|}. \tag{4.14}$$

Remark 1: The oscillating term of Theorem 4.4 is now vanishing, since, for $g\in G$, $S_{Y,g}=0$ when $Y=\{0\}\times(\Sigma_E\cap F_g)$. Moreover, it is easy to see that, since Σ_E is compact and noncritical, zero is isolated in $\mathcal{L}_{E,g}$. Thus the hypothesis $\mathrm{Supp}\,\hat{f}\cap\mathcal{L}_{E,g}=\{0\}$ is fulfilled if $\hat{f}$ is supported close enough to zero.

Remark 2: Theorem 4.5 slightly improves the previous result of El Houakmi given in Ref. 9, by the computation of (4.14). Note that the leading term of $\mathcal{G}_\chi(h)$ is obtained for $g=Id$, and

$$\mathcal{G}_\chi(h)=\frac{d_\chi^2}{|G|}\psi(E)\hat{f}(0)(2\pi h)^{1-d}\frac{1}{2\pi}\int_{\Sigma_E}\frac{\mathrm{d}\Sigma_E}{|\nabla H|}+O(h^{2-d}),\quad \text{as } h\to 0^+.$$

Proof: If $\mathrm{Supp}\,\hat{f}\cap\mathcal{L}_{E,g}=\emptyset$, then $(\mathrm{Supp}(\hat{f})\times\mathbb{R}^{2d})\cap\mathcal{C}_{E,g}=\emptyset$, and by the nonstationary phase theorem, we get the result.

Now suppose that $\mathrm{Supp}\,\hat{f}\cap\mathcal{L}_{E,g}=\{0\}$. Then we have

$$\mathcal{C}_{E,g}\cap(\mathrm{Supp}(\hat{f})\times\mathbb{R}^{2d})=\{0\}\times(\Sigma_E\cap F_g). \tag{4.15}$$

Lemma 4.6: For the rest of the proof, one can assume that G *is composed of isometries.*

Proof: We recall that, since G is compact, there exists some S_0, symmetric $d\times d$ positive definite matrix, such that

$$G_0:=S_0^{-1}GS_0 \text{ is a subgroup of the orthogonal group } O(d,\mathbb{R}). \tag{4.16}$$

Indeed, classically, the following scalar product on $\mathbb{R}^d$:

$$\langle\langle x,y\rangle\rangle:=\frac{1}{|G|}\sum_{g\in G}\langle gx;gy\rangle,\quad \forall\, x,y\in\mathbb{R}^d,$$

is invariant by G, and one can take S_0 such that $\langle\langle x,y\rangle\rangle=\langle S_0^2x,y\rangle$ for all x,y in $\mathbb{R}^d$. Thus, we can define a new G_0-invariant Hamiltonian,

$$H_0(z):=H(M(S_0)z),\quad \textit{where } M(S_0):=\begin{pmatrix}S_0 & 0\\ 0 & {}^tS_0^{-1}\end{pmatrix}.$$

If $\chi\in\hat{G}$, then one can define $\chi_0: G_0\to\mathbb{C}$ by

$$\chi_0(g_0):=\chi(S_0g_0S_0^{-1}).$$

Then it is easy to check that $\chi_0\in\hat{G}_0$ and that the application $\chi\mapsto\chi_0$ is bijective from $\hat{G}$ to $\hat{G}_0$. Moreover, identity (2.2) implies that

$$\mathrm{Op}_h^w(H_0)=\widetilde{M}(S_0)^{-1}\,\mathrm{Op}_h^w(H)\widetilde{M}(S_0).$$

If $\chi\in\hat{G}$, then we can define

$$\widetilde{P}_{\chi_0}:=\frac{d_{\chi_0}}{|G_0|}\sum_{g_0\in G_0}\overline{\chi_0(g_0)}\widetilde{M}(g_0).$$

Then we have $\widetilde{P}_{\chi 0}=\widetilde{M}(S_0)^{-1}P_\chi\widetilde{M}(S_0)$. Therefore, if $f(\hat{H})$ is trace class, then $f(\hat{H}_0)$ also, and we have

$$\mathrm{Tr}(f(\hat{H}_\chi)) = \mathrm{Tr}(f(\hat{H})P_\chi) = \mathrm{Tr}\ (f(\hat{H}_0)\widetilde{P}_{\chi_0})),$$

by cyclicity of trace. This remark can be applied in particular for the trace (1.7). Moreover, if $g \in G$, if $g_0 := S_0^{-1} g S_0$, then $\mathrm{Tr}(f(\hat{H})\widetilde{M}(g)) = \mathrm{Tr}(f(\hat{H}_0)\widetilde{M}(g_0))$. Finally, it is easy to check that hypotheses for (H,G) hold for (H_0,G_0), and that coefficients of the asymptotic have the same expression in terms of (H_0,G_0) as in (H,G). □

From now on, we suppose that G is composed of isometries, without loss of generality. First, we remark that Σ_E and F_g are transverse submanifolds of $\mathbb{R}^{2d}$. Indeed, if $z \in \Sigma_E \cap F_g$, then, by (4.2), since g is an isometry, we have $\nabla H(z) \in F_g$, thus $F_g + [\mathbb{R}\nabla H(z)]^\perp = \mathbb{R}^{2d}$. Therefore

$$\mathcal{T}_{(0,z)}\mathcal{C}_{E,g} = \{0\} \times [F_g \cap [\mathbb{R}\nabla H(z)]^\perp].$$

If $(\tau,\alpha) \in \ker_{\mathbb{R}} \mathrm{Hess}\ \varphi_E(0,z)$ then by Proposition 4.3, $\tau J\nabla H(z) + (M(g) - I_{2d})\alpha = 0$. Then one can take the scalar product of this equality with $J\nabla H(z)$ to obtain $\tau = 0$ and thus, $\ker_{\mathbb{R}} \mathrm{Hess}\ \varphi_E(0,z) = \mathfrak{T}_{(0,z)}\mathcal{C}_{E,g}$. This means that we have the theoretical asymptotic expansion of Theorem 4.5.

Now, we must compute the leading term of this expansion. Here again, we can suppose that g is an isometry, which simplifies the calculus: in particular, $[M(g),J]=0$, when $t=0$, we have $\hat{W}_t = 0$, and $F_z(0) = Id$. By Proposition 4.2, we obtain

$$\mathrm{Hess}\ \varphi_{E,g}(0,z) = \begin{pmatrix} \dfrac{i}{2}|\nabla H(z)|^2 & -{}^t\nabla H(z) \\ -\nabla H(z) & \dfrac{1}{2}J(M(g) - M(g^{-1})) + \dfrac{i}{2}(I - M(g))(I - M(g^{-1})) \end{pmatrix}.$$

We have $\mathcal{N}_{(0,z)}\mathcal{C}_{E,g} = \mathbb{R} \times [F_g^\perp + \mathbb{R}\nabla H(z)]$. Let β_0 be a basis of $F_g^\perp$. We set

$$e_0 := \frac{\partial}{\partial t} = (1,0), \quad \varepsilon_0 := (0,\nabla H(z)).$$

Let β be the basis of $\mathcal{N}_{(0,z)}\mathcal{C}_{E,g}$ made up of (in this order) e_0, ε_0, and β_0. We note that the linear application $\frac{1}{2}J(M(g) - M(g^{-1})) + (i/2)(I - M(g))(I - M(g^{-1}))$ stabilizes the space $F_g^\perp$. Then by calculating the determinant of the restriction of $\mathrm{Hess}\ \varphi_E(0,z)$ to $\mathcal{N}_{(0,z)}\mathcal{C}_{E,g}$ in this basis, we get (noting $\mathcal{N} := \mathcal{N}_{(0,z)}\mathcal{C}_{E,g}$):

$$\det\left(\frac{\varphi''_{E,g}(0,z)_{|_\mathcal{N}}}{i}\right) = |\nabla H(z)|^2 \det\left[\frac{1}{2i}J(M(g) - M(g^{-1})) + \frac{1}{2}(I - M(g))(I - M(g^{-1}))\right]_{\Big| F_g^\perp}.$$

If Π_g is the orthogonal projector on $\widetilde{F}_g$, then we have

$$\frac{1}{|\nabla H(z)|^2}\det\left(\frac{\varphi''_{E,g}(0,z)_{|_\mathcal{N}}}{i}\right) = \begin{pmatrix} \dfrac{1}{2}(I_d - g)(I_d - g^{-1}) + \Pi_g & \dfrac{1}{2i}(g - g^{-1}) \\ -\dfrac{1}{2i}(g - g^{-1}) & \dfrac{1}{2}(I_d - g)(I_d - g^{-1}) + \Pi_g \end{pmatrix}.$$

Then, since g is an isometry, we can suppose that g is block diagonal with blocks I_{p_1}, $-I_{p_2}, R_{\theta_1}, \ldots, R_{\theta_r}$, where $p_1 + p_2 + 2r = d$, θ_j's are not in $\pi\mathbb{Z}$, and $R_\theta := \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right)$. We then use the fact that g commutes with Π_g, and that when $[C,D]=0$, then $\det\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) = \det(AD - BC)$, for any blocks A,B,C,D of same size. A straightforward calculus then gives

$$\det\left(\frac{\varphi''_{E,g}(0,z)_{|\mathcal{N}_{(0,x)}e_{E,g}}}{i}\right)=|\nabla H(z)|^2\det[(I_d-g)_{|\tilde{F}_g^{\perp}}]^2.$$

Since $[\det_*^{-1/2}]^2=\det$, we have

$$\det_*^{-1/2}\left(\frac{\varphi''_{E,g}(0,z)_{|\mathcal{N}_{(0,x)}e_{E,g}}}{i}\right)=\pm|\nabla H(z)||\det(I_d-g)_{|\tilde{F}_g^{\perp}}|.$$

We can prove that the factor ±1 is in fact equal to 1, either by coming back to the calculus of $\det_*^{-1/2}$ with Gaussians, or, classically, by using a weak asymptotic, i.e., by calculating the asymptotic of $\mathrm{Tr}(\varphi(\hat{H})M(g))$, when $\varphi:\mathbb{R}\to\mathbb{R}$ is smooth and $\varphi(\hat{H})$ is trace class.

Using (4.11), the fact that the phase vanishes on $\mathcal{C}_{E,g}$, and that $\dim(\mathcal{C}_{E,g})\cap(\mathrm{Supp}(\hat{f})\times\mathbb{R}^{2d})=2\nu_g-1$, we obtain the result we claimed. This ends the proof of Theorem 4.5. □

As a consequence of Theorem 4.5 near $t=0$, using a well-known Tauberian argument (see Ref. 24), we get the following.

Corollary 4.7: Let G be a finite group of $\mathrm{Gl}(d,\mathbb{R})$, $H:\mathbb{R}^{2d}\to\mathbb{R}$ *be a G-invariant smooth Hamiltonian satisfying (3.5). Let $E_1<E_2$ in $\mathbb{R}$, and $I:=[E_1,E_2]$. Suppose that there exists $\varepsilon>0$ such that $H^{-1}([E_1-\varepsilon,E_2+\varepsilon])$ is compact. Furthermore suppose that E_1 and E_2 are not critical values of H. If $\chi\in\hat{G}$, then the spectrum of H_χ is discrete in I, and we have*

$$N_{1,\chi}(h)=\frac{d_\chi^2}{|G|}(2\pi h)^{-d}\,\mathrm{Vol}[H^{-1}(I)]+O(h^{1-d}),$$

where $N_{I,\chi}(h)$ is the number of eigenvalues of $\hat{H}_\chi$ in I counted with multiplicity.

Remark: One can interpret this result by saying that, semiclassically, the proportion of eigenfunctions of $\hat{H}$ having symmetry χ is $d_\chi^2/|G|$. In particular, the same proportion of eigenvalues has multiplicity greater than d_χ. The more d_χ is high, the more $L^2_\chi(\mathbb{R}^d)$ plays a role in the spectrum of $\hat{H}$.

C. The oscillatory part

If $g\in G$ and γ is a periodic orbit of Σ_E globally stable by $M(g)$, we set

$$\mathcal{L}_{g,\gamma}:=\{t\in\mathrm{Supp}\,\hat{f}:\exists\, z\in\gamma: M(g)\Phi_t(z)=z\}.$$

If $t_0\in\mathcal{L}_{g,\gamma}$, $z\in\gamma$, then P_{γ,g,t_0} denotes the Poincaré map of γ between z and $M(g^{-1})z$ at time t_0, restricted to Σ_E. The characteristic polynomial of $\mathrm{d}P_{\gamma,g,t_0}$ does not depend on $z\in\gamma$. Note that, by iterating formula (4.3), since G is finite, if we have $M(g)\Phi_t(z)=z$, then for all k in $\mathbb{N}$, we have $M(g^k)\Phi_{kt}(z)=z$, and with $k=|G|$, we obtain that z is a periodic point of the Hamiltonian system (1.2).

Theorem 4.8: *Make the same assumptions as in Theorem 4.5, but suppose that $0\notin$ Supp $\hat{f}$. Make the following hypothesis of nondegeneracy: if $\gamma\subset\Sigma_E$, is such that $\exists g\in G$ and $\exists t_0\in\mathcal{L}_{g,\gamma}$, $t_0\neq0$, then 1 is not an eigenvalue of $M(g)\mathrm{d}P_{\gamma,g,t_0}$. Then the set of such γ's is finite and the following expansion holds true modulo $O(h^{+\infty})$, as $h\to0^+$:*

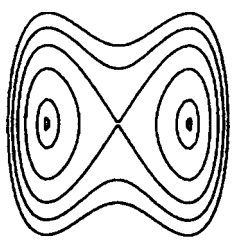
$$\mathcal{G}_\chi(h)\asymp\frac{d_\chi}{|G|}\sum_{\substack{\gamma\text{ periodic}\\ \text{orbit of }\Sigma_E}}\sum_{\substack{g\in G\text{ s.t.}\\ M(g)\gamma=\gamma}}\overline{\chi(g)}\sum_{\substack{t_0\in\mathcal{L}_{g,\gamma}\\ t_0\neq0}}e^{(i/h)S_\gamma(t_0)}\sum_{k\geqslant0}d_k^{\gamma,g,t_0}(\hat{f})h^k. \tag{4.17}$$

The coefficients $\hat{f}\mapsto d_k^{\gamma,g,t_0}(\hat{f})$ define distributions with support in $\{t_0\}$, $S_\gamma(t_0):=\int_0^{t_0}p_s\dot{q}_s\,\mathrm{d}s$, $((q_s,p_s):=\Phi_s(z)$ with $z\in\gamma)$, and

$$d_0^{\gamma,g,t_0}(\hat{f}) = \frac{\psi(E)T_\gamma^* e^{i(\pi/2)\sigma_\gamma(g,t_0)}}{2\pi|\det(M(g)\mathrm{d}P_{\gamma,g,t_0} - Id)|^{1/2}}\hat{f}(t_0),$$

where T_γ^* *is the primitive period of* γ *and* $\sigma_\gamma(g,t_0) \in \mathbb{Z}$.

Example 1: If $d=1$, periodic orbits are always nondegenerate. For example, in the case of a double-well Schrödinger Hamiltonian, one can illustrate the sum of Theorem 4.8 in the diagram below, picturing the classical flow in $\mathbb{R}^2$: some periodic orbits appear only for $g=Id$ in the sum, and others arise for both $g=\pm Id$. One can also fold the picture to compare with the periodic orbits of the reduced space as in Theorem 1.1.



Double-well phase portrait

Example 2: If H is a Schrödinger operator on $\mathbb{R}^d$ with potential $V(x)=\langle Sx,x\rangle$, where S is the diagonal matrix with diagonal nonvanishing $w_1^2,\ldots,w_d^2$, if one assumes that $\forall i \neq j$, $w_i/w_j \notin \mathbb{Q}$, then periodic orbits appear as a union of d planes, with primitive periods $T_j^* = \pi/w_j$ and are all nondegenerate.

As a particular case of this theorem, we get Theorem 1.1.

Proof of Theorem 1.1: If we suppose that G acts freely on Σ_E, then Σ_E/G inherits a structure of smooth manifold such that the canonical projection $\pi:\Sigma_E \twoheadrightarrow \Sigma_E/G$ is smooth, and the dynamical system restricted to Σ_E descends to quotient. If $t_0 \in \mathbb{R}^*$, $g \in G$, and $z \in \Sigma_E$, with orbit γ, are such that $M(g)\Phi_{t_0}(z)=z$, then γ and $\pi(\gamma)$ are periodic. If $P_{\pi(\gamma),\pi(z)}(t_0)$ denotes the Poincaré map of $\pi(\gamma)$ at time t_0, then we have

$$\det(M(g)d_z P_{\gamma,g,t_0} - Id) = \det(d_{\pi(z)}P_{\pi(\gamma),\pi(z)}(t_0) - Id). \tag{4.18}$$

Indeed, if $\tilde{\Phi}_t$ denotes the flow in Σ_E/G, then one can differentiate the following identity on Σ_E with variable z:

$$\pi(M(g)\Phi_{t_0}(z)) = \tilde{\Phi}_{t_0}(\pi(z)),$$

to get the identity:

$$d_z\pi \circ M(g)F_z(t_0) = \tilde{F}_{\pi(z)}(t_0) \circ d_z\pi,$$

where $\tilde{F}_{\pi(z)}(t_0)$ is the differential of $x \mapsto \tilde{\Phi}_{t_0}(x)$ at $\pi(z)$. Moreover, π is a submersion, and by an argument of dimensions it is also an immersion. Thus we have (4.18).

Therefore, the assumptions of Theorem 1.1 imply those of Theorem 4.8. If $z \in \Sigma_E$ is such that the orbit of $\pi(z)$ is periodic with period $t_0 \neq 0$, then there is only one $g = g_\gamma \in G$ such that $M(g)\Phi_{t_0}(z) = z$. If $\mathcal{L}_{\text{red}}$ denotes the set of periods of Σ_E/G, then we resume (4.17) as

$$\sum_{\substack{\gamma \text{ periodic} \\ \text{orbit of } \Sigma_E}} \sum_{\substack{g \in G \text{ s.t.} \\ M(g)\gamma = \gamma}} \sum_{\substack{t_0 \in \mathcal{L}_{g,\gamma} \\ t_0 \neq 0}} \cdots = \sum_{t_0 \in \mathcal{L}_{\text{red}}} \sum_{\substack{\gamma \subset \Sigma_E : \pi(\gamma) \text{ periodic} \\ \text{with } t_0 \text{ for period}}} \sum_{g = g_\gamma} \cdots .$$

If we denote $\text{Stab}(\gamma) := \{g \in G : M(g)\gamma = \gamma\}$, then we have $\text{Stab}(\gamma) = \langle g_\gamma \rangle$ and it is easy to see that $T^*_{\pi(\gamma)} = T^*_\gamma / |\text{Stab}(\gamma)|$. If we denote by $N_{\pi(\gamma)}$ the number of orbits of Σ_E with image $\pi(\gamma)$ by π, then we have $N_{\pi(\gamma)} = |G| / |\text{Stab}(\gamma)|$. Thus we have

$$\mathcal{G}_\chi(h) = d_\chi \sum_{t_0 \in \mathcal{L}_{\text{red}}} \hat{f}(t_0) \sum_{\substack{\gamma \subset \Sigma_E : \pi(\gamma) \text{ periodic} \\ \text{with } t_0 \text{ for period}}} \overline{\chi(g_{\pi(\gamma)}(t_0))} \frac{T^*_{\pi(\gamma)}}{N_{\pi(\gamma)}} \frac{e^{(i/h)S_\gamma(t_0)} e^{i(\pi/2)\sigma_\gamma(g,t_0)}}{2\pi |\det(d_{\pi(z)} P_{\pi(\gamma),\pi(z)}(t_0) - Id)|^{1/2}} + O(h).$$

Then one can show that quantities appearing on the right-hand side do not depend on γ but only on $\pi(\gamma)$, and this proves Theorem 1.1 □

Proof of Theorem 4.8: We fix g in G. If $t_0 \in \mathbb{R}^*$, we set

$$\Gamma_{E,g,t_0} := \{\gamma \text{ orbit of } \Sigma_E : \exists\, z \in \gamma : M(g)\Phi_{t_0}(z) = z\}.$$

Lemma 4.9: Under the nondegeneracy assumptions of Theorem 4.8, $\mathcal{L}_{E,g} \cap \text{Supp}(\hat{f})$ is finite and we have

$$\mathcal{C}_{E,g} \cap (\text{Supp}(\hat{f}) \times \mathbb{R}^{2d}) = \bigcup_{\substack{t_0 \in \mathcal{L}_{E,g} \\ t_0 \neq 0}} \bigcup_{\gamma \in \Gamma_{E,g,t_0}} \{t_0\} \times \gamma. \tag{4.19}$$

Proof: One can adapt the proof of the cylinder theorem of Ref. 1. □

Note that periodic orbits appearing in this critical set are the ones stable by g.

We see that $\mathcal{C}_{E,g} \cap (\text{Supp}(\hat{f}) \times \mathbb{R}^{2d})$ is a submanifold of $\mathbb{R} \times \mathbb{R}^{2d}$ and if $(t_0, z) \in \mathcal{C}_{E,g}$, then we have

$$T_{(t_0,z)}\mathcal{C}_{E,g} = \{0\} \times \mathbb{R} J \nabla H(z).$$

To apply the stationary phase theorem, we must show that $\ker_{\mathbb{R}} \text{Hess}\, \varphi_{E,g}(t_0, z) \subset T_{(t_0,z)}\mathcal{C}_{E,g}$. Let $(\tau, \alpha) \in \ker_{\mathbb{R}} \text{Hess}\, \varphi_{E,g}(t_0, z)$. By Proposition 4.3, we have $\alpha \perp \nabla H(z)$ and

$$\tau J \nabla H(z) + (M(g)F_z(t_0) - I)\alpha = 0. \tag{4.20}$$

If $\lambda \in \mathbb{R}$, we denote by $E_\lambda := \Sigma_{k=1}^{2d} \ker(M(g)F_z(t_0) - Id)^k$. Let γ be the orbit of z. Since 1 is not an eigenvalue of $M(g)\mathrm{d}P_{\gamma,g,t_0}$, 1 is an eigenvalue of $M(g)F_z(t_0)$ of multiplicity 2. Thus $\dim E_1 = 2$. Using (4.5) and (4.20), we have $\alpha \in E_1$. Let $u_2 \in \mathbb{R}^{2d}$ such that $(J\nabla H(z), u_2)$ is a basis of E_1. Note that $\langle u_2, \nabla H(z) \rangle \neq 0$, otherwise we would have $u_2 \in (JE_1)^\perp$, which is equal to $\oplus_{\lambda \neq 1} E_\lambda$ since $M(g)F_z(t_0)$ is symplectic. Since $\alpha \in E_1$ we have λ_1, λ_2 in $\mathbb{R}$ such that

$$\alpha = \lambda_1 J \nabla H(z) + \lambda_2 u_2.$$

Then, using the fact that $\langle \alpha, \nabla H(z)\rangle = 0$, we get $\lambda_2 = 0$ [since $\langle u_2, \nabla H(z)\rangle \neq 0$]. Thus coming back to (4.20), we get $\tau = 0$ and $\alpha \in \mathbb{R}J\nabla H(z)$. Thus $(\tau, \alpha) \in T_{(t_0,z)}\mathcal{C}_{E,g}$.

This shows that we can apply the stationary phase theorem and get a theoretical expansion of $I_g(h)$ and $\mathcal{G}_\chi(h)$. We must now compute the first term of this expansion. We suppose that $(t_0, z) \in \mathcal{C}_{E,g}$. We denote by Π the orthogonal projector on $\mathbb{R}J\nabla H(z)$. We set $F := M(g)F_z(t_0)$ and $W := \hat{W}_{t_0}$. Then we have

$$\det\left(\frac{\varphi''_{E,g}(t_0,z)_{|\mathcal{N}_{(t_0,z)}\mathcal{C}_{E,g}}}{i}\right) = \det\begin{pmatrix} \frac{1}{2}\langle (1-W)J\nabla H(z); J\nabla H(z)\rangle & -\frac{1}{i}{}^t\nabla H(z) + \frac{1}{2}{}^t[({}^tF - I)(I-W)J\nabla H(z)] \\ -\frac{1}{i}\nabla H(z) + \frac{1}{2}({}^tF - I)(I-W)J\nabla H(z) & \frac{1}{2i}[JF + {}^t(JF)] + \frac{1}{2}({}^tF - I)(I-W)(F-I) + \Pi \end{pmatrix}.$$

Since F is symplectic, we have $JF + {}^t(JF) = ({}^tF + I)J(F - I)$. Set

$$K := \frac{1}{2i}({}^tF + I)J + \frac{1}{2}({}^tF + I)(I - W). \tag{4.21}$$

Then, the fourth block is equal to $K(F-I) + \Pi$.

Using (4.5), we note that the third block is equal to $KJ\nabla H(z)$. Let us set

$$X_1 := \tfrac{1}{2}(I - W)J\nabla H(z). \tag{4.22}$$

We then have

$$\det\left(\frac{\varphi''_{E,g}(t_0,z)_{|\mathcal{N}_{(t_0,z)}\mathcal{C}_{E,g}}}{i}\right) = \det\begin{pmatrix} {}^tX_1 J\nabla H(z) & i{}^t\nabla H(z) + {}^tX_1(F-I) \\ KJ\nabla H(z) & K(F-I) + \Pi \end{pmatrix}.$$

The following technical lemma is due to Combescure (see Ref. 5 for the proof).

Lemma 4.10: *K is invertible and* $K^{-1} = \frac{1}{2}[(F-I) + i(F+I)J]$.

Moreover, if we set $F = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix}$, *then* $\det(K) = (-1)^d \det\left(\frac{1}{2}(\tilde{A} + i\tilde{B} - i(\tilde{C} + i\tilde{D}))\right)^{-1}$ Since

$$\det\left(\frac{\varphi''_{E,g}(t_0,z)_{|\mathcal{N}_{(t_0,z)}Y}}{i}\right) = \det\begin{pmatrix} 1 & 0 \\ 0 & K \end{pmatrix}\begin{pmatrix} {}^tX_1 J\nabla H(z) & i{}^t\nabla H(z) + {}^tX_1(F-I) \\ J\nabla H(z) & (F-I) + K^{-1}\Pi \end{pmatrix},$$

and using (4.11) and the preceding lemma, we get

$$d_g(t,z)^{-2} = (-1)^d \det(g^{-1})\det\begin{pmatrix} {}^tX_1 J\nabla H(z) & i{}^t\nabla H(z) + {}^tX_1(F-I) \\ J\nabla H(z) & (F-I) + K^{-1}\Pi \end{pmatrix}. \tag{4.23}$$

We denote by $\alpha := \langle X_1, J\nabla H(z)\rangle$ [note that $\alpha \neq 0$ since $I - W$ is invertible and $J\nabla H(z) \neq 0$] and we use the line operation $L_2 \leftarrow L_2 - (1/\alpha)J\nabla H(z)L_1$, to get

$$d_g(t,z)^{-2} = (-1)^d \alpha \det(D)\det(g^{-1}), \tag{4.24}$$

where

$$D := (F-I) + K^{-1}\Pi - \frac{1}{\alpha}J\nabla H(z)[i{}^t\nabla H(z) + {}^tX_1(F-I)].$$

Then, we compute $\det(D)$ in the basis $\beta_0 := (v_1, \ldots, v_{2d})$ where $v_1 := J\nabla H(z)$, v_2 is such that $v_2 \perp J\nabla H(z)$ and (v_1, v_2) is a basis of $\ker(F-I)^2$. Last $(v_3, \ldots, v_{2d})$ is a basis of $V_z := \oplus_{\lambda \neq 1} E_\lambda$. Let us set $w := (i/2)(F+I)\nabla H(z)$. We have $Dv_1 = -w$ and, using Lemma 4.10,

$$((F-I)+K^{-1}\Pi)v_2=(F-I)v_2, \tag{4.25}$$

$$\frac{1}{\alpha}J\nabla H(z)[i^t\nabla H(z)+{}^tX_1(F-I)]v_2=\frac{1}{\alpha}(i\langle\nabla H(z),v_2\rangle+\langle X_1,(F-I)v_2\rangle)J\nabla H(z). \tag{4.26}$$

Using the fact that $(F-I)v_2\in E_1$, one easily gets that there exists $\lambda_1\in\mathbb{R}$ such that $(F-I)v_2=\lambda_1 J\nabla H(z)$. Thus $\langle X_1,(F-I)v_2\rangle=\lambda_1\alpha$. We obtain, using (4.25) and (4.26):

$$Dv_2=-\frac{i}{2}\langle\nabla H(z),v_2\rangle J\nabla H(z). \tag{4.27}$$

Note that $(F-I)V_z\subset V_z$. Moreover $K^{-1}\Pi$ is of rank 1. Hence, since its image is equal to $K^{-1}\Pi v_1=-w\neq 0$, we can neglect it on others columns than the first column. The same idea holds for $(1/\alpha)J\nabla H(z)[i^t\nabla H(z)+{}^tX_1(F-I)]$, which we neglect in other columns than the second one [since $(1/\alpha)J\nabla H(z)[i^t\nabla H(z)+{}^tX_1(F-I)]v_2\neq 0$]. Therefore

$$\det(D)=\det\begin{pmatrix}-w_1 & -\frac{i}{\alpha}\langle\nabla H(z),v_2\rangle & 0\\ -w_2 & 0 & \\ -w_3 & 0 & \\ \vdots & \vdots & (F-I)_{|V_z}\\ -w_{2d} & 0 & \end{pmatrix},$$

where $(w_1,\ldots,w_{2d})$ are the coordinates of w in the basis β_0.

Hence $\det(D)=-(i/\alpha)w_2\langle\nabla H(z),v_2\rangle\det((F-I)_{|V_z})$.

We write

$$w=\frac{i}{2}(F+I)\nabla H(z)=w_1J\nabla H(z)+w_2v_2+v,$$

where $v\in V_z$, then we take the scalar product with $\nabla H(z)$. Since $E_1=(JV_z)^{\perp}$, we have $\langle v,\nabla H(z)\rangle=0$ and $i|\nabla H(z)|^2=w_2\langle v_2;\nabla H(z)\rangle$. Thus we get

$$\det(D)=\frac{1}{\alpha}|\nabla H(z)|^2\det((F-I)_{|V_x}).$$

Therefore, according to (4.24)

$$d_g(t,z)^{-2}=(-1)^d|\nabla H(z)|^2\det((F-I)_{|V_x})\det(g^{-1}). \tag{4.28}$$

Since $\det(g^{-1})=\pm 1$, there exists $k\in\mathbb{Z}$, depending on g, such that

$$d_g(t,z)=\frac{e^{ik(\pi/2)}}{|\nabla H(z)||\det((F-I)_{|V_z})|^{1/2}}.$$

Moreover, d_g being continuous, k does not depend on $z\in\gamma$. Thus by Theorem 4.4, we have, if $\mathcal{L}_{E,g}:=\{t\in\mathbb{R}:\exists z\in\Sigma_E: M(g)\Phi_t(z)=z\}$,

$$I_g(h)=\sum_{t_0\in\mathcal{L}_{E,g}\cap\mathrm{Supp}(\hat{f})}\sum_{\gamma\in\Gamma_{E,g,t_0}}e^{(i/h)S_\gamma(t_0)}\frac{\psi(E)\hat{f}(t_0)e^{ik(\pi/2)}}{2\pi|\det((F-I)_{|V_z})|^{1/2}}\int_\gamma\frac{\mathrm{d}\gamma}{|\nabla H|}+O(h).$$

Moreover, if $z\in\gamma$, then

$$\int_\gamma \frac{\mathrm{d}\gamma}{|\nabla H|} = \int_0^{T_\gamma^*} |J\nabla H(\phi_t(z))| \frac{\mathrm{d}t}{|\nabla H(\phi_t(z))|} = T_\gamma^*.$$

Last, we sum on $g \in G$ to get the expansion of $\mathcal{G}_\chi(h)$. This ends the proof of Theorem 4.8. □

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APPENDIX: COHERENT STATES

We recall some basic things on coherent states on $\mathbb{R}^{2d}$ in Schrödinger representation. We mainly follow the presentation of Combescure and Robert (cf. Refs. 6, 25, and 5).

Notations: The h-scaling unitary operator $\Lambda_h : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is defined by

$$\Lambda_h \psi(x) = h^{-d/4} \psi(h^{-1/2}x).$$

The phase translation unitary operator associated to $\alpha = (q,p) \in \mathbb{R}^d \times \mathbb{R}^d$ is given by

$$\mathcal{T}_h(\alpha) := \exp\left[\frac{i}{h}(px - qhD_x)\right]. \tag{A1}$$

We classically have $\mathcal{T}_h(\alpha)^* = \mathcal{T}_h(\alpha)^{-1} = \mathcal{T}_h(-\alpha)$ and

$$\mathcal{T}_h(\alpha) f(\alpha) = \exp\left(i\frac{p}{h}\left(x - \frac{q}{2}\right)\right) f(x-q). \tag{A2}$$

The ground state of the harmonic oscillator $-\Delta + |x|^2$ is given by

$$\tilde{\psi}_0(x) := \frac{1}{\pi^{d/4}} \exp\left(-\frac{|x|^2}{2}\right).$$

We set

$$\psi_0(x) := \Lambda_h \tilde{\psi}_0(x) = \frac{1}{(h\pi)^{d/4}} \exp\left(-\frac{|x|^2}{2h}\right). \tag{A3}$$

Then the coherent state associated to $\alpha \in \mathbb{R}^{2d}$ is given by $\varphi_\alpha := \mathcal{T}_h(\alpha)\psi_0$. By (A2), we have

$$\varphi_\alpha(x) = \frac{1}{(h\pi)^{d/4}} \exp\left(i\frac{p}{h}\left(x - \frac{q}{2}\right)\right) \exp\left(-\frac{|x-q|^2}{2h}\right), \tag{A4}$$

and we get easily from (A2) the following formulas:

$$\Lambda_h^* \mathcal{T}_h(\alpha) \Lambda_h = \mathcal{T}_1\left(\frac{\alpha}{\sqrt{h}}\right) \quad \text{and } \Lambda_h^* \operatorname{Op}_h^w(a) \Lambda_h = \operatorname{Op}_1^w(a_h), \quad \text{where } a_\hbar(z) := a(\sqrt{h}z),$$

$$\mathcal{T}_h(\alpha)\mathcal{T}_h(\beta) = e^{(1/2h)\langle J\alpha;\beta\rangle} \mathcal{T}_h(\alpha+\beta) \quad \text{and } \mathcal{T}_h(\alpha)^* \operatorname{Op}_h^w(a) \mathcal{T}_h(\alpha) = \operatorname{Op}_h^w[a(\alpha + \cdot)].$$

A trace formula: If $A \in \mathcal{L}(L^2(\mathbb{R}^d))$ is trace class, then $\int_{\mathbb{R}^{2d}_\alpha} |\langle A\varphi_\alpha; \varphi_\alpha\rangle_{L^2(\mathbb{R}^d)}| \mathrm{d}\alpha < +\infty$, and we have (see Ref. 5)

$$\operatorname{Tr}(A) = (2\pi h)^{-d} \int_{\mathbb{R}^{2d}_\alpha} \langle A\varphi_\alpha; \varphi_\alpha\rangle_{L^2(\mathbb{R}^d)} \, \mathrm{d}\alpha. \tag{A5}$$

Propagation of coherent states: For $z=(q,p)\in\mathbb{R}^d\times\mathbb{R}^d$, let $z_t=(q_t,p_t):=\Phi_t(z)$ be the solution of the Hamiltonian system (1.2) with initial condition z. We introduce the notations

$$S(t,z):=\int_0^t (p_s\cdot\dot{q}_s-H(z_s))\mathrm{d}s, \tag{A6}$$

$$\delta(t,z):=S(t,z)-\frac{q_tp_t-qp}{2}, \tag{A7}$$

where $F_\alpha(t)=\partial_z\Phi_t(\alpha)\in \mathrm{Sp}(d,\mathbb{R})$. We set

$$F_\alpha(t)=\begin{pmatrix} A & B\\ C & D\end{pmatrix} \quad \text{where } A,B,C,D\in M_d(\mathbb{R}). \tag{A8}$$

Theorem 5.1: *Semiclassical propagation of coherent states (Combescure-Robert)* (Refs. 6 and 25). *Let $T>0$. Let $H:\mathbb{R}^{2d}\to\mathbb{R}$ be a smooth Hamiltonian satisfying, for all $\alpha\in\mathbb{N}^{2d}$:*

$$\left|\partial^\alpha H(z)\right|\leqslant C_\alpha\langle x\rangle^{m_\alpha},\quad \textit{where } m_\alpha>0,\quad C_\alpha>0. \tag{A9}$$

Let $\alpha\in\mathbb{R}^{2d}$ be such that the solution with initial condition α of the system $\dot{z}_t=J\nabla H(z_t)$ is defined for $t\in\,]-T,T[$. We denote by $U_h(t):=e^{-i(t/h)H}$ the quantum propagator.

Then, $\forall M\in\mathbb{N}$, $\exists C_{M,T}(\alpha)>0$, independent of h and of $t\in[-T,T]$ such that

$$\left\| U_h(t)\varphi_\alpha-e^{i[(t,\alpha)/h]}\mathcal{T}_h(\alpha_t)\Lambda_h\left[\sum_{j=0}^{M}h^{i/2}b_j(t,\alpha)(x)\cdot e^{(i/2)\langle M_0x,x\rangle}\right]\right\|_{L^2(\mathbb{R}^d)}\leqslant C_{M,T}(\alpha)\cdot h^{(M+1)/2},$$

where $M_0:=(C+iD)(A+iB)^{-1}$, for all $t\in\,]-T,T[$, $b_j(t,\alpha):\mathbb{R}^d\to\mathbb{C}$ is a polynomial independent of h, with degree lower than $3j$, with same parity as j, and smoothly dependent on (t,α). In particular, $b_0(t,\alpha)(x)=\pi^{-d/4}(\det(A+iB))_c^{-1/2}$. Moreover, if the solutions of the Hamiltonian classical system are defined on $[-T,T]$ for initial conditions α in a compact K, then $\alpha\mapsto C_{M,T}(\alpha)$ is upper bounded on K by $\widetilde{C}_{M,T,K}$ independent of $\alpha\in K$.

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Reverse inequalities in μ-deformed Segal-Bargmann analysis

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We prove reverse hypercontractivity inequalities as well as reverse log-Sobolev inequalities in the context of a space of holomorphic functions, which is called the μ-deformed Segal-Bargmann space and arises in the works of Wigner, Rosenblum, and Marron. To achieve this we define μ-deformations of energy and entropy. Our principle results generalize earlier works of Carlen and Sontz. We also show that the semigroup of this theory is L^p bounded, and we conjecture that it is L^p contractive and, even more strongly, that it is hypercontractive. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2186257]

I. INTRODUCTION

Wigner in the very title of his article[29] asked: "Do the equations of motion determine the quantum mechanical commutation relations?" In response to his own question, Wigner gave in that article a parametrized family of inequivalent representations by operators of the equations of motion with the property that the quantum mechanical (i.e., canonical) commutation relation does not hold in those representations for nonzero values of the parameter, which we will denote by μ. Rosenblum in Ref. 20 has extensively studied these representations, which act in an L^2 space of the configuration space and generalize the study of the harmonic oscillator in one dimension in quantum mechanics.

Then in Ref. 14 Marron, a student of Rosenblum, presented in detail a family of Hilbert spaces of holomorphic functions parametrized by the same parameter μ and which carry representations unitarily equivalent to those of Wigner mentioned above. We call these the μ-deformed Segal-Bargmann spaces. These holomorphic Hilbert spaces are proper closed subspaces of an L^2 space associated with the phase space. However, a brief description of these spaces also appears more or less simultaneously in Ref. 21, an unpublished work of Rosenblum. See also Refs. 15 and 17 for earlier related work.

For $\mu=0$, one recovers the usual Segal-Bargmann space. (See Refs. 2 and 22.) In this, the usual context of quantum mechanics, one constructs a number operator N (which is essentially the Hamiltonian of the harmonic oscillator) and its associated contraction semigroup e^{-tN} for $t\geqslant 0$, defined by spectral theory. In this case one finds the following inequalities, called *complex hypercontractivity* or sometimes, more simply, *hypercontractivity*. This says that for $0<p\leqslant q$, $q\leqslant pe^{2t}$ and $f\in\mathcal{B}_0^p$ the operator e^{-tN} satisfies

$$\|e^{-tN}f\|_q \leqslant \|f\|_p$$

and that e^{-tN} is not bounded from $\mathcal{B}_0^p$ to $\mathcal{B}_0^q$ for $q>pe^{2t}$. (Here $\mathcal{B}_0^p$ and $\mathcal{B}_0^q$ are spaces of holomorphic functions, which we will define later. $\mathcal{B}_0^p$ is a subspace of an L^p space and is equipped with its

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norm $\|\cdot\|_p$.) This result is first due to Janson in Ref. 11. Other proofs have been given by Carlen in Ref. 4, Zhou in Ref. 30, Janson in Ref. 12 and Gross in Ref. 9. In the real variable case, Nelson in Ref. 16 has a similar, though not identical, result. It is the work of Nelson that initiated interest in hypercontractivity.

Moreover, Carlen in Ref. 4 obtained another related result, known as *reverse hypercontractivity*. This says that for $0<q<p$, $q<pe^{2t}$, and $f\in\mathcal{B}_0^p$ we have that

$$\|e^{-tN}f\|_q \leqslant C(t,p,q)\|f\|_p,$$

where $C(t,p,q)$ is a finite positive constant. For a discussion about the unknown optimal value of this constant, see Ref. 6. We note that hypercontractivity says that the operator e^{-tN} maps $\mathcal{B}_0^p$ to $\mathcal{B}_0^q$ contractively for $q\geqslant p$ for certain positive values of t. However, reverse hypercontractivity says that the operator e^{-tN} maps $\mathcal{B}_0^p$ to $\mathcal{B}_0^q$ boundedly for $q<p$ for certain values of t, including some negative values. This indicates in what sense the second result is the reverse of the first result. (We will define e^{-tN} for all $t<0$ later on.)

In the context of real variable theory Gross studied in Ref. 8 an inequality known as the *log-Sobolev inequality*. In the case of complex variable theory this says that for all holomorphic functions f in an appropriate space (which is $\mathcal{B}_0^2$ and which will be defined later) we have that

$$S_{\mathcal{B}_0^2}(f) \leqslant \langle f,Nf\rangle,$$

where the entropy $S_{\mathcal{B}_0^2}(f)$ of f will also be defined later on. The term $\langle f,Nf\rangle$ is known as the energy of f.

The second author in Ref. 25 proved an inequality that is known as a *reverse log-Sobolev inequality*. Specifically, this says that for every $c>1$ there exists a number $K(c)>0$ such that

$$\langle f,Nf\rangle \leqslant cS_{\mathcal{B}_0^2}(f) + K(c)\|f\|_2^2$$

for all $f\in\mathcal{B}_0^2$. Note that there is an interchange in the roles of the entropy and the energy in these two types of inequality. The log-Sobolev inequality tells us that finite energy implies finite entropy, while the reverse log-Sobolev inequality tells us precisely the converse.

This paper is a continuation of the works previously mentioned in that we prove reverse hypercontractivity (originally studied by Carlen in Ref. 4) and reverse log-Sobolev inequalities (originally studied by the second author in Ref. 25), but now we do this in the context of the μ-deformed holomorphic function spaces introduced by Rosenblum[21] and Marron[14] in their studies of the works of Rosenblum[20] and Wigner.[29] See Ref. 5 for a study of these reverse inequalities in the context of complex manifolds without μ-deformation. For further studies of μ-deformed Segal-Bargmann analysis, see Refs. 1, 18, and 27.

For the undeformed case $\mu=0$ the relation between log-Sobolev inequalities and hypercontractivity inequalities has been studied extensively, beginning with Ref. 8. Loosely speaking, either one implies the other. Of course, they both involve the number operator N. A similar relation for the case $\mu=0$ between a reverse log-Sobolev inequality and reverse hypercontractivity is to be expected, since again they are both based on the same operator N. But this does not work out as one might wish. (See Ref. 25.) The μ-deformed inequalities are defined in terms of the same μ-deformed number operator (defined later), but as far as we know there is no straightforward relation between the two reverse inequalities. We present them together in this paper, since in a more general approach to deformations of quantum mechanics we would hope to see some underlying connection between them.

An outline of the paper is as follows. In Sec. II we introduce the basic notation and definitions used throughout. In Sec. III we define the basic operators of this theory, namely the μ-deformed number operator N_μ and its associated semigroup e^{-tN_μ}. Then we enter the principle part of the paper in Sec. IV where we discuss reverse hypercontractivity as well as the L^p boundedness of the semigroup. We continue in Sec. V with reverse log-Sobolev inequalities, where we also define μ-deformations of energy and entropy. Then in an Appendix we discuss the relation between the

energy of the μ-deformed harmonic oscillator (described there) and the μ-deformed energy introduced in this paper. Finally, we conclude with a discussion of some problems that remain open.

II. NOTATION AND DEFINITIONS

Let $\mathcal{H}(\mathbb{C})$ denote the space of holomorphic functions $\psi:\mathbb{C}\to\mathbb{C}$, where $\mathbb{C}$ is the field of complex numbers. We also denote by $\mathcal{H}_e(\mathbb{C})$ and $\mathcal{H}_o(\mathbb{C})$ the subspaces of $\mathcal{H}(\mathbb{C})$ of even and odd functions, respectively. We note that $\mathcal{H}(\mathbb{C})=\mathcal{H}_e(\mathbb{C})\oplus\mathcal{H}_o(\mathbb{C})$, where $\oplus$ is the internal direct sum. This is a consequence of the fact that any $\psi\in\mathcal{H}(\mathbb{C})$ can be uniquely written as a sum of an even and an odd function, namely of its even part (notation, ψ_e) and of its odd part (notation, ψ_o). We use this notation throughout without further comment. We also note that μ will always denote a real parameter satisfying $-1/2<\mu<\infty$. One can find an explanation in Ref. 20 of why the region $\mu\leqslant -1/2$ is excluded from this analysis.

We now define the three basic scales of spaces which we will work with in this paper. But before doing so, we comment that we use the usual notation $L^p(\Omega,\nu)$ for the vector space of pth power absolutely integrable functions defined on a measure space Ω with measure ν as well as $\|f\|_p := \|f\|_{L^p(\Omega,\nu)} := (\int_\Omega |f|^p \mathrm{d}\nu)^{1/p}$. We will consider this for $0<p<\infty$. For any $r>1$ we define its *dual index* by $r' := r/(r-1)$.

Definition 2.1: For $0<p<\infty$ we define

$$\mathcal{B}^p_\mu := \{\psi\in\mathcal{H}(\mathbb{C}):\psi_e\in L^p(\mathbb{C},\nu_{e,\mu}),\ \psi_o\in L^p(\mathbb{C},\nu_{o,\mu})\},$$

$$P^p_\mu := \mathcal{H}_e(\mathbb{C})\cap L^p(\mathbb{C},\nu_{e,\mu}) = \mathcal{H}_e(\mathbb{C})\cap\mathcal{B}^p_\mu,$$

$$I^p_\mu := \mathcal{H}_o(\mathbb{C})\cap L^p(\mathbb{C},\nu_{o,\mu}) = \mathcal{H}_o(\mathbb{C})\cap\mathcal{B}^p_\mu.$$

Here

$$\mathrm{d}\nu_{e,\mu}(z) := \kappa_\mu K_{\mu-(1/2)}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y$$

is a probability measure on $\mathbb{C}$,

$$\mathrm{d}\nu_{o,\mu}(z) := \kappa_\mu K_{\mu+(1/2)}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y$$

is a finite measure on $\mathbb{C}$, $\kappa_\mu := 2^{1/2-\mu}/(\pi\Gamma(\mu+1/2))$ *is introduced to simplify notation,* $\Gamma(z)$ *is the Euler gamma function and* $K_\alpha(z)$ *is the Macdonald function of order* α. (*See Ref. 7 or Ref. 13 for information on these special functions.) Finally,* $z\in\mathbb{C}$ *and* $\mathrm{d}x\,\mathrm{d}y$ *is Lebesgue measure on* $\mathbb{C}$.

Proofs that $\mathrm{d}\nu_{e,\mu}$ is a probability measure and that $\mathrm{d}\nu_{o,\mu}$ is a finite measure are given in Refs. 1 and 18. Actually, in Ref. 1 it is shown that $\mathrm{d}\nu_{o,\mu}$ is *not* a probability measure when $\mu\neq 0$. The Macdonald function of order α is characterized by the integral formula

$$K_\alpha(z) = \int_0^\infty e^{-z\cosh u}\cosh(\alpha u)\mathrm{d}u$$

for $\mathrm{Re}(z)>0$ and arbitrary $\alpha\in\mathbb{C}$. This can be found in Lebedev[13] (p. 119), for example. From this integral representation it follows that $K_\alpha(x)>0$ for $x>0$ and that K_α is a monotone decreasing function on $(0,\infty)$. In particular, K_α has no zeros in $(0,\infty)$. A more general definition and discussion of the basic properties of the Macdonald function is given in Refs. 13 and 28. An explanation of how the Macdonald function arises naturally in the context of μ-deformed Segal-Bargmann analysis is given in Ref. 27.

We will be interested in the Macdonald function $K_\alpha(z)$ in the case when z is real and positive and α is real. The asymptotic behavior of the Macdonald function $K_\alpha(x)$ for $x>0$ when $x\to 0^+$ and when $x\to+\infty$ is given as follows. (See Ref. 13, pp. 110 and 136.)

$$K_\alpha(x) \approx \frac{2^{|\alpha|-1}\Gamma(|\alpha|)}{x^{|\alpha|}}, \quad x \to 0^+, \quad \alpha \neq 0, \tag{2.1}$$

$$K_0(x) \approx \log \frac{2}{x}, \quad x \to 0^+, \tag{2.2}$$

$$K_\alpha(x) \approx \left(\frac{\pi}{2x}\right)^{1/2} e^{-x}, \quad x \to +\infty, \quad \text{for all} \quad \alpha \in \mathbb{R}. \tag{2.3}$$

Here we use the standard notation $f(x) \approx g(x)$ when $x \to a$ [and say that $f(x)$ and $g(x)$ are asymptotic when $x \to a$] provided that $\lim_{x\to a} f(x)/g(x) = 1$. Another useful result says that for real α, β satisfying $\beta > |\alpha|$ we have that

$$\int_0^\infty K_\alpha(s) s^{\beta-1}\, \mathrm{d}s = 2^{\beta-2}\Gamma\left(\frac{\beta-\alpha}{2}\right)\Gamma\left(\frac{\beta+\alpha}{2}\right). \tag{2.4}$$

See Eq. (8) on p. 388 in Ref. 28 or Eq. 6.561.16 in Ref. 7.

Definition 2.2: For $\psi \in \mathcal{B}^p_\mu$ and $p > 0$ we define

$$\|\psi\|_{\mathcal{B}^p_\mu} := (\|\psi_e\|^p_{P^p_\mu} + \|\psi_o\|^p_{I^p_\mu})^{1/p},$$

where

$$\|\psi_e\|_{P^p_\mu} := \left(\int_{\mathbb{C}} |\psi_e|^p \, \mathrm{d}\nu_{e,\mu}\right)^{1/p} = \|\psi_e\|_{L^p(\mathbb{C},\nu_{e,\mu})}$$

and

$$\|\psi_o\|_{I^p_\mu} := \left(\int_{\mathbb{C}} |\psi_o|^p \, \mathrm{d}\nu_{o,\mu}\right)^{1/p} = \|\psi_o\|_{L^p(\mathbb{C},\nu_{o,\mu})}.$$

An immediate consequence of these definitions is that these spaces are in fact Banach spaces when they should be, namely, when $p \geqslant 1$. We also include the case $0 < p < 1$ as is usual in the study of holomorphic spaces. Explicitly, we have the following.

Proposition 2.1: If $p \geqslant 1$, then $\|\cdot\|_{\mathcal{B}^p_\mu}$ is a norm and $\mathcal{B}^p_\mu$ equipped with this norm is a Banach space.

Since we will not use this result, we only comment on its proof. First, $\|\cdot\|_{\mathcal{B}^p_\mu}$ is clearly a norm when $p \geqslant 1$. To show that the space is complete in this case, we can adapt an argument for the case $p=2$ and $\mu=0$ from Hall.[10] This identifies $\mathcal{B}^p_\mu$ as a closed subspace of the Banach space $L^p(\mathbb{C}, \nu_{e,\mu}) \oplus L^p(\mathbb{C}, \nu_{o,\mu})$, where $\oplus$ is the external direct sum, and thereby shows $\mathcal{B}^p_\mu$ to be complete. See Ref. 1 for a detailed proof of this result.

Note that for $p=2$ the Banach space $\mathcal{B}^2_\mu$ is actually a Hilbert space with inner product defined by

$$\langle \psi, \phi \rangle_{\mathcal{B}^2_\mu} := \langle \psi_e, \phi_e \rangle_{P^2_\mu} + \langle \psi_o, \phi_o \rangle_{I^2_\mu}.$$

We call this the *μ-deformed Segal-Bargmann space*; it appears in Refs. 14 and 21. When we set $\mu=0$ (as well as $p=2$) we obtain the usual Segal-Bargmann space introduced by Segal[22] and Bargmann.[2]

We warn the reader that in the case $\mu=0$ while the spaces $\mathcal{B}^p_\mu$ are equal to the spaces in Refs. 4 and 25, the norms we have defined are not identical when $p \neq 2$ to the norms used by those authors. However, they are equivalent norms. Since these comments have no bearing on the rest of this paper, we leave their elementary proof to the interested reader.

Definition 2.3: Let (X,ω) *be a finite measure space, that is,* $0<\omega(X)<\infty$. *We define the entropy of any* $f\in L^2(X,\omega)$ *by*

$$S_{L^2(X,\omega)}(f) := \int_X |f(x)|^2 \log|f(x)|^2 \, d\omega(x) - \|f\|_2^2 \log\|f\|_2^2.$$

Here, and in the following, we let log denote the natural logarithm (base e) and set $0\log 0 := 0$. This definition of entropy is due to Shannon in Ref. 23. An application of Jensen's inequality shows that

$$S_{L^2(X,\omega)}(f) \geqslant (-\log \omega(X))\|f\|^2_{L^2(X,\omega)} > -\infty.$$

However, note that $S_{L^2(X,\omega)}(f)=+\infty$ is not excluded. If $f\in\mathcal{H}$, where $\mathcal{H}$ is some closed subspace of $L^2(X,\omega)$ under consideration, we write $S_{\mathcal{H}}(f)$ for this entropy. The first use of Shannon entropy in Segal-Bargmann analysis appears in Ref. 24.

As is usual in analysis, we indifferently use the symbol C for a positive, finite constant whose value can change with each occurrence.

III. THE BASIC OPERATORS

In this section we will define the μ-deformed number operator N_μ and its associated semigroup e^{-tN_μ} in the context of the μ-deformed Segal-Bargmann space $\mathcal{B}^2_\mu$. Our objective is to extend this definition to $\mathcal{H}(C)$. (See Definition 3.5.)

We will start with the following definition, which comes from Rosenblum,[20] p. 372, in order to define later on the canonical orthonormal basis of $\mathcal{B}^2_\mu$.

Definition 3.1: The μ-deformed factorial $\gamma_\mu(n)$ *is defined recursively for integers* $n\geqslant 0$ *by* $\gamma_\mu(0) := 1$ *and by*

$$\gamma_\mu(n) := (n+2\mu\theta_n)\gamma_\mu(n-1) \quad \text{for } n\geqslant 1.$$

Here θ_n *is the characteristic function of the odd integers, that is,* $\theta_n=1$ *if* n *is odd and* $\theta_n=0$ *if* n *is even.*

Note that the standing hypothesis $\mu>-1/2$ implies that $\gamma_\mu(n)>0$. We note that

$$\gamma_\mu(2j) = \frac{2^{2j}\Gamma(j+1)\Gamma(\mu+j+1/2)}{\Gamma(\mu+1/2)} \tag{3.1}$$

and

$$\gamma_\mu(2j+1) = \frac{2^{2j+1}\Gamma(j+1)\Gamma(j+\mu+3/2)}{\Gamma(\mu+1/2)}, \tag{3.2}$$

which can be found in Ref. 20 and are easily checked by induction.

For each integer $n\geqslant 0$ we define the function Ψ^μ_n (actually, holomorphic monomial) by

$$\Psi^\mu_n(z) := \frac{z^n}{(\gamma_\mu(n))^{1/2}}$$

for all $z\in\mathbb{C}$. By direct evaluation of the integrals, using (2.4), (3.1), and (3.2), we have that $\|\Psi^\mu_n\|_{\mathcal{B}^2_\mu}=1$ for all integers $n\geqslant 0$. Next, $\langle\Psi^\mu_n,\Psi^\mu_m\rangle=0$ for $n\neq m$ is quite straightforward. Finally, the set of all these functions forms an orthonormal basis of $\mathcal{B}^2_\mu$ by an argument that closely parallels the proof in Ref. 2 for the case $\mu=0$.

We denote by $\mathcal{D}^2_\mu$ the dense subspace of $\mathcal{B}^2_\mu$ consisting of all finite linear combinations of the Ψ^μ_n. Clearly, $\mathcal{D}^2_\mu$ is the space of all holomorphic polynomials in z.

The following definition is based on formulas in Ref. 20, p. 381.

Definition 3.2: We define the μ-deformed annihilation operator A_μ *as well as the* μ-deformed

creation operator $A_\mu^\star$, *both with domain of definition equal to* $\mathcal{D}_\mu^2$, *by setting for* $n \geqslant 0$,

$$A_\mu \Psi_n^\mu := (n + 2\mu\theta_n)^{1/2} \Psi_{n-1}^\mu,$$

$$A_\mu^\star \Psi_n^\mu := (n + 1 + 2\mu\theta_{n+1})^{1/2} \Psi_{n+1}^\mu,$$

where $\Psi_{-1}^\mu \equiv 0$, *and then extending linearly to all of* $\mathcal{D}_\mu^2$.

The next proposition can be found in Ref. 20, p. 381, though in the context of a different Hilbert space. Since the proof is identical and we will not be needing it, we merely state the result without proving it. The point of this proposition is that the μ-deformed canonical commutation relation, originally given by Wigner in Ref. 29, holds here. (Also see Refs. 14 and 20.) But first, we define the *parity operator* J acting in $\mathcal{B}_\mu^2$ by $J\psi(z) := \psi(-z)$ for all $\psi \in \mathcal{B}_\mu^2$ and all $z \in \mathbb{C}$.

Proposition 3.1: Considered as operators defined with the common domain $\mathcal{D}_\mu^2$ *we have the* μ-deformed canonical commutation relation

$$[A_\mu, A_\mu^\star] = I + 2\mu J \quad \text{or, equivalently,} \quad i[\widetilde{P}_\mu, \widetilde{Q}_\mu] = I + 2\mu J,$$

where $\widetilde{Q}_\mu := 2^{-1/2}(A_\mu + A_\mu^\star)$ *is the definition of the* μ-deformed position operator, $\widetilde{P}_\mu := -i2^{-1/2}(A_\mu - A_\mu^\star)$ *is the definition of the* μ-deformed momentum operator, I *is the identity operator and* J *is the parity operator*.

Note that $\mathcal{D}_\mu^2$ is invariant under the actions of all of A_μ, $A_\mu^\star$, $\widetilde{P}_\mu$, and $\widetilde{Q}_\mu$ so that the commutators are well defined as operators acting on $\mathcal{D}_\mu^2$. Of course, we are using the usual definition $[S,T] := ST - TS$ of the *commutator* of two operators S and T.

We would merely like to note here that the presence of the parity operator J at this basic level of the theory indicates how it comes about that the various function spaces of this theory are defined in terms of the even and odd parts of the functions, which are simply the eigenfunctions of J. More comments about this appear in Ref. 27.

The following definition also is based on Ref. 20 (p. 392), though again in the context of another Hilbert space.

Definition 3.3: We define the μ-deformed number operator N_μ *with domain* $\mathcal{D}_\mu^2$ *by* $N_\mu := A_\mu^\star A_\mu$.

Here the invariance of $\mathcal{D}_\mu^2$ under the action of A_μ tells us that N_μ is well defined. We immediately have for $n \geqslant 0$ that

$$N_\mu \Psi_n^\mu = A_\mu^\star A_\mu \Psi_n^\mu = A_\mu^\star((n + 2\mu\theta_n)^{1/2} \Psi_{n-1}^\mu) = (n + 2\mu\theta_n)\Psi_n^\mu. \tag{3.3}$$

Since the orthonormal basis Ψ_n^μ diagonalizes N_μ, we can use that basis to define functions of N_μ. In particular, this motivates the next definition.

Definition 3.4: For every $t \geqslant 0$, *we define a linear operator* $e^{-tN_\mu}: \mathcal{B}_\mu^2 \to \mathcal{B}_\mu^2$ *as follows. First, we define the operator in the domain* $\mathcal{D}_\mu^2$ *by setting*

$$e^{-tN_\mu} \Psi_n^\mu := e^{-t(n+2\mu\theta_n)} \Psi_n^\mu$$

for every integer $n \geqslant 0$ *and then extending linearly to* $\mathcal{D}_\mu^2$. *Then we can show that* $\|e^{-tN_\mu}\Psi\|_{\mathcal{B}_\mu^2} \leqslant \|\Psi\|_{\mathcal{B}_\mu^2}$ *holds for every* $t \geqslant 0$ *and* $\Psi \in \mathcal{D}_\mu^2$. *Finally, this implies that there is a unique linear extension (still denoted by* e^{-tN_μ}*) to the closure of* $\mathcal{D}_\mu^2$, *namely to* $\mathcal{B}_\mu^2$, *with the same operator norm*.

Let us remark that this definition is what the functional calculus of an unbounded self-adjoint operator also gives. We first note that N_μ with domain $\mathrm{Dom}(N_\mu) = \mathcal{D}_\mu^2$ is a symmetric operator, since the eigenvalues in (3.3) are real. Another straightforward consequence of (3.3) is that each $\Psi_n^\mu \in \mathrm{Ran}(N_\mu \pm i)$, which implies that $\mathrm{Ran}(N_\mu \pm i)$ are dense subspaces in $\mathcal{B}_\mu^2$. So basic functional analysis (Ref. 19, p. 257) tells us that N_μ is essentially self-adjoint. Therefore the functional calculus allows us to evaluate $f_t(\lambda) = e^{-t\lambda}$, where $\lambda \in \mathbb{R}$ and $t \geqslant 0$, on the unique self-adjoint extension $\bar{N}_\mu$ of N_μ. (First, one identifies the spectrum σ of $\bar{N}_\mu$ in order to verify that f_t is bounded

on σ.) By the spectral mapping theorem this bounded operator $f_t(\bar{N}_\mu)$ agrees on the basis elements Ψ_n^μ with the bounded operator e^{-tN_μ} defined above, and so is the same operator acting on $\mathcal{B}_\mu^2$. Alternatively, one can construct $\bar{N}_\mu$ as the Friedrichs extension of N_μ.

The statement and proof of the next proposition are adaptations to this context of a result given by Bargmann in Ref. 2. We present this in detail since we will use this result.

Proposition 3.2: Let $\psi \in \mathcal{H}(\mathbb{C})$ have Maclaurin series (i.e., Taylor series with center at $z=0$),

$$\psi(z) = \sum_{n=0}^{\infty} a_n \Psi_n^\mu(z)$$

written in terms of the monomials Ψ_n^μ. Then

$$\|\psi\|_{\mathcal{B}_\mu^2}^2 = \sum_{n=0}^{\infty} |a_n|^2.$$

In particular, $\psi \in \mathcal{B}_\mu^2$ if and only if $\Sigma_{n=0}^{\infty} |a_n|^2 < \infty$.

Proof: The result is given by the following computation, whose steps are justified afterwards:

$$\begin{aligned}
\|\psi\|_{\mathcal{B}_\mu^2}^2 &= \int_{\mathbb{C}} d\nu_{e,\mu}(z) |\psi_e(z)|^2 + \int_{\mathbb{C}} d\nu_{o,\mu}(z) |\psi_o(z)|^2 = \lim_{R\to\infty} \int_{|z|\le R} d\nu_{e,\mu}(z) \left| \sum_{k=0}^{\infty} a_{2k} \Psi_{2k}^\mu(z) \right|^2 \\
&+ \lim_{R\to\infty} \int_{|z|\le R} d\nu_{o,\mu}(z) \left| \sum_{l=0}^{\infty} a_{2l+1} \Psi_{2l+1}^\mu(z) \right|^2 = \lim_{R\to\infty} \sum_{k,k'=0}^{\infty} a_{2k}^* a_{2k'} \int_{|z|\le R} d\nu_{e,\mu}(z) \Psi_{2k}^\mu(z)^* \Psi_{2k'}^\mu(z) \\
&+ \lim_{R\to\infty} \sum_{l,l'=0}^{\infty} a_{2l+1}^* a_{2l'+1} \int_{|z|\le R} d\nu_{o,\mu}(z) \Psi_{2l+1}^\mu(z)^* \Psi_{2l'+1}^\mu(z) = \lim_{R\to\infty} \sum_{k=0}^{\infty} |a_{2k}|^2 \int_{|z|\le R} d\nu_{e,\mu}(z) \\
&\times |\Psi_{2k}^\mu(z)|^2 + \lim_{R\to\infty} \sum_{l=0}^{\infty} |a_{2l+1}|^2 \int_{|z|\le R} d\nu_{o,\mu}(z) |\Psi_{2l+1}^\mu(z)|^2 = \sum_{k=0}^{\infty} |a_{2k}|^2 \int_{\mathbb{C}} d\nu_{e,\mu}(z) |\Psi_{2k}^\mu(z)|^2 \\
&+ \sum_{l=0}^{\infty} |a_{2l+1}|^2 \int_{\mathbb{C}} d\nu_{o,\mu}(z) |\Psi_{2l+1}^\mu(z)|^2 = \sum_{k=0}^{\infty} |a_{2k}|^2 + \sum_{l=0}^{\infty} |a_{2l+1}|^2 = \sum_{n=0}^{\infty} |a_n|^2.
\end{aligned}$$

The first equality is the definition of the norm. The second equality is by monotone convergence and a simple substitution. The interchange of infinite sum and integral in the third equality is justified by the uniform convergence in the domain of integration. The fourth equality is due to the fact that the off-diagonal integrals vanish as a change of variables to polar coordinates shows. The fifth equality is monotone convergence, while the sixth uses the fact that the functions Ψ_n^μ are normalized. ■

Proposition 3.3: For every $\psi \in \mathcal{B}_\mu^2$ we have

$$e^{-tN_\mu} \psi(z) = \psi_e(e^{-t} z) + e^{-2\mu t} \psi_o(e^{-t} z), \tag{3.4}$$

where $t \ge 0$ and $z \in \mathbb{C}$.

Here $\psi = \psi_e + \psi_o$ is the decomposition of ψ into its even and odd parts.

Proof: We first note for all $n \ge 0$ and $t \ge 0$ that

$$e^{-tN_\mu} \Psi_n^\mu(z) = e^{-t(n+2\mu\theta_n)} \Psi_n^\mu(z) = e^{-t(n+2\mu\theta_n)} z^n / (\gamma_\mu(n))^{1/2} = e^{-2\mu t\theta_n} \Psi_n^\mu(e^{-t} z)$$

follows from the definitions of e^{-tN_μ} and Ψ_n^μ. This is exactly the identity (3.4) we wish to show in the special case when $\psi = \Psi_n^\mu$ for some $n \ge 0$. The rest of the argument consists of an extension of the result to all $\psi \in \mathcal{B}_\mu^2$.

So we let $\psi=\Sigma_{n=0}^{\infty}a_n\Psi_n^{\mu}$ be the Maclaurin series of $\psi\in\mathcal{B}_{\mu}^2$ as before. By the previous proposition we have that $\|\psi\|_{\mathcal{B}_{\mu}^2}^2=\Sigma_{n=0}^{\infty}|a_n|^2$. Since $\psi-\Sigma_{n=0}^{N}a_n\Psi_n^{\mu}=\Sigma_{n=N+1}^{\infty}a_n\Psi_n^{\mu}$ is an element in $\mathcal{B}_{\mu}^2$, the expressions in this computation are finite:

$$\left\|\psi-\sum_{n=0}^{N}a_n\Psi_n^{\mu}\right\|_{\mathcal{B}_{\mu}^2}^2=\left\|\sum_{n=N+1}^{\infty}a_n\Psi_n^{\mu}\right\|_{\mathcal{B}_{\mu}^2}^2=\sum_{n=N+1}^{\infty}|a_n|^2\to 0 \tag{3.5}$$

as $N\to\infty$. Here the second equality is the evaluation of the norm in $\mathcal{B}_{\mu}^2$ by using the previous proposition, but now applied to the function $\Sigma_{n=N+1}^{\infty}a_n\Psi_n^{\mu}\in\mathcal{B}_{\mu}^2$, which is a Maclaurin series. The convergence to zero in (3.5) follows from the fact that $\psi\in\mathcal{B}_{\mu}^2$ and the previous proposition. Therefore (3.5) says that the Maclaurin series $\Sigma_{n=0}^{\infty}a_n\Psi_n^{\mu}$, which is known by complex analysis to converge to ψ uniformly on compact subsets of $\mathbb{C}$, converges to ψ *also* in the norm topology of the Hilbert space $\mathcal{B}_{\mu}^2$. Using this second sense of the convergence of the Maclaurin series to ψ, we immediately see that

$$e^{-tN_{\mu}}\psi=\sum_{n=0}^{\infty}a_ne^{-tN_{\mu}}\Psi_n^{\mu}$$

since $e^{-tN_{\mu}}$ is a bounded operator on the Hilbert space $\mathcal{B}_{\mu}^2$. So we have that

$$\begin{aligned}e^{-tN_{\mu}}\psi(z)&=\sum_{n=0}^{\infty}a_ne^{-tN_{\mu}}\Psi_n^{\mu}(z)=\sum_{n=0}^{\infty}a_ne^{-2\mu t\theta_n}\Psi_n^{\mu}(e^{-t}z)=\sum_{k=0}^{\infty}a_{2k}\Psi_{2k}^{\mu}(e^{-t}z)+\sum_{l=0}^{\infty}a_{2l+1}e^{-2\mu t}\Psi_{2l+1}^{\mu}(e^{-t}z)\\&=\psi_e(e^{-t}z)+e^{-2\mu t}\psi_o(e^{-t}z)\end{aligned}$$

as desired. Here we used the fact that the even (respectively, odd) terms of the Maclaurin series give us the even (respectively, odd) part of the function. ■

Now we extend the definition of $e^{-tN_{\mu}}$, using the previous proposition as our guide.

Definition 3.5: We define $e^{-tN_{\mu}}:\mathcal{H}(\mathbb{C})\to\mathcal{H}(\mathbb{C})$ *by*

$$e^{-tN_{\mu}}\psi(z):=\psi_e(e^{-t}z)+e^{-2\mu t}\psi_o(e^{-t}z), \tag{3.6}$$

where $\psi\in\mathcal{H}(\mathbb{C})$, $z\in\mathbb{C}$, *and* $t\in R$.

Several comments are in order here. First, the previous definition defines the linear operator $e^{-tN_{\mu}}$ with domain given by any of the spaces P_{μ}^p, I_{μ}^p, and $\mathcal{B}_{\mu}^p$ for $0<p<\infty$, and this is what interests us in this paper. By the previous proposition, this generalizes the definition of $e^{-tN_{\mu}}$ for $t\geqslant 0$ given on $\mathcal{B}_{\mu}^2$ in two ways, namely to a larger space and to *all* values $t\in\mathbb{R}$. Actually, the definition also makes sense for all $t\in\mathbb{C}$.

The operator $e^{-tN_{\mu}}$ defined above maps $\mathcal{H}(\mathbb{C})$ to itself continuously (with respect to the topology of uniform convergence on compact subsets) as well as leaving invariant the subspaces $\mathcal{H}_e(\mathbb{C})$ and $\mathcal{H}_o(\mathbb{C})$. The action of $e^{-tN_{\mu}}$ on $\mathcal{H}_e(\mathbb{C})$ is induced exactly by the flow $z\mapsto e^{-t}z$ on $\mathbb{C}$, which is independent of μ. Moreover, on $\mathcal{H}_o(\mathbb{C})$ it is almost induced by the same flow, except that a constant multiplier (depending on μ as well as on t) also appears. Another immediate consequence of the definition is that $e^{-tN_{\mu}}$ for $t\in\mathbb{R}$ is a group of operators acting on $\mathcal{H}(\mathbb{C})$.

Also, let us note that this definition makes sense for *any* function ψ, not just for holomorphic functions. However, in that generality the connection with the operator N_{μ} is obscured. In particular, the proof of Proposition 3.3 depends on the representation of an entire holomorphic function by its Maclaurin series, and the action term by term of $e^{-tN_{\mu}}$ on that series. Another way to understand this is to note that the action of $e^{-tN_{\mu}}$ on the holomorphic polynomials is the starting point of its definition and that these polynomials are dense in $\mathcal{H}(\mathbb{C})$ in its topology of uniform convergence on compact sets. So the extension of the domain of definition of $e^{-tN_{\mu}}$ to $\mathcal{H}(\mathbb{C})$ as given is more or less immediate, while its extension to larger spaces of functions is rather arbitrary.

IV. REVERSE HYPERCONTRACTIVITY

In this section our main goal is to prove reverse hypercontractivity inequalities on the scale of spaces $\mathcal{B}_\mu^p$ for $0<p<\infty$. In order to achieve this goal we will first prove such reverse hypercontractivity inequalities for the even and odd subspaces of $\mathcal{B}_\mu^p$, namely P_μ^p and I_μ^p. This is a technical consideration due to the fact that the definitions of $\mathcal{B}_\mu^p$ and its norm depend on the decomposition of a function into its even and odd parts. And this, as we have noted, comes about from the role that the parity operator plays in this theory.

So, we will prove reverse hypercontractivity inequalities on three scales of spaces: P_μ^p, I_μ^p, and $\mathcal{B}_\mu^p$ where $0<p<\infty$. Specifically, this means we will restrict the action of e^{-tN_μ} for $t\in\mathbb{R}$ to one of these spaces and will ask if the result is a bounded linear map to another one of these spaces indexed by $q<p$. (It need not be a contraction, as is the case in hypercontractivity.) Since e^{-tN_μ} preserves parity and holomorphicity, the problem reduces to finding $q<p$ and $C>0$ for a given value of p such that $\|e^{-tN_\mu}f\|_q\leq C\|f\|_p$ for all f in one of the spaces P_μ^p, I_μ^p or $\mathcal{B}_\mu^p$.

For all the results of this section we use the hypotheses $0<q<p$ and $(1/2)\log(q/p)<t$. We note that they do not depend on the parameter μ. In other words, they are the same hypotheses that appear in the work of Carlen in Ref. 4 on reverse hypercontractivity in the case $\mu=0$. Also, we note that under these hypotheses t can be a negative number.

The method we use originally appeared in Ref. 6 and is also used in Ref. 5.

Theorem 4.1 *(Reverse hypercontractivity for the scale of spaces P_μ^p, $0<p<\infty$):* *For $0<q<p$ and $(1/2)\log(q/p)<t$ we have*

$$\|e^{-tN_\mu}\psi_e\|_{P_\mu^q}\leq A(t,p,q,\mu)\|\psi_e\|_{P_\mu^p} \tag{4.1}$$

for all $\psi_e\in P_\mu^p$, where

$$A(t,p,q,\mu):=e^{(2\mu+3)t/q}\left\{\int_{\mathbb{C}}\left|\frac{K_{\mu-(1/2)}(e^{2t}|w|^2)}{K_{\mu-(1/2)}(|w|^2)}\right|^{p/(p-q)}\mathrm{d}\nu_{e,\mu}(w)\right\}^{(p-q)/pq}<\infty.$$

Remark: Since any $\psi\in P_\mu^p$ is even, $\psi=\psi_e$ holds. So we use the notation ψ_e to denote an arbitrary element in P_μ^p. Similarly, we use ψ_o to denote an arbitrary element in I_μ^p.

Proof: We calculate

$$\begin{aligned}
\|e^{-tN_\mu}\psi_e\|_{P_\mu^q}^q &= \int_{\mathbb{C}}|e^{-tN_\mu}\psi_e(z)|^q\,\mathrm{d}\nu_{e,\mu}(z)=\int_{\mathbb{C}}|\psi_e(e^{-t}z)|^q\kappa_\mu K_{\mu-(1/2)}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y\\
&=\int_{\mathbb{C}}|\psi_e(w)|^q\kappa_\mu K_{\mu-(1/2)}(e^{2t}|w|^2)e^{(2\mu+1)t}|w|^{2\mu+1}e^{2t}\,\mathrm{d}u\,\mathrm{d}v\\
&=e^{(2\mu+3)t}\int_{\mathbb{C}}|\psi_e(w)|^q\frac{K_{\mu-(1/2)}(e^{2t}|w|^2)}{K_{\mu-(1/2)}(|w|^2)}\kappa_\mu K_{\mu-(1/2)}(|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v\\
&\leq e^{(2\mu+3)t}\||\psi_e|^q\|_{P_\mu^r}\left\{\int_{\mathbb{C}}\left|\frac{K_{\mu-(1/2)}(e^{2t}|w|^2)}{K_{\mu-(1/2)}(|w|^2)}\right|^{r'}\kappa_\mu K_{\mu-(1/2)}(|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v\right\}^{1/r'},
\end{aligned}$$

where we have used $K_{\mu-(1/2)}(|w|^2)>0$ for $w\neq 0$, $w=u+iv=e^{-t}z$ and Hölder's inequality for $1<r<\infty$. Taking $r=p/q>1$ [implying that its dual index is $r'=r/(r-1)=p/(p-q)$] and then evaluating the $1/q$ power, we obtain

$$\|e^{tN_\mu}\psi_e\|_{P_\mu^q}\leq e^{(2\mu+3)t/q}\|\psi_e\|_{P_\mu^p}\left\{\int_{\mathbb{C}}\left|\frac{K_{\mu-(1/2)}(e^{2t}|w|^2)}{K_{\mu-(1/2)}(|w|^2)}\right|^{p/(p-q)}\mathrm{d}\nu_{e,\mu}(w)\right\}^{(p-q)/pq}$$

which is the inequality (4.1). Next, to prove that $A(t,p,q,\mu)<\infty$, it is necessary and sufficient to show for $r=p/q$ that

$$\int_{\mathbb{C}} \left| \frac{K_{\mu-(1/2)}(e^{2t}|w|^2)}{K_{\mu-(1/2)}(|w|^2)} \right|^{r'} K_{\mu-(1/2)}(|w|^2)|w|^{2\mu+1}\, du\, dv = \pi \int_0^\infty \left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) s^{\mu+(1/2)}\, ds$$

is finite. And this is equivalent to proving the integrability of the integrand on the right-hand side near 0 and near ∞, since the integrand is a continuous function of $s \in (0,\infty)$. To show the integrability near 0, we use (2.1) which implies that for all $s \in (0,\delta)$ for $\delta > 0$ sufficiently small we have that

$$\left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) \leqslant \frac{C}{s^{|\mu-1/2|}},$$

provided that $\mu \neq 1/2$. When $\mu < 1/2$ this yields

$$\int_0^\delta \left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) s^{\mu+(1/2)}\, ds \leqslant \int_0^\delta \frac{C}{s^{(1/2)-\mu}} s^{\mu+(1/2)}\, ds = C \int_0^\delta s^{2\mu}\, ds < \infty,$$

using the standing hypothesis $\mu > -1/2$. And when $\mu > 1/2$ it gives us

$$\int_0^\delta \left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) s^{\mu+(1/2)}\, ds \leqslant \int_0^\delta \frac{C}{s^{\mu-(1/2)}} s^{\mu+(1/2)}\, ds = C \int_0^\delta s\, ds < \infty.$$

Finally, for $\mu = 1/2$ we take $s \in (0,\delta)$ where $\delta < 2$. We then use (2.2) to obtain that

$$\begin{aligned} \left| \frac{K_0(e^{2t}s)}{K_0(s)} \right|^{r'} K_0(s) &\leqslant C\left(\log \frac{2}{s}\right) \left(\frac{\log \dfrac{2}{e^{2t}s}}{\log \dfrac{2}{s}} \right)^{r'} \\ &= C\left(\log \frac{2}{s}\right) \left(\frac{\log 2/s - 2t}{\log \dfrac{2}{s}} \right)^{r'} \\ &= C\left(\log \frac{2}{s}\right) \left(1 - \frac{2t}{\log \dfrac{2}{s}} \right)^{r'} \leqslant C \log \frac{2}{s}. \end{aligned}$$

Here we used for $t \geqslant 0$ that $\log(2/s) > 0$ and $1 - 2t/\log(2/s) \leqslant 1$, while for $t < 0$ we used $1 - 2t/\log(2/s) < 2$ for δ sufficiently small. Then by elementary calculus we have

$$\int_0^\delta \left| \frac{K_0(e^{2t}s)}{K_0(s)} \right|^{r'} K_0(s) s\, ds \leqslant C \int_0^\delta s \log(2/s) ds < \infty.$$

To show the integrability near ∞ we use (2.3) to show that

$$\left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) \leqslant C \frac{1}{s^{1/2}} e^{-[1-r'(1-e^{2t})]s}$$

for all $s \in (M,\infty)$ for M sufficiently large. Then we get the estimate

$$\int_M^\infty \left| \frac{K_{\mu-(1/2)}(e^{2t}s)}{K_{\mu-(1/2)}(s)} \right|^{r'} K_{\mu-(1/2)}(s) s^{\mu+(1/2)}\, ds \leqslant C \int_M^\infty e^{-[1-r'(1-e^{2t})]s} s^{\mu}\, ds < \infty,$$

since $1-r'(1-e^{2t})>0$ is equivalent to the hypothesis $(1/2)\log(q/p)<t$ given that $r'=p/(p-q)$. ■

Remark: The previous theorem holds for all even functions in $L^p(\mathbb{C},\nu_{e,\mu})$, not just the holomorphic elements, provided that we use the definition in (3.6) for such functions. But, as we commented earlier, such a generalization of the theorem, even though it is true, has nothing to do really with the operator N_μ of interest here. However, we did use the fact that ψ_e is even in the step where we evaluated $e^{-tN_\mu}\psi_e(z)$. The previous theorem also holds with only a slightly modified proof for $0<q<p$ and complex t satisfying $(1/2)\log(q/p)<\mathrm{Re}(t)$. As we also noted before, formula (3.6) defines e^{-tN_μ} for any $t\in\mathbb{C}$. Similar comments hold for the next result, which is about the spaces I^p_μ, and for Theorem 4.3, which is about the spaces $\mathcal{B}^p_\mu$.

Theorem 4.2 *(Reverse hypercontractivity for the scale of spaces I^p_μ, $0<p<\infty$):* *For $0<q<p$ and $(1/2)\log(q/p)<t$ we have that*

$$\|e^{-tN_\mu}\psi_o\|_{I^q_\mu}\leqslant B(t,p,q,\mu)\|\psi_o\|_{I^p_\mu} \tag{4.2}$$

for all $\psi_o\in I^p_\mu$, where

$$B(t,p,q,\mu):=e^{\{[2\mu(1-q)+3]/q\}t}\left\{\int_{\mathbb{C}}\left|\frac{K_{\mu+(1/2)}(e^{2t}|w|^2)}{K_{\mu+(1/2)}(|w|^2)}\right|^{p/(p-q)}\mathrm{d}\nu_{o,\mu}(w)\right\}^{(p-q)/pq}<\infty.$$

Proof: We have that

$$\begin{aligned}\|e^{-tN_\mu}\psi_o\|^q_{I^q_\mu}&=\int_{\mathbb{C}}|e^{-tN_\mu}\psi_o(z)|^q\,\mathrm{d}\nu_{o,\mu}(z)=\int_{\mathbb{C}}|e^{-2\mu t}\psi_o(e^{-t}z)|^q\kappa_\mu K_{\mu+(1/2)}(|z|^2)|z|^{2\mu+1}\,\mathrm{d}x\,\mathrm{d}y\\&=\int_{\mathbb{C}}e^{-2q\mu t}|\psi_o(w)|^q\kappa_\mu K_{\mu+(1/2)}(e^{2t}|w|^2)e^{(2\mu+1)t}|w|^{2\mu+1}e^{2t}\,\mathrm{d}u\,\mathrm{d}v\\&=e^{\{2\mu(1-q)+3\}t}\int_{\mathbb{C}}|\psi_o(w)|^q\frac{K_{\mu+(1/2)}(e^{2t}|w|^2)}{K_{\mu+(1/2)}(|w|^2)}\kappa_\mu K_{\mu+(1/2)}(|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v\\&\leqslant e^{\{2\mu(1-q)+3\}t}\|\,|\psi_o|^q\|_{I^r_\mu}\left(\int_{\mathbb{C}}\left|\frac{K_{\mu+(1/2)}(e^{2t}|w|^2)}{K_{\mu+(1/2)}(|w|^2)}\right|^{r'}\kappa_\mu K_{\mu+(1/2)}(|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v\right)^{1/r'},\end{aligned}$$

where we have used $K_{\mu+(1/2)}(|w|^2)>0$ for $w\neq 0$, $w=u+iv=e^{-t}z$ and Hölder's inequality for $1<r<\infty$. Taking $r=p/q>1$ and then raising to the $1/q$ power we obtain the desired estimate (4.2):

$$\|e^{-tN_\mu}\psi_o\|_{I^q_\mu}\leqslant e^{\{[2\mu(1-q)+3]/q\}t}\|\psi_o\|_{I^p_\mu}\left\{\int_{\mathbb{C}}\left|\frac{K_{\mu+(1/2)}(e^{2t}|w|^2)}{K_{\mu+(1/2)}(|w|^2)}\right|^{p/(p-q)}\mathrm{d}\nu_{o,\mu}(w)\right\}^{(p-q)/pq}.$$

To show that this bound is finite is equivalent to showing that

$$\int_{\mathbb{C}}\left|\frac{K_{\mu+(1/2)}(e^{2t}|w|^2)}{K_{\mu+(1/2)}(|w|^2)}\right|^{r'}K_{\mu+(1/2)}(|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v=\pi\int_0^\infty\left|\frac{K_{\mu+(1/2)}(e^{2t}s)}{K_{\mu+(1/2)}(s)}\right|^{r'}K_{\mu+(1/2)}(s)s^{\mu+(1/2)}\,\mathrm{d}s$$

is finite, where $r=p/q$. As in the previous theorem, it is now a matter of checking that the integrand on the right-hand side is in fact integrable near 0 and near ∞. For $s\in(0,\delta)$ with δ sufficiently small we have that

$$\left| \frac{K_{\mu+(1/2)}(e^{2t}s)}{K_{\mu+(1/2)}(s)} \right|^{r'} K_{\mu+(1/2)}(s) \leqslant C \frac{1}{s^{\mu+(1/2)}},$$

where we have used (2.1) together with the standing hypothesis $\mu+(1/2)>0$. This gives the desired estimate,

$$\int_0^\delta \left| \frac{K_{\mu+(1/2)}(e^{2t}s)}{K_{\mu+(1/2)}(s)} \right|^{r'} K_{\mu+(1/2)}(s) s^{\mu+(1/2)} \, \mathrm{d}s \leqslant \int_0^\delta C \, \mathrm{d}s < \infty.$$

Next, for $s \in [M,\infty)$ with M sufficiently large we apply (2.3) to get

$$\left| \frac{K_{\mu+(1/2)}(e^{2t}s)}{K_{\mu+(1/2)}(s)} \right|^{r'} K_{\mu+(1/2)}(s) \leqslant C \frac{e^{-[1-r'(1-e^{2t})]s}}{s^{1/2}}.$$

Just as in the last estimate in the proof of Theorem 4.1, this then implies that

$$\int_M^\infty \left| \frac{K_{\mu+(1/2)}(e^{2t}s)}{K_{\mu+(1/2)}(s)} \right|^{r'} K_{\mu+(1/2)}(s) s^{\mu+(1/2)} \, \mathrm{d}s \leqslant C \int_M^\infty e^{-[1-r'(1-e^{2t})]s} s^{\mu} \, \mathrm{d}s < \infty,$$

where we have used the inequality $1-r'(1-e^{2t})>0$ which is equivalent to the hypothesis $(1/2)\log(q/p)<t$ together with the fact that $r'=p/(p-q)$. ■

Having shown reverse hypercontractivity for the two scales of spaces P_μ^p and I_μ^p, we now can quickly prove the main goal of this section.

Theorem 4.3 *(Reverse hypercontractivity for the scale of spaces $\mathcal{B}_\mu^p$, $0<p<\infty$):* *For $0<q<p$ and $(1/2)\log(q/p)<t$ we have that*

$$\|e^{-tN_\mu}\psi\|_{\mathcal{B}_\mu^q} \leqslant C(t,p,q,\mu)\|\psi\|_{\mathcal{B}_\mu^p}$$

for every $\psi \in \mathcal{B}_\mu^p$, where

$$C(t,p,q,\mu) := ([A(t,p,q,\mu)]^q + [B(t,p,q,\mu)]^q)^{1/q}$$

and $A(t,p,q,\mu)$ and $B(t,p,q,\mu)$ are defined in Theorems 4.1 and 4.2, respectively.

Proof: For brevity, we write A instead of $A(t,p,q,\mu)$ and so forth. Using the fact that e^{-tN_μ} preserves parity in the second equality, we calculate

$$\begin{aligned}\|e^{-tN_\mu}\psi\|_{\mathcal{B}_\mu^q}^q &= \|(e^{-tN_\mu}\psi)_e\|_{P_\mu^q}^q + \|(e^{-tN_\mu}\psi)_o\|_{I_\mu^q}^q = \|e^{-tN_\mu}\psi_e\|_{P_\mu^q}^q + \|e^{-tN_\mu}\psi_o\|_{I_\mu^q}^q \leqslant A^q\|\psi_e\|_{P_\mu^p}^q + B^q\|\psi_o\|_{I_\mu^p}^q \\ &\leqslant A^q\|\psi\|_{\mathcal{B}_\mu^p}^q + B^q\|\psi\|_{\mathcal{B}_\mu^p}^q = (A^q+B^q)\|\psi\|_{\mathcal{B}_\mu^p}^q = C^q\|\psi\|_{\mathcal{B}_\mu^p}^q.\end{aligned}$$

The first inequality follows from Theorems 4.1 and 4.2, while the first equality and the second inequality follow from the definition of $\|\cdot\|_{\mathcal{B}_\mu^p}$. ■

We conclude this section with a result that is somewhat tangential to the topic of reverse inequalities, but which follows immediately from the results we have just presented. We called this property L^p boundedness before, but we now can give it a more accurate name.

Theorem 4.4 *(Boundedness of the semigroup e^{-tN_μ} on $\mathcal{B}_\mu^p$):* *For $0<p<\infty$ and $t\geqslant 0$ we have that $e^{-tN_\mu}: \mathcal{B}_\mu^p \to \mathcal{B}_\mu^p$ boundedly. Explicitly, we have for all $\psi \in \mathcal{B}_\mu^p$ that*

$$\|e^{-tN_\mu}\psi\|_{\mathcal{B}_\mu^p} \leqslant e^{(2\mu+3)t/p}\|\psi\|_{\mathcal{B}_\mu^p}.$$

Proof: For $\psi_e \in P_\mu^p$ we have from the proof of Theorem 4.1 that

$$\|e^{-tN_\mu}\psi_e\|^p_{P^p_\mu} = e^{(2\mu+3)t}\int_{\mathbb{C}} |\psi_e(w)|^p \kappa_\mu K_{\mu-(1/2)}(e^{2t}|w|^2)|w|^{2\mu+1}\,\mathrm{d}u\,\mathrm{d}v.$$

This holds for $0<p<\infty$ and $t\geqslant 0$. But $K_{\mu-(1/2)}(e^{2t}|w|^2)\leqslant K_{\mu-(1/2)}(|w|^2)$ since the Macdonald function is monotone decreasing and $t\geqslant 0$. Applying this to the previous, we immediately get

$$\|e^{-tN_\mu}\psi_e\|^p_{P^p_\mu} \leqslant e^{(2\mu+3)t}\|\psi_e\|^p_{P^p_\mu}$$

for all $\psi_e \in P^p_\mu$. Similarly, from the identity at the beginning of the proof of Theorem 4.2 and the monotonicity of $K_{\mu+(1/2)}$, we see that for $0<p<\infty$ and $t\geqslant 0$ we have

$$\|e^{-tN_\mu}\psi_o\|^p_{I^p_\mu} \leqslant e^{(2\mu(1-p)+3)t}\|\psi_o\|^p_{I^p_\mu}$$

for all $\psi_o \in I^p_\mu$. The result for general $\psi \in \mathcal{B}^p_\mu$ now follows immediately. ■

This result is far from being sharp. For example, when $\mu=0$, it is known that the semigroup e^{-tN_0} for $t\geqslant 0$ acts contractively on $\mathcal{B}^p_0$. After all, contractivity is just a special case of hypercontractivity. But the bound we get in this case is $e^{3t/p}$. We conjecture that e^{-tN_μ} acts contractively on $\mathcal{B}^p_\mu$ and, even stronger, hypercontractively. This seems reasonable, since it is known to be true for $\mu=0$. Of course, if it is false, then we would have a nice mathematical property that would single out the usual quantization with $\mu=0$ from the deformations with $\mu\neq 0$.

Also note that this result quickly gives us reverse hypercontractivity for $t\geqslant 0$, since then e^{-tN_μ} acting on $\mathcal{B}^p_\mu$ maps its domain to itself boundedly and $\mathcal{B}^p_\mu$ is continuously contained in $\mathcal{B}^q_\mu$ for any $q<p$ by Hölder's inequality. Similar remarks apply to P^p_μ and I^p_μ. So the nontrivial case of reverse hypercontractivity is for negative t, specifically for $t\in((1/2)\log(q/p),0)$.

V. REVERSE LOG-SOBOLEV INEQUALITIES

In this section the goal is to prove a reverse log-Sobolev inequality in the Hilbert space $\mathcal{B}^2_\mu$. As in the preceding section, technical considerations lead us to proving such inequalities first in the Hilbert spaces P^2_μ and I^2_μ. The upshot is that the result for $\mathcal{B}^2_\mu$ is not what one might have expected and, in fact, leads us to a new definition of entropy that is appropriate for $\mathcal{B}^2_\mu$.

The method we use is due to Gross and first appeared in Ref. 26. Also, see Ref. 5 for another use of this method. We start with a definition of a quantity that arises in the next theorem.

Definition 5.1: We define the μ-deformed energy *for* $\psi_e \in P^2_\mu$ *by*

$$E_{e,\mu}(\psi_e) := \int_{\mathbb{C}} |\psi_e(z)|^2|z|^2\,\mathrm{d}\nu_{e,\mu}(z).$$

While we can consider this definition for larger classes of functions, we will comment in detail in an Appendix why we are interested in this quantity in the case that $\psi_e \in P^2_\mu$ and why it is called an energy in that case.

Theorem 5.1 *(Reverse log-Sobolev inequality in the space* P^2_μ*)*: *For* $c>1$ *and* $\psi_e \in P^2_\mu$ *we have that*

$$E_{e,\mu}(\psi_e) \leqslant cS_{P^2_\mu}(\psi_e) + \left(c\log\int_{\mathbb{C}} e^{|z|^2/c}\,\mathrm{d}\nu_{e,\mu}(z)\right)\|\psi_e\|^2_{P^2_\mu}, \tag{5.1}$$

where $S_{P^2_\mu}(\psi_e)$ *is the entropy of* ψ_e *as given in Definition 2.3. Moreover, for* $c>1$ *we have that*

$$1 < \int_{\mathbb{C}} e^{|z|^2/c}\,\mathrm{d}\nu_{e,\mu}(z) < \infty,$$

so that the coefficient of the norm term is positive and finite.

We note that the hypothesis $c>1$ in this and the subsequent theorems in this section does not depend on the parameter μ. In particular, it is the same condition as found by the second author in Ref. 25, where the case $\mu=0$ is studied.

Proof: Consider Young's inequality

$$st \leqslant s \log s - s + e^t,$$

where $s \geqslant 0$ and t are real numbers.

We take $c>1$ and $\psi_e \in P_\mu^2$ and then set $s=c|\psi_e(z)|^2$ and $t=|z|^2/c$ in Young's inequality. Next, we integrate to get

$$E_{e,\mu}(\psi_e) = \int_{\mathbb{C}} |\psi_e(z)|^2 |z|^2 \, \mathrm{d}\nu_{e,\mu}(z) \leqslant \int_{\mathbb{C}} c|\psi_e(z)|^2 \log c|\psi_e(z)|^2 \, \mathrm{d}\nu_{e,\mu}(z) - c\|\psi_e\|_{P_\mu^2}^2 + \int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z)$$

$$= cS_{P_\mu^2}(\psi_e) + (c \log c - c + c \log \|\psi_e\|_{P_\mu^2}^2)\|\psi_e\|_{P_\mu^2}^2 + \int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z),$$

using the definitions of $E_{e,\mu}(\psi_e)$ and $S_{P_\mu^2}(\psi_e)$. Now we replace ψ_e with $\lambda\psi_e$ for $\lambda>0$ and divide by λ^2 to get

$$E_{e,\mu}(\psi_e) \leqslant cS_{P_\mu^2}(\psi_e) + (c \log c - c + c \log \|\psi_e\|_{P_\mu^2}^2 + c \log \lambda^2)\|\psi_e\|_{P_\mu^2}^2 + \frac{1}{\lambda^2}\int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z).$$

Minimizing the right-hand side by varying λ, we obtain the optimal value

$$\lambda^2 = \frac{1}{c\|\psi_e\|_{P_\mu^2}^2}\int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z),$$

if $\psi_e \neq 0$. Substituting this value into the previous inequality and simplifying we get (5.1) in the case when $\psi_e \neq 0$. But (5.1) trivially holds if $\psi_e = 0$.

We still must discuss the integral $\int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z)$. But the integrand is bounded below by 1 and $\nu_{e,\mu}$ is a probability measure, so that $\int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z) > 1$ holds. It remains for us to show that this integral is finite. Since the integrand is continuous, we only must show its integrability near infinity (in the complex plane). We note that by the definition of $\nu_{e,\mu}$ and a simple change of variables we have

$$\int_{\mathbb{C}} e^{|z|^2/c} \, \mathrm{d}\nu_{e,\mu}(z) = \kappa_\mu \int_{\mathbb{C}} e^{|z|^2/c} K_{\mu-(1/2)}(|z|^2)|z|^{2\mu+1} \, \mathrm{d}x \, \mathrm{d}y = \pi\kappa_\mu \int_0^\infty e^{s/c} K_{\mu-(1/2)}(s) s^{\mu+(1/2)} \, \mathrm{d}s. \tag{5.2}$$

So what we must prove is the convergence of this last integral near ∞. But (2.3) implies that for all $s \in [M, \infty)$ for some M sufficiently large, we have that $K_{\mu-1/2}(s) \leqslant Cs^{-1/2}e^{-s}$. Applying this, we find that

$$\int_M^\infty e^{s/c} K_{\mu-(1/2)}(s) s^{\mu+(1/2)} \, \mathrm{d}s \leqslant C \int_M^\infty e^{-(1-1/c)s} s^\mu \, \mathrm{d}s < \infty, \tag{5.3}$$

where we used $c>1$ to conclude that the last integral is finite. ■

Note the the integral on the right-side of (5.2) is exactly calculable as an infinite series by expanding the exponential factor in its Maclaurin series and then using (2.4). This is also given in terms of the hypergeometric function in Eq. 6.621.3 in Ref. 7. We do not present this exact result here, since it seems to be of little interest, unless it should happen to give the unknown optimal coefficient of the norm term in (5.1). So we only present the asymptotic analysis of the integral. This exact result also shows that the integral (5.2) converges if and only if $c>1$, which is

something that an asymptotic analysis gives us as well. In the case $\mu=0$, it is known that the condition $c>1$ in the inequality (5.1) cannot be improved. (See Ref. 25.) It is natural to conjecture that this should be true for all μ. Similar comments apply to Theorem 5.2.

For the subspace of odd holomorphic functions, we have similar results. We start with the definition of the μ-deformation of the energy for this case.

Definition 5.2: We define the μ-deformed energy *for* $\psi_o \in I_\mu^2$ *by*

$$E_{o,\mu}(\psi_o) := \int_{\mathbb{C}} |\psi_o(z)|^2 |z|^2 \, d\nu_{o,\mu}(z).$$

Again, we refer to the Appendix for more details about this concept. It arises in the following theorem, which corresponds to Theorem 5.1 for the space I_μ^2.

Theorem 5.2 *(Reverse log-Sobolev inequality in the space* I_μ^2*)***:** *For* $c>1$ *and* $\psi_o \in I_\mu^2$ *we have*

$$E_{o,\mu}(\psi_o) \leqslant c S_{I_\mu^2}(\psi_o) + \left(c \log \int_{\mathbb{C}} e^{|z|^2/c} \, d\nu_{o,\mu}(z) \right) \|\psi_o\|_{I_\mu^2}^2. \tag{5.4}$$

Here $S_{I_\mu^2}(\psi_o)$ *is the entropy of* ψ_o *as given in Definition 2.3. Furthermore, for* $c>1$ *we have that*

$$\nu_{o,\mu}(C) < \int_{\mathbb{C}} e^{|z|^2/c} \, d\nu_{o,\mu}(z) < \infty, \tag{5.5}$$

so that the coefficient of the norm term is finite.

Proof: The proof of formula (5.4) is the same as the proof of (5.1) in Theorem 5.1, and so it will be omitted. The lower bound in (5.5) follows immediately from the fact that 1 is a lower bound on the integrand. For the upper bound in (5.5) we consider

$$\int_{\mathbb{C}} e^{|z|^2/c} \, d\nu_{o,\mu}(z) = \kappa_\mu \int_{\mathbb{C}} e^{|z|^2/c} K_{\mu+(1/2)}(|z|^2) |z|^{2\mu+1} \, dx \, dy = \pi \kappa_\mu \int_0^\infty e^{s/c} K_{\mu+(1/2)}(s) s^{\mu+(1/2)} \, ds.$$

As in the previous theorem, this integral can be exactly evaluated, but we only do an asymptotic analysis. Since the integrand on the left-hand side is integrable near the origin in the complex plane, the integrand on the right-hand side is integrable near 0. For the integrability on the right-hand side near infinity, we use (2.3) to get $K_{\mu+(1/2)}(s) \leqslant C s^{-1/2} e^{-s}$ for s sufficiently large. Now the proof terminates just as in (5.3), except with $K_{\mu+(1/2)}$ instead of $K_{\mu-(1/2)}$. ■

We comment that for $-1/2<\mu<0$ we have $0<\nu_{o,\mu}(\mathbb{C})<1$. (See Ref. 1.) So the above proof does not exclude the possibility of a negative coefficient of the norm term in (5.4) when $-1/2<\mu<0$. In the case $\mu>0$ we have from Ref. 1 that $\nu_{o,\mu}(\mathbb{C})>1$, so that the coefficient of the norm term in (5.4) is positive. However, we do not know for any pair $\mu>-1/2$ and $c>1$ what is the optimal value of the coefficient of that norm term.

We will use the following concept in the next theorem.

Definition 5.3: We define the total μ-deformed energy *by*

$$E_\mu(\psi) := E_{e,\mu}(\psi_e) + E_{o,\mu}(\psi_o)$$

for all $\psi \in \mathcal{B}_\mu^2$.

Having proved reverse log-Sobolev inequalities in the Hilbert spaces P_μ^2 and I_μ^2, we can now achieve the goal of this section, which is an inequality of that type for $\mathcal{B}_\mu^2$. However, we do not get one entropy term as is the case for a usual reverse log-Sobolev inequality, but rather two.

Theorem 5.3 *(Reverse log-Sobolev inequality in the space* $\mathcal{B}_\mu^2$*)***:** *For all* $c>1$ *there exist real numbers* $M(c,\mu)$ *and* $N(c,\mu)$ *such that for* $\psi \in \mathcal{B}_\mu^2$ *we have*

$$E_\mu(\psi) \leqslant c(S_{P_\mu^2}(\psi_e) + S_{I_\mu^2}(\psi_o)) + M(c,\mu)\|\psi_e\|_{P_\mu^2}^2 + N(c,\mu)\|\psi_o\|_{I_\mu^2}^2.$$

If we set $P(c,\mu) := \max(M(c,\mu), N(c,\mu))$, *then it follows for all* $\psi \in \mathcal{B}_\mu^2$ *that*

$$E_\mu(\psi) \leqslant c(S_{P^2_\mu}(\psi_e) + S_{I^2_\mu}(\psi_o)) + P(c,\mu)\|\psi\|^2_{\mathcal{B}^2_\mu}.$$

The proof of this result is an immediate consequence of Theorems 5.1 and 5.2. The definition of the total μ-deformed energy as the sum of two quadratic forms in $\mathcal{B}^2_\mu$ is neither surprising nor extraordinary. On the other hand, Theorem 5.3 presents us with an expression that is a new type of entropy.

Definition 5.4: For any $\psi \in \mathcal{B}^2_\mu$, *we define its* μ-deformed entropy $S_\mu(\psi)$ *by*

$$S_\mu(\psi) := S_{P^2_\mu}(\psi_e) + S_{I^2_\mu}(\psi_o),$$

where $\psi = \psi_e + \psi_o$ *is the decomposition of* ψ *into its even and odd parts.*

Let us note that this definition is not a particular case of Definition 2.3 of Shannon entropy. As far as we know, this is the first occurrence in the literature of a definition of an entropy of a function that depends on its decomposition into its even and odd parts. Of course, the *μ-deformed even entropy* $S_{P^2_\mu}(\psi_e)$ and the *μ-deformed odd entropy* $S_{I^2_\mu}(\psi_o)$ are Shannon entropies. With this definition the last inequality in Theorem 5.3 now has the compact form:

$$E_\mu(\psi) \leqslant cS_\mu(\psi) + P(c,\mu)\|\psi\|^2_{\mathcal{B}^2_\mu}.$$

VI. CONCLUSION

We note that there is a way to generalize this theory to the case of spaces of holomorphic functions on $\mathbb{C}^n$ for finite n in place of $\mathbb{C}$. We thank C. Pita for telling us about his unpublished work on this subject. This is also presented in Ref. 3. It remains an open problem as to how one might formulate such a theory for an infinite dimensional phase space.

Here are some other problems that are still open in this area. First, one can try to find the optimal constants for the various reverse hypercontractivity and the reverse log-Sobolev inequalities that we have proved. We conjecture that optimizing functions exist for all of these inequalities when the optimal constants are introduced into them, though it remains an open problem to identify these functions explicitly. We recall that a function f_{opt} is an *optimizing function* for an inequality (involving a function f) if that inequality becomes an equality when f_{opt} is substituted for f.

At present we do not even know whether e^{-tN_μ} maps $\mathcal{B}^p_\mu$ to itself contractively for $\mu \neq 0$, $p \neq 2$, and $t > 0$. We conjecture that this is true, but we were only able to prove in Theorem 4.4 that this operator is bounded. In addition we repeat the stronger conjecture made earlier that this semigroup is hypercontractive on the scales of spaces $\mathcal{B}^p_\mu$, a result which is known to be true when $\mu = 0$.

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APPENDIX

We would like to comment in this Appendix about the relationship between the μ-deformed energy and the expected value of the μ-deformed harmonic oscillator energy, to be described below. We begin with an exact formula for the μ-deformed energy for the even case. Let us note that the proof of this formula uses hypotheses that are weaker than $\psi_e \in P_\mu^2$, though the latter is the case of interest.

Proposition 6.1: Suppose that $\psi_e:\mathbb{C}\to\mathbb{C}$ *is an even, holomorphic function with Maclaurin series* $\psi_e(z)=\sum_{j=0}^{\infty}a_{2j}z^{2j}$. *Then we have*

$$E_{e,\mu}(\psi_e)=\sum_{j=0}^{\infty}|a_{2j}|^2 2^{2j+1}\frac{\Gamma(j+3/2)\Gamma(\mu+j+1)}{\Gamma(\mu+1/2)}.$$

In particular, $E_{e,\mu}(\psi_e)$ *is finite if and only if the infinite series on the right-hand side is convergent*.

Proof: We exhibit first the following chain of equalities and give the justifications subsequently:

$$\begin{aligned}
\int_{\mathbb{C}}|\psi_e(z)|^2|z|^2\,\mathrm{d}\nu_{e,\mu}(z) &= \lim_{R\to\infty}\int_{|z|\leqslant R}\left(\sum_j a_{2j}z^{2j}\right)^{\star}\left(\sum_l a_{2l}z^{2l}\right)z^{\star}z\,\mathrm{d}\nu_{e,\mu}(z)\\
&= \lim_{R\to\infty}\int_{|z|\leqslant R}\sum_{j,l}a_{2j}^{\star}a_{2l}(z^{\star})^{2j+1}z^{2l+1}\,\mathrm{d}\nu_{e,\mu}(z)\\
&= \lim_{R\to\infty}\sum_{j,l}a_{2j}^{\star}a_{2l}\int_{|z|\leqslant R}(z^{\star})^{2j+1}z^{2l+1}\,\mathrm{d}\nu_{e,\mu}(z)\\
&= \lim_{R\to\infty}\sum_j|a_{2j}|^2\int_{|z|\leqslant R}|z|^{2(2j+1)}\,\mathrm{d}\nu_{e,\mu}(z)=\sum_j|a_{2j}|^2\int_{\mathbb{C}}|z|^{2(2j+1)}\,\mathrm{d}\nu_{e,\mu}(z)\\
&= \frac{1}{\Gamma(\mu+1/2)}\sum_j|a_{2j}|^2 2^{2j+1}\Gamma(j+3/2)\Gamma(\mu+j+1).
\end{aligned}$$

The introduction of the limit in the first equality is an application of the monotone convergence theorem. The interchange of the integral with the infinite sum in the third equality is allowed by the uniform convergence of the infinite series on the compact domain of integration. The fourth equality holds since the integrals for $j\neq l$ are zero, as one sees by introducing polar coordinates. The fifth equality is again monotone convergence, applied first to the infinite sum and then to the integral. The sixth equality is the evaluation of a finite integral, which we present in a moment. Notice that this chain of inequalities holds also in the case when the integral being evaluated is equal to infinity. Finally for the sixth equality, we have that

$$\begin{aligned}
\int_{\mathbb{C}}|z|^{2(2j+1)}\,\mathrm{d}\nu_{e,\mu}(z) &= \kappa_\mu\int_0^{2\pi}\left(\int_0^{\infty}K_{\mu-(1/2)}(r^2)r^{2\mu+1}r^{2(2j+1)}r\,\mathrm{d}r\right)\mathrm{d}\theta\\
&= \frac{2^{(1/2)-\mu}}{\Gamma(\mu+1/2)}\int_0^{\infty}K_{\mu-(1/2)}(s)s^{\mu+2j+3/2}\,\mathrm{d}s\\
&= \frac{1}{\Gamma(\mu+1/2)}2^{2j+1}\Gamma(j+3/2)\Gamma(\mu+j+1).
\end{aligned}$$

The last equality is an application of the identity (2.4). ■

We now consider the expected value of the μ-deformed harmonic oscillator energy $\langle\psi_e,H_\mu\psi_e\rangle$ for $\psi_e\in P_\mu^2$, where

$$H_\mu := \tfrac{1}{2}(\widetilde{P}_\mu^2 + \widetilde{Q}_\mu^2) = \tfrac{1}{2}(A_\mu A_\mu^\star + A_\mu^\star A_\mu) = N_\mu + \tfrac{1}{2}I + \mu J \tag{A1}$$

is the μ-deformed harmonic oscillator Hamiltonian. (See Ref. 20 and Proposition 3.1.) For $\mu=0$, the relation between the two energies is

$$E_{e,0}(\psi_e) = \langle \psi_e, N_0 \psi_e \rangle + \|\psi_e\|_{\mathcal{B}_0^2}^2 = \langle \psi_e, H_0 \psi_e \rangle + \tfrac{1}{2}\|\psi_e\|_{\mathcal{B}_0^2}^2,$$

where the first equality is an identity of Bargmann in Ref. 2 We therefore expect a relation for general $\mu > -1/2$. Since the identity of Bargmann is just a simple application of the canonical commutation relation (with $\mu=0$), one would expect that an application of the μ-deformed canonical commutation relation starting from the expression $\langle \psi_e, H_\mu \psi_e \rangle$ would lead to some expression involving $E_{e,\mu}(\psi_e)$. But this is not what happens. Instead, the integral $\int_{\mathbb{C}} |\psi_e(z)|^2 |z|^2 \, \mathrm{d}\nu_{o,\mu}(z)$ arises. See Ref. 1 for more about this integral.

We start the analysis of H_μ by noting that $H_\mu \Psi_{2j}^\mu = (2j+\mu+1/2)\Psi_{2j}^\mu$, so that

$$\langle \psi_e, H_\mu \psi_e \rangle = \sum_{j=0}^{\infty} |a_{2j}|^2 \gamma_\mu(2j)(2j+\mu+1/2),$$

where $\psi_e(z) = \Sigma_{j=0}^\infty a_{2j} z^{2j}$ is the Maclaurin series of ψ_e. So using Proposition 6.1, the *conjecture* that

$$E_{e,\mu}(\psi_e) = a_\mu \langle \psi_e, H_\mu \psi_e \rangle + b_\mu \|\psi_e\|_{P_\mu^2}^2$$

for some constants a_μ and b_μ is equivalent to the *conjecture* that

$$\frac{1}{\Gamma(\mu+1/2)} 2^{2j+1} \Gamma(j+3/2)\Gamma(\mu+j+1) = a_\mu \gamma_\mu(2j)(2j+\mu+1/2) + b_\mu \gamma_\mu(2j) \tag{A2}$$

for all integers $j \geqslant 0$, since $\|\psi_e\|_{P_\mu^2}^2 = \Sigma_j |a_{2j}|^2 \gamma_\mu(2j)$. This leads us to consider the quantities

$$Q_{j,\mu} := 2^{2j+1} \frac{\Gamma(j+3/2)\Gamma(\mu+j+1)}{\Gamma(\mu+1/2)\gamma_\mu(2j)}$$

for every integer $j \geqslant 0$.

In particular, the conjecture (A2) is equivalent to saying $Q_{j,\mu} = A_\mu j + B_\mu$ for some constants A_μ and B_μ. To proceed we apply the identity (3.1) to get

$$Q_{j,\mu} := 2\left(\frac{\Gamma(j+3/2)}{\Gamma(j+1)}\right)\left(\frac{\Gamma(\mu+j+1)}{\Gamma(\mu+j+1/2)}\right). \tag{A3}$$

We would like to evaluate this last expression exactly for all values of the parameters, namely for all integers $j \geqslant 0$ and all reals $\mu > -1/2$. This can be done for the first quotient since we have $\Gamma(j+1) = j!$ and $\Gamma(j+3/2) = \pi^{1/2} 2^{-j-1}(2j+1)!!$ by well-known identities. (See Ref. 7) So the problem reduces to calculating the second quotient in (A3). This can be done in either of the following two special cases, since we can again calculate the numerator and denominator separately: (1) $\mu = n$ where $n \geqslant 0$ is an integer. (2) $\mu = n + (1/2)$ (a half-integer) where $n \geqslant 0$ is an integer. We do not write down these formulas here. However, let us note that calculations in the case $\mu = 1/2$ show that the conjecture (A2) is false.

However, for general μ we do not need formulas for the numerator and for the denominator separately, but we only need one formula for the second quotient itself in (A3). And this has the form $\Gamma(\alpha+1/2)/\Gamma(\alpha)$ for $\alpha > 0$. We note the identity

$$\frac{\Gamma(\alpha)}{\Gamma(\alpha+1/2)} = \frac{2}{\pi^{1/2}} \int_0^{\pi/2} (\sin^{2\alpha-1}\theta) \mathrm{d}\theta$$

provided that $\alpha > 0$, which comes from evaluating the beta function $B(1/2, \alpha)$ first in terms of the gamma function (Eq. 8.384.1 in Ref. 7) and then in terms of its usual integral representation (Eq. 8.380.1 in Ref. 7). However, the intent behind this identity is that it gives us a way of evaluating the integral on the right-hand side in terms of the elementary function Γ. For example, see Eq. 3.621.5 in Ref. 7. But here we are interpreting the identity as a way of evaluating a quotient of two values of the Euler gamma function in terms of an integral that does not seem elementary at all, except when α is an integer or a half-integer. And these are exactly the cases when the quotient can be evaluated directly by using identities of the Euler gamma function Γ.

It seems that there is no simpler identity in general for the second quotient in (A3) and that the only thing we can do is to find its asymptotic behavior as $j \to \infty$ with μ fixed. But this is a straightforward application of Stirling's formula, which tells us that $\Gamma(\alpha+1/2) \approx \alpha^{1/2}\Gamma(\alpha)$ as $\alpha \to \infty$. (See Sec. 8.327 and Sec. 8.328, Eq. 2 in Ref. 7.) Since we are only getting the asymptotic behavior of the second quotient in (A3), we will only concern ourselves with the asymptotic behavior (rather than the exact formula) of the first quotient, which has the same form as the second quotient in (A3). So we find for fixed $\mu > -1/2$ that

$$Q_{j,\mu} \approx 2(j+1)^{1/2}(j+\mu+1/2)^{1/2} \approx 2j \approx 2j+\mu+1/2$$

as $j \to \infty$. So there are constants $0 < C_{1,\mu} < C_{2,\mu}$ so that

$$C_{1,\mu}(2j+\mu+1/2) \leqslant Q_{j,\mu} \leqslant C_{2,\mu}(2j+\mu+1/2)$$

for all integers $j \geqslant 0$. This implies that

$$C_{1,\mu}\langle \psi_e, H_\mu \psi_e \rangle \leqslant E_\mu(\psi_e) \leqslant C_{2,\mu}\langle \psi_e, H_\mu \psi_e \rangle.$$

This says that the expected value of the energy of the μ-deformed harmonic oscillator and the μ-deformed energy $E_e(\psi_e)$ are equivalent as quadratic forms. So any inequality involving one of these quadratic forms implies a similar inequality with the other. This explains why we call $E_\mu(\psi_e)$ an energy. Also by using (A1), the expected value of H_μ can be related to the expected value of N_μ.

The analysis for the odd case is quite similar, and we will not present it in full detail. We start by deriving a closed formula for the μ-deformed energy.

Proposition 6.2: Let $\psi_o : \mathbb{C} \to \mathbb{C}$ *be an odd, holomorphic function with Maclaurin series* $\psi_o(z) = \sum_{j=0}^{\infty} b_{2j+1} z^{2j+1}$. *Then we have*

$$E_{o,\mu}(\psi_o) = \sum_{j=0}^{\infty} |b_{2j+1}|^2 2^{2j+2} \frac{\Gamma(j+3/2)\Gamma(\mu+j+2)}{\Gamma(\mu+1/2)}.$$

In particular, $E_{o,\mu}(\psi_o)$ *is finite if and only if the infinite series on the right-hand side is convergent.*

Proof: We note that

$$\begin{aligned}
\int_{\mathbb{C}} |\psi_o(z)|^2 |z|^2 \, \mathrm{d}\nu_{o,\mu}(z) &= \lim_{R\to\infty} \int_{|z|\leqslant R} \left(\sum_j b_{2j+1} z^{2j+2} \right)^{\star} \left(\sum_l b_{2l+1} z^{2l+2} \right) \mathrm{d}\nu_{o,\mu}(z) \\
&= \lim_{R\to\infty} \int_{|z|\leqslant R} \sum_{j,l} b_{2j+1}^{\star} b_{2l+1} (z^{\star})^{2j+2} z^{2l+2} \, \mathrm{d}\nu_{o,\mu}(z) \\
&= \lim_{R\to\infty} \sum_{j,l} b_{2j+1}^{\star} b_{2l+1} \int_{|z|\leqslant R} (z^{\star})^{2j+2} z^{2l+2} \, \mathrm{d}\nu_{o,\mu}(z)
\end{aligned}$$

$$= \lim_{R\to\infty} \sum_j |b_{2j+1}|^2 \int_{|z|\leq R} |z|^{2(2j+2)}\, \mathrm{d}\nu_{o,\mu}(z) = \sum_j |b_{2j+1}|^2 \int_{\mathbb{C}} |z|^{2(2j+2)}\, \mathrm{d}\nu_{o,\mu}(z)$$

$$= \frac{1}{\Gamma(\mu+1/2)} \sum_j |b_{2j+1}|^2 2^{2j+2} \Gamma(j+3/2)\Gamma(\mu+j+2).$$

The justifications of the first five equalities are the same as in the corresponding calculation in Proposition 6.1. For the last equality we have used the evaluation of this finite integral,

$$\int_{\mathbb{C}} |z|^{2(2j+2)}\, \mathrm{d}\nu_{o,\mu}(z) = \kappa_\mu \int_{\mathbb{C}} K_{\mu+1/2}(|z|^2)|z|^{2\mu+1}|z|^{2(2j+2)}\, \mathrm{d}x\, \mathrm{d}y = \pi\kappa_\mu \int_0^\infty K_{\mu+1/2}(s) s^{\mu+2j+5/2}\, \mathrm{d}s$$

$$= \frac{1}{\Gamma(\mu+1/2)} 2^{2j+2} \Gamma(j+3/2)\Gamma(\mu+j+2),$$

where the last equality is an application of (2.4). ■

For $\psi_o \in I^2_\mu$ with Maclaurin series $\psi_o(z) = \Sigma_{j=0}^\infty b_{2j+1} z^{2j+1}$ we have that

$$\|\psi_o\|^2_{I^2_\mu} = \sum_{j=0}^\infty |b_{2j+1}|^2 \gamma_\mu(2j+1),$$

$$\langle \psi_o, H_\mu \psi_o \rangle = \sum_{j=0}^\infty |b_{2j+1}|^2 \gamma_\mu(2j+1)(2j+\mu+3/2).$$

We next define the quantity

$$R_{j,\mu} := \frac{2^{2j+2}\Gamma(j+3/2)\Gamma(\mu+j+2)}{\Gamma(\mu+1/2)\gamma_\mu(2j+1)}.$$

Then using (3.2) we obtain

$$R_{j,\mu} = 2\frac{\Gamma(j+3/2)\Gamma(\mu+j+2)}{\Gamma(j+1)\Gamma(\mu+j+3/2)}.$$

Again, an exact analysis is possible when μ is an integer or half-integer. But in general we are only able to give the asymptotic behavior, which is

$$R_{j,\mu} \approx 2(j+1)^{1/2}(j+\mu+3/2)^{1/2} \approx 2j \approx 2j+\mu+3/2$$

as $j\to\infty$ with μ fixed. Consequently, there exist constants $0 < D_{1,\mu} < D_{2,\mu}$ such that

$$D_{1,\mu}\langle \psi_o, H_\mu \psi_o \rangle \leq E_{o,\mu}(\psi_o) \leq D_{2,\mu}\langle \psi_o, H_\mu \psi_o \rangle$$

for all $\psi_o \in I^2_\mu$. And this tells us that the quadratic form $E_{o,\mu}(\psi_o)$ is equivalent to $\langle \psi_o, H_\mu \psi_o \rangle$. And so in this case too we see that the μ-deformed energy $E_{o,\mu}(\psi_o)$ is equivalent to the expected value of the μ-deformed harmonic oscillator energy.

Thus, the total μ-deformed energy $E_\mu(\psi)$ is equivalent to the μ-deformed harmonic oscillator energy $\langle \psi, H_\mu \psi \rangle$ for all $\psi \in \mathcal{B}^2_\mu$.

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Phase-integral calculation of the phase of the regular Coulomb wave function $F_L(\eta,\rho)$

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The phase of the regular Coulomb wave function $F_L(\eta,\rho)$ is calculated by means of the phase-integral approximation of arbitrary order with a convenient choice of the base function. The result agrees with the most accurate asymptotic expansion of the exact expression, $\arg\Gamma(L+1+i\eta)$, for the phase, truncated at an arbitrary order of approximation. It is seldom the case that the phase-integral expression for a physical quantity can be obtained in an arbitrary order of the approximation, and it is remarkable that in the present case this expression is the same as that obtained from the most accurate asymptotic formula for the quantity in question. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2189196]

I. INTRODUCTION

By means of the phase-integral method, which is described in Chap. 1 of Fröman and Fröman (1993) and in Chap. 2 of Fröman and Fröman (2002), one can in general calculate explicitly only the first few terms in the expansion for a physical quantity. A formula for the general term can, however, be obtained for the phase of the regular Coulomb wave function $F_L(\eta,\rho)$. The purpose of the present paper is to derive this phase with the use of an arbitrary order of the phase-integral approximation and to see how the result is related to asymptotic expansions of the exact expression, $\arg\Gamma(L+1+i\eta)$, for the phase under consideration.

For the background of the present paper we refer to the above-mentioned chapters in Fröman and Fröman (1996, 2002) and to a treatment of Coulomb wave functions in Dzieciol, Yngve, and Fröman (1999).

II. TREATMENT OF THE PROBLEM

Consider the differential equation

$$\frac{d^2\psi}{d\rho^2}+R(\rho)\psi=0 \tag{1}$$

with

$$R(\rho)=1-2\eta/\rho-\frac{L(L+1)}{\rho^2}. \tag{2}$$

The solution of (1) along with (2) that is regular at the origin is proportional to the Coulomb wave function $F_L(\eta,\rho)$, which according to Secs. 14.5.1, 14.5.5, 14.5.6, and 14.5.8 in Abramowitz and Stegun (1972) as $\rho\to+\infty$ behaves as

$$F_L(\eta,\rho)\sim\sin\left[\rho-\eta\ln(2\rho)-\frac{1}{2}L\pi+\sigma_L\right],\quad \rho\to+\infty, \tag{3}$$

where the exact expression for the phase σ_L is given by

$$\sigma_L = \arg \Gamma(L+1+i\eta). \tag{4}$$

Choosing, in our notation,

$$Q^2(\rho) = R(\rho) - \frac{1}{4\rho^2}, \tag{5}$$

Fröman and Yngve (1980) have used the phase-integral method in an arbitrary-order approximation to calculate the phase for the regular solution of a differential equation that becomes identical to (1) along with (2) when one in their paper sets $k=1$ and $b=0$. With this particularization one has according to their equations (10) and (10a, b) in the $(2N+1)$th order of the phase-integral approximation the formulas

$$\sigma_L = \sum_{n=0}^{N} \sigma_L^{(2n+1)} \tag{6}$$

with

$$\sigma_L^{(1)} = \frac{1}{2i}\left[\left(L+\frac{1}{2}+i\eta\right)\ln\left(L+\frac{1}{2}+i\eta\right) - \left(L+\frac{1}{2}-i\eta\right)\ln\left(L+\frac{1}{2}-i\eta\right)\right] - \eta, \tag{7a}$$

$$\begin{aligned}\sigma_L^{(2n+1)} &= \frac{(1-1/2^{2n-1})|B_{2n}|}{4n(2n-1)}\left\{\frac{1}{\left[\eta+i\left(L+\frac{1}{2}\right)\right]^{2n-1}} + \frac{1}{\left[\eta+i\left(L+\frac{1}{2}\right)\right]^{2n-1}}\right\} \\ &= \frac{(-1)^n(1-1/2^{2n-1})|B_{2n}|}{4n(2n-1)}\left\{\frac{1}{i\left(L+\frac{1}{2}+i\eta\right)^{2n-1}} - \frac{1}{i\left(L+\frac{1}{2}-i\eta\right)^{2n-1}}\right\}, \quad n \geqslant 1, \end{aligned} \tag{7b}$$

where B_{2n} are Bernouilli numbers. Noting that according to Secs. 23.1.2, 23.1.18, and 23.1.21 in Abramowitz and Stegun (1972),

$$(-1)^n(1-1/2^{2n-1})|B_{2n}| = (-1)^n(1-1/2^{2n-1})|B_{2n}(0)| = -(1-1/2^{2n-1})B_{2n}(0) = B_{2n}\left(\tfrac{1}{2}\right), n \geqslant 1, \tag{8}$$

where $B_{2n}(0)$ and $B_{2n}\left(\frac{1}{2}\right)$ are Bernouilli polynomials with the arguments 0 and 1/2, respectively, one can write (7b) as

$$\sigma_L^{(2n+1)} = \frac{B_{2n}\left(\frac{1}{2}\right)}{4n(2n-1)}\left\{\frac{1}{i\left(L+\frac{1}{2}+i\eta\right)^{2n-1}} - \frac{1}{i\left(L+\frac{1}{2}-i\eta\right)^{2n-1}}\right\}, \quad n \geqslant 1. \tag{7b$'$}$$

Since

$$L+\frac{1}{2} \pm i\eta = \left[\left(L+\frac{1}{2}\right)^2 + \eta^2\right]^{1/2} \exp\left(\pm i \arctan\frac{\eta}{L+\frac{1}{2}}\right) \tag{9}$$

one can write (7a) as

$$\sigma_L^{(1)} = \eta\left\{\ln\left[\left(L+\frac{1}{2}\right)^2 + \eta^2\right]^{1/2} - 1\right\} + \left(L+\frac{1}{2}\right)\arctan\frac{\eta}{L+\frac{1}{2}}, \tag{10a}$$

and (7b$'$) as

$$\sigma_L^{(2n+1)} = -\frac{B_{2n}\left(\frac{1}{2}\right)}{2n(2n-1)} \operatorname{Re}\left[i\left(L+\frac{1}{2}+i\eta\right)^{-(2n-1)} \right]$$
$$= -\frac{B_{2n}\left(\frac{1}{2}\right)}{2n(2n-1)} \operatorname{Re}\, i\left[\left(L+\frac{1}{2}\right)^2+\eta^2 \right]^{-(2n-1)/2} \exp\left[-i(2n-1)\arctan\frac{\eta}{L+\frac{1}{2}} \right]$$
$$= -\frac{B_{2n}\left(\frac{1}{2}\right)}{2n(2n-1)\left[\left(L+\frac{1}{2}\right)^2+\eta^2\right]^{(2n-1)/2}} \sin\left[(2n-1)\arctan\frac{\eta}{L+\frac{1}{2}} \right], \quad n \geqslant 1. \tag{10b}$$

By means of the phase-integral method we have thus for σ_L obtained the formula (6) along with (7a) and (7b) or alternatively along with (10a) and (10b).

The exact formula for σ_L is

$$\sigma_L = \arg\Gamma(L+1+i\eta) = \frac{1}{2i}[\ln\Gamma(L+1+\eta) - \ln\Gamma(L+1-i\eta)], \tag{11}$$

and the most accurate asymptotic expansion of $\ln\Gamma(L+1\pm i\eta)$, when $L+1\pm i\eta$ tends to infinity, can be obtained from Eq. (5) on p. 32 of Luke (1969), and is

$$\ln\Gamma(L+1\pm i\eta) \sim \left(L+\frac{1}{2}\pm i\eta\right)\left[\ln\left(L+\frac{1}{2}\pm i\eta\right)-1\right] + \ln(2\pi)^{1/2}$$
$$+\sum_{n=1}^{\infty} \frac{B_{2n}\left(\frac{1}{2}\right)}{2n(2n-1)\left(L+\frac{1}{2}\pm i\eta\right)^{2n-1}}, \quad \left|L+\frac{1}{2}\pm i\eta\right| \to \infty. \tag{12}$$

With the use of (12) one obtains from (11) the formula

$$\sigma_L \sim \frac{1}{2i}\left[\left(L+\frac{1}{2}+i\eta\right)\ln\left(L+\frac{1}{2}+i\eta\right) - \left(L+\frac{1}{2}-i\eta\right)\ln\left(L+\frac{1}{2}-i\eta\right)\right] - \eta$$
$$+\sum_{n=1}^{\infty} \frac{B_{2n}\left(\frac{1}{2}\right)}{4n(2n-1)}\left[\frac{1}{i\left(L+\frac{1}{2}+i\eta\right)^{2n-1}} - \frac{1}{i\left(L+\frac{1}{2}-i\eta\right)^{2n-1}}\right], \quad \left|L+\frac{1}{2}\pm i\eta\right| \to \infty, \tag{13}$$

which, when truncated, agrees with the formula (6) along with (7a) and (7b), which was obtained by means of the phase-integral method.

With the use of the asymptotic expansion in Sec. 6.1.40 in Abramowitz and Stegun (1972) one obtains the formula

$$\ln\Gamma(L+1\pm i\eta) \sim \left(L+\frac{1}{2}\pm i\eta\right)\ln(L+1\pm i\eta) - (L+1\pm i\eta) + \ln(2\pi)^{1/2}$$
$$+\sum_{n=1}^{\infty} \frac{B_{2n}}{2n(2n-1)(L+1\pm i\eta)^{2n-1}}, |L+1\pm i\eta| \gg 1, \quad \arg(L+1\pm i\eta) \leqslant \varepsilon \leqslant \pi, \tag{14}$$

which is less accurate than (13). To understand how (14) is related to (12), we consider the first few terms in (14), getting

$$
\begin{aligned}
&\ln\Gamma(L+1\pm i\eta)\\
&\quad\sim\left(L+\frac{1}{2}\pm i\eta\right)\ln(L+1\pm i\eta)-(L+1\pm i\eta)+\ln(2\pi)^{1/2}+\frac{B_2}{2(L+1\pm i\eta)}\\
&\quad=\left(L+\frac{1}{2}\pm i\eta\right)\left\{\ln\left(L+\frac{1}{2}\pm i\eta\right)+\ln\left[1+\frac{1}{2\left(L+\frac{1}{2}\pm i\eta\right)}\right]\right\}\\
&\qquad-(L+1\pm i\eta)+\ln(2\pi)^{1/2}+\frac{B_2}{2(L+1\pm i\eta)}\\
&\quad\approx\left(L+\frac{1}{2}\pm i\eta\right)\left[\ln\left(L+\frac{1}{2}\pm i\eta\right)+\frac{1}{2\left(L+\frac{1}{2}\pm i\eta\right)}-\frac{1}{8\left(L+\frac{1}{2}\pm i\eta\right)^2}\right]\\
&\qquad-\left(L+\frac{1}{2}\pm i\eta\right)-\frac{1}{2}+\ln(2\pi)^{1/2}+\frac{B_2}{2\left(L+\frac{1}{2}\pm i\eta\right)}\\
&\quad=\left(L+\frac{1}{2}\pm i\eta\right)\left[\ln\left(L+\frac{1}{2}\pm i\eta\right)-1\right]+\ln(2\pi)^{1/2}+\frac{B_2-\frac{1}{4}}{2\left(L+\frac{1}{2}\pm i\eta\right)},
\end{aligned}
$$

i.e., when we note that according to Secs. 23.1.3 and 23.1.21 in Abramowitz and Stegun (1972) $B_2-1/4=1/6-1/4=-1/12=B_2(1/2)$,

$$
\ln\Gamma(L+1\pm i\eta)\approx\left(L+\frac{1}{2}\pm i\eta\right)\left[\ln\left(L+\frac{1}{2}\pm i\eta\right)-1\right]+\ln(2\pi)^{1/2}+\frac{B_2\left(\frac{1}{2}\right)}{2\left(L+\frac{1}{2}\pm i\eta\right)}.
$$

This formula agrees with (12), when the sum there is truncated after the first term.

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Motion of a charged particle in a periodic Aharonov-Bohm potential

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In this paper we introduce a periodic Aharonov-Bohm potential, produced by two parallel infinite thin layers. The motion of a quantum charged particle without spin, under the action of this Aharonov-Bohm potential is examined. Finally we introduce a periodic Aharonov-Bohm potential, produced by a system of parallel solenoids and the motion of the charged particle in this field is also examined. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2189199]

I. INTRODUCTION

In the standard interpretation, the Aharonov-Bohm effect is referred to as the phase modification of a quantum particle in the region of space in which the magnetic induction **B** and electric field intensity **E** vanish, but it still exists in a vector potential **A** or an electric potential ϕ.[1–3] The effect was also investigated experimentally.[2]

In a series of recent papers, Audretsch *et al.*,[4,5] Skarzhinsky *et al.*[6] have demonstrated that in an Aharonov-Bohm potential, some other new important effects like the particle electron-positron pair production, bremsstrahlung of relativistic electrons and scattering of neutral atoms with induced electric dipole moments may occur.

It has been found that the action of the Aharonov-Bohm potential produces shift of the energy levels of atoms[7,8] and quantum harmonic oscillators.[9]

In these papers the case of an Aharonov-Bohm potential generated by a magnetic string which produces weak effects has been considered.

Meanwhile, a series of papers were dedicated to the problem of relativistic particles scattering in an Aharonov-Bohm potential, generated by an infinite solenoid,[10,11] or to the time-dependent Aharonov-Bohm potential.[12]

An attempt is made in our paper to define a magnetic structure that produces Aharonov-Bohm potentials more efficient for experimental purposes.

This kind of potential is important because it permits us to obtain more realistic configurations, similar to the free electron laser configurations with undulator magnets.[13]

II. A PERIODIC AHARONOV-BOHM POTENTIAL

Consider a magnetic system consisting in two infinite magnetic layers of thickness δ, lying parallel to the plane *Oyz*. A section of the system in the *Oxy* plane is drawn in Fig. 1. The magnetic layers L_1 and L_2 are situated at a distance *b* from *Oyz* plane.

Consider that the two magnetic layers are magnetized along the *z* axis, and that the magnetic fields have opposite orientations. The magnetic induction will be assumed constant along the *z* axis and having periodic variation along the *y* axis; let λ be the space period and

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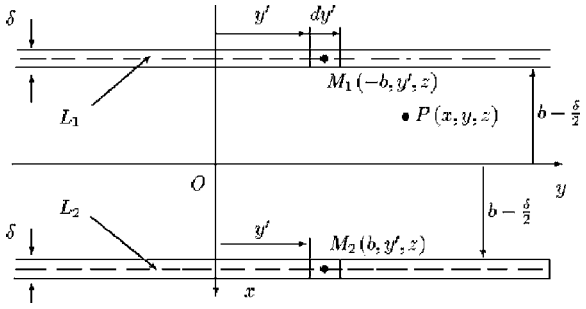

FIG. 1. Magnetic configuration.

$$k = \frac{2\pi}{\lambda},$$

the associated wave vector.

Consider that the magnetic induction in points M_1 and M_2 has the following variation:

$$B_{1z}(x_1, y', z) = -B_0 \cos ky', \quad B_{2z}(x_2, y', z) = B_0 \cos ky',$$

for $x_1 \in [-b-(\delta/2), -b+(\delta/2)]$, $x_2 \in [b-(\delta/2), b+(\delta/2)]$ and that $B_{1j}(-b, y', z) = B_{2j}(b, y', z) = 0$, where $j = x, y$.

Let a pair of magnetic strings, centered in $M_1(-b, y', z)$ and $M_2(b, y', z)$ and directed along the z axis and let $\mathrm{d}S = \delta\, \mathrm{d}y'$ be their cross-section area. These two magnetic strings can be assimilated to a pair of infinite nondispersive solenoids giving rise to the following magnetic fluxes:

$$\mathrm{d}\Phi_1 = B_1 \delta\, \mathrm{d}y', \quad \mathrm{d}\Phi_2 = B_2 \delta\, \mathrm{d}y'.$$

It is known that in an external point $P(x, y, z)$ the vector potential of an infinite nondispersive solenoid, oriented along the z axis is given by[1,2]

$$A_x = -\frac{\Phi}{2\pi} \frac{y}{x^2 + y^2}, \quad A_y = \frac{\Phi}{2\pi} \frac{x}{x^2 + y^2}, \quad A_z = 0,$$

where Φ is the magnetic flux inside the solenoid.

Accordingly, the pair of magnetic strings produces about a point $P(x, y, z)$ (Fig. 1), situated between the magnetic layers, an Aharonov-Bohm vector potential $\mathrm{d}\mathbf{A}$, which has the following components:

$$\mathrm{d}A_x = \frac{B_0 \cos ky' \, \delta\, \mathrm{d}y'}{2\pi} \left[\frac{y - y'}{(x+b)^2 + (y-y')^2} - \frac{y - y'}{(x-b)^2 + (y-y')^2} \right],$$

$$\mathrm{d}A_y = \frac{B_0 \cos ky' \, \delta\, \mathrm{d}y'}{2\pi} \left[\frac{x - b}{(x-b)^2 + (y-y')^2} - \frac{x + b}{(x+b)^2 + (y-y')^2} \right], \tag{1}$$

$$\mathrm{d}A_z = 0.$$

Integrating expressions over $y' \in R$, we obtain the components A_x, A_y, and A_z of the vector potential.

In this view we shall use the Fourier transform after y. Let $\mathcal{F}(k)$ be the Fourier transform of a function $F(y)$. Then, the direct and the inverse Fourier transforms of the function F are

$$\mathcal{F}(k) = \int_{-\infty}^{+\infty} F(y) e^{iky}\, \mathrm{d}y, \quad F(y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathcal{F}(k) e^{-iky}\, \mathrm{d}y.$$

The relations (1) can be generalized if we replace $\cos ky'$ by $e^{iky'}$,

$$dA'_x = \frac{B_0 \exp(iky')\delta\, dy'}{2\pi}\left[\frac{y-y'}{(x+b)^2+(y-y')^2} - \frac{y-y'}{(x-b)^2+(y-y')^2}\right],$$

$$dA'_y = \frac{B_0 \exp(iky')\delta\, dy'}{2\pi}\left[\frac{x-b}{(x-b)^2+(y-y')^2} - \frac{x+b}{(x+b)^2+(y-y')^2}\right], \tag{2}$$

$$dA'_z = 0.$$

Integrating one can obtain A_x, A_y, and A_z taking the real part of the generalized forms of Eq. (2).

Using the residues theorem, we get

$$\int_R \frac{e^{iky'}y'}{y'^2+(x+b)^2}dy' = \pi i\ \mathrm{sign}(k)e^{-|k|(x+b)}, \tag{3}$$

$$\int_R \frac{e^{iky'}y'}{y'^2+(x-b)^2}dy' = \pi i\ \mathrm{sign}(k)e^{|k|(x-b)}, \tag{4}$$

$$\int_R \frac{e^{iky'}(x+b)}{y'^2+(x+b)^2}dy' = \pi\ \mathrm{sign}(k)e^{-|k|(x+b)}, \tag{5}$$

$$\int_R \frac{e^{iky'}(x-b)}{y'^2+(x-b)^2}dy' = -\pi\ \mathrm{sign}(k)e^{|k|(x-b)}. \tag{6}$$

Using Eqs. (3)–(6) and the properties of the Fourier transform,[14] we can integrate (2) and we obtain A'_x, A'_y, and A'_z. Taking the real part of these integrals, the components (1) result as

$$A_j = \mathrm{Real}\ A'_j, \quad j = x,y,z,$$

which, for $k>0$ are

$$A_x(x,y,z) = B_0\delta e^{-kb}\sinh kx \sin ky = A_0 \sinh kx \sin ky,$$

$$A_y(x,y,z) = B_0\delta e^{-kb}\cosh kx \cos ky = A_0 \cosh kx \cos ky, \tag{7}$$

$$A_z(x,y,z) = 0,$$

where $A_0 = B_0\delta e^{-kb}$. The amplitude A_0 can be written as a function of magnetic flux $\mathcal{F}_0$ in a section of a magnetic foil perpendicular on B_0 and having the length equal to one-half of the period along the y axis [i.e., $y \in [0, \lambda/2)$]:

$$A_0 = B_0\delta e^{-kb} = \frac{k}{2}\mathcal{F}_0 e^{-kb}. \tag{8}$$

It is easy to verify that this periodic potential is also an Aharonov-Bohm (AB) potential in the region between the two magnetic layers ($\nabla\mathbf{A}=0$ and $\nabla\times\mathbf{A}=0$), and we may consider that the particle is excluded from the magnetic layers.

In a similar way it is possible to calculate the vector potential outside the layers, i.e., $x \in [b+(\delta/2), \infty)$, $y \in R$, and $x \in [-b-(\delta/2), -\infty)$, $y \in R$. This potential can be useful for the study of the phase difference in a double connected domain (the AB effect).

III. MOTION OF THE CHARGED PARTICLE IN A PERIODIC AHARONOV-BOHM POTENTIAL

Consider a nonrelativistic particle of charge e, mass m and, moving in the region delimited by the two magnetic layers which produces the periodic Aharonov-Bohm potential (7) defined in the preceding section.

The Hamiltonian of the particle can be written as

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2, \tag{9}$$

where $\mathbf{A}$ is given by (7).

The stationary states for the Schrödinger equation of the system (9) can be expressed as

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - 2i\alpha\left(\sinh kx \sin ky \frac{\partial}{\partial x} + \cosh kx \cos ky \frac{\partial}{\partial y}\right) - \alpha^2(\sinh^2 kx \sin^2 ky + \cosh^2 kx \cos^2 ky) + \varepsilon\right]\psi(x,y) = 0, \tag{10}$$

where we used the following notations:

$$\alpha = \frac{eA_0}{c\hbar}, \quad \varepsilon = \frac{2mE}{\hbar^2},$$

in which E is the energy of the stationary states.

Consider that the particle cannot penetrate the magnetic foils domain. Then, it follows that the eigenfunctions $\psi(x,y)$ of (10) must obey the boundary conditions:

$$\psi\left(b - \frac{\delta}{2}, y\right) = 0, \quad \psi\left(-\left(b - \frac{\delta}{2}\right), y\right) = 0. \tag{11}$$

Such a condition was also used in Ref. 15.

In order to find the eigenvalues ε and the eigenfunctions $\psi(x,y)$ of the equation (10) we make the following substitution:

$$u = x + iy, \quad v = x - iy. \tag{12}$$

Accordingly, the Schrödinger equation for the stationary states will be

$$\left[\left(2\frac{\partial}{\partial v} + \alpha \cosh kv\right)\left(2\frac{\partial}{\partial u} - \alpha \cosh ku\right) + \varepsilon\right]\Phi(u,v) = 0, \tag{13}$$

where $\Phi(u,v) = \psi(x,y)$.

The equation (13) is a differential equation with separable variables. Writing the solution under the form

$$\Phi(u,v) = F(u)G(v),$$

we obtain

$$\left[\frac{\left(2\frac{\partial G}{\partial v}+\alpha\cosh kvG\right)}{G}\frac{\left(2\frac{\partial F}{\partial u}-\alpha\cosh kuF\right)}{F}+\varepsilon\right]=0,$$

which, after separation leads to

$$\left(2\frac{\partial}{\partial u}-\alpha\cosh ku\right)F=c_1F,$$

$$\left(2\frac{\partial}{\partial v}+\alpha\cosh kv\right)G=c_2G, \tag{14}$$

$$\varepsilon=-c_1c_2,$$

where c_1 and c_2 are separation constants.

Finally, the solution of Eq. (13),

$$\Phi(u,v)=C\exp\left[\frac{1}{2}(c_1u+c_2v)+\frac{1}{2}\frac{\alpha}{k}(\sinh ku-\sinh kv)\right],$$

where C is the normalization constant. The solution can also be written in terms of variables (x,y) as

$$\psi(x,y)=C\exp\left[\frac{1}{2}(c_1+c_2)x+\frac{1}{2}i(c_1-c_2)y+i\frac{\alpha}{k}\cosh kx\sin ky\right]. \tag{15}$$

Since solution (15) does not comply boundary condition (11) we shall set $c_1=c_2=0$ and examine the more general solution

$$\psi(x,y)=C\exp\left[i\frac{\alpha}{k}\cosh kx\sin ky\right]p(x)q(y), \tag{16}$$

where $p(x)$ and $q(y)$ are unknown functions.

It is noteworthy that the Schrödinger equation (10) is periodic along the y axis with λ and even along the x axis. This implies that the solution $\psi(x,y)$ must fulfill the following conditions:

$$\psi(x,y+\lambda)=\psi(x,y),\quad \psi(-x,y)=\psi(x,y). \tag{17}$$

The factor $\exp[i(\alpha/k)\cosh kx\sin ky]$ in the solution (16) can be expanded in terms of $\exp(iky)$. Due to the property of periodicity it follows from Bloch's theorem that the function $q(y)$ must be periodic with λ.

Finally, we obtain solutions obeying both the conditions (11) and (17), as unbounded states,

$$\psi_{n_1,n_2}(x,y)=N\cos\left(\frac{\pi(2n_1+1)}{2(b-\delta/2)}x\right)\exp\left[in_2ky+i\frac{\alpha}{k}\cosh kx\sin ky\right], \tag{18}$$

where N is the normalization constant. The eigenfunction ψ_{n_1,n_2} is even with respect to the x axis.

The values of n_1, for ψ_{n_1,n_2} must be $n_1=0,1,2,3,\ldots$. The possible values of n_2 are $n_2=0,\pm1,\pm2,\pm3,\ldots$.

Let $|n_1n_2\rangle=\psi_{n_1n_2}$ be the eigenstates (18). It is noteworthy that $|n_1n_2\rangle$ is a set of unbounded states. For this reason, in order to avoid divergent integrals, we can restrict the integration over y to a period, i.e., $y\in[0,2\pi/k]$.

Taking into account this restriction, the scalar product of these states will be

$$\langle n_1 n_2 | n_1' n_2' \rangle = \delta_{n_1,n_1'} \delta_{n_2,n_2'},$$

where δ is the Kronecker symbol. Accordingly, the normalization constant, $N = \sqrt{2/(2b-\delta)}$, and the energy levels will be

$$E_{n_1 n_2} = \frac{\hbar^2}{2m\alpha^2}\left[\left(\frac{\pi}{2b-\delta}\right)^2 (2n_1+1)^2 + k^2 n_2^2\right] = \hbar\,(\omega_x(2n_1+1)^2 + \omega_y n_2^2), \tag{19}$$

where

$$\omega_x = \frac{\hbar c}{ek\mathcal{F}_0}\left(\frac{\pi}{2b-\delta}\right)^2 e^{kb}, \quad \omega_x = \frac{\hbar c}{e\mathcal{F}_0} k e^{kb}.$$

The states ψ_{n_1,n_2} are twofold degenerated with respect to n_1 and n_2, except for $n_2=0$.

Bounded states for Aharonov-Bohm potentials generated by a single solenoid were obtained in a series of previous papers.[7,9,10]

The general solution can also be derived using the variational iteration method of He.[16]

IV. SYSTEM ALGEBRA

We can build the creation and annihilation operators (b_+ and b_-)

$$b_+ = e^{iky}\left[\frac{1}{ik}\left(\frac{\partial}{\partial y} - i\alpha \cosh kx \cos ky\right) + 1\right], \tag{20}$$

$$b_- = \left[\frac{1}{ik}\left(\frac{\partial}{\partial y} - i\alpha \cosh kx \cos ky\right) + 1\right] e^{-iky}, \tag{21}$$

and also a b_0 operator

$$b_0 = \frac{1}{ik}\left(\frac{\partial}{\partial y} - i\alpha \cosh kx \cos ky\right) + \frac{1}{2}, \tag{22}$$

connected to the n_2 quantum number.

The action of these operators on the eigenfunctions $|n_1 n_2\rangle$ is given by

$$\begin{aligned} b_+|n_1,n_2\rangle &= (n_2+1)|n_1,n_2+1\rangle, \\ b_-|n_1,n_2\rangle &= n_2|n_1,n_2-1\rangle, \\ b_0|n_1 n_2\rangle &= \left(n_2+\tfrac{1}{2}\right)|n_1 n_2\rangle. \end{aligned} \tag{23}$$

We also can note that by Hermitian conjugations one can show that

$$b_\pm^\dagger = b_\mp, \quad b_0^\dagger = b_0.$$

These operators obey the commutation relations

$$\begin{aligned} [b_-,b_+] &= 2b_0, \\ [b_0,b_+] &= b_+, \\ [b_0,b_-] &= -b_-. \end{aligned} \tag{24}$$

It is noteworthy that the set of eigenfunctions $|n_1 n_2\rangle$ is separated with respect to n_2 into a set for negative values of n_2 and into a set of positive values of n_2, due to the fact that

$$b_-|n_1 0\rangle = 0, \quad b_+|n_1 - 1\rangle = 0. \tag{25}$$

We can also build a set of creation and annihilation operators $a_\pm$, acting on the quantum number n_1,

$$a_+ = \frac{2b-\delta}{2\pi}\sin\frac{2\pi x}{2b-\delta}\left[\frac{d}{dx} - i\alpha \sinh kx \sin ky\right] + \left(n_1 + \frac{1}{2}\right)\cos\frac{2\pi x}{2b-\delta}, \tag{26}$$

$$a_- = -\frac{2b-\delta}{2\pi}\sin\frac{\pi x}{2b-\delta}\left[\frac{d}{dx} - i\alpha \sinh kx \sin ky\right] + \left(n_1 + \frac{1}{2}\right)\cos\frac{\pi x}{2b-\delta}, \tag{27}$$

and an operator a_0,

$$a_0 = -\left(\frac{2b-\delta}{2\pi}\right)^2\left[\frac{d}{dx} - i\alpha \sinh kx \sin ky\right]^2 - n_1^2 + \frac{1}{4}. \tag{28}$$

It is easy to note that the operators $b_\pm$ are dependent on n_1, i.e., on a state $|n_1 n_2\rangle$ an operator with the same quantum number n_1 must be applied.[17] The action of these operators is given by

$$a_+|n_1,n_2\rangle = \left(n_1 + \tfrac{1}{2}\right)|n_1+1,n_2\rangle, \tag{29}$$

$$a_-|n_1,n_2\rangle = \left(n_1 + \tfrac{1}{2}\right)|n_1-1,n_2\rangle, \tag{30}$$

$$a_0|n_1,n_2\rangle = \left(n_1 + \tfrac{1}{2}\right)|n_1,n_2\rangle. \tag{31}$$

Operators $a_\pm$ and a_0 obey the commutation relations

$$[a_-,a_+] = 2a_0, \tag{32}$$

$$[a_0,a_\pm] = \pm a_\pm. \tag{33}$$

Operators $a_\pm$ can be written in a n_1-independent form using an auxiliary phase type variable ξ ($\xi \in [0,2\pi)$).[18,19] In this representation, the wave functions take the form

$$|n_1 n_2\rangle_\xi = \exp(i n_1 \xi)|n_1 n_2\rangle,$$

and the operators $a_\pm$ (26) and (26) will be

$$a_\pm = \pm e^{\pm i\xi}\frac{2b-\delta}{2\pi}\sin\frac{2\pi x}{2b-\delta}\left[\frac{\partial}{\partial x} - i\alpha \sinh kx \sin ky\right] + e^{\pm i\xi}\cos\frac{2\pi x}{2b-\delta}\left(\frac{1}{i}\frac{\partial}{\partial\xi} + \frac{1}{2}\right), \tag{34}$$

$$a_0 = \left(\frac{1}{i}\frac{\partial}{\partial\xi} + \frac{1}{2}\right). \tag{35}$$

V. COHERENT STATES

We can build the coherent states for the annihilation operator[20,21] as the states $|z_1 z_2\rangle$ (where z_1 and z_2 are complex valued variables, $z_{1,2} \in C$), which are eigenstates for operators a_- and b_-,

$$a_-|z_1 z_2\rangle = z_1|z_1 z_2\rangle, \quad b_-|z_1 z_2\rangle = z_2|z_1 z_2\rangle.$$

These states will be

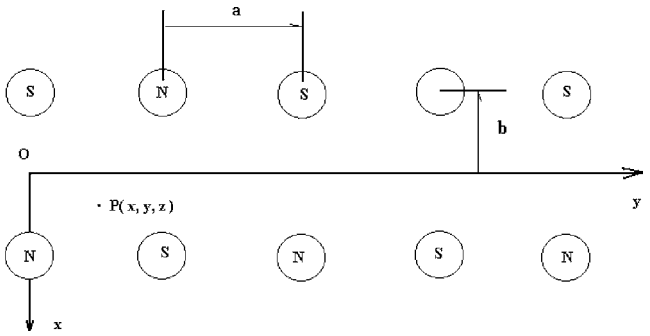

FIG. 2. Periodic structure of solenoids.

$$|z_1 z_2\rangle = d_0 \sum_{n_1=0}^{\infty} \sum_{n_2=-\infty}^{\infty} \frac{z_1^{n_1} z_2^{n_2}}{(3/2)_{n_1} n_2!} |n_1 n_2\rangle, \tag{36}$$

where $(a)_n = a(a+1)(a+2)\cdots(a+n-1)$ and d_0 is a normalization constant equal to

$$d_0 = \left(\sum_{n_1=0}^{\infty} \sum_{n_2=-\infty}^{\infty} \frac{|z_1|^{2n_1} |z_2|^{2n_2}}{(3/2)_{n_1}^2 (n_2\,!)^2} \right)^{-1/2}.$$

We can also build the coherent states for the displacement operators $D_1(\chi_1)$ and $D_2(\chi_2)$ (where $\chi_{1,2} \in C$),

$$D_1(\chi_1) = \exp(\chi_1 a_+ - \chi_1^* a_-), \quad D_2(\chi_2) = \exp(\chi_2 b_+ - \chi_2^* b_-), \tag{37}$$

as[20,21]

$$|\chi_1 \chi_2\rangle = D_1(\chi_1) D_2(\chi_2) |10\rangle. \tag{38}$$

VI. PERIODIC STRUCTURE OF SOLENOIDS

Consider a periodic structure made of solenoids.[22] A section in the plane (x,y) is shown in Fig. 2.

In a point P of the field, situated outside the magnetic flux domain (Fig. 2), the vector potential $\mathbf{A}$ of periodic Aharonov-Bohm structure has the following components:

$$A_x = \frac{F}{2\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left[\frac{y - na}{(x+b)^2 + (y-na)^2} - \frac{y-na}{(x-b)^2 + (y-na)^2} \right],$$

$$A_y = \frac{F}{2\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left[\frac{x-b}{(x-b)^2 + (y-na)^2} - \frac{x+b}{(x+b)^2 + (y-na)^2} \right],$$

$$A_z = 0. \tag{39}$$

In order to put in a restricted form the series expressing the components A_x and A_y of the vector potential, we shall use the Fourier transform with respect to variable y. Then, if $\mathcal{F}(k)$ is the Fourier transform of a function $F(y)$, the Fourier transform of the components A_x and A_y are

$$\mathcal{A}_x(k) = i \frac{F}{4} \operatorname{sign}(k) [e^{-|(x+b)k|} - e^{-|(x-b)k|}] \sum_{n=-\infty}^{+\infty} (e^{in(ka+\pi)} + e^{in(ka-\pi)}), \tag{40}$$

$$\mathcal{A}_y(k) = \frac{F}{4}[\text{sign}(x-b)e^{-|(x-b)k|} - \text{sign}(x+b)e^{-|(x+b)k|}] \sum_{n=-\infty}^{+\infty} (e^{in(ka+\pi)} + e^{in(ka-\pi)}). \tag{41}$$

The above relations contain the following series:

$$S = \sum_{n=-\infty}^{+\infty} (e^{in(ka+\pi)} + e^{in(ka-\pi)}).$$

To express this series, the following identity[14] will be used:

$$\sum_{n=-\infty}^{+\infty} e^{in\omega x} = T \sum_{n=-\infty}^{+\infty} \delta(x - nT). \tag{42}$$

Then, setting $x=[k\pm(\pi/a)]$ and $\omega=2a$, S becomes

$$S = \frac{2\pi}{a} \sum_{n=-\infty}^{+\infty} \left\{ \delta\left[k - (2n+1)\frac{\pi}{a} \right] + \delta\left[k - (2n-1)\frac{\pi}{a} \right] \right\}. \tag{43}$$

Calculating the inverse Fourier transform, observing that $a>0$, and eliminating the negative frequencies, the components of the vector potential can be written as

$$A_x(\mathbf{r}) = \frac{F}{2\pi a} \sum_{n=0}^{+\infty} \left[e^{-2\pi(2n+1)|[(x+b)/2a]|} - e^{-2\pi(2n+1)|[(x-b)/2a]|} \right] \sin\left[2\pi(2n+1)\frac{y}{2a} \right], \tag{44}$$

$$A_y(\mathbf{r}) = \frac{F}{2\pi a} \sum_{n=0}^{+\infty} [\text{sign}(x-b)e^{-2\pi(2n+1)|[(x-b)/2a]|} - \text{sign}(x+b)e^{-2\pi(2n+1)|[(x+b)/2a]|}] \times \cos\left[2\pi(2n+1)\frac{y}{2a} \right], \tag{45}$$

$$A_z(\mathbf{r}) = 0. \tag{46}$$

Taking into account that $x \in [-b, b]$, the components of the vector potential result as

$$A_x(\mathbf{r}) = -\frac{F}{\pi a} \sum_{n=0}^{+\infty} e^{-2\pi(2n+1)(b/2a)} \sinh\left[\frac{2\pi}{2a}(2n+1)x \right] \sin\left[2\pi(2n+1)\frac{y}{2a} \right], \tag{47}$$

$$A_y(\mathbf{r}) = -\frac{F}{\pi a} \sum_{n=0}^{+\infty} e^{-2\pi(2n+1)|(b/2a)|} \cosh\left[\frac{2\pi}{2a}(2n+1)x \right] \cos\left[2\pi(2n+1)\frac{y}{2a} \right]. \tag{48}$$

The *wavelength* (*the spatial period*), of the structure of solenoids, and the corresponding wave number are $\lambda=2a$ and $k=2\pi/\lambda$, respectively.

One can also obtain even harmonics, whose wavelength and wave number are given by

$$\lambda_{2n+1} = \frac{\lambda}{2n+1}, \quad k_{2n+1} = (2n+1)k.$$

The Schrödinger equation for the charged particle under the action of the potential (47) and (48) can be written as

$$\left[\left(\frac{\partial}{\partial x} - \frac{ie}{\hbar c} A_x \right)^2 + \left(\frac{\partial}{\partial y} - \frac{ie}{\hbar c} A_y \right)^2 + \frac{2mE}{\hbar^2} \right] \psi(x,y) = 0. \tag{49}$$

Consider that the particle cannot penetrate the solenoids, i.e., $\psi(x,y)=0$ on the surface of the solenoids.

In terms of variables (u,v), (12), Eq. (49) can be written in a separable form. Then, introducing

$$\epsilon=\frac{2mE}{\hbar^2},\quad \beta=\frac{eF}{\pi a\hbar c},\quad k=\frac{2\pi}{2a},$$

a particular solution $\psi(x,y)$,

$$\psi(x,y)=\exp\left[\frac{1}{2}(c_1+c_2)x+\frac{1}{2}(c_1-c_2)iy-i\frac{\beta}{k}\sum_{n=0}^{\infty}\frac{e^{-kb(2n+1)}}{2n+1}\cosh((2n+1)kx)\sin((2n+1)ky)\right], \tag{50}$$

results.

A more general solution can be written under the form

$$\psi(x,y)=\exp\left[-i\frac{\beta}{k}\sum_{n=0}^{\infty}\frac{e^{-kb(2n+1)}}{2n+1}\cosh((2n+1)kx)\sin((2n+1)ky)\right]h(x,y), \tag{51}$$

where $h(x,y)$ is an unknown function, even with respect to variable x and periodic with respect to variable y, with $\lambda=2a$. Function h must satisfy the differential equation,

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\epsilon\beta^2 h=0.$$

The general solution cannot be found without knowing the solution outside of the region delimited by the solenoid structure.

VII. CONCLUSIONS

In this paper a periodic Aharonov-Bohm potential of magnetic type, generated by two infinite layers of magnetic foil with periodic magnetization is proposed.

This kind of potential is adequate for experimental purposes.

From Eq. (18) one can see that the charged particle has unbounded states with discrete energy levels.

In the early papers on the subject, it has been considered that the Aharonov-Bohm potential produces only phase shift effects in the wave function.

It is easy to see that our periodic potential (7), (47), and (48) does not give phase shift effects for a particle that crosses an integer number of spatial periods $(n2\pi/k)$ along an axis, parallel to the y axis, i.e.,

$$\phi=\frac{e}{\hbar c}\int_0^{n2\pi/k}A_y\,dy=0,$$

since the phase shift per half period is equal but opposite in sign to the phase shift in the next half period.

We estimate that a study of the relativistic oscillator,[23] or of the atom in the presence of the periodic Aharonov-Bohm potential (7) is also possible.

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New multiplicativity results for qubit maps

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Let Φ be a trace-preserving, positivity-preserving (but not necessarily completely positive) linear map on the algebra of complex 2×2 matrices, and let Ω be any finite-dimensional completely positive map. For $p=2$ and $p\geqslant 4$, we prove that the maximal p-norm of the product map $\Phi\otimes\Omega$ is the product of the maximal p-norms of Φ and Ω. Restricting Φ to the class of completely positive maps, this settles the multiplicativity question for all qubit channels in the range of values $p\geqslant 4$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2191787]

I. INTRODUCTION AND STATEMENT OF RESULTS

Qubit maps provide a useful laboratory for exploring methods and conjectures in quantum information theory. In particular they can serve as a testing ground for approaches to the problem of additivity of minimal entropy, and the related issues of Holevo capacity and entanglement of formation.[18] In this article we will focus on the maximal p-norm and consider the question of its multiplicativity for a product map, when one of the factors in the product is a qubit map. For values of p close to one this question is directly related to the additivity of minimal entropy, and hence to the circle of problems mentioned previously.

Recall first that the Schatten norm of a matrix A is defined for $p\geqslant 1$ as

$$\|A\|_p=(\mathrm{Tr}|A|^p)^{1/p}=(\mathrm{Tr}(A^*A)^{p/2})^{1/p}. \tag{1}$$

Let Φ be a linear map on the matrix algebra $\mathbb{C}^{d\times d}$, then the maximal p-norm of Φ is defined as

$$\nu_p(\Phi)=\sup_{\rho}\|\Phi(\rho)\|_p=\sup_{|\psi\rangle}\|\Phi(|\psi\rangle\langle\psi|)\|_p, \tag{2}$$

where the first sup runs over states in $\mathbb{C}^{d\times d}$, the second sup runs over pure states (normalized vectors in $\mathbb{C}^d$), and the second equality follows by convexity of the p-norm. It is natural to define another norm $||\Phi||_{1\to p}$ by instead taking the sup over all matrices A satisfying $||A||_1=1$, and this has been considered in other works;[19,6] however for the applications in this article we are interested only in the quantity defined in (2). In the case $d=2$ we will refer to Φ as a *qubit* map.

Recall that the map Φ is positivity preserving if $\Phi(A)\geqslant 0$ for every $A\geqslant 0$, and trace preserving if $\mathrm{Tr}\,\Phi(A)=\mathrm{Tr}(A)$. The map is completely positive (CP) if in addition $\Phi\otimes I_{d'}$ is positivity preserving for every dimension d'. A *channel* is a CP, trace-preserving map.

Amosov and Holevo[2] conjectured that the maximal p-norm is multiplicative for products of channels, that is for any channels Φ and Ω and for all $p\geqslant 1$

$$\nu_p(\Phi\otimes\Omega)=\nu_p(\Phi)\nu_p(\Omega). \tag{3}$$

Later Werner and Holevo[20] found a family of d-dimensional channels Ψ for which $\nu_p(\Psi\otimes\Psi)>\nu_p(\Psi)^2$ for p sufficiently large ($p>4.78\ldots$ for $d=3$). No such example is known for $d=2$, and the original conjecture (3) survives for the case where at least one of the channels Φ, Ω is a qubit channel.

In our main result we prove (3) for the case where Φ is a trace-preserving, positivity-preserving qubit map, where Ω is any finite-dimensional completely positive map, and where $p=2$ or $p\geqslant 4$. We do *not* assume that Φ is completely positive. Indeed it is essential for our proof

that we consider the larger class of positivity preserving but not completely positive maps. Previous work on entrywise positive maps[14] has provided other examples where multiplicativity holds for a class of non-CP maps, in the range $p \geqslant 2$.

Theorem 1: *Let* Φ *be a trace-preserving, positivity-preserving qubit map, and* Ω *any finite-dimensional completely positive map. Then for* $p=2$ *and for all* $p \geqslant 4$,

$$\nu_p(\Phi \otimes \Omega) = \nu_p(\Phi)\nu_p(\Omega). \tag{4}$$

There has been a lot of work on the additivity and multiplicativity question for quantum channels, and (4) has been established for special classes of qubit channels, including the depolarizing channel,[5,3,7,1] unital qubit channels,[15,10] and some classes of nonunital qubit channels.[11,12,17,8] Theorem 1 settles the question of multiplicativity for all qubit channels, at least in the range $p \geqslant 4$ (the case $p=2$ was proved in Ref. 11). It should be noted that (4) is false in general for positivity-preserving qubit maps if $p<2$, as can be seen with the example $\Phi \otimes I$ where $\Phi(\rho)=\rho^T$. We are not aware of any counterexamples to (4) for $2<p<4$.

The proof of Theorem 1 uses the following matrix inequality which is of independent interest.

Theorem 2: *Let* $A, B, C, D \in \mathbb{C}^{d\times d}$ *for some* $d \geqslant 1$. *Then for* $p=2$ *and for all* $p \geqslant 4$,

$$\left\| \begin{pmatrix} A & B \\ C & D \end{pmatrix} \right\|_p \leqslant \left\| \begin{pmatrix} \|A\|_p & \|B\|_p \\ \|C\|_p & \|D\|_p \end{pmatrix} \right\|_p \tag{5}$$

Inequality (5) was first derived by Nathanson.[16] It had been known previously in the cases where $A=D$ and $B=C$,[4] where $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is positive semidefinite,[12] and where all matrices A, B, C, and D are diagonal.[13] We conjecture that the inequality holds in the interval $2 \leqslant p \leqslant \infty$, and that the reverse inequality holds in the interval $1 \leqslant p \leqslant 2$ (it is easy to see that equality holds at $p=2$). Proving this conjecture would also establish the noncommutative version of Hanner's inequality.[4]

The article is organized as follows. In Sec. II we prove Theorem 1 for a special subclass of qubit maps, making use of the inequality (5). In Sec. III we recall a result of Gorini and Sudarshan[9] on the classification of extreme affine maps on $\mathbb{R}^n$ which map the unit ball into itself. Combining the Gorini-Sudarshan classification with the representation of qubit maps as affine maps on $\mathbb{R}^3$, we derive Lemma 4, which implies that any trace-preserving, positivity-preserving qubit map Φ can be expressed as a convex combination of qubit maps from the subclass of Sec. II, all of which share the same maximal output p-norm as Φ. Using Lemma 4, we then prove Theorem 1 for all qubit maps. Section IV contains the proof of Theorem 2, which makes use of previously known matrix inequalities.[12]

II. PROOF FOR SPECIAL CLASS OF MAPS

In this section we prove Theorem 1 for a special class of positivity-preserving, trace-preserving qubit maps. In order to describe this class we will use the representation of qubit states by points in the Bloch sphere, and qubit maps by affine linear maps on $\mathbb{R}^3$.

A qubit state ρ is represented by a point in the unit ball in $\mathbb{R}^3$ via the relation

$$\rho = \frac{1}{2}\left(I + \sum x_i \sigma_i\right) \mapsto x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \tag{6}$$

where I is the identity matrix and $\{\sigma_1, \sigma_2, \sigma_3\}$ are the Pauli matrices. Positivity of ρ is equivalent to

$$\sum x_i^2 \leqslant 1. \tag{7}$$

A trace-preserving qubit map Φ sends the state $\rho=\frac{1}{2}(I+\Sigma x_i\sigma_i)$ to the state $\Phi(\rho)=\frac{1}{2}(I+\Sigma y_i\sigma_i)$, where $y \in \mathbb{R}^3$ is obtained from x by applying an affine linear map, that is

$$y = Ax + v \tag{8}$$

for some real 3×3 matrix A, and some vector $v \in \mathbb{R}^3$.

Conjugation by a unitary matrix $U \in \mathrm{SU}(2)$ maps ρ to $U\rho U^*$, and this acts on the Bloch sphere by a rotation, sending $x \mapsto R(U)x$ for some $R(U) \in \mathrm{SO}(3)$. If unitary conjugations by matrices U, V are performed on the domain and range of the map Φ respectively, then representation (8) is replaced by

$$y' = R(V)AR(U)x + R(V)v. \tag{9}$$

Since the map $U \mapsto R(U)$ is onto, the singular value decomposition implies that it is always possible to find unitary matrices U, V so that $R(V)AR(U)$ is diagonal (though the diagonal entries need not be all positive). Spectral properties of the map Φ (in particular its maximal output p-norm) are invariant under unitary conjugations in its domain and range, hence there is no loss of generality in assuming that the matrix A in (8) is diagonal. Using representation (8), we will say that Φ is in *diagonal form* if

$$A = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \quad v = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}. \tag{10}$$

Note that Φ is unital if and only if $v=0$ in (8). We now prove Theorem 1 for a special class of maps.

Lemma 3: *Let* Φ *be a positivity-preserving, trace-preserving qubit map in diagonal form* (10), *and suppose that at most one of the numbers* (v_1, v_2, v_3) *is nonzero. Then* (4) *holds for any completely positive map* Ω, *for* $p=2$ *and for* $p \geq 4$.

Proof: By permuting coordinates we can assume that only the third component of v can be nonzero, so that $v_1 = v_2 = 0$. The diagonal entries of A may be positive or negative. However we can change the signs of any two diagonal entries by conjugating with a Pauli matrix, without destroying the diagonal property and without changing the third diagonal entry; for example conjugating with σ_3 changes the signs of λ_1 and λ_2, and leaves λ_3 unchanged. Using this additional freedom we can assume that

$$\lambda_1 \geq 0, \quad \lambda_2 \geq 0. \tag{11}$$

Let ρ_{12} be a bipartite state on $\mathbb{C}^2 \otimes \mathbb{C}^d$ for some d, written in block form

$$\rho_{12} = \begin{pmatrix} X & Y \\ Y^* & Z \end{pmatrix}. \tag{12}$$

Let Ω be a completely positive map on $\mathbb{C}^d$, then

$$(I \otimes \Omega)(\rho_{12}) = \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}, \tag{13}$$

where $A = \Omega(X)$, $B = \Omega(Y)$, and $C = \Omega(Z)$. Since Ω is completely positive, and ρ_{12} is a state, it follows that $(I \otimes \Omega)(\rho_{12})$ is positive semidefinite, and hence $B = A^{1/2} R C^{1/2}$ where R is a contraction. This implies in particular that for all $p \geq 1$

$$\|B\|_p \leq \|A\|_p^{1/2} \|C\|_p^{1/2}. \tag{14}$$

We will encounter the 2×2 matrices of p-norms

$$\begin{pmatrix} \|A\|_p & \|B\|_p \\ \|B\|_p & \|C\|_p \end{pmatrix}, \quad \begin{pmatrix} \|A\|_p & i\|B\|_p \\ -i\|B\|_p & \|C\|_p \end{pmatrix} \tag{15}$$

and we note now that (14) implies the positivity of these matrices, or more generally

$$\begin{pmatrix} \|A\|_p & z\|B\|_p \\ z^*\|B\|_p & \|C\|_p \end{pmatrix} \geqslant 0 \tag{16}$$

for any $z \in \mathbb{C}$ satisfying $|z| \leqslant 1$.

Using the diagonal form (10) and the assumption that v_3 is the only nonzero component of v, we have

$$(\Phi \otimes \Omega)(\rho_{12}) = \begin{pmatrix} c_{++}A + c_{+-}C & \lambda_1 B_1 - i\lambda_2 B_2 \\ \lambda_1 B_1 + i\lambda_2 B_2 & c_{--}A + c_{-+}C \end{pmatrix}, \tag{17}$$

where $B = B_1 - iB_2$ with B_1, B_2 hermitian, and where

$$c_{+\pm} = (1 + v_3 \pm \lambda_3)/2, \quad c_{-\pm} = (1 - v_3 \pm \lambda_3)/2. \tag{18}$$

Since Φ is positivity-preserving, it maps the state $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ into a positive semidefinite matrix, and this implies that

$$c_{++} \geqslant 0, \quad c_{--} \geqslant 0. \tag{19}$$

Similarly it maps the state $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ to a positive semidefinite matrix, hence also

$$c_{+-} \geqslant 0, \quad c_{-+} \geqslant 0 \tag{20}$$

A. The case $p=2$

Using representation (17),

$$\mathrm{Tr}((\Phi \otimes \Omega)(\rho_{12}))^2 = \mathrm{Tr}(c_{++}A + c_{+-}C)^2 + 2(\lambda_1^2 \mathrm{Tr}\, B_1^2 + \lambda_2^2 \mathrm{Tr}\, B_2^2) + \mathrm{Tr}(c_{--}A + c_{-+}C)^2. \tag{21}$$

Using the positivity of the coefficients (19), (20) and convexity of the 2-norm gives

$$\mathrm{Tr}((\Phi \otimes \Omega)(\rho_{12}))^2 \leqslant (c_{++}\|A\|_2 + c_{+-}\|C\|_2)^2 + 2(\lambda_1^2 \mathrm{Tr}\, B_1^2 + \lambda_2^2 \mathrm{Tr}\, B_2^2) + (c_{--}\|A\|_2 + c_{-+}\|C\|_2)^2. \tag{22}$$

Define

$$\lambda = \max\{\lambda_1, \lambda_2\} \tag{23}$$

then it follows that

$$\lambda_1^2 \mathrm{Tr}\, B_1^2 + \lambda_2^2 \mathrm{Tr}\, B_2^2 \leqslant \lambda^2 \mathrm{Tr}\, B^* B = \lambda^2 \|B\|_2^2. \tag{24}$$

Using (24) the right-hand side of (22) can be rewritten as the trace squared of a 2×2 matrix, leading to

$$\mathrm{Tr}((\Phi \otimes \Omega)(\rho_{12}))^2 \leqslant \mathrm{Tr}\begin{pmatrix} c_{++}\|A\|_2 + c_{+-}\|C\|_2 & \lambda\|B\|_2 \\ \lambda\|B\|_2 & c_{--}\|A\|_2 + c_{-+}\|C\|_2 \end{pmatrix}^2 = \mathrm{Tr}\left(\Phi\begin{pmatrix} \|A\|_2 & z\|B\|_2 \\ z^*\|B\|_2 & \|C\|_2 \end{pmatrix}\right)^2, \tag{25}$$

where

$$z = \begin{cases} 1 & \text{if} \quad \lambda = \lambda_1 \\ i & \text{if} \quad \lambda = \lambda_2. \end{cases} \tag{26}$$

As noted in (16) the matrix

$$\begin{pmatrix} \|A\|_2 & z\|B\|_2 \\ z^*\|B\|_2 & \|C\|_2 \end{pmatrix}$$

is positive semidefinite, hence by definition of the maximal 2-norm we get

$$\|(\Phi\otimes\Omega)(\rho_{12})\|_2 \leqslant \left\|\Phi\begin{pmatrix} \|A\|_2 & z\|B\|_2 \\ z^*\|B\|_2 & \|C\|_2 \end{pmatrix}\right\|_2 \leqslant \nu_2(\Phi)\mathrm{Tr}\begin{pmatrix} \|A\|_2 & z\|B\|_2 \\ z^*\|B\|_2 & \|C\|_2 \end{pmatrix}$$
$$= \nu_2(\Phi)(\|A\|_2+\|C\|_2). \tag{27}$$

As $A=\Omega(X)$ and $C=\Omega(Z)$, this yields

$$\|(\Phi\otimes\Omega)(\rho_{12})\|_2 \leqslant \nu_2(\Phi)\nu_2(\Omega)(\mathrm{Tr}\,X+\mathrm{Tr}\,Z) = \nu_2(\Phi)\nu_2(\Omega) \tag{28}$$

as $\mathrm{Tr}\,X+\mathrm{Tr}\,Z=\mathrm{Tr}\,\rho_{12}=1$. As this holds for any state ρ_{12} we deduce that

$$\nu_2(\Phi\otimes\Omega) \leqslant \nu_2(\Phi)\nu_2(\Omega). \tag{29}$$

The inequality in the reverse direction follows by restriction to product states, hence this completes the proof for the case $p=2$.

B. The case $p\geqslant 4$

We apply Theorem 2 to (17) to conclude that for $p\geqslant 4$,

$$\|(\Phi\otimes\Omega)(\rho_{12})\|_p \leqslant \left\|\begin{pmatrix} \|c_{++}A+c_{+-}C\|_p & \|\lambda_1B_1-i\lambda_2B_2\|_p \\ \|\lambda_1B_1+i\lambda_2B_2\|_p & \|c_{--}A+c_{-+}C\|_p \end{pmatrix}\right\|_p. \tag{30}$$

Define the 2×2 real symmetric matrix

$$M=\begin{pmatrix} \|c_{++}A+c_{+-}C\|_p & \|\lambda_1B_1-i\lambda_2B_2\|_p \\ \|\lambda_1B_1+i\lambda_2B_2\|_p & \|c_{--}A+c_{-+}C\|_p \end{pmatrix}, \tag{31}$$

so that (30) can be written

$$\|(\Phi\otimes\Omega)(\rho_{12})\|_p \leqslant \|M\|_p. \tag{32}$$

The positivity results (19) and (20) imply that

$$\begin{aligned} \|c_{++}A+c_{+-}C\|_p &\leqslant c_{++}\|A\|_p + c_{+-}\|C\|_p, \\ \|c_{--}A+c_{-+}C\|_p &\leqslant c_{--}\|A\|_p + c_{-+}\|C\|_p. \end{aligned} \tag{33}$$

Further, recall (23) and suppose first that $\lambda=\lambda_1$, so that $\lambda_1-\lambda_2\geqslant 0$. Then

$$\|\lambda_1B_1-i\lambda_2B_2\|_p = \|(\lambda_1-\lambda_2)B_1+\lambda_2B\|_p \leqslant (\lambda_1-\lambda_2)\|B_1\|_p+\lambda_2\|B\|_p \leqslant \lambda\|B\|_p, \tag{34}$$

where in the last inequality we used $\|B_1\|_p=\frac{1}{2}\|B+B^*\|_p\leqslant\|B\|_p$. A similar argument leads to the same conclusion if $\lambda=\lambda_2$.

We would like to replace the entries of M with the bounds on the right-hand sides of (33) and (34), and argue that $\|M\|_p$ must increase under this substitution. However the matrix M may not be positive semidefinite (since Φ is not necessarily completely positive) so this is not immediately obvious. To see that it does in fact increase, let $p=2q$ so that

$$\|M\|_p = (\|M^2\|_q)^{1/2}. \tag{35}$$

Then the matrix $M^2=M^*M$ is positive semidefinite with positive entries, and it is easy to see that this implies $\|M^2\|_q$ is an increasing function of the entries of M^2. Since M is also entrywise positive, the entries of M^2 are increasing functions of the entries of M, and therefore so is $\|M^2\|_q$.

Therefore $\|M\|_p$ increases when the bounds (33), (34) are inserted in the right-hand side of (32), and we get

$$\|(\Phi \otimes \Omega)(\rho_{12})\|_p \leq \left\| \begin{pmatrix} c_{++}\|A\|_p + c_{+-}\|C\|_p & \lambda\|B\|_p \\ \lambda\|B\|_p & c_{--}\|A\|_p + c_{-+}\|C\|_p \end{pmatrix} \right\|_p. \tag{36}$$

Now we note that the right-hand side of (36) is unchanged if the upper-right entry $\lambda\|B\|_p$ is replaced by $z\lambda\|B\|_p$ and the lower left-hand entry by $z^*\lambda\|B\|_p$ for any $|z|=1$. Hence using the notation (26) again, (36) implies

$$\|(\Phi \otimes \Omega)(\rho_{12})\|_p \leq \left\| \Phi \begin{pmatrix} \|A\|_p & z\|B\|_p \\ z^*\|B\|_p & \|C\|_p \end{pmatrix} \right\|_p. \tag{37}$$

We now repeat the arguments used above in the case $p=2$, to conclude that

$$\|(\Phi \otimes \Omega)(\rho_{12})\|_p \leq \nu_p(\Phi)(\|A\|_p + \|C\|_p) \leq \nu_p(\Phi)\nu_p(\Omega)(\mathrm{Tr}\, X + \mathrm{Tr}\, Z) = \nu_p(\Phi)\nu_p(\Omega). \tag{38}$$

As this holds for any state ρ_{12} we again deduce

$$\nu_p(\Phi \otimes \Omega) \leq \nu_p(\Phi)\nu_p(\Omega) \tag{39}$$

and this completes the proof for the case $p \geq 4$.

III. REDUCTION TO SPECIAL FORM

In this section we will show that the general case of Theorem 1 follows from Lemma 3. Recall that a trace-preserving, positivity-preserving qubit map Φ is represented by an affine linear map on $\mathbb{R}^3$ as in (8), sending the Bloch sphere (the closed unit ball in $\mathbb{R}^3$) into an ellipsoid. We will refer to the latter as the *image ellipsoid* of Φ.

For a positivity-preserving, trace-preserving qubit map Φ, the minimal output entropy and maximal output p-norm are all achieved on the same input state. That is, there is a pure state $|\psi\rangle$ such that for all $p \geq 1$

$$\nu_p(\Phi) = \sup_\rho \|\Phi(\rho)\|_p = \|\Phi(|\psi\rangle\langle\psi|)\|_p. \tag{40}$$

Define the function

$$h_p(r) = \left(\left(\frac{1+r}{2} \right)^p + \left(\frac{1-r}{2} \right)^p \right)^{1/p}. \tag{41}$$

The spectrum of $\Phi(|\psi\rangle\langle\psi|)$ is $\{(1\pm r)/2\}$, for some $0 \leq r \leq 1$. Accordingly the value of (40) is

$$\nu_p(\Phi) = h_p(r). \tag{42}$$

We will denote by $\mathcal{C}_r$ the set of all positivity-preserving, trace-preserving qubit maps whose maximal output p-norm is at most $h_p(r)$, that is

$$\mathcal{C}_r = \{\Phi : \nu_p(\Phi) \leq h_p(r)\}. \tag{43}$$

Note that $\mathcal{C}_r$ does not depend on p. Geometrically, $\mathcal{C}_r$ consists of the positivity-preserving qubit maps for which the image ellipsoid lies inside the sphere of radius r centered at the origin.

It is clear that $\mathcal{C}_r$ is a convex set. The next result shows that the extreme points of $\mathcal{C}_r$ have a simple form. Recall the definition (10) of the diagonal form of a qubit map.

Lemma 4: *Let Φ be an extreme point in $\mathcal{C}_r$, represented in diagonal form by the affine map $x \mapsto Ax+v$ on $\mathbb{R}^3$. Then at most one of the components of v is nonzero.*

Lemma 4 is a consequence of the following Theorem of Gorini and Sudarshan,[9] which classifies all extreme affine maps of $\mathbb{R}^n$ sending the closed unit ball into itself.

Theorem 5: *[Gorini-Sudarshan] Let D_n be the set of affine maps of $\mathbb{R}^n$ which send the closed unit ball into itself. Denote by (B,w) the map $x \mapsto Bx+w$, where $w \in \mathbb{R}^n$ and $B \in \mathbb{R}^{n\times n}$. If (B,w) is an extreme point in D_n, then there are orthogonal matrices $Q_1, Q_2 \in O(n)$, and real numbers $0 \leqslant \kappa \leqslant 1$, $0 < \delta \leqslant 1$ such that*

$$Q_1 w = (0, \ldots, 0, \delta(1-\kappa^2)), \quad Q_1 B Q_2 = \mathrm{Diag}(m, \ldots, m, \kappa m), \tag{44}$$

where $m = \sqrt{1+\kappa^2\delta^2-\delta^2}$ and where $\mathrm{Diag}(d_1, d_2, \ldots)$ denotes the diagonal matrix with entries $d_1, d_2, \ldots$.

To derive Lemma 4 from Theorem 5, we identify $\mathcal{C}_r$ with the set of scaled affine maps $rD_3 = \{(rB, rw) : (B,w) \in D_3\}$. Hence every extreme map Φ in $\mathcal{C}_r$ corresponds to an affine map (rB, rw) where (B,w) satisfies (44). Further, the matrix Q_1 in (44) is in $O(3)$, and hence either $Q_1 \in SO(3)$ or $-Q_1 \in SO(3)$; similarly for Q_2. Since every rotation in $SO(3)$ can be implemented by a unitary conjugation in SU(2) [see the discussion leading up to (9)], this shows that Φ can be written in diagonal form with

$$A = \begin{pmatrix} \pm rm & 0 & 0 \\ 0 & \pm rm & 0 \\ 0 & 0 & \pm r\kappa m \end{pmatrix}, \quad v = \begin{pmatrix} 0 \\ 0 \\ \pm r\delta(1-\kappa^2) \end{pmatrix}, \tag{45}$$

and this proves Lemma 4.

In the remainder of this section we will show that Theorem 1 follows from Lemma 3 and Lemma 4. Accordingly, suppose that Φ is a trace-preserving, positivity-preserving qubit map satisfying (42) for some $0 \leqslant r \leqslant 1$, so that

$$\nu_p(\Phi) = h_p(r). \tag{46}$$

Then it is sufficient to show that for any completely positive map Ω,

$$\nu_p(\Phi \otimes \Omega) \leqslant h_p(r)\,\nu_p(\Omega). \tag{47}$$

Now $\mathcal{C}_r$ is a closed bounded convex subset of $\mathbb{R}^{12}$ (since the matrix A and vector v together have 12 entries), hence by Caratheodory's Theorem any element of $\mathcal{C}_r$ can be written as a convex combination of at most 13 of its extreme points. The map Φ is in $\mathcal{C}_r$, hence there are extreme maps $\{\Phi_i\} \in \mathcal{C}_r$ such that

$$\Phi = \sum_i a_i \Phi_i, \tag{48}$$

where $a_i \geqslant 0$ and $\Sigma a_i = 1$. Since $\{\Phi_i\}$ are in $\mathcal{C}_r$ we also have

$$\nu_p(\Phi_i) \leqslant h_p(r). \tag{49}$$

Further, combining Lemmas 4 and 3, we deduce that

$$\nu_p(\Phi_i \otimes \Omega) = \nu_p(\Phi_i)\,\nu_p(\Omega) \leqslant h_p(r)\,\nu_p(\Omega) \tag{50}$$

for all i. By convexity of the p-norm it follows from (48) and (50) that

$$\nu_p(\Phi \otimes \Omega) \leqslant \sum_i a_i \nu_p(\Phi_i \otimes \Omega) = \sum_i a_i \nu_p(\Phi_i)\,\nu_p(\Omega) \leqslant h_p(r)\,\nu_p(\Omega), \tag{51}$$

and this proves (47).

IV. PROOF OF THEOREM 2

Let $p=2q$ and define

$$M=\begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{52}$$

Then M^*M is positive semidefinite, and we write it in block form as

$$M^*M=\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}. \tag{53}$$

Now we apply the result of Theorem 1(b) from Ref. 12 to the matrix M^*M to deduce that

$$\|M^*M\|_q \leqslant \left\| \begin{pmatrix} \|M_{11}\|_q & \|M_{12}\|_q \\ \|M_{21}\|_q & \|M_{22}\|_q \end{pmatrix} \right\|_q \tag{54}$$

for all $q \geqslant 2$. Further, $M_{11}=A^*A+C^*C$, hence

$$\|M_{11}\|_q \leqslant \|A^*A\|_q + \|C^*C\|_q = \|A\|_p^2 + \|C\|_p^2. \tag{55}$$

Similarly

$$\|M_{12}\|_q = \|M_{21}\|_q \leqslant \|A\|_p \|B\|_p + \|C\|_p \|D\|_p \tag{56}$$

and

$$\|M_{22}\|_q \leqslant \|B\|_p^2 + \|D\|_p^2. \tag{57}$$

For a positive semidefinite 2×2 matrix the q-norm is an increasing function of the entries. Hence combining (54) with (55)–(57) gives

$$\|M^*M\|_q \leqslant \|m^*m\|_q, \tag{58}$$

where

$$m=\begin{pmatrix} \|A\|_p & \|B\|_p \\ \|C\|_p & \|D\|_p \end{pmatrix}. \tag{59}$$

Taking a square root of both sides gives

$$\|M\|_p \leqslant \|m\|_p \tag{60}$$

which is the stated result.

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Superconformal symmetry in the interacting theory of (2,0) tensor multiplets and self-dual strings

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We investigate the concept of superconformal symmetry in six dimensions, applied to the interacting theory of (2,0) tensor multiplets and self-dual strings. The action of a superconformal transformation on the superspace coordinates is found, both from a six-dimensional perspective and by using a superspace with eight bosonic and four fermionic dimensions. The transformation laws for all fields in the theory are derived, as well as general expressions for the transformation of on-shell superfields. Superconformal invariance is shown for the interaction of a self-dual string with a background consisting of on-shell tensor multiplet fields, and we also find an interesting relationship between the requirements of superconformal invariance and those of a local fermionic κ-symmetry. Finally, we try to construct a superspace analogue of the Poincaré dual to the string world-sheet and consider its properties under superconformal transformations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2184810]

I. INTRODUCTION

One of the most interesting discoveries in string/M-theory during the past decade is without doubt the six-dimensional (2,0) theories, named after the supersymmetry algebra under which they are invariant.[1] These are superconformal quantum theories without dynamical gravity, and first appeared in a compactification of Type IIB string theory on a four-dimensional hyper-Kähler manifold.[2] They obey an *ADE* classification (see Ref. 3 for an intrinsically six-dimensional motivation for why the simply laced Lie algebra series A, D, and E appear) but have no other discrete or continuous parameters. However, the theories have a moduli space parametrized by the expectation values of a set of scalar fields.

There is a second origin for the A-series of these theories in terms of M-theory, where they arise as the world-volume theory on a stack of parallel $M5$-branes.[4,5] More specifically, a stack of $r+1$ branes yields the A_r version of (2,0) theory, where r denotes the rank of the associated Lie algebra. The fluctuations of the $M5$-branes are described by r so-called (2,0) tensor multiplets and the $5r$ moduli correspond to the transverse distances between the branes. It is also possible for membranes to stretch between two $M5$-branes;[6–8] the intersections will then appear as self-dual strings from the six-dimensional world-volume perspective on the $M5$-brane. We get in total $r(r+1)/2$ different species of such strings, corresponding to the number of ways to connect the branes. The string tension is proportional to the distance between the branes in question, and is therefore related to the moduli of the theory. Specifically, if the branes coincide, the strings become tensionless. This picture yields in a simple way the different degrees of freedom of (2,0) theory; for a more complete discussion, see, e.g., Ref. 9.

An intrinsically six-dimensional formulation of the (2,0) theories is still lacking, and it is the ultimate goal of our research to find such a definition. In our previous work, we have pursued a program where we consider the theory at a point away from the origin of its moduli space, where

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the strings are tensile. This introduces a scale in the theory and breaks the conformal invariance spontaneously, but also provides a basis for doing perturbation theory, since in the limit of large string tension, the theory describes the well understood free (2,0) tensor multiplet and free self-dual strings. The dimensionless expansion parameter will then be the square of some typical energy divided by the string tension. For simplicity, we have chosen to work in the A_1 version of (2,0) theory, which includes a single type of string and a single tensor multiplet.

In this paper, we consider the hitherto uninvestigated superconformal symmetry of our model. It is well known that superconformal field theories cannot exist in space-times with more than six dimensions. Moreover, in six dimensions, the largest possible supersymmetry consistent with superconformal invariance is $\mathcal{N}=(2,0)$. This means that (2,0) theory, regarded as a superconformal theory, has the largest possible supersymmetry in the highest possible dimension. This observation alone provides a motivation for studying these theories.

The aim of the present paper is first to provide a framework for the study of superconformal invariance in six-dimensional (2,0) theory by using superfields. Second, we want to investigate whether our model[10] for a self-dual string interacting with a tensor multiplet background is superconformally invariant, and in what sense. Finally, we would like to use the new superconformal tools to find some clues on how to formulate the full interacting theory, i.e., when the tensor multiplet fields do not obey their free equations of motion.

It is our intention to make the paper self-contained, thereby reviewing and summarizing some well-known results on conformal and superconformal symmetry. We think that it is worthwhile to include these, in order to understand how the superfield transformations work and how they are derived. It is also, in some cases, nontrivial to adapt the known results to our notations and conventions.

The outline of this paper is as follows: Section II is devoted to the study of (bosonic) conformal transformations in six dimensions, as a warm-up exercise preceding the superconformal model. We find explicit expressions for the action of the conformal group on the space-time coordinates, both from a six-dimensional perspective and by considering a projective hypercone in eight dimensions, where the conformal transformations act linearly. We also study how different fields behave under conformal transformations, especially the ones in the bosonic sector of the (2,0) tensor multiplet. The results of Sec. II are not new, but still useful from a pedagogical point of view.

Section III discusses superconformal symmetry. As in the preceding section, we first find how the transformations act on coordinates, this time in a superspace with six bosonic and 16 fermionic dimensions. The coordinate transformations are also found by considering a projective supercone in a higher-dimensional superspace; a method which, to the best of our knowledge, has not appeared previously in the literature. Next, we use a superfield formalism as a way of compactifying and simplifying the notation and derive how superconformal transformations act on the superfields of the complete (2,0) tensor multiplet and on self-dual spinning strings. The explicit transformation laws are used to show that the model describing a string interacting with a tensor multiplet background is superconformally invariant. We find the new and nontrivial result that the requirements of superconformal symmetry and those of a local fermionic κ-symmetry impose similar restrictions on the possible coupling terms, thereby indicating the uniqueness of the theory.

Finally, Sec. IV discusses the construction of a superspace analogue of the Poincaré dual to the string world-sheet and its properties under superconformal transformations.

II. CONFORMAL INVARIANCE IN THE BOSONIC THEORY

Before discussing the issue of superconformal invariance, it is worthwhile to consider a simpler case, which still contains some important aspects of the problem. Therefore, we begin by working with the model describing a spinless self-dual string interacting with the bosonic part of the (2,0) tensor multiplet in six dimensions.[9] The results in this section have appeared previously in the literature, but it is nevertheless useful to review some aspects in order to get a complete picture. We will also refer (for comparison) to formulas in this section later in this paper, to point out similarities and differences between the bosonic and the superconformal models.

A. Conformal coordinate transformations

In this section, we consider the action of conformal transformations on the coordinates x^μ, $\mu=0,\ldots,5$, in a six-dimensional space-time. These transformations are called *passive*, meaning that they act on the coordinates themselves, rather than on the fields of the theory.

Conformal transformations act on space-time in such a way that the *angle* between two intersecting curves is left invariant. This means that the infinitesimal proper time interval

$$\mathrm{d}\tau^2 = -\,\eta_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu \tag{2.1}$$

transforms according to

$$\mathrm{d}\tau^2 \to \Omega^2(x)\mathrm{d}\tau^2, \tag{2.2}$$

where $\eta_{\mu\nu}$ is the flat space-time metric (with "mostly plus" signature) and $\Omega(x)$ denotes a space-time dependent quantity that also involves the parameters of the conformal transformation. For an infinitesimal transformation, such that $\Omega(x)=1+\Lambda(x)$, this yields that

$$\delta(\mathrm{d}\tau^2) = 2\Lambda(x)\mathrm{d}\tau^2, \tag{2.3}$$

where $\Lambda(x)$ is an infinitesimal function.

It is well known that the most general infinitesimal coordinate transformation that respects Eq. (2.3) is given by

$$\delta x^\mu = a^\mu + \omega^{\mu\nu}x_\nu + \lambda x^\mu + c^\mu x^2 - 2c\cdot x x^\mu, \tag{2.4}$$

where $c\cdot x \equiv \eta_{\mu\nu}c^\mu x^\nu = c_\nu x^\nu$. The (constant) parameters a^μ, $\omega^{\mu\nu}$, λ, and c^μ are related to the different transformations of the conformal group according to the following table:

Symmetry	Generator	Parameter
Translations	$P_\mu=\partial_\mu$	a^μ
Rotations and Lorentz boosts	$M_{\mu\nu}=x_{[\nu}\partial_{\mu]}$	$\omega^{\mu\nu}$
Dilatations	$D=x^\mu\partial_\mu$	λ
Special conformal transformations	$K_\mu=x^2\partial_\mu-2x_\mu x^\nu\partial_\nu$	c^μ

where the differential expressions for the generators make the equation

$$\delta x^\mu = (a^\nu P_\nu + \omega^{\nu\rho}M_{\nu\rho} + \lambda D + c^\nu K_\nu)x^\mu \tag{2.5}$$

valid. In total, we have 28 parameters, in agreement with the dimensionality of the conformal group in six dimensions, denoted by SO(6,2).

From Eq. (2.4), it is easily shown that the differential $\mathrm{d}x^\mu$ transforms according to

$$\delta(\mathrm{d}x^\mu) = (\omega^{\mu\nu} + 4c^{[\mu}x^{\nu]})\mathrm{d}x_\nu + (\lambda - 2c\cdot x)\mathrm{d}x^\mu, \tag{2.6}$$

which implies that the proper time interval indeed transforms according to Eq. (2.3) with $\Lambda(x)=\lambda-2c\cdot x$.

Leaving the coordinate transformations aside for a while, we turn to the commutation relations relating the generators of the conformal group to each other. By direct calculation, it is easily verified that the differential operators defined in the table above obey

$$[P_\mu, M_{\nu\rho}] = -\,\eta_{\mu[\nu}P_{\rho]}, \quad [P_\mu, D] = P_\mu,$$

$$[K_\mu, M_{\nu\rho}] = -\,\eta_{\mu[\nu}K_{\rho]}, \quad [K_\mu, D] = -K_\mu,$$

$$[P_\mu, K_\nu] = -4M_{\mu\nu} - 2\eta_{\mu\nu}D, \quad [M_{\mu\nu}, D] = 0,$$

$$[M_{\mu\nu},M^{\rho\sigma}] = 2\delta_{[\mu}{}^{[\rho}M_{\nu]}{}^{\sigma]}. \tag{2.7}$$

This defines the conformal group SO(6,2) in six dimensions. The SO(6,2) structure may be made more explicit by introducing a new set of generators $J_{\hat{\mu}\hat{\nu}}$, $\hat{\mu},\hat{\nu}=0,\ldots,7$, according to

$$M_{\mu\nu} = J_{\mu\nu},$$

$$P_\mu = 2(J_{7\mu} + J_{6\mu}),$$

$$K_\mu = 2(J_{7\mu} - J_{6\mu}),$$

$$D = 2J_{76}. \tag{2.8}$$

These obey the Lorentz-type commutation relations

$$[J_{\hat{\mu}\hat{\nu}},J_{\hat{\rho}\hat{\sigma}}] = \eta_{\hat{\rho}[\hat{\mu}}J_{\hat{\nu}]\hat{\sigma}} - \eta_{\hat{\sigma}[\hat{\mu}}J_{\hat{\nu}]\hat{\rho}}, \tag{2.9}$$

where the metric $\eta_{\hat{\mu}\hat{\nu}}=\mathrm{diag}(-1,1,1,1,1,1,1,-1)$. Thus, the conformal transformations act as rotations in an eight-dimensional space with two timelike directions.

There is a formulation (first suggested by Dirac,[11] whose work was later continued by Kastrup[12] and by Mack and Salam[13]) in which a d-dimensional space-time is regarded as a projective hypercone in a space with one extra spacelike and one extra timelike dimension, just like the one suggested in the preceding paragraph. In the higher-dimensional space, conformal symmetry acts linearly, i.e., as a rotation with the generator $J_{\hat{\mu}\hat{\nu}}$. Denote the coordinates in this space by $y^{\hat{\mu}}$, and define the projective hypercone by

$$y^2 = \eta_{\hat{\mu}\hat{\nu}}y^{\hat{\mu}}y^{\hat{\nu}} = 0. \tag{2.10}$$

This equation is clearly Lorentz invariant in the eight-dimensional space, and therefore conformally invariant from a six-dimensional point of view.

Next, let the infinitesimal rotation parameters be assembled in the matrix $\pi^{\hat{\mu}\hat{\nu}}$, such that

$$\delta y^{\hat{\mu}} = \pi^{\hat{\rho}\hat{\sigma}}J_{\hat{\rho}\hat{\sigma}}y^{\hat{\mu}} = \pi^{\hat{\mu}\hat{\sigma}}y_{\hat{\sigma}}. \tag{2.11}$$

The last equality follows from the obvious definition

$$J_{\hat{\mu}\hat{\nu}} = y_{[\hat{\nu}}\partial_{\hat{\mu}]}, \tag{2.12}$$

where the derivative acts on the y variables.

To make contact with the six-dimensional space-time, we impose that

$$\pi^{\hat{\rho}\hat{\sigma}}J_{\hat{\rho}\hat{\sigma}} = \omega^{\rho\sigma}M_{\rho\sigma} + a^\rho P_\rho + c^\rho K_\rho + \lambda D, \tag{2.13}$$

which when combined with Eq. (2.8) yields that

$$\omega^{\mu\nu} = \pi^{\mu\nu},$$

$$a^\mu = \tfrac{1}{2}(\pi^{7\mu} + \pi^{6\mu}),$$

$$c^\mu = \tfrac{1}{2}(\pi^{7\mu} - \pi^{6\mu}),$$

$$\lambda = \pi^{76}. \tag{2.14}$$

Next, we parametrize the projective hypercone by

$$y^\mu = \gamma x^\mu,$$

$$y^7 - y^6 = \gamma,$$

$$y^7 + y^6 = \gamma \eta_{\rho\sigma} x^\rho x^\sigma, \tag{2.15}$$

where γ is related to the projectiveness of the hypercone and therefore $\gamma \neq 0$.

Under a conformal transformation as in Eq. (2.11), it turns out that the quantity x^μ introduced in Eq. (2.15) must transform exactly as the coordinates x^μ in Eq. (2.4), while γ transforms according to

$$\delta\gamma = (2\eta_{\mu\nu} c^\mu x^\nu - \lambda)\gamma. \tag{2.16}$$

This shows that the surface of the projective hypercone defined in Eq. (2.10) behaves as the six-dimensional space-time we started with. In this way, we have derived the conformal coordinate transformation in Eq. (2.4) from a higher-dimensional perspective, a viewpoint that will be useful later in this paper as well. The eight-dimensional formulation also suggests a way of formulating manifestly conformally invariant quantities, an observation that hopefully will be pursued in future work.

B. Conformal field transformations

Having discussed the conformal group and its action on the six-dimensional space-time thoroughly, we now turn to the question of how the conformal group generators act on fields defined over this space-time. This action consists of two parts: one due to the dependence of the field in question on the space-time coordinate x^μ and one due to specific properties of the field itself. The latter part consists of the action of the stability subgroup of $x=0$ (the little group) on the fields, e.g., the transformation properties of a vector field under Lorentz transformations. We will (in contrast to our convention in the preceding section) adopt the *active* view on conformal transformations, meaning that the space-time coordinates are fixed but the fields change upon such a transformation. By considering the stability subgroup mentioned before, it can be found[13] that a general field $\phi^i(x)$ (where i denotes some index or indices) transforms according to

$$\begin{aligned}\delta_C \phi^i(x) = {} & a^\mu \partial_\mu \phi^i(x) + \omega^{\mu\nu}[x_\nu \partial_\mu \phi^i(x) + (\Sigma_{\mu\nu}\phi)^i(x)] + \lambda[x^\mu \partial_\mu \phi^i(x) + w\phi^i(x)] \\ & + c^\mu[x^2 \partial_\mu \phi^i(x) - 2x_\mu x^\nu \partial_\nu \phi^i(x) + 4x^\nu (\Sigma_{\mu\nu}\phi)^i(x) - 2x_\mu w \phi^i(x) + (k_\mu \phi)^i(x)],\end{aligned} \tag{2.17}$$

where $\Sigma_{\mu\nu}$, w, and k_μ are defined through

$$[M_{\mu\nu}, \phi^i(0)] = (\Sigma_{\mu\nu}\phi)^i(0),$$

$$[D, \phi^i(0)] = w\phi^i(0),$$

$$[K_\mu, \phi^i(0)] = (k_\mu \phi)^i(0). \tag{2.18}$$

Here, $M_{\mu\nu}$, D, and K_μ should not be confused with the differential expressions in the table above; in these equations (when acting on fields), they denote the full generators of Lorentz transformations, dilatations and special conformal transformations, respectively.

Thus, $\Sigma_{\mu\nu}$ and k_μ correspond to the intrinsic properties of the field under space-time rotations and special conformal transformations, respectively, while w is the conformal weight of the field. Together, these generate the stability subgroup of $x=0$. We also note that a *primary* field corresponds to one having $k_\mu = 0$.

It is convenient to summarize the transformation (2.17) in the expression

$$\delta_C \phi^i(x) = \xi^\mu(x)\partial_\mu \phi^i(x) + \Omega^{\mu\nu}(x)(\Sigma_{\mu\nu}\phi)^i(x) + \Lambda(x) w \phi^i(x) + c^\mu (k_\mu \phi)^i(x), \tag{2.19}$$

where the space-time dependent parameter functions are defined by

$$\xi^\mu(x) \equiv a^\mu + \omega^{\mu\nu} x_\nu + \lambda x^\mu + c^\mu x^2 - 2c \cdot x x^\mu, \tag{2.20}$$

$$\Omega^{\mu\nu}(x) \equiv \omega^{\mu\nu} + 4c^{[\mu} x^{\nu]}, \tag{2.21}$$

$$\Lambda(x) \equiv \lambda - 2c \cdot x. \tag{2.22}$$

This expression is also stated in Ref. 14 and will prove to be useful when dealing with superfields and the superconformal group later in this paper. Note that the expression for $\xi^\mu(x)$ in Eq. (2.20) coincides with the expression for δx^μ in Eq. (2.4), indicating that this part corresponds to the change in the field due to its dependence on the space-time coordinates.

When acting on *fields*, the generators obey the same commutation relations as in Eq. (2.7), but with the opposite sign; this is due to the difference between active and passive transformations.

To conclude, the conformal transformation of a general field is specified by stating its conformal weight (w), its behavior under Lorentz transformations ($\Sigma_{\mu\nu}$) and its properties under special conformal transformations (k_μ).

C. The bosonic tensor multiplet

The next step is to apply the results of the preceding section to the fields in the bosonic sector of the (2,0) tensor multiplet, consisting of five scalar fields and a two-form gauge potential. We denote the scalar fields, transforming in the vector representation of the SO(5) R-symmetry group, by the antisymmetric matrix ϕ^{ab}, $a,b=1,\ldots,4$, satisfying the algebraic condition

$$\Omega_{ab}\phi^{ab} = 0, \tag{2.23}$$

where Ω_{ab} is the SO(5) invariant antisymmetric tensor. Obviously, a and b are SO(5) spinor indices. The two-form potential is denoted b and has an associated field strength $h=\mathrm{d}b$, both R-symmetry scalars. Actually, it is only the self-dual part of the field strength that is part of the tensor multiplet, but in order to give a Lagrangian description of the theory,[15] we include the anti-self-dual part as a spectator field. It is essential to keep this part decoupled when adding interactions to the theory. The field content, along with the reality properties, is more thoroughly discussed in Ref. 16.

The fields have the following properties under conformal transformations:

$$(\Sigma_{\mu\nu}\phi^{ab}) = 0, \quad (k_\mu \phi^{ab}) = 0, \quad w_\phi = 2,$$

$$(\Sigma_{\mu\nu} b)_{\rho\sigma} = \eta_{\mu[\rho} b_{\sigma]\nu} - \eta_{\nu[\rho} b_{\sigma]\mu}, \quad (k_\mu b)_{\rho\sigma} = 0, \quad w_b = 2. \tag{2.24}$$

The conformal weights w_ϕ and w_b are bounded from below by a unitarity condition,[17,18] and due to the BPS property of the tensor multiplet representation, this bound is saturated. The weights coincide with the mass dimensions of the fields.

Using the expression (2.19), this means that the fields of the bosonic theory transform according to

$$\delta_C \phi^{ab}(x) = \xi^\mu(x)\partial_\mu \phi^{ab}(x) + 2\Lambda(x)\phi^{ab}(x), \tag{2.25}$$

$$\delta_C b_{\mu\nu}(x) = \xi^\rho(x)\partial_\rho b_{\mu\nu}(x) + 2\Omega_{[\mu}{}^\rho(x) b_{\nu]\rho}(x) + 2\Lambda(x) b_{\mu\nu}(x), \tag{2.26}$$

$$\delta_C h_{\mu\nu\rho}(x) = \xi^\sigma(x)\partial_\sigma h_{\mu\nu\rho}(x) - 3\Omega_{[\mu}{}^\sigma(x) h_{\nu\ \rho]\sigma}(x) + 3\Lambda(x) h_{\mu\nu\rho}(x), \tag{2.27}$$

where we have required the conformal transformation operator to commute with the exterior derivative, in the sense that

$$\mathrm{d}(\delta_C b) = \delta_C(\mathrm{d}b) = \delta_C h. \tag{2.28}$$

Note that this conformal transformation operator is defined in an abstract sense, acting in different ways on different fields. Specifically, its explicit form is different when acting on the derivative of a field than on the field itself. The relation (2.28) may seem evident here, but it is useful to relate to it when we discuss the superconformal transformations later in this paper.

Comparing Eqs. (2.26) and (2.27), we see that both b and its exterior derivative $h=\mathrm{d}b$ are primary fields, meaning that they have no k_μ piece in their transformation laws, cf. Eq. (2.19). It should be noted that, in general, derivatives of primary fields are not necessarily primary, consider, e.g., the variation

$$\delta_C(\partial_\mu \phi^{ab}(x)) = \partial_\mu(\delta_C \phi^{ab}(x)) \tag{2.29}$$

$$= \xi^\nu(x)\partial_\nu\partial_\mu\phi^{ab}(x) - \Omega_\mu{}^\nu(x)\partial_\nu\phi^{ab}(x) + 3\Lambda(x)\partial_\mu\phi^{ab}(x) - 4c_\mu\phi^{ab}(x), \tag{2.30}$$

where we see that the generators of the conformal group act as expected on a field with a subscript vector index and mass dimension 3, apart from the nonprimary piece with parameter c_μ. Thus, although ϕ^{ab} is a primary field, its derivative is not.

The bosonic model also includes self-dual strings, described by an embedding field X^μ, which is a function of the world-sheet coordinates (labelled σ^i, $i=1,2$) and transforms as a Lorentz vector. In particular, since we have adopted the active viewpoint on conformal transformations, it is natural to conclude that X^μ transforms according to

$$\delta_C X^\mu = -\xi^\mu(X) = -a^\mu - \omega^\mu{}_\nu X^\nu - \lambda X^\mu - c^\mu X^2 + 2c\cdot X X^\mu, \tag{2.31}$$

i.e., in the same way as the space-time coordinate x^μ in Eq. (2.4), but with the opposite sign. This expression does not look as nice as the transformations of the tensor multiplet fields found above, but if we instead consider the variation of the differential $\tilde{\mathrm{d}}X^\mu \equiv \mathrm{d}\sigma^i\,\partial_i X^\mu$ (which is what we will need in explicit calculations), we get that

$$\delta_C(\tilde{\mathrm{d}}X^\mu) = -\Omega^\mu{}_\nu(X)\tilde{\mathrm{d}}X^\nu - \Lambda(X)\tilde{\mathrm{d}}X^\mu, \tag{2.32}$$

in accordance with the expected transformation of a field with a vector index, having conformal weight $w_{\tilde{\mathrm{d}}X}=-1$. Note also, from Eqs. (2.19) and (2.31), that all terms apart from those involving $\Sigma_{\mu\nu}$, w, and k_μ vanish manifestly when transforming the pull-back of a space-time field to the world-sheet of the string.

Using the transformation rules found above, it is a straight-forward task to prove that the interaction described in Ref. 9 is conformally invariant. It should be stressed that this model, because of its electromagnetic coupling, suffers from a classical anomaly.[3] This anomaly is cancelled when fermionic degrees of freedom are included in the model in a supersymmetric way.

III. CONFORMAL INVARIANCE IN THE SUPERSYMMETRIC THEORY

In this section we turn to the complete theory, incorporating fermionic degrees of freedom in the model. We take advantage of the superfield notation in order to simplify expressions and keep them similar and comparable to the bosonic results in the preceding section. This section mixes results that have appeared elsewhere in the literature with new findings. It should also be mentioned that, in some cases, our derivation methods are quite different from those that can be found in previous papers on this subject.

A. Including spinors in the model

In this section, we introduce the notations and conventions used for spinors and state the *bosonic* conformal transformations of the *fermionic* tensor multiplet fields. It summarizes old results, but is included for completeness to keep the paper self-contained.

The (2,0) tensor multiplet includes, apart from the scalars and the two-form potential mentioned in the preceding section, four chiral spinors transforming in the spinor representation of the SO(5) *R*-symmetry group. These are denoted as ψ^a_α where $\alpha=1,\ldots,4$ is an SO(5,1) Weyl spinor index. An anti-Weyl spinor is denoted by a superscript α index. The spinor fields obey a symplectic Majorana reality condition.[19]

It is convenient to use spinor indices also for the bosonic representations of the Lorentz group. This means that we let (by contracting with the appropriate gamma matrices)

$$x^\mu \to x^{\alpha\beta} = x^{[\alpha\beta]}, \tag{3.1}$$

$$\partial_\mu \to \partial_{\alpha\beta} = \partial_{[\alpha\beta]}, \tag{3.2}$$

$$\eta_{\mu\nu} \to \tfrac{1}{2}\epsilon_{\alpha\beta\gamma\delta}, \tag{3.3}$$

$$b_{\mu\nu} \to b_\alpha{}^\beta, \quad \text{such that } b_\alpha{}^\alpha = 0, \tag{3.4}$$

$$h_{\mu\nu\rho} + (*h)_{\mu\nu\rho} \to h_{\alpha\beta} = h_{(\alpha\beta)}, \tag{3.5}$$

$$h_{\mu\nu\rho} - (*h)_{\mu\nu\rho} \to h^{\alpha\beta} = h^{(\alpha\beta)}. \tag{3.6}$$

Note that the last two equations conveniently separate the self-dual and anti-self-dual parts of the three-form h into different representations of the Lorentz group.

As is indicated by Eq. (3.3), pairs of antisymmetric indices may be raised and lowered according to

$$\partial^{\alpha\beta} = \tfrac{1}{2}\epsilon^{\alpha\beta\gamma\delta}\partial_{\gamma\delta}. \tag{3.7}$$

Finally, we introduce the dot product between vectors in the same way as before, such that

$$\partial \cdot x \equiv \partial_{\alpha\beta}x^{\alpha\beta} = 6. \tag{3.8}$$

After these preliminaries, let us return to the conformal group and its generators. Naively, the bosonic differential generators of the table in Sec. II A are translated into

Generator	Parameter
$P_{\alpha\beta}=\partial_{\alpha\beta}$	$a^{\alpha\beta}$
$M_{\alpha\beta;\gamma\delta}=\frac{1}{2}(x_{\gamma\delta}\partial_{\alpha\beta}-x_{\alpha\beta}\partial_{\gamma\delta})$	$\omega^{\alpha\beta;\gamma\delta}$
$D=x^{\alpha\beta}\partial_{\alpha\beta}$	λ
$K^{\alpha\beta}=x^2\partial^{\alpha\beta}-2x^{\alpha\beta}x^{\gamma\delta}\partial_{\gamma\delta}$	$c_{\alpha\beta}$

but it is more convenient to introduce a dual notation for the Lorentz generator M and its corresponding parameter ω, according to

$$M_\alpha{}^\beta = \epsilon^{\beta\gamma\delta\varepsilon}M_{\alpha\gamma;\delta\varepsilon}, \tag{3.9}$$

$$\omega_\alpha{}^\beta = \tfrac{1}{2}\epsilon_{\alpha\gamma\delta\varepsilon}\omega^{\beta\gamma;\delta\varepsilon}, \tag{3.10}$$

in analogy with the notation for the two-form b in Eq. (3.4). This yields that

$$\omega_\beta{}^\alpha M_\alpha{}^\beta = \omega^{\alpha\beta;\gamma\delta} M_{\alpha\beta;\gamma\delta}, \tag{3.11}$$

and the differential operator becomes

$$M_\alpha{}^\beta = x^{\beta\gamma}\partial_{\alpha\gamma} - x_{\alpha\gamma}\partial^{\beta\gamma} = 2x^{\beta\gamma}\partial_{\alpha\gamma} - \tfrac{1}{2}\delta_\alpha{}^\beta x\cdot\partial, \tag{3.12}$$

which is traceless as required.

Under a conformal transformation, the spinor field ψ^a_α transforms according to

$$\delta_C\psi^a_\alpha = \xi^{\gamma\delta}(x)\partial_{\gamma\delta}\psi^a_\alpha + \Omega_\alpha{}^\gamma(x)\psi^a_\gamma + \tfrac{5}{2}\Lambda(x)\psi^a_\alpha, \tag{3.13}$$

where the x-dependent parameter functions are the obvious translations from Sec. II A and become

$$\xi^{\alpha\beta}(x) = a^{\alpha\beta} + \omega_\gamma{}^\alpha x^{\gamma\beta} + \omega_\gamma{}^\beta x^{\alpha\gamma} + (\lambda - 2c\cdot x)x^{\alpha\beta} + c^{\alpha\beta}x^2, \tag{3.14}$$

$$\Omega_\alpha{}^\beta(x) = \omega_\alpha{}^\beta - 4c_{\alpha\gamma}x^{\beta\gamma} + c\cdot x\,\delta_\alpha{}^\beta, \tag{3.15}$$

$$\Lambda(x) = \lambda - 2c\cdot x, \tag{3.16}$$

in terms of which the transformations (2.25) and (2.27) are

$$\delta_C\phi^{ab} = \xi^{\gamma\delta}(x)\partial_{\gamma\delta}\phi^{ab} + 2\Lambda(x)\phi^{ab}, \tag{3.17}$$

$$\delta_C h_{\alpha\beta} = \xi^{\gamma\delta}(x)\partial_{\gamma\delta}h_{\alpha\beta} + \Omega_\alpha{}^\gamma(x)h_{\gamma\beta} + \Omega_\beta{}^\gamma(x)h_{\alpha\gamma} + 3\Lambda(x)h_{\alpha\beta}. \tag{3.18}$$

This ends the discussion concerning the conformal group with only bosonic generators. In the next section, we extend the model to incorporate fermionic generators, thereby forming the full superconformal group.

B. Superconformal coordinate transformations

Since we want to treat a supersymmetric model, it is convenient to supplement the six bosonic space-time coordinates $x^{\alpha\beta}$ by a set of 16 fermionic coordinates θ^α_a, see Ref. 10 for a more thorough introduction of these concepts. The fermionic coordinates are anticommuting, i.e., Grassmann odd, as usual and transform as anti-Weyl spinors under Lorentz rotations and as spinors under R-symmetry transformations.

Following the logic of the preceding section, the obvious next step is to find out what the generators of the conformal group SO(6,2) look like in this *superspace* and how they act on the coordinates. Evidently, the generators must change in comparison to the bosonic case, in order to incorporate the nontrivial action of the conformal group on the fermionic coordinates θ^α_a. For example, since θ^α_a transforms as an anti-Weyl spinor under Lorentz rotations, the corresponding generator ($M_\alpha{}^\beta$) must be modified. The commutation relations in Eq. (2.7) are expected to remain unchanged as expressed in terms of abstract generators.

However, we want to go a bit further and also include the R-symmetry group SO(5), generated by $U^{ab} = U^{(ab)}$, and supersymmetry, which is generated by the fermionic Q^a_α. We are then forced to introduce the generators S^α_a of *special supersymmetry* as well, which arise as the commutator of the supersymmetry and the special conformal symmetry generators. Altogether, we have then arrived at the superconformal group $\mathrm{OSp}(8^*|4)$, which is the expected symmetry group of the complete theory. We will denote the parameters of supersymmetry, R-symmetry and special supersymmetry transformations by η^α_a, v_{ab}, and ρ^a_α, respectively. Note that Q^a_α, S^α_a, η^α_a, and ρ^a_α all are fermionic (Grassmann odd) quantities.

In this section, we will content ourselves with the action of the superconformal group on the coordinates in superspace, postponing their action on fields to the next section. Starting from the purely bosonic parts of the generators of SO(6,2) ($P_{\alpha\beta}$, M^β_α, D, and $K^{\alpha\beta}$) obtained above and the well-known generator of supersymmetry (Q^a_α), we can make suitable ansätze for the unknown but

essential additional parts (including fermionic variables and derivatives) of these generators as well as for the newly introduced generators (S_a^α and U^{ab}). By requiring these generators to obey certain of the commutation relations of the $\mathrm{OSp}(8^*|4)$ group (which is related to the requirement that the algebra should close), the unknown coefficients may be determined and the resulting differential generators are found to be

$$P_{\alpha\beta} = \partial_{\alpha\beta}, \tag{3.19}$$

$$M_\alpha{}^\beta = 2x^{\beta\gamma}\partial_{\alpha\gamma} - \tfrac{1}{2}\delta_\alpha{}^\beta x\cdot\partial + \theta_c^\beta \partial_\alpha^c - \tfrac{1}{4}\delta_\alpha{}^\beta \theta\cdot\partial, \tag{3.20}$$

$$D = x\cdot\partial + \tfrac{1}{2}\theta\cdot\partial, \tag{3.21}$$

$$K^{\alpha\beta} = -4x^{\alpha\gamma}x^{\beta\delta}\partial_{\gamma\delta} - \Omega^{ab}\Omega^{cd}\theta_a^\gamma \theta_b^{[\alpha}\,\theta_c^{\beta]}\theta_d^\delta\partial_{\gamma\delta} + 2\theta_c^{[\alpha}\,(2x^{\beta]\gamma} - i\Omega^{ab}\theta_a^{\beta]}\theta_b^\gamma)\partial_\gamma^c, \tag{3.22}$$

$$Q_\alpha^a = \partial_\alpha^a - i\Omega^{ac}\theta_c^\gamma\partial_{\alpha\gamma}, \tag{3.23}$$

$$S_a^\alpha = \Omega_{ac}(2x^{\alpha\gamma} - i\Omega^{bd}\theta_b^\alpha\theta_d^\gamma)\partial_\gamma^c + 2i\theta_a^\gamma\theta_c^\alpha\partial_\gamma^c - i\theta_a^\gamma(2x^{\delta\alpha} - i\Omega^{bd}\theta_b^\delta\theta_d^\alpha)\partial_{\gamma\delta}, \tag{3.24}$$

$$U^{ab} = \tfrac{1}{2}(\Omega^{ac}\theta_c^\gamma\partial_\gamma^b + \Omega^{bc}\theta_c^\gamma\partial_\gamma^a), \tag{3.25}$$

where the dot product between two fermionic quantities a_a^α and b_β^b is defined by

$$a\cdot b \equiv a_c^\gamma b_\gamma^c. \tag{3.26}$$

Note that the fermions involved in this scalar product are required to have opposite SO(5,1) chirality, i.e., one should be a Weyl spinor and the other an anti-Weyl spinor.

The generators of the superconformal group act on the superspace coordinates $x^{\alpha\beta}$ and θ_a^α in the usual way; the resulting transformation laws are (similar transformations but in a different notation, and derived in a different way, also appear in Ref. 20)

$$\begin{aligned}\delta x^{\alpha\beta} = {} & a^{\alpha\beta} + \omega_\gamma{}^\alpha x^{\gamma\beta} + \omega_\gamma{}^\beta x^{\alpha\gamma} + \lambda x^{\alpha\beta} + 4c_{\gamma\delta}x^{\gamma\alpha}x^{\beta\delta} - i\Omega^{ab}\eta_a^{[\alpha}\,\theta_b^{\beta]} + c_{\gamma\delta}\Omega^{ac}\Omega^{bd}\theta_a^{[\alpha}\,\theta_b^{\beta]}\theta_c^\gamma\theta_d^\delta \\ & - 2i\rho_\gamma^{c}\theta_c^{[\alpha}\,x^{\beta]\gamma} - \rho_\gamma^c\Omega^{ab}\theta_c^{[\alpha}\,\theta_a^{\beta]}\theta_b^\gamma,\end{aligned} \tag{3.27}$$

$$\begin{aligned}\delta\theta_a^\alpha = {} & (\omega_\gamma{}^\alpha - 4c_{\gamma\delta}x^{\alpha\delta} - 2ic_{\gamma\delta}\Omega^{cd}\theta_c^\alpha\theta_d^\delta + 2i\rho_\gamma^c\theta_c^\alpha)\theta_a^\gamma + \tfrac{1}{2}\lambda\theta_a^\alpha + \eta_a^\alpha \\ & + 2\Omega_{ca}\rho_\gamma^c x^{\gamma\alpha} + i\Omega_{ac}\Omega^{bd}\rho_\gamma^c\theta_b^\gamma\theta_d^\alpha + \upsilon_{ac}\Omega^{cd}\theta_d^\alpha,\end{aligned} \tag{3.28}$$

which, as in the bosonic case, look rather messy and complicated. However, it is easily shown that the action on the superspace differentials $e^{\alpha\beta} = \mathrm{d}x^{\alpha\beta} + i\Omega^{ab}\theta_a^{[\alpha}d\theta_b^{\beta]}$ and $\mathrm{d}\theta_a^\alpha$ can be written as

$$\delta e^{\alpha\beta} = \Omega_\gamma{}^\alpha(x,\theta)e^{\gamma\beta} + \Omega_\gamma{}^\beta(x,\theta)e^{\alpha\gamma} + \Lambda(x,\theta)e^{\alpha\beta}, \tag{3.29}$$

$$\delta(\mathrm{d}\theta_a^\alpha) = \Omega_\gamma{}^\alpha(x,\theta)\mathrm{d}\theta_a^\gamma + \tfrac{1}{2}\Lambda(x,\theta)\mathrm{d}\theta_a^\alpha + V^c{}_a(\theta)\mathrm{d}\theta_c^\alpha + 2\Xi_{\gamma,a}(\theta)e^{\alpha\gamma}, \tag{3.30}$$

where the superspace-dependent parameter functions

$$\Omega_\alpha{}^\gamma(x,\theta) = \omega_\alpha{}^\gamma - 4c_{\alpha\delta}x^{\gamma\delta} + c\cdot x\delta_\alpha{}^\gamma - 2ic_{\alpha\delta}\Omega^{cd}\theta_c^\gamma\theta_d^\delta + 2i\rho_\alpha^c\theta_c^\gamma - \frac{i}{2}\delta_\alpha{}^\gamma\rho\cdot\theta, \tag{3.31}$$

$$\Lambda(x,\theta) = \lambda - 2c\cdot x + i\rho\cdot\theta \tag{3.32}$$

are extensions of Eqs. (3.15) and (3.16) to the superconformal case, while the functions

$$V^a{}_d(\theta) = -\Omega^{ac}v_{cd} + 4i\Omega^{ac}c_{\gamma\delta}\theta_c^\gamma\theta_d^\delta - 2i\rho_\gamma^a\theta_d^\gamma + 2i\Omega^{ae}\rho_\gamma^f\theta_e^\gamma\Omega_{fd}, \tag{3.33}$$

$$\Xi_{\alpha,a}(\theta) = 2c_{\alpha\beta}\theta_a^\beta + \Omega_{ab}\rho_\alpha^b \tag{3.34}$$

are new. Naturally, Ω_α^β and V_b^a are traceless, i.e., they obey $\Omega_\alpha{}^\alpha = V^a{}_a = 0$. To the best of our knowledge, this way of presenting the superconformal transformations has not appeared previously in the literature. The advantages of using superspace-dependent parameter functions will be made clearer when we consider transformations of *superfields* in Sec. III C.

The transformations (3.29) and (3.30) contain the expected Lorentz, dilatation and R-symmetry parts (with generalized superspace-dependent parameters), but also a term connecting the variation of $\mathrm{d}\theta_a^\alpha$ to $e^{\alpha\beta}$ with the parameter function $\Xi_{\alpha,a}(\theta)$, containing the (constant) parameters $c_{\alpha\beta}$ and ρ_α^a. This separates special conformal and special supersymmetry transformations from the other transformations, which yield no such possibilities. This issue will be further discussed later in this paper and is a superspace analogue to the nontrivial piece k_μ in Eq. (2.19).

It is also interesting to note that the infinitesimal supersymmetric interval length is preserved up to a superspace-dependent scale factor under superconformal transformations, i.e.,

$$\delta\left(\tfrac{1}{2}\epsilon_{\alpha\beta\gamma\delta}e^{\alpha\beta}e^{\gamma\delta}\right) = \Lambda(x,\theta)\epsilon_{\alpha\beta\gamma\delta}e^{\alpha\beta}e^{\gamma\delta}. \tag{3.35}$$

This relation may in fact be seen as a definition of the superconformal transformations, in analogy with Eq. (2.3) in the bosonic case.

Continuing along the path taken in Sec. II, we calculate the commutation relations for the differential generators in Eqs. (3.19)–(3.25). The result is (similar relations appear, e.g., in Refs. 14 and 20)

$$[P_{\alpha\beta}, M_\gamma{}^\delta] = -2\delta_{[\alpha}{}^\delta P_{\beta]\gamma} - \tfrac{1}{2}\delta_\gamma{}^\delta P_{\alpha\beta}, \quad [P_{\alpha\beta}, U^{ab}] = 0,$$

$$[K^{\alpha\beta}, M_\gamma{}^\delta] = 2\delta_\gamma^{[\alpha}K^{\beta]\delta} + \tfrac{1}{2}\delta_\gamma{}^\delta K^{\alpha\beta}, \quad [K^{\alpha\beta}, U^{ab}] = 0,$$

$$[U^{ab}, D] = 0, \quad [M_\alpha{}^\beta, U^{ab}] = 0,$$

$$[U^{ab}, U^{cd}] = -\Omega^{a(c}U^{d)b} - \Omega^{b(c}U^{d)a}, \quad [P_{\alpha\beta}, D] = P_{\alpha\beta},$$

$$[M_\alpha{}^\beta, D] = 0, \quad [K^{\alpha\beta}, D] = -K^{\alpha\beta},$$

$$[M_\alpha{}^\beta, Q_\gamma^a] = -\delta_\gamma{}^\beta Q_\alpha^a + \tfrac{1}{4}\delta_\alpha{}^\beta Q_\gamma^a, \quad [Q_\alpha^a, D] = \tfrac{1}{2}Q_\alpha^a,$$

$$[M_\alpha{}^\beta, S_a^\gamma] = \delta_\alpha{}^\gamma S_a^\beta - \tfrac{1}{4}\delta_\alpha{}^\beta S_a^\gamma, \quad [S_a^\alpha, D] = -\tfrac{1}{2}S_a^\alpha,$$

$$[K^{\alpha\beta}, Q_\gamma^a] = -2\Omega^{ac}\delta_\gamma^{[\alpha}S_c^{\beta]}, \quad [P_{\alpha\beta}, Q_\gamma^c] = 0,$$

$$[P_{\alpha\beta}, S_a^\gamma] = 2\Omega_{ac}\delta_{[\alpha}{}^\gamma Q^c{}_{\beta]}, \quad [K^{\alpha\beta}, S_a^\gamma] = 0,$$

$$[M_\alpha{}^\beta, M_\gamma{}^\delta] = \delta_\alpha{}^\delta M_\gamma{}^\beta - \delta_\gamma{}^\beta M_\alpha{}^\delta, \quad [U^{ab}, Q_\gamma^c] = \Omega^{c(a}Q_\gamma{}^{b)},$$

$$\{Q_\alpha^a, Q_\beta^b\} = -2i\Omega^{ab}P_{\alpha\beta}, \quad [U^{ab}, S_c^\gamma] = \delta_c^{(a}\Omega^{b)d}S_d^\gamma,$$

$$\{S_a^\alpha, S_b^\beta\} = -2i\Omega_{ab}K^{\alpha\beta},$$

$$\{Q^a_\alpha, S^\beta_b\} = i\delta_\alpha{}^\beta(\delta^a{}_b D - 4\Omega_{bc}U^{ac}) + 2i\delta^a{}_b M_\alpha{}^\beta,$$

$$[P_{\alpha\beta}, K^{\gamma\delta}] = -4\delta_{[\alpha}{}^{[\gamma} M_{\beta]}{}^{\delta]} - 2\delta_{[\alpha}{}^{\gamma}\delta_{\beta]}{}^{\delta} D, \tag{3.36}$$

which together define the superconformal group $\mathrm{OSp}(8^*|4)$. It should be noted that these are the relations that apply when the differential operators act on each other, *not* when the generators act on fields. In the latter case, the sign on the right-hand side of every relation should be changed. It is straightforward to verify that the super-Jacobi identities are satisfied.

In the same way as we compactified the notation in the bosonic case in Eq. (2.9) by extending space-time with one extra spacelike and one extra timelike dimension, we may define new generators $J_{\hat\alpha\hat\beta}$, where $\hat\alpha, \hat\beta = 1, \ldots, 8$ are chiral spinor indices in *eight* dimensions. The hatted indices decompose into subscript and superscript indices in six dimensions, corresponding to Weyl ($\hat\alpha = 1, \ldots, 4$) and anti-Weyl ($\hat\alpha = 5, \ldots, 8$) spinors, respectively. We let

$$J_{\alpha\beta} = \tfrac{1}{2} P_{\alpha\beta},$$

$$J_\alpha{}^\beta = \tfrac{1}{2} M_\alpha{}^\beta + \tfrac{1}{4}\delta_\alpha{}^\beta D = -J^\beta{}_\alpha,$$

$$J^{\alpha\beta} = -\tfrac{1}{2} K^{\alpha\beta}, \tag{3.37}$$

and also define new supercharges $\hat Q^a_{\hat\alpha}$ according to

$$\hat Q^a_\alpha = Q^a_\alpha,$$

$$\hat Q^{a,\alpha} = \Omega^{ab} S^\alpha_b, \tag{3.38}$$

together forming a chiral spinor in eight dimensions.

These generators, together with the unaltered R-symmetry generator U^{ab}, obey the commutation relations

$$\{\hat Q^a_{\hat\alpha}, \hat Q^b_{\hat\beta}\} = -4i(\Omega^{ab} J_{\hat\alpha\hat\beta} + I_{\hat\alpha\hat\beta} U^{ab}), \quad [J_{\hat\alpha\hat\beta}, U^{ab}] = 0,$$

$$[J_{\hat\alpha\hat\beta}, J_{\hat\gamma\hat\delta}] = -I_{\hat\alpha[\hat\gamma} J_{\hat\delta]\hat\beta} + I_{\hat\beta[\hat\gamma} J_{\hat\delta]\hat\alpha}, \quad [J_{\hat\alpha\hat\beta}, \hat Q^a_{\hat\gamma}] = I_{\hat\gamma[\hat\alpha}\, \hat Q^a{}_{\hat\beta]},$$

$$[U^{ab}, U^{cd}] = -\Omega^{a(c}\, U^{d)b} - \Omega^{b(c}\, U^{d)a}, \quad [U^{ab}, \hat Q^c_{\hat\alpha}] = \Omega^{c(a}\, \hat Q^{b)}_{\hat\alpha}, \tag{3.39}$$

where the symmetric matrix $I_{\hat\alpha\hat\beta}$ has components

$$I_{\alpha\beta} = 0,$$

$$I_\alpha{}^\beta = \delta_\alpha{}^\beta = I^\beta{}_\alpha,$$

$$I^{\alpha\beta} = 0; \tag{3.40}$$

it transforms in the singlet representation of SO(6,2). The commutation relations (3.39) contain all the information of Eq. (3.36), but in a much more compact notation.

It is possible to compactify the notation further by considering the generators in a superspace with eight bosonic and four fermionic dimensions. This yields the $\mathrm{OSp}(8^*|4)$ structure in a manifest way; this notation appears in Refs. 14 and 21. Introduce a matrix J_{AB}, where $A = (\hat\alpha, a)$ and

$B=(\hat{\beta},b)$ are $\mathrm{OSp}(8^*|4)$ indices. Note that A and B are superindices, meaning that J_{AB} is symmetric if both indices are fermionic, otherwise it is antisymmetric. We denote this in the standard way by

$$J_{AB}=-(-1)^{AB}J_{BA}. \tag{3.41}$$

J_{AB} contains the different generators of the superconformal group, explicitly we take

$$J_{\hat{\alpha}\hat{\beta}}=J_{\hat{\alpha}\hat{\beta}},$$

$$J_{\hat{\alpha}}{}^{b}=\frac{i}{2\sqrt{2}}\hat{Q}^{b}_{\hat{\alpha}},$$

$$J^{a}{}_{\hat{\beta}}=-\frac{i}{2\sqrt{2}}\hat{Q}^{a}_{\hat{\beta}},$$

$$J^{ab}=iU^{ab}. \tag{3.42}$$

These generators obey the (anti)commutation relations

$$[J_{AB},J_{CD}\}=-\tfrac{1}{2}(I_{BC}J_{AD}-(-1)^{AB}I_{AC}J_{BD}-(-1)^{CD}I_{BD}J_{AC}+(-1)^{AB+CD}I_{AD}J_{BC}) \tag{3.43}$$

where the bracket on the left-hand side is an anticommutator if both entries in it are fermionic, otherwise it is a commutator. The superspace metric $I_{AB}=(-1)^{AB}I_{BA}$ is defined by

$$I_{AB}=\begin{pmatrix}0 & \delta_{\alpha}{}^{\beta} & 0\\ \delta^{\alpha}{}_{\beta} & 0 & 0\\ 0 & 0 & i\Omega^{ab}\end{pmatrix}. \tag{3.44}$$

In order to make the relation

$$I_{AB}I^{BC}=\delta^{C}_{A} \tag{3.45}$$

valid (which is essential if want to raise and lower indices), we also need to define the inverse superspace metric as

$$I^{AB}=\begin{pmatrix}0 & \delta^{\alpha}{}_{\beta} & 0\\ \delta_{\alpha}{}^{\beta} & 0 & 0\\ 0 & 0 & -i\Omega_{ab}\end{pmatrix}. \tag{3.46}$$

Note the resemblance between the (anti)commutation relations in Eq. (3.43) and the well-known Lorentz group commutation relations. This suggests that the superconformal transformations act linearly in a superspace with eight bosonic and four fermionic dimensions.

In Sec. II A, we found the conformal transformations of the bosonic coordinates x^{μ} in an indirect way, by looking at a projective hypercone embedded in an eight-dimensional space with two timelike directions. In this higher-dimensional space, the conformal group acts linearly. Guided by the $\mathrm{OSp}(8^*|4)$ covariant notation introduced above, we would like to perform a similar analysis in the superconformal case.

Let the coordinates in superspace be y_A and introduce a projective supercone by the equation

$$I^{AB}y_Ay_B=0. \tag{3.47}$$

We will parametrize the supercone in a more implicit manner than we did when considering the hypercone in Sec. II A. Consider a point on the supercone, with coordinates $y_A=(y_{\alpha},y^{\alpha},y^{a})$. It is always possible to introduce a fermionic field $\theta^{\alpha}_{a}(y)$ such that for any point on the supercone,

$$y^a = \sqrt{2}\Omega^{ab}\theta_b^\beta y_\beta. \tag{3.48}$$

By requiring θ_a^α to transform as an anti-Weyl spinor under SO(5,1), this field is well-defined in all points on the supercone. In the same manner, we introduce the bosonic field $x^{\alpha\beta}(y) = -x^{\beta\alpha}(y)$ such that

$$y^\alpha = (2x^{\alpha\beta} - i\Omega^{ab}\theta_a^\alpha\theta_b^\beta)y_\beta \tag{3.49}$$

for any point on the supercone.

It is easily verified that all points y_A of this form lie on the supercone defined by Eq. (3.47). Obviously, we may always multiply $x^{\alpha\beta}$ or θ_a^α by a constant and still remain on the supercone. This explains the notion *projective* supercone.

The next step is to vary these coordinates. The transformations are generated by

$$J_{AB} = -y_{[A}\partial_{B]} = (-1)^{AB}y_{[B}\partial_{A]}, \tag{3.50}$$

which satisfies the commutation relations (3.43), given that

$$\partial_A y_B = I_{AB}. \tag{3.51}$$

The coordinates y_A transform according to

$$\delta y_A = \pi^{CD}J_{CD}y_A = (-1)^{C(A+D)}I_{AC}\pi^{CD}y_D, \tag{3.52}$$

where the parameter matrix is given by

$$\pi^{AB} = \begin{pmatrix} 2a^{\alpha\beta} & \omega_\beta{}^\alpha + \frac{1}{2}\lambda\delta_\beta{}^\alpha & -i\sqrt{2}\eta_b^\alpha \\ -\omega_\alpha{}^\beta - \frac{1}{2}\lambda\delta_\alpha{}^\beta & -2c_{\alpha\beta} & -i\sqrt{2}\rho_\alpha^c\Omega_{cb} \\ i\sqrt{2}\eta_a^\beta & i\sqrt{2}\rho_\beta^c\Omega_{ca} & -iv_{ab} \end{pmatrix}, \tag{3.53}$$

chosen such that the relation

$$\pi^{AB}J_{AB} = \omega_\alpha{}^\beta M_\beta{}^\alpha + a^{\alpha\beta}P_{\alpha\beta} + c_{\alpha\beta}K^{\alpha\beta} + \lambda D + \eta_a^\alpha Q_\alpha^a + \rho_\alpha^a S_a^\alpha + v_{ab}U^{ab} \tag{3.54}$$

is valid.

Since Eq. (3.47) is invariant under a transformation of this type, we may require the left-hand and the right-hand sides of Eqs. (3.48) and (3.49) to transform equally. The implicated transformation properties of the fields $x^{\alpha\beta}(y)$ and $\theta_a^\alpha(y)$ when the y coordinates are transformed in this way are found to agree exactly with the superconformal transformations of the coordinates $x^{\alpha\beta}$ and θ_a^α in our original superspace (with six bosonic and 16 fermionic dimensions) in Eqs. (3.27) and (3.28) above. This explains the choice of notation and implies that the rather complicated transformation laws for $x^{\alpha\beta}$ and θ_a^α are a mere consequence of a simple rotation in a superspace with eight bosonic and four fermionic dimensions.

This way of introducing the superspace coordinates and deriving their transformation properties has, as far as we know, not appeared previously in the literature. Presumably, the fact that this works points to some underlying structure of the (2,0) superspace in six dimensions, the nature of which is not clear at the moment.

C. Superfields

Having introduced a superspace (in the remainder of this paper, we will work in the usual (2,0) superspace with six bosonic and 16 fermionic dimensions), the next step is to populate it with superfields. The superfield formulation for the (2,0) tensor multiplet first appeared in Ref. 22; a thorough description of its use in our model can be found in Ref. 10. In this paper, we will content ourselves with a short description of the key aspects.

Define a superfield $\Phi^{ab} = \Phi^{ab}(x,\theta)$, obeying the algebraic constraint

$$\Omega_{ab}\Phi^{ab} = 0 \tag{3.55}$$

and the differential constraint

$$D^a_\alpha \Phi^{bc} + \tfrac{2}{5}\Omega_{de} D^d_\alpha \left(\Omega^{ab}\Phi^{ec} + \Omega^{ca}\Phi^{eb} + \tfrac{1}{2}\Omega^{bc}\Phi^{ea}\right) = 0, \tag{3.56}$$

where D^a_α is the covariant superspace derivative, defined according to

$$D^a_\alpha = \partial^a_\alpha + i\Omega^{ac}\theta^\gamma_c \partial_{\alpha\gamma}. \tag{3.57}$$

It is important to note[10] that the differential constraint (3.56) implies that the lowest component of the superfield must obey the free equations of motion for a massless scalar field, i.e., the Klein-Gordon equation. This reflects the fact that we are dealing with an *on-shell* superfield formulation.

It is convenient to define supplementary superfields according to

$$\Psi^a_\alpha = -\frac{2i}{5}\Omega_{bc} D^b_\alpha \Phi^{ca}, \tag{3.58}$$

$$H_{\alpha\beta} = \tfrac{1}{4}\Omega_{ab} D^a_\alpha \Psi^b_\beta, \tag{3.59}$$

but it should be noted that these contain no new degrees of freedom compared to Φ^{ab}.

By definition, a superfield transforms according to

$$\delta_Q \Phi^{ab} = [\eta \cdot Q, \Phi^{ab}] \tag{3.60}$$

under a supersymmetry transformation. Working out this commutator, with Q as in Eq. (3.23), it can be shown (by comparing with the explicit transformations in Ref. 16) that the lowest components of the superfields Φ^{ab}, Ψ^a_α, and $H_{\alpha\beta}$ are the tensor multiplet fields ϕ^{ab}, ψ^a_α, and $h_{\alpha\beta}$, hence the choice of notation. The differential constraint (3.56) yields the usual free equations of motion for these component fields.

The purpose of this section is to find how the rest of the superconformal transformations act on the superfields. The transformations will, as in the bosonic case, contain one piece including the differential expressions in Eqs. (3.19)–(3.25) and some nondifferential pieces. The latter may be derived by requiring that the transformation of Φ^{ab} must satisfy the differential constraint (3.56) when Φ^{ab} itself does. We also require the abstract transformation operator to commute with the covariant derivative in superspace [in the same way as transformations commute with derivatives in the bosonic case, see Eq. (2.28) and the discussion thereafter]. Note that this approach of course requires the superfields to be on shell. The transformation of (2,0) superfields was also discussed in Ref. 23 using a geometric approach, realizing the transformations as derivations in superspace. We will be more explicit and algebraic in our treatment of the problem, trying to take advantage of the superfield formulation. It is our goal to write the transformations of the superfields in a form similar to the one used in the bosonic case in, e.g., Eq. (3.17), inspired by the transformation properties of the superspace differentials in Eqs. (3.29) and (3.30).

After some quite involved computations, it is found that the superfields transform according to (we are still in the active picture, where we transform the fields rather than the coordinates)

$$\delta_C \Phi^{ab} = \xi^{\gamma\delta}(x,\theta)\partial_{\gamma\delta}\Phi^{ab} + \xi^\gamma_c(x,\theta)\partial^c_\gamma \Phi^{ab} + 2\Lambda(x,\theta)\Phi^{ab} + V^a{}_d(\theta)\Phi^{db} + V^b{}_d(\theta)\Phi^{ad}, \tag{3.61}$$

$$\delta_C \Psi^a_\alpha = \xi^{\gamma\delta}(x,\theta)\partial_{\gamma\delta}\Psi^a_\alpha + \xi^\gamma_c(x,\theta)\partial^c_\gamma \Psi^a_\alpha + \Omega_\alpha{}^\gamma(x,\theta)\Psi^a_\gamma + \tfrac{5}{2}\Lambda(x,\theta)\Psi^a_\alpha + V^a{}_c(\theta)\Psi^c_\alpha - 4\Xi_{\alpha,b}(\theta)\Phi^{ab}, \tag{3.62}$$

$$\delta_C H_{\alpha\beta} = \xi^{\gamma\delta}(x,\theta)\partial_{\gamma\delta}H_{\alpha\beta} + \xi_c^{\gamma}(x,\theta)\partial_\gamma^c H_{\alpha\beta} + \Omega_\alpha{}^\gamma(x,\theta)H_{\gamma\beta} + \Omega_\beta{}^\gamma(x,\theta)H_{\alpha\gamma} + 3\Lambda(x,\theta)H_{\alpha\beta} + 3i\Xi_{\alpha,c}(\theta)\Psi_\beta^c + 3i\Xi_{\beta,c}(\theta)\Psi_\alpha^c, \tag{3.63}$$

where the parameter functions $\Omega_\alpha^\beta(x,\theta)$, $\Lambda(x,\theta)$, $V_b^a(\theta)$, and $\Xi_{\alpha,a}(\theta)$ are those defined in Eqs. (3.31)–(3.34), respectively, while $\xi^{\alpha\beta}(x,\theta)=\delta x^{\alpha\beta}$ and $\xi_a^\alpha(x,\theta)=\delta\theta_a^\alpha$, see Eqs. (3.27) and (3.28). In analogy with the notion of primary fields in the purely bosonic case, we see that the superfield Φ^{ab} is *superprimary* (its transformation does not contain any Ξ-part) while the others are not. Note that the transformations (in this notation) are what one would expect by looking at the indices and mass dimensions of the fields, apart from the parts containing $\Xi_{\alpha,a}(\theta)$, where the numerical coefficients are hard to guess *a priori*.

From these transformations, the transformation laws for the component fields may be read off. The SO(6,2) transformations agree, as expected, with Eqs. (3.13), (3.17), and (3.18), while supersymmetry acts according to

$$\delta_Q\phi^{ab} = i\,\eta_c^\alpha\left(\Omega^{ac}\psi_\alpha^b - \Omega^{bc}\psi_\alpha^a - \tfrac{1}{2}\Omega^{ab}\psi_\alpha^c\right),$$

$$\delta_Q\psi_\alpha^a = \Omega^{ab}\eta_b^\beta h_{\alpha\beta} + 2\partial_{\alpha\beta}\phi^{ab}\eta_b^\beta,$$

$$\delta_Q h_{\alpha\beta} = i\,\eta_a^\gamma(\partial_{\gamma\alpha}\psi_\beta^a + \partial_{\gamma\beta}\psi_\alpha^a), \tag{3.64}$$

in agreement with Ref. 16. The special supersymmetry transformations of the component fields are

$$\delta_S\phi^{ab} = -4ix^{\gamma\delta}\rho_\gamma^{[a}\,\psi_\delta^{b]} - i\Omega^{ab}\Omega_{cd}x^{\gamma\delta}\rho_\gamma^c\psi_\delta^d,$$

$$\delta_S\psi_\alpha^a = -2\rho_\gamma^a x^{\gamma\delta}h_{\delta\alpha} - 4\rho_\alpha^b\Omega_{bc}\phi^{ca} + 4\rho_\gamma^b\Omega_{bc}x^{\gamma\delta}\partial_{\alpha\delta}\phi^{ac},$$

$$\delta_S h_{\alpha\beta} = 2i\Omega_{ab}\rho_\gamma^a x^{\gamma\delta}(\partial_{\delta\alpha}\psi_\beta^b + \partial_{\delta\beta}\psi_\alpha^b) - 3i\Omega_{ab}(\rho_\alpha^a\psi_\beta^b + \rho_\beta^a\psi_\alpha^b), \tag{3.65}$$

while R-symmetry acts according to

$$\delta_U\phi^{ab} = -\Omega^{ac}v_{cd}\phi^{db} - \Omega^{bc}v_{cd}\phi^{ad},$$

$$\delta_U\psi_\alpha^a = -\Omega^{ac}v_{cd}\psi_\alpha^d,$$

$$\delta_U h_{\alpha\beta} = 0, \tag{3.66}$$

as suggested by the index structure of the fields.

This completes the analysis of the superconformal transformations of the free tensor multiplet in superspace, but we should also consider the self-dual string. It is, as before, described by a bosonic embedding field $X^{\alpha\beta}(\sigma)$, but we must supplement it by a second (fermionic) field $\Theta_a^\alpha(\sigma)$ describing the embedding in the fermionic coordinates. The superconformal transformations of these fields are

$$\delta_C X^{\alpha\beta} = -a^{\alpha\beta} - \omega_\gamma{}^\alpha X^{\gamma\beta} - \omega_\gamma{}^\beta X^{\alpha\gamma} - \lambda X^{\alpha\beta} - 4c_{\gamma\delta}X^{\gamma\alpha}X^{\beta\delta} + i\Omega^{ab}\eta_a^{[\alpha}\,\Theta_b^{\beta]} - c_{\gamma\delta}\Omega^{ac}\Omega^{bd}\Theta_a^{[\alpha}\,\Theta_b^{\beta]}\Theta_c^\gamma\Theta_d^\delta + 2i\rho_\gamma^c\Theta_c^{[\alpha}\,X^{\beta]\gamma} + \rho_\gamma^c\Omega^{ab}\Theta_c^{[\alpha}\,\Theta_a^{\beta]}\Theta_b^\gamma, \tag{3.67}$$

$$\delta_C\Theta_a^\alpha = -(\omega_\gamma{}^\alpha - 4c_{\gamma\delta}X^{\alpha\delta} - 2ic_{\gamma\delta}\Omega^{cd}\Theta_c^\alpha\Theta_d^\delta + 2i\rho_\gamma^c\Theta_c^\alpha)\Theta_a^\gamma - \tfrac{1}{2}\lambda\Theta_a^\alpha - \eta_a^\alpha - 2\Omega_{ca}\rho_\gamma^c X^{\gamma\alpha} - i\Omega_{ac}\Omega^{bd}\rho_\gamma^c\Theta_b^\gamma\Theta_d^\alpha - v_{ac}\Omega^{cd}\Theta_d^\alpha, \tag{3.68}$$

which coincide with Eqs. (3.27) and (3.28) for the corresponding coordinates but with the *opposite sign*, in the same manner as in the purely bosonic model. These variations do not have the same structure as the variations of the superfields Φ^{ab}, Ψ_α^a, and $H_{\alpha\beta}$, but if we instead consider the

appropriate differentials of these fields, we get something more familiar. The differentials in question are related in an obvious way to the superfield differentials $e^{\alpha\beta}$ and $\mathrm{d}\theta_a^\alpha$ and are $E^{\alpha\beta}=\tilde{\mathrm{d}}X^{\alpha\beta}+i\Omega^{ab}\Theta_a^{[\alpha}\tilde{\mathrm{d}}\Theta_b^{\beta]}$ and $\tilde{\mathrm{d}}\Theta_a^\alpha$, where $\tilde{d}=\mathrm{d}\sigma^i\partial_i$ denotes a differential operator with respect to the world-sheet parameters σ. The variations of these quantities are

$$\delta_C E^{\alpha\beta}=-\Omega_\gamma{}^\alpha(X,\Theta)E^{\gamma\beta}-\Omega_\gamma{}^\beta(X,\Theta)E^{\alpha\gamma}-\Lambda(X,\Theta)E^{\alpha\beta}, \tag{3.69}$$

$$\delta_C(\tilde{\mathrm{d}}\Theta_a^\alpha)=-\Omega_\gamma{}^\alpha(X,\Theta)\tilde{\mathrm{d}}\Theta_a^\gamma-\tfrac{1}{2}\Lambda(X,\Theta)\tilde{\mathrm{d}}\Theta_a^\alpha-V^d{}_a(\Theta)\tilde{\mathrm{d}}\Theta_d^\alpha-2\Xi_{\gamma,a}(\Theta)E^{\alpha\gamma}, \tag{3.70}$$

which are similar to Eqs. (3.29) and (3.30) but again with the opposite sign. We see that $E^{\alpha\beta}$ transforms as a superprimary quantity while $\tilde{\mathrm{d}}\Theta_a^\alpha$ does not.

In retrospect, what we have done in this section is to generalize the superfield formulation, thereby incorporating the full superconformal group in the formalism. This is a must in order to calculate variations of terms involving superfields under such transformations; using the transformation laws for the component fields would lead us nowhere (we do not even know the explicit expressions for the superfields in terms of component fields to all orders). With the superspace generators, we may in a relatively simple and compact way describe the transformations.

We should also comment on the use of superspace-dependent parameter functions in the transformation laws. This also facilitates the calculations, since Lorentz and *R*-symmetry covariance is manifest through the use of tensor notation. They must, however, be applied with care since these parameter functions generally do not commute with derivatives. To the best of our knowledge, this approach to the superconformal transformations of (2,0) superfields has not appeared previously in the literature.

It would be interesting to consider the problem of finding a field theory in the superspace with eight bosonic and four fermionic dimensions discussed at the end of the preceding section. This theory would, presumably, incorporate manifest superconformal symmetry and probably yield some new insights into the properties of the six-dimensional theory.

D. The supersymmetric interaction terms

In this section, we consider the theory describing the supersymmetric coupling of a self-dual string to a (2,0) tensor multiplet background.[10] As usual, background coupling means that the tensor multiplet fields are taken to be on shell, i.e., they obey their free equations of motion.

The interaction is described by the action terms

$$S^{\mathrm{int}}=-\int_\Sigma d^2\sigma\sqrt{\Phi\cdot\Phi}\sqrt{-G}+\int_D F, \tag{3.71}$$

where the first term is a Nambu-Goto term where the string tension has been replaced by an expression in the superfield Φ^{ab} discussed in the preceding section. Explicitly, the SO(5) invariant scalar product is defined by

$$\Phi\cdot\Phi\equiv\tfrac{1}{4}\Omega_{ac}\Omega_{bd}\Phi^{ab}\Phi^{cd}, \tag{3.72}$$

and its appearance can be understood by considering the relation between the moduli parameters and the string tension mentioned in the introduction. Note that the term involves the *pull-back* of the superfield Φ^{ab} to the string world-sheet Σ. In the second factor of the Nambu-Goto term, G denotes the determinant of the induced metric in superspace, which may be written as

$$G=\tfrac{1}{2}\epsilon^{ik}\epsilon^{jl}G_{ij}G_{kl}, \tag{3.73}$$

where

$$G_{ij} = \tfrac{1}{2}\epsilon_{\alpha\beta\gamma\delta}E_i^{\alpha\beta}E_j^{\gamma\delta}. \tag{3.74}$$

Here $E_i^{\alpha\beta}$ is determined by the relation $E^{\alpha\beta}=\mathrm{d}\sigma^i E_i^{\alpha\beta}$. Naturally, Σ denotes the string world-sheet.

The second term in Eq. (3.71) is of Wess-Zumino type and involves the pull-back of a certain super three-form F to the world-volume of a "Dirac membrane" D attached to the string, satisfying $\partial D=\Sigma$. For a more elaborate discussion of the Dirac membrane and its properties, we refer to Refs. 10 and 24. D is described, similarly to the string, by embedding fields $X^{\alpha\beta}$ and Θ_a^α, but these fields are functions of three parameters instead of two. As an embedding, they naturally transform in the same way as the string embedding fields, i.e., according to Eqs. (3.67) and (3.68), under a superconformal transformation.

The super three-form F is expressed as

$$\begin{aligned} F = {} & \frac{1}{6}e^{\gamma_1\gamma_2}\wedge e^{\beta_1\beta_2}\wedge e^{\alpha_1\alpha_2}\epsilon_{\alpha_2\beta_2\gamma_1\gamma_2}H_{\alpha_1\beta_1} - \frac{i}{2}e^{\gamma_1\gamma_2}\wedge e^{\beta_1\beta_2}\wedge d\theta_a^\alpha\epsilon_{\alpha\beta_1\beta_2\gamma_1}\Psi^a_{\gamma_2} \\ & + \frac{i}{2}e^{\gamma_1\gamma_2}\wedge d\theta_b^\beta\wedge d\theta_a^\alpha\epsilon_{\alpha\beta\gamma_1\gamma_2}\Phi^{ab} \end{aligned} \tag{3.75}$$

in terms of the superfields Φ^{ab}, Ψ^a_α, and $H_{\alpha\beta}$. It was used by us in Ref. 10 but has also appeared (in a slightly different notation) in Refs. 23 and 25. The coefficients in the expression for F make it a closed form in superspace, i.e., $dF=0$, where d is the superspace exterior derivative. The last statement is only true if the superfields obey the differential constraint (3.56), but this is always the case on shell.

The relative coefficient in Eq. (3.71) is determined by requiring invariance under a local fermionic κ-symmetry, which also removes half of the degrees of freedom contained in Θ_a^α, as required by supersymmetry.[10] The closure of F is essential for this to work, but it also implies that the choice of Dirac membrane D, given a string world-sheet $\Sigma=\partial D$, should have no physical significance.

Next, let us consider a superconformal variation of the interaction (3.71). The Nambu-Goto term is clearly invariant; this is easily seen from the expressions (3.61) and (3.69) for the variations of Φ^{ab} and $E^{\alpha\beta}$, respectively. Since all fields are superprimary, the only thing we really need to check is that the conformal weights match appropriately.

The variation of the Wess-Zumino term is a bit more involved, mainly because of the terms involving $\Xi_{\alpha,a}(\theta)$ in the transformation laws for $\tilde{d}\Theta_a^\alpha$, Ψ^a_α, and $H_{\alpha\beta}$. It turns out that the pull-back of the super three-form F to the Dirac membrane world-volume D is superconformally invariant if and only if the coefficients are chosen as in Eq. (3.75), i.e., with the same choice of coefficients that makes it a closed three-form in superspace! This means that the interaction in Eq. (3.71) indeed is superconformally invariant, but *only* with the specific three-form in Eq. (3.75). It should also be stressed that, out of all the transformations in the superconformal group, it is only the special conformal and the special supersymmetry transformations that put any restrictions on the coefficients. With another choice, the theory would still be, e.g., supersymmetric. The model is therefore an example of a theory where special conformal invariance does not follow immediately from dilatational, translational and Lorentz invariance.

Summing up, we have found that the requirement of κ-symmetry and that of superconformal invariance impose equivalent restrictions on the coefficients of the super three-form F, but in different ways. Note, however, that κ-symmetry also determines the relative coefficient between the Nambu-Goto term and the Wess-Zumino term. The superconformal symmetry of the theory has no influence on that. The remarkable agreement between superconformal invariance and κ-symmetry indicates the uniqueness of the theory: the model is tightly constrained by its symmetries. This is arguably the most important result of this paper.

IV. THE POINCARÉ DUAL TO THE STRING WORLD-SHEET

In the preceding section, we worked with an on-shell tensor multiplet. This implied that the super three-form F in Eq. (3.75) was closed and lead us to the conclusion that the choice of Dirac membrane, given a specific string world-sheet Σ, should have no physical significance.

In this section, we try to relax the requirement that F should be closed, as a step in the process of finding a theory where the tensor multiplet fields need not be on shell. We will start in the bosonic case, where the motivation for these ideas is found, and then turn to the superconformal model and try to generalize the concepts introduced in the bosonic theory.

A. The bosonic model

A free two-form gauge field b with a three-form field strength h obeys the Bianchi identity

$$\mathrm{d}h = 0 \tag{4.1}$$

and the equations of motion

$$\mathrm{d} * h = 0, \tag{4.2}$$

where $*$ denotes the Hodge duality operator. For a self-dual three-form h, these two equations coincide.

If we want to couple this field electromagnetically to a self-dual string (with both magnetic and electric charge), this is done by changing the right-hand sides of the equations above. Explicitly, we get

$$\mathrm{d}h = \delta_\Sigma,$$

$$\mathrm{d} * h = \delta_\Sigma, \tag{4.3}$$

where δ_Σ denotes a four-form called the Poincaré dual to the string world-sheet Σ. It is defined by the relation

$$\int_\Sigma b \equiv \int_M \delta_\Sigma \wedge b, \tag{4.4}$$

where the left-hand integral is evaluated over the string world-sheet, while the right-hand integral is over the entire six-dimensional Minkowski space. We also note that the self-dual piece of h, expressed as $h_+ = \frac{1}{2}(h + *h)$, obeys an inhomogeneous equation while the anti self-dual piece $h_- = \frac{1}{2}(h - *h)$ is free and therefore decoupled from the theory, as required. It should be emphasized that Eq. (4.3) does not *imply* self-duality, but it is *consistent* with self-duality.

Explicitly, the Poincaré dual is expressed in terms of the string embedding fields X^μ and the space-time coordinates x^μ according to

$$\delta_\Sigma = \frac{1}{4!}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma \int_\Sigma \tilde{\mathrm{d}}X^\tau \wedge \tilde{\mathrm{d}}X^\varepsilon \, \epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(x - X), \tag{4.5}$$

where $\tilde{\mathrm{d}} \equiv \mathrm{d}\sigma^i \partial_i$ again is the differential with respect to the world-sheet variables σ^i, $i = 1, 2$, and $\delta^{(6)}(x - X)$ is a Dirac delta function in six dimensions. This is somewhat analogous to the coupling of a dyonic relativistic particle to a Maxwell field in four dimensions, in that sense δ_Σ is a generalization of the current four-vector.[24] In our model, we couple to a string and δ_Σ is the dual of a current two-form.

In order for this four-form to be consistent with Eq. (4.3), it must be closed. Applying the exterior derivative to δ_Σ, we get that

$$\begin{aligned}
\mathrm{d}\delta_\Sigma &= \frac{1}{4!}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma \wedge \mathrm{d}x^\kappa \int_\Sigma \tilde{\mathrm{d}}X^\tau \wedge \tilde{\mathrm{d}}X^\varepsilon \, \epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\partial_\kappa \delta^{(6)}(x-X) \\
&= -\frac{2}{5!}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma \wedge \mathrm{d}x^\kappa \int_\Sigma \tilde{\mathrm{d}}X^\tau \wedge \tilde{\mathrm{d}}X^\varepsilon \, \epsilon_{\kappa\mu\nu\rho\sigma\tau}\partial_\varepsilon \delta^{(6)}(x-X) \\
&= -\frac{2}{5!}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma \wedge \mathrm{d}x^\kappa \int_\Sigma \tilde{\mathrm{d}}(\tilde{\mathrm{d}}X^\tau \, \epsilon_{\kappa\mu\nu\rho\sigma\tau}\delta^{(6)}(x-X)) = 0, \qquad (4.6)
\end{aligned}$$

where we used the fact that an antisymmetrization over seven vector indices in six dimensions always is zero. The last equality follows since the integrand is a total derivative and the string world-sheet Σ has no boundary.

Next, we are interested in how these relations and quantities behave under (bosonic) conformal transformations. Consider the variation of the three-form h, which according to Eq. (2.27) equals

$$\delta_C h = \frac{1}{3!}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho (\xi^\sigma(x)\partial_\sigma h_{\mu\nu\rho}(x) - 3\Omega_\mu{}^\sigma(x)h_{\sigma\nu\rho}(x) + 3\Lambda(x)h_{\mu\nu\rho}(x)). \qquad (4.7)$$

However, if we compare this with Eq. (2.6), we see that

$$\delta_C h = \delta_x h, \qquad (4.8)$$

where δ_x denotes a *passive* conformal transformation, i.e., one that acts on the space-time coordinates rather than on the fields. This means that, when dealing with h as a differential form, passive and active transformations yield the same result. We will denote such forms as *primary* differential forms. The statement remains true also when exterior derivatives are applied, i.e., $\delta_C(\mathrm{d}h) = \delta_x(\mathrm{d}h)$, but also for the Hodge dual of h, which means that $\delta_C(*h) = \delta_x(*h)$.

Considering Eq. (4.3), we note that the left-hand sides transform as primary four-forms, therefore the right-hand sides should transform in the same way. Since δ_Σ is an expression in terms of the embedding field X^μ, we may calculate its active transformation explicitly. Before doing this, we want to rewrite the transformation of $\tilde{\mathrm{d}}X^\mu$ in Eq. (2.32) so that all parameter functions are expressed in terms of the space-time coordinates x^μ, rather than in terms of the embedding field X^μ. We find that

$$\delta_C(\tilde{\mathrm{d}}X^\mu) = -\Omega^\mu{}_\nu(x)\tilde{\mathrm{d}}X^\nu - \Lambda(x)\tilde{\mathrm{d}}X^\mu - 2c_\nu \tilde{\mathrm{d}}((x-X)^\mu(x-X)^\nu) + c^\mu \tilde{\mathrm{d}}((x-X)\cdot(x-X)), \qquad (4.9)$$

while the passive variation of this quantity obviously vanishes. We will also need the relation

$$\delta_C(\mathrm{d}x^\mu) = 0 = \delta_x \, \mathrm{d}x^\mu - \Omega^\mu{}_\nu(x)\mathrm{d}x^\nu - \Lambda(x)\mathrm{d}x^\mu. \qquad (4.10)$$

Finally, considering the Dirac delta function we find that

$$\delta_C(\delta^{(6)}(x-X)) = -\delta_C X^\mu \partial_\mu \delta^{(6)}(x-X) = \delta_x(\delta^{(6)}(x-X)) + 6\Lambda(x)\delta^{(6)}(x-X), \qquad (4.11)$$

where we have used the relation

$$x^\mu \partial_\nu \delta^{(6)}(x) = -\delta_\nu{}^\mu \delta^{(6)}(x). \qquad (4.12)$$

Putting all this together, again using the properties of the Dirac delta function, we arrive at the conclusion

$$\delta_C(\delta_\Sigma) = \delta_x(\delta_\Sigma), \qquad (4.13)$$

meaning that our expression (4.5) for δ_Σ transforms as a primary four-form. This shows that Eq. (4.3) is a well-defined equation with respect to conformal symmetry.

B. The superconformal model

Having investigated the bosonic case, we try to generalize these concepts to superspace. We note that the on-shell super three-form F in Eq. (3.75) is primary, i.e.,

$$\delta_C F = \delta_{x,\theta} F, \tag{4.14}$$

where $\delta_{x,\theta}$ obviously denotes a passive conformal transformation in superspace. The validity of this equation is most easily seen from the fact that F yields a superconformally invariant Wess-Zumino term, see Sec. III D.

Let us now try to take F off shell, i.e., relax the requirement $\mathrm{d}F=0$. The equation corresponding to Eq. (4.3) is

$$\mathrm{d}\mathcal{F} = \Delta_\Sigma, \tag{4.15}$$

where d is the exterior derivative in superspace and $\mathcal{F}$ is a super three-form, not necessarily equal to F defined in Eq. (3.75). The super four-form Δ_Σ appearing on the right-hand side is supposed to be a generalization of the Poincaré dual δ_Σ. To find such a quantity is nontrivial, since there is no proper analogue of the Poincaré dual in superspace. The best we can hope for is to find a super four-form that reduces to δ_Σ if all fermionic degrees of freedom are removed, and that transforms in a nice way under superconformal transformations.

Guided by our previous experience, we try to formulate this four-form in terms of superfields. The fundamental superfields involving the embedding fields $X^{\alpha\beta}$ and Θ_a^α are

$$s^{\alpha\beta} \equiv x^{\alpha\beta} - X^{\alpha\beta} - i\Omega^{ab}\theta_a^{[\alpha}\,\Theta_b^{\beta]}, \tag{4.16}$$

$$t_a^\alpha \equiv \theta_a^\alpha - \Theta_a^\alpha; \tag{4.17}$$

the superfield properties of these are easily verified. The superfield $s^{\alpha\beta}$ is a vector and we will, when appropriate, use the alternative notation s^μ for this, employing an SO(5,1) vector index as in the bosonic case. Some important quantities will be stated twice, using both conventions.

We will also need the differential

$$\mathrm{d}s^{\alpha\beta} = \mathrm{d}x^{\alpha\beta} - i\Omega^{ab}\,\mathrm{d}\theta_a^{[\alpha}\,\Theta_b^{\beta]} = e^{\alpha\beta} - i\Omega^{ab}(\theta-\Theta)_a^{[\alpha}\,\mathrm{d}\theta_b^{\beta]}, \tag{4.18}$$

where the second equation follows from the definition of the superspace differential $e^{\alpha\beta}$. Similarly, we may differentiate $s^{\alpha\beta}$ with respect to the parameters defining the string world-sheet, yielding

$$\tilde{\mathrm{d}}s^{\alpha\beta} = -\tilde{\mathrm{d}}X^{\alpha\beta} - i\Omega^{ab}\theta_a^{[\alpha}\,\tilde{\mathrm{d}}\Theta_b^{\beta]} = -E^{\alpha\beta} - i\Omega^{ab}(\theta-\Theta)_a^{[\alpha}\,\tilde{\mathrm{d}}\Theta_b^{\beta]}, \tag{4.19}$$

where $E^{\alpha\beta}$ as before is the bosonic superspace differential expressed in terms of the embedding fields $X^{\alpha\beta}$ and Θ_a^α.

Guided by Eq. (4.5), we introduce

$$\Delta_\Sigma = \frac{1}{4!}\int_\Sigma \mathrm{d}s^\mu \wedge \mathrm{d}s^\nu \wedge \mathrm{d}s^\rho \wedge \mathrm{d}s^\sigma\, \tilde{\mathrm{d}}s^\tau \wedge \tilde{\mathrm{d}}s^\varepsilon\, \epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s) \tag{4.20}$$

$$= \frac{1}{4!}\int_\Sigma \mathrm{d}s^{\delta_1\delta_2} \wedge \mathrm{d}s^{\gamma_1\gamma_2} \wedge \mathrm{d}s^{\beta_1\beta_2} \wedge \mathrm{d}s^{\alpha_1\alpha_2}\, \tilde{\mathrm{d}}s^{\sigma_1\sigma_2} \wedge \tilde{\mathrm{d}}s^{\tau_1\tau_2} \epsilon_{\alpha_1\alpha_2\beta_1\gamma_1}\epsilon_{\gamma_2\delta_1\delta_2\sigma_1}\epsilon_{\sigma_2\tau_1\tau_2\beta_2}\delta^{(6)}(s), \tag{4.21}$$

where the Dirac delta function with a Grassmannian argument containing both "body" and "soul" is defined in terms of its Taylor expansion. It is apparent that this candidate for Δ_Σ reduces to the bosonic δ_Σ in Eq. (4.5) if all fermions are put to zero.

The second requirement on this Δ_Σ is that it should be closed, as is seen immediately from Eq. (4.15). The proof for this is similar to the bosonic case in Eq. (4.6), but slightly more complicated since $\mathrm{d}\,\tilde{\mathrm{d}}s^\mu = \tilde{\mathrm{d}}\,\mathrm{d}s^\mu \neq 0$. However, the changes in the proof are minor and therefore omitted in this text.

We also want to investigate how Δ_Σ transforms under superconformal transformations. As in the bosonic case, we will present the transformations piece by piece. Using the explicit variations of $X^{\alpha\beta}$ and Θ_a^α found above, we find that

$$\delta_C(\mathrm{d}s^{\alpha\beta}) = \delta_{x,\theta}\,\mathrm{d}s^{\alpha\beta} - \tilde{\Lambda}\,\mathrm{d}s^{\alpha\beta} + 2\tilde{\Omega}_\gamma^{\ [\alpha}\,\mathrm{d}s^{\beta]\gamma} + \mathrm{d}\chi^{\alpha\beta}, \tag{4.22}$$

$$\delta_C(\tilde{\mathrm{d}}s^{\alpha\beta}) = \delta_{x,\theta}\,\tilde{\mathrm{d}}s^{\alpha\beta} - \tilde{\Lambda}\,\tilde{\mathrm{d}}s^{\alpha\beta} + 2\tilde{\Omega}_\gamma^{\ [\alpha}\,\tilde{\mathrm{d}}s^{\beta]\gamma} + \tilde{\mathrm{d}}\chi^{\alpha\beta}, \tag{4.23}$$

where we have used the presence of a Dirac delta function in the expression (4.21) to set $s^{\alpha\beta}=0$. Moreover, $\delta_{x,\theta}$ denotes a passive variation in superspace and

$$\tilde{\Omega}_\gamma^{\ \alpha} \equiv \Omega_\gamma^{\ \alpha}(x,\theta) + i\Omega^{cd}\Xi_{c,\gamma}(\theta)t_d^\alpha - \frac{i}{4}\Omega^{cd}\Xi_{c,\delta}(\theta)t_d^\delta\delta_\gamma^{\ \alpha}, \tag{4.24}$$

$$\tilde{\Lambda} \equiv \Lambda(x,\theta) + \frac{i}{2}\Omega^{cd}\Xi_{c,\gamma}(\theta)t_d^\gamma, \tag{4.25}$$

$$\chi^{\alpha\beta} \equiv -\Omega^{ab}\Omega^{cd}\Xi_{a,\gamma}(\theta)t_b^{[\alpha}t_c^{\beta]}t_d^\gamma - c_{\gamma\delta}\Omega^{ab}\Omega^{cd}t_a^\gamma t_b^{[\alpha}t_c^{\beta]}t_d^\delta. \tag{4.26}$$

Alternatively, we may write these variations as

$$\delta_C(\mathrm{d}s^\mu) = \delta_{x,\theta}\,\mathrm{d}s^\mu - \tilde{\Lambda}\,\mathrm{d}s^\mu - \tilde{\Omega}_\nu^\mu\,\mathrm{d}s^\nu + \mathrm{d}\chi^\mu, \tag{4.27}$$

$$\delta_C(\tilde{\mathrm{d}}s^\mu) = \delta_{x,\theta}\,\tilde{\mathrm{d}}s^\mu - \tilde{\Lambda}\,\tilde{\mathrm{d}}s^\mu - \tilde{\Omega}^\mu_{\ \nu}\,\tilde{\mathrm{d}}s^\nu + \tilde{\mathrm{d}}\chi^\mu, \tag{4.28}$$

where we again have introduced a vector index instead of an antisymmetric pair of SO(5,1) spinor indices. We have also introduced $\tilde{\Omega}_\nu^\mu$, the definition of which is apparent from how ω_α^β was defined from $\omega^{\mu\nu}$ in Sec. III A.

The Dirac delta function transforms according to

$$\delta_C(\delta^{(6)}(s)) = \delta_{x,\theta}\delta^{(6)}(s) + 6\tilde{\Lambda}\delta^{(6)}(s) + \chi\cdot\partial\delta^{(6)}(s), \tag{4.29}$$

where we as usual have used the properties of the delta function to set $s^{\alpha\beta}=0$. We have also employed the identity

$$s^{\alpha\gamma}\partial_{\alpha\beta}\delta^{(6)}(s) = -\tfrac{3}{2}\delta_\beta^{\ \gamma}\delta^{(6)}(s), \tag{4.30}$$

which is analogous to Eq. (4.12) in the bosonic model.

Putting all this together, using the vector index notation, we find that the superconformal variation of Δ_Σ is

$$\begin{aligned}\delta_C\Delta_\Sigma = \delta_{x,\theta}\Delta_\Sigma &+ \frac{1}{3!}\int_\Sigma \mathrm{d}s^\mu\wedge\mathrm{d}s^\nu\wedge\mathrm{d}s^\rho\wedge\mathrm{d}\chi^\sigma\,\tilde{\mathrm{d}}s^\tau\wedge\tilde{\mathrm{d}}s^\varepsilon\epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s)\\ &+ \frac{2}{4!}\int_\Sigma \mathrm{d}s^\mu\wedge\mathrm{d}s^\nu\wedge\mathrm{d}s^\rho\wedge\mathrm{d}s^\sigma\,\tilde{\mathrm{d}}s^\tau\wedge\tilde{\mathrm{d}}\chi^\varepsilon\epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s)\\ &+ \frac{1}{4!}\int_\Sigma \mathrm{d}s^\mu\wedge\mathrm{d}s^\nu\wedge\mathrm{d}s^\rho\wedge\mathrm{d}s^\sigma\,\tilde{\mathrm{d}}s^\tau\wedge\tilde{\mathrm{d}}s^\varepsilon\epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\,\chi^\kappa\partial_\kappa\delta^{(6)}(s),\end{aligned} \tag{4.31}$$

which may be rewritten as (our conventions for superderivatives may be found in Ref. 10)

$$\delta_C \Delta_\Sigma = \delta_{x,\theta}\Delta_\Sigma + \mathrm{d}\left[\frac{1}{3!}\int_\Sigma \mathrm{d}s^\mu \wedge \mathrm{d}s^\nu \wedge \mathrm{d}s^\rho\, \tilde{\mathrm{d}}s^\tau \wedge \tilde{\mathrm{d}}s^\varepsilon\, \chi^\sigma \epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s)\right]$$
$$- \frac{2}{4!}\int_\Sigma \tilde{\mathrm{d}}[\mathrm{d}s^\mu \wedge \mathrm{d}s^\nu \wedge \mathrm{d}s^\rho \wedge \mathrm{d}s^\sigma\, \tilde{\mathrm{d}}s^\tau\, \chi^\varepsilon \epsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s)]$$
$$+ \frac{7}{4!}\int_\Sigma \mathrm{d}s^\mu \wedge \mathrm{d}s^\nu \wedge \mathrm{d}s^\rho \wedge \mathrm{d}s^\sigma\, \tilde{\mathrm{d}}s^\tau \wedge \tilde{\mathrm{d}}s^\varepsilon\, \chi^\kappa \epsilon_{[\mu\nu\rho\sigma\tau\varepsilon}\,\partial_{\kappa]}\delta^{(6)}(s). \tag{4.32}$$

In this expression, the last line vanishes since it is an antisymmetrization over seven vector indices in six dimensions, while the second line is zero since it reduces to a boundary term. We are left with

$$\delta_C \Delta_\Sigma = \delta_{x,\theta}\Delta_\Sigma + \mathrm{d}\Lambda_\Sigma, \tag{4.33}$$

where the super three-form Λ_Σ is given by

$$\Lambda_\Sigma = \frac{1}{3!}\int_\Sigma \mathrm{d}s^\mu \wedge \mathrm{d}s^\nu \wedge \mathrm{d}s^\rho\, \tilde{\mathrm{d}}s^\tau \wedge \tilde{\mathrm{d}}s^\varepsilon\, \chi^\sigma \varepsilon_{\mu\nu\rho\sigma\tau\varepsilon}\delta^{(6)}(s) \tag{4.34}$$

$$= \frac{1}{3!}\int_\Sigma \mathrm{d}s^{\gamma_1\gamma_2} \wedge \mathrm{d}s^{\beta_1\beta_2} \wedge \mathrm{d}s^{\alpha_1\alpha_2}\, \chi^{\varepsilon_1\varepsilon_2}\, \tilde{\mathrm{d}}s^{\sigma_1\sigma_2} \wedge \tilde{\mathrm{d}}s^{\tau_1\tau_2}\delta^{(6)}(s)$$
$$\times\left(\varepsilon_{\varepsilon_1\varepsilon_2\beta_1\gamma_1}\varepsilon_{\gamma_2\alpha_1\alpha_2\sigma_1}\varepsilon_{\sigma_2\tau_1\tau_2\beta_2} - \frac{1}{8}\varepsilon_{\varepsilon_1\varepsilon_2\gamma_1\gamma_2}\varepsilon_{\sigma_1\sigma_2\alpha_1\alpha_2}\varepsilon_{\tau_1\tau_2\beta_1\beta_2}\right), \tag{4.35}$$

but this quantity is obviously only well-defined modulo an exact three-form.

Looking back at Eq. (4.13) for the bosonic model, we see that the introduction of fermionic degrees of freedom has altered the relation by adding a d-exact term to the right-hand side. This means that our candidate (4.20) for Δ_Σ does not transform exactly as one would expect when comparing with the bosonic theory, i.e., an active and a passive transformation do not yield the same result. We note that Λ_Σ vanishes if all fermions are removed and that it is localized (by means of the Dirac delta function) to the world-sheet of the string.

This means that the simple generalization of the bosonic case that we have tried in this section did not work out properly. The most probable reason for this failure is that we are required to add a new ingredient, the matrix $\hat{\phi}^{ab}$, to Δ_Σ. This denotes the vacuum expectation value of the field $\phi^{ab}(x)$, normalized to unit modulus with respect to the scalar product in Eq. (3.72). In other words, $\hat{\phi}^{ab}$ is related to the moduli parameters of the theory, denoting the direction in which R-symmetry is broken by the presence of the tensile string. We have seen the appearance of this quantity previously[16] in the discussion concerning the κ-symmetry of the theory. We will not consider how to formulate a superspace generalization of the Poincaré dual including $\hat{\phi}^{ab}$ in this paper, but we hope to return to the matter in a future presentation.

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Friedel theorem for two dimensional relativistic spin-$\frac{1}{2}$ systems

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The Friedel sum rule is generalized to relativistic systems of spin-$\frac{1}{2}$ particles in two dimensions. The change in energy due to the presence of an impurity is studied. The relation of the sum rule with the relativistic Levinson theorem is presented. Density oscillations in such systems are discussed. Since the Friedel theorem has been of major importance in understanding the impurity scattering in materials, the present results may be useful to explain some phenomena in two dimensional fermionic many body systems. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Friedel sum rule (FSR)[1–3] is an important theorem in studying the effects of an impurity on the electron structure in solids, which sets up the relation between the change of the number of states ΔN around the impurity and the phase shift at Fermi energy. In three dimensional (3D) systems, the theorem can be described by

$$\Delta N = \frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\,\delta_l(E_f), \tag{1}$$

where $\delta_l(E_f)$ denotes the phase shift of scattered state in the angular-momentum channel l with energy at the Fermi surface. The result is one of the most interesting results in the theory of impurity. It states that the change of the number of states caused by the potential of an impurity can be quantified in terms of the scattering phase shift at Fermi energy. The subject was then studied by many authors and generalized to include the internal degree of freedom of particles,[4,5] which provides a powerful method in calculating the residual resistance, diamagnetic susceptibility,[2,3] spectral properties of spin-$\frac{1}{2}$ fermions in the presence of an impurity,[6] and so forth. Recently, based on the Dirac equation, the FSR for relativistic spin-$\frac{1}{2}$ particles in 3D systems is proved to be

$$\Delta N = \frac{1}{\pi}\sum_{\kappa=-\infty,\kappa\neq 0}^{\infty} 2|\kappa|\Bigg\{[\delta_\kappa(E_f)-\delta_\kappa(\mu)+\delta_\kappa(-E_f')-\delta_\kappa(-\mu)] + \epsilon_\kappa\frac{\pi(-1)^{|\kappa|}}{2}[\sin^2\delta_\kappa(\mu)-\sin^2\delta_\kappa(-\mu)]\Bigg\}, \tag{2}$$

where $\delta_\kappa(\pm E_\lambda)$ and $\delta_\kappa(\pm\mu)$, classified by the angular momentum $\kappa=\pm(j+1/2)$ and $\epsilon_\kappa\equiv 1(-1)$ for $\kappa>0$ ($\kappa<0$), are the phase shifts of scattering states at Fermi energies ($E_\lambda=E_f$ and $-E_f'$) and zero-momentum ($E_\lambda=\pm\mu$).[7] The result may provide a basis for exploring the effect of an impurity by the FSR for 3D relativistic systems. For 1D systems, the nonrelativistic FSR is given by[8]

$$\Delta N = \frac{2}{\pi} \sum_{p=e,o} \left(\delta_p(E_f) - \delta_p(0) + \epsilon_p \frac{\pi}{2} \sin^2 \delta_p(0) \right), \tag{3}$$

where $\delta_p(0)$ is the phase shift at zero momentum, and the phase shifts $\delta_p(E_\lambda)$ $(p=e,o)$ are classified by even parity (e) and odd parity (o) of wave functions. Its generalization to relativistic spin-$\frac{1}{2}$ particles is shown to relate to the phase shifts $\delta_p(E_\lambda)$ of scattering states at Fermi energies $(E_\lambda = E_f$ and $-E_f')$ and zero momentum $(E_\lambda = \pm\mu)$ as follows:[8]

$$\Delta N = \frac{1}{\pi} \sum_{p=e,o} \left\{ [\delta_p(E_f) - \delta_p(\mu) + \delta_p(-E_f') - \delta_p(-\mu)] - \epsilon_p \frac{\pi}{2} [\sin^2 \delta_p(\mu) - \sin^2 \delta_p(-\mu)] \right\}. \tag{4}$$

where $\epsilon_p = 1(-1)$ for even parity (odd parity). The result is meaningful in 1D nanostructures since the relativistic spectra appear naturally as a low energy effective spectra for electrons in 1D metals.[9]

Over the past two decades, remarkable phenomena have been observed in the 2D electron gas (2DEG), such as the integer and fractional quantum Hall effect.[10,11] On the other hand, a number of interesting physical systems, the effective quantum theory is expected to be described by the 2D Dirac equation[9,12] rather than the Schrödinger equation. The anticipation recently has been confirmed by experiments in perfect graphene,[13,14] which pose new questions on the nature of the electronic properties in such systems and shows a possibility of studying relativistic phenomena in a tabletop experiment. To my knowledge, as one of the most powerful tools in studying effects of impurities, the FSR for 2D Dirac fermions is still lacking. It is our aim in the paper to establish the FSR for 2D relativistic spin-$\frac{1}{2}$ systems. In two dimensions, based on the Schrödinger equation, the nonrelativistic FSR can be proved to be (see the Appendix)

$$\Delta N = \frac{2}{\pi} \sum_{m=-\infty}^{\infty} [\delta_m(E_f) - \delta_m(0)], \tag{5}$$

where $\delta_m(0)$ is the phase shift at the zero momentum in the angular-momentum channel m $(m = 0, \pm 1, \pm 2, \ldots)$. In this paper, we shall generalize the result to relativistic spin-$\frac{1}{2}$ systems.

This paper is organized as follows. In Sec. II, the 2D FRS is generalized to the relativistic spin-$\frac{1}{2}$ particles moving in a short range potential $|V(r)|$ when $r < a$ and $V(r) = 0$ when $r \geqslant a$. The total change of the number of states ΔN around the potential is shown to relate to the phase shifts $\delta_j(E_\lambda)$ of scattering states at Fermi energies $(E_\lambda = E_f$ and $-E_f')$ and zero-momentum $(E_\lambda = \pm\mu)$ as follows:

$$\Delta N = \frac{1}{\pi} \sum_{j=\pm 1/2, \pm 3/2, \ldots} [\delta_j(E_f) - \delta_j(\mu) + \delta_j(-E_f') - \delta_j(-\mu)] \tag{6}$$

where j $(j = \pm 1/2, \pm 3/2, \ldots)$ is the total angular momentum. Section III is used to discuss the change in energy of a relativistic spin-$\frac{1}{2}$ system in the presence of an impurity. In Sec. IV, the relation between the FSR and the 2D relativistic Levinson theorem[15–18] is presented. Density oscillations of relativistic spin-$\frac{1}{2}$ systems are discussed. The FSR for the massless Dirac fermions is also presented here. Our conclusions are summarized in Sec. V.

II. FRIEDEL SUM RULE FOR RELATIVISTIC SPIN-$\frac{1}{2}$ SYSTEMS IN TWO DIMENSIONS

We consider the 2D model. The Dirac equation of a spin-$\frac{1}{2}$ particle with effective mass μ moving in a cylindrically symmetric potential $V(r)$ specified in the previous is given by

$$[\vec{\alpha} \cdot \hat{\mathbf{p}} + \gamma^0 \mu + V(r)] \Psi_\lambda(\mathbf{r}) = E_\lambda \Psi_\lambda(\mathbf{r}), \tag{7}$$

where $\alpha^i = \gamma^0 \gamma^j$ $(i = 1, 2)$ are Dirac matrices. As usual, they are chosen as the Pauli matrices $\gamma^0 = \sigma^3$, $\gamma^1 = i\sigma^1$, and $\gamma^2 = i\sigma^2$ such that the total angular momentum $\hat{J} = \hat{L} + \hat{S}$ with the spin $\hat{S}$

$=(i\epsilon^{ij}\gamma^i\gamma^j)/4$ is conservative. For our purposes it is very convenient to write the spin wave function in a form

$$\Psi_\lambda(\mathbf{r}) = \sum_{j=\pm 1/2,\pm 3/2,\ldots} c_j \Psi_{\lambda j}(\mathbf{r}) = \sum_{j=\pm 1/2,\pm 3/2,\ldots} c_j \begin{pmatrix} f_{\lambda j}(r)\dfrac{e^{i(j-1/2)\varphi}}{\sqrt{2\pi}} \\ g_{\lambda j}(r)\dfrac{e^{i(j+1/2)\varphi}}{\sqrt{2\pi}} \end{pmatrix}. \tag{8}$$

Here c_j's are coefficients dependent on the particular form required for Ψ_λ and j denotes the quantum number of the total angular momentum $\hat{J}$. With (8), it can be shown that the radial equations for spinors $f_{\lambda j}(r)$ and $g_{\lambda j}(r)$ are

$$\left(\frac{d}{dr} - \frac{j-1/2}{r}\right) f_{\lambda j}(r) + [E_\lambda + \mu - V(r)] g_{\lambda j}(r) = 0, \tag{9}$$

$$\left(\frac{d}{dr} + \frac{j+1/2}{r}\right) g_{\lambda j}(r) - [E_\lambda - \mu - V(r)] f_{\lambda j}(r) = 0. \tag{10}$$

At regions of $V=0$, these equations can be decoupled into

$$\frac{d^2}{dr^2} f_{\lambda j}(r) + \frac{1}{r}\frac{d}{dr} f_{\lambda j}(r) + \left(k^2 - \frac{(j-1/2)^2}{r^2}\right) f_{\lambda j}(r) = 0, \tag{11}$$

$$\frac{d^2}{dr^2} g_{\lambda j}(r) + \frac{1}{r}\frac{d}{dr} g_{\lambda j}(r) + \left(k^2 - \frac{(j+1/2)^2}{r^2}\right) g_{\lambda j}(r) = 0, \tag{12}$$

with $k=\sqrt{E_\lambda^2-\mu^2} \geqslant 0$, which turn out to be the Bessel equations. Thus the solution of scattering state of spinor $f_{\lambda j}$ for positive energy ($E_\lambda > \mu$) and a positive quantum number ($j>0$) is given by

$$f_{\lambda j}(r) = [C_1(k) J_{j-1/2}(kr) + C_2(k) N_{j-1/2}(kr)] = A_j(k)[\sin\,\delta_j(k) J_{j-1/2}(kr) + \cos\,\delta_j(k) N_{j-1/2}(kr)], \tag{13}$$

where $J_{j-1/2}(x)$ and $N_{j-1/2}(x)$ are Bessel functions, $\delta_j(k)$ is the phase shift defined by $C_1/C_2 \equiv \tan\,\delta_j(k)$ and $A_j(k)=C_1(k)/\sin\,\delta_j(k)$. The explicit form of $A_j(k)$ is determined by the normalization condition of $\delta(E_\lambda - E_{\lambda'})$ for free particles, which gives $A_j(k)=\sqrt{(E_\lambda+\mu)/2}$. At large distance $r\to\infty$, the asymptotic representation of the spinor reads as

$$f_{\lambda j}(r) \to \sqrt{\frac{(E_\lambda+\mu)}{\pi k r}} \sin\left(kr - \frac{(j-1/2)\pi}{2} - \frac{\pi}{4} + \delta_j\right). \tag{14}$$

Substituting this expression into (9), one obtains

$$g_{\lambda j}(r) \to -\sqrt{\frac{(E_\lambda-\mu)}{\pi k r}} \cos\left(kr - \frac{(j-1/2)\pi}{2} - \frac{\pi}{4} + \delta_j\right). \tag{15}$$

Similarly, the entire asymptotic solutions for particle (positive energy) and antiparticle (negative energy) are found to be

$$f_{\lambda j}(r) \to \sqrt{\frac{(|E_\lambda| \pm \mu)}{\pi k r}} \sin\left(kr - \frac{\kappa\pi}{2} - \frac{\pi}{4} + \delta_j\right), \tag{16}$$

and

$$g_{\lambda j}(r) \to \mp \sqrt{\frac{(|E_\lambda| \mp \mu)}{\pi k r}} \cos\left(kr - \frac{\kappa\pi}{2} - \frac{\pi}{4} + \delta_j\right). \tag{17}$$

Here $\kappa \equiv |j-1/2|$ and the upper and lower signs indicate the scattering states of the particle (positive energy $E_\lambda > \mu$) and antiparticle (negative energy $E_\lambda < -\mu$), respectively. These asymptotic behaviors of spinors will be used to evaluate the change of the number of states around the potential barrier $V(r)$. To approach our aim, we consider a large 2D circular area, radius R, centered on the potential. By multiplying Eq. (7) through by $\Psi_\lambda^\dagger(\mathbf{r})$ and the corresponding equation for $\Psi_\lambda^\dagger(\mathbf{r})$ by $\Psi_\lambda(\mathbf{r})$, it follows that

$$(E_{\lambda'} - E_\lambda)\Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r}) = -i\,\boldsymbol{\nabla}\cdot[\Psi_\lambda^\dagger(\mathbf{r})\vec{\alpha}\Psi_{\lambda'}(\mathbf{r})]. \tag{18}$$

Integrating over the whole area, and using the divergence theorem, one obtains

$$\int d^2r\, \Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r}) = \frac{R}{(E_{\lambda'} - E_\lambda)} \sum_j [f_{\lambda j}^*(R) g_{\lambda' j}(R) - g_{\lambda j}^*(R) f_{\lambda' j}(R)]. \tag{19}$$

To get the equality, the radial component of $\vec{\alpha}$,

$$\frac{\vec{\alpha}\cdot\mathbf{r}}{r} = \begin{pmatrix} 0 & ie^{-i\varphi} \\ -ie^{i\varphi} & 0 \end{pmatrix} \tag{20}$$

is used and one takes $c_j = 1$; since we are only interested in the difference of states its complex nature is of no interest. For free Dirac particles, the above integral can be expanded as

$$\int d^2r\, \Psi_\lambda^{(0)\dagger}(\mathbf{r})\Psi_{\lambda'}^{(0)}(\mathbf{r}) = \frac{R}{(E_{\lambda'} - E_\lambda)} \sum_j [f_{\lambda j}^{(0)*}(R) g_{\lambda' j}^{(0)}(R) - g_{\lambda j}^{(0)*}(R) f_{\lambda' j}^{(0)}(R)], \tag{21}$$

with $f_{\lambda j}^{(0)} = f_{\lambda j}(\delta_j = 0)$, and $g_{\lambda j}^{(0)} = g_{\lambda j}(\delta_j = 0)$. In solids, the electron (hole) states are occupied up to the Fermi energy E_f $(-E_f')$. So the total change of the number of states ΔN around the potential $V(r)$ is obtained by integrating up to the Fermi energy E_f $(-E_f')$,

$$\Delta N = \lim_{R\to\infty} \lim_{E_{\lambda'}\to E_\lambda} \left(\int_{-E_f'}^{-\mu} + \int_{\mu}^{E_f} \right) dE_\lambda \int d^2r [\Psi_\lambda^\dagger(\mathbf{r})\Psi_{\lambda'}(\mathbf{r}) - \Psi_\lambda^{(0)\dagger}(\mathbf{r})\Psi_{\lambda'}^{(0)}(\mathbf{r})], \tag{22}$$

where the lower bound of the Fermi surface for an antiparticle is denoted by $-E_f'$ for accounting of different levels generally. Since at large distances the wave function $\Psi_\lambda(\mathbf{r})$ must be unchanged, except for the phase shifts in the partial waves, the spinors $f_{\lambda j}$ and $g_{\lambda j}$ in (8) can be replaced by the asymptotic representations of (16) and (17). It follows that

$$\begin{aligned} &\frac{R}{(E_{\lambda'} - E_\lambda)} \sum_j [f_{\lambda j}^*(R) g_{\lambda' j}(R) - g_{\lambda j}^*(R) f_{\lambda' j}(R) - f_{\lambda j}^{(0)*}(R) g_{\lambda' j}^{(0)}(R) + g_{\lambda j}^{(0)*}(R) f_{\lambda' j}^{(0)}(R)] \\ &\quad = \frac{C_\pm}{(E_{\lambda'} - E_\lambda)} \sum_j 2\cos\left((k'-k)R + \frac{1}{2}(\delta_{j'} - \delta_j)\right) \sin\left(\frac{1}{2}(\delta_{j'} - \delta_j)\right) \\ &\qquad + \frac{(-1)^\kappa D_\pm}{(E_{\lambda'} - E_\lambda)} \sum_j \left[2\cos[(k'+k)R] \sin^2\left(\frac{1}{2}(\delta_{j'} + \delta_j)\right) + \sin[(k'+k)R] \sin(\delta_{j'} + \delta_j) \right], \end{aligned} \tag{23}$$

where

$$C_\pm = \frac{\epsilon_E}{2\pi\sqrt{kk'}} \{[(|E_\lambda| \pm \mu)(|E_{\lambda'}| \mp \mu)]^{1/2} + [(|E_\lambda| \mp \mu)(|E_{\lambda'}| \pm \mu)]^{1/2}\}, \tag{24}$$

$$D_{\pm}=\frac{1}{2\pi\sqrt{kk'}}\{\pm[(|E_{\lambda}|\mp\mu)(|E_{\lambda'}|\pm\mu)]^{1/2}\mp[(|E_{\lambda}|\pm\mu)(|E_{\lambda'}|\mp\mu)]^{1/2}\}, \tag{25}$$

with $\epsilon_E\equiv 1(-1)$ for $E_{\lambda}\geqslant\mu$ ($E_{\lambda}\leqslant-\mu$). Here subscript "+" ("−") in $C_{\pm}$ corresponds to the particle (antiparticle). Taking the limit $E_{\lambda'}\to E_{\lambda}$, Eqs. (24) and (25) yield $C_{\pm}\to\epsilon_E/\pi$ and $D_{\pm}/(E_{\lambda'}-E_{\lambda})\to-\epsilon_E(\mu/2\pi k^2)$, such that

$$\lim_{E_{\lambda'}\to E_{\lambda}}\frac{C_{\pm}}{(E_{\lambda'}-E_{\lambda})}2\cos\left((k'-k)R+\frac{1}{2}(\delta_{j'}-\delta_j)\right)\sin\left(\frac{1}{2}(\delta_{j'}-\delta_j)\right)\to\frac{\epsilon_E}{\pi}\frac{d\delta_j}{dE_{\lambda}} \tag{26}$$

and

$$\lim_{E_{\lambda'}\to E_{\lambda}}\frac{(-1)^{\kappa}D_{\pm}}{(E_{\lambda'}-E_{\lambda})}\left[2\cos[(k'+k)R]\sin^2\left(\frac{1}{2}(\delta_{j'}+\delta_j)\right)+\sin[(k'+k)R]\sin(\delta_{j'}+\delta_j)\right]$$
$$\to\epsilon_E\frac{-(-1)^{\kappa}\mu}{2\pi k^2}[2\cos(2kR)\sin^2\delta_j+\sin(2kR)\sin(2\delta_j)]. \tag{27}$$

Since in 2D space $\delta_j(k=0)/\pi$ always take integers,[16,17] and $\lim_{R\to\infty}\cos(2kR)$ oscillates, the integral $\lim_{R\to\infty}\int dE_{\lambda}[\cos(2kR)\sin^2\delta_j]/k^2\to 0$. Moreover, due to the fact that $\lim_{R\to\infty}\sin(2kR)/\pi k=\delta(k)$, the integral in the second term in (27) $\lim_{R\to\infty}\int dE_{\lambda}\sin(2kR)\sin(2\delta_j)/\pi k^2\to 0$. Therefore the difference of the number of states finally can be in terms of the phase shifts at Fermi energies and the critical points $\pm\mu$ of zero momentum,

$$\Delta N=\frac{1}{\pi}\sum_{j=\pm 1/2,\pm 3/2,\ldots}[\delta_j(E_f)-\delta_j(\mu)+\delta_j(-E_f')-\delta_j(-\mu)]. \tag{28}$$

This is the FSR for 2D relativistic fermionic systems. One notice that the zero-momentum behavior is quite different from that in Eqs. (2) and (4) for 3D and 1D systems, where half bound states with phase shifts $\pi/2$ are significant.[16] Comparing with the nonrelativistic FSR (5), the antiparticle turns out to be significant. A positive (negative) ion will attract (repulse) electrons (holes), and repulse (attract) holes such that the variance of states is together with the effect of two kinds of particles.

III. THE CHANGE IN ENERGY DUE TO AN IMPURITY IN RELATIVISTIC 2D SYSTEMS

Equations (16) and (17) shows that the wave functions undergo phase shifts. This fact entails a change of the kinetic energy of particles. It can be quantified by the reasonable requirements $\Psi_{\lambda j}^{(0)}(\mathbf{r})|_{\mathrm{B.C.}}=0$ and $\Psi_{\lambda j}(\mathbf{r})|_{\mathrm{B.C.}}=0$ on boundary of the Dirichlet condition, and give

$$kR-\frac{\kappa\pi}{2}-\frac{\pi}{4}=n\pi,\quad n=1,2,\ldots, \tag{29}$$

for spinor $f_{\lambda j}^{(0)}$ and

$$kR-\frac{\kappa\pi}{2}-\frac{\pi}{4}=\frac{(2n+1)\pi}{2},\quad n=0,1,2,\ldots, \tag{30}$$

for spinor $g_{\lambda j}^{(0)}$. Here R is used to denote the boundary of the 2D system. The number dn of allowed states between k and $k+dk$ is given by differentiating both members of (29) and (30), which yield $R\,dk=\pi\,dn$. Thus, the unperturbed density of states for a definite j reads as

$$D(k)=\frac{dn}{dk}=\frac{R}{\pi}. \tag{31}$$

On the other hand, the boundary condition for perturbed wave functions that vanish at $r=R$ yield

$$kR - \frac{\kappa\pi}{2} - \frac{\pi}{4} + \delta_j(k) = n\pi, \quad n = 1,2, \ldots, \tag{32}$$

for spinor $f_{\lambda j}$ and

$$kR - \frac{\kappa\pi}{2} - \frac{\pi}{4} + \delta_j(k) = \frac{(2n+1)\pi}{2}, \quad n = 0,1,2, \ldots, \tag{33}$$

for spinor $g_{\lambda j}$. From (29), (32), (30), and (33), one finds that the change of the wave number Δk of an electron with angular momentum j is $\Delta k \cdot R = -\delta_j(k)$, and the change in energy is

$$\Delta E|_{e^-} = \frac{k\Delta k}{E_\lambda} = \frac{-k\,\delta_j(k)|_{e^-}}{R\sqrt{k^2+\mu^2}}. \tag{34}$$

Similarly, the change in energy for an antiparticle reads as

$$\Delta E|_{e^+} = \frac{k\Delta k}{E_\lambda} = \frac{k\,\delta_j(k)|_{e^+}}{R\sqrt{k^2+\mu^2}}. \tag{35}$$

Here e^- (e^+) is used to denote the particle (antiparticle). Thus, the change in energy due to the presence of an impurity in 2D relativistic spin-$\frac{1}{2}$ systems is given by

$$\begin{aligned}\Delta E &= \sum_{j=\pm 1/2,\pm 3/2,\ldots} \left(\int_0^{k_f} \Delta E|_{e^-} \frac{R}{\pi} dk - \int_0^{k_f'} \Delta E|_{e^+} \frac{R}{\pi} dk \right) \\ &= -\sum_{j=\pm 1/2,\pm 3/2,\ldots} \left(\int_0^{k_f} \frac{k\,\delta_j(k)|_{e^-}}{R\sqrt{k^2+\mu^2}} \frac{R}{\pi} dk + \int_0^{k_f'} \frac{k\,\delta_j(k)|_{e^+}}{R\sqrt{k^2+\mu^2}} \frac{R}{\pi} dk \right),\end{aligned} \tag{36}$$

where R/π is the density of states for j electrons and holes. This result is a 2D relativistic generalization of Fumi theorem,[19] where the change of the kinetic energy due to the impurity for nonrelativistic systems was studied. It is worthy to note that in the massless limit, the change in energy becomes a more compact representation,

$$\Delta E = -\frac{1}{\pi} \sum_{j=\pm 1/2,\pm 3/2,\ldots} \left(\int_0^{k_f} \delta_j(k)|_{e^-}\, dk + \int_0^{k_f'} \delta_j(k)|_{e^+}\, dk \right), \tag{37}$$

which states the variance of system's energy due to the impurity can be completely ascertained as soon as the phase shifts is decided.

IV. DISCUSSIONS

A. The relation with the relativistic Levinson theorem

In 1949, Levinson established a theorem in nonrelativistic quantum mechanics.[15] Well known as the Levinson theorem, it clarifies the relation between the phase shifts of a quantum particle scattered by a short range potential and the number of bound states therein. In 3D systems, the theorem can be described as

$$\delta_l(0) = N_l\pi, \quad l = 0,1,2, \ldots, \tag{38}$$

where $\delta_l(0)$ denotes the phase shift of scattered state with a momentum k at the threshold ($k=0$) in the angular momentum channel l, and N_l is the total number of bound states in the angular momentum channel l allowed by the short range potential. When the angular momentum $l=0$, the theorem must be modified to

$$\delta_0(0) = (N_0 + 1/2)\pi, \tag{39}$$

due to the existence of a zero-energy resonance (a half-bound state).[16] The theorem is one of the most interesting and beautiful results in nonrelativistic quantum theory. For 2D relativistic spin-$\frac{1}{2}$ systems under consideration, there is a very interesting relation between the Levinson theorem and the Friedel sum rule can be established by noting the relationship of completeness of relativistic states,

$$\sum_{\text{discrete}} \psi_{\lambda j}(\mathbf{r})\psi^{\dagger}_{\lambda j}(\mathbf{r}') + \sum_j \left(\int_{-E_f'}^{-\mu} + \int_{\mu}^{E_f} \right) dE_\lambda \, \Psi_{\lambda j}(\mathbf{r})\Psi^{\dagger}_{\lambda j}(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{40}$$

Here $\psi_{\lambda j}(\mathbf{r})$ denotes a discrete bound-state with a definite angular momentum j and energy E_λ allowed by the short range potential. Subtracting the relation from the ones of free particle states $\Psi^{(0)}_{\lambda j}(\mathbf{r})$, setting $\mathbf{r}=\mathbf{r}'$, taking trace, and integrating over the 2D plane, we can find the relation between the total number of bound states N and the difference of scattering states ΔN as follows:

$$N = \sum_j N_j = -\Delta N. \tag{41}$$

The total number of bound states is then given by

$$N = \frac{1}{\pi} \sum_{j=\pm 1/2, \pm 3/2, \ldots} [\delta_j(\mu) - \delta_j(E_f) + \delta_j(-\mu) - \delta_j(-E_f')]. \tag{42}$$

The equality implies the bound-state number for a definite channel of angular momentum j is

$$N_j = \frac{1}{\pi}[\delta_j(\mu) - \delta_j(E_f) + \delta_j(-\mu) - \delta_j(-E_f')]. \tag{43}$$

This result is the Levinson theorem for relativistic spin-$\frac{1}{2}$ particles in 2D many-body systems. Different from the single particle case,[17,18]

$$N_j = \frac{1}{\pi}[\delta_j(\mu) + \delta_j(-\mu)], \tag{44}$$

where the upper bound of the phase is ruled out by the relation $\delta_j(\infty) + \delta_j(-\infty) = 0$. The phase shifts at Fermi energy play an important role here. The relation (41) reflects the completeness of the whole set of states. The total number of states is not altered by an external field, except that some scattering states are pulled down into the bound state region if the external potential is attractive. On the other hand, (41) implies that there is an upper bound on ΔN that depends on the potential $V(r)$. A finite deep potential may have finite bound states such that the change of the number of scattering states is finite.

B. Density oscillation in relativistic systems

Another way to express the change of the number of states that enables us to indicate the variance of the density of states may be expressed as

$$\Delta N = 2\pi \int_0^{\infty} r \, dr[\rho(r) - \rho_0(r)], \tag{45}$$

where $(\rho - \rho_0) \equiv \delta\rho$ is the difference of the density of states given as

$$\delta\rho = \int_{k<k_f} \frac{d^2k}{(2\pi)^2}[|\Psi_\lambda(\mathbf{r})|^2 - |\Psi^{(0)}_\lambda(\mathbf{r})|^2]. \tag{46}$$

At large distances, with (16) and (17), it is shown that

$$\delta\rho = \frac{1}{(2\pi)^2}\sum_j \int_{k<k_f} k\,dk\left((-1)^{\kappa+1}\epsilon_E \frac{2\mu}{\pi k r}\cos(2kr+\delta_j)\sin\,\delta_j\right). \tag{47}$$

The integration about the wave vector is difficult because the phase shifts depend on k. But we can obtain an approximate answer by expending it around the Fermi wave vector as $\delta_j = \delta_j(k_f) + (k - k_f)(d\delta_j/dk)$, which yields

$$\lim_{r\to\infty} \delta\rho = \frac{1}{(2\pi)^2}\sum_j (-1)^{\kappa+1}\frac{\epsilon_E \mu}{\pi}\frac{1}{r^2}\sin[2k_f r + \delta_j(k_f)]\sin\,\delta_j(k_f) + O\left(\frac{1}{r^3}\right). \tag{48}$$

The density oscillates with a period of $2k_f$ and decreases in amplitude as r^{-2}, which describes the density oscillation in 2D systems decay less rapidly than r^{-3} of 3D ones, but more rapidly than r^{-1} of the 1D case.[8] Another remarkable result is that two branches of energy have the opposite oscillating phases. Thus the antiparticle will tend to suppress the oscillation for the same phase shifts.

C. The 2D FSR for massless Dirac fermions

It was pointed out that the Lorentz group often occurs as an approximate symmetry for low energy excitation for 2D fermions in semimetals,[9,12–14] relativistic spectra appear naturally for massless conduction electrons in such systems. It is interesting to discuss the FSR in the condition of the fermion mass tends to zero. From (28), one see that as the effective mass tends to zero, ΔN becomes

$$\Delta N = \sum_{j=\pm 1/2,\pm 3/2,\ldots} [\delta_j(E_f) + \delta_j(-E_f') - 2\delta_j(0)], \tag{49}$$

which indicates the phase shifts of the particle and antiparticle at zero momentum merge to become twice. For systems contain only single carrier type, the Friedel sums become

$$\Delta N_{\text{particle}} = \sum_{j=\pm 1/2,\pm 3/2,\ldots} [\delta_j(E_f) - \delta_j(0)] \tag{50}$$

for the particle and

$$\Delta N_{\text{antiparticle}} = \sum_{j=\pm 1/2,\pm 3/2,\ldots} [\delta_j(-E_f') - \delta_j(0)] \tag{51}$$

for the antiparticle. This is the extreme case of the graphene, where the carrier type can be controlled by the external gate voltage.[13,14] Another interesting result about massless fermions comes from (47). As the effective mass tends to zero, the difference of the density of states at far regions turns into a constant, and is independent of the details of the system. This argument probably enables us to decide the magnitude of effective mass in a nonideal effective relativistic 2D system via Friedel oscillation at far zones.

D. Extension of the potential to the more general case

Although in the procedure of our proof we assume that the potential must be short range, we do not specify the radius a beyond which $V(r)=0$. Hence, we expect that the FSR given in the article should be valid for a very general potential as long as the potential decreases rapidly enough when $r\to\infty$.

E. The control of the change of the total number of states

Since a specified number of bound states in a quantum dot can be realized in the present-day nanotechniques, it seems to us that we can control the number of states around an impurity. This is due to the fact that quantum dots can be carved out of a 2DEG[20] such that the change of the

number of states around them can be counted according to (41). The fact may be very useful in controlling a spin bus (a controllable coupler of many qubits) via Friedel oscillation of spin systems.[20]

V. CONCLUSIONS

In this paper, the 2D Friedel sum rule is generalized to the relativistic spin-$\frac{1}{2}$ systems. The change in energy of the spin-$\frac{1}{2}$ system due to the presence of an impurity is studied. The relation of the rule with the 2D relativistic Levinson theorem is presented. Density oscillation is discussed. Since in 2D semimetals the low energy effective theory for conduction electrons is described by the Dirac's relativistic theory,[9,12–14] we hope that the result is helpful in studying the effects of impurities in the corresponding structures.

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APPENDIX

Here we establish the relation between the Friedel sum rule and Levinson theorem for nonrelativistic particles in 2D systems. Consider the 2D Schrödinger equation in the presence of a central potential $V(r)$

$$\hat{H}\Psi = -\frac{\hbar^2}{2\mu}\nabla^2\Psi + V(r)\Psi = E\Psi. \tag{A1}$$

The solution of (A1) may be expanded as

$$\Psi(r,\varphi) = \sum_{m=-\infty}^{\infty} a_m R_{|m|}(r) e^{im\varphi}, \tag{A2}$$

where $R_m(r)$ satisfies the radial equation,

$$\frac{\partial^2}{\partial r^2}R_m + \frac{1}{r}\frac{\partial}{\partial r}R_m + \left(k^2 - \frac{2\mu V}{\hbar^2} - \frac{m^2}{r^2}\right)R_m = 0, \quad m = 0,1,2,\ldots, \tag{A3}$$

with $k=\sqrt{2\mu E/\hbar^2}$ (we preserve $\hbar$ here for the general convention in nonrelativistic quantum mechanics). Here we need the partial derivative, since R_m is also a function of k. For a short range potential $V(r)=0$ when $r \geqslant a$, the independent scattering solution is given by

$$R_m(kr) = AJ_m(kr) + BN_m(kr). \tag{A4}$$

Using the definition of the phase shifts $B/A=-\tan\delta_m(k)$, one can find the asymptotic representation,

$$R_m(kr) \to \sqrt{\frac{2}{\pi r}}\cos\left(kr - \frac{m\pi}{2} - \frac{\pi}{4} + \delta_m(k)\right), \tag{A5}$$

where the normalization constant is chosen as the function for the free particle normalized to $\delta(k-k')$. For simplicity in deriving the FSR, one defines $R_m=\chi_m/\sqrt{r}$ such that Eq. (A3) reduces to

$$\frac{\partial^2}{\partial r^2}\chi_m - \frac{m^2-1/4}{r^2}\chi_m + \left(k^2 - \frac{2\mu V}{\hbar^2}\right)\chi_m = 0. \tag{A6}$$

The total change of the number of states ΔN around the potential $V(r)$ is obtained by integrating $(|\Psi|^2-|\Psi^{(0)}|^2)$ from 0 to R and up to the Fermi wave vector k_f, which yields

$$\Delta N = \lim_{R\to\infty} \sum_{m=-\infty}^{\infty} \int_0^{k_f} dk \int_0^R dr[|\chi_m(r)|^2 - |\chi_m^{(0)}(r)|^2], \tag{A7}$$

where $\chi_m^{(0)}(r)$ denotes the state of a free particle with a definite angular momentum channel m and we have taken $a_m=1$ since we are only interested in the difference of states its complex nature is of no interest. The integration on r can be evaluated by the following procedures. By multiplying (A6) through by χ_m^* and the corresponding equation for χ_m^* by χ_m, it follows that

$$\frac{\partial}{\partial r}\left(\chi_m^*(k',r)\frac{\partial}{\partial r}\chi_m(k,r) - \chi_m(k,r)\frac{\partial}{\partial x}\chi_m^*(k',r)\right) = (k'^2 - k^2)\chi_m^*(k',r)\chi_m(k,r), \tag{A8}$$

where the dependence of χ_m on the variables k,r is expressed explicitly. By taking the limit $k' \to k$, it can be shown that

$$|\chi_m(r)|^2 = \frac{1}{2k}\frac{\partial}{\partial r}\left(\frac{\partial\chi_m}{\partial r}\frac{\partial\chi_m^*}{\partial k} - \chi_m\frac{\partial^2\chi_m^*}{\partial r\,\partial k}\right). \tag{A9}$$

Thus, for large r, making use of Eq. (A5) and the boundary condition $\chi_m^{(0)}(k,0)=0$, $\chi_m(k,0)=0$, since the wave function should be finite at $r=0$; one finds

$$\begin{aligned}
&\sum_{m=-\infty}^{\infty}\int_0^R dr[|\chi_m(r)|^2 - |\chi_m^{(0)}(r)|^2] \\
&\quad= \frac{1}{\pi}\sum_{m=-\infty}^{\infty}\left[\frac{d\delta_m}{dk} + \frac{1}{2k}\sin\left(2kR - m\pi - \frac{\pi}{2} + 2\delta_m\right) - \sin\left(2kR - m\pi - \frac{\pi}{2}\right)\right] \\
&\quad= \frac{1}{\pi}\sum_{m=-\infty}^{\infty}\left(\frac{d\delta_m}{dk} + \frac{(-1)^m}{\pi k}\sin^2\delta_m\cos(2kR) + \frac{(-1)^m}{2}\sin(2\delta_m)\frac{\sin(2kR)}{\pi k}\right).
\end{aligned} \tag{A10}$$

Since $\lim_{R\to\infty}\sin(2kR)/\pi k = \delta(k)$ and $\lim_{R\to\infty}\cos(2kR)$ oscillates, the integration over k in (A7) can be carried out, which yields the 2D Friedel sum rule,

$$\Delta N = \frac{2}{\pi}\sum_{m=-\infty}^{\infty}[\delta_m(E_f) - \delta_m(0)], \tag{A11}$$

where the factor of 2 is spin degeneracy and we have used the fact that $\delta_m(0)/\pi$ always takes integers in 2D space, such that the integration in the second term in (A10)

$$\lim_{R\to\infty}\int_0^{k_f} dk\frac{1}{k}\sin^2\delta_m\cos(2kR) \to 0. \tag{A12}$$

The interesting relation between the number of bound states (LT) and the change in the scattering states ΔN (FSR) can be established by the completeness relationship

$$\sum_{m=-\infty}^{\infty}\sum_{i=1}^{N_m}\psi_{m,E_i}^*(r)\psi_{m,E_i}(r') + \sum_{m=-\infty}^{\infty}\int_0^{k_f} dk\,\chi_m^*(k,r)\chi_m(k,r') = \delta(r-r'). \tag{A13}$$

Here N_m and $\psi_{m,E_i}(r)$ are the bound-state number and eigenfunction for a definite angular momentum channel. Subtracting the relation from the free particles solutions $\chi_m^{(0)}(k,r)$, setting $r=r'$ and integrating from 0 to R, we obtain the equality

$$N = \sum_{m=-\infty}^{\infty} N_m = -\Delta N, \tag{A14}$$

which implies the total number of the bound states

$$N = \frac{2}{\pi} \sum_{m=-\infty}^{\infty} [\delta_m(0) - \delta_m(E_f)], \tag{A15}$$

with

$$N_m = \delta_m(0) - \delta_m(E_f). \tag{A16}$$

This is the Levinson theorem for nonrelativistic particles in 2D many-body systems. Different from the single particle case, the phase shifts at Fermi energy play an important role.

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The Cauchy problem for the wave equation in the Schwarzschild geometry

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The Cauchy problem is considered for the scalar wave equation in the Schwarzschild geometry. We derive an integral spectral representation for the solution and prove pointwise decay in time. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Recently pointwise decay was proven for solutions of the scalar wave equation in the Kerr geometry.[1,2] The main difficulties in this proof are due to the fact that the metric is only axisymmetric. In particular, the classical energy density may be negative inside the *ergosphere*, a region outside the event horizon in which the Killing vector corresponding to time translations becomes spacelike. This makes it necessary to apply special methods (spectral theory in Pontrjagin spaces, energy splitting estimates, causality arguments) which are technically demanding and not easily accessible. Therefore, it seems worthwile working out the special case of spherical symmetry (Schwarzschild geometry) separately. This is precisely the purpose of the present paper, where we derive an integral representation for the solution of the Cauchy problem and prove pointwise decay for the scalar wave equation in the Schwarzschild geometry. In this case, the classical energy density is positive everywhere outside the event horizon. This gives rise to a positive definite scalar product, making it possible to apply Hilbert space methods.

Recall that in Schwarzschild coordinates (t,r,ϑ,φ), the Schwarzschild metric takes the form

$$\mathrm{d}s^2 = g_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j = \left(1-\frac{2M}{r}\right)\mathrm{d}t^2 - \left(1-\frac{2M}{r}\right)^{-1}\mathrm{d}r^2 - r^2(\mathrm{d}\vartheta^2+\sin^2\vartheta\,\mathrm{d}\varphi^2) \tag{1.1}$$

with $r>0$, $0\leqslant\vartheta\leqslant\pi$, $0\leqslant\varphi<2\pi$. We often use for the angular variables the short notation $x\in S^2$. Obviously, the metric has two singularities at $r=0$ and $r=2M$. The latter is called the *event horizon* and can be resolved by a simple coordinate transformation. In the following we consider only the region $r>2M$ outside the event horizon. The scalar wave equation in the Schwarzschild geometry is given by

$$\Box\phi := g^{ij}\nabla_i\nabla_j\phi = \frac{1}{\sqrt{-g}}\frac{\partial}{\partial x^i}\left(\sqrt{-g}\,g^{ij}\frac{\partial}{\partial x^j}\right)\phi = 0, \tag{1.2}$$

where g denotes the determinant of the metric g_{ij}. We now state our main result.

Theorem 1.1: *Consider the Cauchy problem of the scalar wave equation in the Schwarzschild geometry*

$$\Box\phi = 0, \quad (\phi, i\partial_t\phi)(0,r,x) = \Phi_0(r,x)$$

for smooth initial data $\Phi_0\in C_0^\infty((2M,\infty)\times S^2)^2$ *which is compactly supported outside the event horizon. Then there exists a unique global solution* $\Phi(t)=(\phi(t),i\partial_t\phi(t))\in C^\infty(\mathbb{R}\times(2M,\infty)\times S^2)^2$

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which is compactly supported for all times t. Moreover, for fixed (r,x) *this solution decays as* $t\to\infty$.

There has been considerable work on the wave equation in the Schwarzschild geometry. In 1957, Regge and Wheeler[3] investigated the linear stability of this geometry. Kay and Wald[4] proved boundedness for solutions of the Klein-Gordon equation in this space-time outside and on the event horizon. By heuristic arguments, Price[5] got evidence for polynomial decay of solutions of the scalar wave equation. More recently, Dafermos and Rodnianski[6] gave a mathematical proof for this decay for spherical symmetric initial data. For general initial data they derived decay rates,[7] which are however not sharp. Furthermore, Morawetz and Strichartz type estimates for a massless scalar field without charge in a Reissner Nordstrøm background with naked singularity are developed in Ref. 8. And in Ref. 9 a Morawetz-type inequality was proven for the semilinear wave equation in Schwarzschild.

The paper is organized as follows: First, we introduce the Regge-Wheeler variable and rewrite the wave equation as a first-order Hamiltonian system. The resulting Hamiltonian is a symmetric operator with respect to the scalar product arising from the conserved energy. Exploiting the spherical symmetry of the problem, we may consider the problem for fixed angular modes l and m. We then show that the corresponding Hamiltonian is essentially self-adjoint. More precisely, our goal is to apply Stone's formula, which relates the propagator to an integral over the resolvent. Thus in Sec. IV we give an explicit construction for the resolvent. This construction is based on special solutions of the radial equation, which decay exponentially at $\pm\infty$. In Sec. V we prove the existence of these solutions via the formalism of the Jost equation. Moreover, we obtain appropriate regularity results for these solutions, which lead to an integral representation of the solution operators of the Cauchy problem for fixed l and m. According to the theory of symmetric hyperbolic systems, the Cauchy problem has a unique smooth solution. Thus, summing over the angular modes yields the desired representation of this solution. Combining this representation with a Sobolev imbedding argument, we obtain pointwise decay in time.

II. PRELIMINARIES

In this section we reformulate the wave equation as a first order Hamiltonian system. This will make it possible to analyze the dynamics of the waves with Hilbert space methods.

According to (1.1) and (1.2) the scalar wave equation in the Schwarzschild geometry with respect to Schwarzschild coordinates has the explicit form

$$\left[\frac{\partial^2}{\partial t^2}-\left(1-\frac{2M}{r}\right)\frac{1}{r^2}\left(\frac{\partial}{\partial r}(r^2-2Mr)\frac{\partial}{\partial r}+\Delta_{S^2}\right)\right]\phi=0. \tag{2.1}$$

Here Δ_{S^2} denotes the standard Laplacian on the two sphere, which in the coordinates (ϑ,φ) is given by

$$\Delta_{S^2}=\frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial}{\partial(\cos\vartheta)}\sin^2\vartheta\frac{\partial}{\partial(\cos\vartheta)}. \tag{2.2}$$

In order to bring the equation (2.1) into a more convenient form, we first introduce the Regge-Wheeler coordinate u by

$$u(r):=r+2M\log\left(\frac{r}{2M}-1\right). \tag{2.3}$$

The variable u takes values in the whole interval $(-\infty,\infty)$ as r ranges over $(2M,\infty)$. It satisfies the relations

$$\frac{\mathrm{d}u}{\mathrm{d}r} = \frac{1}{1-\frac{2M}{r}}, \quad \frac{\partial}{\partial u} = \left(1-\frac{2M}{r}\right)\frac{\partial}{\partial r}. \tag{2.4}$$

In what follows the variable r is always implicitly given by u. Using the Regge-Wheeler coordinate, the wave equation (2.1) transforms to

$$\left[\frac{\partial^2}{\partial t^2} - \frac{1}{r}\frac{\partial^2}{\partial u^2}r + \left(1-\frac{2M}{r}\right)\left(\frac{2M}{r^3} - \frac{\Delta_{S^2}}{r^2}\right)\right]\phi = 0. \tag{2.5}$$

To simplify this equation we multiply by r and substitute $\psi = r\phi$. This leads us to the Cauchy problem

$$\left[\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial u^2} + \left(1-\frac{2M}{r}\right)\left(\frac{2M}{r^3} - \frac{\Delta_{S^2}}{r^2}\right)\right]\psi(t,u,x) = 0,$$

$$(\psi, i\partial_t\psi)(0,u,x) = \Psi_0(u,x), \tag{2.6}$$

where the initial data $\Psi_0 \in C_0^\infty(\mathbb{R}\times S^2)^2$ is smooth and compactly supported.

The equation in (2.6) can be reformulated as the Euler-Lagrange equation corresponding to the action

$$S = \int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}u\int_{-1}^{1}d(\cos\vartheta)\int_0^{2\pi}\mathrm{d}\varphi\,\mathcal{L}(\psi,\nabla\psi), \tag{2.7}$$

where the Lagrangian is given by

$$2\mathcal{L} = |\partial_t\psi|^2 - |\partial_u\psi|^2 - \left(1-\frac{2M}{r}\right)\frac{2M}{r^3}|\psi|^2 - \left(1-\frac{2M}{r}\right)\frac{1}{r^2}\left(\frac{1}{\sin^2\vartheta}|\partial_\varphi\psi|^2 + \sin^2\vartheta|\partial_{\cos\vartheta}\psi|^2\right). \tag{2.8}$$

As one sees immediately, the Lagrangian is invariant under time translations, and thus Noether's theorem gives rise to a conserved quantity, the energy E,

$$E[\psi] = \int_{-\infty}^{\infty}\mathrm{d}u\int_{-1}^{1}d(\cos\vartheta)\int_0^{2\pi}\frac{\mathrm{d}\varphi}{\pi}\mathcal{E}, \tag{2.9}$$

where $\mathcal{E}$ is the energy density

$$2\mathcal{E} = 2\left(\frac{\partial\mathcal{L}}{\partial\psi_t}\psi_t - \mathcal{L}\right) = |\partial_t\psi|^2 + |\partial_u\psi|^2 + \left(1-\frac{2M}{r}\right)\left\{\frac{2M}{r^3}|\psi|^2 + \frac{1}{r^2}\left(\frac{1}{\sin^2\vartheta}|\partial_\varphi\psi|^2 + \sin^2\vartheta|\partial_{\cos\vartheta}\psi|^2\right)\right\}. \tag{2.10}$$

It is also easy to check directly that the above energy is conserved in time for all smooth solutions of the wave equation that are compactly supported for all times. Since we consider the wave equation outside the event horizon, i.e., $r>2M$, it is clear that the energy density is positive everywhere.

Next we rewrite the Cauchy problem (2.6) in first-order Hamiltonian form. Letting

$$\Psi = \begin{pmatrix}\psi\\ i\partial_t\psi\end{pmatrix}, \tag{2.11}$$

the Cauchy problem takes the form

$$i\partial_t \Psi = H\Psi, \qquad \Psi|_{t=0} = \Psi_0, \tag{2.12}$$

where H is the Hamiltonian

$$\begin{pmatrix} 0 & 1 \\ A & 0 \end{pmatrix}. \tag{2.13}$$

Here A is the differential operator

$$A = -\partial_u^2 + \left(1 - \frac{2M}{r}\right)\left(\frac{2M}{r^3} - \frac{1}{r^2}\Delta_{S^2}\right). \tag{2.14}$$

We use the energy E in order to introduce a scalar product such that the Hamiltonian H is symmetric with respect to it. More precisely, we endow the space $C_0^\infty(\mathbb{R}\times S^2)^2$ with the *energy scalar product* $\langle .,. \rangle$ by polarizing E, thus

$$\begin{aligned}\langle \Psi, \Phi \rangle := \int_{-\infty}^{\infty} \mathrm{d}u \int_{-1}^{1} d(\cos\vartheta) \int_0^{2\pi} \frac{\mathrm{d}\varphi}{2\pi} \Bigg\{ &\overline{\partial_t \psi} \partial_t \phi + \overline{\partial_u \psi} \partial_u \phi + \left(1 - \frac{2M}{r}\right) \\ &\times \left[\frac{2M}{r^3} \overline{\psi} \phi + \frac{1}{r^2} \left(\frac{1}{\sin^2\vartheta} \overline{\partial_\varphi \psi} \partial_\varphi \phi + \sin^2\vartheta \, \overline{\partial_{\cos\vartheta} \psi} \partial_{\cos\vartheta} \phi \right) \right] \Bigg\},\end{aligned} \tag{2.15}$$

where again $\Psi = (\psi, i\partial_t \psi)^T$ and $\Phi = (\phi, i\partial_t \phi)^T$. Energy conservation implies that for a solution Ψ of the Cauchy problem (2.12) which is compactly supported for all times,

$$0 = \frac{d}{\mathrm{d}t} E[\Psi] = \frac{d}{\mathrm{d}t} \langle \Psi, \Psi \rangle = \langle \dot{\Psi}, \Psi \rangle + \langle \Psi, \dot{\Psi} \rangle = i\langle H\Psi, \Psi \rangle - i\langle \Psi, H\Psi \rangle.$$

Since the initial data $\Psi_0 \in C_0^\infty(\mathbb{R}\times S^2)^2$ can be chosen arbitrarily, polarization yields

$$\langle H\Psi, \Phi \rangle = \langle \Psi, H\Phi \rangle, \quad \text{for all } \Psi, \Phi \in C_0^\infty(\mathbb{R}\times S^2)^2. \tag{2.16}$$

Hence the operator H is symmetric on $C_0^\infty(\mathbb{R}\times S^2)^2$ with respect to $\langle .,. \rangle$.

We will now use the spherical symmetry to simplify the problem. More precisely, we make use of the fact that the angular dependence of the wave equation in the Schwarzschild geometry involves only the Laplacian on the two sphere. It is well known that the spherical harmonics $\{Y_{lm}(\vartheta, \varphi)\}_{l\in\mathbb{N}_0, |m|\leqslant l}$ are smooth eigenfunctions of Δ_{S^2} with the eigenvalues $-l(l+1)$. Moreover, they form an orthonormal basis of the space $L^2(S^2)$. Thus we can decompose an arbitrary $\Psi \equiv (\psi_1, \psi_2)^T \in C_0^\infty(\mathbb{R}\times S^2)^2$ in the following way:

$$\Psi(u, \vartheta, \varphi) = \sum_{l=0}^{\infty} \sum_{|m|\leqslant l} \Psi^{lm}(u) Y_{lm}(\vartheta, \varphi), \tag{2.17}$$

where for each component the sum converges for fixed u in $L^2(S^2)$. Since the $\Psi^{lm} \equiv (\psi_1^{lm}, \psi_2^{lm})^T$ are uniquely determined by $\psi_i^{lm}(u) = \langle Y_{lm}, \psi_i(u) \rangle_{L^2(S^2)}$ it is clear that $\Psi^{lm}(u) \in C_0^\infty(\mathbb{R})^2$ for all l, m. Using this decomposition, we rewrite the norm of Ψ corresponding to the energy scalar product as

$$\begin{aligned}\langle \Psi, \Psi \rangle &= \int_{-\infty}^{\infty} \mathrm{d}u \int_{-1}^{1} d(\cos\vartheta) \int_0^{2\pi} \frac{\mathrm{d}\varphi}{2\pi} \left\{ |\psi_2|^2 + |\partial_u \psi_1|^2 + \overline{\psi_1} \left(1 - \frac{2M}{r}\right)\left(\frac{2M}{r^3} - \frac{1}{r^2}\Delta_{S^2}\right)\psi_1 \right\} \\ &= \sum_{l=0}^{\infty} \sum_{|m|\leqslant l} \int_{-\infty}^{\infty} \mathrm{d}u \left\{ |\psi_2^{lm}(u)|^2 + |\partial_u \psi_1^{lm}(u)|^2 + \left(1 - \frac{2M}{r}\right)\left(\frac{2M}{r^3} + \frac{l(l+1)}{r^2}\right)|\psi_1^{lm}(u)|^2 \right\},\end{aligned} \tag{2.18}$$

where in the first equation we have integrated by parts with respect to (ϑ, φ). The second equation follows from the properties of the Y_{lm}. As one can immediately see, the integrand for every

summand in (2.18) is positive. Hence again by polarizing we obtain for any angular mode l a scalar product $\langle .,. \rangle_l$ on $C_0^\infty(\mathbb{R})^2$ given by

$$\langle \Psi, \Phi \rangle_l = \int_{-\infty}^{\infty} \{\overline{\psi_2}\phi_2 + \overline{\psi_1'}\phi_1' + V_l \overline{\psi_1}\phi_1\} \mathrm{d}u, \tag{2.19}$$

with the potential $V_l(u)$ defined as

$$V_l(u) = \left(1 - \frac{2M}{r}\right)\left(\frac{2M}{r^3} + \frac{l(l+1)}{r^2}\right). \tag{2.20}$$

This definition leads to an isometry

$$(C_0^\infty(\mathbb{R} \times S^2)^2, \langle .,. \rangle) \to \overset{\infty}{\underset{l=0}{\oplus}} \underset{|m|\leqslant l}{\oplus} (C_0^\infty(\mathbb{R})^2, \langle .,. \rangle_l),$$

$$\Psi \mapsto \Psi^{lm}. \tag{2.21}$$

Using (2.17), the Hamiltonian H also decomposes in the following way:

$$H\Psi(u, \vartheta, \varphi) = \sum_{l=0}^{\infty} \sum_{|m|\leqslant l} H_l \Psi^{lm}(u) Y_{lm}(\vartheta, \varphi).$$

Here the H_l act on $C_0^\infty(\mathbb{R})^2$ and are given by

$$H_l = \begin{pmatrix} 0 & 1 \\ -\partial_u^2 + V_l(u) & 0 \end{pmatrix}. \tag{2.22}$$

Thus for fixed angular modes l and m the Cauchy problem (2.12) simplifies to

$$i\partial_t \Psi^{lm} = H_l \Psi^{lm}, \qquad \Psi^{lm}\big|_{t=0} = \Psi_0^{lm}, \tag{2.23}$$

where the initial data is in $C_0^\infty(\mathbb{R})^2$. Moreover, the H_l are symmetric on $C_0^\infty(\mathbb{R})^2$ with respect to $\langle .,. \rangle_l$, because for any $\Psi, \Phi \in C_0^\infty(\mathbb{R})^2$ the functions $\Psi(u)Y_{lm}$ and $\Phi(u)Y_{lm}$ are in $C_0^\infty(\mathbb{R} \times S^2)^2$. Thus

$$\langle H_l \Psi, \Phi \rangle_l = \langle H(\Psi Y_{lm}), \Phi Y_{lm} \rangle = \langle \Psi Y_{lm}, H(\Phi Y_{lm}) \rangle = \langle \Psi, H_l \Phi \rangle_l.$$

In particular, for solutions of (2.23) with compact support in u for all times, the norm with respect to $\langle .,. \rangle_l$ is constant. Therefore we again refer to $\langle .,. \rangle_l$ as the energy scalar product.

Our strategy is to solve for a given inital data $\Psi_0 \in C_0^\infty(\mathbb{R} \times S^2)^2$ the Cauchy problem (2.23) for fixed angular modes l and m, and to sum up the solutions afterwards. Therefore, in what follows we will fix the angular modes l, m and consider the problem (2.23). In order to avoid too many indices, we usually omit the subscript l in the Hamiltonian and energy scalar product.

III. SPECTRAL PROPERTIES OF THE HAMILTONIAN

In the preceding section we introduced the energy scalar product $\langle , \rangle$ on the space $C_0^\infty(\mathbb{R})^2$. Since we cannot expect $C_0^\infty(\mathbb{R})^2$ to be complete with respect to this inner product (and indeed it is not, because the energy scalar product in the second component is just the usual L^2-scalar product), we define the Hilbert space $H^1_{V_l 0}(\mathbb{R})$ as the completion of $C_0^\infty(\mathbb{R})$ within the Hilbert space

$$H^1_{V_l}(\mathbb{R}) = \{u \text{ with } u' \in L^2(\mathbb{R}) \text{ and } V_l^{1/2} u \in L^2(\mathbb{R})\}$$

endowed with the scalar product

$$\langle u,v\rangle_1 := (u',v')_{L^2} + (V_l u, v)_{L^2}.$$

Note that this coincides with the energy scalar product on the first component. Therefore, we choose $\mathcal{H} \equiv H^1_{V_l 0}(\mathbb{R}) \oplus L^2(\mathbb{R})$ endowed with the energy scalar product as the underlying Hilbert space for our Hamiltonian H.

In the preceding section we have seen that the Hamiltonian H is symmetric on $C_0^\infty(\mathbb{R})^2$. Before we can use functional analytic methods, we need to construct a self-adjoint extension of H. In fact, we are able to prove the following lemma.

Lemma 3.1: The operator H with domain $\mathcal{D}(H)=C_0^\infty(\mathbb{R})^2$ is essentially self-adjoint in the Hilbert space $\mathcal{H}$.

In order to prove this lemma, we use the following version of Stone's theorem about strongly continuous one-parameter unitary groups. A proof of this theorem can be found in Ref. 10, Sec. VIII.4. (Also see Ref. 11).

Theorem 3.2: *Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then there is a self-adjoint operator A on $\mathcal{H}$ such that $U(t)=e^{itA}$.*

Furthermore, let D be a dense domain which is invariant under $U(t)$ and on which $U(t)$ is strongly differentiable. Then i^{-1} times the strong derivative of $U(t)$ is essentially self-adjoint on D, and its closure is A.

Now we apply this theorem.

Proof of Lemma 3.1: According to the theory of symmetric hyperbolic systems (cf. Ref. 12, Sec. 5.3) the Cauchy problem

$$(\partial_t^2 - \partial_u^2 + V_l(u))\psi(t,u) = 0,$$

$$\psi|_{t=0} = f, \quad i\partial_t\psi|_{t=0} = g$$

with smooth, compactly supported initial data $f,g \in C_0^\infty(\mathbb{R})$ has a unique solution $\psi(t,u) \in C^\infty(\mathbb{R}\times\mathbb{R})$ which is also compactly supported in u for all times. Using this solution, we define for arbitrary $t \in \mathbb{R}$ the operators

$$U(t): C_0^\infty(\mathbb{R})^2 \to C_0^\infty(\mathbb{R})^2,$$

$$\begin{pmatrix} f \\ g \end{pmatrix} \mapsto \begin{pmatrix} \psi(t,.) \\ i\partial_t\psi(t,.) \end{pmatrix},$$

which leave the dense subspace $C_0^\infty(\mathbb{R})^2 \subseteq \mathcal{H}$ invariant for all times t.

Due to the energy conservation, the $U(t)$ are unitary with respect to the energy scalar product and hence extend to unitary operators on the entire Hilbert space $\mathcal{H}$. Furthermore, since the solution is uniquely determined by the initial data, the $U(t)$ have the following properties:

$$U(0) = Id, \quad U(t+s) = U(t)U(s) \quad \text{for all } t,s \in \mathbb{R},$$

and thus they form a one-parameter unitary group. Due to the fact that smooth initial data yields smooth solutions in t and u, this group is strongly continuous on $\mathcal{H}$ and strongly differentiable on the domain $C_0^\infty(\mathbb{R})^2$. Calculating i^{-1} times the strong derivative one gets

$$i^{-1}\lim_{h\searrow 0}\frac{1}{h}\left(U(h)\begin{pmatrix} f \\ g \end{pmatrix} - \begin{pmatrix} f \\ g \end{pmatrix}\right) = i^{-1}\begin{pmatrix} -ig \\ i(\partial_u^2 - V_l)f \end{pmatrix} = -H\begin{pmatrix} f \\ g \end{pmatrix}$$

for all $f,g \in C_0^\infty(\mathbb{R})$, and the lemma follows from Theorem 3.2.

□

For the further investigations of the Hamiltonian H, we consider its self-adjoint closure which, for the sake of simplicity, we again denote by H. For our purposes, it is not important to know the exact domain of definition $\mathcal{D}(H)$ of the self-adjoint extension.

IV. CONSTRUCTION OF THE RESOLVENT

Stone's formula for the spectral projections of a self-adjoint operator A (cf. Ref. 10 Theorem VII.13),

$$\frac{1}{2}[P_{[a,b]}+P_{(a,b)}]=\text{s-}\lim_{\epsilon\searrow 0}\frac{1}{2\pi i}\int_a^b[(A-\omega-i\epsilon)^{-1}-(A-\omega+i\epsilon)^{-1}]\mathrm{d}\omega, \tag{4.1}$$

relates the spectral projections to the resolvent (here s-lim denotes the strong limit of operators). In view of this relation, it is of interest to derive an explicit representation of the resolvent.

In the preceding section we have seen that there is a domain $\mathcal{D}(H)$ such that our Hamiltonian H is self-adjoint in the Hilbert space $(\mathcal{H},\langle,\rangle)$. From this it immediately follows that the spectrum $\sigma(H)\subseteq\mathbb{R}$ is on the real line and therefore the resolvent $(H-\omega)^{-1}:\mathcal{H}\to\mathcal{H}$ exists for every $\omega\in\mathbb{C}\backslash\mathbb{R}$.

Let us now fix $\omega\in\mathbb{C}\backslash\mathbb{R}$. We often denote the ω-dependence by a subscript ω. We begin by reducing the eigenvalue equation $H\Psi=\omega\Psi$ by substituting the equation for the first component in the second equation. We thus obtain the Schrödinger-type equation

$$(-\partial_u^2+V_\omega(u))\phi(u)=0 \tag{4.2}$$

with the potential

$$V_\omega(u)=-\omega^2+V_l(u)=-\omega^2+\left(1-\frac{2M}{r}\right)\left(\frac{2M}{r^3}+\frac{l(l+1)}{r^2}\right). \tag{4.3}$$

In what follows we refer to this equation simply as the Schrödinger equation. It can be regarded as the radial equation associated to the wave equation in (2.6). Our goal is to construct the resolvent $(H-\omega)^{-1}$ out of special solutions of this equation. We introduce fundamental solutions $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$ of the Schrödinger equation (4.2) which satisfy asymptotic boundary conditions at $u=\pm\infty$ (the existence of these solutions will be proved in Sec. V). More precisely, in the case $\mathrm{Im}(\omega)>0$ we impose that

$$\lim_{u\to-\infty}e^{i\omega u}\acute{\phi}_\omega(u)=1,\quad \lim_{u\to-\infty}(e^{i\omega u}\acute{\phi}_\omega(u))'=0, \tag{4.4}$$

$$\lim_{u\to+\infty}e^{-i\omega u}\grave{\phi}_\omega(u)=1,\quad \lim_{u\to+\infty}(e^{-i\omega u}\grave{\phi}_\omega(u))'=0, \tag{4.5}$$

whereas in the case $\mathrm{Im}(\omega)<0$,

$$\lim_{u\to-\infty}e^{-i\omega u}\acute{\phi}_\omega(u)=1,\quad \lim_{u\to-\infty}(e^{-i\omega u}\acute{\phi}_\omega(u))'=0, \tag{4.6}$$

$$\lim_{u\to+\infty}e^{i\omega u}\grave{\phi}_\omega(u)=1,\quad \lim_{u\to+\infty}(e^{i\omega u}\grave{\phi}_\omega(u))'=0. \tag{4.7}$$

Since the resolvent exists, the map $(H-\omega):\mathcal{D}(H)\to\mathcal{H}$ is bijective and in particular the kernel is trivial. Hence the solutions $\acute{\phi}_\omega$, $\grave{\phi}_\omega$ are linearly independent (otherwise they would give rise to a vector in the kernel due to the exponential decay). Thus $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$ are indeed a system of fundamental solutions with nonvanishing Wronskian

$$w(\acute{\phi}_\omega,\grave{\phi}_\omega):=\acute{\phi}_\omega(u)\grave{\phi}_\omega'(u)-\acute{\phi}_\omega'(u)\grave{\phi}_\omega(u). \tag{4.8}$$

Note that the Wronskian is independent of the variable u, as is easily verified by differentiating with respect to u and substituting the Schrödinger equation.

In the next lemma, we use this fundamental system to derive the Green's function corresponding to (4.2).

Lemma 4.1: The function

$$s_\omega(u,v) := -\frac{1}{w(\acute{\phi}_\omega,\grave{\phi}_\omega)} \times \begin{cases} \acute{\phi}_\omega(u)\grave{\phi}_\omega(v), & \text{if } u \leqslant v, \\ \acute{\phi}_\omega(v)\grave{\phi}_\omega(u), & \text{if } u > v, \end{cases} \tag{4.9}$$

satisfies the distributional equations

$$\left(-\frac{\partial^2}{\partial u^2} + V_\omega(u)\right) s_\omega(u,v) = \delta(u-v) = \left(-\frac{\partial^2}{\partial v^2} + V_\omega(v)\right) s_\omega(u,v).$$

Proof: By definition of the distributional derivative we have for every test function $\eta \in C_0^\infty(\mathbb{R})$,

$$\int_{-\infty}^{\infty} \eta(u)[-\partial_u^2 + V_\omega(u)] s_\omega(u,v)\mathrm{d}u = \int_{-\infty}^{\infty} [(-\partial_u^2 + V_\omega(u))\,\eta(u)] s(u,v)\mathrm{d}u.$$

It is obvious from its definition that the function $s(.,v)$ is smooth except at the point $u=v$, where its first derivative has a discontinuity. Thus, after splitting up the integral, we can integrate by parts twice to obtain

$$\begin{aligned} \int_{-\infty}^{\infty} [(-\partial_u^2 + V_\omega(u))\,\eta(u)] s(u,v)\mathrm{d}u &= \int_{-\infty}^{v} \eta(u)(-\partial_u^2 + V_\omega(u)) s(u,v)\mathrm{d}u + \lim_{u \nearrow v}[\eta(u)\partial_u s(u,v)] \\ &\quad + \int_{v}^{\infty} \eta(u)(-\partial_u^2 + V_\omega(u)) s(u,v)\mathrm{d}u - \lim_{u \searrow v}[\eta(u)\partial_u s(u,v)]. \end{aligned}$$

Since for $u \neq v$, s is a solution of (4.2), the obtained integrals vanish. Computing the limits with the definition (4.9), we get

$$\begin{aligned} \int_{-\infty}^{\infty} [(-\partial_u^2 + V_\omega(u))\,\eta(u)] s(u,v)\mathrm{d}u &= (\lim_{u \nearrow v} - \lim_{u \searrow v})\,\eta(u)\partial_u s(u,v) \\ &= -\frac{1}{w(\acute{\phi}_\omega,\grave{\phi}_\omega)}\,\eta(v)[\acute{\phi}'_\omega(v)\grave{\phi}_\omega(v) - \grave{\phi}'_\omega(v)\acute{\phi}_\omega(v)] = \eta(v), \end{aligned}$$

where in the last step we used the definition of the Wronskian (4.8). This yields the first equation. The second equation is proven exactly in the same way.

□

With this function s we are now able to construct the resolvent. More precisely,

Proposition 4.2: For every $\omega \in \mathbb{C}\backslash\mathbb{R}$, the resolvent $(H-\omega)^{-1}: \mathcal{H} \to \mathcal{H}$ can be represented as an integral operator with the integral kernel

$$k_\omega(u,v) = \delta(u-v)\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + s_\omega(u,v)\begin{pmatrix} \omega & 1 \\ \omega^2 & \omega \end{pmatrix}. \tag{4.10}$$

Proof: We introduce the integral operator S_ω with the integral kernel $k_\omega(u,v)$ on the domain

$$\mathcal{D}(S_\omega) := \{(H-\omega)\Psi \,|\, \Psi \in C_0^\infty(\mathbb{R})^2\}.$$

Let us verify that $\mathcal{D}(S_\omega)$ is a dense subset of $\mathcal{H}$. Let $\phi \in \mathcal{H}$ be an arbitrary vector. Because of the existence of the resolvent, the operator $H-\omega: \mathcal{D}(H) \to \mathcal{H}$ is onto, and thus there is a vector $\psi \in \mathcal{D}(H)$ with $(H-\omega)\psi = \phi$. Then due to the definition of the closure of H, there is a sequence $\{\psi_n\}_{n\in N} \subseteq C_0^\infty(\mathbb{R})^2$ with $\psi_n \to \psi$ and $H\psi_n \to H\psi$ as $n \to \infty$. This shows that

$\{(H-\omega)\psi_n\}_{n\in N}\subseteq\mathcal{D}(S_\omega)$ converges to $(H-\omega)\psi=\phi$. We conclude that $\mathcal{D}(S_\omega)$ is dense. We now calculate the operator product $S_\omega(H-\omega)$ on $C_0^\infty(\mathbb{R})^2$. For an arbitrary $\Psi=(\psi_1,\psi_2)^T\in C_0^\infty(\mathbb{R})^2$ we have

$$(S_\omega(H-\omega)\psi)(u)=\int_{-\infty}^{\infty}k_\omega(u,v)(H-\omega)\psi(v)\mathrm{d}v$$
$$=\begin{pmatrix}0\\-\omega\psi_1+\psi_2\end{pmatrix}(u)+\int_{-\infty}^{\infty}s_\omega(u,v)\begin{pmatrix}-\partial_v^2+V_\omega(v) & 0\\ \omega(-\partial_v^2+V_\omega(v)) & 0\end{pmatrix}\begin{pmatrix}\psi_1\\\psi_2\end{pmatrix}(v)\mathrm{d}v.$$

Hence, according to Lemma 4.1,

$$S_\omega(H-\omega)=Id\quad\text{on } C_0^\infty(\mathbb{R})^2.$$

This yields that $S_\omega=(H-\omega)^{-1}$ on the dense set $\mathcal{D}(S_\omega)$. Since $(H-\omega)^{-1}$ is a bounded operator, the claim follows.

□

As mentioned at the beginning of this section, we can now apply Stone's formula for the spectral projections of H and get for every $\Psi\in\mathcal{H}$,

$$\frac{1}{2}[P_{[a,b]}+P_{(a,b)}]\Psi=\lim_{\epsilon\searrow 0}\frac{1}{2\pi i}\int_a^b[(H-(\omega+i\epsilon))^{-1}-(H-(\omega-i\epsilon))^{-1}]\Psi\,\mathrm{d}\omega,$$

and this yields together with Proposition 4.2,

$$=\lim_{\epsilon\searrow 0}\frac{1}{2\pi i}\int_a^b\left(\int_{\mathbb{R}}(k_{\omega+i\epsilon}(.,v)-k_{\omega-i\epsilon}(.,v))\Psi(v)\mathrm{d}v\right)\mathrm{d}\omega,\tag{4.11}$$

where the limit is with respect to the norm in $\mathcal{H}$. It is therefore of special interest how the kernels $k_{\omega+i\epsilon}(u,v)$ and $k_{\omega-i\epsilon}(u,v)$ behave as $\epsilon\searrow 0$. Since these kernels are given explicitly in terms of the fundamental solutions $\acute{\phi}_{\omega\pm i\epsilon}$ and $\grave{\phi}_{\omega\pm i\epsilon}$, we will discuss their behavior in the next section.

V. THE JOST SOLUTIONS OF THE RADIAL EQUATION

In this section we want to discuss the existence and the behavior of the solutions $\acute{\phi}_\omega$, $\grave{\phi}_\omega$ of the Schrödinger equation (4.2), which in Sec. IV we used for the construction of the resolvent. We will prove the following theorem.

Theorem 5.1:

(i) *For every* $\omega\in D=\{\omega\in\mathbb{C}|\,\mathrm{Im}\,\omega\leqslant 1/4M\}$, *there exists a unique solution* $\phi_1(\omega,u)$ *of the Schrödinger equation (4.2) satisfying the boundary conditions (4.6) such that for every fixed* $u\in\mathbb{R}$ *the function* $\phi_1(\omega,u)$ *is holomorphic in* $\omega\in\mathring{D}$ *and continuous in* D.

(ii) *For every angular momentum number* l, *the solutions* $\grave{\phi}_\omega$ *of the Schrödinger equation (4.2) with boundary conditions (4.7) are well defined and uniquely determined on the set*

$$E=\{\omega\in\mathbb{C}|\mathrm{Im}\,\omega\leqslant 0,\omega\neq 0\}.$$

For each fixed $u\in\mathbb{R}$, *the function* $\grave{\phi}_\omega(u)$ *is holomorphic in* $\omega\in\mathring{E}$ *and continuous in* E. *Furthermore, in the case* $l=0$, $\grave{\phi}_\omega(u)$ *may be continuously extended to* $\omega=0$.

Once having proven this theorem, we simply set

$$\acute{\phi}_\omega(u):=\begin{cases}\overline{\phi_1(\bar{\omega},u)} & \text{if } \mathrm{Im}\,\omega>0,\\ \phi_1(\omega,u) & \text{if } \mathrm{Im}\,\omega\leqslant 0,\end{cases}\tag{5.1}$$

as well as

$$\overleftarrow{\phi}_\omega(u) := \overline{\overrightarrow{\phi}_{\bar{\omega}}(u)} \quad \text{if } \operatorname{Im}\omega > 0, \tag{5.2}$$

to obtain the solutions of Sec. IV. For $\operatorname{Im}\omega < 0$ this is clear by definition. But in the case of $\operatorname{Im}\omega > 0$ the above defined $\overrightarrow{\phi}_\omega(u)$, $\overleftarrow{\phi}_\omega(u)$ are indeed the unique solutions of the Schrödinger equation (4.2) with the desired boundary conditions (4.4) and (4.5), respectively. This follows immediately by complex conjugation of the Schrödinger equation due to the fact that our potential V_l is real.

For the proof of Theorem 5.1 we will formally manipulate the Schrödinger equation with boundary conditions (4.6) and (4.7) in order to get an appropriate integral equation (which in different contexts is called the Jost or Lipman-Schwinger equation). Then we will perform a perturbation expansion and get estimates for all the terms of the expansion. A reference for this method can be found, e.g., in Ref. 13, Sec. XI.8. Since this reference contains only an outline of the proof, it seems worth working out the details.

To introduce the method, we begin with the solutions $\phi_l(\omega, u)$. First we write the Schrödinger equation (4.2) in the form

$$\left(-\frac{d^2}{\mathrm{d}u^2} - \omega^2\right)\phi_\omega(u) = -W(u)\phi_\omega(u), \tag{5.3}$$

where W is a potential in $L^1(\mathbb{R})$ (later on, W will be replaced by V_l). Next we define for $\omega \in \mathbb{C}$ the function $G_\omega(u)$ by

$$G_\omega(u) := \begin{cases} 0 & \text{if } u \leqslant 0, \\ -\dfrac{1}{\omega}\sin(\omega u) & \text{if } u > 0 \text{ and } \omega \neq 0, \\ -u & \text{if } u > 0 \text{ and } \omega = 0. \end{cases} \tag{5.4}$$

A simple computation shows that $G_\omega(u)$ defines a *Green's function* for the operator on the left-hand side of the equation (5.3) in the sense that the distributional equation

$$\left(-\frac{d^2}{\mathrm{d}u^2} - \omega^2\right)G_\omega(u) = \delta(u)$$

holds. In order to build in the boundary condition (4.6), we make in equation (5.3) the substitution $\phi_\omega(u) = e^{i\omega u} + \tilde{\phi}_\omega(u)$ to obtain

$$\left(-\frac{d^2}{\mathrm{d}u^2} - \omega^2\right)\tilde{\phi}_\omega(u) = -W(u)\phi_\omega(u).$$

Solving this equation formally by convoluting the right-hand side with G_ω, we get the formal solution

$$\tilde{\phi}_\omega(u) = ((-W\phi_\omega) * G_\omega)(u) \equiv -\int_{-\infty}^{\infty} G_\omega(u-v)W(v)\phi_\omega(v)\mathrm{d}v.$$

Hence $\phi_\omega(u)$ satisfies the equation

$$\phi_\omega(u) = e^{i\omega u} - \int_{-\infty}^{u} G_\omega(u-v)W(v)\phi_\omega(v)\mathrm{d}v, \tag{5.5}$$

which is referred to as the *Jost equation with boundary conditions at* $-\infty$. Its significance lies in the fact that we can now easily perform a perturbation expansion in the potential W. Namely, making for ϕ_ω the ansatz as the perturbation series

$$\phi_\omega = \sum_{k=0}^{\infty} \phi_\omega^{(k)}, \tag{5.6}$$

we are led to the iteration scheme

$$\phi_\omega^{(0)}(u) = e^{i\omega u},$$

$$\cdots,$$

$$\phi_\omega^{(k+1)}(u) = -\int_{-\infty}^{u} G_\omega(u-v)W(v)\phi_\omega^{(k)}(v)\mathrm{d}v. \tag{5.7}$$

This iteration scheme can be used to construct solutions of the Jost equation.

We remark that under certain assumptions on W like continuity, the Jost equation is equivalent to the corresponding Schrödinger equation with appropriate boundary conditions. We will show this for our special case $W \equiv V_l$. A systematic method to rewrite second-order differential equations with boundary conditions as integral equations can be found, e.g., in Ref. 13. Sec. XI.8 Appendix 2.

We now state a theorem about solutions of the Jost equation. We consider more general potentials W than we have in our case, because it might be of interest by itself.

Theorem 5.2: *Suppose that W is a measurable function obeying for a given $u_0 < 0$ the condition $\int_{-\infty}^{u_0} |W(v)| \mathrm{d}v < \infty$. Define for $u \leqslant u_0$ the function $P_\omega(u)$ by*

$$P_\omega(u) = \int_{-\infty}^{u} \frac{4|v|}{1+|\omega v|} |W(v)| e^{-(\mathrm{Im}\ \omega + |\mathrm{Im}\ \omega|)v}\, \mathrm{d}v. \tag{5.8}$$

Then

(i) *For each $\omega \in E = \{\omega \in \mathbb{C} \,|\, \mathrm{Im}\ \omega \leqslant 0, \omega \neq 0\}$ the Jost equation (5.5) has a unique solution $\phi_\omega(u)$ obeying $\lim_{u\to-\infty} |e^{-i\omega u}\phi_\omega(u)| < \infty$. Moreover, $\phi_\omega(u)$ is continuously differentiable in u on $(-\infty, u_0)$ with $\lim_{u\to-\infty} e^{-i\omega u}\phi_\omega(u) = 1$ and $\lim_{u\to-\infty} e^{-i\omega u}\phi'_\omega(u) = i\omega$. For each fixed u, the functions $\phi_\omega(u)$ and $\phi'_\omega(u)$ are holomorphic in $\overset{\circ}{E}$ and continuous in E. They satisfy the bounds*

$$|\phi_\omega(u) - e^{i\omega u}| \leqslant e^{-u\ \mathrm{Im}\ \omega} |e^{P_\omega(u)} - 1|, \tag{5.9}$$

$$|\phi'_\omega(u) - i\omega e^{i\omega u}| \leqslant e^{-u\ \mathrm{Im}\ \omega} e^{P_\omega(u)} \int_{-\infty}^{u} |W(v)| \mathrm{d}v. \tag{5.10}$$

(ii) *If $\int_{-\infty}^{u_0} |v||W(v)| \mathrm{d}v < \infty$, for every $u \leqslant u_0$ the function $\phi_\omega(u)$ may be continuously extended to $\omega = 0$. Moreover, (5.9) and (5.10) hold also at $\omega = 0$.*

(iii) *If $\int_{-\infty}^{u_0} e^{-mv} |W(v)| \mathrm{d}v < \infty$, for every $u \leqslant u_0$ the function $\phi_\omega(u)$ can be extended to a holomorphic function in $\{\omega \,|\, \mathrm{Im}\ \omega < \frac{1}{2}m\}$, continuous in $\{\omega \,|\, \mathrm{Im}\ \omega \leqslant \frac{1}{2}m\}$. Moreover, in the interval $0 < \mathrm{Im}\ \omega < \frac{1}{2}m$ the inequalities (5.9) and (5.10) are replaced by*

$$|\phi_\omega(u) - e^{i\omega u}| \leqslant \frac{1}{|\omega|} e^{u\ \mathrm{Im}\ \omega} e^{P_\omega(u)} \int_{-\infty}^{u} e^{-2v\ \mathrm{Im}\ \omega} |W(v)| \mathrm{d}v, \tag{5.11}$$

$$|\phi'_\omega(u) - i\omega e^{i\omega u}| \leqslant e^{u\ \mathrm{Im}\ \omega} e^{P_\omega(u)} \int_{-\infty}^{u} e^{-2v\ \mathrm{Im}\ \omega} |W(v)| \mathrm{d}v, \tag{5.12}$$

In each case, ϕ obeys $\overline{\phi_\omega(u)} \equiv \overline{\phi(\omega, u)} = \phi(-\bar{\omega}, u)$.

We call this solution ϕ the *Jost solution*. For the proof of this theorem we need a good estimate for the Green's function G_ω.

Lemma 5.3: For all $u \in \mathbb{C}$,

$$|\sin u| \leqslant \frac{2|u|}{1+|u|} e^{|\mathrm{Im}\, u|}. \tag{5.13}$$

In particular, if $\omega \neq 0$ *and* $v \leqslant u \leqslant 0$,

$$\left| \frac{1}{\omega} \sin(\omega(u-v)) \right| \leqslant \frac{4|v|}{1+|\omega v|} e^{-v|\mathrm{Im}\, \omega| - u\, \mathrm{Im}\, \omega}. \tag{5.14}$$

Proof: In the case $|u| \geqslant 1$, the inequality (5.13) follows directly from the Euler formula $\sin u = (1/2i)(e^{iu} - e^{-iu})$ and the estimate

$$(1+|u|)|\sin u| \leqslant \tfrac{1}{2}(1+|u|) 2 e^{|\mathrm{Im}\, u|} \leqslant 2|u| e^{|\mathrm{Im}\, u|}.$$

In the remaining case $|u| < 1$, we again use the Euler formula to obtain

$$(1+|u|)|\sin u| = \frac{1}{2}(1+|u|)|e^{iu} - e^{-iu}| = \frac{1}{2}(1+|u|) \left| \int_{-1}^{1} iu e^{iu\tau}\, \mathrm{d}\tau \right|,$$

and hence

$$(1+|u|)|\sin u| \leqslant \frac{1}{2}(|u|+|u|^2) \int_{-1}^{1} |e^{iu\tau}| \mathrm{d}\tau \leqslant \frac{1}{2}(|u|+|u|^2) 2 e^{|\mathrm{Im}\, u|}.$$

Now (5.13) follows by the assumption $|u| < 1$.

In order to show (5.14) we use the identity

$$\frac{1}{\omega} \sin(\omega(u-v)) = \frac{1}{\omega} (\sin(\omega u) e^{i\omega v} - \sin(\omega v) e^{i\omega u})$$

and apply (5.13),

$$\begin{aligned} \left| \frac{1}{\omega} \sin(\omega(u-v)) \right| &\leqslant \frac{1}{|\omega|} (|\sin(\omega u) e^{i\omega v}| + |\sin(\omega v) e^{i\omega u}|) \overset{(5.13)}{\leqslant} \frac{2|u|}{1+|\omega u|} e^{|u\, \mathrm{Im}\, \omega|} e^{-v\, \mathrm{Im}\, \omega} \\ &\quad + \frac{2|v|}{1+|\omega v|} e^{|v\, \mathrm{Im}\, \omega|} e^{-u\, \mathrm{Im}\, \omega}. \end{aligned} \tag{5.15}$$

Due to the assumption $0 \geqslant u \geqslant v$, we know that $|v| \geqslant |u|$ and thus

$$\frac{2|u|}{1+|\omega u|} \leqslant \frac{2|v|}{1+|\omega v|}, \qquad -u|\mathrm{Im}\, \omega| - v\, \mathrm{Im}\, \omega \leqslant -v|\mathrm{Im}\, \omega| - u\, \mathrm{Im}\, \omega.$$

Using these inequalities in (5.15) the claim follows.

□

Note that the estimate (5.14) remains valid in the limit $0 \neq \omega \to 0$, if one replaces $(1/\omega)\sin(\omega(u-v))$ by the function $u-v$.

Now we are ready to prove Theorem 5.2.

Proof of Theorem 5.2: Using the perturbation expansion (5.6) together with the iteration scheme (5.7), one easily sees that we have already found a *formal* solution. So our goal is to show that this series is well defined and has the desired properties. To this end, we shall prove inductively that

$$|\phi_\omega^{(k)}(u)| \leqslant e^{-u \operatorname{Im}\omega} \frac{1}{k!} P_\omega(u)^k \quad \text{for all } k \in \mathbb{N}_0, \quad \text{for all } \omega, u \tag{5.16}$$

such that $P_\omega(u)$ is well defined by (5.8). Due to the integrability conditions on the potential W in the statement of the theorem this is the case for $u \leqslant u_0$ and for all $\omega \in E$ [cf. (i)], $\omega \in \bar{E}$ [cf. (ii)], $\omega \in \{\operatorname{Im}\omega \leqslant \frac{1}{2}m\}$ [cf. (iii)], respectively. Furthermore, $P_\omega(u)$ is continuous in u as well as in ω in these domains. The first statement is obvious while the latter is due to the fact that the integrand in the definition (5.8) is continuous in ω and one directly finds an integrable dominating function such that one can apply Lebegue's dominated convergence theorem.

We start the induction with the case $k=0$ for which (5.16) certainly is satisfied. Thus assume that (5.16) holds for a given k. Then, estimating the integral equation in (5.7) using (5.14) and (5.8), we obtain

$$\begin{aligned}
|\phi_\omega^{(k+1)}(u)| &\leqslant \int_{-\infty}^{u} |G_\omega(u-v)||W(v)||\phi_\omega^{(k)}(v)| \mathrm{d}v \\
&\leqslant \int_{-\infty}^{u} \frac{4|v|}{1+|\omega v|} e^{-v|\operatorname{Im}\omega| - u \operatorname{Im}\omega} |W(v)| e^{-v \operatorname{Im}\omega} \frac{1}{k!} P_\omega(v)^k \, \mathrm{d}v \\
&= e^{-u \operatorname{Im}\omega} \frac{1}{k!} \int_{-\infty}^{u} \frac{\mathrm{d}P_\omega}{\mathrm{d}v}(v) P_\omega(v)^k \, \mathrm{d}v = e^{-u \operatorname{Im}\omega} \frac{1}{(k+1)!} P_\omega(u)^{k+1},
\end{aligned}$$

where in the last step we used that $P_\omega(u)$ vanishes when u goes to $-\infty$. This concludes the proof of (5.16).

Summing over k, (5.16) yields the inequality

$$\sum_{k=0}^{\infty} |\phi_\omega^{(k)}(u)| \leqslant e^{-u \operatorname{Im}\omega} e^{P_\omega(u)}. \tag{5.17}$$

Because of the continuity of $P_\omega(u)$, the series (5.6) converges uniformly for u and ω in compact sets. Using the iteration scheme (5.7), this series can be written as

$$\sum_{k=0}^{\infty} \phi_\omega^{(k)}(u) = e^{i\omega u} - \sum_{k=1}^{\infty} \int_{-\infty}^{u} G_\omega(u-v) W(v) \phi_\omega^{(k-1)}(v) \mathrm{d}v,$$

and the bound (5.17) allows us to apply Lebesgue's dominated convergence theorem and to interchange the sum and the integral. Hence the series is indeed a solution of the Jost equation (5.5).

Next we want to show that a solution of the Jost equation is continuously differentiable with respect to u. To this end, we first compute for an arbitrary $u < u_0$ the difference quotient,

$$\frac{1}{h}(\phi_\omega(u+h) - \phi_\omega(u) - e^{i\omega(u+h)} + e^{i\omega u}) \overset{(5.5)}{=}$$

$$\int_{-\infty}^{u+h} \frac{1}{h\omega} [\sin(\omega(u+h-v)) - \sin(\omega(u-v))] W(v) \phi_\omega(v) \mathrm{d}v \tag{5.18}$$

$$+ \frac{1}{h} \int_{u}^{u+h} \frac{1}{\omega} \sin(\omega(u-v)) W(v) \phi_\omega(v) \mathrm{d}v, \tag{5.19}$$

where $h \neq 0$. We may restrict attention to the case $\operatorname{Im}\omega \leqslant 0$ and $h > 0$ (the other cases are analogous). Using the estimate

$$\left|\partial_u\left(\frac{1}{\omega}\sin(\omega(u-v))\right)\right| = |\cos(\omega(u-v))| \leqslant \frac{1}{2}(e^{-u\ \mathrm{Im}\ \omega}e^{v\ \mathrm{Im}\ \omega} + e^{u\ \mathrm{Im}\ \omega}\, e^{-v\ \mathrm{Im}\ \omega})$$

together with (5.17), we can apply the mean value theorem to the first integrand to obtain the dominating function

$$\frac{1}{2}(e^{-\xi(v)\mathrm{Im}\ \omega}e^{v\ \mathrm{Im}\ \omega} + e^{\xi(v)\mathrm{Im}\ \omega}e^{-v\ \mathrm{Im}\ \omega})|W(v)|e^{-v\ \mathrm{Im}\ \omega}e^{P_\omega(v)},$$

where $\xi(v)\in[u,u+h]$. Due to the integrability conditions on W, it is clear that this function is integrable. Hence Lebesgue's dominated convergence theorem allows us to take the limit $h\to 0$ in (5.18). This gives

$$\int_{-\infty}^{u} \cos(\omega(u-v))W(v)\phi_\omega(v)\mathrm{d}v\,.$$

In order to treat the second integral, we choose $h<h_0$, where h_0 is so small that

$$\max_{v\in[u,u+h]}\left|\frac{1}{\omega h}\sin(\omega(u-v))\right| \leqslant 2 \quad \text{for all } h<h_0.$$

This is possible because $\lim_{h\to 0}(1/\omega h)\sin(\omega h)=1$. Thus we can estimate (5.19) by

$$\left|\frac{1}{h}\int_u^{u+h}\frac{1}{\omega}\sin(\omega(u-v))W(v)\phi_\omega(v)\mathrm{d}v\right| \leqslant 2e^{-(u+h)\mathrm{Im}\ \omega}e^{P_\omega(u+h)}\int_{(-\infty,u_0)}|1_{[u,u+h]}(v)W(v)|\mathrm{d}v\,,$$

and the last integral goes to 0 as $h\to 0$ by Lebesgue's monotone convergence theorem using the fact that $W\in L^1(-\infty,u_0)$. Hence (5.19) vanishes.

Altogether we conclude that $\phi_\omega(u)$ is differentiable with derivative

$$\phi'_\omega(u) = i\omega e^{i\omega u} + \int_{-\infty}^{u}\cos(\omega(u-v))W(v)\phi_\omega(v)\mathrm{d}v\,, \tag{5.20}$$

which is continuous on $(-\infty,u_0)$ because of the estimate (5.17).

The estimate (5.9) is a simple consequence of (5.16) together with the perturbation expansion (5.6). For the proof of (5.10) we use the representation of the derivative (5.20) together with the inequality (5.17):

$$|\phi'_\omega(u)-i\omega e^{i\omega u}| \overset{(5.20)}{\leqslant} \int_{-\infty}^{u}|\cos(\omega(u-v))||W(v)||\phi_\omega(v)|\mathrm{d}v \overset{(5.17)}{\leqslant} \int_{-\infty}^{u}\frac{1}{2}(e^{-u\ \mathrm{Im}\ \omega}e^{v\ \mathrm{Im}\ \omega}+e^{u\ \mathrm{Im}\ \omega}e^{-v\ \mathrm{Im}\ \omega})$$

$$\times|W(v)|e^{-v\ \mathrm{Im}\ \omega}e^{P_\omega(v)}\,\mathrm{d}v \leqslant e^{-u\ \mathrm{Im}\ \omega}e^{P_\omega(u)}\int_{-\infty}^{u}|W(v)|\mathrm{d}v\,,$$

where in the last step we used the fact that $P_\omega(v)$ and $e^{-v\ \mathrm{Im}\ \omega}$ (with $\mathrm{Im}\ \omega\leqslant 0$) are monotone increasing. The estimates (5.11) as well as (5.12) are shown in the same way.

Let us now verify that for any fixed u, the function $\phi_\omega(u)$ is holomorphic in ω, and continuous on the domains as specified in (i), (ii), and (iii). Due to the locally uniform convergence of the perturbation series, it suffices to show that every $\phi_\omega^{(k)}(u)$ has the desired properties. We do this inductively, where the case $k=0$ is trivial. Let us now assume that $\phi_\omega^{(k)}(u)$ is holomorphic in $\mathring{E}$ ($\{\mathrm{Im}\ \omega<\frac{1}{2}m\}$, respectively). In order to prove that $\phi_\omega^{(k+1)}$ is holomorphic, we want to apply Morera's theorem. Thus we must show that $\phi_\omega^{(k+1)}(u)$ is continuous in ω and that the integral

$$\oint_\gamma \phi_\omega^{(k+1)}(u)\mathrm{d}\omega \overset{(5.7)}{=} \oint_\gamma \int_{-\infty}^{u} \frac{1}{\omega}\sin(\omega(u-v))W(v)\phi_\omega^{(k)}(v)\mathrm{d}v\,\mathrm{d}\omega \tag{5.21}$$

vanishes for every closed contour γ in $\mathring{E}$ [or in case (iii), for every contour in $\{\mathrm{Im}\,\omega<\frac{1}{2}m\}$, respectively]. Using the above estimates (5.14) and (5.16) together with the monotonicity of $P_\omega(u)$ in u we get the following bound for the integrand

$$\left|\frac{1}{\omega}\sin(\omega(u-v))W(v)\phi_\omega^{(k)}(v)\right| \leqslant |W(v)|\frac{4|v|}{1+|\omega v|}e^{-u\,\mathrm{Im}\,\omega - v|\mathrm{Im}\,\omega| - v\,\mathrm{Im}\,\omega}\frac{1}{k!}P_\omega(u)^k. \tag{5.22}$$

Due to the induction hypothesis, the integrand is continuous in ω. Moreover, for a compact neighborhood $K(\omega_0)$ of a fixed ω_0 contained in the specified domains, (5.22) yields for the family $(1/\omega)\sin(\omega(u-v))W(v)\phi_\omega^{(k)}(v)$, $\omega\in K(\omega_0)$ the uniformly dominating function

$$|W(v)|\frac{4|v|}{1+|v|\min|\omega|}e^{-u\,\mathrm{Im}\,\omega - v\,\max(|\mathrm{Im}\,\omega|+\mathrm{Im}\,\omega)}\frac{1}{k!}P_\omega(u)^k,$$

where the minimum and the maximum are taken in $K(\omega_0)$. This function is integrable for $K(\omega_0)$ chosen sufficiently small due to the integrability conditions on W. This lets us apply Lebesgue's dominated convergence theorem to show the continuity in ω for $\phi_\omega^{(k+1)}(u)$, which is given by the integral (5.7). Moreover, (5.22) together with the continuity in ω of $P_\omega(u)$ yield that the integral

$$\oint_\gamma \int_{-\infty}^{u}\left|\frac{1}{\omega}\sin(\omega(u-v))W(v)\phi_\omega^{(k)}(v)\right|\mathrm{d}v\,\mathrm{d}\omega<\infty$$

exists for an arbitrary closed contour γ in $\mathring{E}$ (or $\{\mathrm{Im}\,\omega<\frac{1}{2}m\}$, respectively). By the theorem of Fubini, we may interchange the orders of integration in (5.21). Because of the induction hypothesis, the integrand of (5.21) on the right-hand side is holomorphic. Thus the integral vanishes due to the Cauchy integral theorem. We conclude that $\phi_\omega^{(k)}$ is holomorphic for every k. Since $\phi_\omega(u)$ is holomorphic, the same argument together with Eq. (5.20) yields that ϕ_ω' is also holomorphic.

It remains to prove uniqueness. Let $\psi_\omega(u)$ be another solution of the Jost equation obeying $\lim_{u\to-\infty}|e^{-i\omega u}\psi_\omega(u)|<\infty$. Then we can find a $c>0$ with $|\psi_\omega(u)|\leqslant ce^{-u\,\mathrm{Im}\,\omega}$ for all $u\leqslant u_0$. Then as above one shows inductively that

$$\left|\psi_\omega(u)-\sum_{l=0}^{N}\phi_\omega^{(k)}(u)\right| \leqslant ce^{-u\,\mathrm{Im}\,\omega}\frac{1}{(N+1)!}P_\omega(u)^{N+1},$$

and taking $N\to\infty$ we obtain $\psi_\omega=\phi_\omega$.

The uniqueness also implies that $\overline{\phi(\omega,u)}=\phi(-\bar{\omega},u)$, concluding the proof.

□

Remark 5.4: In order to treat the Schrödinger equation (4.2) with boundary conditions at infinity (4.7), we derive the corresponding Jost equation with boundary conditions at $+\infty$ using the same procedure as for the solutions ϕ_1,

$$\phi_\omega(u)=e^{-i\omega u}-\int_u^\infty \frac{1}{\omega}\sin(\omega(u-v))W(v)\phi_\omega(v)\mathrm{d}v. \tag{5.23}$$

It is obvious that the solution $\tilde{\phi}_\omega(u)$ of the Jost equation with boundary conditions at $-\infty$ with potential $W(-v)$ constructed in Theorem 5.2 gives rise to a solution ϕ_ω of (5.23) by defining $\phi_\omega(u):=\tilde{\phi}_\omega(-u)$.

With the results of Theorem 5.2 it is now easy to prove Theorem 5.1.

Proof of Theorem 5.1: Let us apply Theorem 5.2 to the potential $V_l(u)$ given by (2.20), which is obviously a smooth function in u. Furthermore, it vanishes on the event horizon $2M$ with the asymptotics $V_l=\mathcal{O}(r-2M)$. Using the definition of the Regge-Wheeler coordinate u (2.3), this

means that $V_l(u)$ decays exponentially as $u \to -\infty$. More precisely, there is a constant $c > 0$ such that

$$|V_l(u)| \leqslant c e^{u/2M} \quad \text{for small } u.$$

Theorem 5.2 (iii) yields for $u \leqslant u_0 < 0$ a solution $\phi_1(\omega, u)$ of the Jost equation (5.5) with the desired properties. It remains to show that ϕ_1 is also a solution of the Schrödinger equation (4.2) for $u \leqslant u_0$. (Due to the Picard-Lindelöf theorem, this solution of the linear equation can be uniquely extended to $u \in \mathbb{R}$; the resulting function is analytic in ω due to the analytical dependence in ω from the coefficients and initial conditions.) But this follows immediately by differentiating equation (5.20) and using that $V_l \equiv W$ is smooth, so that the whole integrand is at least differentiable with respect to v. We have then proven the existence of $\acute{\phi}_\omega$. For the uniqueness, we show that in our special case every solution of (4.2) with boundary conditions (4.6) is a solution of (5.5). This can be done by integration by parts: let $\psi_\omega(u)$ be such a solution. Then

$$\int_{-\infty}^{u} \frac{1}{\omega} \sin(\omega(u-v)) V_l(v) \psi_\omega(v) \mathrm{d}v = \int_{-\infty}^{u} \frac{1}{\omega} \sin(\omega(u-v))(\partial_v^2 + \omega^2)\psi_\omega(v) \mathrm{d}v = \psi_\omega(u) - e^{i\omega u},$$

where the remaining terms vanish due to the boundary conditions. Since we know that the solution of the Jost equation is uniquely determined, this must be also the case for the solution of the Schrödinger equation. Thus we have proven part (i).

For the proof of (ii) we refer to Remark 5.4. In contrast to the exponential decay at $-\infty$, the potential $V_l(u)$ has only polynomial decay at $+\infty$. More precisely, according to the definition of u, $V_l(u) = \mathcal{O}(l(l+1)/u^2)$ for $l \geqslant 1$, $V_0(u) = \mathcal{O}(2M/u^3)$, respectively, as $u \to \infty$. Thus we can apply the analogs of Theorem 5.2 (i), (ii), respectively. This gives the existence and uniqueness of the solution $\grave{\phi}_\omega$ for the Schrödinger equation with the stated properties.

□

When taking the limit $\epsilon \searrow 0$ in Stone's formula (4.11), the behavior of $\grave{\phi}_\omega(u)$ at $\omega = 0$ still causes problems. While in the case $l = 0$ we know from Theorem 5.1 that $\grave{\phi}_\omega$ can be continuously extended there, we do not yet know what happens for $l \neq 0$. The following theorem settles this problem by showing that, after suitable rescaling, the solutions $\grave{\phi}_\omega$ have a well-defined limit at $\omega = 0$.

Theorem 5.5: *For every angular momentum number l, there is a solution ϕ_0 of the Schrödinger equation (4.2) for $\omega = 0$ with the asymptotics*

$$\lim_{u \to \infty} u^l \phi_0(u) = i^l \frac{2^l \sqrt{\pi}}{\Gamma\left(\frac{1}{2} - l\right)} = (-i)^l (2l-1)!!, \tag{5.24}$$

where

$$(2l-1)!! := \begin{cases} (2l-1) \cdot (2l-3) \cdot \cdots \cdot 3 \cdot 1 & \text{if } l \neq 0, \\ 1 & \text{if } l = 0. \end{cases}$$

This solution can be obtained as a limit of the solutions from Theorem 5.1, in the sense that for all $u \in \mathbb{R}$,

$$\phi_0(u) = \lim_{E \ni \omega \to 0} \omega^l \grave{\phi}_\omega(u) \quad \text{and} \quad \phi_0'(u) = \lim_{E \ni \omega \to 0} \omega^l \grave{\phi}_\omega'(u). \tag{5.25}$$

Note that the above properties of the solution ϕ_0 really coincide in the case $l = 0$ with that of the solution $\grave{\phi}_0$ already constructed in Theorem 5.1 (ii).

For the proof of this theorem we use the same method as in the proof for Theorem 5.1. However, the iteration scheme (5.7) does not work for $l \neq 0$ in the limit $\omega \to 0$, because the integral

$$\phi_0^{(1)}(u) = -\int_u^\infty (u-v)V_l(v)\mathrm{d}v$$

diverges [$V_l(u)$ decays only quadratically at infinity for $l \neq 0$]. We avoid this problem by adding the leading asymptotic term of the potential V_l to the unperturbed equation,

$$\left(-\frac{d^2}{\mathrm{d}u^2} - \omega^2 + \frac{\left(l+\frac{1}{2}\right)^2 - \frac{1}{4}}{u^2}\right)\phi_\omega(u) = -W_l(u)\phi_\omega(u). \tag{5.26}$$

Now the perturbation term $W_l(u) = V_l(u) - [l(l+1)/u^2]$ has the asymptotics $W_l(u) = \mathcal{O}(\log u/u^3)$.

Fortunately, the unperturbed differential equation corresponding to (5.26) can still be solved exactly. The solutions can be expressed in terms of Bessel functions. For our further consideration, the two functions

$$h_1(l,\omega,u) = \sqrt{\frac{\pi\omega u}{2}}J_{l+(1/2)}(\omega u), \quad h_2(l,\omega,u) = \sqrt{\frac{\pi\omega u}{2}}J_{-l-(1/2)}(\omega u) \tag{5.27}$$

play an important role. Here the function $J_\nu(u)$ is the Bessel function of the first kind (a good reference for the theory of the Bessel functions is Ref. 14). It solves Bessel's differential equation

$$u^2y''(u) + uy'(u) + (u^2 - \nu^2)y(u) = 0.$$

In addition, it is an analytic function in ν and u for all values of ν and $u \neq 0$ (if $\mathrm{Re}\,\nu \geqslant 0$, it can be analytically extended even to $u=0$). It has the series expansion

$$J_\nu(u) = \sum_{m=0}^\infty \frac{(-1)^m}{m!\Gamma(\nu+m+1)}\left(\frac{u}{2}\right)^{\nu+2m} \tag{5.28}$$

and the following asymptotics for $|u| \gg 1$ (cf. Ref. 14, 7.21):

$$J_\nu(u) \sim \sqrt{\frac{2}{\pi u}}\left[\cos\left(u - \frac{\pi}{2}\left(\nu+\frac{1}{2}\right)\right)\cdot\sum_{m=0}^\infty \frac{(-1)^m(\nu,2m)}{(2u)^{2m}} - \sin\left(u - \frac{\pi}{2}\left(\nu+\frac{1}{2}\right)\right)\cdot\sum_{m=0}^\infty \frac{(-1)^m(\nu,2m+1)}{(2u)^{2m+1}}\right], \tag{5.29}$$

where we have used the notation

$$(\nu,m) := \frac{\Gamma\left(\nu+m+\frac{1}{2}\right)}{m!\Gamma\left(\nu-m+\frac{1}{2}\right)}.$$

Moreover, the derivatives satisfy the recurrence formulas

$$uJ'_\nu(u) = uJ_{\nu-1}(u) - \nu J_\nu(u),$$

$$uJ'_\nu(u) = \nu J_\nu(u) - uJ_{\nu+1}(u).$$

The Wronskian of the functions J_ν, $J_{-\nu}$ (which both solve the same differential equation, since Bessel's differential equation is symmetric in ν) is given by the formula

$$w(J_\nu(u),J_{-\nu}(u)) = -\frac{2\sin(\nu\pi)}{\pi u}. \tag{5.30}$$

This yields that these functions form a fundamental system for Bessel's differential equation provided that ν is not an integer.

In our applications we choose $\nu = l + \frac{1}{2}$. Thus the functions $h_1(l,\omega,u)$ and $h_2(l,\omega,u)$ have the following asymptotics:

$$h_1(l,\omega,u) \sim \begin{cases} \cos\left(\omega u - (l+1)\dfrac{\pi}{2}\right) & \text{if } |\omega u| \gg 1, \\ \dfrac{\sqrt{\pi}}{\Gamma\left(\dfrac{3}{2}+l\right)}\left(\dfrac{\omega u}{2}\right)^{l+1} & \text{if } |\omega u| \ll 1, \end{cases} \tag{5.31}$$

$$h_2(l,\omega,u) \sim \begin{cases} \cos\left(\omega u + l\dfrac{\pi}{2}\right) & \text{if } |\omega u| \gg 1, \\ \dfrac{\sqrt{\pi}}{\Gamma\left(\dfrac{1}{2}-l\right)}\left(\dfrac{\omega u}{2}\right)^{-l} & \text{if } |\omega u| \ll 1. \end{cases} \tag{5.32}$$

Furthermore, the formula (5.30) for the Wronskian simplifies to

$$w(h_1(l,\omega,u),h_2(l,\omega,u)) = (-1)^{l+1}\omega, \quad \text{if } l \text{ is an integer}, \tag{5.33}$$

and this yields that in the case $\omega \neq 0$ the solutions h_1, h_2 form a fundamental system.

Thus for $\omega \neq 0$ we take as the Green's function for the operator on the left-hand side of (5.26) the standard formula

$$S_\omega(u,v) = \Theta(v-u)\frac{1}{w(h_1,h_2)}(h_1(v)h_2(u) - h_1(u)h_2(v)), \tag{5.34}$$

where $h_{1/2}(u) \equiv h_{1/2}(l,\omega,u)$ and Θ denotes the Heaviside function defined by $\Theta(x)=1$ if $x \geqslant 0$ and $\Theta(x)=0$ otherwise. Note that S_ω is also well defined in the limit $\omega \to 0$. For this we use the asymptotics and the value of the Wronskian and get for very small ω,

$$\begin{aligned} \lim_{\omega\to 0} S_\omega(u,v) &= \lim_{\omega\to 0} \frac{(-1)^{l+1}}{\omega} \cdot \frac{\pi\omega}{2\Gamma\left(\dfrac{3}{2}+l\right)\Gamma\left(\dfrac{1}{2}-l\right)}(v^{l+1}u^{-l} - u^{l+1}v^{-l}) \\ &= \frac{(-1)^{l+1}\pi}{2\left(\dfrac{1}{2}+l\right)\Gamma\left(\dfrac{1}{2}+l\right)\Gamma\left(\dfrac{1}{2}-l\right)}(v^{l+1}u^{-l} - u^{l+1}v^{-l}) = \frac{(-1)^{l+1}\pi\cos(\pi l)}{(2l+1)\pi}(v^{l+1}u^{-l} - u^{l+1}v^{-l}) \\ &= -\frac{1}{2l+1}(v^{l+1}u^{-l} - u^{l+1}v^{-l}), \end{aligned}$$

where we have used some elementary properties of the gamma function. This also shows that the Green's function converges to the Green's function $S_0(u,v)$ given by the above formula for the solutions u^{l+1}, u^{-l} of the unperturbed differential operator on the left-hand side of (5.26) for $\omega = 0$.

We now proceed with the perturbation series ansatz

$$\phi_\omega(u) = \sum_{m=0}^{\infty} \phi_\omega^{(m)}(u), \tag{5.35}$$

which, as at the beginning of this section, leads to the iteration scheme

$$\phi_\omega^{(m+1)}(u) = -\int_u^\infty S_\omega(u,v) W_l(v) \phi_\omega^{(m)}(v) \mathrm{d}v. \tag{5.36}$$

As initial function we take

$$\phi_\omega^{(0)}(u) = \omega^l e^{-i(l+1)(\pi/2)} \sqrt{\frac{\pi\omega u}{2}} H^{(2)}_{l+(1/2)}(\omega u),$$

where $H^{(2)}_\nu$ is another solution of Bessels equation (called Bessel function of the third kind or second Hankel function). It is related to J_ν by

$$H^{(2)}_\nu(u) = \frac{J_{-\nu}(u) - e^{\nu\pi i} J_\nu(u)}{-i \sin(\nu\pi)},$$

and has for large $|u|$ the asymptotics

$$H^{(2)}_\nu(u) \sim \sqrt{\frac{2}{\pi u}} e^{-i\{u-(1/2)\pi[\nu+(1/2)]\}} \sum_{m=0}^{\infty} \frac{(\nu,m)}{(2iu)^m}. \tag{5.37}$$

Thus our initial function $\phi_\omega^{(0)}(u)$ solves the unperturbed equation, and we have the relation

$$\phi_\omega^{(0)}(u) = \omega^l((-i)^{l+1} h_1(l,\omega,u) + i^l h_2(l,\omega,u)) \tag{5.38}$$

together with the asymptotics

$$\phi_\omega^{(0)}(u) = \omega^l e^{-i\omega u}\left(1 + \mathcal{O}\left(\frac{1}{u}\right)\right) \text{ if } |u| \gg 1. \tag{5.39}$$

Moreover, the function $\phi_\omega^{(0)}$ converges in the limit $\omega \to 0$ pointwise for all $u \geqslant u_0 > 0$:

$$\lim_{\omega\to 0} \phi_\omega^{(0)}(u) = i^l \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2} - l\right)} \left(\frac{u}{2}\right)^{-l}. \tag{5.40}$$

Since we are interested in statements for $\omega = 0$, it is convenient in what follows to restrict ω to the domain:

$$F := \{\omega \in \mathbb{C} | \mathrm{Im}\ \omega \leqslant 0, |\omega| \leqslant 1\}.$$

The following lemma yields that our perturbation series (5.35) is well defined.

Lemma 5.6: For every $u_0 > 0$, the iteration scheme (5.35), (5.36), and (5.38) *converges locally uniformly for all $u \geqslant u_0$ and $\omega \in F$. In particular, the functions $\phi_\omega(u)$ are for fixed u a continuous family in $\omega \in F$. They satisfy the integral equation*

$$\phi_\omega(u) = \phi_\omega^{(0)}(u) - \int_u^\infty S_\omega(u,v) W_l(v) \phi_\omega(v) \mathrm{d}v. \tag{5.41}$$

Proof: In order to prove the lemma, we need to derive good bounds for the initial function $\phi_\omega^{(0)}(u)$ as well as for the Green's function $S_\omega(u,v)$. To this end, we exploit the asymptotics of h_1, h_2. We thus obtain the bound

$$\frac{1}{C_1} \leqslant |\phi_\omega^{(0)}(u)| e^{-u \operatorname{Im} \omega} \left(\frac{u}{1+|\omega| u} \right)^l \leqslant C_1 . \tag{5.42}$$

Likewise, for the Green's function we have (note that $v \geqslant u > 0$),

$$|S_\omega(u,v)| \leqslant C_2 \left(\frac{u}{1+|\omega| u} \right)^{-l} \left(\frac{v}{1+|\omega| v} \right)^{l+1} \quad \text{if } |\omega v| \ll 1$$

and

$$|S_\omega(u,v)| \leqslant C_3 \frac{v}{1+|\omega| v} e^{v|\operatorname{Im} \omega| + u \operatorname{Im} \omega}, \quad \text{if } |\omega u| \gg 1 .$$

The last inequality follows from the asymptotics

$$|S_\omega(u,v)| \sim \left| \frac{1}{\omega} \sin(\omega(u-v)) \right| \quad \text{if } |\omega u| \gg 1,$$

in the same way as the second inequality of Lemma 5.3. Combining these cases we find a constant such that

$$|S_\omega(u,v)| \leqslant C_4 \left(\frac{u}{1+|\omega| u} \right)^{-l} \left(\frac{v}{1+|\omega| v} \right)^{l+1} e^{v|\operatorname{Im} \omega| + u \operatorname{Im} \omega}. \tag{5.43}$$

Hence defining the function Q_ω by

$$Q_\omega(u) := C_4 \int_u^\infty \frac{v}{1+|\omega| v} |W_l(v)| \mathrm{d}v, \tag{5.44}$$

which is well defined for all $\omega \in F$ and $u \geqslant u_0 > 0$ due to the asymptotic of W_l, it is straightforward to show inductively (cf. proof of Theorem 5.2) that for all $m \in \mathbb{N}$,

$$|\phi_\omega^{(m)}(u)| \leqslant C_1 \left(\frac{u}{1+|\omega| u} \right)^{-l} e^{u \operatorname{Im} \omega} \frac{Q_\omega(u)^m}{m!}. \tag{5.45}$$

Now we proceed exactly as in the proof of Theorem 5.2, where the inequality (5.45) can be considered as the analogue of (5.16). It follows that the series (5.35) converges locally uniformly in ω and u and satisfies the integral equation (5.41). Furthermore, one shows inductively applying Lebesgue's dominated convergence theorem, that for fixed u each $\phi_\omega^{(m)}(u)$ depends continuously of $\omega \in F$. It follows that the same is true for the series due to local uniform convergence.

□

We are now ready to prove Theorem 5.5.

Proof of Theorem 5.5: According to Lemma 5.6, our perturbation series (5.35) satisfies the integral equation (5.41). Using the recurrence formulas for the derivatives of $J_\nu(u)$, one obtains

$$h_1'(l,\omega,u) = -\frac{l}{u} h_1(l,\omega,u) + \omega h_1(l-1,\omega,u),$$

$$h_2'(l,\omega,u) = -\frac{l}{u} h_2(l,\omega,u) - \omega h_2(l-1,\omega,u),$$

respectively. This allows us to estimate the behavior of $\partial_u S_\omega(u,v)$. Exactly as for $S_\omega(u,v)$, we obtain the following asymptotic formulas:

$$|\partial_u S_\omega(u,v)| \leqslant C_5\left(\frac{u}{1+|\omega|u}\right)^{-l-1}\left(\frac{v}{1+|\omega|v}\right)^{l+1} e^{v|\mathrm{Im}\ \omega|+u\ \mathrm{Im}\ \omega}.$$

Following the same arguments of the proofs of Theorems 5.1 and 5.2, and combining them with the above estimates and asymptotic formulas we now have the following results:

(1) One can differentiate $\phi_\omega(u)$ with respect to u, and $\phi'_\omega(u)$ is given by

$$\phi'_\omega(u) = (\phi^{(0)}_\omega)'(u) - \int_u^\infty \partial_u S_\omega(u,v) W_l(v)\phi_\omega(v)\mathrm{d}v.$$

In particular, Lebesgue's dominated convergence theorem yields that for fixed u, $\phi'_\omega(u)$ is continuous in $\omega \in F$.

(2) $\phi_\omega(u)$ and $\phi'_\omega(u)$ obey the following estimates:

$$|\phi_\omega(u) - \phi^{(0)}_\omega(u)| \leqslant C_1\left(\frac{u}{1+|\omega|u}\right)^{-l} e^{u\ \mathrm{Im}\ \omega}(e^{Q_\omega(u)}-1),$$

$$|\phi'_\omega(u) - (\phi^{(0)}_\omega)'(u)| \leqslant C_5\left(\frac{u}{1+|\omega|u}\right)^{-l-1} e^{Q_\omega(u_0)} e^{u\ \mathrm{Im}\ \omega}\int_u^\infty v|W_l(v)|\mathrm{d}v.$$

Thus $\phi_\omega(u) \sim \omega^l e^{-i\omega u}$ and $\phi'_\omega(u) \sim -i\omega^{l+1}e^{-i\omega u}$ as $u \to \infty$.

(3) Differentiating $\phi_\omega(u)$ twice with respect to u shows that $\phi_\omega(u)$ is a solution of the Schrödinger equation (4.2) for all $u \geqslant u_0$. Furthermore, from the asymptotics at infinity combined with the uniqueness statement in Theorem 5.1, we know that

$$\phi_\omega(u) = \omega^l \grave{\phi}_\omega(u), \quad \text{if } \omega \neq 0, u \geqslant u_0. \tag{5.46}$$

Obviously, this extends to all $u \in \mathbb{R}$.

Thus we have proven the continuity statement (5.25) for all $u \geqslant u_0$. On the other hand, we know from the Picard-Lindelöf theorem that for u on compact intervals, the solutions depend continuously on ω. This yields (5.25) for all $u \in \mathbb{R}$.

Finally, the asymptotics (5.24) is a simple consequence of (5.40).

□

VI. AN INTEGRAL SPECTRAL REPRESENTATION

In the preceding section we derived some regularity results for the solutions $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$. We already know (cf. Sec. IV) that these solutions are a system of fundamental solutions of the Schrödinger equation (4.2) in the cases $\mathrm{Im}\ \omega < 0$ and $\mathrm{Im}\ \omega > 0$, respectively. Thus the Wronskian $w(\acute{\phi}_\omega, \grave{\phi}_\omega)$ is nonvanishing in these regions, which implies that the integral kernel $k_\omega(u,v)$ of the resolvent is well defined. Since our next goal is to get the limit in (4.11), we prove in the next lemma that the continuous extension of the solutions $\acute{\phi}_\omega, \grave{\phi}_\omega$ to the real axis again yields a system of fundamental solutions. More precisely we have the following.

Lemma 6.1: The Wronskian $w(\acute{\phi}_\omega, \grave{\phi}_\omega)$ does not vanish for $\omega \in \mathbb{R}\backslash\{0\}$. In particular, $\acute{\phi}_\omega, \grave{\phi}_\omega$ are fundamental solutions for the Schrödinger equation (4.2). *In addition, this remains true for the solutions $\acute{\phi}_0$ and ϕ_0 in the case $\omega = 0$.*

Proof: Let us begin with the statement for $\acute{\phi}_0, \phi_0$.

For $\omega = 0$, the solutions $\acute{\phi}_0(u), \phi_0(u)$ have the asymptotics

$$\lim_{u\to-\infty} \acute{\phi}_0(u) = 1 \quad \text{and} \lim_{u\to\infty} u^l \phi_0(u) = (-i)^l (2l-1)!!.$$

Looking at the construction of these solutions, one sees that $\acute{\phi}_0$ is a real solution, while ϕ_0 is either purely real or imaginary (depending on the value of l). The Schrödinger equation for $\omega=0$ reduces to $\phi''(u)=V_l(u)\phi(u)$ with a everywhere positive potential V_l. Hence, exploiting the special asymptotics, the solution $\acute{\phi}_0$ is convex and Re ϕ_0 (Im ϕ_0, respectively) is either convex or concave depending on l. In any case, we see that $\acute{\phi}_0$ and ϕ_0 are linearly independent, and thus $w(\acute{\phi}_0, \phi_0) \neq 0$.

In order to prove the main part of the lemma, we consider a complex solution $z=z_1+iz_2$ of the Schrödinger equation, where $\{z_1, z_2\}$ is a fundamental system of real solutions, especially $w(z_1, z_2) \equiv c \neq 0$. Setting $y=z'/z$, a simple computation shows that

$$\text{Im } y = \frac{w(z_1, z_2)}{|z|^2},$$

where the right-hand side is well defined because $w(z_1, z_2) \neq 0$ implies that $|z| \neq 0$ everywhere. As a consequence, we have Im $y \neq 0$ everywhere. Thus it follows that for all u either Im $y(u) > 0$ or <0, due to the continuity of the solution z in u.

Applying this result to the solutions $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$, respectively, and exploiting their asymptotics, one sees that Im $\acute{y}_\omega(u)$ and Im $\grave{y}_\omega(u)$ have different signs for all u. Therefore,

$$w(\acute{\phi}_\omega, \grave{\phi}_\omega) = \acute{\phi}_\omega(u)\grave{\phi}'_\omega(u) - \acute{\phi}'_\omega(u)\grave{\phi}_\omega(u) = \acute{\phi}_\omega(u)\grave{\phi}_\omega(u)(\grave{y}_\omega(u) - \acute{y}_\omega(u)) \neq 0.$$

□

As a consequence we have the following.

Corollary 6.2: The function $s_\omega(u,v)$ *given by* (4.9) *is continuous in* (ω,u,v) *for* $\omega \in \{\text{Im } \omega \leqslant 0\}$, $(u,v) \in \mathbb{R}^2$.

Proof: We already know that for fixed $u_0 < 0$, $\acute{\phi}_\omega(u_0)$ is continuous in ω on $\{\text{Im } \omega \leqslant 0\}$. Thus as solutions of the linear differential equation (4.2), which depends analytically on ω and smooth on u, the family $\acute{\phi}_\omega(u)$ is (at least) continuous in (ω,u) in the region $\{\text{Im } \omega \leqslant 0\} \times \mathbb{R}$. Analogously this holds for $\omega^l \grave{\phi}_\omega(u)$ according to Theorems 5.1 and 5.5. Since $s_\omega(u,v)$ is invariant if we substitute $\omega^l \grave{\phi}_\omega(u)$ for $\grave{\phi}_\omega(u)$, the preceding lemma yields the claim.

□

Note that the corollary is also true if ω is in the upper half plane. The essential statement in this corollary is that one can extend $s_\omega(u,v)$ continuously in ω up to the real axis.

From the definitions (5.1) and (5.2), we have for $\omega \in \{\text{Im } \omega \neq 0\}$ the relations

$$\overline{s_\omega(u,v)} = s_{\bar{\omega}}(u,v), \quad \text{hence } \overline{k_\omega(u,v)} = k_{\bar{\omega}}(u,v).$$

This allows us to simplify the expression (4.11). Evaluating for fixed u the right-hand side of (4.11) we obtain for any $\Psi \in \mathcal{H}$ as well as for any bounded interval $[a,b] \subseteq \mathbb{R}$,

$$\lim_{\epsilon \searrow 0} -\frac{1}{\pi} \int_a^b \left(\int_{\mathbb{R}} \text{Im}(k_{\omega - i\epsilon}(u,v)) \Psi(v) \mathrm{d}v \right) \mathrm{d}\omega.$$

According to the above corollary, we know that Im $k_\omega(u,v)$ is continuous in (ω,u,v) for $\omega \in \{\text{Im } \omega \leqslant 0\}$, $(u,v) \in \mathbb{R}^2$. Thus, if we restrict Ψ to the dense set $C_0^\infty(\mathbb{R})^2$, we integrate a continuous integrand over a compact interval. Hence, considering the limit as a pointwise limit for any u, we may interchange the limit and integration. Thus for any $\Psi \in C_0^\infty(\mathbb{R})^2$, $[a,b] \subset \mathbb{R}$ bounded and u the right-hand side of (4.11) converges pointwise to

$$-\frac{1}{\pi}\int_a^b \left(\int_{\text{supp } \psi} \text{Im}(k_\omega(u,v))\psi(v)\mathrm{d}v \right)\mathrm{d}\omega.$$

Hence, together with the norm convergence in (4.11), the spectral projections of H are for every u described by the formula

$$\frac{1}{2}(P_{[a,b]}+P_{(a,b)})\Psi(u) = -\frac{1}{\pi}\int_a^b \left(\int_{\text{supp } \psi} \text{Im}(k_\omega(u,v))\psi(v)\mathrm{d}v \right)\mathrm{d}\omega. \tag{6.1}$$

In particular, this representation yields that $P_{[a,b]} \equiv P_{(a,b)}$.

As an immediate consequence we have the following.

Corollary 6.3: The spectrum $\sigma(H)$ of the operator H is absolutely continuous, i.e., $\sigma(H) \equiv \sigma_{ac}(H)$.

Proof: The corollary is equivalent to the statement that the spectral measure $\langle \Psi, \mathrm{d}P_\omega \Psi\rangle$ of any $\Psi \in \mathcal{H}$ is absolutely continuous. This is clear by (6.1) for any $\Psi \in C_0^\infty(\mathbb{R})^2$. But since this subset is dense, this also holds on the whole Hilbert space $\mathcal{H}$. □

Next we want to write the integrand in (6.1), i.e., $\int_{\text{supp } \Psi} \cdots \mathrm{d}v$, in a more compact way. We first note that for real ω the complex conjugates of $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$ are again solutions of (4.2). Hence, for any $\omega \in \mathbb{R}\backslash\{0\}$ the pair $\{\acute{\phi}_\omega, \overline{\acute{\phi}_\omega}\}$ forms a fundamental system for this equation due to the boundary conditions. Thus we can express $\grave{\phi}_\omega$ as a linear combination of $\acute{\phi}_\omega$ and $\overline{\acute{\phi}_\omega}$,

$$\grave{\phi}_\omega(u) = \lambda(\omega)\acute{\phi}_\omega(u) + \mu(\omega)\overline{\acute{\phi}_\omega(u)} \quad (\omega \in \mathbb{R}\setminus\{0\}),$$

where λ and μ are referred to as *transmission coefficients*. The Wronskian of $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$ can be expressed by

$$w(\acute{\phi}_\omega, \grave{\phi}_\omega) = \mu(\omega) w(\acute{\phi}_\omega, \overline{\acute{\phi}_\omega}) = -2i\omega\mu(\omega),$$

where in the last step we used the asymptotics (4.6). Moreover, we introduce the real fundamental solutions

$$\phi_\omega^1(u) = \text{Re } \acute{\phi}_\omega(u), \quad \phi_\omega^2(u) = \text{Im } \acute{\phi}_\omega(u)$$

and denote the corresponding eigenvectors of the Hamiltonian H by $\Phi_\omega^a(u) = (\phi_\omega^a(u), \omega\phi_\omega^a(u))^T$.

Using the above definitions, a short calculation shows that for $\omega \neq 0$ we can express the imaginary part of the Green's function $s_\omega(u,v)$ by

$$\text{Im } s_\omega(u,v) = -\frac{1}{2\omega}\sum_{a,b=1}^{2} t_{ab}(\omega)\phi_\omega^a(u)\phi_\omega^b(v), \tag{6.2}$$

where the coefficients $t_{ab}(\omega)$ are given by

$$t_{11}(\omega) = 1 + \text{Re}\left(\frac{\lambda}{\mu}(\omega)\right), \quad t_{12}(\omega) = t_{21}(\omega) = -\text{Im}\left(\frac{\lambda}{\mu}(\omega)\right),$$

$$t_{22}(\omega) = 1 - \text{Re}\left(\frac{\lambda}{\mu}(\omega)\right). \tag{6.3}$$

Since we know that $\text{Im } s_\omega(u,v)$ is continuous for $\omega \in \mathbb{R}$ and the expression (6.2) holds for all $\omega \in \mathbb{R}\backslash\{0\}$, it extends to $\omega = 0$. With (6.2), the integrand in (6.1) can be written as

$$-\frac{1}{2\omega}\left(\int_{\text{supp }\Psi}\sum_{a,b=1}^{2} t_{ab}(\omega)\phi^a_\omega(u)\phi^b_\omega(v)\begin{pmatrix}\omega & 1\\ \omega^2 & \omega\end{pmatrix}\Psi(v)\mathrm{d}v\right)$$
$$=-\frac{1}{2\omega^2}\sum_{a,b=1}^{2} t_{ab}(\omega)\Phi^a_\omega(u)\left(\int_{\text{supp }\Psi}\omega^2\phi^b_\omega(v)\psi_1(v)+\omega\phi^b_\omega(v)\psi_2(v)\mathrm{d}v\right),$$

where the ψ_i denote the two components of Ψ.

Using that $\phi^b_\omega(u)$ solves the Schrödinger equation $(-\partial_v^2+V_l(v))\phi^b_\omega(v)=\omega^2\phi^b_\omega(v)$ and integrating by parts, this simplifies to

$$-\frac{1}{2\omega^2}\sum_{a,b=1}^{2} t_{ab}(\omega)\Phi^a_\omega(u)\langle\Phi^b_\omega,\Psi\rangle. \tag{6.4}$$

(Note that in this case the energy scalar product of Φ^b_ω and Ψ is well defined, because Ψ has compact support. Whereas in general this does not exist for arbitrary $\Psi\in\mathcal{H}$, due to the fact that $\Phi^b_\omega\notin\mathcal{H}$.)

With (6.4), we now obtain a more compact representation for the spectral projections. Moreover, we can use (6.4) to express the solution operators e^{-itH}.

Proposition 6.4: Consider the Cauchy problem (2.23) *for compactly supported smooth initial data* $\Psi_0\in C_0^\infty(\mathbb{R})^2$. *Then the solution has the integral representation*

$$\Psi(t)=e^{-itH}\Psi_0=\frac{1}{2\pi}\int_{\mathbb{R}} e^{-i\omega t}\frac{1}{\omega^2}\sum_{a,b=1}^{2} t_{ab}(\omega)\Phi^a_\omega\langle\Phi^b_\omega,\Psi_0\rangle\mathrm{d}\omega. \tag{6.5}$$

Here the integral converges in norm in the Hilbert space $\mathcal{H}$.

Proof: We use the following variation of Stone's formula to obtain for any bounded interval $(c,d)\subseteq\mathbb{R}$,

$$\frac{1}{2}e^{-itH}(P_{[c,d]}+P_{(c,d)})\Psi=\lim_{\epsilon\searrow 0}\int_c^{\mathrm{d}} e^{-i\omega t}[(H-\omega-i\epsilon)^{-1}-(H-\omega+i\epsilon)^{-1}]\Psi\,\mathrm{d}\omega,$$

where the limit is with respect to the norm of $\mathcal{H}$. Since we know that $P_{[c,d]}\equiv P_{(c,d)}$, it follows that this expression is equal to $e^{-itH}P_{(c,d)}\Psi$. Using the explicit formula for the resolvent, for every $u\in\mathbb{R}$ the right-hand side is equal to

$$\lim_{\epsilon\searrow 0}-\frac{1}{\pi}\int_c^{\mathrm{d}} e^{-i\omega t}\left(\int_{\mathbb{R}}\mathrm{Im}(k_{\omega-i\epsilon}(u,v))\Psi(v)\mathrm{d}v\right)\mathrm{d}\omega. \tag{6.6}$$

Due to the continuity of the imaginary part of the kernel $k_\omega(u,v)$, we may take for $\Psi_0\in C_0^\infty(\mathbb{R})^2$ and (c,d) bounded the pointwise limit for any $u\in\mathbb{R}$. Hence, using (6.4) we can simplify (6.6) to

$$\frac{1}{2\pi}\int_c^{\mathrm{d}} e^{-i\omega t}\frac{1}{\omega^2}\sum_{a,b=1}^{2} t_{ab}(\omega)\Phi^a_\omega(u)\langle\Phi^b_\omega,\Psi_0\rangle\mathrm{d}\omega,$$

and together with the norm convergence it follows that this term is equal to $e^{-itH}P_{(c,d)}\Psi_0(u)$. Using the abstract spectral theorem and that e^{-itH} is a unitary operator, it is clear that $e^{-itH}P_{(-n,n)}\Psi_0\to e^{-itH}\Psi_0$ in norm as $n\to\infty$. □

This proposition extends to the following theorem.

Theorem 6.5: *For any fixed* $u\in\mathbb{R}$ *the integrand in the representation* (6.5) *is in* $L^1(\mathbb{R},\mathbb{C}^2)$ *as a function of* ω. *In particular, the representation* (6.5) *of the solutions holds pointwise for every* $u\in\mathbb{R}$, *i.e.*,

$$\Psi(t,u) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{-i\omega t}\frac{1}{\omega^2}\sum_{a,b=1}^{2} t_{ab}(\omega)\Phi^a_\omega(u)\langle\Phi^b_\omega,\Psi_0\rangle \mathrm{d}\omega. \tag{6.7}$$

Moreover, for u fixed, the function $\Psi(t,u)$ *vanishes as* $t\to\infty$.

Proof: Since we know that the integrand is continuous in ω, it is in $L^1([a,b],\mathbb{C}^2)$ for any bounded interval $[a,b]$. Thus it remains to analyze the integrand for large $|\omega|$.

To this end, we must investigate the asymptotic behavior of the fundamental solutions $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$ in ω. We constructed these solutions with the iteration scheme (5.7) as solutions of the Jost equation. For the proof of this, the estimate (5.14) played an essential role. Since in this case we consider real ω with $|\omega|\gg 1$, we can use the simple estimate $|(1/\omega)\sin(\omega(u-v))|\leqslant 1/|\omega|$ instead of (5.14), which now holds for every $u,v\in\mathbb{R}$. Thus, proceeding exactly in the same way as in the proof of Theorem 5.2, we now obtain the following estimates for the several terms in the series expansion (5.6):

$$|\phi^{(k)}_\omega(u)| \leqslant \frac{1}{k!}\hat{P}_\omega(u)^k, \quad \text{where } \hat{P}_\omega(u) := \int_{-\infty}^{u}\frac{1}{|\omega|}V_l(v)\mathrm{d}v,$$

for any $k\in\mathbb{N}$ and $u\in\mathbb{R}$. Thus the solution $\acute{\phi}_\omega(u)$ $(\omega\neq 0)$ is given *for all* $u\in\mathbb{R}$ by this series expansion and obeys the uniform bound

$$|\acute{\phi}_\omega(u) - e^{i\omega u}| \leqslant e^{\hat{P}_\omega(u)} - 1 \leqslant e^{(1/|\omega|)\|V_l\|_{L^1}} - 1,$$

since $V_l\in L^1(\mathbb{R})$. In particular,

$$|\acute{\phi}_\omega(u)| \leqslant 1 + \mathcal{O}\left(\frac{1}{|\omega|}\right) \quad \text{for } |\omega|\gg 1. \tag{6.8}$$

Next we investigate the ω-dependence of $\langle\Phi^b_\omega,\Psi_0\rangle$. We integrate by parts to obtain

$$\langle\Phi^b_\omega,\Psi_0\rangle = \int_{\mathrm{supp}\,\Psi_0}\phi^b_\omega(v)(\omega\psi_2(v) - \psi_1(v)'' + V_l(v)\psi_1(v))\mathrm{d}v,$$

where $\Psi_0=(\psi_1,\psi_2)^T$ [note that the boundary terms drop out, because $\Psi_0\in C^\infty_0(\mathbb{R})^2$]. Since $\phi^b_\omega(u)$ is a solution of the Schrödinger equation (4.2), we substitute $(1/\omega^2)(-\phi^b_\omega(u)''+V_l(u)\phi^b_\omega(u))$ for $\phi^b_\omega(u)$ and integrate by parts twice,

$$= \frac{1}{\omega^2}\int_{\mathrm{supp}\,\Psi_0}\phi^b_\omega(-(\omega\psi_2 - \psi_1'' + V_l\psi_1)'' + V_l(\omega\psi_2 - \psi_1'' + V_l\psi_1))\mathrm{d}v.$$

We can now iterate this procedure as often as we like due to the fact that $\Psi_0\in C^\infty_0(\mathbb{R})^2$ and $V_l\in C^\infty(\mathbb{R})$. Thus using the bound (6.8), we obtain arbitrary polynomial decay in ω for $\langle\Phi^b_\omega,\Psi_0\rangle$.

It remains to control the coefficients $t_{ab}(\omega)$ for large $|\omega|$. According to the definition of the transmission coefficients $\lambda(\omega)$ and $\mu(\omega)$, they satisfy the following relations:

$$w(\grave{\phi}_\omega,\acute{\phi}_\omega) = 2i\mu(\omega) \quad \text{and } w(\grave{\phi}_\omega,\overline{\acute{\phi}_\omega}) = 2i\lambda(\omega).$$

In order to calculate the Wronskians, we substitute the Jost integral equations (5.5) and (5.23) for $\acute{\phi}_\omega$ and $\grave{\phi}_\omega$, respectively, as well as the corresponding integral equations for the derivatives [for instance (5.20) in the case $\acute{\phi}_\omega$] and obtain immediately

$$\mu(\omega) = 1 + \mathcal{O}\left(\frac{1}{\omega}\right), \quad \lambda(\omega) = \mathcal{O}\left(\frac{1}{\omega}\right).$$

Hence the coefficients $t_{ab}(\omega)$ remain (at least) bounded, according to their definition (6.3).

We conclude that the integrand in (6.7) is in $L^1(\mathbb{R},\mathbb{C}^2)$ as a function of ω. Thus the right-hand side in the integral representation (6.5) converges also pointwise and, together with the norm convergence, (6.7) follows.

Since for u fixed, $\Psi(t,u)$ is a Fourier transform of a L^1-function, the Riemann-Lebesgue lemma applies. Hence $\Psi(t,u)$ vanishes as $t\to\infty$.

□

In the next step we extend this proposition to the Cauchy problem (2.6).

Theorem 6.6: *Consider the Cauchy problem (2.6) for smooth and compactly supported initial data. Then there exists a unique smooth solution, which is compactly supported for all times.*

Moreover, decomposing the initial data Ψ_0 *into spherical harmonics, the solution has the representation*

$$\Psi(t,u,\vartheta,\varphi)=\sum_{l=0}^{\infty}\sum_{|m|\leqslant l} e^{-itH_l}\,\Psi_0^{lm}(u)Y_{lm}(\vartheta,\varphi). \tag{6.9}$$

Proof: For the existence and uniqueness of such a solution we apply the theory of linear symmetric hyperbolic systems (cf. Ref. 12). Since the equation in (2.6) is defined on $\mathbb{R}\times\mathbb{R}\times S^2$ we must work in local coordinates for S^2. We demonstrate the idea in the chart $(U,(\vartheta,\varphi))$, where U is an open, relative compact subset of S^2 such that (ϑ,φ) are well defined on $\bar{U}$.

Letting $\Phi=(\partial_t\psi,\partial_u\psi,\partial_{\cos\,\vartheta}\psi,\partial_\varphi\psi,\psi)^T$ we can write the equation as the first order system

$$A^0\partial_t\Phi+A^1\partial_u\Phi+A^2\partial_{\cos\,\vartheta}\Phi+A^3\partial_\varphi\Phi+B\Phi=0,$$

where the matrices A^i,B are given by

$$A^0=\mathrm{diag}\left(1,1,\left(1-\frac{2M}{r}\right)\frac{1}{r^2}\sin^2,\left(1-\frac{2M}{r}\right)\frac{1}{r^2}\frac{1}{\sin^2\vartheta},1\right),$$

$$A^1=(a^1_{ij})\quad\text{with } a^1_{12}=a^1_{21}=-1,$$

$$A^2=(a^2_{ij})\quad\text{with } a^2_{13}=a^2_{31}=-\left(1-\frac{2M}{r}\right)\frac{1}{r^2}\sin^2\vartheta,$$

$$A^3=(a^3_{ij})\quad\text{with } a^3_{14}=a^3_{41}=-\left(1-\frac{2M}{r}\right)\frac{1}{r^2}\frac{1}{\sin^2\vartheta},$$

$$B=(b_{ij})\quad\text{with } b_{13}=\left(1-\frac{2M}{r}\right)\frac{1}{r^2}2\cos\vartheta,$$

$$b_{15}=\left(1-\frac{2M}{r}\right)\frac{2M}{r^3},\quad b_{51}=-1,$$

and all other coefficients vanish. By multiplying this system with $[1-(2M/r)]^{-1}r^2$, we obtain a linear symmetric hyperbolic system on $\mathbb{R}\times\mathbb{R}\times U$ in the sense that the A^i are symmetric and A^0 is uniformly positive definite on $\mathbb{R}\times\mathbb{R}\times U$. Since the initial data Ψ_0 has compact support, we can restrict the system to $\mathbb{R}\times V\times U$, where $V\subseteq\mathbb{R}$ is an open, relative compact set with $\mathrm{supp}\,\Psi_0\subseteq V$. Considering the system on this domain, the matrices A^i,B remain uniformly bounded. Since we can cover S^2 by a finite number of such charts, the theory of symmetric hyperbolic systems yields an $\epsilon_1>0$ such that there is unique and smooth solution $\psi(t,u,x)$ for all $t<\epsilon_1$ on $\mathbb{R}\times V\times S^2$ with initial data Ψ_0.

Moreover, this solution has finite propagation speed, which is independent of u (this is physically clear from causality; it follows mathematically by considering lens-shaped regions for our symmetric hyperbolic systems). Thus there exists an $\epsilon>0$ (possibly smaller than ϵ_1) such that the solution $\psi(t,u,x)$ has compact support in $V\times S^2$ for all times $t\leqslant\epsilon$. Iterating this argument for the Cauchy problem with initial data $(\psi(\epsilon,u,x),i\partial_t\psi(\epsilon,u,x))$ (and choosing $V\subseteq\mathbb{R}$ sufficiently large), we get a unique and smooth solution $\psi(t,u,x)$ with compact support for all $t\leqslant 2\epsilon$ and so forth. Thus we have proven the existence of a global solution $\psi(t,u,x)\in C^\infty(\mathbb{R}\times\mathbb{R}\times S^2)$ which is unique and compactly supported for all times t.

In order to prove the representation (6.9), we consider the restriction of the solution $\Psi(t,u,x)=(\psi(t,u,x),i\partial_t\psi(t,u,x))^T$ of the Cauchy problem (2.12) in Hamiltonian form to fixed modes l,m

$$\Psi^{lm}(t,u)Y_{lm}(\vartheta,\varphi)=\langle\Psi(t,u),Y_{lm}\rangle_{L^2(S^2)}Y_{lm}(\vartheta,\varphi).$$

Then $\Psi^{lm}(t,u)Y_{lm}(\vartheta,\varphi)$ is a solution of (2.12) with initial data $\Psi_0^{lm}(u)Y_{lm}(\vartheta,\varphi)$, which is smooth and compactly supported. Thus $\Psi^{lm}(t,u)$ is a solution of the Cauchy problem (2.23), and due to the uniqueness of such solutions

$$\Psi^{lm}(t,u)=e^{-itH_l}\Psi_0^{lm}(u).$$

Now the uniqueness of the decomposition into spherical harmonics yields (6.9).

□

We are now ready to prove our main theorem.

Proof of Theorem 1.1: The existence and uniqueness of solutions of the Cauchy problem follow directly from Theorem 6.6 after the substitution $\psi=r\phi$. Thus it remains to show the pointwise decay.

The conserved energy for solutions which are compactly supported for all times t implies that for every t,

$$\|\Psi(t,u,\vartheta,\varphi)\|^2=\|\Psi_0(u,\vartheta,\varphi)\|^2=\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}\|\Psi_0^{lm}(u)\|_l^2,$$

where for the second equation we used the isometry (2.21). Hence, defining

$$\Psi^L(t,u,\vartheta,\varphi):=\sum_{l=L}^{\infty}\sum_{|m|\leqslant l}\Psi^{lm}(t,u)Y_{lm}(\vartheta,\varphi),$$

we can find for every $\epsilon>0$ a number L_0 such that

$$\|\Psi^{L_0}(t,u,\vartheta,\varphi)\|^2=\sum_{l=L_0}^{\infty}\sum_{|m|\leqslant l}\|\Psi_0^{lm}(u)\|_l^2<\epsilon.$$

Let us now consider the Cauchy problem (2.6) with initial data

$$H\Psi_0=\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}(H_l\Psi_0^{lm})Y_{lm}.$$

Obviously, this data is also smooth and compactly supported and thus gives rise to the solution

$$\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}(e^{-itH_l}H_l\Psi_0^{lm})Y_{lm}=\sum_{l=0}^{\infty}\sum_{|m|\leqslant l}(H_le^{-itH_l}\Psi_0^{lm})Y_{lm}=H\Psi,$$

where in the second equation we again used the uniqueness of the decomposition into spherical harmonics. Thus for every $\epsilon>0$ there is a L_1 (without restriction $\geqslant L_0$) such that

$$\|H\Psi^{L_1}(t)\| < \epsilon \quad \text{for all times } t.$$

Proceeding inductively, we find for every number N and for every $\epsilon>0$ a number L_N such that

$$\|H^n\Psi^{L_N}(t)\| < \epsilon \quad \text{for all } t \text{ and } n \leqslant N.$$

Let $K\subseteq\mathbb{R}\times S^2$ be an arbitrary compact subset with smooth boundary. Then, due to the definition of the energy, there exists a constant $C_0(K)>0$ such that for $\Psi^{L_N}=(\psi_1^{L_N},\psi_2^{L_N})^T$,

$$\|\psi_1^{L_N}\|_{H^1(K)} + \|\psi_2^{L_N}\|_{L^2(K)} \leqslant C_0(K)\|\Psi^{L_N}\|.$$

Applying the same argument to $H\Psi^{L_N}=(\psi_2^{L_N},A\psi_1^{L_N})^T$, where A is the differential operator given by (2.14), there is a $C_1(K)>0$ such that

$$\|A\psi_1^{L_N}\|_{L^2(K)} + \|\psi_2^{L_N}\|_{H^1(K)} \leqslant C_1(K)\|H\Psi^{L_N}\|.$$

Since the differential operator A is of the form $A=-\Delta+X$, where X is a first order differential operator, it is in particular a second order elliptic partial differential operator. Thus, for $u\in C^\infty(\mathbb{R}\times S^2)$ and for each $U\subset\subset V\subset\subset\mathbb{R}\times S^2$ ($\subset\subset$ denotes relative compact) there is an estimate [cf. Ref. 15, p. 379 (11.3)]

$$\|u\|_{H^{k+2}(U)} \leqslant C\|Au\|_{H^k(V)} + C\|u\|_{H^{k+1}(V)} \quad \text{for all } k\geqslant 0.$$

It follows that there exist new constants $C_0(K),C_1(K)$ such that

$$\|\psi_1^{L_N}\|_{H^2(K)} + \|\psi_2^{L_N}\|_{H^1(K)} \leqslant C_0(K)\|\Psi^{L_N}\| + C_1(K)\|H\Psi^{L_N}\|.$$

Iterating this inequality, we obtain constants $C_0(K),\ldots,C_k(K)$ such that

$$\|\psi_1^{L_N}\|_{H^{k+1}(K)} + \|\psi_2^{L_N}\|_{H^k(K)} \leqslant \sum_{n=0}^{k} C_n(K)\|H^n\Psi^{L_N}\|.$$

In particular, for every $\epsilon>0$ there is a number L such that

$$\|\Psi^L(t)\|_{H^2(K)} < \epsilon \quad \text{for all } t.$$

Thus the Sobolev embedding theorem yields (possibly after enlarging L)

$$\|\Psi^L(t)\|_{L^\infty(K)} < \epsilon \quad \text{for all } t.$$

Furthermore, due to the pointwise decay for fixed modes l,m which was shown in Theorem 6.5, we can find for any $\epsilon>0$ and $(u,x)\in\mathbb{R}\times S^2$ a time t_0 and a number L such that for the solution $\Psi(t,u,x)$ of the Cauchy problem (2.6),

$$|\Psi(t,u,x)| \leqslant \sum_{l=0}^{L-1}\sum_{|m|\leqslant l} |\Psi^{lm}(t,u)Y_{lm}(x)| + |\Psi^L(t,u,x)| < \epsilon \quad \text{for all } t\geqslant t_0.$$

Since $\psi=r\phi$, this concludes the proof.

□

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Space-time matter inflation

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We study a model of power-law inflationary inflation using the space-time-matter theory of gravity for a five-dimensional canonical metric that describes an apparent vacuum. In this approach the expansion is governed by a single scalar (neutral) quantum field. In particular, we study the case where the power of expansion of the universe is $p \gg 1$. This kind of model is more successful than others in accounting for galaxy formation. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A standard mechanism for galaxy formation is the amplification of primordial fluctuations by the evolutionary dynamics of space-time. The inflationary cosmology is based on the dynamics of a quantum field undergoing a phase transition.[1] The exponential expansion of the scale parameter naturally gives a scale-invariant spectrum on cosmological scales, in agreement with experimental data. This is one of the many attractive features of the inflationary universe, particulary in regard to the galaxy formation problem[2] and it arises from the fluctuations of the inflaton, the quantum field which induces inflation. This field can be semiclassically expanded in terms of its expectation value plus other fields, which describe the quantum fluctuations.[3] The quantum to classical transition of quantum fluctuations has been studied thoroughly.[4] The infrared matter field fluctuations are classical and can be described by a coarse-grained field which takes into account only wavelengths larger than the Hubble radius. The dynamics of this coarse-grained field is described by a second order stochastic equation, which can be treated using the Fokker-Planck formalism. This issue has been the subject of intense work during the last two decades.[5] Because of the success of this theory to explain the large-scale structure formation, inflation has become a standard ingredient for the description of the early universe. In fact, it is the unique that solves some of the problems of the standard big-bang scenario and also makes predictions about cosmic microwave background (CMBR) anisotropies, which are being measured with increasing precision.

On the other hand, recently, extra dimensional theories of gravity have received much interest, mainly sparked by works in string[6] and supergravity theories.[7] For the most part, four-dimensional (4D) space-time has been extended by the addition of several extra spatial dimensions, usually taken to be compact. Other very interesting approaches, developed by Wesson and co-workers[8,9] have given new impetus to the study of five-dimensional (5D) gravity. None of the standard dimensional reduction techniques imposed to reduce the number of space-time dimensions to four, are adhered to in their approach; indeed, the extra spatial dimension is not necessarily assumed to be compact. The main question they address in whether the 4D properties of matter can be viewed as being purely geometrical in origin. This idea is not new, and was originally introduced by Einstein.[10]

In this work we are interested in studying the early inflationary dynamics of the universe from the STM theory of gravity. In particular, we are aimed to study power-law inflation, where the

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scale factor of the universe growth as $a \sim t^p$, being $p > 1$ the power of expansion during inflation. To do this, we use the Ponce de Leon metric,[11] in the limital case where the power of expansion is $p \gg 1$, which describe an asymptotic de Sitter expansion of the universe.

II. BASIC STM EQUATIONS

Following the idea suggested by Wesson and co-workers,[8,9] in this section we develop the induced 4D equation of state from the 5D vacuum field equations, $G_{AB}=0 (A,B=0,1,2,3,4)$, which give the 4D Einstein equations $G_{\mu\nu}=8\pi G\, T_{\mu\nu}(\mu,\nu=0,1,2,3)$. In particular, we consider a 5D spatially isotropic and three-dimensional (3D) flat spherically symmetric line element

$$\mathrm{d}S^2 = e^{\alpha(\psi,t)}\,\mathrm{d}t^2 - e^{\beta(\psi,t)}\,\mathrm{d}r^2 - e^{\gamma(\psi,t)}\,\mathrm{d}\psi^2, \tag{1}$$

where $\mathrm{d}r^2=\mathrm{d}x^2+\mathrm{d}y^2+\mathrm{d}z^2$ and ψ is the fifth coordinate. We assume that e^{α}, e^{β}, and e^{γ} are separable functions of the variables ψ and t. The equations for the relevant Einstein tensor elements are

$$G^0{}_0 = -e^{-\alpha}\left[\frac{3\dot{\beta}^2}{4}+\frac{3\dot{\beta}\dot{\gamma}}{4}\right]+e^{-\gamma}\left[\frac{3\overset{\star\star}{\beta}}{2}+\frac{3\overset{\star 2}{\beta}}{2}-\frac{3\overset{\star}{\gamma}\overset{\star}{\beta}}{4}\right], \tag{2}$$

$$G^0{}_4 = e^{-\alpha}\left[\frac{3\overset{\star\cdot}{\beta}}{2}+\frac{3\dot{\beta}\overset{\star}{\beta}}{4}-\frac{3\dot{\beta}\overset{\star}{\alpha}}{4}-\frac{3\overset{\star}{\gamma}\dot{\gamma}}{4}\right], \tag{3}$$

$$\begin{aligned} G^i{}_i = &-e^{-\alpha}\left[\ddot{\beta}+\frac{3\dot{\beta}^2}{4}+\frac{\ddot{\gamma}}{2}+\frac{\dot{\gamma}^2}{4}+\frac{\dot{\beta}\dot{\gamma}}{2}-\frac{\dot{\alpha}\dot{\beta}}{2}-\frac{\dot{\alpha}\dot{\gamma}}{4}\right] \\ &+e^{-\gamma}\left[\overset{\star\star}{\beta}+\frac{3\overset{\star 2}{\beta}}{4}+\frac{\overset{\star\star}{\alpha}}{2}+\frac{\overset{\star 2}{\alpha}}{4}+\frac{\overset{\star}{\beta}\overset{\star}{\alpha}}{2}-\frac{\overset{\star}{\gamma}\overset{\star}{\beta}}{2}-\frac{\overset{\star}{\alpha}\overset{\star}{\gamma}}{4}\right], \end{aligned} \tag{4}$$

$$G^4{}_4 = e^{-\alpha}\left[\frac{3\ddot{\beta}}{2}+\frac{3\dot{\beta}^2}{2}-\frac{3\dot{\alpha}\dot{\beta}}{4}\right]+e^{-\gamma}\left[\frac{3\overset{\star 2}{\beta}}{4}+\frac{3\overset{\star}{\beta}\overset{\star}{\alpha}}{4}\right], \tag{5}$$

where the overstar and the overdot denote, respectively, $\partial/\partial\psi$ and $\partial/\partial t$, and $i=1,2,3$. We shall use the signature $(+,-,-,-)$ for the 4D metric, such that we define $T^0_0=\rho_t$ and $T^1_1=-p$, where ρ_t is the total energy density and p is the pressure. The 5D-vacuum conditions ($G^A_B=0$) are given by[12]

$$8\pi G\rho_t = \tfrac{3}{4}e^{-\alpha}\dot{\beta}^2, \tag{6}$$

$$8\pi G p = e^{-\alpha}\left[\frac{\dot{\alpha}\dot{\beta}}{2}-\ddot{\beta}-\frac{3\dot{\beta}^2}{4}\right], \tag{7}$$

$$e^{\alpha}\left[\frac{3\overset{\star 2}{\beta}}{4}+\frac{3\overset{\star}{\beta}\overset{\star}{\alpha}}{4}\right] = e^{\gamma}\left[\frac{\ddot{\beta}}{2}+\frac{3\dot{\beta}^2}{2}-\frac{\dot{\alpha}\dot{\beta}}{4}\right]. \tag{8}$$

Hence, from Eqs. (6) and (7) and taking $\dot{\alpha}=0$, we obtain the equation of state for the induced matter

$$p = -\left(\frac{4}{3}\frac{\ddot{\beta}}{\dot{\beta}^2} + 1\right)\rho_t. \tag{9}$$

Notice that for $\ddot{\beta}/\dot{\beta}^2 \leqslant 0$ and $|\ddot{\beta}/\dot{\beta}^2| \ll 1$ (or zero), this equation describes an inflationary universe. The particular case $\ddot{\beta}/\dot{\beta}^2 = 0$ corresponds to a 4D de Sitter expansion for the universe.

As in a previous paper,[13] we shall consider power-law inflation, which can be obtained from the metric (1), when α, β, and γ are functions of the following coordinates:

$$\alpha \equiv \alpha(\psi), \quad \beta \equiv \beta(\psi, t), \quad \gamma \equiv \gamma(t). \tag{10}$$

Here, e^{β} is a separable function of ψ and t. The conditions (10) imply that $\dot{\alpha} = \overset{\star}{\gamma} = 0$. Furthermore, we shall consider the case where all the coordinates are independent. The choice (10) implies that only the spatial sphere and the fifth coordinate have squared sizes e^{β} and e^{γ}, respectively, that evolve with time.

III. THE MODEL

In this paper we shall consider the particular case of choosing for the metric (1),

$$e^{\alpha} = \psi^2, \quad e^{\beta} = \left(\frac{t}{t_0}\right)^{2p} \psi^{2p/(p-1)}, \quad e^{\gamma} = \frac{t^2}{(p-1)^2}, \tag{11}$$

which corresponds to the Ponce de Leon metric[11]

$$\mathrm{d}S^2 = \psi^2\,\mathrm{d}t^2 - \left(\frac{t}{t_0}\right)^{2p} \psi^{2p/(p-1)}\,\mathrm{d}r^2 - \frac{t^2}{(p-1)^2}\mathrm{d}\psi^2, \tag{12}$$

for which the absolute value for the determinant of the metric tensor g_{AB} is

$$|^{(5)}g| = \left[\frac{t^{3p+1}\psi^{(4p-1)/(p-1)}}{(p-1)t_0^{3p}}\right]^2.$$

Furthermore, we shall consider an action that describes a free scalar field minimally coupled to gravity

$$I = -\int d^4x\,\mathrm{d}\psi \sqrt{\left|\frac{^{(5)}g}{^{(5)}g_0}\right|}\left[\frac{^{(5)}R}{16\pi G} + {}^{(5)}\mathcal{L}(\varphi, \varphi_{,A})\right], \tag{13}$$

with a Lagrangian

$$L = \sqrt{\frac{^{(5)}g}{^{(5)}g_0}}\mathcal{L}(\varphi, \varphi_{,A}), \tag{14}$$

and the Lagrangian density

$$\mathcal{L} = \tfrac{1}{2}g^{AB}\varphi_{,A}\varphi_{,B}. \tag{15}$$

The scalar $^{(0)}g_0$ in the action (13) is given by $^{(0)}g|_{t=t_0,\psi=\psi_0}$, such that

$$|^{(5)}g_0| = \left(\frac{t_0\psi_0^{(4p-1)/(p-1)}}{(p-1)}\right)^2,$$

where t_0 and ψ_0 are constants. Note that $|^{(5)}g|$ and $|^{(5)}g_0|$ are not well defined for $p=1$. The Lagrange equation is given by

$$\ddot{\varphi}+\frac{3p+1}{t}\dot{\varphi}-\left(\frac{t_0^p\psi^{1/(1-p)}}{t^p}\right)^2\nabla^2\varphi-\psi\frac{(p-1)(4p-1)}{t^2}\varphi_{,\psi}-\psi^2\frac{(p-1)^2}{t^2}\varphi_{,\psi\psi}=0, \tag{16}$$

where the overdot denotes the derivative with respect to the time and $\varphi_{,\psi}=\partial\varphi/\partial\psi$. In order to simplify the structure of this equation we propose the transformation $\varphi=(t_0/t)^{(3p+1)/2}(\psi_0/\psi)^{[(4p-1)/2(p-1)]}\chi$, such that the equation of motion for χ is

$$\ddot{\chi}-\psi^{2/(1-p)}\left(\frac{t_0}{t}\right)^{2p}\nabla^2\chi-\psi^2\frac{(p-1)^2}{t^2}\chi_{,\psi\psi}+\frac{(31p^2-14p+2)}{4t^2}\chi=0. \tag{17}$$

We propose the following Fourier's expansion for χ:

$$\chi(t,\vec{r},\psi)=\frac{1}{(2\pi)^{3/2}}\int d^3k_r\int \mathrm{d}k_\psi[a_{k_rk_\psi}e^{i(\vec{k}_r\cdot\vec{r}+\vec{k}_\psi\cdot\psi)}\xi_{k_rk_\psi}+a^\dagger_{k_rk_\psi}e^{-i(\vec{k}_r\cdot\vec{r}+\vec{k}_\psi\cdot\psi)}\xi^*_{k_rk_\psi}], \tag{18}$$

where the operators $a_{k_rk_\psi}$ and $a^\dagger_{k_rk_\psi}$ describe the algebra

$$[a_{k_rk_\psi},a^\dagger_{k'_rk'_\psi}]=\delta^{(3)}(\vec{k}_r-\vec{k}'_r)\,\delta(\vec{k}_\psi-\vec{k}'_\psi),\quad [a_{k_rk_\psi},a_{k'_rk'_\psi}]=[a^\dagger_{k_rk_\psi},a^\dagger_{k'_rk'_\psi}]=0.$$

The dynamics of the time dependent modes $\xi_{k_rk_\psi}$ is given by

$$\ddot{\xi}_{k_rk_\psi}+\left[\psi^{2/(1-p)}\left(\frac{t_0}{t}\right)^{2p}k_r^2+\frac{\psi^2(p-1)^2}{t^2}\left(k_\psi^2+\frac{(31p^2-14p+2)}{4(p-1)^2\psi^2}-2ik_\psi\frac{\partial}{\partial\psi}-\frac{\partial^2}{\partial\psi^2}\right)\right]\xi_{k_rk_\psi}=0. \tag{19}$$

The commutator between χ and $\dot{\chi}$ is

$$[\chi(t,\vec{r},\psi),\dot{\chi}(t,\vec{r},\psi')]=i\,\delta^{(3)}(\vec{r}-\vec{r})\,\delta(\psi-\psi'), \tag{20}$$

which complies for $\xi_{k_rk_\psi}(t,\psi)\dot{\xi}^*_{k_rk_\psi}(t,\psi')-\xi^*_{k_rk_\psi}(t,\psi')\dot{\xi}_{k_rk_\psi}(t,\psi)=i$, that guarantee the normalization of $\xi_{k_rk_\psi}$. Furthermore, if we make the transformation $\xi_{k_rk_\psi}=e^{-i\vec{k}_\psi\cdot\psi}\tilde{\xi}_{k_rk_\psi}$, we obtain from Eq. (19) the equation of motion for $\tilde{\xi}_{k_rk_\psi}$,

$$\ddot{\tilde{\xi}}_{k_rk_\psi}-\frac{\psi^2}{t^2}(p-1)^2\frac{\partial^2\tilde{\xi}_{k_rk_\psi}}{\partial\psi^2}+\left[\psi^{2/(1-p)}\left(\frac{t_0}{t}\right)^{2p}k_r^2+\frac{(31p^2-14p+1)}{4t^2}\right]\tilde{\xi}_{k_rk_\psi}=0, \tag{21}$$

and the expansion (18) for χ can be rewritten as

$$\chi(t,\vec{r},\psi)=\frac{1}{(2\pi)^{3/2}}\int d^3k_r\int \mathrm{d}k_\psi[a_{k_rk_\psi}e^{i\vec{k}_r\cdot\vec{r}}\tilde{\xi}_{k_rk_\psi}+a^\dagger_{k_rk_\psi}e^{-i\vec{k}_r\cdot\vec{r}}\,\tilde{\xi}^*_{k_rk_\psi}]. \tag{22}$$

4D dynamics of the inflaton field

Now we consider a foliation (choice of a hypersurface) $\psi=\psi_0$ on the metric (12). On this foliation, the effective 4D line element is

$$\mathrm{d}S^2\to\mathrm{d}s^2=\psi_0^2\,\mathrm{d}t^2-\left(\frac{t}{t_0}\right)^{2p}\psi_0^{2p/(p-1)}\,\mathrm{d}r^2, \tag{23}$$

where ψ_0 is a dimensionless constant and the scale factor of the universe is given by $a=a_0(t/t_0)^p$. During inflation $p\gg1$, such that $\ddot{a}>0$ and, for $\dot{\beta}=2H=2\dot{a}/a$ in Eq. (9), the equation of

state describes a quasi-de Sitter (quasivacuum) expansion, $p \simeq \left[\frac{4}{3}(\dot{H}/H^2)+1\right]\rho_t \simeq -\rho_t$. The Lagrangian density (15) can be expanded in the following manner: ${}^{(5)}\mathcal{L} = \frac{1}{2}[g^{\mu\nu}\varphi_{,\mu}\varphi_{,\nu} + g^{\psi\psi}\varphi_{,\psi}\varphi_{,\psi}]$, such that the effective 4D Lagrangian density for the inflaton field on the foliation $\psi = \psi_0$ can be written as

$$ {}^{(4)}\mathcal{L} = \tfrac{1}{2}g^{\mu\nu}\varphi_{,\mu}\varphi_{,\nu} - V(\varphi)\big|_{\psi=\psi_0}, \tag{24}$$

where $V(\varphi)$ is given by

$$ V(\varphi) = -\frac{1}{2}g^{\psi\psi},_{\varphi,\psi}\varphi_{,\psi}\Big|_{\psi=\psi_0} = \frac{(p-1)^2}{2t^2}\left(\frac{\partial\varphi}{\partial\psi}\right)^2\Bigg|_{\psi=\psi_0}. \tag{25}$$

On the other hand, for a foliation $\psi = \psi_0$, the dynamics of the inflaton field holds

$$ \ddot{\varphi} + \frac{(3p+1)}{t}\dot{\varphi} - \left(\frac{t_0}{t}\right)^{2p}\psi^{2/(1-p)}\nabla^2\varphi - \left[\frac{\psi(p-1)(4p-1)}{t^2}\varphi_{,\psi} + \frac{\psi^2(p-1)^2}{t^2}\varphi_{,\psi\psi}\right]\Bigg|_{\psi=\psi_0} = 0, \tag{26}$$

so that we can make the following identification:

$$ V'(\varphi) = \left[\frac{\dot{\varphi}}{t} - \frac{\psi(p-1)(4p-1)}{t^2}\varphi_{,\psi} - \frac{\psi^2(p-1)^2}{t^2}\varphi_{,\psi\psi}\right]\Bigg|_{\psi=\psi_0}. \tag{27}$$

Furthermore, the scalar field χ in Eq. (22) on the foliation $\psi = \psi_0$ now holds

$$ \chi(t,\vec{r},\psi=\psi_0) = \frac{1}{(2\pi)^{3/2}}\int d^3k_r \int \mathrm{d}k_\psi [a_{k_r k_\psi} e^{i\vec{k}_r\cdot\vec{r}}\,\tilde{\xi}_{k_r k_\psi} + \mathrm{c.c.}]\,\delta(k_\psi - k_{\psi_0}). \tag{28}$$

Note that the equation (26) is not separable on the coordinate ψ. However, in the limit $p \gg 1$, which is relevant to study the inflationary expansion of the early universe, the term $(t_0/t)^{2p}\psi^{2/(1-p)}\nabla^2\varphi$ in Eq. (26) tends asymptotically to $(t_0/t)^{2p}\nabla^2\varphi$ as $p \to \infty$. Hence, in this limital case the dynamics for φ is governed by the equation

$$ \ddot{\varphi} + \frac{(3p+1)}{t}\dot{\varphi} - \left(\frac{t_0}{t}\right)^{2p}\nabla^2\varphi - \left[\frac{\psi(p-1)(4p-1)}{t^2}\varphi_{,\psi} + \frac{\psi^2(p-1)^2}{t^2}\varphi_{,\psi\psi}\right]\Bigg|_{\psi=\psi_0} = 0, \tag{29}$$

which is separable on the variable ψ and more easily workable. This particular case will be studied in the next section.

IV. INFLATIONARY EXPANSION ($P \gg 1$)

We consider the case where $p \gg 1$, which describes an inflationary power-law expansion in the very early universe. In this case the equation for the modes, (21), can be approximated to

$$ \ddot{\tilde{\xi}}_{k_r k_\psi} - \frac{\psi^2(p-1)^2}{t^2}\frac{\partial^2\tilde{\xi}_{k_r k_\psi}}{\partial\psi^2} + \left[k_r^2\left(\frac{t_0}{t}\right)^{2p} + \frac{(31p^2-14p+2)}{4t^2}\right]\tilde{\xi}_{k_r k_\psi} \simeq 0. \tag{30}$$

The general solution for this equation on the foliation $\psi = \psi_0$ is

$$ \tilde{\xi}_{k_r k_\psi}(t,\psi) = \alpha\sqrt{\frac{t}{t_0}}\mathcal{H}_\nu^{(1)}[x(t)], \tag{31}$$

where $\nu=\sqrt{(1+4C)}/2(p-1)$, $x(t)=k_r t_0^p t^{1-p}/(p-1)$,

$$\alpha = A_1[M_1\psi_0^{(1/2)+\sqrt{(1/4)+[C/(p-1)^2]}} + M_2\psi_0^{(1/2)-\sqrt{(1/4)+[C/(p-1)^2]}}],$$

$C=C_1+[(31p^2-14p+2)/4]$ and C_1, A_1, M_1, and M_2 are constants of integration. Furthermore, the normalization condition implies that

$$\frac{4(p-1)}{t_0\pi}|\alpha|^2 = 1. \tag{32}$$

To calculate the inflation field fluctuations on the infrared sector, which is relevant for super Hubble scales during inflation, we can make use of the asymptotic representations of the first kind of Hankel function $\mathcal{H}_\nu^{(1)}[x]$ for $x \ll 1$,

$$\mathcal{H}_\nu^{(1)}[x] \simeq \frac{1}{\Gamma(\nu+1)}\left(\frac{x}{2}\right)^\nu + \frac{i}{\pi}\Gamma(\nu)\left(\frac{x}{2}\right)^{-\nu}.$$

With this representation the squared χ fluctuations on cosmological scales are $\langle\chi^2\rangle|_{\mathrm{IR}} = (1/2\pi^2)\int_0^{\epsilon k_0} \mathrm{d}k_r\, k_r^2 \tilde{\xi}_{k_r k_{\psi 0}} \tilde{\xi}^*_{k_r k_{\psi 0}}$ where $k_0(t)=[\sqrt{31p^2-14p+2}/2t_0^p]t^{p-1}$ is the wave number that separates the infrared (IR) and ultraviolet sectors. Making the calculation, we obtain

$$\langle\chi^2\rangle|_{\mathrm{IR}} = \frac{t}{8\pi(p-1)}\left[\frac{1}{\Gamma^2(\nu+1)}\left(\frac{\epsilon^3(31p^2-14p+2)t^{2(p-1)}}{16(p-1)t_0^{2p}}\right)^{2\nu}\frac{1}{(2\nu+3)} - \frac{\Gamma^2(\nu)}{\pi^2(3-2\nu)}\left(\frac{16(p-1)t_0^{2p}t^{-2(p-1)}}{\epsilon^3(31p^2-14p+2)}\right)^{2\nu}\right], \tag{33}$$

and the squared φ fluctuations, which are relevant for us, are

$$\langle\varphi^2\rangle|_{\mathrm{IR}} = \frac{t^{-3p}t_0^{(3p+1)}}{8\pi(p-1)}\left[\frac{1}{\Gamma^2(\nu+1)}\left(\frac{\epsilon^3(31p^2-14p+2)t^{2(p-1)}}{16(p-1)t_0^{2p}}\right)^{2\nu}\frac{1}{(2\nu+3)} - \frac{\Gamma^2(\nu)}{\pi^2(3-2\nu)}\left(\frac{16(p-1)t_0^{2p}t^{-2(p-1)}}{\epsilon^3(31p^2-14p+2)}\right)^{2\nu}\right], \tag{34}$$

which decrease with time as $\langle\varphi^2\rangle|_{\mathrm{IR}} \sim t^{-3p}$. The power spectrum of these fluctuations goes as $\mathcal{P}(k_r) \sim k_r^{3-2\nu}$ which is scale invariant for $C_1=[9(p-1)-2]/8$ and hence for $C=[61p^2-(19p+7)]/8$. This result is very interesting because (with an adequate choice of constant values) we can obtain scale invariance for the power spectrum of $\langle\varphi^2\rangle$ for any $p \gg 1$, independently of some particular value for it.

V. FINAL COMMENTS

In this paper we have studied power-law inflation in the limital case $p \gg 1$ from a STM theory of gravity using the Ponce de Leon metric. In this approach, the inflationary expansion is governed by a single scalar field, that, on a foliation $\psi=\psi_0$ in the 5D metric (12) can be identified as the inflaton field evolving on the effective 4D Friedmann-Robertson-Walker metric (23). In Wesson's theory [called space-time-matter (STM) theory], the, extra dimension is not assumed to be compactified, which is a major departure from earlier multidimensional theories where the cylindricity conditions were imposed. In this theory, the original motivation for assuming the existence of a large extra dimension was to achieve the unification of matter and geometry, i.e., to obtain the properties of matter as a consequence of the extra dimensions. A very important fact in our

approach is that the effective potential $V(\varphi)=-\frac{1}{2}g^{\psi\psi}(\partial\varphi/\partial\psi)^2|_{\psi=\psi_0}$, has a geometrical origin.

In this paper we have studied with major detail the case $p\gg 1$, because this is where the field $\varphi(t,\vec{r},t)$ is separable on the variable ψ and can be more easily treated. However, for cases where the power p is of the order of the unity, the fifth coordinate ψ could play a more important role in the spectrum of the squared φ fluctuations.

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A Morse-theoretical analysis of gravitational lensing by a Kerr-Newman black hole

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Consider, in the domain of outer communication M_+ of a Kerr-Newman black hole, a point p (observation event) and a timelike curve γ (worldline of light source). Assume that γ (i) has no past endpoint, (ii) does not intersect the caustic of the past light cone of p, and (iii) goes neither to the horizon nor to infinity in the past. We prove that then for infinitely many positive integers k there is a past-pointing lightlike geodesic λ_k of (Morse) index k from p to γ, hence an observer at p sees infinitely many images of γ. Moreover, we demonstrate that all lightlike geodesics from an event to a timelike curve in M_+ are confined to a certain spherical shell. Our characterization of this spherical shell shows that in the Kerr-Newman space-time the occurrence of infinitely many images is intimately related to the occurrence of centrifugal-plus-Coriolis force reversal. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2188209]

I. INTRODUCTION

The question of how many images an observer at an event p sees of a light source with worldline γ is equivalent to the question of how many past-pointing lightlike geodesics from p to γ exist. In space-times with many symmetries this question can be addressed, in principle, by directly integrating the geodesic equation. In the space-time around a nonrotating and uncharged black hole of mass m, e.g., which is described by the Schwarzschild metric, all lightlike geodesics can be explicitly written in terms of elliptic integrals; with the help of these explicit expressions, it is easy to verify that in the region outside the horizon, i.e., in the region where $r>2m$, there are infinitely many past-pointing lightlike geodesics from any event p to any integral curve of the Killing vector field ∂_t. This was demonstrated already in 1959 by Darwin.[1] We may thus say that a Schwarzschild black hole acts as a gravitational lens that produces infinitely many images of any static light source. However, already in the Schwarzschild space-time the problem becomes more difficult if we want to consider light sources which are not static, i.e., worldlines γ which are not integral curves of ∂_t.

In this paper we want to investigate this problem for the more general case of a charged and rotating black hole, which is described by the Kerr-Newman metric. More precisely, we want to demonstrate that in the domain of outer communication around a Kerr-Newman black hole, i.e., in the domain outside of the outer horizon, there are infinitely many past-pointing lightlike geodesics from an unspecified event p to an unspecified worldline γ, with as little restrictions on γ as possible. Although the geodesic equation in the Kerr-Newman space-time is completely inte-

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grable, the mathematical expressions are so involved that it is very difficult to achieve this goal by explicitly integrating the geodesic equation. Therefore it is recommendable to use more indirect methods.

Such a method is provided by Morse theory. Quite generally, Morse theory relates the number of solutions to a variational principle to the topology of the space of trial maps. Here we refer to a special variant of Morse theory, developed by Uhlenbeck,[2] which is based on a version of Fermat's principle for a globally hyperbolic Lorentzian manifold (M,g). The trial maps are the lightlike curves joining a point p and a timelike curve γ in M, and the solution curves of Fermat's principle are the lightlike geodesics. If (M,g) and γ satisfy additional conditions, the topology of the space of trial maps is determined by the topology of M. Uhlenbeck's work gives criteria that guarantee the existence of infinitely many past- or future-pointing lightlike geodesics from p to γ. In this paper we will apply her results to the domain of outer communication around a Kerr-Newman black hole which is, indeed, a globally hyperbolic Lorentzian manifold. We will show that the criteria for having infinitely many past-pointing timelike geodesics from p to γ are satisfied for every event p and every timelike curve γ in this region, provided that the following three conditions are satisfied. First, γ must not have a past endpoint; it is obvious that we need a condition of this kind because otherwise it would be possible to choose for γ an arbitrarily short section of a worldline such that trivially the number of past-pointing lightlike geodesics from p to γ is zero. Second, γ must not intersect the caustic of the past light-cone of p; this excludes all cases where p sees an extended image, such as an Einstein ring, of γ. Third, in the past the worldline γ must not go to the horizon or to infinity. Under these (very mild) restrictions on the motion of the light source we will see that the Kerr-Newman black hole acts as a gravitational lens that produces infinitely many images. Moreover, we will also show that all (past-directed) lightlike geodesics from p to γ are confined to a certain spherical shell. For the characterization of this shell we will have to discuss a light-convexity property which turns out to be intimately related to the phenomenon of centrifugal (-plus-Coriolis) force reversal. This phenomenon has been discussed, first in spherically symmetric static and then in more general space-times, in several papers by Abramowicz with various coauthors; material which is of interest to us can be found, in particular, in Abramowicz, Carter, and Lasota,[3] Abramowicz,[4] and Abramowicz, Nurowski, and Wex.[5]

The paper is organized as follows. In Sec. II we summarize the Morse-theoretical results we want to use. Section III is devoted to the notions of centrifugal and Coriolis force in the Kerr-Newman space-time; in particular, we introduce a potential Ψ_+ (respectively, Ψ_-) that characterizes the sum of centrifugal and Coriolis force with respect to corotating (respectively, counterrotating) observers whose velocity approaches the velocity of light. In Sec. IV we discuss multiple imaging in the Kerr-Newman space-time with the help of the Morse theoretical result quoted in Sec. II and with the help of the potential $\Psi_\pm$ introduced in Sec. III. Our results are summarized and discussed in Sec. V.

II. A RESULT FROM MORSE THEORY

In this section we briefly review a Morse-theoretical result that relates the number of lightlike geodesics between a point p and a timelike curve γ in a globally hyperbolic Lorentzian manifold to the topology of this manifold. This result was found by Uhlenbeck[2] and its relevance in view of gravitational lensing was discussed by McKenzie.[6] Uhlenbeck's work is based on a variational principle for lightlike geodesics ("Fermat principle") in a globally hyperbolic Lorentzian manifold, and her main method of proof is to approximate trial paths by broken geodesics. With the help of infinite-dimensional Hilbert manifold techniques Giannoni, Masiello, and Piccione were able to rederive Uhlenbeck's result[7] and to generalize it to certain subsets-with-boundary of space-times that need not be globally hyperbolic.[8] In contrast to Uhlenbeck, they start out from a variational principle for lightlike geodesics that is not restricted to globally hyperbolic space-times. (Such a Fermat principle for arbitrary general-relativistic space-times was first formulated by Kovner;[9] the proof that the solution curves of Kovner's variational principle are, indeed, precisely the lightlike geodesics was given by Perlick[10]). Although for our purpose the original Uhlenbeck result is

sufficient, readers who are interested in technical details are encouraged to also consult the papers by Giannoni, Masiello, and Piccione, in particular because in the Uhlenbeck paper some of the proofs are not worked out in full detail.

Following Uhlenbeck,[2] we consider a four-dimensional Lorentzian manifold (M,g) that admits a foliation into smooth Cauchy surfaces, i.e., a globally hyperbolic space-time. (For background material on globally hyperbolic space-times the reader may consult, e.g., Hawking and Ellis.[11] The fact that the original definition of global hyperbolicity is equivalent to the existence of a foliation into *smooth* Cauchy surfaces was completely proven only recently by Bernal and Sánchez.[12]) Then M can be written as a product of a three-dimensional manifold S, which serves as the prototype for each Cauchy surface, and a time axis,

$$M = S \times \mathbb{R}. \tag{1}$$

Moreover, this product can be chosen such that the metric g orthogonally splits into a spatial and a temporal part,

$$g = g_{ij}(x,t)\mathrm{d}x^i\,\mathrm{d}x^j - f(x,t)\mathrm{d}t^2, \tag{2}$$

where t is the time coordinate given by projecting from $M=S\times\mathbb{R}$ onto the second factor, $x=(x^1,x^2,x^3)$ are coordinates on S, and the summation convention is used for italic indices running from 1 to 3. [We write (2) in terms of coordinates for notational convenience only. We do not want to presuppose that S can be covered by a single coordinate system.] We interpret the direction of increasing t as the future direction on M. Again following Uhlenbeck,[2] we say that the splitting (2) satisfies the *metric growth condition* if for every compact subset of S there is a function F with

$$\int_{-\infty}^{0} \frac{\mathrm{d}t}{F(t)} = \infty, \tag{3}$$

such that for $t\leqslant 0$ the inequality

$$g_{ij}(x,t)v^iv^j \leqslant f(x,t)F(t)^2G_{ij}(x)v^iv^j \tag{4}$$

holds for all x in the compact subset and for all $(v^1,v^2,v^3)\in\mathbb{R}^3$, with a time-independent Riemannian metric G_{ij} on S. It is easy to check that the metric growth condition assures that for every (smooth) curve $\alpha:[a,b]\to S$ there is a function $T:[a,b]\to\mathbb{R}$ with $T(a)=0$ such that the curve $\lambda:[a,b]\to M=S\times\mathbb{R}$, $s\mapsto\lambda(s)=(\alpha(s),T(s))$ is past-pointing and lightlike. In particular, the metric growth condition assures that from each point p in M we can find a past-pointing lightlike curve to every timelike curve that is vertical with respect to the orthogonal splitting chosen. In this sense, the metric growth condition prohibits the existence of *particle horizons*, cf. Uhlenbeck[2] and McKenzie.[6] Please note that our formulation of the metric growth condition is the same as McKenzie's which differs from Uhlenbeck's by interchanging future and past (i.e., $t\mapsto -t$). The reason is that Uhlenbeck in her paper characterizes *future-pointing* lightlike geodesics from a point to a timelike curve whereas we, in view of gravitational lensing, are interested in *past-pointing* ones.

For formulating Uhlenbeck's result we have to assume that the reader is familiar with the notion of *conjugate points* and with the following facts (see, e.g., Perlick[13]). The totality of all conjugate points, along any lightlike geodesic issuing from a point p into the past, makes up the *caustic* of the past light-cone of p. A lightlike geodesic is said to have (Morse) index k if it has k conjugate points in its interior; here and in the following every conjugate point must be counted with its multiplicity. For a lightlike geodesic with two endpoints, the index is always finite. It is our goal to estimate the number of past-pointing lightlike geodesics of index k from a point p to a timelike curve γ that does not meet the caustic of the past light-cone of p. The latter condition is generically satisfied in the sense that, for any γ, the set of all points p for which it is true is dense in M. This condition makes sure that the past-pointing lightlike geodesics from p to γ are

countable, i.e., it excludes gravitational lensing situations where the observer sees a continuum of images such as an Einstein ring.

As another preparation, we recall how the *Betti numbers* B_k of the *loop space* $L(M)$ of a connected topological space M are defined. As a realization of $L(M)$ one may take the space of all continuous curves between any two fixed points in M. The kth Betti number B_k is formally defined as the dimension of the kth homology space of $L(M)$ with coefficients in a field $\mathbb{F}$. (For our purpose we may choose $\mathbb{F}=\mathbb{R}$.) Roughly speaking, B_0 counts the connected components of $L(M)$ and B_k, for $k>0$, counts those "holes" in $L(M)$ that prevent a k sphere from being a boundary. If the reader is not familiar with Betti numbers he or she may consult, e.g., Ref. 14.

After these preparations Uhlenbeck's result that we want to use later in this paper can now be phrased in the following way.

Theorem 1 (Uhlenbeck[2]): *Consider a globally hyperbolic space-time* (M,g) *that admits an orthogonal splitting* (1) and (2) *satisfying the metric growth condition. Fix a point* $p\in M$ *and a smooth timelike curve* $\gamma:\mathbb{R}\to M$ *which, in terms of the above-mentioned orthogonal splitting, takes the form* $\gamma(\tau)=(\beta(\tau),\tau)$, *with a curve* $\beta:\mathbb{R}\to S$. *Moreover, assume that* γ *does not meet the caustic of the past light-cone of* p *and that for some sequence* $(\tau_i)_{i\in N}$ *with* $\tau_i\to-\infty$ *the sequence* $(\beta(\tau_i))_{i\in N}$ *converges in* S. *Then the Morse inequalities*

$$N_k \geqslant B_k \quad \text{for all } k\in\mathbb{N}_0 \tag{5}$$

and the Morse relation

$$\sum_{k=0}^{\infty}(-1)^k N_k=\sum_{k=0}^{\infty}(-1)^k B_k \tag{6}$$

hold true, where N_k *denotes the number of past-pointing lightlike geodesics with index* k *from* p *to* γ, *and* B_k *denotes the* kth *Betti number of the loop space of* M.

Proof: See Uhlenbeck,[2] Sec. IV and Proposition 5.2. □

Please note that the convergence condition on $(\beta(\tau_i))_{i\in N}$ is certainly satisfied if β is confined to a compact subset of S, i.e., if γ stays in a spatially compact set.

The sum on the right-hand side of (6) is, by definition, the Euler characteristic χ of the loop space of M. Hence, (6) can also be written in the form

$$N_+ - N_- = \chi, \tag{7}$$

where N_+ (respectively, N_-) denotes the number of past-pointing lightlike geodesics with even (respectively, odd) index from p to γ.

The Betti numbers of the loop space of $M=S\times\mathbb{R}$ are, of course, determined by the topology of S. Three cases are to be distinguished.

Case A: M is not simply connected. Then the loop space of M has infinitely many connected components, so $B_0=\infty$. In this situation (5) says that $N_0=\infty$, i.e., that there are infinitely many past-pointing lightlike geodesics from p to γ that are free of conjugate points.

Case B: M is simply connected but not contractible to a point. Then for all but finitely many $k\in\mathbb{N}_0$ we have $B_k>0$. This was proven in a classical paper by Serre,[15] cf. McKenzie.[6] In this situation (5) implies $N_k>0$ for all but finitely many k. In other words, for almost every positive integer k we can find a past-pointing lightlike geodesic from p to γ with k conjugate points in its interior. Hence, there must be infinitely many past-pointing lightlike geodesics from p to γ and the caustic of the past light-cone of p must be complicated enough such that a past-pointing lightlike geodesic from p can intersect it arbitrarily often.

Case C: M is contractible to a point. Then the loop space of M is contractible to a point, i.e., $B_0=1$ and $B_k=0$ for $k>0$. In this case (7) takes the form $N_+-N_-=1$ which implies that the total number $N_++N_-=2N_-+1$ of past-pointing lightlike geodesics from p to γ is (infinite or) odd.

The domain of outer communication of a Kerr-Newman black hole has topology $S^2 \times \mathbb{R}^2$ which is simply connected but not contractible to a point. So it is Case B we are interested in when applying Uhlenbeck's result to the Kerr-Newman space-time.

III. CENTRIFUGAL AND CORIOLIS FORCE IN THE KERR-NEWMAN SPACE-TIME

The Kerr-Newman metric is given in Boyer-Lindquist coordinates (see, e.g., Misner, Thorne, and Wheeler,[16] p. 877) by

$$g = -\frac{\Delta}{\rho^2}(\mathrm{d}t - a\sin^2\vartheta\,\mathrm{d}\varphi)^2 + \frac{\sin^2\vartheta}{\rho^2}((r^2+a^2)\mathrm{d}\varphi - a\,\mathrm{d}t)^2 + \frac{\rho^2}{\Delta}\mathrm{d}r^2 + \rho^2\,\mathrm{d}\vartheta^2, \tag{8}$$

where ρ and Δ are defined by

$$\rho^2 = r^2 + a^2\cos^2\vartheta \quad \text{and } \Delta = r^2 - 2mr + a^2 + q^2, \tag{9}$$

and m, q, and a are real constants. We shall assume throughout that

$$0 < m, \quad 0 \leqslant a, \quad \sqrt{a^2+q^2} \leqslant m. \tag{10}$$

In this case, the Kerr-Newman metric describes the space-time around a rotating black hole with mass m, charge q, and specific angular momentum a. The Kerr-Newman metric (8) contains the Kerr metric ($q=0$), the Reissner-Nordström metric ($a=0$) and the Schwarzschild metric ($q=0$ and $a=0$) as special cases which are all discussed, in great detail, in Chandrasekhar;[17] for the Kerr metric we also refer to O'Neill.[18]

By (10), the equation $\Delta=0$ has two real roots,

$$r_\pm = m \pm \sqrt{m^2 - a^2 - q^2}, \tag{11}$$

which determine the two horizons. We shall restrict to the region

$$M_+: \quad r_+ < r < \infty, \tag{12}$$

which is usually called the *domain of outer communication* of the Kerr-Newman black hole. On M_+, the coordinates φ and ϑ range over S^2, the coordinate t ranges over $\mathbb{R}$, and the coordinate r ranges over an open interval which is diffeomorphic to $\mathbb{R}$; hence $M_+ \simeq S^2 \times \mathbb{R}^2$.

From now on we will consider the space-time (M_+, g), where g denotes the restriction of the Kerr-Newman metric (8) with (10) to the domain M_+ given by (12). For the sake of brevity, we will refer to (M_+, g) as to the *exterior Kerr-Newman space-time*. As a matter of fact, (M_+, g) is a globally hyperbolic space-time; the Boyer-Lindquist time coordinate t gives a foliation of M_+ into Cauchy surfaces t=constant. Together with the lines perpendicular to these surfaces, we get an orthogonal splitting of the form (2). Observers with worldlines perpendicular to the surfaces t =constant are called *zero-angular-momentum observers* or *locally nonrotating observers*. In contrast to the worldlines perpendicular to the surfaces t=constant, the integral curves of the Killing vector field ∂_t are *not* timelike on all of M_+; they become spacelike inside the so-called *ergosphere* which is characterized by the inequality $\Delta < a^2\sin^2\vartheta$. For $a \neq 0$ it is impossible to find a Killing vector field which is timelike on all of M_+; in this sense, the exterior Kerr-Newman space-time is *not* a stationary space-time.

In the rest of this section we discuss the notions of centrifugal force and Coriolis force for observers on circular orbits around the axis of rotational symmetry in the exterior Kerr-Newman space-time (M_+, g). For background information on these notions we refer to the work of Abramowicz and his collaborators[3–5] which was mentioned already in the introduction. For our discussion it will be convenient to introduce on M_+ the orthonormal basis

$$E_0 = \frac{1}{\rho\sqrt{\Delta}}((r^2+a^2)\partial_t + a\partial_\varphi),$$

$$E_1 = \frac{1}{\rho \sin \vartheta}(\partial_\varphi + a \sin^2 \vartheta \, \partial_t),$$

$$E_2 = \frac{1}{\rho}\partial_\vartheta, \quad E_3 = \frac{\sqrt{\Delta}}{\rho}\partial_r, \tag{13}$$

whose dual basis is given by the covector fields

$$-g(E_0, \cdot) = \frac{\sqrt{\Delta}}{\rho}(\mathrm{d}t - a \sin^2 \vartheta \, \mathrm{d}\varphi),$$

$$g(E_1, \cdot) = \frac{\sin \vartheta}{\rho}((r^2 + a^2)\mathrm{d}\varphi - a \, \mathrm{d}t),$$

$$g(E_2, \cdot) = \rho \, \mathrm{d}\vartheta, \quad g(E_3, \cdot) = \frac{\rho}{\sqrt{\Delta}}\mathrm{d}r. \tag{14}$$

Henceforth we refer to the integral curves of the timelike basis field E_0 as to the worldlines of the *standard observers* in (M_+, g). For later purpose we list all nonvanishing Lie brackets of the E_i,

$$[E_0, E_2] = -\frac{a^2}{\rho^3} \cos \vartheta \sin \vartheta \, E_0,$$

$$[E_0, E_3] = \left(\frac{r-m}{\rho\sqrt{\Delta}} - \frac{r\sqrt{\Delta}}{\rho^3}\right)E_0 + \frac{2ra \sin \vartheta}{\rho^3}E_1,$$

$$[E_1, E_2] = \frac{(\rho^2 + a^2 \sin^2 \vartheta)\cos \vartheta}{\rho^3 \sin \vartheta}E_1 - \frac{2a\sqrt{\Delta} \cos \vartheta}{\rho^3}E_0,$$

$$[E_1, E_3] = \frac{r\sqrt{\Delta}}{\rho^3}E_1,$$

$$[E_2, E_3] = \frac{r\sqrt{\Delta}}{\rho^3}E_2 + \frac{a^2 \cos \vartheta \sin \vartheta}{\rho^3}E_3. \tag{15}$$

For every $v \in [0,1]$, the integral curves of the vector field

$$U = \frac{E_0 \pm vE_1}{\sqrt{1 - v^2}} \tag{16}$$

can be interpreted as the worldlines of observers who circle along the φ-lines around the axis of rotational symmetry of the Kerr-Newman space-time. The number v gives the velocity (in units of the velocity of light) of these observers with respect to the standard observers. For the upper sign in (16), the motion relative to the standard observers is in the positive φ-direction and thus corotating with the black hole (because of our assumption $a \geqslant 0$), for the negative sign it is in the negative φ-direction and thus counter-rotating. Please note that $g(U,U) = -1$, which demonstrates that the integral curves of U are parametrized by proper time.

In general, U is nongeodesic, $\nabla_U U \neq 0$, i.e., one needs a thrust to stay on an integral curve of U. Correspondingly, relative to a U-observer a freely falling particle undergoes an "inertial acceleration" measured by $-\nabla_U U$. To calculate this quantity, we write

$$-g(\nabla_U U, E_i) = -Ug(U,E_i) + g(U,\nabla_U E_i) = -Ug(U,E_i) + g(U,[U,E_i]). \tag{17}$$

The first term on the right-hand side vanishes, and the second term can be easily calculated with the help of (16) and (15), for $i=0,1,2,3$. We find

$$-g(\nabla_U U, \cdot) = A_{\text{grav}} + A_{\text{Cor}} + A_{\text{cent}}, \tag{18}$$

where the covector fields

$$A_{\text{grav}} = \frac{\Delta r - \rho^2(r-m)}{\rho^2\Delta}\mathrm{d}r + \frac{a^2}{\rho^2}\sin\vartheta\cos\vartheta\,\mathrm{d}\vartheta, \tag{19}$$

$$A_{\text{Cor}} = \pm\frac{v}{(1-v^2)}\frac{2a\sqrt{\Delta}}{\rho^2}\left(\frac{r}{\Delta}\sin\vartheta\,\mathrm{d}r + \cos\vartheta\,\mathrm{d}\vartheta\right), \tag{20}$$

$$A_{\text{cent}} = \frac{v^2}{(1-v^2)}\left(\frac{2r\Delta - \rho^2(r-m)}{\rho^2\Delta}\mathrm{d}r + \frac{(\rho^2 + 2a^2\sin^2\vartheta)\cos\vartheta}{\rho^2\sin\vartheta}\mathrm{d}\vartheta\right) \tag{21}$$

give, respectively, the gravitational, the Coriolis, and the centrifugal acceleration of a freely falling particle relative to the U observers. (Multiplication with the particle's mass gives the corresponding "inertial force.") Here the decomposition of the total inertial acceleration into its three contributions is made according to the same rule as in Newtonian mechanics: The gravitational acceleration is independent of v, the Coriolis acceleration is odd with respect to v, and the centrifugal acceleration is even with respect to v. In Ref. 19 it was shown that, according to this rule, gravitational, Coriolis, and centrifugal acceleration are unambiguous whenever a timelike 2-surface with a timelike vector field has been specified; here we apply this procedure to each 2-surface $(r,\vartheta)=$constant with the timelike vector field E_0.

Up to the positive factor $v/(1-v^2)$, the sum of Coriolis and centrifugal acceleration is equal to

$$\begin{aligned} Z_\pm(v) = {} & \pm\frac{2a\sqrt{\Delta}}{\rho^2}\left(\frac{r}{\Delta}\sin\vartheta\,\mathrm{d}r + \cos\vartheta\,\mathrm{d}\vartheta\right) \\ & + v\left(\frac{2r\Delta - \rho^2(r-m)}{\rho^2\Delta}\mathrm{d}r + \frac{(\rho^2 + 2a^2\sin^2\vartheta)\cos\vartheta}{\rho^2\sin\vartheta}\mathrm{d}\vartheta\right). \end{aligned} \tag{22}$$

If we exclude the Reissner-Nordström case $a=0$, the Coriolis force dominates the centrifugal force for small v. To investigate the behavior for v close to the velocity of light, we consider the limit $v\to 1$. By a straightforward calculation we find that

$$Z_\pm(v) \underset{v\to 1}{\to} \frac{\sin\vartheta}{\rho^2\sqrt{\Delta}}(r^2 + a^2 \pm a\sqrt{\Delta}\sin\vartheta)^2\,\mathrm{d}\Psi_\pm, \tag{23}$$

where

$$\mathrm{d}\Psi_\pm = \frac{2r\Delta - (r-m)\rho^2 \pm 2ar\sqrt{\Delta}\sin\vartheta}{\sqrt{\Delta}\sin\vartheta(r^2 + a^2 \pm a\sqrt{\Delta}\sin\vartheta)^2}\mathrm{d}r + \frac{(\rho^2 + 2a^2\sin^2\vartheta \pm 2a\sqrt{\Delta}\sin\vartheta)\sqrt{\Delta}\cos\vartheta}{\sin^2\vartheta(r^2 + a^2 \pm a\sqrt{\Delta}\sin\vartheta)^2}\mathrm{d}\vartheta \tag{24}$$

is the differential of the function

$$\Psi_{\pm} = \frac{-\frac{1}{\sin\vartheta} \mp \frac{a}{\sqrt{\Delta}}}{\frac{r^2+a^2}{\sqrt{\Delta}} \pm a\sin\vartheta}. \tag{25}$$

Because of $\sin\vartheta$ in the denominator, both Ψ_- and Ψ_+ are singular along the axis. Ψ_+ is negative on all of M_+ whereas Ψ_- is negative outside and positive inside the ergosphere.

From (23) we read that, in the limit $v \to 1$, the sum of Coriolis and centrifugal force is perpendicular to the surfaces $\Psi_{\pm}$=constant and points in the direction of increasing $\Psi_{\pm}$. In this limit, we may thus view the function Ψ_+ (or Ψ_-, respectively) as a Coriolis-plus-centrifugal potential for corotating (or counter-rotating, respectively) observers. The surfaces $\Psi_{\pm}$=constant are shown in Fig. 1.

It is not difficult to see that $\Psi_{\pm}$ is independent of the family of observers with respect to which the inertial accelerations have been defined, as long as their 4-velocity is a linear combination of ∂_t and ∂_φ. We have chosen the standard observers; a different choice would lead to different formulas for the inertial accelerations (19)–(21), but to the same $\Psi_{\pm}$. For the sake of comparison, the reader may consult Nayak and Vishveshwara,[20] where the inertial accelerations are calculated with respect to the zero angular momentum observers. Also, it should be mentioned that the potentials Ψ_+ and Ψ_-, or closely related functions, have been used already by other authors. The quantities $\Omega_{c\pm}$, e.g., introduced by de Felice and Usseglio-Tomasset[21] in their analysis of physical effects related to centrifugal force reversal in the equatorial plane of the Kerr metric, are related to our potentials by $\Omega_{c\pm} = \mp\Psi_{\pm}|_{\vartheta=\pi/2}$.

In the Reissner-Nordström case $a=0$, the Coriolis acceleration (20) vanishes identically and

$$\Psi = \Psi_+ = \Psi_- = -\frac{\sqrt{r^2-2mr+q^2}}{r^2\sin\vartheta} \tag{26}$$

is a potential for the centrifugal acceleration in the sense that A_{cent} is a multiple of $\mathrm{d}\Psi$. In this case, the surfaces Ψ=constant coincide with what Abramowicz[4] calls the *von Zeipel cylinders*. Abramowicz's Fig. 1 in Ref. 4, which shows the von Zeipel cylinders in the Schwarzschild space-time, coincides with the $a \to 0$ limit of our Fig. 1, which shows the surfaces Ψ_+=constant and Ψ_-=constant in the Kerr space-time. (The notion of von Zeipel cylinders has also been defined in the Kerr metric, see Ref. 22, for observers of a specified angular velocity. However, these angular-velocity-dependent von Zeipel cylinders are not related to the potentials Ψ_+ and Ψ_- in the Kerr space-time.)

By construction, the function $\Psi_{\pm}$ has the following property. If we send a lightlike geodesic tangential to a φ-line in the positive (respectively, negative) φ-direction, it will move away from this φ-line in the direction of the negative gradient of Ψ_+ (respectively, Ψ_-). Thus, each zero of the differential $\mathrm{d}\Psi_+$ (respectively, $\mathrm{d}\Psi_-$) indicates a corotating (respectively, counter-rotating) circular lightlike geodesic, i.e., a "photon circle." By (24), $\mathrm{d}\Psi_{\pm}$ vanishes if

$$\cos\vartheta = 0 \quad \text{and } 2r\Delta - (r-m)\rho^2 \pm 2ar\sqrt{\Delta}\sin\vartheta = 0. \tag{27}$$

By writing Δ and ρ^2 explicitly, we see that (27) is true at $\vartheta=\pi/2$ and $r=r_{\pm}^{\text{ph}}$, where $r_{\pm}^{\text{ph}}$ is defined by the equation

$$(r_{\pm}^{\text{ph}})^2 - 3mr_{\pm}^{\text{ph}} + 2a^2 + 2q^2 = \mp 2a\sqrt{(r_{\pm}^{\text{ph}})^2 - 2mr_{\pm}^{\text{ph}} + a^2 + q^2}. \tag{28}$$

For $0 < \sqrt{a^2+q^2} < m$, (28) has exactly one solution for each sign which satisfies

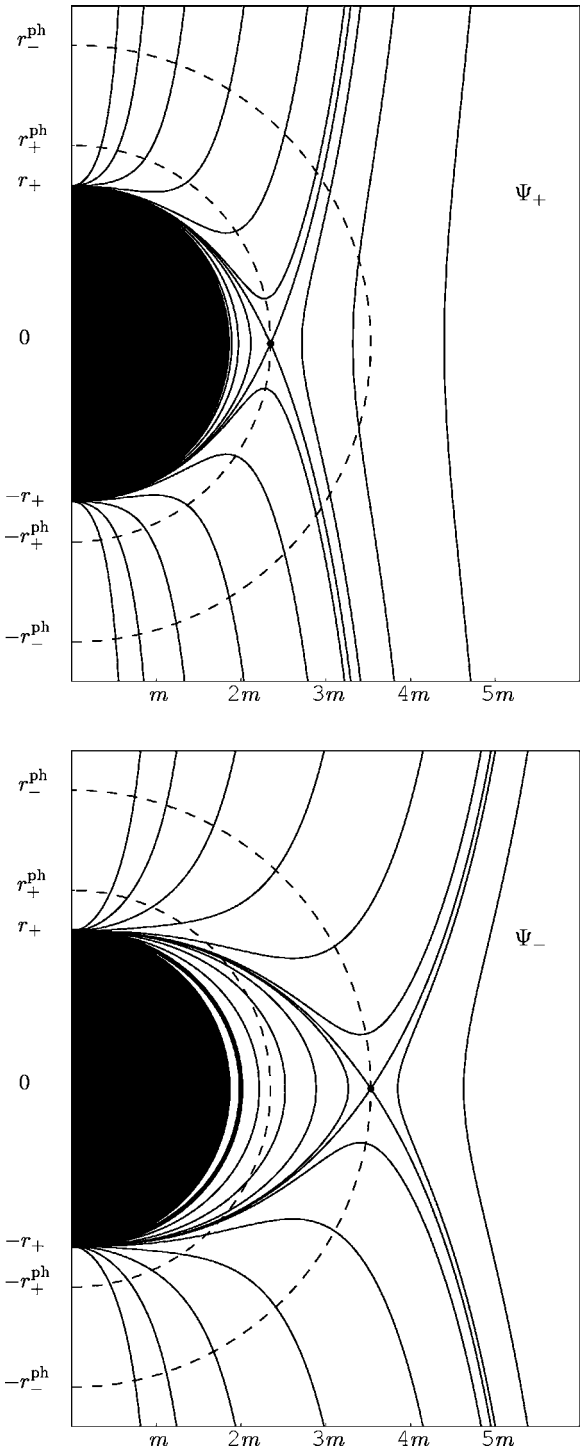

FIG. 1. The surfaces Ψ_+=constant (top) and Ψ_-=constant (bottom) are drawn here for the case $q=0$ and $a=0.5m$. The picture shows the (half-)plane (φ,t)=constant, with $r\sin\vartheta$ on the horizontal and $r\cos\vartheta$ on the vertical axis. The spheres of radius r_+^{ph} and r_-^{ph} are indicated by dashed lines; they meet the equatorial plane in the photon circles. The boundary of the ergosphere coincides with the surface $\Psi_-=0$ and is indicated in the bottom figure by a thick line; it meets the equatorial plane at $r=2m$.

$$r_+ < r_+^{\mathrm{ph}} < \frac{3m}{2} + \sqrt{\frac{9m^2}{4} - 2q^2} < r_-^{\mathrm{ph}} < 2m + 2\sqrt{m^2 - q^2}. \tag{29}$$

So there is exactly one corotating photon circle in M_+, corresponding to the critical point of Ψ_+ at r_+^{ph}, and exactly one counter-rotating photon circle in M_+, corresponding to the critical point of Ψ_- at r_-^{ph}, see Fig. 1. (The relation of photon circles to centrifugal-plus-Coriolis force in the limit $v \to 1$ is also discussed by Stuchlik, Hledik, and Jurán;[23] note, however, that their work is restricted to the equatorial plane of the Kerr-Newman space-time throughout.) In the Reissner-Nordström case, $a=0$, we have

$$r_+^{\mathrm{ph}} = r_-^{\mathrm{ph}} = \frac{3m}{2} + \sqrt{\frac{9m^2}{4} - 2q^2}$$

(cf., e.g., Chandrasekhar,[17] p. 218). If we keep m and q fixed and vary a from 0 to the extreme value $\sqrt{m^2-q^2}$, r_+^{ph} decreases from $\frac{3}{2}m+\sqrt{(9m^2/4)-2q^2}$ to m whereas r_-^{ph} increases from $\frac{3}{2}m+\sqrt{(9m^2/4)-2q^2}$ to $2m+2\sqrt{m^2-q^2}$. As an aside, we mention that, although r_+^{ph} and r_+ both go to m in the extreme case, the proper distance between the corotating photon circle at r_+^{ph} and the horizon at r_+ does not go to zero; for the case $q=0$ this surprising feature is discussed in Ref. 17, p. 340.

From (24) we can read the sign of $\partial_r \Psi_\pm$ at each point. We immediately find the following result.

Proposition 1: Decompose the exterior Kerr space-time into the sets

$$M_{\mathrm{in}}: \quad 2r\Delta - (r-m)\rho^2 < -2ar\sqrt{\Delta}\sin\vartheta, \tag{30}$$

$$K: \quad -2ar\sqrt{\Delta}\sin\vartheta \leqslant 2r\Delta - (r-m)\rho^2 \leqslant 2ar\sqrt{\Delta}\sin\vartheta, \tag{31}$$

$$M_{\mathrm{out}}: \quad 2ar\sqrt{\Delta}\sin\vartheta < 2r\Delta - (r-m)\rho^2, \tag{32}$$

so $M_+ = M_{\mathrm{in}} \cup K \cup M_{\mathrm{out}}$, *see Fig. 2. Then*

$$\partial_r \Psi_+ < 0 \quad \textit{and } \partial_r \Psi_- < 0 \textit{ on } M_{\mathrm{in}}, \tag{33}$$

$$\partial_r \Psi_+ < 0 \quad \textit{and } \partial_r \Psi_- > 0 \textit{ on the interior of } K, \tag{34}$$

$$\partial_r \Psi_+ > 0 \quad \textit{and } \partial_r \Psi_- > 0 \textit{ on } M_{\mathrm{out}}. \tag{35}$$

The inequality $\partial_r \Psi_\pm > 0$ is true for both signs if and only if, for v sufficiently large, the sum of Coriolis and centrifugal force is pointing in the direction of increasing r for corotating and counter-rotating observers. An equivalent condition is that the centrifugal force points in the direction of increasing r and dominates the Coriolis force for v sufficiently large. This is the situation we are familiar with from Newtonian physics. According to Proposition 1, however, in the Kerr-Newman space-time this is true only in the region M_{out}. In the interior of the intermediate region K the direction of centrifugal-plus-Coriolis force for large v is reversed for counter-rotating observers while still normal for corotating observers. In the region M_{in}, finally, it is reversed both for corotating and for counter-rotating observers.

The relevance of the sets M_{out}, M_{in}, and K in view of lightlike geodesics is demonstrated in the following proposition.

Proposition 2: (a) *In the region* M_{out}, *the radius coordinate r cannot have other extrema than strict local minima along a lightlike geodesic.*

(b) *In the region* M_{in}, *the radius coordinate r cannot have other extrema than strict local maxima along a lightlike geodesic.*

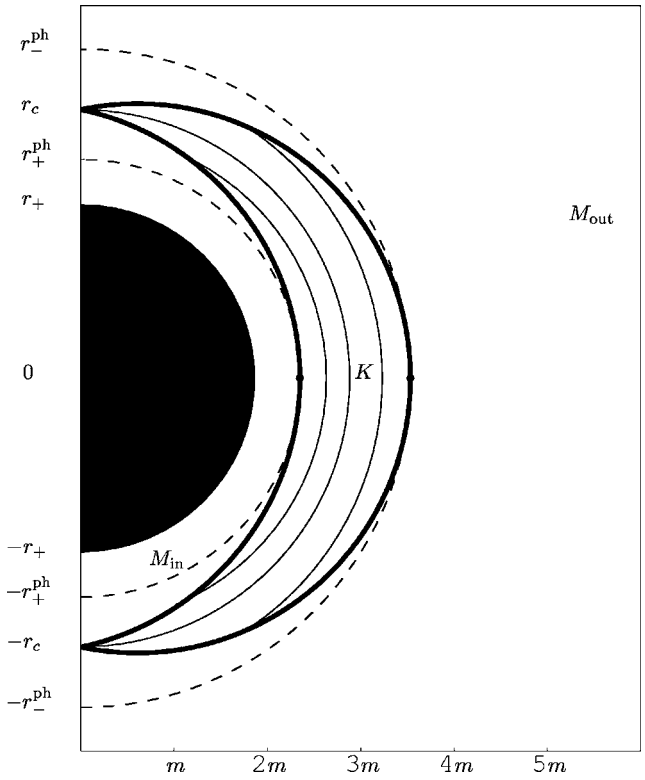

FIG. 2. The regions M_{in}, K, and M_{out} defined in Proposition 1 are shown here for the case $q=0$ and $a=0.5m$. Again, as in Fig. 1, we plot $r\sin\vartheta$ on the horizontal and $r\cos\vartheta$ on the vertical axis. Some of the spherical lightlike geodesics that fill the photon region K are indicated. K meets the equatorial plane in the photon circles at $r=r_+^{\mathrm{ph}}$ and $r=r_-^{\mathrm{ph}}$ and the axis at radius r_c given by $r_c^3-3r_c^2m+r_c(a^2+2q^2)+a^2m=0$. This picture can also be found as Fig. 21 in the online article (Ref. 29).

(c) *Through each point of K there is a spherical lightlike geodesic. (Here "spherical" means that the geodesic is completely contained in a sphere* $r=$constant.)

Proof: Let X be a lightlike and geodesic vector field on (M_+,g), i.e., $g(X,X)=0$ and $\nabla_X X=0$. To prove (a) and (b), we must demonstrate that the implication

$$Xr=0\Rightarrow XXr>0 \tag{36}$$

is true at all points of M_{out} and that the implication

$$Xr=0\Rightarrow XXr<0 \tag{37}$$

is true at all points of M_{in}. Here Xr is to be read as "the derivative operator X applied to the function r." The condition $\nabla_X X=0$ implies

$$XXr=X\,\mathrm{d}r(X)=X\left(\frac{\sqrt{\Delta}}{\rho}g(E_3,X)\right)=\frac{\sqrt{\Delta}}{\rho}g(\nabla_X E_3,X)+\left(X\frac{\sqrt{\Delta}}{\rho}\right)g(E_3,X), \tag{38}$$

where we have used the basis vector field E_3 from (13) and (14). Using these orthonormal basis vector fields, we can write X in the form

$$X=E_0+\cos\alpha\,E_1+\sin\alpha\,E_2 \tag{39}$$

at all points where $Xr=0$. [A nonzero factor of X is irrelevant because X enters quadratically into the right-hand side of (38).] Then (38) takes the form

$$\frac{\rho}{\sqrt{\Delta}}XXr = g(\nabla_{E_0}E_3,E_0) + \sin\alpha\,(g(\nabla_{E_2}E_3,E_0) + g(\nabla_{E_0}E_3,E_2)) + \cos\alpha\,(g(\nabla_{E_1}E_3,E_0) + g(\nabla_{E_0}E_3,E_1))$$
$$+ \sin^2\alpha\, g(\nabla_{E_2}E_3,E_2) + \cos^2\alpha\, g(\nabla_{E_1}E_3,E_1) = g([E_0,E_3],E_0) + \sin\alpha\,(g([E_2,E_3],E_0)$$
$$+ g([E_0,E_3],E_2)) + \cos\alpha\,(g([E_1,E_3],E_0) + g([E_0,E_3],E_1)) + \sin^2\alpha\, g([E_2,E_3],E_2)$$
$$+ \cos^2\alpha\, g([E_1,E_3],E_1). \tag{40}$$

If we insert the Lie brackets from (15) we find

$$\rho^4 XXr = 2r\Delta - (r-m)\rho^2 + 2ar\sqrt{\Delta}\sin\vartheta\cos\alpha. \tag{41}$$

Now we compare this expression with (30)–(32). If $\cos\alpha$ runs through all possible values from -1 to 1, the right-hand side of (41) stays positive on M_{out} and negative on M_{in}. This proves part (a) and part (b). At each point of K there is exactly one value of $\cos\alpha$ such that the right-hand side of (41) vanishes. This assigns to each point of K a lightlike direction such that the integral curves of the resulting direction field are spherical lightlike geodesics. This proves part (c). □

In view of part (c) of Proposition 2 we refer to the closed region K as to the *photon region* of the exterior Kerr-Newman space-time. Along each spherical lightlike geodesic in K the ϑ-coordinate oscillates between extremal values ϑ_0 and $-\vartheta_0$, correponding to boundary points of K, see Fig. 2; the φ-coordinate either increases or decreases monotonically. In the Reissner-Nordström case $a=0$, where (26) is a potential for the centrifugal force, the photon region K shrinks to the *photon sphere* $r=\frac{3}{2}m+\sqrt{(9m^2/4)-2q^2}$ and Proposition 1 reduces to the known fact that centrifugal force reversal takes place at the photon sphere.

We end this section with a word of caution as to terminology. In part (c) of Proposition 2 we have referred to the set $r=$constant as to a sphere. This is indeed justified in the sense that, for each fixed t, fixing the radius coordinate r gives a two-dimensional submanifold of M_+ that is diffeomorphic to the 2-sphere. Moreover, in our Figs. 1 and 2 the sets $r=$constant are represented as (meridional cross sections of) spheres. Note, however, that the Kerr-Newman metric does *not* induce an isotropic metric on these spheres (unless $a=0$), so they are not round spheres in the metrical sense.

IV. MULTIPLE IMAGING IN THE KERR-NEWMAN SPACE-TIME

It is now our goal to discuss multiple imaging in the exterior Kerr-Newman space-time (M_+,g). To that end we fix a point p and a timelike curve γ in M_+ and we want to get some information about the past-pointing lightlike geodesics from p to γ. The following proposition is an immediate consequence of Proposition 2.

Proposition 3: Let p be a point and γ a timelike curve in the exterior Kerr-Newman space-time. Let

$$\Lambda: \quad r_a < r < r_b \tag{42}$$

denote the smallest spherical shell, with $r_+ \leqslant r_a < r_b \leqslant \infty$, such that p, γ and the region K defined by (31) *are completely contained in $\bar{\Lambda}$ (=closure of Λ in M_+). Then all lightlike geodesics that join p and γ are confined within $\bar{\Lambda}$.*

Proof: Along a lightlike geodesic that leaves and reenters $\bar{\Lambda}$ the radius coordinate r must have either a maximum in the region M_{out} or a minimum in the region M_{in}. Proposition 2 makes sure that this cannot happen. □

By comparison with Proposition 1 we see that, among all spherical shells whose closures in M_+ contain p and γ, the shell Λ of Proposition 3 is the smallest shell such that at all points of the boundary of Λ in M_+ the gradient of Ψ_+ and the gradient of Ψ_- are pointing in the direction away from Λ. Based on Proposition 3, we will later see that there is a close relation between multiple imaging and centrifugal-plus-Coriolis force reversal in the Kerr-Newman space-time.

Proposition 3 tells us to what region the lightlike geodesics between p and γ are confined, but it does not tell us anything about the number of these geodesics. To answer the latter question, we now apply Theorem 1 to the exterior Kerr-Newman space-time (M_+,g).

Proposition 4: Consider, in the exterior Kerr-Newman space-time (M_+,g), *a point* p *and a smooth future-pointing timelike curve* $\gamma:]-\infty,\tau_a[\to M_+$, *with* $-\infty<\tau_a\leqslant\infty$, *which is parametrized by the Boyer-Lindquist time coordinate* t, *i.e., the* t*-coordinate of the point* $\gamma(\tau)$ *is equal to* τ. *Assume* (i) *that* γ *does not meet the caustic of the past light-cone of* p, *and* (ii) *that for* $\tau\to-\infty$ *the radius coordinate* r *of the point* $\gamma(\tau)$ *remains bounded and bounded away from* r_+. [*The last condition means that* $\gamma(\tau)$ *goes neither to infinity nor to the horizon for* $\tau\to-\infty$.] *Then there is an infinite sequence* $(\lambda_n)_{n\in\mathbb{N}}$ *of mutually different past-pointing lightlike geodesics from* p *to* γ. *For* $n\to\infty$, *the index of* λ_n *goes to infinity. Moreover, if we denote the point where* λ_n *meets the curve* γ *by* $\gamma(\tau_n)$, *then* $\tau_n\to-\infty$ *for* $n\to\infty$.

Proof: We want to apply Theorem 1 to the exterior Kerr-Newman space-time (M_+,g). To that end, the first thing we must find is an orthogonal splitting of the exterior Kerr-Newman space-time that satisfies the metric growth condition. As in the original Boyer-Lindquist coordinates the t-lines are not orthogonal to the surfaces $t=$constant, we change to new coordinates

$$x^1=r,\quad x^2=\vartheta,\quad x^3=\varphi-u(r,\vartheta)t,\quad t=t, \tag{43}$$

with

$$u(r,\vartheta)=\frac{2mar}{\rho^2\Delta+2mr(r^2+a^2)}. \tag{44}$$

Then the Kerr metric (8) takes the orthogonal splitting form (2), with

$$\begin{aligned} g_{ij}(x,t)\mathrm{d}x^i\,\mathrm{d}x^j=\rho^2&\left(\frac{\mathrm{d}r^2}{\Delta}+\mathrm{d}\vartheta^2\right)\\ &+\frac{\sin^2\vartheta}{\rho^2}((r^2+a^2)^2-\Delta a^2\sin^2\vartheta)\left(t\left(\frac{\partial u(r,\vartheta)}{\partial r}\mathrm{d}r+\frac{\partial u(r,\vartheta)}{\partial\vartheta}\mathrm{d}\vartheta\right)+\mathrm{d}x^3\right)^2 \end{aligned} \tag{45}$$

and

$$f(x,t)=\frac{\rho^2\Delta}{(r^2+a^2)^2-\Delta a^2\sin^2\vartheta}. \tag{46}$$

Clearly, if we restrict the range of the coordinates $x=(x^1,x^2,x^3)$ to a compact set, we can find positive constants A and B such that

$$\frac{g_{ij}(x,t)v^iv^j}{f(x,t)}\leqslant(A+B|t|)^2\delta_{ij}v^iv^j. \tag{47}$$

As $F(t)=A+B|t|$ satisfies the integral condition (3), this proves that our orthogonal splitting satisfies the metric growth condition. Our assumptions on γ guarantee that we can find a curve $\gamma':\mathbb{R}\to M_+$ which, in terms of our orthogonal splitting, is of the form $\gamma'(\tau)=(\beta'(\tau),\tau)$ such that $\gamma'(\tau)=\gamma(\tau)$ for all $]-\infty,\tau_b]$, with some $\tau_b\in\mathbb{R}$. (Introducing γ' is necessary because γ need not be defined on all of $\mathbb{R}$.) As γ does not meet the caustic of the past light-cone of p, we may assure that γ' does not meet the caustic of the past light-cone of p. As γ does not go to the horizon or to infinity for $\tau\to-\infty$, the set $\{\beta'(\tau)\,|-\infty<\tau<\tau_b\}$ is confined to a compact region. Hence, for every sequence $(\tau_i)_{i\in\mathbb{N}}$ with $\tau_i\to-\infty$ the sequence $(\beta'(\tau_i))_{i\in\mathbb{N}}$ must have a convergent subsequence. This shows that all the assumptions of Theorem 1 are satisfied if we replace γ with γ'. Hence, the theorem tells us that $N'_k\geqslant B_k$, where N'_k is the number of past-pointing lightlike geodesics with index k from p to γ' and B_k is the kth Betti number of the loop space of $M_+\simeq S^2\times\mathbb{R}^2$. As $M_+\simeq S^2\times\mathbb{R}^2$ is simply connected but not contractible to a point, the theorem of Serre[15] guarantees

that $B_k > 0$ and, thus, $N_k' > 0$ for all but finitely many $k \in \mathbb{N}$. Hence, for almost all positive integers k there is a past-pointing lightlike geodesic of index k from p to γ'. This gives us an infinite sequence $(\lambda_n)_{n\in\mathbb{N}}$ of mutually different past-pointing lightlike geodesics from p to γ' such that the index of λ_n goes to infinity if $n \to \infty$. We denote the point where λ_n meets the curve γ' by $\gamma'(\tau_n)$. What remains to be shown is that $\tau_n \to -\infty$ for $n \to \infty$; as γ coincides with γ' on $]-\infty, \tau_b]$, this would make sure that all but finitely many λ_n arrive indeed at γ. So we must prove that it is impossible to select infinitely many τ_n that are bounded below. By contradiction, assume that we can find a common lower bound for infinitely many τ_n. As the τ_n are obviously bounded above by the value of the Boyer-Lindquist time coordinate at p, this implies that the τ_n have an accumulation point. Hence, for an infinite subsequence of our lightlike geodesics λ_n the endpoints $\gamma'(\tau_n)$ converge to some point q on γ'. As γ' does not meet the caustic of the past light-cone of p, the past light-cone of p is an immersed three-dimensional lightlike submanifold near q. We have thus found an infinite sequence of points $\gamma'(\tau_n)$ that lie in a three-dimensional lightlike submanifold and, at the same time, on a timelike curve. Such a sequence can converge to q only if all but finitely many $\gamma'(\tau_n)$ are equal to q. So there are infinitely many λ_n that terminate at q. As there is only one lightlike direction tangent to the past light-cone of p at q, all these infinitely many lightlike geodesics must have the same tangent direction at q. As there are no periodic lightlike geodesics in the globally hyperbolic space-time (M_+, g), any two lightlike geodesics from p to q with a common tangent direction at q must coincide. This contradicts the fact that the λ_n are mutually different, so our assumption that there is a common lower bound for infinitely many τ_n cannot be true. □

The proof shows that in Proposition 4 the condition of $\gamma(\tau)$ going neither to infinity nor to the horizon for $\tau \to -\infty$ can be a little bit relaxed. It suffices to require that there is a sequence $(\tau_i)_{i\in\mathbb{N}}$ of time parameters with $\tau_i \to -\infty$ for $i \to \infty$ such that the spatial coordinates of $\gamma(\tau_i)$ converge. This condition is mathematically weaker than the one given in the proposition, but there are probably no physically interesting situations where the former is satisfied and the latter is not.

Proposition 4 tells us that a Kerr-Newman black hole produces infinitely many images for an arbitrary observer, provided that the worldline of the light source satisfies some (mild) conditions. At the same time, this proposition demonstrates that the past light-cone of every point p in the exterior Kerr-Newman space-time must have a nonempty and, indeed, rather complicated caustic; otherwise it would not be possible to find a sequence of past-pointing lightlike geodesics λ_n from p that intersect this caustic arbitrarily often for n sufficiently large. Please note that the last sentence of Proposition 4 makes clear that for the existence of infinitely many images it is essential to assume that the light source exists since arbitrarily early times.

In Proposition 3 we have shown that all lightlike geodesics from p to γ are confined to a spherical shell that contains the photon region K. We can now show that, under the assumptions of Proposition 4, almost all past-pointing lightlike geodesics from p to γ come actually arbitrarily close to K.

Proposition 5: Let U be any open subset of M_+ that contains the region K defined by (31). *Then, if the assumptions of Proposition 4 are satisfied, all but finitely many past-pointing lightlike geodesics from p to γ intersect U.*

Proof: The sequence $(\lambda_n)_{n\in\mathbb{N}}$ of Proposition 4 gives us a sequence $(w_n)_{n\in\mathbb{N}}$ of mutually different lightlike vectors $w_n \in T_pM_+$ with $\mathrm{d}t(w_n) = -1$ and a sequence $(s_n)_{n\in\mathbb{N}}$ of real numbers $s_n \geqslant 0$ such that $\exp_p(s_n w_n)$ is on γ for all $n \in \mathbb{N}$. Here $\exp_p$ denotes the exponential map of the Levi-Civita derivative of the Kerr-Newman metric at the point p. Since the 2-sphere consisting of the lightlike vectors $w \in T_pM_+$ with $\mathrm{d}t(w) = -1$ (which may be regarded as the observer's celestial sphere) is compact, a subsequence of $(w_n)_{n\in\mathbb{N}}$ must converge to some lightlike vector $w_\infty \in T_pM_+$. By Proposition 4, the sequence $(\exp_p(s_n w_n))_{n\in\mathbb{N}}$ cannot have an accumulation point, hence $s_n \to \infty$ for $n \to \infty$. Owing to Proposition 3, the radius coordinate r of all points $\exp_p(s w_n)$ with $s \in [0, s_n]$ is bounded, so the past-pointing past-inextendible lightlike geodesic

$$\lambda_\infty : [0, \infty[\to M_+ \quad ,$$

$$s \mapsto \lambda_\infty(s) = \exp_p(s w_\infty) \tag{48}$$

cannot go to infinity. Let us assume that λ_∞ goes to the horizon. By Proposition 3, this is possible only in the extreme case $a^2+q^2=m^2$. Then along λ_n the radius coordinate r must have local minima arbitrarily close to r_+ for n sufficiently large. As, by Proposition 2, such minima cannot lie in M_{in}, the geodesic λ_n must meet K for n sufficiently large and we are done. Therefore, we may assume for the rest of the proof that λ_∞ does not go to the horizon. So along λ_∞ the coordinate r must either approach a limit value r_∞ or pass through a maximum and a minimum. In the first case, both the first and the second derivative of $s \mapsto r(\lambda_\infty(s))$ must go to zero for $s \to \infty$. This is possible only if λ_∞ comes arbitrarily close to K, because, as we know from the proof of Proposition 2, the implication (36) holds on M_{out} and the implication (37) holds on M_{in}. In the second case, again by Proposition 2, the maximum cannot lie in M_{out} and the minimum cannot lie in M_{in}; hence, both the maximum and the minimum must lie in K. In both cases we have, thus, found that λ_∞ and hence all but finitely many λ_n intersect U. □

V. DISCUSSION AND CONCLUDING REMARKS

We have proven, with the help of Morse theory, in Proposition 4 that a Kerr-Newman black hole acts as a gravitational lens that produces infinitely many images. We emphasize that we made only very mild assumptions on the motion of the light source and that we considered the whole domain of outer communication, including the ergosphere. For the sake of comparison, the reader may consult Sec. 7.2 of Ref. 24 where it is shown, with the help of Morse theory, that a Kerr black hole produces infinitely many images. However, Masiello's work is based on a special version of Morse theory which applies to stationary space-times only; therefore he had to exclude the ergosphere from the discussion, he had to require that the worldline of the light source is an integral curve of the Killing vector field ∂_t, and he had to restrict to the case of slowly rotating Kerr black holes, $0 \leqslant a^2 < a_0^2$ with some a_0 that remained unspecified, instead of the whole range $0 \leqslant a^2 \leqslant m^2$. On the basis of our Proposition 3 one can show that Masiello's a_0 is equal to $m/\sqrt{2}$; this is the value of a where the photon region K reaches the ergosphere (see Fig. 2), i.e., where $r_+^{\text{ph}} = 2m$. For a Kerr space-time with $m \geqslant a \geqslant m/\sqrt{2}$ we can find an event p and a t-line in $M_+ \backslash \{\text{ergosphere}\}$ that can be connected by only finitely many lightlike geodesics in $M_+ \backslash \{\text{ergosphere}\}$.

If an observer sees infinitely many images of a light source, they must have at least one accumulation point on the observer's celestial sphere. This follows immediately from the compactness of the 2-sphere. This accumulation point corresponds to a limit light ray λ_∞. In the proof of Proposition 5 we have demonstrated that λ_∞ comes arbitrarily close to the photon region K and that either λ_∞ approaches a sphere $r=$constant or the radius coordinate along λ_∞ has a minimum and a maximum in K. (In the extreme case $a^2+q^2=m^2$ the ray λ_∞ may go to the inner boundary of M_+.) This is all one can show with the help of Morse theory and the qualitative methods based on the sign of centrifugal-plus-Coriolis force. Stronger results are possible if one uses the explicit first-order form of the lightlike geodesic equation in the Kerr-Newman space-time, making use of the constants of motion which reflect complete integrability. Then one can show that along a lightlike geodesic in M_+ the radius coordinate is either monotonous or has precisely one turning point. (This result can be deduced, e.g., from Calvani and Turolla[25]). Thus, the case that there is a minimum and a maximum in K is, actually, impossible. As a consequence, the limit light ray λ_∞ necessarily approaches a sphere $r=$constant. By total integrability it must then approach a lightlike geodesic with the same constants of motion. Of course, this must be one of the spherical geodesics in K. (In the extreme case $a^2+q^2=m^2$ the limit ray λ_∞ may approach the circular light ray at $r_+^{\text{ph}} = m$ which is outside of M_+.)

Also, it follows from Proposition 4 that the limit curve λ_∞ meets the caustic of the past light cone of p infinitely many times. This gives, implicitly, some information on the structure of the caustic. For the Kerr case, $q=0$, it was shown numerically by Rauch and Blandford[26] that the caustic consists of infinitely many tubes with astroid cross sections. This result was supported by recent analytical results by Bozza, de Luca, Scarpetta, and Sereno.[27]

We have shown, in Proposition 3, that all lightlike geodesics connecting an event p to a timelike curve γ in the exterior Kerr-Newman space-time M_+ are confined to the smallest spherical shell that contains p, γ and the photon region K. If γ satisfies the assumptions of Proposition 4, which guarantees infinitely many past-pointing lightlike geodesics from p to γ, Proposition 5 tells us that all but finitely many of them come arbitrarily close to the photon region K. Thus, our result that a Kerr-Newman black hole produces infinitely many images is crucially related to the existence of the photon region. If we restrict to some open subset of M_+ whose closure is completely contained in either M_{out} or M_{in}, then we are left with finitely many images for any choice of p and γ. In Sec. III we have seen that the decomposition of M_+ into M_{in}, M_{out} and the photon region K plays an important role in view of centrifugal-plus-Coriolis force reversal; if we restrict to an open subset of M_+ that is contained in either M_{out} or M_{in}, then we are left with a space-time on which $\partial_r \Psi_+$ and $\partial_r \Psi_-$ have the same sign, i.e., the centrifugal-plus-Coriolis force for large velocities points either always outwards or always inwards. In an earlier paper[28] we have shown that in a spherically symmetric and static space-time the occurrence of gravitational lensing with infinitely many images is equivalent to the occurrence of centrifugal force reversal. Our new results demonstrate that the same equivalence is true for subsets of the exterior Kerr-Newman space-time, with the only difference that instead of the centrifugal force alone now we must consider the sum of centrifugal and Coriolis force in the limit $v \to 1$. It is an interesting problem to inquire whether this observation carries over to other space-times with two commuting Killing vector fields ∂_t and ∂_φ that span timelike 2-surfaces with cylindrical topology.

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Gravitational magnetic monopoles and Majumdar-Papapetrou stars

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During the 1990s a large amount of work was dedicated to studying general relativity coupled to non-Abelian Yang-Mills type theories. Several remarkable results were accomplished. In particular, it was shown that the magnetic monopole, a solution of the Yang-Mills-Higgs equations can indeed be coupled to gravitation. For a low Higgs mass it was found that there are regular monopole solutions, and that for a sufficiently massive monopole the system develops an extremal magnetic Reissner-Nordström quasihorizon with all the matter fields laying inside the horizon. These latter solutions, called quasi-black holes, although nonsingular, are arbitrarily close to having a horizon, and for an external observer it becomes increasingly difficult to distinguish these from a true black hole as a critical solution is approached. However, at precisely the critical value the quasi-black hole turns into a degenerate space-time. On the other hand, for a high Higgs mass, a sufficiently massive monopole develops also a quasi-black hole, but at a critical value it turns into an extremal true horizon, now with matter fields showing up outside. One can also put a small Schwarzschild black hole inside the magnetic monopole, the configuration being an example of a non-Abelian black hole. Surprisingly, Majumdar-Papapetrou systems, Abelian systems constructed from extremal dust (pressureless matter with equal charge and energy densities), also show a resembling behavior. Previously, we have reported that one can find Majumdar-Papapetrou solutions which are everywhere nonsingular, but can be arbitrarily close of being a black hole, displaying the same quasi-black-hole behavior found in the gravitational magnetic monopole solutions. With the aim of better understanding the similarities between gravitational magnetic monopoles and Majumdar-Papapetrou systems, here we study a particular system, namely a system composed of two extremal electrically charged spherical shells (or stars, generically) in the Einstein-Maxwell-Majumdar-Papapetrou theory. We first review the gravitational properties of the magnetic monopoles, and then compare with the gravitational properties of the double extremal electric shell system. These quasi-black-hole solutions can help in the understanding of true black holes, and can give some insight into the nature of the entropy of black holes in the form of entanglement. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2184766]

I. INTRODUCTION

The coupling of general relativity to Yang-Mills SU(2) non-Abelian theories was studied in detail in the 1990s giving rise to a fuller understanding of the systems involved through a series of remarkable results. This effort started after the paper by Bartnick and McKinnon,[1] which showed that Einstein-Yang-Mills theory has one particle solution, the Bartnick-McKinnon particle, in spite of neither pure gravity nor pure Yang-Mills having a particle solution on their own. Further studies inserted a black hole inside this particle[2,3] with the conclusion that, although unstable, the solution could be an instance of no-hair violation, which in turn motivated new works. Similar systems were then studied, such as, the Einstein-Skyrme system,[4–8] the Einstein-Yang-Mills-dilaton system,[5] the Yang-Mills-Proca system,[6,9] the Einstein-Yang-Mills-Higgs sphaleron system,[6,9] Einstein-Yang-Mills in anti-de Sitter space-times,[10] all these systems have in common that their global electromagnetic type charge is zero, a good review is in Ref. 11. There is yet another very interesting system, which concerns us here, the magnetic monopole which is a solution of the Einstein-Yang-Mills-Higgs system. Indeed, the 't Hooft-Polyakov magnetic monopole, is a solution of the pure Yang-Mills-Higgs system (i.e., Einstein-Yang-Mills-Higgs with zero gravity), when the Yang-Mills and the Higgs fields are in the adjoint SO(3) representation (see the review paper of Goddard and Olive[12]). The 't Hooft-Polyakov magnetic monopole, at large distances, has the same structure of the Dirac monopole, however the core is nonsingular.[12,13] When one couples gravitation, at least weakly, the magnetic monopole solution is still there, as was noticed in Ref. 14, now exerting a small gravitational attraction. For strong gravitational fields the system was studied much later, in the wake of the Bartnick-McKinnon particle, notably by Ortiz,[15] Lee, Nair, and Weinberg,[16,17] Breitenlohner, Forgács, and Maison,[18,19] and Aichelburg and Bizon,[20] among others. A distinctive feature of this system is that it has a global magnetic charge, which of course influences the properties of the space-time. In addition, the Einstein-Yang-Mills-Higgs system has two length scales, one due to the mass of the W particle (the Yang-Mills particle that has eaten some mass in the symmetry breaking process), the other due to the mass of the Higgs. For low Higgs mass, the associated large Compton length scale does not interfere much, and the structure of the monopole is characterized in great extent by the W field features. For this system, the one analyzed in Refs. 15–20, it was found that there are regular solutions, and moreover, for a sufficiently massive monopole the system turns into an extremal quasi-black hole, developing an extremal quasihorizon, with all the nontrivial matter fields inside it. A quasi-black hole is a configuration which is nonsingular but on the verge of having a horizon at some radius r_*. More specifically, quasi-black holes are nonsingular solutions arbitrarily close to having a horizon. For an external observer it becomes increasingly difficult to distinguish a quasi-black hole from a true black hole as a critical solution is approached. At the critical value one must distinguish two situations. In the low Higgs mass situation a horizon never forms, when the configuration has radius r_* the space-time is degenerated, where the time dimension disappears altogether from a region of the space-time. The distinction between a quasi-black hole and a true black hole, as well as the appearance of a degenerated space-time, was not clear in the early works. On the other hand, for high Higgs mass the system behaves differently as was shown later by Lue and Weinberg[21,22] (see also Ref. 23). In this case, for a sufficiently massive monopole the system turns into a quasi-black hole, and at the critical value, a real extremal magnetic Reissner-Nordström black hole appears, developing a true extremal horizon inside the monopole core, and moreover, non-Abelian matter fields stick out of the horizon, in gross violation of the no-hair conjecture. It was further found that one could insert a Schwarzschild black hole inside the monopole without perturbing much its structure, forming a non-Abelian black hole. But when the radius of the Schwarzschild black hole achieved a certain value the horizon would jump into another extremal quasihorizon. This happens both in the low Higgs mass case, as was found by the original authors, as well as in the high Higgs mass case, as was shown by Brihaye, Hartmann, and Kunzin[24] where the continuation of the original program has been carried out. Other studies connected with

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magnetic monopoles in the Einstein-Yang-Mills-Higgs theory can be mentioned: (i) The thermodynamical properties of these monopole black holes were further studied by Maeda *et al.*[25–27] in the low Higgs mass case, and by Lue and Weinberg[22] for high Higgs mass; (ii) Ridgeway and Weinberg found the existence of nonspherically symmetric magnetic monopole configurations;[28] (iii) dyonic solutions were found by Brihaye *et al.*;[29,30] (iv) monopole solutions in other theories were also found, like in a Brans-Dicke theory,[31] and in SU(3), SU(5), and SU(N) gauge theories.[32–34]

Now, in a different context, the study of the Einstein-Maxwell system goes back to the origins of general relativity where Reissner in 1916 and Nordström in 1918 found the Reissner-Nordström solution (see Ref. 35 for the appropriate references), and Weyl studied axisymmetric gravitoelectric vacuum systems in four dimensions.[36] A great development occurred in 1947 when Majumdar[37] and Papapetrou,[38] drawing upon Weyl's results, found new four-dimensional solutions that represent many particles (from one to infinity), each particle with mass equal to charge, located at any desired position, without spatial symmetry in the most generic case [see Ref. 39 for a generalization of Majumdar's[37] and Papapetrou's[38] works to higher dimensional ($d>4$) spacetimes]. The idea is borrowed from Newtonian gravitation: A particle with mass equal to charge is in equilibrium with other mass equal to charge particle, and so with many other such particles, since the gravitational attraction is balanced by the electric repulsion. The Majumdar-Papapetrou solutions are the general relativistic realization of this idea. Now, in Newtonian theory, point particles are point particles, but in general relativity they can be black holes. This was clarified by Hartle and Hawking[40] who showed that the vacuum solution represents extremal Reissner-Nordström black holes at any spatial position. A different development was taken by Das,[41] who relying on the work of Majumdar,[37] put dust particles on the point particles positions, evading the black hole horizons. Several other authors have further analyzed the properties of Majumdar-Papapetrou systems.[42–47] Bonnor and collaborators[48–52] in a series of papers have shown and studied important new solutions of Majumdar-Papapetrou equations and properties of the system. In particular, in Refs. 49–51, spherical extremal matter stars (where extremal matter stars are defined as stars composed of matter with charge density equal to the energy density), with an exterior extremal Reissner-Nordström metric, were found. These are the Bonnor stars. Bonnor stars were further developed by Lemos and Weinberg[53] where new explicit solutions were found. It was also found that these new stars, as well as Bonnor stars, develop a quasi-black-hole behavior, and there are cases that the solution can even display some kind of hair.[53] In addition, in Ref. 54 a thick shell solution was found. In the limit of zero interior radius for this thick shell, the solution is a Bonnor star, in the limit of the thickness going to zero, the solution is a thin shell. These solutions also have quasi-black-hole behavior.

Here we want to explore further the analogy between gravitational magnetic monopoles and Majumdar-Papapetrou stars. In the previous papers,[53,54] the Majumdar-Papapetrou solutions found, although complex did not exhibit the full behavior of the gravitational magnetic monopoles, where there is an interplay between the W-field scale and the Higgs field scale. We construct here a Majumdar-Papapetrou system which shows such a full behavior. Such a system is composed of two infinitesimally thin shells. Majumdar-Papapetrou thin shells have many interesting properties. Let us think first of one thin shell to simplify. We will call it the star, it is a regular solution. Fix the mass of the star, and study the set of formed configurations as one decreases its radius. For a sufficiently small radius the star develops an extremal Reissner-Nordström quasi-black hole. The same happens if instead one fixes the radius and increases the mass. One can go further and put another thin shell inside the thin shell star. One can then ask, when the radii of the system are decreased which shell is going to form a quasihorizon first? The usual case is the outer shell developing a quasihorizon first, the whole system being inside the quasi-black hole. But, depending on the parameters and constraints, the inner shell can develop a quasihorizon first, in which case we have an extremal quasi-black hole in the core of the system, with star matter floating outside. One can also put an extremal Reissner-Nordström true black hole inside the regular star (as was done in the gravitational magnetic monopole case, when one puts a small Schwarzschild black hole inside the magnetic monopole) and then increase the black hole radius

through a set of configurations. At a certain point the whole system jumps into a new extremal Reissner-Nordström quasi-black hole. If we exchange star for monopole, the properties of this Majumdar-Papapetrou system are identical to the properties of the gravitational magnetic monopole system. All these similarities with the gravitational magnetic monopole will be explored in this paper. A similarity which we do not explore, is that both systems permit nonspherically symmetric solutions, in the magnetic monopole case see Ref. 28, in the Majumdar-Papapetrou case see Ref. 52. We note that the Majumdar-Papapetrou solutions, such as the extremal Reissner-Nordström black hole solutions and the Bonnor stars, are also of interest in extensions of general relativity, since the system turns out to be supersymmetric when embedded in a larger theory, such as $N=2$ gauged supergravity (see Ref. 55 for a review of Majumdar-Papapetrou solutions in supergravity and string theories).

The paper is organized as follows. In Sec. II we overview the properties of gravitational magnetic monopoles that most interest us, we give the equations and define the important scales, we review the low Higgs field (low b) case without, and then with, an interior Schwarzschild black hole, and review also the high b case. In Sec. III we study the properties of the Majumdar-Papapetrou two shell system: we give the equations and length scales, assume some constraints for the shells and present the solution, study the equivalent low b behavior without and with an interior extremal Reissner-Nordström true black hole, and then the equivalent high b behavior. A remark: when we write a black hole it means a true extremal Reissner-Nordström black hole, when we write a quasi-black hole it means solutions of matter configurations that are on the verge of being a black hole. In some instances, quasi-black holes turn into degenerated space-times,[16,53] in other instances turn into real black holes.[22]

II. GRAVITATIONAL BEHAVIOR OF MAGNETIC MONOPOLES, AN OVERVIEW

In this section we overview the solutions for gravitational magnetic monopoles. The logical presentation of the material reflects in a unified way the work of the authors on this subject and is suited for comparison with the subsequent analysis on Majumdar-Papapetrou stars.

A. The Einstein-Yang-Mills-Higgs magnetic sector

1. The action and equations of motion

The action of the Einstein-Yang-Mills-Higgs theory is ($G=c=1$)

$$S=\int d^4x\sqrt{-g}\left(-\frac{1}{16\pi}R+\mathcal{L}_{\text{matter}}\right), \tag{1}$$

where R is the scalar curvature, and $\mathcal{L}_{\text{matter}}$ is the Yang-Mills-Higgs Lagrangian given by

$$\mathcal{L}_{\text{matter}}=-\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}+\frac{1}{2}D_\mu\phi^a D^\mu\phi^a-\frac{\lambda}{2}(\phi^{a2}-v^2)^2, \tag{2}$$

$$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu-e\epsilon^a{}_{bc}A^b_\mu A^c_\nu, \tag{3}$$

$$D_\mu\phi^a=\partial_\mu\phi^a-e\epsilon^a{}_{bc}A^b_\mu\phi^c, \tag{4}$$

where e is the gauge coupling constant, λ the Higgs coupling constant, and v the vacuum expectation value of the Higgs field. The Yang-Mills connection A^a and the Higgs field ϕ^a take values on the Lie algebra of the SU(2) group, with a being an internal index. The potential $(\lambda/2)(\phi^{a^2}-v^2)^2$ in the matter Lagrangian has a family of gauge-equivalent minima, given by $\phi^{a2}=v^2$, which breaks spontaneously the SU(2) symmetry down to U(1). One can choose the vacuum to be in the third internal direction $\phi^a=v\delta^{a3}$ (for details see Refs. 12 and 23). The elementary particles of the theory are the electromagnetic U(1) massless gauge field (a photon), two massive W particles with

charge $\pm e$ and mass $m_W = ev$, and the neutral massive field ϕ^3 with mass $m_H = 1/\sqrt{\lambda}v$. There is also the massless graviton.

The monopole configuration is spherically symmetric with metric written generically in terms of two functions $A(r)$ and $B(r)$ as

$$ds^2 = -B(r)dt^2 + A(r)dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2), \tag{5}$$

with a magnetic Yang-Mills field, written in terms of one function $u(r)$, as

$$A_0 = 0, \quad A_i^a = \epsilon_{iaj}\hat{r}^j \frac{1-u(r)}{er}, \tag{6}$$

and a Higgs field, written in terms of one function $h(r)$, as

$$\phi^a = v\hat{r}^a h(r), \tag{7}$$

where ϵ_{iaj} is the Levi-Civita tensor, and $\hat{r}$ is the unit vector in the radial direction. Putting this ansatz into the Einstein-Yang-Mills-Higgs action and varying the action with relation to the four functions yields four equations, two for the gravitational fields $B(r)$ and $A(r)$, one for the Yang-Mills field $u(r)$, and one for the Higgs field $h(r)$. The equations are, respectively (see Ref. 16),

$$\frac{(AB)'}{AB} = 16\pi r\left(\frac{u'^2}{e^2r^2} + \frac{1}{2}v^2h'^2\right), \tag{8}$$

$$\left[r\left(1-\frac{1}{A}\right)\right]' = 8\pi r^2\left[\frac{1}{A}\left(\frac{u'^2}{e^2r^2} + \frac{1}{2}v^2h'^2\right) + \frac{(u^2-1)^2}{2e^2r^4} + \frac{u^2h^2v^2}{r^2} + \frac{\lambda}{2}v^2(h^2-1)^2\right], \tag{9}$$

$$\frac{1}{\sqrt{AB}}\left[\frac{\sqrt{AB}u'}{A}\right]' = \frac{u(u^2-1)}{r^2} + e^2uh^2v^2, \tag{10}$$

$$\frac{1}{r^2\sqrt{AB}}\left[\frac{r^2\sqrt{AB}h'}{A}\right]' = \frac{2hu^2}{r^2} + 2\lambda h(h^2-1)v^2. \tag{11}$$

Sometimes, instead of $A(r)$ the mass function $m(r) = r(1-[1/A(r)])$ is used. There are four parameters in the theory: G (which we have set equal to one), e, λ, and v. With these parameters one can form two dimensionless parameters, α and β. Since v is dimensionless, it is already a sought parameter, $\alpha = v$. The other dimensionless parameter is $\beta = \sqrt{\lambda}/e$. [In passing, note that in these studies of gravitational magnetic monopoles, G is not usually set to one, but rather $G = m_p^{-2} = l_p^2$ ($\hbar = c = 1$), and m_p and l_p are the Planck mass and the Planck length, respectively. Here we are setting $m_p = 1$ and $l_p = 1$, i.e., we are measuring everything in terms of these scales. It is straightforward to move from one system of units to the other: Every time one finds a mass one should divide by m_p, every time one finds a length one should divide by l_p, in the end collect all m_p's and l_p's, transform l_p into m_p by $l_p = m_p^{-1}$, and put back G from $m_p^{-2} = G$.]

2. Some properties and scales of the magnetic monopole

The magnetic monopole solution can be characterized by its mass and radius, and by a secondary mass and a secondary radius. To understand the effects of gravity it is useful to rewrite the parameters α and β, defined above, in terms of two renewed parameters, a and b, defined through the characteristic masses and radii themselves. Indeed, for a weak gravitational field the magnetic charge of the monopole is $Q_m = 1/e$, its radius is given roughly by the Compton wavelength of the Yang-Mills field, $r_m \simeq 1/ev$, and its mass by the magnetic energy $M_m \simeq Q_m^2/r_m = v/e$. Thus, instead of α given above ($\alpha = v$), we can define a parameter a (with $a \sim v^2$) as

$$a \equiv \frac{M_m}{r_m}, \tag{12}$$

which is a useful characterization when we turn on gravitation, and for later comparison. The other parameter b can also be written in similar terms: Since there is the Higgs mass scale, the monopole solution has secondary mass and radius scales. The secondary radius is given by the Compton wavelength of the Higgs field, $r_{m_2} \simeq 1/\sqrt{\lambda}v$, and the secondary mass is given by $M_{m_2} \simeq Q_m^2/r_{m_2} = \sqrt{\lambda}v/e^2$. Thus, instead of β given above ($\beta = \sqrt{\lambda}/e$), we can define a parameter b (with $b \sim \lambda/e^2$) as

$$b \equiv \frac{M_{m_2}/r_{m_2}}{M_m/r_m}, \tag{13}$$

which displays the coupling between both, mass over radius scales. There are three parameters v, e, λ and four quantities, M_m, r_m, M_{m_2}, r_{m_2}, so there is an equation

$$M_m r_m = M_{m_2} r_{m_2}, \tag{14}$$

which constrains the four quantities. For instance, r_{m_2} can be considered as fixed once the other three quantities are known.

B. The gravitational behavior as a function of *a* (gravitation) for low *b* (low Higgs mass)

Here, we overview the solutions found in Refs. 15–19 keeping in mind that we will later want them for comparison. We present the metric and matter functions as a function of radius, discuss the naked horizon behavior and the Coulomb character of this type of solutions, put a Schwarzschild black hole inside, and resketch some diagrams covering the space of solutions.

From the preceding section, low b indicates a small Higgs mass m_H, or large associated Compton wavelength, which means that the Higgs does not participate in the dynamics, it has very little influence on the monopole structure. Reinterpreted through Eq. (13) one can also see the low b case as a monopole with small secondary mass M_{m_2} or large secondary radius r_{m_2}. Given a low b configuration, we want now to understand how the structure changes as gravity is turned on higher and higher, i.e., as the parameter $a = M_m/r_m$ increases.

1. The regular magnetic monopole solution: from no gravitation to the extremal quasi-black hole

Let us start with a [see Eq. (12)] small. This means a highly dispersed magnetic monopole with small mass M_m and large radius r_m. As a increases the solution gets more general relativistic and eventually should get to a black hole, where $a = a_{\text{crit}} \sim 1$ (for instance, if the configuration formed a Schwarzschild black hole $a_{\text{crit}} = \frac{1}{2}$, or if it formed an extremal Reissner-Nordström black hole $a_{\text{crit}} = 1$). It does not happen exactly like this. The solution in the limit of a_{crit} yields a quasi-black hole as defined in Refs. 22 and 53. To get a grip on the solutions we draw in Fig. 1 diagrams showing the metric functions and the matter field functions as a function of r for two values of a, a small, and a_{crit}.[16] The function A signals the existence of a black hole horizon, the function B is the redshift function, the product function $(AB)^{1/2}$ tells whether a horizon is naked or not, and the function u and h report on the hair or no-hair of the solution. More specifically: (i) The function A, or better $1/A$, indicates how strong the curvature is, and in particular indicates the existence of a black hole horizon. At $r = 0$, $1/A$ should be 1 in order that there are no conical singularities, and at $r \to \infty$ should be again 1 for asymptotically flat space-times. Now, for $a \simeq 0$ space-time is flat and $1/A \simeq 1$ for all r. For small a there is a small dip at intermediate r as shown in Fig. 1. For large a the dip is large, and for $a = a_{\text{crit}}$, $1/A$ is zero, indicating that a black hole horizon might have formed, here an extremal one since $1/A$ gets a double zero. In fact, as was first noticed in Ref. 22, a true extremal black never forms. Instead, for a configuration with a radius

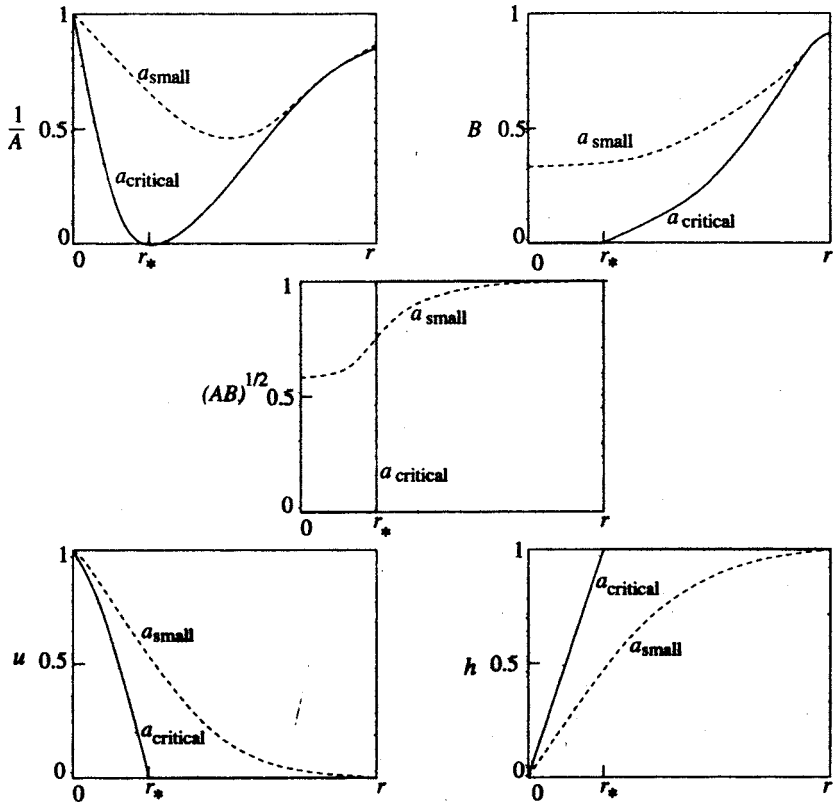

FIG. 1. The graphs of the metric and matter functions, $(1/A, B, (AB)^{1/2}, u, h)$, are plotted as a function of r in the low b case. The curves a small are typical of small gravitational effects, and the curves a critical give the properties of the extremal quasi-black hole. The radius r_* is the radius at which the quasihorizon is formed, see text for details.

arbitrarily near the critical radius, a quasi-black hole forms (i.e., a matter solution whose gravitational properties are virtual indistinguishable from a black hole[22]), and at a_{crit} precisely, a degenerate space-time appears as it is found when one looks to the metric function B. (ii) The metric function B gives the redshift behavior, or the relative behavior of clocks at different spatial positions. It is the function that distinguishes a true black hole from a quasi-black hole, as we will now see. For $a \simeq 0$, one has $B \simeq 1$. For small a, B lowers at the origin showing the existence of a gravitational potential, and goes to 1 at $r \to \infty$. For $a = a_{\text{crit}}$ or very near it, B goes again to one at $r \to \infty$, but now it is zero up to the monopole radius. This is odd, the infinite redshift surface is not a surface it is a three-dimensional region. To be a black hole B should go to zero at a given r only. This means that the solution at $a = a_{\text{crit}}$ does not represent a smooth manifold. Thus, the quasi-black-hole configuration gives rise to a degenerated space-time. For a very near the critical value it is very hard to distinguish the quasi-black-hole solution from a true black hole. The radius of these quasi-black holes is denoted by $r = r_*$, and is arbitrarily near to the radius of the extremal Reissner-Nordström black hole of same mass and charge, see Fig. 1. (iii) One should also pay attention to the behavior of $(AB)^{1/2}$, which says whether the horizon is naked or not, as it will be precised below. For $a \simeq 0$ one has $(AB)^{1/2} \simeq 1$. For a small, $(AB)^{1/2}$ is small at $r = 0$ and 1 at $r \to \infty$. For $a = a_{\text{crit}}$, $(AB)^{1/2}$ is 0 up to $r = r_*$ and then steps into 1, see Fig. 1. It is interesting to comment further on the behavior of $(AB)^{1/2}$ and its consequences. For the Schwarzschild and Reissner-Nordström solutions $(AB)^{1/2}$ is 1 for all radii. However, it is not so here, as can be seen directly in Fig. 1. The fact that $(AB)^{1/2} \to 0$ for $r \leqslant r_*$ at the critical solution implies that the black hole horizon formed has a naked behavior [22]. This means that the components of the Riemann tensor at the horizon in an orthonormal frame blow up at the horizon. It can be understood as follows. Suppose a particle sent in through the monopole, by a distant observer, turns around, and

comes back to the point where it started. Suppose also the monopole is on the verge of forming a horizon, i.e., the monopole surface is a quasihorizon. Due to the very small value of $(AB)^{1/2}$ inside and at the quasihorizon (see Fig. 1), one finds that the proper time the particle takes for the round trip is given by $\Delta\tau \sim r_* \epsilon^q$, where r_* is the radius of the quasihorizon, $\epsilon \equiv (1/A)_{\min}$ is a very small quantity near the critical solution, and q is found by numerical methods to be $\sim 0.7-1.0$.[22] So the particle takes virtual zero time within the quasihorizon. This fact is related to the black hole nakedeness. The Riemann tensor on a particle gives essentially the tidal forces in the particle. It can be shown that the Riemann tensor in these cases is inversely proportional to the square of the proper time it takes the particle to cross the region.[22] Thus if the proper time is zero, the Riemann tensor, and thus the tidal forces are huge, giving rise to a naked behavior, the horizon is exposed. Here $R_{\hat{t}\hat{i}\hat{t}\hat{i}} \sim \epsilon^{-2q}$, where the caret means calculated in the freely falling frame and the indexes i denote spatial indexes. So, these are naked black holes. Note that for the Schwarzschild, Reissner-Nordström, and extremal Reissner-Nordström black holes, the Riemann tensor calculated in the frame falling with the particle is well behaved, so the horizon is well behaved, a result that is known otherwise. The other interesting time to compute in the round trip is the coordinate time. It is given by $\Delta t \sim r_* \epsilon^{-q}$. Thus, for a coordinate observer, the particle takes a long time to return. This coordinate time can be important for entropic considerations.[22] (iv) The function u for the Yang-Mills field shows for a small a $1/r^2$ fall off for large r, and for $a=a_{\text{crit}}$ it disappears for radii greater than $r=r_*$. (v) The function h of the Higgs field for small a is zero and then grows to pick up the Higgs vacuum value at large r. For $a=a_{\text{crit}}$ it grows from 0 at the origin to 1 at the horizon, and stays at 1 up to infinity. This means that there is no hair, outside the horizon, only the trivial magnetic and vacuum Higgs fields. These quasi-black holes have been termed Coulomb type quasi-black holes since they show a Coulomb (no hair) field when they form.[21]

2. Nonregular magnetic monopoles: The Schwarzschild black hole solution inside the monopole

Up to now we have mentioned the behavior of regular gravitating monopoles, i.e., solutions that are regular from the origin to infinity. One can now put a small Schwarzschild black hole, with mass M_{bh} and radius r_{bh}, inside the magnetic monopole. This system is an example of a non-Abelian black hole with hair. One could think that putting a Schwarzschild black hole inside the monopole would disrupt the structure, and turn the monopole solution into a time-dependent one with the Yang-Mills and Higgs fields being accreted onto the black hole. But this is not the case, matter, with energy density ρ and radial pressure component p_{rr}, can coexist with an event horizon at its location as long as $\rho+p_{rr}=0$, a result that follows directly from the conservation equation $T^{\mu\nu}{}_{;\nu}=0$. A well-known example is the Schwarzschild-de Sitter solution, where the cosmological constant term Λ can be seen as a fluid which certainly obeys $\rho+p_{rr}=0$. Following Refs. 16 and 25 one finds that the non-Abelian structure inside the monopole may be approximated as a uniform vacuum energy density ρ_{vac} up to the monopole radius r_m such that the black hole in this region has a metric identical to the Schwarzschild-de Sitter black hole. For small black holes the condition $\rho+p_{rr}=0$ is obeyed and they can inhabit the center of the monopole, i.e., small black holes inside do not perturb much the solution. However, when the Schwarzschild black hole is large enough, such that its mass is of the order of the mass of the system, the system itself collapses giving rise to a magnetically charged extremal Reissner-Nordström quasi-black hole. We note that the literature is not clear whether it forms a true extremal black hole or an extremal quasi-black hole, however by continuity from the regular case one is entitled to infer that it is a quasi-black hole, followed by a degenerated space-time at the critical value. The appearance of this quasi-black hole happens for a critical value of the parameter a, with $a_{\text{crit}} \sim 1$, or alternatively, for a critical value of the total mass M, with $M=M_m+M_{\text{bh}}$. The behavior is thus analogous to the regular monopole in the sense that as one increases gravitation, i.e., as the parameter a or the mass M of the system increases, one finds a a magnetically charged extremal Reissner-Nordström quasi-black hole.

To understand the generic behavior it is helpful to make a plot of the solution space. One such plot is given in a $M_m \times M$, where $M=M_m+M_{\text{bh}}$ is the total mass. This is shown in Fig. 2, see also

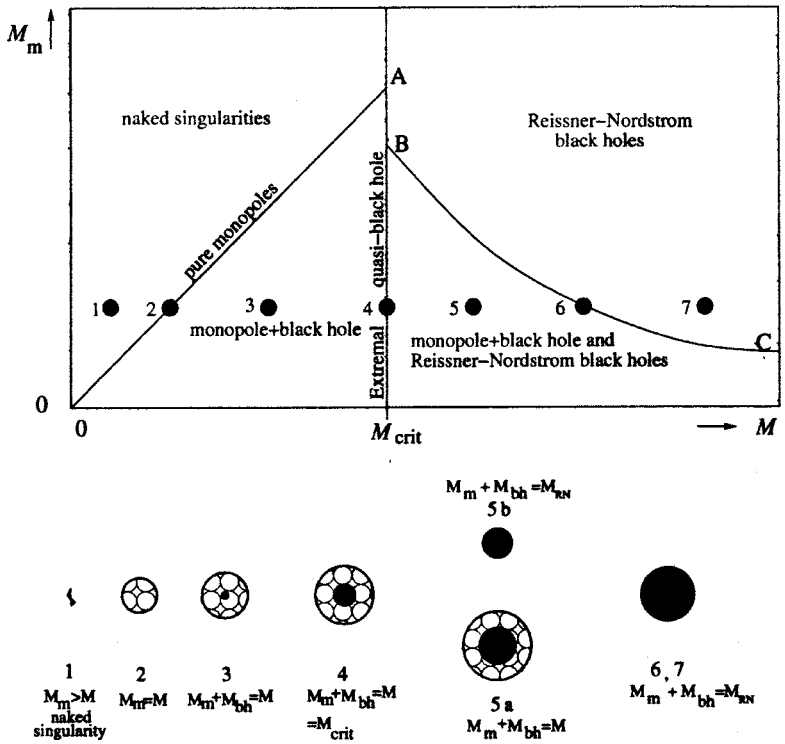

FIG. 2. The space of solutions in a $M_m \times M$, where $M = M_m + M_{\rm bh}$ is the total mass, is plotted (see also Ref. 16). For each point 1–7, along a constant monopole mass, in the diagram, the corresponding configuration is pictorially represented in the bottom part of the figure.

Ref. 16. There are four areas and three lines. The pure monopole line (the regular solutions discussed above) with the total mass equal to the monopole mass, is represented by a line with slope 1. The top-left region represents naked singularities. The center-left area represents monopole+Schwarzschild (non-Abelian) black hole solutions mentioned above. At arbitrarily near the critical mass the solutions are extremal magnetic charged Reissner-Nordström quasi-black holes (and at precisely the critical mass they turn into degenerated solutions). To the right there is a region where monopole+Schwarzschild (non-Abelian) black holes coexist with magnetic (Abelian) Reissner-Nordström black holes. Then to the far right and above there is a region of magnetic (Abelian) Reissner-Nordström black holes alone. In this diagram, solutions with a constant black hole mass are represented by lines parallel to the pure monopole line, i.e., lines of slope 1. Lines of constant monopole mass are horizontal lines. We show pictorially each representative configuration along a constant monopole mass line. Each numbered point (from 1 to 7) in Fig. 2 is represented in the bottom of the figure by a schematic drawing. In this drawing, note that the horizon area of the solution containing a Schwarzschild black hole surrounded by monopole matter (numbered 5a) is larger than the horizon area of the pure magnetic Reissner-Nordström horizon (numbered 5b). Following the area law, the smaller one is prone to be unstable and decay to the larger hairy one. This has interesting implications in the ultimate fate of the black hole through Hawking evaporation.[17]

Another similar but interesting plot is $a \times r_{\rm bh}$ diagram, shown in Fig. 3, see also Ref. 18. There are four areas and four lines. There is the pure monopole line ($r_{\rm bh}=0$), which yields the regular solutions discussed above. The top-left area is the region of no solutions. There is the center-left area of monopole+Schwarzschild (non-Abelian) black hole solutions discussed above, there is the bottom-left area where one finds monopole+Schwarzschild (or non-Abelian) black hole solutions as well as magnetic (Abelian) Reissner-Nordström black holes, and then the right area of magnetic (Abelian) Reissner-Nordström black holes. The other lines are boundaries between these areas.

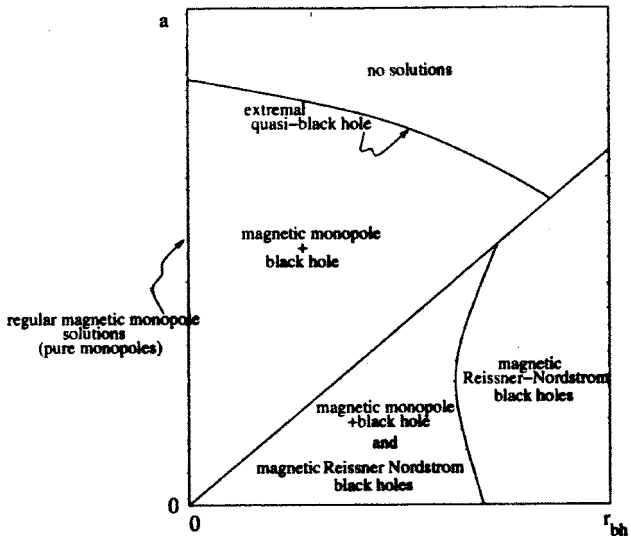

FIG. 3. The space of solutions in a $a \times r_{\rm bh}$ diagram (see also Ref. 18).

C. The gravitational behavior as a function of *a* (gravitation) for high *b* (high Higgs mass)

High Higgs mass reserves surprises. Here we overview the solutions found in Refs. 21 and 22 still keeping in mind that we will later need them for comparison. High b means $b \gtrsim 40$.[21] From Sec. II A, high b indicates a large Higgs mass m_H, or small associated Compton wavelength. This means that the Higgs field does participate in the dynamics, and can have great influence on the monopole structure. Reinterpreted through Eq. (13) one can also see high b as a monopole with large secondary mass M_{m_2}, or small secondary radius r_{m_2}. In order to understand how the structure changes as gravity is turned on higher and higher one must increase the parameter a.

1. The regular magnetic monopole solution: from no gravitation to the extremal black hole

For low a there is not much change in relation to the low b case. Low a represents a highly dispersed magnetic monopole, with small mass M_m and large radius r_m. As a increases the solution gets more general relativistic and eventually gets to a black hole, when $a=a_{\rm crit} \sim 1$. An important difference to the low b case is that instead of passing from a quasihorizon to a degenerate space-time, it passes from a quasihorizon to a true horizon, well inside the core at r_{*2}.[22] To get a grip on the solutions we draw in Fig. 4 diagrams showing the metric functions and the matter field functions as a function of r for two values of a, a small and $a_{\rm crit}$. Specifically the behavior of the functions is (i) The function $1/A$, the metric function that signals the formation of a black hole, shows that very near $a_{\rm crit}$ there are two radial scales, where horizon could be formed, one at r_{*2} (related to the scale set by the Higgs mass), the other at $r=r_*$ (related to the scale set by the W mass), but at $a_{\rm crit}$ the double zero occurs at r_{r^*2}, and an extremal horizon appears there. (ii) The metric function B shows also a zero at r_{*2} signaling the formation of an infinite redshift surface. Note now that B is zero at one point only, r_{r^*2}, not in a whole region as was the case for low b. This means that the configuration quasi-black hole with radius very near r_{*2}, turns into a true extremal black hole rather than to a degenerate space-time as in the low b case. (iii) The behavior of $(AB)^{1/2}$, which tells whether the horizon is naked or not, confirms this behavior. It shows that it is never zero, meaning the horizon is a regular, not a naked one.[22] This means that the components of the Riemann tensor at the horizon in an orthonormal frame are well behaved. In this case a particle that is sent in through the monopole, turns around, and comes back to the point where it started, takes a proper time $\Delta\tau$ which is finite, nonzero. Thus, since the Riemann tensor is pro-

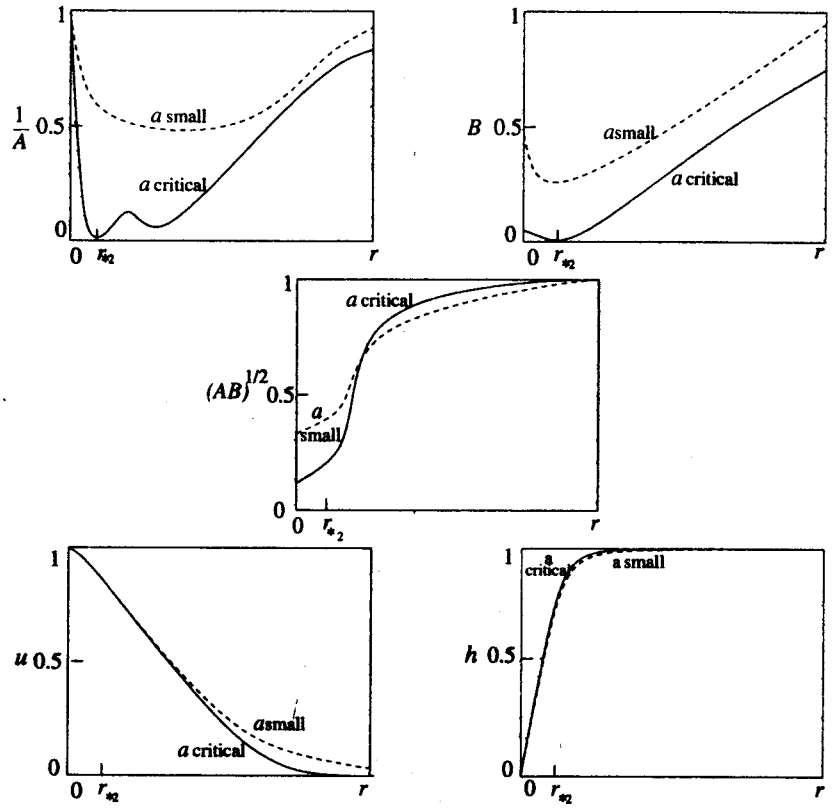

FIG. 4. The graphs of the metric and matter functions, $(1/A, B, (AB)^{1/2}, u, h)$, are plotted as a function of r in the high b case. The curves a small are typical of small gravitational effects, and the curves a critical give the properties of the extremal quasi-black hole. The radius r_* is the radius at which the quasihorizon is formed, see text for details.

portional to $(\Delta\tau)^{-2}$, as discussed in connection to the low b case, there is no funny behavior at the horizon and all behaves well. (iv) The function u for the Yang-Mills field shows that for a_{crit} there is field outside the horizon radius, i.e., there is hair. (v) The function h for the Higgs field, behaves similarly to u. In the critical situation, it only acquires the vacuum value for radii much larger than r_{*2}.

There are three points that are worth commenting. First, we comment further on the behavior of $(AB)^{1/2}$ and its consequences. In terms of the coordinate time, the particle takes for the round trip the time $\Delta t \sim r_{*2}\epsilon^{-1/2}$, where again $\epsilon \equiv (1/A)_{\min}$ is a very small number. Thus the particle takes, as in the low b case, a long time to return to a coordinate observer, and this is important in connection with entropy issues.[22] Indeed, in leading order, this time is determined only from the space-time geometry. An observer finds that the quasi-black hole has an inside which is inaccessible, since probes stay there for an arbitrarily large amount of time, and describes it by a density matrix ρ_{matrix} obtained by tracing over the degrees of freedom inside the quasihorizon, yielding an entropy $S=-\text{Tr}\,(\rho_{\text{matrix}} \ln \rho_{\text{matrix}})$. The calculation of the interior entropy of a field inside a spherical box was performed for a scalar field with the result that $S=\gamma(A/4)$, where γ is an undetermined factor, and A is the area of the box.[56] In this case, the box is the magnetic monopole quasihorizon configuration on the verge of being a black hole. Since one can give a little push from this configuration to the horizon configuration, and in the latter case the entropy is $S=A/4$ one can guess by continuity that the coefficient of proportionality in the quasihorizon case has a dependence on the size of the box $\gamma=\gamma(r_{\text{box}})$ and when a horizon forms, $\gamma(r_{*2})=\frac{1}{4}$.[22] In this sense, the entropy of the extremal black hole is the number of the entangled degrees of freedom inside the horizon. This analysis cannot be applied to the low b case because there is never a true horizon: in the limit, when the object is turning into a black hole it gives a nonsmooth manifold.

Second, another feature of these monopoles is that they have a charge to mass ratio given by $Q/M>1$. Thus if one drops neutral matter onto a regular magnetic monopole one can form an extremal black hole.[22] This is contrary to the case of electric Reissner-Nordström black holes with $Q/M<1$, and where one can drop charged matter, with charge q and mass m obeying $q/m>1$, as much as one wants that one never gets an extremal black hole (this is a version of the third law of black hole mechanics).

Third, one can ask what happens for a higher than the critical value. Following Ref. 22 one finds that there are possibly two branches. One branch is formed of magnetically Abelian charged Reissner-Nordström black holes. The other branch, has non-Abelian matter and hair outside, a horizon, and regular non-Abelian matter inside. Following theorems by Borde[57–59] one finds that these regular solutions may have different inside and outside topologies. This issue should be further explored.

2. The Schwarzschild black hole solution inside the monopole

As in the low b case one can put a Schwarzschild black hole inside. This was done in Ref. 24. The main feature is that again there is hair outside the true horizon. The results are in line with what we have been discussing. Diagrams like those of Figs. 2 and 3 can be drawn, although we have not found them in the literature.

D. Further discussion

Thus, gravitationally there are two distinct behaviors, the low b case and the high b case, the marginal case being at $b\simeq 40$. The low b case has the following main features: when one turns on gravitation (when one increases a) a quasi-black hole appears from the regular monopole, which turns into a degenerate space-time at the critical value $a_{\rm crit}$; it has a naked horizon, and shows no hair, i.e., it is of Coulomb type, the nontrivial fields are hidden inside the horizon. In addition, one can enrich the monopole structure by putting a Schwarzschild black hole inside up to a certain maximum mass. The high b case has also a regular monopole solution which, when one increases the gravitational parameter a, turns into a quasi-black hole, and then at $a_{\rm crit}$ a true extremal black hole appears, with regular horizon and hair. There is a transition between the two cases, a first order type transition. When b is in the transition zone, there is a double double zero, one zero at r_* and the other at r_{*2}. So, the transition is discontinuous in radius, and thus in entropy. It is, however, continuous in mass.[21]

Other features that are also very interesting but not important in our context are the following: (i) For very low b ($b<0.1$ say), the behavior is more complicated near $a_{\rm crit}$.[18] If one increases a from zero, one passes $a_{\rm crit}$ up to an $a_{\rm max}$. But from $a_{\rm crit}$ to $a_{\rm max}$ there are two solutions, one with larger mass M_m (larger radius r_m), the other with smaller values. The one with smaller values is the one that connects continuously with the low mass solutions. The smaller mass solutions are stable, and so the branch which forms black holes is unstable; (ii) for a certain range of the parameters a and b, there are multiple node solutions [nodes appearing in the function $u(r)$ of the Yang-Mills field] of the type found in the Bartnick-Mckinonn solution;[18] (iii) the particular case $b\to\infty$ in the high b sector was analyzed in detail by Aichelburg and Bizon.[20] The solution has a conical singularity at $r=0$ but apart from that it is well behaved. Perhaps, oddly, core behavior in this limit was not found, we will comment on this later on.

This program of studying the gravitational behavior of magnetic monopoles has been continued by Brihaye *et al.*, where the structure of dyonic non-Abelian black holes has been analyzed,[29,30] and gravitational monopoles in SU(3), SU(5), and SU(N) theories have been found.[32–34]

III. GRAVITATIONAL BEHAVIOR OF MAJUMDAR-PAPAPETROU MATTER SYSTEMS: TWO CONCENTRIC SPHERICAL THIN SHELLS

A. The Majumdar-Papapetrou sector of the Einstein-Maxwell-charged dust system

1. The action and equations of motion

We now want to study the Einstein-Maxwell system coupled to some specific electrically charged dust currents as will be described below. By dust one means a fluid with zero pressure. We will compare the configurations found below with the magnetic configurations discussed in Sec. II. A first study in this direction has been done in Ref. 53 (see also Ref. 54). The action for the Einstein-Maxwell-charged dust system is $(G=c=1)$

$$S=\int d^4x\sqrt{-g}\left(\frac{1}{16\pi}R+\mathcal{L}_{\text{matter}}\right), \tag{15}$$

where R is the scalar curvature, and

$$\mathcal{L}_{\text{matter}}=\mathcal{L}_{\text{Maxwell}}+\mathcal{L}_{\text{charged dust}}+\mathcal{L}_{\text{int}}. \tag{16}$$

The Maxwell Lagrangian is

$$\mathcal{L}_{\text{Maxwell}}=-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}, \tag{17}$$

$$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu, \tag{18}$$

where $F_{\mu\nu}$ and A_ν are the electromagnetic field strength and potential, respectively. The charged dust Lagrangian, $\mathcal{L}_{\text{charged dust}}$, is such that the action integral, $S_{\text{dust}}=\int d^4x\sqrt{-g}\mathcal{L}_{\text{dust}}$, gives the energy-momentum tensor for charged dust, i.e.,

$$T^{\mu\nu}_{\text{charged dust}}=-\frac{1}{8\pi}\frac{1}{\sqrt{-g}}\frac{\delta S_{\text{charged dust,}}}{\delta g^{\mu\nu}}=\rho u^\mu u^\nu, \tag{19}$$

where ρ is the dust energy density and u^μ its four-velocity. The interaction Lagrangian $\mathcal{L}_{\text{interaction}}$ is given by

$$\mathcal{L}_{\text{interaction}}=A_\mu j^\mu, \tag{20}$$

where $j^\mu=\rho_e u^\mu$, ρ_e being the electric charge density. The elementary particles are then the electromagnetic massless photon, the massless graviton, and the massive charged dust particles with energy density ρ and charge density ρ_e. The charged dust particles may spread over a given three-dimensional region of space, or can be squeezed into a two-dimensional thin membrane, i.e., a shell. In the latter case the action (15) acquires the form of a bulk action plus a membrane action. These bulk plus membrane systems will be treated now.

The configuration we want to discuss is spherically symmetric, a star type configuration, with metric given again by

$$\mathrm{d}s^2=-B(r)\mathrm{d}t^2+A(r)\mathrm{d}r^2+r^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2), \tag{21}$$

and with the electric Maxwell field given by

$$A_0=\varphi(r),\quad A_i=0. \tag{22}$$

Putting this ansatz into the Einstein-Maxwell-charged dust action (15) and varying the action with relation to the three functions, yields three equations, two for the gravitational field $B(r)$ and $A(r)$, and one for the Maxwell field $\varphi(r)$. The equations are, respectively,

$$\frac{(AB)'}{AB}=8\pi r\rho A, \tag{23}$$

$$\left[r\left(1-\frac{1}{A}\right)\right]' = 8\pi r^2\rho + \frac{r}{AB}\varphi'^2, \tag{24}$$

$$\frac{\sqrt{B}}{r^2\sqrt{AB}}\left[\frac{r^2}{\sqrt{AB}}\varphi'\right]' = -4\pi\rho_e. \tag{25}$$

There are three parameters in the theory: G which we have set equal to one, ρ and ρ_e. Now, ρ and ρ_e have dimensions of length to minus two. Thus one can form in principle two length scales. The ratio of these length scales yields a parameter without dimensions. One particular class of solutions, the one we want to treat, sets

$$\frac{\rho_e}{\rho} = 1. \tag{26}$$

(Note that the charge density ρ_e can have two signs, so strictly speaking one should set $\rho_e = \pm\rho$. In order to not carry this $\pm$ throughout we drop the minus sign, bearing in mind that a $-$ sign can be floating about.) Matter obeying the condition (26), i.e., matter with mass equal to charge, can be called extremal charged dust in analogy with the extremal Reissner-Nordström black holes. The system of equations (23)–(25) with condition (26) is the Majumdar-Papapetrou system.[37,38]

Now, in order to show a behavior analogous to the magnetic monopole of the Einstein-Yang-Mills-Higgs system the Majumdar-Papapetrou system per se is not enough, the parameters do not give enough structure. In order to get more structure we must add new parameters. First assume a given spherical symmetric solution, which we call a star. Then, a new parameter is the radius of the star, $r_{\rm star}$. So now, one has two parameters ρ and $r_{\rm star}$. It is preferable to swap the star's density ρ for the star's mass $M_{\rm star}$, so that the two parameters are $M_{\rm star}$ and $r_{\rm star}$. Then one can form an adimensional parameter

$$a = \frac{M_{\rm star}}{r_{\rm star}}. \tag{27}$$

This is the equivalent to the parameter a in the Einstein-Yang-Mills-Higgs theory, see (12). To simplify the analysis, and without loss of generality, we can think that the star is made of a thin shell of extremal charged dust, with $M_{\rm star}$ and $r_{\rm star}$ being now the mass and the radius of the thin shell. It is not difficult to see that this thin shell is a solution of the Majumdar-Papapetrou system.[54] One can now further bring into the problem a new extremal charged thin shell, called the secondary shell, with two new parameters, the mass M_2 and the radius r_2. One has then two thin shells, one inside the other, a configuration that is also a solution of the Majumdar-Papapetrou system, as will be displayed below. One can then form a new dimensionless parameter b given by

$$b = \frac{M_2/r_2}{M_{\rm star}/r_{\rm star}}. \tag{28}$$

This is equivalent to the secondary parameter of the Einstein-Yang-Mills-Higgs system appearing in Eq. (13). This double shell solution has four parameters $M_{\rm star}$, $r_{\rm star}$, M_2, r_2. In order to produce the required model one should restrict these four parameters through a constraint equation, as in the magnetic monopole case. Generically, the two shells are indistinguishable, one cannot say whether the outer one is the star or the secondary shell. To be definitive, the inner shell is called the secondary shell, the outer shell is the star, and we keep the secondary shell always inside the star, through the constraint

$$r_{\rm star} = 2r_2. \tag{29}$$

The factor 2 in (29) was chosen for convenience, any real number greater than 1 will do. Equation (29) is the equivalent to the constraint (14) in the magnetic monopole case. Thus the system we are going to work with is a Majumdar-Papapetrou system with two extremal charged shells. This

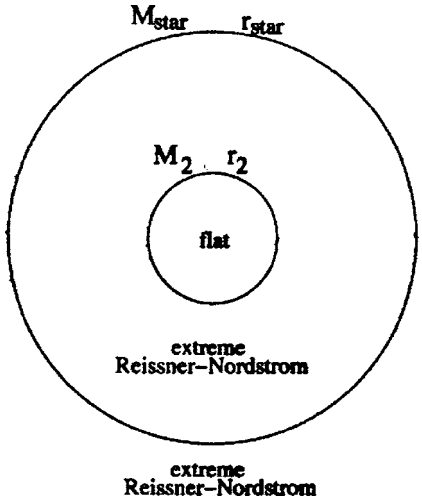

FIG. 5. A schematic drawing of the double shell solution in the Majumdar-Papapetrou system, showing the secondary shell inside the star shell.

simple system mimics a good deal of behavior of the Einstein-Yang-Mills-Higgs system. Instead of working with thin shells, one could work with the thick shell solutions found in Ref. 54 or with the Bonnor stars,[49–51] but this only complicates the technical analysis of the problem without further illuminating it.

2. Some properties and scales of the Majumdar-Papapetrou double shell

We are now ready to put a shell within a shell, and simulate the behavior of the gravitational magnetic monopoles. The star (outer shell) and the secondary shell (inner shell) are considered to be infinitesimally thin, see Fig. 5. Then, the metric valid from $0 \leqslant r < \infty$, for a Majumdar-Papapetrou space-time with two extremal matter thin shells, is given by

$$\mathrm{d}s^2 = -\frac{\left(1-\frac{M}{r_{\mathrm{star}}}\right)^2\left(1-\frac{M_2}{r_2}\right)^2}{\left(1-\frac{M_2}{r_{\mathrm{star}}}\right)^2}\mathrm{d}t^2 + \mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2), \quad 0 \leqslant r \leqslant r_2, \tag{30}$$

$$\mathrm{d}s^2 = -\frac{\left(1-\frac{M}{r_{\mathrm{star}}}\right)^2}{\left(1-\frac{M_2}{r_{\mathrm{star}}}\right)^2}\left(1-\frac{M_2}{r}\right)^2\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{\left(1-\frac{M_2}{r}\right)^2} + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2), \quad r_2 \leqslant r \leqslant r_{\mathrm{star}}, \tag{31}$$

$$\mathrm{d}s^2 = -\left(1-\frac{M}{r}\right)^2\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{\left(1-\frac{M}{r}\right)^2} + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\phi^2), \quad r_{\mathrm{star}} \leqslant r < \infty, \tag{32}$$

where $M = M_{\mathrm{star}} + M_2$ is the total mass of the system. The constants in the g_{tt} components were chosen so that the metric matches at the shells. The electric field is

$$\varphi = 1 - \frac{\left(1 - \frac{M}{r_{\rm star}}\right)\left(1 - \frac{M_2}{r_2}\right)}{\left(1 - \frac{M_2}{r_{\rm star}}\right)}, \quad 0 \leqslant r \leqslant r_2, \tag{33}$$

$$\varphi = 1 - \frac{\left(1 - \frac{M}{r_{\rm star}}\right)\left(1 - \frac{M_2}{r}\right)}{\left(1 - \frac{M_2}{r_{\rm star}}\right)}, \quad r_2 \leqslant r \leqslant r_{\rm star}, \tag{34}$$

$$\varphi = 1 - \left(1 - \frac{M}{r}\right) = \frac{M}{r}, \quad r_{\rm star} \leqslant r < \infty. \tag{35}$$

The fluid field is given by the surface energy densities of the shells. For the secondary thin shell one has that the surface energy density σ_2 is given by

$$\sigma_2 = \frac{M_2}{4\pi r_2^2}, \tag{36}$$

with the corresponding surface electric charge density of the shell σ_{e_2} given by $\sigma_{e_2} = \sigma_2$. For the thin shell star one has that the surface energy density $\sigma_{\rm star}$ is given by

$$\sigma_{\rm star} = \frac{M_{\rm star}}{4\pi r_{\rm star}^2}, \tag{37}$$

with the corresponding surface electric charge density of the shell $\sigma_{e_{\rm star}}$ given by $\sigma_{e_{\rm star}} = \sigma_{\rm star}$. Note that the g_{rr} component of the metric has a step function at r_2 and $r_{\rm star}$. This is no problem, one can smooth it out by considering a shell with small thickness,[54] but for the problem we are considering it is irrelevant.

One important question is which shell, and in which conditions a shell, forms a horizon. We know that a horizon should form when $1/A = 0$. Suppose a b is given, and one starts to increase a. Then it is meaningfull to ask which shell forms first a horizon, the star or the secondary shell? To answer it note that

$$\left(\frac{1}{A}\right)_{r_2} = 1 - \frac{M_2}{r_2} = 1 - ab, \tag{38}$$

$$\left(\frac{1}{A}\right)_{r_{\rm star}} = 1 - \frac{M}{r_{\rm star}} = 1 - \frac{M_{\rm star}}{\rm r_{star}}\left(1 + \frac{M_2/r_2}{M_{\rm star}/r_{\rm star}}\frac{r_2}{r_{\rm star}}\right) = 1 - a\left(1 + \frac{b}{2}\right). \tag{39}$$

It is then clear that there are three cases:

$b < 2$, when a increases an external horizon forms first at $r_{\rm star} = M$, with $a_{\rm crit} = 1/(1 + b/2)$. This is analogous to the behavior of magnetic monopoles with low b, where an external horizon forms outside the core.

$b > 2$, when a increases an interior horizon forms first at $r_2 = M_2$, with $a_{\rm crit} = 1/b$. This is analogous to behavior of magnetic monopoles with high b, where an external horizon forms within the core.

$b = 2$, when a increases a horizon forms at both shells, interior and exterior with $a_{\rm crit} = 1/2$. This divides the two cases above.

As we will show below the solution does not develop a true horizon. Independently of b, upon increasing a, a quasihorizon appears. Then at the critical value one gets a degenerated space-time, and for values of a above the critical one there is no static solution, the shell collapses (see Ref.

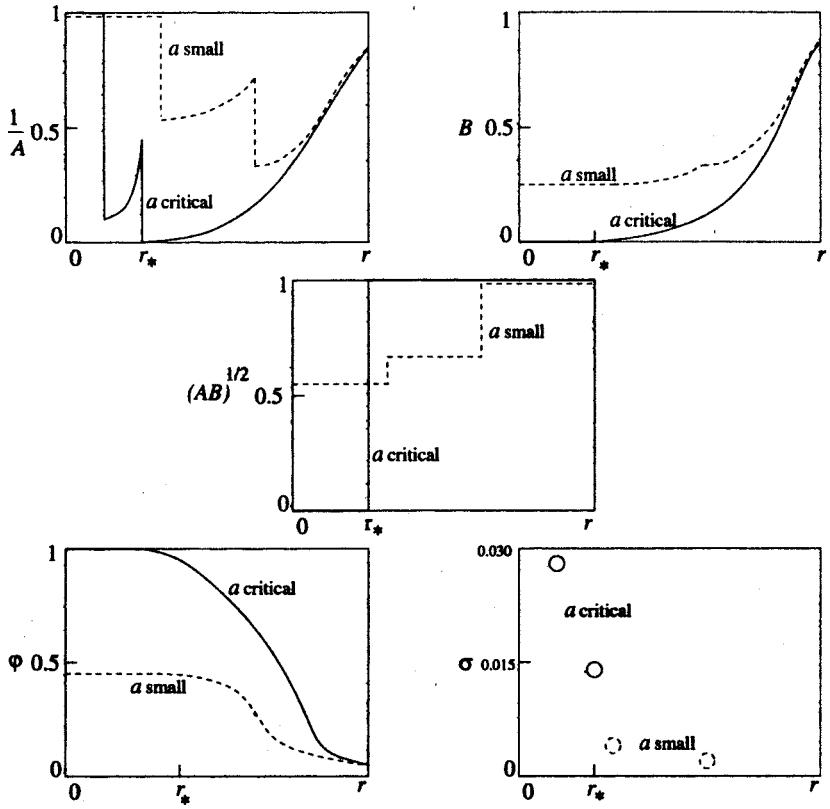

FIG. 6. The graphs of the metric and matter functions, $(1/A, B, (AB)^{1/2}, \varphi, \sigma)$, are plotted as a function of r in the low b ($b<2$) case. The curves a small (dashed lines) are typical of small gravitational effects, and the curves a critical (full lines) give the properties of the extremal electrical quasi-black hole. The radius r_* is r_{star} at the quasihorizon (arbitrarily near the critical radius), see text for details. (In the graphs, we have used $b=1$ as a typical low b case, and have set $M_{\text{star}}=\frac{5}{2}$, $M_2=\frac{5}{4}$, and for a small we have set $r_{\text{star}}=10$, $r_2=5$, while for a critical we have set $r_{\text{star}}=\frac{15}{4}$, $r_2=\frac{15}{8}$.)

60) into a singularity and an extremal Reissner-Nordström black hole forms. In what follows we study each type of configuration. We start with low b, $b<2$, then we do high b, $b>2$.

B. The gravitational behavior as a function of *a* for low *b*

Since $b=(M_2/r_2)/(M_{\text{star}}/r_{\text{star}})$, low b can be seen as a relatively small secondary mass M_2, or large secondary radius r_2, which means that the secondary shell has little influence in the structure. Given a low b configuration, we want to understand how the structure changes as the parameter $a=M_{\text{star}}/r_{\text{star}}$ increases. We present plots giving the behavior of the metric and matter functions as a function of radius for typical cases, discuss the naked horizon behavior and the Coulomb character of these solutions, put an extremal Reissner-Nordström black hole inside, and sketch some diagrams covering the space of solutions.

1. The regular Majumdar-Papapetrou double shell solution: from no gravitation to the extremal quasi-black hole and beyond

We have seen from Eqs. (38) and (39) that for fixed b, with $b<2$, an extremal quasihorizon appears when the parameter a increases, i.e., when one puts more gravitation into the star shell. A small a parameter, i.e., $M_{\text{star}}/r_{\text{star}}$ small, means that the star shell is very dispersed. As a increases, eventually it gets to a stage where a kind of an extremal event horizon forms. Using Eqs. (30)–(39) one can plot the behavior of the metric and matter functions as a function of radius for two values of a, a small, and a arbitrarily near a_{crit}, when a quasihorizon forms, see Fig. 6. Specifically, the behavior of the functions $1/A$, B, $(AB)^{1/2}$, φ, and σ is: (i) the function $1/A$ signals the formation

of a black hole. For a small the function $1/A$ starts at the value 1 (thus there are no conical singularities) drops slightly at the secondary shell, rises and drops again at the star shell, and then rises again to 1 at infinity. When $a=a_{\rm crit}$ (or arbitrarily near it) the function gets a double zero at $r=r_*$ (it would be a double zero had we smoothed out enough of the matter) signaling the formation of a kind of an extremal Reissner-Nordström black hole. (ii) The function B, the redshift function, has the usual behavior for a small. However, for $a_{\rm crit}$ the whole of the region inside r_* gets infinitely redshifted. This means that the manifold is not smooth. Thus the critical case is not a true black hole, it is a degenerated space-time. (iii) The product function $(AB)^{1/2}$ is important to determine whether the forming horizon is naked or not. We find that a particle on a return trip to the star takes a proper time given by $\Delta\tau\sim r_*\epsilon^{1/2}$, where r_* is the radius of the quasihorizon, and, near the critical solution, $\epsilon\equiv(1/A)_{\rm min}$ is a very small quantity.[54] Since this proper time is arbitrarily small, the Riemann tensor diverges at the horizon, and the horizon is naked. For completeness we given the coordinate time Δt taken by the particle in its trip, $\Delta t\sim r_*\epsilon^{-1/2}$, implying that the particle takes a long time to return for a coordinate observer. (iv) The function φ tells whether the solution has hair or not. It starts constant, then decays with $1/r$, with a bump at r_2 and at $r_{\rm star}$. When the horizon forms the field is a pure Coulomb field, showing no-hair. (v) The surface density function σ of the charged dust is also drawn, for completeness. Outside the quasihorizon at r_* there is no matter.

The case $b=0$ is worth discussing because it is the simplest one in the low b sector. There is no secondary shell ($M_2=0$) and so it represents a single thin shell with mass $M_{\rm star}$ and radius $r_{\rm star}$. It is interesting because on one hand it has the same properties of any other low b case, on the other hand, it is easier to figure out what happens above criticality, i.e., for $a>a_{\rm crit}$ ($M_{\rm star}>r_{\rm star}$). We have seen that when the precise equality holds, $a=a_{\rm crit}$, the redshift function B is zero not only at the horizon but also in the whole region inside, meaning that in fact a true black hole does not form, since inside there is no smooth manifold. For $a>a_{\rm crit}$ one has now a shell of matter at $r_{\rm star}$ inside an extremal electrical Reissner-Nordström black hole at $r_{\rm bh}=M_{\rm star}$, the solution being everywhere free from curvature singularities. Following a theorem by Borde,[57] this means that the topology of spacelike slices in this black hole space-time would change from a region where they are noncompact to a region where they are compact, in the interior. In our case this in fact does not happen, there are no solutions with $a>a_{\rm crit}$, i.e., $m>r_{\rm o}$, the shell collapses into a singularity.[60]

2. Nonregular Majumdar-Papapetrou shell solutions: The extremal Reissner-Nordström black hole solution inside the thin shell star

One can put a black hole inside the double thin shell and obtain a structure similar to the one found when one puts a black hole inside a magnetic monopole. For the double thin shell, the extra inner black hole must be an extremal Reissner-Nordström black hole, rather than a Schwarzschild black hole, to keep the solutions within the Majumdar-Papapetrou system. If one puts a nonextremal black hole foreign tensions would develop at the thin shells. So, in order to stick to pure Majumdar-Papapetrou system we stick to an inner extremal Reissner-Nordström black hole. In order to simplify the analysis, we will work with the $b=0$ which is a good simple case for low b. For any other small b, such that $b<2$, the result is analogous. In the $b=0$ case one has $M_2=0$. Thus the system is formed by the star shell with mass $M_{\rm star}$ and radius $r_{\rm star}$, and an inner extremal Reissner-Nordström black hole with mass $M_{\rm bh}$ and radius $r_{\rm bh}$ ($M_{\rm bh}=r_{\rm bh}$). The metric is now

$$ds^2=-\left(1-\frac{M_{\rm bh}}{r}\right)^2\frac{\left(1-\frac{M}{r_{\rm star}}\right)^2}{\left(1-\frac{M_{\rm bh}}{r_{\rm star}}\right)^2}dt^2+\frac{dr^2}{\left(1-\frac{M_{\rm bh}}{r}\right)^2}+r^2(d\theta^2+\sin^2\theta\, d\phi^2),\quad 0\leqslant r\leqslant r_{\rm star},\tag{40}$$

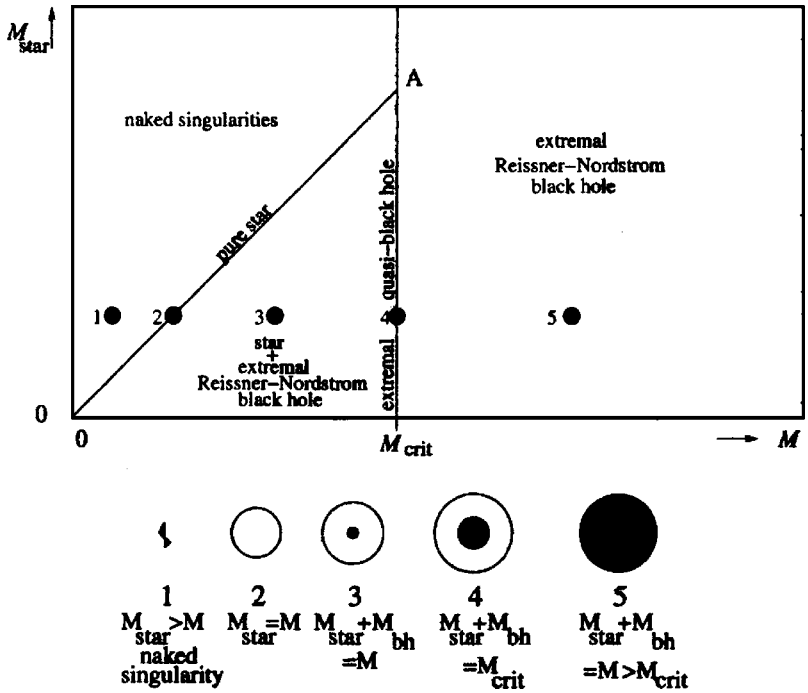

FIG. 7. The space of solutions in a $M_{\text{star}} \times M$, where $M = M_{\text{star}} + M_{\text{bh}}$ is the total mass, is plotted. For each point 1–5, along a constant star mass, in the diagram, the corresponding configuration is pictorially represented in the bottom part of the figure. This is the graph made in Fig. 2 (see also Ref. 16) adapted to the thin shell Majumdar-Papapetrou system.

$$ds^2 = -\left(1 - \frac{M}{r}\right)^2 dt^2 + \frac{dr^2}{\left(1 - \frac{M}{r}\right)^2} + r^2(d\theta^2 + \sin^2\theta\, d\phi^2), \quad r_{\text{star}} \leqslant r, \tag{41}$$

where here $M = M_{\text{star}} + M_{\text{bh}}$ is now the total mass. The electric field $\varphi(r)$ and the charge density field $\rho(r) = \sigma_{\text{star}}(r_{\text{star}})$ profile accordingly.

To understand the generic behavior of this system it is helpful to make a plot of the solution space, similar to the plot made for a Schwarzschild black hole inside the magnetic monopole shown in Fig. 2. We do this in Fig. 7, where we plot the solution space in a $M_{\text{star}} \times M$ diagram for fixed r_{star}. There are three regions and two lines. The pure star line, i.e., the regular solutions discussed above with the total mass equal to the star mass, is represented by a line with slope 1. The top-left region represents extremal charged naked singularities. The center-left region represents star+(extremal Reissner-Nordström black hole) solutions displayed in Eqs. (40) and (41). At values arbitrarily near the critical mass M_{crit} the solutions are extremal electric charged Reissner-Nordström quasi-black holes, which degenerate at the critical value. To the right there is a region of extremal Reissner-Nordström black holes. We show pictorially each representative configuration along a constant star mass line. Each numbered point (from 1 to 5) in Fig. 7 is represented in the bottom of the figure by a schematic drawing. We see that taking M_{star} constant and increasing M we pass through point 1 where M_{star} is greater than M and therefore there is a negative mass at the center, through point 2 where one finds a thin shell solution with $M_{\text{star}} = M$, through point 3 where there is a black hole inside the star, through point 4 which is the case arbitrarily near the critical value where $M_{\text{star}} + M_{\text{bh}} = r_{\text{star}}$, and thus an extremal quasi-black hole appears at r_{star}, finally to point 5 where r_{star} has collapsed inside the horizon radius to form an extremal black hole. Note there is a jump in horizon radius from a point infinitesimally to the left of point 4, to a point infinitesimally to the right of point 4. Note also that this diagram is done for fixed r_{star}. For another value of r_{star}, one gets the same diagram, but with the vertical critical line critical shifted, to the

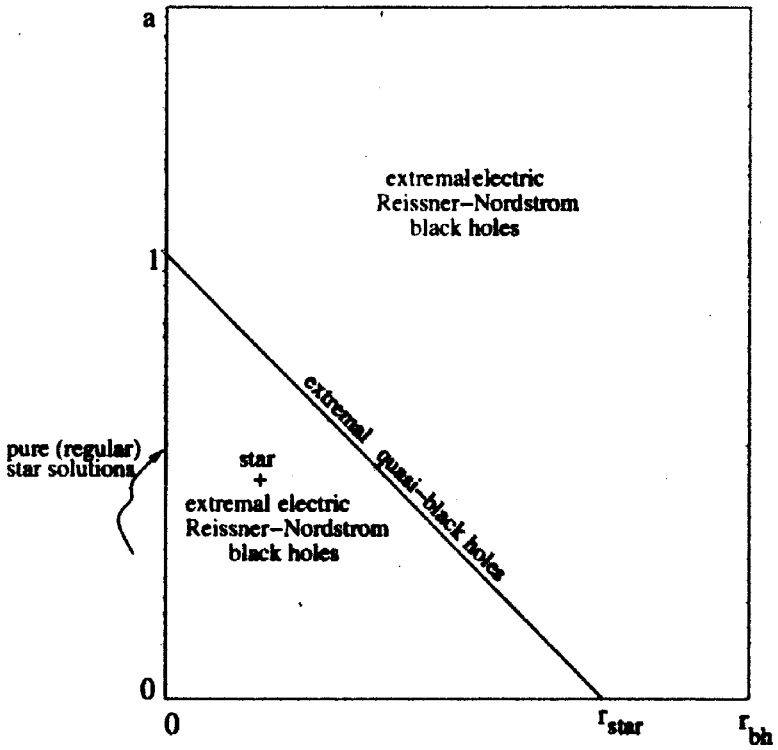

FIG. 8. The space of solutions in an $a \times r_{bh}$ plot. This is the graph made by Fig. 3 (see also Ref. 18) adapted to the thin shell Majumdar-Papapetrou system.

right when the new r_{star} is larger, and to the left when the new r_{star} is smaller than the original value. Comparison of Figs. 2 and 7 shows the similarities between the magnetic monopole and the Majumdar-Papapetrou system.

One can also translate Fig. 3 into this Majumdar-Papapetrou system. This is done in Fig. 8, where we display the important regions in a graph $a \times r_{bh}$ (where again $a = M_{star}/r_{star}$). There are two regions and two lines. There is the vertical line, $r_{bh}=0$, of regular star solutions. There is the region where star+(extremal electric Reissner-Nordström black hole) solutions exist. There is the line where the system forms a quasi-black hole (i.e., a solution arbitrarily near the critical degenerate case). Finally there is the region where an extremal electric black hole exists. These are black holes free from singularities. The naked singularity region, not shown, would appear for negative r_{bh}, i.e., for negative black hole masses, $r_{bh}=M_{bh}<0$.

C. The gravitational behavior as a function of *a* for high *b*

High b can be seen as a relatively large secondary mass M_2, or small secondary radius r_2, which means that the secondary shell has a decisive influence in the structure. Given a high b configuration, we want to understand how the structure changes as the parameter $a = M_{star}/r_{star}$ increases. We present plots giving the behavior of the metric and matter functions as a function of radius for typical cases, discuss the naked horizon behavior and the non-Coulomb character of these solutions, and we briefly comment on putting an extremal Reissner-Nordström black hole inside the high b double shell system.

1. The regular solution: from no gravitation to the extremal quasi-black hole and beyond

In contrast with low b, in the high b case, an extremal quasihorizon forms at the secondary shell r_2, rather than in the star shell. Using Eqs. (30)–(39) one can draw the important field

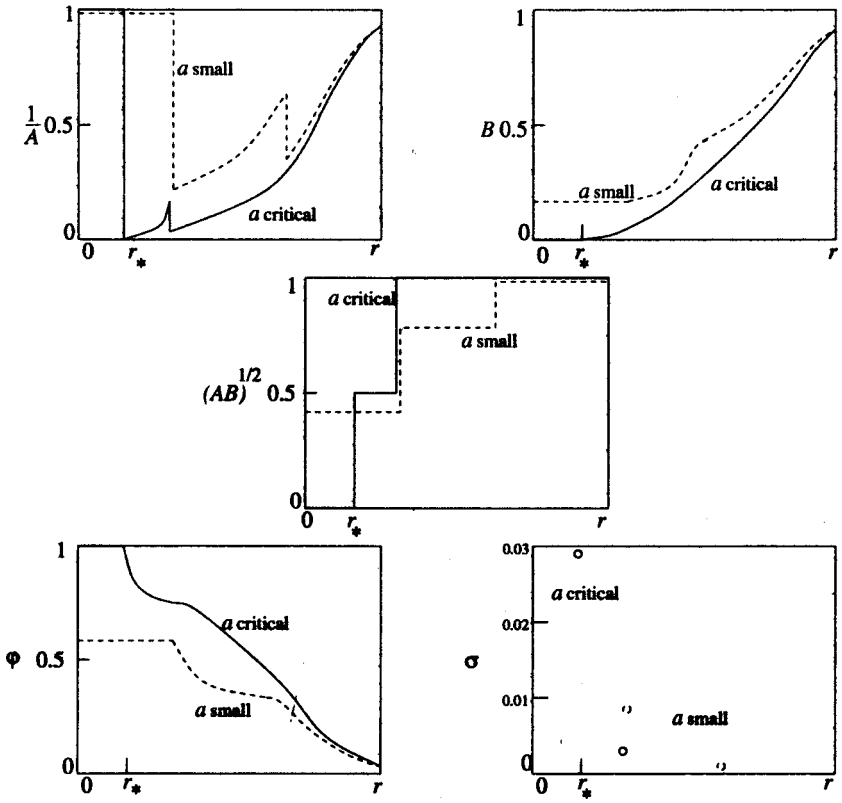

FIG. 9. The graphs of the metric and matter functions, $(1/A, B, (AB)^{1/2}, \varphi, \sigma)$, are plotted as a function of r in the high b ($b>2$) case. The curves a small (dashed lines) are typical of small gravitational effects, and the curves a critical (full lines) give the properties of the extremal quasi-black hole. The radius r_* is now r_2 at the quasihorizon, see text for details. (In the graphs, we have used $b=4$ as a typical high b case, and have set $M_{\text{star}}=\frac{5}{4}$, $M_2=\frac{5}{2}$, and for a small we have set $r_{\text{star}}=10$, $r_2=5$, while for a critical we have set $r_{\text{star}}=5$, $r_2=\frac{5}{2}$.)

functions as a function of r, for a given high b and for two values of a, a small and a critical, see Fig. 9. The behavior of the functions $1/A$, B, $(AB)^{1/2}$, φ, and σ is the following: (i) For a small the function $1/A$ starts at the value 1 drops at the secondary shell, rises and drops slightly at the star shell, and then rises again to 1 at infinity. When a is arbitrarily near a_{crit} the function gets a double zero at $r=r_*$, now situated at the secondary shell r_2, signaling the formation of a quasihorizon. (ii) For a small, the function B has the usual behavior. For a arbitrarily near a_{crit}, B is arbitrarily near zero throughout the region inside r_2. At $a=a_{\text{crit}}$ precisely the manifold is not smooth. Thus again, the critical case is not a true black hole, it is a degenerate manifold. (iii) The function $(AB)^{1/2}$ is zero inside the quasihorizon confirming the existence of a naked behavior. This is not quite the same as the high b behavior for the magnetic monopole, since the magnetic system gets in the high b case a non-naked horizon. (iv) At a arbitrarily near a_{crit}, the function φ does not have a Coulomb type behavior as one can see from Fig. 9, the electric field outside the quasihorizon gets a bump due to the presence of the outer shell. Strictly speaking one cannot talk of a no-hair violation since the no-hair theorem is applied to black holes, not quasi-black holes. (v) The surface density function σ of the charged dust is also drawn, for completeness.

There are two questions that can be asked. The first one is what happens if one increases a past a_{crit}. For $a>a_{\text{crit}}$ one gets an extremal electric Reissner-Nordström black hole outside r_2. This secondary shell then collapses, leaving an extremal black hole with a star shell outside. This is then analogous to the extremal black hole solution inside the star shell discussed previously in the low b case. Upon increasing a further one hits a new critical value, $a_{\text{crit new}}$, where a new horizon forms at the exterior star shell r_{star}.

The second question is what happens when $b \to \infty$. In the magnetic monopole system this case has been analyzed in Ref. 20. When one increases b, keeping a fixed, one finds that r_2 gets relatively smaller and smaller. The behavior is best displayed by looking into the $1/A$ plot of Fig. 9. For a small and fixed, when one increases b the minimum at r_2 is displaced more and more toward $r=0$. Eventually at $b \to \infty$ the minimum hits the $r=0$ line at a point $1/A$ less than 1, which means that the configuration starts at a conical singularity. This example shows why Ref. 20 did not get the high b behavior found in Ref. 21, namely, a smooth black hole formation in the core of the magnetic monopole. What happens is that for $b \to \infty$ a horizon (a kind of singularity) in the inner secondary shell does not form at the core because the initial configuration already possesses at the core ($r=0$) a conical singularity (another kind of singularity which substitutes the horizon in this limit $b \to \infty$). This conical configuration exists for a given typical value of a. Upon increasing a further one hits a critical value for a (corresponding to the $a_{\text{crit new}}$ mentioned above) where a new quasihorizon forms at the exterior star shell r_{star}.

2. The extremal black hole solution inside the system

As in the low b case, where an extremal black hole was put inside the low b shells, one can also put an extremal black hole inside the high b shells. We will not do this here since the behavior is similar to the previous cases. In the magnetic monopole high b case this was done in Ref. 24.

D. Further discussion

(i) *The $b=2$ configuration:* We have treated the cases $b<2$ and $b>2$. The case $b=2$ is also worth commenting as a limiting case. The new feature is that at a_{critical} the function $1/A$ develops two double zeros, one at the secondary shell r_2, the other at the star shell r_{star}. Thus, on going from $b<2$ to $b>2$ the quasihorizon jumps discontinuously in radius at some critical a. If the entropy of this object can be related to the area of the object, as was done in Ref. 22, then the entropy also jumps discontinuously when one passes from $b<2$ to $b>2$. In the transition there is no mass jump, the mass is continuous, so that it is a kind of first order phase transition.

(ii) *More complex configurations:* One can put a third extremal matter shell inside the other two. In this case one has two new parameters, M_3 and r_3, and a new dimensionless parameter c can be given. In analogy with a and b of Eqs. (27) and (28), one finds

$$c = \frac{M_3/r_3}{M_2/r_2}. \tag{42}$$

Assume also as the constraint equation that $r_2=2r_3$. Then, one has

$$\left(\frac{1}{A}\right)_{r_{\text{star}}} = 1 - \frac{M_{123}}{r_{\text{star}}} = 1 - a\left[1 + \frac{b}{2}\left(1 + \frac{c}{2}\right)\right], \tag{43}$$

$$\left(\frac{1}{A}\right)_{r_2} = 1 - \frac{M_{23}}{r_2} = 1 - ab\left(1 + \frac{c}{2}\right), \tag{44}$$

$$\left(\frac{1}{A}\right)_{r_3} = 1 - \frac{M_3}{r_3} = 1 - abc, \tag{45}$$

where $M_{123}=M_{\text{star}}+M_2+M_3$ is the total mass of the system and $M_{23}=M_2+M_3$. Then (I) For $b<4/(2+c)$ and $b<4/(3c-2)$ a quasihorizon forms first at r_{star}, with $a_{\text{crit}}=1/[1+b/2(1+c/2)]$. (II) For $b>4/(2+c)$ and $c<2$ a quasihorizon forms first at r_2, with $a_{\text{crit}}=1/b(1+c/2)$. (III) For the two cases (i) $b<4/(2+c)$ and $b>4/(3c-2)$, and (ii) $b>4/(2+c)$ and $c>2$, a quasihorizon forms first at r_3 with $a_{\text{crit}}=1/(bc)$. Equalities mean that the three quasihorizons form together with $b=1$, $c=2$, and $a_{\text{crit}}=1/2$. Two quasihorizons alone cannot form together.

One can continue to put more shells with the emergence of even more complex behavior in the function $1/A$. This type of behavior should also happen in non-Abelian theories with more Higgs scales.

(iii) *Other configurations:* Other configurations that could be dealt with are a thick shell within a thin shell, with the thick shell being the solution found in Ref. 54. The behavior is similar to what we have been discussing. For the low b case it will give for a_{crit} an extremal naked, Coulomb (no-hair), quasi-black hole. For high b it would give an extremal naked, non-Coulomb (hair), quasi-black hole. One can also put an extremal black hole inside a thick shell, although there is no known exact solution for it.

IV. CONCLUSIONS

We have shown that gravitational magnetic monopoles and Majumdar-Papapetrou stars, in the form of two thin shells, have common properties. We have shown that both systems have extremal quasi-black-hole solutions, some without hair while others developing some type of hair. Both, the monopole system and the two shell Majumdar-Papapetrou system, possess solutions with naked bahavior, i.e., tidal forces tend to infinity at the quasihorizon. At the critical value the interior solution does not give a smooth manifold, indicating a change of topology. For other parameters in the space of solutions of the magnetic monopole system, specifically for high Higgs mass, there are solutions with non-naked behavior, allowing the formation of a true black hole. On the other hand, the two shell Majumdar-Papapetrou system, never shows non-naked behavior, there are only quasi-black-hole solutions. In both systems one can put a black hole inside the configuration without destabilizing the system, for a range of parameters.

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Decoupling of the general scalar field mode and the solution space for Bianchi type I and V cosmologies coupled to perfect fluid sources

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The scalar field degree of freedom in Einstein's plus matter field equations is decoupled for Bianchi type I and V general cosmological models. The source, apart from the minimally coupled scalar field with arbitrary potential $V(\Phi)$, is provided by a perfect fluid obeying a general equation of state $p=p(\rho)$. The resulting ODE is, by an appropriate choice of final time gauge affiliated to the scalar field, reduced to first order, and then the system is completely integrated for arbitrary choices of the potential and the equation of state. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In the past two decades there has been a growing interest in scalar field cosmological models primarily due to the prominent importance of scalar fields for inflationary scenarios.[1] The importance of the coupling between a scalar field and the gravitational field has been further stressed by Madsen,[2] who has shown that it can have nontrivial consequences for the spontaneous breaking of gauge symmetries. A dynamical systems approach has been extensively used in the study of scalar field cosmologies and their asymptotic behavior.[3] See also Ref. 4 for a concise review.

As far as exact solutions of scalar field cosmologies are concerned, Burd and Barrow[5] have studied homogeneous but anisotropic Bianchi models of types III and VI (as well as Kantowski-Sachs models) and have found exact solutions. Lidsey, and Aguirregabiria *et al.*[6] have found exact solutions for Bianchi type I models. Feinstein and Ibanez[7] have found exact solutions for Bianchi models of type III and VI, Moss and Wright, Madsen, and Abreut, Crawford, and Mimoso[8] have studied exact solutions in the setting of conformal scalar field cosmologies. Paul[9] has obtained exact solutions of a higher derivative theory in the presence of an interacting scalar field. The discovery of the BTZ black hole has motivated the study of analytic solutions in the context of scalar field cosmology in (2+1) dimensions,[10] while Russo[11] has obtained the general solution for

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a scalar field cosmology in d dimensions with exponential potentials and a flat Robertson-Walker metric. An early work on exponential potentials has been done by Salopek and Bond[12] while recent treatments are given by Kehagias and Kofinas[13] and Neupane.[14]

Cosmological models containing both a fluid and a scalar field have also been studied. Chimento and Jakubi[15] have given exact solutions of scalar field cosmologies with a perfect fluid and a viscous fluid, respectively. Mendez[16] has obtained an exact solution for the case of an imperfect fluid in a FRW space-time. In the so-called scaling scalar field cosmologies, the energy density due to the scalar field is proportional to the energy density of the perfect fluid. Thus a number of spatially flat, isotropic models in which the energy density of the scalar field is proportional to that of the perfect fluid have been investigated.[17] Billyard, Coley, and van den Hoogen[18] have studied the stability of these scaling solutions within the class of spatially homogeneous cosmological models with a barotropic fluid matter content. Furthermore, they have studied the qualitative behavior of spatially homogeneous models with a barotropic fluid and a noninteracting scalar field with an exponential potential in the class of Bianchi type B models.[19] Saha[20] has obtained exact solutions for a Bianchi type I model with a perfect fluid and dark energy content, while Chimento and Cossarini have studied exact solutions in $1+1$ dimensions using an isotropic perfect fluid source.[21]

In a significant paper, Hawkins and Lidsey[22] have shown that, for a flat FRW geometry, the dynamics of scalar field cosmologies with a perfect fluid matter content can be described by the nonlinear, Ermakov-Pinney equation (which, in turn, leads to tantalizing analogies with the dynamics of Bose-Einstein condensates), while an early work of Barrow also deserves mention in this context. Exact solutions have been obtained in this description.[23] Another kind of decoupling of the scalar field degree of freedom has been initiated in Ref. 24, where a Robertson-Walker background geometry minimally coupled to the scalar field has been investigated. By use of integrals of the motion and of the Klein-Gordon (KG) equation in the quadratic constraint equation, a single, higher-order nonlinear differential equation for the scalar field was obtained.

In the present work we generalize this decoupling for the case of general Bianchi type I and V geometries in the presence of a general perfect fluid source. The advantage is that the resulting ODE is fully integrated and this is achieved for arbitrary choices of the scalar field potential and the fluid equation of state. The paper is organized as follows. In Sec. II the geometry and the matter description as well as the governing equations for the system are presented. In Sec. III the decoupling of the scalar field degree of freedom is performed for Bianchi type I, the reduction of the resulting ODE is given and the system is completely integrated. The corresponding calculations for Bianchi type V are given in Sec. IV. Finally, the conclusions and a discussion of the results obtained are presented in Sec. V.

Throughout we use geometrized units, i.e., $c=8\pi G=1$, while $g_{\mu\nu}$ has the signature $(-,+,+,+)$.

II. THE GOVERNING EQUATIONS AND THE MATTER CONTENT

Our starting point is the line element for a spatially homogeneous geometry,

$$\mathrm{d}s^2=[N^{\alpha}(t)N_{\alpha}(t)-N^2(t)]\mathrm{d}t^2+2N_{\alpha}(t)\sigma_i^{\alpha}(x)\mathrm{d}x^i\,\mathrm{d}t+\gamma_{\alpha\beta}(t)\sigma_i^{\alpha}(x)\sigma_j^{\beta}(x)\mathrm{d}x^i\,\mathrm{d}x^j, \tag{2.1}$$

where $\sigma_i^{\alpha}(x)$ are the basis one-forms satisfying $\sigma_{i,j}^{\alpha}(x)-\sigma_{j,i}^{\alpha}(x)=2C_{\beta\gamma}^{\alpha}\sigma_j^{\beta}(x)\sigma_i^{\gamma}(x)$ (with $C_{\beta\gamma}^{\alpha}$ the structure constants of the Lie algebra of the corresponding three-dimensional isometry group of motion acting simply transitively on the spatial hypersurfaces of simultaneity), $N_{\alpha}(t)$ is the shift vector, $N(t)$ is the lapse function, and $\gamma_{\alpha\beta}(t)$ is the scale factor matrix of the Bianchi type examined.

As explained in Ref. 25 there are special general coordinate transformations mixing space and time in the new space coordinates, whose effect on the line element (2.1) is described by

$$\tilde{\gamma}_{\alpha\beta}(t)=\Lambda_{\alpha}^{\mu}\Lambda_{\beta}^{\nu}a_{\mu\nu}(t),$$

$$\widetilde{N}(t) = N(t)$$

$$\widetilde{N}_\alpha(t) = \Lambda^\beta_\alpha(t)[N_\beta(t) + P^\rho(t)\gamma_{\rho\beta}(t)], \tag{2.2}$$

where $\Lambda^\mu_\nu(t)$, $P^\rho(t)$ satisfy

$$\Lambda^\alpha_\mu C^\mu_{\beta\gamma} = \Lambda^\rho_\beta \Lambda^\sigma_\gamma C^\alpha_{\rho\sigma}, \tag{2.3}$$

$$2P^\mu C^\alpha_{\mu\nu}\Lambda^\nu_\beta = \dot{\Lambda}^\alpha_\beta \tag{2.4}$$

the overdot denoting differentiation with respect to time. Due to (2.3), $\Lambda^\alpha_\beta(t)$ belongs to the automorphism group of the Bianchi type in question and transformations (2.2) describe the gauge freedom of the emanating system of Einstein's field equations in the case of vacuum. So, the three arbitrary functions of time contained in $\Lambda^\alpha_\beta(t)$ and $P^\alpha(t)$ can be used to simplify the line element (2.1) and, thus, also the aforementioned equations. Automorphisms induced by general coordinate transformations have also been considered in Ref. 26, while the rigid gauge symmetries have been analyzed in Ref. 27. Time-dependent automorphisms, seen as tangent space transformations, have also been considered previously,[28,29] while the first (known to us) reference of the relevance of automorphisms to a systematic analysis of Bianchi cosmologies goes back to 1962.[30]

The above result also holds true when the matter content is such that the linear constraints G^0_i do not acquire an extra term T^0_i. For orthogonal perfect fluids and scalar fields depending only on time, T^0_i is indeed zero and therefore we can use the gauge freedom (2.2)–(2.4) to diagonalize $\gamma_{\alpha\beta}(t)$ without losing generality. Therefore, the scale factor matrix is taken to be

$$\gamma_{\alpha\beta}(t) = \mathrm{diag}(a^2, b^2, c^2) \tag{2.5}$$

while for the shift vector we have $N_\alpha(t)=0$. Our choice of time is specified by the gauge condition $N=\sqrt{\det \gamma_{\mu\nu}}$, which is frequently used due to the simplification of the Einstein tensor and whose importance for the decoupling is essential.

The matter content is a minimally coupled scalar field with an arbitrary potential $V(\Phi)$, thus having an energy-momentum tensor

$$T^{(1)}_{\mu\nu} = \Phi_{,\mu}\Phi_{,\nu} - \tfrac{1}{2}g_{\mu\nu}(g^{\kappa\lambda}\Phi_{,\kappa}\Phi_{,\lambda} + 2V(\Phi)) \tag{2.6}$$

and a perfect fluid part

$$T^{(2)}_{\mu\nu} = (p+\rho)u_\mu u_\nu + p g_{\mu\nu}, \tag{2.7}$$

where u^μ is the unit four-velocity vector and a general equation of state $p=p(\rho)$ is adopted. The governing Einstein's field equations are taken to be

$$R^\mu_\nu - \tfrac{1}{2}\delta^\mu_\nu R = T^\mu_\nu, \tag{2.8}$$

where $T_{\mu\nu}=T^{(1)}_{\mu\nu}+T^{(2)}_{\mu\nu}$, while the scalar field equation (Klein-Gordon) is

$$\frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu\Phi) - V'(\Phi) = 0 \tag{2.9}$$

the prime, from now onwards, denoting differentiation with respect to the argument.

The "equation of motion" for the perfect fluid is the conservation of its energy-momentum tensor:

$$T^{(2)\mu}_{\nu;\mu} = 0. \tag{2.10}$$

(The scalar field energy-momentum tensor is separately conserved by virtue of the Klein-Gordon equation).

III. DECOUPLING OF THE SCALAR DEGREE AND THE SOLUTION SPACE FOR BIANCHI TYPE I

The basis one-forms are $\sigma_i^\alpha(x)=\delta_i^\alpha$ and, thus, with (2.5), zero shift and the chosen time gauge, the initial form of the metric is given by

$$g_{\mu\nu}=\begin{pmatrix} -a^2b^2c^2 & 0 & 0 & 0 \\ 0 & a^2 & 0 & 0 \\ 0 & 0 & b^2 & 0 \\ 0 & 0 & 0 & c^2 \end{pmatrix}. \tag{3.1}$$

Spatial homogeneity implies that $\Phi=\Phi(t)$ and $\rho=\rho(t)$. The nonzero components of the Einstein tensor G_ν^μ, and the energy-momentum tensors $T_\nu^{(1)\mu}$, $T_\nu^{(2)\mu}$ (all multiplied by $a^2b^2c^2$) are given by

$$G_0^0=-\frac{\dot{a}\dot{b}}{ab}-\frac{\dot{a}\dot{c}}{ac}-\frac{\dot{b}\dot{c}}{bc}, \tag{3.2}$$

$$G_1^1=\frac{\dot{a}\dot{b}}{ab}+\frac{\dot{b}^2}{b^2}+\frac{\dot{a}\dot{c}}{ac}+\frac{\dot{b}\dot{c}}{bc}+\frac{\dot{c}^2}{c^2}-\frac{\ddot{b}}{b}-\frac{\ddot{c}}{c}, \tag{3.3}$$

$$G_2^2=\frac{\dot{a}^2}{a^2}+\frac{\dot{a}\dot{b}}{ab}+\frac{\dot{a}\dot{c}}{ac}+\frac{\dot{b}\dot{c}}{bc}+\frac{\dot{c}^2}{c^2}-\frac{\ddot{a}}{a}-\frac{\ddot{c}}{c}, \tag{3.4}$$

$$G_3^3=\frac{\dot{a}^2}{a^2}+\frac{\dot{a}\dot{b}}{ab}+\frac{\dot{b}^2}{b^2}+\frac{\dot{a}\dot{c}}{ac}+\frac{\dot{b}\dot{c}}{bc}-\frac{\ddot{a}}{a}-\frac{\ddot{b}}{b}, \tag{3.5}$$

$$T_0^{(1)0}=-a^2b^2c^2V(\Phi)-\tfrac{1}{2}\dot{\Phi}^2, \tag{3.6}$$

$$T_1^{(1)1}=T_2^{(1)2}=T_3^{(1)3}=-a^2b^2c^2V(\Phi)+\tfrac{1}{2}\dot{\Phi}^2, \tag{3.7}$$

$$T_0^{(2)0}=-a^2b^2c^2\rho(t), \tag{3.8}$$

$$T_1^{(2)1}=T_2^{(2)2}=T_3^{(2)3}=a^2b^2c^2p(\rho(t)). \tag{3.9}$$

Due to the equalities (3.7) and (3.9), we can subtract the corresponding Einstein's equations $G_\nu^\mu=T_\nu^{(1)\mu}+T_\nu^{(2)\mu}$, i.e., form the differences (all multiplied by $a^2b^2c^2$) $G_2^2-G_1^1=T_2^{(1)2}+T_2^{(2)2}-T_1^{(1)1}-T_1^{(2)1}$ and $G_3^3-G_1^1=T_3^{(1)3}+T_3^{(2)3}-T_1^{(1)1}-T_1^{(2)1}$ and get the following equations involving only the scale factors:

$$\frac{\dot{a}^2}{a^2}-\frac{\dot{b}^2}{b^2}-\frac{\ddot{a}}{a}+\frac{\ddot{b}}{b}=0, \tag{3.10}$$

$$\frac{\dot{a}^2}{a^2}-\frac{\dot{c}^2}{c^2}-\frac{\ddot{a}}{a}+\frac{\ddot{c}}{c}=0. \tag{3.11}$$

These equations provide the following integrals of motion:

$$b(t)=e^{\lambda t}a(t), \tag{3.12}$$

$$c(t) = e^{\mu t} a(t), \tag{3.13}$$

leaving us with just one undetermined scale factor. At this stage the Klein-Gordon equation (2.9) becomes

$$-V'(\Phi) - \frac{e^{-2(\lambda+\mu)t}\ddot{\Phi}(t)}{a^6(t)} = 0. \tag{3.14}$$

Now, the conservation of the fluid energy-momentum tensor (continuity equation) gives

$$3\frac{\dot{a}}{a} + \frac{\dot{\rho}}{p(\rho)+\rho} + \lambda + \mu = 0. \tag{3.15}$$

It is straightforward to check that the time derivative of the quadratic constraint equation $G_0^0 = T_0^{(1)0} + T_0^{(2)0}$ is identically satisfied by virtue of the remaining spatial equation $G_1^1 = T_1^{(1)1} + T_1^{(2)1}$, the Klein-Gordon equation and the continuity equation [solved for $\ddot{a}(t)$, $\ddot{\Phi}(t)$, $\dot{\rho}(t)$], as expected from the consistency between the aforementioned constraint with the spatial Einstein and the matter equations. Therefore, the equations to be solved are the Klein-Gordon equation (3.14), the continuity equation (3.15) and the constraint equation which, upon multiplication by $-2a^6 e^{2(\lambda+\mu)t}$ reads

$$6\left(\frac{\dot{a}}{a}\right)^2 + 4(\lambda+\mu)\frac{\dot{a}}{a} + 2\lambda\mu - \dot{\Phi}^2 - 2e^{2(\lambda+\mu)t}a^6[V(\Phi)+\rho] = 0. \tag{3.16}$$

In order to have a closed form for the integral of the continuity Eq. (3.15), it is convenient to use the parametrization

$$p(\rho) = \frac{g(\rho)}{g'(\rho)} - \rho \tag{3.17}$$

(the prime denoting differentiation with respect to the argument) through the use of which one obtains the integral

$$\rho = h[\rho_0 a^{-3} e^{-(\lambda+\mu)t}] \tag{3.18}$$

with h being the inverse function to g, i.e., satisfying $h(g(x))=x$.

From the Klein-Gordon equation (3.14) the scale factor and its logarithmic derivative is expressed in terms of the scalar field $\Phi(t)$ and its derivatives as well as $V(\Phi)$,

$$a = \left[-\frac{e^{-2(\lambda+\mu)t}\ddot{\Phi}}{V'(\Phi)}\right]^{1/6}, \tag{3.19}$$

$$\frac{\dot{a}}{a} = \frac{1}{6}\left(\frac{\dddot{\Phi}}{\ddot{\Phi}} - \frac{V''(\Phi)}{V'(\Phi)}\dot{\Phi} - 2(\lambda+\mu)\right). \tag{3.20}$$

The promised decoupling of the scalar field dynamics from the geometry occurs upon inserting (3.18)–(3.20) into (3.16). The result is the following nonlinear, third order ODE for $\Phi(t)$:

$$\left(\frac{\dddot{\Phi}}{\ddot{\Phi}} - \frac{V''(\Phi)}{V'(\Phi)}\dot{\Phi}\right)^2 - 4(\lambda+\mu)^2 + 12\lambda\mu - 6\dot{\Phi}^2 + 12\frac{\ddot{\Phi}}{V'(\Phi)}V(\Phi) + 12\frac{\ddot{\Phi}}{V'(\Phi)}h\left[\rho_0\left(-\frac{\ddot{\Phi}}{V'(\Phi)}\right)^{-1/2}\right] = 0. \tag{3.21}$$

At this stage, any solution to this equation determines, through (3.18) and (3.19) a corresponding solution to the full Einstein plus matter system whose entire space of solution is therefore attained

from the solution space of (3.21). Of course, the price paid, for the moment, is the nonlinearity in the highest time derivative, which has also been raised to third order. Furthermore, normally one would expect that the arbitrary functions h, V need first to be specified before hoping to actually get a solution. Nevertheless, it is quite interesting that further reduction of the order of (3.21), and subsequent complete integration of the whole system, is possible. To this end, we first observe that many terms in (3.21), namely all the nontrivial except the fourth and fifth, are functions of the combination $-\ddot{\Phi}/V'(\Phi)$. We thus define

$$\chi = -\frac{\ddot{\Phi}}{V'(\Phi)} \tag{3.22}$$

and write (3.21) as

$$\left(\frac{\dot{\chi}}{\chi}\right)^2 - 4(\lambda+\mu)^2 + 12\lambda\mu - 6f(\chi) - 12\chi h(\rho_0\chi^{-1/2}) = 0, \tag{3.23}$$

where

$$f(\chi) \equiv \dot{\Phi}^2 + 2\chi V(\Phi) \tag{3.24}$$

implicitly reflects the arbitrariness in choosing $V(\Phi)$. Now (3.23) can be integrated and, by judicious choices for f, h, even give $\chi(t)$ in closed form. Suppose $\chi(t)$ does indeed solve (3.23). Then, multiplying (3.22) by $2\dot{\Phi}V'(\Phi)$ and using (3.24) we get the first order linear differential equation for $f(t)$:

$$\frac{\mathrm{d}f(t)}{\mathrm{d}t} = 2\dot{\chi}(t)V(t) \tag{3.25}$$

and consequently $\Phi(t)$ is given by

$$\frac{\mathrm{d}\Phi(t)}{\mathrm{d}t} = \pm\sqrt{f(\chi(t)) - 2\chi(t)V(t)}. \tag{3.26}$$

Finally, a change of time variable from t to χ [defined in (3.22)] permits the presentation of the entire space of solutions to the system under consideration in closed form. Indeed, considering V, f, Φ as functions of χ one gets from (3.25) and (3.26), respectively,

$$\frac{\mathrm{d}f}{\mathrm{d}\chi} = 2V(\chi), \tag{3.27}$$

$$\frac{\mathrm{d}\Phi(\chi)}{\mathrm{d}\chi}\dot{\chi}(t) = \pm\sqrt{f(\chi) - 2\chi V(\chi)}, \tag{3.28}$$

where the time derivative of χ is given by the constraint (3.23). The integration of these two equations is trivial, yielding f, Φ as

$$f(\chi) = \sigma + 2\int V(\chi)\mathrm{d}\chi, \tag{3.29}$$

$$\Phi(\chi) = \kappa \pm \int \frac{1}{\chi}\sqrt{\frac{f(\chi) - 2\chi V(\chi)}{4(\lambda+\mu)^2 - 12\lambda\mu + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})}}\mathrm{d}\chi. \tag{3.30}$$

The line element in the new time χ reads

$$ds^2 = -\frac{d\chi^2}{\chi[4(\lambda+\mu)^2 - 12\lambda\mu + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})]} + [e^{-2(\lambda+\mu)t(\chi)}\chi]^{1/3}\,dx^2 + [e^{(4\lambda-2\mu)t(\chi)}\chi]^{1/3}\,dy^2 + [e^{(-2\lambda+4\mu)t(\chi)}\chi]^{1/3}\,dz^2 \tag{3.31}$$

with $t(\chi)$ given by the integral form of (3.23),

$$t(\chi) = \pm\int \frac{1}{\chi\sqrt{4(\lambda+\mu)^2 - 12\lambda\mu + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})}}d\chi \tag{3.32}$$

while the density and pressure are given as

$$\rho(\chi) = h(\rho_0\chi^{-1/2}), \quad p(\chi) = \rho_0\chi^{-1/2}h'(\rho_0\chi^{-1/2}) - h(\rho_0\chi^{-1/2}) \tag{3.33}$$

the prime denoting differentiation with respect to the argument. Quite independently of the way these solutions were obtained, one can straightforwardly check (through, say, a symbolic computing facility) that they do satisfy all 10 Einstein's equations, the generalized KG and the continuity equation. Furthermore, since no extra ansatz has been involved in the process of integration of the system (2.8)–(2.10), equations (3.29)–(3.33) represent the full space of solutions to the Einstein plus matter system considered. The functions V, h can be freely specified to obtain special case solutions.

IV. DECOUPLING OF THE SCALAR DEGREE AND THE SOLUTION SPACE FOR THE BIANCHI TYPE V

In this case the basis one-forms are $\sigma^1 = e^{-x}\,dy$, $\sigma^2 = e^{-x}\,dz$, $\sigma^3 = dx$. The $G^0_1 = 0$ Einstein equation [due to spatial homogeneity $\Phi = \Phi(t)$ and $\rho = \rho(t)$ and therefore there is no corresponding component of the matter tensor] implies $c = ab$. Thus the initial metric is taken as

$$g_{\mu\nu} = \begin{pmatrix} -a^3b^3 & 0 & 0 & 0 \\ 0 & ab & 0 & 0 \\ 0 & 0 & a^2e^{-2x} & 0 \\ 0 & 0 & 0 & b^2e^{-2x} \end{pmatrix}. \tag{4.1}$$

The nonzero components of the Einstein tensor G^μ_ν, and the energy-momentum tensors $T^{(1)\mu}_\nu$, $T^{(2)\mu}_\nu$, all multiplied by a^3b^3, are given by

$$G^0_0 = 3a^2b^2 - \frac{\dot{a}^2}{2a^2} - \frac{2\dot{a}\dot{b}}{ab} - \frac{\dot{b}^2}{2b^2}, \tag{4.2}$$

$$G^1_1 = a^2b^2 + \frac{3\dot{a}^2}{2a^2} + \frac{2\dot{a}\dot{b}}{ab} + \frac{3\dot{b}^2}{2b^2} - \frac{\ddot{a}}{a} - \frac{\ddot{b}}{b}, \tag{4.3}$$

$$G^2_2 = a^2b^2 + \frac{\dot{a}^2}{a^2} + \frac{2\dot{a}\dot{b}}{ab} + \frac{2\dot{b}^2}{b^2} - \frac{\ddot{a}}{2a} - \frac{3\ddot{b}}{2b}, \tag{4.4}$$

$$G^3_3 = a^2b^2 + \frac{2\dot{a}^2}{a^2} + \frac{2\dot{a}\dot{b}}{ab} + \frac{\dot{b}^2}{b^2} - \frac{3\ddot{a}}{2a} - \frac{\ddot{b}}{2b}, \tag{4.5}$$

$$T^{(1)0}_0 = -a^3b^3V(\Phi) - \tfrac{1}{2}\dot{\Phi}^2, \tag{4.6}$$

$$T_1^{(1)1} = T_2^{(1)2} = T_3^{(1)3} = -a^3b^3V(\Phi) + \tfrac{1}{2}\dot{\Phi}^2, \tag{4.7}$$

$$T_0^{(2)0} = -a^3b^3\rho(t), \tag{4.8}$$

$$T_1^{(2)1} = T_2^{(2)2} = T_3^{(2)3} = a^3b^3p(\rho(t)). \tag{4.9}$$

The situation is similar to the type I case, and thus forming the difference (multiplied by a^3b^3) $G_2^2 - G_1^1 = T_2^{(1)2} + T_2^{(2)2} - T_1^{(1)1} - T_1^{(2)1}$ we get the following equation involving only the scale factors:

$$-\frac{\dot{a}^2}{2a^2} + \frac{\dot{b}^2}{2b^2} + \frac{\ddot{a}}{2a} - \frac{\ddot{b}}{2b} = 0, \tag{4.10}$$

which can be integrated yielding

$$b(t) = e^{\lambda t}a(t). \tag{4.11}$$

The Klein-Gordon equation (2.9) becomes

$$-V'(\Phi) - \frac{e^{-3\lambda t}\ddot{\Phi}(t)}{a^6(t)} = 0 \tag{4.12}$$

while the conservation of the fluid energy-momentum tensor (continuity equation) gives

$$3\frac{\dot{a}}{a} + \frac{\dot{\rho}}{p(\rho)+\rho} + \frac{3}{2}\lambda = 0. \tag{4.13}$$

Again, the only other equation to be solved is the constraint equation which reads

$$6\left(\frac{\dot{a}}{a}\right)^2 + 6\lambda\frac{\dot{a}}{a} + \lambda^2 - 6e^{2\lambda t}a^4 - \dot{\Phi}^2 - 2e^{3\lambda t}a^6(V(\Phi)+\rho) = 0, \tag{4.14}$$

where the fourth term is the only nontrivial difference from the corresponding equation (3.16) and its presence is due to the nonvanishing curvature of the spatial slice.

Integrating (4.13) [in the parametrization (3.17)] and solving (4.12) for $a(t)$, we obtain the following results for the matter density $\rho(t)$, the scale factor $a(t)$ and its logarithmic derivative

$$\rho = h(\rho_0 a^{-3} e^{-(3/2)\lambda t}), \tag{4.15}$$

$$a = \left(-\frac{e^{-3\lambda t}\ddot{\Phi}}{V'(\Phi)}\right)^{1/6}, \tag{4.16}$$

$$\frac{\dot{a}}{a} = \frac{1}{6}\left(\frac{\dddot{\Phi}}{\ddot{\Phi}} - \frac{V''(\Phi)}{V'(\Phi)}\dot{\Phi} - 3\lambda\right). \tag{4.17}$$

Use of these equations in the quadratic constraint equation (4.14) (multiplied by $-2e^{3\lambda t}a^6$) yields

$$\left(\frac{\dddot{\Phi}}{\ddot{\Phi}} - \frac{V''(\Phi)}{V'(\Phi)}\dot{\Phi}\right)^2 - 3\lambda^2 - 36\left(-\frac{\ddot{\Phi}}{V'(\Phi)}\right)^{2/3} - 6\dot{\Phi}^2 + 12\frac{\ddot{\Phi}}{V'(\Phi)}V(\Phi) + 12\frac{\ddot{\Phi}}{V'(\Phi)}h\left(\rho_0\left(-\frac{\ddot{\Phi}}{V'(\Phi)}\right)^{-1/2}\right) = 0 \tag{4.18}$$

which, with the same definition of χ, translates into

$$\left(\frac{\dot{\chi}}{\chi}\right)^2 - 3\lambda^2 - 36\chi^{2/3} - 6f(\chi) - 12\chi h(\rho_0\chi^{-1/2}) = 0. \tag{4.19}$$

By arguments completely analogous to the previous type I case, the final form of the solution is, in this case

$$f(\chi) = \sigma + 2\int V(\chi)\mathrm{d}\chi, \tag{4.20}$$

$$\Phi(\chi) = \kappa \pm \int \frac{1}{\chi}\sqrt{\frac{f(\chi) - 2\chi V(\chi)}{3\lambda^2 + 36\chi^{2/3} + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})}}\mathrm{d}\chi, \tag{4.21}$$

$$\mathrm{d}s^2 = -\frac{\mathrm{d}\chi^2}{\chi[3\lambda^2 + 36\chi^{2/3} + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})]} + \chi^{1/3}\,\mathrm{d}x^2 + e^{-\lambda t(\chi)-2x}\chi^{1/3}\,\mathrm{d}y^2 + e^{\lambda t(\chi)-2x}\chi^{1/3}\,\mathrm{d}z^2 \tag{4.22}$$

with $t(\chi)$ given by the integral form of (4.19),

$$t(\chi) = \pm\int \frac{1}{\chi\sqrt{3\lambda^2 + 36\chi^{2/3} + 6f(\chi) + 12\chi h(\rho_0\chi^{-1/2})}}\mathrm{d}\chi, \tag{4.23}$$

while the density and pressure are given as

$$\rho(\chi) = h(\rho_0\chi^{-1/2}), \quad p(\chi) = \rho_0\chi^{-1/2}h'(\rho_0\chi^{-1/2}) - h(\rho_0\chi^{-1/2}). \tag{4.24}$$

The remarks at the end of the preceding section apply also here.

V. DISCUSSION AND CONCLUSIONS

We have discussed the dynamics of a scalar field with an arbitrary potential, minimally coupled to a general (anisotropic) Bianchi type I and V geometry, in the presence of a perfect fluid source obeying a general equation of state. In the case of vacuum, the rich structure of outer automorphisms for these two symmetry groups entails the existence of some integrals of motion: Indeed, consider the generators of the rigid symmetries (2.3), i.e., the vector fields in the space of dependent variables $X_I = \lambda^\rho_{I\alpha}\gamma_{\rho\beta}(\partial/\partial\gamma_{\alpha\beta})$ where λ^α_β satisfy $\lambda^\alpha_{I\rho}C^\rho_{\beta\gamma} = \lambda^\rho_{I\beta}C^\alpha_{\rho\gamma} + \lambda^\rho_{I\gamma}C^\alpha_{\beta\rho}$. If one performs the appropriate change of variables $\gamma_{\alpha\beta} \to z_{\alpha\beta}$ which brings one (or more, if possible) generator into each canonical form, say $\partial/\partial z_{11}$, then Einstein's field equations written in the new variables do not explicitly depend on z_{11}. Thus the system becomes of first order in the variable $\dot{z}_{11}$ and therefore an integral of motion arises.

The initial choice of the time gauge in which the lapse is equal to the determinant of the scale factor matrix has a twofold advantage: First, it enables the corresponding integrals of motion (in the presence of the matter content chosen) to be revealed. Second, it makes the Klein-Gordon equation purely algebraic in the scale factor variables. As a result, when the utilization of the integrals of motion has reduced the number of these variables to one, this equation gives this last scale factor as a function of the second derivative of the scalar field, the derivative of the potential with respect to the scalar field, and of time. Substitution of this form of the scale factor into the only equation remaining to be solved, i.e., the quadratic constraint, results in a single ODE for the scalar field (without any explicit time dependence). The utilization of a final time gauge adapted to the scalar field enables the reduction of this equation to first order and subsequently leads to the complete integration of the entire system of Einstein plus matter field equations. The description of the space of solutions contains, in an integral form, the arbitrary functions of the final time χ, $V(\chi)$, and $h(\rho_0\chi^{-1/2})$. The presence of this twofold arbitrariness corresponds to the fact that we have not specified either the form of the potential (as a function of the scalar field) or the equation of state. It is evident that prescribing $V(\chi)$ and $h(\rho_0\chi^{-1/2})$ implicitly corresponds to a choice of

potential form and equation of state. For example, the choice $h=A(\rho_0\chi^{-1/2})^{1+\gamma}$ gives through (4.24) $p=\gamma\rho$, i.e., the barotropic equation of state. For the scalar field, if we take the particular case $\lambda=\mu=\sigma=h(\rho_0\chi^{-1/2})=0$ (i.e., flat Robertson-Walker with no fluid) the choice $V(\chi)=C/\sqrt{\chi}$ corresponds to the functional form $V=\pm Ce^{\sqrt{3}(\kappa-\Phi)}$. If, on the other hand, someone insists in prescribing $V(\Phi)$ and $p(\rho):=p(h)$ then the situation must be dealt with in the following manner: As far as the density is concerned, the equation giving the pressure becomes the holonomic, first order differential equation $p(h)=wh'(w)-h(w)$ with w standing for $\rho_0\chi^{-1/2}$ which can be straightforwardly integrated. For example, a barotropic equation $p:=\gamma\rho$ gives $\rho=A(\rho_0\chi^{-1/2})^{1+\gamma}$. As far as the matter field is concerned, the situation is somewhat more complicated as the results of choosing a particular form $V(\Phi)$ are influenced by the choice of the density h. As an example consider again the case $\lambda=\mu=\sigma=h(\rho_0\chi^{-1/2})=0$ and an arbitrary potential form $V(\Phi)$. Relaxing for a moment (3.30), we get the following Klein-Gordon equation

$$-\frac{V'(\Phi)}{V(\Phi)}+\frac{6\chi}{6\chi^2\Phi'^2(\chi)}[2\chi\Phi''(\chi)-6\chi^2\Phi'^3(\chi)+3\Phi'(\chi)]=0,$$

which may be difficult to solve depending on the choice of $V(\Phi)$. This is the price paid for insisting on prescribing $V(\Phi)$ and not $V(\chi)$ in which case the solution would be given by (3.29)–(3.33) or (4.20)–(4.24) correspondingly. The particular choice $V=V_0e^{-\lambda\Phi}$ corresponds to the case considered in Ref. 11 and the equation above can be dealt with by choosing a new time $\chi=e^{3\tau/2}$, in which the equation becomes the following first order in the derivative $\omega\equiv d\Phi/d\tau$:

$$48\frac{d\omega}{d\tau}-96\omega^3+24\lambda\omega^2-9\lambda=0.$$

Finally, there are two cases which, at first sight, need to be separately examined. The first concerns the case of a constant potential $V(\Phi)\equiv V_0$, i.e., a cosmological constant term. Then, $V'(\Phi)=0$ and the definition of the final time χ in Eq. (3.32) seems to be precarious. However, the Klein-Gordon Eq. (3.14) then implies that also $\ddot{\Phi}=0$ and, surprisingly enough, χ does exist. Indeed, substituting $V(\Phi)\equiv V_0$ in the solutions (3.29)–(3.33) or (4.20)–(4.24) one can see that the solution is still valid. This holds true even for $V_0=0$. The second case arises when the ratio $\ddot{\Phi}/V'(\Phi)=-1/c^6$, for, then, the change of time from t to χ is not valid. In this case, the remaining scale factor is given by $a(t)=ce^{-(\lambda+\mu)t/3}$ in the type I case or $a(t)=ce^{-\lambda t/2}$ in the type V case. The continuity equation [(3.15) or (4.12), respectively] implies that the pressure and density are constants, say, p_0 and ρ_0. The remaining equations dictate $\Phi(t)=At+B$ and $V(\Phi)=V_0$ and there exists a relation between c, p_0, ρ_0, A, and B due to the quadratic constraint.

The general properties of the space of solutions found for both type I and type V cases, e.g., isotropization, attractors and self-similarity, and quintessence, will be examined in a forthcoming paper, in which also particular cases of high interest are to be explicitly elaborated. Possible applications of the method exhibited here can be the cases of $D+1$ spatially homogeneous spacetimes, in which the outer automorphisms are rich enough to provide sufficient integrals of motion. Then the method will be applicable if the matter content is such that the integrals of motion persist.

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Isochronous and partially isochronous Hamiltonian systems are not rare

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A technique is provided that allows to associate to a Hamiltonian another, ω-modified, Hamiltonian, which reduces to the original one when the parameter ω vanishes, and for $\omega>0$ features an *open*, hence *fully dimensional*, region in its phase space where *all* its solutions are *isochronous*, i.e., *completely periodic* with the *same* period. The class of Hamiltonians to which this technique is applicable is large: it includes for instance the Hamiltonian characterizing the classical many-body problem with potentials that are *translation-invariant* but otherwise *completely arbitrary*, which is largely used in this paper to illustrate these findings. We also discuss variants of this technique that yield *partially isochronous* Hamiltonians, which also feature a region in their phase space where *all* solutions are *isochronous*, that region having however a bit less than full dimensionality (for instance codimension one or two) in phase space. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2188211]

I. INTRODUCTION AND OUTLINE OF MAIN FINDINGS

Not too long ago a (so-called) "trick" was introduced,[2] characterized by a *real* parameter ω and capable of transforming an *autonomous* dynamical system (belonging to a fairly large class, see below) into another, as well *autonomous*, system. The ω-modified dynamical system thereby obtained, while reducing to the original system for $\omega=0$, features for $\omega>0$ in its phase space an *open*, hence *fully dimensional*, region in which *all* motions are *completely periodic* with the fixed period

$$T=\frac{2\pi}{\omega}, \tag{1}$$

or possibly with a (generally small) *integer* multiple of this period. Here and hereafter by *completely periodic* we mean that the periodicity property is shared by *all* the dependent variables. Systems featuring such a periodicity property—with a period independent of the initial data provided the initial data belong to some *open, fully dimensional* set of such data—are here called *isochronous*; and we call *partially isochronous* the dynamical systems for which the *complete periodicity* property with a fixed period obtains for a set of initial data having a bit less than full dimensionality in phase space (for instance, for a set of initial data belonging to a manifold in phase space of codimension one or two, see below).

This trick has been extensively exploited to identify and investigate *isochronous* systems.[1–38]

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Here, to illustrate our main findings, we focus mainly on the dynamical system describing an N-body problem, as characterized by the Hamiltonian

$$H(\underline{p},\underline{q}) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + V(\underline{q}) + C, \tag{2}$$

where the *arbitrary* constant C has been introduced for convenience (see below) and the potential $V(\underline{q}) \equiv V(q_1, q_2, \ldots, q_N)$ shall generally be assumed *translation invariant*,

$$V(\underline{q} + a) \equiv V(q_1 + a, q_2 + a, \ldots, q_N + a) = V(\underline{q}), \tag{3a}$$

with a an arbitrary constant, entailing (for infinitesimal a)

$$\sum_{n=1}^{N} \frac{\partial V(\underline{q})}{\partial q_n} = 0. \tag{3b}$$

This is the standard Hamiltonian for the nonrelativistic N-body problem, entailing the standard Hamiltonian equations of motion

$$\dot{q}_n = p_n, \quad \dot{p}_n = -\frac{\partial V(q)}{\partial q_n}, \tag{4}$$

as well as the corresponding Newtonian equations of motion

$$\ddot{q}_n = -\frac{\partial V(\underline{q})}{\partial q_n}, \tag{5}$$

the total momentum conservation formula,

$$P(\underline{p}) = \sum_{n=1}^{N} p_n, \tag{6a}$$

$$\dot{P} = 0, \tag{6b}$$

and the "center-of-mass" evolution

$$Q(\underline{q}) = \frac{1}{N}\sum_{n=1}^{N} q_n, \tag{7a}$$

$$Q(t) = Q(0) + \frac{P}{N}t. \tag{7b}$$

Notation: Here and always below N is a positive integer ($N \geqslant 2$), the (*real*) independent variable t has the significance of *physical time*, superimposed dots indicate differentiations with respect to this variable, indices such as n, m run from 1 to N unless otherwise indicated, underlined symbols denote N-vectors, for instance $\underline{q} \equiv (q_1, \ldots, q_N)$, and of course we use (here and below) the short-hand notation according to which $Q(t) \equiv Q[\underline{q}(t)]$. Note that, for simplicity, we assume here all the particles to have the same mass, and the motions to occur in one-dimensional space; but these restrictions can be dispensed with, see Sec. IV.

In the context of this N-body problem the trick consists of the following change of dependent and independent variables:

$$\breve{q}_n(t) = \exp(i\lambda\omega t) q_n(\tau), \tag{8a}$$

$$\tau = \frac{\exp(i\omega t) - 1}{i\omega}, \tag{8b}$$

where λ is a constant to be chosen appropriately (see below). Note that this change of variables entails the following relations among the initial data for the "old" dependent variables q_n and the "new" dependent variables $\breve{q}_n$:

$$q_n(0) = \breve{q}_n(0), \quad q_n'(0) = \dot{\breve{q}}(0) - i\lambda\omega\breve{q}_n(0). \tag{9}$$

Here and hereafter primes denote differentiations with respect to the argument of the function they are appended to, and of course $q_n'(0)$ denotes the value of $q_n'(\tau) \equiv \mathrm{d}q_n(\tau)/\mathrm{d}\tau$ at $\tau = 0$.

The insertion of this change of variables, (8), in the (*autonomous*) dynamical system characterized by the Newtonian equations of motion (5) yields, as it can be easily verified, the (*autonomous*) dynamical system

$$\ddot{\breve{q}}_n - (2\lambda + 1)i\omega\dot{\breve{q}}_n - \lambda(\lambda + 1)\omega^2\breve{q}_n = -\frac{\partial V(\underline{\breve{q}})}{\partial \breve{q}_n}, \tag{10a}$$

provided the potential $V(\underline{q})$ satisfies the scaling property

$$V(c\underline{q}) = c^{\gamma}V(\underline{q}) \tag{10b}$$

(where c is an arbitrary constant and γ is the exponent characterizing the scaling property) and correspondingly the parameter λ is assigned as follows:

$$\lambda = \frac{2}{\gamma - 2}. \tag{10c}$$

This new system of ODEs (10), determining the time evolution of the new dependent variables $\breve{q}_n \equiv \breve{q}_n(t)$, is the ω-dependent dynamical system and, as we now show, it is generally *isochronous* provided the parameter λ is *real* and *rational*. Note that λ is indeed *real* and *rational* provided γ, see (10b), is itself *real* and *rational* [and different from 2, $\gamma \neq 2$; see (10c)]. Also note that the dynamical variables $\breve{q}_n(t)$ are now necessarily evolving in the *complex* $\breve{q}$-plane; this shall be the case as well for all the evolutions considered hereafter. Of course in order that derivatives with respect to *complex* variables [such as τ, see (8b)] make good sense, one must deal (as we shall always do) with *analytic* functions. On the other hand, any evolution of the N *complex* coordinates $\breve{q}_n(t)$ is completely equivalent to the evolution of the $2N$ coordinates that obtain by considering separately the *real* and the *imaginary* parts of these coordinates; and there are cases (see for instance Chap. 4 of Ref. 3) when such an evolution can, as it were "more physically," be interpreted—by identifying the *complex* plane with a *real* plane—as the evolution of N "physical" pointlike particles in a plane [say, N particles the positions of which are identified by *real* vectors in the *horizontal* plane, $\vec{r}_n(t) \equiv (\mathrm{Re}[\breve{q}_n(t)], \mathrm{Im}[\breve{q}_n(t)], 0)$].

To show that the time evolution entailed by the equations of motion (10) (with λ *real* and *rational*) is indeed *isochronous* we point out to begin with that the change of dependent variable (8b) entails that, as the (*real*) "physical time" variable t evolves from $t = 0$ onwards, the (*complex*) timelike variable τ goes round and round, in the *complex* τ-plane, on the circle C centered at i/ω and having radius $1/\omega$ (draw diagram), traveling a full circle in every time interval T, see (1). Hence, if the functions $q_n(\tau)$ of the *complex* variable τ are *holomorphic* in the (closed) disk D enclosed by the circle C, the corresponding variables $\breve{q}_n(t)$ [see (8) and (1)] are λ-*periodic* with period T,

$$\breve{q}_n(t + T) = \exp(2i\pi\lambda)\breve{q}_n(t), \tag{11}$$

and this entails that they are indeed *periodic* with period T if λ is an *integer*, or with a period which is an *integer multiple* of T if λ is a (*real* and) *rational* number (as we hereafter assume). On

the other hand, the functions $q_n(\tau)$ are just the analytic continuation for *complex time* of the solutions of the Newtonian equations of motion (5)—corresponding to the formal replacement of the *real* variable t by the *complex* variable τ, or equivalently to the replacement of the equations of motion (5) with the analogous equations

$$q_n'' = -\frac{\partial V(q)}{\partial q_n}, \tag{12}$$

where $q_n \equiv q_n(\tau)$ and of course appended primes indicate differentiations with respect to the new (*complex*) independent variable τ. It is then clear that, provided the initial data [see (9)] for these equations of motion are so assigned as to avoid that their right-hand sides be *singular* (at $\tau=0$)—as we shall hereafter assume—their solutions $q_n(\tau)$ are certainly *holomorphic* functions of the *complex* variable τ for $|\tau|<R$ for some $R>0$, namely (at least) inside a circle of *positive* radius R, centered at the origin ($\tau=0$) in the *complex* τ-plane—as implied by the standard theorem guaranteeing the existence, uniqueness and analyticity of the solutions of analytic (systems of) ODEs. The (minimum) value of R depends on the *initial* values of the right-hand sides of the equations (of motion in the *complex* timelike variable τ) (12), on the distances in the (*complex*) q-plane of the *initial* assignments $q_n(0)$ of the dependent variables from the values of these variables that cause the right-hand sides of the ODEs (12) to become *singular*, and on the (moduli of) the *initial* assignments $q_n'(0)$ of the derivatives [see (9)]. But it stands to reason (see examples below, and in the literature quoted above) that there generally exist an *open* set of initial data $\breve{q}_n(0)$ and $\breve{q}_n(0)$ having *full dimensionality* in the (phase) space of these dependent variables such that [via (9)]

$$R > \frac{2}{\omega}. \tag{13}$$

Clearly the analysis we just made implies then that the time evolution of the dependent variables $\breve{q}_n(t)$ resulting from such initial data is *completely periodic*, since this inequality, (13), implies that the circle of radius R centered at the origin in the *complex* τ-plane *encloses* the circular disk D, implying the *holomorphic* character of the functions $q_n(\tau)$ in this (closed) disk.

The development reported so far has tersely reproduced—in the specific context of the standard many-body problem, characterized by the Newtonian equations of motion (5)—the argument associating to a given dynamical system an ω-modified system—in this case, characterized by the Newtonian equations of motions (10)—that has the remarkable property to be *isochronous*. As indicated by the argument reviewed above, the main condition required to obtain such an *isochronous* system is the validity of the scaling property (10b) with γ *real* and *rational* ($\gamma \neq 2$). And let us reemphasize that, as implied by the above argument and as discussed in detail in the literature (see for instance Refs. 8 and 11), in order that the ω-modified system of Newtonian equations (10) be *isochronous* it is by no means required that the original system from which it was obtained [namely, the system of Newtonian equations of motion (5) corresponding to (10) with $\omega=0$] be itself *isochronous* or *integrable*.

But note that it is *far from obvious*—and indeed often *not true*—that the new ω-modified Newtonian equations of motion (10) be *Hamiltonian*, i.e., obtainable from a Hamiltonian.

The main contribution of the present paper is to introduce a technique producing, from a given *Hamiltonian* H, an ω-modified *Hamiltonian* $\tilde{H}$ yielding *isochronous* equations of motion. The main requirement on the original Hamiltonian H for the applicability of this technique is that the dynamics it entails allow the identification of a "collective variable," explicitly defined in terms of the Hamiltonian canonical coordinates and momenta, the time evolution of which is essentially identical to *time* itself. If we denote such a variable as $\Theta(\underline{p},\underline{q})$, it will be characterized by the formula

$$[\Theta(\underline{p},\underline{q}),H(\underline{p},\underline{q})] = 1. \tag{14}$$

Notation: Here and hereafter the *Poisson bracket* $[F,G]$ of two functions $F(\underline{p},\underline{q}),G(\underline{p},\underline{q})$ of the canonical coordinates and momenta is defined in the standard manner,

$$[F(\underline{p},\underline{q}),G(\underline{p},\underline{q})]=\sum_{n=1}^{N}\left[\frac{\partial F(\underline{p},\underline{q})}{\partial q_n}\frac{\partial G(\underline{p},\underline{q})}{\partial p_n}-\frac{\partial F(\underline{p},\underline{q})}{\partial p_n}\frac{\partial G(\underline{p},\underline{q})}{\partial q_n}\right]. \tag{15}$$

The ω-modified Hamiltonian $\widetilde{H}$ yielding *isochronous* motions is then defined as follows:

$$\widetilde{H}(\underline{p},\underline{q};\omega)=u(\underline{p},\underline{q};\omega)H(\underline{p},\underline{q}), \tag{16a}$$

$$u(\underline{p},\underline{q};\omega)=1+i\omega\Theta(\underline{p},\underline{q}). \tag{16b}$$

Let us emphasize that hereafter we only consider the time evolution yielded by this ω-modified Hamiltonian $\widetilde{H}(\underline{p},\underline{q};\omega)$, and therefore the time evolution of functions of the Hamiltonian variables p_n and q_n—such as $H(\underline{p},\underline{q}),P(\underline{p}),Q(\underline{q}),u(\underline{p},\underline{q};\omega)$, see (2), (6a), (7a), and (16b)—obtains via the time dependence of these Hamiltonian variables $p_n\equiv p_n(t),q_n\equiv q_n(t)$ implied by the standard Hamiltonian equations (see below) associated with the Hamiltonian $\widetilde{H}(\underline{p},\underline{q};\omega)$; hence the time evolution of these collective variables is given by the standard formula characterizing the Hamiltonian evolution of any function $F(t)=F[\underline{p}(t),\underline{q}(t)]$ of the Hamiltonian variables,

$$\dot{F}=[F,\widetilde{H}]. \tag{17}$$

In particular it is crucial to note that—as implied by this formula via (16) and (14)—the collective quantities $H(t)$, respectively, $u(t;\omega)$ evolve now as follows:

$$\dot{H}=-i\omega H \tag{18a}$$

entailing

$$H(t)=H(0)\exp(-i\omega t), \tag{18b}$$

respectively,

$$\dot{u}=i\omega u \tag{19a}$$

entailing

$$u(t;\omega)=u(0;\omega)\exp(i\omega t). \tag{19b}$$

Note the consistency, via (16a), of the time evolutions (18b) and (19b) with the obvious fact that the Hamiltonian $\widetilde{H}$ is a constant of motion.

To illustrate our findings in a specific context we now focus again on the (unmodified) N-body Hamiltonian (2), taking advantage of the fact that, as a consequence of its *Galilean invariance*, see (2) and (3), a collective variable Θ satisfying (14) is provided by the following explicit formula:

$$\Theta(\underline{p},\underline{q})=\frac{NQ(\underline{q})}{P(\underline{p})}, \tag{20}$$

see (6a) and (7a). Of course to this quantity one could add an arbitrary function of P, and also of other quantities, if any, which Poisson commute with the (unmodified) Hamiltonian H and are therefore constants of motion for the evolution determined by this Hamiltonian; but for simplicity we refrain from doing so in the following.

In the following Sec. II we demonstrate, for this specific case, the *isochronous* character of the ω-modified Hamilton $\widetilde{H}$, as given by (16) with (2) and (20), (6a) and (7a). Let us emphasize that, quite remarkably, to prove the *isochronous* character of this ω-modified Hamiltonian *no* additional

property of the original N-body Hamiltonian H besides *Galilean invariance* is required, in particular *no* scaling property such as that entailed by the condition (10b)—which was instead essential to allow the transformation via the trick (8) from the (*autonomous*) *Newtonian* equations of motion (5) to the (as well *autonomous*) ω-modified *Newtonian* equations of motion (10). On the other hand the *Newtonian* equations of motion entailed by the ω-modified Hamiltonian $\widetilde{H}$, while having the appealing property to be themselves evidently *Hamiltonian* (which opens the possibility to study the quantized versions of the corresponding N-body problems) and of course to be *isochronous*, seem somewhat less susceptible of a "physical interpretation" than the equations, see (10), yielded by the standard approach based on the application of the trick (8); indeed these novel *Newtonian* equations of motion cannot be generally written in quite explicit form, although the corresponding *Hamiltonian* equations can be quite explicitly exhibited and are indeed relatively neat, see below.

In Sec. III we tersely discuss some specific examples of many-body problems, characterized by specific assignments of the potential $V(\underline{q})$. In Sec. IV we outline various generalizations of our approach, still in the context of nonrelativistic N-body problems: to the case with different masses, and to multidimensional space. In Sec. V we indicate how our approach to generate *isochronous* Hamiltonian systems can be applied in the context of more general Hamiltonian systems than those characterizing the nonrelativistic many-body problem. In Sec. VI we consider (different) variants of our technique [as applied again to the standard many-body problem, see (2), (3), (4) and (5)], yielding (*partially isochronous*) modified Hamiltonians characterized by a time evolution that features a set of initial data—having however a bit less than full generality in phase space, being restricted to lie on a manifold of nonvanishing (but generally small, and in any case N-independent) codimension—out of which emerge motions *all* of which are again *completely periodic* with the *same*, *fixed* period. The paper is concluded by a Sec. VII entitled Outlook, in which we mention further developments (to be pursued in future publications) suggested by the results reported in this paper.

II. THE ISOCHRONOUS *N*-BODY HAMILTONIAN

In this section we demonstrate the *isochronous* character of the time evolution entailed by the ω-modified N-body Hamiltonian $\widetilde{H}(\underline{p},\underline{q};\omega)$ associated to the classical N-body problem, as defined in the preceding section by (16) with (2), (20), (6a), and (7a).

The time evolution associated with the Hamiltonian $\widetilde{H}(\underline{p},\underline{q};\omega)$ is given by the following formulas:

$$\dot{q}_n = [q_n, \widetilde{H}] = \frac{\partial \widetilde{H}}{\partial p_n} = u p_n + \frac{(1-u)H}{P}, \tag{21}$$

$$\dot{p}_n = [p_n, \widetilde{H}] = -\frac{\partial \widetilde{H}}{\partial q_n} = -u\frac{\partial V(\underline{q})}{\partial q_n} - \frac{i\omega H}{P}. \tag{22}$$

From the latter Hamiltonian equations, (22), we get [via (6a) and (3b)]

$$\dot{P} = [P, \widetilde{H}] = -\frac{Ni\omega H}{P}, \tag{23a}$$

entailing, via (18b),

$$P(t) = P(0)\left[\frac{1-\alpha\exp(-i\omega t)}{1-\alpha}\right]^{1/2}. \tag{23b}$$

Here and often below we use the short-hand notation

$$\alpha = \frac{2NH(0)}{2NH(0) - P^2(0)}. \tag{24}$$

Likewise, from the Hamiltonian equations of motion (21) and (7a) we get

$$\dot{Q} = \frac{uP}{N} + \frac{(1-u)H}{P}, \tag{25a}$$

and, via (16b), (20), and (19b),

$$Q(t) = \left[\frac{Q(0)\exp(i\omega t)}{P(0)} + \frac{\exp(i\omega t) - 1}{Ni\omega} \right] P(t), \tag{25b}$$

as well as [from (25a), (16b), and (20)]

$$H = -\frac{P^2\left(\dot{Q} - i\omega Q - \frac{P}{N}\right)}{Ni\omega Q}. \tag{26}$$

Finally we recall that the time evolution of $H(t)$ and $u(t;\omega)$ is provided by the explicit expressions (18) and (19), of course with

$$H(0) = \frac{1}{2}\sum_{n=1}^{N} p_n^2(0) + V(\underline{q}(0)) + C, \tag{27}$$

$$u(0;\omega) = 1 + Ni\omega\frac{Q(0)}{P(0)} = 1 + i\omega\frac{\sum_{n=1}^{N} q_n(0)}{\sum_{n=1}^{N} p_n(0)}. \tag{28}$$

It clearly follows from its explicit expression (23b) that $P(t)$ has (primitive) period T if $|\alpha| < 1$ and has period $2T$ if $|\alpha| > 1$:

$$P(t+T) = P(t) \quad \text{if } |\alpha| < 1, \tag{29a}$$

$$P(t+2T) = P(t) \quad \text{if } |\alpha| > 1. \tag{29b}$$

Note that in the special case when the modulus of α is just unity, $|\alpha| = 1$, clearly $P(t)$, see (23b), vanishes at some finite (*real*) value $t = t_s, P(t_s) = 0$, and clearly at this time t_s the equations of motion (21) and (22) become *singular* due to the blow-up of their right-hand sides. This is not surprising, in view of the appearance of P in the *denominator* in the definition of our Hamiltonian $\tilde{H}(\underline{p}, \underline{q}; \omega)$, see (16) with (20). And of course the periodicity properties of $P(t)$ are as well shared by the center-of-mass coordinate $Q(t)$, see (25b),

$$Q(t+T) = Q(t) \quad \text{if } |\alpha| < 1, \tag{30a}$$

$$Q(t+2T) = Q(t) \quad \text{if } |\alpha| > 1. \tag{30b}$$

Hence we conclude that the motion of the center of mass of our system is *isochronous*, the *isochronicity period* being T or $2T$ depending whether the initial data entail that the modulus of the quantity α, see (24), is smaller or larger than unity [but recall that $H(t)$ and $u(t;\omega)$ are always *periodic* with period T, see (18) and (19)].

Let us now turn to the *relative* motion. To this end let us set

$$p_{n,m} = p_n - p_m, \quad q_{n,m} = q_n - q_m. \tag{31}$$

One then notes by a routine computation [see (20)] that

$$[p_{n,m}, \Theta] = 0, \quad [q_{n,m}, \Theta] = 0, \tag{32}$$

from which it immediately follows that

$$\dot{q}_{n,m} = [q_{n,m}, \widetilde{H}] = [q_{n,m}, H]u = u(0)[q_{n,m}, H]\exp(i\omega t), \tag{33a}$$

$$\dot{p}_{n,m} = [p_{n,m}, \widetilde{H}] = [p_{n,m}, H]u = u(0)[p_{n,m}, H]\exp(i\omega t). \tag{33b}$$

Note that we have more ODEs than independent unknowns. However, these ODEs all follow from the same equations of motion and are hence necessarily consistent: of course only $N-1$ of the ODEs (33b) are independent, and likewise only $N-1$ of the ODEs (33a). To analyze the time evolution of these dependent variables $p_{n,m}(t)$ and $q_{n,m}(t)$ it is now convenient to perform the following change of (independent and dependent) variables [namely, essentially again the trick, see (8), but in the simpler version with $\lambda = 0$]:

$$q_{n,m}(t) = \xi_{n,m}(\tau), \quad p_{n,m}(t) = \pi_{n,m}(\tau), \tag{34a}$$

where the new (*complex*) timelike variable τ is again defined as above [see (8b)],

$$\tau = \frac{\exp(i\omega t) - 1}{i\omega}. \tag{34b}$$

Note that this definition, (34b), entails that $\tau = 0$ for $t = 0$, so that, via (34a), the initial data for the new dependent variables $\xi_{n,m}$ and $\pi_{n,m}$ coincide with the initial data for the original problem:

$$\xi_{n,m}(0) = q_{n,m}(0), \quad \pi_{n,m}(0) = p_{n,m}(0). \tag{35}$$

The time evolution of the dependent variables $\xi_{n,m}(\tau)$ and $\pi_{n,m}(\tau)$ is now given, from (33) via (34), by the following (*autonomous*) equations of motion:

$$\xi'_{n,m} = u(0;\omega)\,\pi_{n,m}, \tag{36a}$$

$$\pi'_{n,m} = -u(0;\omega)\frac{\partial V(\underline{\xi})}{\partial \xi_{n,m}}, \tag{36b}$$

where of course appended primes indicate differentiations with respect to the new (*complex*) independent variable τ. [We hope the attentive reader will pardon the abuse entailed by our use of the notation $\partial V(\underline{\xi})/\partial \xi_{n,m}$ on the right-hand side of the last equation, and will understand the significance of this notation, which is of course permissible thanks to the *translation-invariant* character of the potential $V(\underline{q})$, see (3), entailing that $V(\underline{q})$ is only a function of the difference of the particle coordinates, see (31) and (34a)]. And now, by the standard argument associated with the trick—as tersely reviewed in the preceding section, see the discussion following (12), the adaptation of which to the present circumstances is too obvious to require a detailed treatment—one easily concludes that the (*nonautonomous*) dynamical system characterized by the equations of motion (33) is *isochronous*, there being an open set of initial data $q_{n,m}(0)$, $p_{n,m}(0)$, having full dimensionality in the space of these data, such that the resulting motions are *completely periodic* with period T,

$$q_{n,m}(t+T) = q_{n,m}(t), \quad p_{n,m}(t+T) = p_{n,m}(t). \tag{37}$$

To formulate our final result we need coordinates to describe the *relative* motion. Finding *canonical* coordinates that do this is notoriously awkward, but also not necessary for us here. Let us therefore introduce

$$\tilde{p}_n = p_n - P, \quad \tilde{q}_n = q_n - Q, \tag{38}$$

which are *noncanonical* coordinates describing the *relative* motion. It then follows from (37) that $\tilde{p}_n$ and $\tilde{q}_n$ are all *isochronous*, as they are easily expressed in terms of the $q_{n,m}$ and the $p_{n,m}$:

$$\tilde{q}_n(t+T) = \tilde{q}_n(t), \quad \tilde{p}_n(t+T) = \tilde{p}_n(t). \tag{39}$$

And from this formula, via (38), (29), and (30), we arrive at our fundamental conclusion, namely that the time evolution entailed by the ω-modified Hamiltonian (16) possesses an *open*, hence fully dimensional, set of initial data $\underline{p}(0), \underline{q}(0)$ such that the solutions of the corresponding initial-value problem are *isochronous,*

$$q_n(t+T) = q_n(t), \quad p_n(t+T) = p_n(t) \quad \text{if } |\alpha| < 1, \tag{40a}$$

$$q_n(t+2T) = q_n(t), \quad p_n(t+2T) = p_n(t) \quad \text{if } |\alpha| > 1, \tag{40b}$$

with the constant α defined in terms of the initial data by (24).

Let us end this section by also exhibiting the *Newtonian* equations of motion associated with our *isochronous* dynamical system, that are of course obtained by time differentiating the first of the two Hamiltonian equations, (21), by then using the second, (22), as well as (20), (18b), and (23a), to get rid of all time-differentiated terms on the right-hand side of the resulting equations, and by finally using again (21) to get rid (to the extent possible, see below) of p_n so as to get Newtonian equations of motion that feature on their left-hand sides the "accelerations" $\ddot{q}_n$ and on their right-hand sides the corresponding "forces" expressed in terms of the positions q_m and the velocities $\dot{q}_m$ of the "particles" (moving in the *complex* q-plane). We thus obtain the following equations of motion:

$$\ddot{q}_n - i\omega\dot{q}_n = -\left(1 + Ni\omega\frac{Q}{P}\right)^2 \frac{\partial V(\underline{q})}{\partial q_n} + F, \tag{41a}$$

$$F = -\frac{2i\omega H}{P}\left(1 + \frac{N^2 i\omega Q H}{2P^3}\right) = \ddot{Q} - i\omega\dot{Q}. \tag{41b}$$

Note that the "collective force" F acts equally on *all* the coordinates q_n, and it is moreover easily seen from the results reported above that the time dependence of this force is *periodic* [with period T or $2T$, see (18), (23b), and (25b)]. Moreover, this collective force F induces a collective, *periodic*, motion $Q(t)$ of *all* the canonical coordinates $q_n(t)$, and likewise a collective *periodic* motion $P(t)$ of *all* the canonical momenta $p_n(t)$, the explicit time dependence of which is exhibited above [see (25a) and (23b)].

It should however be noted that these equations, (41), do not quite have yet the *Newtonian* form, because the right-hand sides of (41a), namely, the "forces," are not yet expressed just in terms of the coordinates q_m and the velocities $\dot{q}_m$: a dependence on the canonical momenta p_m still lingers, albeit only via the collective coordinates $P \equiv P(\underline{p})$ and $F \equiv F(\underline{p}, \underline{q})$, see (6a) and (41b) with (2). Actually the second of this collective coordinates can be rather neatly expressed in terms of the first [via (26) and (41)],

$$F = \frac{P^2 - [N(\dot{Q} - i\omega Q) - 2P]^2}{N^2 Q}. \tag{42}$$

But in order to express P in terms of the coordinates q_n and of the velocities $\dot{q}_n$—the first of which actually only enter via $Q(\underline{q})$ and $V(\underline{q})$, see (7a) and (2), while the second enter via $\dot{Q} = Q(\underline{\dot{q}})$ and the collective coordinate K,

$$K \equiv K(\dot{\underline{q}}) = \frac{1}{2}\sum_{n=1}^{N} (\dot{q}_n)^2, \tag{43}$$

see below—one should solve the following algebraic equation (of *fifth* degree in P), obtained from (2) via (21) with (16b) and (20) (to obtain p_n in terms of $\dot{q}_n, Q, P, H$) and then via (26) (to express H in terms of P,Q, and $\dot{Q}$):

$$P^2\left\{-\frac{NS^2}{2} + Ni\omega Qs(s-1)S + K\right\} = (N\omega sQ)^2(V+C), \tag{44a}$$

$$S = \dot{Q} - i\omega sQ = \dot{Q} - i\omega Q - \frac{P}{N}, \tag{44b}$$

$$s = 1 + \frac{P}{Ni\omega Q}. \tag{44c}$$

But let us note that, if the initial data entail that

$$H(0) \equiv H(\underline{p}(0), \underline{q}(0)) = 0, \tag{45a}$$

yielding via (18),

$$H(t) = 0, \tag{45b}$$

the Newtonian equations of motion take instead the much simpler, completely explicit, form

$$\ddot{q}_n - i\omega\dot{q}_n = -\left[\frac{\sum_{n=1}^{N}\dot{q}_n}{\sum_{n=1}^{N}(\dot{q}_n - i\omega q_n)}\right]^2 \frac{\partial V(q)}{\partial q_n}, \tag{46}$$

as entailed by (41a) [with $F=0$, see (41b) with (45) and (25a)] [with (45), (16b) and (20) yielding $P=N(\dot{Q}-i\omega Q)$]; while in the special examples in which the original Hamiltonian H reduces to the free Hamiltonian (i.e., $V+C=0$, see examples below), the Eq. (44) for P becomes a *cubic*.

In view of the significant simplification that obtains (here, and see also below) when the initial data entail the condition (45a), let us note that the requirement that this condition holds restricts the initial data to a hypersurface in the *complex* phase space of (*complex*) codimension one. But this hypersurface can be shifted at will by varying the parameter C in the definition (2) of the original Hamiltonian H. One way to justify this is by considering C itself as an additional dynamical variable rather than a given constant; then the absence in the Hamiltonian $\tilde{H}(\underline{p}, \underline{q}; \omega)$ of the corresponding canonical momentum entails that this quantity C is indeed time independent, namely that C maintains for all time its initial value; which can then be assigned, together with the assignment of all the other initial data, so that (45a) holds. But let us emphasize that, while varying C does not affect the dynamics generated by the original Hamiltonian H, see (2), it does instead modify the dynamics yielded by the ω-modified Hamiltonian $\tilde{H}$, see (16).

III. EXAMPLES

In this section we discuss tersely the results reported above for some cases characterized by specific choices for the potentials $V(\underline{q})$, see (2).

A. No potential

The very simplest case obtains for the choice

$$V(\underline{q}) = 0, \tag{47a}$$

i.e., for the original Hamiltonian

$$H(\underline{p},\underline{q}) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + C, \tag{47b}$$

and the ω-modified Hamiltonian

$$\tilde{H}(\underline{p},\underline{q};\omega) = \left[1 + Ni\omega\frac{Q(\underline{q})}{P(\underline{p})}\right]\left[\frac{1}{2}\sum_{n=1}^{N} p_n^2 + C\right]. \tag{47c}$$

Here and always below the collective coordinates Q and P are of course defined by (7a) and (6a).

The Hamiltonian, respectively, Newtonian equations of motions yielded by this ω-modified Hamiltonian, (47c), read

$$\dot{q}_n = \left[1 + Ni\omega\frac{Q}{P}\right]p_n - \frac{Ni\omega QH}{P^2}, \tag{48a}$$

$$\dot{p}_n = -\frac{i\omega H}{P}, \tag{48b}$$

respectively,

$$\ddot{q}_n - i\omega\dot{q}_n = \frac{P^2 - [N(\dot{Q} - i\omega Q) - 2P]^2}{N^2 Q}. \tag{48c}$$

Also, it is easily seen that the solution of the corresponding initial-value problem reads

$$p_n(t) = p_n(0) + \frac{P(0)}{N}\left\{\left[\frac{1 - \alpha\exp(-i\omega t)}{1 - \alpha}\right]^{1/2} - 1\right\}, \tag{49a}$$

$$q_n(t) = q_n(0) + \frac{NQ(0)}{P(0)}[\exp(i\omega t)p_n(t) - p_n(0)] + p_n(t)\frac{\exp(i\omega t) - 1}{i\omega}, \tag{49b}$$

with α given by (24) and of course [see (48a)] with

$$p_n(0) = \left[1 + Ni\omega\frac{Q(0)}{P(0)}\right]^{-1}\left[\dot{q}_n(0) + \frac{Ni\omega Q(0)H(0)}{P^2(0)}\right] \tag{49c}$$

in the context of the initial-value problem for the Newtonian equation of motions (48c).

The *isochronous* character of this Hamiltonian many-body problem is now evident: its phase space is divided into two parts, that characterized by $|\alpha| < 1$ and by solutions *completely periodic* with period T, see (1), and that characterized by $|\alpha| > 1$ and by solutions *completely periodic* with period $2T$, as stated in (40), while on the *separatrix* between these two phase-space regions, characterized by the formula

$$|\alpha| = 1, \quad \alpha = \exp(i\vartheta), \quad \mathrm{Im}(\vartheta) = 0, \tag{50}$$

the equations of motion become *singular* at the (*real*) time $t_s = (\vartheta/\omega)\mathrm{mod}(T)$ due to the vanishing at that time of the collective coordinate $P, P(t_s) = 0$, see (23b) and (48).

B. Two-body homogeneous potential

Next, let us consider the standard many-body problem characterized by the following *two-body* potentials:

$$V(\underline{q}) = \frac{1}{2} \sum_{n,m=1,n\neq m}^{N} V_{nm}(q_n - q_m), \quad V_{nm}(q) = \frac{g_{nm} q^{2k}}{2k}, \tag{51}$$

where the "coupling constants" g_{nm} satisfy the symmetry condition $g_{nm}=g_{mn}$ and k is an arbitrary *integer* (positive or negative, but *nonvanishing,* and *different from unity* to exclude the uninteresting "harmonic oscillator" case). This choice allows a comparison with the *isochronous* equations of motion of Newtonian type (10)—obtained via the application of the standard trick to the Newtonian equations yielded by the original Hamiltonian H, see (2) with (51)—that in this case read as follows:

$$\ddot{\breve{q}}_n - \left(\frac{k+1}{k-1}\right) i\omega \dot{\breve{q}}_n - \left[\frac{k}{(k-1)^2}\right] \breve{q}_n = -\sum_{m=1,m\neq n}^{N} g_{nm}(\breve{q}_n - \breve{q}_m)^{2k-1}. \tag{52}$$

The (*autonomous*) Newtonian equations of motion (41) yielded by our approach read instead

$$\ddot{q}_n - i\omega \dot{q}_n = -u^2 \sum_{m=1,m\neq n}^{N} g_{nm}(q_n - q_m)^{2k-1} + F, \tag{53}$$

with u, respectively, F expressed in terms of $Q \equiv Q(\underline{q}), P \equiv P(\underline{q})$ and $H \equiv H(\underline{p},\underline{q})$, see (7a), (6a), and (2) with (51), by the formulas (16b) with (20), respectively, (41b) (except that these are not really Newtonian equations of motion, as discussed above; the display of such equations, to the extent it is possible, see above, can be left to the diligent reader).

In this case it is possible to provide explicit conditions on the initial data that are *sufficient* (but of course not *necessary*) to guarantee the *isochronous* behavior of the corresponding solution. The task to exhibit them can be left to the diligent reader, who will find—if need be—guidance in the literature [see for instance Refs. 4, 8, 11, 16, 22, 28, and 32, where analogous computations have been often performed, in particular explicit formulas providing a lower bound to the radius R, see the discussion before and after (13)].

IV. GENERALIZATIONS

In the following two sections we indicate tersely how the treatment of the many-body problem given above can be extended to the cases with different masses and with more dimensions.

A. Different masses

In this section we tersely indicate how the results reported above can be extended to the case with different masses M_n. Since this extension is quite trivial, we simply limit our presentation here to exhibiting, for a few of the key equations of our treatment, their corresponding, extended versions (which of course reduce to the previous equations by setting all the particle masses M_n to unity).

The definition of the unmodified many-body Hamiltonian [see (2)] now reads

$$H(\underline{p},\underline{q}) = \sum_{n=1}^{N} \frac{p_n^2}{2M_n} + V(\underline{q}) + C, \tag{54}$$

and correspondingly the Hamiltonian, respectively, Newtonian equations of motion [see (4), respectively, (5)] read now

$$\dot{q}_n = \frac{p_n}{M_n}, \quad \dot{p}_n = -\frac{\partial V(\underline{q})}{\partial q_n}, \tag{55}$$

respectively,

$$M_n \ddot{q}_n = -\frac{\partial V(\underline{q})}{\partial q_n}. \tag{56}$$

The definition (7a) of the quantity Q is now replaced by

$$Q(\underline{q}) = \frac{\sum_{n=1}^{N} M_n q_n}{\sum_{n=1}^{N} M_n}. \tag{57}$$

We trust the alert reader will have no difficulty to identify which, and how, other equations written above, and below, should be analogously modified, hence we do not devote additional space to this issue.

B. More dimensions

The generalization of the results reported above, and below, to the case with more (say, S) space dimensions is sufficiently simple not to require a detailed treatment: the Hamiltonian coordinates q_n are replaced by S-vectors $\vec{q}_n$, and likewise the corresponding Hamiltonian momenta p_n are replaced by S-vectors $\vec{p}_n$. Again, we trust the alert reader will have no difficulty to see how the standard equations written above, and below, shall be correspondingly modified. But there is one issue in this more general context that warrants some discussion, namely the possibility to introduce a more general definition of the collective variable Θ, see (20), characterized by the validity of the relation (14).

Let us therefore indicate, without many comments, the relevant generalization of our treatment (limiting consideration, for simplicity, to the equal masses case). We generalize (2) to read

$$H(\underline{\vec{p}}, \underline{\vec{q}}) = \frac{1}{2} \sum_{n=1}^{N} (\vec{p}_n \cdot \vec{p}_n) + V(\underline{\vec{q}}) + C \tag{58}$$

[of course always with the translation invariant property (3)], and likewise we generalize (16) to read

$$\tilde{H}(\underline{\vec{p}}, \underline{\vec{q}}; \underline{\vec{a}}; \omega) = u[\vec{P}(\underline{\vec{p}}), \vec{Q}(\underline{\vec{q}}); \underline{\vec{a}}; \omega] H(\underline{\vec{p}}, \underline{\vec{q}}), \tag{59a}$$

$$u(\vec{P}, \vec{Q}; \underline{\vec{a}}; \omega) = 1 + i\omega\Theta(\vec{P}, \vec{Q}; \underline{\vec{a}}) \tag{59b}$$

with [see (20)]

$$\Theta(\vec{P}, \vec{Q}; \underline{\vec{a}}) = \frac{N}{S} \sum_{s=1}^{S} \frac{Q_s}{P_s}, \tag{60}$$

where

$$Q_s = \vec{a}_s \cdot \vec{Q}, \quad P_s = \vec{a}_s \cdot \vec{P}, \tag{61}$$

and of course [see (7a) and (6a)]

$$\vec{Q}(\underline{\vec{q}}) = \frac{1}{N} \sum_{n=1}^{N} \vec{q}_n, \quad \vec{P}(\underline{\vec{p}}) = \sum_{n=1}^{N} \vec{p}_n. \tag{62}$$

The S constant S-vectors $\vec{a}_s$ [see (61)] are *arbitrary*, except for the orthogonality condition (quite useful to simplify the following formulas)

$$\vec{a}_s \cdot \vec{a}_{s'} = a_s^2 \delta_{ss'}. \tag{63}$$

It is then easy to verify that the definition (60) is compatible with the requirement (14). Therefore the properties (18) and (19) continue to hold.

Let us now discuss, as we did in Sec. II, first, the time evolution of the center-of-mass coordinates $\vec{Q}$ and $\vec{P}$, and then the *relative* motions.

To discuss the time evolutions of $\vec{Q}$ and $\vec{P}$ we note first of all that the definitions (61) entail the following formulas, as can be easily verified using the orthogonality relation (63):

$$\vec{Q} = \sum_{s=1}^{S} \frac{Q_s \vec{a}_s}{a_s^2}, \quad \vec{P} = \sum_{s=1}^{S} \frac{P_s \vec{a}_s}{a_s^2}, \tag{64}$$

$$[Q_s, Q_{s'}] = \delta_{ss'} a_s^2, \tag{65}$$

$$\left[\frac{NQ_s}{P_s}, H \right] = 1. \tag{66}$$

It is then easy, following the treatment given in the one-dimensional case (see Sec. II), to obtain the following explicit expressions detailing the time evolution of the quantities $P_s(t)$ and $Q_s(t)$:

$$P_s(t) = P_s(0) \left[\frac{1 - \alpha_s \exp(-i\omega t)}{1 - \alpha_s} \right]^{1/2}, \tag{67a}$$

$$\alpha_s = \frac{2a_s^2 H(0)}{1 - 2a_s^2 H(0)}, \tag{67b}$$

$$Q_s(t) = \left\{ \frac{Q_s(0)}{P_s(0)} + \frac{u(0)[\exp(i\omega t) - 1]}{Ni\omega} \right\} P_s(t). \tag{68}$$

It is thereby seen that the quantities $P_s(t)$ and $Q_s(t)$ are both *periodic*, with period T, respectively, $2T$ if $|\alpha_s| < 1$, respectively, $|\alpha_s| > 1$. Hence we conclude [see (64)] that the quantities $\vec{P}(t)$ and $\vec{Q}(t)$ are both *periodic* with period T if *all* the quantities α_s have modulus less than unity,

$$\vec{Q}(t+T) = \vec{Q}(t), \quad \vec{P}(t+T) = \vec{P}(t) \quad \text{if} \max_{s=1,\ldots,S} |\alpha_s| < 1, \tag{69a}$$

and are *periodic* with period $2T$ otherwise,

$$\vec{Q}(t+2T) = \vec{Q}(t), \quad \vec{P}(t+2T) = \vec{P}(t) \text{ if } \max_{s=1,\ldots,S} |\alpha_s| > 1. \tag{69b}$$

The discussion of the relative motions can then be done just as in the one-dimensional case, see Sec. II, since it is easy to verify that the definition (60) entails the vanishing of the following Poisson brackets:

$$[\vec{q}_n - \vec{q}_m, \Theta(\vec{P}, \vec{Q}; \underline{\vec{a}})] = 0, \quad [\vec{p}_n - \vec{p}_m, \Theta(\vec{P}, \vec{Q}; \underline{\vec{a}})] = 0. \tag{70}$$

Hence, following exactly the same reasoning as in Sec. II one arrives at the formulas:

$$\vec{q}_n(t+T)=\vec{q}_n(t),\quad \vec{p}_n(t+T)=\vec{p}_n(t)\quad \text{if } \max_{s=1,\ldots,S}|\alpha_s|<1, \tag{71a}$$

$$\vec{q}_n(t+2T)=\vec{q}_n(t),\quad \vec{p}_n(t+2T)=\vec{p}_n(t)\quad \text{if } \max_{s=1,\ldots,S}|\alpha_s|>1. \tag{71b}$$

We thereby see that our fundamental conclusion about the *isochronous* character of the dynamics entailed by the ω-modified Hamiltonian (59) is confirmed.

V. GENERAL HAMILTONIANS

In this section we indicate how the approach introduced above can be applied to more general Hamiltonians than that describing the nonrelativistic many-body problem, see (2). This discussion allows a more explicit display of the essential aspects of our technique to manufacture modified Hamiltonians yielding an *isochronous* dynamics.

Let us therefore consider again an ω-modified Hamiltonian defined by (16) with the collective variable $\Theta(\underline{p},\underline{q})$ satisfying (14), but now without making any assumption on the original Hamiltonian H and therefore without being able to provide an explicit form for the dependence of Θ on the Hamiltonian variables. It is nevertheless clear that the time evolution of H and of u is again given by (18) and (19), and therefore that the Hamiltonian equations can now be written in the following (*nonautonomous*) version:

$$\dot{q}_n=i\omega H(0)\exp(-i\omega t)\frac{\partial\Theta(\underline{p},\underline{q})}{\partial p_n}+u(0)\exp(i\omega t)\frac{\partial H(\underline{p},\underline{q})}{\partial p_n}, \tag{72a}$$

$$\dot{p}_n=-i\omega H(0)\exp(-i\omega t)\frac{\partial\Theta(\underline{p},\underline{q})}{\partial q_n}-u(0)\exp(i\omega t)\frac{\partial H(\underline{p},\underline{q})}{\partial q_n}. \tag{72b}$$

Now the first observation is that, if one restricts attention to initial data such that $H(0)$ vanishes, see (45), one gets again an *isochronous* behavior, since then these Hamiltonian equations of motion, (72), take the simpler form

$$\dot{q}_n=u(0)\exp(i\omega t)\frac{\partial H(\underline{p},\underline{q})}{\partial p_n}, \tag{73a}$$

$$\dot{p}_n=-u(0)\exp(i\omega t)\frac{\partial H(\underline{p},\underline{q})}{\partial q_n}, \tag{73b}$$

to which the by now familiar trick can be applied, entailing *isochronicity*. This is however a case of *partial isochronicity* (see Sec. I for this terminology), because the initial data must be restricted to satisfy the condition (45a).

Let us emphasize that this observation—possibly associated with the general possibility to add a constant C to the original Hamiltonian [and see in this respect the discussion at the end of Sec. II of how this possibility can facilitate the implementation of this restriction, (45a)]—entails that the class of Hamiltonians to which our technique can be successfully applied is indeed extremely large, at least as regards manufacturing ω-modified Hamiltonians which are *partially isochronous*.

In the more general case when $H(0)$ does *not* vanish, we conjecture that the motion will be *isochronous* in quite general circumstances, but we do not try to prove this in this paper. We rather restrict attention to systems such that there exists a collective function Θ satisfying (14) that depends on the Hamiltonian coordinates *only* via the two "center of mass" coordinates P and Q, see (6a) and (7a):

$$\Theta(\underline{p},\underline{q}) = \Theta[P(\underline{p}),Q(\underline{q})] \tag{74}$$

(this of course limits substantially the class of Hamiltonians to which this approach is applicable). Then one easily sees that there hold the relations (32) [with (31)], hence proceeding as in Sec. II one concludes that the relative motions are *isochronous.*

To proceed further it is necessary to gain some knowledge on the time evolution of the global "center of mass" quantities $Q(t)$ and $P(t)$. This requires additional information on the explicit form of the function $\Theta(P,Q)$, and moreover on the specific form of the original Hamiltonian, because the time evolution of these quantities, $Q(t)$ and $P(t)$, is determined by the evolution equations [clearly implied by (72)],

$$\dot{Q} = i\omega H(0)\exp(-i\omega t)\Theta_P(P,Q) + \frac{u(0)\exp(i\omega t)}{N}\sum_{n=1}^{N}\frac{\partial H(\underline{p},\underline{q})}{\partial p_n}, \tag{75a}$$

$$\dot{P} = -\frac{i\omega H(0)\exp(-i\omega t)\Theta_Q(P,Q)}{N} - u(0)\exp(i\omega t)\sum_{n=1}^{N}\frac{\partial H(\underline{p},\underline{q})}{\partial q_n}. \tag{75b}$$

VI. PARTIALLY ISOCHRONOUS VARIANTS OF THE MANY-BODY HAMILTONIAN

In this section we discuss—again in the context of the many-body problem characterized by the Hamiltonian (2)—variants of our technique, yielding modified Hamiltonians with enough *completely periodic* solutions to justify calling them *partially isochronous* (see the definition of this term given in Sec. I).

Let us take as starting point of our treatment the modified Hamiltonian

$$\tilde{H}(\underline{p},\underline{q}) = U(P,Q)H(\underline{p},\underline{q}). \tag{76}$$

Notation: largely the same as above, see Secs. I and II, in particular (2), (6a), and (7a). The novelty is that, for the time being, we do not commit ourselves to a specific form of the "modifying multiplicative coefficient" U, except for the assumption that it depend on the Hamiltonian variables *only* via the collective coordinates $P \equiv P(\underline{p})$ and $Q \equiv Q(\underline{q})$; of course for the special choice $U=u$ [see (16) with (20), (6a), and (7a)] the treatment of this section reduces to that given in Secs. I and II. And let us again emphasize, as we did in Sec. I, that hereafter we consider the time evolution entailed by the Hamiltonian $\breve{H}$, both for the Hamiltonian coordinates $q_n(t)$ and $p_n(t)$ and for any collective coordinate—such as P,Q,H,U—the time evolution of which obtains via the time dependence of the Hamiltonian coordinates.

The following evolution equations are then yielded by this modified Hamiltonian (76):

$$\dot{H} = -\frac{PU_Q H}{N}, \tag{77}$$

$$\dot{U} = \frac{PU_Q U}{N}, \tag{78}$$

$$\dot{P} = -U_Q H, \tag{79}$$

$$\dot{Q} = \frac{UP}{N} + U_P H, \tag{80}$$

$$\dot{q}_n = Up_n + U_P H, \tag{81}$$

$$\dot{p}_n = -U\frac{\partial V(\underline{q})}{\partial q_n} - \frac{U_Q H}{N}. \tag{82}$$

Note that here and hereafter we use the short-hand notation U_Q and U_P to denote the (partial) derivatives of the (yet to be assigned) function $U(P,Q)$ with respect to its two arguments:

$$U_Q \equiv \frac{\partial U}{\partial Q}, \quad U_P \equiv \frac{\partial U}{\partial P}. \tag{83}$$

From (79) and (77) we get

$$\dot{P}P = \dot{H}, \tag{84}$$

entailing

$$P = (2H - B^2)^{1/2}, \tag{85a}$$

$$B^2 = 2H(0) - P^2(0). \tag{85b}$$

To proceed further one must make a specific choice for the function $U(P,Q)$. We consider below various possibilities.

A. A simple variant

The first modified Hamiltonian we now consider is characterized by the following "β-modified" variant of the N-body Hamiltonian (2):

$$\breve{H}(\underline{p},\underline{q};\beta) = [1 + i\beta Q(\underline{q})]H(\underline{p},\underline{q}), \tag{86}$$

corresponding to (76) with

$$U(P,Q) \equiv U(Q;\beta) = 1 + i\beta Q \tag{87a}$$

implying

$$U_Q = i\beta, \quad U_P = 0. \tag{87b}$$

Our main result is to show that there exists a set of initial data $q_n(0)$ and $p_n(0)$—having a bit less than full dimensionality in phase space, being restricted by the requirement

$$H(0) \equiv H[\underline{p}(0),\underline{q}(0)] = 0 \tag{88}$$

(and see in this connection the discussion at the end of Sec. II)—yielding motions *all* of which are *completely periodic* with the period

$$\breve{T} = \frac{2\pi}{\Omega}, \quad \Omega = \frac{\beta P(0)}{N} \equiv \frac{\beta P[\underline{p}(0)]}{N}. \tag{89}$$

In this formula $P(\underline{p})$ is of course defined by (6a). Note that this formula entails that the period $\breve{T}$ does depend on the initial data, albeit only via the collective variable $P(\underline{p})$, and of course that we must restrict the initial data so that this period $\breve{T}$, as well as the corresponding circular frequency Ω, be *real*. This entails an *additional* restriction of the initial data $p_n(0)$ to a hypersurface of *real* codimension one. And one can repeat in this respect a completely analogous discussion to that given after (45), up to replacing the role played in that context by the parameter C with the role played in the present context by the parameter β. Note moreover that in this manner—adjusting at one's convenience the value of β [as it were *a posteriori*, after the initial data $p_n(0)$ have been

assigned]—one can in fact even impose that $\breve{T}$ have a given, preassigned value, thereby restoring the property of yielding *isochronous* motions—albeit for a set of initial data having a bit less than full dimensionality in phase space, being restricted to lie on a manifold of (*complex*) codimension *two* in phase space [i.e., the intersection of *two* hypersurfaces each of which of *complex* codimension *one*, that characterized by (88) and that characterized by the requirement that the period $\breve{T}$, or equivalently the circular frequency Ω, see (89), have a *preassigned* real value].

To prove this result we note that the Hamiltonian $\breve{H}(\underline{p},\underline{q};\beta)$, see (86), entails the following time-evolution equations [see (81), (82), (80), (79), and (77) with (87)]:

$$\dot{q}_n = (1 + i\beta Q)p_n, \tag{90a}$$

$$\dot{p}_n = -(1 + i\beta Q)\frac{\partial V(\underline{q})}{\partial q_n} - i\beta H, \tag{90b}$$

$$\dot{Q} = \frac{(1 + i\beta Q)P}{N}, \tag{90c}$$

$$\dot{P} = -i\beta H, \tag{90d}$$

$$\dot{H} = -\frac{i\beta HP}{N}. \tag{90e}$$

The preceding three equations can be easily integrated for general initial data, but we restrict attention here only to the case characterized by the condition (88), in which case the outcome is particularly simple,

$$H(t) = H(0) = 0, \tag{91a}$$

$$P(t) = P(0) \equiv P[\underline{p}(0)], \tag{91b}$$

$$1 + i\beta Q(t) = [1 + i\beta Q(0)]\exp(i\Omega t). \tag{91c}$$

Insertion of the first and last of these formulas in (90a) and (90b) yields the equations that determine the time evolution of the dependent variables $q_n(t)$ and $p_n(t)$,

$$\dot{q}_n = [1 + i\beta Q(0)]\exp(i\Omega t)p_n, \tag{92a}$$

$$\dot{p}_n = -[1 + i\beta Q(0)]\exp(i\Omega t)\frac{\partial V(q)}{\partial q_n}. \tag{92b}$$

From these evolution equations, via the, by now usual, argument based on the trick, one easily concludes that the assertions made at the beginning of this section are valid.

Let us end this section by pointing out that the Hamiltonian $\breve{H}(\underline{p},\underline{q};\beta)$, see (86), is perhaps more susceptible to a "physical interpretation" than the Hamiltonian $\tilde{\tilde{H}}(\underline{p},\underline{q};\omega)$, see (16), inasmuch as $\breve{H}(\underline{p},\underline{q};\beta)$, in contrast to $\tilde{H}(\underline{p},\underline{q};\omega)$, does *not* feature momentum variables in the denominator. This observation is underscored by the possibility to write in this case quite explicitly the *Newtonian* equations of motion that correspond to the *Hamiltonian* equations (90a) and (90b):

$$\ddot{q}_n = \frac{i\beta\dot{Q}\dot{q}_n}{1+i\beta Q} - (1+i\beta Q)^2 \frac{\partial V(\underline{q})}{\partial q_n} - \frac{i\beta(1+i\beta Q)H}{N}, \tag{93}$$

where of course $Q \equiv Q(\underline{q})$ [see (7a)] and $H \equiv H(\underline{p},\underline{q})$ [see (2)] with

$$p_n = \frac{\dot{q}_n}{1+i\beta Q} \tag{94}$$

[see (90a)]. And note moreover that the last term on the right-hand side of the *Newtonian* equations of motion (93) is altogether missing when (88) holds, see (91a).

B. A more general variant

A more general variant—that includes as a special case those treated above—is associated with the observation that—quite generally—the evolution equation (77) with (88) entails the vanishing of H for all time, see (91a), and that—again quite generally, see (79)—the vanishing of H entails that P is time independent, see (91b). This we assume in this section, as in the previous one, hence we consider again a modified Hamiltonian defined by (76) [with (2)], and initial data restricted so that (88) holds. But now we note that (91c) does not generally follow from (91a) and (91b); all that one can assert is that, if (91a) and (91b) hold, then (78) and (80) take the following simpler form:

$$\dot{U} = -\frac{P(0)U_Q U}{N}, \quad \dot{Q} = \frac{P(0)U}{N}. \tag{95}$$

To proceed further, an assumption must again be introduced on the assignment of $U(P,Q)$, although the time-independence of P entails that we can manage with an *ansatz* that allows a certain generality as regards the dependence on this collective variable. For instance let us set

$$U = 1 + \Phi(P)Q + \Psi(P)Q^2, \tag{96a}$$

entailing

$$U_Q = \Phi(P) + 2\Psi(P)Q \tag{96b}$$

[of course the results of the preceding section would be reproduced for $\Phi(P)=i\beta$, $\Psi(P)=0$, although this might involve a nontrivial limiting process; and those of Secs. I and II—with (45)—would be reproduced for $\Phi(P)=Ni\beta/P$, $\Psi(P)=0$]. Then one can easily obtain the following results:

$$U(t) = A\left\{\sin\left[\frac{\Omega(t-t_0)}{2}\right]\right\}^{-2}, \tag{97a}$$

$$A = 1 - \frac{\Phi^2(P)}{4\Psi(P)}, \tag{97b}$$

$$\Omega = \frac{P}{N}[-\Phi^2(P) + 4\Psi(P)]^{1/2}, \tag{97c}$$

$$\sin(t_0) = \left[\frac{A}{1+\Phi(P)Q(0)+\Psi(P)Q^2(0)}\right]^{1/2}. \tag{97d}$$

We then note that, via (91a) and (97), the Hamiltonian equations (81) and (82) now read

$$\dot{q}_n = A\left\{\sin\left[\frac{\Omega(t-t_0)}{2}\right]\right\}^{-2} p_n, \tag{98a}$$

$$\dot{p}_n = -A\left\{\sin\left[\frac{\Omega(t-t_0)}{2}\right]\right\}^{-2} \frac{\partial V(q)}{\partial q_n}, \tag{98b}$$

or equivalently

$$\dot{q}_n = \dot{\tau} p, \quad \dot{p}_n = -\dot{\tau}\frac{\partial V(\underline{q})}{\partial q_n}, \tag{99}$$

provided we set

$$\tau(t) = -\left(\frac{2A}{\Omega}\right)\cot\left[\frac{\Omega(t-t_0)}{2}\right]. \tag{100}$$

It is now clear from (99)—via a generalized version of the trick, the details of which can be easily filled in by the interested reader, being based on the change of independent variables

$$q_n(t) = \breve{q}_n(\tau), \quad p_n(t) = \breve{p}_n(\tau), \tag{101}$$

with the new (*complex*) variable τ related to the (*real*) time variable t by (100)—that this modified Hamiltonian system is *partially isochronous* [with period $2\pi/\Omega$, see (97c)], the initial data having to be restricted, in order to entail *complete periodicity* of the corresponding solutions, by the requirement that (88), hence as well (91a), hold (a restriction of *complex* codimension *one*; but see the remark at the end of Sec. II) and moreover so that Ω be *real* (a restriction of *real* codimension *one*) or have a *preassigned* fixed value (a restriction of *complex* codimension *one*). This last restriction could however be lifted for special choices of the functions $\Phi(P)$ and $\Psi(P)$ that guarantee that Ω have a *fixed real* value independent of P, which is clearly the case if

$$-\Phi^2(P) + 4\Psi(P) = \left(\frac{N\omega}{P}\right)^2, \tag{102}$$

yielding $\Omega = \omega$, see (97c). Note that this restriction, (102), is compatible with $\Phi(P)$ and $\Psi(P)$ being both *real* functions (that yield *real* values whenever their argument, P, is *real*), provided $\Psi(P)$ does not vanish identically [as it instead did in the treatment of Secs. I and II, which indeed involved the *imaginary* function $\Phi(P) = i\omega/P$]. In addition—in order to avoid that the equations of motion run into a *singularity* as the (*real*) time t evolves—the initial data should of course *exclude* that the quantity t_0 be *real* [see (97d) and (98)].

C. Simple examples (no potential)

In this section we exhibit the explicit solutions of the initial-value problems for the models that correspond to the cases treated in the two preceding sections, when the potential is altogether missing, $V(\underline{q}) = 0$. The derivation of these findings is quite straightforward and is therefore left as an exercise for the diligent reader.

The modified Hamiltonian of the first of the two preceding sections reads now as follows:

$$\breve{H}(\underline{p},\underline{q};\beta) = \left[1 + \frac{i\beta}{N}\sum_{n=1}^{N} q_n\right]\left[\frac{1}{2}\sum_{n=1}^{N} p_n^2 + C\right], \tag{103}$$

and, for all initial data satisfying the condition

$$\frac{1}{2}\sum_{n=1}^{N} p_n^2(0) + C = 0, \tag{104}$$

it yields the solution

$$p_n(t) = p_n(0), \quad q_n(t) = q_n(0) + \left[1 + \frac{i\beta}{N}\sum_{n=1}^{N} q_n(0) \right] p_n(0) \frac{\exp(i\Omega t) - 1}{i\Omega}, \tag{105a}$$

$$\Omega = \frac{\beta}{N}\sum_{n=1}^{N} p_n(0), \tag{105b}$$

which is clearly *completely periodic* with period $2\pi/\Omega$ provided Ω is *real* (and *nonvanishing*).

The modified Hamiltonian of the second of the two preceding sections reads now as follows:

$$\tilde{H}(\underline{p},\underline{q};\beta) = [1 + \Phi(P)Q + \Psi(P)Q^2] \left[\frac{1}{2}\sum_{n=1}^{N} p_n^2 + C \right], \tag{106}$$

where of course $P \equiv P(\underline{p})$ and $Q \equiv Q(\underline{q})$, see (6a) and (7a). For all initial data satisfying the condition (104) it yields the solution

$$p_n(t) = p_n(0), \quad q_n(t) = q_n(0) - \frac{2A}{\Omega} p_n(0) \left\{ \cot\left[\frac{\Omega(t - t_0)}{2} \right] + \cot\left[\frac{\Omega t_0}{2} \right] \right\}. \tag{107a}$$

In these formulas we are of course using the notation of the second of the two preceding sections, in particular A, Ω, and t_0 are defined by (97b)–(97d) with $P = P(0)$. This solution is clearly *completely periodic* with period $2\pi/\Omega$ provided Ω is *real* (and *nonvanishing*) and t_0 is instead *not real*.

VII. OUTLOOK

Let us note first of all that the results reported in this paper, see in particular Secs. I, II, V, and VI, do justify the assertion contained in its title, inasmuch as we have shown the existence of a universal procedure applicable to a very broad class of Hamiltonians and yielding *isochronous* dynamics. Indeed let us underline that our treatment entails that the ω-modified Hamiltonian $\tilde{H}(\underline{p},\underline{q};\omega)$, see (16), is *isochronous* [for $\omega > 0$, with basic period T, see (1)] irrespective of any requirement that the original Hamiltonian $H(\underline{p},\underline{q}) = \tilde{H}(\underline{p},\underline{q};0)$ (namely, the unmodified one, corresponding to $\omega = 0$) be special (for instance, *integrable*): the only essential requirement is that there exist a collective variable $\Theta(\underline{p},\underline{q})$ satisfying (14). And conversely, the fact that the solutions of the modified Hamiltonian (with $\omega > 0$) display an *isochronous* behavior generally entails no information on the behavior of the solutions of the unmodified system, at least whenever the *isochronous* character of the solutions of the modified system [with $\omega > 0$, and basic period T, see (1)] prevails only in a subregion (having however full dimensionality, as required in order that the system be indeed classified as *isochronous*) of the phase space, but not in the *entire* phase space (or in the *entire* phase space except for a region of *vanishing* measure, namely having *positive* codimensionality). Only if the *isochronous* character of the solutions of the ω- modified Hamiltonian were to prevail [possibly with a period which is a *finite integer* multiple of the basic period T, see (1)] in the *entire* phase space (or at least in the *entire* phase space except for a region of *vanishing* measure, namely having *positive* codimensionality), then one might well conjecture that the original Hamiltonian be special, perhaps indeed *integrable*.

Two general directions of further research are suggested by the findings reported in this paper.

A first direction, probably of *theoretical* rather than *applicative* relevance, is the investigation of *quantized* versions of modified Hamiltonian models manufactured via the procedure introduced in this paper: in particular the simpler systems, such as those discussed in Secs. III A and VI B that

feature solutions *all* of which are *isochronous* (with the possible exception of a set of solutions of *vanishing* measure in phase space), as well as other, less trivial, systems that are also *isochronous* in the entire phase space (with the possible exception of a set of solutions of *vanishing* measure in phase space) such as those obtained by ω-modifying *integrable* Hamiltonian systems (many such examples can now be easily manufactured). It will be of interest to see whether the *hunch* that there always exist quantized versions of these models that feature *equispaced* spectra is confirmed, and, if so, whether the corresponding eigenfunctions can be *explicitly* exhibited. These investigations are likely to yield some further insight on the quantization issue, which would be further illuminated by the discovery of new *solvable* models, especially such models involving an *arbitrary* number of degrees of freedom.

A second direction of research points instead towards the *applicative* relevance of the findings reported in this paper, as well as in other recent papers which have emphasized that *isochronous dynamical systems are not rare*.[11,17,16,18] It is however likely that such applications be more relevant in other disciplines than physics, and therefore that they will not necessarily involve *Hamiltonian* systems: indeed the domain of natural philosophy that appears to feature the most striking instances of *isochronicity* is *biology*, including key phenomena of human life such as the regular beating of our hearts and the Circadian clocks that subtend the tempo of our biological lives.[39] Whether *mathematical physics* results such as those presented in this paper and in previous ones[2,38] will shed any light on this phenomenology remains to be seen; it certainly does point to an appealing direction of further study.

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Low-frequency currents induced in adjacent spherical cells

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The currents induced inside cells by external electric fields in the frequency range 50–60 Hz are studied analytically by accounting for thin cell membranes with transverse conductivity that is small compared to the conductivity of the saline fluid. A general perturbation scheme is formulated and applied to two adjacent spherical cells of equal radii by using a reflection principle and solving a nonlinear difference equation. The presence of the second cell is found to cause a no more than 10% increase to the current induced in an isolated spherical cell. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2190333]

I. INTRODUCTION

Concerns about the possible health effects of electromagnetic fields generated by power lines have stimulated theoretical studies of the currents induced in the human body when this is exposed to external, extremely-low-frequency fields, in the frequency range 50–60 Hz.[1–11] Over a decade ago Adair[2] asserted that the current induced inside an isolated cell is negligible, because the resistive cell membrane appears to shield the cell interior from incident low-frequency fields.

More recently, King and Wu[4] pointed out that Adair's conclusion, although correct for spherical cells, may not be valid for elongated, cylindrical cells. In the latter case the induced current depends on the length of the cell and the polarization of the incident electric field, so that shielding effects can be significantly reduced as the cell length increases or the incident field becomes parallel to the cell axis. For a typical spherical cell with radius 1 μm, membrane thickness $\delta \approx 5$ nm, membrane conductivity $\sigma_m \approx 10^{-6}$ S/m, and protoplasm (saline-fluid) conductivity $\sigma_0 \approx 0.5$S/m, King and Wu[4] calculated the electric field to be reduced by a factor 10^{-4} inside the cell. By contrast, the electric field inside the elongated, myelinated cell was calculated[4] to be almost equal to the incident field if the length of the cell roughly exceeds 5 mm and the external field is along the cell axis.

The purpose of the present study is to extend previous works[2,4] to more realistic cases where the current induced inside a cell is affected by the presence of neighboring cells. As a starting point, we treat the geometry with two spherical cells by an analytical technique which is directly applicable, although increasingly cumbersome, to many-cell geometries. Our formulation considers disconnected cells and therefore differs from that of Ref. 5 where cells are connected through suitable gap junctions.

The main assumptions underlying our analysis are that the cell membrane thickness is small compared to (i) the cell radius of curvature, and (ii) the length over which the cell curvature varies. So, elongated cells with sharp ends may not be included in the analysis. In addition, the cell curvature is assumed to be a sufficiently smooth and slowly varying function of the surface coordinates. Following Ref. 4 we also assume that the cell membrane is homogeneous and isotropic, with a scalar conductivity σ_m in the range 10^{-5}–10^{-6} S/m. This assumption may pose a limitation on our model, especially because membranes of actual cells have ion channels[12] and thus act as anisotropic media. To avoid complications due to anisotropies and yet preserve the essential physical features of thin membranes we replace the membrane by an "effective" boundary condition that accounts for its thickness and conductivity in the direction transverse to the cell

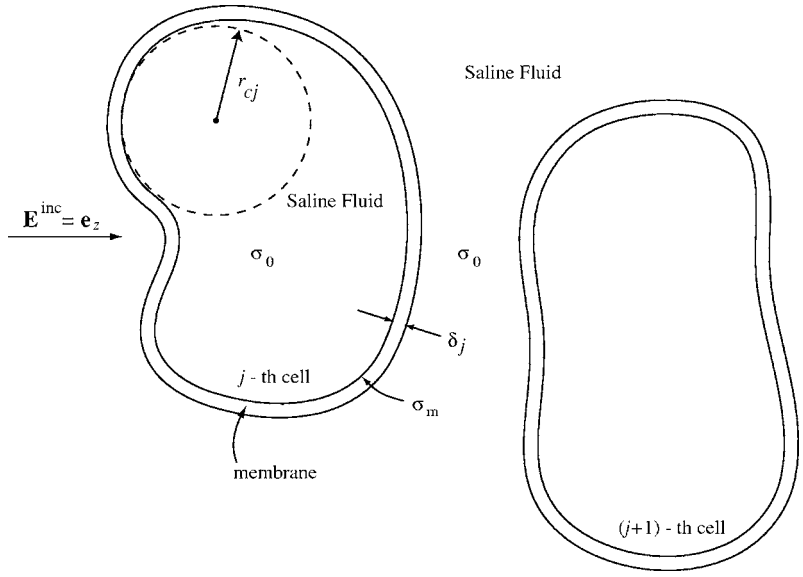

FIG. 1. Schematic of the geometry of arbitrarily shaped cells. The jth cell has radius of curvature r_{cj} and membrane thickness δ_j. The conductivities of the saline fluid and cell membrane are σ_0 and σ_m, respectively. The incident electric field is polarized along the **z** axis.

surface;[4] cf. Eq. (9) below. Similarly, the cell interior is considered as homogeneous and isotropic with conductivity σ_0, typically in the range $0.5-0.8$ S/m, which is taken to be equal to the conductivity of the surrounding saline fluid.

One can argue that the reduction of the electric field in the interior of a cell of reasonably arbitrary shape can be estimated by dimensional analysis. More precisely, the fraction of the penetrating field is expected to be proportional to the *small* factor $\tilde{\epsilon}=(\bar{r}_c/\delta)(\sigma_m/\sigma_0)$, where $\bar{r}_c$ is the cell mean radius of curvature, typically in the range $1-10$ μm, and δ is the membrane thickness, $\delta=2-5$ nm; cf. Fig. 1. This observation motivates the perturbation analysis of this paper because it indicates the dependence of the induced current on the small dimensionless parameter $\tilde{\epsilon}$. A similar technique is described in Ref. 13 for the cell response to a delta-function excitation. The application of perturbation theory, as described below, transcends dimensional analysis because it provides (i) a general mathematical framework to treat systematically problems of low-frequency scattering by cells; and (ii) a closed-form formula for the geometry-dependent prefactor for the field reduction inside a cell for the practically appealing case with two spherical cells of equal radii.

The paper is organized as follows. In Sec. II we describe the general formulation based on perturbation theory to determine currents induced inside cells exposed to uniform electric fields. In Sec. III we apply this formulation to the case with two neighboring spherical cells and derive simple, closed-form formulas for the electric field in the interior of each of the cells. In Sec. IV we discuss other cell geometries where the present framework may serve as a basis of detailed studies. The $e^{-i\omega t}$ time dependence is suppressed throughout the analysis.

II. PERTURBATION THEORY

A. General formulation

We consider a uniform electric field $\mathbf{E}^{\mathrm{inc}}$ parallel to the **z** axis, $\mathbf{E}^{\mathrm{inc}}=E_0\mathbf{e}_z$, and incident upon N cells of reasonably arbitrary shape, where $\mathbf{e}_z$ is the **z**-directed unit vector of the Cartesian coordinate system, and we take $E_0=1$ without loss of generality; cf. Fig. 1. The cells are immersed in saline fluid, an isotropic and homogeneous medium with conductivity σ_0. The interior $\mathcal{R}_j$ of the jth cell[14] is also assumed to be isotropic and homogeneous with a conductivity σ_0, equal to that of the ambient medium. The membrane is sufficiently thin and in principle anisotropic; we take the

membrane conductivity in the direction normal to the boundary to be σ_m, which is small compared to σ_0, $\sigma_m \ll \sigma_0$. At sufficiently low frequencies the effective dielectric constant, ϵ_{eff}, in each medium is dominated by the corresponding conductivity σ,

$$\epsilon_{\text{eff}} \sim \frac{i\sigma}{\omega}, \tag{1}$$

where ω is the radial frequency of the incident field.

The electric field inside each cell depends on the *relative* effective dielectric constant of the membrane because the requisite boundary conditions for the field on the cell surfaces, through which the conductivities enter, are homogeneous; see Appendix A where the problem of a single spherical cell is revisited. Therefore, for later notational convenience we introduce the dimensionless parameter ϵ by

$$\epsilon = \frac{\sigma_m}{\sigma_0}, \tag{2}$$

where ϵ is a small positive number, $0 < \epsilon \ll 1$.

The local radius of curvature, r_{cj}, of the jth cell is assumed to be a positive, sufficiently smooth function of the surface coordinates, and large compared to the membrane thickness δ_j,[15]

$$\tilde{r} = \frac{r_{cj}}{\delta_j} \gg 1. \tag{3}$$

Effective boundary conditions at the boundaries of cells with thin membranes involve the parameter $\tilde{r}\epsilon$.[4] In many cell configurations of interest this parameter is small,

$$\tilde{r}\epsilon \ll 1. \tag{4}$$

Condition (4) is enforced throughout the paper, and enables the application of regular perturbation theory as described below; see also Appendix A where, by virtue of (4), a simplified formula is derived for the current in the interior of an isolated spherical cell.

When the frequency of the incident electromagnetic field is sufficiently low, for instance in the range 50–60 Hz, a mathematically convenient quantity to use is the scalar potential, $\Phi(\mathbf{r})$, which satisfies to a good approximation the Laplace equation,

$$\nabla^2 \Phi(\mathbf{r}) = 0. \tag{5}$$

The electric field $\mathbf{E}(\mathbf{r})$ is approximately decoupled from the magnetic field, and is described by

$$\mathbf{E} = -\nabla\Phi. \tag{6}$$

For the incident field $\mathbf{E}^{\text{inc}} = \mathbf{e}_z$ the condition for $\Phi(\mathbf{r})$ at infinity reads

$$\Phi(\mathbf{r}) \sim -z, \quad r = |\mathbf{r}| \to \infty. \tag{7}$$

Despite the simple form of (5) and (6), mathematical complications may arise because of the special boundary conditions at the membrane separating the cell interior from the saline fluid. Following Ref. 4 we replace the membrane by an effective boundary condition that stems from treating the membrane thickness, δ_j, as properly small compared to the membrane radius of curvature. Next, we rederive briefly and interpret the related result of Ref. 4 by relaxing mathematical elaboration. By integration of (6) across the membrane, the restriction Φ^+ of Φ on the cell boundary from outside the cell and the corresponding restriction Φ^- from inside the cell should satisfy $\Phi^+ - \Phi^- = -E_{m,\perp}\delta_j$; $E_{m,\perp}$ is an appropriate value of the electric field normal to the boundary *inside* the membrane and $\Phi^{\pm}$ are boundary values of Φ *outside* the membrane. For suitably thin membrane, $E_{m,\perp}$ satisfies $\sigma_m E_{m,\perp} = \sigma_0 E_\perp^+ = \sigma_0 E_\perp^-$ by Gauss's law in the absence of surface charge,

where $E_{\perp}^{\pm}$ denote the boundary values of the transverse electric field outside the membrane. The relations of this paragraph yield

$$\frac{\partial\Phi^{+}}{\partial\eta}=\frac{\partial\Phi^{-}}{\partial\eta}\equiv\left.\frac{\partial\Phi}{\partial\eta}\right|_{\partial\mathcal{R}_j}, \tag{8}$$

$$\left.\frac{\partial\Phi}{\partial\eta}\right|_{\partial\mathcal{R}_j}=\frac{1}{\xi_j}[\Phi^{+}(\mathbf{r})-\Phi^{-}(\mathbf{r})], \tag{9}$$

where $\partial\mathcal{R}_j$ is the boundary of region $\mathcal{R}_j$, $\partial\Phi/\partial\eta=\mathbf{e}_\eta\cdot\nabla\Phi$ and $\mathbf{e}_\eta$ is the unit vector normal to the boundary $\partial\mathcal{R}_j$ pointing outward; $\Phi^{+}(\mathbf{r})$ and $\partial\Phi^{+}/\partial\eta$ are the values of Φ and $\partial\Phi/\partial\eta$ as $\mathbf{r}$ approaches $\partial\mathcal{R}_j$ from outside the cell ($\mathbf{r}\to\partial\mathcal{R}_j^{+}$), and $\Phi^{-}(\mathbf{r})$ and $\partial\Phi^{-}/\partial\eta$ are the corresponding values as $\mathbf{r}$ approaches $\partial\mathcal{R}_j$ from inside the cell ($\mathbf{r}\to\partial\mathcal{R}_j^{-}$). The parameter ξ_j has dimensions of length and is defined by

$$\xi_j=\frac{\delta_j}{\epsilon}. \tag{10}$$

Condition (4) ensures that the ξ_j entering boundary condition (9) is large compared to the radius of cell curvature, r_{cj},

$$r_{cj}\ll\xi_j. \tag{11}$$

Next, we describe a perturbation scheme for calculating Φ. The starting point is the expansion[16]

$$\Phi=\Phi_0+\Phi_1+\cdots+\Phi_n+\cdots,\quad n=0,1,\ldots, \tag{12}$$

where the subscript, n, denotes the perturbation order[17] and the ratio of two successive terms is assumed to be[18]

$$\frac{\Phi_n}{\Phi_{n-1}}=O\left(\frac{r_{c1}}{\xi_1},\ldots,\frac{r_{cN}}{\xi_N}\right). \tag{13}$$

Each term Φ_n in expansion (12) is determined iteratively as described below.

1. Zeroth-order approximation, n=0

In the zeroth-order approximation the right-hand side of (9) is set equal to zero. With $\Phi(\mathbf{r})\sim\Phi_0(\mathbf{r})$, Φ_0 satisfies Laplace's equation and the Neumann boundary condition on the cell boundaries, $\partial\mathcal{R}_j$. The boundary-value problem for the cell exterior thus reads

$$\nabla^2\Phi_0(\mathbf{r})=0,\quad \mathbf{r}\in\Omega,\qquad \left.\frac{\partial\Phi_0}{\partial\eta}\right|_{\partial\mathcal{R}_j^{+}}=0,\quad j=1,2,\ldots,N, \tag{14}$$

along with condition (7), where $\Omega=\mathbb{R}^3-\cup_j\mathcal{R}_j-\cup_j\partial\mathcal{R}_j$ is the exterior of all cells ($\mathcal{R}_j$) with exclusion of every $\partial\mathcal{R}_j$; $\mathbb{R}^3$ is the Euclidean space. This problem admits a unique solution for $\Phi_0(\mathbf{r})$.[19] The corresponding problem for the cell interior $\mathcal{R}_j$ has solution

$$\Phi_0(\mathbf{r})=\varphi_{0j},\quad \mathbf{r}\in\mathcal{R}_j, \tag{15}$$

where φ_{0j} ($j=1,2,\ldots,N$) are constants to be determined below. Each of these constants enters the boundary conditions for $\Phi_1(\mathbf{r})$ (in the first-order approximation) and is evaluated as an appropriate surface integral of $\Phi_0(\mathbf{r})$; cf. (19) below.

2. First-order approximation, $n=1$

In this approximation the right-hand side of (9) is replaced by $(\Phi_0^+ - \Phi_0^-)/\xi_j$, and $\Phi(\mathbf{r}) \sim \Phi_0(\mathbf{r}) + \Phi_1(\mathbf{r})$ where $\Phi_0(\mathbf{r})$ is known from (14) above. The boundary-value problem for the cell interior is described by

$$\nabla^2 \Phi_1(\mathbf{r}) = 0, \quad \mathbf{r} \in \mathcal{R}_j, \qquad \left.\frac{\partial \Phi_1}{\partial \eta}\right|_{\mathbf{r} \in \partial \mathcal{R}_j^-} = \frac{1}{\xi_j}(\Phi_0^+ - \varphi_{0j}), \tag{16}$$

along with the condition that $\Phi_1(\mathbf{r})$ be finite in $\mathcal{R}_j$. The Laplace equation with the same boundary conditions on $\partial \mathcal{R}_j$ also apply to the exterior problem. The requisite condition for Φ_1 at infinity becomes

$$\Phi_1(\mathbf{r}) \to 0, \quad r \to \infty. \tag{17}$$

Because the constant φ_{0j} enters the Neumann condition (16), its value must be consistent with the Laplace equation.[19] By integrating $\nabla^2 \Phi_1 = 0$ over $\mathcal{R}_j$ we obtain

$$\oint_{\partial \mathcal{R}_j^-} d\mathbf{r}\, \frac{\partial \Phi_1}{\partial \eta} = 0. \tag{18}$$

By virtue of condition (16),

$$\varphi_{0j} = \frac{1}{\|\partial \mathcal{R}_j\|} \oint_{\partial \mathcal{R}_j} d\mathbf{r}\, \Phi_0^+(\mathbf{r}), \tag{19}$$

where $\|\partial \mathcal{R}_j\|$ denotes the area of the closed surface $\partial \mathcal{R}_j$.

3. nth-order approximation, $n=1,2,\ldots$

It is reasonably straightforward to generalize the first-order approximation in order to carry out the calculations to the next orders in r_{cj}/ξ_j. With $\Phi(\mathbf{r}) \sim \Sigma_{i=0}^{n} \Phi_i(\mathbf{r})$ and $n \geqslant 1$ the boundary-value problem for $\Phi_n(\mathbf{r})$ follows from the preceding discussions of the zeroth- and first-order approximations via the replacements $0 \to n-1$ and $1 \to n$ in the subscripts for Φ. In the cell interior, Φ_n satisfies the boundary-value problem

$$\nabla^2 \Phi_n(\mathbf{r}) = 0, \quad \mathbf{r} \in \mathcal{R}_j, \qquad \left.\frac{\partial \Phi_n}{\partial \eta}\right|_{\partial \mathcal{R}_j^-} = \frac{1}{\xi_j}(\Phi_{n-1}^+ - \Phi_{n-1}^-), \tag{20}$$

where $\Phi_n(\mathbf{r})$ must be bounded everywhere for $n \geqslant 1$. The same differential equation and conditions on $\partial \mathcal{R}_j$ hold for the exterior problem. The condition at infinity reads

$$\Phi_n(\mathbf{r}) \to 0, \quad r \to \infty, \quad n \geqslant 1. \tag{21}$$

In the following we restrict the analysis to the zeroth- and first-order approximations for Φ.

B. Example: Single spherical cell

Next, for comparison and validation purposes we apply the general perturbation scheme of Sec. II A to a single spherical cell with radius a exposed to a uniform field $E^{\mathrm{inc}} = \mathbf{e}_z$. This prototypical case was studied in Refs. 2 and 4. Here, we derive the same result as in Ref. 4 for the electric field inside the cell within the framework of our Sec. II A. For the sake of completeness, the derivation of Ref. 4 for a single cell is revisited in our Appendix A, via the full set of boundary conditions by which the cell membrane is taken to have a finite thickness.

1. Zeroth-order approximation

The potential Φ_0 of the exterior problem satisfies

$$\nabla^2\Phi_0(\mathbf{r}) = 0, \quad r > a, \tag{22}$$

and

$$\frac{\partial\Phi_0}{\partial r} = 0 \quad \text{at } r = a, \quad \Phi_0(r,\theta) \sim -z, \quad r \to \infty. \tag{23}$$

The solution to (22) and (23) is obtained via a reflection principle in Appendix B. The result is

$$\Phi_0(r,\theta) = -\left(r + \frac{a^3}{2r^2}\right)\cos\theta, \quad r > a. \tag{24}$$

In particular, for $r \to a^+$,

$$\Phi_0(a^+,\theta) = \Phi_0^+ = -\frac{3a}{2}\cos\theta. \tag{25}$$

It follows from (15) and (19) that the potential Φ_0 vanishes for $r < a$,

$$\Phi_0(r < a, \theta) \equiv \varphi_0 = 0. \tag{26}$$

2. First-order approximation

In the next order the interior problem is described by

$$\nabla^2\Phi_1(\mathbf{r}) = 0, \quad r < a, \tag{27}$$

$$\frac{\partial\Phi_1}{\partial r} = \frac{1}{\xi}\Phi_0^+ = -\frac{1}{\xi}\frac{3a}{2}\cos\theta \quad \text{at } r = a, \quad \Phi_1(0,\theta)\text{: finite}. \tag{28}$$

Recall that the parameter ξ is defined by (10). Because of rotational symmetry, we apply separation of variables and write $\Phi_1(r,\theta) = g(r)\cos\theta$ where, by (27) and (28), $g(r)$ satisfies

$$r^2\frac{d^2g}{dr^2} + 2r\frac{dg}{dr} - 2g = 0 \quad \text{for } r < a, \quad g(0)\text{: finite}, \quad g(a) = -\frac{3a}{2\xi}, \tag{29}$$

with solution $g(r) = -(3a/2\xi)r$. Hence,

$$\Phi_1(r,\theta) = -\frac{3a}{2\xi}r\cos\theta, \quad r < a, \tag{30}$$

in agreement with (A9) of Appendix A. The electric field $\mathbf{E}$ inside the sphere follows by $\mathbf{E} = -\nabla\Phi$,

$$\mathbf{E}(r,\theta) = \frac{3a}{2\xi}\mathbf{e}_z, \quad r < a. \tag{31}$$

This formula shows that the incident field is reduced by the factor $3a/2\xi$ inside the cell.[2,4]

III. PAIR OF SPHERICAL CELLS

In this section we apply the perturbation scheme introduced in Sec. II to two spherical cells, denoted A and B, with equal radii; cf. Fig. 2 for the geometry of the problem. The radius of each sphere is a and the distance between their centers, O_1 and O_2, is $2d$. The z axis passes through $O_1(0,0,-d)$ and $O_2(0,0,d)$. The extension of our treatment to two spherical cells with different radii, or to three or more spherical cells, is straightforward yet increasingly cumbersome and lies beyond the scope of this paper.

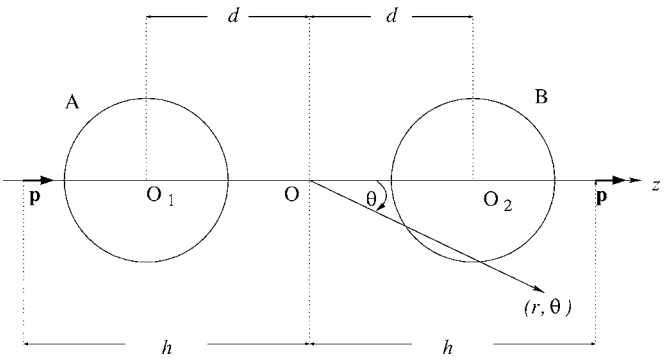

FIG. 2. The geometry of two spherical cells with equal radii, a. The incident, uniform electric field is polarized along the **z** axis. Two dipoles of moment $\mathbf{p}=\mathbf{e}_z$ are placed symmetrically with respect to the origin O in order to produce the incident field in the limit $h\to\infty$.

A. Zeroth-order approximation

The zeroth-order potential Φ_0 satisfies the Neumann boundary condition

$$\frac{\partial\Phi_0}{\partial\eta}=0, \quad \mathbf{r}\in\partial\mathcal{R}_A\cup\partial\mathcal{R}_B, \tag{32}$$

where $\partial\mathcal{R}_A$ and $\partial\mathcal{R}_B$ are the boundaries of spheres $\mathcal{R}_A$ and $\mathcal{R}_B$. In addition, $\Phi_0\sim -r\cos\theta$ as $r\to\infty$. We apply the reflection principle of Appendix B to the boundary-value problem for Φ_0 in the exterior of the cells by replacing the incident electric field by two electric dipoles (sources) of unit moment, $\mathbf{p}=\mathbf{e}_z$, located symmetrically with respect to O, at positions $(0,0,-h)$ and $(0,0,h)$; cf Fig. 2. The uniform incident field of unit amplitude, $\mathbf{E}^{\text{inc}}=\mathbf{e}_z$, is reproduced by taking the limit $h\to\infty$ after multiplying each (unit) dipole moment by πh^3; cf. (B10) of Appendix B. For finite h, the source dipoles generate an infinite number of image dipoles, all lying in the z axis, that are needed to sustain condition (32) on each spherical surface.

Next, we describe the location of image dipoles and their corresponding moments needed to satisfy the Neumann condition on the surface of each sphere, applying the results of Appendix B. Because each time an image dipole is placed inside a sphere the Neumann condition on the other sphere no longer holds, the procedure of placing image dipoles must be repeated *ad infinitum* leading to appropriate sequences of image dipoles inside each sphere. The source dipole at $(0,0,-h)$ induces image dipoles inside sphere A at positions $(0,0,-d-b)$, $(0,0,-d+a_2),\ldots,(0,0,-d+a_{2j})$, and at $(0,0,-d+b_2),\ldots,(0,0,-d+b_{2j})$, and inside sphere B at positions $(0,0,d-a_1),\ldots,(0,0,d-a_{2j-1})$ and at $(0,0,b_1),\ldots,(0,0,d-b_{2j-1})$, where j here is a positive integer and $j\to\infty$. By symmetry, the dipole at $(0,0,h)$ induces images of equal corresponding moments inside sphere B at $(0,0,d+b)$, $(0,0,d-a_2),\ldots,(0,0,d-a_{2j})$ and at $(0,0,d-b_2),\ldots,(0,0,d-b_{2j})$, and inside sphere A at $(0,0,-d+a_1),\ldots,(0,0,-d+a_{2j+1})$ and at $(0,0,-d+b_1),\ldots,(0,0,-d+b_{2j+1})$. According to (B5) of Appendix B, the distance b is defined by

$$b=\frac{a^2}{h-d}. \tag{33}$$

The distances a_m and b_m, where $a_0=d-h$ and $b_0=-b$, separately satisfy the recursion relation

$$\alpha_m=\frac{a^2}{2d-\alpha_{m-1}}, \quad m=1,2,\ldots, \tag{34}$$

where $\alpha_0=a_0$ or $\alpha_0=b_0=-b$. It follows from (B7) of Appendix B that the moments of the image dipoles located at distances a_m from O_1 or O_2 are

$$p_m = (-1)^m \left(\frac{\prod_{i=1}^{m} a_i}{a^m} \right)^3, \quad m = 1,2, \ldots . \tag{35}$$

The dipole moments corresponding to distances b_m from O_1 or O_2 are

$$q_m = (-1)^{m+1} \left(\frac{b\prod_{i=1}^{m} b_i}{a^{m+1}} \right)^3, \quad m = 1,2, \ldots ; \quad q_0 = -(b/a)^3. \tag{36}$$

The difference equation (34) is solved in Appendix C to yield

$$\alpha_m = a \frac{\sinh[m\kappa - \zeta(\alpha_0)]}{\sinh[(m+1)\kappa - \zeta(\alpha_0)]}, \tag{37}$$

where

$$\kappa = \ln \lambda, \quad \lambda = \frac{d + \sqrt{d^2 - a^2}}{a}, \tag{38}$$

$$\zeta(\alpha) = \frac{1}{2} \ln \left[\frac{1 - \lambda a^{-1} \alpha}{1 - (\lambda a)^{-1} \alpha} \right]. \tag{39}$$

It follows from Eqs. (35) and (36) that the strengths of the image dipoles are given explicitly by

$$p_m = (-1)^m \left\{ \frac{\sinh[\kappa - \zeta(a_0)]}{\sinh[(m+1)\kappa - \zeta(a_0)]} \right\}^3, \quad m = 1,2, \ldots , \tag{40}$$

$$q_m = (-1)^{m+1} \left\{ \frac{\sinh \zeta(b_0)}{\sinh[(m+1)\kappa - \zeta(b_0)]} \right\}^3, \quad m = 0,1,2, \ldots . \tag{41}$$

Thus, the zeroth-order potential in the exterior of the cells is furnished by[20]

$$\begin{aligned} 4\pi\Phi^{\mathrm{d}}(\mathbf{r};h) = {} & \frac{\mathbf{e}_z \cdot (h\mathbf{e}_z + \mathbf{r})}{|h\mathbf{e}_z + \mathbf{r}|^3} + \frac{\mathbf{e}_z \cdot (-h\mathbf{e}_z + \mathbf{r})}{|-h\mathbf{e}_z + \mathbf{r}|^3} - \frac{b^3}{a^3} \frac{\mathbf{e}_z \cdot [(d+b)\mathbf{e}_z + \mathbf{r}]}{|(d+b)\mathbf{e}_z + \mathbf{r}|^3} - \frac{b^3}{a^3} \frac{\mathbf{e}_z \cdot [-(d+b)\mathbf{e}_z + \mathbf{r}]}{|-(d+b)\mathbf{e}_z + \mathbf{r}|^3} \\ & + \sum_{m=1}^{\infty} p_m \left[\frac{(d-a_m) + \mathbf{e}_z \cdot \mathbf{r}}{|(d-a_m)\mathbf{e}_z + \mathbf{r}|^3} + \frac{-(d-a_m) + \mathbf{e}_z \cdot \mathbf{r}}{|-(d-a_m)\mathbf{e}_z + \mathbf{r}|^3} \right] + \sum_{m=1}^{\infty} q_m \left[\frac{(d-b_m) + \mathbf{e}_z \cdot \mathbf{r}}{|(d-b_m)\mathbf{e}_z + \mathbf{r}|^3} \right. \\ & \left. + \frac{-(d-b_m) + \mathbf{e}_z \cdot \mathbf{r}}{|-(d-b_m)\mathbf{e}_z + \mathbf{r}|^3} \right] = \sum_{m=0}^{\infty} (-1)^m \left\{ \frac{\sinh[\kappa - \zeta(a_0)]}{\sinh[(m+1)\kappa - \zeta(a_0)]} \right\}^3 \left[\frac{(d-a_m) + \mathbf{e}_z \cdot \mathbf{r}}{|(d-a_m)\mathbf{e}_z + \mathbf{r}|^3} \right. \\ & \left. + \frac{-(d-a_m) + \mathbf{e}_z \cdot \mathbf{r}}{|-(d-a_m)\mathbf{e}_z + \mathbf{r}|^3} \right] + \sum_{m=0}^{\infty} (-1)^{m+1} \left\{ \frac{\sinh \zeta(b_0)}{\sinh[(m+1)\kappa - \zeta(b_0)]} \right\}^3 \left[\frac{(d-b_m) + \mathbf{e}_z \cdot \mathbf{r}}{|(d-b_m)\mathbf{e}_z + \mathbf{r}|^3} \right. \\ & \left. + \frac{-(d-b_m) + \mathbf{e}_z \cdot \mathbf{r}}{|-(d-b_m)\mathbf{e}_z + \mathbf{r}|^3} \right], \end{aligned} \tag{42}$$

where $a_0 = d - h$ and $b_0 = -b$. Recall that b is defined by (33).

In the limit $h \to \infty$ we obtain $a_0 \to -\infty$ and $b_0 \to 0$, and in view of (37) and (39) we find

$$\zeta(a_0) \sim \kappa - \frac{a}{h}\sinh\kappa, \quad \zeta(b_0) \sim \frac{a}{h}\sinh\kappa, \tag{43}$$

and

$$a_{m+1} \sim a\,\frac{\sinh(m\kappa)}{\sinh[(m+1)\kappa]} \equiv \chi_m, \quad b_m \sim \chi_m. \tag{44}$$

After some rearrangement of terms in (42), the potential for $h\to\infty$ reduces to

$$4\pi\Phi^{\mathrm{d}}(\mathbf{r};h) \sim -\frac{4}{h^3}z - 2\frac{a^3}{h^3}(\sinh\kappa)^3\sum_{m=0}^{\infty}\frac{(-1)^m}{[\sinh(m+1)\kappa]^3}\left\{\frac{d-\chi_m+z}{[(d-\chi_m)^2+r^2+2(d-\chi_m)z]^{3/2}}\right.$$
$$\left.+\frac{-(d-\chi_m)+z}{[(d-\chi_m)^2+r^2-2(d-\chi_m)z]^{3/2}}\right\}. \tag{45}$$

The zeroth-order potential $\Phi_0(\mathbf{r})$ is obtained via multiplying Φ^{d} above by πh^3 so that the potential at infinity becomes $-z$:

$$\Phi_0(\mathbf{r}) = \lim_{h\to\infty}(\pi h^3\Phi^{\mathrm{d}}) = -z - \frac{a^3}{2}(\sinh\kappa)^3\sum_{m=0}^{\infty}\frac{(-1)^m}{[\sinh(m+1)\kappa]^3}\left\{\frac{d-\chi_m+z}{[(d-\chi_m)^2+r^2+2(d-\chi_m)z]^{3/2}}\right.$$
$$\left.+\frac{-(d-\chi_m)+z}{[(d-\chi_m)^2+r^2-2(d-\chi_m)z]^{3/2}}\right\}. \tag{46}$$

For nontouching spheres ($d>a$) the terms of the preceding series approach zero exponentially fast as $m\to\infty$.

Equation (46) is simplified considerably when the spheres touch ($d\to a$). With

$$\kappa \sim \sqrt{2}\left(1-\frac{a}{d}\right)^{1/2} \to 0 \quad \text{as } d\to a, \tag{47}$$

(44) furnishes

$$\chi_m = a\,\frac{m}{m+1}. \tag{48}$$

Accordingly, (46) entails

$$\Phi_0(\mathbf{r}) = -z - \frac{a^3}{2}\sum_{m=0}^{\infty}\left\{\frac{z+\dfrac{a}{m+1}}{\left[r^2+\dfrac{a^2}{(m+1)^2}+\dfrac{2az}{m+1}\right]^{3/2}} + \frac{z-\dfrac{a}{m+1}}{\left[r^2+\dfrac{a^2}{(m+1)^2}-\dfrac{2az}{m+1}\right]^{3/2}}\right\}\frac{(-1)^m}{(m+1)^3}. \tag{49}$$

It is worthwhile noting that as $m\to\infty$ terms of this series behave as $O(m^{-3})$, ensuring fast, absolute convergence.

B. First-order approximation

1. Formulas for nontouching spheres, d>a

With $\Phi\sim\Phi_0+\Phi_1$ everywhere the boundary condition for Φ_1 on each spherical surface reads

$$\left.\frac{\partial\Phi_1}{\partial r'}\right|_{r'=a} = \frac{1}{\xi}\,(\Phi_0 - \varphi_0)|_{r'=a}, \tag{50}$$

where (r', θ', ϕ') is the coordinate system with origin at the center of each sphere and φ_0 is given by (19). By expanding Φ_0 in spherical harmonics according to (D1) and (D2) of Appendix D, condition (50) reads

$$\left.\frac{\partial\Phi_1}{\partial r'}\right|_{r'=a} = \frac{1}{\xi}\left[-a\cos\theta' - \frac{a}{2}\sum_{l=1}^{\infty} D_l P_l(\cos\theta)\right], \tag{51}$$

where

$$D_l = D_l^A = (\sinh\kappa)^3 l \sum_{m=0}^{\infty} \frac{(-1)^m}{[\sinh(m+1)\kappa]^3}\left[\left(\frac{\chi_m}{a}\right)^{l-1} + \left(1+\frac{1}{l}\right)\left(\frac{2d-\chi_m}{a}\right)^{-l-2}\right] \tag{52}$$

for sphere A, and

$$D_l = D_l^B = (\sinh\kappa)^3(-1)^{l-1} l \sum_{m=0}^{\infty} \frac{(-1)^m}{[\sinh(m+1)\kappa]^3}\left[\left(\frac{\chi_m}{a}\right)^{l-1} - \left(1+\frac{1}{l}\right)\left(\frac{2d-\chi_m}{a}\right)^{-l-2}\right] \tag{53}$$

for sphere B.

Therefore, Φ_1 is expanded inside each sphere as

$$\Phi_1 = -\frac{a}{\xi} r' \cos\theta' - \frac{a^2}{2\xi}\sum_{l=1}^{\infty}\frac{D_l}{l}\left(\frac{r'}{a}\right)^l P_l(\cos\theta') + \mathcal{C}, \tag{54}$$

where $\mathcal{C}$ is an immaterial constant which is henceforth set to zero, $\mathcal{C}=0$. In view of (52) and (53) along with (D1)–(D3) of Appendix D, carrying out the summation over l gives

$$\begin{aligned}\Phi_1 = -\frac{a}{\xi} z' - \frac{a^2}{2\xi}\sum_{m=0}^{\infty}(-1)^m \frac{(\sinh\kappa)^3}{[\sinh(m+1)\kappa]^3}\left[\frac{r'}{a} T_m\left(\mp\beta_m\frac{r'}{a}, \theta'\right) \pm \gamma_m^3 \frac{r'}{a} T_m\left(\mp\gamma_m\frac{r'}{a}, \theta'\right)\right.\\ \left. + \gamma_m^2 S_m\left(\mp\gamma_m\frac{r'}{a}, \theta'\right)\right],\end{aligned} \tag{55}$$

where the upper (lower) sign corresponds to cell A (B),

$$\beta_m = \frac{\sinh(m\kappa)}{\sinh[(m+1)\kappa]}, \quad \gamma_m = \left(\frac{2d-\chi_m}{a}\right)^{-1}, \tag{56}$$

$$T_m(s,\theta') = \frac{2\cos\theta' + s}{\sqrt{1+2s\cos\theta'+s^2}}\,\frac{1}{1+\sqrt{1+2s\cos\theta'+s^2}}, \tag{57}$$

$$S_m(s,\theta') = \ln\left|\frac{2}{\sin^2\theta'}\frac{1}{s}\right| + \ln\left|\frac{s+\cos\theta' - \cos\theta'\sqrt{1+2s\cos\theta'+s^2}}{1+\sqrt{1+2s\cos\theta'+s^2}}\right|, \tag{58}$$

and χ_m is defined by (44).

The electric field, which is proportional to the current, inside each cell is

$$\mathbf{E}_1 = -\mathbf{e}_{r'}\frac{\partial\Phi_1}{\partial r'} - \mathbf{e}_{\theta'}\frac{1}{r'}\frac{\partial\Phi_1}{\partial\theta'}, \tag{59}$$

where

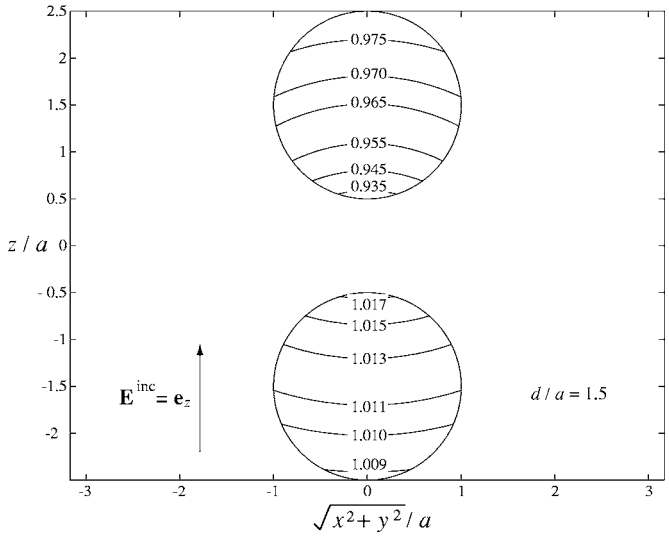

FIG. 3. Contour plots of the magnitude of the normalized electric field, $(3a/2\xi)^{-1}|\mathbf{E}_1|$, inside each cell. Maximum magnitudes are attained at $\theta'=0$; (x,y,z) is the usual Cartesian coordinate system.

$$-\frac{\partial\Phi_1}{\partial r'} = \frac{a}{\xi}\cos\theta' + \frac{a}{2\xi}\sum_{m=0}^{\infty}(-1)^m\frac{(\sinh\kappa)^3}{[\sinh(m+1)\kappa]^3} \times\left[V_m\left(\mp\beta_m\frac{r'}{a},\theta'\right)\pm\gamma_m^3 V_m\left(\mp\gamma_m\frac{r'}{a},\theta'\right)\pm\gamma_m^3 T_m\left(\mp\gamma_m\frac{r'}{a},\theta'\right)\right], \tag{60}$$

and

$$\frac{1}{r'}\frac{\partial\Phi_1}{\partial\theta'} = \frac{a}{\xi}\sin\theta' + \frac{a}{2\xi}\sin\theta'\sum_{m=0}^{\infty}(-1)^m\frac{(\sinh\kappa)^3}{[\sinh(m+1)\kappa]^3} \times\left[U_m\left(\mp\beta_m\frac{r'}{a},\theta'\right)\pm\gamma_m^3 U_m\left(\mp\gamma_m\frac{r'}{a},\theta'\right)\pm\gamma_m^3 W_m\left(\mp\gamma_m\frac{r'}{a},\theta'\right)\right]. \tag{61}$$

In the above,

$$U_m(s,\theta') = \frac{1}{(1+2s\cos\theta'+s^2)^{3/2}}, \tag{62}$$

$$V_m(s,\theta') = \frac{\cos\theta'+s}{(1+2s\cos\theta'+s^2)^{3/2}}, \tag{63}$$

$$W_m(s,\theta') = \frac{1}{\sqrt{1+2s\cos\theta'+s^2}}\,\frac{2\cos\theta'+s}{\cos\theta'(1+\sqrt{1+2s\cos\theta'+s^2})+s}. \tag{64}$$

In Fig. 3 we show contour plots for the magnitude of $\mathbf{E}_1$, normalized by the field $3a/2\xi$ inside an isolated spherical cell of equal radius (cf. Appendix A), inside cells A and B for a fixed value of d/a. In Fig. 4 we show plots for the maximum normalized magnitudes as functions of d/a. Two comments are in order: (i) As expected by close inspection of (59)–(64), for any $d>a$ the maximum $|\mathbf{E}_1|$ is attained for $\theta'=0$ for both spheres. (ii) This maximum value increases with d in sphere A and decreases with d in sphere B; cf. Fig. 4.

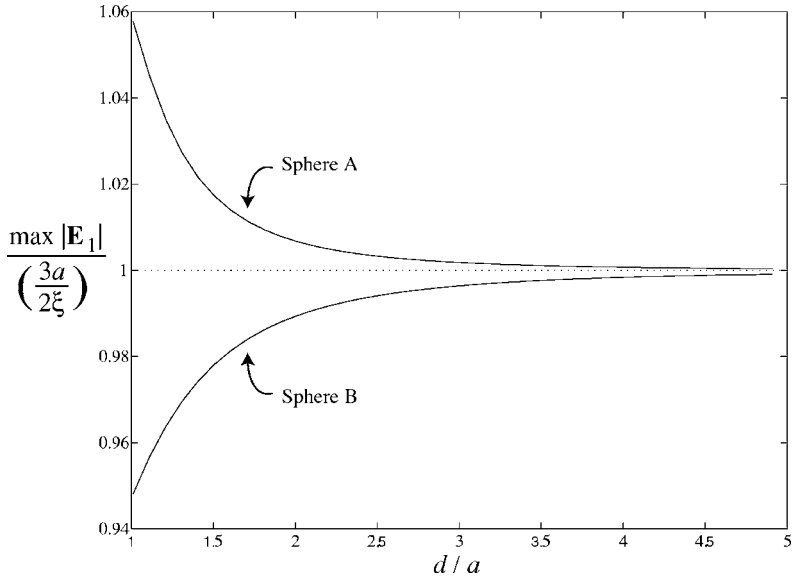

FIG. 4. Plots of the maximum magnitudes of the normalized electric fields inside cells A and B as functions of their normalized distance, d/a; $3a/2\xi$ is the electric field inside an isolated spherical cell of equal radius.

2. Touching spheres, $d \to a$

As mentioned above, a close examination of Eqs. (60) and (61) reveals that for fixed distance d the field magnitude attains its maximum at $\theta' = 0$ inside sphere A (as r' approaches a from left, $r' \to a^-$). A similar situation arises in fluid mechanics.[21] This maximum increases as d approaches a when the spheres tend to touch. In this case, $d \to a$, approximation (47) yields

$$\Phi_1 = -\frac{a}{\xi} z' - \frac{a}{2\xi} \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)^3} \left[\frac{r'}{a} T_m\left(\mp \frac{m}{m+1} \frac{r'}{a}, \theta' \right) \pm \frac{(m+1)^3}{(m+2)^3} \frac{r'}{a} T_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) + \frac{(m+1)^2}{(m+2)^2} S_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) \right]. \tag{65}$$

The corresponding electric field is derived by invoking

$$-\frac{\partial \Phi_1}{\partial r'} = \frac{a}{\xi} \cos\theta' + \frac{a}{2\xi} \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)^3} \left[V_m\left(\mp \frac{m}{m+1} \frac{r'}{a}, \theta' \right) \pm \frac{(m+1)^3}{(m+2)^3} V_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) \pm \frac{(m+1)^3}{(m+2)^3} T_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) \right], \tag{66}$$

and

$$\frac{1}{r'} \frac{\partial \Phi_1}{\partial \theta'} = \frac{a}{\xi} \sin\theta' + \frac{a}{2\xi} \sin\theta' \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)^3} \left[U_m\left(\mp \frac{m}{m+1} \frac{r'}{a}, \theta' \right) \pm \frac{(m+1)^3}{(m+2)^3} U_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) \pm \frac{(m+1)^3}{(m+2)^3} W_m\left(\mp \frac{m+1}{m+2} \frac{r'}{a}, \theta' \right) \right]. \tag{67}$$

It follows that for $d \to a$ the electric field in sphere A along the z axis becomes $\mathbf{E} = (a/\xi)\mathcal{E}_1(z')\mathbf{e}_z$, where $\mathcal{E}_1$ is the positive quantity

$$\mathcal{E}_1(z') = 1 + \frac{1}{2}\sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)^3}\left(1 - \frac{|z'|}{a}\frac{m}{m+1}\right)^{-2} + \frac{1}{2}\sum_{m=0}^{\infty} \frac{(-1)^m}{(m+2)^3}\left(1 - \frac{|z'|}{a}\frac{m+1}{m+2}\right)^{-2}$$
$$+ \frac{1}{2}\sum_{m=0}^{\infty} \frac{(-1)^m}{(m+2)^3}\left(1 - \frac{|z'|}{a}\frac{m+1}{m+2}\right)^{-1}. \tag{68}$$

Hence, $\mathcal{E}_1$ attains its maximum for $z'=a$,

$$\mathcal{E}_{1,\max} = 1 + \frac{1}{2}\sum_{m=0}^{\infty} (-1)^m\left(\frac{1}{m+1} + \frac{1}{m+2} + \frac{1}{(m+2)^2}\right) = 2 - \frac{\pi^2}{24} \approx 1.5888, \tag{69}$$

which is 6% higher than the corresponding value inside the isolated spherical cell of equal radius; compare with (31) of Sec. II.

IV. CONCLUSION

By use of perturbation theory we studied analytically a mathematical model for the scattering of extremely low frequency, uniform electric fields from cells of arbitrary shapes. Two main assumptions in our derivations were that the cell radius of curvature is a slowly varying function of surface coordinates and the cell interior is an isotropic and homogeneous medium. Our results for two spherical cells suggest that the presence of a neighboring cell causes only a small increase to the electric field inside a single cell of reasonably arbitrary shape.

Our analysis, based on suitable application of regular perturbations along with a reflection principle and exact solution of a nonlinear difference equation, can be extended to geometries of many cells but becomes increasingly cumbersome with the number of cells. In this case the solution for the electrostatic potential is obtained by solving a system of tractable difference equations. It is expected, however, that the presence of additional cells will cause only a minor increase in the induced electric field, being sufficiently bounded in the number of cells. This problem is subject of work in progress.

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APPENDIX A: REVISITING THE SINGLE SPHERICAL CELL

In this appendix we review the case with a uniform electric field incident on a single spherical cell, which is also studied in Refs. 2 and 4. The cell interior consists of two concentric spheres of radii a and b, where $b>a$. The effective dielectric constant in the regions $0<r<a$ and $r>b$ is taken to be 1 without loss of generality; the region $a<r<b$ corresponds to the cell membrane and has dielectric constant equal to the ϵ defined by (2). The real parameter ϵ expresses the *relative* dielectric constant for the two media, membrane and protoplasm, and is equal to the ratio of their conductivities, which enter the equations only through the homogeneous boundary conditions given in Eqs. (A5) and (A6) below. For an incident field $\mathbf{E}^{\text{inc}}=\mathbf{e}_z$ the scalar potential Φ at infinity is

$$\Phi(r,\theta) \sim -r\cos\theta, \quad r\to\infty, \tag{A1}$$

where (r,θ,ϕ) are the usual spherical coordinates. The boundary conditions at $r=a,b$ dictate continuity of Φ and $\epsilon(\partial\Phi/\partial r)$ across the spherical boundaries. The scalar potential Φ is thus independent of the azimuthal angle, ϕ, while it satisfies Laplace's equation in free space. With

$$\Phi(r,\theta) = f(r)\cos\theta, \tag{A2}$$

we obtain the equation

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{2}{r^2}\right)f(r)=0, \tag{A3}$$

with general solution $f(r)=Ar+Br^{-2}$. More precisely,

$$f(r)=\begin{cases} A_1 r, & r<a, \\ A_2 r+\dfrac{B_2}{r^2}, & a<r<b, \\ -r+\dfrac{B_3}{r^2}, & r>b, \end{cases} \tag{A4}$$

where the boundary condition (A1) has been used. In order to determine the constants A_1, A_2, B_2, and B_3 we apply the boundary conditions at $r=a$ and $r=b$, and thus obtain the equations

$$A_1 a=A_2 a+\frac{B_2}{a^2}, \quad A_1=\epsilon\left(A_2-\frac{2B_2}{a^3}\right), \tag{A5}$$

$$A_2 b+\frac{B_2}{b^2}=-b+\frac{B_3}{b^2}, \quad \epsilon\left(A_2-\frac{2B_2}{b^3}\right)=-1-\frac{2B_3}{b^3}. \tag{A6}$$

The electric field inside the cell is $-A_1\mathbf{e}_z$, where

$$-A_1=\frac{9\epsilon}{(1+2\epsilon)(2+\epsilon)-2(1-\epsilon)^2(a/b)^3}. \tag{A7}$$

Specifically, if ϵ is small and $a=b-\delta$, $\delta\ll a$, then

$$-A_1\sim\frac{1}{1+\dfrac{2}{3}\dfrac{\delta}{a\epsilon}}=\frac{1}{1+\dfrac{2\xi}{3a}}, \tag{A8}$$

where $\xi=\delta/\epsilon$. The right-hand side of the above equation is small if $\xi\gg a$, and can be expanded as a (convergent) geometric series for $3a/(2\xi)<1$. Specifically,

$$-A_1\sim\frac{3a}{2\xi}, \quad \frac{a}{\xi}\ll 1. \tag{A9}$$

APPENDIX B: REFLECTION PRINCIPLE WITH NEUMANN CONDITION

In this appendix (i) we derive a reflection principle, involving image dipoles, for the problem with a source dipole in the presence of a sphere with Neumann boundary conditions, extending the known analysis with a source charge and Dirichlet boundary conditions;[20] and (ii) we apply this principle to determine the potential Φ for the case with an insulating sphere and incident uniform electric field (cf. Appendix A).

We consider a $\mathbf{z}$-directed electric dipole of moment $\mathbf{p}=p\mathbf{e}_z$ located at $\mathbf{r}_0=(0,0,h)$ in the presence of a sphere with radius a centered at O. In units where $\epsilon_{\text{eff}}=1$, where ϵ_{eff} is the effective dielectric constant of the infinite medium, the ensuing scalar potential $\Phi(\mathbf{r};\mathbf{r}_0|\mathbf{p})$ satisfies the Poisson equation

$$\nabla^2\Phi=p\frac{\partial}{\partial z}\delta(\mathbf{r}-\mathbf{r}_0), \quad r>a, \tag{B1}$$

along with the prescribed Neumann boundary condition

$$\left.\frac{\partial\Phi}{\partial r}\right|_{r=a}=0, \tag{B2}$$

and $\Phi(\mathbf{r};\mathbf{r}_0|\mathbf{p})\to 0$ as $r\to\infty$. The potential Φ is thus determined uniquely in the region $r>a$. Recall that the potential generated by a dipole of moment $\mathbf{p}$ located at the origin is $\mathbf{p}\cdot\mathbf{r}/4\pi r^3$. We next express Φ for $r>a$ as a superposition of the (primary) potential Φ^{pr} generated by the source dipole at $\mathbf{r}_0$ in the absence of the sphere and the (scattered) potential Φ^{sc} of an image dipole with moment $\mathbf{p}'=\nu p\mathbf{e}_z$ at $\mathbf{r}_1=(0,0,h')$ where $h'<a$; ν and h' are to be determined.

Because of condition (B2) it is advantageous to work directly with the electric field $\mathbf{E}=-\nabla\Phi$. For $r>a$ and $|\mathbf{r}-\mathbf{r}_0|>0$,

$$\begin{aligned}\mathbf{E}(\mathbf{r})=\mathbf{E}^{\mathrm{pr}}(\mathbf{r})+\mathbf{E}^{\mathrm{sc}}(\mathbf{r})&=\frac{3[\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_0)](\mathbf{r}-\mathbf{r}_0)-(\mathbf{r}-\mathbf{r}_0)^2\mathbf{p}}{4\pi|\mathbf{r}-\mathbf{r}_0|^5}+\nu\frac{3[\mathbf{p}'\cdot(\mathbf{r}-\mathbf{r}_1)](\mathbf{r}-\mathbf{r}_1)-(\mathbf{r}-\mathbf{r}_1)^2\mathbf{p}'}{4\pi|\mathbf{r}-\mathbf{r}_1|^5}\\&=p\frac{3(r\cos\theta-h)(r\mathbf{e}_r-h\mathbf{e}_z)-(r^2+h^2-2rh\cos\theta)\mathbf{e}_z}{4\pi(r^2+h^2-2rh\cos\theta)^{5/2}}\\&\quad+\nu p\frac{3(r\cos\theta-h')(r\mathbf{e}_r-h'\mathbf{e}_z)-(r^2+h'^2-2rh'\cos\theta)\mathbf{e}_z}{4\pi(r^2+h'^2-2rh'\cos\theta)^{5/2}}.\end{aligned} \tag{B3}$$

Hence,

$$-\left.\frac{\partial\Phi(\mathbf{r})}{\partial r}\right|_{r=a}=p\frac{2(a^2+h^2)\cos\theta-ah(3+\cos^2\theta)}{4\pi(a^2+h^2-2ah\cos\theta)^{5/2}}+\nu p\frac{2(a^2+h'^2)\cos\theta-ah'(3+\cos^2\theta)}{4\pi(a^2+h'^2-2ah'\cos\theta)^{5/2}}. \tag{B4}$$

The substitution

$$\frac{h'}{a}=\frac{a}{h} \tag{B5}$$

yields $|\mathbf{r}-\mathbf{r}_1|=(a/h)|\mathbf{r}-\mathbf{r}_0|$ and reduces (B4) to

$$-\left.\frac{\partial\Phi(\mathbf{r})}{\partial r}\right|_{r=a}=p\left[1+\nu\left(\frac{h}{a}\right)^3\right]\frac{2(a^2+h^2)\cos\theta-ah(3+\cos^2\theta)}{4\pi(a^2+h^2-2ah\cos\theta)^{5/2}}. \tag{B6}$$

Condition (B2) is satisfied if

$$\nu=-\frac{a^3}{h^3}. \tag{B7}$$

This equation concludes the derivation of the reflection principle for a source dipole and Neumann boundary condition on a neighboring sphere.

Next, we apply this principle in order to derive the electrostatic potential for the case with an insulating sphere immersed in a uniform electric field, $E^{\mathrm{inc}}=E_0\mathbf{e}_z$; cf. Appendix A. This potential satisfies the Laplace equation and condition (B2), while the condition at infinity reads

$$\Phi(\mathbf{r})\sim -E_0 r\cos\theta \quad \text{as } r\to\infty. \tag{B8}$$

The uniform incident field is now viewed as the total field of two dipoles located at $(0,0,h)$ and $(0,0,-h)$ in the limit $h\to\infty$, where each dipole has moment $\mathbf{p}=p\mathbf{e}_z$.[22] The scalar potential due to these dipoles in the presence of the insulating sphere and for $r>a$ is

$$\Phi(\mathbf{r}) = \frac{p}{4\pi h^3}\Bigg[\frac{r\cos\theta - h}{\left(1 - \frac{2r}{h}\cos\theta + \frac{r^2}{h^2}\right)^{3/2}} - \frac{a^3}{r^3}\frac{r\cos\theta - \frac{a^2}{h}}{\left(1 - \frac{2a^2}{hr}\cos\theta + \frac{a^4}{r^2h^2}\right)^{3/2}} + \frac{r\cos\theta + h}{\left(1 + \frac{2r}{h}\cos\theta + \frac{r^2}{h^2}\right)^{3/2}}$$
$$- \frac{a^3}{r^3}\frac{r\cos\theta + \frac{a^2}{h}}{\left(1 + \frac{2a^2}{hr}\cos\theta + \frac{a^4}{r^2h^2}\right)^{3/2}}\Bigg] = -\frac{p}{\pi h^3}\left[r + \frac{a^3}{2r^2} + O\left(\frac{a^5}{r^5}\frac{a^2}{h^2}\right)\right]\cos\theta$$
$$\equiv -E_0\left(r + \frac{a^3}{2r^2}\right)\cos\theta, \quad h \to \infty, \tag{B9}$$

in view of (B8), where

$$p = \pi h^3 E_0, \quad h \to \infty. \tag{B10}$$

APPENDIX C: SOLUTION OF NONLINEAR DIFFERENCE EQUATION

In this appendix, the difference equation

$$x_n = \frac{\tilde{a}^2}{1 - x_{n-1}}, \quad n = 1,2,\ldots, \tag{C1}$$

where $0 < \tilde{a} \leqslant 1/2$ and $x_0 < 0$, is solved exactly. The solution is subsequently simplified for $|x_0| \ll 1$.

The substitution $x_n = \tilde{a}(y_n/y_{n+1})$ recasts (C1) to

$$y_n = \tilde{a}(y_{n+1} + y_{n-1}), \quad n = 1,2,\ldots. \tag{C2}$$

This equation is linear and can be solved via the replacement $y_n = \varrho^n$. The variable ϱ satisfies the equation $\tilde{a}\varrho^2 - \varrho + \tilde{a} = 0$ with solutions

$$\varrho = \varrho_\pm = \frac{1 \pm \sqrt{1 - 4\tilde{a}^2}}{2\tilde{a}}. \tag{C3}$$

Note that $\varrho_+\varrho_- = 1$ and $\varrho_+ + \varrho_- = 1/\tilde{a}$. It is inferred that $\varrho_+ \geqslant 1$ and $0 < \varrho_- \leqslant 1$. The solution to (C2) thus reads

$$y_n = c_1\varrho_+^n + c_2\varrho_-^n, \tag{C4}$$

where c_1 and c_2 are constants. Accordingly,

$$x_n = \tilde{a}\lambda\frac{\tilde{c}\lambda^{2n} - 1}{\tilde{c}\lambda^{2(n+1)} - 1}, \quad \lambda = \varrho_+, \quad \tilde{c} = -\frac{c_1}{c_2}. \tag{C5}$$

It follows that

$$\tilde{c} = \frac{\tilde{a} + \lambda^{-1}|x_0|}{\tilde{a} + \lambda|x_0|}, \quad 0 < \tilde{c} < 1. \tag{C6}$$

Let

$$\tilde{c} = e^{-2\zeta}, \quad \lambda = e^{\kappa}, \quad \zeta > 0, \quad \kappa > 0. \tag{C7}$$

Equation (C5) then becomes

$$x_n = \tilde{a}\frac{\sinh(n\kappa - \zeta)}{\sinh[(n+1)\kappa - \zeta]}, \quad n = 0,1,2,\ldots . \tag{C8}$$

It remains to derive an approximation for x_n when $\tilde{a}^{-1}|x_0| \ll 1$. From (C6),

$$\tilde{c} \sim (1 - \tilde{a}^{-1}\lambda^{-1}x_0)(1 + \tilde{a}^{-1}\lambda x_0) \sim 1 + (1 - \lambda^{-2})\tilde{a}^{-1}\lambda x_0, \tag{C9}$$

which in turn leads to

$$x_n \sim \tilde{a}\frac{[1 - (1 - e^{-2\kappa})\tilde{a}^{-1}\lambda|x_0|]e^{n\kappa} - e^{-n\kappa}}{[1 - (1 - e^{-2\kappa})\tilde{a}^{-1}\lambda|x_0|]e^{(n+1)\kappa} - e^{-(n+1)\kappa}} \sim \tilde{a}\frac{\sinh n\kappa}{\sinh(n+1)\kappa}\left(1 - e^{n\kappa}\frac{\sinh\kappa}{\sinh n\kappa}\tilde{a}^{-1}|x_0|\right)$$
$$\times\left[1 + \tilde{a}^{-1}|x_0|e^{(n+1)\kappa}\frac{\sinh\kappa}{\sinh(n+1)\kappa}\right] \sim \tilde{a}\frac{\sinh n\kappa}{\sinh(n+1)\kappa} - \left[\frac{\sinh\kappa}{\sinh(n+1)\kappa}\right]^2|x_0|. \tag{C10}$$

This expression becomes a trivial equality for $n=0$. Note that the coefficient of the correction term $O(x_0)$ is bounded uniformly with n.

APPENDIX D: ELEMENTARY EXPANSION IN LEGENDRE POLYNOMIALS

It is known that[23]

$$(1 + 2\beta x + \beta^2)^{-1/2} = \sum_{l=0}^{\infty}(-1)^l \mathrm{P}_l(x)\begin{cases}\beta^l, & |\beta| < 1,\\ \beta^{-l-1}, & |\beta| > 1,\end{cases} \tag{D1}$$

where $x = \cos\theta$ and $\mathrm{P}_l(x)$ are Legendre polynomials. It follows by differentiation that

$$\frac{x+\beta}{(1 + 2\beta x + \beta^2)^{3/2}} = \sum_{l=0}^{\infty}(-1)^l \mathrm{P}_l(x)\begin{cases}(-l)\beta^{l-1},\\ (l+1)\beta^{-l-2},\end{cases} \tag{D2}$$

for $|\beta| < 1$ or $|\beta| > 1$, respectively.

The term-by-term integration of (D1) yields

$$\sum_{l=1}^{\infty}\frac{\beta^l}{l}\mathrm{P}_l(x) = \int_0^{\beta}\frac{\mathrm{d}t}{t}\left(\frac{1}{\sqrt{1 - 2tx + t^2}} - 1\right), \tag{D3}$$

where $|\beta| < 1$. This integral is elementary; by changing the variable to w according to $t - x = \sqrt{1 - x^2}\sinh w$ we find

$$\sum_{l=1}^{\infty}\frac{\beta^l}{l}\mathrm{P}_l(x) = \ln\left|\frac{2}{1-x^2}\frac{1}{\beta}\frac{\beta - x + x\sqrt{1 - 2\beta x + \beta^2}}{1 + \sqrt{1 - 2\beta x + \beta^2}}\right|. \tag{D4}$$

In the limit $x \to 1^-$ the right-hand side of this formula approaches $-\ln(1-\beta)$, as it should.

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[15] As mentioned in the Introduction, elongated cells may be excluded from our analysis.
[16] The issue of convergence of this expansion is not addressed in this paper. It is expected that the expansion converges for sufficiently small r_c/ξ.
[17] The perturbation order n (subscript in expansion terms) should not be confused with the index j in $\mathcal{R}_j$, $\partial\mathcal{R}_j$ and other symbols of this section; j specifies individual cells.
[18] $A=O(x_1,x_2,\ldots,x_N)$ as $\mathbf{x}=(x_1,x_2,\ldots,x_N)\to 0$ means that $\lim_{\mathbf{x}\to 0}(A/x_k)=O(1)$ if $x_j/x_k=O(1)$ for all $j,k=1,2,\ldots,N$.
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On spatial and material covariant balance laws in elasticity

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This paper presents some developments related to the idea of covariance in elasticity. The geometric point of view in continuum mechanics is briefly reviewed. Building on this, regarding the reference configuration and the ambient space as Riemannian manifolds with their own metrics, a Lagrangian field theory of elastic bodies with evolving reference configurations is developed. It is shown that even in this general setting, the Euler-Lagrange equations resulting from horizontal (referential) variations are equivalent to those resulting from vertical (spatial) variations. The classical Green-Naghdi-Rivilin theorem is revisited and a material version of it is discussed. It is shown that energy balance, in general, cannot be invariant under isometries of the reference configuration, which in this case is identified with a subset of $\mathbb{R}^3$. Transformation properties of balance of energy under rigid translations and rotations of the reference configuration is obtained. The spatial covariant theory of elasticity is also revisited. The transformation of balance of energy under an arbitrary diffeomorphism of the reference configuration is obtained and it is shown that some nonstandard terms appear in the transformed balance of energy. Then conditions under which energy balance is materially covariant are obtained. It is seen that material covariance of energy balance is equivalent to conservation of mass, isotropy, material Doyle-Ericksen formula and an extra condition that we call configurational inviscidity. In the last part of the paper, the connection between Noether's theorem and covariance is investigated. It is shown that the Doyle-Ericksen formula can be obtained as a consequence of spatial covariance of Lagrangian density. Similarly, it is shown that the material Doyle-Ericksen formula can be obtained from material covariance of Lagrangian density. [DOI: 10.1063/1.2190827]

I. INTRODUCTION

Invariance plays an important role in mechanics and in physics. In any continuum theory one has some conservation laws; i.e., quantities that are constant in time, such as mass and energy or balance laws, such as balance of linear and angular momentum. One way of building a continuum theory is to postulate these conservation or balance laws. On the other hand, as we shall recall later, conservation laws and even balance laws can be obtained as a result of postulating invariance of a quantity such as energy or Lagrangian density, under some group of transformations.

Traditionally, continuum mechanics is developed using Euclidean space as the ambient space. This has been motivated by the engineering applications of continuum mechanics and the general tendency of the engineering community to work with the simplest possible spaces. This is of

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course useful and the implicit simplifying assumptions of continuum mechanics have made it applicable to many problems of practical importance. However, being restricted to the misleading and rigid structure of Euclidean space, one should expect to lose important geometric information. For example, for many years there were debates on different stress rates and whether one stress rate is "more objective" than the other one. Putting continuum mechanics in the right geometric setting, one can clearly see that different stress rates in the literature are simply different representations of the same Lie derivative.[28]

Another basic example of the lack of geometry in the traditional formulation of continuum mechanics is the dependence of the well-known balance of linear and angular momenta on the linear structure of Euclidean space. These laws are written in terms of integrals of some vector fields. Of course, integrating a vector field has no intrinsic meaning and is dependent on a linear structure or a specific coordinate choice. One can argue that a geometric point of view has proven useful in, for example, building systematic numerical schemes as well as in bridging length and time scales. For example, geometry has proven useful in Refs. 25, 6, and 3, although much remains to be done in the future.

Following Einstein's idea that physical laws should not depend on any particular choice of coordinate representation of ambient spaces, Marsden and Hughes[28] developed a covariant theory of elasticity building on ideas originated from the work of Naghdi, Green and Rivilin.[19] This work starts from balance of energy, which makes sense intrinsically as it is written in terms of integrals of scalar fields (or more precisely 3-forms). Then they postulate that balance of energy is invariant under arbitrary diffeomorphisms of the ambient space. They observe that this invariance assumption gives all the usual balance laws *plus* the Doyle-Ericksen formula that relates the stress and the metric tensor.

Our motivation for studying spatial and material covariant balance laws was to gain a better understanding of the geometry of configurational forces, which are forces that act in the reference configuration. One may ask the following question. What are the consequences of postulating that balance of energy is *materially* covariant? In the process of answering this question we discovered that such invariance cannot hold in general and this led us to obtain formulas for the way in which balance of energy transforms under material diffeomorphisms. In this paper we also study the connection between spatial and material covariance with Noether's theorem. It will be shown that spatial and material covariance of a Lagrangian density lead to the spatial and material forms of the Doyle-Ericksen formula, respectively.

As was mentioned, one of our motivations for this study was to initiate a geometric study of configurational forces. These forces and their balance laws are important in formulating the evolution of defects in solids in the setting of continuum mechanics. Driving (configurational, material and so forth) forces in continuum mechanics were introduced by Eshelby,[13–15] and many researchers have studied them from different points of view. We mention the work of Knowles,[22] Abeyaratneh and Knowles[1,2] on driving force on a phase interface, Gurtin's work[20,21] on configurational forces by postulating new balance laws, the work of Maugin[31,32] and Maugin and Trimarco[33] on pull-back of balance of standard linear momentum to the reference configuration, etc. However, even after more than five decades after Eshelby's original work there does not seem to be a consensus on the nature of configurational forces and their exact role in continuum mechanics and there are still some controversies in the literature. We believe that the geometric ideas in this paper may be helpful in this direction.

This paper is organized as follows. The geometry of continuum mechanics is reviewed in Sec. II. The Lagrangian field theory of elastic bodies with evolving reference configurations is presented in Sec. III, where deformed bodies and their reference configurations are treated as Riemannian manifolds. Using this setting, the classical Green-Naghdi-Rivilin theorem and a new material version of it are discussed in Sec. IV. Spatial covariant energy balance is revisited in Sec. V. In Sec. VI we obtain the transformation (push-forward) of energy balance under an arbitrary material diffeomorphism. Then, we investigate the consequences of material covariance of energy balance. Section VII studies the connection between covariance and Noether's theorem. It is

shown that spatial and material covariance of a Lagrangian density result in spatial and material versions of the Doyle-Ericksen formula, respectively. Conclusions and future directions are given in Sec. VIII.

II. GEOMETRY OF CONTINUUM MECHANICS

This section recalls some notation from the geometric approach to continuum mechanics that will be needed. It is assumed that the reader is familiar with the basic ideas; refer to, for example, Marsden and Hughes[28] for details. See also Refs. 30 and 29.

If M is a smooth n-manifold, the tangent space to M at a point $p \in M$ is denoted T_pM, while the whole tangent bundle is denoted TM.

We denote by $\mathfrak{B}$ a reference manifold for our body and by $\mathcal{S}$ the space in which the body moves. We assume that $\mathfrak{B}$ and $\mathcal{S}$ are Riemannian manifolds with metrics denoted by $\mathbf{G}$ and $\mathbf{g}$, respectively. Local coordinates on $\mathfrak{B}$ are denoted by X^I and those on $\mathcal{S}$ by x^i. The material body $\mathcal{B}$ is a subset of the material manifold, i.e., $\mathcal{B} \subset \mathfrak{B}$.

A *deformation* of the body is, for purposes of this paper, a C^1 embedding $\varphi: \mathcal{B} \to \mathcal{S}$. The tangent map of φ is denoted $\mathbf{F} = T\varphi: T\mathcal{B} \to T\mathcal{S}$; in the literature it is often called the deformation gradient. In local charts on $\mathcal{B}$ and $\mathcal{S}$, the tangent map of φ is given by the Jacobian matrix of partial derivatives of the components of φ, which we write as

$$\mathbf{F} = T\varphi: T\mathcal{B} \to T\mathcal{S}, \quad T\varphi(X, \mathbf{V}) = (\varphi(X), \mathbf{D}\varphi(X) \cdot \mathbf{V}). \tag{2.1}$$

If $F: \mathcal{B} \to \mathbb{R}$ is a C^1 scalar function, $X \in \mathcal{B}$ and $\mathbf{V}_X \in T_X\mathcal{B}$, then $\mathbf{V}_X[F]$ denotes the derivative of F at X in the direction of $\mathbf{V}_X$, i.e., $\mathbf{V}_X[F] = \mathbf{D}F(X) \cdot \mathbf{V}$. In local coordinates $\{X^I\}$ on $\mathcal{B}$,

$$\mathbf{V}_X[F] = \frac{\partial F}{\partial X^I} V^I. \tag{2.2}$$

For $f: \mathcal{S} \to \mathbb{R}$, the *pull-back* of f by φ is defined by

$$\varphi^* f = f \circ \varphi. \tag{2.3}$$

If $F: \mathcal{B} \to \mathbb{R}$, the *push-forward* of F by φ is defined by

$$\varphi_* F = F \circ \varphi^{-1}. \tag{2.4}$$

If $\mathbf{Y}$ is a vector field on $\mathcal{B}$, then $\varphi_* \mathbf{Y} = T\varphi \circ \mathbf{Y} \circ \varphi^{-1}$, or using the $\mathbf{F}$ notation, $\varphi_* \mathbf{Y} = \mathbf{F} \circ \mathbf{Y} \circ \varphi^{-1}$ is a vector field on $\varphi(\mathcal{B})$ called the *push-forward* of $\mathbf{Y}$ by φ. Similarly, if $\mathbf{y}$ is a vector field on $\varphi(\mathcal{B}) \subset \mathcal{S}$, then $\varphi^* \mathbf{y} = T(\varphi^{-1}) \circ \mathbf{y} \circ \varphi$ is a vector field on $\mathcal{B}$ and is called the pull-back of $\mathbf{y}$ by φ.

The cotangent bundle of a manifold M is denoted T^*M and the fiber at a point $p \in M$ (the vector space of one-forms at p) is denoted by T_p^*M. If β is a one form on $\mathcal{S}$ (that is, a section of the cotangent bundle $T^*\mathcal{S}$), then the one-form on $\mathcal{B}$ defined as

$$(\varphi^* \beta)_X \cdot \mathbf{V}_X = \beta_{\varphi(X)} \cdot (T\varphi \cdot \mathbf{V}_X) = \beta_{\varphi(X)} \cdot (\mathbf{F} \cdot \mathbf{V}_X) \tag{2.5}$$

for $X \in \mathcal{B}$ and $\mathbf{V}_X \in T_X\mathcal{B}$, is called the *pull-back* of β by φ. Likewise, the *push-forward* of a one-form α on $\mathcal{B}$ is the one form on $\varphi(\mathcal{B})$ defined by $\varphi_* \alpha = (\varphi^{-1})^* \alpha$.

We can associate a vector field $\beta^\sharp$ to a one-form β on a Riemannian manifold M through the equation

$$\langle \beta_x, \mathbf{v}_x \rangle = \langle\langle \beta_x^\sharp, \mathbf{v}_x \rangle\rangle_x, \tag{2.6}$$

where $\langle , \rangle$ denotes the natural pairing between the one-form $\beta_x \in T_x^*M$ and the vector $\mathbf{v}_x \in T_xM$ and where $\langle\langle \beta_x^\sharp, \mathbf{v}_x \rangle\rangle_x$ denotes the inner product between $\beta_x^\sharp \in T_xM$ and $\mathbf{v}_x \in T_xM$. In coordinates, the components of $\beta^\sharp$ are given by $\beta^i = g^{ij}\beta_i$.

Traditionally force is thought of as a vector field in the deformed configuration. For example, body force $\mathbf{B}$ per unit undeformed mass is a vector field on $\mathcal{S}$ and its associated one-form can be defined as

$$\langle \beta_x, \delta\mathbf{w}\rangle = \langle\langle \mathbf{B}, \delta\mathbf{w}\rangle\rangle_x \tag{2.7}$$

for all $\delta\mathbf{w} \in T_x\mathcal{S}$. The pull-back of β is defined as

$$\langle (\varphi^* \beta)_X, \delta\mathbf{W}\rangle_X = \langle \beta_x, \mathbf{F}\,\delta\mathbf{W}\rangle_X = \langle\langle \mathbf{B}, \mathbf{F}\,\delta\mathbf{W}_X\rangle\rangle_X = \langle\langle \mathbf{F}^{\mathsf{T}}\mathbf{B}, \delta\mathbf{W}_X\rangle\rangle_X. \tag{2.8}$$

Therefore $\mathbf{F}^{\mathsf{T}}\mathbf{B}$ is the vector field associated with the pull-back of the one-form associated with $\mathbf{B}$.

A type $\binom{p}{q}$-tensor at $X \in \mathcal{B}$ is a multilinear map,

$$\mathbf{T}: \underbrace{T_X^*\mathcal{B} \times \cdots \times T_X^*\mathcal{B}}_{p \text{ copies}} \times \underbrace{T_X\mathcal{B} \times \cdots \times T_X\mathcal{B}}_{q \text{ copies}} \to \mathbb{R}. \tag{2.9}$$

$\mathbf{T}$ is said to be contravariant of order p and covariant of order q. In a local coordinate chart,

$$\mathbf{T}(\alpha^1, \ldots, \alpha^p, \mathbf{V}_1, \ldots, \mathbf{V}_q) = T^{i_1\cdots i_p}{}_{j_1\cdots j_q}\alpha^1_{i_1}\cdots\alpha^p_{i_p}V^{j_1}_1\cdots V^{j_q}_q, \tag{2.10}$$

where $\alpha^k \in T_X^*\mathcal{B}$ and $\mathbf{V}^k \in T_X\mathcal{B}$.

Suppose $\varphi: \mathcal{B} \to \mathcal{S}$ is a regular map and $\mathbf{T}$ is a tensor of type $\binom{p}{q}$. Push-forward of $\mathbf{T}$ by φ is denoted $\varphi_*\mathbf{T}$ and is a $\binom{p}{q}$-tensor on $\varphi(\mathcal{B})$ defined by

$$(\varphi_*\mathbf{T})(x)(\alpha^1, \ldots, \alpha^p, \mathbf{v}_1, \ldots, \mathbf{v}_q) = \mathbf{T}(X)(\varphi^*\alpha^1, \ldots, \varphi^*\alpha^p, \varphi^*\mathbf{v}_1, \ldots, \varphi^*\mathbf{v}_q), \tag{2.11}$$

where $\alpha^k \in T_x^*\mathcal{S}, \mathbf{v}_k \in T_x\mathcal{S}, X = \varphi^{-1}(x), \varphi^*(\alpha^k)\cdot\mathbf{v}_l = \alpha^k\cdot(T\varphi\cdot\mathbf{v}_l)$ and $\varphi^*(\mathbf{v}_l) = T(\varphi^{-1})\mathbf{v}_l$. Similarly, pull-back of a tensor $\mathbf{t}$ defined on $\varphi(\mathcal{B})$ is given by $\varphi^*\mathbf{t} = (\varphi^{-1})_*\mathbf{t}$. In the setting of continuum mechanics push-forward and pull-back of tensors will have the following forms:

$$(\varphi_*\mathbf{T})^{i_1\cdots i_p}{}_{j_1\cdots j_q}(x) = F^{i_1}{}_{I_1}(X)\cdots F^{i_p}{}_{I_p}(X)T^{I_1\cdots I_p}{}_{J_1\cdots J_q}(F^{-1})^{J_1}{}_{j_1}(x)\cdots(F^{-1})^{J_q}{}_{j_q}(x),$$

$$(\varphi^*\mathbf{t})^{I_1\cdots I_p}{}_{J_1\cdots J_q}(X) = (F^{-1})^{I_1}{}_{i_1}(x)\cdots(F^{-1})^{I_p}{}_{i_p}(x)t^{i_1\cdots i_p}{}_{j_1\cdots j_q}F^{j_1}{}_{J_1}(X)\cdots F^{j_q}{}_{J_q}(X).$$

A *two-point tensor* $\mathbf{T}$ of type $\begin{pmatrix} q & q' \\ p & p' \end{pmatrix}$ at $X \in \mathcal{B}$ over a map $\varphi: \mathcal{B} \to \mathcal{S}$ is a multilinear map,

$$T: \underbrace{T_X^*\mathcal{B} \times \cdots \times T_X^*\mathcal{B}}_{p \text{ copies}} \times \underbrace{T_X\mathcal{B} \times \cdots \times T_X\mathcal{B}}_{q \text{ copies}} \times \underbrace{T_x^*\mathcal{S} \times \cdots \times T_x^*\mathcal{S}}_{p \text{ copies}} \times \underbrace{T_x\mathcal{S} \times \cdots \times T_x\mathcal{S}}_{q \text{ copies}} \to \mathbb{R}, \tag{2.12}$$

where $x = \varphi(X)$.

Let $\mathbf{w}: \mathcal{U} \to T\mathcal{S}$ be a vector field, where $\mathcal{U} \subset \mathcal{S}$ is open. A curve $\mathbf{c}: I \to \mathcal{S}$, where I is an open interval, is an *integral curve* of $\mathbf{w}$ if

$$\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t}(r) = \mathbf{w}(\mathbf{c}(r)) \quad \forall\, r \in I. \tag{2.13}$$

If $\mathbf{w}$ depends on time variable explicitly, i.e., $\mathbf{w}: \mathcal{U} \times (-\varepsilon, \varepsilon) \to T\mathcal{S}$, an integral curve is defined by

$$\frac{\mathrm{d}\mathbf{c}}{\mathrm{d}t} = \mathbf{w}(\mathbf{c}(t), t). \tag{2.14}$$

Let $\mathbf{w}:\mathcal{S}\times I\to T\mathcal{S}$ be a vector field. The collection of maps $F_{t,s}$ such that for each s and x, $t\mapsto F_{t,s}(x)$ is an integral curve of $\mathbf{w}$ and $F_{s,s}(x)=x$ is called the flow of $\mathbf{w}$. Let $\mathbf{w}$ be a C^1 vector field on $\mathcal{S}$, $F_{t,s}$ its flow, and $\mathbf{t}$ a C^1 tensor field on $\mathcal{S}$. The *Lie derivative* of $\mathbf{t}$ with respect to $\mathbf{w}$ is defined by

$$\mathbf{L}_{\mathbf{w}}\mathbf{t} = \left.\frac{d}{dt}(F_{t,s}^{*}\mathbf{t})\right|_{t=s}. \tag{2.15}$$

If we hold t fixed in $\mathbf{t}$ then we denote

$$\pounds_{\mathbf{w}}\mathbf{t} = \left.\frac{d}{dt}(F_{t,s}^{*}\mathbf{t})\right|_{t=s}, \tag{2.16}$$

which is called the *autonomous Lie derivative*. Hence

$$\mathbf{L}_{\mathbf{w}}\mathbf{t} = \frac{\partial}{\partial t}\mathbf{t} + \mathfrak{L}_{\mathbf{w}}\mathbf{t}. \tag{2.17}$$

Let $\mathbf{v}$ be a vector field on $\mathcal{S}$ and $\varphi:\mathcal{B}\to\mathcal{S}$ a regular and orientation preserving C^1 map. The *Piola transform* of $\mathbf{v}$ is

$$\mathbf{V} = J\varphi^{*}\mathbf{v}, \tag{2.18}$$

where J is the Jacobian of φ. If $\mathbf{Y}$ is the Piola transform of $\mathbf{y}$, then the *Piola identity* holds,

$$\operatorname{Div}\mathbf{Y} = J(\operatorname{div}\mathbf{y})\circ\varphi. \tag{2.19}$$

A k-form on a manifold M is a skew-symmetric $\binom{0}{k}$-tensor. The space of k-forms on M is denoted $\Omega^k(M)$. If $\varphi:M\to N$ is a regular and orientation preserving C^1 map and $\alpha\in\Omega^k(\varphi(M))$, then

$$\int_{\varphi(M)}\boldsymbol{\alpha} = \int_{M}\varphi^{*}\boldsymbol{\alpha}. \tag{2.20}$$

Geometric continuum mechanics: We next review a few of the basic notions of continuum mechanics from the geometric point of view.

A *body* $\mathcal{B}$ is a submanifold of a Riemannian manifold $\mathfrak{B}$ and a *configuration* of $\mathcal{B}$ is a mapping $\varphi:\mathcal{B}\to\mathcal{S}$, where $\mathcal{S}$ is another Riemannian manifold. The set of all configurations of $\mathcal{B}$ is denoted $\mathcal{C}$. A *motion* is a curve $c:\mathbb{R}\to\mathcal{C};t\mapsto\varphi_t$ in $\mathcal{C}$.

For a fixed t, $\varphi_t(X)=\varphi(X,t)$ and for a fixed X, $\varphi_X(t)=\varphi(X,t)$, where X is position of material points in the undeformed configuration $\mathcal{B}$. The *material velocity* is the map $\mathbf{V}_t:\mathcal{B}\to\mathbb{R}^3$ given by

$$\mathbf{V}_t(X) = \mathbf{V}(X,t) = \frac{\partial\varphi(X,t)}{\partial t} = \frac{d}{dt}\varphi_X(t). \tag{2.21}$$

Similarly, the *material acceleration* is defined by

$$\mathbf{A}_t(X) = \mathbf{A}(X,t) = \frac{\partial\mathbf{V}(\mathbf{X},t)}{\partial t} = \frac{d}{dt}\mathbf{V}_X(t). \tag{2.22}$$

In components

$$A^a = \frac{\partial V^a}{\partial t} + \gamma^a_{bc}V^bV^c, \tag{2.23}$$

where γ^a_{bc} is the Christoffel symbol of the local coordinate chart $\{x^a\}$.

Here it is assumed that φ_t is invertible and regular. The *spatial velocity* of a regular motion φ_t is defined as

$$\mathbf{v}_t:\varphi_t(\mathcal{B}) \to \mathbb{R}^3, \quad \mathbf{v}_t = \mathbf{V}_t \circ \varphi_t^{-1}, \tag{2.24}$$

and the *spatial acceleration* $\mathbf{a}_t$ is defined as

$$\mathbf{a} = \dot{\mathbf{v}} = \frac{\partial \mathbf{v}}{\partial t} + \nabla_{\mathbf{v}}\mathbf{v}. \tag{2.25}$$

In components

$$a^a = \frac{\partial v^a}{\partial t} + \frac{\partial v^a}{\partial x^b}v^b + \gamma^a_{bc}v^b v^c. \tag{2.26}$$

Let $\varphi:\mathcal{B}\to\mathcal{S}$ be a C^1 configuration of $\mathcal{B}$ in $\mathcal{S}$, where $\mathcal{B}$ and $\mathcal{S}$ are manifolds. Recall that the deformation gradient is denoted $\mathbf{F}=T\varphi$. Thus, at each point $X\in\mathcal{B}$, it is a linear map

$$\mathbf{F}(X):T_X\mathcal{B} \to T_{\varphi(X)}\mathcal{S}. \tag{2.27}$$

If $\{x^i\}$ and $\{X^I\}$ are local coordinate charts on $\mathcal{S}$ and $\mathcal{B}$, respectively, the components of $\mathbf{F}$ are

$$F^i{}_J(X) = \frac{\partial \varphi^i}{\partial X^J}(X). \tag{2.28}$$

The deformation gradient may be viewed as a two-point tensor,

$$\mathbf{F}(X):T^*_x\mathcal{S} \times T_X\mathcal{B} \to \mathbb{R}; \quad (\alpha,\mathbf{V}) \mapsto \langle \alpha, T_X\varphi \cdot \mathbf{V}\rangle. \tag{2.29}$$

Suppose $\mathcal{B}$ and $\mathcal{S}$ are Riemannian manifolds with inner products $\langle\langle,\rangle\rangle_X$ and $\langle\langle,\rangle\rangle_x$ based at $X\in\mathcal{B}$ and $x\in\mathcal{S}$, respectively.

Recall that the transpose of $\mathbf{F}$ is defined by

$$\mathbf{F}^{\mathsf{T}}:T_x\mathcal{S} \to T_X\mathcal{B}, \quad \langle\langle \mathbf{F}\mathbf{V},\mathbf{v}\rangle\rangle_x = \langle\langle \mathbf{V},\mathbf{F}^{\mathsf{T}}\mathbf{v}\rangle\rangle_X \tag{2.30}$$

for all $\mathbf{V}\in T_X\mathcal{B}, \mathbf{v}\in T_x\mathcal{S}$. In components,

$$(F^{\mathsf{T}}(X))^J{}_i = g_{ij}(x)F^j{}_K(X)G^{JK}(X), \tag{2.31}$$

where $\mathbf{g}$ and $\mathbf{G}$ are metric tensors on $\mathcal{S}$ and $\mathcal{B}$, respectively. On the other hand, the *dual* of $\mathbf{F}$, a metric independent notion, is defined by

$$\mathbf{F}*(x):T^*_x\mathcal{S} \to T^*_X\mathcal{B}; \quad \langle \mathbf{F}^*(x)\cdot\alpha,\mathbf{W}\rangle = \langle \alpha,\mathbf{F}(X)\mathbf{W}\rangle \tag{2.32}$$

for all $\alpha\in T^*_x\mathcal{S}, \mathbf{W}\in T_X\mathcal{B}$.

Considering bases $\mathbf{e}_a$ and $\mathbf{E}_A$ for $\mathcal{S}$ and $\mathcal{B}$, respectively, one can define the corresponding dual bases $\mathbf{e}^a$ and $\mathbf{E}^A$. The matrix representation of $\mathbf{F}^*$ with respect to the dual bases is the transpose of $F^a{}_A$. $\mathbf{F}$ and $\mathbf{F}^*$ have the following local representations:

$$\mathbf{F} = F^j{}_K\frac{\partial}{\partial x^j}\otimes \mathrm{d}X^K, \quad \mathbf{F}^* = F^j{}_K\,\mathrm{d}X^K \otimes \frac{\partial}{\partial x^j}. \tag{2.33}$$

The *right Cauchy-Green deformation tensor* is defined by

$$\mathbf{C}(X):T_X\mathcal{B} \to T_X\mathcal{B}, \quad \mathbf{C}(X) = \mathbf{F}(X)^T\mathbf{F}(X). \tag{2.34}$$

In components,

$$C^I{}_J = (F^T)^I{}_k F^k{}_J. \tag{2.35}$$

It is straightforward to show that

$$\mathbf{C}^\flat = \varphi^*(\mathbf{g}), \quad \text{i . e . , } C_{IJ} = (g_{ij} \circ \varphi) F^i{}_I F^j{}_J. \tag{2.36}$$

From now on, by $\mathbf{C}$ we mean the tensor with components C_{IJ}. The Finger tensor is defined as $\mathbf{b} = \varphi_{t*}\mathbf{G}$, where $\mathbf{G}$ is the metric of the reference configuration.

To make ideas more concrete, a comment is in order. In the geometric treatment of continuum mechanics one assumes that the material body is a Riemannian manifold $(\mathcal{B}, \mathbf{G})$. Here $\mathcal{B}$ is an embedding of the material body, i.e., material points are identified with their positions in the reference configuration. A deformation of the material body is represented by a mapping $\varphi: \mathcal{B} \to \mathcal{S}$, where $(\mathcal{S}, \mathbf{g})$ is the ambient space, which is another Riemannian manifold. If $\varphi = \mathrm{Id}$, the reference configuration is a trivial embedding of the material body in the ambient space. Physically, in the deformation process the relative distance of material points change in general. In other words, in terms of material points $\mathbf{X}, \mathbf{X} + d\mathbf{X}$ and their positions in the deformed configuration $\mathbf{x}, \mathbf{x} + d\mathbf{x}$ we have

$$d\mathbf{x} \cdot d\mathbf{x} = \mathbf{C}\, d\mathbf{X} \cdot d\mathbf{X} \neq d\mathbf{X} \cdot d\mathbf{X}. \tag{2.37}$$

This means that in general

$$\mathbf{g} \neq \varphi_{t*}\mathbf{G}. \tag{2.38}$$

The following identities will be used frequently in this paper.

$$\frac{\partial g_{ab}}{\partial x^c} = g_{ad}\gamma^d_{bc} + g_{bd}\gamma^d_{ac}, \tag{2.39}$$

$$\frac{\partial G_{AB}}{\partial X^C} = G_{AD}\Gamma^D_{BC} + G_{BD}\Gamma^D_{AC}, \tag{2.40}$$

where γ^d_{bc} and Γ^D_{BC} are the Christoffel symbols associated to the metric tensors $\mathbf{g}$ and $\mathbf{G}$, respectively. The covariant derivative of two-point tensors will also be used frequently in this paper. The following two examples would be useful to clarify the idea. For definition for an arbitrary two-point tensor the reader may refer to Marsden and Hughes,[28]

$$P^{aA}{}_{|B} = \frac{\partial P^{aA}}{\partial X^B} + P^{aC}\Gamma^A_{CB} + P^{bA}F^c{}_A\gamma^a_{bc}, \tag{2.41}$$

$$Q_a{}^A{}_{|B} = \frac{\partial Q_a{}^A}{\partial X^B} + Q_a{}^C\Gamma^A_{CB} - Q_b{}^A F^c{}_A\gamma^b_{ca}. \tag{2.42}$$

Let $\varphi_t: \mathcal{B} \to \mathcal{S}$ be a regular motion of $\mathcal{B}$ in $\mathcal{S}$ and $\mathcal{P} \subset \mathcal{B}$ a k-dimensional submanifold. The *transport theorem* says that for any k-form α on $\mathcal{S}$,

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{P})} \alpha = \int_{\varphi_t(\mathcal{P})} \mathbf{L}_\mathbf{v}\alpha, \tag{2.43}$$

where $\mathbf{v}$ is the spatial velocity of the motion. In a special case when $\alpha = f\, dv$ and $\mathcal{P} = \mathcal{U}$ is an open set,

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{P})} f\, dv = \int_{\varphi_t(\mathcal{P})} \left[\frac{\partial f}{\partial t} + \mathrm{div}(f\mathbf{v})\right] dv. \tag{2.44}$$

We say that a body $\mathcal{B}$ satisfies *balance of linear momentum* if for every nice open set $\mathcal{U} \subset \mathcal{B}$,

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})} \rho\mathbf{v}\, dv = \int_{\varphi_t(\mathcal{U})} \rho\mathbf{b}\, dv + \int_{\partial\varphi_t(\mathcal{U})} \mathbf{t}\, da, \tag{2.45}$$

where $\rho=\rho(\mathbf{x},t)$ is mass density, $\mathbf{b}=\mathbf{b}(\mathbf{x},t)$ is body force vector field and $\mathbf{t}=\mathbf{t}(\mathbf{x},\hat{\mathbf{n}},t)$ is the traction vector. Note that Cauchy's stress theorem tells us that there is a contravariant second-order tensor $\boldsymbol{\sigma}=\boldsymbol{\sigma}(\mathbf{x},t)$ (Cauchy stress tensor) with components σ^{ij} such that $\mathbf{t}=\langle\langle\boldsymbol{\sigma},\hat{\mathbf{n}}\rangle\rangle$. Note that $\langle\langle,\rangle\rangle$ is the inner product induced by the Riemmanian metric $\mathbf{g}$. Equivalently, balance of linear momentum can be written in the undeformed configuration as

$$\frac{d}{dt}\int_{\mathcal{U}} \rho_0\mathbf{V}\, dV = \int_{\mathcal{U}} \rho_0\mathbf{B}\, dV + \int_{\partial\mathcal{U}} \langle\langle\mathbf{P},\hat{\mathbf{N}}\rangle\rangle dA, \tag{2.46}$$

where, $\mathbf{P}=J\varphi^{*}\boldsymbol{\sigma}$ (the first Piola-Kirchhoff stress tensor) is the Piola transform of Cauchy stress tensor. Note that $\mathbf{P}$ is a two-point tensor with components P^{iJ}. Note also that this is the balance of linear momentum in the deformed (physical) space written in terms of some quantities that are defined with respect to the reference configuration.

As was mentioned before, balance of linear momentum has no intrinsic meaning because integrating a vector field is geometrically meaningless. As is standard in continuum mechanics, this balance law makes use of the linear (or affine) structure of Euclidean space.

A body $\mathcal{B}$ is said to satisfy *balance of angular momentum* if for every nice open set $\mathcal{U}\subset\mathcal{B}$,

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})} \rho\mathbf{x}\times\mathbf{v}\, dv = \int_{\varphi_t(\mathcal{U})} \rho\mathbf{x}\times\mathbf{b}\, dv + \int_{\partial\varphi_t(\mathcal{U})} \mathbf{x}\times\langle\langle\boldsymbol{\sigma},\hat{\mathbf{n}}\rangle\rangle da. \tag{2.47}$$

As with balance of linear momentum, balance of angular momentum makes use of the linear structure of Euclidean space and this does *not* transform in a covariant way under a general change of coordinates.

One says that *balance of energy* holds if, for every nice open set $\mathcal{U}\subset\mathcal{B}$,

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})} \rho\left(e+\frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right) dv = \int_{\varphi_t(\mathcal{U})} \rho(\langle\langle\mathbf{b},\mathbf{v}\rangle\rangle + r) dv + \int_{\partial\varphi_t(\mathcal{U})} (\langle\langle\mathbf{t},\mathbf{v}\rangle\rangle + h) da, \tag{2.48}$$

where $e=e(\mathbf{x},t)$, $r=r(\mathbf{x},t)$ and $h=h(\mathbf{x},\hat{\mathbf{n}},t)$ are internal energy per unit mass, heat supply per unit mass and heat flux, respectively.

The geometry of inverse motions: The study of inverse motions in continuum mechanics was started by Shield[38] and further extended by Ericksen[10] and Steinmann.[43,42] Here the idea is to fix spatial points and look at the evolution of material points under the inverse of the deformation mapping. It is known that in inverse motion, Eshelby's tensor has a role similar to that of stress tensor in direct motion. One should note that formulating continuum mechanics in terms of the inverse motion is simply a change in describing the same physical system and so, in general, cannot have any profound consequences. However, in the general relativistic setting, in which it is desireable to have the fields to be defined on space-time and take values in a bundle over space-time, inverse configurations are preferred; see Ref. 5 and references therein.

III. LAGRANGIAN FIELD THEORY OF ELASTIC BODIES WITH EVOLVING REFERENCE CONFIGURATIONS

Suppose the reference configuration evolves in time and assume that this evolution can be represented by a one-parameter family of mappings that map $\mathcal{B}\subset\mathfrak{B}$ (reference configuration at $t=0$) to $\mathcal{B}_t\subset\mathfrak{B}$ (the reference configuration at time t),

$$\Xi_t:\mathcal{B}\to\mathcal{B}_t. \tag{3.1}$$

We call these maps the *configurational deformation maps*. Note that this is not the most general form of reference configuration evolution. In general, one should look at the reference configura-

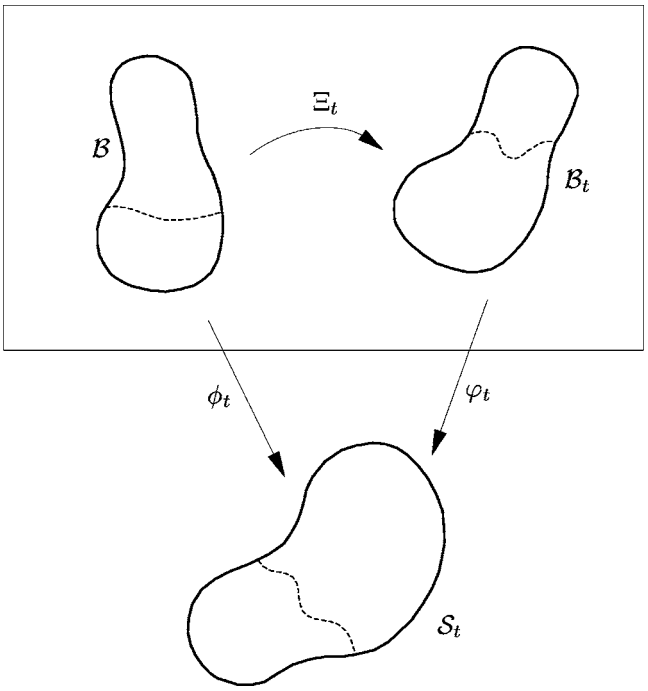


FIG. 1. Configurational and standard deformation maps.

tion evolution locally (see Refs. 9 and 8 for some discussions on this). For the sake of simplicity, we assume a global reference configuration evolution. The *configuration space* for the evolution of the reference configuration is

$$\mathcal{C}^{\text{conf}} = \{\Xi | \Xi : \mathcal{B} \to \mathcal{B}_t\}. \tag{3.2}$$

An *evolution of the reference configuration* is a curve $c : I \to \mathcal{C}^{\text{conf}}$ in $\mathcal{C}^{\text{conf}}$. It is important to put the right restrictions on Ξ_t. It does not seem necessary for Ξ_t to be invertible, in general. Here, we assume that Ξ_t is a diffeomorphism. A standard deformation is represented by a one-parameter family of mappings,

$$\varphi_t : \mathcal{B}_t \to \mathcal{S}. \tag{3.3}$$

The standard configuration space is defined by

$$\mathcal{C} = \{\varphi | \varphi : \mathcal{B}_t \to \mathcal{S}\}. \tag{3.4}$$

Again, a standard deformation is a curve in the standard configuration space. The total deformation map is the composition of standard and configurational deformation maps,

$$\phi_t = \varphi_t \circ \Xi_t : \mathcal{B} \to \mathcal{S}; \tag{3.5}$$

that is, the following diagram commutes:

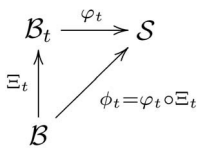
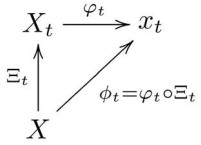


Figure 1 below shows the same idea schematically.

In terms of mapping the material points, $x_t=\varphi_t(X_t)=\varphi_t\circ\Xi_t(X)$, as is shown in the following commutative diagram:



The *configuration space* for the total deformation is defined as

$$\mathcal{C}^{\text{tot}}=\{\phi|\phi=\varphi\circ\Xi,\varphi\in\mathcal{C},\Xi\in\mathcal{C}^{\text{conf}}\}=\mathcal{C}\circ\mathcal{C}^{\text{conf}}. \tag{3.6}$$

A *deformation* is a curve $c:I\to\mathcal{C}^{\text{tot}}$ in the total configuration space. Note that $\Xi_t=\text{Id}$ (identity map) in most of classical continuum mechanics.

Notice that there are two independent deformation mappings φ_t and Ξ_t when reference configuration evolves in time (see Fig. 1). These separate mappings represent independent kinematical processes and hence may correspond to two separate systems of forces, in general.

Definition 3.1 (configurational velocity): The configurational velocity is defined by

$$\mathbf{V}_0(X,t)=\frac{\partial\Xi_t(X)}{\partial t}. \tag{3.7}$$

Definition 3.2: The total material velocity is defined by

$$\tilde{\mathbf{V}}(\mathbf{X},t)=\left.\frac{\partial\phi_t(\mathbf{X}_t)}{\partial t}\right|_{\mathbf{X}\text{ fixed}}=\frac{\partial\varphi_t}{\partial t}+\mathbf{F}\mathbf{V}_0=\mathbf{V}+\mathbf{F}\mathbf{V}_0, \tag{3.8}$$

where, as before, $\mathbf{F}=\partial\varphi_t/\partial\mathbf{X}_t$ *is the deformation gradient* (*holding t fixed*). Note that

$$T\phi_t=T\varphi_t\circ T\Xi_t \quad\text{or}\quad \tilde{\mathbf{F}}=\mathbf{F}\mathbf{F}_0. \tag{3.9}$$

Thus

$$\mathbf{F}_0=\mathbf{F}^{-1}\circ\tilde{\mathbf{F}}. \tag{3.10}$$

Now we may think about postulating the conservation of configurational mass and balance of linear and angular configurational momenta.

Conservation of mass is defined in terms of conservation of mass for deformation mappings Ξ_t and φ_t separately or equivalently for Ξ_t and ϕ_t separately. This makes sense as Ξ_t and φ_t correspond to configurational and standard deformations and should preserve the mass of an arbitrary sub-body.

Definitiion 3.3 (conservation of mass): Suppose $\mathcal{B}$ *is a body and* $\phi_t=\varphi_t\circ\Xi_t$ *is a deformation map. We say that the deformation mapping is mass conserving if for every* $\mathcal{U}\subset\mathcal{B}$,

$$\frac{d}{dt}\int_{\Xi_t(\mathcal{U})}\rho_0(\mathbf{X}_t,t)dV=0 \quad \textit{and} \quad \frac{d}{dt}\int_{\phi_t(\mathcal{U})}\rho(\mathbf{x},t)dv=0, \tag{3.11}$$

where $\rho_0(\mathbf{X}_t,t)$ *is the mass density at point* $X_t\in\mathcal{B}_t$ *and* $\rho(\mathbf{x},t)$ *is the mass density at the point* $\mathbf{x}\in\mathcal{S}$.

Localization of the above equations gives the local form of conservation of mass, namely

$$R_0(\mathbf{X})=\rho_0(\mathbf{X}_t,t)J_0=\rho(\mathbf{x},t)\tilde{J}, \tag{3.12}$$

where $J_0=\det(\mathbf{F}_0)(\sqrt{\det\mathbf{G}}/\sqrt{\det\mathbf{G}_0})$, $\mathbf{F}_0=T\Xi_t$ is the *configurational deformation gradient*, $\mathbf{G}_0$ is the fixed metric of $\mathcal{B}$, $\mathbf{G}$ is the metric of $\mathcal{B}_t$ and R_0 is the mass density at $\mathbf{X}\in\mathcal{B}$ and $\tilde{J}=\det(\tilde{\mathbf{F}})\times(\sqrt{\det\mathbf{g}}/\sqrt{\det\mathbf{G}})=JJ_0$. Note that this is equivalent to

$$R_0 = \rho_0 J_0 \quad \text{and} \quad \rho_0 = \rho J. \tag{3.13}$$

One may be tempted to postulate a balance of configurational linear momentum as follows. A body $\mathcal{B}$ satisfies the balance of configurational linear momentum if for any $\mathcal{U}' \subset \mathcal{B}_t$,

$$\frac{d}{dt}\int_{\mathcal{U}'} \rho_0 \mathbf{V}_0 \, dV = \int_{\mathcal{U}'} \rho_0 \mathbf{B}_0 \, dV + \int_{\partial\mathcal{U}'} \mathbf{P}_0 \mathbf{N} \, dA. \tag{3.14}$$

Localization of this balance law and using Cauchy's theorem gives the following local form of the balance of configurational linear momentum

$$\text{Div}\, \mathbf{P}_0 + \rho_0 \mathbf{B}_0 = \rho_0 \mathbf{A}_0. \tag{3.15}$$

Thinking of configurational deformation mapping Ξ_t as a deformation of a fixed reference configuration, this balance law is similar to the standard balance of linear momentum written in the deformed configuration. Note that postulating such a balance law requires the introduction of two new quantities, namely $\mathbf{P}_0$ and $\mathbf{B}_0$ and does not seem to be of any use at this point.

It should be noted that a configurational change need not be volume preserving. An example is a phase transformation from cubic to tetragonal which has the following configurational deformation gradient (this is called Bain strain or matrix in martensitic phase transformations),

$$\mathbf{F}_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \dfrac{c}{a} \end{pmatrix} \tag{3.16}$$

where $a=b$ and $c>a$ are the tetragonal lattice parameters.

The Lagrangian may be regarded as a map $L: T\mathcal{C} \to \mathbb{R}$, where $\mathcal{C}$ is the space of some sections (for technical details see Ref. 28), associated to the Lagrangian density $\mathcal{L}$ and a volume element $dV(X)$ on $\mathcal{B}$ and is defined as

$$L(\varphi, \dot{\varphi}) = \int_{\mathcal{B}} \mathcal{L}(X, \varphi(X), \dot{\varphi}(X), \mathbf{F}(X), \mathbf{G}(X), \mathbf{g}(\varphi(X))) dV(X). \tag{3.17}$$

Note that here we have assumed an explicit dependence of $\mathcal{L}$ on the material and spatial metrics $\mathbf{G}$ and $\mathbf{g}$. Let us first revisit the classical Lagrangian field theory of elasticity using the above Lagrangian density with explicit dependence on material and spatial metrics. The *action function* is defined as

$$S(\varphi) = \int_{t_0}^{t_1} L(\varphi, \dot{\varphi}) dt. \tag{3.18}$$

Hamilton's principle states that the physical configuration φ is the critical point of the action, i.e.,

$$\mathbf{d}S(\varphi) \cdot \delta\varphi = 0. \tag{3.19}$$

Note that variation in φ leaves the material metric unchanged. The statement of Hamilton's principle can be simplified to read

$$\int_{t_0}^{t_1} \int_{\mathcal{B}} \left(\frac{\partial \mathcal{L}}{\partial \varphi} \cdot \delta\varphi + \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} \cdot \delta\dot{\varphi} + \frac{\partial \mathcal{L}}{\partial \mathbf{F}} : \delta\mathbf{F} + \frac{\partial \mathcal{L}}{\partial \mathbf{g}} : \delta\mathbf{g} \right) dV(X) dt = 0. \tag{3.20}$$

After some manipulations the above integral statement results in

$$\frac{\partial \mathcal{L}}{\partial \varphi^a} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A} - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b^{\ A} F^c{}_A \gamma^b_{ac} + 2\frac{\partial \mathcal{L}}{\partial g_{cd}} g_{bd}\gamma^b_{ac} = 0. \tag{3.21}$$

Noting that

$$\frac{d}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a = \rho_0 (g_{ab}A^b + g_{bc}\gamma^c_{ad}\dot{\varphi}^b\dot{\varphi}^d), \tag{3.22}$$

$$\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A} = -P_a{}^A, \tag{3.23}$$

$$2\frac{\partial \mathcal{L}}{\partial g_{cd}} = \rho_0 \dot{\varphi}^c\dot{\varphi}^d - J\sigma^{cd}, \tag{3.24}$$

Eq. (3.21) can be written as

$$P_a{}^A{}_{|A} + \frac{\partial \mathcal{L}}{\partial \varphi^a} + (F^c{}_A P_b{}^A - J\sigma^{cd}g_{bd})\gamma^b_{ac} = \rho_0 g_{ab}A^b. \tag{3.25}$$

Note that if $\mathcal{L}$ depends on $\mathbf{F}$ and $\mathbf{g}$ through $\mathbf{C}$, then the term in the parentheses would be zero and hence

$$P_a{}^A{}_{|A} + \frac{\partial \mathcal{L}}{\partial \varphi^a} = \rho_0 g_{ab}A^b, \tag{3.26}$$

which is nothing but the familiar equations of motion. [Also note that in (3.25) use was made of Doyle-Ericksen formula (3.24). However, for arriving at (3.26) there is no need for using Doyle-Ericksen formula.]

Now suppose that during the process of deformation the continuum undergoes a continuous material evolution. This means that the deformation mapping φ is the composition of a total deformation mapping and a referential mapping, i.e.,

$$\varphi = \phi \circ \Xi^{-1} \quad \text{or} \quad \phi = \varphi \circ \Xi. \tag{3.27}$$

Note that defining such a composition is ambiguous because there are infinitely many possibilities for decomposing a given deformation mapping ϕ into two mappings φ and Ξ. The new mappings can represent part of the standard deformation and material evolution. To make sure that φ is the standard part of total deformation mapping, the Lagrangian is written as an integral on the current reference configuration $\mathcal{B}_t$

$$L(\varphi, \dot{\varphi}) = \int_{\mathcal{B}_t} \mathcal{L}(X, \varphi(X), \dot{\varphi}(X), \mathbf{F}(X), \mathbf{G}(X), \mathbf{g}(\varphi(X)))\mathrm{d}V(X). \tag{3.28}$$

It would be more convenient to write the Lagrangian as a functional on $\mathcal{B}$ (the fixed initial reference configuration). Let us denote points on $\mathcal{B}$ by U. Note that

$$\dot{\phi}(U) = (\dot{\varphi}\circ\Xi)(U) + T\varphi(\Xi(U))\cdot\dot{\Xi}(U) \quad \text{or} \quad (\dot{\varphi}\circ\Xi)(U) = \dot{\phi}(U) - \mathbf{F}(\Xi(U))\cdot\dot{\Xi}(U). \tag{3.29}$$

Also

$$\mathbf{F}(\Xi(U)) = \mathbf{F}_\phi(U)\mathbf{F}_\Xi^{-1}(\Xi(U)). \tag{3.30}$$

Thus,

$$\mathcal{L} = \mathcal{L}(\Xi(U), \phi(U), \dot{\phi}(U) - \mathbf{F}_\phi(U)\mathbf{F}_\Xi^{-1}(\Xi(U)) \cdot \dot{\Xi}(U), \mathbf{F}_\phi(U)\mathbf{F}_\Xi^{-1}(\Xi(U)), \mathbf{G}(\Xi(U)), \mathbf{g}(\phi(U)))J_\Xi(U), \tag{3.31}$$

where

$$J_\Xi = \det(T\Xi)\frac{\sqrt{\det \mathbf{G}}}{\sqrt{\det \mathbf{G}_0}}, \tag{3.32}$$

and where $\mathbf{G}_0$ is the fixed metric of the fixed reference configuration and $\mathbf{G}$ is the metric of $\mathcal{B}_t$. As before, the action is defined as

$$S(\Xi, \phi) = \int_{t_0}^{t_1} L(\Xi, \dot{\Xi}, \phi, \dot{\phi})\mathrm{d}t. \tag{3.33}$$

Hamilton's principle states that the physical configurations Ξ and ϕ are the critical points of the action, i.e.,

$$\mathbf{d}S(\Xi, \phi) \cdot (\delta\Xi, \delta\phi) = 0. \tag{3.34}$$

For the sake of clarity, we look at the two independent variations separately.

A. Vertical variations

Let us first look at *vertical variations*; that is, we assume that $\delta\Xi = 0$ and see if we can recover the classical Euler-Lagrange equations.

Proposition 3.4: Allowing only vertical variations in Hamilton's principle, one obtains the following equations of motion

$$\frac{\partial \mathcal{L}}{\partial \varphi^a} - \frac{d}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi} \circ \Xi}\right)_a - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |B}^{B} - F^c{}_B \gamma^b_{ac}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b^B + \frac{\partial \mathcal{L}}{\partial g^{bc}}\frac{\partial g^{bc}}{\partial x^a} = 0. \tag{3.35}$$

Proof: The derivative of the action with respect to vertical variations is computed as follows:

$$\begin{aligned}\mathbf{d}S(\Xi, \phi) \cdot (0, \delta\phi) = \int_{t_0}^{t_1}\int_{\mathcal{B}} \Bigg\{ &\frac{\partial \mathcal{L}}{\partial \varphi \circ \Xi} \cdot \delta\phi + \frac{\partial \mathcal{L}}{\partial \dot{\varphi} \circ \Xi} \cdot (\delta\dot{\phi} - \delta[\mathbf{F}_\phi(U)\mathbf{F}_\Xi^{-1}(\Xi(U)) \cdot \dot{\Xi}(U)]) \\ &+ \frac{\partial \mathcal{L}}{\partial \mathbf{F}} : \delta[\mathbf{F}_\phi(U)\mathbf{F}_\Xi^{-1}(\Xi(U))] + \frac{\partial \mathcal{L}}{\partial \mathbf{g}} : \delta\mathbf{g} \circ \phi \Bigg\} J_\Xi(U)\mathrm{d}V(U)\mathrm{d}t = 0.\end{aligned} \tag{3.36}$$

Note that

$$\begin{aligned}\delta(\mathbf{F}_\phi\mathbf{F}_\Xi^{-1} \circ \Xi) &= \delta(\mathbf{F}_\phi\mathbf{F}_\Xi^{-1}) \circ \Xi = T(\delta(\phi \circ \Xi^{-1})) \circ \Xi = T(\delta\phi \circ \Xi^{-1}) \circ \Xi \\ &= (T\delta\phi T\Xi^{-1}) \circ \Xi = D\delta\phi\mathbf{F}_\Xi^{-1} \circ \Xi.\end{aligned} \tag{3.37}$$

Let us assume coordinates $\{U^\alpha\}$, $\{X^A\}$, and $\{x^a\}$ and basis vectors $\mathbf{E}_\alpha$, $\mathbf{e}_A$, and $\mathbf{f}_a$ on $\mathcal{B}$, $\mathcal{B}_t$, and $\mathcal{S}$, respectively. Thus, in coordinates

$$D\delta\phi = \frac{\partial \delta\phi^a}{\partial U^\alpha}\mathbf{f}_a \otimes \mathbf{E}^\alpha. \tag{3.38}$$

The first part of the second term is simplified as

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\delta\dot{\phi}J_{\Xi}(U)\mathrm{d}V(U)=-\int_{t_0}^{t_1}\int_{\mathcal{B}}\left[\frac{d}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a+\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}_a W^B{}_{|B}\right]\delta\phi^a J_{\Xi}\,\mathrm{d}V(U)\mathrm{d}t, \tag{3.39}$$

where

$$\mathbf{W}(U)=\frac{d}{\mathrm{d}t}\Xi(U). \tag{3.40}$$

The second part of the second term in (3.36) can be simplified to

$$\begin{aligned}
&-\int_{t_0}^{t_1}\int_{\mathcal{B}}J_{\Xi}\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}D\delta\phi\mathbf{F}_{\Xi}^{-1}\circ\Xi\cdot\mathbf{W}\,\mathrm{d}V(U)\mathrm{d}t\\
&\quad=\int_{t_0}^{t_1}\int_{\mathcal{B}}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a J_{\Xi}(\mathbf{F}_{\Xi}^{-1}\circ\Xi)^{\beta}{}_B W^B\right]_{|\beta}\delta\phi^a\,\mathrm{d}V(U)\mathrm{d}t\\
&\qquad+\int_{t_0}^{t_1}\int_{\mathcal{B}}\left[J_{\Xi}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_b(\mathbf{F}\circ\Xi)^c{}_A\gamma_{ac}^b W^A\right]\delta\phi^a\,\mathrm{d}V(U)\mathrm{d}t.
\end{aligned} \tag{3.41}$$

Using the Piola identity we have

$$\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a J_{\Xi}(\mathbf{F}_{\Xi}^{-1}\circ\Xi)^{\beta}{}_B W^B\right]_{|\beta}=J_{\Xi}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A\right]_{|A}. \tag{3.42}$$

Also

$$\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A\right]_{|A}=\frac{\partial}{\partial X^A}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A+\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A{}_{|A}-\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_b W^A\gamma_{ac}^b F_A^c. \tag{3.43}$$

Therefore (3.41) is simplified to

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\left[\frac{\partial}{\partial X^A}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A+\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a W^A{}_{|A}\right]\delta\phi^a J_{\Xi}\mathrm{d}V(U)\mathrm{d}t. \tag{3.44}$$

Note that

$$\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a=\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a\circ\Xi^{-1}-\frac{\partial}{\partial X^A}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a\circ\Xi^{-1}W^A. \tag{3.45}$$

Hence adding (3.39) and (3.44) the term corresponding to $\delta\dot{\phi}$ is simplified to

$$\int_{t_0}^{t_1}\int_{\mathcal{B}_t}-\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a\delta\phi^a\circ\Xi^{-1}\,\mathrm{d}V(X)\,\mathrm{d}t. \tag{3.46}$$

After some lengthy manipulations, the third term in (3.36) can be written as

$$-\int_{t_0}^{t_1}\int_{\mathcal{B}}\left[\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}\circ\Xi}\right)_a{}_{|B}^{B}+F^c{}_B\circ\Xi\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}\circ\Xi}\right)_a^B\gamma_{ac}^b\right]\delta\phi^a J_{\Xi}(U)\mathrm{d}V(U)\mathrm{d}t. \tag{3.47}$$

The last term is simplified as

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\mathbf{g}\circ\phi}:\delta\mathbf{g}\circ\phi J_{\Xi}\,\mathrm{d}V(U)\mathrm{d}t=\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial g^{bc}\circ\phi}\frac{\partial g^{bc}}{\partial x^a}\delta\phi^a J_{\Xi}\,\mathrm{d}V(U)\mathrm{d}t=\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\frac{\partial\mathcal{L}}{\partial g^{bc}}\frac{\partial g^{bc}}{\partial x^a}\delta\phi^a$$
$$\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t=-\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\frac{\partial\mathcal{L}}{\partial g^{bc}}(g^{cd}\gamma^b_{ad}+g^{bd}\gamma^c_{ad})\delta\phi^a\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.48}$$

Therefore, adding the above four simplified terms, we obtain

$$\mathbf{d}S(\Xi,\phi)\cdot(0,\delta\phi)=\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left[\frac{\partial\mathcal{L}}{\partial\varphi^a}-\frac{d}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a-\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_{a\ |B}-F^c{}_B\gamma^b_{ac}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_b+\frac{\partial\mathcal{L}}{\partial g^{bc}}\frac{\partial g^{bc}}{\partial x^a}\right]\delta\phi^a$$
$$\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.49}$$

As $\delta\phi^a$ is arbitrary we conclude that

$$\frac{\partial\mathcal{L}}{\partial\varphi^a}-\frac{d}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a-\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_{a\ |B}-F^c{}_B\gamma^b_{ac}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_b+\frac{\partial\mathcal{L}}{\partial g^{bc}}\frac{\partial g^{bc}}{\partial x^a}=0, \tag{3.50}$$

which gives the stated result. □

B. Horizontal variations

Now let us try to find the Euler-Lagrange equations resulting from *horizontal variations*; that is, variations of the configurational deformation mapping Ξ.

Proposition 3.5: Allowing only horizontal variations in Hamilton's principle, one obtains the following configurational equations of motion:

$$\frac{\partial\mathcal{L}}{\partial X^A}+\frac{\partial}{\partial t}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A\right]-\left[\mathcal{L}\delta^B{}_A-\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_a F^a{}_A\right]_{|B}+\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)^B_a F^a{}_C\Gamma^C_{AB}+2G_{CD}\Gamma^D_{AB}\frac{\partial\mathcal{L}}{\partial G_{BC}}=0, \tag{3.51}$$

where Γ^C_{AB} is the Christoffel symbol of a local chart in $\mathcal{B}_t$.

Proof: The derivative of the action with respect to horizontal variations is computed as follows:

$$\mathbf{d}S(\Xi,\phi)\cdot(\delta\Xi,0)=\int_{t_0}^{t_1}\int_{\mathcal{B}}\left(\left[\frac{\partial\mathcal{L}}{\partial\Xi}\cdot\delta\Xi-\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\cdot\delta(\mathbf{F}_{\phi}\mathbf{F}^{-1}_{\Xi}\circ\Xi\cdot\dot{\Xi})+\frac{\partial\mathcal{L}}{\partial\mathbf{F}\circ\Xi}:\delta(\mathbf{F}_{\phi}\mathbf{F}^{-1}_{\Xi}\circ\Xi)\right]J_{\Xi}\right.$$
$$\left.+\frac{\partial\mathcal{L}}{\partial\mathbf{G}\circ\Xi}:\delta\mathbf{G}\circ\Xi+\mathcal{L}\delta J_{\Xi}\right)\mathrm{d}V(U)\mathrm{d}t=0. \tag{3.52}$$

Note that

$$\delta(\mathbf{F}_{\phi}\mathbf{F}^{-1}_{\Xi}\circ\Xi)=\mathbf{F}_{\phi}\delta(\mathbf{F}^{-1}_{\Xi}\circ\Xi). \tag{3.53}$$

But

$$\delta(\mathbf{F}^{-1}_{\Xi}\circ\Xi)=-\mathbf{F}^{-1}_{\Xi}D(\delta\Xi)\mathbf{F}^{-1}_{\Xi}\circ\Xi. \tag{3.54}$$

Thus

$$\delta(\mathbf{F}_{\phi}\mathbf{F}^{-1}_{\Xi}\circ\Xi)=-\mathbf{F}_{\phi}\mathbf{F}^{-1}_{\Xi}D(\delta\Xi)\mathbf{F}^{-1}_{\Xi}\circ\Xi=-\mathbf{F}D(\delta\Xi)\mathbf{F}^{-1}_{\Xi}\circ\Xi. \tag{3.55}$$

Similarly

$$\delta(\mathbf{F}_\phi\mathbf{F}_\Xi^{-1}\circ\Xi\cdot\dot{\Xi}) = -\mathbf{F}D(\delta\Xi)\mathbf{F}_\Xi^{-1}\circ\Xi\cdot\mathbf{W}+\mathbf{F}\circ\Xi\cdot\frac{d}{dt}(\delta\Xi). \tag{3.56}$$

In coordinates,

$$D(\delta\Xi) = \frac{\partial\delta\Xi^A}{\partial U^\beta}\mathbf{e}_A\otimes\mathbf{E}^\beta. \tag{3.57}$$

The second term in (3.52) has two parts which are simplified as follows. The first part is

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\right)_a F^a{}_A\circ\Xi\frac{\partial\delta\Xi^A}{\partial U^\beta}(\mathbf{F}_\Xi^{-1}\circ\Xi)^\beta{}_B W^B J_\Xi\,\mathrm{d}V(U)\mathrm{d}t = -\int_{t_0}^{t_1}\int_{\mathcal{B}'}\frac{\partial}{\partial X^B}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A\right]W^B\delta\Xi^A$$
$$\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t - \int_{t_0}^{t_1}\int_{\mathcal{B}'}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A W^B{}_{|B}\delta\Xi^A\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.58}$$

Similarly, the second part is simplified as

$$-\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\cdot\mathbf{F}\circ\Xi\cdot\frac{d}{dt}(\delta\Xi)J_\Xi\,\mathrm{d}V(U)\mathrm{d}t = \int_{t_0}^{t_1}\int_{\mathcal{B}_t}\frac{d}{dt}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A\right]\delta\Xi^A\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t$$
$$+\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A W^B{}_{|B}\delta\Xi^A\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.59}$$

Adding (3.58) and (3.59), the second term of (3.52) can be written as

$$-\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\dot{\varphi}\circ\Xi}\delta(\mathbf{F}_\phi\mathbf{F}_\Xi^{-1}\circ\Xi\cdot\dot{\Xi})J_\Xi\,\mathrm{d}V(U)\mathrm{d}t = \int_{t_0}^{t_1}\int_{\mathcal{B}_t}\frac{d}{dt}\left[\left(\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}\right)_a F^a{}_A\right]\delta\Xi^A\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.60}$$

After some lengthy manipulations, the third term of (3.52) is simplified to

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\mathbf{F}\circ\Xi}:\delta(\mathbf{F}_\phi\mathbf{F}_\Xi^{-1}\circ\Xi)J_\Xi\,\mathrm{d}V(U)\mathrm{d}t$$
$$=\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left[\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)_a{}^B F^a{}_A\right]_{|B}\delta\Xi^A\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t$$
$$+\int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)_a{}^B F^a{}_C\Gamma^C_{AB}\delta\Xi^A\circ\Xi^{-1}\,\mathrm{d}V(X)\mathrm{d}t. \tag{3.61}$$

The fourth term of (3.52) is simplified to

$$\int_{t_0}^{t_1}\int_{\mathcal{B}}\frac{\partial\mathcal{L}}{\partial\mathbf{G}\circ\Xi}:\delta\mathbf{G}\circ\Xi J_\Xi\,\mathrm{d}V(U)\mathrm{d}t = \int_{t_0}^{t_1}\int_{\mathcal{B}_t}2G_{CD}\Gamma^D_{AB}\frac{\partial\mathcal{L}}{\partial G_{BC}}\mathrm{d}V(X)\mathrm{d}t. \tag{3.62}$$

Note that

$$J_\Xi = (\det\mathbf{F}_\Xi)\sqrt{\frac{\det\mathbf{G}}{\det\mathbf{G}_0}}, \tag{3.63}$$

where $\mathbf{G}_0$ is the fixed Riemannian metric of the fixed reference configuration. Thus,

$$\delta J_\Xi = \delta(\det \mathbf{F}_\Xi)\sqrt{\frac{\det \mathbf{G}}{\det \mathbf{G}_0}} + (\det \mathbf{F}_\Xi)\frac{\delta \det \mathbf{G}}{\det \mathbf{G}_0} = J_\Xi(\mathbf{F}_\Xi^{-1})^\beta{}_B \frac{\partial \delta \Xi^B}{\partial U^\beta} + (\det \mathbf{F}_\Xi)\frac{1}{\sqrt{\det \mathbf{G}_0}}\frac{\partial \sqrt{\det \mathbf{G}}}{\partial \mathbf{X}}\delta\Xi. \tag{3.64}$$

Note that

$$\frac{\partial \sqrt{\det \mathbf{G}}}{\partial \mathbf{X}} = \frac{1}{2}\sqrt{\det \mathbf{G}}\mathbf{G}^{-1}\frac{\partial \mathbf{G}}{\partial \mathbf{X}} = \sqrt{\det \mathbf{G}}\Gamma^B_{AB}\delta\Xi^A. \tag{3.65}$$

Hence

$$\delta J_\Xi = J_\Xi(\mathbf{F}_\Xi^{-1})^\beta{}_B \frac{\partial \delta \Xi^B}{\partial U^\beta} + J_\Xi \Gamma^B_{AB}. \tag{3.66}$$

Thus the last term of (3.52) is simplified to

$$\int_{t_0}^{t_1}\int_{\mathcal{B}} \mathcal{L}\delta J_\Xi \, \mathrm{d}V(U)\mathrm{d}t = -\int_{t_0}^{t_1}\int_{\mathcal{B}_t} (\mathcal{L}\delta_A{}^B)_{|B}\delta\Xi^A \circ \Xi^{-1}\, \mathrm{d}V(X)\mathrm{d}t. \tag{3.67}$$

Now substituting the above five simplified terms into (3.52), we have

$$\begin{aligned}\mathbf{d}S(\Xi,\phi)\cdot(\delta\Xi,0) = \int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left\{\frac{\partial \mathcal{L}}{\partial X^A} + \frac{\partial}{\partial t}\left[\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a F^a{}_A\right] - \left[\mathcal{L}\delta_A{}^B - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_A\right]_{|B}\right\}\delta\Xi^A \\ \circ \Xi^{-1}\, \mathrm{d}V(X)\mathrm{d}t + \int_{t_0}^{t_1}\int_{\mathcal{B}_t}\left\{\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_C\Gamma^C_{AB} + 2G_{CD}\Gamma^D_{AB}\frac{\partial \mathcal{L}}{\partial G_{BC}}\right\}\delta\Xi^A \\ \circ \Xi^{-1}\, \mathrm{d}V(X)\mathrm{d}t = 0.\end{aligned} \tag{3.68}$$

Because $\delta\Xi^A$ is arbitrary, we conclude that

$$\frac{\partial \mathcal{L}}{\partial X^A} + \frac{\partial}{\partial t}\left[\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a F^a{}_A\right] - \left[\mathcal{L}\delta_A{}^B - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_A\right]_{|B} + \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_C\Gamma^C_{AB} + 2G_{CD}\Gamma^D_{AB}\frac{\partial \mathcal{L}}{\partial G_{BC}} = 0. \tag{3.69}$$

□

We now show that this is equivalent to the classical Euler-Lagrange equations and does not give us any new information. After some lengthy manipulations, it can be shown that

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial X^A} + \frac{\partial}{\partial t}\left[\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a F^a{}_A\right] - \left[\mathcal{L}\delta_A{}^B - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_A\right]_{|B} = \left[\frac{\partial \mathcal{L}}{\partial \varphi^a} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}}\right)_a - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^A{}_{|A}\right. \\ \left. - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b{}^A F^c{}_A\gamma^b_{ac} + 2\frac{\partial \mathcal{L}}{\partial g_{cd}}g_{bd}\gamma^b_{ac}\right]F^a{}_A - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^B F^a{}_C\Gamma^C_{AB} - 2G_{CD}\Gamma^D_{AB}\frac{\partial \mathcal{L}}{\partial G_{BC}}.\end{aligned} \tag{3.70}$$

□

[It will be seen in Sec. VI that material covariance of internal energy density implies that the sum of the last two terms is zero. In Sec. VII, it will be shown that material covariance of Lagrangian density results in the same identity. However, at this point there is no such relation and the variational principle does not give us any new information.] This result is known for the case where the underlying metrics are trivial.[25] In conclusion, we have proved the following proposition.

Proposition 3.6: In the absence of discontinuities, i.e., when all the fields are smooth, the configurational and the standard equations of motion are equivalent, even if one is allowed to vary the referential and spatial metrics.

IV. THE GREEN-NAGHDI-RIVILIN THEOREM

Green, Rivilin, and Naghdi[19] realized that conservation of mass and balance of linear and angular momenta can be obtained as a result of postulating invariance of energy balance under isometries of $\mathbb{R}^3$, i.e., rigid translations and rotations in the deformed configuration. Later Marsden and Hughes[28] extended this idea to Riemannian manifolds and diffeomorphisms of the deformed configuration showing that this covariant approach gives the Doyle-Ericksen formula for Cauchy stress as well as conservation of mass and balance of linear and angular momenta. In another relevant work, Šilhavý[39] considered all the densities in the energy balance to be volume densities and assuming (i) invariance of energy balance under Galilean transformations and (ii) boundedness of energy from below, proved the existence of mass, its conservation, balance of linear and angular momenta, transformation of body forces and the splitting of total energy into internal and kinetic energies.

Before discussing the covariant approach to elasticity, let us first discuss the classical Green-Naghdi-Rivilin (GNR) theorem and a nonconventional material form of it. We consider two cases: (i) material energy balance invariance under spatial isometries of $\mathbb{R}^3$ and (ii) material energy balance invariance under material isometries of $\mathbb{R}^3$. We call (i) and (ii) the spatial-material and material-material GNR theorems, respectively.

A. The spatial-material GNR theorem

Consider the material energy balance for a nice subset $\mathcal{U}\subset\mathcal{B}$,

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}}\rho_0\left(\Psi+\frac{1}{2}\mathbf{V}\cdot\mathbf{V}\right)\mathrm{d}V=\int_{\mathcal{U}}\rho_0(\mathbf{B}\cdot\mathbf{V}+R)\mathrm{d}V+\int_{\partial\mathcal{U}}(\mathbf{T}\cdot\mathbf{V}+H)\mathrm{d}A, \tag{4.1}$$

where $\Psi=\Psi(t,\mathbf{X},\mathbf{F})$ is the free energy density per unit mass of the undeformed configuration. Now consider an isometry $\xi_t:\mathbb{R}^3\to\mathbb{R}^3$ of $\mathbb{R}^3$. We postulate that the material energy balance is invariant under ξ_t. For the sake of simplicity we consider translations and rotations separately.

(i) (*Rigid translations*) A spatial rigid translation is defined by

$$\xi_t(\mathbf{x})=\mathbf{x}+(t-t_0)\mathbf{c}, \tag{4.2}$$

where $\mathbf{c}$ is some constant vector field. We now postulate that the material balance of energy holds for the deformation mapping $\varphi_t'=\xi_t\circ\varphi_t$ as well. This balance law is still written on $\mathcal{U}$ but with different fields (primed fields) in general,

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}}\rho_0'\left(\Psi'+\frac{1}{2}\mathbf{V}'\cdot\mathbf{V}'\right)\mathrm{d}V=\int_{\mathcal{U}}\rho_0'(\mathbf{B}'\cdot\mathbf{V}'+R')\mathrm{d}V+\int_{\partial\mathcal{U}}(\mathbf{T}'\cdot\mathbf{V}'+H')\mathrm{d}A. \tag{4.3}$$

Using Cartan's space-time theory, the primed fields are related to the unprimed quantities through the following relations:

$$\rho_0'(\mathbf{X})=\rho_0(\mathbf{X}),\quad R'(\mathbf{X})=R(\mathbf{X}),\quad H'(\mathbf{X})=H(\mathbf{X}),$$

$$\mathbf{V}'|_{t=t_0}=\left.\frac{\partial}{\partial t}\varphi_t'\right|_{t=t_0}=(T\xi_t\mathbf{V}+\mathbf{c})_{t=t_0}=\mathbf{V}+\mathbf{c},$$

$$\mathbf{T}'(\mathbf{X},\mathbf{N})=\mathbf{T}(\mathbf{X},\mathbf{N}). \tag{4.4}$$

Also because

$$\mathbf{b}' - \mathbf{a}' = \xi_{t*}(\mathbf{b} - \mathbf{a}) \quad \text{and} \quad \mathbf{B} - \mathbf{A} = (\mathbf{b} - \mathbf{a}) \circ \varphi_t. \tag{4.5}$$

We have

$$\mathbf{B}' - \mathbf{A}' = \xi_t^*(\mathbf{b} - \mathbf{a}) \circ \varphi_t'. \tag{4.6}$$

Hence

$$(\mathbf{B}' - \mathbf{A}')_{t=t_0} = (\mathbf{b} - \mathbf{a}) \circ \varphi_t = (\mathbf{B} - \mathbf{A}). \tag{4.7}$$

It can be easily shown that

$$\mathbf{F}'(\mathbf{X}) = \mathbf{F}(\mathbf{X}). \tag{4.8}$$

The free energy density would have the following transformation:

$$\Psi'(t, \mathbf{X}, \mathbf{F}'(\mathbf{X})) = \Psi(t, \mathbf{X}, \mathbf{F}(\mathbf{X})). \tag{4.9}$$

Thus,

$$\frac{d}{\mathrm{d}t}\Psi'(t, \mathbf{X}, \mathbf{F}'(\mathbf{X})) = \frac{\partial \Psi}{\partial t}. \tag{4.10}$$

Balance of energy for $\mathcal{U} \subset \mathcal{B}$ for the new deformation mapping at $t = t_0$ can be written as

$$\begin{aligned} &\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\Psi + \frac{1}{2}(\mathbf{V} + \mathbf{c}) \cdot (\mathbf{V} + \mathbf{c})\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\frac{\partial \Psi}{\partial t} + (\mathbf{V} + \mathbf{c}) \cdot \mathbf{A}'|_{t=t_0}\right)\mathrm{d}V \\ &\quad = \int_{\mathcal{U}} \rho_0(\mathbf{B}'|_{t=t_0} \cdot (\mathbf{V} + \mathbf{c}) + R)\mathrm{d}V + \int_{\partial \mathcal{U}} (\mathbf{T} \cdot (\mathbf{V} + \mathbf{c}) + H)\mathrm{d}A, \end{aligned} \tag{4.11}$$

where Div $\mathbf{c} = 0$ was used. Subtracting the material energy balance of the deformation φ_t for $\mathcal{U} \subset \mathcal{B}$ from the above equation and using (4.7) we obtain

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\mathbf{c} \cdot \mathbf{V} + \frac{1}{2}\mathbf{c} \cdot \mathbf{c}\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0 \mathbf{A} \cdot \mathbf{c}\, \mathrm{d}V = \int_{\mathcal{U}} \rho_0 \mathbf{B} \cdot \mathbf{c}\, \mathrm{d}V + \int_{\partial \mathcal{U}} \mathbf{T} \cdot \mathbf{c}\, \mathrm{d}A. \tag{4.12}$$

Because $\mathcal{U}$ and $\mathbf{c}$ are arbitrary one concludes that

$$\frac{\partial \rho_0}{\partial t} = 0, \tag{4.13}$$

$$\mathrm{Div}\, \mathbf{P} + \rho_0 \mathbf{B} = \rho_0 \mathbf{A}. \tag{4.14}$$

(ii) (*Rigid rotations*) Now let us consider a rigid rotation in the ambient space, i.e., $\xi_t : \mathcal{S} \to \mathcal{S}$, where

$$\xi_t(\mathbf{x}) = e^{(t-t_0)\mathbf{\Omega}}\mathbf{x}, \tag{4.15}$$

for some constant skew-symmetric matrix $\mathbf{\Omega}$. Note that

$$T\xi_t|_{t=t_0} = e^{(t-t_0)\mathbf{\Omega}}|_{t=t_0} = \mathrm{Id} \quad \text{and} \quad \left.\frac{\partial}{\partial t}\right|_{t=t_0} \xi_t(\mathbf{x}) = \mathbf{\Omega}\mathbf{x}. \tag{4.16}$$

Also

$$\mathbf{V}'(\mathbf{X})|_{t=t_0} = \mathbf{V} + \mathbf{\Omega}\mathbf{x}(\mathbf{X}). \tag{4.17}$$

Subtracting the balance of energy for $\mathcal{U}$ for deformation mapping φ_t from that of $\varphi'_t = \xi_t \circ \varphi_t$ at time $t=t_0$ results in

$$\int_{\mathcal{U}} \rho_0 \mathbf{\Omega}\mathbf{x}(\mathbf{X}) \cdot (\mathbf{A} - \mathbf{B}) \mathrm{d}V = \int_{\partial\mathcal{U}} \mathbf{T}\mathbf{\Omega}\mathbf{x}(\mathbf{X}) \mathrm{d}A. \tag{4.18}$$

But

$$\int_{\partial\mathcal{U}} \mathbf{T}\mathbf{\Omega}\mathbf{x}(\mathbf{X}) \mathrm{d}A = \int_{\mathcal{U}} (\mathrm{Div}\, \mathbf{P} \cdot \mathbf{\Omega}\mathbf{x} + \mathbf{P}\mathbf{F}^{\mathsf{T}} : \mathbf{\Omega}) \mathrm{d}V. \tag{4.19}$$

Thus

$$\mathbf{P}\mathbf{F}^{\mathsf{T}} = \mathbf{F}\mathbf{P}^{\mathsf{T}}, \tag{4.20}$$

where use was made of balance of linear momentum.

B. The material-material GNR theorem

To our best knowledge, there is no study of invariance of energy balance under isometries of the reference configuration in the literature. It turns out that such an invariance does not hold in general, even in Euclidean space. In this section we study the transformation of balance of energy under rigid translations and rotations of the reference configuration in the Euclidean space context. It will be shown that balance of energy is invariant under translations and rotations of the reference configuration for isotropic materials that satisfy an internal constraint that we call material inviscidity.

Again we consider rigid translations and rigid rotations of the reference configuration separately.

(i) (*Rigid translations*) Consider a time-dependent rigid translation of the reference configuration $\Xi_t : \mathcal{B} \to \mathcal{B}'$. Let

$$\mathbf{X}' = \mathbf{X}_t = \Xi_t(\mathbf{X}) = \mathbf{X} + (t - t_0)\mathbf{W}, \tag{4.21}$$

for some constant vector field $\mathbf{W}$. Note that

$$T\Xi_t = \mathrm{Id}, \quad \mathbf{X} = \Xi_t^{-1}(\mathbf{X}_t) = \mathbf{X}_t - (t - t_0)\mathbf{W}. \tag{4.22}$$

Deformation gradient with respect to the new reference configuration is denoted $\mathbf{F}'$ and,

$$\mathrm{d}\mathbf{x} = \mathbf{F}\, \mathrm{d}\mathbf{X} = \mathbf{F}'\, \mathrm{d}\mathbf{X}'. \tag{4.23}$$

But, $\mathrm{d}\mathbf{X}' = \mathrm{d}\mathbf{X}$ and hence

$$\mathbf{F}\, \mathrm{d}\mathbf{X} = \mathbf{F}'\, \mathrm{d}\mathbf{X} \quad \forall\, \mathrm{d}\mathbf{X}. \tag{4.24}$$

This means that

$$\mathbf{F}'(\mathbf{X}_t) = \mathbf{F}(\mathbf{X}) \quad \text{or} \quad \mathbf{F}' = \mathbf{F} \circ \Xi_t^{-1}. \tag{4.25}$$

In the differential geometry language this means that

$$\mathbf{F}' = \Xi_{t*}\mathbf{F} = \mathbf{F} \circ \Xi_t^{-1}. \tag{4.26}$$

The material velocity with respect to the new reference configuration is

$$\mathbf{V}'(\mathbf{X}_t) = \frac{\partial}{\partial t}\varphi_t \circ \Xi_t^{-1}(\mathbf{X}') = \mathbf{V} \circ \Xi_t^{-1}(\mathbf{X}') - \mathbf{F}\mathbf{W}. \tag{4.27}$$

Thus at $t=t_0$,

$$\mathbf{V}' = \mathbf{V} - \mathbf{F}\mathbf{W}. \tag{4.28}$$

Free energy density is assumed to have the following transformation:

$$\Psi'(\mathbf{X}', \mathbf{F} \circ \Xi_t^{-1}) = \Psi(\mathbf{X}, \mathbf{F}). \tag{4.29}$$

Or

$$\Psi'(\mathbf{X}', \mathbf{F}) = \Psi(\mathbf{X}, \mathbf{F} \circ \Xi_t). \tag{4.30}$$

[Note that this does not put any restrictions on the material properties as here all we assume is that under a change of frame the 3-form $\rho_0\Psi\, \mathrm{d}V$ is transformed to a 3-form $\rho_0'\Psi'\, \mathrm{d}V' = \Xi_{t*}(\rho_0\Psi\, \mathrm{d}V)$.] More precisely,

$$\Xi_t^*\Psi'(\mathbf{X}', \mathbf{F}) = \Psi(\mathbf{X}, \mathbf{F} \circ \Xi_t). \tag{4.31}$$

Thus

$$\frac{d}{\mathrm{d}t}\Psi'(\mathbf{X}', \mathbf{F}) = \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi}{\partial (\mathbf{F} \circ \Xi_t)} : \frac{\partial \mathbf{F}}{\partial \Xi_t(\mathbf{X})} \cdot \mathbf{W}. \tag{4.32}$$

Hence at $t=t_0$

$$\frac{d}{\mathrm{d}t}\Psi'(\mathbf{X}', \mathbf{F}) = \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi}{\partial \mathbf{F}} : \frac{\partial \mathbf{F}}{\partial \mathbf{X}} \cdot \mathbf{W}. \tag{4.33}$$

Material balance of energy for $\mathcal{U} \subset \mathcal{B}$ reads

$$\begin{aligned} &\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\Psi + \frac{1}{2}\langle\langle \mathbf{V}, \mathbf{V}\rangle\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\frac{d}{\mathrm{d}t}\Psi + \langle\langle \mathbf{V}, \mathbf{A}\rangle\rangle\right)\mathrm{d}V \\ &\quad = \int_{\mathcal{U}} \rho_0(\mathbf{B} \cdot \mathbf{V} + R)\mathrm{d}V + \int_{\partial\mathcal{U}} (\mathbf{T} \cdot \mathbf{V} + H)\mathrm{d}A. \end{aligned} \tag{4.34}$$

Let us assume that material balance of energy for $\mathcal{U}' \subset \mathcal{B}'$ reads

$$\begin{aligned} \frac{d}{\mathrm{d}t}\int_{\mathcal{U}'} \rho_0'\left(\Psi' + \frac{1}{2}\mathbf{V}' \cdot \mathbf{V}'\right)\mathrm{d}V' &= \int_{\mathcal{U}'} \rho_0(\mathbf{B}' \cdot \mathbf{V}' + R')\mathrm{d}V' + \int_{\mathcal{U}'} \mathbf{B}_0' \cdot \mathbf{W}_t\, \mathrm{d}V' \\ &\quad + \int_{\partial\mathcal{U}'} (\mathbf{T}' \cdot \mathbf{V}' + H')\mathrm{d}A', \end{aligned} \tag{4.35}$$

for some vector field $\mathbf{B}_0'$ which will be determined shortly. Note that thinking of the integrand of the left-hand side of balance of energy as a 3-form α, we have

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}'} \alpha' = \int_{\mathcal{U}} \frac{d}{\mathrm{d}t}(\Xi_t^*\alpha'). \tag{4.36}$$

But $\Xi_t^*\alpha' = \rho_0(\mathbf{X})\Psi(\mathbf{X}, \mathbf{F} \circ \Xi_t)\mathrm{dV}$, thus material balance of energy for $\mathcal{U}' \subset \mathcal{B}'$ at $t=t_0$ reads

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\Psi + \frac{1}{2}\langle\langle \mathbf{V}-\mathbf{FW}, \mathbf{V}-\mathbf{FW}\rangle\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\left.\frac{d}{\mathrm{d}t}\right|_{t=t_0} \Psi' + \langle\langle \mathbf{V}-\mathbf{FW}, \mathbf{A}'|_{t=t_0}\rangle\rangle\right)\mathrm{d}V$$
$$= \int_{\mathcal{U}} \rho_0\left(\mathbf{B}'|_{t=t_0}\cdot(\mathbf{V}-\mathbf{FW}) + R\right)\mathrm{d}V + \int_{\partial\mathcal{U}} (\mathbf{T}\cdot(\mathbf{V}-\mathbf{FW}) + H)\mathrm{d}A + \int_{\mathcal{U}} \mathbf{B}_0\cdot\mathbf{W}\,\mathrm{d}V, \tag{4.37}$$

where $\mathbf{B}_0$ is an unknown vector field at this point. Note that

$$(\mathbf{B}'-\mathbf{A}')_{t=t_0} = \mathbf{B}-\mathbf{A}. \tag{4.38}$$

Now subtracting the material balance of energy for $\mathcal{U}\subset\mathcal{B}$ from that of $\mathcal{U}'\subset\mathcal{B}'$ at time $t=t_0$ yields

$$\int_{\mathcal{U}} \left(\mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}} + \rho_0\mathbf{F}^{\mathrm{T}}(\mathbf{B}-\mathbf{A}) - \mathbf{B}_0\right)\cdot\mathbf{W}\,\mathrm{d}V + \int_{\partial\mathcal{U}} \mathbf{F}^{\mathrm{T}}\mathbf{T}\cdot\mathbf{W}\mathrm{d}A = 0 \quad \forall\,\mathbf{W}. \tag{4.39}$$

Localization leads to the following conclusion:

$$\mathbf{B}_0 = \mathrm{Div}(\mathbf{F}^{\mathrm{T}}\mathbf{P}) + \rho_0\mathbf{F}^{\mathrm{T}}(\mathbf{B}-\mathbf{A}) + \mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}}. \tag{4.40}$$

Note that

$$\mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}} = \mathrm{Div}(\Psi\mathbf{I}) - \frac{\partial \Psi}{\partial \mathbf{X}}, \tag{4.41}$$

and

$$\mathrm{Div}(\mathbf{F}^{\mathrm{T}}\mathbf{P}) = \mathbf{F}^{\mathrm{T}}\,\mathrm{Div}\,\mathbf{P} + \mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}}. \tag{4.42}$$

Thus (4.40) is equivalent to

$$\mathbf{B}_0 = \mathbf{F}^{\mathrm{T}}[\mathrm{Div}\,\mathbf{P} + \rho_0(\mathbf{B}-\mathbf{A})] + 2\mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}} = 2\mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}}. \tag{4.43}$$

Therefore, the transformed balance of energy is (4.35) with $\mathbf{B}_0' = \Xi_{t*}(\mathbf{B}_0)$.
Invariance of balance of energy under rigid translations of the reference configuration is equivalent to $\mathbf{B}_0 = \mathbf{0}$, i.e.,

$$\mathbf{P}:\frac{\partial \mathbf{F}}{\partial \mathbf{X}} = \mathbf{0}, \tag{4.44}$$

which is equivalent to

$$\mathrm{Div}(\mathbf{F}^{\mathrm{T}}\mathbf{P}) = \mathbf{F}^{\mathrm{T}}\,\mathrm{Div}(\mathbf{P}). \tag{4.45}$$

Obviously, if $\mathbf{F}$ is independent of $\mathbf{X}$, i.e., if the deformation gradient is uniform then this condition is satisfied but as we will see in the sequel this is not necessary. Note that (4.43) is independent of balance of linear momentum. It is seen that an additional constraint must be satisfied for the material energy balance to be invariant under time-dependent rigid referential translations. This shows the very different natures of material and spatial manifolds. We will show at the end of Sec. VI that (4.45) implies that configurational stress tensor is hydrostatic. For this reason we call (4.45) the configurational inviscidity constraint.
Example: Consider a Neo-Hookean rod in uniaxial tension. The deformation gradient is

$$\mathbf{F} = \begin{pmatrix} \lambda^{-1/2} & 0 & 0 \\ 0 & \lambda^{-1/2} & 0 \\ 0 & 0 & \lambda \end{pmatrix}. \tag{4.46}$$

It can be easily shown that the first Piola-Kirchhoff stress tensor has the following representation:

$$\mathbf{P} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \mu\lambda - \dfrac{\mu}{\lambda^2} \end{pmatrix}, \tag{4.47}$$

where $\mu = \mu(\mathbf{X})$. It is now an easy exercise to show that (4.45) is satisfied only if λ is constant, i.e., only if the deformation gradient is uniform. Thus in this case the only possibility would be a uniform deformation gradient for balance of energy to be invariant under rigid translations of the reference configuration.

Example: We know that for an isotropic material

$$S_{AB} = \alpha_0 G_{AB} + \alpha_1 C_{AB} + \alpha_2 C_A^D C_{DB}, \tag{4.48}$$

where α_0, α_1, and α_2 are scalar functions of $\mathbf{X}$ and S_{AB} are components of the second Piola-Kirchhoff stress tensor. For the sake of simplicity, suppose $\alpha_1 = \alpha_2 = 0$. In terms of $\mathbf{P}$ and $\mathbf{F}$ we have

$$P^{aA} = \alpha_0 G^{AB} F^a{}_B. \tag{4.49}$$

When the reference configuration and ambient space are Euclidean the condition $\mathrm{Div}(\mathbf{F}^\mathsf{T}\mathbf{P}) = \mathbf{F}^\mathsf{T}\,\mathrm{Div}(\mathbf{P})$ is equivalent to

$$\alpha_0 F^a{}_B \frac{\partial F^a{}_B}{\partial X^A} = 0. \tag{4.50}$$

Or

$$F^a{}_B \frac{\partial F^a{}_B}{\partial X^A} = F^a{}_B \frac{\partial F^a{}_A}{\partial X^B} = 0. \tag{4.51}$$

Note that, in general, this does not imply that the deformation gradient is uniform and it is simply an internal constraint.

Example: Consider an incompressible perfect fluid (ideal fluid) for which

$$\sigma^{ab} = -pg^{ab} \quad \text{and} \quad J = 1. \tag{4.52}$$

Thus

$$P^{aA} = -J(\mathbf{F}^{-1})^A{}_b p g^{ab}. \tag{4.53}$$

Using Piola identity we have

$$(\mathrm{Div}(\mathbf{F}^\mathsf{T}\mathbf{P}))^A = (-pJG^{AB})_{|B} = -J\frac{\partial p}{\partial x^b} F^b{}_B G^{AB}. \tag{4.54}$$

Also

$$(\mathbf{F}^\mathsf{T}\,\mathrm{Div}(\mathbf{P}))^A = -g_{ab} F^b{}_B G^{AB} J(pg^{ad})_{|d} = -J\frac{\partial p}{\partial x^b} F^b{}_B G^{AB}. \tag{4.55}$$

Thus (4.45) is satisfied for an ideal fluid.

(ii) (*Rigid rotations*) Consider a time-dependent rigid rotation of the reference configuration $\Xi_t:\mathcal{B}\to\mathcal{B}'$ defined as

$$\mathbf{X}'=\mathbf{X}_t=e^{(t-t_0)\mathbf{\Omega}}\mathbf{X}, \tag{4.56}$$

for some constant skew-symmetric matrix $\mathbf{\Omega}$. Note that

$$\mathbf{V}'=V-\mathbf{F}\mathbf{\Omega}\mathbf{X},\quad \mathbf{F}'=\mathbf{F}\circ\Xi_t^{-1}. \tag{4.57}$$

Let us assume that material balance of energy for $\mathcal{U}'\subset\mathcal{B}'$ has the following form:

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}'}\rho_0'\left(\Psi'+\frac{1}{2}\mathbf{V}'\cdot\mathbf{V}'\right)\mathrm{d}V'=\int_{\mathcal{U}'}\rho_0(\mathbf{B}'\cdot\mathbf{V}'+R')\mathrm{d}V'+\int_{\partial\mathcal{U}'}(\mathbf{T}'\cdot\mathbf{V}'+H')\mathrm{d}A'$$
$$+\int_{\mathcal{U}'}(\mathbf{B}_0'\cdot\mathbf{\Omega}\mathbf{X}+\mathbf{C}_0':\mathbf{\Omega})\mathrm{d}V', \tag{4.58}$$

where $\mathbf{C}_0'=\Xi_{t*}\mathbf{C}_0$ and $\mathbf{C}_0$ is an unknown vector field at this point. Material balance of energy for $\mathcal{U}'\subset\mathcal{B}'$ at $t=t_0$ reads

$$\int_{\mathcal{U}}\frac{\partial\rho_0}{\partial t}\left(\Psi+\frac{1}{2}\langle\langle\mathbf{V}-\mathbf{F}\mathbf{\Omega}\mathbf{X},\mathbf{V}-\mathbf{F}\mathbf{\Omega}\mathbf{X}\rangle\rangle\right)\mathrm{d}V$$
$$+\int_{\mathcal{U}}\rho_0\left(\left.\frac{d}{\mathrm{d}t}\right|_{t=t_0}\Psi'+\langle\langle\mathbf{V}-\mathbf{F}\mathbf{\Omega}\mathbf{X},\mathbf{A}'|_{t=t_0}\rangle\rangle\right)\mathrm{d}V$$
$$=\int_{\mathcal{U}}\rho_0(\mathbf{B}'|_{t=t_0}\cdot(\mathbf{V}-\mathbf{F}\mathbf{\Omega}\mathbf{X})+R)\mathrm{d}V+\int_{\partial\mathcal{U}}(\mathbf{T}\cdot(\mathbf{V}-\mathbf{F}\mathbf{\Omega}\mathbf{X})+H)\mathrm{d}A$$
$$+\int_{\mathcal{U}}(\mathbf{B}_0\cdot\mathbf{\Omega}\mathbf{X}+\mathbf{C}_0:\mathbf{\Omega})\mathrm{d}V. \tag{4.59}$$

Subtracting the material balance of energy for $\mathcal{U}\subset\mathcal{B}$ from that of $\mathcal{U}'\subset\mathcal{B}'$ at time $t=t_0$ and considering the relation for $\mathbf{B}_0$ coming from rigid translations of the reference configuration yields

$$\int_{\mathcal{U}}(\mathbf{F}^{\mathsf{T}}\mathbf{P}-\mathbf{C}_0):\Omega\,\mathrm{d}V=0. \tag{4.60}$$

This means that

$$\mathbf{F}^{\mathsf{T}}\mathbf{P}-\mathbf{C}_0=(\mathbf{F}^{\mathsf{T}}\mathbf{P}-\mathbf{C}_0)^{\mathsf{T}}. \tag{4.61}$$

Thus $\mathbf{C}_0=-\mathbf{P}^{\mathsf{T}}\mathbf{F}+\mathbf{S}$ for some symmetric tensor $\mathbf{S}$. This symmetric tensor does not contribute to balance of energy and we can choose it to be $\mathbf{S}=\mathbf{0}$. Thus the transformed balance of energy under rigid rotations of the reference configuration is (4.58) where $\mathbf{C}_0'=\Xi_{t*}(\mathbf{C}_0)$ and $\mathbf{C}_0=-\mathbf{P}^{\mathsf{T}}\mathbf{F}$.

In conclusion, we have proved the following proposition.

Proposition 4.1: Balance of energy is invariant under time-dependent translations and rotations of the reference configuration if $\mathbf{B}_0=\mathbf{C}_0=\mathbf{0}$, i.e., if the reference configuration is both configurationally inviscid and isotropic.

Thus, balance of energy is invariant under material isometries of the reference configuration only under some constraints. As an example, it is seen that balance of energy is invariant under material isometries in the case of ideal fluids.

V. COVARIANT SPATIAL ENERGY BALANCE

In this section we start by a reappraisal of the concept of covariance in elasticity and its consequences. We revisit Marsden and Hughes' theorem[28] and clarify some details in their proof. We then show that the same conclusions can be reached if one assumes that mass density is a 3-form instead of a scalar. A proof is then given for converse of Marsden and Hughes' theorem, i.e., assuming conservation of mass, balance of linear and angular momenta and Doyle-Ericksen formula, balance of energy is invariant under arbitrary spatial diffeomorphisms. At the end of this section, we show that assuming spatial covariance for material energy balance yields results that are identical to those obtained by assuming spatial covariance for spatial energy balance.

A. Covariance and the Doyle-Ericksen formula

First recall that the general notion of covariance of a set of equations is as follows.

Definition 5.1 (Covariance): Suppose a theory has some tensor fields $\mathbf{U},\mathbf{V},\ldots$ *defined on a space* $\mathcal{A}$ *and the governing equations of the theory have the form* $F(\mathbf{U},\mathbf{V},\ldots)=0$. *These governing equations are called covariant if for any diffeomorphism* $\xi:\mathcal{A}\to\mathcal{A}$, $\xi^*(F(\mathbf{U},\mathbf{V},\ldots))=F(\xi^*\mathbf{U},\xi^*\mathbf{V},\ldots)$. *A theory is covariant if all its governing equations are covariant.*

The Doyle-Ericksen formula: Doyle and Ericksen[7] showed the following interesting relation:

$$\boldsymbol{\sigma}=2\rho\frac{\partial e}{\partial \mathbf{g}}, \tag{5.1}$$

i.e., Cauchy's stress tensor is proportional to the partial derivative of the free energy density with respect to the Riemannian metric in the deformed configuration. [Note that (see Ref. 28, p. 198)

$$\frac{\partial e}{\partial \mathbf{g}}=\frac{\partial \psi}{\partial \mathbf{g}}. \tag{5.2}$$

In other words, in Doyle-Ericksen formula internal energy density can be replaced by free energy density because

$$e=\psi+\theta s, \tag{5.3}$$

where θ is absolute temperature and s is entropy density. Thus

$$\frac{\partial e}{\partial \mathbf{g}}=\frac{\partial \psi}{\partial \mathbf{g}}+\frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial \mathbf{g}}+\frac{\partial \theta}{\partial \mathbf{g}}s=\frac{\partial \psi}{\partial \mathbf{g}}, \tag{5.4}$$

as $\partial\psi/\partial\theta=-s$].

Doyle and Ericksen[7] looked at changes of spatial frame passively, i.e., as changes of coordinates while Marsden and Hughes[28] chose the active point of view. The Doyle-Ericksen formula is known to be the essential condition for covariance of energy balance. Later Simo and Marsden[40] found a material version of Doyle-Ericksen formula, which we discuss next. Here by "material version" they mean an analogue of the usual Doyle-Ericksen formula that ensures covariance of material energy balance under spatial diffeomorphisms. [An interesting question to ask would be the condition(s) that ensures covariance of material energy balance under diffeomorphisms of the reference configuration. This will be discussed in Sec. VI.] Simo and Marsden consider a general form of polar decomposition theorem by first associating two Riemannian metrics $\mathbf{G}_0$ and $\mathbf{G}$ to $\mathcal{B}$, where $\mathbf{G}_0$ does not change under spatial diffeomorphisms while $\mathbf{G}$ does change. The polar decomposition theorem states that

$$\mathbf{F}=\mathbf{R}\mathbf{U}, \tag{5.5}$$

where

$$\mathbf{U}(\mathbf{X}):(T_{\mathbf{X}}\mathcal{B},\mathbf{G}_0)\rightarrow(T_{\mathbf{X}}\mathcal{B},\mathbf{G}) \tag{5.6}$$

is the material stretch tensor (a positive-definite symmetric linear map with respect to the given metrics) and

$$\mathbf{R}(\mathbf{X}):(T_{\mathbf{X}}\mathcal{B},\mathbf{G})\rightarrow(T_{\varphi_t(\mathbf{X})}\mathcal{S},\mathbf{g}) \tag{5.7}$$

is, for each $X\in\mathcal{B}$, a $(\mathbf{G},\mathbf{g})$-orthogonal linear transformation. The metric $\mathbf{G}$ is arbitrary and can change under spatial diffeomorphisms,

$$\mathbf{G}=\mathbf{R}^{*}(\mathbf{g}). \tag{5.8}$$

The internal energy density per unit mass of the deformed configuration is

$$e=e(\mathbf{x},t,\mathbf{g}(\mathbf{x})). \tag{5.9}$$

Now define

$$E(\mathbf{X},t,\mathbf{G})=e(\varphi_t(\mathbf{X}),t,\mathbf{R}_{*}(\mathbf{G})). \tag{5.10}$$

Simo and Marsden[40] show that

$$\mathbf{\Sigma}=2\rho\frac{\partial E}{\partial\mathbf{G}}, \tag{5.11}$$

where $\mathbf{\Sigma}$ is the rotated stress tensor defined as

$$\mathbf{\Sigma}=\mathbf{R}^{*}\boldsymbol{\sigma}\quad\text{or}\quad\Sigma^{AB}=(\mathbf{R}^{-1})^{A}{}_{a}\sigma^{ab}(\mathbf{R}^{-1})^{B}{}_{b}. \tag{5.12}$$

In this paper we prove a similar theorem by postulating a balance of energy for an arbitrary reframing of the reference configuration for a special class of materials. It should be noted that there are four possibilities for a covariant energy balance law.

(i) Spatial energy balance law for any reframing of the deformed configuration: This gives the usual Doyle-Ericksen formula.
(ii) Material energy balance law for any reframing of the deformed configuration: This gives the Doyle-Ericksen formula in terms of Kirchhoff stress tensor.
(iii) Material energy balance law for any reframing of the reference configuration: This should give a material form of Doyle-Ericksen formula for Eshelby's stress tensor.
(iv) Spatial energy balance for any reframing of the reference configuration: This should give a spatial form of Doyle-Ericksen formula for Eshelby's stress tensor.

Note that cases (i) and (ii) and also cases (iii) and (iv) are equivalent as the important thing here is the type of the diffeomorphism.

B. Revisiting Marsden and Hughes' theorem

Let us first revisit Marsden and Hughes' covariant energy balance theory.[28] These authors postulate a covariant spatial energy balance, i.e., they consider a motion $\varphi_t:\mathcal{B}\rightarrow\mathcal{S}$ and postulate that balance of energy still holds for any spatial change of frame. Marsden and Hughes consider arbitrary changes of frame for the deformed configuration and postulate that energy balance is invariant under these framings. For a given nice subset $\mathcal{U}\subset\mathcal{B}$, the (spatial) balance of energy reads

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})}\rho\left(e+\frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right)dv=\int_{\varphi_t(\mathcal{U})}\rho(\langle\langle\mathbf{b},\mathbf{v}\rangle\rangle+r)dv+\int_{\partial\varphi_t(\mathcal{U})}(\langle\langle\mathbf{t},\mathbf{v}\rangle\rangle+h)da, \tag{5.13}$$

where e,r, and h are the internal energy function per unit mass, the heat supply per unit mass and the heat flux, respectively. Marsden and Hughes then consider an arbitrary reframing of the deformed configuration, which can be regarded as a motion of $\mathcal{S}$ in $\mathcal{S}$, i.e., $\xi_t:\mathcal{S}\rightarrow\mathcal{S}$. Postulating

the balance of energy (5.13) for such a reframing and considering it for $t=t_0$ they obtain (i) conservation of mass, (ii) balance of linear momentum, (iii) balance of angular momentum, and (iv) the Doyle-Ericksen formula. Conversely, if (i), (ii), (iii), (iv) and balance of energy hold, then balance of energy would hold for any change of spatial frame. We will give a proof for the converse of the theorem in the sequel.

Proposition 5.2 (Transport theorem in a reframing of the deformed configuration): Suppose $f'=\xi_{t*}f$ *is a scalar quantity defined on* $\varphi_t'(\mathcal{U})$, *i.e.*, $f':\varphi_t'(\mathcal{U})\to\mathbb{R}$ *and* $f:\varphi_t(\mathcal{U})\to\mathbb{R}$. [Marsden and Hughes have the following transport theorem on p. 166 of Ref. 28 in the second equation after their Eq. (2), which needs to be corrected:

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})} f\,\mathrm{d}v=\int_{\varphi_t'(\mathcal{U})}(\dot{f}+f\,\mathrm{div}\,\mathbf{v})\mathrm{d}v'. \tag{5.14}$$

In fact, the first $\mathrm{d}v$ should read $\mathrm{d}v'$.] *Then*,

$$\frac{d}{\mathrm{d}t}\bigg|_{t=t_0}\int_{\varphi_t'(\mathcal{U})} f'\,\mathrm{d}v'=\int_{\varphi_t(\mathcal{U})}(\dot{f}+f\,\mathrm{div}\,\mathbf{v})\mathrm{d}v. \tag{5.15}$$

Proof: The usual transport theorem can be written as

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})} f'\,\mathrm{d}v'=\int_{\varphi_t'(\mathcal{U})}(\dot{f}'+f'\,\mathrm{div}'\,\mathbf{v}')\mathrm{d}v', \tag{5.16}$$

where

$$\dot{f}'=\frac{\partial f'}{\partial t}+\frac{\partial f'}{\partial \mathbf{x}'}\cdot\mathbf{v}'=\frac{\partial f'}{\partial t}+\mathrm{d}f'\cdot\mathbf{v}', \tag{5.17}$$

and

$$\mathbf{v}'=\xi_{t*}\mathbf{v}+\mathbf{w}. \tag{5.18}$$

Therefore,

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})} f'\,\mathrm{d}v'=\int_{\varphi_t'(\mathcal{U})}\left[\frac{\partial f'}{\partial t}+\mathrm{d}f'\cdot(\xi_{t*}\mathbf{v}+\mathbf{w})+f'\,\mathrm{div}'\,\mathbf{v}'\right]\mathrm{d}v'. \tag{5.19}$$

Note that

$$\frac{\partial}{\partial \mathbf{x}}=\frac{\partial}{\partial \mathbf{x}'}\circ(T\xi_t)\quad\text{or}\quad\frac{\partial}{\partial \mathbf{x}'}=(T\xi_t)^{-1}\circ\frac{\partial}{\partial \mathbf{x}}. \tag{5.20}$$

This means that

$$\frac{\partial}{\partial \mathbf{x}'}\bigg|_{t=t_0}=\frac{\partial}{\partial \mathbf{x}}. \tag{5.21}$$

Lemma 5.3: If $\xi_t:\mathcal{S}\to\mathcal{S}$ *is a diffeomorphism with the properties*,

$$\xi_t\big|_{t=t_0}=\mathrm{Id},\quad T\xi_t\big|_{t=t_0}=\mathrm{Id}. \tag{5.22}$$

Then

$$(\mathrm{div}'\,\mathbf{v}'\,\mathrm{d}v')\big|_{t=t_0}=\mathrm{div}\,\mathbf{v}\,\mathrm{d}v. \tag{5.23}$$

Proof: We prove the lemma when $\mathcal{S}$ is equipped with an arbitrary volume form μ. This will imply the particular case of a Riemannian manifold with the volume form induced by the Rie-

mannian metric. Recall that the divergence of a vector field $\mathbf{X}$ with respect to μ is defined as

$$\mathbf{L}_{\mathbf{X}}\mu = (\mathrm{div}_{\mu}\,\mathbf{X})\mu. \tag{5.24}$$

Under the spatial change of frame $\mathbf{v}' = \xi_{t*}\mathbf{X} + \mathbf{w}$, $\mu' = \xi_{t*}\mu$. Thus,

$$(\mathrm{div}_{\mu'}\,\mathbf{v}')\mu' = \mathbf{L}_{\mathbf{v}'}(\xi_{t*}\mu) = \xi_{t*}(\mathbf{L}_{\mathbf{v}}\mu), \tag{5.25}$$

where use was made of Theorem 6.19 of Marsden and Hughes[28]. Therefore,

$$(\mathrm{div}'\,\mathbf{v}'\,\mathrm{d}v')\big|_{t=t_0} = \mathrm{div}\,\mathbf{v}\,\mathrm{d}v. \tag{5.26}$$

□

One should be careful with partial time derivatives as $\partial f'/\partial t$ is not equal to $\partial f/\partial t$ at $t=t_0$ because the former is partial time derivative for fixed $\mathbf{x}'$ while the latter is a partial time derivative for fixed $\mathbf{x}$. Note that

$$\left.\frac{\partial f'}{\partial t}\right|_{\mathbf{x}\ \text{fixed}} = \left.\frac{\partial f'}{\partial t}\right|_{\mathbf{x}'\ \text{fixed}} + \mathrm{d}f'\cdot\mathbf{w}_t. \tag{5.27}$$

Hence,

$$\left(\left.\frac{\partial f'}{\partial t}\right|_{\mathbf{x}'\ \text{fixed}}\right)_{t=t_0} = \frac{\partial f}{\partial t} - \mathrm{d}f\cdot\mathbf{w}. \tag{5.28}$$

Therefore (5.19) is simplified to

$$\left.\frac{d}{\mathrm{d}t}\right|_{t=t_0}\int_{\varphi_t'(\mathcal{U})} f'\,\mathrm{d}v' = \int_{\varphi_t(\mathcal{U})}(\dot{f} + f\,\mathrm{div}\,\mathbf{v})\mathrm{d}v. \tag{5.29}$$

□

Now let us take a more natural approach and assume that we are transporting a 3-form. Note that this is more general in the sense that we have not chosen a volume form $\mathrm{d}v$ *a priori*.

Proposition 5.4: Suppose $\alpha' = \xi_{t*}\alpha$ *is a* 3*-form defined on* $\varphi_t'(\mathcal{U})$. *Then*,

$$\left.\frac{d}{\mathrm{d}t}\right|_{t=t_0}\int_{\varphi_t'(\mathcal{U})}\alpha' = \int_{\varphi_t(\mathcal{U})}\mathbf{L}_{\mathbf{v}}\alpha. \tag{5.30}$$

Proof: Using the usual transport theorem for forms we have

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})}\alpha' = \int_{\varphi_t'(\mathcal{U})}\mathbf{L}_{\mathbf{v}'}\alpha'. \tag{5.31}$$

Assuming that α transforms objectively, i.e., $\alpha' = \xi_{t*}\alpha$, using Theorem 6.19 of Marsden and Hughes[28] we have

$$\mathbf{L}_{\mathbf{v}'}\alpha' = \xi_{t*}\mathbf{L}_{\mathbf{v}}\alpha. \tag{5.32}$$

Thus,

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})}\alpha' = \int_{\varphi_t'(\mathcal{U})}\xi_{t*}\mathbf{L}_{\mathbf{v}}\alpha. \tag{5.33}$$

Therefore,

$$\left.\frac{d}{dt}\right|_{t=t_0}\int_{\varphi_t'(\mathcal{U})}\alpha' = \int_{\varphi_t(\mathcal{U})}\mathbf{L}_{\mathbf{v}}\alpha. \tag{5.34}$$

□

Now substitute $\alpha = f\,dv$, where f is a scalar. Note that

$$f'\,dv' = f'\wedge dv' = (\xi_{t*}f)\wedge(\xi_{t*}\,dv) = \xi_{t*}(f\wedge dv) = \xi_{t*}(f\,dv). \tag{5.35}$$

The above proposition now reads

$$\left.\frac{d}{dt}\right|_{t=t_0}\int_{\varphi_t'(\mathcal{U})}f'\,dv' = \int_{\varphi_{t_0}(\mathcal{U})}\mathbf{L}_{\mathbf{v}}(f\,dv). \tag{5.36}$$

Note that $\mathbf{L}$ is a derivation and hence

$$\mathbf{L}_{\mathbf{v}}(f\,dv) = (\mathbf{L}_{\mathbf{v}}f)dv + f(\mathbf{L}_{\mathbf{v}}\,dv) = (\dot{f} + \operatorname{div}\mathbf{v})dv. \tag{5.37}$$

Therefore

$$\left.\frac{d}{dt}\right|_{t=t_0}\int_{\varphi_t'(\mathcal{U})}f'\,dv' = \int_{\varphi_{t_0}(\mathcal{U})}(\dot{f} + f\operatorname{div}\mathbf{v})dv. \tag{5.38}$$

Thus, this approach recovers the same transport equation (5.15).

C. Energy balance in terms of differential forms

In this section we regard ρ as a 3-form and write the energy balance equation as

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})}\rho\left(e + \frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right) = \int_{\varphi_t(\mathcal{U})}\rho(\langle\langle\mathbf{b},\mathbf{v}\rangle\rangle + r) + \int_{\partial\varphi_t(\mathcal{U})}(\langle\langle\mathbf{t},\mathbf{v}\rangle\rangle + h)da. \tag{5.39}$$

[Traction can be thought of as a covector-valued 2-form. There are some technical details involved and we choose to stick to the usual definition of traction.] Under a spatial diffeomorphism $\xi_t:\mathcal{S}\to\mathcal{S}$ we postulate that

$$\frac{d}{dt}\int_{\varphi_t'(\mathcal{U})}\rho'\left(e' + \frac{1}{2}\langle\langle\mathbf{v}',\mathbf{v}'\rangle\rangle\right) = \int_{\varphi_t'(\mathcal{U})}\rho'(\langle\langle\mathbf{b}',\mathbf{v}'\rangle\rangle + r') + \int_{\partial\varphi_t'(\mathcal{U})}(\langle\langle\mathbf{t}',\mathbf{v}'\rangle\rangle + h')da'. \tag{5.40}$$

Let f be the scalar multiplying the density 3-form in the first integrand, i.e., $f := e + \frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle$. Thus

$$\frac{d}{dt}\int_{\varphi_t(\mathcal{U})}\rho f = \int_{\varphi_t(\mathcal{U})}\mathbf{L}_{\mathbf{v}}(\rho f) = \int_{\varphi_t(\mathcal{U})}(\rho\mathbf{L}_{\mathbf{v}}f + f\mathbf{L}_{\mathbf{v}}\rho). \tag{5.41}$$

But

$$\begin{aligned}\mathbf{L}_{\mathbf{v}}f &= \mathbf{L}_{\mathbf{v}}e + \mathbf{L}_{\mathbf{v}}\left(\tfrac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right) = \dot{e} + \frac{\partial}{\partial t}\left(\frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right) + d\left(\frac{1}{2}\langle\langle\mathbf{v},\mathbf{v}\rangle\rangle\right)\cdot\mathbf{v}\\ &= \dot{e} + \left\langle\left\langle\frac{\partial\mathbf{v}}{\partial t},\mathbf{v}\right\rangle\right\rangle + \langle\langle\mathbf{v},\nabla_{\mathbf{v}}\mathbf{v}\rangle\rangle = \dot{e} + \langle\langle\mathbf{v},\mathbf{a}\rangle\rangle.\end{aligned} \tag{5.42}$$

Also,

$$\frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})}\rho' f' = \int_{\varphi_t(\mathcal{U})}\mathbf{L}_{\mathbf{v}'}(\rho' f') = \int_{\varphi_t'(\mathcal{U})}(\rho'\mathbf{L}_{\mathbf{v}'}f' + f'\mathbf{L}_{\mathbf{v}'}\rho'). \tag{5.43}$$

Note that $\mathbf{v}' = \xi_{t*}\mathbf{v} + \mathbf{w}_t$ and thus

$$\mathbf{L}_{\mathbf{v}'}\rho' = \xi_{t*}(\mathbf{L}_{\mathbf{v}}\rho). \tag{5.44}$$

Also,

$$\mathbf{L}_{\mathbf{v}'}f' = \dot{e'} + \left\langle\!\left\langle \mathbf{v}', \frac{\partial \mathbf{v}'}{\partial t} + \nabla_{\mathbf{v}'}\mathbf{v}' \right\rangle\!\right\rangle = \dot{e'} + \langle\langle \mathbf{v}', \mathbf{a}' \rangle\rangle. \tag{5.45}$$

Thus

$$(\mathbf{L}_{\mathbf{v}'}f')\big|_{t=t_0} = \dot{e} + \frac{\partial e}{\partial \mathbf{g}} : \mathfrak{L}_{\mathbf{w}}\mathbf{g} + \langle\langle \mathbf{v}+\mathbf{w}, \mathbf{a}'\big|_{t=t_0}\rangle\rangle, \tag{5.46}$$

$$(\mathbf{L}_{\mathbf{v}'}\rho')\big|_{t=t_0} = \mathbf{L}_{\mathbf{v}}\rho. \tag{5.47}$$

Therefore

$$\begin{aligned}\frac{d}{\mathrm{d}t}\bigg|_{t=t_0}\int_{\varphi_t'(\mathcal{U})}\rho' f' = \int_{\varphi_t(\mathcal{U})}\rho\left(\dot{e} + \frac{\partial e}{\partial \mathbf{g}} : \mathfrak{L}_{\mathbf{w}}\mathbf{g} + \left\langle\!\left\langle \mathbf{v}+\mathbf{w}, \mathbf{a}'\big|_{t=t_0}\right\rangle\!\right\rangle\right) \\ + \int_{\varphi_t(\mathcal{U})}\left(f + \langle\langle \mathbf{v}, \mathbf{w}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{w}, \mathbf{w}\rangle\rangle\right)\mathbf{L}_{\mathbf{v}}\rho.\end{aligned} \tag{5.48}$$

Now subtracting the balance of energy equation for $\varphi_t(\mathcal{U})$ from that of $\varphi_t'(\mathcal{U})$ at $t=t_0$ we obtain

$$\begin{aligned}&\int_{\varphi_t(\mathcal{U})}\rho\left(\frac{\partial e}{\partial \mathbf{g}} : \mathcal{L}_{\mathbf{w}}\mathbf{g} + \langle\langle \mathbf{v}, \mathbf{a}'\big|_{t=t_0} - \mathbf{a}\rangle\rangle + \langle\langle \mathbf{w}, \mathbf{a}'\big|_{t=t_0}\rangle\rangle\right) + \int_{\varphi_t(\mathcal{U})}\left(\langle\langle \mathbf{v}, \mathbf{w}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{w}, \mathbf{w}\rangle\rangle\right)\mathbf{L}_{\mathbf{v}}\rho \\ &= \int_{\varphi_t(\mathcal{U})}(\langle\langle \mathbf{v}, \mathbf{b}'\big|_{t=t_0} - \mathbf{b} + \langle\langle \mathbf{w}, \mathbf{b}'\big|_{t=t_0}\rangle\rangle) + \int_{\partial\varphi_t(\mathcal{U})}\langle\langle \mathbf{w}, \mathbf{t}\rangle\rangle \mathrm{d}a.\end{aligned} \tag{5.49}$$

Using the identity $(\mathbf{b}' - \mathbf{a}')\big|_{t=t_0} = \mathbf{b} - \mathbf{a}$ we have

$$\int_{\varphi_t(\mathcal{U})}\rho\left(\frac{\partial e}{\partial \mathbf{g}} : \mathcal{L}_{\mathbf{w}}\mathbf{g} + \langle\langle \mathbf{w}, \mathbf{a} - \mathbf{b}\rangle\rangle\right) + \int_{\varphi_t(\mathcal{U})}\left(\langle\langle \mathbf{v}, \mathbf{w}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{w}, \mathbf{w}\rangle\rangle\right)\mathbf{L}_{\mathbf{v}}\rho = \int_{\partial\varphi_t(\mathcal{U})}\langle\langle \mathbf{w}, \mathbf{t}\rangle\rangle \mathrm{d}a. \tag{5.50}$$

We know that

$$\int_{\partial\varphi_t(\mathcal{U})}\langle\langle \mathbf{w}, \mathbf{t}\rangle\rangle \mathrm{d}a = \int_{\varphi_t(\mathcal{U})}\left(\langle\langle \operatorname{div}\boldsymbol{\sigma}, \mathbf{w}\rangle\rangle + \boldsymbol{\sigma} : \frac{1}{2}\mathcal{L}_{\mathbf{w}}\mathbf{g} + \boldsymbol{\sigma} : \boldsymbol{\omega}\right)\mathrm{d}v, \tag{5.51}$$

where $\boldsymbol{\omega}$ has the coordinate representation $\omega_{ab} = \frac{1}{2}(w_{a|b} - w_{b|a})$. Let us replace ρ by $\rho\,\mathrm{d}v$ in the first integral of Eq. (5.50),

$$\int_{\varphi_t(\mathcal{U})} \rho\left(\frac{\partial e}{\partial \mathbf{g}}:\mathcal{L}_{\mathbf{w}}\mathbf{g} + \langle\langle \mathbf{w}, \mathbf{a}-\mathbf{b}\rangle\rangle\right)\mathrm{d}v + \int_{\varphi_t(\mathcal{U})}\left(\langle\langle \mathbf{v},\mathbf{w}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{w},\mathbf{w}\rangle\rangle\right)\mathbf{L}_{\mathbf{v}}\rho$$
$$= \int_{\varphi_t(\mathcal{U})}\left(\langle\langle \operatorname{div}\boldsymbol{\sigma},\mathbf{w}\rangle\rangle + \boldsymbol{\sigma}:\frac{1}{2}\mathcal{L}_{\mathbf{w}}\mathbf{g} + \boldsymbol{\sigma}:\boldsymbol{\omega}\right)\mathrm{d}v. \tag{5.52}$$

Since $\mathbf{w}$ is arbitrary we conclude that

$$\mathbf{L}_{\mathbf{v}}\rho = 0, \tag{5.53}$$

$$\boldsymbol{\sigma} = 2\rho\frac{\partial e}{\partial \mathbf{g}}, \tag{5.54}$$

$$\operatorname{div}\boldsymbol{\sigma} + \rho\mathbf{b} = \rho\mathbf{a}, \tag{5.55}$$

$$\boldsymbol{\sigma}^{\mathsf{T}} = \boldsymbol{\sigma}. \tag{5.56}$$

D. Proof of the converse of Marsden and Hughes' theorem

Marsden and Hughes[28] do not give a proof for the converse of the covariant energy balance theorem, i.e., when Eqs. (5.53)–(5.56) are satisfied then energy balance is invariant under $\xi_t:\mathcal{S}\to\mathcal{S}$. Such a proof is nontrivial and is given here.

Let us assume that Eqs. (5.53)–(5.56) are satisfied and define

$$\Delta E(\xi_t) = \frac{d}{\mathrm{d}t}\int_{\varphi_t'(\mathcal{U})}\rho'\left(e' + \frac{1}{2}\langle\langle \mathbf{v}',\mathbf{v}'\rangle\rangle_{\mathbf{g}}\right) - \int_{\varphi_t'(\mathcal{U})}\rho'\left(\langle\langle \mathbf{b}',\mathbf{v}'\rangle\rangle_{\mathbf{g}} + r'\right) - \int_{\partial\varphi_t'(\mathcal{U})}\left(\langle\langle \mathbf{t}',\mathbf{v}'\rangle\rangle_{\mathbf{g}} + h'\right)\mathrm{d}a'. \tag{5.57}$$

Note that balance of energy for $\varphi_t(\mathcal{U})$ can be written as $\Delta E(\mathrm{Id})=0$. We need to prove that for any diffeomorphism ξ_t, $\Delta E(\xi_t)=0$. We know that

$$e'(x',t,\mathbf{g}) = e(x,t,\xi_t^*(\mathbf{g})). \tag{5.58}$$

Let us denote

$$\mathbf{w}_t := \frac{d}{\mathrm{d}t}\xi_t, \quad \mathbf{W}_t = \xi_t^*(\mathbf{w}_t), \quad \mathbf{g}_t = \xi_t^*(\mathbf{g}). \tag{5.59}$$

Note that by definition

$$\int_{\varphi_t'(\mathcal{U})}\rho' r' = \int_{\varphi_t(\mathcal{U})}\rho r, \quad \int_{\partial\varphi_t'(\mathcal{U})} h'\,\mathrm{d}a' = \int_{\partial\varphi_t(\mathcal{U})} h\,\mathrm{d}a. \tag{5.60}$$

Also note that

$$\int_{\partial\varphi_t'(\mathcal{U})}\langle\langle \mathbf{t}',\mathbf{v}'\rangle\rangle_{\mathbf{g}}\,\mathrm{d}a' = \int_{\partial\varphi_t'(\mathcal{U})}\langle\langle \xi_{t*}\mathbf{t}, \xi_{t*}\mathbf{v}+\mathbf{w}_t\rangle\rangle_{\mathbf{g}}\,\mathrm{d}a' = \int_{\partial\varphi_t(\mathcal{U})}\langle\langle \mathbf{t},\mathbf{v}+\mathbf{W}_t\rangle\rangle_{\mathbf{g}_t}\,\mathrm{d}a. \tag{5.61}$$

A straightforward computation shows that

$$\frac{d}{dt}\int_{\varphi_t'(\mathcal{U})}\left(\frac{1}{2}\rho'\langle\langle\mathbf{v}',\mathbf{v}'\rangle\rangle_{\mathbf{g}}-\rho'\langle\langle\mathbf{b}',\mathbf{v}'\rangle\rangle_{\mathbf{g}}\right)=\int_{\varphi_t'(\mathcal{U})}\rho'\langle\langle\xi_{t*}(\mathbf{a}-\mathbf{b}),\xi_{t*}\mathbf{v}+\mathbf{w}_t\rangle\rangle_{\mathbf{g}}=\int_{\varphi_t(\mathcal{U})}\rho\langle\langle\mathbf{a}-\mathbf{b},\mathbf{v}\rangle\rangle_{\mathbf{g}_t}$$
$$+\int_{\varphi_t(\mathcal{U})}\rho\langle\langle\mathbf{a}-\mathbf{b},\mathbf{W}_t\rangle\rangle_{\mathbf{g}_t}, \tag{5.62}$$

where use was made of $\mathbf{L}_{\mathbf{v}}\rho=0$. Note that

$$\frac{d}{dt}\int_{\varphi_t'(\mathcal{U})}\rho'e'=\int_{\varphi_t'(\mathcal{U})}[\rho'\mathbf{L}_{\mathbf{v}'}e'+e'\xi_{t*}(\mathbf{L}_{\mathbf{v}}\rho)]=\int_{\varphi_t'(\mathcal{U})}\rho'\mathbf{L}_{\mathbf{v}'}e'=\int_{\varphi_t'(\mathcal{U})}\rho\xi_t^*(\mathbf{L}_{\mathbf{v}'}e'). \tag{5.63}$$

But

$$\xi_t^*(\mathbf{L}_{\mathbf{v}'}e')=\dot{e}+\frac{\partial e}{\partial\mathbf{g}_t}:\mathcal{L}_{\mathbf{W}_t}\mathbf{g}_t. \tag{5.64}$$

Therefore

$$\Delta E(\xi_t)=\Delta E(\mathrm{Id})+\int_{\varphi_t(\mathcal{U})}\left[\left(2\rho\frac{\partial e}{\partial\mathbf{g}_t}-\boldsymbol{\sigma}\right):\frac{1}{2}\mathcal{L}_{\mathbf{W}_t}\mathbf{g}_t+\boldsymbol{\sigma}:\boldsymbol{\omega}_t\right]dv-\int_{\varphi_t(\mathcal{U})}\langle\langle\mathrm{div}\,\boldsymbol{\sigma}+\rho(\mathbf{b}-\mathbf{a}),\mathbf{W}_t\rangle\rangle_{\mathbf{g}_t}dv$$
$$=0. \tag{5.65}$$

□

E. Spatial covariant material energy balance

Let us consider the material balance of energy

$$\frac{d}{dt}\int_{\mathcal{U}}\rho_0\left(E+\frac{1}{2}\langle\langle\mathbf{V},\mathbf{V}\rangle\rangle\right)=\int_{\mathcal{U}}\rho_0\left(\langle\langle\mathbf{B},\mathbf{V}\rangle\rangle+R\right)+\int_{\partial\mathcal{U}}\left(\langle\langle\mathbf{T},\mathbf{V}\rangle\rangle+H\right)dA, \tag{5.66}$$

where we have assumed that ρ_0 is a 3-form. Physically this is equivalent to the spatial energy balance; material energy balance is simply the spatial energy balance expressed in terms of quantities defined with respect to the reference configuration. Let us postulate that the material energy balance is invariant with respect to diffeomorphisms $\xi_t:\mathcal{S}\to\mathcal{S}$. This is physically equivalent to the postulate of covariant spatial energy balance. The material energy balance for $\varphi_t'(\mathcal{U})\subset\mathcal{S}$ is written as

$$\frac{d}{dt}\int_{\mathcal{U}}\rho_0'\left(E'+\frac{1}{2}\langle\langle\mathbf{V}',\mathbf{V}'\rangle\rangle\right)=\int_{\mathcal{U}}\rho_0'\left(\langle\langle\mathbf{B}',\mathbf{V}'\rangle\rangle+R'\right)+\int_{\partial\mathcal{U}}\left(\langle\langle\mathbf{T}',\mathbf{V}'\rangle\rangle+H'\right)dA. \tag{5.67}$$

Note that for both deformations balance of energy is written for the same subset $\mathcal{U}\subset\mathcal{B}$. The material velocity $\mathbf{V}'$ is related to $\mathbf{V}$ by the following relation:

$$\mathbf{V}'(\mathbf{X})=T\xi_t\circ\mathbf{V}_t+\mathbf{w}_t\circ\varphi_t(\mathbf{X}). \tag{5.68}$$

Thus

$$\mathbf{V}'\big|_{t=t_0}=\mathbf{V}+\mathbf{w}\circ\varphi_{t_0}. \tag{5.69}$$

We know that

$$R=J_{\varphi_t}r\circ\varphi_t,\quad R'=J_{\varphi_t'}r'\circ\varphi_t',\quad r=J_{\xi_t}r'\circ\xi_t. \tag{5.70}$$

Hence

$$J_{\varphi_t'} r' \circ \varphi_t' = (J_{\xi_t} r' \circ \xi_t) \circ \varphi_t J_{\varphi_t} = J_{\varphi_t} r \circ \varphi_t. \tag{5.71}$$

Thus

$$R' = R. \tag{5.72}$$

Similarly

$$H' = H. \tag{5.73}$$

Note that looking at densities as 3-forms

$$\rho_0(\mathbf{X},t) = \varphi_t^* \rho(\mathbf{x},t), \quad \rho_0'(\mathbf{X},t) = (\varphi_t')^* \rho'(\mathbf{x}',t). \tag{5.74}$$

But

$$(\varphi_t')^* \rho'(\mathbf{x}',t) = (\xi_t \circ \varphi_t)^* \rho'(\mathbf{x}',t) = (\varphi_t^* \circ \xi_t^*) \circ \xi_{t*} \rho(\mathbf{x},t) = \varphi_t^* \rho(\mathbf{x},t). \tag{5.75}$$

Thus

$$\rho_0'(\mathbf{X},t) = \rho_0(\mathbf{X},t). \tag{5.76}$$

Because balance of energy is written for the same subset $\mathcal{U} \subset \mathcal{B}$ the same equality holds for densities as scalar fields, i.e., one can replace ρ_0' and ρ_0 by $\rho_0' \, \mathrm{d}V$ and $\rho_0 \, \mathrm{d}V$, respectively. Define

$$E(\mathbf{X},t,\mathbf{g}) = e(\varphi_t(\mathbf{X}),t,\mathbf{g} \circ \varphi_t(\mathbf{X})). \tag{5.77}$$

We know that

$$e'(\mathbf{x}',t,\mathbf{g}) = e(\mathbf{x},t,\xi_t^* \mathbf{g}). \tag{5.78}$$

Thus

$$E'(\mathbf{X},t,\mathbf{g}) = e'(\mathbf{x}',t,\mathbf{g}) = e(\mathbf{x},t,\xi_t^* \mathbf{g}) = E(\mathbf{X},t,\xi_t^* \mathbf{g}). \tag{5.79}$$

Therefore

$$\left. \frac{d}{\mathrm{d}t} \right|_{t=t_0} E' = \frac{\partial E}{\partial t} + \frac{\partial E}{\partial \mathbf{g}} : \mathfrak{L}_{\mathbf{w} \circ \varphi_t} (\mathbf{g} \circ \varphi_t). \tag{5.80}$$

Now the material energy balance for the motion φ_t' at $t = t_0$ can be written as

$$\begin{aligned} &\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t} \left(E + \frac{1}{2} \left\langle \left\langle \mathbf{V} + \mathbf{w} \circ \varphi_{t_0}, \mathbf{V} + \mathbf{w} \circ \varphi_{t_0} \right\rangle \right\rangle \right) \mathrm{d}V + \int_{\mathcal{U}} \left[\rho_0 \left(\frac{\partial E}{\partial t} + \frac{\partial E}{\partial \mathbf{g}} : \mathfrak{L}_{\mathbf{w} \circ \varphi_t} (\mathbf{g} \circ \varphi_t) \right) \right. \\ &\qquad \left. + \rho_0 \langle \langle \mathbf{V} + \mathbf{w} \circ \varphi_{t_0}, \mathbf{A}' |_{t=t_0} \rangle \rangle \right] \mathrm{d}V \\ &= \int_{\mathcal{U}} \rho_0 (\langle \langle \mathbf{B}' |_{t=t_0}, \mathbf{V} + \mathbf{w} \circ \varphi_{t_0} \rangle \rangle + R) \, \mathrm{d}V + \int_{\partial \mathcal{U}} \left(\left\langle \left\langle \mathbf{T}, \mathbf{V} + \mathbf{w} \circ \varphi_{t_0} \right\rangle \right\rangle + H \right) \mathrm{d}A. \end{aligned} \tag{5.81}$$

Subtracting the balance of energy for the motion φ_t from (5.81) one arrives at the following identity:

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\left\langle\left\langle \mathbf{V}, \mathbf{w}\circ\varphi_{t_0}\right\rangle\right\rangle + \frac{1}{2}\left\langle\left\langle \mathbf{w}\circ\varphi_{t_0}, \mathbf{w}\circ\varphi_{t_0}\right\rangle\right\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\frac{\partial E}{\partial \mathbf{g}}:\mathfrak{L}_{\mathbf{w}\circ\varphi_t}(\mathbf{g}\circ\varphi_t) + \left\langle\left\langle \mathbf{w}\circ\varphi_{t_0}, \mathbf{A}\right\rangle\right\rangle\right)\mathrm{d}V$$
$$= \int_{\mathcal{U}} \langle\langle \rho_0 \mathbf{B}, \mathbf{w}\circ\varphi_{t_0}\rangle\rangle \mathrm{d}V + \int_{\partial\mathcal{U}} \langle\langle \mathbf{T}, \mathbf{w}\circ\varphi_{t_0}\rangle\rangle \,\mathrm{d}A. \tag{5.82}$$

Let us denote $\mathbf{W}=\mathbf{w}\circ\varphi_t$ and note that $\mathbf{W}$ is a spatial vector field with components W^a.

Lemma 5.5: *The surface integral term in* (5.82) *is transformed to a volume integral as*

$$\int_{\partial\mathcal{U}} \left\langle\left\langle \mathbf{T}, \mathbf{W}\right\rangle\right\rangle \mathrm{d}A = \int_{\mathcal{U}} \left(\left\langle\left\langle \mathrm{Div}\, \mathbf{P}, \mathbf{W}\right\rangle\right\rangle + \boldsymbol{\tau}:\boldsymbol{\omega} + \boldsymbol{\tau}:\mathbf{k}\right)\mathrm{d}V, \tag{5.83}$$

where, $\tau^{ab}=P^{aB}F^b_B$ *is the Kirchhoff stress and* $\boldsymbol{\omega}$ *and* $\mathbf{k}$ *have the coordinate representations* $k_{ab}=\frac{1}{2}(W_{a|b}+W_{b|a})$ and $\omega_{ab}=\frac{1}{2}(W_{a|b}-W_{b|a})$.

Proof: The integrand has the following component form:

$$T^a g_{ab} W^b = P^{aC} G_{CD} N^D g_{ab} W^b = (P^{aC} g_{ab} W^b) G_{CD} N^D. \tag{5.84}$$

Now using divergence theorem the surface integral is transformed to an integral on $\mathcal{U}$ with an integrand with the following component form:

$$(P^{aC} g_{ab} W^b)_{|C} = P^{aC}{}_{|C} g_{ab} W^b + P^{aC} g_{ab} W^b{}_{|C}, \tag{5.85}$$

where use was made of the fact that $g_{ab|C}=0$. Note that

$$W^b{}_{|C} = \frac{\partial W^b}{\partial X^C} + \gamma^b_{cd} W^c F^d{}_C = W^b{}_{,d} F^d{}_C + \gamma^b_{cd} W^c F^d{}_C = (W^b{}_{,d} + \gamma^b_{cd} W^c) F^d{}_C = W^b{}_{|d} F^d{}_C. \tag{5.86}$$

Therefore,

$$\begin{aligned}(P^{aC} g_{ab} W^b)_{|C} &= P^{aC}{}_{|C} g_{ab} W^b + P^{aC} W_{a|d} F^d{}_C \\ &= P^{aC}{}_{|C} g_{ab} W^b + P^{aC} F^d{}_C \left[\tfrac{1}{2}(W_{a|d} + W_{d|a}) + \tfrac{1}{2}(W_{a|d} - W_{d|a})\right],\end{aligned} \tag{5.87}$$

which proves the lemma. □

Substituting (5.83) into (5.82) yields

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(\left\langle\left\langle \mathbf{V}, \mathbf{W}\right\rangle\right\rangle + \frac{1}{2}\left\langle\left\langle \mathbf{W}, \mathbf{W}\right\rangle\right\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \left(2\rho_0 \frac{\partial E}{\partial \mathbf{g}} - \boldsymbol{\tau}\right):\mathbf{k}\,\mathrm{d}\mathbf{V} - \int_{\mathcal{U}} \boldsymbol{\tau}:\boldsymbol{\omega}\,\mathrm{d}\mathbf{V}$$
$$- \int_{\mathcal{U}} \left\langle\left\langle \mathrm{Div}\, \mathbf{P} + \rho_0 \mathbf{B} - \rho_0 \mathbf{A}, \mathbf{W}\right\rangle\right\rangle \mathrm{d}\mathbf{V} = \mathbf{0}. \tag{5.88}$$

As $\mathbf{W}$ and $\mathcal{U}\subset\mathcal{B}$ are arbitrary we conclude that,

$$\frac{\partial \rho_0}{\partial t} = 0, \tag{5.89}$$

$$\boldsymbol{\tau} = 2\rho_0 \frac{\partial E}{\partial \mathbf{g}}, \tag{5.90}$$

$$\boldsymbol{\tau}^{\mathsf{T}} = \boldsymbol{\tau}, \tag{5.91}$$

$$\mathrm{Div}\,\mathbf{P}+\rho_0\mathbf{B}=\rho_0\mathbf{A}. \tag{5.92}$$

In conclusion, these computations result in the following proposition.

Proposition 5.6: Energy balance written in material form, but still with the assumption of spatial covariance yields results that are identical to those of energy balance written in spatial form, also with covariance under spatial diffeomorphisms.

The converse can be proved similar to what was done in the previous subsection.

VI. TRANSFORMATION OF ENERGY BALANCE UNDER MATERIAL DIFFEOMORPHISMS

As was seen in the preceding section, invariance of balance of energy under an arbitrary change in spatial frame is equivalent to (1) balance of linear momentum, (2) balance of angular momentum, (3) conservation of mass, and (4) Doyle-Ericksen formula. To our best knowledge, there is no material version of this theorem in the literature. Our motivation for studying the possibility of material invariance of energy balance was to gain a better understanding of configurational forces as they are believed to be related to rearrangements of the reference configuration. It turns out that, in general, energy balance cannot be invariant under diffeomorphisms of the reference configuration and what one should be looking for instead is the way in which energy balance transforms under material diffeomorphisms. In this section we first obtain such a transformation formula under an arbitrary time-dependent material diffeomorphism [see Eq. (6.51)] and then obtain the conditions under which balance of energy is materially covariant.

A. The energy balance material transformation formula

We begin with a discussion of how energy balance transforms under material diffeomorphisms. Define

$$E(\mathbf{X},t,\mathbf{G})=\Psi(\mathbf{X},t,\mathbf{C}(\mathbf{F}(\mathbf{X}),\mathbf{g}(\varphi_t(\mathbf{X}))),\mathbf{G}), \tag{6.1}$$

where $\Psi=\Psi(\mathbf{X},t,\mathbf{G},\mathbf{C})$ is the material free energy density. Material (Lagrangian) energy balance can be written as

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}}\rho_0\left(E+\frac{1}{2}\langle\langle\mathbf{V},\mathbf{V}\rangle\rangle\right)\mathrm{d}V=\int_{\mathcal{U}}\rho_0(\langle\langle\mathbf{B},\mathbf{V}\rangle\rangle+R)\mathrm{d}V+\int_{\partial\mathcal{U}}(\langle\langle\mathbf{T},\mathbf{V}\rangle\rangle+H)\mathrm{d}A, \tag{6.2}$$

which can be simplified to read

$$\int_{\mathcal{U}}\frac{d}{\mathrm{d}t}\left[\rho_0\left(E+\frac{1}{2}\langle\langle\mathbf{V},\mathbf{V}\rangle\rangle\right)\right]\mathrm{d}V=\int_{\mathcal{U}}\rho_0\left(\langle\langle\mathbf{B},\mathbf{V}\rangle\rangle+R\right)\mathrm{d}V+\int_{\partial\mathcal{U}}(\langle\langle\mathbf{T},\mathbf{V}\rangle\rangle+H)\mathrm{d}A, \tag{6.3}$$

where $\mathcal{U}$ is an arbitrary nice subset of the reference configuration $\mathcal{B}$, $\mathbf{B}$ is body force per unit undeformed mass, $\mathbf{V}(\mathbf{X},t)$ is the material velocity, $\rho_0(\mathbf{X},t)$ is the material density, $R(\mathbf{X},t)$ is the heat supply per unit undeformed mass, and $H(\mathbf{X},t,\hat{\mathbf{N}})$ is the heat flux across a surface with normal $\hat{\mathbf{N}}$ in the undeformed configuration (normal to $\partial\mathcal{U}$ at $\mathbf{X}\in\partial\mathcal{U}$). It is to be noted that this is balance of energy for a deformed part of the body written in terms of quantities that are defined with respect to the undeformed (reference) configuration. Here we assume that we have a material manifold which is a Riemannian manifold $(\mathfrak{B},\mathbf{G})$ and a given reference configuration $\mathcal{B}\subset\mathfrak{B}$.

Change of reference frame: In this paragraph we consider a change of frame for the reference configuration and look at the transformed quantities for the new reference configuration. A reframing of the reference configuration is a diffeomorphism

$$\Xi_t:(\mathfrak{B},\mathbf{G})\to(\mathfrak{B},\mathbf{G}'). \tag{6.4}$$

A change of frame can be thought of as a change of coordinates in the reference configuration (passive definition) or a rearrangement of microstructure (active definition). Under such a framing, a nice subset $\mathcal{U}$ is mapped to another nice subset $\mathcal{U}'=\Xi_t(\mathcal{U})$ and a material point $\mathbf{X}$ is mapped to

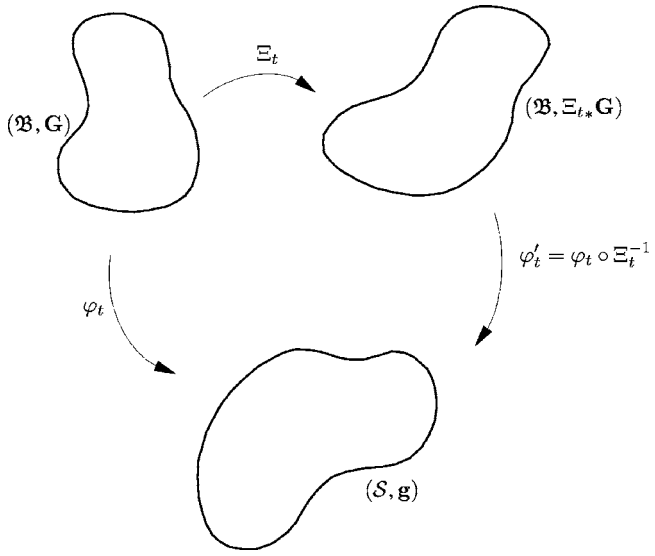


FIG. 2. A material reframing and the corresponding deformation maps.

$\mathbf{X}' = \Xi_t(\mathbf{X})$. Note that $\mathbf{X}$ is the position of a particle in the reference configuration, i.e., material points are identified with their positions in the reference configuration (which is arbitrary). The change of frame is mathematically a mapping between two manifolds and one would expect to define an object on $(\mathfrak{B}, \mathbf{G}')$ as push-forward of the corresponding object on $(\mathfrak{B}, \mathbf{G})$.

The deformation mapping for the new reference configuration is $\varphi'_t = \varphi_t \circ \Xi_t^{-1}$. This can be clearly seen in Fig. 2. The material velocity in $\mathcal{U}'$ is

$$\mathbf{V}'(\mathbf{X}', t) = \frac{\partial}{\partial t}\varphi'_t(\mathbf{X}') = \frac{\partial \varphi_t}{\partial t} \circ \Xi_t^{-1}(\mathbf{X}') + T\varphi_t \circ \frac{\partial \Xi_t^{-1}}{\partial t}(\mathbf{X}'). \tag{6.5}$$

We assume that

$$\Xi_t|_{t=t_0} = \mathrm{Id}, \quad \frac{\partial \Xi_t}{\partial t}(\mathbf{X}) = \mathbf{W}(\mathbf{X}, t). \tag{6.6}$$

Note that $\mathbf{W}$ is the infinitesimal generator of the rearrangement Ξ_t. It can be shown that at $t = t_0$,

$$\frac{\partial \Xi_t^{-1}}{\partial t}(\mathbf{X}')\bigg|_{t=t_0} = -\mathbf{W}(\mathbf{X}, t). \tag{6.7}$$

Thus, at $t = t_0$,

$$\mathbf{V}' = \mathbf{V} - \mathbf{F}\mathbf{W}. \tag{6.8}$$

To find the relation between $\mathbf{G}$ and $\mathbf{G}'$ we note that the Finger tensor $\mathbf{b} = \varphi_{t*}\mathbf{G}$ is a spatial tensor and hence independent of framing of the reference configuration. Thus,

$$\mathbf{b} = \varphi_{t*}\mathbf{G} = (\varphi'_t)_*\mathbf{G}'. \tag{6.9}$$

That is,

$$\mathbf{G}' = (\varphi_t \circ \Xi_t^{-1})^* \circ \varphi_{t*}\mathbf{G} = (\Xi_t^{-1})^* \circ \varphi_t^* \circ \varphi_{t*}\mathbf{G} = (\Xi_t^{-1})^*\mathbf{G} = \Xi_{t*}\mathbf{G} = (T\Xi_t)^{-*}\mathbf{G}(T\Xi_t)^{-1}. \tag{6.10}$$

Note that for an arbitrary $\mathbf{X}_0 \in \mathcal{B}$,

$$\mathbf{F}(\mathbf{X}_0):T_{\mathbf{X}_0}\mathcal{B}\to T_{\varphi_t(\mathbf{X}_0)}\mathcal{S} \quad \text{and} \quad \mathbf{F}'(\mathbf{X}_0'):T_{\mathbf{X}_0'}\mathcal{B}\to T_{\varphi_t'(\mathbf{X}_0')}\mathcal{S}.$$

Given $\mathrm{d}\mathbf{X}\in T_{\mathbf{X}_0}\mathcal{B}$,

$$\mathrm{d}\mathbf{x}=\mathbf{F}(\mathbf{X}_0)\cdot d\mathbf{X} \quad \text{and} \quad \mathrm{d}\mathbf{X}'=T\Xi_t\cdot\mathrm{d}\mathbf{X}.$$

Hence,

$$\mathrm{d}\mathbf{x}=\mathbf{F}'(\mathbf{X}_0')\cdot\mathrm{d}\mathbf{X}'=\mathbf{F}'(\mathbf{X}_0')\circ T\Xi_t\cdot\mathrm{d}\mathbf{X}=\mathbf{F}(\mathbf{X}_0)\cdot\mathrm{d}\mathbf{X}$$

for all $\mathrm{d}\mathbf{X}\in T_{\mathbf{X}_0}\mathcal{B}$. Thus,

$$\mathbf{F}'=\Xi_{t*}\mathbf{F}, \tag{6.11}$$

where

$$\Xi_{t*}\mathbf{F}=\mathbf{F}\circ(T\Xi_t)^{-1}. \tag{6.12}$$

The easier way of proving this is the following:

$$\mathbf{F}'=T\varphi_t'=T(\varphi_t\circ\Xi_t^{-1})=T\varphi_t\circ(\Xi_t)^{-1}=\mathbf{F}\circ(\Xi_t)^{-1}. \tag{6.13}$$

The material internal energy density is assumed to have the following tensorial property:

$$E'(\mathbf{X}',t,\mathbf{G}')=E(\mathbf{X},t,\mathbf{G}). \tag{6.14}$$

Note that this is different from assuming local covariance for internal energy density. This is simply the material analogue of (5.78); all that (6.14) says is that internal energy density at $\mathbf{X}'$ evaluated by the transformed metric $\mathbf{G}'$ is equal to the internal energy density at $\mathbf{X}$ evaluated by the metric $\mathbf{G}$. We know that $\mathbf{G}'=\Xi_{t*}\mathbf{G}$, thus

$$E'(\mathbf{X}',t,\mathbf{G})=E(\mathbf{X},t,\Xi_t^*\mathbf{G}). \tag{6.15}$$

This means that

$$\left.\frac{d}{\mathrm{d}t}\right|_{t=t_0}E'(\mathbf{X}',t,\mathbf{G})=\frac{\partial E}{\partial t}+\frac{\partial E}{\partial\mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G}. \tag{6.16}$$

Remark: Marsden and Hughes[28] defined covariant constitutive equations by looking at isometries of $T_{\mathbf{X}_0}\mathcal{B}$ at a given point $\mathbf{X}_0\in\mathcal{B}$. This is why they did not need to consider an explicit dependence of Ψ on $\mathbf{G}$. Another more general way of defining material covariance for the strain energy function Ψ is to assume that for any local diffeomorphism $\Lambda:T_{\mathbf{X}_0}\mathcal{B}\to T_{\Lambda(\mathbf{X}_0)}\Lambda(\mathcal{B})$ that leaves $\mathbf{X}_0$ fixed,

$$\Psi(\mathbf{X}_0,\mathbf{G},\mathbf{C})=\Psi(\mathbf{X}_0,\Lambda^*\mathbf{G},\Lambda^*\mathbf{C}). \tag{6.17}$$

Note that this is different from the implication of Cartan's space-time, e.g.,

$$\Psi(\mathbf{X}',\mathbf{G}',\mathbf{C}')=\Psi(\mathbf{X},\Xi^*\mathbf{G}',\Xi^*\mathbf{C}'),$$

for an arbitrary diffeomorphism $\Xi:\mathfrak{B}\to\mathfrak{B}$. We emphasize that this relation and similarly (6.14) do not put any restrictions on material properties. Ju and Papadopoulos[26,27] proved that a consequence of (6.17) is the following infinitesimal covariance condition:

$$\mathbf{G}\frac{\partial\Psi}{\partial\mathbf{G}}+\mathbf{C}\frac{\partial\Psi}{\partial\mathbf{C}}=\mathbf{0}, \tag{6.18}$$

which is equivalent to

$$\frac{\partial \Psi}{\partial \mathbf{G}} = -\mathbf{G}^{-1}\mathbf{C}\frac{\partial \Psi}{\partial \mathbf{C}} = -\frac{1}{2}\mathbf{G}^{-1}\mathbf{C}\mathbf{S} = -\frac{1}{2}\mathbf{F}^{\mathrm{T}}\mathbf{P}. \tag{6.19}$$

We will obtain this condition in the sequel as a consequence of assuming material covariance of energy balance.

Example: Consider a (materially uniform) Neo-Hookean material with the following energy density

$$\Psi(\mathbf{X},\mathbf{G},\mathbf{C}) = \mu[\mathrm{tr}(\mathbf{C}) - 3] = \mu(C_{IJ}G^{IJ} - 3). \tag{6.20}$$

We now show that this is an example of a materially covariant material. Note that

$$\left(\mathbf{C}\frac{\partial \Psi}{\partial \mathbf{C}}\right)^{J}_{I} = \mu C_{IK}G^{KJ}. \tag{6.21}$$

Also

$$\left(\mathbf{G}\frac{\partial \Psi}{\partial \mathbf{C}}\right)^{J}_{I} = \mu G_{IK}C_{MN}\frac{\partial G^{MN}}{\partial G_{KJ}} = -\frac{\mu}{2}C_{MN}G_{IK}(G^{MK}G^{JN} + G^{MJ}G^{KN}) = -\mu C_{IK}G^{KJ}, \tag{6.22}$$

i.e.,

$$\mathbf{C}\frac{\partial \Psi}{\partial \mathbf{C}} + \mathbf{G}\frac{\partial \Psi}{\partial \mathbf{G}} = \mathbf{0}. \tag{6.23}$$

□

Spatial covariance of strain energy function (material-frame-indifference) can be defined similarly (see Ref. 41). However, one should note that this is different from Marsden and Hughes point of departure for developing a covariant theory of elasticity; in Marsden and Hughes' theory[28] balance of energy is assumed to be covariant and not the energy function. In covariant energy balance, a global diffeomorphism is considered and energy balance is assumed to be invariant under this global diffeomorphism.

Balance of energy for reframings of the reference configuration: One way to obtain the governing balance equations of a continuum is to use the homogeneity of the ambient space and postulate that if a deformed body satisfies the balance of energy, any framing of it should satisfy the balance of energy as well. This is a postulate and cannot be proved. But, one can justify it (or motivate it) by the fact that the ambient space $\mathcal{S}$ is homogeneous. Invariance of energy balance under framings of the reference configuration is less obvious and, in general, it turns out not to hold. The following is the main conclusion of this section. *Under referential diffeomorphisms, material energy balance has some extra terms in it. The extra terms correspond to some forces that contribute to the rate of change of energy when the reference configuration evolves.*

Consider a deformation mapping $\varphi_t : \mathcal{B} \to \mathcal{S}$ and a referential diffeomorphisms $\Xi_t : \mathfrak{B} \to \mathfrak{B}$. The mapping $\varphi'_t = \varphi_t \circ \Xi_t^{-1} : \mathcal{B}' \to \mathcal{S}$, where $\mathcal{B}' = \Xi_t(\mathcal{B})$, represents the deformation of the new (evolved) reference configuration. We are interested in understanding the form of material energy balance for $\Xi_t(\mathcal{U}) \subset \mathcal{B}'$ for any nice $\mathcal{U} \subset \mathcal{B}$. In addition to contributions from the mapping φ'_t, in general, one should expect to see contributions from the referential mapping Ξ_t as well, i.e., evolution of reference configuration may, in general, contribute to the energy balance. Now the balance of energy should include the following two groups of terms:

(i) Looking at φ'_t as the deformation of $\mathcal{B}'$ in $\mathcal{S}$, one has the usual material energy balance for $\Xi_t(\mathcal{U})$. Transformation of fields from $(\mathfrak{B}, \mathbf{G})$ to $(\mathfrak{B}, \mathbf{G}')$ follows Cartan's space-time theory.

(ii) Nonstandard terms may appear to represent the energy associated with the material evolution.

Here a comment is in order. The mapping that represents all the physical processes is φ_t. This mapping is the composition of φ'_t and Ξ_t and hence it is expected that, in general, both φ'_t and Ξ_t represent part of the physical processes. This means that standard deformation represented by φ'_t and evolution of microstructure (or any other material evolution) represented by Ξ_t should contribute to balance of energy. (This is similar to Gurtin's idea[20,21] of including both standard and nonstandard terms in the expression of working. However, here we consider the full balance of energy.) This rough picture should be enough to convince the reader that the lack of invariance of energy balance under Ξ_t should not be surprising. Lack of invariance implies the appearance of some new terms that are work-conjugate to $\mathbf{W}_t=(\partial/\partial t)\Xi_t$. Let us denote the volume and surface forces conjugate to $\mathbf{W}$ by $\mathbf{B}_0$ and $\mathbf{T}_0$, respectively.

Instead of looking at spatial framings, we fix the deformed configuration and look at framings of the reference configuration. We postulate that energy balance for each nice subset $\mathcal{U}'$ has the following form:

$$\frac{d}{dt}\int_{\mathcal{U}'}\left(E'+\frac{1}{2}\rho'_0\langle\langle\mathbf{V}',\mathbf{V}'\rangle\rangle\right)dV'=\int_{\mathcal{U}'}\rho'_0(\langle\langle\mathbf{B}',\mathbf{V}'\rangle\rangle+R')dV'+\int_{\partial\mathcal{U}'}(\langle\langle\mathbf{T}',\mathbf{V}'\rangle\rangle+H')dA'$$
$$+\int_{\mathcal{U}'}\langle\langle\mathbf{B}'_0,\mathbf{W}_t\rangle\rangle dV'+\int_{\partial\mathcal{U}'}\langle\langle\mathbf{T}'_0,\mathbf{W}_t\rangle\rangle dA', \tag{6.24}$$

where $\mathcal{U}'=\Xi_t(\mathcal{U})$ and $\mathbf{B}'_0$ and $\mathbf{T}'_0$ are unknown vector fields at this point. Using Cartan's space-time theory, it is assumed that the primed quantities have the following relations with the unprimed quantities

$$dV'=\Xi_t{}^*dV\ (J(\Xi_t)dV'=dV),\quad R'(\mathbf{X}',t)=R(\mathbf{X},t),$$

$$\rho'_0(\mathbf{X}',t)=\rho_0(\mathbf{X}),\quad H'(\mathbf{X}',\hat{\mathbf{N}}',t)=H(\mathbf{X},\hat{\mathbf{N}},t), \tag{6.25}$$

$$\mathbf{T}'(\mathbf{X}',\hat{\mathbf{N}}',t)=T\Xi_t(\mathbf{X})\cdot\mathbf{T}(\mathbf{X},\hat{\mathbf{N}},t).$$

We know that

$$\mathbf{B}'-\mathbf{A}'=\Xi_t{}^*(\mathbf{B}-\mathbf{A}). \tag{6.26}$$

Thus

$$(\mathbf{B}'-\mathbf{A}')\big|_{t=t_0}=\mathbf{B}-\mathbf{A}. \tag{6.27}$$

Note that if α is a 3-form on $\mathcal{U}$, then

$$\frac{d}{dt}\bigg|_{t=t_0}\int_{\mathcal{U}'}\alpha'=\int_{\mathcal{U}}\frac{d}{dt}\bigg|_{t=t_0}(\Xi_t^*\alpha'), \tag{6.28}$$

where $\mathcal{U}'=\Xi_t(\mathcal{U})$. Thus

$$\frac{d}{dt}\bigg|_{t=t_0}\int_{\mathcal{U}'}E'dV'=\int_{\mathcal{U}}\frac{d}{dt}\bigg|_{t=t_0}(\Xi_t^*E')dV=\int_{\mathcal{U}}\left(\frac{\partial E}{\partial t}+\frac{\partial E}{\partial\mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G}\right)dV. \tag{6.29}$$

Material balance of energy for $\mathcal{U}'\subset\mathcal{B}'$ at $t=t_0$ reads

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(E+\frac{1}{2}\langle\langle \mathbf{V}-\mathbf{FW},\mathbf{V}-\mathbf{FW}\rangle\rangle\right)\mathrm{d}V+\int_{\mathcal{U}}\rho_0\left(\frac{\partial E}{\partial t}+\frac{\partial E}{\partial \mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G}+\langle\langle \mathbf{V}-\mathbf{FW},\mathbf{A}'|_{t=t_0}\rangle\rangle\right)\mathrm{d}V$$
$$=\int_{\mathcal{U}}\rho_0(\langle\langle \mathbf{B}'|_{t=t_0},\mathbf{V}-\mathbf{FW}\rangle\rangle+R)\mathrm{d}V+\int_{\partial\mathcal{U}}(\langle\langle \mathbf{T},\mathbf{V}-\mathbf{FW}\rangle\rangle+H)\mathrm{d}A+\int_{\mathcal{U}}\langle\langle \mathbf{B}_0,\mathbf{W}\rangle\rangle\mathrm{d}V$$
$$+\int_{\partial\mathcal{U}}\langle\langle \mathbf{T}_0,\mathbf{W}\rangle\rangle\mathrm{d}A. \tag{6.30}$$

Note that $\mathbf{T}_0$ and $\mathbf{B}_0$ are defined on $\mathcal{B}$ and $\mathbf{T}_0'$ and $\mathbf{B}_0'$ are the corresponding quantities defined on $\Xi_t(\mathcal{B})$. Here we assume that $\mathbf{T}_0'=\Xi_{t^*}\mathbf{T}_0$ and $\mathbf{B}_0'=\Xi_{t^*}\mathbf{B}_0$. Subtracting balance of energy for $\mathcal{U}$ from this and noting that $(\mathbf{A}'-\mathbf{B}')_{t=t_0}=\mathbf{A}-\mathbf{B}$ we obtain

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(-\langle\langle \mathbf{V},\mathbf{FW}\rangle\rangle+\frac{1}{2}\langle\langle \mathbf{FW},\mathbf{FW}\rangle\rangle\right)\mathrm{d}V+\int_{\mathcal{U}}\rho_0\left(\frac{\partial E}{\partial \mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G}-\langle\langle \mathbf{FW},\mathbf{A}\rangle\rangle\right)\mathrm{d}V$$
$$=-\int_{\mathcal{U}}\langle\langle \rho_0\mathbf{B},\mathbf{FW}\rangle\rangle\mathrm{d}V-\int_{\partial\mathcal{U}}\langle\langle \mathbf{T},\mathbf{FW}\rangle\rangle\mathrm{d}A+\int_{\mathcal{U}}\langle\langle \mathbf{B}_0,\mathbf{W}\rangle\rangle\mathrm{d}V+\int_{\partial\mathcal{U}}\langle\langle \mathbf{T}_0,\mathbf{W}\rangle\rangle\mathrm{d}A. \tag{6.31}$$

Cauchy's theorem implies that

$$\langle\langle \mathbf{T},\mathbf{FW}\rangle\rangle=\langle\langle \mathbf{FW},\langle\langle \mathbf{P},\hat{\mathbf{N}}\rangle\rangle\rangle\rangle, \tag{6.32}$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor. Similarly

$$\mathbf{T}_0=\langle\langle \mathbf{P}_0,\hat{\mathbf{N}}\rangle\rangle. \tag{6.33}$$

Lemma 6.1: The surface integral in material energy balance has the following transformation:

$$\int_{\partial\mathcal{U}}\langle\langle \mathbf{F}^{\mathsf{T}}\mathbf{T},\mathbf{W}\rangle\rangle\mathrm{d}A=\int_{\mathcal{U}}\mathrm{Div}\langle\langle \mathbf{F}^{\mathsf{T}}\mathbf{P},\mathbf{W}\rangle\rangle\mathrm{d}V=\int_{\mathcal{U}}[\langle\langle \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}),\mathbf{W}\rangle\rangle+\mathbf{F}^{\mathsf{T}}\mathbf{P}:\mathbf{\Omega}+\mathbf{F}^{\mathsf{T}}\mathbf{P}:\mathbf{K}]\mathrm{d}V, \tag{6.34}$$

where

$$\mathbf{\Omega}_{IJ}=\tfrac{1}{2}(G_{IK}W^K{}_{|J}-G_{JK}W^K{}_{|I})=\tfrac{1}{2}(W_{I|J}-W_{J|I}), \tag{6.35}$$

$$\mathbf{K}_{IJ}=\tfrac{1}{2}(G_{IK}W^K{}_{|J}+G_{JK}W^K{}_{|I})=\tfrac{1}{2}(W_{I|J}+W_{J|I}),\quad \mathbf{K}=\tfrac{1}{2}\mathfrak{L}_{\mathbf{W}}\mathbf{G}. \tag{6.36}$$

Proof: In components the integrand can be written as

$$(\mathbf{F}^{\mathsf{T}})^A{}_a T^a G_{AB} W^B. \tag{6.37}$$

But

$$T^a=P^{aC}G_{CD}N^D. \tag{6.38}$$

Hence in components the integrand reads

$$((\mathbf{F}^{\mathsf{T}})^A{}_a P^{aC}G_{AB}W^B)G_{CD}N^D. \tag{6.39}$$

Using the divergence theorem the surface integral is transformed to an integral on $\mathcal{U}$ with the following integrand in components:

$$((\mathbf{F}^{\mathsf{T}})^{A}{}_{a}P^{aC}G_{AB}W^{B})_{|C} = ((\mathbf{F}^{\mathsf{T}}\mathbf{P})^{AC}G_{AB}W^{B})_{|C} = (\mathbf{F}^{\mathsf{T}}\mathbf{P})^{AC}{}_{|C}G_{AB}W^{B} + (\mathbf{F}^{\mathsf{T}}\mathbf{P})^{AC}G_{AB}W^{B}{}_{|C}$$
$$= (\mathbf{F}^{\mathsf{T}}\mathbf{P})^{AC}{}_{|C}G_{AB}W^{B} + (\mathbf{F}^{\mathsf{T}}\mathbf{P})^{AC}\left[\tfrac{1}{2}(G_{AB}W^{B}{}_{|C} + G_{CB}W^{B}{}_{|A}) + \tfrac{1}{2}(G_{AB}W^{B}{}_{|C} - G_{CB}W^{B}{}_{|A})\right], \tag{6.40}$$

where use was made of the fact that $G_{AB|C}=0$. □

Similarly,

$$\int_{\partial\mathcal{U}} \langle\langle \mathbf{T}_0, \mathbf{W}\rangle\rangle \mathrm{d}A = \int_{\mathcal{U}} \mathrm{Div}\langle\langle \mathbf{P}_0, \mathbf{W}\rangle\rangle \mathrm{d}V = \int_{\mathcal{U}} [\langle\langle \mathrm{Div}(\mathbf{P}_0), \mathbf{W}\rangle\rangle + \mathbf{P}_0{:}\boldsymbol{\Omega} + \mathbf{P}_0{:}\mathbf{K}]\mathrm{d}V. \tag{6.41}$$

By definition, at time $t=t_0$ the transformed balance of energy should be the same as the balance of energy for $\mathcal{U}$. Subtracting the material balance of energy for $\mathcal{U}$ from the above balance law and considering conservation of mass, we obtain

$$\int_{\mathcal{U}} \rho_0 \frac{\partial E}{\partial \mathbf{G}}{:}\mathfrak{L}_{\mathbf{W}}\mathbf{G}\mathrm{d}V + \int_{\mathcal{U}} \langle\langle \rho_0 \mathbf{F}^{\mathsf{T}}(\mathbf{B}-\mathbf{A}), \mathbf{W}\rangle\rangle \mathrm{d}V - \int_{\mathcal{U}} \langle\langle \rho_0 \mathbf{B}_0, \mathbf{W}\rangle\rangle \mathrm{d}V + \int_{\partial\mathcal{U}} \langle\langle \mathbf{F}^{\mathsf{T}}\mathbf{T} - \mathbf{T}_0, \mathbf{W}\rangle\rangle \mathrm{d}A = 0. \tag{6.42}$$

Thus

$$\int_{\mathcal{U}} \left(2\rho_0 \frac{\partial E}{\partial \mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0\right){:}\frac{1}{2}\mathfrak{L}_{\mathbf{W}}\mathbf{G}\mathrm{d}V + \int_{\mathcal{U}} (\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0){:}\boldsymbol{\Omega}\mathrm{d}V + \int_{\mathcal{U}} \langle\langle \rho_0 \mathbf{F}^{\mathsf{T}}(\mathbf{B}-\mathbf{A}) - \mathbf{B}_0 + \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) - \mathrm{Div}\,\mathbf{P}_0, \mathbf{W}\rangle\rangle \mathrm{d}V = 0. \tag{6.43}$$

Now using the balance of linear momentum the identity (6.43) simplifies to

$$\int_{\mathcal{U}} \left(2\rho_0 \frac{\partial E}{\partial \mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0\right){:}\frac{1}{2}\mathfrak{L}_{\mathbf{W}}\mathbf{G}\mathrm{d}V + \int_{\mathcal{U}} (\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0){:}\boldsymbol{\Omega}\mathrm{d}V + \int_{\mathcal{U}} \langle\langle \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0) - \mathbf{F}^{\mathsf{T}}\mathrm{Div}\,\mathbf{P} - \mathbf{B}_0, \mathbf{W}\rangle\rangle \mathrm{d}V = 0. \tag{6.44}$$

Because $\mathcal{U}$ and $\mathbf{W}$ are arbitrary

$$\mathbf{P}_0 = 2\rho_0 \frac{\partial E}{\partial \mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P}, \tag{6.45}$$

$$(\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0)^{\mathsf{T}} = \mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0, \tag{6.46}$$

$$\mathbf{B}_0 = \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0) - \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}. \tag{6.47}$$

Note that (6.46) is trivially satisfied after having (6.45). Thus we have

$$\mathbf{P}_0 = 2\rho_0 \frac{\partial E}{\partial \mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P}, \tag{6.48}$$

$$\mathbf{B}_0 = \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0) - \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}. \tag{6.49}$$

Note that $\mathbf{P}_0$ is a measure of anisotropy (deviation from material Doyle-Ericksen formula). This is an interesting result that in a natural way shows the contribution of some nonstandard terms to balance of energy when reference configuration evolves.

Thus we have proven the following theorem.

Theorem 6.2: *Under a referential diffeomorphism* $\Xi_t{:}\mathfrak{B}\to\mathfrak{B}$, *and assuming that material energy density transforms tensorially*, *i.e.*,

$$E'(\mathbf{X}',t,\mathbf{G}) = E(\mathbf{X},t,\Xi_t^*\mathbf{G}), \tag{6.50}$$

material energy balance has the following transformation:

$$\frac{d}{\mathrm{d}t}\int_{\Xi_t(\mathcal{U})}\left(E' + \frac{1}{2}\rho_0'\langle\langle\mathbf{V}',\mathbf{V}'\rangle\rangle\right)\mathrm{d}V' = \int_{\Xi_t(\mathcal{U})}\rho_0'(\langle\langle\mathbf{B}',\mathbf{V}'\rangle\rangle + R')\mathrm{d}V' + \int_{\partial\Xi_t(\mathcal{U})}(\langle\langle\mathbf{T}',\mathbf{V}'\rangle\rangle + H')\mathrm{d}A'$$
$$+ \int_{\Xi_t(\mathcal{U})}\langle\langle\mathbf{B}_0',\mathbf{W}_t\rangle\rangle\mathrm{d}V' + \int_{\partial\Xi_t(\mathcal{U})}\langle\langle\mathbf{T}_0',\mathbf{W}_t\rangle\rangle\mathrm{d}A', \tag{6.51}$$

where

$$\mathbf{T}_0' = \Xi_{t*}\left[\left\langle\left\langle 2\rho_0\frac{\partial E}{\partial\mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P},\hat{\mathbf{N}}\right\rangle\right\rangle\right], \tag{6.52}$$

$$\mathbf{B}_0' = \Xi_{t*}\left[\mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P} - \mathbf{P}_0) - \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}\right], \tag{6.53}$$

and the other quantities are already defined.

B. Consequences of assuming invariance of energy balance

This section shows the consequences of assuming material covariance of energy balance. It turns out that energy balance, in general, cannot be materially covariant.

Material energy balance is invariant under material diffeomorphisms if and only if the following relations hold between the nonstandard terms:

$$\mathbf{P}_0 = \mathbf{0} \quad \text{or} \quad 2\rho_0\frac{\partial E}{\partial\mathbf{G}} = -\mathbf{F}^{\mathsf{T}}\mathbf{P}, \tag{6.54}$$

$$\mathbf{B}_0 = \mathbf{0} \quad \text{or} \quad \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}. \tag{6.55}$$

Equation (6.54) is the material Doyle-Ericksen formula and (6.55) is the configurational inviscidity constraint, which will be defined in the sequel. Let us now start with the "naive" assumption that energy balance is materially covariant and see what its consequences are.

Material covariance of energy balance: Let us postulate that the balance of energy is invariant under a diffeomorphism $\Xi_t:\mathfrak{B}\to\mathfrak{B}$, i.e.,

$$\frac{d}{\mathrm{d}t}\int_{\mathcal{U}'}\rho_0'\left(E' + \frac{1}{2}\langle\langle\mathbf{V}',\mathbf{V}'\rangle\rangle\right)\mathrm{d}V' = \int_{\mathcal{U}'}\rho_0'(\langle\langle\mathbf{B}',\mathbf{V}'\rangle\rangle + R')\mathrm{d}V' + \int_{\partial\mathcal{U}'}(\langle\langle\mathbf{T}',\mathbf{V}'\rangle\rangle + H')\mathrm{d}A'. \tag{6.56}$$

Proposition 6.3: If material energy balance is invariant under arbitrary material diffeomorphisms $\Xi_t:\mathfrak{B}\to\mathfrak{B}$, *then*

$$\frac{\partial\rho_0}{\partial t} = 0, \tag{6.57}$$

$$2\rho_0\frac{\partial E}{\partial\mathbf{G}} = -\mathbf{F}^{\mathsf{T}}\mathbf{P}, \tag{6.58}$$

$$\mathbf{F}^{\mathsf{T}}\mathbf{P} = \mathbf{P}^{\mathsf{T}}\mathbf{F}, \tag{6.59}$$

$$\mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}. \tag{6.60}$$

Conversely, if the above four conditions hold, then material energy balance is invariant under any material diffeomorphism.

Proof: Material balance of energy for $\mathcal{U}' \subset \mathcal{B}'$ at $t=t_0$ reads

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(E + \frac{1}{2}\langle\langle \mathbf{V}-\mathbf{FW}, \mathbf{V}-\mathbf{FW}\rangle\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\frac{\partial E}{\partial t} + \frac{\partial E}{\partial \mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G} + \langle\langle \mathbf{V}-\mathbf{FW}, \mathbf{A}'|_{t=t_0}\rangle\rangle\right)\mathrm{d}V$$

$$= \int_{\mathcal{U}} \rho_0(\langle\langle \mathbf{B}'|_{t=t_0}, \mathbf{V}-\mathbf{FW}\rangle\rangle + R)\mathrm{d}V + \int_{\partial\mathcal{U}} (\langle\langle \mathbf{T}, \mathbf{V}-\mathbf{FW}\rangle\rangle + H)\mathrm{d}A. \tag{6.61}$$

Subtracting balance of energy for $\mathcal{U}\subset\mathcal{B}$ from this and noting that $(\mathbf{A}'-\mathbf{B}')_{t=t_0}=\mathbf{A}-\mathbf{B}$ we obtain

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(-\langle\langle \mathbf{V}, \mathbf{FW}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{FW}, \mathbf{FW}\rangle\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \rho_0\left(\frac{\partial E}{\partial \mathbf{G}}:\mathfrak{L}_{\mathbf{W}}\mathbf{G} - \langle\langle \mathbf{FW}, \mathbf{A}\rangle\rangle\right)\mathrm{d}V$$

$$= -\int_{\mathcal{U}} \langle\langle \rho_0\mathbf{B}, \mathbf{FW}\rangle\rangle \mathrm{d}V - \int_{\partial\mathcal{U}} \langle\langle \mathbf{T}, \mathbf{FW}\rangle\rangle \mathrm{d}A. \tag{6.62}$$

We know that

$$\int_{\partial\mathcal{U}} \langle\langle \mathbf{F}^{\mathsf{T}}\mathbf{T}, \mathbf{W}\rangle\rangle \mathrm{d}A = \int_{\mathcal{U}} \left[\langle\langle \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}), \mathbf{W}\rangle\rangle + \mathbf{F}^{\mathsf{T}}\mathbf{P}:\boldsymbol{\Omega} + \mathbf{F}^{\mathsf{T}}\mathbf{P}:\frac{1}{2}\mathfrak{L}_{\mathbf{W}}\mathbf{G}\right]\mathrm{d}V. \tag{6.63}$$

Thus, (6.62) simplifies to

$$\int_{\mathcal{U}} \frac{\partial \rho_0}{\partial t}\left(-\langle\langle \mathbf{V}, \mathbf{FW}\rangle\rangle + \frac{1}{2}\langle\langle \mathbf{FW}, \mathbf{FW}\rangle\rangle\right)\mathrm{d}V + \int_{\mathcal{U}} \left(2\rho_0\frac{\partial E}{\partial \mathbf{G}} + \mathbf{F}^{\mathsf{T}}\mathbf{P}\right):\frac{1}{2}\mathfrak{L}_{\mathbf{W}}\mathbf{G}\,\mathrm{d}V + \int_{\mathcal{U}} \mathbf{F}^{\mathsf{T}}\mathbf{P}:\boldsymbol{\Omega}\,\mathrm{d}V$$

$$+ \int_{\partial\mathcal{U}} \langle\langle \mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) + \rho_0\mathbf{F}^{\mathsf{T}}(\mathbf{B}-\mathbf{A}), \mathbf{W}\rangle\rangle\,\mathrm{d}V = 0. \tag{6.64}$$

As $\mathcal{U}$ and $\mathbf{W}$ are arbitrary, we have

$$\frac{\partial \rho_0}{\partial t} = 0, \tag{6.65}$$

$$2\rho_0\frac{\partial E}{\partial \mathbf{G}} = -\mathbf{F}^{\mathsf{T}}\mathbf{P}, \tag{6.66}$$

$$\mathbf{F}^{\mathsf{T}}\mathbf{P} = \mathbf{P}^{\mathsf{T}}\mathbf{F}, \tag{6.67}$$

$$\mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) + \rho_0\mathbf{F}^{\mathsf{T}}\mathbf{B} = \rho_0\mathbf{F}^{\mathsf{T}}\mathbf{A}. \tag{6.68}$$

Equation (6.65) is nothing but material conservation of mass. Equation (6.66) is the material Doyle-Ericksen formula. This is what Lu and Papadopoulos[26] call infinitesimal material covariance. Equation (6.67) is balance of configurational angular momentum or isotropy of the material. [Note that if (6.66) holds then (6.67) holds trivially.] Finally, Eq. (6.68) is a condition that must be satisfied for the balance of energy to be invariant under material diffeomorphisms. This constraint is equivalent to

$$\mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}. \tag{6.69}$$

Assuming the above four conditions, it is easy to show that material energy balance is invariant under arbitrary material diffeomorphisms.

Ideal fluids do satisfy all these conditions. In fact, their transformation properties under material diffeomorphisms gives rise to Kelvin's circulation theorem and it is a key ingredient in the geometric approach to fluid mechanics; see the introduction to the Marsden and Ratiu book[29] for a discussion and references to the literature.

C. Material energy balance and defects

We now make a connection between (6.69) and Eshelby's idea of force on a defect. The idea of a driving force in continuum mechanics goes back to Eshelby[13–15] and this notion is important in developing evolution laws for the movement of defects, including dislocations, vacancies, interfaces, cavities, cracks, etc. Driving forces on these defects cause climb and glide of dislocations, diffusion of point defects, migration of interfaces, changing the shape of cavities and propagation of cracks, to mention a few examples. Eshelby defined the force on a defect as the generalized force corresponding to position of the defect (in the reference configuration), which is thought of as a generalized displacement. Eshelby studied inhomogeneities in elastostatic and elastodynamic systems by considering the explicit dependence of the elastic energy density on position in the reference configuration.

Defect forces: Suppose the elastic energy density has an explicit dependence on $\mathbf{X}$ (the position of material points in the undeformed configuration), i.e.,

$$W = W(\varphi, \mathbf{F}, \mathbf{X}), \tag{6.70}$$

where φ and $\mathbf{F}$ are the deformation mapping and the deformation gradient, respectively. Consider an open neighborhood Ω of an isolated defect. Force on the defect in the sense of Eshelby is defined as

$$\mathbf{F}^{\text{defect}} = \int_{\Omega} \left(\frac{\partial W}{\partial \mathbf{X}} \right)_{\text{explicit}} \mathrm{d}V = \int_{\Omega} \operatorname{Div} \mathbf{E} \, \mathrm{d}V = \int_{\partial\Omega} \mathbf{E}\hat{\mathbf{N}} \, \mathrm{d}A, \tag{6.71}$$

where $\mathbf{E} = W\mathbf{I} - \mathbf{F}^{\mathsf{T}}\mathbf{P}$ is Eshelby's energy-momentum tensor. It turns out that for a crack (thought of as a defect) $\mathbf{F}^{\text{defect}}$ is related to the celebrated J-integral;[37] J is the component of $\mathbf{F}^{\text{defect}}$ in the direction of crack propagation.

The following proposition makes an explicit connection between (6.69) and Eshelby's idea of force on a defect.

Proposition 6.4: Suppose an elastic material in an isothermal and quasistatic deformation satisfies the internal constraint $\operatorname{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}} \operatorname{Div} \mathbf{P}$. *In the absence of body forces*, *force on a defect in the sense of Eshelby would be*

$$\mathbf{F}^{\text{defect}} = \int_{\Omega} \left(\frac{\partial W}{\partial \mathbf{X}} \right)_{\text{explicit}} \mathrm{d}V = \int_{\Omega} \operatorname{Div} \mathbf{E} \, \mathrm{d}V = \int_{\partial\Omega} W\hat{\mathbf{N}} \, \mathrm{d}A. \tag{6.72}$$

Proof: Note that

$$\mathbf{F}^{\text{defect}} = \int_{\partial\Omega} \mathbf{E}\hat{\mathbf{N}} \, \mathrm{d}A = \int_{\partial\Omega} W\hat{\mathbf{N}} \, \mathrm{d}A - \int_{\Omega} \mathbf{F}^{\mathsf{T}} \operatorname{Div} \mathbf{P} \, \mathrm{d}V = \int_{\partial\Omega} W\hat{\mathbf{N}} \, \mathrm{d}A.$$

This means that the configurational traction on $\partial\Omega$ is normal to $\partial\Omega$ at all points, i.e., the configurational stress is hydrostatic. For this reason we call the internal constraint $\operatorname{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}} \operatorname{Div} \mathbf{P}$, the configurational inviscidity constraint.

If there is a stationary surface $\mathcal{S}$ across which deformation gradient and other quantities have jump discontinuities, the balance of standard forces reads

$$[\![\mathbf{P}]\!]\hat{\mathbf{N}} = \mathbf{0}. \tag{6.73}$$

Now let us look at the normal jump in Eshelby's energy-momentum tensor,

$$[\![\mathbf{E}]\!]\hat{\mathbf{N}} = [\![\Psi\mathbf{I} - \mathbf{F}^{\mathsf{T}}\mathbf{P}]\!]\hat{\mathbf{N}} = [\![\Psi]\!]\hat{\mathbf{N}} - [\![\mathbf{F}^{\mathsf{T}}]\!]\langle\mathbf{P}\rangle\hat{\mathbf{N}} - \langle\mathbf{F}^{\mathsf{T}}\rangle[\![\mathbf{P}]\!]\hat{\mathbf{N}}, \tag{6.74}$$

where $\langle\cdot\rangle$ denotes average of inner and outer traces. Using Hadamard's compatibility equations,

$$[\![\mathbf{F}]\!]\hat{\mathbf{t}} = \mathbf{0} \quad \text{for all } \hat{\mathbf{t}} \text{ such that } \hat{\mathbf{t}}\cdot\hat{\mathbf{N}} = 0, \tag{6.75}$$

it can be easily shown that

$$\hat{\mathbf{N}}\cdot[\![\mathbf{E}]\!]\hat{\mathbf{N}} = [\![\Psi]\!] - [\![\mathbf{F}]\!]\hat{\mathbf{N}}\cdot\mathbf{P}\hat{\mathbf{N}}, \quad \hat{\mathbf{t}}\cdot[\![\mathbf{E}]\!]\hat{\mathbf{N}} = -\mathbf{F}\hat{\mathbf{t}}\cdot[\![\mathbf{P}]\!]\hat{\mathbf{N}}. \tag{6.76}$$

Now if the balance of standard forces hold one concludes that

$$\hat{\mathbf{t}}\cdot[\![\mathbf{E}]\!]\hat{\mathbf{N}} = 0. \tag{6.77}$$

This means that jump in configurational traction on $\partial\Omega$ is always normal to $\partial\Omega$. However, the previous remark shows that in the absence of body forces the condition $\mathrm{Div}(\mathbf{F}^{\mathsf{T}}\mathbf{P}) = \mathbf{F}^{\mathsf{T}}\,\mathrm{Div}\,\mathbf{P}$ implies that the configurational traction itself is normal to $\partial\Omega$.

Are configurational forces newtonian?: There have been doubts and discussions concerning the nature of configurational forces in the literature already starting from Eshelby himself. Eshelby strongly believed that force on a defect is fictitious and is different from the usual forces in mechanics. He defined force on a defect to be the thermodynamic force conjugate to the generalized coordinates defining the defect, for example, the crack tip position in the case of a crack. Eshelby[16] observed that the configurational force on a disclination in a liquid crystal is a real force. A similar observation was made by Nabarro[34] for dislocations. Kröner[23] and Ericksen[11,12] have similar discussions. Batra[4] argues that force on a defect is equal to the standard force exerted on the boundary of a subbody embracing the defect. Steinmann[42] introduces the spatial signature of a material force. One should note that this viewpoint is not in agreement with Gurtin's theory in which standard and configurational forces have their own balance laws.

Batra[4] proves a theorem that states that force on a defect is equal to the resultant of tractions on the boundary of any region enclosing this single defect. This seems to be a very surprising result. First of all, if body forces are considered resultant of tractions on different regions embodying the defect cannot be independent of the region as in this case stress tensor is not divergence free. Barta suggests that problems involving the J-integral could be reinterpreted using his theorem. As a matter of fact, the J-integral can serve as a counter example for Batra's theorem. The reason is that in the case of a linear elastic material in mode I fracture, for example, the J-integral is quadratic in K_I while the stress is linear in K_I and hence the resultant of tractions acting on the boundary of a small region enclosing the crack would be linear in K_I. This means that the J-integral, which is the component of configurational force in the direction of crack growth, cannot be a real force. The incorrectness of Batra's theorem is because of the way he defines force on a defect. Force on a defect in the sense of Eshelby is the rate of change of potential energy of the elastic body with respect to changes in the position of the defect in the reference configuration. Batra defines force on a defect to be the rate of change of energy with respect to changes of position of the defect in the current configuration. This is the source of his surprising result. One should note that direct and inverse motions describe the same physical process and cannot lead to different conclusions regarding forces. Having the duality picture is useful but one should note that positions of defects in the reference and current configurations are not related by the standard deformation mapping as the evolution of defects is an independent kinematical process.

Standard forces in continuum mechanics are one forms in the deformed configuration, i.e., at each point $x \in \mathcal{S}$, force is an element of $T_x^*\mathcal{S}$. Configurational forces on the other hand are one forms in the reference configuration, i.e., at each point $X \in \mathcal{B}$, configurational force is an element of $T_X^*\mathcal{B}$. Therefore, geometrically it is meaningless to ask if a configurational force is a real force

very much like asking whether the deformation gradient (a two-point tensor) is symmetric. This is why arguments like the one proposed by Steinmann[43] where he defines a spatial signature for a material force do not make sense from the geometric standpoint.

Plasticity and embeddings: A traditional means of introducing configurational forces is based on remapping the reference configuration of the body. However, this approach tacitly assumes that the reference configuration can be embedded in Euclidean space. This approach fails when there is no natural embedding of the reference configuration. A case in point is provided by multiplicative plasticity,[24] where the total deformation gradient at a point x has the representation: $\mathbf{F}(x) = \mathbf{F}^e(x)\mathbf{F}^p(x)$, where $\mathbf{F}^e(x)$ and $\mathbf{F}^p(x)$ are the elastic and plastic deformation gradients, both of which fail to be a gradient in general. The plastic deformation mapping $\mathbf{F}^p(x)$ defines an *intermediate configuration* that defines the reference configuration for the elasticity of the material. In particular, the elastic energy density is assumed to be of the form $W(\mathbf{F}^e, x)$. Since $\mathbf{F}^p(x)$ is not the derivative of a mapping, the intermediate configuration cannot be embedded in Euclidean space. Therefore, remapping cannot be applied to deriving configurational forces directly from $W(\mathbf{F}^e, x)$. By contrast, the present approach can be applied for that purpose, for example, by equipping the intermediate configuration with a constant metric.

The derivation of certain conserved integrals, such as the L-integral that gives the configurational torque on isotropic subbodies, relies on the metric structure of the embedding Euclidean space. In addition, the conventional formulation of material symmetry also presumes the existence of an Euclidian embedding. Such an embedding may not be natural or available in certain models of materials, such as liquid crystals or smectic polymers, where the reference configuration may include a unit director field.

VII. NOETHER'S THEOREM AND BALANCE OF CONFIGURATIONAL FORCES

As is well known, there is a strong connection between conservation laws and symmetries. If the Euler-Lagrange equations are satisfied and the Lagrangian density of a system is invariant under a group of transformations, Noether's theorem gives the corresponding conserved quantity. In this sense, conservation laws are related to symmetries of a given system. Marsden and Hughes[28] consider material invariance in elasticity (in the absence of body forces) and show that invariance of Lagrangian density under rigid translations in the reference configuration results in the following conservation law

$$\frac{\partial}{\partial t}(\partial_{\dot{\phi}}\mathfrak{L}\cdot D\phi\cdot\mathbf{W}) + \mathrm{DIV}(\partial_{\mathbf{F}}\mathfrak{L}\cdot D\phi\cdot\mathbf{W} - \mathfrak{L}\mathbf{W}) = 0. \tag{7.1}$$

This has been obtained assuming that the flow of $\mathbf{W}$ is volume-preserving and that $\mathcal{L}$ does not explicitly depend on X. For a constant $\mathbf{W}$, this equation in our notation reads

$$\mathrm{Div}\left[\left(\Psi - \frac{1}{2}\rho_0|\mathbf{V}|^2\right)\mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{P}\right] = -\frac{\partial}{\partial t}(\rho_0\mathbf{F}^{\mathrm{T}}\mathbf{V}). \tag{7.2}$$

It is seen that this is identical to balance of configurational linear momentum if ρ_0 and Ψ are independent of $\mathbf{X}$ (note that this is stronger that homogeneity of $\mathfrak{L}$). Ignoring the inertial effects, Noether's theorem results in

$$\mathrm{Div}(\Psi\mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{P}) = \mathbf{0}. \tag{7.3}$$

Roughly speaking, Noether's theorem states that when the Euler-Lagrange equations are satisfied, any symmetry of the Lagrangian density corresponds to a conserved quantity. Here we revisit Noether's theorem for nonlinear elasticity assuming that undeformed and deformed configurations are Riemannian manifolds. Writing action in the reference configuration, Lagrangian density has the following explicit independent variables:

$$\mathcal{L} = \mathcal{L}(X^A, \varphi^a, \dot{\varphi}^a, F^a{}_A, G_{AB}, g_{ab}). \tag{7.4}$$

For the sake of clarity, we consider spatial and material symmetries of the Lagrangian density separately.

A. Spatial covariance of Lagrangian density

Theorem 7.1: *If the Lagrangian density is spatially covariant, then the following hold: (i) spatial homogeneity of the Lagrangian density and (ii) the Doyle-Ericksen formula.*

Proof: Suppose ψ_s is a flow on $\mathcal{S}$ generated by a vector field $\mathbf{w}$, i.e.,

$$\left.\frac{d}{\mathrm{d}s}\right|_{s=0} \psi_s \circ \varphi = \mathbf{w} \circ \varphi. \tag{7.5}$$

Invariance of $\mathcal{L}$ means that

$$\mathcal{L}\left(X^A, \psi_s^a(\varphi), \frac{\partial \psi_s^a}{\partial x^b}\dot{\varphi}^b, \frac{\partial \psi_s^a}{\partial x^b}F^b{}_A, G_{AB}, -\frac{\partial \psi_s^c}{\partial x^a}\frac{\partial \psi_s^d}{\partial x^b}g_{cd}\right) = \mathcal{L}(X^A, \varphi^a, \dot{\varphi}^a, F^a{}_A, G_{AB}, g_{ab}). \tag{7.6}$$

[This reminds us of the definition of covariance for internal energy density. So, it would be very natural to expect some connection between Noether's theorem and covariant balance laws.] Now differentiating the above relation with respect to s and then evaluating it at $s=0$ [This is somewhat similar to subtracting two balance relations and evaluating the result at $t=t_0$], one obtains

$$\frac{\partial \mathcal{L}}{\partial \varphi^a}w^a + \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\frac{\partial w^a}{\partial x^b}\dot{\varphi}^b + \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^A \frac{\partial w^a}{\partial x^b}F^b{}_A - 2\frac{\partial \mathcal{L}}{\partial g_{ab}}\frac{\partial w^c}{\partial x^a}g_{bc} = 0. \tag{7.7}$$

Note that

$$\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\frac{\partial w^a}{\partial x^b}\dot{\varphi}^b = \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}w^a\right) - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)w^a. \tag{7.8}$$

After some manipulations, it can be shown that

$$\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^A \frac{\partial w^a}{\partial x^b}F^b{}_A = \left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^A w^a\right]_{|A} - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A} w^a - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b{}^A \gamma^b_{ac}F^c{}_A w^a. \tag{7.9}$$

Also

$$-2\frac{\partial \mathcal{L}}{\partial g_{ab}}\frac{\partial w^c}{\partial x^a}g_{bc} = -\left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a{}^A w^c\right]_{|A} + \left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a{}^A\right]_{|A}^{\ w^c} + 2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bd}\gamma^d_{ac}w^c. \tag{7.10}$$

Therefore, symmetry of $\mathcal{L}$ implies that

$$\begin{aligned}&\left[\frac{\partial \mathcal{L}}{\partial \varphi^a} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)_a - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A} - \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b{}^A F^c{}_A\gamma^b_{ac} + 2\frac{\partial \mathcal{L}}{\partial g_{cd}}g_{bd}\gamma^b_{ac}\right]w^a + \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}w^a\right)\\ &\quad + \left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a{}^A w^a\right]_{|A} - \left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a{}^A w^c\right]_{|A} + \left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a{}^A\right]_{|A} w^c = 0.\end{aligned} \tag{7.11}$$

Note that the term multiplied by w^a is zero if the Euler-Lagrange equations are satisfied. Thus, Noether's theorem states that

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}w^a\right)+\left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A}w^a\right]_{|A}-\left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a^{\ A}w^c\right]_{|A}+\left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a^{\ A}\right]_{|A}w^c=0. \tag{7.12}$$

Note that

$$\left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A}w^a\right]_{|A}=\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}w^a+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A}F^b_{\ A}w^a{}_{|b}. \tag{7.13}$$

Also

$$\left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a^{\ A}w^c\right]_{|A}=\left[2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}(\mathbf{F}^{-1})_a^{\ A}\right]_{|A}w^c+2\frac{\partial \mathcal{L}}{\partial g_{ab}}g_{bc}w^c{}_{|a}. \tag{7.14}$$

Therefore (7.12) is simplified to

$$\left[\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}\right]w^a+\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)\frac{\partial w^a}{\partial t}+\left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A}F^c_{\ A}-2\frac{\partial \mathcal{L}}{\partial g_{bc}}g_{ab}\right]w^a{}_{|c}=0. \tag{7.15}$$

Note that

$$\frac{\partial w^a}{\partial t}=\frac{\partial w^a}{\partial x^c}\dot{\varphi}^c=\dot{\varphi}^c w^a{}_{|c}-\gamma^a_{cd}w^d\dot{\varphi}^c. \tag{7.16}$$

Therefore statement of Noether's theorem, Eq. (7.12) can be rewritten as

$$\left[\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}-\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^d}\gamma^d_{ac}\dot{\varphi}^c\right]w^a+\left[\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_a^{\ A}F^c_{\ A}+\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\dot{\varphi}^c-2\frac{\partial \mathcal{L}}{\partial g_{bc}}g_{ab}\right]w^a{}_{|c}=0. \tag{7.17}$$

Note that

$$\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\dot{\varphi}^c=\rho_0 g_{ab}\dot{\varphi}^b\dot{\varphi}^c. \tag{7.18}$$

If Lagrangian density is covariant, i.e., if $\mathbf{w}$ is arbitrary then (7.17) implies that

$$2\frac{\partial \mathcal{L}}{\partial g_{ab}}=g^{bc}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_c^{\ A}F^a_{\ A}+g^{bc}\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^c}\dot{\varphi}^a, \tag{7.19}$$

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}-\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^d}\gamma^d_{ac}\dot{\varphi}^c=0. \tag{7.20}$$

Equation (7.19) can be rewritten as

$$2\frac{\partial W}{\partial g_{ab}}=g^{bc}\left(\frac{\partial W}{\partial \mathbf{F}}\right)_c^{\ A}F^a_{\ A}, \tag{7.21}$$

which is nothing but the Doyle-Ericksen formula. [Note that this includes balance of angular momentum.] Note that

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}-\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^d}\gamma_{ac}^d\dot{\varphi}^c=\frac{\partial \mathcal{L}}{\partial \varphi^a}-\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b^{\ A}F^c{}_A\gamma_{ac}^b+2\frac{\partial \mathcal{L}}{\partial g_{cd}}g_{bd}\gamma_{ac}^b-\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^b}\dot{\varphi}^c\gamma_{ac}^b. \tag{7.22}$$

But

$$-\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_b^{\ A}F^c{}_A+2\frac{\partial \mathcal{L}}{\partial g_{cd}}g_{bd}=\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^b}\dot{\varphi}^c. \tag{7.23}$$

Thus

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}\right)+\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)_{a\ |A}^{\ A}-\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^d}\gamma_{ac}^d\dot{\varphi}^c=\frac{\partial \mathcal{L}}{\partial \varphi^a}. \tag{7.24}$$

Hence (7.20) implies that

$$\frac{\partial \mathcal{L}}{\partial \varphi^a}=0. \tag{7.25}$$

□

Note that this theorem implies that arbitrary flows and in particular rigid translations cannot be transitive (in the sense of Gotay *et al.*[17,18]) for arbitrary Lagrangian densities.

B. Material covariance of Lagrangian density

Let us first consider the case of Euclidean spaces. Consider a flow Λ_s on $\mathcal{B}$ generated by a vector field $\mathbf{W}$. Invariance of $\mathcal{L}$ with respect to this flow means that

$$\mathcal{L}\left(\Lambda_s^A(X),\varphi^a,\dot{\varphi}^a,\left[\left(\frac{\partial \Lambda_s}{\partial X}\right)^{-1}\right]_A^B F^a{}_B\right)=\mathcal{L}(X^A,\varphi^a,\dot{\varphi}^a,F^a{}_A). \tag{7.26}$$

Differentiating the above relation with respect to s and evaluating the result at $s=0$, one obtains

$$\frac{\partial \mathcal{L}}{\partial X^A}W^A-\frac{\partial \mathcal{L}}{\partial F^a{}_A}\frac{\partial W^B}{\partial X^A}F^a{}_B=0. \tag{7.27}$$

If $\mathbf{W}$ is a constant, then

$$\frac{\partial \mathcal{L}}{\partial X^A}=0, \tag{7.28}$$

i.e., the Lagrangian density must be materially homogeneous. This is also what Nelson[35,36] obtains. After some manipulation and assuming that Euler-Lagrange equations are satisfied (7.27) can be rewritten as

$$\frac{\partial}{\partial X^A}\left(\mathcal{L}W^A-\frac{\partial}{\partial F^a{}_A}F^a{}_BW^B\right)-\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}F^a{}_AW^A\right)-\mathcal{L}\frac{\partial W^A}{\partial X^A}=0, \tag{7.29}$$

where use was made of the fact that $\mathbf{W}$ is time independent. For a volume-preserving flow this gives us

$$\frac{\partial}{\partial X^A}\left(\mathcal{L}W^A - \frac{\partial}{\partial F^a{}_A}F^a{}_B W^B\right) - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}F^a{}_A W^A\right) = 0, \tag{7.30}$$

which is what Marsden and Hughes[28] obtain. Now let us consider the general case of Riemannian manifolds and assume that Λ_s is a flow on the Riemannian manifold $(\mathfrak{B}, \mathbf{G})$ generated by a vector field $\mathbf{W}$, i.e.,

$$\left.\frac{d}{\mathrm{d}s}\right|_{s=0} \Lambda_s(X) = \mathbf{W}(X), \quad X \in \mathcal{B}. \tag{7.31}$$

Theorem 7.2: *If the Lagrangian density is materially covariant then the following hold*: (i) *material homogeneity of the Lagrangian density and* (ii) *material Doyle-Ericksen formula*.

Proof: Invariance of $\mathcal{L}$ with respect to Λ_s means that

$$\begin{aligned}&\mathcal{L}\left(\Lambda_s^A(X), \varphi^a, \dot{\varphi}^a, \left[\left(\frac{\partial \Lambda_s}{\partial X}\right)^{-1}\right]^B_A F^a{}_B, g_{ab}, \left[\left(\frac{\partial \Lambda_s}{\partial X}\right)^{-1}\right]^C_A \left[\left(\frac{\partial \Lambda_s}{\partial X}\right)^{-1}\right]^D_B G_{CD}\right)\\ &\quad = \mathcal{L}(X^A, \varphi^a, \dot{\varphi}^a, F^a{}_A, g_{ab}, G_{AB}).\end{aligned} \tag{7.32}$$

Differentiating the above relation with respect to s and evaluating the result at $s=0$, one obtains

$$\frac{\partial \mathcal{L}}{\partial X^A}W^A - \frac{\partial \mathcal{L}}{\partial F^a{}_A}\frac{\partial W^B}{\partial X^A}F^a{}_B - 2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}\frac{\partial W^C}{\partial X^K} = 0. \tag{7.33}$$

Note that

$$-\frac{\partial \mathcal{L}}{\partial F^a{}_A}\frac{\partial W^B}{\partial X^A}F^a{}_B = -\left(F^a{}_B\frac{\partial \mathcal{L}}{\partial F^a{}_A}W^B\right)_{|A} + \left(F^a{}_B\frac{\partial \mathcal{L}}{\partial F^a{}_A}\right)_{|A}W^B + F^a{}_C\frac{\partial \mathcal{L}}{\partial F^a{}_A}\Gamma^C_{AB}W^B \tag{7.34}$$

and

$$-2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}\frac{\partial W^C}{\partial X^K} = -\left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}W^C\right)_{|K} + \left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}\right)_{|K}W^C + 2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{BD}\Gamma^B_{CK}W^C. \tag{7.35}$$

Also

$$\left(F^a{}_B\frac{\partial \mathcal{L}}{\partial F^a{}_A}\right)_{|A}W^B = \left(\frac{\partial F^a{}_B}{\partial X^A} - F^a{}_C\Gamma^C_{BA}\right)\frac{\partial \mathcal{L}}{\partial F^a{}_A}W^B + F^a{}_A\left[\left(\frac{\partial \mathcal{L}}{\partial F^a{}_B}\right)_{|B} + \frac{\partial \mathcal{L}}{\partial F^b{}_B}F^c{}_B\gamma^b_{ac}\right]W^A. \tag{7.36}$$

Assuming that Euler-Lagrange equations are satisfied and using the above identities after a lengthy series of simplifications, one obtains

$$\left(\mathcal{L}W^A - \frac{\partial \mathcal{L}}{\partial F^a{}_B}W^B\right)_{|A} - \frac{\partial}{\partial t}\left(F^a{}_A\frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a}W^A\right) - \mathcal{L}W^A{}_{|A} - \left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}W^C\right)_{|K} + \left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}\right)_{|K}W^C = 0. \tag{7.37}$$

Note that

$$-\left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}W^C\right)_{|K} + \left(2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}\right)_{|K}W^C = -2\frac{\partial \mathcal{L}}{\partial G_{DK}}G_{DC}W^C_{|K}. \tag{7.38}$$

Therefore in this case Noether's theorem states that

$$\left(\mathcal{L}W^A - \frac{\partial \mathcal{L}}{\partial F^a{}_B} W^B\right)_{|A} - \frac{\partial}{\partial t}\left(F^a_A \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^a} W^A\right) - \mathcal{L}W^A{}_{|A} - 2\frac{\partial \mathcal{L}}{\partial G_{DK}} G_{DC} W^C{}_{|K} = 0. \tag{7.39}$$

Note that

$$\left(F^a{}_B \frac{\partial \mathcal{L}}{\partial F^a{}_A} W^B\right)_{|A} = \frac{\partial}{\partial X^A}\left(F^a{}_B \frac{\partial \mathcal{L}}{\partial F^a{}_A}\right) W^B + F^a{}_B \frac{\partial \mathcal{L}}{\partial F^a{}_A} W^B + F^a{}_B \frac{\partial \mathcal{L}}{\partial F^a{}_A}\left(W^B \Gamma^C_{AC} - W^C \Gamma^B_{CA}\right). \tag{7.40}$$

Using the above relation and some lengthy simplifications, one can rewrite (7.39) as

$$\left[\frac{\partial \mathcal{L}}{\partial X^A} + \left(\frac{\partial \mathcal{L}}{\partial F^a{}_C} F^a{}_B + 2\frac{\partial \mathcal{L}}{\partial G_{CD}} G_{BC}\right)\Gamma^B_{AC}\right] W^A - \left(\frac{\partial \mathcal{L}}{\partial F^a{}_A} F^a{}_B + 2\frac{\partial \mathcal{L}}{\partial G_{AC}} G_{BC}\right) W^B = 0. \tag{7.41}$$

If $\mathcal{L}$ is materially covariant, i.e., if $\mathbf{W}$ is arbitrary, then

$$\frac{\partial \mathcal{L}}{\partial X^A} + \left(\frac{\partial \mathcal{L}}{\partial F^a{}_C} F^a{}_B + 2\frac{\partial \mathcal{L}}{\partial G_{CD}} G_{BC}\right)\Gamma^B_{AC} = 0, \tag{7.42}$$

$$\frac{\partial \mathcal{L}}{\partial F^a{}_A} F^a{}_B + 2\frac{\partial \mathcal{L}}{\partial G_{AC}} G_{BC} = 0. \tag{7.43}$$

Or equivalently

$$\frac{\partial \mathcal{L}}{\partial X^A} = 0, \tag{7.44}$$

$$\frac{\partial W}{\partial F^a{}_A} F^a{}_B + 2\frac{\partial W}{\partial G_{AC}} G_{BC} = 0, \tag{7.45}$$

where W is the material potential energy density. Note that (7.45) is nothing but the material Doyle-Ericksen formula (6.66). □

Remarks: There are some differences between covariant energy balance (CEB) and Lagrangian density covariance (LDC):

(i) CEB is global while LDC is local.
(ii) In CEB the arbitrary vector fields $\mathbf{w}$ and $\mathbf{W}$ are time-dependent (being velocities), in general, while in LDC they are time independent.
(iii) In writing balance of energy in CEB for a material diffeomorphism spatial quantities contribute to energy balance. But in LDC a material flow does not affect the spatial quantities.

VIII. CONCLUSIONS AND FUTURE DIRECTIONS

The results of this paper can be summarized as follows.

(i) We studied continuum mechanics of bodies with global referential evolutions by enlarging the configuration manifold to two Riemannian manifolds with their own metrics. A deformation is then a pair of referential evolution, i.e., a motion in the referential manifold, and a standard motion. We showed that in the absence of discontinuities, configurational and standard equations of motion are equivalent even if the metrics are allowed to vary.

(ii) The classical theorem of Green, Naghdi, and Rivilin[19] was revisited and a material version of it was investigated. We showed that under a referential isometry balance of energy cannot be invariant, in general, and obtained its transformation.

(iii) The idea of covariance in elasticity was reviewed. We revisited a theorem by Marsden and Hughes[28] and some of the details of its proof were clarified and a proof was given for its converse. It was also shown that spatial covariance of material energy balance leads to identical results.

(iv) We posed the question that whether energy balance can be materially covariant. It was shown that, in general, energy balance cannot be invariant under referential diffeomorphisms. We obtained the transformation of energy balance under arbitrary material diffeomorphisms. We found conditions under which energy balance is materially covariant. It was shown that in the absence of body forces the nontrivial condition for material covariance of balance of energy is equivalent to configurational stress tensor (Eshelby's stress tensor) being hydrostatic. It was shown that for ideal fluids energy balance is materially covariant.

(v) An explicit relation between covariance and Noether's theorem was found. We showed that spatial covariance of a Lagrangian density implies spatial homogeneity of the Lagrangian density and the Doyle-Ericksen formula. Similarly, material covariance of a Lagrangian density implies its material homogeneity and the material Doyle-Ericksen formula.

In summary, spatial covariance is reasonable and holds for most materials. The transformation properties of energy balance under material reframings was obtained. However, material covariance of energy balance only holds for special materials, such as ideal fluids.

The main application of the ideas presented in this paper will be in gaining a better understanding of the continuum theory of defects. In particular, if one repeats some of the developments presented in this paper in a space-time setting, one should, in principle, be able to obtain dynamic equations for evolution of defects. Another important relevant problem would be the study of covariance and its meaning in discrete systems. This may lead to a better understanding of "stress" in discrete systems.

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Unified treatment and classification of superintegrable systems with integrals quadratic in momenta on a two-dimensional manifold

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In this paper we prove that the two-dimensional superintegrable systems with quadratic integrals of motion on a manifold can be classified by using the Poisson algebra of the integrals of motion. There are six general fundamental classes of superintegrable systems. Analytic formulas for the involved integrals are calculated in all the cases. All the known superintegrable systems are classified as special cases of these six general classes. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In classical mechanics, an integrable system on a manifold of N dimensions, is a system which has N integrals of motion in evolution. Superintegrable (or maximally integrable) system is a system possessing the maximum number of constants of motion, i.e., $2N-1$ integrals of motion.

The simplest case is the two-dimensional superintegrable problems with integrals of motion, which are linear and quadratic functions of momenta. The investigation of such superintegrable systems on a two-dimensional manifold is a quite old problem, dated in the 19th century. Initially the problem was formulated as a geometry problem. The challenge was to find two-dimensional manifolds whose geodesics are curves which possess additional integrals than the free Hamiltonian. This problem was studied in the four volume treatise of Darboux *Leçons sur la Théorie Générale des Surfaces*.[1] The main result of this study is that, there are five classes of general forms of metrics, whose geodesics have three integrals of motion (the Hamiltonian and two additional functionally independent integrals). These metrics are called "formes essentielles" and they depend on four parameters. All the metrics having more than two integrals of motion can be obtained as partial cases of these "formes essentielles" by choosing appropriate values of the four parameters. The five classes of metrics are tabulated in "Tableau VII" by Koenigs (Ref. 1. Vol. IV, p. 385).

In classical mechanics language, Darboux and Koenigs results can be translated as searching manifolds, where the free Hamiltonian accepts quadratic integrals of motion. The evolution of this problem is to find superintegrable systems, whose Hamiltonian is the free Hamiltonian plus a potential and these systems possess additional quadratic integrals of motion.

The simplest integrable and superintegrable systems are the systems defined on the real plane. A comprehensive review of the real two-dimensional integrable classical systems on the plane is given in Refs. 2 and 3 The complex superintegrable systems with quadratic moments on a flat space were recently catalogued by Kalnins, Miller, Pogosyan *et al.*[4–7] The flat space is a two-dimensional manifold with curvature zero. The Drach potentials are also systems defined on a

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manifold with curvature zero. The Drach systems with quadratic integrals of motion were investigated by Rañada.[8] The superintegrable systems on the hyperbolic plane were studied in Refs. 9 and 10. These systems were studied separately, while they are connected by obvious coordinate transformations. Therefore they are naturally connected, i.e., there is a common classification scheme of all these systems.[9,10]

The case of nonflat space is under current intensive investigation. The superintegrable systems on the sphere were studied in Refs. 8, 9, and 11 and they were classified in Ref. 6 The sphere is a special case of manifold with constant curvature. In Refs. 9 and 10 the superintegrable systems on the sphere and on the hyperbolic plane were studied using a unified formulation.

In the case of manifolds of nonconstant curvature, the known examples of superintegrable systems are those which are defined on manifolds which are surfaces of revolution. The corresponding problem of the geodesics with three quadratic integrals of motion on surfaces of revolution was treated by Koenigs in Ref. 1 Vol. IV, p. 377. Recently Kalnins and collaborators classified the superintegrable systems on a surface of revolution[12,13] using the manifolds which were provided by Koenigs.

In two recent papers Kalnins, Kress, and Miller[14,15] give a comprehensive study of the two-dimensional superintegrable sytems. In Ref. 15, they prove that the general Koenigs essential forms of metrics correspond to the most general forms of superintegrable systems. Also they have shown that every two-dimensional superintegrable system is Stäckel equivalent to a two-dimensional nondegenerate superintegrable system on a constant curvature space.

Kress[16] in collaboration with Kalnins and Miller studied the Stäckel equivalence classes of the superintegrable systems on the spaces of constant curvature, and they have shown that there are six equivalence classes. The general classes of Koenigs classification given by the Table VII in Ref. 1 are five. That means that there is a sixth class which should be added in the Koenigs classification scheme. In this paper we investigate this sixth class, which completes the Koenigs classification. This class is the nondegenerate superintegrable system generated by the case VI_6 of Koenigs.

An interesting question is, whether there could be a general classification scheme of superintegrable systems with quadratic integrals of motion, which contains all the equivalence classes of superintegrable systems on a manifold with constant curvature and the general classes of manifolds, which were introduced by Koenigs. The classification schemes are based on the Darboux relations derived for the invariants, which are defined on a specific manifold. In this paper we propose a classification scheme based on the properties of the Poisson algebra of the integrals of motion. Then we show that there is indeed such a classification scheme, which determines the supporting manifold metric. We must notice that the Kress[16] equivalence classes are derived by classifying the Poisson algebra of integrals of motion. The proposed classes of superintegrable systems in this paper correspond to the equivalent classes studied in Ref. 16. Analytic formulas for the metrics of the permitted manifolds, the potentials and the integrals of motion are calculated.

This paper is organized as follows: In Sec. II the general form of the integrable two-dimensional system with one quadratic integral of motion is derived. The results of this section correspond to the Darboux treatise paragraphs (Ref. 1, No. 593, Vol. III, pp. 30 and 31), but we give a brief modern derivation of the formulas including the potentials in our discussion. These formulas will be used in the following sections. The carrying manifold is a Liouville or a Lie surface. Therefore there are two classes of integrable systems. In a specific coordinate system, which is called Liouville (or Lie) system, the analytic expressions of the potential and the integrals of motion are given and the action is calculated. In Sec. III the Poisson algebra of the integrals of a superintegrable two-dimensional system is discussed. This algebra is a quadratic algebra, the coefficients of the quadratic terms are characteristic of the carrying manifold. In Sec. IV we prove that the coefficients of the Poisson algebra impose the classification of the superintegrable systems with two quadratic integrals in six fundamental classes. The method of analytic calculation of form of the permitted carrying manifolds, the potentials and the integrals of motion are discussed. In this section we prove that the general form of the superintegrable potential can be written as a fraction $V=w(x,y)/g(x,y)$ and the two functions $w(x,y)$ and the metric $g(x,y)$ are two solutions of

the same partial differential equation. The existence of the Poisson algebra was assumed as obvious by several authors.[4–7,17–29] In the Appendix we give a proof of the existence of the Poisson algebra, for two-dimensional superintegrable systems with quadratic integrals of motion. In Sec. V the analytic formulas of the manifolds and integrals are given for all the six fundamental classes of superintegrable systems. From these analytic formulas we can show that there are new superintegrable systems, because they are defined on manifolds which have not constant curvature and are not surfaces of revolution. In Sec. VI the superintegrable systems corresponding to the Koenigs essential forms of Table VII are given. In Sec. VII the superintegrable systems on a surface of revolution are studied. We find that there is a new system which was not revealed by the other classification schemes. In Sec. VIII the superintegrable systems on a manifold with curvature zero are studied and in Sec. IX the systems on a manifold with constant curvature are listed. In Sec. X the systems with a linear and a quadratic integral of motion are discussed. Finally, in Sec. XI the results of the paper are summarized.

II. INTEGRABLE SYSTEMS ON A TWO-DIMENSIONAL MANIFOLD

Let us consider an integrable system defined on a two-dimensional manifold with metric,

$$\mathrm{d}s^2 = E(u,v)\mathrm{d}u^2 + 2F(u,v)\mathrm{d}u\,\mathrm{d}v + G(u,v)\mathrm{d}v^2.$$

There is a conformal coordinate system where the metric can be written as

$$\mathrm{d}s^2 = g(x,y)\mathrm{d}x\,\mathrm{d}y. \tag{1}$$

The passage from the original coordinate system (u,v) to the conformal one (x,y) can be realized by using the Beltrami partial differential equation. We must notice that the choice of the conformal coordinate system is not unique, i.e., there are several conformal coordinate systems for a given metric, these systems are conformally equivalent.

In a conformal coordinate system the general form of the Hamiltonian is

$$H = \frac{p_x p_y}{g(x,y)} + V(x,y), \tag{2}$$

where the Hamiltonian is a quadratic form of the momenta.

Let us consider an integral of motion which is quadratic in momenta. The most general form can be written as

$$I = A(x,y)p_x^2 + B(x,y)p_y^2 - 2p_x p_y \frac{\beta(x,y)}{g(x,y)} + Q(x,y). \tag{3}$$

By definition the Poisson bracket between the Hamiltonian and the integral of motion is zero,

$$\{I,H\}_P = \frac{\partial I}{\partial x}\frac{\partial H}{\partial p_x} - \frac{\partial I}{\partial p_x}\frac{\partial H}{\partial x} + \frac{\partial I}{\partial y}\frac{\partial H}{\partial p_y} - \frac{\partial I}{\partial p_y}\frac{\partial H}{\partial y} = 0. \tag{4}$$

The above equality implies restrictions on the functions involved in Eqs. (2) and (3). The left-hand side of the above equation is an odd function of cubic order in the momenta. The coefficients of p_x^3 and p_y^3 must be zero

$$\frac{\partial A}{\partial y} = 0 \Rightarrow A = A(x),$$

$$\frac{\partial B}{\partial x} = 0 \Rightarrow B = B(y). \tag{5}$$

The coefficients of $p_x^2 p_y$ and $p_y^2 p_x$ in (4) must be indeed zero,

$$\frac{\partial \beta}{\partial y} = A(x)\frac{\partial g}{\partial x} + \frac{g}{2}A'(x), \tag{6}$$

$$\frac{\partial \beta}{\partial x} = B(y)\frac{\partial g}{\partial y} + \frac{g}{2}B'(y). \tag{7}$$

The partial x derivative of the right-hand side in (6) is equal to the y derivative of the right-hand side in Eq. (7), therefore

$$(A''(x) - B''(y))g(x,y) + 3A'(x)\frac{\partial g}{\partial x} - 3B'(y)\frac{\partial g}{\partial y} + 2A(x)\frac{\partial^2 g}{\partial x^2} - 2B(y)\frac{\partial^2 g}{\partial y^2} = 0. \tag{8}$$

The coefficients of p_x and p_y in (4) must be zero,

$$\begin{aligned} \frac{\partial Q}{\partial y} &= 2A(x)\frac{\partial V}{\partial x} + 2\beta(x,y)\frac{\partial V}{\partial y}, \\ \frac{\partial Q}{\partial x} &= 2B(y)\frac{\partial V}{\partial y} + 2\beta(x,y)\frac{\partial V}{\partial y}. \end{aligned} \tag{9}$$

The above relations imply

$$g(x,y)\left(2A(x)\frac{\partial^2 V}{\partial x^2} - 2B(y)\frac{\partial^2 V}{\partial y^2} + 3A'(x)\frac{\partial V}{\partial x} - 3B'(y)\frac{\partial V}{\partial y}\right) + 4\left(A(x)\frac{\partial g}{\partial x}\frac{\partial V}{\partial x} - B(y)\frac{\partial g}{\partial y}\frac{\partial V}{\partial y}\right) = 0. \tag{10}$$

At this point we must distinguish two cases. In the first case $A(x)$ and $B(y)$ are both different from zero, whereas in the second case $B(y)$ is assumed to be zero.

Class I: $A(x)B(y) \neq 0$.

Following the method given in Koenigs original paper, we can choose a new coordinate system

$$\xi = \int \frac{\mathrm{d}x}{\sqrt{A(x)}} \quad \text{and} \quad \eta = \int \frac{\mathrm{d}y}{\sqrt{B(y)}},$$

where the associated momenta are

$$p_\xi = \sqrt{A(x)}p_x \quad \text{and} \quad p_\eta = \sqrt{B(y)}p_y.$$

In this case the metric is written

$$\mathrm{d}s^2 = \hat{g}(\xi,\eta)\mathrm{d}\xi\,\mathrm{d}\eta, \quad \text{where } \hat{g}(\xi,\eta) = g(x,y)\sqrt{A(x)B(y)}.$$

In these new coordinate system (ξ, η) all the above equations are considerably simplified. We can easily show that the formulas are the same by replacing $x \to \xi$, $y \to \eta$ and fixing $A(x)=1$ and $B(y)=1$. For simplicity reasons we omit the hat on the metric $\hat{g}(\xi,\eta) \to g(\xi,\eta)$. Equations (2) and (3) are written

$$\begin{aligned} H &= \frac{p_\xi p_\eta}{g(\xi,\eta)} + V(\xi,\eta), \\ I &= p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{\beta(\xi,\eta)}{g(\xi,\eta)} + Q(\xi,\eta). \end{aligned} \tag{11}$$

We call these specific coordinates (ξ, η) *Liouville coordinates*. In Liouville coordinates the Hamil-

tonian H *and* the integral I are written as it was given in Eq. (11). In the Liouville coordinates, Eq. (8) is considerably simplified,

$$\frac{\partial^2 g}{\partial \xi^2} - \frac{\partial^2 g}{\partial \eta^2} = 0$$

the general solution is

$$g(\xi, \eta) = F(\xi + \eta) + G(\xi - \eta),$$

where $F(u)$ and $G(v)$ are arbitrary functions. The above metric characterizes a surface which is called Liouville surface in the geometry textbooks. Therefore we have shown that a system is integrable in Class I only when the surface is a Liouville surface. The surfaces of constant curvature or the rotation surfaces are Liouville surfaces, but there are Liouville surfaces which have not constant curvature and they are not rotation surfaces.

The function $\beta(\xi, \eta)$ can be calculated from Eq. (6),

$$\frac{\partial \beta}{\partial \xi} = \frac{\partial g}{\partial \eta}, \quad \frac{\partial \beta}{\partial \eta} = \frac{\partial g}{\partial \xi},$$

then

$$\beta(\xi, \eta) = F(\xi + \eta) - G(\xi - \eta). \tag{12}$$

The potential $V(\xi, \eta)$ in Liouville coordinates is the solution of Eq. (10),

$$(F(\xi + \eta) + G(\xi - \eta))\left(\frac{\partial^2 V}{\partial \xi^2} - \frac{\partial^2 V}{\partial \eta^2}\right) + 2F'(\xi + \eta)\left(\frac{\partial V}{\partial \xi} - \frac{\partial V}{\partial \eta}\right) + 2G'(\xi - \eta)\left(\frac{\partial V}{\partial \xi} + \frac{\partial V}{\partial \eta}\right) = 0.$$

The general solution of the above equation in Liouville coordinates is

$$V(\xi, \eta) = \frac{f(\xi + \eta) + g(\xi - \eta)}{F(\xi + \eta) + G(\xi - \eta)}. \tag{13}$$

The functions $f(u)$ and $g(v)$ are arbitrary functions. The function $Q(\xi, \eta)$ is determined from Eqs. (9) and the solution is easily calculated,

$$Q(\xi, \eta) = 4\frac{f(\xi + \eta)G(\xi - \eta) - g(\xi - \eta)F(\xi + \eta)}{F(\xi + \eta) + G(\xi - \eta)}. \tag{14}$$

Usually it is more convenient to use the coordinates u, v, which are defined by

$$\xi = u + iv, \quad \eta = u - iv, \quad p_\xi = \frac{p_u - ip_v}{2}, \quad \text{and } p_\eta = \frac{p_u + ip_v}{2}.$$

The Hamiltonian H and the integral can be written as

$$H = \frac{{p_u}^2 + {p_v}^2 + 4(f(u) + g(v))}{4(F(u) + G(v))},$$

$$I = \frac{{p_u}^2 G(v) - {p_v}^2 F(u)}{F(u) + G(v)} + 4\frac{f(u)G(v) - g(v)F(u)}{F(u) + G(v)}.$$

The above formula has been investigated in a different context in Ref. 30. In these coordinates the action $S(u, v)$ satisfy the following equations:

$$E = H(u,v,p_u,p_v), \quad J = I(u,v,p_u,p_v),$$
$$p_u = \frac{\partial S}{\partial u}, \quad p_v = \frac{\partial S}{\partial v}, \tag{15}$$

and we can find the action $S(u,v)$ by separation of variables,

$$S = -Et + \int \sqrt{4EF(u) + J - 4f(u)}\,\mathrm{d}u + \int \sqrt{4EG(v) - J - 4g(v)}\,\mathrm{d}v.$$

CLass II: $B(y)=0$.

We can choose a new coordinate system

$$\xi = \int \frac{\mathrm{d}x}{\sqrt{A(x)}} \quad \text{and} \quad \eta = y$$

the associated momenta are

$$p_\xi = \sqrt{A(x)}p_x \quad \text{and} \quad p_\eta = p_y.$$

In this case the metric is written

$$\mathrm{d}s^2 = \hat{g}(\xi,\eta)\mathrm{d}\xi\,\mathrm{d}\eta, \quad \text{where } \hat{g}(\xi,\eta) = g(x,y)\sqrt{A(x)}.$$

We can easily show that the formulas are the same by replacing $x \to \xi$, $y \to \eta$ and fixing $A(x)=1$ and $B(y)=0$. For simplicity reasons we omit the hat on the metric $\hat{g}(\xi,\eta) \to g(\xi,\eta)$. Equations (2) and (3) are written

$$H = \frac{p_\xi p_\eta}{g(\xi,\eta)} + V(\xi,\eta),$$
$$I = p_\xi^2 - 2p_\xi p_\eta \frac{\beta(\xi,\eta)}{g(\xi,\eta)} + Q(\xi,\eta). \tag{16}$$

We call these specific coordinates (ξ,η) *Lie coordinates*. In Lie coordinates the Hamiltonian H *and* the integral I are written as it is given in the above equation (16). In Lie coordinates Eq. (18) is written

$$\frac{\partial^2 g}{\partial \xi^2} = 0.$$

The general solution is

$$g(\xi,\eta) = F(\eta)\xi + G(\eta),$$

where $F(\eta)$ and $G(\eta)$ are arbitrary functions. The above metric characterizes a surface which will be called Lie surface. Therefore we have shown that a system is integrable in Case 2 only when the surface is a Lie surface.

Equations (6) imply

$$\left.\begin{aligned} \frac{\partial \beta}{\partial \eta} &= \frac{\partial g}{\partial \xi} \\ \frac{\partial \beta}{\partial \xi} &= 0 \end{aligned}\right\} \Rightarrow \begin{cases} g(\xi,\eta) = F(\eta)\xi + G(\eta), \\ \beta(\xi,\eta) = \int F(\eta)\mathrm{d}\eta. \end{cases} \tag{17}$$

Equation (10) is written

$$(F(\eta)\xi + G(\eta))\frac{\partial^2 V}{\partial \xi^2} + 2F(\eta)\frac{\partial V}{\partial \xi} = 0$$

and the general solution of the above equation is

$$V(\xi,\eta) = \frac{f(\eta)\xi + g(\eta)}{F(\eta)\xi + G(\eta)}. \tag{18}$$

The functions $F(\eta)$, $G(\eta)$, $f(\eta)$, and $g(\eta)$ are arbitrary functions. In this case the solution of the system of equations (9) is given by

$$Q(\xi,\eta) = -2\frac{(f(\eta)\xi + g(\eta))\int F(\eta)\mathrm{d}\eta}{F(\eta)\xi + G(\eta)} + 2\int f(\eta)\mathrm{d}\eta. \tag{19}$$

The action integral in this case can be easily calculated,

$$S = \xi\sqrt{J - 2\left(\int f(\eta)\mathrm{d}\eta - E\int F(\eta)\mathrm{d}\eta\right)} - \int \mathrm{d}\eta \frac{g(\eta) - EG(\eta)}{\sqrt{J - 2(\int f(\eta)\mathrm{d}\eta - E\int F(\eta)\mathrm{d}\eta)}},$$

where

$$E = H(\xi,\eta,p_\xi,p_\eta), \quad J = I(\xi,\eta,p_\xi,p_\eta),$$

$$p_\xi = \frac{\partial S}{\partial \xi}, \quad p_\eta = \frac{\partial S}{\partial \eta}.$$

The integrable systems which belong in Classes I and II are well-known integrable systems (see Ref. 12) the supporting manifold is a Liouville or a Lie surface. We must notice that the Hamiltonian and the integral of an integrable system determine uniquely the Liouville (or Lie) coordinate system. Therefore the use of this privileged system is imposed by the notion of integrability. In the next sections we shall work in this special coordinate system, which is denoted exclusively by the coordinates ξ and η. In Class I integrable systems the system is separable, while in Class II systems there is no separation of variables in general.

III. POISSON ALGEBRA OF SUPERINTEGRABLE SYSTEMS WITH TWO QUADRATIC INTEGRALS OF MOTION

If a system is superintegrable on a two-dimensional manifold, that means that there are three functionally independent integrals of motion H, A, and B. In this section, we assume that these integrals of motion are quadratic functions of the momenta and there are no other integrals of motion, which are linear functions of the momenta. Regarding the Hamiltonian H and the first integral A, we can choose the Liouville coordinate system and in this system,

$$H = \frac{p_\xi p_\eta}{g(\xi,\eta)} + V(\xi,\eta).$$

As we have shown in the preceding section the system is integrable with a square integral of motion in two cases. The integral of motion A in the Liouville coordinate system is written.

$$A = p_\xi^2 + bp_\eta^2 - 2p_\xi p_\eta \frac{\sigma(\xi,\eta)}{g(\xi,\eta)} + \Theta(\xi,\eta),$$

where

$$b = \begin{cases} 1 & \text{in Class I,} \quad \text{where } g(\xi,\eta) = F(\xi+\eta) + G(\xi-\eta) \quad \text{(Liouville system)}, \\ 0 & \text{in Class II,} \quad \text{where } g(\xi,\eta) = F(\eta)\xi + G(\eta) \qquad \text{(Lie system)}. \end{cases}$$

The integral of motion B is assumed to be indeed a quadratic function of momenta, thus the general form in Liouville coordinates is

$$B = A(\xi)p_\xi^2 + B(\eta)p_\eta^2 - 2p_\xi p_\eta \frac{\beta(\xi,\eta)}{g(\xi,\eta)} + Q(\xi,\eta).$$

By definition the following relations are satisfied:

$$\{H,A\}_P = \{H,B\}_P = 0. \tag{20}$$

From the integrals of motion A and B, we can construct the integral of motion

$$C = \{A,B\}_P. \tag{21}$$

The integral of motion C is not a new independent integral of motion, which is a cubic function of the momenta. The integral C is not functionally independent from the integrals H, A, and B as it will be shown later. The fact that, the integral C is a cubic function of momenta, implies the impossibility of expressing C as a polynomial function of the other integrals, which are quadratic functions of momenta. We shall prove that the square of this cubic polynomial is indeed a cubic combination of the integrals. Starting from the integral of motion C, we can construct the (non-independent) integrals $\{A,C\}_P$ and $\{B,C\}_P$. These integrals are quartic functions of the momenta, i.e., functions of fourth order. In the Appendix we show that these integrals can be expressed as quadratic combinations of the integrals H,A, and B. Therefore the following relations are valid:

$$\{A,C\}_P = \alpha A^2 + \beta B^2 + 2\gamma AB + \delta A + \epsilon B + \zeta \tag{22}$$

and

$$\{B,C\}_P = aA^2 + bB^2 + 2cAB + \mathrm{d}A + eB + z. \tag{23}$$

By taking an appropriate rotation of the integrals A and B we can always consider the case $\beta = 0$.

The existence of the Poisson algebra (22) and (23) is not evident. The above form was assumed as obvious by several authors.[4–7,17–29] In Classical mechanics the Poisson algebra was not considered as an important point, but in quantum mechanics the existence of Poisson algebra permits the algebraic treatment of the superintegrable system.[20] In this paper we prove that the superintegrable systems can be classified using the properties of the Poisson algebra. The superintegrability is a global property of the system, and this fact is reflected in the Poisson algebra structure, which is indeed a global property. The mathematical proof of the existence of the algebra (22) and (23) for the two-dimensional superintegrable systems can be found in the Appendix.

The Jacobi equality for the Poisson brackets induces the relation

$$\{A,\{B,C\}_P\}_P = \{B,\{A,C\}_P\}_P.$$

The following relations:

$$b = -\gamma, \quad c = -\alpha, \quad \text{and } e = -\delta$$

must be satisfied.

The integrals A, B, and C satisfy the quadratic Poisson algebra,

$$\{A,B\}_P = C,$$

$$\{A,C\}_P = \alpha A^2 + 2\gamma AB + \delta A + \epsilon B + \zeta, \tag{24}$$

$$\{B,C\}_P = aA^2 - \gamma B^2 - 2\alpha AB + \mathrm{d}A - \delta B + z,$$

where α, γ, a are constants and

$$\delta = \delta(H) = \delta_0 + \delta_1 H,$$

$$\epsilon = \epsilon(H) = \epsilon_0 + \epsilon_1 H,$$

$$\zeta = \zeta(H) = \zeta_0 + \zeta_1 H + \zeta_2 H^2,$$

$$d = d(H) = d_0 + d_1 H,$$

$$z = z(H) = z_0 + z_1 H + z_2 H^2,$$

where δ_i, ϵ_i, ζ_i, d_i, and z_i are constants. The associative algebra, whose generators satisfy Eq. (24), is the general form of the closed Poisson algebra of the integrals of superintegrable systems with integrals quadratic in momenta.

The quadratic Poisson algebra (24) possess a Casimir which is a function of momenta of degree 6 and it is given by

$$K = C^2 - 2\alpha A^2 B - 2\gamma AB^2 - 2\delta AB - \epsilon B^2 - 2\zeta B + \tfrac{2}{3} aA^3 + \mathrm{d}A^2 + 2zA = k_0 + k_1 H + k_2 H^2 + k_3 H^3. \tag{25}$$

Obviously

$$\{K,A\}_P = \{K,B\}_P = \{K,C\}_P = 0.$$

Therefore the integrals of motion of a superintegrable two-dimensional system with quadratic integrals of motion close a constrained classical quadratic Poisson algebra (24), corresponding to a Casimir equal at most to a cubic function of the Hamiltonian (25)

In Ref. 5 the algebra (24) induced by the Casimir (25) can be equivalently formulated as the Poisson algebra generated by

$$C^2 = 2f(A,B,H), \quad C = \{A,B\}_P,$$

$$\{A,C\}_P = \frac{\partial f}{\partial B}, \quad \{C,B\}_P = \frac{\partial f}{\partial A},$$

where $f(A,B,H)$ is a cubic function of A, B, and H.

In the general case of a superintegrable system the integrals are not necessarily quadratic functions of the momenta, but rather polynomial functions of the momenta. The case of the systems with a quadratic and a cubic integral of motion are studied by Tsiganov.[31,32]

IV. CLASSES OF SUPERINTEGRABLE SYSTEMS ON A TWO-DIMENSIONAL MANIFOLD WITH QUADRATIC INTEGRALS OF MOTION

The main result of the preceding section is that the definition of the Casimir of the Poisson algebra, given by Eq. (25) determines uniquely the Poisson algebra. This Poisson algebra is specific for each superintegrable system, therefore it can be used for the classification of the possible superintegrable systems. Usually the proposed classifications of superintegrable systems assumed the definition of the manifold metric and the superintegrable systems were fixed for the given metric. In this paper we propose a classification which is based on the Poisson algebra. Let

us consider a superintegrable system, which is described by a Hamiltonian H and two integrals of motion A and B. The integrability of the system imposes several choices which are determined by two Classes I and II of integrable systems, as it has been shown in Sec. II. These classes of superintegrable systems are the following.

Class I: This class contains superintegrable systems, whose manifold metric and integrals of motion are written in a specific coordinate,

$$ds^2 = g(\xi,\eta)d\xi d\eta, \quad g(\xi,\eta) = F(\xi+\eta) + G(\xi-\eta), \tag{26}$$

$$H = \frac{p_\xi p_\eta}{F(\xi+\eta)+G(\xi-\eta)} + \frac{f(\xi+\eta)+g(\xi-\eta)}{F(\xi+\eta)+G(\xi-\eta)}, \tag{27}$$

and

$$A = p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{F(\xi+\eta)-G(\xi-\eta)}{F(\xi+\eta)+G(\xi-\eta)} + 4\frac{f(\xi+\eta)G(\xi-\eta)-g(\xi-\eta)F(\xi+\eta)}{F(\xi+\eta)+G(\xi-\eta)}. \tag{28}$$

The second integral of motion has the general form

$$B = A(\xi)p_\xi^2 + B(\eta)p_\eta^2 - 2p_\xi p_\eta \frac{\beta(\xi,\eta)}{F(\xi+\eta)+G(\xi-\eta)} + Q(\xi,\eta), \tag{29}$$

where $A(\xi)$ and $B(\eta)$ are not zero.

Class II: This class contains superintegrable systems, whose manifold metric and integrals of motion are written in a specific coordinate,

$$ds^2 = g(\xi,\eta)d\xi d\eta, \quad g(\xi,\eta) = F(\eta)\xi + G(\eta), \tag{30}$$

$$H = \frac{p_\xi p_\eta}{F(\eta)\xi+G(\eta)} + \frac{f(\eta)\xi+g(\eta)}{F(\eta)\xi+G(\eta)}, \tag{31}$$

and

$$A = p_\xi^2 - 2p_\xi p_\eta \frac{\int F(\eta)d\eta}{F(\eta)\xi+G(\eta)} - 2\frac{(f(\eta)\xi+g(\eta))\int F(\eta)d\eta}{F(\eta)\xi+G(\eta)} + 2\int f(\eta)d\eta. \tag{32}$$

The second integral of motion has the general form

$$B = A(\xi)p_\xi^2 + B(\eta)p_\eta^2 - 2p_\xi p_\eta \frac{\beta(\xi,\eta)}{F(\eta)\xi+G(\eta)} + Q(\xi,\eta), \tag{33}$$

where $A(\xi)$ and $B(\eta)$ are not zero. The existence of a second integral of motion B implies that there is another Liouville coordinate system (X,Y) corresponding to the pair of integrals H and B. In this system there are analytic formulas for the second integral of motion. The analytic calculation of these formulas will be given in the following sections.

The Class I superintegrable system is described by the integrals of motion which are given by Eqs. (26)–(29). Correspondingly, the Class II superintegrable system is described by the integrals of motion which are given by Eqs. (30)–(33). These integrals of motion should satisfy the relation (25), which is an identity relation between polynomials of sixth degree for the momenta. The coefficients of p_ξ^6 and p_η^6 in (25) vanish and the following identities are true:

$$6(A'(\xi))^2 = 3\gamma A^2(\xi) + 3\alpha A(\xi) - a, \tag{34}$$

$$6(B'(\eta))^2 = 3\gamma B^2(\eta) + 3\alpha B(\eta) - a.$$

In Eq. (29), the coefficients of p_ξ^2 and p_η^2 in the integral B are determined by the solution of the above equations (34).

The superintegrable systems on a manifold can be classified by the possible solutions of Eqs. (34). The integral of motion A has a standard form, given by Eq. (28), this form is the Liouville form and the coefficients of p_x^2 and p_y^2 are equal to 1. The second integral of motion B can be replaced by any combination of the form

$$B \to qB + rH + sA,$$

where q,r,s are arbitrary constants. From this fact we can show that there are six subclasses of possible solutions of Eq. (34).

Subclass I_1: This class corresponds to

$$\gamma = 0, \quad \alpha = 0, \quad a \neq 0$$

if we choose $a=-6$, then

$$A(\xi) = \xi, \quad B(\eta) = \eta.$$

Subclass I_2: This class corresponds to

$$\gamma = 0, \quad \alpha \neq 0, \quad a = 0$$

if we choose $\alpha=8$, then

$$A(\xi) = \xi^2, \quad B(\eta) = \eta^2.$$

Subclass I_3: This class corresponds to

$$\gamma \neq 0, \quad \alpha = 0, \quad a \neq 0$$

if we choose $\gamma=2$, then we can show that all cases are equivalent to the choice

$$A(\xi) = (e^{\xi} + e^{-\xi})^2, \quad B(\eta) = (e^{\eta} + e^{-\eta})^2.$$

Subclass II_1: This class corresponds to

$$\gamma = 0, \quad \alpha = 0, \quad a = 0$$

then

$$A(\xi) = 1, \quad B(\eta) = 1.$$

Subclass II_2: This class corresponds to

$$\gamma = 0, \quad \alpha = 0, \quad a \neq 0$$

if we choose $a=-6$, then

$$A(\xi) = \xi, \quad B(\eta) = \eta.$$

Subclass II_3: This class corresponds to

$$\gamma = 0, \quad \alpha \neq 0, \quad a = 0$$

if we choose $\alpha=8$, then we can show that

$$A(\xi) = \xi^2, \quad B(\eta) = \eta^2.$$

These classes of solutions will be studied in detail in Sec. V.

A. Class I superintegrable systems

Starting from the definition of functions $A(\xi)$ and $B(\eta)$ we can solve Eqs. (6)–(10) and the superintegrable system is fully determined. This procedure will be sketched in detail in the next paragraphs.

Let us start by the known solutions $A(\xi)$, $B(\eta)$ of Eq. (34).

Equation (8) is written

$$(A''(\xi)-B''(\eta))(F(\xi+\eta)+G(\xi-\eta))+3A'(\xi)(F'(\xi+\eta)+G'(\xi-\eta))-3B'(\eta)(F'(\xi+\eta) - G'(\xi-\eta))+2(A(\xi)-B(\eta))(F''(\xi+\eta)+G''(\xi-\eta))=0. \tag{35}$$

In the next paragraphs we will show that, the above equation can be separated in two second order differential equations for the involved functions $F(u)$ and $G(v)$. The general solution of these equations are given by

$$\begin{aligned} F(u)&=\lambda_1F_1(u)+\lambda_2F_2(u)+\lambda_3F_3(u)+\lambda_4F_4(u),\\ G(v)&=\ell_1G_1(v)+\ell_2G_2(v)+\ell_3G_3(v)+\ell_4G_4(v), \end{aligned} \tag{36}$$

where $F_k(u)$ and $G_k(u)$ are functions which are not generally partial independent solutions of two second order differential equation (8). Between the eight parameters λ_k and ℓ_k for $k=1,2,3,4$ only four among them are independent.

After the calculation of the functions $F(u)$ and $G(v)$ we can calculate the function $\beta(x,y)$ from Eq. (6). The general form of the potential $V(\xi,\eta)$ is given by Eq. (13).

After some elementary (but rather lengthy) algebraic calculation we can show that Eq. (10) leads to a differential equation for the functions $f(u)$ and $g(v)$ which are involved in the definition (13) of the potential,

$$\begin{aligned} &f(\xi+\eta)\{-3B'(\eta)(F'(\xi+\eta)-G'(\xi-\eta))+3A'(\xi)(F'(\xi+\eta)+G'(\xi-\eta))+2(A(\xi)-B(\eta))(F''(\xi\\ &+\eta)+G''(\xi-\eta))\}+g(\xi-\eta)\{-3B'(\eta)(F'(\xi+\eta)-G'(\xi-\eta))+3A'(\xi)(F'(\xi+\eta)+G'(\xi\\ &-\eta))+2(A(\xi)-B(\eta))(F''(\xi+\eta)+G''(\xi-\eta))\}-(F(\xi+\eta)+G(\xi-\eta))\{-3B'(\eta)(f'(\xi+\eta)\\ &-g'(\xi-\eta))+3A'(\xi)(f'(\xi+\eta)+g'(\xi-\eta))+2(A(\xi)-B(\eta))(f''(\xi+\eta)+g''(\xi-\eta))\}=0. \end{aligned}$$

We can eliminate in the above equation the functions $F(u)$ and $G(v)$ which satisfy Eq. (35) and finally the functions involved in the definition of the potential satisfy the following equation:

$$(A''(\xi)-B''(\eta))(f(\xi+\eta)+g(\xi-\eta))+3A'(\xi)(g'(\xi+\eta)+g'(\xi-\eta))-3B'(\eta)(g'(\xi+\eta) - g'(\xi-\eta))+2(A(\xi)-B(\eta))(f''(\xi+\eta)+g''(\xi-\eta))=0. \tag{37}$$

This equation is indeed the same as (35) and the general solution has been given by Eq. (36). Then we have proved the following general proposition.

Proposition 1: The general form of the potential $V(\xi,\eta)$ in Liouville coordinates for a superintegrable system of Class I is given by the general formula:

$$V(\xi,\eta)=\frac{f(\xi+\eta)+g(\xi-\eta)}{F(\xi+\eta)+G(\xi-\eta)},$$

where both pairs of functions $f(u)$, $g(v)$ and $F(u)$, $G(v)$ satisfy the same differential equations (35) and (37).

Therefore the solutions of Eq. (37) are given by

$$f(u)=\rho_1F_1(u)+\rho_2F_2(u)+\rho_3F_3(u)+\rho_4F_4(u), \tag{38}$$

$$g(v) = r_1 G_1(v) + r_2 G_2(v) + r_3 G_3(v) + r_4 G_4(v).$$

The equations of motion do not depend on the shifts of the potential by one constant. This fact explains physically the identity of differential equations (35) and (37).

The calculation of the second integral of motion B is now straightforward. If the functions $A(x)$ and $B(y)$ are fixed as solutions of the characteristic equations (34) then we can introduce the new coordinates,

$$X = \int \frac{\mathrm{d}x}{\sqrt{A(x)}} \quad \text{and} \quad Y = \int \frac{\mathrm{d}y}{\sqrt{B(y)}}. \tag{39}$$

In these coordinates the metric of the manifold can be written

$$\mathrm{d}s^2 = g(x,y)\mathrm{d}x\,\mathrm{d}y = \tilde{g}(X,Y)\mathrm{d}X\,\mathrm{d}Y, \tag{40}$$

where

$$\tilde{g}(X,Y) = g(x,y)\sqrt{A(x)B(y)}$$

and

$$H = \frac{p_x p_y}{g(x,y)} + V(x,y) = \frac{p_X p_Y}{\tilde{g}(X,Y)} + \tilde{V}(X,Y).$$

The integrability of the above Hamiltonian implies

$$\tilde{g}(X,Y) = \tilde{F}(X+Y) + \tilde{G}(X-Y). \tag{41}$$

The above relation implies

$$\tilde{g}\left(\frac{U+V}{2}, \frac{U-V}{2}\right) = \tilde{F}(U) + \tilde{G}(V),$$

$$\tilde{g}\left(\frac{U+d}{2}, \frac{U-d}{2}\right) = \tilde{F}(U) + \tilde{G}(d),$$

$$\tilde{g}\left(\frac{c+V}{2}, \frac{c-V}{2}\right) = \tilde{F}(c) + \tilde{G}(V),$$

$$\tilde{g}\left(\frac{c+d}{2}, \frac{c-d}{2}\right) = \tilde{F}(c) + \tilde{G}(d),$$

where c and d are two arbitrary constants. Therefore the functions $\tilde{F}(U)$ and $\tilde{G}(V)$ are calculated up to one constant by

$$\begin{aligned} \tilde{F}(U) &= \tilde{g}\left(\frac{U+d}{2}, \frac{U-d}{2}\right) - \frac{1}{2}\tilde{g}\left(\frac{c+d}{2}, \frac{c-d}{2}\right) + \mu, \\ \tilde{G}(V) &= \tilde{g}\left(\frac{c+V}{2}, \frac{c-V}{2}\right) - \frac{1}{2}\tilde{g}\left(\frac{c+d}{2}, \frac{c-d}{2}\right) - \mu, \end{aligned} \tag{42}$$

where μ can be an arbitrary chosen constant. Starting from the well-known form of the potential

$$V(x,y)=\frac{w(x,y)}{g(x,y)},\quad w(x,y)=f(x+y)+g(x-y)$$

we can show that

$$V(x,y)=\tilde{V}(X,Y)=\frac{\tilde{w}(X,Y)}{\tilde{g}(X,Y)},$$
$$\tilde{w}(X,Y)=\tilde{f}(X+Y)+\tilde{g}(X-Y)=w(x,y)\sqrt{A(x)B(y)}. \tag{43}$$

The functions $\tilde{f}(U)$ and $\tilde{g}(V)$ are calculated by

$$\tilde{f}(U)=\tilde{w}\left(\frac{U+d}{2},\frac{U-d}{2}\right)-\frac{1}{2}\tilde{w}\left(\frac{c+d}{2},\frac{c-d}{2}\right),$$

$$\tilde{g}(V)=\tilde{w}\left(\frac{c+V}{2},\frac{c-V}{2}\right)-\frac{1}{2}\tilde{w}\left(\frac{c+d}{2},\frac{c-d}{2}\right).$$

Then the second integral of motion in the coordinates X,Y is

$$B=p_X^2+p_Y^2-2p_Xp_Y\frac{\tilde{F}(X+Y)-\tilde{G}(X-Y)}{\tilde{F}(X+Y)+\tilde{G}(X-Y)}+4\frac{\tilde{f}(X+Y)\tilde{G}(X-Y)-\tilde{g}(X-Y)\tilde{F}(X+Y)}{\tilde{F}(X+Y)+\tilde{G}(X-Y)}. \tag{44}$$

After calculating the above integral in the coordinates X,Y, we can compute analytically the second integral B in the original coordinates x,y.

B. Class II superintegrable systems

Equation (8) is written

$$(A''(x)-B''(y))(F(y)x+G(y))+3A'(x)F(y)-3B'(y)(F'(y)x+G'(y))$$
$$+2(A(x)-B(y))(F''(y)x+G''(y))=0. \tag{45}$$

The general solutions of Eq. (45) are given by

$$F(y)=\lambda_1F_1(y)+\lambda_2F_2(y)+\lambda_3F_3(y)+\lambda_4F_4(y),$$
$$G(y)=\ell_1G_1(y)+\ell_2G_2(y)+\ell_3G_3(y)+\ell_4G_4(y), \tag{46}$$

where $F_k(y)$ and $G_k(y)$ are partial independent solutions of two second order differential equations with several constant parameters. Between the eight parameters λ_k and ℓ_k for $k=1,2,3,4$ only four among them are linearly independent.

After the calculation of the functions $F(y)$ and $G(y)$ we can calculate the function $\beta(x,y)$ from Eq. (17). The general form of the potential $V(x,y)$ is given by Eq. (18). After some elementary (but rather complicated) algebraic calculation we can show that, Eq. (19) leads to a differential equation for the functions $f(y)$ and $g(y)$, which are involved in the definition (13) of the potential,

$$(A''(x)-B''(y))(f(y)x+g(y))+3A'(x)f(y)-3B'(y)(f'(y)x+g'(y))$$
$$+2(A(x)-B(y))(f''(y)x+g''(y))=0. \tag{47}$$

Then we have proved the following general proposition.

Proposition 2: The general form of the potential $V(\xi,\eta)$ in Liouville coordinates for a superintegrable system of Class II is given by the general formula

$$V(\xi,\eta)=\frac{f(\eta)\xi+g(\eta)}{F(\eta)\xi+G(\eta)},$$

where both the pairs of functions $f(u)$, $g(v)$ *and* $F(u)$, $G(v)$ *satisfy the same differential equations (45) and (47).*

Therefore the solutions of Eq. (47) are given by

$$\begin{aligned} f(y)&=\rho_1F_1(y)+\rho_2F_2(y)+\rho_3F_3(y)+\rho_4F_4(y),\\ g(y)&=r_1G_1(y)+r_2G_2(y)+r_3G_3(y)+r_4G_4(y). \end{aligned} \tag{48}$$

The equations of motion do not depend on the shifts of the potential by one constant. This fact explains physically the identity of differential equations (35) [or (45)] and (37) [or (47)].

The calculation of the second integral of motion B is now straightforward and we can use the same procedure of solution as it has been described by Eqs. (39)–(44).

V. CLASSIFICATION OF TWO-DIMENSIONAL SUPERINTEGRABLE SYSTEMS WITH TWO QUADRATIC INTEGRALS OF MOTION

In this section we give the analytical solutions for the different classes of superintegrable systems. As we have shown there are two general classes of superintegrable systems, each class has three subclasses.

A. Class I superintegrable systems

1. Subclass I_1 of superintegrable systems

We have

$$A(\xi)=\xi,\quad B(\eta)=\eta,$$

$$F(u)=4\lambda u^2+\kappa u+\nu/2,\quad G(v)=-\lambda v^2+\mu/v^2+\nu/2,$$

$$f(u)=4\ell u^2+ku+n/2,\quad g(v)=-\ell v^2+m/v^2+n/2$$

$$ds^2=(F(\xi+\eta)+G(\xi-\eta))d\xi\,d\eta,\quad H=\frac{p_\xi p_\eta+f(\xi+\eta)+g(\xi-\eta)}{F(\xi+\eta)+G(\xi-\eta)}. \tag{49}$$

The other integral of motion is

$$A=p_\xi^2+p_\eta^2-2p_\xi p_\eta\frac{F(\xi+\eta)-G(\xi-\eta)}{F(\xi+\eta)+G(\xi-\eta)}+4\frac{f(\xi+\eta)G(\xi-\eta)-g(\xi-\eta)F(\xi+\eta)}{F(\xi+\eta)+G(\xi-\eta)}.$$

We introduce the functions

$$\begin{aligned} \tilde F(u)&=\frac{\lambda u^6}{256}+\frac{\kappa u^4}{128}+\frac{\nu u^2}{16}-\frac{\mu}{u^2},\\ \tilde G(v)&=-\frac{\lambda v^6}{256}-\frac{\kappa v^4}{128}-\frac{\nu v^2}{16}+\frac{\mu}{v^2},\\ \tilde f(u)&=\frac{lu^6}{256}+\frac{ku^4}{128}+\frac{nu^2}{16}-\frac{m}{u^2}, \end{aligned} \tag{50}$$

$$\tilde{g}(v) = -\frac{lv^6}{256} - \frac{kv^4}{128} - \frac{nv^2}{16} + \frac{m}{v^2}.$$

The second integral of motion is

$$B = p_X^2 + p_Y^2 - 2p_X p_Y \frac{\tilde{F}(X+Y) - \tilde{G}(X-Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)} + 4\frac{\tilde{f}(X+Y)\tilde{G}(X-Y) - \tilde{g}(X-Y)\tilde{F}(X+Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)},$$

where

$$X = 2\sqrt{\xi}, \quad p_X = \sqrt{\xi}p_\xi, \quad Y = 2\sqrt{\eta}, \quad p_Y = \sqrt{\eta}p_\eta.$$

The constants of the Poisson algebra are

$$\alpha = 0, \quad \beta = 0, \quad \gamma = 0, \quad \delta = 16(\kappa H - k), \quad \epsilon = 256(\lambda H - \ell),$$

$$\zeta = -32(\kappa H - k)(\nu H - n), \quad a = -6, \quad d = 8(\nu H - n),$$

$$z = 8(\nu H - n)^2 - 128(\lambda H - \ell)(\mu H - m),$$

$$K = 32(\nu H - n)^3 + 512(\lambda H - \ell)(\mu H - m)(\nu H - n) - 64(\kappa H - k)^2(\mu H - m).$$

2. Subclass I_2 of superintegrable systems

We have

$$A(\xi) = \xi^2, \quad B(\eta) = \eta^2,$$

$$F(u) = \lambda u^2 + \frac{\kappa}{u^2} + \frac{\nu}{2}, \quad G(v) = -\lambda v^2 + \frac{\mu}{v^2} + \frac{\nu}{2},$$

$$f(u) = \ell u^2 + \frac{k}{u^2} + \frac{n}{2}, \quad g(v) = -\ell v^2 + \frac{m}{v^2} + \frac{n}{2},$$

$$\mathrm{d}s^2 = (F(\xi+\eta) + G(\xi-\eta))\mathrm{d}\xi\,\mathrm{d}\eta, \quad H = \frac{p_\xi p_\eta + f(\xi+\eta) + g(\xi-\eta)}{F(\xi+\eta) + G(\xi-\eta)}. \tag{51}$$

The other integral of motion is

$$A = p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{F(\xi+\eta) - G(\xi-\eta)}{F(\xi+\eta) + G(\xi-\eta)} + 4\frac{f(\xi+\eta)G(\xi-\eta) - g(\xi-\eta)F(\xi+\eta)}{F(\xi+\eta) + G(\xi-\eta)}.$$

We introduce the functions

$$\tilde{F}(u) = 4\lambda e^{2u} + \nu e^u, \quad \tilde{G}(v) = \frac{\kappa e^v}{(1+e^v)^2} + \frac{\mu e^v}{(-1+e^v)^2},$$

$$\tilde{f}(u) = 4\ell e^{2u} + n e^u, \quad \tilde{g}(v) = \frac{k e^v}{(1+e^v)^2} + \frac{m e^v}{(-1+e^v)^2}. \tag{52}$$

The second integral of motion is

$$B = p_X^2 + p_Y^2 - 2p_X p_Y \frac{\tilde{F}(X+Y) - \tilde{G}(X-Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)} + 4\frac{\tilde{f}(X+Y)\tilde{G}(X-Y) - \tilde{g}(X-Y)\tilde{F}(X+Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)},$$

where

$$X = \ln \xi, \quad p_X = \xi p_\xi, \quad Y = \ln \eta, \quad p_Y = \eta p_\eta.$$

The constants of the Poisson algebra are

$$\alpha = 8, \quad \beta = 0, \quad \gamma = 0, \quad \delta = 0, \quad \epsilon = 256(\lambda H - \ell),$$

$$\zeta = -32(\nu H - n)^2 + 256(\lambda H - \ell)((\mu - \kappa)H - (m - k)),$$

$$a = 0, \quad d = 0, \quad z = 32((\kappa + \mu)H - (k + m))(\nu H - n),$$

$$K = 256(\lambda H - \ell)((\kappa + \mu)H - (k + m))^2 + 128((\kappa - \mu)H - (k - m))(\nu H - n)^2.$$

3. Subclass I_3 of superintegrable systems

We have

$$A(\xi) = (e^{\xi} + e^{-\xi})^2, \quad B(\eta) = (e^{\eta} + e^{-\eta})^2,$$

$$\begin{aligned} F(u) &= \frac{\kappa e^{2u}}{(-1 + e^{2u})^2} + \frac{\lambda e^u (1 + e^{2u})}{(-1 + e^{2u})^2}, \quad G(v) = \frac{\mu e^{2v}}{(-1 + e^{2v})^2} + \frac{\nu e^v (1 + e^{2v})}{(-1 + e^{2v})^2}, \\ f(u) &= \frac{k e^{2u}}{(-1 + e^{2u})^2} + \frac{\ell e^u (1 + e^{2u})}{(-1 + e^{2u})^2}, \quad g(v) = \frac{m e^{2v}}{(-1 + e^{2v})^2} + \frac{n e^v (1 + e^{2v})}{(-1 + e^{2v})^2}, \end{aligned} \tag{53}$$

$$\mathrm{d}s^2 = (F(\xi + \eta) + G(\xi - \eta))\mathrm{d}\xi\, \mathrm{d}\eta, \quad H = \frac{p_\xi p_\eta + f(\xi + \eta) + g(\xi - \eta)}{F(\xi + \eta) + G(\xi - \eta)}.$$

The other integral of motion is

$$A = p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{F(\xi + \eta) - G(\xi - \eta)}{F(\xi + \eta) + G(\xi - \eta)} + 4\frac{f(\xi + \eta)G(\xi - \eta) - g(\xi - \eta)F(\xi + \eta)}{F(\xi + \eta) + G(\xi - \eta)}.$$

We introduce the functions

$$\begin{aligned} \tilde{F}(u) &= \frac{(\kappa + 2\lambda)}{4} \tan^2 u + \frac{2\nu - \mu}{4} \cot^2 u + \frac{\lambda + \nu}{2}, \\ \tilde{G}(v) &= \frac{(2\lambda - \kappa)}{4} \tan^2 v + \frac{\mu + 2\nu}{4} \cot^2 v + \frac{\lambda + \nu}{2}, \\ \tilde{f}(u) &= \frac{(k + 2\ell)}{4} \tan^2 u + \frac{2n - m}{4} \cot^2 u + \frac{\ell + n}{2}, \end{aligned} \tag{54}$$

$$\tilde{g}(v) = \frac{(2\ell - k)}{4} \tan^2 v + \frac{m + 2n}{4} \cot^2 v + \frac{\ell + n}{2}.$$

The second integral of motion is

$$B = p_X^2 + p_Y^2 - 2p_X p_Y \frac{\tilde{F}(X+Y) - \tilde{G}(X-Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)} + 4\frac{\tilde{f}(X+Y)\tilde{G}(X-Y) - \tilde{g}(X-Y)\tilde{F}(X+Y)}{\tilde{F}(X+Y) + \tilde{G}(X-Y)},$$

where

$$X = \arctan(e^{\xi}), \quad p_X = (e^{\xi} + e^{-\xi})p_{\xi}, \quad Y = \arctan(e^{\eta}), \quad p_Y = (e^{\eta} + e^{-\eta})p_{\eta}.$$

The constants of the Poisson algebra are

$$\alpha = -32, \quad \beta = 0, \quad \gamma = 8, \quad \delta = 0, \quad \epsilon = 0, \quad \zeta = -32(\lambda H - \ell)(\nu H - n),$$

$$a = 0, \quad d = 64(k - m) - 64(\kappa - \mu)H,$$

$$z = 32((\lambda - \nu)H - (\ell - n))^2 - 32((\kappa H - k)(\mu H - m)\ ,$$

$$K = 64(\kappa H - k)(\nu H - n)^2 - 64(\lambda H - \ell)^2(\mu H - m).$$

B. Class II superintegrable systems

1. Subclass II_1 of superintegrable systems

We have

$$A(\xi) = 1, \quad B(\eta) = 1,$$

$$F(\eta) = \kappa\eta + \lambda, \quad G(\eta) = \mu\eta + \nu,$$

$$f(\eta) = k\eta + \ell, \quad g(\eta) = m\eta + n,$$

$$\mathrm{d}s^2 = g(\xi, \eta)\mathrm{d}\xi\,\mathrm{d}\eta, \quad g(\xi, \eta) = \xi F(\eta) + G(\eta),$$

$$H = \frac{p_{\xi}p_{\eta}}{g(\xi, \eta)} + V(\xi, \eta), \quad V(\xi, \eta) = \frac{w(\xi, \eta)}{g(\xi, \eta)}, \quad w(\xi, \eta) = \xi f(\eta) + g(\eta). \tag{55}$$

The other integral of motion is

$$A = p_{\xi}^2 - \frac{2p_{\xi}p_{\eta}\int F(\eta)\mathrm{d}\eta}{g(\xi, \eta)} - \frac{2(\xi f(\eta) + g(\eta))\int F(\eta)\mathrm{d}\eta}{g(\xi, \eta)} + 2\int f(\eta)\mathrm{d}\eta.$$

We introduce the functions

$$\tilde{F}(u) = \frac{\kappa u^2}{4} + \frac{(\lambda + \mu)u}{2} + \frac{\nu}{2},$$

$$\tilde{G}(v) = -\frac{\kappa v^2}{4} + \frac{(\lambda - \mu)v}{2} + \frac{\nu}{2},$$

$$\tilde{f}(u) = \frac{ku^2}{4} + \frac{(\ell + m)u}{2} + \frac{n}{2}, \tag{56}$$

$$\tilde{g}(v) = -\frac{kv^2}{4} + \frac{(\ell - m)v}{2} + \frac{n}{2}.$$

The second integral of motion is

$$B = p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{\tilde{F}(\xi+\eta) - \tilde{G}(\xi-\eta)}{\tilde{F}(\xi+\eta) + \tilde{G}(\xi-\eta)} + 4\frac{\tilde{f}(\xi+\eta)\tilde{G}(\xi-\eta) - \tilde{g}(\xi-\eta)\tilde{F}(\xi+\eta)}{\tilde{F}(\xi+\eta) + \tilde{G}(\xi-\eta)}.$$

The constants of the Poisson algebra are

$$\alpha = 0, \quad \beta = 0, \quad \gamma = 0, \quad \delta = 8(k - \kappa H), \quad \epsilon = 0, \quad \zeta = 8(\lambda H - \ell)^2,$$

$$a = 0, \quad d = 16(k - \kappa H), \quad z = 8(\lambda H - \ell)^2 - (\mu H - m)^2,$$

$$K = 16(\nu H - n)^2(\kappa H - k) - 32(\lambda H - \ell)(\mu H - m)(\nu H - n).$$

2. Subclass $\mathbf{II_2}$ *of superintegrable systems*

We have

$$A(\xi) = \xi, \quad B(\eta) = \eta,$$

$$F(\eta) = \frac{\kappa}{\sqrt{\eta}} + \lambda, \quad G(\eta) = 3\kappa\sqrt{\eta} + \lambda\eta + \frac{\mu}{\sqrt{\eta}} + \nu,$$

$$f(\eta) = \frac{k}{\sqrt{\eta}} + \ell, \quad g(\eta) = 3k\sqrt{\eta} + \ell\eta + \frac{m}{\sqrt{\eta}} + n,$$

$$\mathrm{d}s^2 = g(\xi,\eta)\mathrm{d}\xi\,\mathrm{d}\eta, \quad g(\xi,\eta) = \xi F(\eta) + G(\eta),$$

$$H = \frac{p_\xi p_\eta}{g(\xi,\eta)} + V(\xi,\eta), \quad V(\xi,\eta) = \frac{w(\xi,\eta)}{g(\xi,\eta)}, \quad w(\xi,\eta) = \xi f(\eta) + g(\eta). \tag{57}$$

The other integral of motion is

$$A = p_\xi^2 - \frac{2p_\xi p_\eta \int F(\eta)\mathrm{d}\eta}{g(\xi,\eta)} - \frac{2(\xi f(\eta) + g(\eta)) \int F(\eta)\mathrm{d}\eta}{g(\xi,\eta)} + 2\int f(\eta)\mathrm{d}\eta.$$

We introduce the functions

$$\tilde{F}(u) = \frac{\lambda u^4}{128} + \frac{\kappa u^3}{16} + \frac{\nu u^2}{16} + \frac{\mu u}{4},$$

$$\widetilde{G}(v) = -\frac{\lambda v^4}{128} + \frac{\kappa v^3}{16} + \frac{\mu v}{4} - \frac{\nu v^2}{16},$$
$$\widetilde{f}(u) = \frac{\ell u^4}{128} + \frac{k u^3}{16} + \frac{n u^2}{16} + \frac{m u}{4}, \tag{58}$$
$$\widetilde{g}(v) = -\frac{\ell v^4}{128} + \frac{k v^3}{16} + \frac{m v}{4} - \frac{n v^2}{16}.$$

The second integral of motion is

$$B = p_X^2 + p_Y^2 - 2p_X p_Y \frac{\widetilde{F}(X+Y) - \widetilde{G}(X-Y)}{\widetilde{F}(X+Y) + \widetilde{G}(X-Y)} + 4\frac{\widetilde{f}(X+Y)\widetilde{G}(X-Y) - \widetilde{g}(X-Y)\widetilde{F}(X+Y)}{\widetilde{F}(X+Y) + \widetilde{G}(X-Y)},$$

where

$$X = 2\sqrt{\xi}, \quad p_X = \sqrt{\xi} p_\xi, \quad Y = 2\sqrt{\eta}, \quad p_Y = \sqrt{\eta} p_\eta.$$

The constants of the Poisson algebra are

$$\alpha = 0, \quad \beta = 0, \quad \gamma = 0, \quad \delta = 4(\ell - \lambda H), \quad \epsilon = 0, \quad \zeta = 8(\kappa H - k)^2,$$

$$a = -6, \quad d = 8(\nu H - n), \quad z = -8(\kappa H - k)(\mu H - m) - 2(\nu H - n)^2,$$

$$K = 8(\lambda H - \ell)(\mu H - m)^2 - 16(\kappa H - k)(\mu H - m)(\nu H - n).$$

3. Subclass II_3 of superintegrable systems

We have

$$A(\xi) = \xi^2, \quad B(\eta) = \eta^2,$$

$$F(\eta) = \lambda \eta + \frac{\kappa}{\eta^3}, \quad G(\eta) = \nu + \frac{\mu}{\eta^2},$$

$$f(\eta) = \ell \eta + \frac{k}{\eta^3}, \quad g(\eta) = n + \frac{m}{\eta^2},$$

$$\mathrm{d}s^2 = g(\xi, \eta)\mathrm{d}\xi\, \mathrm{d}\eta, \quad g(\xi, \eta) = \xi F(\eta) + G(\eta),$$

$$H = \frac{p_\xi p_\eta}{g(\xi, \eta)} + V(\xi, \eta), \quad V(\xi, \eta) = \frac{w(\xi, \eta)}{g(\xi, \eta)}, \quad w(\xi, \eta) = \xi f(\eta) + g(\eta). \tag{59}$$

The other integral of motion is

$$A = p_\xi^2 - \frac{2p_\xi p_\eta \int F(\eta)\mathrm{d}\eta}{g(\xi, \eta)} - \frac{2(\xi f(\eta) + g(\eta)) \int F(\eta)\mathrm{d}\eta}{g(\xi, \eta)} + 2\int f(\eta)\mathrm{d}\eta.$$

We introduce the functions

$$\widetilde{F}(u)=\lambda e^{2u}+\nu e^{u},\quad \widetilde{G}(v)=\kappa e^{2v}+\mu e^{v},$$
$$\widetilde{f}(u)=\ell e^{2u}+ne^{u},\quad \widetilde{g}(v)=ke^{2v}+me^{v}. \tag{60}$$

The second integral of motion is

$$B=p_X^2+p_Y^2-2p_Xp_Y\frac{\widetilde{F}(X+Y)-\widetilde{G}(X-Y)}{\widetilde{F}(X+Y)+\widetilde{G}(X-Y)}+4\frac{\widetilde{f}(X+Y)\widetilde{G}(X-Y)-\widetilde{g}(X-Y)\widetilde{F}(X+Y)}{\widetilde{F}(X+Y)+\widetilde{G}(X-Y)},$$

where

$$X=\ln\xi,\quad p_X=\xi p_\xi,\quad Y=\ln\eta,\quad p_Y=\eta p_\eta.$$

The constants of the Poisson algebra are

$$\alpha=8,\quad \beta=0,\quad \gamma=0,\quad \delta=0,\quad \epsilon=0,\quad \zeta=32(\kappa H-k)(\lambda H-\ell),$$

$$a=0,\quad d=0,\quad z=32(\mu H-m)(\nu H-n),$$

$$K=64(\lambda H-\ell)(\mu H-m)^2-64(\kappa H-k)(\nu H-n)^2.$$

All the above superintegrable systems generally are defined on manifolds which have neither constant curvature nor are they surfaces of revolution. All the known superintegrable systems are defined on manifolds of constant curvature or on surfaces of revolution. Therefore we have proved that there are new superintegrable systems, which have not yet been studied.

VI. SUPERINTEGRABLE SYSTEMS CORRESPONDING TO KOENIGS ESSENTIAL FORMS

Class I_1: Using the coordinate transformation

$$\xi=\frac{1}{2}x^2,\quad p_\xi=\frac{p_x}{x},\quad \eta=\frac{1}{2}y^2,\quad p_\eta=\frac{p_y}{y},$$

the metric of the Class I_2 superintegrable systems is reduced to the metric of the essential form VII.4 (Ref. 1, Vol. IV, p. 385), if

$$\kappa=16A_2,\quad \lambda=16A_3,\quad \mu=-A_0,\quad \nu=4A_1.$$

The corresponding superintegrable system (using the coordinates of Ref. 1) is given by the Hamiltonian,

$$H=\frac{p_xp_y+w(x,y)}{g(x,y)},$$

$$g(x,y)=A_0\left[\frac{1}{(x+y)^2}-\frac{1}{(x-y)^2}\right]+A_1[(x+y)^2-(x-y)^2]+A_2[(x+y)^4-(x-y)^4]$$
$$+A_3[(x+y)^6-(x-y)^6],$$

$$w(x,y)=a_0\left[\frac{1}{(x+y)^2}-\frac{1}{(x-y)^2}\right]+a_1[(x+y)^2-(x-y)^2]+a_2[(x+y)^4-(x-y)^4]$$
$$+a_3[(x+y)^6-(x-y)^6],$$

where only three of the constants a_0, a_1, a_2, a_3 are independent, i.e., we can set one among them

equal to zero. Using relations (50) we have that in x,y coordinates the other integral of motion is

$$A(x,y)=\frac{1}{2}p_x^2+\frac{1}{2}p_y^2-p_xp_y\frac{\tilde{\Phi}(x,y)-\tilde{\Psi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)}+2\frac{\tilde{\phi}(x,y)\tilde{\Psi}(x,y)-\tilde{\psi}(x,y)\tilde{\Phi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)},$$

where

$$\tilde{\Phi}(x,y)=A_0\frac{1}{(x+y)^2}+A_1(x+y)^2+A_2(x+y)^4+A_3(x+y)^6,$$

$$\tilde{\Psi}(x,y)=-A_0\frac{1}{(x-y)^2}-A_1(x-y)^2-A_2(x-y)^4-A_3(x-y)^6,$$

$$\tilde{\phi}(x,y)=a_0\frac{1}{(x+y)^2}+a_1(x+y)^2+a_2(x+y)^4+a_3(x+y)^6,$$

$$\tilde{\psi}(x,y)=-a_0\frac{1}{(x-y)^2}-a_1(x-y)^2-a_2(x-y)^4-a_3(x-y)^6,$$

while using relations (49) we have that in x,y coordinates the second integral of motion is

$$B(x,y)=\frac{1}{x^2}p_x^2+\frac{1}{y^2}p_y^2-2\frac{p_xp_y}{xy}\frac{\Phi(x,y)-\Psi(x,y)}{\Phi(x,y)+\Psi(x,y)}+4\frac{\phi(x,y)\Psi(x,y)-\psi(x,y)\Phi(x,y)}{xy\Phi(x,y)+\Psi(x,y)},$$

where

$$\begin{aligned}\Phi(x,y)=&\tfrac{1}{2}A_1[(x+y)^2-(x-y)^2]+A_2[(x+y)^4-(x-y)^4]+A_3([(x+y)^6-(x-y)^6]\\&+(x+y)^4(x-y)^2-(x+y)^2(x-y)^4),\end{aligned}$$

$$\begin{aligned}\Psi(x,y)=&A_0\left[\frac{1}{(x+y)^2}-\frac{1}{(x-y)^2}\right]+\frac{1}{2}A_1[(x+y)^2-(x-y)^2]-A_3((x+y)^4(x-y)^2\\&-(x+y)^2(x-y)^4),\end{aligned}$$

$$\begin{aligned}\phi(x,y)=&\frac{1}{2}a_1[(x+y)^2-(x-y)^2]+a_2[(x+y)^4-(x-y)^4]+a_3([(x+y)^6-(x-y)^6]\\&+(x+y)^4(x-y)^2-(x+y)^2(x-y)^4),\end{aligned}$$

$$\psi(x,y)=a_0\left[\frac{1}{(x+y)^2}-\frac{1}{(x-y)^2}\right]+\frac{1}{2}a_1[(x+y)^2-(x-y)^2]-a_3((x+y)^4(x-y)^2-(x+y)^2(x-y)^4).$$

Class I_2: Using the coordinate transformation

$$\xi=-\tfrac{1}{2}\cos(2x),\quad p_\xi=\frac{p_x}{\sin(2x)},\quad \eta=-\tfrac{1}{2}\cos(2y),\quad p_\eta=\frac{p_y}{\sin(2y)},$$

the metric of the Class I_2 superintegrable systems is reduced to the metric of the essential form VII.4 (Ref. 1, Vol. IV, p. 385), if

$$\kappa = A_1, \quad \lambda = -8A_3, \quad \mu = -A_0, \quad \nu = -2A_2.$$

The corresponding superintegrable system (using the coordinates of Ref. 1) is given by the Hamiltonian,

$$H = \frac{p_x p_y + w(x,y)}{g(x,y)},$$

where

$$g(x,y) = A_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + A_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right] + A_2[\cos 2(x+y) - \cos 2(x-y)] + A_3[\cos 4(x+y) - \cos 4(x-y)],$$

$$w(x,y) = a_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + a_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right] + a_2[\cos 2(x+y) - \cos 2(x-y)] + a_3[\cos 4(x+y) - \cos 4(x-y)],$$

where only three of the constants a_0, a_1, a_2, a_3 are independent, i.e., we can set one among them equal to zero. Using Relations (52) we have that in x, y coordinates the other integral of motion is

$$A(x,y) = \frac{1}{4}\cot^2(2x)p_x^2 + \frac{1}{4}\cot^2(2y)p_y^2 - \frac{p_x p_y}{2\tan(2x)\tan(2y)}\frac{\tilde{\Phi}(x,y) - \tilde{\Psi}(x,y)}{\tilde{\Phi}(x,y) + \tilde{\Psi}(x,y)} + \frac{1}{\tan(2x)\tan(2y)}\frac{\tilde{\phi}(x,y)\tilde{\Psi}(x,y) - \tilde{\psi}(x,y)\tilde{\Phi}(x,y)}{\tilde{\Phi}(x,y) + \tilde{\Psi}(x,y)},$$

where

$$\tilde{\Phi}(x,y) = A_2[\cos 2(x+y) - \cos 2(x-y)] + A_3[\cos 4(x+y) - \cos 4(x-y)],$$

$$\tilde{\Psi}(x,y) = A_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + A_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right],$$

$$\tilde{\phi}(x,y) = a_2[\cos 2(x+y) - \cos 2(x-y)] + a_3[\cos 4(x+y) - \cos 4(x-y)],$$

$$\tilde{\psi}(x,y) = a_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + a_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right]$$

while using relations (51) we have that in x, y coordinates the second integral of motion is

$$B(x,y) = \frac{1}{\sin^2(2x)}p_x^2 + \frac{1}{\sin^2(2y)}p_y^2 - 2\frac{p_x p_y}{2\sin(2x)\sin(2y)}\frac{\Phi(x,y) - \Psi(x,y)}{\Phi(x,y) + \Psi(x,y)} + 4\frac{1}{\sin(2x)\sin(2y)}\frac{\phi(x,y)\Psi(x,y) - \psi(x,y)\Phi(x,y)}{\Phi(x,y) + \Psi(x,y)},$$

where

$$\Phi(x,y) = A_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right] + \frac{1}{2}A_2[\cos 2(x+y) - \cos 2(x-y)] + 4A_3\cos^2(x+y)\cos^2(x-y)[\cos 2(x+y) - \cos 2(x-y)],$$

$$\Psi(x,y) = A_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + \frac{1}{2}A_2[\cos 2(x+y) - \cos 2(x-y)]$$
$$- 4A_3 \sin^2(x+y)\sin^2(x-y)[\cos 2(x+y) - \cos 2(x-y)],$$

$$\phi(x,y) = a_1\left[\frac{1}{\cos^2(x+y)} - \frac{1}{\cos^2(x-y)}\right] + \frac{1}{2}a_2[\cos 2(x+y) - \cos 2(x-y)]$$
$$+ 4a_3 \cos^2(x+y)\cos^2(x-y)[\cos 2(x+y) - \cos 2(x-y)],$$

$$\psi(x,y) = a_0\left[\frac{1}{\sin^2(x+y)} - \frac{1}{\sin^2(x-y)}\right] + \frac{1}{2}a_2[\cos 2(x+y) - \cos 2(x-y)]$$
$$- 4a_3 \sin^2(x+y)\sin^2(x-y)[\cos 2(x+y) - \cos 2(x-y)].$$

Class I_3: Using the coordinate transformation,

$$\xi = \ln\left(\frac{\frac{\wp(x)-\wp(\omega_1)}{\Delta} - 1}{\frac{\wp(x)-\wp(\omega_1)}{\Delta} + 1}\right) + \frac{1}{2}\ln\left(\frac{\frac{\wp(\omega_1)-\wp(\omega_2)}{\Delta} - 1}{\frac{\wp(\omega_1)-\wp(\omega_2)}{\Delta} + 1}\right), \quad p_\xi = \frac{\wp(2x)-\wp(\omega_1)}{2\Delta}p_x,$$

$$\eta = \ln\left(\frac{\frac{\wp(y)-\wp(\omega_1)}{\Delta} - 1}{\frac{\wp(xy)-\wp(\omega_1)}{\Delta} + 1}\right) + \frac{1}{2}\ln\left(\frac{\frac{\wp(\omega_1)-\wp(\omega_2)}{\Delta} - 1}{\frac{\wp(\omega_1)-\wp(\omega_2)}{\Delta} + 1}\right), \quad p_\eta = \frac{\wp(2y)-\wp(\omega_1)}{2\Delta}p_y,$$

where

$$\Delta^2 = (\wp(\omega_1) - \wp(\omega_2))(\wp(\omega_1) - \wp(\omega_3)),$$

the metric of the Class I_3 superintegrable systems is reduced to the metric of the essential form VII.1 (Ref. 1, Vol. IV, p. 385) if

$$\kappa = 2(A_2 + A_3), \quad \lambda = A_2 - A_3, \quad \mu = -2(A_0 + A_1), \quad \nu = -A_0 + A_1.$$

The corresponding superintegrable system (using the coordinates of Ref. 1) is given by the Hamiltonian,

$$H = \frac{p_x p_y + w(x,y)}{g(x,y)},$$

where

$$g(x,y) = A_0(\wp(x+y) - \wp(x-y)) + A_1(\wp(x+y+\omega_1) - \wp(x-y+\omega_1))$$
$$+ A_2(\wp(x+y+\omega_2) - \wp(x-y+\omega_2)) + A_3(\wp(x+y+\omega_3) - \wp(x-y+\omega_3)),$$

$$w(x,y) = a_0(\wp(x+y) - \wp(x-y)) + a_1(\wp(x+y+\omega_1) - \wp(x-y+\omega_1))$$
$$+ a_2(\wp(x+y+\omega_2) - \wp(x-y+\omega_2)) + a_3(\wp(x+y+\omega_3) - \wp(x-y+\omega_3)),$$

where only three of the constants a_0, a_1, a_2, a_3 are independent, i.e., we can set one among them equal to zero. Using relations (53) we have that in x, y coordinates the other integral of motion is

$$A(x,y)=\frac{1}{4\Delta^2}(\wp(2x)-\wp(\omega_1))p_x^2+\frac{1}{4\Delta^2}(\wp(2y)-\wp(\omega_1))p_y^2$$
$$-\frac{\sqrt{\wp(2x)-\wp(\omega_1)}\sqrt{\wp(2y)-\wp(\omega_1)}p_xp_y}{2\Delta^2}\frac{\Phi(x,y)-\Psi(x,y)}{\Phi(x,y)+\Psi(x,y)}$$
$$+\frac{\sqrt{\wp(2x)-\wp(\omega_1)}\sqrt{\wp(2y)-\wp(\omega_1)}}{\Delta^2}\frac{\phi(x,y)\Psi(x,y)-\psi(x,y)\Phi(x,y)}{\Phi(x,y)+\Psi(x,y)},$$

where

$$\Phi(x,y)=A_2(\wp(x+y+\omega_2)-\wp(x-y+\omega_2))+A_3(\wp(x+y+\omega_3)-\wp(x-y+\omega_3)),$$

$$\Psi(x,y)=A_0(\wp(x+y)-\wp(x-y))+A_1(\wp(x+y+\omega_1)-\wp(x-y+\omega_1)),$$

$$\phi(x,y)=a_2(\wp(x+y+\omega_2)-\wp(x-y+\omega_2))+a_3(\wp(x+y+\omega_3)-\wp(x-y+\omega_3)),$$

$$\psi(x,y)=a_0(\wp(x+y)-\wp(x-y))+a_1(\wp(x+y+\omega_1)-\wp(x-y+\omega_1))$$

while using relations (54) we have that in x, y coordinates the second integral of motion is

$$B(x,y)=\frac{1}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))}(\wp(2x)-\wp(\omega_3))p_x^2$$
$$+\frac{1}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))}(\wp(2y)-\wp(\omega_3))p_y^2$$
$$-2\frac{\sqrt{\wp(2x)-\wp(\omega_3)}\sqrt{\wp(2y)-\wp(\omega_3)}p_xp_y}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))}\frac{\tilde{\Phi}(x,y)-\tilde{\Psi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)}$$
$$+4\frac{\sqrt{\wp(2x)-\wp(\omega_3)}\sqrt{\wp(2y)-\wp(\omega_3)}}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))}\frac{\tilde{\phi}(x,y)\tilde{\Psi}(x,y)-\tilde{\psi}(x,y)\Phi(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)},$$

where

$$\tilde{\Phi}(x,y)=A_1(\wp(x+y+\omega_1)-\wp(x-y+\omega_1))+A_2(\wp(x+y+\omega_2)-\wp(x-y+\omega_2))$$
$$-\frac{1}{2}(A_0+A_1+A_2+A_3)\frac{\sqrt{\wp(2x)-\wp(\omega_3)}\sqrt{\wp(2y)-\wp(\omega_3)}}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))},$$

$$\tilde{\Psi}(x,y)=A_0(\wp(x+y)-\wp(x-y))+A_3(\wp(x+y+\omega_3)-\wp(x-y+\omega_3))$$
$$+\frac{1}{2}(A_0+A_1+A_2+A_3)\frac{\sqrt{\wp(2x)-\wp(\omega_3)}\sqrt{\wp(2y)-\wp(\omega_3)}}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))},$$

$$\tilde{\phi}(x,y)=a_1(\wp(x+y+\omega_1)-\wp(x-y+\omega_1))+a_2(\wp(x+y+\omega_2)-\wp(x-y+\omega_2))$$
$$-\frac{1}{2}(a_0+a_1+a_2+a_3)\frac{\sqrt{\wp(2x)-\wp(\omega_3)}\sqrt{\wp(2y)-\wp(\omega_3)}}{(\wp(\omega_3)-\wp(\omega_1))(\wp(\omega_2)-\wp(\omega_3))},$$

$$\tilde{\psi}(x,y) = a_0(\wp(x+y) - \wp(x-y)) + a_3(\wp(x+y+\omega_3) - \wp(x-y+\omega_3)) + \frac{1}{2}(a_0 + a_1 + a_2 + a_3)\frac{\sqrt{\wp(2x) - \wp(\omega_3)}\sqrt{\wp(2y) - \wp(\omega_3)}}{(\wp(\omega_3) - \wp(\omega_1))(\wp(\omega_2) - \wp(\omega_3))}.$$

Class II_1: This case is not covered by Table VII of Koenigs (Ref. 1, Vol. IV, p. 385). This class corresponds to the Kress[16] equivalence class [0,11] of the nondegenerate superintegrable systems E_{11}, E_{20} of Ref. 6.

The Hamiltonian is

$$H = \frac{p_\xi p_\eta + k\xi\eta + \ell\xi + m\eta + n}{\kappa\xi\eta + \lambda\xi + \mu\eta + \nu},$$

the integrals of motion are

$$A = p_\xi^2 - 2p_\xi p_\eta \frac{\frac{\kappa}{2}\eta^2 + \lambda\eta}{\kappa\xi\eta + \lambda\xi + \mu\eta + \nu} + 2\left(\frac{k\eta^2}{2} + \ell\eta\right) - 2\frac{\left(\frac{\kappa}{2}\eta^2 + \lambda\eta\right)(k\xi\eta + \ell\xi + m\eta + n)}{\kappa\xi\eta + \lambda\xi + \mu\eta + \nu},$$

$$B = p_\xi^2 + p_\eta^2 - 2p_\xi p_\eta \frac{\frac{\kappa}{2}(\xi^2 + \eta^2) + \lambda\eta + \mu\xi}{\kappa\xi\eta + \lambda\xi + \mu\eta + \nu} + 2\left(\frac{k}{2}(\xi^2 + \eta^2) + \ell\eta + m\xi\right) - 2\frac{\left(\frac{\kappa}{2}(\xi^2 + \eta^2) + \lambda\eta + \mu\xi\right)(k\xi\eta + \ell\xi + m\eta + n)}{\kappa\xi\eta + \lambda\xi + \mu\eta + \nu}.$$

The case VI_6 in Table VI (Ref. 1 Vol. IV, p. 384) of Koenigs studied separately the cases where $\kappa=0$ and $\kappa\neq 0$, $\lambda=\mu=0$.

Class II_2: Using the coordinate transformation,

$$\xi = \frac{1}{2}x^2, \quad p_\xi = \frac{p_x}{x}, \quad \eta = \frac{1}{2}y^2, \quad p_\eta = \frac{p_y}{y},$$

the metric of the Class II_2 superintegrable systems is reduced to the metric of the essential form VII.5 (Ref. 1 Vol. IV, p. 385) if

$$\kappa = 2\sqrt{2}A_1, \quad \lambda = 16A_0, \quad \mu = \sqrt{2}A_3, \quad \nu = 4A_2.$$

The corresponding superintegrable system (using the coordinates of Ref. 1) is given by the Hamiltonian

$$H = \frac{p_x p_y + w(x,y)}{g(x,y)},$$

where

$$g(x,y) = A_0[(x+y)^4 - (x-y)^4] + A_1[(x+y)^3 - (x-y)^3] + A_2[(x+y)^2 - (x-y)^2] + A_3[(x+y) - (x-y)],$$

$$w(x,y) = a_0[(x+y)^4 - (x-y)^4] + a_1[(x+y)^3 - (x-y)^3] + a_2[(x+y)^2 - (x-y)^2] + a_3[(x+y) - (x-y)],$$

where only three of the constants a_0, a_1, a_2, a_3 are independent, i.e., we can set one among them

equal to zero. Using relations (58) we have that in x, y coordinates the other integral of motion is

$$A(x,y)=\frac{1}{2}p_x^2+\frac{1}{2}p_y^2-p_xp_y\frac{\tilde{\Phi}(x,y)-\tilde{\Psi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)}+2\frac{\tilde{\phi}(x,y)\tilde{\Psi}(x,y)-\tilde{\psi}\tilde{\Phi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)},$$

where

$$\tilde{\Phi}(x,y)=A_0(x+y)^4+A_1(x+y)^3+A_2(x+y)^2+A_3(x+y),$$

$$\tilde{\Psi}(x,y)=-A_0(x-y)^4-A_1(x-y)^3-A_2(x-y)^2-A_3(x-y),$$

$$\tilde{\phi}(x,y)=a_0(x+y)^4+a_1(x+y)^3+a_2(x+y)^2+a_3(x+y),$$

$$\tilde{\psi}(x,y)=-a_0(x-y)^4-a_1(x-y)^3-a_2(x-y)^2-a_3(x-y),$$

while using relations (57) we have that in x, y coordinates the second integral of motion is

$$B(x,y)=\frac{1}{\sin^2(2y)}p_y^2-2\frac{p_xp_y}{g(x,y)}\int\Phi(x)\mathrm{d}x-2\frac{w(x,y)}{g(x,y)}\int\Phi(x)\mathrm{d}x+2\phi(x)\mathrm{d}x,$$

where

$$\Phi(x)=16A_0x+4A_1,\phi(x)=16a_0x+4a_1.$$

Class II$_3$: Using the coordinate transformation the metric of the Class II$_3$ superintegrable systems is reduced to the metric of the essential form VII.3 (Ref. 1, Vol. IV, p. 385), if

$$\kappa=2(A_1+iA_0),\quad \lambda=2(iA_0-A_1),\quad \mu=-\tfrac{1}{2}(A_3+iA_2),\quad \nu=\tfrac{1}{2}(A_3-iA_2),$$

where

$$\begin{aligned}g(x,y)=&A_0[\sin 4(x+y)-\sin 4(x-y)]+A_1[\cos 4(x+y)-\cos 4(x-y)]\\&+A_2[\sin 2(x+y)-\sin 2(x-y)]+A_3[\cos 2(x+y)-\sin 2(x-y)],\end{aligned}$$

$$\begin{aligned}w(x,y)=&a_0[\sin 4(x+y)-\sin 4(x-y)]+a_1[\cos 4(x+y)-\cos 4(x-y)]\\&+a_2[\sin 2(x+y)-\sin 2(x-y)]+a_3[\cos 2(x+y)-\sin 2(x-y)],\end{aligned}$$

where only three of the constants a_0, a_1, a_2, a_3 are independent, i.e., we can set one among them equal to zero. Using relations (60) we have that in x, y coordinates the other integral of motion is

$$\begin{aligned}A(x,y)=&-\frac{1}{4}p_x^2+\frac{1}{4}\cot^2(2y)p_y^2+\frac{p_xp_y}{2i\tan(2y)}\frac{\tilde{\Phi}(x,y)-\tilde{\Psi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)}\\&-\frac{1}{2i\tan(2y)}\frac{\tilde{\phi}(x,y)\tilde{\Psi}(x,y)-\tilde{\psi}(x,y)\tilde{\Phi}(x,y)}{\tilde{\Phi}(x,y)+\tilde{\Psi}(x,y)},\end{aligned}$$

where

$$\tilde{\Phi}(x,y)=(A_0+iA_1)e^{4ix}\sin(4y)+(A_2+iA_3)e^{2ix}\sin(2y),$$

$$\tilde{\Psi}(x,y)=(A_0-iA_1)e^{-4ix}\sin(4y)+(A_2-iA_3)e^{-2ix}\sin(2y),$$

TABLE I. Essential forms of Table VII in Ref. 1 and equivalence classes of Ref. 16.

Class	κ	λ	μ	ν	Essential from Ref. 1	Classes from Ref. 16
I_1	$16A_2$	$16A_3$	$-A_0$	$4A_1$	VII.4	[3, 2]
I_2	A_1	$-8A_3$	$-A_0$	$-2A_2$	VII.2	[21, 2]
I_3	$2(A_2+A_3)$	A_2-A_3	$-2(A_0+A_1)$	$-A_0+A_1$	VII.1	[111, 1]
II_1						[0, 11]
II_2	$2\sqrt{2}A_1$	$16A_0$	$\sqrt{2}A_3$	$4A_2$	VII.5	[3, 11]
II_3	$2(A_1+iA_0)$	$2(iA_0-A_1)$	$-\frac{1}{2}(A_3+iA_2)$	$\frac{1}{2}(A_3-iA_2)$	VII.3	[21, 0]

$$\tilde{\phi}(x,y) = (a_0 + ia_1)e^{4ix}\sin(4y) + (a_2 + ia_3)e^{2ix}\sin(2y),$$

$$\tilde{\psi}(x,y) = (a_0 - ia_1)e^{-4ix}\sin(4y) + (a_2 - ia_3)e^{-2ix}\sin(2y),$$

while using relations (59) we have that in x, y coordinates the second integral of motion is

$$B(x,y) = \frac{1}{y^2}p_y^2 - 2\frac{p_x p_y}{g(x,y)}\int \Phi(x)\mathrm{d}x - 2\frac{w(x,y)}{g(x,y)}\int \Phi(x)dx + \int \phi(x)\mathrm{d}x,$$

where

$$\Phi(x,y) = -8A_0\cos(4x) + 8A_1\sin(4x),$$

$$\phi(x,y) = -8a_0\cos(4x) + 8a_1\sin(4x).$$

(Also see Table I.)

VII. SUPERINTEGRABLE POTENTIALS ON A SURFACE OF REVOLUTION WITH TWO QUADRATIC INTEGRALS OF MOTION

A manifold which is described by a metric of the form

$$\mathrm{d}s^2 = g(x+y)\mathrm{d}x\,\mathrm{d}y \quad \text{or } \mathrm{d}s^2 = g(x-y)\mathrm{d}x\,\mathrm{d}y$$

is called a surface of revolution.

The above condition is possible only for a specific choice of the parameters κ, λ, μ, and ν. In many cases the superintegrable systems can be calculated by using the general forms which are studied in Sec. V. The general forms of these systems by revolution in many instances are given by the formulas

$$H = \frac{p_\xi p_\eta + f(\xi+\eta) + g(\xi-\eta)}{F(\xi+\eta)} \quad \text{or } H = \frac{p_\xi p_\eta + f(\xi+\eta) + g(\xi-\eta)}{G(\xi-\eta)}$$

and

$$H = \frac{p_X p_Y + \tilde{f}(X+Y) + \tilde{g}(X-Y)}{\tilde{F}(X+Y)} \quad \text{or } H = \frac{p_X p_Y + \tilde{f}(X+Y) + \tilde{g}(X-Y)}{\tilde{G}(X-Y)}.$$

But we must notice that the Liouville or the Lie coordinates are not always the appropriate ones for concluding whether a surface is a surface by revolution. Among the parameters κ, λ, μ, and ν the surfaces of revolution are determined by two independent parameters. In Table II these special values of the parameters κ, λ, μ, and ν are shown. We notice the corresponding potentials given in Refs. 13 and 12. This classification scheme shows that there is the case R_{11} which is not given

TABLE II. Potentials by revolution with two quadratic integrals of motion, (u,v) and (ϕ,ω) are the coordinates, used Ref. 13.

	Class	κ	λ	μ	ν	Potentials from Ref. 13	Potentials from Ref. 12	ξ	η
R_1	I_1	0	0			2[A]		$\frac{1}{2}(v+iu)$	$\frac{1}{2}(v-iu)$
R_2			0	0			(1)	$u+iv$	$u-iv$
R_3	I_2	0	0			2[B]		$\frac{1}{2}(v+iu)$	$\frac{1}{2}(v-iu)$
R_4		0		0		3[B]		$\frac{1}{2}(u+iv)$	$\frac{1}{2}(u-iv)$
R_5			0		0	4[A]		$\frac{1}{2}(x-iy)$	$\frac{1}{2}(x+iy)$
R_6		$-\mu$			0	2[C]		$u+iv$	$u-iv$
R_7	I_3	0	0			4[B]		$v+iu$	$v-iu$
R_8		$-\mu$	ν			4[C]		$\operatorname{arcsinh}(\tan(\phi-i\omega))$	$\operatorname{arcsinh}(\tan(\phi+i\omega))$
R_9	II_1	0	μ				(2)	$u+iv$	$u-iv$
R_{10}			0	0		3[A]		$u+iv$	$u-iv$
R_{11}	II_2	0		0			new	$u+iv$	$u-iv$
R_{12}	II_3		$-\kappa$	$-\nu$		3[D]		$2\sqrt{uv}$	$i\sqrt{\frac{u}{v}}$
R_{13}		$-\mu$	0		0	3[C]		$\frac{v-u}{\sqrt{uv}}$	$\frac{2}{\sqrt{uv}}$

in the above references and it is a new not known superintegrable system. A detailed description of the superintegrable systems R_1 R_{11}.

R_1: *Class* I_1 $\kappa=0$, $\lambda=0$: The form of the Hamiltonian in Liouville coordinates is given by

$$H=\frac{p_\eta p_\xi}{\nu+\dfrac{\mu}{(\xi-\eta)^2}}+\frac{k(\eta+\xi)+4\ell(\eta+\xi)^2-\ell(\xi-\eta)^2+\dfrac{m}{(\xi-\eta)^2}+n}{\nu+\dfrac{\mu}{(\xi-\eta)^2}}.$$

By the coordinate transformation

$$\xi=\frac{v+iu}{2},\quad \eta=\frac{v-iu}{2},\quad p_\xi=p_v-ip_u,\quad p_\eta=pv+ip_u$$

and setting $\mu=-1$, $\nu=1$, the Hamiltonian 2[A] of Ref. 13 is obtained

$$H=\frac{u^2}{u^2+1}\left(p_u^2+p_v^2+kv+4\ell\left(\frac{1}{4}u^2+v^2\right)-\frac{m+n}{u^2}\right)+n.$$

R_{11}: *Class* II_2 $\kappa=0$, $\mu=0$: The form of the Hamiltonian in Liouville coordinates is given by

$$H=\frac{p_\eta p_\xi}{\lambda(\eta+\xi)+\nu}+\frac{n+\dfrac{m+\ell\sqrt{\eta}(\eta+\xi)+k(3\eta+\xi)}{\sqrt{\eta}}}{\lambda(\eta+\xi)+\nu}$$

by the coordinate transformation

$$\xi = u + iv, \quad \eta = u - iv, \quad p_\xi = \tfrac{1}{2}(p_u - ip_v), \quad p_\eta = \tfrac{1}{2}(p_u + ip_v)$$

and setting $\lambda = \frac{1}{2}$, $\nu = 0$, we have

$$H = \frac{p_u^2 + p_v^2}{4u} + \frac{m + (n + 2\ell u)\sqrt{u - iv} + k(4u - 2iv)}{u\sqrt{u - iv}}.$$

For this Hamiltonian the additional integrals of motion have the form

$$A = -\frac{i}{2}X_1 - \frac{K^2}{2} - \frac{2\sqrt{u - iv}\left(\frac{m}{2} + \frac{n\sqrt{u - iv}}{2} - ikv\right)}{u},$$

$$B = X_2 - \frac{2v\left(m\left(iu + \frac{v}{2}\right) + v\left(\frac{n\sqrt{u - iv}}{2} - ikv\right)\right)}{u\sqrt{u - iv}},$$

where K, X_1, X_2 are the three integrals of the free motion of Ref. 12,

$$K = p_v, \quad X_1 = p_u p_v - \frac{v}{2u}(p_u^2 + p_v^2), \quad \text{and } X_2 = p_v(vp_u - up_v) - \frac{v^2}{4u}(p_u^2 + p_v^2).$$

This system was not included in Ref. 12. Therefore it is a new superintegrable system, which is studied here for the first time as far as we know.

VIII. SUPERINTEGRABLE POTENTIALS ON A MANIFOLD WITH CURVATURE ZERO

Let us consider the manifold corresponding to the metric in the Liouville coordinates;

$$ds^2 = g(\xi, \eta)d\xi\, d\eta,$$

the curvature is defined by

$$K = -\frac{1}{2g}\frac{\partial^2}{\partial\xi\partial\eta}\ln g = 0. \tag{61}$$

The above constraint imposes restrictions on the choice of the parameters κ, λ, μ, and ν. In Tables III and IV we can see the possible choices of the values of the above parameters.

In this category there are three families of potentials.

The potentials on the complex E plane corresponding to the Hamiltonian,

$$H = p_x^2 + p_y^2 + V(x,y);$$

these potentials are classified in Ref. 5 and finally the final list of potentials are given in Ref. 6. In this section we follow the enumeration of the potentials given by this exhaustive list.[6]

The Drach potentials corresponding to the Hamiltonian,

$$H = p_x p_y + V(x,y);$$

these potentials are classified in Ref. 8. In this section we follow the enumeration of this reference for the Drach potentials with quadratic integrals of motion.

The potentials on the real hyperbolic plane H_2 corresponding to the Hamiltonian,

$$H = p_x^2 - p_y^2 + V(x,y);$$

these potentials are classified in Ref. 9.

TABLE III. Potentials with curvature zero and two quadratic integrals of motion from Ref. 6.

	Class	κ	λ	μ	ν	Plane potentials from Ref. 6	ξ	η
F_1	I_1	0	0	0		E_2	$x+iy$	$x-iy$
F_2	I_2	0	0	0		E_1	$x+iy$	$x-iy$
F_3		0		0	0	E_{16}	$\sqrt{\frac{x+iy}{2}}$	$\sqrt{\frac{x-iy}{2}}$
F_4	II_1		0	0	0	E_{20}	$\frac{\sqrt{x+\sqrt{x^2+y^2}}+\sqrt{x-\sqrt{x^2+y^2}}}{\sqrt{2}}$	$\frac{\sqrt{x+\sqrt{x^2+y^2}}-\sqrt{x-\sqrt{x^2+y^2}}}{\sqrt{2}}$
F_5		0	0		0	E_{11}	$x+iy$	$2\sqrt{x-iy}$
F_6	II_2	0	0	0		E_9	$x+iy$	$x-iy$
F_7		0	0		0	E_{10}	$x+iy$	$-\frac{(x-iy)^2}{2}$
F_8	II_3	0	0			E_8	$x+iy$	$x-iy$
F_9		0	0			E_7	$\frac{1}{2}(x+iy)$	$\frac{x-iy-\sqrt{(x-iy)^2+16\mu\nu}}{4\nu}$
F_{10}				0	0	E_{17}	$2\sqrt{x-iy}$	$2\sqrt{x+iy}$
F_{11}				0	0	E_{19}	$2\sqrt{x+iy}$	$\sqrt{x-iy+\sqrt{(x-iy)^2-4}}$

Generally the condition (61) restricts the choices of the constants κ, λ, μ, and ν in one independent parameter. These values characterize the permitted metrics in the classification given in Sec. V.

IX. SUPERINTEGRABLE POTENTIALS ON A MANIFOLD WITH CONSTANT CURVATURE

Let us consider the manifold corresponding to the metric in the Liouville coordinates:

$$ds^2 = g(\xi,\eta)d\xi\, d\eta,$$

the curvature is defined by

$$K = -\frac{1}{2g}\frac{\partial^2}{\partial\xi\partial\eta}\ln g = \text{const}. \tag{62}$$

The above constraint imposes restrictions on the choice of the parameters κ, λ, μ, and ν. In Tables V and VI we can see the possible choices of the values of the above parameters.

X. SUPERINTEGRABLE SYSTEMS WITH A LINEAR AND A QUADRATIC INTEGRAL

In the case of a linear integral of motion and a quadratic integral of motion, there is a Liouville coordinate system where the Hamiltonian and the linear integral of motion are written as

TABLE IV. Potentials with curvature zero and two quadratic integrals of motion from Refs. 8 and 9.

	Class	κ	λ	μ	ν	Drach potentials (Ref. 8)	ξ	η	Ref. 9	ξ	η
F_1	I_1	0	0	0		(a) $(r\neq 0)$	$\frac{x}{r}$	y	V^{α}	$x+iy$	$x-iy$
F_2	I_2	0	0	0		(b) $(r\neq 0)$	$\frac{x}{r}$	y	V^{b}	$x+iy$	$x-iy$
F_3		0		0	0	(g) $(r\neq 0)$	$\sqrt{\frac{x}{r}}$	$\sqrt{y}$	V^{c}	$\sqrt{\frac{x+iy}{2}}$	$\sqrt{\frac{x-iy}{2}}$
F_4	II_1		0	0	0	(c)	$2\sqrt{x}$	$2\sqrt{y}$	V^{d}	$\frac{\sqrt{x+\sqrt{x^2+y^2}}+\sqrt{x-\sqrt{x^2+y^2}}}{\sqrt{2}}$	$\frac{\sqrt{x+\sqrt{x^2+y^2}}-\sqrt{x-\sqrt{x^2+y^2}}}{\sqrt{2}}$
F_5		0	0		0	(e) $(r=0)$	x	$2\sqrt{y}$			
F_6	II_2	0	0	0		(e) $(r\neq 0)$	$\frac{x}{r}$	y			
F_7		0	0		0		x	y^2			
F_8	II_3	0	0			(f)	x	y			
F_9		0	0			(i) $(r\neq 0)$	y	$\frac{x+\sqrt{x^2+4\mu\nu}}{2\nu}$			
F_{10}				0	0	(d)	$2\sqrt{y}$	$\frac{2\sqrt{x}}{2\sqrt{x+\sqrt{x^2-r^2}}}$			
F_{11}				0	0	(h) $(r\neq 0)$	$2\sqrt{y}$				

TABLE V. Potentials with constant curvature and two quadratic integrals of motion from Ref. 6. The coordinates $(\sigma,\tau)=(u,v)$ are the horospherical coordinates.

	Class	κ	λ	μ	ν	Ref. 6	ξ	η
C_1	I_1	0	0	$1/K$	0	S_1	$e^{i\phi}\tan\left(\frac{\theta}{2}\right)$	$-e^{i\phi}\cot\left(\frac{\theta}{2}\right)$
C_2	I_2	$-1/K$	0	0	0	S_2	$-\frac{1}{2}ie^{i\phi}\cot\frac{\theta}{2}$	$-\frac{1}{2}ie^{i\phi}\tan\frac{\theta}{2}$
C_3		$-1/K$	0	$1/K$	0	S_4	$2\sqrt{-ie^{i\phi}\cos\left(\frac{\theta}{2}\right)}$	$2\sqrt{ie^{i\phi}\tan\left(\frac{\theta}{2}\right)}$
C_4	I_3	0	0	$4/K$	0			
C_5		0	0	$2/K$	$1/K$	S_9	$\ln\left(e^{i\phi}\tan\left(\frac{\theta}{2}\right)\right)$	$\ln\left(-e^{i\phi}\cot\left(\frac{\theta}{2}\right)\right)$
C_6		$-2/K$	$-1/K$	$2/K$	$-1/K$	S_7	$\operatorname{arcsinh}\left(-ie^{i\phi}\cot\left(\frac{\theta}{2}\right)\right)$	$\operatorname{arcsinh}\left(-ie^{i\phi}\tan\left(\frac{\theta}{2}\right)\right)$
C_7		$-4/K$	0	$4/K$	0	S_8	$\frac{1}{2}\ln\left(\frac{i(-1+\sqrt{1+(\sigma+i\tau)^2})}{\sigma+i\tau}\right)$	$\frac{1}{2}\ln\left(\frac{i(1+\sqrt{1+(\sigma-i\tau)^2})}{\sigma-i\tau}\right)$

$$I=(p_\xi+p_\eta)^2 \quad \text{or } A=(p_\xi-p_\eta)^2$$

and

$$H=\frac{p_\xi p_\eta}{G(\xi-\eta)}+\frac{g(\xi-\eta)}{G(\xi-\eta)} \quad \text{or } H=\frac{p_\xi p_\eta}{F(\xi+\eta)}+\frac{f(\xi+\eta)}{F(\xi+\eta)}.$$

From the forms of the integral of motion, which are given in Sec. V we can find all the possible subclasses corresponding to a linear and quadratic integral of motion in Liouville coordinates. In all the above cases we remark that the potential depends on two parameters among the k, ℓ, m, and n. In Table VII we give the possible cases of superintegrable systems with a linear and a quadratic integral of motion.

In Table VIII, the possible superintegrable systems which are defined on a surface of revolution with a linear and a quadratic integral of motion are listed.

In Table IX, the possible superintegrable systems which are defined on a surface of zero curvature with a linear and a quadratic integral of motion are listed.

In Table X, the possible superintegrable systems which are defined on a surface of constant curvature with a linear and a quadratic integral of motion are listed.

TABLE VI. Potentials with constant curvature ($K=1$) and two quadratic integrals of motion from Ref. 9.

	Class	κ	λ	μ	ν	Ref. 9	ξ	η
C_1	I_1	0	0	$1/K$	0			
C_2	I_2	$-1/K$	0	0	0			
C_3		$-1/K$	0	$1/K$	0			
C_4	I_3	0	0	$4/K$	0	U^c	$\frac{1}{2}\ln\left(-ie^{i\phi}\cot\left(\frac{\theta}{2}\right)\right)$	$\frac{1}{2}\ln\left(ie^{i\phi}\tan\left(\frac{\theta}{2}\right)\right)$
C_5		0	0	$2/K$	$1/K$	U^a	$-i\pi/4+\ln\left(\frac{1+ie^{i\phi}\tan\left(\frac{\theta}{2}\right)}{1-ie^{i\phi}\tan\left(\frac{\theta}{2}\right)}\right)$	$-i\pi/4+\ln\left(\frac{1-ie^{i\phi}\cot\left(\frac{\theta}{2}\right)}{1+ie^{i\phi}\cot\left(\frac{\theta}{2}\right)}\right)$
						U^b	$\ln\left(e^{i\phi}\tan\left(\frac{\theta}{2}\right)\right)$	$\ln\left(-e^{i\phi}\cot\left(\frac{\theta}{2}\right)\right)$
C_6		$-2/K$	$-1/K$	$2/K$	$-1/K$	U^e	$\operatorname{arcsinh}\left(-ie^{i\phi}\cot\left(\frac{\theta}{2}\right)\right)$	$\operatorname{arcsinh}\left(-ie^{i\phi}\tan\left(\frac{\theta}{2}\right)\right)$
C_7		$-4/K$	0	$4/K$	0			

XI. DISCUSSION

The findings of this paper are summarized as follows:

(1) The superintegrable systems with quadratic integrals of motion can be classified in six subclasses. Each subclass depends on seven parameters. Four among these parameters (κ, λ, μ, and ν) determine the metric of the manifold, on which the system is determined. These parameters are characteristic of the system's "kinetic" energy. The remaining three parameters define the potential (the potential depends on four parameters k, ℓ, m, and n but only three among them are independent). For each subclass, the analytic explicit forms of the

TABLE VII. General superintegrable integrable systems with a linear and a quadratic integral of motion.

	Class	κ	λ	μ	ν	k	ℓ	m	n
GL_1	I_1	0	0			0	0		
GL_2			0	0			0	0	
$(\simeq GL_1)$	I_2	0	0			0	0		
GL_3		0		0		0		0	
GL_4			0		0		0		0
GL_5	I_3	0	0			0	0		
$(\simeq GL_1)$		$\kappa=\mp 2\lambda$		$\mu=\pm 2\nu$	$k=\mp 2\ell$		0	$m=\pm 2n$	
GL_6	II_1	0	$\lambda=\pm\mu$			0	$\ell=\pm m$		
GL_7	II_2	0		0		0		0	
$(\simeq GL_3)$	II_3	0		0		0		0	

TABLE VIII. Potentials by revolution with a linear and a quadratic integral of motion.

	Class	κ	λ	μ	ν	k	l	m	n	Potentials by revolution from Ref. 13	Potentials by revolution from Ref. 12
RL_1	I_1	0	0			0	0			2.2[D]	
RL_2			0	0			0	0			3
RL_3	I_2		0		0		0		0	4.2[D]	
RL_4	II_1	0		0		0		0		3.2[E]	

manifold metric, the potential and the integrals of motion are calculated. Also the constants of the quadratic Poisson algebra of integrals of motion are given as functions of the energy and the eight parameters are given.

(2) All the known two-dimensional superintegrable systems are systems defined on surfaces of constant curvature or on surfaces of revolution. All these systems are classified in these six classes. Each class is characterized by the values of four parameters κ, λ, μ, and ν, which are determined by the form of the assumed manifold. If we fix the manifold, let us suppose that the manifold is a manifold with negative constant curvature, the possible values of the parameters κ, λ, μ, and ν are calculated for each subclass. Therefore we can "guess" the existence of the permitted superintegrable systems and to classify these systems in tables. Using this technique we can classify all the possible known superintegrable systems and to investigate the possible missing potentials. With this method a new superintegrable system was found for the class I superintegrable systems by revolution, given in Ref. 5.

(3) Generally for any values of the parameters κ, λ, μ, and ν the associated manifolds are neither surfaces of constant curvature nor surfaces of revolution. Therefore we have investigated superintegrable systems, which are not yet known. We believe that all the possible superintegrable systems with two quadratic integrals of motion are investigated.

(4) The two-dimensional nondegenerate[5] superintegrable systems are classified by the values of the constants of the Darboux equations[9,5] and the constants of the system. The relation of these constants with the constants of the quadratic Poisson algebra is explained.

(5) The six classes of superintegrable systems are the equivalence classes of Stäckel equivalent systems.

From the above discussion several open problems arise.

(i) The superintegrable systems for the case of cubic integrals of motion are under investigation.[8,31–36] The general structure of these systems is recently investigated[14] but the general form and their classification is not yet known for manifolds which carry integrable systems with one third order integral of motion.

TABLE IX. Potentials with curvature zero and with a linear and a quadratic integral of motion.

	Class	κ	λ	μ	ν	k	ℓ	m	n	Potentials from Ref. 6
FL_1	I_1	0	0	0		0	0			E_6
FL_2		0	0	0			0	0		E_5
FL_3	I_2	0	0	0		0		0		E_3
FL_4		0		0	0	0		0		E_{18}
FL_5	II_1	0	0	0		0	0			E_4
FL_6	II_2	0	0	0		0	0			E_{13}
FL_7	II_3	0	0	0		0	0			E_{14}
FL_8		0	0			0	0			E_{12}

TABLE X. Potentials with constant curvature and with a linear and a quadratic integral of motion.

Class	κ	λ	μ	ν	k	l	m	n	Sphere potentials ($K=1$) from Ref. 6
I_1	0	0	$1/K$	0	0	0			S_5
I_2	$-1/K$	0	0	0		0		0	S_3
	$-1/K$	0	$1/K$	0		0		0	S_6

(ii) The quantum counterparts of the general six subclasses of superintegrable systems with quadratic integrals of motion are not yet known. In Sec. II, the separation of variables of these systems has been explicitly written. The form of the separation of Schrödinger equation can be written in a Liouville coordinate system. The solutions of the quantum Schröedinger equation can be calculated. This work is under current investigation. The form of the Poisson algebra can be generalized in a quadratic associative algebra, whose energy eigenvalues are generally calculated by using deformed oscillator techniques.[18–22] From the form of the Poisson algebra, one can guess that the energy eigenvalues of these quantum systems are roots of cubic polynomials.

(iii) The general form of the three-dimensional superintegrable systems with quadratic integrals of motion is not yet known. The Poisson algebras and the associated quantum counterparts for the three-dimensional superintegrable systems are not yet fully studied. Recently[37,38] the quantum quadratic algebras have been written down, which are not generally closed as polynomial algebras. A systematic calculation of energy eigenvalues with algebraic methods has not been performed yet.

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APPENDIX: POLYNOMIAL COMBINATIONS OF INTEGRALS

Let consider a superintegrable system with two quadratic integrals of motion. The general forms of the Hamiltonian and the integrals of motion in Liouville coordinates are

$$H = \frac{p_\xi p_\eta}{g(\xi,\eta)} + V(\xi,\eta),$$

$$A = p_\xi^2 + k p_\eta^2 - 2c(\xi,\eta)\frac{p_\xi p_\eta}{g(\xi,\eta)} + q(\xi,\eta), \quad k = 0 \text{ or } 1, \tag{A1}$$

$$B = a^2(\xi)p_\xi^2 + b^2(\eta)p_\eta^2 - 2\beta(\xi,\eta)\frac{p_\xi p_\eta}{g(\xi,\eta)} + Q(\xi,\eta).$$

In this Appendix we consider that the system has quadratic integrals of motion. We assume that the system has not any linear integral of motion. That assumption excludes the system $H=p_x^2+p_y^2$, because it possesses two linear integrals of motion. In this Appendix, we shall prove the following proposition.

Proposition 3: Let M be an integral of motion, which is a polynomial function of the momenta of even order. We assume that this integral contains only monomials of momenta of even order, i.e.,

$$M = \sum_{k+\ell=even}^{2n} \alpha_{k,\ell}(\xi,\eta) p_\xi^k p_\eta^\ell. \tag{A2}$$

Then M is a polynomial of order n of the integrals H,A,B.

The existence of three integrals of motion implies that the integral M is functionally dependent integral, i.e., there is some smooth function Φ (nongenerally a polynomial one) such that

$$\Phi(M,A,B,H) = 0 \quad \text{or } M = f(A,B,H)$$

but the function $f(A,B,H)$ is not evident that it is a polynomial one. From (A1) we can see that

$$p_\xi^2 = \frac{\begin{vmatrix} A + 2cH - q - 2cV & k \\ B + 2\beta H - Q - 2\beta V & b^2(\xi,\eta) \end{vmatrix}}{\begin{vmatrix} 1 & k \\ a^2(\xi,\eta) & b^2(\xi,\eta) \end{vmatrix}},$$

$$p_\eta^2 = \frac{\begin{vmatrix} 1 & A + 2cH - q - 2cV \\ a^2(\xi,\eta) & B + 2\beta H - Q - 2\beta V \end{vmatrix}}{\begin{vmatrix} 1 & k \\ a^2(\xi,\eta) & b^2(\xi,\eta) \end{vmatrix}},$$

$$p_\xi p_\eta = gH - V.$$

The above equations imply that the momentum monomials $p_\xi^k p_\eta^\ell$ inside the sum sign in (A2) can be written as polynomials of the integrals A,B,H with coefficients, which depend on ξ and η. Therefore the integral of motion M is written

$$M = \sum_{0 \le i+j+k \le n} c_{ijk}(\xi,\eta) A^i B^j H^k.$$

Generally the coefficients c_{ijk} should be constants not depending on the variables ξ,η. If these functions are nonconstant functions $c_{ijk}(\xi,\eta)$ then we choose a fixed value of these parameters ξ_0,η_0. In general there is an infinity of trajectories passing through these position values ξ_0,η_0. Each trajectory is characterized by a special value of the integrals H,A,B, therefore M is a polynomial of fixed constants for an infinity of trajectories. For another pair of parameters ξ_1,η_1 we have another choice of the coefficients in (A2) therefore there is a relation of the form

$$\sum_{0 \le i+j+k \le n} (c_{ijk}(\xi_1,\eta_1) - c_{ijk}(\xi_0,\eta_0)) A^i B^j H^k = 0.$$

The above relations mean that the integrals of motion H,A,B are not functionally independent functions, that is a contradiction to assumption initial regarding the independence of the integrals. Therefore we have proved that the polynomial expansion (A2) of the integral M is indeed unique, when M is an even polynomial of the momenta.

A direct application of Proposition 3 is the following Proposition.

Proposition 4: Let a superintegrable two-dimensional system have even quadratic integrals of motion H,A,B. If we set $C=\{A,B\}$. The integrals $\{A,C\}$ and $\{B,C\}$ can written as quadratic polynomials of the integrals. The integral C^2 is a cubic polynomial of the integrals H,A,B.

The above proposition was taken as a conjecture in the previous work.[18–25] Here we prove that this assumption is indeed true. A generalization of Proposition 4 is indeed true for superintegrable two-dimensional systems with an integral, which is an odd cubic polynomial in momenta.[32,31] This Proposition means that the superintegrable two-dimensional systems with even quadratic integrals

correspond to a quadratic Poisson algebra, which is characteristic for the superintegrable system. The situation in three-dimensional superintegrable systems is not yet clear.[37,38] Recently this problem is studied in complex flat spaces.[39]

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Hamiltonian theory of constrained impulsive motion

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This paper considers systems subject to nonholonomic constraints which are not uniform on the whole configuration manifold. When the constraints change, the system undergoes a transition in order to comply with the new imposed conditions. Building on previous work on the Hamiltonian theory of impact, we tackle the problem of mathematically describing the classes of transitions that can occur. We propose a comprehensive formulation of the transition principle that encompasses the various impulsive regimes of Hamiltonian systems. Our formulation is based on the partial symplectic formalism, which provides a suitable framework for the dynamics of nonholonomic systems. We pay special attention to mechanical systems and illustrate the results with several examples. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2192974]

I. INTRODUCTION

In this paper we consider the problem of mathematically describing impulsive motions (impacts, collisions, reflection, refractions) of Hamiltonian systems subject to nonholonomic constraints. An impulsive behavior takes place when one or more of the basic ingredients of the Hamiltonian dynamical picture undergoes a drastic change. As an example, one may consider the instant of time when the configuration space of the system collapses instantaneously because of an inelastic collision. Another example is given by a ray of light that splits into reflected and refracted rays when passing from one optical media to another, and so on. In situations like these, the phase trajectory of the system becomes discontinuous and the problem of how to describe this discontinuity arises.

The problem of describing impulsive motion has been extensively studied in classical books such as Refs. 2, 29, 31, 32, and 36. In these references, the emphasis is put on the analysis of mechanical systems subject to impulsive forces, and in particular, the study of rigid body collisions by means of Newton and Poisson laws of impact. Impulsive nonholonomic constraints (i.e., constraints whose reaction force is impulsive) are also considered in Refs. 14, 30, 36, and 42, and, from a geometric perspective, in more recent works such as Refs. 13, 20, 23, and 33. If impulsive constraints and impulsive forces are present at the same time, Newton and Poisson approaches have been revealed to be physically inconsistent in certain cases.[8,38] This surprising consequence of the impact laws is only present when the velocity along the impact surface stops or reverses during collision due to the friction. Energetically consistent hypothesis for rigid body collisions with slip and friction are proposed in Refs. 37 and 38. From a design point of view, the interest in systems subject to impulsive forces is linked to the emergence of nonsmooth and hybrid dynamical systems in control theory, i.e., systems where continuous and discrete dynamics coexist, see

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Refs. 7–9 and 40 and references therein. Hybrid mechanical systems that locomote by switching between different constraint regimes and are subject to elastic impacts are studied in Ref. 10. Hyperimpulsive control of mechanical systems is analyzed in Ref. 19.

Here, we aim at a comprehensive analysis of the various situations which can occur concerning impulsive regimes of nonholonomic Hamiltonian systems. In particular, we focus on two different but complementary cases. The first one deals with a drastic change in the nonholonomic constraints imposed on the system. The second one concerns a drastic change of the Hamiltonian function and includes, in particular, collisions and impacts of nonholonomic systems. The proposed solution is given in terms of a generalized version of the *transition principle*. This principle, sketched for the first time in a series of lectures of the second author[6] for discontinuous Hamiltonians, was recently extended to other nonconstrained situations in Refs. 34 and 35 (see also Ref. 17 for a related discussion in an optimal control setting). By its very nature, the transition principle is a direct dynamic interpretation of the geometric data of the problem. This feature distinguishes it from other approaches. For instance, in classical mechanics, the velocity jumps caused by an impact are traditionally derived from some assumptions on the nature of the impulsive forces (see, for instance, Refs. 2 and 24). However, these assumptions are not logical consequences of the fundamental dynamical principles and therefore one should really consider them as additional principles for impulsive problems. The distinguishing feature of the transition principle is that it gives full credit to the geometry of the nonholonomic Hamiltonian system. This seems reasonable for the impulsive regime, keeping in mind the adequacy of the Hamiltonian description to the dynamical behavior of the system in the absence of impulsive motions. In addition, there are some noticeable advantages deriving from the transition principle. First of all, its application gives an exact and direct description of the post-impact state which is of immediate use for both theoretical and computational purposes. Second, it is still valid in some situations where standard methods can hardly be applied. In particular, this is the case of Hamiltonian systems describing the propagation of singularities of solutions of partial differential equations (consider, for instance, the example of geometrical optics).[26,27,41] Clearly, no variational or traditional approach can be applied to this very important class of systems.

A second contribution of this paper concerns the formulation of the dynamics of nonholonomic Hamiltonian systems. We make use of the notion of partial symplectic structures introduced in Ref. 6 and relate this framework with other modern approaches to nonholonomic systems (see Refs. 3–5, 15, 22, 18, 28, and 39 and references therein). One advantage of the partial symplectic formalism is that it allows us to draw clear analogies between the unconstrained and constrained situations. Another advantage is that the treatment of nonlinear constraints can be easily incorporated.

The paper is organized as follows. Section II introduces some geometric preliminaries on distributions, constraint submanifolds and partial symplectic structures. In Sec. III we show how any nonholonomic Hamiltonian system possesses an associated partial symplectic structure, and we use this fact to intrinsically formulate the dynamics. We also analyze systems with instantaneous nonholonomic constraints and systems exhibiting discontinuities. In Sec. IV, we develop a new formulation of the transition principle for systems with constraints. We present the novel notion of focusing points with respect to a constraint submanifold and we also introduce the concept of constrained characteristic. Decisive points are defined for each impulsive regime resorting to in, out, and trapping points. Section V presents a detailed study of the concepts introduced in the preceding sections in the case of mechanical systems. We compute the focusing points and the characteristic curves, and present various results concerning the decisive points. We also prove an appropriate version for generalized constraints of the classical Carnot's theorem for systems subject to impulsive forces: if the constraints are linear, we show that the transition principle always implies a loss of energy. We conclude this section by showing that if the constraints are integrable, then our formulation of the transition principle recovers the solution for completely inelastic collisions.[35] Section VI presents various examples of the application of the above-developed theory. Finally, Sec. VII presents our conclusions and directions for future research.

To ease the exposition, below we make use of the standard notation concerning differential geometry and the Hamiltonian formalism without making explicit reference to any work. In particular, we denote by Λ^i [respectively, $D(M)$] the $C^\infty(M)$-module of ith order differential forms (respectively, of vector fields) on a manifold M. We use $F^*(\varphi)$ to denote the pullback with respect to a smooth map F of a function or differential form φ. If x is a point of M, then the subscript x refers to the value of the corresponding geometric object at x. For instance, X_x stands for the vector field vector $X \in D(M)$ evaluated at x. The interested reader may consult classical books such as Refs. 1, 21, and 25 for further reference. We also assume smoothness of all the objects we are dealing with.

II. PRELIMINARIES

In this paper we deal with Hamiltonian systems defined on the cotangent bundle T^*M of an n-dimensional manifold M. In the particular case of a mechanical system, M and T^*M are, respectively, the configuration space and the phase space of the system. As usual, $\pi_M: T^*M \to M$ (or simply π) stands for the canonical projection from T^*M to M, $H \in C^\infty(T^*M)$ for the Hamiltonian function and $X_H \in D(M)$ for the corresponding Hamiltonian vector field. The canonical symplectic structure on T^*M is denoted by $\Omega = \Omega_M$. In canonical coordinates (q^a, p_a), $a = 1, \ldots, n$ of T^*M, the symplectic form reads $\Omega = \mathrm{d}q^a \wedge \mathrm{d}p_a$.

We say that the Hamiltonian system (M,H) *comes from a Lagrangian system* (M,L) *on* TM if $H = (\mathcal{L}_L^*)^{-1}(E_L)$, where $E_L \in C^\infty(TM)$ is the energy function corresponding to the (hyper-regular) Lagrangian function $L \in C^\infty(TM)$ and $\mathcal{L}_L: TM \to T^*M$ is the associated Legendre map.

If X is a vector field on T^*M, then the map $\alpha_X: T^*M \to TM$ defined by

$$\alpha_X(\theta) = d_\theta \pi(X_\theta) \in T_{\pi(\theta)}, \quad \theta \in T^*M,$$

denotes the *anti-Legendre map associated with* X. In standard coordinates, if $X = A^a(q,p)(\partial/\partial q^a) + B^a(q,p)(\partial/\partial p_a)$, then α_X reads $\alpha_X(q^a, p_a) = (q^a, A^a(q,p))$. For the Hamiltonian vector field $X = X_H$, we write α_H instead of α_{X_H}, so that

$$\alpha_H: (q,p) \mapsto \left(q, v = \frac{\partial H}{\partial p}\right).$$

It is not difficult to see that if the Hamiltonian system (M,H) comes from a Lagrangian system (M,L), then $\alpha_H = \mathcal{L}_L^{-1}$.

A. Distributions and codistributions

Recall that a *distribution* (respectively, *codistribution*) on a manifold M is a vector subbundle of TM (respectively, of T^*M). The *annihilator* of a distribution $\mathcal{D}$ on M is the codistribution $\mathrm{Ann}(\mathcal{D})$ defined by

$$\mathrm{Ann}(\mathcal{D})_x = \{\theta \in T_x^*M \,|\, \theta(\xi) = 0, \ \forall\ \xi \in \mathcal{D}_x\}, \quad x \in M.$$

If $\mathcal{D}$ is $(n-m)$-dimensional, the codistribution $\mathrm{Ann}(\mathcal{D})$ is m-dimensional. The *dual bundle* $\mathcal{D}^*$ *of* $\mathcal{D}$ is canonically identified with the cotangent bundle T^*M modulo $\mathrm{Ann}(\mathcal{D})$. We will also denote by $\mathcal{D}^\perp$ the orthogonal complement of a distribution $\mathcal{D}$ on T^*M with respect to the symplectic form Ω, i.e.,

$$\mathcal{D}_y^\perp = \{\xi \in T_y(T^*M) \,|\, \Omega_y(\xi, \eta) = 0, \ \forall\ \eta \in \mathcal{D}_y\}, \quad y \in T^*M.$$

A vector field $X \in D(M)$ *belongs* to $\mathcal{D}$ if $X_x \in \mathcal{D}_x$ for all $x \in M$. Vector fields belonging to $\mathcal{D}$ constitute a $C^\infty(M)$-module, denoted by $D_{\mathcal{D}}(M)$, which is a submodule of $D(M)$. In the partial symplectic formalism (see Sec. II C below), they are interpreted as "constrained" vector fields. Dually, denote by $\Lambda^1_{\mathcal{D}}(M)$ the $C^\infty(M)$-module of sections of the bundle $\mathcal{D}^*$ and by $\Lambda^i_{\mathcal{D}}(M)$ its ith

exterior product. These are interpreted as "constrained" differential i-forms. We denote the natural restriction map from $\Lambda^i(M)$ to $\Lambda^i_{\mathcal{D}}(M)$ by $r_{\mathcal{D}}$: $\Lambda^i(M)\to\Lambda^i_{\mathcal{D}}(M)$.

The geometric description of nonholonomic systems in the framework of the partial symplectic formalism[6] requires a slight "affine" generalization of these standard notions. Namely, an *affine distribution* on a manifold M is an affine subbundle Δ of TM. This means that the fiber Δ_x of Δ over $x\in M$ is an affine subspace in T_xM. Therefore, Δ_x can be represented in the form $\Delta_x=v+\Delta^0_x$ with $v\in T_xM$ and Δ^0_x being the vector subspace of T_xM canonically associated with Δ_x. In this representation, the *displacement vector* v is unique modulo Δ^0_x. The union $\cup_{x\in M}\Delta^0_x$ constitutes a linear distribution of the tangent bundle TM, denoted by Δ^0, canonically associated with Δ. It is not difficult to see that there always exist a vector field $Y\in D(M)$ such that Y_x is a displacement vector for Δ_x. Such vector fields are called *displacement vector fields of* Δ. Obviously, displacement vector fields differ by another vector field belonging to Δ. In coordinate terms, an $(n-m)$-dimensional affine codistribution is described by a system of linear equations $\Phi_i=0$ with respect to the variables p_a, i.e., $\Phi_i(q,p)=\Phi_{ia}(q)p_a+\Phi_{i0}(q)$, $i=1,\ldots,m$.

Similarly, an *affine codistribution* on M is an affine subbundle $C\subset T^*M$ of the cotangent bundle. As above, one has $C=\Upsilon+C^0$, where C^0 is the unique codistribution on M canonically associated with C, and $\Upsilon\in\Lambda^1(M)$ is a *displacement form*. Point-wisely this means that $C_x=\Upsilon_x+C^0_x$, for all $x\in M$.

1. Linear constraints

In the case of linear constraints, the analogy between free and constrained systems is particularly clear. In fact, it is natural to interpret an affine distribution (respectively, codistribution) on a manifold M as the "constrained" tangent (respectively, cotangent) bundle of M. A linearly constrained Hamiltonian system is then a triple (M,H,C), with $H\in C^\infty(T^*M)$ and C an affine codistribution on M. Similarly, a triple (M,L,Δ), with $L\in C^\infty(TM)$ and Δ an affine distribution on M, is a linearly constrained Lagrangian system. The anti-Legendre map allows one to pass from a constrained Hamiltonian system to the corresponding Lagrangian system and vice versa. More precisely, if (M,H,C) is a linearly constrained Hamiltonian system, the map α_H is linear and (M,H) comes from a Lagrangian system (M,L), then the corresponding linearly constrained Lagrangian system is (M,L,Δ), with $\Delta=\alpha_H(C)$. To go in the opposite direction, one must use the Legendre map $\mathcal{L}_L$ instead of α_H.

Throughout the paper, we distinguish the class of mechanical systems subject to linear constraints because of two reasons. First, classically they have been intensively studied. Second, one can extract from them the motivations for the basic constructions which will be discussed below.

2. Nonlinear constraints

In the Hamiltonian setting, the *nonholonomic constraints* are given by a submanifold (not necessarily a vector subbundle) $C\subset T^*M$. Similarly, *nonholonomic Lagrangian or kinematic constraints* are given by a submanifold $C'\subset TM$. If the Hamiltonian system (M,H) comes from a Lagrangian system (M,L), then $C=\mathcal{L}_L(C')$ if and only if $C'=\alpha_H(C)$. In mechanics, these two approaches correspond to two possible descriptions of nonholonomic constraints: either as limitations imposed on the momenta or as limitations imposed on the velocities, respectively. The fact that C (respectively, C') represents limitations imposed only on the momenta (respectively, velocities), but not on the configurations of the system, implies that the projection π must send C (respectively, C') surjectivity onto M. However, the assumption of "infinitesimal surjectivity" of $\pi|_C$ is more adequate in this context. This means that $\pi|_C$ is a *submersion*, i.e., $d_y(\pi|_C)$: $T_yC\to T_{\pi(y)}M$ is surjective for all $y\in C$. With this motivation, we adopt the following definition.

Definition 2.1: A set of nonholonomic constraints *imposed on a Hamiltonian system* (M,H) *is a submanifold* $C\subset T^*M$ *such that* $\pi|_C$ *is a submersion. The constrained Hamiltonian system is denoted by* (M,H,C).

Since C and $\alpha_H(C)$ are, respectively, interpreted as the constrained cotangent and tangent bundle of the system (M,H,C), we will always assume that they have equal dimensions. It is

worth stressing that the above definition also makes sense for manifolds with boundary. In such a case, the boundary of T^*M is $\pi^{-1}(\partial M)$ and the boundary of C is $\partial C = C \cap \pi^{-1}(\partial M)$.

Remark 2.2: Similarly, *nonholonomic Lagrangian constraints* are represented by submanifolds of TM that project regularly onto M.

In what follows, $\Phi_i(q,p)=0$, $i=1,\ldots,m$, will denote a set of local equations defining C. For a point $x \in M$, we denote by C_x the fiber of C at x,

$$C_x = C \cap T^*_x M = \{y \in C | \pi(y) = x\} = (\pi_{|C})^{-1}(x).$$

3. Instantaneous nonholonomic constraints

Let N be a hypersurface in M. Consider the induced hypersurface $T^*_N M = \pi^{-1}(N)$ of T^*M. Let $C \subset T^*M$ be a set of nonholonomic constraints on M. Instantaneous constraints may be thought as limitations on the momenta (respectively, velocities) of the system that are imposed only at the instant when a trajectory passes through a point of N. Therefore, they are represented by a submanifold C^{inst} of $C \cap T^*_N M$. These constraints are assumed to be additional to the ones already prescribed by C. In order to admit an adequate mechanical interpretation, we also assume that the projection π restricted to C^{inst} is a submersion onto N. From the Lagrangian point of view, instantaneous kinematic constraints are naturally interpreted as a submanifold $C^{\text{inst}'}$ of TN. Based on these considerations, we take the following definition.

Definition 2.3: Let (M,H,C) *be a constrained Hamiltonian system and let N be a hypersurface of M. A set of* instantaneous constraints along *N imposed on* (M,H,C) *is a submanifold* C^{inst} *of* $C \cap T^*_N M$ *such that* π *restricted to* C^{inst} *is a submersion onto N.*

It is worth stressing that, in some cases, a set of instantaneous constraints along N additionally verifies the condition $C^{\text{inst}} \subset \alpha_H^{-1}(TN)$ (here TN is thought to be naturally embedded into TM). In an inelastic scenario, where the nonholonomic motion in M is forced to take place in N after the impact, this latter condition formalizes the parity between the Hamiltonian and Lagrangian approaches: if the Hamiltonian system in question comes from a Lagrangian one, then $C^{\text{inst}} = \mathcal{L}_L(C^{\text{inst}'})$, with $C^{\text{inst}'}$ being the instantaneous kinematic constraints.

B. Dynamics of Hamiltonian systems

As is well known, in the absence of constraints, the dynamics of the Hamiltonian system (M,H) is given by the Hamiltonian vector field X_H, whose coordinate description is

$$\frac{\mathrm{d}q^a}{\mathrm{d}t} = \frac{\partial H}{\partial p_a}, \quad \frac{\mathrm{d}p_a}{\mathrm{d}t} = -\frac{\partial H}{\partial q^a}, \quad a = 1, \ldots, n.$$

In the presence of constraints, the "free" Hamiltonian vector field X_H must be modified along the constraint manifold C in order to become tangent to C. In the traditional approach this goal is achieved by adding to X_H another vector field along C, say, R, interpreted as the *reaction of constraints*. From a purely geometrical point of view, the choice of a vector field that makes X_H tangent to C is far from being unique. Therefore, a new principle must be invoked to select the one that merits being called the "reaction of constraints." The history of this problem (see, for instance, Ref. 30) shows that its solution is not straightforward. By applying, for instance, the Lagrange-d'Alembert principle (see Refs. 4, 15, and 30), one gets the following equations of motion:

$$\frac{\mathrm{d}q^a}{\mathrm{d}t} = \frac{\partial H}{\partial p_a}, \quad \frac{\mathrm{d}p_a}{\mathrm{d}t} = -\frac{\partial H}{\partial q^a} + \lambda_i \frac{\partial \Phi_i}{\partial p_a}, \quad \Phi_i(q^a, p_a) = 0,$$

$a=1,\ldots,n$, $i=1,\ldots,m$, where the "Lagrange multipliers" λ_i's are to be duly determined. Shortcomings of such an approach are that it is not manifestly intrinsic and does not reveal clearly the geometric background of the situation. This is why in our further exposition we shall follow a purely geometric approach, which does not require any discussion of reactions of constraints. It is

based on the concept of *partial symplectic formalism*, which also appears to be more concise from an algorithmic point of view.

C. Partial symplectic structures

The following elementary facts from linear algebra will be most useful. Let V be a vector space, $W\subset V$ a subspace and $b:V\times V\to\mathbb{R}$ a bilinear form on V. Denote by $W_b^\perp$ the b-orthogonal complement of W,

$$W_b^\perp=\{v\in V|b(v,w)=0,\ \forall\, w\in W\}.$$

Note that $W\cap W_b^\perp=0$ if and only if the restriction $b|_W$ of b to W is nondegenerate. The form b is said to be *nondegenerate* on an affine subspace U of V, $U=p_0+W$, $p_0\in V$, if it is nondegenerate on its associated vector space W. In such a case, U can be uniquely represented in the form $U=p_1+W$ with $p_1\in W_b^\perp$ due to the fact that $U\cap W_b^\perp=\{p_1\}$. The vector p_1 is called the *canonical displacement* of U with respect to b. Consider the associated map

$$\mathsf{T}_{W,b}:W\to W^*,\quad \mathsf{T}_{W,b}(w)=b(w,\cdot),\quad w\in W.$$

In other words, $\mathsf{T}_{W,b}(w)(w')=b(w,w')$, for all $w'\in W$. Obviously, $\mathsf{T}_{W,b}$ is an isomorphism if and only if $b|_W$ is nondegenerate.

If b is skew-symmetric and nondegenerate on V, and W is a subspace of V with codimension one, then the kernel of the restricted form $b|_W$, $\ker\, b|_W$ is a one-dimensional subspace, i.e., a *line* in V contained in W. Therefore, $\ker\, b|_W=W_b^\perp$.

Let now Δ be an affine distribution on a manifold Q. A form $\omega\in\Lambda^2(Q)$ is called *nondegenerate* on Δ if $b=\omega_x$ is nondegenerate on $U=\Delta_x$, for all $x\in Q$. In such a case, there exists a unique vector field $Y\in D(Q)$ such that Y_x is the canonical displacement of Δ_x with respect to ω_x, for all $x\in Q$. The vector field $Y=Y_{\Delta,\omega}$ is called the *canonical displacement* of Δ with respect to ω. If $\omega\in\Lambda^2(Q)$ is nondegenerate on Δ, then one has the isomorphism of vector bundles

$$\gamma=\gamma_{\Delta^0,\omega}:\Delta^{0*}\to\Delta^0,\quad \gamma_x=-(\mathsf{T}_{\Delta^0_x,\omega_x})^{-1}:\Delta^{0*}_x\to\Delta^0_x.$$

Passing to sections of these bundles, one gets the isomorphism of $C^\infty(Q)$-modules $\Gamma_{\Delta^0,\omega}:\Lambda^1_{\Delta^0}(Q)\to D_{\Delta^0}(Q)$ defined by

$$\Gamma=\Gamma_{\Delta^0,\omega}(\varrho)(x)=\gamma(\varrho(x)),\quad \varrho\in\Lambda^1_{\Delta^0}(Q). \tag{1}$$

Definition 2.4: A partial symplectic structure *on a manifold Q is a pair (Δ,ω) consisting of an affine distribution Δ on Q and a closed 2-form $\omega\in\Lambda^2(Q)$ which is nondegenerate on Δ.*

Given a partial symplectic structure $\Theta=(\Delta,\omega)$, we will use the subscript Θ to denote the associated objects: $\Delta_\Theta=\Delta$, $\omega_\Theta=\omega$, $Y_\Theta=Y_{\Delta,\omega}$, and Δ^0_Θ for the distribution canonically associated to Δ. We also write

$$r_\Theta=r_{\Delta^0_\Theta},\quad D_\Theta=D_{\Delta^0_\Theta}(Q),\quad \Lambda^1_\Theta=\Lambda^1_{\Delta^0_\Theta}(Q),\quad \Gamma_\Theta=\Gamma_{\Delta^0_\Theta,\omega}:\Lambda^1_\Theta\to D_\Theta.$$

In the partial symplectic formalism, the elements of $C^\infty(Q)$-modules D_Θ and Λ^1_Θ may be viewed as "constrained" vector fields and differential forms, respectively. The *constrained Hamiltonian vector field* associated with a Hamiltonian function $H\in C^\infty(Q)$ is defined as

$$X^\Theta_H=\Gamma_\Theta(r_\Theta(dH))+Y_\Theta. \tag{2}$$

The *almost-Poisson* bracket associated to the partial symplectic structure Θ is

$$\{f,g\}_\Theta=\Gamma_\Theta(r_\Theta(df))(g)=X^\Theta_f-Y_\Theta(g),\quad f,g\in C^\infty(Q).$$

The wording "almost" here refers to the fact that this bracket does not satisfy in general the Jacobi identity. However, it is still skew-symmetric and a bi-derivation.

Definition 2.5: Let $\Theta=(\Delta,\omega)$ *be a partial symplectic structure on a manifold* Q. *A hypersurface* $B\subset Q$ *is* transversal *to* Θ (*or to* Δ) *if the affine subspaces* T_yB *and* Δ_y *of* T_yQ *are transversal for any* $y\in C$.

If B is *transversal* to Θ, then $T_yB\cap\Delta_y$ is of codimension 1 in Δ_y. If Θ is a partial symplectic structure on $C\subset T^*M$, we shall extend this terminology by saying that Θ is *transversal* to a hypersurface $\tilde{B}$ in T^*M if $\tilde{B}$ is transversal to C, so that $B=\tilde{B}\cap C$ is a hypersurface in C, and B is transversal to Θ.

III. DYNAMICS OF NONHOLONOMIC HAMILTONIAN SYSTEMS

In this section, we formulate the dynamics of nonholonomic Hamiltonian systems using the partial symplectic formalism. We show how, under some technical conditions, any Hamiltonian system subject to nonholonomic constraints possesses an associated partial symplectic structure. Then, we analyze the cases of systems with instantaneous nonholonomic constraints, and systems exhibiting discontinuities.

A. The partial symplectic structure associated with a constrained Hamiltonian system

Let (M,H,C) be a constrained Hamiltonian system. Our goal is to associate with it a partial symplectic structure Θ on the "constrained" cotangent bundle C in such a way the corresponding constrained Hamiltonian field X_H^Θ gives the desired nonholonomic dynamics. With this purpose, consider the *constrained symplectic form* defined by the restriction of the "free" symplectic form Ω_M to C,

$$\omega_\Theta=j^*(\Omega_M), \tag{3}$$

with $j:C\hookrightarrow T^*M$ the canonical inclusion. The next step is to construct a suitable affine distribution Δ_Θ on C. A natural nonsingularity requirement on C is asking for the regularity of the map $\alpha_H|_C$. This is the reason why we assume that $\alpha_H|_C$ is an immersion, i.e., that the differential $d_y\alpha_H$ is nonsingular for any $y\in C$. Since $\alpha_H:T^*M\to TM$ is fibered, this assumption implies that the map $(\alpha_H)_x:C_x\to TM$ is an immersion for any $x\in M$ and vice versa.

Let $y\in C$ and $x=\pi(y)$. Let Π_y be the affine subspace of T_xM tangent to $\alpha_H(C_x)$ at $z=\alpha_H(y)$. Since by the above assumption $\alpha_H|_C$ is an immersion, $\dim\Pi_y=\dim C_x=n-m$. Consider the affine distribution Δ_Θ on C defined by

$$\Delta_{\Theta y}=\{\xi\in T_yC|d_y\pi(\xi)\in\Pi_y\}\subset T_yC. \tag{4}$$

Since $d_y(\pi|_C)$ is surjective, the codimension of Δ_{Θ_y} in T_yC is equal to the codimension of Π_y in T_xM, i.e., to m. Therefore, $\dim\Delta_{\Theta_y}=2(n-m)$. It is not difficult to see now that if the form ω_Θ is nondegenerate on the distribution Δ_Θ, then $\alpha_H|_C$ is an immersion.

Proposition 3.1: Let $S=(M,H,C)$ *be a constrained Hamiltonian system. Then,* $\alpha_H|_C$ *is an immersion if the pair* $(\Delta_\Theta,\omega_\Theta)$ *defined by Eqs. (3) and (4) is a partial symplectic structure*.

The converse, however, is in general not true. Since the partial symplectic structure associated with $S=(M,H,C)$ is determined by H and C, we will simply denote it by $\Theta(H,C)=(\Delta_{H,C},\omega_C)$.

For most Hamiltonian systems (including those coming from Mechanics), the anti-Legendre map α_H is regular not only when restricted to C, but on the whole space T^*M. If this is the case, and the Hamiltonian system comes from a Lagrangian system, one can indeed show that the condition of ω_Θ being nondegenerate on the distribution Δ_Θ is equivalent to the so-called *compatibility condition*.[3,18] Therefore, Proposition 3.1 establishes a link between the classical partial symplectic formalism introduced in Ref. 6 and more recent approaches as explained, for instance, in Ref. 15. Also note that the class of mechanical systems automatically verifies the compatibility condition, therefore admitting both formulations. Indeed, for mechanical systems, the conditions in Proposition 3.1 are equivalent.

Definition 3.2: A nonholonomic Hamiltonian system *on a manifold* M *is a constrained system*

(M,H,C), $H\in C^\infty(T^*M)$, $C\subset T^*M$ *such that* $\Theta(H,C)=(\Delta_{H,C},\omega_C)$ *is a partial symplectic structure*.

The dynamics of a nonholonomic Hamiltonian system is given by the constrained Hamiltonian vector field X_H^Θ with respect to the partial symplectic structure $\Theta=\Theta(H,C)$ [cf. Eq. (2)]. This vector field will be denoted by $X_{H,C}$. Under regularity of the map α_H, $X_{H,C}$ reads in canonical coordinates

$$X_{H,C}=\frac{\partial H}{\partial p_a}\frac{\partial}{\partial q^a}-\left(\frac{\partial H}{\partial q^a}+\mathcal{C}_{ij}\left(\frac{\partial H}{\partial p_b}\frac{\partial\Phi^j}{\partial q^b}-\frac{\partial H}{\partial q^b}\frac{\partial\Phi^j}{\partial p_b}\right)\frac{\partial\Phi^i}{\partial p_c}\mathcal{H}_{ca}\right)\frac{\partial}{\partial p_a},$$

where the matrices $(\mathcal{H}_{ab})$ and $(\mathcal{C}_{ij})$ are defined by

$$(\mathcal{H}_{ab})=\left(\frac{\partial^2 H}{\partial p_a\partial p_b}\right)^{-1},\quad (\mathcal{C}_{ij})=\left(\frac{\partial\Phi^i}{\partial p_a}\mathcal{H}_{ab}\frac{\partial\Phi^j}{\partial p_b}\right)^{-1}.$$

Observe that the *force of reaction of nonholonomic constraints* (see Sec. II B) in the partial symplectic framework is defined *a posteriori* as the difference between the constrained and the free Hamiltonian vector fields, $X_{H,C}-X_H$. Also, note that the almost-Poisson bracket associated with the partial symplectic structure $\Theta_{H,C}$ coincides with the so-called nonholonomic bracket.[15,11,39]

Transversality: It is convenient to adapt the terminology related to the notion of transversality discussed in Sec. II C to the context of nonholonomic Hamiltonian systems. First, we shall say that a nonholonomic Hamiltonian system $S=(M,H,C)$ is *transversal* to a hypersurface B in T^*M if the underlying partial symplectic structure $\Theta(H,C)$ is transversal to B. Second, if N is a hypersurface in M, we shall say that S is *transversal* to N if S is transversal to the hypersurface T^*_NM. The following result follows from the definition of the partial symplectic structure $\Theta(H,C)$.

Proposition 3.3: A nonholonomic Hamiltonian system (M,H,C) *is transversal to a hypersurface* $N\subset M$ *if and only if* $\Pi_y\subset T_{\pi(y)}M$, *the affine subspace of* $T_{\pi(y)}M$ *tangent to* $\alpha_H(C_{\pi(y)})$ *at* $z=\alpha_H(y)$, *is transversal to* $T_{\pi(y)}N\subset T_{\pi(y)}M$ *for all* $y\in C$.

B. Instantaneous partial symplectic structures

It is intuitive to think that when a trajectory of a Hamiltonian system (M,H,C) crosses a *critical* hypersurface N in the configuration manifold M, its phase space reduces to T^*N. Moreover, it could possibly be subject to additional instantaneous constraints along N. In the language of our approach, this idea is naturally expressed by saying that all such *critical* states constitute a nonholonomic Hamiltonian system on N. Since T^*N is not naturally embedded into T^*M, a realization of this idea is not completely straightforward. What one really needs is a partial symplectic structure on the manifold of instantaneous constraints C^{inst} which, by definition, is a submanifold of T^*M.

Namely, let C^{inst} be a set of instantaneous constraints along N imposed on (M,H,C) (cf. Definition 2.3). Take $y\in C^{\text{inst}}$. Let $x=\pi(y)$ and denote by Π_y^{inst} the affine subspace of $T_xN\subset T_xM$ tangent to $\alpha_H(C_x^{\text{inst}})$ at $\alpha_H(y)$. Consider the 2-form $\omega_{\Theta^{\text{inst}}}$ and the affine distribution $\Delta_{\Theta^{\text{inst}}}$ on C^{inst} defined by

$$\omega_{\Theta^{\text{inst}}}=j^*(\Omega_M),\quad \Delta_{\Theta^{\text{inst}}y}=\{\xi\in T_yC^{\text{inst}}\,|\,d_y\pi(\xi)\in\Pi_y^{\text{inst}}\}\subset T_yC^{\text{inst}},\tag{5}$$

with $j:C^{\text{inst}}\hookrightarrow T^*M$ the canonical inclusion. We then have the following definition.

Definition 3.4: Let (M,H,C) *be a nonholonomic Hamiltonian system and let* C^{inst} *be a set of instantaneous constraints along a hypersurface* $N\subset M$. *The pair* $(\Delta_{\Theta inst},\omega_{\Theta inst})$ *defined by (5) is called the* instantaneous partial symplectic structure along N *if* $\omega_{\Theta inst}$ *is not degenerate on* $\Delta_{\Theta inst}$. *If this is the case*, C^{inst} *is called a* regular *set of instantaneous constraints*.

Note that this structure is defined by H, C^{inst}, and N. To highlight this fact, we denote $\Theta^{\text{inst}}=\Theta^{\text{inst}}(H,C^{\text{inst}},N)$. Accordingly, we denote by $X_{(H,C^{\text{inst}},N)}$ the constrained Hamiltonian vector field $X_{H^{\text{inst}}}^{\Theta^{\text{inst}}}$, with $H^{\text{inst}}=H|_{C^{\text{inst}}}$.

In general, since $C^{\text{inst}} \subset C$ by definition, one has that $\alpha_H|_{C^{\text{inst}}}$ is an immersion. For mechanical systems, this implies that the 2-form $\omega_{\Theta^{\text{inst}}}$ is nondegenerate on $\Delta_{\Theta^{\text{inst}}}$, and therefore any set of instantaneous constraints is regular.

In what follows, we shall only deal with regular instantaneous nonholonomic constraints. A natural class of instantaneous structures arises in the following situation of particular interest. Assume that the nonholonomic Hamiltonian system $S=(M,H,C)$ is transversal to N and that α_H is regular. Then $\alpha_H^{-1}(TN)$ is transversal to C and, hence,

$$C_{(N,H)} = \alpha_H^{-1}(TN) \cap C$$

is a submanifold of codimension 2 in C. Note that $C_{(N,H)}$ is a set of instantaneous nonholonomic constraints on S along N. By construction, the codimension of $\Delta_{N_y} = \Delta_y \cap T_y(C_{(N,H)})$ in Δ_y is also 2 and Ω_y is nondegenerate when restricted to Δ_{N_y}. Therefore, the affine distribution Δ_N and the 2-form $\Omega|_N$ endow $C_{(N,H)}$ with a partial symplectic structure, which is an instantaneous partial symplectic structure along N. We call it the *trace of S on N* and denote it by $S_{(N,H)}$. In the special case $N=\partial M$, we call it the *boundary of S*, and denote it by ∂S, i.e., $\partial S = S_{(\partial M,H)}$. We will denote the constrained Hamiltonian vector field with respect to the trace (respectively, boundary) as $X^{\text{tr}} = X^{\text{tr}}_{(H,C,N)}$ (respectively, $X^{\partial} = X^{\partial}_{(H,C,\partial M)}$).

C. Discontinuous nonholonomic systems

An impulsive behavior of a Hamiltonian system occurs when its trajectory "tries" to go across a *critical* hypersurface N in the configuration space M. In such an instant, the system may be forced to drastically change its constraints, to pass under the control of another Hamiltonian and/or to be eventually subject to additional instantaneous constraints. Such situations may be interpreted as *discontinuities* on both the constraints and the Hamiltonian of the system. Below, we formalize these concepts properly via the notion of cutting-up.

Definition 3.5: Let $N \subset M$ be a hypersurface of M with $N \cap \partial M = \emptyset$. A pair $(\hat{M}, \varsigma)$, $\varsigma: \hat{M} \to M$, is called a cutting-up of M along N *if*

(i) $\hat{N} = \varsigma^{-1}(N) \subset \partial \hat{M}$,

(ii) ς *maps $\hat{M} \backslash \hat{N}$ diffeomorphically onto $M \backslash N$*,

(iii) $\varsigma|_{\hat{N}}: \hat{N} \to N$ *is a double covering of N.*

Note that, by definition, ς is a local diffeomorphism. Cuttings-up for a given N exist and are equivalent one to each other. If N divides M into two parts, say, M_+ and M_-, i.e., $M = M_+ \cup M_-$, $M_+ \cap M_- = N$, then $\hat{M}$ may be viewed as the disjoint union of M_+ and M_-, and ς as the map that matches them together along the common border N. Locally any cutting-up is of this form.

For our purposes, it is important to realize that, if $(\hat{M}, \varsigma)$ is a cutting-up of M along N, then $(T^*\hat{M}, T^*\varsigma)$ is a cutting-up of T^*M along the hypersurface $T^*_N M$. Here, $T^*\varsigma$ denotes the dual of the inverse of the isomorphism $d_z\varsigma: T_z\hat{M} \to T_{\varsigma(z)}M$, for all $z \in \hat{M}$. In the following definition, we introduce the class of Hamiltonian systems we shall be dealing with throughout this paper.

Definition 3.6: Let $N \subset M$ be a hypersurface of M with $N \cap \partial M = \emptyset$ and let $(\hat{M}, \varsigma)$ be a cutting-up of M along N. A nonholonomic Hamiltonian system discontinuous along N, *denoted $S = (M,H,C|N)$, is the direct image with respect to $T^*\varsigma$ of a nonholonomic Hamiltonian system $(\hat{M}, \hat{H}, \hat{C})$. Such system is called* regular *if $(\hat{M}, \hat{H}, \hat{C})$ is transversal to $\hat{N}$.*

A system of instantaneous nonholonomic constraints on S along N *is the direct image with respect to $T^*\varsigma$ of a set of instantaneous constraints $\hat{C}^{inst}$ along $\hat{N}$ on the associated system $\hat{S} = (\hat{M}, \hat{H}, \hat{C}|\hat{N})$. The* trace of S on N *is the direct image with respect to $T^*\varsigma$ of the trace of $\hat{S}$ along $\hat{N}$.*

According to Definition 3.6, $\hat{H}$ is a smooth function on $T^*\hat{M}$ and $\hat{C}$ is a submanifold of $T^*\hat{M}$.

Therefore, the *direct image* of $\hat{H}$ along the matching map $T^*\varsigma: T^*\hat{M} \to T^*M$ may be viewed as a function on T^*M, which is 1-valued and smooth outside of $T^*_N M$ and 2-valued and smooth on $T^*_N M$. We will continue to use the notation H for this function and will refer to it as a *discontinuous Hamiltonian along N*. Similarly, the direct image $C = T^*\varsigma(\hat{C})$ of $\hat{C}$ will be referred to as *discontinuous nonholonomic constraints along N*. Outside of $T^*_N M$, C is a "good" smooth submanifold of T^*M, whose boundary is an immersed submanifold of $T^*_N M$.

The previous discussion becomes particularly simple when N divides M into two parts, M_+ and M_-, as mentioned above. In such a case, $T^*_N M$ also divides T^*M into two parts, T^*M_+ and T^*M_-, whose common boundary is $T^*_N M$. Then, a discontinuous Hamiltonian H along N may be naturally seen as a pair of Hamiltonians, say, H_+ and H_-, defined on T^*M_+ and T^*M_-, respectively. Similarly, a set of discontinuous nonholonomic constraints along N is regarded as a pair of sets of nonholonomic constraints $C_\pm \subset T^*M_\pm$. Since N always divides M locally, this description constitutes a local picture of a discontinuous nonholonomic Hamiltonian system along N.

We will continue to use the notation C^{inst} (respectively, S^{tr}) for instantaneous nonholonomic constraints (respectively, the trace of S) in the case of discontinuous nonholonomic systems. As before, one may interpret C^{inst} as a 2-valued system of instantaneous nonholonomic constraints along N. In the case when N divides M into two parts, we will distinguish between the two branches using the notation $C^{\text{inst}}_\pm$, and write also $X_{(H,C^{\text{inst}}_\pm,N)}$ (respectively, $X^{\text{tr}}_{(H,C_\pm,N)}$).

Remark 3.7: The impulsive behavior of a Hamiltonian system is not necessarily related to some discontinuity. This type of phenomena occurs, for instance, each time that one of its trajectories "strikes" against the boundary ∂M of the configuration space M. Various kinds of collisions, impacts, etc., in mechanical systems are described in this way. Otherwise said, impulsive behavior is characteristic of Hamiltonian systems *with boundary*. Moreover, systems with boundary may be viewed as a "limit" case of discontinuous systems by dropping the requirement $N \cap \partial M = \emptyset$ and choosing $N = \partial M$, $M_- = \emptyset$, $M_+ = M$. This allows a unified approach to both situations.

IV. THE TRANSITION PRINCIPLE

In this section we discuss the formulation of the transition principle for systems subject to nonholonomic constraints. We first introduce the notions of focusing points, constrained characteristics, and in, out and decisive points. The transition principle builds on these elements to prescribe the behavior of the Hamiltonian system when one or more of its ingredients undergoes a drastic change.

A. Focusing points

The following simple linear result will be key for the subsequent discussion.

Lemma 4.1: Let $y \in T^*M$, *and let* W *be an affine subspace in* $T_y(T^*M)$ *such that* Ω_y *is nondegenerate on* W (*hence*, $\dim W = 2l$ *for certain* l) *and* $\dim d_y\pi(W) = l$. *Denote by* $W^0 \subset T_y(T^*M)$ *and* $d_y\pi(W)^0 = d_y\pi(W^0) \subset T_{\pi(y)}M$ *the linear subspaces associated with the affine spaces* W *and* $d_y\pi(W)$, *respectively. Then the affine subspaces* $W^\bullet = y + \text{Ann}(d_y\pi(W)^0)$ *and* $W_\bullet = y + W^0 \cap T_y(T^*_{\pi(y)}M)$ *in* $T^*_{\pi(y)}M$ *passing through* y *are transversal.*

Proof: Since, by hypothesis, $\dim d_y\pi(W) = l$, one has

$$\dim W^0 \cap T_y(T^*_{\pi(y)}M) = l \quad \text{and} \quad \dim d_y\pi(W)^0 = l.$$

Now, the dimension of $\text{Ann}(d_y\pi(W)^0) \subset T^*_{\pi(y)}M$ is $n-l$. Moreover, $W^0 \cap T_y(T^*_{\pi(y)}M)$ is transversal to $\text{Ann}(d_y\pi(W)^0)$ if one identifies the spaces $T^*_{\pi(y)}M$ and $T_y(T^*_{\pi(y)}M)$. The result now follows. ■

Consider now a nonholonomic Hamiltonian system (M, H, C). Let $y \in C$. Denote by $\Delta = \Delta_{(H,C)}$ be the affine distribution of the corresponding partial symplectic structure $\Theta(H, C)$ (cf. Sec. III A). By Definition 3.2, the affine subspace $W = \Delta_y$ satisfies the assumptions of Lemma 4.1 on W [observe that $d_y\pi(W)$ is precisely Π_y in Eq. (4)]. Therefore, the subspace $W^\bullet = \Delta^\bullet_y$ is well defined and we set

$$K_y = K_y(H,C) = \Delta_y^* \subset T^*_{\pi(y)}M.$$

Moreover, it is not difficult to see that the subspace $W_\bullet = (\Delta_y)_\bullet$ is identical to $T_y C_{\pi(y)}$. This shows that K_y is transversal to C at y, and that $\dim K_y = m$. The *crown of the nonholonomic Hamiltonian system* (M,H,C) is the map

$$\kappa = \kappa_{H,C}: C \to A_m(T^*M), \quad y \mapsto K_y,$$

where $A_k(T^*M)$ denotes the manifold whose elements are k-dimensional affine submanifolds contained in the fibers of the cotangent bundle T^*M. One can see that the graph of the crown κ,

$$\mathrm{Graph}(\kappa) = \{(y,v) \in C \times T^*M | v \in K_y\}$$

is a $2n$-dimensional smooth submanifold of $C \times T^*M$. Note that $\mathrm{Graph}(\kappa)$ is a fiber bundle over C with projection

$$p = p_{(H,C)}: \mathrm{Graph}(\kappa) \to C, \quad (y,v) \mapsto y.$$

The fiber over y of this bundle is precisely K_y. Since $y \in K_y$, the map

$$\sigma: C \to \mathrm{Graph}(\kappa), \quad y \mapsto (y,y),$$

is a section of $p_{(H,C)}$. Since the fibers of $p_{(H,C)}$ are affine spaces, the bundle $\mathrm{Graph}(\kappa) \to C$ has a natural vector bundle structure whose zero section is σ. Moreover, this vector bundle is canonically isomorphic to the normal bundle of C in T^*M. This is due to the fact that, for any $y \in C$, the fiber K_y is transversal to C at y. The same argument also guarantees that the map

$$\Xi = \Xi_{(H,C)}: \mathrm{Graph}(\kappa) \to T^*M, \quad (y,v) \mapsto v,$$

induces a diffeomorphism of a neighborhood of the "zero" section $\sigma(C)$ in $\mathrm{Graph}(\kappa)$ onto its image.

Definition 4.2: Let (M,H,C) *be a nonholonomic Hamiltonian system. Given a point* $u \in T^*M$, *its* (H,C)-focusing locus $F_{(H,C)}(u)$ *is the set of all points* $y \in C$ *such that* $u \in K_y$. *In other words*,

$$F_{(H,C)}(u) = p_{(H,C)}(\Xi^{-1}_{(H,C)}(u)) \subset C_{\pi(u)}.$$

A point in $F_{(H,C)}(u)$ *is called* focusing for u.

Standard arguments show that $\Xi_{(H,C)}$ is regular, i.e., of maximal rank $2n$ almost everywhere, that is, with the exception of a closed subset without interior points. Therefore, for a generic point $u \in T^*M$, the subset $\Xi^{-1}_{(H,C)}(u)$ is discrete, and so is $F_{(H,C)}(u)$ as well. Note also that if $u \in C$, then $u \in F_{(H,C)}(u)$.

Remark 4.3: Focusing points can be understood as *nonintegrable* analogs of the notion of *reducing points* considered in Ref. 35 in connection with the transition principle for inelastic collisions.

Remark 4.4: It is worth noticing that the concept of a focusing point also makes sense in the absence of constraints. Obviously, in this case $F_{(H,C)}(u) = \{u\}$. Therefore there is no need to distinguish between the constrained and nonconstrained cases in the statement of the transition principle.

If the constraints are linear, i.e., $C = \Upsilon + C^0$ with C^0 a linear codistribution and $\Upsilon \in \Lambda^1(M)$ (the displacement form), then for each $y \in T^*M$,

$$T^*_{\pi(y)}M = C^0_{\pi(y)} \oplus \mathrm{Ann}(d_y\pi(\Delta_y)),$$

where $\Delta=\Delta_{(H,C)}$. Denote the corresponding projectors by $\mathcal{P}:T^*_{\pi(y)}M \to C^o_{\pi(y)}$ and $\mathcal{Q}:T^*_{\pi(y)}M \to \mathrm{Ann}(d_y\pi(\Delta_y))$. Given $u \in T^*M$, one has that $z \in F_{(H,C)}(u)$ if and only if $z \in C$ and $\mathcal{P}(z)=\mathcal{P}(u)$. Since $z=\mathcal{P}(z)+\mathcal{Q}(z)=\mathcal{P}(u)+\mathcal{Q}(\Upsilon_y)$, one has the following result.

Proposition 4.5: Let (M,H,C) be a nonholonomic Hamiltonian system with linear constraints. Then, for $u \in T^*_yM$, there is a unique focusing point given by $F_{(H,C)}(u)=\{\mathcal{P}(u)+\mathcal{Q}(\Upsilon_y)\}$.

B. Instantaneous focusing points

We will also need an instantaneous version of the notion of a focusing point introduced in the preceding section. For this purpose, it is sufficient to apply the above construction to instantaneous constraints instead of to the "usual" ones. Namely, let C^{inst} be a system of regular instantaneous constraints along N (see Sec. II A 3) and $\Delta^{\mathrm{inst}}=\Delta_{\Theta^{\mathrm{inst}}}$ be the corresponding affine distribution (see Sec. III B). Following the same reasoning as above, the affine subspace $W=\Delta^{\mathrm{inst}}_y \subset T_y(T^*M)$ satisfies the assumptions of Lemma 4.1. Therefore, the affine subspace $K^{\mathrm{inst}}_y=(\Delta^{\mathrm{inst}})^\bullet$ of $T_y(T^*M)$ is well defined, and we have all the ingredients to define the notion of instantaneous crown and instantaneous focusing point of a system subject to instantaneous nonholonomic constraints. For completeness, we state the latter.

Definition 4.6: Let (M,H,C) be a nonholonomic Hamiltonian system and let C^{inst} be a set of instantaneous constraints along a hypersurface $N \subset M$. Given a point $u \in T^*_NM$, its (H,C^{inst},N)-instantaneous focusing locus $F_{(H,C^{\mathrm{inst}},N)}(u)$ *is the set of all points $y \in C^{\mathrm{inst}}$ such that $u \in K^{\mathrm{inst}}_y$. In other words*,

$$F_{(H,C^{\mathrm{inst}},N)}(u) = p_{(H,C^{\mathrm{inst}})}(\Xi^{-1}_{(H,C^{\mathrm{inst}},N)}(u)) \subset C^{\mathrm{inst}}_{\pi(u)}.$$

A point in $F_{(H,C^{\mathrm{inst}},N)}(u)$ is called instantaneous focusing for u.

As before, if the instantaneous nonholonomic constraints are linear $C^{\mathrm{inst}}=\Upsilon^{\mathrm{inst}}+C^{\mathrm{inst}^o}$, then for each $y \in T^*_NM$,

$$T^*_{\pi(y)}M = C^0_{\pi(y)} \oplus \mathrm{Ann}(d_y\pi(\Delta^{\mathrm{inst}}_y)),$$

where $\Delta^{\mathrm{inst}}=\Delta_{(H,C^{\mathrm{inst}},N)}$. Denoting the corresponding projectors by $\mathcal{P}^{\mathrm{inst}}:T^*_{\pi(y)}M \to C^{\mathrm{inst}^o}{}_{\pi(y)}$ and $\mathcal{Q}^{\mathrm{inst}}:T^*_{\pi(y)}M \to \mathrm{Ann}(d_y\pi(\Delta^{\mathrm{inst}}_y))$, one has the following result.

Proposition 4.7: Let (M,H,C) be a nonholonomic Hamiltonian system and let C^{inst} be a set of instantaneous affine constraints along a hypersurface $N \subset M$. Then, for $u \in T^*_yM$, there is a unique instantaneous focusing point given by $F_{(H,C^{\mathrm{inst}},N)}(u)=\{\mathcal{P}^{\mathrm{inst}}(u)+\mathcal{Q}^{\mathrm{inst}}(\Upsilon^{\mathrm{inst}}_y)\}$.

C. Constrained characteristics

Consider then a partial symplectic structure $\Theta=(\Delta,\omega)$ on a manifold C which is transversal to a hypersurface $B \subset C$ (cf. Definition 2.5). Let Δ^0 denote the linear distribution associated with Δ. For each $y \in B$, consider the linear space $V=\Delta^0_y$, the hyperplane $W=\Delta^0_y \cap T_yB$ of V and the nondegenerate skew-symmetric form $b=\omega_y|_{\Delta^0_y}$. The *characteristic direction at $y \in B$* is defined as

$$l_y = l_y(\Theta,B) = \ker\ b|_W = \ker(\omega_y|_{\Delta^0_y \cap T_yB}) \subset \Delta^0_y \cap T_yB.$$

The proof of the following result is straightforward.

Lemma 4.8: Given a partial symplectic structure $\Theta=(\Delta,\omega)$ on a manifold C and a hypersurface $B \subset C$ transversal to it, the distribution $y \mapsto l_y(\Theta,B)$ is one dimensional.

Definition 4.9: Given a partial symplectic structure $\Theta=(\Delta,\omega)$ on C and a hypersurface $B \subset C$ transversal to it, $y \mapsto l_y(\Theta,B)$ is called the characteristic distribution with respect to (Θ,B), *and its integral curves, denoted by ζ, are the* (Θ,B)-characteristics.

We are particularly interested in the case when we have a nonholonomic Hamiltonian system $S=(M,H,C)$, the partial symplectic structure Θ is $\Theta_{H,C}$, N is a hypersurface in M and $\widetilde{B}=T^*_N M$, $B=T^*_N M\cap C$. We will use the terminology $(S|N)$-or $(H,C|N)$-*characteristic* as a substitute for (Θ,B)-characteristic. It should be emphasized that $(H,C|N)$ characteristics are only defined when S is transversal to N (see Sec. III A).

In the absence of constraints, i.e., when $(C=T^*M,\ \omega=\Omega)$ is a symplectic manifold, and Δ is the trivial distribution $y\mapsto T_y C$ on C, the characteristic curves are precisely the characteristics introduced in Ref. 6. We will refer to *nonconstrained characteristics* and *constrained characteristics* when it is necessary to distinguish between the unconstrained and the constrained cases.

Remark 4.10: Just as nonconstrained characteristics play a key role in describing holonomic elastic collisions, and reflection and refraction phenomena of rays of light,[6,34] the constrained characteristics will be fundamental in describing the "elastic part" of nonholonomic impulsive phenomena. What is meant by "elastic part" will become clear in Sec. IV E when describing decisive points.

If the constraints C are affine, then the $(H,C|N)$-characteristics passing through a point $y\in C$, $\pi(y)\in N$, is described in a particularly simple way. Namely, following Proposition 3.3, it is not difficult to see that the $(H,C|N)$-characteristic passing through y is given by

$$\zeta_y = y + C^0_{\pi(y)} \cap \mathrm{Ann}(d_y\alpha_H(C^0)\cap T_{\pi(y)}N),$$

with C^0 being the linear codistribution associated to C. In particular, in the absence of constraints, $C=T^*M$ and the characteristics are straight lines in $T^*_x M$ parallel to $\mathrm{Ann}(T_x N)$, $x\in N$.

D. In, out and trapping points

Here, we first introduce some concepts concerning the behavior of a vector field in a neighborhood of the boundary of its supporting manifold. We then discuss the notions in, out and trapping points.

Let Q be a manifold with boundary and X a vector field on Q. A point $y\in\partial Q$ is called a jth *order in point for* X if there exists a trajectory of X, $\beta:[0,a]\to Q$, $a>0$ such that

$$y=\beta(0) \quad \text{and } \beta(t)\notin\partial Q \quad \text{for } 0<t\leqslant a,$$

and β is jth order tangent to ∂Q at y. A jth *order out point for* X is a jth order in point for $-X$. In the dynamical context we have in mind, in and out points of 0th order are the most important. It is easy to see that $y\in\partial Q$ is a 0th order in point (respectively, out point) for X if the vector X_y is transversal to ∂Q and directed inside (respectively, outside) of Q. A point that lies on a trajectory of X which is entirely contained in ∂Q is called a *trapping point for* X.

Let $\partial Q^j=\partial Q^j(X)$ denote the subset of all points of ∂Q where X is jth order tangent to ∂Q, and $\partial Q^j_>=\partial Q^j_>(X)$ [respectively, $\partial Q^j_<=\partial Q^j_<(X)$] the set of all jth order in points (respectively, out points) for X. Note that $\partial Q^j\supset\partial Q^{j+1}$ and

$$\partial Q^j\setminus(\partial Q^j_>\cup\partial Q^j_<)\subset\partial Q^{j+1}. \tag{6}$$

In a generic situation, ∂Q^j is a submanifold (with singularities) of codimension j in ∂Q, which is divided by ∂Q^{j+1} into two parts, $\partial Q^j_>\setminus\partial Q^{j+1}_>$ and $\partial Q^j_<\setminus\partial Q^{j+1}_<$. An analytical description of the previous discussion is obtained by choosing a smooth function f on Q with $f\geqslant 0$ and $d_z f\neq 0$, for all $z\in\partial Q$ such that $\partial Q=\{f=0\}$ (which always exists locally). Then

$$\partial Q^j=\{z\in Q|f(z)=0,X(f)(z)=0,\ldots,X^j(f)(z)=0\},$$

$$\partial Q^j_>\setminus\partial Q^{j+1}_>=\partial Q^j\cap\{z\in Q|X^{j+1}(f)(z)>0\},$$

$$\partial Q^j_<\setminus\partial Q^{j+1}_<=\partial Q^j\cap\{z\in Q|X^{j+1}(f)(z)<0\}.$$

The vector field X is said to be *regular with respect to* ∂Q when the inclusion in Eq. (6) is an equality for all $j \geqslant 0$. This is a generic property of vector fields. In such a case, the chain of inclusions

$$\partial Q = \partial Q^0 \supset \partial Q^1 \supset \cdots \supset \partial Q^j \supset \cdots \supset \partial Q^n$$

is a *stratification* of ∂Q whose strata are $\partial Q^j_> \setminus \partial Q^{j+1}_>$ and $\partial Q^j_< \setminus \partial Q^{j+1}_<$. Note also that the set of trapping points precisely corresponds to ∂Q^n.

Consider now a discontinuous nonholonomic Hamiltonian system $(M, H, C|N)$ and the corresponding cutting-up $(\hat{M}, \varsigma)$. Then we can resort to the previous discussion with the manifold $Q = \hat{C} \subset T^*\hat{M}$ and the vector field $X = X_{\hat{H},\hat{C}}$. Recall that $\hat{N} \subset \partial \hat{M}$ and $\partial \hat{C} = \hat{C} \cap T^*_{\partial \hat{M}} \hat{M}$.

Definition 4.11: Let $S = (M, H, C|N)$ *be a discontinuous nonholonomic system and denote by* $(\hat{M}, \varsigma)$ *the associated cutting-up. A point* $y \in T^*_N M$ *is called an* in point (*respectively, an* out point) *of* S *if there exists* $z \in T_{\hat{N}}\hat{M}$ *such that* $y = \varsigma(z)$ *and* z *is an in point (respectively, an out point) of* $X_{\hat{H},\hat{C}}$ *with respect to* $\partial \hat{C}$.

By definition, the map $T^*\varsigma$ restricted to $\partial \hat{C}$ is an immersion. A point in $T^*_N M$ may turn out to be an in and an out point at the same time. To resolve this ambiguity, the branch of $T^*\varsigma$ to which such a point belongs must be taken into consideration. This distinction is easily described in the case when N divides M into two parts. In fact, in this case the system $(M, H, C|N)$ may be viewed as a couple of nonholonomic Hamiltonian systems $(M_\pm, H_\pm, C_\pm)$, with the common boundary $\partial M_\pm = N$, and where $H_\pm \in C^\infty(M_\pm)$ and $C_\pm \subset M_\pm$ (cf. Sec. III C). An in (respectively, out, or trapping) point of the vector field X_{H_+,C_+} with respect to the boundary ∂C_+ is called a *plus-in* (respectively, *plus-out*, or *plus-trapping*) *point*. Analogous definitions are established for $\varepsilon = -$. In this way, the notions of plus-in point, minus-in point, etc., introduced in Ref. 6 for the unconstrained situation are generalized to the constrained case. Finally, we observe that N always divides M locally, and therefore the previous discussion is always valid locally.

E. Decisive points

At this point, we are ready to introduce the key notion of decisive point corresponding to an out point. The construction of decisive points depends on two elements: first, the mode (elastic or inelastic) in which the system passes through the critical state and, second, the continuity and differentiability properties of the Hamiltonian. Below, we will limit our discussion to the two most relevant situations, just to avoid not very instructive technicalities arising in the most general context. The first one is the case when the Hamiltonian is smooth and only the constraints are discontinuous along the critical hypersurface. The second one concerns discontinuous Hamiltonians and not necessarily discontinuous constraints. It is worth stressing that the first situation cannot be considered as a particular case of the second one, i.e., that the notion of a decisive point is not "continuous" in this sense. In what follows, $\varepsilon \in \{+, -\}$ and $\bar{\varepsilon}$ stands for the opposite sign to ε. Throughout the section, instantaneous constraints are assumed to be regular.

1. Elastic mode: change of constraints

Here, we deal with a discontinuous nonholonomic system $(M, H, C|N)$, where the Hamiltonian function is smooth, $H \in C^\infty(M)$.

Definition 4.12 (Decisive points for smooth Hamiltonians and discontinuous constraints): Let $(M, H, C|N)$ *be a regular discontinuous nonholonomic system, with* $H \in C^\infty(M)$ *and consider a set of instantaneous constraints* C^{inst} *along* N. *Let* y *be an* ε*-out point of the system. A sequence* (y_i, ε_i), $i = 0, 1, \ldots, k$, *with* $y_i \in C \cap T^*_N M$ *is called* (y, ε)-admissible*if it verifies the following conditions:*

(i) $(y_0,\varepsilon_0)=(y,\varepsilon)$,
(ii) *for all* $i<k$, y_{i+1} *is a focusing point for* y_i *with respect to either* $C^{inst}_{\varepsilon_{i+1}}$ *or, if instantaneous constraints are absent,* $C_{\varepsilon_{i+1}}$,
(iii) y_i *is an* ε_i*-out point for all* $i<k$ *and* y_k *is either an* ε_k*-in point or an* ε_k*-trapping point*,
(iv) *the sequence of signs* $\{\varepsilon_i\}$ *alternates, i.e.,* $\varepsilon_{i+1}=\bar{\varepsilon}_i$.

The endpoint of an (y,ε)*-admissible sequence,* (y_k,ε_k), *is called* (y,ε)-decisive *and the constrained Hamiltonian vector field* $X_{H,C_{\varepsilon_k}}$ *is referred to as the vector field* corresponding *to it*.

Remark 4.13: The above formal description of decisive points is equivalent to the following iterative procedure. Take, for instance, a plus-out point y. Then, according to Definition 4.12, all focusing with respect to $C^{\text{inst}}_{\bar{\varepsilon}}$ (respectively, to $C_{\bar{\varepsilon}}$) minus-in and minus-trapping points are decisive. On the other hand, the procedure continues by restarting from any of the remaining focusing points that are minus-out points, and so on. In some situations, this process may turn out to be infinite. At the present time, however, it is not clear whether that kind of phenomena can occur, say in propagation of singularities or similar processes.

2. Elastic mode: discontinuous Hamiltonians

In this case, decisive points are constructed on the basis of an iterative procedure whose single steps are either of *reflective* or of *refractive* type, as described below. Consider a regular discontinuous noholonomic system $S=(M,H,C|N)$, which might be subject to additional instantaneous constraints C^{inst} along N. Let $y\in C\cap T^*_NM$ be an ε-out point.

Reflective step:

First move: $y\Rightarrow z$, where z is a point in the constrained characteristic $\zeta_y(H_\varepsilon,C_\varepsilon)$ such that $H_\varepsilon(z)=H_\varepsilon(y)$.

Second move: $z\Rightarrow u$, where u is a focusing point for z with respect to either $C^{\text{inst}}_\varepsilon$ or, if ε-instantaneous constraints are absent, C_ε.

Refractive step:

First move: $y\Rightarrow z$, where z is a point of the constrained characteristic $\zeta_y(H_\varepsilon,C_\varepsilon)$ and such that $H_{\bar{\varepsilon}}(z)=H_\varepsilon(y)$.

Second move: $z\Rightarrow u$, where u is a focusing point for z with respect to either $C^{\text{inst}}_{\bar{\varepsilon}}$ or, if $\bar{\varepsilon}$-instantaneous constraints are absent, $C_{\bar{\varepsilon}}$.

With a slight abuse of language, we shall say that (y,ε) is the *initial point of the step* and (u,ε) [respectively, $(u,\bar{\varepsilon})$] is the *endpoint of the step* if the scenario is reflective (respectively, refractive).

Definition 4.14 (Decisive points for discontinuous Hamiltonians): Consider a regular discontinuous nonholonomic system $(M,H,C|N)$. *Let* C^{inst} *be a set of instantaneous constraints along* N. *Let* y *be an* ε*-out point. A sequence* (y_i,ε_i), $i=0,1,\ldots,k$, *is called* (y,ε)-admissible *if*

(i) $(y_0,\varepsilon_0)=(y,\varepsilon)$,
(ii) (y_i,ε_i) *and* $(y_{i+1},\varepsilon_{i+1})$ *are the initial and the endpoints of a step, respectively*,
(iii) y_i *is an* ε_i*-out point,* $0\leqslant i<k$, *and* y_k *is an* ε_k*-in point or an* ε_k*-trapping point*.

The endpoint (y_k,ε_k) *of an admissible sequence is called* (y,ε)*-decisive and the constrained Hamiltonian vector field* $X_{H,C_{\varepsilon_k}}$ *is referred to as the vector field* corresponding *to it*.

If the Hamiltonian is discontinuous and the constraints are linear, i.e., $C\subset T^*M$ is a smooth linear submanifold, and the instantaneous constraints are absent, the previous definition of decisive points becomes much simpler, as the following result shows.

Proposition 4.15: Let $(M,H,C|N)$ *be a regular discontinuous nonholonomic Hamiltonian system with smooth linear constraints. Let* y *be an* ε*-out point. The* (y,ε)-decisive *points are the in and the trapping points belonging to the intersection of the constrained characteristic* ζ_y *passing through* y *with the set* $\{z\in C|H_\pm(z)=H_\varepsilon(y)\}$.

Proof: Let y be an ε-out point and denote by $\{z_1,\ldots,z_s\}$ (respectively, $\{\bar{z}_1,\ldots,\bar{z}_{\bar{s}}\}$) the points belonging to the intersection of the constrained characteristic ζ_y passing through y with the set

$\{z \in C | H_\varepsilon(z) = H_\varepsilon(y)\}$ [respectively, with $\{z \in C | H_{\bar{\varepsilon}}(z) = H_\varepsilon(y)\}$]. Since the constraints are smooth, then $u = z$ in the second move of both a reflective and a refractive step. Now, for any $j \in \{1, \ldots, s\}$, the intersection of the constrained characteristic passing ζ_{z_j} through z_j with the set $\{z \in C | H_\varepsilon(z) = H_\varepsilon(z_j)\}$ (respectively, with $\{z \in C | H_{\bar{\varepsilon}}(z) = H_\varepsilon(y)\}$) is again $\{z_1, \ldots, z_s\}$ (respectively, $\{\bar{z}_1, \ldots, \bar{z}_{\bar{s}}\}$). The same observation holds for any $\bar{z}_j$, $j \in \{1, \ldots, \bar{s}\}$. The result now follows from Definition 4.14. ■

Remark 4.16: The introduced terminology remains valid for nonholonomic systems with boundary (cf. Remark 3.7). In such a case, one must formally set

$$M_- = \emptyset, \quad M_+ = M, \quad N = \partial M, \quad H_- = \infty, \quad H_+ = H.$$

This type of geometric data occurs in describing various collision phenomena.

3. Inelastic mode: change of constraints

As in the elastic case, we first deal with the case when the Hamiltonian H is smooth. We treat an inelastic behavior of the system as the passage under the control of either the instantaneous discontinuous nonholonomic system or, if instantaneous constraints are absent, the discontinuous boundary system. In this and subsequent sections, the following shorthand notation will be used (cf. Secs. III B and III C):

$$C_\varepsilon^{\mathrm{inst,tr}} = C_\varepsilon^{\mathrm{inst}} \cap \alpha_{H_\varepsilon}^{-1}(TN), \quad X_\varepsilon^{\mathrm{inst,tr}} = X_{(H_\varepsilon, C_\varepsilon^{\mathrm{inst,tr}}, N)},$$

$$C_\varepsilon^{\mathrm{tr}} = C_{\varepsilon(N,H_\varepsilon)}, \quad X_\varepsilon^{\mathrm{tr}} = X_{(H_\varepsilon, C_\varepsilon, N)}^{\mathrm{tr}}.$$

We also use this notation when the Hamiltonian H is smooth, i.e., $H_\pm = H$.

Definition 4.17 (Decisive points for smooth Hamiltonians and discontinuous constraints): Consider a regular discontinuous nonholonomic system $(M, H, C|N)$. Let C^{inst} be a set of instantaneous constraints along N. Let y be an ε-out point. An (y, ε)-decisive point *is a focusing point for y with respect to either $C_\varepsilon^{inst,tr}$ or, if the instantaneous constraints are absent, $C_{\bar{\varepsilon}}^{tr}$. The constrained Hamiltonian vector field $X_{\bar{\varepsilon}}^{inst,tr}$, respectively, $X_{\bar{\varepsilon}}^{tr}$ is referred to as the* corresponding *vector field.*

4. Inelastic mode: discontinuous Hamiltonians

As in the elastic case, decisive points are constructed on the basis of *reflective* or *refractive* steps, as we now describe.

Reflected falling step:

First move: $y \Rightarrow z$, where z is a point of the constrained characteristic $\zeta_y(H_\varepsilon, C_\varepsilon)$ such that $H_\varepsilon(z) = H_\varepsilon(y)$.

Second move: $z \Rightarrow u$, where u is a focusing point for z with respect to either $C_\varepsilon^{\mathrm{inst,tr}}$ or, if ε-instantaneous constraints are absent, $C_\varepsilon^{\mathrm{tr}}$.

Refracted falling step:

First move: $y \Rightarrow z$, where z is a point of the constrained characteristic $\zeta_y(H_\varepsilon, C_\varepsilon)$ such that $H_{\bar{\varepsilon}}(z) = H_\varepsilon(y)$.

Second move: $z \Rightarrow u$, where u is a focusing point for z with respect to $C_{\bar{\varepsilon}}^{\mathrm{inst,tr}}$ or, if $\bar{\varepsilon}$-instantaneous constraints are absent, $C_{\bar{\varepsilon}}^{\mathrm{tr}}$.

We shall refer to (u, ε) [respectively, $(u, \bar{\varepsilon})$] as a *reflected* (respectively, *refracted*) *falling point*.

Definition 4.18 (Decisive points for discontinuous Hamiltonians): Consider a regular discontinuous nonholonomic system $(M, H, C|N)$. Let C^{inst} be a set of instantaneous constraints along N. Let y be an ε-out point. An (y, ε)-decisive *point is a falling point for y. The vector field $X_\varepsilon^{inst,tr}$ (respectively, $X_\varepsilon^{\mathrm{tr}}$ if $C_\varepsilon^{inst} = \emptyset$) is called the vector field* corresponding *to a reflected falling point. The vector field $X_\varepsilon^{inst,tr}$ (respectively, $X_{\bar{\varepsilon}}^{tr}$ if $C_\varepsilon^{inst} = \emptyset$) is called the vector field* corresponding *to a refracted falling point*.

F. Transition principle

From a physical point of view, the transition principle formulated below is an explicit description of the discontinuity of a trajectory of a regular nonholonomic Hamiltonian system S that occurs when it traverses a *critical state*. Such a discontinuity is interpreted as an impact, collision, reflection, refraction, etc., depending on the physical situation modeled by the system S. From a mathematical point of view, the transition principle corresponds to the definition of the trajectory of a regular discontinuous nonholonomic Hamiltonian system.

The elastic or inelastic character of the impulsive motions of an specific physical system must be taken into account when defining the trajectories. Accordingly, there are two different versions of the transition principle that distinguish between the two situations. Let $S=(M,H,C|N)$ stand for a regular discontinuous nonholonomic system and let C^{inst} be eventual instantaneous constraints imposed on S along N. Let $(\hat{M},\varsigma)$ be the associated cutting-up of M along N (cf. Sec. III C). The *regular part of a trajectory of the system* $\hat{S}=(\hat{M},\hat{H},\hat{C})$ is the part of the trajectory of the Hamiltonian vector field $X_{\hat{H},\hat{C}}$ that lies outside $\partial\hat{M}$. The *regular part of a trajectory of* S is the image by ς of the regular part of the corresponding trajectory of $\hat{S}$. At least locally, the regular part may be viewed as a piece of the trajectory of the vector field $X_{H_\varepsilon,C_\varepsilon}$ that lies outside the hypersurface T^*_NM.

Transition principle: Let $S=(M,H,C|N)$ *be a regular discontinuous nonholonomic system and let* C^{inst} *be eventual instantaneous constraints on* S *along* N. *If a regular trajectory of the vector field* $X_{H_\varepsilon,C_\varepsilon}$, $\varepsilon=\pm$ *reaches the critical hypersurface* T_NM *at a point* y, *it then continues its motion from any* (y,ε)*-decisive point according to the chosen mode, elastic or inelastic, under the control of the corresponding constrained Hamiltonian vector field.*

Some features of the transition principle are worth mentioning. First of all, it prescribes a *splitting of the trajectory* when the number of decisive points is greater than one. Of course, it is difficult to imagine that a true mechanical system "goes into pieces" when reaching the critical hypersurface. But it may perfectly happen when a Hamiltonian system describes the propagation of singularities in a field or a continuum media. A classical example one finds in geometrical optics when a light ray passing from one optic medium to another splits into reflected and refracted rays (see, for instance, Ref. 34). The trajectory may also be *trapped* by the critical hypersurface. This happens when an "impact" state y possesses no y-decisive points.

V. MECHANICAL SYSTEMS

In this section, we particularize the preceding discussion to mechanical systems subject to affine constraints. Let g be a Riemannian metric on M and $V\in C^\infty(M)$, and consider the mechanical system whose kinetic energy and potential function are $T(q,v)=\frac{1}{2}g(v,v)$ and V, respectively. The corresponding Lagrangian function is $L(q,v)=T(q,v)-V(q)$ and the Hamiltonian one is

$$H(q,p)=\hat{T}(q,p)+V(q), \tag{7}$$

where $\hat{T}(q,p)=\frac{1}{2}\mathcal{G}(p,p)$, and $\mathcal{G}$ is the cometric, i.e., the metric on the cotangent bundle induced by g. In a local chart q^a on M, the local expressions of g and $\mathcal{G}$ are

$$g=g_{ab}\,\mathrm{d}q^a\otimes\mathrm{d}q^b,\quad \mathcal{G}=g^{ab}\frac{\partial}{\partial q^a}\otimes\frac{\partial}{\partial q^b}.$$

In the mechanical case, the Legendre transform $\mathcal{L}_L:TM\to T^*M$ is a linear bundle mapping whose local description is $\mathcal{L}_L(q^a,\dot{q}^a)=(q^a,g_{ab}\dot{q}^b)$.

Consider an affine distribution $C=C^0+Y$ in T^*M determining some nonholonomic constraints on the system (M,H). The linearity of $\alpha_H=\mathcal{L}_L^{-1}$ implies that the space $\alpha_H(C)=\alpha_H(C^0)+\alpha_H(Y)$ is a distribution of affine spaces on M, or otherwise said, that $\alpha_H(C^0)$ is a linear distribution on M. Throughout this section, we will often resort to the shorthand notation $\mathcal{D}=\alpha_H(C^0)$ and $\Upsilon=\alpha_H(Y)$. Now, it is easy to verify that $T^*_qM=C^0_q\oplus\mathrm{Ann}(\mathcal{D})_q$, with associated projectors

$$\mathcal{P}_q : T_q^*M \to C_q^0, \quad \mathcal{Q}_q : T_q^*M \to \mathrm{Ann}(\mathcal{D})_q, \quad q \in M.$$

Let $\mu_1 = \mu_{1\alpha}\,\mathrm{d}q^a, \ldots, \mu_m = \mu_{ma}\,\mathrm{d}q^a$ be 1-forms such that (locally) $\mathrm{Ann}(\mathcal{D}) = \mathrm{span}\{\mu_1, \ldots, \mu_m\}$. Define the local function $\mu_{i0} : M \to \mathbb{R}$ by $\mu_{i0}(q) = -\mu_i(\Upsilon(q))$. Then $\alpha_H(C)$ is locally defined by the equations

$$\mu_{ia}(q)\dot{q}^a + \mu_{i0}(q) = 0, \quad 1 \leqslant i \leqslant m.$$

Now, consider the matrices

$$G = (g_{ab}), \quad J = (\mu_{ia}), \quad \mathcal{B} = JG^{-1}J^t. \tag{8}$$

From the discussion after Proposition 3.1, recall that $(\Delta_{H,C}, \omega_C)$ is a partial symplectic structure if and only if $\alpha_H|_C$ is an immersion, or, equivalently, if the compatibility condition is verified. Following Ref. 12, the latter is equivalent to the matrix $\mathcal{B}$ being invertible. A direct computation gives the following local expression for the projectors $\mathcal{P}$ and $\mathcal{Q}$:

$$\mathcal{P}(x) = x - \mathcal{Q}(x), \quad \mathcal{Q}(x) = J^t\mathcal{B}^{-1}JG^{-1}x, \quad x \in T^*M.$$

Finally, let $N \subset M$ be a hypersurface and assume that the nonholonomic system $S = (M, H, C)$ is transversal to N. Consider also a set of instantaneous nonholonomic linear constraints $C^{\mathrm{inst}} = (C^{\mathrm{inst}^o}, \Upsilon_{C^{\mathrm{inst}}})$ imposed on S along N. Note that $T_q^*M = C_q^{\mathrm{inst}^o} \oplus \mathrm{Ann}(\mathcal{D}^{\mathrm{inst}})_q$, with associated projectors

$$\mathcal{P}_q^{\mathrm{inst}} : T_q^*M \to C_q^{\mathrm{inst}^o}, \quad \mathcal{Q}_q^{\mathrm{inst}} : T_q^*M \to \mathrm{Ann}(\mathcal{D}^{\mathrm{inst}})_q, \quad q \in N.$$

A. Focusing points

Since the mechanical system is subject to an affine distribution of constraints, Proposition 4.5 implies that for a given $u \in T^*M$, the focusing locus is $F_{(H,C)}(u) = \{\mathcal{P}(u) + \mathcal{Q}(\Upsilon)\}$. Regarding the instantaneous focusing points, according to Proposition 4.7 one has that $F_{(H,C^{\mathrm{inst}},N)}(u) = \{\mathcal{P}^{\mathrm{inst}}(u) + \mathcal{Q}^{\mathrm{inst}}(\Upsilon_{C^{\mathrm{inst}}})\}$.

B. Constrained characteristics

Here we give an explicit description of the characteristic curves. Let N be the critical hypersurface, and assume that (locally) $N = f^{-1}(0)$, with $f \in C^\infty(M)$ verifying that $d_q f \neq 0$ for all $q \in N$. Consider the convector field $\mathcal{P}(\mathrm{d}f)$ along N defined as $q \mapsto \mathcal{P}(\mathrm{d}f)_q = \mathcal{P}_q(d_q f)$, $q \in N$. The transversality assumption between C and N implies that $\mathcal{P}(\mathrm{d}f)_q \neq 0$, for all $q \in N$. Clearly $\mathcal{P}(\mathrm{d}f) \in C^0$. In addition, for $v \in \mathcal{D} \cap TN$,

$$\mathcal{P}(\mathrm{d}f)(v) = (\mathrm{d}f - \mathcal{Q}(\mathrm{d}f))(v) = \mathrm{d}f(v) = 0,$$

and one can conclude that $C^0 \cap \mathrm{Ann}(\mathcal{D} \cap TN) = \mathrm{span}\{\mathcal{P}(\mathrm{d}f)\}$. Therefore, we have the following result.

Lemma 5.1: The constrained characteristic of a mechanical system $(M, H, C|N)$ passing through $y \in C \cap T_N^*M$ is given by $\zeta_y = y + \mathrm{span}\{\mathcal{P}(d_{\pi(y)}f)\} \subset C \cap T_N^*M$.

Note that in the absence of constraints one recovers the standard nonconstrained characteristic $\zeta_y = y + \mathrm{span}\{d_{\pi(y)}f\}$ passing through y.

C. Decisive points: elastic mode

1. Change of constraints

Let $C_\pm \subset T^*M$ be two affine constraint submanifolds. Denote by $\mathcal{P}_\pm$ and $\mathcal{Q}_\pm$ the projectors corresponding to $C_\pm$ and the cometric $\mathcal{G}$. Let $y \in C_\varepsilon \cap T_N^*M$ be a ε-out point, $\varepsilon \in \{+, -\}$. Then,

according to Definition 4.12, an y-admissible sequence, (y_i,ε_i), $i=0,1,\ldots,k$, is necessarily of the form $y_{i+1}=\mathcal{P}_{\varepsilon_{i+1}}(y_i)+\mathcal{Q}_{\varepsilon_{i+1}}(\Upsilon_{C_{\varepsilon_{i+1}}})$. If instantaneous constraints are present, then one must use the projectors $\mathcal{P}_\varepsilon^{\text{inst}}$ and $\mathcal{Q}_\varepsilon^{\text{inst}}$ instead of $\mathcal{P}_\varepsilon$ and $\mathcal{Q}_\varepsilon$, respectively.

Remark 5.2: Mechanical systems subject to generalized constraints are also treated in Ref. 16 in a somehow different context. The approach taken there makes use of generalized (i.e., nonconstant rank) codistributions defining the nonholonomic constraints and a generalized version of Newton's second law. Under appropriate regularity conditions, it can be seen that the post-impact point in Ref. 16 is a decisive point of the Hamiltonian system according to Definition 4.12.

2. Discontinuous Hamiltonian systems

Let $C_\pm\subset T^*M$ be two affine constraint submanifolds. Let $g_\pm$ be a Riemannian metric on $M_\pm$ and $V_\pm\in C^\infty(M_\pm)$ such that

$$H_\pm(q,p)=\hat{T}_\pm(q,p)+V_\pm(q),\quad \hat{T}_\pm(q,p)=\tfrac{1}{2}\mathcal{G}_\pm(p,p). \tag{9}$$

For simplicity, we only treat the case $V_\pm=V|_{M_\pm}$, $V\in C^\infty(M)$. We denote by $\mathcal{P}_\pm$ and $\mathcal{Q}_\pm$ the projectors corresponding to $C_\pm$ and the cometric $\mathcal{G}_\pm$. Additionally, let $C_\pm^{\text{inst}}\subset T_N^*M$ be affine constraint submanifolds corresponding to some instantaneous constraints imposed along N. Denote by $\mathcal{P}_\pm^{\text{inst}}$ and $\mathcal{Q}_\pm^{\text{inst}}$ the projectors corresponding to $C_\pm^{\text{inst}}$ and the cometric $\mathcal{G}_\pm$.

Let $y\in C_\varepsilon\cap T_N^*M$ be an ε-out point. Following Definition 4.14, we first describe the reflective and refractive steps with initial point (y,ε). According to Lemma 5.1, we must look for points of the form

$$x=y+c\mathcal{P}_\varepsilon(d_qf),\quad q=\pi(y),$$

for some c, which in addition belong to the same H-energy level as y.

Reflective step: Concerning the first move, note that $y+c\mathcal{P}_\varepsilon(d_qf)$ and y belong to T_q^*M. Then, the equality $H_\varepsilon(y+c\mathcal{P}_\varepsilon(d_qf))=H_\varepsilon(y)$ implies that $\hat{T}_\varepsilon(y+c\mathcal{P}_\varepsilon(d_qf))=\hat{T}_\varepsilon(y)$. Now,

$$\hat{T}_\varepsilon(y+c\mathcal{P}_\varepsilon(d_qf))=\hat{T}_\varepsilon(y)+c\mathcal{G}_\varepsilon(y,\mathcal{P}_\varepsilon(d_qf))+\frac{c^2}{2}\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(d_qf),\mathcal{P}_\varepsilon(d_qf)),$$

and, therefore, we have

$$c\left(\mathcal{G}_\varepsilon(y,\mathcal{P}_\varepsilon(d_qf))+\frac{c}{2}\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(d_qf),\mathcal{P}_\varepsilon(d_qf))\right)=0,$$

with solutions

$$c_{\varepsilon,1}=0,\quad c_{\varepsilon,2}=-\frac{2\mathcal{G}_\varepsilon(y,\mathcal{P}_\varepsilon(d_qf))}{\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(d_qf),\mathcal{P}_\varepsilon(d_qf))}. \tag{10}$$

An important property of these points is contained in the following lemma.

Lemma 5.3: Let $y\in C_\varepsilon\cap T_N^*M$ and $c_{\varepsilon,2}$ be the constant given by (10). *Then*,

$$\mathcal{G}_\varepsilon(y,d_qf)=\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(y)+\mathcal{Q}_\varepsilon(\Upsilon_q),d_qf),$$

$$\mathcal{G}_\varepsilon(y+c_{\varepsilon,2}\mathcal{P}_\varepsilon(d_qf),d_qf)=\mathcal{G}_\varepsilon(-\mathcal{P}_\varepsilon(y)+\mathcal{Q}_\varepsilon(\Upsilon_q),d_qf).$$

Proof: The first statement follows by noting that if $y\in C_q$, then $y=\mathcal{P}_\varepsilon(y)+\mathcal{Q}_\varepsilon(\Upsilon_q)$. For the second one, notice that

$$\mathcal{G}_\varepsilon(y + c_{\varepsilon,2}\mathcal{P}_\varepsilon(d_q f), d_q f) = \mathcal{G}_\varepsilon(y, d_q f) + c_{\varepsilon,2}\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(d_q f), \mathcal{P}_\varepsilon(d_q f)) = \mathcal{G}_\varepsilon(y, d_q f - 2\mathcal{P}_\varepsilon(d_q f))$$
$$= -\mathcal{G}_\varepsilon(\mathcal{P}_\varepsilon(y), \mathcal{P}_\varepsilon(d_q f)) + \mathcal{G}_\varepsilon(\mathcal{Q}_\varepsilon(y), d_q f) = \mathcal{G}_\varepsilon(-\mathcal{P}_\varepsilon(y) + \mathcal{Q}_\varepsilon(\Upsilon_q), d_q f),$$

which gives the desired result. ■

The second move simply consists of determining the focusing points for points (10) with respect to $C_\varepsilon^{\text{inst}}$ or, if ε instantaneous constraints are absent, with respect to C_ε. This is done in terms of the corresponding projectors, exactly as explained in Sec. V A above.

Refractive step: Concerning the first move, the equality $H_{\bar{\varepsilon}}(y + c\mathcal{P}_\varepsilon(d_q f)) = H_\varepsilon(y)$ implies $\hat{T}_{\bar{\varepsilon}}(y + c\mathcal{P}_\varepsilon(d_q f)) = \hat{T}_\varepsilon(y)$. Now,

$$\hat{T}_{\bar{\varepsilon}}(y + c\mathcal{P}_\varepsilon(d_q f)) = \hat{T}_{\bar{\varepsilon}}(y) + c\mathcal{G}_{\bar{\varepsilon}}(y, \mathcal{P}_\varepsilon(d_q f)) + \frac{c^2}{2}\mathcal{G}_{\bar{\varepsilon}}(\mathcal{P}_\varepsilon(d_q f), \mathcal{P}_\varepsilon(d_q f)).$$

Therefore, one has

$$c\left(\mathcal{G}_{\bar{\varepsilon}}(y, \mathcal{P}_\varepsilon(d_q f)) + \frac{c}{2}\mathcal{G}_{\bar{\varepsilon}}(\mathcal{P}_\varepsilon(d_q f), \mathcal{P}_\varepsilon(d_q f))\right) + \hat{T}_{\bar{\varepsilon}}(y) - \hat{T}_\varepsilon(y) = 0,$$

with solutions $i = 1, 2$,

$$c_{\bar{\varepsilon},i} = \frac{1}{\mathcal{G}_{\bar{\varepsilon}}(\mathcal{P}_\varepsilon(d_q f), \mathcal{P}_\varepsilon(d_q f))}(-\mathcal{G}_{\bar{\varepsilon}}(y, \mathcal{P}_\varepsilon(d_q f))$$
$$\pm \sqrt{\mathcal{G}_{\bar{\varepsilon}}(y, \mathcal{P}_\varepsilon(d_q f))^2 - 2\mathcal{G}_{\bar{\varepsilon}}(\mathcal{P}_\varepsilon(d_q f), \mathcal{P}_\varepsilon(d_q f))(\hat{T}_{\bar{\varepsilon}}(y) - \hat{T}_\varepsilon(y))}). \tag{11}$$

As before, the second move simply consists of computing the focusing points for the solutions (11) with regards to $C_{\bar{\varepsilon}}^{\text{inst}}$ or, if $\bar{\varepsilon}$-instantaneous constraints are absent, $C_{\bar{\varepsilon}}$. This is done in terms of the corresponding projectors according to Sec. V A.

Discontinuous Hamiltonian systems with smooth constraints: In this situation, there is a single constraint submanifold C, and a discontinuous Hamiltonian $H_\pm$ on T^*M. Denote by $\mathcal{P}_\pm$ and $\mathcal{Q}_\pm$ the projectors corresponding to C and the cometrics $\mathcal{G}_\pm$, respectively. According to Proposition 4.15, the decisive points for a given ε-out point $y \in C \cap T_N^*M$ are simply the in and trapping points belonging to the intersection of the constrained characteristic ζ_y passing through y with the set $\{z \in C \,|\, H_\pm(z) = H_\varepsilon(y)\}$. Therefore, as candidate ε-decisive points we have the solution corresponding to $c_{\varepsilon,2}$ in (10), and as candidate $\bar{\varepsilon}$-decisive points we have the solutions corresponding to $c_{\bar{\varepsilon},i}$, $i = 1, 2$, in (11).

Proposition 5.4: Let $y \in C_\varepsilon \cap T_N^*M$ be a ε-out point. If the constraints are linear, $C = C^0$, then the solution corresponding to $c_{\varepsilon,2}$ in (10) *is a ε-decisive point for y.*

Proof: The basic observation is the second order character of the dynamics, both in the presence and in the absence of nonholonomic constraints. This implies that for any $y \in T^*M$ and any distribution of affine constraints C, we have $X_H(f)(y) = X_{H,C}(f)(y)$, since f is only a function of the configurations. Note that if H is of mechanical type, then $X_H(f)(x) = \mathcal{G}(x, d_q f)$, for any $x \in T_q^*M$. Now, from Lemma 5.3, taking $H = H_\varepsilon$, one gets

$$\mathcal{G}_\varepsilon(y + c_2\mathcal{P}_\varepsilon(d_q f), d_q f) = -\mathcal{G}_\varepsilon(y, d_q f).$$

Since y is a ε-out point, then $\mathcal{G}_\varepsilon(y, d_q f) \neq 0$. Consequently, $X_{H_+}(f)(y + c_2\mathcal{P}_+(d_q f)) = -\mathcal{G}_+(d_q f, y)$ has the opposite sign, and hence it is an in point. ■

D. Decisive points: inelastic mode

1. Change of constraints

Let $C_\pm \subset T^*M$ be two affine constraint submanifolds and let C^{inst} be a set of instantaneous affine constraints. We denote by $\mathcal{P}_\pm^{\text{inst}}$ and $\mathcal{Q}_\pm^{\text{inst}}$ the projectors corresponding to $C_\pm^{\text{inst}}$ and the cometric $\mathcal{G}$. If the instantaneous constraints are absent, denote by $\mathcal{P}_\pm$ and $\mathcal{Q}_\pm$ the projectors

corresponding to $C^{\mathrm{tr}}_{\pm}$ and the cometric $\mathcal{G}$. Let $y \in C_\varepsilon \cap T^*_N M$ be a ε-out point, $\varepsilon \in \{+,-\}$. Then, according to Definition 4.17, the unique y-decisive point is $\mathcal{P}^{\mathrm{inst}}_{\bar{\varepsilon}}(y) + \mathcal{Q}^{\mathrm{inst}}_{\bar{\varepsilon}}(\Upsilon_{C_{\bar{\varepsilon}}})$ [or, if there are no instantaneous constraints, $\mathcal{P}_{\bar{\varepsilon}}(y) + \mathcal{Q}_{\bar{\varepsilon}}(\Upsilon_{C_{\bar{\varepsilon}}})$].

2. Discontinuous Hamiltonian systems

As in Sec. V C 2, let $C_\pm \subset T^*M$ be two affine constraint submanifolds, $g_\pm$ a Riemannian metric on $M_\pm$ and $V_\pm \in C^\infty(M_\pm)$ such that Eq. (9) is verified. For simplicity, we only treat the case $V_\pm = V|_{M_\pm}$, $V \in C^\infty(M)$. We denote by $\mathcal{P}_\pm$ and $\mathcal{Q}_\pm$ the projectors corresponding to $C_\pm$ and the cometric $\mathcal{G}_\pm$. Additionally, let $C^{\mathrm{inst}}_\pm \subset T^*_N M$ be affine constraint submanifolds corresponding to some instantaneous constraints imposed along N. We denote by $\mathcal{P}^{\mathrm{inst,tr}}_\varepsilon$ and $\mathcal{Q}^{\mathrm{inst,tr}}_\varepsilon$ the projectors associated with the submanifold $C^{\mathrm{inst,tr}}_\varepsilon$ and the cometric $\mathcal{G}_\varepsilon$. In the absence of instantaneous constraints, we denote by $\mathcal{P}^{\mathrm{tr}}_\varepsilon$ and $\mathcal{Q}^{\mathrm{tr}}_\varepsilon$ the projectors associated with the submanifold $C^{\mathrm{tr}}_\varepsilon$ and the cometric $\mathcal{G}_\varepsilon$. In case $N = \partial M$, we denote the latter with the superscript "∂" instead of "tr."

Let $y \in C_\varepsilon \cap T^*_N M$ be an ε-out point. The points associated with y resulting from the first moves in a reflected or a refracted falling step are given, respectively, by Eqs. (10) and (11). As before, the second move simply consists of computing the focusing points for these solutions with respect to $C^{\mathrm{inst,tr}}_\varepsilon$ for a reflected falling step (respectively, $C^{\mathrm{inst,tr}}_{\bar{\varepsilon}}$ for a refracted falling step) or, if the instantaneous constraints are absent, $C^{\mathrm{tr}}_\varepsilon$ (respectively, $C^{\mathrm{tr}}_{\bar{\varepsilon}}$). This is done in terms of the corresponding projectors according to Sec. V A. According to Definition 4.18, this gives all the y-decisive points.

Proposition 5.5: Let $y \in C_\varepsilon \cap T^*_N M$ be an ε-out point and assume that the constraints are linear. For $N = \partial M$, the unique y-reflected falling point is given by $\mathcal{P}^{inst,\partial}_\varepsilon(y)$ [or, in the absence of ε-instantaneous nonholonomic constraints, $\mathcal{P}^{\partial}_\varepsilon(y)$].

Proof: From the previous discussion, we know that the points in the constrained characteristic passing through y with the same H_ε-energy level are y itself and $y + c_{\varepsilon,2}\mathcal{P}_\varepsilon(d_q f)$, $q = \pi(y)$ [cf. Eq. (10)]. Now, note that $d_q f$ belongs to the $\mathcal{G}_\varepsilon$-orthogonal complement of $\alpha^{-1}_{H_\varepsilon}(T(\partial M))$, i.e.,

$$\mathcal{G}_\varepsilon(d_q f, \beta) = d_q f(\alpha_{H_\varepsilon}(\beta)) = 0, \quad \beta \in \alpha^{-1}_{H_\varepsilon}(T(\partial M)).$$

Using the equality $C^\partial_\varepsilon = C_\varepsilon \cap \alpha^{-1}_{H_\varepsilon}(T(\partial M))$, we have that $d_q f \in \alpha^{-1}_{H_\varepsilon}(T(\partial M))^{\perp_\varepsilon}$ implies $\mathcal{P}^{\mathrm{inst},\partial}_\varepsilon(\mathcal{P}_\varepsilon(d_q f)) = 0$ and $\mathcal{P}^{\partial}_\varepsilon(\mathcal{P}_\varepsilon(d_q f)) = 0$. The result is then a consequence of Definition 4.18. ■

E. Energy behavior

In this section, we discuss the consequences regarding the energy behavior of the system that result from the application of the transition principle.

Lemma 5.6: Given $y \in T^*_N M$, let $x = \mathcal{P}(y) + \mathcal{Q}(\Upsilon_q)$, $q = \pi(y)$, be the associated y-focusing point with respect to a submanifold $C \subset T^*M$. Then

$$\hat{T}(x) \leqslant \hat{T}(y) + \hat{T}(\mathcal{Q}(\Upsilon_q), \mathcal{Q}(\Upsilon_q)),$$

and the equality holds if and only if y belongs to C^0.

Proof: Note that

$$\begin{aligned}\mathcal{G}(\mathcal{P}(y) + \mathcal{Q}(\Upsilon_q), \mathcal{P}(y) + \mathcal{Q}(\Upsilon_q)) &= \mathcal{G}(\mathcal{P}(y), \mathcal{P}(y)) + \mathcal{G}\ (\mathcal{Q}(\Upsilon_q), \mathcal{Q}(\Upsilon_q))) \\ &\leqslant \mathcal{G}(\mathcal{P}(y), \mathcal{P}(y)) + \mathcal{G}(\mathcal{Q}(y), \mathcal{Q}(y)) + \mathcal{G}(\mathcal{Q}(\Upsilon_q), \mathcal{Q}(\Upsilon_q)) \\ &= \mathcal{G}(y, y) + \mathcal{G}(\mathcal{Q}(\Upsilon_q), \mathcal{Q}(\Upsilon_q)),\end{aligned}$$

where we have used that $\mathcal{G}$ is positive-definite, and the fact that C^0 and $\mathrm{Ann}(\mathcal{D})$ are orthogonal spaces with respect to the cometric $\mathcal{G}$. If the equality holds, then $\mathcal{G}(\mathcal{Q}(y), \mathcal{Q}(y)) = 0$, which is equivalent to $y \in C^0$. ■

As a consequence of this simple lemma we can conclude that in the case of linear constraints the transition principle always implies a loss of energy. This is a suitable generalization to constrained systems of the classical Carnot theorem for systems subject to impulsive forces.[36]

Theorem 5.7 (Carnot's theorem for generalized linear constraints): *Suppose that the Hamiltonian system is subject to nonholonomic constraints given by a linear distribution. Then the transition principle implies always a loss of energy as the result of an "impact."*

Proof: Under linear constraints, note that $\Upsilon=0$. From Lemma 5.6, we get $\hat{T}(x)\leqslant\hat{T}(y)$ with $F_{(H,C)}(y)=\{x\}$. The result now follows from the formulation of the transition principle and the definitions of decisive points in Sec. IV E (cf. Definitions 4.12–4.18). ■

Under linear constraints, the trajectory of the system maintains the same energy level after the application of the transition principle in the following cases:

(i) when the decisive points are determined according to Definitions 4.12 and 4.17 and the impact point $y\in T^*_NM$ belongs to $C_+\cap C_-$; and
(ii) when the constraints are smooth, and therefore the decisive points are determined according to Proposition 4.15.

If the decisive points are determined according to Definitions 4.14 and 4.18, then nothing can be said in general. The refractive steps will typically imply an energy decrease.

Remark 5.8: This type of energy arguments also allows to discard as follows the possibility of chattering when computing the y-decisive points if the constraints change (see Definition 4.12 and Remark 4.13 above). Let $N=\{y\in T^*M\,|\,f(y)=0\}$. Assume there is an infinite y-admissible sequence (y_i,ε_i), $i=0,\ldots,\infty$. For each i, we have that $y_i\neq y_{i+1}$, since otherwise

$$X^l_{H,C_{\varepsilon_i+1}}(f)(y_{i+1})=X^l_H(f)(y_{i+1})=X^l_{H,C_{\varepsilon_i}}(f)(y_i)\quad\text{for all } l,$$

which together with the fact that y_i is a ε_i-out point, implies that y_{i+1} is a ε_{i+1}-in point. The latter contradicts the definition of admissible sequence. As a consequence of Lemma 5.6, we then have

$$\hat{T}(y_0)>\hat{T}(y_1)>\hat{T}(y_2)>\cdots>\hat{T}(y_i)\geqslant 0.$$

The limit of this sequence is zero, which implies that the y-decisive point corresponding to such a sequence would be 0, that is, the trajectory would get stuck when reaching N.

F. Integrable constraints

The integrability of the constraints simplifies the application of the transition principle. Consider, for instance, the situation when the mechanical system is unconstrained on M_- and is subject to some generalized linear constraints $C=C^0$ on M_+ that turn out to be holonomic, i.e., $\alpha_H(C^0)=\mathcal{D}$ is integrable. Denote by $\{S_\alpha\}$, α being an m-dimensional parameter, the foliation of M_+ induced by $\mathcal{D}$. Locally this foliation is described by m functions $f_i\in C_\infty(M)$ such that

$$q\in S_\alpha\Leftrightarrow f_i(q)=\alpha_i,\quad 1\leqslant i\leqslant m.$$

A similar situation has been treated in Ref. 35 in the context of totally inelastic collisions (note, however, that in Ref. 35 the integrable distribution is defined only on N, whereas here $\mathcal{D}$ is defined on M_+). The integrable constraints imposed by $\mathcal{D}$ can be interpreted as an abrupt reduction of the phase space of the mechanical system.

By definition, one has that $\mathrm{Ann}(\mathcal{D})=\mathrm{span}\{\mathrm{d}f_1,\ldots,\mathrm{d}f_m\}$. The matrix J in (8) is then given by $J=(\partial f_i/\partial q^a)$ and the projector $\mathcal{P}$ is $\mathcal{P}(x)=(1-J^t\mathcal{B}^{-1}JG^{-1})x$. Let $y\in C_-\cap T^*_NM$ be the impact state of a trajectory $q(t)$ coming from M_-. From the discussion in Sec. V C, we obtain that the unique focusing point associated to y is $x=(1-J^t\mathcal{B}^{-1}JG^{-1})y$. The trajectory will continue its motion in M_+, M_- or N depending on the in/out/trapping character of the focusing point x. If it evolves in M_+ (more precisely, in $S_\alpha\subset M_+$ with α such that $x\in S_\alpha$), we call it the refraction of the original trajectory. If it evolves in M_-, we call it the reflection of the original trajectory.

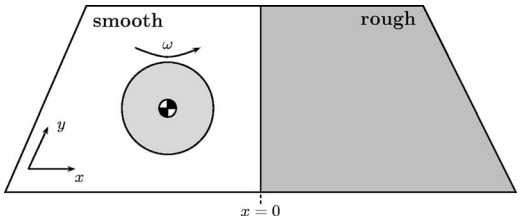

FIG. 1. The rolling sphere on a special surface.

VI. EXAMPLES

In this section we consider four examples to illustrate the theory exposed above. They all present the example of a rolling sphere considered in various constrained situations. The first one is taken from Ref. 16 and is treated here in order to provide a further comparison with previous approaches. The second one combines the presence of smooth nonholonomic constraints with discontinuous Hamiltonians and instantaneous constraints acting on the system along a hypersurface. The third one consists of a ball rolling on a rotating surface whose angular velocity is suddenly changed to a different value, and this is modeled via a discontinuous affine distribution of constraints. Finally, the fourth one presents a two-wheeled system with a rod of variable length and illustrates the application of the transition principle in both the elastic and the inelastic modes.

A. A rolling sphere

Consider a homogeneous sphere rolling on a plane. Assume it has unit mass ($m=1$) and let k^2 be its inertia about any axis. Let (x,y) denote the position of the center of the sphere and let (φ,θ,ψ) denote the Eulerian angles. The configuration space is therefore $Q=\mathbb{R}^2\times \mathrm{SO}(3)$. Assume that the plane is smooth if $x<0$ and absolutely rough if $x>0$ (see Fig. 1). On the smooth half-plane, the motion of the sphere is assumed free, that is, the sphere can slip. On the rough half-plane, the sphere should roll without slipping due to the constraints imposed by the roughness. We are interested in determining the eventual sudden changes in the trajectories of the sphere when it reaches the line separating the smooth and the rough half-planes.

The kinetic energy of the sphere is

$$T=\tfrac{1}{2}(\dot{x}^2+\dot{y}^2+k^2(\omega_x^2+\omega_y^2+\omega_z^2)), \tag{12}$$

where ω_x, ω_y, and ω_z are the angular velocities with respect to the inertial frame, given by

$$\omega_x=\dot{\theta}\cos\psi+\dot{\varphi}\sin\theta\sin\psi,\quad \omega_y=\dot{\theta}\sin\psi-\dot{\varphi}\sin\theta\cos\psi,\quad \omega_z=\dot{\varphi}\cos\theta+\dot{\psi}.$$

The condition of rolling without sliding of the sphere when $x>0$ implies that the point of contact of the sphere and the plane has zero velocity

$$\phi^1=\dot{x}-r\omega_y=0,\quad \phi^2=\dot{y}+r\omega_x=0,$$

where r is the radius of the sphere.

Following the classical procedure,[30] we introduce quasicoordinates q^1, q^2, and q^3 such that $\dot{q}^1=\omega_x$, $\dot{q}^2=\omega_y$, and $\dot{q}^3=\omega_z$. The latter merely have a symbolic meaning in the sense that in the present example, for instance, the partial derivative operators $\partial/\partial q^i$ should be interpreted as linear combinations of the partial derivatives with respect to Euler's angles. Also to the differential forms $\mathrm{d}q^i$ one should attach the appropriate meaning, i.e., they do not represent exact differentials but, instead, we should read them as $\mathrm{d}q^1=\cos\psi\,\mathrm{d}\theta+\sin\theta\sin\psi\,\mathrm{d}\varphi$, etc.

The singular hypersurface N is defined by $N=\{x=0\}$. In this case, the constraints are linear and the nonholonomic distribution $\alpha_H(C)=\mathcal{D}$ on M_+ is given by

$$\mathcal{D}_{(x,y,q^1,q^2,q^3)} = \operatorname{span}\left\{ r\frac{\partial}{\partial x} + \frac{\partial}{\partial q^2}, -r\frac{\partial}{\partial y} + \frac{\partial}{\partial q^1}, \frac{\partial}{\partial q^3} \right\}.$$

Here we are dealing with a single distribution which constrains the motion on M_+.

In the following we compute the decisive points for this example. Let $\lambda \in C_- \cap T^*M$ be a minus-out point. A direct computation shows that the expression of the projector $\mathcal{P}: T^*M \to C$ in local coordinates is

$$\mathcal{P} = \begin{pmatrix} \frac{r^2}{r^2+k^2} & 0 & 0 & \frac{r}{r^2+k^2} & 0 \\ 0 & \frac{r^2}{r^2+k^2} & -\frac{r}{r^2+k^2} & 0 & 0 \\ 0 & \frac{-rk^2}{r^2+k^2} & \frac{k^2}{r^2+k^2} & 0 & 0 \\ \frac{rk^2}{r^2+k^2} & 0 & 0 & \frac{k^2}{r^2+k^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{13}$$

Therefore, the single focusing point for $\lambda \in T^*_N M$ is given by $x = \mathcal{P}(\lambda) \in C \cap T^*_N M$. If we denote $\lambda = (x_0, y_0, q^1_0, q^2_0, q^3_0, (p_x)_0, (p_y)_0, (p_1)_0, (p_2)_0, (p_3)_0)$ and $x = (x, y, q^1, q^2, q^3, p_x, p_y, p_1, p_2, p_3)$, we get

$$p_x = \frac{r^2(p_x)_0 + r(p_2)_0}{r^2+k^2},$$

$$p_y = \frac{r^2(p_y)_0 - r(p_1)_0}{r^2+k^2},$$

$$p_1 = \frac{rk^2(p_y)_0 + k^2(p_1)_0}{r^2+k^2},$$

$$p_2 = \frac{rk^2(p_x)_0 + k^2(p_2)_0}{r^2+k^2},$$

$$p_3 = (p_3)_0.$$

Note also that the focusing point with respect to $C_- = T^*M$ associated with x is x itself. Therefore, if x is a plus-out point, the only admissible sequence for λ is $\{(\lambda,-),(x,+),(x,-)\}$. If x is either a plus-in or a plus-trapping point, then the only admissible sequence for λ is $\{(\lambda,-),(x,+)\}$. The set of plus-trapping points for the dynamics X_{H,C_+} is $\partial(T^*M)^n = \{\mu \in T^*M \,|\, x=0, p_x=0\}$. Consequently, the trajectory is refracted, i.e., the sphere follows its motion on M_+ under the dynamics X_{H,C_+} (rolling without slipping) if $p_x \geqslant 0$. Otherwise (i.e., if $p_x < 0$), the trajectory is reflected by the "roughness" and continues in M_- under the dynamics X_H starting from x.

B. A rolling sphere hitting a wall

This is a classical example[13,20,30] that we treat here for the sake of completeness. Consider again a homogeneous sphere of radius r and unit mass. Assume that the sphere rolls without sliding on a horizontal table, and that at a certain instant of time it hits a wall determined by the plane $x = d > 0$ (cf. Fig. 2). When this happens, the following constraint is instantaneously imposed on the system:

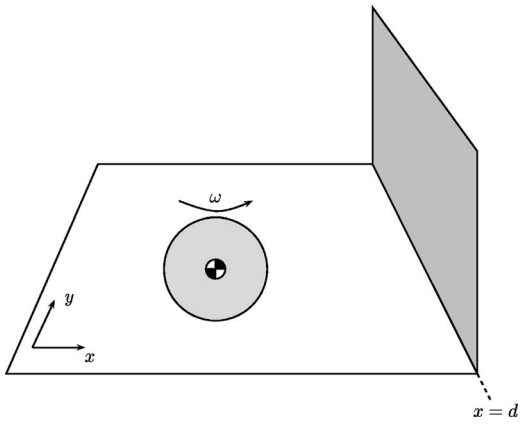

FIG. 2. A rolling sphere that eventually hits a wall.

$$\psi = \dot{y} - r\omega_z = 0.$$

Therefore, we are in the situation explained in Remark 4.16. The configuration space of the system is $M=M_+=\{x<d\}$, with the boundary $N=\{x=d\}$, and the linear constraint submanifold $C=C_+\subset T^*M$ is given by $\alpha_H(C)=\mathcal{D}$,

$$\mathcal{D} = \operatorname{span}\left\{ r\frac{\partial}{\partial x} + \frac{\partial}{\partial q^2}, -r\frac{\partial}{\partial y} + \frac{\partial}{\partial q^1}, \frac{\partial}{\partial q^3} \right\}.$$

The expression for the projector $\mathcal{P}: T^*M \to C$ is given by Eq. (13). The submanifold giving the instantaneous constraints along N is

$$C^{\text{inst}} = \{\lambda \in C | \psi(\alpha_H(\lambda)) = 0\}.$$

The projector $\mathcal{P}^{\text{inst}}=\mathcal{P}_+^{\text{inst}}: T^*M \to C^{\text{inst}}$ is

$$\mathcal{P}^{\text{inst}}(\lambda) = \frac{r\lambda_x + \lambda_2}{r^2 + k^2}(\eta\, dx + k^2\, dq^2) + \frac{-r\lambda_y + \lambda_1 - \lambda_3}{r^2 + 2k^2}(-\eta\, dy + k^2\, dq^1 - k^2\, dq^3). \tag{14}$$

Let $\lambda=(x_0,y_0,q_0^1,q_0^2,q_0^3,(p_x)_0,(p_y)_0,(p_1)_0,(p_2)_0,(p_3)_0) \in C_+ \cap T^*_N M \subset T^*M$ be a plus-out point, i.e., $\mathcal{G}(\lambda, dx) < 0$. We first consider an elastic impact. Since $H_-=\infty$, we only compute the outcome of a reflective step. According to (10), the points in the constrained characteristic passing through λ within the same H_+-energy level are

$$\lambda \quad \text{and } \lambda + c_{+,2}\mathcal{P}(dx), \quad \text{with } c_{+,2} = -2\frac{r^2 + k^2}{r^2}(p_x)_0.$$

The associated focusing points are given by

$$\mathcal{P}^{\text{inst}}(\lambda) \quad \text{and } \mathcal{P}^{\text{inst}}(\lambda) + c_{+,2}\mathcal{P}^{\text{inst}}(\mathcal{P}(dx)). \tag{15}$$

Note that $\mathcal{P}^{\text{inst}}(\mathcal{P}(dx))=\mathcal{P}^{\text{inst}}(dx)=\mathcal{P}(dx)$, and therefore the points in (15) belong to the same constrained characteristic and to the same H_+-energy level. Denoting the coordinates of the point $\mathcal{P}^{\text{inst}}(\lambda)$ by $(x,y,q^1,q^2,q^3,p_x,p_y,p_1,p_2,p_3)$, we get

$$p_x = (p_x)_0,$$

$$p_y = \frac{(r^2 + k^2)(p_y)_0 + r(p_3)_0}{r^2 + 2k^2},$$

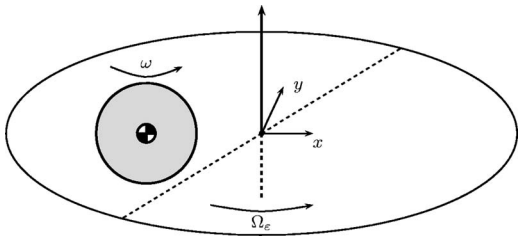

FIG. 3. A rolling sphere on a rotating table.

$$p_1 = -k^2 \frac{(r^2+k^2)(p_y)_0 + r(p_3)_0}{r(r^2+2k^2)},$$

$$p_2 = k^2 \frac{(p_x)_0}{r},$$

$$p_3 = k^2 \frac{(r^2+k^2)(p_y)_0 + r(p_3)_0}{r(r^2+2k^2)}.$$

Now, notice that $\mathcal{P}^{\text{inst}}(\lambda)$ is a plus-out point, because $\mathcal{G}(\mathcal{P}^{\text{inst}}(\lambda), \mathrm{d}x) = \mathcal{G}(\lambda, \mathrm{d}x) < 0$. Therefore, following Proposition 5.4, we conclude that the sequence $\{(\lambda, +), \mathcal{P}^{\text{inst}}(\lambda) + c_{+,2}\mathcal{P}^{\text{inst}}(\mathrm{d}x), +)\}$ is λ-admissible, and $\mathcal{P}^{\text{inst}}(\lambda) + c_{+,2}\mathcal{P}^{\text{inst}}(\mathrm{d}x)$ is a decisive point. The other possible λ-admissible sequence corresponds to

$$\{(\lambda, +), \mathcal{P}^{\text{inst}}(\lambda), \mathcal{P}^{\text{inst}}(\lambda) + c_{+,2}\mathcal{P}^{\text{inst}}(\mathrm{d}x), +)\},$$

but renders the same decisive point.

In the case of an inelastic impact, Proposition 5.5 yields that the unique λ-decisive point is $\mathcal{P}^{\text{inst},\partial}(\lambda)$. After the impact, the ball continues its motion along the wall under the dynamics specified by the vector field $X_+^{\text{inst},\partial}$.

C. A rolling sphere on a rotating table

Consider again a homogeneous sphere of radius r and unit mass. Assume that the sphere rolls without sliding on a horizontal table which is rotating with certain constant angular velocity about a vertical axis through one of its points (see Fig. 3). Let Ω_- and Ω_+ be two angular velocities. Here we consider the following situation: each time the sphere reaches the hypersurface $x=y$, an impulsive force is exerted on the table to put it spinning with a different angular velocity. That is, if the angular velocity of the table was Ω_-, the force applied on its rotation axis changes it to Ω_+ and vice versa. We assume that $\Omega_- < \Omega_+$. This can be modeled as thinking of a system which is subject to two different affine constraint distributions. In order for this model to be consistent, we also assume that the surface of the table is rough enough so that the sphere is rolling without slipping at all times.

The Lagrangian is again given by Eq. (12). The nonholonomic constraints are now affine in the velocities,

$$\dot{x} - r\omega_y = -\Omega y, \quad \dot{y} + r\omega_x = \Omega x.$$

The constraint space $\alpha_H(C)$ is then described by

$$\alpha_H(C) = \mathcal{D} + Y = \operatorname{span}\left\{ r\frac{\partial}{\partial x} + \frac{\partial}{\partial q^2}, -r\frac{\partial}{\partial y} + \frac{\partial}{\partial q^1}, \frac{\partial}{\partial q^3} \right\} + Y,$$

where Y is the vector field defined by

$$Y = -\Omega y\frac{\partial}{\partial x} + \Omega x\frac{\partial}{\partial y}.$$

Note that the projection of $\Upsilon = \mathcal{L}_L(Y)$ to $\mathrm{Ann}(\mathcal{D})$ is given by

$$\mathcal{Q}(\Upsilon) = \frac{\Omega k^2}{r^2 + k^2}(-y\,\mathrm{d}x + x\,\mathrm{d}y - xr\,\mathrm{d}q^1 - yr\,\mathrm{d}q^2).$$

Following the discussion for the case of affine constraints, given $y \in T^*M$, the focusing point with respect to $C_\pm$ is given by

$$x = \mathcal{P}(y) + \mathcal{Q}(\Upsilon_\pm),$$

where $\mathcal{P}$ is the projector in (13).

Assume that the sphere is rolling on the hyperplane $M_- = \{x < y\}$ and that the constant angular velocity of the table is Ω_-. Consider the case when the sphere "hits" the hypersurface $N = \{x = y\}$ with the impact state

$$\lambda = (x_0, y_0, q_0^1, q_0^2, q_0^3, (p_x)_0, (p_y)_0, (p_1)_0, (p_2)_0, (p_3)_0) \in C_- = C_-^0 + \Upsilon_-.$$

Denote the coordinates of the associated focusing point by

$$x = \mathcal{P}(\lambda) + \mathcal{Q}(\Upsilon_+) = (x, y, q^1, q^2, q^3, p_x, p_y, p_1, p_2, p_3).$$

Then

$$\mathcal{G}(\mathrm{d}f, x) = p_x - p_y = (p_x)_0 - (p_y)_0 + \frac{k^2}{r^2 + k^2}(x_0 + y_0)(\Omega_- - \Omega_+). \tag{16}$$

Given that λ is an minus-out point, we have that $\mathcal{G}(\mathrm{d}f, \lambda) = (p_x)_0 - (p_y)_0 > 0$. If $x_0 = y_0 < 0$, then the second term in (16) is also positive, and $\{(\lambda, -), (x, +)\}$ is the unique admissible sequence for λ. In this case, x is the λ-decisive point. On the contrary, for certain values of $x_0 = y_0 > 0$, it might happen that $\mathcal{G}(\mathrm{d}f, x)$ is negative, i.e., that x is a plus-out point. Now, note that the focusing point associated with x is λ itself, since

$$\mathcal{P}(x) + \mathcal{Q}(\Upsilon_-) = \mathcal{P}(\mathcal{P}(\lambda)) + \mathcal{Q}(\Upsilon_-) = \mathcal{P}(\lambda) + \mathcal{Q}(\Upsilon_-) = \lambda.$$

As a consequence, in this case there would not be any λ-decisive point. This problem stems from the fact the modeling of this example as a system subject to affine constraints does not take into account that the jump in the angular velocity of the table takes place *no matter what*. Therefore, after the impact, we should really regard C_+ as the new set of affine constraints acting on the whole configuration manifold. With this interpretation, x would obviously be a plus-in point (and hence decisive). In other words, the trajectory of the ball gets reflected back by the blow of the greater velocity Ω_+.

D. A two-wheeled system with a rod of variable length

Consider a system composed of two wheels of different radii, $r_1 < r_2$, connected by a massless rod of variable length ℓ (see Fig. 4). For simplicity, assume that the two-wheeled system moves along a line, and that both the masses and the momenta of inertia of the wheels are unitary. The wheels are subject to the standard constraints of nonslipping. Assume that the length ℓ of the rod is constrained between a minimum length a and a maximum length b. Here we consider the following two situations: (i) when the length ℓ of the rod becomes extreme, an elastic impact occurs; (ii) when the length ℓ of the rod becomes extreme, an arresting device fixes it, and therefore an inelastic impact occurs.

The Lagrangian of the system is given by the kinetic energy of the wheels

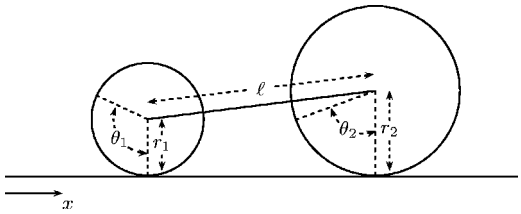

FIG. 4. A two-wheeled system with a rod of variable length.

$$L = \tfrac{1}{2}(\dot{\theta}_1^2 + \dot{\theta}_2^2 + \dot{x}_1^2 + \dot{x}_2^2).$$

The conditions of rolling without sliding are encoded in the constraints

$$\dot{x}_1 - r_1\dot{\theta}_1 = 0, \quad \dot{x}_2 - r_2\dot{\theta}_2 = 0,$$

which, since we are considering the motion of the two-wheeled system only along a line, turn out to be holonomic. The constraint on the length of the rod is given by

$$a \leqslant \ell = \sqrt{(r_2 - r_1)^2 + (x_2 - x_1)^2} \leqslant b.$$

Following Remark 4.16, we set $M_- = \emptyset$, $M_+ = M = \{(x_1, x_2, \theta_1, \theta_2) \in \mathbb{R}^2 \times \mathbb{S}^1 \times \mathbb{S}^1 \,|\, a \leqslant \ell(x_1, x_2, \theta_1, \theta_2) \leqslant b\}$, with boundary set $N = \partial M = \{(x_1, x_2, \theta_1, \theta_2) \in \mathbb{R}^2 \times \mathbb{S}^1 \times \mathbb{S}^1 \,|\, \ell(x_1, x_2, \theta_1, \theta_2) = a \text{ or } \ell(x_1, x_2, \theta_1, \theta_2) = b\}$, and linear constraint submanifold $C = C_+ \subset T^*M$ given by $\alpha_H(C) = \mathcal{D}$,

$$\mathcal{D} = \operatorname{span}\left\{ r_1\frac{\partial}{\partial x_1} + \frac{\partial}{\partial \theta_1}, r_2\frac{\partial}{\partial x_2} + \frac{\partial}{\partial \theta_2} \right\}.$$

The expression for the projector $\mathcal{P}: T^*M \to C$ in local coordinates is given by the following matrix:

$$\mathcal{P} = \begin{pmatrix} \frac{r_1^2}{1+r_1^2} & 0 & \frac{r_1}{1+r_1^2} & 0 \\ 0 & \frac{r_2^2}{1+r_2^2} & 0 & \frac{r_2}{1+r_2^2} \\ \frac{r_1}{1+r_1^2} & 0 & \frac{1}{1+r_1^2} & 0 \\ 0 & \frac{r_2}{1+r_2^2} & 0 & \frac{1}{1+r_2^2} \end{pmatrix}.$$

Let $\lambda \in T^*M_+$ be a plus-out point with $\ell(\lambda) = b$ and $\mathcal{G}(\lambda, \mathrm{d}\ell) > 0$. Since $H_- = \infty$, we only compute the outcome of a reflective step. Following Eq. (10), the points in the constrained characteristic passing through λ with the same H_+-energy level are λ and $\lambda + c_{+,2}\mathcal{P}(\mathrm{d}\ell)$, with

$$c_{+,2} = -\frac{2\mathcal{G}(\lambda, \mathcal{P}(\mathrm{d}\ell))}{\mathcal{G}(\mathcal{P}(\mathrm{d}\ell), \mathcal{P}(\mathrm{d}\ell))}. \tag{17}$$

According to Proposition 5.4, the point $\lambda + c_{+,2}\mathcal{P}(\mathrm{d}\ell)$ is $+$-decisive.

Consider now an inelastic impact, i.e., the case when the length ℓ of the rod becomes fixed after the impact. Since there are no additional instantaneous constraints imposed on the system at the impact state, we compute the decisive points with regards to the boundary of the constraint manifold,

$$C^{\partial} = C \cap \alpha_{H_+}^{-1}(T\partial M) = \{(x_1, x_2, \theta_1, \theta_2, p_{x_1}, p_{x_2}, p_{\theta_1}, p_{\theta_2}) \in T^*M | p_{x_1} = p_{x_2},\ p_{x_1} = r_1 p_{\theta_1},\ p_{x_2} = r_2 p_{\theta_2},\ \ell(x_1, x_2, \theta_1, \theta_2) = a \text{ or } \ell(x_1, x_2, \theta_1, \theta_2) = b\}.$$

As before, we only compute the outcome of a reflective step. Following Proposition 5.5, we deduce that the unique decisive point is $\mathcal{P}^{\partial}(\lambda)$. After the inelastic impact, the length of the rod is fixed forever after, the velocities of the two wheels of the system are reset according to $\mathcal{P}^{\partial}(\lambda)$ and evolve according to $X^{\partial}_{(H,C,N)}$.

VII. CONCLUSIONS

We have developed a generalization of the transition principle to deal with impulsive regimes in general nonholonomic systems, and particularized our discussion to the case of mechanical systems with affine constraints. We have also provided a geometric formulation of the dynamics of nonholonomic Hamiltonian systems via partial symplectic structures. Future work will be devoted to the development of a suitable version of the transition principle for optimal control problems, the comparison of quantitative and qualitative predictions made by the transition principle in specific examples, and the implementation of the results obtained here in numerical schemes for impulsive nonholonomic systems.

ACKNOWLEDGMENT

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Flow acoustics and linearized equations for ideal barotropic fluid flows

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In this paper we analyze the acoustic flow in periodic structures for general time-dependent problems. Mathematically, the acoustic problem reduces to analysis of the linearized Helmholtz equations of an ideal barotropic fluid in the neighbourhood of the stationary background flow. We show that in the linear approximation stationary flows are generally unstable. Explicit unbounded solutions are determined and, in some cases, expressions for the general solution of the acoustic problem are stated. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In periodic structures such as water-air mixtures, the following phenomenon has been observed: due to special arrangement of the two materials, the speed of sound in the mixed structure can drop drastically[17] allowing for several possible applications, see, e.g., Refs. 5, 10, and 13. In Ref. 19, the Bloch theory of acoustic wave propagation in periodically arranged materials has been extended to include the case where a fluid flows in one of the two constituent media. The fluid flow velocity has been assumed to be any function of the coordinates perpendicular to the direction of the flow, i.e., $\mathbf{v}_0=(0,0,v_0(x_1,x_2))$ in Cartesian coordinates x_1,x_2,x_3, while the acoustic materials have been arranged periodically perpendicular to the flow direction.

In this paper we analyze stability of acoustic flows in the general case of flow propagation with respect to the material periodicity and for general time-dependent problems. We consider two cases: when the acoustic materials are arranged perpendicular to the flow direction (homogeneity applies along the flow direction), and when the acoustic materials are arranged periodically also along the flow direction.

Mathematically, the acoustic problem reduces to analysis of the linearized Helmholtz equation of an ideal barotropic fluid (i.e., assuming fluid pressure to be a function of density only) in the neighborhood of the stationary background flow. There have been many works devoted to analysis of stability of stationary fluid flows and loss of smoothness of solutions for incompressible fluids, see, e.g., Refs. 11, 8, 14, 9, and 20, and references therein.

For the case, when the acoustic materials are arranged perpendicular to the flow direction, we study the so-called short-wave asymptotics of perturbations of stationary flows. It has been shown,[2] by studying the Jordan form of the equations, that for incompressible fluids the solutions to linearized equations can be unbounded. We find explicitly these unbounded solutions for our system, and we also expand these results for barotropic fluids: the stationary background flows under consideration are linearly unstable subject to (acoustic) disturbances. In particular, we find that whenever the frequency is an integer times the local flow velocity, unstable solutions to the periodic lattice problem exist in agreement with previous results.[19] In case when the acoustic

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materials are arranged periodically along the flow direction, we also find explicitly the unbounded solutions, and show that the absence of the so-called monofrequency solutions may lead to loss of smoothness of solutions.

In the present analysis, we consider small flows such that pressure drops are negligible, i.e., we consider the ideal case where all flow variables, to a good approximation, can be treated as periodic quantities. At higher flow values this assumption is, however, difficult to establish in practice due to the formation of viscous wakes behind objects.

The instability mechanism in our examples is advective in character, and the growth of solutions is linear (similar to Ref. 2). Usually, the linear growth of solutions to linearized equations is not enough to conclude instability in the nonlinear case. However, here the nonlinear system is also Lyapunov-unstable, and we demonstrate this in the Appendix.

II. MAIN EQUATIONS

Let an ideal compressible barotropic fluid flow on a manifold $M=\mathbb{R}^2\times S^1$, i.e., we assume that the flow velocity and density is periodic in one direction.

We consider the Euler equations in the Helmholtz, or vortex form, see, e.g., Ref. 12,

$$\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v})=0,\quad \frac{\partial\mathbf{w}}{\partial t}+[\mathbf{w},\mathbf{v}]=0, \tag{1}$$

where ρ is the fluid density, $\mathbf{v}$ is the velocity vector field, $\mathbf{w}=(1/\rho)\operatorname{curl}\mathbf{v}$ and $[\mathbf{w},\mathbf{v}]_i=w_j(\partial v_i/\partial x_j)-v_j(\partial w_i/\partial x_j)$ is the commutator of the vector fields.

We assume that the metric on the manifold M is flat. Let $x_1,x_2;x_3(\mathrm{mod}\,2\pi)$ be the (local) Cartesian coordinates on M, thus the volume element being $\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3$.

Let ρ_0, $\mathbf{v}_0$ be the stationary flow of the following type:

$$\mathbf{v}_0=(0,0,v_0(x_1,x_2)),\quad \rho_0=\rho_0(x_1,x_2). \tag{2}$$

Stationary flow (2) will be referred to as a *background flow*. Note that, as $\operatorname{div}\mathbf{v}_0\equiv 0$, the derivative $\partial\rho_0/\partial x_3=0$. The functions $v_0(x_1,x_2)$ and $\rho_0(x_1,x_2)$ can be chosen independently. In our coordinate system the vorticity vector equals

$$\mathbf{w}_0=\frac{1}{\rho_0}\operatorname{curl}\mathbf{v}_0=\frac{1}{\rho_0}\left(\frac{\partial v_0}{\partial x_2},-\frac{\partial v_0}{\partial x_1},0\right).$$

Remark: The Helmholtz equations (1) are not equivalent to the Euler equations

$$\rho\frac{\partial\mathbf{v}}{\partial t}+\rho(\mathbf{v},\nabla)\mathbf{v}=\nabla h(\rho),$$

as there are solutions to the Helmholtz equations that are not the solutions to the Euler equations (but, of course, all solutions to the Euler equation are also solutions to the Helmholtz equations), provided the pressure function $h(\rho)$ is given. For example, our stationary flow is the solution to the Euler equations either if $\rho_0=\mathrm{const}$, or if the pressure function $h(\rho)$ is a constant.

We now denote

$$\mathbf{s}=\mathbf{w}-\mathbf{w}_0,\quad r=\rho-\rho_0,$$

and write down the linearized system,

$$\frac{\partial r}{\partial t}+\operatorname{div}(r\mathbf{v}_0+\rho_0\operatorname{curl}^{-1}(r\mathbf{w}_0+\rho_0\mathbf{s}))=0,$$

$$\frac{\partial \mathbf{s}}{\partial t} + [\mathbf{s}, \mathbf{v}_0] + [\mathbf{w}_0, \mathrm{curl}^{-1}(r\mathbf{w}_0 + \rho_0 \mathbf{s})] = 0. \tag{3}$$

This is the general setup for the flow acoustic problem, see Ref. 19. In writing Eq. (3), we have implicitly assumed that $\mathrm{div}(r\mathbf{w}_0 + \rho_0 \mathbf{s}) = 0$ such that $\mathrm{curl}^{-1}(r\mathbf{w}_0 + \rho_0 \mathbf{s})$ is meaningful.

III. INSTABILITY OF LINEARIZED EQUATIONS

We first notice [see, e.g., Ref. 4, Chap. II, and the discussion following Eq. (9)] that, as $[\mathbf{s}, \mathbf{v}_0]$ is the "strongest" linear operator, comparing with the one containing curl^{-1}, it is reasonable to consider the "shortened" equation

$$\frac{\partial r}{\partial t} + \mathrm{div}(r\mathbf{v}_0) = 0, \quad \frac{\partial \mathbf{s}}{\partial t} + [\mathbf{s}, \mathbf{v}_0] = 0. \tag{4}$$

Proposition 1: For nonuniform background flows (i.e., for $v_0 \neq \mathrm{const}$*), almost all solutions to the shortened equation (4) grow linearly in time.*

Thus the stationary solution (2) is unstable in the linear approximation. Proposition 1 can be deduced from Proposition 5.2 in Ref. 4, Chap. II, if we assume the existence of the "action-angle" variables. We give an independent proof in the Appendix.

Theorem 1: *Let* $\mathbf{w}_0 \neq \mathrm{const}$ *or* $\rho_0 \neq \mathrm{const}$. *Then Eqs. (3) have a solution that grows linearly in time.*

Proof: We search for a solution in the following form:

$$\mathbf{u} = (c_1, c_2, u_3(x_1, x_2, t)), \quad r = r(x_1, x_2, t),$$

where $\mathbf{u} = \mathrm{curl}^{-1}(r\mathbf{w}_0 + \rho_0 \mathbf{s})$. Then

$$\mathbf{s} = \frac{1}{\rho_0} \mathrm{curl}\, \mathbf{u} - \frac{r}{\rho_0} \mathbf{w}_0. \tag{5}$$

From Eq. (3), we formally get that

$$s_1 = -\left(c_1 \frac{\partial w_1}{\partial x_1} + c_2 \frac{\partial w_1}{\partial x_2} \right) t, \quad s_2 = -\left(c_1 \frac{\partial w_2}{\partial x_1} + c_2 \frac{\partial w_2}{\partial x_2} \right) t, \quad s_3 = 0,$$

$$r = -\left(c_1 \frac{\partial \rho_0}{\partial x_1} + c_2 \frac{\partial \rho_0}{\partial x_2} \right) t,$$

where

$$w_1 = \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_2}, \quad w_2 = -\frac{1}{\rho_0} \frac{\partial v_0}{\partial x_1}$$

are the components of the background vorticity. Thus we have found a solution that grows linearly in time, and is zero when $t = 0$. To complete the proof, it is enough to show that from relation (5) the value u_3 can be determined (which means that what we have is actually a solution). From (5) follows that

$$\mathrm{curl}\, \mathbf{u} = \rho_0 \mathbf{s} + r\mathbf{w}_0 = (\rho_0 s_1 + r w_1, \rho_0 s_2 + r w_2, 0).$$

One can verify directly that the divergence of the right-hand side is zero. □

In the Appendix we use the same construction as in Theorem 1 to find an unstable solution for the nonlinear (compressible) case, and to prove the (nonlinear) Lyapunov instability of shear flows on a 3-torus, considered in the linear approximation in Refs. 2 and 4.

Remark: Proposition 1 and Theorem 1 describe a known effect that acoustic waves change their frequency and magnitude while propagating through nonuniform flow, however, the effect is

limited to the area where the flow is really nonuniform, see, e.g., Refs. 6, 7, 15, and 16.

IV. SHORT-WAVE ASYMPTOTICS

We next return to the full set of Eqs. (3). Let us consider periodic solutions (being a subset of possible Bloch solutions for acoustic quantities in the linear approximation). Hence, we expand both $\mathbf{s}$ and r as Fourier series in x_3,

$$\mathbf{s} = \sum_m (A_m(x_1,x_2,t), B_m(x_1,x_2,t), C_m(x_1,x_2,t)) \exp imx_3,$$

$$r = \sum_m D_m(x_1,x_2,t) \exp imx_3. \tag{6}$$

The functions A_m, B_m, C_m, D_m cannot be arbitrary: the vector $r\mathbf{w}_0 + \rho_0\mathbf{s}$ should be divergence-free as mentioned above.

As we are interested in short-wave asymptotics, we take $m \neq 0$. The divergence of the mth term in the series representation of $r\mathbf{w}_0 + \rho_0\mathbf{s}$ is

$$\operatorname{div}\left(\left(\frac{1}{\rho_0} D_m \frac{\partial v_0}{\partial x_2} + \rho_0 A_m, -\frac{1}{\rho_0} D_m \frac{\partial v_0}{\partial x_1} + \rho_0 B_m, \rho_0 C_m\right) \exp imx_3\right) = 0,$$

as the mth term of $r\mathbf{w}_0 + \rho_0\mathbf{s}$ reads

$$r\mathbf{w}_0 + \rho_0\mathbf{s} = \left(D_m \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_2} + \rho_0 A_m, -D_m \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_1} + \rho_0 B_m, \rho_0 C_m\right).$$

Thus,

$$\frac{\partial D_m}{\partial x_1} \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_2} + A_m \frac{\partial \rho_0}{\partial x_1} - D_m \frac{\partial \rho_0}{\partial x_1} \frac{1}{\rho_0^2} \frac{\partial v_0}{\partial x_2} + \rho_0 \frac{\partial A_m}{\partial x_1} + D_m \frac{1}{\rho_0} \frac{\partial^2 v_0}{\partial x_1 \partial x_2} - \frac{\partial D_m}{\partial x_2} \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_1} + B_m \frac{\partial \rho_0}{\partial x_2}$$
$$+ D_m \frac{\partial \rho_0}{\partial x_2} \frac{1}{\rho_0^2} \frac{\partial v_0}{\partial x_1} + \rho_0 \frac{\partial B_m}{\partial x_2} - D_m \frac{1}{\rho_0} \frac{\partial^2 v_0}{\partial x_1 \partial x_2} + im\rho_0 C_m = 0. \tag{7}$$

Therefore one can express C_m as the function of A_m, B_m, and D_m

$$C_m = -\frac{i}{m\rho_0} \left(\frac{\partial D_m}{\partial x_1} \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_2} + A_m \frac{\partial \rho_0}{\partial x_1} - D_m \frac{\partial \rho_0}{\partial x_1} \frac{1}{\rho_0^2} \frac{\partial v_0}{\partial x_2} + \rho_0 \frac{\partial A_m}{\partial x_1} - \frac{\partial D_m}{\partial x_2} \frac{1}{\rho_0} \frac{\partial v_0}{\partial x_1} \right.$$
$$\left. + B_m \frac{\partial \rho_0}{\partial x_2} + D_m \frac{\partial \rho_0}{\partial x_2} \frac{1}{\rho_0^2} \frac{\partial v_0}{\partial x_1} + \rho_0 \frac{\partial B_m}{\partial x_2} \right). \tag{8}$$

We next write a curl^{-1} operator in A_m, B_m, D_m coordinates.

Let $\operatorname{curl} \xi = r\mathbf{w}_0 + \rho_0\mathbf{s}$, and we also assume that

$$\xi = (\xi_1(x_1,x_2,t), \xi_2(x_1,x_2,t), \xi_3(x_1,x_2,t)) \exp imx_3.$$

Then

$$\operatorname{curl} \xi = \left(\frac{\partial \xi_3}{\partial x_2} - im\xi_2, -\frac{\partial \xi_3}{\partial x_1} + im\xi_1, \frac{\partial \xi_2}{\partial x_1} - \frac{\partial \xi_1}{\partial x_2}\right) \exp imx_3.$$

The operator curl^{-1} is defined up to a gradient of a function (the solution to the Euler equations is thus determined by the choice of the pressure function, the boundary conditions and initial conditions, which specify the unique form of the curl^{-1} operator). Here, for simplicity, we choose $\xi_3 \equiv 0$ (which is the correct choice for the incompressible case, as we will see later). In this case we get

$$\xi_1 = \frac{i}{m}\left(D_m \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_1} - \rho_0 B_m\right), \quad \xi_2 = \frac{i}{m}\left(D_m \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_2} + \rho_0 A_m\right). \tag{9}$$

Remark: The expression for curl^{-1} certifies our assumption that $[\mathbf{s}, \mathbf{v}_0]$ is the "strongest" linear operator, compared with the one that contains curl^{-1}: for large values of m the operator curl^{-1} is of order $1/m$, while $[\mathbf{s}, \mathbf{v}_0]$ is of order 1.

We can now write down the linear system for the Fourier coefficients [Eqs. (3)]

$$\frac{\partial D_m}{\partial t} + imv_0 D_m + \frac{\partial \rho_0}{\partial x_1}\xi_1 + \rho_0 \frac{\partial \xi_1}{\partial x_1} + \frac{\partial \rho_0}{\partial x_2}\xi_2 + \rho_0 \frac{\partial \xi_2}{\partial x_2} = 0,$$

$$\frac{\partial A_m}{\partial t} + imv_0 A_m + \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_2}\frac{\partial \xi_1}{\partial x_1} - \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_1}\frac{\partial \xi_1}{\partial x_2} - \xi_1 \frac{\partial}{\partial x_1}\left(\frac{1}{\rho_0}\frac{\partial v_0}{\partial x_2}\right) - \xi_2 \frac{\partial}{\partial x_2}\left(\frac{1}{\rho_0}\frac{\partial v_0}{\partial x_2}\right) = 0,$$

$$\frac{\partial B_m}{\partial t} + imv_0 B_m + \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_2}\frac{\partial \xi_2}{\partial x_1} - \frac{1}{\rho_0}\frac{\partial v_0}{\partial x_1}\frac{\partial \xi_2}{\partial x_2} + \xi_1 \frac{\partial}{\partial x_1}\left(\frac{1}{\rho_0}\frac{\partial v_0}{\partial x_1}\right) + \xi_2 \frac{\partial}{\partial x_2}\left(\frac{1}{\rho_0}\frac{\partial v_0}{\partial x_1}\right) = 0. \tag{10}$$

As we have set $\xi_3 = 0$, the system of Eqs. (10) is a homogeneous linear system in A_m, B_m and D_m. These equations are the most interesting from an acoustic point of view.

We first assume that $\rho_0 = \text{const}$. Thus we can neglect the terms that contain partial derivatives $\partial\rho_0/\partial x$. One can check that Eq. (10) has an "incompressible" solution, $D_m = 0$,

$$A_m = \frac{\partial v_0}{\partial x_1} e^{-imv_0 t}, \quad B_m = \frac{\partial v_0}{\partial x_2} e^{-imv_0 t}.$$

Under our assumptions

$$C_m = \frac{i}{m}\left(\frac{\partial A_m}{\partial x_1} + \frac{\partial B_m}{\partial x_2}\right) = \left(\left(\frac{\partial v_0}{\partial x_1}\right)^2 t + \left(\frac{\partial v_0}{\partial x_2}\right)^2 t + \cdots\right) e^{-imv_0 t},$$

therefore our solution grows at least linearly in time. This solution is indeed incompressible under our choice of the operator curl^{-1}, as

$$\mathrm{div}\ \xi = \frac{i\rho_0}{m}\left(-\frac{\partial B_m}{\partial x_1} + \frac{\partial A_m}{\partial x_2}\right) e^{imx_3} \equiv 0.$$

This is an exact solution, that grows linearly in time, which existence was proved in Ref. 2 for a similar system, by studying the Jordan normal form.

Consider now the case when $v_0 = \text{const}$. Then Eqs. (10) becomes

$$\frac{\partial D_m}{\partial t} + imv_0 D_m + \frac{\partial \rho_0}{\partial x_1}\xi_1 + \rho_0 \frac{\partial \xi_1}{\partial x_1} + \frac{\partial \rho_0}{\partial x_2}\xi_2 + \rho_0 \frac{\partial \xi_2}{\partial x_2} = 0,$$

$$\frac{\partial A_m}{\partial t} + imv_0 A_m = 0, \quad \frac{\partial B_m}{\partial t} + imv_0 B_m = 0. \tag{11}$$

If we have chosen the operator curl^{-1} differently, then the last two equations in system (11) remain the same, but the first one acquires an extra term

$$\frac{\partial D_m}{\partial t} + imv_0 D_m + \frac{\partial \rho_0}{\partial x_1}\xi_1 + \rho_0 \frac{\partial \xi_1}{\partial x_1} + \frac{\partial \rho_0}{\partial x_2}\xi_2 + \rho_0 \frac{\partial \xi_2}{\partial x_2} + im\rho_0 \xi_3 = 0,$$

$$\frac{\partial A_m}{\partial t} + imv_0 A_m = 0, \quad \frac{\partial B_m}{\partial t} + imv_0 B_m = 0. \tag{12}$$

Proposition 2: For almost any choice of the operator curl^{-1}, the general solution to system (12) grows linearly in time.

Proof. All the equations in system (12) are ordinary differential equations, where the coordinates x_1 and x_2 serve as parameters. Instability of the general solution follows from the Jordan form of the system. □

At this point we note that our result giving unstable acoustic solutions whenever $m \neq 0$ is in perfect agreement with previous results obtained in Ref. 19, Eq. (17). In the latter case, it was shown that no stable acoustic solution exists if the wave-vector component m along the flow direction (which is β in the notation of Ref. 19) multiplied by the background flow v_0 equals the sound frequency ω. While the work in Ref. 19 gives emphasis to the small-flow case with large ultrasound frequencies where $|\beta v_0| \ll \omega$ such that acoustic instability is not an issue, the present work is dedicated to the study of acoustic instability in periodic media with background flows.

V. FLOW ACROSS THE PERIODIC STRUCTURE. LINEARIZED EQUATIONS

We consider next the case with flow along the periodic structure which consists of identical infinite cylindrical surfaces, arranged in a periodic rectangular lattice. We assume that both the background flow and the acoustic flow are two dimensional.

We will mostly consider the flows that respect the periodic structure in a sense that they are double periodic, or, formally saying, are invariant under the action of the group $\mathbb{Z}^2$. Thus we can restrict ourselves to studying acoustic flows on 2-tori $\mathbb{T}^2=\mathbb{R}^2/\mathbb{Z}^2$.

In two dimensions, the Helmholtz equation,

$$\frac{\partial \mathbf{w}}{\partial t} + [\mathbf{w}, \mathbf{v}] = 0,$$

reduces to one scalar equation for the *vorticity function* $\omega=\Delta\psi$ and

$$\mathbf{v} = (v_x, v_y) = \left(-\frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial x} \right),$$

$$\frac{\partial \omega}{\partial t} + L_{\mathbf{v}}\omega = 0, \tag{13}$$

with $L_{\mathbf{v}}\omega=v_x(\partial\omega/\partial x)+v_y(\partial\omega/\partial y)$. Note that although the stream function ψ may not be defined *globally* on the torus, Eq. (13) is well defined.

We consider the classical case, when the background flow is potential. To construct such a flow one should solve the Laplace equation with certain boundary conditions. For a special shape of the base of the cylindrical surface this can be done explicitly, see the Appendix: there we give the analytic expression for the background flow in terms of the Weierstrass zeta functions (we first employ the vortex approximation to a flow of an ideal fluid on the 2-torus, and then construct the desired flow).

The flow pattern is shown in Fig. 1. The separatrices form a "Φ"-shape, turned by $\pi/2$. In the exterior of the "Φ" figure we get the background flow.

Let $\mathbf{v}_0$ denote the background potential flow. In our flow region, i.e., in the exterior of the "Φ" figure, curl $\mathbf{v}_0=0$, thus in the linear approximation the Helmholtz equation (13) becomes

$$\frac{\partial \omega}{\partial t} + L_{\mathbf{v}_0}\omega = 0. \tag{14}$$

But this means that the function ω is transported by the flow of the field $\mathbf{v}_0$ (or "frozen" in the flow), which implies that Eq. (14) can be integrated,

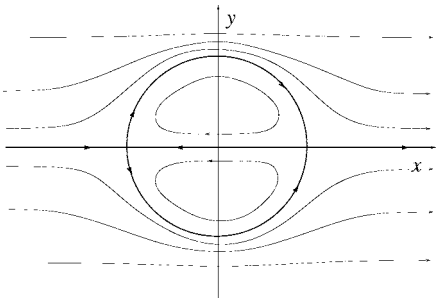

FIG. 1. Flow about the obstacle.

$$\omega(z,t) = \omega^*(g^{-t}_{\mathbf{v}_0} z), \tag{15}$$

where $\omega^*(z)$ is a function on the torus, and $g^t_{\mathbf{v}_0}$ is the phase flow of the vector field $\mathbf{v}_0$.

Let us denote $r=\rho-\rho_0$. We first note that the density function of the background flow ρ_0 is frozen in the flow just like ω. However, from physical considerations, it is natural to consider density as being time independent, as the background flow itself is stationary. Thus $\rho_0(z)$ is a first integral of the flow $g^t_{\mathbf{v}_0}$.

Remark: The operator curl^{-1} *on the plane* is defined for an arbitrary function. However this is not the case for the torus. The reason is that on the torus there are closed 2-forms, that are not exact. As the 2-form $\rho_0\omega^* \mathrm{d}x\wedge\mathrm{d}y$ should be exact (otherwise the d^{-1} operator on forms, that correspond to curl^{-1}, cannot be defined), the integral of the function $\rho_0\omega^*$ over the torus should equal zero—by virtue of the Stokes theorem.

Consider the equation that describes the evolution of r,

$$\frac{\partial r}{\partial t} + L_{\mathbf{v}_0} r + \mathrm{div}(\rho_0 \,\mathrm{curl}^{-1}(\rho_0\omega)) = 0. \tag{16}$$

We denote $\mathrm{div}(\rho_0 \,\mathrm{curl}^{-1}(\rho_0\omega))=f$ and note again that the function $f(z,t)$ should be double periodic in z.

Proposition 3: Let $\partial f/\partial t=0$. *The general solution to Eq. (16) is given by*

$$r(z,t) = r^*(g^{-s}_{\mathbf{v}_0} z) + \int_0^s f(z(\tau))\mathrm{d}\tau - sF(g^{-s}_{\mathbf{v}_0} z) + tF(g^{-s}_{\mathbf{v}_0} z),$$

where s is time passing in going along the phase curve $g^\tau_{\mathbf{v}_0} z$, *that passes through z, from z to the line* $x=0$ *(the integral is also taken along this phase curve), and*

$$F(y) = \int_0^{T(z)} f(z(\tau))\mathrm{d}\tau,$$

where $T(z)$ *is the period of motion along this phase curve.*

Proof: The proposition follows from the general theory of first-order partial differential equations, see, e.g., Ref. 3. The term $sF(g^{-s}_{\mathbf{v}_0} z)$ ensures that the function $\int_0^s f(z(\tau))\mathrm{d}\tau - sF(g^{-s}_{\mathbf{v}_0} z)$ is double periodic in z. □

In general, Eq. (16) has solutions that grow linearly in time. To see this, assume that ρ_0 $=$const and $\omega=0$, while

$$\mathrm{curl}^{-1}(\rho_0\omega) = (0, \cos y),$$

which means that the perturbed flow is potential, but not volume-preserving. The equation for r becomes

$$\frac{\partial r}{\partial t} + L_{\mathbf{v}_0} r - \sin y = 0. \tag{17}$$

For any point z (which does not lie on a separatrix), take a phase curve of the field $\mathbf{v}_0$, that passes through it. Now,

$$F(y) = \int_0^{T(z)} \sin y(\tau) \mathrm{d}\tau,$$

along this curve. The output function F is the function of y only, as the phase curves can be numerated by the y coordinate. Obviously F is not identically zero.

The general solution to Eq. (17) contains the term

$$tF(g_{\mathbf{v}_0}^{-s} z) \neq 0,$$

thus we have found an unbounded solution.

VI. MONOFREQUENCY SOLUTIONS

The usual form for partial solutions to acoustic equations is monofrequency solutions of the type $\omega = \omega(z) \exp i\lambda t$, where $\lambda = \text{const}$, see, e.g., Ref. 19.

Proposition 4: Equation (14) has no smooth (nonzero) monofrequency solutions given by a single-valued function on the torus.

Proof: Let us assume that $\omega = \omega(z) \exp i\lambda t$. Then $\omega(z)$ satisfies the following equation:

$$i\lambda\omega + L_{\mathbf{v}_0}\omega = 0. \tag{18}$$

This equation can be integrated,

$$\omega(z) = e^{i\lambda u(z)} \omega^*(g_{\mathbf{v}_0}^{-s} z), \tag{19}$$

where $\omega(0,x) = \omega^*(y)$, and $u(z)$ is a solution to equation

$$L_{\mathbf{v}_0} u = 1.$$

Solving the latter equation, we get that $u(z) = s$ is the time of the motion along the phase curve $g_{\mathbf{v}_0}^{\tau} z$ from the point z to the line $x = 0$.

If we are looking for a single-valued solution on the torus, we must demand that

$$e^{i\lambda u(2\pi, y)} = e^{i\lambda u(0,y)},$$

i.e., $\lambda u(2\pi, y) = \lambda u(0,y) + 2\pi n$, $n \in \mathbb{Z}$ which for any given point y, is wrong for almost all values of λ. Thus on the torus there are no monofrequency solutions. □

On the other hand, if we let λ depend on the space coordinates, *there may be solutions of the form* (19).

First we notice that if $\lambda = \lambda(z)$ is a first integral of the flow $g_{\mathbf{v}_0}^t$, then the formula (19) does give the solution to Eq. (18). We can now choose λ such that on each phase curve λ equals $1/T$, where T is the period. Then solution (19) is well defined on the torus.

Solutions containing terms of the form $\exp(i\lambda(z)t)$, may lose smoothness for $t \to \infty$: indeed, their *derivative* may contain the terms, linear in t (cf. Ref. 20), which, in our case, provides another source of instability in acoustic flows.

VII. CONCLUSIONS

In this paper we have analyzed the acoustic flow in the general situation, i.e., without assumptions on the monofrequency character of solutions. We have shown that monofrequency solutions, given by single-valued functions on the fluid flow domain, may not exist. We have proved that

general solutions to acoustic equations (that are linearized ideal barotropic fluid equations) usually grow linearly in time. We have found such unbounded solutions explicitly, and in some cases exact expression for the general solution of the acoustic problem were given.

APPENDIX

Proof of Proposition 1

We first write Eq. (4) in our local coordinates,

$$\frac{\partial r}{\partial t} + v_0 \frac{\partial r}{\partial x_3} = 0$$

$$\frac{\partial s_1}{\partial t} + v_0 \frac{\partial s_1}{\partial x_3} = 0, \quad \frac{\partial s_2}{\partial t} + v_0 \frac{\partial s_2}{\partial x_3} = 0,$$

$$\frac{\partial s_3}{\partial t} + v_0 \frac{\partial s_3}{\partial x_3} - s_1 \frac{\partial v_0}{\partial x_1} - s_2 \frac{\partial v_0}{\partial x_2} = 0, \tag{A1}$$

Equation system (A1) has a "wave"-like solution

$$r = \tilde{r}(x_3 - t v_0(x_1, x_2)),$$

$$s_1 = \tilde{s}_1(x_3 - t v_0(x_1, x_2)), \quad s_2 = \tilde{s}_2(x_3 - t v_0(x_1, x_2)),$$

$$s_3 = \tilde{s}_3(x_3 - t v_0(x_1, x_2)) + t\tilde{s}_1(x_3 - t v_0(x_1, x_2)) \frac{\partial v_0}{\partial x_1} + t\tilde{s}_2(x_3 - t v_0(x_1, x_2)) \frac{\partial v_0}{\partial x_2}, \tag{A2}$$

for arbitrary 2π-periodic functions $\tilde{r}(x), \tilde{s}_1(x), \tilde{s}_2(x), \tilde{s}_3(x)$. If we now assume that either $\tilde{s}_1 \partial v_0 / \partial x_1$ or $\tilde{s}_2 \partial v_0 / \partial x_2$ are not identically zero, we get that the function **s** grows linearly in time. Thus almost all solutions to the shortened Eq. (4) grow linearly in time. □

Nonlinear instability

We have shown in Sec. III, that the stationary flow under consideration is generally linearly unstable. In this Appendix, we prove the actual nonlinear instability.

Theorem 2: *Let* $\mathbf{v}_0 \neq const$. *Then the stationary solution (2) is Lyapunov-unstable.*

Proof: We search for a solution to the Helmholtz equations of the following form: $\mathbf{v} = (c_1, c_2, v_3(x_1, x_2, t))$, $\rho = \rho(x_1, x_2, t)$. One can see that for any values of the constants c_1 and c_2, the functions

$$\rho = \rho_0(x_1 - c_1 t, x_2 - c_2 t), \quad v_3 = v_0(x_1 - c_1 t, x_2 - c_2 t), \tag{A3}$$

provide a solution to Eqs. (1). In fact, one can take two arbitrary functions of two variables instead of ρ_0 and v_0. Indeed, the equation for the density reads

$$\frac{\partial \rho}{\partial t} + c_1 \frac{\partial \rho}{\partial x_1} + c_2 \frac{\partial \rho}{\partial x_2} = 0,$$

and it follows that any function $\rho(x_1 - c_1 t, x_2 - c_2 t)$ provides a solution. The same for the vorticity part of Eqs. (1), but now the vector $\mathbf{w}(x_1 - c_1 t, x_2 - c_2 t)$ cannot be arbitrary, as the condition div $\rho \mathbf{w} = 0$ should be satisfied. As this condition is satisfied for the stationary solution, we choose $\rho = \rho_0(x_1 - c_1 t, x_2 - c_2 t)$ and $\mathbf{w} = \mathbf{w}_0(x_1 - c_1 t, x_2 - c_2 t)$.

Now, for any $\epsilon > 0$, choose c_1 and c_2 such that $\|c\|^2 = c_1^2 + c_2^2 = \epsilon^2$. Then the solution (A3) is ϵ-close to the stationary solution (2) at $t = 0$, but then diverges from it for $t = 1/\epsilon$. □

The same result holds for flows on a 3-torus, i.e., when we assume that the velocity and density are periodic in three directions.

Remark: The partial solution we use can be regarded as a special case of solutions studied in Ref. 9 and 18 for incompressible flows. These are solutions that allow decomposition into the "horizontal" and "vertical" components, where both depend only on the "horizontal" coordinates; in our case the "horizontal" component is $(c_1,c_2,0)$, and the "vertical" component is $(0,0,v_3(x_1,x_2,t))$.

Finding a partial solution in the above form is a useful trick: it provides a simple proof for instability of the given stationary solution. As an example, we consider shear flows, studied in Ref. 2 in the linear approximation.

We assume that the flow is incompressible, the flow domain is a 3-torus $\mathbb{T}^3$, and that the stationary solution $\mathbf{v}_0$ is a non-Beltrami solution (the velocity is not proportional to the vorticity). Then both the velocity and vorticity lines lie on 2-tori. We suppose that the 3-torus $\mathbb{T}^3$ is foliated into these 2-tori, and one can choose (local) coordinates ϕ_1,ϕ_2,z, (mod 2π), such that the volume element on $\mathbb{T}^3$ is $\mathrm{d}\phi_1\,\mathrm{d}\phi_2\,\mathrm{d}z$, and

$$\mathbf{v}_0=(v_{1_0}(z),v_{2_0}(z),0).$$

Consider solution to the Euler equation, $\mathbf{v}=(v_1(z,t,\epsilon),v_2(z,t,\epsilon),\epsilon)$,

$$\frac{\partial v_i}{\partial t}+\epsilon\frac{\partial v_i}{\partial z}=0,\quad i=1,2,$$

such that $v_i(0,z)=v_{i_0}(z)$. Then

$$v_1=v_{1_0}(z-\epsilon t),\quad v_2=v_{2_0}(z-\epsilon t).$$

As above, *this solution escapes from the vicinity of the stationary solution, proving that the latter is Lyapunov-unstable*. Moreover, the following result is true.

Proposition 5: Let $\mathbf{v}_0\neq const$, *and let the ratio* v_{1_0}/v_{2_0} *be irrational for* $z=z_0$. *Then for almost all values of* ϵ, *there are trajectories of the vector field* $\mathbf{v}=(v_1(z-\epsilon t),v_2(z-\epsilon t),\epsilon)$, *that are everywhere dense on the torus* $\mathbb{T}^3$.

This proposition proves the nonlinear instability for shear flows in Ref. 2. Notice that the flow can no longer be decomposed into the "horizontal" and "vertical" components as in Ref. 9 and 20.

Proof: Indeed, the equations

$$\dot{\phi}_1=v_{1_0}(z-\epsilon t),\quad \dot{\phi}_2=v_{2_0}(z-\epsilon t),\quad \dot{z}=\epsilon$$

have a solution $z=z_0+\epsilon t$, $\phi_{1,2}=v_{1,2_0}(z_0)t$, which is everywhere dense for almost all ϵ. □

Thus, in general, the trajectories of the velocity field lie no longer on 2-tori. However, all the trajectories of the *vorticity* vector field for the perturbed velocity solution still lie on the same 2-tori, as the original ones ($z=const$), although for big t this field is not close to the vorticity of the stationary flow. Indeed, the z-component of the perturbed vorticity is identically zero: curl $\mathbf{v}=(-\partial v_2/\partial z,\partial v_1/\partial z,0)$.

The vortex approximation to a flow of an ideal fluid

Let $z=(x(\mathrm{mod}\,2\pi),y(\mathrm{mod}\,2\pi))$ be local coordinates on the torus. It is convenient to think of z as a complex number, the velocity $\mathbf{v}$ being a complex-valued function.

In the vortex approximation we assume that the vorticity function is a collection of the Dirac delta functions,

$$\omega(z) = \sum_{i=1}^{N} k_i \delta(z - z_i),$$

where z_i is the coordinate of the ith vortex. The position of the vortices at any given moment of time defines uniquely the fluid velocity field. Assume that the sum $\Sigma_i k_i = 0$. Then the (complex conjugate) velocity field of the fluid is given by a sum of the Weierstrass zeta functions,

$$\frac{d\bar{z}}{dt} = \frac{1}{2\pi i} \sum_{i=1}^{N} k_i \zeta(z - z_i) + C_N, \quad \frac{dz}{dt} = \mathbf{v}, \tag{A4}$$

where C_N does not depend on z, but may depend on instantaneous vortex configuration, see, e.g., Ref. 1, where the exact expression for this constant is provided. Note that although the Weierstrass zeta function is *quasiperiodic* [i.e., $\zeta(z+2\pi m+2\pi i n)=\zeta(z)+mp_1+np_2$, where the constants p_1 and p_2 do not depend on z], their sum is periodic—due to the condition $\Sigma_i k_i = 0$, thus the velocity is a well-defined function on the torus.

The dynamics of the vortices is given by the Hamilton equations

$$\frac{d\bar{z}_i}{dt} = \frac{1}{2\pi i} \sum_{j \neq i}^{N} k_j \zeta(z_i - z_j) + C_N.$$

Analytic expression for the background flow

Let us now consider the velocity field, created by two vortices with intensities $k_1 = -k_2 = k \neq 0$. We assume that the vortices are placed in the points $z_0 = (0, y_0)$ and $\bar{z}_0 = (0, -y_0)$, and that they do not move themselves. Using the expression for the fluid velocity Eq. (A4), we get

$$\frac{d\bar{z}}{dt} = \frac{k}{2\pi i} (\zeta(z - z_0) - \zeta(z + z_0) + \zeta(2z_0)). \tag{A5}$$

Note that there is no single-valued Hamilton function on the torus for our flow.

Remark: The two vortices that we have considered, move with a constant velocity, that equals $-k/2\pi i \zeta(2z_0) + C_N(z_0, \bar{z}_0)$. As we have subtracted this term, we change the coordinate system to the one that moves together with the vortices.

The elliptic function in Eq. (A5) is even ($\mathbf{v}(z) = \mathbf{v}(-z)$), thus if $z = z_1$ is zero of this function, then $z = -z_1$ is also a zero. The number of zero orders of an elliptic function equals the number of pole orders, see, e.g., Ref. 18. Our function $\mathbf{v}(z)$ has two first-order poles, thus it has two zeroes (one zero would be $z_1 = 0$, but one can check that this is not a solution).

We show now explicitly that if $\mathbf{v}(z_1) = 0$, then $\operatorname{Im} z_1 = 0$. Indeed, as $\bar{\zeta}(z) = \zeta(\bar{z})$, $\operatorname{Re} \zeta(iy) = 0$,

$$\frac{2\pi i}{k} \bar{\mathbf{v}}(z_1) = \zeta(x_1 + i(y_1 - y_0)) - \zeta(x_1 + i(y_1 + y_0)) + \zeta(2iy_0) = \bar{\zeta}(x_1 - i(y_1 - y_0)) - \bar{\zeta}(x_1 - i(y_1 + y_0))$$

$$- \bar{\zeta}(2iy_0) = -\bar{\zeta}(-x_1 + i(y_1 - y_0)) + \bar{\zeta}(-x_1 + i(y_1 + y_0)) - \bar{\zeta}(2iy_0) = -\frac{2\pi i}{k} \mathbf{v}(-\bar{z}_1) = 0.$$

Thus, if $\mathbf{v}(z_1) = 0$, then $\mathbf{v}(\bar{z}_1) = 0$. If $\operatorname{Im} z_1 \neq 0$, then we get four distinct points, where our elliptic function satisfies $\mathbf{v}(z) = 0$, which is impossible.

In a similar way as above, one can show that if $\operatorname{Im} z = 0$, then $\operatorname{Im} \mathbf{v}(z) = 0$. As the order of both zeroes of the function $\mathbf{v}(z)$ is one, these are nondegenerate stationary points. Similalry, one can show that if $\operatorname{Im} z = 0$, then $\operatorname{Im} \mathbf{v}(z) = 0$, thus two separatrices, that connect these points, are given by $y = 0$. Together with the to other separatrices, they form a characteristic "Φ"-shape, turned by $\pi/2$, see Fig. 1. In the exterior of the "Φ" figure we get the desired flow about the obstacle.

This way one can describe the potential fluid flow motion about a cylindrical surface. Note that the cross section of this surface is not a circle, still being an analytic curve.

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On metastable regimes in stochastic Lamb system

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We consider the long time behavior of the coupled Hamilton system of one-dimensional string and nonlinear oscillator, in contact with a heat bath modeled by the white noise. For any temperature the system converges to a statistical equilibrium described by the Boltzmann equilibrium measure. The convergence is caused by radiation provided by the nonlinear coupling. If the oscillator potential has more than one well and the temperature is small, the relaxation time is large, and the system goes through a sequence of metastable states located near local minima of the potential. If both, the temperature and the radiation rate are small, the metastable states are distributions among the minima of the potential. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2189198]

I. STRING COUPLED TO A NONLINEAR OSCILLATOR

We will consider a nonlinear oscillator coupled to a heat bath and to a one-dimensional (1D) string. The string is governed by the 1D wave equation

$$\mu\ddot{u}(x,t) = Tu''(x,t), \quad x \in \mathbb{R}\setminus\{0\}, \tag{1.1}$$

where $u(x,t)$ is the real function, $\mu>0$ is the string density, and $T>0$ is its tension. The oscillator is a particle of mass $m>0$ attached to the string at the point $x=0$, so

$$u(0,t) = q(t), \quad t \in \mathbb{R}, \tag{1.2}$$

where $q(t)$ is the deviation of the oscillator. The heat bath is modeled as white noise, so the oscillator is governed by the stochastic equation

$$m\ddot{q}(t) = F(q(t)) + T[u'(0+,t) - u'(0-,t)] + \sqrt{\sigma}\dot{W}(t); \quad q(t) \equiv u(0,t), \tag{1.3}$$

where $F(q)$ stands for the oscillator force function, $W(t)$ is the standard one-dimensional Wiener process, and $\sigma \geqslant 0$ is the temperature of the heat bath. The middle term on the right-hand side of (1.3) descibes the string-oscillator interaction. Roughly speaking, $Tu'(0+,t)$, respectively, $-Tu'(0+,t)$ is the "vertical projection" of the tension of the string to the right-handside, respectively, to the left-handside of the oscillator (see Fig. 1).

The system (1.1)–(1.3) is formally equivalent to a one-dimensional nonlinear wave equation with the nonlinear term concentrated at the single point $x=0$ and with a mass m concentrated at the same point,

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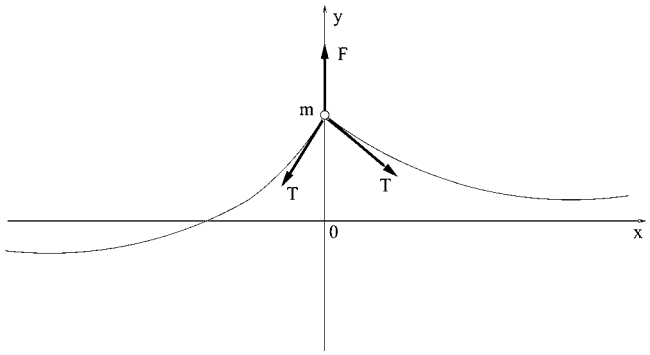

FIG. 1. String with the oscillator.

$$(\mu + m\delta(x))\ddot{u}(x,t) = Tu''(x,t) + \delta(x)[F(u(x,t)) + \sqrt{\sigma}\dot{W}(t)], \quad (x,t) \in \mathbb{R}^2. \tag{1.4}$$

Namely, the equation (1.1) follows from (1.4) with $x \neq 0$, while (1.3) follows by equating the coefficients at the delta function in both sides of (1.4).

For the linear oscillator when $F(q) = -\omega^2 q$ the system (1.1), (1.3) with $\sigma = 0$ was considered originally by Lamb.[11] For general nonlinear force function $F(q)$ and $\sigma = 0$ the system was analyzed in Refs. 8 and 9 (see also Ref. 10, pp. 26–37) where the convergence to stationary states has been proved for all finite energy solutions in the long-time limit $t \to \pm\infty$.

In the present paper we consider the long-time behavior of the Lamb system (1.1)–(1.3) with $\sigma > 0$ modeling the interaction with a heat bath of the temperature σ. We consider the Cauchy problem for the system (1.1)–(1.3) with the initial conditions

$$u|_{t=0} = u_0(x), \quad \dot{u}|_{t=0} = v_0(x), \quad \dot{q}|_{t=0} = p_0. \tag{1.5}$$

We assume that initial functions are compactly supported or decreasing fast enough at infinity. Then one can expect that, due to interplay between the energy dissipation caused by radiation and the incident energy flow from the heat bath, a stationary regime will be established in large time. If the potential $U(q) := -\int F(q)\mathrm{d}q$ has more than one well and the temperature σ is small, the relaxation time is large, and the system goes through a sequence of metastable states.

In generic situation, for a given time scale and an initial point, the system will be situated near certain local minimum of the potential. We consider also the situation when both, the temperature σ and the radiation rate (which can be characterized by the product of the string density and its tension), are small. An "additional stochasticity" appears in this case due to instability near the local maximums of potential. Therefore, even for generic potential, the metastable states are distributions among the minima of the potential. We calculate these limiting distributions.

II. NOTATIONS AND DYNAMICS

Write the Cauchy problem (1.4) and (1.5) in the form

$$\dot{Y}(t) = \mathbf{F}(Y(t),t), \quad t \in \mathbb{R}, \quad Y(0) = Y_0, \tag{2.1}$$

where $Y_0 = (u_0, v_0, p_0)$ and $Y(t) = (u(t), v(t), \dot{q}(t))$.

Let us introduce a phase space $\mathcal{E}$ of finite energy states for the system (1.1)–(1.3). Denote by $\|\cdot\|$, respectively, $\|\cdot\|_R$ the norm in the Hilbert space $L^2 := L^2(\mathbb{R})$, respectively, $L^2(-R,R)$.

Definition 2.1: (i) $\mathcal{E}$ *is the Hilbert space of the triples* $(u(x), v(x), p) \in C(\mathbb{R}) \oplus L^2 \oplus \mathbb{R}$ *with* $u'(x) \in L^2$ *and the* global energy norm

$$\|(u,v,p)\|_{\mathcal{E}} = \|u'\| + |u(0)| + \|v\| + |p|. \tag{2.2}$$

(ii) $\mathcal{E}_F$ *is the space* $\mathcal{E}$ *endowed with the Fréchet topology defined by the* local energy seminorms

$$\|(u,v,p)\|_{\mathcal{E},R} \equiv \|u'\|_R + |u(0)| + \|v\|_R + |p|, \quad R>0. \tag{2.3}$$

(iii) $Y_n \overset{\mathcal{E}_F}{\to} Y$ *iff* $\|Y_n - Y\|_{\mathcal{E},R} \to 0$, $\forall R>0$.

Remark 2.2: This convergence is equivalent to the convergence with respect to the metric

$$\rho(X,Y) = \sum_{R=1}^{\infty} 2^{-R} \frac{\|X-Y\|_{\mathcal{E},R}}{1+\|X-Y\|_{\mathcal{E},R}}, \quad X,Y \in \mathcal{E}. \tag{2.4}$$

We assume that

$$F(q) \in C^1(\mathbb{R}), \tag{2.5}$$

$$U(q) := -\int F(q)\mathrm{d}q \to +\infty, \quad |q| \to \infty. \tag{2.6}$$

Then the system (1.1)–(1.3) for $\sigma=0$ is formally Hamiltonian with the Hamilton functional

$$\mathcal{H}(u,v,p) = \frac{1}{2}\int [|v(x)|^2 + |u'(x)|^2]\mathrm{d}x + m\frac{|p|^2}{2} + U(u(0)) \tag{2.7}$$

for $(u,v,p) \in \mathcal{E}$. We consider solutions $u(x,t)$ such that $Y(t)=(u(\cdot,t),\dot{u}(\cdot,t),\dot{q}(t)) \in C(0,\infty;\mathcal{E})$.

Let us discuss the definition of the Cauchy problem (2.1) for the functions $Y(t) \in C(0,\infty;\mathcal{E})$. At first, $u(x,t) \in C(\mathbb{R}^2)$ due to $Y(t) \in C(0,\infty;\mathcal{E})$. Then the wave equation (1.1) is understood in the sense of distributions. This is equivalent to the d'Alembert decomposition

$$u(x,t) = f_{\pm}(x-at) + g_{\pm}(x+at), \quad \pm x>0, \tag{2.8}$$

where $a=\sqrt{T/\mu}>0$, and $f_- \in C(-\infty,0)$, $g_+ \in C(0,\infty)$, and $f_+, g_- \in C(-\infty,\infty)$. Therefore,

$$\dot{u}(x,t) = -f_{\pm}'(x-at) + g_{\pm}'(x+at), \quad u'(x,t) = f_{\pm}'(x-at) + g_{\pm}'(x+at) \text{ for } \pm x>0,\ t \in \mathbb{R}, \tag{2.9}$$

where all the derivatives are understood in the sense of distributions. The condition $Y(t) \in C(0,\infty;\mathcal{E})$ implies that

$$f_{\pm}', g_{\pm}' \in L^2_{\mathrm{loc}}(\mathbb{R}). \tag{2.10}$$

We now explain the second equation (1.3).

Definition 2.3: In the equation (1.3) *set*

$$u'(0\pm,t) \equiv f_{\pm}'(-at) + g_{\pm}'(at) \in L^2_{\mathrm{loc}}(0,\infty), \tag{2.11}$$

while the derivative $\ddot{q}(t)$ *of* $q(t) \equiv u(0,t) \in C[0,\infty)$ [*or of* $\dot{q}(t) \in L^2_{\mathrm{loc}}[0,\infty)$ *by* (2.10)] *is understood in the sense of distributions.*

Note that the functions $f_{\pm}$ and $g_{\pm}$ in (2.8) are unique up to an additive constant. Hence definition (2.11) is unambiguous.

Proposition 2.4: (*Ref.* 9) *Let the conditions* (2.5), (2.6) *be fulfilled, and* $W(t) \in C(0,\infty;\mathbb{R})$ *is a fixed function. Then*

(i) *For every* $Y_0 \in \mathcal{E}$ *the Cauchy problem* (2.1) *admits a unique solution* $Y(t) \in C(0,\infty;\mathcal{E})$.
(ii) *The map* $U(t): Y_0 \mapsto Y(t)$ *is continuous in* $\mathcal{E}$ *and* $\mathcal{E}_F$.

The proposition is proved in Ref. 9 for the case $W(t) \equiv 0$. The proof for the general case is very similar.

III. GLOBAL ATTRACTOR FOR ZERO TEMPERATURE

The stationary states $S=(s(x),0,0)\in\mathcal{E}$ for (1.1)–(1.3) with $\sigma=0$ are evidently determined. We define for every $c\in\mathbb{R}$ the constant function

$$s_c(x)=c,\quad x\in\mathbb{R}. \tag{3.1}$$

Then the set $\mathcal{S}$ of all stationary states $S\in\mathcal{E}$ is given by

$$\mathcal{S}=\{S_z=(s_z(\cdot),0,0):\ z\in Z\}, \tag{3.2}$$

where $Z=\{z\in\mathbb{R}:\ F(z)=0\}$.

The set S is a global attractor for the Lamb system (1.1)–(1.3) with $\sigma=0$.[9] Our main goal in this paper is to describe the convergence to the statistical equilibrium for the Lamb system with $\sigma>0$, and metastable rejimes for small $\sigma>0$ and $m>0$.

IV. REDUCED EQUATION FOR POSITIVE TEMPERATURE

The Lamb system (1.1)–(1.3) is equivalent to the following reduced equation:

$$m\ddot{q}(t)=F(q(t))-\frac{2T}{a}\dot{q}(t)+\frac{2}{a}\dot{w}_{\rm in}(t)+\sqrt{\sigma}\dot{W}(t),\quad t>0, \tag{4.1}$$

where $w_{\rm in}(t)\in C[0,\infty)$ is determined by the initial conditions (1.5) and the equation is understood in the sense of the corresponding integral equation (or distributions).[9,10]

For $|x|\geqslant at\geqslant 0$ at the solution of the system (1.1)–(1.3) is determined uniquely by the initial functions and is expressed by the d'Alembert formula

$$u(x,t)=\frac{u_0(x-at)+u_0(x+at)}{2}+\frac{1}{2}\int_{x-at}^{x+at}v_0(y)\mathrm{d}y,\quad |x|\geqslant at\geqslant 0. \tag{4.2}$$

For $|x|\leqslant at$ the solution cannot be expressed in the initial functions. Indeed, the waves $f_+(x-at)$, respectively, $g_-(x+at)$ [see (2.8)] in the regions $0<x<at$, respectively, $-at<x<0$ are the *reflected waves* and are not determined by the initial conditions. To determine both these two reflected waves we need two equations: first is the gluing equation $u(0+,t)=u(0-,t)$, and the second is the "jump equation" (1.3). Substituting the d'Alembert representations (2.8) to the equations, we get (see Ref. 9 or Ref. 10, Chap. 1, Lemma 4.6) the reduced equation (4.1), where $w_{\rm in}(t)$ is the sum of the *incident waves* $g_+(x+at)$ and $f_-(x-at)$ at the point $x=0$:

$$w_{\rm in}(t)=g_+(at)+f_-(-at),\quad t\geqslant 0. \tag{4.3}$$

For this function we have

$$\dot{w}_{\rm in}(t)\in L^2(0,\infty) \tag{4.4}$$

since the initial functions belong to the phase space of finite energy states. Moreover, we get the expressions [see Ref. 10, Chap. 1, (4.33)]

$$u(x,t)=\left\{\begin{array}{ll} q(t-x/a)+g_+(x+at)-g_+(at-x), & 0<x<at\\ q(t+x/a)+f_-(x-at)-f_-(-x-at), & -at<x<0\end{array}\right|,\quad t\geqslant 0. \tag{4.5}$$

It is important to note that this formula contains only the incident waves which are constant for large time if the initial functions are constant for large $|x|$. Namely, let us consider the initial functions in (1.5) with

$$u_0(x)=C_\pm,\quad v_0(x)=0,\quad \pm x>R_0. \tag{4.6}$$

Then $g_+(z)=c_+$ for $z>R_0$, and $f_-(z)=c_-$ for $z<-R_0$. Hence (4.3) implies that

$$w_{\text{in}}(t) = 0, \quad t > R_0/a. \tag{4.7}$$

Respectively, (4.1) becomes

$$m\ddot{q}(t) = F(q(t)) - \frac{2T}{a}\dot{q}(t) + \sqrt{\sigma}\dot{W}(t), \quad t > R_0/a, \tag{4.8}$$

and (4.5) implies that

$$u(x,t) = q(t - |x|/a), \quad |x| < R, \quad t \geqslant \frac{R + R_0}{a} \tag{4.9}$$

for every $R > 0$. Finally, take into account the value of a. Then (4.8) reads

$$m\ddot{q}(t) = F(q(t)) - 2\sqrt{\mu T}\dot{q}(t) + \sqrt{\sigma}\dot{W}(t), \quad t > R_0/a. \tag{4.10}$$

Our goal is to describe a long-time behavior of the solution for the cases

$$m \sim \sqrt{\mu T} \ll 1, \quad \sqrt{\sigma} \ll 1. \tag{4.11}$$

V. CONVERGENCE TO EQUILIBRIUM DISTRIBUTION

If the supports of the initial functions $u_0(x)$ and $v_0(x)$ belong to a finite interval $|x| < R_0 < \infty$, then, at least after time $t_0 = R_0/a$, no incident waves come to the origin. So the evolution of the oscillator can be described by Eq. (4.10) which is equivalent to the following system:

$$\begin{aligned} \dot{q}(t) &= p(t), \\ m\dot{p}(t) &= -U'(q(t)) - 2\sqrt{\mu T}p(t) + \sqrt{\sigma}\dot{W}(t), \quad t > t_0. \end{aligned} \tag{5.1}$$

The values $q(t_0)$ and $p(t_0)$ are defined by the initial condition and by the trajectory $W(t)$ for $0 \leqslant t \leqslant t_0$.

The stochastic process $(q(t), p(t))$ defined by (5.1) is a (degenerate) diffusion process governed by the differential operator

$$Lu(q,p) = p\frac{\partial u}{\partial q} - \frac{1}{m}[U'(q) + 2p\sqrt{\mu T}]\frac{\partial u}{\partial p} + \frac{\sigma}{2m^2}\frac{\partial^2 u}{\partial p^2}. \tag{5.2}$$

Solving the stationary Fokker-Planck (forward Kolmogorov) equation $L^* v(q,p) = 0$, we find the stationary Boltzman distribution

$$v(q,p) = \frac{1}{Z}\exp\left\{-\frac{4\sqrt{\mu T}}{\sigma}\left(\frac{mp^2}{2} + U(q)\right)\right\}, \tag{5.3}$$

where Z is a normalizing constant,

$$Z = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left\{-\frac{4\sqrt{\mu T}}{\sigma}\left(\frac{mp^2}{2} + U(q)\right)\right\}\mathrm{d}p\,\mathrm{d}q.$$

Assume that the following condition (*) is satisfied: for some $Q_0 > 0$,

$$U'(q)\,\operatorname{sign} q \geqslant \alpha > 0 \quad \text{for } |q| > Q_0\,. \,(*)$$

This condition, in particular, provides finiteness of the normalizing constant Z.

Proposition 5.1: Let condition (*) *be satisfied. Then*

(i) *There exists a unique stationary solution* $(\bar{q}(t), \bar{p}(t))$ *of system* (5.1). *For any* t, *the*

distribution of $(\bar{q}_t,\bar{p}_t)$ *is given by* (5.3).

(ii) *The solution* $(q(t),p(t))$ *of system* (5.1) *with any initial condition* $q(0)=q_0, p(0)=p_0$, *converges to* $(\bar{q}_t,\bar{p}_t)$ *as time tends to infinity, i.e.*

For every $A>0$, *the distribution of the random process* $(g(T+s),p(T+s)), 0\leqslant s\leqslant A$, *in* $C_{0,A}$ *converges weakly to the distribution of* $(\bar{q}_s,\bar{p}_s)$ *as* $T\to\infty$.

Proof: Without loss of generality, we can assume, that $m=2\sqrt{\mu T}=\sigma=1$. Then the function

$$v(q,p)=\frac{p^2}{2}+(q-\gamma\arctan q)p+v(q)+\int_0^q(s-\gamma\arctan s)\mathrm{d}s+k$$

for a suitable choice of parameters γ,k satisfies the conditions (see Ref. 7, Sec. 3.5) $v(q,p)\geqslant 0, Lv(q,p)<-\alpha<0$ for $|p|+|q|$ large enough, $\lim_{|p|+|q|\to\infty} v(q,p)=\infty$. Here L is defined in (5.2) and α is a positive constant from (*).

As we already mentioned, the Boltzman distribution is invariant for the equation (5.1). To prove uniqueness of the stationary distribution and convergence, one can use the standard construction which goes back to Ref. 7. Therefore we give just a sketch of the proof.

Let $\gamma_A, A>0$ be the boundary of the square $\{(q,p)\in\mathbb{R}^2: |q|<A, |p|<A\}, \Gamma_A=\gamma_{A+1}$. Consider a Markov chain Z_n with the state space γ_A which is defined as follows: Starting from any point $Z_0=(q_0,p_0)\in\gamma_A$, the trajectory of the process $X_t=(q_t,p_t)$ hits at some time Γ_A and then comes back to γ_A. Let τ be the first time when X_t comes to γ_A after hitting Γ_A. Existence of the function $v(q,p)$ constructed above implies that the random variable τ is finite with probability 1, and the expected value $E\tau<\infty$, at least, if A is large enough. Set $Z_1=X_\tau$, so that the chain Z_n in one step jumps from Z_0 to $Z_1=X_\tau$. The standard proof of uniqueness of the stationary distribution and convergence to it is given under nondegeneracy assumption of the operator L.

In our case L is degenerate. But it satisfies the Hörmander conditions, providing the existence of a positive density for X_t. Moreover, one can check that, due to the structure of the operator L, Doeblin conditions for the chain Z_n are satisfied (Ref. 2, Sec. 6.2). This implies that the chain Z_n on γ_A has a unique stationary distribution which is also the limiting distribution for Z_n.

The last property provides uniqueness of the stationary distribution for process (q_t,p_t) and convergence to this distribution (which is the Boltzman distribution) as $t\to\infty$. This implies existence and uniqueness of a stationary process $(\bar{q}_t,\bar{p}_t)$ satisfying equations (5.1) and the last statement of Proposition 5.1. The stationary process $(\bar{q}_t,\bar{p}_t)$ is the solution of (5.1) with the initial point distributed according to the Boltzman distribution.

Theorem 5.1: *Let* (*) *be satisfied, and the initial functions* (1.5) *have a compact support. Then, we have the following*:

(i) *There exists a unique random field* $\bar{u}(t,x)$, $t\in(-\infty,\infty)$, $x\in\mathbb{R}^1$, *such that* $\bar{u}(t,x)$ *is a solution of equation*

$$\mu\frac{\partial^2\bar{u}}{\partial t^2}=T\frac{\partial^2\bar{u}}{\partial x^2},\quad t\in(-\infty,\infty),\quad x\in\mathbb{R}^1\setminus\{0\};\tag{5.4}$$

at $x=0$ *the gluing conditions* (1.2) and (1.3) *are satisfied. The distribution of* $\bar{u}(t,x)$ *is invariant with respect to time shifts*: *for any* $h\in\mathbb{R}^1$, $\bar{u}(t+h,x)$ *and* $\bar{u}(t,x)$ *have the same distribution in the space of continuous functions* $\varphi(t,x)$, $t\in(-\infty,\infty), x\in\mathbb{R}^1$.

(ii) *This unique solution is given by the formula* [cf. (4.9)]

$$\bar{u}(t,x)=\bar{q}\left(t-\frac{|x|}{a}\right),\quad (x,t)\in\mathbb{R}^2,\tag{5.5}$$

where $a=\sqrt{T/\mu}$.

(iii) *For every initial condition with a compact support, the solution* $u(t,x)$ *of problem* (1.1)–(1.3) *converges to the stationary solution* $\bar{u}(t,x)$.

For any $A>0$, the random process $\tilde{u}_T(t,x)=u(T+t,x), 0\leqslant t\leqslant A, |x|\leqslant A$, converges weakly to $\bar{u}(t,x)$ as $T\to\infty$ in the space of continuous functions on $[0,A]\times[|x|\leqslant A]$ provided with uniform topology.

Proof: As it follows from Proposition 5.1, if condition (*) is satisfied, a unique stationary solution $(\bar{q}_t,\bar{p}_t)$ of problem (5.1) exists. Then the function (5.5) satisfies equation (5.4) and the gluing conditions at $x=0$. Since the stochastic process $\bar{q}_t$ is invariant with respect to the time shifts, so is the function $\bar{u}(t,x)$. If another time shift invariant solution $\bar{\bar{u}}(t,x)$ exists, then $\bar{\bar{u}}(t,0)$ should coincide in distribution with $\bar{q}_t$, since problem (5.1) has a unique stationary solution. Convergence of the solution of problem (1.1)–(1.3) with compactly supported initial functions to $\bar{u}(t,x)$ follows by the formula (4.9) from the convergence of $q(t)$ to $\bar{q}_t$.

VI. LOW TEMPERATURE LIMIT

Let us note that the Boltzman equilibrium distribution (5.3) corresponds to the temperature proportional to

$$\frac{\sigma}{\sqrt{\mu T}}. \tag{6.1}$$

Here we discuss low temperature behavior in the Lamb system (1.1)–(1.3), when $\sigma\to 0$ for fixed μ and T.

If the potential $U(q)$ has more than one well, and $\sigma\ll 1$, the convergence to the stationary regime will be slow, and the system will go through a sequence of metastable regimes, where it spends a long time before approaching the stationary solution described above.

The sequence of metastable regimes depends on the equilibrium state of equations (5.1) with $\sigma=0$, to which the system was brought by the initial conditions (1.5). Since we assume that the initial conditions have a compact support, say, they are equal to zero for $|x|>\theta$, no incident waves come to the origin $x=0$ after time $t_0=\theta/a$. Set $u(t_0,0)=q_0^*$, $\dot{u}(t_0,0)=p_0^*$.

Assume that, for system (5.1) with $\sigma=0$, the initial point (q_0^*,p_0^*) is attracted to the stable equilibrium $O_{k(q_0^*,p_0^*)}$. The point $O_{k(q_0^*,p_0^*)}$ in the phase space $\mathbb{R}^2$ has coordinates $(q_{k(q_0^*,p_0^*)},0)$; $q_{k(q_0^*,p_0^*)}$ is a local minimum of the potential $U(q)$.

If $\sigma=0$, then the solution of system (5.1) with initial point (q_0^*,p_0^*) will stay near $O_{k(q_0^*,p_0^*)}$ forever. In the case $0<\sigma\ll 1$, the trajectory (q_t^σ,p_t^σ) of system (5.1) will stay in a neighborhood of $O_{k(q_0^*,p_0^*)}$ a time of order $\exp\{\text{const}/\sigma\}$, and then will switch to another equilibrium of system (5.1) with $\sigma=0$. It will stay there a long time and then again switches to the basin of another equilibrium and so on. It is important to underline that, in the generic case, for each stable equilibrium O_k, there exists exactly one (nonrandom) equilibrium $O_{k'}$, such that, with probability close to 1 for σ small enough, the system switches from O_k to $O_{k'}$. Since we assume that there are just a finite number of minima of $U(q)$, the sequence of transitions, after some time, becomes periodic (see Refs. 3 and 4). Thus we will have a decomposition of the set of local minima of $U(q)$ in cycles of rank 1. Moreover, the transition time $T^\sigma_{k,k'}$ between the basins of O_k and $O_{k'}$ is a random variable, but its logarithmic asymptotics as $\sigma\downarrow 0$ is not random.[3] In time scale larger than transition time in first rank cycles, transitions between the 1-cycles begin. So that in larger time scale, cycles of rank 2 appear, then cycles of rank 3, and so on, until all stable equilibriums of the nonperturbed system will be involved in the transitions.

The cycles of higher rank, as well as the logarithmic asymptotics of transition times between them, are also not random. So that one can speak on quasideterministic approximation for the long-time behavior of a dynamical system perturbed by a small noise. This hierarchy of cycles in a rather general situation was described in Refs. 3 and 4. The construction based on the large deviation theory for dynamical system perturbed by a small noise.[6]

Denote by $\mathcal{E}(O_k,E)$, $E\geqslant U(O_k)$, the connected component of the set $\{q\in\mathbb{R}^1: U(q)\leqslant E\}$ con-

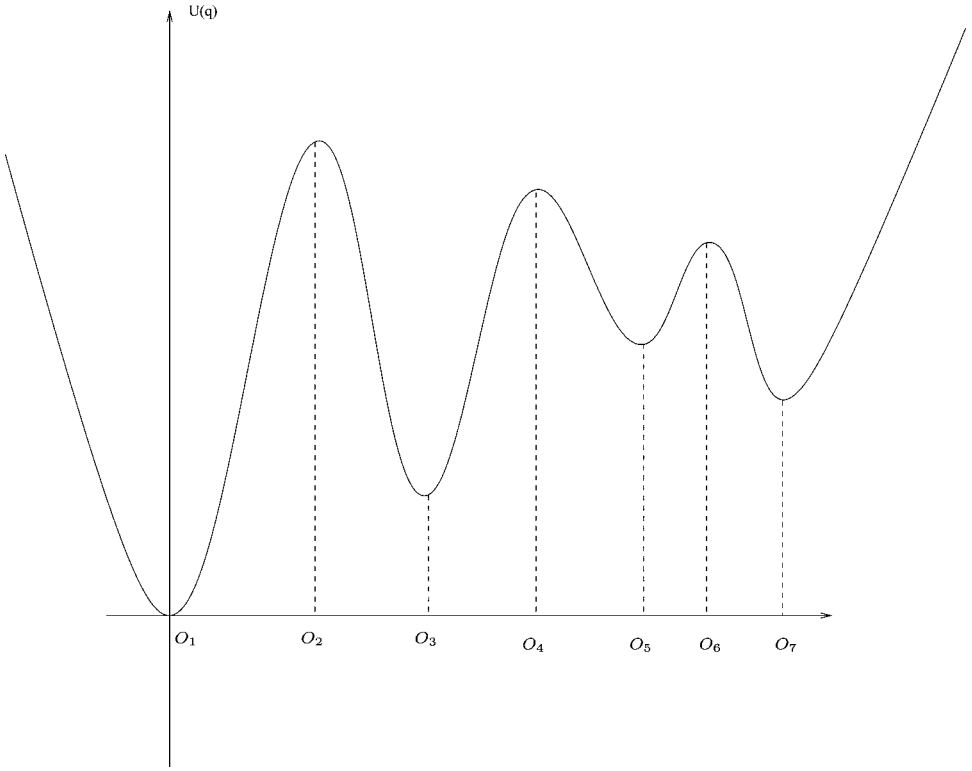

FIG. 2. Potential.

taining the stable equilibrium O_k. Let $O_{k^*(k,E)}$ be the point of $\mathcal{E}(O_k,E)$ such that $\min\{U(q):q \in \mathcal{E}(O_k,E)\}=U(O_{k^*(k,E)})$. We assume that the potential $U(q)$ is generic. Then the equilibrium $O_{k^*(k,E)}$ is defined in a unique way.

It is clear that for E close enough to $U(O_k)$, $O_{k^*(k,E)}=O_k$. If the potential is generic, and O_k is just a local, but not global, minimum of $U(q)$, then one can find E_1 such that $O_{k^*(k,E)}=O_k$ for $E \in (U(O_k),E_1)$, and $O_{k^*(k,E)} \neq O_k$ for $E>E_1$. In general, $E_1<E_2<\cdots<E_m$ exist such that $O_{k^*(k,E)}=O_{\bar{k}}$, $\bar{k}=\bar{k}(k,E_i,E_{i+1})=\text{const}$ for $E \in (E_i,E_{i+1})$, $i \in \{0,\ldots,m\}$, $E_0=U(O_k)$, $E_{m+1}=\infty$. Such an increasing sequence E_i can be defined for any stable equilibrium O_k. If $U(O_k)=\min\{U(q):q \in \mathbb{R}^1\}$, then set $E_1=\infty$.

For example, for the potential shown in Fig. 2 and $O_k=O_5$, $E_1=U(O_6)$, $E_2=U(O_4)$, $E_3=U(O_2)$, and $E_4=\infty$; $\bar{k}(5,U(O_5),E_1)=5$, $\bar{k}(5,E_1,E_2)=7$, $\bar{k}(5,E_2,E_3)=3$, $\bar{k}(5,E_3,E_4)=1$.

Set $\lambda_1=E_1-U(O_k)$, $\lambda_2=E_2-U(O_{\bar{k}(E_1,E_2)}),\ldots,\lambda_l=E_l-U(O_{\bar{k}(k,E_{l-1},E_l)}),\ldots,\lambda_m=E_m-U(O_{\bar{k}(k,E_{m-1},E_m)})$. It is easy to see that $\lambda_1<\lambda_2<\cdots<\lambda_m$.

It follows from Refs. 6 and 4 that in the time scale $T^\sigma \asymp e^{\lambda/\sigma}$, $\lambda_l<\lambda<\lambda_{l+1}$ (here "$\asymp$" is the sign of logarithmic equivalency as $\sigma \downarrow 0$), trajectory (q_t,p_t) of system (5.1) starting at a point from the basin of O_k spends most of the time as $a \downarrow 0$ in a small neighborhood of $O_{\bar{k}(E_l,E_{l+1})}$: For each $\delta>0$, the random variable,

$$\eta_\sigma^\delta=\frac{1}{T^\sigma}\wedge\{t \in [0,T^\sigma]:d((q_t,p_t),O_{\bar{k}(k,E_lE_{l+1})})>\delta\},$$

where $\wedge\{\cdot\}$ stands for the Lebesgue measure in $\mathbb{R}^1$, and $d(\cdot,\cdot)$ is Euclidian distance in $\mathbb{R}^2$, tends to zero in probability as $\sigma \downarrow 0$.

This and formula (4.9) imply the following result.

Theorem 6.1: *Let condition* (*) *be satisfied and the initial functions* (1.5) *have a compact*

support: $u_0(x)=v_0(x)=0$ *for* $|x|\geqslant R_0$. *Suppose the point* $(u(\theta/a,0),\dot{u}(\theta/a,0))$ *belongs to the basin of a stable equilibrium* O_k. *Let* $T^\sigma \asymp e^{-\lambda/\sigma}$, $\lambda \in (\lambda_l,\lambda_{l+1})$, $O^-_{k(k,E_l,E_{l+1})}=(q^-_{k(k,E_l,E_{l+1})},0)$. *Then, for every* $A>0$,

$$\int_{-A}^{A} \mathrm{d}x \int_0^A |u(tT^\sigma,x) - q^-_{k(k,E_l,E_{l+1})}|^2 \,\mathrm{d}t$$

tends to zero in probability as $\sigma \downarrow 0$.

VII. LOW TEMPERATURE AND RADIATION LIMIT

Consider now the case

$$m \ll 1, \quad 2m^{-1}\sqrt{T\mu} \sim 1, \quad k=\frac{\sigma}{m} \ll 1. \tag{7.1}$$

Then the Eq. (4.10) can be written as follows:

$$\ddot{q}(t) = -\frac{1}{m}U'(q(t)) - \dot{q}(t) + \sqrt{\frac{\kappa}{m}}\dot{W}_t. \tag{7.2}$$

Hence, the first two conditions in (7.1) mean that the Hamiltonian vector field is large with respect to the "radiative effects" described by the friction term in (7.2), so we can apply the averaging arguments. The last two conditions in (7.1) mean the low temperature limit $\sigma \to 0$, as above [see (6.1)].

In the preceding section, under certain conditions, we described metastable regimes of our system: For a given initial state and a time scale, the system spends most of the time near certain stationary state of the system without noise (zero temperature). Under conditions of this section, the metastable state, in general, is not a stationary state of the zero temperature system, but a certain distribution among such states. This distribution is determined by the initial conditions and the time scale.

To be specific, we assume that the potential has four minima. Then the Hamiltonian $H(p,q)=p^2/2m+U(q)$ has the wells as it is shown in Fig. 3. The case of general potential can be treated similarly.

The level set $C(z)=\{(q,p):H(q,p)=z\}$ consists, in general of several connected components $C_k(z):C(z)=\cup_{k=1}^N C_k(z)$. We denote by $G_k(z)$ the domain bounded by $C_k(z)$ (compare with Ref. 6, Chap. 8). Let Γ be the graph homeomorphic to the set of connected components of all level sets of the Hamiltonian $H(q,p)$ [Fig. 3(b)] provided with natural topology.

The connected component of the level set of a saddle point O_2, containing O_2, is an eight-shaped curve γ [Fig. 3(c) and 3(d)] consisting of two parts G_1 and G_2.

Equation (7.2) can be written as the system

$$\begin{aligned} \dot{q}^{m,\kappa}(t) &= \frac{1}{\sqrt{m}}p^{m,\kappa}(t), \\ \dot{p}^{m,\kappa}(t) &= -\frac{1}{\sqrt{m}}U'(q^{m,\kappa}(t)) - p^{m,\kappa}(t) + \sqrt{\kappa}\dot{W}(t). \end{aligned} \tag{7.3}$$

Let, first, $m \to 0$, then we are in the situation when the averaging principle should be applied. The fast component of the process $(q^{m,\kappa}(t),p^{m,\kappa}(t))$ is, roughly speaking, the motion along the trajectories of the Hamiltonian system with

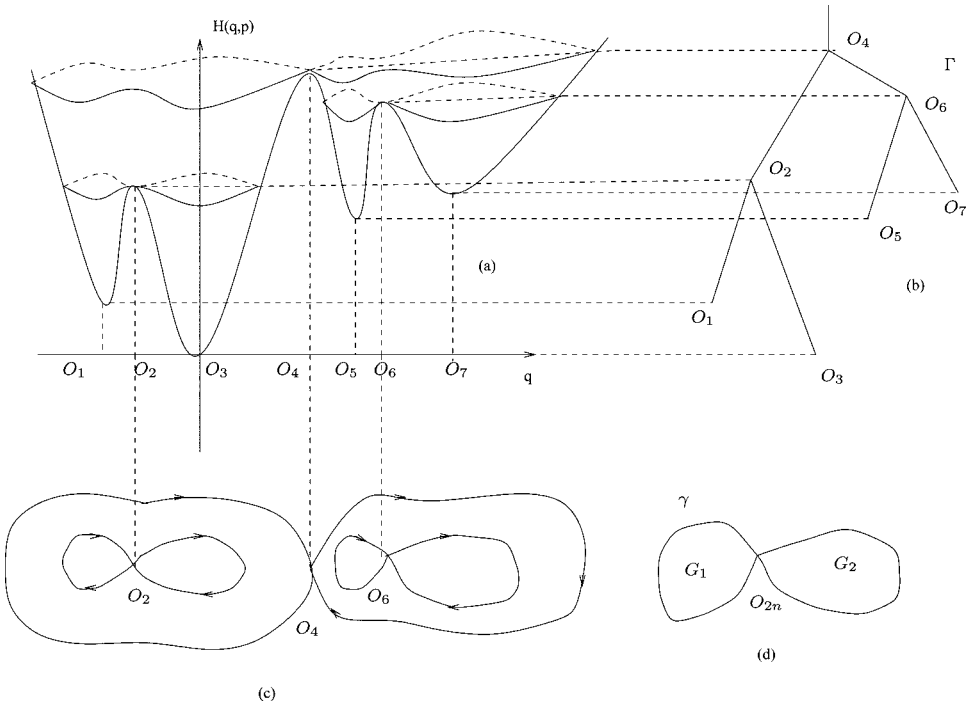

FIG. 3. Hamiltonian, graphs and level sets.

$$H = \frac{p^2}{2} + U(q),$$

and the slow component is the projection $Y(q^{m,\kappa}(t), p^{m,\kappa}(t))$ on the graph Γ: $Y(x)$ is the point of the graph corresponding to the connected component of $H(x)$-level set containing the point $x \in \mathbb{R}^2$.[5,6] It is shown in Ref. 5 that $Y(q^{m,\kappa}(t), p^{m,\kappa}(t))$ converges weakly (in the space of continuous functions on any finite time interval $[0, M]$ with the values in Γ) to a diffusion process $Y^\kappa(t)$ on Γ. The process $Y^\kappa(t)$ is defined by the family of second order operators L_k^κ, one on each edge of the graph, and by gluing conditions at the vertices.

The operator L_k^κ on the edge I_k has the form

$$L_k^\kappa(q,p)f(z) = \frac{\kappa}{2T_k(z)}\frac{d}{dz}\left(\bar{a}_k(z)\frac{df}{dz}\right) - \frac{\bar{\beta}_k(z)}{T_k(z)}\frac{df}{dz},$$

where $T_k(z)$ is the period of rotation along the level set component $C_k(z)$ corresponding to the point (z,k) of the graph: k is the number of the edge containing this point, and z is the corresponding value of the Hamiltonian $H(q,p)$ on the level set of component corresponding to the point of Γ.

Further, $T_k(z) = S'(z)$, where $S_k(z)$ is the area of the domain $G_k(z)$ bounded by $C_k(z)$, and

$$\bar{a}_k(z) = \bar{\beta}_k(z) = S_k(z).$$

To define the process $Y^\kappa(t)$ on Γ in a unique way one should add gluing conditions at the vertices. These conditions were calculated in Ref. 5, but we do not need their form, so we will not describe them here.

Now we want to take κ to zero in the process $Y^\kappa(t)$ on Γ. Then (see Ref. 1) $Y^\kappa(t)$ converges weakly as $\kappa \to 0$ to a process $Y(t)$ on Γ, which has the following structure. Inside an edge $I_k \subset \Gamma$, this is a nonrandom motion with the speed $-\bar{\beta}_k(z)/T_k(z) = -S_k(z)/S_k'(z)$. When a trajectory comes

to a vertex O corresponding to a saddle point (vertices O_2, O_4, and O_6 in Fig. 3), it proceeds without any delay at O in one of the edges below (in energy) of O with certain probabilities $P_1(O)$ and $P_2(O)$, $P_1(O)+P_2(O)=1$. To find these probabilities, one should consider the eight-shaped curve $\gamma(O)$ corresponding to the vertex O [see Fig. 3(d)]. It has two components $G_1(O)$ and $G_2(O)$. Then

$$P_i(O) = \frac{S(G_i)}{S(G_1) + S(G_2)}, \quad i = 1,2,$$

$S(G_i)$ being the area of G_i.

Assume that at time t_0 the oscillator has the energy H_0 greater than the level set of the highest saddle point [$H_0 > H(O_4)$ in Fig. 3]. Then because of "friction" (=radiation) it will lose the energy until it comes to the level $H(O_4)$; this will happen in a finite time. Then trajectory goes to the left (to the edge $[O_2, O_4]$) with probability

$$P_1(O_4) = \frac{S(G_1(O_4))}{S(G_1(O_4)) + S(G_2(O_4))},$$

and to the right (to $[O_4, O_6]$) with probability

$$P_2(O_4) = \frac{S(G_2(O_4))}{S(G_1(O_4)) + S(G_2(O_4))}.$$

Trajectory $Y(t)$ proceeds to go down until it meets the next saddle point (O_2 or O_6). It is scattered on those saddle points and eventually approaches one of the local minima of the potential. In a finite time for every $\delta > 0$ it approaches the δ neighborhood of one of the local minima and stays in the corresponding well a time of order $e^{C/\kappa}$, where

$$C = \min\{U(O_2) - U(O_1), U(O_2) - U(O_3), U(O_6) - U(O_5), U(O_6) - U(O_7)\}.$$

Thus if we observe $(q_t^{m,\kappa}, p_t^{m,\kappa})$ on the time interval $1 \ll t < T_E^\kappa = e^{E/\kappa}$ with $0 < E < C$, it is distributed among the local minima O_1, O_3, O_5, O_7 with probabilities, respectively, equal to

$$\begin{aligned}
m_1 &= \frac{S(G_1(O_4))}{S(G_1(O_4)) + S(G_2(O_4))} \cdot \frac{S(G_1(O_2))}{S(G_1(O_2)) + S(G_2(O_2))}, \\
m_3 &= \frac{S(G_1(O_4))}{S(G_1(O_4)) + S(G_2(O_4))} \cdot \frac{S(G_2(O_2))}{S(G_1(O_2)) + S(G_2(O_2))}, \\
m_5 &= \frac{S(G_2(O_4))}{S(G_1(O_4)) + S(G_2(O_4))} \cdot \frac{S(G_1(O_6))}{S(G_1(O_6)) + S(G_2(O_6))}, \\
m_7 &= \frac{S(G_2(O_4))}{S(G_1(O_4)) + S(G_2(O_4))} \cdot \frac{S(G_2(O_6))}{S(G_1(O_6)) + S(G_2(O_6))},
\end{aligned} \tag{7.4}$$

if, first, $m \downarrow 0$ and then $\kappa \downarrow 0$. This is metastable distribution in the time scale $T_E^\kappa = e^{E/\kappa}$ for $E < C$. In larger time scales, the support of this limiting distribution will become smaller and smaller. To be specific, assume that

$$U(O_6) - U(O_7) < U(O_6) - U(O_5) < U(O_4) - U(O_5) < U(O_2) - U(O_1) < U(O_2) - U(O_3). \tag{7.5}$$

Then if $U(O_6) - U(O_7) < E < U(O_6) - U(O_5)$, trajectory already have enough time to leave O_7 so that the metastable distribution among O_1, O_3, O_5, O_7 in this time scale is $(m_1, m_3, m_5 + m_7, 0)$. If $E \in (U(O_4) - U(O_5), U(O_2) - U(O_1))$, the metastable distribution is

$$\left(\frac{S(G_1(O_2))}{S(G_1(O_2))+S(G_2(O_2))},\frac{S(G_2(O_2))}{S(G_1(O_2))+S(G_2(O_2))},0,0\right).$$

Eventually, if $E>U(O_2)-U(O_1)$, then the distribution is concentrated at point O_3, which is the absolute minimum of the potential.

Together with the equality $u(t,x)=u^{m,\kappa}(t,x)=q^{m,\kappa}(t-|x|/a)$, $a=T/m$, which holds for any $x \in \mathbb{R}^1$ and t large enough, this implies the following result.

Theorem 7.1: Let condition (*) be satisfied, and initial functions (1.5) have a compact support belonging to $\{|x|<\theta\}\subset\mathbb{R}^1$. Let the Hamiltonian $H(p,q)=p^2/2+U(q)$ be as shown in Fig. 3. Let the energy of the oscillator with $\kappa=0$ be greater than $U(O_4)$ at time $t_0=\theta/a$:

$$\frac{m}{2}\left(\frac{\partial u^{m,0}(t_0,0)}{\partial t}\right)^2+U(u^{m,0}(t_0,0))>U(O_4).$$

Assume that inequalities (7.5) are satisfied. Then for any A, $E>0$ and $T_E^\kappa \asymp \exp\{E/\kappa\}$, the random function $u^{m,\kappa}(T_E^\kappa t,x)$, $t\in[0,A]$, $x\in[-A,A]$, converges weakly in $L^2_{[0,A]\times[-A,A]}$ to a random variable η_E as, first, $m\downarrow 0$ and then $\kappa\downarrow 0$.

The random variable η_E has values O_1,O_3,O_5,O_7 with probabilities m_1,m_3,m_5,m_7, respectively, if $0<E<C$, with probabilities $(m_1,m_3,m_5+m_7,0)$ if $E\in(U(O_6)-U(O_7),U(O_6),-U(O_5))$, with probabilities $m_1+m_3,m_5+m_7,0,0)$ if $E\in(U(O_4)-U(O_5),U(O_2)-U(O_1))$, and $P\{\eta_E=O_3\}=1$ if $E>U(O_2)-U(O_1)$.

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On quantum extensions to classical spherical harmonics expansion/Fokker-Planck models

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By following a strategy introduced in previous works, quantum extensions of the classical electron-phonon scattering operator are deduced from first principles. These quantum collision operators satisfy a quantum H-theorem and relax towards quantum equilibria. Then, under an assumption of dominant elastic interactions, a hierarchy of quantum spherical harmonic expansion (SHE) models is derived by a diffusive approximation of collisional Wigner equations. These models are proven entropic and their expansions into powers of the reduced Planck constant $\hbar$ are calculated, leading to $\hbar^2$ corrections for the classical SHE model. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2192968]

I. INTRODUCTION

The transport of charged particles in electronic devices is generally described by kinetic models such as Boltzmann-type equations or macroscopic models of hydrodynamic or diffusion type. Due to the ongoing miniaturization of these devices, reaching the nanometric scale, the reliability of these classical models becomes doubtful as quantum effects become important. Since, at an intermediate scale, collision phenomena remain significant, one of the most challenging areas of investigation in semiconductor modelling deals with the setting-up of quantum transport models which take into account scattering effects. Though many works are concerned with the numerical simulation of ballistic quantum transport models for semiconductors (see, e.g., Refs. 26, 37, 42, 25, 15, and 44), a quantum theory of collisions is still under development (among other works on the quantum theory of scattering, see, e.g., Refs. 3, 12, 24, 38, and 45 and, more recently, Refs. 4, 5, and 27). Furthermore, several attempts were made to adapt existing classical macroscopic models to quantum mechanics[1,2,30–33] but, generally, the link between the so-obtained models and a microscopic quantum description of the particle transport is to a large extent phenomenological.

Recently, a strategy for deriving quantum macroscopic models was introduced in Refs. 21 and 22. It relies on the notion of a quantum local equilibrium (called "quantum Maxwellian"), defined through a Gibbs principle as the minimizer of the quantum entropy under local moment constraints. This approach enabled to write prototypes of collision operators which decrease the quantum entropy and relax towards the quantum local equilibria. By introducing such collision operators in the Wigner equation and by performing formally a hydrodynamic (respectively, diffusive) limit, quantum hydrodynamic (respectively, quantum diffusive) models were derived in Refs. 21 and 19 (these two papers are reviewed in Ref. 20). As a by-product of the method, these

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quantum macroscopic models display some interesting physical properties, such as the preservation of the positivity of the density or an entropy dissipation. The numerical resolution of the simplest of these models, the quantum drift-diffusion model, is investigated in Refs. 28 and 29.

The small size of current semiconductor devices raises another problem. In some regimes, the relevant time and length scales are too small for the cloud of electrons to reach a thermodynamical equilibrium. Therefore, an accurate description of these devices cannot be achieved by models which, like drift-diffusion or hydrodynamic models, rely on the assumption that the system has been driven to an equilibrium with a given profile (of Maxwellian or of Fermi-Dirac type). Intermediate models have been recently introduced, in a classical setting, to fill the gap between precise but numerically expensive models (kinetic models for instance) and numerically affordable but less accurate models such as drift-diffusion models: among others are the spherical harmonics expansion (SHE) models (see, Refs. 6 and 13 for a mathematical description and references). These models are diffusion models in the position-energy space. They have been applied to semiconductor physics,[34,10,11,7,8] neutronics,[35] gas discharge,[46] and plasma physics.[23] Numerical computations have established the relevance of the classical SHE models.[17,9] These models are also referred to as Fokker-Planck models. They consist of a mass balance equation (the continuity equation) for the energy distribution function, and of a constitutive law for the current of particles of given energy. The former governs the transport of the density and the latter describes the effects of the diffusion due to the particle scattering.

The goal of this paper is twofold. On the one hand, following the strategy, described above, which leads to deriving quantum versions of the hydrodynamic (HD), energy-transport (ET), and drift-diffusion (DD) models, we propose quantum SHE models. These models are expected to be better adapted than classical SHE models to situations where quantum phenomena are predominant. Moreover, as in the classical case where SHE models appear as intermediate models between kinetic and macroscopic equations, quantum SHE models fit systems far from Maxwellian-type equilibria better than quantum HD, ET, and DD models.

The derivation of quantum SHE models by a diffusion approximation procedure makes the introduction of quantum collision operators at the kinetic level necessary: this constitutes the second goal of this work. A quantum collision operator is built following ideas first introduced in Refs. 21, 22, and 19 and generalizing the classical electron-phonon scattering operator.[40] Then, in the regime of dominant elastic scattering, several other operators are proposed. All these operators are consistent with the elementary properties which are sought to describe collisions with phonons (conservations, equilibrium states, quantum entropy dissipation).

The paper is organized as follows. Section II recalls some well-known results about the derivation of classical SHE models and emphasizes the importance of the entropy dissipation of the collision operator to obtain an entropic structure for the macroscopic model. Classical features of the linearized electron-phonon collision operator are also recalled. Section III is a first step towards the derivation of a quantum SHE model: we consider the Wigner equation equipped with a classical collision operator and perform the derivation in this setting, which leads to the quasiquantum SHE model. This model does not account for quantum diffusion. Quantum collision operators are introduced in Sec. IV following a heuristic analogy: these operators must fulfill properties analogue to those satisfied by the classical operators given in Sec. II. For this sake, a quantum entropy is given and quantum thermodynamical equilibria are defined as minimizers of this entropy, allowing the introduction of quantum relaxation operators. Then the derivation of a fully quantum SHE model can be performed and this is achieved in Sec. V.

The quantum SHE and quasiquantum SHE models involve pseudodifferential operators and display a nonlocal character. In order to obtain models easier to handle, a formal expansion of these equations with respect to the reduced Planck constant $\hbar$ are given in Secs. III and V. As it was done in Ref. 19 for the quantum energy-transport and the quantum drift-diffusion models, by keeping only the terms up to second order in $\hbar$ in this expansion, we derive quantum correction terms for the classical SHE model.

II. CLASSICAL MODELLING OF ELECTRON-PHONON SCATTERING IN SEMICONDUCTOR DEVICES: A SHORT REVIEW

In this section, we review some well-known features concerning electron-phonon scattering in classical kinetic models. Indeed, having this review in mind will help understand our methodology for establishing quantum collision operators and deriving various quantum SHE models.

A. The Boltzmann equation

The evolution of electrons in semiconductor devices can be described at a microscopic level through classical kinetic equations of Boltzmann type as long as quantum effects are neglected. To that purpose, one introduces the distribution function $f(t,x,p)$ of the electrons. Then f is given as the solution of the initial value problem

$$\begin{gathered}\partial_t f + p\cdot\nabla_x f - \nabla_x V\cdot\nabla_p f = \mathcal{C}(f), \quad x\in\mathbb{R}^3, \quad p\in\mathbb{R}^3, \quad t>0,\\ f(0,x,p) = f_I(x,p),\end{gathered} \tag{2.1}$$

where $V=V(x)$ is a given potential and f_I an initial condition. The collision operator $\mathcal{C}$ models the interactions of the electrons with the medium. All the quantities that will be considered in the sequel are dimensionless. The equation is adimensioned and we set the temperature equal to 1 and the electron mass and elementary charge equal to 1 and -1, respectively. We will note

$$L = p\cdot\nabla_x - \nabla_x V\cdot\nabla_p$$

the classical transport (Liouville) operator. The classical relative entropy usually associated to this kind of equation is

$$H_C(f) = \int_{\mathbb{R}^6} f\left(\ln f - 1 + \frac{|p|^2}{2} + V(x)\right)\mathrm{d}x\,\mathrm{d}p = \int_{\mathbb{R}^6} f\left(\ln\frac{f}{\mathcal{M}} - 1\right)\mathrm{d}x\,\mathrm{d}p$$

where the global Maxwellian $\mathcal{M}$ is defined by

$$\mathcal{M}(x,p) = \exp\left(-\frac{|p|^2}{2} - V(x)\right). \tag{2.2}$$

When the context is clear, we will note as well $\mathcal{M}(x,\varepsilon)=\exp(-\varepsilon - V(x))$, where ε denotes the energy variable ($\varepsilon\geqslant 0$). The following lemma is a classical result on H_C. Its proof is straightforward.

Lemma 2.1: *Let* $\mathcal{C}$ *in* (2.1) *be such that, for any positive measurable function* g, *this inequality holds*,

$$-\int \mathcal{C}(g)\ln\left(\frac{g}{\mathcal{M}}\right)\mathrm{d}x\,\mathrm{d}p \geqslant 0. \tag{2.3}$$

Then, *if* f *is a positive solution of Eq.* (2.1), *the associated entropy satisfies*

$$\frac{\mathrm{d}H_C(f)}{\mathrm{d}t} \leqslant 0. \tag{2.4}$$

According to this lemma, the study of the entropic structure of equations of type (2.1) reduces to proving an inequality on the collision operator $\mathcal{C}$. In this section, several collision operators are introduced in order to model the scattering of electrons in semiconductors. The classical electron-phonon collision operator is introduced and some of its properties are recalled. The limit of a vanishing phonon energy is performed and yields an elastic collision operator. Then, the derivation of a classical SHE model is set out (following Refs. 6 and 13) and its entropic structure is emphasized.

Before achieving these tasks, we introduce the spherical coordinates in momentum space: $\omega = p/|p| \in \mathbb{S}^2$, $\varepsilon = |p|^2/2 > 0$, where $\mathbb{S}^2$ denotes the unit sphere in $\mathbb{R}^3$. For any function f, we note equally $f(p) = f(\varepsilon, \omega)$ and, when the context is unambiguous, $f = f(p)$ and $f' = f(p')$. The following formula holds for any integrable function f:

$$\int_{\mathbb{R}^3} f(p)\mathrm{d}p = \int_{(0,\infty)\times\mathbb{S}^2} f(\varepsilon,\omega)\sqrt{2\varepsilon}\mathrm{d}\varepsilon\,\mathrm{d}\omega$$

and we define

$$\int_{\mathbb{R}^3} f(p')\,\delta(|p'|^2/2-\varepsilon)\mathrm{d}p' = \int_{(0,\infty)\times\mathbb{S}^2} f(\varepsilon',\omega')\,\delta(\varepsilon'-\varepsilon)\sqrt{2\varepsilon'}\mathrm{d}\varepsilon'\,\mathrm{d}\omega := \sqrt{2\varepsilon}\int_{\mathbb{S}^2} f(\varepsilon,\omega')\mathrm{d}\omega'.$$

Let $L^2_{x,p} = L^2(\mathbb{R}^6)$ denote the space of square integrable functions on the phase space $\mathbb{R}^6$. The closed subspace of energy dependent functions will be of considerable interest in the remainder of the paper and is denoted by

$$\mathcal{E} = \{f \in L^2_{x,p} : f(x,p) = f(x,|p|) \text{a . e .}\}$$

and the space orthogonal to $\mathcal{E}$ in $L^2_{x,p}$ is denoted by $\mathcal{E}^\perp$. The projectors on $\mathcal{E}$ and on $\mathcal{E}^\perp$ are, respectively, denoted by $\mathcal{P}$ and $\mathcal{P}^\perp$ and, for any ϕ in $L^2_{x,p}$, they are given by

$$\mathcal{P}(\phi)(\varepsilon) = \frac{1}{N(\varepsilon)}\int_{\mathbb{R}^3} \phi(\varepsilon',\omega')\,\delta(\varepsilon'-\varepsilon)\mathrm{d}p', \quad \mathcal{P}^\perp\phi = (\mathrm{Id}-\mathcal{P})\phi,$$

where Id denotes the identity operator on $L^2_{x,p}$ and $N(\varepsilon)$, the density of state, is defined by

$$N(\varepsilon) = \int_{\mathbb{R}^3} \delta(|p'|^2/2-\varepsilon)\mathrm{d}p' = 4\pi\sqrt{2\varepsilon},$$

so that the projector $\mathcal{P}$ can be written equivalently as

$$\mathcal{P}(\phi)(\varepsilon) = \frac{1}{4\pi}\int_{\mathbb{S}^2} \phi(\varepsilon,\omega')\mathrm{d}\omega'.$$

Note that, for any f and ϕ, $\mathcal{P}(\phi f) = \phi\mathcal{P}(f)$ and $\mathcal{P}^\perp\phi = 0$ as soon as ϕ is a function of the energy ε only. Moreover, $\mathcal{E}^\perp$ is spanned by functions of null angular average.

B. The classical electron-phonon collision operator

We now focus on the expression of the collisions operator $\mathcal{C}(f)$. In semiconductors, electrons undergo mainly three types of collisions against ionized impurities, acoustic phonons, and optical phonons.[47] At large enough energies, optical phonon collisions are dominant and we shall discard the other types of collisions.

Classically (see Ref. 41 for instance), in a low density case, the electron-optical phonon collision operator is linear and can be written, after an appropriate scaling, according to

$$\mathcal{C}_{e\varphi}(f)(p) = \int \Sigma(p,p')\{[(N_0+1)\,\delta(\varepsilon-\varepsilon'+\beta)+N_0\delta(\varepsilon-\varepsilon-\beta)]f(p')$$

$$-[(N_0+1)\,\delta(\varepsilon'-\varepsilon+\beta)+N_0\delta(\varepsilon'-\varepsilon-\beta)]f(p)\mathrm{d}p'$$

with β the scaled phonon energy (which is a constant), $\Sigma(p,p')$ a symmetric function of the form

$$\Sigma(p,p') = C_{\text{opt}}\beta\begin{cases} \dfrac{1}{|p-p'|^2} & \text{(polar interactions)}, \\ 1 & \text{(nonpolar interactions)}, \end{cases} \tag{2.5}$$

where C_{opt} is an appropriate constant. The phonon occupation number N_0 for a lattice temperature $T=1$ is given by the Bose-Einstein statistics as

$$N_0 = \frac{1}{e^{\beta}-1}. \tag{2.6}$$

The collision operator can also be written

$$\mathcal{C}_{e\varphi}(f) = \int \mathcal{S}(p,p')[\delta(\varepsilon'-\varepsilon-\beta)+\delta(\varepsilon'-\varepsilon+\beta)]\left(\frac{f(p')}{M(\varepsilon')}-\frac{f(p)}{M(\varepsilon)}\right)\mathrm{d}p' \tag{2.7}$$

with $M=M(\varepsilon)=\exp(-\varepsilon)$ the Maxwellian and

$$\mathcal{S}(p,p') = \Sigma(p,p')N_0 e^{-(\varepsilon+\varepsilon')/2}e^{\beta/2},$$

which is a symmetric function. The following result can be found in Ref. 40.

Proposition 2.2: *The collision operator* $\mathcal{C}_{e\varphi}$ *defined by* (2.7) *satisfies the following properties*:

(i) *Mass conservation*: $\int \mathcal{C}_{e\varphi}(f)\mathrm{d}p=0$ *for any measurable function* f.

(ii) *Equilibrium states*: *for any measurable function* $f(x,p)$, *we have* $\mathcal{C}_{e\varphi}(f)=0$ *if and only if*

$$f(x,p) = M(|p|^2/2)F(x,|p|^2/2),$$

where F *is such that* $F(x,\varepsilon+\beta)=F(x,\varepsilon)$.

(iii) *Entropy dissipation*: $-\int \mathcal{C}_{e\varphi}(f)\ln(f/\mathcal{M})\mathrm{d}p \geqslant 0$ *for any positive integrable function* f.

Typically, the electron energy in a semiconductor device is of the same order of magnitude as the applied bias, i.e., of the order of 1 V. This is very large compared with the typical optical phonon energy, which is of the order of 10^{-2} V. Therefore, the scaled parameter $\beta \approx 10^{-2}$ is very small and it is meaningful to consider the elastic limit $\beta \to 0$ of the electron-phonon collision operator.

The following operator $\mathcal{C}_{\text{el}}$ can be obtained as the limit of $\mathcal{C}_{e\varphi}$ as $\beta \to 0$:

$$\mathcal{C}_{\text{el}}(f)(p) = N(|p|^2/2)\{\mathcal{P}(\widetilde{\mathcal{S}}(p,\cdot)f(\cdot)) - \mathcal{P}(\widetilde{\mathcal{S}}(p,\cdot))f(p)\}, \tag{2.8}$$

where

$$\widetilde{\mathcal{S}}(p,p') = 2C_{\text{opt}}\begin{cases} \dfrac{1}{|p-p'|^2} & \text{(polar interactions)}, \\ 1 & \text{(nonpolar interactions)}. \end{cases} \tag{2.9}$$

From now on, we drop the tildes. It is straightforward to prove the following.

Proposition 2.3: *The collision operator* $\mathcal{C}_{\text{el}}$ *defined by* (2.8) *satisfies the following properties*:

(i) *Mass conservation*: $\int \mathcal{C}_{\text{el}}(f)\mathrm{d}p=0$ *for any measurable function* f.

(ii) *Equilibrium states*: *for any function* f *in* $L^2_{x,p}$, *we have* $\mathcal{C}_{\text{el}}(f)=0$ *if and only if*

$$f(x,p) = F(x,|p|^2/2),$$

where F *lies in* $\mathcal{E}$.

(iii) *Entropy dissipation*: $-\int \mathcal{C}_{\text{el}}(f)\ln(f/\mathcal{M})\mathrm{d}p \geqslant 0$ *for any positive integrable function* f.

C. Derivation of the classical SHE model (CSHE)

Classical SHE models (CSHE) (also referred to as Fokker-Planck models) are obtained as asymptotic limits of the Boltzmann equation under the assumption of dominant elastic scattering, i.e., when the collision operator [of the type (2.8)] is supposed to be large, say of order $1/\alpha$ where α is a measure of the collision mean-free path in scaled units. We also need to observe the system over large periods of time, i.e., we must rescale the time variable $t \to t/\alpha$ in order to capture the significant dynamics, which is of diffusion type. In this new set of units, the classical Boltzmann equation becomes

$$\alpha \partial_t f^\alpha + (p \cdot \nabla_x - \nabla_x V \cdot \nabla_p) f^\alpha = \frac{1}{\alpha} \mathcal{C}_{\mathrm{el}}(f). \tag{2.10}$$

To ensure boundedness and positivity for the collision operator, we assume the following.

Assumption 2.4: *There exist two positive constants* K, K' *such that* $K < \mathcal{S} < K'$.

Under this assumption, operator $\mathcal{C}_{el}$ is an isomorphism from $\mathcal{E}^\perp$ onto $\mathcal{E}^\perp$ (see Ref. 6 for instance). Then, Eq. (2.10) has solutions according to the Hille-Yosida theorem.

Lemma 2.5: *Under regularity assumptions on the potential V and Assumption 2.4*, *Eq.* (2.10) *with initial datum* f_I *in* $\mathcal{D}(L) := \{f \in L^2_{x,p} : Lf \in L^2_{x,p}\}$ *has a unique solution* f^α in $C^1([0,T], L^2_{x,p}) \cap C^0([0,T], \mathcal{D}(L))$.

We do not enter into details regarding sufficient assumptions on V since the differential operator $\nabla_x V \cdot \nabla_p$ will not be used in this paper, but, instead, an L^2 bounded pseudodifferential operator. The (possibly not optimal) regularity required for V in the quantum case is stated in Assumption 3.2 below.

Proposition 2.6 summarizes some results on the derivation of the CSHE model (see Refs. 6 and 13 for this proposition as well as for precise regularity requirements on the potential V).

Proposition 2.6: *Assumption 2.4 is made and V is supposed regular enough.*

We consider Eq. (2.10) *with initial datum* f_I^α *such that the sequence* (f_I^α) *converges in* $L^2_{x,p}$ *to an element* F_{in} *of* $\mathcal{E}$ *as* $\alpha \to 0$. *By Lemma 2.5*, *this problem has a unique solution* f^α *for all* $\alpha > 0$.

The formal limit F of f^α *as* $\alpha \to 0$ *is the solution of the classical SHE (CSHE) model*,

$$N(\varepsilon)\partial_t F - \tilde{\nabla} \cdot (D \tilde{\nabla} F) = 0,$$

$$F(0,x,\varepsilon) = F_{in}(x,\varepsilon), \tag{2.11}$$

$$\tilde{\nabla} = \nabla_x - \nabla_x V \partial_\varepsilon,$$

$$D = \mathcal{P}(\mathcal{C}_{\mathrm{el}}^{-1}(p) \otimes p) = \frac{|p|^2}{4\pi} \int_{\mathrm{S}^2} \mathcal{C}_{\mathrm{el}}^{-1}(\omega) \otimes \omega \, \mathrm{d}\omega. \tag{2.12}$$

More precisely, *the sequence* $(f^\alpha)_\alpha$ *can be rigorously proved to converge weakly in* $L^\infty((0,T), L^2_{x,p})$ *to a limit* $F \in L^\infty((0,T), \mathcal{E})$ *which is a weak solution of* (2.11), *and* $F \geqslant 0$. *Moreover*, *the following expression*:

$$H_{\mathrm{CSHE}}(F) = \int F \left(\ln \frac{F}{\mathcal{M}} - 1 \right) N(\varepsilon) \mathrm{d}\varepsilon \, \mathrm{d}x$$

is a decreasing function of time.

Proof: The proof of the derivation itself can be found in Refs. 6 and 13 (formal proof) and Ref. 14, for a rigorous proof in the case of a null potential V. When the potential does not vanish, the proof can be adapted from Ref. 18 where the diffusion is driven by particle-wall scattering.□

An interesting case is when the collision kernel is isotropic: $\mathcal{S}(p,p')=\mathcal{S}(|p|,|p'|)$.Then, setting $\mathcal{S}(|p|,|p|)N(|p|^2/2)=\nu$, the collision operator reads

$$\mathcal{C}_{\mathrm{el}}(f)=\nu(\mathcal{P}f-f) \tag{2.13}$$

and the diffusion matrix is a scalar given by

$$D=\frac{4\pi}{3\nu}(2\varepsilon)^{3/2}. \tag{2.14}$$

Remark 2.7: The classical SHE model given by Eq. (2.11) is a degenerate parabolic equation. □

Remark 2.8: Note that, in the definition of this operator (2.13), the projection term $\mathcal{P}f$ can be obtained as the minimizer of the classical entropy $H_C(g)$ under the constraint $\mathcal{P}(g-f)=0$. The definition of a quantum analogue of this relaxation operator in Sec. IV B is inspired by this remark. □

III. CLASSICAL COLLISION OPERATORS AND QUASIQUANTUM SHE MODEL

As a first attempt to introduce quantum phenomenology in the SHE model, the Wigner equation can be substituted to the left-hand side of the Boltzmann equation (2.1). This is our goal in the present section. First, the Wigner-Boltzmann equation (i.e., the Wigner equation with a collisional source term) is introduced. Some notations and properties are given and the resolution of the Cauchy problem for this equation is recalled. Note that in this section, we will focus on the influence of the quantum transport operator. The scattering phenomena are still modeled by a classical collision operator. We emphasize that this approach lacks consistency, as we use a quantum model for transport and still a classical model for collisions. In order to remedy to this inconsistency, we introduce quantum collision operators in Sec. IV.

The so-called quasiquantum SHE (QQSHE) model is rigorously derived from the Wigner-Boltzmann equation in a diffusion asymptotics. As the Wigner equation, the QQSHE model depends on the Planck constant. The expansion of this model with respect to $\hbar$ is investigated and a focus is made on the QQSHE_2 model, that is, the expanded model up to second order terms in $\hbar$. This model is of interest since it introduces correction terms to the CSHE model and may lead to a cheap yet accurate way to introduce quantum corrections in classical SHE models.

A. The Wigner-Boltzmann equation

Let us introduce the Wigner transform and its properties. All the results of this section are given without proof (one can refer to Ref. 39 for instance). To any complex number z we associate its complex conjugate $\bar{z}$. We adopt the following conventions for the Fourier transform $\mathcal{F}$ and the inverse Fourier transform $\mathcal{F}^{-1}$ (in dimension 3):

$$\mathcal{F}(f)(\eta)=\int f(p)e^{-ip\cdot\eta/\hbar}\mathrm{d}p,\quad \mathcal{F}^{-1}(g)(p)=\int g(\eta)e^{ip\cdot\eta/\hbar}\frac{\mathrm{d}\eta}{(2\pi\hbar)^3},$$

where $\hbar$ is the reduced Planck constant. Let ρ denote a trace class non-negative Hermitian operator on $L^2(\mathbb{R}^3)$ and let $\rho(x,y)$ be its integral kernel. Then its Wigner transform is

$$W[\rho](x,p)=\int_{\mathbb{R}^3}\rho\left(x-\frac{\eta}{2},x+\frac{\eta}{2}\right)e^{i\eta\cdot p/\hbar}\,\mathrm{d}\eta,$$

whereas the Weyl quantization of any symbol $a(x,p)$ defines an operator $\mathrm{Op}(a)$,

$$\mathrm{Op}(a)\phi = (2\pi\hbar)^{-3}\int_{\mathbb{R}^6} a\left(\frac{x+y}{2}, p\right)\phi(y)e^{ip\cdot(x-y)/\hbar}\,\mathrm{d}p\,\mathrm{d}y.$$

Then Op and W are formally inverse operations to one another,

$$\mathrm{Op}(W[\rho]) = \rho, \quad W[\mathrm{Op}(a)] = a.$$

For any trace class operator ρ, we denote by $\mathrm{Tr}\,\rho$ its trace and by $\rho^\dagger$ its Hermitian adjoint. We summarize some classical properties of Op and W in the following lemma. We recall that an operator K is a Hilbert-Schmidt operator if there exists a kernel $k \in L^2_{x,p}$ such that, for any $\phi \in L^2_{x,p}$, $K(\phi)(y) = \int k(x,y)\phi(y)\mathrm{d}y$. We note $K \in \mathrm{HS}$.

Lemma 3.1: (Properties of W and Op)

(i) *The Weyl quantization Op(a) of a symbol a is a Hilbert-Schmidt operator if and only if a is in $L^2_{x,p}$. Moreover, Op is an isometry from $L^2_{x,p}$ onto HS.*

(ii) *An operator ρ is Hermitian if and only if $W[\rho]$ is real valued. The Wigner transform W, defined from HS onto $L^2_{x,p}$ is the inverse transform to the Weyl quantization.*

(iii) *For two Hilbert-Schmidt operators ρ and σ, the following formula is a consequence of Plancherel's identity*

$$\mathrm{Tr}\{\rho\sigma^\dagger\} = \frac{1}{(2\pi\hbar)^3}\int W[\rho]\overline{W[\sigma]}\mathrm{d}x\,\mathrm{d}p. \tag{3.1}$$

(iv) *Let $\mathcal{H} = -(\hbar^2/2)\Delta + V$ denote the particle Hamiltonian. Then, for any Hilbert-Schmidt operator ρ, we formally have*

$$\frac{i}{\hbar}W[\mathcal{H},\rho] = (p\cdot\nabla_x - \theta[V])(W[\rho]), \tag{3.2}$$

where $\theta[V]$ denotes the pseudodifferential operator associated with the potential $V(x)$,

$$\begin{aligned}\theta[V]f &= \mathcal{F}^{-1}\left(i\frac{V\left(x+\frac{\eta}{2}\right) - V\left(x-\frac{\eta}{2}\right)}{\hbar}\mathcal{F}(f)\right)\\ &= \frac{i}{(2\pi)^3}\int_{\mathbb{R}^6}\frac{V\left(x+\frac{\hbar}{2}\eta\right) - V\left(x-\frac{\hbar}{2}\eta\right)}{\hbar}f(t,x,p')e^{i(p-p')\cdot\eta}\,\mathrm{d}\eta\,\mathrm{d}p',\end{aligned} \tag{3.3}$$

and $[\rho,\sigma] = \rho\sigma - \sigma\rho$ is the commutator of two operators ρ and σ.

(v) *$Op(|p|^2) = -\hbar^2\Delta$ and, for any symbol s depending only on x, $Op(s)$ is the s-multiplication operator: $Op(s)\varphi: x \to s(x)\varphi(x)$.*

Now we recall the link between the Wigner and the von Neumann equations. The density matrix ρ satisfies the von Neumann equation

$$i\hbar\,\partial_t\rho = [\mathcal{H},\rho] \tag{3.4}$$

if and only if its Wigner transform $f = W[\rho]$ satisfies the Wigner equation

$$\partial_t f + p\cdot\nabla_x f - \theta[V]f = 0 \tag{3.5}$$

as can be seen thanks to Eq. (3.2). The function f cannot be easily interpreted as a distribution function (for instance, it is not necessarily positive), but the classical transport equation $\partial_t f + (p\cdot\nabla_x - \nabla_x V\cdot\nabla_p)f = 0$ can be obtained as the semiclassical limit of the Wigner equation as $\hbar$ tends to 0 (see Ref. 39).

Lemma 3.3 gives some information on the operator $\theta[V]$ if we assume the following.

Assumption 3.2: *The potential V lies in* $W^{2,\infty}(\mathbb{R}^3)$.

Lemma 3.3: *If the potential V satisfies Assumption 3.2, then*

(i) $\theta[V]$ *is a bounded skew-adjoint operator from* $L^2_{x,p}$ *to* $L^2_{x,p}$,
(ii) *for any function* $f \in W^{2,2}(\mathbb{R}^3_x; L^2(\mathbb{R}^3_p))$,

$$\theta[V](f) \in W^{2,2}(\mathbb{R}^3_x, L^2(\mathbb{R}^3_p)),$$

and, for $f \in W^{1,2}(\mathbb{R}^3_x; L^2(\mathbb{R}^3_p))$,

$$\nabla_x \theta[V] f = \theta[\nabla_x V](f) + \theta[V](\nabla_x f),$$

where $\theta[\nabla_x V](f)$ *and* $\theta[V](\nabla_x f)$ *denote, respectively, the two vectors of components* $\theta[\partial_{x_i} V](f)$ *and* $\theta[V](\partial_{x_i} f)$, *for* $i=1,2,3$,
(iii) *for any function* $f \in L^2_{x,p}$ *such that* $pf \in (L^2_{x,p})^3$, $p\theta[V](f)$ *is in* $L^2_{x,p}$,
(iv) *for any function* $F \in \mathcal{E}$, $\theta[V]F$ *belongs to* $\mathcal{E}^{\perp}$.

Equation (3.5) does not take collision phenomena into account. In the remainder of Sec. III it is assumed that the scattering can be modeled through a classical elastic collision operator. Therefore, the collision operator is still $\mathcal{C}_{\mathrm{el}}$, as defined in (2.8). This leads to the following Wigner-Boltzmann equation (after rescaling):

$$\alpha \partial_t f^\alpha + (p \cdot \nabla_x - \theta[V]) f^\alpha = \frac{1}{\alpha} \mathcal{C}_{\mathrm{el}}(f^\alpha). \tag{3.6}$$

We denote by Λ the Wigner operator of domain $\mathcal{D}(\Lambda) = \{g \in L^2_{x,p} : p \cdot \nabla_x g \in L^2_{x,p}\}$ and defined by

$$\Lambda : \mathcal{D}(\Lambda) \to L^2_{x,p},$$
$$g \to (p \cdot \nabla_x - \theta[V]) g.$$

Note that, since $\theta[V]$ is skew-adjoint on $L^2_{x,p}$, so is Λ on $\mathcal{D}(\Lambda)$.

Remark 3.4: It is not clear whether the Wigner-Boltzmann equation equipped with the classical relaxation operator $\mathcal{C}_{\mathrm{el}}$ preserves positivity. In this sense, it is not a consistent quantum model. □

For the study of the QQSHE model, we introduce the following functional spaces:

$$\mathcal{L}^2_{N^k} = \left\{ h(x,\varepsilon) - \text{measurable} : \int_{\mathbb{R}^3_x} \int_{\varepsilon > 0} |h(x,\varepsilon)|^2 (N(\varepsilon))^k \, \mathrm{d}\varepsilon \, \mathrm{d}x < \infty \right\}, \tag{3.7}$$

with $N(\varepsilon) = \sqrt{2\varepsilon}$ and $k \in \mathbb{Z}$. So $\mathcal{E} = \mathcal{L}^2_N$.

Now, we give an existence result for the Wigner-Boltzmann equation (3.6).

Lemma 3.5: *Suppose Assumptions 2.4 and 3.2 hold true.*

Then, for any value of the parameter $\alpha > 0$, *any initial condition* $f^\alpha_I \in \mathcal{D}(\Lambda)$ *and any time* $T > 0$, *there exists a unique solution* $f^\alpha \in C^1([0,T]; L^2_{x,p}) \cap C^0([0,T]; \mathcal{D}(\Lambda))$ *to the initial value problem* (3.6), $f(t=0,x,p) = f^\alpha_I$.

Proof: This is a straightforward consequence of the classical semigroup theory—see, e.g., Refs. 36 and 48. Indeed, Λ is a skew-adjoint operator and generates a unitary group by Stone's theorem. Since $\mathcal{C}_{\mathrm{el}}$ is a bounded perturbation of Λ, $\mathcal{C}_{el} + \Lambda$ with domain $\mathcal{D}(\Lambda)$ generates a group of operators. □

B. The quasiquantum SHE model (QQSHE)

This section is dedicated to the investigation of the limit $\alpha \to 0$ in (3.6). The collision phenomena are modeled by the collision operator $\mathcal{C}_{\mathrm{el}}$ defined by (2.13). For the sake of simplicity, we assume that the collision frequency ν is constant. The main result of this section is the following.

Theorem 3.6: *Assumptions 2.4 and 3.2 are supposed to hold true.*

Let $f^\alpha_I \in L^2_{x,p}$ *be a convergent sequence such that the limit* f_I *be in* $\mathcal{E}$. *We note* $F_I(x, |p|^2/2)$

$=f_I(x,p)$. *Therefore*, F_I *is in* $\mathcal{L}^2_N$. *We assume that the collision frequency* ν *is constant*.

Let f^α *denote the solution of* (3.6), *with initial condition* $f^\alpha(t=0,x,p)=f_I^\alpha(x,p)$, *and with the relaxation operator* $\mathcal{C}_{\mathrm{el}}(f)=\nu(\mathcal{P}(f)-f)$. *Then, as* $\alpha\to 0$, *the sequence* $(f^\alpha)_{\alpha>0}$ *converges* (*up to the extraction of a subsequence*) *weakly in* $L^2(0,T;L^2_{x,p})$ *to a limit* $f\in L^2(0,T;\mathcal{E})$. *We note* $F(t,x,|p|^2/2)=f(t,x,p)$, *so that* $F\in L^2(0,T;\mathcal{L}^2_N)$. *In addition*, F *is a weak solution of*

$$\partial_t F-\frac{1}{\nu}\mathcal{P}(\Lambda(\Lambda(F)))=0, \tag{3.8}$$

$$F(t=0,x,\varepsilon)=F_I(x,\varepsilon). \tag{3.9}$$

Remark 3.7: If the collisions are modeled by the more general collision operator (2.8), then one can prove that the limit equation satisfied by F is

$$\partial_t F-\mathcal{P}(\Lambda(\mathcal{C}_{\mathrm{el}}^{-1}(\Lambda(F))))=0, \tag{3.10}$$

under the condition that the following set of test functions is dense in $L^\infty(0,T;\mathcal{L}^2_N)$:

$$\mathbb{H}=\{\varphi\in W^{1,\infty}(0,T;C_c^\infty(\mathbb{R}^3\times\mathbb{R}^+)):\mathcal{P}(\Lambda(\mathcal{C}_{\mathrm{el}}^{-1}(\Lambda\varphi)))\in L^\infty(0,T;\mathcal{L}^2_N)\}.$$

This condition is obviously fulfilled when $\mathcal{C}_{\mathrm{el}}=\nu(\mathcal{P}f-f)$.

It is possible to insert the expression of Λ into (3.8) [or (3.10)], in order to get a more explicit form of the equation. However, this expression is quite complicated and not very illuminating. We shall derive an explicit expression after using an expansion of Λ in powers of $\hbar$ at Sec. III C. □

Remark 3.8: The quantum (Wigner) transport operator does not preserve the classical entropy. Therefore, there is no (obvious) classical entropy dissipation for the quasiquantum SHE model. Also, the classical relaxation operator $\mathcal{C}_{\mathrm{el}}$ does not decay the quantum entropy introduced below in Sec. IV. This leaves little hope to find a simple entropic structure for this model, at least in the framework presented in this paper.

We have to mention that, unlike the classical SHE model, the QQSHE model has not a clear parabolic (or even degenerate parabolic) structure. Indeed, the Wigner transport operator is a pseudodifferential operator, not a true partial differential operator.

Last, but not least, the quantum relevance of this model is weak since there is no indication whether it admits positive solutions (in the sense of operator positivity). □

Proof: We start from (3.6). We multiply by f^α and integrate with respect to t, x, and p. This yields

$$\|f^\alpha(t)\|^2_{L^2_{x,p}}+\frac{1}{\alpha^2}\int_0^t\|\mathcal{P}^\perp f^\alpha(s)\|^2_{L^2_{x,p}}\,\mathrm{d}s=\|f_I^\alpha\|^2_{L^2_{x,p}}. \tag{3.11}$$

Therefore, the sequence (f^α) is bounded in $L^2_{x,p}$ since (f_I^α) is bounded. There exists f in $L^\infty(0,T;L^2_{x,p})$ such that $f^\alpha\rightharpoonup f$ weakly * in $L^\infty(0,T;L^2_{x,p})$. Moreover, the same estimate (3.11) shows that $\mathcal{P}^\perp f^\alpha$ tends strongly to 0 as $\alpha\to 0$ in the same space. Consequently, the limit f belongs to $\mathcal{E}$ and we can note $F(t,x,|p|^2/2)=f(t,x,p)$.

The Wigner-Boltzmann equation can be written in a weak form, by introducing the following set of test functions:

$$\mathcal{S}=\{\varphi\in W^{1,\infty}(0,T;L^2_{x,p})\cap L^\infty(0,T;\mathcal{D}(\Lambda)):\quad \varphi(T,x,p)=0\}.$$

The weak solutions of (3.6) satisfy

$$\forall\,\varphi\in\mathcal{S}\quad \int_{[0,T]\times\mathbb{R}^6} f^\alpha\left(\partial_t\varphi+\frac{1}{\alpha}\Lambda\varphi+\frac{1}{\alpha^2}\mathcal{C}_{\mathrm{el}}\varphi\right)\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p=\int_{\mathbb{R}^6} f_I^\alpha\varphi(0,x,p)\mathrm{d}x\,\mathrm{d}p. \tag{3.12}$$

In order to prove that F is a weak solution of (3.8), let us introduce a test function $\Phi(t,x,\varepsilon)$ for this equation, in $W^{1,\infty}(0,T;C_c^\infty(\mathbb{R}^3\times\mathbb{R}^+))$. Obviously the function $\varphi_1(t,x,p)$ defined by $\varphi_1(t,x,p)=\Phi(t,x,|p|^2/2)$ belongs to $\mathcal{S}$ and can be taken as a test function in (3.12). We consider the asymptotic behavior of each term in (3.12) as $\alpha\to 0$, in this special case where the test function φ_1 is a function of $(t,x,|p|^2/2)$. The weak convergence of f^α implies

$$\int f^\alpha \partial_t \varphi_1(t,x,p)\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p \to \int N(\varepsilon)F(t,x,\varepsilon)\partial_t\Phi(t,x,\varepsilon)\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\varepsilon$$

and

$$\int f_I^\alpha \varphi_1(0,x,p)\mathrm{d}x\,\mathrm{d}p \to \int N(\varepsilon)F_I(x,\varepsilon)\Phi(0,x,\varepsilon)\mathrm{d}x\,\mathrm{d}\varepsilon.$$

On the other hand, since $\varphi_1(t,\cdot,\cdot)\in\mathcal{E}$, necessarily $\int f^\alpha \mathcal{C}_{\mathrm{el}}\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p=0$.

Let us decompose f^α as follows:

$$f^\alpha = F^\alpha + \alpha g^\alpha,$$

with $F^\alpha=\mathcal{P}f^\alpha$ and $g^\alpha=\mathcal{P}^\perp f^\alpha/\alpha$. According to Lemma 3.3 (iv), $\Lambda\varphi_1$ lies in $\mathcal{E}^\perp$. Therefore, $\int F^\alpha\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p=0$ since $F^\alpha\in\mathcal{E}$ and

$$\frac{1}{\alpha}\int f^\alpha\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = \int g^\alpha\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p. \tag{3.13}$$

We are thus led to investigate the behavior of g^α as $\alpha\to 0$. According to Eq. (3.11), and using the definition of g^α, we have

$$\int_0^t \|g^\alpha(s)\|_{L^2_{x,p}}\,\mathrm{d}s \leqslant C.$$

Therefore, there exists g such that $g^\alpha \rightharpoonup g$ weakly * in $L^\infty(0,T;L^2_{x,p})$ and,

$$\frac{1}{\alpha}\int f^\alpha\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = \int g^\alpha\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p \to \int g\Lambda\varphi_1\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p \tag{3.14}$$

as $\alpha\to 0$. It remains to relate the last integral in (3.14) to F.

To this aim, we come back to (3.12), that we write with another particular test function φ_2 (specified below). Equation (3.12) can be written in terms of g^α and F^α. Since the sequences F^α and g^α are bounded, keeping only the leading order terms in this equation leads to

$$\int g^\alpha\mathcal{C}_{\mathrm{el}}\varphi_2\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = -\int F^\alpha\Lambda\varphi_2\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p + \mathcal{O}(\alpha),$$

or, letting $\alpha\to 0$,

$$\int g\mathcal{C}_{\mathrm{el}}\varphi_2\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = -\int F\Lambda\varphi_2\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p. \tag{3.15}$$

Now, by choosing

$$\varphi_2 = (\mathcal{C}_{\mathrm{el}})^{-1}(\Lambda\varphi_1),$$

we deduce that the last integral in (3.14) can be rewritten

$$\int g\Lambda\varphi_1 \,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = \int g\mathcal{C}_{\mathrm{el}}\varphi_2 \,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p$$

and straightforward calculations lead to

$$\int g\Lambda\varphi_1 \,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}p = -\int NF\mathcal{P}(\Lambda((\mathcal{C}_{\mathrm{el}})^{-1}(\Lambda\varphi_1)))\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\varepsilon.$$

Finally, we get

$$\int NF(\partial_t\Phi - \mathcal{P}(\Lambda((\mathcal{C}_{\mathrm{el}})^{-1}(\Lambda\varphi_1))))\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}\varepsilon = \int NF_I\Phi(0,x,\varepsilon)\mathrm{d}x\,\mathrm{d}\varepsilon \tag{3.16}$$

which is obviously the weak form of (3.10). It remains to check that this formal identification can be made rigorous. Namely, we must prove that, if $\Phi \in W^{1,\infty}(0,T;C_c^\infty(\mathbb{R}^3\times\mathbb{R}^+))$, then $\varphi_2 = (\mathcal{C}_{\mathrm{el}})^{-1}(\Lambda\varphi_1)$ is an admissible test function for (3.12). By Lemma 3.3 (under Assumption 3.2), it is an easy task, since we have

$$(\mathcal{C}_{\mathrm{el}})^{-1}(\Lambda\varphi_1) = -\frac{1}{\nu}\Lambda\varphi_1.$$

□

C. The QQSHE$_2$ model: quantum corrections to the classical SHE model

The explicit form of the diffusion term $\mathcal{P}(\Lambda(\Lambda F))N(\varepsilon)/\nu$ in (3.8) is not easy to handle. As in Ref. 19 we give the expansion of this model in $\hbar$, up to second order terms. This leads to the classical SHE model enriched with quantum correction terms.

In the remainder of this paper, when a function F depends on p through the energy $|p|^2/2$ only, we note equally $F(|p|^2/2)=F(p)$ when the context is clear.

The Wigner transport operator Λ depends on the reduced Planck constant. At usual macroscopic scales, this constant is negligible and the transport operator Λ can be expanded in powers of $\hbar$. Formally, one has

$$\Lambda = L + \hbar^2 L^{(2)} + \mathcal{O}(\hbar^4), \tag{3.17}$$

where $L=p\cdot\nabla_x - \nabla_x V\cdot\nabla_p$ is the classical transport operator and $L^{(2)}$ is a third order differential operator given by

$$L^{(2)} = \tfrac{1}{24}\nabla_x^{\otimes 3}V \vdots \nabla_p^{\otimes 3}.$$

Here the third order tensors are defined as $(\nabla_x^{\otimes 3})_{i,j,k}=\partial^3_{x_i,x_j,x_k}$ (and analogously for $\nabla_p^{\otimes 3}$) and $\vdots$ denotes the third order tensor product. Formula (3.17) gives the leading and second order terms of the so-called Wigner-Moyal expansion (see Ref. 43).

Then the diffusion term becomes

$$N(\varepsilon)\mathcal{P}(\Lambda(\Lambda F)) = N(\varepsilon)\mathcal{P}(L(LF)) + \hbar^2 N(\varepsilon)(\mathcal{P}(L^{(2)}(LF)) + \mathcal{P}(L(L^{(2)}F))) + \mathcal{O}(\hbar^4).$$

Note that $\mathcal{P}(L(LF))$ is the diffusion term that is involved in the CSHE model (2.11), (2.14). Indeed, when F is a function of the position and energy only $LF=p\cdot\tilde{\nabla}F$, where $\tilde{\nabla}$ is the "twisted" gradient operator defined at (2.12). Therefore, $L(LF)=p^{\otimes 2}:\tilde{\nabla}^{\otimes 2}F-\nabla_x V\cdot\tilde{\nabla}F$. Applying projector $\mathcal{P}$ yields

$$N(\varepsilon)\mathcal{P}(L(LF)) = 4\pi\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla}\cdot\tilde{\nabla}F - 4\pi(2\varepsilon)^{1/2}\nabla_x V\cdot\tilde{\nabla}F$$

and one can check that the right-hand side of this equation can be written

$$4\pi\tilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla}F\right)$$

which is the diffusion term in the classical SHE model.

For the computation of the other terms, we refer the reader to Appendix A. They are summarized in the following formal lemma.

Lemma 3.9: *We assume that the collision operator is given by* (2.13). *Up to second order terms in* $\hbar$, *the QQSHE model can be formally approached by the following* QQSHE_2 *model* (*in the case where* ν *is a constant independent of* ε):

$$N(\varepsilon)\partial_t F - \frac{4\pi}{\nu}\tilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla}F\right) - \frac{4\pi\hbar^2}{24\nu}\left\{\frac{\partial^2}{\partial\varepsilon^2}\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\cdot\partial_\varepsilon\tilde{\nabla}F\right)\right.$$
$$\left.+\frac{\partial}{\partial\varepsilon}\tilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\partial_\varepsilon^2 F\right)\right\}=0. \tag{3.18}$$

Remark 3.10: Compared with the CSHE model (2.11), additional terms involving fourth order derivatives appear. They are multiplied by factors involving third order derivatives of the potential, which is natural since these factors appear in the first correction to the classical limit in the Wigner-Moyal expansion.[43] Also, these fourth order derivatives of F involve cross-diffusion terms mixing space and energy derivatives. This is to be related with the cross-diffusion terms that appear in the Fokker-Planck equation used in Ref. 4. □

Given that the coefficients of the fourth order derivatives have no fixed sign, one can wonder about the stability and well-posedness of this model. As for the QQSHE model, there is no clear entropic structure for the QQSHE_2 model. Therefore, no clear indication is given why this model should be well-posed. A linearized stability analysis of this model is in progress to try to answer this question. If the model is found linearly stable, there is good hope that it can be used to efficiently simulate quantum semiconductor devices numerically. □

IV. QUANTUM COLLISION OPERATORS

All the results given in the following section are formal. In Sec. III, the SHE models are of a hybrid type since they are derived from a microscopic equation with a quantum transport term and a classical collision operator. To remedy to this inconsistency, we need to develop a notion of quantum collision operator which allows us to perform the program leading to SHE-type models.

An important property of the collision operators used in classical kinetic theory is the entropy dissipation. Therefore, a natural requirement of a quantum collision operator $\mathcal{Q}$ is that it dissipates quantum entropy and that a quantum kinetic equation such as the Wigner-Boltzmann equation

$$\partial_t f + p\cdot\nabla_x f - \theta[V]f = \mathcal{Q}(f) \tag{4.1}$$

satisfies a quantum analogue to Lemma 2.1.

The collision operator $\mathcal{Q}$ will be derived as a quantum counterpart of the classical electron-phonon collision operator (or its elastic approximation). Therefore, the equilibrium states of this quantum operator will be "quantum" Maxwellian, as the classical operator had ("classical") Maxwellian equilibria. Consequently, the quantum relative entropy associated with the von Neumann equation (3.4) is defined by $H_Q(\rho)=\mathrm{Tr}\{\rho(\ln\rho-1+\mathcal{H})\}$ where $\mathcal{H}=-(\hbar^2/2)\Delta+V$ is the particle Hamiltonian. Lemma 3.1 allows to deduce the expression of quantum entropy in the Wigner framework by

$$H_Q(f)=\frac{1}{(2\pi\hbar)^3}\int f\left(\mathcal{L}\mathrm{n}(f)+\frac{|p|^2}{2}+V-1\right)\mathrm{d}p\,\mathrm{d}x, \tag{4.2}$$

where the "quantum logarithm" $\mathcal{L}\mathrm{n}$ is defined by

$$\mathcal{L}\mathrm{n}(f) = W[\ln(\mathrm{Op}(f))],$$

assuming that $\mathrm{Op}(f) > 0$. Analogously, we define the "quantum exponential" and the quantum Maxwellian $\mathcal{M}\mathrm{ax}$, respectively, by

$$\mathcal{E}\mathrm{xp}(f) = W[\exp(\mathrm{Op}(f))],$$

$$\mathcal{M}\mathrm{ax}(x,p) = W\left[\exp\left(\mathrm{Op}\left(-\frac{|p|^2}{2} - V(x)\right)\right)\right] = \mathcal{E}\mathrm{xp}(-|p|^2/2 - V).$$

Note that $\mathcal{L}\mathrm{n}$ and $\mathcal{E}\mathrm{xp}$ are formal inverses and that $-|p|^2/2 - V = \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}(x,p))$.

Then (4.2) is equivalently written [up to a constant multiplier $(2\pi\hbar)^2$]

$$H_Q(f) = \int f(\mathcal{L}\mathrm{n}(f) - \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}) - 1)\mathrm{d}p\,\mathrm{d}x$$

and appears as the quantum relative entropy with respect to quantum Maxwellian steady states. The following lemma gives a criterion on $\mathcal{Q}$ for Eq. (4.1) to be consistent with the quantum entropy H_Q.

Lemma 4.1: *Let* $\mathcal{Q}$ *in* (4.1) *be such that, for any function* g, *we have*

$$-\int \mathcal{Q}(g)(\mathcal{L}\mathrm{n}(g) - \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}x\,\mathrm{d}p \geqslant 0. \tag{4.3}$$

Then, if f *is a solution of Eq.* (4.1), *the associated quantum entropy satisfies*

$$\frac{\mathrm{d}H_Q(f)}{\mathrm{d}t} \leqslant 0. \tag{4.4}$$

Proof: To begin with, we recall that H_Q is Gâteaux differentiable and its Gâteaux derivative at f in the direction δf is (see Ref. 21)

$$H_Q'(f)\,\delta f = (2\pi\hbar)^3\,\mathrm{Tr}\{(\ln \mathrm{Op}(f) + \mathcal{H})\mathrm{Op}(\delta f)\}$$

or,

$$H_Q'(f)\,\delta f = \int \left(\mathcal{L}\mathrm{n}\, f + \frac{|p|^2}{2} + V\right)\delta f\,\mathrm{d}p\,\mathrm{d}x.$$

Therefore, if f is a solution of (4.1),

$$\begin{aligned}\frac{\mathrm{d}H_Q(f)}{\mathrm{d}t} &= \int \left(\mathcal{L}\mathrm{n}\, f + \frac{|p|^2}{2} + V\right)\partial_t f\,\mathrm{d}p\,\mathrm{d}x = -\int \left(\mathcal{L}\mathrm{n}\, f + \frac{|p|^2}{2} + V\right)\Lambda f\,\mathrm{d}p\,\mathrm{d}x \\ &\quad - \int \left(\mathcal{L}\mathrm{n}\, f + \frac{|p|^2}{2} + V\right)\mathcal{Q}(f)\mathrm{d}p\,\mathrm{d}x \\ &= -\int \left((W[\ln(\mathrm{Op}(f))] + W[\mathcal{H}])\frac{i}{\hbar}W[\mathcal{H}\,\mathrm{Op}(f) - \mathrm{Op}(f)\mathcal{H}]\right)\mathrm{d}p\,\mathrm{d}x \\ &\quad - \int (\mathcal{L}\mathrm{n}(f) - \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\,\mathcal{Q}(f)\mathrm{d}p\,\mathrm{d}x \end{aligned} \tag{4.5}$$

thanks to Lemma (3.1) (iv). Now, using (3.1) (iii), the first integral on the right-hand side can be written

$$(2\pi)^3 i\hbar^2 \operatorname{Tr}\{(\ln(\mathrm{Op}(f)) + \mathcal{H})[\mathcal{H}, \mathrm{Op}(f)]\}$$

or, using the cyclicity of the trace,

$$(2\pi)^3 i\hbar^2 \operatorname{Tr}\{[\mathrm{Op}(f), \ln(\mathrm{Op}(f))]\mathcal{H} + [\mathcal{H}, \mathcal{H}]\mathrm{Op}(f)\}$$

and this trace is obviously null. Finally, the second integral on the right-hand side of (4.5) is non-negative according to (4.3), which completes the proof. □

Consequently, after Ref. 22, what is meant in this paper by quantum collision operators is a class of collision operators $\mathcal{Q}$ that satisfy the following formal properties: for any function $f(x,p)$,

$$\textit{Mass conservation}: \int \mathcal{Q}(f)(p)\mathrm{d}x\,\mathrm{d}p = 0,$$

$$\textit{Entropy dissipation}: -\int \mathcal{Q}(f)(\mathcal{L}\mathrm{n}(f) - \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}x\,\mathrm{d}p \geqslant 0.$$

A. The quantum electron-phonon collision operator

In this section, quantum counterparts of the classical collision operator $\mathcal{C}_{e\varphi}$ and of its elastic approximation $\mathcal{C}_{\mathrm{el}}$ are introduced. They may lead to possibly interesting quantum models for electron-phonon scattering. Moreover, the derivation of a quantum SHE model in Sec. V is performed from a quantum kinetic equation with a relaxation collision operator which can be understood as a relaxation approximation of the operators studied in this section.

Keeping Lemma 4.1 in mind, we introduce the following quantum version of the electron-phonon collision operator $\mathcal{C}_{e\varphi}$ described in Sec. II B (we recall that β is the phonon energy in scaled variables):

$$\mathcal{Q}_{e\varphi}(f) = \int \mathcal{S}(p,p')[\delta(\varepsilon' - \varepsilon - \beta) + \delta(\varepsilon' - \varepsilon + \beta)]\left(\frac{\mathcal{A}(f)'}{M'} - \frac{\mathcal{A}(f)}{M}\right)\mathrm{d}p', \tag{4.6}$$

where

$$\mathcal{A}(f) = \exp W[\ln \mathrm{Op}(f)] = \exp \mathcal{L}\mathrm{n}\, f, \tag{4.7}$$

namely $\mathcal{L}\mathrm{n}\, f = \ln \mathcal{A}(f)$ where ln is the ordinary logarithm. Note that it is not clear what conditions f should satisfy for $\mathcal{A}(f)$ to be a well-defined function. Therefore, the definition of $\mathcal{Q}_{e\varphi}$ is purely formal at this point and all the results stated in this section are formal.

However, we claim that this operator is a natural extension of the classical phonon operator to quantum systems, and that it is consistent with quantum entropy relaxation. Indeed, we have the following.

Proposition 4.2: *The collision operator* $\mathcal{Q}_{e\varphi}$ *defined by* (4.6) *satisfies the following properties*:

(i) *Mass conservation*: $\int \mathcal{Q}_{e\varphi}(f)\mathrm{d}p = 0$ *for any measurable function* f.

(ii) *Equilibrium states*: *for any measurable function* $f(x,p)$, *we have* $\mathcal{Q}_{e\varphi}(f) = 0$ *if and only if*

$$f(x,p) = \mathcal{E}\mathrm{xp}\left(\frac{|\cdot|^2}{2} + \ln F\left(\frac{|\cdot|^2}{2}\right)\right)(x,p) = W\left[\exp\left(-\frac{\hbar^2}{2}\Delta + \mathrm{Op}(\ln F)\right)\right](x,p)$$

where $F = F(\varepsilon)$ *is such that* $F(\varepsilon+\beta) = F(\varepsilon)$.

(iii) *Entropy dissipation*: $-\int \mathcal{Q}_{e\varphi}(f)(\mathcal{L}\mathrm{n}(f) - \mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}p \geqslant 0$ *for any function* f.

Proof: The mass conservation follows from the symmetry of $\mathcal{S}(p,p')$. The equilibria of operator $\mathcal{Q}_{e\varphi}$ can be easily deduced from those of operator $\mathcal{C}_{e\varphi}$ by remarking that $\mathcal{Q}_{e\varphi}(f) = \mathcal{C}_{e\varphi}(\mathcal{A}(f))$. On the other hand, it follows from the symmetry of $\mathcal{S}$ that

$$-\int \mathcal{Q}_{e\varphi}(f)(\mathcal{L}\mathrm{n}(f)-\mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}p$$

$$=\frac{1}{2}\int \mathcal{S}(p,p')(\delta_+ + \delta_-)\left(\frac{\mathcal{A}(f)'}{M'}-\frac{\mathcal{A}(f)}{M}\right)\left(\ln\frac{\mathcal{A}(f)'}{M'}-\ln\frac{\mathcal{A}(f)}{M}\right)\mathrm{d}p\,\mathrm{d}p'\,\mathrm{d}x$$

which is non-negative since ln is an increasing function. □

Like in the case of the classical electron-phonon scattering, we are interested in the elastic limit $\beta\to 0$ of the operator $\mathcal{Q}_{e\varphi}$. More precisely, we let ω_0 tend to zero and get

$$\mathcal{Q}_{\mathrm{el}}(f)(p)=N(|p|^2/2)\{\mathcal{P}(\widetilde{\mathcal{S}}(p,\cdot)\mathcal{A}(f)(\cdot))-\mathcal{P}(\widetilde{\mathcal{S}}(p,\cdot))\mathcal{A}(f)(p)\}, \tag{4.8}$$

where $\widetilde{\mathcal{S}}$ is defined as in Sec. II B by formula (2.9). We drop the tildes in the remainder of the paper. This operator has the properties of a quantum collision operator.

Proposition 4.3: *The collision operator* $\mathcal{Q}_{\mathrm{el}}$ *defined by* (4.8) *satisfies the following properties*:

(i) *Mass conservation*: $\int \mathcal{Q}_{\mathrm{el}}(f)\mathrm{d}p=0$ *for any measurable function* f.

(ii) *Equilibrium states*: *for any measurable function* $f(x,p)$, *we have* $\mathcal{Q}_{\mathrm{el}}(f)=0$ *if and only if there exists a function* $\lambda(x,\varepsilon)$ *of position and energy only such that*

$$f(x,p)=\mathcal{E}\mathrm{xp}(\widetilde{\lambda})(x,p),$$

where $\widetilde{\lambda}(x,p)=\lambda(x,|p|^2/2)$.

(iii) *Entropy dissipation*: $-\int \mathcal{Q}_{\mathrm{el}}(f)(\mathcal{L}\mathrm{n}(f)-\mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}p\geqslant 0$ *for any function* f.

Remark 4.4: Note that f, unlike λ, is *not* a function of the energy only in general. Indeed, it is not clear that the quantum exponential of a function of position and energy $(x,\varepsilon(p))$ remains a function of $(x,\varepsilon(p))$ [with $\varepsilon(p)=|p|^2/2$]. □

Proof: Mass conservation and entropy dissipation can be proven in the same way as for $\mathcal{Q}_{e\varphi}$. For (ii), we consider

$$-\int \mathcal{Q}_{\mathrm{el}}(f)(p)\mathcal{A}(f)(p)\mathrm{d}p=\frac{1}{2}\int \delta\left(\frac{|p'|^2}{2}-\frac{|p|^2}{2}\right)\mathcal{S}(p,p')(\mathcal{A}(f)(p')-\mathcal{A}(f)(p))^2\,\mathrm{d}p'\,\mathrm{d}p\geqslant 0,$$

where $\mathcal{A}$ is defined by (4.7).

Obviously, if $Q_{\mathrm{el}}(f)=0$, then one necessarily has $\mathcal{A}(f)(x,p)=\mathcal{A}(f)(x,p')$ whenever $|p|=|p'|$. Therefore, $\mathcal{A}(f)$ is a function of x and $|p|^2/2$ only. Consequently, $\ln\mathcal{A}(f)$ depends only on $|p|^2/2$ too and, finally, one can set $\lambda(\varepsilon)=\ln\mathcal{A}(f)=\mathcal{L}\mathrm{n}\,f$, or $f=\mathcal{E}\mathrm{xp}\,\lambda$. □

B. The quantum relaxation operator

In classical kinetic theory, an important class of collision operators is constituted by the relaxation operators. The mathematical study of these operators is simpler than for Boltzmann-type collision operators although they share many important properties with them, such as entropy dissipation, mass conservation and the expression of their equilibrium states.

The task in this section is to introduce a consistent notion of quantum relaxation operator that satisfies properties (i), (ii), and (iii) of Proposition 4.3. To this aim, we introduce the following minimization problem:

Given f, find $\mathcal{E}_f$ such that:

$$H_Q(\mathcal{E}_f) = \mathrm{Min}\{H_Q(g)/\mathcal{P}(f-g)=0\}. \tag{4.9}$$

Assuming that, for f in a suitable space, a solution $\mathcal{E}_f$ to this problem exists, we set

$$\mathcal{Q}_{\mathrm{rel}}(f) = \nu(\mathcal{E}_f - f), \tag{4.10}$$

where ν is assumed to be constant in the sequel.

It remains to prove that such an operator has the required properties. We have the following.

Proposition 4.5 The collision operator $\mathcal{Q}_{\mathrm{rel}}$ *defined by* (4.10) *satisfies the following properties:*

(i) *Mass conservation:* $\int \mathcal{Q}_{\mathrm{rel}}(f)\mathrm{d}p=0$ *for any measurable function* f.

(ii) *Equilibrium states: for any measurable function* $f(x,p)$, *we have* $\mathcal{Q}_{\mathrm{rel}}(f)=0$ *if and only if there exists a function* $\lambda(x,\varepsilon)$ *of* x *and the energy only such that*

$$f(x,p) = \mathcal{E}\mathrm{xp}(\tilde{\lambda})(x,p),$$

where $\tilde{\lambda}(x,p)=\lambda(x,|p|^2/2)$.

(iii) *Entropy dissipation:* $-\int \mathcal{Q}_{\mathrm{rel}}(f)(\mathcal{L}\mathrm{n}(f)-\mathcal{L}\mathrm{n}(\mathcal{M}\mathrm{ax}))\mathrm{d}p \geqslant 0$ *for any function* f.

Before proving Proposition 4.5, we state an important property of the solutions of the minimization problem (4.9).

Lemma 4.6: Let f *be a function such that a solution of the minimization problem* (4.9) *exists. We denote such a solution by* $\mathcal{E}_f$. *Then, there exists a function* $\lambda(x,\varepsilon)$ *such that*

$$\mathcal{E}_f(x,p) = \mathcal{E}\mathrm{xp}(\lambda)(x,p).$$

Proof: Since $\mathcal{E}_f$ is the minimizer of $H_Q(g)$ under the constraint $\mathcal{P}(f-g)=0$, there exists a Lagrange multiplier $\mu(x,\varepsilon)$ such that $H_Q'(f)g+\mu\mathcal{P}(g)=0$ for all g. This means that, for all g,

$$\int \left(\mathcal{L}\mathrm{n}(f) + \frac{|p|^2}{2} + V - \mu(x,|p|^2/2)\right) g(x,p)\mathrm{d}p\,\mathrm{d}x = 0,$$

that is $f=\mathcal{E}\mathrm{xp}(\lambda(x,\varepsilon))$ with $\lambda(x,\varepsilon)=\mu(x,\varepsilon)-\varepsilon-V(x)$. □

Proof of Proposition 4.5: Point (i) is obvious since the definition of $\mathcal{E}_f$ implies that $\mathcal{P}(f-\mathcal{E}_f)=0$. Point (ii) is a straightforward consequence of Lemma 4.6. The proof of point (iii) is inspired from Ref. 19. We introduce

$$\Gamma : \gamma \in [0,1] \to \int_{\mathbb{R}^6} \nu(x,\varepsilon) h((1-\gamma)\mathcal{E}_f + \gamma f)\mathrm{d}x\,\mathrm{d}p$$

with $h : f \to f(\mathcal{L}\mathrm{n}\, f - 1 + |p|^2/2 + V)$. Deriving Γ by a chain rule yields

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\gamma}(\gamma) = \int_{\mathbb{R}^6} \nu(x,\varepsilon_p)(f-\mathcal{E}_f)(\mathcal{L}\mathrm{n}((1-\gamma)\mathcal{E}_f + \gamma f) + |p|^2/2 + V)\mathrm{d}x\,\mathrm{d}p.$$

The convexity of h implies that Γ is also convex so that $(\mathrm{d}\Gamma/\mathrm{d}\gamma)(1) \geqslant \Gamma(1)-\Gamma(0)$, which in turn gives

$$-\int \mathcal{Q}_{\mathrm{rel}}(f)(\mathcal{L}\mathrm{n}(f) + |p|^2/2 + V)\mathrm{d}x\mathrm{d}p \geqslant \nu(H_Q(f) - H_Q(\mathcal{E}_f)) \geqslant 0$$

since $\mathcal{E}_f$ is a minimizer of H_Q and ν is a constant. □

Before turning to the derivation of a fully quantum SHE type model, it is important to underline that the collisional Wigner equation equipped with relaxation type operator $\mathcal{Q}_{\mathrm{rel}}$ is a consistent quantum model in the sense that it (formally) preserves positivity. Precisely, the following proposition holds true.

Proposition 4.7: Let the initial datum f_I be positive [in the sense of operators, i.e., *$\rho_I = \mathrm{Op}(f_I)$ is a positive operator]. If the following initial value problem,*

$$\partial_t f + \Lambda f = \mathcal{Q}_{\mathrm{rel}} f, \quad f(t=0,x,p) = f_I(x,p),$$

has a solution $f(t,x,p)$, then this solution is positive [i.e., *$\rho(t) = \mathrm{Op}(f)(t)$ is a positive operator*] *for all time*.

Proof: The proof is very close to the proof of Lemma 2.1 in Ref. 19. We just emphasize on the positivity of operator $\mathrm{Op}(\mathcal{E}_f)$. Indeed, according to Lemma 4.6, to any given function f there can be associated an energy dependent function λ_f such that

$$\mathcal{E}_f = \mathcal{E}\mathrm{xp}(\lambda_f).$$

Consequently, $\mathrm{Op}(\mathcal{E}_f) = \mathrm{Op}(W(\exp \mathrm{Op}(\lambda_f))) = \exp \mathrm{Op}(\lambda_f)$ which obviously is a positive operator.□

This quantum relaxation collision operator will be used for the derivation of the full quantum SHE model. Note that at this point, the existence of a minimizer for (4.9) is an open problem.

V. THE FULL QUANTUM SHE MODEL (QSHE)

In this section, we formally investigate the limit $\alpha \to 0$ in the following rescaled Wigner-Quantum relaxation equation:

$$\alpha \partial_t f^\alpha + \Lambda f^\alpha = \frac{1}{\alpha} \mathcal{Q}_{\mathrm{rel}}(f^\alpha), \tag{5.1}$$

where we recall that $\Lambda = p \cdot \nabla_x - \theta[V]$ is the Wigner operator. In the sequel, we assume the following.

Assumption 5.1: *For any given function f, there exists a solution $\mathcal{E}_f$ to the minimization problem* (4.9), *and this solution is unique*.

The following formal result holds.

Theorem 5.2: *If* (5.1) *admits a solution f^α for all α, and if the so-obtained sequence f^α admits a convergent subsequence, then the limit is denoted by $\mathcal{F}$ and there exists a function λ such that $\tilde{\lambda}: (t,x,p) \to \lambda(t,x,|p|^2/2)$ satisfies*

$$\begin{gathered} \mathcal{F}(t,x,p) = \mathcal{E}\mathrm{xp}(\tilde{\lambda})(t,x,p), \\ N(\varepsilon)\partial_t \mathcal{P}(\mathcal{E}\mathrm{xp}(\tilde{\lambda})) - N(\varepsilon)\mathcal{P}\left(\Lambda\left(\frac{1}{\nu}\Lambda(\mathcal{E}\mathrm{xp}(\tilde{\lambda}))\right)\right) = 0. \end{gathered} \tag{5.2}$$

Furthermore, the quantum entropy decreases with time,

$$\frac{d}{dt} H_{\mathrm{QSHE}}(\mathcal{F}) \leqslant 0, \quad H_{\mathrm{QSHE}}(\mathcal{F}) = \int \mathcal{P}(\mathcal{F})(\lambda + \varepsilon + V - 1) N(\varepsilon) d\varepsilon \, dx. \tag{5.3}$$

Remark 5.3: The main difference between the QQSHE and QSHE models is that the unknown F in the QQSHE model (which is a function of position and energy) is replaced by $\mathcal{E}\mathrm{xp}\,\tilde{\lambda}$ in the QSHE model, where λ is a function of position and energy. This is a true difference since $\mathcal{F} = \mathcal{E}\mathrm{xp}\,\tilde{\lambda}$ is in general *not* a function of position and energy only. This difference makes the QSHE model consistent with *quantum* entropy decay (5.3) rather than classical entropy decay. Again, we do not make this equation more explicit. Indeed, here, it is not possible to make the relation between $\mathcal{E}\mathrm{xp}\,\tilde{\lambda}$ and λ explicit because $\mathcal{E}\mathrm{xp}$ is a nonlinear nonlocal operator. □

Remark 5.4: Equation (5.2) is closed provided the minimization problem (4.9) is uniquely solvable. Indeed, in this case, there is a one to one correspondence between the intensive quantity λ and the extensive quantity $\mathcal{P}(\mathcal{E}\exp\lambda)$. □

Proof: First, letting $\alpha\to 0$ in Eq. (5.1) leads to $\mathcal{Q}_{\mathrm{rel}}(\mathcal{F})=0$ so that, according to Proposition 4.5, there exists $\lambda(x,\varepsilon)$ such that $\mathcal{F}=\mathcal{E}\exp\widetilde{\lambda}$. Now, the Chapman-Enskog expansion of f^α is written

$$f^\alpha=\mathcal{E}_{f^\alpha}+\alpha g^\alpha$$

since f^α is close to the equilibrium when α is small. We assume that $\mathcal{E}_{f^\alpha}$ and g^α are bounded with respect to α in a suitable topology (see Remark 5.5 below). Then, introducing this expansion in Eq. (5.1) yields, at first order in α,

$$\mathcal{P}(\partial_t\mathcal{E}_{f^\alpha}+\Lambda g^\alpha)=\mathcal{O}(\alpha) \tag{5.4}$$

and, at zeroth order in α,

$$\Lambda\mathcal{E}_{f^\alpha}=-\nu g^\alpha+\mathcal{O}(\alpha) \tag{5.5}$$

since $\mathcal{Q}_{\mathrm{rel}}(f^\alpha)=\nu(\mathcal{E}_{f^\alpha}-(\mathcal{E}_{f^\alpha}+\alpha g^\alpha))=-\alpha\nu g^\alpha$. According to (5.5), Eq. (5.4) becomes

$$\mathcal{P}\left(\partial_t\mathcal{E}_{f^\alpha}-\Lambda\left(\frac{1}{\nu}\Lambda\mathcal{E}_{f^\alpha}\right)\right)=\mathcal{O}(\alpha). \tag{5.6}$$

We recall that $\mathcal{E}_{f^\alpha}\to\mathcal{E}\exp\widetilde{\lambda}$ as $\alpha\to 0$. Letting $\alpha\to 0$ in (5.6) leads to (5.2). The entropy decay is obtained by taking the limit $\alpha\to 0$ in (4.4). □

Remark 5.5: At this stage of investigation, any rigorous convergence proof remains speculative. However, in simpler situations, if any, a reasonable proof would at least require that sequences $\mathcal{E}_{f^\alpha}$ and g^α be bounded with respect to α in a suitable topology (precisely the topology in which convergence of sequence f^α would be proven to hold). □

From now on, we drop the tildes and identify λ to $\widetilde{\lambda}$. As in the case of the quasiquantum SHE model, it is interesting to expand the quantum SHE model in powers of $\hbar$ up to second order terms. We recall that $\Lambda=L+\hbar^2L^{(2)}+\mathcal{O}(\hbar^4)$ where $L=p\cdot\nabla_x-\nabla_xV\cdot\nabla_p$ is the classical transport operator and $L^{(2)}=(1/24)\nabla_x^{\otimes 3}V\vdots\nabla_p^{\otimes 3}$. However, unlike in the case of the quasiquantum SHE model, here not only does Λ depend on $\hbar$, but also $\mathcal{E}\exp\lambda$. After Ref. 19, the quantum exponential of any function $f(x,p)$ can be written

$$\mathcal{E}\exp f=\exp f[1+\hbar^2\mathcal{T}f+\mathcal{O}(\hbar^4)], \tag{5.7}$$

$$\mathcal{T}f=\tfrac{1}{8}\left(\nabla_x^{\otimes 2}f:\nabla_p^{\otimes 2}f-\nabla_x\nabla_pf:\nabla_p\nabla_xf+\tfrac{1}{3}(\nabla_x^{\otimes 2}f:\nabla_pf\nabla_pf-2\nabla_x\nabla_pf:\nabla_pf\nabla_xf+\nabla_p^{\otimes 2}f:\nabla_xf\nabla_xf)\right). \tag{5.8}$$

Therefore, the QSHE model is formally approached, up to second order terms, by

$$\begin{aligned}&N(\varepsilon)\partial_tF-N(\varepsilon)\mathcal{P}\left(L\left(\frac{1}{\nu}L(F)\right)\right)+\hbar^2N(\varepsilon)\partial_t[\mathcal{P}(F\mathcal{T}(\ln F))]\\&\quad-\hbar^2N(\varepsilon)\mathcal{P}\left[\left(L\left(\frac{1}{\nu}L^{(2)}\right)+L^{(2)}\left(\frac{1}{\nu}L\right)\right)(F)-L\left(\frac{1}{\nu}L(F\mathcal{T}(\ln F))\right)\right]=0.\end{aligned} \tag{5.9}$$

where we have set $F=\exp\lambda$.

We recall that ν is a constant coefficient. Using the computations already performed to prove Lemma 3.9, we obtain

$$N(\varepsilon)\partial_tF-\frac{4\pi}{\nu}\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{3/2}}{3}\widetilde{\nabla}F\right)$$

$$-\frac{4\pi\hbar^2}{24\nu}\left\{\frac{\partial^2}{\partial\varepsilon^2}\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\cdot\partial_\varepsilon\widetilde{\nabla}F\right)+\frac{\partial}{\partial\varepsilon}\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\partial_\varepsilon^2 F\right)\right\}$$

$$+\hbar^2 N(\varepsilon)\partial_t[\mathcal{P}(F\mathcal{T}(\ln F))]+\frac{\hbar^2 N(\varepsilon)}{\nu}\mathcal{P}[L(L(F\mathcal{T}(\ln F)))]=0.$$

Note that, in this equation, the two first lines correspond to the left-hand side of the QQSHE_2 equation (3.18). Other second order terms appear due to the expansion of the quantum exponential $\mathcal{E}\mathrm{xp}$ into powers of $\hbar$. Since λ is a function of the position and the energy only, after (5.8) $\mathcal{T}\lambda$ can be written as

$$\mathcal{T}\lambda=\tfrac{1}{8}\Big\{\Delta\lambda\partial_\varepsilon\lambda+p^{\otimes 2}{:}(\nabla_x^{\otimes 2}\lambda\partial_\varepsilon^2\lambda-\nabla_x(\partial_\varepsilon\lambda)\nabla_x(\partial_\varepsilon\lambda))+\tfrac{1}{3}[p^{\otimes 2}{:}(\nabla_x^{\otimes 2}\lambda(\partial_\varepsilon\lambda)^2-\partial_\varepsilon(\nabla_x\lambda\nabla_x\lambda)\partial_\varepsilon\lambda$$
$$+\nabla_x\lambda\nabla_x\lambda\partial_\varepsilon^2\lambda)+|\nabla_x\lambda|^2\partial_\varepsilon\lambda]\Big\}. \tag{5.10}$$

According to (5.10), $\mathcal{T}\lambda$ takes the following form:

$$\tfrac{1}{8}(\mathcal{I}_{[\lambda]}+p^{\otimes 2}{:}\mathcal{J}_{[\lambda]}), \tag{5.11}$$

where

$$\mathcal{I}_{[\lambda]}=\Delta\lambda\partial_\varepsilon\lambda+\tfrac{1}{3}|\nabla_x\lambda|^2\partial_\varepsilon\lambda, \tag{5.12}$$

$$\mathcal{J}_{[\lambda]}=\nabla_x^{\otimes 2}\lambda\partial_\varepsilon^2\lambda-\nabla_x(\partial_\varepsilon\lambda)\nabla_x(\partial_\varepsilon\lambda)+\tfrac{1}{3}[\nabla_x^{\otimes 2}\lambda(\partial_\varepsilon\lambda)^2-\partial_\varepsilon(\nabla_x\lambda\nabla_x\lambda)\partial_\varepsilon\lambda+\nabla_x\lambda\nabla_x\lambda\partial_\varepsilon^2\lambda]. \tag{5.13}$$

Therefore, the second order terms in the formal expansion of the QSHE model can be expressed in terms of $\mathcal{I}$ and $\mathcal{J}$.

Lemma 5.6: *We assume that the collision operator is given by* (4.10). *Up to second order terms in* $\hbar$, *the QSHE model can be formally approached by the following* QSHE_2 *model (in the case where* ν *is a constant)*:

$$N(\varepsilon)\partial_t F-\frac{4\pi}{\nu}\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{3/2}}{3}\widetilde{\nabla}F\right)$$

$$-\frac{4\pi\hbar^2}{24\nu}\left\{\frac{\partial^2}{\partial\varepsilon^2}\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\cdot\partial_\varepsilon\widetilde{\nabla}F\right)+\frac{\partial}{\partial\varepsilon}\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\partial_\varepsilon^2 F\right)\right\}$$

$$+\frac{4\pi\hbar^2}{8}\left\{\partial_t\left[F\left(\sqrt{2\varepsilon}\mathcal{I}_{[\ln F]}+\frac{(2\varepsilon)^{2/3}}{3}\mathrm{Trace}\ \mathcal{J}_{[\ln F]}\right)\right]\right.$$

$$+\frac{1}{\nu}\left[\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{3/2}}{3}\widetilde{\nabla}(F\mathcal{I}_{[\ln F]})\right)+2\widetilde{\nabla}^{\otimes 2}{:}\frac{(2\varepsilon)^{5/2}}{15}(F\mathcal{J}_{[\ln F]})\right.$$

$$\left.\left.\widetilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{5/2}}{3}\widetilde{\nabla}(F\ \mathrm{Trace}\ \mathcal{J}_{[\ln F]})\right)\right]\right\}=0,$$

where $\mathcal{I}$ *and* $\mathcal{J}$ *are given by* (5.12) and (5.13), *respectively*, *and* Trace $\mathcal{J}$ *denotes the trace of the second order tensor* $\mathcal{J}$, *namely*

$$\mathrm{Trace}\ \mathcal{J}=\Delta\lambda\ \partial_\varepsilon^2\lambda-|\nabla_x(\partial_\varepsilon\lambda)|^2+\tfrac{1}{3}(\Delta\lambda(\partial_\varepsilon\lambda)^2-\partial_\varepsilon(|\nabla_x\lambda|^2)\partial_\varepsilon\lambda+|\nabla_x\lambda|^2\partial_\varepsilon^2\lambda). \tag{5.14}$$

Remark 5.7: In this equation, we first find the terms involved in the QQSHE_2 model (3.18)

(the first two lines). Then, additional terms arise due to the nonlinear relation between F and $\mathcal{E}\mathrm{xp}\,\tilde{\lambda}$. They still are fourth order terms, but now they are nonlinear. They still involve crossed derivatives. The same stability questions as for the QQSHE_2 model can be posed for this model, completed by the fact that it is now a nonlinear model. The answer to the stability question is therefore even more complex. That this model can be effective for practical computations is not clear. Probably, a direct numerical resolution of the full QSHE model will be more efficient, as it is the case for drift diffusion models (see, e.g., Refs. 28, 29, and 16). □

VI. CONCLUSION

In this paper, we have investigated possible quantum extensions of classical SHE (or Fokker-Planck) models. After a review of the derivation of classical SHE models, two possible extensions have been given: one by using a classical operator at the right-hand side of a quantum Wigner equation, a second one, by using a quantum version of a relaxation operator. The first approach obviously lacks consistency but gives rise to a seemingly tractable equation. The second approach, although more consistent, gives rise to a rather complex model, the practical effectiveness of which is not clear. More work is required to settle the question of stability of these models and to try to find more tractable expressions of them.

APPENDIX A: THE QQSHE_2 MODEL

In the sequel, the following identities are needed (a denotes a fourth order tensor and Einstein's convention is used):

$$\mathcal{P}(1)=1,\quad \mathcal{P}(p)=0,\quad \mathcal{P}(p^{\otimes 2})(\varepsilon)=\frac{2\varepsilon}{3}\delta, \tag{A1}$$

$$(\mathcal{P}(p^{\otimes 4})::a)(\varepsilon)=\frac{(2\varepsilon)^2}{15}(a_{i,i,j,j}+a_{i,j,i,j}+a_{i,j,j,i}), \tag{A2}$$

where δ denotes the second order tensor the components of which are δ^i_j (δ^i_j is the Kronecker symbol). No confusion should arise with the Dirac measure δ. Moreover, :: denotes the fourth order tensor product, defined by

$$a::b=a_{i,j,k,l}b_{i,j,k,l},$$

for two fourth order tensors a and b.

The trace of any second order tensor $\mathcal{G}$ is denoted by $\mathrm{Trace}\,\mathcal{G}$. We recall that we note $\tilde{\nabla}=\nabla_x-\nabla_x V\partial_\varepsilon$.

We first compute the term $\mathcal{P}(L(L^{(2)}F))$, where F depends on p only through the kinetic energy $|p|^2/2$. Obviously then, $\nabla_p F=p\partial_\varepsilon F$. Then,

$$\begin{aligned}\nabla_p^{\otimes 3}F&=\nabla_p\otimes[\nabla_p\otimes(p\partial_\varepsilon F)]\\&=\nabla_p\otimes[\delta\partial_\varepsilon F+p\otimes p\partial_\varepsilon^2 F]\\&=(2\delta\otimes p+p\otimes\delta)\partial_\varepsilon^2 F+p^{\otimes 3}\partial_\varepsilon^3 F\end{aligned}$$

and, since $\nabla_x^{\otimes 3}V$ is a symmetric tensor, we have

$$\nabla_x^{\otimes 3}V\vdots\nabla_p^{\otimes 3}F=3\nabla_x^{\otimes 3}V\vdots p\otimes\delta\partial_\varepsilon^2 F+\nabla_x^{\otimes 3}V\vdots p^{\otimes 3}\partial_\varepsilon^3 F=3p\cdot\nabla_x(\Delta V)\partial_\varepsilon^2 F+\nabla_x^{\otimes 3}V\vdots p^{\otimes 3}\partial_\varepsilon^3 F \tag{A3}$$

since $\mathcal{G}:\delta=\mathrm{Trace}(\mathcal{G})$ for any second order tensor. Now, apply L to $\nabla_x^{\otimes 3}V\vdots\nabla_p^{\otimes 3}F$. First, by (A3),

$$p \cdot \nabla_x(\nabla_x^{\otimes 3} V \vdots \nabla_p^{\otimes 3} F) = 3p^{\otimes 2} : \nabla_x(\nabla_x(\Delta V)\partial_\varepsilon^2 F) + p^{\otimes 4} :: \nabla_x(\nabla_x^{\otimes 3} V \partial_\varepsilon^3 F) \tag{A4}$$

and, on the other hand,

$$\begin{aligned}\nabla_x V \cdot \nabla_p(\nabla_x^{\otimes 3} V \vdots \nabla_p^{\otimes 3} F) &= 3\nabla_x V \nabla_x(\Delta V) : \nabla_p(p\partial_\varepsilon^2 F) + \nabla_x V \nabla_x^{\otimes 3} V :: \nabla_p(p^{\otimes 3}\partial_\varepsilon^3 F) \\ &= 3\nabla_x V \nabla_x(\Delta V) : (\delta \partial_\varepsilon^2 F + p^{\otimes 2}\partial_\varepsilon^3 F) \\ &\quad + \nabla_x V \nabla_x^{\otimes 3} V :: [(\delta p^{\otimes 2} + 2p^{\otimes 2}\delta)\partial_\varepsilon^3 F + p^{\otimes 4}\partial_\varepsilon^4 F].\end{aligned} \tag{A5}$$

We recall that $N(\varepsilon) = 4\pi\sqrt{2\varepsilon}$ and that, for any function $f(p)$ and any function ϕ independent of p or depending on p only through the energy $|p|^2/2$, we have $\mathcal{P}(f\phi) = \mathcal{P}(f)\phi$. Based on this, the projection on $\mathcal{E}$ takes the form

$$\begin{aligned}&N(\varepsilon)\mathcal{P}(p \cdot \nabla_x(\nabla_x^{\otimes 3} V \vdots \nabla_p^{\otimes 3} F))(\varepsilon) \\ &\quad = N(\varepsilon)\mathcal{P}(3p^{\otimes 2}) : \nabla_x(\nabla_x(\Delta V)\partial_\varepsilon^2 F) + N(\varepsilon)\mathcal{P}(p^{\otimes 4}) :: \nabla_x(\nabla_x^{\otimes 3} V \partial_\varepsilon^3 F) \\ &\quad = 4\pi\left\{(2\varepsilon)^{3/2}\nabla_x \cdot (\nabla_x(\Delta V)\partial_\varepsilon^2 F) + \frac{(2\varepsilon)^{5/2}}{5}\nabla_x \cdot (\nabla_x(\Delta V)\partial_\varepsilon^3 F)\right\} \\ &\quad = 4\pi\frac{\partial}{\partial\varepsilon}\nabla_x \cdot \left\{\frac{(2\varepsilon)^{5/2}}{5}(\nabla_x(\Delta V)\partial_\varepsilon^2 F)\right\},\end{aligned}$$

according to (A4) [we have used (A1) and (A2)]. Following (A5), we deduce

$$\begin{aligned}&N(\varepsilon)\mathcal{P}(\nabla_x V \cdot \nabla_p(\nabla_x^{\otimes 3} V \vdots \nabla_p^{\otimes 3} F))(\varepsilon) \\ &\quad = N(\varepsilon)\left\{3\nabla_x V \nabla_x(\Delta V) : (\delta\partial_\varepsilon^2 F + \mathcal{P}(p^{\otimes 2})\partial_\varepsilon^3 F)\right. \\ &\qquad \left. + \nabla_x V \nabla_x^{\otimes 3} V :: [(\delta\mathcal{P}(p^{\otimes 2}) + 2\mathcal{P}(p^{\otimes 2})\delta)\partial_\varepsilon^3 F + \mathcal{P}(p^{\otimes 4})\partial_\varepsilon^4 F]\right. \\ &\quad = 4\pi\frac{\partial}{\partial\varepsilon}\left\{(2\varepsilon)^{3/2}\nabla_x V \cdot \nabla_x(\Delta V)\partial_\varepsilon^2 F + \frac{(2\varepsilon)^{5/2}}{5}\nabla_x V \cdot \nabla_x(\Delta V)\partial_\varepsilon^3 F\right\} \\ &\quad = 4\pi\frac{\partial}{\partial\varepsilon}\nabla_x V \cdot \frac{\partial}{\partial\varepsilon}\left\{\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\partial_\varepsilon^2 F\right\},\end{aligned}$$

where we have used (A1), (A2) and the symmetries of $\nabla_x^3 V$. Therefore,

$$N(\varepsilon)\mathcal{P}(L(L^{(2)}F))(\varepsilon) = \frac{4\pi}{24}\frac{\partial}{\partial\varepsilon}\tilde{\nabla} \cdot \left\{\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\partial_\varepsilon^2 F\right\}.$$

Let us turn to $\mathcal{P}(L^{(2)}(LF))$. First, note that, for any vector $\mathcal{G}(x,\varepsilon)$ depending only on the position and the energy (such as $\tilde{\nabla}F$ and its derivatives with respect to ε), one can write

$$\nabla_p(p \cdot \mathcal{G}) = \mathcal{G} + p(p \cdot \partial_\varepsilon \mathcal{G}). \tag{A6}$$

This will be useful in the following computations. We start from $LF = p \cdot \tilde{\nabla}F$ and apply $\nabla_p^{\otimes 3}$. Using (A6), this gives

$$\nabla_p^{\otimes 3}(p \cdot \tilde{\nabla}F) = \nabla_p^{\otimes 2}(\tilde{\nabla}F + p(p \cdot \partial_\varepsilon\tilde{\nabla}F))$$

$$= \nabla_p(p\partial_\varepsilon\tilde{\nabla}F) + \nabla_p(\delta(p \cdot \partial_\varepsilon\tilde{\nabla}F)) + \nabla_p(p\partial_\varepsilon\tilde{\nabla}F) + \nabla_p(p^{\otimes 2}(p \cdot \partial_\varepsilon^2\tilde{\nabla}F))$$

$$=3\delta\partial_\varepsilon\tilde{\nabla}F+3p^{\otimes 2}\partial_\varepsilon^2\tilde{\nabla}F+(2\delta p+p\delta)(p\cdot\partial_\varepsilon^2\tilde{\nabla}F)+p^{\otimes 3}(p\cdot\partial_\varepsilon^3\tilde{\nabla}F).$$

Using the symmetry of the third order tensor $\nabla_x^{\otimes 3}V$, we get

$$24L^{(2)}(LF)=3\partial_\varepsilon\tilde{\nabla}F\cdot\nabla_x(\Delta V)+3\nabla_x^{\otimes 3}V\vdots p^{\otimes 2}\partial_\varepsilon^2\tilde{\nabla}F$$

$$+3p^{\otimes 2}:\partial_\varepsilon^2\tilde{\nabla}F\nabla_x(\Delta V)+p^{\otimes 4}::\nabla_x^{\otimes 3}V\partial_\varepsilon^3\tilde{\nabla}F.$$

Reminding (A1) and (A2), we have

$$24\mathcal{P}(L^{(2)}(LF))=N(\varepsilon)(3\nabla_x(\Delta V)\cdot\partial_\varepsilon\tilde{\nabla}F)+3N(\varepsilon)\mathcal{P}(p^{\otimes 2}):(\partial_\varepsilon^2\tilde{\nabla}F\nabla_x(\Delta V))$$

$$+3N(\varepsilon)\mathcal{P}(p^{\otimes 2})\partial_\varepsilon^2\tilde{\nabla}F\vdots\nabla_x^{\otimes 3}V+N(\varepsilon)\mathcal{P}(p^{\otimes 4})::\partial_\varepsilon^3\tilde{\nabla}F\nabla_x^{\otimes 3}V$$

$$=4\pi\{3(2\varepsilon)^{1/2}\nabla_x(\Delta V)\cdot\partial_\varepsilon\tilde{\nabla}F+(2\varepsilon)^{3/2}(2\nabla_x(\Delta V)\cdot\partial_\varepsilon^2\tilde{\nabla}F)$$

$$+\frac{(2\varepsilon)^{5/2}}{5}(\tilde{\nabla}(\Delta V)\cdot\partial_\varepsilon^3\tilde{\nabla}F),$$

which finally gives

$$N(\varepsilon)\mathcal{P}(L^{(2)}(LF))(\varepsilon)=\frac{4\pi}{24}\frac{\partial^2}{\partial\varepsilon^2}\left\{\frac{(2\varepsilon)^{5/2}}{5}\nabla_x(\Delta V)\cdot\partial_\varepsilon\tilde{\nabla}F\right\}.$$

APPENDIX B: THE QSHE$_2$ MODEL

Let us note $\lambda=\ln F$ as in Theorem 5.2. The function λ is a function of x and ε only. We shall identify the functions $(x,p)\to\lambda(x,|p|^2/2)$ and λ when no confusion arises. We recall that, for $f(x,p)=\lambda(x,|p|^2/2)$, formula (5.8) can be rewritten as

$$\mathcal{T}\lambda(x,p)=\tfrac{1}{8}(\mathcal{I}+p^{\otimes 2}:\mathcal{J}),$$

where $\mathcal{I}$ and $\mathcal{J}$ are given by (5.12) and (5.13), respectively. The expression of the trace of the second order tensor $\mathcal{J}$ is given by (5.14).

The terms to compute are $\mathcal{P}(F\mathcal{T}(\ln F))$ and $\mathcal{P}(L(L(F\mathcal{T}(\ln F))))$. Since F is a function of the energy only, the first term is equal to $F\mathcal{P}(\mathcal{T}(\ln F))$.

1. Computation of $NF\mathcal{P}(\mathcal{T}(\ln F))$

Here, we only have to project Eq. (5.10). Using formulas (A1) and (A2), this equation becomes [we recall that $N(\varepsilon)=4\pi(2\varepsilon)^{1/2}$]:

$$N(\varepsilon)\mathcal{P}(\mathcal{T}\lambda)=\frac{4\pi}{8}\left(\sqrt{2\varepsilon}\mathcal{I}+\frac{(2\varepsilon)^{3/2}}{3}\text{Trace }\mathcal{J}\right),$$

where Trace $\mathcal{J}$ is explicited in (5.14).

2. Computation of $N\mathcal{P}(L(L(F\mathcal{T}(\ln F))))$

We first give some expressions valid for any function G and second order tensor $\mathcal{G}$ that depend only on the energy. It has been seen that $LG=p\cdot\tilde{\nabla}G$. Then a straightforward computation yields

$$L(LG) = L(p \cdot \tilde{\nabla} G) = p^{\otimes 2} : \tilde{\nabla}^{\otimes 2} G - \nabla_x V \cdot \tilde{\nabla} G,$$

where $L(p) = -\nabla_x V$ has been used. Recalling that $N(\varepsilon) = 4\pi\sqrt{2\varepsilon}$, formula (A1) gives

$$N(\varepsilon)\mathcal{P}(L(LG)) = 4\pi\left(\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla} \cdot \tilde{\nabla}(G) - \sqrt{2\varepsilon}\nabla_x V \cdot \tilde{\nabla} G\right)$$

and, since $\tilde{\nabla}(2\varepsilon)^{(k+1)/2} = (k+1)(2\varepsilon)^{k/2}\nabla_x V$,

$$N(\varepsilon)\mathcal{P}(L(LG)) = 4\pi\tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla} G\right). \tag{B1}$$

On the other hand, since L is a first order tensor, we have

$$L(L(p^{\otimes 2} : \mathcal{G})) = L(L(p^{\otimes 2})) : \mathcal{G} + 2L(p^{\otimes 2}) : L(\mathcal{G}) + p^{\otimes 2} : L(L(\mathcal{G})).$$

Obviously, $Lp = -\nabla_x V$ and $L(\nabla_x V) = p \cdot \nabla_x(\nabla_x V)$. Therefore,

$$\begin{aligned} L(L(p^{\otimes 2})) &= L(-\nabla_x V p - p\nabla_x V) \\ &= [-p \cdot \nabla_x(\nabla_x V)]p - p[p \cdot \nabla_x(\nabla_x V)] + 2\nabla_x V \nabla_x V. \end{aligned} \tag{B2}$$

Since $\mathcal{G}$ depends only on the energy, we have $L\mathcal{G} = p \cdot \tilde{\nabla}(\mathcal{G})$ and, consequently,

$$L(L(\mathcal{G})) = (p^{\otimes 2} : \tilde{\nabla}^{\otimes 2})\mathcal{G} - \nabla_x V \cdot \tilde{\nabla}(\mathcal{G}). \tag{B3}$$

Therefore, reminding that $L(p) = -\nabla_x V$, $L\mathcal{G} = p \cdot \tilde{\nabla}(\mathcal{G})$, that $\mathcal{G}$ is symmetric, and using (B2) and (B3), we obtain

$$\begin{aligned} L(L(p^{\otimes 2} : \mathcal{G})) = {} & [-(2p \cdot \nabla_x(\nabla_x V))p + 2\nabla_x V \nabla_x V] : \mathcal{G} \\ & + 4(-\nabla_x V)p : p \cdot \tilde{\nabla}(\mathcal{G}) + p^{\otimes 4} :: \tilde{\nabla}^{\otimes 2}\mathcal{G} - p^{\otimes 2} : \nabla_x V \cdot \tilde{\nabla}(\mathcal{G}), \end{aligned}$$

which, according to (A1) and (A2), yields

$$\begin{aligned} N(\varepsilon)\mathcal{P}[L(L(p^{\otimes 2} : \mathcal{G}))] = 4\pi\Bigg\{ & 2\left(-\frac{(2\varepsilon)^{3/2}}{3}\nabla_x^{\otimes 2} V + \sqrt{2\varepsilon}\nabla_x V \nabla_x V\right) : \mathcal{G} \\ & + 4\frac{(2\varepsilon)^{3/2}}{3}(-\nabla_x V \tilde{\nabla}) : \mathcal{G} + \frac{(2\varepsilon)^{5/2}}{15}(\tilde{\nabla} \cdot \tilde{\nabla}(\text{Trace } \mathcal{G}) + 2\tilde{\nabla}^{\otimes 2} : \mathcal{G}) \\ & - \frac{(2\varepsilon)^{3/2}}{3}\nabla_x V \cdot \tilde{\nabla}(\text{Trace } \mathcal{G})\Bigg\}. \end{aligned}$$

Finally, using again $\tilde{\nabla}(2\varepsilon)^{(k+1)/2} = (k+1)(2\varepsilon)^{k/2}\nabla_x V$, we have

$$N(\varepsilon)\mathcal{P}[L(L(p^{\otimes 2} : \mathcal{G}))] = 4\pi\left\{2\tilde{\nabla}^{\otimes 2} : \frac{(2\varepsilon)^{5/2}}{15}\mathcal{G} + \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{3}\tilde{\nabla}\ \text{Trace } \mathcal{G}\right)\right\}. \tag{B4}$$

Let us go back to the computation of $N\mathcal{P}(L(L(F\mathcal{I}(\ln F))))$. Taking for G the function $F\mathcal{I}$ and, for $\mathcal{G}$, the second order tensor $F\mathcal{J}$, Eqs. (B1) and (B4) allow to conclude that

$$N\mathcal{P}(L(L(F\mathcal{I}(\ln F)))) = \frac{4\pi}{8}\left\{\tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3}\tilde{\nabla}(F\mathcal{I})\right) + 2\tilde{\nabla}^{\otimes 2} : \frac{(2\varepsilon)^{5/2}}{15}(F\mathcal{J})\right.$$

$$+\tilde{\nabla}\cdot\left(\frac{(2\varepsilon)^{5/2}}{3}\tilde{\nabla}(F\ \mathrm{Trace}\ \mathcal{J})\right)\Bigg\},$$

since by (5.11) we have $F\mathcal{T}(\ln F)=F\mathcal{I}+p^{\otimes 2}:F\mathcal{J}$.

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Novel variable separation solutions and exotic localized excitations via the ETM in nonlinear soliton systems

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In this paper, first, the ETM is applied to obtain variable separation solutions of (2+1)-dimensional systems. A common formula with some arbitrary functions is derived to describe suitable physical quantities for some (2+1)-dimensional models such as the generalized Nizhnik-Novikov-Veselov, Davey-Stewartson, Broer-Kaup-Kupershmidt, Boiti-Leon-Pempinelli, integrable Kortweg-de Vries (KdV), breaking soliton and Burgers models. The universal formula in Tang, Lou, and Zhang [Phys. Rev. E **66**, 046601 (2002)] can be simplified to the common formula in the present paper, which indicates that redundant process is included there since the easier variable separation form can be employed without loss of generality. Second, this method is successfully generalized to (1+1)-dimensional systems, such as coupled integrable dispersionless, long-wave–short-wave resonance interaction and negative KdV models, and obtain another common formula to describe suitable physical fields or potentials of these (1+1)-dimensional models, which is similar to the one in (2+1)-dimensional systems. Moreover, it also is extended to (3+1)-dimensional Burgers system, and find that the common formula in (2+1)-dimensional systems is also appropriate to describe the (3+1)-dimensional Burgers system. The only differences are that the function q is a solution of a constraint equation and p is an arbitrary function of three independent variables. Finally, based on the common formula for (2+1)-dimensional systems and by selecting appropriate multivalued functions, interactions among special dromion, special peakon and foldon are investigated. The interactions between two special dromions, and between two special peakons, both possess novel properties, that is, there exist a multivalued foldon in the process of their collision, which is different from the reported cases in previous literature. Furthermore, the explicit phase shifts for all the local excitations offered by the common formula have been given, and are applied to these novel interactions in detail. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In recent years, increasing attention has been paid to the study of the soliton theory in many natural sciences such as chemistry, biology, mathematics, communication, and particularly in almost all branches of physics like the fluid dynamics, plasma physics, field theory, nonlinear

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optics, and condensed matter physics, etc. How to derive possible exact solutions to a nonlinear model arising from the field of mathematical physics is a popular topic, but solving nonlinear physics problems is much more difficult than solving the linear ones.

In linear physics, it is generally recognized that both the Fourier transformation and the variable separation approach (VSA) are the most universal and powerful means for the study of linear partial differential equations (PDEs). The celebrated inverse scattering transformation, considered as an extension of the Fourier transformation in nonlinear physics, plays an important role in the nonlinear domain.[1] Meanwhile the extension of the variable separation approach to nonlinear field has been a highlight, and there come out some methods: the classical method,[2] the differential Stäckel matrix approach,[3] the ansatz-based method,[2–8] etc. To our excitement, three kinds of "variable separation" procedures have been presented recently. The first method is called the "formal variable separation approach" (FVSA),[4] or equivalently the symmetry constraints.[5] The second one is the procedure to seek for the functional separable solutions[6] and the derivative-dependent functional separable solutions[7] to a PDE via the generalized conditional symmetries.[8] The last one is now called the multilinear variable separation approach (MLVSA) established first in 1996 for the Davey-Stewartsen (DS) equation.[9]

Recently, the MLVSA is developed, and Tang *et al.*[10] presented a universal formula

$$U_1 \equiv \frac{2(a_1a_2 - a_0a_3)P_xQ_y}{(a_0 + a_1P + a_2Q + a_3PQ)^2}, \tag{1}$$

where $P \equiv P(x,t)$ is an arbitrary function of $\{x,t\}$, $Q \equiv Q(y,t)$ may be either an arbitrary function of $\{y,t\}$ for some models like the DS, generalized Nizhnik-Novikov-Veselov (GNNV) and 2DsG systems or an arbitrary solution of a Riccati equation for some other models such as the asymmetric NNV (ANNV), ADS, and the generalized $(N+M)$-component Ablowitz-Kaup-Newell-Segur (AKNS) system. In Ref. 10, a_0, a_1, a_2, and a_3 are taken as arbitrary constants. However, it is clear that a_0, a_1, a_2, and a_3 should satisfy $a_0a_3 \neq a_1a_2$, otherwise the quantity $U_1=0$. More recently, a differential-difference form of the universal formula (1) has also been given for a special differential-difference Toda system and the differential-difference ANNV system.[11] Moreover, The MLVSA is generalized to $(3+1)$-dimensional systems.[12,13] In the past several years, one thought that it is difficult to extend MLVSA to the $(1+1)$-dimensional nonlinear physics systems because the independent variables must be totally separated. However, there are some development recently. This extension of the MLVSA to $(1+1)$-dimensional nonlinear models was presented first by Xu and Zhang in Ref. 14. And then the method was developed to the $(1+1)$-dimensional long-wave–short-wave resonant interaction equation.[15] Shen *et al.* also successfully extended MLVSA to $(1+1)$-dimensional Boiti system[16] and $(N+M)$-component dispersionless system.[17]

In addition, many simple and effective direct methods are developed to solve the nonlinear evolution equations such as the tanh-function method,[18] the sech-function method and the Jacobian-function method,[19] the ETM (ETM) based on mapping method.[20] Now a natural and important issue is whether the variable separation solution based on the former MLVSA can be derived by the latter ETM, which is usually used to search for travelling wave solutions. The crucial question is how to obtain solutions with certain arbitrary functions. Recently, along with variable separation ideas, Zheng *et al.*[21,22] have realized variable separation for the Broer-Kaup-Kupershmidt (BKK) system and dispersive long-wave (DLW) equation by the ETM. However, they actually derived variable separation solutions only for the same kind of $(2+1)$-dimensional system, because the BKK system can be transformed to the DLW equation by using some suitable dependent and independent variable transformations. One finds that it is too difficult to generalize this ETM to obtain variable separation solutions for other $(2+1)$-dimensional systems in virtue of the complexity to solving the over-determined partial differential equations. Therefore, one thinks that this method is not an excellent approach to realize variable separation.

In this paper, we successfully generalize the ETM based on a mapping method to obtain

variable separation solutions of (1+1)-dimensional, (2+1)-dimensional, and (3+1)-dimensional mathematical physics models. Through careful analysis, we first find that there also exists a common formula in (2+1)-dimensional models via this method

$$U_2 \equiv \frac{2p_x q_y}{(p+q)^2}, \tag{2}$$

where $p \equiv p(x,t)$ is an arbitrary function of $\{x,t\}$, q is an arbitrary function of $\{y,t\}$ for some kinds of models like the GNNV and DS systems, or an arbitrary function of $\{y\}$ for the BKK, Boiti-Leon-Pempinelli (BLP) systems, or an arbitrary solution of a constraint equation for integrable Kortweg-de Vries (KdV), breaking soliton (BS) and Burgers models. For nonintegrable KdV equation, neither p or q is arbitrary function, and they must satisfy some constraint equations. Therefore, we can define the solvable models by the ETM: these kinds of models should not be less than an arbitrary function (p or q). The nonintegrable models are also not the solvable models by the ETM. Moreover, there exists also a common formula, which is similar to the formula (2), to describe suitable physical fields or potentials of some (1+1)-dimensional models. The universal formula (2) is also appropriate to describe the (3+1)-dimensional Burgers system. The only differences are that the function q is a solution of a constraint equation and p is an arbitrary function of three independent variables.

Because some arbitrary characteristics, lower dimensional functions (like p), have been included in the universal formula (2), by selecting them appropriately, abundant stable localized structures can be revealed for these models. If the boundary (or initial) conditions of the given localized excitations are considered, one can find that all the (2+1)-dimensional localized solutions of these models are caused by the suitable boundary (or initial) conditions. Namely, the richness of the localized excitations of the (2+1)-dimensional models results from the fact that arbitrary exotic behaviors can propagate along some special characteristics of the models. All rich localized coherent structures discussed by the quantities U_1 expressed by (1), such as nonpropagating solitons, dromion, peakon, compacton, foldon, instanton, ghoston, ring soliton, and the interaction between these solitons, can be rederived by the quantities U_2 expressed by (2).

In the real natural phenomena, there exist very complicated folded phenomena such as the folded protein,[23] folded brain, and skin surfaces, and many other kinds of folded biologic systems.[24] The simplest multivalued (folded) waves may be the bubbles on (or under) a fluid surface. Various ocean waves are really folded waves, too. In Ref. 25 and 26 the authors discussed some simpler cases of multiple-valued solitary waves (folded in all directions and semifoldon). However, nature is extremely colorful and may exhibit quite complicated structures. Of course, at the present stage, it is impossible to make satisfactory analytic descriptions for such complicated folded natural phenomena. But, it is still worth starting with some simpler cases. Dromion and peakon are the focus in the previous discussions. Usually, dromion solutions are driven by two or more nonparallel straight-line ghost solitons. Even more generalized dromion solutions have been found, which are driven by curved and straight line, or curved and curved soliton solutions for some types of (2+1)-dimensional nonlinear models.[9,27] The so-called peakon solution [$u = c\exp(-|x-ct|)$], which is discontinuous at its crest and refers to a weak solution of the celebrated (1+1)-dimensional Camassa-Holm equation, was first given by Camassa and Holm.[28] Within our knowledge, studying the interaction among dromion, peakon and foldon constructed by multivalued functions in higher dimensional physical models is still open. Here we mainly focus on some novel localized coherent structures about multivalued functions, i.e., special dromion, special peakon and foldon, and the interactions among them. The interactions between two special dromions, and between two special peakons, both posses novel properties, that is, there exist a multivalued foldon in the process of their collision, which is different from the reported cases in previous literature. The explicit phase shifts for all the local excitations offered by the common formula have been given, and are applied to these novel interactions in detail.

The paper is arranged as follows. In Sec. II, a remark to MLVSA and ETM is given. In Sec. III, we obtain the variable separation solutions of the GNNV system in detail via the ETM, and list

the known models that can be solved by this method. In Sec. IV, we generalize the ETM to (1 +1)-dimensional systems, and obtain a universal formula. By means of the ETM, variable separation solution of (3+1)-dimensional Burgers system is obtained in Sec. V. Three kind of coherent localized structures and interactions among them are discussed in Sec. VI. Finally, a short summary is presented.

II. REMARK TO MLVSA AND ETM

A. Comments on MLVSA

So far, the procedure of the MLVSA has been established: at first, one may obtain the Bäcklund transformation relation via standard Painlevé expansion. Second, change the model to a multilinear variant form with an arbitrary seed solution. Third, extend the Hirota's two-soliton solution to a general variable separation ansatz $f=a_0+a_1P+a_2Q+a_3PQ$ (see Ref. 10 in detail). Finally, by substituting the variable separation ansatz to the original model and selecting the seed solution appropriately, one may find some nontrivial variable separated solutions. All of the obtained results via MLVSA are remarkable, and it is a very effective method to construct rich localized coherent structures, including dromion,[9] peakon,[10] compacton,[29] foldon,[25] ghoston,[30] ring soliton,[10] and the interaction between these solitons.[10,25,26] Moreover, nonpropagating solitons,[31] chaotic, and fractal patterns,[10] periodic and quasi-periodic wave[32] can be obtained based on the universal formula (1).

In fact, the universal formula (1) obtained via MLVSA can be simplified to another equivalent and terse form

$$U_1 \equiv \frac{2\left(\frac{a_0+a_1P}{a_2+a_3P}\right)_x Q_y}{\left(\frac{a_0+a_1P}{a_2+a_3P}+Q\right)^2} \overset{\text{def}}{=} \frac{2p_xq_y}{(p+q)^2}, \tag{3}$$

where $p(x,t)\equiv(a_0+a_1P)/(a_2+a_3P)$, $q(y,t)\equiv Q$. Equation (3) implies that we can substitute the complicated variable separation forms $a_0+a_1P+a_2Q+a_3PQ$ in Ref. 10 as the simple and direct one $p+q$, which will greatly simplify the operation, and bring some terser constraint conditions than Ricatti equation to some models, such as (2+1)-dimensional DS system, LSRI system and so on. Moreover, the seed solution is very important in MLVSA, because Tang *et al.* employ a smart method to transfer the constraints about arbitrary functions p and q into the constraints about the seed solution in order to preserve the arbitrariness of the arbitrary functions (p or q) in some models. However, it is difficult to seek the seed solution at times. The difficulty can be taken over via ETM, by means of which the variable separation solutions can be derived without considering the seed solution.

B. Comments on ETM

The basic idea of the ETM is that for a given nonlinear partial differential equation (NPDE) with independent variables $x=(x_0=t,x_1,x_2,\ldots,x_m)$, and dependent variable u,

$$L(u,u_t,u_{x_i},u_{x_ix_j},\ldots)=0, \tag{4}$$

where L is in general a polynomial function of its argument, and the subscripts denote the partial derivatives. One assumes that Eq. (4) possesses the following ansatz:

$$u=u(\xi), \quad \xi=\sum_{i=0}^{m} K_ix_i \quad \text{or } \xi=R(x_i), \tag{5}$$

where K_i, $i=0,\ldots,m$ are all arbitrary constants. Substituting Eq. (5) into Eq. (4) yields an ordinary differential equation (ODE): $O(u(\xi),u(\xi)_\xi,u(\xi)_{\xi\xi},\ldots)=0$. Then $u(\xi)$ is expanded into a polynomial in $\phi(\xi)$,

$$u(\xi) = F(\phi(\xi)) = \sum_{j=0}^{n} a_j \phi(\xi)^j, \tag{6}$$

where a_j are constants or arbitrary functions of $\{x_i\}$ to be determined and n is fixed by balancing the linear term of the highest order with the nonlinear term in Eq. (4). If we suppose $\phi(\xi) = \tanh(\xi)$, $\phi(\xi) = \mathrm{sech}(\xi)$ and $\phi(\xi) = \mathrm{sn}(\xi)$ or $\phi(\xi) = \mathrm{cn}(\xi)$, respectively, then the corresponding approach is usually called the tanh-function method, the sech-function method, and the Jacobian-function method. Although the Jacobian elliptic function method is more improved than the tanh-function method and the sech-function method, the repeated calculations are often tedious since the different function $\phi(\xi)$ should be treated in a repeated way. However, this shortcoming is overcome by the ETM based on mapping method, whose virtue is that, without much complicated and repeated calculations, we circumvent integration to directly get solutions in a uniform way. The crucial idea of this ETM is that, $\phi(\xi)$ is not assumed to be a specific function, such as tanh, sech, sn, and cn, etc., but a solution of a mapping equation such as the Riccati equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}R} = l_0 + \phi^2, \tag{7}$$

with its solutions

$$\phi = \begin{cases} -\sqrt{-l_0}\tanh(\sqrt{-l_0}R), & l_0 < 0, \\ -\sqrt{-l_0}\coth(\sqrt{-l_0}R), & l_0 < 0, \\ \sqrt{l_0}\tan(\sqrt{l_0}R), & l_0 > 0, \\ -\sqrt{l_0}\cot(\sqrt{l_0}R), & l_0 > 0, \\ -\dfrac{1}{R}, & l_0 = 0, \end{cases} \tag{8}$$

where l_0 is constant. By means of the mapping relation (7) and the solutions (8), one can obtain many explicit and exact travelling wave solutions or variable separation solutions of system (4).

Actually, these solutions in (8) are not all independent, which can be concluded from the variable separation solutions obtained by Zheng *et al.* for (2+1)-dimensional BKK,[21] DLW,[22] BLP,[33] GBK,[34] and so on. In these solutions of Ref. 21, 22, 33, and 34, only the solutions related to Eq. (2) is essentially effective, while other solutions related to tan, cot, tanh, and coth functions are special cases of Eq. (2). We take the solutions in Ref. 21, for example. Note that there is also some misprints in Ref. 21, and the solutions of the BKK system there should be

$$H_1 = -\frac{\chi_t + \chi_{xx}}{2\chi_x} + \chi_x\sqrt{-\sigma}\tanh(\sqrt{-a}(\chi+\varphi)), \tag{9}$$

$$v_1 = -\chi_x\varphi_y\sigma + \chi_x\varphi_y\sigma\tanh^2(\sqrt{-\sigma}(\chi+\varphi)), \tag{10}$$

$$H_2 = -\frac{\chi_t + \chi_{xx}}{2\chi_x} + \chi_x\sqrt{-\sigma}\coth(\sqrt{-\sigma}(\chi+\varphi)), \tag{11}$$

$$v_2 = -\chi_x\varphi_y\sigma + \chi_x\varphi_y\sigma\coth^2(\sqrt{-\sigma}(\chi+\varphi)), \tag{12}$$

$$H_3 = -\frac{\chi_t + \chi_{xx}}{2\chi_x} - \chi_x\sqrt{\sigma}\tan(\sqrt{\sigma}(\chi+\varphi)), \tag{13}$$

$$v_3 = -\chi_x\varphi_y\sigma - \chi_x\varphi_y\sigma\tan^2(\sqrt{\sigma}(\chi+\varphi)), \tag{14}$$

$$H_4 = -\frac{\chi_t + \chi_{xx}}{2\chi_x} + \chi_x\sqrt{\sigma}\cot(\sqrt{\sigma}(\chi+\varphi)), \tag{15}$$

$$v_4 = -\chi_x\varphi_y\sigma - \chi_x\varphi_y\sigma\cot^2(\sqrt{\sigma}(\chi+\varphi)), \tag{16}$$

$$H_5 = -\frac{\chi_t + \chi_{xx}}{2\chi_x} + \frac{\chi_x}{\chi+\varphi}, \tag{17}$$

$$v_5 = \frac{-\chi_x\varphi_y}{(\chi+\varphi)^2}, \tag{18}$$

with two arbitrary functions $\chi(x,t)$, $\varphi(y)$. The σ in solutions (9)–(18) is just l_0 in (8). By careful analysis, we find that when redefining $\chi=\exp\{-2\sqrt{-\sigma}\chi\}$, $\varphi=\exp\{2\sqrt{-\sigma}\varphi\}$ in solutions (17) and (18), solutions (9) and (10) can be obtained. Similarly, if taking $\chi=-\exp\{-2\sqrt{-\sigma}\chi\}$, $\varphi=\exp\{2\sqrt{-\sigma}\varphi\}$ in solutions (17) and (18), solutions (11) and (12) can be recovered. When considering $\chi=\exp\{-2i\sqrt{\sigma}\chi\}$, $\varphi=\exp\{2i\sqrt{\sigma}\varphi\}$ in solutions (17) and (18), solutions (13) and (14) can be obtained. If letting $\chi=-\exp\{-2i\sqrt{\sigma}\chi\}$, $\varphi=\exp\{2i\sqrt{\sigma}\varphi\}$ in solutions (17) and (18), solutions (15) and (16) can be recovered. Other results for DLW,[22] BLP,[33] and GBK[34] systems have similar relations.

By study, we find that ETM is an alternative approach to derive variable separation solutions without considering the seed solutions, and it is easier to handle than MLVSA to those readers unacquainted with MLVSA. In the following paper, via ETM, we also discuss the variable separation solutions for (1+1)-dimensional and (3+1)-dimensional mathematical physics models, besides (2+1)-dimensional systems.

III. VARIABLE SEPARATION SOLUTIONS FOR THE (2+1)-DIMENSIONAL SYSTEMS

A. (2+1)-dimensional generalized Nizhnik-Novikov-Veselov system

The (2+1)-dimensional generalized Nizhnik-Novikov-Veselov (NNV) equation reads

$$u_t + au_{xxx} + bu_{yyy} + cu_x + du_y - 3a(uv)_x - 3b(uw)_y = 0, \tag{19}$$

$$u_x = v_y, \quad u_y = w_x, \tag{20}$$

where a, b, c, and d are arbitrary constants. For $c=d=0$, the GNNV system will be degenerated to the usual two-dimensional NNV system, which is an isotropic Lax extension of the classical (1+1)-dimensional shallow water-wave KdV model. When $a=1$, $b=c=d=0$ in Eq. (19), we get the asymmetric NNV equation, which may be considered as a model for an incompressible fluid. Some types of the soliton solutions of the GNNV equation have been studied by many authors. For instance, Boiti *et al.*[35] solved the GNNV equation via the inverse scattering transformation. Zhang obtained many exact solution of this system based on an extended homogeneous balance approach.[36] Two new coherent structures for the GNNV equation are discussed in Ref. 37. Recently, a general solution including two arbitrary functions is first obtained for the generalized NNV equation by means of WTC truncation method.[38]

Along with the ETM, we assume that the (2+1)-dimensional NNV equation (19) and (20) possess the solutions of the following form:

$$u(x,y,t) = \sum_{i=0}^{l} a_i\phi^i(R), \quad v(x,y,t) = \sum_{j=0}^{m} b_j\phi^j(R), \quad w(x,y,t) = \sum_{k=0}^{n} c_k\phi^k(R), \tag{21}$$

where ϕ satisfies Eq. (7) with Eq. (8) and $R\equiv R(x,y,t)$, $a_i\equiv a_i(x,y,t)$, $(i=0,1,\ldots,l)$, $b_j\equiv b_j(x,y,t)$, $(j=0,1,\ldots,m)$, $c_k\equiv c_k(x,y,t)$, $(k=0,1,\ldots,n)$ and l_0 is an arbitrary real constant,

while $l=m=n=2$ is obtained by balancing the highest-order derivative terms with the nonlinear terms in Eqs. (19) and (20). Inserting Eqs. (21) and (7) with $l=m=n=2$ into Eqs. (19) and (20), selecting the variable separation ansatz,

$$R = p(x,t) + q(y,t), \tag{22}$$

and eliminating all the coefficients of polynomials of ϕ, one gets a set of partial differential equations

$$12a_2[ap_x(2p_x^2 - b_2) + bq_y(2q_y^2 - c_2)] = 0, \tag{23}$$

$$\begin{aligned}&[6bq_yq_{yy} - 2ap_xb_1 - a(b_1p_x + b_{2,x}) - 2bq_yc_1 + 6ap_xp_{xx} - b(c_1q_y + c_{2y})]a_2\\ &\quad + 2(ap_x^3 + bq_y^3 - 3ap_xb_2 - 3bq_yc_2)a_1 - aa_{2x}b_2 + 6aa_{2x}p_x^2 + 6ba_{2y}q_y^2 - ba_{2y}c_2 = 0,\end{aligned} \tag{24}$$

$$\begin{aligned}&-6(ab_2p_x + bc_2q_y)a_0 + 3(2ap_xp_{xx} - 2ab_1p_x - bc_{2y} - 2bc_1q_y - ab_{2x} + 2bq_yq_{yy})a_1\\ &\quad + (2p_y + 40bl_0q_y^3 + 2cp_x + 2q_t - 12ab_2l_0p_x - 6ap_xb_0 - 6bq_yc_0 + 40al_0p_x^3 - 12bc_2l_0q_y + 2dq_y\\ &\quad + 2bq_{yyy} - 3bc_{1y} + 2ap_{xxx} - 3ab_{1x})a_2 + 6ba_{2y}q_{yy} - 3bc_2a_{1y} + 6aa_{2xx}p_x + 6aa_{1x}p_x^2 - 3ab_1a_{2x}\\ &\quad - 3bc_1a_{2y} + 6aa_{2x}p_{xx} + 6ba_{1y}q_y^2 + 6ba_{2yy}q_y - 3ab_2a_{1x} = 0,\end{aligned} \tag{25}$$

$$2a_2p_x - 2b_2q_y = 0, \tag{26}$$

$$2a_2q_y - 2c_2p_x = 0, \tag{27}$$

$$\begin{aligned}&-3(bc_1q_y + bc_{2y} + ab_1p_x + ab_{2x})a_0 + (ap_{xxx} - 3bq_yc_0 - 9bc_2l_0q_y - 9ab_2l_0p_x - 3ab_{1x} + cp_x + 8al_0p_x^3\\ &\quad + dq_y - 3bc_{1y} - 3ap_xb_0 + bq_{yyy} + 8bl_0q_y^3 + p_t + q_t)a_1 - 3(ab_{0x} - 8bl_0q_yq_{yy} + bc_{0y} - 8al_0p_xp_{xx}\\ &\quad + 3ab_1l_0p_x + 3bc_1l_0q_y)a_2 + a_{2t} + 3ba_{1yy}q_y - 3ab_2a_{0x} + 24ba_{2y}l_0q_y^2 + 3aa_{1,x}p_{xx} + 24aa_{2x}l_0p_x^2\\ &\quad + 3ba_{1y}q_{yy} - 3ab_0a_{2x} - 3bc_0a_{2y} + da_{2y} + aa_{2xxx} + 3aa_{1xx}p_x - 3bc_1a_{1y} - 3ab_1a_{1x} - 3bc_2a_{0y}\\ &\quad + ba_{2yyy} + ca_{2x} = 0,\end{aligned} \tag{28}$$

$$a_{2x} - b_{2y} + a_1p_x - b_1q_y = 0, \tag{29}$$

$$a_{2y} - c_{2x} + a_1q_y - c_1p_x = 0, \tag{30}$$

$$\begin{aligned}&-3(2ab_2l_0p_x + ab_{1x} + bc_{1y} + 2bc_2l_0q_y)a_0 - 3(ab_{0x} + 2ab_1l_0p_x + bc_{0y} - 2al_0p_xp_{xx} - 2bl_0q_yq_{yy}\\ &\quad + 2bc_1l_0q_y)a_1 + 2(al_0p_{xxx} + bl_0q_{yyy} - 3bc_0l_0q_y + cl_0p_x + dl_0q_y - 3ab_0l_0p_x + 8bl_y^2q_y^3 + l_0p_t + l_0q_t\\ &\quad + 8al_0^2p_x^3)a_2 - 3ab_0a_{1x} + 6aa_{2x}l_0p_{xx} + 6aa_{2xx}l_0p_x + aa_{1xxx} + ba_{1yyy} + ca_{1x} + 6ba_{1y}l_0q_y^2\\ &\quad + 6aa_{1x}l_0p_x^2 - 3ab_1a_{0x} + 6ba_{2y}l_0q_{yy} + a_{1t} + 6ba_{2yy}l_0q_y + da_{1y} - 3bc_0a_{1y} - 3bc_1a_{0y} = 0,\end{aligned} \tag{31}$$

$$\begin{aligned}&-3(bc_1l_0q_y + ab_{0x} + bc_{0y} + ab_1l_0p_x)a_0 + (cl_0p_x + dl_0q_y + 2bl_0^2q_y^3 + bl_0q_{yyy} - 3bc_0l_0q_y + al_0p_{xxx}\\ &\quad + l_0q_t + l_0p_t - 3ab_0l_0p_x + 2al_0^2p_x^3)a_1 + 6(al_0^2p_xp_{xx} + bl_0^2q_yq_{yy})a_2 + da_{0y} + ca_{0,x} + aa_{0xxx}\\ &\quad + ba_{0yyy} + 3aa_{1x}l_0p_{xx} + a_{0t} + 6aa_{2x}l_0^2p_x^2 + 3aa_{1xx}l_0p_x + 3ba_{1yy}l_0q_y - 3ab_0a_{0x} + 3ba_{1y}l_0q_{yy}\\ &\quad + 6ba_{2y}l_0^2q_y^2 - 3bc_0a_{0y} = 0,\end{aligned} \tag{32}$$

$$a_{1y} - c_{1x} + 2a_2 l_0 q_y - 2c_2 l_0 p_x = 0, \tag{33}$$

$$a_{1x} - b_{1y} - 2b_2 l_0 q_y + 2a_2 l_0 p_x = 0, \tag{34}$$

$$a_{0x} - b_1 l_0 q_y + a_1 l_0 p_x - b_{0y} = 0, \tag{35}$$

$$a_{0y} - c_1 l_0 p_x + a_1 l_0 q_y - c_{0x} = 0. \tag{36}$$

It is very difficult to solve these prolix and complicated differential equations. Fortunately, by careful analysis and calculation, we derive the special solutions of Eqs. (23)–(36). Based on Eqs. (23), (26), and (27), we obtain

$$a_2 = 2p_x q_y, \quad b_2 = 2p_x^2, \quad c_2 = 2q_y^2. \tag{37}$$

Inserting Eq. (37) into Eqs. (24), (29), and (30) yields

$$a_1 = 0, \quad b_1 = 2p_{xx}, \quad c_1 = 2q_{yy}. \tag{38}$$

Substituting Eqs. (37) and (38) into other partial differential equations, we have

$$a_0 = 2l_0 p_x q_y, \quad b_0 = (3ap_x)^{-1}(p_t + ap_{xxx} + 2al_0 p_x^3 + cp_x), \quad c_0 = (3bq_y)^{-1}(q_t + bq_{yyy} + 2bl_0 q_y^3 + dq_y). \tag{39}$$

Therefore, from Eqs. (21), (8), and (37)–(39), the new types of variable separation solutions of the $(2+1)$-dimensional GNNV equation are of the following form:

Case 1: For $l_0 < 0$,

$$u_1 = 2l_0 p_x q_y - 2l_0 p_x q_y \tanh^2\{\sqrt{-l_0}(p+q)\},$$

$$v_1 = \frac{p_t + ap_{xxx} + cp_x + 2al_0 p_x^3}{3ap_x} - 2\sqrt{-l_0}p_{xx}\tanh\{\sqrt{-l_0}(p+q)\} - 2l_0 p_x^2 \tanh^2\{\sqrt{-l_0}(p+q)\},$$

$$w_1 = \frac{q_t + bq_{yyy} + dq_y + 2bl_0 q_y^3}{3bq_y} - 2\sqrt{-l_0}q_{yy}\tanh\{\sqrt{-l_0}(p+q)\} - 2l_0 q_y^2 \tanh^2\{\sqrt{-l_0}(p+q)\}, \tag{40}$$

$$u_2 = 2l_0 p_x q_y - 2l_0 p_x q_y \coth^2\{\sqrt{-l_0}(p+q)\},$$

$$v_2 = \frac{p_t + ap_{xxx} + cp_x + 2al_0 p_x^3}{3ap_x} - 2\sqrt{-l_0}p_{xx}\coth\{\sqrt{-l_0}(p+q)\} - 2l_0 p_x^2 \coth^2\{\sqrt{-l_0}(p+q)\},$$

$$w_2 = \frac{q_t + bq_{yyy} + dq_y + 2bl_0 q_y^3}{3bq_y} - 2\sqrt{-l_0}q_{yy}\coth\{\sqrt{-l_0}(p+q)\} - 2l_0 q_y^2 \coth^2\{\sqrt{-l_0}(p+q)\}. \tag{41}$$

Case 2: For $l_0 = 0$,

$$u_3 = U_2 = \frac{2p_x q_y}{(p+q)^2}, \tag{42}$$

$$v_3 = \frac{p_t + ap_{xxx} + cp_x}{3ap_x} - \frac{2p_{xx}}{p+q} + \frac{2p_x^2}{(p+q)^2},$$

$$w_3 = \frac{q_t + bq_{yyy} + dq_y}{3bq_y} - \frac{2q_{yy}}{p+q} + \frac{2q_y^2}{(p+q)^2}, \tag{43}$$

where p and q are arbitrary functions of $\{x,t\}$ and $\{y,t\}$, respectively. Here we omit the solutions as $l_0>0$, because they are of fewer significance in soliton theory. The solutions (42) and (43) is similar to the solution given by Darboux transformation in Ref. 39. According to the discussion in Sec. II B, the solutions (40) and (41) are the special examples of solutions (42) and (43). When redefining $p=\exp\{-2\sqrt{-l_0}p\}$, $q=\exp\{2\sqrt{-l_0}q\}$ in solutions (42) and (43), solution (40) can be obtained. Similarly, if taking $p=-\exp\{-2\sqrt{-l_0}p\}$, $q=\exp\{2\sqrt{-l_0}q\}$ in solutions (42) and (43), solution (41) can be recovered. Here we again prove the viewpoint in Sec. II B. Therefore, we only list the variable separation solutions for $l_0=0$ in the following mathematical physics models.

B. (2+1)-dimensional complex systems

(2+1)-dimensional Davey-Stewartson equation. The (2+1)-dimensional DS equation,

$$iU_t + \tfrac{1}{2}(U_{xx} + U_{yy}) - \alpha|U|^2U - UV = 0,$$

$$V_{xx} - V_{yy} - 2\alpha(|U|^2)_{xx} = 0, \tag{44}$$

can be derived from the plasma physics[40] and from the self-dual Yang-Mills field.[41] The DS system has also been proposed as a (2+1)-dimensional model for quantum field theory.[42] The DS equation is an isotropic Lax integrable extension of the well-known (1+1)-dimensional nonlinear Schrödinger equation, and it is IST and Painlevé integrable.

To find some exact solutions with some arbitrary functions of the DS equation, new coordinates X,Y are defined by

$$X = (x+y)/\sqrt{2}, \quad Y = (x-y)/\sqrt{2}, \tag{45}$$

and the transformed DS will be

$$iU_t + \tfrac{1}{2}(U_{XX} + U_{YY}) - \alpha|U|^2U - UV = 0,$$

$$2V_{XY} - \alpha(|U|^2)_{XX} - \alpha(|U|^2)_{YY} - 2\alpha(|U|^2)_{XY} = 0. \tag{46}$$

Introducing the transforms

$$U = u\exp[i(r+s)], \quad V = v, \tag{47}$$

then Eq. (46) changes into

$$-u(r_t + s_t) + \tfrac{1}{2}(u_{XX} + u_{YY}) - \tfrac{1}{2}u({r_X}^2 + {s_Y}^2) + \alpha u^3 - vu = 0,$$

$$u_t + u_X r_X + u_Y s_Y + \tfrac{1}{2}u(r_{XX} + s_{YY}) = 0,$$

$$v_{XY} - \alpha({u_X}^2 + uu_{XX} + {u_Y}^2 + uu_{YY} + 2u_Xu_Y + 2uu_{XY}) = 0, \tag{48}$$

where u, v are arbitrary function of $\{X,Y,t\}$, r and s are arbitrary functions of $\{X,t\}$ and $\{Y,t\}$, respectively.

Similar to the procedure to solve GNNV system, the special variable separation solution of system (46) has the form

$$U=\frac{\delta\sqrt{2\alpha^{-1}p_Xq_Y}}{p+q}\exp[i(r+s)],\quad \delta^2=1, \tag{49}$$

$$V=V_0(x,y,t)-\frac{p_{XX}q_{YY}}{p+q}+\frac{(p_Xq_Y)^2}{(p+q)^2}, \tag{50}$$

with

$$V_0(x,y,t)=\frac{p_{XXX}}{4p_X}+\frac{q_{YYY}}{4q_Y}-\frac{p_{XX}^2}{8p_X^2}-\frac{q_{YY}^2}{8q_Y^2}-r_t-s_t-\frac{1}{2}r_X^2-\frac{1}{2}s_Y^2, \tag{51}$$

and r, s satisfy

$$r_X=-\frac{p_t}{p_X},\quad s_Y=-\frac{q_t}{q_X}, \tag{52}$$

where p and q are arbitrary functions of $\{X,t\}$ and $\{Y,t\}$, respectively. Moreover, the real condition of solution (49) requires

$$2\alpha^{-1}p_Xq_Y\geqslant 0. \tag{53}$$

Especially, for the module square of the field U reads

$$|U|^2=\alpha^{-1}U_2=\frac{2\alpha^{-1}p_Xq_Y}{(p+q)^2}. \tag{54}$$

Clearly, the arbitrary constants $a_0\sim a_3$, which are introduced in MLVSA in Ref. 10, increase the complexity of the constraint conditions to r and s in DS model. However, the terse expressions of the constraint conditions to r and s in (52) make us easily obtain their concrete form.

(2+1)-dimensional long-wave–short-wave resonance interaction equation. The (2+1)-dimensional LSRI equation is of the form

$$i(S_t+S_y)-S_{xx}+LS=0,$$

$$L_t-2(|S|^2)_x=0, \tag{55}$$

where the fields S and L denote short surface wave packets and long interfacial waves, respectively. This system describe the long and short waves propagating at an angle to each other in a two-layer fluid. The above equation has recently been studied[43,44] and its position and one dromion solutions have been generated through the method of coalescence of eigenvalues or wave numbers.[45]

Similar to the procedure to solve DS equation, the special variable separation solution of system (55) reads

$$S=\frac{\delta\sqrt{p_xq_t}}{p+q}\exp[i(r_1+r_2)],\quad \delta^2=1,$$

$$L=\frac{4p_x^2(r_{1y}-r_{1x}^2)-p_{xx}^2+2p_xp_{xxx}}{4p_x^2}-\frac{2p_{xx}}{p+q}+\frac{2p_x^2}{(p+q)^2}, \tag{56}$$

where r_1 satisfies

$$r_{1x} = \frac{p_y + c_y}{2p_x}, \tag{57}$$

and $r_2 \equiv r_2(y-t)$, $q=F(y-t)+c(y)$, and p is an arbitrary function of $\{x,y\}$. Moreover, the real condition of solution (56) requires

$$p_x q_t \geqslant 0. \tag{58}$$

C. Other (2+1)-dimensional integrable systems

In this section, some known models which can be solved via the ETM are listed. With some suitable modifications, they possess a common quantity expressed as Eq. (2).

BKK system: The BKK system,

$$H_{ty} - H_{xxy} + 2(HH_x)_y + 2G_{xx} = 0,$$

$$G_t + G_{xx} + 2(HG)_x = 0, \tag{59}$$

may be derived from the inner parameter-dependent symmetry constraint of the Kadomtsev-Petviashvili (KP) equation.[46] Using some suitable dependent and independent variable transformations, Chen and Li[47] have proved that the (2+1)-dimensional BKKE can be transformed to the (2+1)-dimensional integrable dispersive long-wave equation (DLWE)

$$u_{ty} = -\eta_{xx} - \tfrac{1}{2}(u^2)_{xy},$$

$$\eta_t = -(u\eta + u + u_{xy})_x, \tag{60}$$

and the (2+1)-dimensional integrable Ablowitz-Kaup-Newell-Segur equation (AKNSE)

$$\psi_t = -\psi_{xx} + \psi u,$$

$$\phi_t = \phi_{xx} - \phi u,$$

$$u_y = \psi\phi. \tag{61}$$

When we take $y=x$, the (2+1)-dimensional BKKE is reduced to the usual (1+1)-dimensional BKKE, which can be used to describe the propagation of long wave in shallow water.[48]

For the BKK system, there are special variable solution in the form

$$H = -\frac{p_{xx} + p_t}{2p_x} + \frac{p_x}{p+q},$$

$$G = \frac{U_2}{2} = \frac{p_x q_y}{(p+q)^2}, \tag{62}$$

where p and q are arbitrary functions of $\{x,t\}$ and $\{y\}$, respectively.

Boiti-Leon-Pempinelli system: For the Boiti-Leon-Pempinelli system[49–51]

$$u_{ty} - (u^2 - u_x)_{xy} + 2v_{xxx} = 0,$$

$$v_t - v_{xx} + 2uv_x = 0, \tag{63}$$

special variable separation solutions read

$$u = -\frac{p_{xx} - p_t}{2p_x} + \frac{p_x}{p+q},$$

$$v = \frac{q_y}{p+q}, \tag{64}$$

where p and q are arbitrary functions of $\{x,t\}$ and $\{y\}$, respectively.

From solution (64), the potential v_x satisfies the universal formula, i.e.,

$$v_x = -\frac{U_2}{2} = -\frac{p_x q_y}{(p+q)^2}. \tag{65}$$

(2+1)-dimensional KdV equation: The (2+1)-dimensional KdV equation,

$$u_t + bu_{xxx} + 4b(uv)_x = 0,$$

$$v_y = u_x, \tag{66}$$

was first derived by Boiti *et al.*[35] using the idea of the weak Lax pair. Equation (69) can also be deduced from Jimbo and Miwa hierarchy of nonlinear partial differential equations.[52] The Painlevé property of (69) has been proved by Dorizzi *et al.*[53] The infinite-dimensional symmetries and Lie algebraic structure have been studied.[54]

The variable separation solutions of the (2+1)-dimensional KdV equation (69) possess the form

$$u = -\frac{3}{4}U_2 = -\frac{3p_x q_y}{2(p+q)^2}, \tag{67}$$

$$v = -\frac{p_t + bp_{xxx} + c_t}{4bp_x} + \frac{3p_{xx}}{2(p+q)} - \frac{3p_x^2}{2(p+q)^2}, \tag{68}$$

where p is an arbitrary functions of $\{x,t\}$, and $q(y,t)=F(y)+c(t)$.

(2+1)-dimensional breaking soliton equation: The (2+1)-dimensional BS equation[55–57]

$$u_t + bu_{xxx} + 4b(uv)_x = 0,$$

$$u_y = v_x, \tag{69}$$

have a special variable separation solution

$$u = -\frac{bp_{xxx} + cp_x}{4bp_x} + \frac{3p_{xx}}{2(p+q)} - \frac{3p_x^2}{2(p+q)^2}, \tag{70}$$

$$v = -\frac{3}{4}U_2 = -\frac{3p_x q_y}{2(p+q)^2}, \tag{71}$$

where p is an arbitrary function of $\{x,t\}$ and $q(y,t)=q(y+ct)$.

(2+1)-dimensional Burgers equation: The (2+1)-dimensional Burgers equation[58–60]

$$u_t = uu_y + avu_x + bu_{yy} + abu_{xx} = 0,$$

$$v_y = u_x, \tag{72}$$

have a special variable separation solution

$$u = -\frac{2bq_y}{p+q}, \tag{73}$$

$$v = -\frac{2bp_x}{p+q} + \frac{p_t - abp_{xx}}{ap_x}, \tag{74}$$

where p is an arbitrary function of $\{x,t\}$, and $q(y,t)$ satisfies $q_t = bq_{yy}$.

From solution (73), the potential u_x satisfies the universal formula, i.e.,

$$u_x = bU_2 = \frac{2bp_xq_y}{(p+q)^2}. \tag{75}$$

D. (2+1)-dimensional nonintegrable KdV system

The (2+1)-dimensional nonintegrable KdV equation,

$$u_t + u_{xxx} - auv_x - bvu_x = 0,$$

$$v_y = u_x, \tag{76}$$

is one of the extensions of a (1+1)-dimensional shallow water wave equation.[61] In the real physics problems, a and b in Eq. (76) may be arbitrary constant. This model is completely integrable only for $a=b$.[35]

The variable separation solutions of the (2+1)-dimensional nonintegrable KdV equation (76) possess the form

$$u = \frac{6}{a+b}U_2 = \frac{12p_xq_y}{(a+b)(p+q)^2}, \tag{77}$$

$$v = v_0(x,y,t) - \frac{12p_{xx}}{(a+b)(p+q)} + \frac{12p_x^2}{(a+b)(p+q)^2}, \tag{78}$$

with

$$v_0(x,y,t) = \frac{1}{bp_x}\left\{p_t + \frac{3(a-b)p_{xx}^2}{(a+b)p_x} - \frac{2(a-2b)(p_{xxx}) - K(t)}{a+b}\right\}, \tag{79}$$

where q satisfies

$$q_t = K(t), \tag{80}$$

and p satisfies

$$(a+b)(ap_xv_{0x} + av_0p_{xx} - p_{tx} - p_{xxxx}) - 2bl_0p_x^2p_{xx} = 0. \tag{81}$$

In conclusion, from the solutions (42), (62), (65), (67), (75), (54), and (77), we know that the field quantity satisfy the universal formula U_2 for the GNNV, BKK, integrable KdV, BS, and nonintegrable KdV models, while the potential satisfy the universal formula U_2 for BLP and Burgers models, or the module square of the field quantity satisfy the universal formula U_2 for DS model. For integrable models, such as GNNV, BKK, BLP, integrable KdV, BS, Burgers, DS, and LSRI models, there are not less than an arbitrary function (p or q), while some additional conditions must be introduced to reduce the arbitrariness of the arbitrary functions (both p and q) for the nonintegrable KdV model. Thus we can define the solvable models by the ETM: these kinds of models should not be less than an arbitrary function (p or q). The nonintegrable models are also not the solvable models by the ETM.

Now a subsequent intriguing issue is whether we can generalize the extended tanh-method to the lower $(1+1)$-dimensional and the higher $(3+1)$-dimensional systems? To answer this question, we take the $(1+1)$-dimensional CID, LSRI, negative KdV models and $(3+1)$-dimensional Burgers system as concrete examples.

IV. VARIABLE SEPARATION SOLUTIONS FOR THE (1+1)-DIMENSIONAL SYSTEMS

Coupled integrable dispersionless equations: The coupled integrable dispersionless (CID) equations have the form

$$u_{xt}+(vw)_x=0, \quad v_{xt}-2u_xv=0, \quad w_{xt}-2u_xw=0. \tag{82}$$

These equations were presented and solved by the inverse scattering method.[62] It is shown that the CID systems possess Painlevé property.[63] Starting from the Lagrangian of coupled integrable dispersionless equations, Kakuhata *et al.*[64] derived the Hamiltonian, and conserved quantities associated with the symmetries of the Lagrangian were obtained, which cannot be derived by the inverse scattering method. Alagesan *et al.*[65] investigated the singularity structure analysis of this system. The associated Bäcklund transformation was constructed and Hirota's bilinearization was also obtained through dependent variable transformations.

As in $(2+1)$-dimensional cases, by standard leading term analysis, the ansatz of CID systems is

$$u=a_0(x,t)+a_1(x,t)\phi(R), \quad v=b_0(x,t)+b_1(x,t)\phi(R), \quad w=c_0(x,t)+c_1(x,t)\phi(R), \tag{83}$$

where $\phi(R)$ satisfies Eq. (7) with $R=R(x,t)$. Inserting Eq. (83) with Eq. (7) into Eq. (82), yields a series of partial differential equations, from which we can obtain the variable separation solutions of the $(1+1)$-dimensional coupled integrable dispersionless equations (82),

$$u=-\frac{q_t}{p+q}+u_0(t), \tag{84}$$

$$v=\frac{aq_t}{p+q}-\frac{aq_{tt}}{2q_t}, \tag{85}$$

$$w=\frac{bq_t}{p+q}-\frac{bq_{tt}}{2q_t}, \tag{86}$$

where $q(t)$, $u_0(t)$ are the arbitrary functions of $\{t\}$, $p(x)$ is an arbitrary function of $\{x\}$ and $ab=-1$.

From the solutions (84)–(86), the potential function $G(=u_x=-v_x/a=-w_x/b)$

$$G=\frac{p_xq_t}{(p+q)^2}. \tag{87}$$

Long-wave–short-wave resonant interaction equation: The procedure for the long-wave–short-wave resonant interaction equation (LSRI) reads

$$iS_t+\beta S_{xx}=\gamma LS,$$

$$L_t+\alpha(SS^*)_x=0, \tag{88}$$

where L is the profile of the long wave and S is the envelope of the short wave. α, β, and γ are positive real model constant. Equations (88) were proposed for the time by Zakharov to describe the interaction of Langmuir oscillations with ionic sound in a plasma. The universal equations were obtained for waves on the water surface by Djordjevic and Redekopp[66] and for the model of

a molecular chain in the form of an α-helix by Davydov.[67] The equations were also derived in bubbly liquids by Akhatov and Khismatullin.[68] Reference 69 discussed the Cauahy problem and global solution for this equation.

A general excitation of LSRI system has the form

$$S(x,t) = \pm \frac{\sqrt{-2(\alpha\gamma)^{-1}\beta p_x q_t}}{p+q} \exp\left\{ i\left[c_0 + c_1 t - k \int (2\beta p_x)^{-1}\, \mathrm{d}x \right] \right\}, \tag{89}$$

$$L(x,t) = \frac{-2\beta p_{xx}}{\gamma(p+q)} + \frac{2\beta p_x^2}{\gamma(p+q)^2} + \frac{\beta^2(2p_{xxx}p_x - p_{xx}^2) - k^2}{4\gamma\beta p_x^2} - \gamma^{-1}c_1, \tag{90}$$

where k, c_0, c_1 are arbitrary real constants, p is the arbitrary function of $\{x\}$, and q can be expressed by $q_t = k$. Moreover, the real condition of solution (89) requires

$$-2(\alpha\gamma)^{-1}\beta p_x q_t \geqslant 0. \tag{91}$$

Especially, the module square of S can also be expressed as

$$G = |S|^2 = \frac{-2\beta p_x q_t}{\sigma\gamma(p+q)^2}. \tag{92}$$

Negative KdV model: The negative KdV hierarchy

$$\varphi_{xx} + u\varphi - \lambda\varphi = 0, \quad u_t = (\varphi^n)_x, \tag{93}$$

where $\varphi = \varphi(x,t)$, $u = u(x,t)$, λ and n are arbitrary constants. This model relates to Schrödinger equation[70,71] and has also been proved to relate to the sine-Gordon equation by Miura transformation.[72] By means of the Schrödinger operator, the negative KdV hierarchy can be rewritten to an equivalent differential equation system. As $n = 1, 2$, Eq. (93) is called KdV(−1) and KdV(−2) equations, respectively.

KdV(−1) *model:* As $n = 1$, Eq. (93) is simplified as

$$\varphi_{xx} + u\varphi - \lambda\varphi = 0, \quad u_t = \varphi_x. \tag{94}$$

The general excitation of system (94) has the form

$$\varphi(x,t) = \frac{-6p_x q_t}{(p+q)^2}, \tag{95}$$

$$u(x,t) = -\frac{6p_x^2}{(p+q)^2} + \frac{6p_{xx}}{p+q} - \frac{p_{xxx}}{p_x} + \lambda, \tag{96}$$

where p is the arbitrary function of $\{x\}$, and q is the arbitrary function of $\{t\}$.

KdV(−2) *model:* As $n = 2$, Eq. (93) is simplified as

$$\varphi_{xx} + u\varphi - \lambda\varphi = 0, \quad u_t = (\varphi^2)_x. \tag{97}$$

A special variable separation solution of system (97) reads

$$\varphi(x,t) = \pm \frac{\sqrt{-2p_x q_t}}{p+q}, \tag{98}$$

$$u(x,t) = -\frac{2p_x^2}{(p+q)^2} + \frac{2p_{xx}}{p+q} + \frac{p_{xx}^2 - 2p_{xxx}p_x}{4p_x^2} + \lambda, \tag{99}$$

where p is the arbitrary function of $\{x\}$, and q is the arbitrary function of $\{t\}$. From expression (98), because the real condition of φ,

$$-2p_x q_t \geqslant 0, \tag{100}$$

we must put a constraint on the selections of the functions p, q. In Ref. 14, another special variable separation solution was discussed in detail by MLVSA.

In short, we successfully generalize the ETM to $(1+1)$-dimensional systems. From the expressions (87), (92), (95), and (98), we find that there also exists a common formula

$$U_2' \equiv \frac{p_x q_t}{(p+q)^2}, \tag{101}$$

to describe suitable physical fields or potentials for some $(1+1)$-dimensional models. This formula is similar to the formula U_2 in $(2+1)$-dimensional models.

V. VARIABLE SEPARATION SOLUTION FOR THE (3+1)-DIMENSIONAL BURGERS SYSTEM

The ETM has been successfully generalized to $(1+1)$-dimensional systems, and whether it can be extended to $(3+1)$-dimensional systems? To answer this question, we take the $(3+1)$-dimensional Burgers system,

$$u_t = 2uu_y + 2vu_x + 2wu_x + u_{xx} + u_{yy} + u_{zz},$$

$$u_x = v_y,$$

$$u_z = w_y, \tag{102}$$

as a concrete example. If u is z independent (or $z=x$; $w=u$), (102) will be degenerated to the known $(2+1)$-dimensional Burgers equation (72). Furthermore, if u is both z independent and y independent (or $y=z=x$; $v=w=u$), Eq. (102) is just the well-known $(1+1)$-dimensional Burgers equation which is widely applied in many scientific fields. An alternative potential form of Eq. (102) is obtained from the invertible deformation of the heat conduction equation.[73] In Refs. 12 and 13, the authors extended the VSA to this system.

As in $(2+1)$-dimensional cases, by standard leading term analysis, the ansatz of Burgers system is

$$u = a_0(x,y,z,t) + a_1(x,y,z,t)\phi(R), \quad v = b_0(x,y,z,t) + b_1(x,y,z,t)\phi(R),$$

$$w = c_0(x,y,z,t) + c_1(x,y,z,t)\phi(R), \tag{103}$$

where $\phi(R)$ satisfies Eq. (7) with $R=R(x,y,z,t)$. Inserting Eq. (103) with Eq. (7) into Eq. (102), yields a series of partial differential equations, from which we can obtain the variable separation solution of the $(3+1)$-dimensional Burgers system (102) for $l_0=0$,

$$u = \frac{q_y}{p+q}, \tag{104}$$

$$v = \frac{p_x}{p+q} + \frac{p_t - p_{xx}}{2p_x}, \tag{105}$$

$$w = \frac{p_z}{p+q} - \frac{p_{zz}}{2p_z}, \tag{106}$$

where p is the arbitrary functions of $\{x,z,t\}$, q is an function of $\{y,t\}$ and satisfies $q_t = q_{yy}$.

One of the most important things may be that for the potential $G(=u_x=v_y)$, we have

$$G = -U_2 = -\frac{p_x q_y}{(p+q)^2}, \tag{107}$$

which satisfies the completely same form as the universal quantity (2) in (2+1)-dimensional systems.

VI. SPECIAL LOCALIZED COHERENT STRUCTURES FOR THE COMMON FORMULA (2)

In this section, we will discuss some special types of interesting localized structures for the quantities U_2 expressed by (2). From (2), we know that for general selections of p and q there may be some singularities for the quantity U_2. However, when the arbitrary functions p and q are selected appropriately to avoid the singularities, there may exist abundant excitations for U_2. All rich localized coherent structures discussed by the quantities U_1 expressed by (1), such as nonpropagating solitons, dromion, peakon, compacton, foldon, instanton, ghoston, ring soliton, and the interaction between these solitons, can be rederived by the quantities U_2 expressed by (2). Moreover, if p or q is considered to be a periodic function or a solution of a chaos system like the Lorenz chaos system, then solitons possess periodic or chaotic behaviors. It is well known that there are some lower-dimensional stochastic fractal functions, which may be used to construct higher-dimensional stochastic fractal dromion and lump excitations by the quantities U_2 expressed by (2). Since these similar situations have been widely discussed in some previous literature,[9,10,12–15,26,37,49] the related plots are neglected in our present paper. Here we focus on some novel localized coherent structures about multivalued functions and their interaction cases. For simplification in the following discussions, we merely analyze the expression U_2 without any constraints to p and q.

A. Special dromion, special peakon, and foldon

It is well known that in universal formula (2), dromion, peakon, and foldon can be obtained by selecting p or q single-valued function, piecewise function, and multivalued function, respectively. However, in fact, the single-valued structures, i.e., dromion and peakon can also be derived by selecting p or q multivalued function.[74] Based on the physical quantity (2), special dromion, special peakon, and foldon can be constructed if we select both p and q as the following relations:

$$p_x = \sum_{i=1}^{N} \kappa_i(\zeta - c_i t), \quad x = \zeta + \sum_{i=1}^{N} \chi_i(\zeta - c_i t), \tag{108}$$

$$q_y = \sum_{j=1}^{M} \vartheta_j(\eta - d_j t), \quad y = \eta + \sum_{j=1}^{M} \lambda_j(\eta - d_j t), \tag{109}$$

where $c_i(i=1,2,\ldots,N)$, $d_j(j=1,2,\ldots,M)$ are arbitrary constants, κ_i and χ_i, ϑ_j and λ_j are localized excitations with the properties $\kappa_i(\pm\infty)=0$, $\chi_i(\pm\infty)=\text{const}$, $\vartheta_j(\pm\infty)=0$, $\lambda_j(\pm\infty)=\text{const}$. From Eqs. (108) and (109), one can know that ζ (or η) may be a multivalued function in some suitable regions of x (or y) by choosing the functions χ_i (or λ_j) appropriately. Therefore, the function p_x (or q_y), which is obviously an interaction solution of N (or M) localized excitations due to the property $\zeta|_{x\to\infty}\to\infty$ (or $\eta|_{y\to\infty}\to\infty$), may be a multivalued function of x (or y) in these areas, though it is a single valued function of ζ (or η).

Concretely, p and q are chosen

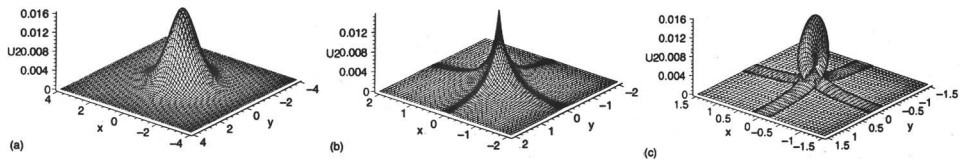

FIG. 1. Special dromion, special peakon and foldon structures for U_2 with conditions (110) and (112), (a) $A=C=0.05$, (b) $A=C=0.95$, (c) $A=C=1.5$ at $t=0$.

$$p_x = \operatorname{sech}^2(\zeta - t), \quad x = \zeta - A\tanh(\zeta), \tag{110}$$

$$q_y = \operatorname{sech}^2(\eta - t), \quad y = \eta - C\tanh(\eta), \tag{111}$$

where A and C are characteristic parameters, whose difference brings the different localized structures. When their values are chosen between 0 and 0.9, 0.9 and 1, and bigger than 1, special dromion, special peakon, and foldon can be derived. Figures 1(a)–1(c) describe three localized structures, special dromion, special peakon, and foldon with $A=C=0.05, 0.95, 1.5$, respectively.

B. Asymptotic behaviors of the localized excitations produced from the formula (2)

In order to discuss the interaction property of these localized excitations related to the physical quantity (2), we first study the asymptotic behaviors of the localized excitations produced from the formula (2) when $t\to\infty$.

In general, if the function p and q [considering Eqs. (108) and (109)] are selected as multilocalized solitonic excitations with ($z_i \equiv \zeta - c_i t$, $Z_j \equiv \eta - d_j t$)

$$p|_{t\to\mp\infty} = \sum_{i=1}^{N} p_i^{\mp}, p_i^{\mp}(z_i) \equiv p_i(\zeta - c_i t) \equiv \int \kappa_i \, \mathrm{d}x|_{z_i\to\mp\infty}, \tag{112}$$

$$q|_{t\to\mp\infty} = \sum_{j=1}^{N} q_j^{\mp}, q_j^{\mp}(Z_j) \equiv q_j(\eta - d_j t) \equiv \int \vartheta_j \, \mathrm{d}y|_{Z_j\to\mp\infty}, \tag{113}$$

where $\{p_i, q_j\}\forall\, i$ and j are localized functions, then the physical quantity expressed by Eq. (2) delivers $M\times N$ (2+1)-dimensional localized excitations with the asymptotic behavior,

$$U_2|_{t\to\mp\infty} \to \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{p_{iz_i}^{\mp} q_{jZ_j}^{\mp}}{(1+\chi_{iz_i}^{\mp})(1+\lambda_{jZ_j}^{\mp})[(p_i^{\mp}(z_i)+\tilde{p}_i^{\mp}) + (q_j^{\mp}(Z_j)+\tilde{q}_j^{\mp})]^2} \equiv \sum_{i=1}^{N}\sum_{j=1}^{M} U_{2,ij}^{\mp}, \tag{114}$$

$$x|_{t\to\mp\infty} \to \zeta + \delta_i^{\mp} + \chi_i^{\mp}(z_i), \tag{115}$$

$$y|_{t\to\mp\infty} \to \eta + \Delta_j^{\mp} + \lambda_j^{\mp}(Z_i), \tag{116}$$

with

$$\tilde{p}_i^{\mp} = \sum_{j<i} p_j(\mp\infty) + \sum_{j>i} p_j(\mp\infty), \tag{117}$$

$$\tilde{q}_i^{\mp} = \sum_{j<i} q_j(\mp\infty) + \sum_{j>i} q_j(\pm\infty), \tag{118}$$

$$\delta_i^{\mp} = \sum_{j<i} \chi_j(\mp\infty) + \sum_{j>i} \chi_j(\pm\infty), \tag{119}$$

$$\Delta_j^{\mp} = \sum_{j<i} \lambda_j(\mp\infty) + \sum_{j>i} \lambda_j(\pm\infty). \tag{120}$$

In the above discussion, it has been assumed, without loss of generality, that $c_i > c_j$, $d_i > d_j$ if $i > j$. From the asymptotic result (114), we discover some important and interesting facts. (i) The ijth localized excitation $U_{2,ij}$ is a travelling wave moving with the velocity c_i along the positive ($c_i > 0$) or negative ($c_i < 0$) x direction, and d_j along the positive ($d_j > 0$) or negative ($d_j < 0$) y direction; (ii) the properties of the ijth localized excitation $U_{2,ij}$ is only determined by p_i of Eq. (112) and q_j of Eq. (113); (iii) the shape of the ijth localized excitation $U_{2,ij}$ will be changed (noncompletely elastic or completely inelastic interaction) if

$$\tilde{p}_i^{+} \neq \tilde{p}_i^{-}, \tag{121}$$

and (or)

$$\tilde{q}_j^{+} \neq \tilde{q}_j^{-}, \tag{122}$$

following the interaction. On the contrary, it will preserve its shape (completely elastic interaction) during the interaction if

$$\tilde{p}_i^{+} = \tilde{p}_i^{-}, \tag{123}$$

$$\tilde{q}_j^{+} = \tilde{q}_j^{-}. \tag{124}$$

(iv) The phase shift of the ijth localized excitation $U_{2,ij}$ reads

$$\delta_i^{+} - \delta_i^{-}, \tag{125}$$

in the x direction and

$$\Delta_j^{+} - \Delta_j^{-}. \tag{126}$$

in the y direction.

The above discussions indicate that localized solitonic excitations for the common quantity U_2 can be produced from the $(1+1)$-dimensional multivalued functions with the properties (112), (113), and (121)–(124). In general terms, if the functions p or q are taken as multiple localized excitations that possess the phase shifts of $(1+1)$-dimensional models then the $(2+1)$-dimensional localized excitations involving formula (2) inherit phase shifts structures.

C. Interaction between the localized coherent excitations produced by multivalued functions

Now we discuss some novel coherent structures for the physical quantity U_2, and focus our attention on interaction between the localized coherent excitations produced by multivalued functions. In Sec. VI A, we present three interesting coherent excitations, i.e., special dromion, special peakon, and foldon. Here we discuss some novel interactions between them. In order to discuss them expediently and reveal the phase shift more clearly and visually, it has proved convenient to fix the one possessing zero velocity. That is to say, if we take the concrete choice $N=2$, $M=1$, $c_1=0.25$, $c_2=0$, $d_1=0$ in Eqs. (112) and (113), one has

$$p_x = 0.5\,\mathrm{sech}^2(\zeta - 0.25t) + 0.8\,\mathrm{sech}^2(\zeta), \quad x = \zeta - A\tanh(\zeta - 0.25t) - B\tanh(\zeta), \tag{127}$$

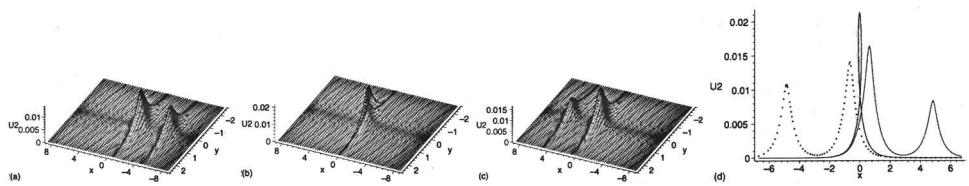

FIG. 2. Interaction between special dromions for U_2 with conditions (127) and (128) and $A=B=C=0.65$, (a) $t=-22$, (b) $t=0.04$, (c) $t=22$. (d) The corresponding sectional view at $y=0$ (dotted, solid, and dashed line denotes before, in, and after collision, respectively).

$$q_y = \mathrm{sech}^2(\eta), \quad y = \eta - C\tanh(\eta), \tag{128}$$

where A, B, and C are characteristic parameters, which determine the type of interactions.

1. Interaction between special dromions

If we take the concrete values $A=B=C=0.65$ in Eqs. (127) and (128), then we successfully construct interaction between special dromions that possess phase shifts for the physical quantity U_2 depicted in Fig. 2. From Fig. 2, we can see that the two special dromion localized excitations possess novel properties, that is, there exists a multivalued foldon in the process of their collision, which is different from the reported cases in previous literature.[75] Moreover, one can find that the interaction between them may exhibit a novel property, which is noncompletely elastic since their shapes are not completely preserved after interaction. Actually, the completely elastic interaction condition (123) and (124) is not satisfied for the common formula (2) with (127) and (128). For the static large dromion,

$$\tilde{p}_2^+ - \tilde{p}_2^- = p_1(+\infty) - p_1(-\infty) = \tfrac{17}{30} \neq 0. \tag{129}$$

For the moving small dromion,

$$\tilde{p}_1^+ - \tilde{p}_1^- = p_2(-\infty) - p_2(+\infty) = -\tfrac{68}{75} \neq 0. \tag{130}$$

The phase shift can also be observed. Prior to interaction, the large dromion has been set to be $\{v_{0x}=c_2=0,\ v_{0y}=0\}$, however, the position located by large dromion is still altered about from $x=-0.65$ to $x=0.65$, then stops at $x=0.65$ and preserves its initial velocities $\{v_x=v_{0x},\ v_y=v_{0y}\}$ after interaction. Therefore the phase shift of the static large dromion is $\delta_2^+ - \delta_2^- = \chi_1(-\infty) - \chi_1(+\infty) = 1.3$. The final velocities V_x and V_y of the moving small dromion also completely preserved its initial velocities $\{V_x=V_{0x}=c_1=0.25,\ V_y=V_{0y}=0\}$. The phase shift of the moving small dromion is $\delta_1^+ - \delta_1^- = \chi_2(+\infty) - \chi_2(-\infty) = -1.3$.

2. Interaction between special peakons

When we fix the concrete values $A=B=C=0.95$ in Eqs. (127) and (128), then we successfully construct interaction between special peakons that possess phase shifts for the physical quantity U_2 depicted in Fig. 3. From Fig. 3, we can see that the two special peakon localized excitations

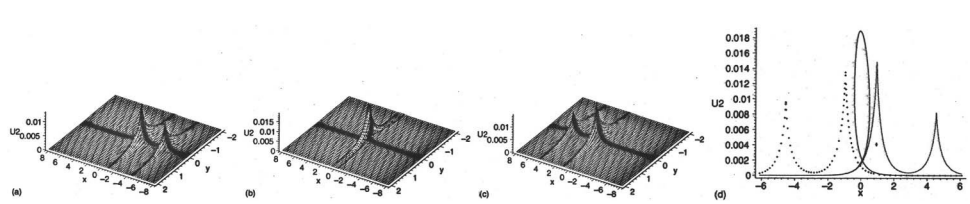

FIG. 3. Interaction between special peakons for U_2 with conditions (127) and (128) and $A=B=C=0.95$, (a) $t=-22$, (b) $t=0.5$, (c) $t=22$. (d) The corresponding sectional view at $y=0$ (dotted, solid, and dashed line denotes before, in, and after collision, respectively).

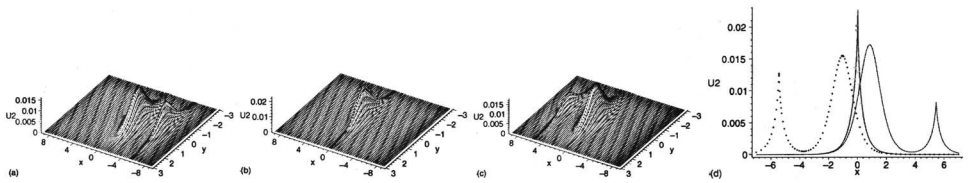

FIG. 4. Interaction between special dromion and peakon for U_2 with conditions (127) and (128) and $A=0.95$, $B=C=0.05$, (a) $t=-22$, (b) $t=0.1$, (c) $t=22$. (d) The corresponding sectional view at $y=0$ (dotted, solid, and dashed line denotes before, in, and after collision, respectively).

possess novel properties, that is, it is noncompletely elastic since their shapes are not completely preserved after interaction and there also exists a multivalued foldon in the process of their collision, which is different from the reported cases in previous literature.[10] The analytical analysis to noncompletely interaction is similar to the case in Sec. VI C 1. For the static large peakon, $\tilde{p}_2^+-\tilde{p}_2^-=\frac{2}{5}\neq 0$. For the moving small peakon, $\tilde{p}_1^+-\tilde{p}_1^-=-\frac{16}{25}\neq 0$. The phase shift can also be observed. Before interaction, the static large peakon is located at $x=-0.95$ and after the interaction, it is shifted to $x=0.95$. Then it stops at $x=0.95$ and preserves its initial velocities $\{v_x=v_{0x}=0, v_y=v_{0y}=0\}$ after interaction. Whereas the moving small peakon also completely preserved its initial velocities $\{V_x=V_{0x}=c_1=0.25, V_y=V_{0y}=0\}$. By careful analysis similar to Sec. VI C 1, we know that the phase shift of the static large peakon is 1.9, and the moving small peakon exists in the phase shift -1.9. These properties are analogous to the case in Sec. VI C 1.

3. Interactions among special dromion, special peakon, and foldon

Along the above ideas and performing a similar analysis, if $A=0.95$, $B=C=0.05$, or $A=1.5$, $B=C=0.05$, or $A=1.5$, $B=C=0.95$ in Eqs. (127) and (128), interactions between special dromion and special peakon, special dromion and foldon, special peakon and foldon can be constructed for the physical quantity U_2 depicted in Figs. 4–6, respectively. From these evolution profiles, one can know that they are all noncompletely elastic since their shapes are not completely preserved after interaction. Moreover, the phase shift can also be observed. In Fig. 4, the phase shift of the static dromion is $\delta_2^+-\delta_2^-=\chi_1(-\infty)-\chi_1(+\infty)=1.9$, and the moving peakon exists phase shift $\delta_1^+-\delta_1^-=\chi_2(+\infty)-\chi_2(-\infty)=-0.1$. In Fig. 5, the phase shift of the static dromion is 3, and the moving foldon exists of phase shift -0.1. In Fig. 6, the phase shift of the static peakon is 3, and the moving foldon exists of phase shift -1.9.

VII. SUMMARY AND DISCUSSION

In summary, the ETM is applied to obtain variable separation solutions of $(1+1)$-dimensional, $(2+1)$-dimensional, and $(3+1)$-dimensional systems. For some $(2+1)$-dimensional integrable models such as the GNNV, DS, BKK, BLP, integrable KdV, BS, and Burgers models, some lower dimensional arbitrary functions can be included in their exact solutions. A common variable separation formula is valid for all these models. For these integrable models, there are not less than an arbitrary function (p or q), whereas for nonintegrable KdV equation, neither p or q is an

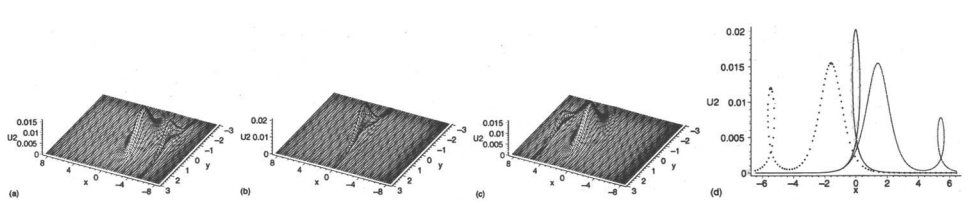

FIG. 5. Interaction between special dromion and foldon for U_2 with conditions (127) and (128) and $A=1.5$, $B=C=0.05$, (a) $t=-22$, (b) $t=0.1$, (c) $t=22$. (d) The corresponding sectional view at $y=0$ (dotted, solid, and dashed line denotes before, in, and after collision, respectively).

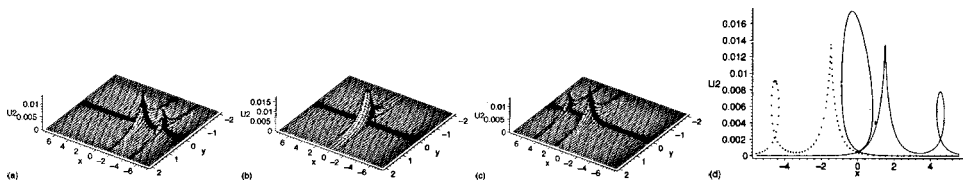

FIG. 6. Interaction between special peakon and foldon for U_2 with conditions (127) and (128) and $A=1.5$, $B=C=0.95$, (a) $t=-22$, (b) $t=-0.2$, (c) $t=22$. (d) The corresponding sectional view at $y=0$ (dotted, solid, and dashed line denotes before, in, and after collision, respectively).

arbitrary function, and they must satisfy some constraint equations. Therefore, we can define the solvable models by the ETM: these kinds of models should not be less than an arbitrary function (p or q). The nonintegrable models are also not the solvable models by the ETM. Moreover, there exists also a common formula, which is similar to the formula (2), to describe suitable physical fields or potentials of some $(1+1)$-dimensional models. The universal formula (2) is suitable to describe the $(3+1)$-dimensional Burgers. The only differences are that the function q is a solution of a constraint equation and p is an arbitrary function of three independent variables. In fact, the common formula (2) is a simplified form of the universal formula (4), i.e., through the transformation $p=(a_0+a_1P)/(a_2+a_3P)$, $q=Q$, we have $U_2=U_1$.

Starting from the common formula (2), all sorts of localized coherent structures discussed by the universal formula (1), such as nonpropagating solitons, dromion, peakon, compaction, foldon, instanton, ghoston, ring soliton, and the interaction between these solitons, can be rederived. Moreover, abundant local excitations with and without completely elastic interaction properties are constructed readily by suitable selecting the arbitrary multivalued functions according the asymptotic result (114). Especially, some novel interactions among special dromion, special peakon, and foldon are investigated both analytically and graphically. The interactions between two special dromions, and between two special peakons, both possess novel properties, that is, there exist a multivalued foldon in the process of their collision, which is different from the reported cases in previous literature. The explicit phase shifts for all the local excitations offered by the common formula have been given, and are applied to these novel interactions in detail.

What we have obtained is also further verification that the ETM is quite useful to generate abundant localized excitations for many models. Besides these systems listed in this paper, we can also obtain the variable separation solutions of $(2+1)$-dimensional Maccari system,[76] $(2+1)$-dimensional nonlinear Schrödinger equation,[77] $(2+1)$-dimensional generalized AKNS system,[78] $(2+1)$-dimensional generalized Burgers system,[79] and $(1+1)$-dimensional Boiti system,[16] and the like. For the limit of length, we do not list them here. It is also known that the DS and the KP equations are the reductions of the self-dual Yang-Mills (SDYM) equation. So both the KP and the SDYM equations may possess quite rich nonlinear excitations with some arbitrary characteristics. The KP equation and $(2+1)$-dimensional Boussinesq equation[80] are other types of important integrable models in the study of integrable models. However, we have not yet found its nontrivial variable separation solutions by ETM. The same cases happen in some known $(1+1)$-dimensional models such as nonlinear Schrödinger equation and KdV, etc. Therefore, how to find the variable separation solutions of these models is an open question. In our future work, we will devote to generalizing this method to these nonlinear systems, the differential-difference equations and other $(3+1)$-dimensional nonlinear systems.

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A spinorial formulation of the maximum clique problem of a graph

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We present a new formulation of the maximum clique problem of a graph in complex space. We start observing that the adjacency matrix A of a graph can always be written in the form $A=B^2$ where B is a complex, symmetric matrix formed by vectors of zero length (null vectors) and the maximum clique problem can be transformed in a geometrical problem for these vectors. This problem, in turn, is translated in spinorial language and we show that each graph uniquely identifies a set of pure spinors, that is vectors of the endomorphism space of Clifford algebras, and the maximum clique problem is formalized in this setting so that, this much studied problem, may take advantage from recent progresses of pure spinor geometry. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2186256]

I. INTRODUCTION

In this paper we propose a new representation of the maximum clique problem in complex space. After a brief review of this famous NP-complete problem, we show how the adjacency matrix of a graph can be expressed as the square of a symmetric complex matrix. The vectors forming this matrix have zero length and Cartan has shown that this geometry can be treated elegantly with spinors. After a brief remind of spinor properties, we show that the adjacency matrix is better decomposed in the Witt basis of complex space. We finish with a formulation of the maximum clique problem in this formalism and show that each graph uniquely identifies a spinor whose properties surely deserve deeper studies.

II. THE MAXIMUM CLIQUE PROBLEM

A. A brief review

Given a graph of size n, a clique is a subgraph with pairwise adjacent vertices and the maximum clique (MC) problem is that of finding the *size k* of the largest clique. It is a well studied NP-complete problem and there are reviews with hundreds references (see, e.g., Refs. 4 and 16).

Given a graph let A be its $n\times n$ adjacency matrix with elements in $\{0,1\}$ and zero diagonal; we will consider only undirected graphs for which A is symmetric. Furthermore, since every undirected graph can be subdivided in connected graphs, we discuss only connected graphs that have irreducible adjacency matrices.

The quadratic form on A ($'$indicates transposition, bold characters, vectors) is bounded by

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$$0 \leqslant \mathbf{x}' A \mathbf{x} \leqslant 1 - \frac{1}{n} \quad \text{for } \mathbf{x} \in K_n,$$

where the simplex $K_n = \{\mathbf{x} \in \mathbb{R}^n : x_i \geqslant 0 \, \forall \, i \text{ and } \mathbf{e}'\mathbf{x} = 1\}$ and $\mathbf{e}' = (1, 1, \ldots, 1)$.

A subgraph with r vertices is uniquely determined by its characteristic vector that is an n dimensional vector whose ith component, by taking values $1/r$ or 0, indicates whether the ith element belongs or not to the subgraph. Characteristic vectors belong to K_n.

In 1965 Motzkin and Straus[14] proved the following.

Theorem 1: *If the MC of graph A has size k then*

$$\max_{\mathbf{x} \in K_n} \mathbf{x}' A \mathbf{x} = 1 - \frac{1}{k} \tag{1}$$

and if $\mathbf{x}_k$ *is the characteristic vector of a MC then* $\mathbf{x}_k' A \mathbf{x}_k = 1 - 1/k$.

Bomze[3] sharpened this result showing that, if $\mathbb{I}$ represents the identity matrix, $\max_{\mathbf{x} \in K_n} \mathbf{x}' (A + \frac{1}{2}\mathbb{I}) \mathbf{x} = 1 - 1/2k$ and moreover that this quadratic form reaches its maximum *if* and *only if* $\mathbf{x}$ is the characteristic vector of a MC.

With this formulation the, essentially combinatorial, MC problem is transposed to the search of the maximum of a quadratic function in a bounded region: a continuous optimization problem with linear constraints. Several authors[11,15,17] used this formulation to find approximate solutions to the MC problem.

B. Decomposition of the adjacency matrix

Any symmetric matrix like A may be expressed in the form (see Appendix for details)

$$A = B'B = BB = B^2, \tag{2}$$

where B is a complex, symmetric matrix that we can think as formed by n complex column vectors $\mathbf{z}_i \in \mathbb{C}^n$,

$$B = (\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n), \quad a_{jk} = (B'B)_{jk} = \mathbf{z}_j' \mathbf{z}_k \tag{3}$$

these vectors are called null vectors since they have zero length since $a_{jj} = \mathbf{z}_j^2 = 0$. Let n_0 be the number of zero eigenvalues of A, then rank A = rank $B = n - n_0$ and this is also the dimension of the space V spanned by the vectors $\mathbf{z}$. With B the quadratic form on A becomes

$$\mathbf{x}' A \mathbf{x} = \mathbf{x}' B' B \mathbf{x} = (B\mathbf{x})^2 := \mathbf{Z}^2,$$

where $\mathbf{Z} = B\mathbf{x} = \Sigma_i x_i \mathbf{z}_i \in \mathbb{C}^n$ is a complex vector with which the MC problem may be reformulated and (1) can be written

$$\max_{\mathbf{x} \in K_n} \mathbf{Z}^2 = 1 - \frac{1}{k}$$

this is the problem of finding the vector of maximum length that can be formed by a convex combination of the $\mathbf{z}$'s. In real space this is the problem of finding the point(s) of the convex hull of the $\mathbf{z}$'s with maximum distance from the origin. We remark that $\mathbf{Z}^2$ is real since x_i and $\mathbf{z}_j' \mathbf{z}_k = a_{jk}$ are all real.

C. Another formulation of the maximum clique problem

The MC problem is tightly connected to the problem of the maximum independent set that is the problem of finding the size of the largest subgraph whose vertices are pairwise nonadjacent. Let $\bar{A}$ represent the adjacency matrix of the complementary graph of A, i.e., the graph with the same vertices and complementary edges; if J is the matrix whose elements are all 1 then $\bar{A} = J - \mathbb{I} - A$. It is simple to verify that every subset of vertices of A that forms a clique form also an

independent set of $\bar{A}$ and vice versa. The cliques of A are thus in one to one correspondence to the independent sets of $\bar{A}$ and if $\mathbf{x}_k$ is the characteristic vector of a clique of A then it is also the characteristic vector of an independent set of $\bar{A}$ and $\mathbf{x}_k'\bar{A}\mathbf{x}_k=0$.

There are several ways to formulate the MC problem of A as the problem of the maximum independent set of $\bar{A}$.[13,16] Indicating $\overline{\mathbf{Z}}=\bar{B}\mathbf{x}$ (from now on we use overstriked symbols to indicate quantities relative to $\bar{A}$) a formulation with appealing properties is

$$\max_{\mathbf{x}\in\{\{0,1\}^n:\overline{\mathbf{Z}}^2=0\}} \mathbf{x}'\mathbf{x}=k. \tag{4}$$

This problem has the following geometrical interpretation: the null vectors $\overline{\mathbf{z}}$ span the space $V\subseteq\mathbb{C}^n$ and any couple of linearly independent vectors $\overline{\mathbf{z}}_j$ and $\overline{\mathbf{z}}_k$ span a two-dimensional space contained in V. If $\overline{\mathbf{z}}_j'\overline{\mathbf{z}}_k=\bar{a}_{jk}=0$ it is easy to verify that this space has the property that all of its elements are null vectors and are all mutually orthogonal: this space is called a totally null plane (TNP). If $\bar{A}$ contains at least one nondiagonal zero element, then V contains at least one two-dimensional TNP.

The solution of the MC problem provides the largest subset $\overline{\mathbf{z}}_{j_1},\overline{\mathbf{z}}_{j_2},\ldots,\overline{\mathbf{z}}_{j_k}$ of $\overline{\mathbf{z}}$'s which define a TNP contained in V. We note that, since for any two of them $\overline{\mathbf{z}}_{j_r}'\overline{\mathbf{z}}_{j_s}=\bar{a}_{j_r j_s}=0$, then not only $\Sigma_{l=1,k}\overline{\mathbf{z}}_{j_l}$, but any of their linear combinations

$$\overline{\mathbf{Z}}=\sum\nolimits_{l=1,k} x_{jl}\overline{\mathbf{z}}_{jl}$$

is a particular null vector that satisfy the constraint $\overline{\mathbf{Z}}^2=0$. Since $\mathbb{C}^n$ cannot contain a TNP of more than $n/2$ dimensions[9] this formulation have already been used to calculate an upper bound for the size of the MC.[5]

III. A BRIEF REVIEW OF SPINORS

It was Cartan who first has shown how the geometry of null vectors may be best dealt with in terms of spinors, nowadays defined as vectors of the representation space of Clifford algebras, whose components are equal (up to a sign) to the square root of linear combinations of null vector components (loosely speaking, spinors are square roots of null vectors). He furthermore has shown how Euclidean geometry may be derived from spinor geometry which then could be the fundamental geometry of space-time and of natural phenomena also because it has the property of linearizing tensor equations, like, for example, Dirac equation linearizes Klein-Gordon equation. It is then appropriate to attempt to reformulate the MC problem in spinorial form.

Following Chevalley[10] spinors may be dealt with in the frame of Clifford algebras.[1,7] Given a $2n$ dimensional complex space $\mathbb{C}^{2n}$, with Euclidean quadratic form and the corresponding Clifford algebra $\mathrm{Cl}(2n)$, let $\gamma_1,\gamma_2,\ldots,\gamma_{2n}$ be the generators of $\mathrm{Cl}(2n)$ with the property

$$[\gamma_j,\gamma_k]_+:=\gamma_j\gamma_k+\gamma_k\gamma_j=2\delta_{jk}\mathbb{I},\quad j,k=1,2,\ldots,2n.$$

$\mathrm{Cl}(2n)$ may be conceived as a direct sum of tensor spaces

$$\mathrm{Cl}(2n)=V^{(0)}\oplus V^{(1)}\oplus\cdots\oplus V^{(2n)}$$

and one can identify $V^{(1)}$ as the image of the vector space $\mathbb{C}^{2n}$ simply substituting the anticommutator with a scalar product and the γ_j with the unit vectors $\mathbf{e}_j$ of a standard orthonormal basis of $\mathbb{C}^{2n}$ with coordinates $(\mathbf{e}_j)_k=\delta_{jk}$.

A remark about notation: we indicated usual vectors in bold, so $\mathbf{v}$ represents a proper vector of $\mathbb{C}^{2n}$ while with v we represent the corresponding element of the Clifford algebra $\mathrm{Cl}(2n)$ belonging to tensor space $V^{(1)}$.

A spinor Φ is a vector belonging to the spaces S of endomorphism of $\mathrm{Cl}(2n)=\mathrm{End}\,S$ and is defined by the Cartan's equation,

$$v\Phi = \left(\sum_{j=1}^{2n} v_j \gamma_j\right)\Phi = 0, \tag{5}$$

where v_j are the orthonormal components of v (and also of $\mathbf{v} \in \mathbb{C}^{2n}$) and $v\Phi$ is a Clifford product $v\Phi = v\rfloor\Phi + v\wedge\Phi$.

A. The Witt basis of Cl(2*n*) and the Fock basis of the associated spinor Φ

Let us define the null, or Witt, basis Cl($2n$) as follows:

$$p_j = \tfrac{1}{2}(\gamma_{2j-1} + i\gamma_{2j}) \quad \text{and} \quad q_j = \tfrac{1}{2}(\gamma_{2j-1} - i\gamma_{2j}), \quad j = 1,2,\ldots,n \tag{6}$$

with the properties

$$[p_j,p_k]_+ = [q_j,q_k]_+ = 0 \quad \text{and} \quad [p_j,q_k]_+ = \delta_{jk}\mathbb{I}. \tag{7}$$

With this basis $\mathbb{C}^{2n}$ is easily seen as the direct sum of two maximal TNP P and Q spanned by null vectors $\{\mathbf{p}_j\}$ and $\{\mathbf{q}_j\}$, respectively,

$$\mathbb{C}^{2n} = P \oplus Q,$$

since $P \cap Q = \varnothing$ each vector $\mathbf{v} \in \mathbb{C}^{2n}$ may be expressed in the form $\mathbf{v} = \Sigma_{i=1}^{n}(\alpha_i\mathbf{p}_i + \beta_i\mathbf{q}_i)$ with α_i and β_i arbitrary complex numbers.

A spinor $\Phi \in S$, defined by Cartan equation (5), may be represented by minimal left ideals (MLI) of Cl($2n$).[10] Consider the 2^n MLI that form the Fock basis in spinor space[8]

$$\omega_0 = p_1 p_2 \ldots p_n,$$

$$\omega_1 = q_1\omega_0, \quad \omega_2 = q_2\omega_0, \quad \omega_4 = q_3\omega_0, \quad \ldots, \quad \omega_{2^{n-1}} = q_n\omega_0,$$

$$\omega_3 = q_1 q_2\omega_0, \quad \omega_5 = q_1 q_3\omega_0, \quad \ldots, \tag{8}$$

$$\ldots,$$

$$\omega_{2^n-1} = q_1 q_2 \ldots q_n\omega_0$$

in which the indexes of the q's always appear in ascending order and the interpretation of the 2^n values of the spinor index s of ω_s is immediate thinking of s as of a binary number of n digits where the jth digit from the right, taking the value 1 or 0, indicates wether q_j is present or not in ω_s. Any spinor Φ may be uniquely expressed in terms of the elements of the Fock basis (8),

$$\Phi = \sum_{s=0}^{2^n-1} \xi_s\omega_s, \tag{9}$$

where the ξ_s are the 2^n complex components of the spinor.

B. Cartan equation in the Fock basis

When we write the Cartan equation (5) in the basis, defined in (6) and (9), we get

$$v\Phi = \left(\sum_{i=1}^{n} \alpha_i p_i + \beta_i q_i\right)\left(\sum_{s=0}^{2^n-1} \xi_s \omega_s\right) = 0 \tag{10}$$

and this equation can be read in two ways depending on whether v or Φ plays the role of the unknown. For example, if $\Phi = \xi_0\omega_0$, i.e., $\Phi = (\xi_0, 0, \ldots, 0)$ (the spinor represented by the MLI ω_0 was named standard by Cartan) it becomes

$$\left(\sum_{i=1}^{n} \alpha_i p_i + \beta_i q_i\right)\xi_0\omega_0 = \left(\sum_{i=1}^{n} \alpha_i p_i + \beta_i q_i\right)\xi_0 p_1 p_2 \cdots p_n = 0$$

and, remembering that from (7) we have,

$$p_i p_i = 0 = q_i q_i, \quad p_i q_i = \mathbb{I} - q_i p_i, \tag{11}$$

one easily finds that the equation is satisfied, for $\xi \neq 0$, if, and only if, all the β_i are zero. Moreover the equation holds for every value taken by the α_i, i.e., for every point of the subspace $P = \mathrm{Span}(\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n)$. It is also simple to work this example the other way round, i.e., given a subspace whose generic vector has the form $\mathbf{v} = \Sigma_{i=1}^{n} x_i \mathbf{p}_i$ one finds that the spinor that satisfies (10) is of the form $\Phi = (\xi_0, 0, \ldots, 0) = \xi_0\omega_0 \ \forall\, \xi_0 \in \mathbb{C}$.

This shows explicitly the correspondence, set up by Cartan equation (10), between spinors and TNP's, in this example between ω_0 and the maximal TNP P of $\mathbb{C}^{2n}$. Similarly one can find that the TNP corresponding to ω_1 is $x_1 q_1 + \Sigma_{i=2}^{n} x_i p_i$ and so on. More generally left-multiplying (10) by v it becomes

$$v^2\Phi = 0$$

showing that v^2 is null for $\Phi \neq 0$ and Eqs. (5) and (10) are linearizations of this relation. Let v' be another solution of $v'\Phi = 0$ for the same Φ, left-multiplying (10) by v' we get

$$v'v\Phi = 0 \quad \text{and similarly} \quad vv'\Phi = 0$$

from which easily derives that

$$[v', v]_+ = 0$$

so v' and v, besides being null, are mutually orthogonal and thus form a TNP.

In general, given a spinor Φ, all the vectors v satisfying (10) are null and mutually orthogonal and define a TNP that we call $M_k(\Phi)$ where $k \leqslant n$ indicates its dimensions. If $k = n$, that is, the dimension of $M_k(\Phi)$ is maximal, the corresponding spinor was called *simple* by Cartan[9] and *pure* by Chevalley,[10] a name now prevailing in the literature. Each one of the 2^n spinors of the Fock basis (8) is pure.

Consequently, from now on, when we indicate with v the solution of $v\Phi = 0$ we actually refer to the entire subspace $M_k(\Phi)$ and not just to one of its vectors.

Pure spinors, as stressed by Cartan, are equivalent, up to a sign, to the corresponding maximal TNP whose null vectors may be bilinearly expressed in terms of them. This equivalence establishes a link between spinors and projective Euclidean geometry (of null vectors) which, being very simple and elegant, might have a crucial role for the explanation of several phenomena in physics. However there is a basic obstacle for setting in evidence this equivalence: while the dimensions of the TNP increase with n, that of the equivalent spinor increase with 2^n and consequently, for large n, their components will have to be subject to $O(2^n)$ constraint relations. In order to overcome this difficulty, Cartan, when discussing the elegant properties and proving the theorems of pure spinor geometry, introduced the concept of standard pure spinors with only one component and therefore not subject to constraint relations.

IV. SPINORIAL FORMULATION OF THE MAXIMUM CLIQUE PROBLEM

We are now ready to give a spinorial formulation of the MC problem and start by introducing the vectors $\overline{\mathbf{z}_i}$ of the matrix $\bar{B}$ defined above, in the Witt basis of $\mathrm{Cl}(2n)$ with the scalar product standing for an anticommutator,

$$\overline{\mathbf{z}_i} = \mathbf{p}_i + \sum_{j=1}^{n} \bar{a}_{ij}\mathbf{q}_j, \quad i = 1,2,\ldots,n.$$

These n vectors have the following properties (immediate to prove):

(i) belong to $\mathbb{C}^{2n}$ and are linearly independent (because of the $\mathbf{p}_i$);
(ii) are null, i.e. $\overline{\mathbf{z}_i}\overline{\mathbf{z}_i}=0$ since $\bar{a}_{ii}=0$;
(iii) satisfy (3) for the complementary matrix, i.e., $\overline{\mathbf{z}_i}\overline{\mathbf{z}_j}=\bar{a}_{ij}$.

In general they span an n dimensional subspace V, which will be partially null. Precisely each $\bar{a}_{ij}=0$ will imply the existence of a two-dimensional TNP in V. V will be totally null only if $\bar{a}_{ij}=0\ \forall ij$ in which case $\overline{\mathbf{z}_i}=\mathbf{p}_i$ and $V=P=\mathrm{Span}(\mathbf{p}_1,\mathbf{p}_2,\ldots,\mathbf{p}_n)$. Differently from (3) now $\bar{B}$ is a $2n\times n$ matrix formed by n linearly independent vectors such that $\bar{A}=\bar{B}'\bar{B}$.

To fully exploit the spinorial formulation we will consider the $\overline{\mathbf{z}_i}$ vectors as representative of the subspace they induce, i.e., $\mathrm{Span}(\mathbf{p}_i,\bar{a}_{i1}\mathbf{q}_1,\ldots,\bar{a}_{in}\mathbf{q}_n)$ of dimension $\Sigma_{j=1}^{n}\bar{a}_{ij}+1$. We do this introducing in the definition arbitrary coefficients α,

$$\overline{\mathbf{z}_i} = \alpha_i\mathbf{p}_i + \sum_{j=1}^{n} \bar{a}_{ij}\alpha_j\mathbf{q}_j, \quad i = 1,2,\ldots,n \tag{12}$$

and we can always get back the representative vectors setting all $\alpha=1$.

The equation $\overline{\mathbf{Z}}^2=0$, representing the constraints of the MC problem in (4), may be linearized formulating the problem in spinorial form:

$$\overline{\mathbf{Z}}\Phi = \bar{B}\mathbf{x}\Phi = \left(\sum_{i=1}^{n} x_i\overline{\mathbf{z}_i}\right)\Phi = 0 \tag{13}$$

or with $\overline{\mathbf{z}_i}$ from (12),

$$\left[\sum_{i=1}^{n} x_i\left(\alpha_i\overline{\mathbf{p}_i} + \sum_{j=1}^{n}\alpha_j\bar{a}_{ij}\mathbf{q}_j\right)\right]\Phi = 0 \tag{14}$$

of the form (10). In this equation, in general, x_i must be interpreted as complex variables, restricted to values in $\{0,1\}$ in the traditional formulation of the MC problem (4).

We thus have a set of n vectors $\overline{\mathbf{z}_i}$ defining an n-dimensional subspace of $\mathbb{C}^{2n}$ and we will look for the spinors Φ that satisfy (13).

A. Some properties of Cartan equation

Before analyzing in detail (14), devoted to graphs, we step back to the general form of Cartan equation (10) and derive some of its properties. First we study the case in which the TNP is not maximal.

Proposition 1: *Given a TNP of dimension $k\leqslant n$, the corresponding spinor Φ, solution of the Cartan equation* (10), *has at least 2^{n-k} nonzero coordinates in the Fock basis.*

Without loss of generality we take $\mathrm{Span}(\mathbf{p}_1,\mathbf{p}_2,\ldots,\mathbf{p}_k)$ as a TNP of dimension k, since given any TNP of dimension k it is always possible, by a proper choice of the basis, make it coincide with $\mathrm{Span}(\mathbf{p}_1,\mathbf{p}_2,\ldots,\mathbf{p}_k)$ (see, e.g, Ref. 8).

We will prove the proposition by induction: we already know that when the TNP is maximal, i.e., of dimension n as in the example in paragraph 3.2, the corresponding spinor can have one component (actually it may have at most two components, see proposition 5 in Ref. 8) and thus satisfies the proposition.

Let us suppose now that we have a TNP of dimension k and that the corresponding spinor Φ has m nonzero components: we will show that when reducing the dimension of the TNP to $k-1$ the new spinor has *at least* $2m$ components. So let us suppose that our spinor Φ has m nonzero components and satisfy

$$\left(\sum_{i=1}^{k} x_i p_i\right)\Phi = \left(\sum_{i=1}^{k-1} x_i p_i + x_k p_k\right)\Phi = 0.$$

Since this relation holds for any value of the x_i it must hold in particular for $x_k=0$ so that we have

$$\left(\sum_{i=1}^{k-1} x_i p_i\right)\Phi = 0$$

from which necessarily derives $p_k\Phi=0$. This implies that q_k does not appear in all the m ω's that are the nonzero components of Φ. Assuming the contrary we could write

$$x_k p_k \sum_s \xi_s \omega_s = x_k p_k \left(\sum_{s\in\{q_k\}} \xi_s \omega_s + \sum_{s\in\{\bar{q}_k\}} \xi_s \omega_s\right) = x_k p_k \sum_{s\in\{q_k\}} \xi_s \omega_s = 0,$$

where by $s\in\{q_k\}$ we indicate the subset of the m values of s such that the term q_k do appear in ω_s and by $s\in\{\bar{q}_k\}$ the complementary subset in which the term q_k do not appear; obviously this second sum vanish when left multiplied by p_k. The generic term of the surviving sum can be easily calculated with (11) and reduces to

$$x_k \sum_{s\in\{q_k\}} \xi_s (-1)^{l_s} (\mathbb{I} - q_k p_k)\omega_{s-2^k} = x_k \sum_{s\in\{q_k\}} \xi_s (-1)^{l_s} \omega_{s-2^k} = 0$$

when q_k is the l_sth of the q's present in ω_s. But this relation cannot hold because it would imply that the components of the Fock basis are linearly dependent (remark that ω_{s-2^k} are all different). Thus we proved that none of the m components of Φ can contain q_k.

Returning to our argument we observe that when we reduce the size of the TNP by 1, setting $x_k\equiv 0$, we have

$$\left(\sum_{i=1}^{k-1} x_i p_i\right)\Phi = 0$$

but also

$$\left(\sum_{i=1}^{k-1} x_i p_i\right)(\Phi + q_k\Phi) = 0$$

and since no component of Φ contains q_k all components of $q_k\Phi$ are different from those of Φ and the spinor $\Phi+q_k\Phi$ has $2m$ nonzero components. This concludes the induction argument proving the proposition. □

An immediate consequence of the arguments of the proof is that Φ relative to $\mathrm{Span}(\mathbf{p}_1,\mathbf{p}_2,\ldots,\mathbf{p}_k)$ cannot have components with any of the $\{q_1,q_2,\ldots,q_k\}$. This allows us to write Φ explicitly: its components are all and only the 2^{n-k} not containing any element of $\{q_1,q_2,\ldots,q_k\}$. This generalizes easily to the case of a TNP of size k of the more general form

$$\left(\sum_i x_i p_i + \sum_j x_j q_j\right)\Phi = 0$$

the corresponding spinor components are all and only the 2^{n-k} components not containing any element of $\{q_i\}$ and containing all of the elements of $\{q_j\}$.

We now consider the more general case of a TNP formed by the span of k null vectors v and show a way to express the corresponding spinor.

Proposition 2: *Given a TNP* $V=Span(v_1,\ldots,v_k)$, *of dimension* k, *the corresponding spinor* $\Phi(v_1,\ldots,v_k)$, *satisfying the Cartan equation* (10), *can be calculated with*

$$\Phi(v_1,\ldots,v_k) = v_1\cdots v_k\Phi(\mathbb{I}), \tag{15}$$

where with $\Phi(\mathbb{I})$ *we represent the most general spinor* (9) *expressed in the Fock basis.*

We start by proving the simpler case in which there is just one vector and moreover this vector coincides with one of the basis, i.e., $v=p_j$ and we prove that

$$\Phi(p_j) = p_j\Phi(\mathbb{I}).$$

To calculate $p_j\Phi(\mathbb{I})$, as in the previous proof, we split the sum over the Fock basis into two parts and get

$$p_j\Phi(\mathbb{I}) = p_j\sum_{s\in\{q_j\}}\xi_s\omega_s + p_j\sum_{s\in\{\bar{q}_j\}}\xi_s\omega_s = p_j\sum_{s\in\{q_j\}}\xi_s\omega_s$$

$$= \sum_{s\in\{q_j\}}\xi_s(-1)^{l_s}(\mathbb{I}-q_jp_j)\omega_{s-2^j} = \sum_{s\in\{q_j\}}\xi_s(-1)^{l_s}\omega_{s-2^j}$$

$$= \sum_{s\in\{\bar{q}_j\}}\xi_{s+2^j}(-1)^{l_{s+2^j}}\omega_s$$

that show that $p_j\Phi(\mathbb{I})$ obviously satisfy $p_j\Phi(p_j)=0$ and has for components the 2^{n-1} in which q_j do not appear in ω_s and thus, given the arbitrary values of the coefficients ξ_s, represents the most general expression for $\Phi(p_j)$, as shown in Proposition 1.

To prove the general proposition we proceed by induction and first extend the proof to a more general null vector $v_1=\Sigma_i\alpha_ip_i+\Sigma_j\beta_jq_j$,

$$\Phi(v_1) = v_1\Phi(\mathbb{I}) = \sum_i \alpha_i\Phi(p_i) + \sum_j \beta_j\Phi(q_j)$$

and

$$v_1\Phi(v_1) = v_1^2\Phi(\mathbb{I}) = 0$$

since, by hypothesis, v_1 is null. Now suppose that we already have

$$\Phi(v_1,\ldots,v_{j-1}) = v_1\cdots v_{j-1}\Phi(\mathbb{I})$$

and we add v_j that form a TNP with previous vectors, we have

$$\left(x_jv_j + \sum_{i=1}^{j-1} x_iv_i\right)v_j\Phi(v_1,\ldots,v_{j-1}) = -v_j\left(\sum_{i=1}^{j-1} x_iv_i\right)\Phi(v_1,\ldots,v_{j-1}) = 0,$$

where we have used the relations $v_j^2=0$ and $v_iv_j=-v_jv_i$ for $i<j$ deriving from the hypothesis that the v's form a TNP. This completes the proof showing also that the order of multiplication of v's in (15) is irrelevant since it can only affect the global sign of the sign of the spinor. □

We conclude with the general case.

Proposition 3: *Given* $V:=Span(v_1,\ldots,v_k)$, *there exists a spinor* Φ, *satisfying the Cartan equation for all values of the coefficients* $x_1,\ldots,x_k$,

$$\left(\sum_{i=1}^{k} x_i v_i\right)\Phi = 0$$

if, and only if, V is a TNP.

To prove it let us suppose the contrary, i.e., that there exists a non-null vector v and $\Phi \neq 0$ satisfying Cartan equation; left-multiplying by v we would get

$$v^2\Phi = 0$$

but since $v^2 \neq 0$ this implies $\Phi=0$ contradicting the initial hypothesis. On the other hand, for any null vector v the spinor $\Phi(v)=v\Phi(\mathbb{I})$ satisfies the Cartan equation since $v\Phi(v)=v^2\Phi(\mathbb{I})=0$. □

B. Back to the graph maximum clique problem

We get back to our form of Cartan equation (14) with an example: let us suppose that $\bar{a}_{12}=0$, this means that $\overline{\mathbf{z}}_1$ and $\overline{\mathbf{z}}_2$ form a TNP and, setting $x_3=x_4=\cdots=x_n=0$, with (12) and Proposition 2 we get

$$(x_1\overline{\mathbf{z}}_1 + x_2\overline{\mathbf{z}}_2)\Phi(\overline{\mathbf{z}}_1\overline{\mathbf{z}}_2) = (x_1\overline{\mathbf{z}}_1 + x_2\overline{\mathbf{z}}_2)\mathbf{p}_1\mathbf{p}_2\cdots\mathbf{q}_i\cdots\Phi(\mathbb{I}) = 0,$$

where with the notation $\cdots\mathbf{q}_i\cdots$ we indicate all different $\mathbf{q}_i$ that appear in $\overline{\mathbf{z}}_1$ and $\overline{\mathbf{z}}_2$. This example shows that it is simple to get particular solutions to (14) the real problem being to find the *set of all solutions*, for which we have the following.

Proposition 4: *The set of nonzero spinors that solve the Cartan equation* (14) *is isomorphic to the set of cliques of A.*

Given a solution of (14) with $\Phi \neq 0$ we will have corresponding values for the coefficients $x_1,\ldots,x_n$. For all $x_i \neq 0$ we can redefine the arbitrary α coefficients in (14) so that $x_i=1$ and the solution can be written in the form $x_i \in \{0,1\}$. The $\overline{\mathbf{z}}_i$ corresponding to $x_i=1$ form necessarily a clique since for any couple of them their scalar product is null. Vice versa given a clique $\overline{\mathbf{z}}_{i_1},\ldots,\overline{\mathbf{z}}_{i_k}$ the corresponding coefficients $x_i \in \{0,1\}$ and the corresponding spinor $\Phi(\overline{\mathbf{z}}_{i_1},\ldots,\overline{\mathbf{z}}_{i_k})$ satisfy the Cartan equation. □

We can now reformulate our initial MC problem (4): it will correspond to that solution of (14) with the maximum intersection with P, i.e.,

$$k = \max_{\Phi:\left(\sum_{i=1}^{n} x_i\bar{z}_i\right)\Phi=0} \dim(P \cap M(\Phi)). \tag{16}$$

This shows also that the problem of finding all possible spinor solutions of (14) is NP complete since, given the set of all solutions, one gets also the solution of the MC problem. With respect to the MC formulation (4) we remark two main differences: the first is that the demanding restriction $\mathbf{x} \in \{0,1\}^n$ can be relaxed since all solutions of (14) necessarily have binary x_i. The second is that the quadratic constraint $\overline{\mathbf{Z}}^2=0$ of (4) is linearized here to $\overline{\mathbf{Z}}\Phi=0$.

C. Definition of the spinor $\Psi(\bar{A})$ corresponding to graph *A*

Even if we cannot determine in general the set of all solutions to our problem (that would mean solving an NP-complete problem) we can try to better characterize the set of spinors satisfying (14). Let us define a null vector $\overline{\mathbf{Z}}_k$, sum of k vectors $\overline{\mathbf{z}}_i$,

$$\overline{\mathbf{Z}}_k = \overline{\mathbf{z}}_{j_1} + \overline{\mathbf{z}}_{j_2} + \cdots + \overline{\mathbf{z}}_{j_k} = \mathrm{Span}(\mathbf{p}_{j_1},\mathbf{p}_{j_2},\ldots,\mathbf{p}_{j_k},\ldots,\mathbf{q}_i\ldots).$$

as *saturated* if it is null and if no other $\overline{\mathbf{z}}_i$ can be added to it without destroying its nullness. In

other words $\overline{\mathbf{Z}}_k$ is saturated if, in its expression, appear exactly n of the $\mathbf{p}_i$ and $\mathbf{q}_i$ vectors all with different indexes. A clique is said to be *maximal* if no other vertex can be added obtaining a new clique (obviously a maximum clique is also maximal). We show that the concepts are identical.

Proposition 5: *The set of saturated vectors formed with the* $\overline{\mathbf{z}}_i$ *is isomorphic to that of the maximal cliques of the corresponding graph.*

Let us suppose that the null vector $\overline{\mathbf{Z}}_k$ is saturated, obviously the set of its $\mathbf{p}_{j_i}$ vectors uniquely identify a subgraph. From its nullness we have $\overline{\mathbf{z}}_{j_i}^{\dagger}\overline{\mathbf{z}}_{j_l}=\bar{a}_{j_i j_l}=0$ for every $j_i j_l$ and the identified subgraph is a clique. To prove that this clique is also maximal let us suppose the contrary, i.e., that the vertex j_{k+1} can be added to it obtaining a larger clique. Then we would necessarily have $\bar{a}_{j_i j_{k+1}}=0$ for all j_i that would mean that the vector $\mathbf{q}_{j_{k+1}}$ would be missing from $\overline{\mathbf{Z}}_k$ violating the hypothesis that $\overline{\mathbf{Z}}_k$ is saturated.

To prove the second part of the proposition let us suppose that we have a maximal clique identified by a vector $\mathbf{x}_k \in \{0,1\}^n$; the vector $\overline{\mathbf{Z}}_k=\bar{B}\mathbf{x}_k$ is null since $0=\bar{a}_{j_i j_l}=\overline{\mathbf{z}}_{j_i}^{\dagger}\overline{\mathbf{z}}_{j_l}$ for every $j_i j_l$. Also $n-k$ of the $\mathbf{q}_i$ appear in it otherwise, as in the preceding part, one can easily contradict the hypothesis that the starting clique is maximal. It follows that $\overline{\mathbf{Z}}_k$ is saturated. □

Each saturated vector $\overline{\mathbf{Z}}_k$, made up by k $\overline{\mathbf{z}}_i$'s, can be thought of as a k-dimensional TNP (remember $\overline{\mathbf{z}}_i$'s are linearly independent) but also, using the more general definition (12), one can use the $\mathbf{p}$'s and $\mathbf{q}$'s that appear in $\overline{\mathbf{Z}}_k$ to build a maximal TNP whose spinor is pure and given by

$$\Phi(\overline{\mathbf{Z}}_k)=\mathbf{p}_{j_1}\cdots\mathbf{p}_{j_k}\cdots\mathbf{q}\cdots\Phi(\mathbb{I}):=\omega_{\bar{Z}_k} \tag{17}$$

so that each saturated vector uniquely identifies one of the pure spinors of the Fock basis (8). Thus, in our formulation, every maximal clique corresponds to a saturated vector $\overline{\mathbf{Z}}_k$ which in turn identifies one of the components of the Fock basis (8).

We remark that the $M(\Phi(\bar{Z}_k))$ has dimension n and the set of the $\mathbf{p}_i$ of $\overline{\mathbf{Z}}_k$ always allow to indicate unambiguously the maximal clique associated with it. In other words, each maximal TNP $M(\Phi(\bar{Z}_k))$ contain one and only one of the saturated vectors and thus just one maximal clique.

We show now the equivalence of the formulation of the Cartan equation.

Proposition 6: *Given a set of* x_{j_i} *that give a solution of the Cartan equation* (14) *and calling* $\overline{\mathbf{Z}}_1,\ldots,\overline{\mathbf{Z}}_p$ *all the saturated vectors such that each of them contains all the* $\overline{\mathbf{z}}_{j_i}$ *we are considering, then*

$$\left(\sum_{i=1}^{k} x_{j_i}\overline{\mathbf{z}}_{j_i}\right)\left(\sum_{l=1}^{p}\Phi(\overline{\mathbf{Z}}_l)\right)=0.$$

First of all we observe that $p\geqslant 1$ since the set of $\overline{\mathbf{z}}_{j_i}$ form a TNP and are thus contained in at least one maximal clique how shown in the constructive proof of Proposition 7. By (17) all $\Phi(\overline{\mathbf{Z}}_l)$ contain all the $\overline{\mathbf{z}}_{j_i}$ of the first sum and the proposition is proved. □

Since, as we prove in the Appendix, each graph is uniquely identified by the set of its maximal cliques it is possible to define uniquely a spinor $\Psi(\bar{A})$ associated to a given graph A: the set of all its maximal cliques defines uniquely a set of saturated vectors $\{\overline{\mathbf{Z}}_l\}$. This set defines in turn a corresponding set $\{\omega_{\mathbf{Z}_l}\}$ in the Fock basis and therefore also a spinor $\Psi(\bar{A})$ of the form (9) uniquely defined by $\bar{A}$,

$$\Psi(\bar{A})=\sum_l \xi_l\Phi(\overline{\mathbf{Z}}_l)=\sum_l \xi_l\omega_{\overline{\mathbf{Z}}_l}. \tag{18}$$

We note that in this formulations not all components are different from zero for all the values of the x_i and we can render explicit this characteristic adding to each components a product of

Kronecker delta that set it to zero when one of the components having positive scalar products with one of the $\overline{\mathbf{Z}}_l$ is present so, calling Q_l the set of the indices of q_i appearing in $\overline{\mathbf{Z}}_l$, we get:

$$\Psi(\bar{A}) = \sum_l \xi_l \omega_{\overline{\mathbf{Z}}_l} \Delta(l, x_1, x_2, \ldots, x_n)$$

with

$$\Delta(l, x_1, x_2, \ldots, x_n) = \prod_{j \in Q_l} \delta_{x_j, 0}$$

and with this definition we can now rewrite (13) as

$$\left(\sum_{i=1}^{n} x_i \overline{\mathbf{z}}_i \right) \Psi(\bar{A}) = 0.$$

For example, if $\bar{A}=0$, $\Psi(\bar{A})=\omega_0$ while for $\bar{A}=J-\mathbb{I}$, $\Psi(\bar{A})=\xi_1\omega_1+\xi_2\omega_2+\xi_4\omega_4+\ldots+\xi_{2^{n-1}}\omega_{2^{n-1}}$. In general $\Psi(\bar{A})$ will have a number of nonzero components lower than 2^n but there exist graphs with an exponential number of maximal cliques.

While $\bar{A}$ uniquely determines $\Psi(\bar{A})$, not every spinor may be conceived as generated by a graph. As an example a spinor $\Psi(\bar{A})$ may not obviously contain components in $\{\omega_1, \omega_3, \omega_7, \ldots\}$. The spinors $\Psi(\bar{A})$ generated by graphs build up a subclass of spinors whose properties should be further analyzed and they will be certainly interesting also for other fields of application of pure spinor geometry, one can conjecture that they fall in the class of generalized spinors studied in Ref. 18.

V. CONCLUSIONS

Spinors were discovered by Cartan in 1913 and soon after introduced in physics for the representation of the electron (and fermions) by Dirac and Weyl. However the geometry of pure spinors was practically ignored after the publication of Chevalley book in 1954.[10] The main motivation is that general spinors are too difficult to deal with because of the exponentially many constraint relations, for large n.

However now, after 50 years, the scenario may change and pure spinors might attract the attention of both theoretical physicists and mathematicians. The main reason of this change is that theoretical physics, since several decades, is facing insormountable difficulties in some of its central sectors like the quantization of the gravitational field or the explanation of some aspects of elementary particles phenomenology (origin of charges, families, etc.). Recently, pure spinors have been discovered to allow to overcome, somehow miraculously, some of these difficulties[2] and to allow to shed some light on some aspects of the obscure phenomenology of elementary particles.[6]

As shown by Cartan the geometry of pure spinors is correlated to that of null vectors and totally null planes, and shares the elegance and simplicity of projective geometry. We have shown that null vectors and TNP are deeply connected to graphs and formulating the MC problem in spinorial language establishes a bridge between these two worlds that, we hope, will allow to cross-fertilize both the fields. If and when, the certainly rich and elegant geometry of the pure spinors will be better known, it might contribute also to the MC problem, once this is formulated in the frame of that geometry, as proposed here.

In this paper, establishing a correspondence between totally null planes and maximal cliques, we have been able to reformulate neatly (16) the maximum clique problem and to define spinors corresponding to graphs (18). Another interesting aspect, which emerges already in this preliminary approach, is that the pure spinor defined by graphs might belong to a subclass less prone to constraint relations.

APPENDIX

Any symmetric matrix like A may be expressed as $A=B^2$ where B is a complex symmetric matrix. Since A is symmetric its eigenvalues are real and it can be diagonalized $A=O'\Lambda O$ with $O'O=OO'=\mathbb{I}$ where Λ is the diagonal matrix of the eigenvalues λ_i and O' is the orthogonal, real, matrix of the eigenvectors. Then, as it is easy to verify, a possible definition of the "square root" of A is $B=O'\sqrt{\Lambda}O$ where $\sqrt{\Lambda}$ is the diagonal matrix whose elements are the square roots of the eigenvalues of A.[12]

We observe that, unless A is semipositive definite ($\lambda_i \geqslant 0$), B is complex and the choice of the signs of the diagonal elements of $\sqrt{\Lambda}$ is arbitrary so, in general, there are at least 2^n different possible B satisfying (2): Moreover when A has multiple eigenvalues, there are infinitely many possible choices of the corresponding eigenvectors, and there are, accordingly, infinitely many possible choices for B.

We conclude by proving the following.

Proposition 7: *Each graph is uniquely identified by the set of its maximal cliques.*

To prove this assertion we provide a constructive algorithm to build A from the set of its maximal cliques. One starts from $A=0$ and add to it (in a Boolean logic fashion) all the links of each maximal clique; it is sufficient to add only the links between the nodes of a maximal clique and these links are all known, since one knows the subset of vertices that forms a maximal clique. This procedure brings to the adjacency matrix of the graph since each link appears in at least one of the maximal cliques. This last statement is proved observing that each maximal clique can be built starting from any link, and the corresponding two nodes, and adding to them, one at the time, other fully connected nodes. This proves that any link must appear in at least one maximal clique and thus the proposition. □

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A formula for the first eigenvalue of the Dirac operator on compact spin symmetric spaces

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Let G/K be a simply connected spin compact inner irreducible symmetric space, endowed with the metric induced by the Killing form of G sign-changed. We give a formula for the square of the first eigenvalue of the Dirac operator in terms of a root system of G. As an example of application, we give the list of the first eigenvalues for the spin compact irreducible symmetric spaces endowed with a quaternion-Kähler structure. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Let G/K be a compact, simply connected, n-dimensional irreducible symmetric space with G compact and simply connected, endowed with the metric induced by the Killing form of G sign-changed. Assume that G and K have the same rank and that G/K has a spin structure. Let T be a common maximal torus of G and K, and let β_k, $k=1,\ldots,p$, be the K-dominant weights with respect to T, occurring in the decomposition into irreducible components of the spin representation under the action of K. In a previous paper, cf. Ref. 9, we proved that the first eigenvalue λ of the Dirac operator verifies

$$\lambda^2 = 2 \min_{1\leqslant k\leqslant p} \|\beta_k\|^2 + n/8, \tag{1}$$

where $\|\cdot\|$ is the norm associated to the scalar product induced by the Killing form of G sign-changed.

The proof was based on a lemma of Parthasarathy in Ref. 10 which allows to express the result in the following way.

Let Φ be the set of nonzero roots of G with respect to T. Let Φ_G^+ be the set of positive roots of G, Φ_K^+ be the set of positive roots of K, with respect to a fixed lexicographic ordering in Φ. Let δ_G (respectively, δ_K) be the half-sum of the positive roots of G (respectively, K). Then the square of the first eigenvalue of the Dirac operator is given by

$$\lambda^2 = 2\min_{w\in W}\|w\cdot\delta_G - \delta_K\|^2 + n/8, \tag{2}$$

where W is the subset of the Weyl group W_G defined by

$$W := \{w \in W_G; w\cdot\Phi_G^+ \supset \Phi_K^+\}. \tag{3}$$

In order to avoid the determination of the subset W for applications, we prove in the following that the square of the first eigenvalue of the Dirac operator is indeed given by

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TABLE I. Compact Quaternion-Kähler Symmetric Spaces

G	K	G/K	$\dim G/K$	Spin structure (cf. Ref. 4)
Sp_{m+1}	$\mathrm{Sp}_m \times \mathrm{Sp}_1$	Quaternionic projective space $\mathbb{H}P^m$	$4m(m \geqslant 1)$	Yes (unique)
SU_{m+2}	$S(\mathrm{U}_m \times \mathrm{U}_2)$	Grassmannian $\mathrm{Gr}_2(\mathbb{C}^{m+2})$	$4m(m \geqslant 1)$	iff m even unique in that case
Spin_{m+4}	$\mathrm{Spin}_m\mathrm{Spin}_4$	Grassmannian $\widetilde{\mathrm{Gr}}_4(\mathbb{R}^{m+4})$	$4m(m \geqslant 3)$	iff m even, unique in that case
G_2	SO_4		8	Yes (unique)
F_4	$\mathrm{Sp}_3\mathrm{SU}_2$		28	No
E_6	$\mathrm{SU}_6\mathrm{SU}_2$		40	Yes (unique)
E_7	$\mathrm{Spin}_{12}\mathrm{SU}_2$		64	Yes (unique)
E_8	$E_7\mathrm{SU}_2$		112	Yes (unique)

$$\lambda^2 = 2 \min_{w \in W_G} \|w \cdot \delta_G - \delta_K\|^2 + n/8. \tag{4}$$

We then give a different expression to use the formula for explicit computations. We obtain

$$\lambda^2 = 2\|\delta_G - \delta_K\|^2 + 4 \sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle + n/8, \tag{5}$$

where Λ is the set

$$\Lambda := \{\theta \in \Phi_G^+; \langle \theta, \delta_K \rangle < 0\}.$$

As an example of application of the above formula, we obtain the list of the first eigenvalues of the Dirac operator for the spin compact irreducible symmetric spaces endowed with a quaternion-Kähler structure. By definition, a Riemannian manifold has a quaternion-Kähler structure if its holonomy group is contained in the group $\mathrm{Sp}_m\mathrm{Sp}_1$. In Ref. 13, Wolf gave the classification of compact quaternion-Kähler symmetric spaces (see Table I).

Note furthermore that all the symmetric spaces in Table I are "inner."

Endowing each symmetric space with the metric induced by the Killing form of G sign-changed, we obtain Table II.

The result was already known for quaternionic projective spaces $\mathbb{H}P^n$,[7] for the Grassmannians $\mathrm{Gr}_2(\mathbb{C}^{m+2})$,[8] and for the symmetric space G_2/SO_4.[11] To our knowledge, the other results are new.

TABLE II. First Eigenvalue of the Dirac Operator on Spin Compact Quaternion-Kähler Symmetric Spaces

G/K	Square of the first eigenvalue of D
$\mathbb{H}P^n = \mathrm{Sp}_{m+1}/(\mathrm{Sp}_m \times \mathrm{Sp}_1)$	$(m+3/m+2)(m/2) = (m+3/m+2)(\mathrm{Scal}/4)$
$\mathrm{Gr}_2(\mathbb{C}^{m+2}) = \mathrm{SU}_{m+2}/S(\mathrm{U}_m \times \mathrm{U}_2)$ (m even)	$(m+4/m+2)(m/2) = (m+4/m+2)(\mathrm{Scal}/4)$
$\widetilde{\mathrm{Gr}}_4(\mathbb{R}^{m+4}) = \mathrm{Spin}_{m+4}/\mathrm{Spin}_m\mathrm{Spin}_4$ (m even)	$[(m^2+6m-4)/m(m+2)](m/2) = [(m^2+6m-4)/m(m+2)](\mathrm{Scal}/4)$
G_2/SO_4	$3/2 = (3/2)(\mathrm{Scal}/4)$
$E_6/(\mathrm{SU}_6\mathrm{SU}_2)$	$41/6 = (41/30)(\mathrm{Scal}/4)$
$E_7/(\mathrm{Spin}_{12}\mathrm{SU}_2)$	$95/9 = (95/72)(\mathrm{Scal}/4)$
$E_8/(E_7\mathrm{SU}_2)$	$269/15 = (269/210)(\mathrm{Scal}/4)$

II. PROOF OF FORMULA (4)

With the notations of the introduction, and since the scalar product is W_G-invariant, one has for any $w \in W_G$,

$$\|w \cdot \delta_G - \delta_K\|^2 = \|\delta_G\|^2 + \|\delta_K\|^2 - 2\langle w \cdot \delta_G, \delta_K\rangle, \tag{6}$$

hence

$$\min_{w \in W} \|w \cdot \delta_G - \delta_K\|^2 = \|\delta_G\|^2 + \|\delta_K\|^2 - 2\max_{w \in W} \langle w \cdot \delta_G, \delta_K\rangle$$

and

$$\min_{w \in W_G} \|w \cdot \delta_G - \delta_K\|^2 = \|\delta_G\|^2 + \|\delta_K\|^2 - 2 \max_{w \in W_G} \langle w \cdot \delta_G, \delta_K\rangle.$$

So we must prove that

$$\max_{w \in W} \langle w \cdot \delta_G, \delta_K\rangle = \max_{w \in W_G} \langle w \cdot \delta_G, \delta_K\rangle. \tag{7}$$

Let

$$\Pi_G := \{\theta_1, \ldots, \theta_r\} \subset \Phi_G^+, \tag{8}$$

be the set of G-simple roots and let

$$\Pi_K := \{\theta'_1, \ldots, \theta'_l\} \subset \Phi_K^+, \tag{9}$$

be the set of K-simple roots.

Let $w_0 \in W_G$ such that

$$\langle w_0 \cdot \delta_G, \delta_K\rangle = \max_{w \in W_G} \langle w \cdot \delta_G, \delta_K\rangle. \tag{10}$$

Suppose that $w_0 \notin W$. Then we claim that there exists a K-simple root θ'_i such that $w_0^{-1} \cdot \theta'_i \notin \Phi_G^+$. Otherwise, if for any K-simple root θ'_i, $w_0^{-1} \cdot \theta'_i \in \Phi_G^+$, then since any K-positive root is a linear combination with non-negative coefficients of K-simple roots, we would have $\forall \theta' \in \Phi_K^+$, $w_0^{-1} \cdot \theta' \in \Phi_G^+$, contradicting the assumption made on w_0.

Now let σ'_i be the reflection across the hyperplane ${\theta'_i}^{\perp}$. Since $\sigma'_i \cdot \delta_K = \delta_K - \theta'_i$, (cf. for instance Corollary of Lemma B, Sec. 10.3 in Ref. 6), one gets by the W_G-invariance of the scalar product

$$\begin{aligned}\langle \sigma'_i w_0 \cdot \delta_G, \delta_K\rangle &= \langle w_0 \cdot \delta_G, \sigma'_i \cdot \delta_K\rangle = \langle w_0 \cdot \delta_G, \delta_K - \theta'_i\rangle \\ &= \langle w_0 \cdot \delta_G, \delta_K\rangle - \langle \delta_G, w_0^{-1} \cdot \theta'_i\rangle.\end{aligned}$$

But since $w_0^{-1} \cdot \theta'_i$ is a negative root of G, one has

$$w_0^{-1} \cdot \theta'_i = -\sum k_j \theta_j, \quad k_j \in \mathbb{N}.$$

Since for any G-simple root θ_j, $\sigma_j \cdot \delta_G = \delta_G - \theta_j$, where σ_j is the reflection across the hyperplane $\theta_j^{\perp}$, one has $\langle \theta_j, \delta_G\rangle = 2\langle \theta_j, \theta_j\rangle > 0$, so

$$-\langle \delta_G, w_0^{-1} \cdot \theta'_i\rangle = \sum k_j \langle \delta_G, \theta_j\rangle > 0,$$

hence

$$\langle \sigma'_i w_0 \cdot \delta_G, \delta_K\rangle > \langle w_0 \cdot \delta_G, \delta_K\rangle,$$

but that is in contradiction with the definition (10) of w_0, hence $w_0 \in W$ and

$$\max_{w\in W_G}\langle w\cdot\delta_G,\delta_K\rangle=\langle w_0\cdot\delta_G,\delta_K\rangle\leqslant\max_{w\in W}\langle w\cdot\delta_G,\delta_K\rangle\leqslant\max_{w\in W_G}\langle w\cdot\delta_G,\delta_K\rangle,$$

hence the result.

III. PROOF OF FORMULA (5)

In order to obtain the formula we will use the following result.

Lemma 3.1: *For any element w of the Weyl group* W_G,

$$w\cdot\delta_G=\delta_G-\sum_{\theta\in\Phi_G^+}k_\theta\theta,\quad k_\theta=0\ or\ 1.$$

Proof: Let $w\in W_G$. With the same notations as in the above proof, we write w in reduced form

$$w=\sigma_{i_1}\cdots\sigma_{i_k},\tag{11}$$

where σ_i is the reflection across the hyperplane $\theta_i^\perp$, $\theta_i\in\Pi_G$, and k is minimal.

Since $\sigma_{i_k}\cdot\delta_G=\delta_G-\theta_{i_k}$, one has

$$w\cdot\delta_G=\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\sigma_{i_k}\cdot\delta_G)=\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\delta_G)-\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\theta_{i_k}).$$

Now, since the expression of w is reduced, $w(\theta_{i_k})$ is a negative root, cf. for instance corollary of Lemma C, Sec. 10.3 in Ref. 6. But $w(\theta_{i_k})=-\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\theta_{i_k})$, hence $\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\theta_{i_k})$ is a positive root.

Now the element $\sigma_{i_1}\cdots\sigma_{i_{k-1}}\in W_G$ is written in reduced form, otherwise the expression (11) of w would not be reduced. Hence we may conclude as above that

$$\sigma_{i_1}\cdots\sigma_{i_{k-1}}(\delta_G)=\sigma_{i_1}\cdots\sigma_{i_{k-2}}(\delta_G)-\sigma_{i_1}\cdots\sigma_{i_{k-2}}(\theta_{i_{k-1}}),$$

where $\sigma_{i_1}\cdots\sigma_{i_{k-2}}(\theta_{i_{k-1}})$ is a positive root.

Proceeding inductively we get

$$w\cdot\delta_G=\delta_G-\sum_{\theta\in\Phi_G^+}k_\theta\theta,\quad k_\theta\in\mathbb{N}.$$

In order to conclude, we must prove that if a G-positive root θ appears in the above sum, then it appears only once.

Suppose that a G-positive root appears at least twice in the above sum, then there exist two integers p and q, $1\leqslant p<q\leqslant k-1$ such that

$$\sigma_{i_1}\cdots\sigma_{i_p}(\theta_{i_{p+1}})=\sigma_{i_1}\cdots\sigma_{i_q}(\theta_{i_{q+1}})$$

applying $\sigma_{i_{p+1}}\sigma_{i_p}\cdots\sigma_{i_1}$ to the two members of the above equation, we get

$$-\theta_{i_{p+1}}=\sigma_{i_{p+2}}\cdots\sigma_{i_q}(\theta_{i_{q+1}})\quad\text{if } p+1<q,$$

$$-\theta_{i_q}=\theta_{i_{q+1}}\quad\text{if } p+1=q.$$

So we get a contradiction, even in the first case, since $\sigma_{i_{p+2}}\cdots\sigma_{i_q}\sigma_{i_{q+1}}\in W_G$ is expressed in reduced form [otherwise the expression (11) of w would not be reduced], hence $\sigma_{i_{p+2}}\cdots\sigma_{i_q}(\theta_{i_{q+1}})$ is a positive root. □

From the above result we deduce the following.

Lemma 3.2: *Let* Λ *be the set*

$$\Lambda:=\{\theta\in\Phi_G^+;\langle\theta,\delta_K\rangle<0\}.\tag{12}$$

One has

$$\max_{w \in W_G} \langle w \cdot \delta_G, \delta_K \rangle = \langle \delta_G, \delta_K \rangle - \sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle,$$

(setting $\Sigma_{\theta \in \Lambda} \langle \theta, \delta_K \rangle = 0$, *if* $\Lambda = \emptyset$*).*

Proof: Suppose $\Lambda \neq \emptyset$. We first prove that there exists $w_0 \in W_G$ such that

$$w_0 \cdot \delta_G = \delta_G - \sum_{\theta \in \Lambda} \theta.$$

Let

$$\Phi_n^+ := \Phi_G^+ \setminus \Phi_K^+.$$

We first remark that any root in Λ belongs to Φ_n^+. Otherwise, if there exists $\theta \in \Lambda \cap \Phi_K^+$, then since θ is a combination with non-negative coefficients of simple K-roots, and since $\langle \delta_K, \theta_i' \rangle > 0$, for any K-simple root θ_i', we would have $\langle \delta_K, \theta \rangle \geqslant 0$, contradicting the fact that $\theta \in \Lambda$.

Now, consider

$$\delta_n := \frac{1}{2} \sum_{\theta \in \Phi_n^+} \theta = \delta_G - \delta_K.$$

Then

$$\delta_G - \sum_{\theta \in \Lambda} \theta = \delta_K + \left(\delta_n - \sum_{\theta \in \Lambda} \theta \right).$$

But,

$$\beta := \delta_n - \sum_{\theta \in \Lambda} \theta,$$

is a weight of the decomposition of the spin representation under the action of K, cf. Sec. 2 in Ref. 10: the weights are just the elements of the form $\delta_n - \Sigma_{\theta \in \Upsilon} \theta$, where Υ is a subset of Φ_n^+.

In fact β is the highest weight of an irreducible component in the decomposition, otherwise we would have

$$\beta + \alpha = \delta_n - \sum_{\theta \in \Upsilon} \theta,$$

where α is a K-positive root and Υ is a subset of Φ_n^+.

Hence setting $\Lambda' := \Lambda \setminus \Upsilon$ and $\Upsilon' := \Upsilon \setminus \Lambda$, we would have

$$-\sum_{\theta \in \Lambda'} \theta + \alpha = -\sum_{\theta \in \Upsilon'} \theta.$$

But since $\Lambda' \subset \Lambda$ and α is a K-positive root,

$$\langle -\sum_{\theta \in \Lambda'} \theta + \alpha, \delta_K \rangle > 0,$$

whereas since $\Upsilon' \subset \Phi_n^+ \setminus \Lambda$,

$$\langle -\sum_{\theta \in \Upsilon'} \theta, \delta_K \rangle \leqslant 0,$$

hence a contradiction.

Now by the result of Lemma 2.2 in Ref. 10, any highest weight in the decomposition of the spin representation has the form

$$w \cdot \delta_G - \delta_K,$$

where w belongs to the subset W of W_G defined in (3). Hence there exists a $w_0 \in W$ such that

$$\beta = w_0 \cdot \delta_G - \delta_K,$$

hence

$$\delta_G - \sum_{\theta \in \Lambda} \theta = \delta_K + \beta = w_0 \cdot \delta_G,$$

hence the result.

Now let w be any element in W_G. By the above lemma,

$$w \cdot \delta_G = \delta_G - \sum_{\theta \in \Phi_G^+} k_\theta \theta, \quad k_\theta = 0 \text{ or } 1,$$

$$= \delta_G - \sum_{\theta \in \Lambda} k_\theta \theta - \sum_{\theta \in \Phi_G^+ \setminus \Lambda} k_\theta \theta.$$

Hence by the definition of Λ,

$$\langle w \cdot \delta_G, \delta_K \rangle \leqslant \langle \delta_G - \sum_{\theta \in \Lambda} k_\theta \theta, \delta_K \rangle \leqslant \langle \delta_G - \sum_{\theta \in \Lambda} \theta, \delta_K \rangle.$$

Thus

$$\max_{w \in W_G} \langle w \cdot \delta_G, \delta_K \rangle \leqslant \langle \delta_G, \delta_K \rangle - \sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle = \langle w_0 \cdot \delta_G, \delta_K \rangle$$

$$\leqslant \max_{w \in W_G} \langle w \cdot \delta_G, \delta_K \rangle,$$

hence the result. □

Now going back to formula (4), we get immediately from (6) the following.

Corollary 3.3: *The first eigenvalue* λ *of the Dirac operator verifies*

$$\lambda^2 = 2\|\delta_G - \delta_K\|^2 + 4 \sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle + n/8.$$

IV. PROOF OF THE RESULTS OF TABLE I

In the following, we note for any integer $n \geqslant 1$, $(e_1, \ldots, e_n)$, the standard basis of $\mathbb{K}^n$, $\mathbb{K} = \mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$, and by (E_{ij}), $1 \leqslant i, j \leqslant n$, the standard basis of the space $\mathrm{M}_n(\mathbb{K})$ of (n,n) matrices with coefficients in $\mathbb{K}$.

A. Quaternionic projective spaces $\mathbb{H}P^n$

Here $G = \mathrm{Sp}_{m+1}$ and $K = \mathrm{Sp}_m \times \mathrm{Sp}_1$, where Sp_{m+1} is the group of symplectic matrices acting on the left on $\mathbb{H}^{n+1}$, (viewed as a right vector space on $\mathbb{H}$), and $\mathrm{Sp}_m \times \mathrm{Sp}_1$ is the subgroup of G formed by matrices of the form $\left(\begin{smallmatrix} A & 0 \\ 0 & q \end{smallmatrix}\right)$, where A is a (n,n) symplectic matrix and q a unit quaternion.

The decomposition of the spin representation into irreducible components under the action of K is known (see Refs. 1 and 12 or 7), so we may conclude with formula (1). However the result may be also simply concluded with formula (5).

We consider the standard maximal torus T of G, which is a common maximal torus of G and K. We denote by $(x_1,\ldots,x_{m+1})$, the basis dual to the standard basis of the Lie algebra $\mathfrak{T}$ of T, and by $(\hat{x}_1,\ldots,\hat{x}_{m+1})$, the corresponding basis of $i\mathfrak{T}^*$. Any vector $\mu\in i\mathfrak{T}^*$ is simply denoted by the $(m+1)$-tuple of its components in this basis: $\mu=(\mu_1,\mu_2,\ldots,\mu_{m+1})$.

The restriction to $\mathfrak{T}$ of the Killing form B of G is given by

$$\forall X\in\mathfrak{T},\ \forall\, Y\in\mathfrak{T},\quad B(X,Y)=4(m+2)\Re(\mathrm{tr}(XY)).$$

Hence the scalar product on $i\mathfrak{T}^*$ induced by the Killing form sign-changed is given by

$$\begin{aligned}&\forall\,\mu=(\mu_1,\ldots,\mu_{m+1})\in i\mathfrak{T}^*,\\ &\forall\,\mu'=(\mu'_1,\ldots,\mu'_{m+1})\in i\mathfrak{T}^*,\end{aligned}\qquad \langle\mu,\mu'\rangle=\frac{1}{4(m+2)}\sum_{k=1}^{m+1}\mu_k\mu'_k. \tag{13}$$

Now, considering the root-spaces decomposition of the complexified Lie algebra of G under the action of T, we may choose as sets of positive roots,

$$\Phi_G^+=\left\{\begin{matrix}\hat{x}_i+\hat{x}_j,\\ \hat{x}_i-\hat{x}_j,\end{matrix}\quad 1\leqslant i\leqslant j\leqslant m+1;2\hat{x}_i,\ 1\leqslant i\leqslant m+1\right\},$$

and

$$\Phi_K^+=\left\{\begin{matrix}\hat{x}_i+\hat{x}_j,\\ \hat{x}_i-\hat{x}_j,\end{matrix}\quad 1\leqslant i\leqslant j\leqslant m;2\hat{x}_i,\ 1\leqslant i\leqslant m+1\right\}.$$

Then

$$\delta_G=\sum_{k=1}^{m+1}(m+2-k)\hat{x}_k=(m+1,m,\ldots,2,1)$$

and

$$\delta_K=\sum_{k=1}^{m}(m+1-k)\hat{x}_k+\hat{x}_{m+1}=(m,m-1,\ldots,1,1).$$

Hence $\delta_G-\delta_K=\Sigma_{k=1}^m\hat{x}_k=(1,1,\ldots,1,0)$, so $\|\delta_G-\delta_K\|^2=m/[4(m+2)]$.

On the other hand, it is easy to verify that the set $\Lambda:=\{\theta\in\Phi_G^+;\langle\theta,\delta_K\rangle<0\}$ is empty, hence by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2=\frac{m}{2(m+2)}+\frac{m}{2}=\frac{m+3}{m+2}\frac{m}{2}.$$

B. Grassmannians $\mathrm{Gr}_2(\mathbb{C}^{m+2})$, m even $\geqslant 2$

Here $G=\mathrm{SU}_{m+2}$ is the group of unitary matrices with determinant 1, and K is the subgroup $S(\mathrm{U}_m\times\mathrm{U}_2)$ formed by matrices of the form $\left(\begin{smallmatrix}A&0\\0&B\end{smallmatrix}\right)$, where A and B are unitary matrices with respective sizes (m,m) and $(2,2)$ such that $\det A\det B=1$.

Here again, the decomposition into irreducible components of the spin representation under the action of K is known,[8] hence the result may be obtained from formula (1). However the result may be also simply concluded with formula (5). The standard maximal torus T of SU_{m+2} is a common maximal torus of G and K. We denote by $(x_1,\ldots,x_{m+1})$, the basis dual to the basis of the Lie algebra $\mathfrak{T}$ of T defined by the vectors $i(E_{ii}-E_{m+2m+2})$, $1\leqslant i\leqslant m+1$, and by $(\hat{x}_1,\ldots,\hat{x}_{m+1})$, the corresponding basis of $i\mathfrak{T}^*$. Any vector $\mu\in i\mathfrak{T}^*$ is denoted by the $(m+1)$-tuple of its components in this basis: $\mu=(\mu_1,\mu_2,\ldots,\mu_{m+1})$.

The restriction to $\mathfrak{T}$ of the Killing form B of G is given by

$$\forall X \in \mathfrak{T}, \quad \forall Y \in \mathfrak{T}, \quad B(X,Y) = 2(m+2)\Re(\mathrm{tr}(XY)).$$

Hence the scalar product on $i\mathfrak{T}^*$ induced by the Killing form sign changed is given by

$$\forall \mu = (\mu_1, \ldots, \mu_{m+1}) \in i\mathfrak{T}^*, \quad \forall \mu' = (\mu'_1, \ldots, \mu'_{m+1}) \in i\mathfrak{T}^*,$$

$$\langle \mu, \mu' \rangle = \frac{1}{2(m+2)} \sum_{k=1}^{m+1} \mu_k \mu'_k - \frac{1}{2(m+2)^2} \left(\sum_{k=1}^{m+1} \mu_k \right) \left(\sum_{k=1}^{m+1} \mu'_k \right). \tag{14}$$

Now, considering the root-spaces decomposition of the complexified Lie algebra of G under the action of T, we may choose as sets of positive roots

$$\Phi_G^+ = \left\{ \hat{x}_i - \hat{x}_j, 1 \leqslant i \leqslant m+1; \hat{x}_i + \sum_{k=1}^{m+1} \hat{x}_k, 1 \leqslant i \leqslant m+1 \right\},$$

and

$$\Phi_K^+ = \left\{ \hat{x}_i - \hat{x}_j, 1 \leqslant i \leqslant m; \hat{x}_{m+1} + \sum_{k=1}^{m+1} \hat{x}_k \right\}.$$

Then

$$\delta_G = \sum_{k=1}^{m+1} (m+2-k)\hat{x}_k = (m+1, m, \ldots, 2, 1)$$

and

$$\delta_K = \frac{1}{2} \left(\sum_{k=1}^{m} (m+2-2k)\hat{x}_k + 2\hat{x}_{m+1} \right) = \frac{1}{2}(m, m-2, m-4, \ldots, 2-m, 2).$$

Hence $\delta_G - \delta_K = \frac{1}{2}(m+2)\Sigma_{k=1}^{m} \hat{x}_k = \frac{1}{2}(m+2)(1, 1, \ldots, 1, 0)$, so $\|\delta_G - \delta_K\|^2 = m/4$.

We now determine the set $\Lambda := \{\theta \in \Phi_G^+; \langle \theta, \delta_K \rangle < 0\}$. Recall that from the proof of Lemma 3.2, if Λ is nonempty, then any $\theta \in \Lambda$ belongs to $\Phi_G^+ \backslash \Phi_K^+$. It is then easy to verify that the elements of Λ are

$$\hat{x}_j - \hat{x}_{m+1}, \quad \frac{m}{2} + 1 \leqslant j \leqslant m, \quad \langle \hat{x}_j - \hat{x}_{m+1}, \delta_K \rangle = \frac{1}{2(m+2)} \left(\frac{m}{2} - j \right),$$

$$\hat{x}_j + \sum_{k=1}^{m+1} \hat{x}_k, \quad \frac{m}{2} + 2 \leqslant j \leqslant m, \quad \langle \hat{x}_j + \sum_{k=1}^{m+1} \hat{x}_k, \delta_K \rangle = \frac{1}{2(m+2)} \left(\frac{m}{2} + 1 - j \right).$$

So

$$\sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle = -\frac{m^2}{8(m+2)}.$$

Hence, by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \frac{m}{2} - \frac{m^2}{2(m+2)} + \frac{m}{2} = \frac{m+4}{m+2}\frac{m}{2}.$$

C. Grassmannians $\widetilde{\mathrm{Gr}}_4(\mathbb{R}^{m+4})$, m even $\geqslant 4$

Here $G=\mathrm{Spin}_{m+4}$ and, identifying $\mathbb{R}^m$ with the subspace of $\mathbb{R}^{m+4}$ spanned by $e_1,\ldots,e_m$, and $\mathbb{R}^4$ with the subspace spanned by $e_{m+1},\ldots,e_{m+4}$, K is the subgroup of G defined by

$$\mathrm{Spin}_m\,\mathrm{Spin}_4 := \{\psi\in\mathrm{Spin}_{m+4};\psi=\varphi\phi,\varphi\in\mathrm{Spin}_m,\phi\in\mathrm{Spin}_4\}.$$

We consider the common maximal torus of G and K defined by

$$T=\left\{\sum_{k=1}^{(m/2)+2}(\cos(\beta_k)+\sin(\beta_k)e_{2k-1}\cdot e_{2k});\beta_1,\ldots,\beta_{(m/2)+2}\in\mathbb{R}\right\}.$$

We denote by $(x_1,\ldots,x_{(m/2)+2})$ the basis dual to the basis $(e_{2j-1}\cdot e_{2j})$, $1\leqslant j\leqslant(m/2)+2$, of the Lie algebra $\mathfrak{T}$ of T, and by $(\hat{x}_1,\ldots,\hat{x}_{(m/2)+2})$ the basis of $i\mathfrak{T}^*$ defined by

$$\hat{x}_k := 2ix_k,\quad k=1,\ldots,\frac{m}{2}+2.$$

Any vector $\mu\in i\mathfrak{T}^*$ is denoted by the $(m/2)+2$-tuple of its components in this basis, $\mu=(\mu_1,\mu_2,\ldots,\mu_{(m/2)+2})$.

The restriction to $\mathfrak{T}$ of the Killing form B of G is given by

$$B(e_{2k-1}\cdot e_{2k},e_{2l-1}\cdot e_{2l})=-8(m+2)\delta_{kl}.$$

Hence the scalar product on $i\mathfrak{T}^*$ induced by the Killing form sign-changed is given by

$$\begin{aligned}&\forall\mu=(\mu_1,\ldots,\mu_{\frac{m}{2}+2})\in i\mathfrak{T}^*,\\&\forall\mu'=(\mu'_1,\ldots,\mu'_{\frac{m}{2}+2})\in i\mathfrak{T}^*,\end{aligned}\quad\langle\mu,\mu'\rangle=\frac{1}{2(m+2)}\sum_{k=1}^{(m/2)+2}\mu_k\mu'_k.\tag{15}$$

Considering the root-spaces decomposition of the complexified Lie algebra of G under the action of T, we may choose as sets of positive roots

$$\Phi_G^+=\left\{\hat{x}_i+\hat{x}_j,\hat{x}_i-\hat{x}_j,1\leqslant i<j\leqslant\frac{m}{2}+2\right\},$$

and

$$\Phi_K^+=\left\{\hat{x}_i+\hat{x}_j,\hat{x}_i-\hat{x}_j,1\leqslant i<j\leqslant\frac{m}{2},\hat{x}_{(m/2)+1}+\hat{x}_{(m/2)+2},\hat{x}_{(m/2)+1}-\hat{x}_{(m/2)+2}\right\}.$$

Then

$$\delta_G=\sum_{k=1}^{(m/2)+2}\left(\frac{m}{2}+2-k\right)\hat{x}_k=\left(\frac{m}{2}+1,\frac{m}{2},\ldots,1,0\right)$$

and

$$\delta_K=\sum_{k=1}^{(m/2)}\left(\frac{m}{2}-k\right)\hat{x}_k+\hat{x}_{(m/2)+1}=\left(\frac{m}{2}-1,\frac{m}{2}-2,\ldots,1,0\right).$$

Hence $\delta_G-\delta_K=2\Sigma_{k=1}^{m/2}\hat{x}_k=2(1,1,\ldots,1,0,0)$, so $\|\delta_G-\delta_K\|^2=m/(m+2)$.

On the other hand, it is easy to verify that the set $\Lambda := \{\theta \in \Phi_G^+; \langle \theta, \delta_K \rangle < 0\}$ has only one element, namely

$$\hat{x}_{(m/2)} - \hat{x}_{(m/2)+1}, \quad \text{with } \langle \hat{x}_{(m/2)} - \hat{x}_{(m/2)+1}, \delta_K \rangle = -1.$$

Hence, by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \frac{2m}{m+2} - \frac{2}{m+2} + \frac{m}{2} = \frac{m^2+6m-4}{2(m+2)}.$$

D. The four exceptional cases

Note first that since all the groups G we consider are simple, their roots system are irreducible so, up to a constant, there is only one W_G-invariant scalar product on the subspace generated by the set of roots, cf. for instance Remark (5.10), Sec. V in Ref. 3.

We use the description of root systems given in Ref. 2. Those root systems are expressed in the simple root basis (α_i). Note that the W_G-invariant scalar product $(,)$ used there is such that $(\alpha, \alpha) = 2$ for any long root α. In order to compare it with the scalar product $\langle , \rangle$ induced by the Killing form sign-changed, we use the "strange formula" of Freudenthal and de Vries, (cf. 47-11 in Ref. 5):

$$\langle \delta_G, \delta_G \rangle = \tfrac{1}{24} \dim G. \tag{16}$$

To determine the set of K-positive roots, we use Theorem 13, Theorem 14, and the proof of Theorem 18 in Ref. 4. By those results, the set Φ_K^+ may be defined as follows. Let $\theta = \Sigma m_i \alpha_i$ be the highest root. In all cases considered, there exists an index j such that $m_j = 2$. Then

$$\Phi_K^+ = \left\{ \sum n_i \alpha_i ; n_j \neq 1 \right\}.$$

1. The symmetric space G_2/SO_4

Using the results of pages 18 and 64 in Ref. 2, we get

$$\delta_G = 3\alpha_1 + 5\alpha_2.$$

By the expression of the Cartan matrix, the scalar product matrix is, in the basis (α_1, α_2), $\left(\begin{smallmatrix} 2 & -1 \\ -1 & 2/3 \end{smallmatrix}\right)$, hence $\|\delta_G\|_{(,)}^2 = \frac{14}{3}$. On the other hand, by the formula of Freudenthal and de Vries, $\|\delta_G\|_{\langle , \rangle}^2 = \frac{7}{12}$, so $\langle , \rangle = \frac{1}{8}(,)$.

The set of K-positive roots is $\Phi_K^+ = \{2\alpha_1 + 3\alpha_2, \alpha_2\}$, hence $\delta_K = \alpha_1 + 2\alpha_2$, so $\delta_G - \delta_K = 2\alpha_1 + 3\alpha_2$. Hence

$$\|\delta_G - \delta_K\|_{\langle , \rangle}^2 = \tfrac{1}{8}\|\delta_G - \delta_K\|_{(,)}^2 = \tfrac{1}{4}.$$

Finally, it is easy to verify that the set $\Lambda := \{\theta \in \Phi_G^+; \langle \theta, \delta_K \rangle < 0\}$ is empty, hence by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \tfrac{1}{2} + 1 = \tfrac{3}{2}.$$

2. The symmetric space $E_6/(SU_6SU_2)$

Using the results of pages 14 and 60 in Ref. 2, we get

$$\delta_G = 8\alpha_1 + 15\alpha_2 + 21\alpha_3 + 15\alpha_4 + 8\alpha_5 + 11\alpha_6.$$

Since all roots have same length equal to 2, we may introduce the fundamental weight basis (ω_i) because $(\omega_i, \alpha_j) = \delta_{ij}$.

Since $\delta_G = \Sigma \omega_i$, we get $\|\delta_G\|^2_{(,)} = 78$, whereas by the formula of Freudenthal and de Vries, $\|\delta_G\|^2_{\langle,\rangle} = \frac{78}{24}$, so $\langle,\rangle = \frac{1}{24}(,)$.

The set of K-positive roots may be defined by $\Phi^+_K = \{\Sigma_{i=1}^6 n_i \alpha_i; n_6 \neq 1\}$.

Then $\delta_K = 3\alpha_1 + 5\alpha_2 + 6\alpha_3 + 5\alpha_4 + 3\alpha_5 + \alpha_6 = \omega_1 + \omega_2 + \omega_3 + \omega_4 + \omega_5 - 4\omega_6$.

Hence $\delta_G - \delta_K = 5\alpha_1 + 10\alpha_2 + 15\alpha_3 + 10\alpha_4 + 5\alpha_5 + 10\alpha_6 = 5\omega_6$. So

$$\|\delta_G - \delta_K\|^2_{\langle,\rangle} = \tfrac{1}{24}\|\delta_G - \delta_K\|^2_{(,)} = \tfrac{25}{12}.$$

On the other hand, it is easy to verify that the set $\Lambda := \{\theta \in \Phi^+_G; \langle \theta, \delta_K \rangle < 0\}$ has seven elements, and that

$$\sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle = \tfrac{1}{24} \sum_{\theta \in \Lambda} (\theta, \delta_K) = -\tfrac{7}{12}.$$

So by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \tfrac{50}{12} - \tfrac{28}{12} + 5 = \tfrac{41}{6}.$$

3. The symmetric space $E_7/(\mathrm{Spin}_{12}\mathrm{SU}_2)$

By the results of pages 15 and 61 in Ref. 2, we get

$$\delta_G = \tfrac{1}{2}(34\alpha_1 + 66\alpha_2 + 96\alpha_3 + 75\alpha_4 + 52\alpha_5 + 27\alpha_6 + 49\alpha_7).$$

Here again, since all roots have the same length equal to 2, we may consider the fundamental weight basis (ω_i). We get $\|\delta_G\|^2_{(,)} = \frac{399}{2}$, whereas by the formula of Freudenthal and de Vries, $\|\delta_G\|^2_{\langle,\rangle} = \frac{133}{24}$, so $\langle,\rangle = \frac{1}{36}(,)$.

The set of K-positive roots may be defined by $\Phi^+_K = \{\Sigma_{i=1}^7 n_i \alpha_i; n_1 \neq 1\}$. Then

$$\delta_K = \tfrac{1}{2}(2\alpha_1 + 18\alpha_2 + 32\alpha_3 + 27\alpha_4 + 20\alpha_5 + 11\alpha_6 + 17\alpha_7)$$

$$= -7\omega_1 + \omega_2 + \omega_3 + \omega_4 + \omega_5 + \omega_6 + \omega_7.$$

Hence $\delta_G - \delta_K = 16\alpha_1 + 24\alpha_2 + 32\alpha_3 + 24\alpha_4 + 16\alpha_5 + 8\alpha_6 + 16\alpha_7 = 8\omega_6$. So

$$\|\delta_G - \delta_K\|^2_{\langle,\rangle} = \tfrac{1}{36}\|\delta_G - \delta_K\|^2_{(,)} = \tfrac{32}{9}.$$

On the other hand, it can be verified that the set $\Lambda := \{\theta \in \Phi^+_G; \langle \theta, \delta_K \rangle < 0\}$ has 13 elements, and that

$$\sum_{\theta \in \Lambda} \langle \theta, \delta_K \rangle = \frac{1}{36} \sum_{\theta \in \Lambda} (\theta, \delta_K) = -\frac{41}{36}.$$

So by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \tfrac{64}{9} - \tfrac{41}{9} + 8 = \tfrac{95}{9}.$$

4. The symmetric space $E_8/(E_7\mathrm{SU}_2)$

By the results of pages 16, 62, and 63 in Ref. 2, we get

$$\delta_G = 29\alpha_1 + 57\alpha_2 + 84\alpha_3 + 110\alpha_4 + 135\alpha_5 + 91\alpha_6 + 46\alpha_7 + 68\alpha_8.$$

Here again, since all roots have the same length equal to 2, we may consider the fundamental weight basis (ω_i). We get $\|\delta_G\|^2_{(,)}=620$, whereas by the formula of Freudenthal and de Vries, $\|\delta_G\|^2_{\langle,\rangle}=\frac{31}{3}$, so $\langle,\rangle=\frac{1}{60}(,)$.

The set of K-positive roots may be defined by $\Phi_K^+=\{\Sigma_{i=1}^8 n_i\alpha_i; n_1 \neq 1\}$. Then

$$\delta_K = \alpha_1 + 15\ \alpha_2 + 28\alpha_3 + 40\alpha_4 + 51\alpha_5 + 35\alpha_6 + 18\alpha_7 + 26\alpha_8$$

$$= -13\omega_1 + \omega_2 + \omega_3 + \omega_4 + \omega_5 + \omega_6 + \omega_7 + \omega_8.$$

Hence

$$\delta_G - \delta_K = 28\alpha_1 + 42\alpha_2 + 56\alpha_3 + 70\alpha_4 + 84\alpha_5 + 56\alpha_6 + 28\alpha_7 + 42\alpha_8 = 14\omega_6.$$

So

$$\|\delta_G - \delta_K\|^2_{\langle,\rangle} = \tfrac{1}{60}\|\delta_G - \delta_K\|^2_{(,)} = \tfrac{98}{15}.$$

On the other hand, it can be verified that the set $\Lambda := \{\theta \in \Phi_G^+; \langle\theta, \delta_K\rangle < 0\}$ has 25 elements, and that

$$\sum_{\theta\in\Lambda} \langle\theta, \delta_K\rangle = \frac{1}{60}\sum_{\theta\in\Lambda} (\theta, \delta_K) = -\frac{137}{60}.$$

So by formula (5), the square of the first eigenvalue λ of the Dirac operator is given by

$$\lambda^2 = \tfrac{196}{15} - \tfrac{137}{15} + 14 = \tfrac{269}{15}.$$

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Trace functions as Laplace transforms

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We study trace functions on the form $t \to \mathrm{Tr}\, f(A+tB)$ where f is a real function defined on the positive half-line, and A and B are matrices such that A is positive definite and B is positive semidefinite. If f is non-negative and operator monotone decreasing, then such a trace function can be written as the Laplace transform of a positive measure. The question is related to the Bessis-Moussa-Villani conjecture. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2186925]

I. INTRODUCTION

The Gibbs density matrix of a system with Hamiltonian H in equilibrium and temperature $kT=1/\beta$ is given by $\exp(-\beta H)$. One would like to study perturbations $H_0+\lambda H_1$ of an exactly solvable Hamiltonian H_0 and see how the thermodynamical quantities are changed. This question was studied by Bessis, Moussa and Villani in Ref. 2 where it is noted that the Padé approximant to the partition function $Z(\beta)=\mathrm{Tr}\exp(-\beta(H_0+\lambda H_1))$ may be efficiently calculated, if the function

$$\lambda \to \mathrm{Tr}\exp(-\beta(H_0+\lambda H_1))$$

is the Laplace transform of a positive measure. The authors then noted that this is indeed true for a system of spinless particles with local interactions bounded from below. The statement also holds if H_0 and H_1 are commuting operators, or if they are just 2×2 matrices. These observations led to the formulation of the following conjecture:

Conjecture (BMV): Let A and B be $n\times n$ matrices for some natural number n, and suppose that A is self-adjoint and B is positive semidefinite. Then there is a positive measure μ with support in the closed positive half-axis such that

$$\mathrm{Tr}\exp(A-tB)=\int_0^\infty e^{-ts}\,d\mu(s)$$

for every $t\geqslant 0$.

The Bessis-Moussa-Villani (BMV) conjecture may be reformulated as an infinite series of inequalities.

Theorem (Bernstein): *Let f be a real C^∞-function defined on the positive half-axis. If f is completely monotone, that is*

$$(-1)^n f^{(n)}(t)\geqslant 0,\quad t>0,\ n=0,1,2,\ldots,$$

then there exists a positive measure μ on the positive half-axis such that

$$f(t)=\int_0^\infty e^{-st}\,\mathrm{d}\mu(s)$$

for every $t>0$.

The BMV conjecture is thus equivalent to saying that the function

$$f(t) = \mathrm{Tr}\exp(A - tB), \quad t > 0$$

is completely monotone. A proof of Bernstein's theorem can be found in Ref. 4.

Assuming the BMV conjecture one may derive a similar statement for free semicircularly distributed elements in a type II_1 von Neumann algebra with a faithful trace. This consequence of the conjecture has been proved by Fannes and Petz.[6] A hypergeometric approach by Drmota, Schachermayer, and Teichmann[5] gives a proof of the BMV-conjecture for some types of 3×3 matrices.

Equivalent formulations: The BMV conjecture can be stated in several equivalent forms.

Theorem 1.1: *The following conditions are equivalent*:

(i) *For arbitrary $n\times n$ matrices A and B such that A is self-adjoint and B is positive semidefinite the function $f(t)=\mathrm{Tr}\exp(A-tB)$, defined on the positive half-axis, is the Laplace transform of a positive measure supported in $[0,\infty)$.*

(ii) *For arbitrary $n\times n$ matrices A and B such that A is self-adjoint and B is positive semidefinite the function $g(t)=\mathrm{Tr}\exp(A+itB)$, defined on the positive half-axis, is of positive type.*

(iii) *For arbitrary positive definite $n\times n$* matrices A and B *the polynomial $P(t)=\mathrm{Tr}(A+tB)^p$ has non-negative coefficients for any $p=1,2,\ldots$.*

(iv) *For arbitrary positive definite $n\times n$ matrices A and B the function $\varphi(t)=\mathrm{Tr}\exp(A+tB)$ is m-positive on some open interval of the form $(-\alpha,\alpha)$.*

The first statement is the BMV-conjecture, and it readily implies the second statement by analytic continuation. The sufficiency of the second statement is essentially Bochner's theorem. The implication (iii)$\Rightarrow$(i) is obtained by applying Bernstein's theorem and approximation of the exponential function by its Taylor expansion. The implication (i)$\Rightarrow$(iii) was proved by Lieb and Seiringer.[15] A function $\varphi:(-\alpha,\alpha)\to\mathbf{R}$ is said to be m-positive, if for arbitrary self-adjoint $k\times k$ matrices X with non-negative entries and spectra contained in $(-\alpha,\alpha)$ the matrix $\varphi(X)$ has non-negative entries. The implication (iii)$\Rightarrow$(iv) follows by approximation, while the implication (iv)$\Rightarrow$(i) follows by Bernstein's theorem and Ref. 8. Theorem 3.3 which states that an m-positive function is real analytic with non-negative derivatives in zero.

II. PRELIMINARIES AND MAIN RESULT

Let f be a real function of one variable defined on a real interval I. We consider for each natural number n the associated matrix function $x\to f(x)$ defined on the set of self-adjoint matrices of order n with spectra in I. The matrix function is defined by setting

$$f(x) = \sum_{i=1}^{p} f(\lambda_i)P_i, \quad \text{where } x = \sum_{i=1}^{p}\lambda_i P_i$$

is the spectral resolution of x. The matrix function $x\to f(x)$ is Fréchet differentiable[7] if I is open and f is continuously differentiable.[3] The norm of the Fréchet differential $\mathrm{d}f(x)$ may be an unbounded function of the order n, cf. Refs. 19 and 18. If however f is assumed to be twice differentiable, then the norm of $\mathrm{d}f(x)$ is bounded independently of the order n for all self-adjoint matrices x with spectra contained in a fixed compact subset of I, cf. Ref. 9 Corollary 2.9 and Ref. 12. We consider in this paper the function

$$\varphi(x) = \mathrm{Tr}\, f(x)$$

defined on the set of self-adjoint matrices of order n with spectra in I. The Fréchet differential is given by $\mathrm{d}\varphi(x)=\mathrm{Tr}\,\mathrm{d}f(x)$, cf. Ref. 10.

The BMV property:

Definition 2.1: A function $f:\mathbf{R}_+\to\mathbf{R}$ is said to have the BMV property, if to each $n=1,2,\ldots$ and each pair of $n\times n$ matrices A and B, such that A is positive definite and B is positive semidefinite, there is a positive measure μ with support in $[0,\infty)$ such that

$$\operatorname{Tr} f(A+tB) = \int_0^\infty e^{-st}\, \mathrm{d}\mu(s)$$

for every $t>0$.

The BMV-conjecture is thus equivalent to the statement that the function $t \to \exp(-t)$ has the BMV property. The main contribution of this paper is the following result.

Main Theorem: *Every non-negative operator monotone decreasing function defined on the open positive half-line has the BMV property*.

III. DIFFERENTIAL ANALYSIS

A simple proof of the following result can be found in Ref. 12, Proposition 1.3.

Proposition 3.1: The Fréchet differential of the exponential operator function $x \to \exp(x)$ *is given by*

$$d\exp(x)h = \int_0^1 \exp(sx)h\exp((1-s)x)\mathrm{d}s = \int_0^1 A(s)\exp(x)\mathrm{d}s,$$

where $A(s)=\exp(sx)h\exp(-sx)$ *for* $s \in \mathbf{R}$.

This is only a small part of the Dyson formula which contains formalisms developed earlier by Tomonaga, Schwinger, and Feynman. The subject was given a rigorous mathematical treatment by Araki in terms of expansionals in Banach algebras. In particular Ref. 1, Theorem 3, the expansional

$$E_r(h;x) = \sum_{n=0}^{\infty} \int_0^1 \int_0^{s_1} \cdots \int_0^{s_{n-1}} A(s_n)A(s_{n-1})\cdots A(s_1)\mathrm{d}s_n\, \mathrm{d}s_{n-1}\cdots \mathrm{d}s_1$$

is absolutely convergent in the norm topology with limit

$$E_r(h;x) = \exp(x+h)\exp(-x).$$

We therefore obtain the pth Fréchet differential of the exponential operator function by the expression

$$d^p \exp(x)h^p = p! \int_0^1 \int_0^{s_1} \cdots \int_0^{s_{p-1}} A(s_p)A(s_{p-1})\cdots A(s_1)\exp(x)\mathrm{d}s_p\, \mathrm{d}s_{p-1}\cdots \mathrm{d}s_1.$$

Divided differences: The following representation of divided differences is due to Hermite,[13] confer also Refs. 17 and 16.

Proposition 3.2: Divided differences can be written in the following form:

$$[x_0,x_1]_f = \int_0^1 f'((1-t_1)x_0 + t_1x_1)\mathrm{d}t_1,$$

$$[x_0,x_1,x_2]_f = \int_0^1 \int_0^{t_1} f''((1-t_1)x_0 + (t_1-t_2)x_1 + t_2x_2)\mathrm{d}t_2\, \mathrm{d}t_1,$$

$$\vdots$$

$$[x_0,x_1,\ldots,x_n]_f = \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} f^{(n)}((1-t_1)x_0 + (t_1-t_2)x_1 + \cdots + (t_{n-1}-t_n)x_{n-1} + t_nx_n)\mathrm{d}t_n \cdots \mathrm{d}t_2\, \mathrm{d}t_1,$$

where f is an n-times continuously differential function defined on an open interval I, and $x_0, x_1, \dots, x_n$ are (not necessarily distinct) points in I.

Lemma 3.3: For $k=1,2,\dots$ and real numbers $\lambda_1, \dots, \lambda_k$ we have

$$\int_0^t e^{-\mu s}[s\lambda_1, \dots, s\lambda_k]_{\exp} s^{k-1}\, \mathrm{d}s = t^k e^{-\mu t}\,[t\lambda_1, \cdots, t\lambda_k, t\mu]_{\exp}$$

for any real μ and $t \geqslant 0$.

Proof: For $k=1$ we calculate

$$\int_0^t e^{-\mu s}[s\lambda_1]_{\exp}\, \mathrm{d}s = \int_0^t e^{s(\lambda_1-\mu)}\, \mathrm{d}s = t\, e^{-\mu t}\,[t\lambda_1, t\mu]_{\exp}.$$

Assuming the formula valid for k we obtain for $k+1$ the expression

$$\begin{aligned}
&\int_0^t e^{-\mu s}\,[s\lambda_1, \dots, s\lambda_{k+1}]_{\exp} s^k\, \mathrm{d}s \\
&\quad = \int_0^t e^{-\mu s} \frac{[s\lambda_1, \dots, s\lambda_k]_{\exp} - [s\lambda_2, \dots, s\lambda_{k+1}]_{\exp}}{s\lambda_1 - s\lambda_{k+1}} s^k\, \mathrm{d}s \\
&\quad = \frac{1}{\lambda_1 - \lambda_{k+1}} (t^k e^{-\mu t}\,[t\lambda_1, \dots, t\lambda_k, t\mu]_{\exp} - t^k e^{-\mu t}\,[t\lambda_2, \dots, t\lambda_{k+1}, t\mu]_{\exp}) \\
&\quad = t^{k+1} e^{-\mu t}\,[t\lambda_1, \dots, t\lambda_{k+1}, t\mu]_{\exp}
\end{aligned}$$

provided $\lambda_1 \neq \lambda_{k+1}$. The case $\lambda_1 = \lambda_{k+1}$ then follows by continuity, and the lemma is proved by induction. Q.E.D.

Theorem 3.4: *Let x and h be operators on a Hilbert space of finite dimension n written on the form*

$$x = \sum_{i=1}^n \lambda_i e_{ii} \quad \text{and } h = \sum_{i,j=1}^n h_{ij} e_{ij},$$

where $\{e_{ij}\}_{i,j=1}^n$ is a system of matrix units, and $\lambda_1, \dots, \lambda_n$ and $h_{i,j}$ for $i,j=1,\dots,n$ are complex numbers. Then the pth derivative

$$\frac{d^p}{\mathrm{d}t^p} \mathrm{Tr} \exp(x+th)\bigg|_{t=0} = p! \sum_{i_1=1}^n \cdots \sum_{i_p=1}^n h_{i_p i_{p-1}} \cdots h_{i_2 i_1} h_{i_1 i_p} [\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_p}, \lambda_{i_p}]_{\exp},$$

where $[\lambda_{i_1}, \lambda_{i_2}, \dots, \lambda_{i_p}, \lambda_{i_p}]_{\exp}$ are divided differences of order $p+1$ of the exponential function.

Proof: We first prove the formulas

$$\begin{aligned}
I_k(s_0) &= \int_0^{s_0} \int_0^{s_1} \cdots \int_0^{s_{k-1}} A(s_k) A(s_{k-1}) \cdots A(s_1)\, \mathrm{d}s_k\, \mathrm{d}s_{k-1} \cdots \mathrm{d}s_1 \\
&= s_0^k \sum_{j=1}^n \sum_{i_1=1}^n \cdots \sum_{i_k=1}^n h_{i_k i_{k-1}} h_{i_{k-1} i_{k-2}} \cdots h_{i_2 i_1} h_{i_1 j}\, e^{-s_0 \lambda_j} [s_0\lambda_{i_1}, \dots, s_0\lambda_{i_k}, s_0\lambda_j]_{\exp}\, e_{i_k j} \qquad (1)
\end{aligned}$$

for natural numbers $k=1,\dots,p$ and real numbers $s_0 \geqslant 0$. For $k=1$ we calculate the integral

$$
\begin{aligned}
I_1(s_0) &= \int_0^{s_0} A(s_1)\mathrm{d}s_1 \\
&= \int_0^{s_0} \exp(s_1 x) h \exp(-s_1 x)\mathrm{d}s_1 \\
&= \sum_{i_1=1}^{n}\sum_{j=1}^{n} h_{i_1 j}\int_0^{s_0} \exp(s_1 x) e_{i_1 j} \exp(-s_1 x)\mathrm{d}s_1 \\
&= \sum_{i_1=1}^{n}\sum_{j=1}^{n} h_{i_1 j}\int_0^{s_0} \exp(s_1(\lambda_{i_1}-\lambda_j)) e_{i_1 j}\, \mathrm{d}s_1 \\
&= s_0 \sum_{j=1}^{n}\sum_{i_1=1}^{n} h_{i_1 j} e^{-s_0\lambda_j}[s_0\lambda_{i_1}, s_0\lambda_j]_{\exp}\, e_{i_1 j}
\end{aligned}
$$

in accordance with (1). For $k \geqslant 2$ and assuming the formulas (1) valid for $k-1$ we obtain the expression

$$
\begin{aligned}
I_k(s_0) &= \int_0^{s_0}\int_0^{s_1}\cdots\int_0^{s_{k-1}} A(s_k)A(s_{k-1})\cdots A(s_1)\mathrm{d}s_k\cdots \mathrm{d}s_2\, \mathrm{d}s_1 \\
&= \int_0^{s_0} I_{k-1}(s_1)A(s_1)\mathrm{d}s_1 \\
&= \int_0^{s_0} s_1^{k-1} \sum_{m,i_2,\cdots,i_k=1}^{n} h_{i_k i_{k-1}}\cdots h_{i_3 i_2} h_{i_2 m}\, e^{-s_1\lambda_m}[s_1\lambda_{i_2}, \ldots, s_1\lambda_{i_k}, s_1\lambda_m]_{\exp}\, e_{i_k m}\, A(s_1)\mathrm{d}s_1.
\end{aligned}
$$

We then insert

$$
A(s_1) = \sum_{i_1=1}^{n}\sum_{j=1}^{n} h_{i_1 j} \exp(s_1(\lambda_{i_1}-\lambda_j)) e_{i_1 j}
$$

and using $e_{i_k m} e_{i_1 j} = \delta(m, i_1) e_{i_k j}$ and the symmetry of the divided difference we obtain the expression

$$
\sum_{j,i_1,i_2,\ldots,i_k=1}^{n} h_{i_k i_{k-1}}\cdots h_{i_2 i_1} h_{i_1 j}\int_0^{s_0} e^{-s_1\lambda_j}[s_1\lambda_{i_1}, s_1\lambda_{i_2}, \ldots, s_1\lambda_{i_k}]_{\exp}\, s_1^{k-1}\, \mathrm{d}s_1\, e_{i_k j}
$$

for $I_k(s_0)$. Finally, using Lemma 3.3 we calculate

$$
I_k(s_0) = s_0^k \sum_{j,i_1,i_2,\ldots,i_k=1}^{n} h_{i_k i_{k-1}}\cdots h_{i_2 i_1} h_{i_1 j} e^{-s_0\lambda_j}\,[s_0\lambda_{i_1}, \ldots, s_0\lambda_{i_k}, s_0\lambda_j]_{\exp}\, e_{i_k j}
$$

which proves (1) by induction. We next observe that

$$
d^p \exp(x) h^p = p!\, I_p(1)\exp(x),
$$

where differentiation is with respect to x when nothing else is indicated. Finally, since

$$
\frac{d^p}{\mathrm{d}t^p}\exp(x+th) = d^p_{x+th}\exp(x+th)h^p
$$

we obtain

$$\frac{d^p}{dt^p}\mathrm{Tr}\exp(x+th)\bigg|_{t=0} = \mathrm{Tr}(d^p\exp(x)h^p) = p!\ \mathrm{Tr}(I_p(1)\exp(x))$$

$$= p!\ \mathrm{Tr}\left[\sum_{j,i_1,i_2,\ldots,i_p=1}^{n} h_{i_p i_{p-1}}\cdots h_{i_2 i_1}h_{i_1 j}e^{-\lambda_j}[\lambda_{i_1},\ldots,\lambda_{i_p},\lambda_j]_{\exp}\, e_{i_p j}\exp(x)\right]$$

$$= p!\sum_{i_1,i_2,\ldots,i_p=1}^{n} h_{i_p i_{p-1}}\cdots h_{i_2 i_1}h_{i_1 i_p}[\lambda_{i_1},\ldots,\lambda_{i_p},\lambda_{i_p}]_{\exp}$$

which is the statement of the theorem. Q.E.D.

Lemma 3.5: Let $f\in C_\infty(\mathbf{R})$, and let x and h be self-adjoint operators on a (possibly infinite dimensional) Hilbert space H. Then the operator function $x\to f(x)$ is infinitely Fréchet differentiable and the pth Fréchet differential is for $p\geqslant 1$ given by

$$d^p f(x)h^p = \int_{-\infty}^{\infty} d_x^p \exp(-isx)h^p\tilde{f}(s)\mathrm{d}s,$$

where d_x indicates differentiation with respect to x and

$$\tilde{f}(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(its)f(t)\mathrm{d}t$$

is the Fourier transform of f.

Proof: We note that the statement is true for $p=1$ by Ref. 12, Theorem 1.5 and assume the statement of the lemma to be valid for p. It follows from the definition of the Fréchet differential that the expression

$$d^p_{x+h}\exp(-is(x+h))h^p - d_x^p\exp(-isx)h^p - d_x(d_x^p\exp(-isx)h^p)h$$

even after division by $\|h\|$ tend to zero as $h\to 0$. We then multiply the above expression by the Fourier transform $\tilde{f}$ and integrate. By Lebesgues's theorem of dominated convergence we therefore obtain that also the expression

$$d^p_{x+h}f(x+h)h^p - d_x^p f(x)h^p - \int_{-\infty}^{\infty} d_x(d_x^p\exp(-isx)h^p)h\tilde{f}(s)\mathrm{d}s,$$

even after division by $\|h\|$, tend to zero as $h\to 0$. Hence

$$d_x^{p+1}f(x)h^{p+1} = \int_{-\infty}^{\infty} d_x^{p+1}\exp(-isx)h^{p+1}\tilde{f}(s)\mathrm{d}s$$

and the lemma is proved by induction. Q.E.D.

In the next corollary we need the identity,

$$t^{p-1}[t\lambda_1,\ldots,t\lambda_p]_f = [\lambda_1,\ldots,\lambda_p]_{f_t},\quad \text{where } f_t(s)=f(ts), \tag{2}$$

valid for p times continuously differentiable functions f. The statement is easily proved by induction after p.

Corollary 3.6: Let $f:I\to\mathbf{R}$ be a C^∞-function defined on an open and bounded interval I, and let x and h be self-adjoint operators on a Hilbert space of finite dimension n written in the forms

$$x=\sum_{i=1}^{n}\lambda_i e_{ii}\quad \textit{and}\ h=\sum_{i,j=1}^{n}h_{ij}e_{ij},$$

where $\{e_{ij}\}_{i,j=1}^n$ is a system of matrix units, and $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of x counted with

multiplicity. If the spectrum of x is in I, then the trace function $t \to \mathrm{Tr}\, f(x+th)$ is infinitely differentiable in a neighborhood of zero and the pth derivative

$$\left.\frac{d^p}{dt^p}\mathrm{Tr}\, f(x+th)\right|_{t=0} = p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} h_{i_1 i_2} h_{i_2 i_3} \cdots h_{i_{p-1} i_p} h_{i_p i_1} [\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_p}, \lambda_{i_1}]_f,$$

where $[\lambda_{i_1}, \lambda_{i_2}, \ldots, \lambda_{i_p}, \lambda_{i_1}]_f$ are divided differences of order $p+1$ of the function f.

Proof: Since the spectrum $\mathrm{Sp}(x)$ is compact, there is an open and bounded interval J such that

$$\mathrm{Sp}(x) \subset J \subset \bar{J} \subset I$$

and we may extend the restriction $f|_J$ to a function $g \in C_\infty(\mathbf{R})$. Since the spectrum $\mathrm{Sp}(x+th)$ is contained in J for small t we obtain

$$\begin{aligned}
\left.\frac{d^p}{dt^p}\mathrm{Tr}\, f(x+th)\right|_{t=0} &= \left.\frac{d^p}{dt^p}\mathrm{Tr}\, g(x+th)\right|_{t=0} \\
&= \int_{-\infty}^{\infty} \left.\frac{d^p}{dt^p}\mathrm{Tr}\exp(-isx-isth)\right|_{t=0} \tilde{g}(s)\,ds \\
&= \int_{-\infty}^{\infty} p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} (-is)^p h_{i_p i_{p-1}} \cdots h_{i_2 i_1} h_{i_1 i_p} \\
&\quad \times [-is\lambda_{i_1}, \ldots, -is\lambda_{i_p}, -is\lambda_{i_p}]_{\exp}\, \tilde{g}(s)\,ds \\
&= p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} h_{i_p i_{p-1}} \cdots h_{i_2 i_1} h_{i_1 i_p} \int_{-\infty}^{\infty} [\lambda_{i_1}, \ldots, \lambda_{i_p}, \lambda_{i_p}]_{\exp(-is\cdot)} \tilde{g}(s)\,ds \\
&= p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} h_{i_p i_{p-1}} \cdots h_{i_2 i_1} h_{i_1 i_p} [\lambda_{i_1}, \ldots, \lambda_{i_p}, \lambda_{i_p}]_g\, ds,
\end{aligned}$$

where $\tilde{g}$ is the Fourier transform of g, and we used (2) and the linearity in g of arbitrary divided differences $[\lambda_1, \ldots, \lambda_p]_g$. The statement now follows by noting that $f=g$ in a neighborhood of the spectrum of x. Q.E.D.

IV. PROOF OF THE MAIN THEOREM

Proposition 4.1: Consider for a constant $c \geqslant 0$ the function

$$g(t) = \frac{1}{c+t}, \quad t > 0.$$

For arbitrary $n \times n$ matrices x and h such that x is positive definite and h is positive semidefinite we have

$$(-1)^p \left.\frac{d^p}{dt^p}\mathrm{Tr}\, g(x+th)\right|_{t=0} \geqslant 0$$

for $p=1,2,\ldots$.

Proof: We first note that the divided differences of g are of the form

$$[\lambda_1,\lambda_2,\ldots,\lambda_p]_g=(-1)^{p-1}g(\lambda_1)g(\lambda_2)\cdots g(\lambda_p),\quad p=1,2,\ldots \tag{3}$$

for arbitrary positive numbers $\lambda_1,\lambda_2,\ldots,\lambda_p$. There is nothing to prove for $p=1$. Assume the statement true for $p\geqslant 2$ and notice that

$$\frac{g(\lambda)-g(\mu)}{\lambda-\mu}=\frac{(c+\lambda)^{-1}-(c+\mu)^{-1}}{\lambda-\mu}=-g(\lambda)g(\mu)$$

for $\lambda\neq\mu$. Therefore

$$\begin{aligned}[\lambda_1,\ldots,\lambda_p,\lambda_{p+1}]_g&=\frac{[\lambda_1,\ldots,\lambda_p]_g-[\lambda_2,\ldots,\lambda_{p+1}]_g}{\lambda_1-\lambda_{p+1}}\\&=(-1)^{p-1}g(\lambda_2)\cdots g(\lambda_p)\frac{g(\lambda_1)-g(\lambda_{p+1})}{\lambda_1-\lambda_{p+1}}\\&=(-1)^p g(\lambda_1)\cdots g(\lambda_p)g(\lambda_{p+1})\end{aligned}$$

for $\lambda_1\neq\lambda_{p+1}$ and the general case follows by approximation. Next, applying Corollary 3.6 we obtain

$$\begin{aligned}&\frac{d^p}{dt^p}\mathrm{Tr}\,g(x+th)\bigg|_{t=0}\\&=p!\sum_{i_1=1}^n\cdots\sum_{i_p=1}^n h_{i_1i_2}h_{i_2i_3}\cdots h_{i_{p-1}i_p}h_{i_pi_1}[\lambda_{i_1},\lambda_{i_2},\ldots,\lambda_{i_p},\lambda_{i_1}]_g\\&=(-1)^p p!\sum_{i_1=1}^n\cdots\sum_{i_p=1}^n h_{i_1i_2}h_{i_2i_3}\cdots h_{i_{p-1}i_p}h_{i_pi_1}g(\lambda_{i_1})g(\lambda_{i_2})\cdots g(\lambda_{i_p})g(\lambda_{i_1}).\end{aligned}$$

Since h is positive semidefinite, it is of the form $h=aa^*$ for some matrix a and therefore

$$h_{ij}=\sum_{m=1}^n a_{im}a_{mj}^*=\sum_{m=1}^n a_{im}\bar{a}_{jm}=(a_i|a_j),\quad i,j=1,\ldots,n,$$

where

$$a_i=(a_{i1}\cdots a_{in})\in\mathbf{C}^n$$

is the ith row in the matrix a. We then set $\xi_i=g(\lambda_i)a_i$ and $b_i=g(\lambda_i)^{1/2}a_i$ for $i=1,\ldots,n$ and calculate

$$\begin{aligned}&\frac{(-1)^p}{p!}\frac{d^p}{dt^p}\mathrm{Tr}\,g(x+th)\bigg|_{t=0}\\&=\sum_{i_1=1}^n\cdots\sum_{i_p=1}^n h_{i_1i_2}h_{i_2i_3}\cdots h_{i_{p-1}i_p}h_{i_pi_1}g(\lambda_{i_1})g(\lambda_{i_2})\cdots g(\lambda_{i_p})g(\lambda_{i_1})\\&=\sum_{i_1=1}^n\cdots\sum_{i_p=1}^n(\xi_{i_1}|b_{i_2})(b_{i_2}|b_{i_3})\cdots(b_{i_{p-1}}|b_{i_p})(b_{i_p}|\xi_{i_1}).\end{aligned}$$

But any sum of the form

$$S=\sum_{i_2=1}^n\cdots\sum_{i_p=1}^n(\xi|b_{i_2})(b_{i_2}|b_{i_3})\cdots(b_{i_{p-1}}|b_{i_p})(b_{i_p}|\xi)$$

is non-negative. It is obvious for $p=2$ since then

$$S = \sum_{i_2=1}^{n} (\xi|b_{i_2})(b_{i_2}|\xi),$$

and for $p=3$ since then

$$\sum_{i_2=1}^{n}\sum_{i_3=1}^{n} (\xi|b_{i_2})(b_{i_2}|b_{i_3})(b_{i_3}|\xi) = \left(\sum_{i_2=1}^{n} (\xi|b_{i_2})b_{i_2}|\sum_{i_3=1}^{n} (\xi|b_{i_3})b_{i_3}\right).$$

For $p\geqslant 4$ we may therefore use induction over either the even or the odd natural numbers by noting that

$$\begin{aligned} S &= \sum_{i_2=1}^{n} \cdots \sum_{i_p=1}^{n} (\xi|b_{i_2})(b_{i_2}|b_{i_3}) \cdots (b_{i_{p-1}}|b_{i_p})(b_{i_p}|\xi) \\ &= \sum_{i_3=1}^{n} \cdots \sum_{i_{p-1}=1}^{n} (\eta|b_{i_3})(b_{i_3}|b_{i_4}) \cdots (b_{i_{p-2}}|b_{i_{p-1}})(b_{i_{p-1}}|\eta), \end{aligned}$$

where the vector

$$\eta = \sum_{i=1}^{n} (\xi|b_i)b_i.$$

This concludes the proof of the statement. Q.E.D.

Proof of the main theorem: Consider again the function

$$g(t) = \frac{1}{c+t}, \quad t>0$$

for $c\geqslant 0$ and arbitrary $n\times n$ matrices x and h such that x is positive definite and h is positive semidefinite. We first note that

$$\left.\frac{d^p}{dt^p}\mathrm{Tr}\, g(x+th)\right|_{t=t_0} = \left.\frac{d^p}{d\varepsilon^p}\mathrm{Tr}\, g(x+t_0h+\varepsilon h)\right|_{\varepsilon=0}$$

for $p=1,2,\ldots$ and $t_0\geqslant 0$. The function $t\to \mathrm{Tr}\, g(x+th)$ is therefore completely monotone. Let now $f:\mathbf{R}_+\to\mathbf{R}$ be a non-negative operator monotone decreasing function. Any operator monotone decreasing function defined on the open positive half-line, thus in particular the function f, is necessarily of the form

$$f(t) = \alpha t + \beta + \int_0^\infty \left(\frac{1}{c+t} - \frac{c}{c^2+1}\right) d\nu(c), \tag{4}$$

where $\alpha\leqslant 0$ and ν is some positive Borel measure with support in $[0,\infty)$ such that the integral $\int (c^2+1)^{-1}\, d\nu(c)$ is finite, cf. Ref. 4 Chap. II, Theorem 1 and Lemma 2. Note that we may write

$$\int_0^\infty \left(\frac{1}{c+t} - \frac{c}{c^2+1}\right) d\nu(c) = \int_0^\infty \frac{1-ct}{c+t}\cdot (c^2+1)^{-1}\, d\nu(c),$$

where for each $t>0$ the function $c\to(1-ct)(c+t)^{-1}$ is decreasing and bounded between $-t$ and t^{-1}. Since f has a finite limit for $t\to\infty$ one may derive that $\alpha=0$, and by appealing to Lebesgues's theorem of monotone convergence we also obtain $\int c(c^2+1)^{-1}\, d\nu(c)<\infty$, hence f allows the representation

$$f(t) = \beta + \int_0^\infty \frac{1}{c+t} \mathrm{d}\nu(c),$$

where we have incorporated the constant contribution from the integral in (4) into β such that

$$\beta = \lim_{t\to\infty} f(t) \geqslant 0.$$

We conclude that the function $t \to \mathrm{Tr}\, f(x+th)$ is completely monotone and thus by Bernstein's theorem is the Laplace transform of a positive measure with support in $[0,\infty)$. Q.E.D.

Further analysis: One may try to use the Hermite expression in Proposition 3.2 to obtain a proof of the BMV conjecture. Applying Theorem 3.4 and calculating the third derivative of the trace function we obtain

$$\begin{aligned}\frac{-1}{3!}\frac{d^3}{\mathrm{d}t^3}\mathrm{Tr}\exp(x-th)\bigg|_{t=0} &= \sum_{p,i,j=1}^n (a_p|a_i)(a_i|a_j)(a_j|a_p)[\lambda_p\lambda_i\lambda_j\lambda_p]_{\exp} \\ &= \int_0^1\int_0^{t_1}\int_0^{t_2}\sum_{p,i,j=1}^n (a_p|a_i)(a_i|a_j)(a_j|a_p)\exp((1-(t_1-t_3))\lambda_p \\ &\quad + (t_1-t_2)\lambda_i + (t_2-t_3)\lambda_j)\mathrm{d}t_3\,\mathrm{d}t_2\,\mathrm{d}t_1,\end{aligned}$$

where $h=aa^*$ and a_i is the ith row in a. Assuming the BMV conjecture this integral should be non-negative, and this would obviously be the case if the integrand is a non-negative function.

Example 4.2: If we evaluate the above integrand in $t_1=t_2=1$ and $t_3=1/3$ we obtain

$$S = \sum_{p,i,j=1}^n (a_p|a_i)(a_i|a_j)(a_j|a_p)\exp\left(\frac{\lambda_p+2\lambda_j}{3}\right)\mathrm{d}t_3\,\mathrm{d}t_2\,\mathrm{d}t_1.$$

If we in addition set

$$a_1 = (1000,-10,1),$$

$$a_2 = (-10,10\,000,1000),$$

$$a_3 = (1,1000,202\,139)$$

and $(\lambda_1,\lambda_2,\lambda_3)=3\log 2\cdot(23,11,0)$, then the sum is an integer with value

$$S = -487\,062\,506\,352\,658\,941\,731\,358\,505\,750.$$

The values of S are extremely sensitive to the chosen figures, and they tend to be overwhelmingly positive. If for example, the third entry in a_3 is changed from 202 139 to 202 138, then

$$S = 376\,189\,230\,591\,238\,013\,538\,921\,396\,773.$$

The result is equally sensitive to changes in the values of $(\lambda_1,\lambda_2,\lambda_3)$.

The above example has not been found by simulation. In fact, millions of simulations with randomly chosen entries have been carried out, without ever hitting a negative value of S. Instead, the example has been obtained by the study and proper modification of an example in Ref. 14 of two positive definite 3×3 matrices A and B such that $\mathrm{Tr}(BABAAB)=-3164$.

Another way forward would be to examine the value of loops of the form

$$(a_1|a_2)(a_2|a_3)\cdots(a_{p-1}|a_p)(a_p|a_1)$$

since they, apart from an alternating sign, are the only possible negative factors in the expression of the derivatives of the trace functions. The value of a loop is a homogeneous function of degree

two in the norm of the vectors, so we only need to consider unit vectors. The value of such a loop is furthermore invariant under unitary transformations and thus takes the minimal value in any subspace of dimension p. By applying a variational principle the lower bound

$$-\cos^p\left(\frac{\pi}{p}\right) \leqslant (a_1|a_2)(a_2|a_3)\cdots(a_{p-1}|a_p)(a_p|a_1)$$

was established in Ref. 11. The lower bound converges very slowly to -1 as p tends to infinity, and it is attained essentially only when all the vectors form a "*fan*" in a two-dimensional subspace.

Remark 4.3: *If we only consider one-dimensional perturbations, that is if* $h=cP$ *for a constant* $c>0$ *and a one-dimensional projection* P, *then* h *is of the form* $h=(\xi_i\overline{\xi}_j)_{i,j=1,\ldots,n}$ *for some vector* $\xi=(\xi_1,\ldots,\xi_n)$ *and each loop*

$$h_{i_1i_2}h_{i_2i_3}\cdots h_{i_{p-1}i_p}h_{i_pi_1} = \|\xi_{i_1}\|^2\cdots\|\xi_{i_p}\|^2$$

is manifestly real and non-negative. This implies that the trace function

$$t \to \mathrm{Tr}\exp(-(x+th)),$$

for any self-adjoint $n\times n$ *matrix* x, *is the Laplace transform of a positive measure with support in* $[0,\infty)$. *The same statement holds, with* x *positive definite, for the trace function* $t\to\mathrm{Tr}\,f(x+th)$ *associated with an arbitrary completely monotone function* f.

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Tri-Hamiltonian extensions of separable systems in the plane

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A method to construct tri-Hamiltonian extensions of a separable system is presented. The procedure is tested for systems, with a Hamiltonian quadratic in the momenta, separable in classical sense in any of the four sets of orthogonal separable coordinates on the Euclidean plane. Some explicit examples are constructed. Finally a conjecture on possible generalizations to other classes of systems is discussed: in particular, the method can be adapted to the 11 orthogonal separable coordinate sets of the Euclidean three-space. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Separation of variables for Hamilton-Jacobi equation is a very effective method to solve Hamiltonian systems. In recent years an increasing interest rose towards this classical topic in analytical mechanics, dated back to the pioneering works of Stäckel, Levi-Civita, and Eisenhart.[12] Starting from these foundations, a number of applications and new results, together with reinterpretations of old ones, have been constructed. A rich and coordinates-independent characterization of separation in the classical framework of cotangent bundles of a Riemannian manifold was developed (see Refs. 2, 9, and 8 and references therein), and some generalizations were proposed. In Ref. 11, Sklyanin presented a recipe to find a separable set of coordinates for systems admitting a Lax matrix with parameter and a corresponding spectral curve. Besides, in Ref. 6 the conditions under which a bi-Hamiltonian system is separable, in the so-called Darboux-Nijenhuis coordinates, are stated. In both these approaches the separation coordinates are general canonical coordinates $\{q^i, p_i\}$ on a $2n$-dimensional symplectic manifold, instead of the coordinates on a Riemannian manifold and their conjugate momenta, as in the classical approach. Moreover, the separability of a family of n Hamiltonians $\{h_k\}$ is characterized through the existence of n function W_i such that

$$W_1(q_1, p_1; \{h_k\}) = 0,$$

$$\cdots,$$

$$W_n(q_n, p_n; \{h_k\}) = 0. \tag{1}$$

The bi-Hamiltonian point of view inspires the results presented in Ref. 5. In this paper it is shown that, given three mutually compatible Poisson tensors P, Q, and R (a *tri-Hamiltonian structure*) with rank $2n$, such that the two Poisson pencils $Q-\lambda P$ and $R-\mu P$ admit a unique polynomial Casimir function $f(\lambda, \mu)$ common to both the pencils, it is possible to find a set of canonical coordinates $\{\lambda_i, \mu_i\}$ that satisfies the relationship

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$$f(\lambda_i, \mu_i; \{h_k\}) = r_i(\lambda_i, \mu_i) \quad \forall\, i = 1, \ldots n, \tag{2}$$

where H_k are the coefficients of $f(\lambda, \mu)$ (restricted to a given symplectic leaf of P), and $r_i(\lambda, \mu)$ are constant functions. This implies that $\{\lambda_i, \mu_i\}$ are separation coordinates (in the generalized sense) for the Hamiltonians h_k, the functions W_i being strictly related to the common Casimir function $f(\lambda, \mu)$. In the same article[5] a class of systems is presented, admitting a Lax matrix with spectral parameter and such that the Casimir function $f(\lambda, \mu)$ is the polynomial defining the spectral curve of the system. This result links the multi-Hamiltonian approach to the Sklyanin one.

Another theory inspired by the bi-Hamiltonian point of view is reviewed in Ref. 3. In that paper the attention is drawn to separable systems in which any conjugate pair of separation coordinates consists of roots of a polynomial. The curve defined by this polynomial is called *separation curve*. A standard form (in separation coordinates) is found for this kind of system, and a pair of compatible Poisson tensors P and Q setting the coefficients of the polynomial in a Lenard recurrence relation are constructed. The standard form and the Poisson structures depend on the number and the position of the Casimir functions for P inside the recurrence relation between the coefficients: in *split type systems* the recurrence relation can be divided in different Lenard chains, otherwise one has *unsplit type systems*.

The aim of the present work is to introduce, in the simple case of the Euclidean plane, a recipe for constructing tri-Hamiltonian (and consequently bi-Hamiltonian) extensions of an orthogonally separable natural Hamiltonian. Although referred to a particular case, the results of the present paper give hints on more general issues.

First, the similarities between the two approaches presented in Refs. 3 and 5 raise a natural question about the relation between the separation curve and the common Casimir function of a tri-Hamiltonian structure. The present work shows a link between the two approaches: at least in the Euclidean plane, the separation curve can be obtained through a reduction procedure from the common Casimir function associated to a tri-Hamiltonian structure.

Second, starting from a tri-Hamiltonian extension of a separable system in the plane, it is possible to construct two different bi-Hamiltonian extensions, whose recursion relations are in a case of unsplit type, while in the other case of split type. This suggests the possibility to deal with both cases in a unified way.

Third, until now very few examples of tri-Hamiltonian systems are known: the recipe proposed in this paper can, in principle, produce a whole class of them, starting from any separable system. Moreover, if one of the questions answered in Ref. 5 was "how to construct separable coordinates for a tri-Hamiltonian system?," this paper gives a partial answer to the opposite question: "does any separable system admit a tri-Hamiltonian interpretation?"

Eventually, the properties of the tri-Hamiltonian systems obtained in this paper cast light on the general theory of tri-Hamiltonian separability: in fact only the Hamiltonians separable in asymmetric coordinate systems (parabolic and elliptic-hyperbolic) produce a tri-Hamiltonian structure admitting a unique common Casimir function such that (2) holds; but the explained procedure can be applied even to systems separable in symmetric coordinate systems (Cartesian and polar), and the tri-Hamiltonian structures obtained in these cases admit more Casimir functions. This indicates a possible generalization of the method to find separation coordinates for a tri-Hamiltonian system.

The main open question is the possibility of extending the partial results presented in the paper: although the method looks promising also for the separable coordinate systems of the Euclidean three-space, the extension of the procedure to any orthogonally separable system has still to be performed.

The paper is organized in the following way: in the second section the general separation theory in the classical framework is briefly reviewed. The four separable sets of coordinates on the Euclidean plane are presented together with the associated pairs of quadratic Hamiltonians. These systems are, in different coordinates, the four types of integrable systems in the plane with two quadratic first integrals listed in Ref. 10. In Sec. III the basic concepts of the bi-Hamiltonian and tri-Hamiltonian framework are summarized. The procedure for constructing a tri-Hamiltonian

extension is presented first for the two asymmetric coordinate systems, and then for the two symmetric ones. Finally, in Sec. IV some explicit examples are shown. In particular the one-Casimir extensions of Hénon-Heiles and Kepler systems presented in Ref. 3 is recovered from a tri-Hamiltonian point of view and it is shown, in the Kepler case, how multiple sets of separation coordinates lead to different tri-Hamiltonian extensions of the same Hamiltonian. The paper ends with an appendix that shows how to adapt to the extension method the Stäckel matrices for the sets of orthogonally separable coordinates in the Euclidean space.

II. ORTHOGONAL SEPARATION OF VARIABLES

A. General theory

Let (Q,g) be a n-dimensional Riemannian manifold with coordinates $q=\{q^1,\ldots q^n\}$, T^*Q is its cotangent bundle, with canonical coordinates given by $\{q^i\}$ and by the momenta $p=\{p_1,\ldots,p_n\}$. In this paper only Hamiltonian functions depending quadratically on the momenta are considered. The Hamiltonian functions constructed with the metric tensor

$$H(q,p)=\tfrac{1}{2}g^{ij}p_ip_j+V(q)=G(q,p)+V(q), \tag{3}$$

are particularly important and are called *natural*. The function G is called the *geodesic part* of the Hamiltonian. One should observe that a *point transformation of coordinates*,

$$Q^i=Q^i(q), \quad P_i=\frac{\partial q^j}{\partial Q^i}p_j$$

sends any natural Hamiltonian in a natural one. In this paper only this kind of transformation is considered.

In the following the basic facts about the classical theory of separation of variables are recalled. Proofs and a more systematic review can be found in Refs. 2 and 4.

A complete solution $W(q;\{a^i\})$ of the (time-independent) Hamilton-Jacobi equation

$$H\left(q,\frac{\partial W}{\partial q}\right)=E$$

associated to a natural Hamiltonian is called *separated* in the coordinates $\{q^i\}$ if $W=\Sigma_iW_i(q^i)$ where any function W_i depends only on the coordinate q^i. A *separated change of coordinates* (i.e., a transformation such that any new coordinate Q^i depends only on the old coordinate q^i) sends a separated solution of the Hamilton-Jacobi equation in another separated solution. Thus, instead of a coordinate system, it is more appropriate to consider the associated web, i.e., the n families of hypersurfaces given by the level set of the coordinates: webs, indeed, are invariant under separated change of variables.

The natural Hamiltonian (3) is separable in a given set of coordinates only if its geodesic part G is separable. Therefore it is possible to determine the sets of coordinates in which a certain Hamiltonian may be separated through the study of all separable coordinate systems associated to the metric g. If the separation is performed in an orthogonal set of coordinates, then it is called *orthogonal separation*, otherwise it is called *general separation*. Orthogonal separation is quite important not only because it is simpler, but even because general separation is always equivalent to orthogonal separation in a Riemannian manifold of constant curvature.

The keystone of the separability theory of Stäckel and Eisenhart[12] is the concept of Stäckel matrix: Stäckel proved that a geodetic Hamiltonian is separable in a set of orthogonal coordinates if and only if an invertible $n\times n$ matrix S exists, such that each element S_i^j belonging to the ith row of the matrix depends only on the coordinate q^i, and the diagonal controvariant components g^{ii} of the metric tensor form a row of the inverse of S,

$$g^{ii} = (S^{-1})^i_j \quad \text{for a fixed } j.$$

The existence of a Stäckel matrix is equivalent to the existence of a family of $n-1$ Killing tensors $K_{(l)}$ that together with the metric g have n common normal eigenvectors. The vector space spanned by g and this family is the *Killing-Stäckel algebra* associated to the orthogonal coordinate systems. Conversely, from a Killing-Stäckel algebra it is possible to reconstruct the Stäckel matrix of the coordinate system. Finally, also the separability of a natural Hamiltonian with potential, $H=G+V$, can be related to the Stäckel matrix: the Killing-Stäckel algebra allows to construct a family of $n-1$ potentials $V_{(l)}$ such that the Hamiltonians

$$H_{(l)} = K^{ij}_{(l)} p_i p_j + V_{(l)}$$

are in involution both mutually and with H. An alternative way to restate these results is the following: a family of n Hamiltonians H_i is orthogonally separable if and only if there exists a Stäckel matrix S and a set of n functions Φ_i, each depending only on the ith coordinate and its momentum and forming the so-called *Stäckel vector*, such that

$$S \begin{pmatrix} H_1 \\ \vdots \\ H_n \end{pmatrix} = \begin{pmatrix} \Phi_1(q_1,p_1) \\ \vdots \\ \Phi_n(q_n,p_n) \end{pmatrix}. \tag{4}$$

It is important to remark that, if a family of Hamiltonians is separable in a set of coordinates, then any their linear combination is separable in the same coordinates. Therefore the separability is a property related not just to a given metric tensor g, and to the associated natural Hamiltonian, but to the whole Killing-Stäckel algebra.

These classical results have been set in a more handy form in Ref. 1, where it has been proved that a natural Hamiltonian is orthogonally separable if and only if a Killing tensor K with n normal and simple eigenvalues exists such that $\mathrm{d}(K\,\mathrm{d}V)=0$. A stronger result can be proved if Q is also equipped with a *conformal Killing tensor* with vanishing *Nijenhuis torsion*, i.e., a tensor L of type (1,1) satisfying

$$[LX,LY] - L[LX,Y] - L[X,LY] + L^2[X,Y] = 0$$

for all vector fields X and Y on Q, and

$$\{L^{ij} p_i p_j, g^{ij} p_i p_j\} = c g^{ij} p_i p_j.$$

In this case, indeed, the whole Killing-Stäckel algebra can be generated by a recursion formula. This kind of systems are called *Benenti systems* or *L-systems*.

B. Orthogonal separable systems in the plane

It is well known that in the Euclidean plane only four systems of orthogonal coordinates exist, that allow the separation of the Hamilton-Jacobi equation associated to a natural Hamiltonian (see, for example, Ref. 4). If x and y denote the Cartesian coordinates then the other three coordinate systems are

(i) parabolic coordinates,

$$x = \frac{u+v}{2}, \quad u = x + \sqrt{x^2+y^2},$$

$$y = \sqrt{-uv}, \quad v = x - \sqrt{x^2+y^2}$$

with a web made up of two families of confocal parabolae with focus in the origin and symmetric with respect to the x axis;

(ii) elliptic-hyperbolic coordinates,

$$x = \frac{\mathrm{d}s}{2k}, \quad s = \sqrt{(x+k/2)^2 + y^2} + \sqrt{(x-k/2)^2 + y^2},$$

$$y = \frac{\sqrt{-(d^2-k^2)(s^2-k^2)}}{2k}, \quad d = \sqrt{(x+k/2)^2 + y^2} - \sqrt{(x-k/2)^2 + y^2}$$

with a web made up of a family of confocal hyperbolas and a family of confocal ellipses. The common foci of these conic sections lie on the x axis with coordinate $\pm k/2$;

(iii) polar coordinates,

$$x = r\cos\theta, \quad r = \sqrt{x^2 + y^2},$$

$$y = r\sin\theta, \quad \theta = \arctan(y/x),$$

centered at the origin.

A pair of Hamiltonian functions, H and K, can be constructed for each separable coordinate system (more precisely for each web underlying the coordinate system), through the associated Killing tensors.[4] These functions are in involution with respect to the canonical Poisson bracket on the contangent bundle of $\mathbb{R}^2$: hence they define four canonical types of completely integrable system. Both H and K are separable in the given coordinates, as it is ensured by the Stäckel relation.

1. Cartesian coordinates

Hamiltonian functions,

$$H = \tfrac{1}{2}p_x^2 + \phi_1(x),$$

$$K = \tfrac{1}{2}p_y^2 + \phi_2(y).$$

Stäckel relation,

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} \frac{1}{2}p_x^2 + \phi_1(x) \\ \frac{1}{2}p_y^2 + \phi_2(y) \end{pmatrix}. \tag{5}$$

2. Parabolic coordinates

Hamiltonian functions,

$$H = \frac{\left(\frac{1}{2}p_u^2 + \phi_1(u)\right)u - \left(\frac{1}{2}p_v^2 + \phi_2(v)\right)v}{u - v},$$

$$K = \frac{\left(\frac{1}{2}p_v^2 - \frac{1}{2}p_u^2 + \phi_2(v) - \phi_1(u)\right)uv}{u - v}.$$

Stäckel relation,

$$\begin{pmatrix} 1 & \frac{1}{u} \\ 1 & \frac{1}{v} \end{pmatrix}\begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} \frac{1}{2}p_u^2 + \phi_1(u) \\ \frac{1}{2}p_v^2 + \phi_2(v) \end{pmatrix}. \tag{6}$$

3. Elliptic-hyperbolic coordinates

Hamiltonian functions,

$$H = \frac{\left(\frac{1}{2}p_s^2 + \phi_1(s)\right)(s^2 - k^2) - \left(\frac{1}{2}p_d^2 + \phi_2(d)\right)(d^2 - k^2)}{s^2 - d^2},$$

$$K = \frac{\left(\frac{1}{2}p_d^2 - \frac{1}{2}p_s^2 + \phi_2(d) - \phi_1(s)\right)(s^2 - k^2)(d^2 - k^2)}{s^2 - d^2}.$$

Stäckel relation,

$$\begin{pmatrix} 1 & \frac{1}{s^2 - k^2} \\ 1 & \frac{1}{d^2 - k^2} \end{pmatrix} \begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} \frac{1}{2}p_s^2 + \phi_1(s) \\ \frac{1}{2}p_d^2 + \phi_2(d) \end{pmatrix}. \tag{7}$$

4. Polar coordinates

Hamiltonian functions,

$$H = \frac{1}{2}p_r^2 + \phi_1(r) + \frac{1}{r^2}\left(\frac{1}{2}p_\theta^2 + \phi_2(\theta)\right),$$

$$K = -\frac{1}{2}p_\theta^2 - \phi_2(\theta).$$

Stäckel relation,

$$\begin{pmatrix} 1 & \frac{1}{r^2} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} \frac{1}{2}p_r^2 + \phi_1(r) \\ -\frac{1}{2}p_\theta^2 - \phi_2(\theta) \end{pmatrix}. \tag{8}$$

In Cartesian coordinates, the two alternative Hamiltonian functions,

$$\hat{H} = \frac{1}{2}(p_x^2 + p_y^2) + \phi_1(x) + \phi_2(y),$$

$$\hat{K} = \frac{1}{2}p_y^2 + \phi_2(y),$$

with Stäckel matrix

$$S = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$$

are sometimes preferred. Indeed $\hat{H}$ is a natural Hamiltonian associated to the Euclidean metric, while H is not natural. The Hamiltonians H and K used in the present work are trivial recombinations of the Hamiltonians $\hat{H}$ and $\hat{K}$, hence they are still separable in Cartesian coordinates. The reason for choosing the two Hamiltonians H and K, instead of $\hat{H}$ and $\hat{K}$, is to put the Stäckel matrix in a form such that in the ith row only different powers of a suitable function of the coordinate q^i appear. In order to extend the procedure presented in this paper to more general cases, one of the key points is to characterize the class of Stäckel matrix that can be put in this form.

The method to construct a tri-Hamiltonian extension of the previous systems is slightly different for the asymmetric coordinate systems (parabolic and elliptic-hyperbolic) and for the sym-

metric ones (polar and Cartesian). This is due to the different form of the Stäckel matrix in the two cases, as it can be seen in the formulas from (5)–(8). In fact, for asymmetric coordinate systems all the rows of the Stäckel matrix have the same form, whereas for symmetric coordinate systems different rows of the Stäckel matrix have different forms. Therefore, the algorithm used in the asymmetric case needs to be adapted to each symmetric coordinate system in a specific way.

III. TRI-HAMILTONIAN EXTENSION

A. Separation of tri-Hamiltonian systems

The idea of a tri-Hamiltonian extension of separable systems is suggested by the construction of bi-Hamiltonian extension of Benenti systems presented in Ref. 7, and by some results about tri-Hamiltonian systems, briefly summarized in this section (see Ref. 5 for proofs). Let P, Q, and R be three Poisson structures mutually compatible, with rank $2n$, on a manifold of dimension $2n+k$. Let, moreover, f be a simultaneous Casimir function for the two Poisson pencils $Q-\lambda P$ and $R-\mu P$, and a polynomial in λ and μ. Then, it can be proved that all the coefficients h_k of this polynomial are functions mutually in involution with respect to all the three Poisson structures, and satisfy a recurrence scheme determined by the form of the polynomial f. Under some further hypotheses, it is possible to find out a set of coordinates $\{\lambda_i, \mu_i, c_\alpha\}$ with the following characteristics:

(1) c_α are k Casimir functions for P;
(2) λ_i, μ_i are $2n$ Darboux-Nijenhuis coordinates for both the Nijenhuis tensors obtained, through a deformation procedure, from the two Poisson pencils $Q-\lambda P$ and $R-\mu P$;
(3) λ_i, μ_i satisfy the n relations,

$$f(\lambda_i, \mu_i; \{h_k\}, c_\alpha) = r_i(\lambda_i, \mu_i) \tag{9}$$

in which the functions $r_i(\lambda, \mu)$ are constant functions on the manifold.

The relations (9) imply the separability, in the sense (1) of Sklyanin, of the Hamiltonians h_k. It is then natural to ask if it is possible, starting from a classical separable system, to obtain an adapted tri-Hamiltonian structure.

A special case is important for the next sections: set $n=2$ and consider the common Casimir function $f=h_1+\lambda h_2+\hat{f}(\lambda, \mu; \{c_\alpha\})$, where $\hat{f}$ is a polynomial in λ, μ and in the Casimir functions c_α, then the relations (9) become

$$\begin{aligned} h_1 + \lambda_1 h_2 + \hat{f}(\lambda_1, \mu_1; \{c_\alpha\}) &= r_1(\lambda_1, \mu_1), \\ h_1 + \lambda_2 h_2 + \hat{f}(\lambda_2, \mu_2; \{c_\alpha\}) &= r_2(\lambda_2, \mu_2). \end{aligned} \tag{10}$$

For any fixed value of the Casimir functions c_α the formula (10) gives a separation relation in the sense of (1).

B. Asymmetric coordinate systems

The separation relations encoded by the Stäckel matrix in asymmetric coordinate systems are very similar to relations (10). Indeed with the symplectic (and separated) transformations:

$$\lambda_1 = u, \quad \lambda_2 = v, \quad \mu_1 = p_u, \quad \mu_2 = p_v$$

for parabolic coordinates and

$$\lambda_1 = s^2 - k^2, \quad \lambda_2 = d^2 - k^2, \quad \mu_1 = \frac{p_s}{2s}, \quad \mu_2 = \frac{p_d}{2d}$$

for elliptic-hyperbolic coordinates, the relations extracted from Stäckel matrix become

$$\begin{pmatrix} \lambda_1 & 1 \\ \lambda_2 & 1 \end{pmatrix} \begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} r_1(\lambda_1, \mu_1) \\ r_2(\lambda_1, \mu_1) \end{pmatrix},$$

that is

$$K + \lambda_i H = r_i(\lambda_i, \mu_i), \tag{11}$$

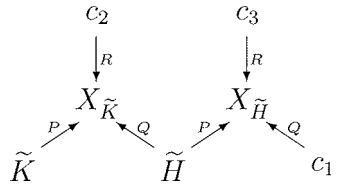
where the functions $r_i(\lambda, \mu)$ are, respectively, in the two coordinate systems,

$$r_i(\lambda, \mu) = \tfrac{1}{2}\lambda\mu^2 + \lambda\phi_i(\lambda), \tag{12}$$

$$r_i(\lambda, \mu) = 2\mu^2(\lambda^2 + \lambda k^2) + \lambda\phi_i(\sqrt{\lambda + k^2}). \tag{13}$$

Relations (10) and (11) differ only in the lack of the Casimir function c_α in (11). A set of Casimir functions are also necessary to construct a recurrence relation with a finite number of elements. In order to add Casimir functions and to obtain a set of relations analogous to (10), it is necessary to extend the phase space of the system $\mathbb{R}^4 = T^*\mathbb{R}^2$ to $\mathbb{R}^{4+k}$, with k extra coordinates c_α. Obviously the phase space $\mathbb{R}^4$ can be identified with the level surface $\mathcal{S} = \{c_\alpha = 0\}$ of the extended space. On $\mathbb{R}^{4+k}$, a Poisson structure P should be defined such that the new coordinates c_α are its Casimir functions, and the reduction of P on the symplectic leaf $\mathcal{S}$ gives the canonical Poisson bracket of $\mathbb{R}^4$. An extension of a given function g on $\mathbb{R}^2$ is any function $\tilde{g}$ on $\mathbb{R}^{4+k}$ such that $\tilde{g}|_{\mathcal{S}} = g$. In this framework the relations (11) can be thought of as a restriction of relations (10) on the symplectic leaf $\mathcal{S}$.

The simplest tri-Hamiltonian recursion relation involving two vector fields and compatible with the relations (11) is



(14)

where $\tilde{H}$ and $\tilde{K}$ are extensions of the Hamiltonians H and K and three extra coordinates are introduced. The recurrence scheme (14) corresponds to the common Casimir function.

$$f = \tilde{K} + \lambda\tilde{H} + c_1\lambda^2 + \mu c_2 + \lambda\mu c_3. \tag{15}$$

In the scheme (14), the notation $g \xrightarrow{P} X_g$ means that the vector field X_g is obtained from the differential of the function g, through the extended Poisson structure P given by

$$P = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{16}$$

The next step of the procedure is to require that λ_i, μ_i satisfy the two relations (10). This implies that $\tilde{H}$ and $\tilde{K}$ must solve the linear system

$$f(\lambda_i,\mu_i;\tilde{K},\tilde{H},c_\alpha)=r_i(\lambda_i,\mu_i).$$

Therefore the solution, using the function (15), is

$$\tilde{H}=\frac{r_2(\lambda_2,\mu_2)-r_1(\lambda_1,\mu_1)}{\lambda_2-\lambda_1}-(\lambda_1+\lambda_2)c_1+\frac{(\mu_2-\mu_1)}{\lambda_1-\lambda_2}c_2+\frac{(\mu_2\lambda_2-\mu_1\lambda_1)}{\lambda_1-\lambda_2}c_3, \tag{17}$$

$$\tilde{K}=\frac{\lambda_2 r_1(\lambda_1,\mu_1)-\lambda_1 r_2(\lambda_2,\mu_2)}{\lambda_2-\lambda_1}+\lambda_2\lambda_1 c_1+\frac{(\lambda_2\mu_1-\mu_2\lambda_1)}{\lambda_1-\lambda_2}c_2+\frac{\lambda_2\lambda_1(\mu_2-\mu_1)}{\lambda_2-\lambda_1}c_3, \tag{18}$$

where the two functions r_i are related to the two arbitrary functions ϕ_i by the expression (12) in the case of parabolic coordinates, and by the expression (13) in the case of elliptic-hyperbolic coordinates.

It is important to point out some aspects of the construction just presented. First, it is possible to reduce the number of new coordinates needed, by omitting the "vertical" part of the recurrence scheme and looking for a function in the form

$$f=\tilde{K}+\lambda\tilde{H}+\lambda^2 c_1.$$

This approach is followed in Refs. 7 and 3, but it allows to obtain only a bi-Hamiltonian recursion. This bi-Hamiltonian extension can be recovered in the tri-Hamiltonian approach through a reduction process.

Second, it is possible, both in the bi-Hamiltonian (as in Ref. 3) and in the tri-Hamiltonian case, to add to the function (15) a "redundant" Casimir function common to all the Poisson structures, by setting

$$\bar{f}=f+\lambda^n c_4 \quad \text{with } n>2.$$

In this way another pair of extended Hamiltonians $\tilde{H}$ and $\tilde{K}$ and a new tri-Hamiltonian structure are constructed. The new Hamiltonians and Poisson structures can be related to the old ones, through the reduction on the level set $c_4=0$.

Besides these digressions, the last step, in order to obtain the desired recursion scheme, is to construct two further Poisson structures. For this purpose a method similar to Ref. 5 is implemented. One starts by defining the two Poisson tensors represented by the 7×7 matrices

$$Q_d=\begin{pmatrix}0 & \Lambda & 0\\ -\Lambda & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\quad R_d=\begin{pmatrix}0 & M & 0\\ -M & 0 & 0\\ 0 & 0 & 0\end{pmatrix},$$

where the null matrices have the appropriate dimensions and

$$\Lambda=\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix},\quad M=\begin{pmatrix}\mu_1 & 0\\ 0 & \mu_2\end{pmatrix}.$$

Then, one constructs the two vector fields,

$$X_Q=\sum_\alpha F_\alpha\frac{\partial}{\partial c_\alpha},\quad X_R=\sum_\alpha G_\alpha\frac{\partial}{\partial c_\alpha}, \tag{19}$$

where the functions F_α and G_α satisfy the relations $P\,\mathrm{d}F_\alpha=Q\,\mathrm{d}c_\alpha$ and $P\,\mathrm{d}G_\alpha=R\,\mathrm{d}c_\alpha$ in the recurrence scheme (14). Hence one has $F_1=\tilde{H}$, $F_2=F_3=0$ and $G_1=0$, $F_2=\tilde{K}$, $F_3=\tilde{H}$, and the two vector fields become

$$X_Q = \tilde{H}\frac{\partial}{\partial c_1}, \quad X_R = \tilde{K}\frac{\partial}{\partial c_2} + \tilde{H}\frac{\partial}{\partial c_3},$$

where the Hamiltonians $\tilde{H}$ and $\tilde{K}$ are already known by formulas (17) and (18).

Eventually, the two further tensors needed to realize the recursion scheme (14) are given by

$$Q = Q_d - L_{X_Q}P, \quad R = R_d - L_{X_R}P. \tag{20}$$

The surprising result of this complicated construction is the following fact, proved by direct computation.

Fact 1: The tensors Q and R, defined by (20), are compatible Poisson tensors independently of the choice of the functions $r_i(\lambda,\mu)$. *Moreover, the function f given by (15) is a common Casimir function for the two Poisson pencils* $Q-\lambda P$ *and* $R-\lambda P$, *thus realizing the recursion scheme (14).*

Since c_2 and c_3 are Casimir functions for both P and Q, these two Poisson structures can be reduced on the level surface $\{c_2=c_3=0\}$. On this surface the function (15) reduces to

$$\tilde{K} + \lambda\tilde{H} + \lambda^2 c_1$$

and the tri-Hamiltonian recursion scheme (14) becomes a simply bi-Hamiltonian one. Moreover, since the separation relations (10) for the reduced system become

$$\tilde{K} + \lambda_1\tilde{H} + \lambda_1^2 c_1 = r_1(\lambda_1,\mu_1),$$

$$\tilde{K} + \lambda_2\tilde{H} + \lambda_2^2 c_1 = r_2(\lambda_2,\mu_2),$$

if $\phi_1=\phi_2$ (and so $r_1=r_2=r$) then the function

$$\tilde{K} + \lambda\tilde{H} + \lambda^2 c_1 - r(\lambda,\mu)$$

defines an unsplitted separation curve in the sense of Ref. 3.

Conversely, a splitted bi-Hamiltonian recursion chain is obtained by reducing the function f and the Poisson structures P and R on the level surface $\{c_1=0\}$ of their common Casimir function c_1.

C. Symmetric coordinate systems

The procedure described above cannot be directly applied to Hamiltonians that are separable in a symmetric coordinate system, i.e., in polar or Cartesian coordinates. In these cases, actually, the rows of the Stäckel matrix are of different form, and therefore do not identify an unique polynomial, from whom to construct a Casimir function common to the two Poisson pencils $Q-\lambda P$ and $R-\lambda P$. This difficulty can be overcome by observing that a tri-Hamiltonian structure does not admit necessarily only one common Casimir function for the two Poisson pencils. Therefore, it will be sufficient to build a different common Casimir function for each of the different polynomial relations generated by the Stäckel matrix.

In the case of polar coordinates, through the symplectic transformations,

$$\lambda_1 = r^2, \quad \lambda_2 = \tan\theta, \quad \mu_1 = \frac{p_r}{2r}, \quad \mu_2 = \cos^2\theta p_\theta$$

the Stäckel relationships can be rewritten with the two equations

$$\begin{aligned} K + \lambda_1 H &= r_1(\lambda_1,\mu_1), \\ K &= r_2(\lambda_2,\mu_2), \end{aligned} \tag{21}$$

where the functions $r_i(\lambda,\mu)$ are

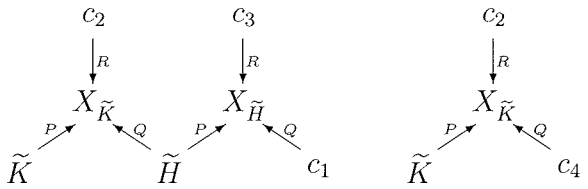
$$r_1(\lambda,\mu) = 2\mu^2\lambda^2 + \lambda\phi_1(\sqrt{\lambda}),$$

$$r_2(\lambda,\mu) = -\tfrac{1}{2}(1+\lambda^2)^2\mu^2 - \phi_2(\arctan\lambda).$$

Hence it is necessary to build two functions in the form

$$f_1 = \widetilde{K} + \lambda\widetilde{H} + \lambda^2 c_1 + \mu c_2 + \lambda\mu c_3,$$
$$f_2 = \widetilde{K} + \lambda c_4 + \mu c_2 \tag{22}$$

that realize the tri-Hamiltonian recursion scheme:



(23)

The expressions for $\widetilde{H}$ and $\widetilde{K}$ can be obtained solving the system

$$\widetilde{K} + \lambda_1\widetilde{H} + \lambda_1^2 c_1 + \mu_1 c_2 + \lambda_1\mu_1 c_3 = r_1(\lambda_1,\mu_1),$$

$$\widetilde{K} + \lambda_2 c_4 + \mu_2 c_2 = r_2(\lambda_2,\mu_2),$$

whose solution is

$$\widetilde{H} = \frac{r_1(\lambda_1,\mu_1) - r_2(\lambda_2,\mu_2)}{\lambda_1} - \lambda_1 c_1 + \frac{\mu_2-\mu_1}{\lambda_1}c_2 - \mu_1 c_3 + \frac{\lambda_2}{\lambda_1}c_4, \tag{24}$$

$$\widetilde{K} = r_2(\lambda_2,\mu_2) - \mu_2 c_2 - \lambda_2 c_4. \tag{25}$$

The Poisson tensor P used in this case is analogous to (16) but it has four Casimir functions. The structures Q and R are obtained, similarly to the asymmetric case

$$Q = Q_d - L_{X_Q}P, \quad R = R_d - L_{X_R}P, \tag{26}$$

where the vector fields X_Q and X_R are again constructed according to the formulas (19), but using the four functions $c_1,\ldots,c_4$. Hence from the recursion scheme (23) one obtains

$$X_Q = \widetilde{H}\frac{\partial}{\partial c_1} + \widetilde{K}\frac{\partial}{\partial c_4}, \quad X_R = \widetilde{K}\frac{\partial}{\partial c_2} + \widetilde{H}\frac{\partial}{\partial c_3}. \tag{27}$$

By direct computation the following fact can be proved:

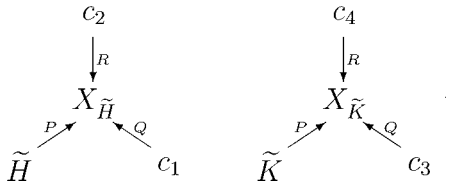
Fact 2: The tensors Q and R, defined by (26) with vector fields (27), are compatible Poisson tensors independently of the choice of the functions $r_i(\lambda,\mu)$. Moreover, the functions f_1 and f_2 given by (22) are two common Casimir functions for the two Poisson pencils $Q-\lambda P$ and $R-\lambda P$, thus realizing the recursion scheme (23).

Finally, in the case of Cartesian coordinates, the starting point is the construction of two functions of the form

$$f_1 = \widetilde{H} + c_1\lambda + \mu c_2,$$
(28)

$$f_2 = \tilde{K} + \lambda c_3 + \mu c_4,$$

that realize the tri-Hamiltonian recursion scheme,



(29)

By solving the linear system,

$$\tilde{H} + c_1\lambda_1 + \mu_1 c_2 = r_1(\lambda_1, \mu_1),$$

$$\tilde{K} + \lambda_2 c_3 + \mu_2 c_4 = r_2(\lambda_2, \mu_2),$$

one finds out the Hamiltonians

$$\tilde{H} = r_1(\lambda_1, \mu_1) - c_1\lambda_1 - \mu_1 c_2, \tag{30}$$

$$\tilde{K} = r_2(\lambda_2, \mu_2) - \lambda_2 c_3 - \mu_2 c_4, \tag{31}$$

where the arbitrary functions r_1, r_2 are linked to the functions ϕ_1, ϕ_2 in (5) by

$$r_1(\lambda_1(x), \mu_1(p_x, x)) = \tfrac{1}{2}p_x^2 + \phi_1(x),$$

$$r_2(\lambda_2(y), \mu_2(p_y, y)) = \tfrac{1}{2}p_y^2 + \phi_2(y).$$

The vector fields obtained from the recursion scheme (29) are the following:

$$X_Q = \tilde{H}\frac{\partial}{\partial c_1} + \tilde{K}\frac{\partial}{\partial c_3}, \quad X_R = \tilde{H}\frac{\partial}{\partial c_2} + \tilde{K}\frac{\partial}{\partial c_4}. \tag{32}$$

A result analogous to Fact 1 and Fact 2 is true also in this case, and it takes the following form.

Fact 3: The tensors Q and R, defined by (26) with vector fields (32), are compatible Poisson tensors independently of the choice of the functions $r_i(\lambda, \mu)$. Moreover, the functions f_1 and f_2 given by (28) are two common Casimir functions for the two Poisson pencils $Q - \lambda P$ and $R - \lambda P$, thus realizing the recursion scheme (29).

IV. EXAMPLES

A. Tri-Hamiltonian extension of Hénon-Heiles system

An application of the recipe presented above is given by the Hénon-Heiles system, already considered in Ref. 3. Its Hamiltonian expressed in natural coordinates is

$$H = \tfrac{1}{2}(p_1^2 + p_2^2) + V, \quad V = \tfrac{1}{2}q_1 q_2^2 + q_1^3. \tag{33}$$

This system is separable in the parabolic coordinate system given by

$$q_1 = \lambda_1 + \lambda_2, \quad q_2 = 2\sqrt{-\lambda_1\lambda_2},$$

$$p_1 = \frac{\lambda_1\mu_1 - \lambda_2\mu_2}{\lambda_1 - \lambda_2}, \quad p_2 = \sqrt{-\lambda_1\lambda_2}\frac{\mu_1 - \mu_2}{\lambda_1 - \lambda_2}.$$

If the Hénon-Heiles Hamiltonian (33) is compared with the general Hamiltonian (17), with $c_1=c_2=c_3=0$, one finds

$$V(\lambda_1,\lambda_2) = \frac{\lambda_2\phi(\lambda_2) - \lambda_1\phi(\lambda_1)}{\lambda_2 - \lambda_1}.$$

Any choice of the two functions ϕ_1 and ϕ_2 gives a separable potential and a suitable tri-Hamiltonian extension. On the contrary, a pair of functions ϕ_1, ϕ_2 is associated to any potential separable in the coordinates $\{\lambda_i, \mu_i\}$, also if the potential contains additional terms with respect to (33). Under the assumption that both $\phi_i(z)$ are continuous for $z=0$ one has

$$\phi_1(z) = V(z,0), \quad \phi_2(z) = V(0,z).$$

One should observe that the choice of the arbitrary functions is not unique: in fact, the pair $\phi_i(z)+(k/z)$ produce the same potential as the pair $\phi_i(z)$. The potential (33) is obtained by choosing

$$\phi_1(z) = \phi_2(z) = z^3.$$

The corresponding extended Hamiltonians are found by substituting in the general formulas (17) and (18):

$$\tilde{H} = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}q_1q_2^2 + q_1^3 - q_1c_1 - 2\frac{p_2}{q_2}c_2 - p_1c_3,$$

$$\tilde{K} = \frac{1}{2}(q_2p_1p_2 - q_1p_2^2) + \frac{1}{4}q_1^2q_2^2 + \frac{1}{16}q_2^4 - \frac{1}{4}q_2^2c_1 + \left(2\frac{q_1p_2}{q_2} - p_1\right)c_2 - \frac{1}{2}q_2p_2c_3.$$

They are set in the recursion scheme (14) by the three Poisson structures,

$$P = \begin{pmatrix} 0_{2\times2} & 1_{2\times2} & 0_{2\times3} \\ -1_{2\times2} & 0_{2\times2} & 0_{2\times3} \\ 0_{3\times2} & 0_{3\times2} & 0_{3\times3} \end{pmatrix},$$

$$Q=\begin{pmatrix} 0 & 0 & q_1 & \frac{1}{2}q_2 & p_1-c_3 & 0 & 0 \\ 0 & 0 & \frac{1}{2}q_2 & 0 & p_2-2\frac{c_2}{q_2} & 0 & 0 \\ -q_1 & -\frac{1}{2}q_2 & 0 & \frac{1}{2}p_2 & c_1-3q_1^2-\frac{1}{2}q_2^2 & 0 & 0 \\ -\frac{1}{2}q_2 & 0 & -\frac{1}{2}p_2 & 0 & -q_1q_2-2\frac{p_2}{q_2^2}c_2 & 0 & 0 \\ c_3-p_1 & 2\frac{c_2}{q_2}-p_2 & 3q_1^2+\frac{1}{2}q_2^2-c_1 & q_1q_2+2\frac{p_2}{q_2^2}c_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R=\begin{pmatrix} 0 & 0 & p_1 & p_2 & 0 & Y_1 & X_1 \\ 0 & 0 & p_2 & p_1-2\frac{p_2q_1}{q_2} & 0 & Y_2 & X_2 \\ -p_1 & -p_2 & 0 & \frac{p_2^2}{q_2} & 0 & Y_3 & X_3 \\ -p_2 & 2\frac{q_1p_2}{q_2}-p_1 & -\frac{p_2^2}{q_2} & 0 & 0 & Y_4 & X_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -Y_1 & -Y_2 & -Y_3 & -Y_4 & 0 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 \end{pmatrix},$$

where $X=X_{\tilde{H}}=P\,\mathrm{d}\tilde{H}$ and $Y=X_{\tilde{K}}=P\,\mathrm{d}\tilde{K}$. It is worth to observe that both P and Q can be reduced by restriction on the level surface $c_2=c_3=0$ and the reduced Hamiltonians and Poisson structures are those considered in Ref. 3. On the contrary the structure R is not reducible, so the reduced system appears to be just a one-Casimir bi-Hamiltonian extension of the Hénon-Heiles system. An advantage of the knowledge of a tri-Hamiltonian extension of the system is the possibility to perform a reduction on the level set $c_1=0$, thus producing a different, two-Casimir bi-Hamiltonian extension of the system, whose Poisson structures are the reductions of P and R.

B. Tri-Hamiltonian extension of Kepler system in the plane

The Kepler system in the plane is separable in three different sets of coordinates: the parabolic, the elliptic-hyperbolic and the polar coordinate systems. A different second constant of motion (related to the Killing tensor of the coordinate system) and a different tri-Hamiltonian extension can be associated to each of these coordinate systems.

In the case of parabolic coordinates, the transformation between the natural and the $\{\lambda_i,\mu_i\}$ coordinates is given by

$$q_1=2\sqrt{-\lambda_1\lambda_2},\quad q_2=\lambda_1+\lambda_2,$$

$$p_1=\frac{\sqrt{-\lambda_1\lambda_2}(\mu_1-\mu_2)}{\lambda_1-\lambda_2},\quad p_2=\frac{\lambda_1\mu_1-\lambda_2\mu_2}{\lambda_1-\lambda_2}.$$

If one sets

$$\phi_1(z) = \frac{a}{2z}, \quad \phi_2(z) = -\frac{a}{2z},$$

the extended Hamiltonians (17) and (18) become

$$\widetilde{H} = \frac{1}{2}(p_1^2 - p_2^2) - \frac{a}{\sqrt{q_1^2 + q_2^2}} - q_2 c_1 - 2\frac{p_1}{q_1} c_2 - p_2 c_3,$$

$$\widetilde{K} = \frac{1}{2}(q_1 p_1 p_2 - q_2 p_1^2) + \frac{a q_2}{2\sqrt{q_1^2 + q_2^2}} - \frac{1}{4} q_1^2 c_1 + \frac{2q_2 p_1 - q_1 p_2}{q_1} c_2 - \frac{1}{2} q_1 p_1 c_3.$$

They are set in the recursion scheme (14) by the three Poisson structures,

$$P = \begin{pmatrix} 0_{2\times 2} & 1_{2\times 2} & 0_{2\times 3} \\ -1_{2\times 2} & 0_{2\times 2} & 0_{2\times 3} \\ 0_{3\times 2} & 0_{3\times 2} & 0_{3\times 3} \end{pmatrix},$$

$$Q = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{2}q_1 & X_1 & 0 & 0 \\ 0 & 0 & \frac{1}{2}q_1 & q_2 & X_2 & 0 & 0 \\ 0 & -\frac{1}{2}q_1 & 0 & -\frac{1}{2}p_1 & X_3 & 0 & 0 \\ -\frac{1}{2}q_1 & -q_2 & \frac{1}{2}p_1 & 0 & X_4 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & p_2 - 2\frac{p_1 q_2}{q_1} & p_1 & 0 & Y_1 & X_1 \\ 0 & 0 & p_1 & p_2 & 0 & Y_2 & X_2 \\ 2\frac{p_1 q_2}{q_1} - p_2 & -p_1 & 0 & -\frac{p_1^2}{q_1} & 0 & Y_3 & X_3 \\ -p_1 & -p_2 & \frac{p_1^2}{q_1} & 0 & 0 & Y_4 & X_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -Y_1 & -Y_2 & -Y_3 & -Y_4 & 0 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 \end{pmatrix},$$

where $X = X_{\widetilde{H}} = P\,\mathrm{d}\widetilde{H}$ and $Y = X_{\widetilde{K}} = P\,\mathrm{d}\widetilde{K}$. As it can be easily seen, the one-Casimir extension considered in Ref. 3 is obtained by reducing the Poisson structures P and Q and the Hamiltonians on the level set $c_2 = c_3 = 0$. It is important to observe that the separation coordinates used do not seem to originate a unique "separation curve" because the two functions ϕ_1 and ϕ_2 are different.

In the case of the elliptic-hyperbolic coordinates, the transformation from the natural coordinates is

$$q_2 = \frac{\sqrt{-\lambda_1\lambda_2}}{k}, \quad q_1 = \frac{\sqrt{(\lambda_1 + k^2)(\lambda_2 + k^2)}}{k} + k,$$

$$p_1 = 2\frac{(\lambda_1\mu_1 - \lambda_2\mu_2)\sqrt{(\lambda_1 + k^2)(\lambda_2 + k^2)}}{k(\lambda_1 - \lambda_2)}, \quad p_2 = 2\frac{\mu_1(\lambda_1 + k^2) - \mu_2(\lambda_2 + k^2)}{k(\lambda_1 - \lambda_2)}\sqrt{-\lambda_1\lambda_2}$$

and the two arbitrary functions are

$$\phi_1(z) = \phi_2(z) = \frac{az}{k^2 - z^2}.$$

The two extended Hamiltonians (17) and (18) turn out to be

$$\tilde{H} = \frac{1}{2}(p_1^2 + p_2^2) - \frac{a}{\sqrt{q_1^2 + q_2^2}} - (q_1^2 + q_2^2 - 2q_1k)c_1 + \frac{1}{2k^2}\left(\frac{p_1}{(q_1 - k)} - \frac{p_2}{q_2}\right)c_2 - \frac{p_1}{2(q_1 - k)}c_3,$$

$$\tilde{K} = (q_1 - k)q_2p_1p_2 - \frac{1}{2}q_1(q_1 - 2k)p_2^2 - \frac{1}{2}q_2^2p_1^2 - \frac{akq_1}{\sqrt{q_1^2 + q_2^2}} - q_2^2k^2c_1 + \frac{1}{2k^2}\left(\frac{q_1^2 + q_2^2 - 2q_1k}{q_2}p_2 - \frac{(q_1 - k)^2 + q_2^2}{(q_1 - k)}p_1\right)c_2 + \frac{1}{2}\left(\frac{q_2^2p_1}{q_1 - k} - q_2p_2\right)c_3,$$

and the three Poisson structures are

$$P = \begin{pmatrix} 0_{2\times2} & 1_{2\times2} & 0_{2\times3} \\ -1_{2\times2} & 0_{2\times2} & 0_{2\times3} \\ 0_{3\times2} & 0_{3\times2} & 0_{3\times3} \end{pmatrix},$$

$$Q = \begin{pmatrix} 0 & 0 & q_1(q_1 - 2k) & (q_1 - k)q_2 & X_1 & 0 & 0 \\ 0 & 0 & (q_1 - k)q_2 & q_2^2 & X_2 & 0 & 0 \\ q_1(2k - q_1) & (k - q_1)q_2 & 0 & (q_1 - k)p_2 - q_2p_1 & X_3 & 0 & 0 \\ (k - q_1)q_2 & -q_2^2 & (k - q_1)p_2 + q_2p_1 & 0 & X_4 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & \frac{(q_2^2 + k^2)p_1}{2k^2(q_1 - k)} - \frac{q_2p_2}{2k^2} & \frac{(q_1 - k)p_2 - q_2p_1}{2k^2} & 0 & Y_1 & X_1 \\ 0 & 0 & -\frac{(q_1 - k)p_2 - q_2p_1}{2k^2} & \frac{(q_1 - k)p_1}{2k^2} - \frac{q_1(q_1 - 2k)p_2}{2q_2k^2} & 0 & Y_2 & X_2 \\ \frac{(q_2^2 + k^2)p_1}{2k^2(k - q_1)} + \frac{q_2p_2}{2k^2} & \frac{(k - q_1)p_2 + q_2p_1}{2k^2} & 0 & \frac{(q_1 - k)^2p_2^2 + p_1^2q_2^2}{2q_2k^2(q_1 - k)} - \frac{p_2p_1}{k^2} & 0 & Y_3 & X_3 \\ \frac{(k - q_1)p_2 + q_2p_1}{2k^2} & \frac{(k - q_1)p_1}{2k^2} + \frac{q_1(q_1 - 2k)p_2}{2q_2k^2} & \frac{(q_1 - k)^2p_2^2 + p_1^2q_2^2}{2k^2q_2(q_1 - k)} + \frac{p_2p_1}{k^2} & 0 & 0 & Y_4 & X_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -Y_1 & -Y_2 & -Y_3 & -Y_4 & 0 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 \end{pmatrix},$$

where $X = X_{\tilde{H}} = P\,\mathrm{d}\tilde{H}$ and $Y = X_{\tilde{K}} = P\,\mathrm{d}\tilde{K}$.

Finally, in the case of polar coordinates, the transformation between the natural and the $\{\lambda_i, \mu_i\}$ coordinates is given by

$$q_1 = \sqrt{\frac{\lambda_1}{1+\lambda_2^2}}, \quad q_2 = \lambda_2 \sqrt{\frac{\lambda_1}{1+\lambda_2^2}},$$

$$p_1 = \frac{2\mu_1\lambda_1 - \mu_2\lambda_2^3 - \lambda_2\mu_2}{\sqrt{\lambda_1(1+\lambda_2^2)}}, \quad p_2 = \frac{\mu_2\lambda_2^2 + 2\lambda_1\lambda_2\mu_1 + \mu_2}{\sqrt{\lambda_1(1+\lambda_2^2)}}.$$

With the choice

$$\phi_1(z) = -\frac{a}{z}, \quad \phi_2(z) = 0$$

the extended Hamiltonians (24) and (25) become

$$\widetilde{H} = \frac{1}{2}(p_1^2 + p_2^2) - \frac{a}{\sqrt{q_1^2+q_2^2}} - (q_1^2+q_2^2)c_1 - \frac{q_1p_1 + q_2p_2 - 2q_1^2(q_1p_2 - q_2p_1)}{2(q_1^2+q_2^2)^2}c_2 - \frac{q_1p_1+q_2p_2}{2(q_1^2+q_2^2)^2}c_3 + \frac{q_2c_4}{q_1(q_1^2+q_2^2)},$$

$$\widetilde{K} = q_1q_2p_1p_2 - \frac{1}{2}(q_2^2p_1^2 + q_1^2p_2^2) - q_1^2\frac{q_1p_2 - q_2p_1}{q_1^2+q_2^2}c_2 - \frac{q_2}{q_1}c_4.$$

They are set in the recursion scheme (23) by the three Poisson structures,

$$P = \begin{pmatrix} 0_{2\times2} & 1_{2\times2} & 0_{2\times4} \\ -1_{2\times2} & 0_{2\times2} & 0_{2\times4} \\ 0_{4\times2} & 0_{4\times2} & 0_{4\times4} \end{pmatrix},$$

$$Q = \begin{pmatrix} 0 & 0 & q_1^2 + \frac{q_2^3}{q_1(q_1^2+q_2^2)} & q_1q_2 - \frac{q_2^2}{q_1^2+q_2^2} & X_1 & 0 & 0 & Y_1 \\ 0 & 0 & q_1q_2 - \frac{q_2^2}{q_1^2+q_2^2} & q_2^2 + \frac{q_1q_2}{q_1^2+q_2^2} & X_2 & 0 & 0 & Y_2 \\ -q_1^2 - \frac{q_2^3}{q_1(q_1^2+q_2^2)} & \frac{q_2^2}{q_1^2+q_2^2} - q_1q_2 & 0 & q_1p_2 - q_2p_1 - \frac{q_2(q_1p_2-q_2p_1)}{q_1(q_1^2+q_2^2)} & X_3 & 0 & 0 & Y_3 \\ \frac{q_2^2}{q_1^2+q_2^2} - q_1q_2 & -q_2^2 - \frac{q_1q_2}{q_1^2+q_2^2} & q_2p_1 - q_1p_2 - \frac{q_2(q_2p_1-q_1p_2)}{q_1(q_1^2+q_2^2)} & 0 & X_4 & 0 & 0 & Y_4 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -Y_1 & -Y_2 & -Y_3 & -Y_4 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R = \begin{pmatrix} 0 & 0 & A & B & 0 & Y_1 & X_1 & 0 \\ 0 & 0 & B & C & 0 & Y_2 & X_2 & 0 \\ -A & -B & 0 & D & 0 & Y_3 & X_3 & 0 \\ -B & -C & -D & 0 & 0 & Y_4 & X_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -Y_1 & -Y_2 & -Y_3 & -Y_4 & 0 & 0 & 0 & 0 \\ -X_1 & -X_2 & -X_3 & -X_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where $X = X_{\widetilde{H}} = P\,\mathrm{d}\widetilde{H}$, $Y = X_{\widetilde{K}} = P\,\mathrm{d}\widetilde{K}$, and

$$A = q_1^2 \frac{q_1p_1 + q_2p_2 + 2q_2^2(q_1p_2 - q_2p_1)}{2(q_1^2 + q_2^2)^2},$$

$$B = q_1q_2 \frac{q_1p_1 + q_2p_2 - 2q_1^2(q_1p_2 - q_2p_1)}{2(q_1^2 + q_2^2)^2},$$

$$C = \frac{q_2^2(q_1p_1 + q_2p_2) + 2q_1^4(q_1p_2 - q_2p_1)}{2(q_1^2 + q_2^2)^2},$$

$$D = (q_1p_2 - q_2p_1) \frac{q_1p_1 + q_2p_2 - 2q_1^2(q_1p_2 - q_2p_1)}{2(q_1^2 + q_2^2)^2}.$$

V. FINAL REMARKS

In this paper a procedure to construct tri-Hamiltonian extensions of classical separable systems has been presented. This procedure has been tested in the particularly simple case of the Euclidean plane; however in principle it may be applied also to more general cases. It is articulated in the following steps:

(1) Write down the separation relations of a given system with n degree of freedom in the form involving the Stäckel matrix of the separation coordinates,

$$\begin{pmatrix} a_{11}(q_1) & \cdots & a_{1n}(q_1) \\ a_{21}(q_2) & \cdots & a_{2n}(q_2) \\ \vdots & & \vdots \\ a_{n1}(q_n) & \cdots & a_{nn}(q_n) \end{pmatrix} \begin{pmatrix} \hat{H}_1(\{p_i,q_i\}) \\ \hat{H}_2(\{p_i,q_i\}) \\ \vdots \\ \hat{H}_n(\{p_i,q_i\}) \end{pmatrix} = \begin{pmatrix} \Phi_1(p_1,q_1) \\ \Phi_2(p_2,q_2) \\ \vdots \\ \Phi_n(p_n,q_n) \end{pmatrix}.$$

(2) Transform, through a transformation to a suitable system of coordinates $\{\lambda_i, \mu_i\}$ (and in some case a linear combination of the Hamiltonians) the Stäckel relation in such a way that the ith row contains only different powers of λ_i. This is the most troublesome step: in fact it is not clear if all the Stäckel matrix can be put in this form. However this is possible for all the 11 orthogonal separable webs in $\mathbb{R}^3$, as it is shown in the Appendix.

(3) The separation relation encoded by the ith row of Stäckel matrix is now given by a polynomial in the coordinate λ_i: its coefficients are a set of Hamiltonians H_j obtained from the recombination of the $\hat{H}_j$. These polynomials can be grouped on the basis of their form: a polynomial function is associated to each different form, together with the corresponding tri-Hamiltonian recursion scheme between the H_j. In general there will be $m \leqslant n$ of such functions, labeled $f_1, \ldots, f_m$. The coefficients of the polynomial functions f_l are the extended Hamiltonians $\tilde{H}_j$ and a suitable number of Casimir functions.

(4) Solve the n equations (linear in the n extended Hamiltonians)

$$f_1(\lambda_1;\{\tilde{H}_j\}) = r_1(\lambda_1,\mu_1), \quad \cdots, \quad f_m(\lambda_n;\{\tilde{H}_j\}) = r_n(\lambda_n,\mu_n)$$

so that the explicit form of the extended Hamiltonians is obtained.

(5) The Poisson tensor P on the extended space is obtained in a trivial way from the canonical Poisson tensor. Moreover, from the extended Hamiltonian and the recursion scheme, it is possible to construct the two vector fields X_Q and X_R, and then the two tensors $Q = Q_d - L_{X_Q}P$ and $R = R_d - L_{X_R}P$.

The *conjecture* (proved in the Euclidean plane) suggested by this recipe is that the three tensors P, Q, and R are Poisson tensors mutually compatible; and that, moreover, the m functions

$f_l(\lambda,\mu)$ are common Casimir functions for the two Poisson pencils $Q-\lambda P$ and $R-\mu P$. As a consequence, the extended Hamiltonians $\tilde{H}_j$ satisfy the required tri-Hamiltonian recursion scheme.

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APPENDIX: STÄCKEL MATRICES IN $\mathbb{R}^3$

The aim of this appendix is only to show how to set the Stäckel matrices, for the orthogonally separable coordinate systems in $\mathbb{R}^3$ with the Euclidean metric, in a form suitable for the application of the extension method. The existence of a tri-Hamiltonian extension will not be discussed. Actually, this issue is a particular case of the more general conjecture suggested by the results in the Euclidean plane. In the following list on the left-hand side there are the standard Stäckel matrix and separable Hamiltonians (derived, with minor modifications, from Ref. 4), while on the right-hand side there is the form adapted to the extension algorithm. The Stäckel vector is omitted. In most cases the transformations in the ith row of the Stäckel matrix is multiplied by a suitable function of the ith coordinate only, this operation preserves the separation relation.

Cartesian coordinates,

$$\begin{pmatrix} 1 & 1 & -1 \\ 1 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1+\hat{H}_2-\hat{H}_3$, $H_2=\hat{H}_1-\hat{H}_2-\hat{H}_3$, $H_3=\hat{H}_3$. The coordinates are just renamed.

Elliptic-hyperbolic cylindrical coordinates,

$$\begin{pmatrix} 1 & \dfrac{1}{d^2-k^2} & \dfrac{d^2+3k^2}{d^2-k^2} \\ 1 & \dfrac{1}{s^2-k^2} & \dfrac{s^2+3k^2}{s^2-k^2} \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 1 & 0 \\ \lambda_2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1+\hat{H}_3$, $H_2=\hat{H}_2+4k^2\hat{H}_3$, $H_3=\hat{H}_3$. It is also set $\lambda_1=d^2-k^2$, $\lambda_2=s^2-k^2$.

Circular cylindrical coordinates,

$$\begin{pmatrix} 1 & \dfrac{1}{r^2} & \dfrac{1+r^2}{r^2} \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1+\hat{H}_3$, $H_2=\hat{H}_2+\hat{H}_3$, $H_3=\hat{H}_3$. It is also set $\lambda_1=r^2$.

Parabolic cylindrical coordinates,

$$\begin{pmatrix} 1 & \dfrac{1}{d_+} & 1 \\ 1 & \dfrac{1}{d_-} & 1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 1 & 0 \\ \lambda_2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1+\hat{H}_3$, $H_2=\hat{H}_2$, $H_3=\hat{H}_3$. The coordinates are just renamed.

Prolate spheroidal coordinates,

$$\begin{pmatrix} \dfrac{d^2}{d^2-k^2} & \dfrac{1}{d^2-k^2} & \dfrac{1}{(d^2-k^2)^2} \\ \dfrac{s^2}{s^2-k^2} & \dfrac{1}{s^2-k^2} & \dfrac{1}{(s^2-k^2)^2} \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1^2 & \lambda_1 & 1 \\ \lambda_2^2 & \lambda_2 & 1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1$, $H_2=\hat{H}_2+k^2\hat{H}_1$, $H_3=\hat{H}_3$. It is also set $\lambda_1=d^2-k^2$, $\lambda_2=s^2-k^2$.

Oblate spheroidal coordinates,

$$\begin{pmatrix} 1 & \dfrac{1}{d^2-k^2} & \dfrac{1}{d^2(d^2-k^2)} \\ 1 & \dfrac{1}{s^2-k^2} & \dfrac{1}{s^2(s^2-k^2)} \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix}$$

multiplying the first row by $d^2(d^2-k^2)$ and the second by $s^2(s^2-k^2)$, the Stäckel relation is equivalent to

$$\begin{pmatrix} d^4-k^2d^2 & d^2 & 1 \\ s^4-k^2s^2 & s^2 & 1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1^2 & \lambda_1 & 1 \\ \lambda_2^2 & \lambda_2 & 1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the new Hamiltonians are $H_1=\hat{H}_1$, $H_2=\hat{H}_2-k^2\hat{H}_1$, $H_3=\hat{H}_3$. It is also set $\lambda_1=d^2$, $\lambda_2=s^2$.

Spherical coordinates,

$$\begin{pmatrix} 1 & \dfrac{1}{r^2} & 0 \\ 0 & 1 & \dfrac{1}{\sin^2\theta} \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 1 & 0 \\ 0 & 1 & \lambda_2 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where it is set $\lambda_1=r^2$, $\lambda_2=\sin^2\theta$.

Parabolic coordinates,

$$\begin{pmatrix} 1 & \frac{1}{d_+} & \frac{1}{d_+^2} \\ 1 & \frac{1}{d_-} & \frac{1}{d_-^2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1 & 1 & 0 \\ \lambda_2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the coordinates are just renamed.

Ellipsoidal coordinates,

$$\begin{pmatrix} \frac{u^2}{\Pi_i(u-a_i)} & \frac{u}{\Pi_i(u-a_i)} & \frac{1}{\Pi_i(u-a_i)} \\ \frac{v^2}{\Pi_i(v-a_i)} & \frac{v}{\Pi_i(v-a_i)} & \frac{1}{\Pi_i(v-a_i)} \\ \frac{w^2}{\Pi_i(w-a_i)} & \frac{w}{\Pi_i(w-a_i)} & \frac{1}{\Pi_i(w-a_i)} \end{pmatrix} \begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1^2 & \lambda_1 & 1 \\ \lambda_2^2 & \lambda_2 & 1 \\ \lambda_3^2 & \lambda_3 & 1 \end{pmatrix} \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the coordinates are just renamed.

Paraboloidal coordinates,

$$\begin{pmatrix} \frac{u^2}{(u^2-k^2)} & \frac{u}{(u^2-k^2)} & \frac{1}{(u^2-k^2)} \\ \frac{v^2}{(v^2-k^2)} & \frac{v}{(v^2-k^2)} & \frac{1}{(v^2-k^2)} \\ \frac{w^2}{(w^2-k^2)} & \frac{w}{(w^2-k^2)} & \frac{1}{(w^2-k^2)} \end{pmatrix} \begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} \lambda_1^2 & \lambda_1 & 1 \\ \lambda_2^2 & \lambda_2 & 1 \\ \lambda_3^2 & \lambda_3 & 1 \end{pmatrix} \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the coordinates are just renamed.

Spherical-conical coordinates,

$$\begin{pmatrix} 0 & \frac{u}{\Pi_i(u-a_i)} & \frac{1}{\Pi_i(u-a_i)} \\ 0 & \frac{v}{\Pi_i(v-a_i)} & \frac{1}{\Pi_i(v-a_i)} \\ \frac{1}{w} & \frac{1}{w^2} & 0 \end{pmatrix} \begin{pmatrix} \hat{H}_1 \\ \hat{H}_2 \\ \hat{H}_3 \end{pmatrix} \to \begin{pmatrix} 0 & \lambda_1 & 1 \\ 0 & \lambda_2 & 1 \\ \lambda_3 & 1 & 0 \end{pmatrix} \begin{pmatrix} H_1 \\ H_2 \\ H_3 \end{pmatrix},$$

where the coordinates are just renamed.

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The very unusual properties of the resolvent, heat kernel, and zeta function for the operator $-d^2/dr^2-1/(4r^2)$

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In this paper we analyze the resolvent, the heat kernel and the spectral zeta function of the operator $-d^2/dr^2-1/(4r^2)$ over the finite interval. The structural properties of these spectral functions depend strongly on the chosen self-adjoint realization of the operator, a choice being made necessary because of the singular potential present. Only for the Friedrichs realization standard properties are reproduced, for all other realizations highly nonstandard properties are observed. In particular, for $k \in \mathbb{N}$ we find terms like $(\log t)^{-k}$ in the small-t asymptotic expansion of the heat kernel. Furthermore, the zeta function has $s=0$ as a logarithmic branch point.
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I. INTRODUCTION

A. Zeta functions and an unusual example

It is well known that the zeta function of a Laplacian over a smooth compact manifold, with or without boundary, defines a meromorphic function on $\mathbb{C}$ with simple poles at prescribed half-integer values depending on the dimension of the manifold.[21] (For a manifold with boundary, we put local boundary conditions, e.g., Dirichlet conditions.) These properties have far reaching applications in physics as well as mathematics, e.g., in the context of Casimir energies, effective actions and analytic torsion; see, for example, Refs. 12–14, 25, 28, and 41.

Surprisingly, there is a completely natural example of a zeta function for which the described properties break down and which has no meromorphic extension to $\mathbb{C}$. Let $\Omega \subset \mathbb{R}^2$ be any compact region and take polar coordinates $(x,y) \leftrightarrow (r,\theta)$ centered at any fixed point in Ω. Then in these coordinates, the standard Laplacian on $\mathbb{R}^2$ takes the form

$$\Delta_{\mathbb{R}^2} = -\partial_x^2 - \partial_y^2 = -\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\theta^2,$$

and the measure transforms to $dx\,dy = r\,dr\,d\theta$. A short computation shows that

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$$\Delta_{\mathbb{R}^2}\phi = \left(-\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\theta^2\right)\phi = \mathcal{R}^{-1}\left(-\partial_r^2 + \frac{1}{r^2}\left(-\partial_\theta^2 - \frac{1}{4}\right)\right)\mathcal{R}\phi,$$

where $\mathcal{R}$ is the multiplication map by $r^{1/2}$, which is an isometry from $L^2(\Omega, r\,\mathrm{d}r\,\mathrm{d}\theta)$ to $L^2(\Omega, \mathrm{d}r\,\mathrm{d}\theta)$. Hence, the following two operators are equivalent under $\mathcal{R}$:

$$\Delta_{\mathbb{R}^2} \leftrightarrow -\partial_r^2 + \frac{1}{r^2}A, \quad \text{where } A = -\partial_\theta^2 - \frac{1}{4}.$$

In the zero eigenspace of $-\partial_\theta^2$, we obtain the operator of the form $-\partial_r^2 - (1/4r^2)$. Then this Laplace type operator has many different self-adjoint realizations parametrized by angles $\theta \in [0, \pi)$; the angle $\theta = \pi/2$ corresponds to the so-called Friedrichs realization. Each realization has a discrete spectrum.[35] Consider any one of the realizations, say Δ_θ, with $\theta \neq \pi/2$ and form the corresponding zeta function,

$$\zeta(s, \Delta_\theta) := \sum_{\lambda_j \neq 0} \frac{1}{\lambda_j^s},$$

where the λ_j's are the eigenvalues of Δ_θ. The shocking fact is that *every* such zeta function corresponding to an angle $\theta \in [0, \pi)$, except $\theta = \pi/2$, does not have a meromorphic extension to $\mathbb{C}$; in fact each such zeta function has a logarithmic branch cut with $s = 0$ as the branch point.

B. Self-adjoint realizations

The properties of the Laplace operator considered above boil down to the main object of consideration in this paper,

$$\Delta := -\frac{d^2}{\mathrm{d}r^2} - \frac{1}{4r^2} \quad \text{over } [0, R]. \tag{1.1}$$

In Sec. II we work out an explicit description of the maximal domain of Δ. In order to choose a self-adjoint realization of Δ, we first fix a boundary condition for Δ at $r = R$; it turns out that any such boundary condition for $\phi \in \mathcal{D}_{\max}(\Delta)$ must be of the form (see Sec. IV)

$$\cos\theta_2 \phi'(R) + \sin\theta_2 \phi(R) = 0. \tag{1.2}$$

In other words, the boundary conditions we can choose at $r = R$ are parametrized by angles $\theta_2 \in [0, \pi)$. Note that the Dirichlet condition is when $\theta_2 = \pi/2$ and the Neumann condition is when $\theta_2 = 0$. Let us henceforth *fix* an angle $\theta_2 \in [0, \pi)$ and consider Δ with the condition in (1.2). At $r = 0$, the operator Δ is singular and a limiting procedure $r \to 0$ must be used to define boundary conditions. As shown in Sec. III (see also Sec. IV), the self-adjoint realizations of Δ with the condition (1.2) are again parametrized by angles $\theta_1 \in [0, \pi)$; the paper by Kochubeĭ[31] is perhaps one of the earliest references to contain such a parametrization. It turns out that $\theta_1 = \pi/2$ corresponds to the Friedrichs realization.

As we will show in Theorem 2.1, $\phi \in \mathcal{D}_{\max}(\Delta)$ if and only if it can be written in the form

$$\phi = c_1(\phi) r^{1/2} + c_2(\phi) r^{1/2} \log r + \mathcal{O}(r^{3/2}),$$

where $c_1(\phi)$ and $c_2(\phi)$ are constants depending on ϕ. In terms of these constants, given angles $\theta_1, \theta_2 \in [0, \pi)$, we consider the operator

$$\Delta_L := \Delta : \mathcal{D}_L \to L^2([0, R]),$$

where

$$\mathcal{D}_L = \{\phi \in \mathcal{D}_{\max}(\Delta) | \cos\,\theta_1 c_1(\phi) + \sin\,\theta_1 c_2(\phi) = 0, \cos\,\theta_2 \phi'(R) + \sin\,\theta_2 \phi(R) = 0\}.$$

Here, the subscript "L" represents the two-dimensional subspace $L \subset \mathbb{C}^4$ defined by

$$L := \{(z_1, z_2, z_3, z_4) \in \mathbb{C}^4 | \cos\,\theta_1 z_1 + \sin\,\theta_1 z_2 = 0, \cos\,\theta_2 z_3 + \sin\,\theta_2 z_4 = 0\}.$$

This vector space is a Lagrangian subspace of $\mathbb{C}^4$ with respect to a natural Hermitian symplectic form intimately related to self-adjoint realizations of Δ; see Sec. III. For general references on this relation see; Refs. 23, 24, 27, and 31–34. For a study of adjoints of "cone operators" (in the sense of Schulze) see Ref. 19. For properties of resolvents of cone operators see, for example, Refs. 20 and 42.

C. The resolvent, heat kernel, and zeta function

When $\theta_1 = \pi/2$ (the Friedrichs realization), the following properties concerning the resolvent, heat kernel, and zeta function are well known; see for example, Brüning and Seeley,[7,8] Falomir *et al.*,[15] or Mooers.[38] With $\theta_1 = \pi/2$, the following properties hold.

Theorem 1.1 (cf. Refs. 8, 15, and 38): *Fixing a boundary condition* (1.2) *at* $r=R$, *let* Δ_L *denote the corresponding Friedrichs realization* (*that is, take* $\theta_1 = \pi/2$). *Then*

(1) *Let* $\Lambda \subset \mathbb{C}$ *be any sector (solid angle) not intersecting the positive real axis. Then as* $|\lambda| \to \infty$ *with* $\lambda \in \Lambda$, *we have*

$$\mathrm{Tr}(\Delta_L - \lambda)^{-1} \sim \sum_{k=1}^{\infty} a_k (-\lambda)^{-k/2}.$$

(2) *As* $t \to 0$, *we have*

$$\mathrm{Tr}(e^{-t\Delta_L}) \sim \sum_{k=0}^{\infty} \beta_k t^{(k-1)/2}.$$

(3) *The zeta function*

$$\zeta(s, \Delta_L) = \mathrm{Tr}(\Delta_L^{-s})$$

extends from $\Re s > 1/2$ *to a meromorphic function on* $\mathbb{C}$ *with poles at* $s = 1/2 - k$ *for* $k = 0, 1, 2, \ldots$.

These properties are "usual" in that they remain valid, with appropriate changes, to Laplace-type operators on compact manifolds (with or without boundary); see for example, Gilkey's book[21] for a thorough treatment. The first result of this paper shows that for *any* other realization, these properties are completely destroyed; see also Ref. 29.

Theorem 1.2: *With any boundary condition* (1.2) *fixed at* $r=R$, *choose a self-adjoint realization* Δ_L *of the resulting operator that is not the Friedrichs realization*. (*That is, take* $\theta_1 \neq \pi/2$). *Let* $\kappa = \log 2 - \gamma - \tan\,\theta_1$ *where* γ *is the Euler constant*. *Then the following properties hold*:

(1) *Let* $\Lambda \subset \mathbb{C}$ *be any sector (solid angle) not intersecting the positive real axis*. *Then as* $|\lambda| \to \infty$ *with* $\lambda \in \Lambda$, *we have*

$$\mathrm{Tr}(\Delta_L - \lambda)^{-1} \sim \frac{1}{(-\lambda)(\log(-\lambda) - 2\kappa)} + \sum_{k=1}^{\infty} b_k (-\lambda)^{-k/2}.$$

(2) *As* $t \to 0$, *we have* (*here* $\Im$ *denotes* "*imaginary part of*")

$$\mathrm{Tr}(e^{-t\Delta_L}) \sim \frac{1}{\pi} \Im \left(\int_1^{\infty} e^{-tx} \frac{1}{x(\log x + i\pi - 2\kappa)} dx \right) + \sum_{k=0}^{\infty} \beta_k t^{(k-1)/2}.$$

(3) *The zeta function* $\zeta(s,\Delta_L)$ *can be written in the form*

$$\zeta(s,\Delta_L) = -\frac{e^{-2s\kappa}\sin \pi s}{\pi}\log s + \zeta_L(s),$$

where $\zeta_L(s)$ *extends from* $\Re s > 1/2$ *to a holomorphic function on* $\mathbb{C}$ *with poles at* $s = 1/2 - k$ *for* $k = 0,1,2,\ldots$. *In particular,* $\zeta(s,\Delta_L)$ *has* $s=0$ *as a logarithmic branch point*

Remark 1.3: The authors have never seen a natural *geometric* differential operator with discrete spectrum on a compact manifold having a spectral zeta function with properties of the sort described in this theorem.

Remark 1.4: The first term in assertion (1) can be expanded further if needed. In the formulation of this theorem we leave it in this more useful compact form.

Remark 1.5: The same kind of remark holds for the first term in assertion (2). Expanding further we obtain the following expansion: As $t \to 0$, we have

$$\mathrm{Tr}(e^{-t\Delta_L}) \sim \sum_{k=1}^{\infty} \alpha_k (\log t)^{-k} + \sum_{k=0}^{\infty} \beta_k t^{(k-1)/2} \tag{1.3}$$

with the α_k's depending on κ via (here $\Im$ denotes "imaginary part of")

$$\alpha_k = -\frac{1}{k\pi}\Im\left(\int_1^{\infty} e^{-x}(\log x + i\pi - 2\kappa)^k \, \mathrm{d}x\right), \quad k = 1,2,3,\ldots .$$

The expansion (1.3) is misleading as written because for $k>1$, the terms $\beta_k t^{(k-1)/2}$ are subleading to any of the inverse log terms. However, we interpret the first sum in the expansion (1.3) to mean that for all N, we have

$$\frac{1}{\pi}\Im\left(\int_1^{\infty} e^{-tx}\frac{1}{x(\log x + i\pi - 2\kappa)}\mathrm{d}x\right) = \sum_{k=1}^{N} \alpha_k (\log t)^{-k} + \mathcal{O}((\log t)^{-N-1}).$$

D. Explicit formula for the zeta determinant

Our second result is an explicit formula for a regularized determinant. For concreteness, we shall impose the Dirichlet boundary condition at $r=R$. That is, given an angle $\theta \in [0,\pi)$ with $\theta \neq \pi/2$, we consider the operator

$$\Delta_\theta := \Delta : \mathcal{D}_\theta \to L^2([0,R]),$$

where

$$\mathcal{D}_\theta = \{\phi \in \mathcal{D}_{\max}(\Delta) \,|\, \cos\theta c_1(\phi) + \sin\theta c_2(\phi) = 0, \phi(R) = 0\}.$$

Then from Theorem 1.2, the zeta function $\zeta(s,\Delta_\theta)$ has the following form:

$$\zeta(s,\Delta_\theta) = -\frac{e^{-2s\kappa}\sin \pi s}{\pi}\log s + \zeta_\theta(s),$$

where $\zeta_\theta(s)$ extends from $\Re s > 1/2$ to a holomorphic function on $\mathbb{C}$ with poles at $s = 1/2 - k$ for $k = 0,1,2,\ldots$.

In particular, $\zeta(s,\Delta_\theta)$ has the form

$$\zeta(s,\Delta_\theta) \sim -s\log s + \mathcal{O}(s^2\log s) + \text{holomorphic} \quad \text{as } s\to 0. \tag{1.4}$$

In particular,

$$\zeta'(s,\Delta_\theta) \sim -\log s + \mathcal{O}(s\log s) + \text{holomorphic} \quad \text{as } s\to 0,$$

so the ζ-regularized determinant $\det(\Delta_\theta) := \exp(-\zeta'(0,\Delta_\theta))$ is *not* defined However, from (1.4), we see that

$$\zeta_{\text{reg}}(s,\Delta_\theta) := \zeta(s,\Delta_\theta) + s\log s$$

does have a well-defined derivative at $s=0$. For this reason, we define

$$\det{}_{\text{reg}}(\Delta_\theta) := \exp(-\zeta'_{\text{reg}}(0,\Delta_\theta)).$$

In the following theorem, we give a beautiful explicit formula for this regularized determinant.

Theorem 1.6: *For any* $\theta\in[0,\pi)$ *with* $\theta\neq\pi/2$, *we have*

$$\det{}_{\text{reg}}(\Delta_\theta) = \begin{cases} 2\sqrt{2\pi R}\,e^{\gamma}(\tan\theta - \log R), & \tan\theta \neq \log R, \\ \sqrt{\dfrac{\pi R}{2}}\,e^{\gamma}R^2, & \tan\theta = \log R. \end{cases}$$

We remark that when $\theta=\pi/2$, the zeta function $\zeta(s,\Delta_\theta)$ is regular at $s=0$ and we can also compute the (usual) ζ-regularized determinant: For $\theta=\pi/2$, we have

$$\det(\Delta_\theta) = \sqrt{2\pi R},$$

a well known result, see, e.g., Theorem 2.3 of Ref. 36, Proposition 5.2 of Ref. 37.

We now outline this article. In Secs. II–IV we study the self-adjoint realizations of our main operator using the Hermitian symplectic theory due to Gelfand (Ref. 39, p. 1); cf. also Refs. 15, 31–33, 37, 38, and 40. Although some of this material can be found piecemeal throughout the literature, we present all the details here in order to keep our paper elementary, self-contained, and "user-friendly." In Secs. V–VIII we prove Theorem 1.2 in the special case that the Dirichlet boundary condition is chosen at $r=R$ and in Sec. IX we prove Theorem 6, all using the contour integration method developed in Refs. 3–5. In Sec. X we prove Theorem 1.2 in full generality. Finally, in the Appendix, we explicitly calculate the resolvent of Δ_θ, which is needed at various places in our analysis.

II. THE MAXIMAL DOMAIN

Our first order of business is to characterize the self-adjoint realizations of the operator in (1.1); for general references on self-adjoint realizations and their applications to physics see, e.g., Refs. 2, 6, 10, 11, 16–18, 31–34, 40, and 44 To do so, we first need to determine the maximal domain of Δ:

$$\mathcal{D}_{\max}(\Delta) := \{\phi\in L^2([0,R]) \,|\, \Delta\phi\in L^2([0,R])\}.$$

For a quick review, $\Delta\phi$ is understood in the distributional sense; thus, $\Delta\phi$ is the functional on test functions $C_c^\infty((0,R))$ defined by

$$(\Delta\phi)(\xi) := \int_0^R \Delta\xi(r)\overline{\phi(r)}\mathrm{d}r \quad \text{for all } \xi\in C_c^\infty((0,R)).$$

Then $\Delta\phi\in L^2([0,R])$ means that the distribution $\Delta\phi: C_c^\infty((0,R))\to\mathbb{C}$ is represented by an L^2 function in the sense that there is a function $f\in L^2([0,R])$ such that

$$\int_0^R \Delta\xi(r)\overline{\phi(r)}\mathrm{d}r = \langle \xi, f\rangle \quad \text{for all } \xi \in C_c^\infty((0,R)),$$

where $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product (conjugate linear in the second slot) on $L^2([0,R])$. The following theorem is inspired by Falomir *et al.* (Ref. 15, Lemma 2.1).

Theorem 2.1: *$\phi \in \mathcal{D}_{\max}(\Delta)$ if and only if ϕ can be written in the form*

$$\phi = c_1(\phi)r^{1/2} + c_2(\phi)r^{1/2}\log r + \tilde{\phi}, \tag{2.1}$$

where $c_1(\phi), c_2(\phi)$ are constants and $\tilde{\phi}$ is a continuously differentiable function on $[0,R]$ such that $\tilde{\phi}(r) = \mathcal{O}(r^{3/2})$, $\tilde{\phi}'(r) = \mathcal{O}(r^{1/2})$, and $\Delta\tilde{\phi} \in L^2([0,R])$.

Proof: Since

$$\Delta(c_1 r^{1/2} + c_2 r^{1/2}\log r) = 0,$$

it follows that any ϕ of the stated form is in $\mathcal{D}_{\max}(\Delta)$. Now let $\phi \in \mathcal{D}_{\max}(\Delta)$; then $\Delta\phi = f \in L^2([0,R])$. Let us define $\psi := r^{-1/2}\phi$ so that $\phi = r^{1/2}\psi$. Then

$$f = -\phi'' - \frac{1}{4r^2}\phi = \frac{1}{4}r^{-3/2}\psi - r^{-1/2}\psi' - r^{1/2}\psi'' - \frac{1}{4}r^{-3/2}\psi = -r^{-1/2}\psi' - r^{1/2}\psi''.$$

After multiplication by $r^{1/2}$, we get

$$\psi' + r\psi'' = -r^{1/2}f \Rightarrow (r\psi')' = -r^{1/2}f.$$

Since $r^{1/2}$ and f are in $L^2([0,R])$, by the Cauchy-Schwartz inequality, we know that $r^{1/2}f$ is in $L^1([0,R])$, therefore we can conclude that

$$\psi' = \frac{c_2}{r} - \frac{1}{r}\int_0^r t^{1/2}f(t)\mathrm{d}t. \tag{2.2}$$

Notice that by Cauchy-Schwartz,

$$\left|\int_0^r t^{1/2}f(t)\mathrm{d}t\right| \leqslant \sqrt{\int_0^r t\,\mathrm{d}t}\cdot\|f\|_2 = \frac{r}{\sqrt{2}}\|f\|_2. \tag{2.3}$$

Thus, the second term on the right-hand side in (2.2) is in $L^1([0,R])$. Therefore, from (2.2) we see that

$$\psi(r) = c_1 + c_2\log r - \int_0^r \frac{1}{x}\int_0^x t^{1/2}f(t)\mathrm{d}t\,\mathrm{d}x,$$

or, since $\phi = r^{1/2}\psi$, we get

$$\phi(r) = c_1 r^{1/2} + c_2 r^{1/2}\log r + \tilde{\phi}, \quad \tilde{\phi} := -r^{1/2}\int_0^r \frac{1}{x}\int_0^x t^{1/2}f(t)\mathrm{d}t\,\mathrm{d}x.$$

By (2.3), we have

$$\left|\int_0^r \frac{1}{x}\int_0^x t^{1/2}f(t)\mathrm{d}t\,\mathrm{d}x\right| \leqslant \int_0^r \frac{1}{\sqrt{2}}\|f\|_2\,\mathrm{d}x = \frac{r}{\sqrt{2}}\|f\|_2.$$

From this estimate, it follows that $\tilde{\phi}(r) = \mathcal{O}(r^{3/2})$ and $\tilde{\phi}'(r) = \mathcal{O}(r^{1/2})$. □

III. SELF-ADJOINT REALIZATIONS

Choosing a linear subspace $\mathcal{D}\subset\mathcal{D}_{\max}(\Delta)$, we say that

$$\Delta_{\mathcal{D}} := \Delta:\mathcal{D}\to L^2([0,R])$$

is *self-adjoint* (in which case $\Delta_{\mathcal{D}}$ is called a *self-adjoint realization* of Δ) if

$$\{\psi\in\mathcal{D}_{\max}(\Delta)|\langle\Delta\phi,\psi\rangle=\langle\phi,\Delta\psi\rangle \text{ for all } \phi\in\mathcal{D}\}=\mathcal{D};$$

in other words, Δ is symmetric on $\mathcal{D}$ and adding any elements to $\mathcal{D}$ will destroy this symmetry.

In order to determine if Δ has any self-adjoint realization, we need to analyze the quadratic form

$$\langle\phi,\Delta\psi\rangle-\langle\Delta\phi,\psi\rangle \quad \text{for } \phi,\psi\in\mathcal{D}_{\max}(\Delta).$$

It turns out that this difference is related to finite-dimensional symplectic linear algebra. Let us define

$$\omega:\mathbb{C}^4\times\mathbb{C}^4\to\mathbb{C}$$

by

$$\omega(v,w) := v_1\overline{w_2}-v_2\overline{w_1}+v_3\overline{w_4}-v_4\overline{w_3}. \tag{3.1}$$

The function ω is Hermitian antisymmetric and nondegenerate; for this reason, ω is called a *Hermitian symplectic form*.

Theorem 3.1: *Let* $\phi,\psi\in\mathcal{D}_{\max}(\Delta)$ *be written in the form* (2.1), *i.e.*,

$$\phi=c_1(\phi)r^{1/2}+c_2(\phi)r^{1/2}\log r+\tilde{\phi},$$

where $\tilde{\phi}$ *is continuously differentiable with* $\tilde{\phi}(r)=\mathcal{O}(r^{3/2})$, $\tilde{\phi}'(r)=\mathcal{O}(r^{1/2})$, *and* $\Delta\tilde{\phi}\in L^2([0,R])$, *and with a similar formula holding for* ψ. *Then*,

$$\langle\phi,\Delta\psi\rangle-\langle\Delta\phi,\psi\rangle=\omega(\vec{\phi},\vec{\psi}),$$

where ω *is the Hermitian symplectic form defined above and* $\vec{\phi},\vec{\psi}\in\mathbb{C}^4$ *are the vectors*

$$\vec{\phi} := (c_1(\phi),c_2(\phi),\phi'(R),\phi(R)), \quad \vec{\psi} := (c_1(\psi),c_2(\psi),\psi'(R),\psi(R)).$$

Proof: We have

$$\begin{aligned}\langle\phi,\Delta\psi\rangle-\langle\Delta\phi,\psi\rangle &= \lim_{\varepsilon\to0}\int_\varepsilon^R(\phi(r)\overline{\Delta\psi(r)}-\Delta\phi(r)\overline{\psi(r)})\mathrm{d}r=\lim_{\varepsilon\to0}\int_\varepsilon^R\frac{d}{\mathrm{d}r}(-\phi(r)\overline{\psi'(r)}+\phi'(r)\overline{\psi(r)})\mathrm{d}r\\ &=\lim_{\varepsilon\to0}(\phi(\varepsilon)\overline{\psi'(\varepsilon)}-\phi'(\varepsilon)\overline{\psi(\varepsilon)})+(\phi'(R)\overline{\psi(R)}-\phi(R)\overline{\psi'(R)}).\end{aligned} \tag{3.2}$$

Recall that

$$\phi=c_1(\phi)r^{1/2}+c_2(\phi)r^{1/2}\log r+\tilde{\phi}, \quad \psi=c_1(\psi)r^{1/2}+c_2(\psi)r^{1/2}\log r+\tilde{\psi},$$

where $\tilde{\phi}$ and $\tilde{\psi}$ are continuously differentiable functions on $[0,R]$ such that $\tilde{\phi}(r),\tilde{\psi}(r)=\mathcal{O}(r^{3/2})$, $\tilde{\phi}'(r),\tilde{\psi}'(r)=\mathcal{O}(r^{1/2})$. Taking derivatives, we get

$$\phi'=\frac{c_1(\phi)}{2}r^{-1/2}+\frac{c_2(\phi)}{2}r^{-1/2}(\log r+2)+\tilde{\phi}'$$

and similarly for ψ'. It follows that

$$\phi(\varepsilon)\overline{\psi'(\varepsilon)} = \frac{c_1(\phi)\overline{c_1(\psi)}}{2} + \frac{c_1(\phi)\overline{c_2(\psi)}}{2}(\log\varepsilon + 2) + \frac{c_2(\phi)\overline{c_1(\psi)}}{2}\log\varepsilon + \frac{c_2(\phi)\overline{c_2(\psi)}}{2}\log\varepsilon(\log\varepsilon + 2) + o(1)$$

and similarly for $\phi'(\varepsilon)\overline{\psi(\varepsilon)}$. Subtracting, we get

$$\phi(\varepsilon)\overline{\psi'(\varepsilon)} - \phi'(\varepsilon)\overline{\psi(\varepsilon)} = c_1(\phi)\overline{c_2(\psi)} - c_2(\phi)\overline{c_1(\psi)} + o(1).$$

Combining this with (3.2) proves our result. □

Recall that a subspace $L \subset \mathbb{C}^4$ is called *Lagrangian* if $L^{\perp_\omega} = L$ where $L^{\perp_\omega}$ is the orthogonal complement of L with respect to ω; explicitly, L is Lagrangian means

$$\{w \in \mathbb{C}^4 | \omega(v,w) = 0 \text{ for all } v \in L\} = L.$$

We now have our main result.

Theorem 3.2: *Self-adjoint realizations of* Δ *are in one-to-one correspondence with Lagrangian subspaces of* $\mathbb{C}^4$ *in the sense that given any Lagrangian subspace* $L \subset \mathbb{C}^4$, *defining*

$$\mathcal{D}_L := \{\phi \in \mathcal{D}_{\max}(\Delta) | \vec{\phi} \in L\}$$

the operator

$$\Delta_L := \Delta : \mathcal{D}_L \to L^2([0,R])$$

is self-adjoint and any self-adjoint realization of Δ *is of the form* $\mathcal{D}_L$ *for some Lagrangian* $L \subset \mathbb{C}^4$.

Proof: By definition,

$$\Delta_{\mathcal{D}} := \Delta : \mathcal{D} \to L^2([0,R])$$

is *self-adjoint* means

$$\{\psi \in \mathcal{D}_{\max}(\Delta) | \langle \Delta\phi, \psi\rangle = \langle \phi, \Delta\psi\rangle \text{ for all } \phi \in \mathcal{D}\} = \mathcal{D}.$$

By Theorem 3.1, we can write this as: $\Delta_{\mathcal{D}}$ is self-adjoint if and only if

$$\omega(\vec{\phi}, \vec{\psi}) = 0 \text{ for all } \phi \in \mathcal{D} \Leftrightarrow \psi \in \mathcal{D}. \tag{3.3}$$

Suppose that $\Delta_{\mathcal{D}}$ is self-adjoint and define $L := \{\vec{\phi} \in \mathbb{C}^4 | \phi \in \mathcal{D}\}$; we shall prove that L is Lagrangian. Let $w \in L$ and choose $\psi \in \mathcal{D}$ such that $\vec{\psi} = w$. Then by (3.3), $\omega(\vec{\phi}, w) = 0$ for all $\phi \in \mathcal{D}$. Therefore, $\omega(v, w) = 0$ for all $v \in L$. Conversely, let $w \in \mathbb{C}^4$ and assume that $\omega(v, w) = 0$ for all $v \in L$. Choose $\psi \in \mathcal{D}_{\max}(\Delta)$ such that $\vec{\psi} = w$; e.g., if $w = (w_1, w_2, w_3, w_4)$, then

$$\psi := w_1 r^{1/2} + w_2 r^{1/2}\log r + (w_3 - w_4)(r - R) + w_4 r \tag{3.4}$$

will do. Then $\omega(v, w) = 0$ for all $v \in L$ implies that $\omega(\vec{\phi}, \vec{\psi}) = 0$ for all $\phi \in \mathcal{D}$, which by (3.3), implies that $\psi \in \mathcal{D}$, which further implies that $w = \vec{\phi} \in L$.

Now let $L \subset \mathbb{C}^4$ be Lagrangian; we shall prove that Δ_L is self-adjoint, that is, (3.3) holds. Let $\psi \in \mathcal{D}_L$. Then, since L is Lagrangian, we automatically have $\omega(\vec{\phi}, \vec{\psi}) = 0$ for all $\phi \in \mathcal{D}_L$. Conversely, let $\psi \in \mathcal{D}_{\max}(\Delta)$ and assume that $\omega(\vec{\phi}, \vec{\psi}) = 0$ for all $\phi \in \mathcal{D}_L$. By the construction (3.4) given any $v \in L$ we can find a $\phi \in \mathcal{D}_{\max}(\Delta)$ such that $\vec{\phi} = v$. Therefore, $\omega(\vec{\phi}, \vec{\psi}) = 0$ for all $\phi \in \mathcal{D}_L$ implies that $\omega(v, \vec{\psi}) = 0$ for all $v \in L$, which by the Lagrangian condition on L, implies that $\vec{\psi} \in L$. This shows that $\psi \in \mathcal{D}_L$ and our proof is complete. □

IV. MORE ON LAGRANGIAN SUBSPACES

The symplectic form $\omega : \mathbb{C}^4 \times \mathbb{C}^4 \to \mathbb{C}$ defined in (3.1) is naturally separated into two parts:

$$\omega(v,w) = \omega_0((v_1,v_2),(w_1,w_2)) + \omega_0((v_3,v_4),(w_3,w_4)), \tag{4.1}$$

where

$$\omega_0{:}\mathbb{C}^2 \times \mathbb{C}^2 \to \mathbb{C} \text{ is defined by } \omega_0(v,w) = v_1\overline{w_2} - v_2\overline{w_1}.$$

The first ω_0 appearing in (4.1) corresponds to the singularity at $r=0$ and the second ω_0 in (4.1) corresponds to the boundary $r=R$. For this reason, it is natural to focus on Lagrangian subspaces $L\subset\mathbb{C}^4$ of the form $L=L_1\oplus L_2$ where $L_i\subset\mathbb{C}^2$ is Lagrangian with respect to ω_0. With this in mind, let us characterize all such Lagrangian subspaces of $\mathbb{C}^2$. First, we observe the following.

Lemma 4.1: We can write

$$\omega_0(v,w) = \langle Gv,w\rangle \text{ for all } v,w \in \mathbb{C}^2,$$

where $\langle,\rangle$ *denotes the inner product on* $\mathbb{C}^2$ *and* $G=\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)$.

Recalling that $L\subset\mathbb{C}^2$ is Lagrangian means that

$$\{w \in \mathbb{C}^2 | \omega_0(v,w) = 0 \text{ for all } v \in L\} = L,$$

from this lemma, it is straightforward to show that

$$L \subset \mathbb{C}^2 \text{ is Lagrangian if and only if } GL^{\perp} = L,$$

where $L^{\perp}$ is the orthogonal complement of L with respect to the inner product $\langle,\rangle$. From this, one can easily prove the following main result in this section.

Theorem 4.2: *$L\subset\mathbb{C}^2$ is Lagrangian if and only if $L=L_\theta$ for some $\theta\in\mathbb{R}$ where*

$$L_\theta = \{(x,y) \in \mathbb{C}^2 | \cos\theta x + \sin\theta y = 0\}.$$

Notice that we can restrict to $0\leqslant\theta<\pi$ in Theorem 4.2. Let θ_1,θ_2 be two such angles and set $L:=L_{\theta_1}\oplus L_{\theta_2}$. As in (2.1), we write $\phi\in\mathcal{D}_{\max}(\Delta)$ as

$$\phi = c_1(\phi)r^{1/2} + c_2(\phi)r^{1/2}\log r + \tilde{\phi},$$

where $\tilde{\phi}$ is continuously differentiable with $\tilde{\phi}(r)=\mathcal{O}(r^{3/2})$, $\tilde{\phi}'(r)=\mathcal{O}(r^{1/2})$, and $\Delta\tilde{\phi}\in L^2([0,R])$. Then as a consequence of Theorem 3.2, we know that

$$\Delta_L := \Delta{:}\mathcal{D}_L \to L^2([0,R]) \tag{4.2}$$

is self-adjoint, where

$$\mathcal{D}_L = \{\phi \in \mathcal{D}_{\max}(\Delta) | \cos\theta_1 c_1(\phi) + \sin\theta_1 c_2(\phi) = 0, \cos\theta_2\phi'(R) + \sin\theta_2\phi(R) = 0\}.$$

When $\theta_1=\pi/2$, then we are requiring $c_2(\phi)$ vanish so that near $r=0$, we have

$$\phi = c_1(\phi)r^{1/2} + \tilde{\phi};$$

that is, no log terms; in Ref. 8, Brüning and Seeley prove that $\theta_1=\pi/2$ is the Friedrichs realization of the operator Δ acting on smooth functions supported away from $r=0$ with the boundary condition $\cos\theta_2\phi'(R)+\sin\theta_2\phi(R)=0$ at $r=R$. As seen in Theorem 1.1 in the Introduction, this self-adjoint realization gives rise to the "usual" resolvent, heat kernel, and zeta function properties. When $\theta_1\neq\pi/2$, we get very pathological properties as shown in Theorem 1.2. In the following sections we enter in the proof of Theorem 1.2.

V. EIGENVALUES WITH DIRICHLET CONDITIONS AT $r=R$

As shown in detail in Sec. X, the strange behaviors depicted in Theorem 1.2 do not depend on the choice of the Lagrangian L_2 (that is, the choice of boundary condition at $r=R$). For this reason, we shall use $\theta_2=0$ for the Lagrangian L_2 in (4.2); thus, we shall consider the self-adjoint operator $\Delta_\theta := \Delta : \mathcal{D}_\theta \to L^2([0,R])$, where $0 \leqslant \theta < \pi$ and $\theta \neq \pi/2$, and

$$\mathcal{D}_\theta = \{\phi \in \mathcal{D}_{\max}(\Delta) | \cos\theta c_1(\phi) + \sin\theta c_2(\phi) = 0, \phi(R) = 0\};$$

so we are simply imposing the Dirichlet condition at $r=R$.

We now find an explicit formula for the eigenfunctions and a transcendental equation, which determines the spectrum of Δ_θ. We begin with the following eigenvalue equation:

$$(\Delta_\theta - \mu^2)\phi = 0 \Leftrightarrow \phi'' + \frac{1}{4r^2}\phi + \mu^2\phi = 0.$$

We can turn this into a Bessel equation via the usual trick by setting $\phi = r^{1/2}\psi(\mu r)$. Then,

$$\phi'' = -\tfrac{1}{4}r^{-3/2}\psi(\mu r) + \mu r^{-1/2}\psi'(\mu r) + \mu^2 r^{1/2}\psi''(\mu r),$$

so

$$\phi'' + \frac{1}{4r^2}\phi + \mu^2\phi = 0 \Leftrightarrow \mu r^{-1/2}\psi'(\mu r) + \mu^2 r^{1/2}\psi''(\mu r) + \mu^2 r^{1/2}\psi(\mu r) = 0,$$

or

$$(\mu r)^2\psi''(\mu r) + (\mu r)\psi'(\mu r) + (\mu r)^2\psi(\mu r) = 0.$$

For fixed μ, the solutions to this equation are linear combinations of J_0 and Y_0 (with Y_0 the Bessel function of the second kind), so

$$\phi = C_1 r^{1/2} J_0(\mu r) + C_2 r^{1/2} Y_0(\mu r).$$

Using that (Ref. 1, p. 360)

$$\frac{\pi}{2}Y_0(z) := (\log z - \log 2 + \gamma)J_0(z) - \sum_{k=1}^{\infty} \frac{H_k\left(-\frac{1}{4}z^2\right)^k}{(k!)^2}, \tag{5.1}$$

where $H_k := 1 + \frac{1}{2} + \cdots + (1/k)$, the form (2.1) for $\phi \in \mathcal{D}_{\max}(\Delta)$ is obtained by choosing the constants C_1 and C_2 in such a way that

$$\phi = c_1(\phi) r^{1/2} J_0(\mu r) + c_2(\phi) r^{1/2}\left(\frac{\pi}{2}Y_0(\mu r) - (\log\mu - \log 2 + \gamma)J_0(\mu r)\right).$$

By definition of the Bessel function (Ref. 1, p. 360) we have as $z \to 0$,

$$J_v(z) = \frac{z^v}{2^v}\sum_{k=0}^{\infty} \frac{\left(-\frac{1}{4}z^2\right)^k}{k!\Gamma(v+k+1)} = \frac{z^v}{2^v\Gamma(1+v)}\left(1 - \frac{z^2}{4(1+v)} + \frac{z^4}{32(1+v)(2+v)} - + \cdots\right) \tag{5.2}$$

and by (5.1)), we see that

$$\phi = c_1(\phi)r^{1/2} + c_2(\phi)r^{1/2}\log r + \mathcal{O}((\mu r)^2),$$

where $\mathcal{O}((\mu r)^2)$ is a power series in $(\mu r)^2$ vanishing like $(\mu r)^2$ as $r\to 0$. Therefore, by definition of $\mathcal{D}_\theta$, we have

$$\cos\theta c_1(\phi) + \sin\theta c_2(\phi) = 0. \tag{5.3}$$

To satisfy the Dirichlet condition at $r=R$, we must have

$$c_1(\phi)J_0(\mu R) + c_2(\phi)\left(\frac{\pi}{2}Y_0(\mu R) - (\log\mu - \log 2 + \gamma)J_0(\mu R)\right) = 0.$$

It follows that

$$\det\begin{pmatrix} \cos\theta & \sin\theta \\ J_0(\mu R) & \dfrac{\pi}{2}Y_0(\mu R) - (\log\mu - \log 2 + \gamma)J_0(\mu R) \end{pmatrix} = 0,$$

or $(\pi/2)Y_0(\mu R) - (\log\mu - \log 2 + \gamma)J_0(\mu R) = \tan\theta J_0(\mu R)$. We summarize our findings in the following proposition.

Proposition 5.1: The transcendental equation,

$$F(\mu) := \frac{\pi}{2}Y_0(\mu R) - (\log\mu - \kappa)J_0(\mu R) = 0, \quad \kappa = \log 2 - \gamma - \tan\theta, \tag{5.4}$$

determines the eigenvalues of Δ_θ.

In the following theorem we state various properties of the eigenvalues of Δ_θ; note that in Ref. 15, p. 4572 it is stated that there are no negative eigenvalues; however, it turns out that, for example, when $\pi/2 < \theta < \pi$ and $R \geqslant 1$, there is *always* a negative eigenvalue.

Theorem 5.2: *For* $0 \leqslant \theta < \pi$ *with* $\theta \neq \pi/2$,

(1) Δ_θ *has a zero eigenvalue if and only if* $\log R = \tan\theta$.
(2) Δ_θ *has a unique negative eigenvalue if and only if* $\tan\theta < \log R$.

Proof: Using (5.1) and the expansion

$$J_0(z) = \sum_{k=0}^{\infty} \frac{\left(-\frac{1}{4}z^2\right)^k}{(k!)^2}, \tag{5.5}$$

the eigenvalue equation $(\pi/2)Y_0(\mu R) - (\log\mu - \log 2 + \gamma)J_0(\mu R) = \tan\theta J_0(\mu R)$ can be written as

$$-\sum_{k=1}^{\infty} \frac{H_k\left(-\frac{1}{4}\mu^2R^2\right)^k}{(k!)^2} = (-\log R + \tan\theta)\sum_{k=0}^{\infty} \frac{\left(-\frac{1}{4}\mu^2R^2\right)^k}{(k!)^2}. \tag{5.6}$$

Thus, $\mu = 0$ solves this equation if and only if $\log R = \tan\theta$.

Now Δ_θ has a negative eigenvalue means that $\mu = ix$ for x real solves (5.6):

$$-\sum_{k=1}^{\infty} \frac{H_k\left(\frac{1}{4}x^2R^2\right)^k}{(k!)^2} = (-\log R + \tan\theta)\sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}x^2R^2\right)^k}{(k!)^2}. \tag{5.7}$$

If $(-\log R + \tan\theta) > 0$, then (5.7) has no solutions because the right-hand side of (5.7) will be strictly positive for all real x while the left-hand side of (5.7) is nonpositive. Thus, we may assume that $\alpha := \log R - \tan\theta > 0$. Then we can write (5.7) as

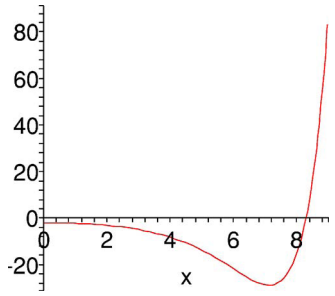

FIG. 1. (Color online) Graph of $f(x)$ when $R=1$ and $\tan\theta=-2$.

$$f(xR)=0 \quad \text{where } f(x)=\sum_{k=1}^{\infty}\frac{H_k x^{2k}}{4^k(k!)^2}-\sum_{k=0}^{\infty}\frac{\alpha x^{2k}}{4^k(k!)^2};$$

thus, we just have to prove that $f(x)=0$ has a unique solution. To prove this, observe that since the harmonic series $1+\frac{1}{2}+\frac{1}{3}+\cdots$ diverges, we can choose $N\in\mathbb{N}$ such that $H_N>\alpha>H_{N-1}$. We now write

$$f(x)=\sum_{k=N}^{\infty}\frac{(H_k-\alpha)x^{2k}}{4^k(k!)^2}-\left(\sum_{k=0}^{N-1}\frac{(\alpha-H_k)x^{2k}}{4^k(k!)^2}\right),$$

where $H_0:=0$, and note that $f(x)=0$ if and only if $g(x)=0$ where

$$g(x):=x^{-2N}f(x)=\sum_{k=N}^{\infty}\frac{(H_k-\alpha)x^{2(k-N)}}{4^k(k!)^2}-\left(\sum_{k=0}^{N-1}\frac{(\alpha-H_k)}{4^k(k!)^2x^{2(N-k)}}\right).$$

Because of the powers of x in the denominator the second sum on the right-hand side, we see that $g(0+)=-\infty$ while because of the first sum on the right-hand side, we see that $\lim_{x\to\infty}g(x)=\infty$. In particular, by the intermediate value theorem, $g(x)=0$ for some $0<x<\infty$. Since

$$g'(x)=\sum_{k=N+1}^{\infty}\frac{(H_k-\alpha)2(k-N)x^{2(k-N)-1}}{4^k(k!)^2}+\left(\sum_{k=0}^{N-1}\frac{2(N-k)(\alpha-H_k)}{4^k(k!)^2x^{2(N-k)+1}}\right)>0$$

the function g is strictly increasing, so there is only one $x>0$ such that $g(x)=0$. It follows that $f(x)=0$ for a unique $x>0$ and our proof is now complete. A graph of $f(x)$ for $R=1$ and $\tan\theta=-2$ is shown in Fig. 1. □

VI. THE ζ-FUNCTION WITH DIRICHLET CONDITIONS AT $r=R$

Let $0\leqslant\theta<\pi$ with $\theta\neq\pi/2$. We now analyze the zeta function using the contour integral techniques developed in Refs. 4, 5, 28, and 30.

In the Appendix, Theorem A.1, we have shown that

$$\mathrm{Tr}(\Delta_\theta-\mu^2)^{-1}=-\frac{1}{2\mu}\frac{d}{d\mu}\log F(\mu).$$

Therefore, for $\Re s>1/2$, by *definition* the zeta function is given by

$$\zeta(s,\Delta_\theta)=\frac{1}{2\pi i}\int_\gamma \mu^{-2s}\frac{d}{d\mu}\log F(\mu)d\mu=\frac{1}{2\pi i}\int_\gamma \mu^{-2s}\frac{F'(\mu)}{F(\mu)}d\mu, \tag{6.1}$$

where γ is a contour in the plane shown in Fig. 2.

To analyze properties of the zeta function, we need the following technical lemma.

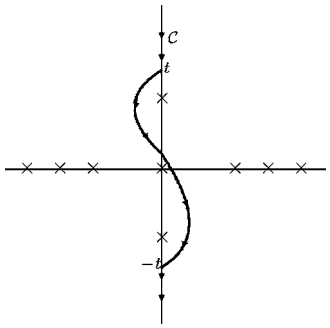

FIG. 2. The contour γ for the zeta function. The $\times$'s represent the zeros of $F(\mu)$. The squares of the $\times$'s on the imaginary axis represent the negative eigenvalues of Δ_θ. Here, t is on the imaginary axis and is larger in absolute value than the absolute value of the negative eigenvalue of Δ_θ (if one exists). The contour γ_t goes from t to $-t$.

Lemma 6.1: Let $0 \leqslant \theta < \pi$ *with* $\theta \neq \pi/2$ *and* $\Upsilon \subset \mathbb{C}$ *be a sector (closed angle) in the right-half plane. Then as* $|x| \to \infty$ *with* $x \in \Upsilon$, *we have*

$$F(ix) \sim -\frac{1}{\sqrt{2\pi}}(\log x - \kappa)(xR)^{-1/2}e^{xR}\left(1 + \frac{1}{8xR} + \frac{9}{2(8xR)^2} + \mathcal{O}(x^{-3})\right), \tag{6.2}$$

where $\mathcal{O}(x^{-3})$ *is a power series in* x^{-1} *starting from* x^{-3}, *and*

$$\frac{d}{dx}\log F(ix) \sim \frac{1}{x(\log x - \kappa)} + R - \frac{1}{2x} - \frac{1}{8x^2R} + \mathcal{O}(x^{-3}), \tag{6.3}$$

with the same meaning for $\mathcal{O}(x^{-3})$. *Finally,* $F(\mu)$ *is an even function of* μ, *and as* $\mu \to 0$, *we have*

$$F(\mu) \sim (\log R - \tan\theta) + \frac{1}{4}\mu^2R^2(1 + \tan\theta - \log R) + \mathcal{O}(\mu^4). \tag{6.4}$$

Proof: From (5.1), we have

$$\frac{\pi}{2}Y_0(ix) = (\log(ix) - \log 2 + \gamma)J_0(ix) - \sum_{k=1}^{\infty}\frac{H_k\left(-\frac{1}{4}(ix)^2\right)^k}{(k!)^2}$$

$$= \left(\log x + i\frac{\pi}{2} - \log 2 + \gamma\right)I_0(x) - \sum_{k=1}^{\infty}\frac{H_k\left(\frac{1}{4}x^2\right)^k}{(k!)^2} = i\frac{\pi}{2}I_0(x) - K_0(x),$$

where $I_0(x)$ is the modified Bessel function of the first kind, and

$$K_0(x) := -(\log x - \log 2 + \gamma)I_0(x) + \sum_{k=1}^{\infty}\frac{H_k\left(\frac{1}{4}x^2\right)^k}{(k!)^2}$$

is the modified Bessel function of the second kind. Therefore,

$$F(ix) = \frac{\pi}{2}Y_0(ixR) - (\log(ix) - \kappa)J_0(ixR) = i\frac{\pi}{2}I_0(xR) - K_0(xR) - \left(\log x + i\frac{\pi}{2} - \kappa\right)I_0(xR)$$

$$= -(\log x - \kappa)I_0(xR) - K_0(xR).$$

By Ref. 1, p. 377, as $|x| \to \infty$ for $x \in \Upsilon$, we have

$$I_0(x) \sim \frac{e^x}{\sqrt{2\pi x}}\left(1+\frac{1}{8x}+\frac{9}{2(8x)^2}+\mathcal{O}(x^{-3})\right),$$

where $\mathcal{O}(x^{-3})$ is a power series in x^{-1} starting with x^{-3}; furthermore (Ref. 1, p. 378), as $|x|\to\infty$ for $x\in\Upsilon$,

$$K_0(x) \sim \sqrt{\frac{2}{\pi x}}e^{-x}\left(1-\frac{1}{8x}+\frac{9}{2(8x)^2}+\mathcal{O}(x^{-3})\right).$$

Therefore, as $|x|\to\infty$ for $x\in\Upsilon$, we have

$$F(ix) \sim -(\log x-\kappa)I_0(xR) \sim -\frac{1}{\sqrt{2\pi}}(\log x-\kappa)(xR)^{-1/2}e^{xR}\left(1+\frac{1}{8xR}+\frac{9}{2(8xR)^2}+\mathcal{O}(x^{-3})\right),$$

which proves (6.2). Taking logarithms, we see that as $|x|\to\infty$ for $x\in\Upsilon$, we have

$$\log F(ix) \sim c+\log(\log x-\kappa)-\frac{1}{2}\log x+xR+\log\left(1+\frac{1}{8xR}+\frac{9}{2(8xR)^2}+\mathcal{O}(x^{-3})\right),$$

where c is a constant. Since $\log(1+z)=z-(z^2/2)+(z^3/3)-+\dots$, we have

$$\log F(ix) \sim c+\log(\log x-\kappa)-\frac{1}{2}\log x+xR+\frac{1}{8xR}+\mathcal{O}(x^{-2}).$$

Taking the derivative of this we get (6.3).

To determine the asymptotics as $\mu\to 0$, recalling that $\kappa=\log 2-\gamma-\tan\theta$, we see that

$$\begin{aligned}F(\mu) &= \frac{\pi}{2}Y_0(\mu R)-(\log\mu-\kappa)J_0(\mu R) = \frac{\pi}{2}Y_0(\mu R)-(\log\mu-\log 2+\gamma)J_0(\mu R)-\tan\theta J_0(\mu R)\\ &= \frac{1}{4}\mu^2R^2+(\log R-\tan\theta)+(\tan\theta-\log R)\cdot\frac{1}{4}\mu^2R^2+\mathcal{O}(\mu^4)\\ &= (\log R-\tan\theta)+\frac{1}{4}\mu^2R^2(1+\tan\theta-\log R)+\mathcal{O}(\mu^4),\end{aligned}$$

where we used (5.1) and (5.5) in passing from the second to the third line. In particular, the second line with (5.1) and (5.5) shows that $F(\mu)$ is an even function of μ. This completes our proof. □

We need one more lemma.

Lemma 6.2: We have

$$\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x = -e^{-2s\kappa}\log s-e^{-2s\kappa}(\gamma+\log(2(\log|t|-\kappa))+\mathcal{O}(s)),$$

where $\mathcal{O}(s)$ is an entire function of s that is $\mathcal{O}(s)$ at $s=0$.

Proof: In the integral we assume that $\log|t|>\kappa$ so that the integral is well defined. Now to analyze this integral we make the change of variables $u=\log x-\kappa$ or $x=e^{\kappa}e^{u}$, and obtain

$$\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x = e^{-2s\kappa}\int_{\log|t|-\kappa}^{\infty}e^{-2su}\frac{\mathrm{d}u}{u}.$$

Making the change of variables $y=2su$, we get

$$\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x = e^{-2s\kappa}\int_{2s(\log|t|-\kappa)}^{\infty}e^{-y}\frac{\mathrm{d}y}{y}.$$

Recall that the *exponential integral* is defined by (see Ref. 22, Sec. 8.2)

$$\mathrm{Ei}(z) := -\int_{-z}^{\infty} e^{-y}\frac{\mathrm{d}y}{y}.$$

Therefore,

$$\int_{|t|}^{\infty} x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x = -e^{-2s\kappa}\,\mathrm{Ei}(-2s(\log|t|-\kappa)).$$

Also from Ref. 22, p. 877, we have

$$\mathrm{Ei}(z) = \gamma + \log(-z) + \sum_{k=1}^{\infty}\frac{z^k}{k\cdot k!},$$

therefore

$$\begin{aligned}\int_{|t|}^{\infty} x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x &= -e^{-2s\kappa}(\gamma+\log(2s(\log|t|-\kappa))+\mathcal{O}(s))\\ &= -e^{-2s\kappa}\log s - e^{-2s\kappa}(\gamma+\log(2(\log|t|-\kappa))+\mathcal{O}(s)),\end{aligned} \tag{6.5}$$

where $\mathcal{O}(s)$ is an entire function of s that is $\mathcal{O}(s)$ at $s=0$. This completes our proof. □

We now determine the structure of the zeta function.

Proposition 6.3: The zeta function $\zeta(s,\Delta_\theta)$ can be written in the form

$$\zeta(s,\Delta_\theta) = -\frac{e^{-2s\kappa}\sin\pi s}{\pi}\log s + \zeta_\theta(s),$$

where $\kappa=\log 2-\gamma-\tan\theta$ and $\zeta_\theta(s)$ extends from $\Re s>1/2$ to a holomorphic function on $\mathbb{C}$ with poles at $s=1/2-k$ for $k=0,1,2,\ldots$. In particular, $\zeta(s,\Delta_\theta)$ has $s=0$ as a logarithmic branch point.

Proof: Recalling (6.1), we write

$$\int_{\gamma} = -\int_{t}^{0+i\infty} + \int_{-t}^{0-i\infty} + \int_{\gamma_t},$$

where γ_t is the part of γ from t to $-t$, and using that

$$i^{-2s} = (e^{i\pi/2})^{-2s} = e^{-i\pi s} \text{ and } (-i)^{-2s} = (e^{-i\pi/2})^{-2s} = e^{i\pi s},$$

we obtain the integral

$$\begin{aligned}\zeta(s,\Delta_\theta) &= \frac{1}{2\pi i}\int_{\gamma}\mu^{-2s}\frac{d}{\mathrm{d}\mu}\log F(\mu)\mathrm{d}\mu = \frac{1}{2\pi i}\left\{-\int_{|t|}^{\infty}(ix)^{-2s}\frac{d}{\mathrm{d}x}\log F(ix)\mathrm{d}x\right.\\ &\quad\left.+\int_{|t|}^{\infty}(-ix)^{-2s}\frac{d}{\mathrm{d}x}\log F(-ix)\mathrm{d}x\right\}+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}\mathrm{d}\mu\\ &= \frac{1}{2\pi i}(-e^{-i\pi s}+e^{i\pi s})\int_{|t|}^{\infty}x^{-2s}\frac{d}{\mathrm{d}x}\log F(ix)\mathrm{d}x+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}\mathrm{d}\mu,\end{aligned}$$

or,

$$\zeta(s,\Delta_\theta)=\frac{\sin \pi s}{\pi}\int_{|t|}^{\infty} x^{-2s}\frac{d}{dx}\log F(ix)dx+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}d\mu, \tag{6.6}$$

a formula that will be analyzed in a moment. The second integral here is over a finite contour so an entire function of $s\in\mathbb{C}$, so we are left to analyze the analytic properties of the first integral. To do so, recall from (6.3) that for $x\to\infty$, we have

$$\frac{d}{dx}\log F(ix)\sim\frac{1}{x(\log x-\kappa)}+\sum_{k=0}^{\infty}\beta_k x^{-k},$$

for some constants β_k. Since

$$\frac{\sin \pi s}{\pi}\int_{|t|}^{\infty} x^{-2s-k}\,dx=\frac{\sin \pi s}{\pi}\left.\frac{x^{-2s-k+1}}{-2s-k+1}\right|_{x=|t|}^{\infty}=\frac{\sin \pi s}{\pi}\frac{|t|^{-2s-k+1}}{2s+k-1}$$

which has poles at $s=(1-k)/2$ for $s\notin\mathbb{Z}$, it follows that the expansion $\Sigma_{k=0}^{\infty}\beta_k x^{-k}$ will contribute to the function $\zeta_\theta(s)$ in the statement of this proposition where $\zeta_\theta(s)$ extends from $\Re s>1/2$ to a holomorphic function on $\mathbb{C}$ with poles at $s=1/2-k$ for $k=0,1,2,\ldots$. Lemma 6.2 applied to the integral

$$\frac{\sin \pi s}{\pi}\int_{|t|}^{\infty} x^{-2s}\frac{1}{x(\log x-\kappa)}dx$$

now completes our proof. □

Remark 6.4: The existence of the logarithmic branch point at $s=0$ has been missed in Ref. 15. *The error occurs in Eq. (A13) where certain antiderivatives [specifically $xY_1(x)$ and $x^2Y_1^2$] were accidentally set equal to zero at $s=0$.*

VII. TRACE OF THE RESOLVENT WITH DIRICHLET CONDITIONS AT *r=R*

Using the Theorem A.1, we can now prove Theorem 1.2 (1) for Δ_θ. We have chosen to present the results in a form where the first term has been expanded further; Theorem 1.2 (1) is contained in Eq. (7.1) of the proof and the explanation of the meaning of the expansion is similar to that found in Remark 1.5.

Proposition 7.1: Let $\theta\neq\pi/2$ and $\kappa=\log 2-\gamma-\tan\theta$, furthermore let $\Lambda\subset\mathbb{C}$ be any sector (solid angle) not intersecting the positive real axis. Then as $|\lambda|\to\infty$ with $\lambda\in\Lambda$, we have

$$\mathrm{Tr}(\Delta_\theta-\lambda)^{-1}\sim(-\lambda)^{-1}\sum_{k=0}^{\infty}a_k(\log(-\lambda))^{-k-1}+\sum_{k=1}^{\infty}b_k(-\lambda)^{-k/2},$$

where $a_k=(2\kappa)^k$ for $k=0,1,2,\ldots$ (in particular, $a_0=1\neq 0$).

Proof: Setting $\lambda=-x^2$ with $x\in\Upsilon\subset\mathbb{C}$ a sector in the right-half plane, it suffices to prove that as $|x|\to\infty$ with $x\in\Upsilon$, we have

$$\mathrm{Tr}(\Delta_\theta+x^2)^{-1}\sim x^{-2}\sum_{k=0}^{\infty}\frac{\kappa^k}{2}(\log x)^{-k-1}+x^{-1}\sum_{k=0}^{\infty}b_k x^{-k},$$

or after multiplication by $2x$, we just have to prove that

$$2x\,\mathrm{Tr}(\Delta_\theta+x^2)^{-1}\sim x^{-1}\sum_{k=1}^{\infty}\kappa^k(\log x)^{-k-1}+\sum_{k=0}^{\infty}\beta_k x^{-k}.$$

To prove this, we recall from Theorem A.1 that

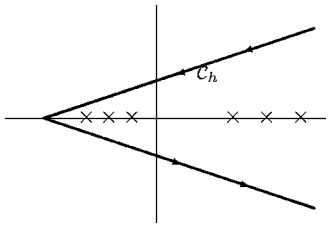

FIG. 3. The contour γ.

$$2x\,\mathrm{Tr}(\Delta_\theta + x^2)^{-1} = \frac{d}{dx}\log F(ix).$$

By Lemma 6.1 [see (6.3)] we know that as $|x|\to\infty$ for $x\in\Upsilon$,

$$\frac{d}{dx}\log F(ix) \sim \frac{1}{x(\log x - \kappa)} + \sum_{k=0}^{\infty}\beta_k x^{-k}. \tag{7.1}$$

Finally, the expansion

$$\frac{1}{x(\log x-\kappa)} = \frac{1}{x\log x}\cdot\frac{1}{(1-\kappa(\log x)^{-1})} = \frac{1}{x\log x}\sum_{k=0}^{\infty}\kappa^k(\log x)^{-k} = x^{-1}\sum_{k=0}^{\infty}\kappa^k(\log x)^{-k-1},$$

concludes our result. □

As shown in the proof, for $|x|\to\infty$ with $x\in\Upsilon$, where Υ is a sector in the right-half plane, we have

$$2x\,\mathrm{Tr}(\Delta_\theta + x^2)^{-1} = \frac{d}{dx}\log F(ix) \sim \frac{1}{x(\log x-\kappa)} + \sum_{k=0}^{\infty}\beta_k x^{-k}, \tag{7.2}$$

or with $\lambda=-x^2$, as $|\lambda|\to\infty$ with $\lambda\in\Lambda\subset\mathbb{C}$, a sector not intersecting the positive real axis, we have

$$\mathrm{Tr}(\Delta_\theta-\lambda)^{-1} \sim \frac{1}{(-\lambda)(\log(-\lambda)-2\kappa)} + \sum_{k=1}^{\infty} b_k(-\lambda)^{-k/2}. \tag{7.3}$$

This fact will be used in the next section.

VIII. THE HEAT TRACE WITH DIRICHLET CONDITIONS AT $r=R$

To determine the small-time heat asymptotics, we write

$$\mathrm{Tr}(e^{-t\Delta_\theta}) = \frac{i}{2\pi}\int_\gamma e^{-t\lambda}\,\mathrm{Tr}(\Delta_\theta-\lambda)^{-1}\,d\lambda,$$

where γ is a counter-clockwise contour in the plane surrounding the eigenvalues of Δ_θ; see Fig. 3. This is the starting point to show Theorem 1.2 (2) for Δ_θ. Again we have chosen to present the results in a form where the first term has been expanded further. This makes the actual structure of the small-t expansion more explicit; Theorem 1.2 (2) is contained in Eq. (8.2) of the proof.

Proposition 8.1: As $t\to 0$, we have

$$\mathrm{Tr}(e^{-t\Delta_\theta}) \sim \sum_{k=1}^{\infty}\alpha_k(\log t)^{-k} + \sum_{k=0}^{\infty}\beta_k t^{(k-1)/2}$$

with the *α_k's depending on κ via*

$$\alpha_k = -\frac{1}{k\pi}\Im\left(\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k \, dx\right).$$

Proof: The small-time asymptotics are determined by the large-spectral parameter asymptotics of the resolvent. Now recall from (7.3) that as $|\lambda|\to\infty$ with λ in a sector not intersecting the positive real axis, we have

$$\mathrm{Tr}(\Delta_\theta - \lambda)^{-1} \sim \frac{1}{(-\lambda)(\log(-\lambda) - 2\kappa)} + \sum_{k=1}^{\infty} b_k(-\lambda)^{-k/2}.$$

Since (making the change of variables $\lambda \mapsto t^{-1}\lambda$)

$$\int e^{-t\lambda}(-\lambda)^{-k/2}\, d\lambda = t^{-1+k/2}\int e^{-\lambda}(-\lambda)^{-k/2}\, d\lambda$$

the series $\Sigma_{k=1}^{\infty} b_k(-\lambda)^{-k/2}$ gives rise to a small time expansion

$$\sum_{k=1}^{\infty} \beta_k t^{-1+k/2}.$$

Therefore, we just have to analyze the behavior of

$$\frac{i}{2\pi}\int_\gamma e^{-t\lambda}\frac{1}{(-\lambda)(\log(-\lambda) - 2\kappa)}d\lambda.$$

Deforming γ to the real line, the integral here is, modulo a term that is a smooth function of t at $t=0$, equal to

$$-\int_1^\infty e^{-tx}\frac{1}{(-x)(\log(-(x+i0)) - 2\kappa)}dx + \int_1^\infty e^{-tx}\frac{1}{(-x)(\log(-(x-i0)) - 2\kappa)}dx,$$

or after simplification, this sum becomes

$$\int_1^\infty e^{-tx}\frac{1}{x(\log x - i\pi - 2\kappa)}dx - \int_1^\infty e^{-tx}\frac{1}{x(\log x + i\pi - 2\kappa)}dx.$$

(The reason we start at $x=1$ is that $1/(x[\log x \pm i\pi - 2\kappa])$ is not integrable near $x=0$.) Since for any complex number z, we have $i(\bar{z}-z)=2\Im z$, we see that modulo a term that is a smooth function of t at $t=0$,

$$\frac{i}{2\pi}\int_\gamma e^{-t\lambda}\frac{1}{(-\lambda)(\log(-\lambda) - 2\kappa)}d\lambda \equiv \frac{1}{\pi}\Im\left(\int_1^\infty e^{-tx}\frac{1}{x(\log x + i\pi - 2\kappa)}dx\right) = \frac{1}{\pi}\Im\ell(t), \quad (8.1)$$

where

$$\ell(t) := \int_1^\infty e^{-tx}\frac{1}{x(\log x + i\pi - 2\kappa)}dx.$$

In summary, we have proved that

$$\mathrm{Tr}(e^{-t\Delta_\theta}) \sim \frac{1}{\pi}\Im\ell(t) + \sum_{k=0}^{\infty}\beta_k t^{(k-1)/2}, \quad (8.2)$$

which is exactly the statement of Theorem 1.2 (2).

We shall compute the asymptotics of $\ell(t)$ as $t\to 0$. To do so, observe that

$$\ell'(t) := -\int_1^\infty e^{-tx}\frac{1}{(\log x + i\pi - 2\kappa)}\mathrm{d}x.$$

Now $1/\log x$ is integrable near $x=0$, so we can write

$$\ell'(t) = f(t) + g(t),$$

where

$$f(t) := -\int_0^\infty e^{-tx}\frac{1}{(\log x + i\pi - 2\kappa)}\mathrm{d}x, \quad g(t) := \int_0^1 e^{-tx}\frac{1}{(\log x + i\pi - 2\kappa)}\mathrm{d}x.$$

Note that $g(t)$ is smooth at $t=0$. We will now determine the asymptotics of $f(t)$ near $t=0$. To this end, we make the change of variables $x\mapsto t^{-1}x$,

$$f(t) = -t^{-1}\int_0^\infty e^{-x}\frac{1}{(\log(x/t) + i\pi - 2\kappa)}\mathrm{d}x = t^{-1}(\log t)^{-1}\int_0^\infty e^{-x}\frac{1}{1 - \dfrac{\log x + i\pi - 2\kappa}{\log t}}\mathrm{d}x.$$

Since $(1-r)^{-1} = \Sigma_{k=0}^{N} r^k + r^{N+1}(1-r)^{-1}$ for any $N \in \mathbb{N}$, we see that for any $N \in \mathbb{N}$,

$$f(t) = t^{-1}(\log t)^{-1}\sum_{k=0}^{N}(\log t)^{-k}\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k\,\mathrm{d}x$$
$$+ t^{-1}(\log t)^{-1}\cdot(\log t)^{-N-1}\int_0^\infty e^{-x}\frac{(\log x + i\pi - 2\kappa)^{N+1}}{1 - \dfrac{\log x + i\pi - 2\kappa}{\log t}}\mathrm{d}x.$$

The last integral here is bounded in t as $t\to 0$. Since N is arbitrary, it follows that

$$f(t) \sim t^{-1}\sum_{k=0}^{\infty}(\log t)^{-k-1}\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k\,\mathrm{d}x.$$

Therefore, since $\ell'(t) = f(t) + g(t)$, as $t\to 0$ we have

$$\ell'(t) \sim t^{-1}\sum_{k=0}^{\infty}(\log t)^{-k-1}\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k\,\mathrm{d}x + \sum_{k=0}^{\infty}\gamma_k t^k.$$

Integrating both sides, using that

$$\int t^{-1}(\log t)^{-1}\,\mathrm{d}t = \log|\log t|, \quad \int t^{-1}(\log t)^{-k-1}\,\mathrm{d}t = -\frac{1}{k}(\log t)^{-k} \quad \text{for } k > 0,$$

we get

$$\ell(t) \sim \log|\log t| - \sum_{k=1}^{\infty}\frac{1}{k}(\log t)^{-k}\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k\,\mathrm{d}x + \sum_{k=0}^{\infty}\delta_k t^k.$$

Finally, in view of (8.1), we see that as $t\to 0$,

$$\frac{i}{2\pi}\int_\gamma e^{-t\lambda}\frac{1}{(-\lambda)(\log(-\lambda)-2\kappa)}\mathrm{d}\lambda \sim \frac{1}{\pi}\mathfrak{I}\ell(t) \sim -\sum_{k=1}^{\infty}\frac{1}{k\pi}(\log t)^{-k}\mathfrak{I}\left(\int_0^\infty e^{-x}(\log x + i\pi - 2\kappa)^k\,\mathrm{d}x\right) + \sum_{k=0}^{\infty}\epsilon_k t^k.$$

□

IX. THE ZETA DETERMINANT

By Proposition 6.3, we have

$$\zeta(s,\Delta_\theta) = -\frac{e^{-2s\kappa}\sin\pi s}{\pi}\log s + \zeta_\theta(s),$$

where $\zeta_\theta(s)$ extends from $\Re s > 1/2$ to a holomorphic function on $\mathbb{C}$ with poles at $s = 1/2 - k$ for $k = 0,1,2,\ldots$. Since $e^{-2s\kappa}\sin\pi s/\pi = s + \mathcal{O}(s^2)$, it follows that

$$\zeta_{\mathrm{reg}}(s,\Delta_\theta) := \zeta(s,\Delta_\theta) + s\log s$$

has a derivative at $s=0$. Therefore, we can define

$$\det{}_{\mathrm{reg}}(\Delta_\theta) := \exp(-\zeta'_{\mathrm{reg}}(0,\Delta_\theta)),$$

which is computed in this section.

Recall that $0 \leqslant \theta < \pi$ with $\theta \neq \pi/2$. The idea here is to make the first term in

$$\zeta(s,\Delta_\theta) = \frac{\sin\pi s}{\pi}\int_{|t|}^\infty x^{-2s}\frac{d}{\mathrm{d}x}\log F(ix)\mathrm{d}x + \frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}\mathrm{d}\mu$$

regular at $s=0$, as the second term (being entire) is already regular at $s=0$. In order to analytically continue the first term, we add and subtract off the leading asymptotics of $F(ix)$. Thus, recalling Lemma 6.1 [see (6.3)]

$$F(ix) \sim C_0(\log x - \kappa)x^{-1/2}e^{xR}\left(1 + \mathcal{O}\left(\frac{1}{x}\right)\right) \quad \text{as } x \to \infty,$$

where $C_0 = -1/\sqrt{2\pi R}$, we consider

$$\int_{|t|}^\infty x^{-2s}\frac{d}{\mathrm{d}x}\log F(ix)\mathrm{d}x = \int_{|t|}^\infty x^{-2s}\frac{d}{\mathrm{d}x}\log\left(\frac{F(ix)}{C_0(\log x-\kappa)x^{-1/2}e^{xR}}\right)\mathrm{d}x + \int_{|t|}^\infty x^{-2s}\frac{d}{\mathrm{d}x}\log(C_0(\log x - \kappa)x^{-1/2}e^{xR})\mathrm{d}x.$$

The second integral can be computed explicitly,

$$\int_{|t|}^\infty x^{-2s}\frac{d}{\mathrm{d}x}\log(C_0(\log x-\kappa)x^{-1/2}e^{xR})\mathrm{d}x = \int_{|t|}^\infty x^{-2s}\frac{1}{x(\log x-\kappa)}\mathrm{d}x - \frac{|t|^{-2s}}{4s} + \frac{|t|^{-2s+1}}{2s-1}R.$$

Therefore,

$$\zeta(s,\Delta_\theta)=\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{d}{dx}\log\left(\frac{F(ix)}{C_0(\log x-\kappa)x^{-1/2}e^{xR}}\right)dx+\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}dx$$
$$-\frac{\sin\pi s}{\pi}\frac{|t|^{-2s}}{4s}+\frac{\sin\pi s}{\pi}\frac{|t|^{-2s+1}}{2s-1}R+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}d\mu.$$

Hence, as $\zeta_{\mathrm{reg}}(s,\Delta_\theta)=\zeta(s,\Delta_\theta)+s\log s$, we see that

$$\zeta_{\mathrm{reg}}(s,\Delta_\theta)=\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{d}{dx}\log\left(\frac{F(ix)}{C_0(\log x-\kappa)x^{-1/2}e^{xR}}\right)dx+\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}dx$$
$$+s\log s-\frac{\sin\pi s}{\pi}\frac{|t|^{-2s}}{4s}+\frac{\sin\pi s}{\pi}\frac{|t|^{-2s+1}}{2s-1}R+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}d\mu.$$

By Lemma 6.2, we have

$$\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{1}{x(\log x-\kappa)}dx=-\frac{e^{-2s\kappa}\sin\pi s}{\pi}\log s-\frac{e^{-2s\kappa}\sin\pi s}{\pi}(\gamma+\log(2(\log|t|-\kappa))+\mathcal{O}(s))$$
$$=-s\log s-s(\gamma+\log(2(\log|t|-\kappa))+\mathcal{O}(s\log s)).$$

Thus,

$$\zeta_{\mathrm{reg}}(s,\Delta_\theta)=\frac{\sin\pi s}{\pi}\int_{|t|}^{\infty}x^{-2s}\frac{d}{dx}\log\left(\frac{F(ix)}{C_0(\log x-\kappa)x^{-1/2}e^{xR}}\right)dx-s(\gamma+\log(2(\log|t|-\kappa))$$
$$+\mathcal{O}(s^2\log s))-\frac{\sin\pi s}{\pi}\frac{|t|^{-2s}}{4s}+\frac{\sin\pi s}{\pi}\frac{|t|^{-2s+1}}{2s-1}R+\frac{1}{2\pi i}\int_{\gamma_t}\mu^{-2s}\frac{F'(\mu)}{F(\mu)}d\mu.$$

The first integral on the right-hand side is regular at $s=0$ due to the asymptotics found in Lemma 6.1. Therefore, using that

$$\frac{\sin(\pi s)}{\pi}\bigg|_{s=0}=0,\quad \frac{d}{ds}\ \frac{\sin(\pi s)}{\pi}\bigg|_{s=0}=1,\qquad \frac{\sin(\pi s)}{\pi s}\bigg|_{s=0}=1,\quad \frac{d}{ds}\ \frac{\sin(\pi s)}{\pi s}\bigg|_{s=0}=0,$$

we see that

$$\zeta'_{\mathrm{reg}}(0,\Delta_\theta)=\int_{|t|}^{\infty}\frac{d}{dx}\log\left(\frac{F(ix)}{C_0(\log x-\kappa)x^{-1/2}e^{xR}}\right)dx-(\gamma+\log(2(\log|t|-\kappa))+\frac{1}{2}\log|t|-|t|R$$
$$-\frac{1}{\pi i}\int_{\gamma_t}\log\mu\frac{F'(\mu)}{F(\mu)}d\mu=-\log\left(\frac{F(i|t|)}{C_0}\right)-\gamma-\log 2-\frac{1}{\pi i}\int_{\gamma_t}\log\mu\frac{F'(\mu)}{F(\mu)}d\mu.$$

Therefore,

$$\det{}_{\mathrm{reg}}(\Delta_\theta)=2e^{\gamma}\frac{F(t)}{C_0}\cdot\exp\left(\frac{1}{\pi i}\int_{\gamma_t}\log\mu\frac{F'(\mu)}{F(\mu)}d\mu\right).\tag{9.1}$$

This formula is derived, *a priori*, when t is on the upper half of the imaginary axis. However, the right-hand side is a *holomorphic* function of $t\in\mathcal{D}$, where $\mathcal{D}$ is the set of complex numbers minus the negative real axis and the zeros of $F(\mu)$. Therefore (9.1) holds for all $t\in\mathcal{D}$. Here, we recall that γ_t is any curve in $\mathcal{D}$ from t to $-t$. As before, the trick now is to let $t\to 0$ in (9.1).

First, assume that $\log R-\tan\theta\neq 0$ so that Δ_θ has no zero eigenvalue by Theorem 5.2. We determine the limit as $t\to 0$ of the exponential $\exp(1/\pi i)\int_{\gamma_t}\log\mu[F'(\mu)/F(\mu)]d\mu)$. Let's take $t\to 0$ in $\mathcal{D}$ from the upper half plane as shown in Fig. 4. In view of Fig. 4, it follows that

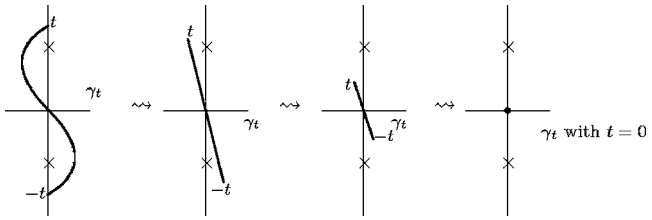

FIG. 4. The contour γ_t as we let $t \to 0$ in $\mathcal{D}$ from the upper half plane.

$$\exp\left(\frac{1}{\pi i}\int_{\gamma_t} \log \mu \frac{F'(\mu)}{F(\mu)} \mathrm{d}\mu\right) \to \exp(0) = 1.$$

Recalling (6.4), as $\mu \to 0$, we have

$$F(\mu) \sim (\log R - \tan\theta) + \tfrac{1}{4}\mu^2 R^2(1 + \tan\theta - \log R) + \mathcal{O}(\mu^4).$$

In this case $F(0) = \log R - \tan\theta$. In conclusion, taking $t \to 0$ in (9.1), we see that

$$\det_{\mathrm{reg}}(\Delta_\theta) = 2\sqrt{2\pi R}\, e^{\gamma}(\tan\theta - \log R). \tag{9.2}$$

Second, assume now that $\log R - \tan\theta = 0$ so that as $\mu \to 0$, we have

$$F(\mu) \sim \tfrac{1}{4}\mu^2 R^2(1 + \mathcal{O}(\mu^2)).$$

Let us set

$$\widetilde{F}(\mu) := \frac{F(\mu)}{\mu^2};$$

then $\widetilde{F}(\mu)$ is nonzero at $\mu = 0$ with value $R^2/4$, and

$$\zeta(s, \Delta_\theta) = \frac{\sin \pi s}{\pi}\int_{|t|}^{\infty} x^{-2s}\frac{d}{\mathrm{d}x}\log \widetilde{F}(ix)\mathrm{d}x + \frac{1}{2\pi i}\int_{\gamma_t} \mu^{-2s}\frac{\widetilde{F}'(\mu)}{\widetilde{F}(\mu)}\mathrm{d}\mu.$$

By Lemma 6.1 [see (6.2)], we have

$$\widetilde{F}(ix) \sim \frac{C_0(\log x - \kappa)x^{-1/2}e^{xR}}{-x^2} = \widetilde{C}_0(\log x - \kappa)x^{-5/2}e^{xR}, \quad \text{where } \widetilde{C}_0 = \frac{1}{\sqrt{2\pi R}}.$$

Now following the argument above used to prove (9.1), we can show

$$\det_{\mathrm{reg}}(\Delta_\theta) = 2e^{\gamma}\frac{\widetilde{F}(t)}{\widetilde{C}_0}\cdot \exp\left(\frac{1}{\pi i}\int_{\gamma_t} \log \mu \frac{\widetilde{F}'(\mu)}{\widetilde{F}(\mu)}\mathrm{d}\mu\right).$$

Finally, taking $t \to 0$ as we did before, yields in the $\tan\theta = \log R$ case, the result

$$\det_{\mathrm{reg}}(\Delta_\theta) = 2e^{\gamma}\frac{R^2}{4\widetilde{C}_0} = \frac{R^2}{2}e^{\gamma}\sqrt{2\pi R} = \sqrt{\frac{\pi R}{2}}e^{\gamma}R^2.$$

X. GENERAL BOUNDARY CONDITIONS AT $r = R$

We now prove Theorem 1.2. Let us briefly recall the setup. Let $0 \leqslant \theta_1, \theta_2 < \pi$ with $\theta_1 \neq \pi/2$ and set $L := L_{\theta_1} \oplus L_{\theta_2}$. Then as a consequence of Theorem 3.2, we know that

$$\Delta_L := \Delta : \mathcal{D}_L \to L^2([0,R])$$

is self-adjoint, where

$$\mathcal{D}_L = \{\phi \in \mathcal{D}_{\max}(\Delta) | \cos\theta_1 c_1(\phi) + \sin\theta_1 c_2(\phi) = 0, \cos\theta_2 \phi'(R) + \sin\theta_2 \phi(R) = 0\}.$$

The trick to proving Theorem 1.2 is to write the resolvent $(\Delta_L - \lambda)^{-1}$ in terms of $(\Delta_{\theta_1} - \lambda)^{-1}$ (same self-adjoint condition at $r=0$ but with the Dirichlet condition at $r=R$). To do so, let $\varrho(r) \in C^\infty((-\infty,\infty))$ be a nondecreasing function such that $\varrho(r)=0$ for $r \leqslant 1/4$ and $\varrho(r)=1$ for $r \geqslant 3/4$. Given any real numbers $\alpha < \beta$, we define

$$\varrho_{\alpha,\beta}(r) := \varrho((r-\alpha)/(\beta-\alpha)). \tag{10.1}$$

Then $\varrho_{\alpha,\beta}(r)=0$ on a neighborhood of $\{r \leqslant \alpha\}$ and $\varrho_{\alpha,\beta}(r)=1$ on a neighborhood of $\{r \geqslant \beta\}$. We define

$$\psi_1(r) = \varrho_{R/2,3R/4}(r), \quad \psi_2(r) = 1 - \psi_1(r),$$

$$\varphi_1(r) = \varrho_{R/4,R/2}(r), \quad \varphi_2(r) = 1 - \varrho_{3R/4,R}(r). \tag{10.2}$$

Let $\Delta' := -(d^2/dr^2) - (1/4r^2)$ over $[R/4,R]$ with the Dirichlet condition at $r=R/4$ and the condition $\cos\theta_2\phi'(R) + \sin\theta_2\phi(R)=0$ at $r=R$; note that since $r \geqslant R/4$ over $[R/4,R]$, the operator Δ' is a true smooth elliptic operator over this interval with no singularities. We define

$$Q(\lambda) := \varphi_1(\Delta' - \lambda)^{-1}\psi_1 + \varphi_2(\Delta_{\theta_1} - \lambda)^{-1}\psi_2. \tag{10.3}$$

It follows that $Q(\lambda)$ maps into the domain $\mathcal{D}_L$ of Δ_L, and

$$\begin{aligned}(\Delta_L - \lambda)Q(\lambda) &= (\Delta_L - \lambda)\varphi_1(\Delta' - \lambda)^{-1}\psi_1 + (\Delta_L - \lambda)\varphi_2(\Delta_{\theta_1} - \lambda)^{-1}\psi_2 \\ &= \varphi_1(\Delta' - \lambda)(\Delta' - \lambda)^{-1}\psi_1 + \varphi_2(\Delta_{\theta_1} - \lambda)(\Delta_{\theta_1} - \lambda)^{-1}\psi_2 + K_0(\lambda) \\ &= \psi_1 + \psi_2 + K_0(\lambda) = \mathrm{Id} + K_0(\lambda),\end{aligned}$$

where

$$K_0(\lambda) = [\Delta, \varphi_1](\Delta' - \lambda)^{-1}\psi_1 + [\Delta, \varphi_2](\Delta_{\theta_1} - \lambda)^{-1}\psi_2.$$

Because the supports of $[\Delta, \varphi_i]$ and ψ_i, where $i=1,2$, are disjoint, using the explicit formula (A3) for the resolvent $(\Delta_{\theta_1} - \lambda)^{-1}$ and the properties of the resolvent of $(\Delta' - \lambda)^{-1}$ found in the work of Seeley[43] it is straightforward to check that $K_0(\lambda)$ is trace-class operator that vanishes to infinite order as $|\lambda| \to \infty$ for λ in any sector Λ of $\mathbb{C}$ not intersecting the positive real axis; we shall fix such a sector Λ from now on. In particular, forming the Neumann series, it follows that $\mathrm{Id} + K_0(\lambda)$ is invertible for $|\lambda|$ large with $\lambda \in \Lambda$ with

$$(\mathrm{Id} + K_0(\lambda))^{-1} = \mathrm{Id} + K(\lambda),$$

where $K(\lambda)$ has the same properties as $K_0(\lambda)$. Thus, multiplying both sides of $(\Delta_L - \lambda)Q(\lambda) = \mathrm{Id} + K_0(\lambda)$ by $\mathrm{Id} + K(\lambda)$, we see that

$$(\Delta_L - \lambda)^{-1} = Q(\lambda) + Q(\lambda)K(\lambda).$$

Therefore, as $|\lambda| \to \infty$ for $\lambda \in \Lambda$, we see that Proposition 7.1 holds also for $\mathrm{Tr}(\Delta_L - \lambda)^{-1}$. Now using the resolvent asymptotics, we can proceed to copy the proofs of Proposition 8.1 and 6.3. The proof of Theorem 1.2 is now complete.

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APPENDIX: THE RESOLVENT WITH DIRICHLET CONDITIONS AT $r=R$

In this Appendix, we compute the trace of the resolvent by explicitly finding the Schwartz kernel of the Bessel function. To do so, recall that the resolvent kernel of the differential operator $\Delta_\theta-\mu^2$ with given boundary conditions at $r=0$ and $r=R$ can be expressed as follows (see Lemma 4.1 in Ref. 9 or Ref. 26, Sec. 3.3 for an elementary account):

$$\frac{-1}{W(p,q)}\begin{cases} p(r,\mu)q(s,\mu) & \text{for } r\leqslant s,\\ p(s,\mu)q(r,\mu) & \text{for } r\geqslant s,\end{cases}$$

where $p(r,\mu)$ and $q(r,\mu)$ are solutions of $(\Delta_L-\mu^2)\phi=0$ satisfying the given boundary conditions at $r=0$ and $r=R$, respectively and where $W(p,q)$ is the Wronskian of (p,q). Recall that the general solution to $(\delta_L-\mu^2)\phi=0$ is

$$\phi=c_1(\phi)r^{1/2}J_0(\mu r)+c_2(\phi)r^{1/2}\left(\frac{\pi}{2}Y_0(\mu r)-(\log\mu-\log 2+\gamma)J_0(\mu r)\right).$$

To satisfy the boundary condition at $r=0$, we must have [see (5.3)]:

$$\cos\theta c_1(\phi)+\sin\theta c_2(\phi)=0.$$

Thus, we can take $c_2(\phi)=1$ and $c_1(\phi)=-\tan\theta$; this gives

$$p(r,\mu)=r^{1/2}\left(\frac{\pi}{2}Y_0(\mu r)-(\log\mu-\kappa)J_0(\mu r)\right), \tag{A1}$$

where $\kappa=\log 2-\gamma-\tan\theta$. To determine $q(r,\mu)$ we use the less fancy formulation of the general solution:

$$\phi=C_1r^{1/2}J_0(\mu r)+C_2r^{1/2}Y_0(\mu r).$$

To satisfy the Dirichlet condition at $r=R$, we therefore take

$$q(r,\mu)=r^{1/2}(Y_0(\mu R)J_0(\mu r)-J_0(\mu R)Y_0(\mu r)). \tag{A2}$$

The Wronskian is easily computed using that $W(r^{1/2}J_0(\mu r),r^{1/2}Y_0(\mu r))=2/\pi$ (see Ref. 45):

$$\begin{aligned}W(p,q)&=\frac{\pi}{2}Y_0(\mu R)W(r^{1/2}Y_0(\mu r),r^{1/2}J_0(\mu r))+(\log\mu-\kappa)J_0(\mu R)W(r^{1/2}J_0(\mu r),r^{1/2}Y_0(\mu r))\\&=-Y_0(\mu R)+\frac{2}{\pi}(\log\mu-\kappa)J_0(\mu R).\end{aligned}$$

Therefore,

$$(\Delta_\theta-\mu^2)^{-1}(r,s)=\frac{1}{F(\mu)}\begin{cases} p(r,\mu)q(s,\mu) & \text{for } r\leqslant s,\\ p(s,\mu)q(r,\mu) & \text{for } r\geqslant s,\end{cases} \tag{A3}$$

where p and q are given in (A1) and (A2), respectively, and where

$$F(\mu):=Y_0(\mu R)-\frac{2}{\pi}(\log\mu-\kappa)J_0(\mu R).$$

We now need to compute $\int_0^R p(r,\mu)q(r,\mu)\mathrm{d}r$; that is,

$$\int_0^R r\left(\frac{\pi}{2}Y_0(\mu r)-(\log\mu-\kappa)J_0(\mu r)\right)(Y_0(\mu R)J_0(\mu r)-J_0(\mu R)Y_0(\mu r))\mathrm{d}r$$
$$=\frac{\pi}{2}Y_0(\mu R)\int_0^R rY_0(\mu r)J_0(\mu r)\mathrm{d}r-\frac{\pi}{2}J_0(\mu R)\int_0^R rY_0(\mu r)^2\,\mathrm{d}r+(\log\mu$$
$$-\kappa)J_0(\mu R)\int_0^R rJ_0(\mu r)Y_0(\mu r)\mathrm{d}r-(\log\mu-\kappa)Y_0(\mu R)\int_0^R rJ_0(\mu r)^2\,\mathrm{d}r. \tag{A4}$$

We next use the indefinite integrals

$$\int rJ_0(\mu r)^2\,\mathrm{d}r=\frac{r^2}{2}(J_0(\mu r)^2+J_1(\mu r)^2),$$

$$\int rY_0(\mu r)^2\,\mathrm{d}r=\frac{r^2}{2}(Y_0(\mu r)^2+Y_1(\mu r)^2),$$

$$\int rY_0(\mu r)J_0(\mu r)\mathrm{d}r=\frac{r^2}{2}(Y_0(\mu r)J_0(\mu r)+Y_1(\mu r)J_1(\mu r)),$$

which we need to evaluate between $r=0$ and $r=R$. Recalling (5.2), $zJ_0(z)$ and $zJ_1(z)$ vanish at $z=0$. Also, by (5.1) $zY_0(z)$ also vanishes at $z=0$. However, it is a remarkable fact, which may be easily overlooked, that since

$$\frac{\pi}{2}Y_1(z)=-\frac{1}{z}J_0(z)+(\log z-\log 2+\gamma)J_1(z)-\frac{1}{2}z\sum_{k=1}^{\infty}\frac{kH_k\left(-\frac{1}{4}z^2\right)^{k-1}}{(k!)^2},$$

where we used that $Y_1(z)=-Y_0'(z)$ and $J_1(z)=-J_0'(z)$ from Ref. 1 p. 361, we have

$$(zY_1(z))|_{z=0}=-\frac{2}{\pi}\Rightarrow\ (z^2Y_1(z)^2)|_{z=0}=\frac{4}{\pi^2}.$$

Therefore,

$$\int_0^R rJ_0(\mu r)^2\,\mathrm{d}r=\frac{R^2}{2}(J_0(\mu R)^2+J_1(\mu R)^2)$$

$$\int_0^R rY_0(\mu r)^2\,\mathrm{d}r=\frac{R^2}{2}(Y_0(\mu R)^2+Y_1(\mu R)^2)-\frac{1}{2}\ \ (r^2Y_1(\mu r)^2)|_{r=0})$$
$$=\frac{R^2}{2}(Y_0(\mu R)^2+Y_1(\mu R)^2)-\frac{2}{\pi^2\mu^2}$$

$$\int_0^R rY_0(\mu r)J_0(\mu r)\mathrm{d}r=\frac{R^2}{2}(Y_0(\mu R)J_0(\mu R)+Y_1(\mu R)J_1(\mu R)).$$

Plugging these integrals into (A4) and using the identity (Ref. 1, p. 360)

$$J_1(z)Y_0(z) - J_0(z)Y_1(z) = \frac{2}{\pi z}$$

to simplify the expression obtained, we eventually arrive that

$$\int_0^R p(r,\mu)q(r,\mu)\mathrm{d}r = \frac{R}{2\mu}\left(Y_1(\mu R) - \frac{2}{\pi}(\log\mu - \kappa)J_1(\mu R)\right) + \frac{1}{\pi\mu^2}J_0(\mu R)$$

$$= \frac{R}{2\mu}\left(Y_1(\mu R) - \frac{2}{\pi}(\log\mu - \kappa)J_1(\mu R) + \frac{2}{\pi\mu R}J_0(\mu R)\right).$$

Using the fact that $J_0'(z) = -J_1(z)$ and $Y_0'(z) = -Y_1(z)$, we can write this as

$$\int_0^R p(r,\mu)q(r,\mu)\mathrm{d}r = -\frac{1}{2\mu}\frac{d}{\mathrm{d}\mu}\left(Y_0(\mu R) - \frac{2}{\pi}(\log\mu - \kappa)J_0(\mu R)\right) = -\frac{1}{2\mu}\frac{d}{\mathrm{d}\mu}F(\mu),$$

where we recall that

$$F(\mu) \coloneqq Y_0(\mu R) - \frac{2}{\pi}(\log\mu - \kappa)J_0(\mu R).$$

Since [see (A3)]

$$(\Delta_\theta - \mu^2)^{-1}(r,s) = \frac{1}{F(\mu)}\begin{cases} p(r,\mu)q(s,\mu) & \text{for } r \leqslant s, \\ p(s,\mu)q(r,\mu) & \text{for } r \geqslant s, \end{cases}$$

we have proved the following theorem.

Theorem A.1: *With* $F(\mu) \coloneqq Y_0(\mu R) - (2/\pi)(\log\mu - \kappa)J_0(\mu R)$, *we have*

$$\mathrm{Tr}(\Delta_\theta - \mu^2)^{-1} = -\frac{1}{2\mu}\frac{1}{F(\mu)}\frac{d}{\mathrm{d}\mu}F(\mu) = -\frac{1}{2\mu}\frac{d}{\mathrm{d}\mu}\log F(\mu).$$

This theorem has been used to analyze the zeta function, resolvent, and heat kernel of Δ_θ in Secs. VI–VIII.

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Quaternionic root systems and subgroups of the Aut(F_4)

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Cayley-Dickson doubling procedure is used to construct the root systems of some celebrated Lie algebras in terms of the integer elements of the division algebras of real numbers, complex numbers, quaternions, and octonions. Starting with the roots and weights of SU(2) expressed as the real numbers one can construct the root systems of the Lie algebras of SO(4), SP(2)$\approx$SO(5), SO(8), SO(9), F_4 and E_8 in terms of the discrete elements of the division algebras. The roots themselves display the groups structures besides the octonionic roots of E_8 which form a closed octonion algebra. The automorphism group Aut(F_4) of the Dynkin diagram of F_4 of order 2304, the largest crystallographic group in four-dimensional Euclidean space, is realized as the direct product of two binary octahedral group of quaternions preserving the quaternionic root system of F_4. The Weyl groups of many Lie algebras, such as, G_2, SO(7), SO(8), SO(9), SU(3)*X*SU(3), and SP(3)$\times$SU(2) have been constructed as the subgroups of Aut(F_4). We have also classified the other non-parabolic subgroups of Aut(F_4) which are not Weyl groups. Two subgroups of orders 192 with different conjugacy classes occur as maximal subgroups in the finite subgroups of the Lie group G_2 of orders 12096 and 1344 and proves to be useful in their constructions. The triality of SO(8) manifesting itself as the cyclic symmetry of the quaternionic imaginary units e_1, e_2, e_3 is used to show that SO(7) and SO(9) can be embedded, triply symmetric way in SO(8) and F_4 in respectively. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2190334]

I. INTRODUCTION

There are a few celebrated Lie algebras which seem to be playing important roles in understanding the underlying symmetries of the unified theory of all interactions. The most popular ones are the exceptional Lie groups G_2, F_4, E_6, E_7, and E_8 and the related groups.[1] The groups Spin7 and G_2 are proposed as the holonomy groups for the compactification of the M-theory from 11 to four dimensional space-time.[2] It is also well known that two orthogonal groups SO(8) and SO(9) are the little groups of the massless particles of string theories in 10-dimensions and the M-theory in 11-dimensions, respectively. The fact that SO(9) can be embedded in the exceptional Lie group F_4 in a triply symmetric way and the noncompact $F_{4(-25)}$ can be embedded in the Lorenz group SO(25,1) indicates the importance of the exceptional group F_4.[3] The largest exceptional group E_8 which had been suggested as the unified theory of the electroweak and strong interactions with three generations of lepton-quark families[4] naturally occurred as the gauge symmetry of the $E_8 \times E_8$ heterotic string theory.[5] It has many novel mathematical aspects[6] which has not been ex-

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ploited in physics. It was known that a non-compact version of E_7 manifests itself as a global symmetry of the 11-dimensional supergravity.[7] Some of its maximal subgroups show themselves as local symmetries.[8] The E_6 has been suggested as a unified theory of electroweak and strong interactions.[9]

The Weyl groups of these groups are also important for the invariants of the Lie groups can be deduced using the related Weyl groups. The Weyl groups of the exceptional Lie groups F_4, E_6, E_7, and E_8 correspond to some finite subgroups of the Lie groups of O(4), O(6), O(7), and O(8), respectively.[10]

It has been shown in some details that the finite subgroups of O(4) can be classified as direct products of finite subgroups of quaternions,[11] isomorphic to the finite subgroups of SU(2), which is the double cover of SO(3). Therefore the relevant Weyl groups of the Lie groups F_4, SO(9), and SO(8) correspond to some finite subgroups of O(4).[12] Similarly, the Weyl groups of some rank-3 Lie algebras can be obtained from the finite subgroups of O(3). Interestingly enough, the relevant root systems can be represented as discrete quaternions and the Weyl groups can be realized as the left-right actions of the quaternions on the root systems. When one considers the finite subgroups of O(8) it is natural to encounter with the discrete octonions which represent the root system of E_8 where the root system of E_7 is described by imaginary octonions.[13] The automorphism group of octonionionic root system of E_7 turns out to be a finite subgroup of G_2 of order 12096.[14] In what follows we will restrict ourselves to the quaternionic root system of F_4, SO(9), SO(8), SO(7), SP(3) and construct explicitly their Weyl groups as finite subgroups of O(4). The largest group of interest here is the Aut(F_4) of order $2304=48\times 48$ which is the direct product of the binary octahedral group with itself.[15] We follow a chain of decomposition of Aut(F_4) into its relevant subgroups, some of which are maximal subgroups in the finite subgroups of G_2 of orders 12096 and 1344.[16]

The paper is organized as follows. In Sec. II we start with the scaled roots ± 1 0 and the weights $\pm\frac{1}{2}$ of SU(2) and using the Cayley-Dickson doubling procedure we construct the roots of SO(4) and SP(2)$\approx$SO(5) in terms of complex numbers. Further doubling of the roots of SP(2) $\approx$SO(5) leads to the quaternionic roots of SO(8).[13,16] The eight-dimensional vector and spinor representations of Spin-8 constitute the short roots of F_4. Doubling of two sets of quaternionic roots of F_4 leads to the octonionic roots of E_8. The triality of SO(8) is then coded in the cyclic symmetry of the quaternionic imaginary units. In Sec. III we introduce the finite subgroups of SU(2) in terms of quaternions and explain their geometric properties. We explain how to construct the Aut(F_4) and the Weyl groups of F_4, SO(9), and SO(8).[15]In Sec. IV we construct the root systems of SO(7) and G_2 by folding the Coxeter-Dynkin diagram of SO(8),[17] which displays the threefold embeddings of SO(7) into SO(8). The Weyl groups of SO(7), G_2, and SP(3) are constructed in terms of quaternions. In Sec. V we discuss the subgroup chains of Aut(F_4) and find out the explicit expressions of the groups down to the groups of order 192. A particular emphasis is given to two groups of orders 192 since they appear as the maximal subgroups in the finite subgroups of G_2 of orders 12096 and 1344. Finally in Sec. VI we further elaborate the geometric aspects of the symmetries discussed in the preceding sections.

II. ROOT SYSTEMS WITH THE CAYLEY-DICKSON DOUBLING PROCEDURE

The Cayley-Dickson doubling is a procedure to build the elements of division algebras starting with the real numbers. Let us denote by p, q, r, s the elements of a division algebra other than the octonions. Then the pairs (p,q) and (r,s) with the multiplication rule

$$(p,q)(r,s) = (pr - s\bar{q}, rq + \bar{p}s) \tag{1}$$

constitute the elements of a division algebra in higher dimension. The celebrated Hurwitz's theorem[18] states that there are only four division algebras, namely, real numbers, complex numbers, quaternions, and octonions. Starting with the complex numbers at every higher level of division algebras one introduces one complex number, say, e_1, e_2, and e_7 which anticommute with each other and satisfy the relation $e_1^2=e_2^2=e_7^2=-1$. Doubling of the real numbers constitutes the

complex numbers, two sets of complex numbers define the quaternions and finally a pair of quaternions defines the octonions under the definition (1). Let us revise the work of Ref. 13 by starting with the roots ±1 0 and the weights $\pm\frac{1}{2}$ of SU(2). A pair of set ±1 0 leads to the roots of SO(4):

$$(\pm 1,0) = \pm 1,(0,\pm 1) = \pm e_1(\text{we use } e_1 \text{ for the imaginary number } i). \tag{2}$$

The nonzero roots ± 1 $\pm e_1$ of SO(4) form a cyclic group of order 4. The weights of the spinor representation $(\underline{2},\underline{2})$ of SO(4) can be taken as

$$\left(\pm\tfrac{1}{2},\pm\tfrac{1}{2}\right) = \tfrac{1}{2}(\pm 1 \pm e_1). \tag{3}$$

The roots in (2) and the weights in (3) constitute the scaled roots of $\mathrm{SP}(2) \approx \mathrm{SO}(5)$,

$$\mathrm{SP}(2) \approx \mathrm{SO}(5): \pm 1, \pm e_1, \tfrac{1}{2}(\pm 1 \pm e_1). \tag{4}$$

When the short roots are scaled to the unit norm then the roots of SP(2) form a cyclic group of order 8. A nontrivial structure will arise when two sets of the roots of SP(2) are paired as $(\mathrm{SP}(2),\mathrm{SP}(2))$ where the long roots match with the zero roots while the short roots match with the short roots leading to the quaternionic roots of SO(8):

$$T:\left\{\pm 1, \pm e_1, \pm e_2, \pm e_3, \tfrac{1}{2}(\pm 1 \pm e_1 \pm e_2 \pm e_3)\right\}, \tag{5}$$

where we have used $e_3e_1=-e_1e_3=e_2$. If we include the pairing of the short roots with the zero roots we obtain

$$V_1':\left(\tfrac{1}{2}(\pm 1 \pm e_1),0\right) = \tfrac{1}{2}(\pm 1 \pm e_1),\left(0,\tfrac{1}{2}(\pm 1 \pm e_1)\right) = \tfrac{1}{2}(\pm e_2 \pm e_3). \tag{6}$$

These are the weights of the eight-dimensional representation of SO(8) and together with the roots in (5) they represent the roots of SO(9). The cyclic symmetry of the quaternionic imaginary units would lead to the weights of the two eight-dimensional spinor representations of SO(8) which represent the weights of the 16-dimensional spinor representation of SO(9):

$$\begin{aligned} V_2':&\left\{\tfrac{1}{2}(\pm 1 \pm e_2), \quad \tfrac{1}{2}(\pm e_3 \pm e_1)\right\}, \\ V_3':&\left\{\tfrac{1}{2}(\pm 1 \pm e_3), \quad \tfrac{1}{2}(\pm e_1 \pm e_2)\right\}. \end{aligned} \tag{7}$$

The set of quaternions in (5)–(7) constitutes the scaled roots of F_4. A further doubling the set of roots of F_4 will lead to the octonionic roots of E_8,[13]

$$\begin{aligned} &(T,0) = T, \quad (0,T) = e_7T, \\ &(V_1',V_1') = V_1' + e_7V_1', \\ &(V_2',V_3') = V_2' + e_7V_3', \\ &(V_3',V_2') = V_3' + e_7V_2', \end{aligned} \tag{8}$$

where one can define $e_4=e_7e_1$, $e_5=e_7e_2$, $e_6=e_7e_3$. We note that when the roots in (6) and (7) are multiplied by $\sqrt{2}$ to make the norm 1 then the 48 sets of quaternions are the elements of the binary octahedral group O of SU(2) where T represents the binary tetrahedral subgroup of order 24.

III. BINARY OCTAHEDRAL GROUP AND THE Aut(F_4)

Some of the material of this section have been discussed in Ref. 12. The finite subgroups of SO(3) are well known: icosahedral group of order 60, octahedral group of order 24, tetrahedral group of order 12, and dihedral and cyclic groups of various orders.[19] Their double covers are the

TABLE I. Multiplication table of the binary octahedral group.

	V_0	V_+	V_-	V_1	V_2	V_3
V_0	V_0	V_+	V_-	V_1	V_2	V_3
V_+	V_+	V_-	V_0	V_3	V_1	V_2
V_-	V_-	V_0	V_+	V_2	V_3	V_1
V_1	V_1	V_2	V_3	V_0	V_+	V_-
V_2	V_2	V_3	V_1	V_-	V_0	V_+
V_3	V_3	V_1	V_2	V_+	V_-	V_0

finite subgroups of quaternions which are related to the ADE series of the Lie algebras through the McKay correspondence.[20] Our interests here solely are constrained to the binary octahedral group whose direct product with itself is isomorphic to the Aut(F_4) which can be realized as the left and right actions of the quaternionic elements on the quaternionic roots of F_4. The root system of F_4 has very interesting geometrical structures which has not been discussed in the literature. We classify the elements of the binary octahedral group as sets of the hyperoctahedra in four dimensions,[21]

$$\begin{aligned} V_0 &= \{\pm 1, \pm e_1, \pm e_2, \pm e_3\} \\ T{:}V_+ &= \left\{\tfrac{1}{2} \pm 1 \pm e_1 \pm e_2 \pm e_3\right\}, \quad \text{even number of } (+) \text{ signs} \\ V_- &= \overline{V_+} = \left\{\tfrac{1}{2} \pm 1 \pm e_1 \pm e_2 \pm e_3\right\}, \quad \text{odd number of } (+) \text{ signs}, \end{aligned} \tag{9}$$

where $\overline{V_+}$ is the quaternionic conjugate of V_+.

$$\begin{aligned} V_1 &= \left\{\frac{1}{\sqrt{2}}(\pm 1 \pm e_1), \frac{1}{\sqrt{2}}(\pm e_2 \pm e_3)\right\} \\ T'{:}V_2 &= \left\{\frac{1}{\sqrt{2}}(\pm 1 \pm e_2), \frac{1}{\sqrt{2}}(\pm e_3 \pm e_1)\right\} \\ V_3 &= \left\{\frac{1}{\sqrt{2}}(\pm 1 \pm e_3), \frac{1}{\sqrt{2}}(\pm e_1 \pm e_2)\right\} \end{aligned} \tag{10}$$

$$O{:}T \oplus T'. \tag{11}$$

Here each of V_0, V_+, and V_- represents the vertices of a hyperoctahedron in four-dimensions and any two hyperoctahedra form a hypercube in four dimensions with 16 vertices. The set of quaternions T in (9) not only constitute the nonzero roots of SO(8) but also represent a polytope 3,4,5 called 24-cell.[21] The set of quaternions in T' are the duals of T; consequently any $V_i(i=1,2,3)$ is a hyperoctahedron and any two hyperoctahedra form the vertices of a hypercube. We give the multiplication table of these sets of quaternions in Table I to understand the structure of the binary octahedral group. Here V_0 is the quaternion group and forms an invariant subgroup both in T and O.

A general element of $\mathrm{O}(4) \approx \mathrm{SU}(2) \times \mathrm{SU}(2)$ can be defined as follows. Denote by p,q the quaternions of unit norm acting on an arbitrary quaternion $r=r_0+r_1e_1+r_2e_2+r_3e_3$,

$$^{[29]}r \to prq{:}[p,q], \tag{12}$$

$$r \to p\bar{r}q{:}[p,q]^*, \tag{13}$$

where $\bar{r}$ is the quaternion conjugate $\bar{r}=r_0-r_1e_1-r_2e_2-r_3e_3$. For arbitrary quaternions p,q with unit norm the elements $[p,q]$ and $[p,q]^*$ form a six parameter group leaving the norm $r\bar{r}=\bar{r}r$ invariant. When written in terms of matrices the group elements $[p,q]$ and $[p,q]^*$ have determinants +1 and

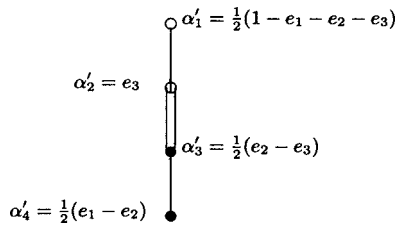

FIG. 1. The Coxeter-Dynkin diagram of F_4.

-1, respectively. Therefore the elements $[p,q]$ form a subgroup $\mathrm{SO}(4) \approx \mathrm{SU}(2) \times \mathrm{SU}(2)/Z_2$ of $\mathrm{O}(4)$. In Ref. 12 we have proven that the Weyl group $W(F_4)$ can be compactly written as the union of elements,

$$W(F_4) = [T,T] \oplus [T',T'] \oplus [T,T]^* \oplus [T',T']^*. \tag{14}$$

The automorphism group $\mathrm{Aut}(F_4)$ is the semidirect product of the Weyl group $W(F_4)$ with the Z_2 symmetry of the Coxeter-Dynkin diagram of F_4,

$$^{[30]}\mathrm{Aut}(F_4) \equiv (O,O) \oplus (O,O)^* \approx W(F_4){:}Z_2. \tag{15}$$

The generators of $\mathrm{Aut}(F_4)$ can be obtained from the Coxeter-Dynkin diagram of F_4 where the simple roots are given in terms of scaled quaternions (Fig. 1).

The regular simple roots α_i are related to α_i' by $\alpha_i = \sqrt{2}\alpha_i' (i=1,2,3,4)$. The $\mathrm{Aut}(F_4)$ is generated by the elements

$$[\alpha_1', -\alpha_1']^*, [\alpha_2', -\alpha_2']^*, [\alpha_3, -\alpha_3]^*, [\alpha_4, -\alpha_4]^*, \left[\frac{1}{\sqrt{2}}(e_2 + e_3), -e_2\right]. \tag{16}$$

The first four generators in (16) represent the reflections in the roots $\alpha_i (i=1,2,3,4)$ and generate the Weyl group $W(F_4)$ and the last term stands for the diagram symmetry of F_4 which transforms, by conjugation, $\alpha_1' \leftrightarrow \alpha_4'$ and $\alpha_2' \leftrightarrow \alpha_3'$. An extended Coxeter-Dynkin diagram of F_4 can be used to obtain the Coxeter-Dynkin diagrams of its maximal Lie algebras. We will discuss all starting with SO(9).

A. The parabolic subgroups of F_4

1. SO(9)

We have shown in Ref. 12 that the Weyl group $W(\mathrm{SO}(9))$ can be represented by the set of group elements

$$[V_0, V_0], [V_+, V_+], [V_-, V_-], [V_0, V_0]^*, [V_+, V_+]^*, [V_-, V_-]^*, \tag{17}$$

$$[V_1, V_1], [V_2, V_3], [V_3, V_2], [V_1, V_1]^*, [V_2, V_3]^*, [V_3, V_2]^*. \tag{18}$$

This is a group of order 384. The $W(\mathrm{SO}(9))$ can be embedded in the $W(F_4)$ triply symmetric way by permuting the quaternionic imaginary units e_1, e_2, e_3 in the cyclic order. It is an inner automorphism of $W(F_4)$ which replaces the elements in (18) by the corresponding elements where the indices 1,2,3 are permuted in the cyclic order. This permutation of the indices leaves the set of elements in (17) invariant as expected. Actually the set of elements in (17) constitute the elements of the Weyl group $W(\mathrm{SO}(8))$. The Weyl group $W(\mathrm{SO}(9))$ has a very interesting geometrical aspect; it is the largest symmetry preserving the four-dimensional hyperoctahedron. One can show that the group elements in (17) and (18) leave the set of elements in V_1 invariant which is one of those six hyperoctahedra of the 48 roots of F_4. This must be expected anyway because the set of roots $V_1/\sqrt{2}$ are the short roots of SO(9) and must be rotated to each other by the elements of $W(\mathrm{SO}(9))$.

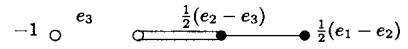

FIG. 2. The Coxeter-Dynkin diagram of $SU(2)\times SP(3)$.

Since the weights of the 16-dimensional spinor representation are represented by the quaternions $(1/\sqrt{2})(V_2+V_3)$ corresponding to the vertices of a cube in four-dimensions they are also preserved by the elements of $W(SO(9))$ in (14). Embedding $W(SO(9))$ in $\mathrm{Aut}(F_4)$ can be made with a sixfold cyclic symmetry under the conjugation, say, by $[V_+,V_1]W(SO(9))[V_-,V_1]$ where $[V_+,V_1]^6=[V_0,V_0]$. This leads to six conjugate representations of $W(SO(9))$ in $\mathrm{Aut}(F_4)$ in each of which one of the six hyperoctahedra $V_0,V_\pm,V_i(i=1,2,3)$ is left invariant by $W(SO(9))$. There are other subgroups of $\mathrm{Aut}(F_4)$ of order 384 not isomorphic to the Weyl group $W(SO(9))$. We will discuss them in Sec. V. Now we discuss the Weyl group of the maximal subalgebra $SU(2)\times SP(3)$ of F_4.

2. SU(2)×SP(3)

The algebra $SU(2)\times SP(3)$ can be represented by the Coxeter-Dynkin diagram shown in Fig. 2.

The reflection generators on the simple roots are represented by

$$r_0=[1,-1]^*,\quad r_1=[e_3,-e_3]^*,\quad r_2=\left[\frac{1}{\sqrt{2}}(e_2-e_3),-\frac{1}{\sqrt{2}}(e_2-e_3)\right]^*,$$
$$r_3=\left[\frac{1}{\sqrt{2}}(e_1-e_2),-\frac{1}{\sqrt{2}}(e_1-e_2)\right]^* \tag{19}$$

and will generate the set of roots

$$\begin{array}{cc} \mathrm{SU}(2) & \mathrm{SP}(3) \\ \pm 1 & \pm e_1,\pm e_2,\pm e_3 \\ & \frac{1}{2}(\pm e_1\pm e_2) \\ & \frac{1}{2}(\pm e_2\pm e_3) \\ & \frac{1}{2}(\pm e_3\pm e_1). \end{array} \tag{20}$$

The long roots $\pm e_1$, $\pm e_2$, $\pm e_3$ of SP(3) form the vertices of an octahedron. Therefore the Weyl group $W(SP(3))$ is the symmetry of the octahedron in three-dimensions. Since the product of two reflections is a rotation around some axis the proper rotation subgroup of $W(SP(3))$ is generated by

$$R=r_1r_2=\left[\frac{1}{\sqrt{2}}(1-e_1),\frac{1}{\sqrt{2}}(1+e_1)\right],S=r_2r_3=[\bar{t},t] \tag{21}$$

with $t=\frac{1}{2}(1+e_1+e_2+e_3)$. Here the generators satisfy the generation relations of an octahedral group[23]

$$R^4=S^3=(RS)^2=[1,1]. \tag{22}$$

It is one of the finite subgroups of SO(3) isomorphic to the symmetric group S_4. Another generator $(r_1r_2r_3)^3=[1,1]^*$ commutes with the generators R and S so that the maximal group of the SP(3) roots is the group $W(SP(3))\approx S_4\times Z_2$, a group of order 48. The Z_2 group of $W(SU(2))$ is generated by $[1,-1]^*$ which commutes with the generators of $W(SP(3))$. Therefore the Weyl group $W(SU(2))\times W(SP(3))$ is isomorphic to the group $S_4\times Z_2^2$ of order 96. The group elements are represented by the pair of quaternions

$$[p,\pm\bar{p}],[p',\pm\bar{p}'],[p,\pm\bar{p}]^*,[p',\pm\bar{p}']^*;p\in T,p'\in T'. \tag{23}$$

FIG. 3. The Coxeter-Dynkin diagram of $SU(3)\times SU(3)$. Here $\bar{t}=\frac{1}{2}(1-e_1-e_2-e_3)$, $s_1'=\frac{1}{2}(e_1-e_2)$, and $s_2'=\frac{1}{2}(e_2-e_3)$.

Since the vertices of the octahedron are represented by the imaginary quaternions $\pm e_1, \pm e_2, \pm e_3$ one can naturally ask the question: what is the maximal group which preserves the quaternion algebra of the set of quaternions $\pm e_1, \pm e_2, \pm e_3$? It is well known that when p is the unit quaternion with nonzero real component then the transformation $e_i'=pe_i\bar{p}$ is the only transformation which preserves the quaternion algebra and is isomorphic to the group SO(3). This implies that the finite subgroup of SO(3) which preserves the set of quaternions $\pm e_1, \pm e_2, \pm e_3$ is the octahedral group represented by the elements $[p,\bar{p}],[p',\bar{p}]$ which is isomorphic to the symmetric group S_4.

3. SU(3)×SU(3)

From the extended Coxeter-Dynkin diagram of F_4 we obtain the Coxeter-Dynkin diagram of $SU(3)\times SU(3)$ (Fig. 3).

Note that one of the SU(3) is represented by the short roots. The nonzero roots of $SU(3)\times SU(3)$ are given by

$$\pm 1, \pm t, \pm \bar{t}, \pm s_1', \pm s_2', \pm s_3', \tag{24}$$

where $s_3'=\frac{1}{2}(e_3-e_1)$. Using the standard technique one can form the elements of $W(SU(3))\times W(SU(3))$ of order 36 which is the direct product of two symmetric groups S_3. A further symmetry is the diagram automorphism of $SU(3)\times SU(3)$ which can be made by an element $c=[1,(1/\sqrt{2})(e_1-e_2)]$ which permutes the simple roots and preserve the Cartan matrix of the algebra $SU(3)\times SU(3)$. An extension of the Weyl group $W(SU(3))\times W(SU(3))$ by the element $c=[1,(1/\sqrt{2})(e_1-e_2)]$ leads to, up to conjugation, the group $\mathrm{Aut}(SU(3)\times SU(3))\approx[W(SU(3))\times W(SU(3))]:Z_4$ (Ref. 24) where Z_4 is the cyclic group of order 4 generated by the element c. The set of elements can be represented by $[p,q]\oplus[p,q]^*$ where p,q take arbitrary values from the set of scaled roots $p,q\in\{\pm 1,\pm t,\pm\bar{t},\pm s_1,\pm s_2,\pm s_3\}$ where $s_i=\sqrt{2}s_i'(i=1,2,3)$.

IV. SO(8) AND ITS SUBGROUPS

The SO(8) algebra plays a special role when embedding in F_4 since the long roots of F_4 are the roots of SO(8). Its Coxeter-Dynkin diagram illustrates the triality in terms of the cyclic symmetry of the quaternionic imaginary units.

The Weyl group $W(SO(8))$ is represented by the set of elements (17) and the $\mathrm{Aut}(S(O(8))$ is isomorphic to the Weyl group $W(F_4)$. Since in Ref. 12 we have worked SO(8) in some detail here we will deal with its two special subgroups SO(7) and G_2 (Fig. 4).

A. SO(7)

The SO(7) diagram can be obtained from that of SO(8) by folding two branches and averaging the corresponding simple roots.[17]

Denote by the reflection generators r_1, r_2, r_3 of SO(7) (Fig. 5) corresponding to the simple roots e_1, $\bar{t}=\frac{1}{2}(1-e_1-e_2-e_3)$, $\frac{1}{2}(e_2+e_3)$, respectively, which can be expressed as

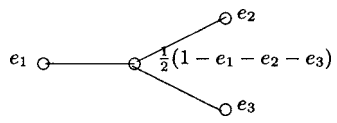

FIG. 4. The Coxeter-Dynkin diagram of SO(8).

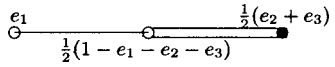

FIG. 5. The Coxeter-Dynkin diagram of SO(7).

$$r_1=[e_1,-e_1]^*,\quad r_2=[\bar{t},-\bar{t}]^*,\quad r_3=\left[\frac{1}{\sqrt{2}}(e_2+e_3),-\frac{1}{\sqrt{2}}(e_2+e_3)\right]^*. \tag{25}$$

One can also express r_3 in terms of the simple roots of SO(8) as the product of reflection generators corresponding to e_2 and e_3 rather than the one in (25). That would give us $r_3=[e_2,-e_2]^*[e_3,-e_3]^*=[e_1,-e_1]$ which gives the same result when acting on the roots of SO(7). If we define $d_1=(1/\sqrt{2})(e_2-e_3)$ then we can write the $W(\mathrm{SO}(7))$ generators as

$$r_1=[e_1,-d_1\bar{e}_1\bar{d}_1]^*,\quad r_2=[\bar{t},-d_1t\bar{d}_1]^*,\quad r_3=[e_1,-d_1\bar{e}_1\bar{d}_1]. \tag{26}$$

The generators $a=r_1r_2$ and $b=(r_1r_2r_3)^2$ satisfy the generation relation

$$a^3=b^3=(ab)^2=[1,1] \tag{27}$$

which is the generation relation of the tedrahedral group of order 12 isomorphic to the group A_4 of the even permutations of four letters.[23] The group elements can be written as

$$[p,d_1\bar{p}\bar{d}_1],p\in T. \tag{28}$$

One can check that the elements

$$[1,-1],[1,\pm 1]^* \tag{29}$$

preserve the simple roots by conjugation. This means that the tetrahedral group in (28) can be extended by the elements in (29) so that the whole set of elements will read

$$[p,\pm d_1\bar{p}\bar{d}_1],[p,\pm d_1\bar{p}\bar{d}_1]^*. \tag{30}$$

We note that the set of elements

$$[p,d_1\bar{p}\bar{d}_1],[p,d_1\bar{p}\bar{d}_1]^* \tag{31}$$

form a group isomorphic to the octahedral group S_4. The element $[1,-1]$ commutes with the elements of S_4 in (31). Therefore the set of elements represent a group isomorphic to the group $S_4\times Z_2$ which is the Weyl group $W(\mathrm{SO}(7))$ of order 48. This is the group isomorphic to $W(\mathrm{SP}(3))$ represented by (30) and (31). We could have different foldings of SO(8) diagram other than the one shown in Fig. 5. This would lead to replacing the quaternion d_1 in (30) by $d_2=\frac{1}{2}(e_3-e_1)$ and $d_3=\frac{1}{2}(e_1-e_2)$. By replacing d_1 by d_2 and d_3 in (30) we obtain three different embeddings of SO(7) in SO(8). When we stick to the representation of $W(\mathrm{SO}(7))$ in (30) we can show that the 24 nonzero roots of SO(8) can be decomposed as

$$\pm 1,\pm e_1,e_2,-e_3,\tfrac{1}{2}(\pm 1\pm e_1\pm(e_2+e_3)),\tfrac{1}{2}(\pm 1\pm e_1+(e_2-e_3)) \tag{32}$$

which represent 18 nonzero roots of SO(7) and the remaining ones are the six nonzero weights of the seven-dimensional representation of SO(7),

$$-e_2,e_3,\tfrac{1}{2}(\pm 1\pm e_1-(e_2-e_3)). \tag{33}$$

Three different embeddings of SO(7) in SO(8) can be realized by permuting the indices (1,2,3) in (32) and (33) in the cyclic order.

FIG. 6. The Coxeter-Dynkin diagram of G_2.

B. G_2

The Coxeter-Dynkin diagram of G_2 can be obtained from that of SO(8) by folding three branches and taking the average of the outer simple roots[17] (Fig. 6).

Let us denote by $I=(1/\sqrt{3})(e_1+e_2+e_3)$ with $I^2=-1$. The simple roots scaled by $\sqrt{2}$ are given by $\alpha_1=\frac{1}{2}(1-\sqrt{3}I)=e^{-(\pi/3)I}$, $\alpha_2=I/\sqrt{3}$ and the reflection generators read $r_1=[e^{-(\pi/3)I},-e^{-\pi I/3}]^*$, $r_2=[I,-I]^*$. The group $W(G_2)$ generated by r_1 and r_2 is the dihedral group D_6 of order 12. One can obtain the 12 nonzero roots of G_2 by acting the generators r_1 and r_2 on the simple roots. The weights of the seven-dimensional representation can be obtained from the highest weight $\sqrt{\frac{2}{3}}e^{(\pi/6)I}$.

A remark is in order. We can summarize the discussion in this section that the SO(7) can be embedded in SO(8) triply symmetric way and the G_2 takes place in the intersection of these three SO(7) in SO(8) (Fig. 7).[25]

V. NONPARABOLIC SUBGROUPS OF Aut(F_4)

So far we have discussed the parabolic subgroups of Aut(F_4) related with the Lie subalgebras of F_4. As we have mentioned before the Aut(F_4) is the largest crystallographic group in four dimensions and deserves further analysis regarding its chain decomposition through its maximal subgroups which could be useful for the crystallography in four dimensions. First we discuss the maximal subgroups of Aut(F_4). We will give the group elements in terms of quaternions and distinguish the groups by their orders and conjugacy classes. The group orders and conjugacy classes are not sufficient to understand the group structures. Since we will write down the group elements explicitly in terms of quaternions the distinguishing the groups of the same order will not create a problem. Nevertheless we will denote a group of interest with its order together with its conjugacy classes in a parentheses and display the group elements in terms of quaternions. For example, the group Aut(F_4), being of order 2304 with 29 conjugacy classes will be shortly denoted by 2304(29) and its quaternionic representation will follow the group notation. We know that this is not a proper group notation; it should rather have a decomposition involving invariant subgroups. Since we denote each group by their elements the order with the conjugacy classes would be sufficient.

A. Maximal subgroups of Aut(F_4)

We have three maximal subgroups of Aut(F_4) of order 1152.

1. $W(F_4)$ of order 1152(25)

It is a subgroup of O(4). We have discussed this group in details which was represented by the quaternions in (14),

$$W(F_4)=[T,T]\oplus[T',T']\oplus[T,T]^*\oplus[T',T']^*.$$

Note that the group $W(F_4)$ is invariant under the transformation $T\leftrightarrow T'$.

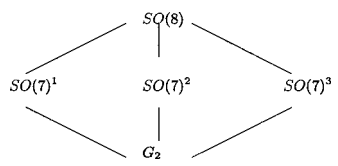

FIG. 7. Threefold embedding of SO(7) in SO(8).

2. The group 1152(19)

It is a subgroup of O(4) and its quaternionic structure can be written as follows:

$$[T,T] \oplus [T',T'] \oplus [T,T']^* \oplus [T',T]^*. \tag{34}$$

We know that the first two sets of elements form a subgroup of order 576. One can show that the set of elements in (30) is closed by noting that

$$[T,T']^*[T,T']^* = [T',T]^*[T',T]^* = [T,T], \quad [T,T']^*[T',T]^* = [T',T']. \tag{35}$$

It is clear that it is a maximal subgroup of $\mathrm{Aut}(F_4)$ and will be left invariant under the transformation $T \leftrightarrow T'$.

3. The group 1152(34)

This is the largest crystallographic group in four dimensions with proper rotations. That means it is a finite subgroup of SO(4). Naturally, it involves only nonstar elements of $\mathrm{Aut}(F_4)$

$$[T,T] \oplus [T',T'] \oplus [T,T'] \oplus [T',T]. \tag{36}$$

Its closure property is straightforward. Some of its subgroups of order 192 will be of our special interest for they appear as maximal subgroups in some of the finite subgroups of the Lie group G_2.[26] It is also invariant under the transformation $T \leftrightarrow T'$.

Now we discuss, in turn, the maximal subgroups classified under the subclasses A, B, C.

B. The maximal subgroups of $W(F_4)$

Its parabolic subgroups have been already discussed in Sec. IV. Besides those groups there are two maximal subgroups of order 576 with the conjugacy classes 20 and 23. The group 576(23) is the extension of the Weyl group $W(\mathrm{SO}(8))$ by a cyclic symmetry of the simple roots represented by imaginary quaternions. The group 576(20) is also a maximal subgroup of the groups 1152(19) and 1152(34).

1. The group 576(23)

It is the extension of the group $W(\mathrm{SO}(8))$ by a cyclic group of order 3 and its elements can be written as

$$[T,T] \oplus [T,T]^* \approx [T,T] \oplus [T',T']^*. \tag{37}$$

It can be shown that the group can be written as a semidirect product of the Weyl group of SO(8) and the cyclic group Z_3,

$$W(\mathrm{SO}(8)){:}Z_3,$$

where the cyclic symmetry permutes the outer simple roots of SO(8).

2. The group 576(20)

It has the structure

$$[T,T] \oplus [T',T']. \tag{38}$$

It is also a maximal subgroup in the crystallographic subgroup of SO(4) denoted by 1152(34) and the group 1152(19). No doubt that the elements in (38) closes under multiplication. We simply note the nontrivial case, namely,

$$[T',T']^2 = [T,T].$$

C. The maximal subgroups of the group 1152(19)

1. The group 576(20)

This group is just discussed in the above.

2. The group 192(17)

This group occurs also in the subgroup decomposition of the group 1152(34) and will be discussed in the following.

D. The maximal subgroups of the group 1152(34)

1. The group 576(29)

It has the structure

$$[T,T]\oplus[T,T']\approx[T,T]\oplus[T',T]. \tag{39}$$

Since the group 576(29) is an index 2 group in the group 1152(34) it should have two conjugates subgroups which is reflected in the isomorphism above.

2. The group 384(31)

We have the following structure of the group:

$$[V_0,T]\oplus[V_1,T]\oplus[V_0,T']\oplus[V_1,T']. \tag{40}$$

This is certainly a maximal subgroup of the group 1152(34) because $V_0\oplus V_1$ form a maximal subgroup of order 16 in the binary octahedral group $T\oplus T'$. It can be embedded in the group 1152(34) triply symmetric way by replacing V_1 by V_2 and V_3 in (40) in a similar manner where $W(\mathrm{SO}(9))$ is embedded in $W(F_4)$.

3. The group 288(24)

When we examine the parent group $[O,O]$ we know that the binary octahedral group O has many maximal subgroups, one of which is the dicyclic group (binary dihedral group) of order 12. It can be generated by two elements $a=\frac{1}{2}(1-e_1-e_2-e_3)$ and $b=(1/\sqrt{2})(e_1-e_2)$ where $a^6=b^4=1$ satisfying the generation relation $ba^n\bar{b}=\bar{a}^n(n=1,\ldots,6)$. The group can be denoted by $2D_3$ where D_3 is the dihedral group of order 6. When $2D_3$ acts on the left and the binary octahedral group acts on the right we obtain the group 288(24) which reads in our notation

$$[2D_3,O]. \tag{41}$$

We can further continue to determine the maximal subgroups of the groups discussed in the series A, B, and C.

4. The maximal subgroups of $W(\mathrm{SO}(8)):Z_3$

A1.1. The group 288(25):This is the group $[T,T]$ occurring in many groups discussed above.

A1.2. The group $192(13)\approx W(\mathrm{SO}(8))$: It has been discussed before and shown to be the Weyl group of SO(8)

$$[V_0,V_0]\oplus[V_+,V_+]\oplus[V_-,V_-]\oplus[V_0,V_0]^*\oplus[V_+,V_+]^*\oplus[V_-,V_-]^* \tag{42}$$

which is invariant under the cyclic symmetry Z_3. The action of the group elements on the hyperoctahedra V_0, V_+, V_- are as follows:

(i) $[V_0,V_0]$ leaves each hyperoctahedra invariant.
(ii) $[V_+,V_+]$ permutes the three octahedra in the cycylic order and $[V_-,V_-]$ does the same in the reverse order.

(iii) The element $[V_i,V_i]^*(i=0,+,-)$ leaves the hyperoctahedron V_i invariant but interchanges the other two. These properties indicate that the $[V_0,V_0]$ form an invariant subgroup where the factor group is the symmetric group of order 6,

$$\frac{W(\mathrm{SO}(8))}{[V_0,V_0]} \approx S_3.$$

The group 192(16): It can be represented in three equivalent ways and can be proven that they are the conjugate groups

(i) $[V_0,V_0]\oplus[V_+,V_-]\oplus[V_-,V_+]\oplus[V_0,V_0]^*\oplus[V_+,V_-]^*\oplus[V_-,V_+]^*$,
(ii) $[V_0,V_0]\oplus[V_+,V_-]\oplus[V_-,V_+]\oplus[V_+,V_+]^*\oplus[V_-,V_0]^*\oplus[V_0,V_-]^*$,
(iii) $[V_0,V_0]\oplus[V_+,V_-]\oplus[V_-,V_+]\oplus[V_-,V_-]^*\oplus[V_+,V_0]^*\oplus[V_0,V_+]^*$.

Interestingly enough that each of these conjugate groups leaves one of the hyperoctahedra invariant. One can easily show that the groups in (i), (ii), and (iii) leave V_0, V_+, and V_- invariant, respectively. Embedding of the group 192(16) in the group $W(\mathrm{SO}(8)):Z_3$ follows the cyclic symmetry of quaternionic units e_1,e_2,e_3.

5. The maximal subgroups of the group 576(20)

B1.1. The group 288(25): It has been discussed in Sec. Vd4a.

B1.2. The group 288(24): This group was discussed in Sec. Vd3a.

B1.3. The group 192′(13): It has the same order and the same number of conjugacy classes with $W(\mathrm{SO}(8))$ but not isomorphic to it. It has the structure

$$[V_0,V_0]\oplus[V_+,V_+]\oplus[V_-,V_-]\oplus[V_1,V_1]\oplus[V_2,V_3]\oplus[V_3,V_2]. \tag{43}$$

An important difference is that $W(\mathrm{SO}(8))$ is a subgroup of O(4) whereas this group is a subgroup of SO(4). The group 192′(13) has an index 6 in the group 1152(34). Its conjugate groups can be obtained by the conjugation of the element $[V_+,V_1]$ which permutes the six hyperoctahedra in the cyclic order $V_0\to V_3\to V_-\to V_1\to V_+\to V_2\to V_0$. This would yield the six conjugate representations of (43). This group turns out to be a maximal subgroup of the finite subgroup of G_2 of order 1344 preserving the octonion algebra of the set $\pm e_i(i=1,2,\ldots,7)$.[26]

6. Maximal subgroups of the group 576(29)

All its maximal subgroups which have not been discussed so far also occur as the maximal subgroups of the group 384(31) and will be discussed below.

7. Maximal subgroups of the group 384(31)

C2.1. The group 192(26): It has the structure

$$[V_0,T]\oplus[V_1,T]. \tag{44}$$

*C2.2. The group 192(23)*It can be represented by

$$[V_0,T]\oplus[V_0,T']. \tag{45}$$

C2.3. The group 192(20): This group has an interesting structure which can be written as

$$[a,T]\oplus[b,T'], \tag{46}$$

where the set of elements of a is generated by $(1/\sqrt{2})(1+e_1)$ and the set $b=e_3a$. The set $[a,T]$ forms an invariant subgroup of order 96. The set of elements a and b generate a dicyclic group of order 16 as we discussed before, however, as a and b are paired with different subsets of the binary octahedral group the dicyclic group is not a subgroup of the group 192(20). The set of elements of a and b are given by

$$a=\left\{\pm 1,\pm e_1,\frac{1}{\sqrt{2}}(\pm 1\pm e_1)\right\},\quad b=\left\{\pm e_2,\pm e_3,\frac{1}{\sqrt{2}}(\pm e_2\pm e_3)\right\}. \tag{47}$$

C2.4. The group 192(17): It can be represented by

$$[V_0,T]\oplus[V_1,T'] \tag{48}$$

which is also a subgroup of the group 576(20). It is one of the maximal subgroup of the finite subgroup of the Lie group of G_2 order 12096 which leaves the quaternion decomposition of the octonionic root system of the exceptional Lie algebra E_7 (Ref. 26) invariant.

VI. CONCLUSION

The automorphism group $\mathrm{Aut}(F_4)$ of the root system of the exceptional Lie algebra F_4 is the largest crystallographic group in four-dimensions which has not been discussed in the literature using quaternions. This work not only relates this crystallographic group to the Coxeter-Dynkin diagram of F_4 but also discusses its relevance to other Lie algebraic structures as well as to the four-dimensional Euclidean geometry. We have discussed the decomposition of $\mathrm{Aut}(F_4)$ down to the groups of order 192 and shown that a number of groups of order 192 have different structures related to different geometries. It is perhaps also interesting to continue the same decomposition to determine the groups acting in three-dimensions. In this context we have discussed only the Weyl groups $W(S(7))\approx W(\mathrm{SP}(3))$.

We have noted that two groups of order 192, namely, the groups $192'(13)$ and 192(17), occur as maximal subgroups in the finite subgroups of the Lie group G_2. The group $192'(13)$ is a maximal subgroup of a group $Z_2^3\cdot PSL_2(7)$ of order 1344 which is a finite subgroup of G_2 preserving the set of imaginary octonions $\pm e_i(i,1,2,\ldots,7)$.[16] Here $PSL_2(7)$ is the famous Klein's simple group of order 168 and $Z_2^3=Z_2\times Z_2\times Z_2$ is the elementary Abelian group of order 8. The group 192(17) is the maximal subgroup of the Chevalley group $G_2(2)$ of order 12096 which leaves the octonionic roots of the Lie algebra E_7 invariant.

The Weyl group $W(\mathrm{SO}(8))$ which is the group 192(13) is also a maximal subgroup of a group $Z_2^3{:}PSL_2(7)$ of order 1344 which is, in turn, a maximal subgroup of the simple group A_8, even permutations of eight letters. The group A_8 is related to the Weyl group $W(E_7)$ through $W(\mathrm{SU}(8))$ and is a maximal subgroup of the Chevalley group $\mathrm{SO}_7(2)$.[27] It is also interesting to note that some finite subgroups of SO(4) also occur in the phase transitions of the liquid helium ^{3}He.[28]

We believe that the group structures and their quaternionic representations will be useful in various fields of physics which may need the finite subgroups of O(4).[29,30]

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BRST quantization of quasisymplectic manifolds and beyond

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We consider a class of *factorizable* Poisson brackets which includes almost all reasonable Poisson structures. A particular case of the factorizable brackets are those associated with symplectic Lie algebroids. The BRST theory is applied to describe the geometry underlying these brackets as well as to develop a deformation quantization procedure in this particular case. This can be viewed as an extension of the Fedosov deformation quantization to a wide class of *irregular* Poisson structures. In a more general case, the factorizable Poisson brackets are shown to be closely connected with the notion of n-algebroid. A simple description is suggested for the geometry underlying the factorizable Poisson brackets based on construction of an odd Poisson algebra bundle equipped with an Abelian connection. It is shown that the zero-curvature condition for this connection generates all the structure relations for the n-algebroid as well as a generalization of the Yang-Baxter equation for the symplectic structure. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The deformation quantization of a Poisson manifold $(M,\{\cdot,\cdot\})$ is the construction of a local one-parameter deformation of the commutative algebra of functions $C^\infty(M)$ respecting associativity.[1,2] The deformed product is usually denoted by $*$, and the deformation parameter is the Plank constant $\hbar$. In each order in $\hbar$ the $*$-product is given by a bidifferential operator (locality) and the skew-symmetric part of the first $\hbar$ order coincides with the Poisson bracket of functions (correspondence principle).

Very early it appeared that the complexity of the deformation quantization program essentially depends on whether a given Poisson manifold is regular or not. In the regular case, i.e., where the rank of the Poisson tensor is constant, one can introduce an affine symmetric connection respecting the Poisson structure (a Poisson connection). Clearly, in the irregular case such a connection cannot exist. The relevance of the Poisson connection for constructing $*$-products had been already discussed in Ref. 2, but in its full strength, the connection was first exploited by Fedosov in his seminal paper[3] on the deformation quantization of symplectic and regular Poisson manifolds (see also Ref. 4).

The existence of deformation quantization for general Poisson manifolds, not necessarily regular, was proved by Kontsevich[5] as a consequence of his Formality Theorem. An explicitly covariant version of the Kontsevich quantization has been given in Ref. 6 (see also Ref. 7, where both covariant and equivariant versions of the formality theorem have been presented). It should be noted that the Kontsevich quantization is based on completely different ideas and involves a

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more complicated algebraic technique as compared to the Fedosov quantization. A nice "physical explanation" of the Kontsevich quantization formula was given in Ref. 8 by applying the BV quantization method[9] to the Poisson sigma model.

Recently, it was recognized that the method of Fedosov's quantization can further be extended to include a certain class of irregular Poisson manifolds even though no Poisson connection can exist in this case. To give an idea about the manifolds in question let us write the following expression describing the general structure of the corresponding Poisson brackets:

$$\{f,g\} = \omega^{ab}(X_a^\mu \partial_\mu f)(X_b^\nu \partial_\nu g), \quad \det(\omega^{ab}) \neq 0. \tag{1.1}$$

The matrices X and ω are subject to certain conditions ensuring the Jacobi identity. The geometric meaning of these conditions as well as the precise mathematical status of X and ω will be explained in the next section. Here we would like to mention that, no *a priori* assumption is made about the rank of the matrix X, so the Poisson brackets (1.1) may well be irregular.

In the case where the matrix X is the anchor of a Lie algebroid the manifolds under consideration are something intermediate between symplectic and general Poisson manifolds. For this reason, we refer to them as *quasisymplectic* Poisson manifolds (not to be confused with the quasi-Poisson manifolds introduced in Ref. 10). Being closely related with the notion of a dynamical r-matrix, these manifolds may be of immediate interest in the theory of integrable systems.

The generalization of the Fedosov deformation quantization to the case of symplectic Lie algebroids was first given by Nest and Tsygan.[11] They also proved corresponding classification theorems. Fedosov's quantization method was also described in the work[12] for the same class of manifolds in the language of symplectic ringed spaces. Particular classes of quasisymplectic manifolds have been quantized in Refs. 13–15 making use of various ideas, including BRST theory.

The aim of this work is twofold. In the first part of the paper we put the deformation quantization of quasisymplectic manifolds in the framework of BFV-BRST theory.[16–18] For the (constrained) Hamiltonian systems on symplectic manifolds, the relationship has been already established between the BFV-BRST and the Fedosov quantizations.[19,20] Here we reshape this technology to make it work in a more general case of quasisymplectic manifolds. The second part of the paper is devoted to a possible generalization of the notion of a quasisymplectic manifold to the case of n algebroids or, in other terminology, NQ manifolds.[21–24] This generalization essentially relaxes the restrictions on the structure functions X and ω, entering factorization (1.1), and covers almost all reasonable Poisson structures.

The paper is organized as follows. In Sec. II we give the definition of a quasisymplectic Poisson manifold and discuss some examples. Here we also construct a simple counterexample to existence of a quasisymplectic representation for any Poisson bracket. Section III deals with realization of quasisymplectic manifolds as coisotropic surfaces in the total space of vector bundles associated with symplectic Lie algebroids. In Sec. IV this realization is exploited to perform the BRST quantization of the resulting gauge system. We prove that the quantum multiplication in the algebra of physical observables induces an associative $*$-product on the initial quasisymplectic manifold. In Sec. V we generalize the notion of a quasisymplectic manifold to a wider class of factorizable Poisson brackets. Under reasonable restrictions this class of Poisson structures is proved to be closely connected with n algebroids. Using the 2-algebroid as an example, we show how the geometry underlying factorizable Poisson brackets can be described in terms of a supervector bundle equipped with a fiberwise odd Poisson structure and a compatible Abelian connection.

II. QUASISYMPLECTIC MANIFOLDS: DEFINITION AND EXAMPLES

The most concise and geometrically transparent way to define the quasisymplectic manifolds is to use the notion of a *Lie algebroid*.[25]

Definition: A Lie algebroid over a manifold M is a (real) vector bundle $\mathcal{E}\to M$ equipped with the following additional structures:

(1) There is a (real) Lie algebra structure on the linear space of sections $\Gamma(\mathcal{E})$.
(2) There is a bundle map $\rho:\mathcal{E}\to TM$ such that the Lie algebra and $C^\infty(M)$-module structures on $\Gamma(\mathcal{E})$ are compatible in the following sense:

$$[s_1,fs_2]=f[s_1,s_2]+(\rho_*(s_1)f)s_2,\quad \forall\, f\in C^\infty(M),\quad \forall\, s_1,s_2\in\Gamma(\mathcal{E}). \tag{2.1}$$

The map ρ is called the *anchor* of the Lie algebroid $\mathcal{E}\to M$.

The last relation can be viewed as the Leibniz rule for the Lie algebroid bracket. Using this relation and the Jacobi identity for the bracket it is not hard to see that the anchor map $\rho:\mathcal{E}\to TM$ defines a Lie algebra homomorphism on sections, i.e.,

$$\rho_*([s_1,s_2])=[\rho_*(s_1),\rho_*(s_2)],\quad \forall\, s_1,s_2\in\Gamma(\mathcal{E}), \tag{2.2}$$

where the brackets on the right-hand side (rhs) stand for the commutator of vector fields.

It is instructive to look at the local coordinate expression of the above relations. Let x^μ be a coordinate system on a trivializing chart $\mathcal{U}\subset M$ and let s_a be a frame of $\mathcal{E}|_{\mathcal{U}}$. By definition, we have

$$\begin{gathered}[s_a,s_b]=f_{ab}^c(x)s_c,\quad \rho_*(s_a)=X_a^\mu(x)\partial_\mu,\\ \mu=1,\ldots,\dim M,\quad a=1,\ldots,\operatorname{rank}\mathcal{E}.\end{gathered} \tag{2.3}$$

In view of Relations (2.2) and (2.1) the structure functions f_{ab}^c, $X_a^\mu\in C^\infty(U)$ meet the following conditions:

$$[X_a,X_b]^\nu:=X_a^\mu\partial_\mu X_b^\nu-X_b^\mu\partial_\mu X_a^\nu=f_{ab}^cX_c^\nu, \tag{2.4}$$

$$f_{ab}^df_{dc}^e-X_c^\mu\partial_\mu f_{ab}^e+\operatorname{cycle}(a,b,c)=0. \tag{2.5}$$

Notice that the second relation is automatically satisfied for any vector bundle $\mathcal{E}$ of rank 1 or 2, whereas in the case of rank $\mathcal{E}>2$ it becomes an actual restriction on the structure functions f_{ab}^c.

In general, $\rho(\mathcal{E})$ is not a smooth subbundle of TM as the rank of the distribution $\rho(\mathcal{E})$ may vary from point to point. Nonetheless, in view of (2.2), $\rho(\mathcal{E})$ generates a (singular) integrable distribution in the sense of Sussman:[26] for each $p\in M$ there is a smooth submanifold $\Sigma_p\subset M$ such that $p\in\Sigma_p$ and $T_q\Sigma_p=\rho(\mathcal{E}_q)$ for any $q\in\Sigma_p$. The corresponding foliation will be denoted by $F(M)$.

Example: Any tangent bundle TM may be viewed as a Lie algebroid with the Lie bracket given by the commutator of vector fields and the anchor $\rho=\mathrm{id}:TM\to TM$.

A. Differential geometry of Lie algebroids

One can regard the concept of a Lie algebroid as a tool for transferring all the usual differential-geometric constructions from a tangent bundle to an abstract vector bundle. In particular, it is possible to define the Lie-algebroid counterpart of the exterior calculus. Denote by $\Lambda(\mathcal{E})=\oplus\Lambda^p(\mathcal{E})$ the exterior algebra of sections $\Gamma(\wedge^\bullet\mathcal{E}^*)$, $\mathcal{E}^*$ being the bundle dual to $\mathcal{E}$. Consider the following nilpotent operator $d:\Lambda^p(\mathcal{E})\to\Lambda^{p+1}(\mathcal{E})$:

$$\mathrm{d}\alpha(s_0,\ldots,s_p)=\sum_{k=0}^{p}(-1)^k\rho_*(s_k)(\alpha(s_0,\ldots,\hat{s}_k,\ldots,s_p))$$
$$+\sum_{k<n=1}^{p}(-1)^{k+n}\alpha([s_k,s_n],s_0,\ldots,\hat{s}_k,\ldots,\hat{s}_n,\ldots,s_p), \tag{2.6}$$

for all $s_0,s_1,\ldots,s_p\in\Gamma(\mathcal{E})$. Since $d^2=0$, we have a generalization of the De Rham complex. We will refer to elements of $\Lambda^p(\mathcal{E})$ as $\mathcal{E}$-p-forms, or just p-forms when it cannot lead to confusion. Note that $\Lambda^0(\mathcal{E})$ is naturally identified with $C^\infty(M)$.

More generally, one may consider the tensor product $\mathcal{E}\otimes V$, where $V\to M$ is a vector bundle with connection ∇. Then, ∇ induces the covariant derivative $\nabla_\rho:\Lambda^p(\mathcal{E},V)\to\Lambda^{p+1}(\mathcal{E},V)$ on the space $\Lambda(M,\mathcal{E})=\Lambda(\mathcal{E})\otimes\Gamma(V)$ of $\Gamma(V)$-valued $\mathcal{E}$ forms,

$$\nabla_\rho\omega(s_0,\ldots,s_p)=\sum_{k=0}^{p}(-1)^k\nabla_{\rho_*(s_k)}(\omega(s_0,\ldots,\hat{s}_k,\ldots,s_p))$$
$$+\sum_{k<n=1}^{p}(-1)^{k+n}\alpha([s_k,s_n],s_0,\ldots,\hat{s}_k,\ldots,\hat{s}_n,\ldots,s_p). \tag{2.7}$$

The curvature of ∇_ρ is defined in the usual way,

$$R=\nabla_p^2:\Gamma(V)\to\Lambda^2(\mathcal{E},V). \tag{2.8}$$

One may verify that

$$R(fu)=fRu,\quad \forall f\in C^\infty(M),\quad \forall u\in\mathcal{E}, \tag{2.9}$$

so that in each coordinate chart the curvature R is given by a matrix-valued 2-form determining a $C^\infty(M)$-linear automorphism of $\Gamma(V)$. Like the curvature of the bundle connection ∇, R satisfies the *Bianchi identity*,

$$[\nabla_\rho,\nabla_\rho^2]=0\Leftrightarrow\nabla_\rho R=0. \tag{2.10}$$

(To write the last formula we extend the action of ∇ from V to the tensor product $V\otimes V^*$ by the usual formulas of differential geometry.)

In what follows we will mostly deal with the case $V=\mathcal{E}$. Then, in addition to the curvature, one more covariant of the connection can be introduced. The *torsion* T of a Lie algebroid connection ∇_ρ is an element of $\Lambda^2(\mathcal{E},\mathcal{E})$ defined by the rule

$$\Gamma(\mathcal{E})\ni T(u,v)=\nabla_{\rho_*(u)}v-\nabla_{\rho_*(v)}u-[u,v],\quad \forall u,v\in\Gamma(\mathcal{E}). \tag{2.11}$$

If $\Gamma^a_{\mu b}$ are coefficients of the connection ∇ with respect to local coordinates x^μ and a frame s_a, then the components of the torsion tensor read

$$T^c_{ab}=X^\mu_a\Gamma^c_{\mu b}-X^\mu_b\Gamma^c_{\mu a}-f^c_{ab}. \tag{2.12}$$

The components of the curvature tensor R are

$$R^d_{abc}=X^\mu_aX^\nu_bR^d_{\mu\nu c}, \tag{2.13}$$

where

$$R^d_{\mu\nu c}=\partial_\mu\Gamma^d_{\nu c}-\partial_\nu\Gamma^d_{\mu c}+\Gamma^d_{\mu a}\Gamma^a_{\nu c}-\Gamma^d_{\nu a}\Gamma^a_{\mu c} \tag{2.14}$$

is the curvature of ∇. There is a simple formula relating the exterior and covariant derivatives:

$$\mathrm{d}\alpha(s_0,\ldots,s_p)=\sum_{k=0}^{p}(-1)^k(\nabla_{\rho_*(s_k)}\alpha)(s_0,\ldots,\hat{s}_k,\ldots,s_p)$$
$$+\sum_{k<n=1}^{p}(-1)^{k+n}\alpha(T(s_k,s_n),s_0,\ldots,\hat{s}_k,\ldots,\hat{s}_n,\ldots,s_p); \tag{2.15}$$

here we use the isomorphism $\Lambda^p(\mathcal{E})\simeq\Lambda^0(\mathcal{E},\wedge^p\mathcal{E})$. A straightforward computation yields the *torsion Bianchi identity*

$$\nabla_c T^d_{ab}+R^d_{abc}+\mathrm{cycle}(a,b,c)=0, \tag{2.16}$$

where $\nabla_a:=\nabla_{\rho^*(s_a)}$.

In this paper we are interested in the Lie algebroids endowed with a closed and nondegenerate 2-form $\omega\in\Lambda^2(\mathcal{E})$. A 2-form ω is called nondegenerate if the equality

$$\omega(u,v)=0,\quad \forall\, u\in\Gamma(\mathcal{E}), \tag{2.17}$$

implies $v=0$. In terms of local coordinates the closedness condition $\mathrm{d}\omega=0$ reads

$$X^\mu_c\partial_\mu\omega_{ab}+\omega_{cd}f^d_{ab}+\mathrm{cycle}(a,b,c)=0, \tag{2.18}$$

where $\omega_{ab}:=\omega(s_a,s_b)$. Extending the analogy with classical differential geometry, we refer to ω as the *symplectic form* and call the triple $(\mathcal{E},\rho,\omega)$ the *symplectic Lie algebroid*. (This is a particular example of *triangular Lie bialgebroids* studied in Ref. 27.)

B. Quasisymplectic manifolds

It is well known that any symplectic structure on a Lie algebroid $\mathcal{E}\to M$ gives rise to a Poisson structure on the base manifold M. It is this Poisson structure we are going to quantize by the BFV-BRST method.

Proposition 2.1: Let $(\mathcal{E},\rho,\omega)$ be a symplectic Lie algebroid, then M is a Poisson manifold with respect to the following Poisson bracket:

$$\{f,g\}=\omega^{-1}(\mathrm{d}f,\mathrm{d}g),\quad \forall\, f,g\in C^\infty(M)\simeq\Lambda^0(\mathcal{E}); \tag{2.19}$$

here ω^{-1} is the bisection inverse to the symplectic form $\omega\in\Lambda^2(\mathcal{E})$ and $\mathrm{d}f$, $\mathrm{d}g\in\Lambda^1(\mathcal{E})$ are the differentials defined by (2.6).

Proof: In terms of local coordinates the Poisson bivector determining the bracket (2.19) has the form

$$\alpha=\omega^{ab}c_a\wedge X_b\in\wedge^2 TM,\quad \{f,g\}=\alpha^{\mu\nu}\partial_\mu f\partial_\nu g, \tag{2.20}$$

where $X_a:=X^\mu_a\partial_\mu$, $\omega^{ac}\omega_{cb}=\delta^a_b$, and $\alpha^{\mu\nu}=\omega^{ab}X^\mu_aX^\nu_b$. The Jacobi identity for α follows immediately from the Lie algebroid relations (2.4) and the closedness condition (2.18). Indeed, using the Leibniz rule for the Schouten bracket of α with itself, we get

$$\tfrac{1}{4}[\alpha,\alpha]=\omega^{ab}\omega^{cd}X_a\wedge[X_b,X_c]\wedge X_d+\omega^{ab}[X_b,\omega^{cd}]X_a\wedge X_c\wedge X_d$$
$$=(\omega^{am}f^b_{mn}\omega^{nc}+\omega^{am}X^u_m\partial_\mu\omega^{bc})X_a\wedge X_b\wedge X_c=(\mathrm{d}\omega)_{abc}X^a\wedge X^b\wedge X^c=0. \tag{2.21}$$

The indices are lowered and raised with the help of the symplectic form ω and its inverse.

Since the rank of the anchor distribution may vary through M, the induced Poisson structure (2.20) is irregular in general (though it involves a nondegenerate bivector $\omega^{-1}\in\wedge^2\mathcal{E}$). For this reason and following the terminology of Ref. 12 we refer to (M,α) as the *quasisymplectic manifold*. Accordingly, relation (2.19) is said to define a *quasisymplectic representation* for the Poisson bivector α.

Given a symplectic Lie algebroid, we have two (singular) foliations on M: the anchor foliation $F(M)$ and the symplectic foliation $S(M)$ associated with the induced Poisson structure (2.20). Clearly, the latter foliation is subordinated to the former one in the sense that any symplectic leaf belongs to a leaf of the anchor foliation.

Remark: A natural question to ask is as follows: Given a Poisson bivector (2.20), where ω_{ab} is some nondegenerate 2-form and X_a is an integrable distribution, are these data sufficient to define a symplectic Lie algebroid? In general, the answer is negative, since we do not require the local vector fields X_a to be linearly independent. Nonetheless, if X's are linearly independent on an everywhere dense domain in M, the answer is positive. In that case the structure equations (2.5) and (2.18) follow immediately from the Jacobi identities for the Schouten commutators of the local vector fields (2.4) and the Poisson bivector (2.20). We will discuss this question in more detail in Sec. V.

C. Symplectic connection and curvature

The deformation quantization of quasisymplectic Poisson manifolds to be developed in the next sections involves one more geometric ingredient, a *symplectic connection*. This is defined as a torsion-free Lie-algebroid connection respecting a symplectic 2-form, i.e.,

$$\nabla_\rho \omega = 0. \tag{2.22}$$

Here we consider ω as a section of $\Lambda^0(\mathcal{E}, \wedge^2\mathcal{E})$.

Proposition 2.2: Any symplectic Lie algebroid admits a symplectic connection.

Proof: We are looking for a symplectic connection of the form $\nabla + \Delta\Gamma$, where ∇ is an arbitrary connection and $\Delta\Gamma \in \Gamma(\mathcal{E}\otimes\mathcal{E}^*\otimes\mathcal{E}^*)$. In terms of local coordinates the compatibility condition (2.22) reads

$$\nabla_c \omega_{ab} = \Delta\Gamma_{cab} - \Delta\Gamma_{cba}, \tag{2.23}$$

where $\Delta\Gamma_{abc} = \Delta\Gamma^d_{ab}\omega_{dc}$. Obviously, these equations cannot have a unique solution: any tensor $\Delta\Gamma'_{abc}$, symmetric in bc, satisfies the homogeneous equation and therefore it can be added to a given solution $\Delta\Gamma_{abc}$ to produce another one. A particular solution to Eq. (2.23) is given by

$$\Delta\Gamma^c_{ab} = -\tfrac{1}{2}\omega^{cd}\nabla_a \omega_{db}. \tag{2.24}$$

Now let ∇_ρ be an arbitrary Lie-algebroid connection which respects ω and has torsion T. By making use of the aforementioned ambiguity, one can define the new connection $\nabla'_\rho = \nabla_\rho + \Delta\Gamma'$,

$$\Delta\Gamma'_{abc} = -\tfrac{1}{3}(T_{abc} + T_{acb}), \quad T_{abc} = T^d_{ab}\omega_{dc}, \tag{2.25}$$

which is also compatible with ω. By definition (2.12), we have

$$T'^c_{ab} = T^c_{ab} + \Delta\Gamma'^c_{ab} - \Delta\Gamma'^c_{ba}. \tag{2.26}$$

Substituting (2.25) into (2.26) and lowering the upper index with the help of ω we get

$$T'_{abc} = T_{acb} + \mathrm{cycle}(a,b,c) = 0. \tag{2.27}$$

The last equality follows immediately from (2.15) with ω in place of α. Thus, ∇'_ρ is a symplectic connection.

Let R^d_{abc} be the curvature of a symplectic connection. By analogy with Riemannian geometry we can define the *covariant curvature tensor* just lowering upper index with the help of the symplectic 2-form, $R_{abcd} = R^n_{abc}\omega_{nd}$. The following symmetry properties take place:

$$R_{abcd} = -R_{bacd}, \quad R_{abcd} = R_{abdc}, \quad R_{abcd} + R_{bcad} + R_{cabd} = 0. \tag{2.28}$$

The first equality is obvious, the second one follows from the definition (2.8) and the fact that ∇_ρ respects ω, the third equality is just the Bianchi identity (2.16).

D. Examples

Let us give some examples of symplectic Lie algebroids and the corresponding quasisymplectic Poisson brackets. More examples of Lie algebroids, with or without symplectic structure, can be found in Refs. 12 and 25.

Example 1: Any symplectic manifold (M,ω) gives rise to the symplectic Lie algebroid $(TM,$ id, $\omega)$. The quasisymplectic Poisson structure is given by

$$\alpha = (\omega^{-1})^{\mu\nu}\partial_\mu \wedge \partial_\nu. \tag{2.29}$$

To get a less trivial quasisymplectic representation for α consider an almost complex structure J compatible with ω. Recall that an almost complex structure is a smooth field of automorphisms $J:TM\to TM$ obeying conditions

$$J^2 = -\,\mathrm{id}, \quad \omega(JX,JY) = \omega(X,Y), \tag{2.30}$$

where X,Y are arbitrary vector fields. J being nondegenerate, we get a quasisymplectic representation for the Poisson bivector α associated with the symplectic Lie algebroid (TM,J,ω),

$$\alpha = (\omega^{-1})^{\mu\nu}J_\mu \wedge J_\nu. \tag{2.31}$$

Here $J=\mathrm{d}x^\mu J^\nu_\mu \partial_\nu$ and $J_\mu = J^\nu_\mu \partial_\nu$.

Example 2: Generalizing the previous example, consider a pair of Schouten-commuting bivectors β and ω, where the former is a Poisson one and the latter is nondegenerate. The triple (T^*M,β,ω) defines a symplectic Lie algebroid with the structure functions

$$[\beta(\mathrm{d}x^\mu),\beta(\mathrm{d}x^\nu)] = \partial_\lambda \beta^{\mu\nu}\beta(\mathrm{d}x^\lambda), \quad \beta(\mathrm{d}x^\mu) = \beta^{\mu\nu}\partial_\nu.$$

The induced Poisson structure on M is given by

$$\alpha = (\omega^{-1})_{\mu\nu}\beta^{\mu\gamma}\beta^{\nu\lambda}\partial_\gamma \wedge \partial_\lambda. \tag{2.32}$$

Example 3: Recall that a Lie algebra L is called *quasi-Frobenius*[28] if it admits a nondegenerate central extension L_c of the form

$$[p_a,p_b] = f^d_{ab}p_d + \omega_{ab}c, \quad [c,p_a] = 0, \quad \det(\omega_{ab}) \neq 0.$$

The Jacobi identity for L_c requires the nondegenerate matrix ω_{ab}, determining the central extension, to be a 2-cocycle of the Lie algebra $L \simeq L_c/c$.

Given an action $\rho: L\to \mathrm{Vect}(M)$ of the Lie algebra L on M by smooth vector fields $X_a = \rho(p_a)$, one can define a symplectic Lie algebroid associated with the trivial vector bundle $M \oplus L$, anchor ρ, and symplectic form ω_{ab}. The induced quasisymplectic structure on M reads

$$\alpha = \omega^{ab}X_a \wedge X_b, \quad \omega^{ac}\omega_{cd} = \delta^a_d. \tag{2.33}$$

A simple quantization procedure for such Poisson brackets has been proposed in Ref. 15.

Example 4: Let (M,α) be a two-dimensional Poisson manifold. We say that the bivector α is *quasihomogeneous* if there exist a volume form ω and a vector field Y such that the function $h = \omega(\alpha)$ obeys condition $Yh=h$.

It turns out that any quasihomogeneous Poisson manifold is also a quasisymplectic one. Namely, a simple computation yields

$$\alpha = X \wedge Y, \quad [X,Y] = (1 - \mathrm{div}_\omega Y)X. \tag{2.34}$$

Here X is the Hamiltonian vector field associated with the Hamiltonian h and the symplectic (volume) form ω. The structure equations (2.5) and (2.18) are automatically satisfied by the reason of dimension and we get a symplectic Lie algebroid associated with the trivial vector bundle $M \oplus \mathbb{R}^2$.

For instance, the following polynomial Poisson brackets on 2-plane,

$$\{x,y\} = x^m y^n + x^k y^l,$$
$$\delta = nk - lm \neq 0, \quad m,n,k,l \in \mathbb{N}, \tag{2.35}$$

are quasihomogeneous with respect to $\omega = \mathrm{d}x \wedge \mathrm{d}y$ and

$$Y = \delta^{-1}(n-l)x\partial_x + \delta^{-1}(k-m)y\partial_y,$$
$$X = (mx^{m-1}y^n + kx^{k-1}y^l)\partial_y - (nx^m y^{n-1} + lx^k y^{l-1})\partial_x. \tag{2.36}$$

In accordance with (2.34),

$$[Y,X] = (1 - \delta^{-1}(n+k-l-m))X, \tag{2.37}$$

and we arrive at the symplectic Lie algebroid associated with the two-dimensional quasi-Frobenius Lie algebra (2.37) (see the previous example).

E. Counterexample

As we have seen the quasisymplectic manifolds constitute a wide class of Poisson manifolds. Here is an example of a Poisson manifold that does not admit any quasisymplectic representation (even locally).

Proposition 2.3: The Lie-Poisson bracket on the dual of so(3) *algebra does not admit a quasisymplectic representation*.

Proof: The Poisson bracket in question is of the form

$$\{x^i,x^j\} = \sum_k \epsilon^{ijk}x^k, \tag{2.38}$$

where x^i are linear coordinates in $\mathbb{R}^3$ and ϵ^{ijk} is the Levi-Civita tensor. The only irregular point is $0 \in \mathbb{R}^3$, where the rank of the Poisson bracket is equal to zero; at the other points the rank equals 2. The leaves of the symplectic foliation $S(\mathbb{R}^3)$ are exactly the level sets of the Casimir function $(x^1)^2+(x^2)^2+(x^3)^2$, i.e., spheres centered at the origin.

Since any vector bundle $\mathcal{E}$ over $\mathbb{R}^3$ is trivial, we may look for an anchor being just an integrable vector distribution $X_a \in \mathrm{Vect}(\mathbb{R}^3)$. For the same reason, any symplectic 2-$\mathcal{E}$-form is given by an invertible skew-symmetric matrix $\omega_{ab}(x)$ on $\mathbb{R}^3$. Clearly, each sphere from $S(\mathbb{R}^3)$ is entirely contained in some leaf of the anchor foliation $F(\mathbb{R}^3)$; so, we write $S(\mathbb{R}^3) \subset F(\mathbb{R}^3)$. The existence of a quasisymplectic representation is expressed by the equality

$$X^i_a \omega^{ab} X^j_b = \sum_k \epsilon^{ijk}x^k. \tag{2.39}$$

The key to the analysis of this equation lies with the rank r of the vector distribution at the origin. *A priori*, r may take any value from 0 to 3. Let us show that any assumption about r leads to a contradiction.

The case $r=0$: This possibility is ruled out by comparing the order of zero on both sides of the equality (2.39). Indeed, since all X's must vanish at $x=0$, the order of zero on the left-hand side (lhs) is of at least 2, while the rhs tends to zero linearly.

The cases $r=1,2$: There is an integral leaf of dimension 1 or 2 passing through the origin and intersecting *transversally* at least one of the symplectic spheres. (Otherwise, this leaf would be entirely contained in one of the spheres, and thus, could not reach the origin.) But this contradicts to the inclusion $S(\mathbb{R}^3) \subset F(\mathbb{R}^3)$.

The case $r=3$: Passing, if necessary, to another basis we may assume that $X_a=(X_i,X_\alpha)$, where $X_i=\partial_i$ and $X_\alpha=0$. Then the matrix ω^{ab} takes the block form

$$\begin{pmatrix} \omega^{ij} & \omega^{i\beta} \\ \omega^{\alpha j} & \omega^{\alpha\beta} \end{pmatrix} \tag{2.40}$$

with $\omega^{ij}=\Sigma\epsilon^{ijk}x^k$. Among various equations on the matrix elements of (2.40), expressing the fact of closedness of ω, one can find the following one:

$$\omega^{\alpha k}\partial_k\omega^{ij}+\omega^{ik}\partial_k\omega^{j\alpha}-\omega^{jk}\partial_k\omega^{i\alpha}=0. \tag{2.41}$$

Since $\omega^{ij}(0)=0$ and $\partial_k\omega^{ij}(0)=\epsilon^{ijk}$, the last equation implies that $\omega^{\alpha i}(0)=0$, and hence the entire matrix (2.40) must degenerate at the origin. This contradiction concludes the proof.

III. POISSON DESCRIPTION OF SYMPLECTIC LIE ALGEBROIDS

In order to construct as well as physically interpret the deformation quantization of quasisymplectic manifolds it is convenient to think of (M,α) as the phase space of some (gauge invariant) mechanical system with zero Hamiltonian. In what follows we will use the standard terminology from the theory of constrained systems: first and second class constraints, gauge-fixing conditions, ghost variables, BRST charge, etc.[18] It should be noted that unlike the common practice we will consider Hamiltonian constraints that are defined by a *section* of some vector bundle $\mathcal{E}\to M$ rather than scalar functions on M. To provide the covariance of the quantization with respect to the bundle automorphisms an appropriate linear connection is needed, and that requires some modification of the conventional BRST formalism.[16–18] In particular, it will be convenient to use noncanonical commutation relations for ghost variables. The details will be explained below.

Now let us outline the basic steps of our approach. The main idea is to quantize a quasisymplectic manifold M by means of its suitable embedding into a certain supermanifold endowed with "a more simple" Poisson structure. The construction of such an embedding involves a quite standard machinery of the Hamiltonian BRST theory;[17,18,29] it can be subdivided into three steps. First, using the Lie algebroid structure, we represent (M,α) as a second-class constrained system on the vector bundle $\mathcal{E}^*$ dual to the Lie algebroid $\mathcal{E}$. As the next step, the second-class constrained system on $\mathcal{E}^*$ is converted into an equivalent gauge system on the direct sum of vector bundles $\mathcal{N}=\mathcal{E}^*\oplus\mathcal{E}$. The equivalence just means that the Poisson algebra of physical observables on $\mathcal{N}$ is isomorphic to the Poisson algebra of smooth functions on (M,α). Finally, the classical gauge system is covariantly quantized by the BFV-BRST method. The key point is that the space of physical observables on $\mathcal{N}$, being identified with a certain BFV-BRST cohomology in ghost number zero, carries a simple Poisson structure which can easily be quantized. By construction, the associative product on the algebra of quantum observables on $\mathcal{N}$ induces a $*$-product on the original quasisymplectic manifold (M,α).

For the case of symplectic manifolds, including second-class constrained system, such a program was first implemented in Refs. 19 and 20 establishing detailed correspondence between the key ingredients of the BRST theory and the Fedosov deformation quantization.

A. Symplectic embedding

We start with the description of a sympletic embedding of (M,α) into the dual bundle of the corresponding Lie algebroid. It is well known that $\mathcal{E}^*$ carries a natural Poisson structure, which is dual to the Lie algebroid structure.[25,30] A proper modification of this Poisson structure in the presence of a symplectic 2-form is offered by the next proposition.

Proposition 3.1: Let $(\mathcal{E},\rho,\omega)$ be a symplectic Lie algebroid corresponding to a quasisymplectic manifold (M,α). Then $C^\infty(\mathcal{E}^*)$ can be equipped with the following Poisson brackets:

$$\{x^\mu,x^\nu\}=0,\quad \{p_a,x^\mu\}=X_a^\mu,\quad \{p_a,p_b\}=f_{ab}^c p_c+\omega_{ab}. \tag{3.1}$$

Here x^μ are local coordinates on M and p_a are linear coordinates on the fibers of $\mathcal{E}^*$. The Poisson manifold (M,α) is symplectically imbedded into $\mathcal{E}^*$ as zero section.

Remark: Although the definition of the brackets on $\mathcal{E}^*$ involves local coordinates, the Poisson structure (3.1) is actually coordinate independent, so the relationship between the Lie algebroid

structure on $\mathcal{E}$ and the Poisson bivector on $\mathcal{E}^*$ is intrinsic. The Jacobi identity for (3.1) generates the full set of the Lie algebroid axioms as well as the closedness condition for the symplectic structure.

In terms of local coordinates (x^μ, p_a) one may identify the base manifold M with those points of $\mathcal{E}^*$ for which

$$p_a = 0. \tag{3.2}$$

Since

$$\det(\{p_a, p_b\})\big|_{p=0} = \det(\omega_{ab}) \neq 0, \tag{3.3}$$

the canonical imbedding $M \hookrightarrow \mathcal{E}^*$ defined by (3.2) is symplectic, and the induced Poisson structure on M reads

$$\{f, g\} = \omega^{ab}(X_a^\mu \partial_\mu f)(X_b^\nu \partial_\nu g), \quad \forall f, g \in C^\infty(M). \tag{3.4}$$

From the physical viewpoint, this bracket can be thought of as the Dirac bracket associated with the second-class constraints (3.2), where f and g are taken to be p-independent functions on $\mathcal{E}^*$.

B. Classical conversion

Choosing a symplectic connection ∇_ρ, one can extend the Poisson structure (3.1) on $\mathcal{E}^*$ to that on the direct sum $\mathcal{N}=\mathcal{E}\otimes\mathcal{E}^*$. Namely, if y^a are linear coordinates on the fibers of $\mathcal{E}$, then the corresponding Poisson brackets read

$$\begin{gathered}\{x^\mu, x^\nu\} = 0, \quad \{p_a, x^\mu\} = X_a^\mu(x), \\ \{x^\mu, y^a\} = 0, \quad \{p_a, y^b\} = -\Gamma_{ac}^b(x) y^c, \\ \{y^a, y^b\} = \omega^{ab}(x), \quad \{p_a, p_b\} = \omega_{ab}(x) + f_{ab}^c(x) p_c - \tfrac{1}{2} R_{abcd}(x) y^c y^d.\end{gathered} \tag{3.5}$$

Here Γ_{ab}^c are the coefficients of the connection ∇_ρ and R_{abcd} is the corresponding curvature tensor.

The brackets (3.5) are well defined and meet the Jacobi identity. Verifying the Jacobi identity, one gets the compatibility condition (2.22), the definition of the curvature tensor (2.13), the Bianchi identity (2.10), and the axioms of a symplectic Lie algebroid.

Now we aim to replace the second-class constrained system (3.1) and (3.2) on $\mathcal{E}^*$ with an equivalent gauge system on the extended Poisson manifold $\mathcal{N}$. In the Hamiltonian formalism a reparametrization invariant gauge system is completely specified by a set of first class constraints $T_a=0$ defining some coisotropic submanifold $\Sigma \subset \mathcal{N}$ (a constraint surface). The quotient of Σ by the Hamiltonian action of T's is assumed to be isomorphic to the quasisymplectic manifold (M, α) and this is the sense in which the equivalence will be established between the original Poisson manifold and the effective gauge theory. In fact, for the purposes of deformation quantization it is sufficient to work with a *formal gauge system* on $\mathcal{N}$ in the sense that the first class constraints T_a are allowed to be given by formal power series in y's. It is required, however, that the canonical projection of the formal coisotropic submanifold Σ onto $\mathcal{E}^*$ to coincide with the well-defined constraint surface (3.2), i.e., with M. This allows one to assign a precise meaning to the Hamiltonian reduction by the formal first class constraints.

Thus, we are looking for a set of Hamiltonian constraints $T_a(x, p, y)$ obeying conditions

$$\{T_a, T_b\} = U_{ab}^c T_c, \quad T_a(x,p,y)\big|_{\mathcal{E}} = T_a(x,p,0) = p_a, \tag{3.6}$$

where $U_{ab}^c(x, p, y)$ are some structure functions. Geometrically, one can think of T's as a section of the vector bundle $\pi: \mathcal{E}\oplus\mathcal{E}^* \to \mathcal{E}$ over the base $\mathcal{E}$, with π being the canonical projection onto the first factor.

Proposition 3.2: The equations (3.6) have a solution of the form

$$T_a = p_a + \sum_{n=1}^{\infty} T_a^n, \quad T_a^n = t_{ab_1\cdots b_n}(x) y^{b_1}\cdots y^{b_n}, \tag{3.7}$$

where the coefficients $t_{ab_1\cdots b_n}(x)$ *do not depend on* p's.

Remark: In the physical literature, the passage from a given second-class constrained system to an equivalent first-class one is known as the *conversion procedure*; accordingly, y's are called *conversion variables*. In the local setting, i.e., for a sufficiently small domain in the extended phase space, the existence of the conversion is ensured by a fairly general theorem.[29] Moreover, passing, if necessary, to an equivalent basis of second class constraints, it is possible to have a solution with $U_{ab}^c = 0$ (Abelian conversion). Here, however, we concern with account of global geometry that requires to consider a non-Abelian conversion in general.

Proof: Substituting the expansion (3.7) into the involution relations (3.6) and extracting contribution to zero order in y's, we find

$$(f_{ab}^c - U_{ab}^c) p_c + t_{an}\omega^{nm} t_{bm} + \omega_{ab} = 0. \tag{3.8}$$

A particular solution to this equation is obvious

$$U_{ab}^c = f_{ab}^c, \quad t_{ab} = -\omega_{ab}. \tag{3.9}$$

Taking this solution, one gets the following chain of equations for higher orders in y's:

$$F_{ab}^s := \partial_{[a} T_{b]}^{s+1} - B_{ab}^s = 0, \quad s \geqslant 1, \tag{3.10}$$

where

$$B_{ab}^1 = (X_{[a}^i \partial_i \omega_{b]c} + \omega_{d[a}\Gamma^d_{b]c} + f_{ab}^d \omega_{dc}) y^c,$$

$$B_{ab}^2 = \{p_{[a}, T_{b]}^2\} + f_{ab}^c T_c^2 - \tfrac{1}{2} R_{abcd} y^c y^d, \tag{3.11}$$

$$B_{ab}^s = \{p_{[a}, T_{b]}^s\} + f_{ab}^c T_c^s + \sum_{n=2}^{s} \{T_a^n, T_b^{s+2-n}\}, \quad s \geqslant 3.$$

Hereinafter the square brackets denote antisymmetrization of indices and ∂_a is the partial derivative with respect to y^a. The form of the equations (3.10) suggests to interpret T_a^s as the components of 1-form $T^s = T_a^s \, \mathrm{d}y^a$ defined on the linear space of y's. Thus, we can write

$$F^s = \mathrm{d}T^{s+1} - B^s = 0, \quad s \geqslant 1, \tag{3.12}$$

where d is the usual exterior differential with respect to y's, and B^s is a given 2-form provided the 1-forms $T^1, \ldots, T^s$ have been already determined. According to the Poincaré lemma, Eqs. (3.12) are consistent iff the 2-forms B^s are closed. In this case, the general solution to (3.10) reads

$$T_a^{s+1} = \frac{1}{s+2} y^b B_{ba}^s + \partial_a C^s, \tag{3.13}$$

C^s being an arbitrary monomial of degree $s+2$. The closedness of B's is now proved by induction in s. Consider the identity

$$\{\bar{T}_a^s, \bar{T}_b^s\} - f_{ab}^d \bar{T}_d^s = \sum_{n=0}^{s-1} F_{ab}^n + B_{ab}^s + \cdots, \tag{3.14}$$

where $\bar{T}_a^s = p_a + \Sigma_{n=1}^s T_a^n$ and dots stand for the terms of order higher than s. Taking the Poisson bracket of this relation with $\bar{T}_c^s$ and using the Jacobi identity

$$\{\{\bar{T}^s_a,\bar{T}^s_b\},\bar{T}^s_c\}+\mathrm{cycle}(a,b,c)=0, \tag{3.15}$$

we can write

$$(f^d_{ab}\{\bar{T}^s_c,\bar{T}^s_d\}+\{\bar{T}_c,f^d_{ab}\}\bar{T}_d)\mathrm{d}y^a\wedge\mathrm{d}y^b\wedge\mathrm{d}y^c=\left(\sum_{n=0}^{s-1}\{F^n_{ab},\bar{T}^s_c\}-\{B^s_{ab},\bar{T}^s_c\}+\cdots\right)\mathrm{d}y^a\wedge\mathrm{d}y^b\wedge\mathrm{d}y^c. \tag{3.16}$$

With account of (3.5) and the Lie algebroid relations (2.5), the contribution to the $(s-1)$th order of the last equation is given by

$$\mathrm{d}B^s=\left(f^d_{ab}F^{s-1}_{dc}+\sum_{n=0}^{s-1}\{F^n_{ab},T^{s-n+2}_c\}\right)\mathrm{d}y^a\wedge\mathrm{d}y^b\wedge\mathrm{d}y^c. \tag{3.17}$$

But the rhs of this relation vanishes by the induction hypothesis. Thus, B^s is a closed 2-form and the recurrent formula (3.13) gives the general solution for T_a.

Notice that the ambiguity concerning the choice of arbitrary functions C^s, entering the general solution for T_a, can be removed by imposing the y-transversality condition

$$y^aT^s_a=0,\quad s\geqslant 1. \tag{3.18}$$

Then it follows from Eq. (3.13) that

$$y^a\partial_aC^s(x,y)=(s+2)C^s(x,y)=0\Rightarrow C^s(x,y)=0.$$

Remark: For the case of symplectic manifolds, the convergence of the series (3.7) in a tubular neighborhood of M was proved in Ref. 31 under assumptions of analyticity and compactness. It seems that the same arguments are applicable to any quasisymplectic manifold provided all the structure functions are real-analytical and M is compact.

Now to see the equivalence of the constructed gauge system on $\mathcal{N}$ to the original Hamiltonian system on M it suffices to note that equations $\chi^a:=y^a=0$ are well-defined gauge-fixing conditions for the first class constraints $T_a=0$. Indeed,

$$\det\left.\begin{pmatrix}\{T_a,T_c\} & \{T_a,\chi^d\}\\ \{\chi^b,T_c\} & \{\chi^b,\chi^d\}\end{pmatrix}\right|_{T=\chi=0}=\det\begin{pmatrix}0 & -\delta^d_a\\ \delta^b_c & \omega^{bd}\end{pmatrix}=1. \tag{3.19}$$

Therefore, the reduced Poisson manifold (physical phase space) is isomorphic to the constraint surface $T_a=\chi^b=0$. The last equations are obviously equivalent to $p_a=y^a=0$, i.e., defines the canonical projection $\varphi:\mathcal{N}\to M$. The explicit description of the resulting Poisson structure on M can be obtained by introducing the Dirac bracket for the second-class constraints (T_a,χ^b). Identifying the space of smooth functions on M with the subspace of p- and y-independent functions on $\mathcal{N}$, it is easy to see that $\varphi:\mathcal{N}\to M$ is a Poisson map relating the Dirac bracket $\{\cdot,\cdot\}_D$ on $\mathcal{N}$ with the initial quasisymplectic bracket on M, i.e.,

$$\varphi_*(\{f,g\}_D)=\{\varphi_*(f),\varphi_*(g)\}_M. \tag{3.20}$$

IV. QUANTIZATION

Having realized the quasisymplectic manifold (M,α) as a formal gauge system on $\mathcal{N}$ we are ready to perform its BRST quantization. As usual, this implies further enlargement of the phase space of the system by ghost variables, constructing a nilpotent BRST charge, and identifying physical observables with certain BRST cohomology classes.

A. Ghost variables and the classical BRST charge

With each first class constraint T_a we associate the pair of anticommuting (Grassman odd) ghost variables $(\mathcal{C}^a,\mathcal{P}_b)$ subject to the canonical Poisson bracket relations

$$\{\mathcal{C}^a,\mathcal{P}_b\}=\delta^a_b,\quad \{\mathcal{C}^a,\mathcal{C}^b\}=\{\mathcal{P}_a,\mathcal{P}_b\}=0. \tag{4.1}$$

It is quite natural to treat $\mathcal{C}^a$ and $\mathcal{P}_b$ as linear coordinates on the fibers of the vector bundles $\Pi\mathcal{E}$ and $\Pi\mathcal{E}^*$, respectively. Here by Π we denote the parity reversion operation: being applied to a vector bundle it transforms the bundle into the supervector bundle with the same base manifold and transition functions, and the fibers being the Grassman odd vector spaces. Thus, the phase space of our gauge system is extended to the direct sum of (super-)vector bundles $\mathcal{M}=\mathcal{N}\oplus\Pi\mathcal{N}$. This geometric interpretation places the ghosts on equal footing with the conversion variables y's and suggests the following extension of the Poisson structure from $\mathcal{N}$ to $\mathcal{M}$:

$$\{p_a,\mathcal{C}^b\}=-\Gamma^b_{ac}(x)\mathcal{C}^c,\quad \{p_a,\mathcal{P}_b\}=\Gamma^c_{ab}(x)\mathcal{P}_c. \tag{4.2}$$

The brackets of the ghosts with x^μ and y^a are equal to zero. To meet the Jacobi identity one must modify the Poisson brackets of p's by ghost terms as follows:

$$\{p_a,p_b\}=\omega_{ab}(x)+f^c_{ab}(x)p_c-\tfrac{1}{2}R_{abcd}(x)y^cy^d-R^d_{abc}(x)\mathcal{C}^c\mathcal{P}_d. \tag{4.3}$$

The other Poisson brackets (3.5) remain intact.

Remark: At this point we slightly deviate from the usual line of the BRST scheme, where the ghost variables are assumed to Poisson commute with functions on the original phase space ($\mathcal{N}$ in our case) and, in particular, with the first class constraints. In principle, it is possible to work with the canonical Poisson brackets for ghosts, setting the rhs of (4.2) to zero and omitting the last term in (4.3), but this leads to nonlinear transformations of p_a under bundle automorphisms (p's are mixed with the ghost bilinears $\mathcal{C}^a\mathcal{P}_b$). We refer to Ref. 19 for the details of this construction in the case where M is a symplectic manifold (2.29). As we will see below, these noncanonical Poisson brackets of ghosts can be naturally incorporated into the BRST quantization procedure making it explicitly covariant.

Let $\mathcal{F}(M)$ denote the super-Poisson algebra of functions on the supermanifold $\mathcal{M}$; the elements of $\mathcal{F}(\mathcal{M})$ are superfunctions of the form (in what follows we omit the prefix "super" whenever possible)

$$A(x,p,y,\mathcal{C},\mathcal{P})=\sum A^{b_1\cdots b_m}_{a_1\cdots a_k d_1\cdots d_n}(x)y^{a_1}\cdots y^{a_k}\mathcal{C}^{d_1}\cdots\mathcal{C}^{d_n}\mathcal{P}_{b_1}\cdots\mathcal{P}_{b_m}, \tag{4.4}$$

where $A^{b_1\cdots b_m}_{a_1\cdots a_k d_1\cdots d_n}(x)$ are $\mathcal{E}$ tensors. In addition to the usual $\mathbb{Z}_2$ grading, associated with the Grassman parity,

$$\epsilon(\mathcal{C}^a)=\epsilon(\mathcal{P}_b)=1,\quad \epsilon(x^i)=\epsilon(p_a)=\epsilon(y^b)=0\pmod 2, \tag{4.5}$$

the space $\mathcal{F}(\mathcal{M})$ is endowed with an additional $\mathbb{Z}$ grading by prescribing the following *ghost numbers* to the local coordinates:

$$\mathrm{gh}(\mathcal{C}^a)=1,\quad \mathrm{gh}(\mathcal{P}_a)=-1,\quad \mathrm{gh}(x^i)=\mathrm{gh}(p_a)=\mathrm{gh}(y^a)=0. \tag{4.6}$$

The ghost number just counts the difference between powers of $\mathcal{C}$'s and $\mathcal{P}$'s, entering homogeneous elements of $\mathcal{F}(\mathcal{M})$, and is additive with respect to the Poisson algebra operations,

$$\mathrm{gh}(AB)=\mathrm{gh}(A)+\mathrm{gh}(B),\quad \mathrm{gh}(\{A,B\})=\mathrm{gh}(A)+\mathrm{gh}(B). \tag{4.7}$$

In particular, functions with zero ghost number form a subalgebra in the Poisson algebra $\mathcal{F}(\mathcal{M})$.

The classical BRST charge $Q\in\mathcal{F}(\mathcal{M})$ is defined as an odd function of ghost number 1 obeying the *classical master equation*

$$\{Q,Q\}=0, \tag{4.8}$$

and the standard boundary conditions

$$Q|_{\mathcal{P}=0}=\mathcal{C}^a T_a. \tag{4.9}$$

A function $A\in\mathcal{F}(\mathcal{M})$ is said to be BRST invariant if

$$DA:=\{Q,A\}=0, \quad \mathrm{gh}(A)=0. \tag{4.10}$$

Clearly, $D^2=0$. The space of *physical observables* is identified with the zero-ghost-number cohomology of the BRST operator D. The Poisson algebra structure on $\mathcal{F}(\mathcal{M})$ induces that on the space of physical observables.

According to general theorems of the BRST theory,[18] (i) Eq. (4.8) is always soluble, and (ii) the Poisson algebra of physical observables is isomorphic to that obtained by the Hamiltonian reduction by the first class constraints. In the case at hand, these statements can be refined as follows.

Proposition 4.1: The classical master equation (4.8) admits the following solution:

$$Q=\mathcal{C}^a T_a. \tag{4.11}$$

The Poisson algebra of physical observables on $\mathcal{M}$ is isomorphic to that on the quasisymplectic manifold (M,α). Each physical observable can be represented by a BRST invariant element from $\mathcal{F}(\mathcal{M})$ that does not depend on the ghost variables.

Proof: The first part of the proposition is easily verified by straightforward calculations. Notice that, unlike what one has in the standard BRST theory, the first class constraints T_a are no longer in involution as we have modified the Poisson brackets of p's by the ghost-dependent term (4.3). Luckily, this term does not contribute to the nilpotency condition due to the symmetry properties of the curvature tensor (2.28).

The rest of the proposition will follow from the classical limit of the analogous statement for the quantum BRST observables to be considered in the next section. Here we just show that each physical observable $A(x,p,y,\mathcal{C},\mathcal{P})$ on $\mathcal{M}$ is uniquely determined by its projection $A(x,0,0,0,0)$ on M. Speaking informally, this implies that the space of physical observables is not larger than $C^\infty(M)$. In order to see this, let us introduce the following *homotopy operator* $h:\mathcal{F}(\mathcal{M})\to\mathcal{F}(\mathcal{M})$:

$$h=\mathcal{P}_a\frac{\partial}{\partial\bar{p}_a}+y^a\frac{\partial}{\partial\mathcal{C}^a}, \tag{4.12}$$

where $\bar{p}_a:=p_a-\omega_{ab}y^b$. From the explicit expression for the BRST charge (4.11) it follows that

$$D=\bar{p}_a\frac{\partial}{\partial\mathcal{P}_a}+\mathcal{C}^a\frac{\partial}{\partial y^a}+\cdots. \tag{4.13}$$

Here the dots stand for the terms that increase the total degree when acting on monomials in y, $\mathcal{C}$, $\mathcal{P}$, and p. Then

$$Dh+hD=N, \tag{4.14}$$

where $N=N_0+\cdots$, and

$$N_0=y^a\frac{\partial}{\partial y^a}+\bar{p}_a\frac{\partial}{\partial\bar{p}_a}+\mathcal{C}^a\frac{\partial}{\partial\mathcal{C}^a}+\mathcal{P}_a\frac{\partial}{\partial\mathcal{P}_a}. \tag{4.15}$$

Obviously, $\ker N_0=C^\infty(M)\subset\mathcal{F}(\mathcal{M})$, and hence the operator N_0 is invertible on the subspace $\mathcal{F}_0=\mathcal{F}(\mathcal{M})\backslash C^\infty(M)$ and so is the operator N. This implies that the BRST cohomology is centered in the subspace $C^\infty(M)$; for any BRST invariant B from the complementary subspace $\mathcal{F}_0$ we have

$$B = DC, \quad C = h(N|_{\mathcal{F}_0})^{-1}B. \tag{4.16}$$

To conclude this section, let us depict the diagram of maps describing the path from the original quasisymplectic manifold (M,α) to the super-Poisson manifold $\mathcal{M}$,

$$\mathcal{M} = \mathcal{N} \oplus \Pi\mathcal{N} \to \mathcal{N} = \mathcal{E} \oplus \mathcal{E}^* \to \mathcal{E} \to M. \tag{4.17}$$

All the arrows are canonical projections.

B. Quantization of the super-Poisson manifold $\mathcal{M}$

In the general case, it is not easy to quantize the irregular Poisson brackets (3.5) and (4.1)–(4.3). Fortunately, for our purposes, it is sufficient to deal with a special Poisson subalgebra $\mathcal{A} \subset \mathcal{F}(\mathcal{M})$. This is given by functions of x^μ, y^a, $\mathcal{C}^a$ and $p := \mathcal{C}^a p_a$. Since $p^2 = 0$, the generic element of $\mathcal{A}$ has the form

$$A(x,y,p,\mathcal{C}) = a(x,y,\mathcal{C}) + b(x,y,\mathcal{C})p, \tag{4.18}$$

where a, b belong to the Poisson subalgebra $\mathcal{A}_0$ of p-independent elements of $\mathcal{A}$. The elements of $\mathcal{A}_0$ are given thus by formal power series in y's and $\mathcal{C}$'s with coefficients in $\Lambda(\mathcal{E}, S(\mathcal{E}))$, $S(\mathcal{E})$ being the space of symmetric tensor powers of $\mathcal{E}$. With this geometrical interpretation the basic Poisson bracket relations in $\mathcal{A}$ can be written as

$$\{p,p\} = R + \omega, \quad \{p,a\} = \nabla a, \quad \{a,b\} = \omega^{cd}\frac{\partial a}{\partial y^c}\frac{\partial b}{\partial y^d}, \quad a,b \in \mathcal{A}_0. \tag{4.19}$$

Here

$$\nabla a = \mathcal{C}^d \nabla_d a = \mathcal{C}^a \left(X^\mu_a \frac{\partial}{\partial x^\mu} - y^b \Gamma^d_{ab}\frac{\partial}{\partial y^d} - \mathcal{C}^b \Gamma^d_{ab}\frac{\partial}{\partial \mathcal{C}^d} \right) a \tag{4.20}$$

is the covariant derivative in $\mathcal{A}_0$ induced by the symplectic connection ∇_ρ on $\Lambda(\mathcal{E}, S(\mathcal{E}))$, and

$$R = -\tfrac{1}{2} R_{abcd}\mathcal{C}^a\mathcal{C}^b y^c y^d, \quad \omega = \omega_{ab}\mathcal{C}^a\mathcal{C}^b, \quad R,\omega \in \mathcal{A}_0, \tag{4.21}$$

are the covariant curvature tensor and the symplectic form written in the frame $(y^a, \mathcal{C}^a)$.

In view of Proposition (4.1), the algebra $\mathcal{A}$ contains the classical BRST charge (5.23) as well as all the physical observables of the effective gauge system. It is the reason why one can restrict consideration to the subalgebra $\mathcal{A}$ when the goal is to quantize the algebra of physical observables.

Proceeding to quantization, we introduce the formal deformation parameter $\hbar$ and extend the Poisson algebra $\mathcal{A}$ to the tensor product

$$\hat{\mathcal{A}} = \mathcal{A} \otimes [[\hbar]], \tag{4.22}$$

where $[[\hbar]]$ denotes the space of formal power series in $\hbar$ with coefficients in $\mathbb{C}$. Accordingly, denote by $\hat{\mathcal{A}}_0 := \mathcal{A}_0 \otimes [[\hbar]]$ the subalgebra of p-independent elements of $\hat{\mathcal{A}}$. There is an almost obvious quantum product giving rise to deformation quantization of the Poisson algebra $\hat{\mathcal{A}}$. For any two elements a, $b \in \hat{\mathcal{A}}_0$ we just use the Weyl-Moyal formula

$$(a \circ b)(x,y,\mathcal{C},\hbar) = \exp\left(-\frac{i\hbar}{2}\omega^{ab}\frac{\partial}{\partial y^a}\frac{\partial}{\partial z^b} \right) a(x,y,\mathcal{C},\hbar)\, b(x,z,\mathcal{C},\hbar)|_{y=z}, \tag{4.23}$$

and then extend this $\circ$-product to the whole algebra $\hat{\mathcal{A}}$ by associativity setting

$$p \circ a = pa - i\hbar\, \nabla a, \quad a \circ p = ap, \quad p \circ p = -i\hbar(R + \omega). \tag{4.24}$$

Clearly, the $\circ$-product respects both the Grassman and the ghost-number gradings.

As for any graded associative algebra, we can endow $\hat{\mathcal{A}}$ with the structure of super-Lie algebra with respect to the supercommutator

$$[A,B] = A \circ B - (-1)^{\epsilon(A)\epsilon(B)} B \circ A, \tag{4.25}$$

A, B being homogeneous elements of $\hat{\mathcal{A}}$.

For further purposes let us introduce one more useful grading on $\hat{\mathcal{A}}$ by prescribing the following degrees to the variables:

$$\deg(x^\mu) = \deg(\mathcal{C}^a) = 0, \quad \deg(y^a) = 1, \quad \deg(p) = \deg(\hbar) = 2. \tag{4.26}$$

Since this grading involves essentially the deformation parameter we will refer to it as *ħ-grading*.

C. Quantum BRST charge

This is defined as an element $\hat{Q} \subset \hat{\mathcal{A}}$ of ghost number 1 satisfying the *quantum master equation*

$$[\hat{Q},\hat{Q}] = 2\hat{Q} \circ \hat{Q} = 0 \tag{4.27}$$

with the boundary condition

$$\hat{Q}|_{\mathcal{P}=\hbar=0} = \mathcal{C}^a T_a. \tag{4.28}$$

The adjoint action of $\hat{Q}$ defines the nilpotent derivation $\hat{D}: \hat{\mathcal{A}} \to \hat{\mathcal{A}}$:

$$\hat{D}a = \frac{i}{\hbar}[\hat{Q},a], \quad a \in \hat{\mathcal{A}}. \tag{4.29}$$

The operator $\hat{D}$ increases the ghost number by 1 preserving the subalgebra $\hat{\mathcal{A}}_0$.

By definition, the space of *quantum physical observables* is identified with the zero-ghost-number cohomology of the operator $\hat{D}$.

Let us show the existence of a quantum BRST charge $\hat{Q}$ whose classical limit coincides with the classical BRST charge Q. Technically, instead of finding $\hbar$ corrections to Q, it is more convenient to build up $\hat{Q}$ using recursion on the total $\hbar$ degree (4.26). In order to do this we introduce the pair of Fedosov's operators changing the $\hbar$ degree by 1 unit. The first operator is given by

$$\delta a = \mathcal{C}^a \frac{\partial a}{\partial y^a}, \quad \delta^2 = 0 \tag{4.30}$$

for any $a \in \hat{\mathcal{A}}_0$. Since

$$\delta a = \frac{i}{\hbar}[\mathcal{C}^a \omega_{ab} y^b, a], \tag{4.31}$$

it is an internal derivation of $\hat{\mathcal{A}}_0$. The second operator is defined by its action on homogeneous functions,

$$\delta^* a_{mn} = \frac{1}{n+m} y^a \frac{\partial a}{\partial \mathcal{C}^a}, \quad n+m \neq 0,$$
$$\delta^* a_{00} = 0, \tag{4.32}$$

where $a_{nm} = a_{a_1 \cdots a_n, b_1 \cdots b_m}(x, \hbar) y^{a_1} \cdots y^{a_n} \mathcal{C}^{b_1} \cdots \mathcal{C}^{b_m}$. Like δ, the operator δ^* is nilpotent, though it is not a derivation of the $\circ$-product. One can regard δ^* as a homotopy operator:

$$a|_{\mathcal{C}=y=0} + \delta\delta^* a + \delta^* \delta a = a, \quad \forall\, a \in \hat{\mathcal{A}}_0. \tag{4.33}$$

The last relation resembles the usual Hodge-De Rham decomposition for the exterior algebra of differential forms.

Proposition 4.2: The quantum master equation (4.27) has a solution of the form

$$\hat{Q} = \sum_{r=1}^{\infty} Q_r, \quad \deg(Q_r) = r, \tag{4.34}$$

where

$$Q_1 = -\mathcal{C}^a \omega_{ab} y^b, \quad Q_2, = p, \quad \textit{and } Q_r \in \hat{\mathcal{A}}_0, \quad \forall\, r > 2, \tag{4.35}$$

which is unique if we require

$$\delta^* Q_r = 0, \quad \forall\, r > 2. \tag{4.36}$$

Proof: The first three terms in the expansion (4.34) coincide with those in the classical BRST charge (4.11), and this proves the validity of Eq. (4.27) in the lowest order in $\hbar$ degree. For $r \geqslant 4$ Eq. (4.27) implies

$$\delta Q_{r+1} = B_r, \tag{4.37}$$

where

$$B_r = -\frac{i}{2\hbar} \sum_{s=0}^{r-2} [Q_{r+2}, Q_{r-s}], \quad \deg(B_r) = r. \tag{4.38}$$

In view of the Hodge-De Rham decomposition (4.33), Eq. (4.37) is soluble iff $\delta B_r = 0$. In this case we have the unique solution

$$Q_{r+1} = \delta^* B_r \tag{4.39}$$

subject to the extra condition $\delta^* Q_{r+1} = 0$. So, it remains to show that $\delta B_r = 0$. Proceeding by induction, we assume that Eq. (4.27) is valid up to the sth order in $\hbar$ degree. Then, extracting the $(s+3)$-order in the Jacobi identity

$$[Q^s, [Q^s, Q^s]] = 0, \quad Q^s = \sum_{k=1}^{s} Q_k, \tag{4.40}$$

one gets $\delta B_s = 0$, that completes the proof.

Since $\mathrm{gh}(Q) = 1$, the ansatz (4.34) implies the following structure of the quantum BRST charge: $Q = \mathcal{C}^a \hat{T}_a(x, y, \hbar)$, where $\hat{T}_a$ are the "quantum" first class constraints. Then relation (4.36) is just another form of the y-transversality condition (3.18), which allows one to extract a unique solution both at the classical and quantum levels.

D. Quantum observables and star-product

In Sec. IV A we have shown that the space of physical observables of the classical gauge system on $\mathcal{N}$ is not larger than $C^\infty(M)$ in the sense that any physical observable is uniquely determined by its projection on M. In this section we prove the inverse: any physical observable on M has a unique BRST-invariant extension to a zero-ghost-number function from $\mathcal{A}_0$. Moreover, this picture takes place at the quantum level as well if we replace $C^\infty(M)\to C^\infty(M)\otimes[[\hbar]]$ and $\mathcal{A}_0\to\hat{\mathcal{A}}_0$. Therefore, it is sufficient to consider only the quantum case, the classical statement will follow from the classical limit.

Proposition 4.3: For any $a\in C^\infty(M)$ there is a unique $\hat{a}\in\hat{\mathcal{A}}_0$ obeying conditions

$$[\hat{Q},\hat{a}]=0,\quad \hat{a}|_{y=0}=a. \tag{4.41}$$

Proof: Consider the expansion of $\hat{a}\in\hat{\mathcal{A}}_0$ according to the $\hbar$ degree,

$$\hat{a}=\sum_{s=0}^{\infty}a_s,\quad \deg(a_s)=s. \tag{4.42}$$

The second condition in (4.41) says that $a_0=a(x)$. Substituting this expansion into the first equation, one gets

$$\delta a_{s+1}=B_s,\quad s>1, \tag{4.43}$$

where

$$B^s=\frac{i}{\hbar}\sum_{k=0}^{s-2}[Q^{k+2},a^{s-k}],\quad \deg(B^s)=s. \tag{4.44}$$

In view of the Hodge-De Rham decomposition (4.33) and the boundary condition (4.41), Eq. (4.43) has the unique solution

$$a^{s+1}=\delta^* B^s, \tag{4.45}$$

provided the rhs is δ-closed. The equality $\delta B^s=0$ follows by induction from the $(s+3)$-order of the identity

$$[\hat{Q},[\hat{Q},\hat{a}]]=0. \tag{4.46}$$

Corollary: There is a linear isomorphism between the spaces of quantum observables on M, i.e., $C^\infty(M)\otimes[[\hbar]]$, *and the zero-ghost-number cohomology of the BRST-differential $\hat{D}:\hat{\mathcal{A}}_0\to\hat{\mathcal{A}}_0$.*

Proof: Equation (4.41), being linear, has a unique solution even though we allow $\hat{a}|_{y=0}$ to depend formally on $\hbar$. Therefore, we can replace $C^\infty(M)$ with $C^\infty(M)\otimes[[\hbar]]$.

Clearly, the $\circ$-product on $\hat{\mathcal{A}}_0$ descends to the BRST cohomology and, in view of the corollary, induces an associative $*$-product on $C^\infty(M)\otimes[[\hbar]]$. Explicitly,

$$a*b=(\hat{a}\circ\hat{b})|_{y=0}=\sum_{n=1}^{\infty}\hbar^n D_n(a,b),\quad \forall\, a,b\in C^\infty(M)\otimes[[\hbar]], \tag{4.47}$$

where

$$D_0(a,b)=ab,\quad D_1(a,b)=-\frac{i}{2}\{a,b\}_M, \tag{4.48}$$

and the "hat" stands for the BRST-invariant lift from M to $\mathcal{M}$ (the existence and uniqueness of such a lift are ensured by Proposition 4.3). The higher orders in $\hbar$, being recurrently constructed by (4.39) and (4.45), involve also the symplectic connection and curvature.

Remark: By construction, the bidifferential operators D_n entering the $*$-product (4.47) have a rather peculiar structure. Namely, they are determined by repeated differentiations along the anchor distribution $\{X_a\}$,

$$D_n(a,b) = \sum_{k,l\leqslant n} D_n^{c_1\cdots c_k d_1\cdots d_l}(x)(X_{c_1}\cdots X_{c_k}a)(X_{d_1}\cdots X_{d_l}b). \tag{4.49}$$

Here the structure functions $D^{c_1\cdots c_k d_1\cdots d_l}(x)$ are *universally* expressed via the data of a symplectic Lie algebroid and a Lie algebroid connection. The differential operators of the form (4.49) are called the $\mathcal{E}$-differential operators; accordingly, the $*$-product (4.47) is called the $\mathcal{E}$-deformation of M. As was shown in Ref. 11, any $\mathcal{E}$ deformation of M can be induced by an $\mathcal{E}$ deformation of the commutative algebra of $\mathcal{E}$ jets. Conversely, the $\mathcal{E}$ deformation of M, given by the formula (4.47), admits a canonical extension to the space of $\mathcal{E}$ jets (by universality). In Ref. 15 such an extension was used to derive the universal deformation formula for triangular Lie bialgebras.

V. FACTORIZABLE POISSON BRACKETS BEYOND SYMPLECTIC LIE ALGEBROIDS

As we have seen, the concept of a symplectic Lie algebroid gives rise to an interesting class of Poisson brackets. Not any Poisson bracket comes in this way, but when it does, we have a simple quantization procedure generalizing the Fedosov quantization. In this section we would like to discuss, in a sense, an inverse problem: To what extent the factorization (2.20) of a Poisson bivector α defines a symplectic Lie algebroid?

The precise formulation of the problem is as follows. Let $\mathcal{E}\to M$ be a vector bundle over a smooth manifold M, ω a section of $\mathcal{E}\wedge\mathcal{E}$, and X a section of $\mathcal{E}^*\otimes TM$. By a slight abuse of notation, we will use the same letters ω and X to denote the corresponding bundle homomorphisms $\omega:\mathcal{E}^*\to\mathcal{E}$ and $X:\mathcal{E}\to TM$. Let us also suppose that the $\mathcal{E}$-bivector ω is nondegenerate (defines an isomorphism between $\mathcal{E}$ and its dual $\mathcal{E}^*$) and X is involutive. The latter means that in each trivializing coordinate chart $\mathcal{U}\subset M$ with frame $s_\alpha\in\Gamma(\mathcal{E}|_{\mathcal{U}})$, the local vector fields $X_\alpha = X_\alpha^i\partial_i \in \mathrm{Vect}(\mathcal{U})$ form an involutive distribution,

$$[X_\alpha, X_\beta] = f_{\alpha\beta}^\gamma X_\gamma, \tag{5.1}$$

$f_{\alpha\beta}^\gamma$ being smooth functions on $\mathcal{U}$. Clearly, the property of $\{X_\alpha\}$ to be involutive does not depend on a frame, and hence, $\{X_a\}$ generates a (singular) foliation $F(M)$. Suppose now that the bivector

$$\alpha = \omega^{\alpha\beta}X_\alpha\wedge X_\beta \in \wedge^2 TM \tag{5.2}$$

satisfies the Jacobi identity

$$[\alpha,\alpha] = 0. \tag{5.3}$$

Question: What is the most general geometric structure underlying Eqs. (5.1)–(5.3).

A particular solution to these equations is delivered by a symplectic Lie algebroid $\mathcal{E}\to M$ with anchor X and symplectic 2-form ω. In this case (M,α) is just a quasisymplectic manifold considered in the preceding sections.

Explicitly, the Jacobi identities for the local vector fields X_a and the Poisson bivector α read

$$(f_{\alpha\beta}^\delta f_{\delta\gamma}^\mu - X_\gamma f_{\alpha\beta}^\mu + \mathrm{cycle}(\alpha,\beta,\gamma))X_\mu = 0, \tag{5.4}$$

$$\begin{gathered}(\omega_{\gamma\delta}f_{\alpha\beta}^\delta - X_\gamma\omega_{\alpha\beta})X^\alpha\wedge X^\beta\wedge X^\gamma = 0,\\ X^\alpha = \omega^{\alpha\beta}X_\beta,\quad \omega_{\alpha\gamma}\omega^{\gamma\beta} = \delta_\alpha^\beta.\end{gathered} \tag{5.5}$$

If the map $X:\mathcal{E}\to TM$ is injective on an everywhere dense domain in M, the expressions in parentheses (5.5) must vanish by continuity, and we arrive at a symplectic Lie algebroid $(\mathcal{E},X,\omega)$. In the opposite case the lhs of Eqs. (5.4) and (5.5) cannot be "divided" by X_a so simply, and thus,

more general solutions for the structure functions $f^{\gamma}_{\alpha\beta}$, $\omega_{\alpha\beta}$, and X^i_α are possible. To further study these equations, we impose a certain regularity condition on X. In what follows we will assume that the space $\Gamma(TM)$, considered as a $C^\infty(M)$-module, admits a resolution of the form

$$0 \leftarrow TM \xleftarrow{d_1} \mathcal{E}_1 \xleftarrow{d_2} \mathcal{E}_2 \leftarrow \cdots \leftarrow \mathcal{E}_{n-1} \xleftarrow{d_n} \mathcal{E}_n \leftarrow 0, \tag{5.6}$$

where $\mathcal{E}_k \to M$ and d_k are sequences of vector bundles over M and their M-morphisms with $\mathcal{E}_1 = \mathcal{E}$ and $d_1 = X$. [A sequence of homomorphisms of modules (5.6) is called a resolution of the module $\Gamma(TM)$, if $\operatorname{im} d_{k+1} = \ker d_k$. In other words, the sequence (5.6) is just a cochain complex, which is exact, exclusive of maybe the first term.] Here we do not require the morphisms d_k to have constant ranks, but since $n < \infty$, their ranks must be constant on an open everywhere dense domain in M. In particular, the last structure map $d_k : \mathcal{E}_k \to \mathcal{E}_{k-1}$ should be injective on an everywhere dense domain in M. By analogy with ordinary Lie algebroids, we will refer to the first structure map $d_1 = X$ as anchor.

In order to clarify the meaning of the regularity condition, let us choose an open domain $\mathcal{U} \subset M$ such that for all $k = 1, \ldots, n$, $\mathcal{E}_k|_{\mathcal{U}}$ is a trivial vector bundle with frame s_{α_k}. Upon restriction on $\mathcal{U}$, the morphisms d_k are represented by matrices $d^{\alpha_{k-1}}_{\alpha_k}$, so that $d^{\alpha_{k-1}}_{\alpha_k} d^{\alpha_k}_{\alpha_{k+1}} = 0$. Since the complex (5.6) is exact starting with $\mathcal{E}_1$, the equality $f^{\alpha_k} d^{\alpha_{k-1}}_{\alpha_k} = 0$, f^{α_k} being a section of $\mathcal{E}_k$, implies that $f^{\alpha_k} = g^{\alpha_{k+1}} d^{\alpha_k}_{\alpha_{k+1}}$ for some section $g^{\alpha_{k+1}}$ of $\mathcal{E}_{k+1}$.

Example 0: Consider the adjoint representation of so(3). Identifying the carrier space so(3) with $\mathbb{R}^3$ we get a set of three linear vector fields on $\mathbb{R}^3$ generating the so(3)-algebra action:

$$\mathrm{ad}_i = \epsilon_{ijk} x_j \partial_k, \quad [\mathrm{ad}_i, \mathrm{ad}_j] = -\epsilon_{ijk}\, \mathrm{ad}_k. \tag{5.7}$$

Clearly, the rank of the anchor $\mathrm{ad} : \mathbb{R}^3 \times \mathrm{so}(3) \to T\mathbb{R}^3$ equals 2 in general position and vanishes at the origin $0 \in \mathbb{R}^3$. Since the equation $f^i(x)\mathrm{ad}_i = 0$ implies $f^i(x) = g(x)x^i$, for some smooth function g, while the equation $x^i h(x) = 0$ has the unique solution $h = 0$, we get the following resolution:

$$0 \leftarrow T\mathbb{R}^3 \xleftarrow{\mathrm{ad}} \mathbb{R}^3 \times \mathrm{so}(3) \xleftarrow{d_2} \mathcal{E}_2 \leftarrow 0, \tag{5.8}$$

were $\mathcal{E}_2$ is a linear bundle over $\mathbb{R}^3$ and $d_2 = (x^i)$.

Given an anchor X satisfying the regularity condition, one can solve the Jacobi identity (5.4) in the following form:

$$f^{\delta}_{\alpha\beta} f^{\mu}_{\delta\gamma} - X_\gamma f^{\mu}_{\alpha\beta} + \mathrm{cycle}(\alpha,\beta,\gamma) = f^{a}_{\alpha\beta\gamma} d^{\mu}_{a}, \tag{5.9}$$

where $f^{\alpha}_{\alpha\beta\gamma}$ are smooth functions on $\mathcal{U}$, skew-symmetric in $\alpha\beta\gamma$, and d^{α}_{a} is the matrix of the second structure map d_2 in (5.6). By definition, we have

$$d^{\gamma}_{a} X_\gamma = 0. \tag{5.10}$$

In order to solve the Jacobi identity for α, we assume the anchor foliation $F(M)$ to be regular (this technical restriction can be weakened), i.e., $\operatorname{im} X$ is an integrable subbundle of TM. Then

$$\omega_{\gamma\delta} f^{\delta}_{\alpha\beta} - X_\gamma \omega_{\alpha\beta} + \mathrm{cycle}(\alpha,\beta,\gamma) = W^{a}_{\alpha\beta} d_{a\gamma} + \mathrm{cycle}(\alpha,\beta,\gamma), \quad d_{a\gamma} = \omega_{\gamma\beta} d^{\beta}_{a}, \tag{5.11}$$

$W^{a}_{\alpha\beta} = -W^{a}_{\beta\alpha}$ being smooth functions on $\mathcal{U}$. Examining compatibility of these equations with the involution relations (5.1), one obtains an infinite set of higher structure functions and structure relations to be studied below.

Let us forget for a moment about the Poisson bivector α, focusing at the anchor distribution X. Commuting (5.10) with X_β, we find

$$X_\beta d^{\alpha}_{a} + f^{\alpha}_{\beta\gamma} d^{\gamma}_{a} = -f^{b}_{\beta a} d^{\alpha}_{b}, \tag{5.12}$$

f^{β}_{ba} being local functions. Contracting the last identity with d^{β}_{c} and symmetrizing in the indices ac, we get

$$d_c^\beta f_{\beta a}^b + d_a^\beta f_{\beta c}^d = f_{ca}^A d_A^b, \tag{5.13}$$

where d_A^b is the matrix of the third structure map in (5.6), so that $d_A^b d_b^\alpha = 0$. Proceeding in the same manner one can derive the other structure relations.

There is a nice way to generate all these relations systematically using the language of *NQ manifolds*. Let us recall the basic definitions.[21–24] An *N manifold* is a non-negatively integer graded supermanifold, whose *N* grading is compatible with the underlying $\mathbb{Z}_2$ grading (Grassman parity). In other words, an *N* manifold is just a supermanifold with a privileged class of atlases in which particular coordinates are assigned non-negative integer degrees (even coordinates have even degrees, while odd ones have odd degrees) so that the changes of coordinates respect these degrees. The highest degree of coordinates is called the *degree* of an *N* manifold. For example, if $\deg M = 0$, then *M* is just an ordinary manifold. Finally, an *NQ* manifold is an *N* manifold endowed with integrable vector field *Q* of degree 1, called a *homological vector field*. Since *Q* is odd, the integrability condition $[Q,Q] = 2Q^2 = 0$ is nontrivial. The classical example of an *NQ* manifold of degree 1 is the anticotangent bundle ΠTM (cotangent bundle with the reverse parity of fibers). The functions on ΠTM are just inhomogeneous differential forms on *M* and *Q* is the usual exterior differential. More generally, an *NQ* manifold of degree 1 is the same as Lie algebroid. For this reason it is natural to name the *NQ* manifolds of degree *n* as *n algebroids*.[24]

A general homological vector field looks like (all derivatives are assumed to be acting on the left)

$$Q = c^{\alpha_1} X_{\alpha_1}^i(x) \frac{\partial}{\partial x^i} + \sum_{k=1}^{\deg \mathcal{M}} c^{\alpha_{k+1}} d_{\alpha_{k+1}}^{\alpha_k}(x) \frac{\partial}{\partial c^{\alpha_k}} + \cdots, \tag{5.14}$$

where $\deg(x^i) = 0$, $\deg(c^{\alpha_k}) = k$, and dots stand for higher orders in the positively graded variables c^{α_k}. Evaluating the equation $Q^2 = 0$ at the first order in *c*'s one recovers the cochain complex axioms $d_{\alpha_m}^{\alpha_{m-1}} d_{\alpha_{m+1}}^{\alpha_m} = 0$, the second order in c^{α_1} reproduces the involution relations (5.1), relation (5.9) contributes to the cubic order, and so on. [Notice, that any *n* algebroid can also be viewed as an $(n+1)$-algebroid whose higher structure functions are just equal to zero.] Thus, we see that the resolution (5.6) for the involutive distribution $X: \mathcal{E} \to TM$ is just a regular *n* algebroid.

Although the language of *NQ* manifolds is quite convenient to describe the structure of *n* algebroids as such, it becomes unappropriated when one tries to incorporate the symplectic structure entering the factorization (2.20). Here we would like to present a new geometric framework providing a uniform description for both *n*-algebroid and symplectic structures underlying factorizable Poisson brackets. For the sake of simplicity we restrict our consideration to the case of 2-algebroids. The general construction will be developed elsewhere. Before going into details let us give two examples which are of interest by themselves.

Example 1: (Poisson-Lie algebras.) Consider an invariant Poisson bracket on a Lie group *G* associated with the bivector

$$\alpha = r^{ij}(L_i \wedge L_j - R_i \wedge R_j). \tag{5.15}$$

Here L_i, R_j are left and right invariant vector fields on *G*, and the matrix (r^{ij}) obeys the Yang-Baxter equation

$$f_{ml}^i (r^{jn} f_{ns}^l r^{sk} + \mathrm{cycle}(j,l,k)) + \mathrm{cycle}(i,j,k) = 0, \tag{5.16}$$

f_{ij}^k being the structure constants of the corresponding Lie algebra $L(G)$. If $\det(r^{ij}) \neq 0$, we have the Poisson bivector α associated with the symplectic structure r^{ij} and the 2-algebroid,

$$0 \leftarrow TG \xleftarrow{(L,R)} TG \oplus TG \xleftarrow{d_2} TG \leftarrow 0, \tag{5.17}$$

where $d_2 = (1, A)$, and *A* is the automorphism of the tangent bundle *TG* relating the left and right invariant vector fields, $L_i = A_i^j R_j$.

Example 2: (Universal factorization.) Any Poisson bivector $\alpha=\alpha^{ij}\partial_i\wedge\partial_j$ can be factorized in a skew-symmetric product of Hamiltonian and coordinate vector fields,

$$\alpha = P_i \wedge Q^i, \quad P_i = \partial_i, \quad Q^i = \alpha^{ij}\partial_j. \tag{5.18}$$

The local vector distribution (P_j, Q^j) is obviously transitive and hence involutive. Moreover, there is a one-parameter ambiguity in writing the involution relations,

$$[P_i, P_j] = 0,$$

$$[P_i, Q^j] = \partial_i\alpha^{jk}P_k, \tag{5.19}$$

$$[Q^i, Q^j] = t\partial_k\alpha^{ij}Q^k + (1-t)\partial_k\alpha^{ij}\alpha^{kn}P_n, \quad t\in\mathbb{R}.$$

This ambiguity is due to linear dependence of the local vector fields,

$$Q^i = \alpha^{ij}P_j. \tag{5.20}$$

The last equations are already independent and we arrive at the following cochain complex:

$$0 \leftarrow TM \xleftarrow{(P,Q)} TM\oplus T^*M \xleftarrow{(1,\alpha)} TM \leftarrow 0, \tag{5.21}$$

which is exact provided α is nondegenerate on an everywhere dense domain in M.

Consider now a general NQ-manifold $\mathcal{M}$ of degree 2. As for usual manifolds, the structure of $\mathcal{M}$ can be described in terms of coordinate charts and transition functions gluing together individual N-graded domains $U\in\mathcal{M}$. Without loss of generality we can assume that each U is given by a direct product $\mathcal{U}\times\mathbb{R}^n_1\times\mathbb{R}^m_2$, where $\mathcal{U}\in M$ is an open contractible domain on the base manifold with local coordinates x^i, $\mathbb{R}^n_1$ and $\mathbb{R}^m_2$ are vector spaces with linear coordinates c^α and c^a, respectively. We set $\deg(x^i)=0$, $\deg(c^\alpha)=1$, $\deg(c^a)=2$, so that x^i and c^a are commuting, while c^α are anticommuting coordinates on $U\in\mathcal{M}$. If now U and U' are two graded domains with nonempty intersection, then the most general form of transition functions, compatible with the N grading, is given by

$$x'^i = f^i(x), \quad c'^\alpha = A^\alpha_\beta(x)c^\beta, \quad c'^a = B^a_b(x)c^b + \tfrac{1}{2}F^a_{\alpha\beta}(x)c^\alpha c^\beta, \tag{5.22}$$

f^i, A^α_β, B^a_b and $F^a_{\alpha\beta}$ are smooth functions on $\mathcal{U}\cap\mathcal{U}'$. The first equation defines transformation of local coordinates on the base manifold M. Disregarding the F term, we see that the second and third equations are similar to those defining transition functions for (graded) vector bundles. Moreover, the matrix-valued functions A and B do really obey the standard cocycle conditions on overlaps of two and three coordinate charts, defining thus the direct sum $\mathcal{E}_1\oplus\mathcal{E}_2$ of two graded vector bundles.

In terms of local coordinates the most general homological vector field on $\mathcal{M}$ reads

$$Q = c^\alpha X^i_\alpha\frac{\partial}{\partial x^i} + c^a d^\alpha_a\frac{\partial}{\partial c^\alpha} + \frac{1}{2}c^\beta c^\alpha f^\gamma_{\alpha\beta}\frac{\partial}{\partial c^\gamma} + c^\alpha c^a f^b_{\alpha a}\frac{\partial}{\partial c^b} + c^\gamma c^\beta c^\alpha f^a_{\alpha\beta\gamma}\frac{\partial}{\partial c^a}. \tag{5.23}$$

Using relations (5.22) one can derive transformation properties for the structure functions X^i_α, d^γ_a, $f^\gamma_{\alpha\beta}$, $f^b_{a\beta}$, $f^a_{\alpha\beta\gamma}\in C^\infty(\mathcal{U})$ under coordinate changes. In particular, the F term induces the shift

$$f^\gamma_{\alpha\beta} \to f^\gamma_{\alpha\beta} + F^a_{\alpha\beta}d^\gamma_a, \tag{5.24}$$

which reflects an inherent ambiguity concerning the choice of the structure functions (5.1) whenever X_α are linearly dependent. Also, it is not hard to see that X^i_α and d^γ_a transform homogeneously, i.e., as sections of the associated vector bundles $\mathcal{E}^*_1\oplus TM$ and $\mathcal{E}^*_2\oplus\mathcal{E}_1$.

Now suppose that $\mathcal{M}$ defines a 2-algebroid factorizing a Poisson bivector α. Our aim is to give a unified description for both the 2-algebroid and the symplectic structure entering this

factorization. It turns out that all structure relations underlying the factorization (5.2) can be described in terms of an Abelian connection (covariant derivative) acting on a bundle of odd Poisson algebras over M. The construction goes as follows.

Let $E_0 \oplus E_1$ be a $\mathbb{Z}_2$-graded vector bundle over M defined by the aforementioned gluing cocycles A and $(B^{-1})^*$, that is $E_1 = \mathcal{E}_1$, $E_0 = \mathcal{E}_2^*$. If c^α and π_a are linear coordinates in the fibers of E_1 and E_0 over a trivializing domain $\mathcal{U} \in M$, we set $\epsilon(c^\alpha) = 1$, $\epsilon(\pi_a) = \epsilon(x^i) = 0$. It is convenient to think of this bundle as a formal supermanifold $\mathcal{N}$ with even coordinates x^i, π_a and odd coordinates c^α. The word "formal" reflects the fact that we allow the functions on $\mathcal{N}$ to be given by formal power series in π's. These functions form a supercommutative algebra $\mathcal{F}$ with the generic element

$$f(x,c,\pi) = \sum_{k,n} f^{a_1 \cdots a_k}_{\alpha_1 \cdots \alpha_n}(x)\, \pi_{a_1} \cdots \pi_{a_k} c^{\alpha_1} \cdots c^{\alpha_n}. \tag{5.25}$$

The algebra $\mathcal{F} = \oplus \mathcal{F}_{n,m}$ is naturally bigraded with respect to powers of c's and π's and is isomorphic to the tensor algebra of sections of the associated vector bundle $S^\bullet E_0^* \otimes \Lambda^\bullet E_1^*$.

The space $\mathcal{F}$ can also be endowed with the structure of odd Poisson algebra. To this end, we introduce the odd Laplacian $\Delta : \mathcal{F}_{m,n} \to \mathcal{F}_{m-1,n-1}$,

$$\Delta f = d_a^\alpha(x) \frac{\partial^2 f}{\partial c^\alpha \partial \pi_a}. \tag{5.26}$$

Clearly, $\Delta^2 = 0$. The odd Poisson bracket $(\cdot,\cdot) : \mathcal{F}_{n,m} \oplus \mathcal{F}_{k,l} \to \mathcal{F}_{n+k-1,m+l-1}$ is defined by the rule

$$(-1)^{\epsilon(f)}(f,g) = \Delta(f \cdot g) - \Delta f \cdot g - (-1)^{\epsilon(f)} f \cdot \Delta g. \tag{5.27}$$

It obeys the standard identities which may be taken as the axioms of an odd Poisson manifold,

$$\begin{gathered} \epsilon(f,g) = \epsilon(f) + \epsilon(g) + 1 \pmod 2, \\ (f,g) = -(g,f)(-1)^{(\epsilon(f)+1)(\epsilon(g)+1)} \quad \text{(symmetry)}, \\ (f,gh) = (f,g)h + (f,h)g(-1)^{\epsilon(g)\epsilon(h)} \quad \text{(Leibnitz rule)}, \\ (f,(g,h))(-1)^{(\epsilon(f)+1)(\epsilon(h)+1)} + \text{cycle}(f,g,h) = 0 \quad \text{(Jacobi identity)}. \end{gathered} \tag{5.28}$$

Notice that Δ respects the odd Poisson bracket (5.27) in the sense that

$$\Delta(f,g) = (\Delta f, g) + (-1)^{\epsilon(f)+1}(f, \Delta g). \tag{5.29}$$

The algebra $\mathcal{F}$ contains a special element $\omega = \frac{1}{2}\omega_{\alpha\beta} c^\alpha c^\beta \in \mathcal{F}_{2,0}$ associated with the symplectic structure. The adjoint action of ω gives rise to the nilpotent differentiation $\delta : \mathcal{F}_{n,m} \to \mathcal{F}_{n+1,m-1}$,

$$\delta f = (\omega, f) = -c^\alpha \omega_{\alpha\beta} d_a^\beta \frac{\partial f}{\partial \pi_a}, \quad \delta^2 = 0. \tag{5.30}$$

It is easy to see that the δ-cohomology is trivial when evaluated on $\mathcal{F}_{\bullet,k}$ with $k > 0$.

Now we would like to endow the bundle of odd Poisson algebras $\mathcal{F}$ with a sort of partial connection $\nabla : \mathcal{F}_{m,n} \to \mathcal{F}_{m+1,n}$ making possible parallel transport along the leaves of the anchor foliation $F(M)$. Treating ∇ as an odd vector field on $\mathcal{N}$, we set

$$\nabla a = c^\alpha \left(X^i_\alpha \frac{\partial}{\partial x^i} + \frac{1}{2} c^\beta f^\gamma_{\alpha\beta} \frac{\partial}{\partial c^\gamma} + \pi_a f^\alpha_{ab} \frac{\partial}{\partial \pi_b} \right) a + (W_1, a), \tag{5.31}$$

where the structure functions X^i_α, $f^\gamma_{\alpha\beta}$, $f^a_{\alpha b}$ are the same as in Eq. (5.23) and $W_1 = c^\alpha c^\beta W^a_{\alpha\beta} \pi_a \in \mathcal{F}_{2,1}$ is given by the rhs of Eq. (5.11). Using the definition of ∇, one can rewrite Eq. (5.11) as

$$\nabla\omega = 0 \tag{5.32}$$

or, equivalently,

$$\nabla\delta + \delta\nabla = 0. \tag{5.33}$$

The main property of the local vector field ∇ is that it respects the odd Poisson bracket, i.e.,

$$\nabla(f,g) = -(\nabla f,g) + (-1)^{\epsilon(f)+1}(f,\nabla g), \tag{5.34}$$

for any $f,g \in \mathcal{F}|_U$. Squaring ∇, we get an internal derivation of the odd Poisson algebra,

$$\nabla^2 f = (R,f), \tag{5.35}$$

where one can thought of the odd function $R = c^\gamma c^\beta c^\alpha f^a_{\alpha\beta\gamma}\pi_a \in \mathcal{F}_{3,1}$ as the curvature of ∇. Like a curvature, R obeys the Bianchi identity

$$\nabla R = 0. \tag{5.36}$$

Now we can extend ∇ from a local coordinate chart U to the whole $\mathcal{N}$. To this end, we choose a trivializing covering $\{\mathcal{U}_i\}$ of M together with local connections ∇_i on $(E_0 \oplus E_1)|_{\mathcal{U}_i}$. It follows from (5.32) that on each nonempty intersection $\mathcal{U}_i \cap \mathcal{U}_j$,

$$\nabla_i - \nabla_j = (\delta\phi_{ij}, \cdot), \tag{5.37}$$

for some $\phi_{ij} \in \mathcal{F}_{1,2}|_{\mathcal{U}_i\cap\mathcal{U}_j}$. Then, on each nonempty intersection $\mathcal{U}_i \cap \mathcal{U}_j \cap \mathcal{U}_k$ the functions ϕ_{ij} satisfy the relation

$$\delta(\phi_{ij} + \phi_{jk} + \phi_{ki}) = 0. \tag{5.38}$$

Since the δ-cohomology is trivial on $\mathcal{F}_{1,2}$ we conclude that

$$\phi_{ij} + \phi_{jk} + \phi_{ki} = \delta\psi_{ijk} \quad \text{on } \mathcal{U}_i \cap \mathcal{U}_j \cap \mathcal{U}_k, \tag{5.39}$$

for some $\chi_{ijk} \in \mathcal{F}_{0,3}|_{\mathcal{U}_i\cap\mathcal{U}_j\cap\mathcal{U}_k}$. Again, from the last equation it follows that on each nonempty intersection $\mathcal{U}_i \cap \mathcal{U}_j \cap \mathcal{U}_k \cap \mathcal{U}_l$ of four domains one has

$$\chi_{ijk} - \chi_{jkl} + \chi_{kli} - \chi_{lij} = 0. \tag{5.40}$$

Notice that Eq. (5.37) does not define ϕ_{ij} uniquely as we are free to add to them any δ-closed terms $\delta\psi_{ij} \in \mathcal{F}_{1,2}$. This modifies the rhs of Eq. (5.39) as follows:

$$\chi_{ijk} \to \chi_{ijk} - (\psi_{ij} + \psi_{jk} + \psi_{ki}). \tag{5.41}$$

Equations (5.40) and (5.41) imply that to any collection of local connections ∇_i we have associated an element χ of the second Čech cohomology group with coefficients in $\mathcal{F}_{0,3}$. Since this group is completely determined by the second De Rham's cohomology group of M we can think of χ as an element of $H^2(M)$.

Given a partition of unity $\{h^i\}$ subordinated to the covering $\{\mathcal{U}_i\}$, we set

$$\phi_i = \phi_{ij}h^j. \tag{5.42}$$

It is not hard to check, using relation (5.39), that the new local connections $\nabla'_i = \nabla_i - (\delta\phi_i, \cdot)$ already coincide on each intersection $\mathcal{U}_i \cap \mathcal{U}_j \neq \emptyset$. Thus, there are no topological obstructions to introducing a partial connection of the form (5.31) and we can regard $\chi \in H^2(M)$ as an invariant of ∇.

Combining now the action of ∇ with internal differentiations of the odd Poisson algebra $\mathcal{F}$, one can construct a more general connection $D: \mathcal{F}_{n,\bullet} \to \mathcal{F}_{n+1,\bullet}$,

$$Da = \delta a + \nabla a - (W,a) = \nabla a + (\omega - W,a), \tag{5.43}$$

W being an element of $\mathcal{F}_{2,\bullet}$, if $D^2=0$, we refer to D as an Abelian connection. The condition of D to be an Abelian connection is equivalent to the following equation:

$$\delta W = R + \nabla W + \tfrac{1}{2}(W,W). \tag{5.44}$$

The existence of an Abelian connection follows from the solubility of (5.44). Indeed, substituting expansion

$$W = \sum_{k=2}^{\infty} W_k, \quad W_k \in \mathcal{F}_{2,k}, \tag{5.45}$$

into (5.44) one gets

$$\begin{aligned} \delta W_2 &= R, \\ \delta W_{n+1} &= \nabla W_n + \frac{1}{2}\sum_{k=2}^{n} (W_{n-k+2}, W_k), \quad n \geqslant 2. \end{aligned} \tag{5.46}$$

Since the δ-cohomology is trivial when evaluated on $\mathcal{F}_{2,k}$ with $k>0$, the first equation is soluble provided $\delta R=0$. But the last condition immediately follows from the identities $0=\nabla^2\omega=(R,\omega)=-\delta R$. Proceeding by induction, one can see that the rhs of the $(n+1)$th equation is δ closed (and thus is δ exact) provided all the previous equations for $W_2,\ldots,W_n$ have been satisfied.

The main results of this section can be summarized as follows.

Proposition 5.1: Suppose we are given the following data:

(1) *a short exact sequence*

$$0 \to \mathcal{E}_2 \xrightarrow{d} \mathcal{E}_1 \xrightarrow{X} F \to 0,$$

where $\mathcal{E}_1 \to M$, $\mathcal{E}_2 \to M$ are vector bundles over a smooth manifold M, F is an integrable subbundle of the tangent bundle TM, and d, X are M-morphisms of the vector bundles (not necessarily of constant rank);

(2) *a nondegenerate, skew-symmetric, bilinear form ω on $\mathcal{E}_1$ inducing a Poisson bivector field on the base manifold*,

$$\alpha = \langle \omega, X \wedge X \rangle \in \wedge^2 TM, \quad [\alpha,\alpha] = 0.$$

(Here we identify $X:\mathcal{E}_1 \to F \subset TM$ with a section of $\mathcal{E}_1^* \otimes TM$.)

Then to each set of such data one can associate

(1) *an invariant χ taking value in the second group of De Rham's cohomology of M, and*
(2) *a bundle of odd Poisson algebras $\mathcal{F}$ over M together with an Abelian connection D differentiating $\mathcal{F}$ such that the condition $D^2=0$ generates all structure relations arising from the integrability of F and the Jacobi identity for α.*

The generating procedure stated above could be viewed as starting point for quantizing general factorizable brackets associated with symplectic 2-algebroids along the lines of Secs. III and IV.

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Discrete reductive perturbation technique

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We expand a partial difference equation (PΔE) on multiple lattices and obtain the PΔE which governs its far field behavior. The perturbative-reductive approach is here performed on well-known nonlinear PΔEs, both integrable and nonintegrable. We study the cases of the lattice modified Korteweg-de Vries (mKdV) equation, the Hietarinta equation, the lattice Volterra-Kac-Van Moerbeke equation and a nonintegrable lattice KdV equation. Such reductions allow us to obtain many new PΔEs of the nonlinear Schrödinger type. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Problems involving the evolution of nonlinear phenomena, both continuous and discrete, have become of increasing interest in various branches of science and engineering. Nonlinear waves, without dissipation and dispersion give rise in a finite time to a discontinuity. A typical example of nonlinear wave is the shock wave produced by a supersonic object. Dissipation and dispersion play an important role in balancing the steepening due to nonlinearity, so that when these effects are present, a steep but smooth solitary wave may be formed and then propagates for all times. The solitary wave phenomenon has actually been observed for many years in the form of a surface wave in shallow water. A model equation of nonlinear dispersive phenomena may, in general, be very complicated. The soliton may appear only in the asymptotics, after a long transient period. Thus to be able to put in evidence the solitons, Taniuti and collaborators[11,12] introduced an asymptotic method which makes it possible to reduce general nonlinear evolution equations to some more tractable nonlinear equations. This method go under the denomination of *reductive perturbation technique*. Under the assumption that the amplitude of the waves are small, one is able to reduce the starting hyperbolic system to a few simple equations, such as the Burgers equation, the Korteweg-de Vries equation, the nonlinear Schrödinger equation and few others.

In the reductive perturbation method, the space and time coordinates are stretched in terms of a small expansion parameter and we introduce the concept of *far field*, as the field governing the asymptotic behavior of the reduced equation. To give a simple idea of the reasoning underlining this concept, let us consider, as an example, the familiar wave equation in two variables:

$$\phi_{,tt} - \phi_{,xx} = 0. \tag{1}$$

The general solution of Eq. (1) can be expressed as the superposition of waves moving to the right and to the left. In general these two waves are excited simultaneously by an arbitrary initial condition. However, if the initial condition is localized, after a certain finite time the disturbance separates in a progressive wave propagating to the right and one to the left, and they are solutions

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to a first order equation, i.e., an equation of one fewer degree of freedom:

$$\phi_{,x} \pm \phi_{,t} = 0.$$

We call the solutions of the first order equation the *far field solutions* of the original wave equation. The concept of far field came from the idea of finding properties of a given evolution equation which do not depend in a sensitive manner on the details of the initial conditions, but correspond to a wide class of initial conditions.

As an example of the simplification obtained by considering the reductive perturbation method, let us consider a Riemann wave,

$$\phi_{,t} + \lambda(\phi)\phi_{,x} = 0. \tag{2}$$

When the wave function is small we may find the solution ϕ by a perturbation calculation. Let ϵ be a small parameter and let us expand the solution around the constant solution $\phi^{(0)}$,

$$\phi = \phi^{(0)} + \epsilon\phi^{(1)} + O(\epsilon^2).$$

Expanding in powers of ϵ we get from Eq. (2) the following results:

$$\epsilon^0, \quad \phi^{(1)}_{,t} + \lambda_0 \phi^{(1)}_{,x} = 0,$$

$$\epsilon^1, \quad \phi^{(2)}_{,t} + \lambda_0 \phi^{(2)}_{,x} = -\lambda_{,\phi^{(0)}} \phi^{(1)} \phi^{(1)}_{,x},$$

with

$$\lambda_0 \doteq \lambda(\phi^{(0)}), \quad \lambda_{,\phi^{(0)}} \doteq \left(\frac{d\lambda}{d\phi}\right)_{\phi=\phi^{(0)}}.$$

Introducing the new variables $x' = x - \lambda_0 t$, $t' = \epsilon t$, we can rewrite Eq. (2), up to the second order in ϵ, as

$$\phi^{(1)}_{,t'} + \lambda_{,\phi^{(0)}} \phi^{(1)} \phi^{(1)}_{,x'} = 0. \tag{3}$$

If we consider a nonlinear dispersive system, like, for example, the Euler equation, instead of Eq. (3) we get

$$\phi_{,t'} = \phi_{,x'x'x'} + 6\phi\phi_{,x'}, \tag{4}$$

that is the Korteweg-de Vries (KdV) equation.

The nonlinear system at the lowest order approximation can admit a solution given by monocromatic wave packets, i.e., $\phi^{(0)} = A \exp[kx - \omega(k)t]$. Then it is reasonable to consider perturbations of such solution and to turn the nonlinear system into a set of equations for the complex envelope of these packets. The characteristic packet size and wavelength play the role of different scales for this system.

Let us consider, for example, the KdV equation (4) for a small amplitude field ϕ of order ϵ. The linear equations admits a monocromatic solution with dispersion relation $\omega(k) = -k^3$. Then the solution of the KdV equation can be written as

$$\phi = \sum_{n=-\infty}^{+\infty} \epsilon^{\alpha_{|n|}} v_n(x', t') e^{in(kx - \omega(k)t)}, \quad v_n^* = v_{-n},$$

with

$$x' = \epsilon(x + 3k^2 t), \quad t' = -6\epsilon^2 kt,$$

$$\alpha_0 = 1, \quad \alpha_n = n - 1, \quad n \geqslant 1,$$

and v_1 will satisfy the well-known integrable nonlinear Schrödinger (NLS) equation

$$v_{1,t'} + \tfrac{1}{2} v_{1,x'x'} - k^2 v_1 |v_1|^2 = 0. \tag{5}$$

It is important to notice that these multiscale expansions are structurally strong and can be applied to both integrable and nonintegrable systems. Zakharov and Kuznetsov in the introduction of their paper[14] say: *If the initial system is not integrable, the result can be both integrable and nonintegrable. But if we treat the integrable system properly, we again must get from it an integrable system.*

Calogero and Eckhaus[3] used similar ideas starting from generic hyperbolic systems to prove in 1987 the necessary conditions for the integrability of nonlinear partial differential equations (PDEs). Later Degasperis and Procesi[4] introduced the notion of *asymptotic integrability of order n* by requiring that the multiscale expansion be verified up to order n.

Also in the case of differential equations on a lattice, we would like to have a reliable reductive perturbative method which would produce reduced discrete systems. As the far field solution implies the introduction of a new variable which combines the continuous time with the discrete lattice, it is natural to get from a differential-difference equation by the reductive perturbation technique a continuous NLS equation (5). Leon and Manna[7] and later Levi and Heredero[9] proposed a set of tools which allows to perform multiscale analysis for a discrete evolution equation. These tools rely on the definition of a large grid scale via the comparison of the magnitude of related difference operators and on the introduction of a slow varying condition for functions defined on the lattice. Their results, however, are not very promising as the reduced models are neither simpler nor as integrable as the original ones. Starting from an integrable model, like the Toda lattice, Leon and Manna[7] produce a nonintegrable differential-difference equation of the discrete NLS type. Levi and Heredero[9] from the integrable differential-difference NLS equation obtain a nonintegrable system of differential-difference equations of KdV type.

In the present paper we consider the case of nonlinear partial difference equations (PΔEs). To be able to carry out the discrete reductive perturbation technique, in Sec. II we introduce multiple lattice variables and give a definition of slow varying functions on the lattice. Section III is devoted to the application of the perturbative expansions introduced to the case of a set of integrable and nonintegrable equations, i.e., the lattice modified Korteweg-de Vries (mKdV) equation, the Hietarinta equation, the lattice Volterra-Kac-Van Moerbeke (VKVM) equation and a nonintegrable lattice KdV equation. Section IV is devoted to some conclusive remarks.

II. MULTIPLE SCALES ON THE LATTICE AND FUNCTIONAL VARIATION ON THEM

The aim of this section is to fix the notation and to introduce the mathematical formulas necessary to reduce integrable and nonintegrable lattice equations in the framework of the perturbative-reductive approach. In doing so we will partly follow Ref. 8, trying to present a clearer and simpler derivation of all necessary formulas.

A. Slow varying variables on the lattice

Given a lattice defined by a constant lattice spacing h, we will denote by n the running index of the points separated by h. In correspondence with the lattice variable n, we can introduce the real variables $x = hn$.

We can define on the same lattice a set of slow varying variables by introducing a small parameter $\epsilon = N^{-1}$ and requiring that

$$n_j = \epsilon^j n. \tag{6}$$

This is equivalent to sampling points from the original variables which are situated at a distance of $N^j h$ between them and then setting them on a lattice of spacing h. The corresponding slowly varying real variables x_j are related to the variable x by the equation $x_j = \epsilon^j x$.

B. Expansion of slowly varying functions

Let us study the relation between functions living on the different lattices defined in Sec. II A. We consider a function $f \doteq f_n$ defined on the points of a lattice of index n. Let us assume that $f_n = g_{n_1,n_2,\ldots,n_K}$, i.e., f depends on a finite number K of slow varying lattice variables n_j $j=1,2,\ldots,K$ defined as in (6). We want to get explicit expressions for, say, f_{n+1} in terms of $g_{n_1,n_2,\ldots,n_K}$ evaluated on the points of the $n_1,n_2,\ldots,n_K$ lattices. At first let us consider the case, studied in Ref. 6, when we have only two different lattices, i.e., $K=1$. Using the results obtained in this case we will then consider the case corresponding to $K=2$. The general case will then be obvious.

(I) $K=1$ ($f_n = g_{n_1}$): In this case we use the following result presented in Ref. 6:

$$\Delta^k g_{n_1} \doteq \sum_{i=0}^{k} (-1)^{k-i} \binom{k}{i} g_{n_1+i} = \sum_{i=k}^{\infty} \frac{k!}{i!} P(i,k) \Delta^i f_n. \tag{7}$$

Here the coefficients $P(i,k)$ are given by

$$P(i,j) = \sum_{\alpha=j}^{i} \omega^{\alpha} S_i^{\alpha} \mathfrak{S}_{\alpha}^{j}, \tag{8}$$

where ω is the ratio of the increment in the lattice of variable n with respect to that of variable n_1. In this case, taking into account Eq. (6), $\omega = N$. The coefficients S_i^{α} and $\mathfrak{S}_{\alpha}^{j}$ are the Stirling numbers of the first and second kind, respectively.[2] Formula (7) allow us to express a difference of order k in the lattice of variable n_1 in terms of an infinite number of differences on the lattice of variable n. The result (7) can be inverted and we get

$$\Delta^k f_n = \sum_{i=k}^{\infty} \frac{k!}{i!} Q(i,k) \Delta^i g_{n_1}, \tag{9}$$

where the coefficients $Q(i,k)$ are given by (8) with $\omega = N^{-1} = \epsilon$.

To get from Eqs. (7) and (9) a finite approximation of the variation of $g_{n_1} \doteq f_n$ we need to truncate the expansion on the right-hand side (rhs) by requiring a slow varying condition for the function f_n. Let us introduce the following definition.

Definition: The function f_n is a slow varying function of order p iff $\Delta^{p+1} f_n = 0$.

From Sec. II A it follows that a slow varying function of order p is a polynomial of degree p in n. From Eqs. (7) and (9) we see that also the following statement holds.

Theorem: *f_n is a slow varying function of order p iff $\Delta^{p+1} g_{n_1} = 0$, namely g_{n_1}, is of order p.*

Equation (9) provides us with the formulas for f_{n+1} in terms of g_{n_1} and its neighboring points in the case of slow varying functions of any order. Let us write down explicitly these expressions in the case of g_{n_1} of order 1, 2, and 3.

(i) $p=1$. The formula (9) reduces to

$$\Delta f_n = \frac{1}{N} \Delta g_{n_1},$$

i.e., f_{n+1} reads

$$f_{n+1} = g_{n_1} + \frac{1}{N}(g_{n_1+1} - g_{n_1}) + O(N^{-2}).$$

(ii) $p=2$: From Eq. (9) we get

$$\Delta f_n = \frac{1}{N}\Delta g_{n_1} + \frac{1-N}{2N^2}\Delta^2 g_{n_1},$$

and thus f_{n+1} reads

$$f_{n+1} = g_{n_1} + \frac{1}{2N}(-g_{n_1+2} + 4g_{n_1+1} - 3g_{n_1}) + \frac{1}{2N^2}(g_{n_1+2} - 2g_{n_1+1} + g_{n_1}) + O(N^{-3}). \quad (10)$$

(iii) $p=3$: From Eq. (9) we get

$$\Delta f_n = \frac{1}{N}\Delta g_{n_1} + \frac{1-N}{2N^2}\Delta^2 g_{n_1} + \frac{(1-N)(1-2N)}{6N^3}\Delta^3 g_{n_1},$$

and thus f_{n+1} reads

$$f_{n+1} = g_{n_1} + \frac{1}{6N}(2g_{n_1+3} - 9g_{n_1+2} + 13g_{n_1+1} - 6g_{n_1}) + \frac{1}{2N^2}(-g_{n_1+3} + 4g_{n_1+2} - 5g_{n_1+1} + 2g_{n_1})$$
$$+ \frac{1}{6N^3}(g_{n_1+3} - 3g_{n_1+2} + 3g_{n_1+1} - g_{n_1}) + O(N^{-4}).$$

In the next sections we will consider mainly the reduction of integrable discrete equations and we will be interested in obtaining from them integrable discrete equations. It is known[13] that a scalar differential-difference equation can possess higher conservation laws and thus be integrable only if it depends symmetrically on the discrete variable, i.e., if the discrete equation is invariant with respect to the inversion of the lattice index. The results contained in (9) do not provide us with symmetric formulas. To get symmetric formulas we start from Eq. (7) and take into account the following remarks:

(1) Formula (7) holds also if h is negative;
(2) For a slow varying function of order p, we have $\Delta^p f_n = \Delta^p f_{n+\ell}$, for all $\ell \in \mathbb{Z}$.

When f_n is a slow varying function of odd order we are not able to construct completely symmetric derivatives using just an odd number of points centered around the n_1 point and thus $f_{n\pm1}$ can never be expressed in a symmetric form.

Using the above remarks we can construct the symmetric version of (10). From (7) we get

$$g_{n_1+1} = g_{n_1} + N\Delta f_n + \tfrac{1}{2}N(N-1)\Delta^2 f_n, \quad (11)$$

where $\Delta^2 f_n = f_{n+1} - 2f_n + f_{n-1}$ thanks to the remark 2. Using the remark 1 we can also write

$$g_{n_1-1} = g_{n_1} + N\Delta_{-1} f_n + \tfrac{1}{2}N(N-1)\Delta^2 f_n, \quad (12)$$

where $\Delta_{-1} f_n \doteq f_{n-1} - f_n$. From Eqs. (11) and (12) we obtain the following form for f_{n+1}:

$$f_{n+1} = g_{n_1} + \frac{1}{2N}(g_{n_1+1} - g_{n_1-1}) + \frac{1}{2N^2}(g_{n_1+1} - 2g_{n_1} + g_{n_1-1}) + O(N^{-3}). \quad (13)$$

(II) $K=2$ ($f_n = g_{n_1,n_2}$): The derivation of the formulas in this case is done in the same spirit as for the symmetric expansion presented above, see Eq. (13). Let us just consider the case when $p=2$, as this is the lowest value of p for which we can consider f_n as a function of the two scales n_1 and n_2. From Eq. (11) we get

$$g_{n_1+1,n_2} = g_{n_1,n_2} + N\Delta_1 f_{n,n} + \tfrac{1}{2}N(N-1)\Delta_1^2 f_{n,n}, \quad (14)$$

$$g_{n_1,n_2+1} = g_{n_1,n_2} + N^2\Delta_2 f_{n,n} + \tfrac{1}{2}N^2(N^2-1)\Delta_2^2 f_{n,n}. \tag{15}$$

Here the symbols Δ_1 and Δ_2 denote difference operators which acts on the first and, respectively, on the second index of the function $f_{n,n} \doteq g_{n_1,n_2}$, e.g., $\Delta_1 f_{n,n} \doteq f_{n+1,n} - f_{n,n}$ and $\Delta_2 f_{n,n} = f_{n,n+1} - f_{n,n}$.

Let us now consider a function g_{n_1,n_2} where one shifts both indices by 1. From Eq. (14), taking into account that, from Eq. (6), for example, $g_{n_1+1,n_2} = f_{n+N,n}$, one has

$$g_{n_1+1,n_2+1} = g_{n_1,n_2+1} + N\Delta_1 f_{n,n+N^2} + \tfrac{1}{2}N(N-1)\Delta_1^2 f_{n,n+N^2}, \tag{16}$$

and using the result (15) we can write Eq. (16) as

$$\begin{aligned} g_{n_1+1,n_2+1} &= g_{n_1,n_2} + N^2\Delta_2 f_{n,n} + \tfrac{1}{2}N^2(N^2-1)\Delta_2^2 f_{n,n} + N\Delta_1\left[f_{n,n} + N^2\Delta_2 f_{n,n} + \tfrac{1}{2}N^2(N^2-1)\Delta_2^2 f_{n,n}\right] \\ &\quad + \tfrac{1}{2}N(N-1)\Delta_1^2\left[f_{n,n} + N^2\Delta_2 f_{n,n} + \tfrac{1}{2}N^2(N^2-1)\Delta_2^2 f_{n,n}\right] \\ &= g_{n_1,n_2} + N^2\Delta_2 f_{n,n} + \tfrac{1}{2}N^2(N^2-1)\Delta_2^2 f_{n,n} + N\Delta_1 f_{n,n} + N^3\Delta_1\Delta_2 f_{n,n} + \tfrac{1}{2}N^3(N^2-1)\Delta_1\Delta_2^2 f_{n,n} \\ &\quad + \tfrac{1}{2}N(N-1)\Delta_1^2 f_{n,n} + N^3(N-1)\Delta_1^2\Delta_2 f_{n,n} + \tfrac{1}{4}N^3(N^2-1)(N-1)\Delta_1^2\Delta_2^2 f_{n,n}. \end{aligned} \tag{17}$$

As, using the second remark, the second difference of $f_{n,n}$ depends just on its nearest neighboring points, the right-hand side of Eq. (17) depends, apart from $f_{n,n} = g_{n_1,n_2}$, on $f_{n,n+1}$, $f_{n,n-1}$, $f_{n+1,n}$, $f_{n-1,n}$, $f_{n+1,n+1}$, $f_{n+1,n-1}$, $f_{n-1,n+1}$, and $f_{n-1,n-1}$, i.e., eight unknowns. Starting from Eqs. (14), (15), and (17) we can write down eight equations, using the first remark, which defines g_{n_1+1,n_2}, g_{n_1-1,n_2}, g_{n_1,n_2+1}, g_{n_1,n_2-1}, g_{n_1+1,n_2+1}, g_{n_1+1,n_2-1}, g_{n_1-1,n_2+1}, and g_{n_1-1,n_2-1} in terms of the functions $f_{n+i,n+j}$ with $(i,j) = 0, \pm 1$. Inverting this system of equations we get $f_{n\pm1}$ in term of g_{n_1,n_2} and its shifted values:

$$\begin{aligned} f_{n\pm1} &= g_{n_1,n_2} \pm \frac{1}{2N}(g_{n_1+1,n_2} - g_{n_1-1,n_2}) + \frac{1}{2N^2}(g_{n_1+1,n_2} - 2g_{n_1,n_2} + g_{n_1-1,n_2}) \pm \frac{1}{2N^2}(g_{n_1,n_1+1} - g_{n_1,n_2-1}) \\ &\quad + \frac{1}{4N^3}(g_{n_1+1,n_2+1} - g_{n_1-1,n_2+1} - g_{n_1+1,n_2-1} + g_{n_1-1,n_2-1}) + O(N^{-4}). \end{aligned} \tag{18}$$

It is worthwhile to notice that the two lowest order (in N^{-1}) terms of the expansion (18) are just the sum of the first symmetric differences of g_{n_1} and g_{n_2}. Thus in the continuous limit, when we divide by h and send h to zero in such a way that $x = hn$, $x_1 = hn_1$, and $x_2 = hn_2$ be finite, we will have

$$f_{,x} = \epsilon g_{x_1} + \epsilon^2 g_{x_2}.$$

Extra terms appear at the order N^{-3} and contain shifts in both n_1 and n_2.

When f_n is a slow varying function of order 2 in n_1 it can also be of order 1 in n_2. In such a case Eq. (15) is given by

$$g_{n_1,n_2+1} = g_{n_1,n_2} + N\Delta_2 f_{n,n}. \tag{19}$$

Starting from Eqs. (14) and (19) and a modified (17) we can get a set of eight equations which allows us to get $f_{n\pm1}$ in terms of g_{n_1,n_2} and its shifted values. In such a case $f_{n\pm1}$ reads

$$\begin{aligned} f_{n\pm1} &= g_{n_1,n_2} \pm \frac{1}{2N}(g_{n_1+1,n_2} - g_{n_1-1,n_2}) + \frac{1}{N^2}(g_{n_1,n_2\pm1} - g_{n_1,n_2}) + \frac{1}{2N^2}(g_{n_1+1,n_2} - 2g_{n_1,n_2} + g_{n_1-1,n_2}) \\ &\quad + O(N^{-3}). \end{aligned} \tag{20}$$

It is possible to introduce two parameters in the definition of n_1, n_2 in terms of n. Let us define

$$n_1 = \frac{nM_1}{N}, \quad n_2 = \frac{nM_2}{N^2},$$

where M_1 and M_2 are divisors of N and N^2 so that n_1 and n_2 are integers numbers. In such a case, Eq. (18) reads

$$f_{n\pm1} = g_{n_1,n_2} \pm \frac{M_1}{2N}(g_{n_1+1,n_2} - g_{n_1-1,n_2}) + \frac{M_1^2}{2N^2}(g_{n_1+1,n_2} - 2g_{n_1,n_2} + g_{n_1-1,n_2}) \pm \frac{M_2}{2N^2}(g_{n_1,n_2+1} - g_{n_1,n_2-1})$$
$$+ \frac{M_1M_2}{4N^3}(g_{n_1+1,n_2+1} - g_{n_1-1,n_2+1} - g_{n_1+1,n_2-1} + g_{n_1-1,n_2-1}) + O(N^{-4}) \tag{21}$$

and Eq. (20) accordingly.

When we consider partial difference equations we have more than one independent variable. Let us consider the case of two independent lattices and a function $f_{n,m}$ defined on them. As the two lattices are independent the formulas presented above apply independently on each of the lattice variables. So, for instance, the variation $f_{n+1,m}$ when the function $f_{n,m}$ is a slowly varying function of order 2 of a lattice variable n_1 reads

$$f_{n+1,m} = g_{n_1,m} + \frac{1}{2N}(g_{n_1+1,m} - g_{n_1-1,m}) + \frac{1}{2N^2}(g_{n_1+1,m} - 2g_{n_1,m} + g_{n_1-1,m}) + O(N^{-3}). \tag{22}$$

A slightly less obvious situation appears when we consider $f_{n+1,m+1}$, as new terms will appear. We consider here just the case we will need later when

$$n_1 = \frac{M_1 n}{N}, \quad m_1 = \frac{M_2 m}{N}, \quad m_2 = \frac{n}{N^2}. \tag{23}$$

If $f_{n,m}$ is a slow varying function of first order in m_2 and of second order in both n_1 and m_1, from Eqs. (21) and (22) the variation $f_{n+1,m+1}$ reads

$$f_{n+1,m+1} = g_{n_1,m_1,m_2} + \frac{M_1}{2N}(g_{n_1+1,m_1,m_2} - g_{n_1-1,m_1,m_2}) + \frac{M_2}{2N}(g_{n_1,m_1+1,m_2} - g_{n_1,m_1-1,m_2}) + \frac{M_1^2}{2N^2}(g_{n_1+1,m_1,m_2}$$
$$+ g_{n_1-1,m_1,m_2} - 2g_{n_1,m_1,m_2}) + \frac{M_2^2}{2N^2}(g_{n_1,m_1+1,m_2} + g_{n_1,m_1-1,m_2} - 2g_{n_1,m_1,m_2})$$
$$+ \frac{M_1M_2}{4N^2}(g_{n_1+1,m_1+1,m_2} + g_{n_1-1,m_1-1,m_2} - g_{n_1+1,m_1-1,m_2} - g_{n_1-1,m_1+1,m_2}) + \frac{1}{N^2}(g_{n_1,m_1,m_2+1}$$
$$- g_{n_1,m_1,m_2}) + O(N^{-3}).$$

III. MULTISCALE REDUCTION OF NONLINEAR PARTIAL DIFFERENCE EQUATIONS

In the following we will apply the formulas obtained in Sec. II to some well-known partial difference equations. Some of those are known to have a Lax pair and are associated to integrable partial differential equations. Others are concocted so as to have a real dispersion relation but with no particular reason why they should be integrable. The integrable equations we will consider here, the lattice modified KdV (mKdV), presented in Sec. III A, the Hietarinta equation, presented in Sec. III B and the lattice Volterra-Kac-Van Moerbeke (VKVM) equation, presented in Sec. III C, are defined on four lattice points and are PΔEs *consistent around a cube*.[5] From this property one can derive their Lax equation.

The lattice mKdV is an integrable equation of the same class of the lattice potential KdV and KdV (Ref. 3) and it possesses a Lax pair.[10] As from KdV we get by multiscale reduction the NLS,[14] the same we may expect here. To get an integrable discrete equation we expect a resulting

discrete equation which is somehow symmetric. At least when $h_t \to 0$ with $t=mh_t$ the differential difference equation we obtain must be symmetric in terms of the inversion of n_j, i.e., if it contains n_{j+k} it will contain also n_{j-k}.

The nonintegrable KdV equation presented in Sec. III D is obtained by a straightforward discretization using the symmetric representation of the derivatives so as to get a real dispersion relation.

In all the cases considered we will expand the solution of the nonlinear lattice equation around a wave solution of the linear part. In doing so we require that the wave solution be always bounded so that a perturbative expansion with slowly variable coefficients is meaningful. This can be always achieved if the dispersion relation is real. This is always true if the equation can be rewritten in terms of symmetric derivatives. Moreover to get a meaningful reduction we need to have a nontrivial nonlinear dispersion relation.

A. Reduction of the lattice mKdV

The discrete analogue of the modified Korteweg-de Vries (mKdV) equation is given by the following nonlinear PΔE:[10]

$$p(u_{n,m}u_{n,m+1} - u_{n+1,m}u_{n+1,m+1}) - q(u_{n,m}u_{n+1,m} - u_{n,m+1}u_{n+1,m+1}) = 0. \tag{24}$$

This equation involves just four points which lay on two orthogonal infinite lattices and are the vertices of an elementary square. In Eq. (24) $u_{n,m}$ is the dynamical field (real) variable at site $(m,n) \in \mathbb{Z}\times\mathbb{Z}$ and $p,q \in \mathbb{R}$ are the lattice parameters. These are assumed different from zero and will go to zero in the continuous limit so as to get the continuous mKdV.

Carrying out the change of variable $u_{n,m} \mapsto 1+u_{n,m}$, one can separate the linear and nonlinear parts of Eq. (24),

$$\begin{aligned} &p(u_{n,m} + u_{n,m+1} - u_{n+1,m} - u_{n+1,m+1}) - q(u_{n,m} + u_{n+1,m} - u_{n,m+1} - u_{n+1,m+1}) \\ &\quad = q(u_{n,m}u_{n+1,m} - u_{n,m+1}u_{n+1,m+1}) - p(u_{n,m}u_{n,m+1} - u_{n+1,m}u_{n+1,m+1}). \end{aligned} \tag{25}$$

Let us consider the linear part of Eq. (25), namely

$$p(u_{n,m} + u_{n,m+1} - u_{n+1,m} - u_{n+1,m+1}) - q(u_{n,m} + u_{n+1,m} - u_{n,m+1} - u_{n+1,m+1}) = 0. \tag{26}$$

Given any initial condition $u_{n,0}$ the general solution of Eq. (26) is given by

$$u_{n,m} = \frac{1}{2\pi i}\sum_{j=-\infty}^{\infty} u_{j,0} \oint_{|z|=1} \left[\frac{(p-q)-(p+q)z}{(p-q)z-(p+q)}\right]^m z^{n-j-1}\,\mathrm{d}z. \tag{27}$$

Equation (27) can be rewritten in a more natural way (from the continuous point of view) by defining

$$z \doteq e^{ik}, \quad \Omega \doteq e^{-i\omega} = \frac{(p-q)-(p+q)z}{(p-q)z-(p+q)}. \tag{28}$$

In such a case the solution (27) is written as a superposition of linear waves

$$E_{n,m} = e^{i[kn-\omega(k)m]} = z^n\Omega^m. \tag{29}$$

The dispersion relation for these linear waves is given by

$$\omega = -2\arctan\left[\frac{p}{q}\tan\left(\frac{k}{2}\right)\right], \tag{30}$$

the same as for the lattice potential KdV (pKdV) equation.[8] From Eqs. (28) and (30), by differentiation with respect to k, we get the group velocity $\omega_{,k}$,

$$\omega_{,k} = \frac{4pqz}{[(p-q)z-(p+q)][(p+q)z-(p-q)]} = \frac{2pq}{p^2+q^2-(p^2-q^2)\cos k}. \tag{31}$$

The linear part of the PΔE (25), i.e., Eq. (26), is solved in terms of harmonics (29) if ω is given by (30). The nonlinearity will couple the harmonics. This suggests to look for solutions of the PΔE (25) written as a combination of modulated waves,

$$u_{n,m} = \sum_{s=0}^{\infty} \epsilon^{\beta_s} \psi_{n,m}^{(s)} (E_{n,m})^s + \sum_{s=1}^{\infty} \epsilon^{\beta_s} \bar{\psi}_{n,m}^{(s)} (\bar{E}_{n,m})^s, \tag{32}$$

where the functions $\psi_{n,m}^{(s)}$ are slowly varying functions on the lattice, i.e., $\psi_{n,m}^{(s)} = \psi_{n_1,m_1,m_2}^{(s)}$ and $\epsilon^{\gamma} = N^{-1}$. By $\bar{b}$ we mean the complex conjugate of a complex quantity b so that, for example, $\bar{E}_{n,m} = (E_{n,m})^{-1}$. The positive numbers β_s are to be determined in such a way that

(1) $\beta_1 \leqslant \beta_s \ \forall s = 0, 2, 3, \ldots, \infty$. In general it is possible to set $\beta_1 = 1$.
(2) In the equation for $\psi_{n,m}^{(1)} = \psi_{n,m}$, we require that the lowest order nonlinear terms should match the slow time derivative of the linear part after having solved all linear equations. This will provide a relation between γ and the β_s.

The fact that the second summation in Eq. (32) starts from $s=1$ and contains the complex conjugates of the terms of the first summation is due to the reality condition for the solutions of the PΔE (24).

After introducing the expansion (32) in the PΔE (25) and analyzing the coefficients of the various harmonics $(E_{n,m})^s$ for $s=1$, $s=2$, and $s=0$ (as, assuming that β_s increases with s, the nonlinear terms will depend only on the lowest s terms) we came to the conclusion that we can choose

$$\gamma = 1, \quad \beta_0 = 2, \quad \beta_s = s, \quad s \geqslant 1. \tag{33}$$

The discrete slow varying variables n_1, m_1, and m_2 are defined in terms of n and m by Eq. (23).

Having fixed the constants β_s according to Eq. (33) we can introduce the ansatz (32) into Eq. (25) and get the determining equations.

For $s=1$ we get, at lowest order in ϵ,

$$\psi_{n_1,m_1,m_2}[(q-p)(1-z\Omega)-(p+q)(\Omega-z)] = 0,$$

which is identically solved by the dispersion relation (28).

At ϵ^2 we get the linear equation

$$M_1 z[(p-q)\Omega+(p+q)](\psi_{n_1+1,m_1,m_2} - \psi_{n_1-1,m_1,m_2}) + M_2\Omega[(p-q)z-(p+q)](\psi_{n_1,m_1+1,m_2} - \psi_{n_1,m_1-1,m_2}) = 0, \tag{34}$$

whose solution is given by

$$\psi_{n_1,m_1,m_2} = \phi_{n_2,m_2}, \quad n_2 = n_1 - m_1.$$

provided that the integers M_1 and M_2 are chosen as

$$M_1 = S\Omega[(p-q)z-(p+q)], \quad M_2 = Sz[(p-q)\Omega+(p+q)], \tag{35}$$

where $S \in \mathbb{C}$ is a constant; S cannot be completely arbitrary since M_1 and M_2 are to be integer numbers. We will show in Appendix A how it is possible to choose the complex constant S in such a way that M_1 and M_2 are in fact integer numbers as required by Eq. (23). Substituting the expression of Ω given in (28) into Eq. (35), we can rewrite M_1 and M_2 as

$$M_1 = -S[(p+q)z-(p-q)], \quad M_2 = \frac{4pqSz}{[(p+q)-z(p-q)]}. \tag{36}$$

From Eqs. (31) and (36) we get

$$\omega_{,k} = \frac{M_2}{M_1}, \tag{37}$$

i.e., the ratio M_2/M_1 is the group velocity. As M_1 and M_2 are integers, it follows that not all values of k are admissible as $\omega_{,k} \in \mathbb{Q}$. Let us notice that also $n_2 = n_1 + m_1$ solves Eq. (34) by an appropriate choice of M_1 and M_2.

At ϵ^3 we get a nonlinear equation for ϕ_{n_2,m_2} which depends on $\psi^{(2)}_{n_2,m_2}$,

$$\phi_{n_2,m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+2,m_2} + \phi_{n_2-2,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + c_3\psi^{(2)}_{n_2,m_2}\bar{\phi}_{n_2,m_2} = 0, \tag{38}$$

where

$$c_1 = pq(p-q)S^2z^2\frac{(p-q)-(p+q)z}{[(p-q)z-(p+q)]^2},$$

$$c_2 = 2pq(p-q)S^2z\frac{(p+q)(1+z^2)-2(p-q)z}{[(p-q)z-(p+q)]^2},$$

$$c_3 = \frac{2pq(p^2-q^2)(1-z^2)^3}{z[(p-q)z-(p+q)]^2[(p+q)z-(p-q)]^2}. \tag{39}$$

Using the form of the complex constant S obtained in Appendix A, the coefficients (39) read

$$c_1 = -\frac{M_2^2(p-q)}{16pq}[(p+q)(\cos k + i\sin k)-(p-q)],$$

$$c_2 = \frac{M_2^2(p-q)}{4pq}[(p+q)\cos k-(p-q)],$$

$$c_3 = i\frac{2pq(p^2-q^2)\sin^3 k}{[(p^2+q^2)-(p^2-q^2)\cos k]^2}. \tag{40}$$

The coefficients (40) depend on the integer constant M_2. The integer M_1 is then written out in terms of M_2 and reads

$$M_1 = M_2\frac{p^2+q^2-(p^2-q^2)\cos k}{2pq},$$

so that not all values of k are admissible as M_1 must be also an integer. See Appendix A for details.

The lowest order equations for the harmonic $s=2$ appear at ϵ^2 and give

$$\psi^{(2)}_{n_2,m_2} = \tfrac{1}{2}(\phi_{n_2,m_2})^2.$$

It is easy to see that the choice (33) implies that the coefficients of all other harmonics are expressed in terms of ϕ_{n_2,m_2} and $\bar{\phi}_{n_2,m_2}$.

Taking these results into account the nonlinear equation PΔE (38) for ϕ_{n_2,m_2} reads

$$i(\phi_{n_2,m_2+1}-\phi_{n_2,m_2})=C_1(\phi_{n_2+2,m_2}+\phi_{n_2-2,m_2}-2\phi_{n_2,m_2})+C_2(\phi_{n_2+1,m_2}+\phi_{n_2-1,m_2}-2\phi_{n_2,m_2})+C_3\phi_{n_2,m_2}|\phi_{n_2,m_2}|^2, \tag{41}$$

where $C_i=-ic_i$, $i=1,2$, $C_3=-ic_3/2$, and the coefficients c_i's are given by Eq. (40). It is easy to see that C_3 is a real coefficient.

The PΔE (41) is a *completely discrete and local* NLS equation depending on the first and second neighboring lattice points. At difference from the Ablowitz and Ladik[1] discrete NLS, the nonlinear term in (41) is completely local. The PΔE (41) has a natural semicontinuous limit when $m_2\to\infty$ as $H_2\to 0$ in such a way that $t_2=m_2\,H_2\in\mathbb{R}$ is finite. Setting $n_2\doteq n$ and $t_2\doteq t$ one gets the following nonlinear differential-difference equation:

$$i\frac{\partial\phi_n}{\partial t}=C_1(\phi_{n+2}+\phi_{n-2}-2\phi_n)+C_2(\phi_{n+1}+\phi_{n-1}-2\phi_n)+C_3\phi_n|\phi_n|^2. \tag{42}$$

The continuous limit of the PΔE (41) is obtained if we consider in Eq. (42) the limit $n\to\infty$ as $H_1\to 0$ in such a way that $x=nH_1\in\mathbb{R}$ is finite. The resulting NLS equation reads

$$i\phi_{,t}=(4C_1+C_2)\phi_{,xx}+C_3\phi|\phi|^2, \tag{43}$$

where

$$4C_1+C_2=-\frac{M_2^2(p^2-q^2)\sin k}{4pq}. \tag{44}$$

As the coefficient (44) is real, Eq. (43) is just the well-known integrable NLS equation.

B. Reduction of the Hietarinta equation

In Ref. 5 Hietarinta introduces a new *consistent around a cube* PΔE,

$$\frac{u_{n,m}+e_2}{u_{n,m}+e_1}\frac{u_{n+1,m+1}+o_2}{u_{n+1,m+1}+o_1}-\frac{u_{n+1,m}+e_2}{u_{n+1,m}+o_1}\frac{u_{n,m+1}+o_2}{u_{n,m+1}+e_1}=0, \tag{45}$$

where the four constants $e_i,o_i\in\mathbb{R}$, $1\leqslant i\leqslant 2$, are lattice parameters.

By a direct calculation one can separate the linear and the nonlinear parts of Eq. (45),

$$\begin{aligned}&o_1o_2(e_1-e_2)u_{n,m}+e_1e_2(o_1-o_2)u_{n+1,m+1}+e_1o_2(e_2-o_1)u_{n+1,m}+e_2o_1(o_2-e_1)u_{n,m+1}\\&=[(o_2-e_1)u_{n+1,m}+(e_2-o_1)u_{n,m+1}]u_{n,m}u_{n+1,m+1}+[(o_1-o_2)u_{n,m}+(e_1-e_2)u_{n+1,m+1}]u_{n+1,m}u_{n,m+1}\\&\quad+[o_1(e_2-o_2)u_{n,m+1}+o_2(o_1-e_1)u_{n+1,m}]u_{n,m}+[e_2(e_1-o_1)u_{n,m+1}+e_1(o_2-e_2)u_{n+1,m}]u_{n+1,m+1}\\&\quad+(o_2e_2-o_1e_1)(u_{n,m}u_{n+1,m+1}-u_{n+1,m}u_{n,m+1}).\end{aligned} \tag{46}$$

Let us now solve the linear part of the PΔE (46),

$$o_1o_2(e_1-e_2)u_{n,m}+e_1e_2(o_1-o_2)u_{n+1,m+1}+e_1o_1(e_2-o_2)u_{n+1,m}+e_2o_2(o_1-e_1)u_{n,m+1}=0. \tag{47}$$

Defining

$$z\doteq e^{ik},\quad \Omega\doteq e^{-i\omega}=\frac{o_2[e_1(e_2-o_1)z+o_1(e_1-e_2)]}{e_2[e_1(o_2-o_1)z+o_1(e_1-o_2)]},$$

the (complex) dispersion relation for these linear waves is given by

$$\omega = 2 \arctan\left\{ \frac{ie_1o_1(o_2 - e_2)\tan(k/2)}{[o_1o_2(e_1 - e_2) + e_1e_2(o_1 - o_2)]\tan(k/2) + ie_2o_2(e_1 - o_1)} \right\}.$$

The dispersion relation is a real function of k if the following condition holds:

$$o_1o_2(e_1 - e_2) + e_1e_2(o_1 - o_2) = 0. \tag{48}$$

To give a meaning to the expansion (32) we must require that the dispersion relation $\omega(k)$ be a real function for k real. From Eq. (48) we can write o_2 in terms of o_1, e_1, e_2, and get

$$\Omega \doteq e^{-i\omega} = \frac{e_1(e_2 - o_1)z + o_1(e_1 - e_2)}{o_1(e_1 - e_2)z + e_1(e_2 - o_1)}, \tag{49}$$

so that the real dispersion relation reads

$$\omega = 2 \arctan\left[\frac{e_2(e_1 + o_1) - 2e_1o_1}{e_2(o_1 - e_1)} \tan\left(\frac{k}{2}\right) \right]. \tag{50}$$

From Eq. (49), by differentiation with respect to k, we get the real group velocity $\omega_{,k}$,

$$\omega_{,k} = \frac{e_2(o_1 - e_1)[2e_1o_1 - e_2(e_1 + o_1)]z}{[e_1(o_1 - e_2)z + o_1(e_2 - e_1)][o_1(e_1 - e_2)z + e_1(e_2 - o_1)]}. \tag{51}$$

The PΔE (47) has a bounded wave solution given by Eq. (29), where Ω is given by Eq. (49). So we can look for solutions of the PΔE (46) in the form of a combination of modulated waves (32), where the functions $\psi^{(s)}_{n,m}$ are slowly varying functions on the lattice, i.e., $\psi^{(s)}_{n,m} = \psi^{(s)}_{n_1,m_1,m_2}$ and $\epsilon^\gamma = N^{-1}$.

Introducing the expansion (32) in the Hietarinta equation (46) and considering the equations for $s=1$, $s=2$, and $s=0$ harmonics we deduce that the choice (33) is still valid. Moreover, the discrete slow varying variables n_1, m_1 and m_2 are defined in terms of n and m by Eq. (23).

Having fixed the constants β_s we can now introduce the ansatz (32) into Eq. (46) and pick out the coefficients of the various harmonics $(E_{n,m})^s$ to get the determining equations.

For $s=1$, having defined $\psi^{(1)}_{n,m} \doteq \psi_{n,m}$, we obtain an equation at the first order in ϵ which is identically solved by the dispersion relation (50).

At ϵ^2 we get the linear equation

$$M_1 z[o_1(e_1 - e_2)\Omega + e_1(o_1 - e_2)](\psi_{n_1+1,m_1,m_2} - \psi_{n_1-1,m_1,m_2}) + M_2\Omega[o_1(e_1 - e_2)z - e_1(o_1 - e_2)] \times (\psi_{n_1,m_1+1,m_2} - \psi_{n_1,m_1-1,m_2}) = 0,$$

whose solution is given by

$$\psi_{n_1,m_1,m_2} = \phi_{n_2,m_2}, \quad n_2 = n_1 - m_1$$

provided that the integers M_1 and M_2 are chosen as

$$M_1 = S\Omega[o_1(e_1 - e_2)z - e_1(o_1 - e_2)], \quad M_2 = Sz[o_1(e_1 - e_2)\Omega + e_1(o_1 - e_2)], \tag{52}$$

where $S \in \mathbb{C}$ is a constant. Inserting Ω given by Eq. (49) in Eq. (52) we can show that the ratio M_2/M_1 coincides with the group velocity (51).

At ϵ^3 we get a nonlinear equation for ϕ_{n_2,m_2} which depends on $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$. It reads

$$\phi_{n_2,m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+2,m_2} + \phi_{n_2-2,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + c_3\phi_{n_2,m_2}|\phi_{n_2,m_2}|^2 + c_4\psi^{(0)}_{n_2,m_2}\phi_{n_2,m_2} + c_5\psi^{(2)}_{n_2,m_2}\bar{\phi}_{n_2,m_2} = 0, \tag{53}$$

where the coefficients c_i, $1 \leqslant i \leqslant 5$, depend on z, S and the lattice parameters e_1, e_2, o_1 and are given in Appendix B as their expressions are rather complicated.

The functions $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ that appear in Eq. (53) are obtained by considering the equations for the harmonics $s=0$, at the third order in ϵ, and $s=2$ at the second one. From them we get

$$\psi^{(2)}_{n_2,m_2} = p_1(\phi_{n_2,m_2})^2, \tag{54}$$

$$\psi^{(0)}_{n_2+1,m_2} - \psi^{(0)}_{n_2-1,m_2} = p_2[\bar{\phi}_{n_2,m_2}(\phi_{n_2+1,m_2} - \phi_{n_2-1,m_2}) + \phi_{n_2,m_2}(\bar{\phi}_{n_2+1,m_2} - \bar{\phi}_{n_2-1,m_2})], \tag{55}$$

with

$$p_1 = \frac{e_1 z - o_1}{e_1 o_1 (z-1)}, \quad p_2 = \frac{e_1 + o_1}{e_1 o_1}.$$

From Eqs. (54) and (55) we evince that both $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ are expressed in term of ϕ_{n_2,m_2}. In particular, we notice that $\psi^{(2)}_{n_2,m_2}$ depends from ϕ_{n_2,m_2} in a local way while $\psi^{(0)}_{n_2,m_2}$ depends from ϕ_{n_2,m_2} in a nonlocal way through a summation, namely

$$\psi^{(0)}_{n_2,m_2} = (-1)^{n_2}\left[w_1 + p_2 \sum_{j=n_2}^{\infty} (-1)^j (\bar{\phi}_{j,m_2}\phi_{j+1,m_2} + \phi_{j,m_2}\bar{\phi}_{j+1,m_2}) \right] + w_2, \tag{56}$$

where w_1, w_2 are two arbitrary summation constants.

Inserting $\psi^{(2)}_{n_2,m_2}$ given by Eq. (54) in Eq. (53) we get

$$\phi_{n_2 m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+2,m_2} + \phi_{n_2-2,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + \hat{c}_3\phi_{n_2,m_2}|\phi_{n_2,m_2}|^2 + c_4\psi^{(0)}_{n_2,m_2}\phi_{n_2,m_2} = 0, \tag{57}$$

where, using the form of the complex constant S, see Appendix A, and the fact that $z \doteq e^{ik}$, the coefficients are

$$c_1 = \frac{P_2[P_1(\cos k + i \sin k) + P_2]}{4(P_2^2 - P_1^2)} M_2^2,$$

$$c_2 = \frac{P_2(P_1 \cos k + P_2)}{P_2^2 - P_1^2} M_2^2,$$

$$\hat{c}_3 = \frac{2(P_1 - P_2)[P_1(e_1 - e_2) + P_2(e_2 - o_1)](\cos k - 1)}{e_2(o_1 e_2 + P_2)(P_1^2 + P_2^2 + 2P_1 P_2 \cos k)},$$

$$c_4 = -\frac{2(P_1 - P_2)(P_1 - e_2^2 + o_1 e_2)(\cos k - 1)}{e_2(P_1^2 + P_2^2 + 2P_1 P_2 \cos k)},$$

with

$$P_1 = e_1(e_2 - o_1), \quad P_2 = o_1(e_1 - e_2).$$

Here M_2 is an arbitrary integer number, while M_1 is given by (see Appendix A)

$$M_1 = M_2 \frac{P_1^2 + P_2^2 + 2P_1P_2 \cos k}{P_2^2 - P_1^2}.$$

C. Reduction of the lattice VKVM equation

The completely discrete version of the Volterra-Kac-Van Moerbeke (VKVM) equation is given by the following PΔE:[10]

$$\frac{u_{n,m+1}}{u_{n+1,m}} = \frac{\alpha u_{n,m} - 1}{\alpha u_{n+1,m+1} - 1}. \tag{58}$$

Here α is a real lattice parameter and $u_{n,m}$ is a real field.

The dispersion relation of the linear part of Eq. (58) is trivial. So, we carry out the change of variable $u_{n,m} \mapsto 1 + u_{n,m}$. Then one can split Eq. (58) into the linear and nonlinear parts:

$$\alpha(u_{n+1,m+1} - u_{n,m}) + (1-\alpha)(u_{n+1,m} - u_{n,m+1}) = \alpha(u_{n,m}u_{n+1,m} - u_{n+1,m+1}u_{n,m+1}). \tag{59}$$

The dispersion relation for the linear waves is given by

$$\Omega = \frac{\alpha(z+1) - z}{\alpha(z+1) - 1}, \quad \omega = \arctan\left[\frac{(2\alpha - 1)\sin k}{(2\alpha^2 - 2\alpha + 1)\cos k + 2\alpha(\alpha - 1)}\right]. \tag{60}$$

From Eq. (60), by differentiation with respect to k, we get the group velocity $\omega_{,k}$,

$$\omega_{,k} = \frac{(2\alpha - 1)z}{[\alpha(z+1) - z][\alpha(z+1) - 1]} = \frac{(2\alpha - 1)}{2\alpha(\alpha - 1)(\cos k + 1) + 1}. \tag{61}$$

We now consider a solution of the PΔE (59) in the form of a combination of modulated waves, see Eq. (32), where $E_{n,m}$ is given by Eq. (29) with Ω as in Eq. (60). As in the previous cases the functions $\psi^{(s)}_{n,m}$ are to be slowly varying functions on the lattice, i.e., $\psi^{(s)}_{n,m} = \psi^{(s)}_{n_1,m_1,m_2}$ and $\epsilon^\gamma = N^{-1}$.

Introducing the expansion (32) in the lattice VKVM equation (59) and considering the equations for $s=1$, $s=2$, and $s=0$ we deduce that the choice (33) is still valid. The discrete slow varying variables n_1, m_1 and m_2 are defined in terms of n and m by the positions (23), where $M_1, M_2 \in \mathbb{Z}$.

For $s=1$ we obtain an equation at the first order in ϵ which is identically solved by the dispersion relation (60).

At ϵ^2 we get a linear equation

$$M_1 z[\alpha(\Omega - 1) + 1](\psi_{n_1+1,m_1,m_2} - \psi_{n_1-1,m_1,m_2}) + M_2 \Omega[\alpha(z+1) - 1](\psi_{n_1,m_1+1,m_2} - \psi_{n_1,m_1-1,m_2}) = 0,$$

whose solution is given by

$$\psi_{n_1,m_1,m_2} = \phi_{n_2,m_2}, \quad n_2 = n_1 - m_1$$

provided that the integers M_1 and M_2 are chosen as

$$M_1 = S\Omega[\alpha(z+1) - 1], \quad M_2 = Sz[\alpha(\Omega - 1) + 1], \tag{62}$$

where $S \in \mathbb{C}$ is a constant. Inserting Ω given by Eq. (60) in Eq. (62) we get that the ratio M_2/M_1 coincides with the group velocity (61). As shown in Appendix A it is possible to choose the complex constant S in such a way that M_1 and M_2 are in fact integer numbers.

At ϵ^3 we get a nonlinear equation for ϕ_{n_2,m_2} which depends on $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$. It reads

$$\phi_{n_2,m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+2,m_2} + \phi_{n_2-2,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + c_3\psi^{(0)}_{n_2,m_2}\phi_{n_2,m_2} + c_4\psi^{(2)}_{n_2,m_2}\bar{\phi}_{n_2,m_2} = 0, \tag{63}$$

where the coefficients c_i, $1 \leqslant i \leqslant 4$, are

$$c_1 = \alpha S^2 z^2 \frac{(1-2\alpha)[\alpha(z+1)-z]}{4[\alpha(z+1)-1]^2},$$

$$c_2 = \alpha S^2 z \frac{(2\alpha-1)[\alpha(z+1)^2 - z^2 - 1]}{2[\alpha(z+1)-1]^2},$$

$$c_3 = \frac{\alpha(1-z^2)}{[\alpha(z+1)-z][\alpha(z+1)-1]},$$

$$c_4 = \frac{\alpha(1-z^2)(z^2-z+1)}{[\alpha(z+1)-z][\alpha(z+1)-1]z}.$$

The functions $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ that appear in Eq. (63) are obtained by considering the equations for the harmonics $s=0$, at the second order in ϵ, and $s=2$, at the third one. We get the following equations:

$$\psi^{(2)}_{n_2,m_2} = p_1(\phi_{n_2,m_2})^2, \tag{64}$$

$$\psi^{(0)}_{n_2+1,m_2} - \psi^{(0)}_{n_2-1,m_2} = p_2[\bar{\phi}_{n_2,m_2}(\phi_{n_2+1,m_2} - \phi_{n_2-1,m_2}) + \phi_{n_2,m_2}(\bar{\phi}_{n_2+1,m_2} - \bar{\phi}_{n_2-1,m_2})], \tag{65}$$

with

$$p_1 = \frac{(1-2\alpha)z}{\alpha(z+1)^2 - z^2 - 1}, \quad p_2 = \frac{2\alpha(1+z^2) - z^2 - 1}{(1-z^2)(\alpha-1)}.$$

From Eqs. (64) and (65) we evince that both $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ are expressed in term of ϕ_{n_2,m_2}. In particular $\psi^{(0)}_{n_2,m_2}$ admits a nonlocal expansion as in Eq. (56). Inserting $\psi^{(2)}_{n_2,m_2}$ given by Eq. (64) in Eq. (63) we get

$$\phi_{n_2,m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+2,m_2} + \phi_{n_2-2,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + c_3\psi^{(0)}_{n_2,m_2}\phi_{n_2,m_2} + \hat{c}_4\phi_{n_2,m_2}|\phi_{n_2,m_2}|^2 = 0, \tag{66}$$

where $\hat{c}_4 = c_4 p_1$.

Let us write the coefficients that appear in Eq. (66), i.e., $c_1, c_2, c_3, \hat{c}_4$, using the form of the complex constant S, see Appendix A, and the fact that $z \doteq e^{ik}$. We get

$$c_1 = -\alpha \frac{(\alpha-1)(\cos k + i \sin k) + \alpha}{4(2\alpha-1)} M_2^2,$$

$$c_2 = \alpha \frac{(\alpha-1)\cos k + \alpha}{2\alpha-1} M_2^2,$$

$$c_3 = -i \frac{2\alpha \sin k}{2\alpha(\alpha-1)(\cos k + 1) + 1},$$

$$\hat{c}_4 = i\frac{(2\cos k - 1)\sin k}{(\alpha - 1)(\cos k - 1)[2\alpha(\alpha - 1)(\cos k + 1) + 1]}.$$

As in the previous cases we can choose the integer number M_2, while M_1 is given by (see Appendix A)

$$M_1 = M_2\frac{2\alpha(\alpha - 1)(\cos k + 1) + 1}{2\alpha - 1}.$$

D. Reduction of a nonintegrable lattice KdV equation

Let us now consider the following nonintegrable lattice KdV equation:

$$u_{n,m+1} - u_{n,m-1} = \frac{\alpha}{4}(u_{n+3,m} - 3u_{n+1,m} + 3u_{n-1,m} - u_{n-3,m}) + \beta[(u_{n+1,m})^2 - (u_{n-1,m})^2], \tag{67}$$

where $\alpha, \beta \in \mathbb{R}$ are the lattice parameters and $u_{n,m}$ is a real field.

As we did for previous cases we apply the standard discrete Fourier transform procedure introducing $u_{n,m} = z^n\Omega^m$ into the linear part of the lattice equation (67). Here $z \doteq e^{ik}$ and $\Omega \doteq e^{-i\omega}$. We easily get

$$\Omega - \Omega^{-1} = \frac{\alpha}{4}(z - z^{-1})^3. \tag{68}$$

Hence the dispersion relation reads

$$\omega = \arcsin(\alpha \sin^3 k)$$

and the corresponding group velocity is

$$\omega_{,k} = -\frac{3}{4}\frac{\alpha\Omega}{1 + \Omega^2}\frac{(z^4 - 1)(z^2 - 1)}{z^3} = \frac{3\alpha\cos k \sin^2 k}{\sqrt{1 - \alpha^2 \sin^6 k}}. \tag{69}$$

Introducing the expansion (32) into the PΔE (67), where $E_{n,m}$ is given by Eq. (29) and taking into account that

$$f_{n\pm k} = g_{n_1} \pm \frac{k}{2N}(g_{n_1+1} - g_{n_1-1}) + \frac{k^2}{4N^2}(g_{n_1+1} + g_{n_1-1} - 2g_{n_1}) + O(N^{-3}),$$

we get the standard choice (33).

Let us consider now the equations for the harmonics $s = 1$. The equation at the order ϵ is identically satisfied by taking into account the dispersion relation (68). The equation at the order ϵ^2 is satisfied if we introduce the index $n_2 = n_1 - m_1$ when M_1 and M_2 are chosen as

$$M_1 = S\left(\Omega + \frac{1}{\Omega}\right), \quad M_2 = -\frac{3}{4}S\alpha\frac{(z^4 - 1)(z^2 - 1)}{z^3}. \tag{70}$$

We notice that the group velocity $\omega_{,k}$ (69) coincides again with the ratio M_2/M_1, as in Eq. (37). From Eq. (70), using the fact that $z \doteq e^{ik}$ and $\Omega \doteq e^{-i\omega}$, we obtain

$$M_1 = -2S\cos\omega, \quad M_2 = -6S\alpha\cos k \sin^2 k.$$

We can now fix the (real) constant S in such a way that M_1 is an integer number; M_2 will be an integer if the group velocity is a rational number. Hence not all values of k are admissible, but only those which make $\omega_{,k}$ (69) rational.

The equation at the order ϵ^3 is given by

$$\phi_{n_2 m_2+1} - \phi_{n_2,m_2} + c_1(\phi_{n_2+1,m_2} + \phi_{n_2-1,m_2} - 2\phi_{n_2,m_2}) + c_2(\phi_{n_2,m_2}\phi^{(0)}_{n_2,m_2} + \bar{\phi}_{n_2,m_2}\phi^{(2)}_{n_2,m_2}) = 0, \tag{71}$$

where $\phi_{n_2,m_2} = \psi_{n_1,m_1,m_2}$, $n_2 = n_1 - m_1$, and c_1, c_2 are known, easy to compute but too complicated to write down, complex coefficients depending on z and on the lattice parameter α. The functions $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ that appear in Eq. (71) are obtained by considering the equations for the harmonics $s=0$, at the third order in ϵ, and $s=2$, at the second one. We get the following equations:

$$\psi^{(2)}_{n_2,m_2} = p_1(\phi_{n_2,m_2})^2, \tag{72}$$

$$\psi^{(0)}_{n_2+1,m_2} - \psi^{(0)}_{n_2-1,m_2} = p_2[\bar{\phi}_{n_2,m_2}(\phi_{n_2+1,m_2} - \phi_{n_2-1,m_2}) + \phi_{n_2,m_2}(\bar{\phi}_{n_2+1,m_2} - \bar{\phi}_{n_2-1,m_2})], \tag{73}$$

where p_1, p_2 are known complex coefficients depending on z and on the lattice parameters. From Eqs. (72) and (73) we evince that both $\psi^{(0)}_{n_2,m_2}$ and $\psi^{(2)}_{n_2,m_2}$ are expressed in term of ϕ_{n_2,m_2}. As in the previous cases $\psi^{(0)}_{n_2,m_2}$ admits a nonlocal expansion as in Eq. (56). Hence the PΔE (71) is a well-defined lattice equation in the field variable ϕ_{n_2,m_2}.

IV. CONCLUSIVE REMARKS

In this paper we have shown that we can construct a well-defined procedure to carry out the reductive perturbation technique on the lattice. In this case, at difference with respect to the differential-difference case, we are able to solve all linear equations and thus can obtain a final nonlinear difference equation. To do so we had to apply some nontrivial but at the end obvious tricks which consist in the introduction of appropriate lattice variables so as to be able to perform the symmetric reduction of the linear discrete wave equation.

Applying the perturbative-reductive technique to some integrable and nonintegrable equations we obtain some new completely discrete NLS equations. As some of these equations (41), (57), and (66) come from the reduction of integrable equations we expect them to be also integrable. However they are very different from the Ablowitz-Ladik discrete-discrete NLS (Ref. 1) as all contains, apart from the nearest neighboring points, also the points $n\pm 2$ and either they are completely local or they have nonlocal completely irregular terms [depending on $(-1)^n$].

So we are at the moment, from one side extending our analysis to other well-known integrable equations, like the discrete time Toda lattice, the sine-Gordon and the Volterra equations and from the other using the integrability properties of the starting nonlinear equations (i.e., Lax pairs or generalized symmetries) to show the integrability of the derived equations. If our equation are integrable than we have presented a very important tool for obtaining new integrable equations and for analyzing the far field behavior of physical problems described by differential-difference or partial difference equations.

In the derivation we introduced the request that the far field expansion of a slow varying function on the lattice should depend on the discrete asymptotic variables in a symmetric way. As a consequence of this ansatz we find that the nonlocal resulting equation depends on $(-1)^n$. This may not be a necessary ansatz and work is in progress in this direction.

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APPENDIX A

From Eqs. (35), (52), and (62) we get that the coefficients M_1 and M_2 can always be written in the following general form:

$$M_1 = S\Omega(Pz - Q), \quad M_2 = Sz(P\Omega + Q), \tag{A1}$$

where $S \in \mathbb{C}$ is a suitable constant such that $M_1, M_2 \in \mathbb{Z}$, $\Omega \doteq e^{-i\omega}$, $z \doteq e^{ik}$ and $P, Q \in \mathbb{R}$ are given by

$$P = p - q, \quad Q = p + q, \quad \text{lattice mKdV equation},$$

$$P = o_1(e_1 - e_2), \quad Q = e_1(o_1 - e_2), \quad \text{Hietarinta equation},$$

$$P = \alpha, \quad Q = 1 - \alpha, \quad \text{lattice VKVM equation}.$$

The (real) dispersion relation for the linear parts of the above lattice equations can be written in the form

$$\Omega = \frac{P - Qz}{Pz - Q}. \tag{A2}$$

Let us now define the complex constant S as $S \doteq \rho e^{i\theta}$, with $\rho \in \mathbb{R}_+$ and $-\pi \leqslant \theta < \pi$. From Eqs. (A1) and (A2) we get

$$\mathrm{Re}(M_1) = \rho[P\cos(\theta) - Q\cos(\theta + k)], \tag{A3}$$

$$\mathrm{Im}(M_1) = \rho[P\sin(\theta) - Q\sin(\theta + k)], \tag{A4}$$

$$\mathrm{Re}(M_2) = \frac{\rho(P^2 - Q^2)}{P^2 + Q^2 - 2PQ\cos k}[P\cos(\theta) - Q\cos(\theta + k)], \tag{A5}$$

$$\mathrm{Im}(M_2) = \frac{\rho(P^2 - Q^2)}{P^2 + Q^2 - 2PQ\cos k}[P\sin(\theta) - Q\sin(\theta + k)]. \tag{A6}$$

Since $M_1, M_2 \in \mathbb{Z}$ we must require that $\mathrm{Im}(M_1) = \mathrm{Im}(M_2) = 0$. From Eqs. (A4) and (A6) we obtain

$$\theta = -\arctan\left(\frac{Q\sin k}{Q\cos k - P}\right) + \ell\pi, \quad \ell \in \mathbb{Z}. \tag{A7}$$

We must now require that $M_1 = \mathrm{Re}(M_1)$, $M_2 = \mathrm{Re}(M_2) \in \mathbb{Z}$. According to Eqs. (A3), (A5), and (A7), we get

$$M_1 = (-1)^\ell \rho(P^2 + Q^2 - 2PQ\cos k)^{1/2}, \tag{A8}$$

$$M_2 = (-1)^\ell \rho \frac{(P^2 - Q^2)}{(P^2 + Q^2 - 2PQ\cos k)^{1/2}}. \tag{A9}$$

We can fix arbitrarily the integer number M_2 (or equivalently M_1) and express M_1 (or M_2) in terms of it,

$$M_1 = M_2 \frac{P^2 + Q^2 - 2PQ\cos k}{P^2 - Q^2}. \tag{A10}$$

From (A10) we can see that not all values of k are admissible since M_1 must be integer.

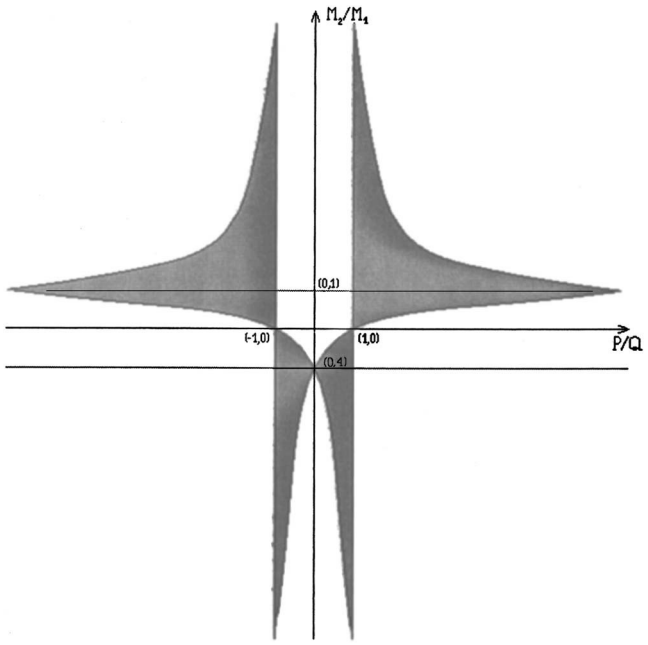

FIG. 1. The grey zones denote the allowed regions for the ratio M_2/M_1 in terms of the ratio P/Q.

Let us finally notice that the fact that Eq. (A10) contains $\cos(k)$ implies that the ratios M_2/M_1 and P/Q are constrained as $-1 \leqslant \cos(k) \leqslant 1$. We have the following cases (see Fig. 1):

$$P/Q \in (1,\infty) \Rightarrow M_2/M_1 \in [(P/Q-1)/(P/Q+1),(P/Q+1)/(P/Q-1)] \in \mathbb{Q},$$

$$P/Q \in (0,1) \Rightarrow M_2/M_1 \in [(P/Q+1)/(P/Q-1),(P/Q-1)/(P/Q+1)] \in \mathbb{Q},$$

$$P/Q \in (-1,0) \Rightarrow M_2/M_1 \in [(P/Q-1)/(P/Q+1),(P/Q+1)/(P/Q-1)] \in \mathbb{Q},$$

$$P/Q \in (-\infty,-1) \Rightarrow M_2/M_1 \in [(P/Q+1)/(P/Q-1),(P/Q-1)/(P/Q+1)] \in \mathbb{Q}.$$

APPENDIX B

The coefficients c_i, $1 \leqslant i \leqslant 5$ that appear in Eq. (53) are

$$c_1 = S^2 z^2 \frac{P_2(P_1^2 - P_2^2)(P_1 z + P_2)}{4(P_1 + P_2 z)^2},$$

$$c_2 = -S^2 z \frac{P_2(P_1^2 - P_2^2)[P_1(1+z^2) + 2P_2 z]}{2(P_1 + P_2 z)^2},$$

$$c_3 = \frac{(z-1)(P_1 - P_2)[Q_1 z^5 + Q_2 z^4 + Q_3 z^3 + Q_4 z^2 + Q_5 z + Q_6]}{e_2(P_1 - e_1 e_2)(P_1 + P_2 z)^2 (P_1 z + P_2)^2 z},$$

$$c_4 = \frac{(z-1)^2(P_1 - P_2)(e_2^2 - e_1 e_2 + P_2)}{e_2(P_2 z + P_1)(P_1 z + P_2)},$$

$$c_5 = \frac{(z-1)^2(P_1 - P_2)[R_1 z^4 + R_2 z^3 + R_3 z + R_4]}{e_2(P_1 + P_2 z)^2(P_1 z + P_2)^2 z},$$

with

$$P_1 = e_1(e_2 - o_1),$$

$$P_2 = o_1(e_1 - e_2),$$

$$Q_1 = P_1 P_2(P_1 e_1 + P_2 e_2),$$

$$Q_2 = P_1^3(e_1 - e_2) + P_2^3(e_2 - o_1) + P_1 P_2(P_2 e_1 + 2P_1 e_2 - P_1 o_1),$$

$$Q_3 = -P_1[P_1^2(e_1 - e_2) + P_2^2(e_1 + 4o_1 - 3e_2) + P_1 P_2(3e_2 - e_1)],$$

$$Q_4 = -P_2[P_1^2(4e_1 - 3e_2 + o_1) + P_2^2(o_1 - e_2) + P_1 P_2(3e_2 - o_1)],$$

$$Q_5 = -P_1^3(e_1 - e_2) - P_2^3(e_2 - o_1) - P_1 P_2(P_2 e_1 - 2P_1 e_2 - P_1 o_1),$$

$$Q_6 = P_1 P_2(P_1 e_2 + P_2 o_1),$$

$$R_1 = P_2[P_1^2 + P_2^2 + P_1 P_2 + P_2(e_2^2 - e_1 e_2)],$$

$$R_2 = P_2^3 + (e_2^2 - e_1 e_2)(P_2^2 - P_1^2) + P_1 P_2(e_2^2 - e_1 e_2 + P_1 + 3P_2),$$

$$R_3 = -P_2^3 - (e_2^2 - e_1 e_2)(P_2^2 - P_1^2) - P_1 P_2(e_2^2 - e_1 e_2 + P_1 + P_2),$$

$$R_4 = P_1(P_1 e_2^2 - P_2^2 - P_1 e_1 e_2).$$

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On the Euler angles for SU(*N*)

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In this paper we reconsider the problem of the Euler parametrization for the unitary groups. After constructing the generic group element in terms of generalized angles, we compute the invariant measure on SU(N) and then we determine the full range of the parameters, using both topological and geometrical methods. In particular, we show that the given parametrization realizes the group SU($N+1$) as a fibration of U(N) over the complex projective space $\mathbb{CP}^n$. This justifies the interpretation of the parameters as generalized Euler angles. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2190898]

I. INTRODUCTION

The importance of group theory in all branches of physics is a well-known fact. Explicit realizations of group representations are often necessary technical tools. Often it is finite dimensional and compact Lie groups and then the knowledge of the associated algebra, which describes the group in a neighborhood of the identity, is enough for this purpose.

There are however cases where an explicit expression of the full global group structure is needed, as, for example, when nonperturbative computations come into play. In most of these cases, the main objectives are two: First, one would like to find a relative simple parametrization, making all the computations manageable. Second, one needs to determine the full range of the parameters, in order to be able to handle global questions.

If both such points can seem unnecessary at an abstract level, they become essential at a most concrete level, e.g., in instantonic calculus or in nonperturbative lattice gauge theory computations. The necessary computer memory for simulations is in fact drastically diminished.

The case of SU(N) was first considered and solved by Tilma and Sudarshan, in Ref. 1. There, they provide a parametrization, in terms of angular parameters, for the unitary groups. In particular, in the first paper they consider special groups, SU(N), together with some applications to qubit and qutrit configurations. In the second paper, they give an extension to U(N) groups, using the fibration structure of SU($N+1$) as U(N) fiber over the complex projective space $\mathbb{CP}^n$.

In this paper we reconsider the problem of finding a generalized Euler parametrization for special unitary groups. The intent is to provide a fully explicit and elementary (which does not mean short) proof of the beautiful results of Ref. 1. Our motivation is that the determination of the range of the parameters is a quite difficult task, so that disagreements are present in the literature

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even for SU(3) (for example, in Ref. 2). Therefore, we think that a careful deduction is necessary in order to corroborate the results of Tilma and Sudarshan. Also, all our proofs based essentially on inductive procedures, and they are explicit, in order to be easily accessible to anyone who needs them.

Our construction is quite different from Ref. 1, and as a result our parametrization differs slightly from theirs. However, this does not affect the final expression of the invariant measure.

To illustrate the spirit of our construction, let us start by taking a look at the Euler parametrization for SU(2).

Starting from the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.1}$$

it is known that the generic element of SU(2) can be written as

$$g = e^{i\phi\sigma_3} e^{i\theta\sigma_2} e^{i\psi\sigma_3}. \tag{1.2}$$

Here $\phi \in [0,\pi]$, $\theta \in [0,\pi/2]$, $\psi \in [0,2\pi]$ are the so-called Euler angles for SU(2). They are related to the well-known Euler angles traditionally used in classical mechanics to describe the motion of a spin. From the point of view of the structure of the representation, (1.2) is obtained starting from a one parameter subgroup $\exp(i\theta\sigma_2)$ and then acting on it both from the left and from the right with a maximal subgroup of SU(2) which does not contain the first subgroup. We can rewrite it in the schematic form $g=\mathrm{U}(1)\exp(i\theta\sigma_2)\mathrm{U}(1)$. On the other hand, the group SU(2) is topologically equivalent to the three-sphere S^3, and admits a Hopf fibration structure with fiber S^1 over the base $S^2 \simeq \mathbb{CP}^1$.

To recognize this fibration structure in (1.2), we can apply the methods used in Refs. 3 and 4. After introducing the metric $\langle A|B\rangle = \frac{1}{2}\mathrm{Tr}(AB)$ on the algebra, the metric on the group can be computed as $\mathrm{d}s^2 = \frac{1}{2}\,\mathrm{Tr}\, J\otimes J$, where $J=-ig^{-1}\,\mathrm{d}g$ are the left-invariant currents. Following Ref. 3, it is possible to separate the fiber from the base by writing $g=h\mathrm{U}(1)$, where $h=e^{i\phi\sigma_3}e^{i\theta\sigma_2}$ and $\mathrm{U}(1)=e^{i\psi\sigma_3}$. To find the metric on the fiber, let us fix the point on the base and compute the currents along the fiber, $J_F=-i\mathrm{U}(1)^{-1}d\mathrm{U}(1)=\mathrm{d}\psi\sigma_3$. The metric on the fiber is then simply given by $\mathrm{d}s_F^2=\mathrm{d}\psi^2$. To determine the metric on the base, we first must project out from the current $J_B=-ih^{-1}\,\mathrm{d}h$ the component along the fiber, in order to be left with the reduced current on the basis $\tilde{J}_B=\mathrm{d}\psi\sigma_2+\sin(2\psi)\mathrm{d}\psi\,\sigma_1$, which then in turn provides the metric

$$\mathrm{d}s_B^2 = \tfrac{1}{4}[d(2\psi)^2 + \sin^2(2\psi)d(2\phi)^2]. \tag{1.3}$$

This corresponds in fact with the metric of a sphere of radius $\frac{1}{2}$. It is easy to see that, introducing the complex coordinates $z=\tan\psi e^{i\phi}$ and their complex conjugates, the metric $\mathrm{d}s_B^2$ reduces to the standard Fubini-Study metric for $\mathbb{CP}^1$.

This shows that the Euler parametrization captures the Hopf fibration structure of SU(2), which is the starting point for our construction. Mimicking what we said about SU(2), let us write the generic element of SU($N+1$) as $g=\mathrm{U}(N)e(\theta)\mathrm{U}(N)$, where $e(\theta)$ is a one parameter subgroup not contained in U(N). The first difficulty we must face here is that this expression for a generic SU($N+1$) group has redundancies, which must be eliminated. After this problem is solved, we then must show that the parametrization respects the Hopf fibration structure of SU($N+1$).

II. THE SU(N) ALGEBRA

The generators of su(N) are all the $N\times N$ traceless Hermitian matrices. A convenient choice for a base are the generalized Gell-Mann matrices as explained in Ref. 1. Let us remind how they can be constructed using an inductive procedure. Let $\{\lambda_i\}_{i=1}^{N^2-1}$ be the Gell-Mann base for su(N): They are $N\times N$ matrices which can be embedded in su($N+1$) adding a null column and a null row

$$\tilde{\lambda}_i = \begin{pmatrix} \lambda_i & \vec{0} \\ \vec{0} & 0 \end{pmatrix}. \tag{2.1}$$

We will omit the tilde from now on. The dimension of SU(N) being $(N+1)^2-1$, we must add $2N+1$ matrices to obtain a Gell-Mann base for su($N+1$). This can be done as follows: Set

$$\begin{aligned} \{\lambda_{N^2+2a-2}\}_{\alpha\beta} &= \delta_{\alpha,a}\delta_{\beta,N+1} + \delta_{\alpha,N+1}\delta_{\beta,a}, \\ \{\lambda_{N^2+2a-1}\}_{\alpha\beta} &= i(-\delta_{\alpha,a}\delta_{\beta,N+1} + \delta_{\alpha,N+1}\delta_{\beta,a}), \end{aligned} \tag{2.2}$$

for $a=1,\ldots,N$. The last matrix we need is diagonal and traceless so that we can take $\lambda_{(N+1)^2-1} = \epsilon_{N+1}\,\mathrm{diag}\{1,\ldots,1,-N\}$.

One can easily verify that the base of matrices $\{\lambda_I\}_{I=1}^{(N+1)^2-1}$ so obtained satisfies the normalization condition $\mathrm{Trace}\{\lambda_I\lambda_J\}=2\delta_{IJ}$ if we choose $\epsilon_{N+1}=\sqrt{2/[(N+1)^2-(N+1)]}$.

These are exactly the matrices we need to generate the group elements.

III. THE EULER PARAMETRIZATION FOR SU($N+1$): INDUCTIVE CONSTRUCTION

It is a well-known fact that special unitary groups SU($N+1$) can be geometrically understood as U(N) fibration over the complex projective space $\mathbb{CP}^N$. Now U(N) is generated by the first N^2-1 generalized Gell-Mann matrices plus the last one $\lambda_{(N+1)^2-1}$. Using the fact that all the remaining generators of SU($N+1$) can be obtained from the commutators of these matrices with λ_{N^2+1}, one is tempted to write the general element of SU($N+1$) in the form

$$\mathrm{SU}(N+1) = \mathrm{U}(N)e^{ix\lambda_{N^2+1}}\mathrm{U}(N). \tag{3.1}$$

However to describe SU($N+1$) we need $(N+1)^2-1$ parameters, while in the rhs they are $2N^2+1$: There are $(N-1)^2$ redundancies. Inspired at first by dimensional arguments, we propose that an U($N-1$) subgroup can be subtracted from the left U(N) in the following way. Let us write U(N) in the form $\mathrm{U}(N)=\mathrm{SU}(N)e^{i\psi\lambda_{(N+1)^2-1}}$. Inductively, we can think that also SU(N) can be recovered from $\mathrm{U}(N-1)e^{i\phi\lambda_{(N-1)^2+1}}\,\mathrm{U}(N-1)$ eliminating the redundant parameters, so that it will have the form $\mathrm{SU}(N)=he^{i\phi\lambda_{(N-1)^2+1}}\,\mathrm{SU}(N-1)e^{i\theta\lambda_{N^2-1}}$. We then choose to eliminate the appearing SU($N-1$) together with the phase $e^{i\psi\lambda_{(N+1)^2-1}}$. In this way the SU($N+1$) group element can be written in the form $\mathrm{SU}(N+1)=he^{i\phi\lambda_{(N-1)^2+1}}e^{i\theta\lambda_{N^2-1}}e^{ix\lambda_{N^2+1}}\,\mathrm{U}(N)$. By induction, assuming $N\geqslant 2$ we arrive to the final form of our Ansatz about the parametrization of the general element $g \in \mathrm{SU}(N+1)$,

$$g = e^{i\theta_1\lambda_3}e^{i\phi_1\lambda_2}\prod_{a=2}^{N}[e^{i(\theta_a/\epsilon_a)\lambda_{a^2-1}}e^{i\phi_a\lambda_{a^2+1}}]\mathrm{U}(N)[\alpha_1,\ldots,\alpha_{N^2}], \tag{3.2}$$

where $\mathrm{U}(N)[\alpha_1,\ldots,\alpha_{N^2}]$ is a parametrization of U(N) which in turn can be obtained inductively using the fact

$$\mathrm{U}(N) = [\mathrm{SU}(N)\times\mathrm{U}(1)]/\mathbb{Z}_N. \tag{3.3}$$

The Ansatz (3.2) contains the correct number of parameters. However, we need to show that it is a good Ansatz, meaning that at least locally it must generate the whole tangent space to the identity. Using the Backer-Campbell-Hausdorff formula and some properties of the Gell-Mann matrices, (essentially the fact that the commutators of $\lambda_{(k-1)^2+1}$ with the first $(k-1)^2-1$ matrices generate all the remaining matrices of the su(k) algebra but the last one) it is easy to show that

$$e^{i\theta_1\lambda_1}e^{i\phi_1\lambda_3}\prod_{a=2}^{N}\left[e^{i(\theta_a/\epsilon_a)\lambda_{a^2-1}}e^{i\phi_a\lambda_{a^2+1}}\right]=e^{i\sum_{j=1}^{(N+1)^2-2}a_j\lambda_j}, \tag{3.4}$$

where a_j are all nonvanishing functions of the $2N$ parameters θ_a,ϕ_a. Thus in a change of coordinates (from the θ_a,ϕ_a to the a_j) only $2N$ of the a_j can be chosen as independent parameters. We could choose the last ones, corresponding to the coefficients of the matrices $\{\lambda_k\}_{k=N^2}^{N^2+2N-1}$. In this way, the N^2 free parameters for the remaining matrices come out exactly from the U(N) factors in (3.2).

We have not entered into details here because a second simple proof of the validity of this parametrization will be given by constructing a nonsingular invariant measure from our Ansatz.

IV. INVARIANT MEASURE AND THE RANGE OF THE PARAMETERS

A. The invariant measure

To construct the invariant measure for the group starting from (3.2), we will adopt the same method used in Ref. 3, with $U:=\mathrm{U}(N)$ as the fiber group. Let us then write (3.2) as

$$g=h\cdot U. \tag{4.1}$$

Starting from the computation of the left invariant currents $j_h=-ih^{-1}\,\mathrm{d}h$, we can define the one forms

$$e^l:=\tfrac{1}{2}\mathrm{Tr}[j_h\cdot\lambda_{N^2+l-1}],\quad l=1,\ldots,2N, \tag{4.2}$$

which turns out to give the Vielbein one forms of the base space of the fibration. If $\underline{e}$ denotes the corresponding Vielbein matrix, the invariant measure for SU($N+1$) will then take the form

$$\mathrm{d}\mu_{\mathrm{SU}(N+1)}=\det\underline{e}\cdot\mathrm{d}\mu_{U(N)}, \tag{4.3}$$

$\mathrm{d}\mu_{U(N)}$ being the invariant measure for U(N). Using (3.3) with $\mathrm{U}(1)=e^{i(\omega/\epsilon_{N+1})\lambda_{(N+1)^2-1}}$ we obtain the recursion relation (note that here ω is allowed to vary in the range $[0,2\pi/N]$)

$$\mathrm{d}\mu_{\mathrm{SU}(N+1)}=\det\underline{e}\cdot\mathrm{d}\mu_{\mathrm{SU}(N)}\frac{\mathrm{d}\omega}{\epsilon_{N+1}}. \tag{4.4}$$

Then we will concentrate on the $\det\underline{e}$ term. To this end let us write (3.2) in the form

$$g=h_{N+1}[\theta_a,\phi_a]\cdot U[\alpha_i]. \tag{4.5}$$

Here we will consider $N\geqslant 3$ so that the relation

$$h_{N+1}=h_N e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}e^{i\phi_N\lambda_{N^2+1}}, \tag{4.6}$$

is true. If we introduce the right currents $J_{h_{N+1}}=-ih_{N+1}^{-1}\,\mathrm{d}h_{N+1}$ then the Vielbein (4.2) takes the form

$$\begin{aligned}e_l^{\{N\}}&=\frac{1}{2}\mathrm{Tr}\{J_{h_{N+1}}\lambda_l\}=\mathrm{d}\phi_N\delta_{l,N^2+1}+\frac{1}{2\epsilon_N}\mathrm{d}\theta_N\,\mathrm{Tr}\{e^{-i\phi_N\lambda_{N^2+1}}\lambda_{N^2-1}e^{i\phi_N\lambda_{N^2+1}}\lambda_{N^2+l}\}\\&+\frac{1}{2}\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}}J_{h_N}e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}e^{i\phi_N\lambda_{N^2+1}}\lambda_{N^2+l}e^{-i\phi_N\lambda_{N^2+1}}\},\end{aligned} \tag{4.7}$$

and using the relations in Appendix A we find

$$\underline{e}^{\{N\}} = \begin{pmatrix} \mathrm{d}\phi_N & 0 & 0 \\ 0 & \sin\phi_N \cos\phi_N \,\mathrm{d}\theta_N & \sin\phi_N \cos\phi_N \frac{1}{2}\sum_{a=2}^{N} \mathrm{Tr}\left[\frac{1}{\alpha_a} J_{h_N} \lambda_{a^2-1}\right] \\ 0 & 0 & \frac{1}{2}\sin\phi_N \,\mathrm{Tr}[e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}} \underline{M}] \end{pmatrix}, \tag{4.8}$$

where we introduced the $\{N\}$ index to remember that this is a $2N\times 2N$ matrix associated to the group SU$(N+1)$. Here $\underline{M}$ is a column of matrices, $M_{2j-1}=\lambda_{j^2+1}$, $M_{2j}=\lambda_{j^2}$, $j=1,2,\ldots,N-1$. Formula (4.8) then reads as follows: J_{h_N} is a 1-form with components $J_{h_N,c}$, $c=1,2,\ldots,2n-2$, with respects to the coordinates X^c, defined as $X^{2j-1}=\theta_j$, $X^{2j}=\phi_j$. To find the component (r,c) of (4.8) one must then take the cth component of $J_{h_N,c}$ and the rth component of $\underline{M}$ before to compute the trace.

The invariant measure is then

$$\det \underline{e}^{\{N\}} = \mathrm{d}\phi_N \,\mathrm{d}\theta_N \cos\theta_N \sin^{2N-1}\phi_N \det\left(\frac{1}{2}\mathrm{Tr}[e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}} \underline{M}]\right). \tag{4.9}$$

We now use the recurrence relation

$$\begin{aligned} J_{h_N} = {} & \lambda_{(N-1)^2+1}\,\mathrm{d}\phi_{N-1} + \frac{1}{\epsilon_{N-1}} e^{-i\phi_{N-1}\lambda_{(N-1)^2+1}} \lambda_{(N-1)^2-1} e^{i\phi_{N-1}\lambda_{(N-1)^2+1}}\,\mathrm{d}\theta_{N-1} \\ & + e^{-i\phi_{N-1}\lambda_{(N-1)^2+1}} e^{-i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} J_{h_{N-1}} e^{i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} e^{i\phi_{N-1}\lambda_{(N-1)^2+1}}. \end{aligned} \tag{4.10}$$

Computing the traces different cases arise depending on whether $j=N-1$ or $j<N-1$; using again the relations in Appendix A it is not too difficult to show that the last determinant is equal to

$$\begin{aligned} & \det\begin{pmatrix} \mathrm{d}\phi_{N-1}\cos(N\theta_N) & -\frac{1}{2}\sin(N\theta_N)\sin(2\phi_{N-1})\mathrm{d}\theta_{N-1} \\ \mathrm{d}\phi_{N-1}\sin(N\theta_N) & \frac{1}{2}\cos(N\theta_N)\sin(2\phi_{N-1})\mathrm{d}\theta_{N-1} \end{pmatrix} \\ & \times \det\left(\frac{1}{2}\cos\phi_{N-1}\,\mathrm{Tr}[e^{-i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} J_{h_{N-1}} e^{i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} \underline{M}]\right), \end{aligned}$$

which set into (4.9) in turn yields the recurrence relation

$$\det \underline{e}^{\{N\}} = \mathrm{d}\phi_N \,\mathrm{d}\theta_N \frac{\sin^{2N-1}\phi_N}{\tan^{2N-4}\phi_{N-1}} \det \underline{e}^{\{N-1\}}, \tag{4.11}$$

which can be solved to give

$$\det \underline{e}^{\{N\}} = 2\,\mathrm{d}\theta_N \,\mathrm{d}\phi_N \cos\phi_N \sin^{2N-1}\phi_N \prod_{a=1}^{N-1} [\sin\phi_a \cos^{2a-1}\phi_a \,\mathrm{d}\theta_a \,\mathrm{d}\phi_a]. \tag{4.12}$$

This is the same result as found in Ref. 1.

B. The range of the parameters

At this point we are able to determine the range of the parameters in such a way as to cover the whole group. We will do this only for the base space: The remaining ranges for the fiber can be determined recursively, as discussed above, remembering in particular that the U(1) phase in U(k) can be taken in $[0,2\pi/k]$.

We then proceed as in Ref. 3. We first choose the ranges so as to generate a closed $[(N+1)^2-1]$-dimensional closed manifold which then must wrap around the group manifold of

SU($N+1$) an integer number of times. This can be done by looking at the measure (4.12) on the base manifold and noticing that it is nonsingular when $0<\phi_a<\pi/2$, whereas θ_a can take all the period values $\theta_a \in [0,2\pi]$, for all $a=1,\ldots,N$. However, note that the angles θ_1,ϕ_1,θ_2 generate the whole SU(2) group when $0\leqslant\theta_1\leqslant\pi$, $0<\phi_a<\pi/2$ and $0\leqslant\theta_2\leqslant 2\pi$. We can then restrict $\theta_1 \in [0,\pi]$. The rest of the variety is generated by the remaining U(N) part.

If we call V_{N+1} the manifold obtained this way we then find

$$\begin{aligned}\mathrm{Vol}(V_{N+1}/\mathrm{U}(N)) &= \int_0^{\pi} \mathrm{d}\theta \prod_{a=2}^{N} \int_0^{2\pi} \mathrm{d}\theta_a \prod_{b=1}^{N} \int_0^{\pi/2} \mathrm{d}\phi_b \left\{ \cos\phi_N \sin^{2N-1}\phi_N \prod_{c=1}^{N-1} [\sin\phi_c \cos^{2c-1}\phi_c] \right\} \\ &= \frac{\pi^N}{N!},\end{aligned} \tag{4.13}$$

or equivalently

$$\mathrm{Vol}(V_{N+1}) = \mathrm{Vol}(\mathrm{U}(N))\frac{\pi^N}{N!}. \tag{4.14}$$

This is exactly the recursion relation found in Appendix B. Therefore, it is the correct range of the parameters for every $N\geqslant 2$, if we have $V_3=\mathrm{SU}(3)$, as can be easily checked directly or by comparison with the results given in Appendix A of Ref. 2 (see also Appendix B of Ref. 4). The next step is to determine the parametrization of SU($N+1$) for every value of N. It is given by (3.2) with

$$\begin{gathered}0\leqslant\theta_1\leqslant\pi, \quad 0\leqslant\theta_a\leqslant 2\pi, a=2,\ldots,N, \\ 0\leqslant\omega\leqslant\frac{2\pi}{N}, \quad 0\leqslant\phi_a\leqslant\frac{\pi}{2}, a=1,\ldots,N,\end{gathered} \tag{4.15}$$

and the remaining parameters which cover SU(N) (determined inductively).

To prove that our parametrization is well defined we can do more: We are in fact able to show that the induced metric on the base manifold is exactly the Fubini-Study metric over $\mathbb{CP}^N$.

V. THE GEOMETRIC ANALYSIS OF THE FIBRATION

We will now show that the metric induced on the base space takes exactly the form of the Fubini-Study metric in trigonometric coordinates as given in Appendix C. To do so we will again use inductive arguments.

The metric on the base is $\mathrm{ds}_B^2=[\underline{e}^{\{N\}}]^T\otimes\underline{e}^{\{N\}}$, where T indicates transposition and $\underline{e}^{\{N\}}$ is given in (4.8). Using the relations in Appendix A and defining

$$X_N = \frac{1}{2}\sum_{a=2}^{N} \mathrm{Tr}[J_{h_N}\epsilon_a\lambda_{a^2-1}] \tag{5.1}$$

the metric takes the form

$$\begin{aligned}\mathrm{ds}_B^2 = d^2\phi_N + \sin^2\phi_N \Bigg\{ [\mathrm{d}\theta_N + X_N]^2 + \sum_{j=1}^{N-1} \left[\frac{1}{2}\mathrm{Tr}(e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}) \lambda_{j^2} \right]^2 \\ + \sum_{j=1}^{N-1} \left[\frac{1}{2}\mathrm{Tr}(e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}) \lambda_{j^2+1} \right]^2 \Bigg\} - \sin^4\phi_N [\mathrm{d}\theta_N + X_N]^2.\end{aligned} \tag{5.2}$$

This is an encouraging form, which upon comparison with (C3) suggests the identification $\xi=\phi_N$. With this identification in mind, let us first remark that the following recursion relation holds:

$$X_N = \cos^2 \phi_{N-1}(\mathrm{d}\theta_{N-1} + X_{N-1}), \tag{5.3}$$

which can be shown by inserting (4.10) in (5.1) and then applying (A6) and (A11). A direct computation yields

$$X_3 = \cos^2 \phi_2(\mathrm{d}\theta_2 + \cos(2\phi_1)\mathrm{d}\theta_1), \tag{5.4}$$

from which, through repeated application of the recurrence relation (5.3), we obtain

$$X_N = \sum_{k=1}^{N-3} \left[\prod_{i=1}^{k} \cos^2 \phi_{N-i} \right] \mathrm{d}\theta_{N-k} + \left[\prod_{i=1}^{N-2} \cos^2 \phi_{N-i} \right] (\mathrm{d}\theta_2 + \cos(2\phi_1)\mathrm{d}\theta_1). \tag{5.5}$$

At this point we must to compare $\mathrm{d}\theta_N + X_N$ with the coefficient of $\sin^4 \xi$ in (C3). In fact, to bring $\mathrm{d}\theta_N + X_N$ to the desired form $\Sigma_{i=1}^{N} (\widetilde{R}^i)^2 \, \mathrm{d}\psi_i$, one is tempted to just set $\theta_i = \psi_i$ and $\phi_\mu = \omega_\mu$. However, this cannot be the case because the $\widetilde{R}^i$ does not satisfy the condition $\Sigma(\widetilde{R}^i)^2 = 1$.

These observations, together with explicit calculations for the case $N=4$ and $N=5$, suggest that we should simply take some linear combination $\psi_i = \psi_i(\theta_j)$. This can be done as follows: Let us introduce new variables $\widetilde{\theta}_K$, $k=1, \ldots, N$, such that

$$\begin{gathered} \widetilde{\theta}_N = \theta_N, \quad \theta_{N-k} = \widetilde{\theta}_{N-k} - \widetilde{\theta}_{N-k+1}, \quad k = 1, \ldots, N-3, \\ \theta_1 + \theta_2 = \widetilde{\theta}_1 - \widetilde{\theta}_3, \quad \theta_1 - \theta_2 = \widetilde{\theta}_3 - \widetilde{\theta}_2. \end{gathered} \tag{5.6}$$

In this way $\mathrm{d}\theta_N + X_N$ takes the desired form

$$\mathrm{d}\theta_N + X_N = \sum_{i=1}^{N} (R^i(\omega_\mu))^2 \, \mathrm{d}\psi_i \tag{5.7}$$

with $\omega_\mu = \phi_\mu$, $\mu = 1, \ldots N-1$, $\psi_i = \widetilde{\theta}_{N-i+1}$, $i=1, \ldots, N$ and

$$\begin{gathered} R_1 = \sin \phi_{N-1}, \quad R_k = \sin \phi_{N-k} \prod_{i=1}^{k-1} \cos \phi_{N-i}, \quad k = 2, \ldots, N-1, \\ R_N = \prod_{i=1}^{N-1} \cos \phi_{N-i}. \end{gathered} \tag{5.8}$$

These formulas agree with the expressions in Appendix C. As the last step, in Appendix D we finally show that, after performing the change of variables described above, the coefficients of $\sin^2 \xi$ and $\sin^2 \phi_N$ also agree. This proves that the metric induced on the base $\mathbb{CP}^N$ of the U(N) fibration by the invariant metric on SU($N+1$) is nothing else but the natural Fubini-Study metric in trigonometric coordinates.

We can now use this result as a different method to fix the range of the parameters. In fact, $(R^1, \ldots, R^N)$ parametrize the positive orthant of a sphere, if $0 < \phi_i < \pi/2$, $i=1, \ldots, N-1$. Moreover, the identification of ϕ_N with ξ yields $\phi \in [0, \pi/2]$. Finally, it is easy to show that the conditions $\widetilde{\theta}_i \in [0, 2\pi]$ are equivalent to $\theta_1 \in [0, \pi]$ and $\theta_i \in [0, 2\pi]$, $i=2, \ldots, N$. These are the same results obtained in (4.15).

VI. CONCLUSIONS

In this paper, we have reconsidered the problem of constructing a generalized Euler parametrization for SU(N). The parametrization we find differs slightly from the one described by Tilma and Sudarshan. In fact, comparing our results with the expression (18) in Ref. 1, it is possible to

see that we have chosen $\lambda_{(k-1)^2-1}$ instead of λ_3. Furthermore, we have computed the corresponding invariant measure, which turns out to coincide with the result in Ref. 1, despite the slight differences in the choice of the parametrization.

To determine the range of the parameters, we have used two distinct methods, both yielding the same result. To better motivate the name "Euler angles," we have carefully shown that the parametrization captures the Hopf fibration structure of the SU(N) groups. In particular the change of coordinate we found to evidentiate the fibrations, gives an explicit map between the Euler coordinates introduced starting from the generalized Gell-Mann matrices, and the ones introduced in Ref. 5 using geometrical considerations.

We have given a quite explicit proof of every assertion. Apart from corroborating the results of Tilma and Sudarshan, we think that our work is providing a complete toolbox of computation techniques useful in applied theoretical physics as well as for experimental physicists.

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APPENDIX A: SOME COMMUTATORS

Using the explicit form of the generalized Gell-Mann matrices constructed with the conventions of Sec. II, we find the useful commutators

$$\begin{aligned}[\lambda_{N^2+1},\lambda_{N^2+2j}] &= -i\lambda_{j^2},\\ [\lambda_{N^2+1},\lambda_{N^2+2j+1}] &= i\lambda_{j^2+1},\end{aligned} \tag{A1}$$

when $j=1,\ldots,N-1$.

Others interesting relations easy to check are

$$\begin{aligned}[\lambda_{N^2+1},\lambda_{N^2}] &= -i(N+1)\epsilon_{N+1}\lambda_{(N+1)^2-1} - i\sum_{a=2}^{N}\epsilon_a\lambda_{a^2-1},\\ [\lambda_{N^2+1},\lambda_{a^2-1}] &= i\epsilon_a\lambda_{N^2},\\ [\lambda_{N^2+1},\lambda_{(N+1)^2-1}] &= i(N+1)\epsilon_{N+1}\lambda_{N^2},\end{aligned} \tag{A2}$$

where $a=1,\ldots,N$, from which remembering that $\epsilon_k=\sqrt{2/k(k-1)}$, one also finds

$$[\lambda_{N^2+1},[\lambda_{N^2+1},\lambda_{N^2}]] = 4\lambda_{N^2}. \tag{A3}$$

From the first two commutators we find the very useful relations

$$e^{ix\lambda_{N^2+1}}\lambda_{j^2+1}e^{-ix\lambda_{N^2+1}} = \frac{1}{\sin x}\lambda_{N^2+2j+1} - \frac{1}{\tan x}e^{ix\lambda_{N^2+1}}\lambda_{N^2+2j+1}e^{-ix\lambda_{N^2+1}},$$

$$e^{ix\lambda_{N^2+1}}\lambda_{j^2}e^{-ix\lambda_{N^2+1}} = -\frac{1}{\sin x}\lambda_{N^2+2j} + \frac{1}{\tan x}e^{ix\lambda_{N^2+1}}\lambda_{N^2+2j}e^{-ix\lambda_{N^2+1}}, \tag{A4}$$

when $j=1,\ldots,N-1$.

Other useful relations easy to prove using the previous relations are

$$\sum_{a=2}^{N}\epsilon_a^2 + (N+1)^2\epsilon_{N+1}^2 = 4, \tag{A5}$$

$$\sum_{a=2}^{N}\epsilon_a^2 + (N+1)\epsilon_{N+1}^2 = 2, \tag{A6}$$

$$\mathrm{Tr}[e^{-ix\lambda_{N^2+1}}\lambda_{N^2-1}e^{ix\lambda_{N^2+1}}\lambda_{N^2+I}] = \epsilon_N\delta_{I0}\sin(2x), \tag{A7}$$

$$\frac{1}{2}\mathrm{Tr}[\lambda_a e^{ix\lambda_{N^2+1}}\lambda_{N^2+2i}e^{-ix\lambda_{N^2+1}}] = \delta_{a,i^2}\sin x,\ a \leqslant N^2-1,\ i=1,\ldots,N-1, \tag{A8}$$

$$\frac{1}{2}\mathrm{Tr}[\lambda_a e^{ix\lambda_{N^2+1}}\lambda_{N^2+2i-1}e^{-ix\lambda_{N^2+1}}] = -\delta_{a,i^2+1}\sin x,\ a \leqslant N^2-1,\ i=1,\ldots,N-1, \tag{A9}$$

$$\frac{1}{2}\mathrm{Tr}\left[e^{ix\lambda_{N^2+1}}\lambda_{N^2}e^{-ix\lambda_{N^2+1}}\sum_{a=1}^{N^2-1}C^a\lambda_a\right] = \sin(2x)\frac{1}{2}\sum_{b=2}^{N}\mathrm{Tr}[C^{b^2-1}\epsilon_{b^2-1}], \tag{A10}$$

$$\sum_{a=2}^{N}\mathrm{Tr}[Ae^{ix\lambda_{(N-1)^2+1}}\lambda_{a^2-1}e^{-ix\lambda_{(N-1)^2+1}}] = \cos^2 x\sum_{a=2}^{N}\mathrm{Tr}[A\epsilon_a\lambda_{a^2-1}], \tag{A11}$$

$$e^{ix\lambda_{N^2-1}}\lambda_{(N-1)^2}e^{-ix\lambda_{N^2-1}} = \cos(N\epsilon_N x)\lambda_{(N-1)^2} - \sin(N\epsilon_N x)\lambda_{(N-1)^2+1}, \tag{A12}$$

$$e^{ix\lambda_{N^2-1}}\lambda_{(N-1)^2+1}e^{-ix\lambda_{N^2-1}} = \cos(N\epsilon_N x)\lambda_{(N-1)^2+1} + \sin(N\epsilon_N x)\lambda_{(N-1)^2}, \tag{A13}$$

where we used $A := \Sigma_{i=1}^{(N-1)^2-1}A^i\lambda_i$.

APPENDIX B: THE TOTAL VOLUME OF SU(*k*)

The total volume for the groups SU(k) can be found following Macdonald in Ref. 6. First remember that, in the sense of rational cohomology, SU(k) is equivalent to the product of odd dimensional spheres

$$\mathrm{SU}(k+1) \sim \prod_{j=1}^{k} S^{2i+1}, \tag{B1}$$

where we choosen $k+1$ to obtain recursive relations. The total volume of the group is then uniquely determined when a metric is established on the Lie algebra. We chose the metric induced by the scalar product $(A|B)=\frac{1}{2}\mathrm{Tr}(AB)$, for $A,B\in\mathrm{su}(k+1)$. In this way the Gell-Mann generators are orthonormal. The formula for the total volume is (Ref. 6)

$$\mathrm{Vol}(\mathrm{SU}(k+1)) = \prod_{j=1}^{k} \mathrm{Vol}(S^{2i+1}) \cdot \mathrm{Vol}(\mathbb{T}_k) \prod_{\alpha>0} |\alpha^\vee|^2, \tag{B2}$$

where $\alpha^\vee$ are the coroots associated to positive roots and $\mathrm{Vol}(\mathbb{T}_k)$ is the volume of the torus generated by the simple coroots.

For su$(k+1)$ the simple coroots are $s_i = L_i - L_{i+1}$, $i=1,\ldots,k$ where L_i is the diagonal matrix with the only nonvanishing entry $\{L_i\}_{ii}=1$. After writing s_i in terms of λ_j, as

$$s_i = \sum_{a=1}^{k} \frac{1}{2} \mathrm{Tr}\{s_i \lambda_{(a+1)^2-1}\} \lambda_{(a+1)^2-1}, \tag{B3}$$

it is easy to prove the recursive relation

$$\mathrm{Vol}(\mathbb{T}_k) = \sqrt{\frac{k+1}{2k}} \mathrm{Vol}(\mathbb{T}_{k-1}). \tag{B4}$$

From this we find

$$\mathrm{Vol}(\mathrm{SU}(k+1)) = \mathrm{Vol}(\mathrm{SU}(k)) 2 \frac{\pi^{k+1}}{k!} \sqrt{\frac{k+1}{2k}}, \tag{B5}$$

where we used the fact that all the positive coroots have unitary length. If we note that the phase $e^{i(\theta_k/\epsilon_k)\lambda_{(k+1)^2-1}}$ generates a U(1) group of volume $2\pi\sqrt{k(k+1)/2}$ and that $\mathrm{U}(k) = [\mathrm{SU}(k) \times \mathrm{U}(1)]/Z_k$, we can finally write

$$\mathrm{Vol}(\mathrm{SU}(k+1)) = \mathrm{Vol}(\mathrm{U}(k)) \frac{\pi^k}{k!}, \tag{B6}$$

APPENDIX C: THE FUBINI-STUDY METRIC FOR $\mathbb{CP}^N$

$\mathbb{CP}^N$ is a Kähler manifold of complex dimension N. In a local chart, which uses holomorphic inhomogeneous coordinates $\{z^i\}_{i=1}^N \in \mathbb{C}$, the Kähler potential is $K(z^i, \overline{z^j}) = k/2 \log(1+\Sigma_{i=1}^N |z^i|^2)$ with k a constant. The associated Kähler metric $g_{i\bar{j}} = \partial^2 K / \partial z^i \partial \overline{z^j}$ is then

$$\mathrm{d}s^2_{\mathbb{CP}^N} = k \left(\frac{\sum_{i=1}^N \mathrm{d}z^i \, \mathrm{d}\overline{z^i}}{1+\sum_{i=1}^N |z^i|^2} - \frac{\sum_{i,j=1}^N z^i \, \mathrm{d}\overline{z^i} \, \overline{z^j} \, \mathrm{d}z^j}{(1+\sum_{i=1}^N |z^i|^2)^2} \right). \tag{C1}$$

Notice that obviously it is not possible to cover the whole space with a single chart, but the set of points which cannot be covered has vanishing measure. For our purpose it is therefore enough to consider a single chart.

Let us now search for a trigonometric coordinatization. To this aim let us introduce the new real coordinates ξ, ω_μ, ψ_i, $\mu=1,\ldots,N-1$, $i=1,\ldots,N$, such that

$$z^i = \tan \xi R^i(\omega_\mu) e^{i\psi_i}. \tag{C2}$$

Here $R^i(\omega_\mu)$ is a parametrization of the unit sphere S^{n-1}, construced as an immersion in $\mathbb{R}^N$, where $\Sigma_{i=1}^N (R^i)^2 = 1$ and ω_μ are the angles of the sphere. However, notice that we are restricted to the positive orthant only: $R_i > 0$. If ω_μ are the standard angles (starting, for example, with the azimuthal one ω_1), then $\omega_\mu \in [0, \pi/2]$, $\xi \in [0, \pi/2]$, and $\psi_i \in [0, 2\pi]$. This choice of coordinates finally gives

$$ds^2_{\mathbb{C}P^N} = d\xi^2 + \sin^2\xi\left[\sum_{i=1}^{N} dR^i\, dR^i + \sum_{i=1}^{N} (R^i)^2 d^2\psi_i\right] - \sin^4\xi\left[\sum_{i=1}^{N} (R^i)^2\, d\psi_i\right]^2. \tag{C3}$$

In particular notice that the coefficient of $\sin^2\xi$ yields a metric for (the positive orthant of) the sphere S^{N-1}.

APPENDIX D: FINAL CHECKS

Here we verify that the change of variables introduced in Sec. V transforms the terms

$$[d\theta_N + X_N]^2 + \sum_{j=1}^{N-1}\left[\frac{1}{2}\mathrm{Tr}(e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}})\lambda_{j^2}\right]^2 + \sum_{j=1}^{N-1}\left[\frac{1}{2}\mathrm{Tr}(e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}})\lambda_{j^2+1}\right]^2, \tag{D1}$$

into the coefficient of $\sin^2\xi$ in (C3).

First, using (4.10) and the relations in Appendix A, it is possible to show that

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{j^2}\} = \cos\phi_{N-1}\,\mathrm{Tr}\{e^{-i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} J_{h_{N-1}} e^{i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N^2-1)-1}}\lambda_{j^2}\}, \quad j < N-1,$$

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{j^2+1}\} = \cos\phi_{N-1}\mathrm{Tr}\{e^{-i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}} J_{h_{N-1}} e^{i(\theta_{N-1}/\epsilon_{N-1})\lambda_{(N-1)^2-1}}\lambda_{j^2+1}\}, \quad j < N-1,$$

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{(N-1)^2}\} = \sin(2\phi_{N-1})\cos(N\theta_N)[d\theta_{N-1} + X_{N-1}] - 2\sin(N\theta_N)d\phi_{N-1},$$

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{(N-1)^2+1}\} = \sin(2\phi_{N-1})\sin(N\theta_N)[d\theta_{N-1} + X_{N-1}] + 2\cos(N\theta_N)d\phi_{N-1}. \tag{D2}$$

Note that these are true for $N \geqslant 3$, if we define $X_2 := \cos(2\phi_1)d\theta_1$. From these relations we find

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{j^2}\} = \left[\prod_{k=j+1}^{N-1}\cos\phi_k\right][\sin(2\phi_j)\cos[(j+1)\theta_{j+1}](d\theta_j + X_j) - 2\sin[(j+1)\theta_{j+1}]d\phi_j],$$

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_{j^2+1}\} = \left[\prod_{k=j+1}^{N-1}\cos\phi_k\right][\sin(2\phi_j)\sin[(j+1)\theta_{j+1}](d\theta_j + X_j) + 2\cos[(j+1)\theta_{j+1}]d\phi_j],$$

with $j = 2, \ldots, N-1$. For $j = 1$,

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}} J_{h_N} e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_1\} = \left[\prod_{k=2}^{N-1}\cos\phi_k\right][\sin(2\phi_1)\cos(2\theta_2)d\theta_1 - \sin(2\theta_2)d\phi_1],$$

$$\mathrm{Tr}\{e^{-i(\theta_N/\epsilon_N)\lambda_{N^2-1}}J_{h_N}e^{i(\theta_N/\epsilon_N)\lambda_{N^2-1}}\lambda_2\} = \left[\prod_{k=2}^{N-1}\cos\phi_k\right][\sin(2\phi_1)\sin(2\theta_2)\mathrm{d}\theta_1 + \cos(2\theta_2)\mathrm{d}\phi_1].$$

Thus we see that (D2) takes the form $S_N + U_N$, where

$$S_N = \mathrm{d}\phi_{N-1}^2 + \sum_{j=1}^{N-2}\left[\prod_{k=j+1}^{N-1}\cos^2\phi_k\right]\mathrm{d}\phi_j^2, \tag{D3}$$

$$U_N = (\mathrm{d}\theta_N + X_N)^2 + \sum_{j=2}^{N-1}\sin^2\phi_j\left[\prod_{k=j}^{N-1}\cos^2\phi_k\right](\mathrm{d}\theta_j + X_j)^2 + \prod_{k=2}^{N-1}\cos^2\phi_k\sin^2(2\phi_1)\mathrm{d}\theta_1^2. \tag{D4}$$

First, we show that

$$S_N = \sum_{j=1}^{N}\mathrm{d}R^j\mathrm{d}R^j, \tag{D5}$$

with R^j as in (5.8). To this aim let us define the N-dimensional vector $\vec{R}_N = (R^1, \ldots, R^N)$. Such a vector has unit length, and satisfies the recurrence relation $\vec{R}_N = (\sin\phi_{N-1}, \cos\phi_{N-1}\vec{R}_{N-1})$, from which we find

$$\mathrm{d}\vec{R}_N \cdot \mathrm{d}\vec{R}_N = \mathrm{d}\phi_{N-1}^2 + \cos^2\phi_{N-1}\,\mathrm{d}\vec{R}_{N-1}\cdot\mathrm{d}\vec{R}_{N-1}. \tag{D6}$$

Here the dot indicates the scalar product in N dimensions. Now, from (D3), we also have

$$S_N = \mathrm{d}\phi_{N-1}^2 + \cos^2\phi_{N-1}S_{N-1}. \tag{D7}$$

As S_N and $\mathrm{d}\vec{R}_N\cdot\mathrm{d}\vec{R}_N$ both satisfy the same recurrence relation, the thesis follows because of $S_2 = \mathrm{d}\vec{R}_2\cdot\mathrm{d}\vec{R}_2$.

The second and last step of our proof consists in showing that after the change of coordinates (5.6) the Eq. (D4) takes the form

$$U_N = \sum_{i=1}^{N}(R^i)^2\mathrm{d}\psi_i^2. \tag{D8}$$

The structure of (D4) suggests that it is convenient to make the change of variables starting from θ_N and θ_{N-1} step by step. Note that X_{N-1} is invariant under this transformation, so that we have

$$(\mathrm{d}\theta_N + X_N)^2 + \sin^2\phi_{N-1}\cos^2\phi_{N-1}(\mathrm{d}\theta_{N-1} + X_{N-1})^2 = \sin^2\phi_{N-1}\mathrm{d}\tilde{\theta}_N^2 + \cos^2\phi_{N-1}(\mathrm{d}\tilde{\theta}_{N-1} + X_{N-1})^2. \tag{D9}$$

Here we have used (5.3) to express X_N in terms of X_{N-1}. Then U_N takes the form

$$U_N = \sin^2\phi_{N-1}\mathrm{d}\tilde{\theta}_N^2 + \cos^2\phi_{N-1}[(\mathrm{d}\tilde{\theta}_{N-1} + X_{N-1})^2 + \sin^2\phi_{N-2}\cos^2\phi_{N-2}(\mathrm{d}\theta_{N-2} + X_{N-2})^2] + \cdots. \tag{D10}$$

Now it is possible to use (D9) with $N-1$ in place of N in order to write θ_{N-2} in terms of $\tilde{\theta}_{N-2}$. In fact, this relation can be applied recursively up to $\mathrm{d}\theta_3$, obtaining

$$U_N = \sin^2\phi_{N-1}\,\mathrm{d}\tilde{\theta}_N^2 + \sum_{j=2}^{N-4}\sin^2\phi_{N-j}\left[\prod_{l=N-j+1}^{N-1}\cos^2\phi_l\right]\mathrm{d}\tilde{\theta}_{N-j+1}^2 + \left[\prod_{l=3}^{N-1}\cos^2\phi_l\right](\mathrm{d}\tilde{\theta}_3 + X_3)^2$$
$$+ \sin^2\phi_2\left[\prod_{k=2}^{N-1}\cos^2\phi_k\right](\mathrm{d}\theta_2 + \cos(2\phi_1)\mathrm{d}\theta_1)^2 + \left[\prod_{k=2}^{N-1}\cos^2\phi_k\right]\sin^2(2\phi_1)\theta_1^2. \tag{D11}$$

At this point we can perform the last two changes of coordinates in (5.6), to show that

$$\mathrm{d}\tilde{\theta}_3 + X_3 = \sin^2\phi_2\,\mathrm{d}\tilde{\theta}_3 + \cos^2\phi_2(\sin^2\phi_1\tilde{\theta}_2 + \cos^2\phi_1\,d\tilde{\theta}_1), \tag{D12}$$

and this completes the proof.

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Superintegrable quantum u(3) systems and higher rank factorizations

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A class of two-dimensional superintegrable systems on a constant curvature surface is considered as the natural generalization of some well known one-dimensional factorized systems. By using standard methods to find the shape-invariant intertwining operators we arrive at a so(6) dynamical algebra and its Hamiltonian hierarchies. We pay attention to those associated to certain unitary irreducible representations that can be displayed by means of three-dimensional polyhedral lattices. We also discuss the role of superpotentials in this new context. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2191360]

I. INTRODUCTION

This work deals with a class of superintegrable Hamiltonian systems, in the framework of the Schrödinger equation of quantum mechanics, and its connections with the factorization method. We will restrict ourselves to a particular case where the underlying symmetry is the Lie algebra u(3), but its main features can be directly implemented to higher dimensional systems.

The main objective of this study is to show a natural extension to higher dimensional spaces of the intertwining (or Darboux) transformations from a well known class of one-dimensional factorized systems. In fact, we want to set the higher rank u(n) systems corresponding to those having as dynamical algebra the Lie algebra u(2). We will show in detail that the application of procedures familiar in one dimension to a concrete two-dimensional system will lead us to a wide set of operators closing a dynamical Lie algebra. We also consider discrete symmetry operators quite important to perform equivalences. All these operators connect eigenstates that can be drawn as points in a three-dimensional lattice giving rise to polyhedrons representing degenerate series of u(3) irreducible representations. Each of these series corresponds to the same energy and can be embedded in just one representation of the Lie algebra so(6).

The notion of superpotential will also be re-examined inside the higher rank formalism. Thus, the usual procedure to look for solutions with separable variables can be better appreciated under this point of view.

Thus, we try to implement the program of generalization of the factorizable one-dimensional systems involving Lie algebras of rank one as dynamical algebras, as can be seen, for instance, in the classical paper by Infeld and Hull.[1] We also hope that this work will be useful when dealing with other integrable systems, but not necessarily maximally integrable, for instance not enjoing so many factorizations, or even not having a system of separable variables, but still allowing for algebraic methods.[2–7]

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The organization of this article is as follows. In Sec. II we will introduce a two-dimensional superintegrable system and find some separable solutions by standard procedures. Although these polynomial solutions are known and can be found in other references, this will serve us to recall some aspects of the usual factorization technique and to specify the operators of the Lie algebra u(2) related with the Lie algebra so(4), and their support spaces. Next, in Sec. III, we will look for other sets of intertwining operators, corresponding to the Lie algebras u(3) and so(6), taking also into account discrete symmetries. We characterize the eigenfunctions belonging to irreducible representations that will be depicted as the points on octahedrons and the interpretation of some of its planar sections. The analog of the superpotentials and their relation with certain types of solutions will be considered in Sec. IV. Some conclusions and perspective for future work will close the article.

II. A SUPERINTEGRABLE u(3)-HAMILTONIAN SYSTEM

We will fix our attention on a superintegrable Hamiltonian system defined inside a three-dimensional Euclidean ambient space.[8–11] In fact, our system lives on the two-sphere $\mathcal{S}$

$$\mathcal{S} \equiv (s_0)^2 + (s_1)^2 + (s_2)^2 = 1, \quad (s_0, s_1, s_2) \in \mathbb{R}^3.$$

In the frame of the Schrödinger equation, this Hamiltonian takes the form

$$H = -(J_0^2 + J_1^2 + J_2^2) + \frac{l_0^2 - 1/4}{(s_0)^2} + \frac{l_1^2 - 1/4}{(s_1)^2} + \frac{l_2^2 - 1/4}{(s_2)^2}, \tag{2.1}$$

where $(l_0, l_1, l_2) \in \mathbb{R}^3$, and $J_i = -\epsilon_{ijk} s_j \partial_k$ [note that the J_i's operators generate the rotation Lie algebra so(3)]. We can parameterize $\mathcal{S}$ by means of spherical coordinates (ϕ_1, ϕ_2) around the s_2 axis given by

$$s_0 = \cos\phi_2 \cos\phi_1, \quad s_1 = \cos\phi_2 \sin\phi_1, \quad s_2 = \sin\phi_2. \tag{2.2}$$

Then, the eigenvalue problem

$$H\Phi = E\Phi$$

after substituting the coordinates (2.2), takes the form of a separable differential equation

$$\left[-\partial_{\phi_2}^2 + \tan\phi_2 \partial_{\phi_2} + \frac{l_2^2 - 1/4}{\sin^2\phi_2} + \frac{1}{\cos^2\phi_2} \left[-\partial_{\phi_1}^2 + \frac{l_0^2 - 1/4}{\cos^2\phi_1} + \frac{l_1^2 - 1/4}{\sin^2\phi_1} \right] \right] \Phi = E\Phi. \tag{2.3}$$

The solutions separated in the variables ϕ_1 and ϕ_2, i.e.

$$\mathbf{\Phi}(\phi_1, \phi_2) = f(\phi_1) g(\phi_2)$$

after replacing in (2.3) originate the equations

$$\left[-\partial_{\phi_1}^2 + \frac{l_0^2 - 1/4}{\cos^2\phi_1} + \frac{l_1^2 - 1/4}{\sin^2\phi_1} \right] f(\phi_1) = \alpha f(\phi_1), \tag{2.4}$$

$$\left[-\partial_{\phi_2}^2 + \tan\phi_2 \partial_{\phi_2} + \frac{\alpha}{\cos^2\phi_2} + \frac{l_2^2 - 1/4}{\sin^2\phi_2} \right] g(\phi_2) = E g(\phi_2), \tag{2.5}$$

where α is a separating constant. Next we will solve each of these two equations through standard factorizations giving rise to polynomials. The key point is that the results obtained for the first equation will match in a certain way with those of the second one originating degenerate levels.

A. The ϕ_1 factorization

The one-dimensional Hamiltonian (2.4) in the variable ϕ_1 is a well known example in the theory of factorizations.[1] So, in the following we will restrict ourselves to give a list of the relevant results. We will see later, in Sec. III, how to make use of these considerations in a broader context.

The second order operator at the left-hand side of Eq. (2.4) can be cast as a product of first order operators

$$H^{\phi_1}_{(0)} = A^+_0 A^-_0 + \lambda_0$$

being

$$A^\pm_0 = \pm \partial_{\phi_1} - (l_0 + 1/2)\tan\phi_1 + (l_1 + 1/2)\cot\phi_1, \quad \lambda_0 = (l_0 + l_1 + 1)^2.$$

These elements are part of a family of operators $\{A^+_m, A^-_m, \lambda_m, H^{\phi_1}_{(m)}\}$, $m \in \mathbb{Z}$, where

$$A^\pm_m = \pm \partial_{\phi_1} - (l_0 + m + 1/2)\tan\phi_1 + (l_1 + m + 1/2)\cot\phi_1, \tag{2.6}$$

$$\lambda_m = (l_0 + l_1 + 2m + 1)^2,$$

$$H^{\phi_1}_{(m)} = -\partial^2_{\phi_1} + \frac{(l_0 + m)^2 - 1/4}{\cos^2\phi_1} + \frac{(l_1 + m)^2 - 1/4}{\sin^2\phi_1}. \tag{2.7}$$

They originate the one-dimensional Hamiltonian hierarchy (2.7), starting from $H^{\phi_1}_{(0)}$. The Hamiltonians $H^{\phi_1}_{(m)}$ satisfy the fundamental relation

$$H^{\phi_1}_{(m)} = A^+_m A^-_m + \lambda_m = A^-_{m-1} A^+_{m-1} + \lambda_{m-1} \tag{2.8}$$

so that $A^\pm_m$ are shape invariant intertwining operators, i.e.,

$$A^-_m H^{\phi_1}_{(m)} = H^{\phi_1}_{(m+1)} A^-_m, \quad A^+_m H^{\phi_1}_{(m+1)} = H^{\phi_1}_{(m)} A^+_m. \tag{2.9}$$

Hence, from a formal point of view, the operators $A^\pm_m$ acting on a Hamiltonian eigenfunction will give another eigenfunction of a consecutive Hamiltonian in the hierarchy with the same eigenvalue. If we design the eigenfunction spaces of $H^{\phi_1}_{(m)}$ (as differential operators) by $\mathcal{H}^{\phi_1}_m$, then we have

$$A^-_m : \mathcal{H}^{\phi_1}_m \to \mathcal{H}^{\phi_1}_{m+1}, \quad A^+_m : \mathcal{H}^{\phi_1}_{m+1} \to \mathcal{H}^{\phi_1}_m.$$

In principle, the discrete spectrum and the physical eigenstates of $H^{\phi_1}_{(0)}$ could be obtained from the fundamental states $f^0_{(m)}$ and their eigenvalues of all the Hamiltonians in the hierarchy $\{H^{\phi_1}_{(m)}\}$. These fundamental states are determined by $A^-_m f^0_{(m)} = 0$, giving the solutions (up to a normalization constant)

$$f^0_{(m)}(\phi_1) = \cos^{l_0+m+1/2}\phi_1 \, \sin^{l_1+m+1/2}\phi_1$$

with eigenvalues $\lambda_m = (l_0 + l_1 + 2m + 1)^2$. Often the intertwining operators (2.6) are written in the form

$$A^\pm_m = \pm \partial_{\phi_1} + \omega_m(\phi_1), \quad \omega_m(\phi_1) = \frac{\partial_{\phi_1} f^0_{(m)}(\phi_1)}{f^0_{(m)}(\phi_1)}, \tag{2.10}$$

where $\omega_m(\phi_1)$ is called superpotential function.

In order to go from the ground eigenstate, $f^0_{(m)}$ of $H^{\phi_1}_{(m)}$, up to the excited eigenfunction, $f^m_{(0)}$ of $H^{\phi_1}_{(0)}$, with the same eigenvalue, we apply consecutive operators A^+

$$f^m_{(0)} = A^+_0 A^+_1 \cdots A^+_{m-1} f^0_{(m)} \tag{2.11}$$

obtaining explicitly

$$f^m_{(0)} = N \sin^{l_1+1/2} \phi_1 \cos^{l_0+1/2} \phi_1 P^{(l_1,l_0)}_m(\cos(2\phi_1)), \tag{2.12}$$

where $P^{(a,b)}_n(x)$ are Jacobi polynomials and N is a normalization constant. Therefore, the spectrum of the first separating Hamiltonian (2.4) is given by

$$\alpha = \lambda_m = (l_0 + l_1 + 2m + 1)^2, \quad m \in \mathbb{Z}^+. \tag{2.13}$$

The following two subsections are devoted to characterize the Lie algebras of shape invariant intertwining operators for the one-dimensional Hamiltonian hierarchies. They will constitute a useful pattern for the two-dimensional Hamiltonians of Sec. III.

B. The dynamical algebra u(2)

Starting from the operators $A^\pm_m$ let us define free-index operators $A^\pm$ acting inside the total space $\oplus_m \mathcal{H}_m$, in the following way:[12,13]

$$\begin{aligned} A^+ f_{(m+1)} &:= \tfrac{1}{2} A^+_m f_{(m+1)} \propto \tilde{f}_{(m)}, \\ A^- f_{(m)} &:= \tfrac{1}{2} A^-_m f_{(m)} \propto \tilde{f}_{(m+1)}, \\ A f_{(m)} &:= -\tfrac{1}{2}(l_0 + l_1 + 2m) f_{(m)} \propto f_{(m)}, \end{aligned} \tag{2.14}$$

where $f_{(m)}$ (or $\tilde{f}_{(m)}$) denotes an eigenfunction of $H_{(m)}$. This action can be extended to linear combinations of eigenfunctions by linearity. With this convention we can rewrite (2.8) and (2.14) simply as the commutators

$$[A, A^\pm] = \pm A^\pm, \quad [A^-, A^+] = -2A \tag{2.15}$$

assuming that the action is on any (linear combination of) $f_{(m)}$. The commutators (2.15) close the Lie algebra su(2), whose Casimir element is given by $\mathcal{C} = A^+A^- + A(A-1)$. The eigenvalues of $\mathcal{C}$, labeling the irreducible unitary representations (IUR), are $j(j+1)$, where $2j \in \mathbb{Z}^+$. The dimension of the support spaces of these IURs is, obviously, $2j+1$. We make use of the standard notation $|j,s\rangle$ for an A eigenvector with eigenvalue s, inside the "j-representation."

Now, we can identify the eigenstates of the Hamiltonians $H^{\phi_1}_{(m)}$ in terms of representation vectors $|j,s\rangle$. First, let us consider the ground states $f^0_{(m)}$ characterized by

$$A^- f^0_{(m)} = 0, \quad A f^0_{(m)} = -[(l_0 + l_1 + 2m)/2] f^0_{(m)} \tag{2.16}$$

following notation (2.14). These relations suggest the identification (up to a normalization constant)

$$f^0_{(m)} = |j_m, -j_m\rangle, \quad j_m = (l_0 + l_1 + 2m)/2.$$

To see that indeed this is the case we need to define the whole representation space as well as an inner product. Thus, consider the space $\mathcal{L}^2[0, \pi/2]$ of square integrable functions in the interval $[0, \pi/2]$. Then, the wave functions obtained from the ground state $f^0_{(m)}$ by the consecutive action of the operator A^+ will span the representation space of a j_m representation, with $j_m = (l_0 + l_1 + 2m)/2$, provided that both $l_0 + m$ and $l_1 + m$ belong to $\mathbb{Z}^+$. The wave functions of the space so

generated vanish at the end points, and the hermiticity relations $(A^-)^\dagger = A^+$, $A^\dagger = A$ are implemented in all the space. Hence, under these conditions, $(A^+)^k f^0_{(m)}$ can be identified, up to normalization, with the vector state $|j_m, -j_m + k\rangle$.

As a consequence, the excited states obtained in this way for any Hamiltonian in a factorization hierarchy where l_0 and l_1 are positive integers, correspond to IUR-vector states. For instance, the eigenstate of the kth excited level of $H^{\phi_1}_{(0)}$ is

$$f^k_{(0)} \equiv |j_k + k, -j_k + k\rangle, \quad j_k = (l_0 + l_1 + 2k)/2, \quad k = 0, 1, 2, \ldots,$$

and $H^{\phi_1}_{(0)}$ (as well as any $H^{\phi_1}_{(m)}$) can be expressed in terms of the su(2)-Casimir $\mathcal{C}$ acting on such representations

$$H^{\phi_1}_{(0)} = 4(\mathcal{C} + 1/4).$$

Therefore, the eigenvalue equation for any of the excited states can be written as follows

$$H^{\phi_1}_{(0)} f^k_{(0)} \equiv 4(\mathcal{C} + 1/4)|j_0 + k, -j_0 + k\rangle = 4(j_0 + k + 1/2)^2 |j_0 + k, -j_0 + k\rangle = (l_0 + l_1 + 2k + 1)^2 f^k_{(0)}$$

with $k = 0, 1, 2, \ldots$.

It will be convenient to consider a new diagonal operator D, to be added to the generators of su(2) (2.14), defined by

$$D f_{(m)} := (l_0 - l_1) f_{(m)}.$$

It is immediate to see that D commutes with any other operator of su(2) giving rise to the Lie algebra u(2). In this way any eigenstate in the Hamiltonian hierarchy can be characterized completely by an eigenfunction of an u(2)-IUR. Without D we would have an ambiguity due to the fact that different fundamental states with values of l_0 and l_1 giving the same $j_0 = (l_0 + l_1)/2$ would lead to the same j representation of su(2).

It is worth noting that when l_0 or l_1 are not in $\mathbb{Z}^+$ the eigenfunctions and spectrum of the Hamiltonian hierarchies are still given by (2.12) and (2.13), but these states belong to nonunitary representations of u(2).

C. The dynamical algebra so(4)

As we have just seen in the previous subsection the eigenstates sharing the same energy of the one-dimensional Hamiltonian hierarchies in the variable ϕ_1 are given in terms of IURs of the dynamical algebra u(2). However, in this respect, there is a point not quite satisfactory: different u(2) IURs may correspond to states with the same energy. We would prefer a larger dynamical algebra with a simpler correspondence, i.e., such that only one of its IURs gives all the eigenstates with the same energy in the hierarchy.

In order to build up a dynamical algebra having these properties, let us introduce the two-dimensional parameter space (l_0, l_1). Any operator with one subindex defined in Secs. II A and II B will change to a two-subindex notation in the following way.

(1) The one-dimensional Hamiltonian (2.4) will be denoted by $H_{(l_0,l_1)}$

$$H^{\phi_1}_{(l_0,l_1)} = -\partial^2_{\phi_1} + \frac{l_0^2 - 1/4}{\cos^2 \phi_1} + \frac{l_1^2 - 1/4}{\sin^2 \phi_1}.$$

Its eigenfunctions will be designed by $f_{(l_0,l_1)}$.

(2) The factor operators $A^\pm_0$ in (2.6) will be rewritten as $A^\pm_{(l_0,l_1)}$

$$A^\pm_{(l_0,l_1)} = \pm \partial_{\phi_1} - (l_0 + 1/2)\tan \phi_1 + (l_1 + 1/2)\cot \phi_1, \quad A_{(l_0,l_1)} = -\tfrac{1}{2}(l_0 + l_1).$$

Now, in this way, relations (2.9) can be expressed as

$$A^-_{(l_0,l_1)}H^{\phi_1}_{(l_0,l_1)} = H^{\phi_1}_{(l_0+1,l_1+1)}A^-_{(l_0,l_1)}, \quad A^+_{(l_0,l_1)}H^{\phi_1}_{(l_0+1,l_1+1)} = H^{\phi_1}_{(l_0,l_1)}A^+_{(l_0,l_1)}. \tag{2.17}$$

With this convention we can also define the free-subindex operators $A^{\pm}$, A, D as in (2.14).

On the other hand, notice that each two-parameter Hamiltonian $H^{\phi_1}_{(l_0,l_1)}$ is invariant under the reflections

$$I_0 := (l_0,l_1) \to (-l_0,l_1), \quad I_1:(l_0,l_1) \to (l_0,-l_1).$$

This property gives rise to a second factorization (see also Refs. 14–16) via conjugation of the operators of the first factorization by the reflection operators

$$I_0A^{\pm}I_0 = \widetilde{A}^{\pm}, \quad I_0AI_0 = \widetilde{A}, \quad I_0DI_0 = \widetilde{D},$$

$$\widetilde{I}_1A^{\pm}I_1 = \widetilde{A}^{\mp}, \quad I_1AI_1 = -\widetilde{A}, \quad I_1DI_1 = -\widetilde{D}.$$

Explicitly

$$\widetilde{A}^{\pm}_{(l_0,l_1)} = \pm\partial_{\phi_1} + (l_0 - 1/2)\tan\phi_1 + (l_1 + 1/2)\cot\phi_1, \quad \widetilde{A}_{(l_0,l_1)} = -\tfrac{1}{2}(-l_0 + l_1). \tag{2.18}$$

The above-mentioned operators $\{\widetilde{A},\widetilde{A}^{\pm}\}$ generate a Lie algebra isomorphic to su(2) denoted by $\widetilde{\mathrm{su}}(2)$. Since su(2) and $\widetilde{\mathrm{su}}(2)$ commute and, essentially, D and $\widetilde{D}$ coincide with $\widetilde{A}$ and A, respectively, the complete dynamical algebra has the structure of a direct sum $\mathrm{su}(2)\oplus\widetilde{\mathrm{su}}(2)\approx\mathrm{so}(4)$.

If we allow to act with the so(4) generators on an Hamiltonian $H_{(l_0,l_1)}$ we will get a two-dimensional parameter lattice of Hamiltonians which constitute a so(4) hierarchy fixed by the initial values (l_0,l_1): $\{H_{l_0-n+m,l_1+n+m}\}$, $m, n \in \mathbb{Z}$. Each energy level of this Hamiltonian hierarchy is degenerated and the eigenstates belong to so(4) representations.

Let us concentrate on the hierarchies associated to IURs of so(4). Now, these so(4) IURs are fixed by the fundamental (or lowest weight) states satisfying

$$A^-_{(l_0,l_1)}f^0_{(l_0,l_1)} = \widetilde{A}^-_{(l_0,l_1)}f^0_{(l_0,l_1)} = 0. \tag{2.19}$$

These are realized, up to a constant, by the wave functions

$$f^0_{(0,n)} = \cos^{1/2}\phi_1 \sin^{n+1/2}\phi_1, \quad n \in \mathbb{Z}^+, \tag{2.20}$$

where we have taken $l_0=0$ and $l_1=n$. We see also that the state (2.20) is stable under I_0 (i.e., $I_0f^0_{(l_0,l_1)}=f^0_{(l_0,l_1)}$), and comes into the other fundamental state (annihilated by A^+ and $\widetilde{A}^+$: the highest weight) of the same representation. Hence, these representations will be invariant under I_0 and I_1. Therefore, the so(4) IURs obtained from (2.20) are symmetric tensor products that can be denoted by

$$j \otimes j, \quad j = l_1/2 = n/2, \quad n \in \mathbb{Z}^{\geqslant 0},$$

where "j" stands for a j representation of su(2). In this way the degenerancy of the nth energy level is $(n+1)\times(n+1)$, which is composed of $n+1$ IURs of u(2) each of them of dimension $n+1$.

The Hamiltonians in this hierarchy can be expressed in terms of any of the su(2) [or $\widetilde{\mathrm{su}}(2)$] Casimir operators $H_{(l_0,l_1)}=4(\mathcal{C}+1/4)=4(\widetilde{\mathcal{C}}+1/4)$. With the help of all the discrete reflections we get directly its expression also in terms of the so(4) Casimir

$$\begin{aligned} H_{(l_0,l_1)} &= (\mathcal{C}+1/4) + I_0(\mathcal{C}+1/4)I_0 + I_1(\mathcal{C}+1/4)I_1 + I_0I_1(\mathcal{C}+1/4)I_0I_1 \\ &= \{A^+,A^-\} + 2A^2 + \{\widetilde{A}^+,\widetilde{A}^-\} + 2\widetilde{A}^2 + 1 = \{A^+,A^-\} + \{\widetilde{A}^+,\widetilde{A}^-\} + {L_0}^2 + {L_1}^2 + 1, \end{aligned}$$

where the diagonal operators L_0 and L_1 are defined by

$$L_0 f_{(l_0,l_1)} = l_0 f_{(l_0,l_1)}, \quad L_1 f_{(l_0,l_1)} = l_1 f_{(l_0,l_1)}.$$

Certainly, some so(4) hierarchies (those corresponding to the IURs previously described) may have Hamiltonians whose explicit expressions coincide

$$H_{(l_0,l_1)} = H_{(-l_0,l_1)} = H_{(l_0,-l_1)}$$

and the same happens with their corresponding eigenstates. But we cannot get rid of this multiplicity unless we enlarge the ambient space.

Another natural question is whether there are other intertwining shape-invariant operators inside the so(4) hierarchy. We can build, for instance, other pairs of operators through the composition of those already known

$$\mathcal{X}^{\pm} = A^{\pm}\tilde{A}^{\pm}, \quad \mathcal{Y}^{\pm} = A^{\pm}\tilde{A}^{\mp}.$$

These kinds of shape-invariant operators change two units, either the parameter l_0 or l_1 (but not both at the same time). When we restrict to $l_0=0$ or $l_1=0$ there are also first order intertwining operators changing one unit the nonvanishing parameter. This feature is not so special; it is also shared by the "radial oscillator" hierarchies[17] (which are closely related to the ones presented here).

For other Hamiltonian so(4) hierarchies the physical eigenstates are described by nonunitary representations that are not invariant under both reflections. In this respect, their description becomes more involved, so that one must be very careful in these cases.

D. The ϕ_2 factorization

Now, let us return to the separation process started in Sec. II A. The second equation (2.5) obtained from the initial separation of variables can be dealt with along the same lines, substituting the eigenvalues obtained from the previous factorization, $\alpha=\lambda_m=(l_0+l_1+2m)^2$. The most relevant fact, here, is that the new factorization leads to a degeneration of the energy levels which suggest that the underlying dynamical symmetry could be larger, as it will be confirmed in the next section. Thus, substituting in (2.5), we have

$$\begin{aligned} H^{\phi_2}_{(0)} &= -\partial^2_{\phi_2} + \tan(\phi_2)\partial_{\phi_2} + \frac{(l_0+l_1+2m+1)^2}{\cos^2(\phi_2)} + \frac{(l_2^2-1/4)}{\sin^2(\phi_2)} \\ &= \{\partial_{\phi_2} - (l_0+l_1+2(m+1))\tan(\phi_2) + (l_2+1/2)\cot(\phi_2)\} \\ &\quad \times \{-\partial_{\phi_2} - (l_0+l_1+2m+1)\tan(\phi_2) + (l_2+1/2)\cot(\phi_2)\} \\ &\quad + (l_2+l_0+l_1+2m+3/2)(l_2+l_0+l_1+2m+5/2) \\ &\equiv M_0^+ M_0^- + \mu_0. \end{aligned} \tag{2.21}$$

This is the first one of the Hamiltonian hierarchy $H^{\phi_2}_{(n)}$ in the variable ϕ_2,

$$H^{\phi_2}_{(n)} = M_n^+ M_n^- + \mu_n = M_{n-1}^- M_{n-1}^+ + \mu_{n-1},$$

where

$$M_n^{\pm} = \pm\partial_{\phi_2} - (l_0+l_1+2(m+1)+n)\tan(\phi_2) + (l_2+n+1/2)\cot(\phi_2),$$

$$\mu_n = (l_1+l_0+l_2+2n+2m+3/2)(l_2+l_1+l_0+2n+2m+5/2).$$

Now, the values for the energy (closely following the same arguments in Sec. II A) are given by

$$E = \mu_n = (l_1 + l_0 + l_2 + 2n + 2m + 3/2)(l_2 + l_1 + l_0 + 2n + 2m + 5/2). \tag{2.22}$$

The fundamental states $g^0_{(n)}$ for this factorization are

$$g^0_{(n)}(\phi_2) = N \cos^{l_1+l_0+2m+1} \phi_2 \sin^{l_2+n+1/2} \phi_2$$

and the eigenfunctions $g^n_{(0)}$ of the initial Hamiltonian (2.21) can be written in the form

$$g^n_{(0)}(\phi_2) = \cos^{l_1+l_0+2m+1} \phi_2 \sin^{l_2+1/2} \phi_2 P_n^{(l_2+1/2, l_1+l_0+2m+1)}(\cos 2\phi_2). \tag{2.23}$$

The commutation relation for the relevant free-index operators $M^{\pm}$, defined in a similar way as $A^{\pm}$ in (2.14), is again that of su(2),

$$[M^-, M^+] = -4(l_1 + l_0 + l_2 + 2m + 2n + 1) \equiv -2M.$$

Eigenfunctions (2.23) are square integrable, but the representations are unitary provided that, besides the previous conditions on l_0 and l_1, the parameter l_2 be also a positive integer number.

In summary, if we finally join the results of both factorizations, the square integrable eigenfunctions of Hamiltonian (2.3) in the separable variables (ϕ_1, ϕ_2) are given by the products

$$\Phi_{m,n}(\phi_1, \phi_2) = f^m_{(0)}(\phi_1) g^n_{(0)}(\phi_2), \quad m, n \in \mathbb{Z}^+, \tag{2.24}$$

where the components have the polynomial expressions (2.12) and (2.23). The corresponding eigenvalues given in (2.22) are degenerated for those values of m and n whose sum $m+n$ keeps constant (see also, for instance, Ref. 11).

III. DYNAMICAL SYMMETRIES

The spectrum obtained by the methods of Sec. II suggests the existence of a bigger dynamical algebra of the Hamiltonian hierarchy. This is the point that we want to address here developing exhaustively the concept of intertwining (shape invariant) operators for this kind of Hamiltonians. Such operators will supply us with a more consistent picture of the spectrum and eigenfunctions. Thus, based on the considerations of Secs. II B and II C, we will introduce three sets of intertwining operators closing the Lie algebra u(3). Then, in the following subsection, we will enlarge this algebra to so(6) by means of the relevant reflections.

A. The Hamiltonian u(3) hierarchies

1. The set $\{A^+, A^-, A\}$

As we will use some properties of Sec. II in a different direction, it is convenient to introduce another notation more appropriate to rewrite some previous results. The Hamiltonian (2.1) characterized by the parameters $\ell \equiv (l_0, l_1, l_2)$ will be referred to as $H_{(l_0,l_1,l_2)}$, and the operators defined by (2.6) will be taken henceforth with a threefold subindex

$$A^{\pm}_{(l_0,l_1,l_2)} = \pm \partial_{\phi_1} - (l_0 + 1/2)\tan \phi_1 + (l_1 + 1/2)\cot \phi_1. \tag{3.1}$$

As differential operators (2.6) and (3.1) depend only on the variable ϕ_1, they do not affect the part in the total Hamiltonian (2.1) depending on the second separable variable ϕ_2. So that, in the same way as (2.17) we have the intertwining relations

$$A^-_{(l_0,l_1,l_2)} H_{(l_0,l_1,l_2)} = H_{(l_0+1,l_1+1,l_2)} A^-_{(l_0,l_1,l_2)},$$

$$A^{+}_{(l_0,l_1,l_2)}H_{(l_0+1,l_1+1,l_2)} = H_{(l_0,l_1,l_2)}A^{+}_{(l_0,l_1,l_2)}.$$

This means that now $A^{-}_{(l_0,l_1,l_2)}$ is acting on eigenstates of $H_{(l_0,l_1,l_2)}$ leading to eigenstates of $H_{(l_0+1,l_1+1,l_2)}$ whereas $A^{+}_{(l_0,l_1,l_2)}$ does it in the opposite way (later we will comment on the square-integrability conditions through unitary representations).

If we include the normalizing constant just as in (2.14), and define global operators acting on eigenfunctions of this class of Hamiltonians in the forms

$$A^{+}\Phi_{(l_0+1,l_1+1,l_2)} := \tfrac{1}{2}A^{+}_{(l_0,l_1,l_2)}\Phi_{(l_0+1,l_1+1,l_2)} \propto \tilde{\Phi}_{(l_0,l_1,l_2)},$$

$$A^{-}\Phi_{(l_0,l_1,l_2)} := \tfrac{1}{2}A^{-}_{(l_0,l_1,l_2)}\Phi_{(l_0,l_1,l_2)} \propto \tilde{\Phi}_{(l_0+1,l_1+1,l_2)},$$

$$A\Phi_{(l_0,l_1,l_2)} := -\tfrac{1}{2}(l_0+l_1)\Phi_{(l_0,l_1,l_2)},$$

we are led to the standard su(2) commutators (2.15). Here, we want to stress again that now these operators are acting on the total wave function of complete Hamiltonians like $H_{(l_0,l_1,l_2)}$, not just on a factor function in only one variable.

In order to introduce other sets of operators we will use the fact that the Hamiltonian (2.1) can be separated in other coordinate systems. Since the axes (s_0,s_1,s_2) play a symmetric role in the Hamiltonian, we will take their cyclic rotations to get two other sets of coordinates and, hence, new sets of intertwining operators.

2. The set $\{B^{+},B^{-},B\}$

We will take the spherical coordinates choosing as third axis not s_2, but s_1, i.e.,

$$s_2 = \cos\xi_2\cos\xi_1, \quad s_0 = \cos\xi_2\sin\xi_1, \quad s_1 = \sin\xi_2. \tag{3.2}$$

Then, the initial Hamiltonian is also separated in the coordinates (ξ_1,ξ_2). In particular, we can build the operators $B^{\pm}_{(l_0,l_1,l_2)}$ in a similar way as $A^{\pm}_{(l_0,l_1,l_2)}$. From coordinate systems (2.2) and (3.2) we easily arrive at the following expressions for the new set in terms of the initial coordinates (ϕ_1,ϕ_2):

$$B^{\pm}_{(l_0,l_1,l_2)} = \pm(\sin\phi_1\tan\phi_2\partial_{\phi_1} + \cos\phi_1\partial_{\phi_2}) - (l_2+1/2)\cos\phi_1\cot\phi_2 + (l_0+1/2)\sec\phi_1\tan\phi_2. \tag{3.3}$$

These operators intertwine the pair of Hamiltonians

$$B^{-}_{(l_0,l_1,l_2)}H_{(l_0,l_1,l_2)} = H_{(l_0+1,l_1,l_2+1)}B^{-}_{(l_0,l_1,l_2)},$$

$$B^{+}_{(l_0,l_1,l_2)}H_{(l_0+1,l_1,l_2+1)} = H_{(l_0,l_1,l_2)}B^{+}_{(l_0,l_1,l_2)}.$$

The "global" operators, defined by

$$B^{+}\Phi_{(l_0+1,l_1,l_2+1)} := \tfrac{1}{2}B^{+}_{(l_0,l_1,l_2)}\Phi_{(l_0+1,l_1,l_2+1)} \propto \tilde{\Phi}_{(l_0,l_1,l_2)},$$

$$B^{-}\Phi_{(l_0,l_1,l_2)} := \tfrac{1}{2}B^{-}_{(l_0,l_1,l_2)}\Phi_{(l_0,l_1,l_2)} \propto \tilde{\Phi}_{(l_0+1,l_1,l_2+1)},$$

$$B\Phi_{(l_0,l_1,l_2)} := -\tfrac{1}{2}(l_0+l_2)\Phi_{(l_0,l_1,l_2)},$$

also close a new su(2).

3. The set $\{C^+, C^-, C\}$

Finally, taking the spherical coordinates around the s_0 axis,

$$s_1 = \cos\theta_2 \cos\theta_1, \quad s_2 = \cos\theta_2 \sin\theta_1, \quad s_0 = \sin\theta_2$$

the Hamiltonian is also separated in the variables $\{\theta_1, \theta_2\}$ and we get a new pair of operators, that written in terms of the initial ϕ_1 and ϕ_2 variable, take the expression

$$C^{\pm}_{(l_0,l_1,l_2)} = \pm(\cos\phi_1 \tan\phi_2 \partial_{\phi_1} - \sin\phi_1 \partial_{\phi_2}) + (l_1 - 1/2)\csc\phi_1 \tan\phi_2 + (l_2 + 1/2)\sin\phi_1 \cot\phi_2. \tag{3.4}$$

These operators act as intertwiners of the Hamiltonians in the following way:

$$C^-_{(l_0,l_1,l_2)} H_{(l_0,l_1,l_2)} = H_{(l_0,l_1-1,l_2+1)} C^-_{(l_0,l_1,l_2)},$$

$$C^+_{(l_0,l_1,l_2)} H_{(l_0,l_1-1,l_2+1)} = H_{(l_0,l_1,l_2)} C^+_{(l_0,l_1,l_2)}.$$

The global operators are defined by

$$C^+\Phi_{(l_0,l_1-1,l_2+1)} := \tfrac{1}{2} C^+_{(l_0,l_1,l_2)} \Phi_{(l_0,l_1-1,l_2+1)} \propto \tilde{\Phi}_{(l_0,l_1,l_2)},$$

$$C^-\Phi_{(l_0,l_1,l_2)} := \tfrac{1}{2} C^-_{(l_0,l_1,l_2)} \Phi_{(l_0,l_1,l_2)} \propto \tilde{\Phi}_{(l_0,l_1-1,l_2+1)},$$

$$C\Phi_{(l_0,l_1,l_2)} := -\tfrac{1}{2}(-l_1 + l_2)\Phi_{(l_0,l_1,l_2)},$$

closing the third algebra su(2). Notice that $C = B - A$.

In fact, as we saw in Sec. II, each separable system gives rise to two sets of intertwining operators (in that section distinguished by means of the tilde). However, here we have made a "good" choice of the previous three sets that will close a Lie algebra (on this point see Sec. III B).

4. The complete algebra u(3)

Now, we can join all the above-defined transformations, $A^{\pm}$, A, $B^{\pm}$, B, $C^{\pm}$, C, and commute any two of them to check that indeed they close a Lie algebra su(3). The nonvanishing commutators are

$$[A^3, A^{\pm}] = \pm A^{\pm}, \quad [A^-, A^+] = 2A, \quad [A^+, B^-] = C^-, \quad [A^+, B] = -A^+/2,$$

$$[A^+, C^+] = -B^+, \quad [A^+, C] = A^+/2, \quad [A^-, B^+] = -C^+, \quad [A^-, B] = A^-/2,$$

$$[A^+, C^+] = B^-, \quad [A^-, C] = -A^-/2, \quad [A, B^+] = B^+/2, \quad [A, C^+] = -C^+/2,$$

$$[A, C^-] = C^-/2, \quad [B, B^{\pm}] = \pm B^{\pm}, \quad [B^-, B^+] = 2B, \quad [B^+, C^-] = -A^+,$$

$$[B^+, C] = -B^+/2, \quad [B^-, C^+] = C^+/2, \quad [B^-, C] = B^-/2, \quad [B, C^+] = C^+/2,$$

$$[B, C^-] = C^-/2, \quad [C, C^{\pm}] = \pm C^{\pm}, \quad [C^+, C^-] = 2C, \quad [A^-, C^-] = B^-.$$

The Casimir operator is given by

$$\mathcal{C} = A^+A^- + B^+B^- + C^+C^- + \tfrac{2}{3}A(A-3/2) + \tfrac{2}{3}B(B-3/2) + \tfrac{2}{3}C(C-3/2). \tag{3.5}$$

In order to complete an algebra u(3) we can add a diagonal operator D commuting with all the above-mentioned transformations. It is a central operator, i.e.,

$$D := l_0 - l_1 - l_2, \quad [D, \cdot\,] = 0.$$

We can also adopt the global operator convention H for the Hamiltonians in the hierarchy by defining its action on the eigenfunctions $\Phi_{(l_1,l_2,l_3)}$ of $H_{(l_1,l_2,l_3)}$ by

$$H\Phi_{(l_1,l_2,l_3)} := H_{(l_1,l_2,l_3)}\Phi_{(l_1,l_2,l_3)}.$$

In this way we can express the Hamiltonian H in terms of both operators $\mathcal{C}$ and D

$$H = 4\mathcal{C} - \tfrac{1}{3}D^2 + \tfrac{15}{4}. \tag{3.6}$$

In the case of one-dimensional systems, one (first order) intertwining set $\{A^\pm\}$ for the Hamiltonian gives rise to its factorization. However, for Hamiltonians with more degrees of freedom (more components, or in more dimensions) the relationship of H with these operators, in general, turns out to be more complex. In our case the set $\{A^\pm, B^\pm, C^\pm\}$ according to expressions (3.5) and (3.6) is enough to express the Hamiltonian as a certain quadratic function $H=h(A^+A^-, B^+B^-, C^+C^-)$ generalizing the usual factorization.

In summary, we have built an algebra u(3) of intertwining operators that, once fixed the initial Hamiltonian with parameter values (l_0, l_1, l_2), gives rise to a two-parameter Hamiltonian hierarchy

$$\{H_{(l_0+m, l_1+m-n, l_2+n)}\}, \quad m,n \in \mathbb{Z}$$

where the points (l_0+m, l_1+m-n, l_2+n) lie on a certain plane $D=d_0$. In this subsection we will consider this special hierarchy, together with its eigenstates, connected to the IURs of u(3). The states of such representations are square integrable and, therefore, should take part of the physical eigenfunctions whose energy eigenvalues belong to the spectrum.

In order to build an IUR we start from a fundamental state Φ annihilated by A^- and C^- [two simple roots of su(3)]

$$A^-_\ell \Phi_\ell = C^-_\ell \Phi_\ell = 0 \tag{3.7}$$

with $\ell=(l_0, l_1, l_2)$. Such states exist only when $l_1=0$, taking the explicit form

$$\Phi_\ell(\phi_1, \phi_2) = N \cos^{l_0+1/2}\phi_1 \sin^{1/2}\phi_1 \cos^{l_0+1}\phi_2 \sin^{l_2+1/2}\phi_2, \tag{3.8}$$

where N is a normalizing constant. The diagonal operators A and C act on Φ_ℓ as

$$A\Phi_\ell = -l_0/2\Phi_\ell, \quad l_0 = m, \quad l_1 = 0, \quad m = 0,1,2,\ldots,$$

$$C\Phi_\ell = -l_2/2\Phi_\ell, \quad l_2 = n, \quad n = 0,1,2,\ldots. \tag{3.9}$$

This means that Φ_ℓ is a fundamental state of the representations $j_1=m/2$ of the subalgebra su(2) generated by $\{A^\pm, A\}$, and $j_2=n/2$ of the corresponding su(2) determined by $\{C^\pm, C\}$. Such a representation of su(3) will be denoted (m,n) with $m,n \in \mathbb{Z}^+$. The points labeling the states of this representation obtained from Φ_ℓ lie on the plane $D=m-n$ inside the ℓ-parameter space.

The energy for the states of the IURs determined by the fundamental state (3.9) with the parameters $(l_0, 0, l_2)$, according to (3.6) is given by

$$E = (l_0 + l_2 + 3/2)(l_0 + l_2 + 5/2) = (m + n + 3/2)(m + n + 5/2). \tag{3.10}$$

Therefore, the IURs fixed by (m,n) with the same value $m+n$ will lead to states with the same energy. We call such IURs an isoenergy series and they will be examined under the light of the algebra so(6) in the following section. The values for the energy (3.10) coincide with the ones

computed by the method of variable separation of Sec. II, as can be seen from (2.22) once the replacement $l_1=1/2$ is performed. We can also check that in this case the ground state (2.24) coincides with those fixing an IUR (3.8).

B. The so(6) hierarchy

Following the pattern and motivation of Sec. II C, we will consider the relevant discrete symmetries in order to find a larger dynamical algebra.

It is obvious that the Hamiltonian $H_{(l_0,l_1,l_2)}$ is invariant under reflections in the parameter space $\{(l_0,l_1,l_2)\}$

$$I_0{:}(l_0,l_1,l_2)\to(-l_0,l_1,l_2),\quad I_1{:}(l_0,l_1,l_2)\to(l_0,-l_1,l_2),\quad I_2{:}(l_0,l_1,l_2)\to(l_0,l_1,-l_2).$$

Each of these symmetries can be directly implemented in the eigenfunction space, leading through conjugation to another set of intertwining operators that close a Lie algebra isomorphic to u(3) and denoted by ${}_i\mathrm{u}(3)$

$${}_iX=I_iXI_i,\quad X\in\mathrm{u}(3),\quad {}_iX\in{}_i\mathrm{u}(3),\quad i=0,1,2.$$

The intertwining operators of ${}_i\mathrm{u}(3)$ connect eigenstates of Hamiltonians whose parameters (l_0,l_1,l_2) belong to the planes ${}_iD=k_i$, k_i being certain real constants. We will choose the following convention for the resulting generators

$$\{A^{\pm},B^{\pm},C^{\pm}\}\xrightarrow{I_0}\{\tilde{A}^{\mp},\tilde{B}^{\mp},C^{\pm}\},$$

$$\{A^{\pm},B^{\pm},C^{\pm}\}\xrightarrow{I_1}\{\tilde{A}^{\pm},B^{\pm},\tilde{C}^{\pm}\},$$

$$\{A^{\pm},B^{\pm},C^{\pm}\}\xrightarrow{I_2}\{A^{\pm},\tilde{B}^{\pm},\tilde{C}^{\mp}\},$$

where, for instance, the sets $\{A^{\pm},A\}$ and $\{\tilde{A}^{\pm},\tilde{A}\}$ close the two commuting Lie algebras su(2) of Sec. II. The explicit expression for the new operators (labeled with a tilde) can be easily obtained in the same way as it was done in (2.18). The set of all the generators obtained in this process close the Lie algebra of rank 3, so(6). In the eigenfunction space it is enough to consider three independent diagonal operators $\{L_0,L_1,L_2\}$ defined by

$$L_i\Phi_{(l_0,l_1,l_2)}=l_i\Phi_{(l_0,l_1,l_2)}.$$

The Hamiltonian can be expressed in terms of the so(6)-Casimir operator by means of the "symmetrization" of the u(3) Hamiltonian (3.6)

$$\begin{aligned}H_{\mathrm{so}(6)}&=\tfrac{1}{8}\Big(H_{\mathrm{u}(3)}+\sum_j I_jH_{\mathrm{u}(3)}I_j+\sum_{j\neq k}I_jI_kH_{\mathrm{u}(3)}I_jI_k+I_0I_1I_2H_{\mathrm{u}(3)}I_0I_1I_2\Big)\\&=\{A^+,A^-\}+\{B^+,B^-\}+\{C^+,C^-\}+\{\tilde{A}^+,\tilde{A}^-\}+\{\tilde{B}^+,\tilde{B}^-\}+\{\tilde{C}^+,\tilde{C}^-\}+{L_0}^2+{L_1}^2+{L_2}^2+\tfrac{41}{12}.\end{aligned}$$

Henceforth we remove the subindex so(6) of the Hamiltonian.

The intertwining generators of so(6) give rise to larger three-dimensional Hamiltonian hierarchies

$$\{H_{(l_0+m+p,l_1+m-n-p,l_2+n)}\},\quad m,n,p\in\mathbb{Z},$$

each one including a class of the previous ones coming from u(3). The eigenstates of these Hamiltonian hierarchies can be classified in terms of so(6) representations. Let us fix our attention in those determined by the so(6) IURs. These IURs are built from the fundamental states annihilated by the simple roots $A^-,C^-,\tilde{A}^-$

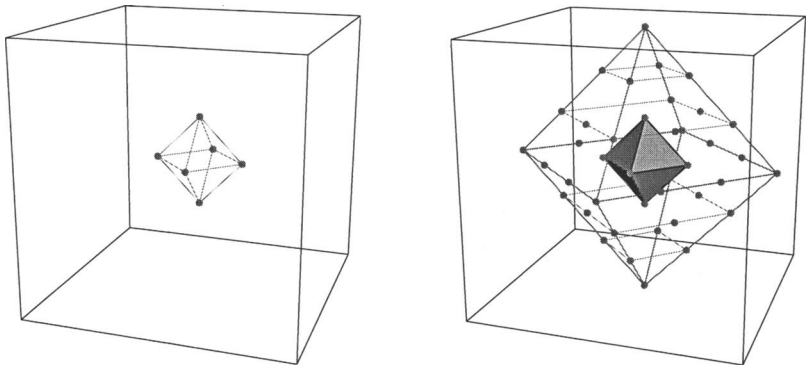

FIG. 1. Plot of the points representing the states of two odd IURs with (left) $q=1$ and (right) $q=3$. The 6 ($q=1$) eigenstates share the energy $E=\frac{5}{2}\cdot\frac{3}{2}$. The 50 ($q=3$) eigenstates share the energy $E=\frac{7}{2}\cdot\frac{5}{2}$ (the points corresponding to $q=3$ include those of $q=1$, of the inner octahedron, which are doubly degenerated).

$$A^-\Phi_\ell^{(0)} = C^-\Phi_\ell^{(0)} = \tilde{A}^-\Phi_\ell^{(0)} = 0.$$

The equations for the operators A^- and C^- have been used in (3.7), whereas the one for $\tilde{A}^-$ were already applied in (2.19). Therefore, the wave functions of the highest weight vectors take the form

$$\Phi_\ell^{(0)}(\phi_1,\phi_2) = N\cos^{1/2}\phi_1 \sin^{1/2}\phi_1 \cos\phi_2 \sin^{l_2+1/2}\phi_2$$

characterized by the eigenvalues of the diagonal operators,

$$L_0\Phi_\ell = L_1\Phi_\ell = 0, \quad L_2\Phi_\ell = n\Phi_\ell, \quad n \in \mathbb{Z}^+.$$

This fundamental state is invariant under the inversions I_0 and I_1, and the representation, so obtained, is also invariant under I_2. Thus, in this way we arrive at two classes of symmetric IURs of so(6)

(a) $(l_0=0,\ l_1=0,\ l_2=0)$; $\{H_{(m+p,m-n-p,n)}\}$, $n,\ m,\ p \in \mathbb{Z}$ (even IURs) and
(b) $(l_0=0,\ l_1=0,\ l_2=1)$; $\{H_{(m+p,m-n-p,1+n)}\}$, $n,\ m,\ p \in \mathbb{Z}$ (odd IURs).

Each of these IURs is described in the parameter space by an octahedral lattice of points such that it will include an isoenergy su(3) [or ${}_i$su(3)] series of representations, quoted in the previous subsection, which correspond to parallel exterior faces of the octahedron and some of its sections. Such sections are determined by the values of the diagonal operator D (or ${}_iD$) whose values fix the corresponding u(3) representations.

For instance, the so(6) representation labeled by $q=1$, corresponding to the odd hierarchy, includes the first su(3) series, (1, 0) and (0, 1) described by the opposite faces of an elemental octahedron. The so(6) representation of the even hierarchy fixed by $q=2$ includes the su(3) series made of (2, 0), (1, 1), and (0, 2). Those associated to (2, 0) and (0, 2) correspond to opposite triangular faces, whereas (1, 1) is described by the parallel hexagonal section through the origin. These features can be better appreciated in Figs. 1 and 2.

In general, the so(6) IURs fixed by the parameter q will include the isoenergy series of the su(3) representations labeled by (m,n) with $m+n=q$. This is the degeneration explained by the larger algebra so(6). A similar discussion can be done with respect to the representations of the su(2) $\oplus$ $\tilde{\text{su}}$(2) subalgebra. They can be identified with square sections of the octahedron.

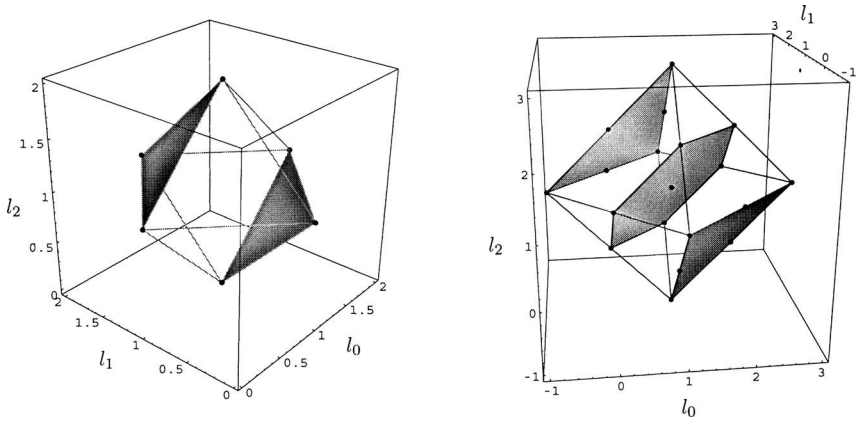

FIG. 2. (Left) $q=1$ IUR of so(6) where the triangular opposite faces correspond to two IURs of su(3). (Right) Points of a $q=3$ IUR of so(6). The three sections describe three IURs of su(3).

IV. EIGENSTATES AND FACTORIZATIONS

Let H_ℓ and $H_{\ell'}$ be two Hamiltonians related by means of a differential operator X in the following form

$$XH_\ell = H_{\ell'}X \Rightarrow X^\dagger H_{\ell'} = H_\ell X^\dagger, \tag{4.1}$$

where the dagger denotes adjoint differential operators. Then, it is said that X is an intertwining operator connecting H_ℓ with $H_{\ell'}$.

In a formal way, the eigenfunctions of H_ℓ are transformed by X into eigenfunctions of $H_{\ell'}$, but one must be careful about the behavior of some properties, such as square-integrability, singularities, or boundary conditions, which might be altered by X. The intertwining problem just as introduced in (4.1), which applies to the u(3) system of Sec. III, takes into account shape invariance, in the sense that the partner Hamiltonian $H_{\ell'}$ differs from the initial H_ℓ simply by changing the values of the parameters: $\ell \to \ell'$. In general, shape invariance leads to an algebraic structure of the intertwining operators as it happens in our present case.

Now, we will discuss in this section the form of the su(3) intertwining operators of Sec. III and its relation to certain eigenstates [similar considerations also apply to so(6)]. First of all, note that we can write such operators [see expressions (3.1), (3.3), and (3.4)] as

$$A_\ell^\pm = a^\pm + \alpha_\ell, \quad B_\ell^\pm = b^\pm + \beta_\ell, \quad C_\ell^\pm = c^\pm + \gamma_\ell \tag{4.2}$$

where $a^\pm$, $b^\pm$, and $c^\pm$ stand for vector fields (expressed, for instance, in the variables ϕ_1, ϕ_2) defined on the sphere and α_ℓ, β_ℓ, γ_ℓ design functions also defined on the sphere. Notice that

$$a^+ = (a^-)^\dagger = J_2, \quad b^+ = (b^-)^\dagger = J_1, \quad c^+ = (c^-)^\dagger = J_0$$

where J_0, J_1, and J_2 close the rotation algebra so(3). Moreover, taking the hermitian conjugate we have made use of the invariant measure on the sphere. If we write the Hamiltonians in the hierarchy displaying the kinetic (or free) part and the potential as

$$H_\ell = H^{(\mathrm{kin})} + V_\ell$$

we see that the vector fields originate the kinetic term, i.e.,

$$H^{(\mathrm{kin})} = a^+a^- + b^+b^- + c^+c^-$$

and the components α_ℓ, β_ℓ, and γ_ℓ (defined on the sphere) give rise to the potential $V_\ell(\phi_1, \phi_2)$, labeled by the parameters $\ell \equiv (l_0, l_1, l_2)$. Substituting (4.2) into Hamiltonian (3.6) and taking into account (3.5), we get the expression

$$V_\ell(\phi_1,\phi_2) = (a_\ell)^2 + (a^+\alpha_\ell) + (\beta_\ell)^2 + (b^+\beta_\ell) + (\gamma_\ell)^2 + (c^+\gamma_\ell) + \lambda_\ell, \tag{4.3}$$

where γ_ℓ is a number depending on l_0, l_1, l_2. Equation (4.3) can be considered as a nonlinear partial differential equation linking the unknowns $\{\alpha_\ell,\beta_\ell,\gamma_\ell\}$ with the potential, in a quite similar way to the Riccati equation for the superpotential ω in the one-dimensional Schrödinger equation. For this reason, we sometimes will refer to $\{\alpha_\ell,\beta_\ell,\gamma_\ell\}$ as superpotential functions. This is in agreement with a more general result[2,3] where the first order intertwining is built by dressing the symmetries of the Laplacian operator with certain functions.

The basic property of the one-dimensional superpotential ω was that it could be considered as the logarithmic derivative of a Hamiltonian eigenstate [see (2.10)]. Here, we have something similar with respect to the superpotentials $\{\alpha_\ell,\beta_\ell,\gamma_\ell\}$ but first we want to settle this problem in general terms. If we know an intertwining operator X satisfying (4.1) it can help us in computing certain eigenfunctions of H_ℓ. Notice that if we define the kernel, $\mathcal{K}_X$, of X as the linear manifold of wave-functions annihilated by X,

$$X\psi = 0, \quad \forall\ \psi \in \mathcal{K}_X$$

then, such a space is invariant under the Hamiltonian operator H_ℓ. Thus, we can look for eigenfunctions inside $\mathcal{K}_X$, in general a much simpler problem. But, in the case of X being a partial differential operator, its kernel includes certain arbitrary functions, so it is still an infinite dimensional space. This is in sharp contrast with ordinary first order differential operators where the kernel is one-dimensional.

Another option we have at hand is the following. The intertwining relation (4.1) implies the commutation

$$X^\dagger X H_\ell = H_\ell X^\dagger X.$$

This means that we can look for eigenfunctions of H_ℓ inside any eigenfunction space of $X^\dagger X$, not necessarily that one annihilated by X, as was the case just considered previously. In this case, however, a similar expression to (2.10) in terms of such eigenfunctions is no longer valid for ω. When we know several intertwining operators, as in the present case, we can apply them in different ways according to the above-mentioned comments.

(i) *Superpotentials associated to a global fundamental eigenstate of* $\{A^-,B^-,C^-\}$. We consider the intersection of the kernels of all the intertwining operators. Assuming that this subspace is one-dimensional we have just one eigenstate (up to a factor) Φ_0 annihilated by all the lowering operators $\{A^-,B^-,C^-\}$, so that we obtain the following expressions quite similar to (2.10)

$$\alpha_\ell = -\frac{(a^-\Phi_0)}{\Phi_0}, \quad \beta_\ell = -\frac{(b^-\Phi_0)}{\Phi_0}, \quad \gamma_\ell = -\frac{(c^-\Phi_0)}{\Phi_0}. \tag{4.4}$$

This mechanism corresponds to the IURs characterized in Sec. III.

(ii) *Superpotentials associated to a partial fundamental eigenstate*. If the previous subspace is the trivial null space, we can still restrict ourselves to the kernel subspace of anyone of the intertwining operators, for example A^-. Thus, let Φ be an eigenfunction of H_ℓ with $\Phi \in \mathcal{K}_{A^-}$, i.e., $A^-\Phi = 0$. This allows us to set

$$\alpha_\ell = -(a^-\Phi)/\Phi.$$

From this equation we can also separate variables in Φ, so that the eigenfunction equation $H\Phi = E\Phi$ leads to a second order ordinary differential equation whose solution can be easily obtained.

However, we must outline that in this case the remaining superpotential functions β_ℓ, γ_ℓ

have not a simultaneous expression (4.4) in terms of the same Φ, they need different eigenfunctions. Under this point of view, Sec. II constitutes an illustration of how this option leads to eigenfunctions separated in the variables ϕ_1, ϕ_2.

(iii) *Other excited eigenstates*. The second option is to solve, for instance, the eigenvalue problem $A^+A^-\Phi=\alpha\Phi$, requiring at the same time Φ to be also a Hamiltonian eigenfunction. In terms of the ambient coordinates s_0, s_1, s_2 this equation is (see also Ref. 11)

$$\left\{-\left(s_1\frac{\partial}{\partial s_0}-s_0\frac{\partial}{\partial s_1}\right)^2+(l_0-1/4)\frac{s_0^2+s_1^2}{s_0^2}+(l_1-1/4)\frac{s_0^2+s_1^2}{s_1^2}\right\}\Phi=\alpha\Phi.$$

The same procedure can be applied with other more general sets of operators commuting with the Hamiltonian. For instance, we can diagonalize H inside the subspace

$$(e_2A^+A^-+e_1B^+B^-+e_0C^+C^-)\Phi=\alpha\Phi$$

where the e_i's are constant coefficients. This leads to eigenfunctions separated in elliptic coordinates, that we do not consider here.[11]

V. CONCLUSIONS

We have shown how to deal with the u(3) [and the general u(n) case[9,18] follows the same pattern[19]] analog of a class of factorizable one-dimensional potentials with underlying dynamical algebra u(2). The higher rank systems in consideration are well known inside the class of superintegrable Hamiltonians and, of course, our objective was not to compute original eigenfunctions. Our interest was to apply a different point of view to understand some properties in a new context. For instance, the classification of the irreducible representations of su(3) in series corresponding to so(6) octahedrons, and the relations involved in this framework is a nontrivial result that could be best appreciated inside the intertwining technique. The relation of the unitary representations with a special form of the superpotential functions, or the separable eigensolutions determined in terms of intertwining operators clarifies some of the known procedures.

We have seen how the elements of one-dimensional factorizations must be adapted to the new context. For example, the relation of superpotentials and a whole class of eigenfunctions (not just one), the expression of the Hamiltonian operator is not just a simple factorization, the lattice of states must be drawn in a three-dimensional space, etc.

There are several problems that can be addressed using the present procedure. The systems underlying noncompact algebras u(p,q), inhomogeneous Lie algebras $iu(p,q)$ and contracted algebras[20] are among the first applications that we expect to report in a near future. But, in general, other integrable Hamiltonian systems could also allow for this treatment, with or without variable separation. This application would be of most interest.

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Discrete and continuous sine transform generalized to semisimple Lie groups of rank two

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A new continuous group transform, together with its discretization over a lattice of any density and admissible symmetry, is defined and described for the four compact semisimple Lie groups of rank 2. In the case of rank 1, the discrete version is the sine transform. Properties of the expansion functions of the transform, called *S*-functions, are studied. Digital data processing is our motivating application.
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I. INTRODUCTION

The present paper is the concluding but independent part of a series of three articles.[1,2] Previous papers, which also include Refs. 3–7, dealt with properties of *C*-functions [see Eq. (3.2)]. General comments and motivation to our study are found in those papers. Originally the *C*-functions of this paper were called "orbit functions" or "orbit sums."[8]

Our subject in this paper are analogous properties of *S*-functions [see Eq. (3.1)]. Both types of functions are based on compact semisimple Lie groups. The rank of the group is the number of continuous variables of the *C*- and *S*-functions. Since our main motivation are two-dimensional applications, we are focused on Lie groups of rank 2, although most of the properties of *S*-functions described in Sec. III are general as to the type and rank of semisimple compact Lie group.

The *S*-functions are known in Lie theory mainly from the Weyl character formula, where an irreducible character of a representation labeled by its highest weight λ, is written as the ratio of two *S*-functions, say $S_{\lambda+\rho}$ and S_ρ, where ρ is the half-sum of positive roots of the Lie group. In this article we make use of the *S*-functions in a very different way. Apparently, no group transforms based on *S*-functions, either continuous or discrete, have been considered elsewhere in the literature (except in Ref. 9).

Let us point out that recently a third type of generalization of one-dimensional group transforms was introduced.[9] The expansion functions in that case, called *E*-functions, are multidimensional generalizations of the exponential function. Their properties will be studied elsewhere.[10]

Among the possible applications, the most interesting to us in this paper, is decomposition of class functions on a compact semisimple Lie group. Such a decomposition takes place on the fundamental region *F* of the Lie group where each conjugacy class of the group is represented by precisely one point. It is a basic problem of Fourier analysis which in theory is solved by decomposition of the functions into series of irreducible characters of the group. In practice that is hardly ever done even in one dimension for a number of reasons. Let us point out at least two of them.

First, characters are complicated functions. Their complexity rapidly increases without limits, the higher is the underlying irreducible representation. They are built either as a ratio of polyno-

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mials of ever increasing degree, or as integer linear combination of *C*-functions.[7] Coefficients of the linear combinations are the multiplicities of dominant weights. Finding the coefficients is a laborious computational task. Look-up tables[11] offer only limited help.

Our second objection is related to the behavior of irreducible characters (and also *C*-functions) at the boundary ∂F of F. Both are symmetric with respect to reflection in any side of F of maximal dimension, i.e., $n-1$. Thus both being continuous functions, their normal derivative at ∂F must be zero (Neumann conditions). Clearly functions on F which have a different behavior at ∂F cannot be satisfactorily decomposed either into series of irreducible characters or *C*-functions. The *S*-functions are antisymmetric with respect to reflections in the sides of F. Therefore, being continuous, they go through zero at ∂F.

In two dimensions there are four families of *C*-functions and four families of *S*-functions. The families are determined by compact semisimple Lie groups.

There are three compact simple Lie groups of rank 2, namely the following: SU(3), O(5) or Sp(4), and G(2). There is only one nonsimple but semisimple compact Lie group: $\mathrm{SU}(2)\times\mathrm{SU}(2)$. In this article, we use the notation more familiar in Lie algebra theory:

$$\mathrm{A}_1 \leftrightarrow \mathrm{SU}(2),$$

and

$$\mathrm{A}_1 \times \mathrm{A}_1 \leftrightarrow \mathrm{SU}(2) \times \mathrm{SU}(2), \quad \mathrm{A}_2 \leftrightarrow \mathrm{SU}(3),$$

$$\mathrm{C}_2 \leftrightarrow \mathrm{O}(5) \text{ or } \mathrm{Sp}(4), \quad \mathrm{G}_2 \leftrightarrow \mathrm{G}(2).$$

In principle, one could also consider the compact Lie groups of rank 2 $\mathrm{U}(1)\times\mathrm{U}(1)$ and $\mathrm{U}(1)\times\mathrm{SU}(2)$, which are not semisimple, and which only lead to the traditional Fourier decompositions. Here we disregard those cases.

Two and two of the four groups of rank 2 are related by their root and weight lattices. Specifically, for $\mathrm{A}_1\times\mathrm{A}_1$ and C_2 the lattices are rectangular, whereas they are triangular for A_2 and G_2.

Discrete expansions of functions given on the fundamental region of a compact semisimple Lie group in terms of *S*-functions are described here for the first time. It turns out that the discretization of *C*-function expansions laid out in Ref. 8 is valid also for *S*-functions with only minimal modifications. In the one-dimensional case the transforms are known and are called cosine and sine transforms, respectively.[12]

The main goal of this article is to describe properties of the *S*-functions, and their exploitation for continuous and discrete expansions of class functions of the corresponding Lie group of rank 2, into a series of *S*-functions. We provide such a description in an explicit ready-to-use form. Apparently such expansions have not been considered in the literature. Crucial property for the expansions is the orthogonality of *S*-functions, both continuous and discrete. For rank 2 that is shown by direct computation. In general, for compact semisimple Lie groups of any rank $n<\infty$, it is proven elsewhere.[13]

In one dimension the underlying group is the group A_1. Expansion functions in this case are the familiar ones:

$$C\text{-functions of } \mathrm{A}_1\text{:} \quad C_m(z) \overset{\text{def}}{=} 2\cos(\pi m z), \quad m \in \mathbb{Z}^{\geqslant 0}, z \in \mathbb{R},$$

$$S\text{-functions of } \mathrm{A}_1\text{:} \quad S_m(z) \overset{\text{def}}{=} 2i\sin(\pi m z), \quad m \in \mathbb{N}, z \in \mathbb{R}.$$

In higher dimensions, *C*-functions generalize cosines, whereas the *S*-functions generalize sines. From that we take the terms *C*- and *S*-functions.

An observation, important for the generalization, is that in 1-dimension the functions inside of either family are orthogonal not only when integrated over $0 \leqslant z \leqslant 2$, but already when they are integrated over $0 \leqslant z \leqslant 1$. That range of z is the fundamental region F of A_1.

Let us point out properties of the (continuous) C- and S-functions which they have in common and where they differ.

(a) Minimal domains of their orthogonality coincide. It is the fundamental region F of the corresponding Lie group.
(b) C- and S-functions with the same dominant weight have the same number of exponential constituents.
(c) The symmetry properties of C- and S-functions with respect of the affine Weyl group coincide up to a sign.
(d) C- and S- functions are eigenfunctions of the same Laplace operators. Their eigenvalues are up to a constant equal to the square length of their dominant weights.
(e) Discretizations of both families is made on identically defined grids in F.
(f) Products of any two C-functions decompose into a sum of C-functions with positive integer coefficients. Products of any C- and S-function decomposes into a sum of S-functions with positive integer coefficients. Products of any two S-functions decompose into a sum of C-functions with integer coefficients. Only the highest and the lowest terms in such decompositions are easily determined. Efficient and general algorithms for the decompositions are yet to be found.
(g) Dominant weights labeling C-functions are in the positive Weyl chamber P^+ of the weight lattice P. Dominant weights labeling S-functions are restricted to the interior P^{++} of P^+. More precisely, S-functions with dominant weight at the boundary of P^+ turn out to be zero. One has $P^{++} \subset P^+ \subset P$.

Let us underline some notations used throughout the article. The symbols $\mathbb{C}$, $\mathbb{R}$, $\mathbb{Z}$, and $\mathbb{N}$ denote complex, real, integer, and positive integer numbers, respectively. In a real Euclidean space $\mathbb{R}^2$ of dimension two the form $\langle a|b\rangle$ denotes the scalar product of $a,b \in \mathbb{R}^2$, whereas in the complex space of functions, it denotes a Hermitian form.

In Sec. II we present a brief introduction to one-dimensional S-functions and an overview of the one-dimensional S-function transform; Sec. III describes the S-functions in the general case, whereas the cases for the four compact semisimple groups of rank two are described in Sec. IV; polynomials derived from C- and S-functions are briefly presented in Sec. V; Sec. VI contains the discretization of the S-function transforms for all the two-dimensional cases; some comparative examples are given in Sec. VII; and, finally, the concluding remarks are found in Sec. VIII.

II. THE GROUP A_1

The rank 1 case is transparent without reference to the underlying simple Lie group A_1.

A. The continuous case

The S-functions of A_1 happen to be the familiar periodic functions

$$S_m(z) = 2i \sin(\pi m z), \quad m \in \mathbb{N}, \quad z \in \mathbb{R}. \tag{2.1}$$

In particular

$$S_m(0) = S_m(1) = \cdots = S_m(k) = 0, \quad \forall\, k \in \mathbb{Z}.$$

Note that $m=0$ is excluded from consideration in Eq. (2.1). The functions are pairwise orthogonal. Indeed, the Hermitian form of two S-functions

$$\langle S_m(z)|S_{m'}(z)\rangle \overset{\text{def}}{=} \int_0^1 S_m(z)\overline{S_{m'}(z)}\mathrm{d}z = \int_0^1 4\sin(\pi m z)\sin(\pi m' z)\mathrm{d}z \sim \delta_{m,m'}.$$

Consequently, the continuous sine transform is the expansion of functions over $0 \leqslant z \leqslant 1$ and its inversion,

$$f(z) = \sum_{m=1}^{\infty} d_m S_m(z),$$

where the expansion coefficients d_m are obtained from

$$d_m \sim \langle f(z)|S_m(z)\rangle = \int_0^1 f(z)\cdot(-2i\sin(\pi m z))\mathrm{d}z.$$

Somewhat more generally, the expansion and its inversion would hold for any $a \leqslant z \leqslant a+1$ with $a \in \mathbb{R}$.

We refrain from recalling well known properties of S-functions in this case even if they become rather non-trivial in subsequent generalizations.

B. Discretization in one dimension

Fixing $M \in \mathbb{N}$, determines an equidistant grid of $M+1$ points F_M

$$F_M \overset{\text{def}}{=} \left\{ s = \frac{s_1}{M} \mid s_0 + s_1 = M > 0, s_0, \quad s_1 \in \mathbb{Z}^{\geqslant 0} \right\}$$

by running the values of nonnegative integers s_0 and s_1 through their admissible values. Thus we have explicitly

$$F_M = \left\{ 0, \frac{1}{M}, \frac{2}{M}, \frac{3}{M}, \ldots, \frac{M-1}{M}, 1 \right\}.$$

The values of S-functions on the points of the grid F_M are thus

$$S_m(s) = 2i\sin(\pi m s), \quad s \in F_M, \quad m \in \mathbb{N}.$$

Since the values of the S-functions are always equal to 0 on the points $k\pi$, $k \in \mathbb{Z}$, it makes sense to exclude such points from F_M. Thus we obtain a grid of $M-1$ points which we define by F_M^-

$$F_M^- \overset{\text{def}}{=} \left\{ s = \frac{s_1}{M} \mid s_0 + s_1 = M, \quad s_0, s_1 \in \mathbb{N} \right\} = F_M \setminus \partial F.$$

Discrete orthogonality for $0 < m, m' < M$ is defined on F_M^- using a discrete version of the Hermitian form

$$\langle S_m|S_{m'}\rangle_M \overset{\text{def}}{=} \sum_{s \in F_M^-} S_m(s)\overline{S_{m'}(s)} = 2M\delta_{m,m'}.$$

Our aim in developing the formalism so far, is to use it for expansion of functions $f(s)$, given by its values on the grid F_M^-.

We have the discrete sine transform of A_1,

$$f(s) = \sum_{m=1}^{M-1} a_m S_m(s), \quad a_m = \frac{1}{2M}\sum_{s \in F_M^-} f(s)\overline{S_m(s)}, \tag{2.2}$$

and its continuous extension

$$f(z) = \sum_{m=1}^{M-1} a_m S_m(z), \quad \text{for } z \in \mathbb{R}. \tag{2.3}$$

A remarkable property of the continuous extension [Eq. (2.3)] is how smoothly it interpolates the values of $f(s)$ between the points of the grid F_M^-. Analogous property of continuous extension of cosine transform was established in Refs. 3, 14, and 15, see also Refs. 1 and 2.

III. HIGHER RANK CASES IN GENERAL

Most of the tools and properties we need can be presented in a uniform way for any dimension $n < \infty$. In this section we recall to some of the facts brought forward in the first two parts of the series.[1,2]

Such are α- and ω-bases, the bases of simple roots and fundamental weights, respectively, their duals, whenever those are different, corresponding root and weight lattices, Q and P, respectively, the positive chamber $P^+ \subset P$; the finite Weyl groups W and their orbits W_λ, the infinite affine Weyl groups W^{aff} and its fundamental region F (colloquially called also the fundamental region of the Lie group).

A. Definition of *S*-functions (Ref. 9)

The definitions of S- and C-function, $S_\lambda(z)$ and $C_\lambda(z)$, respectively, involve both $\lambda \in P^+$ and $z \in \mathbb{R}^n$. It requires also the W-orbit W_λ of λ. The compact semisimple Lie group enters only through its Weyl group and through the fact that the functions are formed as sums of exponential functions, constituents of irreducible characters. One has,

$$S_{\lambda+\rho}(z) \overset{\text{def}}{=} \sum_{\mu \in W_{\lambda+\rho}} (-1)^{p(\mu)} e^{2\pi i \langle \mu | z \rangle}, \tag{3.1}$$

$$C_\lambda(z) \overset{\text{def}}{=} \sum_{\mu \in W_\lambda} e^{2\pi i \langle \mu | z \rangle}, \quad \lambda \in P^+, \quad z \in \mathbb{R}^n. \tag{3.2}$$

Here $p(\mu)$ is the number of elementary reflections of W one needs to transform $\lambda+\rho$ to μ. The symbol ρ is the half-sum of positive roots of the Lie group. Relative to the ω-basis, it happens to be the vector

$$\rho = \sum_{k=1}^{n} \omega_k = (1,1,\ldots,1)$$

for every semisimple Lie group of rank $1 \leqslant n < \infty$.

The number of summands in Eqs. (3.1) and (3.2) is finite. It is equal to the number of weights in the corresponding Weyl group orbit. That number varies for C-functions (it is always one of the divisors of the order of the Weyl group). More precisely, the number of terms in W_λ is equal to the ratio

$$|W_\lambda| = \frac{|W|}{|\text{Stab}_W \lambda|}.$$

However, for S-functions, the number of summands in Eq. (3.1) always coincides with the order of the Weyl group because the stabilizer of $\lambda+\rho$ is always 1. That is, a weight $\lambda+\rho$, with $\lambda \in P^+$, has only the trivial stabilizer in W.

B. Orthogonality of *S*- and *C*-functions

Suppose that the S- and C-functions belong to the same Weyl group (equivalently to the same compact semisimple Lie group). Then we have the orthogonality relations:

$$\langle S_{\lambda+\rho}(z)|S_{\lambda'+\rho}(z)\rangle \overset{\text{def}}{=} \int_F S_{\lambda+\rho}(z)\overline{S_{\lambda'+\rho}(z)}\mathrm{d}z \sim \delta_{\lambda,\lambda'},$$

$$\langle C_{\lambda}(z)|C_{\lambda'}(z)\rangle \overset{\text{def}}{=} \int_F C_{\lambda}(z)\overline{C_{\lambda'}(z)}\mathrm{d}z \sim \delta_{\lambda,\lambda'},$$

where the overbar denotes complex conjugation.

C. Decomposition of functions on *F*

Continuous *S*-transform of a function $f(z)$ on F, is the decomposition

$$f(z) = \sum_{\lambda \in P^+} b_\lambda S_{\lambda+\rho}(z) = \sum_{\lambda \in P^{++}} b_\lambda S_{\lambda+\rho}(z), \quad \text{for } z \in F$$

and its inversion

$$b_\lambda = \frac{1}{\langle S_{\lambda+\rho}|S_{\lambda+\rho}\rangle}\int_F f(z)\overline{S_{\lambda+\rho}(z)}\mathrm{d}F.$$

Since $S_{\lambda+\rho}(z)=0$ when z is at the boundary ∂F of F, the *S*-transform is appropriate for functions $f(z)$ having zero values at ∂F.

D. Weyl group antisymmetries of *S*-functions

Important antisymmetry properties of *S*-functions are the following three:

$$S_{\lambda+\rho}(r_k z) = -S_{\lambda+\rho}(z), \quad k = 1,2,\ldots,n,$$

$$S_{\lambda+\rho}(r_j r_k z) = S_{\lambda+\rho}(z), \quad j,k = 1,2,\ldots,n,$$

$$S_{\lambda+\rho}(R_{\xi_h} z) = -S_{\lambda+\rho}(z),$$

where r_k, $k=1,2,\ldots,n$ are the Weyl group reflections and R_{ξ_h} is the affine reflection with respect to the highest root ξ_h, see Refs. 1 and 2.

E. Laplace operator

The *C*- and *S*-functions are eigenfunctions of the same Laplace operator. Moreover, the eigenvalues of $C_\mu(z)$ and $S_{\lambda+\rho}(z)$, coincide if $\mu=\lambda+\rho$. They are determined, up to a constant, by the square length of the weight of the Weyl group orbit.

Special cases of type A_2 (in our notation) are found in the literature, see Refs. 16–19.

Consider the application of the following operator on *S*-functions:

$$LS_{\lambda+\rho}(z) = \left(\sum_{k=1}^{n} \alpha_k \partial_k\right)^2 S_{\lambda+\rho}(z) = \sum_{j=1}^{n}\sum_{k=1}^{n} \langle \alpha_j|\alpha_k\rangle \partial_j\partial_k S_{\lambda+\rho}(z) = -4\pi^2\langle \lambda+\rho|\lambda+\rho\rangle S_{\lambda+\rho}(z).$$

Here we take ∂_k as acting on the kth coordinates of z in $\check{\omega}$-basis.

On the boundary ∂F of F one has

$$S_{\lambda+\rho}(z) = 0, \quad z \in \partial F.$$

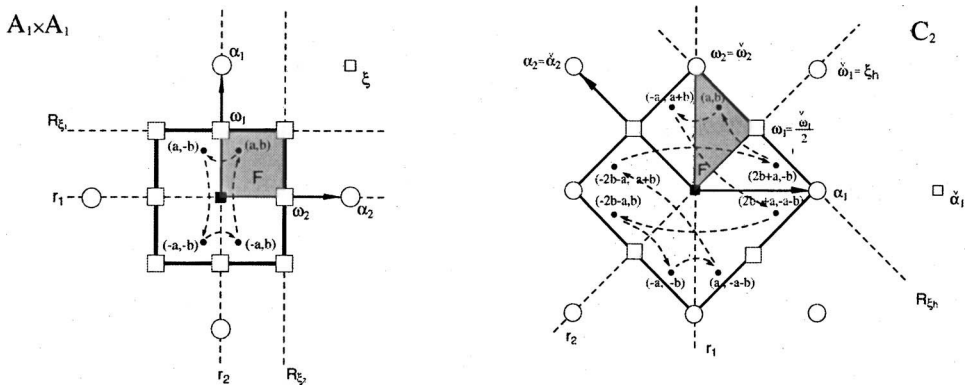

FIG. 1. The simple roots, the fundamental weights, along with their duals, and the fundamental region for the cases $A_1 \times A_1$ and C_2. The thick line square encloses the proximity cell to origin of the dual root lattice in each case. The dots are points of a generic Weyl group orbit for a, b not integers.

F. Decomposition of products of *S*- and *C*-functions

Products of *S*- and *C*-functions referring to the same Lie group and for the same z are completely decomposable into their linear combination. More precisely, products of *S*- and *C*-functions decompose into finite sums of *S*-functions,

$$S_{\lambda+\rho}C_{\lambda'} = S_{\lambda+\lambda'+\rho} + \cdots$$

It is a computational problem to find the remaining terms of the sum and their multiplicities in each case.

Products of two *S*-functions decompose into finite linear combinations of *C*-functions with integer coefficients of both signs, in general.

$$S_{\lambda+\rho}S_{\lambda'+\rho} = C_{\lambda+\lambda'+2\rho} + \cdots$$

We have seen in Refs. 1 and 2 that also products of *C*-functions decompose into sums of *C*-functions

$$C_{\lambda}C_{\lambda'} = C_{\lambda+\lambda'} + \cdots$$

with positive integer coefficients.

IV. THE TWO-DIMENSIONAL CONTINUOUS CASES

A. The group $A_1 \times A_1$

This is a straightforward concatenation of two A_1 cases of Sec. II.

Lengths and angles of the simple roots are given by the scalar products

$$\langle \alpha_1 | \alpha_2 \rangle = 0, \quad \langle \alpha_1 | \alpha_1 \rangle = \langle \alpha_2 | \alpha_2 \rangle = 2.$$

The Cartan matrix and its inverse are

$$C = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \quad C^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}.$$

Consequently, $\alpha_1 = 2\omega_1$ and $\alpha_2 = 2\omega_2$. Also $\check{\alpha}_j = \alpha_j$ and $\check{\omega}_j = \omega_j$ for $j = 1, 2$. Further, the root system $\Delta = \{\pm\alpha_1, \pm\alpha_2\}$ geometrically represents vertices of a square, see Fig. 1. The fundamental region F is the Cartesian product of two fundamental regions of A_1, namely, the square $[0,1] \times [0,1]$.

The *S*-functions are defined for W_λ-orbits with only a trivial stabilizer in W, i.e., such that $\lambda = a\omega_1 + b\omega_2 \in P^{++} \subset P^+$, where $a, b \in \mathbb{N}$. Then the Weyl group orbit W_λ is given by

$$W_\lambda \equiv W_{(a,b)} = \{\pm(a,b), \pm(a,-b)\}.$$

The S-functions of $A_1 \times A_1$, with $\lambda = a\omega_1 + b\omega_2$ and $z = x\omega_1 + y\omega_2$ are products of two S-functions of A_1

$$S_{(a,b)}(x,y) = S_a(x)S_b(y) = -4\sin(\pi a x)\sin(\pi b y), \quad a,b \in \mathbb{N} \text{ and } x,y \in \mathbb{R}.$$

The orthogonality relation of the S-functions of $A_1 \times A_1$ is expressed by the following:

$$\int_F S_{(a,b)}(x,y)S_{(c,d)}(x,y)\mathrm{d}F = \int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y S_{(a,b)}(x,y)S_{(c,d)}(x,y) = 4\delta_{a,c}\delta_{b,d}.$$

B. The group C_2

First we recall standard information about α- and ω-bases in this case. Lengths and angles of the simple roots are given by

$$\langle \alpha_1 | \alpha_2 \rangle = -1, \quad \langle \alpha_1 | \alpha_1 \rangle = 1, \quad \langle \alpha_2 | \alpha_2 \rangle = 2.$$

The Cartan matrix and its inverse are

$$C = \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix}, \quad C^{-1} = \begin{pmatrix} 1 & \frac{1}{2} \\ 1 & 1 \end{pmatrix}.$$

Consequently,

$$\begin{aligned} \alpha_1 &= 2\omega_1 - \omega_2, & \omega_1 &= \alpha_1 + \tfrac{1}{2}\alpha_2, & \check{\omega}_1 &= 2\omega_1, \\ \alpha_2 &= -2\omega_2 + 2\omega_2, & \omega_2 &= \alpha_1 + \alpha_2, & \check{\omega}_2 &= \omega_2. \end{aligned}$$

The root system $\Delta = \{\pm(2\alpha_1 + \alpha_2), \pm(\alpha_1 + \alpha_2), \pm\alpha_1, \pm\alpha_2\}$ geometrically represents vertices and midpoints of a square. The highest root is $\xi_h = 2\alpha_1 + \alpha_2$.

Put $\lambda = a\omega_1 + b\omega_2 \in P^{++}$. Then the Weyl group orbit W_λ consists of the following eight points:

$$W_\lambda \equiv W_{(a,b)} = \{\pm(a,b), \pm(-a,a+b), \pm(a+2b,-b), \pm(a+2b,-a-b)\}.$$

The S-functions of C_2, with $\lambda = a\omega_1 + b\omega_2$ and $z = x\check{\omega}_1 + y\check{\omega}_2$, are all real-valued, namely the following:

$$\begin{aligned} S_{(a,b)}(x,y) = {} & 2\cos(\pi(2(a+b)x + (a+2b)y)) - 2\cos(\pi(2(a+b)x) + ay) \\ & - 2\cos(\pi(2bx + (a+2b)y)) + 2\cos(\pi(-2bx + ay)), \end{aligned}$$

where $a,b \in \mathbb{N}$ and $x,y \in \mathbb{R}$.

The fundamental region $F(C_2)$ is described by

$$F(C_2) = \{x\check{\omega}_1 + y\check{\omega}_2 \mid 0 \leqslant x,y;\ 1 \geqslant 2x + y\}.$$

The orthogonality relation of the S-functions of C_2 is expressed by the following:

$$\int_F S_{(a,b)}(x,y)S_{(c,d)}(x,y)\mathrm{d}F = \int_0^{1/2} dx \int_0^{1-2x} S_{(a,b)}(x,y)S_{(c,d)}(x,y)\mathrm{d}y = 2\delta_{a,c}\delta_{b,d}.$$

C. The group A_2

Lengths and angles of the simple roots are given by

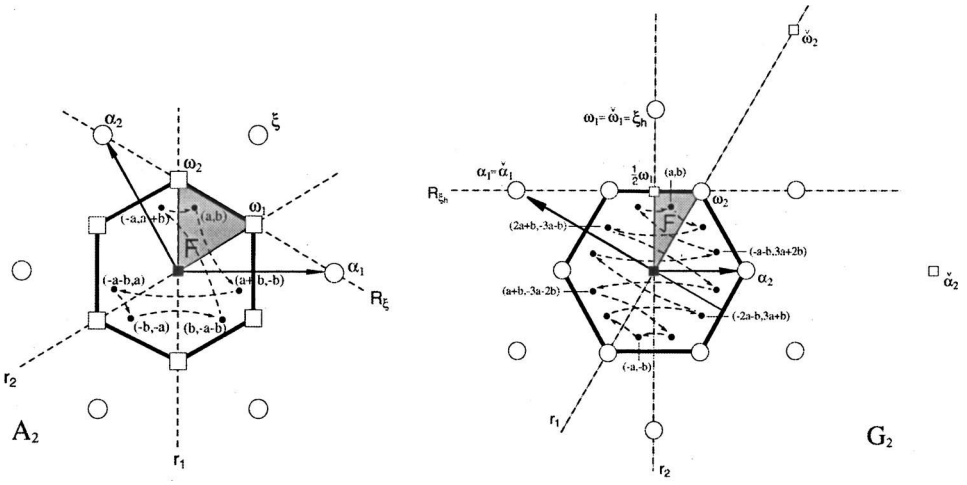

FIG. 2. The simple roots, the fundamental weights, along with their duals, and the fundamental region for the cases A_2 and G_2. The thick line hexagon encloses the proximity cell to origin of the dual root lattice in each case. The dots are points of a generic Weyl group orbit for a, b not integers.

$$\langle \alpha_1 | \alpha_2 \rangle = -1, \quad \langle \alpha_1 | \alpha_1 \rangle = \langle \alpha_2 | \alpha_2 \rangle = 2.$$

The Cartan matrix and its inverse are

$$C = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \quad C^{-1} = \tfrac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Consequently,

$$\alpha_1 = 2\omega_1 - \omega_2, \quad \omega_1 = \tfrac{1}{3}(2\alpha_1 + \alpha_2),$$

$$\alpha_2 = -\omega_2 + 2\omega_2, \quad \omega_2 = \tfrac{1}{3}(\alpha_1 + 2\alpha_2).$$

Also $\check{\alpha}_j = \alpha_j$ and $\check{\omega}_j = \omega_j$ for $j = 1, 2$.

The root system $\Delta = \{\pm(\alpha_1 + \alpha_2), \pm\alpha_1, \pm\alpha_2\}$ geometrically represents vertices of a regular hexagon, see Fig. 2.

Put $\lambda = a\omega_1 + b\omega_2 \in P^{++}$. Then the Weyl group orbit W_λ consists of the points given here in ω-basis

$$W_\lambda \equiv W_{(a,b)} = \{(a,b),(-a,a+b),(a+b,-b),(-b,-a),(b,-a-b),(-a-b,a)\}.$$

The S-functions of A_2 are then defined

$$\begin{aligned} S_{(a,b)}(x,y) = {} & e^{(2\pi i/3)((2a+b)x+(a+2b)y)} - e^{(2\pi i/3)((-a+b)x+(a+2b)y)} \\ & - e^{(2\pi i/3)((2a+b)x+(a-b)y)} + e^{-(2\pi i/3)((a-b)x+(2a+b)y)} \\ & + e^{-(2\pi i/3)((a+2b)x+(b-a)y)} - e^{-(2\pi i/3)((2b+a)x+(b+2a)y)}, \end{aligned}$$

$$S_{(a,a)}(x,y) = -2i(\sin(2\pi a y) + \sin(2\pi a y) - 2\sin(2\pi a(x+y))),$$

where $a, b \in \mathbb{N}$ and $x, y \in \mathbb{R}$.

The fundamental region $F(A_2)$ is described by

$$F(A_2) = \{x\omega_1 + y\omega_2 \mid 0 \leqslant x, y; \quad 1 \geqslant x + y\}.$$

The orthogonality relation of the S-functions of A_2 is expressed by

$$\int_F S_{(a,b)}(x,y)\overline{S_{(c,d)}(x,y)}\mathrm{d}x\mathrm{d}y = \frac{1}{\sqrt{3}}\int_0^1 \mathrm{d}x \int_0^{1-x} S_{(a,b)}(x,y)\overline{S_{(c,d)}(x,y)}\mathrm{d}y = \sqrt{3}\,\delta_{a,c}\delta_{b,d}.$$

Recall that for A_2 complex conjugation, denoted here by overbar, is also achieved by interchange of the subscripts, $S_{(a,b)}(x,y)=\overline{S_{(b,a)}(x,y)}$.

D. The group G_2

Lengths and angles of the simple roots are given by

$$\langle\alpha_1|\alpha_2\rangle = -1, \quad \langle\alpha_1|\alpha_1\rangle = 2, \quad \langle\alpha_2|\alpha_2\rangle = \tfrac{2}{3}.$$

The Cartan matrix and its inverse are

$$C = \begin{pmatrix} 2 & -3 \\ -1 & 2 \end{pmatrix}, \quad C^{-1} = \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix}.$$

Consequently,

$$\alpha_1 = 2\omega_1 - 3\omega_2, \quad \omega_1 = 2\alpha_1 + 3\alpha_2, \quad \check{\omega}_1 = \omega_1, \quad \check{\alpha}_1 = \alpha_1,$$

$$\alpha_2 = -\omega_2 + 2\omega_2, \quad \omega_2 = \alpha_1 + 2\alpha_2, \quad \check{\omega}_2 = 3\omega_2, \quad \check{\alpha}_2 = 3\alpha_2.$$

Note that in this case, $\alpha_1,\ \alpha_2 \in P$. Hence the root and weight lattices coincide.

The root system

$$\Delta = \{\pm(2\alpha_1 + 3\alpha_2), \pm(\alpha_1 + 3\alpha_2), \pm(\alpha_1 + 2\alpha_2), \pm(\alpha_1 + \alpha_2), \pm\alpha_1, \pm\alpha_2\}$$

geometrically represents the twelve vertices of a regular hexagonal star, see Fig. 2.

Let $\lambda = a\omega_1 + b\omega_2 \in P^{++}$. Then the Weyl group orbit W_λ is given by

$$W_\lambda \equiv W_{(a,b)} = \{\pm(a,b), \pm(-a,3a+b), \pm(a+b,-b),$$
$$\pm(2a+b,-3a-b), \pm(-a-b,-3a+2b), \pm(2a+b,-3a-2b)\}.$$

The S-functions of G_2, with $\lambda = a\omega_1 + b\omega_2$ and $z = x\check{\omega}_1 + y\check{\omega}_2$, are all real:

$$\begin{aligned} S_{(a,b)}(x,y) = {} & 2\cos(2\pi((a+b)x+by)) + 2\cos(2\pi((2a+b)x+(3a+2b)y)) \\ & - 2\cos(2\pi(ax-by)) - 2\cos(2\pi((a+b)x+(3a+2b)y)) \\ & - 2\cos(2\pi((2a+b)x+(3a+b)y)) + 2\cos(2\pi(ax+(3a+b)y)), \end{aligned}$$

where $a,b \in \mathbb{N}$ and $x,y \in \mathbb{R}$.

The fundamental region $F(G_2)$ is described by

$$F(G_2) = \{x\check{\omega}_1 + y\check{\omega}_2 \mid 0 \leqslant x,y;\ 1 \geqslant 2x+3y\}.$$

The orthogonality relation of the S-functions of G_2 is expressed by the following:

$$\int_F S_{(a,b)}(x,y)S_{(c,d)}(x,y)\mathrm{d}F = \sqrt{3}\int_0^{1/2} dx \int_0^{2/3-(1/2)x} S_{(a,b)}(x,y)S_{(c,d)}(x,y)\mathrm{d}y = \sqrt{3}\,\delta_{a,c}\delta_{b,d}.$$

V. *C*- AND *S*-POLYNOMIALS IN TWO VARIABLES

The *C*- and *S*-functions can be viewed also as polynomials.[1,2,7] From a narrow perspective of our functions, variables of such polynomials take values on an n-dimensional torus. However, it is natural to enlarge one's perspective and consider the variables as taking any complex values.

In general, properties of the polynomials arising from the *C*-, *S*-, and *E*-functions[9,10] will be studied elsewhere. In here we just point out the structure of these polynomials and their relation to semisimple Lie groups. For a more general approach, see Refs. 20 and 21.

A. *S*-polynomials

Assuming that $a,b \in \mathbb{N}$, and after a suitable substitution of variables, the *S*-functions are converted to polynomials, say in X and Y. Thus, for example, the substitutions

$$X = e^{(2\pi i/3)(2x+y)}, \quad Y = e^{(2\pi i/3)(x+2y)}, \quad \text{for } x,y \in \mathbb{R},$$

convert the generic *S*-function of A_2 into the corresponding polynomial.

The *S*-polynomials $S_{(a,b)}(X,Y)$ of compact semisimple Lie groups of rank two are the following ones.

$$\begin{aligned}
\mathrm{A}_1 \times \mathrm{A}_1\colon\ & X^aY^b - X^{-a}Y^b - X^aY^{-b} + X^{-a}Y^{-b},\\
\mathrm{A}_2\colon\ & X^aY^b - X^{-a}Y^{a+b} - X^{a+b}Y^{-b} + X^bY^{-a-b}\\
& + X^{-a-b}Y^a - X^{-b}Y^{-a},\\
\mathrm{C}_2\colon\ & X^aY^b - X^{-a}Y^{a+b} - X^{a+2b}Y^{-b}\\
& + X^{a+2b}Y^{-a-b} + X^{-a-2b}Y^{a+b}\\
& - X^{-a-2b}Y^b - X^aY^{-a-b} + X^{-a}Y^{-b},\\
\mathrm{G}_2\colon\ & X^aY^b - X^{-a}Y^{3a+b} - X^{a+b}Y^{-b} + X^{2a+b}Y^{-3a-b}\\
& + X^{a-b}Y^{3a+2b} - X^{-2a-b}Y^{3a+2b} - X^{-2a-b}Y^{3a+b}\\
& + X^{-a+b}Y^{-3a-b} + X^{2a+b}Y^{-3a-2b} - X^{-a-b}Y^b\\
& - X^aY^{-3a-b} + X^{-a}Y^{-b}.
\end{aligned}$$

Although the *S*-functions are defined for a and b strictly positive, one sees from the above polynomials that they turn to zero whenever either $a=0$ or $b=0$.

B. *C*-polynomials

A *C*-polynomial $C_\lambda(z)$ differs from an *S*-polynomial $S_\lambda(z)$ for the same group of rank 2, in two ways. Both are formed by the same monomials, but in the case of $C_\lambda(z)$ all signs are positive. Second, $C_\lambda(z)$ is also different from zero for $\lambda=(0,b)$, $(a,0)$, and $(0,0)$.

VI. DISCRETIZATION OF 2-DIMENSIONAL TRANSFORMS

We recall the essentials of the discretization in the case of *S*-functions even if it closely parallels that of *C*-functions.[1,2] In fact it is noticeably simpler. That is related to $S_\lambda(z)$ being equal to zero when $z \in \partial F$. Therefore points z at the boundary of F do not contribute to the value of a scalar product (or Hermitian form if the values are complex) of two *S*-functions.

A. Equidistant grids of points in the fundamental region

The fundamental region F can be used to tile the entire plane $\mathbb{R}^2$ by reflecting it repeatedly in its sides. A grid F_M of discrete points in F of any density is fixed by a positive integer M. One requires that the grid extends to a lattice during the tiling of $\mathbb{R}^2$ by copies of F.

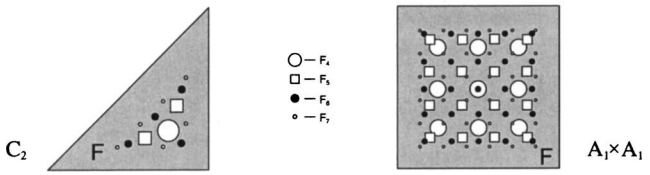

FIG. 3. The lattice points of F_4^-, F_5^-, F_6^-, and F_7^- in the fundamental region F for the cases $A_1 \times A_1$ and C_2.

The points $z_s \in F_M$ are conveniently described in barycentric coordinates. That is, by fixing nonnegative integers, s_0, s_1, and s_2 such that

$$F_M \overset{\text{def}}{=} \left\{ \left(\frac{s_1}{M}, \frac{s_2}{M} \right) \mid s_0, s_1, s_2 \in \mathbb{Z}^{\geqslant 0}, \quad s_0 + q_1 s_1 + q_2 s_2 = M > 0 \right\},$$

where $z_s = (s_1/M, s_2/M) = (s_1/M)\check{\omega}_1 + (s_2/M)\check{\omega}_2$. The constants q_1 and q_2 are given by the highest root $\xi_h = q_1\alpha_1 + q_2\alpha_2$ of the group. Specifically,

$$A_2: \quad q_1 = q_2 = 1,$$

$$C_2: \quad q_1 = 2, \quad q_2 = 1,$$

$$G_2: \quad q_1 = 2, \quad q_2 = 3.$$

Since the S-functions are always equal to 0 on the boundary ∂F of the fundamental region F, it makes sense to exclude those points from F_M. Thus we obtain a subgrid of points which we define by F_M^-

$$F_M^- \overset{\text{def}}{=} \left\{ \left(\frac{s_1}{M}, \frac{s_2}{M} \right) \mid s_0, s_1, s_2 \in \mathbb{N}, \; s_0 + q_1 s_1 + q_2 s_2 = M \right\} = \{ s \in F_M, \text{ where } s \notin \partial F \}. \tag{6.1}$$

See Figs. 3 and 4 for examples of such grids.

B. Sesquilinear form on F_M

Given the set of points F_M in the fundamental region, and two functions $f(s)$ and $h(s)$ given by their values at the points $s \in F_M$. One defines a Hermitian form as follows.

$$\langle f | h \rangle_M \overset{\text{def}}{=} \sum_{s \in F_M} c_s f(s) \overline{h(s)}.$$

The overbar stands for complex conjugation. The coefficients c_s are positive integers specific for each Lie group. They are listed in Refs. 1 and 2 for the groups of rank 2. They do not intervene in this article because they are all equal on F_M^- to the order of the Weyl group,

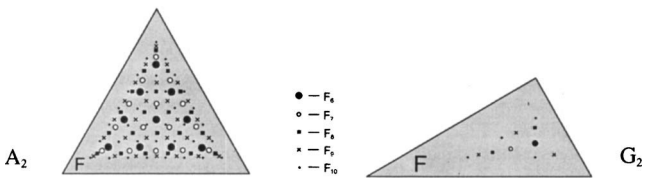

FIG. 4. The lattice points of F_6^-, F_7^-, F_8^-, F_9^-, and F_{10}^- in the fundamental region F for the cases A_2 and G_2.

$$c_s \equiv c, \quad s \in F_M^-,$$

hence would influence only the normalization of the form.

Besides, since S_λ are always 0 on the boundary ∂F of F, therefore, for the purpose of discretization in this paper, we can freely use

$$\langle f|h\rangle_M = c \sum_{s\in F_M^-} f(s)\overline{h(s)}$$

for any functions f and h.

C. Discrete orthogonality of *S*-functions

For a fixed value of $M \in \mathbb{N}$, the crucial property of S-functions is their discrete orthogonality on $F_M^- \subset F$:

$$\langle S_{(a,b)}|S_{(a',b')}\rangle_M = c \sum_{s\in F_M^-} S_{(a,b)}(s)\overline{S_{(a',b')}(s)} = \delta_{a,a'}\delta_{b,b'}\langle S_{(a,b)}|S_{(a,b)}\rangle_M. \tag{6.2}$$

It holds for (a,b), (a',b') from a finite subset S_M^- of S-functions. One has $S_{a,b} \in S_M^-$, provided a and b satisfy the inequality

$$a,b \in \mathbb{N}, \quad aq_2 + bq_1 < M \Leftrightarrow S_{(a,b)} \in S_M^-,$$

The numbers $\langle S_{(a,b)}|S_{(a,b)}\rangle_M$ in Eq. (6.2) take only integer multiples of M^2 for each M. Subsequently we provide them for all of the cases considered in this article and for all $0<a,b<\infty$.

D. Discretization in the case of $A_1 \times A_1$

This is a simple combination of two A_1-discretizations already described in Sec. II, in two orthogonal directions.

In the general case, the density of points $s \in F_{M,M'}^-$ is chosen by fixing positive integers M and M'. A rectangular lattice $F_{M,M'}^-$, of orders M in the ω_1-direction and M' in the ω_2-direction, is built on F the following way:

$$F_{M,M'}^-(A_1 \times A_1) = \left\{ \frac{s_1}{M}\omega_1 + \frac{s_1'}{M'}\omega_2 \mid s_0 + s_1 = M,\ s_0' + s_1' = M',\ s_0,s_1,s_0',s_1' \in \mathbb{N} \right\}.$$

In this case the coefficient $c=4$.

The S-functions are discretely orthogonal, i.e., for $S_{(a,b)}, S_{(a',b')} \in S_{M,M'}^-(A_1\times A_1) = \{S_{(a,b)}|a,b\in\mathbb{N}, a<M, b<M'\}$:

$$\langle S_{(a,b)}|S_{(a',b')}\rangle_{M,M'} = 4 \sum_{s\in F_{M,M'}^-} S_{(a,b)}(s)S_{(a',b')}(s) = \begin{cases} 0 & \text{if } a \neq a' \text{ or } b \neq b' \\ 16MM' & \text{otherwise,} \end{cases}$$

with the higher S-functions repeating the values of the functions in $S_{M,M'}^-$.

For simplicity, we choose $M=M'$ in our examples, and for simplicity, in such cases we denote the $F_{M,M'}^-$ by only F_M^- and $S_{M,M'}^-$ by S_M^-.

Examples: $F_4^-(A_1\times A_1)$ is a square grid with $M=M'=4$ that consists of the nine points (see Fig. 3) given as $[s_0,s_1],[s_0',s_1'] = (s_1/4, s_1'/4)$:

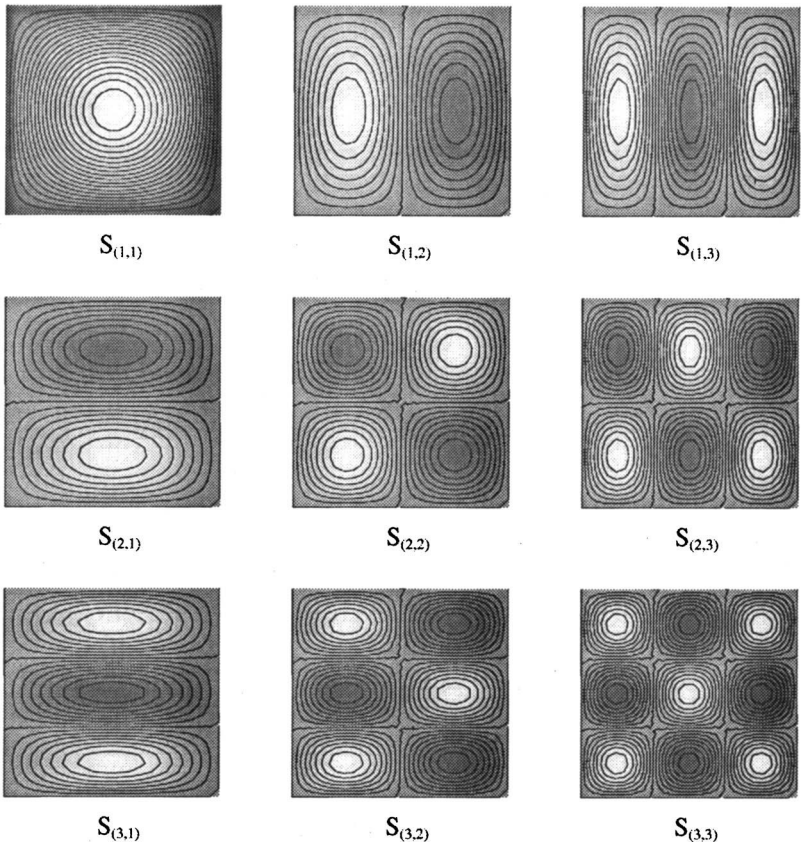

FIG. 5. The set of nine lowest pairwise orthogonal S-functions of $A_1 \times A_1$ for the grid $F_4^-(A_1 \times A_1)$.

$$
\begin{aligned}
&[3,1],[3,1]=\left(\tfrac{1}{4},\tfrac{1}{4}\right), \quad [3,1],[2,2]=\left(\tfrac{1}{4},\tfrac{1}{2}\right), \quad [3,1],[1,3]=\left(\tfrac{1}{4},\tfrac{3}{4}\right),\\
&[2,2],[3,1]=\left(\tfrac{1}{2},\tfrac{1}{4}\right), \quad [2,2],[2,2]=\left(\tfrac{1}{2},\tfrac{1}{2}\right), \quad [2,2],[1,3]=\left(\tfrac{1}{2},\tfrac{3}{4}\right),\\
&[1,3],[3,1]=\left(\tfrac{3}{4},\tfrac{1}{4}\right), \quad [1,3],[2,2]=\left(\tfrac{3}{4},\tfrac{1}{2}\right), \quad [1,3],[1,3]=\left(\tfrac{3}{4},\tfrac{3}{4}\right),
\end{aligned}
$$

whereas $F_3^-(A_1 \times A_1)$ has only four points:

$$
[2,1],[2,1]=\left(\tfrac{1}{3},\tfrac{1}{3}\right), \quad [1,2],[2,1]=\left(\tfrac{2}{3},\tfrac{1}{3}\right), \quad [2,1],[1,2]=\left(\tfrac{1}{3},\tfrac{2}{3}\right), \quad [1,2],[1,2]=\left(\tfrac{2}{3},\tfrac{2}{3}\right).
$$

See Fig. 5 for examples of S-functions of $A_1 \times A_1$.

E. Discretization in the case of A_2

Individual points $s \in F_M^-$ are given by triplets $s=[s_0,s_1,s_2] \equiv (s_1/M, s_2/M)$ of positive integers that satisfy the following A_2 sum rule:

$$
s_0 + s_1 + s_2 = M, \quad s_0,s_1,s_2 \in \mathbb{N}. \tag{6.3}
$$

All points of $F_M^- \subset F$ are obtained by letting the three positive integers run through all the values compatible with Eq. (6.3). Equivalently,

$$
F_M^-(A_2) = \left\{ \frac{s_1}{M}\omega_1 + \frac{s_2}{M}\omega_2 \mid s_0,s_1,s_2 \in \mathbb{N}, s_0+s_1+s_2=M \right\}.
$$

In this case the coefficient $c=6$.

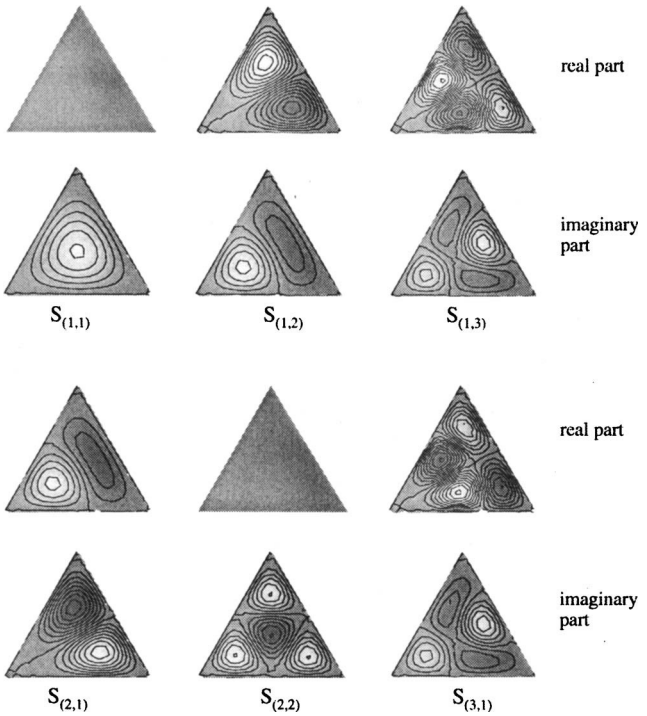

FIG. 6. The set of six lowest S-functions of A_2 which are pairwise orthogonal on the grid $F_5^-(A_2)$.

The S-functions are discretely orthogonal, i.e., for $S_{(a,b)}, S_{(a',b')} \in S_M^-(A_2) = \{S_{(a,b)} | a,b \in \mathbb{N}, a+b < M\}$:

$$\langle S_{(a,b)} | S_{(a',b')} \rangle_M = \begin{cases} 0 & \text{if } a \neq a' \text{ or } b \neq b' \\ 18M^2 & \text{otherwise,} \end{cases}$$

with the higher S-functions repeating the values of the functions in S_M^-.

Examples: $F_5^-(A_2)$ consists of the following six points (see Fig. 4) given as $[s_0, s_1, s_2] \equiv (s_1/M, s_2/M)$:

TABLE I. Values of several S-functions of A_2 at the six points of $F_5^-(A_2)$. Notation: $\kappa = 2i(-2\sin(2\pi/5) + \sin(\pi/5))$, $\zeta = -2i(\sin(2\pi/5) + 2\sin(\pi/5))$, and $\eta = e^{2\pi i/6}$.

z_s	$\left(\frac{1}{5},\frac{1}{5}\right)$	$\left(\frac{1}{5},\frac{2}{5}\right)$	$\left(\frac{1}{5},\frac{3}{5}\right)$	$\left(\frac{2}{5},\frac{1}{5}\right)$	$\left(\frac{2}{5},\frac{2}{5}\right)$	$\left(\frac{3}{5},\frac{1}{5}\right)$
$S_{(1,1)}(z_s)$	κ	ζ	κ	ζ	ζ	κ
$S_{(1,2)}(z_s)$	ζ	$\kappa\eta^5$	$\zeta\eta^4$	$\kappa\eta$	$\kappa\eta^3$	$\zeta\eta^2$
$S_{(1,3)}(z_s)$	κ	$\zeta\eta^4$	$\kappa\eta^2$	$\zeta\eta^2$	ζ	$\kappa\eta^4$
$S_{(2,1)}(z_s)$	ζ	$\kappa\eta$	$\zeta\eta^2$	$\kappa\eta^5$	$\kappa\eta^3$	$\zeta\eta^4$
$S_{(2,2)}(z_s)$	ζ	$\kappa\eta^3$	ζ	$\kappa\eta^3$	$\kappa\eta^3$	ζ
$S_{(3,1)}(z_s)$	κ	$\zeta\eta^2$	$\kappa\eta^4$	$\zeta\eta^4$	ζ	$\kappa\eta^2$
$S_{(4,2)}(z_s)$	κ	$\zeta\eta^2$	$\kappa\eta^4$	$\zeta\eta^4$	ζ	$\kappa\eta^2$
$S_{(3,3)}(z_s)$	ζ	$\kappa\eta^3$	ζ	$\kappa\eta^3$	$\kappa\eta^3$	ζ
$S_{(4,3)}(z_s)$	ζ	$\kappa\eta$	$\zeta\eta^2$	$\kappa\eta^5$	$\kappa\eta^3$	$\zeta\eta^4$
$S_{(2,4)}(z_s)$	κ	$\zeta\eta^4$	$\kappa\eta^2$	$\zeta\eta^2$	ζ	$\kappa\eta^4$
$S_{(3,4)}(z_s)$	ζ	$\kappa\eta^5$	$\zeta\eta^4$	$\kappa\eta$	$\kappa\eta^3$	$\zeta\eta^2$
$S_{(4,4)}(z_s)$	κ	ζ	κ	ζ	ζ	κ

$$[1,1,3]=\left(\tfrac{1}{5},\tfrac{3}{5}\right),\quad [1,2,2]=\left(\tfrac{2}{5},\tfrac{2}{5}\right),\quad [1,3,1]=\left(\tfrac{3}{5},\tfrac{1}{5}\right),$$
$$[2,1,2]=\left(\tfrac{1}{5},\tfrac{2}{5}\right),\quad [2,2,1]=\left(\tfrac{2}{5},\tfrac{1}{5}\right),\quad [3,1,1]=\left(\tfrac{1}{5},\tfrac{1}{5}\right).$$

In Table I several S-functions are found along with their values at the points of $F_5^-(\mathrm{A}_2)$. The first six belong to $S_5^-(\mathrm{A}_2)$. However, a closer inspection reveals presence of another orthogonal set obtained from $S_5^-(\mathrm{A}_2)$ by affine reflection $R_{(5,5)}$ applied to all its elements.

Using the entries of Table I, where $\kappa=2i(-2\sin(2\pi/5)+\sin(\pi/5))$, $\zeta=-2i(\sin(2\pi/5)+2\sin(\pi/5))$, and $\eta=e^{2\pi i/6}$, let us calculate the products:

$$\begin{aligned}\langle S_{1,1}|S_{1,2}\rangle_5 &= 6(\kappa\cdot\bar{\zeta}+\zeta\cdot\overline{\kappa\eta^5}+\kappa\cdot\overline{\zeta\eta^4}+\zeta\cdot\overline{\kappa\eta}+\zeta\cdot\overline{\kappa\eta^3}+\kappa\cdot\overline{\zeta\eta^2})\\ &= 6(\kappa\bar{\zeta}\cdot(\overline{1+\eta^2+\eta^4})+\zeta\bar{\kappa}\cdot(\overline{\eta+\eta^3+\eta^5}))=0;\end{aligned}$$

$$\begin{aligned}\langle S_{1,2}|S_{1,2}\rangle_5 &= 6(\zeta\cdot\bar{\zeta}+\kappa\eta^5\cdot\overline{\kappa\eta^5}+\zeta\eta^4\cdot\overline{\zeta\eta^4}+\kappa\eta\cdot\overline{\kappa\eta}+\kappa\eta^3\cdot\overline{\kappa\eta^3}+\zeta\eta^2\cdot\overline{\zeta\eta^2})\\ &= 6.3(\kappa\bar{\kappa}+\zeta\bar{\zeta})=18(20(\sin(2\pi/5))^2+20(\sin(\pi/5))^2)\\ &= 18\cdot 25=450.\end{aligned}$$

See Fig. 6 for examples of S-functions of A_2.

F. Discretization in the case of C_2

The highest root of C_2 is $\xi_h,=2\alpha_1+2\alpha_2$, therefore the individual points $s\in F_M^-$ are given by triplets $s=[s_0,s_1,s_2]=(s_1/M,s_2/M)$ of positive integers that satisfy the following C_2 sum rule:

$$s_0+2s_1+s_2=M,\quad s_0,s_1,s_2\in\mathbb{N}. \tag{6.4}$$

All points of $F_M^-\subset F$ are obtained by letting the three positive integers run through all the values compatible with Eq. (6.4). Equivalently,

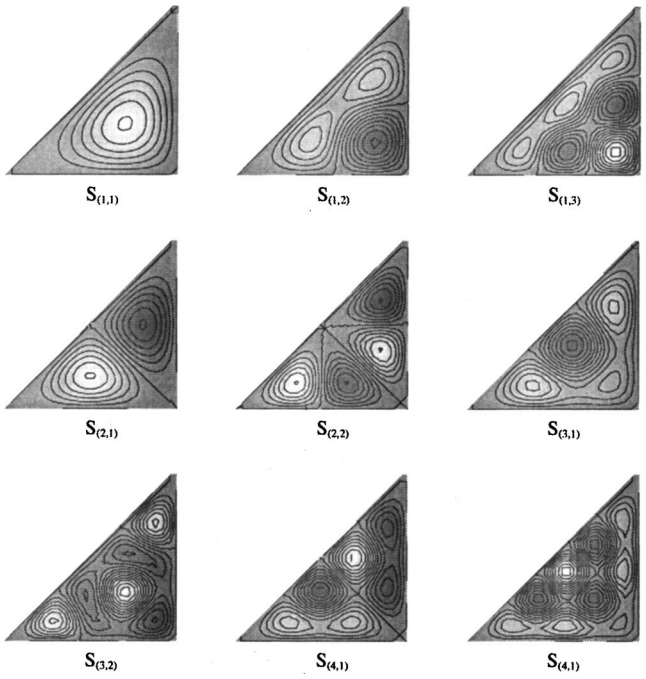

FIG. 7. The set of nine lowest S-functions of C_2 which are pairwise orthogonal on the grid $F_8^-(\mathrm{C}_2)$.

$$F_M^-(\mathrm{C}_2) = \left\{ \frac{s_1}{M}\check{\omega}_1 + \frac{s_2}{M}\check{\omega}_2 \mid s_0, s_1, s_2 \in \mathbb{N}, \quad s_0 + 2s_1 + s_2 = M \right\}.$$

In this case the coefficient $c=8$.

The S-functions are discretely orthogonal, i.e., for $S_{(a,b)}, S_{(a',b')} \in S_M^-(\mathrm{C}_2) = \{S_{(a,b)} | a, b \in \mathbb{N}, a + 2b < M\}$:

$$\langle S_{(a,b)} | S_{(a',b')} \rangle_M = \begin{cases} 0 & \text{if } a \neq a' \text{ or } b \neq b' \\ 16M^2 & \text{otherwise,} \end{cases}$$

with the higher S-functions repeating the values of the functions in S_M^-.

Examples: $F_7^-(\mathrm{C}_2)$ consists of the following six points given as $[s_0, s_1, s_2] \equiv (s_1/M, s_2/M)$:

$$[1,1,4] = \left(\tfrac{1}{7}, \tfrac{4}{7}\right), \quad [1,2,2] = \left(\tfrac{2}{7}, \tfrac{2}{7}\right), \quad [2,1,3] = \left(\tfrac{1}{7}, \tfrac{3}{7}\right),$$
$$[2,2,1] = \left(\tfrac{2}{7}, \tfrac{1}{7}\right), \quad [3,1,2] = \left(\tfrac{1}{7}, \tfrac{2}{7}\right), \quad [4,1,1] = \left(\tfrac{1}{7}, \tfrac{1}{7}\right).$$

See Fig. 7 for examples of S-functions of C_2.

G. Discretization in the case of G_2

As before, the value of M fixes the grid of discretization. The highest root of G_2 is $\xi_h = 2\alpha_1 + 3\alpha_2$, therefore the individual points $s \in F_M^-$ are given by triplets $s = [s_0, s_1, s_2] \equiv (s_1/M, s_2/M)$ of positive integers that satisfy the following G_2 sum rule:

$$s_0 + 2s_1 + 3s_2 = M, \quad s_0, s_1, s_2, \in \mathbb{N}. \tag{6.5}$$

All points of $F_M^- \subset F$ are obtained by letting the three positive integers run through all the values compatible with Eq. (6.5). Equivalently,

$$F_M^-(\mathrm{G}_2) = \left\{ \frac{s_1}{M}\check{\omega}_1 + \frac{s_2}{M}\check{\omega}_2 \mid s_0, s_1, s_2 \in \mathbb{N}, \quad s_0 + 2s_1 + 3s_2 = M \right\}.$$

In this case the coefficient c is equal to 12.

The S-functions are discretely orthogonal, i.e., for $S_{(a,b)}, S_{(a',b')}, \in S_M^-(\mathrm{G}_2) = \{S_{(a,b)} | a, b \in \mathbb{N}, 3a + 2b < M\}$:

$$\langle S_{(a,b)} | S_{(a',b')} \rangle_M = \begin{cases} 0 & \text{if } a \neq a' \text{ or } b \neq b' \\ 12M^2 & \text{otherwise,} \end{cases}$$

with the higher S-functions repeating the values of the functions in S_M^-.

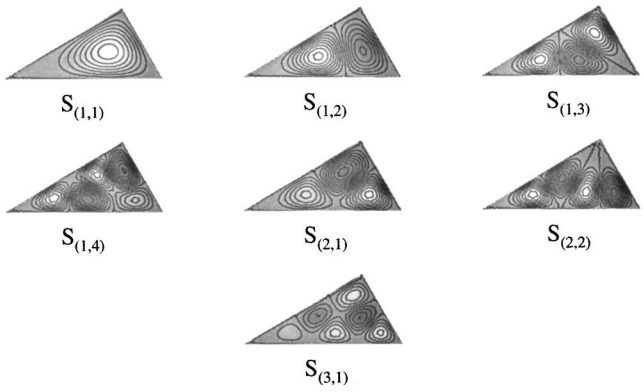

FIG. 8. The set of seven lowest S-functions of G_2 which are pairwise orthogonal on the grid $F_{12}^-(\mathrm{G}_2)$.

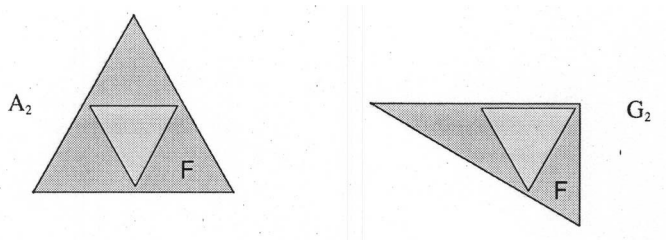

FIG. 9. The triangular step function [Eq. (7.2)] placed in the fundamental regions of A_2 and G_2.

Examples: $F_{14}^{-}(G_2)$ consists of the following ten points given as $[s_0,s_1,s_2]\equiv(s_1/M,s_2/M)$:

$$[1,2,3]=\left(\tfrac{1}{7},\tfrac{3}{14}\right),\quad [1,5,1]=\left(\tfrac{5}{14},\tfrac{1}{14}\right),\quad [2,3,2]=\left(\tfrac{3}{14},\tfrac{1}{7}\right),\quad [3,1,3]=\left(\tfrac{1}{14},\tfrac{3}{14}\right),$$
$$[3,4,1]=\left(\tfrac{2}{7},\tfrac{1}{14}\right),\quad [4,2,2]=\left(\tfrac{1}{7},\tfrac{1}{7}\right),\quad [5,3,1]=\left(\tfrac{3}{14},\tfrac{1}{14}\right),\quad [6,1,2]=\left(\tfrac{1}{14},\tfrac{1}{7}\right),$$
$$[7,2,1]=\left(\tfrac{1}{7},\tfrac{1}{14}\right),\quad [9,1,1]=\left(\tfrac{1}{14},\tfrac{1}{14}\right).$$

See Fig. 8 for examples of *S*—functions of G_2.

VII. MOTIVATING EXAMPLES

Comparison of expansions of class functions into series of *S*-functions of all groups considered here will require further study. Related results/questions are illustrated by the following examples.

There are two examples shown in this section, involving decomposition of the square function $f_{sq}(x,y)$ and a triangular function $f_{tr}(x,y)$ into series of *S*-functions of $A_1\times A_1$ and C_2, and A_2 and G_2, respectively. The goal of the examples is: (i) to illustrate discrete decomposition of a given function followed by the continuous extension and (ii) to compare the continuous extensions in both cases at compatible densities of the grids.

In order to make the comparison, for the cases $A_1\times A_1$ and C_2 we set up the vertices of the two fundamental regions as follows (relative to an orthonormal basis),

$$F(A_1\times A_1)=\{(0,0),(0,1),(1,1),(1,0)\},$$

$$F(C_2)=\{(0,0),(1,1),(1,0)\}.$$

Thus, the area of $F(A_1\times A_1)$ is exactly half of the area of $F(C_2)$.

We choose for $f_{sq}(x,y)$ a square step function with sharp edges with vertices in $(0,0),\left(0,\frac{1}{2}\right)$, $\left(\frac{1}{2},\frac{1}{2}\right)$, and $\left(\frac{1}{2},0\right)$:

$$f_{sq}(x,y)=\begin{cases}1 & \text{for } (x,y)\in\left\{(0,0),\left(0,\frac{1}{2}\right),\left(\frac{1}{2},\frac{1}{2}\right),\left(\frac{1}{2},0\right)\right\}\\ 0 & \text{elsewhere in } F.\end{cases}\tag{7.1}$$

For the cases A_2 and G_2, we set up the vertices of the two fundamental regions as follows (relative to an orthonormal basis):

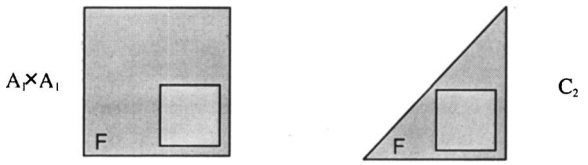

FIG. 10. The square step function [Eq. (7.1)] placed in the fundamental regions of $A_1\times A_1$ and C_2.

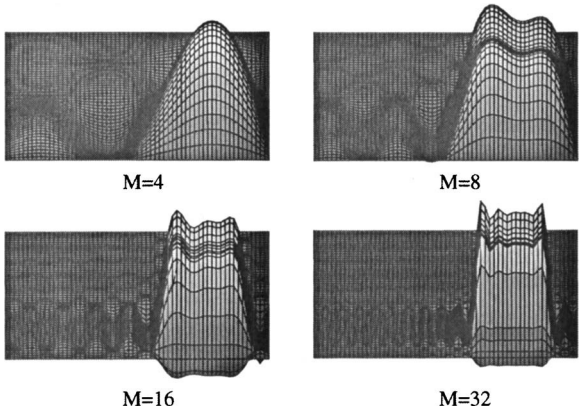

FIG. 11. Decomposition and continuous extension of a square step function placed in the fundamental region of $A_1 \times A_1$ on the grids of orders $M=4$, 8, 16, and 32.

$$F(A_2) = \left\{(0,0),(1,0),\left(\tfrac{1}{2},\tfrac{\sqrt{3}}{2}\right)\right\}$$

$$F(G_2) = \left\{\left(-\tfrac{1}{4},\tfrac{\sqrt{3}}{4}\right),\left(\tfrac{3}{4},\tfrac{\sqrt{3}}{4}\right),\left(\tfrac{3}{4},\tfrac{\sqrt{3}-2}{4}\right)\right\}$$

Thus, the area of $F(G_2)$ is also exactly half of the area of $F(A_2)$.

Here, we choose for $f_{\mathrm{tr}}(x,y)$ a triangular step function with sharp edges with vertices in $\left(\frac{1}{4},\frac{\sqrt{3}}{4}\right)$, $\left(\frac{3}{4},\frac{\sqrt{3}}{4}\right)$, and $\left(\frac{1}{2},0\right)$:

$$f_{\mathrm{tr}}(x,y) = \begin{cases} 1 & \text{for } (x,y) \in \left\{\left(\frac{1}{4},\frac{\sqrt{3}}{4}\right),\left(\frac{3}{4},\frac{\sqrt{3}}{4}\right),\left(\frac{1}{2},0\right)\right\} \\ 0 & \text{elsewhere in } F. \end{cases} \tag{7.2}$$

Chosen as such, $f_{\mathrm{tr}}(x,y)$ and $f_{\mathrm{sq}}(x,y)$ fit into the fundamental regions F of the four groups as shown in Figs. 9 and 10. Further, in order to have the same density of grid points, the orders of the grids are taken with the ratio $M_{A_1\times A_1}=M_{C_2}$ and $M_{G_2}=2M_{A_2}$. Figures 3 and 4 demonstrate the difference of densities of the grids of the same order for the four cases. It also helps to demonstrate the reason of the choice of the example functions and their placement into the fundamental regions in order to ensure a fair comparison of the cases.

Figures 11–14 contain results of our two examples. The values of the two functions $f_{\mathrm{sq}}(x,y)$ and $f_{\mathrm{tr}}(x,y)$ are sampled at the points s of the grids F_M^- 6.1 and taken as our digital data $f_{\mathrm{sq}}(s)$ and $f_{\mathrm{tr}}(x,y)$. Then the functions are expanded 2.2 into S-functions on the corresponding grids F_M^-, i.e.,

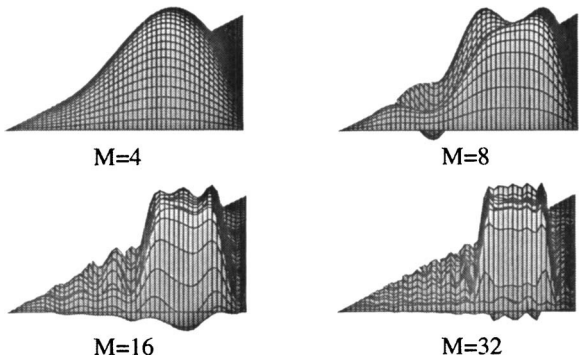

FIG. 12. Decomposition and continuous extension of a triangular step function placed in the fundamental region of C_2 on the grids of orders $M=4$, 8, 16, and 32.

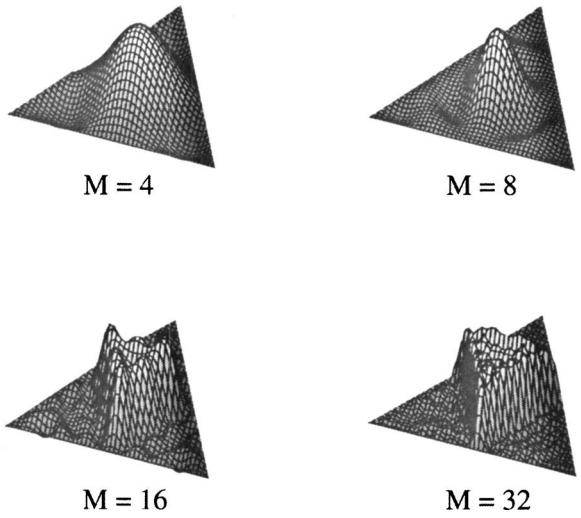

FIG. 13. Decomposition and continuous extension of a triangular step function placed in the fundamental region of A_2 on the grids of orders $M=4$, 8, 16, and 32.

expansion coefficients are calculated. After that, continuous extensions of the discrete expansions of $f_{\mathrm{sq}}(s)$ and $f_{\mathrm{tr}}(x,y)$ are made 2.3 by replacing the S-functions of the discrete argument s in the expansions by the same functions of the continuous argument, while keeping the expansion coefficients unchanged. Figures 11–14 show the functions $f_{\mathrm{sq\ cont}}(x,y)$ and $f_{\mathrm{tr\ cont}}(x,y)$ resulting from the continuous extension of discrete expansions. More precisely, four different continuous extensions are shown. They differ by the densities of the grid F_M^-, namely $M_{\mathrm{A}_1\times\mathrm{A}_1}=4$, 8, 16, 32, $M_{\mathrm{C}_2}=4$, 8, 16, 32, $M_{\mathrm{A}_2}=4$, 8, 16, 32, and $M_{\mathrm{G}_2}=8$, 16, 32, 64, from which the continuous extension is made. For these values the densities of grid points in the sample function are the same. The points of the grids are not shown in Figs. 11–14.

Inspecting and comparing the results, one readily observes the following:

1. As in Ref. 1, increasing density of the grid, i.e., increasing the value M, makes the continuous extension to match more closely the given model functions $f_{\mathrm{sq}}(x,y)$ of Eq. (7.1) and $f_{\mathrm{tr}}(x,y)$ of Eq. (7.2).
2. Quality of the extension, i.e., the match between the continuous extensions $f_{\mathrm{sq\ cont}}(x,y)$, $f_{\mathrm{tr\ cont}}(x,y)$, and the original functions $f_{\mathrm{sq}}(x,y)$, $f_{\mathrm{tr}}(x,y)$, is comparable for the same density of the grid in both cases, though C_2 and G_2 expansion may be slightly superior, as noticeable by comparing the two at the highest values of M in Figs. 11–14.

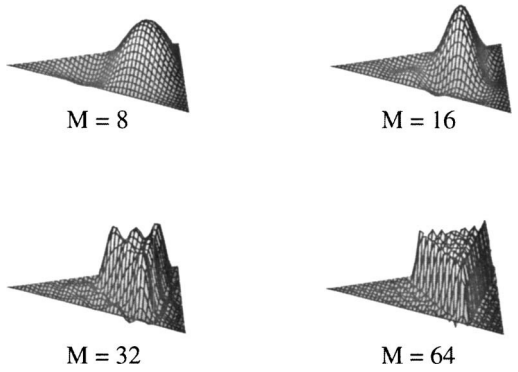

FIG. 14. Decomposition and continuous extension of a triangular step function placed in the fundamental region of G_2 on the grids of orders $M=8$, 16, 32 and 64.

3. The calculations of complex-valued functions in the case of A_2 took much longer time compared to the other cases, which gives them an obvious advantage in the discretization of real-valued functions, whereas A_2 is more useful for processing complex-valued information.

VIII. CONCLUDING COMMENTS

Comparison of the properties of *C*-functions of Refs. 1 and 2 with the properties of *S*-functions in this article reveals a far going parallel. Both families were described in the special case of two dimensions only, but both generalize to any finite dimension through the underlying compact semisimple Lie group *G*. The number of variables/dimension equals the rank of *G*.

Discretization in both families coincide: Identical grids are defined in the fundamental region *F* of *G*. Their symmetry is determined by the choice of *G*, their density is fixed by the positive integer *M*. Extended by the action of the affine Weyl group into the entire space, the grids automatically form a lattice because the points of F_M can also be interpreted[22] as representative of conjugacy classes of an Abelian subgroup of the maximal torus of *G* generated by the elements of order *M*.

The difference between the two families stems from their behavior under the action of the Weyl group *W* of *G*. Although *C*-functions are symmetric with respect to the reflections *r*, generating *W*, the *S*-functions are antisymmetric. Geometrically it is equivalent to the behavior of the functions with respect to their reflections in any side of *F*. Flipping $C_\lambda(z)$ values for $z \in F$ to its adjacent copy of *F*, flips also their values, $C_\lambda(rz)=C_\lambda(z)$, $r \in W$. Under the same operations the *S*-functions are antisymmetric, $S_\lambda(rz)=-S_\lambda(z)$. Thus, one is justified taking *C*- and *S*-functions as multidimensional generalizations of cosine and sine, respectively. A natural question of what then would be the multidimensional generalization of the exponential function has been answered in Ref. 9. Properties of *E*-functions of compact semisimple Lie groups will be studied elsewhere.[10]

Since our motivating application has been the decomposition of functions on *F* into a series of *C*- and/or *S*-functions, practically important for us is the behavior of the functions on the boundary of *F*. The *C*-transform requires that the normal derivatives at ∂F are zero, whereas the *S* transforms apply to functions that take zero value at ∂F.

Comparison of various decompositions of functions of two variables, using *C*- and *S*-functions of different groups is evidently of practical interest. In order to get an idea of the efficiency of the decomposition, we choose to consider continuous extension of model functions with sharp edges, more precisely cylinders, with zero value in the neighborhood of the boundary ∂F of *F*. Thus the value of the model function and its normal derivatives are both zero at ∂F. Sampling the functions at grids of comparable densities yields digital model data to work with. Continuous extension of such model data can then be visually inspected and compared.

Comparison of the functions plotted on Figs. 5 and 6 of Ref. 1 and Figs. 9 and 10 here, as well as the functions on Figs. 6 and 7 of Ref. 2 with Figs. 13 and 14 here, leads one to a qualitative conclusion that for the same grids (same value of *M*) the *C*- and *S*-functions are equally appropriate and, more importantly, that the interpolation of the digital data in both cases is equally good.

Similarly as with common discrete Fourier expansions one has continuous expansions (Fourier integral), it would be interesting to explore integral expansions based on *C*- or *S*-functions, where the variable λ takes continuous values from the *n* dimensional space rather than from an *n* dimensional lattice.

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Representations of simple finite Lie conformal superalgebras of type *W* and *S*

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I. INTRODUCTION

Lie conformal superalgebras encode the singular part of the operator product expansion of chiral fields in two-dimensional quantum field theory.[8] On the other hand, they are closely connected to the notion of formal distribution Lie superalgebra $(\mathfrak{g},\mathcal{F})$, that is a Lie superalgebra $\mathfrak{g}$ spanned by the coefficients of a family $\mathcal{F}$ of mutually local formal distributions. Namely, to a Lie conformal superalgebra R one can associate a formal distribution Lie superalgebra (Lie R,R) which establishes an equivalence between the category of Lie conformal superalgebras and the category of equivalence classes of formal distribution Lie superalgebras obtained as quotients of Lie R by irregular ideals.[8]

Finite simple Lie conformal algebras were classified in Ref. 6 and all their finite irreducible representations were constructed in Ref. 4. According to Ref. 6, any finite simple Lie conformal algebra is isomorphic either to the current Lie conformal algebra Cur$\mathfrak{g}$, where $\mathfrak{g}$ is a simple finite-dimensional Lie algebra, or to the Virasoro conformal algebra.

However, the list of finite simple Lie conformal superalgebras is much richer, mainly due to existence of several series of super extensions of the Virasoro conformal algebra. The complete classification of finite simple Lie conformal superalgebras was obtained in Ref. 7. The list consists of current Lie conformal superalgebras Cur$\mathfrak{g}$, where $\mathfrak{g}$ is a simple finite-dimensional Lie superalgebra, four series of "Virasoro like" Lie conformal superalgebras W_n $(n\geqslant 0)$, $S_{n,b}$ and $\widetilde{S}_n$ $(n\geqslant 2, b\in\mathbb{C})$, K_n $(n\geqslant 0)$, and the exceptional Lie conformal superalgebra CK_6.

All finite irreducible representations of the simple Lie conformal superalgebras Cur$\mathfrak{g}$, K_0 = Vir and K_1 were constructed in Ref. 4 and those of $S_{2,0}$, $W_1=K_2$, K_3, K_4 in Ref. 5.

The main result of the present paper is the construction of all finite irreducible modules over the Lie conformal superalgebras W_n, $S_{n,b}$, and $\widetilde{S}_n$. The proof relies on the method developed in Ref. 4, that is, the observation that representation theory of Lie conformal superalgebras is controlled by the representation theory of the (extended) annihilation superalgebra, and a lemma from Ref. 1. In our cases, this reduces to the study of certain representations of the Lie superalgebra $W(1,n)_+$

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of all vector fields on a superline (an affine superspace of dimension $(1|n)$) and the Lie superalgebra $S(1,n)_+$ of such vector fields with zero divergence. As in Refs. 9 and 10, we follow the approach developed for representations of infinite-dimensional simple linearly compact Lie algebras by A.R. in Ref. 11. The problem reduces to the description of the so-called degenerate modules, and for the latter we have to study singular vectors.

The paper is organized as follows. In Sec. II, we recall the notions and some basic facts on formal distributions, Lie conformal superalgebras, and their modules. In Sec. III, we recall some simple facts of the representation theory of infinite-dimensional simple linearly compact Lie superalgebras. In Sec. IV, we describe the conformal Lie superalgebra W_n and we classify its finite irreducible conformal modules by studying the corresponding singular vectors. In Sec. V, we obtain similar results for the Lie conformal superalgebra $S_n = S_{n,0}$. Finally, in Sec. VI, we complete the cases $S_{n,b}$ and $\widetilde{S}_n$. In all cases (as in Ref. 11) the answer has a geometric meaning: all finite irreducible modules are either "nondegenerate" tensor modules, or occur as cokernels of the differential in the conformal de Rham complex, or are duals of the latter.

Note that similar results for arbitrary non-super Lie pseudoalgebras of types W and S have been obtained in Ref. 2.

The remaining cases of the Lie conformal superalgebras K_n and CK_6 will be worked out in the subsequent publication.

II. FORMAL DISTRIBUTIONS, LIE CONFORMAL SUPERALGEBRAS, AND THEIR MODULES

First we introduce the basic definitions and notations, see Refs. 8 and 6. Let $\mathfrak{g}$ be a Lie superalgebra. A $\mathfrak{g}$-valued *formal distribution* in one indeterminate z is a series in the indeterminate z,

$$a(z) = \sum_{n \in \mathbb{Z}} a_n z^{-n-1}, \quad a_n \in \mathfrak{g}.$$

The vector superspace of all formal distributions, $\mathfrak{g}[[z,z^{-1}]]$, has a natural structure of a $\mathbb{C}[\partial_z]$-module. We define

$$\mathrm{Res}_z a(z) = a_0.$$

Let $a(z), b(z)$ be two $\mathfrak{g}$-valued formal distributions. They are called *local* if

$$(z-w)^N [a(z), b(w)] = 0 \quad \text{for } N \gg 0.$$

Let $\mathfrak{g}$ be a Lie superalgebra, a family $\mathcal{F}$ of $\mathfrak{g}$-valued formal distributions is called a *local family* if all pairs of formal distributions from $\mathcal{F}$ are local. Then, the pair $(\mathfrak{g}, \mathcal{F})$ is called a *formal distribution Lie superalgebra* if $\mathcal{F}$ is a local family of $\mathfrak{g}$-valued formal distributions and $\mathfrak{g}$ is spanned by the coefficients of all formal distributions in $\mathcal{F}$. We define the *formal δ-function* by

$$\delta(z-w) = z^{-1} \sum_{n \in \mathbb{Z}} \left(\frac{w}{z} \right)^n.$$

Then it is easy to show (Ref. 8, Corollary 2.2), that two local formal distributions are local if and only if the bracket can be represented as a finite sum of the form

$$[a(z), b(w)] = \sum_j [a(z)_{(j)} b(w)] \partial_w^j \delta(z-w)/j!,$$

where $[a(z)_{(j)} b(w)] = \mathrm{Res}_z (z-w)^j [a(z), b(w)]$. This is called the *operator product expansion*. Then we obtain a family of operations $_{(n)}$, $n \in \mathbb{Z}_+$, on the space of formal distributions. By taking the generating series of these operations, we define the λ-bracket:

$$[a_\lambda b] = \sum_{n \in \mathbb{Z}_+} \frac{\lambda^n}{n!} [a_{(n)} b].$$

The properties of the λ-bracket motivate the following definition:

Definition 2.1: A *Lie conformal superalgebra* R is a left $\mathbb{Z}/2\mathbb{Z}$-graded $\mathbb{C}[\partial]$-module endowed with a $\mathbb{C}$-linear map,

$$R \otimes R \to \mathbb{C}[\lambda] \otimes R, \quad a \otimes b \mapsto [a_\lambda b]$$

called the λ-bracket, and satisfying the following axioms $(a, b, c \in R)$,

Conformal sesquilinearity	$[\partial a_\lambda b] = -\lambda [a_\lambda b], \quad [a_\lambda \partial b] = (\lambda + \partial)[a_\lambda b],$
Skew-symmetry	$[a_\lambda b] = -(-1)^{p(a)p(b)} [b_{-\lambda-\partial} a],$
Jacobi identity	$[a_\lambda [b_\mu c]] = [[a_\lambda b]_{\lambda+\mu} c] + (-1)^{p(a)p(b)} [b_\mu [a_\lambda c]].$

Here and further $p(a) \in \mathbb{Z}/2\mathbb{Z}$ is the parity of a.

A Lie conformal superalgebra is called *finite* if it has finite rank as a $\mathbb{C}[\partial]$-module. The notions of homomorphism, ideal and subalgebras of a Lie conformal superalgebra are defined in the usual way. A Lie conformal superalgebra R is *simple* if $[R_\lambda R] \neq 0$ and contains no ideals except for zero and itself.

Given a formal distribution Lie superalgebra $(\mathfrak{g}, \mathcal{F})$ denote by $\bar{\mathcal{F}}$ the minimal subspace of $\mathfrak{g}[[z, z^{-1}]]$ which contains $\mathcal{F}$ and is closed under all jth products and invariant under ∂_z. Due to Dong's lemma, we know that $\bar{\mathcal{F}}$ is a local family as well. Then $\mathrm{Conf}(\mathfrak{g}, \mathcal{F}) := \bar{\mathcal{F}}$ is the Lie conformal superalgebra associated to the formal distribution Lie superalgebra $(\mathfrak{g}, \mathcal{F})$.

In order to give the (more or less) reverse functorial construction, we need the notion of *affinization* $\widetilde{R}$ of a conformal algebra R (which is a generalization of that for vertex algebras[3]). We let $\widetilde{R} = R[t, t^{-1}]$ with $\widetilde{\partial} = \partial + \partial_t$ and the λ-bracket:[8]

$$[af(t)_\lambda bg(t)] = [a_{\lambda+\partial_t} b] f(t) g(t') \big|_{t'=t}. \tag{2.1}$$

The 0-th product is

$$[at^n_{(0)} bt^m] = \sum_{j \in \mathbb{Z}_+} \binom{m}{j} [a_j b] t^{m+n-j}. \tag{2.2}$$

Observe that $\widetilde{\partial}\widetilde{R}$ is an ideal of $\widetilde{R}$ with respect to the 0-th product. We let $\mathrm{Alg}R = \widetilde{R}/\widetilde{\partial}\widetilde{R}$ with the 0-th product and let

$$\mathcal{R} = \left\{ \sum_{n \in \mathbb{Z}} (at^n) z^{-n-1} = a\delta(t - z) \,|\, a \in R \right\}.$$

Then $(\mathrm{Alg}R, \mathcal{R})$ is a formal distribution Lie superalgebra. Note that Alg is a functor from the category of Lie conformal superalgebras to the category of formal distribution Lie superalgebras. One has[8]

$$\mathrm{Conf}(\mathrm{Alg}R) = R, \quad \mathrm{Alg}(\mathrm{Conf}(\mathfrak{g}, \mathcal{F})) = (\mathrm{Alg}\bar{\mathcal{F}}, \bar{\mathcal{F}}).$$

Note also that $(\mathrm{Alg}R, \mathcal{R})$ is the *maximal formal distribution superalgebra* associated to the conformal superalgebra R, in the sense that all formal distribution Lie superalgebras $(\mathfrak{g}, \mathcal{F})$ with $\mathrm{Conf}(\mathfrak{g}, \mathcal{F}) = R$ are quotients of $(\mathrm{Alg}R, \mathcal{R})$ by irregular ideals (that is, an ideal I in $\mathfrak{g}$ with no nonzero $b(z) \in \mathcal{R}$ such that $b_n \in I$). Such formal distribution Lie superalgebras are called *equivalent*.

We thus have an equivalence of categories of conformal Lie superalgebras and equivalence classes of formal distribution Lie superalgebras. So the study of formal distribution Lie superalgebras reduces to the study of conformal Lie superalgebras.

An important tool for the study of Lie conformal superalgebras and their modules is the (extended) annihilation algebra. The *annihilation algebra* of a Lie conformal superalgebra R is the subalgebra $\mathcal{A}(R)$ (also denoted by $(\mathrm{Alg}R)_+$) of the Lie superalgebra Alg$R$ spanned by all elements at^n, where $a \in R, n \in \mathbb{Z}_+$. It is clear from (2.2) that this is a subalgebra, which is invariant with respect to the derivation $\partial = -\partial_t$ of Alg$R$. The *extended annihilation algebra* is defined as

$$\mathcal{A}(R)^e = (\mathrm{Alg}R)^+ := \mathbb{C}\,\partial \ltimes (\mathrm{Alg}R)_+.$$

Introducing the generating series

$$a_\lambda = \sum_{j \in \mathbb{Z}_+} \frac{\lambda^j}{j!}(at^j), \tag{2.3}$$

we obtain from (2.2):

$$[a_\lambda, b_\mu] = [a_\lambda b]_{\lambda+\mu}, \quad \partial(a_\lambda) = (\partial a_\lambda) = \lambda(a_\lambda). \tag{2.4}$$

Now let $\mathfrak{g}$ be a Lie superalgebra, and let V be a $\mathfrak{g}$-module. Given a $\mathfrak{g}$-valued formal distribution $a(z)$ and a V-valued formal distribution $v(z)$ we may consider the formal distribution $a(z)v(w)$ and the pair $(a(z), v(z))$ is called *local* if $(z-w)^N(a(z)v(w)) = 0$ for $N \gg 0$. As before, we have an expansion of the form:

$$a(z)v(w) = \sum_j (a(z)_{(j)}v(w))\partial_w^j \delta(z-w)/j\,!\,,$$

where $a(w)_{(j)}v(w) = \mathrm{Res}_z (z-w)^j a(z)v(w)$ and the sum is finite. By taking the generating series of these operations, we define the λ-*action of* $\mathfrak{g}$ *on* V:

$$a(w)_\lambda v(w) = \sum_{n \in \mathbb{Z}_+} \frac{\lambda^n}{n!}(a(w)_{(n)}v(w)) \quad \text{(finite sum)}.$$

It has the following properties:

$$\partial_z a(z)_\lambda v(z) = -\lambda a(z)_\lambda v(z), \quad a(z)_\lambda \partial_z v(z) = (\partial_z + \lambda)(a(z)_\lambda v(z)),$$

and

$$[a(z)_\lambda, b(z)_\mu]v(z) = [a(z)_\lambda b(z)]_{\lambda+\mu} v(z).$$

This motivates the following definition:

Definition 2.2: A *module* M over a Lie conformal superalgebra R is a $\mathbb{Z}/2\mathbb{Z}$-graded $\mathbb{C}[\partial]$-module endowed with a $\mathbb{C}$-linear map $R \otimes M \to \mathbb{C}[\lambda] \otimes M$, $a \otimes v \mapsto a_\lambda^M v$, satisfying the following axioms $(a, b \in M;\ v \in M)$,

$$(\mathrm{M1})_\lambda \qquad (\partial a)_\lambda^M v = [\partial^M, a_\lambda^M]v = -\lambda a_\lambda^M v,$$
$$(\mathrm{M2})_\lambda \qquad [a_\lambda^M, b_\mu^M]v = [a_\lambda b]_{\lambda+\mu}^M v.$$

An R-module M is called *finite* if it is finitely generated over $\mathbb{C}[\partial]$. An R-module M is called *irreducible* if it contains no nontrivial submodule, where the notion of submodule is the usual one.

As before, if $\mathcal{F} \subset \mathfrak{g}[[z, z^{-1}]]$ is a local family and $\mathcal{E} \subset V[[z, z^{-1}]]$ is such that all pairs $(a(z), v(z))$, where $a(z) \in \mathcal{F}$ and $v(z) \in \mathcal{E}$, are local, let $\bar{\mathcal{E}}$ be the minimal subspace of $V[[z, z^{-1}]]$ which contains E and all $a(z)_{(j)}v(z)$ for $a(z) \in \mathcal{F}$ and $v(z) \in \mathcal{E}$, and is ∂_z-invariant. Then it is easy to show that all pairs $(a(z), v(z))$, where $a(z) \in \bar{\mathcal{F}}$ and $v(z) \in \bar{\mathcal{E}}$, are local and $a(z)_{(j)}(\bar{\mathcal{E}}) \subset \bar{\mathcal{E}}$ for all $a(z) \in \bar{\mathcal{F}}$.

Let $\mathcal{F}$ be a local family that spans $\mathfrak{g}$ and let $\mathcal{E} \subset V[[z, z^{-1}]]$ be a family that span V. Then $(V, \mathcal{E})$ is called a *formal distribution module* over the formal distribution Lie superalgebra $(\mathfrak{g}, \mathcal{F})$ if all pairs $(a(z), v(z))$, where $a(z) \in \mathcal{F}$ and $v(z) \in \mathcal{E}$, are local. It follows that a formal distribution

module $(V,\mathcal{E})$ over a formal distribution Lie superalgebra $(\mathfrak{g},\mathcal{F})$ gives rise to a module $\mathrm{Conf}(V,\mathcal{E}):=\bar{\mathcal{E}}$ over the conformal Lie superalgebra $\mathrm{Conf}(\mathfrak{g},\mathcal{F})$.

In the same way as above, we have an equivalence of categories of modules over a Lie conformal superalgebra R and equivalence classes of formal distribution modules over the Lie superalgebra Alg$R$. Namely, given an R-module M, one defines its *affinization* $\tilde{M}=M[t,t^{-1}]$ as an $\tilde{R}$-module with $\tilde{\partial}=\partial+\partial_t$ and the λ-action similar to (2.1):

$$af(t)_\lambda vg(t)=(a_{\lambda+\partial_t^{(t)}}v)f(t)g(t')\big|_{t'=t}. \tag{2.5}$$

The 0-th action is

$$at^n_{(0)}vt^m=\sum_{j\in\mathbb{Z}_+}\binom{m}{j}(a_jv)t^{m+n-j}. \tag{2.6}$$

Observe that $\tilde{\partial}\tilde{M}$ is invariant with respect to the 0-th action and $(\tilde{\partial}\tilde{R})_{(0)}\tilde{M}=0$, hence the 0-th action of $\tilde{R}$ on $\tilde{M}$ induces a representation of the Lie superalgebra $\mathrm{Alg}R=\tilde{R}/\tilde{\partial}\tilde{R}$ on $V(M):=\tilde{M}/\tilde{\partial}\tilde{M}$. Let $\mathcal{M}=\{v\,\delta(z-t)\,|\,v\in M\}$. Then $(V(M),\mathcal{M})$ is a formal distribution module over the formal distribution Lie superalgebra $(\mathrm{Alg}R,\mathcal{R})$, which is maximal in the sense that all conformal $(\mathrm{Alg}R,\mathcal{R})$ modules $(V,\mathcal{E})$ such that $\bar{\mathcal{E}}\simeq M$ as R-modules are quotients of $(V(M),\mathcal{M})$ by irregular submodules. Such formal distribution modules are called equivalent, and we get an equivalence of categories of R-modules and equivalence classes of formal distribution $(\mathrm{Alg}R,\mathcal{R})$-modules.

Formula (2.4) implies the following important proposition relating modules over a Lie conformal superalgebra R to continuous modules over the corresponding extended annihilation Lie superalgebra $(\mathrm{Alg}R)^+$.

Proposition 2.3: (Ref. 4) A module over a Lie conformal superalgebra R is the same as a continuous module over the Lie superalgebra $(\mathrm{Alg}R)^+$, *i.e. it is an* $(\mathrm{Alg}R)^+$*-module satisfying the property*

$$a_\lambda m\in\mathbb{C}[\lambda]\otimes M\quad \textit{for any } a\in R,m\in M. \tag{2.7}$$

(*One just views the action of the generating series* a_λ *of* $(\mathrm{Alg}R)^+$ *as the* λ*-action of* $a\in R$).

Denote by $V(M)_+$ the span of elements $\{vt^n\,|\,v\in M,n\in\mathbb{Z}_+\}$ in $V(M)$. It is clear from (2.5) that $V(M)^+$ is an $(\mathrm{Alg}R)^+$ submodule, hence an R -module by Proposition 2.3. We denote by $V(M)_+^*$ the restricted dual of $V(M)_+$, i.e., the space of all linear functions on $V(M)_+$ which vanish on all but finite number of subspaces Mt^n, with $n\in\mathbb{Z}_+$. This is an $(\mathrm{Alg}R)^+$-module and hence an R-module as well. The *conformal dual* M^* to an R-module M is defined as

$$M^*=\{f_\lambda:M\to\mathbb{C}[\lambda]\,|\,f_\lambda(\partial m)=\lambda f_\lambda(m)\},$$

with the structure of $\mathbb{C}[\partial]$-module $(\partial f)_\lambda(m)=-\lambda f_\lambda(m)$, with the following λ-action of R:

$$(a_\lambda f)_\mu(m)=-(-1)^{p(a)(p(f)+1)}f_{\mu-\lambda}(a_\lambda m),\quad a\in R,m\in M.$$

Given a homomorphism of conformal R-modules $T:M\to N$, we define the transpose homomorphism $T^*:N^*\to M^*$ by

$$[T^*(f)]_\lambda(m)=-f_\lambda(T(m)).$$

Proposition 2.4: Let $T:M\to N$ *be an injective homomorphism of R-modules such that* $N/\mathrm{Im}\,T$ *is finitely generated torsion-free* $\mathbb{C}[\partial]$*-module. Then* T^* *is surjective*.

Proof: Since $L=N/\mathrm{Im}\,T$ is finitely generated torsion-free, then it is free and therefore a projective $\mathbb{C}[\partial]$-module. Hence, the short exact sequence $0\to\mathrm{Im}\,T\to N\to N/\mathrm{Im}\,T\to 0$ is split and $N=\mathrm{Im}\,T\oplus L$ as $\mathbb{C}[\partial]$-module. Now, given $\alpha\in M^*$, we define $\beta\in N^*$ as follows:

$$\beta_\lambda(T(m)) = \alpha_\lambda(m), \quad m \in M, \quad \beta_\lambda(l) = 0, \quad l \in L.$$

Then β is well-defined since T is injective and β belongs to N^* since L is a complementary $\mathbb{C}[\partial]$-submodule, finishing the proof. □

Remark 2.5: Observe that the injectivity is not enough (cf. Remark 4.12). Namely, let $R = \mathrm{Vir} = \mathbb{C}[\partial]L$ be the Virasoro conformal algebra with λ-bracket $[L_\lambda L] = (2\lambda + \partial)L$. Consider the following Vir-modules:

$$\Omega_0 = \mathbb{C}[\partial]m, \quad \text{with } L_\lambda m = (\lambda + \partial)m, \quad \Omega_1 = \mathbb{C}[\partial]n \quad \text{with } L_\lambda n = \partial n.$$

Then it is easy to see that the map $d: \Omega_0 \to \Omega_1$ given by $d(m) = \partial n$ is an injective homomorphism of R-modules, but the dual map $d^*: \Omega_1^* \to \Omega_0^*$ given by $d^*(m^*) = \partial n^*$ is not surjective.

Proposition 2.6: Let $T: M \to N$ be a homomorphism of R-modules such that $N/\mathrm{Im}\, T$ is finitely generated torsion-free $\mathbb{C}[\partial]$-module. Then the standard map $\psi: N^*/\mathrm{Ker}\, T^* \to (M/\mathrm{Ker}\, T)^*$, given by $[\psi(\bar{f})]_\lambda(\bar{m}) = f_\lambda(T(m))$ (where by the bar we denote the corresponding class in the quotient) is an isomorphism of R-modules.

Proof: Using Proposition 2.4 the proof follows by standard arguments. □

Proposition 2.7: If M is an R-module finitely generated (over $\mathbb{C}[\partial]$), then $M^{**} \simeq M$.

Proof: Let $M = \oplus \mathbb{C}[\partial]m_i$ (finite sum), with $a_\lambda m_j = \Sigma_k P_{jk}(\lambda, \partial)m_k$. Then $M^* = \oplus \mathbb{C}[\partial]m_i^*$, with $(m_i^*)_\lambda(m_k) = \delta_{i,k}$ and

$$(a_\lambda m_i^*)_\mu(m_j) = -(m_i^*)_{\mu-\lambda}(a_\lambda m_j) = -\sum_k (m_i^*)_{\mu-\lambda}(P_{jk}(\lambda, \partial)m_k) = P_{ji}(\lambda, \mu - \lambda).$$

Therefore,

$$(a_\lambda m_i^*) = -\sum_j P_{ji}(\lambda, -\partial - \lambda)m_j^*,$$

and the last formula shows that by taking the dual again we obtain

$$(a_\lambda m_i^{**}) = \sum_j P_{ij}(\lambda, \partial)m_j^{**}.$$

Hence the map $m_i \mapsto m_i^{**}$ gives us the isomorphism between M and M^{**}. □

Proposition 2.8: (*a*) *The map $M \to V(M)/V(M)_+$ given by $v \mapsto vt^{-1}$ mod $V(M)_+$ is an isomorphism of* $(\mathrm{Alg}R)^+$- (*and R-*)*modules.*

(*b*) *The map $V(M)_+^* \to M^*$ defined by $f \mapsto f_\lambda$, where*

$$f_\lambda(m) = \sum_{j \in \mathbb{Z}_+} \frac{(-\lambda)^j}{j!} f(mt^j),$$

is an isomorphism of $(\mathrm{Alg}R)^+$- (*and R-*)*modules.*

Proof: A direct verification. □

Assuming that R is finite, choose a finite set of generators of this $\mathbb{C}[\partial]$-module: $\{a^i \mid i \in I\}$, and for each $m \in \mathbb{Z}_+$, denote by $(\mathrm{Alg}R)^+_{(m)}$ the $\mathbb{C}$-span of all elements $a^i t^j, i \in I, j \geqslant m$ of $(\mathrm{Alg}R)^+$. This defines a descending filtration of $(\mathrm{Alg}R)^+$ by subspaces of finite codimension:

$$(\mathrm{Alg}R)^+ \supset (\mathrm{Alg}R)_+ = (\mathrm{Alg}R)_{(0)} \supset (\mathrm{Alg}R)_{(1)} \supset \dots . \tag{2.8}$$

It is easy to see from (2.2) that there exists $s \in \mathbb{Z}_+$ such that for all $k, r \in \mathbb{Z}_+$ one has

$$[(\mathrm{Alg}R)_{(k)}, (\mathrm{Alg}R)_{(r)}] \subset (\mathrm{Alg}R)_{(k+r-s)}. \tag{2.9}$$

In particular, $(\mathrm{Alg}R)_r := (\mathrm{Alg}R)_{(r+s)}$ is a filtration of $(\mathrm{Alg}R)^+$ by subalgebras of finite codimension.

Given an R-module M, it is an $(\mathrm{Alg}R)^+$-module (by Proposition 2.3), and we let for $j \in \mathbb{Z}_+$:

$$M_{(j)} = \{v \in M | (\mathrm{Alg}R)_{(j)} v = 0\}. \tag{2.10}$$

The subspaces $M_{(j)}$ form an ascending filtration of M by $(\mathrm{Alg}R)_0$-invariant subspaces. The following proposition is a special case of Lemma 14.4 from Ref. 1.

Proposition 2.9: Let R be a finite Lie conformal superalgebra and let M be a finite R-module such that

$$M^R = \{m \in M | R_\lambda m = 0\} (= M_{(0)})$$

is finite dimensional (over $\mathbb{C}$). Then all subspaces $M_{(j)}$ are finite-dimensional. In particular M is locally finite as an $(\mathrm{Alg}R)_0$-module, meaning that any $m \in M$ is contained in a finite-dimensional $(\mathrm{Alg}R)_0$-invariant subspace.

This Proposition together with the results of the following section will provide a characterization of all finite irreducible modules over a finite Lie conformal superalgebra in terms of certain (quotients of) induced modules over the extended annihilation algebra.

III. GENERAL REMARKS ON REPRESENTATIONS OF LINEARLY COMPACT LIE SUPERALGEBRAS

We follow the approach developed for representations of infinite-dimensional simple linearly compact Lie algebras by A.R. in Ref. 11. In this section we will follow Ref. 9.

We shall consider continuous representations in spaces with discrete topology. The continuity of a representation of a linearly compact Lie superalgebra L in a vector space V with discrete topology means that the stabilizer $L_v = \{g \in L | gv = 0\}$ of any $v \in V$ is an open (hence of finite codimension) subalgebra of L.

Let L be a simple linearly compact Lie superalgebra. In some cases (the examples studied in the following sections), L has a $\mathbb{Z}$-gradation of the form

$$L = \oplus_{m \geqslant -1} L_m, \tag{3.1}$$

this gives a triangular decomposition

$$L = L_- \oplus L_0 \oplus L_+ \quad \text{with } L_\pm = \oplus_{\pm m > 0} L_m. \tag{3.2}$$

Let $L_{\geqslant 0} = L_{>0} \oplus L_0$. Denote by $P(L, L_{\geqslant 0})$ the category of all continuous L-modules V, where V is a vector space with discrete topology, that are $L_{\geqslant 0}$-locally finite, that is any $v \in V$ is contained in a finite-dimensional $L_{\geqslant 0}$-invariant subspace. When talking about representations of L, we shall always mean modules from $P(L, L_{\geqslant 0})$. Modules in this category are called *finite continuous L-modules*.

In most cases of simple L, for example if L is of W or S type, by taking $L_{\geqslant 0}$ certain maximal open subalgebra, one can choose L_- to be a subalgebra. Taking an ordered basis of L_-, we denote by $U(L_-)$ the span of all PBW monomials in this basis. We have $U(L) = U(L_-) \otimes U(L_{\geqslant 0})$, as vector spaces (here and in the following $U(L)$ stands for the universal enveloping algebra of the Lie superalgebra L). It follows that any irreducible L-module V in the category $P(L, L_{\geqslant 0})$ is finitely generated over $U(L_-)$:

$$V = U(L_-)E$$

for some finite-dimensional subspace E. This property is very important in the theory of conformal modules.[4]

Given an $L_{\geqslant 0}$-module F, we may consider the associated induced L-module

$$M(F) = \mathrm{Ind}_{L_{\geqslant 0}}^{L} F = U(L) \otimes_{U(L_{\geqslant 0})} F,$$

called the *generalized Verma module* associated to F. Sometimes, we shall omit L and $L_{\geqslant 0}$, and simply denote it as $\mathrm{Ind}\, F$.

Let V be an L-module. The elements of the subspace

$$\mathrm{Sing}(V) := \{v \in V | L_{>0} v = 0\}$$

are called *singular vectors*. For us the most important case is when $V=M(F)$. The $L_{\geqslant 0}$-module F is canonically an $L_{\geqslant 0}$-submodule of $M(F)$, and $\mathrm{Sing}(F)$ is a subspace of $\mathrm{Sing}(M(F))$, called the *subspace of trivial singular vectors*. Observe that $M(F)=F\oplus F_+$, where $F_+=U_+(L_-)\otimes F$ and $U_+(L_-)$ is the augmentation ideal in the symmetric algebra $U(L_-)$. Then

$$\mathrm{Sing}_+(M(F)) := \mathrm{Sing}(M(F)) \cap F_+$$

are called the *nontrivial singular vectors*.

Theorem 3.1: (Refs. 9 and 11) (*a*) *If F is a finite-dimensional $L_{\geqslant 0}$-module, then $M(F)$ is in $P(L,L_{\geqslant 0})$.*

(*b*) *In any irreducible finite-dimensional $L_{\geqslant 0}$-module F the subalgebra L_+ acts trivially.*

(*c*) *If F is an irreducible finite-dimensional $L_{\geqslant 0}$-module, then $M(F)$ has a unique maximal submodule.*

(*d*) *Denote by $I(F)$ the quotient by the unique maximal submodule of $M(F)$. Then the map $F\mapsto I(F)$ defines a bijective correspondence between irreducible finite-dimensional L_0-modules and irreducible L-modules in $P(L,L_{\geqslant 0})$, the inverse map being $V\mapsto Sing(V)$.*

(*e*) *An L-module $M(F)$ is irreducible if and only if the L_0-module F is irreducible and $M(F)$ has no nontrivial singular vectors.*

Remark 3.2: The correspondence defined in Theorem 3.1(d) provides the classification of irreducible modules of the category $P(L,L_{\geqslant 0})$. Also, we would like to remark that in general $\mathrm{Sing}_+(M(F))$ generates a proper submodule in the L-module $M(F)$, but the factor by this submodule is not necessarily irreducible, there could appear new nontrivial singular vectors. However this happens very rarely (see Ref. 10 for an example and cf. Remark 4.8) and in most cases it can be proven that the factor module will be irreducible.

IV. LIE CONFORMAL SUPERALGEBRA W_n AND ITS FINITE IRREDUCIBLE MODULES

A. Definition of W_n and the induced modules

According to Ref. 6, any finite simple Lie conformal algebra is isomorphic either to $\mathrm{Cur}\mathfrak{g}$, where $\mathfrak{g}$ is a simple finite-dimensional Lie algebra, or to the Virasoro conformal algebra.

However, the list of finite simple Lie conformal superalgebras is much richer, mainly due to existence of several series of super extensions of the Virasoro conformal algebra, see Ref. 7.

The first series is associated to the Lie superalgebra $W(1,n)$ $(n\geqslant 1)$. More precisely, let $\Lambda(n)$ be the Grassmann superalgebra in the n odd indeterminates $\xi_1,\xi_2,\ldots,\xi_n$. Set $\Lambda(1,n)=\mathbb{C}[t,t^{-1}]\otimes\Lambda(n)$, then

$$W(1,n)=\left\{ a\partial_t+\sum_{i=1}^{n} a_i\partial_i | a,a_i \in \Lambda(1,n) \right\}, \tag{4.1}$$

where $\partial_i=\partial/\partial\xi_i$ and $\partial_t=\partial/\partial t$ are odd and even derivations, respectively. Then $W(1,n)$ is a formal distribution Lie superalgebra with spanning family of (pairwise local) formal distributions:

$$\mathcal{F}=\{\delta(t-z)a | a\in W(n)\}\cup\{\delta(t-z)f\partial_t | f\in\Lambda(n)\},$$

where $W(n)=\{\Sigma_{i=1}^{n} a_i\partial_i \,|\, a_i\in\Lambda(n)\}$ is the (finite-dimensional) Lie superalgebra of all derivations of $\Lambda(n)$. The associated Lie conformal superalgebra W_n is defined as

$$W_n=\mathbb{C}[\partial]\otimes(W(n)\oplus\Lambda(n)). \tag{4.2}$$

The λ-bracket is defined as follows $(a,b\in W(n);f,g\in\Lambda(n))$:

$$[a_\lambda b]=[a,b],\quad [a_\lambda f]=a(f)-(-1)^{p(a)p(f)}\lambda fa,\quad [f_\lambda g]=-(\partial+2\lambda)fg. \tag{4.3}$$

The Lie conformal algebra W_n is simple for $n\geqslant 0$ and has rank $(n+1)2^n$.

The annihilation subalgebra is

$$\mathcal{A}(W_n) = W(1,n)_+ = \left\{ a\partial_t + \sum_{i=1}^{n} a_i\partial_i | a, a_i \in \Lambda(1,n)_+ \right\}, \tag{4.4}$$

where $\Lambda(1,n)_+ = \mathbb{C}[t] \otimes \Lambda(n)$. The extended annihilation subalgebra is

$$\mathcal{A}(W_n)^e = W(1,n)^+ = \mathbb{C}\partial_t \ltimes W(1,n)_+,$$

and therefore it is isomorphic to the direct sum of $W(1,n)_+$ and a commutative one-dimensional Lie algebra.

The $\mathbb{Z}$-gradation in (3.1) is obtained by letting

$$\deg t = \deg \xi_i = 1 = -\deg \partial_t = -\deg \partial_i.$$

If $L = W(1,n)_+$, then $L_{-1} = \langle \partial_t, \partial_1, \ldots, \partial_n \rangle$, where ∂_t is an even element and $\partial_1, \ldots, \partial_n$ are odd elements of a basis in L_{-1}. Note also that $L_0 \simeq gl(1|n)$.

From now on, we shall use the notation $\partial_0 = \partial_t$. Explicitly, we have

$$L_0 = \langle \{ t\partial_i, \xi_i\partial_j : 0 \leqslant i, j \leqslant n \} \rangle.$$

In order to write explicitly weights for vectors in $W(1,n)_+$-modules, we would consider the basis

$$t\partial_0; t\partial_0 + \xi_1\partial_1, \ldots, t\partial_0 + \xi_n\partial_n$$

for the Cartan subalgebra H in $W(1,n)_+$, and we write the weight of an eigenvector for the Cartan subalgebra H as a tuple

$$\bar{\mu} = (\mu; \lambda_1, \ldots, \lambda_n)$$

for the corresponding eigenvalues of the basis.

B. Modules of Laurent differential forms

1. Restricted dual

Our algebra $L = W(1,n)_+$, and in the last section $S(1,n)_+$, are $\mathbb{Z}$-graded (super)algebras and the modules we intend to study are graded modules, i.e., an L-module V is a direct sum $V = \oplus_{m \in \mathbb{Z}} V_m$ of finite-dimensional subspaces V_m, and $L_k \cdot V_m \subset V_{k+m}$. For a graded module V we define the *restricted dual module* $V^\#$ as

$$V^\# = \oplus_{m \in \mathbb{Z}} (V_m)^*.$$

Hence $V^\#$ is a subspace of V^* and it is invariant with respect to the contragradient action, so it defines an L-module structure. Observe that $(V^\#)^\# = V$.

In our situation, we have $L_{-1} = \langle \partial_0, \partial_1, \ldots, \partial_n \rangle$, then any L-module becomes a $\mathbb{C}[\partial_0, \partial_1, \ldots, \partial_n]$-module. Hence, a module V is a free $\mathbb{C}[\partial_0, \partial_1, \ldots, \partial_n]$-module if and only if $V^\#$ is a cofree module, i.e., it is isomorphic to a direct sum of copies of the standard module $\mathbb{C}[z, \rho_1, \ldots, \rho_n]$, with $\partial_0 \cdot f = (\partial/\partial z) f$, and $\partial_i \cdot f = (\partial/\partial \rho_i) f$.

An induced module $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F$ is by definition a free $\mathbb{C}[\partial_0, \partial_1, \ldots, \partial_n]$-module, so the co-induced (or produced) module

$$\mathrm{Cnd} F^\# = (\mathrm{Ind} F)^\#$$

will be cofree.

2. Differential forms modules

In order to define the differential forms one considers an odd variable dt and even variables $d\xi_1,\dots,d\xi_n$ and defines the differential forms to be the (super)commutative algebra freely generated by these variables over $\Lambda(1,n)_+=\mathbb{C}[t]\otimes\Lambda(n)$, or

$$\Omega_+=\Lambda(1,n)_+[d\xi_1,\dots,d\xi_n]\otimes\Lambda[dt].$$

Generally speaking Ω_+ is just a polynomial (super)algebra over a big set of variables

$$t,\xi_1,\dots,\xi_n,dt,d\xi_1,\dots,d\xi_n,$$

where the parity is

$$p(t)=0,\quad p(\xi_i)=1,\quad p(dt)=1,\quad p(d\xi_i)=0.$$

These are called (*polynomial*) *differential forms*, and we define the *Laurent differential forms* to be the same algebra over $\Lambda(1,n)=\mathbb{C}[t,t^{-1}]\otimes\Lambda(n)$:

$$\Omega=\Lambda(1,n)[d\xi_1,\dots,d\xi_n]\otimes\Lambda[dt].$$

We would like to consider a fixed complementary subspace Ω_- to Ω_+ in Ω chosen as follows:

$$\Omega_-=t^{-1}\mathbb{C}[t^{-1}]\otimes\Lambda(n)\otimes\mathbb{C}[d\xi_1,\dots,d\xi_n]\otimes\Lambda[dt].$$

For the differential forms we need the usual differential degree that measure only the involvement of the differential variables $dt,d\xi_1,\dots,d\xi_n$, that is

$$\deg t=0,\quad \deg\xi_i=0,\quad \deg dt=1,\quad \deg d\xi_i=1.$$

As a result, the degree of a function is zero and it gives us the *standard* $\mathbb{Z}$*-gradation* both on Ω and $\Omega_\pm$. As usual, we denote by $\Omega^k,\Omega^k_\pm$ the corresponding graded components.

We denote by Ω^k_c the special subspace of differential forms with constant coefficients in Ω_k.

The operator d is defined on Ω as usual by the rules $d\cdot t=dt,d\cdot\xi_i=d\xi_i,d\cdot d\xi_i=0$, and the identity

$$d(fg)=(df)g+(-1)^{p(f)}fdg.$$

Observe that d maps both Ω_+ and Ω_- into themselves.

As usual, we extend the natural action of $W(1,n)_+$ on $\Lambda(1,n)$ to the whole Ω by imposing the property

$$D\cdot d=(-1)^{p(D)}d\cdot D,\quad D\in W(1,n)_+,$$

that is, D (super)commutes with d. It is clear that Ω_+ and all the subspaces Ω^k are invariant. Hence Ω^k_+ and Ω^k are $W(1,n)_+$-modules, which are called the *natural representations* of $W(1,n)_+$ in differential forms.

We define the action of $W(1,n)_+$ on Ω_- via the isomorphism of Ω_- with the factor of Ω by Ω_+. Practically this means that in order to compute $D\cdot f$, where $f\in\Omega_-$, we apply D to f and "disregard terms with non-negative powers of t."

The operator d restricted to $\Omega^k_\pm$ defines an odd morphism between the corresponding representations. Clearly the image and the kernel of such a morphism are submodules in $\Omega^k_\pm$.

Let $\Theta^k_c=(\Omega^k_c)^\#$ and $\Theta^k_+=(\Omega^k_+)^\#$. In the rest of this section, we consider $L=W(1,n)_+$.

Proposition 4.1: For $L=W(1,n)_+$ *we have*:

(1) *The* L_0*-module* $\Theta^k_c,k\geqslant 0$ *is irreducible with highest weight*

$$(0;0,\dots,0,-k),\quad k\geqslant 0.$$

(2) *The L-module* Θ^k_+, $k\geqslant 0$ *contains* Θ^k_c *and this inclusion induces the isomorphism*

$$\Theta_+^k = \mathrm{Ind}\,\Theta_c^k.$$

(3) *The dual maps* $d^{\#}: \Theta_+^{k+1} \to \Theta_+^k$ *are morphisms of L-modules. The kernel of one of them is equal to the image of the next one and it is a nontrivial proper submodule in* Θ_+^k.

Proof: (1) It is well known that Ω_c^k are irreducible and thus Θ_+^k are also irreducible. Observe that the lowest vector in Ω_c^k is $(d\xi_n)^k$ and it has the weight $(0;0,\ldots,0,k)$. Now the sign changes as we go to the dual module and so we get the highest weight of Θ_c^k.

(2) By the definition of the restricted dual, it is the sum of the dual of all the graded components of the initial module. In our case Ω_c^k is the component of the minimal degree in Ω_+^k, so Θ_c^k becomes the component of the maximal degree in Θ_+^k. This implies that $L_{>0}$ acts trivially on Θ_c^k, so the morphism $\mathrm{Ind}\,\Theta_c^k \to \Theta_+^k$ is defined. Clearly Ω_+^k is isomorphic to

$$\Omega_c^k \otimes \mathbb{C}[t,\xi_1,\ldots,\xi_n],$$

so it is a cofree module. Then the module Θ_+^k is a free $\mathbb{C}[\partial_0,\partial_1,\ldots,\partial_n]$-module and the morphism

$$\mathrm{Ind}\,\Theta_c^k \to \Theta_+^k$$

is therefore an isomorphism.

(3) This statement follows immediately from the fact that d commutes with the action of vector fields. □

Corollary 4.2: The $W(1,n)_+$*-modules* Ω_+^k *of differential forms are isomorphic to the coinduced modules*

$$\Omega_+^k = \mathrm{Cnd}\,\Omega_c^k.$$

Let us now study the $L=W(1,n)_+$-modules Ω_-^k. First, notice that these modules are free as $\mathbb{C}[\partial_0,\partial_1,\ldots,\partial_n]$-modules. Let

$$\xi_* = \xi_1 \cdots \xi_n, \quad \text{and} \quad \bar{\Omega}_c^k = t^{-1}\xi_* \Omega_c^k \subset \Omega_-^k. \tag{4.5}$$

Proposition 4.3: For $L=W(1,n)_+$*, we have:*

(1) $\bar{\Omega}_c^k$ *is an irreducible* L_0*-submodule in* Ω_-^k *with highest weight*

$$\begin{aligned} &(-1;0,0,\ldots,0) && \text{for } k=0,\\ &(0;k,1,\ldots,1) && \text{for } k>0, \end{aligned}$$

and $L_{>0}$ *acts trivially on* $\bar{\Omega}_c^k$.

(2) *There is an isomorphism* $\Omega_-^k = \mathrm{Ind}_{L_{\geqslant 0}}^{L} \bar{\Omega}_c^k$.

(3) *The differential d gives us L-module morphisms on* Ω_-^k *and the kernel and image of d are L-submodules in* Ω_-^k.

(4) *The kernel of d and image of d in* Ω_-^k *for* $k \geqslant 2$ *coincide, in* Ω_-^1 *we have* $\mathrm{Ker}\,d = \mathbb{C}(t^{-1}dt) + \mathrm{Im}\,d$*, and in* Ω_-^0*, we have* $\mathrm{Ker}\,d = 0$ (*and the image does not exist*).

Proof: (1) First of all, $\bar{\Omega}_c^k$ is the maximum total degree component in Ω_-^k, so any element from $L_{>0}$ moves it to zero. Also, as L_0-module $\bar{\Omega}_c^k$ is isomorphic to Ω_c^k multiplied by the one-dimensional module $\langle t^{-1}\xi_* \rangle$. This permits us to see that its highest vectors are

$$\begin{aligned} &\langle t^{-1}\xi_* \rangle && \text{for } k=0,\\ &\langle t^{-1}\xi_* dt \rangle && \text{for } k=1,\\ &\langle t^{-1}\xi_* dt (d\xi_1)^{k-1} \rangle && \text{for } k>1. \end{aligned}$$

The values of the highest weights are easy to compute.

(2) It is straightforward to see that Ω_-^0 is a free rank 1 $\mathbb{C}[\partial_0,\partial_1,\ldots,\partial_n]$-module. Now, the action of $\partial_0,\partial_1,\ldots,\partial_n$ on Ω_-^k is coefficient-wise and the fact that Ω_-^k is a free

$\mathbb{C}[\partial_0,\partial_1,\ldots,\partial_n]$-module follows. This gives us the isomorphism $\Omega^k_-=\mathrm{Ind}^L_{L_{\geqslant 0}}\bar{\Omega}^k_c$. Parts (3) and (4) are left to the reader. □

The above statement shows us that there are nontrivial submodules in $\Omega^k_\pm$ and Θ^k_+. In fact, these are "almost all" proper submodules and the respective factors are irreducible. These results are discussed in Sec. IV D. In order to get this result we need to study singular vectors.

C. Singular vectors of W_n-modules

Having in mind the results of Sec. III, we introduce the following modules. Given a $gl(1|n)$-module V, we have the associated tensor field $W(1,n)$-module $\mathbb{C}[t,t^{-1}]\otimes\Lambda(n)\otimes V$, which is a formal distribution module spanned by a collection of fields $E=\{\delta(t-z)fv\,|\,f\in\Lambda(n),v\in V\}$. The associated conformal W_n-module is

$$\mathrm{Tens}(V)=\mathbb{C}[\partial]\otimes(\Lambda(n)\otimes V) \tag{4.6}$$

with the following λ-action:

$$a_\lambda(g\otimes v)=a(g)\otimes v+(-1)^{p(a)}\sum_{i,j=1}^n(\partial_i f_j)g\otimes(E_{ij}-\delta_{ij})(v)-\lambda(-1)^{p(g)}\sum_{j=1}^n f_j g\otimes E_{0j}(v), \tag{4.7}$$

$$f_\lambda(g\otimes v)=(-\partial)(fg\otimes v)+(-1)^{p(fg)}\sum_{i=1}^n(\partial_i f)g\otimes E_{i0}(v)+\lambda(fg\otimes E_{00}(v)), \tag{4.8}$$

where $a=\Sigma_{i=1}^n f_i\partial_i\in W(n),f,g\in\Lambda(n),v\in V$, and $E_{ij}\in gl(1|n)$ are matrix units (they correspond to the level 0 elements $\xi_i\partial_j$ with the notation $\xi_0=t$ and $\partial_0=\partial_t$).

In this case, the modules $M(F)=\mathrm{Ind}^L_{L_{\geqslant 0}}F$ defined in Sec. III, correspond to the W_n-module $\mathrm{Tens}(F)$, with F a finite-dimensional (irreducible) $gl(1|n)$-module. When we discuss the highest weight of vectors and singular vectors, we always mean with respect to the upper Borel subalgebra in $L=W(1,n)_+$ generated by $L_{>0}$ and the elements of L_0:

$$t\partial_i,\quad \xi_i\partial_j\ i<j. \tag{4.9}$$

Therefore, in the module $M(V)$, viewed as a module over the annihilation algebra $W(1,n)_+$ (see Proposition 2.3), a vector $m\in M(V)$ is a singular vector if and only if the following conditions are satisfied ($g=\xi_{i_1}\cdots\xi_{i_s}\in\Lambda(n)$, and $\partial_0=\partial_t$)

$$\begin{aligned}&\text{(s1) } t^n g\partial_i\cdot m=0 \quad \text{for } n>1,\\ &\text{(s2) } t^1 g\partial_i\cdot m=0 \quad \text{except for } g=1 \text{ and } i=0,\\ &\text{(s3) } t^0 g\partial_j\cdot m=0 \quad \text{for } s>1 \text{ or } g=\xi_i \text{ with } i<j.\end{aligned} \tag{4.10}$$

We shall frequently use the notation

$$\xi_I=\xi_{i_1}\cdots\xi_{i_s}\in\Lambda(n),\quad \text{with } I=\{i_1,\ldots,i_s\}. \tag{4.11}$$

Therefore, these conditions on a singular vector $m\in\mathrm{Tens}(V)$ translate in terms of the λ-action to (cf. (2.3)):

(S1) $d^2/d\lambda^2(f_\lambda m)=0$ for all $f\in\Lambda(n)$,
(S2) $d/d\lambda(a_\lambda m)=0$ for all $a\in W(n)$,
(S3) $d/d\lambda(f_\lambda m)|_{\lambda=0}=0$ for all $f\in\Lambda(n)$ with $f\neq 1$,
(S4) $(a_\lambda m)|_{\lambda=0}=0$ for all $a=\xi_I\partial_j\in W(n)$ with $|I|>1$ or $a=\xi_i\partial_j$ with $i<j$,
(S5) $(f_\lambda m)|_{\lambda=0}=0$ for all $f=\xi_I\in\Lambda(n)$ with $|I|>1$.

In order to classify the finite irreducible W_n-modules we should solve these equations (S1–5) to obtain the singular vectors.

Let $m \in \mathrm{Tens}(V) = \mathbb{C}[\partial] \otimes \Lambda(n) \otimes V$, then

$$m = \sum_{k=0}^{N} \sum_{I} \partial^k (\xi_I \otimes v_{I,k}) \quad \text{with } v_{I,k} \in V. \tag{4.12}$$

In order to obtain the singular vectors, we need some reduction lemmas:

Lemma 4.4: If $m \in \mathrm{Tens}(V)$ is a singular vector, then the degree of m in ∂ is at most 1.

Proof: Using (4.7), we have for $a = \sum_{i=1}^{n} f_i \partial_i$ that

$$\frac{d}{d\lambda}(a_\lambda m) = \sum_{k=1}^{N} \sum_{I} k(\lambda + \partial)^{k-1} [a(\xi_I) \otimes v_{I,k} + (-1)^{p(a)} \sum_{i,j=1}^{n} (\partial_i f_j) \xi_I \otimes (E_{ij} - \delta_{ij})(v_{I,k}) - \lambda (-1)^{|I|} \sum_{j=1}^{n} f_j \xi_I \otimes E_{0j}(v_{I,k})] - \sum_{k=0}^{N} \sum_{I} (\lambda + \partial)^k (-1)^{|I|} \sum_{j=1}^{N} f_j \xi_I \otimes E_{0j}(v_{I,k}). \tag{4.13}$$

Taking $a = \partial_j$, condition (S2) becomes

$$0 = \sum_{k=1}^{N} \sum_{I | j \in I} k(\lambda + \partial)^{k-1} (\xi_{i_1} \cdots \hat{\xi}_j \cdots \xi_{i_s} \otimes v_{I,k}) - \lambda \sum_{k=1}^{n} \sum_{I} (-1)^{|I|} k(\lambda + \partial)^{k-1} (\xi_I \otimes E_{0j}(v_{I,k})) - \sum_{k=0}^{N} \sum_{I} (\lambda + \partial)^k (-1)^{|I|} (\xi_I \otimes E_{0j}(v_{I,k})). \tag{4.14}$$

Now, viewed as a polynomial in λ, we obtain

$$E_{0j}(v_{I,k}) = 0, \quad \forall\, I, k = 1, \ldots, N, \quad \text{and } j = 1, \ldots, n. \tag{4.15}$$

Using it in (4.14) and taking the coefficients in $\lambda + \partial$, we get

$$v_{I,k} = 0 \quad \text{for all } I \neq \emptyset, \text{ and } k \geqslant 2.$$

Hence, $m = \sum_{k=0}^{1} \sum_{I} \partial^k (\xi_I \otimes v_{I,k}) + \sum_{k=2}^{N} \partial^k (1 \otimes v_{\emptyset,k})$.

Using (4.8) and condition (S1) for $f = 1$, we have

$$0 = \frac{d^2}{d\lambda^2}(f_\lambda m) = 2 \sum_{I} (\xi_I \otimes E_{00}(v_{I,1})) - \sum_{k=2}^{N} (k-1)k(\lambda + \partial)^{k-2}\, \partial\, (1 \otimes v_{\emptyset,k}) + \sum_{k=2}^{N} (2k(\lambda + \partial)^{k-1} + \lambda k(k-1)(\lambda + \partial)^{k-2})(1 \otimes E_{00}(v_{\emptyset,k})). \tag{4.16}$$

Then, viewed as a polynomial in λ, we have $E_{00}(v_{\emptyset,k}) = 0$ for all $k \geqslant 2$. Hence the last term in (4.16) is 0. Now, viewed as a polynomial in $(\lambda + \partial)$, we obtain $v_{\emptyset,k} = 0$ for all $k \geqslant 2$, finishing the proof. □

Observe that the coefficient in $(\lambda + \partial)^0$ in (4.16), gives us the following useful identity:

$$E_{00}(v_{I,1}) = 0 \quad \text{for all } I. \tag{4.17}$$

We will use the following notation: $[1, n] = \{1, \ldots, n\}$.

Lemma 4.5: If m is a singular vector, then

$$m = \partial(\xi_{[1,n]} \otimes w) + \sum_{l=1}^{n} (\xi_{[1,n]-\{l\}} \otimes v_l) + \xi_{[1,n]} \otimes v_0.$$

Proof: By the previous lemma, we have

$$m = \sum_{I} [\partial(\xi_I \otimes v_{I,1}) + (\xi_I \otimes v_{I,0})].$$

Now (S5) gives us

$$0=(f_\lambda m)_{|_{\lambda=0}}=\sum_I((-\partial)(f\xi_I\otimes v_{I,0})-(-1)^{|I|}\sum_{i=1}^n(\partial_i f)\xi_I\otimes E_{i0}(v_{I,0}))$$
$$+\sum_I((-\partial^2)(f\xi_I\otimes v_{I,1})-(-1)^{|I|}\sum_{i=1}^n\partial((\partial_i f)\xi_I\otimes E_{i0}(v_{I,1}))) \tag{4.18}$$

for any $f=\xi_J$ with $|J|>1$. Considering the coefficient of ∂^2 and taking $f=\xi_l\xi_k$, we obtain $v_{I,1}=0$ for all I with $|I|\leqslant n-2$. Using this and considering the coefficient of ∂ with $f=\xi_l\xi_k\xi_s$, we obtain $v_{I,0}=0$ for all I with $|I|\leqslant n-3$. With this reduction, the coefficient of ∂ with $f=\xi_i\xi_j$ $(i\neq j)$ is

$$0=-(\xi_{[1,n]}\otimes v_{[1,n]-\{i,j\},0})+(-1)^{n-1}(\xi_{[1,n]}\otimes E_{i0}(v_{[1,n]-\{j\},1})),$$

obtaining

$$E_{i0}(v_{[1,n]-\{j\},1})=(-1)^{n-1}v_{[1,n]-\{i,j\},0}\quad\text{for all } i\neq j. \tag{4.19}$$

Computing (S3), we have

$$0=\frac{d}{d\lambda}(f_\lambda m)_{|_{\lambda=0}}=\sum_{|I|\geqslant n-1}((-\partial)(f\xi_I\otimes v_{I,1})-(-1)^{|I|}\sum_{i=1}^n(\partial_i f)\xi_I\otimes E_{i0}(v_{I,1}))$$
$$+\partial\sum_{|I|\geqslant n-1}f\xi_I\otimes E_{00}(v_{I,1})+\sum_{|I|\geqslant n-2}f\xi_I\otimes E_{00}(v_{I,0}).$$

Now, taking $f=\xi_i$, using (4.17), and considering the coefficient in ∂, we have

$$v_{I,1}=0\quad\text{for all } |I|=n-1,$$

and using it in (4.19), we have

$$v_{I,0}=0\quad\text{for all } |I|=n-2,$$

finishing the proof. □

Let $\xi_*:=\xi_{[1,n]}$ and $\xi^l:=\xi_{[1,n]-\{l\}}$. Due to the previous lemma, any singular vector has the form

$$m=\partial(\xi_*\otimes w)+\sum_{l=1}^n(\xi^l\otimes v_l)+\xi_*\otimes v_0.$$

Then, it is easy to see that conditions (s1–3) are equivalent to the following list

(s1):

$$E_{00}(w)=0, \tag{4.20}$$

$$E_{0i}(w)=0,\quad i=1,\ldots,n. \tag{4.21}$$

(s2):

$$E_{ji}(w)+E_{0i}(v_j)=0,\quad i,j=1,\ldots,n, \tag{4.22}$$

$$E_{0i}(v_0)=0,\quad i=1,\ldots,n, \tag{4.23}$$

$$E_{0i}(v_j)=0,\quad i,j=1,\ldots,n,\quad i\neq j, \tag{4.24}$$

$$E_{0j}(v_j)=-w,\quad j=1,\ldots,n. \tag{4.25}$$

$$E_{i0}(w)=E_{00}(v_i),\quad i=1,\ldots,n. \tag{4.26}$$

(s3):

$$E_{i0}(v_j) = E_{j0}(v_i), \quad i,j = 1, \ldots, n, \quad i \neq j. \tag{4.27}$$

$$E_{ij}(v_l) = E_{lj}(v_i), \quad i,j,l = 1, \ldots, n, \quad i \neq l. \tag{4.28}$$

$$E_{ij}(w) = 0, \quad i,j = 1, \ldots, n, \quad i < j, \tag{4.29}$$

$$E_{ij}(v_0) = 0, \quad i,j = 1, \ldots, n, \quad i < j, \tag{4.30}$$

$$E_{ij}(v_l) = 0, \quad i,j,l = 1, \ldots, n, \quad i < j, l \neq j, \tag{4.31}$$

$$E_{ij}(v_j) = v_i, \quad i,j = 1, \ldots, n, \quad i < j. \tag{4.32}$$

Now replacing (4.24) and (4.25) on (4.22), we obtain

$$E_{ij}(w) = \delta_{ij} w, \quad i,j = 1, \ldots, n. \tag{4.33}$$

Recall that we are considering the basis $(\partial_0 = \partial_t)$

$$t\partial_0; t\partial_0 + \xi_1\partial_1, \ldots, t\partial_0 + \xi_n\partial_n$$

for the Cartan subalgebra H in $W(1,n)_+$, and we write the weight of an eigenvector for the Cartan subalgebra H as a tuple

$$\bar{\mu} = (\mu; \lambda_1, \ldots, \lambda_n) \tag{4.34}$$

for the corresponding eigenvalues of the basis.

Using the above conditions, we can prove the following:

Proposition 4.6: Let $n \geqslant 2$ *and* m *be a nontrivial singular vector in* Tens V *with weight* $\bar{\mu}_m$, *then we have one of the following:*

(*a*) $m = \xi^n \otimes v_n$, $\bar{\mu}_m = (0; 0, \ldots, 0, -k)$ *with* $k \geqslant 0$, v_n *is a highest weight vector in* V *with weight* $(0; 0, \ldots, 0, -k-1)$, *and* m *is uniquely defined by* v_n.

(*b*) $m = \Sigma_{l=1}^n \xi^l \otimes v_l$, $\bar{\mu}_m = (0; k, 1, \ldots, 1)$ *with* $k \geqslant 2$, v_1 *is a highest weight vector in* V *with weight* $(0; k-1, 1, \ldots, 1)$, *and* m *is uniquely defined by* v_1.

(*c*) $m = \partial(\xi_* \otimes w) + \Sigma_{l=1}^n \xi^l \otimes v_l$, $\bar{\mu}_m = (-1; 0, \ldots, 0)$, w *is a highest weight vector in* V *with weight* $(0; 1, \ldots, 1)$, *and* m *is uniquely defined by* w.

Proof: By computing $E_{00} \cdot m = (t\partial) \cdot m$ and using (4.20) and (4.26) on it, we obtain the following conditions:

If $w = 0$, then

$$E_{00} \cdot m = 0 \quad \text{and} \quad E_{00}(v_0) = 0. \tag{4.35}$$

If $w \neq 0$, then

$$E_{00} \cdot m = -m, \tag{4.36}$$

$$E_{00}(v_l) = -v_l, \quad l = 0, \ldots, n, \tag{4.37}$$

and using (4.26), in this case $(w \neq 0)$ we have

$$E_{i0}(w) = -v_i, \quad i = 1, \ldots, n. \tag{4.38}$$

Similarly, observe that $E_{ii} \cdot m = (\xi_i \partial_i) \cdot m$. Now this action can be easily computed, and using (4.33) on it, we have the following:

If $w \neq 0$, then

$$E_{ii}\cdot m = m, \quad i = 1, \ldots, n,$$

$$\begin{aligned} E_{ii}(v_l) &= v_l, \quad l, i = 1, \ldots, n, l \neq i, \\ E_{ii}(v_i) &= 2v_i, \quad i = 1, \ldots, n, \end{aligned} \tag{4.39}$$

$$E_{ii}(v_0) = v_0, \quad i = 1, \ldots, n.$$

Using this and Eqs. (4.36), (4.20), and (4.33), we obtain for the case $w \neq 0$, that the corresponding weights are

$$\bar{\mu}_m = (-1; 0, \ldots, 0) \quad \text{and} \quad \bar{\mu}_w = (0; 1, \ldots, 1).$$

This result together with (4.38) give us the proof of case (c) in the proposition.

For the rest of the proof, we assume $w=0$, let us show that the only possible cases are (a) and (b).

Observe that replacing (4.32) in (4.28), we get

$$E_{jj}(v_i) = v_i \quad \forall\, i < j. \tag{4.40}$$

Now, Eq. (4.32) shows that if $v_l=0$ for some l with $1 \leqslant l \leqslant n$, then $v_j=0$ for all $j<l$. In order to finish the proof, we should show that only the two extreme cases are possible, that is $v_l \neq 0$ for all l or $v_l=0$ except for $l=n$.

Now, suppose that there exist $l>1$ such that $v_j=0$ for all $j<l$ and $v_l \neq 0$, then using (4.28) we have that

$$E_{ii}(v_k) = 0, \quad i < l \leqslant k. \tag{4.41}$$

Then by (4.41) and (4.40), we obtain that

$$E_{ii}\cdot m = \alpha m \quad \text{with } \alpha = 0 \text{ or } 1, \quad \text{if } i < l \text{ or } i > l, \text{ respectively.}$$

Therefore, using this and (4.35) we get

$$\bar{\mu}_m = (0; 0, \ldots, 0, k, 1, \ldots, 1)$$

where $E_{ll}\cdot m = km$. But the space V, from which we are inducing is finite-dimensional and a singular vector generates a finite-dimensional L_0-submodule, then (recall notation (4.34))

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$$

is a highest weight, and because of that only two extreme positions of k are possible (recall that $n>1$). This gives us the cases (a) and (b). In order to finish the proof we need to complete the computation of weights in each case.

If $v_1 \neq 0$, then using (4.26) and (4.40) we obtain

$$\bar{\mu}_m = (0; k, 1, \ldots, 1) \quad \text{and} \quad \bar{\mu}_{v_1} = (0; k-1, 1, \ldots, 1) \quad \text{with } k \geqslant 1,$$

getting case (b).

If $v_l=0$ except for $l=n$, then using (4.26) and (4.41) we obtain

$$\bar{\mu}_m = (0; 0, \ldots, 0, k) \quad \text{and} \quad \bar{\mu}_{v_n} = (0; 0, \ldots, 0, k-1) \quad \text{with } k \leqslant 0$$

obtaining case (c). Case (d) is immediate. □

D. Irreducible induced $W(1,n)_+$-modules

In this section we consider $L=W(1,n)_+$, with $n\geqslant 2$. Now, we have the following:

Theorem 4.7: *Let $n\geqslant 2$ and F be an irreducible L_0-module with highest weight $\bar{\mu}_*$. Then the L-modules $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F$ are irreducible finite continuous modules except for the following cases*:

(*a*) $\bar{\mu}_*=(0;\bar{0},\ldots,0,-m), m\geqslant 0$, *where* $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F=\Theta_+^m$ *and the image* $d^{\#}\Theta_+^{m+1}$ *is the only nontrivial proper submodule.*

(*b*) $\bar{\mu}_*=(0;k,1,\ldots,1), k\geqslant 1$, *where* $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F=\Omega_-^k$. *For* $k\geqslant 2$ *the image* $d\Omega_-^{k-1}$ *is the only nontrivial proper submodule. For* $k=1$, *both* $\mathrm{Im}(d)$ *and* $\mathrm{Ker}(d)$ *are proper submodules*. $\mathrm{Ker}(d)$ *is a maximal submodule.*

Remark 4.8: Let F be an irreducible L_0-module with highest weight $\bar{\mu}_*=(-1;0,\ldots,0)$. Then $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F=\Omega_-^0$ is an irreducible L-module. Note that the image of $d:\Omega_-^0\to\Omega_-^1$ is the submodule in Ω_-^1 generated by the singular vector corresponding to the case (c) in Proposition 4.6, but it is not a maximal submodule (see Proposition 4.3 (4)).

Proof: We know from Theorem 3.1 that in order for $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F$ to be reducible it has to have nontrivial singular vectors and the possible highest weights of F in this situation are listed in Proposition 4.6 above.

The fact that the induced modules are actually reducible in those cases is known because we have got nice realizations for these induced modules in Propositions 4.1 and 4.3 together with morphisms defined by $d, d^{\#}$, so kernels and images of these morphisms become submodules.

The subtle thing is to prove that a submodule is really a maximal one. We notice that in each case the factor is isomorphic to a submodule in another induced module so it is enough to show that the submodule is irreducible. This can be proved as follows, a submodule in the induced module is irreducible if it is generated by any highest singular vector that it contains. We see from our list of nontrivial singular vectors that there is at most one such vector for each case and the images and kernels in question are exactly generated by those vectors, hence they are irreducible. □

Corollary 4.9: The theorem gives us a description of finite continuous irreducible $W(1,n)_+$-modules for $n\geqslant 2$. Such a module is either $\mathrm{Ind}_{L_{\geqslant 0}}^{L} F$ for an irreducible finite-dimensional L_0-module F where the highest weight of F does not belong to the types listed in (a), (b) of the theorem or the factor of an induced module from (a), (b) by its submodule $Ker(d)$.

E. Finite irreducible W_n-modules

In order to give an explicit construction and classification, we need the following notation. Recall that $W(1,n)$ acts by derivations on the algebra of differential forms $\Omega=\Omega(1,n)$, and note that this is a conformal module by taking the family of formal distributions

$$E=\{\delta(z-t)\omega \quad \text{and} \quad \delta(z-t)\omega dt \,|\, \omega\in\Omega(n)\}.$$

Translating this and all other attributes of differential forms, like de Rham differential, etc., into the conformal algebra language, we arrive at the following definitions.

Recall that given an algebra A, the associated current formal distribution algebra is $A[t,t^{-1}]$ with the local family $F=\{a(z)=\Sigma_{n\in\mathbb{Z}}(at^n)z^{-n-1}=a\delta(z-t)\}_{a\in A}$. The associated conformal algebra is $\mathrm{Cur}A=\mathbb{C}[\partial]\otimes A$ with multiplication defined by $a_\lambda b=ab$ for $a,b\in A$ and extended using sesquilinearity. This is called the *current conformal algebra*, see Ref. 8 for details.

The conformal algebra of differential forms Ω_n is the current algebra over the commutative associative superalgebra $\Omega(n)+\Omega(n)dt$ with the obvious multiplication and parity, subject to the relation $(dt)^2=0$:

$$\Omega_n=\mathrm{Cur}(\Omega(n)+\Omega(n)dt).$$

The de Rham differential $\tilde{d}$ of Ω_n (we use the tilde in order to distinguish it from the de Rham differential d on $\Omega(n)$) is a derivation of the conformal algebra Ω_n such that

$$\widetilde{d}(\omega_1 + \omega_2 dt) = d\omega_1 + d\omega_2 dt - (-1)^{p(\omega_1)}\,\partial\,(\omega_1 dt). \tag{4.42}$$

Here and further $\omega_i \in \Omega(n)$.

The standard $\mathbb{Z}_+$-gradation $\Omega(n) = \oplus_{j\in\mathbb{Z}_+}\Omega(n)^j$ of the superalgebra of differential forms by their degree induces a $\mathbb{Z}_+$-gradation

$$\Omega_n = \oplus_{j\in\mathbb{Z}_+}\Omega_n^j, \quad \text{where } \Omega_n^j = \mathbb{C}[\partial]\otimes(\Omega(n)^j + \Omega(n)^{j-1}dt),$$

so that $\widetilde{d}:\Omega_n^j \to \Omega_n^{j+1}$.

The contraction ι_D for $D = a + f \in W_n$ is a conformal derivation of Ω_n such that:

$$(i_a + f)_\lambda \quad (\omega_1 + \omega_2 dt) = i_a\omega_1 + (-1)^{p(f)} f\omega_2.$$

Here and further, as before, $a \in W(n)$, $f \in \Lambda(n)$. The Lie derivative $\widetilde{L}_D$ for $D \in W_n$ is a conformal derivation of Ω_n such that:

$$(\widetilde{L}_a)_\lambda(\omega_1 + \omega_2 dt) = L_a\omega_1 + (L_a\omega_2)dt,$$

$$(\widetilde{L}_f)_\lambda\omega = -(\partial + \lambda)(f\omega), \tag{4.43}$$

$$(\widetilde{L}_f)_\lambda(\omega dt) = (-1)^{p(f)+p(\omega)}(df)\omega - \partial(f\omega dt).$$

The properties of $\Omega(1,n)$ imply the corresponding properties of Ω_n given by the following proposition.

Proposition 4.10:

(a) $\widetilde{d}^2 = 0$.

(b) *The complex* $(\Omega_n, \widetilde{d}) = \{0 \to \Omega_n^0 \to \cdots \to \Omega_n^j \to \cdots\}$ *is exact at all terms* Ω_n^j, *except for* $j = 1$. *One has*: $\operatorname{Ker}\widetilde{d}_{|\Omega_n^1} = \widetilde{d}\Omega_n^0 \oplus \mathbb{C}dt$.

(c) $\iota_{D_1}\iota_{D_2} + p(D_1, D_2)\iota_{D_2}\iota_{D_1} = 0$.

(d) $\widetilde{L}_D\widetilde{d} = (-1)^{p(D)}\widetilde{d}\widetilde{L}_D$.

(e) $\widetilde{L}_D = \widetilde{d}\iota_D + (-1)^{p(D)}\iota_D\widetilde{d}$.

(f) *The map* $D \mapsto \widetilde{L}_D$ *defines a* W_n*-module structures on* Ω_n, *preserving the* $\mathbb{Z}_+$*-gradation and commuting with* $\widetilde{d}$.

Proof: Only the proof of (b) requires a comment. Following Proposition 3.2.2 of Ref. 8, we construct $\mathbb{C}[\partial]$-linear maps $K:\Omega_n \to \Omega_n$ (a homotopy operator) and $\epsilon:\Omega_n \to \Omega_n$ by the formulas ($\omega \in \Omega(n) + \Omega(n)dt$):

$$K(d\xi_n\omega) = \xi_n\omega, \quad K(\omega) = 0 \quad \text{if } \omega \text{ does not involve } d\xi_n,$$

$$\epsilon(d\xi_n\omega) = \epsilon(\xi_n\omega) = 0, \quad \epsilon(\omega) = \omega \quad \text{if } \omega \text{ does not involve both } d\xi_n \text{ and } \xi_n.$$

One checks directly that

$$K\widetilde{d} + \widetilde{d}K = 1 - \epsilon.$$

Therefore, if $\omega \in \Omega_n$ is a closed form, we get $\omega = \widetilde{d}(K\omega) + \epsilon(\omega)$. It follows by induction on n that $\omega = \widetilde{d}\omega_1 + P(\partial)dt$ for some $\omega_1 \in \Omega_n$ and a polynomial $P(\partial)$. But it is clear from (4.42) that $P(\partial)dt$ is always closed, and it is exact iff $P(\partial)$ is divisible by ∂. □

Since the extended annihilation algebra $W(1,n)^+$ is a direct sum of $W(1,n)_+$ and a one-dimensional Lie algebra $\mathbb{C}a$, any irreducible $W(1,n)^+$-module is obtained from a $W(1,n)_+$-module M by extending to $W(1,n)^+$, letting $a \mapsto -\alpha$, where $\alpha \in \mathbb{C}$. Translating into the conformal language

(see Proposition 2.3), we see that all W_n-modules are obtained from conformal $W(1,n)_+$-modules by taking for the action of ∂ the action of $-\partial_t+\alpha I, \alpha\in\mathbb{C}$. We denote by $\mathrm{Tens}_\alpha V$ and $\Omega_{k,\alpha}, \alpha\in\mathbb{C}$, the W_n-modules obtained from Tens V and Ω_k by replacing in (4.7) and (4.8), respectively, ∂ by $\partial+\alpha$.

Now, Theorem 4.7 and Corollary 4.9, along with Sec. III and Propositions 2.3, 2.8, 2.6, and 2.9 give us a complete description of finite irreducible W_n-modules.

Theorem 4.11: *The following is a complete list of nontrivial finite irreducible W_n-modules* $(n\geqslant 2, \alpha\in\mathbb{C})$:

(a) $\mathrm{Tens}_\alpha V$, *where V is a finite-dimensional irreducible $gl(1|n)$-module different from* $\Lambda^k(\mathbb{C}^{1|n})^*$, $k=1,2,\ldots$ *and* $\bar{\Omega}^k_c$ (*see* (4.5)), $k=1,2,\ldots$,
(b) $\Omega^*_{k,\alpha}/\mathrm{Ker}\,\tilde{d}^*, k=1,2,\ldots$, *and the same modules with reversed parity*,
(c) W_n*-modules dual to* (*b*), *with* $k>1$.

Remark 4.12: (a) Using Proposition 4.3, we have that the kernel of $\tilde{d}$ and the image of $\tilde{d}$ coincide in Ω_k for $k\geqslant 2$. Now, since Ω_{k+2} is a free $\mathbb{C}[\partial]$-module of finite rank and $\Omega_{k+1}/\mathrm{Im}\,\tilde{d}=\Omega_{k+1}/\mathrm{Ker}\,\tilde{d}\simeq \mathrm{Im}\,\tilde{d}\subset\Omega_{k+2}$, we obtain that $\Omega_{k+1}/\mathrm{Im}\,\tilde{d}$ is a finitely generated free $\mathbb{C}[\partial]$-module. Therefore, we can apply Proposition 2.6, and we have that

$$\Omega^*_{k+1,\alpha}/\mathrm{Ker}\,\tilde{d}^*\simeq(\Omega_{k,\alpha}/\mathrm{Ker}\,\tilde{d})^*. \tag{4.44}$$

for $k\geqslant 1$.

(b) Observe that we cannot apply the previous argument for $k=0$ since, by Proposition 4.3, the image of $\tilde{d}$ has codimension one (over $\mathbb{C}$) in $\mathrm{Ker}\,\tilde{d}$. In fact, (4.44) is not true for $k=0$. For example, this can be easily seen for $W_0=\mathrm{Vir}$ using the differential map which is explicitly written in Remark 2.5.

(c) Observe that $\Omega_{0,\alpha}$ is an irreducible tensor module ($\mathrm{Ker}\,\tilde{d}=0$, cf. Proposition 4.3), that is why this module is included in case (a) of Theorem 4.11.

(d) Since for a finite rank module M over a Lie conformal superalgebra we have $M^{**}=M$ (see Proposition 2.7), the W_n-modules in case (c) of Theorem 4.11 are isomorphic to $\Omega_{k,\alpha}/ker\tilde{d}$, $k=2,3,\ldots$.

(e) Observe that $(\mathrm{Tens}\,V)^*$ is not isomorphic to Tens V^*. For example, consider the case of W_1. We have, using the notation below, that $M(a,b)=\mathrm{Tens}V_{a,b}$. It is easy to see that for the case $a+b\neq 0$, $(\mathrm{Tens}V_{a,b})^*=\mathrm{Tens}V_{-a,-b}$, but $(V_{a,b})^*=V_{1-a,-b-1}$.

Now we will present the case $n=1$ in detail and we shall see that our result agrees with the classification given in Ref. 5 for $K_2\simeq W_1$. Let us fix some notations. We have

$$W_1=\mathbb{C}[\partial]\otimes(\Lambda(1)\oplus W(1))=\mathbb{C}[\partial]\{1,\xi,\partial_1,\xi\partial_1\}.$$

In Ref. 5, the conformal Lie superalgebra K_2 is presented as the freely generated module over $\mathbb{C}[\partial]$ by $\{L,J,G^\pm\}$. An isomorphism between K_2 and W_1 is explicitly given by

$$L\mapsto -1+\frac{1}{2}\,\partial\,\xi\partial_1,\quad J\mapsto\xi\partial_1,\quad G^+\mapsto 2\xi,\quad G^-\mapsto-\partial_1. \tag{4.45}$$

The irreducible modules of W_1 are parametrized by finite-dimensional irreducible representations of $gl(1,1)$ (and the additional twist by alpha that, for simplicity, shall be omitted in the formulas to follow). The irreducible representations of $gl(1,1)$, denoted by $V_{a,b}$, are parametrized by a and b, the corresponding eigenvalues of e_{11} and e_{22} on the highest weight vector.

If both parameters are equal to zero, the representation is trivial one-dimensional. Otherwise, either $a+b=0$, the dimension of the $gl(1,1)$-representation is 1, and the corresponding representation of W_1 is one of the tensor modules of rank 2. Or else $a+b$ is nonzero, the dimension of the $gl(1,1)$-representation is 2, and the corresponding tensor module has rank 4.

Explicitly, consider the set of $\mathbb{C}[\partial]$-generators of $W_1\{1,\xi,\partial_1,\xi\partial_1\}$. Let a and b such that $a+b\neq 0$. Let $V_{a,b}=\mathbb{C}-\text{span}\{v_0,v_1\}$, where v_0 is a highest weight vector. Let $M(a,b)=M(V_{a,b})=\mathbb{C}[\partial]\{v_0,v_1,w_1=\partial_1 v_0,w_0=\partial_1 v_1\}$ be the tensor W_1-module and denote by $L(a,b)$ the irreducible quotient. The action of W_1 in $M(a,b)$ is given explicitly by the following formulas:

$$\begin{gathered}
1_\lambda v_0=(a\lambda-\partial)v_0,\quad 1_\lambda v_1=((a-1)\lambda-\partial)v_1,\\
1_\lambda w_1=(a\lambda-\partial)w_1,\quad 1_\lambda w_0=((a-1)\lambda-\partial)w_0,\\
\xi_\lambda v_0=v_1,\quad \xi_\lambda v_1=0,\\
\xi_\lambda w_1=(a\lambda-\partial)v_0-w_0,\quad \xi_\lambda w_0=((a-1)\lambda-\partial)v_1,\\
\partial_{1\lambda}v_0=w_1,\quad \partial_{1\lambda}v_1=(a+b)\lambda v_0+w_0,\\
\partial_{1\lambda}w_1=0,\quad \partial_{1\lambda}w_0=-(a+b)\lambda w_1\\
\xi\partial_{1\lambda}v_0=bv_0,\quad \xi\partial_{1\lambda}v_1=(b+1)v_1,\\
\xi\partial_{1\lambda}w_1=(b-1)w_1,\quad \xi\partial_{1\lambda}w_0=-(a+b)\lambda v_0+bw_0.
\end{gathered}\tag{4.46}$$

If $a+b\neq 0$ and $a\neq 0$, then $M(a,b)$ is irreducible of rank 4, and the explicit action is given by (4.45). The proof of this statement is in the following way (the proof of the other statements below are much simpler): Take $v=p(\partial)v_0+q(\partial)w_0+r(\partial)v_1+s(\partial)w_1$ in a submodule of $M(a,b)$. Denote by w the coefficient of the highest power in λ of $\xi_\lambda v$ and by y the coefficient of the highest power in λ of $\xi_\lambda w$.

If $a\neq 1$ then $y=v_1$ (up to a constant factor), therefore v_1 lies in the submodule. If $a=1$, then by taking the coefficient of the highest power in λ of $\xi\partial_{1\lambda}y$ and using that in this case $b\neq -1$, we also obtain that v_1 lies in the submodule.

Therefore, in any case we have that v_1 lies in any submodule, and by the formulas for the actions on v_1 it is immediate that the other generators also belong to any submodule, proving that $M(a,b)$ is irreducible in this case.

If $a+b\neq 0$ but $a=0$, it is easy to show as above that $N=\mathbb{C}[\partial]w_1\oplus\mathbb{C}[\partial](\partial v_0+w_0)$ is a submodule of $M(0,b)$. The irreducible quotient of $M(0,b)$ by N is $L(0,b)=\mathbb{C}[\partial]v_0\oplus\mathbb{C}[\partial]v_1$, of rank 2, and the action here is explicitly, as follows:

$$\begin{gathered}
1_\lambda v_0=(-\partial)v_0,\quad 1_\lambda v_1=(-\lambda-\partial)v_1,\\
\xi_\lambda v_0=v_1,\quad \xi_\lambda v_1=0,\\
\partial_{1\lambda}v_0=0,\quad \partial_{1\lambda}v_1=(b\lambda-\partial)v_0,\\
\xi\partial_{1\lambda}v_0=bv_0,\quad \xi\partial_{1\lambda}v_1=(b+1)v_1.
\end{gathered}\tag{4.47}$$

If $a+b=0$, but $a\neq 0$, it is easy to show as above that $M(a,-a)=C[\partial]\{v_0,w_1\}$ is irreducible of rank 2 and the action of W_1 here is given by

$$\begin{gathered}
1_\lambda v_0=(a\lambda-\partial)v_0,\quad 1_\lambda w_1=(a\lambda-\partial)w_1,\\
\xi_\lambda v_0=0,\quad \xi_\lambda w_1=(a\lambda-\partial)v_0,\\
\partial_{1\lambda}v_0=w_1,\quad \partial_{1\lambda}w_1=0,\\
\xi\partial_{1\lambda}v_0=-av_0,\quad \xi\partial_{1\lambda}w_1=(-a-1)w_1.
\end{gathered}\tag{4.48}$$

Thus we obtain

Corollary 4.13: *The W_1-module $L(a,b)$ as a $\mathbb{C}[\partial]$-module has rank*: 4 *if* $a+b\neq 0$ *and* $a\neq 0$, 2 *if* $a+b\neq 0$ *and* $a=0$, 2 *if* $a+b=0$ *and* $a\neq 0$, 0 *if* $a=b=0$. *These are all nontrivial finite irreducible W_1-modules*.

Remark 4.14: In Ref. 5, the irreducible representations of K_2 are classified in terms of parameters Λ and Δ. Using the isomorphism between K_2 and W_1 in (4.45), these parameters are related to ours as follows:

$$a=-\Delta-\frac{\Lambda}{2},\quad b=\Lambda.$$

Then it can be easily checked that the above corollary corresponds to Theorem 4.1 in Ref. 5, and explicit formulas for the λ-action given at the end of Sec. IV in Ref. 5, corresponds to ours in each case.

V. LIE CONFORMAL SUPERALGEBRA S_n AND ITS FINITE IRREDUCIBLE MODULES

Recall that the *divergence* of a differential operator $D=\Sigma_{i=0}^{n}a_i\partial_i\in W(1,n)$, with $a_i\in\Lambda(1,n)$ and $\partial_0=\partial_t$ is defined by the formula

$$\operatorname{div} D=\partial_0 a_0+\sum_{i=1}^{n}(-1)^{p(a_i)}\partial_i a_i.$$

The basic property of the divergence is ($D_1,D_2\in W(1,n)$)

$$\operatorname{div}[D_1,D_2]=D_1(\operatorname{div} D_2)-(-1)^{p(D_1)p(D_2)}D_2(\operatorname{div} D_1).$$

It follows that

$$S(1,n)=\{D\in W(1,n):\operatorname{div} D=0\}$$

is a subalgebra of the Lie superalgebra $W(1,n)$. Similarly,

$$S(1,n)_+=\{D\in W(1,n)_+:\operatorname{div} D=0\}$$

is a subalgebra of $W(1,n)_+$. We have

$$S(1,n)\ (\text{respectively, } S(1,n)_+)=S(1,n)'\ (\text{respectively, } S(1,n)'_+)\oplus\mathbb{C}\xi_1\cdots\xi_n\partial_0,\qquad(5.1)$$

where $S(1,n)'$ (respectively, $S(1,n)'_+$) denotes the derived subalgebra. It is easy to see that $S(1,n)'$ is a formal distribution Lie superalgebra, see Ref. 7, Example 3.5.

In order to describe the associated Lie conformal superalgebra, we need to translate the notion of divergence to the "conformal" language as follows. It is a $\mathbb{C}[\partial]$-module map $\operatorname{div}: W_n\to\operatorname{Cur}\Lambda(n)$, given by

$$\operatorname{div} a=\sum_{i=1}^{n}(-1)^{p(f_i)}\partial_i f_i,\quad \operatorname{div} f=-\partial\otimes f,$$

where $a=\Sigma_{i=1}^{n}f_i\partial_i\in W(n)$ and $f\in\Lambda(n)$. The following identity holds in $\mathbb{C}[\partial]\otimes\Lambda(n)$, where $D_1,D_2\in W_n$:

$$\operatorname{div}[D_{1\lambda}D_2]=(D_1)_\lambda(\operatorname{div} D_2)-(-1)^{p(D_1)p(D_2)}(D_2)_{-\lambda-\partial}(\operatorname{div} D_1).\qquad(5.2)$$

Therefore,

$$S_n=\{D\in W_n:\operatorname{div} D=0\}$$

is a subalgebra of the Lie conformal superalgebra W_n. It is known that S_n is simple for $n\geqslant 2$, and finite of rank $n2^n$. Furthermore, it is the Lie conformal superalgebra associated to the formal

distribution Lie superalgebra $S(1,n)'$. The annihilation algebra and the extended annihilation algebra is given by

$$\mathcal{A}(S_n) = S(1,n)'_+ \quad \text{and} \quad \mathcal{A}(S_n)^e = \mathbb{C}ad(\partial_0) \ltimes S(1,n)'_+.$$

Now, we have to study representations of $S(1,n)_+$ and of its derived algebra $S(1,n)'_+$ which has codimension 1. Observe that $S(1,n)_+$ inherits the $\mathbb{Z}$-gradation in $W(1,n)_+$, and denoting by $L=S(1,n)_+$ (for the rest of this section), we have that $L_{-1}=\langle \partial_0, \ldots, \partial_n \rangle$ as in $W(1,n)_+$ but the other graded components are strictly smaller than these of $W(1,n)_+$. Observe that $L_0=sl(1|n)$.

In order to consider weights of vectors in $S(1,n)_+$-modules, we take the basis

$$t\partial_0 + \xi_1\partial_1, \ldots, t\partial_0 + \xi_n\partial_n$$

for the Cartan subalgebra. And the weights are written as $\bar{\lambda}=(\lambda_1, \ldots, \lambda_n)$ for the corresponding eigenvalues.

Propositions 4.1 and 4.3, and Corollary 4.2 hold for $L=S(1,n)_+$ with the following minor modification: all highest weights are the same as in the W case, except for the first coordinate that should be removed.

Similarly, if V is an $sl(1|n)$-module, then formulas (4.7) and (4.8) define an S_n-module structure in Tens(V). Indeed, elements $(-1)^{p(f)}\partial(f\partial_i)+\partial_i f$, with $f \in \Lambda(n)$ generate S_n as a $\mathbb{C}[\partial]$-module, and it is easy to see that for the action of these elements defined by (4.7) and (4.8), one needs only $E_{ij}(v)$ for $i \neq j$ and $(E_{00}+E_{ii})(v)$ for $i>0$.

As in the W-case, the classification is reduced to the study of singular vectors in Tens(V), where V is an $sl(1|n)$-module. Observe that the reduction Lemma 4.4 hold in this case, and the proof is basically the same. Therefore, analogous computations give as the following

Proposition 5.1: *Let $n \geqslant 2$ and V an irreducible finite-dimensional $sl(1|n)$-module. If m is a nontrivial singular vector in the $S(1,n)_+$-module* Tens V *with weight $\bar{\lambda}_m$, then we have one of the following*:

(*a*) $m=\xi^n \otimes v_n$, $\bar{\lambda}_m=(0, \ldots, 0, -k)$ *with* $k \geqslant 0$, v_n *is a highest weight vector in* V *with weight* $(0, \ldots, 0, -k-1)$, *and* m *is uniquely defined by* v_n.

(*b*) $m=\sum_{l=1}^n \xi^l \otimes v_l$, $\bar{\lambda}_m=(k, 1, \ldots, 1)$ *with* $k \geqslant 2$, v_1 *is a highest weight vector in* V *with weight* $(k-1, 1, \ldots, 1)$, *and* m *is uniquely defined by* v_1.

(*c*) $m=\partial(\xi_* \otimes w)+\sum_{l=1}^n \xi^l \otimes v_l$, $\bar{\lambda}_m=(0, \ldots, 0)$, w *is a highest weight vector in* V *with weight* $(1, \ldots, 1)$, *and* m *is uniquely defined by* w.

(*d*) $m=\partial(\xi^n \otimes w)+\sum_{l=1}^{n-1} \xi_{[l,n]-\{l,n\}} \otimes v_l + \xi^n \otimes v_n$, $\bar{\lambda}_m=(0, \ldots, 0, -1)$, w *is a highest weight vector in* V *with weight* $(1, \ldots, 1)$, *and* m *is uniquely defined by* w.

Using the above proposition, we have

Theorem 5.2: *Let $L=S(1,n)_+$ $(n \geqslant 2)$ and F be an irreducible L_0-module with highest weight $\bar{\lambda}_*$. Then the L-modules* $\mathrm{Ind}_{L_{\geqslant 0}}^L F$ *are irreducible finite continuous modules except for the following cases*:

(*a*) $\bar{\lambda}_*=(0, \ldots, 0, -p), p \geqslant 0$, *where* $\mathrm{Ind}_{L_{\geqslant 0}}^L F=\Theta_+^p$ *and the image* $d^{\#}\Theta_+^{p+1}$ *is the only nontrivial proper submodule*.

(*b*) $\bar{\lambda}_*=(q, 1, \ldots, 1), q \geqslant 1$, *where* $\mathrm{Ind}_{L_{\geqslant 0}}^L F=\Omega_-^q$. *For* $q \geqslant 2$ *the image* $d\Omega_-^{q-1}$ *is the only nontrivial proper submodule. For* $q=1$, *the proper submodules are* $\mathrm{Im}(d)$, $\mathrm{Ker}(d)$ *and* $\mathrm{Im}(\alpha)$, *where* α *is the composition*

$$\alpha: \Theta_+^1 \xrightarrow{d^{\#}} \Theta_+^0 \simeq \Omega_-^0 \xrightarrow{d} \Omega_-^1,$$

and $\mathrm{Ker}(d)$ *is the maximal proper submodule*.

Proof: Similar to the case of $W(1,n)_+$, the modules $\mathrm{Ind}_{L_{\geqslant 0}}^L F$ are irreducible except when they have a singular vector and the highest weights of such F, when it could happen, are listed in (a), (b), (c), and (d) of the above Proposition 5.1. The weight $(1, \ldots, 1)$ is special here because it is

relevant to (b), (c), and (d). There are three types of singular vectors possible in this case. The corresponding module $\mathrm{Ind}(F)=\Omega^1_-$ has three different submodules and all three vectors are present. The same argument as for $W(1,n)_+$-modules allows us easily to conclude that the listed submodules are the only ones and the factors are irreducible. □

Corollary 5.3: *The theorem gives us a description of finite continuous irreducible* $S(1,n)_+$*-modules when* $n\geqslant 2$. *Such a module is either* $\mathrm{Ind}^L_{L_{\geqslant 0}}F$ *for an irreducible finite-dimensional* L_0*-module* F *where the highest weight of* F *does not belong to the types listed in* (*a*), (*b*) *of the theorem or the factor of an induced module from* (*a*), (*b*) *by the submodule* $\mathrm{Ker}(d)$.

Corollary 5.4: *The Lie superalgebras* $S(1,n)_+$ *and* $S(1,n)'_+$ *have the same finite continuous irreducible modules*, *and they are described by the previous corollary*.

Proof: In order to see that Theorem 5.2 also holds for $S(1,n)'_+$, it is basically enough to see that Proposition 5.1 holds in this case. But, if we check the proof in the classification of singular vectors, we see that the element $\xi_1\cdots\xi_n\partial_0$ (cf. (5.1)) appears only in the condition (s3) in (4.10) in the special case $g=\xi_1\cdots\xi_n$ and $j=0$. If we track the details of the proof, we see that this special constraint only produces Eq. (4.27) for $n=2$, but in any case, this equation is not used in the rest of the proof. Therefore, the singular vectors are the same for both Lie superalgebras $S(1,n)'_+$ and $S(1,n)_+$, finishing the proof. □

Now, as in the W_n case, Theorem 5.2 and Corollary 5.4, along with Sec. III and Propositions 2.3, 2.8, and 2.9 give us a complete description of finite irreducible S_n-modules ($n\geqslant 2$): it is given by Theorem 4.11 in which W_n is replaced by S_n and $gl(1|n)$ is replaced by $sl(1|n)$.

Remark 5.5: Under the standard isomorphism between S_2 and small $N=4$ conformal superalgebra it is easy to see that our result agrees with the classification given in Ref. 5. Indeed, in Ref. 5 (Theorem 6.1) the classification of irreducible modules was given in terms of parameters Λ and Δ, and these parameters are related to ours as follows:

$$\lambda_1=-\Delta+\frac{\Lambda}{2}, \tag{5.3}$$

$$\lambda_2=-\Delta-\frac{\Lambda}{2}. \tag{5.4}$$

Therefore, the case $2\Delta-\Lambda=0$ ($\Lambda\in\mathbb{Z}_+$) corresponds to the family $\Omega^*_{\Lambda,\alpha}/\mathrm{Ker}\,\tilde{d}^*$ of rank 4Λ, and the case $2\Delta+\Lambda+2=0$ ($\Lambda\in\mathbb{Z}_+$) corresponds to $\Omega_{\Lambda+1,\alpha}/\mathrm{Ker}\,\tilde{d}$ of rank $4\Lambda+8$. Therefore, we have one module of rank 4 that corresponds to $\Omega^*_1/\mathrm{Ker}\,\tilde{d}^*$, and by Remark 4.12, the dual of this module is Ω_0 (Ker is trivial in this case) and (using Proposition 4.3) Ω_0 is the tensor module $\mathrm{Tens}(V)$ where V is the trivial representation, therefore it is reducible with a maximal submodule of codimension 1 (over $\mathbb{C}$).

VI. LIE CONFORMAL SUPERALGEBRAS $S_{n,b}$ AND $\tilde{S}_n$, AND THEIR FINITE IRREDUCIBLE MODULES

Case $S_{n,b}$:

For any $b\in\mathbb{C}$, $b\neq 0$, we take

$$S(1,n,b)=\{D\in W(1,n)\,|\,\mathrm{div}(e^{bx}D)=0\}.$$

This is a formal distribution subalgebra of $W(1,n)$. The associated Lie conformal superalgebra is constructed explicitly as follows. Let $D=\sum_{i=1}^n P_i(\partial,\xi)\partial_i+f(\partial,\xi)$ be an element of W_n. We define the deformed divergence as

$$\mathrm{div}_b D=\mathrm{div}\,D+bf.$$

It still satisfies Eq. (5.2), therefore

$$S_{n,b} = \{D \in W_n | \mathrm{div}_b D = 0\}$$

is a subalgebra of W_n, which is simple for $n \geqslant 2$ and has rank $n2^n$. Since $S_{n,0} = S_n$ has been discussed in the previous section, we can (and will) assume that $b \neq 0$.

If $b \neq 0$, the extended annihilation algebra is given by

$$(\mathrm{Alg}(S_{n,b}))^+ = \mathbb{C}ad\left(\partial_0 - b\sum_{i=1}^{n} \xi_i \partial_i\right) \ltimes S(1,n)_+ \simeq CS(1,n)'_+$$

where $CS(1,n)'_+$ is obtained from $S(1,n)'_+$ by enlarging $sl(1,n)$ to $gl(1,n)$ in the 0-th-component.

Therefore, the construction of all finite irreducible modules over $S_{n,b}$ is the same as that for W_n, but without twisting by α. Hence, using Theorem 4.11, we have

Theorem 6.1: *The following is a complete list of finite irreducible $S_{n,b}$-modules* ($n \geqslant 2, b \in \mathbb{C}, b \neq 0$):

(a) $\mathrm{Tens}\, V$, *where V is a finite-dimensional irreducible $gl(1|n)$-module different from* $\Lambda^k(\mathbb{C}^{1|n})^*$, $k=1,2,\ldots$ *and* $\Lambda^k(\mathbb{C}^{1|n})$, $k=0,1,2,\ldots$,

(b) $\Omega_k^*/\mathrm{Ker}\, \tilde{d}^*$, $k=1,2,\ldots$, *and the same modules with reversed parity*,

(c) *$S_{n,b}$-modules dual to* (*b*), *with* $k>1$.

Case $\widetilde{S}_n$:

Let $n \in \mathbb{Z}_+$ be an even integer. We take

$$\widetilde{S}(1,n) = \{D \in W(1,n) | \mathrm{div}((1+\xi_1 \ldots \xi_n)D) = 0\}.$$

This is a formal distribution subalgebra of $W(1,n)$. The associated Lie conformal superalgebra $\widetilde{S}_n$ is constructed explicitly as follows:

$$\widetilde{S}_n = \{D \in W_n | \mathrm{div}((1+\xi_1 \ldots \xi_n)D) = 0\} = (1-\xi_1 \ldots \xi_n)S_n.$$

The Lie conformal superalgebra $\widetilde{S}_n$ is simple for $n \geqslant 2$ and has rank $n2^n$.

The extended annihilation algebra is given by

$$(\mathrm{Alg}(\widetilde{S}_n))^+ = \mathbb{C}ad(\partial_0 - \xi_1 \ldots \xi_n \partial_0) \ltimes S(1,n)'_+ \simeq S(1,n)_+.$$

Therefore, the construction of all finite irreducible modules over $\widetilde{S}_n$ is the same as that for S_n, but without the twist by α.

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Second order superintegrable systems in conformally flat spaces. IV. The classical 3D Stäckel transform and 3D classification theory

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This article is one of a series that lays the groundwork for a structure and classification theory of second order superintegrable systems, both classical and quantum, in conformally flat spaces. In the first part of the article we study the Stäckel transform (or coupling constant metamorphosis) as an invertible mapping between classical superintegrable systems on different three-dimensional spaces. We show first that all superintegrable systems with nondegenerate potentials are multiseparable and then that each such system on any conformally flat space is Stäckel equivalent to a system on a constant curvature space. In the second part of the article we classify all the superintegrable systems that admit separation in generic coordinates. We find that there are eight families of these systems. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2191789]

I. INTRODUCTION

This is a continuation of the series[1–3] whose purpose is to lay the groundwork for a structure and classification theory of second order superintegrable systems, both classical and quantum, in complex conformally flat spaces. Real spaces are considered as restrictions of these to the various real forms. In Refs. 1 and 3 we have given examples in two and three dimensions, described the background as well as the interest and importance of these systems in mathematical physics and given many applications relevant to such systems on conformally flat spaces. Observed features of the systems are multiseparability, closure of the quadratic algebra of second order symmetries at order 6, use of representation theory of the quadratic algebra to derive spectral properties of the quantum Schrödinger operator, and a close relationship with exactly solvable and quasiexactly solvable problems. Our approach is, rather than focus on particular spaces and systems, to use a general theoretical method based on integrability conditions to derive structure common to all systems. In distinction to the two-dimensional (2D) case, there are relatively few papers considering superintegrability on spaces of dimension $\geqslant 3$. A few exceptions are Refs. 4–13. Except for our own work, no one appears to have studied the detailed structure and classification theory for these higher dimensional systems.

In the first part of this article we study the Stäckel transform, or coupling constant metamorphosis,[14,15] for three-dimensional (3D) classical superintegrable systems. Recall that for a classical 3D system on a conformally flat space we can always choose local coordinates x, y, z, not unique, such that the Hamiltonian takes the form $H=(p_1^2+p_2^2+p_3^2)/\lambda(x,y,z)+V(x,y,z)$. This

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system is *second order superintegrable with nondegenerate* potential $V=V(x,y,z,\alpha,\beta,\gamma,\delta)$ if it admits five functionally independent quadratic constants of the motion (i.e., generalized symmetries) $S_k=\Sigma_{ij}a^{ij}_{(k)}p_ip_j+W_{(k)}(x,y,\alpha,\beta,\gamma)$. As described in Ref. 3, the potential V is *nondegenerate* if it satisfies a system of coupled partial differential equations of the form

$$V_{22}=V_{11}+A^{22}V_1+B^{22}V_2+C^{22}V_3,\quad V_{33}=V_{11}+A^{33}V_1+B^{33}V_2+C^{33}V_3,$$

$$V_{12}=A^{12}V_1+B^{12}V_2+C^{12}V_3,\quad V_{13}=A^{13}V_1+B^{13}V_2+C^{13}V_3, \tag{1}$$

$$V_{23}=A^{23}V_1+B^{23}V_2+C^{23}V_3,$$

whose integrability conditions are satisfied identically. The analytic functions A^{ij},B^{ij},C^{ij} are determined uniquely from the Bertrand-Darboux equations for the five constants of the motion and are analytic except for a finite number of poles. At any regular point $\mathbf{x}_0=(x_0,y_0,z_0)$, i.e., a point where the A^{ij}, B^{ij}, and C^{ij} are defined and analytic and the constants of the motion are functionally independent, we can prescribe the values of $V(\mathbf{x}_0),V_1(\mathbf{x}_0),V_2(\mathbf{x}_0),V_3(\mathbf{x}_0),V_{11}(\mathbf{x}_0)$ arbitrarily and obtain a unique solution of (1). Here, $V_1=\partial V/\partial x$, $V_2=\partial V/\partial y$, etc. The four parameters for a nondegenerate potential (in addition to the usual additive constant) are the maximum number of parameters that can appear in a superintegrable system. If the number of parameters is fewer than four, we say that the superintegrable potential is *degenerate*.

The 3D Stäckel transform is a conformal transformation of a superintegrable system on one conformally flat 3D space to a superintegrable system on another such space. We discuss some of the properties of this transform for a classical system and then prove two fundamental results: (1) We show that every superintegrable system with nondegenerate potential is multiseparable. This result uses the structure theory for such systems that we worked out in Ref. 3. (2) We prove that all nondegenerate 3D superintegrable systems are Stäckel transforms of constant curvature systems. Thus, to obtain all nondegenerate conformally flat superintegrable systems, it is sufficient to classify those of constant curvature. The proofs of these fundamental results rest on results obtained in Ref. 3, and the careful reader of this article will need to keep Ref. 3 at hand.

In the second part of the article we use the results of the first part and our explicit knowledge of all separable coordinate systems on 3D constant curvature spaces to make a major advance in the classification of all separable systems with nondegenerate potential on a conformally flat space. Among the separable systems for 3D complex Euclidean space there are seven that are "generic." We give a precise definition later, but, essentially this means that the coordinates belong to a multiparameter family. The ultimate generic coordinates are the Jacobi elliptic coordinates from which all others can be obtained by limiting processes.[16,17] We show that each of the generic separable systems uniquely determines a nondegenerate superintegrable system that contains it. We obtain a similar result for the five generic separable systems on the complex three-sphere. However, four of these turn out to be Stäckel transforms of Euclidean generic systems. Thus we find eight Stäckel inequivalent generic systems on constant curvature spaces and all generic systems on 3D conformally flat spaces must be Stäckel equivalent to one of these. (In addition there are two nondegenerate superintegrable systems in Euclidean space that are only weakly functionally independent and these give rise to similar systems on a variety of conformally flat spaces.) Thus we exhibit ten families of superintegrable systems in conformally flat spaces. This does not solve the classification problem completely, but it is a major advance. Any remaining nondegenerate superintegrable systems must be multiseparable but separate *only* in degenerate separable coordinates. This remaining problem is still complicated, but much less so than the original problem. This is a technically detailed proof, but the results are quite explicit and easy to grasp. We derive and give a simple characterization of eight families of separable systems whose Stäckel transforms yield nondegenerate superintegrable systems on a variety of conformally flat spaces.

The next article in this series will extend all of our classical 2D and 3D results to the quantum case. This is very easy in the 2D case but requires some machinery in 3D.

Second order conformal Killing tensors: There is a close relationship between the second-order Killing tensors of a conformally flat space in 3D and the second order conformal Killing tensors of flat space. A second order conformal Killing tensor for a space M_3 with metric $ds^2=\lambda(x_1,x_2,x_3)(dx_1^2+dx_2^2+dx_3^2)$ and free Hamiltonian $\mathcal{H}=(p_1^2+p_2^2+p_3^2)/\lambda$ is a quadratic form $\mathcal{S}=\Sigma a^{ij}(x_1,x_2,x_3)p_ip_j$ such that $\{\mathcal{H},\mathcal{S}\}=f(x_1,x_2,x_3)\mathcal{H}$, for some function f. Since f is arbitrary, it is easy to see that $\mathcal{S}$ is a conformal Killing tensor for M_3 if and only if it is a conformal Killing tensor for flat space $dx_1^2+dx_2^2+dx_3^2$. The conformal Killing tensors for flat space are very well known, e.g., Ref. 18. The space of conformal Killing tensors is infinite dimensional.[19] It is spanned by products of the conformal Killing vectors

$$p_1,\quad p_2,\quad p_3,\quad x_3p_2-x_2p_3,\quad x_1p_3-x_3p_1,\quad x_2p_1-x_1p_2,\quad x_1p_1+x_2p_2+x_3p_3,$$

$$(x_1^2-x_2^2-x_3^2)p_1+2x_1x_3p_3+2x_1x_2p_2,\quad (x_2^2-x_1^2-x_3^2)p_2+2x_2x_3p_3+2x_2x_1p_1,$$

$$(x_3^2-x_1^2-x_2^2)p_3+2x_3x_1p_1+2x_3x_2p_2,$$

and terms $g(x_1,x_2,x_3)(p_1^2+p_2^2+p_3^2)$, where g is an arbitrary function. Since every Killing tensor is also a conformal Killing tensor, we see that every second-order Killing tensor for M_3 can be expressed as a linear combination of these second-order generating elements though, of course, the space of Killing tensors is only finite dimensional. This shows in particular that every a^{ij} and every $a^{ii}-a^{jj}$ with $i\neq j$ is a polynomial of order at most four in x_1, x_2, x_3, no matter what is the choice of λ.

A straightforward, though tedious, computation from the above-mentioned results yields the expressions

$$\begin{aligned}
a_{11}^{12}&=-a_{22}^{12}=\alpha_3(x_1^2-x_2^2)+(\delta_1+\gamma_2)x_1x_2-\alpha_1x_1x_3-\alpha_2x_2x_3+\phi_3x_1+\xi_3x_2+\mu_3x_3+\nu_3,\\
a_{11}^{13}&=-a_{33}^{13}=\alpha_2(x_1^2-x_3^2)-\alpha_1x_1x_2+\gamma_2x_1x_3-\alpha_3x_2x_3+\phi_2x_1+\xi_2x_2+\mu_2x_3+\nu_2,\\
\alpha_{33}^{23}&=-a_{22}^{23}=\alpha_1(x_2^2-x_3^2)-\alpha_2x_1x_2+\alpha_3x_1x_3+\delta_1x_2x_3+\phi_1x_1+\xi_1x_2+\mu_1x_3+\nu_1,
\end{aligned}\tag{2}$$

where α_j, δ_j, γ_j, ϕ_j, ξ_j, μ_j, and ν_j are constants. Further $(a^{ii}-a^{jj})_i=2a_j^{ij}$ for $i\neq j$, and $a_3^{12}+a_2^{13}+a_1^{23}=0$.

It is useful to pass to new variables a^{11}, a^{24}, a^{34}, a^{12}, a^{13}, a^{23} for the Killing tensor, where $a^{24}=a^{22}-a^{11}$, $a^{34}=a^{33}-a^{11}$. Then we see that a^{24}, a^{34}, a^{12}, a^{13}, a^{23} are polynomials of order $\leqslant 4$. The remaining conditions can be expressed in the form

$$\begin{aligned}
(a^{11}\lambda)_1&=-\lambda_2a^{12}-\lambda_3a^{13},\quad (a^{11}\lambda)_2=-\lambda_1a^{12}-(a^{24}\lambda)_2-\lambda_3a^{23},\\
(a^{11}\lambda)_3&=-\lambda_1a^{13}-\lambda_2a^{23}-(a^{34}\lambda)_3.
\end{aligned}\tag{3}$$

Theorem 1: *Necessary and sufficient conditions that the quadratic form* $\mathcal{S}=\Sigma_{ij}a^{ij}p_ip_j+W$ *be a second order constant of the motion for the space with metric* $ds^2=\lambda(dx_1^2+dx_2^2+dx_3^2)$ *and potential V are*

(1) $\Sigma_{ij}a^{ij}p_ip_j$ *is a conformal Killing tensor on the flat space with metric* $dx_1^2+dx_2^2+dx_3^2$.
(2) *The integrability conditions for (3) hold:*

$$\begin{aligned}
(\lambda_2a^{12}+\lambda_3a^{13})_2&=(\lambda_1a^{12}+(a^{24}\lambda)_2+\lambda_3a^{23})_1,\\
(\lambda_2a^{12}+\lambda_3a^{13})_3&=(\lambda_1a^{13}+\lambda_2a^{23}+(a^{34}\lambda)_3)_1,\\
(\lambda_1a^{12}+(a^{24}\lambda)_2+\lambda_3a^{23})_3&=(\lambda_1a^{13}+\lambda_2a^{23}+(a^{34}\lambda)_3)_2.
\end{aligned}\tag{4}$$

(3) *The Bertrand-Darboux conditions for the potential hold:*

$$\sum_{s=1}^{3} [V_{sj}\lambda a^{s\ell} - V_{s\ell}\lambda a^{sj} + V_s((\lambda a^{s\ell})_j - (\lambda a^{sj})_\ell)] = 0. \tag{5}$$

These are just the conditions $\partial_{x_\ell} W_j = \partial_{x_j} W_\ell$ *for* $j \neq \ell$.

II. THE STÄCKEL TRANSFORM FOR 3D SYSTEMS

The Stäckel transform[14] or coupling constant metamorphosis[15] plays a fundamental role in relating superintegrable systems on different manifolds. Suppose we have a superintegrable system

$$H = \frac{p_1^2 + p_2^2 + p_3^2}{\lambda(x,y,z)} + V(x,y,z) \tag{6}$$

in local orthogonal coordinates, with nondegenerate potential $V(x,y,z)$:

$$V_{33} = V_{11} + A^{33}V_1 + B^{33}V_2 + C^{33}V_3, \quad V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2 + C^{22}V_3,$$

$$V_{23} = A^{23}V_1 + B^{23}V_2 + C^{23}V_3, \quad V_{13} = A^{13}V_1 + B^{13}V_2 + C^{13}V_3, \tag{7}$$

$$V_{12} = A^{12}V_1 + B^{12}V_2 + C^{12}V_3$$

and suppose $U(x,y,z)$ is a particular solution of Eqs. (7), nonzero in an open set. Then the transformed system $\tilde{H} = (p_1^2 + p_2^2 + p_3^2)/\tilde{\lambda} + \tilde{V}$ with nondegenerate potential $\tilde{V}(x,y,z)$:

$$\tilde{V}_{33} = \tilde{V}_{11} + \tilde{A}^{33}\tilde{V}_1 + \tilde{B}^{33}\tilde{V}_2 + \tilde{C}^{33}\tilde{V}_3, \quad \tilde{V}_{22} = \tilde{V}_{11} + \tilde{A}^{22}\tilde{V}_1 + \tilde{B}^{22}\tilde{V}_2 + \tilde{C}^{22}\tilde{V}_3,$$

$$\tilde{V}_{23} = \tilde{A}^{23}\tilde{V}_1 + \tilde{B}^{23}\tilde{V}_2 + \tilde{C}^{23}\tilde{V}_3, \quad \tilde{V}_{13} = \tilde{A}^{13}\tilde{V}_1 + \tilde{B}^{13}\tilde{V}_2 + \tilde{C}^{13}\tilde{V}_3, \tag{8}$$

$$\tilde{V}_{12} = \tilde{A}^{12}\tilde{V}_1 + \tilde{B}^{12}\tilde{V}_2 + \tilde{C}^{12}\tilde{V}_3,$$

is also superintegrable, where

$$\tilde{\lambda} = \lambda U, \quad \tilde{V} = \frac{V}{U}, \quad \tilde{A}^{33} = A^{33} + 2\frac{U_1}{U}, \quad \tilde{C}^{33} = C^{33} - 2\frac{U_3}{U},$$

$$\tilde{A}^{22} = A^{22} + 2\frac{U_1}{U}, \quad \tilde{B}^{22} = B^{22} - 2\frac{U_2}{U}, \quad \tilde{B}^{23} = B^{23} - \frac{U_3}{U}, \quad \tilde{C}^{23} = C^{23} - \frac{U_2}{U},$$

$$\tilde{A}^{13} = A^{13} - \frac{U_3}{U}, \quad \tilde{C}^{13} = C^{13} - \frac{U_1}{U}, \quad \tilde{A}^{12} = A^{12} - \frac{U_2}{U}, \quad \tilde{B}^{12} = B^{12} - \frac{U_1}{U},$$

and $\tilde{A}^{23} = A^{23}$, $\tilde{B}^{33} = B^{33}$, $\tilde{B}^{13} = B^{13}$, $\tilde{C}^{22} = C^{22}4$, $\tilde{C}^{12} = C^{12}$. Let $S = \Sigma a^{ij}p_ip_j + W = S_0 + W$ be a second order symmetry of H and $S_U = \Sigma a^{ij}p_ip_j + W_U = S_0 + W_U$ be the special case that is in involution with $(p_1^2 + p_2^2 + p_3^2)/\lambda + U$. Then $\tilde{S} = S_0 - (W_U/U)H + (1/U)H$ is the corresponding symmetry of $\tilde{H}$. Since one can always add a constant to a nondegenerate potential, it follows that $1/U$ defines an inverse Stäckel transform of $\tilde{H}$ to H. See Ref. 14 for many examples of this transform.

III. MULTISEPARABILITY AND STÄCKEL EQUIVALENCE

From the general theory of variable separation for Hamilton-Jacobi equations, e.g., Refs. 20 and 21 we know that second order symmetries L_1, L_2 define a separable system for the equation

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{\lambda(x,y,z)} + V(x,y,z) = E$$

if and only if (1) the symmetries H, L_1, L_2 form a linearly independent set as quadratic forms, (2) $\{L_1, L_2\}=0$, and, (3) the three quadratic forms have a common eigenbasis of differential forms. This last requirement means that, expressed in coordinates x, y, and z, at least one of the matrices $\mathcal{A}_{(j)}(\mathbf{x})$ (of the quadratic form associated with L_j) can be diagonalized by conjugacy transforms in a neighborhood of a regular point and that $[\mathcal{A}_{(2)}(\mathbf{x}), \mathcal{A}_{(1)}(\mathbf{x})]=0$. However, for nondegenerate superintegrable potentials in a conformally flat space we see that $\{L_1, L_2\}=0 \leftrightarrow [\mathcal{A}_{(2)}(\mathbf{x}_0), \mathcal{A}_{(1)} \times(\mathbf{x}_0)]=0$, $\mathcal{F}(\mathbf{x}_0)=0$ at a single regular point $\mathbf{x}_0$, see Sec. V of Ref. 3, so that the intrinsic conditions for the existence of a separable coordinate system are simplified.

Let $\mathcal{A}=\Sigma_{i\leqslant j} a^{ij}\mathcal{A}^{ij}$, $\mathcal{B}=\Sigma_{i\leqslant j} b^{ij}\mathcal{A}^{ij}$, be the matrices of two symmetries at the point $\mathbf{x}_0$. Here, $\mathcal{A}^{ij}=\frac{1}{2}(\mathcal{E}^{ij}+\mathcal{E}^{ji})$ where $\mathcal{E}^{ij}$ is the 3×3 matrix with matrix element 1 in row i, column j, and 0 everywhere else. From the table in Sec. V of Ref. 3 we see that the corresponding symmetries are in involution if and only if the matrices $\mathcal{A}, \mathcal{B}$ commute and the additional condition

$$\begin{aligned}
&(a^{12}b^{11} - b^{12}a^{11})(C^{33} - B^{23} - A^{13}) + (a^{22}b^{12} - a^{12}b^{22})(C^{33} - 2B^{23}) \\
&\quad + (a^{13}b^{11} - a^{11}b^{13})(B^{33} + 2A^{12} - B^{22}) + (a^{33}b^{13} - a^{13}b^{33})(2B^{33} + 2A^{12} - B^{22}) \\
&\quad + (a^{23}b^{22} - a^{22}b^{23})(-2B^{12} - A^{33}) + (a^{33}b^{23} - b^{33}a^{23})(-2B^{12} + A^{22} - 2A^{33}) \\
&\quad + 2(a^{11}b^{22} - a^{22}b^{11} + a^{33}b^{11} - a^{11}b^{33} + a^{22}b^{33} - a^{33}b^{22})A^{23} + (a^{23}b^{11} - a^{11}b^{23})(A^{22} - A^{33}) \\
&\quad + (a^{33}b^{12} - a^{12}b^{33})(B^{23} - A^{13}) + (a^{13}b^{22} - a^{22}b^{13})B^{33} = 0
\end{aligned} \tag{9}$$

holds. Note that the metric G does not appear in these conditions.

Theorem 2: *Let V be a superintegrable nondegenerate potential in a 3D conformally flat space. Then V defines a multiseparable system.*

Proof: From (9) we see that the second order symmetries with matrices $\mathcal{A}^{(33)}$ and $\alpha\mathcal{A}^{(11)} + \beta\mathcal{A}^{(12)}$ will be in involution if and only if $2\alpha A^{23} + \beta(B^{23} - A^{13}) = 0$ at the regular point $\mathbf{x}_0$. If $A^{23}(\mathbf{x}_0)=0$ we can set $\alpha=1$, $\beta=0$ and the symmetries $\mathcal{A}^{(33)}$, $\mathcal{A}^{11}$ will define a separable system. If $A^{23}(\mathbf{x}_0)\neq 0$ we can set $\alpha=-(B^{23}-A^{13})/2A^{23}$, $\beta=1$. Then the symmetries with nonzero matrices $\mathcal{A}^{(33)}$ and $\alpha\mathcal{A}^{(11)}+\beta\mathcal{A}^{(12)}$ will be in involution. The second case must occur for some regular point $\mathbf{x}_0$ unless $A^{23}(\mathbf{x})=0$ for all $\mathbf{x}$. In this last eventuality we can perform a suitable Euclidean rotation (with arbitrarily small complex rotation angle) so that A^{23} does not vanish identically in the rotated coordinate system. It is a straightforward exercise to show that this transformation is not possible if and only if

$$B^{33} = C^{22} = 0, \quad A^{13} = B^{23}, \quad A^{12} = C^{23}, \quad A^{22} = A^{33}. \tag{10}$$

In this eventuality, we can set $\alpha=0$, $\beta=1$ and find a solution. Thus we can always find a linear combination of these matrices, corresponding to $\beta=1$ and with three distinct eigenvalues, so they will determine separable coordinates. We could have carried through this same construction for the second order symmetries with matrices $\mathcal{A}^{(22)}$ and $\gamma\mathcal{A}^{(11)}+\delta\mathcal{A}^{(13)}$ and for the second order symmetries with matrices $\mathcal{A}^{(11)}$ and $\mu\mathcal{A}^{(22)}+\xi\mathcal{A}^{(23)}$ and shown that we could always find solutions with $\delta=\xi=1$. Thus the system is multiseparable (in at least three coordinate systems). Q.E.D.

Corollary 1: Let V be a superintegrable nondegenerate potential in a 3D conformally flat space. Then there is a continuous one-parameter (or multiparameter) family of separable systems for V, spanning at least a five-dimensional subspace of symmetries.

Proof: We follow the method of proof of the theorem.

Case I: Suppose $A^{23}(\mathbf{x}_0)\neq 0$. From (9) we can verify that the symmetries with matrices

$$\mathcal{A}=\begin{pmatrix}0 & 0 & 0\\ 0 & f^2 & -f\\ 0 & -f & 1\end{pmatrix},\quad \mathcal{B}=\begin{pmatrix}g & 1/2 & f/2\\ 1/2 & 0 & 0\\ f/2 & 0 & 0\end{pmatrix}, \tag{11}$$

are in involution provided

$$-4f^2B^{23}+2f^2C^{33}+3fB^{33}+4fA^{12}-2fB^{22}+fB^{23}-4f^2gA^{23}-4fgA^{22}$$
$$+4fgA^{33}+4gA^{23}+2B^{23}-2A^{13}-2f^3B^{33}=0.$$

As $A^{23}(\mathbf{x}_0)\neq 0$ this equation can be solved for g as a function of f for f in some open set. The resulting symmetries $\mathcal{A},\mathcal{B}$ are in involution and have eigenvalues $(0,0,f^2+1)$ and $\left(0,\frac{1}{2}[g+\sqrt{f^2+g^2+1}],\frac{1}{2}[g-\sqrt{f^2+g^2+1}]\right)$, respectively. Thus they determine a one-parameter family of separable coordinates. Moreover, as f varies in an open set, the space spanned by the symmetries (including the Hamiltonian) has dimension six.

Case II: If $A^{23}(\mathbf{x}_0)=0$, we can assume that Eq. (10) holds. Then the problem breaks up into a series of special cases. Suppose first that $C^{33}-2A^{13}=\ell\neq 0$. Then we can verify that the symmetries with matrices

$$\mathcal{A}=\begin{pmatrix}0 & 2gk/K & 0\\ 2gk/K & 1 & -g/K\\ 0 & -g/K & g^2/K\end{pmatrix},\quad \mathcal{B}=\begin{pmatrix}f & g/2 & 1/2\\ g/2 & 0 & 0\\ 1/2 & 0 & k\end{pmatrix}, \tag{12}$$

are in involution provided $K=1-4fk\neq 0$ and g satisfies

$$-g(2A^{12}-B^{22})+2k(A^{22}+2B^{12})=\ell.$$

If $2A^{12}-B^{22}\neq 0$ then there is a nonzero solution expression g as a function of k. Since f,k are essentially arbitrary, they determine a five-dimensional space spanned by the symmetries and a two-parameter family of separable coordinates. If $2A^{12}-B^{22}=0$, $A^{22}+2B^{12}\neq 0$ then k is a nonzero constant and f,g are essentially arbitrary, so they again determine a five-dimensional space spanned by the symmetries and a two-parameter family of separable coordinates. If $2A^{12}-B^{22}=0$, $A^{22}+2B^{12}=0$, then the symmetries with matrices

$$\mathcal{A}=\begin{pmatrix}0 & H/K & 0\\ H/K & 1 & 0\\ 0 & 0 & L/K\end{pmatrix},\quad \mathcal{B}=\begin{pmatrix}f & g/2 & 1/2\\ g/2 & 0 & h/2\\ 1/2 & h/2 & k\end{pmatrix}, \tag{13}$$

where $K=1-4fk-h^2-2hgf\neq 0$, and

$$H=-h+2gk+hg^2,\quad G=-g+2fh+gh^2,\quad L=g^2-h^2+2hg(k-f),$$

are in involution provided $f=(g/2h-h/2g)$. (This implies $G=0$ and $L=Hh$.) They determine a six-dimensional space spanned by the symmetries and a three-parameter family of separable coordinates. This covers all cases where $\ell\neq 0$.

Now suppose $\ell=0$, i.e., $C^{33}=2A^{13}$. Then the symmetries with matrices (13) are in involution provided

$$(2A^{12}-B^{22})(h^2-g^2+2hgf-2hkg)+(A^{22}+2B^{12})(-h+2kg+hg^2)=0.$$

If $2A^{12}-B^{22}\neq 0$ then we can solve this equation to express f as a nonzero function of g,h,k. This yields at least a five-dimensional space spanned by the symmetries and a three-parameter family of separable coordinates. Finally, suppose in addition that $2A^{12}-B^{22}=0$. Then we can verify that the symmetries with matrices

$$\mathcal{A}=\begin{pmatrix}0 & 0 & 0\\ 0 & f^2 & -f\\ 0 & -f & 1\end{pmatrix},\quad \mathcal{B}=\begin{pmatrix}g & 1/2 & f/2\\ 1/2 & 0 & 0\\ f/2 & 0 & 0\end{pmatrix}, \tag{14}$$

are in involution with no conditions on f,g. Again, as f,g vary in an open set, the space spanned by the symmetries (including the Hamiltonian) has dimension six. Q.E.D.

In Ref. 17 the following result was obtained.

Theorem 3: *Let u_1,u_2,u_3 be an orthogonal separable coordinate system for a 3D conformally flat space with metric $\mathrm{d}\tilde{s}^2$. Then there is a function f such that $f\mathrm{d}\tilde{s}^2=\mathrm{d}s^2$ where $\mathrm{d}s^2$ is a constant curvature space metric and $\mathrm{d}s^2$ is orthogonally separable in exactly these same coordinates u_1,u_2,u_3. The function f is called a Stäckel multiplier with respect to this coordinate system.*

Thus the possible separable coordinate systems for a conformally flat space are all obtained, modulo a Stäckel multiplier, from separable systems on 3D flat space or on the three sphere.

Theorem 4: *Every superintegrable system with nondegenerate potential on a 3D conformally flat space is Stäckel equivalent to a superintegrable system on either 3D flat space or the three sphere.*

Proof: Suppose we have a superintegrable system with nondegenerate potential on a conformally flat space. Then by Corollary 1 this system separates in a one- or multiparameter family of coordinate systems spanning a five-dimensional subspace of symmetries. By Theorem 3 each of these three systems is conformal to a separable system in flat space or on the three sphere. Thus from Ref. 19, p. 85, the metric for the space in standard Cartesian-like coordinates x, y, z is simultaneously conformal to three systems corresponding to the following possible choices for the metric function $\lambda(x,y,z)$, namely

$$1,\quad 1/(x+iy)^2,\quad 1/r^4\quad \text{(flatspace)};\quad 1/x^2,\quad 1/(1+r^2/4)^2\quad \text{(three sphere)}; \tag{15}$$

in the same coordinates, and each of the conformal factors is a Stäckel multiplier with respect to the corresponding separable coordinates. From the Corollary we see that we can find two separable systems such that the factor (15) is the same, i.e., the metric must take the form $\mathrm{d}\tilde{s}^2=f\mathrm{d}s^2$, where $\mathrm{d}s^2$ is the metric on a single constant curvature space, either 3D flat space or the three sphere, and the constant curvature space separates in these same two coordinate systems. Further the space of symmetries spanned by the two sets is at least five dimensional.

Then we have $(\tilde{\mathcal{H}}+\tilde{V})/f=\mathcal{H}+V$, where $\tilde{\mathcal{H}}+\tilde{V}$ is the original superintegrable system, $\mathcal{H}$ is the Hamiltonian on a constant curvature space, and V is the induced multiparameter potential. Under the transform f each of the commuting second order symmetries $\mathcal{S}$ of the original system that defines a coordinate separation transforms to a symmetry of the form $\mathcal{S}+g_S\mathcal{H}$ for g_S a function. There are at least five such functionally linearly independent symmetries arising from separation in two coordinate systems, so the constant curvature space system admits five functionally linearly independent symmetries. Thus the potential V must satisfy the Bertrand–Darboux equations for these symmetries. It follows that V is nondegenerate and by Theorem 2 of Ref. 3 that the system $\mathcal{H}+V$ is itself superintegrable with nondegenerate potential. The function f is simultaneously a Stäckel multiplier with respect to the two coordinate systems whose symmetries completely characterize the superintegrable system $\mathcal{H}+V$. That is, f satisfies the Bertrand–Darboux equations for five functionally linearly independent symmetries. Hence f itself satisfies the equations that determine the nondegenerate potential V. This means that the system $\tilde{\mathcal{H}}+\tilde{V}$ is Stäckel equivalent to the constant curvature space superintegrable system. Q.E.D.

IV. CLASSIFICATION OF NONDEGENERATE SYSTEMS

A. Separable systems in complex Euclidean space

It is a difficult task to list all 3D conformally flat superintegrable systems with nondegenerate potential and to show that the classification is complete. However, we now have tools to simplify the problem. First, as every such system is Stäckel equivalent to a system on Euclidean space or the complex sphere, we can restrict ourselves to those two spaces. Second, since every such

system is multiseparable, we can bring to bear our knowledge of all orthogonal separable coordinates on these spaces. These results can be gleaned from the books[20,16] and many papers of the authors, e.g., Ref. 17. Thus in principle, we have enough information to accomplish our task, though the details are formidably complicated.

We begin by summarizing the full list of orthogonal separable systems in complex Euclidean space and the associated symmetry operators. Here, a "natural" basis for first order symmetries is given by $p_1 \equiv p_x$, $p_2 \equiv p_y$, $p_3 \equiv p_z$, $J_1 = yp_z - zp_y$, $J_2 = zp_x - xp_z$, $J_3 = xp_y - yp_x$ in the classical case and $p_1 = \partial_x$, $p_2 = \partial_y$, $p_3 = \partial_z$, $J_1 = y\partial_z - z\partial_y$, $J_2 = z\partial_x - x\partial_z$, $J_3 = x\partial_y - y\partial_x$ in the quantum case. (In the operator characterizations for the quantum case, the classical product of two constants of the motion is replaced by the symmetrized product of the corresponding operator symmetries.) The Hamiltonian is $H = p_1^2 + p_2^2 + p_3^2$. In each case below we list the coordinates followed by the constants of the motion that characterize them.

Note: The bracket notation used to describe generic coordinates in three-dimensional Euclidean space is due to Bôcher and is an adaptation of the notation used to describe the elementary divisors of two quadratic forms one of which is the quadratic form associated with Euclidean space and the second with the quadratic form of the coordinate curves describing the coordinate system. In order to do this in three dimensions and also deal with separable solutions of Laplace's equation we use the symbol $[p_0, p_1, \ldots, p_r]$ where $\Sigma_{i=0}^{r} p_i = 5$ and $p_0 \geqslant 2$. (See Ref. 16 for further details). This determines a coordinate system whose infinitesimal distance is of the form

$$\mathrm{d}s^2 = \frac{1}{(u-v)(u-w)} P(u) p_u^2 + \frac{1}{(v-u)(v-w)} P(v) p_v^2 + \frac{1}{(w-v)(w-u)} P(w) p_w^2,$$

where $P(\lambda) = (\lambda - e_1)^{p_1} \cdots (\lambda - e_r)^{p_r}$. The index p_0 is associated with ∞.

$$[2111] \quad x^2 = c^2 \frac{(u-e_1)(v-e_1)(w-e_1)}{(e_1-e_2)(e_1-e_3)}, \quad y^2 = c^2 \frac{(u-e_2)(v-e_2)(w-e_2)}{(e_2-e_1)(e_2-e_3)},$$

$$z^2 = c^2 \frac{(u-e_3)(v-e_3)(w-e_3)}{(e_3-e_1)(e_3-e_2)},$$

$$L_1 = J_1^2 + J_2^2 + J_3^2 + c^2((e_1+e_2)p_3^2 + (e_1+e_3)p_2^2 + (e_3+e_2)p_1^2),$$

$$L_2 = e_1 J_1^2 + e_2 J_2^2 + e_3 J_3^2 + c^2(e_1 e_2 p_3^2 + e_1 e_3 p_2^2 + e_3 e_2 p_1^2).$$

$$[211] \quad x^2 + y^2 = -c^2 \left[\frac{(u-e_1)(v-e_1)(w-e_1)}{(e_1-e_2)^2} \right] - \frac{c^2}{e_1-e_2}[(u-e_1)(v-e_1) + (u-e_1)(w-e_1) + (v-e_1)(w-e_1)],$$

$$(x-iy)^2 = c^2 \frac{(u-e_1)(v-e_1)(w-e_1)}{e_1-e_2}, \quad z^2 = c^2 \frac{(u-e_2)(v-e_2)(w-e_2)}{(e_2-e_1)^2}.$$

$$L_1 = J_1^2 + J_2^2 + J_3^2 + c^2((e_1-e_2)(p_1+ip_2)^2 + 2e_2 p_3^2 + (e_1+e_2)(p_1^2+p_2^2)),$$

$$L_2 = e_2(J_1^2 + J_2^2) + (e_2-e_1)(J_1+iJ_2)^2 + e_1 J_3^2 + c^2((e_1 e_2(p_1^2+p_2^2) + e_1(e_1-e_2)(p_1+ip_2)^2 + e_2^2 p_3^2)).$$

$$[23] \quad x - iy = \frac{1}{2} c \left(\frac{u^2+v^2+w^2}{uvw} - \frac{1}{2} \frac{u^2v^2 + u^2w^2 + v^2w^2}{u^3v^3w^3} \right),$$

$$z=\frac{1}{2}c\left(\frac{uv}{w}+\frac{uw}{v}+\frac{vw}{u}\right),\quad x+iy=cuvw.$$

$$L_1=J_1^2+J_2^2+J_3^2+2c^2(p_1+ip_2)p_3,\quad L_2=-2J_3(J_1+iJ_2)+c^2(p_1+ip_2)^2.$$

$$[311]\quad x=\frac{c}{4}\left(u^2+v^2+w^2+\frac{1}{u^2}+\frac{1}{v^2}+\frac{1}{w^2}\right)+\frac{3}{2}c,$$

$$y=-\frac{c}{4}\frac{(u^2-1)(v^2-1)(w^2-1)}{uvw},\quad z=i\frac{c}{4}\frac{(u^2+1)(v^2+1)(w^2+1)}{uvw}.$$

$$L_1=c(J_3p_2-J_2p_3)+c^2(p_1^2-p_2^2),\quad L_2=-\frac{1}{4}J_1^2-cJ_2p_3-c^2p_3^2.$$

$$[32]\quad x+iy=uvw,\quad x-iy=-\left(\frac{uv}{w}+\frac{uw}{v}+\frac{vw}{u}\right),\quad z=\frac{1}{2}(u^2+v^2+w^2).$$

$$L_1=-c(J_2+iJ_1)(p_1+ip_2)-c(J_2-iJ_1)(p_1-ip_2)-c^2(p_1+ip_2)^2,$$

$$L_2=J_3^2-2c(J_2-iJ_1)(p_1+ip_2).$$

$$[41]\quad x+iy=u^2v^2+u^2w^2+v^2w^2-\tfrac{1}{2}(u^4+v^4+w^4),\quad x-iy=c^2(u^2+v^2+w^2),\quad z=2icuvw.$$

The symmetries that describe this system are

$$L_1=-iJ_3(p_1-ip_2)+(J_2+iJ_1)p_3+\tfrac{1}{4}c^4(p_1+ip_2)^2,\quad L_2=-(J_1-iJ_2)^2-2ic^4(J_1+iJ_2)p_3.$$

$$[5]\quad x+iy=c(u+v+w),\quad x-iy=\frac{c}{4}(u-v-w)(u+v-w)(u+w-v),$$

$$z=-\frac{c}{4}(u^2+v^2+w^2-2(uv+uw+vw)).$$

$$L_1=iJ_3(p_1+ip_2)+(J_2-iJ_1)p_3+cp_3(p_1-ip_2),$$

$$L_2=\frac{1}{4}(J_2-iJ_1)^2-c(2(J_2+iJ_1i(p_1+ip_2)+i(p_1-ip_2)(J_1+iJ_2))+\frac{c^2}{4}(p_1-ip_2)^2.$$

We summarize the remaining degenerate separable coordinates:

Euclidean coordinates: All of these have one symmetry in common: $L_1=p_3^2$. The seven systems are, polar, Cartesian, light cone, elliptic, parabolic, hyperbolic, and semihyperbolic.

Complex sphere coordinates: These all have the symmetry $L_1=J_1^2+J_2^2+J_3^2$ in common. The five systems are spherical, horospherical, elliptical, hyperbolic, and semicircular parabolic.

Rotational types of coordinates: There are three of these systems, each of which is characterized by the fact that one defining symmetry is a perfect square.

Nonorthogonal heat type coordinates: Each of these nonorthogonal systems corresponds to one first order symmetry. Hence it cannot arise for systems with nondegenerate potentials.

Note that the first seven separable systems are generic, i.e., they occur in one-, two- or three-parameter families, whereas the remaining systems are special limiting cases of the generic ones. We shall show that each of the generic separable systems uniquely determines a nondegenerate superintegrable system.

B. Generic 3D Euclidean superintegrable systems

Each of the seven generic Euclidean separable systems depends on a scaling parameter c and up to three parameters e_1, e_2, e_3. For each such set of coordinates we shall show that there is exactly one nondegenerate superintegrable system that admits separation in these coordinates *simultaneously for all values of the parameters* c, e_j.

Consider the system in Ref. 23, for example. If a nondegenerate superintegrable system separates in these coordinates for all values of the parameter c, then the space of second order symmetries must contain the five symmetries

$$\mathcal{H} = p_x^2 + p_y^2 + p_z^2 + V, \quad \mathcal{S}_1 = J_1^2 + J_2^2 + J_3^2 + f_1, \quad \mathcal{S}_2 = J_3(J_1 + iJ_2) + f_2,$$

$$\mathcal{S}_3 = (p_x + ip_y)^2 + f_3, \quad \mathcal{S}_4 = p_z(p_x + ip_y) + f_4.$$

It is straightforward to check that the 12×5 matrix of coefficients of the second derivative terms in the twelve Bertrand-Darboux equations associated with symmetries $\mathcal{S}_1, \ldots, \mathcal{S}_4$ has rank five in general. Thus, there is at most one nondegenerate superintegrable system admitting these symmetries. Solving the Bertrand-Darboux equations for the potential we find the unique solution

$$V(\mathbf{x}) := \alpha(x^2 + y^2 + z^2) + \frac{\beta}{(x+iy)^2} + \frac{\gamma z}{(x+iy)^3} + \frac{\delta(x^2 + y^2 - 3z^2)}{(x+iy)^4}.$$

Finally, we can use the symmetry conditions for this potential to obtain the full six-dimensional space of second order symmetries. This is the superintegrable system III on the following table. The other six cases yield corresponding results.

Theorem 5: *Each of the seven generic Euclidean separable systems determines a unique nondegenerate superintegrable system that permits separation simultaneously for all values of the scaling parameter c and any other defining parameters* e_j. *For each of these systems there is a basis of five (strongly) functionally independent and six linearly independent second order symmetries. The corresponding nondegenerate potentials and basis of symmetries are (the* f_j *are functions of* x_1, x_2, x_3):

$$\text{I } [2111] \quad V = \frac{\alpha_1}{x^2} + \frac{\alpha_2}{y^2} + \frac{\alpha_3}{z^2} + \delta(x^2 + y^2 + z^2), \tag{16}$$

$$\mathcal{P}_i = \partial_{x_i}^2 + \delta x_i^2 + \frac{\alpha_i}{x_i^2}, \quad \mathcal{J}_{ij} = (x_i p_{x_j} - x_j p_{x_i})^2 + \alpha_i^2 \frac{x_j^2}{x_i^2} + \alpha_j^2 \frac{x_i^2}{x_j^2}, \quad i \geqslant j.$$

$$\text{II } [221] \quad V = \alpha(x^2 + y^2 + z^2) + \beta\frac{x - iy}{(x+iy)^3} + \frac{\gamma}{(x+iy)^2} + \frac{\delta}{z^2}, \tag{17}$$

$$\mathcal{S}_1 = J \cdot J + f_1, \quad \mathcal{S}_2 = p_z^2 + f_2, \quad \mathcal{S}_3 = J_3^2 + f_3,$$

$$\mathcal{S}_4 = (p_x + ip_y)^2 + f_4, \quad L_5 = (J_2 - iJ_1)^2 + f_5.$$

$$\text{III [23]} \quad V=\alpha(x^2+y^2+z^2)+\frac{\beta}{(x+iy)^2}+\frac{\gamma z}{(x+iy)^3}+\frac{\delta(x^2+y^2-3z^2)}{(x+iy)^4}, \tag{18}$$

$$\mathcal{S}_1=J\cdot J+f_1,\quad \mathcal{S}_2=(J_2-iJ_1)^2+f_2,\quad \mathcal{S}_3=J_3(J_2-iJ_1)+f_3,$$

$$\mathcal{S}_4=(p_x+ip_y)^2+f_4,\quad \mathcal{S}_5=p_z(p_x+ip_y)+f_5.$$

$$\text{IV [311]} \quad V=\alpha(4x^2+y^2+z^2)+\beta x+\frac{\gamma}{y^2}+\frac{\delta}{z^2}, \tag{19}$$

$$\mathcal{S}_1=p_x^2+f_1,\quad \mathcal{S}_2=p_y^2+f_2,\quad \mathcal{S}_3=p_zJ_2+f_3,$$

$$\mathcal{S}_4=p_yJ_3+f_4,\quad \mathcal{S}_5=J_1^2+f_5.$$

$$\text{V [32]} \quad V=\alpha(4x^2+y^2+z^2)+\beta x+\frac{\gamma}{(y+iz)^2}+\frac{\delta(y-iz)}{(y+iz)^3}, \tag{20}$$

$$\mathcal{S}_1=p_x^2+f_1,\quad \mathcal{S}_2=J_1^2+f_2,\quad \mathcal{S}_3=(p_z-ip_y)(J_2+iJ_3)+f_3,$$

$$\mathcal{S}_4=p_zJ_2-p_yJ_3+f_4,\quad \mathcal{S}_5=(p_z-ip_y)^2+f_5.$$

$$\text{VI [41]} \quad V=\alpha(z^2-2(x-iy)^3+4(x^2+y^2))+\beta(2(x+iy)-3(x-iy)^2)+\gamma(x-iy)+\frac{\delta}{z^2}, \tag{21}$$

$$\mathcal{S}_1=(p_x-ip_y)^2+f_1,\quad \mathcal{S}_2=p_z^2+f_2,\quad \mathcal{S}_3=p_z(J_2+iJ_1)+f_3,$$

$$\mathcal{S}_4=J_3(p_x-ip_y)-\frac{i}{4}(p_x+ip_y)^2+f_4,\quad \mathcal{S}_5=(J_2+iJ_1)^2+4ip_zJ_1+f_5.$$

$$\begin{aligned}\text{VII [5]} \quad V=&\alpha(x+iy)+\beta\left(\tfrac{3}{4}(x+iy)^2+\tfrac{1}{4}z\right)+\gamma\left((x+iy)^3+\tfrac{1}{16}(x-iy)+\tfrac{3}{4}(x+iy)z\right)\\&+\delta\left(\tfrac{5}{16}(x+iy)^4+\tfrac{1}{16}(x^2+y^2+z^2)+\tfrac{3}{8}(x+iy)^2z\right),\end{aligned} \tag{22}$$

$$\mathcal{S}_1=(J_1+iJ_2)^2+2iJ_1(p_x+ip_y)-J_2(p_x+ip_y)+\tfrac{1}{4}(p_y^2-p_z^2)-iJ_3p_z+f_1,$$

$$\mathcal{S}_2=J_2p_z-J_3p_y+i(J_3p_x-J_1p_z)-\frac{i}{2}p_yp_z+f_2,\quad \mathcal{S}_3=(p_x+ip_y)^2+f_4,$$

$$\mathcal{S}_4=J_3p_z+iJ_1p_y+iJ_2p_x+2J_1p_x+\frac{i}{4}p_z^2+f_3,\quad \mathcal{S}_5=p_z(p_x+ip_y)+f_5.$$

Note that in the complete list of orthogonal separable coordinate systems for complex 3D Euclidean space there are some other systems besides the first seven that have parameter depen-

dence, e.g., cylindrical elliptic coordinates $L_1=p_3^2$, $L_2=J_3^2+c^2p_1^2$. However, for all of these other coordinates the corresponding Bertrand-Darboux equations have only rank four, hence they do not uniquely determine a possible superintegrable system.

C. Interbasis expansions for Euclidean systems

To proceed with the classification of nondegenerate Euclidean superintegrable systems we need to look more closely at the relationship between a standard basis of symmetries for such a system and the natural basis written in terms of the linear and angular momentum generators p_k, J_k, $k=1,\ldots,3$.

Let us denote our preferred Cartesian coordinate system by $\mathbf{x}=(u,v,w)$ and let $\mathbf{x}_0=(x,y,z)$, be a fixed regular point. We define the translated Cartesian coordinates (X,Y,Z) by $u=x+X$, $v=y+Y$, $w=z+Z$. Then, near the regular point (x,y,z) we have a basis of "natural symmetries" $p_1=p_X$, $p_2=p_Y$, $p_3=p_Z$, $J_1=Yp_z-Zp_Y$, $J_2=Zp_X-Xp_Z$, $J_3=Xp_Y-Yp_X$. Now suppose we have a Euclidean superintegrable system with nondegenerate potential. Then there will exist fifteen rational functions $A^{ij}(x,y,z)$, $B^{ij}(x,y,z)$, $C^{ij}(x,y,z)$, that completely characterize the superintegrable system. In particular, only 10 of these are linearly independent [see relations (A2)],

$$A^{22},\ A^{33},\ B^{22},\ B^{33},\ C^{33},\ A^{12},\ B^{12},\ A^{13},\ A^{23},\ B^{23}, \tag{23}$$

and they are subject to the five quadratic conditions (A3) with $G\equiv 0$. These functions are related to the symmetries $\mathcal{S}=\Sigma a^{ij}p_ip_j+W$ via the conditions (A1). Recall that the second order basis symmetries at the regular point $\mathcal{S}^{(\ell m)}_{\mathbf{x}_0}(\mathbf{x})=\Sigma a^{ij}_{(\ell m)}(\mathbf{x})p_ip_j+f_{(\ell m)}$ take the form $\mathcal{S}^{(\ell m)}_{\mathbf{x}_0}(\mathbf{x}_0)=p_ip_j+f_{(\ell m)}(\mathbf{x}_0)$ when evaluated at the point. Thus we can expand each standard basis symmetry in terms of the natural basis at the point via

$$\begin{aligned}\mathcal{S}^{(\ell m)}_{\mathbf{x}_0}=&\,p_\ell p_m+\alpha_3^{(\ell m)}J_1^2+\alpha_4^{(\ell m)}J_2^2+\alpha_5^{(\ell m)}J_3^2+\alpha_6^{(\ell m)}p_1J_1+\alpha_7^{(\ell m)}p_2J_2+\alpha_8^{(\ell m)}p_1J_2+\alpha_9^{(\ell m)}p_1J_3\\&+\alpha_{10}^{(\ell m)}p_2J_1+\alpha_{11}^{(\ell m)}p_2J_3+\alpha_{12}^{(\ell m)}p_3J_1+\alpha_{13}^{(\ell m)}p_3J_2+\alpha_{14}^{(\ell m)}J_1J_2+\alpha_{15}^{(\ell m)}J_1J_3\\&+\alpha_{16}^{(\ell m)}J_2J_3+W^{(\ell m)}(\mathbf{x}),\end{aligned} \tag{24}$$

where the $\alpha_k^{(\ell m)}$ are constants in X,Y,Z but rational functions of the parameters x, y, z of the regular point. [This notation for the expansion coefficients α_s is not completely logical, but since all of our software programs use the same notation we continue to use it to avoid (our) confusion.]

We conclude that all of the expansion constants $\alpha_k^{(\ell m)}$ can be expressed in terms of the ten numbers (23). However, we shall not embark on this straightforward task but instead restrict ourselves to expanding the two symmetries

$$\begin{aligned}\mathcal{S}^{(12)}_{\mathbf{x}_0}=&\,p_1p_2+\alpha_3J_1^2+\alpha_4J_2^2+\alpha_5J_3^2+\alpha_6p_1J_1+\alpha_7p_2J_2+\alpha_8p_1J_2+\alpha_9p_1J_3+\alpha_{10}p_2J_1+\alpha_{11}p_2J_3\\&+\alpha_{12}p_3J_1+\alpha_{13}p_3J_2+\alpha_{14}J_1J_2+\alpha_{15}J_1J_3+\alpha_{16}J_2J_3+W^{(12)}(\mathbf{x}),\end{aligned} \tag{25}$$

$$\begin{aligned}\mathcal{S}^{(13)}_{\mathbf{x}_0}=&\,p_1p_3+\alpha'_3J_1^2+\alpha'_4J_2^2+\alpha'_5J_3^2+\alpha'_6p_1J_1+\alpha'_7p_2J_2+\alpha'_8p_1J_2+\alpha'_9p_1J_3+\alpha'_{10}p_2J_1+\alpha'_{11}p_2J_3\\&+\alpha'_{12}p_3J_1+\alpha'_{13}p_3J_2+\alpha'_{14}J_1J_2+\alpha'_{15}J_1J_3+\alpha'_{16}J_2J_3+W^{(13)}(\mathbf{x}).\end{aligned} \tag{26}$$

(Here, $\alpha_s=\alpha_s^{(12)}$, $\alpha'_s=\alpha_s^{(13)}$.) Indeed it is easy to verify that the six Bertrand-Darboux equations for these two symmetries have rank five (an illustration of Lemma 1 of Ref. 3). Thus these two symmetries completely determine the A^{ij}, B^{ij}, C^{ij}, hence the superintegrable system.

If $a^{ij}(\mathbf{x})$ is the quadratic form associated with $\mathcal{S}^{(12)}(\mathbf{x})$ it is straightforward to verify that

$$a_1^{11}(\mathbf{x}_0)=0,\quad a_2^{11}(\mathbf{x}_0)=-\alpha_9,\quad a_3^{11}(\mathbf{x}_0)=\alpha_8,$$

$$a_1^{22}(\mathbf{x}_0)=\alpha_{11},\quad a_2^{22}(\mathbf{x}_0)=0,\quad a_3^{22}(\mathbf{x}_0)=-\alpha_{10},$$

$$
\begin{gathered}
a_1^{33}(\mathbf{x}_0) = -\alpha_{13}, \quad a_2^{33}(\mathbf{x}_0) = \alpha_{12}, \quad a_3^{33}(\mathbf{x}_0) = 0, \\
a_1^{12}(\mathbf{x}_0) = \tfrac{1}{2}\alpha_9, \quad a_2^{12}(\mathbf{x}_0) = -\tfrac{1}{2}\alpha_{11}, \quad a_3^{12}(\mathbf{x}_0) = \tfrac{1}{2}(\alpha_7 - \alpha_6), \\
a_1^{13}(\mathbf{x}_0) = -\tfrac{1}{2}\alpha_8, \quad a_2^{13}(\mathbf{x}_0) = \tfrac{1}{2}\alpha_6, \quad a_3^{13}(\mathbf{x}_0) = \tfrac{1}{2}\alpha_{13}, \\
a_1^{23}(\mathbf{x}_0) = -\tfrac{1}{2}\alpha_7, \quad a_2^{23}(\mathbf{x}_0) = \tfrac{1}{2}\alpha_{10}, \quad a_3^{23}(\mathbf{x}_0) = -\tfrac{1}{2}\alpha_{12},
\end{gathered}
\tag{27}
$$

where $a_k^{ij}(\mathbf{x}_0) = \partial_k a^{ij}(\mathbf{x})|_{\mathbf{x}_0}$. There are identical relations for the other symmetries $\mathcal{S}^{(\ell m)}(\mathbf{x})$. Using (27) and the identities (A2) and (A1) we can express the expansion coefficients $\alpha_6, \ldots, \alpha_{13}$ in terms of the ten numbers (23) at $\mathbf{x}_0$:

$$
\begin{gathered}
\alpha_6 = \tfrac{1}{3}(2A^{13} - B^{23}), \quad \alpha_7 = \tfrac{1}{3}(A^{13} - 2B^{23}), \quad \alpha_8 = -\tfrac{1}{3}A^{23}, \\
\alpha_9 = \tfrac{1}{3}A^{22}, \quad \alpha_{10} = \tfrac{1}{3}A^{23}, \quad \alpha_{11} = \tfrac{1}{3}B^{22}, \\
\alpha_{12} = \tfrac{1}{3}(B^{12} - A^{22} + A^{33}), \quad \alpha_{13} = -\tfrac{1}{3}(B^{33} + A^{12}).
\end{gathered}
\tag{28}
$$

The corresponding results for the expansion coefficients $\alpha'_6, \ldots, \alpha'_{13}$ of $\mathcal{S}^{(13)}$ are

$$
\begin{gathered}
\alpha'_6 = -\tfrac{1}{3}(2A^{12} + B^{33}), \quad \alpha'_7 = -\tfrac{1}{3}(A^{12} + 2B^{23}), \quad \alpha'_8 = -\tfrac{1}{3}A^{33}, \\
\alpha'_9 = \tfrac{1}{3}A^{23}, \quad \alpha'_{10} = -\tfrac{1}{3}B^{12}, \quad \alpha'_{11} = \tfrac{1}{3}B^{23}, \\
\alpha'_{12} = -\tfrac{1}{3}A^{23}, \quad \alpha'_{13} = -\tfrac{1}{3}C^{33}.
\end{gathered}
\tag{29}
$$

The expansion coefficients of the terms of the form $J_\ell J_m$, i.e., $\alpha_3, \alpha_4, \alpha_5, \alpha_{14}, \alpha_{15}, \alpha_{16}$ can be expressed in terms of second derivatives of the associated quadratic form, evaluated at the regular point $\mathbf{x}_0$. For example, $\alpha_{14} = 2a_{23}^{13}(\mathbf{x}_0) = -a_{33}^{12}(\mathbf{x}_0) = -a_{12}^{33}(\mathbf{x}_0)$. For a superintegrable system the integrability conditions for the symmetry relations (A1) are satisfied identically, so these equations can be differentiated to compute the second derivatives $a_{k\ell}^{ij}(\mathbf{x}_0)$ as a quadratic expression in the ten basic constants [subject to the five quadratic identities (A3)]. Though straightforward, these computations are tedious. The only relations that we will use here are those for the expansion coefficients $\alpha_{14}^{(\ell m)}$. We have

$$
\begin{gathered}
\alpha_{14}^{(11)} = \tfrac{1}{9}(4A^{23}(B^{33} - B^{22}) - 4B^{23}(A^{23} - A^{22}) - 2A^{13}B^{12} + 2A^{12}A^{23}), \\
\alpha_{14}^{(22)} = \tfrac{1}{9}(4A^{12}A^{23} + 2B^{12}B^{23} + 2A^{23}B^{33} - 2A^{13}B^{12} - 2B^{23}A^{33} + 2B^{23}A^{22} - 4B^{12}B^{23}), \\
\alpha_{14}^{(33)} = \tfrac{1}{9}(2B^{23}(A^{22} - A^{33} + B^{12}) - 4A^{13}B^{12} + 2A^{23}(A^{12} - 2B^{22} + B^{33})), \\
\begin{aligned}
\alpha_{14}^{(12)} = \tfrac{1}{9}((2B^{23} - A^{13})(B^{33} - B^{22}) - 2(B^{33} + A^{12} - B^{22})B^{23} \\
- A^{23}B^{12} + (2B^{23} + A^{13})A^{12} + 2B^{33}A^{13} - A^{23}A^{33}),
\end{aligned}
\end{gathered}
\tag{30}
$$

$$
\begin{aligned}
\alpha_{14}^{(13)} = \tfrac{1}{18}(7(B^{33})^2 + (A^{33})^2 - 2A^{22}B^{12} - (A^{23})^2 + 4A^{12}B^{33} - A^{13}C^{33} - 3(A^{12})^2 - 5(B^{12})^2 - 4A^{33}B^{12} \\
- 7B^{22}B^{33} - 7B^{23}C^{33} + 2A^{13}B^{23} + 7(B^{23})^2 - A^{22}A^{33}),
\end{aligned}
$$

$$\alpha_{14}^{(23)} = \tfrac{1}{9}(A^{23}(-B^{23}+C^{33}) + (A^{23}-A^{22}+B^{12})(A^{12}+B^{22}-B^{33})).$$

Note that since the Hamiltonian is $\mathcal{S}^{(11)}+\mathcal{S}^{(22)}+\mathcal{S}^{(33)}$ and the coefficient of J_1J_2 in the Hamiltonian is 0, we must have $\alpha_{14}^{(11)}+\alpha_{14}^{(22)}+\alpha_{14}^{(33)}=0$, which can be verified directly from the above-mentioned expressions.

As a result of the previous discussion we have the result

Theorem 6: *For a nondegenerate superintegrable system the expansion coefficients* $\alpha_k^{(\ell m)}$ *expressing the standard basis* $\mathcal{S}^{\ell m}$ *in terms of the natural basis* p_hp_k, p_hJ_k, J_hJ_k *are explicit linear and quadratic expressions in the ten terms (23).*

D. The significance of generic Euclidean systems

Suppose we have a nondegenerate Euclidean superintegrable system with potential V that is separable with respect to some orthogonal coordinates. (Since every superintegrable system is multiseparable, we know that such coordinates exist.) By performing an Euclidean transformation, if necessary, we can assume that the separable coordinates are in a standard form determined by two constants of the motion in involution,

$$L_1 = \sum a^{ij}p_ip_j + f_1, \quad L_2 = \sum b^{ij}p_ip_j + f_2.$$

Clearly, L_1 and L_2 lie in the six-dimensional space of second order symmetries for the superintegrable system. Thus, the quadratic form a^{ij}, for example, satisfies the three Bertrand-Darboux equations for potential V. Since V is nondegenerate we can express the second derivatives $V_{jj}-V_{kk}$ and V_{jk} with $j\neq k$ in the Bertrand-Darboux equations as linear combinations of the first derivatives V_h. Equating coefficients of V_1, V_2, V_3 separately in each of the three equations, we end up with nine linear conditions for the ten constants $A^{22},\ldots,B^{23}$ at each regular point. A typical example of one of these conditions is

$$A^{13}(3a^{11}-3a^{33}) + B^{23}(0) + A^{23}(-3a^{12}) + A^{22}(0) + B^{22}(0) + B^{12}(0) + A^{33}(-3a^{13}) + B^{33}(0) + A^{12}(-3a^{23}) + C^{33}(0) = -a_1^{13} + a_3^{11}.$$

Here, $B^{23}(0)=0$, etc. For the second symmetry there will be nine more linear conditions with a^{ij} replaced by b^{ij}. Thus we will have eighteen linear equations (not linearly independent) for the ten quantities $A^{22},\ldots,B^{23}$. Another source of conditions is obtained by writing the symmetry L_1 in terms of the standard basis:

$$a^{ij}(\mathbf{x}) = \sum_{\ell\leq m} a^{\ell m}(\mathbf{x}_0)\mathcal{A}^{ij}_{(\ell,m)}(\mathbf{x}),$$

where $\mathcal{A}^{ij}_{(\ell,m)}$ is the quadratic form associated with the standard basis symmetry $\mathcal{S}^{(\ell,m)}$ at $\mathbf{x}_0$. Expanding both sides of this equation in terms of the natural basis we obtain linear and quadratic conditions on the ten basic quantities. For example if we equate coefficients of the natural basis element J_1J_2 we find the quadratic conditions for L_1 and L_2:

$$2a_{23}^{13}(\mathbf{x}_0) = \sum_{\ell\leq m} a^{\ell m}(\mathbf{x}_0)\alpha_{14}^{(\ell m)}, \quad 2b_{23}^{13}(\mathbf{x}_0) = \sum_{\ell\leq m} b^{\ell m}(\mathbf{x}_0)\alpha_{14}^{(\ell m)}. \tag{31}$$

Though there are many other quadratic conditions for L_1, L_2 to belong to the symmetry algebra, we shall use only these two and the five fundamental quadratic identities (A3) that hold independent of any choice of L_1, L_2. Note that by equating coefficients of natural basis elements of the form p_iJ_k we could obtain linear identities. However, these are equivalent to the linear conditions for a^{ij}, b^{ij} already discussed previously.

We give an example to show how this works. Suppose we have a nondegenerate superintegrable system that admits separation for some special choice of ellipsoidal coordinates [2111]. (Here we do *not* assume that the system separates for all values of the parameters c, e_1, e_2, e_3, but only for one value.) By performing an Euclidean transformation and a change of scale we can

assume that the coordinates are in the standard form [2111] in our table and that $c=1$, $e_1=0$, $e_2=1$, and $e_3=a$ where a is any fixed complex number such that $a(a-1)\neq 0$. It follows that

$$a^{11}=y^2+z^2+a+1,\quad a^{22}=x^2+z^2+a,\quad a^{33}=x^2+y^2+1,$$

$$a^{12}=-xy,\quad a^{13}=-xz,\quad a^{23}=-yz,\quad b^{11}=ay^2+z^2+a,$$

$$b^{22}=ax^2,\quad b^{33}=x^2,\quad b^{12}=-axy,\quad b^{13}=-xz,\quad b^{23}=0,$$

at any regular point with coordinates (x,y,z). Substituting these expressions into the 18 linear conditions discussed previously, with the help of the computer algebra system MAPLE, we find that there are exactly seven independent linear conditions. Thus the ten quantities $A^{22},\ldots,B^{23}$ can be expressed linearly in terms of three of these quantities. Substituting this result into the five fundamental quadratic identities (A3) we find that these identities yield a single *linear* relation for the remaining three unknowns. Finally we substitute our expressions in terms of the three unknowns and (30) into (50) and obtain (with the help of MAPLE) two more independent linear conditions. Thus we end up with ten independent linear conditions for our ten unknowns, and we obtain the unique solution

$$A^{12}=B^{12}=A^{23}=B^{23}=A^{13}=B^{33}=0,\quad A^{33}=A^{22}=\frac{3}{x},\quad C^{33}=-\frac{3}{z},\quad B^{22}=-\frac{3}{y},$$

which corresponds to the nondegenerate potential [I],

$$V=\frac{\alpha}{x^2}+\frac{\beta}{y^2}+\frac{\gamma}{z^2}+\delta(x^2+y^2+z^2).$$

Note that it was obvious that our conditions would have solutions, since we already knew that system [I] separated simultaneously for all choices of the parameters c, e_1, e_2, e_3. What was far from obvious is the fact that *no other* nondegenerate superintegrable system separates for *any* special case of ellipsoidal coordinates.

Theorem 7: *A 3D Euclidean nondegenerate superintegrable system admits separation in a special case of the generic coordinates [2111], [221], [23], [311], [32], [41], or [5], respectively, if and only if it is equivalent via a Euclidean transformation to system [I], [II], [III], [IV], [V], [VI], or [VII], respectively.*

The proof (complicated but straightforward) proceeds exactly as the case [2111] described previously. For each case [221]–[5] we use the symmetries a^{ij}, b^{ij} listed. The eighteen linear conditions discussed previously reduce to exactly seven independent linear conditions. Thus always the ten quantities $A^{22},\ldots,B^{23}$ can be expressed linearly in terms of three of these quantities. Substituting into the five fundamental quadratic identities (A3) we find that these identities yield a single *linear* relation for the remaining three unknowns. Substituting our expressions in terms of the three unknowns and (30) into (50) we obtain two more independent linear conditions. Thus we end up with ten independent linear conditions for our ten unknowns, and a unique solution, the corresponding generic superintegrable system.

This does not settle the problem of classifying all 3D nondegenerate superintegrable systems in complex Euclidean space, for we have not excluded the possibility of such systems that separate only in degenerate separable coordinates. In fact we have already studied two such systems in:[3]

$$[O]\quad V(x,y,z)=\alpha x+\beta y+\gamma z+\delta(x^2+y^2+z^2),$$

$$[OO]\quad V(x,y,z)=\frac{\alpha}{2}\left(x^2+y^2+\frac{1}{4}z^2\right)+\beta x+\gamma y+\frac{\delta}{z^2}. \tag{32}$$

However, both of these nondegenerate superintegrable systems are only weakly functionally independent, in contrast to systems [I]–[VII]. Thus we consider $[O]$ and $[OO]$ as associate members of the superintegrable family, not regular members. An investigation of other possible Euclidean systems is in progress.

E. Generic superintegrable systems on the three sphere

An important task remaining is to classify the possible systems on the three sphere (particularly those three-sphere systems not Stäckel equivalent to a flat space system). We choose a standardized Cartesian-like coordinate system $\{x,y,z\}$ on the three sphere such that the metric and Hamiltonian are

$$\mathrm{d}s^2=\frac{1}{\left(1+\frac{r^2}{4}\right)^2}(\mathrm{d}x^2+\mathrm{d}y^2+\mathrm{d}z^2),\quad \mathcal{H}=\left(1+\frac{r^2}{4}\right)^2(p_x^2+p_y^2+p_z^2)+V, \tag{33}$$

where $r^2=x^2+y^2+z^2$. These coordinates can be related to the standard realization of the sphere via complex coordinates $\mathbf{s}=(s_1,s_2,s_3,s_4)$ such that $\Sigma_{j=1}^4 s_j^2=1$ and $\mathrm{d}s^2=\Sigma_j \mathrm{d}s_j^2$ via

$$s_1=\frac{4x}{4+r^2},\quad s_2=\frac{4y}{4+r^2},\quad s_3=\frac{4z}{4+r^2},\quad s_4=\frac{4-r^2}{4+r^2} \tag{34}$$

with inverse $x=2s_1/(1+s_4)$, $y=2s_2/(1+s_4)$, $z=2s_3/(1+s_4)$. Here x,y,z are local coordinates in a neighborhood of the pole $\mathbf{P}=(0,0,0,1)$ on the three sphere. A basis of Killing vectors for the zero potential system is J_h, K_h, $h=1,2,3$ where

$$J_1=yp_z-zp_y,\quad J_2=zp_x-xp_z,\quad J_3=xp_y-yp_x,$$

$$K_1=\left(1+\frac{x^2-y^2-z^2}{4}\right)p_x+\frac{xy}{2}p_y+\frac{xz}{2}p_z,\quad K_2=\left(1+\frac{y^2-x^2-z^2}{4}\right)p_y+\frac{xy}{2}p_x+\frac{yz}{2}p_z, \tag{35}$$

$$K_3=\left(1+\frac{z^2-x^2-y^2}{4}\right)p_z+\frac{xz}{2}p_x+\frac{yz}{2}p_y.$$

The commutation relations are

$$\{J_1,J_2\}=J_3,\quad \{K_1,K_2\}=J_3,\quad \{K_1,J_2\}=K_3 \tag{36}$$

and their cyclic permutations. The relation between this basis and the standard basis of rotation generators on the sphere $I_{\ell m}=s_\ell p_m-s_m p_\ell=-I_{m\ell}$ is

$$J_1=I_{23},\quad J_2=I_{31},\quad J_3=I_{12},\quad K_1=I_{41},\quad K_2=I_{42},\quad K_3=I_{43}. \tag{37}$$

We shall use the x,y,z coordinates as standard but we also need to see how these coordinates relate to analogous Cartesian-like coordinates centered at any point $\mathbf{T}$ on the sphere. We can always find a complex orthogonal matrix O, not unique, such that $\mathbf{T}=O\mathbf{P}$. If X,Y,Z, (34), define local Cartesian-like coordinates near $\mathbf{P}$ then via $\mathbf{t}=Os(X,Y,Z)$ they also define local coordinates in a neighborhood of $\mathbf{T}=(T_1,T_2,T_3,T_4)$. Moreover, since O is orthogonal we have

$$\mathrm{d}s^2=\mathrm{d}\mathbf{t}\cdot\mathrm{d}\mathbf{t}=\mathrm{d}O\mathbf{s}\cdot\mathrm{d}O\mathbf{s}=\mathrm{d}\mathbf{s}\cdot\mathrm{d}\mathbf{s}=\frac{1}{\left(1+\frac{R^2}{4}\right)^2}(\mathrm{d}X^2+\mathrm{d}Y^2+\mathrm{d}Z^2),$$

so we can consider X,Y,Z as Cartesian-like coordinates in a neighborhood of $\mathbf{T}$. We can also require that the coordinate axes line up so that differentiation of $\mathbf{s}$ by X,Y,Z, respectively, at $\mathbf{P}$ corresponds to (normalized) differentiation of $\mathbf{t}$ by x,y,z, respectively, at $\mathbf{T}$, i.e., so that p_X corresponds to $(1+r^2/4)p_x$, etc. Thus,

$$\left(\frac{2}{1+t_4}\partial_x \mathbf{t}\right)\Big|_{\mathbf{t}=\mathbf{T}} = O\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad \left(\frac{2}{1+t_4}\partial_y \mathbf{t}\right)\Big|_{\mathbf{t}=T} = O\begin{pmatrix}0\\1\\0\\0\end{pmatrix},$$

$$\left(\frac{2}{1+t_4}\partial_z \mathbf{t}\right)\Big|_{\mathbf{t}=T} = O\begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad \mathbf{T} = O\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

This determines O uniquely, since the column vectors on the left-hand sides of these expressions are mutually orthogonal unit vectors. We find

$$O_T = \begin{pmatrix} -\frac{T_1^2 - T_4 - 1}{T_4+1} & -\frac{T_2 T_1}{T_4+1} & -\frac{T_3 T_1}{T_4+1} & T_1 \\ -\frac{T_1 T_2}{T_4+1} & -\frac{T_2^2 - T_4 - 1}{T_4+1} & -\frac{T_3 T_2}{T_4+1} & T_2 \\ -\frac{T_1 T_3}{T_4+1} & -\frac{T_2 T_3}{T_4+1} & -\frac{T_3^2 - T_4 - 1}{T_4+1} & T_3 \\ -T_1 & -T_2 & -T_3 & T_4 \end{pmatrix}. \tag{38}$$

In the **P**-based coordinate system the coordinates of **t** are u, v, w where $u=2t_1/(1+t_4)$, $v=2t_2/(1+t_4)$, $w=2t_3/(1+t_4)$. From the equation $\mathbf{t}=O_T\mathbf{s}$ we can solve for u, v, w to obtain

$$u = \frac{4[r^2 X - 2x(xX+yY+zZ) + 4(x+X) - xR^2]}{16 - 8(xX+yY+zZ) + r^2R^2},$$

$$v = \frac{4[r^2 Y - 2y(xX+yY+zZ) + 4(y+Y) - yR^2]}{16 - 8(xX+yY+zZ) + r^2R^2}, \tag{39}$$

$$w = \frac{4[r^2 Z - 2z(xX+yY+zZ) + 4(z+Z) - zR^2]}{16 - 8(xX+yY+zZ) + r^2R^2}.$$

To recapitulate: **t** is a point on the complex unit sphere, (x,y,z) are the coordinates of **T** in the **P**-based system, (u,v,w) are the coordinates of **t** in the **P**-based system, and (X,Y,Z) are the coordinates of **t** in the **T**-based system. Thus, for fixed **T**, Eq. (39) defines the coordinate transformation between (u,v,w) and (X,Y,Z). We can write Eq. (39) in a simpler form by introducing the supplementary variables

$$U = \frac{u-x}{1+\frac{r^2}{4}}, \quad V = \frac{v-y}{1+\frac{r^2}{4}}, \quad W = \frac{v-z}{1+\frac{r^2}{4}}, \quad Q^2 = U^2 + V^2 + W^2.$$

Then

$$U = \frac{1 - \frac{1}{2}xX}{1 - \frac{1}{2}(xX+yY+zZ) + \frac{r^2R^2}{16}},$$

$$V=\frac{1-\frac{1}{2}yY}{1-\frac{1}{2}(xX+yY+zZ)+\frac{r^2R^2}{16}},\quad W=\frac{1-\frac{1}{2}zZ}{1-\frac{1}{2}(xX+yY+zZ)+\frac{r^2R^2}{16}},\tag{40}$$

with inverse

$$X=\frac{U+\frac{x}{4}Q^2}{1+\frac{1}{2}(xU+yV+zW)+\frac{r^2Q^2}{16}},$$

$$Y=\frac{V+\frac{y}{4}Q^2}{1+\frac{1}{2}(xU+yV+zW)+\frac{r^2Q^2}{16}},\quad Z=\frac{W+\frac{z}{4}Q^2}{1+\frac{1}{2}(xU+yV+zW)+\frac{r^2Q^2}{16}}.\tag{41}$$

In Ref. 22 we have determined all orthogonal separable coordinate systems on the complex unit three sphere. Of the 21 systems listed those that are generic, in the sense we used for Euclidean separable systems, are given as follows with coordinates followed by defining constants of the motion. (Here we take the Hamiltonian as $\mathcal{L}_0=I_{12}^2+I_{13}^2+I_{14}^2+I_{23}^2+I_{24}^2+I_{34}^2$, and we recall the identity $I_{23}I_{41}+I_{31}I_{42}+I_{12}I_{43}=0$.)

[1111] (system (17) in Ref. [22])

$$s_1^2=\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_2)(e_1-e_3)(e_1-e_4)},\quad s_2^2=\frac{(x_1-e_2)(x_2-e_2)(x_3-e_2)}{(e_2-e_1)(e_2-e_3)(e_2-e_4)},$$

$$s_3^2=\frac{(x_1-e_3)(x_2-e_3)(x_3-e_3)}{(e_3-e_1)(e_3-e_2)(e_3-e_4)},\quad s_4^2=\frac{(x_1-e_4)(x_2-e_4)(x_3-e_4)}{(e_4-e_2)(e_4-e_3)(e_4-e_1)},$$

$$\mathcal{L}_1=(e_1+e_2)I_{12}^2+(e_1+e_3)I_{13}^2+(e_1+e_4)I_{14}^2+(e_2+e_3)I_{23}^2+(e_2+e_4)I_{24}^2+(e_3+e_4)I_{34}^2,$$

$$\mathcal{L}_2=e_1e_2I_{12}^2+e_1e_3I_{13}^2+e_1e_4I_{14}^2+e_2e_3I_{23}^2+e_2e_4I_{24}^2+e_3e_4I_{34}^2.$$

[211] (system (18) in Ref. [22])

$$(is_1+s_2)^2=-2\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_3)(e_1-e_4)},$$

$$s_1^2+s_2^2=-\partial_{e_1}\left(\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_3)(e_1-e_4)}\right),$$

$$s_3^2=-\frac{(x_1-e_3)(x_2-e_3)(x_3-e_3)}{(e_3-e_1)^2(e_3-e_4)},\quad s_4^2=-\frac{(x_1-e_4)(x_2-e_4)(x_3-e_4)}{(e_4-e_1)^2(e_4-e_3)};$$

$$\mathcal{L}_1=(I_{14}+iI_{24})^2+(I_{13}+iI_{23})^2+2e_1(2I_{12}^2+I_{14}^2+I_{24}^2+I_{13}^2+I_{23}^2)+2e_3(I_{34}^2+I_{13}^2+I_{23}^2)$$
$$+2e_4(I_{14}^2+I_{24}^2+I_{34}^2),$$

$$\mathcal{L}_2=e_1^2I_{12}^2+e_1e_3(I_{13}^2+I_{23}^2)+e_1e_4(I_{14}^2+I_{24}^2)+e_3e_4I_{34}^2+\frac{e_3}{2}(I_{13}+iI_{23})^2+\frac{e_4}{2}(I_{14}+iI_{24})^2.$$

[22] (system (19) in Ref. [22])

$$(s_1+is_2)^2=-2\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_3)^2},$$

$$(s_3+is_4)^2=-2\frac{(x_1-e_3)(x_2-e_3)(x_3-e_3)}{(e_1-e_3)^2},\quad s_1^2+s_2^2=-\frac{\partial}{\partial e_1}\left(\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_3)^2}\right);$$

$$\mathcal{L}_1=-I_{24}^2+I_{13}^2+iI_{13}I_{23}+iI_{14}I_{24}+iI_{23}I_{24}+iI_{13}I_{14}+(e_1-e_3)[I_{12}^2-I_{34}^2]+e_2,$$

$$\mathcal{L}_2=e_1^2I_{12}^2+e_3^2I_{34}^2+e_1e_3[I_{13}^2+I_{24}^2+I_{14}^2+I_{23}^2]+\frac{1}{4}[I_{13}^2+I_{24}^2-I_{14}^2-I_{23}^2+2iI_{13}I_{23}+2iI_{13}I_{14}-2iI_{14}I_{24}$$
$$-2iI_{23}I_{24}-4I_{13}I_{24}-2I_{12}I_{34}]+\frac{e_1}{2}[I_{13}^2-I_{24}^2-I_{14}^2+I_{23}^2+2iI_{13}I_{14}+2iI_{23}I_{24}]+\frac{e_3}{2}[-I_{24}^2+I_{13}^2+I_{14}^2$$
$$-I_{23}^2+2iI_{13}I_{23}+2iI_{14}I_{24}].$$

[31] (system (20) in Ref. in [22])

$$(s_1+is_2)^2=-2\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_4)},\quad s_4^2=-\frac{(x_1-e_4)(x_2-e_4)(x_3-e_4)}{(e_4-e_1)^3},$$

$$\sqrt{2}s_3(s_1+is_2)=-\frac{\partial}{\partial e_1}\left(\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_4)}\right),$$

$$s_1^2+s_2^2+s_3^2=-\frac{1}{2}\frac{\partial^2}{\partial e_1^2}\frac{(x_1-e_1)(x_2-e_1)(x_3-e_1)}{(e_1-e_4)};$$

$$\mathcal{L}_1=\sqrt{2}(I_{14}I_{34}-I_{12}I_{23}+iI_{24}I_{34}+iI_{12}I_{13})+e_1(I_{12}^2+I_{13}^2+I_{23}^2)+e_4(I_{34}^2+I_{14}^2+I_{24}^2),$$

$$\mathcal{L}_2=-\frac{1}{2}I_{13}^2+\frac{1}{2}I_{23}^2-iI_{13}I_{23}+e_1e_4(I_{34}^2+I_{14}^2+I_{24}^2)=e_1^2(I_{12}^2+I_{13}^2+I_{23}^2)-\frac{e_1}{\sqrt{2}}(-2iI_{12}I_{13}+2I_{12}I_{23})$$
$$+\sqrt{2}e_4(I_{14}I_{34}+iI_{24}I_{34}).$$

[4] (system (21) in [22])

$$(s_1+is_2)^2=-2(x_1-e_1)(x_2-e_2)(x_3-e_3),$$

$$(s_1+is_2)(s_3+is_4)=-\frac{\partial}{\partial e_1}((x_1-e_1)(x_2-e_1)(x_3-e_1)),$$

$$2(s_1+is_2)(s_3-is_4)+(s_3+is_4)^2=-\frac{\partial^2}{\partial e_1^2}((x_1-e_1)(x_2-e_1)(x_3-e_1));$$

$$\mathcal{L}_1=\frac{1}{2}(2I_{34}I_{14}+2I_{12}I_{14}-2I_{23}I_{34}-2I_{12}I_{23}-I_{24}^2+I_{23}^2-I_{14}^2+I_{13}^2+2iI_{13}I_{14}+2iI_{23}I_{24}+2iI_{12}I_{24}$$
$$+2iI_{13}I_{34}+2iI_{24}I_{34}+2iI_{12}I_{13}),$$

$$\mathcal{L}_2 = -I_{14}^2 - I_{23}I_{34} - \frac{1}{4}I_{24}^2 + \frac{1}{4}I_{23}^2 + \frac{1}{4}I_{14}^2 - \frac{1}{4}I_{13}^2 - \frac{i}{2}I_{13}I_{23} - \frac{i}{2}I_{23}I_{24}\frac{i}{2}I_{14}I_{24} + \frac{i}{2}I_{13}I_{14} - iI_{24}I_{34} + iI_{13}I_{34}$$
$$- \frac{1}{2}I_{13}I_{34} - \frac{1}{2}I_{14}I_{23}.$$

We now show that each generic separable system on the three sphere uniquely determines a superintegrable system with nondegenerate potential. The proof is, in most part, analogous to that for the Euclidean case. Consider system (1111). If we have a superintegrable system that admits the symmetries $\mathcal{L}_1$, $\mathcal{L}_2$ for all values of the parameters $e_1, \ldots, e_4$ then it must have the basis of symmetries

$$\text{VIII} \quad \mathcal{S}_0 = I_{12}^2 + f_0, \quad \mathcal{S}_1 = I_{13}^2 + f_1, \quad \mathcal{S}_2 = I_{14}^2 + f_2, \quad \mathcal{S}_3 = I_{32}^2 + f_3,$$

$$\mathcal{S}_4 = I_{24}^2 + f_4, \quad \mathcal{S}_5 = I_{34}^2 + f_5.$$

The system of Bertrand-Darboux equations associated with these symmetries has rank five so the potential is uniquely determined. Solving the Bertrand-Darboux equations we obtain the nondegenerate potential on the three sphere

$$V(s) = \frac{\alpha}{s_1^2} + \frac{\beta}{s_2^2} + \frac{\gamma}{s_3^2} + \frac{\delta}{s_4^2}. \tag{42}$$

This potential is not Stäckel equivalent to a potential on Euclidean space.

Three of the four remaining systems can be obtained in the same way. However there is an alternative approach which enables us to obtain systems 2, 3, and 4 from 1 via well defined limiting processes. These are discussed elsewhere, e.g., Refs. 16 and 17, but we content ourselves with an example of how to obtain [211] from [1111]. If we make the transformations

$$s_1 \to \frac{1}{\sqrt{-\epsilon}}y_1, \quad s_2 \to \frac{1}{\sqrt{\epsilon}}(y_1 + \epsilon y_2), \quad \alpha \to -\sqrt{\beta}2\epsilon^2, \quad \beta \to \frac{\alpha}{\epsilon} - \frac{\beta}{2\epsilon^2}$$

then we deduce the relations

$$y_1^2 = -\frac{(u-e_1)(v-e_1)(w-e_1)}{(e_1-e_2)(e_1-e_3)}, \quad 2y_1y_2 = \frac{\partial}{\partial e_1}y_1^2.$$

The coordinates on the sphere can be represented using the identifications $y_1=(s_1+is_2)/\sqrt{2}$, $y_2=(s_1-is_2)/\sqrt{2}$, $y_3=s_3$, $y_4=s_4$ where $2y_1y_2+y_3^2+y_4^2=s_1^2+s_2^2+s_3^2+s_4^2=1$. We then transform the potential according to $\alpha/s_1^2+\beta/s_2^2+\gamma/s_3^2+\delta/s_4^2 \to \alpha/y_1^2+\beta y_2/y_1^3+\gamma/y_3^2+\delta/y_4^2$.

An exactly similar approach leads to the coordinates, constants of the motion and nondegenerate potential for the system [22]. Here the limit is taken in the form $e_2=e_1+\epsilon$, $e_4=e_3+\epsilon'$ where $\epsilon, \epsilon' \to 0$. For the system [31] we set $e_2=e_1+\epsilon$, $e_3=e_1+\epsilon'$ and allow $\epsilon, \epsilon' \to 0$, whereas for system [4] we set $e_2=e_1+\epsilon$, $e_3=e_1+\epsilon_1$, $e_4=e_1+\epsilon_2$ and allow $\epsilon, \epsilon_1, \epsilon_2 \to 0$. In all cases except [4] the requirement that we have separation for all values of the parameters e_j yields a set of six linearly independent second-order constants of the motion that can be verified to correspond to a nondegenerate superintegrable system. In the case [4] the constants of the motion do not depend on e_1 and we have only three independent symmetries. However, there is a unique potential that is obtained as the limit of the nondegenerate potential for case [1111]. By writing down the Bertrand-Darboux equations for this limit potential we can directly verify that it admits six linearly independent symmetries and is nondegenerate.

Theorem 8: *Each of the five generic three-sphere separable systems determines a unique nondegenerate superintegrable system that permits separation simultaneously for all values of the parameters e_j. For each of these systems there is a basis of five (strongly) functionally independent and six linearly independent second order symmetries. In addition to system [VIII] above there are*

the following superintegrable systems (nondegenerate potential, followed by a basis of constants of the motion):

I′ [211] (Stäckel equivalent to the Euclidean superintegrable system [I])

$$V=\frac{\alpha_1}{(s_1+is_2)^2}+\frac{\alpha_2(s_1-is_2)}{(s_1+is_2)^3}+\frac{\alpha_3}{s_3^2}+\frac{\alpha_4}{s_4^2};$$

$$\mathcal{S}_0=I_{12}^2+f_0,\quad \mathcal{S}_1=I_{34}^2+f_1,\quad \mathcal{S}_2=I_{13}^2+I_{23}^2+f_2, \tag{43}$$

$$\mathcal{S}_3=I_{14}^2+I_{24}^2+f_3,\quad \mathcal{S}_4=I_{13}(I_{13}+iI_{23})+f_4,\quad \mathcal{S}_5=I_{14}(I_{14}+iI_{24})+f_5.$$

II′ [22] (Stäckel equivalent to the Euclidean superintegrable system [II])

$$V=\frac{\alpha_1}{(s_1+is_2)^2}+\frac{\alpha_2(s_1-is_2)}{(s_1+is_2)^3}+\frac{\alpha_3}{(s_3+is_4)^2}+\frac{\alpha_4(s_3-is_4)}{(s_3+is_4)^3};$$

$$\begin{gathered}\mathcal{S}_0=I_{12}^2+f_0,\quad \mathcal{S}_1=I_{34}^2+f_1,\quad \mathcal{S}_2=I_{13}^2+I_{14}^2+I_{23}^2+I_{24}^2+f_2,\\ \mathcal{S}_3=I_{13}^2+I_{14}^2+i(I_{13}I_{23}+I_{14}I_{24})+f_3,\quad \mathcal{S}_4=I_{13}^2+I_{23}^2+i(I_{13}I_{14}+I_{23}I_{24})+f_4,\end{gathered} \tag{44}$$

$$\mathcal{S}_5=I_{13}^2+I_{24}^2+i(I_{13}I_{14}+I_{13}I_{23}-I_{14}I_{24}-I_{23}I_{24})-2I_{13}I_{24}-I_{12}I_{34}+f_5.$$

IV′ [31] (Stäckel equivalent to the Euclidean superintegrable system [IV])

$$V=\frac{\alpha_1}{(s_1+is_2)^2}+\frac{\alpha_2 s_3}{(s_1+is_2)^3}+\frac{\alpha_3(s_1^2+s_2^2-3s_3^2)}{(s_1+is_2)^4}+\frac{\alpha_4}{s_4^2};$$

$$\begin{gathered}\mathcal{S}_0=I_{12}^2+I_{13}^2+I_{23}^2+f_0,\quad \mathcal{S}_1=I_{14}^2+I_{24}^2+I_{34}^2+f_1,\quad \mathcal{S}_2=(I_{23}-iI_{13})^2+f_2,\\ \mathcal{S}_3=I_{12}(I_{23}-iI_{13})+f_3,\quad \mathcal{S}_4=I_{34}(I_{14}+iI_{24})+f_4,\end{gathered} \tag{45}$$

$$\mathcal{S}_5=I_{14}I_{34}-I_{12}I_{23}+i(I_{24}I_{34}+I_{12}I_{13})+f_5.$$

VI′ [4] (Stäckel equivalent to the Euclidean superintegrable system [VI])

$$\begin{aligned}V=&\frac{\alpha_1}{(s_1+is_2)^2}+\frac{\alpha_2(s_3+is_4)}{(s_1+is_2)^3}+\frac{\alpha_3\left[(s_1+is_2)(s_3-is_4)-\frac{3}{2}(s_3+is_4)^2\right]}{(s_1+is_2)^4}\\&+\frac{\alpha_4\left[(s_1+is_2)\left(s_1^2+s_2^2-\frac{3}{2}(s_3^2+s_4^2)+(s_3+is_4)^3\right]\right.}{(s_1+is_2)^5};\end{aligned}$$

$$\mathcal{S}_0=I_{12}^2+I_{13}^2+I_{14}^2+I_{23}^2+I_{24}^2+I_{34}^2+V,$$

$$\mathcal{S}_1=(I_{13}-I_{24}+iI_{23}+iI_{14})^2+f_1,$$

$$\begin{aligned}\mathcal{S}_2=&4(I_{23}I_{34}+I_{14}I_{34}+I_{13}I_{24})+4i(I_{24}I_{34}-I_{13}I_{34})+2i(I_{13}I_{23}-I_{14}I_{24}-I_{13}I_{14}+I_{23}I_{24})-2I_{12}I_{34}+I_{13}^2\\&+I_{24}^2-I_{14}^2-I_{23}^2+f_2,\end{aligned}$$

$$\mathcal{S}_3 = 2(I_{12}I_{23} + I_{23}I_{34} - I_{12}I_{14} - I_{14}I_{34}) - 2i(I_{23}I_{24} + I_{13}I_{14} + I_{13}I_{34} + I_{24}I_{34} + I_{12}I_{24} + I_{12}I_{13}) - I_{13}^2 + I_{24}^2 + I_{14}^2 - I_{23}^2 + f_3,$$

$$\mathcal{S}_4 = (I_{13} - I_{24} + iI_{23} + iI_{14})(I_{13} + I_{24} + iI_{23} - iI_{14}) + f_4,$$

$$\mathcal{S}_5 = (I_{13} - I_{24} + iI_{23} + iI_{14})(I_{34} - I_{12}) + f_5. \tag{46}$$

We also mention that the nongeneric superintegrable system on the three sphere with potential

$$\mathbf{00'} \quad V = \frac{\alpha}{(s_1 + is_2)^2} + \frac{\beta s_3}{(s_1 + is_2)^3} + \frac{\gamma s_4}{(s_1 + is_2)^3} + \frac{\delta(1 - 4s_3^2 - 4s_4^2)}{(s_1 + is_2)^4}$$

is Stäckel equivalent to the Euclidean superintegrable system [00].

F. Interbasis expansions for three-sphere systems

In analogy with our treatment of Euclidean systems, to proceed with the classification of nondegenerate superintegrable systems on the three sphere we need to look more closely at the relationship between a standard basis of symmetries and the natural basis written in terms of the angular momentum generators J_ℓ, K_ℓ $\ell = 1, \ldots, 3$. Then, near the regular point $\mathbf{T}$, i.e., (x, y, z), we have a basis of "natural symmetries" $J_1 = Yp_Z - Zp_Y$, $J_2 = Zp_X - Xp_Z$, $J_3 = Xp_Y - Yp_X$, $K_1 = K_X$, $K_2 = K_Y$, $K_3 = K_Z$. At the point itself we have $(1 + r^2/4)p_u = p_X$, $(1 + r^2/4)p_v = p_Y$, $(1 + r^2/4)p_w = p_Z$. Now suppose we have a three-sphere superintegrable system with nondegenerate potential. Then there will exist fifteen rational functions $A^{ij}[x, y, z]$, $B^{ij}[x, y, z]$, $C^{ij}[x, y, z]$, [with respect to the (X, Y, Z) coordinates and restricted to the point $(X, Y, Z) = (0, 0, 0)$, that completely characterize the superintegrable system]. In particular, only ten of these, (23), are linearly independent, see relations (A2), and they are subject to the five quadratic conditions (A3) with $G(X, Y, Z) = \ln \lambda = -2 \ln(1 + R^2/4)$. These functions are related to the symmetries $\mathcal{S} = \Sigma a^{ij} p_i p_j + W$ via the conditions (A1). The second order basis symmetries at the regular point $\mathcal{S}_{\mathbf{x}_0}^{(\ell m)}(\mathbf{X}) = \Sigma a_{(\ell m)}^{ij}(\mathbf{X}) p_i p_j + f_{(\ell m)}(\mathbf{X})$ take the form $\mathcal{S}_{\mathbf{x}_0}^{(\ell m)}(0, 0, 0) = p_i p_j + f_{(\ell m)}(0, 0, 0)$ when evaluated at the point. Thus we can expand each standard basis symmetry in a neighborhood of the point (x, y, z) in terms of the natural basis at the point via

$$\begin{aligned}\mathcal{S}_{\mathbf{x}_0}^{(\ell m)} = {} & K_\ell K_m + \alpha_3^{(\ell m)} J_1^2 + \alpha_4^{(\ell m)} J_2^2 + \alpha_5^{(\ell m)} J_3^2 + \alpha_6^{(\ell m)} K_1 J_1 + \alpha_7^{(\ell m)} K_2 J_2 + \alpha_8^{(\ell m)} K_1 J_2 + \alpha_9^{(\ell m)} K_1 J_3 \\ & + \alpha_{10}^{(\ell m)} K_2 J_1 + \alpha_{11}^{(\ell m)} K_2 J_3 + \alpha_{12}^{(\ell m)} K_3 J_1 + \alpha_{13}^{(\ell m)} K_3 J_2 + \alpha_{14}^{(\ell m)} J_1 J_2 + \alpha_{15}^{(\ell m)} J_1 J_3 \\ & + \alpha_{16}^{(\ell m)} J_2 J_3 + W^{(\ell m)}(\mathbf{X}),\end{aligned} \tag{47}$$

where the $\alpha_k^{(\ell m)}$ are constants in X, Y, Z but rational functions of the parameters x, y, z of the regular point. Here we are taking into account the identity $\Sigma_{h=1}^3 K_h J_h = 0$ and the fact that $K_h = p_h$ at the point $(X, Y, Z) = (0, 0, 0)$. Again, nondegenerate superintegrable system is uniquely determined by the ten numbers (23), and these numbers themselves are subject to five quadratic identities (A3). (Note that G and all of its first and second derivatives vanish when $X = Y = Z = 0$, except that $G_{ii} = -1$, $i = 1, 2, 3$. Further, we can use relations (40) to express the derivatives of V at the regular point with respect to the (X, Y, Z) coordinates in terms of derivatives with respect to (u, v, w). Thus the numbers (23) can be expressed as linear combinations of the corresponding numbers with respect to the (u, v, w) coordinates.)

Although all of the expansion constants $\alpha_k^{(\ell m)}$ can be expressed in terms of these ten numbers, we shall restrict ourselves to expanding the two symmetries

$$\begin{aligned}\mathcal{S}_{\mathbf{x}_0}^{(12)} = {} & K_1 K_2 + \alpha_3 J_1^2 + \alpha_4 J_2^2 + \alpha_5 J_3^2 + \alpha_6 K_1 J_1 + \alpha_7 K_2 J_2 + \alpha_8 K_1 J_2 + \alpha_9 K_1 J_3 + \alpha_{10} K_2 J_1 + \alpha_{11} K_2 J_3 \\ & + \alpha_{12} K_3 J_1 + \alpha_{13} K_3 J_2 + \alpha_{14} J_1 J_2 + \alpha_{15} J_1 J_3 + \alpha_{16} J_2 J_3 + W^{(12)}(\mathbf{X}),\end{aligned} \tag{48}$$

$$\mathcal{S}^{(13)}_{\mathbf{x}_0} = K_1K_3 + \alpha'_3J_1^2 + \alpha'_4J_2^2 + \alpha'_5J_3^2 + \alpha'_6K_1J_1 + \alpha'_7K_2J_2 + \alpha'_8K_1J_2 + \alpha'_9K_1J_3 + \alpha'_{10}K_2J_1 + \alpha'_{11}K_2J_3$$
$$+ \alpha'_{12}K_3J_1 + \alpha'_{13}K_3J_2 + \alpha'_{14}J_1J_2 + \alpha'_{15}J_1J_3 + \alpha'_{16}J_2J_3 + W^{(13)}(\mathbf{X}). \tag{49}$$

(Here, $\alpha_s=\alpha_s^{(12)}$, $\alpha'_s=\alpha_s^{(13)}$.) Since the six Bertrand-Darboux equations for these two symmetries have rank five, the symmetries completely determine the A^{ij}, B^{ij}, C^{ij}, hence the superintegrable system.

From (39)–(41) we have (with $J_w=up_v-vp_u$ and cyclic permutations)

$$J_1 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1+\frac{x^2}{4}-\frac{y^2}{4}-\frac{z^2}{4}\right)J_u + \frac{zx}{2}J_w + \frac{yx}{2}J_v - yK_w + zK_v\right),$$

$$J_2 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1-\frac{x^2}{4}+\frac{y^2}{4}-\frac{z^2}{4}\right)J_v + \frac{xy}{2}J_u + \frac{zy}{2}J_w - zK_u + xK_w\right),$$

$$J_3 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1-\frac{x^2}{4}-\frac{y^2}{4}+\frac{z^2}{4}\right)J_w + \frac{yz}{2}J_v + \frac{xz}{2}J_u - xK_v + yK_u\right),$$

$$K_1 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1+\frac{x^2}{4}-\frac{y^2}{4}-\frac{z^2}{4}\right)K_u + \frac{yx}{2}K_v + \frac{zx}{2}K_w - yJ_w + zJ_v\right),$$

$$K_2 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1-\frac{x^2}{4}+\frac{y^2}{4}-\frac{z^2}{4}\right)K_v + \frac{xy}{2}K_u + \frac{zy}{2}K_w - zJ_u + xJ_w\right),$$

$$K_3 = \frac{1}{1+\frac{r^2}{4}}\left(\left(1-\frac{x^2}{4}-\frac{y^2}{4}+\frac{z^2}{4}\right)K_w + \frac{xz}{2}K_u + \frac{yz}{2}K_v - xJ_v + yJ_u\right).$$

The inverse of these relations takes almost exactly the same form. Now, suppose we have a nondegenerate three-sphere superintegrable system with potential V, that is separable with respect to some orthogonal coordinates. (As every superintegrable system is multiseparable, we know that such coordinates exist.) By performing an Euclidean transformation, if necessary, we can assume that the separable coordinates are in some standard form determined by two constants of the motion in involution, $L_1=\Sigma a^{ij}p_ip_j+f_1$, $L_2=\Sigma b^{ij}p_ip_j+f_2$. Clearly, L_1 and L_2 lie in the six-dimensional space of second order symmetries for the superintegrable system. Thus, the quadratic form a^{ij}, for example, satisfies the three Bertrand-Darboux equations for potential V. Since V is nondegenerate we can express the second derivatives $V_{jj}-V_{kk}$ and V_{jk} with $j\neq k$ in the Bertrand-Darboux equations as linear combinations of the first derivatives V_h. Equating coefficients of V_1, V_2, V_3 separately in each of the three equations, we end up with nine linear conditions for the ten constants $A^{22},\ldots,B^{23}$ at each regular point. If we choose the Cartesian-like coordinates X, Y, Z that vanish at the regular point, then we obtain the same 18 conditions as in the Euclidean case. Indeed, the first derivatives G_i all vanish at the regular point.

For the second symmetry there will be nine more such linear conditions with a^{ij} replaced by b^{ij}. Thus we will have eighteen linear equations (not linearly independent) for the ten quantities $A^{22},\ldots,B^{23}$.

The five fundamental quadratic identities (A3) are identical to those for the Euclidean case. This is because the only nonzero terms in the metric for the three sphere are $G_{ii}=-1$ and all such terms occur in the form $G_{ii}-G_{jj}=0$ in the five quadratic conditions.

Another source of conditions is obtained by writing the symmetry L_1 in terms of the standard basis: $a^{ij}(\mathbf{x})=\Sigma_{\ell\leqslant m}a^{\ell m}(\mathbf{x}_0)\mathcal{A}^{ij}_{(\ell,m)}(\mathbf{x})$, where $\mathcal{A}^{ij}_{(\ell,m)}$ is the quadratic form associated with the standard basis symmetry $\mathcal{S}^{(\ell,m)}$ at $\mathbf{x}_0$. Expanding both sides of this equation in terms of the natural

basis we obtain linear and quadratic conditions on the ten basic quantities. In this case there is a difference between the Euclidean and three-sphere expressions. For example if we equate coefficients of the natural basis element J_1J_2 we find the quadratic conditions for L_1 and L_2

$$-a_{12}^{33}(\mathbf{x}_0)=\sum_{\ell\leqslant m}a^{\ell m}(\mathbf{x}_0)\alpha_{14}^{(\ell m)},\quad -b_{12}^{33}(\mathbf{x}_0)=\sum_{\ell\leqslant m}b^{\ell m}(\mathbf{x}_0)\alpha_{14}^{(\ell m)}. \tag{50}$$

It is no longer true that $-a_{12}^{33}=2a_{23}^{13}$ as in the Euclidean case. The expressions for the terms $\alpha_{14}^{(\ell m)}$ can be computed from the basic formulas (A1). They involve the terms G_{ii} and differ from the Euclidean case. For example, from (A1) and formulas for the derivatives $\partial_i A^{jk}$, $\partial_i B^{jk}$, $\partial_i C^{jk}$ we can calculate $-a_{12}^{33}(\mathbf{x}_0)$ corresponding to the basis symmetry $\mathcal{S}^{(12)}$ and obtain

$$\begin{aligned}-3\alpha_{14}^{(12)}=&\tfrac{1}{3}B^{22}C^{23}-\tfrac{2}{3}(C^{13})^2-\tfrac{2}{3}C^{13}A^{22}+\tfrac{1}{6}(A^{23})^2+\tfrac{1}{3}C^{33}\left(\tfrac{7}{2}B^{23}-2C^{22}\right)+\tfrac{3}{2}-\tfrac{1}{2}(B^{33})^2+\tfrac{5}{6}B^{33}B^{22}\\&+\tfrac{5}{6}(B^{12})^2+A^{33}B^{12}-\tfrac{1}{2}(B^{23})^2+\tfrac{1}{6}(A^{12})^2-\tfrac{1}{3}B^{33}A^{12}-\tfrac{1}{6}A^{22}A^{33}+\tfrac{1}{6}(A^{33})^2-\tfrac{1}{6}C^{33}A^{13}.\end{aligned}$$

Though there are many other quadratic conditions for L_1, L_2 to belong to the symmetry algebra, we shall use only these two.

G. Significance of generic three-sphere systems

Suppose we have a nondegenerate superintegrable system that admits separation for some special choice of ellipsoidal coordinates [1111]. (Here we do *not* assume that the system separates for all values of the parameters c, e_1, e_2, e_3, e_4, but only for one value.) By performing an Euclidean transformation and a change of scale we can assume that the coordinates are in the standard form [1111] in our table and that $e_1=0$, $e_2=1$, $e_3=a$, and $e_4=b$ where a, b are any fixed complex numbers such that $ab(a-1)(b-1)(b-a)\neq 0$. We follow the same method given before in the Euclidean case. We evaluate the a^{ij}, b^{ij} at any regular point with coordinates (x, y, z). Substituting these expressions into the eighteen linear conditions, with the help of MAPLE, we find that there are exactly seven independent linear conditions. Thus the ten quantities $A^{22}, \ldots, B^{23}$ can be expressed linearly in terms of three of these quantities. Substituting this result into the five fundamental quadratic identities (A3) we find that these identities yield exactly two solutions. Finally we substitute each of these solutions into (50) and find conditions that rule out one of these solutions. Thus only one solution exists and it must be the one that we already knew: System [VIII] that separates simultaneously for all choices of the parameters $e_1, \ldots, e_4$. What was far from obvious is the fact that *no other* nondegenerate superintegrable system separates for *any* special case of ellipsoidal coordinates on the three sphere.

Theorem 9: *A three-sphere nondegenerate superintegrable system admits separation in a special case of the generic coordinates [1111], [211], [22], [31], or [4], respectively, if and only if it is equivalent via a complex rotation to system [VII],* [*I′*], [*II′*], [*IV′*], *or* [*VI′*], *respectively*.

We have indicated the proof for coordinates [1111]. The other generic coordinates are Stäckel transforms of generic coordinates in Euclidean space so the proof for them follows immediately from Theorem 7.

APPENDIX

This is a list of some important results from Ref. 3. Using the nondegenerate potential condition and the Bertrand-Darboux equations we can solve for all of the first partial derivatives a_i^{jk} of a quadratic symmetry to obtain the defining conditions [with $\lambda=\exp(G)$]

$$a_1^{11}=-G_1a^{11}-G_2a^{12}-G_3a^{13},$$

$$a_2^{22}=-G_1a^{12}-G_2a^{22}-G_3a^{23},$$

$$a_3^{33}=-G_1a^{13}-G_2a^{23}-G_3a^{33},$$

$$3a_1^{12} = a^{12}A^{22} - (a^{22} - a^{11})A^{12} - a^{23}A^{13} + a^{13}A^{23} + G_2a^{11} - 2G_1a^{12} - G_2a^{22} - G_3a^{23},$$

$$3a_2^{11} = -2a^{12}A^{22} + 2(a^{22} - a^{11})A^{12} + 2a^{23}A^{13} - 2a^{13}A^{23} - 2G_2a^{11} + G_1a^{12} - G_2a^{22} - G_3a^{23},$$

$$3a_3^{13} = -a^{12}C^{23} + (a^{33} - a^{11})C^{13} + a^{23}C^{12} - a^{13}C^{33} - G_1a^{11} - G_2a^{12} - 2G_3a^{13} + G_1a^{33},$$

$$3a_1^{33} = 2a^{12}C^{23} - 2(a^{33} - a^{11})C^{13} - 2a^{23}C^{12} + 2a^{13}C^{33} - G_1a^{11} - G_2a^{12} + G_3a^{13} - 2G_1a^{33},$$

$$3a_2^{23} = a^{23}(B^{33} - B^{22}) - (a^{33} - a^{22})B^{23} - a^{13}B^{12} + a^{12}B^{13} - G_1a^{13} - 2G_2a^{23} - G_3a^{33} + G_3a^{22},$$

$$3a_3^{22} = -2a^{23}(B^{33} - B^{22}) + 2(a^{33} - a^{22})B^{23} + 2a^{13}B^{12} - 2a^{12}B^{13} - G_1a^{13} + G_2a^{23} - G_3a^{33} - 2G_3a^{22},$$

$$3a_1^{13} = -a^{23}A^{12} + (a^{11} - a^{33})A^{13} + a^{13}A^{33} + a^{12}A^{23} - 2G_1a^{13} - G_2a^{23} - G_3a^{33} + G_3a^{11},$$

$$3a_3^{11} = 2a^{23}A^{12} + 2(a^{33} - a^{11})A^{13} - 2a^{13}A^{33} - 2a^{12}A^{23} + G_1a^{13} - G_2a^{23} - G_3a^{33} - 2G_3a^{11},$$

$$3a_2^{33} = -2a^{13}C^{12} + 2(a^{22} - a^{33})C^{23} + 2a^{12}C^{13} - 2a^{23}(C^{22} - C^{33}) - G_1a^{12} - G_2a^{22} + G_3a^{23} - 2G_2a^{33},$$

$$3a_3^{23} = a^{13}C^{12} - (a^{22} - a^{33})C^{23} - a^{12}C^{13} - a^{23}(C^{33} - C^{22}) - G_1a^{12} - G_2a^{22} - 2G_3a^{23} + G_2a^{33},$$

$$3a_2^{12} = -a^{13}B^{23} + (a^{22} - a^{11})B^{12} - a^{12}B^{22} + a^{23}B^{13} - G_1a^{11} - 2G_2a^{12} - G_3a^{13} + G_1a^{22},$$

$$3a_1^{22} = 2a^{13}B^{23} - 2(a^{22} - a^{11})B^{12} + 2a^{12}B^{22} - 2a^{23}B^{13} - G_1a^{11} + G_2a^{12} - G_3a^{13} - 2G_1a^{22},$$

$$3a_1^{23} = a^{12}(B^{23} + C^{22}) + a^{11}(B^{13} + C^{12}) - a^{22}C^{12} - a^{33}B^{13} + a^{13}(B^{33} + C^{23}) - a^{23}(C^{13} + B^{12}) - 2G_1a^{23} + G_2a^{13} + G_3a^{12}.$$

$$3a_3^{12} = a^{12}(-2B^{23} + C^{22}) + a^{11}(C^{12} - 2B^{13}) - a^{22}C^{12} + 2a^{33}B^{13} + a^{13}(-2B^{33} + C^{23}) + a^{23}(-C^{13} + 2B^{12}) - 2G_3a^{12} + G_2a^{13} + G_1a^{23}.$$

$$3a_2^{13} = a^{12}(B^{23} - 2C^{22}) + a^{11}(B^{13} - 2C^{12}) + 2a^{22}C^{12} - a^{33}B^{13} + a^{13}(B^{33} - 2C^{23}) + a^{23}(2C^{13} - B^{12}) - 2G_2a^{13} + G_1a^{23} + G_3a^{12}, \tag{A1}$$

plus the linear relations

$$A^{23} = B^{13} = C^{12}, \quad B^{23} - A^{31} - C^{22} = 0,$$
$$B^{12} - A^{22} + A^{33} - C^{13} = 0, \quad B^{33} + A^{12} - C^{23} = 0. \tag{A2}$$

Using the linear relations we can express C^{12}, C^{13}, C^{22}, C^{23}, and B^{13} in terms of the remaining ten functions. Finally, requiring that the integrability conditions for (A1) hold identically, we obtain exactly five quadratic identities for the ten independent functions:

$$-A^{23}B^{23} - A^{12}A^{23} + A^{13}B^{12} + B^{22}A^{23} + B^{23}A^{33} + \frac{1}{2}A^{22}G_3 - \frac{1}{2}A^{33}G_3 - \frac{1}{2}B^{12}G_3 - \frac{1}{2}G_1G_3 - \frac{1}{2}A^{13}G_1 + \frac{3}{2}G_{13} - \frac{1}{2}A^{23}G_2 - A^{22}B^{23} = 0, \tag{A3a}$$

$$(A^{33})^2 + B^{12}A^{33} - A^{33}A^{22} - B^{33}A^{12} - C^{33}A^{13} + B^{22}A^{12} - B^{12}A^{22} + A^{13}B^{23} - (A^{12})^2 + \frac{3}{2}G_{22} - \frac{1}{2}G_y^2$$
$$- \frac{3}{2}G_{33} + \frac{1}{2}A^{13}G_3 + \frac{1}{2}B^{33}G_2 - \frac{1}{2}A^{22}G_1 + \frac{1}{2}A^{33}G_1 - \frac{1}{2}B^{23}G_3 - \frac{1}{2}B^{22}G_2 + \frac{1}{2}C^{33}G_3 + \frac{1}{2}(G_3)^2 = 0, \tag{A3b}$$

$$- (B^{33})^2 - B^{33}A^{12} + B^{33}B^{22} + B^{12}A^{33} + B^{23}C^{33} - (B^{23})^2 + (B^{12})^2 + \frac{1}{2}(G_1)^2 - \frac{3}{2}G_{11} + \frac{3}{2}G_{33}$$
$$- \frac{1}{2}B^{33}G_2 - \frac{1}{2}A^{33}G_1 - \frac{1}{2}(G_3)^2 - \frac{1}{2}C^{33}G_3 = 0, \tag{A3c}$$

$$- B^{12}A^{23} - A^{33}A^{23} + A^{13}B^{33} + A^{12}B^{23} + \frac{3}{2}G_{23} - \frac{1}{2}A^{23}G_1 - \frac{1}{2}A^{12}G_3 - \frac{1}{2}B^{23}G_2 - \frac{1}{2}G_2G_3$$
$$- \frac{1}{2}B^{33}G_3 = 0, \tag{A3d}$$

$$A^{12}B^{12} + C^{33}A^{23} - A^{23}B^{23} + B^{33}A^{22} - B^{33}A^{33} + \frac{3}{2}G_{12} - \frac{1}{2}G_1G_2 - \frac{1}{2}A^{12}G_1 - \frac{1}{2}B^{12}G_2 - \frac{1}{2}A^{23}G_3 = 0. \tag{A3e}$$

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The performance of the OSRC method for concentric penetrable circular cylinder

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In this paper we consider the scattering of a wave by concentric penetrable circular cylinder to examine the performance of higher order SRCs up to the L_4 operator in two dimensions. We assume that in the rectangular Cartesian axes, (x,y,z), the z axis coincides with the axis of a cylinder and an incident wave propagates in a direction perpendicular to the cylinder. All the field quantities are then independent of z. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2186923]

I. INTRODUCTION

Approximate techniques have been introduced to study the scattering of waves by obstacles. The aim of these methods is to reduce the labor involved in solving an integral equation or any appropriate formulation of the problem. The on-surface radiation condition (OSRC) method, has been devised by Kriegsmann, Taflove, and Umashankar, to investigate electromagnetic scattering problems involving cylindrical convex objects. The main concept in this method is the application of a radiation condition, connecting the field and its normal derivative, directly onto the surface of the scatterer to determine approximately the surface field or its derivative in terms of the given field. The calculation of the scattered field is then reduced to quadratures. As is demonstrated in references for a wide variety of two-dimensional obstacles, results are in confirmity with exact analysis or numerical methods over a wide range of frequencies. The approach has been employed to derive radiation boundary conditions (RBCs). The method is based on the idea of killing the terms of the expansion of the scattering field satisfying the Helmholtz equation and Sommerfeld radiation condition. An nth order RBC operator which annihilates the first n terms in the expansion is obtained either on a large circular cylinder enclosing a cylindrical convex object, or on a large sphere enclosing a finite convex object, depending on the geometrical dimensions of the problem. These RBCs can be generalized so that they can be used in the OSRC method for constructing the approximate solution of a scattering problem involving an arbitrary convex object. Until now, only the first and second order RBCs have been generalized and used in conjunction with the OSRC method.[1–9] It seems that the main obstacle to such a generalization is the difficulty in interpreting the terms properly.

In this work we apply the higher-order SRCs to scattering plane waves by a concentric penetrable circular cylinder. The results are compared with those of second- and fourth-order SRCs.

This paper is organized as follows. The formulation of the problem is described in Sec. II. In Sec. III the exact and approximate solutions of these equations with OSRC method are presented and calculated and the Appendix has some concluding remarks. In the Appendix the higher order radiation conditions are found.

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II. FORMULATION

Elliptic boundary value problems governed by the Helmholtz equation in exterior regions arise in many branches of continuum physics. An example is the scattering of a time harmonic acoustic wave u^i by an obstacle occupying the region $\mathcal{B}_2$ with a boundary surface Σ_1. Let us denote the region outside Σ_1 by $\mathcal{B}_1$. We assume that $\mathcal{B}_1$ is a homogeneous isotropic medium with sound speed c_1 and constant density ρ_1.

The scattering of plane waves by a two-layered penetrable circular cylinder is examined. The concentric case is considered. We denote the outer and inner layers by $\mathcal{B}_2$ with sound speed c_2 and constant density ρ_2 and $\mathcal{B}_3$ with sound speed c_3 and constant density ρ_3, respectively. The interface between them is the circular cylinder Σ_2 of radius r_2. The radius of the circular cylinder between the exterior region $\mathcal{B}_1$ and the region $\mathcal{B}_2$ is r_1, i.e., $\mathcal{B}_1=\{r>r_1\}$, $\mathcal{B}_2=\{r_1<r<r_2\}$, $\mathcal{B}_3=\{r<r_3\}$. A plane wave incident in the direction of the positive x axis can be written as $u^i=e^{-ik_1 r\cos\theta}=\sum_{n=-\infty}^{\infty}J_n(k_1r)e^{in[\theta-(\pi/2)]}$.

The scattering problem for a two layered cylinder is described by the following equations and boundary conditions:

$$\nabla^2 u_l + k_l^2 u_l = 0, \quad \mathbf{x}\in\mathcal{B}_l \quad \text{for } k_l=\frac{w}{c_l}, \quad l=1,2,3, \tag{2.1}$$

$$u_1+u^i=u_2 \quad \text{and} \quad \frac{\partial}{\partial r}(u_1+u^i)=\xi_1\frac{\partial u_2}{\partial r} \quad \text{on } \Sigma_1, \tag{2.2}$$

$$u_2=u_3 \quad \text{and} \quad \frac{\partial u_2}{\partial r}=\xi_2\frac{\partial u_3}{\partial r} \quad \text{on } \Sigma_2, \tag{2.3}$$

where $\zeta_1=\rho_1/\rho_2$, $\zeta_2=\rho_2/\rho_3$. In addition, at infinity the scattered field u_1 must have the form of a radiating wave, i.e., the following Sommerfeld radiation condition must be satisfied:

$$\lim_{r\to\infty} r^{1/2}\left(\frac{\partial u_1}{\partial r}+ik_1u_1\right)=0. \tag{2.4}$$

The solutions for u_1, u_2, and u_3 are defined as follows:

$$u_1=\sum_{n=-\infty}^{\infty}a_nH_n(k_1r)e^{in[\theta-(\pi/2)]}, \tag{2.5}$$

$$u_2=\sum_{n=-\infty}^{\infty}[b_nJ_n(k_2r)+c_nH_n(k_2r)]e^{in[\theta-(\pi/2)]}, \tag{2.6}$$

$$u_3=\sum_{n=-\infty}^{\infty}d_nJ_n(k_3r)e^{in[\theta-(\pi/2)]}. \tag{2.7}$$

Using boundary conditions (2.2) and (2.3) the coefficients a_n, b_n, c_n, and d_n are found to be

$$J_n(k_1r_1)+a_nH_n(k_1r_1)=b_nJ_n(k_2r_1)+c_nH_n(k_2r_1), \tag{2.8}$$

$$k_1J_n'(k_1r_1)+a_nk_1H_n'(k_1r_1)=\xi_1k_2b_nJ_n'(k_2r_1)+\xi_1k_2c_nH_n'(k_2r_1), \tag{2.9}$$

$$b_nJ_n(k_2r_2)+c_nH_n(k_2r_2)=d_nJ_n(k_3r_2), \tag{2.10}$$

$$k_2 b_n J_n'(k_2 r_2) + k_2 c_n H_n'(k_2 r_2) = \xi_2 k_3 d_n J_n'(k_3 r_2), \tag{2.11}$$

$$a_n = \frac{\Delta_1}{\Delta}, \quad b_n = \frac{\Delta_2}{\Delta}, \quad c_n = \frac{\Delta_3}{\Delta}, \quad d_n = \frac{\Delta_4}{\Delta}, \tag{2.12}$$

where

$$\begin{aligned}\Delta = {} & [\xi_1 k_2 H_n(k_1 r_1) J_n'(k_2 r_1) - k_1 H_n'(k_1 r_1) J_n(k_2 r_1)][\xi_2 k_3 H_n(k_2 r_2) J_n'(k_3 r_2) - k_2 H_n'(k_2 r_2) J_n(k_3 r_2)] \\ & - [\xi_1 k_2 H_n(k_1 r_1) H_n'(k_2 r_1) - k_1 H_n'(k_1 r_1) H_n(k_2 r_1)][\xi_2 k_3 J_n(k_2 r_2) J_n'(k_3 r_2) - k_2 J_n'(k_2 r_2) J_n(k_3 r_2)],\end{aligned} \tag{2.13}$$

$$\begin{aligned}\Delta_1 = {} & [\xi_1 k_2 J_n(k_1 r_1) H_n'(k_2 r_1) - k_1 J_n'(k_1 r_1) H_n(k_2 r_1)][\xi_2 k_3 J_n(k_2 r_2) J_n'(k_3 r_2) - k_2 J_n'(k_2 r_2) J_n(k_3 r_2)] \\ & - [\xi_1 k_2 J_n(k_1 r_1) J_n'(k_2 r_1) - k_1 J_n'(k_1 r_1) J_n(k_2 r_1)][\xi_2 k_3 H_n(k_2 r_2) J_n'(k_3 r_2) - k_2 H_n'(k_2 r_2) J_n(k_3 r_2)],\end{aligned} \tag{2.14}$$

$$\Delta_2 = \frac{2i}{\pi r_1}[\xi_2 k_3 H_n(k_2 r_2) J_n'(k_3 r_2) - k_2 H_n'(k_2 r_2) J_n(k_3 r_2)],$$

$$\Delta_3 = \frac{-2i}{\pi r_1}[\xi_2 k_3 J_n(k_2 r_2) J_n'(k_3 r_2) - k_2 J_n'(k_2 r_2) J_n(k_3 r_2)], \tag{2.15}$$

$$\Delta_4 = \frac{-4}{\pi^2 r_1 r_2}.$$

The radiation boundary conditions have been derived at the phase fronts and on these surfaces establish approximate (asymptotic) between the derivative of u in the direction of the normal to u and their tangential derivatives. Hence these relations will be valid wherever there is a wave front. Kriegsmann, Taflove, and Umashankar[3] assume that these expressions are also valid on Σ_1 and replace $\partial/\partial n$ with $\partial/\partial s$ at $L_1 u$ and $L_2 u$. Therefore at the representation in two dimensions of the radiation boundary conditions given replacing $\partial/\partial s$ by $\partial/\partial n$ and writing $u = u_1$, the following relation is given between the normal derivative of scattering field and tangential derivative on Σ_1.

The relation

$$\frac{\partial u_1}{\partial n} = \Lambda^{(m)} u_1, \quad m = 2,3,4 \tag{2.16}$$

based on behavior local to a wave front is derived where $\Lambda^{(m)} u_1$ denotes all terms out of $\partial u/\partial s$ at radiation boundary conditions. Boundary condition on Σ_1 from (2.4) is

$$u_1 = u_2 - u^i, \quad \frac{\partial u_1}{\partial n} = \zeta \frac{\partial u_2}{\partial n} - \frac{\partial u^i}{\partial n}.$$

Then the relation is obtained as follows:

$$\zeta \frac{\partial u_2}{\partial n} - \Lambda^{(m)} u_2 = \frac{\partial u^i}{\partial n} - \Lambda^{(m)} u^i. \tag{2.17}$$

$\nabla^2 u_2 + k_2^2 u_2 = 0$ and (2.17) defines an interior problem for u_2. This condition and

$$u_2 = u_3, \quad \frac{\partial u_2}{\partial n} = \zeta_2 \frac{\partial u_3}{\partial n}, \quad \text{on } r = r_1$$

conditions constitute an interior elliptic boundary value problem with

$$\nabla^2 u_l + k_l^2 u_l = 0, \quad \mathbf{x} \in \mathcal{B}_l, \quad l = 2,3$$

equations. Defining $v_2(\theta) = u_2(a, \theta)$ and $w_2(\theta) = (1/k_2)(\partial u_2/\partial r)$ the boundary conditions (2.2) can be written as

$$v_1 + v^i = v_2 \quad \text{and} \quad k_1(w_1 + w^i) = k_2 \zeta w_2. \tag{2.18}$$

Using these equations, v_1 and w_1 can be eliminated from the SRCs given in the Appendix by (A13) to obtain

$$\alpha_1^{(m)} \frac{d^4 v_2}{\mathrm{d}\theta^4} + \alpha_2^{(m)} \frac{d^2 v_2}{\mathrm{d}\theta^2} + \alpha_3^{(m)} v_2 - \frac{k_2}{k_1} \zeta \left\{ \alpha_4^{(m)} \frac{d^2 w_2}{\mathrm{d}\theta^2} + \alpha_5^{(m)} w_2 \right\}$$

$$= \alpha_1^{(m)} \frac{d^4 v^i}{\mathrm{d}\theta^4} + \alpha_2^{(m)} \frac{d^2 v^i}{\mathrm{d}\theta^2} + \alpha_3^{(m)} v^i - \frac{k_2}{k_1} \zeta \left\{ \alpha_4^{(m)} \frac{d^2 w^i}{\mathrm{d}\theta^2} + \alpha_5^{(m)} w^i \right\}. \tag{2.19}$$

The use of SRCs (A13) together with (2.18) yields the impedance conditions (2.19) with $\zeta = \xi_1$. The impedance condition (2.19) together with

$$\nabla^2 u_l + k_l^2 u_l = 0, \quad \mathbf{x} \in \mathcal{B}_l, \quad l = 2,3, \tag{2.20}$$

$$u_2 = u_3 \quad \text{and} \quad \frac{\partial u_2}{\partial r} = \xi_2 \frac{\partial u_3}{\partial r}. \tag{2.21}$$

constitute an interior boundary value problem for u_2 and u_3,

$$u_2 = \sum_{n=-\infty}^{\infty} [B_n J_n(k_2 r) + C_n H_n(k_2 r)] e^{in[\theta - (\pi/2)]}, \tag{2.22}$$

$$u_3 = \sum_{n=-\infty}^{\infty} D_n J_n(k_3 r) e^{in[\theta - (\pi/2)]}. \tag{2.23}$$

Once u_2 and u_3 have been determined, v_1 and w_1 are found from (2.18). If we use boundary conditions (2.2) and (2.3) the coefficients B_n, C_n, and D_n are found.

For the approximate solution, the coeffcients B_n, C_n, and D_n are found using (2.17) and (2.19) ($\varepsilon = k_1 r_1$),

$$\Theta^{(l)}(\varepsilon)\{B_n J_n(k_2 r_1) + C_n H_n(k_2 r_1)\} - \frac{k_2}{k_1} \xi_1 \{B_n J_n'(k_2 r_1) + C_n H_n'(k_2 r_1)\}$$

$$= \Theta^{(l)}(\varepsilon) J_n(\varepsilon) - J_n'(\varepsilon), \tag{2.24}$$

$$B_n J_n(k_2 r_2) + k_2 C_n H_n(k_2 r_2) = D_n J_n(k_3 r_2), \tag{2.25}$$

$$k_2 B_n J_n'(k_2 r_2) + k_2 C_n H_n'(k_2 r_2) = \xi_2 k_3 D_n J_n'(k_3 r_2), \tag{2.26}$$

$$B_n = \frac{\tilde{\Delta}_2}{\tilde{\Delta}}, \quad C_n = \frac{\tilde{\Delta}_3}{\tilde{\Delta}}, \quad D_n = \frac{\tilde{\Delta}_4}{\tilde{\Delta}}, \tag{2.27}$$

where

$$\tilde{\Delta} = [\xi_1 k_2 J_n'(k_2 r_1) - k_1 \Theta^{(l)}(\varepsilon) J_n(k_2 r_1)][\xi_2 k_3 H_n(k_2 r_2) J_n'(k_3 r_2) - k_2 H_n'(k_2 r_2) J_n(k_3 r_2)] - [\xi_1 k_2 H_n'(k_2 r_1) - k_1 \Theta^{(l)}(\varepsilon) H_n(k_2 r_1)][\xi_2 k_3 J_n(k_2 r_2) J_n'(k_3 r_2) - k_2 J_n'(k_2 r_2) J_n(k_3 r_2)], \tag{2.28}$$

$$\tilde{\Delta}_2 = -k_1[\Theta^{(l)}(\varepsilon) J_n(\varepsilon) - J_n'(\varepsilon)][\xi_2 k_3 H_n(k_2 r_2) J_n'(k_3 r_2) - k_2 H_n'(k_2 r_2) J_n(k_3 r_2)], \tag{2.29}$$

$$\tilde{\Delta}_3 = k_1[\Theta^{(l)}(\varepsilon) J_n(\varepsilon) - J_n'(\varepsilon)][\xi_2 k_3 J_n(k_2 r_2) J_n'(k_3 r_2) - k_2 J_n'(k_2 r_2) J_n(k_3 r_2)] \tag{2.30}$$

$$\tilde{\Delta}_4 = k_1 k_2[\Theta^{(l)}(\varepsilon) J_n(\varepsilon) - J_n'(\varepsilon)][J_n(k_2 r_2) H_n'(k_2 r_2) - J_n'(k_2 r_2) J_n(k_2 r_2)], \tag{2.31}$$

and

$$\Theta^{(m)}(\varepsilon) = -\frac{n^4 \alpha_1^{(m)} - n^2 \alpha_2^{(m)} + \alpha_3^{(m)}}{n^2 \alpha_4^{(m)} - \alpha_5^{(m)}}. \tag{2.32}$$

III. COMPARISON

It is observed that the replacement of $\Theta^{(m)}(\varepsilon)$ by $H_n'(\varepsilon)/H_n(\varepsilon)$ in the approximate solutions and using $H_n(z)J_n'(z) - H_n'(z)J_n(z) = 2i/\pi z$ the Wronskian relation also yields the exact ones. It is shown that the expressions $\tilde{\Delta}$, $\tilde{\Delta}_2$, $\tilde{\Delta}_3$, $\tilde{\Delta}_4$, are transformed to Δ, Δ_2, Δ_3, Δ_4. Thus, for the problem under consideration the SRC method is equivalent to introducing the approximation

$$\frac{H_n'(\varepsilon)}{H_n(\varepsilon)} \approx \Theta^{(m)}(\varepsilon) \tag{3.1}$$

and therefore, this result is independent of the boundary conditions prescribed on the surface of the circular cylinder Σ_1. Hence, the accuracy of the method for the cylinder problems will depend on the accuracy of the approximation in (3.1). Hence, the accuracy of the method for the cylinder problems will depend on the accuracy of the approximation in (3.1).

Comparisons were made between the exact answer of the problem and the SRC solutions. It is observed that introductions of higher-order radiation conditions improve the approximation considerably in comparison to results obtained by the use of a second-order radiation condition, especially in cases which creeping waves are less pervasive.

The characterization of the region and the wave within this region given in Fig. 1 and graphs (a) and (b) for $\varepsilon = 1, 10$, respectively, are as follows: $k_3 = (c_1/c_3)k_1$, $k_2 = (c_1/c_2)k_1$, $\xi_1 = \rho_1/\rho_2$, $\xi_2 = \rho_2/\rho_3$,

$$\rho_1 = 1.2, \quad c_1 = 340, \quad \rho_2 = 1000, \quad c_2 = 1480, \quad \rho_3 = 1200, \quad c_3 = 1600. \tag{3.2}$$

Whenever the regions are, respectively, air, water, and a region denser than water from outside to inside the results of the second and fourth order SRCs for the parameters in (3.2) are depicted together with the exact curve for $\varepsilon = 1, 10$. It can be seen that the performance of the higher-order SRCs give better results than the second-order SRC. Note that the existence of dissipation improves the results to a certain extent. It should be noted that in the cases given in the graphs the concentric penetrable cylinder behaves nearly as a hard cylinder.[10]

The characterization of the region and the wave within this region given in Fig. 2 and graphs (a) and (b) for $\varepsilon = 1, 10$, respectively, are as follows:

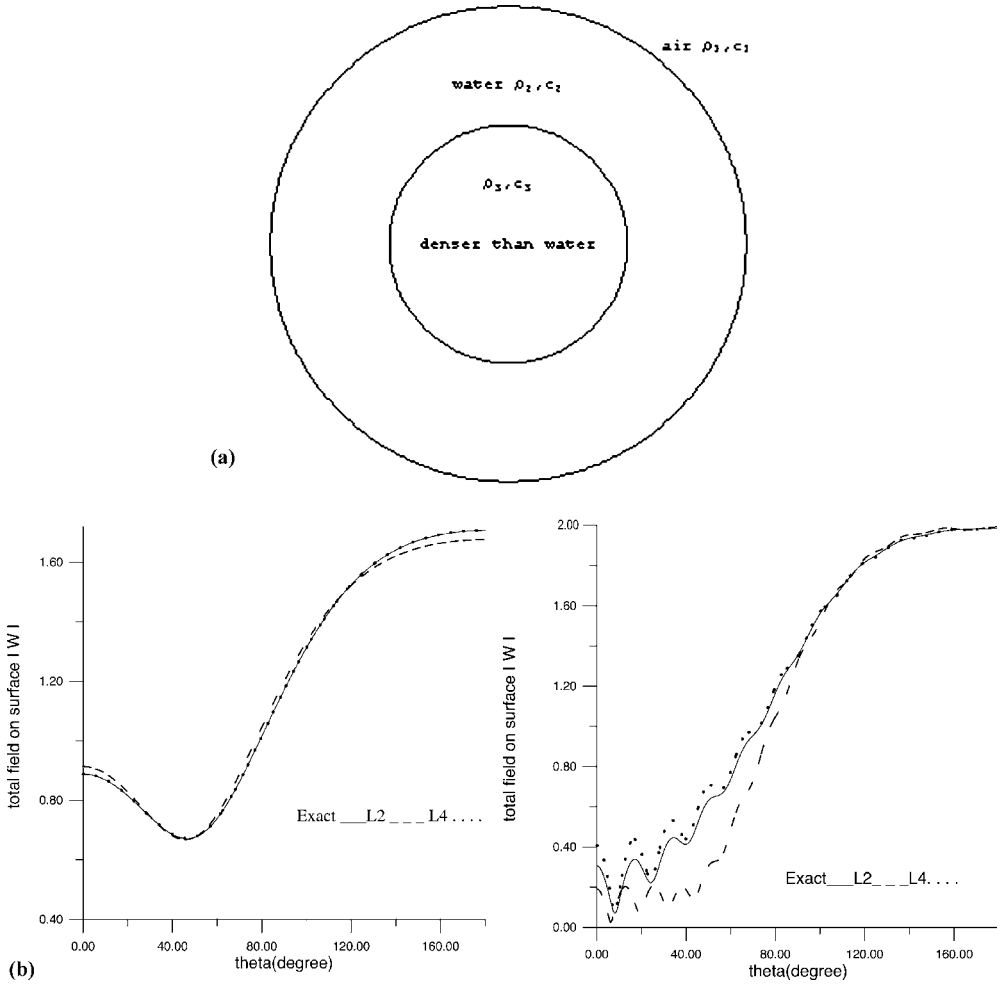

FIG. 1.

$$\rho_1 = 1000, \quad c_1 = 1480, \quad \rho_2 = 1.2, \quad c_2 = 340, \quad \rho_3 = 1.0, \quad c_3 = 280. \tag{3.3}$$

Figure 2 shows the results of the second- and fourth-order SRCs for the parameters in (3.3) for $\varepsilon = 1, 10$. It can be seen that for $\varepsilon = 1, 10$ the performance of the fourth-order SRCs are perfect, and they offer an improvement, although in these cases the second-order SRCs also produce quite good results. It should be noted that in the cases given in the graphs, the concentric penetrable cylinder behaves nearly as a soft cylinder.[11]

In a different manner from Figs. 1 and 2 whenever the densities of the first two regions are similar and the density of the smaller third region is greater than those, the case specific parameters and graphs (a) and (b) of Figure 3 for $\varepsilon = 1, 10$, respectively, are as follows:

$$\rho_1 = 1,2, \quad c_1 = 340, \quad \rho_2 = 1.4, \quad c_2 = 400, \quad \rho_3 = 1000, \quad c_3 = 1480. \tag{3.4}$$

As opposed to Fig. 3, whenever the densities of the first two regions are similar between them and lower than the third region the case specific parameters and graphs (a) and (b) of Figure 4 for $\varepsilon = 1, 10$, respectively, are as follows:

$$\rho_1 = 1200, \quad c_1 = 1600, \quad \rho_2 = 1000, \quad c_2 = 1480, \quad \rho_3 = 1.2, \quad c_3 = 340. \tag{3.5}$$

In Figs. 3 and 4 we see almost the same results of the problem according to the parameters in (3.4) and (3.5) as in (3.2) and (3.3), respectively.

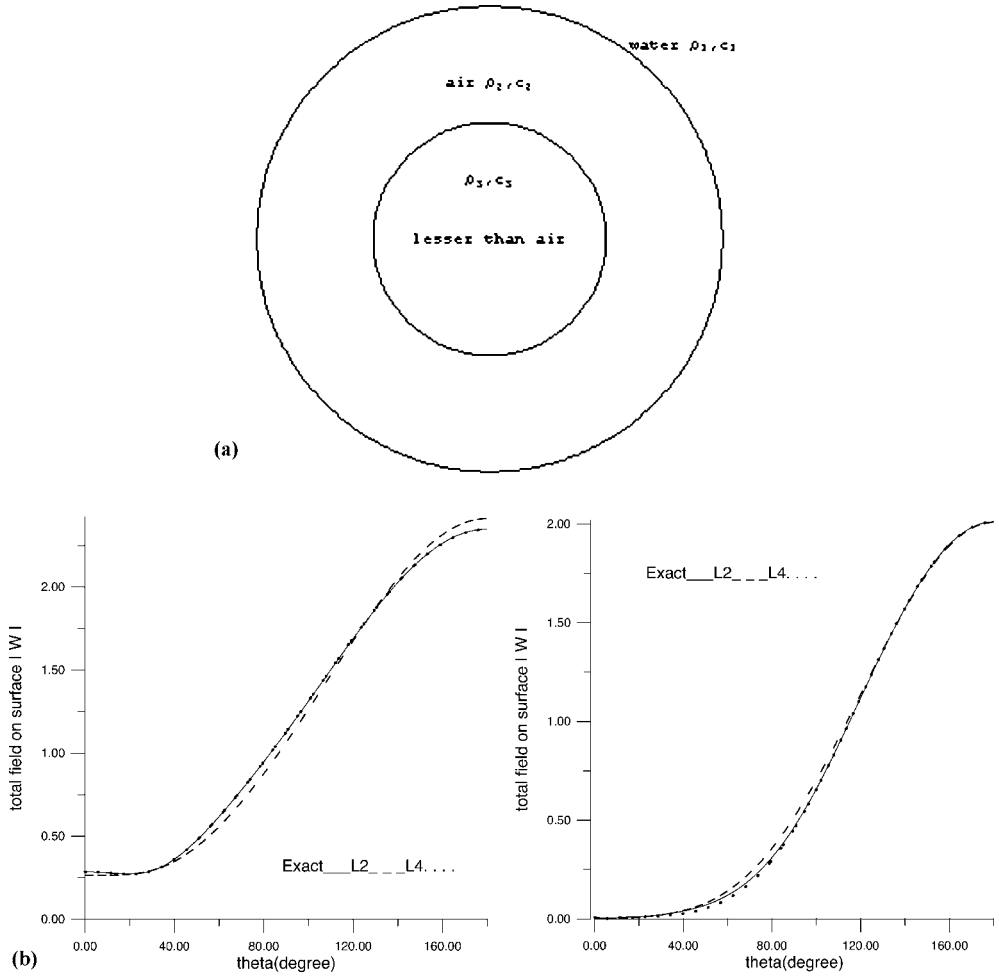

FIG. 2.

From all the graphics related to Figs. 1–4 it can be seen that the fourth-order SRC produces the most accurate results for all of the frequencies. It is known that the creeping waves are less pervasive for the case in Fig. 1 objects and therefore the results are more accurate in the high-frequency range. Nevertheless the fourth-order SRC improves the SRC approximation considerably for both Figs. 1 and 2 and also for all frequencies.

APPENDIX

It is well known that the solution of the Helmholtz equation satisfying the Sommerfeld radiation condition can be represented by the series which is convergent in $\mathcal{B}_1$ and is

$$u = H_0^{(2)}(kr)\sum_{n=0}^{\infty}\frac{F_n(\theta)}{r^n} + H_1^{(2)}(kr)\sum_{n=0}^{\infty}\frac{G_n(\theta)}{r^n}. \tag{A1}$$

For large values, the asymptotic expansion for u is

$$u \approx \sqrt{\frac{2}{\pi kr}}e^{-i(kr-\pi/4)}\sum_{n=0}^{\infty}\frac{f_n(\theta)}{r^n}. \tag{A2}$$

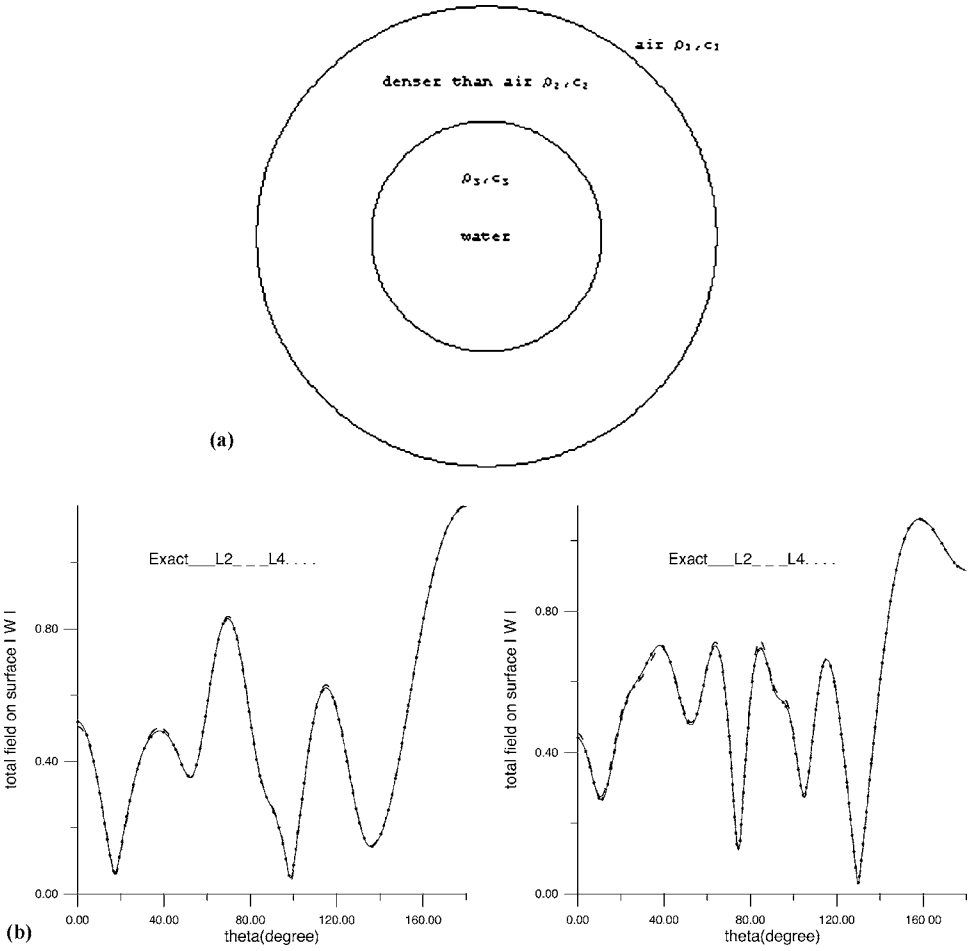

FIG. 3.

If we want to solve the problem numerically by direct methods; we must first make the region $\mathcal{B}_1$ finite. This can be done by means of a Σ_2 curve which includes Σ_1 curve and whose center is in $\mathcal{B}_2$ and has radius r_1. With these assumptions the problem is reduced to finding the solution of the Helmholtz equation on the region bounded by Σ_1 and Σ_2 the solution must satisfy the empedance condition on Σ_1 and the boundary condition must be satisfied on Σ_2 which will play the role of the Sommerfeld radiation condition. How ever this condition is as yet unknown and the first thing that comes to mind is to carry the Sommerfeld condition over to Σ_2. That is,

$$\left(\frac{\partial u}{\partial r} + iku\right)_{r=r_1} = 0. \tag{A3}$$

Howewer, this is a wrong approach. It can be immediately seen that even for the first term of expansion (A2), (A3) is not definite,

$$\left(\frac{\partial}{\partial r} + ik\right)\sqrt{\frac{2}{\pi kr}}e^{-i(kr-\pi/4)}f_0(\theta) = \vartheta(r^{-3/2}). \tag{A4}$$

If the operator $L_1 = (\partial/\partial r) + ik + (1/2r)$ is used instead of $[(\partial/\partial r) + ik]$

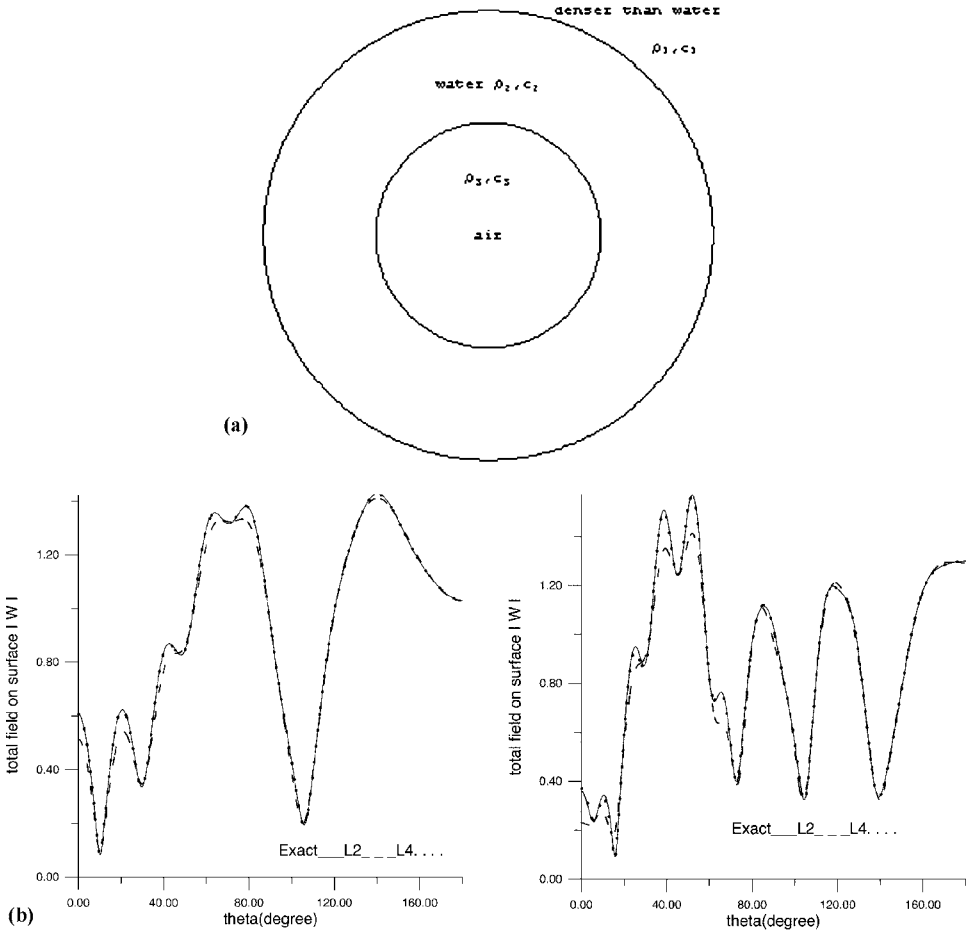

FIG. 4.

$$L_1\left(\sqrt{\frac{2}{\pi kr}}e^{-i(kr-\pi/4)}f_0(\theta)\right)=0 \tag{A5}$$

will be found. This result will be true for

$$\frac{e^{-i(kr)}}{\sqrt{kr}}F(\theta), \tag{A6}$$

where $F(\theta)$ is an arbitrary function and for (A2) the following will be valid:

$$(L_1u)_{r=r_1}=\vartheta(r^{-5/2}) \tag{A7}$$

That is when L_1 is applied to u, a result less erroneous then the Sommerfeld radiation condition is obtained. Similarly, higher order boundary condition operators can be obtained from Ref. 6 and are given by

$$L_m=\left(\frac{\partial}{\partial r}+ik+\frac{4m-3}{2r}\right)L_{m-1}. \tag{A8}$$

The first four operators in polar coordinates for the Helmholtz equations, which are used in this paper, are

$$L_1 u = \frac{\partial u}{\partial r} + iku + \frac{u}{2r}, \tag{A9}$$

$$L_2 u = 2\left(\frac{1}{r} + ik\right)\frac{\partial u}{\partial r} - \left(2k^2 + \frac{3}{4r^2} + \frac{3ik}{r}\right)u - \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}, \tag{A10}$$

$$L_3 u = \left(\frac{23}{4r^2} + \frac{12ik}{r} - 4k^2\right)\frac{\partial u}{\partial r} + \left(\frac{15}{8r^3} + \frac{45ik}{4r^2} - \frac{14k^2}{r} - 4ik^3\right)u + \left(\frac{-9}{2r^3} - \frac{3ik}{r^2}\right)\frac{\partial^2 u}{\partial \theta^2} - \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\left(\frac{\partial u}{\partial r}\right), \tag{A11}$$

and

$$\begin{aligned} L_4 u = {} & \left(\frac{22}{r^3} + \frac{71ik}{r^2} - \frac{48k^2}{r} - 8ik^3\right)\frac{\partial u}{\partial r} + \left(\frac{105}{16r^4} + \frac{105ik}{2r^3} - \frac{94k^2}{r^2} - \frac{52ik^3}{r} + 8k^4\right)u \\ & + \left(\frac{-43}{2r^4} - \frac{30ik}{r^3} + \frac{8k^2}{r^2}\right)\frac{\partial^2 u}{\partial \theta^2} + \left(\frac{-8}{r^3} - \frac{4ik}{r^2}\right)\frac{\partial^2}{\partial \theta^2}\left(\frac{\partial u}{\partial r}\right) + \frac{1}{r^4}\frac{\partial^4 u}{\partial \theta^4}, \end{aligned} \tag{A12}$$

respectively.

For a cylinder the second-, third-, and fourth-order radiation conditions are found to be

$$\alpha_1^{(m)}\frac{d^4 v_1}{d\theta^4} + \alpha_2^{(m)}\frac{d^2 v_1}{d\theta^2} + \alpha_3^{(m)} v_1 = \alpha_4^{(m)}\frac{d^2 w_1}{d\theta^2} + \alpha_5^{(m)} w_1, \quad m = 2,3,4, \tag{A13}$$

where

$$v_1(\theta) = u_1(a,\theta) \quad \text{and} \quad w_1(\theta) = \frac{1}{k_1}\frac{\partial u_1}{\partial r}(a,\theta) \tag{A14}$$

and $\alpha_q^{(m)}$ are functions of $\varepsilon = k_1 a$. In (A13) the superscript m denotes the order. $\alpha_q^{(m)}$ are defined as

$$\alpha_1^{(2)} = 0, \quad \alpha_2^{(2)} = 1, \quad \alpha_3^{(2)} = -\frac{3}{4} - 3i\epsilon + 2\epsilon^2, \quad \alpha_4^{(2)} = 0, \quad \alpha_5^{(2)} = 2\epsilon(1 + i\epsilon),$$

$$\alpha_1^{(3)} = 0, \quad \alpha_2^{(3)} = -3i\epsilon - \frac{9}{2}, \quad \alpha_3^{(3)} = \frac{15}{8} + \frac{45}{4}i\epsilon - 14\epsilon^2 - 4i\epsilon^3,$$

$$\alpha_4^{(3)} = \epsilon, \quad \alpha_5^{(3)} = -\epsilon\left(\frac{23}{4} + 12i\epsilon - 4\epsilon^2\right), \tag{A15}$$

$$\alpha_1^{(4)} = 1, \quad \alpha_2^{(4)} = -\frac{43}{2} - 30i\epsilon + 8\epsilon^2, \quad \alpha_3^{(4)} = \frac{105}{16} + \frac{105i\epsilon}{2} - 94\epsilon^2 - 52i\epsilon^3 + 8\epsilon^4,$$

$$\alpha_4^{(4)} = 4\epsilon(2 + i\epsilon), \quad \alpha_5^{(4)} = -\epsilon(22 + 71i\epsilon - 48\epsilon^2 - 8i\epsilon^3).$$

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Quantum entanglement and geometry of determinantal varieties

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Quantum entanglement was first recognized as a feature of quantum mechanics in the famous paper of Einstein, Podolsky, and Rosen. Recently it has been realized that quantum entanglement is a key ingredient in quantum computation, quantum communication, and quantum cryptography. In this paper, we introduce algebraic sets, which are determinantal varieties in the complex projective spaces or the products of complex projective spaces, for the mixed states on bipartite or multipartite quantum systems as their invariants under local unitary transformations. These invariants are naturally arised from the physical consideration of measuring mixed states by separable pure states. Our construction has applications in the following important topics in quantum information theory: (1) separability criterion, it is proved that the algebraic sets must be a union of the linear subspaces if the mixed states are separable; (2) simulation of Hamiltonians, it is proved that the simulation of semipositive Hamiltonians of the same rank implies the projective isomorphisms of the corresponding algebraic sets; (3) construction of bound entangled mixed states, examples of the entangled mixed states which are invariant under partial transpositions (thus PPT bound entanglement) are constructed systematically from our new separability criterion. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2194629]

I. INTRODUCTION

A bipartite pure quantum state $|\psi\rangle \in H=H_A^m \otimes H_B^n$, where H_A^m, H_B^n are finite dimensional Hilbert spaces of dimensions m and n, and the tensor inner product is used on H, is called entangled if it cannot be written as $|\psi\rangle=|\psi_A\rangle \otimes |\psi_B\rangle$ for some $|\psi_A\rangle \in H_A^m$ and $|\psi_B\rangle \in H_B^n$. A mixed state (or a density matrix) ρ, which is a semipositive definite operator on H with trace 1, is called entangled if it cannot be written as

$$\rho = \Sigma_i p_i P_{|\psi_i^A\rangle} \otimes P_{|\psi_i^B\rangle}, \tag{1}$$

for some set of states $|\psi_i^A\rangle \in H_A^m$, $|\psi_i^B\rangle \in H_B^n$, and $p_i \geqslant 0$. Here P_v for a state (unit vector) v means the (rank 1) projection operator to the vector v. If the mixed state ρ can be written in the form of (1), it is called separable (see Refs. 28, 39, and 41).

For the mixed state ρ on $H=H_A^m \otimes H_B^n$, we have the following partial transposition ρ^{PT} and the partial trace $\mathrm{tr}_B(\rho)$ on H_A^m [$\mathrm{tr}_A(\rho)$ on H_B^n can be defined similarly] defined as follows:

$$\langle ij|\rho^{\mathrm{PT}}|kl\rangle = \langle il|\rho|kj\rangle,$$

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$$\langle i|\mathrm{tr}_B(\rho)|k\rangle = \Sigma_j \langle ij|\rho|kj\rangle, \tag{2}$$

where $\{|1\rangle,\ldots,|m\rangle\}$, $\{|1\rangle,\ldots,|n\rangle\}$, $\{|11\rangle,\ldots|1n\rangle,\ldots|m1\rangle,\ldots,|mn\rangle\}$ are orthogonal bases of $H'_A H^n_B$ and H, respectively. We observe that the partial transposition of a separable mixed state is again a separable mixed state, this implies that the partial transposition of a separable mixed state is semi positive definite. This is the famous Peres PPT criterion of separability (see Ref. 38).

For multipartite quantum systems, there are similar definitions of entangled and separable mixed states (see Refs. 28, 39, and 41). We restrict ourselves to the tripartite case. Let ρ be a mixed state on $H=H^m_A\otimes H^n_B\otimes H^l_C$. ρ is called separable if it can be written as

$$\rho = \Sigma_i p_i P_{|\psi^A_i\rangle}\otimes P_{|\psi^B_i\rangle}\otimes P_{|\psi^C_i\rangle}, \tag{3}$$

for some set of states $|\psi^A_i\rangle\in H^m_A$, $|\psi^B_i\rangle\in H^n_B, |\psi^C_i\rangle\in H^l_C$, and $p_i\geqslant 0$. If the mixed state ρ cannot be written in the form of (3), it is called entangled. Sometimes we also consider the separability relative to the cut $A:BC$ ($B:AC$, etc.), that means ρ is considered as a mixed state on the bipartite quantum system $H=H^m_A\otimes(H^n_B\otimes H^l_C)$.

For a n-party quantum system $H=H^{m_1}_{A_1}\otimes\cdots\otimes H^{m_n}_{A_n}$, local unitary transformations (acting on a mixed state ρ by $U\rho U^\dagger$, where $\dagger$ is the adjoint) are those unitary transformations of the form $U=U_{A_1}\otimes\cdots\otimes U_{A_n}$, where U_{A_i} is a unitary transformation on $H^{m_i}_{A_i}$ for $i=1,\ldots,n$. We can check that all eigenvalues (spectra) of ρ (global spectra) and, $\mathrm{tr}_{A_{i_1}\cdots A_{i_l}}(\rho)$ of mixed states ρ, where $i_1,\ldots,i_l\in\{1,\ldots,n\}$, (local spectra) are invariant under local unitary transformations, and the invariants in the examples of Refs. 33 and 34 are more or less spectra-involved. It is clear that separability (or being entangled) is an invariant property under local unitary transformations. For a mixed state ρ, to judge whether it is entangled or separable and decide its entangled class (i.e., the equivalent class of all entangled (or separable) mixed states which are equivalent to ρ by local unitary transformations) is a fundamental problem in the study of quantum entanglement.[28,41] Thus for the purpose to quantify entanglement, any good measure of entanglement must be invariant under local transformations.[33,34,28,41] Another important concept is the distillable mixed state, which means that some singlets can be extracted from it by local operations and classical communication (LOCC) (see Ref. 28). A mixed state ρ on H is distillable if and only if for some t, there exists projections $P_A:H^{\otimes t}_A\to H^2$ and $P_B:H^{\otimes t}_B\to H^2$, where H^2 is a two-dimensional Hilbert space, such that the mixed state $(P_A\otimes P_B)\rho^{\otimes t}(P_A\otimes P_B)^\dagger$ is an entangled state in $H^2\otimes H^2$ (see Ref. 28). A mixed state which cannot be distilled is called bound entangled mixed state.

The phonomenon of quantum entanglement lies at the heart of quantum mechanics since the famous Einstein, Podolsky, and Rosen[16] paper (see Refs. 8, 28, and 39). Its importance lies not only in philosophical consideration of the nature of quantum theory, but also in applications where it has emerged recently that quantum entanglement is the key ingredient in quantum computation[20] and communication[4] and plays an important role in cryptography (Ref. 19). These new applications of quantum entanglement have stimulated tremendous studies of quantum entanglements of both pure and mixed states from both theoretical and experimental view, for surveys we refer to Refs. 8, 28, 32, 39, and 41.

To find good necessary conditions of separability (separability criterion) is a fundamental problem in the study of quantum entanglement.[28,41] Bell-type inequalities[28] and entropy criterion[28] are well-known numerical criterion of separable states. In 1996, Peres[38] gave a striking simple criterion which asserts that a separable mixed state ρ necessarily has (semi) positive definite partial transposition (PPT), which has been proved by Horodeckis[25] also a sufficient condition of separability in 2×2 and 2×3 systems. The significance of PPT property is also reflected in the facts that PPT mixed states satisfy Bell inequalities[44] and cannot be distilled,[28,26] thus the first several examples of the PPT entangled mixed states[24] indicated the new phenomenon that there is bound entanglement in nature.[26] These examples were constructed from the so-called range criterion of Horodecki (see Refs. 24 and 28). However, constructing PPT entangled mixed states (thus bound entanglement) is an exceedingly difficult task,[6] and the only known systematic way of such construction is the context of unextendible product base (UPB) in Ref. 6, which works in both the

bipartite and multipartite case and is also based on Horodecki's range criterion. The most recent disorder criterion of separability in Ref. 37, which is stronger than entropy criterion, was proved by the mathematics of majorization.

It has been realized that the entanglement of tripartite pure quantum states is not a trivial extension of the entanglement of bipartite pure quantum states.[21] Recently Bennett *et al.*,[5] studied the exact and asymptotic entanglement measure of multipartite pure states, which showed essential difference to that of bipartite pure states. On the other hand Carteret *et al.*,[12] proved a generalization of Schmidt decomposition for pure multipartite states. Basically, the understanding of multipartite quantum entanglement for both pure and mixed states, is much less advanced.

It is clear that any separability criterion for bipartite mixed states, such as Peres PPT criterion[38] and Horodecki range criterion,[24,28] can be applied to multipartite mixed states for their separability under various cuts. For example, from Peres PPT criterion, a separable multipartite mixed state necessarily has all its partial transpositions semipositive. In Ref. 27, Horodeckis studied the separability criterion of multipartite mixed states by linear maps. Classification of triqubit mixed states was studied in Ref. 2.

There have been many interesting works (Refs. 10, 11, 30, 35, and 43) for understanding quantum entanglement and related problems from the view of representation theory and topology.

The physical motivation of this paper is as follows. We consider the following situation. Alice and Bob share a bipartite quantum system $H_A^m \otimes H_B^n$, and they have a mixed state ρ. Now they want to understand the entanglement properties of ρ. It is certain that they can prepare any separable pure state $|\phi_1\rangle \otimes |\phi_2\rangle$ separately. Now they measure ρ with this separable pure state, the expectation value is $\langle \phi_1 \otimes \phi_2 | \rho | \phi_1 \otimes \phi_2 \rangle$. If Alice's pure state $|\phi_1\rangle$ is fixed, then $\langle \phi_1 \otimes \phi_2 | \rho | \phi_1 \otimes \phi_2 \rangle$ is a Hermitian bilinear form on Bob's pure states (i.e., on H_B^n). We denote this bilinear form by $\langle \phi_1 | \rho | \phi_1 \rangle$. Intuitively the *degenerating locus* $V_A^k(\rho) = \{|\phi_1\rangle \in P(H_A^m) : \mathrm{rank}(\langle \phi_1 | \rho | \phi_1 \rangle) \leqslant k\}$, where $P(H_A^m)$ is the projective space of all pure states in H_A^m, should contain the physical information of ρ and it is almost obvious that these *degenerating locus* are invariant under local unitary transformations. For a multipartite quantum system, a similar consideration leads to some Hermitian bilinear forms on some of its parts and similarly we can consider the *degenerating locus* of these Hermitian bilinear forms. We prove that these *degenerating locus* are algebraic sets, which are determinantal varieties, for the mixed states on both bipartite and multipartite quantum systems. They have the following properties.

(1) When we apply local unitary transformations on the mixed state the corresponding algebraic sets are changed by local (unitary) linear transformations, and thus these invariants can be used to distinguish inequivalent mixed states under local unitary transformations.

(2) The algebraic sets must be linear (a union of some linear subspaces) if the mixed state is separable, and thus we give a new separability criterion.

(3) The algebraic sets are independent of eigenvalues and only measure the positions of eigenvectors of the mixed states.

(4) These algebraic sets can be calculated easily.

From our construction here, we establish a connection between quantum entanglement and algebraic geometry. Actually from our results below, we can see that if the Fubini-Study metric of the projective complex space is used, the metric properties of these algebraic sets are also preserved when local unitary transformations are applied on the mixed state. Hence we establish a connection between quantum entanglement and both the algebraic geometry and complex differential geometry. Any algebraic geometric or complex differential geometric invariant of the algebraic set of the mixed state is an invariant of the mixed state under local unitary transformations.

The determinantal varieties (Ref. 23 Lecture 9 and Ref. 3 Chap. II) have been studied from different motivations such as geometry of curves,[3,18] geometry of determinantal varieties,[17] Hodge theory,[22] commutative algebra,[15] and even combinatorics.[1] It is interesting to see that it can be useful even in quantum information theory. We refer to Refs. 23 and 3 for the standard facts about determinantal varieties.

The paper is organized as follows. We define the algebraic sets of the mixed states and prove their basic properties including the separability criteria based on these algebraic sets in Sec. II. In

Sec. III, we indicate briefly how numerical invariants of the bipartite or multipartite mixed states under local unitary transformations can be derived from these algebraic sets. As an easiest example, Schmidt rank of a pure state on bipartite quantum systems, a classical concept in quantum entanglement, is shown to be the codimension of the algebraic set. Many examples of entangled mixed states corresponding to the famous determinantal varieties in algebraic geometry, such as Segre varieties, rational normal scrolls and generic determinantal varieties are constructed in Sec. IV. We also show that a well-known theorem of Eisenbud[17] can help us to construct many entangled bipartite mixed states of low ranks. In Sec. V we introduce a family of the generalized Smolin states, which is a natural extension of Smolin's physical construction[40] from algebraic-geometric view. In Secs. VI and VII, it is proved that these algebraic sets are nonempty for low rank mixed states, and indicate how a *finer* result with the same idea (Theorem 9′) can be potentially used to treat the entanglement properties of high rank mixed states. Based on the algebraic sets introduced in Sec. II, a necessary condition about the simulating Hamiltonians efficiently using local unitary transformations is given in Sec. VIII. In Sec. IX, we give a continuous family of bipartite mixed states, tripartite pure states, and bipartite Hamiltonians with the property that the eigenvalues (spectra) of them and their partial traces are constant, however, their entanglement properties are distinct. This offers strong evidence that it is hopeless to characterize the entanglement properties by only using eigenvalue spectra. In Sec. X, we illustrate by an explicit example that our separability criterion can be used to construct PPT entangled mixed states (thus bound entanglement) systematically.

II. INVARIANTS AND SEPARABILITY CRITERIA

Now we define the invariants and give the coordinate form. Let $H=H_A^m\otimes H_B^n$, $\{|ij\rangle\}$, where $i=1,\ldots,m$ and $j=1,\ldots,n$, be an orthogonal base and ρ be a mixed state on H. We represent the matrix of ρ in the bases $\{|11\rangle,\ldots|1n\rangle,\ldots,|m1\rangle,\ldots,|mn\rangle\}$, and consider ρ as a blocked matrix $\rho=(\rho_{ij})_{1\leqslant i\leqslant m,1\leqslant j\leqslant m}$ with each block ρ_{ij} a $n\times n$ matrix corresponding to the $|i1\rangle,\ldots,|in\rangle$ rows and the $|j1\rangle,\ldots,|jn\rangle$ columns. For any pure state $|\phi_1\rangle=r_1|1\rangle+\cdots+r_m|m\rangle\in P(H_A^m)$ the matrix of the Hermitian linear form $\langle\phi_1|\rho|\phi_1\rangle$ with the basis $|1\rangle,\ldots,|n\rangle$ is $\Sigma_{i,j}r_ir_j^*\rho_{ij}$. Thus the *degenerating locus* are as follows.

Definition 1: We define

$$V_A^k(\rho)=\{|\phi_1\rangle\in P(H_A^m):\mathrm{rank}(\langle\phi_1|\rho|\phi_1\rangle)\leqslant k\}=\{(r_1,\ldots,r_m)\in CP^{m-1}:\mathrm{rank}(\Sigma_{i,j}r_ir_j^*\rho_{ij})\leqslant k\},\tag{4}$$

where $k=0,1,\ldots,n-1$. *Similarly* $V_B^k(\rho)\subseteq CP^{n-1}$, *where* $k=0,1,\ldots,m-1$, *can be defined.*

Example 1: Let $\rho=(1/mn)I_{mn}$ be the maximally mixed state, we easily have $V_A^k(\rho)=\{(r_1,\ldots,r_m):\mathrm{rank}(\Sigma r_ir_i^*I_n)\leqslant k\}=\varnothing$ for $k=0,1,\ldots,n-1$, where $*$ is the complex conjugate.

Example 2: Let $H=H_A^2\otimes H_B^n$, T_1,T_2 be 2 $n\times n$ matrices of rank $n-1$ such that the $n\times(2n)$ matrix (T_1,T_2) has rank n. Let T' be a $2n\times 2n$ matrix with 11 block T_1, 22 block T_2, 12 and 21 blocks 0. Its rows correspond to the orthogonal base $|11\rangle,\ldots,|1n\rangle,|21\rangle,\ldots,|2n\rangle$ of H. Let $\rho=(1/D)TT^\dagger$ (where D is a normalizing constant) be a mixed state on H. It is easy to check that ρ is of rank $2n-2$ and $V_A^{n-1}(\rho)=\{(r_1,r_2):r_1r_2=0\}$.

Let $H=H_A^m\otimes H_B^n\otimes H_C^l$. Take an orthogonal base of H, $|ijk\rangle$, where, $i=1,\ldots,m$, $j=1,\ldots,n$, and $k=1,\ldots,l$, and ρ is a mixed state on H. We represent the matrix of ρ in the base $\{|111\rangle,\ldots|11l\rangle,\ldots,|mn1\rangle,\ldots,|mnl\rangle\}$ as $\rho=(\rho_{ij,i'j'})_{1\leqslant i,i'\leqslant m,1\leqslant j,j'\leqslant n}$, and $\rho_{ij,i'j'}$ is a $l\times l$ matrix. Consider H as a bipartite system as $H=(H_A^m\otimes H_B^n)\otimes H_C^l$, then we have $V_{AB}^k(\rho)=\{(r_{11},\ldots,r_{mn})\in CP^{mn-1}:\mathrm{rank}(\Sigma r_{ij}r_{i'j'}^\dagger\rho_{ij,i'j'})\leqslant k\}$ defined as above. This set is actually the *degenerating locus* of the Hermitian bilinear form $\langle\phi_{12}|\rho|\phi_{12}\rangle$ on H_C^l for the given pure state $|\phi_{12}\rangle=\Sigma_{i,j}^{m,n}r_{ij}|ij\rangle\in P(H_A^m\otimes H_B^n)$. When the finer cut $A:B:C$ is considered, it is natural to take $|\phi_{12}\rangle$ as a separable pure state $|\phi_{12}\rangle=|\phi_1\rangle\otimes|\phi_2\rangle$, i.e., there exist $|\phi_1\rangle=\Sigma_ir_i^1|i\rangle\in P(H_A^m)$ and $|\phi_2\rangle=\Sigma_jr_j^2|j\rangle\in P(H_B^n)$ such that $r_{ij}=r_i^1r_j^2$. In this way the tripartite mixed state ρ is measured by tripartite separable pure states $|\phi_1\rangle\otimes|\phi_2\rangle\otimes|\phi_3\rangle$. Thus it is natural that we define $V_{A:B}^k(\rho)$ as follows. It is the *degenerating locus* of the bilinear form $\langle\phi_1\otimes\phi_2|\rho|\phi_1\otimes\phi_2\rangle$ on H_C^l.

Definition 2: Let $\phi: CP^{m-1} \times CP^{n-1} \to CP^{mn-1}$ *be the mapping defined by*

$$\phi(r_1^1, \ldots r_m^1, r_1^2, \ldots, r_n^2) = (r_1^1 r_1^2, \ldots, r_i^1 r_j^2, \ldots r_m^1 r_n^2) \tag{5}$$

(i.e., $r_{ij} = r_i^1 r_j^2$ *is introduced).*

Then $V_{A:B}^k(\rho)$ *is defined as the preimage* $\phi^{-1}(V_{AB}^k(\rho))$.

Similarly $V_{B:C}^k(\rho), V_{A:C}^k(\rho)$ can be defined. In the following statement we just state the result for $V_{A:B}^k(\rho)$. The conclusion holds similarly for other V's.

For the mixed state ρ on the multipartite system $H = H_{A_1}^{m_1} \otimes \cdots \otimes H_{A_k}^{m_k}$, we want to study the entanglement under the cut $A_{i_1}: A_{i_2}: \cdots : A_{i_l} : (A_{j_1} \cdots A_{j_{k-l}})$, where $\{i_1, \ldots, i_l\} \cup \{j_1, \ldots, j_{k-l}\} = \{1, \ldots, k\}$. We can define the set $V_{A_{i_1}: \cdots : A_{i_l}}^k(\rho)$ similarly.

It is obvious we have the following results about the "invariance" under local unitary transformations.

Theorem 1: *Let* $T = U_A \otimes U_B$, *where* U_A *and* U_B *are the unitary transformations on* H_A^m *and* H_B^n, *respectively. Then* $V_A^k(T(\rho)) = U_A^{-1}(V_A^k(\rho))$, *that is* $V_A^k(\rho)$ [*respectively,* $V_B^k(\rho)$] *is an "invariant" up to a linear transformation of* CP^{m-1} *of the mixed state* ρ *under local unitary transformations.*

Theorem 1′: *Let* $T = U_A \otimes U_B \otimes U_C$, *where* U_A, U_B, *and* U_C *are unitary transformations on* H_A^m, H_B^n, *and* H_C^l, *respectively. Then* $V_{A:B}^k(T(\rho)) = U_A^{-1} \times U_B^{-1}(V_{A:B}^k(\rho))$, *that is* $V_{A:B}^k(\rho)$ *is an "invariant" up to a linear transformation of* $CP^{m-1} \times CP^{n-1}$ *of the mixed state* ρ *under local unitary transformations.*

Theorem 1″: *Let* $T = U_{A_{i_1}} \otimes \cdots \otimes U_{A_{i_l}} \otimes U_{j_1 \cdots j_{k-l}}$, *where* $U_{A_{i_1}}, \ldots, U_{A_{i_l}}, U_{j_1 \cdots j_{k-l}}$ *are unitary transformations on* $H_{A_{i_1}}^{m_{i_1}}, \ldots, H_{A_{i_l}}^{m_{i_l}}$ *and* $(H_{A_{j_1}}^{m_{j_1}} \otimes \cdots \otimes H_{A_{j_{k-l}}}^{m_{j_{k-l}}})$, *respectively. Then* $V_{A_{i_1}: \cdots : A_{i_l}}^k(T(\rho)) = U_{A_{i_1}}^{-1} \times \cdots \times U_{A_{i_l}}^{-1}(V_{A_{i_1}: \cdots : A_{i_l}}^k(\rho))$.

Remark 1: Since $U_{A_{i_1}}^{-1} \times \cdots \times U_{A_{i_l}}^{-1}$ certainly preserves the standard Euclid metric of complex linear space and hence the (product) Fubini-Study metric of the product of projective complex spaces, all metric properties of $V_{A_{i_1}: \cdots : A_{i_l}}^k(\rho)$ are preserved when the local unitary transformations are applied to the mixed state ρ.

Moreover from the proof it is easy to see that all algebraic-geometric properties [since $V_A^k(\rho)$, $V_B^k(\rho)$ are algebraic sets as proved in Theorem 2] of $V_A^k(\rho)$ [respectively, $V_B^k(\rho)$] are preserved even under local linear inversible transformations (i.e., $T = T_A \otimes T_B$ where T_A, T_B are just linear inversible operators of H_A^m, H_B^n)

We observe $V_A^k(\rho^{\mathrm{PT}}) = (V_A^k(\rho))^*$, here * is the conjugate mapping of CP^{m-1} defined by $(r_1, \ldots, r_m)^* = (r_1^*, \ldots, r_m^*)$. It is clear that this property holds for other V's invariants.

Theorem 2: $V_A^k(\rho)$ [*respectively*, $V_B^k(\rho)$] *is an algebraic set in* CP^{m-1} (*respectively*, CP^{n-1}).

From Definition 2 and Theorem 2 we immediately have the following result.

Theorem 2′: $V_{A:B}^k(\rho)$ *is an algebraic set in* $CP^{m-1} \times CP^{n-1}$.

The general result can be stated as follows.

Theorem 2″: $V_{A_{i_1}: \cdots : A_{i_l}}^k(\rho)$ *is an algebraic set in* $CP^{m_{i_1}-1} \times \cdots \times CP^{m_{i_l}-1}$.

It is easy to see from Definitions that we just need to prove Theorem 2.

Theorem 3: *If* ρ *is a separable mixed state,* $V_A^k(\rho)$ [*respectively*, $V_B^k(\rho)$] *is a linear subset in* CP^{m-1} (*respectively*, CP^{n-1}), *i.e., it is a union of the linear subspaces.*

In the following statement we give the separability criterion of the mixed state ρ under the cut $A:B:C$. The "linear subspace of $CP^{m-1} \times CP^{n-1}$" means the product of a linear subspace in CP^{m-1} and a linear subspace in CP^{n-1}.

Theorem 3′: *If* ρ *is a separable mixed state on* $H = H_A^m \otimes H_B^n \otimes H_C^l$ *under the cut* $A:B:C$, $V_{A:B}^k(\rho)$ *is a linear subset in* $CP^{m-1} \times CP^{n-1}$, *i.e., it is a union of the linear subspaces.*

The general result can be stated as follows.

Theorem 3″: *If* ρ *is a separable mixed state on* $H = H_{A_1}^{m_1} \otimes \cdots \otimes H_{A_k}^{m_k}$ *under the cut* $A_{i_1}: A_{i_2}: \cdots : A_{i_l} : (A_{j_1} \cdots A_{j_{k-l}})$, $V_{A_{i_1}: \cdots : A_{i_l}}^k(\rho)$ *is a linear subset in* $CP^{m_{i_1}-1} \times \cdots \times CP^{m_{i_l}-1}$, *i.e., it is a union of the linear subspaces.*

We just proved Theorem 3 and Theorem 3′. The proof of Theorem 3″ is similar.

For the purpose to prove Theorems 2 and 3 we need the following lemmas.

Lemma 1: Let $\{e_1,\ldots,e_h\}$ *be an orthogonal base of a h dimension Hilbert space H,* $\rho=\Sigma_{l=1}^{t}p_lP_{v_l}$, *where* v_l *is unit vector in H for* $l=1,\ldots,t$, $v_l=\Sigma_{k=1}^{h}a_{kl}e_k$, *and* $A=(a_{kl})_{1\leqslant k\leqslant h,1\leqslant l\leqslant t}$ *is the* $h\times t$ *matrix. Then the matrix of* ρ *with the base* $\{e_1,\ldots,e_h\}$ *is* $APA^{\dagger}$, *where P is the diagonal matrix with diagonal entries* $p_1,\ldots,p_t$.

Proof: We note that the matrix of P_{v_l} with the basis is $\alpha_l\alpha_l^{\dagger}$ where $\alpha_l=(a_{1l},\ldots,a_{hl})^{\tau}$ is just the expansion of v_l with the basis. The conclusion follows immediately.

The following conclusion is a direct matrix computation from Lemma 1 or see Ref. 24.

Corollary 1: Suppose $p_i>0$, *then the image of* ρ *is the linear span of vectors* $v_1,\ldots,v_t$.

From Corollary 1 it is clear that the ranges of the separable mixed states and its partial transposition are the linear span of separable pure states. This is the so-called range criterion of Horodecki (see Refs. 24 and 28).

Now let H be the $H_A^m\otimes H_B^n$, $\{e_1,\ldots,e_{mn}\}$ be a orthogonal bases $\{|11\rangle,\ldots,|1n\rangle,\ldots,|m1\rangle,\ldots,|mn\rangle\}$ and $\rho=\Sigma_{l=1}^{t}p_lP_{v_l}$ with positive p_l's be a mixed state on H. We may consider the $mn\times t$ matrix A as a $m\times 1$ blocked matrix with each block A_w, where $w=1,\ldots,m$, a $n\times t$ matrix corresponding to $\{|w1\rangle,\ldots,|wn\rangle\}$. Then it is easy to see $\rho_{ij}=A_iPA_j^{\dagger}$, where $i=1,\ldots,m$, $j=1,\ldots,m$. Thus

$$\Sigma r_ir_j^{*}\rho_{ij}=(\Sigma r_iA_i)P(\Sigma r_iA_i)^{\dagger}. \tag{6}$$

Lemma 2: $\Sigma r_ir_j^{*}\rho_{ij}$ *is a (semi) positive definite* $n\times n$ *matrix. Its rank equals the rank of* (Σr_iA_i).

Proof: The first conclusion is clear. The matrix $\Sigma r_ir_j^{*}\rho_{ij}$ is of rank k if and only if there exist $n-k$ linear independent vectors $c^j=(c_1^j,\ldots,c_n^j)$ with the property,

$$c^j(\Sigma_{ij}r_ir_j^{*}\rho_{ij})(c^j)^{*}=(\Sigma_i r_ic^jA_i)P(\Sigma_i r_ic^jA_i)^{\dagger}=0. \tag{7}$$

Since P is a strictly positive definite matrix, our conclusion follows immediately.

Proof of Theorem 2: From Lemma 1, we know that $V_A^k(\rho)$ is the zero locus of all determinants of $(k+1)\times(k+1)$ submatrices of (Σr_iA_i). The conclusion is proved.

Because the determinants of all $(k+1)\times(k+1)$ submatrices of (Σr_iA_i) are homogeneous polynomials of degree $k+1$, thus $V_A^k(\rho)$ [respectively, $V_B^k(\rho)$] is an algebraic subset (called determinantal varieties in algebraic geometry[16,17]) in CP^{m-1} [respectively, CP^{n-1}].

The point here is for different representations of ρ as $\rho=\Sigma_j p_jP_{v_j}$ with p_j's positive real numbers, the determinantal varieties from their corresponding $\Sigma_i r_iA_i$'s are the same.

Now suppose that the mixed state ρ is separable, i.e., there are unit product vectors $a_1\otimes b_1,\ldots,a_s\otimes b_s$ such that $\rho=\Sigma_{l=1}^{s}q_lP_{a_l\otimes b_l}$, where $q_1,\ldots,q_s$ are positive real numbers. Suppose $a_u=a_u^1|1\rangle+\cdots+a_u^m|m\rangle$, $b_u=b_u^1|1\rangle+\cdots+b_u^n|n\rangle$ for $u=1,\ldots,s$. Hence the vector representation of $a_u\otimes b_u$ with the standard basis is $a_u\otimes b_u=\Sigma_{ij}a_u^ib_u^j|ij\rangle$. Consider the corresponding $mn\times s$ matrix C of $a_1\otimes b_1,\ldots,a_s\otimes b_s$ as in Lemma 1, we have $\rho=CQC^{\dagger}$, where Q is diagonal matrix with diagonal entries $q_1,\ldots,q_s$. As before we consider C as $m\times 1$ blocked matrix with blocks C_w, $w=1,\ldots,m$. Here C_w is a $n\times s$ matrix of the form $C_w=(a_j^wb_j^i)_{1\leqslant i\leqslant n,1\leqslant j\leqslant s}=BT_w$, where $B=(b_j^i)_{1\leqslant i\leqslant n,1\leqslant j\leqslant s}$ is a $n\times s$ matrix and T_w is a diagonal matrix with diagonal entries $a_1^w,\ldots,a_s^w$. Thus from Lemma 1, we have $\rho_{ij}=C_iQC_j^{\dagger}=B(T_iQT_j^{\dagger})B^{\dagger}=BT_{ij}B^{\dagger}$, where T_{ij} is a diagonal matrix with diagonal entries $q_1a_1^i(a_1^j)^{\dagger},\ldots,q_sa_s^i(a_s^j)^{\dagger}$.

Proof of Theorem 3: As in the proof of Theorem 2, we have

$$\Sigma r_ir_j^{\dagger}\rho_{ij}=\Sigma r_ir_j^{\dagger}BT_{ij}B^{\dagger}=B(\Sigma r_ir_j^{\dagger}T_{ij})B^{\dagger}. \tag{8}$$

Here we note $\Sigma r_ir_j^{\dagger}T_{ij}$ is a diagonal matrix with diagonal entries $q_1(\Sigma r_ia_1^i)\times(\Sigma r_ia_1^i)^{\dagger},\ldots,q_s(\Sigma r_ia_s^i)(\Sigma r_ia_s^i)^{\dagger}$. Thus $\Sigma r_ir_j^{*}\rho_{ij}=BGQG^{\dagger}B^{\dagger}$, where G is a diagonal matrix with diagonal entries $\Sigma r_ia_1^i,\ldots,\Sigma r_ia_s^i$. Because Q is a strictly positive definite matrix, from Lemma 1 we know that $\Sigma r_ir_j^{\dagger}\rho_{ij}$ is of rank smaller than $k+1$ if and only if the rank of BG is strictly smaller than $k+1$. Note that BG is just the multiplication of s diagonal entries of G (which are linear forms

of $r_1,\ldots,r_m$) on the s columns of B, thus the determinants of all $(k+1)\times(k+1)$ submatrices of BG (in the case $s\geqslant k+1$, otherwise automatically linear) are the multiplications of a constant (possibly zero) and $k+1$ linear forms of $r_1,\ldots,r_m$. Thus the conclusion is proved.

From Lemma 1 and the proof of Theorems 2 and 3, $\Sigma_i r_i A_i$ play a key role. If we take the standard $\rho=\Sigma_{j=1}^{r} p_j P_{\varphi_j}$, where $p_j,\varphi_j, j=1,\ldots,r$ are eigenvalues and eigenvectors, the corresponding $\Sigma_i r_i A_i$ measures the *geometric positions* of eigenvectors in $H_A^m\otimes H_B^n$. It is obvious from the proof of Theorem 2, the invariants defined in Definition 1 are independent of $p_1,\ldots,p_r$, the global eigenvalue spectra of the mixed states.

Proof of Theorem 3′: We first consider the separability of ρ under the cut $AB:C$, i.e., $\rho=\Sigma_{f=1}^{g} p_f P_{a_f\otimes c_f}$, where $a_f\in H_A^m\otimes H_B^n$ and $c_f\in H_C^l$ for $f=1,\ldots,g$. Consider the separability of ρ under the cut $A:B:C$, we have $a_f=a_f'\otimes a_f''$, $a_f'\in C_A^m, a_f''\in C_B^m$. Let $a_f=(a_f^1,\ldots,a_f^{mn})$, $a_f'=(a_f'^1,\ldots,a_f'^m)$, and $a_f''=(a_f''^1,\ldots,a_f''^n)$ be the coordinate forms with the standard orthogonal basis $\{|ij\rangle\}$, $\{|i\rangle\}$, and $\{|j\rangle\}$, respectively, we have that $a_f^{ij}=a_f'^i a_f''^j$. Recall the proof of Theorem 3, the diagonal entries of G in the proof of Theorem 3 are

$$\Sigma_{ij} r_{ij} a_f^{ij}=\Sigma_{ij} r_i^1 a_f'^i r_j^2 a_f''^j=(\Sigma_i r_i^1 a_f'^i)(\Sigma_j r_j^1 a_f''^j). \tag{9}$$

Thus as argued in the proof of Theorem 3, $V_{A:B}^k(\rho)$ must be the zero locus of the multiplications of the linear forms in (9). The conclusion is proved.

III. NUMERICAL INVARIANTS

It is a standard fact in algebraic geometry that V's defined in Sec. II are the sum of irreducible algebraic varieties (components). Suppose $V_A^k(\rho)=V_1\cup\cdots\cup V_t$. From Theorem 1 and Remark 1, we know that t is a numerical invariant of ρ when local linear inversible transformations are applied to ρ. Actually, since there are a lot of numerical algebraic-geometric invariants of these components, e.g., dimensions, cohomology classes [represented by V_i's in $H^*(CP^{m-1})$], cohomology rings of V_i's, etc. We can get many numerical invariants of the mixed state when local linear inversible transformations are applied to them. In this way, we get a very powerful tool of numerical invariants to distinguish the entangled classes of the mixed states in composite quantum systems.

On the other hand, if local unitary transformations are applied to the mixed states, it is known that even the metric properties of V's (the metric on V is from the standard Fubini-Study metric of projective spaces) are invariant. Thus any complex differential geometric quantity, such as the volumes of V_i's, the integrations (over the whole component) of some curvature functions of V_i's, are the invariants of the mixed states under local unitary transformations.

For any given pure state $|v\rangle$ on a bipartite quantum system, $|v\rangle\in H_A^m\otimes H_B^n$, there exist orthogonal basis $|\phi_1\rangle,\ldots,|\phi_m\rangle$ of H_A^m and orthogonal basis $|\psi_1\rangle,\ldots,|\psi_n\rangle$ of H_B^n, such that $|v\rangle=\lambda_1|\phi_1\rangle\otimes|\psi_1\rangle+\cdots+\lambda_d|\phi_d\rangle\otimes|\psi_d\rangle$, where $d\leqslant\min\{m,n\}$. This is Schmidt decomposition (see Ref. 39). It is clear that d is an invariant under local unitary transformations. This number is called the Schmidt rank of the pure state $|v\rangle$. It is clear that $|v\rangle$ is separable if and only if its Schmidt rank is 1. Schmidt rank of pure states on a bipartite quantum system is a classical concept in the theory of quantum entanglement, it is actually the codimension of the invariant $V_A^0(\rho)$ for the pure state $\rho=P_{|v\rangle}$.

Let $\rho=P_{|v\rangle}$ be a pure state on $H_A^m\otimes H_B^n$ with $m\leqslant n$. From Theorem 1 about the invariance of $V_A^0(\rho)$, we can compute it from its Schmidt decomposition $|v\rangle=\Sigma_{i=1}^{d}\lambda_i|\phi_i\rangle\otimes|\psi_i\rangle$. It is clear that $V_A^0(\rho)=\{(r_1,\ldots,r_m)\in CP^{m-1}:(\lambda_1 r_1,\ldots,\lambda_d r_d,0,\ldots,0)^\tau=0\}$.

Proposition 1: For the pure state $\rho=P_{|v\rangle}$, $d=m$ *if and only if* $V_A^0(\rho)=\varnothing$ *and* $d=m-1-dim(V_A^0(\rho))=n-1-dim(V_B^0(\rho))$ *if* $d\leqslant m-1$.

In this way we show that the Schmidt rank of a pure state is just the codimension of the algebraic set, and thus it seems interesting to study the quantity $m-1-\dim(V_A^k(\rho))$ for mixed states, since it is nonlocal invariant and the generalization of the classical concept of Schmidt rank of pure states.[14,42]

IV. EXAMPLES

Now we give some examples to show how to use Theorems 1, 2, and 3 to construct and distinguish the entangled classes of the mixed states.

Example 3: Let $H=H_A^m\otimes H_B^n$ and $\rho_{a_1,\ldots,a_n}=(1/n)(\Sigma_{i=1}^n P_{a_i\otimes|i\rangle})$, where a_i, $i=1,\ldots,n$, are unit vectors in H_A^m. This is a rank n separable mixed state. Suppose $a_i=(a_i^1,\ldots,a_i^m)$, $i=1,\ldots,n$, the expansion with respect to the standard basis $|1\rangle,\ldots,|m\rangle$ of H_A^m. Let $l_i(r_1,\ldots,r_m)=a_i^1r_1+\cdots+a_i^mr_m$ for $i=1,\ldots,n$ be n linear forms. It is easy to check that $V_A^{n-1}(\rho)=\{(r_1,\ldots,r_m):l_1\cdots l_n=0\}$.

Proposition 2: The mixed states $\rho_{a_1,\ldots,a_n}$ and $\rho_{b_1,\ldots,b_n}$ are equivalent under the local unitary transformations if and only if there exists a unitary transformation U_A on H_A^m such that the n vectors $b_1,\ldots,b_n$ are exactly $U_A(a_1),\ldots,U_A(a_n)$, i.e., $b_i=U_A(a_{i_j})$, where $\{i_1,\ldots,i_n\}=\{1,\ldots,n\}$.

Proof: The "if" part is clear. Let $l_i'(r_1,\ldots,r_m)=b_i^1r_1+\cdots+b_i^mr_m$ for $i=1,\ldots,n$. Then $V_A^{n-1}(\rho_{a_1,\ldots,a_n})$ [respectively, $V_A^{n-1}(\rho_{b_1,\ldots,b_n})$] are the union of n hyperplanes defined by $l_i=0$ (respectively $l_i'=0$) for $i=1,\ldots,n$. It should be noted here that these hyperplanes are counted with multiplicities. From Theorem 1 we get the conclusion.

Segre variety $\Sigma_{n,m}$, which is the image of the following map, $\sigma:CP^n\times CP^m\to CP^{(n+1)(m+1)-1}$ where $\sigma([X_0,\ldots,X_n],[Y_0,\ldots,Y_m])=[\ldots,X_iY_j,\ldots]$, is a famous determinantal variety (see Ref. 23, pp. 25 and 26). It is clear that Segre variety is irreducible and not a linear subvariety. We consider the Segre variety $\Sigma_{1,m}$ in the case $n=1$, actually $\Sigma_{1,m}=\{(r_1,\ldots,r_{2n}):\mathrm{rank}(M)\leqslant 1\}$ where M is the following matrix:

$$\begin{pmatrix} r_1 & r_2 & \cdots & r_n \\ r_{n+1} & r_{n+2} & \cdots & r_{2n} \end{pmatrix}. \tag{10}$$

Example 4 (entangled mixed state from Segre variety): Let $H=H_A^{2m}\otimes H_B^2$, $|\phi_i\rangle=(1/\sqrt{2})(|i1\rangle+|(m+i)2\rangle)$ for $i=1,\ldots,m$ and $\rho=(1/m)(P_{|\phi_1\rangle}+\cdots+P_{|\phi_m\rangle})$. This is a mixed state of rank m. By computing $\Sigma_i r_iA_i$ as in the proof of Theorem 2, we get $V_A^1(\rho)=\Sigma_{1,m}$. Thus ρ is an entangled mixed state.

The rank 1 locus $X_{l,n-l-1}=\{\mathrm{rank}(R)\leqslant 1\}$ of the following $2\times(n-1)$ matrix R:

$$\begin{pmatrix} r_0 & \ldots & r_{l-1} & r_{l+1} & \ldots & r_{n-1} \\ r_1 & \ldots & r_l & r_{l+2} & \ldots & r_n \end{pmatrix}$$

is the rational normal scroll (see p. 106 of Ref. 23). The mixed states corresponding to them are as follows.

Example 5 (entangled mixed state from rational normal scroll): Let $H=H_A^{n+1}\otimes H_B^2$ and $|\phi_1\rangle=(1/\sqrt{2})(|01\rangle+|12\rangle),\ldots,|\phi_i\rangle=(1/\sqrt{2})(|(i-1)1\rangle+|i2\rangle),\ldots,|\phi_l\rangle=(1/\sqrt{2})(|(l-1)1\rangle+|l2\rangle),|\phi_{l+1}\rangle=(1/\sqrt{2})(|(l+1)1\rangle+|(l+2)2\rangle),\ldots,|\phi_j\rangle=(1/\sqrt{2})(|j1\rangle+|(j+1)2\rangle),\ldots,|\phi_{n-1}\rangle=(1/\sqrt{2})(|(n-1)1\rangle+|n2\rangle)$. We consider the mixed state $\rho_l=[1/(n-1)](P_{|\phi_1\rangle}+\cdots+P_{|\phi_{n-1}\rangle})$ of rank $n-1$ on H. It is clear from Sec. II that $V_A^1(\rho)=X_{l,n-l-1}\subset CP^n$. From the well-known fact in algebraic geometry (see pp. 92 and 93 of Ref. 23) we have the following result.

Proposition 3. The mixed states $\rho_l, l=1,\ldots,[(n-1)/2]$ are entangled and ρ_l and $\rho_{l'}$ for $l\neq l'$ are not equivalent under local unitary transformations.

We need to recall a well-known result in the theory of determinantal varieties (see Proposition on p. 67 of Ref. 8). Let $M(m,n)=\{(x_{ij}):1\leqslant i\leqslant m,1\leqslant j\leqslant n\}$ (isomorphic to CP^{mn-1}) be the projective space of all $m\times n$ matrices. For an integer $0\leqslant k\leqslant min\{m,n\}$, $M(m,n)_k$ is defined as the locus $\{A=(x_{ij})\in M(m,n):\mathrm{rank}(A)\leqslant k\}$. $M(m,n)_k$ is called generic determinantal varieties.

Proposition 4: $M(m,n)_k$ is an irreducible algebriac subvariety of M of codimension $(m-k)\times(n-k)$.

Suppose $m\leqslant n$, we now construct a mixed state ρ with $V_A^{m-1}(\rho)=M(m,n)_{(m-1)}$.

Example 6 (generic entangled mixed state): Let $H=H_A^{mn}\otimes H_B^m$, where $m\leqslant n$, and A_{ij}, $i=1,\ldots,m$, $j=1,\ldots n$ be $m\times n$ matrix with only nonzero entry at ij position equal to 1. Let A be a blocked $mn\times 1$ matrix with ij block A_{ij}. Here the kth row of A_{ij} in A corresponds to the vector $|(ij)k\rangle$ in the standard basis of H. Hence A is a size $m^2n\times n$ matrix. Let $\rho=(1/D)AA^\dagger$ be a mixed

state on H. (Here D is a normalizing constant.) It is a rank n mixed state.

It is easy to compute $\Sigma_{ij} r_{ij} A_{ij} = (r_{ij})_{1 \leqslant i \leqslant m, 1 \leqslant j \leqslant n}$ (up to a constant). Thus we have $V_A^{m-1}(\rho) = M(m,n)_{(m-1)}$. From Proposition 4 and Theorem 3, ρ is an entangled mixed state.

Example 7: Let $H = H_A^m \otimes H_B^n \otimes H_C^m$, $|\phi_l\rangle = (1/m)\Sigma_{i=1}^m |ili\rangle$ for $l = 1, \ldots, n$ and $\rho = (1/n)(P_{|\phi_1\rangle} + \cdots + P_{|\phi_n\rangle})$ be a rank n mixed state on H. It is clear that under the cut $B:AC$, ρ is separable. However, under the cut $AB:C$, we can check that ρ is just the mixed state in Example 6 and thus entangled. Similarly under the cut $A:BC$, ρ is also the mixed state in Example 6 and thus entangled. Hence this is a mixed state on tripartite quantum system with the property that it is separable under $B:AC$ cut and entangled under $AB:C$ and $A:BC$ cuts.

Example 8 (entangled mixed states from Eisenbud theorem (Ref. 17): Let $H = H_A^h \otimes H_B^m$, where $h \geqslant nm - m + 2$ and $n \geqslant m$ are positive integers, A_i, $i = 1, \ldots, h$ be $m \times n$ matrix with the property: the space M of linear forms (of $r_1, \ldots, r_h$) span by the entries of $T(r_1, \ldots, r_h) = \Sigma_i r_i A_i$ is of dimension h. Let A be the $hm \times n$ matrix with ith block A_i. Here the kth row of A_i in A corresponds to the vector $|ik\rangle$ in the standard basis of H. Let $\rho = (1/D)AA^\dagger$ (D is a normalizing constant) be a (rank n) mixed state on H. From the proof of Theorem 2 we have $V_A^{m-1}(\rho) = \{(r_1, \ldots, r_h) : \mathrm{rank}(T(r_1, \ldots, r_h)) \leqslant m-1\}$. We observe that when $h = mn$ it is just the mixed state in Example 6.

Theorem 6: *ρ is an entangled mixed state.*

Proof: It is clear that $M(m,n)$ is 1-generic (see Ref. 17, p. 548). We can see that the space M has codimension [in $M(m,n)$] smaller or equal to $m-1$ (here $v = n$, $w = m$, $k = m-1$ as referred to Theorem 2.1 on p. 552 of Ref. 17). From definition it is clear that $V_A(\rho)$ is just M_{m-1}, which is reduced and irreducible and of codimension $n-m+1$ in $M(m,n)$ from Theorem 2.1 of Ref. 17. The conclusion is proved.

Eisenbud theorem (Theorem 2.1 in Ref. 17 and thus Theorem 6 here) gives us a general method to construct many entangled states of low ranks, since the condition about M is not a very strong restriction.

Example 9 (Bennett-DiVincenzo-Mor-Shor-Smolin-Terhal mixed state from UPB (Ref. 7)): Let $H = H_A^2 \otimes H_B^2 \otimes H_C^2$, $|\phi_+\rangle = (1/\sqrt{2})(|1\rangle + |2\rangle)$, $|\phi_-\rangle = (1/\sqrt{2})(|1\rangle - |2\rangle)$. Consider the linear subspace T spaned by the following four vectors $|1\rangle \otimes |2\rangle \otimes |\phi_+\rangle$, $|2\rangle \otimes |\phi_+\rangle \otimes |1\rangle$, $|\phi_+\rangle \otimes |1\rangle \otimes |2\rangle$, $|\phi_-\rangle \otimes |\phi_-\rangle \otimes |\phi_-\rangle$. Now P is the projection to the complementary space $T^\perp$ of T and $\rho = (1/D)P$ is a rank 4 PPT mixed state on H for any bipartite cut (see Ref. 7). It is proved in Ref. 7 that ρ is entangled under the cut $A:B:C$ (thus bound entanglement), however, it is separable under the cuts $A:BC, B:AC, C:AB$. Now we can compute its invariants $V_{AB}^1(\rho)$ and $V_{A:B}^1(\rho)$. It is easy to see from Theorem 3 that $V_{AB}^1(\rho)$ should be linear, however we can see that $V_{A:B}^1(\rho)$ is also linear from our computation below, though it is entangled under the cut $A:B:C$.

It is easy to check that the following four vectors $|010\rangle - |011\rangle$, $|100\rangle - |110\rangle$, $|001\rangle - |101\rangle$, $|000\rangle - |111\rangle$ are the base of $T^\perp$. Thus the matrix A is of the following form (with rows corresponding to $|000\rangle$, $|001\rangle$, $|010\rangle$, $|011\rangle$, $|100\rangle$, $|101\rangle$, $|110\rangle$, $|111\rangle$):

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{11}$$

and $\Sigma_{ij} r_{ij} A_{ij}$ is of the following form:

$$\begin{pmatrix} r_{01} & r_{10} - r_{11} & 0 & r_{00} \\ -r_{01} & 0 & r_{00} - r_{10} & -r_{11} \end{pmatrix}. \tag{12}$$

Thus $V^1_{AB}(\rho)$ is the union of the following three points (1:1:0:0), (0:1:0:1), (0:0:1:0) in CP^3 and $V^1_{A:B}(\rho)$ is union of $CP^1\times(1:0)$, $(0:1)\times CP^1$, and $(1:0)\times(0:1)$ in $CP^1\times CP^1$.

V. GENERALIZED SMOLIN STATE

Smolin[40] introduced a rank 4 mixed state $\rho=\frac{1}{4}(P_{|v_1\rangle}+P_{|v_2\rangle}+P_{|v_3\rangle}+P_{|v_4\rangle})$ on 4-party quantum system $H^2_A\otimes H^2_B\otimes H^3_C\otimes H^2_D$, where

$$|v_1\rangle=\tfrac{1}{2}(|0000\rangle+|0011\rangle+|1100\rangle+|1111\rangle),$$

$$|v_2\rangle=\tfrac{1}{2}(|0000\rangle-|0011\rangle-|1100\rangle+|1111\rangle),$$

$$|v_3\rangle=\tfrac{1}{2}(|0101\rangle+|0110\rangle+|1001\rangle+|1010\rangle),$$

$$|v_4\rangle=\tfrac{1}{2}(|0101\rangle-|0110\rangle-|1001\rangle+|1010\rangle).$$

This mixed state ρ is a bound entangled state when four parties A,B,C,D are isolated.

The following example, which is a continuous family (depending on eight parameters) of mixed state on the four-party quantum system $H^2_A\otimes H^2_B\otimes H^2_C\otimes H^2_D$ separable for any 2:2 cut but entangled for any 1:3 cut (thus bound entangled mixed state when A,B,C,D are isolated), can be thought of as a generalization of Smolin's mixed state in Ref. 40. We prove that the generic members in this family of mixed states are not equivalent under local unitary transformations (Theorem 7 below).

Example 10: Let $H=H^2_A\otimes H^2_B\otimes H^2_C\otimes H^2_D$ and h_1,h_2,h_3,h_4 (understood as row vectors) be four mutually orthogonal unit vectors in C^4 and $a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8$ be eight nonzero real parameters satisfying $a_1a_8=a_2a_7=a_3a_6=a_5a_4$. Consider the 16×4 matrix T with 16 rows as $T=(a_1h_1^\tau,0,0,a_2h_2^\tau,0,a_3h_3^\tau,a_4h_4^\tau,0,0,a_5h_4^\tau,a_6h_3^\tau,0,a_7h_2^\tau,0,0,a_8h_1^\tau)^\tau$. Let $|\phi_1'\rangle$, $|\phi_2'\rangle$, $|\phi_3'\rangle$, $|\phi_4'\rangle$ be four vectors in H whose expansions with the basis $|0000\rangle$, $|0001\rangle$, $|0010\rangle$, $|0011\rangle$, $|0100\rangle$, $|0101\rangle$, $|0110\rangle$, $|0111\rangle$, $|1000\rangle$, $|1001\rangle$, $|1010\rangle$, $|1011\rangle$, $|1100\rangle$, $|1101\rangle$, $|1110\rangle$, $|1111\rangle$ are exactly the four columns of the matrix T. Let $\rho=(1/D)TT^\dagger$ (D is a normalizing constant) be the mixed states (matrix with respect to the standard base of H as above).

It is easy to check that when $h_1=(1/\sqrt{2})(1,1,0,0)$, $h_2=(1/\sqrt{2})(1,-1,0,0)$, $h_3=(1/\sqrt{2})\times(0,0,1,1)$, $h_4=(1/\sqrt{2})(0,0,1,-1)$ and all a_i's are 1, it is just the Smolin's mixed state in Ref. 40.

Now we prove that ρ is invariant under the partial transposes of the cuts $AB:CD,AC:BD,AD:BC$.

Let the "representation" matrix $T=(b^t_{ijkl})_{i=0,1,j=0,1,k=0,1,l=0,1,t=1,2,3,4}$ be the matrix with columns corresponding the expansions of $\phi_1,\phi_2,\phi_3,\phi_4$. Then we can consider that $T=(T_1,T_2,T_3,T_4)^\tau$ as a blocked matrix of size 4×1 with each block $T_{ij}=(b^t_{kl})_{k=0,1,l=0,1,=1,2,3,4}$ a 4×4 matrix, where $ij=00,01,10,11$. Because h_1,h_2,h_3,h_4 are mutually orthogonal unit vectors we can easily check that $T_{ij}T^\dagger_{i'j'}=T_{i'j'}T^\dagger_{ij}$ from the condition $a_1a_8=a_2a_7=a_3a_6=a_5a_4$. Thus it is invariant when the partial transpose of the cut $AB:CD$ is applied.

With the same methods we can check that ρ is invariant when the partial transposes of the cuts $AC:BD$, $AD:BC$ are applied. Hence ρ is PPT under the cuts $AB:CD$, $AC:BD$, $AD:BC$. Thus from a result in Ref. 31 which claims that the PPT mixed states on $H^m_T\otimes H^n_S$ with their ranks not bigger than $\max\{m,n\}$ are separable, we know ρ is separable under these cuts $AB:CD$, $AC:BD$, $AD:BC$.

Now we want to prove ρ is entangled under the cut $A:BCD$ by computing $V^1_{BCD}(\rho)$. From the previous arguments, we can check that $V^1_{BCD}(\rho)$ is the locus of the condition: $a_1h_1r_{000}+a_2h_2r_{011}+a_3h_3r_{101}+a_4h_4r_{110}$ and $a_7h_1r_{100}+a_8h_2r_{111}+a_5h_3r_{001}+a_6h_4r_{010}$ are linear dependent. This is equivalent to the condition that the matrix (8) is of rank 1,

$$\begin{pmatrix} a_7r_{100} & a_8r_{111} & a_5r_{001} & a_6r_{010}\\ a_1r_{000} & a_2r_{011} & a_3r_{101} & a_4r_{110}\end{pmatrix}.$$

From Ref. 23, pp. 25 and 26 we can check that $V^1_{BCD}(\rho)$ is exactly the famous Segre variety in algebraic geometry. It is irreducible and thus cannot be linear. From Theorem 3, ρ is entangled under the cut $A:BCD$. Similarly we can prove that ρ is entangled under the cuts $B:ACD$, $C:ABD$, $D:ABC$.

Now we compute $V^3_{A:B}(\rho)$. From the previous arguments and Definition 2, it is just the locus of the condition that the vectors $h_1(a_1r^1_0r^2_0+a_7r^1_1r^2_1)$, $h_3(a_3r^1_0r^2_1+a_5r^1_1r^2_0)$, $h_4(a_4r^1_0r^2_1+a_6r^1_1r^2_0)$, $h_2(a_2r^1_0r^2_0+a_8r^1_1r^2_1)$ are linear dependent. Since h_1,h_2,h_3,h_4 are mutually orthogonal unit vectors, we have

$$V^3_{A:B}(\rho)=\{(r^1_0,r^1_1,r^2_0,r^2_1)\in CP^1\times CP^1:\\ (a_1r^1_0r^2_0+a_7r^1_1r^2_1)(a_3r^1_0r^2_1+a_5r^1_1r^2_0)(a_4r^1_0r^2_1+a_6r^1_1r^2_0)(a_2r^1_0r^2_0+a_8r^1_1r^2_1)=0\}.$$

Set $\lambda_1=a_1/a_7=a_2/a_8$ and $\lambda_2=a_3/a_5=a_4/a_6$, we know that $V^3_{A:B}(\rho)$ is the union of V_1 and V_2 with multiplicity 2, where

$$V_1=\{(r^1_0,r^1_1,r^2_0,r^2_1)\in CP^1\times CP^1:r^1_0r^2_0-\lambda_1r^1_1r^2_1=0\},$$

$$V_2=\{(r^1_0,r^1_1,r^2_0,r^2_1)\in CP^1\times CP^1:r^1_0r^2_1-\lambda_2r^1_1r^2_0=0\}.$$

From Theorem 3 we know that ρ is entangled for the cut $A:B:CD$, $A:C:BD$, and $A:D:BC$ for generic parameters, since $r^1_0r^2_0+\lambda_1r^1_1r^2_1$, etc., cannot be factorized to two linear forms for generic λ_1. This provides another proof that the mixed state is entangled if the four parties are isolated.

Theorem 7: *The generic members in this continuous family of mixed states are inequivalent under the local unitary transformations on* $H=H^2_A\otimes H^2_B\otimes H^2_C\otimes H^2_D$.

Proof: From the above computation, $V^3_{A:B}(\rho_{\lambda_{1,2}})$ is the union of V_1 and V_2 with multiplicity 2. From Theorem 1′, if $\rho_{\lambda_{1,2}}$ and $\rho\lambda'_{1,2}$ are equivalent by a local operation, there must exist two fractional linear transformations T_1,T_2 of CP^1 such that $T=T_1\times T_2$ (acting on $CP^1\times CP^1$) transforms the two varieties V_1,V_2 of $\rho_{\lambda_{1,2}}$ to the two varieties V'_1,V'_2 of $\rho\lambda'_{1,2}$, i.e., $T(V_i)=V'_j$.

Introduce the inhomogeneous coordinates $x_1=r^1_0/r^1_1$, $x_2=r^2_0/r^2_1$. Suppose $T(V_i)=V'_i$ $i=1,2$ without loss of generality. Then we have $\lambda_1\lambda_2=1$. This means that there are some algebraic relations of parameters if the T exists. This implies that there are some algebraic relations on parameters if $\rho_{\lambda_{1,2}}$ and $\rho\lambda'_{1,2}$ are equivalent by local unitary transformations. Hence our conclusion follows immediately.

VI. NONEMPTY THEOREM

In this section, we prove that the algebraic set invariants introduced in Sec. II are not empty for low rank mixed states.

Theorem 8: *Let* $H=H^m_A\otimes H^n_B$ *be a bipartite quantum system and* ρ *is a rank* r *mixed state on* H *with* $r\leqslant m+n-2$. *Then* $V^{n-1}_A(\rho)$ *and* $V^{m-1}_B(\rho)$ *are not empty.*

Proof: We take "the standard representation" $\rho=\Sigma^r_{i=1}p_iP_{v_i}$, where $p_1,\ldots,p_r$, $v_1,\ldots,v_r$ are eigenvalues and eigenvectors of ρ and $r=\mathrm{rank}(\rho)$. Recall the proof of Theorem 2, $V^{n-1}_A(\rho)$ is the locus of the condition that $\Sigma_ir_tA_i$ (a $n\times r$ matrix) has its rank smaller than n. From Proposition 4 the variety of *generic* $n\times r$ matrices of rank less than or equal to $n-1$ has its codimension smaller or equal to $(n-(n-1))(r-(n-1))=r-n+1$, we know that the codimension of $V^{n-1}_A(\rho)$ in CP^{m-1} is smaller or equal to $r-n+1$. Hence $\dim(V_A(\rho))\geqslant m-1-r+n-1\geqslant 0$ and $V^{n-1}_A(\rho)$ is not empty. The conclusion for $V^{m-1}_B(\rho)$ can be proved similarly.

VII. A RELATION OF DETERMINANTS

As indicated in Sec. II, we can have the following statement from Lemma 2.

Theorem 9: *Let* $H=H^m_A\otimes H^n_B$ *be a bipartite quantum system and* $\rho=\Sigma^t_{l=1}p_lP_{v_l}=\Sigma^s_{l=1}q_lP_{v'_l}$ *be a mixed state with two "representations" as convex combinations of projections with* $p_1,\ldots,p_t,q_1,\ldots,q_s>0$. *Let* A *(respectively,* A'*) be the* $mn\times t$ *(respectively,* $mn\times s$*) matrix of*

vectors $v_1,\ldots,v_t$ *(respectively,* $v_1',\ldots,v_s'$*) in the standard basis* $|11\rangle,\ldots,|1n\rangle,\ldots,|m1\rangle,\ldots,|mn\rangle$ *as in Lemma 1. We represent A (respectively,* A'*) as* $m\times 1$ *blocked matrix with blocks* $A_1,\ldots,A_m$ *(respectively,* $A_1',\ldots,A_m'$*). Then the determinantal varieties defined by the conditions that the ranks of* $R=\Sigma_i r_i A_i$ *and* $R'=\Sigma_i r_i A_i'$ *are smaller than* $k,k=0,1,\ldots,n-1$*, are the same.*

Actually we can get more information about the determinants of $n\times n$ submatrices of $\Sigma_i r_i A_i$ and $\Sigma_i r_i A_i'$ from the proof of Theorems 2 and 3. This relation seems to be helpful to extract information of ρ's one unknown "representation" from its another known "representation," as in the proof of Theorem 3.

Theorem 9′: *Let* $H,\rho,p_1,\ldots p_t,q_1,\ldots,q_s,A,A',R,R'$ *be as above and* $R_{i_1,\ldots i_n}$ *(respectively,* $R'_{i_1'},\ldots,i_n'$*) be the* $n\times n$ *submatrix of R (respectively,* R'*) consisting of* $i_1<\cdots<i_n$ *(respectively,* $i_1'<\cdots<i_n'$)th *columns, where* $i_1,\ldots,i_n\in\{1,\ldots t\}$ *and* $i_1',\ldots,i_n'\in\{1,\ldots,s\}$ *are distinct indices. Then we have*

$$\Sigma_{i_1<\cdots<i_n} p_{i_1}\cdots p_{i_n}|R_{i_1,\ldots,i_n}|^2=\Sigma_{i_1'<\cdots<i_n'} q_{i_1'}\cdots q_{i_n'}|R'_{i_1',\ldots,i_n'}|^2. \tag{13}$$

The above result follows from the following lemma immediately, since both sides of the equality are just $\det(\Sigma_{ij} r_i r_j^\dagger \rho_{ij})$.

Lemma 3 (Binet-Cauchy formula): Let B be a $n\times t$ *matrix with* $t>n$ *and* $B_{i_1,\ldots,i_n}$ *be the* $n\times n$ *submatrix of B consisting of* $i_1<\cdots<i_n$-th *columns. Then* $\det(BB^\dagger)=\Sigma_{i_1<\cdots<i_n}|\det B_{i_1,\ldots,i_n}|^2$.

It is clear that Theorems 2 and 3 follow from Theorem 8′ here immediately.

The following result was previously known in Refs. 29 and 31.

Proposition 5: Let $H=H_A^n\otimes H_B^n$, $\rho=(1/n)\Sigma_{i=1}^n p_i P_{a_i\otimes b_i}$ *where* $a_1,\ldots,a_n$ *(respectively,* $b_1,\ldots,b_n$*) are linearly independent unit vectors in* H_A^n *(respectively,* H_B^n*). Suppose that* $\rho=(1/t)\Sigma_{i=1}^t q_i P_{c_i\otimes d_i}$ *is another representation of* ρ *as a convex combination with* q_i*'s positive, then actually we have* $t=n$ *and* $\{a_1\otimes b_1,\ldots,a_n\otimes b_n\}=\{c_1\otimes d_1,\ldots,c_n\otimes d_n\}$.

Proof: We apply Theorem 9′ to the 2 "representations" here. First of all, we know that $\det(\Sigma_{ij} r_i r_j^\dagger \rho_{ij})$ is (up to a nonzero constant) the square of the absolute value of a multiplication of linear forms $b_i(r_1,\ldots,r_n)=\Sigma_j b_1^j r_j$, where $b_i=\Sigma_j b_i^j|j\rangle$ is the coordinate form of b_i for $i=1,\ldots,n$, from one known "representation." Thus we know from Theorem 8′ that there are at least n vectors in $\{d_1,\ldots,d_t\}$, without loss of generality, suppose they are $d_1,\ldots,d_n$, are just $b_1,\ldots,b_n$. Using Theorem 9′ for the second factor and consider the first through nth columns of R', this implies that the multiplication of the linear forms $c_1(r_1,\ldots,r_n),\ldots,c_n(r_1,\ldots,r_n)$ are just the multiplication of the linear forms $a_1(r_1,\ldots,r_n),\ldots,a_n(r_1,\ldots,r_n)$. Hence we know that the set $\{c_1,\ldots,c_n\}$ are just the set $\{a_1,\ldots,a_n\}$.

On the other hand, it is easy to see that $a_i\otimes b_j$ with $i\neq j$ is not in the linear span of $a_1\otimes b_1,\ldots,a_n\otimes b_n$, since $a_1,\ldots,a_n$ (respectively, $b_1,\ldots,b_n$) are linear independent. Thus $c_i=a_i$ from Corollary 1.

Applying Theorem 9′ to other columns of R and R' by a similar argument, we have $c_j\in\{a_1,\ldots,a_n\}$ and $d_j\in\{b_1,\ldots,b_n\}$. Since $a_i\otimes b_j$ with $i\neq j$ cannot be in the image of ρ, $c_j\otimes d_j$ must be the form $a_{i_j}\otimes b_{i_j}$. The conclusion is proved.

Remark 2: If we compute $V_A^{n-1}(\rho)$ from the representation of ρ's standard form, i.e., linear sum of projections to its eigenvectors, it can be seen that our invariants defined in Sec. II are independent of eigenvalues ($p_1,\ldots,p_t$ in Sec. II). However the information of $p_1,\ldots,p_t$ or eigenvalues is certainly reflected in Theorem 9′ here. Thus Theorem 9′ might be more useful in determining whether a given mixed state is entangled or not, provided that we know how to extract sufficient information from Theorem 9′.

Remark 3: As shown in Example 1, our invariants might be an empty set for high rank mixed states, however it seems that Theorem 9′ is still useful in determining whether a given high rank mixed state is entangled or not in this case, provided that we know how to extract information from Theorem 9′.

VIII. SIMULATION OF HAMILTONIANS

Historically, the idea of simulating Hamiltonian (self-adjoint operators on the Hilbert space corresponding to the quantum system, see Ref. 39) time evolutions was the first motivation for quantum computation because of the famous paper of Feynman. Recently the ability of nonlocal Hamiltonians to simulate one another is a popular topic, which has applications in quantum control theory, quantum computation, and the task of generating entanglement. For the general treatment of this topic and the references, we refer to Ref. 5.

We say, for two bipartite Hamiltonians H and H' on $H_A^m \otimes H_B^n$, H' can be efficiently simulated by H with local unitary operations, write as $H' \prec_{LU} H$, if H' can be written as a convex combination of conjugates of H by local unitary operations, $H' = p_1(U_1 \otimes V_1)H(U_1 \otimes V_1)^\dagger + \cdots + p_s(U_s \otimes V_s)H(U_s \otimes V_s)^\dagger$, where $p_1, \ldots, p_s$ are positive real numbers such that $p_1 + \cdots + p_s = 1$, $U_1, \ldots, U_s$, and $V_1, \ldots, V_s$ are unitary operations on H_A^m and H_B^n, respectively. Here we use $\dagger$ for the adjoint. This is equivalent to the notion "infinitesimal simulation" in Ref. 5. In Ref. 5 it is shown that "local terms" like $I \otimes K_B$ and $K_A \otimes I$ are irrelevant to the simulation problem up to the second order, thus they considered the simulation problem for Hamiltonians without local terms' effect. Our definition here is more restricted without neglecting the local terms.

We can have the following necessary conditions about the simulation of semipositive Hamiltonians based on the algebraic set invariants introduced in Sec. II.

Theorem 10: *Let H and H' be two semipositive Hamiltonians on the bipartite quantum system $H_A^m \otimes H_B^n$. Suppose $H' \prec_{LU} H$, that is, H' can be simulated by H efficiently by using local unitary transformations. Then there are projective isomorphisms U_1 of CP^{m-1} and V_1 of CP^{n-1} such that $U_1(V_A^k(H')) \subset V_A^k(H)$ for $k = 0, \ldots, n-1$ and $V_1(V_B^k(H')) \subset V_B^k(H)$ for $k = 0, \ldots, m-1$.*

The following observation about the computation of $V_A^k(\rho)$ is the key point of the proof of Theorem 10 and Corollary 3. From Corollary 1 if $\rho = \Sigma_i^t p_i P_{v_i}$ with p_i's positive real numbers, the range of ρ is the linear span of vectors $v_1, \ldots, v_t$. We take some vectors in the set $\{v_1, \ldots, v_t\}$, say they are $v_1, \ldots, v_s$. Let B be the $mn \times s$ matrix with columns corresponding to the s vectors $v_1, \ldots, v_s$'s coordinates in the standard basis of $H_A^m \otimes H_B^n$. We consider B as $m \times 1$ blocked matrix with blocks $B_1, \ldots, B_m$ $n \times s$ matrix as in Sec. II. It is clear that $V_A^k(\rho)$ is an algebraic subset of the zero locus of the determinants of all $(k+1) \times (k+1)$ submatrices of $\Sigma_i^m r_i B_i$, since $\Sigma_i^m r_i B_i$ is a submatrix of $\Sigma_i^m r_i A_i$. On the other hand, if $v_1, \ldots, v_s$ are linear independent and $s = \dim(\text{range}(\rho))$, $V_A^k(\rho)$ is just the zero locus of the determinants of all $(k+1) \times (k+1)$ submatrices of $\Sigma_i^m r_i B_i$, since any column in $\Sigma_i r_i A_i$ is a linear combination of columns in $\Sigma_i r_i B_i$ [$\text{rank}(\Sigma_i r_i A_i) \leqslant k$ is equivalent to $\text{rank}(\Sigma_i r_i B_i) \leqslant k$].

Proof of Theorem 10: Suppose $H' \prec_{LU} H$, then there exist positive numbers $p_1, \ldots, p_s$ and local unitary transformations $U_1 \otimes V_1, \ldots, U_s \otimes V_s$, such that $\Sigma_i p_i U_i \otimes V_i H(U_i \otimes V_i)^\dagger = H'$. Let $H = \Sigma_i^s q_i P_{\psi_i}$, where $s = \dim(\text{range}(H))$, $q_1, \ldots, q_s$ are eigenvalues of H and $\psi_1, \ldots, \psi_s$ are eigenvectors of H. Then it is clear that $(U_i \otimes V_i)H(U_i \otimes V_i)^\dagger = \Sigma_j^s q_j P_{(U_i \otimes V_i)\psi_j}$ and thus $H' = \Sigma_{i,j} p_i q_j P_{(U_i \otimes V_i)\psi_j}$. This is a representation of H' as a convex combination of projections. From our above observation $V_A^k(H')$ is an algebraic subset in $V_A^k((U_1 \times V_1)H)$ [which can be computed from vectors $(U_1 \otimes V_1)\psi_1, \ldots, (U_1 \otimes V_1)\psi_s$]. Thus the conclusion follows from Theorem 1.

Corollary 3 (see Ref. 13): Let H and H' be two semipositive Hamiltonians on the bipartite quantum system $H_A^m \otimes H_B^n$ of the same rank, i.e., $\dim(\text{range}(H)) = \dim(\text{range}(H'))$. Suppose $H' \prec_{LU} H$, that is, H' can be simulated by H efficiently by using local unitary transformations. Then $V_A^k(H') = V_A^k(H)$ for $k = 0, \ldots, n-1$ and $V_B^k(H') = V_B^k(H)$ for $k = 0, \ldots, m-1$. Here the equality of the algebraic sets means they are isomorphic via projective linear transformations of complex projective spaces.

Proof: Suppose $H' \prec_{LU} H$, then there exist positive numbers $p_1, \ldots, p_s$ and local unitary transformations $U_1 \otimes V_1, \ldots, U_s \otimes V_s$, such that, $\Sigma_i p_i U_i \otimes V_i H(U_i \otimes V_i)^\dagger = H'$. Let $H = \Sigma_i^s q_i P_{\psi_i}$, where $s = \dim(\text{range}(H))$, $q_1, \ldots, q_s$ are eigenvalues of H and $\psi_1, \ldots, \psi_s$ are eigenvectors of H. Then it is clear that $(U_i \otimes V_i)H(U_i \otimes V_i)^\dagger = \Sigma_j^s q_j P_{(U_i \otimes V_i)\psi_j}$ and thus $H' = \Sigma_{i,j} p_i q_j P_{(U_i \otimes V_i)\psi_j}$. This is a representation of H' as a convex combination of projections. From our above observation $V_A^k(H')$ can be computed from vectors $(U_1 \otimes V_1)\psi_1, \ldots, (U_1 \otimes V_1)\psi_s$, since they are linear independent and s

$=\dim(\mathrm{range}(H'))$. Hence $V_A^k(H')=V_A^k((U_1\otimes V_1)H)$ from the definition. Thus the conclusion follows from Theorem 1.

Let S be the swap operator on the bipartite system $H_A^n\otimes H_B^n$ defined by $S|ij\rangle=|ji\rangle$. For any Hamiltonian H, $S(H)=SHS^\dagger$ corresponds to the Hamiltonian evolution of H with A and B interchanged. It is very interesting to consider the problem if H can be simulated by $S(H)$ efficiently. This led to some important consequences in the discussion VII of Ref. 5. For example it was shown there are examples that H and $S(H)$ cannot be simulated efficiently with one another in higher dimensions ($n\geqslant 3$). Thus in higher dimensions nonlocal degrees of freedom of Hamiltonians cannot be characterized by quantities that are symmetric with respect to A and B, such as eigenvalues. This conclusion is also obtained from our example and Corollary 5 in the next section. From Corollary 3 we have the following necessary condition about $H\prec_{LU}S(H)$.

Corollary 4: Let H be a semipositive Hamiltonian on $H_A^n\otimes H_B^n$. *Suppose* $H\prec_{LU}S(H)$. *Then* $V_A^k(H)=V_B^k(H)$ *for* $k=0,\ldots,n-1$.

The following is a Hamiltonian H on 3×3 system for which H cannot be simulated efficiently by $S(H)$.

Example 11: $H=P_{|\phi_1\rangle}+P_{|\phi_2\rangle}+P_{|\phi_3\rangle}$, where

$$|\phi_1\rangle=\frac{1}{\sqrt{3}}(|11\rangle+|21\rangle+|32\rangle),$$

$$|\phi_2\rangle=\frac{1}{\sqrt{1+|v|^2}}(|12\rangle+v|22\rangle), \tag{14}$$

$$|\phi_3\rangle=\frac{1}{\sqrt{1+|\lambda|^2}}(|13\rangle+\lambda|23\rangle).$$

Then it is easy to compute that $V_A^2(H)$ is the sum of three lines in CP^2 defined by $r_1+r_2=0$, $r_1+vr_2=0$, and $r_1+\lambda r_2=0$ for $v\neq\lambda$ and both v,λ are not 1, and $V_B^2(H)$ is the sum of 2 lines in CP^2 defined by $r_2=0$ and $r_3=0$. Thus we cannot have $H\prec_{LU}S(H)$.

IX. A CONTINUOUS FAMILY OF STATES AND HAMILTONIANS RELATED TO ELLIPTIC CURVES

From a physical point of view, it is very interesting to have isospectral [i.e., eigenvalues of $\rho,\mathrm{tr}_A(\rho),\mathrm{tr}_B(\rho)$ are the same] mixed states, but they are not equivalent under local unitary transformations. This phenomenon indicates that we cannot obtain a complete understanding of a bipartite quantum system by just studying the local and global properties of the spectra of the system. Some examples of such mixed states have been found by several authors (see Nielsen and Kempe[37] and references therein). Their result would imply the existence of continuously many isospectral no-local-equivalent mixed states. Here we give a continuous family of such mixed states by the theory of elliptic curves.[9]

Let $H=H_A^3\otimes H_B^3$ and $\rho_{\eta_1,\eta_2,\eta_3}=\frac{1}{3}(P_{|v_1\rangle}+P_{|v_2\rangle}+P_{|v_3\rangle})$ (η_1,η_2,η_3 are real parameters), a continuous family of mixed states on H, where

$$|v_1\rangle=\frac{1}{\sqrt{3}}(e^{i\eta_1}|11\rangle+|22\rangle+|33\rangle),$$

$$|v_2\rangle=\frac{1}{\sqrt{3}}(e^{i\eta_2}|12\rangle+|23\rangle+|31\rangle), \tag{15}$$

$$|v_3\rangle=\frac{1}{\sqrt{3}}(e^{i\eta_3}|13\rangle+|21\rangle+|32\rangle).$$

It is easy to calculate that Σr_iA_i (up to a constant) is the following 3×3 matrix:

$$\begin{pmatrix} e^{i\eta_1}r_1 & r_3 & r_2 \\ r_2 & e^{i\eta_2}r_1 & r_3 \\ r_3 & r_2 & e^{i\eta_3}r_1 \end{pmatrix}.$$

Thus $V_A^2(\rho_{\eta_1,\eta_2,\eta_3})$ is defined by $e^{i(\eta_1+\eta_2+\eta_3)}r_1^3+r_2^3+r_3^3-(e^{i\eta_1}+e^{i\eta_2}+e^{i\eta_3})r_1r_2r_3=0$ in CP^2. With $e^{i(\eta_1+\eta_2+\eta_3)/3}r_1=r_1'$ we have $r_1'^3+r_2^3+r_3^3-[(e^{i\eta_1}+e^{i\eta_2}+e^{i\eta_3})/(e^{i(\eta_1+\eta_2+\eta_3)/3})]r_1'r_2r_3=0$. This is a family of elliptic curves.

It is easy to check that three nonzero eigenvalues of $\rho_{\eta_1,\eta_2,\eta_3}, \mathrm{tr}_A(\rho_{\eta_1,\eta_2,\eta_3}), \mathrm{tr}_B(\rho_{\eta_1,\eta_2,\eta_3})$ are all the same value $\frac{1}{3}$ for different parameters. In this case we have a family of isospectral (both global and local) mixed states $\rho_{\eta_1,\eta_2,\eta_3}$. Set $g(\eta_1,\eta_2,\eta_3)=(e^{i\eta_1}+e^{i\eta_2}+e^{i\eta_3})/(e^{i(\eta_1+\eta_2+\eta_3)/3})$.

Theorem 11: *$\rho_{\eta_1,\eta_2,\eta_3}$ is entangled mixed state when $(g(\eta_1,\eta_2,\eta_3))^3\neq 27$. Moreover $\rho_{\eta_1,\eta_2,\eta_3}$ and $\rho_{\eta_1',\eta_2',\eta_3'}$ are not equivalent under local unitary transformations if $k(g(\eta_1,\eta_2,\eta_3))\neq k(g(\eta_1',\eta_2',\eta_3'))$, where $k(x)=x^3(x^3+216)^3/(-x^3+27)^3$ is the moduli function of elliptic curves.*

Proof: The conclusion follows from Theorem 3, Theorem 1 and the well-known fact about elliptic curves (see Ref. 9).

In Ref. 36 Nielsen gave a beautiful necessary and sufficient condition for the bipartite pure state $|\psi\rangle$ that can be transformed to the pure state $|\phi\rangle$ by local operations and classical communication (LOCC) based on the majorization between the eigenvalue vectors of the partial traces of $|\psi\rangle$ and $|\phi\rangle$. In Ref. 7 an example was given, from which we know that Nielsen's criterion cannot be generalized to multipartite case, **3EPR** and **2GHZ** are understood as pure states in a $4\times4\times4$ quantum system, they have the same eigenvalue vectors when traced over any subsystem. However it is proved that they are LOCC incomparable in Ref. 7.

In the following example, a continuous family $|\{\phi\}_{\eta_1,\eta_2,\eta_3}\rangle$ of pure states in tripartite quantum system $H_{A_1}^3\otimes H_{A_2}^3\otimes H_{A_3}^3$ is given, the eigenvalue vectors of $\mathrm{tr}_{A_i}(P_{|\phi_{\eta_1,\eta_2,\eta_3}\rangle}), \mathrm{tr}_{A_iA_j}(P_{|\phi_{\eta_1,\eta_2,\eta_3}\rangle})$ are independent of parameters η_1,η_2,η_3. However, the *generic* pure states in this family are entangled and LOCC incomparable. This gives stronger evidence that it is hopeless to characterize the entanglement properties of multipartite pure states by only using the eigenvalue spectra of their partial traces.

Let $H=H_{A_1}^3\otimes H_{A_2}^3\otimes H_{A_3}^3$ be a tripartite quantum system and $|\phi_{\eta_1,\eta_2,\eta_3}\rangle=(1/\sqrt{3})(|v_1\rangle\otimes|1\rangle+|v_2\rangle\otimes|2\rangle+|v_3\rangle\otimes|3\rangle)$, where $|v_1\rangle,|v_2\rangle,|v_3\rangle$ are as in (15). This is a continuous family of pure states in H parametrized by three real parameters. We can check that the eigenvalue vector of any partial trace of $P_{|\phi_{\eta_1,\eta_2,\eta_3}\rangle}$ is a constant vector. On the other hand, it is clear that $\mathrm{tr}_{A_3}(P_{|\phi_{\eta_1,\eta_2,\eta_3}\rangle})=\frac{1}{3}(P_{|v_1\rangle}+P_{|v_2\rangle}+P_{|v_3\rangle})$ is a rank 3 mixed state in $H_{A_1}^3\otimes H_{A_2}^3$. $|\phi_{\eta_1,\eta_2,\eta_3}\rangle$ and $|\phi_{\eta_1',\eta_2',\eta_3'}\rangle$ are not equivalent under local unitary transformations if $k(g(\eta_1,\eta_2,\eta_3))\neq k(g(\eta_1',\eta_2',\eta_3'))$, since their corresponding traces over A_3 are not equivalent under local unitary transformations of $H_{A_1}^3\otimes H_{A_2}^3$ from Theorem 11. Hence the *generic* members of this family of pure states in tripartite quantum system H are entangled and LOCC incomparable from Theorem 1 in Ref. 7.

We can also consider the following continuous family of semipositive Hamiltonians depending on three real parameters, $H_{\eta_1,\eta_2,\eta_3}=P_{|v_1\rangle}+P_{|v_2\rangle}+P_{|v_3\rangle}$, where v_1,v_2,v_3 are as in (15). As calculated above, $V_A^2(H_{\eta_1,\eta_2,\eta_3})$ is just the elliptic curve in CP^2 defined by $r_1^3+r_2^3+r_3^3-[(e^{i\eta_1}+e^{i\eta_2}+e^{i\eta_3})/(e^{i(\eta_1+\eta_2+\eta_3)/3})]r_1r_2r_3=0$. The elliptic curve $V_A^2(H_{\eta_1,\eta_2,\eta_3})$ is not isomorphic to the elliptic curve $V_A^2(H_{\eta_1',\eta_2',\eta_3'})$ if $k(g(\eta_1,\eta_2,\eta_3))\neq k(g(\eta_1',\eta_2',\eta_3'))$. Thus we have the following Corollary of Theorem 9.

Corollary 5: $H_{\eta_1',\eta_2',\eta_3'}$ cannot be simulated by H_{η_1,η_2,η_3} efficiently by using local unitary transformations, i.e., we cannot have $H_{\eta_1',\eta_2',\eta_3'}\prec_{LU}H_{\eta_1,\eta_2,\eta_3}$, if $k(g(\eta_1,\eta_2,\eta_3))\neq k(g(\eta_1',\eta_2',\eta_3'))$, though the three nonzero eigenvalues of H_{η_1,η_2,η_3}, $H_{\eta_1',\eta_2',\eta_3'}$ and their partial traces are all 1.

X. CONSTRUCTING ENTANGLED PPT MIXED STATES

As mentioned in the Introduction, the first several entangled PPT mixed states were constructed in Ref. 24 based on Horodecki's range criterion of separable states, which asserts that a separable mixed state must include sufficiently many *separable pure states* in its own range (see Refs. 24 and 28). This range criterion of separable mixed states was also the base to construct PPT entangled mixed states in the context of unextendible product base (UPB) studied by Bennett, DiVincenzo, Mor, Shor, Smolin, and Terhal in Ref. 6. (We should mention that unextendible product bases also have other physical significance *nonlocality without entanglement*, see Refs. 6 and 28.) It is always interesting and important to have more methods to construct entangled PPT mixed states. In this section, we give an example to show how our separability criterion Theorem 3 can be used to construct entangled mixed states which are invariant under partial transposition (thus PPT and bound entanglement) systematically.

In the following example we construct a family of rank 7 mixed states $\{\rho_{e_1,e_2,e_3}\}$ (e_1,e_2,e_3 are real parameters) with $\rho_{e_1,e_2,e_3}=\rho^{\mathrm{PT}}_{e_1,e_2,e_3}$ (hence PPT automatically) on $H=H_A^4\otimes H_B^6$. We prove that they are entangled by Theorem 3 (thus bound entanglement) for generic parameters e_1,e_2,e_3 and parameters $(e_1,e_2,e_3)=(0,0,1)$. This family and the method used here can be easily generalized to construct entangled mixed states with $\rho=\rho^{\mathrm{PT}}$ systematically.

Consider the following four 6×7 matrices:

$$A_1=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 2 & 0 & 0 & 1\\ 0 & 0 & 0 & 0 & 2 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \end{pmatrix},$$

$$A_2=\begin{pmatrix} 0 & 1 & 1 & -1 & 0 & 0 & 1\\ 1 & 0 & 1 & 0 & 0 & 0 & 0\\ 1 & 1 & 0 & 0 & 0 & 0 & 0\\ -1 & 0 & 0 & 0 & 1 & 1 & 0\\ 0 & 0 & 0 & 1 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{pmatrix},$$

$$A_3=\begin{pmatrix} e_2+e_3 & e_1 & 0 & 0 & 0 & 0 & 0\\ e_1 & e_2 & e_3 & 0 & 0 & 0 & 0\\ 0 & e_3 & e_1+e_2 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & e_2+e_3 & e_1 & 0 & 0\\ 0 & 0 & 0 & e_1 & e_2 & e_3 & 0\\ 0 & 0 & 0 & 0 & e_3 & e_1+e_2 & 0 \end{pmatrix},$$

where e_1,e_2,e_3 are real parameters, and $A_4=(I_6,0)$, where I_6 is the 6×6 unit matrix.

Let A be a 24×7 matrix with four blocks A_1,A_2,A_3,A_4 where the 24 rows correspond to the standard basis $\{|11\rangle,\ldots,|16\rangle,\ldots,|41\rangle,\ldots,|46\rangle\}$. Let ρ_{e_1,e_2,e_3} be $(1/D)AA^\dagger$ (where D is a normalizing constant), a mixed state on H. It is easy to check that $A_iA_j^\dagger=A_jA_i^\dagger$, hence ρ_{e_1,e_2,e_3} is invariant under partial transposition and thus PPT.

Let $|\psi_1\rangle,\ldots,|\psi_7\rangle\in H_A^4\otimes H_B^6$ be seven vectors corresponding to seven columns of the matrix A. It is clear that the range of ρ_{e_1,e_2,e_3} is the linear span of $|\psi_1\rangle,\ldots,|\psi_7\rangle$. When $e_1=e_2=0$, $e_3=1$,

$|\psi_2\rangle - |\psi_3\rangle = (|1\rangle + |4\rangle - |2\rangle) \otimes (|2\rangle - |3\rangle)$. Thus there are some separable pure states in the range of $\rho_{0,0,1}$. We will show that $\rho_{0,0,1}$ and ρ_{e_1,e_2,e_3} for generic parameters e_1, e_2, e_3 are entangled by our separability criterion Theorem 3.

As in the proof of Theorem 2 it is easy to compute $F = r_1A_1 + r_2A_2 + r_3A_3 + r_4A_4$,

$$\begin{pmatrix} u_1 & r_2+e_1r_3 & r_2 & -r_2 & 0 & 0 & r_2 \\ r_2+e_1r_3 & u_1' & r_2+e_3r_3 & 0 & 0 & 0 & 0 \\ r_2 & r_2+e_3r_3 & u_1'' & 0 & 0 & 0 & 0 \\ -r_2 & 0 & 0 & u_2 & r_2+e_1r_3 & r_2 & r_1 \\ 0 & 0 & 0 & r_2+e_1r_3 & u_2' & r_2+e_3r_3 & 0 \\ 0 & 0 & 0 & r_2 & r_2+e_3r_3 & u_2'' & 0 \end{pmatrix} \tag{16}$$

where $u_1 = r_1 + r_4 + (e_2+e_3)r_3$, $u_1' = r_1 + r_4 + e_2r_3$, $u_1'' = r_1 + r_4 + (e_1+e_2)r_3$ and $u_2 = 2r_1 + r_4 + (e_2+e_3)r_3$, $u_2' = 2r_1 + r_4 + e_2r_3$, $u_2'' = 2r_1 + r_4 + (e_1+e_2)r_3$.

We consider the following matrix F' which is obtained by adding the seventh column of F to the fourth column of F and adding r_2/r_1 of the seventh column to the first column,

$$\begin{pmatrix} v_1 & r_2+e_1r_3 & r_2 & 0 & 0 & 0 & r_2 \\ r_2+e_1r_3 & u_1' & r_2+e_3r_3 & 0 & 0 & 0 & 0 \\ r_2 & r_2+e_3r_3 & u_1'' & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & v_2 & r_2+e_1r_3 & r_2 & r_1 \\ 0 & 0 & 0 & r_2+e_1r_3 & u_2' & r_2+e_3r_3 & 0 \\ 0 & 0 & 0 & r_2 & r_2+e_3r_3 & u_2'' & 0 \end{pmatrix}, \tag{17}$$

where $v_1 = r_1 + r_4 + (e_2+e_3)r_3 + (r_2^2/r_1)$, $v_2 = 3r_1 + r_4 + (e_2+e_3)r_3$.

It is clear that the determinantal varieties defined by F and F' are the same in the affine chart C^3 defined by $r_1 \neq 0$. Consider the zero locus Z_1 defined by the condition that the determinants of the two diagonal 3×3 submatrices of the first 6×6 submatrix in (17) are zero, locus Z_2 defined by the condition that the first three rows in (17) are linear dependent and the locus Z_3 defined by the condition that the last three rows in (17) are linear dependent, it is clear that $V_A^5(\rho_{e_1,e_2,e_3}) \cap C^3$ is the sum of Z_1, Z_2, Z_3. We can use the affine coordinates $r_2' = r_2/r_1$, $r_3' = r_3/r_1$, $r_4' = r_4/r_1$ on the affine chart C^3 of CP^3 defined by $r_1 \neq 0$. In this affine coordinate system all r_2, r_3, r_4 should be replaced by r_2', r_3', r_4' and r_1 should be replaced by 1 in (17). Now we analyze $V_A^5(\rho_{0,0,1})$. It is clear that the following two planes $H_1 = \{(r_2', r_3', r_4') : r_2' = r_4' + 1\}$, $H_2 = \{(r_2', r_3', r_4') : r_2' = r_4' + 2\}$ are in $V_A^5(\rho_{0,0,1}) \cap C^3$, since in the case $r_2' = r_4' + 1$ the second and the third rows of (17) are linearly dependent and in the case $r_2' = r_4' + 2$ the fifth and sixth rows of (17) are linearly dependent. The determinants of two 3×3 diagonal submatrices of the first 6×6 submatrix of (17) are

$$(r_2' - r_4' - 1)((r_2')^3 + (r_2')^2 r_4' - (r_2')^2 + (r_4')^2 + r_2'r_3' + r_2'r_4' + r_3'r_4' + r_2' + r_3' + 2r_4' + 1)$$

and

$$(r_2' - r_4' - 2)((r_4')^2 - 2(r_2')^2 + r_2'r_3' + r_2'r_4' + r_3'r_4' + 3r_2' + 2r_3' + 5r_4' + 6).$$

Let X_1 and X_2 be the zero locus of the second factors of the above two determinants. It is obvious that $X_1 \cap X_2$ is in $V_A^5(\rho_{0,0,1}) \cap C^3$, we want to show that $X_1 \cap X_2 \backslash H_1 \cup H_2$ is a curve, not a line. Take the point $P = (0, 2, -1) \in X_1 \cap X_2 \cap H_1$, the tangent plane H_3 of X_2 at P is defined by $4r_2' + r_3' + 5r_4' = -3$. If $X_1 \cap X_2$ is a line around the point P, this line is contained in $H_3 \cap X_2$. However we can easily find that $H_3 \cap X_2$ is defined by $3(r_2')^2 + 2(r_4')^2 + 4r_2'r_4' + 4r_4' = 0$. This polynomial is irreducible and thus $H_3 \cap X_2$ is a curve around the point P. Thus $X_1 \cap X_2$ is a curve around the point P. It is easy to check that $X_1 \cap X_2$ is not contained in H_1 around the point P. This implies that $V_A^5(\rho_{e_1,e_2,e_3}) \cap C^3$ (actually the locus Z_1) contains a curve (not a line) for generic parameters e_1, e_2, e_3 (including parameters 0,0,1) from algebraic geometry. Thus if $V_A^5(\rho_{e_1,e_2,e_3}) \cap C^3$ is the sum

of (affine) linear subspaces, it must contain a dimension 2 affine linear subspace H_4 other than H_1 and H_2 of the affine chart C^3. Thus the determinants of all 6×6 submatrices of (17) must contain a (fixed) affine linear form (i.e., a degree one polynomial of r_2, r_3, r_4 which may contain a constant term) other than r_2-r_4-1 and r_2-r_4-1 as one of their factors. This affine linear form defines that dimension 2 linear affine subspace H_4 of C^3. However it is easy to check that this is impossible for generic parameters e_1, e_2, e_3 (including parameters 0,0,1). We know that $V_A^5(\rho_{e_1,e_2,e_3})\cap C^3$ cannot be the sum of (affine) linear subspaces of C^3 for generic e_1, e_2, e_3 (including parameters 0,0,1). Thus from Theorem 3, ρ_{e_1,e_2,e_3} is entangled for generic parameters e_1, e_2, e_3 (including parameters 0,0,1).

Theorem 12: *The mixed states* ρ_{e_1,e_2,e_3}*'s, which are invariant under partial transposition, are entangled for generic parameters and* $(e_1, e_2, e_3)=(0,0,1)$.

Remark 4: $\rho_{0,0,1}$ is the first example of PPT entangled mixed state (thus bound entanglement) with some separable pure states in its range.

From the construction in this example we can see if $A_1, \ldots, A_m$ are $mn\times t$ matrices satisfying $A_iA_j^\dagger = A_jA_i^\dagger$, A is the $m\times 1$ matrix with ith block A_i and the rows of A correspond to the basis $|11\rangle, \ldots, |1n\rangle, \ldots, |m1\rangle, \ldots, |mn\rangle$ of $H_A^m\otimes H_B^n$, then the mixed state $\rho=(1/D)AA^\dagger$, where D is a normalized constant, is invariant under partial transpose. It is not very difficult to find such matrices. For the purpose that the constructed mixed state ρ is entangled (thus a bound entangled mixed state), we just need that the determinantal variety $\{(r_1, \ldots, r_m): \mathrm{rank}(\Sigma r_iA_i)\leqslant n-1\}$ is not linear. We know from algebraic geometry, it is not very hard to find such matrices $A_1, \ldots, A_m$. However, as illustrated in this Example we do need some explicit calculation to prove this point. Thus our separability criterion and the method used in this Example offer a new systematic way to construct PPT bound entangled mixed states.

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Observables of angular momentum as observables on the Fedosov quantized sphere

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In this paper we construct quantum mechanical observables of a single free particle that lives on the surface of the two-sphere $\mathbb{S}^2$ by implementing the Fedosov $*$-formalism. The Fedosov $*$ is a generalization of the Moyal star product on an arbitrary symplectic manifold. After their construction we show that they obey the standard angular momentum commutation relations in ordinary nonrelativistic quantum mechanics. The purpose of this paper is threefold. One is to find an exact, nonperturbative solution of these observables. The other is to verify that the commutation relations of these observables correspond to angular momentum commutation relations. The last is to show a more general computation of the observables in Fedosov $*$-formalism; essentially an undeformation of Fedosov's algorithm. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2195529]

I. INTRODUCTION

The Moyal star product formalism is an equivalent way to do quantum mechanics.[1] The idea is that instead of using abstract linear operators on a Hilbert space such as position $\hat{x}$ and momentum $\hat{p}$, we may use classical variables x and p however we change the product so that the commutation relations are the same as in the Hilbert space formalism. Namely,

$$[\hat{x}^a,\hat{p}_b]=i\hbar\,\delta^a_b,\quad [\hat{x}^a,\hat{x}^b]=0=[\hat{p}_a,\hat{p}_b],$$

become

$$[x^a,p_b]_*=i\hbar\,\delta^a_b,\quad [x^a,x^b]_*=0=[p_a,p_b]_*$$

we use the convention that the lower case indices run from $1,\ldots,n$ and capital ones run from $1,\ldots,2n$ and

$$[f,g]_*=f*g-g*f,$$

where f and g are any 2 functions of x and p.

We note that the limit $\hbar\to 0^+$ gives the ordinary product of functions.

The definition of the Moyal star for $\mathbb{R}^{2n}$ explicitly is

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$$f * g = f e^{(i\hbar/2)\omega^{AB}\overleftarrow{\partial}_A\overrightarrow{\partial}_B} g = fg + \frac{i\hbar}{2}\omega^{AB}(\partial_A f)(\partial_B g) - \frac{\hbar^2}{8}\omega^{CE}\omega^{AB}(\partial_C\partial_A f)(\partial_E\partial_B g) + \cdots ,$$

where $\partial_A = (\partial/\partial x^a, \partial/\partial p_a)$ and the arrow determines the direction that the derivative acts and the operator $\omega^{AB}\overleftarrow{\partial}_A\overrightarrow{\partial}_B$ is called the Poisson bracket.

There is an invertible map called the Weyl transform $\mathcal{W}$ that translates from the Hilbert space formalism to the Moyal formalism. The main property of this transform is that an arbitrary Taylor series operator on the Hilbert space (note that this is effectively an arbitrary operator since we can use the commutators to rearrange each term so that the x's are to the left and the p's are to the right):

$$\hat{A} = \sum_{m,n} A_{a_1\cdots a_m}{}^{b_1\cdots b_n}\hat{x}^{a_1}\cdots\hat{x}^{a_m}\hat{p}_{b_1}\cdots\hat{p}_{b_n}$$

becomes by applying the Weyl transform

$$\mathcal{W}(\hat{A}) = A = \sum_{m,n} A_{a_1\cdots a_m}{}^{b_1\cdots b_n}x^{a_1} * \cdots * x^{a_m} * p_{b_1} * \cdots * p_{b_n}$$

in a mechanical way by simply replacing each $\hat{x}$ with x, $\hat{p}$ with p and placing stars between each of them as is done above.[1]

The trace over an operator of compact support goes to

$$\mathrm{Tr}(\hat{A}) \overset{\mathcal{W}}{\leftrightarrow} \mathrm{Tr}_*(A) := \frac{1}{(2\pi\hbar)^n}\int \frac{\omega^n}{n!}A.$$

So if we are given the Hamiltonian $\hat{H}$ and the density matrix $\hat{\rho}$ we may map

$$\hat{H} \overset{\mathcal{W}}{\leftrightarrow} H, \quad \hat{\rho} \overset{\mathcal{W}}{\leftrightarrow} \rho.$$

We thus can get the time-independent Schrödinger equation by mapping

$$\hat{H}\hat{\rho}_n = E_n\hat{\rho}_n, \quad [\hat{H},\hat{\rho}_n] = 0$$

to

$$H * \rho_n = E_n\rho_n, \quad [H,\rho_n]_* = 0,$$

where ρ_n are called the Wigner functions. This also works with the time-dependent Schrödinger equation. (See Fedosov for clarification.[2])

Also expectation values become

$$\mathrm{Tr}(\hat{\rho}\hat{A}) \leftrightarrow \mathrm{Tr}_*(\rho * A).$$

The Moyal $*$ has been generalized to an arbitrary smooth symplectic manifold $(\mathcal{N},\omega,D)$ endowed with a preserved two-form ω (called the symplectic form) and a phase-space connection D by Fedosov[2] (an excellent summary is Ref. 3). For any such manifold $(\mathcal{N},\omega,D)$ he gives a perturbative expansion for his $*$-product. However, the convergence issues of the Fedosov $*$, in general, remain unknown.

The properties of the Fedosov $*$ are

(i) It is an associative (but not commutative) map $*: C^\infty(\mathcal{N})\times C^\infty(\mathcal{N}) \to C^\infty(\mathcal{N})$.
(ii) Invariant under *all* smooth coordinate transformations of the phase-space variables x and p.
(iii) No assumed Hamiltonian.
(iv) The Fedosov $*$ is given perturbatively given any symplectic manifold $(\mathcal{N},\omega,D)$.
(v) In the limit $\hbar \to 0^+$, $*$ becomes the ordinary pointwise multiplication of functions on $\mathcal{N}$.
(vi) To first order in $\hbar$ the commutator is the Poisson bracket $[f,g]_* = i\hbar\{f,g\} + \mathcal{O}(\hbar^2)$.

(vii) When $\mathcal{N}=T^*\mathbb{E}^n$ (i.e., the phase space or the cotangent bundle of $\mathbb{E}^n$) (here $\mathbb{E}^n$ stands for Euclidean n-dimensional space) we get the Moyal $*$.

In this paper we restrict $\mathcal{N}$ to be the cotangent bundle of a manifold with metric g $(\mathcal{M},g)$ denoted $T^*\mathcal{M}$. (The cotangent bundle of any manifold is known to be a symplectic manifold.) The reason to do this is that the cotangent bundle of a manifold is the phase space of that manifold (i.e., the space of all coordinates x and momentum p). In quantum mechanics using the Moyal $*$ the phase space is the arena for quantization by giving proper $*$-commutation relations between the x's and p's. The importance of the Fedosov $*$-formalism is that it is a coordinate invariant way of constructing these commutation relations on general $T^*\mathcal{M}$ in such a way that they patch consistently to any coordinate map of the cotangent bundle. Also another important point is that it can be constructed at least perturbatively for any cotangent bundle.

However unlike Fedosov who defines a formulation based on the deformation of covectors (i.e., covectors equipped with a Moyal-type product between them) we will not. We will introduce a Heisenberg algebra generated by $\tilde{s}$ and $\tilde{k}$ ($[\tilde{s}^i,\tilde{s}^j]=[\tilde{k}_i,\tilde{k}_j]=0$, $[\tilde{s}^i,\tilde{k}_j]=i\hbar\delta^i_j$ where i and j run from 1 through $2n$) at every point of our phase-space $T^*\mathcal{M}$. The motivation to do this instead of Fedosov's way is to make a more direct connection between ordinary quantum mechanics involving Heisenberg algebras and the state spaces that the algebra acts on called Hilbert spaces. We then define this algebra to be linear operators on a Hilbert space which, of course, will eventually contain our states. This new construction will still preserve all of the essential properties of the original Fedosov $*$ albeit reformulated so as to apply to different objects. It will be a quantization procedure, i.e., a map of the variables on the phase-space x and p to the observables $\hat{x}$ and $\hat{p}$ which are linear operators on the Hilbert space.

The properties of the Fedosov $*$-quantization in our construction are

(i) $\hat{x}$ and $\hat{p}$ form an associative but noncommutative algebra.
(ii) The map from $(x,p)\rightarrow(\hat{x},\hat{p})$ is invariant under *all* smooth canonical coordinate transformations of the phase-space variables x and p.
(iii) No assumed Hamiltonian.
(iv) We can construct the $\hat{x}$ and $\hat{p}$ perturbatively given any $(T^*\mathcal{M},\omega,D)$.
(v) In the limit $\hbar\rightarrow 0^+$, $\hat{x}$ and $\hat{p}$ become x and p, respectively, i.e., the ordinary variables on $T^*\mathcal{M}$.
(vi) To first order in $\hbar$ the commutator is the Poisson bracket $[\hat{f},\hat{g}]=i\hbar\{\hat{f},\hat{g}\}+\mathcal{O}(\hbar^2)$.
(vii) When $\mathcal{M}=\mathbb{R}^n$ we get the ordinary quantum mechanics.

In the present work we take as our symplectic manifold $T^*\mathbb{S}^2$, the phase space of a single particle on the 2-sphere, $\mathbb{S}^2$. For this space we construct the Fedosov observables nonperturbatively. The advantage of choosing $\mathbb{S}^2$ is that we had suspected previous to the calculation that the commutators are the same as the usual angular momentum commutators in nonrelativistic quantum mechanics. Saying in fact that the theory of angular momentum is the quantization of the two-sphere without the need for it to be embedded in $\mathbb{R}^3$.

Outline: We will follow the basic scheme of keeping derivations sufficiently general so as to apply to a completely general manifold with metric $(\mathcal{M},g)$ and then state results from our specific case of the sphere.

In Sec. II we introduce the phase-space connection. We introduce the basis of covectors of matrices/operators $\hat{y}^A$ on the cotangent bundle in Sec. III. In Sec. IV we attempt to motivate and solve for a new derivation $\hat{D}$. Also we talk a bit about $\hat{D}$'s ambiguities. Moving into Sec. V we explicitly compute the quantities $\hat{x}$ and $\hat{p}$. In Sec. VI we compute the commutators $[\hat{x}^a,\hat{x}^b]$, $[\hat{x}^a,\hat{p}_b]$, and $[\hat{p}_a,\hat{p}_b]$ using the explicit forms of the operators. Section VII explains how one would construct states of angular momentum on $T^*\mathbb{S}^2$ by finally introducing the standard Hamiltonian in ordinary nonrelativistic quantum mechanics. Up until this point no Hamiltonian was assumed.

II. THE PHASE-SPACE CONNECTION FOR $T^*\mathbb{S}^2$

Before we begin, we note the use of the convention that the lower case are the indices of $\mathcal{M}$ (these run from $1,\ldots,n$) and capital ones are the indices of the phase-space $T^*\mathcal{M}$ (these run from $1,\ldots,2n$).

We start with the phase space of a single classical particle confined to a general manifold $(\mathcal{M},g)$. The objects needed are the phase space, $T^*\mathcal{M}$ which is the cotangent bundle of $\mathcal{M}$, an affine connection on the phase space D and the symplectic form ω of $T^*\mathcal{M}$.

A phase-space connection's action on all functions $f(x,p)\in T^*\mathcal{M}$ and a basis of covectors $\Theta^A\in T^*T^*\mathcal{M}$ are

$$Df = \mathrm{d}f = \frac{\partial f}{\partial x^a}\mathrm{d}x^a + \frac{\partial f}{\partial p_a}\mathrm{d}p_a,$$

$$D\otimes\Theta^A = \Gamma^A_B\otimes\Theta^B = \Gamma^A_{BC}\Theta^C\otimes\Theta^B$$

in such a way as to preserve the symplectic form $\omega=\mathrm{d}p_a\wedge\mathrm{d}x^a$ on $T^*\mathbb{S}^2$ $(D\otimes\omega=0)$ where $D=\Theta^C D_C$, $D_C\Theta^A=\Gamma^A_{BC}\Theta^B$ and Γ^A_{BC} is the Christoffel symbol in this basis.

Additionally we impose that D be torsion-free $(D^2f=0)$ and that it corresponds to the Levi-Civita connection on $\mathcal{M}$ when it acts on functions of x and $\mathrm{d}x$. Of course we extend to vectors and higher tensors by the Leibnitz rule.

In the specific case of $\mathbb{S}^2$ $(T^*\mathbb{S}^2)$ we employ the convention that the lower/upper-case indices be of the embedding space $\mathbb{E}^3$ $(T^*\mathbb{E}^3)$ running from 1, 2, 3 (1,…,6) instead of 1, 2 (1,…,4). We note before continuing that the calculation of the Fedosov observables is *inherently* two space-time dimensional. The third coordinate is merely for convenience. We see this fact manifest itself by the two conditions (e.g., $\underline{x}\cdot\underline{x}=1$ and $\underline{x}\cdot\underline{p}=0$) on the three coordinates every step of the way.

The natural objects and quantities on $T^*\mathbb{S}^2$ are

(i) The induced $\mathbb{S}^2$ metric g by the $\mathbb{E}^3$ embedding metric δ.
(ii) The induced $T^*\mathbb{S}^2$ symplectic form ω by the $T^*\mathbb{E}^3$ embedding symplectic form.
(iii) Also the equations defining $T^*\mathbb{S}^2$ inside of $T^*\mathbb{E}^3$, $\underline{x}\cdot\underline{x}=\delta_{ab}x^ax^b=1$ and $\underline{x}\cdot\underline{p}=x^ap_a=0$.
(iv) A torsion-free phase-space connection $D=\Theta^AD_A$ on $T^*\mathbb{S}^2$ that preserves all of the above conditions along with the symplectic form ω and there subsequent derivatives. In other words,

$$D^l\otimes g = D^l\otimes\omega = D^l(\delta_{ab}x^ax^b) = D^l(x^ap_a) = 0$$

for all positive integers l where $g=g_{ab}\,\mathrm{d}x^a\vee\mathrm{d}x^b$, $\omega=\omega_{AB}\Theta^A\wedge\Theta^B$, where Θ^A is basis of forms and $\vee$, $\wedge$ are the symmetric, antisymmetric tensor products, respectively, that we will omit because it will be clear when we mean the one or the other.

We define a basis of covectors or forms by

$$\Theta^A = (\theta^a,\alpha_a),$$

where the θ's are the first three Θ's and the α's are the last three Θ's. θ and α are defined to be

$$\underline{\alpha} := \underline{x}\times\mathrm{d}\underline{p},$$

$$\underline{\theta} := \underline{x}\times\mathrm{d}\underline{x}.$$

The metric on $\mathbb{S}^2$ is

$$g = \underline{\theta}\cdot\underline{\theta}.$$

The phase-space connection we use for $T^*\mathbb{S}^2$ is

$$D\underline{x} := \mathrm{d}\underline{x} = \underline{\theta} \times \underline{x},$$

$$D\underline{p} := \mathrm{d}\underline{p} = \underline{\alpha} \times \underline{x} - \underline{p} \times \underline{\theta},$$

$$D \otimes \underline{\theta} = \underline{\theta} \otimes_{\times} \underline{\theta}, \quad (D\theta)$$

$$D \otimes \underline{\alpha} = \underline{\theta} \otimes_{\times} \underline{\alpha} - \tfrac{2}{3}(\underline{\theta} \times \underline{x}) \otimes (\underline{p} \cdot \underline{\theta}) + \tfrac{1}{3}(\underline{p} \cdot \underline{\theta}) \otimes (\underline{\theta} \times \underline{x}), \quad (D\alpha)$$

and its corresponding curvature

$$D^2\underline{x} := 0,$$

$$D^2\underline{p} := 0,$$

$$D^2 \otimes \underline{\theta} = \tilde{\omega} \otimes (\underline{x} \times \underline{\theta}), \quad (D^2\theta)$$

$$D^2 \otimes \underline{\alpha} = \tilde{\omega} \otimes (\underline{x} \times \underline{\alpha}) + \tfrac{1}{3}(\underline{\alpha}(\underline{\theta} \otimes_{\cdot} \underline{\theta}) - \underline{\theta}(\underline{\alpha} \otimes_{\cdot} \underline{\theta}) - 2\omega \otimes \underline{\theta}). \quad (D^2\alpha)$$

III. INTRODUCING THE $\hat{y}$'s

Following Fedosov, we are going to introduce some machinery namely the operators $\hat{y}$'s to calculate the observables on general manifold $\mathcal{M}$. However, unlike Fedosov who defines these $\hat{y}$'s as covectors equipped with a Moyal-type product between them we choose a different starting point. We define the $\hat{y}$'s at fixed point to be a Heisenberg algebra $[\hat{y}^A, \hat{y}^B] = i\hbar\omega^{AB}$ where ω^{AB} is the inverse of ω_{AB} with $\omega^{AB}\omega_{BC} = \delta^A_C$. More explicitly $\hat{y}$'s are huge (infinite dimensional) matrices that act on a Hilbert space

$$\hat{y}^A = \begin{pmatrix} y^A_{11}(x,p) & y^A_{12}(x,p) & \cdots \\ y^A_{21}(x,p) & y^A_{22}(x,p) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix},$$

where for each A, j, and k $y^A_{jk} \in C^\infty(T^*\mathcal{M})$.

To make a connection with a more familiar form of the Heisenberg algebra we use Darboux's theorem. Darboux's theorem says that in the neighborhood of each point of $q \in T^*\mathcal{M}$ there exist $2n$ local coordinates $(\tilde{x}^1, \ldots, \tilde{x}^n, \tilde{p}_1, \ldots, \tilde{p}_n)$ [note that these $2n$ coordinates are different from the $2n+2$ embedding coordinates (x^μ, p_μ)], called canonical or Darboux coordinates, such that the symplectic form ω may be written by means of these coordinates as $\omega = \mathrm{d}\tilde{p}_1\,\mathrm{d}\tilde{x}^1 + \cdots + \mathrm{d}\tilde{p}_n\,\mathrm{d}\tilde{x}^n$. Thus in this coordinate system at q the $\hat{y}$'s are expressed as $2n$ operators $(\tilde{s}^1, \ldots, \tilde{s}^n, \tilde{k}_1, \ldots, \tilde{k}_n)$ which have the commutators $[\tilde{s}^i, \tilde{s}^j] = [\tilde{k}_i, \tilde{k}_j] = 0$, $[\tilde{s}^i, \tilde{k}_j] = i\hbar\delta^i_j$ where i and j run from 1 through $2n$. And so at each point the $\hat{y}$'s establish a Heisenberg algebra which acts on a Hilbert space.

Important note: Fedosov actually begins with the $\hat{y}$'s as being an arbitrary basis of ordinary covectors with a Moyal-type product between themselves.[1] We take the point of view that the specific form of the product is irrelevant. All that matters is that we have an algebra with the same commutation relations and the action of the connection is the same on the $\hat{y}$'s.

Defining properties of $\hat{y}$,

$$[\hat{y}^A, \hat{y}^B] = i\hbar\omega^{AB},$$

$$D\hat{y}^A = \Gamma^A{}_B\hat{y}^B = \Gamma^A{}_{BC}\Theta^C\hat{y}^B, \quad \Theta^A = (\theta^a, \alpha_a).$$

The $\hat{y}$'s commute with the set of quantities $\{x, p, \mathrm{d}x, \mathrm{d}p, g, \omega, \hbar, i\}$ where i is the complex unit.

Note: The action of the phase-space connection on $\hat{y}$ is the same as the one on Θ ($D\otimes\Theta^A=\Gamma^A_{BC}\Theta^C\otimes\Theta^B$) and so we regard it as a basis of operator or matrix-valued covectors. [One may be tempted to quantize the manifold by mapping $(x^1,x^2,x^3,p_1,p_2,p_3)$ to the matrices $(\hat{y}^1,\hat{y}^2,\hat{y}^3,\hat{y}^4,\hat{y}^5,\hat{y}^6)$, but we want a coordinate independent formalism and, in general, this is not coordinate independent.] This tells us how to parallel transport the Heisenberg algebra (the $\hat{y}$'s) at one point to the Heisenberg algebra of every other point in a consistent way.

Introducing terminology: In this paper when we say f is a function/form we define it to be a complex Taylor series in its variables. (The set of all of these type of functions is sometimes called the enveloping algebra of its arguments.) Explicitly,

$$f(u,\ldots,v)=\sum_{l,j\text{'s}} f_{j_1\cdots j_l}u^{j_1}\cdots v^{j_l}\quad (j\text{ 's are powers not indices}),$$

where $f_{j_1\cdots j_l}$ are constants while u and v could be any of the set $\{x,p,\mathrm{d}x,\mathrm{d}p,\omega,\hbar,i\}$.

So if f is a function/form of some subset or all of the quantities x, p, $\mathrm{d}x$, $\mathrm{d}p$, ω, $\hbar$, and i it then commutes with the $\hat{y}$'s and will be called a complex-valued function/form. On the contrary a matrix-valued function/form is a complex Taylor series in $\hat{y}$ and possibly some subset or all of the quantities x, p, $\mathrm{d}x$, $\mathrm{d}p$, ω, $\hbar$, and i.

So if $f\,(x,p,\mathrm{d}x,\mathrm{d}p,\omega,\hbar,i)$ is a complex-valued function/form it then commutes with the $\hat{y}$'s. More explicitly with the matrix indices written

$$(\hat{y}^A\hat{y}^B)_{jk}=\Sigma_l\hat{y}^A_{jl}\hat{y}^B_{lk},$$

$$([\hat{y}^A,f])_{jk}:=\hat{y}^A_{jk}f-f\hat{y}^A_{jk}=0.$$

On the contrary a matrix-valued function/form does not. From now on we will not write the matrix indices explicitly.

The end goal: The idea for Fedosov's introduction of the $\hat{y}$'s is to associate to each $f(x,p)\in C^\infty(T^*\mathcal{M})$ a unique observable $\hat{f}(x,p,\hat{y})$,

$$\hat{f}(x,p,\hat{y})=\sum_l f_{A_1\cdots A_l}\hat{y}^{A_1}\cdots\hat{y}^{A_l},\quad (\hat{f})$$

where $f_{A_1\cdots A_l}$ are some unknown functions of x and p to be determined.

Important note: Most of the rest of the sections will be dedicated to finding a solution for $\hat{f}$ (i.e., the coefficients functions $f_{A_1\cdots A_l}$) for each $f(x,p)\in C^\infty(T^*\mathbb{S}^2)$ up to some "reasonable" ambiguity (discussed in Secs. IV and V).

$T^*\mathbb{S}^2$ *explicitly:* Specifically for $T^*\mathbb{S}^2$ we have the induced symplectic form ω of $T^*\mathbb{R}^3$ onto $T^*\mathbb{S}^2$ being

$$\omega=\underline{\alpha}\cdot\underline{\theta}=(\delta^a_b-x^ax_b)\alpha_a\theta^b.$$

We make the convention

$$\hat{y}^A=(s^a,k_a),$$

where the s's are the first three $\hat{y}$'s and the k's are the last three $\hat{y}$'s. [Note that the indices go from 1 to $2n+2$ and are different from the $2n$ operators defined above by $(\tilde{s}^1,\ldots,\tilde{s}^n,\tilde{k}_1,\ldots,\tilde{k}_n)$. The difference between them is the same as the difference between the embedding coordinates $(x^1,\ldots,x^{n+1},p_1,\ldots,p_{n+1})$ and $(\tilde{x}^1,\ldots,\tilde{x}^n,\tilde{p}_1,\ldots,\tilde{p}_n)$.] Using the above formulas we then write the commutation relations

$$[s^a,s^b]=0=[k_a,k_b],\quad [s^a,k_b]=i\hbar(\delta^a_b-x^ax_b).$$

We may assume that $\underline{x}\cdot\underline{s}=\underline{x}\cdot\underline{k}=0$ because we observe that the only part of s and k that affect the commutators are the parts that are perpendicular to x. The irrelevance of the part of s and k

parallel to x stems from the above relations because $[x_a s^a, k_b]=0$ and $[s^a, k_b x^b]=0$ and so we could always subtract off the part of s and k parallel to x and get the same commutators. Since $\underline{x}\cdot\underline{s}=\underline{x}\cdot\underline{k}=0$ we have four independent operators which are required (one for each direction on $T^*\mathbb{S}^2$).

The action of the connection and curvature acting on $\underline{s}$ and $\underline{k}$ is written down directly from the equations $(D\theta)$, $(D\alpha)$, $(D^2\theta)$, and $(D^2\alpha)$,

$$D\underline{s} = \underline{\theta}\times\underline{s},$$

$$D\underline{k} = \underline{\theta}\times\underline{k} - \tfrac{2}{3}\underline{\theta}\times\underline{x}(\underline{p}\cdot\underline{s}) + \tfrac{1}{3}(\underline{p}\cdot\underline{\theta})(\underline{s}\times\underline{x}),$$

$$D^2\underline{s} = \tilde{\omega}(\underline{x}\times\underline{s}),$$

$$D^2\underline{k} = \tilde{\omega}(\underline{x}\times\underline{k}) + \tfrac{1}{3}(\underline{\alpha}(\underline{s}\cdot\underline{\theta}) + (\underline{s}\cdot\underline{\alpha})\underline{\theta} - 2\omega\underline{s}).$$

IV. CONSTRUCTING THE GLOBAL DERIVATION $\hat{D}$

Following Fedosov, we now introduce a global derivation as a matrix commutator $\hat{D}=[\hat{Q},\cdot]$ which is central to constructing the coefficients $f_{A_1\cdots A_l}$ in equation $(\hat{f})$ for each $f(x,p)\in C^\infty(T^*\mathcal{M})$. One possible physical motivation for $\hat{D}$ is that in the next section we will require that all observables $\hat{f}$ must satisfy the equation $(D-\hat{D})\hat{f}(x,p,\hat{y})=0$. We see that on $\hat{f}$ $\hat{D}$ is an infinitesimal translation matrix operator equivalent to D. We then reason that matrix operators corresponding to infinitesimal translations on the cotangent bundle should exist, i.e., $\hat{D}$. The reason that we require that they must exist is because we are constructing the set of *all* physical matrix operators on states and certainly infinitesimal translations are in this set. If this reasoning is correct then the equation $(D-\hat{D})\hat{f}=0$ must be satisfied for all observables $\hat{f}$. Also the case of $T^*\mathbb{R}^n$ may provide some insight since it is the overlap of this formalism and quantum mechanics using the Moyal $*$ (see Appendix D for the example of $T^*\mathbb{R}^n$).

Define the derivation $\hat{D}$ by the graded commutator [graded commutators have the property that $[\hat{Q}_A\Theta^A,w]=[\hat{Q}_A,w]\Theta^A=(\hat{Q}_A w - w\hat{Q}_A)\Theta^A$ where w is an l-form with coefficients $w_{A_1\cdots A_l}$ which are complex-valued functions of the variables x, p, and $\hat{y}$.]

$$\hat{D}=[\hat{Q},\cdot]=[\hat{Q}_A\Theta^A,\cdot], \quad (\hat{D})$$

$$\hat{Q}_A=\sum_l Q_{AA_1\cdots A_l}\hat{y}^{A_1}\cdots\hat{y}^{A_l},$$

where $\Theta^A=(\theta^a,\alpha_a)$ and $Q_{AA_1\cdots A_l}$ are complex-valued functions of x and p that need to be determined. We reiterate that complex-valued functions are not matrices hence they commute with the $\hat{y}$'s.

Again following Fedosov, we can partially determine the functions $Q_{AA_1\cdots A_l}$ by the mysterious equation

$$(D-\hat{D})^2\hat{y}^A=0. \quad (\text{cond } \hat{D})$$

[Fedosov adds an additional condition that makes his $\hat{D}$ unique from a fixed D being $\hat{d}^{-1}r_0=0$ where $\hat{d}^{-1}$ is what he calls δ^{-1} (an operator used in a de Rham decomposition) and r_0 is the first term in the recursive solution. We regard this choice as being artificial and thus omit it from the paper.]

The physical motivation for this equation is still unclear and may lurk in the work of Fedosov. One reason for the above requirement is that in the next section we want to solve the equation $(D-\hat{D})\hat{f}=0$ for $\hat{f}$ and the above is an integrability condition for the solvability of this equation.

We now let $\hat{Q}$ be the sum of two parts the first being the solution in the case of $T^*\mathbb{R}^n$ (Christoffels$=\Gamma=0$),

$$\hat{Q}_A\Theta^A = \omega_{AB}\hat{y}^A\Theta^B + r, \quad (\hat{Q})$$

where

$$r = \sum_l r_{AA_1\cdots A_l}\Theta^A\hat{y}^{A_1}\cdots\hat{y}^{A_l},$$

and $r_{AA_1\cdots A_l}$ are complex-valued functions of x and p that need to be determined. In general, we assume that r has terms that are cubic or higher powers in the $\hat{y}$'s (see Appendix B and Fedosov[2] for clarification).

We rewrite the condition (cond $\hat{D}$) as

$$(D-\hat{D})^2\hat{y}^A = [\Omega - Dr + \hat{\mathrm{d}}r + r^2, \hat{y}^A] = 0,$$

where $\Omega := (1/2i\hbar)\omega_{FN}R^F_{BCE}\Theta^C\Theta^E\hat{y}^N\hat{y}^B$ is the phase-space curvature $(D^2\otimes\Theta^A = R^A_{BCE}\Theta^C\Theta^E\otimes\Theta^B)$ as a commutator and $\hat{\mathrm{d}}h = (1/i\hbar)[\omega_{AB}\hat{y}^A\Theta^B, h]$ where h is a matrix-valued function of x p, dx dp, and $\hat{y}$ (see Appendix A for the proof).

From now on we let

$$\Omega - Dr + \hat{\mathrm{d}}r + r^2 = 0, \quad (r)$$

and keep it in the back of our minds that we could add something that commutes with all $\hat{y}$'s to $\Omega - Dr + \hat{\mathrm{d}}r + r^2$.

Important: To emphasize the importance of this equation the reader should note that the whole Fedosov $*$-formalism hinges on this r existing. We know solutions exists perturbatively in general [Fedosov has the recursive solution for it (Ref. 2, p. 144)], however convergence issues still remain unresolved. On a technical note we have found that solving for r to be the hardest point of the computation of the Fedosov observables because of the need for the right ansatz and the nonlinear equation (r) above that it must solve.

Specifically for the case of $T^*\mathbb{S}^2$ the solution for the curvature as a commutator Ω is

$$\Omega := \tfrac{1}{3}((\underline{s}\cdot\underline{\alpha})(\underline{s}\cdot\underline{\theta}) - s^2\omega) + (\underline{x}\times\underline{k})\cdot\underline{s}\widetilde{\omega}.$$

We then verify that it gives the curvature as commutators,

$$[\Omega, \underline{s}] = [-\underline{k}\cdot(\underline{x}\times\underline{s})\widetilde{\omega}, \underline{s}] = \widetilde{\omega}(\underline{x}\times\underline{s}),$$

$$[\Omega, \underline{k}] = \tfrac{1}{3}(\underline{\alpha}(\underline{s}\cdot\underline{\theta}) + (\underline{s}\cdot\underline{\alpha})\underline{\theta} - 2\omega\underline{s}) + (\underline{x}\times\underline{k})\widetilde{\omega}.$$

To simplify the calculations we set $i\hbar = 1$ which we will eventually put back in the end.

Fedosov at this point would implement an algorithm to construct r perturbatively, however rather than do this we will make an ansatz for r by exploiting the rotational symmetry of the sphere. This will give us an exact solution for r. (On a technical note: we ran the Fedosov algorithm a few times to help us see what form the ansatz should take. Also remember that we require $\Omega - Dr + \hat{\mathrm{d}}r + r^2 = 0$ modulo terms that commute with the $\hat{y}$'s.)

Our ansatz for r is

$$r = r_0 + f(s^2)\underline{z}\cdot\underline{s}(\underline{x}\times\underline{s})\cdot\underline{\theta} + g(s^2)\underline{z}\cdot(\underline{x}\times\underline{s})\underline{s}\cdot\underline{\theta} + h(s^2)\underline{s}\cdot\underline{\theta}, \quad (r \text{ ansatz})$$

where $\underline{z}=\underline{p}-\underline{x}\times\underline{k}$ and $r_0=\frac{1}{3}((\underline{k}\cdot\underline{\theta})s^2-\underline{k}\cdot\underline{s}(\underline{s}\cdot\underline{\theta}))$.

We will now state the results of our calculations because the calculations are just too space consuming and yet at the same time straightforward. Given the formulas for r and Ω and performing lengthy calculations eventually we get

$$Dr = \left(\frac{1}{9}-\frac{2g}{3}+\frac{f}{3}\right)s^2\underline{p}\cdot\underline{s}\tilde{\omega} + f\underline{\alpha}\cdot(\underline{x}\times\underline{s})(\underline{x}\times\underline{s})\cdot\underline{\theta} - g(\underline{s}\cdot\underline{\alpha})\underline{s}\cdot\underline{\theta},$$

$$\hat{\mathrm{d}}r = -\Omega + (2f's^2+3f+g)\underline{z}\cdot\underline{s}\tilde{\omega} - g(\underline{s}\cdot\underline{\alpha})\underline{s}\cdot\underline{\theta} + f\underline{\alpha}\cdot(\underline{x}\times\underline{s})(\underline{x}\times\underline{s})\cdot\underline{\theta},$$

$$r^2 = \left(\frac{1}{9}-\frac{2g}{3}+\frac{f}{3}\right)s^2\underline{p}\cdot\underline{s}\tilde{\omega} + \left(2gf's^2+gf-f^2-\frac{2f}{3}+\frac{g}{3}-\frac{1}{9}\right)s^2\underline{z}\cdot\underline{s}\tilde{\omega},$$

where $f'=\partial f/\partial(s^2)$ for all functions.

Putting these into the equation (r) we obtain a condition for g,

$$g = \frac{s^2\left(\left(f+\frac{1}{3}\right)^2-2f'\right)-3f}{s^2\left(\left(f+\frac{1}{3}\right)+2s^2f'\right)+1}$$

while f and h are left arbitrary as long as g is well defined. This is a necessary and sufficient condition for the equation (r) to hold.

We note that $f=-\frac{1}{3}$, $g=1$ and $f=-\frac{1}{12}$, $g=\frac{1}{4}$ are the only solutions where f and g are constant. We will choose to work with the $f=-\frac{1}{3}$ $g=1$, $h=0$ solution from now on. We choose this solution for the sake of clarity because it turns out to be the easiest to use in the next few sections. However, the reader should note that we calculated the commutators for the general solutions for g, f, and h and obtained the same result for all of them. See Sec. VI for the exact result of the commutators for the particular solution $f=-\frac{1}{3}$, $g=1$, $h=0$ (and hence the solution for the general solutions for g f, and h).

The solution for r for $f=-\frac{1}{3}$, $g=1$, $h=0$ is

$$r = -\tfrac{1}{3}(\underline{p}\cdot\underline{s})((\underline{x}\times\underline{s})\cdot\underline{\theta}) + \underline{z}\cdot(\underline{x}\times\underline{s})\underline{s}\cdot\underline{\theta}. \quad (r \text{ soln})$$

Ambiguities in r: It is worth while to note that the condition (cond $\hat{D}$) does not uniquely define $\hat{D}$ given a fixed D. [Fedosov adds an additional condition that makes his $\hat{D}$ unique from a fixed D being $\hat{d}^{-1}r_0=0$ where $\hat{d}^{-1}$ is what he calls δ^{-1} (an operator used in a de Rham decomposition) and r_0 is the first term in the recursive solution. We regard this choice as being artificial and thus omit it from the paper.]

It appears however that most of the ambiguities in constructing $\hat{D}$ when given a fixed phase space connection D can be absorbed by a basis change (in other words a gauge transformation). It is easy to see this in a Darboux chart because the connection may be expressed as a commutator,

$$\tilde{D}\hat{y}^A = [\tilde{Q},\hat{y}^A],$$

where $\tilde{D}=D-\hat{D}$, $\tilde{Q}=Q-\hat{Q}$, and $D=[Q,\cdot]$. The gauge transformation takes the form

$$\hat{y}^A \to \hat{y}^A_{\text{new}} := U\hat{y}^AU^{-1}, \quad \tilde{D}\hat{y}^A \to \tilde{D}_{\text{new}}\hat{y}^A_{\text{new}} := [U\tilde{Q}U^{-1},U\hat{y}^AU^{-1}] = U(\tilde{D}\hat{y}^A)U^{-1},$$

where U is some invertible function of the x's, p's, and $\hat{y}$'s. Thus the physical content of this theory is independent of U because the commutators remain unchanged.

This can be seen as follows:

$$r \to r + r',$$

where r is a solution to the equation (r) and r' is some unknown series,

$$r' = \sum_l r'_{AA_1\cdots A_l} \Theta^A \hat{y}^{A_1} \cdots \hat{y}^{A_l}.$$

Setting $r \to r+r'$ into (r) we obtain

$$\Omega - D(r+r') + [\underline{s}\cdot\underline{\alpha} - \underline{k}\cdot\underline{\theta}, (r+r')] + (r+r')^2 = 0$$

modulo the equation (r) to get

$$-Dr' + [\underline{s}\cdot\underline{\alpha} - \underline{k}\cdot\underline{\theta}, r'] + (r')^2 + [r,r'] = 0 \Rightarrow \tilde{D}r' - (r')^2 = 0.$$

This tells us that if r' is of the form

$$r' = (\tilde{D}U)U^{-1}$$

for any U which corresponds to a gauge transformation in the enveloping algebra then the resulting $r_{\text{new}} = r + r'$ will solve equation (r). In other words once we have one solution we have actually have huge class of equivalent solutions. We suspect this class of equivalent solutions are all of the solutions for a simply connected manifold.

Note: There is another source of ambiguity namely the ambiguity in the phase-space connection D. Given a connection D we may add to it a tensor Δ^A_{BC} where if we lower by $\Delta_{ABC} = \omega_{AE}\Delta^E_{BC}$ it is symmetric in all three indices. The new connection still preserves the symplectic form ω. Our curvature becomes

$$(D+\Delta)^2 = D^2 + D(\Delta) + \Delta^2.$$

It is unclear what this ambiguity means so we will leave it for a future discussion.

V. COMPUTING $\hat{x}$ AND $\hat{p}$

At this point in Fedosov's algorithm we have all the tools in place to associate an observable $\hat{f}$ to every $f \in C^\infty(T^*\mathcal{M})$. Following Fedosov we require that every observable $\hat{f}(x,p,\hat{y})$ must satisfy the equation

$$(D - \hat{D})\hat{f}(x,p,\hat{y}) = 0,$$

where $f_{A_1\cdots A_l}$ are some unknown functions of x and p such that

$$\ell o(\hat{f}(x,p,\hat{y})) = f(x,p)$$

ℓo (short for leading order in $\hat{y}$ and $\hbar$) picks out the term which has no $\hat{y}$'s and no $\hbar$'s in it. Explicitly,

$$\hat{f}(x,p,\hat{y}) = f(x,p) + \mathcal{O}(\hat{y},\hbar),$$

where f has no $\hbar$'s in it.

And so the condition to solve (we believe unique up to unitary transformations) for an observable $\hat{f}$ for every $f \in C^\infty(T^*\mathcal{M})$ is

$$(D - \hat{D})\hat{f}(x,p,\hat{y}) = 0, \quad \ell o(\hat{f}(x,p,\hat{y})) = f(x,p). \quad (\text{cond } \hat{f})$$

If we have determined our D and $\hat{D}$ we can find solutions for the operators $\hat{x}^a$ and $\hat{p}_a$ (i.e., their coefficients $b^a_{A_1\cdots A_l}$ and $c_{aA_1\cdots A_l}$),

$$\hat{x}^a = \sum_l b^a_{A_1\cdots A_l}\hat{y}^{A_1}\cdots\hat{y}^{A_l}, \quad (\hat{x})$$

$$\hat{p}_a = \sum_l c_{aA_1\cdots A_l}\hat{y}^{A_1}\cdots\hat{y}^{A_l}, \quad (\hat{p})$$

where $b^a_{A_1\cdots A_l}$ and $c_{aA_1\cdots A_l}$ are complex-valued functions of x and p [which are the coefficients $f_{A_1\cdots A_l}$ in equation $(\hat{f})$ where the first terms in the series is $f=b^a=x^a$ or $f=c_a=p_a$, respectively] and will be determined by the equations:

$$(D-\hat{D})\hat{x}^a = 0, \quad \ell o(\hat{x}^a) = x^a, \quad (\text{cond } \hat{x})$$

$$(D-\hat{D})\hat{p}_a = 0, \quad \ell o(\hat{p}_a) = p_a\,. \quad (\text{cond } \hat{p})$$

Again see the example in Appendix D for solutions to $\hat{x}$ and $\hat{p}$ in the case of $T^*\mathbb{R}^n$ where $D=d$.

If we invert the equations $(\hat{x})$ and $\hat{p})$ once we have solved for the coefficients $b^a_{A_1\cdots A_l}$ and $c^a_{A_1\cdots A_l}$ to get $\hat{y}$ as matrix-valued function of x, p, $\hat{x}$, and $\hat{p}$ [i.e., $\hat{y}^A=\hat{y}^A(x,p,\hat{x},\hat{p})$] and then substitute it into the equation for an arbitrary observable $(\hat{f})$ and get

$$\hat{f}(\hat{x},\hat{p}) = \sum_{lm} f^{b_1\cdots b_m}_{a_1\cdots a_l}\hat{x}^{a_1}\cdots\hat{x}^{a_l}\hat{p}_{b_1}\cdots\hat{p}_{b_m}, \quad (\hat{f}\text{ soln})$$

where $f^{b_1\cdots b_m}_{a_1\cdots a_l}$ are constant coefficients. (To prove this act $D-\hat{D}$ on this equation.)

However, once we have our $\hat{x}$ and $\hat{p}$ there is the ambiguity of how to order each variable when you map a function $f(x,p)$ to $\hat{f}(\hat{x},\hat{p})$. For example, does the function $f(x,p)=x^1p_1$ go to $\hat{x}^1\hat{p}_1$, $\hat{p}_1\hat{x}^1$ or some linear combination of the two? We should expect this in any well-defined quantization procedure because such ordering ambiguities arise in quantum mechanics. We will, for now, regard the ordering of each $\hat{f}$ to be undetermined. (Fedosov chooses Weyl ordering.)

$T^*\mathbb{S}^2$ explicitly: Fedosov at this point would implement an algorithm to construct $\hat{x}$ and $\hat{p}$ perturbatively (Ref. 2, p. 146) for our specific case of $T^*\mathbb{S}^2$. We instead try to find exact solutions to them. (We, again, ran the Fedosov algorithm a few times to help us see what for the ansatz we should take.) Specifically for the case of $T^*\mathbb{S}^2$ we have the ansatz for both $\hat{x}$ and $\hat{p}$ as

$$\hat{\underline{x}} = v(s^2)\underline{x} + w(s^2)\underline{x}\times\underline{s} + y(s^2)\underline{s},$$

$$\hat{\underline{p}} = (\underline{z}\cdot\underline{s}t(s^2) + \underline{z}\cdot(\underline{x}\times\underline{s})q(s^2))\underline{x} + \underline{z}n(s^2) + \underline{z}\times\underline{x}u(s^2)$$

with some functions v, w, y, t, q, n, and u to be determined and the requirements that $\ell o(\hat{\underline{x}})=\underline{x}$ and $\ell o(\hat{\underline{p}})=\underline{p}$.

The conditions (cond $\hat{x}$) and (cond $\hat{p}$) become the following equations:

$$\begin{aligned}0 = (D-\hat{D})\hat{\underline{x}} &= ((-2v'(s^2+1)+w)(\underline{s}\cdot\underline{\theta}) - y(\underline{x}\times\underline{s})\cdot\underline{\theta})\underline{x}\\ &+\left(\left(-\frac{v}{s^2}-2w'(s^2+1)-w\left(1+\frac{1}{s^2}\right)\right)(\underline{s}\cdot\underline{\theta}) - y\frac{1}{s^2}(\underline{x}\times\underline{s})\cdot\underline{\theta}\right)\underline{x}\times\underline{s}\\ &+\left(\left(\frac{v}{s^2}+w\frac{1}{s^2}\right)(\underline{x}\times\underline{s})\cdot\underline{\theta} + \left(-2y'(s^2+1)-y\left(1+\frac{1}{s^2}\right)\right)(\underline{s}\cdot\underline{\theta})\right)\underline{s}\end{aligned}$$

and

$$
0=(D-\hat{D})\underline{\hat{p}}=\left(\begin{array}{c}\left(\begin{array}{c}-2\underline{z}\cdot\underline{s}t'(s^2+1)-(\underline{z}\cdot\underline{s})\dfrac{1}{s^2}t-2\underline{z}\cdot(\underline{x}\times\underline{s})q'(s^2+1)\\ +\underline{z}\cdot(\underline{x}\times\underline{s})\left(1-\dfrac{1}{s^2}\right)q-(\underline{z}\cdot\underline{s})\dfrac{1}{s^2}u+\underline{z}\cdot(\underline{x}\times\underline{s})\dfrac{1}{s^2}n\end{array}\right)(\underline{s}\cdot\underline{\theta})\\ \left(\begin{array}{c}-\left(\underline{z}\cdot(\underline{x}\times\underline{s})\left(1+\dfrac{1}{s^2}\right)\right)t+(\underline{z}\cdot\underline{s})\dfrac{1}{s^2}q\\ +\underline{x}\cdot(\underline{z}\times\underline{s})\dfrac{1}{s^2}u-(\underline{z}\cdot\underline{s})\dfrac{1}{s^2}n\end{array}\right)(\underline{x}\times\underline{s})\cdot\underline{\theta}\end{array}\right)\underline{x}
$$

$$
+\left(\begin{array}{c}\left(\begin{array}{c}-\underline{z}\cdot\underline{s}t-\underline{z}\cdot(\underline{x}\times\underline{s})q+2\underline{z}\cdot(\underline{x}\times\underline{s})n\\ -(\underline{z}\cdot\underline{s})u+2(\underline{z}\cdot\underline{s})(s^2+1)u'-2(\underline{z}\times\underline{x})\cdot\underline{s}(s^2+1)n'\end{array}\right)(\underline{s}\cdot\underline{\theta})\\ +\underline{z}\cdot(\underline{x}\times\underline{s})(\underline{x}\times\underline{s})\cdot\underline{\theta}u\end{array}\right)\frac{1}{s^2}\underline{x}\times\underline{s}
$$

$$
+\left(\begin{array}{c}\left(\begin{array}{c}2\underline{z}\cdot(\underline{x}\times\underline{s})u+(\underline{z}\cdot\underline{s})n\\ -2(\underline{z}\cdot\underline{s})(s^2+1)n'-2((\underline{z}\times\underline{x})\cdot\underline{s})(s^2+1)u'\end{array}\right)\underline{s}\cdot\underline{\theta}\\ +(\underline{z}\cdot\underline{s}t+\underline{z}\cdot(\underline{x}\times\underline{s})q-\underline{z}\cdot(\underline{x}\times\underline{s})n)(\underline{x}\times\underline{s})\cdot\underline{\theta}\end{array}\right)\frac{1}{s^2}\underline{s}.
$$

So the conditions that $\tilde{D}\underline{\hat{x}}=0$ and $\tilde{D}\underline{\hat{p}}=0$ becomes 6+6 equations because $(\underline{s}\cdot\underline{\theta})^2=0=((\underline{x}\times\underline{s})\cdot\underline{\theta})^2$ and $(\underline{s}\cdot\underline{\theta})(\underline{x}\times\underline{s})\cdot\underline{\theta}=\tilde{\omega}$ where $\tilde{\omega}_{ab}$ is invertible. We then solve the subsequent differential equations for the functions v,w,y,t,q,n, and u along with requiring that they have the correct term with no $\hat{y}$'s [$\ell o(\underline{\hat{x}})=\underline{x}$ and $\ell o(\underline{\hat{p}})=\underline{p}$] in the Taylor expansion to obtain the solutions

$$
\underline{\hat{x}}=(\underline{x}-\underline{x}\times\underline{s})(s^2+1)^{-1/2},\quad(\hat{x}\text{ soln})
$$

$$
\underline{\hat{p}}=(\underline{z}\cdot(\underline{x}\times\underline{s})\underline{x}+\underline{z})(s^2+1)^{1/2},\quad(\hat{p}\text{ soln})
$$

where $\underline{z}=\underline{p}-\underline{x}\times\underline{k}$ with the following conditions holding:

$$
\begin{array}{l}\ell o(\underline{\hat{x}})=\underline{x},\ \ell o(\underline{\hat{p}})=\underline{p},\\ \underline{\hat{p}}\cdot\underline{\hat{x}}=\underline{\hat{x}}\cdot\underline{\hat{p}}-2i\hbar=0.\end{array}\quad(\hat{x}\hat{p}\text{ conds})
$$

We note at this point that there is not much insight looking at these formulas except for what we get for the commutators in the next section.

VI. THE COMMUTATORS $[\hat{x}^a,\hat{x}^b]$, $[\hat{x}^a,\hat{p}_b]$, AND $[\hat{p}_a,\hat{p}_b]$

Once we have $\hat{x}^a$ and $\hat{p}_a$, i.e., the coefficients $b^a_{A_1\cdots A_l}$ and $c^a_{A_1\cdots A_l}$ we work out the commutation relations $[\hat{x}^a,\hat{x}^b]$, $[\hat{x}^a,\hat{p}_b]$, and $[\hat{p}_a,\hat{p}_b]$ using the formulas $(\hat{x})$ and $(\hat{p})$ in the previous section in a brute force calculation. Remember that the $*$-commutators is the Poisson bracket on $T^*\mathcal{M}$ to first order in $\hbar$,

$$
[\hat{f}(\hat{x},\hat{p}),\hat{g}(\hat{x},\hat{p})]=\hat{h}(\hat{x},\hat{p})
$$

$$
[f_*(x,p),g_*(x,p)]_*=h_*(x,p)=i\hbar\{f,g\}_{\mathcal{M}}+\mathcal{O}(\hbar^2)\quad(*\text{-comm})
$$

where $\hat{f},\hat{g},\hat{h}$ and f_*,g_*,h_* are functions defined by:

$$
\hat{f}(\hat{x},\hat{p})=\sum_{Im}f^{b_1\cdots b_m}_{ja_1\cdots a_l}\hbar^j\hat{x}^{a_1}\cdots\hat{x}^{a_1}\hat{p}_{b_1}\cdots\hat{p}_{b_m}
$$

$$f_*(x,p) = \sum_{Im} f_{ja_1\cdots a_l}^{b_1\cdots b_m} \hbar^j x^{n_1} * \cdots * x^{a_1} * p_{b_1} * \cdots * p_{b_m}$$

where $f_{ja_1\cdots a_l}^{b_1\cdots b_m}$ are constants.

These two sets, one of all f_*'s $\{f_*\}$ and one of all $\hat{f}$'s $\{\hat{f}\}$ defined above are isomorphic.

$T^*\mathbb{S}^2$ explicitly: In our case of $T^*\mathbb{S}^2$ we find

$$[\hat{x}^a,\hat{x}^b] = 0,$$

$$[\hat{x}^a,\hat{p}_b] = i\hbar(\delta_b^a - \hat{x}^a\hat{x}_b),$$

$$[\hat{p}_a,\hat{p}_b] = 2i\hbar\hat{x}_{[b}\,\hat{p}_{a]},$$

$$\underline{\hat{x}}\cdot\underline{\hat{x}} = 1, \quad \underline{\hat{p}}\cdot\underline{\hat{x}} = \underline{\hat{x}}\cdot\underline{\hat{p}} - 2i\hbar = 0.$$

We now define $\underline{\hat{L}}$ because we argue below that it is a more "natural" momentum,

$$\underline{\hat{L}} := -\underline{\hat{p}}\times\underline{\hat{x}} = \underline{\hat{x}}\times\underline{\hat{p}} = \underline{x}\times\underline{z} + (\underline{z}\cdot\underline{s})\underline{x} - \underline{z}\cdot(\underline{x}\times\underline{s})\underline{s}$$

again with the computed conditions

$$\underline{\hat{L}}\cdot\underline{\hat{x}} = \underline{\hat{x}}\cdot\underline{\hat{L}} = 0, \quad \underline{\hat{x}}\cdot\underline{\hat{x}} = 1,$$

$$\ell o(\underline{\hat{L}}) = \underline{L} = \underline{x}\times\underline{p}.$$

We easily recognize that $\underline{\hat{L}}$ is the more "natural" variable compared to $\underline{\hat{p}}$. This is because $\underline{\hat{p}}\cdot\underline{\hat{x}}=0$ and $\underline{\hat{x}}\cdot\underline{\hat{p}}=2i\hbar$ are very "unnatural" conditions since there is no physical reason why it should not be $\underline{\hat{x}}\cdot\underline{\hat{p}}=0$ and $\underline{\hat{p}}\cdot\underline{\hat{x}}=-2i\hbar$. We could define $\underline{\hat{p}}_{\text{new}}=\underline{\hat{p}}+A\underline{\hat{x}}$ where A is an arbitrary constant and obtain the same commutators. On the other hand, the symmetry between $\underline{\hat{L}}\cdot\underline{\hat{x}}=\underline{\hat{x}}\cdot\underline{\hat{L}}=0$ seems to suggest that $\underline{\hat{L}}$ should be the preferred quantity over $\underline{\hat{p}}$. In other words, the relevant component of $\underline{\hat{p}}$ is the one perpendicular to $\underline{\hat{x}}$ which is precisely what $\underline{\hat{L}}$ is.

Therefore the part of $\hat{p}$ parallel to $\hat{x}$ is irrelevant,

$$\underline{\hat{x}} = (\underline{x} - \underline{x}\times\underline{s})(s^2+1)^{-1/2}, \quad (\hat{x}\text{ soln})$$

$$\underline{\hat{L}} = \underline{x}\times\underline{z} + (\underline{z}\cdot\underline{s})\underline{x} - \underline{z}\cdot(\underline{x}\times\underline{s})\underline{s}, \quad (\hat{L}\text{ soln})$$

where $\underline{z}=\underline{p}-\underline{x}\times\underline{k}$ with conditions

$$\underline{\hat{L}}\cdot\underline{\hat{x}} = \underline{\hat{x}}\cdot\underline{\hat{L}} = 0, \quad \underline{\hat{x}}\cdot\underline{\hat{x}} = 1\,. \quad (\hat{x}\hat{L}\text{ conds})$$

Again we note at this point that there is not much insight looking at these formulas except for what we get for the commutators in the remainder of this section.

We compute the commutators,

$$[\hat{x}^a,\hat{x}^b] = 0, \quad (xx)$$

$$[\hat{x}^a,\hat{L}_b] = i\hbar\varepsilon^a{}_{bc}\hat{x}^c, \quad (xL)$$

$$[\hat{L}_a, \hat{L}_b] = i\hbar \varepsilon^c{}_{ab} \hat{L}_c, \quad (LL)$$

along with

$$\underline{\hat{x}} \cdot \underline{\hat{x}} = 1, \underline{\hat{L}} \cdot \underline{\hat{x}} = \underline{\hat{x}} \cdot \underline{\hat{L}} = 0 . \quad (\text{cond } xL)$$

Once we know these relations we know the whole algebra of functions since the algebra is associative. And thus we are done.

And so in the case of $T^*\mathbb{S}^2$ a general element $\hat{f}$ [the function $(\hat{f})$ we were looking for and the specific form of the solution ($\hat{f}$ soln)] in the space of all observables of $\hat{x}$ and $\hat{L}$ is

$$\hat{f}(\hat{x}, \hat{L}) = \sum_{lm} f^{b_1 \cdots b_m}_{a_1 \cdots a_l} \hat{x}^{a_1} \cdots \hat{x}^{a_l} \hat{L}_{b_1} \cdots \hat{L}_{b_m},$$

where $f^{b_1 \cdots b_m}_{a_1 \cdots a_l}$ are constants. This is the enveloping algebra of the operators of angular momentum and position on a Hilbert space.

Clearly we see that the $\hat{L}$'s generate the standard angular momentum algebra and the $\hat{x}$'s transform properly under rotations. However both the $\hat{x}$'s and the $\hat{L}$'s form a constrained version of the standard $\mathbb{R}^3$ Euclid algebra with invariant constraints given by the last equations.

VII. ANGULAR MOMENTUM STATES

Since we now have the algebra of observables we can ask about Hamiltonians and states. The free single quantum particle Hamiltonian in ordinary quantum mechanics is $\hat{H} = \hat{p}^2/2m = (\hat{p}_r^2/2m) + (\hat{\underline{L}} \cdot \hat{\underline{L}}/mr^2)$ where $\hat{p}_r$ is the radial component of momentum and $\hat{\underline{L}}$ is the angular momentum. In other words, the natural choice for the Hamiltonian on our $\mathbb{S}^2$ (which we are free to choose) is $\hat{H} = \hat{\underline{L}} \cdot \hat{\underline{L}}$, $r=1, m=1$ because it is just the restricted version of the $\mathbb{E}^3$ free particle Hamiltonian onto $\mathbb{S}^2$. We then construct our angular momentum states in the usual way by solving the eigenvalue equation

$$\hat{H}|\phi\rangle = E|\phi\rangle, \quad (\text{Schrödinger})$$

where $E \in \mathbb{R}$.

We will not do it because it is standard physics that one is able to do as an undergraduate physics student.

VIII. CONCLUSIONS

We have explicitly constructed an exact nonperturbative solutions to the observables in the Fedosov $*$-formalism on $T^*\mathbb{S}^2$ and showed that they obeyed the angular momentum commutation relations. In other words, we took the phase space of a single classical particle confined to a sphere, quantized it and got the quantum angular momentum algebra (which we expected). This is done by starting with a chosen phase-space connection D and constructing an explicit formula for $\hat{D}$. Via the equation $(D - \hat{D})\hat{f} = 0$ that defines the algebra, i.e., the algebra of all $\hat{f}$'s we then explicitly constructed $\underline{\hat{x}}$ and $\underline{\hat{p}}$ (the operator analogues of $\underline{x}$ and $\underline{p}$) and computed their commutators. We realized (by defining $\hat{\underline{L}} = \underline{\hat{x}} \times \underline{\hat{p}}$) that the enveloping algebra of all $\underline{\hat{x}}$'s and $\underline{\hat{p}}$'s gives the angular momentum algebra.

Subsequently we defined a Hamiltonian $\hat{\underline{L}} \cdot \hat{\underline{L}}$ that would have eigenstates of angular momentum, however we did not explicitly construct it because it is standard physics.

Another main point was that most of the ambiguity given a fixed phase-space connection D of the construction of $\hat{D}$, it seemed, stemmed from the freedom of a change of basis $(\hat{f} \to U\hat{f}U^{-1})$ given by the argument in Sec. IV. Finally the matrix form of the $\hat{y}$'s did not change anything from a Moyal-type object as is done in deformation quantization.

We conclude that we would arrive at the same answer given any algebraic object $\hat{y}$ that had the same commutators along with the same action of the connection on them. We then view the Fedosov $*$-formalism as a general algebraic construction and less tied to the deformation aspect of its original formulation. Thus our formulation using Heisenberg algebras and their subsequent representation spaces (Hilbert spaces) makes a more direct connection to the standard formulation of ordinary quantum mechanics.[4–12]

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APPENDIX A

We now show that the equation $(D-\hat{D})^2\hat{y}^A=0$ is equivalent to $[\Omega-Dr+\hat{\mathrm{d}}r+r^2,\hat{y}^A]=0$.

Proof:

$$(D-\hat{D})^2\hat{y}^A=(D^2-D\hat{D}-\hat{D}D+\hat{D}^2)\hat{y}^A,$$

$$(D\hat{D}+\hat{D}D)\hat{y}^A=[D(\omega_{AB}\hat{y}^A\Theta^B+r),\hat{y}^A]=[Dr,\hat{y}^A],$$

$$\begin{aligned}\hat{D}^2\hat{y}^A=[\hat{Q},[\hat{Q},\hat{y}^A]]=\hat{Q}(\hat{Q}\hat{y}^A-\hat{y}^A\hat{Q})+(\hat{Q}\hat{y}^A-\hat{y}^A\hat{Q})\hat{Q}=[\hat{Q}^2,\hat{y}^A]_-=[(\omega_{AB}\hat{y}^A\Theta^B+r)^2,\hat{y}^A]_-\\=[(\omega_{AB}\hat{y}^A\Theta^B)^2+[\omega_{AB}\hat{y}^A\Theta^B,r]+r^2,\hat{y}^A]_-,\end{aligned}$$

$$\begin{aligned}2(\omega_{AB}\hat{y}^A\Theta^B)^2=[\omega_{AB}\hat{y}^A\Theta^B,\omega_{CE}\hat{y}^C\Theta^E]=[\hat{y}^A,\hat{y}^C]\omega_{AB}\Theta^B\omega_{CE}\Theta^E=\omega_{AB}\Theta^A\Theta^B\\\Rightarrow\hat{D}^2\hat{y}^A=[[\omega_{AB}\hat{y}^A\Theta^B,r]+r^2,\hat{y}^A]_-,\end{aligned}$$

where $[A,B]_-=AB-BA$ for any A and B.

The curvature D^2 acting on Θ^A is

$$D^2\otimes\Theta^A=R_B{}^A\otimes\Theta^B.$$

Thus the curvature D^2 acting on $\hat{y}^A$ is

$$D^2\hat{y}^A=R_B{}^A\hat{y}^B.$$

Knowing this we define Ω as the curvature D^2 acting on $\hat{y}^A$ as a commutator, namely,

$$\frac{1}{i\hbar}[\Omega,\hat{y}^A]=R_B{}^A\hat{y}^B,$$

we can immediately write a solution for Ω knowing $[\hat{y}^A,\hat{y}^B]=i\hbar\omega^{AB}$, $\omega^{AB}\omega_{BC}=\delta^A_C$ and using the symmetries of the curvature tensor,

$$\Omega:=-\tfrac{1}{2}\omega_{AC}R_B{}^A\hat{y}^B\hat{y}^C.$$

Thus we may rewrite the condition $(D-\hat{D})^2\hat{y}^A=0$ as

$$(D-\hat{D})^2\hat{y}^A=[\Omega-Dr+\hat{\mathrm{d}}r+r^2,\hat{y}^A]=0.$$

APPENDIX B

Here we present an argument as to why r only has terms that are cubic or higher powers in the $\hat{y}$'s. Given

$$\hat{D} = [\hat{Q}, \cdot\,] = [\hat{Q}_A \Theta^A, \cdot\,],$$

$$\hat{Q}_A = \sum_l Q_{AA_1\cdots A_l} \hat{y}^{A_1} \cdots \hat{y}^{A_l},$$

we require

$$(D - \hat{D})^2 \hat{y}^A = 0.$$

If we let

$$\hat{Q}_A \Theta^A = \omega_{AB} \hat{y}^A \Theta^B + r,$$

$$r = \sum_l r_{AA_1\cdots A_l} \Theta^A \hat{y}^{A_1} \cdots \hat{y}^{A_l}.$$

If we want r to be globally defined for *all* manifolds we must define it out of nondegenerate tensors namely the metric, the symplectic form and the curvature. This is because Ω is degree 2 in the $\hat{y}$'s (i.e., $\Omega := -\frac{1}{2}\omega_{AC} R^A_{BDE} \hat{y}^B \hat{y}^C$ has 2 $\hat{y}$'s). The degree is defined by

$$\deg(a) = (\text{number of } \hat{y}\text{'s}) + 2(\text{number of } \hbar\text{'s}).$$

A linear r would yield

$$\underbrace{\Omega}_{2} - \underbrace{Dr}_{1} + \underbrace{\hat{d}r}_{0} + \underbrace{r^2}_{1}$$

and this cannot be zero for $\Omega \neq 0$. This means that r must have a quadratic term in it.

If r is quadratic ($r = \Sigma_{l=0}^{2} r_{AA_1\cdots A_l} \Theta^A \hat{y}^{A_1} \cdots \hat{y}^{A_l}$), in general, there is no way to construct the degree 2 coefficient $r_{AA_1A_2}$ out of invariant tensors. Thus we require that r has terms that are cubic or higher powers in the $\hat{y}$'s. Fedosov mentions this fact also.[2]

For a specific manifold there might be an r that is quadratic. The argument above is meant for an r in a *general* construction for a *general* manifold and so we give a counterexample in the case when the manifold $\mathcal{M}$ is $\mathbb{E}^n$.

There is always the trivial solution to r,

$$r = -\tfrac{1}{2}\omega_{CB} \Gamma^C{}_A \hat{y}^A \hat{y}^B,$$

where $\Gamma^C_A = \Gamma^C_{BA} \Theta^B$ are the Christoffel symbols associated to D. One can easily observe that this is a solution knowing $[\hat{y}^A, \hat{y}^B] = i\hbar\omega^{AB}$, $\omega^{AB}\omega_{BC} = \delta^A_C$ and using the symmetries of the Christoffel symbols. However, the Γ's are not necessarily globally defined and if we find an r in one coordinate patch on $T^*\mathcal{M}$ there is no guarantee that it will be well defined in another. However if $\mathcal{M} = \mathbb{E}^n$ then this is a global r.

APPENDIX C

Useful identities,

$$\mathrm{d}\underline{p} = \underline{\alpha} \times \underline{x} - \underline{p} \times \underline{\theta},$$

$$\theta^a \theta^b = \tilde{\omega} \varepsilon^{abc} x_c,$$

$$\underline{z} \times \underline{x} = \underline{p} \times \underline{x} - \underline{k},$$

$$\underline{z} = \underline{p} - \underline{x} \times \underline{k},$$

$$\theta^a \theta^b = \theta^{[a}\ \theta^{b]} = \tfrac{1}{2}\varepsilon^{abc}(\underline{\theta} \times \underline{\theta})_c = \tilde{\omega}\varepsilon^{abc}x_c,$$

$$(\underline{v} \times \underline{w}) \times \underline{u} = \delta_{ab}v^a \underline{w} u^b - \underline{v}(\underline{w} \cdot \underline{u}),$$

$$\underline{v} \times (\underline{w} \times \underline{u}) = \delta_{ab}v^a \underline{w} u^b - (\underline{v} \cdot \underline{w})\underline{u},$$

for all 3D vectors assuming nothing about $[v_a, w_b]$, $[v_a, u_b]$ or $[w_a, u_b]$,

$$(\underline{v} \cdot \underline{\theta})(\underline{x} \times \underline{w}) \cdot \underline{\theta} = \tilde{\omega}(\underline{v} \cdot \underline{w})$$

for all 3D vectors assuming $[\theta^a, v_b] = [\theta^a, w_b] = 0$ and assuming nothing about $[v_a, w_b]$. For two vectors such that $\underline{v} \cdot \underline{x} = \underline{w} \cdot \underline{x} = 0$ we have the identities

$$\underline{v} \times \underline{w} = ((\underline{v} \times \underline{w}) \cdot \underline{x})\underline{x} \sim \underline{x},$$

$$\underline{z} \cdot (\underline{x} \times \underline{s}) = \underline{p} \cdot (\underline{x} \times \underline{s}) - t,$$

$$[s^2, (\underline{x} \times \underline{k}) \cdot \underline{s}] = 0,$$

$$s_a f(\underline{k} \cdot \underline{s}) = f(\underline{k} \cdot \underline{s} + 1)s_a,$$

$$[r_0, \underline{s}] = \tfrac{1}{3}((\underline{s} \cdot \underline{\theta})\underline{s} - s^2 \underline{\theta}),$$

$$[r_0, (\underline{s} \cdot \underline{\theta})] = 0,$$

$$[r_0, s^2] = 0 = [\underline{z} \cdot \underline{s}, s^2],$$

$$[r_0, \underline{k}] = \tfrac{1}{3}(2\underline{s}(\underline{k} \cdot \underline{\theta}) - \underline{\theta} t - (\underline{s} \cdot \underline{\theta})\underline{k}),$$

$$[r_0, \underline{z}] = \tfrac{1}{3}((\underline{s} \cdot \underline{\theta})\underline{x} \times \underline{k} - \underline{\theta} \times \underline{x} t - 2\underline{x} \times \underline{s}(\underline{k} \cdot \underline{\theta})),$$

$$\tilde{D}\underline{s} = \underline{\theta} \times \underline{s} - \left(1 + \frac{1}{s^2}\right)(\underline{s} \cdot \underline{\theta})\underline{s} - \frac{1}{s^2}((\underline{x} \times \underline{s}) \cdot \underline{\theta})\underline{x} \times \underline{s},$$

$$\tilde{D}\underline{x} = D\underline{x} = \underline{\theta} \times \underline{x} = \frac{1}{s^2}((\underline{x} \times \underline{s}) \cdot \underline{\theta})\underline{s} - (\underline{s} \cdot \underline{\theta})\underline{x} \times \underline{s},$$

$$\tilde{D}\underline{z} = \underline{\theta} \times \underline{z} + ((\underline{z} \cdot \underline{s})(\underline{s} \cdot \underline{\theta}) - \underline{z} \cdot (\underline{x} \times \underline{s})((\underline{x} \times \underline{s}) \cdot \underline{\theta}))\frac{1}{s^2}\underline{s} + 2\underline{z} \cdot (\underline{x} \times \underline{s})(\underline{s} \cdot \underline{\theta})\frac{1}{s^2}\underline{x} \times \underline{s}.$$

APPENDIX D: $T^*\mathbb{R}^n$

In the case of $T^*\mathbb{R}^n$ we solve equation (r) above for r when $D \otimes \Theta^A = 0$ therefore $D\hat{y}^A = 0$ and hence $\Omega = 0$ and get the solution $r = 0$. This gives us $\hat{D}$ by the formulas $(\hat{D})$ and $(\hat{Q})$,

$$\hat{D} = \frac{1}{i\hbar}[\omega_{AB}\hat{y}^A\Theta^B, \cdot\,] = \frac{1}{i\hbar}[\underline{s}\cdot \mathrm{d}\underline{p} - \underline{k}\cdot \mathrm{d}\underline{x}, \cdot\,] = \frac{1}{i\hbar}[(\underline{x}+\underline{s})\cdot \mathrm{d}\underline{p} - (\underline{p}+\underline{k})\cdot \mathrm{d}\underline{x}, \cdot\,],$$

where s and k are the first n $\hat{y}$'s and the last n $\hat{y}$'s, respectively [i.e., $\hat{y}^A=(s^a,k_a)$] also we have $[s^a,s^b]=0=[k_a,k_b],[s^a,k_b]=i\hbar\,\delta^a_b$, and $Ds^a=0=Dk_a$.

All operators are required to satisfy

$$\frac{\partial \hat{f}}{\partial x^a}\mathrm{d}x^a + \frac{\partial \hat{f}}{\partial p_a}\mathrm{d}p_a - \hat{D}\hat{f} = 0$$

$$\Rightarrow \frac{\partial \hat{f}}{\partial x^a}\mathrm{d}x^a + \frac{\partial \hat{f}}{\partial p_a}\mathrm{d}p_a = \frac{1}{i\hbar}[(\underline{x}+\underline{s})\cdot \mathrm{d}\underline{p} - (\underline{p}+\underline{k})\cdot \mathrm{d}\underline{x}, \hat{f}].$$

This equation is the specific case of the equation (cond $\hat{f}$) for $T^*\mathbb{R}^n$ introduced in Sec. II. The above equation tells us that $\hat{f}$ is a function of $\hat{x}^a=x^a+s^a$ and $\hat{p}_a=p_a+k_a$ $[\hat{f}=\hat{f}(\hat{x},\hat{p})]$ which are solutions to the equation (cond $\hat{f}$), i.e., the coefficients $b^a_{A_1\ldots A_l}$ and $c_{aA_1\ldots A_l}$ in the case of $T^*\mathbb{R}^n$ introduced in Sec. II when $\ell o(\hat{f})=x^a$ and $\ell o(\hat{f})=p_a$, respectively. The equation above implies that $(1/i\hbar)[\cdot,\hat{p}_a]$ generates the translation on the cotangent bundle in the x^a direction and $(1/i\hbar)\times[\hat{x}^a,\cdot\,]$ generates the translation on the cotangent bundle in the p_a direction on all observables $\hat{f}$. See Fedosov for more details on motivating the need for $\hat{D}$.[2] □

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Semiclassical expansion of Wigner functions

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We show that the time evolved Wigner function of a quantum particle under the action of a smooth potential can be formally expanded in powers of $\hbar$, where each term of the expansion can be computed in terms of the corresponding classical flow. Moreover the solution can be approximated by the N-order truncation with an error $O(\hbar^{N+1})$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2200143]

I. INTRODUCTION

WKB methods (see, e.g., Refs. 6–8, and references quoted therein) provide an asymptotic expansion of the solutions to the Schrödinger equation:

$$i\varepsilon\partial_t\Psi = -\frac{\varepsilon^2}{2}\Delta\Psi + U\Psi, \tag{1.1}$$

in powers of $\varepsilon=\hbar$, $\hbar=h/2\pi$, h being the Planck constant. Here we consider a quantum system whose corresponding classical Hamiltonian is

$$H(x,p) = \frac{p^2}{2} + U(x), \tag{1.2}$$

where $x \in \mathbb{R}^d$ is a configuration of the system. The initial state is usually assumed of the form:

$$\Psi(x) = a(x)e^{iS(x)/\varepsilon} \tag{1.3}$$

where a and S are real functions of the configurational space.

The main disadvantage of the WKB methods is that they easily work for a short time, while extensions to arbitrary times require significant technical efforts. In fact assuming the solution to the problem (1.1) of the form

$$\Psi(x,t) = a(x,t)e^{iS(x,t)/\varepsilon}, \tag{1.4}$$

we find, at zero order in ε, the following equations for a and S:

$$\partial_t a + \tfrac{1}{2}a\,\mathrm{div}(\nabla S) + \nabla S\cdot\nabla a = 0, \tag{1.5}$$

$$\partial_t S + \tfrac{1}{2}|\nabla S|^2 + U = 0. \tag{1.6}$$

Setting $u=\nabla S$ and $n=a^2$, from (1.5) and (1.6) we obtain the pressureless Euler equations:

$$\partial_t n + \mathrm{div}(un) = 0, \tag{1.7}$$

$$\partial_t u + u\cdot\nabla u + \nabla U = 0. \tag{1.8}$$

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It is well known that Eqs. (1.7) and (1.8) deliver, in general, singularities in a finite time, therefore we find difficulties in justifying Eq. (1.4) globally in time, even at zero order in ε.

On the other hand we can introduce the Wigner transform (see Ref. 11) of a quantum state described by the integral kernel $\rho=\rho(x;y)$. It is a function in the classical phase space defined by

$$f_\rho(x,v)=\left(\frac{1}{2\pi}\right)^d\int \mathrm{d}y e^{iv\cdot y}\rho\left(x-\frac{\varepsilon}{2}y;x+\frac{\varepsilon}{2}y\right) \tag{1.9}$$

reducing to

$$f_\Psi(x,v)=\left(\frac{1}{2\pi}\right)^d\int \mathrm{d}y e^{iv\cdot y}\Psi\left(x-\frac{\varepsilon}{2}y\right)\bar{\Psi}\left(x+\frac{\varepsilon}{2}y\right) \tag{1.10}$$

whenever $\rho(x;y)=\bar{\Psi}(x)\Psi(y)$, that is the quantum state is pure and described by the wave function Ψ. The quantum evolution usually given in terms of the Heisenberg (or the Schrödinger) equation is equivalently described by the so-called Wigner-Liouville equation which we shall introduce later on. At zero order in ε such an equation reduces to the classical Liouville equation

$$(\partial_t+v\cdot\nabla_x)f+F\cdot\nabla_v f=0, \tag{1.11}$$

where $F=-\nabla U$ is the force field.

The Wigner transform of the initial state (1.3) is, at zero order in ε,

$$f(x,v)=n(x)\delta(v-u(x)), \tag{1.12}$$

where $u=\nabla S$ and $n=a^2$. Now, by using the characteristics of the Hamiltonian flow generated by the Hamiltonian (1.2), we can construct a global solution to Eq. (1.11), with initial state (1.12), provided that U is sufficiently smooth. Therefore, at least at zero order in ε, the Wigner formalism works globally in time. As a consequence it seems natural to go further, namely to find an asymptotic expansion for the solution to the Wigner-Liouville equation, which is expected to work globally. However, in doing this we have to pay a price: we cannot pretend to recover the WKB wave function globally in time. Indeed the solution to Eq. (1.11) has the hydrodynamical representation

$$f(x,v;t)=n(x,t)\delta(v-u(x,t)) \tag{1.13}$$

only locally in time because Eq. (1.13) holds if and only if the pair n,u solves the problem (1.7) and (1.8) which, as we said, has unique smooth solution for a short time only. This is well known and has been pointed out in recent works (see, e.g., Ref. 9, and references quoted therein).

On the other side the loss of a clear wave function picture is compensated by the fact that we can compute, at least in principle, the asymptotic expansion of the physical observables, which are moments of the Wigner measure. For instance the current and the current density are given by

$$n(x)=|\psi(x)|^2=\int f(x,v)\mathrm{d}v, \tag{1.14}$$

$$\varepsilon\ \mathrm{Im}\ \bar{\psi}\nabla\ \psi(x)=J(x)=\int vf(x,v)\mathrm{d}v, \tag{1.15}$$

respectively.

The formal expansion we present here (see Sec. II) is not new. It corresponds to the well-known Egorov theorem and has been previously used by different authors (see, e.g., Refs. 2, 5, and 10 and also Ref. 1 for a geometrical description of the propagator of the time evolved Wigner function). However it is somehow surprising that a rigorous analysis of the semiclassical expansion of the Wigner function is apparently absent, as far as we know, from the current literature. The main purpose of the present paper is to fill this gap.

We mention that Wigner function approaches have been invoked in connection with compactness methods also to weaken the usual regularity assumptions (see, e.g., Refs. 3 and 4). Here we use a different and complementary point of view: we assume smoothness on the potential and analyze the coefficients of the formal expansion in power of ε of the solution. Then we control the remainder showing that it is $O(\varepsilon^{N+1})$ if N is the order of approximation.

We point out that the present method works for a large class of initial states including WKB and coherent states.

Our regularity assumptions are severe. We believe that they can be relaxed, however we prefer to privilege the simplicity in this context.

II. THE FORMAL EXPANSION

The Wigner-Liouville equation for our quantum system described by the Wigner function $f(x,v)$ on the classical phase space, reads as

$$(\partial_t + v \cdot \nabla_x) f = Tf, \tag{2.1}$$

where

$$Tf(x,v) = \frac{i}{\varepsilon} \sum_{\sigma=\pm 1} \sigma \int \mathrm{d}k \hat{U}(k) e^{ik\cdot x} f\left(x, v + \frac{\sigma}{2}\varepsilon k\right). \tag{2.2}$$

We find it convenient to express T in the following equivalent divergence form, namely,

$$T = i \int_{-1/2}^{1/2} \mathrm{d}\lambda \int \mathrm{d}k \hat{U}(k) e^{ik\cdot x} k \cdot \nabla_v f(x, v + \varepsilon\lambda k). \tag{2.3}$$

By using the Taylor formula:

$$f(x,v+\varepsilon\lambda k) = \sum_{n=0}^{N} (k\cdot\nabla_v)^n f(x,v) \frac{(\varepsilon\lambda)^n}{n!} + \frac{(\varepsilon)^{N+1}}{N!} \int_0^{\lambda} \mathrm{d}\mu (k\cdot\nabla_v)^{N+1} f(x, v+\varepsilon\mu k) \mu^N, \tag{2.4}$$

we expand T in the formal power series in ε,

$$T = T_0 + \varepsilon T_1 + \varepsilon^2 T_2 + \cdots, \tag{2.5}$$

where

$$T_{2n} = i\left(\frac{1}{2}\right)^{2n} \frac{1}{(2n+1)!} \int \mathrm{d}k \hat{U}(k) e^{ik\cdot x} (k\cdot\nabla_v)^{2n+1} f(x,v), \quad n = 0,1\ldots \tag{2.6}$$

and

$$T_{2n+1} = 0, \quad n = 0,1\ldots. \tag{2.7}$$

Note that odd powers vanish and that:

$$T_0 = \nabla_x U \cdot \nabla_v f \tag{2.8}$$

is the classical interaction part of the Liouville operator.

Now let f_0 be the initial state. We assume that f_0 has the following formal power expansion:

$$f_0 = f_0^{(0)} + \varepsilon f_0^{(1)} + \varepsilon^2 f_0^{(2)} + \cdots. \tag{2.9}$$

We expand also the solution $f(t)$ to Eq. (2.1) accordingly

$$f(t) = f^{(0)}(t) + \varepsilon f^{(1)}(t) + \varepsilon^2 f^{(2)}(t) + \cdots \tag{2.10}$$

and, using (2.5) in (2.1), we find at zero order:

$$(\partial_t + v \cdot \nabla_x) f^{(0)} = T_0 f^{(0)}, \tag{2.11}$$

that is the classical Liouville equation with initial condition $f_0^{(0)}$. More generally at order ε^n we have

$$(\partial_t + v \cdot \nabla_x) f^{(n)} = T_0 f^{(n)} + \sum_{k=1}^{n} T_k f^{(n-k)}, \tag{2.12}$$

with initial condition $f_0^{(n)}$.

Equation (2.11) has the solution expressed in terms of the classical Hamiltonian flow $\phi^t(x,v)$ generated by the Hamiltonian (1.2), namely $\phi^t(x,v)=(x(t),v(t))$ where

$$\dot{x}(t) = v(t), \quad \dot{v}(t) = -\nabla_x U(x(t)), \tag{2.13}$$

with initial condition $x(0)=x$, $v(0)=v$. Then the solution to (2.11) is

$$f^{(0)}(x,v;t) = f_0^{(0)}(\phi^{-t}(x,v)). \tag{2.14}$$

Equation (2.12) can be solved for $n>0$ by recurrence. In fact the Duhamel formula gives us

$$f^{(n)}(x,v;t) = f_0^{(n)}(\phi^{-t}(x,v)) + \int_0^t \mathrm{d}\tau S_n(\phi^{-(t-\tau)},\tau), \tag{2.15}$$

where

$$S_n = \sum_{k=1}^{n} T_k f^{(n-k)} \tag{2.16}$$

is known by the previous steps.

It is remarkable that each term of the expansion can be computed in terms of the classical flow $\phi^t(x,v)$ and its derivative with respect to the initial velocities.

The formal algebra we present in this section corresponds to the semiclassical Egorov theorem (see, e.g., Ref. 8). It gives the formal expansion, in power of ε, of the symbol of the time evolution of a quantum observable. In other words the Weyl quantization formula (see Eq. (4.1)) of Eq. (2.10) yields the power expansion of the time evolved quantum density matrix.

III. INITIAL STATES

The expansions introduced in the previous section are formal and presumably diverging as a power series in ε. For a rigorous analysis we truncate the series and estimate the remainder. To do this, however, we first want to see which reasonable hypotheses we have to do on the expansion at time zero. If it is given by a wave function Ψ not depending on ε, the Wigner transform $f_0 = f_\Psi$ given by Eq. (1.10) is gently varying with ε and has a series expansion

$$f_0 = f_0^{(0)} + \varepsilon f_0^{(1)} + \varepsilon^2 f_0^{(2)} + \cdots \tag{3.1}$$

in which all the coefficients $f_0^{(k)}$ are smooth. These initial data, however, do not exhaust all cases of physical interest. For instance WKB states have a quickly oscillating phase. Let us compute the coefficient of the expansion (3.1) starting with the simplest case, namely the one in which the phase is a linear function of the configuration:

$$S(x) = p \cdot x, \quad p \in \mathbb{R}^d. \tag{3.2}$$

Then the Wigner transform of the wave function (1.3) is

$$f_0(x,v) = \left(\frac{1}{2\pi}\right)^d \int \mathrm{d}y e^{i(v-p)\cdot y} a\left(x - \frac{\varepsilon}{2}y\right) a\left(x + \frac{\varepsilon}{2}y\right) \tag{3.3}$$

(assuming a real). Inserting in (3.3) the Taylor expansion

$$a\left(x \pm \frac{\varepsilon}{2}y\right) = \sum_{n\geqslant 0} (y\cdot\nabla_x)^n a(x) \frac{(\pm 1)^n}{n!}\left(\frac{\varepsilon}{2}\right)^n \tag{3.4}$$

we find

$$f_0(x,v) = \sum_{n\geqslant 0}\left(\frac{\varepsilon}{2}\right)^n \sum_{k\leqslant n} \frac{(-1)^k}{k!}\frac{1}{(n-k)!} \times \sum_{j_1\ldots j_n=1}^{\mathrm{d}} \frac{\partial^k}{\partial_{x_{j_1}}\ldots\partial_{x_{j_k}}} a(x) \frac{\partial^{n-k}}{\partial_{x_{j_{k+1}}}\ldots\partial_{x_{j_n}}} a(x) \int \mathrm{d}y y_{j_1}\ldots y_{j_n} e^{i(v-p)\cdot y}. \tag{3.5}$$

Therefore the coefficients, which are explicitly given by

$$f_0^{(n)}(x,v) = \left(\frac{-i}{2}\right)^n \sum_{k=0}^{n} \frac{1}{k!}\frac{1}{(n-k)!}(-1)^k \sum_{j_1\ldots j_n} \frac{\partial^k}{\partial_{x_{j_1}}\ldots\partial_{x_{j_k}}} a(x) \frac{\partial^{n-k}}{\partial_{x_{j_{k+1}}}\ldots\partial_{x_{j_n}}} a(x) \frac{\partial^n}{\partial_{v_{j_1}}\ldots\partial_{v_{j_n}}} \delta(v-p), \tag{3.6}$$

are distributions in v, no matter how a is assumed smooth.

When S is not a linear function of x, we can proceed analogously by expanding also the exponential of the oscillating phase. The calculations are slightly more involved but again the coefficients are smooth as regards the x dependence and derivatives of δ functions as regards the v dependence. The explicit form of the coefficients is not particularly relevant in the present context and hence we omit the details.

Let us now analyze the case of a coherent state of the form:

$$\Psi(x) = \left(\frac{1}{\pi\varepsilon}\right)^{d/4} e^{(i/\epsilon)v_0\cdot x} \exp\left(\frac{(x-x_0)^2}{2\varepsilon}\right) \tag{3.7}$$

whose Wigner transform is

$$f_\Psi(x,v) = \left(\frac{1}{\pi\varepsilon}\right)^d \exp\left(-\frac{(x-x_0)^2}{2\varepsilon}\right)\exp\left(-\frac{(v-v_0)^2}{2\varepsilon}\right). \tag{3.8}$$

Given a test function $\varphi(x,v)$, setting $z=(x,v)$ and $z_0=(x_0,v_0)$, we obtain

$$\langle f_\Psi,\varphi\rangle = \left(\frac{1}{\pi}\right)^d \int_{\mathbb{R}^{2d}} \mathrm{d}z e^{-z^2}\varphi(z_0+\sqrt{\varepsilon}z) = \left(\frac{1}{\pi}\right)^d \sum_{n\geqslant 0}\frac{1}{(2n)!}\varepsilon^n \int_{\mathbb{R}^{2d}} \mathrm{d}z e^{-z^2}(z\cdot\nabla_z)^{2n}\varphi(z_0). \tag{3.9}$$

Hence:

$$f_\Psi(x,v) = \delta(x-x_0)\delta(v-v_0) + \varepsilon\sum_{i=1}^{d}\left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial v_i^2}\right)\delta(x-x_0)\delta(v-v_0) + \cdots. \tag{3.10}$$

Thus the expansion at order n of the Wigner function of a coherent state involved derivatives of order $2n$ of δ functions. On the other hand a mixture of coherent states by means of a smooth probability density on (x_0,v_0) can be expanded in terms of smooth coefficients. Therefore we are led to consider initial expansions (2.9) with smooth and distributional coefficients.

IV. H_s ESTIMATES FOR THE WIGNER FUNCTION

We start by reviewing some well-known facts concerning the solution to the Wigner-Liouville Eq. (2.1).

Equation (1.9) can be inverted, namely we have

$$\rho(x,y)=\left(\frac{1}{2\pi}\right)^d\int \mathrm{d}v e^{i(v/\varepsilon)(x-y)}f\left(\frac{x+y}{2};v\right). \tag{4.1}$$

Actually the operator $\hat{\rho}$, whose integral kernel is given by (4.1), is the Weyl quantization of the classical observable f defined on the phase space.

Consider now the Hamiltonian $H=-(\varepsilon^2/2)\Delta+U$. Under a suitable assumption on U (for instance $U\in L_\infty$) H is self-adjoint on a suitable domain and $V(t)=\exp(it/\varepsilon)H$ is a strongly continuous group of unitaries in $L_2(\mathbb{R}^d)$. The time evolution of $\hat{\rho}$ is $\hat{\rho}(t)=V(t)\hat{\rho}V(-t)$. Therefore, given $f\in L_2(x,v)$ we can define the time evolution mapping $f\to f(t)$ by means of the following steps:

$$f\to\hat{\rho}\to\hat{\rho}(t)\to f(t)\equiv\Omega(t)f$$

where the above actions are the Weyl quantization (4.1), the quantum time evolution and the Wigner transform, respectively. The family of transformations $\Omega(t)$ is a one-parameter group of unitaries whose generator extends $-v\cdot\nabla+T$ as an anti-self-adjoint operator. Therefore Eq. (2.1) may be seen as an equation in $L_2(x,v)$.

Remark: Here f is considered as a classical observable and $\hat{\rho}$ a quantum observable obtained by means of the Weyl quantization. Of course a probability density f does not correspond necessarily to a physical admissible state. Conversely the Wigner transform of a quantum state is not, in general, a probability density.

Now we look for further regularity. Let $f=f(x,v;t)$ be the solution to the Wigner-Liouville equation, with initial datum $f_0\in H_s(x,v)$, where $H_s(x,v)$ is the Sobolev space of order s and s is a positive integer. In this section we show that $f(t)\in H_s(x,v)$, provided that the potential energy U is sufficiently smooth. In proving this we exploit the antisymmetry of the operators $v\cdot\nabla_x$ and T using straightforward L_2 estimates.

For any multi-index $\alpha=\{\alpha_1\ldots\alpha_d\}$, we introduce the standard notation:

$$D_x^\alpha=\frac{\partial^{|\alpha|}}{\partial^{\alpha_1}x_1\ldots\partial^{\alpha_d}x_d}, \tag{4.2}$$

where $|\alpha|=\Sigma_j\alpha_j$. Analogously we set:

$$D_v^\alpha=\frac{\partial^{|\alpha|}}{\partial^{\alpha_1}v_1\ldots\partial^{\alpha_d}v_d}, \tag{4.3}$$

and define the scalar product:

$$(f,g)_n=\sum_{\substack{\alpha,\beta:\\ |\alpha|+|\beta|\le n}}(D_v^\alpha D_x^\beta f,D_v^\alpha D_x^\beta g)_{L_2(x,v)}, \tag{4.4}$$

and the associated norm $\|f\|_n=\sqrt{(f,f)_n}$. The Hilbert space equipped with the scalar product (4.4) is denoted by H_n.

In order to estimate $\|f(t)\|_n$ we compute $\partial_t D_v^\alpha D_x^\beta f$ with $|\alpha|+|\beta|\le n$. We have

$$\partial_t D_v^\alpha D_x^\beta f = D_v^\alpha D_x^\beta(-v\cdot\nabla_x + T)f = (-v\cdot\nabla_x + T)D_v^\alpha D_x^\beta f + \sum_{\substack{\alpha'<\alpha:\\ |\alpha'|=1}} C_{\alpha,\alpha'} D_v^{\alpha'} v\cdot\nabla_x D_v^{\alpha-\alpha'} D_x^\beta f$$

$$+ i\sum_{\substack{\beta'<\beta:\\ |\beta'|>0}} C_{\beta,\beta'} \int_{-1/2}^{1/2} \mathrm{d}\lambda \int \mathrm{d}k \hat{U}(k) D_x^{\beta'} e^{ik\cdot x}(k\cdot\nabla_v) D_v^\alpha D_x^{\beta-\beta'} f(x, v+\varepsilon\lambda k), \tag{4.5}$$

where $C_{\alpha,\alpha'}$ is a suitable combinatorial coefficient and $\alpha'<\alpha$ means $\alpha'_j \leqslant \alpha_j$ with $|\alpha'|<|\alpha|$. Finally $\beta-\beta' = \{\beta_j - \beta'_j\}_{j=1}^d$.

Note that the second term on the right-hand side of (4.5) is absent when $|\alpha|=0$.

We have now that

$$(g, v\cdot\nabla_x g)_{L_2(x,v)} = (g, Tg)_{L_2(x,v)} = 0 \tag{4.6}$$

for any g smooth enough. Then, for f real:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(D_v^\alpha D_x^\beta f, D_v^\alpha D_x^\beta f)_{L_2(x,v)} = (D_v^\alpha D_x^\beta f, D_v^\alpha D_x^\beta f \partial_t f)_{L_2(x,v)}. \tag{4.7}$$

Inserting (4.5) in (4.7) we realize that, by virtue of (4.6), the first term on the right-hand side of (4.5) (namely that with higher order derivatives) does not give any contribution. By the Schwarz inequality, for $|\alpha|\geqslant 1$:

$$(D_v^\alpha D_x^\beta f, D_v^{\alpha'} v\cdot\nabla_x D_v^{\alpha-\alpha'} D_x^\beta f)_{L_2} \leqslant C\|f\|_n^2, \tag{4.8}$$

because $|\alpha|-|\alpha'|+|\beta|+1\leqslant n$. Analogously the last term on the right-hand side of (4.5) is bounded in the L_2 norm, by

$$\int \mathrm{d}k |\hat{U}(k)||k|^{(|\beta'|+1)} \|\nabla_v D_v^\alpha D_x^{\beta-\beta'} f\|_{L_2} \leqslant C\|f\|_n \tag{4.9}$$

because $|\alpha|+|\beta|-|\beta'|+1\leqslant n$. In conclusion,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|f\|_n^2 \leqslant C\|f\|_n^2, \tag{4.10}$$

provided that

$$\int \mathrm{d}k |\hat{U}(k)||k|^n \leqslant C < +\infty. \tag{4.11}$$

Summarizing we proved the following.

Theorem 4.1: Let $f=f(t)$ be the solution to Eq. (2.1) with initial datum $f_0 \in H_n(x,v)$ with $n \geqslant 0$ and suppose that the potential U satisfies condition (4.11). Then $f(t) \in H_n(x,v)$ and

$$\|f(t)\|_n \leqslant \|f_0\|_n e^{Ct},$$

where the constant C (which depends on n) is independent of ε. For $n=0$ we have $C=1$, namely the L_2 norm is conserved.

V. CONTROLLING THE REMAINDER

In this section we present the main results of this paper. We show that the formal expansion (2.10) can be truncated at an arbitrary order N and the error we make is $O(\varepsilon^{N+1})$.

The discussion in Sec. III on the initial data suggests to consider separately the case of smooth and distributional coefficients (for instance when dealing with a suitable mixture of coherent states and WKB or coherent pure states, respectively). We need first to establish a few preliminary estimates. We introduce the operator $\mathcal{T}_N$ by

$$\mathcal{T}_N = T - \sum_{j=0}^{N} T_j \varepsilon^j = i\varepsilon^{N+1} \int \mathrm{d}k \hat{U}(k) e^{ik\cdot x} \int_{-1/2}^{1/2} \mathrm{d}\lambda \int_0^{\lambda} \mathrm{d}\mu \frac{\mu^N}{N!} (k\cdot\nabla_v)^{N+2} f(x, v+\mu\varepsilon k) \tag{5.1}$$

and set:

$$u(n) = \int \mathrm{d}k |\hat{U}(k)| (1+|k|)^n. \tag{5.2}$$

Then if $g \in H_{N+s+2}(x,v)$ and if U is sufficiently smooth, from (5.1) we get

$$\|\mathcal{T}_N g\|_s \leqslant C\varepsilon^{N+1} u(s+N+2) \|g\|_{N+s+2}. \tag{5.3}$$

Here and in the sequel C denotes any positive constant depending on N, the Sobolev indices $n, s, \ldots$ and time, but not on ε. Estimate (5.3) follows easily by the definition. In the same way we obtain

$$\|T_n g\|_s \leqslant C u(s+n+1) \|g\|_{n+s+1}. \tag{5.4}$$

Finally setting

$$\widetilde{\mathcal{D}} = \bigcap_{s\in\mathbb{N}^+} H_s(x,v), \tag{5.5}$$

we can prove the following:

Theorem 5.1: Consider $f(t)$ the solution to the initial value problem (2.1) with initial condition

$$f_0 = \sum_{n=0}^{N} \varepsilon^n f_0^{(n)} + R_N(0), \tag{5.6}$$

for some integer $N \geqslant 1$. Assume that $f_0^{(n)} \in \widetilde{\mathcal{D}}$ for all $n \geqslant 0 \ldots N$ and that $R_N(0) \in \widetilde{\mathcal{D}}$ with the bound

$$\|R_N(0)\|_s \leqslant C\varepsilon^{N+1}, \quad s = 0, 1, \ldots . \tag{5.7}$$

If $u(n) < C_n < +\infty$ for any $n \geqslant 1$, then

$$f(t) = \sum_{n=0}^{N} \varepsilon^n f^{(n)}(t) + R_N(t) \tag{5.8}$$

with $f^{(n)}(t)$ given by (2.14). Furthermore the following bound on the remainder holds:

$$\|R_N(t)\|_s \leqslant C\varepsilon^{N+1} \tag{5.9}$$

for any $s \geqslant 0$.

Proof: By Eq. (2.1), assuming for the solution the representation (5.8), we have

$$(\partial_t + v\cdot\nabla_x)\sum_{n=0}^{N}\varepsilon^n f^{(n)} + (\partial_t + v\cdot\nabla_x)R_N = \sum_{n=0}^{N}\varepsilon^n T f^{(n)} + TR_N = \sum_{\substack{s,n=0:\\ s+n\leqslant N}}^{N}\varepsilon^{n+s}T_s f^{(n)} + \sum_{n=0}^{N}\varepsilon^n \mathcal{T}_N f^{(n)} + \sum_{\substack{s,n=0:\\ s+n>N}}^{N}\varepsilon^{n+s}T_s f^{(n)} + TR_N. \tag{5.10}$$

By construction the first terms on the left- and right-hand sides of (5.10) compensate, so that the equation for the remainder $R_N(t)$ is

$$(\partial_t + v\cdot\nabla_x)R_N(t) = TR_N(t) + S_N^R(t), \tag{5.11}$$

where

$$S_N^R = \sum_{n=0}^{N}\varepsilon^n \mathcal{T}_N f^{(n)} + \sum_{\substack{s,n=0:\\ s+n>N}}^{N}\varepsilon^{n+s}T_s f^{(n)}. \tag{5.12}$$

By Eq. (2.15) and Theorem 4.1 we have, for any $s\geqslant 0$,

$$\|f^{(n)}(t)\|_s \leqslant C\|f_0^{(n)}\|_s + C\int_0^t \mathrm{d}\tau \|S_n(\tau)\|_s. \tag{5.13}$$

Moreover, by (2.16) and (5.4):

$$\|S_n(\tau)\|_s = \sum_{k=1}^{n}\|T_k f^{(n-k)}(\tau)\|_s \leqslant C\sum_{k=1}^{n}\|f^{(n-k)}(\tau)\|_{s+k+1}. \tag{5.14}$$

Therefore $\sup_{t\leqslant t_0}\|f^{(n)}(t)\|_s \leqslant C$ for all $s\geqslant 0$ provided that the same estimate holds for $0,1,\ldots n-1$. By Theorem 4.1 if $f_0^{(0)}\in\widetilde{\mathcal{D}}$ then $\sup_{t\leqslant t_0}\|f^{(0)}(t)\|_s \leqslant C$ for all $s\geqslant 0$. Therefore we can inductively conclude that

$$\sup_{t\leqslant t_0}\|f^{(n)}(t)\|_s \leqslant C$$

for all s and n.

By (5.11) and the Duhamel formula:

$$R_N(t) = \Omega(t)R_N(0) + \int_0^t \mathrm{d}\tau\,\Omega(t-\tau)S_N^R(\tau). \tag{5.15}$$

By Theorem 4.1 we have

$$\|R_N(t)\|_s \leqslant C\|R_N(0)\|_s + C\int_0^t \mathrm{d}\tau\|S_N^R(\tau)\|_s \tag{5.16}$$

and finally, by (5.12), (5.3), and (5.4):

$$\|S_N^R(\tau)\|_s \leqslant \sum_{n=0}^{N}\varepsilon^n\|\mathcal{T}_N f^{(n)}(\tau)\|_s + \sum_{\substack{s,n=0:\\ s+n>N}}^{N}\varepsilon^{n+s}\|T_s f^{(n)}(\tau)\|_s \leqslant C\varepsilon^{N+1}. \tag{5.17}$$

This concludes the proof. ■

We remark that the hypotheses under which we proved Theorem 5.1 could be considerably relaxed. Indeed if N is not arbitrary but given, we can prove (5.9) with $s=0$, provided that $f_0^{(n)} \in H_{N+1}$ for all $n \leqslant N$ and $u(N+1) < C$.

We now rephrase Theorem 5.1 for Sobolev spaces with negative indices to include WKB or coherent states.

We start by observing that H_{-s} solutions to Eq. (2.1), for initial condition $f_0 \in H_{-s}$, can be defined by duality:

$$(g, f(t)) = (\Omega(-t)g, f_0) \tag{5.18}$$

for all $g \in H_s$. Theorem 4.1 makes the above definition meaningful and provides the bound

$$\|f(t)\|_{-s} \leqslant C\|f_0\|_{-s}. \tag{5.19}$$

We can also extend estimates (5.3) and (5.4) by duality:

$$\|\mathcal{T}_N g\|_{-s} \leqslant C\varepsilon^{N+1} u(s+N+2)\|g\|_{-(s-N-2)}, \tag{5.20}$$

$$\|T_n g\|_s \leqslant Cu(s+n+1)\|g\|_{-(s-n-1)}. \tag{5.21}$$

Obviously Eqs. (5.20) and (5.21) make sense provided that $g \in H_{-(s-N-2)}$ and $g \in H_{-(s-n-1)}$, respectively.

Theorem 5.2: Let $f(t)$ be the solution to the initial value problem (2.1) with initial condition

$$f_0 = \sum_{n=0}^{N} \varepsilon^n f_0^{(n)} + R_N(0), \tag{5.22}$$

for some integer $N \geqslant 1$. Assume that $f_0^{(n)} \in H_{-(r+2n)}$, for some $r \geqslant 0$ and all $n \geqslant 0 \ldots N$ and that $R_N(0) \in H_{-(r+4N)}$ with the bound

$$\|R_N(0)\|_{-(r+4N)} \leqslant C\varepsilon^{N+1}. \tag{5.23}$$

If $u(r+4N+2) < C < +\infty$, then

$$f(t) = \sum_{n=0}^{N} \varepsilon^n f^{(n)}(t) + R_N(t) \tag{5.24}$$

with $f^{(n)}(t)$ given by (2.15). Furthermore:

$$\|R_N(t)\|_{-(r+4N)} \leqslant C\varepsilon^{N+1}. \tag{5.25}$$

Proof: We proceed as in the proof of Theorem 5.1. By (2.15) and (5.22), for fixed arbitrary t_0, if $t \leqslant t_0$:

$$\|f^{(n)}(t)\|_{-(r+2n)} \leqslant C\|f_0^{(n)}\|_{-(r+2n)} + C \sup_{\tau < t_0} \|S_n(\tau)\|_{-(r+2n)}. \tag{5.26}$$

Moreover, by (2.16) and (5.21):

$$\|S_n(\tau)\|_{-(r+2n)} \leqslant \sum_{k=1}^{n} \|T_k f^{(n-k)}(\tau)\|_{-(r+2n)} \leqslant C \sum_{k=1}^{n} \|f^{(n-k)}(\tau)\|_{-(r+2n-k-1)}. \tag{5.27}$$

Assuming, by inductive hypothesis, that for all $k < n$,

$$\sup_{t<t_0}\|f^{(k)}(t)\|_{-(r+2k)} = C \tag{5.28}$$

[note that Eq. (5.28) is known to hold for $k=0$ by (5.19)] then, using (5.28) in (5.27), we conclude that

$$\|S_n(\tau)\|_{-(r+2n)} \leqslant C\sum_{k=1}^{n} \|f^{(n-k)}(\tau)\|_{-(r+2(n-k))} \leqslant C \tag{5.29}$$

and hence (5.28) holds for any $k \leqslant N$.

Furthermore by (5.15), (5.11), and (5.12):

$$\|R_N(t)\|_{-(r+4N)} \leqslant C\|R_N(0)\|_{-(r+4N)} + C\sup_{t<t_0}\|S_N^R(\tau)\|_{-(r+4N)}, \tag{5.30}$$

$$\begin{aligned}\|S_N^R(\tau)\|_{-(r+4N)} &\leqslant \sum_{n=0}^{N} \varepsilon^n \|\mathcal{T}_N f^{(n)}(\tau)\|_{-(r+4N)} + \sum_{\substack{s,n=0:\\ s+n>N}}^{N} \varepsilon^{n+s}\|T_s f^{(n)}(\tau)\|_{-(r+4N)} \\ &\leqslant \varepsilon^{N+1}\sum_{s,n=0}^{N} \|f^{(n)}(\tau)\|_{-(r+2n)} \leqslant \varepsilon^{N+1}.\end{aligned} \tag{5.31}$$

This concludes the proof. ■

To comment on the result we note that if A is a quantum observable with kernel $A(x,y)$ and symbol $a(x,v)$, then:

$$(\Psi, A\Psi)_{L_2(x)} = (f_\Psi, a)_{L_2(x,v)} \tag{5.32}$$

where

$$a(x,v) = \left(\frac{\varepsilon}{2\pi}\right)^3 \int \mathrm{d}y e^{iv\cdot y} A\left(x+\varepsilon\frac{y}{2}; x-\varepsilon\frac{y}{2}\right), \tag{5.33}$$

where a is the symbol of A (which is its Weyl quantization). For many fundamental observables (like momentum, energy, angular momentum, etc.) the symbol a is independent of ε. In this case $(\Psi, A\Psi)_{L_2(x)}$ can be easily expanded:

$$(\Psi, A\Psi)_{L_2(x)} = \sum_n A_n(t)\varepsilon^n, \tag{5.34}$$

where

$$A_n(t) = \int \mathrm{d}x \int \mathrm{d}v a(x,v) f_\Psi^{(n)}(x,v;t). \tag{5.35}$$

For instance for the current density we have

$$J(x,t) = \sum_n J_n(x,t)\varepsilon^n,$$

where

$$J_n(x,t) = \int \mathrm{d}v v f_\Psi^{(n)}(x,v;t).$$

However, in principle, other observables A can have symbols which depend on ε. In this case we have to combine the semiclassical expansion of the symbol:

$$a(x,v,\varepsilon) = \sum_n a_n(x,v)\varepsilon^n$$

with the expansion (2.10) for f_Ψ, namely we have to replace (5.35) by

$$A_n(t) = \sum_{k=0}^{n} \int dx \int dv a_k(x,v) f_\Psi^{(n-k)}(x,v;t). \tag{5.36}$$

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Fisher information of *D*-dimensional hydrogenic systems in position and momentum spaces

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The spreading of the quantum-mechanical probability distribution density of *D*-dimensional hydrogenic orbitals is quantitatively determined by means of the local information-theoretic quantity of Fisher in both position and momentum spaces. The Fisher information is found in closed form in terms of the quantum numbers of the orbital. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Fisher information, originally introduced by R. A. Fisher in the theory of statistical estimation,[1,2] is the main theoretic tool of the extreme physical information principle, a general variational principle which allows one to derive numerous fundamental equations of physics:[3–5] Maxwell equations, the Einstein field equations, the Dirac and Klein-Gordon equations, various laws of statistical physics and some laws governing nearly incompressible turbulent fluid flows. Applications to a large variety of problems in theoretical physics have received a strong impulse when it was realized that the spatial distribution of the single-particle probability density $\rho(\vec{r})$ of a many-particle system, which is the basic variable of the density functional theory,[6,7] can be quantitatively measured by its translationally invariant Fisher information in a different and complementary manner as the Shannon entropy. Both quantities characterize the information-theoretic content of the density $\rho(\vec{r})$ which describes the physical state under consideration. The Shannon entropy[8,9] is a logarithmic functional of the density, so that it is a global measure of disorder or smoothness of $\rho(\vec{r})$. The Fisher information is the gradient functional of the density

$$I_\rho = \int_{\mathbb{R}^3} \frac{[\vec{\nabla}\rho(\vec{r})]^2}{\rho(\vec{r})} d\vec{r}, \tag{1}$$

so it has a property of locality because it is sensitive to local rearrangements of the position variable $\vec{r}$.[3,10] The higher this quantity is, the more concentrated the single-particle density, the smaller the uncertainty and the higher the accuracy is in predicting the localization for the particle.[3,11]

The Fisher information I_ρ has been shown to be closely connected with other density functionals which characterize a number of macroscopic properties of fundamental character as well as physical observables;[3,7,12,13] in particular, it represents, a constant apart, the Weiszäcker energy functional of the many-particle system.[7,13] Moreover, it has been used (i) to build up uncertainty relations stronger than the variance-based Heisenberg principle (e.g., the Cramer-Rao

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relation),[3,11,14] (ii) to analyze the correlation problem of the many-electron systems,[15] and (iii) to identify the most distinctive nonlinear spectral phenomena (the avoided crossings) of electronic systems in external fields.[16]

However, the analytical determination of the Fisher information from first principles has not been undertaken yet, even for single-particle systems. In this paper we shall calculate the Fisher information of a D-dimensional hydrogenic system in terms of D quantum numbers which characterize its orbitals not only in the position but also in the momentum representation. Emphasis will be on momentum hydrogenic orbitals, i.e., the solution to the nonrelativistic, time-independent Schrödinger equation in momentum space describing the quantum-mechanics for the motion of an electron in the Coulomb field of a nucleus with charge $+Ze$. This is not only because the momentum orbitals have usually been avoided in favor of the position orbitals but also because of (i) their conceptual importance, (ii) the distribution of momenta for real ($D=3$) atomic systems and specifically for hydrogen atom[17–19] is nowadays experimentally accessible in atomic, molecular, and nuclear experiments, especially since the advent of the modern spectroscopy (e,e'),[19] (iii) the scattering phenomena are most conveniently viewed in numerical simulations by means of momentum orbitals (see, e.g., Ref. 20), and (iv) they play a very relevant role in numerous other physical processes with atoms and molecules which are governed by simple functions of the momentum transfer.[21,22] Moreover, the D-dimensional hydrogenic orbitals are of interest as many-electron Sturmians.[23,24] For further details and motivation see Refs. 25–38.

The position and momentum hydrogenic orbitals in D-dimensions in polar coordinates are known to be composed of an angular part and a radial part.[25,39–42] The angular part, which is common to both position and momentum cases, corresponds to hyperspherical harmonics because of the radially symmetric character of the Coulomb potential. The radial part is controlled by the Laguerre and Gegenbauer polynomials in the position and momentum representations, respectively. This is not accidental; it is associated with the well-known $O(3)$ and $O(4)$ symmetries of the hydrogen atom.[43–46]

The paper is structured as follows. First in Sec. II the known position and momentum wave functions of the hydrogenic system in D dimensions are described in detail, and the corresponding probability densities are explicitly shown. Then in Secs. III and IV we find closed expressions for the Fisher information of the hydrogenic orbitals in terms of the D quantum numbers which characterize them in position and momentum spaces, respectively. Finally, some concluding remarks are given.

II. THE HYDROGENIC PROBLEM IN *D* DIMENSIONS

In the following we fix our notation and we describe in hyperspherical polar coordinates the wave functions of the D-dimensional hydrogenic orbitals (i.e., the solutions to the nonrelativistic, time-independent Schrödinger equation in D dimensions describing the quantum mechanics for the motion of an electron in the Coulomb field of a nucleus with charge $+Ze$) in the configuration (or position) and momentum spaces, as well as the associated probability densities.

A. *D*-dimensional position orbitals

The position hydrogenic orbitals $\Psi(\vec{r})$ are the solutions of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}_D^2-\frac{Ze^2}{r}\right)\Psi(\vec{r})=E\Psi(\vec{r}), \tag{2}$$

where μ is the reduced mass, the position vector $\vec{r}=(x_1,x_2,\ldots,x_D)$, and $\vec{\nabla}_D^2$ is the Laplacian operator in the D-dimensional space, $D\geqslant 2$. By use of the polar coordinates $(r,\theta_1,\theta_2,\ldots,\theta_{D-2},\varphi)$ defined by

$$x_1=r\sin\theta_1\sin\theta_2\ldots\sin\theta_{D-2}\cos\varphi,$$

$$x_2 = r \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{D-2} \sin\varphi,$$

$$x_3 = r \sin\theta_1 \sin\theta_2 \ldots \cos\theta_{D-2},$$

$$\vdots$$

$$x_{D-1} = r \sin\theta_1 \cos\theta_2,$$

$$x_D = r \cos\theta_1,$$

with $0 \leqslant \theta_j \leqslant \pi$, $j=1,\ldots,D-2$, and $0 \leqslant \varphi \leqslant 2\pi$, one has that Eq. (2) transforms as

$$\left[-\frac{\hbar^2}{2\mu_e}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{D-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\Lambda^2}{r^2} \right) - \frac{Ze^2}{r} \right] \Psi(\vec{r}) = E\Psi(\vec{r}),$$

where Λ^2 is the D-dimensional generalization of the square of the angular momentum operator[26,40,47] which only depends on the $D-1$ angular coordinates $\theta_1, \theta_2, \ldots, \theta_{D-2}$, and φ of a D-dimensional sphere. The technique of separation of variables is known to provide the bound state solutions $\{E, \Psi(\vec{r})\}$ for this problem. The energies are given (see, e.g., Ref. 36) by

$$E = -\frac{Z^2e^2}{a_\mu}\frac{1}{2\eta^2} = -\frac{Z^2e^2}{a_0}\frac{\mu}{m_e}\frac{1}{2\eta^2}, \tag{3}$$

where $a_\mu = \hbar^2/\mu e^2 = (m_e/\mu)a_0$, and $a_0 = \hbar^2/m_e e^2$ is the Bohr radius, and

$$\eta = n + \frac{D-3}{2}, \quad n = 1,2,3,\ldots . \tag{4}$$

The associated eigenfunctions $\Psi(\vec{r})$ have a radial part $R(r)$ and an angular part $Y(\Omega_{D-1})$ so that

$$\Psi(\vec{r}) = R(r)Y(\Omega_{D-1}), \tag{5}$$

where $Y(\Omega_{D-1})$ are the hyperspherical harmonics, i.e., the eigenfunctions of the nonradial part of the Hamiltonian, Λ^2, i.e.,

$$\Lambda^2 Y_{l,\{\mu\}}(\Omega_{D-1}) = l(l+D-2)Y_{l,\{\mu\}}(\Omega_{D-1}), \quad l = 0,1,2,\ldots .$$

Each hyperspherical harmonic is determined by the $D-1$ quantum numbers $(l \equiv \mu_1, \mu_2, \ldots, \mu_{D-1}) \equiv (l, \{\mu\})$, which may have all values consistent with the inequalities $l \equiv \mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_{D-1} \equiv |m| \geqslant 0$. These functions have the form

$$Y_{l,\{\mu\}}(\Omega_{D-1}) = \frac{1}{\sqrt{2\pi}} A_{l,\{\mu\}} e^{im\varphi} \prod_{j=1}^{D-2} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}} \equiv \frac{1}{\sqrt{2\pi}} e^{im\varphi} \prod_{j=1}^{D-2} Y_{\mu_j,\mu_{j+1}}^{(j)}(\theta_j), \tag{6}$$

with the normalization constant

$$|A_{l,\{\mu\}}|^2 = \prod_{j=1}^{D-2} \frac{(\alpha_j+\mu_j)(\mu_j-\mu_{j+1})![\Gamma(\alpha_j+\mu_{j+1})]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j+\mu_j+\mu_{j+1})} \equiv \prod_{j=1}^{D-2} A_{\mu_j,\mu_{j+1}}^{(j)}, \tag{7}$$

where $2\alpha_j = D-j-1$ and $C_k^\lambda(t)$ is the Gegenbauer polynomial of degree k and parameter λ. In addition, we have used the notation

$$Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j) = A^{(j)}_{\mu_j,\mu_{j+1}} C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_j+1}.$$

Remark that for $D=2$ there are no products, so that the corresponding spherical harmonic is just $e^{im\varphi}/(2\pi)$. The spherical harmonics satisfy the orthonormalization condition

$$\int_{-1}^{1} \mathrm{d}\Omega_{D-1} Y_{l',\{\mu'\}}(\Omega_{D-1}) Y_{l,\{\mu\}}(\Omega_{D-1}) = \delta_{ll'}\delta_{\{\mu\}\{\mu'\}}. \tag{8}$$

The radial eigenfunctions $R(r)$, i.e., the solutions of the radial Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{D-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+D-2)}{r^2}\right) - \frac{Ze^2}{r}\right] R(r) = ER(r), \tag{9}$$

have the form

$$R_{\eta,L}(r) = N_{\eta,L}\left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right]^{1/2} L^{2L+1}_{\eta-L-1}(\tilde{r}), \tag{10}$$

where the grand orbital angular momentum quantum number L and the adimensional parameter $\tilde{r}$ are

$$L = l + \frac{D-3}{2}, \quad l = 0,1,2,\ldots,$$

$$\tilde{r} = \frac{r}{\lambda} \quad \text{with } \lambda = \frac{\eta\hbar^2}{2Z\mu e^2} = \frac{\eta a_\mu}{2Z},$$

and $\omega_\alpha(\tilde{r}) = \tilde{r}^\alpha e^{-\tilde{r}}$ denotes the weight function with respect to which the Laguerre polynomials $L^\alpha_k(\tilde{r})$ are orthogonal on the interval $[0,\infty)$. And the normalization constant is given by

$$N_{\eta,L} = \lambda^{-D/2}\left\{\frac{(\eta-L-1)!}{2\eta[(\eta+L)!]^3}\right\}^{1/2} = \left\{\left(\frac{2Z}{a_\mu\left(n+\frac{D-3}{2}\right)}\right)^D \frac{(n-l-1)!}{2\left(n+\frac{D-3}{2}\right)[(n+l+D-3)!]^3}\right\}^{1/2} \equiv N_{n,l}.$$

Then, the complete energy eigenfunctions of the D-dimensional hydrogen atom are

$$\Psi_{\eta,L,\{\mu\}}(\vec{r}) = R_{\eta,L}(r) Y_{L,\{\mu\}}(\Omega_{D-1}) = N_{\eta,L}\left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right]^{1/2} L^{2L+1}_{\eta-L-1}(\tilde{r}) Y_{L,\{\mu\}}(\Omega_{D-1}),$$

or, also the form

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = R_{n,l}(r) Y_{l,\{\mu\}}(\Omega_{D-1}) = N_{n,l}\left(\frac{r}{\lambda}\right)^l e^{-(r/2\lambda)} L^{2l+D-2}_{n-l-1}\left(\frac{r}{\lambda}\right) Y_{l,\{\mu\}}(\Omega_{D-1}). \tag{11}$$

So, the probability density of the system in the configuration space $\rho(\vec{r}) = |\Psi(\vec{r})|^2$ has the form

$$\begin{aligned}\rho(\vec{r}) &= R^2_{nl}|Y_{l,\{\mu\}}(\Omega_{D-1})|^2 = N^2_{\eta,L}\left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right][L^{2L+1}_{\eta-L-1}(\tilde{r})]^2 |Y_{L,\{\mu\}}(\Omega_{D-1})|^2 \\ &= N^2_{n,l}\tilde{r}^{2l}e^{-\tilde{r}}[L^{2l+D-2}_{n-l-1}(\tilde{r})]^2 |Y_{l,\{\mu\}}(\Omega_{D-1})|^2,\end{aligned} \tag{12}$$

where Eqs. (5), (10), and (11) were taken into account, and the notation $\tilde{r} = r/\lambda$ given by Eq. (9) has been used. It is worth noticing that this expression reduces to the well-known position eigenfunctions for the three-dimensional hydrogenic atom when $D=3$.

B. *D*-dimensional momentum orbitals

By means of a generalization of the Fock method[48] (see also Refs. 40–42 and 49) to *D*-dimensional hydrogenic atoms or, alternatively, by computing the *D*-dimensional Fourier transform of the configuration eigenfunction $\Psi_{nl\{\mu\}}(\vec{r})$[25,50,51] it is obtained that the *D*-dimensional hydrogen eigenfunction in momentum space $\Psi_{nl\{\mu\}}(\vec{p})$ has the form

$$\Psi_{nl\{\mu\}}(\vec{p}) = M_{\eta,L}(p) Y_{l\{\mu\}}(\Omega_{D-1}), \tag{13}$$

when

$$M_{\eta,l}(p) = K_{\eta,L} \frac{(\eta p)^l}{(1+\eta^2 p^2)^{L+2}} C_{\eta-L-1}^{L+1}\left(\frac{1-\eta^2 p^2}{1+\eta^2 p^2}\right). \tag{14}$$

Here the electron momentum p is assumed to be expressed in units of Zp_μ, where $p_\mu=(\mu/m)p_0$, with the atomic momentum unit $p_0=\hbar/a_0$. And the normalization constant

$$K_{\eta,L} = \left(\frac{(\eta-L-1)!}{2\pi(\eta+L)!}\right)^{1/2} 2^{2L+3}\Gamma(L+1)\,\eta^{(D+1)/2}. \tag{15}$$

Then, the corresponding probability density in momentum space $\gamma(\vec{p})=|\Psi_{nl\{\mu\}}(\vec{p})|^2$ is expressed as

$$\gamma(\vec{p}) = K_{nl}^2 \frac{(\eta p)^{2l}}{(1+\eta^2 p^2)^{2l+D+1}} \left[C_{n-l-1}^{l+(D-1)/2}\left(\frac{1-\eta^2 p^2}{1+\eta^2 p^2}\right)\right]^2 |Y_{l\{\mu\}}(\Omega_D)|^2.$$

Here again, for $D=3$ this expression reduces to the corresponding momentum density of the three-dimensional hydrogenic atom.[52]

III. THE FISHER INFORMATION IN POSITION SPACE

In this section we compute the Fisher information of the *D*-dimensional hydrogenic orbital in configuration space, characterized by the quantum numbers $(n,l,\mu_2,\ldots,\mu_{D-1})\equiv(n,l,\{\mu\})$, i.e.,

$$I_\rho(D) := \int_{\mathbb{R}^D} \frac{[\vec{\nabla}_D \rho(\vec{r})]^2}{\rho(\vec{r})} \mathrm{d}^D r, \tag{16}$$

where $\rho(\vec{r})$ is the position probability density of the orbital as given by Eq. (12), $\vec{\nabla}_D$ denotes the *D*-dimensional gradient operator given by

$$\vec{\nabla}_D = \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\sum_{i=1}^{D-2} \frac{1}{\prod_{k=1}^{i-1} \sin\theta_k} \frac{\partial}{\partial\theta_i}\theta_i + \frac{1}{r\prod_{i=1}^{D-2}\sin\theta_i}\frac{\partial}{\partial\varphi}\hat{\varphi}, \tag{17}$$

in the polar coordinates $(r,\theta_1,\theta_2,\ldots,\theta_{D-2},\varphi)$, and the volume element in the *D*-dimensional space is

$$\mathrm{d}\vec{r} = r^{D-1}\mathrm{d}r\mathrm{d}\Omega_{D-1}; \mathrm{d}\Omega_{D-1} = \left(\prod_{j=1}^{D-2}(\sin\theta_j)^{2\alpha_j}\mathrm{d}\theta_j\right)\mathrm{d}\varphi.$$

Taking into account that

$$\rho(\vec{r}) = |\Psi_{n,l,\{\mu\}}(r,\theta_1,\theta_2,\ldots,\theta_{D-2},\varphi)|^2 = |\Psi_{n,l,\{\mu\}}(r,\theta_1,\theta_2,\ldots,\theta_{D-2},0)|^2,$$

one has that

$$I_\rho(D) = 4\int_{\Re^D} [\vec{\nabla}_D \Psi_{n,l,\{\mu\}}(r,\theta_1,\theta_2,\ldots,\theta_{D-2},0)]^2 \mathrm{d}^D r. \tag{18}$$

The use of Eqs. (11) and (17) into this expression allows us to write that

$$\begin{aligned} I_\rho(D) &= 4\int_0^\infty \left[\frac{\partial}{\partial r} R_{nl}(r)\right]^2 r^{D-1}\mathrm{d}r + 4\int_0^\infty r^{-2} R_{nl}^2(r) r^{D-1}\mathrm{d}r \\ &\times \sum_{i=1}^{D-2} \int_{\Omega_{D-1}} \left[\frac{1}{\prod_{k=1}^{i-1} \sin\theta_k} \frac{\partial}{\partial\theta_i} Y_{l,\{\mu\}}(\theta_1,\theta_2,\ldots,\theta_{D-2},0)\right]^2 \mathrm{d}\Omega_{D-1} \\ &\equiv I_R(D) + \langle r^{-2}\rangle \sum_{i=1}^{D-2} I_{\theta_i}(D), \end{aligned} \tag{19}$$

where we have used the orthonormalization condition (8) of the hyperspherical harmonics in the first equality, and the expectation value

$$\langle f(r)\rangle = \int_{\Re^D} f(r)\rho(\vec{r})\mathrm{d}^D r = \int_0^\infty f(r) R_{nl}^2(r) r^{D-1}\mathrm{d}r, \tag{20}$$

for $f(r)=r^{-2}$ in the second equality. As well we have used the notations

$$I_R(D) \equiv 4\int_0^\infty \left[\frac{\mathrm{d}}{\mathrm{d}r} R_{nl}(r)\right]^2 r^{D-1}\mathrm{d}r, \tag{21}$$

for the radial component of the Fisher information $I_\rho(D)$, and

$$I_{\theta_i}(D) \equiv 4\int_{\Omega_{D-1}} \left[\frac{1}{\prod_{k=1}^{i-1} \sin\theta_k} \frac{\partial}{\partial\theta_i} Y_{l,\{\mu\}}(\theta_1,\theta_2,\ldots,\theta_{D-2},0)\right]^2 \mathrm{d}\Omega_{D-1}, \tag{22}$$

for the ith part of the angular component.

In the following we are going to show that the radial integral $I_R(D)$ has the value

$$I_R(D) = \frac{4Z^2}{a_\mu^2 \eta^3}\left[\eta - 2\frac{l(l+D-2)}{2l+D-2}\right] = \frac{4Z^2}{a_\mu^2\eta^3}\left\{\eta - \frac{2}{2L+1}\left[L(L+1) - \frac{1}{4}(D-1)(D-3)\right]\right\}, \tag{23}$$

where we have used that $l(l+D-2)=L(L+1)-\frac{1}{4}(D-1)(D-3)$, and that the angular component $I_{\theta_i}(D)$ is given by

$$I_{\theta_i}(D) = 4\left[\mu_i(\mu_i+D-i-1) - \mu_{i+1}(\mu_{i+1}+D-i-2)\frac{2\mu_i+D-i-1}{2\mu_{i+1}+D-i-2}\right] \times \prod_{k=1}^{i-1} \frac{2\mu_k+D-k-1}{2\mu_{k+1}+D-k-2}. \tag{24}$$

Taking into account that the product

$$\prod_{k=1}^{i-1} \frac{2\mu_k+D-k-1}{2\mu_{k+1}+D-k-2} = \frac{2\mu_1+D-2}{2\mu_i+D-i-1}, \tag{25}$$

one has that Eq. (24) reduces as

$$I_{\theta_i}(D) = 4\left[\mu_i(\mu_i + D - i - 1) - \mu_{i+1}(\mu_{i+1} + D - i - 2)\frac{2\mu_i + D - i - 1}{2\mu_{i+1} + D - i - 2}\right] \times \frac{2\mu_1 + D - 2}{2\mu_i + D - i - 1}. \tag{26}$$

Consideration of Eqs. (19), (23), and (26), and that the expectation value

$$\langle r^{-2}\rangle = \frac{2Z^2}{a_\mu^2 \eta^3}\frac{1}{2l + D - 2} = \frac{2Z^2}{a_\mu^2 \eta^3}\frac{1}{2L + 1}, \tag{27}$$

we have found the following value for the Fisher information of the D-dimensional hydrogenic orbital in the configuration space:

$$I_\rho(D) = \frac{4Z^2}{a_\mu^2 \eta^3}\left\{\eta - \frac{2}{2L+1}\left[L(L+1) - \frac{1}{4}(D-1)(D-3) - \sum_{i=1}^{D-2}\left(\mu_i(\mu_i + D - i - 1) - \frac{\mu_{i+1}(\mu_{i+1} + D - i - 2)(2\mu_i + D - i - 1)}{2\mu_{i+1} + D - i - 2}\right) \times \frac{2\mu_1 + D - 2}{2\mu_i + D - i - 1}\right]\right\}. \tag{28}$$

Straightforward algebraic manipulations lead to the following simple expression for the D-dimensional position Fisher information

$$I_\rho(D) = \frac{4Z^2}{a_\mu^2 \eta^3}[\eta - \mu_{D-1}], \tag{29}$$

valid for $D \geqslant 2$. Remark that for $D=2$, the summation is empty, so that it does not contribute.

It is observed that the Fisher information, as the ionization energy [see Eq. (3)], behaves as η^{-2} with respect to the generalized principal quantum number η [see Eq. (4)]. Remark that the Fisher information depends on the grand principal quantum number η and the grand magnetic quantum number $\mu_{D-1} = |m|$. It is worth noticing that for $D=3$ this expression boils down to

$$I_\rho(D=3) = \frac{4Z^2}{a_\mu^2}\frac{n - |m|}{n^3},$$

recently obtained by other means.[53,54] One observes that the Fisher information of the real hydrogenic system, as well as the level energy, does not depend on the familiar orbital quantum number, but it does depend on the magnetic quantum number m.

Let us first compute the radial integral $I_R(D)$ given by Eq. (21). The integration by parts leads us to the expression

$$I_R(D) = 4\int_0^\infty r^{D-1}R'\,\mathrm{d}R = -4(D-1)\int_0^\infty r^{D-2}RR'\,\mathrm{d}r - 4\int_0^\infty r^{D-1}RR''\,\mathrm{d}r.$$

The use of the radial Schrödinger equation (9) expressed as

$$R''(r) = a_1(r)R'(r) + a_2(r)R(r), \tag{30}$$

with

$$a_1(r) = \frac{1-D}{r}, \tag{31}$$

$$a_2(r) = \frac{2Z}{a_\mu r} + \frac{2E}{a_\mu e^2} - \frac{l(l+D-2)}{r^2}, \tag{32}$$

allows us to write

$$\begin{aligned} I_R(D) &= -4(D-1)\int_0^\infty r^{D-2} RR' \mathrm{d}r - 4\int_0^\infty r^{D-1} R[a_1(r)R' + a_2(r)R]\mathrm{d}r \\ &= -4\int_0^\infty [(D-1)r^{D-2} + a_1(r)r^{D-1}]RR' \mathrm{d}r - 4\int_0^\infty a_2(r)R^2 r^{D-1}\mathrm{d}r \\ &= -2\int_0^\infty [(D-1)r^{D-2} + a_1(r)r^{D-1}]\mathrm{d}R^2 - 4\int_0^\infty a_2(r)R^2 r^{D-1}\mathrm{d}r. \end{aligned}$$

And the integration by parts in the first integral gives rise to

$$\begin{aligned} I_R(D) &= \int_0^\infty \left\{ 2(D-1)\left[(D-2)r^{-2} + \frac{a_1(r)}{r} \right] + 2a_1'(r) - 4a_2(r) \right\} R^2 r^{D-1}\mathrm{d}r \\ &= \left\langle 2(D-1)\left[(D-2)r^{-2} + \frac{a_1(r)}{r} \right] + 2a_1'(r) - 4a_2(r) \right\rangle \\ &= 2(D-1)\left[(D-2)\langle r^{-2}\rangle + \left\langle \frac{a_1(r)}{r} \right\rangle \right] + 2\langle a_1'(r)\rangle - 4\langle a_2(r)\rangle, \end{aligned} \tag{33}$$

where we have used of the expectation value of $f(r)$ given by Eq. (20).

The use of Eqs. (31) and (32) allows us to write

$$\left\langle \frac{a_1(r)}{r} \right\rangle = (1-D)\langle r^{-2}\rangle, \quad \langle a_1'(r)\rangle = (D-1)\langle r^{-2}\rangle \langle a_2(r)\rangle = \frac{2Z}{a_\mu}\langle r^{-1}\rangle + \frac{2E}{a_\mu e^2} - l(l+D-2)\langle r^{-2}\rangle,$$

so that the radial integral $I_R(D)$ is equal to

$$I_R(D) = \frac{8Z}{a_\mu}\langle r^{-1}\rangle + \frac{8E}{a_\mu e^2} - 4l(l+D-2)\langle r^{-2}\rangle.$$

And taking into account the virial theorem

$$E = -\frac{Ze^2}{2}\langle r^{-1}\rangle,$$

one has that

$$I_R(D) = \frac{8Z}{2a_\mu}\langle r^{-1}\rangle - 4l(l+D-2)\langle r^{-2}\rangle. \tag{34}$$

Then, since $\langle r^{-1}\rangle = Z/a_\mu \eta^2$ and $\langle r^{-2}\rangle$ has the value (27), it is straightforward to obtain the searched expression (23) for the radical position Fisher information of the hydrogenic orbital.

Let us now compute the angular integral $I_{\theta_i}(D)$ given by Eq. (22). To do that, according to Eq. (6) we express the involved hyperspherical harmonics as

$$Y_{l,\{\mu\}}(\theta_1, \theta_2, \ldots, \theta_{D-2}, 0) = \frac{1}{2\pi}\prod_{j=1}^{D-2} Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j),$$

where

$$Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j) \equiv A^{(j)}_{\mu_j,\mu_{j+1}} C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\,\theta_j)(\sin\,\theta_j)^{\mu_j+1},$$

where the constant $A^{(j)}_{\mu_j,\mu_{j+1}}$ was defined by Eq. (7).

These functions satisfy the following properties: the normalization condition

$$\int_0^\pi [Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j)]^2(\sin\,\theta_j)^{D-j-1}\mathrm{d}\theta_j = 1,$$

and the differential equation (see, e.g., Ref 26):

$$\frac{\partial}{\partial\theta_j}\left[(\sin\,\theta_j)^{D-j-1}\frac{\partial}{\partial\theta_j}Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j)\right]$$
$$= -(\sin\,\theta_j)^{D-j-1}\left[\mu_j(\mu_j+D-j-1) - \frac{\mu_{j+1}(\mu_{j+1}+D-j-2)}{\sin^2\,\theta_j}\right]Y^{(j)}_{\mu_j,\mu_{j+1}}(\theta_j).$$

Use of these considerations into Eq. (22) allows us to write

$$I_{\theta_i}(D) = I^{(1)}_{\theta_i}(D)\cdot\prod_{k=1}^{i-1}\int_0^\pi [Y^{(k)}_{\mu_k,\mu_{k+1}}(\theta_k)]^2(\sin\,\theta_k)^{D-k-3}\mathrm{d}\theta_k$$

where

$$I^{(1)}_{\theta_i}(D) = \int_0^\pi\left[\frac{\partial}{\partial\theta_i}Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)\right]^2(\sin\,\theta_i)^{D-i-1}\mathrm{d}\theta_i = -\int_0^\pi\frac{\partial}{\partial\theta_i}\left[(\sin\,\theta_i)^{D-i-1}\frac{\partial}{\partial\theta_i}Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)\right]Y^i_{l,\{\mu\}}\mathrm{d}\theta_i$$
$$= \mu_i(\mu_i+D-i-1)\int_0^\pi [Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)]^2(\sin\,\theta_i)^{D-i-1}\mathrm{d}\theta_i$$
$$-\mu_{i+1}(\mu_{i+1}+D-i-2)\int_0^\pi [Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)]^2(\sin\,\theta_i)^{D-i-3}\mathrm{d}\theta_i,$$

where an integration by parts has been performed in the second equality, and the orthogonalization condition of the harmonics $Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)$ were taken into account in the second equality. The normalization of these functions and the value of the integral

$$\int_0^\pi [Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)]^2(\sin\,\theta_i)^{D-i-3}\mathrm{d}\theta_i = \frac{2\mu_i+D-i-1}{2\mu_{i+1}+D-i-2}, \tag{35}$$

has allowed us to find the value given by Eq. (24) for the searched angular integral $I_{\theta_i}(D)$. The integral (35) can be obtained by the use of the relation between the involved spherical harmonics and the associated Legendre function $P^m_n(x)$, together with the expression

$$\int_{-1}^{+1}(1-x^2)^{-1}[p^m_n(x)]^2\mathrm{d}x = \frac{(n+m)!}{m(n-m)!}.$$

IV. THE FISHER INFORMATION IN MOMENTUM SPACE

Here we calculate the Fisher information of D-dimensional hydrogenic orbital in momentum space given by

$$I_\gamma(D) \coloneqq \int_{\Re^D} \frac{|\vec{\nabla}_D \gamma(\vec{p})|^2}{\gamma(\vec{p})} \mathrm{d}^D p, \tag{36}$$

where

$$\gamma(\vec{p}) = |\Psi_{\eta,l,\{\mu\}}(\vec{p})|^2 = |\Psi_{\eta,l,\{\mu\}}(p,\theta_1,\theta_2,\ldots,\theta_{D-1})|^2 = [\Psi_{\eta,l,\{\mu\}}(p,\theta_1,\theta_2,\ldots,\theta_{D-2},0)]^2,$$

so that, after an integration by parts, one has

$$I_\gamma(D) = 4\int_{\Re^D} [\vec{\nabla}_D \Psi_{\eta,l,\{\mu\}}(p,\theta_1,\theta_2,\ldots,\theta_{D-2},0)]^2 \mathrm{d}^D p.$$

Remark that the spherical polar angles of the momentum vector $\vec{p}$ are denoted with the same symbols as in the position vector. The D-dimensional gradient operator in momentum space has the same formal expression as given by Eq. (17) with the only change $r \leftrightarrow p$, so that

$$\begin{aligned} I_\gamma(D) &= 4\int_0^\infty \left[\frac{\mathrm{d}}{\mathrm{d}p} M_{\eta,L}(p)\right]^2 p^{D-1}\mathrm{d}p + 4\int_0^\infty p^{-2} M_{\eta,L}^2(p) p^{D-1}\mathrm{d}p \\ &\quad \times \sum_{i=1}^{D-2} \int_{\Omega_{D-1}} \left[\frac{1}{\prod_{k=1}^{i-1} \sin\theta_k} \frac{\partial}{\partial\theta_i} Y_{l,\{\mu\}}(\theta_1,\theta_2,\ldots,\theta_{D-2},0)\right]^2 \mathrm{d}\Omega_{D-1} \\ &\equiv 4J_R(D) + 4\langle p^{-2}\rangle \sum_{i=1}^{D-2} I_{\theta_i}(D), \end{aligned} \tag{37}$$

where the angular integral $I_{\theta_i}(D)$ has been shown to have the value (26) in the previous section and the expectation value $\langle p^{-2}\rangle$ is given by

$$\langle p^{-2}\rangle = \int_0^\infty p^{-2} M_{\eta,L}^2(p) p^{D-1}\mathrm{d}p = \eta^2 \frac{8\eta - 6L - 3}{(2L+1)}. \tag{38}$$

Let us now compute the radial integral $J_R(D)$ given by

$$J_R(D) = \int_0^\infty \left[\frac{\mathrm{d}}{\mathrm{d}p} M_{\eta,L}(p)\right]^2 p^{D-1}\mathrm{d}p = \left(\frac{1}{\eta}\right)^{D-2} \int_0^\infty \left[\frac{\mathrm{d}M_{\eta,L}(x)}{\mathrm{d}x}\right]^2 x^{D-1}\mathrm{d}x,$$

where $x = \eta p$, and

$$M_{\eta,L}(x) = K_{n,l} \frac{x^l}{(1+x^2)^{L+2}} C_{\eta-L-1}^{L+1}\left(\frac{1-x^2}{1+x^2}\right).$$

The change of the variable $x \to y : y = (1-x^2)/(1+x^2)$, so that $\mathrm{d}x = (1-y)^{-3/2}(1+y)^{-1/2}\mathrm{d}y$, allows us to write

$$J_R(D) = \left(\frac{1}{\eta}\right)^{D-2} \int_{-1}^{+1} \left[\frac{\mathrm{d}M_{\eta,L}(y)}{\mathrm{d}y}\right]^2 (1+y)^{D/2}(1-y)^{-(D-4)/2}\mathrm{d}y, \tag{39}$$

where

$$M_{\eta,L}(y) = \frac{K_{\eta,L}}{2^{L+2}} (1+y)^{L/2-(D-3)/4} (1-y)^{L/2+(D-5)/4} C_{\eta-L-1}^{L+1}(y). \tag{40}$$

This integral can be decomposed into a sum of functionals of Gegenbauer polynomials whose members can be calculated following a modus operandi similar to that described in Ref. 51. This is done in the Appendix. We have found the value

$$J_R(D) = \eta^2 \frac{[(2L-D+3)(2L+D-1)(6L-8\eta+3)]}{4(2L+1)} + \frac{\eta^2}{2}(1+5\eta^2-3L(L+1)). \tag{41}$$

Gathering together in Eq. (37) the values for the radial integral $J_R(D)$, the expectation value $\langle p^{-2}\rangle$ and the angular integral $I_{\theta_i}(D)$ given by Eqs. (41), (38), and (26), respectively, one finally obtains the following expression for the Fisher information of a D-dimensional hydrogenic orbital in momentum space [see Eq. (36)]:

$$I_\gamma(D) = \eta^2 \Bigg\{ \frac{[(2L-D+3)(2L+D-1)(6L-8\eta+3)]}{(2L+1)} + 2(1+5\eta^2-3L(L+1)) + 4\frac{8\eta-6L-3}{2L+1} \cdot \times \sum_{i=1}^{D-2} \left[\mu_i(\mu_i+D-i-1) - \mu_{i+1}(\mu_{i+1}+D-i-2)\frac{2\mu_i+D-i-1}{2\mu_{i+1}+D-i-2} \right] \times \frac{2\mu_1+D-2}{2\mu_i+D-i-1} \Bigg\}. \tag{42}$$

A straightforward algrebraic manipulation leads to the more compact expression

$$I_\gamma(D) = 2\eta^2[5\eta^2 - 3L(L+1) - (8\eta-6L-3)\mu_{D-1}],$$

valid for $D \geqslant 2$. Here again for $D=2$ the term containing the summation does not contribute since the sum is empty. In the case $D=3$ this expression reduces as

$$I_\gamma(D=3) = 2n^2[5n^2+1-3l(l+1)+3(2l+1)|m| - 8n|m|],$$

which provides the Fisher information of the momentum distribution of a hydrogenic state characterized by the quantum numbers (n,l,m), already found by other means.[54]

V. CONCLUDING REMARKS

The translationally invariant Fisher information for D-dimensional hydrogenic systems, which is an information-theoretic measure of the localization of the quantum-mechanical distribution density of these systems all over the space, has been determined in a closed and compact form for both position and momentum spaces in terms of the dimension parameter D, the nuclear charge Z and the quantum numbers η, L and $\mu_{D-1}=|m|$ of the physical state under consideration.

Finally, let us point out that this information-theoretic quantity remains to be calculated for multidimensional hydrogenic Sturmians of nonspherical character (e.g., parabolic, elliptic)[55–57] in the two complementary spaces. This work is presently being done by the authors.

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APPENDIX: CALCULATION OF THE MOMENTUM RADIAL INTEGRAL $J_R(D)$

Here we shall prove that the radial integral $J_R(D)$ given by Eqs. (39) and (40) has the value given by Eq. (41). From Eqs. (39) and (40) one has that $J_R(D)$ can be decomposed into six different integrals as

$$J_R(D) = J_{R_1} + J_{R_2} + J_{R_3} + J_{R_4} + J_{R_5} + J_{R_6}. \tag{A1}$$

With the notation $\omega_{L+1}(y)=(1-y^2)^{L+1/2}$ for the weight function of the Gegenbauer polynomials $C_m^{L+1}(y)$, these integrals have the following values:

$$J_{R_1}=\frac{K_{\eta,L}^2}{2^{2L+4}}\left(\frac{1}{\eta}\right)^{D-2}(2L-D+3)^2\int_{-1}^{+1}[C_{\eta-L-1}^{L+1}(y)]^2\omega_{L+1}(y)(1+y)^{-1}\mathrm{d}y=\frac{2\eta^3(2L-D+3)^2}{2L+1},$$

$$J_{R_2}=\frac{K_{\eta,L}^2}{2^{2L+4}}\left(\frac{1}{\eta}\right)^{D-2}\left[\frac{(D+1)^2}{4}-(2L-D+3)^2\right]\int_{-1}^{+1}[C_{\eta-L-1}^{L+1}(y)]^2\omega_{L+1}(y)\mathrm{d}y$$
$$=\eta^2\left[\frac{(D+1)^2}{4}-(2L-D+3)^2\right],$$

$$J_{R_3}=\frac{K_{\eta,L}^2}{2^{2L+4}}\left(\frac{1}{\eta}\right)^{D-2}[L(D-3L-11)+2D-10]\times\int_{-1}^{+1}[C_{\eta-L-1}^{L+1}(y)]^2\omega_{L+1}(y)y^2\mathrm{d}y$$
$$=\frac{\eta^2}{2}[L(D-3L-11)+2D-10]\frac{\eta^2-1-L(L+1)}{\eta^2-1},$$

$$J_{R_4}=\frac{K_{\eta,L}^2}{2^{2L+2}}\left(\frac{1}{\eta}\right)^{D-2}(L+1)^2\int_{-1}^{+1}[C_{\eta-L-2}^{L+2}(y)]^2\omega_{L+2}(y)(1-y)^3\mathrm{d}y$$
$$=\eta^2[\eta^2-(L+1)^2]\left[1+\frac{3}{2}\frac{\eta^2-3-L(L+3)}{\eta^2-1}\right],$$

$$J_{R_5}=-8\frac{K_{\eta,L}^2}{2^{2L+4}}\left(\frac{1}{\eta}\right)^{D-2}(2L-D+3)(L+1)\int_{-1}^{+1}[C_{\eta-L-1}^{L+1}(y)][C_{\eta-L-2}^{L+2}(y)]\omega_{L+1}(y)y\mathrm{d}y$$
$$=-4\eta^2(2L-D+3)(\eta-L-1),$$

and

$$J_{R_6}=2\frac{K_{\eta,L}^2}{2^{2L+4}}\left(\frac{1}{\eta}\right)^{D-2}(6L-D+11)(L+1)\int_{-1}^{+1}[C_{\eta-L-1}^{L+1}(y)][C_{\eta-L-2}^{L+2}(y)]\omega_{L+2}(y)y\mathrm{d}y$$
$$=\frac{\eta^2}{2}(6L-D+11)(L+1)\frac{\eta^2-(L+1)^2}{\eta^2-1}.$$

To compute the integrals included in the six expressions considered above, we have made an intensive use of the special properties which characterize the Gegenbauer polynomials (e.g., the three-term recurrence relation, the orthogonality relation, etc.).

Gathering all these J-expressions together in Eq. (A1), one obtains the searched value given by Eq. (41) for $J_R(D)$; namely,

$$J_R(D)=\eta^2\frac{[(2L-D+3)(2L+D-1)(6L-8\eta+3)]}{4(2L+1)}+\frac{\eta^2}{2}(1+5\eta^2-3L(L+1)).$$

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Combinatorics of *n*-point functions via Hopf algebra in quantum field theory

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We use a coproduct on the time-ordered algebra of field operators to derive simple relations between complete, connected and 1-particle irreducible *n*-point functions. Compared to traditional functional methods our approach is much more intrinsic and leads to efficient algorithms suitable for concrete computations. It may also be used to efficiently perform tree level computations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196239]

I. INTRODUCTION

It may be said that time-ordered *n*-point functions are at the heart of (perturbative) quantum field theory. These determine the S-matrix that in turn allows to calculate experimentally observable scattering cross sections. Besides the complete *n*-point functions which are expectation values of time-ordered products of field operators, a key role is played by connected and by 1-particle irreducible (1PI) *n*-point functions. In particular, the latter play a prominent role in the process of renormalization, as it is enough to renormalize 1PI *n*-point functions. Furthermore, they are intimately related to the effective action. The different classes of *n*-point functions correspond directly to different sums over Feynman graphs, namely all graphs (excluding vacuum graphs), connected graphs and 1PI graphs.

The relations between these different classes of *n*-point functions (and thus sums over Feynman graphs) are traditionally expressed by using functional methods. While having an undeniable elegance, a disadvantage of these methods is the need for auxiliary sources and associated generating functions. These, as well as functional derivatives used in the process are often purely formal and have no rigorous mathematical existence. Consequently, they are only indirectly related to concrete calculations of *n*-point functions one may wish to perform.

In the present paper we describe the relation between these classes of *n*-point functions directly on the level of the algebra of time-ordered field operators. The key structure we will make use of is the natural *coproduct* on this algebra, making it into a *Hopf algebra*. Ensembles of time-ordered *n*-point functions are simply linear forms on this algebra. We show that the convolution product (induced by the coproduct) provides an extremely concise and elegant way of relating complete and connected *n*-point functions. Indeed, this relation is simply given by the convolution exponential (or, conversely, the logarithm).

Our second (and perhaps main) result concerns the relation of connected and 1PI *n*-point functions. As is well known, the former are expressible in terms of the latter as the sum over all tree graphs with 1PI vertices. We present a simple recursion formula using the coproduct, which generates exactly all tree diagrams. Moreover, the result takes an algebraic form which can be directly evaluated on 1PI functions so as to yield the connected functions. We proceed to derive an alternative recursion formula which relates directly components of connected *n*-point functions

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ordered by vertex number. Moreover, these same formulas can be alternatively applied to calculate the tree level contribution to the connected n-point functions, using the interaction terms of the Lagrangian.

A key feature of our results is their close relation to algorithmic descriptions of the computations involved. Indeed, it is easy to read off from our recursion relations not only algorithms to perform the computations, but even data structures relevant for an implementation. Our algorithm for generating trees also seems to be particular efficient as it allows to impose a lower bound on the number of legs per vertex from the outset.

The present paper may be seen as part of a program laid out in Ref. 1 and rooted in Ref. 2–4, with the aim of formulating and understanding the key structures of quantum field theory and their combinatorics in terms of the Hopf algebra of field operators. The focus of Ref. 1 were the different products of field operators (normal product, canonical product, and time-ordered product), uncovering their relation through Drinfeld twists via certain 2-cocycles in Hopf algebra cohomology. At the same time the relation between products and associated n-point functions was elucidated, again using Hopf algebra cohomology. The present paper complements this by investigating with the same means the relation between different classes of n-point functions that correspond to different classes of Feynman diagrams.

While Hopf algebras and coproducts have a long history in combinatorics, their use in combinatorial problems in quantum field theory is rather recent. The first instance probably was Kreimer's Hopf algebraic explanation of the Bogoliubov formula of renormalization and of Zimmermann's solution,[5] subsequently developed together with Connes.[6] We caution the reader, however, that the Hopf algebras used by Kreimer and Connes, while also being related to Feynman graphs, are quite distinct from the Hopf algebra of field operators used here.

Section II starts with recalling the different classes of n-point functions and their relation to Feynman graphs. Then, the basic algebraic formalism used in this paper is introduced, in particular the coproduct. Section III deals with the relation between complete and connected n-point function, Sec. IV with that between connected and 1PI n-point functions. An alternative recursion formula for the latter is derived in Sec. V. In Sec. VI various generalizations (e.g., tree level calculations) and related issues are discussed. Some Conclusions are offered in Sec. VII. The appendix shows all tree graphs with up to seven vertices with weight factors computed according to Sec. IV.

No knowledge of Hopf algebras is required to read this paper.

II. BASIC DEFINITIONS

We shall be concerned in the following with a generic perturbative quantum field theory. We denote the basic field operators by $\phi(x)$, where x represents a label that completely determines the operator. In a position representation x would specify a point in Minkowski space, possibly together with internal indices. While our notation suggests a field theory with a single scalar field, this is just a convenience. Although our results are general, we limit ourselves in the following exposition to a purely bosonic theory for simplicity. We return in Sec. VI D to a discussion of the general case, including fermionic fields.

A. Feynman graphs and *n*-point functions

We review here essentials about (classes of) Feynman graphs and n-point functions. For more information on these and the standard functional approach used to manipulate them we refer the reader to standard textbooks such as Ref. 7.

Definition 1: *A graph is a finite collection of* vertices *and* edges (*also called* legs), *such that any end of an edge may be connected to a vertex. Edges that are connected to vertices at both ends are called* internal, *while edges with at least one free end are called* external. *The* valence *of a vertex is the number of ends of edges connected to the vertex. A* tree *(graph) is a connected graph that has no cycles.*

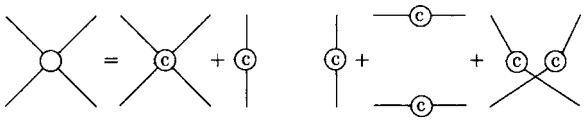

FIG. 1. Decomposition of the complete 4-point function in terms of connected functions.

Feynman graphs are graphs that carry certain labels on vertices and edges. The former correspond to the interaction terms of the Lagrangian while the latter may correspond to momenta and internal indices (usually indicated by different styles of lines, e.g., straight for fermions, wiggly for bosons, etc.). We shall only consider labels attached to (open ends) of external legs, assuming internal labels to be summed or integrated over.

Definition 2: *A* labeled *graph is a graph whose (ends of) external legs are labeled by field operator labels.*

In the following we shall consider only such labeled graphs, i.e., from now on *graph* really means *labeled graph*. A Feynman graph has a (usually complex) value as a function of the labels on the external legs.

We denote by $G^{(n)}(x_1,\ldots,x_n)$ the *complete* n-point function. This is the vacuum expectation value of the time-ordered product of n field operators, i.e.,

$$G^{(n)}(x_1,\ldots,x_n)=\langle 0|T\phi(x_1)\cdots\phi(x_n)|0\rangle.$$

In terms of Feynman graphs it is the sum of the values of all graphs with external legs labeled by $x_1,\ldots,x_n$. Let us denote by Γ^n the set of all Feynman graphs of the given theory with n legs (with vacuum graphs, i.e., graphs containing pieces not connected to any external leg already excluded). [Whether one considers the bare or renormalized (including counter terms) theory does not matter to us here. Of course, in the former case quantities might be infinite and manipulations therefore formal.] For a given graph $\gamma\in\Gamma^n$ we denote by $\gamma(x_1,\ldots,x_n)$ its value for the given labelings. Then,

$$G^{(n)}(x_1,\ldots,x_n)=\sum_{\gamma\in\Gamma^n}\gamma(x_1,\ldots,x_n). \tag{1}$$

Of particular importance is the Feynman propagator $G_F(x,y)$ which is the value of the graph that consists of an edge only, its two ends labeled by x and y, respectively. Note that the Feynman propagator is symmetric in its arguments $G_F(x,y)=G_F(y,x)$ as suggested by the corresponding symmetry of the graph. We also define its inverse G_F^{-1} which is determined by the equation

$$\int \mathrm{d}y G_F(x,y)G_F^{-1}(y,z)=\delta(x,z). \tag{2}$$

(Here as in the following we use a notation that suggests merely an integration over space–time. However, appropriate summations over internal indices are also implied, but not written explicitly.)

Consider the restricted class Γ_c of Feynman graphs that are connected. The n-point functions $G_c^{(n)}$ defined by the corresponding restriction of (1) are called the *connected* n-point functions. The relation between complete and connected n-point functions can be described in a simple way. Partition the set of external legs of the complete n-point function in all possible ways. The sum over the product of connected functions for each partition yields the complete n-point function,

$$G^{(n)}(x_1,\ldots,x_n)=\sum_{k=1}^{n}\sum_{I_1\cup\cdots\cup I_k=\{x_1,\ldots,x_n\}}\prod_{j=1}^{k}G_c(I_j). \tag{3}$$

Here $I_1,\ldots,I_k$ denote nonempty subsets of $\{x_1,\ldots,x_n\}$ forming a partition. Note also that the partitions are *unordered*, i.e., the subsets $I_1,\ldots,I_k$ are not distinguished. As an example, Fig. 1

FIG. 2. Decomposition of the connected propagator in terms of 1PI functions. Only part of the infinite sum is shown.

shows the decomposition of the complete 4-point function in terms of connected functions. The former is indicated by an empty circle, while the latter are indicated by circles carrying the letter "c."

We turn to consider the restriction of the class of connected Feynman graphs to that of *1-particle irreducible (1PI)* Feynman graphs, denoted by $\Gamma_{1\mathrm{PI}}$. These are Feynman graphs which are connected and remain connected when any one of their internal edges is cut. We define $G_{1\mathrm{PI}}$ in analogy to (1) for this restricted class. The relation between 1PI functions and connected ones may now be described as follows. The connected n-point function is the sum over all tree graphs with the given external legs, where the value of each vertex is given by $G_{1\mathrm{PI}}$. Since the latter carry Feynman propagators on all their legs, internal edges connecting two vertices need to carry the inverse Feynman propagator G_F^{-1} to cancel one superfluous Feynman propagator. As an example, Fig. 2 shows the infinite decomposition of the connected 2-point function (propagator) in terms of 1PI ones. The 1PI vertices are drawn as shaded discs.

One variant of the 1PI functions is of interest. Namely, replace the Feynman propagator G_F on the external legs of a 1PI function by the connected propagator $G_c^{(2)}$. We denote these modified 1PI functions by $\hat{G}_{1\mathrm{PI}}$. The relation between G_c and $\hat{G}_{1\mathrm{PI}}$ is the same as that between G_c and $G_{1\mathrm{PI}}$ described above, except that internal edges now carry the inverse $(G_c^{(2)})^{-1}$ of the connected propagator [defined analogous to (2)]. A crucial property of the modified 1PI functions is that the 2-point function $\hat{G}_{1\mathrm{PI}}^{(2)}$ vanishes by definition. This means that only trees with vertices that have valence at least three can occur in the sum. In particular, this makes the sum over trees finite for any given set of external legs. Figure 3 shows the decomposition of the connected 4-point function in terms of modified 1PI functions. The fact that the legs now carry the connected propagator is indicated with little circles.

Note that we assume all 1-point functions to vanish.

B. Field operator algebra and coproduct

We turn to introduce the basic algebraic definitions and elementary formalism employed in this paper. While our basic setup is largely the same as that in Ref. 1 we give an adapted and self-contained description here.

Let V be the vector space of linear combinations of elementary field operators $\phi(x)$. That is, elements of V take the form $\lambda_1\phi(x_1)+\lambda_2\phi(x_2)+\cdots+\lambda_n\phi(x_n)$, where λ_i are complex numbers and x_i denote field operator labels. Consider now the commutative algebra $\mathsf{S}(V)$ generated by those field operators with the *time-ordered* product. In Ref. 1 the same algebra was considered, but with the *normal ordered* product. This makes no difference to its structure. It is just more convenient in the present context to start immediately with time-ordered product. A general element in $\mathsf{S}(V)$ takes the form

$$\lambda_1\phi(x_{1,1})\phi(x_{1,2})\cdots\phi(x_{1,k_1})+\lambda_2\phi(x_{2,1})\phi(x_{2,2})\cdots\phi(x_{2,k_2})+\cdots.$$

Note that we do not explicitly indicate the time-ordering prescription, but it is always understood. Let us denote by V^k the vector space of k-fold products of field operator. Then, $\mathsf{S}(V)$ is the direct sum of the spaces V^k, i.e., $\mathsf{S}(V)=\oplus_{k=0}^{\infty}V^k$. We denote the identity operator spanning V^0 by $\mathbf{1}$.

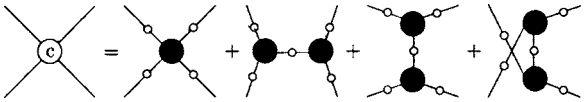

FIG. 3. Decomposition of the complete 4-point function in terms of modified 1PI functions.

In mathematical terms, $\mathsf{S}(V)$ is called the *symmetric algebra* over V. In our current notation a time-ordered n-point function is a linear map $V^n \to \mathbb{C}$. Thus, the ensemble of time-ordered n-point functions (of a given type) determines a linear map $\mathsf{S}(V) \to \mathbb{C}$. Recalling the various types of n-point functions introduced in the preceding section we denote the corresponding linear maps $\mathsf{S}(V) \to \mathbb{C}$ as follows:

$$\rho(\phi(x_1)\cdots\phi(x_n)) := G^{(n)}(x_1,\ldots,x_n),$$

$$\sigma(\phi(x_1)\cdots\phi(x_n)) := G_c^{(n)}(x_1,\ldots,x_n),$$

$$\tau(\phi(x_1)\cdots\phi(x_n)) := G_{1\mathrm{PI}}^{(n)}(x_1,\ldots,x_n),$$

$$\hat{\tau}(\phi(x_1)\cdots\phi(x_n)) := \hat{G}_{1\mathrm{PI}}^{(n)}(x_1,\ldots,x_n).$$

The assumption that all 1-point functions vanish means that $\rho(\phi(x))=\sigma(\phi(x))=\tau(\phi(x))=\hat{\tau}(\phi(x))=0$. For completeness, we also need to define 0-point functions. Since $\rho(\mathbf{1})=\langle 0|0\rangle$ we need to set $\rho(\mathbf{1})=1$. We shall see that the consistent choice for the other 0-point functions is $\sigma(\mathbf{1})=\tau(\mathbf{1})=\hat{\tau}(\mathbf{1})=0$. Also, the 2-point function $\hat{\tau}(\phi(x)\phi(y))$ vanishes by construction.

$\mathsf{S}(V)$ is not only an algebra, but also a *coalgebra* in a natural way. This means that there exists a linear *coproduct* map $\Delta:\mathsf{S}(V)\to\mathsf{S}(V)\otimes\mathsf{S}(V)$ with certain properties. One way to think about this coproduct map is as a way to split a product of field operators into two parts in all possible ways. For example,

$$\Delta(\mathbf{1}) = \mathbf{1}\otimes\mathbf{1}, \tag{4}$$

$$\Delta(\phi(x)) = \phi(x)\otimes\mathbf{1} + \mathbf{1}\otimes\phi(x), \tag{5}$$

$$\Delta(\phi(x)\phi(y)) = \phi(x)\phi(y)\otimes\mathbf{1} + \phi(x)\otimes\phi(y) + \phi(y)\otimes\phi(x) + \mathbf{1}\otimes\phi(x)\phi(y). \tag{6}$$

The general formula for the coproduct is

$$\Delta(\phi(x_1)\cdots\phi(x_n)) = \sum_{I_1\cup I_2=\{\phi(x_1),\ldots,\phi(x_n)\}} T(I_1)\otimes T(I_2). \tag{7}$$

Here the sum runs over partitions of the set of field operators $\{\phi(x_1),\ldots,\phi(x_n)\}$ into two sets I_1 and I_2. T denotes the time-ordered product of the field operators in the corresponding partition.

The coproduct has the property that it is an algebra map. This means that $\Delta(\phi(x_1)\cdots\phi(x_n))=\Delta(\phi(x_1)\cdots\phi(x_k))\cdot\Delta(\phi(x_{k+1})\cdots\phi(x_n))$. Here, the product in $\mathsf{S}(V)$ is extended to a product in $\mathsf{S}(V)\otimes\mathsf{S}(V)$ in the obvious way. The property of the coproduct to be an algebra map together with (4) and (5) completely determines it. Formula (7) can be derived from these properties.

Another important structure is the *counit* $\epsilon:\mathsf{S}(V)\to\mathbb{C}$. It is defined by $\epsilon(\mathbf{1})=1$ and $\epsilon(\phi(x_1)\cdots\phi(x_n))=0$ for $n>0$. The characterizing property of the counit is the equality $(\epsilon\otimes\mathrm{id})\circ\Delta=\mathrm{id}=(\mathrm{id}\otimes\epsilon)\circ\Delta$. The algebra $\mathsf{S}(V)$ together with unit, counit, coproduct, and antipode (which is another map that we do not need here) forms a *Hopf algebra*, see Ref. 1.

We shall also need iterated coproducts. First note that the coproduct satisfies the equality $(\Delta\otimes\mathrm{id})\circ\Delta=(\mathrm{id}\otimes\Delta)\circ\Delta$. That is, after applying the coproduct once, a second application either on the first or on the second component yield the same result. This is called *coassociativity*. We define the map $\Delta^k:\mathsf{S}(V)\to\mathsf{S}(V)^{\otimes k+1}$ as the k-fold application of the coproduct. Here, $\mathsf{S}(V)^{\otimes k+1}$ denotes the $(k+1)$-fold tensor product of $\mathsf{S}(V)$. Thus, $\Delta^0=\mathrm{id}$ and $\Delta^{k+1}=(\Delta\otimes\mathrm{id}^{\otimes k})\circ\Delta^k$. Here, the latter equation could be written in $k+1$ different ways (corresponding to different positions of the application of the coproduct) which are all equivalent due to coassociativity. The map Δ^k generalizes (7) as follows:

$$\Delta^k(\phi(x_1)\cdots\phi(x_n)) = \sum_{I_1\cup\cdots\cup I_{k+1}=\{\phi(x_1),\ldots,\phi(x_n)\}} T(I_1)\otimes\cdots\otimes T(I_{k+1}). \tag{8}$$

The difference to the single coproduct is that the set of field operators is now split into $k+1$ partitions. Note also that the partitions are *ordered*, i.e., the sets $I_1\ldots I_{k+1}$ are distinguishable.

A further definition we will require is the following. Given linear maps $\alpha:\mathsf{S}(V)\to\mathbb{C}$ and $\beta:\mathsf{S}(V)\to\mathbb{C}$ their *convolution product* is the map $\alpha\star\beta:\mathsf{S}(V)\to\mathbb{C}$ defined by $(\alpha\otimes\beta)\circ\Delta$. That is, we apply the coproduct followed by the application of α to its first and β to its second component. Note that the coassociativity of the coproduct implies associativity of the convolution product. Thus, we can write multiple convolution products without needing to specify brackets. In particular, we may write an iterated convolution product using the iterated coproduct,

$$\alpha_1\star\cdots\star\alpha_k = (\alpha_1\otimes\cdots\otimes\alpha_k)\circ\Delta^{k-1}. \tag{9}$$

The convolution product makes $(\mathsf{S}(V))^*$, the space of complex linear functions on $\mathsf{S}(V)$, into an algebra. This algebra has a unit which is given by the counit ϵ of $\mathsf{S}(V)$. Furthermore, any element α which satisfies $\alpha(\mathbf{1})\neq 0$ is invertible in this algebra, i.e., has an inverse with respect to the convolution product.

III. COMPLETE AND CONNECTED *n*-POINT FUNCTIONS

The first instance where we shall apply the Hopf algebraic approach to capture the combinatorics of quantum field theory is in the relation between the complete and the connected n-point functions.

As the (iterated) coproduct (8) is intimately related to partitions it seems predestined to express the relation between complete and connected n-point functions (3). Indeed, the relation between the two is very compactly and elegantly expressed using the convolution product (and thus implicitly the coproduct).

Proposition 3: *The complete n-point functions may be expressed in terms of the connected ones through the convolution exponential,* $\rho=\exp_\star\sigma$. *The convolution exponential is defined in terms of its power series expansion.*

Proof: We explicitly perform the power series expansion on a given argument in the subspace $V^n\subset\mathsf{S}(V)(n>0)$,

$$(\exp_\star(\sigma))(\phi(x_1)\cdots\phi(x_n)) = \sum_{k=0}^{\infty}\frac{1}{k!}\sigma^{\star k}(\phi(x_1)\cdots\phi(x_n))$$

$$=\sum_{k=1}^{\infty}\frac{1}{k!}(\sigma\otimes\cdots\otimes\sigma)\circ\Delta^{k-1}(\phi(x_1)\cdots\phi(x_n))$$

$$=\sum_{k=1}^{n}\frac{1}{k!}\sum_{I_1\cup\cdots\cup I_k=\{\phi(x_1),\ldots,\phi(x_n)\}}\prod_{j=1}^{k}\sigma(T(I_j)).$$

Here, $\sigma^{\star k}$ denotes the k-fold convolution product of σ with itself. In particular, $\sigma^{\star 0}=\epsilon$ by definition. Since $\epsilon(\phi(x_1)\cdots\phi(x_n))=0$ the first summand is zero in the first line and we may omit it. In going from the second to the third line we insert the definition of the iterated coproduct (8). Note that by definition $\sigma(\mathbf{1})=0$. This implies that all partitions where at least one partitioning set I_j is empty do not contribute. In particular, all summands of the outer sum with $k>n$ must vanish. The only difference to the partitioning in (3) is that the latter are unordered. However, the number of occurrences of each unordered partition in the set of ordered ones is exactly $k!$. Thus, the factor $1/k!$ establishes equality with $\rho(\phi(x_1)\cdots\phi(x_n))$. To complete the proof, note that $\rho(\mathbf{1})=\sigma^{\star 0}(\mathbf{1})=\epsilon(\mathbf{1})=1$ since $\sigma(\mathbf{1})=0$ and thus $\sigma^{\star k}(\mathbf{1})=0$ for $k>0$. □

Let us emphasize that although the power series defining the exponential is formally infinite, on any given element of $\mathsf{S}(V)$ it is truncated to a finite and thus well defined sum as shown in the proof above. Thus, the relation $\rho=\exp_\star \sigma$ is completely well-defined algebraically. Indeed, we may even invert it.

Corollary 4: *The connected n-point functions may be expressed in terms of the complete ones through the convolution logarithm,* $\sigma=\log_\star 0$. *The convolution logarithm is defined in terms of its power series expansion in* $\rho-\epsilon$.

Proof: By definition

$$\log_\star \rho = \sum_{k=0}^{\infty} (-1)^k \frac{1}{k} (\rho - \epsilon)^{\star k}.$$

Note that $(\rho-\epsilon)(\mathbf{1})=0$. This implies as in the proof of Proposition 3 that the sum truncates to a finite sum on any given element in $\mathsf{S}(V)$. One may show that the operations $\exp_\star$ and $\log_\star$ are mutually inverse by inserting one power series into the other. Since the procedure and result is exactly the same as in the usual arithmetic of complex numbers (say) we do not perform it explicitly here. However, it is crucial that the truncation of the power series for any given argument in $\mathsf{S}(V)$ makes it algebraically well defined in the present context. □

The attentive reader will notice that the present method of relating the complete and connected *n*-point functions shows certain similarities to the conventional one. Namely, in the conventional method one also finds that the relation is given by the exponential and the logarithm respectively, see e.g., Ref. 7. The difference is of course that the conventional method uses sources while the present one uses the coproduct to define exponential and logarithm.

IV. CONNECTED AND 1PI *n*-POINT FUNCTIONS

We now turn to the relation between connected and 1PI *n*-point functions. To state our Hopf algebraic formulation of this relation we need to define a few auxiliary structures first.

Define the formal element $R \in \mathsf{S}(V) \otimes \mathsf{S}(V)$ using the inverse Feynman propagator (2) as follows [R is formal insofar as it really lives in a completion of the tensor product $\mathsf{S}(V) \otimes \mathsf{S}(V)$. However, this fact is largely irrelevant for our purposes]:

$$R := \int \mathrm{d}x\, \mathrm{d}y\, G_F^{-1}(x,y)(\phi(x) \otimes \phi(y)). \tag{10}$$

Using the product in $\mathsf{S}(V) \otimes \mathsf{S}(V)$ we may view R as an operator acting on this space by multiplication. Define now the map $Q: \mathsf{S}(V) \to \mathsf{S}(V) \otimes \mathsf{S}(V)$ as the composition of R with the coproduct together with a factor of $1/2$:

$$Q := \tfrac{1}{2} R \circ \Delta. \tag{11}$$

We generalize Q to maps $Q_i: \mathsf{S}(V)^{\otimes k} \to \mathsf{S}(V)^{\otimes k+1}$. Namely, let Q_i be the application of Q on the ith component only, i.e.,

$$Q_i := \mathrm{id}^{\otimes i-1} \otimes Q \otimes \mathrm{id}^{\otimes k-i}.$$

Finally, we define maps $\Lambda^k: \mathsf{S}(V) \to \mathsf{S}(V)^{\otimes k+1}$ for $k \in \mathbb{N}_0$ recursively as follows:

$$\Lambda^0 := \mathrm{id},$$

$$\Lambda^k := \frac{1}{k} \sum_{i=1}^{k} Q_i \circ \Lambda^{k-1}. \tag{12}$$

We are now ready to state our main result.

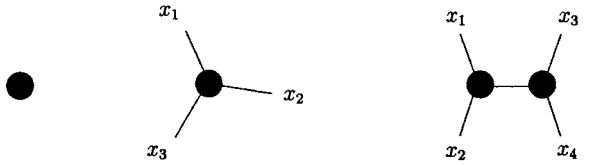

FIG. 4. Examples for the correspondence of graphs with elements of $\mathsf{S}(V)^{\otimes k}$.

Theorem 5: *The connected n-point functions may be expressed in terms of the 1PI ones through the formula*

$$\sigma = \sum_{k=1}^{\infty} \sigma^k, \text{ with } \sigma^k := \tau^{\otimes k} \circ \Lambda^{k-1}. \tag{13}$$

The remainder of this section will be devoted to the proof of this result.

Recall from the description in Sec. II A that the connected n-point functions are expressible as the sum over all tree graphs with 1PI n-point functions as vertices. Since the latter are represented by τ we see that the sum in formula (13) must correspond to the sum over the number of such vertices k. In turn, the map Λ^k must contain the information about all tree graphs with k vertices. We proceed to explain this.

We first generalize the definition of R given in (10) to an element (or operator) $R_{i,j} \in \mathsf{S}(V)^{\otimes k}$ with $1 \leqslant i < j \leqslant k$ via

$$R_{i,j} := \int \mathrm{d}x\, \mathrm{d}y\, G_F^{-1}(x,y)(\mathbf{1}^{\otimes i-1} \otimes \phi(x) \otimes \mathbf{1}^{\otimes j-i-1} \otimes \phi(y) \otimes \mathbf{1}^{\otimes k-j}). \tag{14}$$

In other words, the field operators $\phi(x)$ and $\phi(y)$ are inserted at the ith and jth position, respectively.

We proceed to establish a correspondence between graphs with k vertices and certain elements of $\mathsf{S}(V)^{\otimes k}$. Each tensor factor of $\mathsf{S}(V)^{\otimes k}$ corresponds to one vertex. A product $\phi(x_1)\cdots\phi(x_n)$ in a given tensor factor corresponds to external legs labeled by $x_1, \ldots, x_n$. The element $R_{i,j} \in \mathsf{S}(V)^{\otimes k}$ corresponds to an internal edge connecting the ith vertex with the jth vertex. Combining several internal edges and external legs by multiplying the respective expressions in $\mathsf{S}(V)^{\otimes k}$ allows to build arbitrary graphs with k vertices. Figure 4 shows some examples. Applying $\tau^{\otimes k}$ to the resulting expression obviously yields the value of the respective graph with the vertices being 1PI functions. Thus, the graphs we just discussed are exactly those that are to enter into expressing the connected functions in terms of the 1PI ones.

The ordering of the tensor factors of $\mathsf{S}(V)^{\otimes k}$ induces an ordering of the vertices of the graph, i.e., we may think of them as labeled with numbers $1, \ldots, k$. However, when applying $\tau^{\otimes k}$ the ordering is "forgotten." Indeed, it is not relevant for the interpretation of graphs, but only plays a role at the level of their algebraic representation here. For short, we call a graph *ordered* if its vertices are ordered. In the following, we will encounter elements of $\mathsf{S}(V)^{\otimes k}$ that are linear combinations of expressions corresponding to ordered graphs. Alternatively, we might think of such elements as linear combinations of unordered graphs by considering different ordered graphs that correspond to the same unordered graph as the same. We call *weight* of the graph the scalar multiplying the expression for a given graph. Clearly, the weight of an unordered graph is the sum of the weights of all corresponding ordered graphs.

We see now what is required to prove Theorem 5. Namely, we need to show that $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n)) \in \mathsf{S}(V)^{\otimes k}$ corresponds exactly to the sum over all tree graphs with k (unordered) vertices and external legs labeled by $x_1, \ldots, x_n$, each with weight one. Actually, we need to

show something slightly weaker, namely, the statement needs to apply only to graphs where all of the vertices have valence at least two. This is because the 0-point and 1-point 1PI functions are zero. Indeed, we will see in the process that the more general statement is false.

Consider the coproduct applied to the ith component of $\mathsf{S}(V)^{\otimes k}$, i,e., $\Delta_i := \mathrm{id}^{\otimes i-1} \otimes \Delta \otimes \mathrm{id}^{\otimes k-i}$ as a map $\mathsf{S}(V)^{\otimes k} \to \mathsf{S}(V)^{\otimes k+1}$. Recalling the formula (7) we see that Δ_i converts a graph with k vertices into a sum over graphs with $k+1$ vertices by *splitting* the ith vertex into two in all possible ways. That is, the ith vertex is replaced by two vertices (numbered i and $i+1$) and its legs (considered as distinguishable) are distributed between the two new vertices in all possible ways. Note that the two new vertices are distinguished due to the ordering of the tensor factors. Thus, to obtain the corresponding operation for unordered graphs we need to divide by a factor of 2. This factor corresponds to the two different relative orderings of the new vertices with which each unordered configuration occurs. The only exception to this is the case when the split vertex has no legs at all. No overcounting happens in this case. The meaning of the map Q_i given by (11) becomes clear now in terms of graphs. Namely, it splits the ith vertex into two and subsequently reconnects the two new vertices with an edge. Dividing by 2 compensates for the double counting as described above if we are interested in unordered graphs (assuming the set of legs of the split vertex is not empty).

Lemma 6: *Fix integers $k \geqslant 1$ and $n \geqslant 0$ as well as field operator labels $x_1, \ldots, x_n$. (a) $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ corresponds in the manner described above to a sum of weighted graph with k vertices and n external legs labeled by $x_1, \ldots, x_n$. (b) Each of these graphs is connected. (c) Each of these graphs is a tree graph. (d) Any free graph with k unlabeled vertices and the given external legs occurs in $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ with some positive weight.*

Proof: First, it is clear that $\Lambda^0(\phi(x_1)\cdots\phi(x_n))$ corresponds to the graph with one vertex and the external legs labeled by $x_1, \ldots, x_n$. Second, $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ is generated from this by sums of multiple applications of maps Q_i and scalar factors. But Q_i converts a term corresponding to a graph to a sum over terms corresponding to graphs. Thus, $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ is a sum of terms each of which corresponds to a graph (with some weight). This completes the proof of (a).

Given a connected graphs, splitting a vertex produces at most two disconnected pieces. Reconnecting the new vertices with an edge yields again a connected graph. Thus, Q_i produces connected graphs from connected ones. Evidently, $\Lambda^0(\phi(x_1)\cdots\phi(x_n))$ corresponds to a connected graph. This proves (b).

Splitting a vertex of a tree graph necessarily yields two disconnected graphs. Reconnecting the new vertices with an edge thus cannot introduce a cycle. Therefore, Q_i produces tree graphs from tree graphs. Evidently, $\Lambda^0(\phi(x_1)\cdots\phi(x_n))$ corresponds to a tree graph. This proves (c).

To prove (d) we use a recursive argument. Evidently, for $k=1$ the statement is true. Now assume that any tree graph with $k-1$ unlabeled vertices and the given external legs occurs in $\Lambda^{k-2}(\phi(x_1)\cdots\phi(x_n))$ with positive weight. Consider a tree graph with k unlabeled vertices and the given external legs. Choose an arbitrary internal edge. Shrinking this edge and fusing the vertices it connects yields a tree graph that corresponds by assumption to a term in $\Lambda^{k-2}(\phi(x_1)\cdots\phi(x_n))$. Say, the fused vertex has position i. Applying Q_i to this term will yield a sum over terms one of which will correspond to the original tree graph. By the recursive definition of $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ it thus contains this term with positive weight. This completes the proof. □

What remains in order to prove Theorem 5 is to show that the term corresponding to each tree graph (with all vertices of valence at least two) has weight exactly 1. We start with a more restricted result.

Lemma 7: *Fix integers $k \geqslant 1$ and $n \geqslant k$ and field operator labels $x_1, \ldots, x_n$. Consider a tree with k vertices, external legs labeled by $x_1, \ldots, x_n$ and the property that each vertex has at least one external leg. Then, the term in $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ corresponding to that tree has weight 1.*

Proof: We proceed by induction on the number of vertices. Clearly, the statement is true for $k=1$. Now assume that $\Lambda^{k-2}(\phi(x_1)\cdots\phi(x_n))$ contains each tree graph with $k-1$ vertices and external legs labeled by $x_1, \ldots, x_n$ and the property that each vertex carries at least one external leg with weight exactly 1. (Of course it may in addition contain terms corresponding to other graphs.) Consider a tree graph γ with k vertices, external legs labeled by $x_1, \ldots, x_n$ and the property that

each vertex carries at least one external leg. We proceed to show that it occurs with weight exactly 1 in $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$. To this end we check from which graphs with $k-1$ vertices γ is generated by the recursion formula (12) and in how many ways. Translated into the language of graphs, the formula prescribes that a given graph is split and reconnected at every of its vertices. The resulting terms are summed over and multiplied by $1/k$. Conversely, this implies that γ is generated from all the graphs that are obtained by shrinking one of its internal edges. Since there are k edges these are a priori k graphs. These graphs are indeed all distinct, since the external legs attached to each vertex force them to be distinguishable. Furthermore, each of these graphs generates γ in only one way, i.e., as one resulting graph in the splitting and reconnecting of only one of its vertices (again due to the forced distinguishability of the vertices). Since by assumption each generating graph has weight one, the multiplicity k cancels exactly with the factor $1/k$ in (12) to produce weight 1 for γ. This completes the proof. □

To describe the weight of arbitrary tree graphs we will need to consider symmetries of graphs.

Definition 8: *Consider a tree graph γ with ordered vertices*. A symmetry *of γ is a permutation of the ordering of its vertices that yields the (topologically) same ordered graph. The number of symmetries, i.e., order of the group of permutations leaving the graph invariant, is called the* symmetry factor *of the graph*.

Since the symmetry factor is the same for any ordering of the vertices of a graph the concept makes sense for unordered graphs as well.

We also need the following property of Λ^k.

Lemma 9: *Fix integers $k,n\geqslant 0$ and operator labels $x_1,\ldots,x_n$. Then, Λ^k satisfies the factorization property*

$$\Lambda^k(\phi(x_1)\cdots\phi(x_n)) = \Lambda^k(\mathbf{1})\cdot\Delta^k(\phi(x_1)\cdots\phi(x_n)).$$

Proof: This follows immediately from the multiplicativity of the coproduct and the recursive definition (12). □

We can now state the generalization of Lemma 7.

Lemma 10: *Fix integers $k\geqslant 1$ and $n\geqslant 0$ and field operator labels $x_1,\ldots,x_n$. Consider a tree γ with k vertices and external legs labeled by $x_1,\ldots,x_n$. Let s be the symmetry factor of γ. Then, the term in $\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))$ corresponding to that tree has weight $1/s$.*

Proof: If γ has external legs attached to every of its vertices we simply recall Lemma 7 and note that a graph with this property has no nontrivial symmetries. Thus, we may now assume that γ has m vertices to which no external leg is attached. Consider a graph γ' which is constructed from γ by attaching an external leg to every vertex without external legs, choosing arbitrary but fixed labels $y_1,\ldots,y_m$ for the legs in the process. By Lemma 9 and the multiplicativity of Δ and thus Δ^j we have

$$\Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n)\phi(y_1)\cdots\phi(y_m)) = \Lambda^{k-1}(\phi(x_1)\cdots\phi(x_n))\cdot\Delta^{k-1}(\phi(y_1)\cdots\phi(y_m)).$$

By Lemma 7, the graph γ' occurs in the term on left-hand side with weight 1. By Lemma 6, the graph γ occurs in the first factor on the right-hand side with some nonzero weight, say α. Every summand of $\Delta^{k-1}(\phi(y_1)\cdots\phi(y_m))$ [recall the formula (8)] which places the external legs at the designated vertices of γ to produce γ' contributes to the weight of γ' in terms of that of γ. Any different ways this can happen define a symmetry of γ. Furthermore, γ can have no more than these symmetries, since its vertices that already carry external legs are distinguishable and thus held fixed under any symmetry. Therefore, we obtain the formula $1=\alpha\cdot s$ for the weights, or $\alpha=1/s$. This completes the proof. □

The appendix shows the result of computing all tree graphs without external legs as weighted contributions to $\Lambda^{k-1}(\mathbf{1})$, for vertex number $k\leqslant 7$.

The proof of Theorem 5 is completed with the following lemma.

Lemma 11: *Consider a tree graph γ, all of whose vertices have valence at least two. Then, γ has no nontrivial, symmetries*.

Proof: Consider a vertex v of γ. We show that any symmetry must leave v invariant. If v

carries an external leg it must be invariant since it is distinguishable. Thus, assume v carries no external leg. Choose one internal edge e connected to v. Cut γ into two by removing e. This yields two tree graphs γ_1 and γ_2. Each of these must have at least one external leg to satisfy the valence requirement. Say e_1 is an external leg of γ_1 and e_2 an external leg of γ_2. Since γ is a tree there is exactly one path to connect e_1 with e_2. Since the vertices connected with e_1 and e_2 are held fixed under any symmetry so is the whole chain of vertices formed by the path. However, v is part of this chain by construction and thus held fixed by any symmetry. □

V. FURTHER RECURSION RELATIONS

We may extend the results of the preceding section to obtain further interesting recursion relations. Recall from (13) the decomposition of σ into components σ^k according to vertex number k.

Proposition 12: *σ^k may be determined recursively via $\sigma^1=\tau$ and with the recursion equation for $k>1$,*

$$\sigma^k = \frac{1}{k-1}\sum_{i=1}^{k-1} (\sigma^i \otimes \sigma^{k-i}) \circ Q.$$

Given the definition of σ^k in (13) Proposition 12 is implied by the following lemma.

Lemma 13:

$$\Lambda^{k-1} = \frac{1}{k-1}\sum_{i=1}^{k-1} (\Lambda^{i-1} \otimes \Lambda^{k-i-1}) \circ Q \quad \forall\, k>1.$$

Proof: As a first step to the proof, we "commute" the R-operator contained in Q through the tensor product $\Lambda^{i-1}\otimes\Lambda^{k-i-1}$. To this end, recall the multiplicativity of the (iterated coproduct) together with the factorization property of Λ (Lemma 9). We obtain the equivalent expression

$$\begin{aligned}\Lambda^{k-1} &= \frac{1}{2(k-1)}\sum_{i=1}^{k-1} ((\Delta^{i-1} \otimes \Delta^{k-i-1})R) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i-1}) \circ \Delta \\ &= \frac{1}{2(k-1)}\sum_{i=1}^{k-1} \left(\sum_{a=1}^{i}\sum_{b=i+1}^{k} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i-1}) \circ \Delta. \end{aligned} \tag{15}$$

Before proceeding with the proof we note that this formula has a straight forward interpretation in terms of sums over weighted tree diagrams following the correspondence of Sec. IV. Namely, the formula states that the weighted sum over trees with k vertices is given by summing over all ordered pairs of weighted trees with total number of vertices equal to k, connecting them in all possible ways with an edge and dividing by $2(k-1)$. [Indeed, it would be possible to base the proof of Lemma 7 on the recursion formula for Λ given here instead of (12). The argument would then roughly proceed by considering all $k-1$ ways to cut a tree with k vertices into two by removing an internal edge. The factor 2 accounts for the relative ordering of the two subtrees.]

The equation (15) is proved by induction. We verify it for $k=2$,

$$\Lambda^1 = \frac{1}{2}R \cdot (\Lambda^0 \otimes \Lambda^0) \circ \Delta = \frac{1}{2}R \cdot \Delta,$$

and assume it hold for general order k. Then, (12) yields

$$
\begin{aligned}
\Lambda^k &= \frac{1}{k}\left(\sum_{j=1}^{k} Q_j\right) \circ \Lambda^{k-1} \\
&= \frac{1}{k}\left(\sum_{j=1}^{k} Q_j\right) \frac{1}{2(k-1)} \left(\sum_{i=1}^{k-1} \left(\sum_{a=1}^{i} \sum_{b=i+1}^{k} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i-1})\right) \circ \Delta \\
&= \frac{1}{2k(k-1)} \sum_{i=1}^{k-1} \left(\left(\sum_{j=1}^{i} Q_j\right)\left(\left(\sum_{a=1}^{i} \sum_{b=i+1}^{k} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-1-i})\right)\right. \\
&\quad \left. + \left(\sum_{j=i+1}^{k} Q_j\right)\left(\left(\sum_{a=1}^{i} \sum_{b=i+1}^{k} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-1-i})\right)\right) \circ \Delta \\
&= \frac{1}{2k(k-1)} \sum_{i=1}^{k-1} \left(\sum_{j=1}^{i} \left(\left(\Delta_j \sum_{a=1}^{i} \sum_{b=i+1}^{k} R_{a,b}\right) \cdot Q_j\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-1-i})\right. \\
&\quad \left. + \sum_{j=i+1}^{k} \left(\left(\Delta_j \sum_{a=1}^{i} \sum_{b=i+1}^{k} R_{a,b}\right) \cdot Q_j\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-1-i})\right) \circ \Delta \\
&= \frac{1}{2k(k-1)} \sum_{i=1}^{k-1} \left(i\left(\sum_{a=1}^{i+1} \sum_{b=i+2}^{k+1} R_{a,b}\right) \cdot (\Lambda^{i} \otimes \Lambda^{k-1-i})\right. \\
&\quad \left. + (k-i)\left(\sum_{a=1}^{i} \sum_{b=i+1}^{k+1} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i})\right) \circ \Delta \\
&= \frac{1}{2k}\left(\left(\sum_{a=1}^{k} R_{a,k+1}\right) \cdot (\Lambda^{k-1} \otimes \Lambda^{0}) + \sum_{i=2}^{k-1} \left(\sum_{a=1}^{i} \sum_{b=i+1}^{k+1} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i})\right. \\
&\quad \left. + \left(\sum_{b=2}^{k+1} R_{1,b}\right) \cdot (\Lambda^{0} \otimes \Lambda^{k-1})\right) \circ \Delta \\
&= \frac{1}{2k} \sum_{i=1}^{k} \left(\sum_{a=1}^{i} \sum_{b=i+1}^{k+1} R_{a,b}\right) \cdot (\Lambda^{i-1} \otimes \Lambda^{k-i}) \circ \Delta .
\end{aligned}
$$

□

VI. EXTENSIONS AND APPLICATIONS

A. Modified 1PI functions

In Sec. II A we have discussed two versions of 1PI functions, the standard one, denoted $G_{1\mathrm{PI}}$, and a modified one, denoted $\hat{G}_{1\mathrm{PI}}$. Recall that the connected n-point functions G_c are expressible in terms of $G_{1\mathrm{PI}}$ and of $\hat{G}_{1\mathrm{PI}}$ essentially in the same way, as a sum over all tree graphs, the difference being that for $\hat{G}_{1\mathrm{PI}}$ the (inverse) Feynman propagator G_F is replaced by the (inverse) connected propagator $G_c^{(2)}$ for all edges. Thus, the results of Secs. IV and V immediately carry over to the relation between connected functions and modified 1PI functions. We only need to modify the definition of R by replacing G_F^{-1} with $G_c^{(2)-1}$ in (10); call the new version $\hat{R}$. We denote the induced modifications of Q and Λ by $\hat{Q}$ and $\hat{\Lambda}$, respectively.

Corollary 14: *The connected n-point functions may be expressed in terms of the modified 1PI ones through the formula*

$$
\sigma = \sum_{k=1}^{\infty} \hat{\sigma}^k, \quad \textit{with} \quad \hat{\sigma}^k := \hat{\tau}^{\otimes k} \circ \hat{\Lambda}^{k-1}. \tag{16}
$$

Corollary 15: *$\hat{\sigma}^k$ may be determined recursively via $\hat{\sigma}^1=\hat{\tau}$ and with the recursion equation for $k>1$,*

$$\hat{\sigma}^k=\frac{1}{k-1}\sum_{i=1}^{k-1}(\hat{\sigma}^i\otimes\hat{\sigma}^{k-i})\circ\hat{Q}.$$

Recall that for the modified 1PI functions not only 0- and 1-point functions vanish, but also 2-point functions. This implies that only trees contribute which have the property that all their vertices have valence at least three. For a given number of external legs, there are only finitely many such trees. Thus, in contrast to (13) the sum in (16) is finite for each given set of external legs, i.e., for each element of $\mathsf{S}(V)$ to which it is applied.

B. Tree level contributions

Another context in quantum field theory, where we sum over all tree diagrams is of course when we wish to evaluate merely the tree level contribution to an *n*-point function. Let us indicate the tree level contribution by a lower index "*T*." Thus, the tree level contributions to the algebraic *n*-point functions are denoted ρ_T,σ_T, and τ_T for the complete, connected and 1PI *n*-point functions, respectively. Of course, the latter are now nothing but the interaction terms of the Lagrangian. The results of Sec. III carry over immediately.

Corollary 16: *$\rho_T=\exp_\star\sigma_T$, where the convolution exponential is defined in terms of its power series expansion.*

Corollary 17: *$\sigma_T=\log_\star\rho_T$, where the convolution logarithm is defined in terms of its power series expansion in $\rho_T-\epsilon$.*

The results of Secs. IV and V take the following form.

Corollary 18: *The tree level connected n-point functions may be expressed in terms of the interaction vertices through the formula*

$$\sigma_T=\sum_{k=1}^{\infty}\sigma_T^k\quad\text{with }\sigma_T^k:=\tau_T^{\otimes k}\circ\Lambda^{k-1}. \tag{17}$$

Corollary 19: *σ_T^k may be determined recursively via $\sigma_T^1=\tau_T$ and with the recursion equation for $k>1$,*

$$\sigma_T^k=\frac{1}{k-1}\sum_{i=1}^{k-1}(\sigma_T^i\otimes\sigma_T^{k-i})\circ Q.$$

Not only the 0- and 1-point, but also the 2-point contribution to τ_T vanishes by definition. Thus, as in the case of the modified 1PI functions, only finitely many tree graphs with given external legs contribute and the sum (17) is finite on any given element of $\mathsf{S}(V)$.

C. Algorithmic considerations

A key feature of the Hopf algebraic approach to *n*-point functions presented here is the close relation of the obtained algebraic relations to concrete algorithms. In Sec. IV the recursive definition (12) mirrors an algorithm to construct all tree graphs. Tree graphs with $k+1$ vertices are created from those with k vertices by taking each graph in turn and applying the following procedure: Take every vertex of the graph in turn and split it into two vertices, distributing the legs in all possible ways and reconnecting the two new vertices.

Of course, the actual algorithm is slightly more complicated as symmetries have to be taken into account and the correct weights must be obtained. However, the recursion relation (12) even suggests an implementation of data structures. For example, we may represent $\mathsf{S}(V)^{\otimes n}$ by an array, each element of which corresponds to a graph in the sense of Sec. IV. Such an element would contain a rational scalar (the weight) and an array, each element of which would correspond to one

tensor factor in $\mathsf{S}(V)^{\otimes n}$ or equivalently to one vertex. In turn each element would be a set of symbolic elements representing external or internal legs. The coproduct and the R-operator are then very simple operations distributing or adding pairs of symbolic elements.

In this context a certain property of the recursion algorithm represented by (12) is rather interesting. Namely, it is easy to see that a graph containing at least one vertex with valence 1 will in a recursion step only generate graphs that contain at least one vertex with valence 1. Conversely, this means that if we are not interested in such graphs we may exclude them at each recursion step without losing any relevant graphs. What is more, we may implement this removal of "irrelevant" graphs through a *truncated coproduct*. Recall from (7) that the coproduct restricted to the subspace $V^n \subset \mathsf{S}(V)$ is a map $V^n \to \oplus_{i=0}^n V^i \otimes V^{n-i}$. Removing those components of the direct sum where at least one of the target tensor factors is V^0 we obtain a map $V^n \to \oplus_{i=0}^{n-1} V^i \otimes V^{n-i}$. We call this the truncated coproduct $\Delta_{\geqslant 1}$. For example,

$$\Delta_{\geqslant 1}(\mathbf{1}) = 0, \quad \Delta_{\geqslant 1}(\phi(x)) = 0,$$

$$\Delta_{\geqslant 1}(\phi(x)\phi(y)) = \phi(x) \otimes \phi(y) + \phi(y) \otimes \phi(x).$$

In the recursion process (12) the number of legs of a vertex changes when the Q-operator is applied to it. The only terms corresponding to 1-point vertices arise from those terms in the coproduct where one of the new vertices receives no legs at all and has thus, after reconnecting with R, only one leg. Thus, replacing the coproduct Δ by the truncated coproduct $\Delta_{\geqslant 1}$ exactly eliminates the irrelevant trees with 1-point vertices.

If we limit the allowed valence of vertices even more, we can push the truncation prescription even further. Assume we are interested only in trees with vertices of valence at least three (as in the case of modified 1PI functions or tree level calculations). By extension of the above discussion it is clear that the removal of all irrelevant trees is achieved by a further truncation of the coproduct. Namely, remove from the coproduct map $V^n \to \oplus_{i=0}^n V^i \otimes V^{n-i}$ the components with tensor factors V^0 and V^1. We denote the truncated coproduct defined in this way by $\Delta_{\geqslant 2}$. It is then obvious that using this truncated coproduct to define Q and in turn Λ produces only trees all of whose vertices have valence at least three. In particular, this means that for given external legs the algorithm sketched above for calculating all trees terminates after finitely many steps. As in the above case, it never creates a tree that would need to be discarded later. Note that this procedure may be extended to any lower bound n on the valence of vertices by using the corresponding $(n-1)$-truncated coproduct $\Delta_{\geqslant n-1}$ defined in the obvious way.

D. Fermions

Recall that we have limited ourselves above to a purely bosonic theory. However, as already mentioned, this limitation is purely one of convenience and simplicity. Indeed, all of our arguments and results apply equally to fermionic fields. However, the underlying formalism becomes slightly more complicated. The vector space V will in general be a $\mathbb{Z}_2$-*graded* vector space, a direct sum of a bosonic and a fermionic part. In turn, the algebra $\mathsf{S}(V)$ is the $\mathbb{Z}_2$-*graded* symmetric algebra over V. As special cases, if V is completely bosonic we recover the usual commutative symmetric algebra (as above); if V is completely fermionic we recover the usual anticommutative exterior algebra. As a Hopf algebra $\mathsf{S}(V)$ is in general a $\mathbb{Z}_2$-*graded* or *super*-Hopf algebra. In particular, the coproduct becomes graded. This simply means that a minus sign appears as soon as odd elements are commuted, e.g.,

$$\Delta(ab) = ab \otimes \mathbf{1} + \mathbf{1} \otimes ab + a \otimes b + (-1)^{|a||b|} b \otimes a.$$

Here, $|a|$ is defined to be 0 or 1 depending on whether a is bosonic or fermionic. We refer to Ref. 1 for more details on the structure of $\mathsf{S}(V)$ in general.

However, all formulas appearing in Theorems, Propositions, and Corollaries generalize completely unchanged. The graded structure is completely implicit there. The only explicitly changing formulas are indeed those that involve explicit evaluations of the coproduct such as (6)–(8). The

underlying reason is that our constructions are completely "functorial" and could indeed be generalized to arbitrary (reasonable) symmetric categories. (For a generalization of certain *n*-point functions to nonsymmetric categories see Ref. 4.)

VII. CONCLUSIONS

Functional methods used to handle the combinatorics of quantum field theory, while having a certain elegance, have some serious drawbacks. While appearing to be analytic, they are really formal as the mathematical objects involved usually do not actually exist. In particular, the source terms appearing in functional expressions are usually merely a book keeping device, rather than actual mathematical (or physical) entities. We hope to have convinced the reader that at least certain combinatorial aspects of quantum field theory can be handled in a much more intrinsic and (we think) at least as elegant language. Indeed, our main object is nothing but the rather concrete time-ordered algebra of field operators. Its coproduct, while perhaps an unusual structure for quantum field theorists, is well known to mathematicians. It is thus natural to use it instead of more indirect and formal functional methods.

Another advantage of our algebraic approach over a functional one is its closeness to algorithmic descriptions of the processes involved. Recall from Sec. VI C how easy it is to translate the recursion relation underlying the correspondence between connected and 1PI *n*-point functions into an algorithm, which moreover appears to be rather efficient.

As mentioned in the introduction, the present paper shares a common program with Ref. 1, namely to employ the full Hopf algebraic structure of the algebra of field operators in describing and understanding quantum field theory. Thus, it is natural to combine the results of the present paper with those of Ref. 1. Indeed, the functorial nature of the Drinfeld twist employed in Ref. 1 to relate different products and their (complete) *n*-point functions should make it possible to induce the corresponding transformation on the corresponding connected or 1PI *n*-point functions using the results presented here. This, of course, goes beyond the scope of the present paper.

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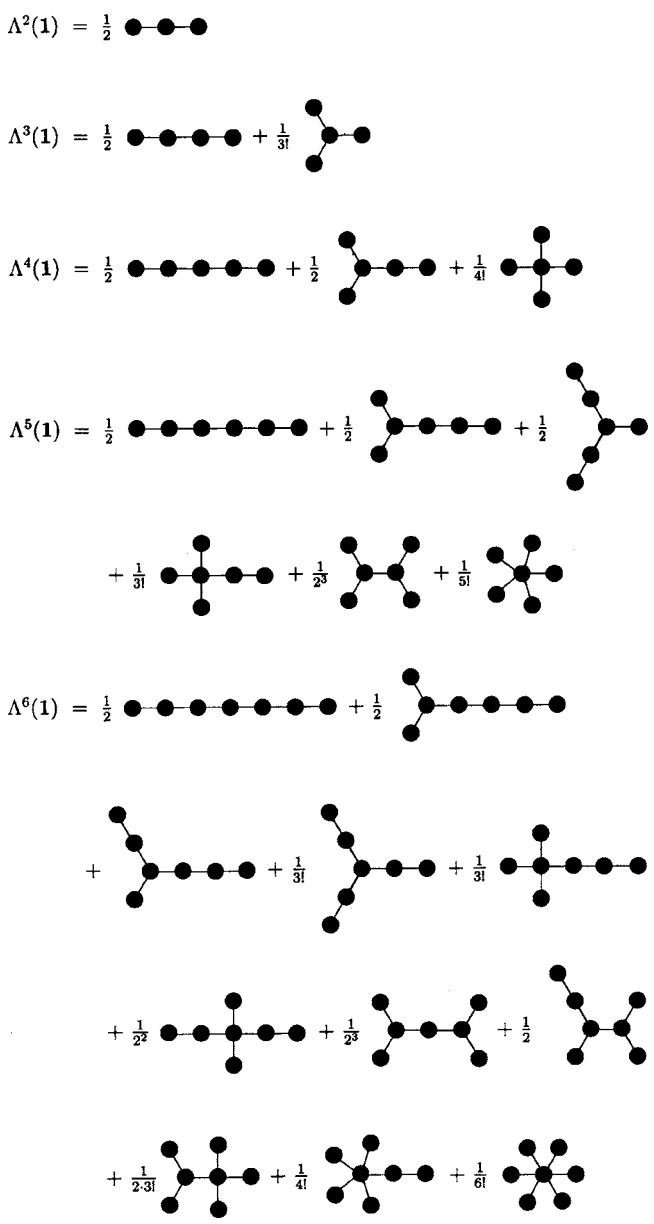
APPENDIX

This appendix shows all tree graphs without external legs and with up to seven vertices, computed as contributions to $\Lambda^k(\mathbf{1})$ via (12). The factors in front are the inverses of the symmetry factors of Definition 8, see Lemma 10.

$\Lambda^0(\mathbf{1}) =$

$\Lambda^1(\mathbf{1}) = \frac{1}{2}$ 



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Investigation of the Nicole model

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We study soliton solutions of the Nicole model—a non-linear four-dimensional field theory consisting of the CP^1 Lagrangian density to the non-integer power $\frac{3}{2}$—using an ansatz within toroidal coordinates, which is indicated by the conformal symmetry of the static equations of motion. We calculate the soliton energies numerically and find that they grow linearly with the topological charge (Hopf index). Further we prove this behavior to hold exactly for the ansatz. On the other hand, for the full three-dimensional system without symmetry reduction we prove a sublinear upper bound, analogously to the case of the Faddeev–Niemi model. It follows that symmetric solitons cannot be true minimizers of the energy for sufficiently large Hopf index, again in analogy to the Faddeev–Niemi model. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2199089]

I. INTRODUCTION

In the last few years there has been rising interest in non-linear field theories which allow for the existence of ringlike, or, more generally, knotlike solitons. On the one hand, this interest is due to the fact that there may exist physical applications for such models, as is the case, for instance, for the Faddeev–Niemi model, which finds some applications both as a candidate for a low-energy effective theory for Yang-Mills theory and in condensed matter physics. On the other hand, the rising interest is related to the advance of more powerful computer facilities which allow for reliable numerical calculations of those solitons in cases when an analytical solution is not available (which happens quite often). In addition, there is some intrinsical mathematical interest in theories with knot solitons.

In the simplest case the field of the theory describes a map from one-point compactified three-dimensional space $\mathbb{R}^3_0$ to the two-sphere S^2. $\mathbb{R}^3_0$ is topologically equivalent to the three-sphere S^3, therefore such maps are characterized by the third homotopy group of the target space S^2, which is nontrivial, $\pi_3(S^2)=\mathbb{Z}$. As a consequence, fields which describe maps $\mathbb{R}^3_0 \to S^2$ fall into different homotopy classes, and a soliton is a field configuration which minimizes a given energy functional within a fixed homotopy class. The topological index characterizing the homotopy class is called Hopf index, the corresponding map is called a Hopf map, and the minimizers are sometimes called Hopf solitons. For details on the Hopf map we refer to Appendix A.

The probably best-known theory which allows for Hopf solitons is the Faddeev–Niemi model[1,2] with Lagrangian density

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$$\mathcal{L}_{\mathrm{FN}} = \mathcal{L}_2 - \lambda \mathcal{L}_4, \tag{1}$$

where λ is a dimensionful coupling constant, $\mathcal{L}_2$ is

$$\mathcal{L}_2 = 4\frac{\partial_\mu u \partial^\mu \overline{u}}{(1+u\overline{u})^2}, \tag{2}$$

and $\mathcal{L}_4$ is

$$\mathcal{L}_4 = 4\frac{(\partial^\mu u \partial_\mu \overline{u})^2 - (\partial^\mu u \partial_\mu u)(\partial^\nu \overline{u} \partial_\nu \overline{u})}{(1+u\overline{u})^4}. \tag{3}$$

Further, u is a complex field which parametrizes the stereographic projection of the target S^2, see Appendix A. The Faddeev–Niemi model is the S^2 restriction of Skyrme theory and so circumvents Derrick's theorem, because it consists of two terms such that their corresponding energies behave oppositely under a scale transformation. The existence of (static) soliton solutions for the lowest Hopf indices has been confirmed by numerical calculations.[3–6]

There are two more models which can be constructed from the two Lagrangian densities $\mathcal{L}_2$ and $\mathcal{L}_4$ separately by choosing appropriate (non-integer) powers of these Lagrangians such that the corresponding energies are scale invariant. For $\mathcal{L}_4$ the appropriate choice is

$$\mathcal{L}_{\mathrm{AFZ}} = -(\mathcal{L}_4)^{3/4} \tag{4}$$

and for this model infinitely many analytic soliton solutions were found by Aratyn, Ferreira, and Zimerman (AFZ) by using an ansatz with toroidal coordinates.[7,8] We shall, therefore, refer to this model as the AFZ model in the sequel. The analysis of the AFZ model was carried further in Ref. 9, where, among other results, all the space-time and (geometric) target space symmetries of the AFZ model were determined, and, further, the use of the ansatz with toroidal coordinates was related to the conformal symmetry of the model (more precisely, of the static equations of motion). It turns out that the AFZ model has infinitely many target space symmetries and, moreover, realizes the notion of classical integrability in a rather strict sense, because the static equations of motion (e.o.m.) resulting from the ansatz with toroidal coordinates may be solved by simple integration. Let us also mention here that the model with Lagrangian $\mathcal{L}_4$ has the same (infinitely many) target space symmetries and, in addition, a scale invariant action, leading thereby to analytic time-dependent solutions[10].

The other model is

$$\mathcal{L}_{\mathrm{Ni}} = (\mathcal{L}_2)^{3/2}. \tag{5}$$

This model was first proposed by Nicole,[11] and it was shown in the same paper that the simplest Hopf map with Hopf index 1 is a soliton solution for this model. We, therefore, call this model the Nicole (Ni) model in this paper. This model is, in fact, the restriction to S^2 target space of a nonpolynomial SU(2) model which was studied first in Ref. 12 as a possible candidate for a pion model. The Nicole model shares the conformal symmetry with the AFZ model, therefore, again the ansatz with toroidal coordinates may be used to simplify the static e.o.m. (to reduce them to an ordinary differential equation). However, the Nicole model only has the obvious symmetries—the conformal base space symmetries (in the static case) and the modular target space symmetries, see Ref. 13. Consequently, the e.o.m. are no longer integrable, and the solutions are no longer available in closed, analytic form (except for the simplest case with Hopf index one—exact solitons with higher Hopf index have been found in modified Nicole models[14]). It is the main purpose of this paper to analyze these soliton solutions with higher Hopf index by developing the analytical treatment as far as possible and by performing numerical calculations where it is necessary.

The AFZ and Nicole models currently do not have direct physical applications, but they can serve as useful test labors for the understanding of generic features of models with knot solitons. This is all the more true as analytic results—already for solitons, but even more so for time-

dependent problems like soliton scattering—are notoriously difficult to obtain for realistic models like the Faddeev–Niemi model. Both the AFZ and the Nicole model are much easier to treat, and for time-dependent problems the Nicole model even has one advantage over the AFZ model. The infinitely many symmetries of the former—which provide its integrability on the one hand—imply that the moduli space for multi-soliton configurations is infinite dimensional. This most likely makes an adiabatic treatment of soliton scattering problematic. On the other hand, that problem is absent for the Nicole model which may, therefore, probably serve as a natural test labor for an adiabatic study of the scattering of knot-like solitons. A further issue which may be useful for the study of time-dependent problems is provided by the observation that all field configurations within the toroidal ansatz belong to an integrable subsector of the Nicole model (i.e., to a sector with infinitely many conservad currents), see Sec. III.

The paper is organized as follows. In Sec. II we provide the static e.o.m. of the Nicole model as well as the non-linear ODE resulting from the ansatz with toroidal coordinates. Then we analyze the latter equation in detail, establishing some properties analytically. In a next step we calculate the energies of the corresponding solitons numerically with high precision. We provide all energies for solitons with sufficiently small Hopf index. Further, we calculate some energies for larger Hopf index in order to establish some generic behavior. We prove that this generic behavior is in accordance with exact energy estimates for the ansatz in toroidal coordinates.

In Sec. III we show that for all the solutions of Sec. II there exist infinitely many conserved currents, that is to say, all these field configurations belong to an integrable subsector of the Nicole model.

In Sec. IV A we prove an upper bound for the energies of field configurations with given Hopf index, of the type $E_Q \leqslant C_2 Q^{3/4}$, and provide an explicit value for the constant C_2. In Sec. IV B we derive an analogous bound for the AFZ and Faddeev–Niemi model, which is easily achieved with the help of the results of Sec. IV A. The discussion of the possibility to find a corresponding lower bound $E_Q \geqslant C_1 Q^{3/4}$ for the Nicole model, analogous to the Vakulenko-Kapitansky bound for the Faddeev–Niemi model, is presented in Appendix C. We show where a Vakulenko-Kapitansky type proof needs to be refined for the Nicole (and also for the AFZ) model and leave this lower bound as a conjecture for the moment.

Section V contains our conclusions, where we comment on the relevance of our results for issues like stability, and on the relation to the corresponding results for the other two models (Faddeev–Niemi and AFZ). In Appendix A we collect useful results and facts about Hopf maps which we use throughout the paper. Appendix B contains some proofs which we need in the main sections. In Appendix C we discuss the lower energy bound.

II. SOLITONS IN THE NICOLE MODEL

A. Equation of motion

The static e.o.m. for the Nicole model (5) is

$$\frac{1}{2}(u_{jk}\overline{u_j}u_k + \overline{u_{jk}}u_j u_k) + u_j\overline{u_j}u_{kk} - \frac{u_j\overline{u_j}}{1+u\overline{u}}(u_k\overline{u_k}u + 3u_k u_k\overline{u}) = 0, \tag{6}$$

where $u_k \equiv \partial_\mu u$, etc., and the Einstein summation convention is understood. We now introduce toroidal coordinates (η, ξ, φ) via

$$\begin{gathered} x = q^{-1}\sinh\eta\cos\varphi, \quad y = q^{-1}\sinh\eta\sin\varphi, \\ z = q^{-1}\sin\xi, \quad q = \cosh\eta - \cos\xi. \end{gathered} \tag{7}$$

Further, we choose for u the ansatz

$$u = f(\eta)e^{im\varphi+in\xi}, \quad m,n \in \mathbb{Z}, \tag{8}$$

which is compatible with the e.o.m. for the Nicole model as well as for the AFZ model. The reason for this ansatz may, in fact, be understood from the symmetries of the model. More precisely, the presence of the conformal symmetry on base space implies that the ansatz (8) is an "educated guess" for a solution to Eq. (6) in the sense of the Lie theory of symmetry. That is to say, if we choose a rotation about the z axis and a certain combination of proper conformal transformation along the z axis and translation along the z axis as a maximal set of two commuting base space transformations, then the corresponding infinitesimal symmetry generators (vectors $\mathbf{v}^i$) are precisely given by the tangent vectors along φ and ξ, $\mathbf{v}^1=\partial_\varphi$, and $\mathbf{v}^2=\partial_\xi$. The ansatz (8) is invariant under a combination of these base space transformations and phase transformations of the target space variable u, i.e., under the action of the vector fields $\tilde{\mathbf{v}}^1=\partial_\varphi - imu\partial_u$ and $\tilde{\mathbf{v}}^2=\partial_\xi - inu\partial_u$, which provides precisely the educated guess according to Lie. A concise discussion of these points can be found in Ref. 9, where the symmetries of the AFZ model are discussed in great detail.

We need the gradient in toroidal coordinates

$$\nabla = (\nabla\eta)\partial_\eta + (\nabla\xi)\partial_\xi + (\nabla\varphi)\partial_\varphi = q\left(\hat{e}_\eta\partial_\eta + \hat{e}_\xi\partial_\xi + \frac{1}{\sinh\,\eta}\hat{e}_\varphi\partial_\varphi\right), \tag{9}$$

where $(\hat{e}_\eta,\hat{e}_\xi,\hat{e}_\varphi)$ form an orthonormal frame in $\mathbb{R}^3$. Further we need the relations

$$\nabla\cdot\hat{e}_\eta = -\sinh\,\eta + \frac{1-\cosh\,\eta\cos\,\xi}{\sinh\,\eta}, \quad \nabla\cdot\hat{e}_\xi = -2\sin\,\xi, \quad \nabla\cdot\hat{e}_\varphi = 0. \tag{10}$$

Inserting now the ansatz (8) into the static e.o.m. (6) we find, after a straight-forward calculation, that the ansatz is indeed compatible with the static e.o.m. and that f has to obey the non-linear ODE

$$\begin{aligned} &2f''f'^2 + f''f^2\left(n^2+\frac{m^2}{\sinh^2\,\eta}\right) + (f'^3 + n^2f'f^2)\frac{\cosh\,\eta}{\sinh\,\eta} - f^3\left(n^2+\frac{m^2}{\sinh^2\,\eta}\right)^2 \\ &\quad - f\frac{f'^2 + f^2\left(n^2+\frac{m^2}{\sinh^2\,\eta}\right)}{1+f^2}\left(4f'^2 - 2f^2\left(n^2+\frac{m^2}{\sinh^2\,\eta}\right)\right) = 0, \end{aligned} \tag{11}$$

where $f' \equiv \partial_\eta f$, etc. It may be checked without difficulty that the simplest Hopf map

$$u = \sinh\,\eta e^{i\xi+i\varphi} \Rightarrow f = \sinh\,\eta, \quad m=n=1 \tag{12}$$

indeed solves the above equation.

For technical reasons it is preferable to introduce the new variable

$$t \equiv \sinh\,\eta \tag{13}$$

in terms of which the above-noted e.o.m. can be expressed as a pure polynomial in the independent and dependent variables t, f, f_t, f_{tt},

$$\begin{aligned} F(t,f,f_t,f_{tt}) \equiv\ & t^2(1+t^2)(1+f^2)(2t^2(1+t^2)f_t^2 + (n^2t^2+m^2)f^2)f_{tt} - 4t^4(1+t^2)^2ff_t^4 + t^3(1 \\ & + 3t^2)(1+t^2)(1+f^2)f_t^3 - 2t^2(1+t^2)(n^2t^2+m^2)f^3f_t^2 \\ & + t^3(m^2+n^2(1+2t^2))(1+f^2)f^2f_t - (n^2t^2+m^2)^2f^3(1-f^2) = 0 \end{aligned} \tag{14}$$

where $f_t \equiv \partial_t f$, etc. Further, we need the energy functional $E[f]$ which results for the ansatz (8) after the integration with respect to the variables ξ,φ. With

$$dV \equiv d^3r = q^{-3}\sinh\,\eta\,d\eta\,d\xi\,d\varphi \tag{15}$$

we find

$$E[f] = 32\pi^2 \int_0^\infty d\eta \sinh\eta \frac{\left(f_\eta^2 + f^2\left(n^2 + \frac{m^2}{\sinh^2\eta}\right)\right)^{3/2}}{(1+f^2)^3}$$

$$= 32\pi^2 \int_0^\infty dt\, t(1+t^2) \frac{\left(f_t^2 + \left(n^2 + \frac{m^2}{t^2}\right)\frac{f^2}{1+t^2}\right)^{3/2}}{(1+f^2)^3}. \tag{16}$$

For $n=m=1$ for the solution $f(t)=t$ the energy may be calculated analytically,

$$E = 32\pi^2 2^{3/2} \int_0^\infty \frac{dtt}{(1+t^2)^2} = 32\pi^2\sqrt{2}. \tag{17}$$

If we calculate the energy for the field configuration $f(t)=ct$ instead, we find

$$E = 32\pi^2\sqrt{2}\frac{1}{2}\left(c + \frac{1}{c}\right), \tag{18}$$

which certainly has a minimum at $c=1$ but also shows clearly that the one-soliton sector is indeed separated from the trivial sector (with Hopf index zero) by an infinite energy barrier.

Next we have to fix the boundary conditions which f has to obey. The u of Eq. (8) has to take values in the whole target space $\mathbb{C}_0$ in order to be a Hopf map. This implies that f has to take values in the whole positive real numbers, including zero, i.e., in the whole $\mathbb{R}_{+0}$. It follows that the possible boundary conditions on f are restricted to one of the two following options. Either $f(0)=0$, $f(\infty)=\infty$ or $f(0)=\infty$, $f(\infty)=0$. The reason for this is that the values $f=0$ and $f=\infty$ correspond to the north and south pole of the target space S^2, respectively. Consequently, their preimages in the base space $\mathbb{R}_0^3$ must be one-dimensional objects (closed lines). But the only two values $\eta=\eta_0=$const (or $t=t_0=$const) which correspond to lines rather than surfaces (tori) are the values $\eta=0$ ($t=0$) and $\eta=\infty$ ($t=\infty$). Therefore we assume

$$f(\eta=0) = f(t=0) = 0, \quad f(\eta=\infty) = f(t=\infty) = \infty, \tag{19}$$

which is general, because the other option is related to this one by a symmetry transformation.

B. Asymptotic behavior and numerical evaluation

In a next step we want to determine the asymptotic behavior of the function $f(t)$ for small and large values of t from the differential equation (14). For small t we assume that $f(t) \sim t^\alpha + o(t^\beta)$ where $\beta > \alpha > 0$. From Eq. (14) we get

$$F(t,f,f_t,f_{tt}) \sim (2\alpha^4 - \alpha^3 + \alpha^2 m^2 - \alpha m^2 - m^4)t^{3\alpha} + o(t^{3\alpha+2}) + o(t^{3\beta}) \equiv 0. \tag{20}$$

The condition that the leading (i.e., smallest) order $t^{3\alpha}$ is absent therefore leads to

$$2\alpha^4 - \alpha^3 + \alpha^2 m^2 - \alpha m^2 - m^4 = 0, \tag{21}$$

which has four solutions for α of which only one is acceptable (real and positive), namely

$$\alpha_m \equiv \tfrac{1}{4}(1 + \sqrt{8m^2+1}). \tag{22}$$

In the same fashion we may determine the subleading (higher order) contributions to f for small t in an iterative manner. We find

$$f = t^{\alpha_m} P^{(0)}(t, t^{\alpha_m}) \quad \text{for } t \ll 1, \tag{23}$$

where $P^{(0)}(t,t^{\alpha_m})$ is a polynomial of its arguments, which is determined up to a multiplicative constant,

$$P^{(0)}(t,t^{\alpha_m}) = \sum_{k,l=0}^{\infty} c_{kl}^{(0)} t^k t^{l\alpha_m}. \tag{24}$$

Here it is possible to determine the higher coefficients $c_{kl}^{(0)}$ in terms of m, n, and $c_{00}^{(0)}$. Unfortunately, it is not possible to determine $c_{00}^{(0)}$, i.e., an overall constant remains undetermined by this asymptotic analysis.

We repeat the same asymptotic analysis for large values of t. We assume that $f(t) \sim t^{\alpha} + o(t^{\beta})$ where now $\alpha > \beta > 0$ and find

$$F(t,f,f_t,f_{tt}) \sim (2\alpha^4 - \alpha^3 + \alpha^2 n^2 - \alpha n^2 - n^4) t^{5\alpha+4} + o(t^{5\alpha+2}) + o(t^{5\beta+4}) \equiv 0 \tag{25}$$

and therefore the same condition for α like for small t with the only replacement $m \to n$. We may again determine f asymptotically up to an overall constant,

$$f = t^{\alpha_n} P^{(\infty)}(t^{-1}, t^{-\alpha_n}) \quad \text{for } t \gg 1, \tag{26}$$

where

$$P^{(\infty)}(t^{-1}, t^{-\alpha_n}) = \sum_{k,l=0}^{\infty} c_{kl}^{(\infty)} t^{-k} t^{-l\alpha_n} \tag{27}$$

and again the higher coefficients $c_{kl}^{(\infty)}$ are determined in terms of m, n, and $c_{00}^{(\infty)}$. Again, $c_{00}^{(\infty)}$ remains undetermined.

Next we turn to the numerical evaluation of the soliton energies for general m, n. For this purpose it is preferable to minimize the energy functional (16). The problem is that standard evolution procedures for the differential equation (14) cannot be used because of the singular nature of this equation at $t=0$. We proceed as follows with the minimization. We first factorize the leading behavior, e.g., we choose

$$f(t) \equiv t^{\alpha_m} (1+t^2)^{(\alpha_n - \alpha_m)/2} g(t), \tag{28}$$

where g obeys

$$g > 0 \; \forall \; t, \quad g(0) = g_0, \quad g(\infty) = g_{\infty}. \tag{29}$$

Then we make a finite parameter ansatz for g of the form

$$g(t) = \frac{g_0 + g_{\infty} t^2}{1+t^2} \frac{1 + \sum_{i=1}^{k} a_i t^{2i} + t^{k+2}}{1 + \sum_{j=1}^{k} b_j t^{2j} + t^{k+2}}, \tag{30}$$

where g_0, g_{∞}, a_i, and b_j are the parameters with respect to which we minimize the energy functional (16). For each value of m, n we increase the number of parameters (i.e., the integer number k), until we reach stability (i.e., until the energies do not change further with the increase of the number of parameters). We do not choose a full numerical minimization of the energy functional for the following reason. It turns out that the leading behavior (i.e., $g(t)=\text{const}$), already provides rather good results for the corresponding energies. This implies that the energy functional, when viewed as a functional of g, is rather shallow. As a consequence, a full numerical minimization which implements the derivatives numerically has the tendency to produce false minima unless the numerical minimization grid is chosen very finely (and consumes a lot of computer time). On the other hand, within our finite parameter ansatz we are able to perform the derivatives analytically, and therefore this problem is absent.

We show our numerical results in Table I for all $(m,n)=(1,1),\ldots,(5,5)$ as well as for some higher values. Further we plot the energies versus the Hopf index $Q=mn$ in Fig. 1. From our results it is obvious that the energies grow linearly in Q to a very good accuracy. More precisely, the energies for $m=n$ lie on a straight line in Fig. 1 almost exactly. The energies for $m \neq n$ lie

TABLE I. The rescaled energies $E^*=(32\pi^2)^{-1}E$ of solutions for selected values of m and n.

n	m	E^*	n	m	E^*
1	1	1.413 621 93	4	1	6.524 502 66
1	2	2.626 150 91	4	2	9.033 849 01
1	3	4.133 387 23	4	3	12.743 662 4
1	4	5.373 494 09	4	4	16.789 796
1	5	7.541 507 89	4	5	20.886 948
2	1	2.647 535 48	5	1	9.486 800 75
2	2	4.522 499 73	5	2	11.890 141 5
2	3	6.629 259 43	5	3	15.978 639 9
2	4	8.853 709 29	5	4	20.893 791 5
2	5	10.951 318 4	5	5	25.975 942
3	1	4.282 322 66	6	6	37.201 786 9
3	2	6.649 418 01	8	8	65.771 712
3	3	9.640 594 35	9	9	83.116 75
3	4	12.730 713 6	10	10	102.501 125
3	5	15.867 283 6	20	20	408.581 244
			5	10	51.899 074 7
			6	15	96.058 593 3
			14	7	103.670 713

slightly above, whereas no energy lies below this line. It is in fact possible to prove the linear growth of energies with the Hopf charge for solutions of the ansatz (8). This we show for the simplest case $m=n$ in the next section.

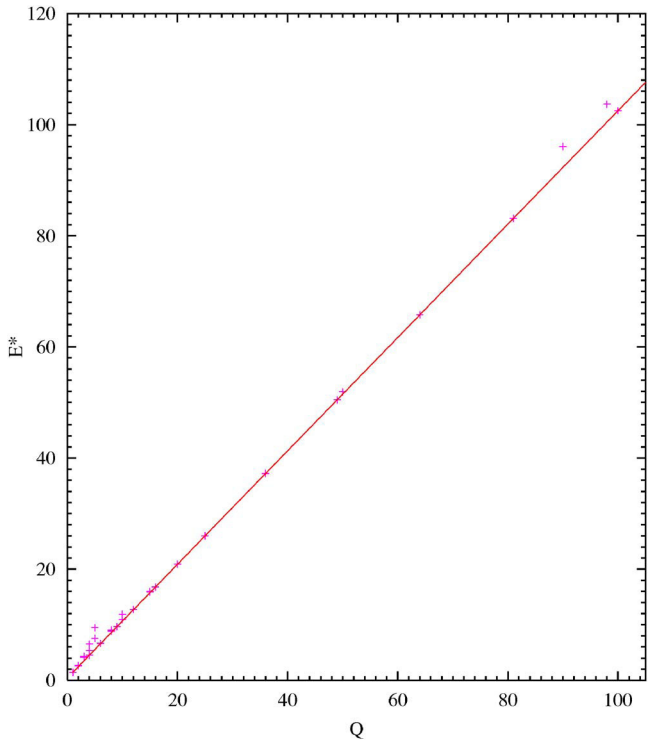

FIG. 1. (Color online) The rescaled energies $E^*=(32\pi^2)^{-1}E$ (vertical axis) are plotted vs the Hopf index $Q=mn$. The straight line connects energies for $m=n$. The energies for $m\neq n$ lie slightly above this line.

On the other hand, for the full model the sublinear upper bound $E \leqslant C_2 Q^{3/4}$ holds, which we prove in Sec. IV. It follows that the solutions we found for the symmetric ansatz (8) *cannot* be true solitons, i.e., global minima of topological sectors with fixed Q for sufficiently large values of Q. This is akin to the situation in the Faddeev–Niemi model and differs from the situation in the AFZ model (see our discussion in Sec. V).

C. Upper and lower bounds for the torus ansatz

In this section we prove the bounds $c_1 Q \leqslant E[f_{m,n}]$ and, for the special case $m=n$, $E[f_{m,m}] \leqslant c_2 m^2$ (with explicit values for the constants c_1 and c_2) in order to further support our numerical results. Here $E[f]$ is the energy functional (16) and $f_{m,n}$ is the corresponding solution of the equation of motion. We first prove the lower bound. We use the inequality

$$(a+b)^{3/2} \geqslant \frac{3\sqrt{3}}{2} a^{1/2} b \quad \text{for } a,b \geqslant 0, \tag{31}$$

which we prove in Appendix B (here $3\sqrt{3}/2$ is an optimal value). We choose $a=f_t^2$ and $b=(n^2+m^2/t^2)f^2/(1+t^2)$ and introduce

$$Q = mn, \quad \mu = \frac{m}{n} \tag{32}$$

to get

$$\begin{aligned} E[f] &= 32\pi^2 \int_0^\infty dt t(1+t^2) \frac{\left(f_t^2 + Q\left(\frac{1}{\mu} + \frac{\mu}{t^2}\right)\frac{f^2}{1+t^2}\right)^{3/2}}{(1+f^2)^3} \\ &\geqslant 32\pi^2 Q \frac{3\sqrt{3}}{2} \int_0^\infty dt \left(\frac{t}{\mu} + \frac{\mu}{t}\right) |f_t| \frac{f^2}{(1+f^2)^3} \\ &\geqslant 32\pi^2 Q 3\sqrt{3} \int_0^\infty dt f_t \frac{f^2}{(1+f^2)^3} \equiv \tilde{E}[f], \end{aligned} \tag{33}$$

where we used $(t/\mu+\mu/t) \geqslant 2$. Up to now we have in fact used inequalities for the energy densities, i.e., these inequalities hold for given, fixed functions f. However, if we evaluate the last expression for its minimizer $f_{\min}$ then the inequality holds for arbitrary f and, consequently, for the solutions $f_{m,n}$. The minimization of the last expression is simplified by the observation that it is a total derivative. Therefore it is minimized for all f which obey the required boundary conditions $f(0)=0$ and $f(\infty)=\infty$. Explicitly we get

$$\tilde{E}[f] = 32\pi^2 Q 3\sqrt{3} \left[-\frac{f}{4(1+f^2)^2} + \frac{f}{8(1+f^2)} + \frac{1}{8} \arctan f \right]_{f=0}^{f=\infty} = 32\pi^2 Q 3\sqrt{3} \frac{\pi}{16} = 1.02 \times 32\pi^2 Q. \tag{34}$$

Comparing with Table I, we see that for larger values of m, n our lower bound gets very close to the numerical values, especially for $m=n$ (e.g., better than 1% for $m=n=10$ or $m=n=20$). This demonstrates the very good accuracy of our numerical results.

For the derivation of an upper bound we restrict to the simpler case $m=n$. We simply insert a trial function $f_{m,m}^{\mathrm{tr}}$ into the energy functional $E[f]$. Concretely we choose $f_{m,m}^{\mathrm{tr}} = t^m$ and get

$$E[t^m] = 32\pi^2 \int_0^\infty dt t(1+t^2) \frac{m^3 t^{3m-3} 2^{3/2}}{(1+t^{2m})^3} \tag{35}$$

and, with the substitution $u=t^m$,

$$E[t^m] = 32\pi^2 m^2 2^{3/2} \int_0^\infty du(u^{1/m} + u^{-1/m}) \frac{u^2}{(1+u^2)^3} = 32\pi^2 m^2 2^{3/2} \frac{1}{8} \left(1 - \frac{1}{m^2}\right) \frac{\pi}{\cos \frac{\pi}{2m}}. \quad (36)$$

The function $(1-1/m^2)/(\cos(\pi/2m))$ is a monotonously decreasing function in m and may, therefore, be estimated by its value at $m=2$ for the range $m \geqslant 2$. With

$$\left(1 - \frac{1}{4}\right) \frac{1}{\cos \frac{\pi}{4}} = \frac{3}{4}\sqrt{2} \quad (37)$$

we therefore get

$$E[t^m] \leqslant 32\pi^2 m^2 \frac{3\pi}{8} = 1.18 \times 32\pi^2 m^2 \quad \text{for } m \geqslant 2 \quad (38)$$

which, for large m, is about 15% above the numerical value. By using Eq. (36) instead of the order m^2 estimate (38), we get slightly better results which, for large m, are less than 10% above the numerical values.

In short, we established the bounds $c_1 m^2 \leqslant E[f_{m,m}] \leqslant c_2 m^2$ with $c_1 = 1.02 \times 32\pi^2$ and $c_2 = 1.18 \times 32\pi^2$, as announced.

III. INFINITELY MANY CONSERVED CURRENTS

In this section we want to demonstrate that the ansatz (8) belongs to a subsector of the Nicole model with infinitely many conserved currents for arbitrary profile function $f(\eta)$. The integrability condition defining this subsector exists for a wide class of models, and discussing it for the whole class does not complicate matters (for a more detailed discussion, and especially for the geometric meaning of the integrability condition, we refer to Ref. 15; the concept of higher dimensional integrability, which is at the basis of these discussions, was introduced in Ref. 16). Therefore, we start with the general class of Lagrangian densities

$$\mathcal{L}(u, \overline{u}, u_\mu, \overline{u_\mu}) = F(a,b,c), \quad (39)$$

where

$$a = u\overline{u}, \quad b = u_\mu \overline{u^\mu}, \quad c = (u_\mu \overline{u^\mu})^2 - u_\mu^2 \overline{u_\nu^2} \quad (40)$$

and F is an arbitrary real function of its arguments. Obviously, the Nicole model belongs to this class, $\mathcal{L}_{\mathrm{Ni}} = [4(1+a)^{-1}b]^{3/2}$.

Further, we define the currents

$$K^\mu = h(a)\overline{\Pi}^\mu, \quad (41)$$

where h is an arbitrary given real function of its argument, and Π^μ and $\overline{\Pi}^\mu$ are the conjugate four-momenta of u and $\overline{u}$, i.e.,

$$\Pi_\mu \equiv \mathcal{L}_{u^\mu} = \overline{u}^\mu F_b + 2(u^\lambda \overline{u}_\lambda \overline{u}_\mu - \overline{u}_\lambda^2 u_\mu) F_c. \quad (42)$$

Finally, we define the infinitely many Noether currents

$$J_\mu^G = i(G_u K_\mu - G_{\overline{u}} \overline{K}_\mu), \quad (43)$$

where G is an arbitrary real function of u and $\overline{u}$, and $G_u \equiv \partial_u G$.

Now we want to study the conditions which one has to impose in order to make the divergence $\partial^\mu J_\mu^G$ vanish. A simple calculation reveals

$$\partial^\mu J^G_\mu = ih\left(\left[\left(\frac{h'}{h}\overline{u}G_u + G_{uu}\right)u_\mu^2 - \left(\frac{h'}{h}uG_{\overline{u}} + G_{\overline{uu}}\right)\overline{u}_\mu^2\right]F_b + (uG_u - \overline{u}G_{\overline{u}})\left[\frac{h'}{h}(bF_b + 2cF_c) + F_a\right]\right), \tag{44}$$

where the prime denotes the derivative with respect to a.

The second term at the right-hand side of Eq. (44) certainly vanishes if

$$uG_u - \overline{u}G_{\overline{u}} = 0 \tag{45}$$

with the general solution

$$G(u,\overline{u}) = \widetilde{G}(u\overline{u}) \equiv \widetilde{G}(a). \tag{46}$$

Without taking condition (46) into account, the first term on the right-hand side of Eq. (44) vanishes for the integrability condition

$$u_\mu^2 = 0, \tag{47}$$

i.e., the complex eikonal equation (it also vanishes for some more complicated integrability conditions which we do not discuss here, see Refs. 17 and 18). However, by using condition (46) we may re-express the first term like

$$(h'G' + hG'')F_b[\overline{u}^2 u_\mu^2 - u^2\overline{u}_\mu^2] \tag{48}$$

and, therefore, we find, instead of the complex eikonal equation, the weaker integrability condition

$$\overline{u}^2 u_\mu^2 - u^2\overline{u}_\mu^2 = 0. \tag{49}$$

The meaning of this condition becomes especially transparent when we re-express u in terms of its modulus and phase like

$$u = \exp(\Sigma + i\Lambda). \tag{50}$$

Then the complex eikonal equation is equivalent to the two real equations

$$\Sigma_\mu^2 = \Lambda_\mu^2 \tag{51}$$

and

$$\Sigma^\mu \Lambda_\mu = 0 \tag{52}$$

whereas the weaker condition (49) becomes Eq. (52) alone or, for time-independent u,

$$(\nabla\Sigma)\cdot(\nabla\Lambda) = 0. \tag{53}$$

Remark: The condition $G(u,\overline{u}) = \widetilde{G}(u\overline{u})$, Eq. (46), restricts the space of allowed G to a subspace which is still infinite-dimensional, therefore the integrability condition (49) really defines a subsector with infinitely many conserved currents.

Remark: The ansatz (8) obeys the integrability condition (53) for arbitrary profile function $f(\eta)$, as is obvious from the orthonormality of the basis vectors $(\hat{e}_\eta, \hat{e}_\xi, \hat{e}_\varphi)$. Therefore, all our solutions of Sec. II really belong to the subsector of the Nicole model defined by condition (49) with infinitely many conserved currents. This is in contrast to the complex eikonal equation (47), which leads to a non-linear ODE for the profile function which is not compatible with the Nicole model field equation except for the simplest Hopf map $m=n=1$, see Ref. 19.

Remark: Both condition (46) and the integrability condition (49) do not restrict the Lagrangian density, therefore the corresponding integrable subsectors with infinitely many conservation laws exist for all Lagrangians of the type (39). So they may be of interest for other models like, e.g., the Faddeev–Niemi model.

IV. ENERGY ESTIMATES FOR THE FULL MODEL

In this section we study upper bounds on the energies of solitons with a given Hopf index, of the type $E_Q \leqslant C_2 Q^{3/4}$. In Sec. IV A we prove the upper bound $E_Q \leqslant C_2 Q^{3/4}$ by following the method used in Ref. 20 for the Faddeev–Niemi model. Further, we provide an explicit value for the constant C_2. In Sec. IV B, we briefly derive the analogous upper bounds for the AFZ and the Faddeev–Niemi models, again with explicit values for the constants C_2. They easily follow from our results from Sec. IV A. The issue of a lower bound $C_1 Q^{3/4} \leqslant E_Q$ is discussed in Appendix C. There we show where a naive Vakulenko-Kapitansky type proof does not work and needs some refinement in our case, leaving open for the moment the problem of rigorously establishing such a lower bound.

A. The estimate $E_Q \leqslant C_2 Q^{3/4}$

In this section we use the unit vector $\vec{n}$ to denote Hopf maps, because this has some technical advantages (components of the vector $\vec{n}$ can be easily estimated, whereas the complex function u may take arbitrary values). In our proof we will closely follow the method used in Ref. 20 for the proof of an analogous result for the Faddeev–Niemi model. However, we will use explicit expressions for certain functions instead of using just their existence, which enables us to provide an explicit value for the constant C_2 in our estimate.

For a Hopf index which is a square, $Q=l^2$, a Hopf map is constructed in Ref. 20 which is a composition of a Hopf map $\vec{n}(\vec{r})$ with Hopf index 1 and a map $\vec{N}(\vec{n}):S^2 \to S^2$ with winding number $w=l$. The Hopf map $\vec{n}(\vec{r})$ is constructed such that it varies smoothly from $\vec{n}=(0,0,1)$ at $\vec{r}=0$ to $\vec{n}=(0,0,-1)$ at $|\vec{r}|=R$ and remains at this value for $r>R$. This implies, by Eq. (A20), that it has indeed Hopf index 1. Further, the gradient $|\nabla^{\mathbb{R}^3}\vec{n}|$ may be estimated like $|\nabla^{\mathbb{R}^3}\vec{n}| \leqslant c/R$ for $r \leqslant R$ and by $|\nabla^{\mathbb{R}^3}\vec{n}|=0$ for $r>R$ (here and below c denotes an unspecified constant). The map $\vec{N}(\vec{n}):S^2 \to S^2$ is constructed such that $\vec{N}$ varies smoothly over l nonintersecting geodesic discs covering the base S^2, where $\vec{N}=(0,0,1)$ in the center of each disc and $\vec{N}=(0,0,-1)$ at the boundary of each disc and between the discs. Each disc contributes a winding number 1 for the map $\vec{N}(\vec{n})$, therefore the total winding number is l. Further, the geodesic radius of each disc can be chosen (not larger than) $R_g=cl^{-1/2}$ in order to be able to put l nonintersecting discs on one unit S^2. The gradient may be again estimated by the inverse (geodesic) radius, $|\nabla^{S^2}\vec{N}(\vec{n})| \leqslant cl^{1/2}$, and with the help of the chain rule one finds for the gradient of $\vec{N}$ that $|\nabla^{\mathbb{R}^3_0}\vec{N}(\vec{n}(\vec{r}))| \leqslant cR^{-1}l^{1/2}$ and for the energy density $\mathcal{E}_{\mathrm{Ni}}(\vec{r}) \sim |\nabla^{\mathbb{R}^3_0}\vec{N}|^3 \leqslant cR^{-3}l^{3/2}$. The energy E_{Ni}, which is the integral over all space of $\mathcal{E}_{\mathrm{Ni}}(\vec{r})$, may in the case at hand be calculated by integrating over the ball B^R of radius R with the result that $E_{\mathrm{Ni}} \leqslant cl^{3/2} \equiv cQ^{3/4}$ which is the announced estimate for $Q=l^2$.

Before rederiving this result in more detail and with explicit choices for the above described maps, it may be useful to have a geometric picture of the above-noted composition of maps. In fact, the map $\vec{N}(\vec{n}(\vec{r}))$ describes l nonintersecting, full tori confined to the ball B^R, where, in addition, each full torus is linked with all other tori. In the center of each torus there is a closed line along which $\vec{N}$ takes the value $\vec{N}=(0,0,1)$. From the center to the surface of each full torus, $\vec{N}$ varies smoothly from $\vec{N}=(0,0,1)$ to $\vec{N}=(0,0,-1)$. At the surface of each full torus (which has the topology of the two-torus T^2) as well as in the space between the tori and outside the ball B^R, $\vec{N}$ remains at the value $\vec{N}=(0,0,-1)$.

Now for the detailed derivation, where we still assume $Q=l^2$ for the moment. For the map $\vec{n}(\vec{r})=(\sin\vartheta\cos\phi, \sin\vartheta\sin\phi, \cos\vartheta)$ with Hopf index 1 we assume that it has cylindrical symmetry, as in Eq. (A24). For the profile function $\rho(r)$ we want to find a choice which varies as smoothly as possible from 0 to π as r varies from 0 to R, in order to be able to estimate it with a number as small as possible. The smoothest choice $\rho=\pi r/R$ for $r \leqslant R$ and $\rho=\pi$ for $r>R$ does not have a continuous first derivative at $r=R$, which we need for the energy density, but there is a simple generalization which does have one. We choose

$$\rho_\epsilon(r) = \pi F_\epsilon(x), \quad x \equiv \frac{r}{R}, \tag{54}$$

where

$$F_\epsilon(x) = F_\epsilon^<(x) \equiv \frac{2}{2-\epsilon}x \quad \text{for } 0 \leqslant x \leqslant 1-\epsilon,$$

$$F_\epsilon(x) = F_\epsilon^>(x) \equiv 1 - \frac{1}{\epsilon(2-\epsilon)}(x-1)^2 \quad \text{for } 1-\epsilon < x \leqslant 1, \tag{55}$$

$$F_\epsilon(x) = 1 \quad \text{for } x > 1,$$

and ϵ is a sufficiently small, positive nonzero parameter. It may be checked easily that $\rho_\epsilon(r)$ is continuous and has continuous first derivatives everywhere. Further, the following estimates hold:

$$|F_\epsilon(x)| \leqslant k(\epsilon)x \quad \text{for } 0 \leqslant x \leqslant 1,$$

$$|F_\epsilon(x)| \leqslant k(\epsilon) \quad \text{for } 1 < x < \infty, \tag{56}$$

$$|F'_\epsilon(x)| \leqslant k(\epsilon) \quad \text{for } 0 \leqslant x < \infty,$$

where

$$k(\epsilon) \equiv \frac{2}{2-\epsilon} > 0. \tag{57}$$

For the map $\vec{N}(\vec{n})$ with winding number l we choose l nonintersecting geodesic discs on the base S^2 such that $\vec{N}$ varies smoothly from $\vec{N}=(0,0,1)$ in the center of each disc to $\vec{N}=(0,0,-1)$ at the boundary of each disc and remains at this value in between the discs. The geodesic radius ϑ_0 of these geodesic discs has to be chosen sufficiently small so that it is possible to put l nonintersecting discs with this geodesic radius on the base S^2. We prove in Appendix B that the choice

$$\vartheta_0 = \frac{\pi}{4\sqrt{l}} \tag{58}$$

is sufficient. Next we give an explicit expression for the map $\vec{N}$ for one geodesic disc which is chosen symmetric about the north pole. With

$$\vec{N} = (\sin\chi\cos\sigma, \sin\chi\sin\sigma, \cos\chi) \tag{59}$$

and

$$\vec{n} = (\sin\vartheta\cos\phi, \sin\vartheta\sin\phi, \cos\vartheta) \tag{60}$$

we get

$$\chi(\vartheta) = \pi F_\epsilon(\tilde{\vartheta}), \quad \tilde{\vartheta} \equiv \frac{\vartheta}{\vartheta_0} \tag{61}$$

and

$$\sigma = \phi, \tag{62}$$

where $F_\epsilon(\cdot)$ is defined in (55) (with the additional restriction that here $\tilde{\vartheta} \leqslant 4\sqrt{l}$ because $\vartheta \leqslant \pi$). The above-defined $\vec{N}$ has winding number 1, and to reach winding number l we have to require that it is nonconstant over $l-1$ further geodesic discs. We do not need, however, explicit expressions for the contribution of these further discs to $\vec{N}$, because their gradients on S^2, $|\nabla^{S^2}\vec{N}|$ can be estimated by the same majorants as the above explicit expression. The reason for this is that the above-noted symmetrically chosen disc is related to an arbitrary disc with the same geodesic radius by a rotation of the base space S^2, and the gradient $|\nabla^{S^2}\vec{N}|$ is invariant under such rotations. All that changes is that more regions of the base S^2 provide nonzero contributions to the gradient.

Next we want to estimate the energy density $\mathcal{E}_{\mathrm{Ni}}(\vec{r}) \sim |\nabla\vec{N}|^3$. Here we first estimate (Einstein summation convention is understood, $k, a = 1, \ldots, 3$)

$$|\nabla\vec{N}|^2 = (\nabla_k N^a)^2 = \chi_\vartheta^2 (\nabla_k \vartheta)^2 + \sin^2\chi (\nabla_k \sigma)^2, \tag{63}$$

where we used (59), and $\chi_\vartheta \equiv \partial_\vartheta \chi$. The first term may be estimated by

$$\chi_\vartheta^2 \leqslant \left(\frac{\pi}{\vartheta_0}\right)^2 k(\epsilon)^2 \tag{64}$$

and, with the help of spherical polar coordinates, by

$$(\nabla_k\vartheta)^2 = \vartheta_r^2 + \frac{1}{r^2}\vartheta_\theta^2 = \frac{4\rho_r^2 \cos^2\rho \sin^2\theta}{1-\sin^2\rho\sin^2\theta} + \frac{\sin^2\rho}{r^2}\frac{4\cos^2\theta}{1-\sin^2\rho\sin^2\theta} \leqslant 4\rho_r^2 + 4\frac{\rho^2}{r^2} \leqslant 8\pi^2\frac{k(\epsilon)^2}{R^2}, \tag{65}$$

where we used

$$\frac{\cos^2\alpha}{1-\sin^2\alpha\sin^2\beta} \leqslant 1, \quad \sin\alpha \leqslant \alpha \tag{66}$$

as well as Eqs. (54) and (56). For the second term we find

$$\sin^2\chi \leqslant \sin^2\left(\pi k(\epsilon)\frac{\vartheta}{\vartheta_0}\right) \leqslant \left(\frac{\pi k(\epsilon)}{\vartheta_0}\right)^2 \sin^2\vartheta, \tag{67}$$

where we used

$$\sin ax \leqslant a \sin x \quad \text{for } a \geqslant 1, \quad x \in \left[0, \frac{\pi}{2}\right] \tag{68}$$

which we prove in Appendix B. Further we find, using $\sigma = \phi$ and the expression for ϕ in Eq. (A24)

$$\sin^2\vartheta(\nabla_k\phi)^2 = 4\sin^2\rho\sin^2\theta(1-\sin^2\rho\sin^2\theta) \tag{69}$$

$$\cdot\left(\frac{1}{r^2\sin^2\theta} + \frac{\rho_r^2\cos^2\theta + (1/r^2)\cos^2\rho\sin^2\rho\sin^2\theta}{(1-\sin^2\rho\sin^2\theta)^2}\right) \tag{70}$$

$$= 4\frac{\sin^2\rho}{r^2}(1-\sin^2\rho\sin^2\theta) \tag{71}$$

$$+ 4\sin^2\rho\sin^2\theta\rho_r^2\frac{\cos^2\theta}{1-\sin^2\rho\sin^2\theta} \tag{72}$$

$$+4\sin^2\rho\sin^4\theta\frac{\sin^2\rho}{r^2}\frac{\cos^2\rho}{1-\sin^2\rho\sin^2\theta} \tag{73}$$

$$\leqslant 4\left(\frac{\pi k(\epsilon)}{R}\right)^2+4\left(\frac{\pi k(\epsilon)}{R}\right)^2+4\left(\frac{\pi k(\epsilon)}{R}\right)^2=12\left(\frac{\pi k(\epsilon)}{R}\right)^2. \tag{74}$$

Putting everything together, we therefore find

$$|\nabla\vec{N}|^2\leqslant 20\left(\frac{\pi^2 k(\epsilon)^2}{\vartheta_0 R}\right)^2=20l\left(\frac{4\pi k(\epsilon)^2}{R}\right)^2. \tag{75}$$

Taking the power of $\frac{3}{2}$ and integrating over the ball B^R we estimate the energy by

$$E_{\mathrm{Ni}}=\int d^3r|\nabla\vec{N}|^3\leqslant\int_{B^R}d^3r5^{3/2}l^{3/2}\left(\frac{8\pi k(\epsilon)^2}{R}\right)^3=\frac{4\pi}{3}5^{3/2}l^{3/2}(8\pi k(\epsilon)^2)^3. \tag{76}$$

Finally, for the estimate it is sufficient if the estimating field configuration is a distribution. Therefore we may now perform the limit $\lim_{\epsilon\to 0}k(\epsilon)=1$ and get, for $Q=l^2$,

$$E_{\mathrm{Ni}}\leqslant\frac{4\pi}{3}(8\pi)^3 5^{3/2}l^{3/2}. \tag{77}$$

In the cases when the Hopf index Q is not a square, we shall find a slightly weaker bound (i.e., a slightly larger value for the constant C_2). Again following Ref. 20, we write Q as

$$Q=l^2+m,\quad m\in[1,2l] \tag{78}$$

and estimate the energy by the following Hopf map. It maps the ball B^R with radius R about the origin to the two-sphere with a contribution of l^2 to the Hopf index in exactly the way constructed above for the case $Q=l^2$. Further, it maps m balls B_i^1, $i=1,\ldots,m$ with unit radius to the S^2 such that each ball contributes one unit to the Hopf index. Here the m unit balls are chosen such that they intersect neither each other nor the ball B^R. The map from B^R contributes exactly the above-calculated expression (77) to the energy, whereas the m maps from the B_i^1 contribute the energy of a unit Hopf map each. One might think to take just the energy (77) with $l=1$ for each energy contribution, but we can do better. The reason is that we were forced to choose ϑ_0 rather small in Eq. (58) to ensure that we can put l geodesic discs on one S^2. But here we are only interested in a map with winding number one, therefore we can choose the "geodesic disc" equal to the full S^2, i.e., $\vartheta_0=\pi$. This leads to the following energy estimate:

$$E_{\mathrm{Ni}}\leqslant\frac{4\pi}{3}(8\pi)^3 5^{3/2}l^{3/2}+\frac{4\pi}{3}(2\pi)^3 5^{3/2}m, \tag{79}$$

which we want to estimate in terms of Q again, i.e.,

$$c_2 l^{3/2}+c_3 m\leqslant c_4(l^2+m)^{3/4}. \tag{80}$$

Here the left-hand side grows linearly in m, whereas the right-hand side grows sublinearly, therefore the inequality certainly holds for all $m\in[1,2l]$ if it holds for the maximum value $m=2l$, i.e.,

$$c_2 l^{3/2}+2c_3 l\leqslant c_4(l^2+2l)^{3/4}. \tag{81}$$

With the help of the inequality

$$c_2 + 2c_3 l^{-1/2} \leqslant c_2 + 2c_3 \leqslant (c_2 + 2c_3)\left(1 + \frac{2}{l}\right)^{3/4} \tag{82}$$

we see that the above-noted inequality certainly holds for $c_4 = c_2 + 2c_3$. Inserting the concrete numbers from (79) we therefore get

$$E_{\mathrm{Ni}} \leqslant \frac{4\pi}{3}(2\pi)^3(4^3+2)5^{3/2}Q^{3/4} \tag{83}$$

as our final estimate for general Q.

B. Upper bounds for the AFZ and Faddeev–Niemi models

We may use our result to obtain upper bounds for the energies of the AFZ and Faddeev–Niemi models, as well. For the bound on the AFZ model we use the simple inequality for the energy densities

$$\mathcal{E}_4 \leqslant \tfrac{1}{2}\mathcal{E}_2^2, \tag{84}$$

which is obvious from the (ϑ, ϕ) parametrization, see Eqs. (A25) and (A26). It follows immediately that $E_{\mathrm{AFZ}} \leqslant (\frac{1}{2})^{3/4} E_{\mathrm{Ni}}$ and, therefore,

$$E_{\mathrm{AFZ}} \leqslant \left(\frac{1}{2}\right)^{3/4}\frac{4\pi}{3}(2\pi)^3(4^3+2)5^{3/2}Q^{3/4}. \tag{85}$$

For the Faddeev–Niemi model with energy density $\mathcal{E}_{\mathrm{FN}} = \mathcal{E}_2 + \lambda\mathcal{E}_4$ we consider the case $Q = l^2$ of a square Hopf index first. We use Eq. (75) for the density $\mathcal{E}_2$ and the inequality (84) and find

$$\begin{aligned} E_{\mathrm{FN}} &= \int_{B^R} d^3r(\mathcal{E}_2 + \lambda\mathcal{E}_4) \leqslant \int_{B^R} d^3r\left(20l\left(\frac{4\pi}{R}\right)^2 + \frac{\lambda}{2}(20l)^2\left(\frac{4\pi}{R}\right)^4\right) \\ &= \frac{4\pi}{3}R^3\left(20l\left(\frac{4\pi}{R}\right)^2 + \frac{\lambda}{2}(20l)^2\left(\frac{4\pi}{R}\right)^4\right) \end{aligned} \tag{86}$$

and, with the choice

$$R = R_0\sqrt{l}, \tag{87}$$

we get

$$E_{\mathrm{FN}} \leqslant 20\frac{4\pi}{3}(4\pi)^2 l^{3/2}\left(R_0 + 10(4\pi)^2\frac{\lambda}{R_0}\right). \tag{88}$$

For a neat estimate we now minimize the expression in brackets with respect to R_0 which leads to

$$R_0 = 4\pi\sqrt{10\lambda} \tag{89}$$

and to

$$E_{\mathrm{FN}} \leqslant 40\frac{4\pi}{3}(4\pi)^3\sqrt{10\lambda}\, l^{3/2}. \tag{90}$$

Here we have separated a factor $(4\pi)^3$ because it can be replaced by π^3 for winding number one, exactly as in the estimate for the Nicole model, which we need for general Q. Again we write $Q = l^2 + m$ and estimate

$$E_{\mathrm{FN}} \leqslant 40\frac{4\pi}{3}(4\pi)^3\sqrt{10\lambda}l^{3/2} + 40\frac{4\pi}{3}\pi^3\sqrt{10\lambda}m \tag{91}$$

and finally by

$$E_{\mathrm{FN}} \leqslant 40\frac{4\pi}{3}\pi^3\sqrt{10\lambda}(4^3+2)Q^{3/4} \tag{92}$$

in complete analogy to the Nicole model.

Note added: after finishing this paper we became aware of Ref. 21, where an analogous bound $E_{\mathrm{FN}} \leqslant C_2 Q^{3/4}$ was derived for the Faddeev–Niemi model. There the authors found a better (i.e., lower) value for C_2 by a combination of analytical and numerical methods.

V. CONCLUSIONS

Combining numerical and analytical techniques, we found the energies for static solutions of the Nicole model within the symmetric ansatz (8) for a wide (in principle arbitrary) range of the integers m and n. It turns out that the energies of these symmetric solutions grow linearly with the Hopf index $Q=mn$ within a very good accuracy. Together with the sublinear growth inequality of Sec. IV, $E \leqslant C_2 Q^{3/4}$ this implies that, for sufficiently large values of Q, the symmetric solutions we found cannot be global minima within their respective topological sectors with fixed Hopf index Q. It is of some interest to compare this result with the corresponding results for the AFZ and Faddeev–Niemi models.

For the AFZ model all solutions for the symmetric ansatz (8) and their corresponding energies can be calculated exactly.[8] The energies are

$$E_{\mathrm{AFZ}} = 8\sqrt{2}\pi^2\sqrt{|m||n|(|m|+|n|)} = 8\sqrt{2}\pi^2 Q^{3/4}\sqrt{\mu+\frac{1}{\mu}}, \quad \mu^2 \equiv \left|\frac{m}{n}\right| \tag{93}$$

and, for $m=n$ ($\mu=1$) perfectly fit within the upper bound $E_{\mathrm{AFZ}} \leqslant C_2 Q^{3/4}$ which holds also for the AFZ model (see Sec. IV). It is, therefore, plausible to conjecture that these solutions might be true minima for $m=n$ (and, maybe, even for $m \neq n$ provided that m and n do not differ too much).

For the Faddeev–Niemi model the ansatz (8) is not compatible with the equations of motion (due to the lack of conformal symmetry of the latter), but the cylindrically symmetric ansatz

$$u = f(\eta,\xi)e^{im\varphi} \tag{94}$$

for complex f is compatible and leads to an equation in the two independent variables η and ξ. Numerical investigation of the full e.o.m. in three variables shows that the solutions for the ansatz (94) are true minima only for the lowest values $Q=1,2$ of the Hopf index.[4] In this respect, therefore, the Nicole model bears more similarity with the Faddeev–Niemi model than with the AFZ model. It is tempting to speculate at this instant that the different behavior of the AFZ model—i.e., the possibility that the symmetric solutions (93) are true minima for arbitrary Q—is related to the integrability properties of the latter. But at the moment this is, of course, only speculation which deserves further investigation.

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APPENDIX A: FACTS ABOUT HOPF MAPS

A Hopf map is a map from the three-sphere S^3 to the two-sphere S^2. The third homotopy group of the two-sphere is nontrivial, $\Pi_3(S^2)=\mathbb{Z}$, therefore Hopf maps are characterized by an integer topological index, the so-called Hopf index Q. The three-sphere is topologically equivalent to one-point compactified three-dimensional Euclidean space $\mathbb{R}^3_0$, therefore, for each Hopf map $S^3\to S^2$ there exists a corresponding map $\mathbb{R}^3_0\to S^2$, which we shall call Hopf map, as well, and which has the same Hopf index (due to the metric independence of a topological index). Explicitly, a Hopf map $\mathbb{R}^3_0\to S^2$ may be given by a three-component unit vector field

$$\vec{n}(\vec{r}):\mathbb{R}^3_0\to S^2,\quad \vec{n}^2=1,\quad \lim_{\vec{r}\to\infty}=\vec{n}_0=\text{const}, \tag{A1}$$

where the tip of the unit vector field spans the unit two-sphere, or via stereographic projection

$$\vec{n}=\frac{1}{1+|u|^2}(u+\overline{u},-i(u-\overline{u}),1-u\overline{u}),\quad u=\frac{n_1+in_2}{1+n_3} \tag{A2}$$

by a complex field

$$u(\vec{r}):\mathbb{R}^3_0\to\mathbb{C}_0,\quad \lim_{\vec{r}\to\infty}=u_0=\text{const}, \tag{A3}$$

where our conventions are such that the projection is from the south pole to the equatorial plane of the two-sphere. Further, $\mathbb{C}_0$ is the one-point compactified complex plane. A third possibility to parametrize a Hopf map is by the spherical angles $\phi\in[0,2\pi]$, $\vartheta\in[0,\pi]$, which are related to the unit vector $\vec{n}$ and complex field u via

$$u=\tan\frac{\vartheta}{2}e^{i\phi},\quad \vec{n}=(\sin\vartheta\cos\phi,\sin\vartheta\sin\phi,\cos\vartheta). \tag{A4}$$

The geometry behind the Hopf map may be visualized as follows. The pre-images under the inverse of the Hopf map u of points in the target space S^2 (or, equivalently, $\mathbb{C}_0$) are closed curves in $\mathbb{R}^3_0$ (in general, knots), where each two curves corresponding to two different points in target space are linked exactly Q times. An analytic expression for the Hopf index Q is

$$Q=\frac{1}{16\pi^2}\int d^3r\vec{\mathcal{A}}\cdot\vec{\mathcal{B}}, \tag{A5}$$

where $\vec{\mathcal{B}}$ is the Hopf curvature

$$\vec{\mathcal{B}}=\frac{2}{i}\frac{\nabla u\times\nabla\overline{u}}{(1+u\overline{u})^2}=-\frac{1}{2}\epsilon^{abc}n^a\nabla n^b\times\nabla n^c=-\sin\vartheta\nabla\vartheta\times\nabla\phi \tag{A6}$$

and $\vec{\mathcal{A}}$ is the gauge potential for the "magnetic field" $\vec{\mathcal{B}}$, $\vec{\mathcal{B}}=\nabla\times\vec{\mathcal{A}}$. There is no local expression for $\vec{\mathcal{A}}$ in terms of the Hopf map u alone (however, there certainly exist nonlocal expressions for certain gauges, as is obvious from the analogy with electrodynamics, by choosing, e.g., the Coulomb gauge $\nabla\cdot\vec{\mathcal{A}}=0$ which implies $\vec{\mathcal{A}}=\nabla\times\int d^3r'\Delta^{-1}(\vec{r}-\vec{r}')\vec{\mathcal{B}}(\vec{r}')$).

Geometrically, $\vec{\mathcal{B}}$ is the Hodge dual of the pullback of the area two-form on S^2 under the Hopf map u, i.e.,

$$\mathcal{B}\equiv\mathcal{B}_k dr^k=*\mathcal{F}, \tag{A7}$$

$$\mathcal{F}\equiv\tfrac{1}{2}\mathcal{F}_{jk}dr^j dr^k,\quad \mathcal{B}_k=\varepsilon_{klm}\mathcal{F}_{lm}, \tag{A8}$$

where

$$\mathcal{F} = u^*(\Omega), \quad \Omega = \frac{2}{i}\frac{d\zeta d\bar{\zeta}}{(1+\zeta\bar{\zeta})^2}, \quad \int_{S^2} \Omega = 4\pi. \tag{A9}$$

The second cohomology group of the three-sphere is trivial, $H_2(S^3)=0$, therefore the closed two-form $\mathcal{F}$ must be exact, $\mathcal{F}=d\mathcal{A}$. It follows that the gauge potential $\vec{\mathcal{A}}$ is globally well-defined for appropriately chosen gauges (e.g., in the Couloumb gauge).

The simplest Hopf map with Hopf index 1 is

$$u = i\frac{2(x+iy)}{2z+i(r^2-1)} \tag{A10}$$

(the irrelevant factor i has been introduced to be in exact agreement with the simplest Hopf map of Eq. (12)). Its level curves (i.e., the pre-images of points $u=$const) are circles which lie on tori, and each two different circles are linked precisely once.

There are different ways to construct Hopf maps explicitly. One method which we shall need is to compose a given Hopf map with a map $S^2 \to S^2$,

$$\vec{N}(\vec{n}(\vec{r})):\mathbb{R}^3_0 \xrightarrow{\vec{n}(\vec{r})} S^2 \xrightarrow{\vec{N}(\vec{n})} S^2. \tag{A11}$$

If the Hopf map $\vec{n}(\vec{r})$ has Hopf index Q and the map $\vec{N}(\vec{n})$ has winding number w, then the composition map $\vec{N}(\vec{n}(\vec{r}))$ has Hopf index $Q'=w^2Q$.

A method to construct all possible Hopf maps starts from maps $S^3 \to S^3$ (or, equivalently, maps $\mathbb{R}^3_0 \to S^3$). The third homotopy group of S^3 is nontrivial, $\Pi_3(S^3)=\mathbb{Z}$, therefore such maps are classified by a topological index, the winding number W. It is possible to construct Hopf maps $\mathbb{R}^3_0 \to S^2$ from maps $\mathbb{R}^3_0 \to S^3$ such that the Hopf index equals the winding number. Explicitly a map $\mathbb{R}^3_0 \to S^3$ may be given by a four component unit vector field

$$(e_1(\vec{r}),e_2(\vec{r}),e_3(\vec{r}),e_4(\vec{r})):\mathbb{R}^3_0 \to S^3, \quad e_\alpha e_\alpha = 1, \quad \alpha = 1,\ldots,4 \tag{A12}$$

$$\lim_{\vec{r}\to\infty} e_\alpha = e^0_\alpha = \text{const} \tag{A13}$$

then the corresponding Hopf map is given in terms of u as

$$u = \frac{e_1+ie_2}{e_3+ie_4} \tag{A14}$$

or in terms of $\vec{n}$ as

$$\vec{n} = (2e_1e_3+2e_2e_4, -2e_1e_4+2e_2e_3, e_3^2+e_4^2-e_1^2-e_2^2). \tag{A15}$$

Further, it is now possible to give an explicit, local expression for the gauge potential $\vec{\mathcal{A}}$, in terms of the e_α, as

$$\vec{\mathcal{A}} = \frac{2}{i}[(e_1-ie_2)\,\nabla\,(e_1+ie_2)+(e_3-ie_4)\,\nabla\,(e_3+ie_4)]. \tag{A16}$$

It may be checked without difficulty that indeed $\nabla\times\vec{\mathcal{A}}=\vec{\mathcal{B}}$ where $\vec{\mathcal{B}}$ is the Hopf curvature (A6).

As the group manifold of SU(2) is equivalent to the three-sphere S^3, we may use maps $\mathbb{R}^3_0 \to \mathrm{SU}(2)$ instead. Indeed, with the group element

$$U = e_4 - i\vec{e}\cdot\vec{\sigma} \equiv \exp[-i\rho\vec{k}\cdot\vec{\sigma}], \quad \lim_{\vec{r}\to\infty} U = U_0 = \text{const} \tag{A17}$$

$$e_4 = \cos\rho, \quad \vec{e} = \sin\rho\vec{k}, \quad \vec{k}^2 = 1 \tag{A18}$$

(where $\vec{e}=(e_1,e_2,e_3)$ and $\vec{\sigma}$ are the Pauli matrices) the Hopf map (A15) may be expressed like

$$\vec{n} = \tfrac{1}{2}\mathrm{tr}\sigma_3 U^\dagger \vec{\sigma} U. \tag{A19}$$

This latter representation may be used to produce ansaetze for Hopf maps with cylindrical symmetry from maps $\mathbb{R}^3_0 \to \mathrm{SU}(2)$ with rotational symmetry. Indeed, for

$$\vec{k} = \hat{r} \equiv \vec{r}/r, \quad \rho = \rho(r), \quad \rho(0) = 0, \quad \lim_{r\to\infty} \rho = \pi W, \quad W \in \mathbb{Z} \tag{A20}$$

(the conditions on $\rho(r)$ are to ensure a well-defined U on all $\mathbb{R}^3_0$, and they provide, at the same time, a winding number equal to W for the corresponding map $\mathbb{R}^3_0 \to S^3$ or $\mathbb{R}^3_0 \to \mathrm{SU}(2)$), the resulting group element $U(\rho(r),\hat{r})$ is rotationally invariant in the sense that any rotation in $\mathbb{R}^3_0$ can be compensated by a SU(2) transformation,

$$U(\rho(r),O\hat{r}) \equiv \cos\rho(r) - i\sin(\rho(r)\vec{\sigma}\cdot(O\hat{r}) = V^\dagger U(\rho(r),\hat{r})V, \tag{A21}$$

where O is a rotation matrix acting on $\hat{r}$ and V is the SU(2) matrix corresponding to the rotation O. Within this ansatz, and using spherical polar coordinates $\hat{r}=(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, we get for the complex field u

$$u = \frac{\sin\rho\sin\theta e^{i\varphi}}{\sin\rho\cos\theta + i\cos\rho}, \tag{A22}$$

which has cylindrical symmetry in the sense that any rotation $\varphi \to \varphi+\varphi_0$ can be compensated by a phase transformation $u \to e^{i\varphi_0}u$. Further, u is a Hopf map with Hopf index equal to the winding number W. For technical reasons we prefer to use a u which is multiplied by $-i$ in our main calculation, i.e.,

$$u = -i\frac{e_1+ie_2}{e_3+ie_4} = \frac{\sin\rho\sin\theta}{\sqrt{\sin^2\rho\cos^2\theta+\cos^2\rho}} e^{i\varphi + i\arctan[\tan\rho\cos\theta]}. \tag{A23}$$

With $u=\tan(\vartheta/2)e^{i\phi}$ this leads to

$$\sin\vartheta = 2\sin\rho\sin\theta\sqrt{1-\sin^2\rho\sin^2\theta}, \quad \phi = \varphi + \arctan[\tan\rho\cos\theta]. \tag{A24}$$

Finally, we display the energy densities of the Nicole and AFZ models in the three different parametrizations, $\mathcal{E}_{\mathrm{Ni}}=\mathcal{E}_2^{3/2}$ with

$$\mathcal{E}_2 = |\nabla\vec{n}|^2 \equiv |\nabla_k n^a|^2 = 4\frac{\nabla u\cdot\nabla\overline{u}}{(1+u\overline{u})^2} = (\nabla\vartheta)^2 + \sin^2\vartheta(\nabla\phi)^2 \tag{A25}$$

and $\mathcal{E}_{\mathrm{AFZ}}=\mathcal{E}_4^{3/4}$ with

$$\begin{aligned}\mathcal{E}_4 = \vec{\mathcal{B}}^2 &= \frac{1}{2}((\nabla n^b\cdot\nabla n^b)^2 - (\nabla n^b\cdot\nabla n^c)^2) \\ &= 4\frac{(\nabla u\cdot\nabla\overline{u})^2 - (\nabla u)^2(\nabla\overline{u})^2}{(1+u\overline{u})^4} = \sin^2\vartheta((\nabla\vartheta)^2(\nabla\phi)^2 - (\nabla\vartheta\cdot\nabla\phi)^2).\end{aligned} \tag{A26}$$

APPENDIX B

Proof that

$$(a+b)^{3/2} \geqslant ca^{1/2}b \quad \text{for } a,b \geqslant 0, \quad c \leqslant \sqrt{3}\frac{3}{2}. \tag{B1}$$

By squaring the above expression and subtracting the right-hand side we get

$$a^3 + 3a^2b + 3(1-d^2)ab^2 + b^3 \geqslant 0, \quad d^2 \equiv \frac{c^2}{3} \tag{B2}$$

or, by introducing the variable $x=a/b$,

$$h(x) \equiv x^3 + 3x^2 + 3(1-d^2)x + 1 \geqslant 0 \quad \text{for } x \geqslant 0. \tag{B3}$$

This problem we solve by first calculating the minimum $x_{\min}$ of $h(x)$ for $x \geqslant 0$, and by then requiring that $h(x_{\min})=0$. The minimum is at

$$h'(x) = 3(x^2 + 2x + (1-d^2)) \equiv 0 \Rightarrow x_{\min} = d - 1 \tag{B4}$$

and the condition $h(x_{\min})=0$ finally leads to

$$h(x_{\min}) = d^2(3-2d) \equiv 0 \wedge d \geqslant 1 \Rightarrow d = \tfrac{3}{2} \tag{B5}$$

which implies (B1). QED

Proof that one may cover the unit sphere with l nonintersecting discs with geodesic radius $\vartheta_0 = \pi/4\sqrt{l}$. First we study the case where l is a square, $l=k^2$. We divide the northern hemisphere of the two-sphere into segments by circles which are concentric about the north pole and are given by

$$\vartheta = \frac{m\pi}{2k}, \quad m = 1, \ldots, k. \tag{B6}$$

This divides the northern hemisphere into one disc with geodesic radius $\pi/2k$ about the north pole (on which one geodesic disc with geodesic radius $\vartheta_0 = \pi/4k$ certainly does fit) and into sphere segments such that the boundary circles have a geodesic distance of $\pi/2k$. Therefore discs with geodesic diameter $2\vartheta_0 = \pi/2k$ exactly fit in between. Further, $2m+1$ geodesic discs fit on the segment between the circles at $\vartheta = m\pi/2k$ and at $\vartheta = [(m+1)\pi]/2k$. This is because the central circle of the segment has a circumference which is bigger than the sum of $m+1$ diameters of the geodesic discs, i.e.,

$$2\pi \sin\left(\left(m+\frac{1}{2}\right)\frac{\pi}{2k}\right) \geqslant 2\pi\frac{2}{\pi}\left(\left(m+\frac{1}{2}\right)\frac{\pi}{2k}\right) = (2m+1)\frac{\pi}{k} \geqslant (2m+1)\frac{\pi}{2k}, \tag{B7}$$

where we used

$$\sin x \geqslant \frac{2}{\pi}x \quad \text{for } x \in \left[0, \frac{\pi}{2}\right]. \tag{B8}$$

Finally, summing over all discs on all segments (including the first disc at the segment which is itself a disc) we find

$$\sum_{m=0}^{k-1} (2m+1) = \sum_{m=1}^{k} (2m-1) = k^2, \tag{B9}$$

therefore we may indeed distribute k^2 nonintersecting geodesic discs with geodesic radius $\vartheta_0 = \pi/4k$ on the northern hemisphere.

It remains to study the case where l is not a square. Then we write $l=k^2+j$. We distribute the k^2 discs on the northern hemisphere as just described. Further, we distribute the remaining j discs on the southern hemisphere. This is obviously possible as long as $k^2 \geqslant j$. So we cover all cases except the case $l=3$. This latter case may be proven easily with the help of elementary geometry. QED

Proof that

$$\sin ax \leqslant a \sin x \quad \text{for } a \geqslant 1, \quad x \in \left[0, \frac{\pi}{2}\right]. \tag{B10}$$

We introduce $a \equiv 1+\epsilon$, $\epsilon \geqslant 0$ and write

$$\sin((1+\epsilon)x) = \sin x \cos \epsilon x + \cos x \sin \epsilon x \leqslant \sin x + \epsilon x \cos x \leqslant \sin x + \epsilon \sin x \equiv a \sin x, \tag{B11}$$

where we used $\cos x \leqslant 1$, $\sin x \leqslant x$ for $x \geqslant 0$, and

$$x \cos x \leqslant \sin x \Rightarrow \tan x \geqslant x \quad \text{for } x \in \left[0, \frac{\pi}{2}\right] \tag{B12}$$

which is obviously true. QED

APPENDIX C: ON THE POSSIBILITY OF A LOWER BOUND $C_1 Q^{3/4} \leqslant E_Q$

It may be useful to briefly comment on the problem of deriving a lower bound for the energy of the type $C_1 Q^{3/4} \leqslant E_Q$, analogously to the case of the Faddeev–Niemi model, where this bound can be proven (Vakulenko-Kapitansky bound, see, e.g., Refs. 22–24). In the case of the Faddeev–Niemi model, the first step in the proof is Hoelder's inequality (we use the conventions of Ref. 25, where all inequalities of this appendix can be found; further, we assume that $\vec{\mathcal{A}}$ and $\vec{\mathcal{B}}$ belong to the appropriate Sobolev spaces such that all integrals below exist)

$$16\pi^2 Q \equiv \int d^3r \vec{\mathcal{A}} \cdot \vec{\mathcal{B}} \leqslant \left(\int d^3r |\vec{\mathcal{A}}|^p\right)^{1/p} \left(\int d^3r |\vec{\mathcal{B}}|^q\right)^{1/q} \tag{C1}$$

$$\frac{1}{p} + \frac{1}{q} = 1. \tag{C2}$$

For the Faddeev–Niemi model one has to choose $p=6$, $q=\frac{6}{5}$ and may estimate the first term with the help of the Gagliardo-Nirenberg-Sobolev (GNS) inequality,

$$\left(\int d^3r |\vec{\mathcal{A}}|^6\right)^{1/6} \leqslant c \left(\int d^3r |\nabla |\vec{\mathcal{A}}||^2\right)^{1/2} \tag{C3}$$

(here and below c is an unspecified constant) and, when the Couloumb gauge condition $\nabla \cdot \vec{\mathcal{A}} = 0$ is imposed, the integrand can be reexpressed like

$$|\nabla |\vec{\mathcal{A}}||^2 \leqslant c \left|\sum_{jk} \partial_j \mathcal{A}_k\right|^2 = c(|\nabla \times \vec{\mathcal{A}}|^2 + \nabla \cdot \vec{\Lambda}), \tag{C4}$$

where

$$\Lambda_1 = (\mathcal{A}_2 \partial_2 + \mathcal{A}_3 \partial_3)\mathcal{A}_1 - \mathcal{A}_1(\partial_2 \mathcal{A}_2 + \partial_3 \mathcal{A}_3) \tag{C5}$$

and Λ_2, Λ_3 follow by permutation. Therefore, the integrand is the sum of $\vec{\mathcal{B}}^2$ and a total divergence which does not contribute to the integral (for $\vec{\mathcal{A}}$ which decay sufficiently fast in the limit $|\vec{r}| \to \infty$; this is automatically satisfied by the class of $\vec{\mathcal{A}}$ we consider). The proof continues with the interpolation inequality

$$\left(\int d^3r|\vec{\mathcal{B}}|^{6/5}\right)^{5/6} \leqslant \left(\int d^3r|\vec{\mathcal{B}}|\right)^{2/3}\left(\int d^3r|\vec{\mathcal{B}}|^2\right)^{1/6} \tag{C6}$$

for the second term. This leads to

$$16\pi^2 Q \leqslant c\left(\int d^3r|\vec{\mathcal{B}}|^2\right)^{2/3}\left(\int d^3r|\vec{\mathcal{B}}|\right)^{2/3} \tag{C7}$$

and, together with $|\vec{\mathcal{B}}|^2=\mathcal{E}_4$ and $|\vec{\mathcal{B}}|\leqslant(1/\sqrt{2})\mathcal{E}_2$, to

$$16\pi^2 Q \leqslant c\lambda^{-2/3}\left[\left(\lambda\int d^3r\mathcal{E}_4\right)^{1/2}\left(\int d^3r\mathcal{E}_2\right)^{1/2}\right]^{4/3} \leqslant c\lambda^{-2/3}\left[\lambda\int d^3r\mathcal{E}_4+\int d^3r\mathcal{E}_2\right]^{4/3}, \tag{C8}$$

where we used Cauchy's inequality in the last step. The Vakulenko–Kapitansky bound follows immediately by taking the above inequality to the power $\frac{3}{4}$.

Now let us point out where the analogous proof fails for the AFZ and Nicole models. One again starts with Hoelder's inequality (C1), but now one would have to choose $p=3$ and $q=\frac{3}{2}$. With the GNS inequality one can again estimate the first term

$$\left(\int d^3r|\vec{\mathcal{A}}|^3\right)^{1/3} \leqslant c\left(\int d^3r|\nabla|\vec{\mathcal{A}}||^{3/2}\right)^{2/3} \tag{C9}$$

but now the integrand is

$$|\nabla|\vec{\mathcal{A}}||^{3/2} \leqslant c\left|\sum_{jk}\partial_j\mathcal{A}_k\right|^{3/2} = c(|\nabla\times\vec{\mathcal{A}}|^2+\nabla\cdot\vec{\Lambda})^{3/4} \tag{C10}$$

and therefore no longer a total derivative, and we cannot express the integrand in terms of the Hopf curvature alone. We have not been able to overcome this difficulty. For our main results, however, the upper bound is more important, which shows that for sufficiently high Hopf index our solutions of Sec. II cannot be true minimizers of the energy.

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The two-loop massless $(\lambda/4!)\varphi^4$ model in nontranslational invariant domain

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We study the $(\lambda/4!)\varphi^4$ massless scalar field theory in a four-dimensional Euclidean space, where all but one of the coordinates are unbounded. We are considering Dirichlet boundary conditions in two hyperplanes, breaking the translation invariance of the system. We show how to implement the perturbative renormalization up to two-loop level of the theory. First, analyzing the full two and four-point functions at the one-loop level, we show that the bulk counterterms are sufficient to render the theory finite. Meanwhile, at the two-loop level, we must also introduce surface counterterms in the bare Lagrangian in order to make finite the full two and also four-point Schwinger functions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this paper we are interested to show how to implement the renormalization procedure up to two-loop level in the massless $(\lambda/4!)\varphi^4$ scalar field theory, defined in a four-dimensional Euclidean space with one compactified dimension. Our aim is to shed light on the renormalization procedure in a system defined in a domain where translational symmetry is broken, which must be done, for example, in the high temperature dimensional reduced quantum chromodynamics (QCD), defined in a finite region.

Quantum chromodynamics is a non-Abelian Yang-Mills theory with gauge group SU(3). Since it is assumed that the fermions of the theory transform according to the fundamental representation of the gauge group, each flavor of quark is a triplet of the color group SU(3). Gauge bosons transform according to the adjoint representation. The interaction between the quarks is mediated by the gluons. Due to the non-Abelian structure of the theory, the gluons couple not only with the quarks but have also cubic and quartic self-interaction. The self-interaction of the gluons provides the antiscreening of the color charge in QCD. This is responsible for asymptotic freedom and presumably confinement.

The confinement-deconfinement phase transition in QCD may occur in usual matter at sufficiently high temperature or if it is strongly compressed.[1–3] In ultrarelativistic heavy ion collisions, we expect that the plasma of quarks and gluons can be produced. We would like to stress that, although nonequilibrium processes occur in the quark-gluon plasma in the heavy ion collisions, for

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simplicity in a first approximation we can assume a static situation. Just after the collision hot and compressed nuclear matter is confined in a small region of the space and in such circumstances the volume and surface effects become very important.

In the above described physical situation there are two important points: the first one is that the thermodynamic limit of the infinite volume system cannot be used and therefore finite volume effects should be investigated and taken into account. The second point is that the quark-gluon plasma exists in a situation of high temperature, where using the Matsubara formalism to describe high temperature QCD, dimensional reduction must occur.[4–7] Dimensional reduction is based on the Appelquist-Carrazone decoupling theorem.[8] From a more fundamental theory, the effective Lagrangian density of this theory can be obtained as some low-energy limit of the fundamental theory where the heavy modes have been removed. There are some interesting physical situations where the decoupling theorem can be used. First, for scalar fields without spontaneous symmetry breaking. Second, in quantum electrodynamics, where a derivative expansion of the photon effective action can be obtained by integrating out the fermionic fields. Also in QCD at least in lowest order in perturbation theory the decoupling theorem works. The decoupling theorem is not valid, for example, in spontaneous broken gauge theories. It is important to stress that the nonvalidity of the decoupling theorem means that low-energy experiments can provide information about the high energy physics.

Going back to the heavy-ions collision situation, we can assume that the following scenario appears: in the situation where dimensional reduction occurs, we have an effective theory for the gluons field and also finite size effects for these bosonic fields. To shed light on the renormalization procedure in systems defined in domain where translational symmetry is broken, as for example, the high temperature dimensional reduced QCD, in this paper we are interested to investigate scalar models, impose classical boundary condition over the fields. We hope that this study will give us some insight over the most interesting and also more complicated situation as the one mentioned above. Therefore, in this paper we analyze how to implement the perturbative renormalization up to two-loop level of $(\lambda/4!)\varphi^4$ massless scalar field model defined in a four-dimensional Euclidean space with one compactified dimension.

Finite size effects and the presence of macroscopic structures in different field theory models have been extensively studied in the literature. The critical behavior of the O(N) model in the presence of a surface was a target of intense investigations.[9] The same O(N) model was studied in two different geometries: the periodic cube and the cylinder along one dimension (the time) and finite and periodic in the $(d-1)$ remaining dimensions by Brezin and Zinn-Justin.[10] Finite size effects in QCD[11] and also in different field theory models have also been extensively studied in the literature. Assuming periodic or antiperiodic boundary conditions for bosonic and fermionic models, respectively, the translation symmetry is maintained, and surface effects are avoided. Therefore, to avoid surface effects, quantum fields defined in manifolds with periodic or anti-periodic boundary conditions in the spatial section were preferred by many authors.[12] Nevertheless, the case of boundaries conditions that break the translational symmetry deserves our attention.

In the case of hard boundary conditions as, for example, Dirichlet-Dirichlet (DD) or Neumann-Neumann (NN), the translational invariance is lacking. This fact makes the Feynman diagrams harder to compute than in an unbounded space. Moreover the renormalization program is implemented in a different way from unbounded or translational invariance systems since some surface divergence appears.[13] For translational invariant systems, one can use the momentum space representation, which is a more convenient framework to analyze the ultraviolet divergences of a theory. Translational invariance is preserved for momentum conservation conditions. For nontranslational invariant systems a more convenient representation for the n-point Schwinger functions is a mixed momentum coordinate space.

Fosco and Svaiter considered the anisotropic scalar model in a d-dimensional Euclidean space, where all but one of the coordinates are unbounded. Translational invariance along the bounded coordinate which lies in the interval $[0,L]$ is broken because the choice of boundary condition chosen for the hyperplanes at $z=0$ and $z=L$. Two different possibilities of boundary conditions were considered: (DD) and also (NN), and the renormalization of the two-point func-

tion was achieved in the one-loop approximation.[14] Further, the renormalization of the four-point function was achieved in the one-loop approximation by Caicedo and Svaiter.[15] Finally Svaiter[16] studied the renormalization of the $(\lambda/4!)\varphi^4$ massless scalar field model in the one-loop approximation in finite size systems assuming that the system is in thermal equilibrium with a reservoir. Also, still studying surface, edge, and corners effects, Rodrigues and Svaiter[17] analyzed first the renormalized vacuum fluctuations associated with a massless real scalar field, confined in the interior or a rectangular infinitely long waveguide. A closed form of the analytic continuation of the local zeta function in the interior of the waveguide was obtained and a detailed study of the surface and edge divergences was presented. Next, these authors[18] studied the renormalized stress tensor associated with an electromagnetic field in the interior of a rectangular infinitely long waveguide.

In this paper we will consider an interacting massless scalar model, in a four-dimensional Euclidean space, where the first three coordinates are unbounded and the last one lies in the interval $[0,L]$. We analyze only DD boundary conditions. First, we present an algebraic expression in coordinate space for the free propagator which let us identify the divergences of the *n*-point Schwinger functions for the interacting theory. This algebraic expression agrees with the result obtained by Lukosz.[19] We would like to stress that instead of assuming hard boundary conditions, some authors assumed soft boundary conditions and also treated the boundary as a quantum mechanical object.[20] Here, we prefer to keep hard classical boundary conditions.

The organization of the paper is as follows: In Sec. II we discuss the slab configurations, obtaining some important expressions for the free propagator in order to understand some procedures in the divergence identification. In Sec. III the regularization program is implemented in the one-loop approximation. In Sec. IV the regularization program is implemented in the two-loop approximation. Section V contains our conclusions. In the Appendix, an expression for the free propagator is introduced. Throughout this paper we use $\hbar=c=1$.

II. CLASSICAL BOUNDARY CONDITIONS AND SOME PROPERTIES OF THE FREE PROPAGATOR

Let us consider a neutral scalar field with a $(\lambda\varphi^4)$ self-interaction, defined in a *d*-dimensional Minkowski space-time. The vacuum persistence functional is the generating functional of all vacuum expectation value of time-ordered products of the theory. The Euclidean field theory can be obtained by analytic continuation to imaginary time allowed by the positive energy condition for the relativistic field theory. In the Euclidean field theory, we have the Euclidean counterpart for the vacuum persistence functional, that is, the generating functional of complete Schwinger functions. The $(\lambda\varphi^4)_d$ Euclidean theory is defined by these Euclidean Green's functions. The Euclidean generating functional $Z(h)$ is formally defined by the following functional integral:

$$Z(h)=\int [\mathrm{d}\varphi]\exp\left(-S_0-S_I+\int d^dx h(x)\varphi(x)\right), \tag{1}$$

where the action that describes a free scalar field is

$$S_0(\varphi)=\int d^dx\left(\frac{1}{2}(\partial\varphi)^2+\frac{1}{2}m_0^2\varphi^2(x)\right), \tag{2}$$

and the interacting part, defined by the non-Gaussian contribution, is

$$S_I(\varphi)=\int d^dx\frac{\lambda}{4!}\varphi^4(x). \tag{3}$$

In Eq. (1), $|\mathrm{d}\varphi|$ is a translational invariant measure, formally given by $|\mathrm{d}\varphi|=\Pi_x \mathrm{d}\varphi(x)$. The terms λ and m_0^2 are, respectively, the bare coupling constant and mass squared of the model.

Finally, $h(x)$ is a smooth function that we introduce to generate the Schwinger functions of the theory by means of functional derivatives. Note that we are using the same notation for functionals and functions, for example, $Z(h)$ instead of the usual notation $Z[h]$.

In the weak-coupling perturbative expansion, we perform a formal perturbative expansion with respect to the non-Gaussian terms of the action. As a consequence of this formal expansion, all the n-point unrenormalized Schwinger functions are expressed in a power series of the bare coupling constant g_0. Let us summarize how to perform the weak-coupling perturbative expansion in the $(\lambda\varphi^4)_d$ theory. The Gaussian functional integral $Z_0(h)$ associated with the Euclidean generating functional $Z(h)$ is

$$Z_0(h) = \mathcal{N} \int [\mathrm{d}\varphi] \exp\left(-\frac{1}{2}\varphi K \varphi + h\varphi\right). \tag{4}$$

We are using a compact notation and the first term on the right-hand side of Eq. (4) is given by

$$\varphi K \varphi = \int d^d x \int d^d y \varphi(x) K(m_0; x, y) \varphi(y). \tag{5}$$

The term that couples linearly the field with the external source is

$$h\varphi = \int d^d x \varphi(x) h(x). \tag{6}$$

As usual $\mathcal{N}$ is a normalization factor and the symmetric kernel $K(m_0; x, y)$ is defined by

$$K(m_0; x, y) = (-\Delta + m_0^2)\delta^d(x - y), \tag{7}$$

where Δ denotes the Laplacian in the Euclidean space R^d. As usual, the normalization factor is defined using the condition $Z_0(h)|_{h=0} = 1$. Therefore $\mathcal{N} = (\det(-\Delta + m_0^2))^{1/2}$ but, in the following, we are absorbing this normalization factor in the functional measure. It is convenient to introduce the inverse kernel, i.e., the free two-point Schwinger function $G_0(m_0; x-y)$ which satisfies the identity

$$\int d^d z G_0(m_0; x - z) K(m_0; z - y) = \delta^d(x - y). \tag{8}$$

Since Eq. (4) is a Gaussian functional integral, simple manipulations, performing only Gaussian integrals, gives

$$\int [\mathrm{d}\varphi] e^{-S_0 + \int d^d x h(x)\varphi(x)} = \exp\left[\frac{1}{2}\int d^d x \int d^d y h(x) G_0^{(2)}(m_0; x - y) h(y)\right]. \tag{9}$$

Therefore, we have an expression for $Z_0(h)$ in terms of the inverse kernel $G_0^{(2)}(m_0; x-y)$, i.e., in terms of the free two-point Schwinger function. This construction is fundamental to perform the weak-coupling perturbative expansion with the Feynman diagramatic representation of the perturbative series. The non-Gaussian contribution in a perturbation with regard to the remaining terms of the action. It is important to point out that the weak-coupling perturbative expansion can be defined in arbitrary geometries, and classical boundary conditions must be implemented in the two-point Schwinger function. Another way is to restrict the space of functions that appear in the functional integral.

We are interested in studying finite size systems, where the translational invariance is broken. In this situation, we are analyzing the perturbative renormalization for the $(\lambda/4!)\varphi^4$ massless scalar field model, in the two-loop approximation. Therefore, let us assume boundary conditions over the plates for the massless field $\varphi(x)$. For simplicity we are assuming Dirichlet-Dirichlet boundary conditions, i.e.,

$$\varphi(\vec{r},z)\big|_{z=0} = \varphi(\vec{r},z)\big|_{z=L} = 0, \tag{10}$$

for the free field. Since the translational invariance is not preserved, let us use a Fourier expansion of the fields in the following form:

$$\varphi(\vec{r},z) = \frac{1}{(2\pi)^{(d-1)/2}} \int d^{d-1}p \sum_n \phi_n(\vec{p}) e^{i\vec{p},\vec{r}} u_n(z), \tag{11}$$

where the set $u_n(z)$ are the orthonormalized eigenfunctions associated to the operator $-d^2/\mathrm{d}z^2$, $[-d/\mathrm{d}z^2 u_n(z) = k_n^2 u_n(z)]$, and $k_n = n\pi/L$, $n = 1,2,\ldots$. The orthonormal set corresponding to the eigenfunctions of the Hermitian operator $-d^2/\mathrm{d}z^2$ defined on a finite interval is given by

$$u_n(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi z}{L}\right), \; n = 1,2,\ldots \; . \tag{12}$$

These eigenfunctions satisfy the completeness and orthonormality relations, i.e.,

$$\sum_n u_n(z) u_n^*(z') = \delta(z - z') \tag{13}$$

and

$$\int_0^L \mathrm{d}z \, u_n(z) u_{n'}^*(z) = \delta_{n,n'}. \tag{14}$$

Since we are interested in performing the weak coupling expansion, let us first write the free two-point Schwinger function. This free two-point Schwinger function can be expressed in the following form:

$$G_0^{(2)}(\vec{r},z,z') = \frac{1}{(2\pi)^{d-1}} \int d^{d-1}p \sum_n e^{i\vec{p}.\vec{r}} u_n(z) u_n^*(z') G_{0,n}(\vec{p}), \tag{15}$$

where $G_{0,n}(\vec{p})$ is given by

$$G_{0,n}(\vec{p}) = (\vec{p}^2 + k_n^2 + m^2)^{-1}. \tag{16}$$

Next, we will present some properties of the two-point free Schwinger function in order to understand the behavior of the interacting field theory in the presence of macroscopic structures. Therefore, in order to understand some procedures used in the identification of the divergences in the Schwinger functions that will appear in the next section, let us analyze some properties of the free two-point Schwinger function. Substituting Eq. (12) and Eq. (16) in Eq. (15) we get that the free propagator $G_0^{(2)}(\vec{r}_1 - \vec{r}_2, z_1, z_2)$ can be written as

$$G_0^{(2)}(\vec{r}_1 - \vec{r}_2, z_1, z_2) = \frac{2}{L} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi z_1}{L}\right) \sin\left(\frac{n\pi z_2}{L}\right) \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \frac{e^{i\vec{p}.(\vec{r}_1 - \vec{r}_2)}}{\left(\vec{p}^2 + \left(\frac{n\pi}{L}\right)^2 + m^2\right)}. \tag{17}$$

The next step is to show that the two-point free Schwinger function can be written in terms of the variables: r_{12}, z_{12}^- and finally z_{12}^+, where $r_{12} = (|\vec{r}_1 - \vec{r}_2|)/L$, $z_{12}^- = (z_1 - z_2)/L$, and $z_{12}^+ = (z_1 + z_2)/L$, respectively. Working in the four-dimensional case and also in the massless situation, a straightforward calculation (see the Appendix) gives us that $G_0^{(2)}(\vec{r}_1 - \vec{r}_2, z_1, z_2)$ can be written as

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{1}{16\pi^2L^2}\sum_{k=-\infty}^{\infty}\left\{\frac{1}{\left(k-\frac{|z_{12}^-|}{2}\right)^2+\left(\frac{r_{12}}{2}\right)^2}-\frac{1}{\left(k-\frac{|z_{12}^+|}{2}\right)^2+\left(\frac{r_{12}}{2}\right)^2}\right\}. \tag{18}$$

The former expression for the two-point Schwinger function was obtained also by Lukosz[19] using the image method. Performing the summations in Eq. (18) (see the Appendix), it is possible to find a closed expression for $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$. We get

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{\sinh(\pi r_{12})}{16\pi L^2 r_{12}}\left\{\frac{\sin\left(\frac{\pi z_1}{L}\right)\sin\left(\frac{\pi z_2}{L}\right)}{\left[\sinh^2\left(\frac{\pi r_{12}}{2}\right)+\sin^2\left(\frac{\pi z_{12}^-}{2}\right)\right]\left[\sinh^2\left(\frac{\pi r_{12}}{2}\right)+\sin^2\left(\frac{\pi z_{12}^+}{2}\right)\right]}\right\}. \tag{19}$$

It is not difficult to show that the two-point Schwinger function $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$ satisfies the following properties:

(i) The free two-point Schwinger function is not negative, i.e., $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)\geqslant 0$, for $z_1,z_2\in[0,L]$ and $\vec{r}_1$, $\vec{r}_2\in\mathcal{R}^3$, since we are working in a Euclidean space.

(ii) The free two-point Schwinger function is zero when one of its points are evaluated on the boundaries

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,0,z_2)=G_0^{(2)}(\vec{r}_1-\vec{r}_2,L,z_2)=G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,0)=G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,L)=0,$$

since we are assuming Dirichlet boundary conditions.

(iii) The free two-point Schwinger function contain the usual bulk divergences, i.e., when $(\vec{r}_1,z_1)=(\vec{r}_2,z_2)$, it is singular. From Eq. (18) we can identify three singular terms. Splitting the free two-point Schwinger function in the singular and regular terms we have

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{1}{4\pi^2L^2}\left\{\frac{1}{(z_{12}^-)^2+r_{12}^2}-\frac{1}{(z_{12}^+)^2+r_{12}^2}-\frac{1}{(2-z_{12}^+)^2+r_{12}^2}\right\}$$

$$+\frac{1}{4\pi^2L^2}\left\{\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}\frac{1}{(2k-|z_{12}^-|)^2+r_{12}^2}-\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}\frac{1}{(2k-|z_{12}^+|)^2+r_{12}^2}\right\}. \tag{20}$$

The first term on the right-side of the last equation, is singular only when $\vec{r}_1=\vec{r}_2$ and $z_1=z_2$. This is the term that carries the usual bulk divergences. The second term is singular only when $z_1=z_2=0$ and $\vec{r}_1=\vec{r}_2$. The third term is singular only when $z_1=z_2=L$ and $\vec{r}_1=\vec{r}_2$. These two terms mentioned previously carries surface divergences. Finally the two last terms do not have singularities.

(iv) When $|\vec{r}_1-\vec{r}_2|/L\gg 1$ the free propagator behaves like

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)\sim\frac{1}{2\pi L^2}\frac{e^{-\pi r_{12}}}{r_{12}}\sin\left(\frac{\pi z_1}{L}\right)\sin\left(\frac{\pi z_2}{L}\right), \tag{21}$$

which shows an exponential convergence behavior.

(v) The integral of the variable $\{\vec{r},z\}$ on a neighborhood around $\{\vec{r}',z'\}$ of the free propagator is finite, i.e., $\int_R d^3r\,\mathrm{d}_z\,G_0^{(2)}(\vec{r}-\vec{r}',z,z')<\infty$. See Fig. 1.

Property (v) allows us to show that the external legs of the Feynman diagrams do not create divergences. Let us suppose we have the integral corresponding to some Feynman diagram,

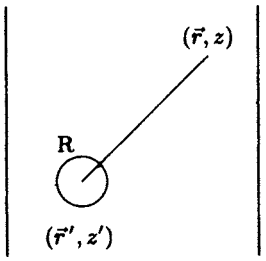

FIG. 1. The integral of the variable $\{\vec{r},z\}$ on a neighborhood around $\{\vec{r}';z'\}$.

$$\int_R d^3r\, \mathrm{dz}\, G_0^{(2)}(\vec{r}-\vec{r}',z,z')F(\vec{r}',z'), \tag{22}$$

where $G_0^{(2)}(\vec{r}-\vec{r}',z,z')$ is some external leg and $F(\vec{r}',z')$ describes the remainder part of the diagram. Now in order to proceed we must use the following statement: for two continuous and positives functions $f(\vec{x})$ and $g(\vec{x})$ defined in a finite region R with the exception of the point $\vec{x}_1$ where $f(\vec{x})$ diverges, then the integral $I=\int_R d^dx f(\vec{x})g(\vec{x})$ is finite, if and only if $I'=\int_V d^dx f(\vec{x})$ is finite on some neighborhoods V of the point $\vec{x}_1$. With the property (v) and the statement before we can see that external legs from the Feynman diagrams do not generate divergences.

III. REGULARIZED TWO- AND FOUR-POINT SCHWINGER FUNCTIONS AT ONE-LOOP ORDER

In this section we identify the divergent contribution in the two- and four-point Schwinger function at one-loop level. Essentially we use Eq. (20) in the 1PI diagrams of the Green functions considering their external legs, and the integrations in the coordinate space. We write Eq. (20) as

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{1}{4\pi^2L^2}\left[\frac{1}{(z_{12}^-)^2+r_{12}^2}-\frac{1}{(z_{12}^+)^2+r_{12}^2}-\frac{1}{(2-z_{12}^+)^2+r_{12}^2}+h(r_{12},z_1,z_2)\right], \tag{23}$$

where $h(r_{12},z_1,z_2)$ is given by

$$h(r_{12},z_1,z_2)=\frac{1}{4}\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}\frac{1}{\left(k-\frac{|z_{12}^-|}{2}\right)^2+\left(\frac{r_{12}2}{2}\right)}-\frac{1}{4}\sum_{\substack{k=-\infty\\k\neq 0,1}}^{\infty}\frac{1}{\left(k-\frac{z_{12}^+}{2}\right)^2+\left(\frac{r_{12}2}{2}\right)}. \tag{24}$$

From the property (iii) we see that the three first contributions on the right-hand side of Eq. (23) have singularities. Otherwise, the last term is finite in the whole domain where we defined the model. After this brief introduction, we are able to study the interacting theory. Let us start analyzing the tadpole diagram, displayed in Fig. 2, from which we can write the expression for the

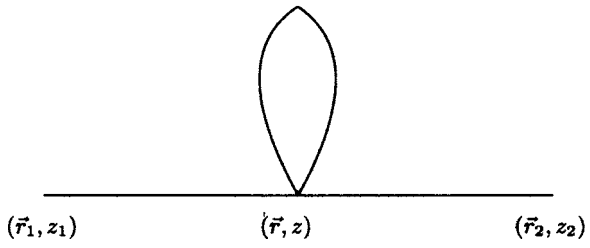

FIG. 2. The two-point function at one-loop level.

one-loop two-point Schwinger function $G_1^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$. We have that

$$G_1^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{\lambda}{2}\int d^3r\,\mathrm{d}z\,G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(0,z,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z). \tag{25}$$

In the following we are generalizing the results obtained by Fosco and Svaiter.[14] Let us begin studying the quantity $G_0^{(2)}(0,z,z)$ that appears in the tadpole defined in Eq. (25). From Eq. (20) we get that $G_0^{(2)}(0,z,z)$ can be written as

$$G_0^{(2)}=(0,z,z)=\frac{1}{4\pi^2L^2}\left[A-\frac{1}{(2z/L)^2}-\frac{1}{(2-2z/L)^2}+\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}\frac{1}{(2k)^2}-\sum_{\substack{k=-\infty\\k\neq 0,1}}^{\infty}\frac{1}{(2k-2z/L)^2}\right], \tag{26}$$

where A is given by

$$A=\lim_{(z_1,\vec{r}_1)\to(z_2,\vec{r}_2)}\frac{L^2}{(z_1-z_2)^2+|\vec{r}_1-\vec{r}_2|^2}$$

$$=\lim_{\Lambda\to\infty}\frac{L^2S_4}{8\pi^2}\Lambda^2, \tag{27}$$

$S_d=[2\pi^{d/2}/\Gamma(d/2)]$ and Λ is an ultraviolet cutoff. In the same way, from Eq. (26) by performing the summations, we-get for $G_0^{(2)}(0,z,z)$,

$$G_0^{(2)}(0,z,z)=\frac{1}{4\pi^2L^2}\left[A+\frac{\pi^2}{12}-\frac{\pi^2}{4}\frac{1}{\sin^2(\pi z/L)}\right]. \tag{28}$$

Substituting Eq. (27) in Eq. (28) we obtain

$$G_0^{(2)}(0,z,z)=\lim_{\Lambda\to\infty}\frac{S_4}{32\pi^4}\Lambda^2+\frac{1}{48L^2}-\frac{1}{16L^2}\frac{1}{\sin^2(\pi z/L)}. \tag{29}$$

The first term in Eq. (29) is a bulk divergence. Substituting Eq. (29) in Eq. (25) we get

$$\begin{aligned}G_1^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=&\lim_{\Lambda\to\infty}\frac{\lambda S_4}{64\pi^4}\Lambda^2\int_R d^3r\,\mathrm{d}z\,G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)\\&+\frac{\lambda}{96L^2}\int_R d^3r\,\mathrm{d}z\,G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)\\&-\frac{\lambda}{32L^2}\int_R d^3r\,\mathrm{d}z\frac{G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)}{\sin^2(\pi z/L)}\end{aligned} \tag{30}$$

The first term on the right-hand side carries a bulk divergence. The second term is finite. To see this we analyze the integral by sectors. Therefore we have

$$\int_R d^3r\,\mathrm{d}z\,G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)=\int_{R_1}+\int_{R_2}+\int_{R_3}+\int_{R_4}+\int_{R_5}, \tag{31}$$

where each integral is defined in different regions displayed in Fig. 3, where the points $(\vec{r}_1,z_1)$ and $(\vec{r}_2,z_2)$ are the centers of the regions R_1 and R_2, respectively. Using the property (v) we have that the integrals on R_1 and R_2 are finite. Since the free propagators $G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)$ and $G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)$ presented in Eq. (31) do not have divergences on R_3 and this region is compact, then the integral on R_3 is finite. The integrals defined in regions R_4 and R_5 also are finite since from the property (iv) the propagator decreases exponentially when one of its points becomes far from the

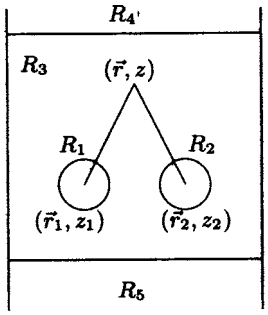

FIG. 3. Regions of integration R_i.

other. Thus the integral defined by Eq. (31) is finite. Finally we must study the third integral on the right-hand side of Eq. (30). Note that the term $1/\sin^2(\pi z/L)$ diverges when z is evaluated on the boundaries.

Nevertheless this integral is convergent, because the products of $G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)$ and $G_0^{(2)}\times(\vec{r}_2-\vec{r},z_2,z)$ take away the divergence. Using Eq. (19), we have that the third integral on the right-hand side of Eq. (30) is finite. Therefore the one-loop two-point Schwinger function only has bulk divergence.

Our next step is to analyze the four-point Schwinger function in the one-loop level (see Fig. 4). Since the free propagator only has singularities when its two points are equal or also when the two points joined are evaluated at the boundaries, we continue our analysis of the integrals only in the domains where the two external points of the free propagators take the same values. The complete four-point function at one-loop level is given by

$$G_1^{(4)}(\vec{r}_1,z_1,\vec{r}_2,z_2,\vec{r}_3,z_3,\vec{r}_4,z_4)=\frac{\lambda^2}{2}\int d^{d-1}r\int d^{d-1}r'\int_0^L \mathrm{d}z\int_0^L \mathrm{d}z'\; G_0^{(2)}(\vec{r}_1-\vec{r},z_1,z)G_0^{(2)}(\vec{r}_2-\vec{r},z_2,z)$$
$$\times\left[G_0^{(2)}(\vec{r}-\vec{r}',z,z')\right]^2 G_0^{(2)}(\vec{r}_3-\vec{r}',z_3,z')G_0^{(2)}(\vec{r}_4-\vec{r}',z_4,z'). \qquad (32)$$

For simplicity, in Fig. 5 we define three different regions between the boundaries. The first one, R_1 is concerned when $\{\vec{r}',z'\}$ is close to $\{\vec{r},z\}$. In this region the contribution coming from $[G_0^{(2)}(\vec{r}-\vec{r}',z,z')]^2$ is singular. Nevertheless, we still must analyze if this divergent behavior will appear in the integral defined by Eq. (32). We will show that the singularities will appear only as bulk divergences. In the region R_2 ($z,z'\to 0$ and $\vec{r}'\to\vec{r}$) the term $[G_0^{(2)}(\vec{r}-\vec{r}',z,z')]^2$ is also divergent. As we will see, this divergent behavior disappears when we compute the complete four-point function at one-loop order, defined by Eq. (32). In the region R_3 ($z,z'\to L$ and $\vec{r}'\to\vec{r}$) the situation is identical as in the region R_2. Using the same argument that we used before to analyze the convergence of the integral denned by Eq. (22), we can study the convergence of the integral defined by Eq. (32) with the amputated external legs. Therefore we must study Eq. (32) with the external legs amputated. Therefore we must study the quantity $\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'[G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2$. Substituting Eq. (23) in the former equation we get

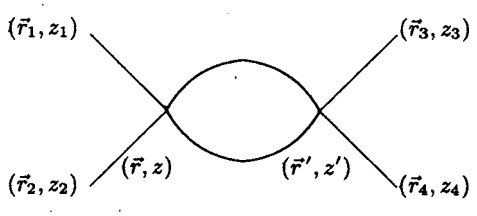

FIG. 4. The four-point function at one loop.

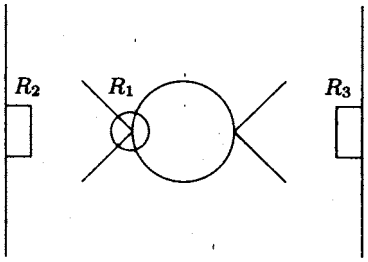

FIG. 5. Regions of integration for the four-point function.

$$\int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[G_0^{(2)}(\vec{r}'-\vec{r},z',z)\right]^2 = \frac{1}{(4\pi^2L^2)^2}\left(I_1+I_2+I_3+I_4+I_5\right) + \text{finite part}, \tag{33}$$

where the integrals $I_i, i=1,2,\ldots,$ are given by

$$I_1 = \int d^3r'\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{1}{\left[(z_{12}^-)^2+r_{12}^2\right]^2}, \tag{34}$$

$$I_2 = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[-\frac{1}{\left[(z_{12}^+)^2+r_{12}^2\right]^2} + \frac{1}{\left[(2-z_{12}^+)^2+r_{12}^2\right]^2}\right], \tag{35}$$

$$I_3 = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[-\frac{2}{\left[(z_{12}^-)^2+r_{12}^2\right]\left[(z_{12}^+)^2+r_{12}^2\right]} - \frac{2}{\left[(z_{12}^-)^2+r_{12}^2\right]\left[(2-z_{12}^+)^2+r_{12}^2\right]}\right] \tag{36}$$

$$I_4 = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{2}{\left[(z_{12}^+)^2+r_{12}^2\right]\left[(2-z_{12}^+)^2+r_{12}^2\right]}, \tag{37}$$

$$I_5 = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[\frac{1}{(z_{12}^-)^2+r_{12}^2} - \frac{1}{(z_{12}^+)^2+r_{12}^2} - \frac{1}{(2-z_{12}^+)+r_{12}^2}\right] h(r_{12},z_1,z_2). \tag{38}$$

Let us investigate each term of Eq. (33). The integral I_1 must be analyzed only in the region R_1. For this purpose we need an auxiliary result. We can prove that a continuous and positive function $f(x)$ which does not have singularities except for $x=0$, and $M=\int_{-\vec{\epsilon}}^{\vec{\epsilon}} d^dx f(w^2)$ where $w^2=|\vec{w}|^2$, then there exist ϵ' such that $M=S_d\int_0^{\epsilon'} \mathrm{d}w\, w^{d-1} f(w^2)$ where $\epsilon<\epsilon'<\sqrt{d}\epsilon$. Then we get

$$I_1 = \int_{R_1} d^3r'\, \mathrm{d}z' \frac{1}{[(z_{12}^-)^2+r_{12}^2]^2} = \int_{\vec{r}-\vec{\epsilon}}^{\vec{r}+\vec{\epsilon}} d^3r' \int_{z-\epsilon}^{z+\epsilon} \mathrm{d}z' \frac{1}{[(z-z')^2+|\vec{r}-\vec{r}'|^2]^2}$$

$$= \int_{-\vec{\epsilon}}^{\vec{\epsilon}} \frac{d^4w}{w^4} = S_4 \int_0^{\epsilon'} \mathrm{d}w \frac{w^3}{w^4} = S_4 \ln w \Big|_0^{\epsilon'}. \tag{39}$$

Therefore I_1 contributes with a bulk divergence of the type as the one that appears in the theory without boundaries. In the usual renormalization procedure, the contribution coming from I_1 can be eliminated by the usual counterterms. Concerning the contribution coming from I_2 we have that the first term $1/[(z_{12}^+)^2+r_{12}^2]^2$ is not singular in the region R_1. In the region R_2, using the same auxiliary result that we used before, we can obtain an upper bound to the contribution coming from this term. We get

$$\int_{R_2} d^3r\, dz\, d^3r\, dz' \frac{1}{[(z+z')^2+|\vec{r}-\vec{r}'|^2]^2} < \int d^3r \int_{\vec{r}-\vec{\epsilon}}^{\vec{r}+\vec{\epsilon}} d^3r' \int_0^{\epsilon}\int_0^{\epsilon} dz\, dz' \frac{1}{[z^2+z'^2+|\vec{r}-\vec{r}'|^2]^2}$$

$$< \frac{1}{4}\int d^3r \int_{-\vec{\epsilon}}^{\vec{\epsilon}} d^5w \frac{1}{w^2} = \frac{1}{12} S_5 \epsilon'^3 \int_{R'} d^3r. \tag{40}$$

Since the region $R' \subset R_2$ is finite this integral is convergent. Next, let us analyze the term $1/[(2-z_{12}^+)^2+r_{12}^2]^2$ of I_2 in the region R_3. Since the behavior of the field in each plates (for $z=0$ and $z=L$) is the same, then the analysis follows the same lines as previous ones and therefore this contribution is also finite. To study I_3, we consider first the term $2/[(z_{12}^-)^2+r_{12}^2][(z_{12}^+)^2+r_{12}^2]$. This expression must be studied in the regions R_1 and R_2, respectively. In R_1 we can see that the convergence of

$$\int_{R_1} d^3r dz d^3r' dz' \frac{1}{[(z-z')^2+|\vec{r}-\vec{r}'|^2]\underbrace{[(z+z')^2+|\vec{r}-\vec{r}'|^2]}_{\text{finite in } R_1}}, \tag{41}$$

depends on the convergence of

$$\int_{R_1} d^3r\, dz\, d^3r'\, dz' \frac{1}{(z-z')^2+|\vec{r}-\vec{r}'|^2}. \tag{42}$$

From the above arguments we have that Eq. (42) can be written as

$$\int_{-\vec{\epsilon}}^{\vec{\epsilon}} \frac{d^4w}{w^2} = S_4 \int_0^{\epsilon'} dw\, w = \frac{S_4 \epsilon'^2}{2}, \tag{43}$$

thus Eq. (42) gives a finite contribution. Now we consider the first term of I_3 in the region R_2. For this purpose we will use the following property. Let us take a continuous and positive function $f(x)$ which does not have singularities except for $x=0$, and $N=\int_0^{\vec{\epsilon}}\int_0^{\vec{\epsilon}} d^l y d^m z f(y^2+z^2)$ then there exist ϵ' in such a way that $N=(S_{l+m+2}/S_{l+1}S_{m+1})\int_0^{\epsilon'} dw\, w^{l+m+1} f(w^2)$ where $\epsilon'>0$. Using this property, we have for the first term of Eq. (35), in the region R_2, that

$$\int d^3r \int_0^{\epsilon} dz \int_z^{z+\epsilon} dz' \int_{\vec{r}-\vec{\epsilon}}^{\vec{r}+\vec{\epsilon}} d^3r' \frac{1}{[(z-z')^2+|\vec{r}-\vec{r}'|^2][(z+z')^2+|\vec{r}-\vec{r}'|^2]}$$

$$< \int d^3r \int_0^{\epsilon} dz \int_0^{\epsilon} du \int_{-\vec{\epsilon}}^{\vec{\epsilon}} d^3v \frac{1}{(u^2+v^2)(z^2+u^2+v^2)}$$

$$< \frac{1}{4} S_4 \int d^3r \int_0^{\epsilon} dz \int_0^{\epsilon'} dw \frac{w}{(z^2+w^2)} = \frac{S_3 S_4}{2 S_1 S_2} \epsilon''. \tag{44}$$

Therefore the first term of I_3 is also finite in R_2. The second term $2/[((z_{12}^-)^2+r_{12}^2)((2-z_{12}^+)^2+r_{12}^2)]$ in I_3 must be analyzed also in the regions R_1 and R_3. This analysis follows the same lines as the last case, therefore the contribution coming from this term is also finite.

We have now to study the term I_4. Note that $2/[((z_{12}^+)^2+r_{12}^2)((2-z_{12}^+)^2+r_{12}^2)]$ must be analyzed in the regions R_2 and R_3, respectively. Let us start with the region R_2. Using previous arguments we have that the convergence of I_4 depends on the convergence of the following expression:

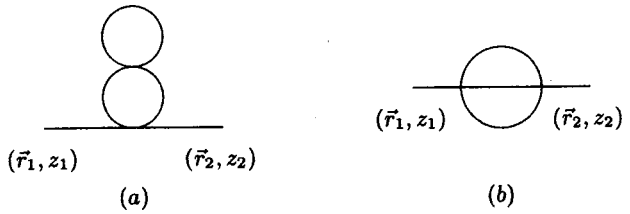

FIG. 6. Two-point Schwinger functions at two-loop level.

$$\int_0^\epsilon \int_0^\epsilon \mathrm{d}z\, \mathrm{d}z' \int_{\vec{r}-\vec{\epsilon}}^{\vec{r}+\vec{\epsilon}} d^3r' \frac{1}{z^2+z'^2+|\vec{r}-\vec{r}'|^2} = \frac{S_5}{4}\int_0^{\epsilon'} \mathrm{d}w \frac{w^4}{w^2} = \frac{S_5}{12}\epsilon'^3, \tag{45}$$

which is finite. In the region R_3 our analysis follows the same lines as in the region R_2, thus the integral in the region. R_3 is also finite.

Using the same argument that we used before, it is not difficult to show that the contribution coming from I_5 is also finite. We conclude that the integrals given by Eq. (32) only have bulk divergences. In this way we can conclude that at the one-loop level the bulk counterterms are sufficient to render the complete connected Schwinger functions finite. In the next section we will identify the divergent contribution in the connected two-point Schwinger functions at the two-loop order.

IV. THE DIVERGENCES IN THE TWO-POINT SCHWINGER FUNCTIONS AT TWO-LOOP LEVEL

In this section we will generalize some results obtained by Fosco and Svaiter[14] and also by Caicedo and Svaiter.[15] We will identify the divergent contribution in the connected two-point Schwinger functions at the two-loop order. The diagrams that we are interested to analyze are displayed in Fig. 6. The expression that corresponds to Fig. 6(a) is given by

$$\frac{\lambda^2}{4}\int d^3r'\, \mathrm{d}z'\, d^3r\, \mathrm{d}z\, G_0^{(2)}(\vec{r}_1-\vec{r}',z_1,z')\left[G_0^{(2)}(\vec{r}'-\vec{r},z',z)\right]^2 G_0^{(2)}(0,z,z) G_0^{(2)}(\vec{r}_2-\vec{r}',z_2,z'). \tag{46}$$

Since the external legs in Eq. (46) do not contribute to generate divergences, let us consider only the following integral:

$$\int d^3r\, \mathrm{d}z [G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2 G_0^{(2)}(0,z,z). \tag{47}$$

Replacing Eq. (29) in Eq. (47) we get

$$\begin{aligned}\int d^3r\, \mathrm{d}z [G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2 G_0^{(2)}(0,z,z) = \lim_{\Lambda\to\infty} \frac{S_4}{32\pi^4}\Lambda^2 \int d^3r\, \mathrm{d}z [G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2 \\ + \frac{1}{48L^2}\int d^3r\, \mathrm{d}z [G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2 \\ - \frac{1}{16L^2}\int d^3r\, \mathrm{d}z [G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2 \frac{1}{\sin^2(\pi z/L)}.\end{aligned} \tag{48}$$

The first term and the second one in Eq. (48) can be renormalized introducing only bulk counterterms. The most interesting behavior appears in the last term of this equation. Note that this unrenormalized quantity contains only bulk divercences, since the contribution coming from

$[G_0^{(2)}(\vec{r}'-\overline{r},z',z)]^2$ cancels the surface divergent behavior generated by the $1/\sin^2(\pi z/L)$ term. Nevertheless, after the introduction of a bulk counterterm to render the contribution $[G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^2$ finite between the plates, surface divergences appear. Thus this surface divergence must be renormalized. After the introduction of surface and bulk counterterms, the finite contribution coming from the last term of Eq. (48), up to a finite renormalization constant, is given by

$$\frac{1}{16L^2}\int d^3r\,\mathrm{d}z\left[(G_0^{(2)}(\vec{r}'-\vec{r},z',z))^2-\frac{1}{(4\pi^2L^2)^2}\frac{1}{[(z_{12}^-)^2+r_{12}^2]^2}\right]\left[\frac{1}{\sin^2(\pi z/L)}-\frac{L^2}{(\pi z)^2}-\frac{L^2}{\pi^2(L-z)^2}\right]. \tag{49}$$

Therefore this term contains an overlapping between bulk and surface counterterms.

We still must analyze the sunset diagram. The expression corresponding to Fig. 6(b) is given by

$$\frac{\lambda^2}{6}\int d^3r'\,\mathrm{d}z'\,d^3r\,\mathrm{d}z\,G_0^{(2)}(\vec{r_1}-\vec{r}',z_1z')\left[G_0^{(2)}(\vec{r}'-\vec{r},z',z)\right]^3G_0^{(2)}(\vec{r}_2-\vec{r}',z_2,z'). \tag{50}$$

Again, the external legs do not contribute to generate divergences, and therefore let us study the amputated diagram, i.e., without external legs. We have

$$\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'[G_0^{(2)}(\vec{r}'-\vec{r},z',z)]^3=\frac{1}{(4\pi^2L^2)^3}(I_1+I_2+\cdots+I_{12})+\text{finite part}, \tag{51}$$

where

$$I_1=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{1}{[(z_{12}^-)^2+r_{12}^2]^3}, \tag{52}$$

$$I_2=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\,\frac{1}{[(z_{12}^+)^2+r_{12}^2]^3}, \tag{53}$$

$$I_3=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{1}{[(2-z_{12}^+)^2+r_{12}^2]^3}, \tag{54}$$

$$I_4=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{2}{[(z_{12}^-)^2+r_{12}^2]^2[(z_{12}^+)^2+r_{12}^2]}, \tag{55}$$

$$I_5=\int d^3r\,\mathrm{d}z\,d^3r'\mathrm{d}z'\,\frac{2}{[(z_{12}^-)^2+r_{12}^2]^2[(2-z_{12}^+)^2+r_{12}^2]}, \tag{56}$$

$$I_6=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{2}{[(z_{12}^-)^2+r_{12}^2][(z_{12}^+)^2+r_{12}^2]^2}, \tag{57}$$

$$I_7=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{2}{[(z_{12}^-)^2+r_{12}^2][(2-z_{12}^+)^2+r_{12}^2]^2}, \tag{58}$$

$$I_8=\int d^3r\,\mathrm{d}z\,d^3r'\,\mathrm{d}z'\frac{2}{[(z_{12}^+)^2+r_{12}^2]^2[(2-z_{12}^+)^2+r_{12}^2]}, \tag{59}$$

$$I_9 = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{2}{[(z_{12}^+)^2 + r_{12}^2][(2 - z_{12}^+)^2 + r_{12}^2]^2}, \tag{60}$$

$$I_{10} = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{6}{[(z_{12}^-)^2 + r_{12}^2][(z_{12}^+)^2 + r_{12}^2][(2 - z_{12}^+)^2 + r_{12}^2]}, \tag{61}$$

$$I_{11} = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[\frac{1}{(z_{12}^-)^2 + r_{12}^2} - \frac{1}{(z_{12}^+)^2 + r_{12}^2} - \frac{1}{(2 - z_{12}^+)^2 + r_{12}^2} \right]^2 h(r_{12}, z_1, z_2), \tag{62}$$

$$I_{12} = \int d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \left[\frac{1}{(z_{12}^-)^2 + r_{12}^2} - \frac{1}{(z_{12}^+)^2 + r_{12}^2} - \frac{1}{(2 - z_{12}^+)^2 + r_{12}^2} \right] h^2(r_{12}, z_1, z_2), \tag{63}$$

Let us analyze each contribution coming from each term of Eq. (51). The first integral I_1 given by Eq. (52) is divergent in R_1. In general we can show that

$$\int_{R_1} d^3r'\, \mathrm{d}z' \frac{1}{[(z_{12}^-)^2 + r_{12}^2]^n} = \begin{cases} \text{finite}, & n < 2, \\ \infty, & n \geqslant 2. \end{cases} \tag{64}$$

Using the above result we can see that the integrals I_3, I_4 and the first integral of I_{11} are divergent. These integrals contain bulk divergences which must be removed introducing bulk counterterms. Next let us analyze the contribution coming from the integral I_2 in the region R_2. Using previous arguments and considering the external legs we get

$$\int_{R_2} d^3r\, \mathrm{d}z\, \mathrm{d}^3r'\, \mathrm{d}z' \frac{zz'}{[(z_{12}^+)^2 + r_{12}^2]^3} < \int d^3r \int_{-\vec{\epsilon}}^{\vec{\epsilon}} \int_0^{\epsilon} \int_0^{\epsilon} d^3u\, \mathrm{d}z\, \mathrm{d}z' \frac{zz'}{(z^2 + z'^2 + w^2)^3} < \frac{S_7}{S_2^2} \epsilon' \int d^3r. \tag{65}$$

Therefore this term gives a finite contribution to Eq. (50). The contribution from the integral I_6 to the integral must be studied in region R_2. In this case we must consider the external legs, and the property: let us take a function $f(x,y)$ positive which does not have singularities except for $(x,y)=(0,0), I=\int_0^{\epsilon}\int_0^{\epsilon} \mathrm{d}x\, \mathrm{d}y\, f(x,y)$ then, $I < \int_0^{\epsilon} \mathrm{d}x \int_x^{x+\epsilon} \mathrm{d}y\, f(x,y) + \int_0^{\epsilon} \mathrm{d}y \int_y^{y+\epsilon} \mathrm{d}y f(x,y)$, we get

$$\int_{R_2} d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{zz'}{[(z_{12}^-)^2 + r_{12}^2][(z_{12}^+)^2 + r_{12}^2]^2} < 2 \int d^3r \int_{-\vec{\epsilon}}^{\vec{\epsilon}} d^3w \int_0^{\epsilon} \mathrm{d}z \int_0^{\epsilon} \mathrm{d}u \frac{z(z+u)}{(u^2 + w^2)(u^2 + z^2 + w^2)^2}. \tag{66}$$

From the above arguments we have that the contribution from the integral I_6 is smaller than

$$S_4 \int d^3r \int_0^{\epsilon} \mathrm{d}z \int_0^{\epsilon'} \mathrm{d}s \frac{z^2 s}{(s^2 + z^2)^2} + 2S_3 \int d^3r \int_0^{\epsilon} \mathrm{d}z \int_0^{\epsilon} \mathrm{d}u \int_0^{\epsilon'} \mathrm{d}s \frac{zus^2}{(u^2 + s^2)(u^2 + s^2 + z^2)^2}$$

$$< \frac{S_4 S_5}{S_2 S_3}\epsilon'' \int d^3r + 2\frac{(S_5)^2}{(S_2)^2 S_3}\int d^3r \int_0^{\epsilon'''} \mathrm{d}w \frac{w^4}{w^4} < \left(\frac{S_4 S_5}{S_2 S_3}\epsilon'' + 2\frac{(S_5)^2}{(S_2)^2 S_3}\epsilon'''\right)\int d^3r. \tag{67}$$

We conclude that the integral I_6 is finite. Also integrating the contribution coming from the term I_8 on R_2 we get

$$\int_{R_2} d^3r dz d^3r' dz' \frac{1}{[(z_{12}^+)^2 + r_{12}^2]^2 \underbrace{[(2 - z_{12}^+)^2 + r_{12}^2]}_{\text{finite}}}. \tag{68}$$

Using the fact that the integral $\int_{R_2} d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z'\, 1/[(z_{12}^+)^2 + r_{12}^2]^2$ is finite, we have that this integral also is convergent in R_2. The contribution from the term I_{10} on R_2 is given by

$$\int_{R_2} d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{1}{[(z_{12}^-)^2 + r_{12}^2][(z_{12}^+)^2 + r_{12}^2]\underbrace{[(2 - z_{12}^+)^2 + r_{12}^2]}_{\text{finite}}}. \tag{69}$$

Since the integral $\int_{R_2} d^3r\, \mathrm{d}z\, d^3r'\, \mathrm{d}z' \frac{1}{[(z_{12}^-)^2 + r_{12}^2][(x_{12}^+) + r_{12}^2]}$ is finite, then the integral defined by Eq. (69) is convergent in R_2. The contribution coming from the terms I_{11} contain only a bulk divergence. Otherwise, the contributions coming from the terms I_{12} are finite. We conclude that we need only bulk counterterms to render the integral defined by Eq. (50) finite. The same analysis can be done for the four-point Schwinger function in the two-loop approximation. We obtained that only bulk divergences appear in the full four-point function.

V. CONCLUSIONS

In this paper we are interested to show how to implement the renormalization procedure in systems where the translational invariance is broken by the presence of macroscopic structures. For the sake of simplicity we are studying the self-interacting massless scalar field theory in a four-dimensional Euclidean space. We impose that one coordinate is defined in a compact domain, introducing two parallel mirrors where we are assuming Dirichlet-Dirichlet boundary conditions. Note that although that there are some similarities with the finite temperature field theory using the Matsubara formalism, in thermal systems there appears only bulk divergences, as for example, in the case of the system where we assume periodic boundary conditions. In nontranslational invariant systems, in general, to render the theory finite it is necessary to introduce surface counterterms.

In this work we generalize some results obtained by Fosco and Svaiter[14] and also by Caicedo and Svaiter.[15] We identify the divergences of the Schwinger functions in the massless self-interacting scalar field theory up to the two-loop approximation. First, analyzing the full two- and four-point Schwinger functions at the one-loop level, we show that the bulk counterterms are sufficient to render the theory finite. Second, at the two-loop level, we must introduce surface counterterms in the bare Lagrangian in order to make finite the full two- and also four-point Schwinger functions. The most interesting behavior appears in the "double scoop" diagram given by Eq. (46). The amputated diagram is given by Eq. (47) and we are interested in the last term of Eq. (48). This unrenormalized quantity contains only bulk divergences. Nevertheless, after the introduction of a bulk counterterm to render the contribution finite between the plates, surface divergences appear. Thus this surface divergence must be renormalized. Therefore this term contains an overlapping between bulk and surface counterterms. This procedure can be generalized to the n-loop level. The inclusion of the counterterm in the Lagrangian up to two-loop level with the full renormalized action and the general algorithm to identify the surface and bulk conterterms in the n-loop level will be left to future work.

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APPENDIX

In this Appendix we will derive a useful representation for the free two-point Schwinger function. Starting from Eq. (17), we have that $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$ is given by

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{2}{(2\pi)^{d-1}L}\sum_{n=1}^{\infty}\int d^{d-1}p\,\sin\left(\frac{n\pi z_1}{L}\right)\sin\left(\frac{n\pi z_2}{L}\right)\frac{e^{i\vec{p}\cdot(\vec{r}_1-\vec{r}_2)}}{\left[\vec{p}^2+\left(\frac{n\pi}{L}\right)^2+m^2\right]}. \tag{A1}$$

Using the variables $u=(z_1-z_2)/L$ and $v=(z_1+z_2)/L$ defined, respectively, in the region $u\in[-1,1]$ and $v\in[0,2]$, and also making use of a trigonometric identity and performing the sum that appears in Eq. (A1) we obtain[21]

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{1}{2}\int\frac{d^{d-1}p}{(2\pi)^{d-1}}\frac{e^{i\vec{p}}\cdot(\vec{r}_1-\vec{r}_2)}{(\vec{p}^2+m^2)^{1/2}}\left[\frac{\cosh(L(1-|u|)(\vec{p}^2+m^2)^{1/2})}{\sinh(L(\vec{p}^2+m^2)^{1/2})}-\frac{\cosh(L(1-v)(\vec{p}^2+m^2)^{1/2})}{\sinh(L(\vec{p}^2+m^2)^{1/2})}\right]. \tag{A2}$$

Taking $m=0,d=4$, and integrating the angular part, it is possible to show that $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$ can be written as

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{-i}{2(2\pi)^2r'L^2}\int_0^{\infty}dx(e^{ixr'}-e^{-ixr'})\left[\frac{\cosh((1-|u|)x)}{\sinh x}-\frac{\cosh((1-v)x)}{\sinh x}\right], \tag{A3}$$

where the variable r' is defined by $r'\equiv(|\vec{r}_1-\vec{r}_2|)/L$. Making use of the following integral representation of the product between the gamma function and the Riemann zeta function[21]

$$\int_0^{\infty}dx\frac{x^{z-1}e^{-\beta x}}{e^{px}-1}=\frac{\Gamma(z)}{p^z}\zeta\left(z,\frac{\beta}{p}+1\right), \tag{A4}$$

where $\mathrm{Re}(z)>1,\mathrm{Re}(\beta/p)>-1$ and the Riemann zeta function $\zeta(z,q)$ is defined by

$$\zeta(z,q)=\sum_{k=0}^{\infty}\frac{1}{(k+q)^z},\quad q\neq 0,-1,-2,\ldots, \tag{A5}$$

then, it is possible to write $G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)$ as

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2)=\frac{1}{16\pi^2L^2}\left[\sum_{k=-\infty}^{\infty}\frac{1}{\left(k-\frac{|u|}{2}\right)^2+\left(\frac{r'}{2}\right)^2}-\sum_{k=-\infty}^{\infty}\frac{1}{\left(k-\frac{v}{2}\right)^2+\left(\frac{r'}{2}\right)^2}\right]. \tag{A6}$$

Finally, using the following identity:

$$\sum_{k=-\infty}^{\infty} \frac{1}{(k-z)^2+r^2} = \frac{\pi}{2r}\frac{\sinh(2\pi r)}{\sinh^2(\pi r)+\sin^2(\pi z)}, \tag{A7}$$

we obtain the expression for the two-point Schwinger function that we need to proceed in our analysis. Using the above equation in Eq. (A6) we get

$$G_0^{(2)}(\vec{r}_1-\vec{r}_2,z_1,z_2) = \frac{\sinh(\pi r')}{16\pi L^2 r'}\left[\frac{\sin\left(\frac{\pi z_1}{L}\right)\sin\left(\frac{\pi z_2}{L}\right)}{\left[\sinh^2\left(\frac{\pi r'}{2}\right)+\sin^2\left(\frac{\pi u}{2}\right)\right]\left[\sinh^2\left(\frac{\pi r'}{2}\right)+\sin^2\left(\frac{\pi v}{2}\right)\right]}\right]. \tag{A8}$$

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On the quantum mechanics for one photon

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This paper revisits the quantum mechanics for one photon from the modern viewpoint and by the geometrical method. Especially, besides the ordinary (rectangular) momentum representation, we provide an explicit derivation for the other two important representations, called the cylindrically symmetrical representation and the spherically symmetrical representation, respectively. These other two representations are relevant to some current photon experiments in quantum optics. In addition, the latter is useful for us to extract the information on the quantized black holes. The framework and approach presented here are also applicable to other particles with arbitrary mass and spin, such as the particle with spin $\frac{1}{2}$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2200572]

I. INTRODUCTION

From the modern viewpoint, relativistic quantum mechanics originates from the natural marriage of special relativity and quantum theory: The Hilbert space for one particle quantum wave functions forms the unitary representation of the Poincare group, which is the isometric transformation group of the Minkowski spacetime. Especially, as realized on the Minkowski spacetime, the quantum wave functions need to satisfy the field equation of motion.[1–5] Not only does it provide a basis for relativistic quantum field, i.e., the quantum field operator is just defined on the Fock space associated with the Hilbert space of one particle states, but relativistic quantum mechanics itself is of significance in those cases which do not involve particle creation and annihilation, such as free propagations for in states before interaction and out states after interaction. It is here that relativistic quantum mechanics demonstrates its most striking properties such as quantum superposition and quantum entanglement, and thus acquires many invaluable applications such as quantum information and quantum computation.[6] Moreover, the information on the interaction can be extracted by comparing out states with in states.

Obviously, light occupies a special position in our attempts to understand nature both relativistically and quantum mechanically. It was light that initiated the great birth of both special relativity and quantum theory. Furthermore, the quantum mechanics on the photon and its interaction with matters has been developed into an individual discipline with wide applications, now called quantum optics.[7] By the geometric method, this paper is mainly intended to revisit the quantum mechanics for one photon from the modern viewpoint mentioned in the beginning. In particular, besides the momentum representation, we explicitly provide the other two important

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representations, i.e., the cylindrically symmetrical representation and the spherically symmetrical one. These other two representations are very relevant to some of the current research in quantum optics.[8–11] Especially, the latter is significant to the multi-pole radiation and electro-magnetic scattering around such a central potential as the Schwarzschild black hole. Furthermore, based on Hod's corresponding principle, it acquires a new application in the quantized black holes.[12]

It is worth noting that although all the three representations are known, they are treated here in a uniform framework and on an equal footing. (The first and third can be found in many of advanced textbooks such as Ref. 13, but the second was obtained for the first time in Ref. 14.) Especially, for the derivation of the later two representations, our method is obviously different from that used before.[13,14] We here employ the spin weighted harmonics functions and the corresponding spin weighted raising(lowering) operators, which have advantage of providing a straightforward and unified formalism applicable to particles of any spin.

The paper is organized as follows. In the next section, we construct the Hilbert space for one photon states from the solutions to the Maxwell equation. Based on the Killing field realization of the Poincare Lie algebra, Sec. III well defines the relevant conserved observables on the Hilbert space for one photon states, which is thus indicated to form the unitary representation of the Poincare group. The three representations are presented in Sec. IV, where the explicit derivation is given. We conclude with some implications and extensions in Sec. V.

Our notation and conventions follow those in Ref. 3. In particular, the index is raised or lowered by the Minkowski metric η_{ab}. We denote the covariant derivative and volume element compatible with the metric by ∇_a and ϵ_{abcd}, respectively. The d'Alembertian is defined as $\Box = \nabla_a \nabla^a$. The Lorentz coordinate system is specially denoted by $\{x^\mu | \mu = 0,1,2,3\}$, and the spatial vectors are indicated by letters in boldface.

II. THE HILBERT SPACE FOR ONE PHOTON STATES

Start with the source free Maxwell equation on the Minkowski spacetime

$$\nabla_{[a} F_{bc]} = 0, \qquad \nabla^a F_{ab} = 0, \tag{1}$$

where F_{ab} is a skew tensor field, called field strength. It is obvious that the solutions to the Maxwell equation form a complex vector space, denoted by H. (More precisely, we define H to be the complex vector space of solutions which vanish rapidly at spatial infinity.) To introduce an inner product on our complex vector space, we first define a conserved current as

$$j_a[A,A'] = i[\overline{F}_{ab} A'^b - \overline{A}^b F'_{ab}], \tag{2}$$

where A_a is the vector potential, satisfying

$$F_{ab} = 2\nabla_{[a} A_{b]}. \tag{3}$$

Whence the inner product can be defined as

$$(F,F') = (A,A') = \int_\Sigma j^a[A,A'] \epsilon_{abcd}. \tag{4}$$

Note that the conservation of $j_a[A,A']$ implies that this inner product is independent of choice of the Cauchy surface Σ. (This point also implies the unitarity of the evolution of source free fields.) Thus, for later convenience, we choose the surface of constant x^0 as Σ once and for all. Moreover, Eq. (4) can be written as

$$(F,F') = (A,A') = \int_{\Sigma} \left(\frac{\partial}{\partial x^0}\right)^a j_a[A,A']\tilde{\epsilon}_{bcd}, \tag{5}$$

where $\tilde{\epsilon}_{bcd} = (\partial/\partial x^0)^a \epsilon_{abcd}$ is the induced spatial volume element on Σ.

In addition, by Eq. (2), Eq. (5), and the second part of Eq. (1), the Stokes theorem shows that the inner product is invariant under gauge transformations

$$\begin{aligned} A_a &\to A_a + \nabla_a \Lambda, \\ A'_a &\to A'_a + \nabla_a \Lambda', \end{aligned} \tag{6}$$

where Λ and Λ' are both arbitrary scalar fields. However, this inner product is not always non-negative on our whole complex vector space. We next restrict H to its subvector space which guarantees the non-negativity of the above inner product. We denote this subvector space by H^+, which is just the Hilbert space for one photon states.

III. CONSERVED OBSERVABLES FROM THE POINCARE LIE ALGEBRA

As is well known, the Poincare Lie algebra can be realized by the Killing vector fields on the Minkowski spacetime as follows:

$$\begin{aligned} P_\mu &= i\left(\frac{\partial}{\partial x^\mu}\right)^a, \\ M_{\mu\nu} &= i\left[x_\mu\left(\frac{\partial}{\partial x^\nu}\right)^a - x_\nu\left(\frac{\partial}{\partial x^\mu}\right)^a\right]. \end{aligned} \tag{7}$$

According to the fact that the covariant derivative commutes with the Lie derivatives via Killing vector fields, the operators from the Poincare Lie algebra, i.e.,

$$\begin{aligned} \hat{P}^\mu F_{ab} &= \mathcal{L}_{P^\mu} F_{ab}, \\ \hat{M}_{\mu\nu} F_{ab} &= \mathcal{L}_{M_{\mu\nu}} F_{ab}, \end{aligned} \tag{8}$$

are well defined on H. Moreover, it can also be shown that they are well defined on the Hilbert space for one photon states indeed. (It seems easier to prove in the rectangular momentum representation.) Later, employing the Leibnitz rule, the conservation of $j_a[A,A']$, and the Stokes theorem, we find that the above operators are Hermitian with respect to the inner product (5). In addition, since the inner product (5) is independent of the choice of Σ, the above-noted operators are also conserved observables. Furthermore, taking into account $[\mathcal{L}_u, \mathcal{L}_v] = \mathcal{L}_{[u,v]}$ with u and v arbitrary vector fields, we can obtain

$$[\hat{P}_\mu, \hat{P}_\nu] = 0, \tag{9}$$

$$[\hat{P}_\mu, \hat{M}_{\rho\sigma}] = 2i\,\eta_{\mu[\rho}\hat{P}_{\sigma]}, \tag{10}$$

$$[\hat{M}_{\mu\nu}, \hat{M}_{\rho\sigma}] = 2i(\eta_{\mu[\rho}\hat{M}_{\sigma]\nu} - \eta_{\nu[\rho}\hat{M}_{\sigma]\mu}). \tag{11}$$

Here, $\hat{P}^\mu$ is the four-momentum operator. By Eq. (1), we have

$$\hat{P}_\mu \hat{P}^\mu = -\ \Box\ = 0, \tag{12}$$

which shows that the eigenvalue of the four-momentum operator is null. Furthermore, $\{\hat{L}_1 \equiv \hat{M}_{23}, \hat{L}_2 \equiv \hat{M}_{31}, \hat{L}_3 \equiv \hat{M}_{12}\}$ are the total angular momentum operators.

We next introduce the Pauli-Lubanski spin vector operator

$$\hat{S}_\mu = \tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}\hat{P}^\nu \hat{M}^{\rho\sigma}. \tag{13}$$

Resorting to Eq. (1) and after a straightforward calculation, we can obtain (the reader is suggested to follow the steps described in Ref. 15)

$$\hat{S}_\mu = \hat{P}_\mu \hat{S}, \tag{14}$$

where $\hat{S}$ is the helicity operator, defined by

$$\hat{S}F_{ab} = (-i)^* F_{ab} = -\frac{i}{2}\epsilon_{abcd}F^{cd}. \tag{15}$$

Based on the fact that the Lie derivatives via Killing vector fields annihilate the volume element, $\hat{S}$ commutes with both $\hat{P}_\mu$ and $\hat{M}_{\mu\nu}$. Furthermore, we have

$$\hat{S}^2 = 1, \tag{16}$$

which implies that the possible eigenvalue of the helicity operator takes ± 1.

IV. THREE REPRESENTATIONS IN THE COULOMB GAUGE

In this section, we shall employ the vector potential in the Coulomb gauge. In terms of the vector potential, the Maxwell equation can be written as

$$\Box A_a = 0, \tag{17}$$

where the Coulomb gauge

$$\begin{aligned} \nabla^a A_a &= 0, \\ \left(\frac{\partial}{\partial x^0}\right)^a A_a &= 0, \end{aligned} \tag{18}$$

has been employed. In this case, the inner product (5) is equivalent to

$$(F,F') = (A,A') = \int_\Sigma \left(\frac{\partial}{\partial x^0}\right)^a j'_a[A,A']\tilde{\epsilon}_{bcd}, \tag{19}$$

where the conserved current

$$j'_a[A,A'] = i[\nabla_a \overline{A_b})A'^b - \overline{A^b}\nabla_a A'_b]. \tag{20}$$

Later, according to the commutation relations in the last section, we can choose $\{\hat{P}^1, \hat{P}^2, \hat{P}^3, \hat{S}\}$ as a complete observable set, which forms the ordinary rectangular momentum representation. Similarly, the complete observable set $\{\hat{P}^0, \hat{P}^3, \hat{L}_3, \hat{S}\}$ forms the cylindrically symmetrical representation, and $\{\hat{P}^0, \hat{\mathbf{L}}^2, \hat{L}_3, \hat{S}\}$ forms the spherically symmetrical representation.

A. The rectangular momentum representation

Since the details of the rectangular momentum representation have appeared in the literature, we will only recall the main results without entering into the explicit derivations. First, according to Eqs. (17) and (18), any vector potential can be written as

$$A_a(x) = \frac{1}{\sqrt{(2\pi)^3}}\left\{\int_{p^0>0}\frac{d^3\mathbf{p}}{p^0}[\acute{A}_+(\mathbf{p})(\varepsilon^+)_a(\mathbf{p}) + \acute{A}_-(\mathbf{p})(\varepsilon^-)_a(\mathbf{p})]e^{-ip_bx^b} + \int_{p^0<0}\frac{d^3\mathbf{p}}{p^0}[\grave{A}_+(\mathbf{p})(\varepsilon^+)_a(\mathbf{p}) + \grave{A}_-(\mathbf{p})(\varepsilon^-)_a(\mathbf{p})]e^{-ip_bx^b}\right\}. \tag{21}$$

Here $p^a = p^u(\partial/\partial x^\mu)^a$ is a constant real null vector field, and $x^a = x^\mu(\partial/\partial x^\mu)^a$ is the position vector field. In addition, $(\varepsilon^\pm)_a(\mathbf{p})$ are constant null fields and complex conjugate with each other, satisfying

$$p^a(\varepsilon^\pm)_a(\mathbf{p}) = 0,$$

$$\left(\frac{\partial}{\partial x^0}\right)^a(\varepsilon^\pm)_a(\mathbf{p}) = 0, \tag{22}$$

$$\epsilon_{abcd} = -\frac{i}{p^0}(dx^0)_a \wedge p_b \wedge (\varepsilon^+)_c(\mathbf{p}) \wedge (\varepsilon^-)_d(\mathbf{p}).$$

Later, substituting Eq. (21) into Eq. (19), we have

$$(F,F') = (A,A') = \int d^3\mathbf{x}\left(\frac{\partial}{\partial x^0}\right)aj'_a[A,A'] = 2\left\{\int_{p^0>0}\frac{d^3\mathbf{p}}{p^0}[\overline{\acute{A}}_+(\mathbf{p})\acute{A}'_+(\mathbf{p}) + \overline{\acute{A}}_-(\mathbf{p})\acute{A}'_-(\mathbf{p})] + \int_{p^0<0}\frac{d^3\mathbf{p}}{p^0}[\overline{\grave{A}}_+(\mathbf{p})\grave{A}'_+(\mathbf{p}) + \overline{\grave{A}}_-(\mathbf{p})\grave{A}'_-(\mathbf{p})]\right\}. \tag{23}$$

Whence H^+ is just the positive energy solutions to the Maxwell equation, as is also what we expect. Therefore, we shall restrict ourselves to the case of $p^0>0$ in all of the following discussions. Furthermore, the orthonormal basis for H^+ in the rectangular momentum representation is given by

$$|\mathbf{p},s = \pm 1\rangle = \frac{1}{\sqrt{(2\pi)^3}}\frac{1}{\sqrt{2p^0}}(\varepsilon^\pm)_a(\mathbf{p})e^{-ip_bx^b}, \tag{24}$$

where $\mathbf{p}$ is the eigenvalue of three-momentum operator, and s is the eigenvalue of the helicity operator.

B. The cylindrically symmetrical representation

It is convenient to provide the cylindrically symmetrical representation in the cylindrical coordinate system, i.e.,

$$x^0 = t,$$

$$x^1 = \varrho\cos\phi,$$

$$x^2 = \varrho \sin \phi,$$

$$x^3 = z. \tag{25}$$

Whence the Minkowski metric reads

$$ds^2 = dt^2 - dz^2 - d\varrho^2 - \varrho^2 d\phi^2, \tag{26}$$

and

$$P^0 = i\left(\frac{\partial}{\partial t}\right)^a,$$

$$P^3 = -i\left(\frac{\partial}{\partial z}\right)^a, \tag{27}$$

$$L_3 = -i\left(\frac{\partial}{\partial \phi}\right)^a.$$

Define a pair of null covariant vector fields as

$$(\varepsilon^{\mp})_a = \frac{1}{\sqrt{2}}[(d\varrho)_a \pm i\varrho(d\phi)_a], \tag{28}$$

then according to the second part in Eq. (18), any vector potential can be written as

$$A_a = A_z(dz)_a + A_-(\varepsilon^-)_a + A_+(\varepsilon^+)_a, \tag{29}$$

where, A_z has spin weight 0, A_- with spin weight -1, and A_+ with spin weight 1.[16] From

$$\nabla_a(dz)_b = 0,$$

$$\nabla_a(\varepsilon^-)_b = \frac{1}{\sqrt{2}\varrho}[(\varepsilon^+)_a - (\varepsilon^-)_a](\varepsilon^-)_b, \tag{30}$$

$$\nabla_a(\varepsilon^+)_b = \frac{1}{\sqrt{2}\varrho}[(\varepsilon^-)_a - (\varepsilon^+)_a](\varepsilon^+)_b,$$

it can be shown that the Maxwell equation reads

$$\begin{aligned}\Box A_a = &\left(-\bar{\eth}\,\eth A_z + \frac{\partial^2 A_z}{\partial t^2} - \frac{\partial^2 A_z}{\partial z^2}\right)(dz)_a \\ &+ \left(-\bar{\eth}\,\eth A_- + \frac{\partial^2 A_-}{\partial t^2} - \frac{\partial^2 A_-}{\partial z^2}\right)(\varepsilon^-)_a + \left(-\bar{\eth}\,\eth A_+ + \frac{\partial^2 A_+}{\partial t^2} - \frac{\partial^2 A_+}{\partial z^2}\right)(\varepsilon^+)_a = 0,\end{aligned} \tag{31}$$

together with

$$\nabla^a A_a = -\frac{\partial A_z}{\partial z} + \frac{1}{\sqrt{2}}(\eth A_- + \bar{\eth} A_+) = 0. \tag{32}$$

Here $\eth, \bar{\eth}$ are operators acting on a quantity f with spin weight n, i.e.,

$$\eth f = -\left(\frac{\partial}{\partial \varrho} + \frac{i}{\varrho}\frac{\partial}{\partial \phi} - \frac{n}{\varrho}\right)f,$$

$$\bar{\eth} f = -\left(\frac{\partial}{\partial \varrho} - \frac{i}{\varrho}\frac{\partial}{\partial \phi} + \frac{n}{\varrho}\right) f. \tag{33}$$

Then, $\eth f$ and $\overline{\eth f}$ have spin weight $n+1$ and $n-1$, respectively.[16] Later, it is easy to check that the Lie derivatives of $\{(dz)_a, (\varepsilon^{\mp})_a\}$ via $\{P^0, P^3, L_3\}$ all vanish, thus the simultaneous eigensolutions of $\{\hat{P}^0, \hat{P}^3, \hat{L}_3\}$ to Eq. (31) with the corresponding eigenvalue $\{p^0, p^3, m\}$ must take the form

$$\begin{aligned} A_z &= a_{00} Z_{\alpha m}(\varrho, \phi) e^{-i(p_0 t + p_3 z)}, \\ A_- &= a_{--1} Z_{\alpha m}(\varrho, \phi) e^{-i(p_0 t + p_3 z)}, \\ A_+ &= a_{+1} Z_{\alpha m}(\varrho, \phi) e^{-i(p_0 t + p_3 z)}, \end{aligned} \tag{34}$$

where a_0, a_-, and a_+ are all constant coefficients; ${}_nZ_{\alpha m}$ is the spin-weighted cylindrical harmonics with spin weight n such that[16]

$$\begin{aligned} \eth {}_nZ_{\alpha m} &= \alpha_{n+1} Z_{\alpha m}, \\ \bar{\eth} {}_nZ_{\alpha m} &= -\alpha_{n-1} Z_{\alpha m}, \\ \hat{L}_{3n} Z_{\alpha m} &= m_n Z_{\alpha m} \end{aligned} \tag{35}$$

with $\alpha = \sqrt{p_0^2 - p_3^2}$. Moreover, by the boundary condition, here p_3 is a real constant, and

$${}_nZ_{\alpha m} = J_{m+n}(\alpha \varrho) e^{im\phi}, \tag{36}$$

where J_{m+n} is the first kind of Bessel function of order $m+n$ with $\alpha \geq 0$ and m an integer.

Substituting Eq. (34) into Eq. (32), we have

$$ip_3 a_0 + \frac{\alpha}{\sqrt{2}}(a_- - a_+) = 0. \tag{37}$$

Next combine it with the eigenequations of the helicity operator, i.e.,

$$\begin{aligned} ip_0 a_0 - s\frac{\alpha}{\sqrt{2}}(a_- + a_+) &= 0, \\ i(p_0 - sp_3) a_+ + s\frac{\alpha}{\sqrt{2}} a_0 &= 0, \\ i(p_0 + sp_3) a_- + s\frac{\alpha}{\sqrt{2}} a_0 &= 0, \end{aligned} \tag{38}$$

where $s = \pm 1$ is the eigenvalue of the helicity operator. Thus we have

$$\begin{aligned} a_- &= \frac{isa_0}{\sqrt{2}\alpha}(p_0 - sp_3), \\ a_+ &= \frac{isa_0}{\sqrt{2}\alpha}(p_0 + sp_3). \end{aligned} \tag{39}$$

Furthermore, note

$$\int_0^\infty \mathrm{d}\varrho\,\varrho J_m(\alpha\varrho)J_m(\alpha'\varrho) = \frac{1}{\alpha}\delta(\alpha-\alpha') \tag{40}$$

with $\alpha \leq \alpha'$.[20] Then it follows that the orthonormal basis with respect to the inner product (19) in the cylindrically symmetrical representation reads

$$|p^0,p^3,m,s\rangle = \frac{\alpha}{4\pi p_0}\Bigg\{ J_m(\alpha\varrho)e^{im\phi}e^{-i(p_0t+p_3z)}(\mathrm{dz})_a + \frac{i}{\sqrt{2}\alpha}[(sp_0-p_3)J_{m-1}(\alpha\varrho)e^{im\phi}e^{-i(p_0t+p_3z)}(\varepsilon^-)_a + (sp_0+p_3)J_{m+1}(\alpha\varrho)e^{im\phi}e^{-i(p_0t+p_3z)}(\varepsilon^+)_a]\Bigg\}, \tag{41}$$

which satisfies

$$\langle p^0,p^3,m,s|p'^0,p'^3,m',s'\rangle = \delta(p^0-p'^0)\delta(p^3-p'^3)\delta_{mm'}\delta_{ss'}. \tag{42}$$

Finally, we would like to point out that $|p^0,p^3,m,s\rangle$ vanishes for $m \neq \pm 1$ in the case of $\alpha=0$.

C. The spherically symmetrical representation

To provide the spherically symmetrical representation, we would like to use the spherical coordinate system, i.e.,

$$\begin{aligned} x^0 &= t, \\ x^1 &= r\sin\theta\cos\varphi, \\ x^2 &= r\sin\theta\sin\varphi, \\ x^3 &= r\cos\theta. \end{aligned} \tag{43}$$

In this case, the Minkowski metric takes the form

$$\mathrm{d}s^2 = \mathrm{d}t^2 - \mathrm{d}r^2 - r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2), \tag{44}$$

and

$$\begin{aligned} P^0 &= i\left(\frac{\partial}{\partial t}\right)^a, \\ L_\pm &\equiv L_1 \pm iL_2 = \pm e^{\pm i\varphi}\left[\left(\frac{\partial}{\partial\theta}\right)^a \pm i\cot\theta\left(\frac{\partial}{\partial\varphi}\right)^a\right], \\ L_3 &= -i\left(\frac{\partial}{\partial\varphi}\right)^a. \end{aligned} \tag{45}$$

Define a pair of null covariant vector fields as

$$(\varepsilon^\mp)_a = \frac{r}{\sqrt{2}}[(\mathrm{d}\theta)_a \pm i\sin\theta(\mathrm{d}\varphi)_a], \tag{46}$$

then from the second part in Eq. (18), any vector potential reads

$$A_a = A_r(\mathrm{d}r)_a + A_-(\varepsilon^-)_a + A_+(\varepsilon^+)_a, \tag{47}$$

where A_r has spin weight 0, A_- with -1, and A_+ with 1.[17–19] Using

$$\nabla_a(\mathrm{d}r)_b = \frac{1}{r}[(\varepsilon^-)_a(\varepsilon^+)_b + (\varepsilon^+)_a(\varepsilon^-)_b],$$

$$\nabla_a(\varepsilon^-)_b = \frac{1}{r}\left\{\frac{\cot\theta}{\sqrt{2}}[(\varepsilon^+)_a - (\varepsilon^-)_a](\varepsilon^-)_b - (\varepsilon^-)_a(\mathrm{d}r)_b\right\}, \tag{48}$$

$$\nabla_a(\varepsilon^+)_b = \frac{1}{r}\left\{\frac{\cot\theta}{\sqrt{2}}[(\varepsilon^-)_a - (\varepsilon^+)_a](\varepsilon^+)_b - (\varepsilon^+)_a(\mathrm{d}r)_b\right\},$$

it follows that

$$\begin{aligned}\Box A_a = &\left[\frac{-1}{2r^2}(\eth\bar{\eth} + \bar{\eth}\,\eth)A_r + \frac{\partial^2 A_r}{\partial t^2} - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{2}{r^2}\right)A_r - \frac{\sqrt{2}}{r^2}(\eth A_- + \bar{\eth}A_+)\right](\mathrm{d}r)_a \\ &+ \left[\frac{-1}{2r^2}(\eth\bar{\eth} + \bar{\eth}\,\eth)A_- + \frac{\partial^2 A_-}{\partial t^2} - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\right)A_- + \frac{\sqrt{2}}{r^2}\bar{\eth}A_r\right](\varepsilon^-)_a \\ &+ \left[\frac{-1}{2r^2}(\eth\bar{\eth} + \bar{\eth}\,\eth)A_+ + \frac{\partial^2 A_+}{\partial t^2} - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\right)A_+ + \frac{\sqrt{2}}{r^2}\eth A_r\right](\varepsilon^+)_a = 0,\end{aligned} \tag{49}$$

and

$$\nabla_a A^a = -\left(\frac{\partial}{\partial r} + \frac{2}{r}\right)A_r + \frac{1}{\sqrt{2}r}(\eth A_- + \bar{\eth}A_+) = 0. \tag{50}$$

Here $\eth, \bar{\eth}$ are operators acting on a quantity f with spin weight n, i.e.,

$$\begin{aligned}\eth f &= -\left(\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\varphi} - n\cot\theta\right)f, \\ \bar{\eth}f &= -\left(\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\varphi} + n\cot\theta\right)f.\end{aligned} \tag{51}$$

Then, $\eth f$ and $\bar{\eth}f$ have spin weight $n+1$ and $n-1$, respectively.[19]

On the other hand, we have

$$\hat{L}_\pm(\mathrm{d}r)_a = L_\pm^b\partial_b(\mathrm{d}r)_a + (\mathrm{d}r)_b\partial_a L_\pm^b = 0,$$

$$\hat{L}_\pm(\varepsilon^-)_a = L_\pm^b\partial_b(\varepsilon^-)_a + (\varepsilon^-)_b\partial_a L_\pm^b = e^{\pm i\varphi}(\varepsilon^-)_a, \tag{52}$$

$$\hat{L}_\pm(\varepsilon^+)_a = L_\pm^b\partial_b(\varepsilon^+)_a + (\varepsilon^+)_b\partial_a L_\pm^b = -e^{\pm i\varphi}(e^+)_a,$$

where ∂_a is the ordinary derivative associated with the spherical coordinate system. Thus

$$\hat{L}_\pm A_a = (\hat{L}_\pm A_r)(\mathrm{d}r)_a + (\hat{L}_\pm A_- + e^{\pm i\varphi}\csc\theta A_-)(\varepsilon^-)_a + (\hat{L}_\pm A_+ - e^{\pm i\varphi}\csc\theta A_+)(\varepsilon^+)_a. \tag{53}$$

Similar, it is easy to check that the Lie derivatives of $\{(\mathrm{d}r)_a, (\varepsilon^\pm)_a\}$ via $\{P^0, L_3\}$ all vanish. Whence the simultaneous eigensolutions of $\{\hat{P}^0, \hat{\mathbf{L}}^2, \hat{L}_3\}$ to Eq. (49) with the corresponding eigenvalue $\{p^0, l(l+1), m\}$ must satisfy

$$A_r = R_0(r)_0 Y_{lm}(\theta,\varphi)e^{-ip_0 t},$$

$$A_- = R_-(r)_{-1}Y_{lm}(\theta,\varphi)e^{-ip_0t},$$

$$A_+ = R_+(r)_1Y_{lm}(\theta,\varphi)e^{-ip_0t}. \tag{54}$$

Here ${}_nY_{lm}$ is the spin weighted spherical harmonics with l non-negative integers and $m=-l,-l+1,\ldots,l$, such that

$${}_0Y_{lm} = Y_{lm},$$

$$\eth_nY_{lm} = \sqrt{(l-n)(l+n+1)}{}_{n+1}Y_{lm},$$

$$\bar{\eth}_nY_{lm} = -\sqrt{(l+n)(l-n+1)}{}_{n-1}Y_{lm}, \tag{55}$$

$$(\hat{L}_\pm - ne^{\pm i\varphi}\csc\theta){}_nY_{lm} = \sqrt{(l\mp m)(l\pm m+1)}{}_nY_{lm\pm1},$$

$$\hat{L}_{3n}Y_{lm} = m_nY_{lm},$$

where Y_{lm} is the ordinary spherical harmonics, and ${}_nY_{lm}$ with $l<|n|$ vanishes.[19]

We next substitute Eq. (54) into Eq. (49) to obtain the radial equations

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{2}{r^2}\right)R_0 + p_0^2R_0 - \frac{l(l+1)}{r^2}R_0 + \frac{\sqrt{2l(l+1)}}{r^2}(R_- - R_+) = 0,$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)R_- + p_0^2R_- - \frac{l(l+1)}{r^2}R_- + \frac{\sqrt{2l(l+1)}}{r^2}R_0 = 0, \tag{56}$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)R_+ + p_0^2R_+ - \frac{l(l+1)}{r^2}R_+ - \frac{\sqrt{2l(l+1)}}{r^2}R_0 = 0.$$

Furthermore, Eq. (50) requires

$$-\left(\frac{d}{dr}+\frac{2}{r}\right)R_0 + \frac{\sqrt{l(l+1)}}{\sqrt{2}r}(R_- - R_+) = 0. \tag{57}$$

It can be shown that Eqs. (56) and (57) are equivalent to

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)(R_- + R_+) + p_0^2(R_- + R_+) - \frac{l(l+1)}{r^2}(R_- + R_+) = 0,$$

$$\left(\frac{d^2}{dr^2}+\frac{4}{r}\frac{d}{dr}+\frac{2}{r^2}\right)R_0 + p_0^2R_0 - \frac{l(l+1)}{r^2}R_0 = 0, \tag{58}$$

$$R_- - R_+ - \frac{\sqrt{2}r}{\sqrt{l(l+1)}}\left(\frac{d}{dr}+\frac{2}{r}\right)R_0 = 0.$$

By the boundary condition, the solutions to Eq. (58) are given by

$$R_- + R_+ = b\frac{j_{l+1/2}(p_0 r)}{\sqrt{p_0 r}},$$

$$R_0 = b_0\frac{j_{l+1/2}(p_0 r)}{(\sqrt{p_0 r})^3},$$

$$R_- - R_+ = b_0\frac{\sqrt{2}}{\sqrt{l(l+1)}}\left[\frac{J_{l-1/2}(p_0 r)}{\sqrt{p_0 r}} - l\frac{J_{l+1/2}(p_0 r)}{(\sqrt{p_0 r})^3}\right], \tag{59}$$

where b and b_0 are both constant coefficients; $J_{l\pm1/2}$ is the first kind of Bessel function of order $l\pm 1/2$.[20]

Substituting Eq. (59) into the eigenequations of the helicity operator with the eigenvalue $s = \pm 1$, i.e.,

$$ip_0 R_0 - s\frac{\sqrt{l(l+1)}}{\sqrt{2}r}(R_- + R_+) = 0,$$

$$ip_0 R_- + s\frac{\sqrt{l(l+1)}}{\sqrt{2}r}R_0 - s\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r}\right)R_- = 0, \tag{60}$$

$$ip_0 R_+ + s\frac{\sqrt{l(l+1)}}{\sqrt{2}r}R_0 + s\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r}\right)R_+ = 0.$$

We obtain

$$b = isb_0\frac{\sqrt{2}}{\sqrt{l(l+1)}}. \tag{61}$$

Note

$$\int_{4\pi} d\varphi d\theta \sin\theta_n \overline{Y}_{lmn} Y_{l'm'} = \delta_{ll'}\delta_{mm'} \tag{62}$$

with $l \geq |n|$,[19] and

$$\int_0^\infty \mathrm{d}r r J_{l+1/2}(p_0 r) J_{l+1/2}(p_0' r) = \frac{1}{p_0}\delta(p_0 - p_0'),$$

$$\int_0^\infty \mathrm{d}r \frac{1}{r} J_{l+1/2}(p_0 r) J_{l+1/2}(p_0' r) = \frac{1}{2l+1}\left(\frac{p_0}{p_0'}\right)^{l+1/2},$$

$$\int_0^\infty \mathrm{d}r J_{l-1/2}(p_0 r) J_{l+1/2}(p_0' r) = \frac{1}{p_0}\left(\frac{p_0}{p_0'}\right)^{l+1/2}, \tag{63}$$

$$\int_0^\infty \mathrm{d}r J_{l-1/2}(p_0' r) J_{l+1/2}(p_0 r) = 0,$$

$$\int_0^\infty \mathrm{d}r J_{l-1/2}(p_0 r) J_{l+1/2}(p_0 r) = \frac{1}{2p_0}$$

with $p_0 \leq p_0'$.[20] Thus it follows that the orthonormal basis with respect to the inner product (19) in the spherical symmetrical representation reads

$$\begin{aligned}|p^0,l,m,s\rangle = \frac{\sqrt{l(l+1)}}{2\sqrt{r}}\Bigg\{ & \frac{J_{l+1/2}(p_0 r)}{p_0 r}{}_0Y_{lm}(\theta,\varphi)e^{-ip_0 t}(\mathrm{d}r)_a \\ & + \frac{1}{\sqrt{2l(l+1)}}\Bigg[\left(\frac{isp_0 r - l}{p_0 r}J_{l+\frac{1}{2}}(p_0 r) + J_{l-\frac{1}{2}}(p_0 r)\right){}_{-1}Y_{lm}(\theta,\varphi)e^{ip_0 t}(\varepsilon^-)_a \\ & + \left(\frac{isp_0 r + l}{p_0 r}J_{l+\frac{1}{2}}(p_0 r) - J_{l-\frac{1}{2}}(p_0 r)\right){}_1Y_{lm}(\theta,\varphi)e^{-ip_0 t}(\varepsilon^+)_a\Bigg]\Bigg\},\end{aligned} \tag{64}$$

which satisfies

$$\langle p^0,l,m,s|p'^0,l',m',s'\rangle = \delta(p^0 - p'^0)\delta_{ll'}\delta_{mm'}\delta_{ss'}. \tag{65}$$

It is obvious that $|p^0,l,m,s\rangle$ vanishes in the case of $l=0$, which implies that the angular quantum number l of one photon only takes positive integers.

V. DISCUSSIONS

We would like to stress that the framework and method presented here are also applicable to other particles with arbitrary mass and spin such as neutrino and electron. In addition, after a simple modification, our results obtained here are easy to be generalized to those cavities with the suitable boundaries, which is important not only to the investigation of the Casimir effect, but also to understanding the relationship between the holographic entropy bound and local quantum field theory.[21]

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Noncommutative geometry and the standard model vacuum

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The space of Dirac operators for the Connes-Chamseddine spectral action for the standard model of particle physics coupled to gravity is studied. The model is extended by including right-handed neutrino states, and the S^0-reality axiom is not assumed. The possibility of allowing more general fluctuations than the inner fluctuations of the vacuum is proposed. The maximal case of all possible fluctuations is studied by considering the equations of motion for the vacuum. While there are interesting nontrivial vacua with Majorana-type mass terms for the leptons, the conclusion is that the equations are too restrictive to allow solutions with the standard model mass matrix. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A. The noncommutative geometry of the standard model

Connes discovered a geometric principle which unifies the metric tensor of general relativity with the classical fields of particle physics—both bosons and fermions—in one geometric structure.[1] The principle is similar to the Kaluza and Klein idea of extending Einstein's space–time geometry to incorporate an internal space at each point in space–time so that the geometry of the extra dimensions is determined by the matter fields of particle physics.[2] Connes' principle is both a generalization of this idea and a simplification. It is more general because the internal space is allowed to be a noncommutative space, whereas it is at the same time simpler because the internal space is 0-dimensional. This is possible because in the noncommutative world 0-dimensional spaces have a much richer structure than in the commutative world of Kaluza and Klein, for whom a 0-dimensional space would have been merely an uninteresting discrete set of points. A noncommutative 0-dimensional space is characterized by a finite-dimensional matrix algebra, which turns out to be just what is required to produce non-Abelian gauge fields.

In fact, noncommutative geometry explains the geometrical structure of the standard model of particle physics.[3] One of the most striking features of this is the discovery that the Higgs field and the gauge bosons are both part of a connection on the total geometry—space–time plus internal space. The Higgs field is the part of the connection in the internal space directions. These directions are actually discrete, so one can think of the Higgs field as providing the parallel transport for hops from left-to right-handed particles, and vice-versa. This geometrical picture extends to a unified formula for the particle physics action, the famous quartic "mexican hat" potential for the Higgs being nothing other than part of the (quartic) Yang-Mills action for the connection on the total geometry. Another striking feature is the extension of the Yang-Mills gauge group to a matrix algebra. For example, SU(3) becomes $M_3(\mathbb{C})$, the algebra of all 3×3 matrices, which contains SU(3), but has a more restricted representation theory. The fact that the fermions fall into representations of the matrix algebra provides a deep explanation of the ad hoc pattern of charges which

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appears in the usual formulation of the standard model. These insights are very striking and suggest that noncommutative geometry is an important part of particle physics.

Connes' spectral triple formulation of a noncommutative geometry contains the following elements: A Hilbert space $\mathcal{H}$ with an involution γ and an antilinear involution J, a real *-algebra $\mathcal{A}$ of bounded operators in $\mathcal{H}$, and a Dirac operator D. Here we would like to give a brief description of these for the standard model; more details are given below in Sec. II.

The Hilbert space $\mathcal{H}$ is the space of classical fermion fields on the space–time manifold M. This is a finite number of Dirac spinors, one for each elementary fermion (left-handed leptons and quarks, right-handed leptons and quarks, and their antiparticles). Thus $\mathcal{H}=\mathcal{H}_M\otimes\mathcal{H}_F$, where $\mathcal{H}_M$ is the Hilbert space of Dirac spinors on M and $\mathcal{H}_F$ is the finite-dimensional Hilbert space with the basis of the elementary fermions.

The algebra $\mathcal{A}=\mathcal{A}_M\otimes\mathcal{A}_F$ is the algebra of coordinates on the total space, the product of the space–time with the internal space. While the functions on space–time $\mathcal{A}_M$ commute as usual, the internal space is noncommutative, so that its algebra of coordinates $\mathcal{A}_F$ is a matrix algebra. The operator J is charge conjugation, while γ is the chirality operator. Finally the Dirac operator contains all the bosonic fields (metric, gauge fields and Higgs), as well as the parameters for the fermion masses and their mixing angles.

In Ref. 4, Connes and Chamseddine formulated a very simple formula for the action for this data, called the spectral action. The action is

$$\mathrm{Tr}(\chi(D^2)) + (\psi, D\psi) \tag{1}$$

with $\psi\in\mathcal{H}$ the fermion field and χ a cutoff function on the spectrum of D^2 which interpolates between 1 below a very high-energy cutoff scale (possibly the Planck scale), and 0 above it. Amazingly, there is a class of Dirac operators for which this unpacks to give the very long formula for the full standard model Lagrangian coupled to gravity.

Impressive as this is, there are a number of issues that need to be resolved before it can have a greater impact in particle physics. In the Lagrangian of Ref. 4.

(1) The space–time metric has Euclidean signature.
(2) The fermions are quadrupled. For example, there are separate Dirac spinors for the left-handed electron, right-handed electron and their antiparticles, whereas physically there should be only one.[5,6]
(3) The bare Weinberg angle is predicted as $\sin^2\theta=\frac{3}{8}$. In Ref. 4 this is assumed to be the high energy value, which changes under renormalization. However renormalization does not give the correct experimental value.[7]
(4) The neutrinos are massless. While this is correct for the standard model, observational evidence shows that neutrinos have mass, and so the noncommutative geometry should be extended to account for neutrino masses.

In addition to this, there are some further theoretical puzzles about seemingly ad hoc features of the action. In contrast to the above, these points do not indicate problems with the physics of the model, but raise questions about the mathematical formulation and about the understanding of the standard model in terms of noncommutative geometry.

(5) To obtain the standard model, it is necessary to remove a U(1) gauge field in D by the unimodularity constraint.[1,8,9] It is known that this is equivalent to the requirement that the resulting quantum field theory is anomaly free,[10,11] but the reason for this equivalence is mysterious.
(6) To obtain the standard model, a particular vacuum Dirac operator D_0 is chosen. Are there any theoretical constraints on this choice, or are there many other (nonphysical) variants of the standard model?
(7) Is there an intrinsic definition (in terms of noncommutative geometry) of the set of Dirac operators that the action (1) applies to?

B. Sets of Dirac operators

Our main observation is that the theoretical puzzles are all questions about which is the set of Dirac operators to which the spectral action should be applied. Our contribution is to study what happens when the set of Dirac operators is enlarged to the maximum extent allowed by the axioms.

Accordingly, we first explain the class of Dirac operators which appears in Connes' standard model. In Connes' construction, given a metric (and spin structure) g on M, a vacuum geometry is defined by the Dirac operator on $\mathcal{H}=\mathcal{H}_M\otimes\mathcal{H}_F$,

$$D_0 = D_M \otimes I + \gamma_M \otimes D_F, \tag{2}$$

where D_M is the usual Dirac first-order differential operator of g with the Levi-Civita connection, γ_M is the chirality operator on (M,g) (often denoted γ_5) and D_F is a certain matrix which encodes the vacuum Higgs fields and the fermion mass matrix. The details of D_F are explained below in Sec. II. Then the gauge and Higgs fields for this metric are obtained by the process of internal fluctuations determined by the 1-forms $A=A^*=\Sigma_i a_i[D_0,b_i]$ given a finite set of elements $a_i,b_i \in \mathcal{A}$. The result is the set of Dirac operators

$$\mathcal{D}^g = \{D_0 + A + JAJ^{-1}\}. \tag{3}$$

Note: in an arbitrary dimension the correct formula is $D_0+A+\epsilon' JAJ^{-1}$, where $\epsilon'=\pm 1$ is determined by $JDJ^{-1}=\epsilon' D$; $\epsilon'=1$ in all even dimensions. However the unimodular condition must be taken account of. This restricts to a smaller set of Dirac operators $\mathcal{D}'^g \subset \mathcal{D}^g$ obtained by removing a U(1) gauge field that has charge +1 for all quarks, 0 for leptons, and −1 for antiquarks. Finally, the set of all Dirac operators for the Connes-Chamseddine spectral action is the union of these for all metrics and spin structures,

$$\mathcal{D}_{\mathrm{CC}} = \bigcup_g \mathcal{D}'^g.$$

It appears that a similar construction could be carried out starting with any matrix D_F. The only difficulty would be deciding exactly how the unimodularity condition generalizes; the most physical generalization would be a condition that guarantees the absence of anomalies in the corresponding perturbative quantum field theory.

An answer to question (6) is provided by the observation that the vacuum Dirac operator should be a stationary point for the spectral action. Therefore there are equations which restrict D_0. These equations require that the Higgs fields in D_F are actually at a stationary point of the Higgs potential. There are no constraints on the parameters of the fermion mass matrix.

From the point of view of noncommutative geometry, the Connes-Chamseddine class of Dirac operators is very strange, as its description uses the underlying commutative description of the fields and requires an unexplained choice of D_F which is rather special. From the point of view of physics one can describe this by saying that the Connes-Chamseddine class of Dirac operators treats the gravitational and the bosonic matter degrees of freedom differently; for the bosons the internal fluctuations are used but for the gravitational degrees of freedom, all possible fluctuations of the Dirac operator are used, the internal fluctuations being trivial. This undermines the idea of a geometric unification of matter and gravity.

A much more natural class of operators (alluded to in Ref. 1) is the set $\mathcal{D}$ of all Dirac operators for the standard model $\mathcal{A}$ and $\mathcal{H}$. From a physical point of view, this class is almost certainly too big; however understanding the consequences of choosing $\mathcal{D}$ for the spectral action is a necessary first step towards investigating whether there is a natural class which is larger than $\mathcal{D}_{\mathrm{CC}}$ but smaller than $\mathcal{D}$.

Enlarging the set of Dirac operators for the action has two effects. First, some of the parameters in D_0 which were previously constants now become variables. Second, there are an equal number of new equations of motion which, in the generic situation, will therefore fix the vacuum values of this number of constants. So, for example, taking the extreme case where the set of Dirac

operators is just one Dirac operator, $\{D_0\}$, then there are no equations of motion and so no constraints on any of the parameters in D_F. Then enlarging the class of Dirac operators to the set $\mathcal{D}^g$ given by the internal fluctuations of a vacuum D_0, results in promoting the Higgs vacuum parameters to fields. The corresponding new equations of motion, as noted above, demand that the vacuum values of these parameters lie at the stationary points of the Higgs potential, which is a significant constraint. The gauge fields have equations of motion of course, but these are all compatible with the vacuum values zero, and the unimodularity constraint does not affect the vacuum either. Looking at the class $\mathcal{D}_{\mathrm{CC}}$, one has in addition the Einstein equations for the variation of the metric g.

Enlarging the class further brings the prospect of further Higgs fields and further constraint equations. The danger is that the additional equations may rule out the standard model vacuum, or provide additional fields which contradict phenomenology. However if these dangers do not materialize, there is the major benefit that further equations will provide previously unknown relations between the parameters of the standard model in the fermion mass matrix, and in models which are extended to allow neutrino masses, may have predictive power in constraining the form of the neutrino sector.

In this paper we consider the set $\mathcal{D}$ of all Dirac operators for the given $\mathcal{H}$ and $\mathcal{A}$ for the standard model, and also for the model where $\mathcal{H}$ is enlarged to allow a right-handed neutrino. This approach contrasts with that of Ref. 12, where enlarging the set of Dirac operators was considered by enlarging the algebra $\mathcal{A}$ but staying with the class of inner fluctuations. We assume the vacuum is of the form (2), with g a flat metric. Thus we are essentially ignoring the Einstein equations, which of course would be important on a macroscopic scale (e.g., in cosmology), but not microscopically. We calculate the equations of motion for D_F by requiring that it is stationary for all variations of the action in this class and classify the possible vacua under some simplifying assumptions. Finally the physical relevance of the equations and the vacua we have found is addressed in the concluding remarks.

II. DETAILS OF THE STANDARD MODEL

The internal Hilbert space is

$$\mathcal{H}_F = \mathcal{H}_L \oplus \mathcal{H}_R \oplus \mathcal{H}_L^c \oplus \mathcal{H}_R^c, \tag{4}$$

where

$$\mathcal{H}_L = (\mathbb{C}^2 \otimes \mathbb{C}^n \otimes \mathbb{C}^3) \oplus (\mathbb{C}^2 \otimes \mathbb{C}^n),$$

$$\mathcal{H}_R = ((\mathbb{C} \oplus \mathbb{C}) \otimes \mathbb{C}^n \otimes \mathbb{C}^3) \oplus (\mathbb{C} \otimes \mathbb{C}^n).$$

A basis of $\mathcal{H}_F$ is labelled by the elementary fermions and their antiparticles. The symbol c is used to indicate the subspace represented by the antiparticles, which duplicates the particle space. In either case of $\mathcal{H}_L$ and $\mathcal{H}_R$, the first direct summand is the quarks and the second, the leptons. The first factor in the tensor product is the down/up (or electron/neutrino) doublet, the second factor is the space of n generations, and the third factor, for quarks, is color.

Since the fermions are left or right handed, $\mathcal{H}_F$ is $\mathbb{Z}/2$ graded by the chirality operator $\gamma_F = \mathrm{diag}(1,-1,1,-1)$, using the decomposition (4). The right-handed neutrino ν_R does not occur in the standard model, but we include it as an extension of the standard model which allows neutrino masses. Results for models without the right-handed neutrino can be easily obtained by setting the relevant matrix entries in D_F to zero and dropping the equations obtained by varying them. In the following, explicit matrices are written and so we need a convention for the order of the rows and columns: the quark basis is (d_L, u_L, d_R, u_R), each of which is reproduced in three colors, and a similar basis of singlets for the leptons (e_L, ν_L, e_R, ν_R). The antiparticle bases are correspondingly $(d_L^c, u_L^c, d_R^c, u_R^c)$ and $(e_L^c, \nu_L^c, e_R^c, \nu_R^c)$.

The standard model algebra is

$$\mathcal{A}_F = \mathbb{H} \oplus \mathbb{C} \oplus M_3(\mathbb{C}),$$

where $\mathbb{H}$ are the quaternions. The action of an element (q, λ, m) of $\mathcal{A}_F$ is

$$\rho = \begin{pmatrix} \rho_L & 0 & 0 & 0 \\ 0 & \rho_R & 0 & 0 \\ 0 & 0 & \rho_L^c & 0 \\ 0 & 0 & 0 & \rho_R^c \end{pmatrix}, \tag{5}$$

where $\rho_L = q$ acting on isospin, $\rho_R = \Lambda = \begin{pmatrix} \overline{\lambda} 0 \\ 0 \lambda \end{pmatrix}$ acting on the two isospin scalars, (d_R, u_R) or (e_R, ν_R). The action on the antiparticles is $\rho_L^c = \rho_R^c = m$ acting on the color index for quarks, and $\rho_L^c = \rho_R^c = \lambda$ for leptons. The action is the same for each generation, and we refer to the analogs of the down, up, electron and neutrino in the other generations by the same names.

A real spectral triple possesses a real structure given by an operator J that takes particles into antiparticles and charge conjugation,

$$J \begin{pmatrix} \psi_1 \\ \psi_2^c \end{pmatrix} = \begin{pmatrix} \overline{\psi_2^c} \\ \overline{\psi_1} \end{pmatrix} \in \mathcal{H}.$$

It turns the Hilbert space into a bimodule,

$$a \psi b = a J b^* J^{-1} \psi. \tag{6}$$

Note that

$$[a, J b^* J^{-1}] = 0. \tag{7}$$

Also, J commutes with $\gamma = \gamma_M \otimes \gamma_F$.

This data satisfies an axiom called Poincaré duality, which is the generalization of the familiar Poincaré duality of manifolds to noncommutative geometry. While this axiom is a natural generalization from the mathematical point of view, its physical meaning for the internal space is unclear. Applied to the internal geometry, the axiom is satified for the standard model but not if there is the same number of left- and right-handed neutrinos.[13] However it is satisfied if one of the generations does not have a right-handed neutrino but the other two do. In the following we do not require that the Poincaré duality axiom holds.

So far, we have explained some of the axioms relating to the Hilbert space and the algebra for the standard model finite triple. The final ingredient is the Dirac operator. A Dirac operator must satisfy the first order condition:

$$[[D, a], J b^* J^{-1}] = 0 \tag{8}$$

for all $a, b \in \mathcal{A}$ in order that D be a first order differential operator.[14] Note that due to (7), this implies that also $[[D, J b^* J^{-1}], a] = 0$.

The choice made for D_F in Ref. 4 in order that the spectral action principle reproduces the standard model is

$$D_F = \begin{pmatrix} 0 & M^* & 0 & 0 \\ M & 0 & 0 & 0 \\ 0 & 0 & 0 & M^T \\ 0 & 0 & \overline{M} & 0 \end{pmatrix}, \tag{9}$$

where $M = Q \otimes 1_3 \oplus L$

$$Q^* = \begin{pmatrix} k_d\phi_1 & k_u\overline{\phi}_2 \\ k_d\phi_2 & -k_u\overline{\phi}_1 \end{pmatrix},$$

$$L^* = \begin{pmatrix} k_e\phi_1 & 0 \\ k_e\phi_2 & 0 \end{pmatrix},$$

with

$$k_u = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_c & 0 \\ 0 & 0 & m_t \end{pmatrix}, \quad k_d = V_{\mathrm{CKM}} \begin{pmatrix} m_d & 0 & 0 \\ 0 & m_s & 0 \\ 0 & 0 & m_b \end{pmatrix},$$

$$k_e = \begin{pmatrix} m_e & 0 & 0 \\ 0 & m_\mu & 0 \\ 0 & 0 & m_\tau \end{pmatrix}.$$

M^T denotes the transpose, M^* denotes Hermitian conjugate, $\overline{M}$ denotes the complex conjugate matrix, m_x are the Yukawa couplings of the elementary fermions, V_{CKM} is the Cabibbo-Kobayashi-Maskawa generation mixing matrix, and (ϕ_1, ϕ_2) is the Higgs scalar doublet.

III. THE GENERAL D_F

The problem of finding the vacua reduces in essence to considering a single point of space–time. We simplify the action formula (1) by removing all terms involving the space–time curvature, and all kinetic terms, and set the gauge fields to zero. This is equivalent to varying the Dirac operator over all operators of the form (2), with a fixed D_M. By inspecting the heat expansion detailed in Ref. 15 we find that the action we are looking for is

$$S = \mathrm{Tr}(D_F^4 - 2D_F^2). \tag{10}$$

This formula gives the Higgs potential for internal fluctuations of the standard model vacuum. However it applies to the wider class of operators $\mathcal{D}$.

In order to find the most general D_F for the standard model internal space, we employ the constraints given by the axioms for a 0-dimensional noncommutative space. Only the axioms involving the Dirac operator are listed here.

(i) Self-adjointness, $D_F = D_F^*$.

(ii) Reality, $[D_F, J] = 0$.
These first two imply that, splitting the Dirac operator into four blocks corresponding to the particle/antiparticle split of the basis,

$$D_F = \begin{pmatrix} Y & Z \\ \overline{Z} & \overline{Y} \end{pmatrix}, \tag{11}$$

where $Y = Y^*$ and $Z = Z^T$.

(iii) Orientability, $D_F\gamma_F + \gamma_F D_F = 0$, implies that

$$D_F = \begin{pmatrix} Y & Z \\ \overline{Z} & \overline{Y} \end{pmatrix} = \begin{pmatrix} 0 & M^* & 0 & G \\ M & 0 & G^T & 0 \\ 0 & \overline{G} & 0 & M^T \\ G^* & 0 & \overline{M} & 0 \end{pmatrix} \tag{12}$$

using a further split of each block into the left/right subspaces. In this formula M and G are general matrices with complex coefficients, M giving a generalization of the mass matrix of the standard model and G having the interpretation of Majorana mass terms and other interactions.

If the vacuum Dirac operator generates Majorana masses then the model is no longer the standard model but a modification of it. In this modified model, the generation of Majorana masses involves symmetry breaking with new scalar fields, in addition to the Higgs fields. This introduction of new fields is not necessarily undesirable because any new physics of fermion masses must necessarily go beyond the standard model.

The remaining axiom is the following.

(iv) First order condition, $[[D_F, a], Jb^*J^{-1}]=0$. The effect of applying the first order condition to (12) is to determine which elements of M and G are nonzero.

In Ref. 16, Krajewski shows that for any finite dimensional spectral triple, the Dirac operator solves the first order condition uniquely in the form of the sum, $D_F=D_L+D_R$ where D_R commutes with any element $b^o=Jb^*J^{-1}$ in the opposite algebra and D_L commutes with any element in the algebra. See also Ref. 17. Using these formulas

$$D_L a - aD_L = 0, \quad D_R b^o - b^o D_R = 0 \tag{13}$$

and using the representation as given above (5) we find that

$$D_L = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & G^T & 0 \\ 0 & \overline{G} & 0 & M^T \\ 0 & 0 & \overline{M} & 0 \end{pmatrix} \tag{14}$$

and

$$D_R = \begin{pmatrix} 0 & M^* & 0 & G \\ M & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ G^* & 0 & 0 & 0 \end{pmatrix} \tag{15}$$

with $M=Q\otimes 1_3 \oplus L$, a direct sum of a quark matrix Q which commutes with color, and a lepton matrix L. Both Q and L are arbitrary 4×4 complex matrices (for one generation). For three generations, these become arbitrary 12×12 matrices. The other matrix is in block form

$$G = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & U & 0 & N \end{pmatrix}, \tag{16}$$

using the basis explained in Sec. II, i.e., a map $(d_R^c, u_R^c, e_R^c, \nu_R^c) \mapsto (d_L, u_L, e_L, \nu_L)$. The nonzero entries are the blocks U and N. These are maps

$$U: u_R^c \mapsto (e_L, \nu_L)$$

and

$$N: \nu_R^c \mapsto (e_L, \nu_L).$$

Their appearance results from the fact that u_R^c, ν_R^c, and e_L and ν_L are all in the same representation of the opposite algebra $\mathcal{A}^o$, multiplication by the complex number λ. The other entries of G are zero because they are intertwining inequivalent representations. Note that the matrix $\overline{G}$ gives maps $u_R \mapsto (e_L^c, \nu_L^c)$ and $\nu_R \mapsto (e_L^c, \nu_L^c)$.

Explicitly, for one generation we use the matrices

$$Q = \begin{pmatrix} d & c \\ b & a \end{pmatrix}, \quad L = \begin{pmatrix} q & r \\ s & t \end{pmatrix}, \tag{17}$$

$$U = \begin{pmatrix} x & u & g \\ y & v & h \end{pmatrix}, \quad N = \begin{pmatrix} j \\ l \end{pmatrix}, \tag{18}$$

(x,u,g), (y,v,h) are three-dimensional color vectors and j, l are color singlets.

It is also convenient to split Q and L into smaller blocks corresponding to the gauge-invariant split of the right-handed fermions into down/up or electron/neutrino:

$$Q = \begin{pmatrix} Q_d \\ Q_u \end{pmatrix}, \quad L = \begin{pmatrix} L_e \\ L_\nu \end{pmatrix}. \tag{19}$$

For example, for one generation this means that $L_e = (q\ r)$, etc.

The nonzero entries give rise to terms in the fermionic part of the action (1) given, for one generation, by

$$(\psi_L^c, \overline{G}\psi_R) = (e_L^c, (\overline{x,u,g}) \cdot u_R) + (\nu_L^c, (\overline{y,v,h}) \cdot u_R) + (e_L^c, \overline{j}\nu_R) + (\nu_L^c, \overline{l}\nu_R),$$

$$(\psi_R^c, G^*\psi_L) = (\nu_R^c, \overline{j}e_L) + (\nu_R^c, \overline{l}\nu_L) + (u_R^c, (\overline{x,u,g})e_L) + (u_R^c, (\overline{y,v,h})\nu_L),$$

plus the Hermitian conjugate of each term, which are $(\psi_R, G^T\psi_L^c)$ and $(\psi_L, G\psi_R^c)$, respectively. Thus the action contains, for example,

$$(\nu_R^c, \overline{l}\nu_L) + (\nu_L^c, \overline{l}\nu_R) + (\nu_L, l\nu_R^c) + (\nu_R, l\nu_L^c).$$

This action is plausibly the Euclidean analog of a Majorana mass term; but note that significant differences between the Euclidean and Minkowskian formulation mean that this is somewhat heuristic. The fields U have been studied before in the context of the noncommutative standard model and are called leptoquarks,[18] while the N are new fields which are of course absent if the right-handed neutrino is not included in the model.

Relatively recently there has been new experimental evidence for neutrinos being massive. There are two possibilities for theoretical neutrino mass generation, the Dirac mass and the Majorana mass term. For a particle to have a Dirac mass, both chiralities must be present, so this would require ν_R and thus a modification of the standard model. To justify existence of the ν_R, there must be an explanation as to why it remains undetected; it must either be extremely massive or sterile (not interacting). A Majorana mass term is possible without ν_R, but it requires an SU(2) Higgs triplet; many models include ν_R and a combination of Majorana and Dirac mass terms to render ν_R very heavy while leaving ν_L relatively light.

IV. EQUATIONS OF MOTION

The overall aim is to see if the standard model vacuum D_F can be found as a solution of the internal space equations without making any assumptions other than the axioms themselves, instead of making the choice (9) motivated from laboratory evidence. To this end, we need to vary *all* the degrees of freedom of D_F which means that the Yukawa couplings, and generation mixing

angles (plus all the other fluctuations) are no longer viewed as constants but as dynamical variables. In other words, we let $\mathcal{D}=\{D_F\}$ form the configuration space of the theory and calculate the internal space equations of motion.

To calculate the internal space equations of motion, we minimize the action (10) with respect to the degrees of freedom of both M and G. The action is

$$\begin{aligned} S &= \mathrm{Tr}(-2D_F^2 + (D_F)^4) \\ &= \mathrm{Tr}(-2(G^*G + M^*M) + (M^*M)^2 + (G^*G)^2 + 2(M^*MGG^* + MM^*G^T\overline{G} + MG\overline{MG})) \\ &= \mathrm{Tr}\Big(-(LL^* + 3QQ^* + UU^* + NN^*) + \tfrac{1}{2}((L^*L)^2 + 3(Q^*Q)^2 + (UU^* + NN^*)^2) \\ &\quad + L^*L(UU^* + NN^*) + L_\nu L_\nu^* N^T\overline{N} + (Q_u Q_u^* \otimes I_3)U^T\overline{U}\Big). \end{aligned} \tag{20}$$

The results for varying with respect to Q, L, U, and N are, respectively,

$$Q^*\left(-3I + 3QQ^* + \begin{pmatrix} 0 & 0 \\ 0 & \mathrm{Tr}_{\mathrm{col}}(U^T\overline{U}) \end{pmatrix}\right) = 0, \tag{21}$$

$$-L^* + L^*LL^* + (UU^* + NN^*)L^* + (0\ L_\nu^* N^T\overline{N}) + (0\ N\overline{L_\nu}\,\overline{N}) = 0, \tag{22}$$

$$U^*(-I + UU^* + NN^* + L^*L) + (\overline{Q_u}Q_u^T \otimes I_3)U^* = 0, \tag{23}$$

$$-N^* + N^*UU^* + N^*NN^* + N^*L^*L + \overline{L_\nu}L_\nu^T N^* + \overline{L_\nu}\,\overline{N}L_\nu = 0. \tag{24}$$

In Eq. (21), the matrix is split into blocks according to the down/up split of the basis, and $\mathrm{Tr}_{\mathrm{col}}$ denotes the trace over color degrees of freedom. Thus each matrix block has size $n\times n$, where n is the number of generations.

In the following we analyze the solutions of these equation in various special cases, and then make some remarks about the general case.

V. SOLUTIONS WITH $G=0$

With $U=0$ and $N=0$, the equations of motion reduce to

$$Q^*(QQ^* - I) = 0, \tag{25}$$

$$L^*(LL^* - I) = 0. \tag{26}$$

By multiplying (25) on the left by Q, we see that QQ^* is a self-adjoint projection, and by multiplying the conjugate on the left by Q^* that Q^*Q is also a projector. Therefore, by definition, $Q \in M_n(\mathbb{C})$ is a partial isometry. Another characterization of a partial isometry is that it is a projector multiplied by a unitary matrix. Obviously the same conclusion applies for L.

These equations are the same as the ones obtained from assuming the additional S^0-reality axiom,[3] which has the effect that U and N are equal to zero in the action.

The standard model vacuum (9) is clearly not a solution of our equations. To see this, we write down MM^*,

$$\begin{pmatrix} k_d^* k_d(|\phi_1|^2+|\phi_2|^2) & 0 & 0 \\ 0 & k_u^* k_u(|\phi_1|^2+|\phi_2|^2) & 0 \\ 0 & 0 & k_e^* k_e(|\phi_1|^2+|\phi_2|^2) \\ 0 & 0 & 0 \end{pmatrix} \tag{27}$$

so the vacua satisfying our equations of motion have degenerate fermion masses that are either 0 or 1 (times a constant, which has been omitted from the action). We note that in the case in which ν_R is absent, the left-handed neutrino is necessarily massless. This is a consequence of the fact that L is not a square matrix in that case.

The impact of the following sections is to explore the way in which lifting the assumption of S^0-reality allows further vacua with U or N not equal to zero.

VI. SOLUTIONS WITH $G \neq 0$

A. General

Throughout we assume that the quark mass matrix Q is nondegenerate. This means that Q^* can be cancelled from (21) to give

$$-3I + 3QQ^* + \begin{pmatrix} 0 & 0 \\ 0 & \mathrm{Tr}_{\mathrm{col}}(U^T\overline{U}) \end{pmatrix} = 0. \tag{28}$$

This equation can be solved for QQ^*, and thus for Q, up to multiplication on the right-hand side by a unitary operator, which is a symmetry. One very important feature (not always shared by the degenerate case) is that QQ^* is block diagonal. This is an important feature of the standard model vacuum. Indeed, using the split (19), the equation becomes the three equations

$$Q_d Q_d^* = I,$$

$$Q_d Q_u^* = 0,$$

$$Q_u Q_u^* = I - \tfrac{1}{3}\mathrm{Tr}_{\mathrm{col}}(U^T\overline{U})$$

which shows that the down-quark masses are all equal to 1, the block-diagonal feature, and that the up-quark masses are split by a nonzero U. It is worth noting that the condition $Q_d Q_u^* = 0$ fixes the form of Q_u in the standard model vacuum (9) if Q_d is given the correct form. However there is no equation which constrains Q_d to have the special form of (9).

B. One generation

For one generation of fermions, we use the explicit matrices of (17) and (18). The equations of motion are written out in the appendix. Equation (21) becomes (A1)–(A4) and (22) becomes (A5)–(A8) and (23) becomes (A9)–(A14) and (24) becomes (A15) and (A16).

The equation (28) becomes the following:

$$|c|^2 + |d|^2 - 1 = 0, \tag{29}$$

$$a\overline{c} + \overline{b}d = 0, \tag{30}$$

$$3|a|^2 + 3|b|^2 + |g|^2 + |u|^2 + |x|^2 + |h|^2 + |v|^2 + |y|^2 - 3 = 0. \tag{31}$$

As above, (30) implies that QQ^* is a diagonal matrix.

1. Solutions with $U=0$, $N\neq 0$

In this case, Q decouples from the other fields and its equation reduces to (25). Thus Q is a unitary matrix and the quark masses are all equal to 1. To present the solutions to these equations we have used the symmetry afforded by a 2×2 unitary matrix acting on e_L and ν_L to simplify one of the vectors (q,r), (s,t) or (j,l).

The possible solutions are all equivalent to

(i) $q=1$, $s=t=r=0$, $j=0$, $|l|=1$,
(ii) $q=r=s=0$, $|t|^2+|j|^2=1$, $l=0$,
(iii) $q=1$, $s=r=0$, $|t|=1/2$, $j=0$, $|l|=1/2$,
(iv) $q=0$, $s=r=0$, $|t|=1/2$, $j=0$,$|l|=1/2$,
(v) $r=s=t=0$, $|q|^2+|j|^2=1$, $l=0$.

The proof that these are the only solutions is to consider combining the equations $N^*(22)-(24)L^*$. This leads to a set of algebraic conditions which reduce to the given solutions when substituted into the full equations of motion.

2. Solutions with $U\neq 0$

We have been unable to find any explicit one-generation solutions with nonzero leptoquarks U. For the case where the quark and electron masses in the mass matrix M are nonzero, we can prove that there are no such solutions. This has the corollary that there are no solutions where the matrix M takes the form of a one-generation version of the standard model vacuum (9).

The argument is as follows. Using a symmetry as above, we may assume that $r=0$ and $q\neq 0$. Combining (A6), (A5), and (A9) shows that $g=0$, since $|a|^2+|b|^2\neq 0$. Similarly, $u=x=0$. Then (A10) and (31) imply either $h=0$ or $\frac{2}{3}(|v|^2+|h|^2+|y|^2)+|l|^2+|t|^2=0$, which also implies $h=0$. A similar argument shows $v=y=0$. Hence $U=0$.

If additionally, $N=0$, then the same conclusion also holds if the electron mass $q=0$ (see Sec. VI C below).

It is worth noting that the solutions considered here in the case that $L_\nu=0$ are the same as for the system obtained by omitting the right-handed neutrino ν_R from the action.

C. Three generations

For three generations we do not have complete results but note that the equations are of course solved by aggregating three one-generation solutions. In addition we outline some general features of the solutions. We continue to assume that the quark masses are all nonzero; thus the remarks of Sec. VI A continue to hold. A general feature of the solutions to the equations can be found by taking the combination of equations $U^*(22)-(23)L^*$. This gives the equation

$$L_e U=0.$$

In the case where $N=0$, it also shows that

$$L_\nu U=0$$

and Eq. (23) reduces to

$$\left(U^*U-\tfrac{1}{3}\mathrm{Tr}_{\mathrm{col}}(U^*U)\otimes I_3\right)U^*=0$$

from which follows that

$$U^*U=C\otimes I_3$$

for some 3×3 matrix C. Since the rank of U^*U is at most 6, C has rank at most 2. As a consequence, only two out of the three up quarks, charm and top are given different masses from that of the three down-family quarks.

The corresponding argument for one generation shows that the rank of U^*U is at most 2, and hence C must be zero. This agrees with the result found explicitly in the preceding section, and holds even if $q=0$.

VII. CONCLUSIONS

We have attempted to understand the standard model vacuum from a fundamental point of view involving noncommutative geometry. In particular, the question is: why does nature pick one particular vacuum geometry, i.e., one particular set of parameters in the fermion mass matrix? To attack this question, we investigated the simplest possible Ansatz for the set of Dirac operators in the action which is to promote all the degrees of freedom of the internal geometry, including the mass parameters, to be dynamical fields. This gives additional equations of motion which complement the usual Einstein and matter equations. The conclusion is that these equations exclude the standard model vacuum. Therefore there is something unexplained about either the physics of the standard model or the geometry of spectral triples. This is our overall conclusion.

The main problem is that the simplest solutions involve an unwanted degeneracy in the masses of the fermions. However there are some quite complicated vacua in which this problem is partially alleviated. Allowing an extension of the model to include a right-handed neutrino lifts the degeneracy of the lepton Dirac masses via Eq. (22) in some solutions. The potential occurence of leptoquark fields lifts the degeneracy of the up-quark Dirac masses to some extent, but the degeneracy of the down quarks remains. In practice it seems to be hard to find vacua with nonzero values of the leptoquark field. With one generation and reasonable assumptions, the leptoquarks are always equal to zero. This is in a sense reassuring because the leptoquarks would break color symmetry, but it does not help with the problem of quark mass degeneracy. With three generations, leptoquark fields are possible but we have found solutions affecting at most two out of the three generations, thus giving some sort of consistency with the one-generation result.

Some features of the very special standard model vacuum are automatically incorporated, whereas others are not. In particular there are typically many Higgs fields and there appears to be no constraint which forces the Higgs for the leptons and the quarks to be the same field. One can see this in our results for one generation. Since it is not possible to diagonalize both Q and L with a single unitary transformation, the parameters q, r, a, and b are independent, providing two Higgs doublets.

The extension to include the right-handed neutrino also introduces potential Majorana mass terms for the leptons. The explicit solutions we found allow (i) a Dirac mass for the electron and a Majorana mass for the neutrino, (ii) a Dirac mass for the neutrino and a mixing between ν_R and e_L, (iii) a Dirac mass for the electron and a neutrino with both Dirac and Majorana mass terms, (iv) a massless electron with a neutrino with both Dirac and Majorana mass terms, and (v) a Dirac mass for the electron and a massless neutrino with a mixing between ν_R and e_L. Further calculations show that in each case the Majorana term is such that the eigenvalues of D always remain 0 or $+/-1$. However it is worth emphasizing that there are differences between the Euclidean and Lorenzian formulations for fermions which make it difficult to draw conclusions from this for the physical Lorentzian case. In spite of this our overall conclusion that the masses are too degenerate stands, and this points to the need for modifications to the formalism if the overall objectives are to be retained. In the future this could possibly be carried out by adding more constraints to the space of Dirac operators or by additional terms to the spectral action.

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APPENDIX

The equations of motion for one generation and three colored quarks are the following:

$$\overline{a}(3|a|^2+3|c|^2+3|b|^2+|g|^2+|u|^2+|x|^2+|h|^2+|v|^2+|y|^2-3)+3\overline{c}\overline{b}\overline{d}=0, \tag{A1}$$

$$\overline{b}(3|b|^2+3|d|^2+|g|^2+|u|^2+|x|^2+|h|^2+|v|^2+|y|^2+3|a|^2-3)+3\overline{a}\overline{d}\overline{c}=0, \tag{A2}$$

$$\overline{c}(|a|^2+|c|^2+|d|^2-1)+\overline{a}\overline{d}\overline{b}=0, \tag{A3}$$

$$\overline{d}(|b|^2+|d|^2+|c|^2-1)+\overline{c}\overline{b}\overline{a}=0, \tag{A4}$$

$$\overline{q}(|q|^2+|s|^2+|r|^2+|g|^2+|u|^2+|x|^2+|j|^2-1)+\overline{r}(\overline{h}\overline{g}+\overline{v}\overline{u}+\overline{y}\overline{x}+\overline{l}\overline{j}+\overline{s}\overline{t})=0, \tag{A5}$$

$$\overline{r}(|r|^2+|t|^2+|q|^2+|h|^2+|v|^2+|y|^2+|l|^2-1)+\overline{q}(\overline{g}\overline{h}+\overline{u}\overline{v}+\overline{x}\overline{y}+\overline{j}\overline{l}+\overline{t}\overline{s})=0, \tag{A6}$$

$$\overline{s}(3|j|^2+|q|^2+|s|^2+|t|^2+|g|^2+|u|^2+|x|^2+|l|^2-1)+\overline{t}(\overline{h}\overline{g}+\overline{v}\overline{u}+\overline{y}\overline{x}+2\overline{l}\overline{j}+\overline{q}\overline{r})=0, \tag{A7}$$

$$\overline{t}(3|l|^2+|r|^2+|t|^2+|s|^2+|h|^2+|v|^2+|y|^2+|j|^2-1)+\overline{s}(\overline{g}\overline{h}+\overline{u}\overline{v}+\overline{x}\overline{y}+2\overline{j}\overline{l}+\overline{r}\overline{q})=0, \tag{A8}$$

$$\overline{g}(|g|^2+|u|^2+|x|^2+|h|^2+|j|^2+|q|^2+|s|^2+|a|^2+|b|^2-1)+\overline{h}(\overline{r}\overline{q}+\overline{x}\overline{y}+\overline{u}\overline{v}+\overline{t}\overline{s}+\overline{j}\overline{l})=0, \tag{A9}$$

$$\overline{h}(|g|^2+|v|^2+|h|^2+|y|^2+|l|^2+|r|^2+|t|^2+|a|^2+|b|^2-1)+\overline{g}(\overline{q}\overline{r}+\overline{y}\overline{x}+\overline{v}\overline{u}+\overline{s}\overline{t}+\overline{l}\overline{j})=0, \tag{A10}$$

$$\overline{u}(|u|^2+|g|^2+|x|^2+|v|^2+|j|^2+|q|^2+|s|^2+|a|^2+|b|^2-1)+\overline{v}(\overline{r}\overline{q}+\overline{x}\overline{y}+\overline{g}\overline{h}+\overline{t}\overline{s}+\overline{j}\overline{l})=0, \tag{A11}$$

$$\overline{v}(|u|^2+|v|^2+|h|^2+|y|^2+|l|^2+|r|^2+|t|^2+|a|^2+|b|^2-1)+\overline{u}(\overline{q}\overline{r}+\overline{y}\overline{x}+\overline{h}\overline{g}+\overline{s}\overline{t}+\overline{l}\overline{j})=0, \tag{A12}$$

$$\overline{x}(|u|^2+|g|^2+|x|^2+|y|^2+|j|^2+|q|^2+|s|^2+|a|^2+|b|^2-1)+\overline{y}(\overline{r}\overline{q}+\overline{u}\overline{v}+\overline{g}\overline{h}+\overline{t}\overline{s}+\overline{j}\overline{l})=0, \tag{A13}$$

$$\overline{y}(|x|^2+|v|^2+|h|^2+|y|^2+|l|^2+|r|^2+|t|^2+|a|^2+|b|^2-1)+\overline{x}(\overline{q}\overline{r}+\overline{v}\overline{u}+\overline{h}\overline{g}+\overline{s}\overline{t}+\overline{l}\overline{j})=0, \tag{A14}$$

$$\overline{j}(3|s|^2+|j|^2+|g|^2+|u|^2+|x|^2+|l|^2+|t|^2+|q|^2-1)+\overline{l}(\overline{r}\overline{q}+2\overline{t}\overline{s}+\overline{g}\overline{h}+\overline{u}\overline{v}+\overline{x}\overline{y})=0, \tag{A15}$$

$$\overline{l}(3|t|^2+|h|^2+|v|^2+|y|^2+|j|^2+|l|^2+|r|^2+|s|^2-1)+\overline{j}(\overline{q}\overline{r}+2\overline{s}\overline{t}+\overline{h}\overline{g}+\overline{v}\overline{u}+\overline{y}\overline{x})=0. \tag{A16}$$

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Motion in Kaluza-Klein type theories

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Path and path deviation equations for charged, spinning and spinning charged objects in different versions of Kaluza-Klein (KK) theory using a modified Bazanski Lagrangian have been derived. The significance of motion in five dimensions, especially for a charged spinning object, has been examined. We have also extended the modified Bazanski approach to derive the path and path deviation equations of a test particle in a version of non-symmetric KK theory. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196749]

I. INTRODUCTION

In an attempt to unify gravity and electromagnetism Kaluza (1921) introduced a fifth dimension to describe electromagnetism. Klein (1926) added a stringent cylindrical condition, which keeps the extra dimension compact.[1] Following the scheme of compactification many theories have developed Kaluza-Klein (KK) ideas and extended the process of compactification to include higher dimensions as a way to unify many fields.[2] However, Wesson *et al.*[3] have considered unification of geometry with matter by dropping the cylindrical condition, and introducing non-compact theories of higher dimensions based geometrically on the Campbell-Magaard theorem. This approach has been emerged into two classes of non-compact theories: brane theories[4] and space-time-matter theories.[5]

From this perspective, path and path deviation equations play a vital part to interpret the behavior of any particle describing any of the above-mentioned theories. These equations offer a way to test the new physics coming from the introduction of extra dimensions.[6] The behavior of test particles and extended objects could be used for examining additional phenomena embedded in higher dimensions. Accordingly, we present a study of path and path deviation equations for charged, spinning, and spinning charged objects using different theories of KK. The path and path deviation equations could also be used to detect the cosmological variation of spin, and to study the evolution of the angular momentum of galaxies, pulsars, and high energy primordial objects[7] using a gyroscopic motion in five dimensions. KK theories have been extended to include different types of non-symmetric theory of gravity. One such trial has been done by Kalinowski to unify gravity and gauge fields using a multidimensional manifold in the Jordan-Thirry manner.[8]

The aim of the present work is to extend the Bazanski approach[9] into five dimensions (5D) in order to derive some versions of path and path deviation equations in multidimensional space for different objects such as charged, spinning, and spinning charged particles, with taking the status of extra dimension as either compact or non-compact. The paper is organized into the following steps:

(1) Describing path equations and their corresponding path deviation equations in four dimensions (4D).
(2) Extending these equations into 5D.

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II. MOTION IN 4D

A. Path and path deviation equations in Riemannian geometry

Geodesic and geodesic deviation equations can be obtained simultaneously by applying the action principle on the Bazanski Lagrangian:[9]

$$L = g_{\alpha\beta} U^{\alpha} \frac{D\Psi^{\beta}}{Ds}, \tag{1}$$

where D/Ds is the covariant derivative. This can be done if one takes the variation with respect to the deviation vector Ψ^{ρ} in order to derive the geodesic equation:

$$\frac{dU^{\alpha}}{ds} + \left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\} U^{\mu} U^{\nu} = 0, \tag{2}$$

where $\left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\}$ is the Christoffel symbol. If one takes the variation with respect to the unit tangent vector U^{ρ}, one derives the geodesic deviation equation:

$$\frac{D^2\Psi^{\alpha}}{Ds^2} = R^{\alpha}_{.\beta\gamma\delta} U^{\beta} U^{\gamma} \Psi^{\delta}, \tag{3}$$

where $R^{\alpha}_{\beta\gamma\delta}$ is the Riemann-Christoffel curvature tensor. It is worth mentioning that the Bazanski approach has been successfully applied in geometries different from the Riemannian.[10,11] Now, Lagrangian (1) can be amended to describe path and path deviation equations of charged, spinning, and spinning charged particles if we introduce the following Lagrangian:

$$L = g_{\alpha\beta} U^{\alpha} \frac{D\Psi^{\beta}}{Ds} + f_{\beta} \Psi^{\beta} \tag{4}$$

such that

$$f_{\beta} = a_1 F_{\alpha\beta} U^{\beta} + a_2 R_{\alpha\beta\gamma\delta} S^{\gamma\delta} U^{\alpha},$$

where a_1 and a_2 are parameters that may take the values e/m and $1/2m$, respectively, $F^{\mu}_{.\nu}$ is an electromagnetic tensor and $S^{\gamma\delta}$ is the spin tensor. These parameters have to be adjusted with their counterparts in the original Lorentz force equation,[12] the Papapetrou equation,[13] and the Dixon equation.[14]

Applying the Bazanski approach for obtaining path and path deviation equations on Lagrangian (4) we get the following.

(i) The Lorentz charged equation (for $a_1 = e/m$ and $a_2 = 0$),

$$\frac{\mathrm{d}U^{\alpha}}{ds} + \left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\} U^{\mu} U^{\nu} = \frac{e}{m} F^{\mu}_{.\nu} U^{\nu}, \tag{5}$$

and the charged deviation equation:[15]

$$\frac{D^2\Psi^{\alpha}}{Ds^2} = R^{\alpha}_{.\mu\nu\rho} U^{\mu} U^{\nu} \Psi^{\rho} + \frac{e}{m} \left(F^{\alpha}_{.\nu} \frac{D\Psi^{\nu}}{Ds} + F^{\alpha}_{.\nu;\rho} U^{\nu} \Psi^{\rho} \right). \tag{6}$$

(ii) The Papapetrou equation for spinning objects (for $a_1 = 0$ and $a_2 = 1/2m$)

$$\frac{\mathrm{d}U^{\alpha}}{\mathrm{d}s} + \left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\} U^{\mu} U^{\nu} = \frac{1}{2m} R^{\alpha}_{.\mu\nu\rho} S^{\nu\rho} U^{\mu}. \tag{7}$$

The spinning deviation equation becomes[16]

$$\frac{D^2\Psi^\alpha}{Ds^2} = R^\alpha_{.\mu\nu\rho}U^\mu U^\nu\Psi^\rho + \frac{1}{2m}\left(R^\alpha_{.\mu\nu\rho}S^{\nu\rho}\frac{D\Psi^\mu}{Ds} + R^\alpha_{\mu\nu\lambda}S^{\nu\lambda}_{\ \ :\rho}U^\mu\Psi^\rho + R^\alpha_{\mu\nu\lambda;\rho}S^{\nu\lambda}U^\mu\Psi^\rho\right). \tag{8}$$

(iii) The Dixon equation for spinning charged objects (for $a_1=e/m$ and $a_2=1/2m$)[14]

$$\frac{\mathrm{d}U^\alpha}{\mathrm{d}s} + \left\{\begin{matrix}\alpha\\ \mu\nu\end{matrix}\right\}U^\mu U^\nu = \frac{e}{m}F^\mu_{\ .\nu}U^\nu + \frac{1}{2m}R^\alpha_{.\mu\nu\rho}S^{\nu\rho}U^\mu, \tag{9}$$

and its spinning charged deviation equation becomes

$$\frac{D^2\Psi^\alpha}{Ds^2} = R^\alpha_{.\mu\nu\rho}U^\mu U^\nu\Psi^\rho + \frac{e}{m}\left(F^\mu_{\ .\nu}\frac{D\Psi^\nu}{Ds} + F^\mu_{\ .\nu;\rho}U^\nu\Psi^\rho\right)$$
$$+ \frac{1}{2m}\left(R^\alpha_{.\mu\nu\rho}S^{\nu\rho}\frac{D\Psi^\mu}{Ds} + R^\alpha_{.\mu\nu\lambda;\rho}S^{\nu\lambda}U^\mu\Psi^\rho + R^\alpha_{.\mu\nu\lambda}S^{\nu\lambda}_{\ \ ;\rho}U^\mu\Psi^\rho\right). \tag{10}$$

Papapetrou[17] has derived an equation describing a spinning object which is able to precess:

$$\frac{D}{Ds}\left(mU^\alpha + U_\rho\frac{DS^{\alpha\rho}}{Ds}\right) = \frac{1}{2}R^\alpha_{.\mu\nu\rho}S^{\nu\rho}U^\mu. \tag{11}$$

Using the Bazanski approach, we can suggest the following Lagrangian:

$$L = g_{\alpha\beta}\left(mU^\alpha + U_\rho\frac{DS^{\alpha\rho}}{Ds}\right)\frac{D\Psi^\beta}{Ds} + R_{\alpha\beta\gamma\delta}S^{\gamma\delta}U^\beta\Psi^\alpha, \tag{12}$$

which can be used to derive Eq. (11) and to obtain its corresponding deviation equation in the following way:

$$\frac{D^2\Psi^\alpha}{Ds^2} = R^\alpha_{.\mu\nu\rho}U^\mu\left(mU^\nu + U_\beta\frac{DS^{\nu\beta}}{Ds}\right)\Psi^\rho + g^{\alpha\sigma}g_{\nu\lambda}\left(mU^\lambda + U_\beta\frac{DS^{\lambda\beta}}{Ds}\right)_{;\sigma}\frac{D\Psi^\nu}{Ds} + R^\alpha_{.\mu\nu\rho}S^{\nu\rho}\frac{D\Psi^\mu}{Ds}$$
$$+ R^\alpha_{\mu\nu\lambda}S^{\nu\lambda}_{\ \ :\rho}U^\mu\Psi^\rho + R^\alpha_{\mu\nu\lambda;\rho}S^{\nu\lambda}U^\mu\Psi^\rho. \tag{13}$$

B. Path and path deviation equations in non-symmetric geometries

Path equations in one of the versions of non-symmetric geometries, e.g., Legaré and Moffat, have been derived from following Lagrangian:[18]

$$L = g_{(\mu\nu)}U^\mu U^\nu + \lambda\hat{A}_\nu U^\nu, \tag{14}$$

by taking the variation with respect to U^σ to give

$$\frac{dU^\alpha}{ds} + \left\{\begin{matrix}\alpha\\ \mu\nu\end{matrix}\right\}U^\mu U^\nu = \lambda g^{(\alpha\mu)}f_{[\mu\nu]}U^\nu, \tag{15}$$

where $g_{(\mu\nu)}$ is the symmetric part of the gravitational potential tensor, λ is a parameter and, $f_{[\mu\nu]}=\hat{A}_{\mu,\nu}-\hat{A}_{\nu,\mu}$ is a skew symmetric tensor related to the Yukawa force.

Applying the Bazanski approach, we can derive (15) from the following Lagrangian:

$$L = g_{(\alpha\beta)}U^\alpha\frac{D\Psi^\beta}{Ds} + \lambda f_{\nu\rho}\Psi^\nu U^\rho. \tag{16}$$

Using the same approach, we can show its corresponding deviation equation to be

$$\frac{D^2\Psi^\alpha}{Ds^2} = R^\alpha_{.\mu\nu\rho}U^\mu U^\nu\Psi^\rho + \lambda\left(f^\alpha_{\ .\nu}\frac{D\Psi^\nu}{Ds} + f^\alpha_{\ .\nu;\rho}U^\nu\Psi^\rho\right). \tag{17}$$

But, if we consider the following Lagrangian:

$$L = \mathbf{g}_{\mu\nu} U^{\mu} \frac{D\Psi^{\nu}}{D\tau} + \lambda f_{\nu\rho} \Psi^{\nu} U^{\rho}, \tag{18}$$

where $\mathbf{g}_{\mu\nu} = g_{(\mu\nu)} + g_{[\mu\nu]}$, and follow the Bazanski approach to get the path and path deviation equations related to this type of geometry by taking the variation with respect to Ψ^{σ} and U^{σ}, respectively, we can obtain:

$$\frac{\mathrm{d}U^{\alpha}}{\mathrm{d}s} + \left\{ \begin{matrix} \alpha \\ \mu\nu \end{matrix} \right\} U^{\mu} U^{\nu} = \lambda \mathbf{g}^{\alpha\mu} f_{[\mu\nu]} U^{\nu} + \mathbf{g}^{\alpha\sigma} g_{[\nu\sigma];\rho} U^{\nu} U^{\rho}, \tag{19}$$

and the path deviation equation becomes

$$\frac{D^2\Psi^{\alpha}}{Ds^2} = R^{\alpha}_{\cdot\mu\nu\rho} U^{\mu} U^{\nu} \Psi^{\rho} + 2\mathbf{g}^{\sigma\alpha} (g_{[\nu[\sigma];\rho]}) \frac{D\Psi^{\nu}}{Ds} U^{\rho} + \lambda \left(f^{\alpha}_{\cdot\nu} \frac{D\Psi^{\nu}}{Ds} + f^{\alpha}_{\cdot\nu;\rho} U^{\nu} \Psi^{\rho} \right). \tag{20}$$

It is clear that the difference between (15) and (19) is related to absence of the spin of the source in (15). Thus, from (19) it is possible to find an interaction between the spin of the source and the skew field.[19] Kalinowski[20] has extended Moffat's version[21] which is described in Einstin-Cartan geometry, to establish a relation between the mass and fermion current curve space-time while the spin of the source is twisting it.

Moreover, Wanas and Kahil have extended the Bazanski approach, applying it in Einstein non-symmetric geometries[22] to reach the conclusion that paths in these geometries are naturally quantized (in the Planck sense of quantization).[10] This type of natural quantization of paths exists in absolute parallelism geometries as well.[11]

III. MOTION IN 5D

The problem of motion in higher dimensions is an intriguing problem. The significance of motion in higher dimensions may yield some indications with regards to the principles that should be followed when describing motion in 4D, i.e., an equation which governs the motion in $4D$[6]. In the present work, we will examine the effect of non gravitational forces on the current motion, i.e., should this motion be absorbed into the extra dimension or remain unchanged from the usual equation of motion in 4D space apart from increasing the dimensions?

A. The Bazanski approach in five dimensions

In an attempt to derive path and path deviation equations in five dimensions, we extend the Bazanski Lagrangian to 5D:

$$L = g_{AB} U^{A} \frac{D\Psi^{B}}{DS} \tag{21}$$

where $(A=1,2,3,4,5)$. By taking the variation with respect to the deviation vector Ψ^{C} and the tangent vector U^{C}, we obtain the geodesic and geodesic deviation equations, respectively,

$$\frac{dU^{C}}{dS} + \left\{ \begin{matrix} C \\ AB \end{matrix} \right\} U^{A} U^{B} = 0, \tag{22}$$

and

$$\frac{D^2\Psi^{C}}{DS^2} = R^{C}_{\cdot ABD} \Psi^{D} U^{A} U^{B}. \tag{23}$$

B. Compact spaces

The process to unify electromagnetism (gauge fields) and gravity depends on extra component(s) of the metric using the cylinder condition.[1] Some authors believe that compact dimensions can be tested, for example, by examining the rate of energy released as a result of gravitational waves from binary pulsars.[23]

In our study, we derive the same geodesic and geodesic deviation equations given by Kerner *et al.*[15] using the Bazanski approach:

$$\frac{dU^{\mu}}{dS}+\left\{\begin{matrix}\mu\\ \nu\lambda\end{matrix}\right\}U^{\nu}U^{\lambda}+\left(\frac{dx^{5}}{dS}+A_{\nu}\frac{dx^{\nu}}{dS}\right)F^{\mu}_{\cdot\lambda}U^{\lambda}=0, \tag{24}$$

$$\frac{d}{dS}\left(\frac{dx^{5}}{dS}+A_{\mu}\frac{dx^{\mu}}{dS}\right)=0. \tag{25}$$

where $Q\equiv dx^{5}/dS+A_{\mu}dx^{\mu}/dS$ is constant along the 5D geodesics, i.e.,

$$\frac{q}{m}=\frac{dx^{5}}{dS}+A_{\mu}\frac{dx^{\mu}}{dS}.$$

Consequently, (24) becomes

$$\frac{dU^{\mu}}{dS}+\left\{\begin{matrix}\mu\\ \nu\lambda\end{matrix}\right\}U^{\nu}U^{\lambda}+\frac{q}{m}F^{\mu}_{\cdot\lambda}U^{\mu}=0, \tag{26}$$

with $ds^{2}=(1-Q^{2})dS^{2}$ and its corresponding path deviation equation becomes:

$$\frac{D^{2}\Psi^{\mu}}{DS^{2}}=R^{\mu}_{\cdot\rho\nu\lambda}U^{\rho}U^{\nu}\Psi^{\lambda}+\frac{q}{m}\left(F^{\mu}_{\cdot\nu;\rho}U^{\nu}\Psi^{\rho}+F^{\mu}_{\cdot\nu}\frac{D\Psi^{\nu}}{DS}\right)+F^{\mu}_{\cdot\lambda}U^{\lambda}\left(\frac{d}{dS}(A_{\lambda}\Psi^{\lambda}+\Psi^{5})+F_{\nu\rho}U^{\nu}\Psi^{\rho}\right) \tag{27}$$

and

$$\frac{d}{dS}((\Psi^{5}+A_{\lambda}\Psi^{\lambda})+F_{\lambda\rho}U^{\rho}\Psi^{\lambda})=0 \tag{28}$$

A charged particle whose behavior is described by the Lorentz equation in 4D behaves as a test particle moving on a geodesic in 5D. This result is obtained from the usual Basanski method in 5D rather than its modified method in 4D.

C. Noncompact spaces

In an attempt to unify geometry and matter, Wesson and his collaborators[3] have assumed that $g_{AB,5}\neq 0$, which is applied in the brane world models[4] and space-time-matter theories.[5] The idea of non-compact spaces is based upon the Campbell-Maagard theorem.[24] Using this approach, Wesson[25] has found that: (1) Massive particles traveling on a time-like geodesic in 4D can be regarded as traveling on a null-geodesic in 5D. This is obvious as an implication of the behavior of wave-like particles in a double slits experiment.

(2) Massive particles traveling on any path may exhibit changes their rest mass because there is a direct contact with the fifth force. In this case, the path equation will be a generalization of the problem of moving particles having variable mass in classical mechanics.

It is well known that the path equation of a charged object described in non-compact space[26] is given by

$$\frac{dU^{\alpha}}{dS}+\left\{\begin{matrix}\alpha\\ \mu\nu\end{matrix}\right\}U^{\mu}U^{\nu}=nF^{\alpha}_{\mu}U^{\nu}U^{\nu}+\epsilon n^{2}\frac{\Phi^{;\alpha}}{\Phi^{3}}-A^{\alpha}\frac{dn}{dS}-g^{\alpha\lambda}\frac{dx^{5}}{dS}\left(nA_{\lambda,5}+g_{\lambda\mu,5}\frac{dx^{\mu}}{dS}\right) \tag{29}$$

and

$$\frac{d}{dS}\epsilon\Phi^{2}\left(\frac{dx^{5}}{dS}+A_{\mu}\frac{dx^{\mu}}{dS}\right)=0, \tag{30}$$

where $n=\epsilon\Phi^{2}(dx^{5}/dS+A_{\mu}U^{\mu})$, Φ is a scalar potential, and $\epsilon=\pm 1$ depending on whether the extra dimension is space-like or time-like, respectively. This leads to $q/m=\epsilon\Phi^{2}(dx^{5}/dS+A_{\mu}U^{\mu})$ in which its scalar field affects the ratio of charge to mass.

However, the above equation has two main defects: *it is not gauge invariant*, and *the additional extra force from an extra dimension is parallel to the four vector velocity* i.e., $f_{\mu}U^{\mu}\neq 0$.

Ponce de Leon[26] has dealt with these two defects by using various types of transformations in order to make (29) and (30) like the geodesic equation in its usual form:

$$\frac{d^{2}\xi^{A}}{dS^{2}}+\left\{\begin{matrix}A\\ BC\end{matrix}\right\}\frac{d\xi^{B}}{dS}\frac{d\xi^{C}}{dS}=0, \tag{31}$$

where ξ^{A} is the projected 5D velocity. This allows us to introduce its corresponding Bazanski Lagrangian:

$$L=g_{AB}\frac{d\xi^{A}}{dS}\frac{D\Psi^{B}}{DS} \tag{32}$$

which gives its geodesic deviation equation as

$$\frac{D^{2}\Psi^{A}}{DS^{2}}=0 \tag{33}$$

D. Path and path deviation equations of nonsymmetric geometries in 5D

We now consider the following Lagrangian:

$$L=\mathbf{g}_{AB}U^{A}\frac{D\Psi^{B}}{DS}+\lambda f_{CE}\Psi^{C}U^{E}, \tag{34}$$

Applying the Bazanski approach to derive the path and path deviation equations by taking the variation with respect to Ψ^{D} and U^{D}, respectively, we obtain:

$$\frac{dU^{A}}{dS}+\left\{\begin{matrix}A\\ BC\end{matrix}\right\}U^{B}U^{C}=\lambda\mathbf{g}^{AD}f_{[DC]}U^{C}+\mathbf{g}^{AD}g_{[CD];M}U^{C}U^{M}, \tag{35}$$

and

$$\frac{D^{2}\Psi^{A}}{DS^{2}}=R^{A}_{.BCD}U^{B}U^{C}\Psi^{D}+2\mathbf{g}^{DA}(g_{[A[D];M]})\frac{D\Psi^{C}}{DS}U^{M}+\lambda\mathbf{g}^{DA}\left(f_{A_{.C}}\frac{D\Psi^{C}}{Ds}+f_{AC;M}U^{C}\Psi^{M}\right). \tag{36}$$

In one version of KK Non-symmetric theory of gravity, Kalinowski[8] has summarized the role of the extra dimension in the following matter: mass and fermion current curve the four dimensions, the spin of the source and the electromagnetic potential twist the fifth dimension.

IV. ROTATION IN 5D

The concept of rotation in higher dimensions is related to obtaining the governing equation of the current spinning object.[27] For a spinning gyroscope it is well known that the fifth equation is testing the rate of precession.[28] Some authors believe that the study of two nearby free-falling gyroscopes could be used to examine the question of the existence of gravitational waves.[16]

We may apply the Bazanski approach on the following Lagrangian:

$$L = g_{AB}U^A\frac{D\Psi^B}{DS} + \frac{1}{2m}R_{ABCD}S^{CD}U^B\Psi^A \tag{37}$$

to derive the path equation of a spinning object in 5D:

$$\frac{\mathrm{d}U^C}{\mathrm{d}S} + \begin{Bmatrix} C \\ AB \end{Bmatrix} U^A U^B = \frac{1}{2m}R^C_{.ABD}S^{BD}U^A. \tag{38}$$

The above equation describes spinning objects in compact spaces which satisfy the cylinder condition, i.e., $g_{AB,5}=0$. This is identical to the Dixon equation if we project it into four dimensions. The fifth coordinate will contribute the electromagnetic tensor, which has already appeared in the Dixon equation.

Also, the original Papapetrou equation in 5D will be as follows:

$$\frac{D}{DS}\left(mU^A + U_E\frac{DS^{AE}}{DS}\right) = \frac{1}{2}R^A_{.BCD}S^{CD}U^B \tag{39}$$

and its corresponding deviation equation will take the following form:

$$\frac{D^2\Psi^A}{DS^2} = R^A_{.BCD}U^B\left(mU^C + U_E\frac{DS^{CE}}{DS}\right)\Psi^D + g^{AC}g_{BE}\left(mU^E + U_O\frac{DS^{EO}}{DS}\right)_{;C}\frac{D\Psi^B}{DS} + R^A_{.BCD}S^{CD}\frac{D\Psi^B}{DS} + R^A_{BCE}S^{CE}_{.;D}U^B\Psi^D + R^A_{BCE;D}S^{CE}U^B\Psi^D. \tag{40}$$

These equations could be used to study the behavior of spinning charged objects that exhibit precession, e.g., neutron stars, compact objects, etc.

In non-compact spaces with $R_{ABCD}=0$, it is found that a spinning particle is moving on a geodesic in 5D rather than the Papapetrou equation.[29] This leads us to suggest that in non-compact spaces, satisfying the Campbell-Magaard theorem, spinning particles and spinning charged particles as well as test particles are moving along geodesics in 5D. But if we consider the original Papapetrou equation in 5D, we can find out that it is different from the usual geodesic equation, i.e.,

$$\frac{D}{DS}\left(mU^A + U_B\frac{DS^{AB}}{DS}\right) = 0. \tag{41}$$

On the contrary, its corresponding deviation equation is identical to (33).

V. DISCUSSION AND CONCLUSION

The Lagrangian required to derive the path and path deviation equations in higher dimensions becomes the conventional Bazanski Lagrangian if the extra fields are described in the fifth (higher) dimension. Path equations of different particles in 4D can be considered as the projection of the geodesic equation in 5D on 4D. But if the extra effect, non-gravitational force, is not totally absorbed in the higher dimensional equations then the Bazanski Lagrangian should be amended like their counterparts in four-dimension, which is seen in the 5D Papapertrou's equation (38).

It has been shown in this paper that the effect of the compactness of the extra dimension(s) can be clearly perceived on moving objects. Also, we find that the effect of precession may distinguish between tops and test particles moving in a background whose 5D curvature has vanished.

In our study we have shown that the apparent Papapetrou equation in 5D is merely the projection of the Dixon equation in 4D. But if the space does not include electromagnetism as an extra dimension, the Papapetrou equation in 4D remains the same in 5D unless the extra dimension space is not compact satisfying the Campbell-Magaard theorem. Also, as can be seen from (25) and (30) the path equations in compact and non-compact spaces display a contradictory aspect: the ratio of charge to mass is constant in the case of compact space, while it is variable depending on the scalar field in case of non-compact spaces, which can be explored due to the effect of the cylinder condition on higher dimensions.

It was shown that in 4D, the Bazanski Lagrangian can be modified to describe path equations for charged, spinning, and spinning charged particles, as well as for spinning objects with precession and their corresponding path deviation equation. In an attempt to find the path and path deviation equations of the above-mentioned particles in 5D, we have found that the Bazanski Lagrangian could remain unmodified if the non-gravitational force could be absorbed into the higher dimension. Otherwise, the Bazanski Lagrangian must be amended.

In our study, we have also found that in non-compact spaces, spinning objects and the non-precessing ones are not following the same trajectory, although their path deviation equations are the same.

We have applied the Bazanski approach to determine path and path deviation equations of one version of the Einstein non-symmetric theories of gravity in 5D. This work could be extended to study the effect of compactness on the path equations in our future work.

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Gravitational radiation, vorticity and the electric and magnetic part of Weyl tensor

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The electric and the magnetic part of the Weyl tensor, as well as the invariants obtained from them, are calculated for the Bondi vacuum metric. One of the invariants vanishes identically and the other only exhibits contributions from terms of the Weyl tensor containing the static part of the field. It is shown that the necessary and sufficient condition for the spacetime to be purely electric is that such spacetime be static. It is also shown that the vanishing of the electric part implies Minkowski spacetime. Unlike the electric part, the magnetic part does not contain contributions from the static field. Finally a speculation about the link between the vorticity of world lines of observers at rest in a Bondi frame, and gravitational radiation, is presented. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The study of the electric $E_{\alpha\beta}$ and magnetic $H_{\alpha\beta}$ parts of Weyl tensor has attracted the attention of researchers for many years (see Refs. 1–19, and references therein).

Particularly intriguing is the eventual relationship of the magnetic part of the Weyl tensor, with rotation[2,9] and with gravitational radiation.[1,5,8,10–12]

On the other hand, the link has been established between gravitational radiation and vorticity of world lines of observers at rest in a Bondi spacetime.[20,21] Specifically, it has been shown that the leading term in the vorticity (in an expansion of powers of $1/r$) is expressed through the news function in such a way that it will vanish if and only if there is no news (no radiation). This suggests the possibility of detecting gravitational waves by means of gyroscopes.[20,22]

In order to delve deeper into these issues, we shall calculate in this work the electric and the magnetic part of the Weyl tensor, as well as the two invariants obtained from them, in the field of gravitational radiation.

From the obtained expressions, it follows that the vanishing of the magnetic part, implies the vanishing of the news function and also the vanishing of nonradiative but time-dependent field, except for a very peculiar class of solutions, called by Bondi "non-natural, non-radiative moving systems." This result, together with the known fact[6] that static Weyl metrics are purely electric,

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implies, if we exclude by physical reasons the class of solutions mentioned before, that the necessary and sufficient condition for a Bondi spacetime to be purely electric is that such spacetime be static.

The vanishing of the electric part of the Weyl tensor is shown to imply that the spacetime is Minkowski. Thus there is no purely magnetic vacuum Bondi spacetimes, in agreement with the conjecture that purely magnetic vacuum spacetimes do no exist.[6,7,9,18,19]

It is also obtained that one of the invariants ($Q \equiv E^{\alpha\beta}H_{\alpha\beta}$) vanishes identically whereas the other ($L \equiv E^{\alpha\beta}E_{\alpha\beta} - H^{\alpha\beta}H_{\alpha\beta}$) has a leading term with contributions only from the coefficients in the expansion of the Weyl tensor which contain the static part of the field. Coefficients containing purely radiative and/or nonradiative but time-dependent part of the field, do not enter in L.

Finally, we shall speculate that the fact that gravitational radiation produces vorticity of a time-like congruence might be explained by a mechanism similar to the one suggested to explain the vorticity of a time-like congruence in the field of a charged static magnetic dipole.[23]

We shall carry out our calculations using the Bondi's formalism[24] which has, among other things, the virtue of providing a clear and precise criterion for the existence of gravitational radiation (see also Ref. 25). Namely, if the news function is zero over a time interval, then there is no radiation during that interval.

The formalism has as its main drawback[26] the fact that it is based on a series expansion which could not give closed solutions and which raises unanswered questions about convergence and appropriateness of the expansion.

However we shall restrain ourselves to a region sufficiently far from the source, so that we shall need in our calculations only the leading terms in the expansion of metric functions. Furthermore, since the source is assumed to radiate during a finite interval, then no problem of convergence appears.[27]

A brief resume of Bondi's formalism is given in the next section, together with the expression of the vorticity of a time-like congruence of observers at rest in a Bondi frame. In Sec. III we present the result of the calculations of the electric and a magnetic part as well as the invariants Q and L, and in the last section results are discussed.

II. BONDI'S FORMALISM

The general form of an axially and reflection symmetric asymptotically flat metric given by Bondi is[24]

$$ds^2 = \left(\frac{V}{r}e^{2\beta} - U^2r^2e^{2\gamma}\right)du^2 + 2e^{2\beta}du dr + 2Ur^2e^{2\gamma}du d\theta - r^2(e^{2\gamma}d\theta^2 + e^{-2\gamma}\sin^2\theta d\phi^2), \quad (1)$$

where V, β, U, and γ are functions of u, r, and θ.

We number the coordinates $x^{0,1,2,3} = u, r, \theta, \phi$, respectively. u is a timelike coordinate such that $u = constant$ defines a null surface. In flat spacetime this surface coincides with the null light cone open to the future. r is a null coordinate ($g_{rr} = 0$) and θ and ϕ are two angle coordinates (see Ref. 24 for details).

Regularity conditions in the neighborhood of the polar axis ($\sin\theta = 0$), imply that as $\sin\theta -> 0$,

$$V, \beta, U/\sin\theta, \gamma/\sin^2\theta, \quad (2)$$

each equals a function of $\cos\theta$ regular on the polar axis.

The four metric functions are assumed to be expanded in series of $1/r$, then using the field equations Bondi gets

$$\gamma = cr^{-1} + \left(C - \tfrac{1}{6}c^3\right)r^{-3} + \cdots, \quad (3)$$

$$U = -(c_\theta + 2c\cot\theta)r^{-2} + [2N + 3cc_\theta + 4c^2\cot\theta]r^{-3}\cdots, \tag{4}$$

$$V = r - 2M - \left(N_\theta + N\cot\theta - c_\theta^2 - 4cc_\theta\cot\theta - \tfrac{1}{2}c^2(1 + 8\cot^2\theta)\right)r^{-1} + \cdots, \tag{5}$$

$$\beta = -\tfrac{1}{4}c^2r^{-2} + \cdots, \tag{6}$$

where c, C, N, and M are functions of u and θ, letters as subscripts denote derivatives, and

$$4C_u = 2c^2c_u + 2cM + N\cot\theta - N_\theta. \tag{7}$$

The three functions c, M, and N are further related by the supplementary conditions

$$M_u = -c_u^2 + \tfrac{1}{2}(c_{\theta\theta} + 3c_\theta\cot\theta - 2c)_u, \tag{8}$$

$$-3N_u = M_\theta + 3cc_{u\theta} + 4cc_u\cot\theta + c_uc_\theta. \tag{9}$$

In the static case M equals the mass of the system whereas N and C are closely related to the dipole and quadrupole moment, respectively.

Next, Bondi defines the mass $m(u)$ of the system as

$$m(u) = \frac{1}{2}\int_0^\pi M\sin\theta d\theta \tag{10}$$

which by virtue of (8) and (2) yields

$$m_u = -\frac{1}{2}\int_0^\pi c_u^2\sin\theta d\theta. \tag{11}$$

Let us now recall the main conclusions emerging from Bondi's approach.

1. If γ, M, and N are known for some $u=a$ (constant) and c_u (the news function) is known for all u in the interval $a \leqslant u \leqslant b$, then the system is fully determined in that interval. In other words, whatever happens at the source, leading to changes in the field, it can only do so by affecting c_u and vice versa. In the light of this comment the relationship between news function and the occurrence of radiation becomes clear.
2. As it follows from (11), the mass of a system is constant if and only if there are no news.

Now, for an observer at rest in the frame of (1), the four-velocity vector has components

$$u^\alpha = \left(\frac{1}{A}, 0, 0, 0\right) \tag{12}$$

with

$$A \equiv \left(\frac{V}{r}e^{2\beta} - U^2r^2e^{2\gamma}\right)^{1/2}. \tag{13}$$

Then, it can be shown that for such an observer the vorticity vector may be written as (see Ref. 20 for details)

$$\omega^\alpha = (0, 0, 0, \omega^\phi) \tag{14}$$

with

$$\omega^{\phi} = -\frac{e^{-2\beta}}{2r^2 \sin\theta}\left[2\beta_{\theta}e^{2\beta} - \frac{2e^{2\beta}A_{\theta}}{A} - (Ur^2e^{2\gamma})_r + \frac{2Ur^2e^{2\gamma}}{A}A_r + \frac{e^{2\beta}(Ur^2e^{2\gamma})_u}{A^2} - \frac{Ur^2e^{2\gamma}}{A^2}2\beta_u e^{2\beta}\right] \tag{15}$$

and for the absolute value of ω^{α} we get

$$\Omega \equiv (-\omega_{\alpha}\omega^{\alpha})^{1/2} = \frac{e^{-2\beta-\gamma}}{2r}\left[2\beta_{\theta}e^{2\beta} - 2e^{2\beta}\frac{A_{\theta}}{A} - (Ur^2e^{2\gamma})_r + 2Ur^2e^{2\gamma}\frac{A_r}{A} + \frac{e^{2\beta}}{A^2}(Ur^2e^{2\gamma})_u - 2\beta_u\frac{e^{2\beta}}{A^2}Ur^2e^{2\gamma}\right]. \tag{16}$$

Feeding back (3)–(6) into (16) and keeping only the two leading terms, we obtain

$$\Omega = -\frac{1}{2r}(c_{u\theta} + 2c_u\cot\theta) + \frac{1}{r^2}[M_{\theta} - M(c_{u\theta} + 2c_u\cot\theta) - cc_{u\theta} + 6cc_u\cot\theta + 2c_uc_{\theta}]. \tag{17}$$

Therefore, up to order $1/r$, a gyroscope at rest in (1) will precess as long as the system radiates ($c_u \neq 0$). Observe that if

$$c_{u\theta} + 2c_u\cot\theta = 0 \tag{18}$$

then

$$c_u = \frac{F(u)}{\sin^2\theta}, \tag{19}$$

which implies

$$F(u) = 0 \Rightarrow c_u = 0 \tag{20}$$

in order to ensure regularity conditions, mentioned earlier, in the neighborhood of the polar axis ($\sin\theta = 0$). Thus the leading term in (17) will vanish if and only if $c_u = 0$.

The order $1/r^2$ contains, beside the terms involving c_u, a term not involving news, namely M_{θ}. This last term represents the class of nonradiative motions discussed by Bondi[24] and may be thought of as corresponding to the tail of the wave, appearing after the radiation process.[26]

Let us now assume that initially (before some $u = u_0 = \text{constant}$) the system is static, in which case

$$N_u = c_u = 0 \tag{21}$$

which implies, because of (9),

$$M_{\theta} = 0 \tag{22}$$

and $\Omega = 0$ (actually, in this case $\Omega = 0$ at any order) as expected for a static field (for the electrovacuum case however, this may change[23]). Then let us suppose that at $u = u_0$ the system starts to radiate ($c_u \neq 0$) until $u = u_f$, when the news vanish again. For $u > u_f$ the system is not radiating although (in general) $M_{\theta} \neq 0$ implying (see for example (9)) time dependence of metric functions (nonradiative motions[24]).

For $u > u_f$ there is a vorticity term of order $1/r^2$ describing the effect of the tail of the wave. This in turn provides "observational" evidence for the violation of the Huygens's principle, a problem largely discussed in the literature (see, for example Refs. 24 and 26, and references therein).

III. THE ELECTRIC AND MAGNETIC PARTS OF WEYL TENSOR

The electric and magnetic parts of Weyl tensor, $E_{\alpha\beta}$ and $H_{\alpha\beta}$, respectively, are formed from the Weyl tensor $C_{\alpha\beta\gamma\delta}$ and its dual $\tilde{C}_{\alpha\beta\gamma\delta}$ by contraction with the four velocity vector given by (12):[28]

$$E_{\alpha\beta} = C_{\alpha\gamma\beta\delta} u^{\gamma} u^{\delta}, \tag{23}$$

$$H_{\alpha\beta} = \tilde{C}_{\alpha\gamma\beta\delta} u^{\gamma} u^{\delta} = \tfrac{1}{2} \epsilon_{\alpha\gamma\epsilon\delta} C^{\epsilon\delta}_{\beta\rho} u^{\gamma} u^{\rho}, \quad \epsilon_{\alpha\beta\gamma\delta} \equiv \sqrt{-g}\, \eta_{\alpha\beta\gamma\delta}, \tag{24}$$

where $\eta_{\alpha\beta\gamma\delta} = +1$ for $\alpha, \beta, \gamma, \delta$ in even order, -1 for $\alpha, \beta, \gamma, \delta$ in odd order, and 0 otherwise. Also note that

$$\sqrt{-g} = r^2 \sin\theta e^{2\beta} \approx r^2 \sin\theta \exp\left(-\frac{c^2}{2r^2}\right) \approx r^2 \sin\theta + O(1).$$

Since the obtained expressions are fairly long, in order to check our results we have calculated the magnetic and electric parts in two different ways and then compared results, excluding thereby any possible error. On the one hand we have calculated with MAPLE the components of Weyl tensor and from them, "by hand" its electric and magnetic part from (23) and (24). We do not include here the detailed expressions of Weyl components, but they are available upon request. The only nonvanishing components of Weyl tensor are

$$C_{0101}, C_{0102}, C_{0112}, C_{0202}, C_{0212}, C_{0303},$$

$$C_{0313}, C_{0323}, C_{1212}, C_{1313}, C_{1323}, C_{2323}.$$

However they are not independent, since the following relations between them exist:

$$\frac{r^4 \sin^2\theta}{e^{2\beta}} C_{1010} = e^{2\gamma}(V - r^4 e^{2\gamma - 2\beta}) C_{1313} - 2r^2 e^{2\gamma} C_{0313}, \tag{25}$$

$$\frac{r^2 \sin^2\theta}{e^{2\gamma}} C_{0112} = e^{2\beta} C_{1323} - r^2 e^{2\gamma} C_{1313}, \tag{26}$$

$$\frac{2r^2 \sin^2\theta}{e^{2\gamma}} C_{0212} = e^{2\beta} C_{2323} - r e^{2\gamma} C_{1313}, \tag{27}$$

$$\sin^2\theta C_{1212} = -e^{4\gamma} C_{1313}. \tag{28}$$

On the other hand, we have calculated the magnetic and electric part using GRTENSOR. Thus, one has for the components of the magnetic Weyl tensor, up to the order $1/r^3$:

$$H^0_0 = H^0_1 = H^0_2 = H^1_0 = H^1_1 = H^1_2 = H^2_0 = H^2_1 = H^2_2 = H^3_0 = H^3_3 = 0, \tag{29}$$

$$\begin{aligned} H^0_3 = &-\frac{1}{r}(2c_u \cos\theta + c_{\theta u} \sin\theta) \\ &+ \frac{1}{r^2}\left\{ 4c_u(c - M)\cos\theta + \left[\frac{3}{2}(N_u + M_\theta + c_u c_\theta) + \frac{7}{2} c c_{\theta u} - 2M c_{\theta u} \right] \sin\theta \right\} \\ &+ \frac{1}{r^3}\left\{ -\frac{N}{\sin\theta}(1 + 2c_u) + \left[8M c_u (c - M) + N_\theta (1 - 2c_u) + \frac{5}{2} c^2 c_u - N c_{\theta u} - P_u - 4Mc \right] \right. \end{aligned}$$

$$\times\cos\theta+\left[2(N-Mc_\theta)-c_{\theta u}\left(7Mc-4M^2-N_\theta-\frac{7}{4}c^2\right)+3M(N_u+M_\theta)\right.$$
$$\left.-\frac{1}{2}P_{\theta u}-3cM_\theta+N_{\theta\theta}+c_u\left(8N+3Mc_\theta+\frac{5}{2}cc_\theta\right)\right]\sin\theta\Bigg\}, \tag{30}$$

$$H_3^1=\frac{1}{r}[(c_\theta c_{uu}+c_{\theta u})\sin\theta+2(cc_{uu}+c_u)\cos\theta]+\frac{1}{r^2}\Bigg\{\frac{4cc_u\cos\theta}{\sin^2\theta}+\frac{2c_uc_\theta-cc_{\theta u}}{\sin\theta}$$
$$+\left[-\frac{1}{2}c_\theta c_{\theta\theta u}+(2M-3c)c_\theta c_{uu}-\frac{5}{2}(cc_{\theta u}+c_uc_\theta)-2Nc_{uu}-\frac{3}{2}(N_u+M_\theta)\right]$$
$$\times\sin\theta+\left[-6cc_u+4c(M-c)c_{uu}-\frac{1}{2}c_\theta c_{\theta u}-cc_{\theta\theta u}\right]\cos\theta\Bigg\}$$
$$+\frac{1}{r^3}\Bigg\{\frac{8cc_u(M-c)\cos\theta}{\sin^2\theta}+\frac{1}{\sin\theta}[c_uc_\theta(4M-3c)+N-2cN_u+2Ncc_{uu}$$
$$+cc_{\theta u}(7c-2M)-4c_uN-cM_\theta]+\left[\frac{1}{2}P_{\theta u}-N_{\theta\theta}-2N+4cM_\theta-4c_uN+2cN_u\right.$$
$$+c_uc_\theta\left(-\frac{9}{2}c-M+cc_u+\frac{1}{2}c_{\theta\theta}\right)+c_\theta\left(2M-cM_u+P_{uu}+N_{\theta u}+\frac{1}{2}M_{\theta\theta}\right)$$
$$+c_{\theta u}\left(-\frac{19}{4}c^2+2c_\theta^2+2Mc\right)+c_{\theta\theta u}(N+3cc_\theta-Mc_\theta)$$
$$\left.+c_\theta c_{uu}\left(-6Mc+\frac{1}{2}c^2+N_\theta+4M^2\right)-2Nc_{uu}(c+2M)\right]\sin\theta$$
$$+\left[2c\left(2M+N_{\theta u}+P_{uu}-cM_u+\frac{1}{2}M_{\theta\theta}\right)+c_u\left(-2Mc-\frac{3}{2}c^2+2c^2c_u+\frac{3}{2}c_\theta^2+cc_{\theta\theta}\right)\right.$$
$$+c_{\theta u}(N-Mc_\theta+8cc_\theta)+c_{uu}(c^3+2cN_\theta+Nc_\theta-8Mc^2+8M^2c)$$
$$\left.+cc_{\theta\theta u}(5c-2M)-c_\theta\left(\frac{1}{2}M_\theta+N_u\right)+P_u-N_\theta\right]\cos\theta\Bigg\}, \tag{31}$$

$$H_3^2=\frac{1}{r}(\sin\theta c_{uu})+\frac{1}{r^2}\left\{\frac{2c_u}{\sin\theta}-\frac{1}{2}c_{\theta u}\cos\theta+\left[2c_{uu}(M-c)-c_u-\frac{1}{2}c_{\theta\theta u}\right]\sin\theta\right\}$$
$$+\frac{1}{r^3}\Bigg\{4c_u\frac{M-c}{\sin\theta}+\left[\frac{3}{2}c_uc_\theta-N_u-\frac{1}{2}M_\theta+Nc_{uu}+\left(\frac{7}{2}c-M\right)c_{\theta u}\right]\cos\theta$$
$$+\left[\left(\frac{5}{2}c-M\right)c_{\theta\theta u}+\left(\frac{1}{2}c_{\theta\theta}-M\right)c_u+2c_\theta c_{\theta u}+c_{uu}\right.$$
$$\left.\times(2c^2+4M^2-4Mc+N_\theta)+\frac{1}{2}M_{\theta\theta}-cM_u+N_{\theta u}+P_{uu}+cc_u^2\right]\sin\theta\Bigg\}, \tag{32}$$

$$H_1^3=\frac{1}{r^3}\frac{2c_u\cos\theta+c_{\theta u}\sin\theta}{\sin^2\theta}, \tag{33}$$

$$H_2^3=\frac{1}{r\sin\theta}\frac{c_{uu}}{}+\frac{1}{r^2\sin\theta}\Bigg[2c_{uu}(c+M)-c_u-\frac{1}{2}c_{\theta\theta u}-\frac{1}{2}\cot\theta c_{\theta u}+2\frac{c_u}{\sin^2\theta}\Bigg]$$
$$+\frac{1}{r^3\sin\theta}\Bigg\{\frac{4Mc_u}{\sin^2\theta}+\cot\theta\Bigg[-N_u+Nc_{uu}-\frac{1}{2}c_uc_\theta-\left(\frac{1}{2}c+M\right)c_{\theta u}-\frac{1}{2}M_\theta\Bigg]$$
$$+c_{uu}(N_\theta+4Mc+4M^2+2c^2)+cc_u^2+\left(\frac{1}{2}c_{\theta\theta}-M\right)c_u+\left(\frac{1}{2}c-M\right)c_{\theta\theta u}$$
$$+P_{uu}+\frac{1}{2}M_{\theta\theta}+c_\theta c_{\theta u}-cM_u+N_{\theta u}\Bigg\}. \tag{34}$$

Regarding the electric part, one gets, up to the order $1/r^3$:

$$E_0^0=E_3^0=E_0^1=E_3^1=E_0^2=E_3^2=E_0^3=E_1^3=E_2^3=0, \tag{35}$$

$$E_1^0=\frac{2(cc_u+M)}{r^3}, \tag{36}$$

$$E_2^0=\frac{2c_u\cos\theta+c_{\theta u}\sin\theta}{r\sin\theta}+\frac{1}{2\sin\theta r^2}$$
$$\times\{8Mc_u\cos\theta+[c_{\theta u}(4M-3c)-3(M_\theta+c_uc_\theta+N_u)]\sin\theta\}$$
$$+\frac{1}{4r^3}\Bigg\{(1+2c_u)\frac{4N}{\sin^2\theta}+\cot\theta[4(Nc_{\theta u}+P_u-N_\theta)+c_u(32M^2+8N_\theta-42c^2)]$$
$$+4(N-3cN_u-N_{\theta\theta})-12M(M_\theta+N_u)+c_{\theta u}(4N_\theta+16M^2-13c^2-12Mc)$$
$$-c_u(30cc_\theta+12Mc_\theta+32N)+2P_{\theta u}\Bigg\}, \tag{37}$$

$$E_1^1=-\frac{2cc_u(1+\cos^2\theta)+(c_\theta c_{\theta u}+2M)\sin^2\theta+2\sin\theta\cos\theta(c_uc_\theta+cc_{\theta u})}{r^3\sin^2\theta}, \tag{38}$$

$$E_2^1=-\frac{2(cc_{uu}+c_u)\cos\theta+(c_\theta c_{uu}+c_{\theta u})\sin\theta}{r\sin\theta}+\frac{1}{2r^2}$$
$$\times\Bigg\{3(N_u+M_\theta)+c_{uu}(2cc_\theta-4Mc_\theta+4N)+5c_\theta c_u+c_\theta c_{\theta\theta u}+cc_{\theta u}$$
$$+\cot\theta[2c(c_{\theta\theta u}+2c_u-4Mc_{uu})+c_\theta c_{\theta u}]+\frac{2}{\sin^2\theta}(cc_{\theta u}-2c_\theta c_u)-\frac{8}{\sin^3\theta}cc_u\cos\theta\Bigg\}$$
$$-\frac{1}{r^3}\Bigg\{8cc_u(M-c)\frac{\cos\theta}{\sin^3\theta}+\frac{1}{\sin^2\theta}\Big[(4M-7c)c_uc_\theta-4c_uN+2Ncc_{uu}$$
$$+(c^2-2Mc)c_{\theta u}+N-c(M_\theta+2N_u)\Big]+\cot\theta\Bigg[c_u\left(-\frac{1}{2}c_\theta^2-2Mc+cc_{\theta\theta}+2c^2c_u-\frac{15}{2}c^2\right)$$
$$+c_\theta\left(c_{uu}N+(3c-M)c_{\theta u}-N_u-\frac{1}{2}M_\theta\right)+cc_{uu}(8M^2-3c^2+2N_\theta)$$
$$+cc_{\theta\theta u}(3c-2M)+c_{\theta u}N+cM_{\theta\theta}+P_u-N_\theta+2c(P_{uu}+N_{\theta u}-M-cM_u)\Bigg]$$
$$+c_{uu}\Bigg[c_\theta\left(-\frac{7}{2}c^2+N_\theta-2Mc+4M^2\right)-6Nc-4MN\Bigg]$$

$$+c_u\left[c_\theta\left(\frac{1}{2}c_{\theta\theta}-\frac{9}{2}c-M+cc_u\right)-4N\right]+c_{\theta u}\left(c_\theta^2+2Mc-\frac{15}{4}c^2\right)+c_{\theta\theta u}(N-Mc_\theta+2cc_\theta)$$
$$+c_\theta\left(\frac{1}{2}M_{\theta\theta}-M+N_{\theta u}+P_{uu}-M_uc\right)-N_{\theta\theta}+\frac{1}{2}P_{\theta u}-cN_u+N+cM_\theta\Bigg\}, \tag{39}$$

$$E_1^2=-\frac{2c_u\cos\theta+c_{\theta u}\sin\theta}{r^3\sin\theta}, \tag{40}$$

$$E_2^2=-\frac{c_{uu}}{r}+\frac{1}{2r^2}\left(c_{\theta\theta u}-4Mc_{uu}+2c_u+\cot\theta c_{\theta u}-\frac{4c_u}{\sin^2\theta}\right)$$
$$+\frac{1}{r^3}\Bigg\{M_uc-\frac{1}{2}M_{\theta\theta}+M-N_{\theta u}-P_{uu}+\cot\theta\left[Mc_{\theta u}+\frac{1}{2}M_\theta+N_u-\frac{1}{2}cc_{\theta u}+\frac{1}{2}c_\theta c_u-Nc_{uu}\right]$$
$$+c_u\left[\frac{4(c-M)}{\sin^2\theta}+M-c-cc_u-\frac{1}{2}c_{\theta\theta}\right]-c_{uu}(4M^2+N_\theta)-c_\theta c_{\theta u}+c_{\theta\theta u}\left(M-\frac{3}{2}c\right)\Bigg\}, \tag{41}$$

$$E_3^3=\frac{c_{uu}}{r}-\frac{1}{2r^2}\left(c_{\theta\theta u}-4Mc_{uu}+2c_u+\cot\theta c_{\theta u}-\frac{4c_u}{\sin^2\theta}\right)$$
$$+\frac{1}{r^3}\Bigg\{M+N_{\theta u}+P_{uu}+\frac{1}{2}M_{\theta\theta}-cM_u+\cot\theta\left[\frac{5}{2}cc_{\theta u}-\frac{1}{2}M_\theta-N_u+Nc_{uu}-Mc_{\theta u}+\frac{3}{2}c_uc_\theta\right]$$
$$+c_u\left[\frac{4M}{\sin^2\theta}+cc_u-M+\frac{1}{2}c_{\theta\theta}-c\right]+c_{uu}(4M^2+N_\theta)+2c_\theta c_{\theta u}+\left(\frac{3}{2}c-M\right)c_{\theta\theta u}\Bigg\}, \tag{42}$$

where

$$P\equiv C-\frac{c^3}{6}. \tag{43}$$

We shall now provide expressions for the two algebraic invariants associated to the electric and magnetic parts of the Weyl tensor, namely

$$Q=H^\alpha_\beta E^\beta_\alpha,\quad L=E^\alpha_\beta E^\beta_\alpha-H^\alpha_\beta H^\beta_\alpha. \tag{44}$$

As it turns out, the invariant Q vanishes identically, i.e.,

$$Q=0, \tag{45}$$

whereas the first nonvanishing order in L is $1/r^6$ and one then has

$$L=\frac{2}{r^6}\left[3(cc_u+M)^2+(c^3+6P)c_{uu}+6N(c_{\theta u}+2c_u\cot\theta)\right]+O(1/r^7). \tag{46}$$

IV. DISCUSSION

We are now ready to try to answer the main questions which motivated this work, in the context of the Bondi metric, namely:

- What consequences emerge from the vanishing of the magnetic part of the Weyl tensor?
- What consequences emerge from the vanishing of the electric part of the Weyl tensor?
- How do different types of fields (radiative, nonradiative but time dependent, and static) enter into the electric and magnetic part of the Weyl tensor, and into the corresponding invariants?

- Why does gravitational radiation produce vorticity?

Let us start with the first question. If we put $H^{\alpha}_{\beta}=0$ then it follows from the coefficient of $1/r$ in (30) that

$$c_{\theta u}\sin\theta+2c_u\cos\theta=0, \tag{47}$$

which according to (19) and (20) implies

$$c_u=0. \tag{48}$$

Thus the field is nonradiative. Next, the vanishing of the coefficient $1/r^2$ in (30) implies in turn that

$$M_{\theta}=N_u=0, \tag{49}$$

where we have used (9).

Finally from the vanishing of the coefficient of the $1/r^3$ in (30) it follows that

$$N_{\theta\theta}\sin^2\theta+N_{\theta}\sin\theta\cos\theta-N\cos 2\,\theta-(2cM\sin^2\theta)_{\theta}=0 \tag{50}$$

whose general solution is

$$N=\left(\int\frac{2cM}{\sin\theta}d\theta+\sigma\right)\sin\theta \tag{51}$$

where σ is a constant.

Feeding back (51) into (7) and using (48), it follows that

$$C_u=0. \tag{52}$$

It can be easily checked that no further information can be obtained from (31) and (34). Therefore up to order $1/r^3$ in γ, the metric is static, and the mass, the "dipole" (N), and the "quadrupole" (C) moments correspond to a static situation. However, the time dependence might enter through coefficients of higher order in γ, giving rise to what Bondi calls "non-natural non-radiative moving system" (nnnrms). In this later case, the system keeps the three first moments independent of time, but allows for time dependence of higher moments. As unlikely as this situation may be from the physical point of view, we were not able not rule it out mathematically. On the other hand it is known that static spacetimes are purely electric. Accordingly, we conclude that, excluding nnnrms, the necessary and sufficient condition for a Bondi metric to be purely electric is to be static.

The second question has a simple answer. Indeed assuming $E^{\alpha}_{\beta}=0$ and using regularity conditions, we find from the coefficient of order $1/r$ in (37)

$$c_u=0, \tag{53}$$

then it follows at once from (36) that $M=0$. If we exclude the possibility of negative masses, then the spacetime must be Minkowski, giving further support to the conjecture that there are no purely magnetic vacuum spacetimes.[9]

The third question also has a simple answer. The electric part contains all kinds of contributions, radiative, nonradiative but time dependent (nrtd), and static. At order $1/r$ only radiative contributions appear, whereas nrtd terms appear at order $1/r^2$, and higher and contributions from the static field enter in the $1/r^3$ order, and higher. However the magnetic part does not contain contribution from the static field. Only radiative (at order $1/r$ and higher) and nrtd terms (at order $1/r^2$ and higher) appear.[28]

On the other hand, the only nonvanishing invariant (L) has a leading term of order $1/r^6$ implying that purely radiative and nrtd terms in the Weyl tensor do not contribute to L. This is in agreement with the fact that for purely radiative spacetimes, both invariants Q and L vanish.[8]

Finally, let us consider the last question. With this purpose in mind, it is worth recalling a result obtained by Bonnor[23] concerning the dragging of inertial frames by a charged magnetic dipole. To explain the appearance of vorticity in such spacetimes, Bonnor notices that the corresponding electromagnetic Poynting vector has a nonvanishing component, describing a flow of electromagnetic energy round in circles where frame-dragging occurs.[29] He then suggests that such a flow of energy affects inertial frames by producing vorticity of congruences of particles, relative to the compass of inertia.

One could speculate about a similar mechanism in our case, i.e., a flow of gravitational radiation in the ϕ direction. However for testing such a conjecture we should have available a unique expression for a "gravitational" Poynting vector, which is still an open question in general relativity.

Thus for example, the super-Poynting vector based on the Bel–Robinson tensor, as defined in Ref. 15, is

$$P_\alpha = \epsilon_{\alpha\beta\gamma\delta} E^\beta_\rho H^{\gamma\rho} u^\delta \tag{54}$$

giving in our case $P^\phi = 0$. However, besides the ambiguity problem in the definition of energy, this negative result may be caused by the reflection symmetry of the Bondi metric, which intuitively seems to be incompatible with the presence of a circular flow of energy in the ϕ direction. In order to clarify this situation, P^ϕ should be calculated for the general radiative metric without reflection symmetry,[30] but this of course is out of the scope of the present work.

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Local Cauchy problem for the nonlinear Dirac and Dirac-Klein-Gordon equations on Kerr space–time

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We prove the local existence of solutions of nonlinear Dirac and Dirac-Klein-Gordon equations in Kerr metric with regular Cauchy initial datas. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196240]

I. INTRODUCTION

This paper deals with the Cauchy problem for nonlinear Dirac and Dirac-Klein-Gordon equations in Kerr space–time. This curved space–time is one of physical relevant space–time solution of Einstein equations in vacuum. More precisely in Boyer-Lindquist coordinates on $\mathcal{M}:=\mathbb{R}_t \times \mathbb{R}_r \times S^2_\omega$, we have

$$g_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu = \left(1-\frac{2Mr}{\rho^2}\right)\mathrm{d}t^2 + \frac{4aMr\sin^2\theta}{\rho^2}\mathrm{d}t\,\mathrm{d}\varphi - \frac{\rho^2}{\Delta}\mathrm{d}r^2 - \rho^2\,\mathrm{d}\theta^2 - \frac{\sigma^2}{\rho^2}\sin^2\theta\,\mathrm{d}\varphi^2,$$

$$\sigma^2 := (r^2+a^2)\rho^2 + 2Mra^2\sin^2\theta, \quad \Delta := r^2 - 2Mr + a^2,$$

$$\rho^2 := r^2 + a^2\cos^2\theta. \tag{1}$$

The manifold $(\mathcal{M},g)$ describes a rotating uncharged black hole where M is its mass and a is its angular momentum per unit mass. Briefly, we remark that we have two types of singularities: a true curvature singularity, the space of points $\{\rho;\rho^2=0\}$, and the coordinates singularities, the sphere(s) where Δ vanishes. This last property defines the horizon of the black-hole. Roughly speaking the sphere-horizon are the regions for which an observer does not cross and comes back them without a speed greater than the light. Finally the number of real roots of Δ ($\leqslant 2$) define three types of Kerr black hole:

(i) Δ has no real root, i.e., for $|a|>M$, there are no horizon and the ring $\{\rho;\rho^2=0\}$ is a naked singularity.
(ii) Δ has double root, i.e., for $|a|=M$, $\{r=M\}$ is the only horizon, this is the extreme Kerr space–time.
(iii) For $0<|a|<M$, Δ has two real roots,

$$r_\pm = M \pm \sqrt{M^2-a^2}, \tag{2}$$

so there are two horizons $\{r=r_-\}$ and $\{r=r_+\}$. This is the slow Kerr space–time.

In the sequel we consider this last type of Kerr black-hole. Hence the two horizons define three regions of the space–time. The block III ($\mathcal{B}_{\mathrm{III}}$), $\{r<r_-\}$ contains the ring singularity and a time machine. The block II ($\mathcal{B}_{\mathrm{II}}$), $\{r_-<r<r_+\}$, is a dynamic region where an inertial observer is dragged toward the horizon $\{r=r_-\}$. The block I ($\mathcal{B}_{\mathrm{I}}$), $\{r>r_+\}$ is the exterior of the black-hole.

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Moreover, $\mathcal{B}_{\mathrm{I}}$ is not stationary, i.e., the killing vector field $K:=\partial/\partial t$ is not timelike in all block I. The region $\mathcal{E}\subset\mathcal{B}_{\mathrm{I}}$ where K is spacelike in $\mathcal{B}_{\mathrm{I}}$ ($g_{tt}<0$) is called the ergosphere,

$$\mathcal{E} := \{(t,r,\theta,\varphi): r_+ < r < M + \sqrt{M^2 - a^2\cos^2\theta}\}.$$

We study on $(\mathcal{B}_{\mathrm{I}},g)$ the solutions of the nonlinear Dirac equation (NLD):

$$i\gamma^\mu\nabla_\mu\Psi - m_d\Psi = k(\Psi^*\mathcal{V}_1\Psi)\Psi, \tag{3}$$

where $m_d>0$ is the mass of the spin-1/2 field, $\mathcal{V}_1$ a matrix and $k\in L^\infty(\mathcal{B}_{\mathrm{I}})$. γ^μ are the Dirac matrices. We also study the Dirac-Klein-Gordon system (DKG),

$$i\gamma^\mu\nabla_\mu\Psi - m_d\Psi = \Phi\mathcal{V}_2\Psi,$$

$$\Box_g\Phi + m_{kg}^2\Phi = \Psi^*\mathcal{V}_3\Psi, \tag{4}$$

where $m_{kg}>0$ is the mass of the spin-0 field, $\mathcal{V}_2$, $\mathcal{V}_3$ two matrices and $\Box_g$ the Laplacian for the Lorentzian metric g.

The difficulties of these studies on this type of space–time are principally due to the fact that we must work with a curved manifold with less symmetries than flat space–time. Moreover in $\mathcal{B}_{\mathrm{I}}$ of Kerr black-hole and for the spin-0 fields (wave, Klein-Gordon equations) the phenomenon of the super-radiance takes place. It is a consequence of the absence of globally defined timelike Killing vector field that implies the nonexistence of positive-definite conserved quantities useful to define a functional framework to study the field equation. The super-radiance is the analogue for spin-0 fields of the Penrose experience of extraction of energy from the ergosphere. On the other hand, the spin-1/2 field always possess a conserved current inducing a positive-definite inner product. Therefore the super-radiance seems not to be a real problem to prove the existence of the solutions of (3) unlike of (4) since the system consists in the Klein-Gordon field of spin-0.

The first paper about Cauchy problem for a nonlinear field equation in the black-hole background concerns the Klein-Gordon equation.[32] Later, the author extended in Ref. 34 his first work for the nonlinear Klein-Gordon equation in Schwarzschild metric [$a=0$ in (1)] to the Kerr metric. To overcome the problem of the super-radiance, he used the geometrical 3+1 decomposition (ADM) of the Block I. It consists in adopt the coordinates of fixed observer with the respect to infinity. Indeed, we recall that the exterior of the black-hole $\mathcal{B}_{\mathrm{I}}$ is dynamic, i.e., an inertial observer turns with the black hole. Using the ADM decomposition we have outside the black hole

$$\mathcal{B}_{\mathrm{I}} = \mathbb{R}_\tau\times\Sigma, \quad g = N^2\,\mathrm{d}\tau^2 - h(\tau), \tag{5}$$

where N is called the lapse function and h is the spacelike metric. We prove that $N\to 0$ at the horizon and that $h(\tau)$ is equivalent uniform in space and locally uniform in time to the euclidean metric outside a unit closed ball in $\mathbb{R}^3$ ($\Sigma\cong\mathbb{R}^3\backslash\bar{B}(0,1)$). In this framework the Klein-Gordon equation [but also our equations (3) and (4)] have the form of an evolution problem on natural Hilbert space. The norm of this Hilbert space is not *a priori* conserved but it is controlled by an energy estimate. The author of Ref. 34 proves the global existence and the uniqueness for weakly regular initial data (energy data $H^1\oplus L^2$). Indeed this regularity is sufficient to give sense of an equivalent integral formulation of the nonlinear Cauchy problem since we have a cubic nonlinearity and the Sobolev embedding $H^1\hookrightarrow L^6$. Moreover the globalization is obtained thanks to an energy estimate.

For our problems, the charge spaces are L^2 for (NLD) and $L^2\oplus H^1\oplus L^2$ for (DKG). These regularities do not allow us to control the nonlinear terms of the equations. Hence, we take the more regular data for our study: H^2 for (NLD) and $H^2\oplus H^2\oplus H^1$ for (DKG). The important property that $h(t)$ is equivalent to the euclidean metric outside a unit closed ball gives, thanks to the flat Sobolev embedding in $\mathbb{R}^3, H^2\hookrightarrow L^\infty$, the same embedding for the curved space. This allows us to control the nonlinear terms. The global existence is much more difficult since for our equations, we do not have the conservation or control of the norm H^2 for (NLD) or $H^2\oplus H^2$

$\oplus H^1$ for (DKG). Usually for (3) and (4) in the flat space-time, we obtain the global existence for the sufficiently small initial data in often using the sharper estimations. See this as well as possible exhaustive list of papers: For Dirac semilinear equation, Refs. 35, 36, and 19. For nonlinear Dirac equation, Refs. 30, 27, 28, 37, 31, 15, 4, 5, 27, 16, 17, 14, 13, 12, and 11. For Dirac-Klein-Gordon, Refs. 20, 29, 26, 8, 7, 6, 40, 18, 3, 2, 1, 39, 38, 10, and 9. Obviously the sharp estimates in curved space–time (like Strichartz) are a problem of great complexity, and in ours case there are not proved.

The paper is organized as follows. The second section concerns the $3+1$ decomposition. In the third and fourth we treat, respectively, of Cauchy problem for Dirac and Dirac-Klein-Gordon equation.

II. THE ADM 3+1 DECOMPOSITION OF THE KERR BLOCK I

Usually, to describe the Kerr space-time we adopt the Boyer-Lindquist coordinates $(t,r,\omega) \in \mathbb{R}_t \times \mathbb{R}_r^+ \times S_\omega^2$. We have a time function t globally defined in Block I, i.e., ∇t is a timelike future oriented vector field in $\mathcal{B}_\mathrm{I}$. This function provides a foliation $\{\Sigma_t\}_{t\in\mathbb{R}}$ of $\mathcal{B}_\mathrm{I}$ by its level Cauchy hypersurfaces. Moreover, $K=a\,.\,\partial/\partial t$, $a\in\mathbb{R}$, is the only Killing vector field timelike near spacelike infinity. It fixes the product structure $\mathcal{B}_\mathrm{I}:=\mathbb{R}_t\times\Sigma$, i.e., the identification of points of Σ_t along the integral lines of K. We remark that $\partial/\partial t$ is not timelike everywhere in $\mathcal{B}_\mathrm{I}$. Indeed, $g_{tt}\leqslant 0$ if $(t,r,\omega)\in\mathcal{E}$ and $g_{tt}\geqslant 0$ if $(t,r,\omega)\in\mathcal{B}_\mathrm{I}\backslash\mathcal{E}$. Hence, there exists no global timelike Killing vector field in $\mathcal{B}_\mathrm{I}$. Therefore, this space–time is not stationary. We know that the function t of the Boyer-Lindquist coordinates is a time function. Hence t can be used as time parameter in an evolution equation on $\mathcal{B}_\mathrm{I}=\mathbb{R}_t\times\Sigma$,

$$\Sigma = \,]\, r_+, +\infty[\, \times S_\omega^2. \tag{6}$$

Since the metric g is time independent in the Boyer Lindquist coordinates ($\partial/\partial t$ is a Killing vector field), then the coefficients of the field equation are also time independent.

Now, we point out the difficulties linked to the Boyer-Lindquist coordinates to study a Cauchy problem for equations (3) and (4). These difficulties are mainly due to the nonglobally timelike definition of the Killing vector field $\partial/\partial t$. Indeed, we consider $T_{\mu\nu}$ the stress-energy-momentum tensor for the following scalar field u such that

$$\Box_g u + m^2 u = 0, \quad \nabla^\mu T_{\mu\nu} = 0. \tag{7}$$

Since $\partial/\partial t$ is a Killing vector then the 1-form $T_{\mu 0}\,\mathrm{d}x^\mu$ is closed. Now, we denote by $\mathbf{T}$ the unit future oriented vector field which is normal to Σ_t such that

$$\mathbf{T}^\mu \frac{\partial}{\partial x^\mu} = \sqrt{\frac{\sigma^2}{\Delta\rho^2}}\left(\frac{\partial}{\partial t} + \frac{2aMr}{\sigma^2}\frac{\partial}{\partial\varphi}\right). \tag{8}$$

Then the energy of the field measured by an observer (static at infinity) whose 4-velocity vector is $\partial/\partial t$ is given by

$$E(u,t) := \int_{\Sigma_t} \mathbf{T}^\mu T_{\mu 0}\mathrm{dVol}, \quad \mathrm{dVol} = \sqrt{\frac{\rho^2\sigma^2}{\Delta}}\mathrm{d}r\,\mathrm{d}\omega \tag{9}$$

where dVol is the volume measure on Σ. Hence,

$$E(u,t) = \int_\Sigma \left(|\partial_t u(t)|^2 + \frac{\Delta^2}{\sigma^2}|\partial_r u(t)|^2 + \frac{\Delta}{\sigma^2}|\partial_\theta u(t)|^2 + \frac{\rho^2-2Mr}{\sigma^2\sin^2\theta}|\partial_\varphi u(t)|^2 + \frac{\Delta\rho^2 m^2}{\sigma^2}|u(t)|^2\right)\frac{\sigma^2}{\Delta}\mathrm{d}r\,\mathrm{d}\omega. \tag{10}$$

Clearly, the fourth term is positive outside the ergosphere and negative inside. Hence the energy is not positive definite in all $\mathcal{B}_\mathrm{I}$. This property allows superradiance to take place outside the black

hole. Hence we do not choose this energy space to study the Cauchy problem with a system which contains a spin-0 field as (4). Then, the study is more difficult but not impossible, see, for example, the strategy used in Ref. 24. Roughly speaking, it consists in finding a new energy norm positive definite such that its growth is controlled by an energy estimate. Finally in the sequel, we adopt this approach but the choice of the new energy space is naturally given by the geometry thanks to the $3+1$ decomposition. Although in the case of the spin-$1/2$ the phenomenon of superradiance does not take place, we show in the following paragraph that the $3+1$ decomposition is nevertheless useful for this field.

The space–time $(\mathcal{B}_{\mathrm{I}}, g)$ is globally hyperbolic. This means that there exists a time function t globally defined on $\mathcal{B}_{\mathrm{I}}$ (providing of foliation of $\mathcal{B}_{\mathrm{I}}$ by the hypersurfaces Σ_t) and that any points of $\mathcal{B}_{\mathrm{I}}$ can be reached from Σ_{t_0} along a nonspacelike curve (see Geroch[22]). Each Σ_t are homeomorphic to a given 3-manifold Σ. Now, we choose $\mathbf{T}$ the unit timelike oriented vector normal to Σ_t defined in (8) to fixed the product structure $\mathcal{B}_{\mathrm{I}}=\mathbb{R}\times\Sigma$, i.e., the points on different hypersurfaces Σ_t are identified along the integral lines of $\mathbf{T}$. This construction induces an explicit system of coordinates that is referred to as the point of view of locally non rotating observers:

$$\tau = t, \quad R = r, \quad \Theta = \theta, \quad \Phi = \varphi - t\alpha, \quad \alpha := -\frac{g_{t\varphi}}{g_{\phi\phi}} = \frac{2aMr}{\sigma^2}. \tag{11}$$

Now, we decompose the metric g as the sum of its orthogonal projection along $\mathbf{T}$ and $(\mathbf{T})^{\perp} = T_p\Sigma_t$,

$$g_{\mu\nu}\,\mathrm{d}x^{\mu}\,\mathrm{d}x^{\nu} = N^2\,\mathrm{d}\tau^2 - h(\tau), \quad N := \sqrt{g_{tt} - \frac{g_{t\varphi}^2}{g_{\varphi\varphi}}} = \sqrt{\frac{\Delta\rho^2}{\sigma^2}}, \tag{12}$$

where N is the lapse function, and

$$h(\tau) = -g_{rr}\,\mathrm{d}R^2 - g_{\theta\theta}\,\mathrm{d}\Theta^2 - g_{\varphi\varphi}\left(\mathrm{d}\Phi + \tau\frac{\partial\alpha}{\partial R}\mathrm{d}R + \tau\frac{\partial\alpha}{\partial\Theta}\mathrm{d}\Theta\right)^2. \tag{13}$$

The definition of g in these new coordinates leads to simple form of hyperbolic evolution equation without crossed terms depending on t and φ since $g_{t\varphi}=0$ (unlike to the Boyer-Lindquist coordinates form for g). This is the main motivation to use the $3+1$ decomposition for spin-$1/2$ fields. But we remark that the metric is not time independent anymore. Henceforth, the evolution equation is defined with the help of time-dependent Hamiltonian. The following proposition state that the dependence on t is rather nice (see Ref. 33.)

Proposition 2.1:

(i) $\Sigma_\tau=(\Sigma, h(\tau))$ *is a* C^∞*-Riemannian manifold for all* $\tau\in\mathbb{R}$ *with smooth boundary* $\partial\Sigma=\{r_+\}\times S^2_\omega$.

(ii) *The lapse function* N *is strictly positive on* Σ, *vanishes on* $\partial\Sigma$, *is independent of* τ, C^∞ *and uniformly bounded on* $\bar{\Sigma}$ *as well as all its derivatives*.

(iii) $h_{\mu\nu}\in C^\infty(\mathbb{R}_\tau; C_b^\infty(\Sigma; T_{\mu\nu}\mathcal{M}))$, $h^{\mu\nu}\in C^\infty(\mathbb{R}_\tau; C_b^\infty(\Sigma; T^{\mu\nu}\mathcal{M}))$. *All slice* Σ_τ *have the same geometry (*g *is independent of* t *in Boyer-Lindquist coordinates) and* $h(\tau)$ *is obtained from* $h(0)$ *by a rotation around the axis of the black hole whose angle is* $\tau\alpha$ *with* α *defined in (11).*

$$h(0) = \frac{\rho^2}{R^2}\mathrm{d}u^2 + \frac{\rho^2}{(1+u)^2}(1+u)^2\,\mathrm{d}\Theta^2 + \frac{(R^2+a^2)\rho^2 + 2MRa^2\sin^2\Theta}{\rho^2(1+u)^2}(1+u)^2\sin^2\Theta\,\mathrm{d}\Phi^2 \tag{14}$$

with u *the h-distance to the horizon such that*

$$u:\left[r_+,+\infty\right[_R \mapsto \mathbb{R}, \quad u(R) := \int_{r_+}^{R} \frac{s}{\sqrt{\Delta}} \mathrm{d}s. \tag{15}$$

Hence, we remark that $h(\tau)$ is equivalent to the Euclidian metric on $\mathbb{R}^3 \backslash \bar{B}(0,1)$,

$$\mathrm{d}u^2 + (1+u)^2\, \mathrm{d}\Theta^2 + (1+u)^2 \sin^2\Theta\, \mathrm{d}\Phi^2. \tag{16}$$

(iv) *$|h|$, the determinant of the metric $h(\tau)$, is independent of τ and $|g| := |\det g| = -N^2|h|$.*

III. LOCAL CAUCHY PROBLEM FOR NONLINEAR DIRAC EQUATION OUTSIDE A KERR BLACK HOLE

In this section we study the local Cauchy problem for the nonlinear Dirac equation (3). We use the 3+1 decomposition to defined an evolution problem in $\mathcal{B}_{\mathrm{I}}$. A result of Nicolas[33] gives the existence of a propagator for a solution of the linear part of (3). For the nonlinear equation, a Duhamel formula and a Sobolev embedding $H^2 \hookrightarrow L^\infty$ are useful to obtain the result.

We describe more precisely the Dirac equation in 3+1 decomposition framework. Since $(\mathcal{B}_{\mathrm{I}}, g)$ is a globally hyperbolic spacetime then it admits a spin structure (Refs. 21 and 23). We denote by $\mathbb{S}$ the bundle over $\mathcal{B}_{\mathrm{I}}$ of negative spinors and by $\bar{\mathbb{S}}$ the bundle of positive spinors i.e., the complex structure in $\mathbb{S}$ simply replaced by its opposite. We also, respectively, denote by the $\mathbb{S}^*$ and $\bar{\mathbb{S}}^*$ the dual of $\mathbb{S}$ and $\bar{\mathbb{S}}$. Finally the complexified tangent bundle to $\mathcal{B}_{\mathrm{I}}$ is recovered as the tensor product of $\mathbb{S}$ and $\bar{\mathbb{S}}$,

$$T\mathcal{B}_{\mathrm{I}} \otimes \mathbb{C} = \mathbb{S} \otimes \bar{\mathbb{S}}, \quad T^*\mathcal{B}_{\mathrm{I}} \otimes \mathbb{C} = \mathbb{S}^* \otimes \bar{\mathbb{S}}^*. \tag{17}$$

We define the Dirac equation on the block I. The bundle of Dirac spinors on $\mathcal{B}_{\mathrm{I}}$ is described as

$$\mathbb{S}_D := \mathbb{S}^* \oplus \bar{\mathbb{S}}. \tag{18}$$

On space–time $\mathcal{B}_{\mathrm{I}}$, we choose a local orthogonal Lorentz frame $\{e_0, e_1, e_2, e_3\}$ such that

$$g(e_0, e_0) = 1, \quad g(e_a, e_a) = -1, \quad a = 1,2,3, \quad g(e_a, e_b) = 0, \quad a \neq b. \tag{19}$$

Obviously in the 3+1 decomposition framework, we choose for the basis $\{e_0, e_1, e_2, e_3\}$

$$e_0{}^a := \frac{1}{\sqrt{2}} T^a, \quad e_1, e_2, e_3 \in T\Sigma_t. \tag{20}$$

Hence, we define the Dirac operator on $\mathcal{B}_{\mathrm{I}}$ by

$$\mathbf{D} := \sum_{a=0}^{3} e_a \,.\, \nabla_{e_a} \tag{21}$$

where ∇_{e_a} is the directional convariante derivative along e_a and e_a. The Clifford product by the vector e_a. More presicely by a choice of spin-frame or Newman-Penrose tetrad, the Clifford multiplication of a Dirac spinor $\Psi \in \mathbb{S}_D$ by e_a is described as the multiplication by a Dirac matrices γ^a satisfying the following relation:

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}\mathbf{1}_4, \quad \mu, \nu = 0,1,2,3,4. \tag{22}$$

The Dirac equation for a spin-1/2 particle with mass $m_d > 0$ takes the following form with Einstein notation:

$$i\gamma^\mu \nabla_{e_\mu} \Psi - m_d \Psi = (\mathbf{D} - m_d)\Psi = 0. \tag{23}$$

From (20) and (23), we write the Dirac equation as an evolution system

$$ie_0 \,.\, \nabla_{e_0}\Psi = -i\sum_{a=1}^{3} e_a \,.\, \nabla_{e_a}\Psi + m_d\Psi \tag{24}$$

or

$$\nabla_{e_0}\Psi = -\sum_{a=1}^{3} e_0 \,.\, e_a \,.\, \nabla_{e_a}\Psi - im_d\Psi. \tag{25}$$

We introduce the Dirac-Witten operator $\mathbf{D}_w(\tau)$ on Σ_τ (extrinsic geometry) such that

$$\mathbf{D}_w(\tau) = \sum_{a=1}^{3} e_a \,.\, \nabla_{e_a}. \tag{26}$$

We also define $\mathbf{D}_\Sigma(\tau)$ the Dirac operator associated to the Levi-Civita connection on $(\Sigma_\tau, h(\tau))$ such that

$$\mathbf{D}_w(\tau) = \mathbf{D}_\Sigma(\tau) + \frac{1}{2\sqrt{2}}Ke_0, \tag{27}$$

where K is the $\sqrt{2}$ times the trace of the extrinsic curvature. This operator is symmetric on $C_0^\infty(\Sigma_t, \mathbb{S}_D)$ for the inner product

$$\langle \Psi, \Phi \rangle_{L^2_{\Sigma_\tau}} := \int_\Sigma \langle \Psi, \Phi \rangle \mathrm{dVol}_{h_\tau}, \tag{28}$$

where

$$\langle \Psi, \Phi \rangle := \Psi_1\bar{\Phi}_1 + \Psi_2\bar{\Phi}_2 + \Psi_3\bar{\Phi}_3 + \Psi_4\bar{\Phi}_4 \tag{29}$$

when we choose a spin-frames adapted to the foliation Σ_τ. According to Proposition 2.1, this inner product is in fact τ-independent since the determinent of g is also τ-independent. Finally, we write the Dirac equation in the following form, i.e., as a first order symmetric hyperbolic system on Σ,

$$\nabla_{e_0}\Psi = -e_0 \cdot \mathbf{D}_\Sigma(\tau)\Psi - \frac{1}{2\sqrt{2}}K\Psi - im_d\Psi, \tag{30}$$

and the operator

$$\mathbf{D}_D := e_0 \cdot \mathbf{D}_\Sigma(\tau), \quad e_0 = \frac{1}{\sqrt{2}}\mathbf{T}^\mu\partial_\mu \tag{31}$$

being formally skew-adjoint on $L^2(\Sigma; \mathbb{S}_D)$. By choosing a adapted Newman-Penrose tetrad (a spin frame adapted to foliation Σ_τ) equation (30) becomes (see Appendix A in Ref. 33)

$$\frac{\partial\Psi}{\partial\tau} = \mathcal{A}_D(\tau)\Psi, \quad \mathcal{A}_D(\tau) := -\frac{N}{\sqrt{2}}\left(\mathbf{D}_\Sigma(\tau) + \frac{1}{2\sqrt{2}}K + im_d\gamma^0 + B(\tau)\right), \tag{32}$$

where B is a matrix containing the connections terms of ∇_{a_0}, N the lapse function and

$$\gamma^0 = i\begin{pmatrix} 0 & \mathbf{1}_2 \\ -\mathbf{1}_2 & 0 \end{pmatrix}. \tag{33}$$

We introduce the functional framework. On Σ_τ we define the Sobolev space $H_0^k(\Sigma_\tau; \mathbb{S}_D)$ as the completion of $C_0^\infty(\Sigma; \mathbb{S}_D)$ for the norm

$$\|\Psi\|_{H_0^k(\Sigma_\tau)} = \left(\sum_{p=0}^{k} \int_\Sigma \langle (D_\tau)^p \Psi, (D_\tau)^p \Psi \rangle \mathrm{dVol}_h \right)^{1/2}, \tag{34}$$

where D_τ is the Levi-Civita connection on $(\Sigma, h(\tau))$. According Proposition 2.1, we remark that for all $\tau \in \mathbb{R}$, $\mathrm{dVol}_h = \mathrm{dVol}_{h(\tau)}$ and the norms in $H_0^k(\Sigma_\tau; \mathbb{S}_D)$ and $H_0^k(\Sigma_{\tau_0}; \mathbb{S}_D)$ are locally uniformly in time equivalent (the constants in the norms estimates are time dependent and locally bounded in time). Hence, we simply denote by $H_0^k(\Sigma, \mathbb{S}_D)$ the Sobolev space associated with the norm

$$\left\| \cdot \right\|_{(k)} := \left\| \cdot \right\|_{H_0^k(\Sigma_{\tau_0})}$$

and the metric $h(\tau_0)$.

Proposition 3.1:

We define the following norm for all $\tau \in \mathbb{R}$:

$$\|\Psi\|_{k,\tau} := \left(\sum_{p=0}^{k} \int_\Sigma \langle (\mathbf{D}_\Sigma)^p(\tau)\Psi, (\mathbf{D}_\Sigma)^p(\tau)\Psi \rangle \mathrm{dVol}_h \right)^{1/2}, \quad \forall\, \Psi \in H_0^k(\Sigma; \mathbb{S}_D). \tag{35}$$

Then the norm $\|\cdot\|_{(k)}$ *and* $\|\cdot\|_{k,\tau}$ *are locally uniformly in time equivalent on* $H_0^k(\Sigma; \mathbb{S}_D)$.

This proposition is a consequence of Proposition 2.1 and the Bochner-Lichnerowicz-Weitzenböck formula

$$(\mathbf{D}_\Sigma(\tau))^* \mathbf{D}_\Sigma(\tau) = (\mathbf{D}_\Sigma)^2 = D_\tau^* D_\tau + \tfrac{1}{4} R_{h(\tau)} = -\Delta_{h(\tau)} + \tfrac{1}{4} R_{h(\tau)}, \tag{36}$$

where $R_{h(\tau)}$ is the scalar curvature of $(\Sigma, h(\tau))$. The following theorem concerns the Cauchy problem on Block I for the linear equation (32) (see Ref. 33).

Theorem 3.1: *For any initial data* $\Psi_0 \in H_0^k(\Sigma; \mathbb{S}_D)$, $k \in \mathbb{N}$, *the system (32) has a unique solution* Ψ *satisfying*

$$\Psi \in \bigcap_{l=0}^{k} C^l(\mathbb{R}_\tau; H_0^{k-l}(\Sigma; \mathbb{S}_D)). \tag{37}$$

Moreover, there exits a propagator $\mathcal{U}_D$ *such that*

(i) $\mathcal{U}_D(\tau, \tau_0) : \Psi_0 \mapsto \Psi(\tau)$.

(ii) $\forall t, s \mathbb{R}$, $\mathcal{U}_D(t,s) \in \mathcal{L}(H_0^k(\Sigma; \mathbb{S}_D))$, $\mathcal{U}_D$ *is strongly continuous on* $\mathbb{R}^2_{ts}$ *to* $\mathcal{L}(H_0^k(\Sigma; \mathbb{S}_D))$.

(iii) $\mathcal{U}_D(t,t) = \mathrm{Id}$, $\mathcal{U}_D(t,s) = \mathcal{U}_D(t,r)\mathcal{U}_D(r,s)$ *for all* $t, s, r \in \mathbb{R}$.

(iv) *we have in the sense of distributions on* $\mathbb{R} \times \Sigma$,

$$\frac{\partial}{\partial \tau} \mathcal{U}_D(\tau, \tau_0)\Psi_0 = \mathcal{A}_D(\tau)\mathcal{U}_D(\tau, \tau_0)\Psi_0, \tag{38}$$

$$\frac{\partial}{\partial \tau_0} \mathcal{U}_D(\tau, \tau_0)\Psi_0 = -\mathcal{U}_D(\tau, \tau_0)\mathcal{A}_D(\tau_0)\Psi_0, \tag{39}$$

(v) *We have also the unitary evolution in* $L^2(\Sigma; \mathbb{S}_D)$,

$$\|\Psi(\tau)\|_{L^2(\Sigma; \mathbb{S}_D)} = \|\Psi_0\|_{L^2(\Sigma; \mathbb{S}_D)}. \tag{40}$$

(vi) *There exists a continuous, strictly positive function* α_k *such that*

$$\|\Psi(\tau)\|_{k,\tau} \leqslant \alpha_k(\tau, \tau_0)\|\Psi_0\|_{k,\tau_0}, \quad \alpha_k(\tau, \tau) = 1, \tag{41}$$

and a continuous, strictly positive function κ *such that*

$$\|\Psi(\tau)\|_{(k)} \leqslant \kappa_k(\tau,\tau_0)\|\Psi_0\|_{(k)}, \quad \kappa_k(\tau,\tau)=1, \tag{42}$$

According to the 3+1 decomposition, we consider the nonlinear problem (3) in the new equivalent form

$$\frac{\partial\Psi}{\partial\tau}=\mathcal{A}_D(\tau)\Psi+\mathcal{J}_D(\Psi), \quad \mathcal{J}_D(\Psi):=i\frac{N}{\sqrt{2}}k(\Psi^*\gamma^0\Psi)\gamma^0\Psi. \tag{43}$$

In the sequel, we present a proof of the local Cauchy problem for the previous nonlinear equation with $H_0^2(\Sigma;\mathbb{S}_D)$ initial data. First, we prove the following lemma.

Lemma 3.1: There exists a constant $C\geqslant 0$ such that,

$$\|\mathcal{J}_D(\Psi)\|_{(2)} \leqslant C\|\Psi\|_{(2)}^3, \quad \Psi,\Phi\in H_0^2(\Sigma;\mathbb{S}_D), \tag{44}$$

$$\|\mathcal{J}_D(\Psi)-\mathcal{J}_D(\Phi)\|_{(2)} \leqslant C(\|\Psi\|_{(2)}^2+\|\Phi\|_{(2)}^2)\|\Psi-\Phi\|_{(2)}, \tag{45}$$

Proof: We only prove (45), since (44) is (45) with $\Phi\equiv 0$. We have

$$\begin{aligned}\mathcal{J}_D(\Psi)-\mathcal{J}_D(\Phi)=\frac{N}{\sqrt{2}}k[&(\Psi^*\gamma^0\Psi)\gamma^0\Psi-(\Phi^*\gamma^0\Psi)\gamma^0\Psi+(\Phi^*\gamma^0\Psi)\gamma^0\Psi+(\Phi^*\gamma^0\Phi)\gamma^0\Psi\\&-(\Phi^*\gamma^0\Phi)\gamma^0\Psi-(\Phi^*\gamma^0\Phi)\gamma^0\Phi],\end{aligned}$$

$$=\frac{N}{\sqrt{2}}k[([\Psi^*-\Psi^*]\gamma^0\Psi)\gamma^0\Psi+(\Phi^*\gamma^0[\Psi-\Phi])\gamma^0\Psi+(\Phi^*\gamma^0\Phi)\gamma^0[\Psi-\Phi]]. \tag{46}$$

Now, we remark that $H^2(\mathbb{R}^3)\hookrightarrow L^\infty(\mathbb{R}^3)$. Then, since $h(\tau)$ is equivalent to the Euclidian metric on $\mathbb{R}^3\backslash\bar{B}(0,1)$, we have for $\Psi\in H_0^2(\Sigma;\mathbb{S}_D)$

$$\|\Psi\|_{L^\infty(\Sigma;\mathbb{S}_D)} \leqslant C_1\|\Psi\|_{(2)}, \quad C_1>0. \tag{47}$$

Therefore, according to (46) and (47), since $N,k\in L^\infty$, we have

$$\begin{aligned}\|\mathcal{J}_D(\Psi)-\mathcal{J}_D(\Phi)\|_{(2)} &\leqslant C_3(\|\Psi\|_{L^\infty(\Sigma;\mathbb{S}_D)}^2+\|\Psi\|_{L^\infty(\Sigma;\mathbb{S}_D)}\|\Phi\|_{L^\infty(\Sigma;\mathbb{S}_D)}+\|\Phi\|_{L^\infty(\Sigma;\mathbb{S}_D)}^2)\|\Psi-\Phi\|_{(2)}\\&\leqslant C(\|\Psi\|_{(2)}^2+\|\Phi\|_{(2)}^2)\|\Psi-\Phi\|_{(2)}, \quad C_3,C>0.\end{aligned} \tag{48}$$

■

Now, we study the following problem:

$$\Psi(\tau)=S(\Psi)(\tau),$$

$$S(\Psi)(\tau):=\mathcal{U}_D(\tau,\tau_0)\Psi_0+\int_{\tau_0}^{\tau}\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))\mathrm{d}s, \quad \Psi\in C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D)). \tag{49}$$

to solve the local Cauchy problem

$$\begin{aligned}&\frac{\partial\Psi}{\partial\tau}=\mathcal{A}_D(\tau)\Psi+\mathcal{J}_D(\Psi),\\&\Psi(\tau_0)=\Psi_0\in H_0^2(\Sigma;\mathbb{S}_D), \quad \Psi\in C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D)).\end{aligned} \tag{50}$$

Theorem 3.2: *For* $\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D)$, *there exists* $T(\|\Psi_0\|_{(2)})>0$ *such that (43) admits a unique solution* Ψ *such that*

$$\Psi(\tau_0)=\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D), \quad \Psi \in C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D)). \tag{51}$$

Proof: The operator S in (49) is well defined if $\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D)$. Indeed, if $\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D)$ then $\mathcal{U}_D(\tau,\tau_0)\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D)$ by (42) and

$$\|\mathcal{U}_D(\tau,s+h)\mathcal{J}_D(\Psi(s+h))-\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))\|_{(2)}, \quad K:=\max\{\kappa_2(\sigma,\tau),\sigma,\tau\in[\tau_0,\tau_0+T]\},$$

$$\leqslant \|\mathcal{U}_D(\tau,s+h)(\mathcal{J}_D(\Psi(s+h))-\mathcal{J}_D(\Psi(s)))\|_{(2)}+\|(\mathcal{U}_D(\tau,s+h)-\mathcal{U}_D(\tau,s))\mathcal{J}_D\ (\Psi(s)))\|_{(2)}$$
$$\leqslant K\|\mathcal{J}_D(\Psi(s+h))-\mathcal{J}_D(\Psi(s))\|_{(2)}+K\|(\mathcal{U}_D(s,s+h)-1)\mathcal{J}_D(\Psi(s))\|_{(2)}.$$

Hence $s\mapsto\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))$ is continuous on $H_0^2(\Sigma;\mathbb{S}_D)$, thanks to (44) and (45) and since $\mathcal{U}_D$ is strongly continuous on $H_0^2(\Sigma;\mathbb{S}_D)$.

Moreover, $C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D))$ is stable by S,

$$\|S(\Psi)(\tau+h)-S(\Psi)(\tau)\|_{(2)}\leqslant\|\mathcal{U}_D(\tau+h,\tau_0)\Psi_0-\mathcal{U}_D(\tau,\tau_0)\Psi_0\|_{(2)}+\int_{\tau_0}^{\tau}\|\mathcal{U}_D(\tau+h,s)\mathcal{J}_D(\Psi(s))$$
$$-\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))\|_{(2)}\,\mathrm{d}s+\int_{\tau+h}^{\tau}\|\mathcal{U}_D(\tau+h,s)\mathcal{J}_D(\Psi(s))\|_{(2)}\,\mathrm{d}s \tag{52}$$

This norm vanishes as $h\to 0$, since $\mathcal{U}$ is strongly continuous on $H_0^2(\Sigma;\mathbb{S}_D)$ for the first term on right on side, thanks to the same property, the Lebesgue theorem and (45) for the second. The last is bounded by $Kh\sup_{s\in[\tau,\tau+h]}\|\Psi(s)\|^3_{H_0^2(\Sigma;\mathbb{S}_D)}$, $K:=\max\{\kappa_2(\sigma,\tau),\sigma,\tau\in[\tau_0,\tau_0+T]\}$ thanks to (44).

Now, we define the convex closed of $C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D))$,

$$V_{T,\Psi_0}:=\{\Psi\in C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D));\Psi(\tau_0)=\Psi_0,\ \|\Psi\|_T\leqslant 2K\|\Psi_0\|_{(2)}\}, \tag{53}$$

$$K:=\max\{\kappa_2(\sigma,\tau),\sigma,\tau\in[s,s+T]\}, \tag{54}$$

with

$$\|\Psi\|_T=\sup_{[\tau_0,\tau_0+T[_\tau}\|\Psi\|_{(2)}. \tag{55}$$

For T small $S(V_{T,\Psi_0})\subset V_{T,\Psi_0}$. Indeed, according to (45) and (53), we have

$$\|S(\Psi)\|_T\leqslant K(1+8TCK^2\|\Psi_0\|^2_{(2)})\|\Psi_0\|_{(2)}, \quad \Psi\in V_{T,\Psi_0}, \tag{56}$$

and we choose

$$T<(8CK^2\|\Psi_0\|^2_{(2)})^{-1}. \tag{57}$$

Moreover, we obtain with (45).

$$\|S(\Psi)-S(\Phi)\|_T\leqslant TK\|\mathcal{J}_D(\Psi)-\mathcal{J}_D(\Phi)\|_T\leqslant 4TK^2C\|\Psi_0\|^2_{(2)}\|\Psi-\Phi\|_T, \quad \Psi,\Phi\in V_{T,\Psi_0}. \tag{58}$$

Then, if we choose

$$T<\min(8CK^2\|\Psi_0\|^2_{(2)})^{-1}, \quad (4TK^2C\|\Psi_0\|^2_{(2)})^{-1}) \tag{59}$$

by the Banach fixed point theorem there exists a solution of (49).

Now we study the uniqueness of this problem. Given $T>0$, $\Psi_0 \in H_0^2(\Sigma;\mathbb{S}_D)$ and two solutions $\Psi_1, \Psi_2 \in C^0([\tau_0, \tau_0+T[_\tau, H_0^2(\Sigma;\mathbb{S}_D))$ associated to Ψ_0, then with $K := \max\{\kappa_2(\sigma,\tau), \sigma, \tau \in [\tau_0, \tau_0+T]\}$

$$\|\Psi_1(\tau)-\Psi_2(\tau)\|_{(2)} \leqslant K\int_{\tau_0}^{\tau} \|\mathcal{J}_D(\Psi_1(s))-\mathcal{J}_D(\Psi_2(s))\|_{(2)}\,\mathrm{d}s \leqslant K(\|\Psi\|_T^2+\|\Phi\|_T^2) \times \int_{\tau_0}^{\tau} \|\Psi_1(s)-\Psi_2(s)\|_{(2)}\,\mathrm{d}s. \tag{60}$$

Then by Gronwall lemma we have $\Psi_1=\Psi_2$.

First, we prove that the problems (49) and (50) are equivalent. If Ψ is solution of (49) then Ψ, satisfies equation (50). Indeed, according to the properties of $\mathcal{U}_D$ we have

$$\frac{\partial\Psi}{\partial\tau}(\tau) = \mathcal{A}_D(\tau)\mathcal{U}_D(\tau,\tau_0)\Psi + \int_{\tau_0}^{\tau} \mathcal{A}_D(\tau)\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))\mathrm{d}s + \mathcal{J}_D(i(\tau)) = \mathcal{A}_D(\tau)\Psi(\tau) + \mathcal{J}_D(\Psi(\tau))$$

since $s \mapsto \mathcal{A}_D(\tau)\mathcal{U}_D(\tau,s)\mathcal{J}_D(\Psi(s))$ is bounded on $H_0^2(\Sigma;\mathbb{S}_D)$ by (44) and (42) and also $\mathcal{A}_D(\tau)$ is closed for each τ. The inverse is straightforward. The uniqueness follows from the Gronwall lemma. ■

Remark 3.1:

(1) *Theorem 3.2 is in fact valid for* $\Psi_0 \in H_0^s(\Sigma;\mathbb{S}_D)$, $s \geqslant 2$. *Indeed, it is easy to prove thanks to the Sobolev embedding* $H^s(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)$ *an equivalent lemma of Lemma 3.1 for* $H_0^s(\Sigma;\mathbb{S}_D)$. *The proof of the theorem with* $\Psi_0 \in H_0^s(\Sigma;\mathbb{S}_D)$ *is essentially the same.*

(2) *Theorem 3.2 is still valid with the following non linearity,*

$$\mathcal{J}_D^p(\Psi) := i\frac{N}{\sqrt{2}}k|(\Psi^*\gamma^0\Psi)|^{(p-1)/2}\gamma^0\Psi, \quad p \geqslant 3. \tag{61}$$

Then, we obtain the following estimates:

$$\|\mathcal{J}_D^p(\Psi)\|_{(s)} \leqslant C\|\Psi\|_{(s)}^p, \quad \Psi,\Phi \in H_0^s(\Sigma;\mathbb{S}_D), \tag{62}$$

$$\|\mathcal{J}_D^p(\Psi)-\mathcal{J}_D^p(\Phi)\|_{(s)} \leqslant C(\|\Psi\|_{(s)}^{p-1}+\|\Phi\|_{(s)}^{p-1})\|\Psi-\Phi\|_{(s)}. \tag{63}$$

As above, the proof with this nonlinearity remains essentially the same.

IV. LOCAL CAUCHY PROBLEM FOR THE DIRAC-KLEIN-GORDON EQUATION OUTSIDE A KERR BLACK HOLE

In this section we study the local Cauchy problem for the Dirac-Klein-Gordon equation (4). As above, we use the 3+1 decomposition to defined an evolution problem in $\mathcal{B}_I$. To prove the existence of local solutions, we use a Duhamel formula and a Sobolev embedding $H^s(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)$, $s \geqslant 2$.

According to the 3+1 decomposition, the preceding section and the following definition:

$$\Box_g = \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^\mu}\left(\sqrt{|g|}g^{\mu\nu}\frac{\partial}{\partial x^\nu}\right), \tag{64}$$

Eq. (4) is equivalent to

$$\frac{\partial\Psi}{\partial\tau} = \mathcal{A}_D(\tau)\Psi + i\frac{N}{\sqrt{2}}\Phi\gamma^0\mathcal{V}_2\Psi, \tag{65}$$

$$\frac{\partial^2\Phi}{\partial\tau^2} = \mathcal{A}_{\mathrm{KG}}(\tau)\Phi + N^2\Psi^*\mathcal{V}_3\Psi, \quad \mathcal{A}_{\mathrm{KG}}(\tau) := N^2\Delta_h - N^2 m_{kg}^2, \tag{66}$$

where

$$\Delta_h := \frac{1}{N\sqrt{|h|}}\frac{\partial}{\partial x^a}\left(N\sqrt{|h|}h^{ab}\frac{\partial}{\partial x^b}\right) \tag{67}$$

and $\mathcal{A}_D(\tau)$ defined in (32). Now we put this equation in Hamiltonian form such that

$$\frac{\partial U}{\partial\tau} = \mathcal{A}_{\mathrm{DKG}}(\tau)U + \mathcal{J}_{\mathrm{DKG}}(U), \quad U={}^t(\Psi,\Phi,\partial_\tau\Phi), \tag{68}$$

where

$$\mathcal{A}_{\mathrm{DKG}}(\tau) := \begin{pmatrix} \mathcal{A}_D(\tau) & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \mathcal{A}_{\mathrm{KG}}(\tau) & 0 \end{pmatrix}, \quad \mathcal{J}_{\mathrm{DKG}}(U) := \begin{pmatrix} i\frac{N}{\sqrt{2}}\Phi\gamma^0\mathcal{V}_2\Psi \\ 0 \\ N^2\Psi^*\mathcal{V}_3\Psi \end{pmatrix}. \tag{69}$$

First, we remark some properties for the linear part of the equation (66) (i.e., $\mathcal{V}_3=0$). According to a result due to Leray,[25] we have for this linear equation.

Theorem 4.1: *For initial data $\Phi_0,\Phi_1\in C_0^\infty(\Sigma)$ in $\tau_0\in\mathbb{R}$, the equation (66) with $V_3=0$ has a solution $\Phi\in C^\infty(\mathbb{R}_\tau,C_0^\infty(\Sigma))$ satisfying $\Phi(\tau_0)=\Phi_0$ and $\partial_\tau\Phi(\tau_0)=\Phi_1$.*

The proof of the following proposition consists in multiplying the equation by $\partial_\tau\Phi$ and integrating by part on $[\tau_0,\tau]\times\Sigma$:

Proposition 4.1: There exists a continuous, strictly positive function ξ such that $\xi(\tau,\tau)=1$ and for each $\Phi\in C^\infty(\mathbb{R}_\tau,C_0^\infty(\Sigma))$ solution of the equation (68) with $V_3=0$, we have for any $\tau,\tau_0\in\mathbb{R}$

$$E_{3+1}(\Phi,\tau) \leqslant \xi(\tau,\tau_0)E_{3+1}(\Phi,\tau_0) \tag{70}$$

with

$$E_{3+1}(\Phi,\tau) := \int_{\Sigma_\tau}(|\partial_t\Phi|^2 + N^2h^{ab}\partial_a\Phi\partial_b\bar{\Phi} + N^2m_{kg}^2|\Phi|^2)\frac{1}{N}\mathrm{dVol}. \tag{71}$$

According to Proposition 2.1, we consider $\eta=h(0)$ on $\bar{\Sigma}$ and we introduce the Hilbert space $\mathcal{H}_0^{1,0}(\Sigma)$ as the completion of $C_0^\infty(\Sigma)\oplus C_0^\infty(\Sigma)$ for the norm

$$\|(u,v)\|_{[1,0]}^2 := \int_\Sigma(|v|^2 - \mathcal{A}_{\mathrm{KG}}u\bar{u})\frac{1}{N}\mathrm{dVol} = \int_\Sigma(|v|^2 + N^2|\nabla u|^2 + N^2m_{kg}^2|u|^2)\frac{1}{N}\mathrm{dVol},$$
$$|\nabla u|^2 = \eta^{ab}\partial_a u\partial_b\bar{u}. \tag{72}$$

With these two last results, we deduce the following.

Proposition 4.2: For any initial data $U_0 := {}^t(\Phi_0, \Phi_1) \in \mathcal{H}_0^{1,0}(\Sigma)$ *in* $\tau_0 \in \mathbb{R}$, *the equation (66) with* $V_3 = 0$ *has an unique solution* $U \in C^0(\mathbb{R}_\tau, \mathcal{H}_0^{1,0}(\Sigma))$ *satisfying* $U(\tau_0) = {}^t(\Phi_0, \Phi_1)$. *Moreover, we have the existence of a propagator* $\mathcal{U}_{\mathrm{KG}}$ *such that:*

(i) *For all* $\tau, \sigma \in \mathbb{R}$, $\mathcal{U}_{\mathrm{KG}}(\tau, \sigma) \in \mathcal{L}(\mathcal{H}_0^{1,0})$, $\|\mathcal{U}_{\mathrm{KG}}(\tau, \sigma)\|_{\mathcal{L}(\mathcal{H}_0^{1,0}(\Sigma))} \leqslant \xi(\sigma, \tau)$ *where* ξ *is the function defined in (70).*

(ii) $\mathcal{U}_{\mathrm{KG}}(\tau, \tau) = 1$, $\mathcal{U}_{\mathrm{KG}}(\tau, s) = \mathcal{U}_{\mathrm{KG}}(t, r)\mathcal{U}_{\mathrm{KG}}(r, s)$ *for all* $t, s, r \in \mathbb{R}$.

(iii) *We have in the sense of distributions on* $\mathbb{R} \times \Sigma$,

$$\frac{\partial}{\partial \tau}\mathcal{U}_{\mathrm{KG}}(\tau, \tau_0)U_0 = \mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau)\mathcal{U}_{\mathrm{KG}}(\tau, \tau_0)U_0, \quad \mathcal{M}_{\mathcal{A}_{\mathrm{KG}}} = \begin{pmatrix} 0 & 1 \\ \mathcal{A}_{\mathrm{KG}} & 0 \end{pmatrix}, \tag{73}$$

$$\frac{\partial}{\partial \tau_0}\mathcal{U}_{\mathrm{KG}}(\tau, \tau_0)U_0 = -\mathcal{U}_{\mathrm{KG}}(\tau, \tau_0)\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau_0)U_0. \tag{74}$$

We introduce $\tilde{\mathcal{A}}_{\mathrm{KG}}$ such that

$$\tilde{\mathcal{A}}_{\mathrm{KG}} := N^2\Delta_\eta - 1. \tag{75}$$

Now, we define $\mathcal{H}_0^{2,1}(\Sigma)$ as the completion of $C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma)$ for the norm

$$\|(u, v)\|_{[2,1]}^2 := \int_\Sigma (|\tilde{\mathcal{A}}_{\mathrm{KG}}u|^2 - \mathcal{A}_{\mathrm{KG}}u\bar{u} - \mathcal{A}_{\mathrm{KG}}v\bar{v})\frac{1}{N}\mathrm{dVol},$$

$$= \int_\Sigma (N^2|\nabla v|^2 + N^2 m_{kg}^2|v|^2 + |N^2\Delta_\eta u - u|^2 + N^2|\nabla u|^2 + N^2 m_{kg}^2|u|^2)\frac{1}{N}\mathrm{dVol} = \int_\Sigma (N^2|\nabla v|^2 + N^2 m_{kg}^2|v|^2$$

$$+ N^4|\Delta_\eta u|^2 + (1 + m_{kg}^2)N^2|\nabla u|^2 + (m_{kg}^2 N^2 + 1)|u|^2)\frac{1}{N}\mathrm{dVol}.$$

But, for a regular solution U^{KG} of (66) with $V_3 = 0$ associated to the initial data $U_0^{\mathrm{KG}} \in C_0^\infty(\Sigma) \oplus C_0^\infty(\Sigma)$, we have

$$\partial_\tau(\mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)U^{\mathrm{KG}}(\tau)) = \mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau)(\mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)U^{\mathrm{KG}}(\tau)) + ((\partial_\tau\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau)) + [\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau), \mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)])U^{\mathrm{KG}}(\tau)$$

where

$$[\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau), \mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)] = \begin{pmatrix} \tilde{\mathcal{A}}_{\mathrm{KG}} - \mathcal{A}_{\mathrm{KG}} & 0 \\ 0 & \mathcal{A}_{\mathrm{KG}} - \tilde{\mathcal{A}}_{\mathrm{KG}}, \end{pmatrix} = (N^2 - 1)\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{76}$$

Hence, we obtain the integral formula

$$\mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)U^{\mathrm{KG}}(\tau) = \mathcal{U}_{\mathrm{KG}}(\tau, \tau_0)(\mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(au_0)U^{\mathrm{KG}}(\tau_0)) + \int_{\tau_0}^{\tau} \mathcal{U}_{\mathrm{KG}}(\tau, \sigma)G(\sigma)\mathrm{d}\sigma, \tag{77}$$

with

$$G(\sigma) := ((\partial_\tau\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\sigma)) + [\mathcal{M}_{\mathcal{A}_{\mathrm{KG}}}(\tau), \mathcal{M}_{\tilde{\mathcal{A}}_{\mathrm{KG}}}(\tau)])U^{\mathrm{KG}}(\sigma). \tag{78}$$

But thanks to Proposition 2.1 we have

$$\|G(\sigma)\|_{[1,0]} \leqslant C(\sigma)\|U^{\mathrm{KG}}(\sigma)\|_{[2,1]}, \tag{79}$$

where C is a continuous positive function on $\mathbb{R}$ independent of U^{KG}. Hence, by formula (77) and the Gronwall lemma we obtain the estimate

$$\|U^{\mathrm{KG}}(\tau)\|_{[2,1]} \leqslant C'(\tau,\tau_0)\|U_0^{\mathrm{KG}}\|_{[2,1]}, \tag{80}$$

where C' is a continuous function such that $C'(\tau,\tau)=1$. Now, we introduce $H_0^{2,1}(\Sigma)$ as the completion of $C_0^\infty(\Sigma)\oplus C_0^\infty(\Sigma)$ for the norm

$$\|(u,v)\|_{(2,1)}^2 := \int_\Sigma (N^2|\nabla v|^2 + |v|^2 + N^4|\Delta_\eta u|^2 + N^2|\nabla u|^2 + |u|^2)\frac{1}{N}\mathrm{dVol}. \tag{81}$$

This space, smaller than $\mathcal{H}_0^{2,1}(\Sigma)$ allow us to use the Sobolev embedding. Clearly $H_0^{2,1}(\Sigma)\hookrightarrow\mathcal{H}_0^{2,1}(\Sigma)$. Moreover, if we consider the initial data $U_0^{\mathrm{KG}}\in C_0^\infty(\Sigma)\oplus C_0^\infty(\Sigma)$ in some initial time $\tau_0\in\mathbb{R}$, we have $U^{\mathrm{KG}}\in C^\infty(\mathbb{R}_\tau; C_0^\infty(\Sigma)\oplus C_0^\infty(\Sigma))$ and

$$\|U^{\mathrm{KG}}(\tau)\|_{(2,1)} \leqslant C_1(\|U^{\mathrm{KG}}(\tau)\|_{[2,1]} + \|\Phi(\tau)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})} + \|\partial_\tau\Phi(\tau)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})}), \quad C_1>0. \tag{82}$$

But

$$\|\Phi(\tau)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})} \leqslant \|\Phi(\tau_0)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})} + \int_{\tau_0}^{\tau}\|\partial_\tau\Phi(\sigma)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})}\mathrm{d}\sigma \tag{83}$$

$$\leqslant \|U^{\mathrm{KG}}(\tau_0)\|_{(2,1)} + \int_{\tau_0}^{\tau}\|U^{\mathrm{KG}}(\sigma)\|_{(2,1)}\,\mathrm{d}\sigma \tag{84}$$

and

$$\|\partial_\tau\Phi(\tau)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})} \leqslant \|\partial_\tau\Phi(\tau_0)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})} + \int_{\tau_0}^{\tau}\|\partial_\tau^2\Phi(\sigma)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})}\mathrm{d}\sigma \tag{85}$$

$$\leqslant \|U^{\mathrm{KG}}(\tau_0)\|_{(2,1)} + \int_{\tau_0}^{\tau}\|\mathcal{A}_{\mathrm{KG}}\Phi(\sigma)\|_{L^2(\Sigma;N^{-1}\,\mathrm{dVol})}\mathrm{d}\sigma \tag{86}$$

$$\leqslant \|U^{\mathrm{KG}}(\tau_0)\|_{(2,1)} + \int_{\tau_0}^{\tau}\|U^{\mathrm{KG}}(\sigma)\|_{(2,1)}\mathrm{d}\sigma. \tag{87}$$

Hence, thanks to (80) and the two previous estimates, we deduce with (82) that

$$\|U^{\mathrm{KG}}(\tau)\|_{(2,1)} \leqslant C'(\tau,\tau_0)\|U^{\mathrm{KG}}(\tau_0)\|_{(2,1)} + C_2\|U^{\mathrm{KG}}(\tau_0)\|_{(2,1)} + C_2\int_{\tau_0}^{\tau}\|U^{\mathrm{KG}}(\sigma)\|_{(2,1)}\mathrm{d}\sigma, \quad C_2>0 \tag{88}$$

and by the Gronwall lemma

$$\|U^{\mathrm{KG}}(\tau)\|_{(2,1)} \leqslant C''(\tau,\tau_0)\|U_0^{\mathrm{KG}}\|_{(2,1)}, \tag{89}$$

with C'' a continuous positive function on $\mathbb{R}$ independent of U^{KG}. This last estimate allows us to extend $\mathcal{U}_{\mathrm{KG}}$ as a propagator on $H_0^{2,1}(\Sigma)$. Hence, with the Theorem 3.1 and the preview result we deduce the existence of a progator for the linear part of equation (68) on $H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma)$:

Proposition 4.3: For any initial data $U_0\in H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma)$, *the system (68) with* $\mathcal{J}_{\mathrm{DKG}}$

$=0$ *has a unique solution* U *satisfying*

$$U \in C^0(\mathbb{R}_\tau; H_0^2(\Sigma;\mathbb{S}_D) \oplus H_0^{2,1}(\Sigma)). \tag{90}$$

Moreover, there exits a propagator $\mathcal{U}_{\mathrm{DKG}}$ *such that*

(i) $\mathcal{U}_{\mathrm{DKG}}(\tau,\tau_0): U_0 \mapsto U(\tau)$, $\mathcal{U}_{\mathrm{DKG}} := {}^t(\mathcal{U}_D, \mathcal{U}_{\mathrm{KG}})$.
(ii) $\forall t,s \in \mathbb{R}$, $\mathcal{U}_{\mathrm{DKG}}(t,s) \in \mathcal{L}(H_0^2(\Sigma;\mathbb{S}_D) \oplus H_0^{2,1}(\Sigma))$.
(iii) $\mathcal{U}_{\mathrm{DKG}}$ *is strongly continuous on* $\mathbb{R}^2_{ts}$ *to* $\mathcal{L}(H_0^2(\Sigma;\mathbb{S}_D) \oplus H_0^{2,1}(\Sigma))$.
(iv) $\mathcal{U}_{\mathrm{DKG}}(t,t) = \mathrm{Id}$, $\mathcal{U}_{\mathrm{DKG}}(t,s) = \mathcal{U}_{\mathrm{DKG}}(t,r)\mathcal{U}_{\mathrm{DKG}}(r,s)$ *for all* $t,s,r \in \mathbb{R}$.
(iv) *There exists a continuous, strictly positive function* κ_{DKG} *such that*

$$\|U(\tau)\|_{(2,2,1)} := \|\Psi(\tau)\|_{(2)} + \|(\Phi(\tau), \partial_\tau \Phi(\tau))\|_{(2,1)} \leqslant \kappa_{\mathrm{DKG}}(\tau,\tau_0)\|U_0\|_{(2,2,1)}, \quad \kappa_{\mathrm{DKG}}(\tau,\tau) = 1. \tag{91}$$

To study the nonlinear Cauchy problem for (DKG), we establish the following lemma about the continuity of $\mathcal{J}_{\mathrm{DKG}}$ on $H_0^2(\Sigma;\mathbb{S}_D) \oplus H_0^{2,1}(\Sigma)$.

Lemma 4.1: There exists a constant $C \geqslant 0$ *such that,* $U_i = (\Psi_i, V_i) = (\Psi_i, \Phi_i, \partial_\tau \Phi_i) \in H_0^2(\Sigma;\mathbb{S}_D) \oplus H_0^{2,1}(\Sigma)$ *and* $\cup_i \mathrm{supp}(\Phi_i) \subset [R,+\infty] \times S_\omega$, $R > 0$,

$$\|\mathcal{J}_{\mathrm{DKG}}(U_1)\|_{(2,2,1)} \leqslant C\|U_1\|^2_{(2,2,1)}, \tag{92}$$

$$\|\mathcal{J}_{\mathrm{DKG}}(U_1) - \mathcal{J}_{\mathrm{DKG}}(U_2)\|_{(2,2,1)} \leqslant C(\|U_1\|_{(2,2,1)} + \|U_2\|_{(2,2,1)})\|U_1 - U_2\|_{(2,2,1)}. \tag{93}$$

Proof: We prove (93), indeed (92) is (93) with $U_2 \equiv 0$. We have

$$\mathcal{J}_{\mathrm{DKG}}(U_1) - \mathcal{J}_{\mathrm{DKG}}(U_2) = \begin{pmatrix} i\dfrac{N}{\sqrt{2}}(\Phi_2 \gamma^0 \mathcal{V}_2(\Psi_1 - \Psi_2) + (\Phi_1 - \Phi_2)\gamma^0 \mathcal{V}_2 \Psi_1) \\ 0 \\ N^2(\Psi_2^* \mathcal{V}_3(\Psi_1 - \Psi_2) + (\Psi_1^* - \Psi_2^*)\mathcal{V}_3 \Psi_1) \end{pmatrix}. \tag{94}$$

We estimate the first component of the previous difference. We introduce $H_0^2(\Sigma)$ as the completion of $C_0^\infty(\Sigma)$ in the norm

$$\|\Phi\|_{H^2(\Sigma)} := \int_\Sigma |\Phi|^2 + |\nabla\Phi|^2 + |\underline{\Delta}_\eta|^2 \, \mathrm{dVol}, \quad \underline{\Delta}_\eta := \frac{1}{\sqrt{|\eta|}} \frac{\partial}{\partial x^a}\left(\sqrt{|\eta|}\,\eta^{ab}\frac{\partial}{\partial x^b}\right). \tag{95}$$

Since $H^2(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)$ and $h(\tau)$ is equivalent to the Euclidian metric on $\mathbb{R}^3 \backslash \bar{B}(0,1)$, we obtain as in Lemma 3.1,

$$\|\Phi\|_{L^\infty(\Sigma)} \leqslant C_1\|\Phi\|_{H^2(\Sigma)}, \quad C_1 > 0, \quad \Phi \in H_0^2(\Sigma). \tag{96}$$

Moreover, for $\Phi \in C_0^\infty(\Sigma)$,

$$N\Delta_\eta \Phi = N\underline{\Delta}_\eta \Phi + \nabla N \,.\, \nabla\Phi \tag{97}$$

and

$$\underline{\Delta}_\eta(N\Phi) = N\underline{\Delta}_\eta\Phi + 2\,\nabla N \,.\, \nabla\Phi + (\underline{\Delta}_\eta N)\Phi. \tag{98}$$

Therefore, for $V = {}^t(\Phi, \partial_\tau\Phi) \in H_0^{2,1}(\Sigma)$ with $\mathrm{supp}(\Phi) \subset [R,+\infty[\times S_\omega, R > 0$ and since on $\mathrm{supp}(\Phi)$ there exists $C_i > 0$ such that $C_1 \leqslant N \leqslant C_2$, we have

$$\|N\Phi\|_{L^\infty(\Sigma)} \leqslant C_2\|V\|_{(2,1)}, \quad C_2 > 0, \quad V = {}^t(\Phi, \partial_\tau\Phi) \in H_0^{2,1}(\Sigma). \tag{99}$$

Hence

$$\left\| i\frac{N}{\sqrt{2}}(\Phi_2\mathcal{V}_2(\Psi_1-\Psi_2)+(\Phi_1-\Phi_2)\mathcal{V}_2\Psi_1)\right\|_{(2)} \leqslant C_2(\|V_2\|_{(2,1)}\|\Psi_1-\Psi_2\|_{(2)}+\|V_1-V_2\|_{(2,1)}\|\Psi_1\|_{(2)})$$
$$\leqslant C_2(\|U_1\|_{(2,2,1)}+\|U_2\|_{(2,2,1)})\|U_1-U_2\|_{(2,2,1)}. \tag{100}$$

Moreover with (47), we have

$$\|(0,N^2(\Psi_2^*\gamma^0\mathcal{V}_3(\Psi_1-\Psi_2)+(\Psi_1^*-\Psi_2^*)\gamma^0\mathcal{V}_3\Psi_1))\|_{(2,1)} \leqslant C_3(\|U_1\|_{(2,2,1)}+\|U_2\|_{(2,2,1)})\|U_1-U_2\|_{(2,2,1)}, \tag{101}$$

$$C_3>0$$

and with (100) we deduce the result. ■

According to Theorem 4.3, $\mathcal{U}_{\mathrm{DKG}}\in\mathcal{L}(H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma))$ and satisfies (91). Moreover, for $U_0:=(\Psi_0,\Phi_0,\Phi_1)\in H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma)$ at $\tau_0>0$ and $\cup_i \mathrm{supp}(\Phi_i)\subset[R,+\infty[\times S_\omega$, $R>0$, we have $\mathrm{supp}(\mathcal{U}(\tau,\tau_0)U_0)\subset[R'(R,\tau,\tau_0),+\infty[\times S_\omega$, $R'(R,\tau,\tau_0)<R$ since the system (68) with $\mathcal{J}_{\mathrm{DKG}}=0$ is hyperbolic. Hence, in the integral formulation of the Cauchy problem, we can apply Lemma 4.1 for $\mathcal{U}(\tau,\tau_0)U_0$. By an identical proof of Theorem 3.2, we have the following theorem.

Theorem 4.2: *For* $U_0:=(\Psi_0,\Phi_0,\Phi_1)\in H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma)$ *at* $\tau_0>0$ *and* $\cup_i \mathrm{supp}(\Phi_i)\subset[R,+\infty[\times S_\omega$, $R>0$, *there exists* $T(\|U_0\|_{(2,2,1)})>0$ *such that system (68) admits a unique solution* U *such that*

$$U(\tau_0)=U_0\in H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma),\quad U\in C^0([\tau_0,\tau_0+T[_\tau,H_0^2(\Sigma;\mathbb{S}_D)\oplus H_0^{2,1}(\Sigma)). \tag{102}$$

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The determination of all syzygies for the dependent polynomial invariants of the Riemann tensor. II. Mixed invariants of even degree in the Ricci spinor

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We continue our analysis of the polynomial invariants of the Riemann tensor in a four-dimensional Lorentzian space. We concentrate on the mixed invariants of even degree in the Ricci spinor $\Phi_{AB\dot{A}\dot{B}}$ and show how, using constructive graph-theoretic methods, arbitrary scalar contractions between copies of the Weyl spinor Ψ_{ABCD}, its conjugate $\bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$ and an even number of Ricci spinors can be expressed in terms of paired contractions between these spinors. This leads to an algorithm for the explicit expression of dependent invariants as polynomials of members of the complete set. Finally, we rigorously prove that the complete set as given by Sneddon [J. Math. Phys. **39**, 1659–1679 (1998)] for this case is both complete and minimal.
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I. INTRODUCTION

This paper continues our recent work on the classic problem of determining a complete set of polynomial invariants of the Riemann tensor in a four-dimensional Lorentzian space.[1] Recall that a set, $I=\{I_1,I_2,\ldots I_n\}$, of invariants is said to be a complete set in the usual classical sense if any polynomial invariant can be expressed as a *polynomial* in $I_1,I_2,\ldots I_n$, and no invariant in the set can be so expressed in terms of the remaining I_i. It then seems natural to ask the following questions:

(i) How does one find a complete set of invariants for the Riemann tensor, and prove that this set is both complete and minimal?
(ii) How does one construct the polynomial syzygies[2] relating any other invariant to the members of this set?

The first question has received a significant amount of attention recently.[3–11] However, none of the existing work fully solves the problem without introducing additional restrictions.

It will be convenient to partition the set of Riemann tensor invariants into two subsets. The set $\mathcal{E}$ consists of invariants that are even in polynomial degree in the Ricci spinor, and the set $\mathcal{O}$ consists of invariants that are odd in polynomial degree in the Ricci spinor. We shall refer to members of $\mathcal{E}$ and $\mathcal{O}$ as "even invariants" and "odd invariants," respectively. The pure Weyl invariants, $\mathcal{W}$, and the even-degree pure Ricci invariants are subsets of $\mathcal{E}$, whereas the odd-degree pure Ricci invariants form a subset of $\mathcal{O}$.

Bonanos investigated the subset of even invariants formed by contractions between arbitrary products of Ψ_{ABCD} and the Weyl-type square of the Ricci spinor, $\Phi_{(AB}{}^{\dot{C}\dot{D}}\Phi_{CD)\dot{C}\dot{D}}$, with the additional requirement that all contractions involve pairs of indices.[11] All such invariants could be expressed in terms of traces of products of two symmetric matrices, and the problem was reduced to finding a complete set for these traces. Bonanos also conjectured that scalars formed via different types of spinor index contractions between Ψ_{ABCD} and $\Phi_{(AB}{}^{\dot{C}\dot{D}}\Phi_{CD)\dot{C}\dot{D}}$ can be expressed in terms of these traces.[12]

Sneddon's work on the even invariants was also similarly restricted to scalars formed solely via paired index contractions between Ψ_{ABCD}, $\Phi_{AB\dot{A}\dot{B}}\Phi_{CD}{}^{\dot{A}\dot{B}}$, $\Phi_{AB\dot{A}\dot{B}}\bar{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\Phi_{CD}{}^{\dot{C}\dot{D}}$, $\Phi_{AB\dot{A}\dot{B}}\bar{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\bar{\Psi}^{\dot{C}\dot{D}}{}_{\dot{E}\dot{F}}\Phi_{CD}{}^{\dot{E}\dot{F}}$ and their complex conjugates.[7,8] The problem of expressing even invariants formed via different types of spinor index contractions in terms of this subset was not explicitly addressed. In a subsequent work, Sneddon argued that the odd invariants are expressible in terms of the restricted even invariants and a subset of the odd invariants. This subset of odd invariants contains invariants which have exactly one factor of ϵ^{ABC} and exactly one factor of $\epsilon^{\dot{A}\dot{B}\dot{C}}$, where A, B, and C are rotor (bivector) indices that run from 1 to 3.[9] It is still unclear how to construct the functions relating arbitrary invariants to these subsets.

The *algebraically complete* set of Carminati and Zakhary is complete in a less restrictive sense: no invariant in their set can be expressed in an algebraic, as opposed to polynomial, relation with the remaining elements of the set.[3–5]

The second question has hardly been addressed at all in the literature. With the exception of Bonanos,[11] these existing results established completeness using nonconstructive methods and therefore provide no insight on how to relate invariants outside the complete sets to those within these sets.

In the first part of this series, which will be referred to throughout this paper as "paper I," we introduced a correspondence between directed multigraphs and pure Weyl and pure Ricci invariants.[1] This correspondence allowed the development of a graph-theoretic algorithm for the construction of syzygies relating *any* pure invariant in terms of members of their complete sets. A constructive proof of Bonanos' conjecture for the special case of the pure Weyl invariants is a corollary of these results.[1]

In this paper, we extend the graphical representation of invariants to cover mixed invariants, and investigate the completeness problem for mixed invariants which are of even degree in the Ricci spinor. Unless otherwise stated, the notation and terminology used is that of our previous paper.[1]

II. GRAPHICAL REPRESENTATION OF MIXED INVARIANTS

In the case of the mixed invariants, we need to uniquely associate the invariants with directed multigraphs possessing three distinct classes of vertices corresponding to the Ricci spinor, the Weyl spinor and the conjugate Weyl spinor. We accomplish this using the following definition:

Definition 1: The directed multigraph G_N uniquely associated with each invariant N consists of the following:

(i) *A vertex set $V=\{v_1,v_2,\ldots,v_n\}$, where each element of V is uniquely associated with each spinor contracted to form N.*

(ii) *A vertex characteristic function $\varphi: V\rightarrow\{4,4i,2+2i\}$ such that*

$$\varphi(v_j)=\begin{cases}2+2i, & \text{iff } v_j \text{ is a Ricci spinor}\\ 4, & \text{iff } v_j \text{ is a Weyl spinor}\\ 4i, & \text{iff } v_j \text{ is a conjugate Weyl spinor},\end{cases}$$

(iii) *An arc set $E=V\times V$, and*

(iv) *Two multiplicity functions, $m^S: V\times V\rightarrow\{0,1,2,3,4\}$, and $m^D: V\times V\rightarrow\{0,1,2,3,4\}$, such that each arc $(v_j,v_k)\in E$ is associated with two multiplicities: the number of contractions between lower undotted indices on the spinor v_j and upper undotted indices on the spinor v_k is $m^S(v_j,v_k)$, whereas the number of contractions between lower dotted indices on the spinor v_j and upper dotted indices on the spinor v_k is $m^D(v_j,v_k)$.*

In the figures, vertices of characteristic 4, $4i$ and $2+2i$ are depicted using the symbols Ψ, $\bar{\Psi}$, and Φ, respectively. Recall that we use two types of arcs to depict the two multiplicity functions: contractions between undotted indices are represented by solid arcs, and contractions between dotted indices are represented by dashed arcs. For example, the invariants I_1

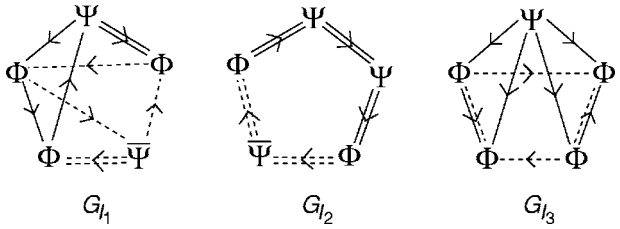

FIG. 1. Directed multigraphs associated with the invariants I_1, I_2, and I_3.

$=\Psi_{A\dot{A}DE}\Phi^{DE\dot{A}\dot{B}}\bar{\Psi}_{\dot{B}\dot{D}\dot{E}}\Phi_{B}{}^{C\dot{D}\dot{E}}\Phi_{C\dot{C}}{}^{A\dot{A}}$, $I_2=\Psi^{AB}{}_{CD}\Psi^{CD}{}_{EF}\Phi^{EF}{}_{\dot{E}\dot{F}}\bar{\Psi}^{\dot{E}\dot{F}}{}_{\dot{C}\dot{D}}\Phi_{AB}{}^{\dot{C}\dot{D}}$, and $I_3=\Psi_{ABCD}\Phi^{AE\dot{A}\dot{B}}\Phi^{B}{}_{E\dot{A}\dot{C}}\Phi^{CF\dot{C}\dot{D}}\Phi^{D}{}_{F\dot{D}\dot{B}}$ are associated with the graphs G_{I_1}, G_{I_2}, and G_{I_3}, respectively, in Fig. 1.

Adopting vertex orderings as given in the contraction sequences of I_1, I_2, and I_3 in the preceding paragraph, we can represent these graphs as their adjacency matrices, where the entry in row j and column k is the total multiplicity of the arcs from vertex j to vertex k. The generalized definition of total multiplicity given in paper I is applicable to the mixed invariants.[1]

$$A(G_N)=[a_{jk}],$$

$$a_{jk}=m(v_j,v_k)=m^S(v_j,v_k)+im^D(v_j,v_k),\quad j,k=1,2,\ldots,n, \tag{1}$$

$$A(G_{I_1})=\begin{bmatrix}0&2&0&0&1\\0&0&0&0&i\\0&i&0&2i&0\\1&0&0&0&0\\0&0&i&1&0\end{bmatrix},$$

$$A(G_{I_2})=\begin{bmatrix}0&2&0&0&0\\0&0&2&0&0\\0&0&0&2i&0\\0&0&0&0&2i\\2&0&0&0&0\end{bmatrix},$$

$$A(G_{I_3})=\begin{bmatrix}0&1&1&1&1\\0&0&0&0&0\\0&1+i&0&i&0\\0&0&0&0&0\\0&i&0&1+i&0\end{bmatrix}.$$

We can assume without loss of generality that no loops are present in these graphs, i.e., for all $v_j\in V(G_N), a_{jj}=m(v_j,v_j)=0$, because self-contracted Weyl and Ricci spinors are identically zero. Using the convention introduced in our previous paper, the sum of the outdegrees and the indegrees at each vertex depends on whether it is associated with a Ricci spinor, Weyl spinor, or conjugate Weyl spinor. The following condition holds for the sum of outdegrees and indegrees at v_j:

$$\sum_{k=1}^{n}(a_{jk}+a_{kj})=\varphi(v_j),\quad j=1,2,\ldots,n. \tag{2}$$

Equivalently, the degrees of the vertices of the underlying undirected graph, U_N, of G_N are equal to their respective characteristics.

As per our previous paper, we associate each invariant N with its oriented form N' by reorienting arcs in G_N to form $G_{N'}$, which satisfies the condition $m(v_j,v_k)=0$ whenever $m(v_k,v_j)\neq 0$ for all $j\neq k$. N' is equivalent to N up to a sign, depending on whether the number of arcs reoriented to form $G_{N'}$ from G_N is even or odd.

We say that the graph G_N, which possesses two types of arcs, is connected iff at least one path exists between any pair of vertices when the types and the directions of the arcs are both disregarded. We can now describe an invariant N as being connected iff G_N is a connected graph.

By directly extending Definition 1 in an obvious manner, we can use graphs to represent spinors with free indices, up to a sign. While the directions of contractions between pairs of indices are specified, we note that the correspondence in Definition 1 would not provide any information on the covariant or contravariant nature of the free indices. It is possible to augment the correspondence to account for the nature of these indices. However, we shall not do so here as this is not required in any of the subsequent discussion in this paper.

Unlike the graphs associated with the invariants, the graph G_ξ associated with the p-spinor ξ possesses *deficient vertices*, which are associated with the component spinors of ξ that possess free indices. Assuming ξ is formed via contractions between the Weyl, conjugate Weyl and Ricci spinors, we may associate with each vertex of G_ξ a vertex deficiency, $\mathcal{D}:V\rightarrow\{0,1,2,3,4,i,2i,3i,4i,1+i,1+2i,2+i,2+2i\}$, where

$$\mathcal{D}(v_j)=\varphi(v_j)-\sum_{k=1}^{n}(a_{jk}+a_{kj}),\quad j=1,2,\ldots,n.$$

$\mathrm{Re}(\mathcal{D}(v_j))$ and $\mathrm{Im}(\mathcal{D}(v_j))$ are the number of free undotted and dotted indices on the spinor associated with v_j, respectively. It immediately follows that

$$\sum_{j=1}^{n}[\mathrm{Re}(\mathcal{D}(v_j))+\mathrm{Im}(\mathcal{D}(v_j))]=p.$$

We are now in a position to state that ξ is *connected* iff G_ξ is connected. A disconnected spinor may be expressed as a product of connected spinors and invariants, where each factor corresponds to a connected subgraph of G_ξ. For example, $\Psi_{ABEF}\Psi_{CGH}{}^{E}\Psi_{D}{}^{FGH}$ is connected, whereas $\Psi_{AEFG}\Phi_{BH\dot{B}\dot{H}}\Psi_{C}{}^{EFG}\Phi_{D}{}^{H\dot{B}\dot{H}}$ is disconnected, and is the product of two connected spinors, $\Psi_{AEFG}\Psi_{C}{}^{EFG}$ and $\Phi_{BH\dot{B}\dot{H}}\Phi_{D}{}^{H\dot{B}\dot{H}}$.

The following result holds for oriented graphs associated with any mixed invariant.

Lemma 1: The total number of odd-multiplicity arcs of a given type which are incident with each vertex of $G_{N'}$ is even (or zero).

Proof: Each vertex of $G_{N'}$ is incident with an even number of (or zero) arcs of either type. It immediately follows that any vertex of $G_{N'}$ cannot be incident with an odd number of odd-multiplicity arcs of either type. ■

We introduced unpaired subgraphs in paper I when discussing the construction of syzygies involving the pure Weyl invariants.[1] The concept is readily extendable to the mixed case: consider the subgraphs, $S^S_{N'}$ and $S^D_{N'}$, of the oriented directed graph, $G_{N'}$ where $m_{S^S_{N'}}(v_j,v_k)=1$ iff $\mathrm{Re}(m_{G_{N'}}(v_j,v_k))$ is odd, and $m_{S^S_{N'}}(v_j,v_k)=0$ otherwise; while $m_{S^D_{N'}}(v_j,v_k)=i$ iff $\mathrm{Im}(m_{G_{N'}}(v_j,v_k))$ is odd, and $m_{S^D_{N'}}(v_j,v_k)=0$ otherwise. Thus, the oriented graph $G_{N'}$ associated with a mixed invariant may be considered to be the union of three edge-disjoint subgraphs: $G_{N'}=S^S_{N'}\cup S^D_{N'}\cup G^S_{N'}$, where the subgraph $G^S_{N'}$ consists solely of solid and dashed arcs of even multiplicity. The adjacency matrices of these subgraphs satisfy the following conditions:

$$A(S^S_{N'})=[\mathrm{Re}(a'_{jk})\bmod 2],$$

$$A(S^D_{N'}) = [i(\mathrm{Im}(a'_{jk}) \bmod 2)], \tag{3}$$

$$A(G^S_{N'}) = A(G_{N'}) - (A(S^S_{N'}) + A(S^D_{N'})),$$

and the subgraphs $S^S_{N'}$ and $S^D_{N'}$ satisfy the following property.

Lemma 2: The arcs in $S^S_{N'}$ and $S^D_{N'}$ may be reoriented to form $S^S_{N''}$ and $S^D_{N''}$ respectively, such that each connected component of $S^S_{N''}$ and $S^D_{N''}$ has a directed Euler circuit.

Proof: This immediately follows from Lemma 1, which implies that the degrees of every vertex of $S^S_{N'}$ and $S^D_{N'}$ are divisible by two. ■

III. PROPERTIES OF EVEN AND ODD INVARIANTS

Consider the sets $\mathcal{E}^c \subset \mathcal{E}$ and $\mathcal{O}^c \subset \mathcal{O}$, which are the connected invariants within $\mathcal{E}$ and $\mathcal{O}$, respectively. We observe that an invariant $N \in \mathcal{E}$ either belongs to $\mathcal{E}^c$ or is the product of elements of $\mathcal{E}^c$ and/or an even number of elements of $\mathcal{O}^c$, whereas an invariant $N \in \mathcal{O}$ either belongs to $\mathcal{O}^c$ or is the product of an element of $\mathcal{O}^c$ and an element of $\mathcal{E}$.

Lemma 3: When $N \in \mathcal{E}$, G_N possesses an even number of solid arcs and an even number of dashed arcs. Furthermore, the number of distinct odd-multiplicity arcs of each type in $G_{N'}$ is either zero, or even and greater than or equal to four.

Proof: N has the general form $\Psi^n \Phi^{2m} \bar{\Psi}^p$. The sum of the degrees of all vertices in the underlying undirected graph, U_N, of G_N is $4n+2m(2+2i)+(4p)i$. It follows that the sums of all solid arc multiplicities, and of all dashed arc multiplicities in G_N are even, being $2(n+m)$ and $2(m+p)$, respectively. Hence, there must be an even number of (or zero) odd-multiplicity arcs of each type in G_N. Suppose we had some $G_{N'}$ possessing only two odd-multiplicity arcs of a given type. By Lemma 2, it follows that both these arcs must connect one pair of vertices v_j and v_k, where both $m(v_j, v_k)$ and $m(v_k, v_j)$ are odd. This contradicts the fact that $G_{N'}$ is oriented. Thus, if the number of distinct odd-multiplicity arcs of a given type in $G_{N'}$ is nonzero, the minimum number of such odd-multiplicity arcs is four. ■

Lemma 4: When $N \in \mathcal{O}$, G_N possesses an odd number of solid arcs and an odd number of dashed arcs. Furthermore, the number of distinct odd-multiplicity arcs of each type in $G_{N'}$ is odd and greater than or equal to three.

Proof: N has the form $\Psi^n \Phi^{2m+1} \bar{\Psi}^p$. The sum of the degrees of all vertices in the underlying undirected graph, U_N, of G_N is $4n+(2m+1)(2+2i)+(4p)i$. It follows that the number of solid and dashed arcs in G_N are $2(n+m)+1$ and $2(m+p)+1$, respectively. Hence, there must be an odd number of odd-multiplicity arcs of each type in G_N. Suppose we had some $G_{N'}$ possessing exactly one odd-multiplicity arc of a given type. By Lemma 2, it follows that this arc forms a loop at a single vertex, which implies that $N \equiv 0$. Thus, the minimum number of such odd-multiplicity arcs in $G_{N'}$ is three. ■

We shall concentrate on finding a complete set of invariants for $\mathcal{E}$ in this paper, and address the determination of a complete set for $\mathcal{O}$ in a subsequent presentation. We define the set $\hat{\mathcal{E}} \subset \mathcal{E}$ such that an even invariant N belongs to $\hat{\mathcal{E}}$ iff all contractions in N are *even*, i.e., all contractions between spinors in N occur pairwise, and the contractions belonging to each pair have the same direction. This is equivalent to saying that every arc in G_N possesses multiplicities that are divisible by 2. The invariant I_2 represented in Fig. 1 is a member of this set.

The set $\hat{\mathcal{E}}^c \subset \hat{\mathcal{E}}$ consists of the connected invariants within $\hat{\mathcal{E}}$. We note that $\hat{\mathcal{W}} \subset \hat{\mathcal{E}}$, and $\hat{\mathcal{W}}^c \subset \hat{\mathcal{E}}^c$. The even-degree pure Ricci invariants belonging to $\hat{\mathcal{E}}^c$ are associated with "polygon-shaped" graphs with alternating solid and dashed arcs of multiplicity two.

Lemma 5: An invariant $N \in \hat{\mathcal{E}}$ either belongs to $\hat{\mathcal{E}}^c$, or is expressible as a product of elements of $\hat{\mathcal{E}}^c$.

Proof: Suppose $N \in \hat{\mathcal{E}}$. If G_N is connected, then $N \in \hat{\mathcal{E}}^c$. Suppose G_N is disconnected and it possesses a connected subgraph, S_{odd} containing an odd number of vertices of vertex characteristic

$2+2i$. It follows from Lemma 4 that S_{odd} possesses an odd number of arcs of either arc type. Hence the multiplicity of every arc in G_N is not divisible by 2, contradicting the fact that $N \in \hat{\mathcal{E}}$. Thus, if G_N is disconnected, each of its connected components must possess an even number of vertices of characteristic $2+2i$, and given that the multiplicity of every arc in G_N must be divisible by 2, it follows that each connected component is associated with a member of $\hat{\mathcal{E}}^c$. ■

We are now in a position to state the main result of this section. Following the convention introduced in Paper I, we use the symbol $\oplus$ in the graphical representation to denote addition of the associated invariants of two graphs.[1,13]

Theorem 1: *For any invariant $N \in \mathcal{E}$, $S^S_{N'}$ and $S^D_{N'}$ are expressible, using the identity, as a finite sum of graphs, $\tilde{S}^S_j$ and $\tilde{S}^D_l$, consisting only of even-multiplicity arcs which are solid and dashed, respectively,*

$$S^S_{N'} \equiv \mathop{\oplus}_{j=1}^{n} b_j \tilde{S}^S_j, \tag{4}$$

$$S^D_{N'} \equiv \mathop{\oplus}_{l=1}^{m} c_l \tilde{S}^D_l, \tag{5}$$

where the coefficients b_j and c_l are rational numbers.

The graph $G_{N'}$ may then be expressed as

$$G_{N'} \equiv \mathop{\oplus}_{j=1}^{n} \mathop{\oplus}_{l=1}^{m} b_j c_l G_{X_{jl}}, \tag{6}$$

where

$$G_{X_{jl}} = G^S_{N'} \cup \tilde{S}^S_j \cup \tilde{S}^D_l. \tag{7}$$

The invariant N' then obeys the following identity:

$$N' = \sum_{j=1}^{n} \sum_{l=1}^{m} b_j c_l X_{jl}, \tag{8}$$

where $X_{jl} \in \hat{\mathcal{E}}$, $j=1,2,\ldots,n$; $l=1,2,\ldots,m$.

Proof: By Lemma 2, the unpaired subgraphs $S^S_{N'}$ and $S^D_{N'}$ are reorientable to $S^S_{N''}$ and $S^D_{N''}$ where each connected component of $S^S_{N''}$ and $S^D_{N''}$ are Euler circuits. $S^S_{N''}$ and $S^D_{N''}$ are equivalent to $S^S_{N'}$ and $S^D_{N'}$, respectively, up to a sign modulo union with $G^S_{N'}$ in the graphical representation, depending on whether the total number of arcs reoriented is even or odd. Lemma 3 requires that the sums of lengths of the solid circuits in $S^S_{N''}$ and of the dashed circuits in $S^D_{N''}$ must both be even.

Case 1: Both $S^S_{N''}$ and $S^D_{N''}$ are connected.

Let $S^S_{N''}$ be a single solid k-circuit, and $S^D_{N''}$ be a single dashed k^*-circuit, where both k and k^* are even. Following the argument presented in Case 1 of the proof of Theorem 1 in Paper I,[1] and incorporating a sign change if an odd number of arcs were reoriented to form $S^S_{N''}$ from $S^S_{N'}$, it is possible to reexpress $S^S_{N''}$ as written in Eq. (4). A direct extension of this method to dashed arcs yields Eq. (5). Each individual term, $G_{X_{jl}}$ in the graphical decomposition of $G_{N'}$ [Eq. (6)] is constructed by forming the union of $G^S_{N'}$ with $\tilde{S}^S_j$ and $\tilde{S}^D_l$, as shown in Eq. (7). The equivalent expression in spinor form expresses N' as a polynomial of members of $\hat{\mathcal{E}}$ [Eq. (8)].

Case 2: At least one of $S^S_{N''}$ or $S^D_{N''}$ is not connected.

When $S^S_{N''}$ is not connected, it is reducible to the connected case using the procedure described in Case 2 of the proof of Theorem 1 in Paper I.[1] The extension towards the reduction of $S^D_{N''}$ to the connected case is trivial. ■

Bonanos' full conjecture[11] is a corollary of this result. We note that Theorem 1 holds for both connected and disconnected members of $\mathcal{E}$, and applying the decomposition process outlined in the proof to disconnected members of $\mathcal{E}$ yields *algebraic* syzygies involving connected invariants. Sneddon has suggested that squares of odd invariants, and products of any two odd invariants, will be expressible as polynomials of even invariants.[8] In fact, this will be true for any product containing an even number of odd invariants. We have now provided a means of explicitly constructing such syzygies, and an example is provided in Appendix A. Polynomial syzygies relating odd invariants to members of $\hat{\mathcal{O}}^c$ and $\hat{\mathcal{E}}^c$ will be explored in detail in the next part of this series.

IV. DETERMINATION OF THE BASIS ELEMENTS OF $\hat{\mathcal{E}}^c$

Lemma 5 and Theorem 1 reduce the problem of finding a polynomial basis for $\mathcal{E}$ to that of finding one for $\hat{\mathcal{E}}^c$. Ultimately, we also wish to explicitly construct the syzygies relating any member of $\mathcal{E}$ to the basis. To achieve these objectives, we construct spinorial objects that constitute fundamental building blocks for the elements of $\hat{\mathcal{E}}^c$, and examine the structures of these elements in terms of the building blocks. We make the following definition.

Definition 2: A Υ*-spinor is any connected 4-indexed spinor* Υ_{ABCD} *which may be formed solely from even dotted contractions between copies of the Weyl, conjugate Weyl and Ricci spinors.*

Apart from the trivial Υ-spinor, Ψ_{ABCD}, the Υ-spinors can only be formed using the conjugate Weyl and Ricci spinors. All of the available dotted indices must be completely exhausted using even dotted contractions. Furthermore, a Υ-spinor must have four free undotted indices, and not contain any undotted contractions. Therefore, all nontrivial Υ-spinors contain exactly two copies of the Ricci spinor, and can be described as a contiguous sequence of even dotted contractions beginning with a Ricci spinor, continuing with an arbitrary number of conjugate Weyl spinors, and ending with another Ricci spinor: $\Phi\bar{\Psi}^p\Phi$. It will be convenient to describe the Υ-spinors as having two types of symmetries: index-pair symmetry $\Upsilon_{ABCD}=\Upsilon_{BACD}=\Upsilon_{ABDC}$, and block symmetry $\Upsilon_{ABCD}=\Upsilon_{CDAB}$.

Every Υ-spinor has a dyad expansion of the following form:

$$
\begin{aligned}
{}^j\Upsilon_{ABCD} = {}&{}^j\Upsilon_{00}\iota_A\iota_B\iota_C\iota_D - 4{}^j\Upsilon_{01}\iota_{(A}\iota_B\iota_C o_{D)} + {}^j\Upsilon_{02}(o_A o_B\iota_C\iota_D + o_C o_D\iota_A\iota_B) + {}^j\Upsilon_{11}(o_A o_C\iota_B\iota_D + o_A o_D\iota_B\iota_C \\
&+ o_B o_C\iota_A\iota_D + o_B o_D\iota_A\iota_C) - 4{}^j\Upsilon_{12}o_{(A}o_B o_C\iota_{D)} + {}^j\Upsilon_{22}o_A o_B o_C o_D,
\end{aligned}
$$

where

$$
\begin{aligned}
{}^j\Upsilon_{00} &= {}^j\Upsilon_{0000}, \\
{}^j\Upsilon_{01} &= {}^j\Upsilon_{0001} = {}^j\Upsilon_{0010} = {}^j\Upsilon_{0100} = {}^j\Upsilon_{1000}, \\
{}^j\Upsilon_{02} &= {}^j\Upsilon_{0011} = {}^j\Upsilon_{1100}, \\
{}^j\Upsilon_{11} &= {}^j\Upsilon_{1010} = {}^j\Upsilon_{1001} = {}^j\Upsilon_{0110} = {}^j\Upsilon_{0101}, \\
{}^j\Upsilon_{12} &= {}^j\Upsilon_{0111} = {}^j\Upsilon_{1011} = {}^j\Upsilon_{1101} = {}^j\Upsilon_{1110}, \\
{}^j\Upsilon_{22} &= {}^j\Upsilon_{1111},
\end{aligned}
\tag{9}
$$

and the prefix j distinguishes distinct Υ-spinors.

Taking the conjugates of the Υ-spinors yield the $\bar{\Upsilon}$-spinors. Apart from the trivial $\bar{\Upsilon}$-spinor, $\bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$, all $\bar{\Upsilon}$-spinors have the form of a contiguous sequence of even undotted contractions beginning with a Ricci spinor, continuing with an arbitrary number of Weyl spinors, and ending with another Ricci spinor: $\Phi\Psi^{p}\Phi$.

We now establish that the Υ-spinors and the $\bar{\Upsilon}$-spinors constitute fundamental building blocks for the invariants belonging to $\hat{\mathcal{E}}^{c}$.

Lemma 6: A connected invariant N belongs to $\hat{\mathcal{E}}^{c}$ iff it is expressible in at least one of the following ways:

(i) *solely as even contractions between copies of* Υ*-spinors, or*
(ii) *solely as even contractions between copies of* $\bar{\Upsilon}$*-spinors.*

Proof: The graph G_N associated with any such N only possesses arcs of even multiplicity. The lemma is trivially true for the quadratic invariants: $\Psi_{ABCD}\Psi^{ABCD}$, $\bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}\bar{\Psi}^{\dot{A}\dot{B}\dot{C}\dot{D}}$, and $\Phi_{AB\dot{A}\dot{B}}\Phi^{AB\dot{A}\dot{B}}$. Hence we can assume without loss of generality that each spinor in N is evenly contracted to exactly two other distinct spinors. It is then clear from the structure of G_N that N is a cyclic sequence of such even contractions. Suppose contractions between pairs of undotted indices are present. These undotted contractions can be viewed to separate this cyclic sequence of even contractions into connected 4-indexed compound spinors formed solely from even dotted contractions. Thus, we obtain a contractive partitioning of N into copies of Υ-spinors. Similarly, contractions between pairs of dotted indices yield a contractive partitioning of N into copies of $\bar{\Upsilon}$-spinors. The converse follows immediately from the fact that besides Ψ_{ABCD} and $\bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$, every Υ-spinor and $\bar{\Upsilon}$-spinor contain exactly two copies of the Ricci spinor. ■

For example, the invariant $\Psi_{ABCD}\Phi^{CD\dot{C}\dot{D}}\bar{\Psi}_{\dot{C}\dot{D}\dot{E}\dot{F}}\Phi^{AB\dot{E}\dot{F}}$ can be formed by even undotted contractions between the Υ-spinors Ψ_{ABCD} and $\Phi_{CD\dot{C}\dot{D}}\bar{\Psi}^{\dot{C}\dot{D}\dot{E}\dot{F}}\Phi_{AB\dot{E}\dot{F}}$, or by even dotted contractions between the $\bar{\Upsilon}$-spinors $\bar{\Psi}_{\dot{C}\dot{D}\dot{E}\dot{F}}$ and $\Phi_{AB\dot{E}\dot{F}}\Psi^{ABCD}\Phi_{CD\dot{C}\dot{D}}$. The pure Weyl invariants belonging to $\hat{\mathcal{W}}^{c}$ and their conjugates both form subsets of $\hat{\mathcal{E}}^{c}$. The former is expressible only in terms of Υ-spinors, and the latter only in terms of $\bar{\Upsilon}$-spinors. However, all other invariants belonging to $\hat{\mathcal{E}}^{c}$ possess both undotted and dotted contractions. Thus for these invariants we can obtain both a Υ-*structure* and a $\bar{\Upsilon}$-*structure*. This existence of two distinct structures of the mixed invariants belonging to $\hat{\mathcal{E}}^{c}$ will play a significant role in the subsequent basis determination.

It will be useful to define the Γ-spinors to be connected 4-spinors formed by sequential pairwise undotted contractions between copies of Υ-spinors, and $\bar{\Gamma}$-spinors to be the conjugates of Γ-spinors. All Γ-spinors possess index-pair symmetry, but a Γ-spinor will not possess block symmetry unless it is formed from a palindromic sequence of Υ-spinors. Every Γ-spinor has a dyad expansion of the following form:

$$
\begin{aligned}
{}^{j}\Gamma_{ABCD} = {}&{}^{j}\Gamma_{00}\iota_A\iota_B\iota_C\iota_D - 2{}^{j}\Gamma_{10}\iota_C\iota_D\iota_{(A}o_{B)} - 2{}^{j}\Gamma_{01}\iota_A\iota_B\iota_{(C}o_{D)} + {}^{j}\Gamma_{20}o_Ao_B\iota_C\iota_D + {}^{j}\Gamma_{02}o_Co_D\iota_A\iota_B \\
&+ {}^{j}\Gamma_{11}(o_Ao_C\iota_B\iota_D + o_Ao_D\iota_B\iota_C + o_Bo_C\iota_A\iota_D + o_Bo_D\iota_A\iota_C) - 2{}^{j}\Gamma_{12}o_Co_Do_{(A}\iota_{B)} \\
&- 2{}^{j}\Gamma_{21}o_Ao_Bo_{(C}\iota_{D)} + {}^{j}\Gamma_{22}o_Ao_Bo_Co_D,
\end{aligned}
$$

where

$$
{}^{j}\Gamma_{00} = {}^{j}\Gamma_{0000},
$$

$$
{}^{j}\Gamma_{01} = {}^{j}\Gamma_{0001} = {}^{j}\Gamma_{0010},
$$

$$
{}^{j}\Gamma_{10} = {}^{j}\Gamma_{0100} = {}^{j}\Gamma_{1000},
$$

$$
\begin{aligned}
{}^{j}\Gamma_{02} &= {}^{j}\Gamma_{0011},\\
{}^{j}\Gamma_{20} &= {}^{j}\Gamma_{1100},\\
{}^{j}\Gamma_{11} &= {}^{j}\Gamma_{1010} = {}^{j}\Gamma_{1001} = {}^{j}\Gamma_{0110} = {}^{j}\Gamma_{0101},\\
{}^{j}\Gamma_{12} &= {}^{j}\Gamma_{0111} = {}^{j}\Gamma_{1011},\\
{}^{j}\Gamma_{21} &= {}^{j}\Gamma_{1101} = {}^{j}\Gamma_{1110},\\
{}^{j}\Gamma_{22} &= {}^{j}\Gamma_{1111},
\end{aligned}
\tag{10}
$$

and the prefix j distinguishes distinct Γ-spinors.

Lemma 6 implies that all scalars constructed from evenly contracting Γ-spinors belong to $\hat{\mathcal{E}}^c$. We shall specify these scalars as a list, $[j_1,j_2,j_3,\ldots]$, of the prefixes of the sequence of Γ-spinors evenly contracted in a cyclic manner to form the scalar. For example, the scalar ${}^{1}\Gamma_{ABCD}\,{}^{3}\Gamma^{CD}{}_{EF}\,{}^{3}\Gamma^{EF}{}_{GH}\,{}^{4}\Gamma^{GHAB}$ would be denoted as [1, 2, 3, 4]. Obviously, the scalar denoted by $[j_1,j_2,j_3,\ldots,j_n]$ is equivalent to the scalars represented by any cyclic permutation of that list. In the special case where all of the spinors denoted by $j_1,j_2,j_3,\ldots,j_n$ are Υ-spinors, the scalar denoted by $[j_1,j_2,j_3,\ldots,j_n]$ is also equivalent to the scalars represented by any cyclic permutation of the reversal of that list, $[j_n,\ldots,j_3,j_2,j_1]$. For convenience, we shall drop the commas whenever this will not create any ambiguities and rewrite $[A,B,C,D]$ as $[ABCD]$. Additionally, we will further simplify the representation by indicating a contiguous, evenly contracted sequence of n copies of ${}^{j}\Gamma$ as j^n within the square brackets. For example, we will write $[AAAB]$ and $[AABB]$ as $[A^3B]$ and $[A^2B^2]$, respectively.

One can verify the following scalar identity using Eq. (10):

$$
\begin{aligned}
&[ABCD]+[ABDC]+[ACBD]+[ACDB]+[ADBC]+[ADCB]\\
&\quad-[A][BCD]-[A][BDC]-[B][ACD]-[B][ADC]-[C][ABD]\\
&\quad-[C][ADB]-[D][ABC]-[D][ACB]-[AB][CD]-[AC][BD]\\
&\quad-[AD][BC]+[AB][C][D]+[AC][B][D]+[AD][B][C]\\
&\quad+[BC][A][D]+[BD][A][C]+[CD][A][B]-[A][B][C][D]\equiv 0.
\end{aligned}
\tag{11}
$$

Equation (11), which obviously also holds when A, B, C, and D are all $\bar{\Gamma}$-spinors, is a polynomial identity relating invariants of the form $[ABCD]$ to other members of $\hat{\mathcal{E}}^c$. The form of this equation is readily justified by associating each Γ-spinor, Γ_{ABCD}, with a 3×3 complex matrix, $\Gamma_{\alpha\beta}$, which transforms under the $\mathrm{SO}(3,\mathbb{C})$ representation. The elements of $\Gamma_{\alpha\beta}$ are the components of Γ_{ABCD} with respect to the orthonormal basis,[14]

$$
\begin{aligned}
{}^{1}\delta_{AB} &= -\frac{i}{\sqrt{2}}(o_A o_B - \iota_A \iota_B),\\
{}^{2}\delta_{AB} &= \frac{1}{\sqrt{2}}(o_A o_B + \iota_A \iota_B),\\
{}^{3}\delta_{AB} &= \frac{i}{\sqrt{2}}(o_A \iota_B + \iota_A o_B),
\end{aligned}
$$

such that

$$\Gamma_{\alpha\beta} = \Gamma^{ABCD} \overset{\alpha}{\delta}_{AB} \overset{\beta}{\delta}_{CD}.$$

In terms of the dyad components of Γ_{ABCD}, the matrix $\Gamma_{\alpha\beta}$ has the following form:

$$\Gamma_{\alpha\beta} = \begin{bmatrix} \frac{1}{2}(\Gamma_{02}+\Gamma_{20}-\Gamma_{00}-\Gamma_{22}) & \frac{i}{2}(\Gamma_{20}+\Gamma_{22}-\Gamma_{00}-\Gamma_{02}) & \Gamma_{01}-\Gamma_{21} \\ \frac{i}{2}(\Gamma_{02}+\Gamma_{22}-\Gamma_{00}-\Gamma_{20}) & \frac{1}{2}(\Gamma_{00}+\Gamma_{02}+\Gamma_{20}+\Gamma_{22}) & (\Gamma_{01}+\Gamma_{21})i \\ \Gamma_{10}-\Gamma_{12} & (\Gamma_{10}+\Gamma_{12})i & -2\Gamma_{11} \end{bmatrix},$$

and performing a similar calculation on Υ_{ABCD} yields the analogous matrix $\Upsilon_{\alpha\beta}$,

$$\Upsilon_{\alpha\beta} = \begin{bmatrix} \Upsilon_{02}-\frac{1}{2}(\Upsilon_{00}+\Upsilon_{22}) & \frac{i}{2}(\Upsilon_{22}-\Upsilon_{00}) & \Upsilon_{01}-\Upsilon_{12} \\ \frac{i}{2}(\Upsilon_{22}-\Upsilon_{00}) & \Upsilon_{02}+\frac{1}{2}(\Upsilon_{00}+\Upsilon_{22}) & (\Upsilon_{01}+\Upsilon_{12})i \\ \Upsilon_{01}-\Upsilon_{12} & (\Upsilon_{01}+\Upsilon_{12})i & -2\Upsilon_{11} \end{bmatrix}.$$

Equtation (11) is equivalent to the statement that antisymmetrizing over four indices annihilates any product of 3×3 matrices, $\Gamma^{[\alpha}{}_{\beta}\Gamma^{\beta}{}_{\gamma}\Gamma^{\gamma}{}_{\delta}\Gamma^{\delta]}{}_{\alpha} \equiv 0$. The derivation of the corresponding matrix identity from the Cayley-Hamilton theorem has been reported by Spencer and Rivlin, who subsequently used various versions of this identity to construct bases for matrix polynomials in up to five 3×3 matrices.[15–17]

Setting $D=A$ and $D=C=A$ in Eq. (11) gives the special cases Eqs. (12) and (13), respectively,

$$\begin{aligned} &2[A^2BC]+2[A^2CB]+2[ABAC]-2[A][ABC]-2[A][ACB]-2[B][A^2C]-2[C][A^2B]-[A^2][BC] \\ &-2[AB][AC]+[A^2][B][C]+2[AB][A][C]+2[AC][A][B]+[BC][A]^2-[A]^2[B][C]\equiv 0, \end{aligned} \tag{12}$$

$$6[A^3B]-6[A][A^2B]-2[B][A^3]-3[A^2][AB]+3[A^2][A][B]+3[AB][A]^2-[A]^3[B]\equiv 0. \tag{13}$$

Given that Υ-spinors are a specialized form of Γ-spinors, it is immediately obvious that Eqs. (11)–(13) also hold when A, B, C, and D are all Υ-spinors, or all $\bar{\Upsilon}$-spinors. Equation (13) states that whenever three or more identical Υ-spinors are contracted sequentially within the Υ-structure of an invariant, this invariant is then expressible as a polynomial function of lower-degree invariants. We define an invariant $N \in \hat{\mathcal{E}}^c$ to be Υ-*irreducible* if it does not possess a Υ-structure or if its Υ-structure is not expressible as a function of lower-degree invariants modulo Eq. (13). Simliarly, if N does not possess a $\bar{\Upsilon}$-structure or if its $\bar{\Upsilon}$-structure is not expressible as a function of lower-degree invariants modulo Eq. (13), then N is said to be $\bar{\Upsilon}$-*irreducible*. We shall make use of this result, which follows immediately from Eq. (13).

Lemma 7: An invariant $N \in \hat{\mathcal{E}}^c$ is either Υ-irreducible or expressible as a polynomial function of Υ-irreducible elements of $\hat{\mathcal{E}}^c$. Furthermore, N is either $\bar{\Upsilon}$-irreducible or expressible as a polynomial function of $\bar{\Upsilon}$-irreducible elements of $\hat{\mathcal{E}}^c$.

We are now in a position to introduce the following specific Υ-spinors:

$${}^1\Upsilon_{ABCD} = \Psi_{ABCD},$$

$${}^2\Upsilon_{ABCD} = \Phi_{AB\dot{A}\dot{B}}\Phi_{CD}{}^{\dot{A}\dot{B}},$$

$$^{3}\Upsilon_{ABCD} = \Phi_{AB\dot{A}\dot{B}}\bar{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\Phi_{CD}{}^{\dot{C}\dot{D}},$$

$$^{4}\Upsilon_{ABCD} = \Phi_{AB\dot{A}\dot{B}}\bar{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\bar{\Psi}^{\dot{C}\dot{D}}{}_{\dot{E}\dot{F}}\Phi_{CD}{}^{\dot{E}\dot{F}},$$

which are the four lowest-degree Υ-spinors, and the respective spinorial counterparts of the matrices A, B, C, and D in Sneddon's paper.[8] The dyad components of $^{1}\Upsilon$, $^{2}\Upsilon$, $^{3}\Upsilon$, and $^{4}\Upsilon$ are presented in Appendix B. From this point onwards, we shall follow Sneddon's notation and use the symbols A, B, C, and D to represent the symmetric 3×3 matrix representations of $^{1}\Upsilon$, $^{2}\Upsilon$, $^{3}\Upsilon$, and $^{4}\Upsilon$, respectively, and the list notation to denote the traces of matrix products. For example, the scalar invariant $\Psi_{AB}{}^{CD}\Psi_{CD}{}^{EF}\Phi_{EF}{}^{\dot{E}\dot{F}}\Phi^{AB}{}_{\dot{E}\dot{F}}$ is equivalent to the trace of the matrix product A^2B, and shall be denoted as $[A^2B]$. Sneddon has suggested that any even invariant is expressible in terms of traces of products of the matrices A, B, C, and D, and their conjugates.[8] The following result, in conjunction with Theorem 1, formally justifies a stronger version of this claim.

Theorem 2: *Any invariant $N\in\hat{\mathcal{E}}^{c}$ is expressible as a polynomial function of $\overline{[A^2]}$, $\overline{[A^3]}$ and traces of products of the matrices A, B, C, and D.*

Proof: Theorem 1 in paper I[1] immediately implies that this statement is true for all pure Weyl and conjugate-Weyl invariants. Hence, without loss of generality, we only consider the remaining invariants belonging to $\hat{\mathcal{E}}^{c}$. Consider any such $N\in\hat{\mathcal{E}}^{c}$. It possesses both a Υ-structure and a $\bar{\Upsilon}$-structure. There are two cases.

Case 1: N is $\bar{\Upsilon}$-irreducible.

Here, N will never contain contiguous, evenly contracted sequences of more than two copies of the conjugate Weyl spinor. Thus, Lemma 6 implies that its Υ-structure will contain only copies of $^{1}\Upsilon$, $^{2}\Upsilon$, $^{3}\Upsilon$, and $^{4}\Upsilon$; and the theorem is established in this case.

Case 2: N is $\bar{\Upsilon}$-reducible.

Here, N is a polynomial function of $\bar{\Upsilon}$-irreducible elements of $\hat{\mathcal{E}}^{c}$, by Lemma 7. Apart from the pure conjugate Weyl invariants $\overline{[A^2]}$ and $\overline{[A^3]}$, every other $\bar{\Upsilon}$-irreducible invariant possesses a Υ-structure, and the problem is reduced to Case 1. ■

The concept of reducibility modulo Eq. (13) thus reduces the general problem to one of determining the basis of the set of all product traces of four symmetric 3×3 complex matrices, $^{1}\Upsilon$, $^{2}\Upsilon$, $^{3}\Upsilon$, $^{4}\Upsilon$. Spencer and Rivlin have derived the following basis, which we shall call $\mathcal{S}$, for product traces of four arbitrary symmetric 3×3 matrices, A, B, C, and D, under the orthogonal transformation group.[15–17]

Degree 1: $[A],[B],[C],[D]$.
Degree 2: $[A^2],[AB],[AC],[AD],[B^2],[BC],[BD],[C^2],[CD],[D^2]$.
Degree 3: $[A^3],[A^2B],[A^2C],[A^2D],[AB^2],[ABC],[ABD],[AC^2],[ACD],[AD^2],[B^3]$,
$[B^2C],[B^2D],[BC^2],[BCD],[BD^2],[C^3],[C^2D],[CD^2],[D^3]$.
Degree 4: $[A^2B^2],[A^2BC],[A^2BD],[A^2C^2],[A^2CD],[A^2D^2],[AB^2C],[AB^2D]$,
$[ABC^2],[ABCD],[ABDC],[ABD^2],[AC^2D],[ACD^2],[B^2C^2],[B^2CD]$,
$[B^2D^2],[BC^2D],[BCD^2],[C^2D^2]$
Degree 5: $[A^2B^2C],[A^2B^2D],[A^2BC^2],[A^2BCD],[A^2BDC],[A^2BD^2]$,
$[A^2C^2D],[A^2CD^2],[AB^2C^2],[AB^2CD],[AB^2D^2],[ABC^2D]$,
$[ABCD^2],[ABDC^2],[ACB^2D],[ACBD^2],[AC^2D^2],[B^2C^2D]$,
$[B^2CD^2],[BC^2D^2]$.
Degree 6: $[A^2BACD],[A^2B^2CD],[A^2CBD^2],[A^2C^2BD],[AB^2CBD]$,
$[ABC^2DC],[ABC^2D^2],[ACB^2D^2],[AC^2B^2D],[ADBCD^2]$

The proofs of Lemmas 1–3 and Theorem 1 in Ref. 15 and Sec. V in Ref. 16 are able to be implemented as an algorithm that allows the trace of any product of A, B, C, and D to be systematically expressed in terms of $\mathcal{S}$ using only variations of Eq. (11).[18]

In our case, $[A] \equiv 0$ owing to the trace-free character of ${}^{1}\Upsilon$. Furthermore, the matrices A, B, C, D are not independent, and the complete set for $\mathcal{E}$ will be a proper subset of $\mathcal{S}$. We say that an element of $\hat{\mathcal{E}}^c$ is minimal with respect to the Υ-structure, or Υ-*minimal* iff it does not possess a Υ-structure or its Υ-structure corresponds to an element in $\mathcal{S}$. With the exception of $[A^2]$ and $[A^3]$, the remaining Υ-minimal elements also possess $\bar{\Upsilon}$-structures. It can be easily verified that their $\bar{\Upsilon}$-structures contain only $\overline{{}^{1}\Upsilon}$, $\overline{{}^{2}\Upsilon}$, $\overline{{}^{3}\Upsilon}$, and $\overline{{}^{4}\Upsilon}$; therefore these invariants also belong in the space of product traces of $\bar{A}$, $\bar{B}$, $\bar{C}$, and $\bar{D}$. It immediately follows that the set $\bar{\mathcal{S}}$ of conjugates of the elements of $\mathcal{S}$ form the basis of this space, and an element of $\hat{\mathcal{E}}^c$ is $\bar{\Upsilon}$-*minimal* iff it does not possess a $\bar{\Upsilon}$-structure or its $\bar{\Upsilon}$-structure corresponds to an element in $\bar{\mathcal{S}}$.

For example, the invariant $N = \Psi_{ABCD}\Phi^{CD\dot{C}\dot{D}}\Phi_{EF\dot{C}\dot{D}}\Phi^{EF\dot{E}\dot{F}}\Phi_{AB}{}^{\dot{E}\dot{F}}$ possesses the Υ-structure $[AB^2]$ and the $\bar{\Upsilon}$-structure $\overline{[BC]}$. Therefore N is both Υ-minimal and $\bar{\Upsilon}$-minimal. On the other hand, the Υ-minimal invariant $[CD]$ possesses the $\bar{\Upsilon}$-structure $\overline{[A^2BAB]}$, and can be expressed in terms of $\bar{\Upsilon}$-minimal invariants as follows:

$$\overline{[A^2BAB]} = \tfrac{1}{6}(\overline{[A^3]}[B]^2 - \overline{[A^3]}\overline{[B^2]}) + \overline{[AB]}\overline{[A^2B]}.$$

In accordance with Theorem 2, we can rewrite $\overline{[A^2BAB]}$, $\overline{[B]}$, $\overline{[B^2]}$, $\overline{[AB]}$, and $\overline{[A^2B]}$ in terms of their Υ-structures to give

$$[CD] = \tfrac{1}{6}(\overline{[A^3]}[B]^2 - \overline{[A^3]}[B^2]) + [C][D].$$

It is straightforward to verify that every invariant on the right-hand side is both Υ-minimal and $\bar{\Upsilon}$-minimal. Analyzing every member of $\mathcal{S}$ in this manner yields the set of even invariants which are both Υ-minimal and $\bar{\Upsilon}$-minimal, $\mathcal{J}_{\mathcal{E}} = \{[A^2], [A^3], \overline{[A^2]}, \overline{[A^3]}, [B], [B^2], [B^3], [C], [D], [AB], [AC], [AD], [BC], [BD], [A^2B], [A^2C], [A^2D], [AB^2], [ABC], [ABD], [A^2B^2], [A^2BC], [A^2BD], [AB^2C], [AB^2D], [A^2B^2C], [A^2B^2D], [A^2BACD]\}$.

An even invariant belonging to the complete set for $\mathcal{E}$ is necessarily a member of $\mathcal{J}_{\mathcal{E}}$ and it remains to be established whether every member of $\mathcal{J}_{\mathcal{E}}$ belongs to the complete set for $\mathcal{E}$. Sneddon has previously specialized the set $\mathcal{S}$ towards the determination of a complete set, $\mathcal{J}$, for the even invariants,[8] and the set $\mathcal{J}_{\mathcal{E}}$ is identical to his complete set $\mathcal{J}$. In Sec. VI of his subsequent paper concerning the odd invariants, Sneddon examined new syzygies that arose from multiplying syzygies of the odd invariants with other odd invariants.[9] These results led him to argue that $\mathcal{J}_{\mathcal{E}}$ is a minimal basis for $\mathcal{E}$. Now, every four-dimensional Lorentzian manifold belongs to one of 15 different possible Segre types. Therefore, we may explicitly demonstrate the minimality of $\mathcal{J}_{\mathcal{E}}$, without needing to consider the odd invariants, by showing that each invariant is necessary as a basis element for at least one of the 15 different Segre types.

For each Segre type, a canonical frame[4,5] was selected and the members of $\mathcal{J}_{\mathcal{E}}$ were expressed in terms of the Newman-Penrose curvature components. Trial polynomial syzygies of the form $I_n = \Sigma a_j P_j$ were then constructed, where P_j were all products of invariants within $\mathcal{J}_{\mathcal{E}} - \{I_n\}$ of the same polynomial degree in Ψ_{ABCD}, $\bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$, and $\Phi_{AB\dot{A}\dot{B}}$ as I_n. Attempts were then made to solve for the coefficients a_j. If no solution existed for a particular I_n in a given Segre type, then I_n is necessarily a member of the complete set for that particular Segre type. The complete sets and polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$ for all 15 Segre types are given in Appendix C, and it is apparent that *no member of* $\mathcal{J}_{\mathcal{E}}$ *is a polynomial function of the remaining members of* $\mathcal{J}_{\mathcal{E}}$ *for every Segre type*. Hence, every member of $\mathcal{J}_{\mathcal{E}}$ belongs to the complete set for $\mathcal{E}$, and it follows that $\mathcal{J}_{\mathcal{E}}$ is a minimal complete set for $\mathcal{E}$.

The 10 real and 18 complex members of $\mathcal{J}_{\mathcal{E}}$ are depicted graphically in Figs. 2 and 3, respectively. Sneddon worked exclusively in the space of 3×3 complex matrices in his derivation of his complete set $\mathcal{J}$.[8] To the best of our knowledge, there is no explicit justification in the literature for the assertion that *every* even invariant is expressible as polynomials of traces of 3×3 complex matrix products. Furthermore, a general method to construct polynomial syzygies expressing the dependent invariants in terms of $\mathcal{J}$ is not available. We have provided a rigorous

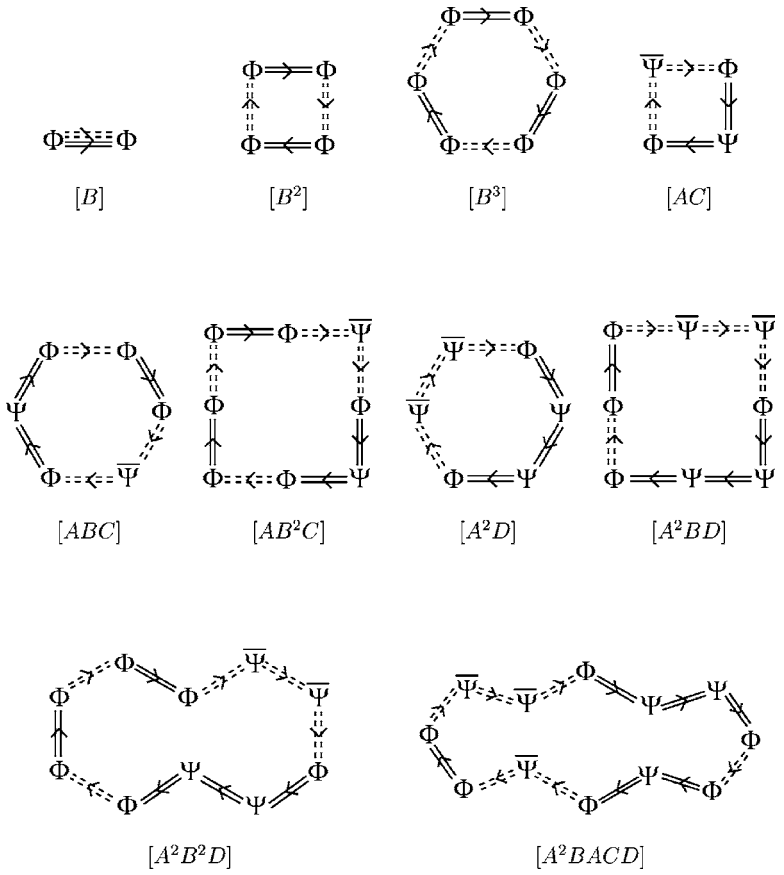

FIG. 2. Real invariants belonging to $\mathcal{J}_{\mathcal{E}}$.

derivation of a complete set for the even invariants in a manner that resolves the aforementioned problems, and we can now explicitly construct the syzygies expressing any even invariant as a polynomial function of the elements in $\mathcal{J}_{\mathcal{E}}$.

V. SYZYGY CONSTRUCTION

The proof of Theorem 1 provides a general algorithm for constructing the polynomial syzygies relating any even invariant $N \notin \hat{\mathcal{E}}^c$ in terms of elements of $\hat{\mathcal{E}}^c$, given N in the form of its associated oriented matrix $A(G_{N'})$. The characteristics of each vertex in the ordering defined by $A(G_{N'})$ are provided by Eq. (2). $A(G_{N'})$ is partitioned into $A(G^S_{N'})$, $A(S^S_{N'})$, and $A(S^D_{N'})$ using the conditions of Eq. (3). The subgraphs $S^S_{N'}$ and $S^D_{N'}$ can be decomposed separately into the forms specified by Eqs. (4) and (5) via the method of permutations of vertex sequences described in Sec. V of paper I.[1] The adjacency matrices $A(G_{X_{jl}})$ associated with each component of the syzygy are obtained by adapting Eq. (3),

$$A(G_{X_{jl}}) = A(G^S_{N'}) + A(\tilde{S}^S_j) + A(\tilde{S}^D_l).$$

It is then straightforward to obtain X_{jl} and construct the first syzygy expressing N in terms of elements of $\hat{\mathcal{E}}^c$ according to Eq. (8).

Lemma 7 guarantees that we can use Eq. (13) to express any invariant belonging to $\hat{\mathcal{E}}^c$ as a polynomial function of Υ-irreducible invariants, or of $\bar{\Upsilon}$-irreducible invariants; and we then make

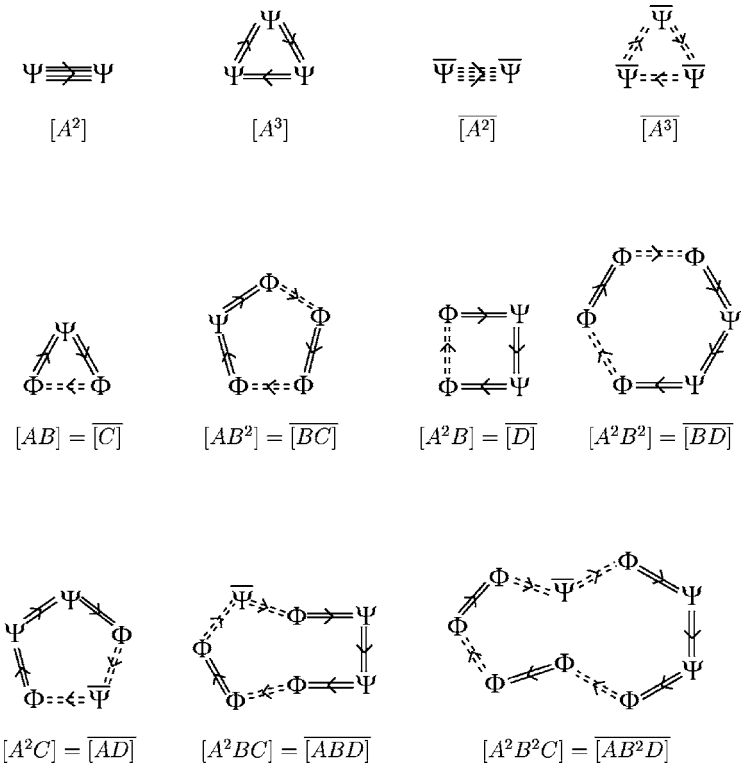

FIG. 3. Complex invariants belonging to $\mathcal{J}_\mathcal{E}$.

use of the fact that every $\bar{\Upsilon}$-irreducible invariant other than $\overline{[A^2]}$ and $\overline{[A^3]}$ is expressible in terms of Υ-irreducible invariants to express N in the manner specified by Theorem 2.

An implementation[18] of the Spencer and Rivlin solution of the basis problem for four symmetric 3×3 matrices, is then used to express N in terms of $\overline{[A^2]}$, $\overline{[A^3]}$ and the elements of $\mathcal{S}$. N is now expressed entirely in terms of Υ-minimal invariants. Each individual term is examined and decomposed further into $\bar{\Upsilon}$-minimal invariants if it is not already $\bar{\Upsilon}$-minimal. Each new term is reexamined for Υ-minimality and reduced if necessary. This alternate checking for Υ-minimality and $\bar{\Upsilon}$-minimality is repeated until every term is both Υ-minimal and $\bar{\Upsilon}$-minimal. We then have the polynomial syzygy expressing N in terms of the elements of $\mathcal{J}_\mathcal{E}$. This algorithm is guaranteed to terminate because in each step, invariants which are not Υ-minimal or $\bar{\Upsilon}$-minimal are reexpressed in terms of invariants of lower polynomial degree in the Weyl, conjugate Weyl and Ricci spinors.

We now give an example of this decomposition process applied to an even invariant for $N' = \bar{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}\Phi_{AB}{}^{\dot{A}\dot{B}}\Phi^{A}{}_{C}{}^{\dot{C}}{}_{\dot{E}}\Phi^{B}{}_{D}{}^{\dot{E}}{}_{\dot{F}}\Psi^{CD}{}_{EF}\Phi^{EF}{}_{\dot{G}\dot{H}}\Phi_{GH}{}^{\dot{G}\dot{H}}\Phi^{GHD\dot{F}}$. The graph $G_{N'}$ is drawn and its vertices labeled as shown in Fig. 4.

Partitioning the arc set of $G_{N'}$ using Eq. (3) yields the subgraphs $S^S_{N'}$ and $S^D_{N'}$, which are then decomposed separately as described earlier in this section. The graphical representations of Eqs. (4) and (5) for this particular example are depicted in Fig. 5.

Constructing the double sum described in Eqs. (7) and (8) yields a syzygy of nine terms which simplifies to the following expression:

$$N' = \tfrac{1}{4}([B][ABC] - 2[ABCB]),$$

$[ABCB]$ is not Υ-minimal, and is rewritten using a relation with the form of Eq. (12) to give

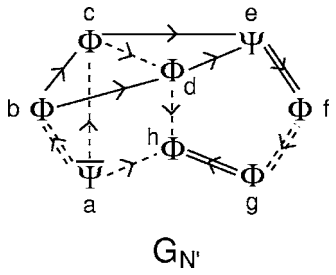

FIG. 4. The graph $G_{N'}$ associated with the example invariant N'.

$$N' = [AB^2C] + \tfrac{1}{4}([B]^2[AC] - [AC][B^2] + 2[B][C][AB] - 2[AB][BC] - 2[C][AB^2] - 3[B][ABC]).$$

It is easily verified that every invariant on the right-hand side is both Υ-minimal and $\bar{\Upsilon}$-minimal, and hence N' is expressed as a polynomial function of elements of $\mathcal{J}_{\mathcal{E}}$.

VI. CONCLUDING REMARKS

We have extended our work in paper I and provided a graph-theoretic algorithm that constructs the polynomial syzygies relating any even invariant to the even invariants formed solely via paired spinor index contractions. This fills in a significant gap in previous work by others. In our determination of the basis for this subset of even invariants, we have confirmed Sneddon's earlier insights and placed them on a rigorous footing.

This concludes the complete analysis of the polynomial syzygies of the even invariants. The solution of the complete problem requires a similar study of the odd invariants and their relationships with the even invariants. We have managed to derive a graph-theoretic algorithm to express odd invariants in terms of restricted subsets and work is currently underway to determine the basis of these subsets. This work will appear in a forthcoming presentation.

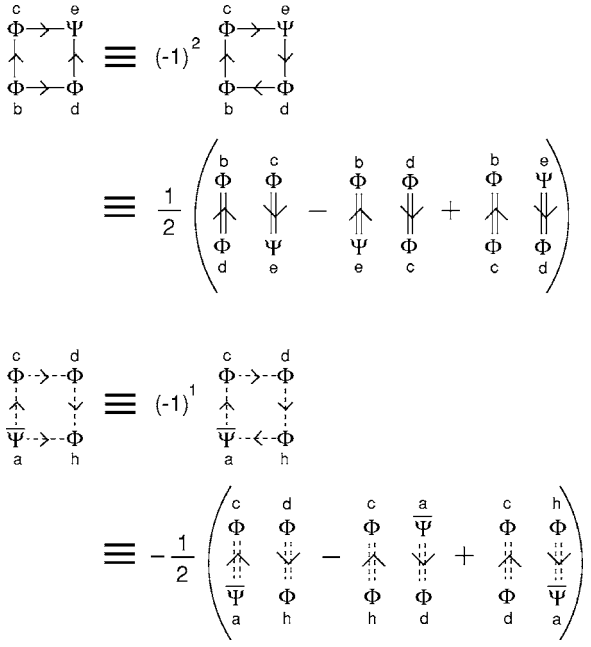

FIG. 5. Decomposition of $S^S_{N'}$ and $S^D_{N'}$ for the example in this section.

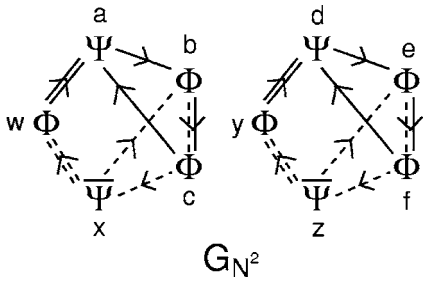

FIG. 6. The graph G_{N^2} associated with the example invariant N^2.

APPENDIX A: GENERATION OF AN ALGEBRAIC SYZYGY

We shall apply the results of this paper to construct an algebraic syzygy relating the square of the odd invariant $N=\bar{\Psi}_{\dot{A}\dot{B}\dot{D}}{}^{\dot{E}}\Phi_{AB}{}^{\dot{A}\dot{B}}\Psi^{AB}{}_{C}{}^{E}\Phi^{C}{}_{D\dot{C}}{}^{\dot{D}}\Phi_{E}{}^{D\dot{C}}{}_{\dot{E}}$ to members of the set $\mathcal{J}_{\mathcal{E}}$. The graph G_{N^2} associated with the quantity N^2 is shown in Fig. 6. The solid unpaired subgraph $S^S_{N^2}$ consists of two disjoint 3-circuits, and is rewritten as the difference between two 6-circuits using the procedure described in Case 2 of the proof of Theorem 1 in Paper I.[1] Subsequent application of the arc-pairing procedure (Case 1) yields 15 terms, each consisting solely of paired arcs, for each 6-circuit. After collecting like terms, $S^S_{N^2}$ is equivalently rewritten as the six terms shown in Fig. 7. The dashed unpaired subgraph $S^D_{N^2}$ is rewritten as a combination of six paired-arc terms in a very similar manner.

Constructing the double sum in Eq. (6) yields a 36-term expression for N^2 in terms of members of $\hat{\mathcal{E}}^c$. After collecting like terms, this simplifies to

$$N^2=[B][AC]^2-2[AC][ABC]+[A^2CBC]-[B][A^2C^2]+[ABAC^2]+[AB^2AD]$$
$$-[B][ABAD]+\frac{[A^2D]}{2}([B]^2-[B^2]).$$

The procedure outlined in Sec. V is used to rewrite nonminimal invariants in terms of invariants that are both Υ-minimal and $\bar{\Upsilon}$-minimal, resulting in the final algebraic syzygy relating N to elements of $\mathcal{J}_{\mathcal{E}}$,

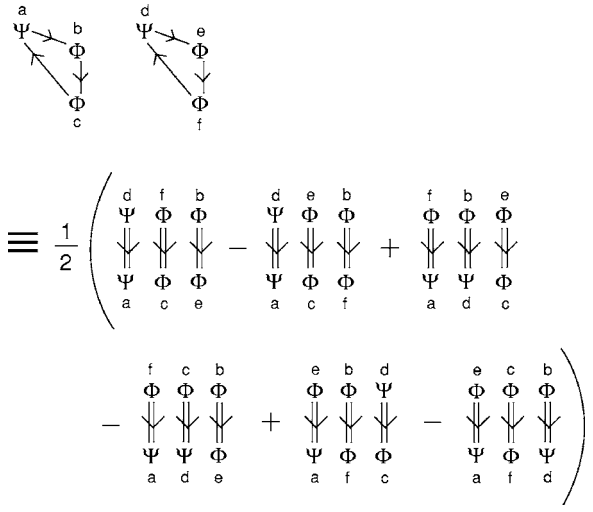

FIG. 7. Decomposition of $S^S_{N^2}$.

$$
\begin{aligned}
N^2 = {} & [D][AB]^2 - 2[C][A^2BC] - 2[AB][ABD] - 6[A^2B^2D] + [AD][AB^2] + [D][A^2B^2] + [A^2C][BC] \\
& + 4[B][A^2BD] + [A^2B]([C]^2 + [BD] - [B][D]) + [AC]([B][AC] - 2[ABC] + [C][AB]) \\
& + \frac{[A^2D]}{2}(5[B^2] - 3[B]^2) - \frac{\overline{[A^2]}[A^2B]}{4}([B]^2 + [B^2]) + \frac{[A^2]\overline{[A^2]}}{12}(5[B]^3 - 12[B][B^2] + 7[B^3]) \\
& + \frac{[A^2]}{4}(2[BC][C] + 2[B][BD] - [B]^2[D] - [B^2][D] - 2[C]^2[B]) \\
& + \frac{\overline{[A^2]}}{2}([AB^2][AB] + [B][A^2B^2] - [B][AB]^2).
\end{aligned}
$$

APPENDIX B: DYAD COMPONENTS OF $^1\Upsilon$, $^2\Upsilon$, $^3\Upsilon$, AND $^4\Upsilon$

Below are the dyad components of the Υ-spinors $^1\Upsilon$, $^2\Upsilon$, $^3\Upsilon$ and $^4\Upsilon$ when they are written in the form of Eq. (9).

$$^1\Upsilon_{00} = \Psi_0,$$

$$^1\Upsilon_{01} = {}^1\Upsilon_{10} = \Psi_1,$$

$$^1\Upsilon_{02} = {}^1\Upsilon_{20} = {}^1\Upsilon_{11} = \Psi_2,$$

$$^1\Upsilon_{12} = {}^1\Upsilon_{21} = \Psi_3,$$

$$^1\Upsilon_{22} = \Psi_4,$$

$$^2\Upsilon_{00} = 2\Phi_{00}\Phi_{02} - 2\Phi_{01}^2,$$

$$^2\Upsilon_{01} = {}^2\Upsilon_{10} = \Phi_{10}\Phi_{02} + \Phi_{12}\Phi_{00} - 2\Phi_{11}\Phi_{01},$$

$$^2\Upsilon_{02} = {}^2\Upsilon_{20} = \Phi_{22}\Phi_{00} + \Phi_{20}\Phi_{02} - 2\Phi_{01}\Phi_{21},$$

$$^2\Upsilon_{11} = 2\Phi_{10}\Phi_{12} - 2\Phi_{11}^2,$$

$$^2\Upsilon_{12} = {}^2\Upsilon_{21} = \Phi_{10}\Phi_{22} + \Phi_{12}\Phi_{20} - 2\Phi_{21}\Phi_{11},$$

$$^2\Upsilon_{22} = 2\Phi_{20}\Phi_{22} - 2\Phi_{21}^2,$$

$$^3\Upsilon_{00} = 4\bar{\Psi}_2\Phi_{01}^2 + \bar{\Psi}_0\Phi_{02}^2 + \bar{\Psi}_4\Phi_{00}^2 + 2\bar{\Psi}_2\Phi_{00}\Phi_{02} - 4\bar{\Psi}_3\Phi_{00}\Phi_{01} - 4\bar{\Psi}_1\Phi_{01}\Phi_{02},$$

$$
\begin{aligned}
^3\Upsilon_{01} = {}^3\Upsilon_{10} = {} & \bar{\Psi}_0\Phi_{12}\Phi_{02} - 2\bar{\Psi}_3\Phi_{00}\Phi_{11} + \bar{\Psi}_2\Phi_{10}\Phi_{02} + \bar{\Psi}_2\Phi_{00}\Phi_{12} - 2\bar{\Psi}_1\Phi_{12}\Phi_{01} + \bar{\Psi}_4\Phi_{00}\Phi_{10} \\
& + 4\bar{\Psi}_2\Phi_{11}\Phi_{01} - 2\bar{\Psi}_1\Phi_{11}\Phi_{02} - 2\bar{\Psi}_3\Phi_{01}\Phi_{10},
\end{aligned}
$$

$$
\begin{aligned}
^3\Upsilon_{02} = {}^3\Upsilon_{20} = {} & 4\bar{\Psi}_2\Phi_{21}\Phi_{01} - 2\bar{\Psi}_3\Phi_{00}\Phi_{21} + \bar{\Psi}_0\Phi_{02}\Phi_{22} + \bar{\Psi}_4\Phi_{20}\Phi_{00} + \bar{\Psi}_2\Phi_{20}\Phi_{02} - 2\bar{\Psi}_3\Phi_{01}\Phi_{20} \\
& + \bar{\Psi}_2\Phi_{00}\Phi_{22} - 2\bar{\Psi}_1\Phi_{01}\Phi_{22} - 2\bar{\Psi}_1\Phi_{21}\Phi_{02},
\end{aligned}
$$

$$
{}^{3}\Upsilon_{11} = 4\bar{\Psi}_2\Phi_{11}^2 - 4\bar{\Psi}_1\Phi_{11}\Phi_{12} + \bar{\Psi}_4\Phi_{10}^2 - 4\bar{\Psi}_3\Phi_{10}\Phi_{11} + \bar{\Psi}_0\Phi_{12}^2 + 2\bar{\Psi}_2\Phi_{10}\Phi_{12},
$$

$$
\begin{aligned}
{}^{3}\Upsilon_{12} = {}^{3}\Upsilon_{21} &= \bar{\Psi}_4\Phi_{20}\Phi_{10} - 2\bar{\Psi}_1\Phi_{22}\Phi_{11} + \bar{\Psi}_2\Phi_{10}\Phi_{22} + \bar{\Psi}_2\Phi_{20}\Phi_{12} + 4\bar{\Psi}_2\Phi_{11}\Phi_{21} + \bar{\Psi}_0\Phi_{12}\Phi_{22} \\
&\quad - 2\bar{\Psi}_1\Phi_{12}\Phi_{21} - 2\bar{\Psi}_3\Phi_{20}\Phi_{11} - 2\bar{\Psi}_3\Phi_{10}\Phi_{21},
\end{aligned}
$$

$$
{}^{3}\Upsilon_{22} = \bar{\Psi}_4\Phi_{20}^2 + 2\bar{\Psi}_2\Phi_{20}\Phi_{22} + \bar{\Psi}_0\Phi_{22}^2 - 4\bar{\Psi}_3\Phi_{20}\Phi_{21} + 4\bar{\Psi}_2\Phi_{21}^2 - 4\bar{\Psi}_1\Phi_{21}\Phi_{22},
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{00} &= 4\bar{\Psi}_1\bar{\Psi}_2\Phi_{01}\Phi_{02} + 2\bar{\Psi}_2^2\Phi_{00}\Phi_{02} - 2\bar{\Psi}_3^2\Phi_{00}^2 + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{02}^2 - 8\bar{\Psi}_2^2\Phi_{01}^2 - 4\bar{\Psi}_0\bar{\Psi}_3\Phi_{01}\Phi_{02} \\
&\quad - 4\bar{\Psi}_1\bar{\Psi}_4\Phi_{00}\Phi_{01} + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{00}^2 + 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{01}^2 + 4\bar{\Psi}_2\bar{\Psi}_3\Phi_{00}\Phi_{01} - 2\bar{\Psi}_1^2\Phi_{02}^2 + 2\bar{\Psi}_0\bar{\Psi}_4\Phi_{00}\Phi_{02} \\
&\quad - 4\bar{\Psi}_1\bar{\Psi}_3\Phi_{00}\Phi_{02},
\end{aligned}
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{01} = {}^{4}\Upsilon_{10} &= \bar{\Psi}_2^2\Phi_{10}\Phi_{02} - 8\bar{\Psi}_2^2\Phi_{11}\Phi_{01} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{10}\Phi_{01} - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{12}\Phi_{00} + \bar{\Psi}_2^2\Phi_{12}\Phi_{00} \\
&\quad + \bar{\Psi}_0\bar{\Psi}_4\Phi_{12}\Phi_{00} + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{02}\Phi_{12} + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{10}\Phi_{01} + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{10}\Phi_{00} + 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{11}\Phi_{01} \\
&\quad - 2\bar{\Psi}_1^2\Phi_{02}\Phi_{12} - 2\bar{\Psi}_3^2\Phi_{00}\Phi_{10} - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{02}\Phi_{10} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{11}\Phi_{00} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{12}\Phi_{01} \\
&\quad + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{11}\Phi_{00} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{11}\Phi_{02} + 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{11}\Phi_{02} + 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{12}\Phi_{01} + \bar{\Psi}_0\bar{\Psi}_4\Phi_{02}\Phi_{10},
\end{aligned}
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{02} = {}^{4}\Upsilon_{20} &= \bar{\Psi}_2^2\Phi_{22}\Phi_{00} - 2\bar{\Psi}_3^2\Phi_{20}\Phi_{00} - 2\bar{\Psi}_1^2\Phi_{22}\Phi_{02} - 8\bar{\Psi}_2^2\Phi_{21}\Phi_{01} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{21}\Phi_{00} + \bar{\Psi}_2^2\Phi_{02}\Phi_{20} \\
&\quad + 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{21}\Phi_{01} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{21}\Phi_{02} + 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{21}\Phi_{02} + \bar{\Psi}_0\bar{\Psi}_4\Phi_{22}\Phi_{00} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{01}\Phi_{22} \\
&\quad + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{01}\Phi_{20} - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{22}\Phi_{00} + 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{22}\Phi_{01} + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{22}\Phi_{02} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{01}\Phi_{20} \\
&\quad + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{20}\Phi_{00} + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{21}\Phi_{00} + \bar{\Psi}_0\bar{\Psi}_4\Phi_{02}\Phi_{20} - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{02}\Phi_{20},
\end{aligned}
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{11} &= 2\bar{\Psi}_0\bar{\Psi}_4\Phi_{10}\Phi_{12} - 2\bar{\Psi}_1^2\Phi_{12}^2 + 2\bar{\Psi}_2^2\Phi_{10}\Phi_{12} - 2\bar{\Psi}_3^2\Phi_{10}^2 + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{12}^2 + 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{11}^2 \\
&\quad - 4\bar{\Psi}_1\bar{\Psi}_4\Phi_{11}\Phi_{10} + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{10}^2 + 4\bar{\Psi}_2\bar{\Psi}_3\Phi_{11}\Phi_{10} - 8\bar{\Psi}_2^2\Phi_{11}^2 + 4\bar{\Psi}_1\bar{\Psi}_2\Phi_{11}\Phi_{12} \\
&\quad - 4\bar{\Psi}_1\bar{\Psi}_3\Phi_{12}\Phi_{10} - 4\bar{\Psi}_0\bar{\Psi}_3\Phi_{11}\Phi_{12},
\end{aligned}
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{12} = {}^{4}\Upsilon_{21} &= 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{11}\Phi_{22} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{11}\Phi_{22} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{11}\Phi_{20} + \bar{\Psi}_0\bar{\Psi}_4\Phi_{22}\Phi_{10} - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{22}\Phi_{10} \\
&\quad + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{11}\Phi_{20} - 2\bar{\Psi}_3^2\Phi_{10}\Phi_{20} - 2\bar{\Psi}_1^2\Phi_{22}\Phi_{12} + \bar{\Psi}_0\bar{\Psi}_4\Phi_{12}\Phi_{20} + \bar{\Psi}_2^2\Phi_{12}\Phi_{20} + \bar{\Psi}_2^2\Phi_{10}\Phi_{22} \\
&\quad - 2\bar{\Psi}_1\bar{\Psi}_3\Phi_{12}\Phi_{20} - 8\bar{\Psi}_2^2\Phi_{11}\Phi_{21} - 2\bar{\Psi}_0\bar{\Psi}_3\Phi_{12}\Phi_{21} - 2\bar{\Psi}_1\bar{\Psi}_4\Phi_{10}\Phi_{21} + 2\bar{\Psi}_1\bar{\Psi}_2\Phi_{12}\Phi_{21} \\
&\quad + 2\bar{\Psi}_2\bar{\Psi}_3\Phi_{10}\Phi_{21} + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{12}\Phi_{22} + 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{11}\Phi_{21} + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{10}\Phi_{20},
\end{aligned}
$$

$$
\begin{aligned}
{}^{4}\Upsilon_{22} &= 8\bar{\Psi}_1\bar{\Psi}_3\Phi_{21}^2 - 2\bar{\Psi}_3^2\Phi_{20}^2 + 2\bar{\Psi}_0\bar{\Psi}_2\Phi_{22}^2 + 4\bar{\Psi}_1\bar{\Psi}_2\Phi_{21}\Phi_{22} - 4\bar{\Psi}_0\bar{\Psi}_3\Phi_{21}\Phi_{22} - 4\bar{\Psi}_1\bar{\Psi}_4\Phi_{20}\Phi_{21} \\
&\quad - 4\bar{\Psi}_1\bar{\Psi}_3\Phi_{20}\Phi_{22} + 2\bar{\Psi}_2\bar{\Psi}_4\Phi_{20}^2 + 2\bar{\Psi}_2^2\Phi_{20}\Phi_{22} - 2\bar{\Psi}_1^2\Phi_{22}^2 + 2\bar{\Psi}_0\bar{\Psi}_4\Phi_{20}\Phi_{22} - 8\bar{\Psi}_2^2\Phi_{21}^2 \\
&\quad + 4\bar{\Psi}_2\bar{\Psi}_3\Phi_{20}\Phi_{21}.
\end{aligned}
$$

APPENDIX C: COMPLETE SETS AND POLYNOMIAL SYZYGIES WITHIN $\mathcal{J}_{\mathcal{E}}$ FOR ALL SEGRE TYPES

1. PP type O

a. Segre type [(1,111)]

Ricci components in a canonical frame: $\Phi_{ab}=0$.
Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]}\}$.

b. Segre type [(2,11)]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{12}=\Phi_{11}=0,\quad \Phi_{22}\neq 0.$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[AC],[AD],[A^2C],[A^2D]\}$.

c. Segre type [(1,11)1]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{12}=\Phi_{22}=0\quad \Phi_{02}=-2\Phi_{11}\neq 0.$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$3[B^2]=[B]^2,\quad 9[B^3]=[B]^3,$$

$$3[D]=[B]\overline{[A^2]},\quad 9[BD]=[B]^2\overline{[A^2]},$$

$$3[A^2B]=[B][A^2],\quad 3[ABC]=[B][AC],$$

$$3[ABD]=[B][AD],\quad 9[A^2B^2]=[B]^2[A^2],$$

$$3[A^2BC]=[B][A^2C],\quad 3[A^2BD]=[B][A^2D],$$

$$9[AB^2C]=[B]^2[AC],\quad 9[AB^2D]=[B]^2[AD],$$

$$9[A^2B^2C]=[B]^2[A^2C],\quad 9[A^2B^2D]=[B]^2[A^2D],$$

$$324[A^2BACD]=[B]^2(4[A^3]\overline{[A^3]}[B]+9[A^2]\overline{[A^2]}[AC]).$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[AC],[AD],[A^2C],[A^2D]\}$.

d. Segre type [1,(111)]

Ricci components in a canonical frame:

$$\Phi_{01}=\Phi_{02}=\Phi_{12}=0,\quad \Phi_{00}=2\Phi_{11}=\Phi_{22}\neq 0,$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$ and complete set are the same as for Segre type [(1,11)].

2. PP type N

a. Segre type [(3,1)]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{11}=\Phi_{22}=0,\quad \Phi_{12}\neq 0.$$

Syzygy within $\mathcal{J}_{\mathcal{E}}$, $2[\underline{A^2BACD}]=[\underline{C}][AD][A^2B]+[D][AB][A^2C]$.
Complete set: $\{[A^2],[\overline{A^2}],[A^3],[\overline{A^3}],[C],[AB],[D],[A^2B],[AC],[AD],[A^2C],[A^2D]\}$.

b. Segre type [(2,1)1]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{12}=0,\quad \Phi_{02}=-2\Phi_{11}\neq 0,\quad \Phi_{22}\neq 0.$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$3[B^2]=[B]^2,\quad 9[B^3]=[B]^3,$$

$$3[BC]=2[B][C],\quad 9[BD]=[B](6[D]-[B][\overline{A^2}]),$$

$$3[AB^2]=2[B][AB],\quad 9[A^2B^2]=[B](6[A^2B]-[B][A^2]),$$

$$9[AB^2C]=[B](6[ABC]-[B][AC]),\quad 9[AB^2D]=[B](6[ABD]-[B][AD]),$$

$$9[A^2B^2C]=[B](6[A^2BC]-[B][A^2C]),\quad 9[A^2B^2D]=[B](6[A^2BD]-[B][A^2D]).$$

Complete set: $\{[A^2],[\overline{A^2}],[A^3],[\overline{A^3}],[B],[C],[D],[AB],[AC],[AD],[A^2B],[A^2C],[A^2D],[ABC],[ABD],[A^2BC],[A^2BD],[A^2BACD]\}$.

3. PP type III

a. Segre type [3,1]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{22}=0,\quad \Phi_{02}=-2\Phi_{11}\neq 0,\quad \Phi_{12}\neq 0.$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$3[B^2]=[B]^2,\quad 9[B^3]=[B]^3.$$

Complete set: $\{[A^2],[\overline{A^2}],[A^3],[\overline{A^3}],[B],[C],[D],[AB],[AC],[AD],[BC],[BD],[A^2B],[A^2C],[A^2D],[AB^2],[ABC],[ABD],[A^2B^2],[A^2BC],[A^2BD],[AB^2C],[AB^2D],[A^2B^2C],[A^2B^2D],[A^2BACD]\}$.

4. PP type D

a. Segre type [(1,1)(11)]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{12}=\Phi_{22}=0,\quad \Phi_{11}\neq 0.$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$[B^2]=[B]^2,\quad [B^3]=[B]^3,$$

$$[BC]=[B][C],\quad [BD]=[B][D],$$

$$[AB^2]=[B][AB],\quad [ABC]=[B][AC]=[C][AB],$$

$$[ABD]=[B][AD]=[D][AB],\quad [A^2B^2]=[B][A^2B],$$

$$[A^2BC]=[B][A^2C]=[C][A^2B],\quad [A^2BD]=[B][A^2D]=[D][A^2B],$$

$$[AB^2C]=[B][C][AB]=[B]^2[AC],\quad [AB^2D]=[B][D][AB]=[B]^2[AD],$$

$$[A^2B^2C]=[B][C][A^2B]=[B]^2[A^2C],\quad [A^2B^2D]=[B][D][A^2B]=[B]^2[A^2D],$$

$$[A^2BACD]=[B][AC][A^2D]=[B][AD][A^2C]=[C][AB][A^2D]=[C][AD][A^2B]$$
$$=[D][AB][A^2C]=[D][AC][A^2B].$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[C],[D],[AB],[AC],[AD],[A^2B],[A^2C],[A^2D]\}$.

b. Segre type [(1,1)11]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{12}=\Phi_{22}=0,\quad \Phi_{02}\neq 0,\quad \Phi_{02}\neq \pm 2\Phi_{11}$$

Generic case: $\Phi_{11}\neq 0$.
Complete set: $\mathcal{J}_{\mathcal{E}}$ (no polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$).
Special case: $\Phi_{11}=0$.
Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$2[B^2]=[B]^2,\quad 4[B^3]=[B]^3,$$

$$2[BC]=[B][C],\quad 2[BD]=[B][D],$$

$$2[AB^2]=[B][AB],\quad 2[ABC]=[B][AC],$$

$$2[ABD]=[B][AD],\quad 2[A^2B^2]=[B][A^2B],$$

$$2[A^2BC]=[B][A^2C],\quad 2[A^2BD]=[B][A^2D],$$

$$4[AB^2C]=[B]^2[AC],\quad 4[AB^2D]=[B]^2[AD],$$

$$4[A^2B^2C]=[B]^2[A^2C],\quad 4[A^2B^2D]=[B]^2[A^2D],$$

$$144[A^2BACD]=36[B][AC][A^2D]-36[B][AD][A^2C]+[B]^3[A^3]\overline{[A^3]}+72[C][AD][A^2B]$$
$$+72[D][AB][A^2C]+12[B][C][D][A^3]+12[B][AB][A^2B]\overline{[A^3]}.$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[C],[D],[AB],[AC],[AD],[A^2B],[A^2C],[A^2D]\}$.

c. Segre type [2,(11)]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{12}=0,\quad \Phi_{22}\neq 0,\quad \Phi_{11}\neq 0.$$

Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$[B^2]=[B]^2,\quad [B^3]=[B]^3,$$

$$[BC]=[B][C],\quad [BD]=[B][D],$$

$$[AB^2]=[B][AB],\quad [A^2B^2]=[B][A^2B],$$

$$[AB^2C]=[B][ABC],\quad [AB^2D]=[B][ABD],$$

$$[A^2B^2C]=[B][A^2BC],\quad [A^2B^2D]=[B][A^2BD],$$

$$4[A^2BACD]=[B][AD][A^2C]-[B][AC][A^2D]+2[C][AD][A^2B]+2[D][AB][A^2C]$$
$$-2[A^2C][ABD]+2[A^2D][ABC]-2[AD][A^2BC]+2[AC][A^2BD].$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[C],[D],[AB],[AC],[AD],[A^2B],[A^2C],[A^2D],[ABC],[ABD],[A^2BC],[A^2BD]\}$.

d. Segre type [$Z\bar{Z}$,(11)]

Ricci components in a canonical frame:

$$\boldsymbol{\Phi_{01}=\Phi_{02}=\Phi_{12}=0,\quad \Phi_{22}=-\Phi_{00}\neq 0.}$$

Generic case: $\Phi_{11}\neq 0$.
Complete set: $\mathcal{J}_{\mathcal{E}}$ (no polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$).
Special case: $\Phi_{11}=0$.
Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$2[B^2]=[B]^2,\quad 4[B^3]=[B]^3,$$

$$2[BC]=[B][C],\quad 2[BD]=[B][D],$$

$$2[AB^2]=[B][AB],\quad 2[ABC]=[B][AC],$$

$$2[ABD]=[B][AD],\quad 2[A^2B^2]=[B][A^2B],$$

$$2[A^2BC]=[B][A^2C],\quad 2[A^2BD]=[B][A^2D],$$

$$4[AB^2C]=[B]^2[AC],\quad 4[AB^2D]=[B]^2[AD],$$

$$4[A^2B^2C]=[B]^2[A^2C],\quad 4[A^2B^2D]=[B]^2[A^2D],$$

$$144[A^2BACD]=36[B][AC][A^2D]-36[B][AD][A^2C]+[B]^3[A^3]\overline{[A^3]}+72[C][AD][A^2B]$$
$$+72[D][AB][A^2C]+12[B][C][D][A^3]+12[B][AB][A^2B]\overline{[A^3]}.$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[C],[D],[AB],[AC],[AD],[A^2B],[A^2C],[A^2D]$.

e. Segre type [1,1(11)]

Ricci components in a canonical frame:

$$\Phi_{01}=\Phi_{02}=\Phi_{12}=0,\quad \Phi_{22}=\Phi_{00}\neq 0,\quad \Phi_{00}\neq \pm 2\Phi_{11}.$$

Generic case: $\Phi_{11}\neq 0$.
Complete set: $\mathcal{J}_{\mathcal{E}}$ (no polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$).
Special case: $\Phi_{11}=0$.
Syzygies within $\mathcal{J}_{\mathcal{E}}$ and complete set are the same as for the $\Phi_{11}=0$ case of Segre type $[Z\bar{Z},(11)]$.

5. PP type II

a. Segre type [2,11]

Ricci components in a canonical frame:

$$\Phi_{00}=\Phi_{01}=\Phi_{12}=0,\quad \Phi_{02}\neq 0,\quad \Phi_{22}\neq 0,\quad \Phi_{02}\neq \pm 2\Phi_{11}.$$

Generic case: $\Phi_{11}\neq 0$.
Complete set: $\mathcal{J}_{\mathcal{E}}$ (no polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$).
Special case: $\Phi_{11}=0$.
Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$2[B^2]=[B]^2,$$

$$4[B^3]=[B]^3,$$

$$4[AB^2C]=[B](4[ABC]-[B][AC]),$$

$$4[AB^2D]=[B](4[ABD]-[B][AD]),$$

$$4[A^2B^2C]=[B](4[A^2BC]-[B][A^2C]),$$

$$4[A^2B^2D]=[B](4[A^2BD]-[B][A^2D]),$$

$$\begin{aligned}144[A^2BACD]=&[B]^3[A^3]\overline{[A^3]}-12[C][BD][A^3]-12[D][BC][A^3]-12[AB]\overline{[A^3]}[A^2B^2]\\&-72[A^2C][ABD]+72[A^2D][ABC]+72[AC][A^2BD]+72[C][AD][A^2B]\\&+72[D][AB][A^2C]+36[B][AD][A^2C]-36[B][AC][A^2D]-72[AD][A^2BC]\\&-12[A^2B][AB^2]\overline{[A^3]}+24[B][C][D][A^3]+24[B][AB][A^2B]\overline{[A^3]}.\end{aligned}$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[C],[D],[AB],[AC],[AD],[BC],[BD],[A^2B],[A^2C],[A^2D],[AB^2],[ABC],[ABD],[A^2B^2],[A^2BC],[A^2BD]\}$.

6. PP type I

a. Segre type [$Z\bar{Z}$,11]

Ricci components in a canonical frame:

$$\boldsymbol{\Phi_{01}=\Phi_{12}=0,\quad \Phi_{02}\neq 0,\quad \Phi_{22}=-\Phi_{00}\neq 0.}$$

Generic case: $\Phi_{11}\neq 0$.
Complete set: $\mathcal{J}_{\mathcal{E}}$ (no polynomial syzygies within $\mathcal{J}_{\mathcal{E}}$).
Special case: $\Phi_{11}=0$.
Syzygies within $\mathcal{J}_{\mathcal{E}}$,

$$2[B^3]=[B](3[B^2]-[B]^2),$$

$$2[AB^2C]=2[B][ABC]+[AC]([B^2]-[B]^2),$$

$$2[AB^2D]=2[B][ABD]+[AD]([B^2]-[B]^2),$$

$$2[A^2B^2C]=2[B][A^2BC]+[A^2C]([B^2]-[B]^2),$$

$$2[A^2B^2D] = 2[B][A^2BD] + [A^2D]([B^2] - [B]^2),$$

$$\begin{aligned}72[A^2BACD] = {} & 12[B][C][D][A^3] + 36[C][AD][A^2B] + 36[D][AB][A^2C] + 18[B][AD][A^2C] \\ & - 18[B][AC][A^2D] + [B]^3[A^3]\overline{[A^3]} + 12[B][AB][A^2B]\overline{[A^3]} - 6[C][BD][A^3] \\ & - [B][B^2][A^3]\overline{[A^3]} + 36[ABC][A^2D] - 36[AD][A^2BC] - 36[A^2C][ABD] \\ & + 36[AC][A^2BD] - 6[D][BC][A^3] - 6[AB][A^2B^2]\overline{[A^3]} - 6[A^2B][AB^2]\overline{[A^3]}.\end{aligned}$$

Complete set: $\{[A^2],\overline{[A^2]},[A^3],\overline{[A^3]},[B],[B^2],[C],[D],[AB],[AC],[AD],[BC],[BD],[A^2B],[A^2C],[A^2D],[AB^2],[ABC],[ABD],[A^2B^2],[A^2BC],[A^2BD]\}$.

b. Segre type [1,111]

Ricci components in a canonical frame:

$$\Phi_{01} = \Phi_{12} = 0, \quad \Phi_{02} \neq 0, \quad \Phi_{22} = \Phi_{00} \neq 0.$$

Generic case: $\Phi_{11} \neq 0$.

Complete set: $\mathcal{J}_\mathcal{E}$ (no polynomial syzygies within $\mathcal{J}_\mathcal{E}$).

Special case: $\Phi_{11}=0$.

Syzygies within $\mathcal{J}_\mathcal{E}$, and complete set are the same for the $\Phi_{11}=0$ case of Segre type $[Z\overline{Z},(11)]$.

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Uniform attractors for nonautonomous incompressible non-Newtonian fluid with locally uniform integrable external forces

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This paper discusses the long time behavior of solutions for a two-dimensional (2D) nonautonomous incompressible non-Newtonian fluid in 2D bounded domains. When the external force $g_0(x,t)$ is locally uniform integrable (see Definition 1.1) in $L^2_{\mathrm{loc}}(\mathbf{R};H)$, the authors obtain the existence and structure of uniform attractors in space V for the family of processes associated with the fluid. Moreover, when $\|g_0\|_{L^2_b}$ is properly small, they provide some interesting corollaries. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2200145]

I. INTRODUCTION

In the past decades there was considerable progress in the research of infinite dimensional dynamical systems. There arose some well-known works in this area (see e.g., Refs. 7, 10, 20, 21, 24, and 25). In Ref. 21, Temam studied systematically the notation of global attractor, as well as many concrete autonomous equations arising in mathematical physics. Later on, Chepyzhov and Vishik[7] presented a general theory that is well valid to deal with nonautonomous equations. When one studies the uniform attractor for some nonautonomous equations, the construction of the skew-product flow plays the main role in this theory which makes it possible to reduce the problem to the study of an attractor of some semigroup acting in an extended function phase space.[9,17] Moreover, this theory reveals that the uniform attractor could be represented as the union of kernel sections of the family of processes. Generally speaking, one can obtain the strongly compact uniform attractor for some systems with symbols of strongly compact hull, in other words, to obtain the strongly compact uniform attractor, one usually assumes that the symbol $g_0(x,t)=g_0(t)$ of the addressed equations is translation compact (tr.c.) in some Banach space, i.e., the strong closure of the set $\{g_0(t+h):h\in\mathbf{R}\}$ is compact in the Banach space. Recently, Lu *et al.*,[15] used the definition of measure of noncompactness and uniformly ω-limit compactness to discuss the two-dimensional (2D) Navier-Stokes equations and obtained some new result, which showed that it is possible to obtain the strongly compact uniform attractor for the system with symbols of weakly compact hull (see later for definitions).

In the present paper, we will develop the idea of Ref. 15 to obtain the uniform attractors and to reveal their structure for the family of processes corresponding to the following 2D nonautonomous incompressible fluid:

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$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u + \nabla p = \nabla \cdot \tau(e(u)) + g(x,t), \quad x = (x_1,x_2) \in \Omega, \quad t \in \mathbf{R}, \tag{1.1}$$

$$\nabla \cdot u = 0, \tag{1.2}$$

where Ω is a smooth bounded subset of $\mathbf{R}^2$, the unknown function $u=u(x,t)=(u_1,u_2)$ represents the velocity of the fluid, $g(x,t)=g(t)=(g_1,g_2)$ is the time-dependent external force, and the scalar function p is the pressure. Equation (1.1) describes the motion of an isothermal, incompressible viscous fluid, where $\tau(e(u))=(\tau_{ij}(e(u)))_{2\times 2}$, which is usually called the extra stress tensor for the fluid, is a matrix of order 2×2 in which

$$\begin{aligned} &\tau_{ij}(e(u)) = 2\mu_0(\varepsilon + |e|^2)^{-\alpha/2}e_{ij} - 2\mu_1\Delta e_{ij}, \quad i,j = 1,2, \\ &\text{and} \quad e_{ij} = e_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad |e|^2 = \sum_{i,j=1}^{2} |e_{ij}|^2, \end{aligned} \tag{1.3}$$

and $\mu_0, \mu_1, \alpha, \varepsilon$ are parameters which generally depend on the temperature and pressure. In this paper we assume that $\mu_0, \mu_1, \varepsilon$ are positive constants and $0<\alpha<1$. In (1.3) if the dependence of $\tau_{ij}(e(u))$ on $e(u)$ is linear then we say systems (1.1) and (1.2) satisfy the Stokes law and the corresponding fluid is called a Newtonian one. Incompressible fluid whose extra stress tensor cannot be adequately described by the Stokes law is usually called non-Newtonian fluid (see, Ref. 16). We refer to Refs. 3–5, 13, 16, and 18 and references therein for detailed background. Obviously, if $\alpha=\mu_1=0$, (1.1) and (1.2) turn into the famous Navier-Stokes equations; if $\mu_1=\mu_0=0$, (1.1) and (1.2) reduce to the well-known Euler equations.

We consider the initial boundary value problem of (1.1) and (1.3) as follows:

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u + \nabla p = \nabla \cdot (2\mu_0(\varepsilon + |e|^2)^{-\alpha/2}e - 2\mu_1\Delta e) + g(x,t), \quad x \in \Omega, \quad t > \tau, \tag{1.4}$$

$$\nabla \cdot u = 0, \tag{1.5}$$

$$u|_{\partial\Omega} = 0, \tag{1.6}$$

$$u|_{t=\tau} = u_\tau, \quad \tau \in \mathbf{R}. \tag{1.7}$$

There are many works concerning the unique existence, regularity, and long time behavior of solutions to Eqs. (1.4)–(1.7) or its associated version (see, e.g., Refs. 2, 6, 8, 11, 26, and 27). The main objective of the present paper is to construct the uniform attractors and to reveal their structure for the family of processes corresponding to Eqs. (1.4)–(1.7). We consider the classical mathematical setting of problem (1.4)–(1.7). Set

$$\mathcal{V} = \{\varphi = (\varphi_1,\varphi_2) \in C_0^\infty(\bar{\Omega}) \times C_0^\infty(\bar{\Omega}), \nabla \cdot \varphi = 0\},$$

$$H = \text{the closure of } \mathcal{V} \text{ in } L^2(\Omega) \times L^2(\Omega),$$

$$V = \text{the closure of } \mathcal{V} \text{ in } H^2(\Omega) \times H^2(\Omega).$$

We use H' and V' to denote the dual space of H and V, respectively. If one identifies H' with H itself, then $V \hookrightarrow H = H' \hookrightarrow V'$. Also $(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle$ represent the inner product in H and the dual pairing between V' and V, respectively. Moreover we have (see Ref. 22) $(f,u)=\langle f,u\rangle, \forall f \in H, u \in V$. Eliminating the pressure p, we can express problem (1.4)–(1.7) as follows (see Refs. 5 and 26):

$$\frac{\partial u}{\partial t} + 2\mu_1 Au + B(u) + N(u) = g(x,t), \quad t > \tau, \tag{1.8}$$

$$u|_{t=\tau} = u_\tau, \quad \tau \in \mathbf{R}. \tag{1.9}$$

The definitions of the operators $A, B(\cdot)$ and $N(\cdot)$ will be introduced in Sec. II. The time-dependent external force $g(\cdot,t)$ will be taken as the time symbol of the equation.

To state our main result clearly, we introduce some notations. Let E be some Banach space. A function $g(t) \in L^2_{\mathrm{loc}}(\mathbf{R};E)$ is said to be translation bounded (tr.b.) in $L^2_{\mathrm{loc}}(\mathbf{R};E)$ if

$$\|g\|^2_{L^2_b(\mathbf{R};E)} = \|g\|^2_{L^2_b} = \sup_{t\in\mathbf{R}} \int_t^{t+1} \|g(s)\|^2_E \mathrm{d}s < +\infty.$$

We denote by $L^2_b(\mathbf{R};E)$ the union of tr.b. functions in $L^2_{\mathrm{loc}}(\mathbf{R};E)$. We say that a function $g(t) \in L^2_{\mathrm{loc}}(\mathbf{R};E)$ is tr.c. in $L^2_{\mathrm{loc}}(\mathbf{R};E)$ if $\mathcal{H}_s(g)$ is compact in $L^2_{\mathrm{loc}}(\mathbf{R};E)$, where $\mathcal{H}_s(g)$ refers that the set $\mathcal{H}_0(g)=\{g(t+h): h\in\mathbf{R}\}$ takes closure with respect to (w.r.t.) the strong topology of $L^2_{\mathrm{loc}}(\mathbf{R};E)$. The collection of tr.c. functions in $L^2_{\mathrm{loc}}(\mathbf{R};E)$ is denoted by $L^2_c(\mathbf{R};E)$.

Definition 1.1: A function $g(t) \in L^2_{\mathrm{loc}}(\mathbf{R};E)$ is said to be locally uniform integrable, if for any $\epsilon>0$ there exists $\eta=\eta(\epsilon)>0$ such that

$$\sup_{t\in\mathbf{R}} \int_t^{t+\eta} \|g(s)\|^2_E \mathrm{d}s \leqslant \epsilon. \tag{1.10}$$

We use $L^2_{\mathrm{lui}}(\mathbf{R};E)$ to denote the union of locally uniform integrable functions in $L^2_{\mathrm{loc}}(\mathbf{R};E)$. We remark that Definition (1.1) originates from Ref. 15, which pointed out that $L^2_c(\mathbf{R};E) \subset L^2_{\mathrm{lui}}(\mathbf{R};E) \subset L^2_b(\mathbf{R};E)$. In this paper, we assume some fixed external force $g_0(t)$ that is locally uniform integrable in $L^2_{\mathrm{loc}}(\mathbf{R};H)$ and take the symbol space $\Sigma=\mathcal{H}_w(g_0)$, where $\mathcal{H}_w(g_0)$ refers that the set $\mathcal{H}_0(g_0)=\{g_0(t+h): h\in\mathbf{R}\}$ takes closure w.r.t. the weak topology of $L^2_{\mathrm{loc}}(\mathbf{R};E)$. Obviously, $\mathcal{H}_w(g_0)$ is weakly compact in $L^2_{\mathrm{loc}}(\mathbf{R};H)$.

Our main result reads as follows.

Theorem 1.1: *If the external force $g_0(t)$ of Eq. (1.8) is locally uniform integrable in $L^2_{\mathrm{loc}}(\mathbf{R};H)$. Then the family of processes $\{U_g(t,\tau)\}, g\in\mathcal{H}_w(g_0)$, corresponding to Eqs. (1.8) and (1.9) has a compact uniform (w.r.t. $g\in\mathcal{H}_w(g_0)$) attractor $\mathcal{A}_{\mathcal{H}_w(g_0)}$ in space V, which uniformly (w.r.t. $g\in\mathcal{H}_w(g_0)$) attracts any bounded sets of H in norm of V. Also the process $\{U_{g_0}(t,\tau)\}$, the family of processes $\{U_g(t,\tau)\}, g\in\mathcal{H}_0(g_0)$, corresponding to Eqs. (1.8) and (1.9) possesses, respectively, the compact uniform (w.r.t. $\tau\in\mathbf{R}$, w.r.t. $g\in\mathcal{H}_0(g_0)$, respectively) attractor $\mathcal{A}_0$ and $\mathcal{A}_{\mathcal{H}_0(g_0)}$. Moreover,*

$$\mathcal{A}_0 = \mathcal{A}_{\mathcal{H}_0(g_0)} = \mathcal{A}_{\mathcal{H}_w(g_0)} = \bigcup_{g\in\mathcal{H}_w(g_0)} \mathcal{K}_g(0) = \omega_{0,\mathcal{H}_w(g_0)}(B_1), \tag{1.11}$$

where $\mathcal{K}_g(0)$ is the kernel section at time moment $t=0$, $\mathcal{K}_g$ is the kernel of the process $\{U_g(t,\tau)\}$, and $\mathcal{K}_g$ is nonempty for all $g\in\mathcal{H}_w(g_0)$; B_1 is the bounded uniformly (w.r.t. $g\in\mathcal{H}_w(g_0)$) absorbing set defined by (2.30) and $\omega_{0,\mathcal{H}_w(g_0)}(B_1)$ is its uniform (w.r.t. $g\in\mathcal{H}_w(g_0)$) ω-limit set.

This result shows that we can obtain the strongly compact uniform attractor for the family of processes corresponding to the incompressible non-Newtonian fluid with weakly compact hull. This is essentially caused by the particular extra stress tensor $\tau(e(u))$ in the equation of the fluid.

We arrange the paper as follows. In Sec. II we introduce some definitions and show the unique existence and some estimations of the solutions. In Sec. III, we first prove the uniform (w.r.t. $g\in\mathcal{H}_w(g_0)$) ω-limit compactness and $(V\times\mathcal{H}_w(g_0), V)$ weak continuity for the associated family of processes. Then we prove Theorem 1.1 and provide some interesting corollaries.

In this paper we use the stand norms of vector-valued functional spaces (see Ref. 1). If no confusion arises, we denote by $X=X\times X$, and $\|\cdot\|_X$ stands for the norm of the Banach space $X\times X$. For instance, $L^2(\Omega)=L^2(\Omega)\times L^2(\Omega)$, $\|\cdot\|_{L^2(\Omega)}$ denotes the norm of $L^2(\Omega)\times L^2(\Omega)$; especially,

$\|\cdot\|=\|\cdot\|_{L^2(\Omega)}$. In addition, $\mathrm{dist}_{\mathcal{M}}(X,Y)=\sup_{x\in X}\inf_{y\in Y}\mathrm{dist}(x,y)$ denotes the semidistance from $X\subset\mathcal{M}$ to $Y\subset\mathcal{M}$ in the metric space $\mathcal{M}$. "$\rightharpoonup$" denotes the convergence in weak topology. The summation convention of repeated indices is used in the whole paper.

II. *A PRIORI* ESTIMATES AND BOUNDED UNIFORMLY ABSORBING SET

In this section, we first introduce the definitions of the operators A, $B(\cdot)$, $N(\cdot)$ and show some properties of them. Then we prove the unique existence and some estimations of the solutions to Eqs. (1.8) and (1.9). Lastly we use these estimations to construct the bounded uniformly (w.r.t. $g\in\mathcal{H}_w(g_0)$) absorbing set in V.

Set

$$a(u,v)=\sum_{i,j,k=1}^{2}\left(\frac{\partial e_{ij}(u)}{\partial x_k},\frac{\partial e_{ij}(v)}{\partial x_k}\right)=\sum_{i,j,k=1}^{2}\int_\Omega\frac{\partial e_{ij}(u)}{\partial x_k}\frac{\partial e_{ij}(v)}{\partial x_k}\mathrm{d}x,\quad u,v\in V. \tag{2.1}$$

Lemma 2.1: (Bloom and Hao[5]) *There exists a positive constant C_1 that depends only on Ω such that*

$$C_1\|u\|_V^2\leqslant a(u,u)\leqslant\|u\|_V^2,\quad \forall\, u\in V. \tag{2.2}$$

Lemma 2.1 implies that $a(\cdot,\cdot)$ defines a positive definite symmetric bilinear form on V. As a consequence of the Lax-Milgram Lemma we obtain an isometric operator $A\in\mathcal{L}(V,V')$, via

$$\langle Au,v\rangle=a(u,v),\quad \forall\, u,v\in V.$$

Let $D(A)=\{\varphi\in V:A\varphi\in H\}$, then $D(A)$ is a Hilbert space and A is also a positive and self-adjoint operator from $D(A)=V\cap H^4(\Omega)$ to H. In fact, $A=P\Delta^2$, where P is the Leray projector from $L^2(\Omega)$ into H. Moreover, for any $u\in D(A)$ we have

$$C_1\|u\|_V\leqslant\|Au\|, \tag{2.3}$$

hereafter C_1 is the constant from Lemma 2.1. In fact, for any $u\in D(A)$, we have by using Lemma 2.1 that

$$C_1\|u\|_V^2\leqslant a(u,u)=\langle Au,u\rangle=(Au,u)\leqslant\|Au\|\|u\|\leqslant\|Au\|\|u\|_V.$$

Thus we obtain (2.3).

Now we define a continuous trilinear form on $H_0^1(\Omega)$ as follows.

$$b(u,v,w)=\sum_{i,j=1}^{2}\int_\Omega u_i\frac{\partial v_j}{\partial x_i}w_j\mathrm{d}x,\quad u,v,w\in H_0^1(\Omega). \tag{2.4}$$

In fact, one can easily check

$$b(u,v,w)=-b(u,w,v),\quad \forall\, u,v,w\in H_0^1(\Omega), \tag{2.5}$$

$$b(u,v,v)=0,\quad \forall\, u,v\in H_0^1(\Omega). \tag{2.6}$$

Since $V\subset H_0^1(\Omega)$, $b(u,v,w)$ is also continuous on V. Moreover, for any $u\in V$,

$$\langle B(u),w\rangle=b(u,u,w),\quad \forall\, w\in V, \tag{2.7}$$

defines a continuous functional $B(u)$ from $V\times V$ to V'. For further details on the operator $B(u)$ one can refer to Refs. 7 and 21–23.

Lastly we introduce the operator $N(\cdot)$ acting on V. For $u\in V$, we set

$$\mu(u) = 2\mu_0(\varepsilon + |e(u)|^2)^{-\alpha/2}$$

and define $N(u)$ by

$$\langle N(u), v\rangle = \sum_{i,j=1}^{2} \int_\Omega \mu(u) e_{ij}(u) e_{ij}(v) \mathrm{d}x, \quad \forall\, v \in V. \tag{2.8}$$

Then the functional $N(u)$ is continuous from V to V'. Moreover, when $u \in D(A)$, $N(u)$ can be extended to H via $\langle N(u), v\rangle = -\int_\Omega \{\nabla \cdot [\mu(u)e(u)]\} \cdot v \mathrm{d}x$, $\forall v \in H$.

With the above definitions, we can formulate the weak form of problem (1.4)–(1.7) as (1.8) and (1.9) in the sense of distributions (see Refs. 5, 14, and 23).

We now begin to show the unique existence and some estimations of the solutions to Eqs. (1.8) and (1.9).

Lemma 2.2: (*i*) *Suppose* $g(x,t) \in L_b^2(\mathbf{R}; H)$, *then for any* $\tau \in \mathbf{R}$ *and* $u_\tau \in H$ *Eqs. (1.8) and (1.9) possess a unique solution* $u(t)$ *satisfying*

$$u \in C([\tau, +\infty); H) \cap L^2_{\mathrm{loc}}([\tau, +\infty); V), \quad u_t \in L^2_{\mathrm{loc}}([\tau, +\infty); V'). \tag{2.9}$$

Moreover,

$$\|u(t)\|^2 \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}\left(1 + \frac{1}{\delta}\right)\|g\|^2_{L_b^2}, \tag{2.10}$$

$$\|u(t)\|^2 + C_1\mu_1 \int_\tau^t \|u(s)\|_V^2 \mathrm{d}s \leqslant \|u_\tau\|^2 + \frac{2}{C_1\mu_1}\int_\tau^t \|g(s)\|^2 \mathrm{d}s, \tag{2.11}$$

where the positive constant δ *essentially depends only on* Ω *and* μ_1.

(*ii*) *Suppose* $g(x,t) \in L_b^2(\mathbf{R}; H)$, *then for any* $\tau \in \mathbf{R}$ *and* $u_\tau \in V$ *Eqs. (1.8) and (1.9) possess a unique solution* $u(t)$ *satisfying*

$$u \in C([\tau, +\infty); V) \cap L^2_{\mathrm{loc}}([\tau, +\infty); D(A)), \quad u_t \in L^2_{\mathrm{loc}}([\tau, +\infty); H). \tag{2.12}$$

Moreover,

$$(t-\tau)\|u(t)\|_V^2 \leqslant Q_1\left(t-\tau, \|u_\tau\|^2, \int_\tau^t \|g(s)\|^2 \mathrm{d}s\right), \quad t \geqslant \tau, \quad \tau \in \mathbf{R}, \tag{2.13}$$

where $Q_1(z_1, z_2, z_3)$ *is a monotone continuous function of* $z_1 = t-\tau$, z_2 *and* z_3.

Proof of (i): One can use the Galerkin method to prove the unique existence and regularity of solutions to Eqs. (1.8) and (1.9). Since the method is classical and the proof is essentially the same as that in Ref. 5, we omit it and here we only prove the estimations (2.10) and (2.11). Let $u(t)$ be the unique solution corresponding to initial data $u_\tau \in H$. Using $u(t)$ to multiply Eq. (1.8), we obtain, using (2.6) and the positive definiteness of the term $\langle N(u), u\rangle$,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 + 2C_1\mu_1\|u(t)\|_V^2 \leqslant \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 + 2\mu_1 a(u,u) + \langle N(u), u\rangle = (g(t), u(t)). \tag{2.14}$$

Now from the definition of norm for Sobolev space we see $\|u\|^2 \leqslant \|u\|_V^2$ holds for any $u \in V$. Thus by (2.14) we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 + 2C_1\mu_1\|u(t)\|^2 \leqslant (g(t), u(t)) \leqslant \frac{\|g(t)\|^2}{C_1\mu_1} + \frac{3C_1\mu_1}{2}\|u(t)\|^2,$$

i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 + C_1\mu_1\|u(t)\|^2 \leqslant \frac{2\|g(t)\|^2}{C_1\mu_1}. \tag{2.15}$$

Applying Gronwall inequality to (2.15) and taking some transformation in the integral, we have

$$\|u(t)\|^2 \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}\int_\tau^t e^{-\delta(t-s)}\|g(s)\|^2\mathrm{d}s \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}\Bigg[\int_{t-1}^t e^{-\delta(t-s)}\|g(s)\|^2\mathrm{d}s + \int_{t-2}^{t-1} e^{-\delta(t-s)}$$
$$\times\|g(s)\|^2\mathrm{d}s + \cdots\Bigg] \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}\Bigg[\int_{t-1}^t \|g(s)\|^2\mathrm{d}s + e^{-\delta}\int_{t-2}^{t-1}\|g(s)\|^2\mathrm{d}s$$
$$+ e^{-2\delta}\int_{t-3}^{t-2}\|g(s)\|^2\mathrm{d}s + \cdots\Bigg] \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}[1 + e^{-\delta} + e^{-2\delta} + \cdots]\|g\|_{L_b^2}^2 \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)}$$
$$+ \frac{2}{\delta}(1 - e^{-\delta})^{-1}\|g\|_{L_b^2}^2 \leqslant \|u_\tau\|^2 e^{-\delta(t-\tau)} + \frac{2}{\delta}\left(1 + \frac{1}{\delta}\right)\|g\|_{L_b^2}^2,$$

where $\delta = C_1\mu_1 > 0$. Obviously, δ depends essentially only on Ω and μ_1. Thus (2.10) holds. Now from (2.14) we easily have

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 + C_1\mu_1\|u(t)\|_V^2 \leqslant \frac{2\|g(t)\|^2}{C_1\mu_1}. \tag{2.16}$$

Equation (2.11) follows directly from (2.16) by integrating it over $[\tau, t]$. The proof of (i) is completed.

In the sequel, we use C to denote a generic constant that maybe depends on Ω, μ_0, μ_1, α, ε, and C_1, also maybe depend on the Sobolev embedding coefficient between spaces (and thus essentially depends on Ω), but is independent of u. We allow C to take different value in different place.

Proof of (ii): Similar to the proof of (i), we only establish the estimation (2.13). For the sake of brevity, we set $\tau = 0$ and thus $t \geqslant 0$. Multiplying Eq. (1.8) by tAu, we obtain

$$\left(\frac{\partial u}{\partial t}, tAu\right) + 2\mu_1 t(Au, Au) + \langle B(u), tAu\rangle + \langle N(u), tAu\rangle = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[ta(u,u)] - \frac{1}{2}a(u,u) + 2\mu_1 t\|Au\|^2$$
$$+ t\langle B(u), Au\rangle + t\langle N(u), Au\rangle = t(g(t), Au) \leqslant \frac{1}{2}\mu_1 t\|Au\|^2 + \frac{2t}{\mu_1}\|g(t)\|^2. \tag{2.17}$$

At the same time, using Hölder inequality, Gagliardo-Nirenberg inequality, and (2.3), we obtain

$$t\langle B(u), Au\rangle \leqslant t\|B(u)\|\|Au\| \leqslant Ct\|u\|_{L^4(\Omega)}\|\nabla u\|_{L^4(\Omega)}\|Au\| \leqslant Ct\|u\|_V^{1/2}\|u\|_{H^1(\Omega)}\|u\|^{1/2}\|Au\|$$
$$\leqslant Ct\|Au\|^{3/2}\|u\|^{1/2}\|u\|_{H^1(\Omega)} \leqslant \tfrac{1}{2}\mu_1 t\|Au\|^2 + Ct\|u\|^2\|u\|_{H^1(\Omega)}^4, \tag{2.18}$$

where C is a positive constant independent of u. Also we have

$$t\langle N(u), Au\rangle = -t\int_\Omega \{\nabla\cdot[\mu(u)e(u)]\}\cdot Au\,\mathrm{d}x. \tag{2.19}$$

To estimate (2.19), we set

$$F(s) = (\varepsilon + |s|^2)^{-\alpha/2}s, \quad \text{where } s = \begin{pmatrix} s_1 & s_2 \\ s_3 & s_4 \end{pmatrix}, \quad s_i \in \mathbf{R},\ i = 1,2,3,4.$$

By computation we see that the first-order Frechét derivative of $F(s)$ satisfies

$$\|DF(s)\| \leqslant \sqrt{4+\frac{12}{\varepsilon}}\varepsilon^{-\alpha/2} \leqslant C\varepsilon^{-\alpha/2}, \quad \forall\, s_i \in \mathbf{R},\ i=1,2,3,4. \tag{2.20}$$

Using (2.20), we deduce from (2.19) that

$$\begin{aligned} t\langle N(u),Au\rangle &\leqslant 2\mu_0 Ct\sqrt{4+\frac{12}{\varepsilon}}\varepsilon^{-\alpha/2}\|\nabla u\|\|Au\| + 2\mu_0 Ct\varepsilon^{-\alpha/2}\|\Delta u\|\|Au\| \\ &\leqslant Ct\|u\|_{H^1(\Omega)}\|Au\| + Ct\|u\|_V\|Au\| \\ &\leqslant \frac{\mu_1 t}{2}\|Au\|^2 + Ct\|u\|^2_{H^1(\Omega)} + Ct\|u\|^2_V. \end{aligned} \tag{2.21}$$

Combining (2.17), (2.18), and (2.21), we obtain by using Lemma 2.1 and (2.3) that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}[ta(u,u)] + \mu_1 t\|Au\|^2 &\leqslant a(u,u) + \frac{4t}{\mu_1}\|g(t)\|^2 + Ct\|u\|^2\|u\|^4_{H^1(\Omega)} + Ct\|u\|^2_{H^1(\Omega)} + Ct\|u\|^2_V \\ &\leqslant a(u,u) + \frac{4t}{\mu_1}\|g(t)\|^2 + Ct\|u\|^2\|u\|^4_V + Ct\|u\|^2_V \\ &\leqslant a(u,u) + \frac{4t}{\mu_1}\|g(t)\|^2 + ta(u,u)[Ca(u,u)\|u\|^2 + C]. \end{aligned}$$

Therefore, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}H(t) \leqslant K(t)H(t) + I(t), \tag{2.22}$$

where

$$H(t) = ta(u(t),u(t)), \quad K(t) = Ca(u(t),u(t))\|u(t)\|^2 + C, \quad I(t) = a(u(t),u(t)) + \frac{4t}{\mu_1}\|g(t)\|^2.$$

Applying Gronwall inequality to (2.22), we obtain

$$H(t) \leqslant \left[H(0) + \int_0^t I(s)\mathrm{d}s\right]\exp\left\{\int_0^t K(s)\mathrm{d}s\right\} = \int_0^t I(s)\mathrm{d}s\,\exp\left\{\int_0^t K(s)\mathrm{d}s\right\}. \tag{2.23}$$

Now using Lemma 2.1 and estimation (2.11), we have

$$\begin{aligned} \int_0^t I(s)\mathrm{d}s = \int_0^t\left[a(u(s),u(s)) + \frac{4s}{\mu_1}\|g(s)\|^2\right]\mathrm{d}s &\leqslant \int_0^t\|u(t)\|^2_V\mathrm{d}s + \frac{4t}{\mu_1}\int_0^t\|g(s)\|^2\mathrm{d}s \leqslant \frac{1}{C_1\mu_1}\|u(0)\|^2 \\ + \left[\frac{2}{C_1^2\mu_1^2} + \frac{4t}{\mu_1}\right]\int_0^t\|g(s)\|^2\mathrm{d}s &\leqslant C\left(\|u(0)\|^2 + (1+t)\int_0^t\|g(s)\|^2\mathrm{d}s\right), \end{aligned} \tag{2.24}$$

where

$$C = \max\left\{\frac{1}{C_1\mu_1}, \frac{2}{C_1^2\mu_1^2}, \frac{4}{\mu_1}\right\}.$$

Similarly, using (2.10) and (2.11), we get

$$\int_0^t K(s)\mathrm{d}s = \int_0^t [Ca(u(s),u(s))\|u(s)\|^2 + C]\mathrm{d}s \leqslant C\int_0^t \|u(t)\|_V^2\|u(s)\|^2\mathrm{d}s + Ct$$
$$\leqslant C\left\{\left(\|u(0)\|^2 + \int_0^t \|g(s)\|^2\mathrm{d}s\right)^2 + t\right\}. \tag{2.25}$$

Equations (2.3) and (2.23)–(2.25) imply

$$t\|u(t)\|_V^2 \leqslant C\left(\|u(0)\|^2 + (1+t)\int_0^t \|g(s)\|^2\mathrm{d}s\right) \times \exp\left\{C\left[\left(\|u(0)\|^2 + \int_0^t \|g(s)\|^2\mathrm{d}s\right)^2 + t\right]\right\}$$
$$\doteq Q_1\left(t, \|u(0)\|^2, \int_0^t \|g(s)\|^2\mathrm{d}s\right), \tag{2.26}$$

where $Q_1(z_1,z_2,z_3)=C[z_2+(1+z_1)z_3]\exp\{C[(z_2+z_3)^2+z_1]\}$. We complete the proof (*ii*) of this lemma.

The proof of Lemma 2.2 is completed. □

Obviously, if $g_0 \in L_b^2(\mathbf{R};H)$, then

$$\|g\|_{L_b^2}^2 \leqslant \|g_0\|_{L_b^2}^2 < +\infty, \quad \forall\, g \in \mathcal{H}_w(g_0). \tag{2.27}$$

In other words, $g_0 \in L_b^2(\mathbf{R};H)$ implies $g \in L_b^2(\mathbf{R};H)$ for all $g \in \mathcal{H}_w(g_0)$. Thus, according to Lemma 2.2(*ii*), we can define the process $\{U_{g_0}(t,\tau)\}: U_{g_0}(t,\tau)V \mapsto V$, $U_{g_0}(t,\tau)u_\tau = u(t)$, where $u(t)$ is the solution of Eqs. (1.8) and (1.9) with symbol g_0 and initial condition $u_\tau \in V$. Similarly, the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, and $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_0(g_0)$, can be defined on V, respectively.

Lemma 2.3: Suppose $g_0(x,t) \in L_b^2(\mathbf{R};H)$, then the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, corresponding to Eqs. (1.8) and (1.9) has a bounded uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbing set $B_1 \subset V$, which uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbs any bounded sets of H in norm of V.

Proof. By (2.10) and (2.27), we see that the set

$$B_0 = \left\{u \in H: \|u\|^2 \leqslant \frac{4}{\delta}\left(1 + \frac{1}{\delta}\right)\|g_0\|_{L_b^2}^2 \doteq R_0^2\right\} \tag{2.28}$$

is a bounded uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbing set in H, that is, for any bounded sets B of H, there exists $t_0 = t_0(\tau,B) \geqslant \tau$ such that

$$\bigcup_{g\in\mathcal{H}_w(g_0)} U_g(t,\tau)B \subset B_0, \quad \forall\, t \geqslant t_0(\tau,B). \tag{2.29}$$

Now set

$$B_1 = \bigcup_{g\in\mathcal{H}_w(g_0)} U_g(\tau+1,\tau)B_0. \tag{2.30}$$

Then we can derive from (2.13), (2.27), and (2.28) that B_1 is bounded in V. Precisely, we have

$$\|u\|_V^2 \leqslant Q_1(1,R_0^2,\|g_0\|_{L_b^2}^2) \doteq R_1^2, \quad \forall\, u \in B_1. \tag{2.31}$$

Clearly, $B_1 \subset V$ is the bounded uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbing set of the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, which uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbs any bounded sets of H in norm of V. The proof is completed. □

III. UNIFORM ω-LIMIT COMPACTNESS AND WEAK CONTINUITY

In this section we prove that the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$ is uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) ω-limit compact and is $(V \times \mathcal{H}_w(g_0), V)$ weakly continuous. Then we briefly establish Theorem 1.1.

Let E be a Banach space and $\mathcal{B}(E)$ be the union of all bounded sets of E. Also let Σ be the symbol space of some family of processes $\{U_\sigma(t,\tau\}$, $\sigma\in\Sigma$, defined on E. For the sake of brevity, we set

$$B_t=\bigcup_{\sigma\in\Sigma}\bigcup_{s\geqslant t}U_\sigma(s,\tau)B.$$

Definition 3.1: The set $\omega_{\tau,\Sigma}(B)=\cap_{t\geqslant\tau}\bar{B}_t$ *is called the uniform (w.r.t.* $\sigma\in\Sigma$*)* ω*-limit set of* $B\subset E$*. A family of processes* $\{U_\sigma(t,\tau)\}$, $\sigma\in\Sigma$, *is said to be uniformly (w.r.t.* $\sigma\in\Sigma$*)* ω*-limit compact if for any* $\tau\in\mathbf{R}$ *and any* $B\in\mathcal{B}(E)$*, the set* B_t *is bounded and* $\lim_{t\to+\infty}\alpha(B_t)=0$*, where* $\alpha(B)$ *denotes the Kuratowski measure of noncompactness which is defined by*

$$\alpha(B)=\inf\{\gamma>0\text{: }B\text{ admits a finite cover by sets of diameters}\leqslant\gamma\}.$$

Lemma 3.1: Let $g_0\in L^2_{\mathrm{lui}}(\mathbf{R};H)$*, then for any* $\tau\in\mathbf{R}$*, there holds*

$$\lim_{\lambda\to+\infty}\sup_{t\geqslant\tau}\int_\tau^t e^{-\lambda(t-\tau)}\|g(s)\|^2\mathrm{d}s=0 \tag{3.1}$$

uniformly w.r.t. $g\in\mathcal{H}_w(g_0)$.

This lemma is a directly corollary of Lemma 3.1 in Ref. 15.

Lemma 3.2: Let $g_0\in L^2_{\mathrm{lui}}(\mathbf{R};H)$*. Then the family of processes* $\{U_g(t,\tau)\}$, $g\in\mathcal{H}(g_0)$*, corresponding to Eqs. (1.8) and (1.9) is uniformly (w.r.t.* $g\in\mathcal{H}(g_0)$*)* ω*-limit compact in* V.

Proof: According to Theorem 2.3 in Ref. 15, we only need to prove the following assertion: for any fixed $\tau\in\mathbf{R}$, any $B\in\mathcal{B}(V)$ and any $\epsilon>0$, there exist $t_1=t_1(\tau,B,\epsilon)$ and a finite dimensional subspace V_m of V such that

$$P\Big(\bigcup_{g\in\mathcal{H}_w(g_0)}\bigcup_{t\geqslant t_1}U_g(t,\tau)B\Big)\text{ is bounded in }V, \tag{3.2}$$

$$\text{and }\Big\|(I-P)\Big(\bigcup_{g\in\mathcal{H}_w(g_0)}\bigcup_{t\geqslant t_1}U_g(t,\tau)x\Big)\Big\|_V\leqslant\epsilon,\quad\forall\,x\in B, \tag{3.3}$$

where I is the identity operator and P is a bounded projector from V into V_m.

In fact, by the classical spectral theory of elliptic operators (see e.g., Ref. 16), there exist a sequence $\{\lambda_n\}_{n=1}^\infty$ satisfying

$$0<\lambda_1\leqslant\lambda_2\leqslant\cdots\leqslant\lambda_n\leqslant\cdots,\quad\lambda_n\to+\infty\text{ as }n\to+\infty, \tag{3.4}$$

and a family of elements $\{w_n\}_{n=1}^\infty\subset D(A)$, which form a basis of V and are orthonormal in H, such that

$$Aw_n=\lambda_n w_n,\quad\forall\,n\in\mathbf{N}. \tag{3.5}$$

Let $V_m=\mathrm{span}\{w_1,\ldots,w_m\}$, then V_m is a finite dimensional subspace of V. Denote by P_m the orthogonal projector from V into V_m and we obviously have $\|P_m\|\leqslant1$ for each $m\in\mathbf{N}$. Now for any $u\in D(A)\subset V$, we set

$$u=P_mu+(I-P_m)u\doteq u_1+u_2.$$

Using Au_2 to take inner product with (1.8) in H, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}a(u_2,u_2)+2\mu_1(Au_2,Au_2)+\langle B(u),Au_2\rangle+\langle N(u),Au_2\rangle=(g,Au_2). \tag{3.6}$$

Now using the definition of $B(\cdot)$, Hölder inequality and Gagliardo-Nirenberg inequality, we have

$$|\langle B(u),Au_2\rangle| \leqslant \|u\|_{L^4(\Omega)}\|\nabla u\|_{L^4(\Omega)}\|Au_2\| \leqslant C\|u\|^{1/2}\|\nabla u\|^{1/2}\|u\|^{1/4}\|\Delta u\|^{3/4}\|Au_2\|$$
$$\leqslant C\|u\|^{3/4}\|u\|^{1/2}_{H^1(\Omega)}\|u\|^{3/4}_V\|Au_2\| \leqslant \frac{3}{8}\mu_1\|Au_2\|^2 + \frac{8C}{3\mu_1}\|u\|^{3/2}\|u\|_{H^1(\Omega)}\|u\|^{3/2}_V$$
$$\leqslant \frac{3}{8}\mu_1\|Au_2\|^2 + \frac{C}{\mu_1}\|u\|^{3/2}\|u\|^{5/2}_V, \tag{3.7}$$

here and in the following C denotes the generic constant that has been mentioned in Sec. II. Also we have by using (2.20) and Hölder inequality that

$$|\langle N(u),Au_2\rangle| = \left|-\int_\Omega \{\nabla\cdot[\mu(u)e(u)]\}\cdot Au_2 \mathrm{d}x\right| \leqslant 2C\mu_0\varepsilon^{-\alpha/2}\sqrt{4+\frac{12}{\varepsilon}}\|\nabla u\|\|Au_2\| + 2C\mu_0\varepsilon^{-\alpha/2}\|\Delta u\|$$
$$\times\|Au_2\| \leqslant \frac{C}{\mu_1}\|u\|^2_{H^1(\Omega)} + \frac{3}{4}\mu_1\|Au_2\|^2 + \frac{C}{\mu_1}\|u\|^2_V \leqslant \frac{3}{4}\mu_1\|Au_2\|^2 + \frac{C}{\mu_1}\|u\|^2_V. \tag{3.8}$$

It is clear that

$$(g,Au_2) \leqslant \|Au_2\|\|g\| \leqslant \frac{3}{8}\mu_1\|Au_2\|^2 + \frac{8}{3\mu_1}\|g\|^2. \tag{3.9}$$

Taking (3.6)–(3.9) into account, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}a(u_2,u_2) + \mu_1(Au_2,Au_2) \leqslant \frac{C}{\mu_1}\|u\|^{3/2}\|u\|^{5/2}_V + \frac{C}{\mu_1}\|u\|^2_V + \frac{16}{3\mu_1}\|g\|^2. \tag{3.10}$$

Now (3.4) and (3.5) and Lemma 2.1 imply

$$\|Au_2\|^2 \geqslant \lambda_{m+1}\|u_2\|^2_V \geqslant \lambda_{m+1}a(u_2,u_2). \tag{3.11}$$

Combining (3.10) and (3.11) and Lemma 2.3, we see that $t \geqslant t_0+1$ implies

$$\frac{\mathrm{d}}{\mathrm{d}t}a(u_2(t),u_2(t)) + \mu_1\lambda_{m+1}a(u_2(t),u_2(t)) \leqslant \frac{C}{\mu_1}R_0^{3/2}R_1^{5/2} + \frac{C}{\mu_1}R_1^2 + \frac{16}{3\mu_1}\|g\|^2, \tag{3.12}$$

where t_0 is the constant from Lemma 2.3. Applying Gronwall inequality to (3.12), we obtain

$$a(u_2(t),u_2(t)) \leqslant a(u_2(t_0+1),u_2(t_0+1))e^{-\mu_1\lambda_{m+1}(t-t_0-1)} + \frac{C}{\mu_1^2\lambda_{m+1}}(R_0^{3/2}R_1^{5/2}+R_1^2)$$
$$+ \frac{C}{\mu_1^2\lambda_{m+1}}\int_{t_0+1}^t e^{-\mu_1\lambda_{m+1}(s-t_0-1)}\|g(s)\|^2\mathrm{d}s, \quad \forall\, t \geqslant t_0+1. \tag{3.13}$$

By (3.4) and Lemma 3.1, we derive that for any $\epsilon>0$, there exists $m_0\in\mathbf{N}$ such that

$$\frac{C}{\mu_1^2\lambda_{m+1}}(R_0^{3/2}R_1^{5/2}+R_1^2) \leqslant \frac{C_1\epsilon}{3}, \quad m \geqslant m_0, \tag{3.14}$$

$$\frac{C}{\mu_1^2\lambda_{m+1}}\int_{t_0+1}^t e^{-\mu_1\lambda_{m+1}(s-t_0-1)}\|g(s)\|^2\mathrm{d}s \leqslant \frac{C_1\epsilon}{3}, \quad m \geqslant m_0, \quad \forall\, g\in\mathcal{H}_w(g_0). \tag{3.15}$$

Now we set

$$\tilde{t} = \tilde{t}(\tau, B, \epsilon) = t_0 + 1 + \frac{1}{\mu_1 \lambda_{m+1}} \ln\left(\frac{3R_1^2}{C_1 \epsilon}\right),$$

then

$$a(u_2(t_0+1), u_2(t_0+1)) e^{-\mu_1 \lambda_{m+1}(t-t_0-1)} \leqslant \frac{C_1 \epsilon}{3}, \quad \forall\, t \geqslant \tilde{t}. \tag{3.16}$$

Choose $t_1 = t_1(\tau, B, \epsilon) = \max\{\tilde{t}, t_0+1\}$ and we combine Lemma 2.1 and (3.13)–(3.16) to obtain (when $m \geqslant m_0$)

$$\|u_2(t)\|_V^2 \leqslant \frac{1}{C_1} a(u_2(t), u_2(t)) \leqslant \frac{1}{C_1}\left(\frac{C_1\epsilon}{3} + \frac{C_1\epsilon}{3} + \frac{C_1\epsilon}{3}\right) = \epsilon, \quad \forall\, t \geqslant t_1, \quad \forall\, g \in \mathcal{H}_w(g_0).$$

Therefore, we have established the assertion formulated in the beginning of the proof. The proof of this lemma is completed. □

Lemma 3.3: Let $g_0 \in L^2_{\mathrm{lui}}(\mathbf{R}; H)$. Then the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, corresponding to Eqs. (1.8) and (1.9) is $(V \times \mathcal{H}_w(g_0), V)$ weakly continuous, i.e., for any $t \geqslant \tau$, $\tau \in \mathbf{R}$, the mapping $U_g(t,\tau): (u,g) \mapsto U_g(t,\tau)u$ is weakly continuous from $V \times \mathcal{H}_w(g_0)$ to V.

Proof: Let $u_0^{(n)} \rightharpoonup u_0$ in V and $g_n \rightharpoonup g_0$ in $L^2_{\mathrm{loc}}(\mathbf{R}; H)$. For any $\tau \in \mathbf{R}$, we set $u^{(n)}(t) = U_{g_n}(t,\tau)u_0^{(n)}$ and $u(t) = U_{g_0}(t,\tau)u_0$. Analogous with Lemma 2.2(*ii*), we can prove that $\{u^{(n)}\}$ is bounded in $C([\tau, +\infty); V) \cap L^2_{\mathrm{loc}}([\tau, +\infty); D(A))$ and $\{u_t^{(n)}\}$ is bounded in $L^2_{\mathrm{loc}}([\tau, +\infty); H)$. The rest is essentially the same as the proof of Lemma 2.2 in Ref. 12 or of Lemma 2.1 in Ref. 19. So we omit it here. □

Proof of Theorem 1.1; Since $g_0 \in L^2_{\mathrm{lui}}(\mathbf{R}; H) \subset L^2_b(\mathbf{R}; H)$, $\mathcal{H}_w(g_0)$ is weakly compact in $L^2_{\mathrm{loc}}(\mathbf{R}; H)$. At the same time, Lemma 3.3 shows that the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, corresponding to Eqs. (1.8) and (1.9) is $(V \times \mathcal{H}_w(g_0), V)$ weakly continuous. Moreover, Lemma 2.3 shows that $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, has a bounded uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) absorbing set in V and Lemma 3.2 implies that $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, is uniformly (w.r.t. $g \in \mathcal{H}_w(g_0)$) ω-limit compact. It is clear that for any $h \geqslant 0$, we have $T(h)\mathcal{H}_w(g_0) = \mathcal{H}_w(g_0)$ and $U_{T(h)g}(t,\tau) = U_g(t+h, \tau+h)$, $\forall t \geqslant \tau$, $\tau \in \mathbf{R}$, $g \in \mathcal{H}_w(g_0)$, where $\{T(h)\}_{h \geqslant 0}$ is the natural translation semigroup (see Ref. 7 for details). These results show that the family of processes $\{U_g(t,\tau)\}$, $g \in \mathcal{H}_w(g_0)$, satisfies all conditions of Theorem 2.6 in Ref. 15 and thus we obtain Theorem 1.1. The proof is completed. □

In Ref. 28 the authors of the present paper assumed that the external force g_0 is tr.c in $L^2_{\mathrm{loc}}(\mathbf{R}; H)$ and obtained the existence and structure of the uniform attractor in space H for the family of processes corresponding to Eqs. (1.8) and (1.9). The result of this paper extends that of Ref. 28. The following corollaries could be proved essentially in the same way as that in Ref. 28. Here we only list them out and omit the proofs.

Corollary 3.1: Assume $g_0 \in L^2_{\mathrm{lui}}(\mathbf{R}; H)$ and $\|g_0\|^2_{L^2_b} < \hat{C}$, where $\hat{C}$ depends only on Ω and μ_1. Then for all $g \in \mathcal{H}_w(g_0)$ Eqs. (1.8) and (1.9) possess a unique bounded solution $\hat{u}(t) \in V$, $t \in \mathbf{R}$, which is asymptotically stable in H, that is,

$$\|\hat{u}(t) - u(t)\|^2 \leqslant \|\hat{u}(\tau) - u_\tau\|^2 K_0 e^{-\beta(t-\tau)}, \quad t \geqslant \tau, \quad \tau \in \mathbf{R},$$

where $u_\tau \in H$ is arbitrary and $u(t)$ is the corresponding solution; the positive constants K_0 and β are both independent of u_τ.

Corollary 3.2: Let g_0 satisfy the conditions of Corollary 3.1. If g_0 is a periodic function, then $\hat{u}(t)$ is also a periodic function with the same period.

Corollary 3.3: Let the conditions of Corollary 3.1 be satisfied and let $\hat{u}(t)$, $t \in \mathbf{R}$, be the bounded solution of Eqs. (1.8) and (1.9) with symbol g_0. Then

$$\mathcal{A}_0 = \mathcal{A}_{\mathcal{H}_w(g_0)} = \mathcal{A}_{\mathcal{H}_0(g_0)} = \{\hat{u}(t) : t \in \mathbf{R}\} = [\{\hat{u}(t) : t \in \mathbf{R}\}]_V,$$

where $[\cdot]_V$ *denotes taking closure w.r.t. strong topology of* V.

Corollary 3.4: If $g_0 \in L^2_{\mathrm{lui}}(\mathbf{R};H)$, *then*

$$\mathcal{A}_0 = \mathcal{A}_{\mathcal{H}_w(g_0)} = \mathcal{A}_{\mathcal{H}_0(g_0)} \subseteq B_{R_1}(0),$$

where $B_{R_1}(0)$ *is the ball in* V *centered at* 0 *with radius* R_1 *defined in (2.31).*

Remark 3.1: When $g_0 \in L^2_c(\mathbf{R};H)$,[28] constructed the uniform attractor $\mathcal{A}_{\mathcal{H}_s(g_0)} \subset H$ for the family of processes corresponding to the non-Newtonian fluid. Indeed, if $g_0 \in L^2_c(\mathbf{R};H)$, then Theorem 1.1 also holds true and we can deduce from Theorem 1.1 and Theorem 3.1 in Ref. 28 that $\mathcal{A}_{\mathcal{H}_s(g_0)} \subset \mathcal{A}_{\mathcal{H}_w(g_0)} \subset V$, which implies the regularity of uniform attractors and thus reveals the asymptotic smoothing effect of solutions in the sense that the solutions become eventually more regular than the initial data.

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A new energy method for the Boltzmann equation

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An energy method for the Boltzmann equation was proposed by Liu, Yang, and Yu [Physica D **188**, 178–192 (2004)] based on the decomposition of the Boltzmann equation and its solution around the local Maxwellian. The main idea is to rewrite the Boltzmann equation as a fluid-type dynamics system with the nonfluid component appearing in the source terms, coupled with an equation for the time evolution of the nonfluid component. In this paper, we will elaborate this method and our main observation is that the microscopic projection of the local Maxwellian with respect to a given global Maxwellian is not linear but quadratic. Based on this and by analyzing the fluid-type system using the analytic techniques for the system of conservation laws, we can indeed control the conserved quantities $\rho, \rho u$, and $\rho(\frac{1}{2}u^2+\mathcal{E})$ of the Boltzmann equation by the microscopic projection of the solution of the Boltzmann equation with respect to the global Maxwellian, which is sufficient to deduce the energy estimates for the solution of the Boltzmann equation. The main purpose here is to show that there is no need to perform two sets of energy estimates with respect to the local and a global Maxwellian as in the previous works. In fact, one set of energy estimates with respect to the global Maxwellian is sufficient for closing the energy estimates. Therefore, it not only simplifies the analysis in the previous works, but also shed some light on the stability analysis in some complicated systems, such as the Vlasov-Poisson-Boltzmann and Vlasov-Maxwell-Boltzmann systems. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Consider the Boltzmann equation

$$f_t + \xi \cdot \nabla_x f = \frac{1}{\kappa} Q(f,f), \quad (f,t,x,\xi) \in \mathbf{R}^+ \times \mathbf{R}^+ \times \mathbf{R}^3 \times \mathbf{R}^3, \tag{1.1}$$

where $f=f(t,x,\xi)$ represents the distributional density of particles at space–time (x,t) with velocity ξ, κ is the Knudsen number proportional to the mean free path, and $Q(f,f)$ is the collision operator given by the following bilinear form, cf. Ref. 1,

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$$Q(f,g)(\xi)=\int_{\mathbf{R}^3}\int_{\mathbf{S}^2_+}(f(\xi')g(\xi'_*)+f(\xi'_*)g(\xi')-f(\xi)g(\xi_*)-f(\xi_*)g(\xi))B(|\xi-\xi_*|,\theta)\mathrm{d}\xi_*\,\mathrm{d}\Omega,$$

with θ being the angle between the relative velocity and the unit vector Ω, i.e., $\cos\theta=(\xi-\xi_*)\cdot\Omega/|\xi-\xi_*|$. Here $\mathbf{S}^2_+=\{\Omega\in\mathbf{S}^2:(\xi-\xi_*)\cdot\Omega\geqslant 0\}$. The conservation of momentum and energy gives the following relation between velocities before and after collision:

$$\xi'=\xi-[(\xi-\xi_*)\cdot\Omega]\Omega,\quad \xi'_*=\xi_*+[(\xi-\xi_*)\cdot\Omega]\Omega.$$

Throughout this paper, the collision kernel $B(|V|,\theta)$ is assumed to satisfy the following two conditions:

(A1) There is $0\leqslant\delta_1<1$ such that

$$0\leqslant B(|V|,\theta)\leqslant C_1(|V|+|V|^{-\delta_1})|\cos\theta|. \tag{1.2}$$

(A2) There are constants $0<\beta\leqslant 1$ such that

$$C_2(1+|\xi|)^{\beta}\leqslant\nu(\xi)\leqslant C_3(1+|\xi|)^{\beta}, \tag{1.3}$$

where $C_i>0(i=1,2,3)$ are positive constants and $\nu(\xi)$ is the collision frequency defined by (cf. Ref. 6)

$$\nu(\xi)=\int_{\mathbf{R}^3}\int_{\mathbf{S}^2}\mathbf{M}(\xi)B(|\xi-\xi_*|,\theta)\mathrm{d}\xi_*\,\mathrm{d}\Omega. \tag{1.4}$$

Notice that both the hard sphere model and the hard potential model with angular cutoff satisfy the above two conditions (A1) and (A2).

In this paper, we consider the Boltzmann equation (1.1) in the whole space with its initial data given by

$$f(0,x,\xi)=f_0(x,\xi). \tag{1.5}$$

Here $f_0(x,\xi)$ is assumed to be a small perturbation of a given global Maxwellian $\overline{\mathbf{M}}=\mathbf{M}_{[\bar\rho,\bar u,\bar\theta]}$ for any given constant $\bar\rho>0$, $\bar u\in\mathbf{R}^3$, $\bar\theta>0$. Without loss of generality, we can let $\bar u=0$ in the rest of this paper.

For a solution around a global Maxwellian or a nontrivial solution profile, the solution spaces for the Boltzmann equation can be in $L^\infty_{x,\xi}$, $L^1_{x,\xi}$, and $H^s_x(L^2_\xi)$, respectively. The solution in $L^\infty_{x,\xi}$ is proved based on the spectral analysis and the bootstrapping argument from Grad[6] to Ukai.[21] The important contribution of DiPerna and Lions[4] is the establishment of the renormalized solutions in $L^1_{x,\xi}$ space using the Boltzmann's celebrated **H** theorem and the averaging lemma. Recently, the existence of solutions in the $H^s_x(L^2_\xi)$ space was proved by energy method for the study on the stability of solution profiles and the large time behavior of the solutions related to fluid dynamics. For this, the decomposition of the solution and the equation around a global Maxwellian was introduced in Ref. 17 for the stability analysis of the shock profiles. And it was also used in the study on the space periodic solutions.[7,8] For the study of the nontrivial solution profiles, a decomposition of the solution into the local Maxwellian and the nonfluid component was used in Ref. 15 so that the Boltzmann equation can be rewritten as a new fluid-type system and an equation for the nonfluid component. So far, the stability of each basic wave pattern, i.e., shock wave, rarefaction wave and contact discontinuity, and the solution profiles for Boltzmann equation with external force and the Vlasov-Poisson-Boltzmann system have been investigated by the energy method through the above decomposition on both the solution and the Boltzmann equation, cf. Refs. 11, 12, 15–17, and 22–24.

However, in all the above analysis through the decomposition around the local Maxwellian, two sets of energy estimates are used. One is with respect to the local Maxwellian and another with respect to a global Maxwellian chosen appropriately. The reason to use two sets of energy

estimates is that the collision frequency is of the order of $(1+|\xi|)^{\beta}$ with $\beta \leqslant 1$ for $|\xi|$ large, while the differentiation on the local Maxwellian may generate a factor as a polynomial of ξ of order greater than 1. And the set of the energy estimates with respect to the global Maxwellian is to absorb the polynomial in ξ, while the energy estimates with respect to the local Maxwellian $\mathbf{M}$ is used by applying the orthogonality of $\mathbf{P}_0^{\mathbf{M}} f$ and $L_{\mathbf{M}}(\mathbf{P}_1^{\mathbf{M}} f)$ with respect to the local Maxwellian $\mathbf{M}$.

The main purpose of this paper is to give a new way of obtaining energy estimates so that only one set of energy estimates is needed. Our main observation is that the microscopic projection of the local Maxwellian $\mathbf{M}$ with respect to the global Maxwellian $\overline{\mathbf{M}}$ is not linearly but quadratic. Based on this and by analyzing the fluid-type system (2.13) using the analytic techniques for the system of conservation laws, we can indeed control the conserved quantities ρ, ρu, and $\rho\left(\frac{1}{2}u^2+\mathcal{E}\right)$ of the Boltzmann equation (1.1) by $\mathbf{P}_1^{\bar{M}} f$ besides the initial data, which is the microscopic projection of the solution $f(t,x,\xi)$ to the Boltzmann equation (1.1) with respect to the global Maxwellian $\overline{\mathbf{M}}$. Hence, it is sufficient to close the energy estimates for the solution of the Boltzmann equation (1.1) by performing the energy estimates on the original equation (1.1) with respect to the global Maxwellian $\overline{\mathbf{M}}$. Therefore, it indeed provides a clear energy method for the study of Boltzmann equation not only simplifies all the previous works in the direction, but also give a clear-cut relation of the Boltzmann equation with the corresponding fluid dynamics. Moreover, in some cases, it gives the optimal results.

The relation of the Boltzmann equation for rarefied gas with the systems of the fluid dynamics is well known since Boltzmann's derivation of this fundamental equation from statistics physics. In fact, the Hilbert expansion in 1912 gives the system of the compressible Euler equations as the first order approximation, while the Chapman-Enskog expansion in 1916–1917 yields the system of the compressible Navier-Stokes equations in the second order approximation, cf. Refs. 3 and 10. By using the decomposition around the local Maxwellian,[15] the derived system of fluid-type equations is not an approximation but an exact system for the time evolution of the fluid components in the solution with a source in terms of the nonfluid component. Moreover, even though the decomposition of the solution into the local Maxwellian and the nonfluid component is known since Maxwell,[19] the analysis on its time evolution and the solution behavior becomes much clearer until recently.[9,11,12,15–17,22–24]

The rest of the paper will be organized as follows. In the next section, we will review the decomposition and rewrite Boltzmann equation as in Ref. 15. In Sec. III, the new energy method is given by the estimation on the fluid component through the fluid-type system and the original equation for the nonfluid component where a basic estimate on the projection of the local Maxwellian with respect to the global Maxwellian is crucially used.

II. REFORMULATION

For completeness and the convenience of the readers, in this section, we give reformulation of the Boltzmann equation through the decomposition introduced in Ref. 15.

Let $f(t,x,\xi)$ be the solution to the Boltzmann equation, we decompose it into the macroscopic, fluid part, the local Mawellian $\mathbf{M}=\mathbf{M}(x,t,\xi)=\mathbf{M}_{[\rho,u,\theta]}(\xi)$, and the microscopic, nonfluid part $\mathbf{G}=\mathbf{G}(x,t,\xi)$,

$$f(t,x,\xi)=\mathbf{M}(t,x,\xi)+\mathbf{G}(t,x,\xi). \tag{2.1}$$

Here, $\mathbf{M}(t,x,\xi)$ is defined by the five conserved quantities, the mass density $\rho(t,x)$, momentum $m(t,x)=\rho(t,x)u(t,x)$ and energy density $\mathcal{E}(t,x)+|u(t,x)|^2/2$,

$$\rho(t,x) \equiv \int_{\mathbf{R}^3} f(t,x,\xi)\mathrm{d}\xi,$$

$$m^i(t,x) \equiv \int_{\mathbf{R}^3} \psi_i(\xi) f(t,x,\xi) \mathrm{d}\xi, \quad i = 1,2,3,$$

$$\left[\rho\left(\mathcal{E} + \tfrac{1}{2}|u|^2\right)\right](t,x) \equiv \int_{\mathbf{R}^3} \psi_4(\xi) f(t,x,\xi) \mathrm{d}\xi, \tag{2.2}$$

in the form of

$$\mathbf{M} \equiv \mathbf{M}_{[\rho,u,\theta]}(\xi) \equiv \frac{\rho}{\sqrt{(2\pi R\theta)^3}} \exp\left(-\frac{|\xi - u|^2}{2R\theta}\right). \tag{2.3}$$

Here $\theta(t,x)$ is the temperature which is related to the internal energy $\varepsilon(t,x)$ through the gas constant R, $\mathcal{E} = \frac{3}{2}R\theta$, and $u(t,x) = (u^1(t,x), u^2(t,x), u^3(t,x))$ is the fluid velocity. Also $\psi_\alpha(\xi)$, $\alpha = 0,1,\ldots,4$, are the five collision invariants,[1]

$$\psi_0(\xi) \equiv 1,$$

$$\psi_i(\xi) \equiv \xi^i, \quad i = 1,2,3, \tag{2.4}$$

$$\psi_4(\xi) \equiv \tfrac{1}{2}|\xi|^2.$$

For any given Maxwellian $\tilde{\mathbf{M}} = \tilde{\mathbf{M}}_{[\tilde{\rho},\tilde{u},\tilde{\theta}]}$, we define an inner product in $\xi \in \mathbf{R}^3$ as

$$\langle h, g \rangle_{\tilde{\mathbf{M}}} \equiv \int_{\mathbf{R}^3} \frac{h(\xi) g(\xi)}{\tilde{\mathbf{M}}} \mathrm{d}\xi,$$

for functions h and g of ξ such that the integral is well defined. Using this inner product with respect to this Maxwellian, the subspace spanned by the collision invariants has the following set of orthogonal basis:

$$\begin{aligned}
\chi_0^{\tilde{\mathbf{M}}} &= \chi_0(\xi;\tilde{\rho},\tilde{u},\tilde{\theta}) \equiv \frac{1}{\sqrt{\tilde{\rho}}}\tilde{\mathbf{M}}, \\
\chi_i^{\tilde{\mathbf{M}}} &= \chi_i(\xi;\tilde{\rho},\tilde{u},\tilde{\theta}) \equiv \frac{\xi^i - \tilde{u}^i}{\sqrt{R\tilde{\theta}\tilde{\rho}}}\tilde{\mathbf{M}}, \quad i = 1,2,3, \\
\chi_4^{\tilde{\mathbf{M}}} &= \chi_4(\xi;\tilde{\rho},\tilde{u},\tilde{\theta}) \equiv \frac{1}{\sqrt{6\tilde{\rho}}}\left(\frac{|\xi - \tilde{u}|^2}{R\theta} - 3\right)\tilde{\mathbf{M}},
\end{aligned} \tag{2.5}$$

$$\langle \chi_\alpha^{\tilde{\mathbf{M}}}, \chi_\beta^{\tilde{\mathbf{M}}} \rangle_{\tilde{\mathbf{M}}} = \delta_{\alpha\beta}, \quad \text{for } \alpha,\beta = 0,1,2,3,4.$$

With this basis, we can define the macroscopic projection $\mathbf{P}_0^{\tilde{\mathbf{M}}}$ and microscopic projection $\mathbf{P}_1^{\tilde{\mathbf{M}}}$ by

$$\mathbf{P}_0^{\tilde{\mathbf{M}}} h \equiv \sum_{\alpha=0}^{4} \langle h, \chi_\alpha^{\tilde{\mathbf{M}}} \rangle_{\tilde{\mathbf{M}}} \chi_\alpha^{\tilde{\mathbf{M}}},$$

$$\mathbf{P}_1^{\tilde{\mathbf{M}}} h \equiv h - \mathbf{P}_0^{\tilde{\mathbf{M}}} h.$$

Notice that the operators $\mathbf{P}_0^{\tilde{\mathbf{M}}}$ and $\mathbf{P}_1^{\tilde{\mathbf{M}}}$ are projections, that is,

$$\mathbf{P}_0^{\tilde{\mathbf{M}}}\mathbf{P}_0^{\tilde{\mathbf{M}}} = \mathbf{P}_0^{\tilde{\mathbf{M}}}, \quad \mathbf{P}_1^{\tilde{\mathbf{M}}}\mathbf{P}_1^{\tilde{\mathbf{M}}} = \mathbf{P}_1^{\tilde{\mathbf{M}}}, \quad \mathbf{P}_0^{\tilde{\mathbf{M}}}\mathbf{P}_1^{\tilde{\mathbf{M}}} = \mathbf{P}_1^{\tilde{\mathbf{M}}}\mathbf{P}_0^{\tilde{\mathbf{M}}} = 0.$$

Now, the system of conservation laws

$$\int_{\mathbf{R}^3} \psi_\alpha (f_t + \xi \cdot \nabla_x f) \mathrm{d}\xi = 0, \quad \alpha = 0,1,\ldots,4, \tag{2.6}$$

takes the following form:

$$\rho_t + \mathrm{div}_x\, m = 0,$$

$$m_t^i + \left(\sum_{j=1}^3 u^j m^i \right)_{x^j} + p_{x^i} + \int_{\mathbf{R}^3} \psi_i(\xi)(\xi \cdot \nabla_x \mathbf{G}) \mathrm{d}\xi = 0, \quad i = 1,2,3, \tag{2.7}$$

$$\left[\rho \left(\frac{|u|^2}{2} + \mathcal{E} \right) \right]_t + \sum_{j=1}^3 \left\{ u^j \left[\rho \left(\frac{|u|^2}{2} + \mathcal{E} \right) + p \right] \right\}_{x^j} + \int_{\mathbf{R}^3} \psi_4(\xi)(\xi \cdot \nabla_x \mathbf{G}) \mathrm{d}\xi = 0.$$

The equation of the state is that for the monatomic gas, with the gas constant R chosen to be $\frac{3}{2}$ without loss of generality, cf. Ref. 16,

$$p = \tfrac{2}{3}\rho e.$$

And the macroscopic entropy S is given by

$$S = -\tfrac{2}{3} \ln \rho + \ln\left(\tfrac{4}{3}\pi\theta\right) + 1.$$

The microscopic equation is obtained by applying the microscopic projection $\mathbf{P}_1^{\mathbf{M}}$ to the Boltzmann equation (1.1):

$$\mathbf{G}_t + \mathbf{P}_1^{\mathbf{M}}(\xi \cdot \nabla_x \mathbf{G} + \xi \cdot \nabla_x \mathbf{M}) = \frac{1}{\kappa} L_{\mathbf{M}} \mathbf{G} + \frac{1}{\kappa} Q(\mathbf{G}, \mathbf{G}), \tag{2.8}$$

where $L_{\mathbf{M}}$ is the linearized collision operator defined by

$$L_{\mathbf{M}} g = L_{\mathbf{M}_{[\rho,u,\theta]}} g \equiv Q(\mathbf{M}_{[\rho,u,\theta]} + g, \mathbf{M}_{[\rho,u,\theta]} + g) - Q(g,g). \tag{2.9}$$

From (2.8) we have

$$\mathbf{G} = \kappa L_{\mathbf{M}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi \cdot \nabla_x \mathbf{M})) + L_{\mathbf{M}}^{-1}(\kappa(\partial_t \mathbf{G} + \mathbf{P}_1^{\mathbf{M}} \xi \cdot (\nabla_x \mathbf{G})) - Q(\mathbf{G}, \mathbf{G})) = \kappa L_{\mathbf{M}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi \cdot \nabla_x \mathbf{M})) + \Theta. \tag{2.10}$$

By substituting (2.10) into (2.7) yields the following fluid-type system for the macroscopic components:

$$\rho_t + \mathrm{div}_x\, m = 0,$$

$$m_t^i + \left(\sum_{j=1}^3 u^j m^i \right)_{x^j} + p_{x^i} + \kappa \int_{\mathbf{R}^3} \psi_i(\xi)(\xi \cdot \nabla_x L_{\mathbf{M}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi \cdot \nabla_x \mathbf{M}))) \mathrm{d}\xi$$

$$+ \int_{\mathbf{R}^3} \psi_i(\xi)(\xi \cdot \nabla_x \Theta) \mathrm{d}\xi = 0, \quad i = 1,2,3,$$

$$\left[\rho\left(\frac{|u|^2}{2}+\mathcal{E}\right)\right]_t+\sum_{j=1}^{3}\left\{u^j\left[\rho\left(\frac{|u|^2}{2}+\mathcal{E}\right)+p\right]\right\}_{x^j}+\kappa\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}}^{-1}(\mathrm{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M})))\mathrm{d}\xi$$
$$+\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x\Theta)\mathrm{d}\xi=0. \tag{2.11}$$

Notice also that in the above system, the terms

$$-\kappa\int_{\mathbf{R}^3}\psi_i(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M})))\mathrm{d}\xi$$

$$=-\kappa\int_{\mathbf{R}^3}\psi_i(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}_{[\rho,u,\theta]}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M}_{[\rho,u,\theta]})))\mathrm{d}\xi$$

$$=-\kappa\int_{\mathbf{R}^3}\psi_i(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}_{[1,u,\theta]}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M}_{[1,u,\theta]})))\mathrm{d}\xi,\quad i=1,2,3,$$

$$-\kappa\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M})))\mathrm{d}\xi$$

$$=-\kappa\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}_{[\rho,u,\theta]}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M}_{[\rho,u,\theta]})))\mathrm{d}\xi$$

$$=-\kappa\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x L_{\mathbf{M}_{[1,u,\theta]}}^{-1}(\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{M}_{[1,u,\theta]})))\mathrm{d}\xi$$

are the viscosity and heat conductivity terms which are the same as those in the compressible Navier-Stokes equations; and they are independent of the density gradient $\nabla_x\rho$. In fact, with the Burnett functions A and B, the viscosity coefficient $\mu(\theta)$ and heat conductivity coefficient $\kappa(\theta)$ can be represented by

$$A_j(\xi)=\frac{|\xi|^2-5}{2}\xi^j,\quad j=1,2,3,$$

$$B_{ij}(\xi)=\xi^i\xi^j-\tfrac{1}{3}\delta_{ij}|\xi|^2,\quad i,j=1,2,3,$$
$$\mu(\theta)=-\kappa R\theta\int_{\mathbf{R}^3}B_{ij}\left(\frac{\xi}{\sqrt{R\theta}}\right)L_{\mathbf{M}_{[1,u,\theta]}}^{-1}\left(B_{ij}\left(\frac{\xi}{\sqrt{R\theta}}\right)\mathbf{M}_{[1,u,\theta]}\right)\mathrm{d}\xi>0,\quad i\neq j, \tag{2.12}$$

$$\kappa(\theta)=-\kappa R^2\theta\int_{\mathbf{R}^3}A_l\left(\frac{\xi}{\sqrt{R\theta}}\right)L_{\mathbf{M}_{[1,u,\theta]}}^{-1}\left(A_l\left(\frac{\xi}{\sqrt{R\theta}}\right)\mathbf{M}_{[1,u,\theta]}\right)\mathrm{d}\xi>0,$$

and the fluid-type system (2.11) can be rewritten as

$$\rho_t+\mathrm{div}_x\, m=0,$$

$$m_t^i+\sum_{j=1}^{3}(u^j m^i)_{x^j}+p_{x^i}=\sum_{j=1}^{3}\left[\mu(\theta)\left(u^i_{x^j}+u^j_{x^i}-\tfrac{2}{3}\delta_{ij}\,\mathrm{div}_x\, u\right)\right]_{x^j}-\int_{\mathbf{R}^3}\psi_i(\xi)(\xi\cdot\nabla_x\Theta)\mathrm{d}\xi,\quad i=1,2,3,$$

$$\left[\rho\left(\tfrac{1}{2}|u|^2+\mathcal{E}\right)\right]_t+\sum_{j=1}^{3}\left(u^j\left(\rho\left(\tfrac{1}{2}|u|^2+\mathcal{E}\right)+p\right)\right)_{x^j}=\sum_{i,j=1}^{3}\left\{\mu(\theta)u^i\left(u^i_{x^j}+u^j_{x^i}-\tfrac{2}{3}\delta_{ij}\,\mathrm{div}_x\,u\right)\right\}_{x^j}$$
$$+\sum_{j=1}^{3}\left(\kappa(\theta)\theta_{x^j}\right)_{x^j}-\int_{\mathbf{R}^3}\psi_4(\xi)(\xi\cdot\nabla_x\Theta)\mathrm{d}\xi. \tag{2.13}$$

From this fluid-type system, one can easily see the structure of the compressible Euler and the compressible Navier-Stokes equations. For instance, when the Knudsen number κ is set zero, the system (2.13) becomes the compressible Euler equations. On the other hand, when Θ is set to be zero in (2.13), it becomes the compressible Navier-Stokes equations. These fluid equations as derived through the Hilbert and Chapman-Enskog expansions are approximations to the Boltzmann equation.[3] However, the above system is part of the Boltzmann equation. Nevertheless, this reformulation is consistent in spirit with these expansions in that the higher order terms beyond first order in the expansions must be microscopic. The above analysis also indicates that if we deduce the compressible Navier-Stokes equations from the Boltzmann equation, the viscosity coefficient $\mu(\theta)>0$ and the heat conductivity coefficient $\kappa(\theta)>0$ are smooth functions of the temperature θ.

III. ENERGY METHOD

This section is devoted to the energy method for the Boltzmann equation (1.1). For simplicity, we assume from now on that the Knudsen number $\kappa=1$.

We first state some basic inequalities for later use. The first lemma is concerned with some inequalities of Sobolev type.

Lemma 3.1: For $g(x)\in H^1(\mathbf{R}^3)$, we have

$$\|g(x)\|_{L^6(\mathbf{R}^3)}\leqslant C_0\|\nabla_x g(x)\|, \tag{3.1}$$

where C_0 is a positive constant independent of $g(x)$. Consequently, for $g(x)\in H^2(\mathbf{R}^3)$, there exists a positive constant C_1 independent of $g(x)$ such that

$$\|g(x)\|_{L^\infty(\mathbf{R}^3)}\leqslant C_1\|\nabla_x g(x)\|_1,$$
$$\|g(x)\|_{L^4(\mathbf{R}^3)}\leqslant C_1\|\nabla_x g(x)\|^{\frac{3}{4}}\|g(x)\|^{\frac{1}{4}}. \tag{3.2}$$

Here and in the sequel, $\|\cdot\|$ and $\|\cdot\|_s$ denote the standard $L^2(\mathbf{R}^3)$-norm and $H^s(\mathbf{R}^3)$-norm, respectively.

In the following, we will give some inequalities on the nonlinear and linearized collision operators $Q(f,f)$ and $L_{\mathbf{M}}\mathbf{G}$. The first lemma is from Ref. 5.

Lemma 3.2: Suppose that $B(|\xi-\xi_*|,\theta)$ satisfies (A1) and (A2), then there exists a positive constant $C_2>0$ such that

$$\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}Q(f,g)^2}{\tilde{\mathbf{M}}}\mathrm{d}\xi\leqslant C_2\left\{\int_{\mathbf{R}^3}\frac{\nu(\xi)f^2}{\tilde{\mathbf{M}}}\mathrm{d}\xi\cdot\int_{\mathbf{R}^3}\frac{g^2}{\tilde{\mathbf{M}}}\mathrm{d}\xi+\int_{\mathbf{R}^3}\frac{f^2}{\tilde{\mathbf{M}}}\mathrm{d}\xi\cdot\int_{\mathbf{R}^3}\frac{\nu(\xi)g^2}{\tilde{\mathbf{M}}}\mathrm{d}\xi\right\}, \tag{3.3}$$

where $\tilde{\mathbf{M}}$ is any Maxwellian such that the above integrals are well defined.

As pointed out before, to perform the energy estimates for the Boltzmann equation (1.1), for $\mathbf{P}_1^{\mathbf{M}_0}f$, the microscopic projection of its solution $f(t,x,\xi)$ with respect to a given Maxwellian $\mathbf{M}_0$, the dissipative effect through the microscopic **H** theorem should be used. In short, the microscopic **H** theorem states that the linearized collision operator $L_{\mathbf{M}_0}$ around a fixed Maxwellian state $\mathbf{M}_0$ is negative definite on the nonfluid element $\mathbf{P}_1^{\mathbf{M}_0}f$,[2] i.e.,

$$-\int_{\mathbf{R}^3}\frac{\mathbf{P}_1^{\mathbf{M}_0} f L_{\mathbf{M}_0}(\mathbf{P}_1^{\mathbf{M}_0} f)}{\mathbf{M}_0}\mathrm{d}\xi \geqslant \sigma\int_{\mathbf{R}^3}\frac{\nu(\xi)|\mathbf{P}_1^{\mathbf{M}_0} f|^2}{\mathbf{M}_0}\mathrm{d}\xi,$$

for a positive constant σ. Furthermore, one can vary the background for linearization and the weight function. That is, we also have the following result whose proof is based on Lemma 3.2, cf. Ref. 16.

Lemma 3.3: If $\theta/2<\widetilde{\theta}$ and the assumptions in Lemma 3.2 are satisfied, then there exist two positive constants $\bar{\sigma}=\bar{\sigma}(u,\theta;\widetilde{u},\widetilde{\theta})$ and $\eta_0=\eta_0(u,\theta;\widetilde{u},\widetilde{\theta})$ such that if $|u-\widetilde{u}|+|\theta-\widetilde{\theta}|<\eta_0$, we have for $h(\xi)\in\mathcal{N}^{\perp}$,

$$-\int_{\mathbf{R}^3}\frac{hL_{\mathbf{M}}h}{\widetilde{\mathbf{M}}}\mathrm{d}\xi \geqslant \bar{\sigma}\int_{\mathbf{R}^3}\frac{\nu(\xi)h^2}{\widetilde{\mathbf{M}}}\mathrm{d}\xi. \tag{3.4}$$

Here $\mathbf{M}\equiv\mathbf{M}_{[\rho,u,\theta]}(\xi)$, $\widetilde{\mathbf{M}}=\widetilde{\mathbf{M}}_{[\widetilde{\rho},\widetilde{u},\widetilde{\theta}]}(\xi)$ and

$$\mathcal{N}^{\perp}=\left\{f(\xi):\quad \int_{\mathbf{R}^3}\psi_j(\xi)f(\xi)\mathrm{d}\xi=0,\quad j=0,1,2,3,4\right\}.$$

Remark 3.1: The constant η_0 is some positive constant depending on the first nonzero eigenvalue of the linearized operator $L_{\mathbf{M}}$. Note that η_0 is not necessary to be small, cf. Ref. 16.

A direct consequence of Lemma 3.3 and the Cauchy inequality is the following corollary, cf. Ref. 16.

Corollary 3.1: Under the assumptions in Lemma 3.3, we have for $h(\xi)\in\mathcal{N}^{\perp}$,

$$\int_{\mathbf{R}^3}\frac{\nu(\xi)}{\widetilde{\mathbf{M}}}|L_{\mathbf{M}}^{-1}h|^2\,\mathrm{d}\xi \leqslant \bar{\sigma}^{-2}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}h^2(\xi)}{\widetilde{\mathbf{M}}}\mathrm{d}\xi. \tag{3.5}$$

Before performing the energy estimates for the Boltzmann equation (1.1), we first give the function space for the solutions considered in this paper

$$\mathbf{H}_{x,\xi}^N([0,T])=\left\{g(t,x,\xi)\;\middle|\;\begin{array}{c}\dfrac{\partial_t^\beta\partial_x^\alpha g(t,x,\xi)}{\sqrt{\overline{\mathbf{M}}(\xi)}}\in\mathbf{BC}_t([0,T],L^2_{x,\xi}(\mathbf{R}^3\times\mathbf{R}^3))\\ \dfrac{\sqrt{\nu(\xi)}\partial_t^\beta\partial_x^\alpha g(t,x,\xi)}{\sqrt{\overline{\mathbf{M}}(\xi)}}\in L^2_{t,x,\xi}([0,T]\times\mathbf{R}^3\times\mathbf{R}^3),\quad \text{for } |\alpha|+|\beta|>0\\ 0\leqslant t\leqslant T,\quad |\alpha|+|\beta|\leqslant N\end{array}\right\}.$$

Here $g(t,x,\xi)=f(t,x,\xi)-\overline{\mathbf{M}}(\xi)$.

Now we deduce an estimate on the conserved quantities $\rho(t,x)$, $m(t,x)\equiv\rho(t,x)u(t,x)$, $\rho(t,x)\left(\frac{1}{2}u^2(t,x)+\mathcal{E}(t,x)\right)$ by using the analytic techniques for the systems of conservation laws, cf. Refs. 13, 15, and 18, based on the following *a priori* assumption:

$$\begin{aligned}N(t)^2\equiv&\sup_{0\leqslant\tau\leqslant t}\sum_{|\alpha|+|\beta|\leqslant 4}\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(\rho(\tau,x)-\bar{\rho},u(\tau,x),\theta(\tau,x)-\bar{\theta})|^2\,\mathrm{d}x\\&+\sup_{0\leqslant\tau\leqslant t}\sum_{|\alpha|+|\beta|\leqslant 4}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f(\tau,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\\&+\sum_{1\leqslant|\alpha|+|\beta|\leqslant 4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta(f(\tau,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\leqslant\varepsilon^2.\end{aligned}\tag{3.6}$$

Here, the small parameter $\varepsilon>0$ will be given in terms of the strength of the initial data $f_0(x,\xi)$,

and the discussion is in $\mathbf{H}^4_{x,\xi}([0,T])$ space which can be readily generalized to the $\mathbf{H}^s_{x,\xi}([0,T])$ space for $s>4$.

It is easy to see from (3.6), the conservation laws (2.7) and Sobolev's inequality that

$$N(0) \leqslant O(1)\mathcal{E}(f_0) \quad \text{with } \mathcal{E}(f_0)^2 \equiv \sum_{|\alpha|+|\beta|\leqslant 4} \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{|\partial_x^\alpha \partial_t^\beta (f_0(x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x \tag{3.7}$$

and

$$\begin{aligned} &\sup_{0\leqslant\tau\leqslant t, x\in\mathbf{R}^3}\left(\sum_{|\alpha|+|\beta|\leqslant 2} |\partial_x^\alpha \partial_t^\beta(\rho(\tau,x)-\bar{\rho}, u(\tau,x), \theta(\tau,x)-\bar{\theta})|^2\right) \\ &\quad + \sup_{0\leqslant\tau\leqslant t, x\in\mathbf{R}^3}\left(\sum_{|\alpha|+|\beta|\leqslant 2}\int_{\mathbf{R}^3} \frac{|\partial_x^\alpha \partial_t^\beta (f(\tau,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\right) \leqslant O(1)\varepsilon^2. \end{aligned} \tag{3.8}$$

Here and in the sequel, we will use $O(1)$ to denote a generic positive constant independent of t and x.

Let $\mathbf{m}=(m^0,m,m^4)^t=(m^0,m^1,m^2,m^3,m^4)=\left(\rho,m,\rho\left(\frac{1}{2}u^2+\mathcal{E}\right)\right)^t$, as in Ref. 15, we construct a convex entropy-entropy flux pair (η,q) around the global Maxwellian $\overline{\mathbf{M}}$ as follows:

$$\begin{aligned} \eta &= \tfrac{3}{2}\left\{\rho\theta - \bar{\theta}\rho S + \rho\left[\left(\bar{S}-\tfrac{5}{3}\right)\bar{\theta}+\frac{|u|^2}{2}\right]+\tfrac{2}{3}\bar{\rho}\bar{\theta}\right\}, \\ q_j &= u_j\eta + u_j(\rho\theta-\bar{\rho}\bar{\theta}), \quad j=1,2,3. \end{aligned} \tag{3.9}$$

Notice that for $\mathbf{m}$ in any closed bounded region $\mathcal{D}\subset\Sigma=\{\mathbf{m}:\rho>0,\theta>0\}$, there exists a positive constant C_3 depending on $\mathcal{D}$ such that the entropy-entropy flux thus constructed satisfies (cf. Refs. 15 and 16)

$$c_3^{-1}|\mathbf{m}-\overline{\mathbf{m}}|^2 \leqslant \eta \leqslant C_3|\mathbf{m}-\overline{\mathbf{m}}|^2. \tag{3.10}$$

The (η,q_1,q_2,q_3) solves the following partial differential equation:

$$\begin{aligned} \eta_t + \mathrm{div}_x\, q &= \sum_{i,j=1}^3 \eta_{m^i}(\mathbf{m})\left[\mu(\theta)\left(u^i_{x^j}+u^j_{x^i}-\tfrac{2}{3}\delta_{ij}\,\mathrm{div}_x\, u\right)\right]_{x^j} \\ &\quad + \sum_{i,j=1}^3 \eta_{m^4}(\mathbf{m})\left[\mu(\theta)u^i\left(u^i_{x^j}+u^j_{x^i}-\tfrac{2}{3}\delta_{ij}\,\mathrm{div}_x\, u\right)\right]_{x^j} + \sum_{j=1}^3 \eta_{m^4}(\mathbf{m})(\kappa(\theta)\theta_{x^j})_{x^j} \\ &\quad - \int_{\mathbf{R}^3} \nabla_{\mathbf{m}}\eta(\mathbf{m})\cdot(0,\psi_1(\xi),\psi_2(\xi),\psi_3(\xi),\psi_4(\xi))(\xi\cdot\nabla_x\Theta)\mathrm{d}\xi. \end{aligned} \tag{3.11}$$

Since

$$\nabla_{\mathbf{m}}\eta(\mathbf{m}) = -\frac{3}{2}\bar{\theta}\left(S+\frac{|u|^2}{2\theta}-\bar{S}, -\frac{u^1}{\theta}, -\frac{u^2}{\theta}, -\frac{u^3}{\theta}, -\frac{\theta-\bar{\theta}}{\theta\bar{\theta}}\right), \tag{3.12}$$

we have by integrating (3.11) with respect to t and x over $[0,t]\times\mathbf{R}^3$, and using the Cauchy-Schwarz inequality and (3.10) that

$$\|(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^2(t) + \int_0^t \|\nabla_x(u,\theta)\|^2(\tau)\mathrm{d}\tau$$

$$\leqslant O(1)\|(\rho_0(x)-\bar{\rho},u_0(x),\theta_0(x)-\bar{\theta})\|^2+O(1)\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}|\xi|^4|\Theta|^2\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau. \tag{3.13}$$

If we choose ε sufficiently small such that

$$\varepsilon<\min\left\{\frac{\eta_0}{2},\bar{\theta}\right\}, \tag{3.14}$$

then for any θ_- satisfying

$$\bar{\theta}<\theta_-<\bar{\theta}+\varepsilon, \tag{3.15}$$

we have

$$\begin{gathered}\theta\leqslant\bar{\theta}+|\theta-\bar{\theta}|<\bar{\theta}+\varepsilon<2\bar{\theta}<2\theta_-,\\ |u|+|\theta-\theta_-|\leqslant(|u|+|\theta-\bar{\theta}|)+\theta_--\bar{\theta}<2\varepsilon<\eta_0.\end{gathered} \tag{3.16}$$

Denote $\mathbf{M}_-=\mathbf{M}_{[\bar{\rho},0,\theta_-]}$, we have from Lemma 3.2, Corollary 3.1, (1.3), (2.10), (3.6), (3.8), and (3.16) that

$$\begin{aligned}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}|\xi|^4|\Theta|^2\,\mathrm{d}\xi\,\mathrm{d}x&\leqslant O(1)\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|L_{\mathbf{M}}^{-1}(\mathbf{G}_t\mathbf{P}_1^{\mathbf{M}}(\xi\cdot\nabla_x\mathbf{G})-Q(\mathbf{G},\mathbf{G}))|^2}{\mathbf{M}_-}\mathrm{d}\xi\,\mathrm{d}x\\ &\leqslant O(1)\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}(|\mathbf{G}_t|^2|\xi|^2|\nabla_x\mathbf{G}|^2+|Q(\mathbf{G},\mathbf{G})|^2)}{\mathbf{M}_-}\mathrm{d}\xi\,\mathrm{d}x\\ &\leqslant O(1)\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{(|\mathbf{G}_t|^2+|\nabla_x\mathbf{G}|^2)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\\ &\quad+O(1)\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)\mathbf{G}^2}{\mathbf{M}_-}\mathrm{d}\xi\int_{\mathbf{R}^3}\frac{\mathbf{G}^2}{\mathbf{M}_-}\mathrm{d}\xi\,\mathrm{d}x\\ &\leqslant O(1)\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{1}{\underline{\underline{\mathbf{M}}}}(\mathbf{G}_t^2+|\nabla_x\mathbf{G}|^2+\varepsilon^2\mathbf{G}^2)\mathrm{d}\xi\,\mathrm{d}x.\end{aligned} \tag{3.17}$$

Setting (3.13) and (3.17) together gives

$$\begin{aligned}&\|(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^2(t)+\int_0^t\|\nabla_x(u,\theta)\|^2(\tau)\mathrm{d}\tau\\ &\leqslant O(1)\|(\rho_0(x)-\bar{\rho},u_0(x),\theta_0(x)-\bar{\theta})\|^2\\ &\quad+O(1)\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{1}{\underline{\underline{\mathbf{M}}}}(\mathbf{G}_t^2+|\nabla_x\mathbf{G}|^2+\varepsilon^2\mathbf{G}^2)\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau.\end{aligned} \tag{3.18}$$

To obtain the higher order estimates on the conserved quantities, we first note that the system (2.13) can be rewritten as

$$\rho_t=-(\rho-\bar{\rho})\mathrm{div}_x\,u-\nabla_x(\rho-\bar{\rho})\cdot u-\bar{\rho}\,\mathrm{div}_x\,u, \tag{3.19a}$$

$$u_t^i + \sum_{j=1}^{3} u^j u_{x^j}^i + \frac{2}{3\rho}(\rho\theta - \bar{\rho}\bar{\theta})_{x^i} = -\int_{\mathbf{R}^3} \frac{\psi_i(\xi\cdot\nabla_x\Theta)}{\rho}\mathrm{d}\xi + \frac{1}{\rho}\sum_{j=1}^{3}\left\{\mu(\theta)\left(u_{x^j}^i + u_{x^i}^j - \frac{2}{3}\delta_{ij}\mathrm{div}_x u\right)\right\}_{x^j}, \tag{3.19b}$$

$$i = 1,2,3,$$

$$\theta_t + \sum_{j=1}^{3}\left(u^j\theta_{x^j} + \frac{2}{3}\theta u_{x^j}^j\right) = -\int_{\mathbf{R}^3}\frac{\psi_4 - \xi\cdot u}{\rho}(\xi\cdot\nabla_x\Theta)\mathrm{d}\xi + \frac{1}{\rho}\left\{\sum_{j=1}^{3}(\kappa(\theta)\theta_{x^j})_{x^j} + \frac{1}{2}\mu(\theta)\sum_{i,j=1}^{3}(u_{x^j}^i + u_{x^i}^j)^2 - \frac{2}{3}\mu(\theta)(\mathrm{div}_x u)^2\right\}. \tag{3.19c}$$

Similar to the analysis in Ref. 18, 14, and 20 for the compressible Navier-Stokes equations, we have by applying $\partial^\gamma(1\leqslant|\gamma|\leqslant 3)$ to (3.19b) and (3.19c), multiplying the resulting identities by $\rho\partial^\gamma u_i$ and $\bar{\rho}/\theta\partial^\gamma\theta$, taking the summation with respect to i from 1 to 3, and integrating the resulting equations with respect to t and x over $[0,t]\times\mathbf{R}^3$ that, for $j=1,2,3$,

$$\begin{aligned}
&\sum_{|\alpha|+|\beta|=j}\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho},u,\theta)|^2\,\mathrm{d}x + \sum_{|\alpha|+|\beta|=j}\int_0^t\int_{\mathbf{R}^3}|\nabla_x\partial_x^\alpha\partial_t^\beta(u,\theta)|^2\,\mathrm{d}x\,\mathrm{d}\tau\\
&\leqslant O(1)\varepsilon(f_0)^2 + O(1)\sum_{|\gamma|=j}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{(|\partial_x^\alpha\partial_t^\beta\mathbf{G}_t|^2 + |\nabla_x\partial_x^\alpha\partial_t^\beta\mathbf{G}|^2)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\
&\quad + O(1)\varepsilon\sum_{1\leqslant|\alpha|+|\beta|\leqslant j+1}\int_0^t\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho},u,\theta)|^2\,\mathrm{d}x\,\mathrm{d}\tau\\
&\quad + O(1)\varepsilon\sum_{|\alpha|+|\beta|\leqslant j}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathbf{G}|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau.
\end{aligned} \tag{3.20}$$

It is worthy to point out that, compared with those estimates in Ref. 18, the only difference is that we need to deal with the terms containing Θ. This can be estimated suitably as in the proof of (3.17) by using Lemma 3.2, Corollary 3.1, (1.3), (2.10), (3.6), (3.8), and (3.16) and the following basic estimate on the collision operator $Q(f,g)$ (cf. Corollary 3.1 of Ref. 22),

$$\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}|\partial_x^\alpha\partial_t^\beta Q(\mathbf{G},\mathbf{G})|^2}{\mathbf{M}_-}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau \leqslant O(1)\varepsilon\sum_{|\alpha'|+|\beta'|\leqslant 4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^{\alpha'}\partial_t^{\beta'}\mathbf{G}|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau.$$

Here $|\alpha|+|\beta|\leqslant 4$.

To get the $L^2_{t,x}$ estimates on $\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho})$ for $1\leqslant|\alpha|+|\beta|\leqslant 4$, we use the conservation laws (2.13) as in Refs. 13 and 15 to deduce that

$$\sum_{|\alpha|+|\beta|=j+1}\int_0^t\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho})|^2\,\mathrm{d}x\,\mathrm{d}\tau \tag{3.21}$$

$$\leqslant O(1)\varepsilon(f_0)^2 + O(1)\int_{\mathbf{R}^3}\left(\sum_{|\alpha|+|\beta|=j+1}|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho})|^2 + \sum_{|\alpha|+|\beta|=j}|\partial_x^\alpha\partial_t^\beta u|^2\right)\mathrm{d}x$$
$$+ O(1)\sum_{1\leqslant|\alpha|+|\beta|\leqslant j+1}\int_0^t\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(u-\theta)|^2\,\mathrm{d}x\,\mathrm{d}\tau$$
$$+ O(1)\varepsilon\sum_{1\leqslant|\alpha|+|\beta|\leqslant j}\int_0^t\int_{\mathbf{R}^3}|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho})|^2\,\mathrm{d}x\,\mathrm{d}\tau$$
$$+ O(1)\sum_{|\alpha|+|\beta|\leqslant j+1}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathrm{G}|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau,\quad j=0,1,2,3.$$

A suitable linear combination of (3.18), (3.20), and (3.21) yields an estimate on the conserved quantities, $\rho, m, \rho\frac{1}{2}|u|^2+\varepsilon$ which is controlled by $\mathbf{G}$ besides the initial data, the microscopic projection of the solution $f(t,x,\xi)$ of the Boltzmann equation (1.1) with respect to the local Maxwellian $\mathbf{M}$.

Lemma 3.4: Under the a priori assumption (3.6) *we have*

$$\sum_{|\alpha|+|\beta|\leqslant 3}\|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^2(t) + \sum_{1\leqslant|\alpha|+|\beta|\leqslant 4}\int_0^t\|\partial_x^\alpha\partial_t^\beta(\rho,u,\theta)\|^2(\tau)\mathrm{d}\tau$$
$$\leqslant O(1)\varepsilon(f_0)^2 + O(1)\sum_{|\alpha|+|\beta|\leqslant 4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathbf{G}|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau. \tag{3.22}$$

Since we want to close the energy estimates for the solution $f(t,x,\xi)$ of the Boltzmann equation (1.1) by performing the energy estimates on the original equation (1.1) with respect to the global Maxwellian $\overline{\mathbf{M}}$, we need to transform the estimates on $\mathbf{G}$, the microscopic projection of $f(t,x,\xi)$ with respect to the local Maxwellian $\mathbf{M}$ into $\mathbf{P}_1^{\overline{\mathbf{M}}}f$, the microscopic projection of $f(t,x,\xi)$ with respect to the global Maxwellian $\overline{\mathbf{M}}$. For this purpose, by noticing

$$\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{G} = \mathbf{G},\quad \mathbf{P}_1^{\overline{\mathbf{M}}}f = \mathbf{G} + \mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M}, \tag{3.23}$$

we only need to obtain an estimate on $\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M}$ which is presented in the following lemma.

Lemma 3.5: Under the assumptions of Lemma 3.4, we can deduce

$$\int_{\mathbf{R}^3}\frac{\nu(\xi)^k|\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M}|^2}{\mathbf{M}_0}\mathrm{d}\xi \leqslant O(1)|(\rho-\bar{\rho},u,\theta-\bar{\theta})|^4. \tag{3.24}$$

Here $k>0$ *is any positive constant and* $\mathbf{M}_0=\mathbf{M}_{[\rho_0,u_0,\theta_0]}$ *can be any Maxwellian satisfying* $\theta_0 > \frac{1}{2}\max\{\theta,\bar{\theta}\}$.

Consequently, we have for all $|\alpha|+|\beta|\leqslant 4$ *that*

$$\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathbf{G}|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau \leqslant \int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}f|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau$$
$$+ O(1)\varepsilon\sum_{1\leqslant|\alpha|+|\beta|\leqslant 4}\int_0^t\|\partial_x^\alpha\partial_t^\beta(\rho,u,\theta)\|^2(\tau)\mathrm{d}\tau. \tag{3.25}$$

Proof: We only prove (3.24) since (3.25) follows immediately from (3.23), (3.24), Lemma 3.1 and the *a priori* assumption (3.6).

To prove (3.24), first notice that $\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M}$ is a smooth function of ρ, u, θ, and

$$\nabla_{(\rho,u,\theta)}\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M} = \mathbf{P}_1^{\overline{\mathbf{M}}}(\nabla_{(\rho,u,\theta)}\mathbf{M}).$$

Since

$$\mathbf{P}_1^{\overline{\mathbf{M}}}(\nabla_{(\rho,u,\theta)}\mathbf{M})|_{(\rho,u,\theta)=(\bar{\rho},0,\bar{\theta})} = 0,$$

we can easily deduce that $\mathbf{P}_1^{\overline{\mathbf{M}}}\mathbf{M}$ is quadratic with respect to $(\rho-\bar{\rho},u,\theta-\bar{\theta})$ and (3.24) follows immediately. This completes the proof of Lemma 3.5.

The following corollary is a direct consequence of Lemma 3.4 and Lemma 3.5.

Corollary 3.2: Under the assumptions in Lemma 3.3, we have

$$\sum_{|\alpha|+|\beta|\leqslant 3}\|\partial_x^\alpha\partial_t^\beta(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^2(t) + \sum_{1\leqslant|\alpha|+|\beta|\leqslant 4}\int_0^t\|\partial_x^\alpha\partial_t^\beta(\rho,u,\theta)\|^2(\tau)\mathrm{d}\tau$$

$$\leqslant O(1)\varepsilon(f_0)^2 + O(1)\sum_{|\alpha|+|\beta|\leqslant 4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}f|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau. \tag{3.26}$$

Now we can finalize the energy estimates on the solutions $f(t,x,\xi)$ of the Boltzmann equation (1.1). To this end, since $g(t,x,\xi)=f(t,x,\xi)-\overline{\mathbf{M}}(\xi)$ solves

$$g_t + \xi\cdot\nabla_x g = L_{\overline{\mathbf{M}}}(\mathbf{P}_1^{\overline{\mathbf{M}}}g) + Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_1^{\overline{\mathbf{M}}}g) + 2Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}})) + Q(\mathbf{P}_1^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}),\mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}})), \tag{3.27}$$

we have by applying $\partial_x^\alpha\partial_t^\beta(|\alpha|+|\beta|\leqslant 4)$ to (3.27) and integrating its product with $\partial_x^\alpha\partial_t^\beta g/\overline{\mathbf{M}}$ over $[0,t]\times\mathbf{R}\times\mathbf{R}^3$ that

$$\begin{aligned}\frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\Bigg|_0^t &= \int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta g\cdot\partial_x^\alpha\partial_t^\beta L_{\overline{\mathbf{M}}}(\mathbf{P}_1^{\overline{\mathbf{M}}}g)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\ &+\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta g\,.\,\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_1^{\overline{\mathbf{M}}}g)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\ &+2\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta g\,.\,\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}))}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\ &+\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta g\,.\,\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}),\mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}))}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau.\\ &:=\sum_{j=1}^4 I_j.\end{aligned} \tag{3.28}$$

Here $I_i(i=1,2,3,4)$ are the corresponding terms in the above equation without any ambiguity.

Since $\overline{\mathbf{M}}$ is independent of t and x, we have

$$\begin{aligned}\mathbf{P}_1^{\overline{\mathbf{M}}}(\partial_x^\alpha\partial_t^\beta g) &= \partial_x^\alpha\partial_t^\beta g\mathbf{P}_1^{\overline{\mathbf{M}}}g,\\ \partial_x^\alpha\partial_t^\beta L_{\overline{\mathbf{M}}}(\mathbf{P}_1^{\overline{\mathbf{M}}}g) &= L_{\overline{\mathbf{M}}}(\partial_x^\alpha\partial_t^\beta g\mathbf{P}_1^{\overline{\mathbf{M}}}g).\end{aligned} \tag{3.29}$$

Thus from Lemma 3.2, Lemma 3.3, and (3.6), I_1 and I_2 can be estimated as follows:

$$I_1=\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g\cdot L_{\overline{\mathbf{M}}}(\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\leqslant-\sigma\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau,\tag{3.30}$$

$$\begin{aligned}I_2&=\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g\cdot\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_1^{\overline{\mathbf{M}}}g)}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\leqslant\frac{\sigma}{4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau+O(1)\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}|\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_1^{\overline{\mathbf{M}}}g)|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\leqslant\frac{\sigma}{4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\quad+O(1)\varepsilon\sum_{|\alpha|+|\beta'|\leqslant4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}|\partial_x^{\alpha'}\partial_t^{\beta'}\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau.\end{aligned}\tag{3.31}$$

Here we have used the inequality

$$\begin{aligned}&\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)^{-1}|\partial_x^\alpha\partial_t^\beta Q(\mathbf{P}_1^{\overline{\mathbf{M}}}g,\mathbf{P}_1^{\overline{\mathbf{M}}}g)|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\qquad\leqslant O(1)\varepsilon\sum_{|\alpha|+|\beta'|\leqslant4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^{\alpha'}\partial_t^{\beta'}\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau,\end{aligned}\tag{3.32}$$

which follows similarly to the Corollary 3.1 of Ref. 22.

For I_3 and I_4, we want to prove the following estimates;

$$\begin{aligned}I_3&\leqslant\frac{\sigma}{4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\quad+O(1)\varepsilon\sum_{|\alpha'|+|\beta'|\leqslant4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^{\alpha'}\partial_t^{\beta'}\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau\\&\quad+O(1)\varepsilon\sum_{1\leqslant|\alpha'|+|\beta'|\leqslant4}\int_0^t\int_{\mathbf{R}^3}|\partial_x^{\alpha'}\partial_t^{\beta'}(\rho,u,\theta)|^2\mathrm{d}x\,\mathrm{d}\tau.\end{aligned}\tag{3.33}$$

and

$$I_4\leqslant\frac{\sigma}{4}\int_0^t\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{\nu(\xi)|\partial_x^\alpha\partial_t^\beta\mathbf{P}_1^{\overline{\mathbf{M}}}g|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}\tau+O(1)\varepsilon\sum_{1\leqslant|\alpha'|+|\beta'|\leqslant4}\int_0^t\int_{\mathbf{R}^3}|\partial_x^{\alpha'}\partial_t^{\beta'}(\rho,u,\theta)|^2\mathrm{d}x\,\mathrm{d}\tau.\tag{3.34}$$

For illustration, we only prove (3.34) because similar argument holds for (3.33). For this, we have from Lemma 3.2, (3.6), (3.8), and (3.29) that

$$
\begin{aligned}
I_4 = & \sum_{(\alpha',\beta')\leqslant(\alpha,\beta)} C_{\alpha,\beta}^{\alpha',\beta'} \int_0^t \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \\
& \times \frac{\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g \cdot Q(\partial_x^{\alpha'} \partial_t^{\beta'} \mathbf{P}_1^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}), \partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'} \mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}))}{\overline{\mathbf{M}}} \mathrm{d}\xi \, \mathrm{d}x \, \mathrm{d}\tau \\
\leqslant & \frac{\sigma}{4} \int_0^t \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\nu(\xi) |\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \, \mathrm{d}x \, \mathrm{d}\tau \\
& + O(1) \sum_{(\alpha',\beta')\leqslant(\alpha,\beta)} \int_0^t \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\nu(\xi)^{-1} |Q(\partial_x^{\alpha'} \partial_t^{\beta'} \mathbf{P}_1^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}), \partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'} \mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}}))|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \, \mathrm{d}x \, \mathrm{d}\tau \\
\leqslant & \frac{\sigma}{4} \int_0^t \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\nu(\xi) |\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \, \mathrm{d}x \, \mathrm{d}\tau \\
& + O(1) \sum_{(\alpha',\beta')\leqslant(\alpha,\beta)} \int_0^t \int_{\mathbf{R}^3} \left(\int_{\mathbf{R}^3} \frac{\nu(\xi)^{-1} |\partial_x^{\alpha'} \partial_t^{\beta'} \mathbf{P}_1^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}})|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \right. \\
& \left. \cdot \int_{\mathbf{R}^3} \frac{|\partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'} \mathbf{P}_0^{\overline{\mathbf{M}}}(\mathbf{M}-\overline{\mathbf{M}})|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \right) \mathrm{d}x \, \mathrm{d}\tau \\
\leqslant & \frac{\sigma}{4} \int_0^t \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\nu(\xi) |\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi \, \mathrm{d}x \, \mathrm{d}\tau \\
& + O(1)\varepsilon \sum_{1\leqslant|\alpha'|+|\beta'|\leqslant 4} \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2 \, \mathrm{d}x \, \mathrm{d}\tau \\
& + O(1) \sum_{(\alpha',\beta')\leqslant(\alpha,\beta)} \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2 |\partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'}(\rho,u,\theta)|^2 \mathrm{d}x \, \mathrm{d}\tau. \qquad (3.35)
\end{aligned}
$$

Denote

$$
I_{\alpha,\beta}^{\alpha',\beta'} = \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2 |\partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'}(\rho,u,\theta)|^2 \mathrm{d}x \, \mathrm{d}\tau. \qquad (3.36)
$$

We estimate $I_{\alpha,\beta}^{\alpha',\beta'}$ by considering the following three cases.

Case 1: $(\alpha',\beta')=(\alpha,\beta)=(0,0)$.

For this case, we have from Lemma 3.1 and the *a priori* assumption (3.6) that

$$
\begin{aligned}
I_{0,0}^{0,0} = & \int_0^t \int_{\mathbf{R}^3} |(\rho-\bar{\rho},u,\theta-\bar{\theta})|^4 \mathrm{d}x \, \mathrm{d}\tau \\
\leqslant & O(1) \int_0^t \|(\rho-\bar{\rho},u,\theta-\bar{\theta})\| \|\nabla_x(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^3 \mathrm{d}\tau \\
\leqslant & O(1)\varepsilon \int_0^t \|\nabla_x(\rho-\bar{\rho},u,\theta-\bar{\theta})\|^2 \mathrm{d}\tau. \qquad (3.37)
\end{aligned}
$$

Case 2: $0\leqslant|\alpha'|+|\beta'|\leqslant 2$, $(\alpha',\beta')<(\alpha,\beta)$.

In this case, we have from (3.8) that

$$I_{\alpha,\beta}^{\alpha',\beta'} \leqslant O(1)\varepsilon \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha-\alpha'} \partial_t^{\beta-\beta'}(\rho,u,\theta)|^2 \mathrm{d}x\, \mathrm{d}\tau. \tag{3.38}$$

Case 3: $2<|\alpha'|+|\beta'|\leqslant 4$.

In this case, we have $|\alpha-\alpha'|+|\beta-\beta'|\leqslant 1$ because $|\alpha|+|\beta|\leqslant 4$. Similar to Case 2, we have

$$I_{\alpha,\beta}^{\alpha',\beta'} \leqslant O(1)\varepsilon \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2 \mathrm{d}x\, \mathrm{d}\tau. \tag{3.39}$$

Setting (3.37), (3.38), and (3.39) together yields

$$I_{\alpha,\beta}^{\alpha',\beta'} \leqslant O(1)\varepsilon \sum_{1\leqslant|\alpha'|+|\beta'|\leqslant 4} \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2 \mathrm{d}x\, \mathrm{d}\tau. \tag{3.40}$$

Plugging (3.40) into (3.35) gives (3.34) immediately. This completes the proof of (3.33) and (3.34).

Now substituting (3.30), (3.31), (3.33), and (3.34) into (3.28) yields

$$\begin{aligned}
&\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{|\partial_x^\alpha \partial_t^\beta g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x + \int_0^t \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\nu(\xi)|\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}\tau \\
&\quad \leqslant O(1)\varepsilon (f_0)^2 + O(1)\varepsilon \sum_{|\alpha'|+|\beta'|\leqslant 4} \int_0^t \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\nu(\xi)|\partial_x^{\alpha'} \partial_t^{\beta'} \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x\, \mathrm{d}\tau \\
&\quad + O(1)\varepsilon \sum_{1\leqslant|\alpha'|+|\beta'|\leqslant 4} \int_0^t \int_{\mathbf{R}^3} |\partial_x^{\alpha'} \partial_t^{\beta'}(\rho,u,\theta)|^2\, \mathrm{d}x\, \mathrm{d}\tau.
\end{aligned} \tag{3.41}$$

Thus

$$\begin{aligned}
&\sum_{|\alpha|+|\beta|\leqslant 4} \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{|\partial_x^\alpha \partial_t^\beta g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x + \sum_{|\alpha|+|\beta|\leqslant 4} \int_0^4 \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\nu(\xi)|\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} g|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x\, \mathrm{d}\tau \\
&\quad \leqslant O(1)\varepsilon (f_0)^2 + O(1)\varepsilon \sum_{1\leqslant|\alpha|+|\beta|\leqslant 4} \int_0^t \int_{\mathbf{R}^3} |\partial_x^\alpha \partial_t^\beta(\rho,u,\theta)|^2\, \mathrm{d}x\, \mathrm{d}\tau.
\end{aligned} \tag{3.42}$$

Multiplying (3.42) by a suitably large positive constant C_4 and adding the result to (3.26) yields

$$\begin{aligned}
&\sum_{|\alpha|+|\beta|\leqslant 4} \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{|\partial_x^\alpha \partial_t^\beta (f-\overline{\mathbf{M}})|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x + \sum_{|\alpha|+|\beta|\leqslant 4} \int_{\mathbf{R}^3} |\partial_x^\alpha \partial_t^\beta(\rho-\bar{\rho},u,\theta-\bar{\theta})|^2\, \mathrm{d}x \\
&\quad + \sum_{|\alpha|+|\beta|\leqslant 4} \int_0^t \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\nu(\xi)|\partial_x^\alpha \partial_t^\beta \mathbf{P}_1^{\overline{\mathbf{M}}} f|^2}{\overline{\mathbf{M}}} \mathrm{d}\xi\, \mathrm{d}x\, \mathrm{d}\tau + \sum_{1\leqslant|\alpha|+|\beta|\leqslant 4} \int_0^t \int_{\mathbf{R}^3} |\delta_x^\alpha \delta_t^\beta(\rho,u,\theta)|^2 \mathrm{d}x\, \mathrm{d}\tau \\
&\quad \leqslant O(1)\varepsilon (f_0)^2.
\end{aligned} \tag{3.43}$$

This closes the *a priori* assumption (3.6) provided that we choose $\delta_0>0$ sufficiently small such that

$$\begin{aligned}
&\varepsilon(f_0) < \delta_0, \\
&O(1)\delta_0^2 < \varepsilon^2.
\end{aligned} \tag{3.44}$$

The above analysis yields the following energy estimates for the solution $f(t,x,\xi)$ of the Boltzmann equation (1.1) with initial data $f_0(x,\xi)$.

Lemma 3.6 (Energy estimates): Assume that $f(t,x,\xi)\in \mathbf{H}^4_{x,\xi}([0,T])$ *is a solution of the Cauchy problem* (1.1) and (1.5) *for some constant* $T>0$. *Then there exist two sufficiently small positive constants* ε, δ_0 *such that if* $\varepsilon(f_0)<\delta_0$ *we have*

$$N(T)<\varepsilon. \tag{3.45}$$

In order to use the above energy estimates and the continuity argument to get the global existence result for the Cauchy problem (1.1) and (1.5), we need the local existence result in $\mathbf{H}^4_{x,\xi}([0,T])$ from Refs. 9 and 22.

Lemma 3.7 (Local existence result): For any sufficiently small constant $M>0$, *there exists a positive constant* $T^*(M)>0$ *such that if* $\varepsilon(f_0)\leqslant M$, *then the Cauchy problem* (1.1) and (1.5) *admits a unique classical solution* $f(t,x,\xi)\in \mathbf{H}^4_{x,\xi}([0,T^*(M)))$ *on* $[0,T^*(M))\times\mathbf{R}^3\times\mathbf{R}^3$ *such that* $f(t,x,\xi)\geqslant 0$ *and*

$$\sup_{0\leqslant t\leqslant T^*(M)}\sum_{|\alpha|+|\beta|\leqslant 4}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f(t,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}(\xi)}\mathrm{d}\xi\,\mathrm{d}x\leqslant C_5M, \tag{3.46}$$

for some positive constant C_5.

Remark 3.2: Notice that even for the local existence, the smallness of the initial data $g_0(x,\xi)=f_0(x,\xi)-\overline{\mathbf{M}}(\xi)$ *is needed.*

By combining Lemma 3.6 with Lemma 3.7, the main result in this paper can be stated as in the following theorem.

Theorem 3.1: Let $N\geqslant 4$ *be an integer and* $\overline{\mathbf{M}}(\xi)$ *be any given global Maxwellian, then there exist two sufficiently small positive constants* δ_0 *and* ε *such that if*

$$\varepsilon(f_0)\equiv\sum_{|\alpha|+|\beta|\leqslant N}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f_0(x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x<\delta_0, \tag{3.47}$$

the Cauchy problem (1.1) and (1.5) *admits a unique global classical solution* $f(t,x,\xi)\in\mathbf{H}^N_{x,\xi}(\mathbf{R}^+)$ *satisfying* $f(t,x,\xi)\geqslant 0$ *and*

$$\begin{aligned}&\sum_{|\alpha|+|\beta|\leqslant N}\sup_{t\in\mathbf{R}^+}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f(t,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}}\mathrm{d}\xi\,\mathrm{d}x\leqslant\varepsilon,\\ &\lim_{t\to\infty}\sup_{x\in\mathbf{R}^3}\sum_{|\alpha|+|\beta|\leqslant N-3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f(t,x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\overline{\mathbf{M}}(\xi)}\mathrm{d}\xi=0.\end{aligned} \tag{3.48}$$

Remark 3.3: The above analysis only shows that Theorem 3.1 *holds for* $N=4$. *But the case* $s>4$ *can be discussed similarly. It is worthy to point out that the assumption* $N\geqslant 4$ *is to guarantee that* $H^N_{x,\xi}([0,T])$ *is a Banach algebra.*

Before concluding this paper, we point out the main difference of this work from the previous ones on the stability analysis. The nonlinear stability of the global Maxwellian $\overline{\mathbf{M}}$ is studied in Ref. 15 based on the decomposition of the Boltzmann equation (1.1) and its solution $f(t,x,\xi)$ around the local Maxwellian $\mathbf{M}(t,x,\xi)$. The fluid component $\mathbf{P}_0^{\mathbf{M}}f$ and nonfluid component $\mathbf{P}_1^{\mathbf{M}}f$ are estimated separately. The energy estimates are closed with respect to some suitably chosen global Maxwellian $\mathbf{M}_-=\mathbf{M}_{[\rho_-,u_-,\theta_-]}$. Because of the technicality, it requires, among others, that

$$\theta_-<\bar{\theta},$$

and the initial data $f_0(x,\xi)$ satisfies

$$\sum_{|\alpha|+|\beta|\leqslant N}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{|\partial_x^\alpha\partial_t^\beta(f_0(x,\xi)-\overline{\mathbf{M}}(\xi))|^2}{\mathbf{M}_-}\mathrm{d}\xi\,\mathrm{d}x<\delta_0,$$

for some sufficiently small positive constant δ_0. Hence, it is easy to see that the assumptions imposed on the initial data in Ref. 15 is stronger than those in this paper.

On the other hand, the energy estimate is also closed with respect to the global Maxwellian $\overline{\mathbf{M}}$ in Ref. 9 and the key point there is to use the positivity of the linearized collision operator $L_{\overline{\mathbf{M}}}$ for the solution $f(t,x,\xi)$ with small amplitude to the Boltzmann equation (1.1). Precisely, based on the macroscopic projection

$$\mathbf{P}_0^{\overline{\mathbf{M}}}f=\left(a(t,x)+\sum_{j=1}^{3}b^j(t,x)\xi^j+c(t,x)|\xi|^2\right)\overline{\mathbf{M}},$$

the author in Ref. 9 gave a set of equations for the macroscopic quantities $a(t,x),b^j(t,x)(j=1,2,3)$ and $c(t,x)$. And the proof of the positivity of $L_{\overline{\mathbf{M}}}$ for the solution $f(t,x,\xi)$ with small amplitude to the Boltzmann equation (1.1) is then obtained by some delicate estimates on the macroscopic quantities $a(t,x),b^j(t,x)(j=1,2,3)$, and $c(t,x)$. However, the time evolution of the conserved quantities $\rho,m,\rho\frac{1}{2}|u|^2+\varepsilon$ is not clearly presented by just analyzing the macroscopic quantities $a(t,x),b^j(t,x)(j=1,2,3)$, and $c(t,x)$ as in Ref. 9.

The main observation in this paper is to close the energy estimates with respect to the global Maxwellian $\overline{\mathbf{M}}$ by estimating the conserved quantities $\rho,\rho u,\rho\frac{1}{2}|u|^2+\varepsilon$ governed by the well-known compressible Navier–Stokes equations with the nonfluid component $\mathbf{P}_1^{\mathbf{M}}f$ appearing in the source terms. Hence, the analytic techniques for the system of the compressible Navier–Stokes equations can be used to deduce the desired estimates on the conserved quantities. Therefore, it not only simplifies the analysis in the previous works, but also sheds some light on the stability analysis in some complicated systems, such as the Vlasov-Poisson-Boltzmann and Vlasov-Maxwell-Boltzmann systems.

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Semidirect sums of Lie algebras and discrete integrable couplings

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A relation between semidirect sums of Lie algebras and integrable couplings of lattice equations is established, and a practicable way to construct integrable couplings is further proposed. An application of the resulting general theory to the generalized Toda spectral problem yields two classes of integrable couplings for the generalized Toda hierarchy of lattice equations. The construction of integrable couplings using semidirect sums of Lie algebras provides a good source of information on complete classification of integrable lattice equations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2194630]

I. INTRODUCTION

Integrable couplings have been receiving growing attention recently. A few ways to construct integrable couplings are presented by using perturbations,[1–3] enlarging spectral problems,[4,5] and creating new loop Lie algebras.[6,7]

The problem of integrable couplings can be expressed as follows:[2] *For a given integrable system, how can we construct a nontrivial system of differential equations which is still integrable and includes the original integrable system as a subsystem?* Obviously, a change of orders of equations in a system does not lose integrability of the system. Therefore, up to a permutation, an integrable coupling of a given integrable system $u_t=K(u)$ is given by a bigger and triangular system:

$$u_t = K(u), \quad v_t = S(u,v).$$

The vector-valued function S should satisfy the nontriviality condition $\partial S/\partial[u]\neq 0$, where $[u]=(u,D_x u,D_x^2 u,\ldots)$ and $D_x^n u$ denotes a vector consisting of all derivatives of u of order n with respect to the space variable x. The above nontriviality condition means that the second subsystem involves the dependent variables of the first subsystem (i.e., the original system), and thus it guarantees that trivial diagonal systems with $S(u,v)=S(v)$ are not within our discussion.

A basic integrable coupling of an integrable system $u_t=K(u)$ is given by

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$$u_t = K(u), \quad v_t = K'(u)[v], \tag{1.1}$$

which can be generated by a perturbation around a solution of the system $u_t = K(u)$.[1] In the above system and elsewhere throughout this paper, $P'(u)[v]$ denotes the Gateaux derivative of $P(u) \equiv P(u, D_x u, \ldots)$ with respect to u in a direction v, i.e.,

$$P'(u)[v] = \frac{\partial}{\partial \varepsilon} P(u + \varepsilon v)|_{\varepsilon=0} = \frac{\partial}{\partial \varepsilon} P(u + \varepsilon v, D_x u + \varepsilon D_x v, \ldots)|_{\varepsilon=0}.$$

Obviously, the second subsystem $v_t = K'(u)[v]$ in the above integrable coupling (1.1) is linear with respect to v. Moreover, a symmetry $S(u)$ of the system $u_t = K(u)$ leads to a solution $(u, S(u))$ to the integrable coupling (1.1). However, the second component v of a solution (u, v) to the integrable coupling (1.1) is generally not a symmetry of the system $u_t = K(u)$. This is because v satisfies the linearized system $v_t = K'(u)[v]$ only for one solution, not for all solutions of the system $u_t = K(u)$. Therefore, the simple integrable coupling (1.1) is already a generalization of the symmetry problem. Another basic integrable coupling of an integrable system $u_t = K(u)$ reads as

$$u_t = K(u), \quad v_t = K'(u)[v] + K(u). \tag{1.2}$$

This system has a set of hereditary recursion operators[2]

$$\Phi(\beta_1, \beta_2) = \begin{pmatrix} \beta_1 \Phi(u) & 0 \\ \beta_1 \Phi'(u)[v] + \beta_2 \Phi(u) & \beta_1 \Phi(u) \end{pmatrix}$$

with two arbitrary constants β_1 and β_2, if the original system $u_t = K(u)$ has a hereditary recursion operator $\Phi(u)$. Therefore, integrable couplings possess richer integrable structures than the original integrable systems.

The study of integrable couplings provides clues towards complete classification of integrable systems. Let us first observe classification of square matrix spectral problems through the Jordan blocks under similar transformations of matrices. Each triangular Jordan block corresponds to an undecomposable subsystem in a given integrable system. Now, note that an arbitrary Lie algebra has a semidirect sum structure of a solvable Lie algebra and a semisimple Lie algebra,[8] and we will see that semidirect sums of Lie algebras can result in integrable couplings. These imply that the study of integrable couplings through semidirect sums of Lie algebras is an inevitable step towards complete classification of integrable systems with an arbitrary number of components, from a point of view of Lie algebras.

The study of integrable couplings also generates interesting mathematical structures such as Lax pairs with several spectral parameters,[9,10,2] integrable constrained flows with higher multiplicity,[11,12] local bi-Hamiltonian structures in higher dimensions[13] and hereditary recursion operators of higher order.[2,14] Very recently, we have proposed a relation between semidirect sums of Lie algebras and integrable couplings of continuous soliton equations, which provides an interesting and systematic approach to integrable couplings of continuous soliton equations.[15] In this paper, we would like to discuss the problem of discrete integrable couplings and develop a theory for constructing discrete integrable couplings by use of semidirect sums of Lie algebras.

Throughout our discussion, we denote by E the shift operator, write

$$(E^m x)(n) = x^{(m)}(n) = x(m+n), \quad \text{where } x: \mathbb{Z} \to \mathbb{R}, \ m, n \in \mathbb{Z}, \tag{1.3}$$

and adopt an inverse of the difference operator $E-1$ as follows:

$$(E-1)^{-1} = \frac{1}{2}\left(\sum_{k=-\infty}^{-1} - \sum_{k=0}^{\infty} \right) E^k. \tag{1.4}$$

Let G be a matrix Lie algebra with the standard Lie bracket $[A, B] = AB - BA$, and closed under matrix multiplication: $AB \in G$ for all $A, B \in G$. We assume that an integrable lattice equation (or system) of evolution type

$$u_t = K(u) = K(u, Eu, E^{-1}u, \dots) \tag{1.5}$$

is associated with G, where $u=u(n,t)$ is a dependent variable. More precisely, there is a pair of square matrices U and V in G, called a Lax pair, so that the discrete spatial matrix spectral problem

$$E\phi = U\phi = U(u,\lambda)\phi \tag{1.6}$$

and the associated discrete temporal matrix spectral problem

$$\phi_t = V\phi = V(u, Eu, E^{-1}u, \dots; \lambda)\phi, \tag{1.7}$$

where λ is a spectral parameter and ϕ is an eigenfunction, generate[16,17] the integrable lattice equation (1.5) through their isospectral (i.e., $\lambda_t=0$) compatibility condition

$$U_t = (EV)U - UV, \tag{1.8}$$

which is called a discrete zero curvature equation. In other words, we have

$$U'(u)[K] = (EV)U - UV, \tag{1.9}$$

where $U'(u)[K]$ denotes the Gateaux derivative as above. In a nonisospectral case, e.g., $\lambda_t=f(\lambda)$, then we have

$$U'(u)[K] + fU_\lambda = (EV)U - UV, \tag{1.10}$$

where U_λ is a partial derivative of U with respect to λ. Based on (1.6) and (1.7), the lattice equation (1.5) can often be solved by the inverse scattering transform (for example, see Ref. 18). There are also a few interesting Lie algebraic structures hidden behind the equation (1.10) (see Ref. 17 for more information). An integrable hierarchy and its master symmetry hierarchy usually correspond to the isospectral case and the nonisospectral case $\lambda_t=\lambda^n$, $n\geqslant 0$, respectively. These two hierarchies constitute a semidirect sum of Lie algebras, each of which consists of symmetries in one hierarchy. The spatial matrix spectral problem (1.6) is our starting point in constructing discrete integrable couplings. The closure property of the Lie algebra G under matrix multiplication guarantees that $(EV)U-UV$ is still in G so that the discrete zero curvature equation (1.8) makes sense.

In what follows, we are going to establish a relation between semidirect sums of Lie algebras and integrable couplings of lattice equations and a technically practicable way to generate integrable couplings through semidirect sums of Lie algebras. The resulting general theory will be used to generate two classes of integrable couplings for the generalized Toda hierarchy presented in Ref. 19. It will also be indicated that the construction of integrable couplings using semidirect sums of Lie algebras provides a good source of information about classification of integrable lattice equations. A few concluding remarks will be given in the last section.

II. CONSTRUCTING INTEGRABLE COUPLINGS USING SEMIDIRECT SUMS OF LIE ALGEBRAS

A. Generating scheme

Assume that the lattice equation (1.5) has a Lax pair (U,V) in a matrix Lie algebra G closed under matrix multiplication.

To construct an integrable coupling of the lattice equation (1.5), we use semidirect sums of Lie algebras to enlarge the original Lie algebra G. Take another matrix Lie algebra G_c closed under matrix multiplication and then form a semidirect sum $\overline{G}$ of G and G_c:

$$\overline{G} = G \dotplus G_c. \tag{2.1}$$

The notion of semidirect sums means that G and G_c satisfy

$$[G, G_c] \subseteq G_c, \tag{2.2}$$

where $[G, G_c] = \{[A, B] | A \in G, B \in G_c\}$. Obviously, G_c is an ideal Lie subalgebra of $\overline{G}$. The subscript c here indicates a contribution to the construction of couplings. We also require that the closure property between G and G_c under matrix multiplication,

$$GG_c, G_cG \subseteq G_c, \tag{2.3}$$

where $G_1G_2 = \{AB | A \in G_1, B \in G_2\}$, to guarantee that a Lax pair from the semidirect sum $\overline{G}$ can generate a coupling system. Note that the two different binary operations were used in the above closure properties in (2.2) and (2.3).

Now choose a pair of new Lax matrices in the semidirect sum $\overline{G}$ of Lie algebras:

$$\overline{U} = U + U_c, \quad \overline{V} = V + V_c, \quad U_c, V_c \in G_c, \tag{2.4}$$

and make a pair of enlarged discrete spatial matrix spectral problems

$$\begin{aligned} E\overline{\phi} &= \overline{U}\overline{\phi} = \overline{U}(\overline{u}, \lambda)\overline{\phi}, \\ \overline{\phi}_t &= \overline{V}\overline{\phi} = \overline{V}(\overline{u}, E\overline{u}, E^{-1}\overline{u}, \ldots; \lambda)\overline{\phi}, \end{aligned} \tag{2.5}$$

where the matrix U_c in $\overline{U}$ introduces additional dependent variables and $\overline{u}$ consists of both the original dependent variables and the additional dependent variables. In addition, the matrix U_c could depend on the spectral parameter λ, and the matrix V_c in $\overline{V}$ really does almost in all cases. Based on the closure properties of G, G_c and between G and G_c, it is easy to see that

$$\begin{aligned} (E\overline{V})\overline{U} - \overline{UV} &= [(EV)U - UV] + \{[(EV)U_c - U_cV] + [(EV_c)U - UV_c] + [(EV_c)U_c - U_cV_c]\} \\ &\in G \oplus G_c. \end{aligned}$$

Therefore, under $u_t = K(u)$, the corresponding enlarged discrete zero curvature equation

$$\overline{U}_t = (E\overline{V})\overline{U} - \overline{UV} \tag{2.6}$$

precisely presents

$$\begin{aligned} U_t &= (EV)U - UV, \\ U_{c,t} &= [(EV)U_c - U_cV] + [(EV_c)U - UV_c] + [(EV_c)U_c - U_cV_c]. \end{aligned} \tag{2.7}$$

The first equation above is equivalent to the lattice equation (1.5), and hence, this is a coupling system for the lattice equation (1.5).

The whole construction process above shows that semidirect sums of a given Lie algebra G with new Lie algebras provide a great choice of candidates of integrable couplings for the lattice equation (1.5) generated from the Lie algebra G.

B. Realizations by particular semi-direct sums

To shed light on the above general scheme of constructing coupling systems, let us introduce the following particular class of semidirect sums of Lie algebras:

$$\bar{G} = G \oplus G_c, \quad G = \{\mathrm{diag}(\underbrace{A, \ldots, A}_{\mu}, \underbrace{0, \ldots, 0}_{\nu-\mu+1})\},$$

$$G_c = \left\{ \begin{pmatrix} 0 & & & & \\ & \ddots & & B_{ij} & \\ & & 0 & & \\ & & & B_{\mu+1,\mu+1} & \\ & 0 & & & \ddots \\ & & & & & B_{\nu+1,\nu+1} \end{pmatrix} \right\}, \tag{2.8}$$

where A, B_{ii} are arbitrary square matrices, A is of the same order as U and the partitions of matrices in G and G_c are the same. Obviously, $B_{ij}, j \leqslant \mu$, are square but $B_{ij}, j \geqslant \mu+1$, may not; and all closure conditions of G, G_c and between G and G_c under matrix multiplication are satisfied.

Define

$$U_G := \operatorname{diag}(\underbrace{U, \ldots, U}_{\mu}, \underbrace{0, \ldots, 0}_{\nu-\mu+1}), \quad V_G := \operatorname{diag}(\underbrace{V, \ldots, V}_{\mu}, \underbrace{0, \ldots, 0}_{\nu-\mu+1}).$$

Note that U_G and V_G in G generate the same lattice equation as U and V, and thus for integrable couplings, the corresponding enlarged spectral matrices $\overline{U}$ and $\overline{V}$ in the semidirect sum $G \dotplus G_c$ can be chosen as

$$\overline{U} = U_G + U_{G,c} := \begin{pmatrix} U & & & & \\ & \ddots & & U_{ij} & \\ & & U & & \\ & & & U_{\mu+1,\mu+1} & \\ & 0 & & & \ddots \\ & & & & & U_{\nu+1,\nu+1} \end{pmatrix}$$

$$\overline{V} = V_G + V_{G,c} := \begin{pmatrix} V & & & & \\ & \ddots & & V_{ij} & \\ & & V & & \\ & & & V_{\mu+1,\mu+1} & \\ & 0 & & & \ddots \\ & & & & & V_{\nu+1,\nu+1} \end{pmatrix},$$

where the first two matrices U_G and V_G play the (U,V)-part and the second two matrices $U_{G,c}$ and $V_{G,c}$ play the (U_c, V_c)-part in the pair of $\overline{U}$ and $\overline{V}$ defined in (2.4). It is not difficult to see that the resulting coupling system (2.7) becomes

$$U_t = (EV)U - UV,$$

$$(U_{i+1,i+1})_t = (EV_{i+1,i+1})U_{i+1,i+1} - U_{i+1,i+1}V_{i+1,i+1}, \quad \mu \leqslant i \leqslant \nu, \tag{2.9}$$

$$U_{ij,t} = \sum_{k=i}^{j} [(EV_{ik})U_{kj} - U_{ik}V_{kj}], \quad 1 \leqslant i < j \leqslant \nu + 1,$$

where $U_{ii} = U$ and $V_{ii} = V$, $1 \leqslant i \leqslant \mu$.

In particular, first, if we take

$$\overline{U}=\begin{pmatrix} U & U_{12} & \cdots & U_{1,\mu+1} \\ & \ddots & \ddots & \vdots \\ & & U & U_{\mu,\mu+1} \\ 0 & & & 0 \end{pmatrix}, \quad \overline{V}=\begin{pmatrix} V & V_{12} & \cdots & V_{1,\mu+1} \\ & \ddots & \ddots & \vdots \\ & & V & V_{\mu,\mu+1} \\ 0 & & & 0 \end{pmatrix},$$

then the coupling system (2.9) becomes

$$\begin{aligned} U_t &= (EV)U - UV, \\ U_{ij,t} &= \sum_{k=i}^{j} [(EV_{ik})U_{kj} - U_{ik}V_{kj}], \quad 1 \leqslant i < j \leqslant \mu+1, \end{aligned} \tag{2.10}$$

where $U_{ii}=U$, $V_{ii}=V$, $1 \leqslant i \leqslant \mu$, and $U_{ii}=V_{ii}=0$, $i=\mu+1$. Second, if we take

$$\overline{U}=\begin{pmatrix} U & U_{a_1} & \cdots & U_{a_\nu} \\ & U & \ddots & \vdots \\ & & \ddots & U_{a_1} \\ 0 & & & U \end{pmatrix}, \quad \overline{V}=\begin{pmatrix} V & V_{a_1} & \cdots & V_{a_\nu} \\ & V & \ddots & \vdots \\ & & \ddots & V_{a_1} \\ 0 & & & V \end{pmatrix},$$

then the coupling system (2.9) becomes

$$\begin{aligned} U_t &= (EV)U - UV, \\ U_{a_i,t} &= \sum_{k+l=i,k,l\geqslant 0} [(EV_{a_k})U_{a_l} - U_{a_l}V_{a_k}], \quad 1 \leqslant i \leqslant \nu, \end{aligned} \tag{2.11}$$

where $U_{a_0}=U$ and $V_{a_0}=V$.

We remark that here we have just presented one class of semidirect sums of Lie algebras, together with two specific examples. It is interesting to construct other possible realizations, especially those which could carry essential information for keeping integrable properties of the original lattice equations.

C. Linearly dependent case on the spectral parameter

Let us now assume that the spatial spectral matrix U depends linearly on the spectral parameter λ (see, for example, Refs. 17 and 19–21):

$$U = U(u,\lambda) = \lambda U_0 + U_1, \quad \frac{\partial U_0}{\partial \lambda} = \frac{\partial U_1}{\partial \lambda} = 0. \tag{2.12}$$

Consider two specific examples of the enlarged spatial spectral matrices introduced in the last section,

$$\overline{U_1}=\begin{pmatrix} U & U_a \\ 0 & 0 \end{pmatrix}, \quad \overline{U_2}=\begin{pmatrix} U & U_a \\ 0 & U \end{pmatrix}, \quad \frac{\partial U_a}{\partial \lambda} = 0. \tag{2.13}$$

Note that the submatrices U_a in the above two enlarged spatial spectral matrices could be of different sizes. As in the continuous cases,[4,15] suppose that

$$\overline{W_1}=\begin{pmatrix} W & W_a \\ 0 & 0 \end{pmatrix}, \quad \overline{W_2}=\begin{pmatrix} W & W_a \\ 0 & W \end{pmatrix}$$

with

$$W=\sum_{i\geqslant 0} W_i\lambda^{-i},\quad W_a=\sum_{i\geqslant -n_0} W_{a,i}\lambda^{-i},\quad \frac{\partial W_i}{\partial\lambda}=0,\quad \frac{\partial W_{a,i}}{\partial\lambda}=0, \tag{2.14}$$

where $n_0\geqslant 0$ is a proper integer, solve the corresponding enlarged discrete stationary zero curvature equations

$$(E\overline{W}_i)\overline{U}_i-\overline{U}_i\overline{W}_i=0,\quad i=1,2, \tag{2.15}$$

respectively.

Then for each $m\geqslant 0$, choose

$$\overline{V}_1^{[m]}=\begin{pmatrix} V^{[m]} & V_a^{[m]}\\ 0 & 0\end{pmatrix}=(\lambda^m\overline{W}_1)_+ +\overline{\Delta}_m,\quad \overline{\Delta}_m=\begin{pmatrix}\Delta_m & \Delta_{m,a}\\ 0 & 0\end{pmatrix},$$

where Δ_m and $\Delta_{m,a}$ do not depend on λ and satisfy

$$(E\Delta_m)U_0-U_0\Delta_m=0,\quad U_0\Delta_{m,a}=0, \tag{2.16}$$

and choose

$$\overline{V}_2^{[m]}=\begin{pmatrix} V^{[m]} & V_a^{[m]}\\ 0 & V^{[m]}\end{pmatrix}=(\lambda^m\overline{W}_2)_+ +\overline{\Delta}_m,\quad \overline{\Delta}_m=\begin{pmatrix}\Delta_m & \Delta_{m,a}\\ 0 & \Delta_m\end{pmatrix},$$

where Δ_m and $\Delta_{m,a}$ do not depend on λ and satisfy

$$(E\Delta_m)U_0-U_0\Delta_m=0,\quad (E\Delta_{m,a})U_0-U_0\Delta_{m,a}=0. \tag{2.17}$$

The subscript $+$ above denotes to select the polynomial part in λ. Based on (2.10) and (2.11) and using (2.15), we can directly show that the enlarged discrete zero curvature equations

$$\overline{U}_{i,t_m}=(E\overline{V}_i^{[m]})\overline{U}_i-\overline{U}_i\overline{V}_i^{[m]},\quad i=1,2,$$

namely,

$$U_{t_m}=(EV^{[m]})U-UV^{[m]},$$

$$U_{a,t_m}=(EV^{[m]})U_a-UV_a^{[m]},$$

and

$$U_{t_m}=(EV^{[m]})U-UV^{[m]},$$

$$U_{a,t_m}=(EV^{[m]})U_a+(EV_a^{[m]})U-UV_a^{[m]}-U_aV^{[m]},$$

present

$$\begin{aligned} U_{t_m}&=(\Delta_m)_x+[U_0,W_{m+1}]-[U_1,\Delta_m],\\ U_{a,t_m}&=U_0W_{a,m+1}+(E\Delta_m)U_a-U_1\Delta_{m,a},\end{aligned} \tag{2.18}$$

and

$$U_{t_m}=(\Delta_m)_x+[U_0,W_{m+1}]-[U_1,\Delta_m], \tag{2.19a}$$

$$U_{a,t_m} = U_0 W_{a,m+1} - (EW_{a,m+1})U_0 + (E\Delta_m)U_a - U_a\Delta_m + (E\Delta_{m,a})U_1 - U_1\Delta_{m,a}, \qquad (2.19b)$$

respectively.

We remark that these two enlarged hierarchies in (2.18) and (2.19) share the enlarged discrete spectral problems

$$E\overline{\phi} = \overline{U}_1\overline{\phi}, \quad E\overline{\phi} = \overline{U}_2\overline{\phi},$$

respectively. Thus, all lattice equations in each of the two enlarged hierarchies can possess infinitely many common conserved densities except the original ones (see Refs. 22–24 for a few concrete examples). Moreover, one can construct a specific nondegenerate bilinear form on $\overline{G}$ with the invariance property, to present Hamiltonian structures of the enlarged lattice equations by a generalized trace identity. The detailed analysis on those integrable properties will be left to a future presentation.

To sum up, each system of lattice equations in the hierarchy (2.18) or (2.19) can provide an integrable coupling for its first subsystem of lattice equations. In the next section, we will only discuss two examples of constructing enlarged lattice hierarchies, in the generalized Toda case presented in Ref. 19.

III. INTEGRABLE COUPLINGS OF THE GENERALIZED TODA HIERARCHY

A. The generalized Toda equations

Let us here recall the generalized Toda hierarchy.[19] The corresponding discrete spatial spectral problem reads

$$E\phi = U(u,\lambda)\phi, U(u,\lambda) = \begin{pmatrix} 0 & 1 \\ (\alpha\lambda+\beta)r & \lambda+s \end{pmatrix}, \quad u = \begin{pmatrix} r \\ s \end{pmatrix}, \qquad (3.1)$$

where λ is a spectral parameter, and α and β are two arbitrary constants satisfying $\alpha^2+\beta^2 \neq 0$. When $\alpha=0$ and $\beta=-1$, (3.1) becomes the Toda spectral problem.[16]

Its stationary discrete zero curvature equation

$$(EW)U - UW = 0 \qquad (3.2)$$

has the solution

$$W = \begin{pmatrix} a & b \\ (\alpha\lambda+\beta)c & -a \end{pmatrix}, \qquad (3.3)$$

with

$$a = \sum_{i\geqslant 0} a_i\lambda^{-i}, \quad b = \sum_{i\geqslant 0} b_i\lambda^{-i}, \quad c = \sum_{i\geqslant 0} c_i\lambda^{-i},$$

where the coefficients are defined by the initial conditions

$$a_0 = -\tfrac{1}{2}, \quad b_0 = 0, \quad c_0 = 0,$$

and the recursion relation

$$c_{i+1} - rb_{i+1}^{(1)} = 0, \quad i \geqslant 0, \qquad (3.4a)$$

$$b_{i+1}^{(1)} + sb_i^{(1)} + (a_i^{(1)} + a_i) = 0, \quad i \geqslant 0, \qquad (3.4b)$$

$$(a_{i+1}^{(1)} - a_{i+1}) + s(a_i^{(1)} - a_i) + \alpha(rb_{i+1} - c_{i+1}^{(1)}) + \beta(rb_i - c_i^{(1)}) = 0, \quad i \geqslant 0, \tag{3.4c}$$

which are all difference polynomials in u with respect to the lattice variable n. Under the initial-value conditions

$$a_1|_{u=0} = c_1|_{u=0} = 0, \quad a_i|_{u=0} = b_i|_{u=0} = c_i|_{u=0} = 0, \quad i \geqslant 2,$$

the recursion relation (3.4) uniquely determines the lattice functions a_i, b_i, and c_i, $i \geqslant 1$. The first few lattice functions are

$$a_1 = \alpha r, \quad b_1 = 1, \quad c_1 = r,$$

$$a_2 = -\alpha^2 r^{(1)} r - \alpha^2 r^2 - \alpha^2 r r^{(-1)} - \alpha r s - \alpha r s^{(-1)} + \beta r,$$

$$b_2 = -\alpha r - \alpha r^{(-1)} - s^{(-1)}, \quad c_2 = -rs - \alpha r^2 - \alpha r r^{(1)}.$$

As usual, choose that

$$V_m = \begin{pmatrix} (\lambda^m a)_+ & (\lambda^m b)_+ \\ (\alpha\lambda + \beta)(\lambda^m c)_+ & -(\lambda^m a)_+ \end{pmatrix}, \quad m \geqslant 0. \tag{3.5}$$

Then it follows from (3.4) that

$$(EV_m)U - UV_m = \begin{pmatrix} 0 & -b_{m+1}^{(1)} \\ (\alpha\lambda + \beta)c_{m+1} & \beta(c_m^{(1)} - rb_m) - s(a_m^{(1)} - a_m) \end{pmatrix}.$$

Take a modification

$$\Delta_m = \begin{pmatrix} b_{m+1} & 0 \\ 0 & 0 \end{pmatrix},$$

and define the temporal spectral matrices

$$V^{[m]} = V_m + \Delta_m, \quad m \geqslant 0. \tag{3.6}$$

Then, a direct calculation leads to the following matrix:

$$(EV^{[m]})U - UV^{[m]} = \begin{pmatrix} 0 & 0 \\ (\alpha\lambda + \beta)(c_{m+1} - rb_{m+1}) & \beta(c_m^{(1)} - rb_m) - s(a_m^{(1)} - a_m) \end{pmatrix}.$$

This is consistent with U_{t_m}, and thus, making the evolution laws

$$\phi_{t_m} = V^{[m]}\phi, \quad m \geqslant 0, \tag{3.7}$$

the compatibility conditions

$$U_{t_m} = (EV^{[m]})U - UV^{[m]}, \quad m \geqslant 0,$$

of the discrete spatial spectral problem (3.1) and the associated discrete temporal spectral problems (3.7) give rise to the following hierarchy of lattice equations:

$$\begin{aligned} r_{t_m} &= c_{m+1} - rb_{m+1}, \\ s_{t_m} &= -\alpha(c_{m+1}^{(1)} - rb_{m+1}) + (a_{m+1}^{(1)} - a_{m+1}), \end{aligned} \quad m \geqslant 0. \tag{3.8}$$

This generalized Toda hierarchy is Liouville integrable,[19] and its Hamiltonian structure leads to infinitely many conservation laws and symmetries for every system in the hierarchy.

Obviously, the first nonlinear lattice equation in the hierarchy is

$$r_{t_1} = r(s^{(-1)} - s) + \alpha r(r^{(-1)} - r^{(1)}),$$
$$s_{t_1} = \alpha s(r - r^{(1)}) + \beta(r^{(1)} - r). \tag{3.9}$$

When $\alpha=0$ and $\beta=-1$, (3.9) becomes the Toda lattice equation,[25]

$$r_{t_1} = r(s^{(-1)} - s), \quad s_{t_1} = r - r^{(1)}, \tag{3.10}$$

and when $\alpha=1$ and $\beta=0$, (3.9) becomes the following lattice equation presented in Ref. 26:

$$r_{t_1} = r(s^{(-1)} - s) + r(r^{(-1)} - r^{(1)}), \quad s_{t_1} = s(r - r^{(1)}). \tag{3.11}$$

The lattice equation (3.11) is linearly independent of the Toda lattice equation (3.10). There exist a voluminous literature on the Toda lattice equation, and its generalizations and solution structures (for example, see Refs. 27–32).

B. Integrable couplings from specific semidirect sums

The generalized Toda spectral problem (3.1) linearly depends on the spectral parameter λ, and thus we can write

$$U = \begin{pmatrix} 0 & 1 \\ (\alpha\lambda + \beta)r & \lambda + s \end{pmatrix} = U_0\lambda + U_1, \quad U_0 = \begin{pmatrix} 0 & 0 \\ \alpha r & 1 \end{pmatrix}, \quad U_1 = \begin{pmatrix} 0 & 1 \\ \beta r & s \end{pmatrix}. \tag{3.12}$$

We will also see that there is a difference between the two cases of $\alpha=0$ and $\alpha\neq 0$ in computing integrable couplings.

Let us first consider the semidirect sum of Lie algebras of 3×3 matrices,

$$G \dot{+} G_c, \quad G = \left\{ \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} | A \in \mathbb{C}[\lambda,\lambda^{-1}] \otimes M_{2\times 2} \right\}, \quad G_c = \left\{ \begin{pmatrix} 0 & B \\ 0 & 0 \end{pmatrix} | B \in \mathbb{C}[\lambda,\lambda^{-1}] \otimes M_{2\times 1} \right\},$$

where $\mathbb{C}[\lambda,\lambda^{-1}]\otimes M_{m\times n} = \mathrm{span}\{\lambda^k A | k \in \mathbb{Z}, A \in M_{m\times n}\}$. In this case, G_c is an Abelian ideal of $G \dot{+} G_c$. We define the corresponding enlarged spatial spectral matrix as

$$\overline{U} = \overline{U}(\overline{u},\lambda) = \begin{pmatrix} U & U_a \\ 0 & 0 \end{pmatrix} \in G \dot{+} G_c, \quad U_a = U_a(v) = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \tag{3.13}$$

where v_1 and v_2 are new dependent variables and

$$v = (v_1, v_2)^T, \quad \overline{u} = (u^T, v^T)^T = (r, s, v_1, v_2)^T.$$

Upon setting

$$\overline{W} = \begin{pmatrix} W & W_a \\ 0 & 0 \end{pmatrix}, \quad W_a = W_a(\overline{u},\lambda) = \begin{pmatrix} e \\ f \end{pmatrix},$$

where W is a solution to $(EW)U - UW = 0$, defined by (3.3), the corresponding enlarged discrete stationary zero curvature equation $(E\overline{W})\overline{U} - \overline{UW} = 0$ becomes

$$(EW)U_a - UW_a = 0, \tag{3.14}$$

which is equivalent to

$$W_a = WU^{-1}U_a,$$

namely,

$$f = a^{(1)}v_1 + b^{(1)}v_2, \tag{3.15a}$$

$$(\alpha\lambda+\beta)re=(\alpha\lambda+\beta)c^{(1)}v_1-a^{(1)}v_2-(\lambda+s)f. \tag{3.15b}$$

This system determines a solution for e and f as follows:

$$e=\sum_{i\geqslant -n_0} e_i\lambda^{-i},\quad f=\sum_{i\geqslant 0} f_i\lambda^i,$$

where $n_0=1$ if $\alpha=0$ and $n_0=0$ if $\alpha\neq 0$ [see (2.14) for introduction of n_0]. Now define the enlarged temporal spectral matrix as

$$\overline{V}^{[m]}=\begin{pmatrix} V^{[m]} & V_a^{[m]} \\ 0 & 0 \end{pmatrix},\quad V_a^{[m]}=(\lambda^m W_a)_+ +\Delta_{m,a},\quad m\geqslant 0, \tag{3.16}$$

where $V^{[m]}$ is defined as in (3.6). To satisfy (2.16), choose $\Delta_{m,a}$ as

$$\Delta_{m,a}=\begin{pmatrix} h_m \\ -\alpha r h_m \end{pmatrix},\quad h_m-\text{arbitrary},\quad m\geqslant 0. \tag{3.17}$$

Then based on (3.15), we can compute that

$$\begin{aligned}(EV^{[m]})U_a-UV_a^{[m]}&=(EV_m)U_a-U(\lambda^m W_a)_+ +(E\Delta_m)U_a-U_1\Delta_{m,a}=\begin{pmatrix} 0 \\ -\alpha c_{m+1}^{(1)}v_1+\alpha r e_{m+1}+f_{m+1}\end{pmatrix}\\ &\quad+\begin{pmatrix} b_{m+1}^{(1)}v_1 \\ 0\end{pmatrix}-\begin{pmatrix} -\alpha r h_m \\ \beta r h_m-\alpha r s h_m\end{pmatrix}\\ &=\begin{pmatrix} b_{m+1}^{(1)}v_1+\alpha r h_m \\ -\alpha c_{m+1}^{(1)}v_1+\alpha r e_{m+1}+f_{m+1}-\beta r h_m+\alpha r s h_m\end{pmatrix},\quad m\geqslant 0.\end{aligned}$$

Therefore, the mth enlarged discrete zero curvature equation

$$\overline{U}_{t_m}=(E\overline{V}^{[m]})\overline{U}-\overline{U}\overline{V}^{[m]}$$

leads to

$$v_{t_m}=\begin{pmatrix} v_1 \\ v_2\end{pmatrix}_{t_m}=S_m(u,v)=\begin{pmatrix} b_{m+1}^{(1)}v_1+\alpha r h_m \\ -\alpha c_{m+1}^{(1)}v_1+\alpha r e_{m+1}+f_{m+1}-\beta r h_m+\alpha r s h_m\end{pmatrix}, \tag{3.18}$$

together with the mth generalized Toda equation in (3.8). Therefore, we obtain a hierarchy of coupling systems defined by (2.18),

$$\overline{u}_{t_m}=\begin{pmatrix} u \\ v\end{pmatrix}_{t_m}=\overline{K}_m(u)=\begin{pmatrix} K_m(u) \\ S_m(u,v)\end{pmatrix},\quad m\geqslant 0 \tag{3.19}$$

for the generalized Toda hierarchy (3.8).

Let us second consider the semidirect sum of Lie algebras of 4×4 matrices,

$$G\oplus G_c,\quad G=\left\{\begin{pmatrix} A & 0 \\ 0 & A\end{pmatrix}|A\in\mathbb{C}[\lambda,\lambda^{-1}]\otimes M_{2\times 2}\right\},\quad G_c=\left\{\begin{pmatrix} 0 & B \\ 0 & 0\end{pmatrix}|B\in\mathbb{C}[\lambda,\lambda^{-1}]\otimes M_{2\times 2}\right\}.$$

In this case, G_c is an Abelian ideal of $G\oplus G_c$, too. We define the corresponding enlarged spatial spectral matrix as

$$\overline{U}=\overline{U}(\overline{u},\lambda)=\begin{pmatrix} U & U_a \\ 0 & U\end{pmatrix}\in G\oplus G_c,\quad U_a=U_a(v)=\begin{pmatrix} v_1 & v_2 \\ v_3 & v_4\end{pmatrix}, \tag{3.20}$$

where v_i, $1\leqslant i\leqslant 4$, are new dependent variables and

$$v=(v_1,v_2,v_3,v_4)^T,\quad \overline{u}=(u^T,v^T)^T=(r,s,v_1,v_2,v_3,v_4)^T.$$

If we set

$$\overline{W}=\begin{pmatrix} W & W_a \\ 0 & W \end{pmatrix},\quad W_a=W_a(\overline{u},\lambda)=\begin{pmatrix} e & f \\ g & -e \end{pmatrix},$$

where W is a solution to $(EW)U-UW=0$, defined by (3.3), then the corresponding enlarged discrete stationary zero curvature equation $(E\overline{W})\overline{U}-\overline{UW}=0$ becomes

$$(EW)U_a+(EW_a)U-UW_a-U_aW=0, \tag{3.21}$$

which is equivalent to

$$\begin{aligned}
&(e^{(1)}+e)+(\lambda+s)f^{(1)}+(a^{(1)}+a)v_2+b^{(1)}v_4-bv_1=0,\\
&-(\alpha\lambda+\beta)r(e^{(1)}+e)-(\lambda+s)g+(\alpha\lambda+\beta)(c^{(1)}v_1-cv_4)-(a^{(1)}+a)v_3=0,\\
&g^{(1)}-(\lambda+s)(e^{(1)}-e)-(\alpha\lambda+\beta)(rf-c^{(1)}v_2)-(a^{(1)}-a)v_4-bv_3=0.
\end{aligned} \tag{3.22}$$

This system can determine a solution for e, f, and g as follows:

$$e=\sum_{i\geqslant 0}e_i\lambda^{-i},\quad f=\sum_{i\geqslant 0}f_i\lambda^{-i},\quad g=\sum_{i\geqslant 0}g_i\lambda^{-i}.$$

Now, we define the enlarged temporal spectral matrix as

$$\overline{V}^{[m]}=\begin{pmatrix} V^{[m]} & V_a^{[m]} \\ 0 & V^{[m]} \end{pmatrix},\quad V_a^{[m]}=(\lambda^mW_a)_+ +\Delta_{m,a},\quad m\geqslant 0, \tag{3.23}$$

where $V^{[m]}$ is defined as in (3.6). To satisfy (2.17), choose $\Delta_{m,a}$ as

$$\Delta_{m,a}=\begin{pmatrix} h_m & 0 \\ -\alpha rh_m & 0 \end{pmatrix},\quad h_m-\text{arbitrary},\quad m\geqslant 0. \tag{3.24}$$

Then based on (3.22), we can compute that

$$\begin{aligned}
&(EV^{[m]})U_a+(EV_a^{[m]})U-UV_a^{[m]}-U_aV^{[m]}\\
&\quad=[(EV_m)U_a+(E(\lambda^mW_a)_+)U-U(\lambda^mW_a)_+-U_aV_m]\\
&\qquad+[(E\Delta_m)U_a-U_a\Delta_m]+[(E\Delta_{m,a})U_1-U_1\Delta_{m,a}]\\
&\quad=\begin{pmatrix} -\alpha c_{m+1}v_2+\alpha rf_{m+1}^{(1)} & f_{m+1}^{(1)} \\ \alpha c_{m+1}^{(1)}v_1-\alpha c_{m+1}v_4-\alpha r(e_{m+1}^{(1)}+e_{m+1})-g_{m+1} & \alpha c_{m+1}^{(1)}v_2-\alpha rf_{m+1}-(e_{m+1}^{(1)}-e_{m+1}) \end{pmatrix}\\
&\qquad+\begin{pmatrix} (b_{m+1}^{(1)}-b_{m+1})v_1 & b_{m+1}^{(1)}v_2 \\ -b_{m+1}v_3 & 0 \end{pmatrix}+\begin{pmatrix} \alpha rh_m & h_m^{(1)} \\ r(\alpha s-\beta)h_m & -\alpha r^{(1)}h_m^{(1)} \end{pmatrix}\\
&\quad=\begin{pmatrix} -\alpha c_{m+1}v_2+\alpha rf_{m+1}^{(1)}+(b_{m+1}^{(1)}-b_{m+1})v_1+\alpha rh_m, \\ \alpha c_{m+1}^{(1)}v_1-\alpha c_{m+1}v_4-\alpha r(e_{m+1}^{(1)}+e_{m+1})-g_{m+1}-b_{m+1}v_3+r(\alpha s-\beta)h_m, \\ f_{m+1}^{(1)}+b_{m+1}^{(1)}v_2+h_m^{(1)} \\ \alpha c_{m+1}^{(1)}v_2-\alpha rf_{m+1}-(e_{m+1}^{(1)}-e_{m+1})-\alpha r^{(1)}h_m^{(1)} \end{pmatrix}.
\end{aligned}$$

Then the mth enlarged discrete zero curvature equation

$$\overline{U}_{t_m} = (E\overline{V}^{[m]})\overline{U} - \overline{U}\overline{V}^{[m]}$$

leads to

$$v_{t_m} = (v_1, v_2, v_3, v_4)^T_{t_m} = T_m(u,v)$$
$$= \begin{pmatrix} -\alpha c_{m+1} v_2 + \alpha r f^{(1)}_{m+1} + (b^{(1)}_{m+1} - b_{m+1}) v_1 + \alpha r h_m \\ f^{(1)}_{m+1} + b^{(1)}_{m+1} v_2 + h^{(1)}_m \\ \alpha c^{(1)}_{m+1} v_1 - \alpha c_{m+1} v_4 - \alpha r (e^{(1)}_{m+1} + e_{m+1}) - g_{m+1} - b_{m+1} v_3 + r(\alpha s - \beta) h_m \\ \alpha c^{(1)}_{m+1} v_2 - \alpha r f_{m+1} - (e^{(1)}_{m+1} - e_{m+1}) - \alpha r^{(1)} h^{(1)}_m \end{pmatrix}, \quad (3.25)$$

together with the mth generalized Toda equation in (3.8). Therefore, we obtain a hierarchy of coupling systems defined by (2.19),

$$\overline{u}_{t_m} = \begin{pmatrix} u \\ v \end{pmatrix}_{t_m} = \overline{K}_m(u) = \begin{pmatrix} K_m(u) \\ T_m(u,v) \end{pmatrix}, \quad m \geqslant 0 \quad (3.26)$$

for the generalized Toda hierarchy (3.8).

C. Illustrative examples

We now work out two concrete examples as follows, one in each of the two above cases.

Case of $\alpha=1$ and $\beta=0$: Let us first compute an example of the hierarchy (3.19). Assume that $\alpha=1$ and $\beta=0$ for convenience, which corresponds to the lattice hierarchy presented in Ref. 26. In this case, we have $n_0=0$ in (2.14).

It directly follows from (3.15) that

$$f_i = a^{(1)}_i v_1 + b^{(1)}_i v_2,$$

$$re_{i+1} = c^{(1)}_{i+1} v_1 - a^{(1)}_i v_2 - f_{i+1} - s f_i,$$

where $i \geqslant 0$ and $re_0 = c^{(1)}_0 v_1 - f_0$. We can then obtain that

$$f_0 = -\tfrac{1}{2} v_1, \quad f_1 = r^{(1)} v_1 + v_2,$$

$$f_2 = -[r^{(2)} r^{(1)} + (r^{(1)})^2 + r^{(1)} r + r^{(1)} s^{(1)} + r^{(1)} s] v_1 - (r^{(1)} + r + s) v_2;$$

$$re_0 = \tfrac{1}{2} v_1, \quad re_1 = \tfrac{1}{2} s v_1 - \tfrac{1}{2} v_2, \quad re_2 = r^{(1)} r v_1 + r v_2.$$

If we choose

$$h_1 = 2\xi f_0 f_1 = -\xi v_1 (r^{(1)} v_1 + v_2), \quad \xi = \text{const},$$

then the vector-valued function S_1 defined by (3.18) becomes

$$S_1(u,v) = \begin{pmatrix} -(r^{(1)} + r + s) v_1 - \xi r v_1 (r^{(1)} v_1 + v_2) \\ -r^{(1)} s v_1 - (r^{(1)} + s) v_2 - \xi r s v_1 (r^{(1)} v_1 + v_2) \end{pmatrix}.$$

Therefore, the integrable coupling of the generalized Toda lattice equation (3.11), defined by (3.19), reads as

$$r_{t_1} = r(s^{(-1)} - s) + r(r^{(-1)} - r^{(1)}),$$

$$
\begin{aligned}
s_{t_1} &= s(r - r^{(1)}),\\
v_{1,t_1} &= -(r^{(1)} + r + s)v_1 - \xi r v_1 (r^{(1)} v_1 + v_2),\\
v_{2,t_1} &= -r^{(1)} s v_1 - (r^{(1)} + s)v_2 - \xi r s v_1 (r^{(1)} v_1 + v_2),
\end{aligned}
\tag{3.27}
$$

the second subsystem of which is nonlinear with respect to both subsets of dependent variables when $\xi \neq 0$.

Case of $\alpha=0$ and $\beta=1$: Let us second compute an example of the hierarchy (3.26). Assume that $\alpha=0$ and $\beta=1$ for convenience, which corresponds to the Toda lattice hierarchy. In this case, we have $n_0=1$ in (2.14).

We take the initial set of functions as follows:

$$f_0 = g_0 = 0, \quad e_0 = -\tfrac{1}{2}.$$

Obviously from (3.22), we can have

$$f_{i+1}^{(1)} = -s f_i^{(1)} - (e_i^{(1)} + e_i) - (a_i^{(1)} + a_i)v_2 - b_i^{(1)} v_4 + b_i v_1,$$

$$g_{i+1} = -s g_i - r(e_i^{(1)} + e_i) - (a_i^{(1)} + a_i)v_3 + c_i^{(1)} v_1 - c_i v_4,$$

$$e_{i+1}^{(1)} - e_{i+1} = -s(e_i^{(1)} - e_i) + g_i^{(1)} - r f_i - (a_i^{(1)} - a_i)v_4 + c_i^{(1)} v_2 - b_i v_3,$$

where $i \geqslant 0$. It then follows that

$$f_1 = 1 + v_2^{(-1)}, \quad g_1 = r + v_3, \quad e_1 = v_3 + r(1 + v_2^{(-1)}),$$

$$f_2 = -(s^{(-1)} + r)(1 + v_2^{(-1)}) - v_3 - v_3^{(-1)} - r^{(-1)}(1 + v_2^{(-2)}) - v_4^{(-1)} + v_1^{(-1)},$$

$$g_2 = -s(r + v_3) - r[v_3^{(1)} + v_3 + r^{(1)}(1 + v_2) + r(1 + v_2^{(-1)})] + r^{(1)} v_1 - r v_4,$$

$$e_2^{(1)} - e_2 = (1 - s)(r^{(1)} - r + v_3^{(1)} - v_3 + r^{(1)} v_2 - r v_2^{(-1)}).$$

We can use the inverse formula (1.4) to compute e_2 here, but as we will see, this is not necessary for computing the corresponding integrable coupling.

Now if we choose

$$h_1 = \eta v_1 e_1 = \eta v_1 [v_3 + r(1 + v_2^{(-1)})], \quad \eta = \text{const},$$

then the vector-valued function T_1 defined by (3.25) becomes

$$
T_1(u,v) = \begin{pmatrix}
-(s - s^{(-1)})v_1,\\
-s v_2 - (s + r^{(1)})(1 + v_2) - r(1 + v_2^{(-1)}) + v_1 - v_3^{(1)}\\
-v_3 - v_4 + \eta v_1^{(1)}[v_3^{(1)} + r^{(1)}(1 + v_2)],\\
(s^{(-1)} + s)v_3 + rs + r[v_3^{(1)} + v_3 + r^{(1)}(1 + v_2) + r(1 + v_2^{(-1)})]\\
-r^{(1)} v_1 + r v_4 - \eta r v_1 [v_3 + r(1 + v_2^{(-1)})],\\
(s - 1)(r^{(1)} - r + v_3^{(1)} - v_3 + r^{(1)} v_2 - r v_2^{(-1)})
\end{pmatrix}.
$$

Therefore, the integrable coupling of the Toda lattice equation (3.10), defined by (3.26), reads as

$$r_{t_1} = r(s^{(-1)} - s), \quad s_{t_1} = r^{(1)} - r,$$

$$v_{1,t_1} = -(s - s^{(-1)})v_1,$$

$$\begin{aligned} v_{2,t_1} &= -sv_2 - (s + r^{(1)})(1 + v_2) - r(1 + v_2^{(-1)}) + v_1 - v_3^{(1)} - v_3 - v_4 + \eta v_1^{(1)}[v_3^{(1)} + r^{(1)}(1 + v_2)], \\ v_{3,t_1} &= (s^{(-1)} + s)v_3 + rs + r[v_3^{(1)} + v_3 + r^{(1)}(1 + v_2) + r(1 + v_2^{(-1)})] \\ &\quad - r^{(1)}v_1 + rv_4 - \eta r v_1[v_3 + r(1 + v_2^{(-1)})], \end{aligned} \tag{3.28}$$

$$v_{4,t_1} = (s - 1)(r^{(1)} - r + v_3^{(1)} - v_3 + r^{(1)}v_2 - rv_2^{(-1)}),$$

the second subsystem of which is nonlinear with respect to both subsets of dependent variables when $\eta \neq 0$.

IV. CONCLUSIONS AND REMARKS

A feasible approach to construct integrable couplings of discrete soliton equations has been proposed by taking advantage of semidirect sums of Lie algebras, and the resulting theory has been applied to the generalized Toda hierarchy of lattice equations to generate integrable couplings for the hierarchy. The key point in our generating scheme is to establish a relation between semidirect sums of Lie algebras and integrable couplings of discrete soliton equations. The underlying discrete matrix spectral problems are generated from semidirect sums of Lie algebras, and the discrete Lax spectral matrices associated with given soliton equations play the nonideal part in the semidirect sums.

In our analysis of the two specific semidirect sums, we have seen that there is always an arbitrary modified term $\Delta_{n,a}$. This indicates that higher order matrix spectral problems have more degrees of freedom in generating integrable systems. On the other hand, in all additional spectral submatrices such as U_{a_i}, one can take their dependence on the spectral parameter into consideration, and this will bring much more diverse integrable couplings.

There are also other questions about integrable properties of the resulting enlarged lattice equations, even in the case where additional spectral submatrices are independent of the spectral parameter. For example, can we solve the enlarged lattice equations by the inverse scattering transform? The class of Lie algebras in (2.8) provides a few realizations of semidirect sums of Lie algebras. Other possible realizations are still interesting, especially those which could carry significant information about integrable properties. Reductions of the presented cases of semidirect sums, which keep the uniqueness property of discrete spectral problems (see Ref. 17), could be good examples.

We would especially like to emphasize that we have been considering the problem of integrable couplings and the key is semidirect sums of Lie algebras. The initial Lie algebras G associated with given integrable systems in our construction can be simple (e.g., see Refs. 29 and 30), but semidirect sums of Lie algebras $\overline{G}$ are normally nonsimple (see Ref. 15). Our examples in Sec. II are all nonsimple, since the Killing forms on those semidirect sums of Lie algebras $\overline{G}$ are degenerate. However, there still exist specific nondegenerate bilinear forms on the Lie algebras $\overline{G}$, with nice invariance properties, and their corresponding generalized trace identities, which present Hamiltonian structures of the enlarged lattice equations.

To conclude, semidirect sums of Lie algebras provide a good source of matrix spectral problems for generating integrable systems, and thus the study of integrable couplings using semidirect sums of Lie algebras will enhance our understanding of classification of integrable systems. We are expecting to see more research on related topics.

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Tzitzéica transformation is a dressing action

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We classify the simplest rational elements in a twisted loop group, and prove that dressing actions of them, on proper indefinite affine spheres, give the classical Tzitzéica transformation and its dual. We also give the group point of view of the permutability theorem, construct complex Tzitzéica transformations, and discuss the group structure for these transformations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2195527]

I. INTRODUCTION

In 1910, Tzitzéica published a classical paper[21] on hyperbolic surfaces in $\mathbb{R}^3$ whose Gauss curvature at any point p is proportional to the fourth power of the distance from a fixed point to the tangent plane at p. He proved

$$w_{xy} = e^{w} - e^{-2w} \tag{1.1}$$

is the structure equation, and also constructed a geometric transformation of such surfaces that is similar to the well-known Bäcklund transformation of surfaces with constant negative curvature. These surfaces are invariant under affine transformations, and they are now known as (proper) affine spheres in affine differential geometry.

The classical Tzitzéica equation (1.1) was rediscovered in many mathematical and physical contexts afterwards (see, e.g., Refs. 5, 7, and 8). In recent years, techniques from soliton theory have been applied to this equation extensively by, e.g., Rogers and Schief in the context of gas dynamics,[15] Kaptsov and Shan'ko on multisoliton formulas,[11] Dorfmeister and Eitner on Weierstrass-type representation,[6] and Bobenko and Schief on its discretizations.[3,4] Terng and Uhlenbeck[20] gave a systematic method to construct Bäcklund-type transformations via dressing actions of simple rational loop group elements. It is natural to ask whether the classical Tzitzéica transformation is a dressing action of some loop element, whether there are new transformations of affine spheres, and what is the group structure of these transformations. This paper answers these questions.

In Sec. II, we give a brief review of classical results and provide the Lax pair of the structure equations. In Sec. III, we review the reality conditions for this Lax pair and give the loop group description of indefinite affine spheres. We then classify the simplest rational elements in this loop group and compute their dressing actions on affine spheres in Sec. IV. These rational elements cannot be constructed by projections as in Ref. 20 and the computation is harder. It turns out that one class of dressing action provides exactly the Tzitzéica transformation and the other provides the dual transformation. In Sec. V, we present the group point of view of the classical permutability theorem, construct complex Tzitzéica transformations and discuss the group structure of these transformations. Some examples are presented in the last section.

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II. INDEFINITE AFFINE SPHERE AND ITS LAX REPRESENTATION

Classical affine differential geometry studies the properties of surfaces in $\mathbb{R}^3$ invariant under the (equi) affine transformations $x \to Ax+v$, where $A \in \mathrm{SL}(3,\mathbb{R})$ and $x,\ v \in \mathbb{R}^3$. There are three fundamental affine invariants: the affine (or Blaschke) metric, the Fubini-Pick cubic form, and the third fundamental form (or the affine shape operator). These invariants satisfy certain compatibility equations and the fundamental theorem states that they then determine a surface uniquely up to affine transformations. Let us first review the definitions of these invariants (for more details see, e.g., Refs. 2, 13, and 18). The reader may also refer to Refs. 2–4 or 17 for an elementary description of affine spheres.

Let $X: M \hookrightarrow \mathbb{R}^3$ be an immersed surface with nondegenerate second fundamental form. Let $E=(e_1,e_2,e_3)$ be a local $\mathrm{SL}(3,\mathbb{R})$-frame on M such that e_1,e_2 are tangent to M, and e_3 is transversal to M. Let ω_1,ω_2 denote the dual coframe of e_1,e_2, i.e.,

$$\mathrm{d}X = e_1 \otimes \omega_1 + e_2 \otimes \omega_2.$$

Let (ω_{AB}) denote the $\mathrm{sl}(3,\mathbb{R})$-valued 1-form $E^{-1}\,\mathrm{d}E$, i.e.,

$$\mathrm{d}e_A = \sum_{B=1}^{3} e_B \otimes \omega_{BA}.$$

Then we have the structure equation

$$\begin{aligned} \mathrm{d}\omega_A &= -\sum\nolimits_B \omega_{AB} \wedge \omega_B, \\ \mathrm{d}\omega_{AB} &= -\sum\nolimits_C \omega_{AC} \wedge \omega_{CB}. \end{aligned} \tag{2.1}$$

Since $\omega_3=0$ on M, (2.1) implies that for $i=1,2$,

$$\omega_{3,i} = h_{i1}\omega_1 + h_{i2}\omega_2, \quad \text{with } h_{ij} = h_{ji}. \tag{2.2}$$

A direct computation shows that the quadratic form

$$g := |\det(h_{ij})|^{-1/4} \sum_{i,j=1}^{2} h_{ij}\omega_i\omega_j \tag{2.3}$$

is invariant under change of affine frames, and it is called the *affine metric* of M. M is said to be *definite* or *indefinite* if the affine metric is definite or indefinite, respectively.

The *affine normal* is $\xi := \triangle X/2$, where $\triangle$ is the Laplacian of g. It satisfies two natural geometric conditions,

(i) $\mathrm{d}\xi(\cdot) \in \mathrm{T}M$,
(ii) $i_\xi\,\mathrm{d}V = \mathrm{dvol}_g$ (the volume form of g);

and is essentially determined by them.

Take the exterior differentiation of (2.2) to get

$$\sum_j (\mathrm{d}h_{ij} + h_{ij}\omega_{3,3} - h_{ik}\omega_{kj} - h_{kj}\omega_{ki}) \wedge \omega^j = 0, \tag{2.4}$$

and define h_{ijk} by

$$\sum_k h_{ijk}\omega_k = \mathrm{d}h_{ij} + h_{ij}\omega_{3,3} - h_{ik}\omega_{kj} - h_{kj}\omega_{ki}. \tag{2.5}$$

Then (2.2) and (2.4) imply that h_{ijk} is symmetric in i,j,k. *The Fubini-Pick cubic form* is defined as

$$J := \sum_{i,j,k} h_{ijk}\omega_i\omega_j\omega_k,$$

which is an affine invariant.

We choose $e_3=\xi$. Then $\omega_{3,3}=0$. Exterior differentiate it to get

$$\omega_{13}\wedge\omega_{31}+\omega_{23}\wedge\omega_{32}=0.$$

Thus the following form

$$\mathrm{III} := |\det(h_{ij})|^{1/4}(\omega_{13}\omega_{31}+\omega_{23}\omega_{32})$$

is symmetric. This is the *third fundamental form*. Equivalently, we can first define the *affine shape operator* S,

$$S(u) := \mathrm{d}\xi(u), \quad \forall\, u\in T_pM,$$

then $\mathrm{III}(u,v)=g(S(u),v)=g(u,S(v))$. The *affine mean curvature* H and the *affine Gauss curvature* K are defined as $H=\mathrm{Tr}\,S/2$, $K=\det S$.

Definition 2.1: An *affine sphere* is a surface all of whose affine normals meet at a common point.

An equivalent definition is $S=H\cdot\mathrm{Id}$, i.e., the shape operator is a scalar multiple of the identity map and H is then the affine mean curvature. It follows from the structure equations that H must be constant. When $H=0$, all affine normals are parallel and the center is at infinity. Such surface is called *improper affine sphere* and has been completely classified in Ref. 2. When $H\neq 0$, it is called *proper affine sphere* and we can move the center to the origin and normalize H to 1 by scaling the ambient space and changing the orientation if necessary. Then $e_3=\xi=X$.

From now on we will only consider proper indefinite affine spheres in $\mathbb{R}^3$ with $\xi=X$. First note that there exists local asymptotic coordinate system (x,y) and a smooth function $w(x,y)$ such that the affine metric is

$$g = e^w(\mathrm{d}x\otimes\mathrm{d}y+\mathrm{d}y\otimes\mathrm{d}x).$$

We choose a frame $e_1=X_x$, $e_2=e^{-w}X_y$, and $e_3=\xi=X$. Then $\det(e_1,e_2,e_3)=1$, and

$$\omega_1=\mathrm{d}x=\omega_{13}=\omega_{32}, \qquad \omega_2=e^w\,\mathrm{d}y=\omega_{23}=\omega_{31},$$
$$\omega_{33}=0, \qquad (h_{ij})=\begin{pmatrix}0&1\\1&0\end{pmatrix}.$$

A direct computation using the formula (2.5) shows

$$\omega_{21}=a\,\mathrm{d}x, \quad \omega_{12}=be^{-2w}\,\mathrm{d}y \quad \text{for some functions } a,\ b;$$
$$J=-2a\,\mathrm{d}x^3-2b\,\mathrm{d}y^3.$$

Finally from $\mathrm{d}\omega_A+\Sigma_B\omega_{AB}\wedge\omega_B=0$ we get

$$\omega_{11}=-\omega_{22}=w_x\,\mathrm{d}x.$$

We have obtained the flat $\mathrm{sl}(3,\mathbb{R})$-valued 1-form

$$\omega = E^{-1}\,\mathrm{d}E=\begin{pmatrix} w_x\,\mathrm{d}x & be^{-2w}\,\mathrm{d}y & \mathrm{d}x\\ a\,\mathrm{d}x & -w_x\,\mathrm{d}x & e^w\,\mathrm{d}y\\ e^w\,\mathrm{d}y & \mathrm{d}x & 0\end{pmatrix}.$$

The compatibility equations are

$$d\omega + \omega \wedge \omega = 0 \Leftrightarrow \begin{cases} w_{xy} = e^w - abe^{-2w}, \\ a_y = 0, \quad b_x = 0. \end{cases} \tag{2.6}$$

When $ab \neq 0$ we may reparametrize the asymptotic coordinates to make $a=b=1$. Then (2.6) is simplified to the classical Tzitzéica equation.

Remark 2.2: It is known that ruled proper indefinite affine spheres correspond to the case $ab=0$ and they have been well understood (see Ref. 13). For nonruled case, the points at which $ab=0$ are called *planar points*.

The following observation is crucial for the integrability of proper indefinite affine spheres: The system (2.6) is invariant under the transformation

$$a \to \gamma a, \quad b \to \gamma^{-1} b$$

with $\gamma \in \mathbb{C}\backslash\{0\}$. Thus a family of flat connections is obtained,

$$\omega_\gamma = \begin{pmatrix} w_x\, dx & \gamma^{-1} b e^{-2w}\, dy & dx \\ \gamma a\, dx & -w_x\, dx & e^w\, dy \\ e^w\, dy & dx & 0 \end{pmatrix}.$$

The zero curvature equation of ω_γ is called the *Lax representation* of (2.6).

When we solve E_γ from

$$E_\gamma^{-1}\, dE_\gamma = \omega_\gamma \tag{2.7}$$

for any $\gamma \in \mathbb{R}\backslash\{0\}$, the last column of E_γ gives a family of affine spheres, whose affine fundamental invariants are

$$g = 2e^w\, dx\, dy, \quad S = \mathrm{Id}, \quad J = -2\gamma a\, dx^3 - \frac{2}{\gamma} b\, dy^3.$$

Let us recall the classical *duality relation* for indefinite affine spheres. Let $h=e^\omega$. Then Tzitzéica equation becomes

$$(\ln h)_{xy} = h - \frac{1}{h^2}, \quad \text{or } h_{xy}h - h_x h_y = h^3 - 1. \tag{2.8}$$

Classically (2.7) with $a=b=1$ was written as a linear system for X,

$$\begin{aligned} X_{xx} &= \frac{h_x}{h} X_x + \frac{\gamma}{h} X_y, \\ X_{xy} &= hX, \\ X_{yy} &= \frac{1}{\gamma h} X_x + \frac{h_y}{h} X_y. \end{aligned} \tag{2.9}$$

If X solves (2.9), then we can check that

$$X^* := \frac{1}{h} X_x \times X_y$$

is a solution of (2.9) with γ replaced by $-\gamma$. Here $\times$ is the vector cross product in $\mathbb{R}^3$. This is clearly a duality relation $(X^*)^* = X$.

Finally let us recall the classical Tzitzéica transformation.

Theorem 2.3 (Ref. 21). *Given a solution* (h, X) *of* (2.8) and (2.9), *and* ϕ_1 *any scalar solution of* (2.9) *with parameter* γ_1, *then the following transformation produces a new solution* (h_1, X_1) *of* (2.8) and (2.9):

$$h_1 := h - 2(\ln \phi_1)_{xy},$$
$$X_1 := \frac{(\gamma - \gamma_1)hX - 2\gamma(\ln \phi_1)_x X_y + 2\gamma_1(\ln \phi_1)_y X_x}{(\gamma + \gamma_1)h}. \tag{2.10}$$

III. THE REALITY CONDITIONS AND LOOP GROUP DESCRIPTION

Henceforth we assume $a=b=1$. To further reveal the hidden symmetry, let $\lambda = \sqrt[3]{\gamma}$ and change the frame E_γ to

$$F_\lambda = E_\gamma \operatorname{diag}(1/\lambda, \lambda, 1).$$

The gauged family of flat connections is then

$$\theta_\lambda = F_\lambda^{-1}\, dF_\lambda = \begin{pmatrix} w_x & 0 & \lambda \\ \lambda & -w_x & 0 \\ 0 & \lambda & 0 \end{pmatrix} dx + \lambda^{-1} \begin{pmatrix} 0 & e^{-2w} & 0 \\ 0 & 0 & e^{w} \\ e^{w} & 0 & 0 \end{pmatrix} dy. \tag{3.1}$$

For any $g \in \mathrm{SL}(3,\mathbb{C})$, we need to define $\tau(g) := \bar{g}$ and define σ by

$$\sigma(g) := T(g^t)^{-1}T^{-1}, \quad \text{where } T = \begin{pmatrix} 0 & 1 & 0 \\ -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon^2 \end{pmatrix}, \quad \epsilon = e^{\pi i/3}.$$

The automorphism σ has order 6 and induces the following automorphism (still denoted by σ) on the Lie algebra $\mathrm{sl}(3,\mathbb{C})$: $\sigma(A) = -TA^tT^{-1}$. Therefore σ gives the eigenspace decomposition: $\mathrm{sl}(3,\mathbb{C}) = \oplus_{j=0}^{5}\mathcal{G}_j$, where $\mathcal{G}_j$ is of eigenvalue ϵ^j. We compute that $X_j \in \mathcal{G}_j$ if and only if

$$X_0 = \begin{pmatrix} x_{11} & 0 & 0 \\ 0 & -x_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_1 = \begin{pmatrix} 0 & 0 & x_{13} \\ x_{21} & 0 & 0 \\ 0 & x_{13} & 0 \end{pmatrix},$$

$$X_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & x_{23} \\ -x_{23} & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} x_{11} & 0 & 0 \\ 0 & x_{11} & 0 \\ 0 & 0 & -2x_{11} \end{pmatrix},$$

$$X_4 = \begin{pmatrix} 0 & 0 & x_{13} \\ 0 & 0 & 0 \\ 0 & -x_{13} & 0 \end{pmatrix}, \quad X_5 = \begin{pmatrix} 0 & x_{12} & 0 \\ 0 & 0 & x_{23} \\ x_{23} & 0 & 0 \end{pmatrix}.$$

Note that $\sigma\tau = \tau^{-1}\sigma^{-1}$ implies that $\oplus_{j=0}^{5}(\mathrm{sl}(3,\mathbb{R}) \cap \mathcal{G}_j)$ is the corresponding eigenspace decomposition of $\mathrm{sl}(3,\mathbb{R})$.

The θ_λ in (3.1) satisfies two reality conditions (first given in Ref. 12),

$$\tau(\theta_\lambda) = \theta_{\bar{\lambda}}, \quad \sigma(\theta_\lambda) = \theta_{\epsilon\lambda}. \tag{3.2}$$

When we solve F_λ in (3.1) uniquely with the initial condition $F(0,0,\lambda) = I$, it is easy to show that F_λ also satisfies the reality conditions (3.2).

Let $\mathbb{C}_* := \mathbb{C}\backslash\{0\}$. We adopt the following notations for loop groups:

$$\Lambda G = \{\text{holomorphic maps from } \mathbb{C}_* \cap (\mathcal{O}_r \cup \mathcal{O}_{1/r}) \text{ to } G\},$$

$$\Lambda_+ G = \{\text{holomorphic maps from } \mathbb{C}_* \text{ to } G\},$$

$$\Lambda_{-}G = \{\text{holomorphic maps } f \text{ from } \mathcal{O}_r \cup \mathcal{O}_{1/r} \text{ to } G \text{ with } f(\infty) = I\},$$

where $0 < r < 1$ is sufficiently small and

$$\mathcal{O}_r = \{\lambda \in \mathbb{C} : |\lambda| < r\}, \quad \mathcal{O}_{1/r} = \{\lambda \in \mathbb{C} \cup \{\infty\} : |\lambda| > 1/r\}.$$

Similar notations also apply to their Lie algebras. Let $\Lambda^{\tau,\sigma}G$ denote the subgroup of $g \in \Lambda G$ satisfying the reality conditions (3.2). Then θ_λ in (3.1) is a $\Lambda_+^{\tau,\sigma}\mathrm{sl}(3,\mathbb{C})$-valued flat connection, and the corresponding frame F_λ for indefinite affine spheres lies in $\Lambda_+^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C})$. Conversely, given any smooth map F from a domain in $\mathbb{R}^2$ to $\Lambda_+^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C})$ satisfying

$$F^{-1}F_x = A\lambda + B, \quad F^{-1}F_y = C\lambda^{-1} + D \tag{3.3}$$

with $A_{32}C_{31} \neq 0$, the last column of F then gives an affine sphere with $h = A_{32}C_{31}$ and F differs from F_λ in (3.1) by a simple gauge. This is the loop group description for indefinite affine spheres (for details, see Refs. 3 and 6).

IV. DRESSING ACTIONS OF SIMPLE RATIONAL ELEMENTS

Let us briefly review the method of dressing action (the original idea went back to Ref. 22 but see Refs. 9 or 19 for an elementary introduction). Let $G = \mathrm{SL}(3,\mathbb{C})$, $g(\lambda) \in \Lambda_-^{\tau,\sigma}G$, and $F(x,y,\lambda) \in \Lambda_+^{\tau,\sigma}G$ the frame of an associated family of indefinite affine spheres. Assume we can do the following factorization for each fixed (x,y):

$$g(\lambda)F(x,y,\lambda) = \widetilde{F}(x,y,\lambda)\widetilde{g}(x,y,\lambda), \tag{4.1}$$

with $\widetilde{F} \in \Lambda_+^{\tau,\sigma}G$ and $\widetilde{g} \in \Lambda_-^{\tau,\sigma}G$. Then $\widetilde{F}$ also satisfies (3.3) and generates new affine spheres. We sketch the proof here. It suffices to prove that $\widetilde{F}^{-1}(\widetilde{F})_x$ and $\widetilde{F}^{-1}(\widetilde{F})_y$ are linear in λ and λ^{-1}, respectively. But

$$\widetilde{F}^{-1}(\widetilde{F})_x = \widetilde{g}F^{-1}g^{-1}(gF\widetilde{g}^{-1})_x = \widetilde{g}(F^{-1}F_x)\widetilde{g}^{-1} + \widetilde{g}(\widetilde{g}^{-1})_x = \widetilde{g}(A\lambda + B)\widetilde{g}^{-1} - \widetilde{g}_x\widetilde{g}^{-1}.$$

On the left-hand side, $\widetilde{F}^{-1}(\widetilde{F})_x$ is holomorphic in $\lambda \in \mathbb{C}\backslash\{0\}$; on the right it has a simple pole at ∞ since $g(\infty) = \widetilde{g}(\infty) = I$. So

$$\widetilde{F}^{-1}(\widetilde{F})_x = \widetilde{A}\lambda + \widetilde{B}.$$

Similarly, $\widetilde{F}^{-1}(\widetilde{F})_y$ is linear in $1/\lambda$. This completes the proof.

Furthermore, $g * F := \widetilde{F}$ defines a group action of $\Lambda_-^{\lambda,\sigma}G$ on the frames of affine spheres, which is called the *dressing action*.

The factorization (4.1) can indeed be done on a dense open subset of $\Lambda^{\tau,\sigma}G$ (see Refs. 1 and 14). There is no explicit construction for general g, but when g is a rational element, the factorization can be carried out using residue calculus (see Ref. 20). In search of simple rational elements in $\Lambda_-^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C})$, it helps to write $\sigma = \nu \circ \mu$ as the composition of two commuting automorphisms, where

$$\nu(g) := QgQ^{-1} \quad \text{with } Q = \mathrm{diag}(\epsilon^4, \epsilon^2, 1),$$

$$\mu(g) := P(g^t)^{-1}P \quad \text{with } P = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Here ν has been called the Coxeter-Killing automorphism, and the involution μ is the unique outer automorphism of $\mathrm{SL}(3,\mathbb{C})$ modulo inner ones. We observe that an element $g(\lambda) \in \Lambda G$ lies in $\Lambda^{\tau,\sigma}G$ if and only if

$$\tau(g_\lambda^-) = g_\lambda, \quad \nu(g_\lambda) = g_{\epsilon^4\lambda}, \quad \mu(g_\lambda) = g_{-\lambda}. \tag{4.2}$$

Remark 4.1: τ and μ define a symmetric space $\mathrm{SL}(3,\mathbb{R})/\mathrm{SO}(2,1)$. Here $\mathrm{SO}(2,1)$ is the isometry group of the quadratic form given by the symmetric matrix P, i.e., $2x_1x_2+x_3^2$ on $\mathbb{R}^3$. It was proved in Ref. 19 that if F_λ is the frame of an associated family of indefinite affine spheres, then $F_{-1}F_1^{-1}$ is a harmonic map from $\mathbb{R}^{1,1}$ to the symmetric space $\mathrm{SL}(3,\mathbb{R})/\mathrm{SO}(2,1)$.

We will first study rational elements in $\Lambda_-^\sigma G$. Due to the ν-reality condition in (4.2), the simplest rational element in $\Lambda_-^\sigma G$ may have only three simple poles $\{\alpha, \epsilon^2\alpha, \epsilon^4\alpha\}$ with $\alpha \in \mathbb{C}_*$. The element can always take the following special form:

$$g(\lambda) = I + \frac{2\alpha}{\lambda-\alpha}A + \frac{2\epsilon^2\alpha}{\lambda-\epsilon^2\alpha}B + \frac{2\epsilon^4\alpha}{\lambda-\epsilon^4\alpha}C. \tag{4.3}$$

Plug it into (ν,μ)-reality conditions in (4.2) and compare the residues, at each pole, we obtain that $g \in \Lambda_-^\sigma G$ if and only if

$$\begin{gathered} B = Q^{-1}AQ, \quad C = QAQ^{-1}, \\ A^tP(I - A - 2\epsilon B + 2\epsilon^2 C) = 0. \end{gathered} \tag{4.4}$$

Write $A=(a_{ij})$, and we compute that

$$(I - A - 2\epsilon B + 2\epsilon^2 C) = \begin{pmatrix} 1-3a_{11} & -3a_{12} & 3a_{13} \\ 3a_{21} & 1-3a_{22} & -3a_{23} \\ -3a_{31} & 3a_{32} & 1-3a_{33} \end{pmatrix}. \tag{4.5}$$

If the rank of A is 3, we get $A=I/3$ and $g(\lambda)$ is trivial. So there are two types left for A: rank 1 type and rank 2 type. A long but not hard computation implies that the **rank** 1 **type** is as follows:

$$A = \frac{1}{3}\begin{pmatrix} \dfrac{b}{2ab-1} \\ a \\ 1 \end{pmatrix}(a \quad b \quad 1) = \frac{1}{3}\begin{pmatrix} \dfrac{ab}{2ab-1} & \dfrac{b^2}{2ab-1} & \dfrac{b}{2ab-1} \\ a^2 & ab & a \\ a & b & 1 \end{pmatrix}, \tag{4.6}$$

with the corresponding loop group element

$$g(\lambda) = I + \frac{2}{\lambda^3-\alpha^3}\begin{pmatrix} \dfrac{\alpha^3 ab}{2ab-1} & \dfrac{\alpha\lambda^2 b^2}{2ab-1} & \dfrac{\alpha^2\lambda b}{2ab-1} \\ \alpha^2\lambda a^2 & \alpha^3 ab & \alpha\lambda^2 a \\ \alpha\lambda^2 a & \alpha^2\lambda b & \alpha^3 \end{pmatrix}; \tag{4.7}$$

and the rank 2 type [*thus the matrix* (4.5) *has rank* 1] is as follows:

$$A = \frac{1}{3}\begin{pmatrix} \dfrac{ab-1}{2ab-1} & \dfrac{-b^2}{2ab-1} & \dfrac{b}{2ab-1} \\ a^2 & 1-ab & -a \\ -a & b & 0 \end{pmatrix}, \tag{4.8}$$

with the corresponding loop group element

$$g(\lambda) = I + \frac{2}{\lambda^3 - \alpha^3}\begin{pmatrix} \frac{\alpha^3(ab-1)}{2ab-1} & \frac{-\alpha\lambda^2 b^2}{2ab-1} & \frac{\alpha^2\lambda b}{2ab-1} \\ \alpha^2\lambda a^2 & \alpha^3(1-ab) & -\alpha\lambda^2 a \\ -\alpha\lambda^2 a & \alpha^2\lambda b & 0 \end{pmatrix}. \tag{4.9}$$

Both types must meet the constraint $2ab \neq 1$.

Remark 4.2: We compute that $\det g$ is $[(\lambda^3+\alpha^3)/(\lambda^3-\alpha^3)]^{\mathrm{rank}(A)}$, i.e., only depending on the poles and the rank of the residues. A scaling by $(\det g)^{-1/3}$ will make them lie in $\mathrm{SL}(3,\mathbb{C})$, though not rational any more. Since the scaling does not affect the factorization and the dressing action, we will ignore this step henceforth.

Let $l := (a,b,1)$, ℓ be the line $\mathbb{C}\cdot l$, and introduce the following cone:

$$\Delta := \{(z_1,z_2,z_3) \in \mathbb{C}^3 \mid 2z_1z_2 = z_3^2, \text{ or } z_3 = 0\}.$$

Then $2ab \neq 1$ is equivalent to $\ell \subsetneq \Delta$. We observe that $\ell^t = \mathrm{Image}(\mathrm{Res}_\alpha g^t)$ for rank 1 type and $\ell^t = \mathrm{Kernel}(\mathrm{Res}_\alpha g\, P)$ for rank 2 type (here ℓ^t means $\mathbb{C}\cdot l^t$). Conversely, a line ℓ not in Δ determines the residue A and thus the simple element g uniquely in both types. Henceforth we always use $g_{\alpha,\ell}$ to denote the rank 1 type element (4.7) and use $h_{\alpha,\ell}$ to denote the rank 2 type element (4.9). We have proved the following theorem.

Theorem 4.3: *The simplest rational element in* $\Lambda_-^\sigma \mathrm{GL}(3,\mathbb{C})$ *is either* $g_{\alpha,\ell}$ *of rank* 1 *type* (4.7) *or* $h_{\alpha,\ell}$ *of rank* 2 *type* (4.9), *where* $\alpha \in \mathbb{C}_*$ *and* $\ell \subsetneq \Delta$.

Imposing the τ-reality condition $g(\bar{\lambda}) = g(\lambda)$ on both types, we obtain that one pole, say α, must be real and so is the residue A there. It is convenient in this case to let ℓ denote the real line $\mathbb{R}\cdot(a,b,1)$ in $\mathbb{R}^3$ and let Δ_0 denote $\Delta \cap \mathbb{R}^3$. We then have the following.

Corollary 4.4: The simplest rational element in $\Lambda_-^{\tau,\sigma}\mathrm{GL}(3,\mathbb{C})$ *is either* $g_{\alpha,\ell}$ *of rank* 1 *type or* $h_{\alpha,\ell}$ *of rank* 2 *type*, *where* $\alpha \in \mathbb{R}_*$ *and the real line* $\ell \subsetneq \Delta_0$.

We are ready to compute the dressing action of these simple elements.

Lemma 4.5: Let $g_{\alpha,\ell} \in \Lambda_-^{\tau,\sigma}\mathrm{GL}(3,\mathbb{C})$ *as in* (4.7), *and* $F \in \Lambda_+^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C})$. *If* $\ell := \ell F(\alpha) \subsetneq \Delta_0$, *then* $g_{\alpha,\ell}\cdot F$ *can be factored uniquely as*

$$g_{\alpha,\ell}\cdot F = \widetilde{F}\cdot g_{\alpha,\widetilde{\ell}} \in \Lambda_+^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C}) \times \Lambda_-^{\tau,\sigma}\mathrm{GL}(3,\mathbb{C}).$$

Proof: It suffices to prove that $\widetilde{F} := g_{\alpha,\ell}\cdot F\cdot g_{\alpha,\widetilde{\ell}}^{-1}$ lies in $\Lambda_+^{\tau,\sigma}\mathrm{SL}(3,\mathbb{C})$. Since $\widetilde{F}$ satisfies the reality conditions (4.2) and is holomorphic in $\mathbb{C}_*$ except for possible simple poles coming from the poles of $g_{\alpha,\ell}$ and $g_{\alpha,\widetilde{\ell}}^{-1}$, we only need to prove that the residues of $\widetilde{F}$ are zero at both α and $-\alpha$. But

$$\mu(g_{\alpha,\ell}(\lambda)) = g_{\alpha,\ell}(-\lambda) \Leftrightarrow P = g_{\alpha,\ell}(\lambda)Pg_{\alpha,\ell}(-\lambda)^t,$$

whose residue is zero at α implies that $\ell P g_{\alpha,\ell}(-\alpha)^t = 0$, or equivalently $g_{\alpha,\ell}(-\alpha)P\ell^t = 0$. These two equations are also true for $\widetilde{\ell}$. Therefore $(a,b,1)F(\alpha) \in \widetilde{\ell}$ and the special form of A in (4.6) imply that

$$\mathrm{Res}_\alpha \widetilde{F} = 2\alpha A F(\alpha) P g_{\alpha,\widetilde{\ell}}(-\alpha)^t P = 0,$$

and $F(-\alpha)P(\widetilde{a},\widetilde{b},1)^t \in [F(-\alpha)PF(\alpha)^t]\ell^t = P\ell^t$ implies that

$$\mathrm{Res}_{-\alpha} \widetilde{F} = 2\alpha g_{\alpha,\ell}(-\alpha)F(-\alpha)P\widetilde{A}^t P = 0.$$

The proof is completed once we notice that $\det \widetilde{F} = 1$ by Remark 4.2. □

Theorem 4.6: *The dressing action of rank* 1 *type* $g_{\alpha,\ell}$ *on the affine frames* $F(x,y,\lambda)$ *of proper indefinite affine spheres gives the classical Tzitzéica transformation*, *provided an open condition that* $\ell F(x,y,\alpha) \subsetneq \Delta_0$. *The dressing action of rank* 2 *type* $h_{\alpha,\ell}$ *gives the dual transformation.*

Proof: By Lemma 4.5, for fixed (x,y), we have the factorization

$$g_{\alpha,\ell}(\lambda)\cdot F(x,y,\lambda)=\tilde{F}(x,y,\lambda)\cdot g_{\alpha,\tilde{\ell}}(\lambda)$$

with $\tilde{\ell}=\ell F(x,y,\alpha)$. From $F(x,y,\alpha)=((X_\alpha)_x/\alpha,\alpha(X_\alpha)_y/h,X_\alpha)$, we get

$$(a,b,1)F(x,y,\alpha)=(\phi_x/\alpha,\alpha\phi_y/h,\phi)\in\tilde{\ell},$$

where $\phi:=(a,b,1)X_\alpha$ is a scalar solution of (2.9) with parameter α. Note that a constant scaling of ϕ does not change Tzitzéica transformation (2.10), and the solution space of the linear system (2.9) has dimension 3. Therefore, by varying ℓ,ϕ can be a generic scalar solution up to a constant multiple.

By the discussion at the beginning of this section, the third column of $\tilde{F}$ produces new affine sphere, so does the affine transformation of it by $g_{\alpha,\ell}^{-1}$,

$$\begin{aligned}\hat{X}&:=g_{\alpha,\ell}^{-1}(\tilde{F})_3=(F(\lambda)g_{\alpha,\tilde{\ell}}(\lambda)^{-1})_3\\&=(F(\lambda)Pg_{\alpha,\tilde{\ell}}(-\lambda)^tP)_3\\&\overset{(4.7)}{=}(X_x/\lambda,\lambda X_y/h,X)\cdot\frac{1}{\lambda^3+\alpha^3}\cdot\begin{pmatrix}2\alpha^3\lambda\phi_y/(h\phi)\\-2\lambda^2\phi_x/\phi\\\lambda^3-\alpha^3\end{pmatrix}\\&=\frac{(\lambda^3-\alpha^3)hX-2\lambda^3(\ln\phi)_xX_y+2\alpha^3(\ln\phi)_yX_x}{(\lambda^3+\alpha^3)h}.\end{aligned}$$

The corresponding solution to Tzitzéica equation is given by

$$\hat{h}=\hat{X}_{xy}/\hat{X}=h-2(\ln\phi)_{xy}.$$

This is exactly the classical Tzitzéica transformation (2.10) with

$$\gamma=\lambda^3,\quad \gamma_1=\alpha^3,\quad \phi_1=\phi.$$

In rank 2 type case, there is a similar factorization $h_{a,\ell}\cdot F=\tilde{F}\cdot h_{\alpha,\tilde{\ell}}$ when $\tilde{\ell}:=\mathrm{Kernel}^t(AF(\alpha)P)\subsetneq\Delta_0$. We omit the details and present the corresponding transformation on affine spheres

$$\tilde{X}=\frac{(\lambda^3+\alpha^3)hX-2\lambda^3(\ln\phi)_xX_y-2\alpha^3(\ln\phi)_yX_x}{(\lambda^3-\alpha^3)h},$$

where ϕ is the same scalar solution as the rank 1 type case. We see that

$$\hat{X}_\lambda=-\tilde{X}_{-\lambda},$$

i.e., $-\tilde{X}$ gives the dual of $\hat{X}$. This completes the proof. □

V. PERMUTABILITY THEOREM AND COMPLEX TZITZÉICA TRANSFORMATIONS

Let us briefly review the classical description of the permutability theorem. In Theorem 2.3, let ϕ_1,ϕ_2 be the scalar solution of (2.9) with parameter γ_1,γ_2, respectively. Then using ϕ_1 to apply Tzitzéica transformation on h, we get a new solution to Tzitzéica equation,

$$h_1:=h-2(\ln\phi_1)_{xy}.$$

Applying Tzitzéica transformation (2.10) to (ϕ_2,γ_2), we obtain

$$\phi_{12} := \frac{(\gamma_2 - \gamma_1)h\phi_2 - 2\gamma_2(\ln \phi_1)_x(\phi_2)_y + 2\gamma_1(\ln \phi_1)_y(\phi_2)_x}{(\gamma_2 + \gamma_1)h} \tag{5.1}$$

as a scalar solution to (2.9) with new h_1 and parameter γ_2. Therefore we can use ϕ_{12} to apply Tzitzéica transformation again on the new h_1, i.e.,

$$h_{12} = h_1 - 2(\ln \phi_{12})_{xy}$$

will give another solution to Tzitzéica equation. In this two step iteration, we may interchange the roles of ϕ_1 and ϕ_2 to obtain h_{21} as another new solution. The permutability theorem claims $h_{12} = h_{21}$. Similarly we can apply this two step iteration to the affine sphere X to obtain X_{12} and X_{21}, respectively, and the equality $X_{12} = X_{21}$ still holds.

We will give a group point of view to this permutability theorem.

Lemma 5.1: Let $g_{\alpha_i,\ell_i}(\lambda)(i=1,2)$ *be of rank* 1 *type with* $\alpha_1^3 \neq \pm\alpha_2^3$. *If both* $\tilde{\ell}_1 := \ell_1 g_{\alpha_2,\ell_2}(\alpha_1)^{-1}$ *and* $\tilde{\ell}_2 := \ell_2 g_{\alpha_1,\ell_1}(\alpha_2)^{-1}$ *are not in* Δ, *then*

$$g_{\alpha_2,\tilde{\ell}_2} g_{\alpha_1,\ell_1} = g_{\alpha_1,\tilde{\ell}_1} g_{\alpha_2,\ell_2}. \tag{5.2}$$

Proof: It is equivalent to prove that $f := g_{\alpha_1,\tilde{\ell}_1} g_{\alpha_2,\ell_2} g_{\alpha_1,\ell_1}^{-1}$ equals $g_{\alpha_2,\tilde{\ell}_2}$. First of all, they both are rational elements in the group $\Lambda^{\sigma}_{-}\mathrm{GL}(3,\mathbb{C})$. It suffices to prove that their poles and residues are the same.

Let $l_i=(a_i,b_i,1)$ and $\tilde{l}_i=(\tilde{a}_i,\tilde{b}_i,1)$ span ℓ_i and $\tilde{\ell}_i$, respectively. Similar to the proof of Lemma 4.5, we compute that

$$\mathrm{Res}_{\alpha_1} f = 2\alpha_1 \tilde{A}_1 g_{\alpha_2,\ell_2}(\alpha_1) P g_{\alpha_1,\ell_1}(-\alpha_1)^t P = 0$$

since $\tilde{l}_1 g_{\alpha_2,\ell_2}(\alpha_1) \in \ell_1$, and

$$\mathrm{Res}_{-\alpha_1} f = -2\alpha_1 g_{\alpha_1,\tilde{\ell}_1}(-\alpha_1) g_{\alpha_2,\ell_2}(-\alpha_1) P A_1^t P = 0$$

since $g_{\alpha_2,\ell_2}(-\alpha_1) P l_1^t \in [g_{\alpha_2,\ell_2}(-\alpha_1) P g_{\alpha_2,\ell_2}(\alpha_1)^t]\tilde{\ell}_1^t = P\tilde{\ell}_1^t$. Thus f has only three simple poles $\{\alpha_2, \epsilon^2\alpha_2, \epsilon^4\alpha_2\}$, same as $g_{\alpha_2,\tilde{\ell}_2}$.

Now due to the ν reality condition in (4.2), we only need to prove that their residues at α_2 are the same. But

$$\mathrm{Image}(\mathrm{Res}_{\alpha_2} f^t) = \mathrm{Image}(g_{\alpha_1,\ell_1}(\alpha_2)^{-1})^t A_2^t g_{\alpha_1,\tilde{\ell}_1}(\alpha_2)^t = (g_{\alpha_1,\ell_1}(\alpha_2)^{-1})^t \ell_2^t = \tilde{\ell}_2^{\,t} = \mathrm{Image}(\mathrm{Res}_{\alpha_2} g^t_{\alpha_2,\tilde{\ell}_2}).$$

Then $\mathrm{Res}_{\alpha_2} f$ must be the same as $\mathrm{Res}_{\alpha_2}(g_{\alpha_2,\tilde{\ell}_2})$ since rank 1 type residue is uniquely determined by the above image. This completes the proof. □

Example 5.2: Choose two nonzero poles α_1, α_2 such that $\alpha_1^3 \neq \pm\alpha_2^3$, and let $\ell_i = \mathbb{C}\cdot(0,b_i,1)$ for $i=1,2$. Then $g_{\alpha_2,\tilde{\ell}_2} g_{\alpha_1,\ell_1} = g_{\alpha_1,\tilde{\ell}_1} g_{\alpha_2,\ell_2}$ holds for $\tilde{\ell}_i = \mathbb{C}\cdot(0,\tilde{b}_i,1)$ with

$$\tilde{b}_1 = \frac{(\alpha_1^3 + \alpha_2^3)b_1 - 2\alpha_1\alpha_2^2 b_2}{(\alpha_1^3 - \alpha_2^3)}, \quad \tilde{b}_2 = \frac{2\alpha_1^2\alpha_2 b_1 - (\alpha_1^3 + \alpha_2^3)b_2}{(\alpha_1^3 - \alpha_2^3)}.$$

Theorem 5.3: *Use the same notation and the factorization formula* (5.2) *in Lemma 5.1. Let all* α_i, ℓ_i *be real. Let* $F_1 := g_{\alpha_1,\ell_1} * F$ *and* $F_2 := g_{\alpha_2,\ell_2} * F$, *where* * *is the dressing action on the frames* $F(x,y,\lambda)$ *of affine spheres. Then the following holds and implies the classical permutability theorem*:

$$(g_{\alpha_2,\tilde{\ell}_2} g_{\alpha_1,\ell_1}) * F = g_{\alpha_2,\tilde{\ell}_2} * F_1 (=: F_{12}) = (g_{\alpha_1,\tilde{\ell}_1} g_{\alpha_2,\ell_2}) * F = g_{\alpha_1,\tilde{\ell}_1} * F_2 (=: F_{21}). \tag{5.3}$$

Proof: Because the dressing action is a group action, (5.3) certainly holds by (5.2). Let $l_i = (a_i,b_i,1)$ and $\tilde{l}_i=(\tilde{a}_i,\tilde{b}_i,1)$ span ℓ_i and $\tilde{\ell}_i$, respectively. From the proof of Theorem 4.6, F_1:

$=g_{\alpha_1,\ell_1}*F$ means in classical terms the following: Tzitzéica transformation via $\phi_1:=l_1(F(\alpha_1))_3$ on $X=(F)_3$ gives a new affine sphere $X_1:=g^{-1}_{\alpha_1,\ell_1}(F_1)_3$. Therefore $F_{12}:=g_{\alpha_2,\tilde{\ell}_2}*F_1$ implies that Tzitzéica transformation via $\phi_{12}:=\tilde{l}_2(F_1(\alpha_2))_3$ on $(F_1)_3=g_{\alpha_1,\ell_1}X_1$ gives a new affine sphere $g^{-1}_{\alpha_2,\tilde{\ell}_2}(F_{12})_3$. We observe that

$$\phi_{12}:=\tilde{l}_2(F_1(\alpha_2))_3=c_0 l_2 g_{\alpha_1,\ell_1}(\alpha_2)^{-1}(F_1(\alpha_2))_3=c_0 l_2 X_1(\alpha_2),$$

which coincides with the classical formula (5.1) except for a negligible constant c_0 when we plug in $\phi_2:=l_2X(\alpha_2)$.

So Tzitzéica transformation via ϕ_{12} on $X_1=g^{-1}_{\alpha_1,\ell_1}(F_1)_3$ produces

$$X_{12}=g^{-1}_{\alpha_1,\ell_1}(g^{-1}_{\alpha_2,\bar{\ell}_2}F_{12})_3=(g^{-1}_{\alpha_1,\ell_1}g^{-1}_{\alpha_2,\bar{\ell}_2}F_{12})_3.$$

Similarly $X_{21}=(g^{-1}_{\alpha_2,\ell_2}g^{-1}_{\alpha_1,\tilde{\ell}_1}F_{21})_3$. Therefore, by (5.2) and (5.3) we obtain the classical permutability theorem: $X_{12}=X_{21}$, which automatically implies $h_{12}=h_{21}$ for the corresponding affine metrics.□

There is some rational element in $\Lambda^{\tau,\sigma}_{-}\mathrm{GL}(3,\mathbb{C})$ which has six simple poles but none of them are real. The poles must form two conjugate triples as $\{\alpha,\epsilon^2\alpha,\epsilon^4\alpha\}$ and $\{\bar{\alpha},\epsilon^2\bar{\alpha},\epsilon^4\bar{\alpha}\}$, where we may assume $0<\arg(\alpha)<\pi/3$ without loss of generality. So such element is not a product of *real* rank 1 or 2 type elements. In fact, we can use Lemma 5.1 to construct them.

Proposition 5.4: Let $\alpha\in\mathbb{C}_*$ *with* $\arg(\alpha)\in(0,\pi/6)\cup(\pi/6,\pi/3)$. *Let* $\ell\subsetneq\Delta$. If $\ell^*:=\ell\cdot g_{\alpha,\ell}(\bar{\alpha})^{-1}\subsetneq\Delta$, *then* $f_{\alpha,\ell}:=g_{\bar{\alpha},\ell^*}g_{\alpha,\ell}\in\Lambda^{\tau,\sigma}_{-}\mathrm{GL}(3,\mathbb{C})$.

Proof: We first observe that $f_{\alpha,\ell}$ lies in $\Lambda^{\sigma}_{-}\mathrm{GL}(3,\mathbb{C})$. It suffices to verify $f(\bar{\lambda})=f(\lambda)$, which is

$$g_{\alpha,\bar{\ell}^*}g_{\bar{\alpha},\bar{\ell}}=g_{\bar{\alpha},\ell^*}g_{\alpha,\ell}.$$

Since $\ell^*=\bar{\ell}\cdot g_{\alpha,\ell}(\bar{\alpha})^{-1}\subsetneq\Delta$ implies $\bar{\ell}^*=\ell\cdot g_{\bar{\alpha},\bar{\ell}}(\alpha)^{-1}\subsetneq\Delta$ and $\arg(\alpha)\neq\pi/6$ implies $\alpha^3\neq-\bar{\alpha}^3$, the above factorization holds by Lemma 5.1. □

The dressing action of $f_{\alpha,\ell}$ on affine spheres can be viewed as the composition of two conjugate complex Tzitzéica transformations, which produces a real solution in the end. The permutability Theorem 5.3 can be applied to compute this action. Solutions from this construction are often called breather type solutions.

It is not hard to show, by a similar residue calculus as before, that any rational element with six simple poles as above can be constructed from Proposition 5.4. What would be much messier, if not harder, to prove is that the subgroup of all rational elements in $\Lambda^{\tau,\sigma}_{-}\mathrm{GL}(3,\mathbb{C})$ is generated by $g_{\alpha,\ell}$'s, $f_{\alpha,\ell}$'s, and their rank 2 type brothers. This subgroup can then be regarded as the group of Tzitzéica transformations on affine spheres. We will leave this interesting problem for future study.

VI. BASIC EXAMPLES

In this section, we use x,y,z as the standard $\mathbb{R}^3$ coordinates to represent the immersion X, and use u,v to denote the asymptotic coordinates of the affine spheres.

Example 6.1 (*the vacuum solution):* The vacuum solution to Tzitzéica equation (see also Refs. 6 and 15) is $\omega_0\equiv0$ (or $h_0\equiv1$). One can integrate (3.1) to obtain the whole family of frames. The Cartesian equation of the surface is then obtained by the determinant

$$x^3+y^3+z^3-3xyz=1.$$

Note that it is independent of the parameter λ. So this family is really a family of parametrizations of the same affine sphere.

A general scalar solution of system (2.9) with parameter $\gamma=\lambda^3$ is

$$\phi(\lambda)=c_0R(\lambda)+c_1R(\epsilon^2\lambda)+c_2R(\epsilon^4\lambda),\tag{6.1}$$

where $R(\lambda):=\exp(\lambda u+\lambda^{-1}v)$.

Therefore we may choose the following asymptotic parametrizations of the vacuum affine sphere after certain affine transformations:

$$X_0(u,v,\lambda)=\begin{pmatrix}\exp[-(\lambda u+\lambda^{-1}v)/2]\cos[\sqrt{3}(\lambda u-\lambda^{-1}v)/2]\\ \exp[-(\lambda u+\lambda^{-1}v)/2]\sin[\sqrt{3}(\lambda u-\lambda^{-1}v)/2]\\ \frac{2}{3\sqrt{3}}\exp(\lambda u+\lambda^{-1}v)\end{pmatrix},$$

which is a surface of revolution (Note that Jonas has classified all affine spheres of revolution in Ref. 10 using elliptic functions).

Example 6.2 (*the one-soliton solution):* Apply Tzitzéica transformation to the vacuum solution we obtain the one-soliton solution h_1. By (6.1), $\phi_1=\phi(\lambda_1)$ is a scalar solution of system (2.9) with parameter $\gamma_1=\lambda_1^3$. It is real when $c_0\in\mathbb{R}$, $c_1=\overline{c_2}$, and $\lambda_1\in\mathbb{R}_*$. Compute $h_1=1-2\ (\ln\phi_1)_{uv}$:

$$h_1=1-\frac{6\beta_0\exp(3s_1/2)\cos(\sqrt{3}t_1/2+\theta_0)+1.5}{[\beta_0\exp(3s_1/2)+\cos(\sqrt{3}t_1/2+\theta_0)]^2},$$

where $c_1=\rho_0 e^{i\theta_0}$, $\beta_0=c_0/(2\rho_0)$, $s_1=\lambda_1 u+\lambda_1^{-1}v$, and $t_1=\lambda_1 u-\lambda_1^{-1}v$. The family of affine spheres $X_1(u,v,\lambda)$ has a long expression given by (2.10).

When $\beta_0=0$ (i.e., $c_0=0$), we have the special solution

$$h_1=1-1.5\sec^2[\sqrt{3}(\lambda_1 u-\lambda_1^{-1}v)/2+\theta_0]. \tag{6.2}$$

We give explicit formula for this family of affine spheres,

$$\begin{aligned}X_1(u,v,\lambda)=&\frac{(\lambda^3-\lambda_1^3)}{(\lambda^3+\lambda_1^3)}X_0(u,v,\lambda)\\&+\frac{\sqrt{3}\lambda\lambda_1\tan(\sqrt{3}t_1/2+\theta_0)}{(\lambda^3+\lambda_1^3)}.\begin{pmatrix}e^{-s/2}[\lambda\cos(\sqrt{3}t/2+4\pi/3)+\lambda_1\cos(\sqrt{3}t/2+2\pi/3)]\\ e^{-s/2}[\lambda\sin(\sqrt{3}t/2+4\pi/3)+\lambda_1\sin(\sqrt{3}t/2+2\pi/3)]\\ 2e^{s}(\lambda+\lambda_1)/(3\sqrt{3}).\end{pmatrix}\end{aligned} \tag{6.3}$$

Note that ϕ_1 need not be real to produce real h_1. For example, (6.2) will be a real hyperbolic function solution when λ_1 and θ_0 are pure imaginary. In this case the real (or imaginary) part of (6.3) still produces affine spheres, among which are the stationary and traveling one-soliton affine sphere shown in Ref. 16. Some pictures have already been shown in Refs. 15 and 16. In terms of dressing action, λ_1 is the pole of some rank 1 type simple element $g_{\lambda 1,\ell}$. So dressing actions of $g_{\lambda 1,\ell}$ with a pure imaginary pole (or a pole whose argument is $\pm\pi/6$) may also produce new real affine spheres sometime.

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Gravitation theory in a fractal space-time

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Assimilating the physical space-time with a fractal, a general theory is built. For a fractal dimension $D=2$, the virtual geodesics of this space-time implies a generalized Schrödinger type equation. Subsequently, a geometric formulation of the gravitation theory on a fractal space-time is given. Then, a connection is introduced on a tangent bundle, the connection coefficients, the Riemann curvature tensor and the Einstein field equation are calculated. It results, by means of a dilation operator, the equivalence of this model with quantum Einstein gravity. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196747]

I. INTRODUCTION

A fractal structure is a manifestation of the universality of self-organization processes, a result of a sequence of spontaneous symmetry breaking. Space-time itself may be a fractal. Some arguments in favor of the universality of a fractal structure of space-time and matter at small and large scales are given in Refs. 1 and 2: "(i) Fractal trajectories in space with Hausdorff dimension two (a Peano-Moore curve) exhibit both an uncertainty principle and a de Broglie relation. Quantum particles move statistically on such a fractal (Feynman) paths. Thus, the Schrödinger equation may be interpreted as a fractal signature of space-time; (ii) The formal analytic continuation ($t \rightarrow it$) which relates the Schrödinger and diffusion equations has a physical alternative: there is a (classical and quantum) stochastic fluid which can be either a fluid of probability for a unique element or a real fluid composed of elements undergoing quasi-Brownian motion. A (composite) particle (corpuscle with internal structure) may be one or a small cluster of stochastic elements. There is a sort of democracy (statistical self-similarity) between the stochastic element constituting the particle. As regards the cause of the randomness, the parton model involves a fragmentation of the partons. The diffusion may be considered as a Brownian (random) motion which is superimposed on the Hamiltonian time development. This leads to a Langevin equation which is equivalent to a Fokker-Planck equation for distribution function $\rho(\xi,t)$ in the phase space, $\partial\rho/\partial t + \{H,\rho\} - (D/2)\Delta^H\rho = 0$, where $-\Delta^H\rho$ is a positive semidefinite second order differential operator which is determined by the Hamiltonian dynamics and a sympletic metric $g^{\alpha\beta} = \langle \Delta\xi^\alpha \Delta\xi^\beta \rangle$ on phase space; (iii) Nature does not 'fractalize' (and quantize); it is intrinsically fractal (and quantum). Wave function of the Universe is a solution of the Weller-DeWitt equation of quantum cosmology and corresponds to the Schrödinger equation. This can be related to the fact that observations of the galaxy-galaxy and cluster-cluster correlations, as well as other large-scale structure can be fit with a fractal with $D_f \approx 1.2$ which may have grown from two-dimensional sheet-like objects such as domain walls or string wakes. The fractal dimension D_f can serve as a constraint on the properties of the stochastic motion responsible for limiting the fractal structure; (iv) The non-

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linear (soliton) equation corresponds to a (linear) Schrödinger equation coupled to a medium with specific nonlocal response. Physically, this model is similar to a simple case of linear propagation of thin beams in a wave-guide. Thus, a free photon in (fractal) space represents in fact a "bouncing ball" in a wave-guide. In other words, space-time is structured as a (fractal) web if optical fibers (channels) which represents a skeleton of space-time; (v) The proper wave-function $(\psi_1, \psi_2, \psi_3, \ldots)$ describing the hydrogen-like atom are similar to the electromagnetic models $(\mathrm{TEM}_0, \mathrm{TEM}_1, \mathrm{TEM}_2, \ldots)$ in optical resonating cavities; (vi) It is known that in quasi-crystalline phase there exists atomic clusters with hierarchical and quasi-periodic packing which display a scale-invariance under appropriate inflation/deflation transformation. In the case of a one-dimensional quasi-periodic chain there appears a new type of electronic ('critical') state which manifests a multifractal nature."

In particular, $\epsilon^{(\infty)}$ Cantorian fractal space-time is constructed as an infinite numbers of elementary Cantor sets with all conceivable Hausdorff dimension. This space has three dimensions, the formal dimension $n_f=\infty$, the topological dimension $n_T=4$, and the Hausdorff dimension $\langle d_c \rangle = 4 + \phi^3 = 4.236\,067\,977$.[3] A fractal path in the Cantorian space time has always a fractal Hausdorff dimension of $d_H=2$, and can be considered a two-dimensional projection of a fractal string [in three-dimensional (3D) space] which may represent a cosmic string. Then, the stability of the solitonic objects (strings and vortices) in quantum fields theory implies instantons.[4,5] An instanton may be interpreted as a tunneling transition and it is effectively an unusual transition between the energy levels of Dirac's sea. This remarkable construction was subsequently used by 't Hooft to resolve the $U(I)$ problem of the standard model and to explain the mass of the η meson. However, seen from the $\epsilon^{(\infty)}$ symplictic vacuum point of view, such "event," are completely natural and go on all the time to ensure the symplictic topology of the vacuum (VAK) as the ultimate source of all of the physics particles.[4] It might be possible to interpret supersymmetry (SUSY) and exotic particles in an analogous way.[4,5]

The Cantorian gravity is effectively the quantum gravity of $\epsilon^{(\infty)}$ theory (El Naschie's Cantorian gravity).[4,6] In turn Cantorian-fractal gravity is an effect that is, in essence, analogous to the van der Waals forces and may therefore be understood in terms of what has been termed the Feynman—El Naschie conjecture.[4] In short, the idea is the following[4]: It is well known that the speed at which "time flows" could be slowed down by a gravitational field. If this is true, and it is true according to Einstein's theory, then the converse is also true. This means that by changing the "speed" of the passing of time, one can "create" a gravitational effect. Put in a different way, a fluctuation in time creates a fluctuation in gravity and vice versa. Now the fundamental idea in the El Naschie's theory is that space-time is a random Cantorian fractal, which means that "time" is also a fractal. Since even a regular fractal possesses an "intrinsic fluctuation" which may clearly be seen from a parametric representation of say a Peano curve, the random fractal nature of Cantorian time must be seen as the cause for gravitational fluctuation. Similar to van der Waals forces the expectation or mean value of this fluctuation at the VAK level is a nonzero quantity and is that the origin of "fractal" gravity which we can now link to mass via Einstein's equivalence principle. The preceding discussion could be summarized in one single sentence; the fractalness of space-time is the origin of massiveness. A simple logical consequence of the previous discussion seems to be that "particles" for which times does not pass could not possibly have any rest mass. Thus the photon for which times does not pass as far as our classical theories tell us, must be "massless".

In this article we give a geometric formulation of the gravitation theory in a fractal space-time.

II. A MATHEMATICAL MODEL OF THE FRACTAL SPACE-TIME

Let us suppose that the motion of the various physical objects takes place on continuous, but nowhere differentiable, curves, hence on fractals. In order to save the differential equations of physics, we consider, for a real fractalic function $f(x)$,[5] its approximation obtained from smoothing it or averaging at various resolutions

$$f(x,\epsilon) = \int_{-\infty}^{+\infty} \phi(x,y,\epsilon) f(y) \mathrm{d}y, \tag{1}$$

where $\phi(x,y,\epsilon)$ is a smoothing function centered on x. Now we impose $\lim_{\epsilon\to 0} \phi(x,y,\epsilon) = \delta_{x-y}$ hence

$$\lim_{\epsilon\to 0} f(x,\epsilon) = f(x). \tag{2}$$

$f(x,\epsilon)$ can be everywhere differentiable and $f(x)$ is the so-called *fractal function*.[5] In this treatment we have a new variable (a new dimension), the *resolution* ϵ.

Let us consider an infinitesimal dilatation

$$\epsilon \to \epsilon' = \epsilon(1 + \mathrm{d}\rho) = \epsilon + \epsilon\, \mathrm{d}\rho \tag{3}$$

to the resolution. Omitting the x dependence of a function $\mathcal{L}$ (e.g., the length) we have

$$\mathcal{L}(\epsilon') = \mathcal{L}(\epsilon + \epsilon\, \mathrm{d}\rho) = \mathcal{L}(\epsilon) + \epsilon \frac{\partial \mathcal{L}(\epsilon)}{\partial \epsilon} \mathrm{d}\rho, \tag{4}$$

or

$$\mathcal{L}(\epsilon') = (1 + D\, \mathrm{d}\rho)\mathcal{L}(\epsilon). \tag{5}$$

Here

$$D = \epsilon\, \partial/\partial\epsilon = \partial/\partial \ln \epsilon \tag{6}$$

as

$$\partial/\partial\epsilon = (\partial \ln \epsilon/\partial\epsilon)(\partial/\partial \ln \epsilon) = (1/\epsilon)\, \partial/\partial \ln \epsilon \tag{7}$$

with D the dilation operator.

From the previous equations it is obvious that the intrinsic variable of resolution is not ϵ, but $\ln \epsilon$. This claim has an important consequence. Since both the argument of the logarithm and the exponent of the exponential function must be nondimensional, the same feature must have the variables of the fractal functions (in the aforementioned case x and ϵ). It does not mean that we cannot work with variables like distance, or time, but they are divided as constants of the same physical dimension, having the unitary dimension. For example, the time t measured in seconds is in fact divided by $t_0 = 1$ s.

The nondifferentiable nature of space-time implies some dramatic consequences.

(i) A breaking of differential time reflection invariance. Let us consider indeed the usual definition of the derivative of a given function with respect to time

$$\left(\frac{\mathrm{d}f}{\mathrm{d}t}\right) = \lim_{\mathrm{d}t\to 0} \frac{f(t + \mathrm{d}t) - f(t)}{\mathrm{d}t} = \lim_{\mathrm{d}t\to 0} \frac{f(t) - f(t - \mathrm{d}t)}{\mathrm{d}t}. \tag{8}$$

The two definitions are equivalent in the differentiable case. One passes from one to the other by the transformation $dt \to -dt$ (time reflection invariance at the infinitesimal level). In the nondifferentiable situation considered here, both definitions fail, since the limits are no longer defined. The fractal method solves this problem in the following way: we attribute to the differential element $\mathrm{d}t$ the new meaning of a variable, identified with a time resolution, $\mathrm{d}t = \delta t$. The passage to the limit $dt \to 0$ is actually devoid of physical meaning (an infinite energy would be needed to really perform a measurement at zero time resolution interval). The physics is now in the behavior of the function during the "zoom" operation on $\mathrm{d}t$. The two functions f'_+ and f'_- are now defined as explicit functions of t and of $\mathrm{d}t$:

$$f'_+(t,\mathrm{d}t)=\frac{f(t+\mathrm{d}t,\mathrm{d}t)-f(t,\mathrm{d}t)}{\mathrm{d}t}, \tag{9a}$$

$$f'_-(t,\mathrm{d}t)=\frac{f(t,\mathrm{d}t)-f(t-\mathrm{d}t,\mathrm{d}t)}{\mathrm{d}t}. \tag{9b}$$

(ii) We can write:

$$\mathrm{d}X^i_\pm=\mathrm{d}x^i_\pm+\mathrm{d}\xi^i_\pm \tag{10}$$

for the forward process (+) and backward process (−), respectively. Here $\mathrm{d}x^i_\pm$ are the right and left differentials of the classical variables, and $\mathrm{d}\xi^i_\pm$ describe the fractal behavior. So that

$$\langle dX^i_\pm\rangle=dx^i_\pm, \tag{11a}$$

$$\langle d\xi^i_\pm\rangle=0. \tag{11b}$$

If a point like body along a fractal curve moves, the parameter t of the time could establish the place where the moving object is at a given moment. Since $d\xi^i_\pm$ describes the fractal properties of the considered curve which has the fractal dimension D,[5] it is natural to impose $(d\xi^i_\pm)^D$ to be proportional to $\mathrm{d}t$, i.e.,

$$(\mathrm{d}\xi^i_\pm)^D\sim\mathrm{d}t, \tag{12a}$$

or

$$(\mathrm{d}\xi^i_\pm)^D=\mathcal{D}\,\mathrm{d}t, \tag{12b}$$

where $\mathcal{D}$ is a coefficient of proportionality. From our earlier discussion, the fluctuation $d\xi_\pm$ is written:

$$\langle \mathrm{d}\xi^i_\pm \mathrm{d}\xi^j_\pm\rangle=\pm\,\delta^{ij}(\mathcal{D}\,\mathrm{d}t)^{2/D}. \tag{13}$$

This relation is invariant under translations and rotations in space between Cartesian coordinate systems. If $i\neq j$ relation (13) is zero, due to the independence of $d\xi^i$ on $d\xi^j$.

(iii) We must introduce two velocities (v_+,v_-) instead of one even when going back to the classical domain. Such a two valuedness of the velocity vector is a new, specific consequence of nondifferentiability that has no standard counterpart (in the sense of differential physics), since it finds its origin in a breaking of the symmetry $(\mathrm{d}t\rightarrow-\mathrm{d}t)$. Such a symmetry was considered self-evident up to now in physics (since the differential element $\mathrm{d}t$ disappears when passing to the limit), so that it has not been analyzed on the same footing as the other well-known symmetries. Note that it is actually different from the time reflection symmetry T, even though infinitesimal irreversibility implies global irreversibility. Now, at the level of our description, we have no way to favor v_+ rather than v_-. Both choices are equally qualified for the description of the laws on nature. The only solution to this problem is to consider both the forward $(\mathrm{d}t>0)$ and backward $(\mathrm{d}t<0)$ processes together. The number of degrees of freedom is doubled with respect to the classical, differentiable description (six velocity components instead of three).

We define average forward (+) and backward (−) derivatives, which, once applied to x^i, yield the above-mentioned forward and backward mean velocities

$$\frac{\mathrm{d}_+x^i(t)}{\mathrm{d}t}=v^i_+, \tag{14a}$$

$$\frac{\mathrm{d}_- x^i(t)}{\mathrm{d}t} = v_-^i, \tag{14b}$$

where $v_\pm^i$ are the components of the "forward" velocity, and v_-^i the components of the "backward" velocity. The average of the fractal velocities $\langle \mathrm{d}\xi_\pm^i/\mathrm{d}t\rangle$ is zero. Yet, if $(v_+^i+v_-^i)/2$ may be considered as classical velocity, the difference between them, more precisely $(v_+^i-v_-^i)/2$ is due to the fractal movement. In order to emphasize the latter from the former, we introduce a complex velocity

$$\mathcal{V}^i = \frac{v_+^i + v_-^I}{2} - i\frac{v_+^i - v_-^i}{2} = \frac{dx_+^i + dx_-^i}{2dt} - i\frac{dx_+^i - dx_-^i}{2dt}. \tag{15}$$

Such procedures are quite often in the theoretical physics (see, e.g., the dumping factor of the oscillations).

Let us make now a change in our parameters. Instead of $\mathrm{d}x_\pm$, we put $\mathrm{d}_\pm x$. Then (15) becomes

$$\mathcal{V}^i = \left(\frac{\mathrm{d}_+ + \mathrm{d}_-}{2\mathrm{d}t} - i\frac{\mathrm{d}_+ - \mathrm{d}_-}{2\mathrm{d}t}\right)x^i, \tag{16}$$

which justifies the definition of the operator

$$d = \frac{\mathrm{d}_+ + \mathrm{d}_-}{\mathrm{d}t} - i\frac{\mathrm{d}_+ - \mathrm{d}_-}{2\mathrm{d}t}. \tag{17}$$

(iv) Let us assume now that the fractal curve[5] is immersed in a 3D space, and $\boldsymbol{X}$ of components $X^i(i=\overline{1,3})$ is the position vector of a point on the curve. Let us consider now a function $f(\boldsymbol{X},t)$ and the following Taylor series expansion up to the second order. This second order term we consider rest term; without entering into deep mathematics, we have

$$\mathrm{d}f = f(X^i + \mathrm{d}X^i, t + \mathrm{d}t) - f(X^i, \mathrm{d}t)$$

$$= \nabla f \cdot d\boldsymbol{X} + \frac{\partial f}{\partial t}\mathrm{d}t + \frac{1}{2}\frac{\partial^2 f}{\partial X^i\,\partial X^j}\mathrm{d}X^i\mathrm{d}X^j + \frac{\partial^2 f}{\partial X^i\,\partial t}\mathrm{d}X^i dt + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}(\mathrm{d}t)^2. \tag{18}$$

The right and left average values of this equation reads

$$\langle \mathrm{d}_\pm f\rangle = \langle \nabla f \cdot \mathrm{d}_\pm \boldsymbol{X}\rangle + \left\langle \frac{\partial f}{\partial t}\mathrm{d}t \right\rangle + \frac{1}{2}\left\langle \frac{\partial^2 f}{\partial X^i\,\partial X^j}\mathrm{d}X_\pm^i \mathrm{d}X_\pm^j \right\rangle + \left\langle \frac{\partial^2 f}{\partial X^i\,\partial t}\mathrm{d}X_\pm^i \mathrm{d}t \right\rangle + \frac{1}{2}\left\langle \frac{\partial^2 f}{\partial t^2}(\mathrm{d}t^2) \right\rangle. \tag{19}$$

We make now the following stipulations: the mean values of the function f and its derivatives coincide with themselves, and the differentials $\mathrm{d}X_\pm^i$ and $\mathrm{d}t$ are independent, therefore the averages of their products coincide with the product of averages. Thus (19) becomes

$$\mathrm{d}_\pm f = \frac{\partial f}{\partial t}\mathrm{d}t + \nabla f \cdot \langle \mathrm{d}_\pm \boldsymbol{X}\rangle + \frac{1}{2}\frac{\partial^2 f}{\partial X^i\,\partial X^j}\langle \mathrm{d}X_\pm^i \mathrm{d}X_\pm^j\rangle + \frac{\partial^2 f}{\partial X^i\,\partial t}\langle \mathrm{d}X_\pm^i\rangle\langle \mathrm{d}t\rangle + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}\langle (\mathrm{d}t)^2\rangle. \tag{20}$$

In what follows we use (11a). Consequently it results

$$\mathrm{d}_\pm f = \frac{\partial f}{\partial t}\mathrm{d}t + \nabla f \cdot \mathrm{d}x_\pm + \frac{1}{2}\frac{\partial^2 f}{\partial X^i\,\partial X^j}\left\{\mathrm{d}x_\pm^i \mathrm{d}x_\pm^j + \langle \mathrm{d}\xi_\pm^i \mathrm{d}\xi_\pm^j\rangle\right\} + \frac{\partial^2 f}{\partial X^i\,\partial t}\mathrm{d}x^i\mathrm{d}t + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}(\mathrm{d}t)^2, \tag{21}$$

where we took into account the fact that $\langle d\xi^i\rangle = 0$ [see (11b)].

Now we make a choice and a specification. The choice concerns the dimension $D=2$ of the fractal curve, i.e., of the Peano type curves. Now (13) becomes

$$\langle \mathrm{d}\xi_{\pm}^{i}\mathrm{d}_{\pm}^{j}\rangle = \pm \delta^{ij}\mathcal{D}\,\mathrm{d}t. \tag{22}$$

The specification relates to the sign: since $\langle \mathrm{d}\xi_{\pm}^{i}\mathrm{d}\xi_{\pm}^{j}\rangle \geqslant 0$, and $\mathrm{d}t$ is negative for the vectors taken to the left, we have put $\pm$ in front of $\mathrm{d}t$ for the two cases.

Now (21) becomes

$$\mathrm{d}_{\pm}f = \frac{\partial f}{\partial t}\mathrm{d}t + \nabla f\cdot \mathrm{d}x_{\pm} + \frac{1}{2}\frac{\partial^2 f}{2\,\partial X^i\,\partial X^j}\mathrm{d}x_{\pm}^{i}\mathrm{d}x_{\pm}^{j} \pm \frac{\partial^2 f}{\partial X^i\,\partial X^j}\delta^{ij}\mathcal{D}\,\mathrm{d}t + \frac{\partial^2 f}{\partial X^i\,\partial t}\mathrm{d}x^i\mathrm{d}t + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}\langle(\mathrm{d}t)^2\rangle. \tag{23}$$

If we now divide by $\mathrm{d}t$ and neglect the terms which still contain differential factors, (23) is reduced to

$$\frac{\mathrm{d}_{\pm}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \nabla f\cdot\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} \pm \frac{\mathcal{D}}{2}\Delta f. \tag{24}$$

The last term is specific to fractality. Let us calculate, under these circumstances $df/\mathrm{d}t$. Taking into account (24), we have

$$\frac{df}{\mathrm{d}t} = \frac{1}{2}\left\{\frac{\mathrm{d}_{+}f}{\mathrm{d}t} + \frac{\mathrm{d}_{-}f}{\mathrm{d}t} - i\left[\frac{\mathrm{d}_{+}f}{\mathrm{d}t} - \frac{\mathrm{d}_{-}f}{\mathrm{d}t}\right]\right\}$$

$$= \frac{1}{2}\left\{\left(\frac{\partial f}{\partial t} + \nabla f\cdot\boldsymbol{v}_{+} + \frac{\mathcal{D}}{2}\Delta f\right) + \left(\frac{\partial f}{\partial t} + \nabla f\cdot + \boldsymbol{v}_{-} - \frac{\mathcal{D}}{2}\Delta f\right)\right.$$

$$\left. - i\left[\left(\frac{\partial f}{\partial t} + \nabla f\cdot\boldsymbol{v}_{+} + \frac{\mathcal{D}}{2}\Delta f\right) - \left(\frac{\partial f}{\partial t} + \nabla f\cdot\boldsymbol{v}_{-} - \frac{\mathcal{D}}{2}\Delta f\right)\right]\right\}$$

$$= \frac{\partial f}{\partial t} + \nabla f\cdot\frac{\boldsymbol{v}_{+}+\boldsymbol{v}_{-}}{2} - i\left(\nabla f\cdot\frac{\boldsymbol{v}_{+}-\boldsymbol{v}_{-}}{2} + \frac{\mathcal{D}}{2}\Delta f\right),$$

or using (15)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \boldsymbol{\mathcal{V}}\cdot\nabla f - i\mathcal{D}\Delta f. \tag{25}$$

This relation allows us to also give the definition of the fractal operator

$$\frac{d}{\mathrm{d}t} = \frac{\partial}{\partial t} + \boldsymbol{\mathcal{V}}\cdot\nabla - i\mathcal{D}\Delta. \tag{26}$$

We now apply the principle of scale covariance, and postulate that the passage from classical (differentiable) mechanics to the new nondifferentiable mechanics that is considered here can be implemented by replacing the standard time derivative $\mathrm{d}/\mathrm{d}t$ by the new complex operator $d/\mathrm{d}t$. As a consequence, we are now able to write the equation of geodesics of the fractal space under its covariant form $d\boldsymbol{\mathcal{V}}/dt=0$. Equivalent results was given in Refs. 4–6.

III. A GENERALIZED SCHRÖDINGER EQUATION

Now, let us consider the covariant derivative (26) and the following $\boldsymbol{\mathcal{V}}$ complex velocity concretization

$$\boldsymbol{\mathcal{V}} = -2i\mathcal{D}\,\nabla\,\ln\psi. \tag{27}$$

Applying the $d/\mathrm{d}t$ covariant derivative to the $\boldsymbol{\mathcal{V}}$ complex velocity, we obtain

$$(d/\mathrm{d}t)\boldsymbol{\mathcal{V}} = \partial_t \boldsymbol{\mathcal{V}} + \nabla\left[(\boldsymbol{\mathcal{V}}^2/2) - i\mathcal{D}\,\nabla\cdot\boldsymbol{\mathcal{V}}\right]$$

$$= -2i\mathcal{D}\left[\partial_t(\nabla \ln \psi) - 2i\mathcal{D}(\nabla \ln \psi\cdot\nabla)(\nabla \ln \psi) - i\mathcal{D}\Delta(\nabla \ln \psi)\right] \tag{28}$$

or still, considering the identity

$$\nabla(\Delta\psi/\psi) = \Delta(\nabla \ln \psi) + 2(\nabla \ln \psi\cdot\nabla)(\nabla \ln \psi),$$

we have

$$(d/\mathrm{d}t)\boldsymbol{\mathcal{V}} = -2\mathcal{D}\,\nabla\,[i(\partial_t, \psi/\psi) + \mathcal{D}(\Delta\psi/\psi)]. \tag{29}$$

Now, Newton's second principle takes the form

$$m(d/\mathrm{d}t)\boldsymbol{\mathcal{V}} = -\nabla U \tag{30}$$

or explicitly

$$\nabla U = \nabla\left[2im\mathcal{D}(\partial_t\psi/\psi) + 2m\mathcal{D}^2(\Delta\psi/\psi)\right] \tag{31}$$

with U the potential. Integrating this equation yields

$$\mathcal{D}^2\Delta\psi + i\mathcal{D}\partial_t\psi = \frac{U}{2m}\psi \tag{32}$$

up to an arbitrary phase factor $\alpha(t)$ which may be set to zero by a suitable choice of the phase of ψ. If there is no external field, $U=0$, the covariance is explicit, since Newton's equation of inertial motion is $(d/\mathrm{d}t)\boldsymbol{\mathcal{V}}=0$. The statistical meaning of the wave function (Born postulate) can now be deduced from the very construction of the theory.[4] Even in the case of only one particle, the virtual geodesic family is infinite (this remains true even in the zero particle case, i.e., for the vacuum field). The particle properties are assimilated to those of a random subset of the geodesics in the family, and its probability to be found at a given position must be proportional to the density of the geodesic fluid. This density can easily be calculated in our formalism, since the imaginary part of Eq. (32) writes in terms of $\rho=\psi\psi^*, \partial_t\rho+\nabla\cdot[\rho(\boldsymbol{\mathcal{V}}+\boldsymbol{\mathcal{V}}^*)/2=0]$, where $(\boldsymbol{\mathcal{V}}+\boldsymbol{\mathcal{V}}^*)/2$ is the real part of the complex velocity, which is identified, at the classical limit, with the classical velocity.

IV. A COVARIANT MECHANICAL MODEL

We assume that any mechanical system can be characterized by a Lagrange function $L(x, \boldsymbol{\mathcal{V}}, t)$ from which an action S is defined

$$S = \int_1^2 L(x, \mathcal{V}, t)\mathrm{d}t. \tag{33}$$

In a general way, the Lagrange function is expected to be a function of the variables x and their derivatives $\dot{x}=v$. We have found that the number of velocity components v is doubled, so that we led to write $L=L(x, v_+, v_-, t)$. Instead, we have made the choice to write the Lagrange function as $L=L(x, \mathcal{V}, t)$. We now justify this choice by the covariance principle. Re-expressed in terms of v_+ and v_- the Lagrange function writes

$$L = L\left(x, \frac{1-i}{2}v_+ + \frac{1+i}{2}v_-, t\right). \tag{34}$$

Therefore we obtain

$$\frac{\partial L}{\partial v_+} = \frac{1-i}{2}\frac{\partial L}{\partial \mathcal{V}}, \tag{35a}$$

$$\frac{\partial L}{\partial v_-} = \frac{1+i}{2}\frac{\partial L}{\partial \boldsymbol{\mathcal{V}}}, \tag{35b}$$

whereas the new covariant time derivative operator writes

$$d/\mathrm{d}t = \frac{1-i}{2}\frac{\mathrm{d}_+}{\mathrm{d}t} + \frac{1+i}{2}\frac{\mathrm{d}_-}{\mathrm{d}t}. \tag{36}$$

Let us write the stationary action principle in terms of the Lagrange function $\delta S = \delta\int_1^2 L(x, \boldsymbol{\mathcal{V}}, t)\mathrm{d}t = 0$. It becomes

$$\int_1^2 \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial v_+}\delta v_+ + \frac{\partial L}{\partial v_-}\delta v_-\right)\mathrm{d}t = 0. \tag{37}$$

As $\delta v_+ = \mathrm{d}_+(\delta x)/\mathrm{d}t$ and $\delta v_- = \mathrm{d}_-(\delta x)/\mathrm{d}t$ it takes the form

$$\int_1^2 \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \mathcal{V}}\left[\frac{1-i}{2}\frac{\mathrm{d}_+}{\mathrm{d}t} + \frac{1+i}{2}\frac{\mathrm{d}_-}{\mathrm{d}t}\right]\delta x\right)\mathrm{d}t = 0, \tag{38}$$

i.e.,

$$\int_1^2 \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \mathcal{V}}\frac{d}{\mathrm{d}t}\delta x\right)\mathrm{d}t = 0 \tag{39}$$

The subsequent demonstration of the Lagrange equations relies on an integration by parts. Now such an operation involves the Leibniz rule for the covariant derivative operator $d/\mathrm{d}t$. As $d/\mathrm{d}t = \partial/\partial t + \boldsymbol{\mathcal{V}}\cdot\nabla - iD\Delta$ is a linear combination of first and second order derivatives, the same is true of its Leibniz rule. This implies the appearance of an additional term in the expression for the derivative of a product:

$$\frac{d}{\mathrm{d}t}\left[\frac{\partial L}{\partial \mathcal{V}}\cdot\delta x\right] = \frac{d}{\mathrm{d}t}\frac{\partial L}{\partial \boldsymbol{\mathcal{V}}}\cdot\delta x + \frac{\partial L}{\partial \boldsymbol{\mathcal{V}}}\frac{d}{\mathrm{d}t}\delta x - 2iD\,\nabla\frac{\partial L}{\partial \boldsymbol{\mathcal{V}}}\cdot\nabla\delta x. \tag{40}$$

As $\delta x(t)$ is not a function of x, the additional term vanishes. After having defined a new integration as the inverse of the covariant derivation, i.e. $\int df = f$, the integral reduces to

$$\int_1^2 \left(\frac{\partial L}{\partial x} - \frac{d}{\mathrm{d}t}\frac{\partial L}{\partial \boldsymbol{\mathcal{V}}}\right)\delta x\,\mathrm{d}t = 0. \tag{41}$$

Finally the Euler-Lagrange equations write

$$\frac{d}{\mathrm{d}t}\frac{\partial L}{\partial \boldsymbol{\mathcal{V}}} = \frac{\partial}{\partial x}. \tag{42}$$

Therefore, thanks to the transformation $\mathrm{d}/\mathrm{d}t \to d/\mathrm{d}t$, they take exactly their standard classical form. This results reinforced the identification of our tool with a "quantum-covariant" representation, since, as we have shown in previous paragraph and as we recall in what follows, this Euler-Lagrange equation can be integrated in the form of a Schrödinger equation.

Assuming homogeneity of space in the mean lead to define a generalized complex momentum given by $P = \partial L/\partial \boldsymbol{\mathcal{V}}$. If we consider the action as a functional of the upper limit of integration in Eq. (41), the variation of the action from a trajectory to another nearby trajectory yields a generalization of another well-known relation of standard mechanics $P = \nabla S$.

V. THE GEOMETRY OF THE FRAME

Physics, both experimental and theoretical, is in fact based on the referential concept. The position, or more general, the motion of a body cannot be described but relative to certain referential. From the experimental point of view, the referential is given by a system of bodies or, with a certain degree of abstraction, by points "relatively fixed" one from each other, system which is the core of the measurements of distance and direction. The intervention of speculative thinking subsequently led to the detaching of the notion of coordinates of a point in a given referential: spatially speaking, the point is localized by three real numbers—its coordinates—if it is moving, also by means of the time when it is localized, i.e., by the moment of time read by a clock attached to the referential.

Theoretically speaking the events or phenomena may be described by coordinates which ease up most of the computations. Usually, the system of coordinates are chosen as to satisfy a certain type of symmetry, or as to the results of the computations to be able to be reported in terms directly testable by experiments.

In principle, the computations may be performed in any coordinate system, the result being equivalent: the geometry found here has an entire arsenal of formula of transformation from one system of coordinates to another. This reciprocal transformability led subsequently to the detachment of the notion of referential from the pure experimental one mentioned above. A referential frequently used in geometry is the referential of the vectors tangent to the lines of coordinates (the so-called natural referential.[7]) Due to the fact that the crossings between several such referentials are easy to be expressed through derivatives of some unknown functions, the referential transformations are called "olonomous." Related to such referentials, pure mathematical, the physical one defined previously, is marked by a high degree of arbitrariness: not always its abstract defining elements—the basis vectors—may define lines of coordinates relatively to where they must be tangent. As a result, it is said that the basis of such referentials is nonolonomous.[8,9] However, clearly, these referentials are those used in the experimental physics, the olonomous being in general, only abstractions necessary to the calculus, as we will try to show in what follows.

Physically speaking, for a system of coordinates to correspond to reality: it is necessary to be measurable or interpretable in terms of measurable parameters. Although, in the quasitotality of the cases the coordinates are not measurable. For example, in astronomy, the position of a star may be reported in spherical or Cartesian coordinates: azimuth, height, and distance from the star. In both cases we deal with parameters with unknown significance, or effectively measured value. For example, the Cartesian coordinates are not measurable even if we consider the space absolutely Euclidian. The manner of work in astronomy consists of a second set of coordinates, for which the radial distance, deduced from physical considerations, is affected by a large arbitrariness, quantitatively speaking. Then even qualitatively, if the space is non-Euclidian, it has not the significance which was given. In this last case, even the angles do not give the real direction anymore, but a local, apparent one. Nevertheless, they keep a certain significance—as we tried to mention to emphasize in—which is not related to translations, but only to rotations of the moving referential or of some portions of it (which to play, eventually, the part of "theodolite"). Let us not forget this fact, since we will use it in what follows.

This, because, among all the other notions used in physics, the notion of direction is endowed apparently with a certain transcendence. For example, in quantum mechanics, the experimental device must obey with enough accuracy, to the classical laws. This refers to the fact that the difference between the classical laws [applicable to the measurement gauges and the quantum laws (applicable to the microobjects)], is extended in what concerns the measuring scale of masses, lengths and times and, in general, over any parameters which imply displacements, not over the directions, which implies only rotations. This has here two aspects: the first one concerns the intuitive fact that a direction, no matter how it has been established, may serve as referential both for microscopic, and for macroscopic ones, and the second one, concerns the fact that the imprecision relations which complies angular variables and associated operators, need a plus of precautions in definition,[10] which might indicate a certain "classicism" of the respective variables.

The indiscernability of the coordinate systems, as well as the fact that in measurements one

uses the nonolonomous physical referentials indicate, clearly, the necessity of reporting the calculus to these last ones. Hence, only these are used, e.g., in the operational definition of the space-time metric element or, as it is underlined in Refs. 11–13, even the models of universe defined by ingenious operational methods, as is the kinematic model of Milne, may be reformulated with the help of the notion of metrics. For the metric theories there is a strong basis: the general relativity theory of Einstein. In our opinion, what lacks in order to overcome the state of fact in physics (or in cosmology, with a higher restraint) is the physical interpretation, i.e., a physical referential, of the coordinates which enter in metrics. In other words, if usually a coordinates system may determine a referential (of the tangent vectors), the problem which arises is exactly inverse: given a referential, one has to detect a coordinate system compatible with it. The theory of the complex potential[9,14,15] allows us to reach to some extent the solving of this problem, as from here, it is clear that the only olonomous coordinates cannot be but the three-dimensional ambient metrics, which could be a working hypothesis.

Therefore, these coordinates have a relation with what is measuring (which is e.g., a potential), only through a certain function solution of a partial derivative equation. This supposes yet an extension of the operational processes beyond the ones used habitually: the distance measurement, even by light signals, and the watch synchronization by the same signals. These being intrinsically linked to each other, since synchronization is marked by a high degree of arbitrariness, the same will happen with the definition of the distance.

A first way of defining a measurement process related to the physical referential, as it was accepted previously, resides in a speculation which has at its basis the quantum measurability, i.e., by means of hermitic operators, whose eigenvalues represent values measured of the parameters which has operators attached. In order to explain such a point of view, we must first accept that on a physical referential one can establish directions independent of the phenomenological frame where we are fixed (micro- or macro-cosmos). Specifically we admit that, artificially (with rational intervention) or intrinsically, a physical referential is endowed with "theodolitic apparatus," which may be oriented anyhow independently on the referential and, mostly, of the way this is taken into consideration (e.g., indifferently of the orientation of the three Cartesian axis attached to it). Obviously, such a theodolitic apparatus "points to" something. Rising to some degree of abstraction, in its interior some interactions happen, due to the fields captured from the pointing direction, interactions through which one measures some parameters related to this field. Pointing to various directions, the apparatus "measures" in the same way: what it measures (what it evidences) does not depend in its nature on the direction it is pointing to, or on the parameters associated to this direction in the considered physical referential. In one word, the internal process through which the measurement is achieved is independently on the direction. Under these circumstances, a theodolit must be characterized by a hermitic operator which may depend on the direction, but which—in any case—has eigenvalues, independent on it. One may build such operators using the S^3 sphere.

The S^3 sphere can be parameterized in terms of either Cartesian coordinates $x^m (m=1,2,3,4)$, complex variables (u,v), or ρ and angles (θ,α,β). If the radius of S^3 is equal to ρ, then

$$(x^1)^2 + (x^2)^2 + (x^3)^2 + (x^4)^2 = \rho^2. \tag{43}$$

We will set ρ equal to unity $(\rho=1)$ wherever possible. The inverse radius ρ^{-1} can be considered as a mass scale in this space.[16] The connection between different variables is of the form

$$u = x^1 + ix^2 = \rho \cos\theta e^{i\alpha}, \tag{44a}$$

$$\mathcal{V} = x^3 + ix^4 = \rho \sin\theta e^{i\beta}, \tag{44b}$$

with the angular volume element

$$d\Omega = \frac{1}{2\pi^2} \sin\theta \cos\theta \, d\theta \, d\alpha \, d\beta. \tag{45}$$

The manifold S^3 has an $O(4)$ symmetry, whose algebra is $SU(2) \times SU(2)$. S^3 is itself the manifold of the group SU(2), and the two subgroups correspond to left and right multiplications acting on the manifold. As a consequence, there are two independent frames $e_i^{(1)}$ and $e_i^{(2)}$ ($i = 1,2,3$) possible on S^3, each of which is smooth everywhere and can be used to define the spatial derivatives. The particular choice of one or another of these frames has no physical consequences.

Throughout this article we choose the frame $e_i^{(1)}$, and the corresponding derivatives will be denoted by ∂_i ($i=1,2,3$):

$$\partial_1 = \frac{i}{\rho}\left(u\frac{\partial}{\partial \nu^*} - \nu\frac{\partial}{\partial u^*} + \nu^*\frac{\partial}{\partial u} - u^*\frac{\partial}{\partial \nu}\right)$$

$$= \frac{1}{\rho}\left[-\sin(\alpha+\beta)\frac{\partial}{\partial\theta} + \cos(\alpha+\beta)\left(\tan\theta\frac{\partial}{\partial\alpha} - \cot\theta\frac{\partial}{\partial\beta}\right)\right], \tag{46a}$$

$$\partial_2 = \frac{1}{\rho}\left(u\frac{\partial}{\partial \nu^*} - \nu\frac{\partial}{\partial u^*} - \nu^*\frac{\partial}{\partial u} + u^*\frac{\partial}{\partial \nu}\right)$$

$$= \frac{1}{\rho}\left[\cos(\alpha+\beta)\frac{\partial}{\partial\theta} + \sin(\alpha+\beta)\left(\tan\theta\frac{\partial}{\partial\alpha} - \cot\theta\frac{\partial}{\partial\beta}\right)\right], \tag{46b}$$

$$\partial_3 = \frac{i}{\rho}\left(u^*\frac{\partial}{\partial u^*} - u\frac{\partial}{\partial u} + \nu^*\frac{\partial}{\partial u^*} - \nu\frac{\partial}{\partial \nu}\right) = -\frac{1}{\rho}\left(\frac{\partial}{\partial\alpha} - \frac{\partial}{\partial\beta}\right). \tag{46c}$$

Note that these derivatives do not commute

$$[\partial_i, \partial_j] = \frac{2}{\rho}\varepsilon_{ijk}\partial_k, \tag{47}$$

where ε_{ijk} is the antisymmetric tensor of rank 3 with $\varepsilon_{123}=1$. If we consider the derivatives

$$\partial_\mu = \left(\partial_i, \partial_4 = \left(\frac{\partial}{\partial\xi_\pm}\right)^D = \frac{1}{\mathcal{D}}\frac{\partial}{\partial t}\right),$$

then we have

$$[\partial_\mu, \partial_\nu] = C^\gamma_{\mu\nu}\partial_\gamma = -\frac{2}{\rho}\varepsilon^\gamma_{\mu\nu 4}\partial_\gamma, \tag{48a}$$

$$\varepsilon_{1234} = -1, \tag{48b}$$

$$\mu = 1,2,3,4. \tag{48c}$$

The quantities $C^\gamma_{\mu\nu}$ are the structure constants for the Lie algebra of the group $SU(2) \times T$, were T is the group of fractal time translations. In the works of Carmeli and Marlin[17–22] one uses the angular momentum components $L_i (i=1,2,3)$ as derivatives in S^3. They satisfy the commutation relations

$$[L_i, L_j] = -\varepsilon_{ijk}L_k \tag{49}$$

which are equivalent up to a factor with (47). In this case we have $C^\gamma_{\mu\nu} = (2/\rho)\varepsilon^\gamma_{\mu\nu 4}$

VI. THE LINEAR CONNECTION ON THE FRACTAL SPACE-TIME

Let $\bar{T}$ be the tangent bundle over the fractal space-time and ∇ a linear connection on this manifold. It is known that ∇ is a derivative on the bundle $\bar{T}$. We define then a Riemannian structure on the fractal space-time by introducing a metric form on $\bar{T}$ (Ref. 23)

$$g:(X,Y) \to g(X,Y), \tag{50}$$

which is symmetric, nondegenerate, and positive. Here X and Y are vector fields over the fractal space-time.

If we use the derivatives $\partial_\mu, \mu=0,1,2,3$, then the vector fields X,Y can be written under the form[23]

$$X = X^\mu \partial_\mu, \quad Y = Y^\mu \partial_\mu. \tag{51}$$

In this case the metric form g becomes

$$g(X,Y) = g(X^\mu \partial_\mu, Y^\nu \partial_\nu) = X^\mu Y^\nu g(\partial_\mu, \partial_\nu). \tag{52}$$

If we introduce the metric coefficients

$$g_{\mu\nu} = g(\partial_\mu, \partial_\nu) \tag{53}$$

then relation (52) can be written as

$$g(X,Y) = g_{\mu\nu} X^\mu Y^\nu. \tag{54}$$

Because g is symmetric, the metric coefficient has the property

$$g_{\mu\nu} = g_{\nu\mu}. \tag{55}$$

To describe the gravitational field, we suppose that the connection ∇ is Riemannian, i.e., the covariant derivative of g is null:

$$(\nabla_x g)(Y,Z) = 0. \tag{56}$$

This condition combined with the property of null torsion for Riemannian manifold yields:

$$2g(\nabla_x Y,Z) = X(g(Y,Z)) - Y(g(Z,X)) - Z(g(X,Y)) + g([X,Y],Z) + g([Z,X],Y) - g([Y,Z],X). \tag{57}$$

In a local chart we choose the vector fields X,Y, and Z to be ∂_μ, ∂_ν, and ∂_γ, respectively. Then, using, (48a)–(48c) Eq. (57) becomes

$$2g(\nabla_{\partial_\mu} \partial_\nu, \partial_\gamma) = \partial_\mu g_{\nu\gamma} + \partial_\nu g_{\gamma\mu} - \partial_\gamma g_{\mu\nu} + g([\partial_\mu, \partial_\nu], \partial_\gamma) + g([\partial_\gamma, \partial_\mu]\partial_\nu) - g([\partial_\nu, \partial_\gamma]\partial_\mu). \tag{58}$$

We introduce now the connection coefficient $\Gamma^\omega_{\mu\nu}$ by the definition

$$\nabla_{\partial_\mu} \partial_\nu = \Gamma^\omega_{\mu\nu} \partial_\omega. \tag{59}$$

Then, using (48a)–(48c) and (53), we can write (58) in the form

$$2\Gamma^\omega_{\mu\nu} g_{\omega\gamma} = \partial_\mu g_{\nu\gamma} + \partial_\nu g_{\gamma\mu} - \partial_\gamma g_{\mu\nu} + C^\rho_{\mu\nu} g_{\rho\gamma} + C^\rho_{\gamma\nu} g_{\rho\nu} - C^\rho_{\nu\gamma} g_{\rho\mu}. \tag{60}$$

Finally, if we observe that $g_{\omega\gamma}g^{\gamma\lambda}=\partial^{\omega}_{\lambda}$, then from Eq. (60) we obtain

$$\Gamma^{\lambda}_{\mu\nu}=\tfrac{1}{2}g^{\gamma\lambda}(\partial_{\mu}g_{\nu\gamma}+\partial_{\nu}g_{\gamma\mu}-\partial_{\gamma}g_{\mu\nu})+\tfrac{1}{2}g^{\gamma\,\lambda}(C^{\rho}_{\mu\nu}g_{\rho\gamma}+C^{\rho}_{\gamma\nu}g_{\rho\nu}-C^{\rho}_{\nu\gamma}g_{\rho\mu}). \tag{61}$$

This result differs from the result of Carmeli and Malin[22] by the last three terms on the right-hand side. These terms, containing the structure constants $C^{\gamma}_{\mu\nu}$ are determined by the noncommutativity of the derivatives ∂_{μ}.

It is easy to verify that

$$\Gamma^{\lambda}_{\mu\nu}-\Gamma^{\lambda}_{\nu\mu}-C^{\lambda}_{\mu\nu}=0. \tag{62}$$

This result shows that the torsion of the Riemannian connection ∇ introduced in fractal space-time is null. Indeed, from the definition of torsion[23] we have

$$T(\partial_{\mu},\partial_{\nu})=\nabla_{\partial_{\mu}}\partial_{\nu}-\nabla_{\partial_{\nu}}\partial_{\mu}-\lfloor\partial_{\mu},\partial_{\nu}\rfloor$$

$$=(\Gamma^{\lambda}_{\mu\nu}-\Gamma^{\lambda}_{\nu\mu}-C^{\lambda}_{\mu\nu})\partial_{\lambda} \tag{63}$$

and, by using the definition of the torsion tensor components

$$T^{\lambda}_{\mu\nu}\partial_{\lambda}=T(\partial_{\mu},\partial_{\nu})$$

we obtain

$$T^{\lambda}_{\mu\nu}=\Gamma^{\lambda}_{\mu\nu}-\Gamma^{\lambda}_{\nu\mu}-C^{\lambda}_{\mu\nu}=0. \tag{64}$$

Now, we can write the covariant derivative of a covariant vector by using the property

$$\nabla_{X}(fY)=f\nabla_{X}Y+(Xf)Y, \tag{65}$$

where f is a differentiable function defined on the fractal space-time. If we choose X as ∂_{μ} and put $Y=\partial_{\nu}$ and $f=V^{\nu}$, then

$$\nabla_{\partial_{\mu}}(V^{\nu}\partial_{\nu})=V^{\nu}\nabla_{\partial_{\mu}}\partial_{\nu}+(\partial_{\mu}V^{\nu})\partial_{\nu}=(\partial_{\mu}V^{\nu}+\Gamma^{\nu}_{\mu\rho}V^{\rho})\partial_{\nu}$$

or

$$\nabla_{\mu}V^{\nu}=\partial_{\mu}V^{\nu}+\Gamma^{\nu}_{\mu\rho}V^{\rho}. \tag{66}$$

This result coincides with that given in Ref. 22 for the covariant derivative.

We calculated now the Riemann curvature tensor $R^{\sigma}_{\rho\mu\nu}$ by using the definition of the curvature two-form $R(X,Y)$.[23] If we choose X,Y, and Z as $\partial_{\mu},\partial_{\nu}$, and ∂_{γ}, respectively, then

$$R(\partial_{\mu},\partial_{\nu})\partial_{\gamma}=\nabla_{\partial_{\mu}}\nabla_{\partial_{\nu}}\partial_{\gamma}-\nabla_{\partial_{\nu}}\nabla_{\partial_{\mu}}\partial_{\gamma}-\nabla_{[\partial_{\mu},\partial_{\nu}]}\partial_{\gamma}. \tag{67}$$

Using (48a)–(48c) and (59), we write expression (67) as

$$R(\partial_{\mu},\partial_{\nu})\partial_{\gamma}=\nabla_{\partial_{\mu}}(\Gamma^{\sigma}_{\nu\gamma}\partial_{\sigma})-\nabla_{\partial_{\nu}}(\Gamma^{\sigma}_{\mu\gamma}\partial_{\sigma})-C^{\sigma}_{\mu\nu}\nabla_{\partial_{\sigma}}\partial_{\gamma}. \tag{68}$$

If we define now the Riemann curvature tensor $R^{\sigma}_{\rho\mu\nu}$ by

$$R(\partial_{\mu},\partial_{\nu})\partial_{\gamma}=R^{\sigma}_{\gamma\mu\nu}\partial_{\sigma} \tag{69}$$

then from Eq. (68) we obtain

$$R^{\sigma}_{\gamma\mu\nu}=\partial_{\mu}\Gamma^{\sigma}_{\nu\gamma}-\partial_{\nu}\Gamma^{\sigma}_{\mu\gamma}+\Gamma^{\sigma}_{\mu\rho}\Gamma^{\rho}_{\nu\gamma}-\Gamma^{\sigma}_{\nu\rho}\Gamma^{\sigma}_{\mu\gamma}-C^{\sigma}_{\mu\nu}\Gamma^{\sigma}_{\rho\gamma}. \tag{70}$$

This result differs also from that of Ref. 22 by the term $C^{\rho}_{\mu\nu}\Gamma^{\sigma}_{\rho\gamma}$, and is determined by the noncommutativity of the derivative ∂_{μ}.

VII. EINSTEIN'S FIELD EQUATIONS

The parametrization (44a) and (44b) is consistent, leading to the metric

$$d\sigma^2 = \rho^2\left[\cos^2\theta\, d\alpha^2 + \sin^2\theta\, d\beta^2 + d\theta^2\right] \tag{71}$$

and to the everywhere continuous right-handed triad $e_i=\partial_i$—see (46a)–(46c) whose corresponding dual base is[24]

$$\omega^1 = (\rho/2)\cos(\alpha+\beta)\sin(2\theta)(d\alpha - d\beta) - \rho\sin(\alpha+\beta)d\theta, \tag{72a}$$

$$\omega^2 = (\rho/2)\sin(\alpha+\beta)\sin(2\theta)(d\alpha - d\beta) - \rho\cos(\alpha+\beta)d\theta, \tag{72b}$$

$$\omega^3 = -\rho(\cos^2\theta\, d\alpha + \sin^2\theta\, d\beta). \tag{72c}$$

The Lorentzian metric for the $S^3\times T$ space-time being

$$ds^2 = d\sigma^2 - dt^2, \tag{73}$$

the orthonormal frame is defined by $\{\partial_\mu\}=\{\partial_1,\partial_2,\partial_3,\partial_4=\partial/\mathcal{D}\partial t\}$, whereas the corresponding dual orthonormal base consists of $\{\omega^\mu\}=\{\omega^1,\omega^2,\omega^3,\omega^4=\mathcal{D}\,dt\}$.

The above-introduced pseudo-orthonormal tetradic fields satisfy the $SU(2)\times T$ algebra (48a)–(48c). Using the tetradic field one-forms $\{\omega^\mu\}$ one can obtain the line element as[12,25]

$$ds^2 = g_{\mu\nu}\omega^\mu\omega^\nu, \tag{74}$$

where $g_{\mu\nu}=\mathrm{diag}(1,1,1,-1)=\eta_{\mu\nu}$ denotes the usual "flat" metric. In this choice of the tetrad, exploiting the group properties of the manifold, the Cartan formalism leads to important results which will be presented in the sequel.

Thus, the algebraically essential coefficients of the Levi-Civita connection are easily obtained as

$$\Gamma_{ijk} = -\varepsilon_{ijk}, \tag{75a}$$

$$\Gamma_{4ij} = 0, \tag{75b}$$

$$i,j,k = \overline{1,3}. \tag{75c}$$

Considering $\rho=f(\mathcal{D}t)$ to be a function of time alone, we generalize the previous results to a time-dependent radius of curvature. With this assumption, the structure constants for the algebra (48a)–(48c) read

$$C_{ijk} = (2/f)\varepsilon_{ijk}, \tag{76a}$$

$$C_{ii4} = -C_{i4i} = f'/f, \tag{76b}$$

$$C_{4ii} = 0, \tag{76c}$$

where prime marks fractal time derivatives.

Using the first torsionless Cartan equation[12,25]

$$d\omega^\mu = -\Gamma^\mu_\nu \wedge \omega^\nu \tag{77}$$

we obtain the connection coefficients as

$$\Gamma^i_{jk} = -(1/f)\varepsilon^i_{jk}, \quad \Gamma^i_{41} = \Gamma^4_{ii} = -f'/f, \quad \Gamma^i_{i4} = 0. \tag{78}$$

From the second Cartan equation[12,25]

$$\mathrm{d}\Gamma_{\mu\nu} + \Gamma_{\mu\alpha} \wedge \Gamma^{\alpha}_{\nu} = (1/2) R_{\mu\nu\alpha\beta} \omega^{\alpha} \wedge \omega^{\beta} \tag{79}$$

we get the following essential Riemann tensor components:

$$\begin{gathered} R_{1212} = R_{1313} = R_{2323} = 1/f^2 + (f'/f)^2, \\ R_{1414} = R_{2424} = R_{3434} = -f''/f^2, \end{gathered} \tag{80}$$

which enable us to compute the Ricci tensor

$$\begin{gathered} R_{11} = R_{22} = R_{33} = 2/f^2 + f''/f + 2(f'/f)^2, \\ R_{44} = -3f''/f, \end{gathered} \tag{81}$$

and the scalar curvature

$$R = \eta^{\mu\nu} R_{\mu\nu} = 6[1/f^2 + f''/f + (f'/f)^2]. \tag{82}$$

For $f(\mathcal{D}t) = \rho = \text{const.}$, one can obtain from (82) the well-known geometrical result $R = 6/\rho^2$.[13]

Using (81) and (82), we compute the components of the Einstein tensor $G_{\mu\nu} = R_{\mu\nu} - (1/2)\eta_{\mu\nu} R$, obtaining

$$G_{ii} = -[1/f^2 + 2f''/f + (f'/f)^2], \tag{83a}$$

$$G_{44} = (3/f^2)(1 + f'^2). \tag{83b}$$

In the following we analyze the Einstein equations, for the dynamized metric, in two physically important cases. The exact solutions are derived and some considerations on particular cases are made.

Considering the Einstein field equations

$$G_{\mu\nu} = kT_{\mu\nu} \tag{84}$$

with the matter-energy-momentum tensor of an ideal fluid

$$T_{\mu\nu} = (w + p) u_{\mu} u_{\nu} + p \eta_{\mu\nu}, \tag{85}$$

where p is the pressure and w is the energy density. The concrete expressions for the components (83a) and (83b) suggest the use of the well-known relation $w = 3p$. So, the ideal fluid may be identified with an electromagnetic field of pure radiation, and (85) can be written in the form

$$T_{\mu\nu} = (w/3)(4\delta^4_{\mu}\delta^4_{\nu} + \eta_{\mu\nu}). \tag{86}$$

Introducing (83a), (83b), and (86) in (84), we get

$$1/f^2 + 2f''/f + (f'/f)^2 = -kw/3, \tag{87a}$$

$$(3/f^2)(1 + f'2) = kw. \tag{87b}$$

which lead to the following different equation for f:

$$f''f + f'2 + 1 = 0 \tag{88}$$

with the general solution

$$f(\mathcal{D}t) = \pm [f_0^2 - (\mathcal{D}t - \mathcal{D}t_0)^2]^{1/2}, \tag{89}$$

where f_0 and t_0 are integration constants.

The (88) result in the form

$$\frac{\partial \mathcal{L}}{\partial \ln \varepsilon} = -2,$$

where

$$\mathcal{L} = \ln(p^2 + 1), p = f' \text{ and } \varepsilon = f$$

leads to a continuous scale invariance—see Refs. 4 and 5. In this case, the scale dimension is given by the eigenvalues of the dilation operator (6)

$$\mathcal{D}\mathcal{L} = \lambda \mathcal{L}$$

and indicates, according to the general theory of the fractal space-time—see Refs. 4 and 5 that it is valuable at the microscopic scale since $\lambda = -2$. Moreover, the fractalic dimension $D = -\lambda = 2$ show that this model becomes the quantum Einstein gravity.[26,27]

Replacing (89) in (87a) and (87b), we obtain the energy density for the electromagnetic field of pure radiation as

$$w = \pm (3\rho/k)[f_0^2 - (\mathcal{D}t - \mathcal{D}t_0)^2]^{1/2}. \tag{90}$$

For comparison, it is worthwhile analyzing the simplest case of a cosmological dust whose energy-momentum tensor is $T_{\mu\nu} = w u_\mu u_\nu$ [derived from (85) for $p = 0$] and possesses, with respect to the co-moving frame $u_i = 0$, a single nonvanishing component, $T_{44} = w$. Under these hypotheses, the Einstein's field equations (84) concretely become

$$l/f^2 + 2f''/f + (f'/f)^2 = 0, \tag{91a}$$

$$(3/f^2)(1 + f'^2) = kw, \tag{91b}$$

whose general solution is expressed through the transcendent dependence of the sphere radius on time

$$\mathcal{D}t = \mathcal{D}t_0 \pm \lfloor f_0 \sqrt{(f/f_0)(1 - f/f_0)} + (\sqrt{f_0}/2)\arcsin\sqrt{1 - f/f_0} \rfloor, \tag{92}$$

where t_0 and f_0 are integration constants.

Equation (91b) provides the energy density

$$w = 3f_0/(kf^3) \tag{93}$$

in perfect agreement with Ref. 13.

VIII. CONCLUSIONS

The main conclusions of the present paper are the following: (i) Assimilating the physical space-time with a fractal, a general theory is built. For a fractal dimension $D = 2$, the virtual geodesics of this space-time impliesh a generalized Schrödinger type equation and (ii) A geometric formulation of the gravitation theory on a fractal space-time is given. Then, a connection is introduced on a tangent bundle, the connection coefficients, the Riemann curvature tensor and the Einstein field equation are calculated. It results, by means of the a dilation operator, the equivalence of this model with quantum Einstein gravity.

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Hilbert spaces built on a similarity and on dynamical renormalization

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We develop a Hilbert-space framework for a number of general multiscale problems from dynamics. The aim is to identify a spectral theory for a class of systems based on iterations of a non-invertible endomorphism. We are motivated by the more familiar approach to wavelet theory which starts with the two-to-one endomorphism $r:z\mapsto z^2$ in the one-torus $\mathbb{T}$, a wavelet filter, and an associated transfer operator. This leads to a scaling function and a corresponding closed subspace V_0 in the Hilbert space $L^2(\mathbb{R})$. Using the dyadic scaling on the line $\mathbb{R}$, one has a nested family of closed subspaces V_n, $n\in\mathbb{Z}$, with trivial intersection, and with dense union in $L^2(\mathbb{R})$. More generally, we achieve the same outcome, but in different Hilbert spaces, for a class of non-linear problems. In fact, we see that the geometry of scales of subspaces in Hilbert space is ubiquitous in the analysis of multiscale problems, e.g., martingales, complex iteration dynamical systems, graph-iterated function systems of affine type, and subshifts in symbolic dynamics. We develop a general framework for these examples which starts with a fixed endomorphism r (i.e., generalizing $r(z)=z^2$) in a compact metric space X. It is assumed that $r:X\to X$ is onto, and finite-to-one. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We study a class of endomorphisms $r:X\to X$, where X is a metric space. The endomorphism is assumed onto, and finite-to-one. We build a spectral theory on a Hilbert space associated naturally with (X,r). Our focus is on the case when X is assumed to carry a certain strongly invariant measure ρ, see (2.3).

Continuing our earlier work[13] we consider basis constructions in a general context of dynamical systems; the case of endomorphisms, i.e., non-reversible dynamics. Our framework will include wavelet bases, as well as algorithmic basis constructions in Hilbert spaces built on fractals or on Julia sets of rational functions in one complex variable. In fact, these examples motivated our results.

First recall that in the real variable case of standard wavelets (in one or several variables, i.e., the d-dimensional Lebesgue measure), there is a separate generalizations of standard dyadic wavelets, again based on translation and scaling: See for example Ref. 1 for such an approach to the construction of generalized wavelet bases in the Hilbert space $L^2(\mathbb{R}^d)$, i.e., of orthogonal bases in $L^2(\mathbb{R}^d)$, or just frame wavelet bases, but still in $L^2(\mathbb{R}^d)$.

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It is the purpose of this paper to develop a geometric context of this viewpoint which applies to any kind of dynamics which is based on an iterated scale of selfsimilarity. Hence our paper will offer a Hilbert-space framework which goes beyond the setting of scale similarity, and our results will offer a new viewpoint even in the case of the more familiar selfsimilarity which is based on a cascade of affine scales.

The best know instance of this is $d=1$, and dyadic wavelets.[10] In that case, the two operations on the real line $\mathbb{R}$ are translation by the group $\mathbb{Z}$ of the integers, and scaling by powers of 2, i.e., $x\mapsto 2^j x$, as j runs over $\mathbb{Z}$. This is the approach to wavelet theory which is based on multiresolutions and filters from signal processing. In higher dimensions d, the scaling is by a fixed matrix, and the translations by the rank-d lattice $\mathbb{Z}^d$. Again we will need scaling by all integral powers. We view points x in $\mathbb{R}^d$ as column vectors, and we then consider the group of scaling transformations, $x\mapsto A^j x$ as j ranges over $\mathbb{Z}$.

Suitable spectral conditions will be imposed on A. In particular we note that if A is integral, i.e., the entries in A are in $\mathbb{Z}$, then $x\mapsto Ax$ passes to the quotient $\mathbb{R}^d/\mathbb{Z}^d$. Since $\mathbb{R}^d/\mathbb{Z}^d$ is a copy of the compact d-torus $\mathbb{T}^d$ via a familiar identification, we see that A induces an endomorphism r_A in $\mathbb{T}^d$. If further A is invertible, then r_A is finite-to-one, and maps $\mathbb{T}^d$ onto itself. In fact, for every x in $\mathbb{T}^d$, the inverse image $r_A^{-1}(x)$ has cardinality $=|\det A|=:N$,

$$\frac{1}{\sqrt{\det A}}\varphi(A^{-1}x)=\sum_{k\in\mathbb{Z}^d} a_k\varphi(x-k)\quad (x\in\mathbb{R}^d). \tag{1.1}$$

So our starting point is a given finite-to-one endomorphism $r: X\to X$ in a compact space X. Our aim is threefold: (1) to build an associated Hilbert space which admits wavelet decompositions; (2) to show that the corresponding computations can be done with a geometric algorithm; and finally (3) we offer concrete examples from dynamics where our approach leads to new insight. So in addition to the endomorphism (X,r), our initial setup will include a scalar function m_0; an analog of the function from wavelet theory which determines low-pass filters.

Details: Set $W(x):=|m_0|^2/\#r^{-1}(x)$. We say that m_0 satisfies a *low-pass* condition if $W(0)=1$. (In the special case of (1.1) above, the relationship between the function m_0 and the coefficients $\{a_k\}$ is that the a_k numbers will be the d-Fourier coefficients of m_0 when m_0 is viewed as a function on the compact quotient $X=\mathbb{R}^d/\mathbb{Z}^d$. This explains the summation over $\mathbb{Z}^d$ in (1.1).)

Suppose for some p, and $x\in X$, that $r^p(x)=x$. Then we say that the finite set of points $C=\{x,r(x),\ldots,r^{p-1}(x)\}$ is a *cycle*. A cycle C is called a *W-cycle* if $W(y)=1$ for all $y\in C$.

We will extend to the context of endomorphisms the following general principle from wavelets in the Hilbert space $L^2(\mathbb{R}^d)$: A generalized wavelet basis (also called a Parseval-frame, see e.g., Ref. 1) will have the stronger orthonormal basis (ONB)property when the only one W-cycle is $C=\{0\}$. On the other hand, the presence of non-trivial W-cycles is consistent with wavelet systems that form frame-bases. The reader is referred to Ref. 6 for details regarding these more general wavelet bases. It was proved in Ref. 6 that the presence of W-cycles is consistent with a class of certain *super-wavelets*. This wavelet basis involves an additional cyclic structure which we will develop in the paper.

This setup arose earlier for the familiar linear multiresolution analysis (MRA) approach to wavelets: Recall[10] that dyadic wavelets represent a special basis for the Hilbert space $L^2(\mathbb{R})$, but they are generated by a subspace V_0 in $L^2(\mathbb{R})$ which is the closed linear span of a single function φ and its translates by the integers $\mathbb{Z}$. The function φ satisfies a certain scaling identity

$$\frac{1}{\sqrt{2}}\varphi(x/2)=\sum_{k\in\mathbb{Z}} a_k\varphi(x-k)\quad (x\in\mathbb{R}), \tag{1.2}$$

which implies that the scaling operator $Uf(x):=1/\sqrt{2}f(x/2)$ maps V_0 into itself. A solution φ is called a scaling function. Using a terminology from optics, we say that functions on $\mathbb{R}$ represent signals or images, and that the subspace V_0 initializes a fixed resolution.

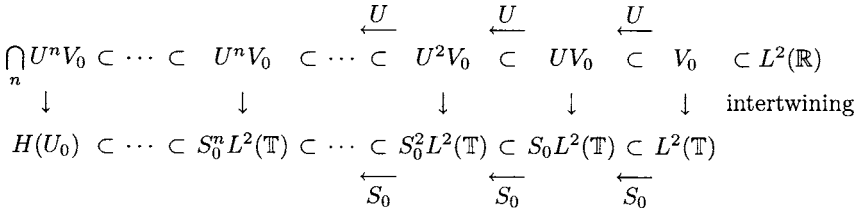

FIG. 1. Multiresolutions.

A special case: $X=\mathbb{T}=\{z\in\mathbb{C}\,|\,|z|=1\}=\mathbb{R}/\mathbb{Z}$, $r(z)=z^2$, and m_0 is the function on $\mathbb{T}$ with Fourier coefficients equal to the masking coefficients a_k from (1.2), i.e., $m_0(z)=\Sigma_{k\in\mathbb{Z}}a_k z^k$. The function m_0 is called a filter function because of an analogy to a setting in signal processing. One of the axioms for m_0 (the *quadrature-mirror-filter* axiom) from wavelet theory amounts to the fact that the associated linear operator, $S_0h(z):=m_0(z)h(z^2)$ is isometric in $L^2(\mathbb{T},$ Haar measure); see Fig. 1,

In this paper, we state a version of the scaling identity (1.2), for the case of an endomorphism $r:X\to X$, and we show that it admits a solution in certain Hilbert spaces built on (X,r). It turns out that the variant of (1.2) which arises by the Fourier transform, i.e.,

$$\sqrt{2}\hat{\varphi}(t)=m_0(e^{it/2})\hat{\varphi}(t/2)\quad(t\in\mathbb{R}),\tag{1.3}$$

is more suggestive of the generalization we have in mind; see Theorem 2.14 for details.

While the standard MRA approach to wavelets (see Ref. 17) restricts the functions m_0 in (1.3) by assuming that m_0 is in some regularity class, e.g., is Lipschitz, we shall not do this here. Moreover, there is a rich class of wavelet systems where m_0 is typically only known *a priori* to be L^∞. This is the case, for example, for the frequency localized wavelets studied in Refs. 1 and 21. (In this last case, m_0 is in fact matrix-valued.)

The scaling identity (1.2) implies that there is a natural intertwining of the isometry S_0 on $L^2(\mathbb{T})$ with the restriction of U to the subspace V_0 in $L^2(\mathbb{R})$. A second axiom for m_0 from wavelet theory (called *low-pass*) implies that S_0 is a *pure* shift isometry, i.e., that the intersection $S_0^n(L^2(\mathbb{T}))$, for n in $\mathbb{N}$ is $\{0\}$, see Fig. 1. Because of the intertwining relation, this fact guarantees that the standard functions that make up a wavelet basis really do form a basis for the whole Hilbert space $L^2(\mathbb{R})$. See Fig. 1. And the purity of S_0 is also what yields a certain martingale system, i.e., a nested family of spaces, or of sigma-algebras.

It is the purpose of this paper to generalize this setting to that of endomorphisms, and to realize a natural scaling function, as a generating vector in a Hilbert space which corresponds to $L^2(\mathbb{R})$ for the special case of wavelets. For this purpose we introduce a solenoid X_∞ built on X, and a family of repelling cycles for the system (X,r,m_0). Our Hilbert space is built as an L^2-space on certain infinite paths starting at X. In Theorem 2.14, we solve the corresponding scaling identity, and write the scaling function as an infinite product. As one should expect by analogy to wavelets, a central theme in our present analysis is a characterization of those filter functions m_0 on X for which the scaling identity has non-trivial solutions in a Hilbert space of functions of X_∞.

A concrete example of this wavelet technique used on a particular graph dynamical system (The Golden mean shift) is presented in Proposition 2.18 below. Our aim is to present this as a systematic tool for dynamics outside the traditional context of wavelets in $L^2(\mathbb{R})$.

In recent papers,[11,13] the co-authors have adapted this MRA technique to a related but different problem, the problem of creating a spectral theory for a class of non-linear iterated function systems (IFS), but in those cases, there is not a direct analog to the scaling identity. Our construction here parallels the one we outlined briefly for the standard dyadic MRA wavelet constructions.[17] (We have sketched the standard wavelet construction only in the dyadic case, and only in one dimension, i.e., for $\mathbb{R}$, but it is known that this construction carries over *mutatis mutandis* to $\mathbb{R}^d$ with $d>1$, and when $x\mapsto 2x$, is replaced with matrix scaling $x\mapsto Ax$ in $\mathbb{R}^d$ where A is a d by d matrix over $\mathbb{Z}$ with eigenvalues λ such that $|\lambda|>1$. Moreover our results apply to the kind of multiwavelets studied recently in Ref. 1.)

Our present paper is not about $\mathbb{R}^d$-wavelets but instead about a class of non-linear dynamics $r:X\to X$. Specifically, now we start with $r:X\to X$, and the function m_0 is defined on X. We will also call m_0 a *filter function* because of known analogy to subband filtering in signal processing. When m_0 is given then S_0 given by $S_0h(x):=m_0(x)h(r(x))$ is isometric in $L^2(X)$, subject to a technical condition on m_0. So by Wold's theorem,[31] it is then the orthogonal sum of a shift operator S and a unitary operator U_0; i.e., the Hilbert space $L^2(X)$ on which S_0 acts is the direct sum of two Hilbert spaces $H(S)$ and $H(U_0)$ such that (i) each space invariant for S_0, (ii) the restriction to $H(S)$ is a shift S, and the restriction to $H(U_0)$ a unitary operator. We say that S_0 is *pure* if $H(U_0)=\{0\}$. (See Fig. 1.) This will be equivalent to the fact that the intersection of the multiresolution subspaces is trivial.

This means that S_0 is itself a shift operator on $L^2(X)$. Our Theorem 3.9 gives a simple condition for the isometry S_0 to be pure.

The first step in our construction is an extension from the initial endomorphism $r:X\to X$, to a new invertible system $\hat{r}:X_\infty\to X_\infty$, i.e., with $\hat{r}$ invertible on X_∞. When r is assumed finite-to-one, this can be done such that there is a quotient X_∞/X which becomes a Cantor space. The extension space X_∞ is called a solenoid. For the case when (X,r) is a one-sided subshift,[24] we work out (in Sec. II D) an explicit model for this solenoid.

In fact the notion of a solenoid (for the study of dynamics of an endomorphism and extension to an automorphism) was used already in a pioneering paper by Lawton[19] in 1973. Lawton considered groups with expansive automorphisms; see also Ref. 20. Motivated by applications, we note that our present analysis is not restricted to groups.

The use of solenoids in the study of particular systems with scale similarity was initiated in Ref. 8, and was continued in Ref. 7. The context of Ref. 8 is a class of algebraic irrational numbers and an associated C^*-algebraic crossed product. In a general context of non-linear dynamics, this work was continued in Refs. 11 and 13.

II. COVARIANT REPRESENTATIONS

Let X be a compact metric space with a non-invertible endomorphism $r:X\to X$ such that r is measurable, onto and finite to one, i.e., $0<\#r^{-1}(x)<\infty$ for all $x\in X$.

We have shown in Refs. 12 and 13 that, for certain filter functions m_0 on X, one can construct multiresolutions and scaling functions in Hilbert spaces of functions on X_∞ (see (2.1)).

In Ref. 13 we proved that to get useful multiresolutions, the function m_0 must have certain extreme cycles (see Definition 2.10). In this case the measure on X_∞ is actually supported on a smaller set $\mathbf{N}_C$ (see (2.4) below).

A. The ground space

An (infinite) *path* starting at x is a sequence $(z_1,z_2,\dots)$ of points in X such that $r(z_1)=x$, $r(z_{n+1})=z_n$ for $n\geqslant 1$. We denote by Ω_x the set of paths starting at x. We denote by X_∞ the set of all paths,

$$X_\infty=\cup_{x\in X}\Omega_x. \tag{2.1}$$

Note that a path $(z_1,z_2,\dots)$ in Ω_x can be identified with the doubly infinite sequence $(z_n)_{n\in\mathbb{Z}}$, where $z_0:=x$ and $z_{-n}=r^n(x)$ for $n\geqslant 0$.

$X_\infty\subset X^{\mathbb{Z}}$ inherits the usual Tychonoff topology from $X^{\mathbb{Z}}$.

The maps $\theta_n:X_\infty\to X$ are defined for all $n\in\mathbb{Z}$, by

$$\theta_n((z_k)_{k\in\mathbb{Z}})=z_n.$$

The endomorphism r can be extended to the automorphism $\hat{r}$ defined on X_∞ by

$$\hat{r}(z_n)_{n\in\mathbb{Z}}=(z_{n-1})_{n\in\mathbb{Z}}.$$

These maps satisfy the following relations:

$$\theta_n \circ \hat{r} = \theta_{n-1} \quad \theta_0 \circ \hat{r} = r \circ \theta_0.$$

For a function g on X we define

$$g^{(n)}(x) := g(x)g(r(x)) \cdots g(r^{n-1}(x)) \quad (n \geqslant 1). \tag{2.2}$$

For a function ξ on X_∞, we define $\xi^{(0)}=1$,

$$\xi^{(n)} := \xi\xi \circ \hat{r} \cdots \xi \circ \hat{r}^{n-1},$$

and if ξ is not vanishing on X_∞, then

$$\xi^{(-n)} = \frac{1}{\xi \circ \hat{r}^{-1}\xi \circ \hat{r}^{-2} \cdots \xi \circ \hat{r}^{-n}} \quad (n \geqslant 1).$$

We can identify functions g on X with functions on X_∞ by $g \leftrightarrow g \circ \theta_0$. (Note that the two definitions for $g^{(n)}$ will coincide.)

Consider $r: X \to X$ and suppose ρ is a *strongly invariant* probability measure on X, i.e.,

$$\int_X f(x)d\rho(x) = \int_X \frac{1}{\#r^{-1}(x)} \sum_{y \in r^{-1}(x)} f(y)d\rho(x) \quad (f \in L^\infty(\rho)). \tag{2.3}$$

Let $C=\{x_0, x_1, \ldots, x_{p-1}\} \subset X$ be a *cycle* of length p, i.e., the points x_i are distinct and $r(x_{i+1}) = x_i$, $r(x_0)=x_{p-1}$.

We define the set

$$\mathbf{N}_C(x) := \{\omega = (z_1, z_2, \ldots) \in \Omega_x | \lim_{n\to\infty} z_{pn} \in C\}. \tag{2.4}$$

For each $x \in X$ and $\omega=(z_1, z_2, \ldots) \in \mathbf{N}_C(x)$, define $i(\omega) \in \{0, \ldots, p-1\}$ by $i(\omega) := i$ if $\lim_{k\to\infty} z_{kp} = x_i$.

An inspection reveals that each $\mathbf{N}_C(x)$ is countable.

Define the measure λ_C on X_∞ by

$$\int_{X_\infty} f d\lambda_C = \int_X \sum_{\omega \in \mathbf{N}_C(x)} f(\omega)d\rho(x). \tag{2.5}$$

To simplify the notation we write $\mathfrak{c}(x) = \# r^{-1}(r(x))$.

Proposition 2.1: For all $\xi \in L^1(X_\infty, \lambda_C)$ and $n \in \mathbb{Z}$, we have

$$\int_{X_\infty} \mathfrak{c}^{(n)} \xi \circ \hat{r}^n d\lambda_C = \int_{X_\infty} \xi d\lambda_C.$$

Proof: It is enough to prove this for $n=1$, the rest follows by induction,

$$\begin{aligned}
\int_{X_\infty} \mathfrak{c}\xi \circ \hat{r} d\lambda_C &= \int_X \# r^{-1}(r(x)) \sum_{\omega \in \mathbf{N}_C(x)} \xi(\hat{r}(x,\omega))d\rho(x) \\
&= \int_X \frac{1}{\#r^{-1}(x)} \sum_{y \in r^{-1}(x)} \# r^{-1}(r(y)) \sum_{\omega \in \mathbf{N}_C(y)} \xi(\hat{r}(y,\omega))d\rho(x) \\
&= \int_X \sum_{\omega \in \mathbf{N}_C(x)} \xi(x,\omega)d\rho(x) = \int_{X_\infty} d\lambda_C.
\end{aligned}$$

□

B. The operators

In this section we show that when (X,r) is given as above, there is a natural covariant representation (U,π) acting on the Hilbert space $L^2(X_\infty,\lambda_C)$, i.e., with r inducing a unitary operator U, and π a representation of $L^\infty(X)$ by multiplication operators, such that the relation (2.8) is satisfied on $L^2(X_\infty,\lambda_C)$. (The operators on $L^2(X_\infty,\lambda_C)$ are equipped with the strong operator topology (SOT).)

Let $\alpha_0,\ldots,\alpha_{p-1}$ be a set of complex numbers of absolute value 1.

Let U be the operator on $L^2(X_\infty,\lambda_C)$ defined by

$$U\xi(x,\omega)=\alpha_{i(\omega)}\sqrt{\#r^{-1}(r(x))}\,\xi\circ\hat{r}(x,\omega)\quad(\xi\in L^2(X_\infty,\lambda_C),x\in X,\omega\in\Omega_x). \tag{2.6}$$

For $f\in L^\infty(X,\rho)$ define the operator $\pi(f)$ on $L^2(X_\infty,\lambda_C)$ by

$$\pi(f)\xi(x,\omega)=f(x)\xi(x,\omega)\quad(\xi\in L^2(X_\infty,\lambda_C),x\in X,\omega\in\Omega_x). \tag{2.7}$$

Proposition 2.2: The operator U is unitary, π is a representation of the algebra $L^\infty(X,\rho)$ and the following covariance relation is satisfied:

$$U\pi(f)U^{-1}=\pi(f\circ r)\quad(f\in L^\infty(X,\rho)). \tag{2.8}$$

For any function $f\in L^\infty(X,\rho)$ and $n\geqslant 1$, the operator $U^{-n}\pi(f)U^n$ is the operator of multiplication by $f\circ\theta_n$. The union of the algebras $\{U^{-n}\pi(f)U^n|f\in L^\infty(X,\rho)\}$ is SOT-dense in the algebra $L^\infty(X_\infty,\lambda_C)$ (seen as multiplication operators on $L^2(X_\infty,\lambda_C)$). An operator S on $L^2(X_\infty,\lambda_C)$ commutes with U and $\pi(f)$ for all $f\in L^\infty(X,\rho)$ if and only if there exists a function $F\in L^\infty(X_\infty,\lambda_C)$ such that $F=F\circ\hat{r}$ and S is the operator of multiplication by F.

Proof: The fact that U is an isometry follows form Proposition 2.1.

The inverse of U is

$$U^{-1}\xi(x,\omega)=\alpha^{-1}_{i(\hat{r}(\omega))}\frac{1}{\sqrt{\#r^{-1}(x)}}\xi\circ\hat{r}^{-1}(x,\omega).$$

Some simple computations prove the other relations.

Note that the algebra $\{U^{-n}\pi(f)U^nf\in L^\infty(X,\rho)\}$ is the algebra of operators of multiplication by functions which depend only on the first n coordinates. Since any function in $L^\infty(X,\rho)$ can be pointwise and uniformly boundedly approximated by such functions, it follows that the union of these algebras is dense in $L^\infty(X_\infty,\lambda_C)$.

Since $L^\infty(X_\infty,\lambda_C)$ is maximal Abelian, if S commutes with U and π then S commutes with the multiplication operators, so it is a multiplication operator itself, $S=M_F$. Since S commutes with U, it follows that $F=F\circ\hat{r}$. □

Our formula for the measure λ_C in (2.5) shows that the Hilbert space $L^2(X_\infty,\lambda_C)$ fibers over functions on X as follows: for a dense space of functions $\xi,\eta\in L^2(X_\infty,\lambda_C)$, the sum

$$\langle\xi|\eta\rangle(x):=\sum_{\omega\in\mathbf{N}_C(x)}\xi(\omega)\overline{\eta}(\omega)$$

defines a $C(X)$-valued inner product as in Refs. 28 and 16 and

$$\int_X\langle\xi|\eta\rangle(x)d\rho(x)=\langle\xi|\eta\rangle_{L^2(X_\infty,\lambda_C)}.$$

C. A direct integral decomposition

We now resume our discussion of cycles C for the endomorphism.

The cycle $C=\{x_0,\ldots,x_{p-1}\}$ generates p points in X_∞:

$$\omega_C := (x_0,x_1,\ldots,x_{p-1},x_0,\ldots) \quad \text{and} \quad \hat{r}^k(\omega_C), k \in \{1,\ldots,p-1\},$$

i.e., ω_C is the path that goes through the cycle infinitely many times. We may write $\omega_C := CC\cdots = C^\infty$.

Definition 2.3: A fixed point x_0 for r is called repelling if there is $0<c<1$ and $\delta>0$ such that for all $x \in X$ with $d(x,x_0)<\delta$, one has $d(r(x),x_0)>c^{-1}d(x,x_0)$.

A cycle $C=\{x_0,\ldots,x_{p-1}\}$ is called repelling if each point x_i is repelling for r^p.

Definition 2.4: A subset A of X_∞ is called a *cross section* if for every path $\omega \in \cup_{x\in X}\mathbf{N}_C(x)\backslash\{\hat{r}^k(\omega_C)\,|\,k\in\{0,\ldots,p-1\}\}$, the intersection $A\cap\{\hat{r}^k(\omega)\ k\in\mathbb{Z}\}$ contains exactly one point.

Proposition 2.5: If C is repelling, and r is continuous at the points in C, then there exists a cross section.

Proof: Using the continuity of r and the fact that the cycle is repelling, we can find a small $\delta>0$ and $0<c<1$ such that $r^i(B(x_0,\delta))\cap B(x_0,\delta)=\emptyset$, for $i\in\{1,\ldots,p-1\}$, $r^{-p}(x_0)\cap B(x_0,\delta)=\{x_0\}$, and such that $d(r^p(x),x_0)\geq c^{-1}d(x,x_0)$ for $x\in B(x,\delta)$.

Define

$$A := \{(z_k)_{k\in\mathbb{Z}} \in X_\infty | z_0 \in r^p(B(x_0,\delta))\setminus B(x_0,\delta), \quad \text{and} \quad z_{kp}\in B(x_0,\delta) \text{ for } k\geq 1\}.$$

It is enough to prove that, for every path $(z_k)_{k\in\mathbb{Z}}$ in $\mathbf{N}_C(x)$, except the special ones ω_C and the others, there is a unique $k_0\in\mathbb{Z}$ such that

$$z_{k_0}\in r^p(B(x_0,\delta))\setminus B(x_0,\delta), \quad \text{and} \quad z_{kp}\in B(x_0,\delta) \quad \text{for } k\geq 1. \tag{2.9}$$

Since ω is in $\mathbf{N}_C(x)$, the sequence $\{z_{kp}\}$ converges to one of the points x_i. Then, using the continuity of r, $\{z_{kp+p-i}\}$ converges to x_0.

Take the first $k_0\in\mathbb{Z}$ such that $z_{kp+k_0}\in B(x_0,\delta)$, for all $k\geq 1$. We still have to justify why there is a first one.

If not, then $z_{-kp+k_0}\in B(x_0,\delta)$ for all $k\geq 0$. Then, using the fact that x_0 is repelling for r^p, there is a c such that $0<c<1$, and for all $k\geq 0$,

$$\delta > d(z_{-kp+k_0},x_0) = d(r^{kp}(z_{k_0}),x_0) \geq c^{-k}d(z_{k_0},x_0).$$

But then let $k\to\infty$, and obtain that $z_{k_0}=x_0$. So, $z_{k_0-l}=r^l(x_0)=x_{l \bmod p}$ for all $l\geq 0$. Also, since $z_{k_0+p}\in B(x_0,\delta)\cap r^{-p}(x_0)$, we get $z_{k_0+p}=x_0$. By induction we obtain then that ω is one of the special points in the orbit of ω_C, which yields the contradiction.

Since $z_{k_0+p}\in B(x_0,\delta)$, $z_{k_0}=r^p(z_{k_0+p})$ is in $r^p(B(x_0,\delta))$ but not in $B(x_0,\delta)$.

Since $z_{k_0+kp}\in B(x_0,\delta)$ for $k\geq 1$, this proves that k_0+kp does not have the property (2.9).

Since $z_{k_0}\notin B(x_0,\delta)$, this proves that k_0-kp does not have the property (2.9) for $k\geq 1$.

Since for $k\geq 0$, $z_{k_0+kp+p}\in B(x_0,\delta)$, it follows that for $i\in\{1,\ldots,p-1\}$, one has $z_{k_0+kp+i}\in r^{p-i}(B(x_0,\delta))$ so it is not in $B(x_0,\delta)$, and therefore k does not satisfy (2.9) when $k\not\equiv k_0 \bmod p$.

This proves that A is a cross section. □

Our present notion of cross section, and our next theorem are motivated in part by an earlier theorem of Lim, Packer, and Taylor[21] on direct integral decompositions of a class of wavelet representations: This is the class of wavelets for which the Fourier transform $\hat{\psi}$ of the wavelet mother-function ψ is the indicator function of a measurable subset in $\mathbb{R}^d$. Both our present direct integral decomposition theorem, and that in Ref. 21 are motivated by Mackey's theory of unitary representations of non-Abelian groups. In fact, our representation of the covariant system (U,π) may be viewed as a single representation of a certain non-Abelian crossed product $\mathfrak{A}_{\hat{r}}$

$:= C(X_\infty) \ltimes_{\hat{r}} \mathbb{Z}$ (see Ref. 8), and our simultaneous direct integral decomposition of U and π in Theorem 2.6 below, is also a direct integral decomposition of a single representation of the crossed product group.

Assume now that A is a cross section. For each $\omega \in A$, define the operators U_ω and $\pi_\omega(f)$, $f \in L^\infty(X,\rho)$ on $l^2(\mathbb{Z})$ by

$$U_\omega \xi(k) = \alpha_{i(r^k(\omega))} \xi(k+1) \quad (\xi \in l^2(\mathbb{Z}), k \in \mathbb{Z}),$$

$$\pi_\omega(f)\xi(k) = f(z_{-k})\xi(k) \quad (\xi \in l^2(\mathbb{Z}), k \in \mathbb{Z}).$$

The representation π_ω extends to a representation of $C(X_\infty)$ defined by

$$\pi_\omega(f)\xi(k) = f(\hat{r}^k(\omega))\xi(k) \quad (f \in C(X_\infty), \xi \in l^2(\mathbb{Z}), k \in \mathbb{Z}).$$

The covariance relation is satisfied:

$$U_\omega \pi_\omega(f) U_\omega^{-1} = \pi_\omega(f \circ \hat{r}) \quad (f \in C(X_\infty)).$$

Theorem 2.6: *Let A be a cross section, and assume that $\rho(C)=0$. The map $\Phi: L^2(X_\infty, \lambda_C) \to L^2(A, \lambda_C) \otimes l^2(\mathbb{Z})$ defined by*

$$(\Phi(f))(\omega,k) = \sqrt{\mathfrak{c}^{(k)}(z_0)} f(\hat{r}^k(\omega)) \quad (f \in L^2(X_\infty, \lambda_C), \omega = (z_k)_{k\in\mathbb{Z}} \in A, k \in \mathbb{Z})$$

is an isometric isomorphism which intertwines the operators U and $\int_A^\oplus U_\omega d\lambda_C(\omega)$, and also the representations π and $\int_A^\oplus \pi_\omega d\lambda_C(\omega)$. The representations (U_ω, π_ω) on $l^2(\mathbb{Z})$ are irreducible for all $\omega \in A$.

Proof: The fact that Φ is isometric follows from Proposition 2.1. The inverse of Φ is defined as follows: for each $\omega \in \cup_x \mathbf{N}_C(x)$, (except the special ones which have measure 0, so do not matter), there exists a unique $k(\omega) \in \mathbb{Z}$ and $\eta(\omega) \in A$ such that $\omega = \hat{r}^{k(\omega)}(\eta(\omega))$. Then

$$\Phi^{-1}(f)(\omega) = \frac{1}{\sqrt{\mathfrak{c}^{(k(\omega))}(\eta(\omega)_0)}} f(\eta(\omega), k(\omega)).$$

Everything follows by direct computation.

We prove now that the representation (U_ω, π_ω) is irreducible for all $\omega = (z_k)_{k\in\mathbb{Z}} \in A$.

Note first that $\pi_\omega(f)$ is a diagonal operator F with entries $F_{kk} = f(z_{-k})$, $k \in \mathbb{Z}$.

We claim that for $k \neq l$ big enough, we have $z_k \neq z_l$. Since ω is in $\mathbf{N}_C(z_0)$, it follows that z_{kp} converges to one of the points of the cycle. Also, for k big enough, the points z_k cannot be in C, because, this path ω_C was removed from A. Suppose now that for any m we can find $k, l \geqslant m$, such that $k > l$ and $z_k = z_l$. Then this implies that z_k is periodic, therefore also $z_{k-1} = r(z_k), z_{k-2}, \ldots, z_l$ are periodic, and since m is arbitrary, it follows that all the points z_m are periodic. The orbit of the two periodic points z_0 and z_k intersect, because $r^k(z_k) = z_0$, therefore the two orbits must be the same. Thus the path $(z_k)_{k\in\mathbb{Z}}$ is an infinite repetition of the periodic orbit of z_0: $(z_0, z_1, \ldots, z_{p_0-1}, z_0, z_1, \ldots)$. However, this cannot converge to the cycle C.

Take now $k \neq l$ small enough. Then $z_{-k} \neq z_{-l}$ so we can pick a function continuous function f such that $F_{kk} = f(z_{-k}) \neq f(z_{-l}) = F_{ll}$. If $T = (T_{ij})_{i,j\in\mathbb{Z}}$ is an operator on $l^2(\mathbb{Z})$ that commutes with U_ω and π_ω, then $T_{kl}F_{ll} = F_{kk}T_{kl}$. So $T_{kl} = 0$ for $k \neq l$ small enough.

Note that $(U_\omega^{-1}\pi_\omega(f)U_\omega\xi)(k) = f(z_{-k+1})\xi(k)$, so the conjugation with U_ω shifts the diagonal entries of $\pi_\omega(f)$. Therefore, with the previous argument, we obtain that $T_{kl} = 0$ for all $k \neq l$. So T is a diagonal operator. Since, T commutes with U_ω, we obtain that $T_{kk} = T_{k+1,k+1}$. So T is a constant multiple of the identity. This proves that the representation (U_ω, π_ω) is irreducible. □

We show in Theorem 2.7 below that the harmonic analysis of covariant systems (U, π) as in (2.8) is completely equivalent to that of single representations $\hat{\pi}$ of a certain C^*-algebraic crossed product $\mathfrak{A}_{\hat{r}}$. With this identification $(U, \pi) \leftrightarrow \hat{\pi}$, we note in particular that the operators in the

commutant of the pair (U,π) coincide with the commutant of the representation $\hat{\pi}$. Our main conclusion in Theorem 2.7 is that the representation $\hat{\pi}$ of $\mathfrak{A}_{\hat{r}}$ is faithful, i.e., that the kernel of $\hat{\pi}$ is trivial.

Theorem 2.7: *Assume that for every $x \in X$, there exists a path $(z_i)_{i\geqslant 1}$ that starts at x and with $\lim_{i\to\infty} z_{pi} \in C$, (i.e., $\mathbf{N}_C(x)$ is non-empty). Then the operators U and M_f, $(f \in C(X_\infty))$ on $L^2(X_\infty,\lambda_C)$ form a faithful representation of the crossed-product $\mathfrak{A}_{\hat{r}} := C(X_\infty) \ltimes_{\hat{r}} \mathbb{Z}$.*

Proof: The C^*-algebraic crossed product $\mathfrak{A}_{\hat{r}}$ (Ref. 29) is the C^*-algebraic completion of formal symbols $\{(f,k)\,|\,f \in C(X_\infty), k \in \mathbb{Z}\}$ with product

$$(f,k)\cdot(g,l) = (fg\circ \hat{r}^k, k+l) \quad (f,g \in C(X_\infty), k,l \in \mathbb{Z}).$$

The representation is defined by

$$\hat{\pi}:(f,k) \mapsto \pi(f)U^k.$$

We saw in Proposition 2.2 and its proof that the covariance relation is satisfied, so we have to check only that this representation is faithful. If not, using a result from Ref. 32, we see that there is a non-zero element in $\mathfrak{A}_{\hat{r}}$ of the form $(\Sigma_{k\in\mathbb{Z}} c_k(f,k))$ with $\Sigma_{k\in\mathbb{Z}}|c_k| < \infty$, $f \in C(X_\infty)$ such that this element is mapped to 0 under $\hat{\pi}$.

This means that $\pi(f)\Sigma_{k\in\mathbb{Z}} c_k U^k = 0$. With Theorem 2.6 it follows that for almost all $\omega \in A$ and all $\xi \in l^2(\mathbb{Z})$, $l \in \mathbb{Z}$, one has

$$f(\hat{r}^l(\omega)) \sum_{k\in\mathbb{Z}} c_k \xi(k+l) = 0.$$

Take $\xi = \delta_i$ and get $f(\hat{r}^l(\omega))c_{i-l} = 0$ which implies that either $f(\hat{r}^l(\omega)) = 0$ for all l, or $c_l = 0$ for all l. But, if $c_l = 0$ for all l then this contradicts that the element in the crossed-product is non-zero.

Thus, for almost all $\omega = (z_i)_{i\in\mathbb{Z}} \in A$, we have that $f(\hat{r}^l(\omega)) = 0$ for all l.

This implies that f is 0 on almost all $\cup_x \mathbf{N}_C(x)$. We know that non-empty open sets in X have positive ρ-measure (see Ref. 13). Hence, since the measure on each $\mathbf{N}_C(x)$ is atomic, every non-empty open set in $\cup_x \mathbf{N}_C(x)$ has positive measure. This implies that f has to be 0 on all $\cup_x \mathbf{N}_C(x)$. We claim that this set is dense in X_∞.

Take $\omega := (z_1, z_2, \ldots) \in X_\infty$ and $n \geqslant 1$ fixed. Since $\mathbf{N}_C(z_n)$ is not empty, there exists a path $(y_1, y_2, \ldots)$ that starts at z_n and is convergent to the cycle. Then, $(z_1, z_2, \ldots, z_n, y_1, y_2, \ldots)$ is in $\mathbf{N}_C(x)$ and coincides with the initial path on the first n components. Thus, the path ω can be approximated with paths in $\mathbf{N}_C(x)$.

Hence $\cup_x \mathbf{N}_C(x)$ is dense in X_∞, and this implies that $f = 0$. The contradiction yields the result. □

Remark 2.8: [Iteration of rational functions]

Let $r: \mathbb{S}^2 \to \mathbb{S}^2$ be a rational function viewed as an endomorphism of the Riemann sphere $\mathbb{S}^2$, or $\mathbb{C}^\infty = \mathbb{C} \cup \{\infty\}$; and suppose the degree of r is bigger than 2. Let $X = X(r)$ be the *Julia set* of r, i.e., X is the complement of the largest open subset $\mathcal{U}$ such that $\{r^n|_{\mathcal{U}} \,|\, n \geqslant 1\}$ is a normal family. It is known that X is non-empty, compact, and that (X,r) carries a unique strongly invariant probability measure; see Refs. 5 and 9.

Our present general result for cycles is motivated by the following specific theorems for rational mappings:

Let r be a rational mapping of degree at least 2.

- Let C be a p-cycle for r. Then C is repelling if and only if $|(r^p)'(z)| > 1$ for all $z \in C$. Moreover, $(r^p)'(z) = \Pi_{w\in C} r'(w)$, $z \in C$, so $(r^p)'$ has the same value for all points z on the cycle C.
- Every repelling cycle C lies in the Julia set X.
- The Julia set X is the closure of the repelling periodic points, see Ref. 25.

D. The scaling function

We now turn to a theorem which is analogous to the existence theorem for the scaling function in the classical theory of wavelets. As outlined in Ref. 10, the wavelet scaling function φ in $L^2(\mathbb{R})$ depends on a filter function m_0 with m_0 defined on $\mathbb{T}=\mathbb{R}/\mathbb{Z}$. In fact, in the wavelet theory, it is the Fourier transform $\hat{\varphi}$ which is an infinite product of scaled versions of m_0. As is well known, this representation requires that the function m_0 satisfies two conditions: one is called the *quadrature condition*, and the second is called the *low-pass* condition. Both of these conditions are motivated directly from the probabilistic interpretation that $|m_0|^2$ enjoys in signal processing.

In our theorem below we identify the analog of these two conditions for the function $m_0: X \to \mathbb{C}$ which is associated to an endomorphism $r: X \to X$. The quadrature condition takes the form (2.10), and the low-pass condition takes the form (2.11). The reason for the name quadrature is that $r(z)=z^2$ in the wavelet case, and the reason for the name low-pass, is that points on $\mathbb{T}=\mathbb{R}/\mathbb{Z}$ correspond to frequencies, and $x=0$ is the lowest frequency.

In the general setting of the endomorphism r, the analog of low frequencies are points in cycles C for r, and in this setting low-pass means that $|m_0|^2$ attains its maximum on C. This is exactly what condition (2.11) is saying.

In the case of endomorphism, we will therefore expect to represent a scaling function as an infinite product built out of m_0 and iterated shifts applied to m_0. The fact that this can be done is the main conclusion in the theorem.

Definition 2.9: A complex valued function f on a metric space X is called β-Lipschitz at a point x_0 if there is a non-decreasing function $\beta: [0,\infty) \to [0,\infty)$ such that for all $A>0$ and $c<1$,

$$\sum_{k=1}^{\infty} \beta(Ac^k) < \infty,$$

and

$$|f(x) - f(x_0)| \leq \beta(d(x,x_0)),$$

for all x in some neighborhood of x.

Definition 2.10: Let $W: X \to [0,1]$ be a given function, and set

$$R_W f(x) := \sum_{r(y)=x} W(y) f(y) \quad (x \in X).$$

We say that R_W is a *transfer operator*, or a *Ruelle operator*. A function h on X is said to be *harmonic* with respect to R_W if $R_W h = h$. A cycle C for r is said to be a W-cycle if $W(x)=1$ for all $x \in C$.

The operator in Definition 2.10 plays a role in many areas of mathematics and physics. Some of its recent uses are highlighted in Ref. 30, where it is key to Ruelle's thermodynamical formalism.

Lemma 2.11: There is a unique family of measures P_x supported on Ω_x, $x \in X$, satisfying the following relation: for all measurable sets $E \subset X_\infty$ and all $x \in X$,

$$\sum_{r(y)=x} W(y) P_y(\Omega_y \cap \hat{r}^{-1}(E)) = P_x(\Omega_x \cap E).$$

Proof: It is enough to define P_x on cylinder sets: for a fixed $(a_1, a_2, \ldots, a_n, \ldots) \in \Omega_x$ and $n \geq 2$,

$$E := \{(z_1, z_2, \ldots) \in \Omega_x | z_1 = a_1, \ldots, z_n = a_n\}.$$

Then $P_x(E \cap \Omega_x) = \prod_{k=1}^{n} W(a_k)$.

The extension of P_x to the sigma-algebra generated by the cylinder sets now follows from Kolmogorov's theorem. See Ref. 13 for more details.

Also, for $y \in r^{-1}(x)$, one has that $\hat{r}^{-1}(E) \cap \Omega_y$ is empty unless $y = a_1$, in which case $P_y(\hat{r}^{-1}(E) \cap \Omega_y) = \Pi_{k=2}^{n} W(a_k)$. The lemma follows. □

Lemma 2.12: The function $h_C(x) := P_x(\mathbf{N}_C(x))$ is harmonic with respect to R_W.

Proof: We have the following disjoint union $\cup_{r(y)=x} \mathbf{N}_C(y) = \hat{r}^{-1}(\mathbf{N}_C(x))$. The lemma follows then from Lemma 2.11. Indeed,

$$(R_W h_C)(x) = \sum_{r(y)=x} W(y) h_C(y) = \sum_{r(y)=x} W(y) P_y(\Omega_y \cap \mathbf{N}_C(y))$$

$$= \sum_{r(y)=x} W(y) P_y(\Omega_y \cap \hat{r}^{-1}\mathbf{N}_C(x)) = P_x(\Omega_x \cap \mathbf{N}_C(x)) = h_C(x).$$

□

Definition 2.13: We call $h_C(x) := P_x(\mathbf{N}_C(x))$ the harmonic function associated to the cycle C. See also Ref. 13 for more details.

In our next theorem, we prove that each repelling cycle C generates a covariant operator system on the corresponding Hilbert space $L^2(X_\infty, \lambda_C)$. Moreover, under two conditions on a given filter function m_0, we show that the corresponding scaling equation has a natural solution $\hat{\varphi}_C$ in $L^2(X_\infty, \lambda_C)$.

Theorem 2.14: *Assume now that the cycle C is repelling and the functions r and $x \mapsto \# r^{-1}(x)$ are continuous at the points in C. Let $m_0 \in L^\infty(X, \rho)$ be a function which is β-Lipschitz at the points in C and which satisfies the conditions*

$$\frac{1}{\# r^{-1}(x)} \sum_{y \in r^{-1}(x)} |m_0(y)|^2 = 1, \quad (x \in X), \tag{2.10}$$

and

$$m_0(x_i) = \alpha_i \sqrt{\# r^{-1}(r(x_i))}, \quad (i \in \{0, \ldots, p-1\}). \tag{2.11}$$

Define the function $\hat{\varphi}$ by

$$\hat{\varphi}(x, (z_k)_{k \geqslant 1}) := \prod_{k=1}^{\infty} \frac{\alpha_{i(\omega)+k}^{-1} m_0(z_k)}{\sqrt{\# r^{-1}(r(z_k))}}, \quad (x \in X, (z_k)_{k \geqslant 1} \in \mathbf{N}_C(x)). \tag{2.12}$$

Then $\hat{\varphi}$ is in $L^2(X_\infty, \lambda_C)$ and it satisfies the following relation:

$$U\hat{\varphi} = \pi(m_0)\hat{\varphi}. \tag{2.13}$$

If $W(x) := |m_0(x)|^2 / \# r^{-1}(r(x))$, then C is a W-cycle, and if h_C is the harmonic function associated to this W-cycle, then

$$\langle \pi(f)\hat{\varphi} | \hat{\varphi} \rangle = \int_X f h_C d\rho. \tag{2.14}$$

Set $V_0 := \overline{\{\pi(f)\hat{\varphi} | f \in L^\infty(X, \rho)\}}^{L^2}$, and $V_n := U^{-n} V_0$, for $n \in \mathbb{Z}$. Then $V_n \subset V_{n+1}$,

$$\overline{\cup_{n \in \mathbb{Z}} V_n} = L^2(X_\infty, \lambda_C), \quad \cap_{n \in \mathbb{Z}} V_n = \{0\}.$$

Proof: First we check that the infinite product (2.12) is convergent. Take $x \in X$, $\omega = (z_1, z_2, \ldots) \in \mathbf{N}_C(x)$. Then the sequence $\{z_{kp}\}$ converges to one of the points of the cycle C,

namely $x_{i(\omega)}$. Applying r, which is continuous at these points, we obtain that, for all l, the sequence $\{z_{kp+l}\}$ is convergent to $x_{i(\omega)+l}$.

Now we use the fact that the cycle is repelling. For k large enough, the path ω enters the neighborhood where the cycle is repelling (see Definition 2.3). Therefore, there are constants $0<c_l<1$, $0\leqslant m_l<\infty$ such that for k large enough $d(z_{kp+l},x_{i(\omega)+l})\leqslant c_l^k m_l$, for all $l\in\{0,\dots,p-1\}$. Take $c=\max\{\sqrt[p]{c_l}\}\in(0,1)$ and $M:=c^{-p}\max\{m_l\}$. Then for k large enough

$$d(z_k,x_{i(\omega)+k})\leqslant c^k M.$$

Since the function $\#r^{-1}(r(\cdot))$ is continuous at the points of the cycle, we get that for k large, $\#r^{-1}(r(z_k))=\#r^{-1}(r(x_{i(\omega)+k}))=:A_k\geqslant 1$.

Let β be the function given by the β-Lipschitz condition for m_0 at all the points of the cycle (Take the minimum of these functions over all the points of the cycle). Using the condition (2.11), we have

$$\left|\frac{\alpha_{i(\omega)+k}^{-1}m_0(z_k)}{\sqrt{\#r^{-1}(r(z_k))}}-1\right|=\frac{1}{\sqrt{A_k}}|m_0(z_k)-m_0(x_{i(\omega)+k})|$$

$$\leqslant\beta(d(z_k,x_{i(\omega)+k}))\leqslant\beta(c^kM).$$

This implies that the sum over the terms on the left-hand side of this inequality is convergent, which in turn implies that the infinite product is absolutely convergent.

Next we check (2.14). It is clear that C is a W-cycle. Also note that

$$|\hat{\varphi}(x,(z_k)_{k\geqslant 1})|^2=\prod_{k=1}^{\infty}W(z_k)=P_x(\{(z_k)_{k\geqslant 1}\}).$$

(See Ref. 13). Then

$$h_C(x)=P_x(\mathbf{N}_C(x))=\sum_{\omega\in\mathbf{N}_C(x)}|\hat{\varphi}(x,\omega)|^2, \tag{2.15}$$

and Eq. (2.14) follows. Since $h_C\leqslant 1$, this also implies that $\hat{\varphi}$ is in $L^2(X_\infty,\lambda_C)$.

We check Eq. (2.13). For $\omega=(z_1,z_2,\dots)\in\mathbf{N}_C(x)$,

$$U\hat{\varphi}(x,\omega)=\sqrt{\#r^{-1}(r(x))}\,\alpha_{i(\omega)}\prod_{k=1}^{\infty}\frac{\alpha_{i(\hat{r}(\omega))+k}^{-1}m_0(z_{k-1})}{\sqrt{\#r^{-1}(r(z_{k-1}))}}$$

$$=\sqrt{\#r^{-1}(r(x))}\,\alpha_{i(\omega)}\frac{\alpha_{i(\omega)}^{-1}m_0(x)}{\sqrt{\#r^{-1}(r(x))}}\prod_{k=2}^{\infty}\frac{\alpha_{i(\omega)+k-1}^{-1}m_0(z_{k-1})}{\sqrt{\#r^{-1}(r(z_{k-1}))}}=m_0(x)\hat{\varphi}(x,\omega).$$

The scaling equation (2.13) and the covariance equation (2.8) imply that $V_{-1}\subset V_0$. This implies that the sequence of subspaces $\{V_n\}$ is increasing.

To check that their union is dense, we note that the closure of this union is invariant for U and for $\pi(f)$, $f\in L^\infty(X,\rho)$. Therefore the projection P onto this space is in the commutant $\{U,\pi\}'$. But, then, with Proposition 2.2, we obtain a function F in $L^\infty(X_\infty,\lambda_C)$ such that $F=F\circ\hat{r}$ and $P=M_F$. In particular, $F\hat{\varphi}=\hat{\varphi}$ and F is the characteristic function of some set $\mathcal{F}$ which is invariant for $\hat{r}$.

However, the previous argument shows that, if $\omega=(z_1,z_2,\dots)\in\mathbf{N}_C(x)$ has z_i close enough to the cycle C, for all $i\geqslant 1$, then $\hat{\varphi}(x,\omega)$ is close to 1. Now, take $\omega=(z_1,z_2,\dots)\in\mathbf{N}_C(x)\setminus\mathcal{F}$. Then $\hat{r}^{-n}(\omega)$ is outside $\mathcal{F}$. Because $\omega\in\mathbf{N}_C(x)$, for n large enough, all the points $z_{n+1},z_{n+2},\dots$ are close to the cycle, so $\hat{\varphi}(\hat{r}^{-n}(\omega))$ is close to 1. But $\hat{\varphi}(\hat{r}^{-n}(\omega))=\hat{\varphi}(\hat{r}^{-n}(\omega))\chi_{\mathcal{F}}(\hat{r}^{-n}(\omega))=0$, a contradiction. It follows that $\mathcal{F}$ has complement of measure 0 so $P=M_F$ is the identity, and therefore the union of the multiresolution subspaces is dense.

It remains to check that the intersection $\cap V_n$ is trivial. We use the following lemma:

Lemma 2.15: Define $\mathcal{J}: L^2(X, h_C d\rho) \to V_0$ *by*

$$\mathcal{J}(f) = \pi(f)\hat{\varphi}, \quad (f \in L^\infty(X,\rho)).$$

Define the operator S_0 *on* $L^2(X, h_C d\rho)$ *by* $S_0 f = m_0 f \circ r$. *Then* $\mathcal{J}$ *is an isometric isomorphism such that* $U\mathcal{J} = \mathcal{J}S_0$.

The proof of the lemma requires just some simple computations. The fact that S_0 is an isometry is proved in Theorem 3.9.

With this lemma, the assertion follows from Theorem 3.9. □

Let $(X, \mathfrak{B}, \rho)$ be a measure space with ρ some fixed probability measure defined on the sigma-algebra $\mathfrak{B}$ on X. Let π be a representation of $L^\infty(X, \mathfrak{B})$ on a Hilbert space $\mathcal{H}$, and suppose that the measure $f \mapsto \langle \pi(f)\psi | \psi \rangle$ is absolutely continuous with respect to ρ for all $\psi \in \mathcal{H}$, i.e., there exists $h_\psi \in L^1(X, \mathfrak{B})$ such that $\langle \pi(f)\psi | \psi \rangle = \int_X f h_\psi d\rho$, $f \in L^\infty(X, \mathfrak{B})$.

By the spectral multiplicity theorem (Refs. 2, 15, and 31), there is a measurable function $d: X \to \{1, 2, \ldots, \infty\}$ such that if $X_k := \{x \in X | d(x) \geqslant k\}$, then the spectral representation of π takes the form of an isometric isomorphism $\mathcal{J}: \mathcal{H} \to \Sigma^{\oplus}_{k \in \mathbb{N}} L^2(X_k, \mathfrak{B}, \rho)$, such that $\mathcal{J}_k \pi(f)\psi = f \mathcal{J}_k \psi = M_f \mathcal{J}_k \psi$ for all $f \in L^\infty(X, \mathfrak{B})$ and all $\psi \in \mathcal{H}$.

We say that d is the *multiplicity function* of the representation π.

Corollary 2.16: Let $V_0 \subset L^2(X_\infty, \lambda_C)$, *be the subspace from Lemma 2.15 and Theorem 2.14, and let* π_n, $n \in \mathbb{N}$, *be the restriction of the representation* π *of* $L^\infty(X, \mathfrak{B})$ *to* $U^{-n}V_0$. *Then*

$$d_{U^{-n}V_0}(x) = \#\left(r^{-n}(x) \cap \{z \in X | h_C(z) \neq 0\}\right) \quad (x \in X).$$

Proof: Since $\langle \pi(f)\hat{\varphi} | \hat{\varphi} \rangle = \int_X f h_C d\rho$, it follows that $d_{V_0}(x) = \chi_{\{z \in X | h_C(z) \neq 0\}} =: \chi_{E_C}$.

From Ref. 12, we know that

$$d_{U^{-n}V_0}(x) = \sum_{r^n(y)=x} d_{V_0}(y) = \sum_{r^n(y)=x} \chi_{E_C}(y) = \#\left(r^{-n}(x) \cap E_C\right).$$

□

Example 2.17: Let A be a square matrix with $0-1$ entries. Suppose every column of A contains at least one entry 1. Then we show that the two systems $(X_\infty, \hat{r})$ and (X, r) may be realized as two-sided, respectively one-sided subshifts.

Let I be the index set for the rows and columns of A. Let

$$X_\infty(A) := \{(x_i)_{i \in \mathbb{Z}} \in I^{\mathbb{Z}} | A(x_i, x_{i+1}) = 1\}.$$

Let

$$\hat{r}((x_i)_{i \in \mathbb{Z}}) = (x_{i+1})_{i \in \mathbb{Z}}.$$

Define $\theta_0((x_i)_{i \in \mathbb{Z}}) = (x_i)_{i \geqslant 0}$, and set $X(A) = \theta_0(X_\infty(A))$.

Then there is an endomorphism $r = r_A: X(A) \to X(A)$ such that $r \circ \theta_0 = \theta_0 \circ \hat{r}$.

Specifically,

$$x = (x_i)_{i \in \mathbb{Z}} = \ldots x_{-2}x_{-1}x_0x_1x_2 \ldots$$

with $x_i \in I$;

$$\theta_0((x_i)_{i \in \mathbb{Z}}) = (x_i)_{i \geqslant 0} = x_0x_1x_2 \ldots;$$

and $r(x_0x_1x_2\ldots) = (x_1x_2x_3\ldots)$ for $x \in X(A)$.

For $x, y \in X(A)$, let $x \wedge y$ be the longest initial block in $I \times I \times \cdots$ common to both x and y, and let $|x \wedge y|$ be the length of this block. Let $0 < c < 1$, and set $d_c(x, y) = c^{|x \wedge y|}$. Then d_c is a metric, and $(X(A), d_c)$ is a compact metric space whose open sets are generated by the cylinder sets in $X(A)$.

Moreover, $d_c(r(x),r(y)) \leqslant c^{-1}d_c(x,y)$ holds for all $x,y \in X(A)$. If $x \in X(A)$, then $r^{-1}(x) = \{(ix) \mid A(i,x_0)=1\}$, and for the transfer operator $\mathcal{L}_A : C(X(A)) \to C(X(A))$,

$$(\mathcal{L}_A f)(x) = \frac{1}{\#r^{-1}(x)} \sum_{r(y)=x} f(y),$$

we have

$$(\mathcal{L}_A f)(x) = \frac{1}{\#\{i \mid A(i,x_0)=1\}} \sum_{A(i,x_0)=1} f(ix).$$

By Ref. 24, Chap. 2, there is a unique probability measure $\rho=\rho_A$ on $X(A)$ such that $\rho(\mathcal{L}_A f) = \rho(f)$ for all $f \in C(X(A))$; i.e., $\rho=\rho_A$ is the unique strongly invariant probability measure on $X(A)$.

It follows that all the results in this setting apply; in particular, if $C \subset X(A)$ is a cycle, then $L^2(X_\infty(A),\lambda_C)$ is defined by

$$\int_{X_\infty(A)} |f|^2 d\lambda_C = \int_{X(A)} \sum_{\omega \in \mathbf{N}_C(x)} |f(\omega)|^2 d\rho(x) < \infty .$$

Note also that $\mathbf{N}_C(x)$ consists of doubly infinite words in $X_\infty(A)$ that start with an infinite repetition of the cycle C. Specifically, for $x=(x_0x_1x_2\ldots) \in X(A)$, $\mathbf{N}_C(x)=\{(\omega_i)_{i\in\mathbb{Z}} \in X_\infty(A) \mid \exists k \in \mathbb{N}$ such that $(\omega_I)_{i\leqslant -k}$ is C^∞, $(\omega_i)_{-k<i\leqslant -1}$ is some finite word, and $\omega_i=x_i$ for $i \geqslant 0\}$.

We now turn to a concrete example. Let the index set I be $\{1,2\}$ and let $A=\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$. This is called the golden mean shift (see Ref. 22, p. 37).

Proposition 2.18: Let m_0 be the function on $X(A)$ determined by

$$m_0(11\ldots)=\sqrt{2}, \quad m_0(21\ldots)=0, \quad m_0(12\ldots)=1, \tag{2.16}$$

and C be the cycle $\{111\ldots\}$. Then m_0 satisfies (2.10) *and* (2.11) *and defines a scaling vector $\hat{\varphi} \in L^2(X_\infty,\lambda_C)$ with $h_C=1$.*

Proof: It is easy to verify the two conditions (2.10) and (2.11). The scaling function $\hat{\varphi}$ is defined by the infinite product (2.12). (We set $\alpha_i=1$.) If ω is in $\mathbf{N}_C(x_0x_1\ldots)$, then it has the form $\ldots 111x_{-n}x_{-n+1}\ldots x_{-1}x_0x_1\ldots$. Note that if one of the letters x_{-k} is 2 ($k \geqslant 1$) then the next one has to be 1. Therefore, shifting the word to the right will bring the 21 to the central position, and m_0 is 0 on words that start with 21. Therefore the infinite product is non-zero only when $x_{-k}=1$ for all $k \geqslant 1$. Then, an analysis of the possibilities for x_0 shows that $\hat{\varphi}$ is 1 in this case.

Therefore $\hat{\varphi}(\omega)=1$, if $x_{-k}=1$ for all $k \geqslant 1$, and $\hat{\varphi}(\omega)=0$ otherwise.

Then by (2.15)

$$h_C(x_0x_1\ldots) = \sum_{\omega \in \mathbf{N}_C(x_0x_1\ldots)} |\hat{\varphi}(\omega)|^2 = 1.$$

An interesting consequence of (2.10) and (2.11) for this example is that an admissible m_0 cannot be of the form $m_0=\sqrt{2}\chi_E$ for a subset E of $X(A)$ (because $|m_0(21\ldots)|^2=1$). This contrasts a known wavelet, the Shannon wavelet, see Refs. 17 and 1. □

III. ERGODIC PROPERTIES AND THE WOLD DECOMPOSITION

In our analysis of the intersection of the multiresolution spaces V_n, we are forced to study some convergence properties for the measure ρ and the filter m_0. The main tool in this study will be Doob's convergence theorems for reversed martingales, see e.g., Ref. 27.

Even though we are mainly interested in the strongly invariant measure ρ, our analysis works in the following more general case.

Definition 3.1: Let $V \geqslant 0$ be a measurable function on X such that

$$\sum_{r(y)=x} V(y) = 1 \quad (x \in X).$$

A probability measure ν on X such that

$$\int_X f d\nu = \int_X \sum_{r(y)=x} V(y) f(y) d\nu(x) \quad (f \in L^1(X,\nu)) \tag{3.1}$$

is called a Perron-Frobenius measure for the corresponding Ruelle operator

$$(R_V f)(x) := \sum_{r(y)=x} V(y) f(y) \quad (x \in X).$$

For example, when $V(x) = 1/\#r^{-1}(r(x))$, then (3.1) is equivalent to the strong invariance of ν.

Note that a Perron-Frobenius measure ν is also invariant for r, because

$$\int_X f \circ r d\nu = \int_X \sum_{r(y)=x} V(y) f(r(y)) d\nu(x) = \int_X f(x) \sum_{r(y)=x} V(y) d\nu(x) = \int_X f d\nu.$$

Let $\mathfrak{B}$ be the sigma-algebra of measurable subsets of X.

Definition 3.2: Let $\mathfrak{B}$ be a sigma-algebra on X and let ν be a probability measure on $(X,\mathfrak{B})$. Let $\mathfrak{C} \subset \mathfrak{B}$ be a sub-sigma-algebra. Then the $\mathfrak{C}$-conditional expectation $E_{\mathfrak{C}}$ is defined by

$$\int_X E_{\mathfrak{C}} f g d\nu = \int_X f g d\nu,$$

for $f \in L^1(\mathfrak{B},\nu)$, $g \in L^\infty(\mathfrak{C})$; and $E_{\mathfrak{C}} L^1(\mathfrak{B},\nu) = L^1(\mathfrak{C},\nu)$.

Proposition 3.3: The operator E_n^V defined on $L^1(X,\nu)$ by

$$E_n^V(f)(x) = \sum_{r^n(y)=r^n(x)} V^{(n)}(y) f(y) \quad (x \in X),$$

defines the conditional expectation of $\mathfrak{B}$ with respect to $r^{-n}(\mathfrak{B})$.

Proof: First note that if a function g on X is $r^{-n}(\mathfrak{B})$-measurable, then $g(x) = g(y)$ whenever $r^n(x) = r^n(y)$. Take now $g \in L^2(r^{-n}(\mathfrak{B}))$ and $f \in L^1(\mathfrak{B})$. Using the invariance of ν and (3.1), we have

$$\int_X E_n^V(f) g d\nu = \int_X \sum_{r^n(x)=r^n(y)} V^{(n)}(y) f(y) g(x) d\nu(x)$$

$$= \int_X \sum_{r^n(y)=x} V^{(n)}(y) f(y) g(y) d\nu(x) = \int_X f g d\nu.$$

This shows that E_n^V is the conditional expectation. □

We note the relation between the Ruelle operator R_V and the conditional expectation E_n^V:

$$E_n^V(f) = (R_V^n) \circ r^n \quad (n \geqslant 1, f \in L^1(X,\nu)). \tag{3.2}$$

The sigma-algebras $r^{-n}(\mathfrak{B})$ form a decreasing sequence, and we denote their intersection by $\mathfrak{B}_\infty$. Denote by E_∞^V the conditional expectation of $\mathfrak{B}$ with respect to $\mathfrak{B}_\infty$. Doob's theorems for reverse martingales can be applied now directly and we obtain the following theorem:

Theorem 3.4: *If $f \in L^p(X,\nu)$, $(1 \leqslant p < \infty)$, then $E_n^V(f)$ converges pointwise ν-a.e. and in $L^p(X,\rho)$ to $E_\infty^V(f)$.*

Definition 3.5: We say that r is *averaging* (with respect to the measure ν), if $L^1(\mathfrak{B}_\infty)$ contains only functions which are constant ν-a.e., (or, equivalently, the sigma-algebra $\mathfrak{B}_\infty$ contains only sets of ν-measure 0 or 1).

Proposition 3.6: If r is averaging with respect to ν then it is also ergodic with respect to ν.

Proof: If A is a completely invariant set for r then, for any two points x,y such that $r^n(x)=r^n(y)$ for some $n\geqslant 0$ $\chi_A(x)=\chi_A(r^n(x))=\chi_A(r^n(y))=\chi_A(y)$, so $\chi_A\in L^1(\mathfrak{B}_\infty)$, therefore $\nu(A)$ is 0 or 1. □

Corollary 3.7: If r is averaging with respect to ν, then for all $f\in L^p(X,\nu)$, $1\leqslant p<\infty$, the sequence $E_n^V(f)$ converges pointwise ν-a.e. and in $L^p(X,\nu)$ to $\int_X f d\nu$.

Next, we will derive an ergodic property for a function m_0 satisfying (2.10).

Theorem 3.8: *Assume that the strongly invariant measure ρ is ergodic with respect to r. Let $m_0\in L^\infty(X,\rho)$ be a function that satisfies* (2.10) *and such that $|m_0|\neq 1$ on a set of positive measure. Then*

$$A := \int_X \ln|m_0(x)|d\rho(x) \in [-\infty,0).$$

Then

$$\lim_{n\to\infty}|m_0(x)\cdots m_0(r^{n-1}(x))|^{\frac{1}{n}}=e^A \quad \textit{for } \rho\text{-a.e. } x\in X.$$

Proof: We have, using the strong invariance of ρ:

$$\begin{aligned}\int_X \ln|m_0(x)|d\rho(x)&=\frac{1}{2}\int_X \ln|m_0(x)|^2 d\rho(x)=\int_X \frac{1}{\#r^{-1}(x)}\sum_{r(y)=x}\ln|m_0(y)|^2 d\rho(x)\\&=\int_X \ln\Big(\prod_{r(y)=x}|m_0(y)|^2\Big)^{1/\#r^{-1}(x)}d\rho(x)\\&\leqslant\int_X \ln\Big(\frac{1}{\#r^{-1}(x)}\sum_{r(y)=x}|m_0(y)|^2\Big)d\rho(x)=\int_X \ln(1)=0.\end{aligned}$$

If we have equality in this chain, then we get that for ρ-a.e., $x\in X$, $|m_0(y)|=|m_0(y')|$ for all $y,y'\in r^{-1}(x)$, which implies that

$$1=\frac{1}{\#r^{-1}(r(x))}\sum_{r(y)=r(x)}|m_0(y)|^2=|m_0(x)|,\quad \text{for a.e. } x.$$

This contradicts the hypothesis. Thus $A\in[-\infty,0)$.

Assume now, that $A>-\infty$. Then, using Birkhoff's ergodic theorem, we obtain that

$$\lim_{n\to\infty}\ln\Big(\frac{|m_0(x)\cdots m_0(r^{n-1}(x))|^{1/n}}{e^A}\Big)=\lim_{n\to\infty}\frac{1}{n}\sum_{k=0}^{n-1}\ln|m_0(r^k(x))|-A$$

$$=\int_X \ln|m_0(x)|d\rho(x)-A=0.$$

This yields the conclusion in the case $A>-\infty$.

When $A=-\infty$, take $0>B>-\infty$ arbitrary and choose a bounded measurable function f, with $|f|\geqslant|m_0|$ and such that $-\infty<\int_X\ln|f(x)|\,d\rho(x)=B$. Then apply the previous argument to conclude that $|f(x)f(r(x))\cdots f(r^{n-1}(x))|^{1/n}$ converges a.e. to e^B. Then

$$\limsup_n|m_0(x)\cdots m_0(r^{n-1}(x))|^{1/n}\leqslant e^B$$

and, as B is arbitrary this implies that the limit is $e^{-\infty}=0$. □

With these results, we are now able to derive the result about the Wold decomposition[31] of the isometry S_0 associated to m_0.

Theorem 3.9: *Let ρ be a strongly invariant measure for r. Let $m_0 \in L^\infty(X,\rho)$ be a function that satisfies* (2.10). *Let $h \in L^\infty(X,\rho)$ be a function such that $h \geqslant 0$ and*

$$\frac{1}{\#r^{-1}(x)} \sum_{r(y)=x} |m_0(y)|^2 h(y) = h(x) \quad (x \in X). \tag{3.3}$$

Then the operator S_0 on $L^2(X,hd\rho)$ defined by

$$S_0 f = m_0 f \circ r$$

is an isometry.

Assume in addition that r is averaging with respect to ρ, and that $|m_0| \neq 1$ on a set of positive measure ρ. Then

$$\cap_{k \geqslant 1} S_0^k (L^2(X,hd\rho)) = \{0\}.$$

Proof: The fact that S_0 is an isometry follows from the fact that ρ is strongly invariant and from the relation (3.3):

$$\int_X |m_0(x)|^2 |f(r(x))|^2 h(x) d\rho(x) = \int_X \frac{1}{\#r^{-1}(x)} \sum_{r(y)=x} |m_0(y)|^2 |f(r(y))|^2 h(y) d\rho(x)$$

$$= \int_X |f(y)|^2 d\rho(x).$$

Denote by

$$c(x) := \frac{1}{\#r^{-1}(r(x))} \quad (x \in X).$$

Note that

$$R_{m_0}^k f(x) = \sum_{r^k(y)=x} c^{(k)}(y) |m_0^{(k)}(y)|^2 f(y),$$

where R_{m_0} is the Ruelle operator associated to $W(x) := |m_0(x)|^2 / \#r^{-1}(r(x))$.

In particular

$$\sum_{r^k(y)=x} c^{(k)}(y) |m_0^{(k)}(y)|^2 = 1.$$

Take now $\xi \in \cap_k S_0^k (L^2(X,hd\rho))$. Then for all $k \geqslant 1$, there exists $f_k \in L^2(X,hd\rho)$ such that $\xi = m_0^{(k)} f_k \circ r^k$. This implies that for all $x \in X$:

$$|\xi(x)|^2 = |m_0^{(k)}(x)|^2 |f_k(r^k(x))|^2 \sum_{r^k(y)=r^k(x)} c^{(k)}(y) |m_0^{(k)}(y)|^2$$

$$= |m_0^{(k)}(x)|^2 \sum_{r^k(y)=r^k(x)} c^{(k)}(y) |m_0^{(k)}(y) f_k(r^k(y))|^2$$

$$= |m_0^{(k)}(x)|^2 \sum_{r^k(y)=r^k(x)} c^{(k)}(y) |\xi(y)|^2$$

$$= |m_0^{(k)}(x)|^2 E_k^c(|\xi|^2).$$

With Theorem 3.8 and Corollary 3.7, if we let $k \to \infty$, we can conclude that $\xi = 0$, ρ-a.e. This proves the theorem. □

Remark 3.10: It is conceivable that the last conclusion in Theorem 3.9 above may hold slightly more generally; possibly when only ergodicity is assumed for (X, r, ρ). But for the applications we have in mind, our present assumption of strong invariance is appropriate, i.e., the averaging assumption we place on the system (X, r, ρ).

Some conditions for r to be averaging. We will give some necessary conditions for r to averaging. For this we will relate the expectation E_V^n to the Ruelle operator R_V.

Just as before, assume $V \geqslant 0$ is a measurable function such that

$$\sum_{r(y)=x} V(y) = 1 \quad (x \in X),$$

and let ν be a measure such that

$$\int_X R_V f d\nu = \int_X f d\nu.$$

Proposition 3.11: Suppose there exists a family of functions $\mathcal{F}$ which is dense in $L^1(X, \nu)$ such that for all $f \in \mathcal{F}$,

$$\lim_{n\to\infty} \left\| R_V^n(f) - \int_X f d\nu \right\|_1 = 0.$$

Then, for all $f \in L^1(X, \nu)$.

$$\lim_{n\to\infty} R_V^n(f) = \int_X f d\nu = E_\infty^V(f).$$

In particular r is averaging with respect to ν.

Proof: Take $f \in L^1(X, \nu)$, and $\epsilon > 0$. There exists $g \in \mathcal{F}$, such that $\|f - g\|_1 < \epsilon$. Then, using the fact that ν is invariant for r, and also for R_V, we have, with the aid of (3.2):

$$\left\| E_n^V(f) - \int_X f d\nu \right\|_1 = \left\| R_V^n f - \int_X f d\nu \right\|_1$$

$$\leqslant \|R_V^n(f-g)\|_1 + \left\| R_V^n g - \int_X g d\nu \right\|_1 + \left\| \int_X (g-f) d\nu \right\|_1$$

$$\leqslant 2\|f-g\|_1 + \left\| R_V^n g - \int_X g \right\|_1 < 3\epsilon,$$

for n large enough. This proves the first assertion. Since $E_\infty^V(f)$ is constant for all $f \in L^1(X, \nu)$, it follows that $L^1(\mathfrak{B}_\infty)$ contains only constant functions so r is averaging. □

Remark 3.12: The conditions of Proposition 3.11 are satisfied in many cases of interest. This is a consequence of Ruelle's theorem (see Refs. 3 and 14). For example, if r is locally expanding (i.e., there exists $b > 0$ and $\lambda > 1$ such that $d(r(x), r(y)) \geqslant \lambda d(x, y)$ when $d(x, y) < b$), and mixing (i.e., for every open set U in X, there exists n such that $r^n(U) = X$), and if $V > 0$ and is Lipschitz, then $\mathcal{F}$ can be taken to be the set of continuous functions, and $R_V^n f$ converges uniformly to $\int_X f d\nu$, where ν is the unique probability measure invariant for R_V.

In particular, this is satisfied, for subshifts of finite type.

Also, consider the case when r is a rational map on $\mathbb{C}$ and X is its Julia set. Take $V=1/N$ where N is the degree of the map r. Then $\nu=\rho$ is the unique strongly invariant measure and we may take again $\mathcal{F}$ to be the set of continuous functions (see Ref. 23).

Given our assumptions above, the existence and the uniqueness of the measure ν follows from the conclusion in Ruelle's theorem, applied to R_V.

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Jacobi identity for vertex algebras in higher dimensions

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Vertex algebras in higher dimensions, introduced previously by Nikolov, provide an algebraic framework for investigating axiomatic quantum field theory with global conformal invariance. We develop further the theory of such vertex algebras by introducing formal calculus techniques and investigating the notion of polylocal fields. We derive a Jacobi identity which together with the vacuum axiom can be taken as an equivalent definition of vertex algebra. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2197687]

I. INTRODUCTION

Two-dimensional conformal field theory is important in physics as providing models of quantum field theory (QFT). It also plays a role in other areas of mathematical physics as well as in statistical physics and condensed matter physics. A *vertex algebra* is essentially the same as a *chiral algebra* in conformal field theory (see Refs. 7 and 20 and Ref. 12). In more details, the field content in two-dimensional conformal field theories splits into two chiral parts consisting of fields that depend separately on one of the two light-cone variables. Observable chiral fields have commutators supported on the diagonal, i.e., vanishing for noncoinciding arguments. It turns out that chiral fields form a purely algebraic structure under their *operator product expansion*, which is called a vertex algebra. Axiomatically, the notion of vertex algebra was first introduced by Borcherds.[8] Vertex algebras arose naturally in the representation theory of infinite-dimensional Lie algebras and in the construction of the "moonshine module" for the Monster finite simple group.[8,19] Now the theory of vertex algebras is a rapidly developing area of mathematics (see Refs. 19, 21, 17, and 24). "Multidimensional" generalizations of vertex algebras were considered in Refs. 9, 23, 26, and 28.

The vertex algebras introduced in Ref. 28 for higher space–time dimension arose naturally within a one-to-one correspondence with axiomatic QFT models satisfying the additional symmetry condition of *global conformal invariance* (GCI). The incorporation of GCI within the framework of axiomatic QFT, together with the problem of finding (nonperturbatively) such models in higher dimensions, has been studied previously in, e.g., Refs. 31, 30, 32, and 29 [see also the groundbreaking early work (Ref. 34)]. In this way constructing models of higher-dimensional QFT with GCI becomes a purely algebraic problem. Let us point out that even for general QFT (without GCI) there are not any known models that satisfy the Wightman axioms in space–time dimension greater or equal to 4, which cannot be realized by free or generalized free (Heisenberg) fields. In fact, this problem has remained open for more than 50 years.

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On the other hand, even in dimension one (i.e., in chiral conformal field theory), vertex algebras are far from full classification and are quite intricate in general. A different algebraic structure known as a *vertex Lie algebra* has been introduced by Kac[21] (see also Refs. 33, 17, and 14) (it is also called a "conformal algebra" but we will not use this terminology here since it can be confused with the usual conformal Lie algebra in higher dimensions). This is the structure formed by the commutators of fields, i.e., by the singular part of their operator product expansion. Thus the relationship between vertex Lie algebras and vertex algebras is somewhat similar to the relationship between Lie algebras and associative algebras. It turns out that this new algebraic structure is more tractable and, in particular, classification results for vertex Lie (super)algebras can be obtained[11,15] (see also Refs. 21 and 22). The theory of vertex Lie algebras was further developed in, e.g., Refs. 10 and 4, and a "multidimensional" generalization was considered in Ref. 1.

In the present paper we initiate an investigation of the notion of vertex Lie algebra for the vertex algebras in higher dimensions of Ref. 28. In dimension one, the main axiom for vertex Lie algebras is the so-called *Jacobi identity*, which is related to the Jacobi identity of Ref. 19 for vertex algebras (and the Borcherds identity of Ref. 21). Recall that in dimension one vertex algebras can be defined in terms of the Jacobi identity (see Refs. 19, 18, 21, and 24). The main result of the present paper is a generalization of this Jacobi identity to higher dimensions. In addition, we show that together with the vacuum axiom this identity can be taken as a definition of vertex algebra equivalent to the definition of Ref. 28.

As in dimension one, we derive our Jacobi identity from certain "commutativity" and "associativity" identities (cf. Refs. 18, 25, 2, and 24). However, in the one-dimensional case the Jacobi identity can be simplified so that it does not involve external sufficiently large parameters. This is no longer the case in higher dimensions, and our Jacobi identity entails the same degree of difficulty as the "associativity" identity. The main difference with the one-dimensional case is that now the singular part of the operator product expansion contains infinitely many terms. Nevertheless, it follows from our Jacobi identity that the singular modes close an algebraic structure under the commutator, which would be the higher-dimensional analog of vertex Lie algebra.

The paper is organized as follows. The next two sections are devoted to an important technical preparation, which can be useful not only for this work but also for future investigations of vertex algebras in higher dimensions. This includes an introduction of several spaces of *formal series* in Sec. II and a higher-dimensional *residue functional* in Sec. III (additional material is contained in the Appendix). In Sec. IV we recall the notions of fields, locality and operator product expansion in higher dimensions, mainly following Ref. 28, but extending our considerations also to *polylocal fields*. Our main result, the *Jacobi identity*, is contained in Sec. V, together with several integral versions and a *commutator formula*. Concluding remarks are presented in Sec. VI.

II. SPACES OF FORMAL SERIES

In this section we introduce various spaces of formal series, which will be used throughout the paper. In particular, we define the notion of a formal distribution, and we discuss formal series expansions.

A. Notation

In this section we fix some notation to be used throughout the paper, mostly following the notation of Ref. 28. We fix a positive integer D, which will play the role of *space–time dimension*, and we denote by z, z_i, w, etc., D-component variables,

$$\mathrm{z} = (z^1, \dots, z^D), \quad \mathrm{z}_i = (z_i^1, \dots, z_i^D), \quad \mathrm{w} = (w^1, \dots, w^D). \tag{2.1}$$

We will denote by z_{ij} the difference

$$\mathrm{z}_{ij} := \mathrm{z}_i - \mathrm{z}_j = (z_i^1 - z_j^1, \dots, z_i^D - z_j^D), \tag{2.2}$$

and not a new variable. We introduce the standard scalar product,

$$\mathrm{z}_1 \cdot \mathrm{z}_2 := \sum_{\alpha=1}^{D} z_1^\alpha z_2^\alpha, \quad \mathrm{z}^2 := \mathrm{z} \cdot \mathrm{z}. \tag{2.3}$$

Note that z^2 stands for the Euclidean square of the vector z, while z^2 is its second component.

For concreteness we will work over the field $\mathbb{C}$ of complex numbers, even though all of our results hold over an arbitrary field of characteristic 0. For a vector space V, let $V[\mathrm{z}]$ (respectively, $V[\![\mathrm{z}]\!]$) be the space of polynomials (respectively, formal power series) in z with coefficients in V. For a one-component variable ϱ, we denote by $V[\![\varrho, \varrho^{-1}]\!]$ the space of formal power series in ϱ and ϱ^{-1} with coefficients in V, and by $V[\![\varrho]\!]_\varrho \equiv V[\![\varrho]\!][\varrho^{-1}]$ the space of formal Laurent series involving finitely many negative powers of ϱ.

Note that $V[\mathrm{z}]$ is a $\mathbb{C}[\mathrm{z}]$-module and $V[\![\mathrm{z}]\!]$ is a $\mathbb{C}[\![\mathrm{z}]\!]$-module. We denote by $\mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$ (respectively, $\mathbb{C}[\![\mathrm{z}]\!]_{\mathrm{z}^2}$) the localization of $\mathbb{C}[\mathrm{z}]$ (respectively, $\mathbb{C}[\![\mathrm{z}]\!]$) with respect to the multiplicative system $\{(\mathrm{z}^2)^k\}_{k=1,2,\ldots}$. Let $V[\mathrm{z}]_{\mathrm{z}^2}$ and $V[\![\mathrm{z}]\!]_{\mathrm{z}^2}$ be the localizations of the corresponding modules. Then $V[\mathrm{z}]_{\mathrm{z}^2}$ (respectively, $V[\![\mathrm{z}]\!]_{\mathrm{z}^2}$) is a module over $\mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$ (respectively, $\mathbb{C}[\![\mathrm{z}]\!]_{\mathrm{z}^2}$).

We introduce the formal derivatives on $V[\mathrm{z}]$ and $V[\![\mathrm{z}]\!]$,

$$\partial_{\mathrm{z}} := (\partial_{z^1}, \ldots, \partial_{z^D}), \quad \partial_{z^\alpha} := \frac{\partial}{\partial z^\alpha}, \tag{2.4}$$

and the Euler and Laplace operators

$$\mathrm{z} \cdot \partial_{\mathrm{z}} = \sum_{\alpha=1}^{D} z^\alpha \partial_{z^\alpha}, \quad \partial_{\mathrm{z}}^2 = \sum_{\alpha=1}^{D} (\partial_{z^\alpha})^2. \tag{2.5}$$

Then a polynomial $f(\mathrm{z}) \in V[\mathrm{z}]$ is **homogeneous** of degree m iff $(\mathrm{z}\cdot\partial_{\mathrm{z}} - m)f(\mathrm{z}) = 0$; it is **harmonic** iff $\partial_{\mathrm{z}}^2 f(\mathrm{z}) = 0$. We denote by $V[\mathrm{z}]^{\mathrm{har}}$ (respectively, $V[\![\mathrm{z}]\!]^{\mathrm{har}}$) the spaces of harmonic polynomials (respectively, formal power series). Note that a formal power series is harmonic if and only if each of its homogeneous components is a harmonic polynomial.

Finally, we denote by $\mathbb{Z}_+$ the set of non-negative integers, and by $\mathbb{N}$ the set of positive integers. The notation $N \gg 0$ means that $N > 0$ is sufficiently large.

B. Harmonic decomposition

The classical harmonic decomposition is the fact that every polynomial of $\mathrm{z} \in \mathbb{C}^D$ can be divided by z^2 with a unique harmonic remainder. One can view this in a more abstract way as follows. Let V be an arbitrary vector space. It is easy to see that the linear operators ∂_{z}^2, z^2 and $\mathrm{z}\cdot\partial_{\mathrm{z}} + D/2$ generate a representation of $\mathfrak{sl}_2$ on $V[\mathrm{z}]$, namely

$$[\partial_{\mathrm{z}}^2, \mathrm{z}^2] = 2\mathrm{z} \cdot \partial_{\mathrm{z}} + D, \quad [\mathrm{z} \cdot \partial_{\mathrm{z}}, \partial_{\mathrm{z}}^2] = -2\partial_{\mathrm{z}}^2, \quad [\mathrm{z} \cdot \partial_{\mathrm{z}}, \mathrm{z}^2] = 2\mathrm{z}^2. \tag{2.6}$$

In particular, we have the following useful formula:

$$[\partial_{\mathrm{z}}^2, (\mathrm{z}^2)^n] = 4n(\mathrm{z}^2)^{n-1}(n - 1 + \mathrm{z} \cdot \partial_{\mathrm{z}} + D/2). \tag{2.7}$$

It follows from the representation theory of $\mathfrak{sl}_2$ that every homogeneous polynomial $\phi(\mathrm{z}) \in V[\mathrm{z}]$ of degree k can be written uniquely in the form

$$\phi(\mathrm{z}) = \sum_{2n+m=k} (\mathrm{z}^2)^n h_m(\mathrm{z}), \tag{2.8}$$

where $h_m(\mathrm{z})$ are harmonic homogeneous polynomials of degree m (see, e.g., Ref. 28, Lemma 1.1 for a direct proof). There is a similar harmonic decomposition for elements $\phi(\mathrm{z})$ of the localized space $V[\mathrm{z}]_{\mathrm{z}^2}$; the only difference is that we allow k and n to be negative (and the sum is still finite).

If we allow infinite sums, the largest space that we get is the space $V[\![\mathrm{z}, 1/\mathrm{z}^2]\!]$ of formal series (see Ref. 28)

$$\phi(\mathrm{z}) = \sum_{n\in\mathbb{Z}} \sum_{m=0}^{\infty} \sum_{\sigma=1}^{\mathfrak{h}_m} \phi_{\{n,m,\sigma\}} (\mathrm{z}^2)^n h_{m,\sigma}(\mathrm{z}), \quad \phi_{\{n,m,\sigma\}} \in V. \tag{2.9}$$

Here $\{h_{m,\sigma}(\mathrm{z})\}_{\sigma=1,\ldots,\mathfrak{h}_m}$ is a basis of the space of harmonic homogeneous polynomials of degree m and

$$\mathfrak{h}_m = \binom{m+D-1}{D-1} - \binom{m+D-3}{D-1}. \tag{2.10}$$

Note that the localized space $V[\![\mathrm{z}]\!]_{\mathrm{z}^2}$ introduced in Sec. II A can be naturally embedded in $V[\![\mathrm{z}, 1/\mathrm{z}^2]\!]$ as the set of elements (2.9) for which the sum over n is bounded from below.

Elements (2.9) are called V-valued **formal distributions**, and the coefficients $\phi_{\{n,m,\sigma\}}$ in expansion (2.9) are called modes of $\phi(\mathrm{z})$. The space $V[\![\mathrm{z}, 1/\mathrm{z}^2]\!]$ has a natural structure of a **differential module** over the algebra $\mathbb{C}[z]_{\mathrm{z}^2}$ (see Ref. 28 Sec. 1), i.e., a $\mathbb{C}[z]_{\mathrm{z}^2}$-module equipped with a compatible action of $\mathbb{C}[\partial_z]$ so that the Leibniz rule for differentiation is satisfied. We will review and generalize this in the next section.

C. Differential module structure

In this section we will describe the algebraic structure of the space $V[\![\mathrm{z}, 1/\mathrm{z}^2]\!]$ in a way that can be generalized to more general vector spaces of "formal functions."

As a consequence of harmonic decomposition (2.8), the vector space $V[\mathrm{z}]$ is naturally isomorphic to $V[\varrho][\mathrm{z}]^{\mathrm{har}}$, the vector spaces of harmonic polynomials with coefficients polynomials in a one-component variable $\varrho \equiv \mathrm{z}^2$. Similarly, we have $V[\mathrm{z}]_{\mathrm{z}^2} \cong V[\varrho, \varrho^{-1}][\mathrm{z}]^{\mathrm{har}}$ and

$$V[\![\mathrm{z}]\!]_{\mathrm{z}^2} \cong V[\![\varrho]\!]_{\varrho}[\mathrm{z}]^{\mathrm{har}}, \quad V[\![\mathrm{z}, 1/\mathrm{z}^2]\!] \cong V[\![\varrho, \varrho^{-1}]\!][\![\mathrm{z}]\!]^{\mathrm{har}}, \tag{2.11}$$

using the notation of Secs. II A and II B.

We will now describe the differential module structures of the spaces $V[\mathrm{z}]$ and $V[\mathrm{z}]_{\mathrm{z}^2}$ (over the algebras $\mathbb{C}[\mathrm{z}]$ and $\mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$, respectively) in a way that is applicable to the space $V[\![\mathrm{z}, 1/\mathrm{z}^2]\!]$ and is suitable for generalization. Set $R = V[\varrho]$ or $V[\varrho, \varrho^{-1}]$, respectively. Let $f(\varrho) \in R$ and let $h(\mathrm{z}) \in R[\mathrm{z}]^{\mathrm{har}}$ be a harmonic homogeneous polynomial of degree m. Then for each $\alpha = 1, \ldots, D$, the polynomials $\partial_{z^\alpha} h(\mathrm{z})$ and

$$(A_\alpha h)(\mathrm{z}) := z^\alpha h(\mathrm{z}) - (D + 2m - 2)^{-1} \mathrm{z}^2 \partial_{z^\alpha} h(\mathrm{z}) \tag{2.12}$$

are harmonic as well. Indeed, for $(A_\alpha h)(\mathrm{z})$ this follows from (2.7). Note that the right-hand side of (2.12) is well defined for $m = 0$ since in this case $\partial_{z^\alpha} h(\mathrm{z}) = 0$. We deduce that the action of z^α and ∂_{z^α} on $R[\mathrm{z}]^{\mathrm{har}}$ is given by the formulas

$$z^\alpha (f(\varrho) h(\mathrm{z})) = f(\varrho)(A_\alpha h)(\mathrm{z}) + (D + 2m - 2)^{-1} \varrho f(\varrho)(\partial_{z^\alpha} h)(\mathrm{z}), \tag{2.13}$$

$$\partial_{z^\alpha} (f(\varrho) h(\mathrm{z})) = f(\varrho)(\partial_{z^\alpha} h)(\mathrm{z}) + 2 z^\alpha (f'(\varrho) h(\mathrm{z})), \tag{2.14}$$

where $\varrho \equiv \mathrm{z}^2$ and $f'(\varrho)$ denotes the derivative $\mathrm{d}f(\varrho)/\mathrm{d}\varrho$, and in the right-hand side of (2.14) one must apply (2.13) in order to get a result in $R[\mathrm{z}]^{\mathrm{har}}$.

Now we observe that by linearity Eqs. (2.13), (2.14) give rise to a well-defined action of z^α and ∂_{z^α} on the space of harmonic formal power series $R[\![\mathrm{z}]\!]^{\mathrm{har}}$. This follows from the fact that the linear operators A_α and ∂_{z^α} on $R[\![\mathrm{z}]\!]^{\mathrm{har}}$ are *graded* (of degree +1 and −1, respectively) with respect to the polynomial degree in z. We also notice that the right-hand sides of Eqs. (2.13) and (2.14) involve only the differential $\mathbb{C}[\varrho]$-module structure of R. These observations are summarized in the following statement.

Proposition 2.1: Let R be a differential module over $\mathbb{C}[\varrho]$ *with a derivation* $f \mapsto f'$. *Then Eqs.* (2.13) and (2.14) *define on* $R[\mathrm{z}]^{\mathrm{har}}$ *and* $R[\![\mathrm{z}]\!]^{\mathrm{har}}$ *structures of differential modules over* $\mathbb{C}[\mathrm{z}]$ *with derivations* ∂_{z^α}. *If R is a differential* $\mathbb{C}[\varrho, \varrho^{-1}]$*-module, then* $R[\mathrm{z}]^{\mathrm{har}}$ *and* $R[\![\mathrm{z}]\!]^{\mathrm{har}}$ *are differential*

$\mathbb{C}[z]_{z^2}$*-modules*.

Proof: We must check that for every $\phi(z) \in R[z]^{\mathrm{har}}$ or $R[\![z]\!]^{\mathrm{har}}$, the following relations are satisfied:

$$z^\alpha z^\beta \phi(z) = z^\beta z^\alpha \phi(z), \quad \sum_{\alpha=1}^{D} (z^\alpha)^2 \phi(z) = z^2 \phi(z),$$

$$\partial_{z^\alpha}\partial_{z^\beta}\phi(z) = \partial_{z^\beta}\partial_{z^\alpha}\phi(z), \quad \partial_{z^\alpha}(z^\beta \phi(z)) = z^\beta \partial_{z^\alpha}\phi(z) + \delta^\beta_\alpha \phi(z),$$

$$\partial_{z^\alpha}((z^2)^{-1}\phi(z)) = (z^2)^{-1}\partial_{z^\alpha}\phi(z) - 2(z^2)^{-2} z^\alpha \phi(z).$$

This can be verified by a straightforward computation, or can be deduced from the fact that these relations hold for $R = V[\varrho]$ and $V[\varrho, \varrho^{-1}]$. □

In particular, using isomorphism (2.11) and taking $R = V[\![\varrho, \varrho^{-1}]\!]$ in the above proposition, we obtain a structure of a differential $\mathbb{C}[z]_{z^2}$-module on the space $V[\![z, 1/z^2]\!]$ of formal distributions (cf. Ref. 28). Note that $V[\![z]\!]$ is also a $\mathbb{C}[z]$-module, and $V[\![z]\!]_{z^2}$ is a $\mathbb{C}[z]_{z^2}$-module. However, $V[\![z, 1/z^2]\!]$ is *not* a $\mathbb{C}[z]$-module because $V[\![\varrho, \varrho^{-1}]\!]$ is not a $\mathbb{C}[\varrho]$-module. Although obvious, the next remark plays an important role in the theory.

Remark 2.1: The action of $\mathbb{C}[\![z]\!]_{z^2}$ on $V[\![z]\!]_{z^2}$ does not have zero divisors. In other words, if $p(z)\,\phi(z) = 0$ for $p(z) \in \mathbb{C}[\![z]\!]_{z^2}$, $\phi(z) \in V[\![z]\!]_{z^2}$, then either $p(z) = 0$ or $\phi(z) = 0$. Note that this is not the case for the $\mathbb{C}[z]_{z^2}$-module $V[\![z, 1/z^2]\!]$ (see Ref. 28, Example 1.1).

D. Generalized formal distributions

As another application of Proposition 2.1, we will define spaces of formal distributions that involve nonintegral powers of z^2. We will take R to be a space of formal series in real powers of ϱ,

$$R = V[\![\varrho^\Gamma]\!] := \left\{ f(\varrho) = \sum_{\gamma \in \Gamma} f_\gamma \varrho^\gamma \,\middle|\, f_\gamma \in V \right\}, \tag{2.15}$$

where Γ is a $\mathbb{Z}$-invariant subset of $\mathbb{R}$, i.e., such that

$$\Gamma + \mathbb{Z} := \{\gamma + m \,|\, \gamma \in \Gamma, m \in \mathbb{Z}\} \subseteq \Gamma. \tag{2.16}$$

Then R is a differential $\mathbb{C}[\varrho, \varrho^{-1}]$-module [with $(\varrho^\gamma)' = \gamma \varrho^{\gamma-1}$], and $R[\![z]\!]^{\mathrm{har}}$ is a differential $\mathbb{C}[z]_{z^2}$-module, which we denote as $V[\![z, (z^2)^\Gamma]\!]$. We can view the elements of $V[\![z, (z^2)^\Gamma]\!]$ as infinite series [cf. (2.9) and (2.11)]

$$\phi(z) = \sum_{\gamma \in \Gamma} \sum_{m=0}^{\infty} \sum_{\sigma=1}^{\mathfrak{h}_m} \phi_{\{\gamma,m,\sigma\}} (z^2)^\gamma h_{m,\sigma}(z), \quad \phi_{\{n,m,\sigma\}} \in V. \tag{2.17}$$

For $\Gamma = \mathbb{Z}$, the above-defined module $V[\![z, (z^2)^{\mathbb{Z}}]\!]$ coincides with $V[\![z, 1/z^2]\!]$. We will call elements (2.17) (generalized) **formal distributions**. Note that this construction works also for subsets $\Gamma \subseteq \mathbb{C}$ but we will restrict our considerations to $\mathbb{R}$. We define inductively the vector spaces

$$V[\![z_1, (z_1^2)^{\Gamma_1}; \ldots; z_n (z_n^2)^{\Gamma_n}]\!] := (V[\![z_1, (z_1^2)^{\Gamma_1}; \ldots; z_{n-1}, (z_{n-1}^2)^{\Gamma_{n-1}}]\!])[\![z_n, (z_n^2)^{\Gamma_n}]\!] \tag{2.18}$$

of formal distributions in several D-dimensional vector variables $z_1, \ldots, z_n$. When all $\Gamma_i = \mathbb{Z}$, we will denote the space (2.18) as $V[\![z_1, 1/z_1^2; \ldots; z_n, 1/z_n^2]\!]$.

Remark 2.2: Choosing instead $R = V[\varrho^\Gamma]$ in the above construction, we obtain a differential $\mathbb{C}[z]_{z^2}$-module $R[z]^{\mathrm{har}}$ denoted as $V[z, (z^2)^\Gamma]$; it consists of all finite sums of the form (2.17).

Remark 2.3: Note that Eq. (2.7) is valid for $n \in \Gamma$, and it implies

$$\partial_z^2((z^2)^\gamma h_{m,\sigma}(z)) = 4\gamma\left(\gamma + m + \frac{D}{2} - 1\right)(z^2)^{\gamma-1} h_{m,\sigma}(z). \tag{2.19}$$

In particular, $(z^2)^\gamma h_{m,\sigma}(z)$ is harmonic if and only if $\gamma=0$ or $\gamma=-(D/2)+1-m$.

Example 2.1: Let us consider the case $D=1$. Then $z=z$ is a one-component variable and the harmonic polynomials are just the affine polynomials $a+bz$. Thus, every element of $V[\![z,(z^2)^\Gamma]\!]$ has the form

$$\phi(z) = \sum_{\gamma\in\Gamma} (z^2)^\gamma (a_\gamma + b_\gamma z), \quad a_\gamma, b_\gamma \in V. \tag{2.20}$$

It is easy to see that when Γ is an additive subgroup of $\mathbb{R}$ containing $\frac{1}{2}\mathbb{Z}$, we have the following direct sum of differential $\mathbb{C}[z]_{z^2}$-modules:

$$V[\![z,(z^2)^\Gamma]\!] = (1+(z^2)^{-1/2}z)V[\![z,(z^2)^\Gamma]\!] \oplus (1-(z^2)^{-1/2}z)V[\![z,(z^2)^\Gamma]\!]. \tag{2.21}$$

Note that here $(z^2)^{-1/2}z$ is viewed as an element of $V[\![z,(z^2)^\Gamma]\!]$, and is not equal to 1.

E. Γ-Localization

The vector space of localized formal power series $V[\![z]\!]_{z^2}$ can be embedded in $V[\![z, 1/z^2]\!]$ as the subspace of all elements (2.9) for which the sum over n is bounded from below. This space is a (differential) module over the localized algebra $\mathbb{C}[\![z]\!]_{z^2}$. We will later need the following generalizations of these spaces.

Let $\Gamma_1,\dots,\Gamma_s$ be additive subgroups of $\mathbb{R}$ containing $\mathbb{Z}$; then each Γ_i is automatically $\mathbb{Z}$-invariant [see (2.16)]. Let A be a commutative associative algebra, and let $f_1,\dots,f_s$ be some fixed elements of A. Then we define

$$A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}} := (\mathbb{C}[\Gamma_1]\otimes_{\mathbb{C}}\cdots\otimes_{\mathbb{C}}\mathbb{C}[\Gamma_s]\otimes_{\mathbb{C}}A)/J, \tag{2.22}$$

where $\mathbb{C}[\Gamma_i]$ is the group algebra of Γ_i (with elements denoted as e^γ) and J is the ideal generated by elements of the form

$$e^{\gamma_1'}\otimes\cdots\otimes e^{\gamma_s'}\otimes g - e^{\gamma_1''}\otimes\cdots\otimes e^{\gamma_s''}\otimes g \tag{2.23}$$

for which there exist $\gamma_i\in\Gamma_i$ such that $\gamma_i+\gamma_i', \gamma_i+\gamma_i''\in\mathbb{Z}_+$ $(i=1,\dots,s)$ and

$$f_1^{\gamma_1+\gamma_1'}\cdots f_s^{\gamma_s+\gamma_s'} g = f_1^{\gamma_1+\gamma_1''}\cdots f_s^{\gamma_s+\gamma_s''} g \tag{2.24}$$

in the algebra A. The so-defined commutative associative algebra $A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$ will be called the $(\Gamma_1,\dots,\Gamma_s)$-**localization** of A with respect to $f_1,\dots,f_s$. When all groups Γ_i are equal to Γ, we will just call it Γ-localization. The image in $A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$ of an element $e^{\gamma_1}\otimes\cdots\otimes e^{\gamma_s}\otimes g$ will be denoted as $f_1^{\gamma_1}\cdots f_s^{\gamma_s} g$.

Obviously, the $\mathbb{Z}$-localization of A with respect to $f_1,\dots,f_s$ coincides with the localized algebra $A_{f_1\cdots f_s}$. In this case the localization with respect to a set $\{f_1,\dots,f_s\}$ is naturally isomorphic to the localization with respect to the product $f_1\cdots f_s$. For general Γ this is not true.

If M is an A-module, then in the same way one defines the localization $M_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$ as an $A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$-module. In addition, if M is a differential A-module, then the localization $M_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$ is a differential $A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$-module with the same set of derivations. Indeed, every derivation of A extends by the Leibniz rule to $A_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$ since J is an invariant subspace. We note also that if M has no zero divisors the same is true for $M_{f_1^{\Gamma_1}\dots f_s^{\Gamma_s}}$(cf. Remark 2.1).

As a special case of the above construction, we get a differential $\mathbb{C}[\![z]\!]_{(z^2)^\Gamma}$-module $V[\![z]\!]_{(z^2)^\Gamma}$. The latter can be identified with the $\mathbb{C}[z]_{z^2}$-submodule of $V[\![z,(z^2)^\Gamma]\!]$ consisting of all elements (2.17) for which the sum over γ is over the union of *finitely* many sets of the form $\{\gamma_i+\mathbb{Z}_+\}$.

F. Formal expansions

Let Γ be an additive subgroup of $\mathbb{R}$ containing $\mathbb{Z}$, and let V be a vector space. Recall the Γ-localizations defined in Sec. II E and the spaces of formal series defined by (2.17), (2.18). There are obvious embeddings

$$\mathbb{C}[\![z,w]\!]_{(z^2)^\Gamma(w^2)^\Gamma} \subsetneqq \mathbb{C}[\![z]\!]_{(z^2)^\Gamma}[\![w]\!]_{(w^2)^\Gamma} \subsetneqq \mathbb{C}[\![z,(z^2)^\Gamma;w,(w^2)^\Gamma]\!]. \tag{2.25}$$

We emphasize that the spaces $\mathbb{C}[\![z]\!]_{z^2}[\![w]\!]_{w^2}$ and $\mathbb{C}[\![w]\!]_{w^2}[\![z]\!]_{z^2}$ are different, because elements of the former space have only finitely many negative powers of w^2 but possibly infinitely many negative powers of z^2. Note also that the first two spaces in (2.25) are rings, and hence the second one is a module over the first.

For $\gamma\in\Gamma$, we define $\iota_{z,w}((z-w)^2)^\gamma$ as the Taylor expansion of $((z-w)^2)^\gamma$ in w around 0, to wit

$$\iota_{z,w}((z-w)^2)^\gamma := e^{-w\cdot\partial_z}(z^2)^\gamma = \sum_{k=0}^{\infty}\frac{(-w\cdot\partial_z)^k}{k!}(z^2)^\gamma \in \mathbb{C}[\![z]\!]_{(z^2)^\Gamma}[\![w]\!]. \tag{2.26}$$

One defines $\iota_{z,w}((z+w)^2)^\gamma$ in the same way, while $\iota_{w,z}((z-w)^2)^\gamma$ is defined using the identifications

$$((z-w)^2)^\gamma \equiv ((w-z)^2)^\gamma, \quad ((-z)^2)^\gamma \equiv (z^2)^\gamma. \tag{2.27}$$

More generally, for $\psi(z,w)\in V[\![z,w]\!]_{(z^2)^\Gamma(w^2)^\Gamma}$ we set

$$\iota_{z,w}(\psi(z,w)((z-w)^2)^\gamma) := \psi(z,w)\iota_{z,w}((z-w)^2)^\gamma, \tag{2.28}$$

thus obtaining a $\mathbb{C}[\![z,w]\!]_{(z^2)^\Gamma(w^2)^\Gamma}$-linear map

$$\iota_{z,w}: V[\![z,w]\!]_{(z^2)^\Gamma(w^2)^\Gamma((z-w)^2)^\Gamma} \to V[\![z]\!]_{(z^2)^\Gamma}[\![w]\!]_{(w^2)^\Gamma}. \tag{2.29}$$

Note that the map $\iota_{z,w}$ commutes with all partial derivatives ∂_{z^α} and ∂_{w^α}.

We define another version of $\iota_{z,w}$ as follows:

$$\begin{gathered}\iota_{z,w}: V[\![z-w]\!]_{((z-w)^2)^\Gamma}[\![w]\!]_{(w^2)^\Gamma} \to V[\![z]\!]_{(z^2)^\Gamma}[\![w]\!]_{(w^2)^\Gamma},\\ \phi(z-w,w)\mapsto e^{-w'\cdot\partial_z}\phi(z,w)\big|_{w'=w},\end{gathered} \tag{2.30}$$

where on the left-hand side $z-w$ is viewed as an independent variable. Equation (2.30) is well defined because $e^{-w'\cdot\partial_z}\phi(z,w)\in V[\![z]\!]_{(z^2)^\Gamma}[\![w,w']\!]_{(w^2)^\Gamma}$ (while an analogous formal expansion $\iota_{z,w}$ on $V[\![w]\!]_{(w^2)^\Gamma}[\![z-w]\!]_{((z-w)^2)^\Gamma}$ does not make sense). Obviously, maps (2.29) and (2.30) agree with each other on the intersection of their domains. The two versions of $\iota_{z,w}$ can be related to each other by the following statement.

Proposition 2.2: (Taylor's formula) *For every* $\phi(z,w)\in V[\![z,w]\!]_{(z^2)^\Gamma(w^2)^\Gamma((z-w)^2)^\Gamma}$ *we have*

$$\iota_{z,w}\iota_{z-w,w}\phi((z-w)+w,w) = \iota_{z,w}\phi(z,w). \tag{2.31}$$

Proof: It suffices to prove (2.31) for $\phi(z,w)=(z^2)^\gamma$, $\gamma\in\Gamma$. Then, according to Eqs. (2.26) and (2.30), we have

$$\iota_{z,w}\iota_{z-w,w}(((z-w)+w)^2)^\gamma = \iota_{z,w}\left(e^{w'\cdot\partial_z}((z-w)^2)^\gamma\big|_{w'=w}\right)$$

$$= e^{-w''\cdot\partial_z}e^{w'\cdot\partial_z}(z^2)^\gamma\big|_{w'=w''=w} = (z^2)^\gamma,$$

which completes the proof. □

We define the spaces of successively localized formal series

$$V[\![z_1]\!]_{(z_1^2)^\Gamma}\cdots[\![z_1]\!]_{(z_n^2)^\Gamma} := (V[\![z_1]\!]_{(z_1^2)^\Gamma}\cdots[\![z_{n-1}]\!]_{(z_{n-1}^2)^\Gamma})[\![z_n]\!]_{(z_n^2)^\Gamma}, \tag{2.32}$$

which will be used in the sequel. The space (2.32) is a module over the algebra $\mathbb{C}[\![z_1]\!]_{(z_1^2)^\Gamma}\cdots[\![z_1]\!]_{(z_n^2)^\Gamma}$. Again, one should keep in mind that in (2.32) one would get a different space if the variables are put in different order.

III. RESIDUE FUNCTIONAL

In this section we introduce an important linear functional on the spaces of formal distributions, which we call the residue functional. We discuss its fundamental properties and we prove an analog of the Cauchy formula. A geometric interpretation of the residue is given in the Appendix.

A. Definition and main properties

In this section we introduce, for an arbitrary vector space V, an important linear map $V[\![z,(z^2)^{\mathbb{R}}]\!]\to V$, which will be denoted as $\phi(z)\mapsto \mathrm{Res}_z\,\phi(z)$ and will be called the residue. Observing that every element of $V[\![z,(z^2)^{\mathbb{R}}]\!]$ can be uniquely represented as a formal series of the form

$$\phi(z)=\sum_{\gamma\in\mathbb{R}}(z^2)^\gamma\phi_\gamma(z)\quad \text{with } \phi_\gamma(z)\in V[\![z]\!]^{\mathrm{har}}, \tag{3.1}$$

we define

$$\mathrm{Res}_z\sum_{\gamma\in\mathbb{R}}(z^2)^\gamma\phi_\gamma(z) := \phi_{-D/2}(0). \tag{3.2}$$

Theorem 3.1: (a) *The linear map* (3.2) *is* ∂_z-invariant *in the sense that*

$$\mathrm{Res}_z\,\partial_{z^\alpha}\phi(z)=0 \tag{3.3}$$

for all $\phi(z)\in V[\![z,(z^2)^{\mathbb{R}}]\!]$ *and* $\alpha=1,\dots,D$.

(b) *The bilinear form*

$$\langle f,g\rangle := \mathrm{Res}_z f(z)g(z),\quad f,g\in\mathbb{C}[z,(z^2)^{\mathbb{R}}], \tag{3.4}$$

is nondegenerate.

(c) *Let* $h_m(z)$ *and* $h'_{m'}(z)$ *be harmonic homogeneous polynomials of degrees* m *and* m', *respectively. Then*

$$\langle (z^2)^\gamma h_m(z),h'_{m'}(z)\rangle=0\quad \textit{if}$$

$$m\neq m'\quad \textit{or}\quad 2\gamma+m+m'\neq -D, \tag{3.5}$$

and in the opposite case this coincides with the unique, up to a multiplicative constant, $\mathrm{O}(D)$*-invariant scalar product on the vector space of harmonic homogeneous polynomials of degree* $m(=m')$ *given by*

$$\langle (z^2)^{-m-(D/2)}h_m(z),h'_m(z)\rangle. \tag{3.6}$$

Proof: (a) Let $h(z)$ be a harmonic homogeneous polynomial of degree m. From Eqs. (2.12)–(2.14) we deduce the harmonic decomposition

$$\partial_{z^\alpha}((z^2)^\gamma h(z)) = 2\gamma(z^2)^{\gamma-1}(A_\alpha h)(z) + (1+2\gamma(D+2m-2)^{-1})(z^2)^\gamma\partial_{z^\alpha}h(z).$$

Now let us apply Res_z to the right-hand side of this equation. The first term will give zero, because

$(A_\alpha h)(0)=0$. Similarly, the second term can give a nonzero result only if $m=1$ and $\gamma=-D/2$ but then the coefficient vanishes.

(b), (c) Property (3.5) follows from the harmonic decomposition

$$h_m(\mathrm{z})h'_{m'}(\mathrm{z}) = \sum_{n=0}^{\min(m,m')} (\mathrm{z}^2)^n h''_{m+m'-2n}(\mathrm{z}),$$

where $h''_{m''}(\mathrm{z})$ are uniquely determined harmonic homogeneous polynomials of degree $m''=|m-m'|,\ldots,m+m'$. It is known that for $m=m'$, the constant polynomial $h''_0 \in \mathbb{C}$ defines an $\mathrm{O}(D)$-invariant nondegenerate scalar product on the space of harmonic polynomials of degree m. This proves the remaining statements. □

From now on, we will assume that the bases $\{h_{m,\sigma}(\mathrm{z})\}_{\sigma=1,\ldots,\mathfrak{h}_m}$ of harmonic homogeneous polynomials of degree m are *orthonormal*, so that

$$\mathrm{Res}_{\mathrm{z}}(\mathrm{z}^2)^\gamma h_{m,\sigma}(\mathrm{z})h_{m',\sigma'}(\mathrm{z}) = \delta_{\gamma,-(D/2)-m}\delta_{m,m'}\delta_{\sigma,\sigma'}, \tag{3.7}$$

in accord with Theorem 3.1(c). Consequently, the modes of a formal series $\phi(\mathrm{z})$ given by (2.17) can be recovered as residues,

$$\phi_{\{\gamma,m,\sigma\}} = \mathrm{Res}_{\mathrm{z}}\, \phi(\mathrm{z})(\mathrm{z}^2)^{-(D/2)-\gamma-m}h_{m,\sigma}(\mathrm{z}). \tag{3.8}$$

This justifies the name "formal distributions."

Corollary 3.2: Let Γ *be a* $\mathbb{Z}$*-invariant subset of* $\mathbb{R}$ (*i.e.*, $\Gamma+\mathbb{Z}\subseteq\Gamma$), *and set*

$$\Gamma' = -\Gamma + \frac{D}{2} \coloneqq \left\{ -\gamma + \frac{D}{2} \,\middle|\, \gamma \in \Gamma \right\}. \tag{3.9}$$

Then

$$V[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!] \cong \mathrm{Hom}_{\mathbb{C}}(\mathbb{C}[\mathrm{z},(\mathrm{z}^2)^{\Gamma'}],V) \tag{3.10}$$

as differential $\mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$*-modules. In particular,* $\mathbb{C}[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!]$ *is the dual* $\mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$*-module of* $\mathbb{C}[\mathrm{z},(\mathrm{z}^2)^{\Gamma'}]$.

Note that by the recursive definition (2.18) the residue functional is defined also on formal distributions in several D-dimensional variables. For instance, we have

$$V[\![\mathrm{z},(\mathrm{z}^2)^{\mathbb{R}};\mathrm{w},(\mathrm{w}^2)^{\mathbb{R}}]\!] \xrightarrow{\mathrm{Res}_{\mathrm{w}}} V[\![\mathrm{z},(\mathrm{z}^2)^{\mathbb{R}}]\!] \xrightarrow{\mathrm{Res}_{\mathrm{z}}} V. \tag{3.11}$$

Then under the natural isomorphism

$$V[\![\mathrm{z},(\mathrm{z}^2)^{\mathbb{R}};\mathrm{w},(\mathrm{w}^2)^{\mathbb{R}}]\!] \cong V[\![\mathrm{w},(\mathrm{w}^2)^{\mathbb{R}};\mathrm{z},(\mathrm{z}^2)^{\mathbb{R}}]\!] \tag{3.12}$$

the "Fubini theorem" is satisfied, namely,

$$\mathrm{Res}_{\mathrm{z}}\,\mathrm{Res}_{\mathrm{w}}\,\phi(\mathrm{z},\mathrm{w}) = \mathrm{Res}_{\mathrm{w}}\,\mathrm{Res}_{\mathrm{z}}\,\phi(\mathrm{z},\mathrm{w}) \tag{3.13}$$

for $\phi(\mathrm{z},\mathrm{w}) \in V[\![\mathrm{z},(\mathrm{z}^2)^{\mathbb{R}};\mathrm{w},(\mathrm{w}^2)^{\mathbb{R}}]\!]$.

The following proposition describes all ∂_{z}-invariant linear functionals $V[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!] \to V$ [cf. (3.3)].

Proposition 3.3: Let Γ *be a* $\mathbb{Z}$*-invariant subset of* $\mathbb{R}$, *and let* $\Omega: V[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!] \to V$ *be a linear map that is* ∂_{z}*-invariant, i.e., such that* $\Omega(\partial_{\mathrm{z}^\alpha}\phi)=0$ *for all* $\phi \in V[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!]$ *and* $\alpha=1,\ldots,D$.

(a) *If* $D\geqslant 2$, *then there exists a complex constant* C *such that* $\Omega(\phi)=C\,\mathrm{Res}_{\mathrm{z}}\,\phi$ *for all* $\phi \in V[\![\mathrm{z},(\mathrm{z}^2)^\Gamma]\!]$. *In particular, if* $D/2 \notin \Gamma$ *then* $\Omega=0$.

(b) *If* $D=1$, *then there exist complex constants* C *and* C' *such that* $\Omega(\phi)=C\,\mathrm{Res}_z\,\phi + C'\,\mathrm{Res}'_z\,\phi$ *for all* $\phi \in V[\![z,(z^2)^\Gamma]\!]$ (z *is now one-component variable*), *where* Res'_z *is defined by*

$$\mathrm{Res}'_z \sum_{\gamma\in\mathbb{R}} (z^2)^\gamma (a_\gamma + b_\gamma z) := b_{-1} \tag{3.14}$$

(*see Example 2.1*).

Proof: The space of all ∂_z-invariant linear maps $\Omega: V[\![z,(z^2)^\Gamma]\!] \to V$ is isomorphic to the vector space

$$\mathrm{Hom}_{\mathbb{C}}(V[\![z,(z^2)^\Gamma]\!]/\partial_z V[\![z,(z^2)^\Gamma]\!], V),$$

where

$$\partial_z V[\![z,(z^2)^\Gamma]\!] := \partial_{z^1} V[\![z,(z^2)^\Gamma]\!] + \cdots + \partial_{z^D} V[\![z,(z^2)^\Gamma]\!].$$

Fix $\gamma \in \Gamma$ and a harmonic homogeneous polynomials $h(z)$ of degree m. We will prove that for $D \geqslant 2$ one has

$$(z^2)^\gamma h(z) \in \partial_z V[\![z,(z^2)^\Gamma]\!] \quad \text{if } (\gamma,m) \neq \left(-\frac{D}{2},0\right), \tag{3.15}$$

while for $D=1$ one has

$$(z^2)^\gamma h(z) \in \partial_z V[\![z,(z^2)^\Gamma]\!] \quad \text{if} \quad (\gamma,m) \neq \left(-\frac{1}{2},0\right) \quad \text{or } (\gamma,m) \neq (-1,1). \tag{3.16}$$

Indeed, using the equalities [see (2.19)]

$$\partial_z^2((z^2)^{\gamma+1}h(z)) = 4(\gamma+1)\left(\gamma+m+\frac{D}{2}\right)(z^2)^\gamma h(z)$$

and

$$\sum_{\alpha=1}^{D} \partial_{z^\alpha}((z^2)^{\gamma+1}\partial_{z^\alpha}h(z)) = 2m(\gamma+1)(z^2)^\gamma h(z),$$

we conclude that $(z^2)^\gamma h(z) \in \partial_z V[\![z,(z^2)^\Gamma]\!]$ if $\gamma \neq -1$ and $(\gamma,m) \neq (-D/2,0)$. Finally, in the case $\gamma=-1$, we have

$$\sum_{\alpha=1}^{D} \partial_{z^\alpha}((z^2)^{-1}z^\alpha h(z)) = (D+m-2)(z^2)^{-1}h(z).$$

This proves (3.15) and (3.16).

Now observing that by Theorem 3.1(a) we have $(z^2)^{-D/2} \notin \partial_z V[\![z,(z^2)^\Gamma]\!]$, we complete the proof of part (a). To prove part (b), it remains to check that Res'_z is ∂_z-invariant, which is straightforward. □

Example 3.1: Let $D=1$; then elements of $V[\![z,(z^2)^\Gamma]\!]$ have the form (2.20). In particular, for $\Gamma=\mathbb{Z}$, we can write every element $\phi(z) \in V[\![z,1/z^2]\!]$ uniquely as

$$\phi(z) = \sum_{n\in\mathbb{Z}} c_n z^n, \quad c_n \in V. \tag{3.17}$$

In other words, $V[\![z,1/z^2]\!]$ can be identified with the space of formal series $V[\![z,z^{-1}]\!]$. The functional Res_z vanishes on a series (3.17), while the functional Res'_z coincides with the usual residue, $\mathrm{Res}'_z\, \phi(z) = c_{-1}$.

B. Translation invariance and Cauchy formula

Let V be a vector space, as before. One of the most important properties of the residue map (3.2) is its translation invariance.

Proposition 3.4: (Formal translation invariance)

$$\mathrm{Res}_z\, \iota_{z,w}\phi(z+w) = \mathrm{Res}_z\, \phi(z), \quad \phi(z) \in V[\![z]\!]_{(z^2)^{\mathbb{R}}}. \tag{3.18}$$

This equation is also valid for elements of $V[\![z,(z^2)^{\mathbb{R}}]\!]$.

Proof: Recall that, by definition [cf. (2.26)], $\iota_{z,w}\phi(z+w)=e^{w\cdot\partial_z}\phi(z)$. Then Eq. (3.18) follows from Theorem 3.1(a). □

We proceed to finding an analog of the Cauchy kernel for our residue functional.

Proposition 3.5: For $\psi(z) \in V[\![z]\!]$, $\gamma \in \mathbb{R}$, $n \in \mathbb{N}$, *we have*

$$\mathrm{Res}_z (z^2)^{\gamma}\psi(z) = 0 \quad \textit{if } \gamma + \frac{D}{2} > 0 \quad \textit{or } \gamma + \frac{D}{2} \notin \mathbb{Z}, \tag{3.19}$$

$$\mathrm{Res}_z (z^2)^{-D/2}\psi(z) = \psi(0), \tag{3.20}$$

and

$$\mathrm{Res}_z (z^2)^{-(D/2)-n}\psi(z) = K_n^{-1}((\partial_z^2)^n\psi)(0), \tag{3.21}$$

where

$$K_n := 2^{2n}\prod_{k=1}^{n} k\left(k + \frac{D}{2} - 1\right). \tag{3.22}$$

Proof: Equations (3.19) and (3.20) are straightforward from the definition of the residue functional. To prove (3.21), it is enough to assume that $\psi(z)$ is a homogeneous polynomial of degree $2n$. Then we apply induction on n, starting with (3.20), and using the ∂_z-invariance (3.3) and the relation

$$\sum_{\alpha=1}^{D} \partial_{z^\alpha}((z^2)^{-(D/2)-n+1}(\partial_{z^\alpha}\psi)(z)) = -4n\left(n + \frac{D}{2} - 1\right)(z^2)^{-(D/2)-n}\psi(z) + (z^2)^{-(D/2)-n+1}(\partial_z^2\psi)(z).$$

This completes the proof. □

As a corollary of Proposition 3.5, for *even D* we have a local formula for the residue of an element $\phi(z) \in V[\![z]\!]_{z^2}$,

$$\mathrm{Res}_z\, \phi(z) = K_N^{-1}(\partial_z^2)^N((z^2)^{N+D/2}\phi(z))|_{z=0}, \quad N \gg 0. \tag{3.23}$$

Proposition 3.6: (Higher-dimensional "Cauchy formula")

$$\mathrm{Res}_z\, \iota_{z,w}((z-w)^2)^{-D/2}\psi(z) = \psi(w) \quad \textit{for } \psi(z) \in V[\![z]\!]. \tag{3.24}$$

Proof: Consider the formal series

$$\phi(z,w) := \iota_{z,w}((z-w)^2)^{-D/2}\psi(z) \in V[\![z]\!]_{z^2}[\![w]\!].$$

By (3.18), we have

$$\mathrm{Res}_z\, \phi(z,w) = \mathrm{Res}_z\, \iota_{z,w'}\phi(z+w',w).$$

We can set $w'=w$ on the right-hand side and obtain

$$\mathrm{Res}_z\, \iota_{z,w}\phi(z+w,w) = \mathrm{Res}_z\, \iota_{z,w}(z^2)^{-D/2}\psi(z+w) = \psi(w),$$

using (3.20). □

C. Harmonic decomposition of $\iota_{z,w}((z-w)^2)^\gamma$

As before, let $\{h_{m,\sigma}(z)\}$ be an *orthonormal* basis of the space of harmonic homogeneous polynomials of degree m [see (3.7)]. Introduce the polynomials

$$H_m(z,w) := \sum_{\sigma=1}^{\mathfrak{h}_m} h_{m,\sigma}(z)h_{m,\sigma}(w). \tag{3.25}$$

Note that $H_m(z,w)$ is the unique, up to a multiplicative constant, $O(D)$-invariant polynomial that is separately harmonic and homogeneous in z and w of degree m. Combining Eq. (3.7) with the Cauchy formula (3.24), we obtain that

$$\iota_{z,w}((z-w)^2)^{-D/2} = \sum_{m,n=0}^{\infty} (z^2)^{-(D/2)-m-n}(w^2)^n H_m(z,w). \tag{3.26}$$

Recall that for every $\gamma \in \mathbb{R}$ and $n \in \mathbb{Z}_+$ the binomial coefficient $\binom{\gamma}{n}$ is defined as $\gamma(\gamma-1)\cdots(\gamma-n+1)/n!$ and is a polynomial of γ of degree n.

Proposition 3.7: For every $\gamma \in \mathbb{R}$, we have

$$\iota_{z,w}((z-w)^2)^\gamma = \sum_{m,n=0}^{\infty} K_{m,n}(\gamma)(z^2)^{\gamma-m-n}(w^2)^n H_m(z,w), \tag{3.27}$$

where

$$K_{m,n}(\gamma) := \frac{(-1)^n}{\binom{-\frac{D}{2}}{m+n}} \binom{\frac{D}{2}-1+\gamma}{n} \binom{\gamma}{m+n}. \tag{3.28}$$

Proof: It follows from definition (2.26) and the $O(D)$-invariance that $\iota_{z,w}((z-w)^2)^\gamma$ has the form (3.27). Moreover, it is clear from (2.26) that for each fixed $m,n \in \mathbb{Z}_+$, the coefficient $K_{m,n}(\gamma)$ is a polynomial of γ. Then to establish (3.28) it will suffice to prove it for infinitely many values of γ.

We will prove by induction that formula (3.28) holds for all γ such that $-(D/2)-\gamma \in \mathbb{Z}_+$. For $\gamma=-D/2$ it gives $K_{m,n}(-D/2)=1$, which agrees with (3.26). Next, assume that (3.27) and (3.28) hold for some γ. Apply the Laplace operator ∂_z^2 to both sides of (3.27) and use (2.19) to find

$$\gamma\left(\gamma+\tfrac{D}{2}-1\right)\iota_{z,w}((z-w)^2)^{\gamma-1} = \sum_{m,n=0}^{\infty} K_{m,n}(\gamma)(\gamma-m-n)\left(\gamma-n+\tfrac{D}{2}-1\right)(z^2)^{\gamma-1-m-n}(w^2)^n H_m(z,w).$$

Comparing this to (3.27) with $\gamma-1$ instead of γ, we obtain that (3.28) holds for $\gamma-1$. This completes the proof. □

For $\gamma=-(D/2)+1$, expansion (3.27) takes the particularly simple form

$$\iota_{z,w}((z-w)^2)^{-(D/2)+1} = \sum_{m=0}^{\infty} \frac{\frac{D}{2}-1}{\frac{D}{2}-1+m}(z^2)^{-(D/2)+1-m}H_m(z,w). \tag{3.29}$$

Note that both sides of this equation are harmonic with respect to both z and w (see Remark 2.3). Let us also point out that for fixed $\gamma \in \mathbb{Z}_+$, the coefficient $K_{m,n}(\gamma)$ vanishes whenever $m+n>\gamma$. Using (3.27) for $\gamma=0,1,2,\ldots$, one can find the polynomials $H_m(z,w)$ recursively; for example,

$$H_0(z,w)=1,\quad H_1(z,w)=Dz\cdot w,$$
$$H_2(z,w)=\left(\tfrac{D}{2}+1\right)(D(z\cdot w)^2-z^2w^2). \tag{3.30}$$

D. Formal delta-function

In this section we define a formal distribution in two variables, which plays the role of the delta distribution. Let us consider the $\mathbb{Z}$-invariant set $\mathbb{Z}'\coloneqq(D/2)+\mathbb{Z}$ [cf. (3.9)], which coincides with $\mathbb{Z}$ when D is even. We define the following formal distribution in two variables:

$$\delta(z,w)\coloneqq\sum_{n\in\mathbb{Z}}\sum_{m=0}^{\infty}(z^2)^{-(D/2)-m-n}(w^2)^nH_m(z,w)\in\mathbb{C}[[z,(z^2)^{\mathbb{Z}'};w,(w^2)^{\mathbb{Z}}]]. \tag{3.31}$$

Proposition 3.8: The above-defined $\delta(z,w)$ *is the unique element of* $\mathbb{C}[[z,(z^2)^{\mathbb{Z}'};w,(w^2)^{\mathbb{Z}}]]$ *with the property that*

$$\mathrm{Res}_z\,\phi(z)\delta(z,w)=\phi(w)\quad \textit{for all}\ \phi(z)\in\mathbb{C}[z]_{z^2}. \tag{3.32}$$

In addition, it satisfies

$$\phi(z)\delta(z,w)=\phi(w)\delta(z,w),\quad \phi(z)\in\mathbb{C}[z]_{z^2} \tag{3.33}$$

and

$$\partial_{z^\alpha}\delta(z,w)=-\partial_{w^\alpha}\delta(z,w),\quad \alpha=1,\dots,D. \tag{3.34}$$

Proof: Property (3.32) and the uniqueness of $\delta(z,w)$ follow from the orthogonality relation (3.7) (cf. Corollary 3.2). Then Eq. (3.32) and the ∂_z-invariance of the residue (3.3) imply that, for every $\phi(z)\in\mathbb{C}[z]_{z^2}$,

$$\mathrm{Res}_z\,\phi(z)(\partial_{z^\alpha}+\partial_{w^\alpha})\delta(z,w)=-\mathrm{Res}_z(\partial_{z^\alpha}\phi(z))\delta(z,w)+\partial_{w^\alpha}\mathrm{Res}_z\,\phi(z)\delta(z,w)=0.$$

This proves (3.34). Similarly, (3.33) follows from the equalities:

$$\mathrm{Res}_z\,\psi(z)\phi(z)\delta(z,w)=\psi(w)\phi(w)=\mathrm{Res}_z\,\psi(z)\phi(w)\delta(z,w),$$

for all $\psi(z),\phi(z)\in\mathbb{C}[z]_{z^2}$. □

Remark 3.1: Let Γ be any $\mathbb{Z}$-invariant subset of $\mathbb{R}$, and let $\Gamma'=-\Gamma+\frac{D}{2}$ [see (3.9)]. Corollary 3.2 implies that there exists a unique element $\delta_\Gamma(z,w)\in\mathbb{C}[[z,(z^2)^{\Gamma'};w,(w^2)^{\Gamma}]]$ such that Eq. (3.32) holds for $\delta_\Gamma(z,w)$ and all $\phi(z)\in\mathbb{C}[z]_{(z^2)\Gamma}$. Then (3.34) is satisfied as well, while the analog of (3.33) holds only when Γ is a subgroup of $\mathbb{R}$ (this is needed for $\mathbb{C}[z]_{(z^2)\Gamma}$ to be a ring). Finally, note that $\delta_\Gamma(z,w)=\delta_\Gamma(w,z)$ when $\Gamma=\Gamma'$.

Observe that $\delta(z,w)$ is symmetric, i.e., $\delta(z,w)=\delta(w,z)$, if and only if D is even. Switching z and w in (3.26) and using (2.27), we obtain that for even D we have

$$\delta(z,w)=\iota_{z,w}((z-w)^2)^{-D/2}+\iota_{w,z}((z-w)^2)^{-D/2}+\sum_{m=0}^{\infty}\sum_{n=1}^{(D/2)-1+m}(z^2)^{-(D/2)-m+n}(w^2)^{-n}H_m(z,w). \tag{3.35}$$

This splitting of $\delta(z,w)$ as a sum of three terms suggests the introduction of a natural partition of the space of formal distributions (without assuming that D is even). For a formal distribution $\phi(z)\in V[[z,1/z^2]]$, written as in (2.9), we define its parts $\phi(z)_+$, $\phi(z)_-$, and $\phi(z)_\sim$, as follows. We let $\phi(z)_+$ be given by (2.9) with the sum over $n\in\mathbb{Z}$ restricted to $n\geqslant 0$, $n\in\mathbb{Z}$. For $\phi(z)_-$ we restrict

the sum to $n \leqslant -(D/2)-m$, $n \in \mathbb{Z}$ (we first sum over m and then over n). For $\phi(z)_\sim$ we restrict the sum to $-(D/2)+1-m \leqslant n \leqslant -1$, $n \in \mathbb{Z}$. We call $\phi(z)_+$ the regular part of $\phi(z)$, and we define the singular part as

$$\phi(z)_{s.p.} := \phi(z)_- + \phi(z)_\sim. \tag{3.36}$$

Then, obviously, $\phi(z)_+ \in V[[z]]$ and

$$\phi(z) = \phi(z)_+ + \phi(z)_- + \phi(z)_\sim = \phi(z)_+ + \phi(z)_{s.p.}. \tag{3.37}$$

It is important that the above partition of the space of formal distributions is $\mathbb{C}[\partial_z]$-invariant, i.e.,

$$(\partial_z{}^{(\alpha)}\phi(z))_\star = \partial_z{}^{(\alpha)}\phi(z)_\star \quad \text{for } \star = +, -, \sim, \text{s.p.} \quad \text{and } \alpha = 1, \ldots, D. \tag{3.38}$$

Let us point out that the product $\phi(z)\iota_{z,w}((z-w)^2)^{-D/2}$ is well defined and belongs to the space $V[[z,1/z^2]][[w]]$. Then we can generalize Cauchy formula (3.24), using Eq. (3.26), to obtain

$$\mathrm{Res}_z\, \phi(z)\iota_{z,w}((z-w)^2)^{-D/2} = \phi(w)_+, \quad \phi(z) \in V[[z,1/z^2]]. \tag{3.39}$$

Thus, $\iota_{z,w}((z-w)^2)^{-D/2}$ may be called $\delta^+(z,w)$, and one can also introduce formal distributions $\delta^-(z,w)$ and $\delta^\sim(z,w)$ that give the $-$ and $\sim$ parts of $\phi(w)$, respectively, and such that $\delta(z,w) = \delta^+(z,w)+\delta^-(z,w)+\delta^\sim(z,w)$. In the case when D is even, this splitting of $\delta(z,w)$ coincides with the one in Eq. (3.35).

Remark 3.2: Introduce the formal distribution [cf. (3.26)]

$$\delta^+_{\mathrm{har}}(z,w) := (z^2-w^2)\iota_{z,w}((z-w)^2)^{-D/2} = \sum_{m=0}^{\infty} (z^2)^{-(D/2)+1-m} H_m(z,w).$$

It is harmonic with respect to both z and w, and has the property that

$$\mathrm{Res}_z\, h(z)\delta^+_{\mathrm{har}}(z,w) = h(w) \quad \text{for all } h(z) \in \mathbb{C}[z]^{\mathrm{har}}.$$

It follows from (3.31) that $\delta(z,w) = \delta_1(z^2-w^2)\delta^+_{\mathrm{har}}(z,w)$, where

$$\delta_1(x-y) := \sum_{n\in\mathbb{Z}} x^{-1-n}y^n \in \mathbb{C}[[x,x^{-1};y,y^{-1}]]$$

is the formal delta distribution in the usual $D=1$ theory of vertex algebras (see, e.g., Refs. 19, 21, and 24). Notice that, even though $(z^2-w^2)\delta_1(z^2-w^2)=0$, one cannot conclude from here that $\delta(z,w)=0$, because the product $\delta_1(z^2-w^2)\iota_{z,w}((z-w)^2)^{-D/2}$ is not well defined [see the discussion in Ref. 24, Sec. 2.1 and in particular Eq. (2.1.17)].

E. Transformation properties

For completeness, in this section we will investigate the transformation properties of the residue functional and the ι-operation under the *conformal inversion* $z \mapsto z/z^2$.

We observe that the substitution $\phi(z) \mapsto \phi(z/z^2)$ is a well-defined involution of $V[[z,(z^2)^{\mathbb{R}}]]$ if we set $((z/z^2)^2)^\gamma := (z^2)^{-\gamma}$. Explicitly, if $\phi(z)$ is given by (2.17), then

$$\phi\left(\frac{z}{z^2}\right) := \sum_{\gamma\in\Gamma}\sum_{m=0}^{\infty}\sum_{\sigma=1}^{\mathfrak{h}_m} \phi_{\{\gamma,m,\sigma\}}(z^2)^{-\gamma-m}h_{m,\sigma}(z), \tag{3.40}$$

because $h_{m,\sigma}(z/z^2) = (z^2)^{-m}h_{m,\sigma}(z)$. Clearly, under this isomorphism, the $\mathbb{C}[z]_{z^2}$-module $V[[z,(z^2)^\Gamma]]$ is mapped onto $V[[z,(z^2)^{-\Gamma}]]$.

Now let Γ be an additive subgroup of $\mathbb{R}$ containing $\mathbb{Z}$. For $\gamma \in \Gamma$, we define

$$\left(\left(\frac{z}{z^2}-\frac{w}{w^2}\right)^2\right)^{\gamma} := (z^2)^{-\gamma}(w^2)^{-\gamma}((z-w)^2)^{\gamma}, \tag{3.41}$$

which agrees with the usual formula for $\gamma=1$. Then the substitution $\psi(z,w)\mapsto\psi(z/z^2,w/w^2)$ defines an automorphism of $V[z,w]_{(z^2)^{\Gamma}(w^2)^{\Gamma}((z-w)^2)^{\Gamma}}$.

Proposition 3.9: Let $\phi(z)\in V[\![z,(z^2)^{\mathbb{R}}]\!]$ *and* $\psi(z,w)\in V[z,w]_{(z^2)^{\Gamma}(w^2)^{\Gamma}((z-w)^2)^{\Gamma}}$. *Then we have*

$$\mathrm{Res}_z\,\phi\left(\frac{z}{z^2}\right)=\mathrm{Res}_z(z^2)^{-D}\phi(z) \tag{3.42}$$

and

$$\iota_{z,w}\left(\psi\left(\frac{z}{z^2},\frac{w}{w^2}\right)\right)=(\iota_{w',z'}\psi(z',w'))\Big|_{z'=z/z^2,w'=w/w^2}. \tag{3.43}$$

Proof: Equation (3.42) is immediate from the definition of the residue [cf. (2.17), (3.40)]. To prove (3.43), it suffices to check it for $\psi(z,w)=((z-w)^2)^{\gamma}$, in which case the statement follows from (2.27), (3.27), and (3.41). □

One can define involutive automorphisms

$$\phi(z)\mapsto\phi(-z),\quad \psi(z,w)\mapsto\psi(-z,-w) \tag{3.44}$$

of $V[\![z,(z^2)^{\mathbb{R}}]\!]$ and $V[z,w]_{(z^2)^{\Gamma}(w^2)^{\Gamma}((z-w)^2)^{\Gamma}}$ by setting [cf. (2.27)]

$$(z^2)^{\gamma_1}(w^2)^{\gamma_2}((z-w)^2)^{\gamma_3}f(z,w)\mapsto(z^2)^{\gamma_1}(w^2)^{\gamma_2}((z-w)^2)^{\gamma_3}f(-z,-w) \tag{3.45}$$

for $f(z,w)\in V[\![z,w]\!]$. By the definition of $\iota_{z,w}$ and $\iota_{w,z}$ (see Sec. II F), the so-defined operation commutes with both of them. It is also clear that it anticommutes with all partial derivatives ∂_{z^α}, ∂_{w^α}, and satisfies

$$\mathrm{Res}_z\,\phi(-z)=\mathrm{Res}_z\,\phi(z),\quad \phi(z)\in V[\![z,(z^2)^{\mathbb{R}}]\!]. \tag{3.46}$$

Remark 3.3: In analogy with the above automorphism (3.45), one can define an automorphism Θ by setting

$$\Theta:(z^2)^{\gamma_1}(w^2)^{\gamma_2}((z-w)^2)^{\gamma_3}f(z,w)\mapsto e^{2\pi i(\gamma_1+\gamma_2+\gamma_3)}(z^2)^{\gamma_1}(w^2)^{\gamma_2}((z-w)^2)^{\gamma_3}f(z,w)$$

for $f(z,w)\in V[\![z,w]\!]$. Then Θ commutes with the ι-operations and with the partial derivatives, and instead of (3.46) one has $\mathrm{Res}_z(\Theta\phi)(z)=(-1)^D\,\mathrm{Res}_z\,\phi(z)$.

IV. FIELDS AND LOCALITY

In this section we investigate the notions of fields, locality, and operator product expansion in higher dimensions, mainly following Ref. 28. We give the definition of vertex algebra and we provide two examples of vertex algebras.

A. Polylocal fields

In this section we introduce the notion of a field of several variables, and we generalize the results of Ref. 28, Sec. 2 about the existence of operator product expansion.

Let $V=V_{\bar{0}}\oplus V_{\bar{1}}$ be a $\mathbb{Z}_2$-graded vector space (i.e., a *superspace*). Then $\mathrm{End}\,V=(\mathrm{End}\,V)_{\bar{0}}\oplus(\mathrm{End}\,V)_{\bar{1}}$ is a $\mathbb{Z}_2$-graded associative algebra, and we will denote its Lie super bracket by

$$[A,B]:=AB-(-1)^{pq}BA,\quad \text{for } A\in(\mathrm{End}\,V)_p,\quad B\in(\mathrm{End}\,V)_q. \tag{4.1}$$

We will suppose that V is endowed with an action of mutually commuting even endomorphisms $T_1,\ldots,T_D$ (called **translation endomorphisms**) and with an even vector $|0\rangle$ (called **vacuum**), such that $T_1|0\rangle=\cdots=T_D|0\rangle=0$.

Let $A(z_1,\dots,z_m)$ be an (End V)-valued formal distribution; in other words, let

$$A(z_1,\dots,z_m) \in (\mathrm{End}\ V)[[z_1,1/z_1^2;\dots;z_m,1/z_m^2]]. \tag{4.2}$$

It is called a **field** in $z_1,\dots,z_m$ (or just an m-field) iff for every $v \in V$ one has

$$A(z_1,\dots,z_m)v \in V[[z_1,\dots,z_m]]_{z_1^2\cdots z_m^2}. \tag{4.3}$$

This means that for every $v \in V$ there is a non-negative integer $N_{A,v}$ such that

$$A(z_1,\dots,z_m)v = (z_1^2\cdots z_m^2)^{-N_{A,v}}\psi_{A,v}(z_1,\dots,z_m) \tag{4.4}$$

for some $\psi_{A,v}(z_1,\dots,z_m) \in V[[z_1,\dots,z_m]]$.

If A is an m-field, then for every partition

$$\{1,\dots,m\} = J_1 \sqcup \cdots \sqcup J_r \quad \text{(disjoint union)}, \tag{4.5}$$

the restriction

$$\widetilde{A}(u_1,\dots,u_r)v := ((z_1^2\cdots z_m^2)^{-N_{A,v}}\psi_{A,v}(z_1,\dots,z_m))\big|_{z_j:=u_s \text{ for } j\in J_s} \tag{4.6}$$

makes sense and defines again a field.

An m-field [or, more generally, an (End V)-valued formal distribution] A is called **translation invariant** iff

$$[T_\alpha, A(z_1,\dots,z_m)] = \sum_{k=1}^{m} \partial_{z_k^\alpha} A(z_1,\dots,z_m) \tag{4.7}$$

for every $\alpha = 1,\dots,D$.

Let us point out that a product $A(z_1,\dots,z_m)B(w_1,\dots,w_n)$ of two fields is *not* a field in general. Indeed, by the above definition, for every $v \in V$ we have

$$A(z_1,\dots,z_m)B(w_1,\dots,w_n)v \in V[[z_1,\dots,z_m]]_{z_1^2\cdots z_m^2}[[w_1,\dots,w_n]]_{w_1^2\cdots w_n^2}, \tag{4.8}$$

and it may contain infinitely many negative powers of $z_1^2,\dots,z_m^2$. As a consequence, the restriction of the product (4.8) for coinciding arguments is not well defined in general. We will show below that one can "regularize" this product to make a field if the following definition is satisfied.

Two fields [or, more generally, (End V)-valued formal distributions] A and B are called **mutually local** iff there exists a non-negative integer $N_{A,B}$ such that

$$\left(\prod_{j=1}^{m}\prod_{k=1}^{n}(z_j-w_k)^2\right)^{N_{A,B}} [A(z_1,\dots,z_m),B(w_1,\dots,w_n)] = 0. \tag{4.9}$$

A 1-field that is local with respect to itself is usually called a **local** field; a 2-field that is local with respect to itself is called a **bilocal** field. An m-field, for general m, which is local with respect to itself, is called a **polylocal** field.

In the following statement we sum up some consequences of the above definitions.

Theorem 4.1: *Let* $A(z_1,\dots,z_m)$ *and* $B(z_1,\dots,z_n)$ *be an m-field and an n-field, respectively, which are mutually local as above.*

(a) *Every restriction* (4.6) *of A is also a field and is mutually local with respect to B.*
(b) *If the field A is translation invariant, then its restrictions* (4.6) *are also translation invariant fields.*
(c) *If A is translation invariant, then* $A(z_1,\dots,z_m)|0\rangle \in V[[z_1,\dots,z_m]]$.
(d) *Every partial derivative* $\partial_{z_k^\alpha}A$ *is a field and is mutually local with respect to B. If the field A is translation invariant, then* $\partial_{z_k^\alpha}A$ *is also translation invariant.*
(e) *The formal distribution*

$$F_{A,B}(\mathrm{z}_1,\dots,\mathrm{z}_m,\mathrm{w}_1,\dots,\mathrm{w}_n) := \left(\prod_{j=1}^{m}\prod_{k=1}^{n}(\mathrm{z}_j-\mathrm{w}_k)^2\right)^{N_{A,B}} A(\mathrm{z}_1,\dots,\mathrm{z}_m)B(\mathrm{w}_1,\dots,\mathrm{w}_n) \quad (4.10)$$

is an $(m+n)$-field. If the fields A and B are local with respect to a p-field $C(\mathrm{z}_1,\dots,\mathrm{z}_p)$, then $F_{A,B}$ is also local with respect to C. If both fields A and B are translation invariant, then $F_{A,B}$ is also translation invariant.

Proof: Statements (a) and (b) follow easily from definitions.

Statement (c) for $m=1$ is proved in Ref. 32, Proposition 3.2(a), and that proof can be straightforwardly generalized for general m (note that one can take $h_2=h_1$ there).

To prove (d), one "commutes" the derivative $\partial_{\mathrm{z}_k}^{\alpha}$ through the polynomial $((\mathrm{z}_k-\mathrm{w}_j)^2)^N$, as it is done in a more general case in Ref. 28, Lemma 2.3.

(e) Note that, by (4.8) and (4.9), for every $v\in V$ the series $F_{A,B}(\mathrm{z}_1,\dots,\mathrm{z}_m,\mathrm{w}_1,\dots,\mathrm{w}_n)v$ belongs to the intersection

$$V[\![\mathrm{z}_1,\dots,\mathrm{z}_m]\!]_{\mathrm{z}_1^2\cdots\mathrm{z}_m^2}[\![\mathrm{w}_1,\dots,\mathrm{w}_n]\!]_{\mathrm{w}_1^2\cdots\mathrm{w}_n^2} \cap V[\![\mathrm{w}_1,\dots,\mathrm{w}_n]\!]_{\mathrm{w}_1^2\cdots\mathrm{w}_n^2}[\![\mathrm{z}_1,\dots,\mathrm{z}_m]\!]_{\mathrm{z}_1^2\cdots\mathrm{z}_m^2}$$

which is exactly $V[\![\mathrm{z}_1,\dots,\mathrm{z}_m,\mathrm{w}_1,\dots,\mathrm{w}_n]\!]_{\mathrm{z}_1^2\cdots\mathrm{z}_m^2\mathrm{w}_1^2\cdots\mathrm{w}_n^2}$. But this means, by definition, that $F_{A,B}$ is an $(m+n)$-field. The remaining part of the statement is straightforward. □

As a corollary of Theorem 4.1, every m-field $A(\mathrm{z}_1,\dots,\mathrm{z}_m)$ can be expanded in 1-fields as follows. Consider for $v\in V$ the formal expansion

$$\begin{aligned}&\iota_{\mathrm{z},\mathrm{w}_1}\cdots\iota_{\mathrm{z},\mathrm{w}_{m-1}}A(\mathrm{z}+\mathrm{w}_1,\dots,\mathrm{z}+\mathrm{w}_{m-1},\mathrm{z})v\\ &\quad := \exp(\mathrm{w}_1\cdot\partial_{\mathrm{z}_1}+\cdots+\mathrm{w}_{m-1}\cdot\partial_{\mathrm{z}_{m-1}})A(\mathrm{z}_1,\dots,\mathrm{z}_m)v\big|_{\mathrm{z}_1=\cdots=\mathrm{z}_m=\mathrm{z}}\\ &\quad \in V[\![\mathrm{z}]\!]_{\mathrm{z}^2}[\![\mathrm{w}_1,\dots,\mathrm{w}_{m-1}]\!].\end{aligned} \quad (4.11)$$

This is a formal power series in $\mathrm{w}_1,\dots,\mathrm{w}_{m-1}$ with coefficients of the form $\psi_i(\mathrm{z})v\in V[\![\mathrm{z}]\!]_{\mathrm{z}^2}$ for some uniquely defined fields $\psi_i(\mathrm{z})$ (i running over some index set). All $\psi_i(\mathrm{z})$ are fields because they are obtained from $A(\mathrm{z}_1,\dots,\mathrm{z}_m)$ by the operations of differentiation and restriction. If, in addition, A is translation invariant and is local with respect to some other fields B, C, etc., then all the fields $\psi_i(\mathrm{z})$ are also translation invariant and local with respect to B, C, etc.

The formal expansion (4.11) is called the **operator expansion** of $A(\mathrm{z}_1,\dots,\mathrm{z}_m)$. Applying this expansion to the field $F_{A,B}$ (4.10), we get what is called the **operator product expansion** (OPE) of two mutually local fields A and B.

Example 4.1: Let us consider, for comparison, the $D=1$ case of OPE. Recall from Example 3.1 that now $\mathrm{z}=z$ is a one-component variable and the space of (End V)-valued formal distributions is identified with (End V)$[\![z,z^{-1}]\!]$. Then our notions of *fields* and *locality* coincide with the ones used in vertex algebra theory (see Refs. 20, 13, 25, 21, and 24). For two mutually local fields $a(z)$ and $b(z)$ with parities p_a and p_b, respectively, one introduces their nth product for $n\in\mathbb{Z}$ by

$$(a(w)_{(n)}b(w))c := \mathrm{res}_z\, a(z)b(w)c\iota_{z,w}(z-w)^n-(-1)^{p_ap_b}\mathrm{res}_z\, b(w)a(z)c\iota_{w,z}(z-w)^n, \quad (4.12)$$

where $\mathrm{res}_z\, z^k := \delta_{k,-1}$ is the usual residue functional (it corresponds to our Res'_z; see Example 3.1). By the Cauchy theorem for res_z (see Refs. 19, 21, and 24), one gets an equivalent definition

$$(a(w)_{(n)}b(w))c = \frac{1}{N!}\partial_z^N((z-w)^{N+n+1}a(z)b(w)c)\big|_{z=w}, \quad N\gg 0, \quad (4.13)$$

where the right-hand side is independent of N. Our approach to the OPE of $a(z)$ and $b(z)$ corresponds precisely to definition (4.13). Then *Dong's lemma*, the fact that the field $a(z)_{(n)}b(z)$ is local with respect to every field $c(z)$ local with respect to a and b, is a simple corollary of Theorem 4.1 (e), (d), (a).

B. Completeness and state-field correspondence: Definition of vertex algebra

The translation invariance and locality properties allow us to introduce a state-field correspondence for a vertex algebra in higher dimensions, as in Secs. 3 and 4 of Ref. 28. Here we will reproduce these results in a more concise way.

As in the previous section, let V be a superspace endowed with an action of mutually commuting even endomorphisms T_α ($\alpha=1,\dots,D$) and a vacuum vector $|0\rangle$. A system of fields $\{\phi_i(z)\}_{i\in\mathcal{I}}$ is called **local** iff $\phi_i(z)$ and $\phi_j(z)$ are mutually local for every $i,j\in\mathcal{I}$. The system $\{\phi_i(z)\}$ is called **translation invariant** iff every $\phi_i(z)$ is translation invariant. Finally, the system $\{\phi_i(z)\}$ is called **complete** (with respect to the vacuum $|0\rangle$) iff the coefficients of all formal series $\phi_{i_1}(z_1)\cdots\phi_{i_n}(z_n)|0\rangle$ ($n\in\mathbb{N}$)together with $|0\rangle$ span the whole vector space V. In other words, the system $\{\phi_i(z)\}$ is complete iff the vacuum $|0\rangle$ is a cyclic vector for the associative subalgebra of End V generated by the modes of all fields $\phi_i(z)$.

Theorem 4.2: Let $\{\phi_i(z)\}_{i\in\mathcal{I}}$ *be a translation invariant, local, and complete system of fields. Then for every* $a\in V$ *there exists a unique field, denoted as* $Y(a,z)$, *which is translation invariant, local with respect to all* $\phi_i(z)$, *and such that*

$$Y(a,z)|0\rangle\big|_{z=0}=a. \tag{4.14}$$

Proof: Let us consider the vector space $\mathcal{F}$ of all translation invariant 1-fields that are local with respect to $\phi_i(z)$ for all $i\in\mathcal{I}$. By Theorem 4.1(c), there is a well-defined linear map

$$\mathcal{F}\to V,\quad \chi(z)\mapsto\chi(z)|0\rangle\big|_{z=0}. \tag{4.15}$$

It follows from translation invariance that

$$\chi(z)|0\rangle=e^{z\cdot T}(\chi(w)|0\rangle\big|_{w=0}),\quad z\cdot T:=z^1T_1+\cdots+z^DT_D.$$

Then Theorem 3.1 from Ref. 28 implies that map (4.15) is injective. The theorem will be proved as soon as we show that map (4.15) is surjective.

Consider for every fixed $m=1,2,\dots$ and $i_1,\dots,i_m\in\mathcal{I}$ the m-field

$$A(z_1,\dots,z_m):=\Bigg(\prod_{1\le k<l\le m}(z_{kl}^2)^{N_{kl}}\Bigg)\phi_{i_1}(z_1)\cdots\phi_{i_m}(z_m),$$

where $z_{kl}=z_k-z_l$ and N_{kl} are the integers fulfilling the locality condition (4.9) for ϕ_{i_k} and ϕ_{i_l}. We then claim that all coefficients of $A(z_1,\dots,z_m)|0\rangle$ belong to the image of (4.15). To prove this, first note that by Theorem 4.1(e) A is a translation invariant m-field that is local with respect to $\phi_i(z)$ for all $i\in\mathcal{I}$. Then all coefficients $\psi_i(z)$ in the operator expansion of A are contained in $\mathcal{F}$ [see (4.11)]. It follows from Theorem 4.1(c) that for $v=|0\rangle$ the right-hand side of (4.11) is simply the Taylor expansion of

$$A(z+w_1,\dots,z+w_{m-1},z)|0\rangle\in V[\![z,w_1,\dots,w_{m-1}]\!].$$

Then it is clear that all coefficients of $A(z_1,\dots,z_m)|0\rangle$ belong to the image of (4.15).

On the other hand, iterating (4.8) we obtain that [cf. (2.32)]:

$$\phi_{i_1}(z_1)\cdots\phi_{i_m}(z_m)|0\rangle\in V[\![z_1]\!]_{z_1^2}\cdots[\![z_m]\!]_{z_m^2}. \tag{4.16}$$

The right-hand side of (4.16) is a module over the algebra $\mathbb{C}[\![z_1]\!]_{z_1^2}\cdots[\![z_m]\!]_{z_m^2}$, in which the polynomial $\Pi_{k<l}(z_{kl}^2)^{N_{kl}}$ is invertible: its inverse is given by applying the expansion $\Pi_{k<l}\,\iota_{z_k,z_l}$ (see Sec. II F). Therefore,

$$\phi_{i_1}(z_1)\cdots\phi_{i_m}(z_m)|0\rangle=\Bigg(\prod_{1\le k<l\le m}\iota_{z_k,z_l}(z_{kl}^2)^{-N_{kl}}\Bigg)A(z_1,\dots,z_m)|0\rangle\,.$$

This implies that every coefficient of (4.16) can be expressed as a linear combination of coefficients of $A(\mathrm{z}_1,\ldots,\mathrm{z}_m)|0\rangle$, and hence belongs to the image of map (4.15). But by completeness the coefficients of (4.16) span V; therefore, (4.15) is surjective. □

Corollary 4.3: Let $\chi(\mathrm{z})$ *be a translation invariant field, which is local with respect to a translation invariant, local, and complete system of fields* $\{\phi_i(\mathrm{z})\}$. *Then* $\chi(\mathrm{z})$ *is a local field and* $\chi(\mathrm{z})=Y(a,\mathrm{z})$ *for* $a=\chi(\mathrm{z})|0\rangle|_{\mathrm{z}=0}$.

Theorem 4.2 leads naturally to the following definition.[28]

Definition 4.1: A **vertex algebra** V over $\mathbb{C}^D$ is a superspace V endowed with

(a) an action of mutually **commuting, even** endomorphisms $T_1,\ldots,T_D$ (translation endomorphisms),
(b) an **even** vector $|0\rangle$ (vacuum) such that $T_1|0\rangle=\cdots=T_D|0\rangle=0$,
(c) a **parity preserving** linear map (state-field correspondence)

$$V\to(\mathrm{End}\,V)[\![\mathrm{z},1/\mathrm{z}^2]\!],\quad a\mapsto Y(a,\mathrm{z}),$$

such that $\{Y(a,\mathrm{z})\}_{a\in V}$ is a **translation invariant, local** system of **fields** and $a=Y(a,\mathrm{z})|0\rangle|_{\mathrm{z}=0}$ for all $a\in V$.

Corollary 4.4: Every translation invariant, local, and complete system of fields $\{\phi_i(\mathrm{z})\}$ *generates on V a unique structure of a vertex algebra.*

Note that when $D=1$, Definition 4.1 is equivalent to the definition of a usual (chiral) vertex algebra (see, e.g., Refs. 21 and 24). We will use the notation

$$a(\mathrm{z})\equiv Y(a,\mathrm{z}) \tag{4.17}$$

as it is customary in the usual $D=1$ theory of vertex algebras. For a vertex algebra V and elements $a,b\in V$, we denote by $N(a,b)$ the smallest non-negative integer fulfilling the locality condition for $a(\mathrm{z})$ and $b(\mathrm{z})$, i.e.,

$$N(a,b):=\min\{N\in\mathbb{Z}_+|((\mathrm{z}-\mathrm{w})^2)^N[a(\mathrm{z}),b(\mathrm{w})]=0\}. \tag{4.18}$$

Remark 4.1: One can introduce a more general notion of vertex algebra that involves nonintegral powers of z^2 in the definition of a field and in the notion of locality. For $D=1$ this would correspond to the "generalized vertex algebras" of Refs. 16, 13, and 27, as explained in Ref. 3. For $D=2$, a related notion was introduced in Ref. 23.

C. Examples of vertex algebras

For completeness, in this section we present two simple examples of vertex algebras. We refer to Refs. 28, 32, 5, and 6 for additional examples.

Our first example shows that the notion of a vertex algebra includes as a special case that of a (super)commutative associative algebra (cf. Ref. 8). We call a vertex algebra V over $\mathbb{C}^D$ holomorphic if $Y(a,\mathrm{z})\in(\mathrm{End}\,V)[\![\mathrm{z}]\!]$ for all $a\in V$. The following statement is a straightforward generalization of the corresponding one in the case $D=1$ (see Refs. 8, 21, and 24).

Proposition 4.5: (a) *If V is a holomorphic vertex algebra over* $\mathbb{C}^D$, *then* $a\star b:=Y(a,z)b|_{\mathrm{z}=0}$ *defines on V the structure of supercommutative associative algebra with a unit* $|0\rangle$ *and even derivations* $T_1,\ldots,T_D$.

(b) *Conversely, given a supercommutative associative algebra V with a product* $\star$, *a unit* $|0\rangle$, *and with mutually commuting even derivations* $T_1,\ldots,T_D$, *then* $Y(a,\mathrm{z})b:=(e^{\mathrm{z}\cdot\mathrm{T}}a)\star b$ *defines the structure of a holomorphic vertex algebra on V.*

Our second example is the vertex algebra generated by a harmonic scalar free field $\varphi(\mathrm{z})$ in *even* space–time dimensions $D>2$ (see Ref. 28 Sec. 5 for a more general construction). Consider a new formal variable $\mathrm{p}:=(p_1,\ldots,p_D)$ and introduce the vector spaces

$$P := \mathbb{C}[\mathrm{p}]/\mathrm{p}^2\mathbb{C}[\mathrm{p}] \cong \mathbb{C}[\mathrm{p}]^{\mathrm{har}}, \quad V := \mathbb{C}[P]. \tag{4.19}$$

Here V is defined as the algebra of all polynomials of the elements of P, i.e., it is the symmetric algebra of P. We will denote by $[f(\mathrm{p})]$ the equivalence class of a polynomial $f(\mathrm{p}) \in \mathbb{C}[\mathrm{p}]$ in P. Then V is the linear span over $\mathbb{C}$ of all monomials of the form $[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})]$ (note that $[f_1(\mathrm{p})][f_2(\mathrm{p})] \neq [f_1(\mathrm{p})f_2(\mathrm{p})]$ in V).

We define an (End V)-valued formal distribution $\varphi(\mathrm{z})$ by the formula

$$\varphi(\mathrm{z})[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})] := \sum_{k=0}^{\infty} \frac{1}{k!}[(\mathrm{z}\cdot\mathrm{p})^k][f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})] + \sum_{l=1}^{n} f_l(-\partial_{\mathrm{z}})(\mathrm{z}^2)^{-\frac{D}{2}+1}[f_1(\mathrm{p})]\cdots\widehat{[f_l(\mathrm{p})]}\cdots[f_n(\mathrm{p})], \tag{4.20}$$

where a hat over a term means that it is omitted in the product. This does not depend on the choice of representatives $f_l(\mathrm{p})$ because $\partial_{\mathrm{z}}^2(\mathrm{z}^2)^{-(D/2)+1}=0$. Since the right-hand side of (4.20) contains only finitely many negative powers of z^2, it follows that $\varphi(\mathrm{z})$ is a field. After a straightforward computation, one finds

$$\varphi(\mathrm{z}_1)\varphi(\mathrm{z}_2)[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})] = e^{-\mathrm{z}_2\cdot\partial_{\mathrm{z}_1}}(\mathrm{z}_1^2)^{-(D/2)+1}[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})] + \cdots, \tag{4.21}$$

where the remaining terms are symmetric under the exchange of z_1 and z_2. Hence,

$$[\varphi(\mathrm{z}_1),\varphi(\mathrm{z}_2)] = (\iota_{\mathrm{z}_1,\mathrm{z}_2}(\mathrm{z}_{12}^2)^{-(D/2)+1} - \iota_{\mathrm{z}_2,\mathrm{z}_1}(\mathrm{z}_{12}^2)^{-(D/2)+1})\mathrm{id}_V, \tag{4.22}$$

where $\mathrm{z}_{12}=\mathrm{z}_1-\mathrm{z}_2$. Therefore, $\varphi(\mathrm{z})$ is a *local field*, since

$$(\mathrm{z}_{12}^2)^{(D/2)-1}[\varphi(\mathrm{z}_1),\varphi(\mathrm{z}_2)] = 0. \tag{4.23}$$

We define endomorphisms $T_1,\ldots,T_D$ of V by the formula

$$T_\alpha[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})] := \sum_{l=1}^{n} [p_\alpha f_l(\mathrm{p})][f_1(\mathrm{p})]\cdots\widehat{[f_l(\mathrm{p})]}\cdots[f_n(\mathrm{p})] \tag{4.24}$$

for $\alpha=1,\ldots,D$. In particular, $T_\alpha|0\rangle=0$, where $|0\rangle$ is the constant polynomial $1\in V$. One can easily verify that the endomorphisms $T_1,\ldots,T_D$ commute with each other, and the field $\varphi(\mathrm{z})$ is *translation invariant*. Let us point out that $\varphi(\mathrm{z})|0\rangle=[e^{\mathrm{z}\cdot\mathrm{p}}]=e^{\mathrm{z}\cdot\mathrm{T}}[1]$, and $\varphi(\mathrm{z})|0\rangle|_{\mathrm{z}=0}=[1]\neq 1=|0\rangle$.

Using (4.20), one can prove by induction on n that every monomial $[f_1(\mathrm{p})]\cdots[f_n(\mathrm{p})]$ is a linear combination of the coefficients of $\varphi(\mathrm{z}_1)\cdots\varphi(\mathrm{z}_n)|0\rangle$. Therefore, the field $\varphi(\mathrm{z})$ is *complete*, and one can apply Corollary 4.4 to generate on V the structure of a vertex algebra over $\mathbb{C}^D$. Finally, we note that the field $\varphi(\mathrm{z})$ is *harmonic*, i.e., it satisfies the Laplace equation $\partial_{\mathrm{z}}^2\varphi(\mathrm{z})=0$. This follows from (4.19), (4.20) and the fact that the function $(\mathrm{z}^2)^{-(D/2)+1}$ is harmonic.

V. JACOBI IDENTITY

This section contains the main results of the paper. We first prove certain "formal commutativity and associativity" relations, and then use them to derive our Jacobi identity. Integral versions of the Jacobi identity are also presented. We show that together with a partial vacuum axiom it can be taken as an equivalent definition of the notion of vertex algebra over $\mathbb{C}^D$. We derive a formula for the commutator of two fields, and we prove that the singular parts of fields close a substructure under the commutator.

A. Commutativity and associativity

In this section we will extend the "associativity" of Ref. 28, Theorem 4.3 by giving a connection between the degrees of the poles in a product $a(z)b(w)$ of two fields and the integers $N(a,b)$ introduced in (4.18). In the case of usual $D=1$ vertex algebras our results agree with the "formal commutativity and associativity" of Refs. 17 and 24.

Theorem 5.1: ("Formal commutativity and associativity.") *Let V be a vertex algebra, and let $a,b,c \in V$, where a and b have parities p_a and p_b, respectively. Then there exists a localized formal series*

$$\mathcal{Y}_{a,b,c}(z_1,z_2) = \frac{\psi_{a,b,c}(z_1,z_2)}{(z_1^2)^{N(a,c)}(z_2^2)^{N(b,c)}(z_{12}^2)^{N(a,b)}}, \tag{5.1}$$

where

$$\psi_{a,b,c}(z_1,z_2) \in V[[z_1,z_2]], \quad z_{12} = z_1 - z_2,$$

such that

$$\mathcal{Y}_{a,b,c}(z_1,z_2) = (-1)^{p_a p_b}\mathcal{Y}_{b,a,c}(z_2,z_1) \tag{5.2}$$

and

$$a(z_1)b(z_2)c = \iota_{z_1,z_2}\mathcal{Y}_{a,b,c}(z_1,z_2), \tag{5.3}$$

$$b(z_2)a(z_1)c = (-1)^{p_a p_b}\iota_{z_2,z_1}\mathcal{Y}_{a,b,c}(z_1,z_2), \tag{5.4}$$

$$(a(z_3)b)(z_2)c = \iota_{z_2,z_3}\mathcal{Y}_{a,b,c}(z_2+z_3,z_2). \tag{5.5}$$

Proof: Equations (5.2)–(5.5) follow from Proposition 4.2 and Theorem 4.3 of Ref. 28. The explicit form (5.1) of $\mathcal{Y}_{a,b,c}(z_1,z_2) \in V[[z_1,z_2]]_{z_1^2 z_2^2 z_{12}^2}$ follows from Eq. (4.18) and the following lemma, which provides another description of the numbers $N(a,b)$. □

Lemma 5.2: For any two elements a and b in a vertex algebra V, we have

$$N(a,b) = \min\{N \in \mathbb{Z}_+ | (z^2)^N a(z)b \in V[[z]]\}. \tag{5.6}$$

Proof: Denote the right-hand side of (5.6) by $N'(a,b)$, and consider the formal distribution

$$F_{a,b}(z_1,z_2) := (z_{12}^2)^{N(a,b)}a(z_1)b(z_2).$$

Due to Theorem 4.1(e), (c), $F_{a,b}$ is a translation invariant, bilocal field and $F_{a,b}(z_1,z_2)|0\rangle \in V[[z_1,z_2]]$. Therefore, setting $z_2=0$ we find from $b(z_2)|0\rangle|_{z_2=0}=b$ that $N'(a,b) \leqslant N(a,b)$.

Consider now the formal distribution

$$F'_{a,b}(z_1,z_2) := (z_{12}^2)^{N'(a,b)}a(z_1)b(z_2).$$

As in the proof of Theorem 4.1(e), $F'_{a,b}$ is translation invariant and local (as a formal distribution) with respect to all fields $c(z)$ for $c \in V$. It follows from translation invariance that

$$F'_{a,b}(z_1,z_2)|0\rangle = e^{z_2\cdot T}((z_{12}^2)^{N'(a,b)}a(z_{12})b) \in V[[z_{12},z_2]] \equiv V[[z_1,z_2]]. \tag{5.7}$$

On the other hand, by locality (assuming that $c \in V$ has a fixed parity p_c) we get

$$((z_1-w)^2(z_2-w)^2)^N F'_{a,b}(z_1,z_2)c(w)|0\rangle = ((z_1-w)^2(z_2-w)^2)^N(-1)^{(p_a+p_b)p_c}c(w)F'_{a,b}(z_1,z_2)|0\rangle$$

for $N \gg 0$. It follows from Eq. (5.7) and Theorem 4.1 that both sides of the above equation belong to the intersection of $V[[z_1, 1/z_1^2; z_2, 1/z_2^2]][[w]]$ and $V[[w]]_{w^2}[[z_1,z_2]]$. But the latter space is exactly $V[[z_1,z_2,w]]$. Therefore,

$$((z_1-w)^2(z_2-w)^2)^N F'_{a,b}(z_1,z_2)c(w)|0\rangle \in V[[z_1,z_2,w]],$$

and setting $w=0$ we find that $F'_{a,b}$ is a field.

In the same way one proves that

$$F'_{b,a}(z_1,z_2) := (z_{12}^2)^{N'(a,b)} b(z_2)a(z_1)$$

is a field; note that $N'(a,b)=N'(b,a)$ because of the "quasisymmetry" relation

$$a(z)b = (-1)^{p_a p_b} e^{z\cdot T}(b(-z)a), \quad a,b \in V \tag{5.8}$$

(see Ref. 28, Proposition 4.4). Locality for $a(z)$ and $b(z)$ implies that

$$(z_{12}^2)^N (F'_{a,b}(z_1,z_2) - (-1)^{p_a p_b} F'_{b,a}(z_1,z_2))c = 0, \quad N \gg 0.$$

On the other hand, since $F'_{a,b}$ and $F'_{b,a}$ are fields,

$$(F'_{a,b}(z_1,z_2) - (-1)^{p_a p_b} F'_{b,a}(z_1,z_2))c \in V[[z_1,z_2]]_{z_1^2 z_2^2},$$

which is a $\mathbb{C}[z_1,z_2]_{z_1^2 z_2^2}$-module with *no zero divisors*. Hence, $F'_{a,b}=(-1)^{p_a p_b}F'_{b,a}$ and $N(a,b) \leqslant N'(a,b)$. □

From the proof of Lemma 5.2 and from Theorem 4.1, we deduce the following corollary.

Corollary 5.3: Let V be a vertex algebra, and let $A(z_1,\dots,z_m)$ be an (End V)*–valued formal distribution, which is translation invariant and local with respect to all fields $Y(c,z)(c \in V)$. Then A is an m-field if and only if $A(z_1,\dots,z_m)|0\rangle \in V[[z_1,\dots,z_m]]$.*

Next, we will derive from Theorem 5.1 an "associativity" property, which generalizes Eqs. (4.2) and (7.3) from Ref. 2 (see also Refs. 13 and 24).

Proposition 5.4: ("Associativity") *For every three elements a,b,c in a vertex algebra V and for $L \geqslant N(a,c)$, we have*

$$((z+w)^2)^L (a(z)b)(w)c = ((z+w)^2)^L \iota_{z,w} a(z+w)b(w)c, \tag{5.9}$$

$$(z^2)^L a(z)b(w)c = [((u+z-w)^2)^L \iota_{z,w}(a(z-w)b)(u)c]_{u=w}, \tag{5.10}$$

where the expression under the substitution on the right-hand side of (5.10) *belongs to $\iota_{z,w}V[[z,w,u]]_{(z-w)^2u^2}$ and setting $u=w$ makes sense.*

Proof: We can assume without loss of generality that $L=N(a,c)$. Then, by Theorem 5.1, the left-hand side of (5.9) is equal to

$$\frac{\psi_{a,b,c}(z+w,w)}{(z^2)^{N(a,b)}(w^2)^{N(b,c)}} \in V[[z,w]]_{z^2w^2},$$

while the right-hand side is

$$\iota_{z,w}\iota_{z+w,w}\frac{\psi_{a,b,c}(z+w,w)}{(((z+w)-w)^2)^{N(a,b)}(w^2)^{N(b,c)}}.$$

Then Eq. (5.9) follows from Taylor's formula (2.31). The proof of Eq. (5.10) is simpler: its sides are equal to

$$\iota_{z,w}\frac{\psi_{a,b,c}(z,w)}{((z-w)^2)^{N(a,b)}(w^2)^{N(b,c)}} \quad \text{and} \quad \iota_{z,w}\frac{\psi_{a,b,c}(u+z-w,u)}{((z-w)^2)^{N(a,b)}(u^2)^{N(b,c)}},$$

respectively, and obviously they become equal after the substitution $u=w$. □

B. Jacobi identity

In this section, for any three elements in a vertex algebra over $\mathbb{C}^D$, we derive an identity that generalizes the Jacobi identity of Ref. 19 (and the Borcherds identity of Ref. 21) for usual $D=1$ vertex algebras.

Theorem 5.5: ("Jacobi identity") *Let V be a vertex algebra, and let $a,b,c \in V$, where a and b have fixed parities p_a and p_b, respectively. Then for $L \geqslant N(a,c)$ and for every $F(\mathrm{z},\mathrm{w}) \in \mathbb{C}[[\mathrm{z},\mathrm{w}]]_{(\mathrm{z}^2)^{\mathbb{R}}(\mathrm{w}^2)^{\mathbb{R}}((\mathrm{z}-\mathrm{w})^2)^{\mathbb{R}}}$, we have*

$$\begin{aligned} &a(\mathrm{z})b(\mathrm{w})c\iota_{\mathrm{z},\mathrm{w}}F(\mathrm{z},\mathrm{w}) - (-1)^{p_a p_b}b(\mathrm{w})a(\mathrm{z})c\iota_{\mathrm{w},\mathrm{z}}F(\mathrm{z},\mathrm{w}) \\ &\quad = (\mathrm{z}^2)^{-L}[((\mathrm{u}+\mathrm{z}-\mathrm{w})^2)^L(\iota_{\mathrm{z},\mathrm{w}} - \iota_{\mathrm{w},\mathrm{z}})(a(\mathrm{z}-\mathrm{w})b)(\mathrm{u})cF(\mathrm{z},\mathrm{w})]_{\mathrm{u}=\mathrm{w}}, \end{aligned} \tag{5.11}$$

where the expression under the substitution on the right-hand side belongs to $(\iota_{\mathrm{z},\mathrm{w}}-\iota_{\mathrm{w},\mathrm{z}})V[[\mathrm{z},\mathrm{w},\mathrm{u}]]_{(\mathrm{z}^2)^{\mathbb{R}}(\mathrm{w}^2)^{\mathbb{R}}((\mathrm{z}-\mathrm{w})^2)^{\mathbb{R}}\mathrm{u}^2}$ and setting $\mathrm{u}=\mathrm{w}$ makes sense.

Proof: By the same argument as in the proof of Eq. (5.10) above, one finds separately

$$a(\mathrm{z})b(\mathrm{w})c\iota_{\mathrm{z},\mathrm{w}}F(\mathrm{z},\mathrm{w}) = (\mathrm{z}^2)^{-L}[((\mathrm{u}+\mathrm{z}-\mathrm{w})^2)^L\iota_{\mathrm{z},\mathrm{w}}(a(\mathrm{z}-\mathrm{w})b)(\mathrm{u})cF(\mathrm{z},\mathrm{w})]_{\mathrm{u}=\mathrm{w}}, \tag{5.12}$$

$$(-1)^{p_a p_b}b(\mathrm{w})a(\mathrm{z})c\iota_{\mathrm{w},\mathrm{z}}F(\mathrm{z},\mathrm{w}) = (\mathrm{z}^2)^{-L}[((\mathrm{u}+\mathrm{z}-\mathrm{w})^2)^L\iota_{\mathrm{w},\mathrm{z}}(a(\mathrm{z}-\mathrm{w})b)(\mathrm{u})cF(\mathrm{z},\mathrm{w})]_{\mathrm{u}=\mathrm{w}} \tag{5.13}$$

for $L \geqslant N(a,c)$. Taking the difference we obtain (5.11). □

The main subtlety of Eq. (5.11) is that on the right-hand side one cannot make the substitution $\mathrm{u}=\mathrm{w}$ in each of the factors separately. It is only after we multiply them that this substitution makes sense. The reason is that, in contrast to the case $D=1$, the expression $(\iota_{\mathrm{z},\mathrm{w}}-\iota_{\mathrm{w},\mathrm{z}})a(\mathrm{z}-\mathrm{w})b$ involves an infinite sum, and hence in general $(\iota_{\mathrm{z},\mathrm{w}}-\iota_{\mathrm{w},\mathrm{z}})(a(\mathrm{z}-\mathrm{w})b)(\mathrm{w})c$ is not well defined. We refer to Secs. V D and V E below for additional discussion.

It is clear from the proof of Eq. (5.10) that if we multiply the right-hand sides of Eqs. (5.12) and (5.13) by $(\mathrm{u}^2)^M$ for $M \geqslant N(b,c)$, they will become regular in u (i.e., not containing negative powers of u^2). Then we will be able to represent the substitution $\mathrm{u}=\mathrm{w}$ by Cauchy formula (3.24). Thus we obtain the following equivalent integral form of Jacobi identity (5.11).

Corollary 5.6: For every element a,b,c in a vertex algebra V, a and b having fixed parities p_a and p_b, respectively, and for every $L \geqslant N(a,c)$, $M \geqslant N(b,c)$, we have

$$\begin{aligned} &a(\mathrm{z})b(\mathrm{w})c\iota_{\mathrm{z},\mathrm{w}}F(\mathrm{z},\mathrm{w}) - (-1)^{p_a p_b}b(\mathrm{w})a(\mathrm{z})c\iota_{\mathrm{w},\mathrm{z}}F(\mathrm{z},\mathrm{w}) \\ &\quad = \mathrm{Res}_{\mathrm{u}}(\mathrm{z}^2)^{-L}(\mathrm{w}^2)^{-M}((\mathrm{u}+\mathrm{z}-\mathrm{w})^2)^L(\mathrm{u}^2)^M\iota_{\mathrm{u},\mathrm{w}}((\mathrm{u}-\mathrm{w})^2)^{-D/2} \\ &\qquad \times (\iota_{\mathrm{z},\mathrm{w}} - \iota_{\mathrm{w},\mathrm{z}})((a(\mathrm{z}-\mathrm{w})b)(\mathrm{u})cF(\mathrm{z},\mathrm{w})) \end{aligned} \tag{5.14}$$

for $F(\mathrm{z},\mathrm{w}) \in \mathbb{C}[[\mathrm{z},\mathrm{w}]]_{(\mathrm{z}^2)^{\mathbb{R}}(\mathrm{w}^2)^{\mathbb{R}}((\mathrm{z}-\mathrm{w})^2)^{\mathbb{R}}}$.

Proof: It remains to note that the right-hand side of (5.14) makes sense. Indeed, the product of the Cauchy kernel $\iota_{\mathrm{u},\mathrm{w}}((\mathrm{u}-\mathrm{w})^2)^{-D/2}$ and the third line in (5.14) is well defined in the space $(\iota_{\mathrm{z},\mathrm{w}} - \iota_{\mathrm{w},\mathrm{z}})V[[\mathrm{u}]]_{\mathrm{u}^2}[[\mathrm{z},\mathrm{w}]]_{(\mathrm{z}^2)^{\mathbb{R}}(\mathrm{w}^2)^{\mathbb{R}}((\mathrm{z}-\mathrm{w})^2)^{\mathbb{R}}}$. □

Remark 5.1: One can give an alternative proof of Theorem 5.5 by using "associativity" relation (5.9), "quasisymmetry" relation (5.8), and generalizing the arguments of Ref. 2, Sec. 7 to the case of arbitrary D (see also Refs. 18, 25, and 24). With obvious modifications, Eq. (5.11) remains valid for generalized vertex algebras (see Remark 4.1 and Refs. 16, 13, 27, and 3).

We will show in Sec. V D below that Jacobi identity (5.11), together with a partial vacuum axiom, can be taken as an equivalent definition of vertex algebra over $\mathbb{C}^D$.

C. Integral Borcherds formula

In this section we will derive an integral version of Jacobi identity (5.11), which in particular gives a formula for the commutator of modes that generalizes the Borcherds commutator formula from Ref. 8 (see also Refs. 19, 18, 21, and 24).

Let us introduce the following additive subgroup of $\mathbb{R}$:

$$\hat{\mathbb{Z}} := \mathbb{Z} + \tfrac{D}{2}\mathbb{Z} = \begin{cases} \mathbb{Z} & \text{if } D \text{ is even,} \\ \frac{1}{2}\mathbb{Z} & \text{if } D \text{ is odd.} \end{cases} \tag{5.15}$$

As a consequence of Corollary 3.2, every $(\mathrm{End}\, V)$–valued formal distribution $\phi(z) \in (\mathrm{End}\, V)[[z, 1/z^2]]$ can be considered as a linear map

$$\mathbb{C}[z]_{(z^2)\hat{z}} \to \mathrm{End}\, V, \quad f(z) \mapsto \mathrm{Res}_z \phi(z) f(z). \tag{5.16}$$

Thus $\mathbb{C}[z]_{(z^2)\hat{z}}$ plays the role of a vector space of *test functions*, and for even space–time dimension D it is exactly $\mathbb{C}[z]_{z^2} \equiv \mathbb{C}[z]_{(z^2)\mathbb{Z}}$. According to Eq. (3.8), the modes of $\phi(z)$ can be obtained by integrating $\phi(z)$ (with Res_z) against appropriate test functions.

Now let us take $\mathrm{Res}_z \mathrm{Res}_w$ of both sides of Eqs. (5.12) and (5.13) for $F(z,w) \in \mathbb{C}[[z,w]]_{(z^2)\hat{z}(w^2)\hat{z}((z-w)^2)\hat{z}}$, and represent the substitution $u=w$ as Res_u as done in Eq. (5.14). We are going to rewrite the resulting identities in the form

$$\mathrm{Res}_z \mathrm{Res}_w\, a(z)b(w)c\iota_{z,w}F(z,w) = \mathrm{Res}_z \mathrm{Res}_w\, \mathcal{K}^+_{L,M}(z,w;F)(a(z)b)(w)c, \tag{5.17}$$

$$\mathrm{Res}_z \mathrm{Res}_w\, b(w)a(z)c\iota_{w,z}F(z,w) = (-1)^{p_a p_b}\mathrm{Res}_z \mathrm{Res}_w \mathcal{K}^-_{L,M}(z,w;F)(a(-z)b)(w)c, \tag{5.18}$$

where $\mathcal{K}^{\pm}_{L,M}$ are to be determined. To arrive at the above formulas, we will use translation invariance of the residue to replace z with $z+w$ in (5.12) and w with $w+z$ in (5.13). More precisely, we have the following lemma.

Lemma 5.7: For every $G(z,w) \in V[[z,w]]_{(z^2)\hat{z}(w^2)\hat{z}((z-w)^2)\hat{z}}$ we have

$$\mathrm{Res}_z \mathrm{Res}_w\, \iota_{z,w}G(z,w) = \mathrm{Res}_z \mathrm{Res}_w\, \iota_{z,w}G(z+w,w). \tag{5.19}$$

Proof: Translation invariance of the residue [see (3.18)] implies the identity

$$\mathrm{Res}_z \mathrm{Res}_w\, \iota_{z,w}G(z,w) = \mathrm{Res}_z \mathrm{Res}_w\, \iota_{z,u}\iota_{z+u,w}G(z+u,w).$$

Then since the expression under the residue on the right-hand side belongs to the space $V[[z]]_{(z^2)\hat{z}}[[w,u]]_{(w^2)\hat{z}}$, we can set there $u=w$. But

$$\iota_{z,w}\iota_{z+w,w}G(z+w,w) = \iota_{z,w}G(z+w,w)$$

by "Taylor formula" (2.31). □

Applying Lemma 5.7 to the right-hand side of (5.12), we obtain (5.17) with

$$\mathcal{K}^+_{L,M}(z,w;F) := \mathrm{Res}_u\, \iota_{z,u}F(u+z,u)((u+z)^2)^{-L}(u^2)^{-M}\iota_{w,u}((w-u)^2)^{-D/2}((z+w)^2)^L(w^2)^M. \tag{5.20}$$

Similarly, after a renaming of the variables, (5.13) leads to (5.18) with

$$\mathcal{K}^-_{L,M}(z,w;F) := \mathrm{Res}_u\, \iota_{z,u}F(u,u+z)((u+z)^2)^{-M}(u^2)^{-L}\iota_{w,u+z}((w-(u+z))^2)^{-D/2}((w-z)^2)^L(w^2)^M. \tag{5.21}$$

Notice that the expressions after Res_u on the right-hand sides of (5.20) and (5.21) are well-defined elements of $\mathbb{C}[[w]]_{(w^2)\hat{z}}[[z]]_{(z^2)\hat{z}}[[u]]_{(u^2)\hat{z}}$, and in fact the former belongs to $\mathbb{C}[[z,w]]_{(z^2)\hat{z}(w^2)\hat{z}}[[u]]_{(u^2)\hat{z}}$. Then (5.20) and the formula

$$\mathcal{K}^-_{L,M}(z,w;F) = \iota_{w,z}\mathcal{K}^+_{L,M}(z,w-z;F^{\mathrm{op}}), \quad F^{\mathrm{op}}(z,w) := F(w,z) \tag{5.22}$$

imply that

$$\mathcal{K}^+_{L,M}(z,w;F) \in \mathbb{C}[[z,w]]_{(z^2)\hat{z}(w^2)\hat{z}}, \quad \mathcal{K}^-_{L,M}(z,w;F) \in \mathbb{C}[[w]]_{(w^2)\hat{z}}[[z]]_{(z^2)\hat{z}}. \tag{5.23}$$

Taking the difference of Eqs. (5.17) and (5.18), and using (3.46), we obtain the following result.

Theorem 5.8: *With the above notation, in any vertex algebra, we have*

$$\begin{aligned}&\mathrm{Res}_{\mathrm{z}}\,\mathrm{Res}_{\mathrm{w}}\, a(\mathrm{z})b(\mathrm{w})c\,\iota_{\mathrm{z,w}}F(\mathrm{z},\mathrm{w}) - (-1)^{p_a p_b}\,\mathrm{Res}_{\mathrm{z}}\,\mathrm{Res}_{\mathrm{w}} b(\mathrm{w})a(\mathrm{z})c\,\iota_{\mathrm{w,z}}F(\mathrm{z},\mathrm{w})\\ &\quad=\mathrm{Res}_{\mathrm{z}}\,\mathrm{Res}_{\mathrm{w}}\,\mathcal{K}_{L,M}(\mathrm{z},\mathrm{w};F)(a(\mathrm{z})b)(\mathrm{w})c,\end{aligned}\tag{5.24}$$

where

$$\mathcal{K}_{L,M}(\mathrm{z},\mathrm{w};F) := \mathcal{K}^{+}_{L,M}(\mathrm{z},\mathrm{w};F) - \mathcal{K}^{-}_{L,M}(-\mathrm{z},\mathrm{w};F).\tag{5.25}$$

In particular, when $F(\mathrm{z},\mathrm{w})=f(\mathrm{z})g(\mathrm{w})$ is a product of two test functions, Eq. (5.24) gives a formula for the commutator of modes, generalizing the Borcherds formula.

D. The Jacobi identity as alternative axiom and the case $D=1$

In this section we derive some consequences of our Jacobi identity (5.11). We prove that together with a partial vacuum axiom it can be taken as an equivalent definition of vertex algebra over $\mathbb{C}^D$. We also show that for $D=1$ it reduces to (an equivalent form of) the Jacobi identity of Ref. 19.

First of all, it is clear from the definitions that if $(\mathrm{z}^2)^N a(\mathrm{z})b \in V[\![\mathrm{z}]\!]$, then $(\iota_{\mathrm{z,w}}-\iota_{\mathrm{w,z}})a(\mathrm{z}-\mathrm{w})b((\mathrm{z}-\mathrm{w})^2)^N=0$. Therefore, Jacobi identity (5.11) implies locality. Our next step is to show that it also implies "associativity."

Lemma 5.9: Let V be a vector space, let c be an element of V, and let $a(\mathrm{z})$, $b(\mathrm{w})$ be two fields on V. Assume that Eq. (5.11) *holds for some fixed p_a, p_b, L and for all $F(\mathrm{z},\mathrm{w}) \in \mathbb{C}[\![\mathrm{z},\mathrm{w}]\!]_{\mathrm{z}^2\mathrm{w}^2((\mathrm{z}-\mathrm{w})^2)\hat{\mathrm{z}}}$ [see* (5.15)*]. Then Eq.* (5.9) *holds for some $L' \geqslant L$.*

Proof: Let $L' \geqslant L$ be large enough so that $(\mathrm{z}^2)^{L'} a(\mathrm{z})c \in V[\![\mathrm{z}]\!]$. Obviously, if Eq. (5.11) holds for some L then it holds for all $L' \geqslant L$, so let us just assume $L'=L$. Applying $\mathrm{Res}_{\mathrm{z}}$ to both sides of (5.11) with $F(\mathrm{z},\mathrm{w})=(\mathrm{z}^2)^L f(\mathrm{z}-\mathrm{w})$, where $f(\mathrm{z}) \in \mathbb{C}[\![\mathrm{z}]\!]_{(\mathrm{z}^2)\hat{\mathrm{z}}}$ is an arbitrary test function, we obtain

$$\mathrm{Res}_{\mathrm{z}}(\mathrm{z}^2)^L a(\mathrm{z})b(\mathrm{w})c\,\iota_{\mathrm{z,w}} f(\mathrm{z}-\mathrm{w}) = \mathrm{Res}_{\mathrm{z}}[((\mathrm{u}+\mathrm{z}-\mathrm{w})^2)^L \iota_{\mathrm{z,w}}(a(\mathrm{z}-\mathrm{w})b)(\mathrm{u})c f(\mathrm{z}-\mathrm{w})]_{\mathrm{u}=\mathrm{w}}.$$

Now using the translation invariance of the residue [see (3.18)], we get

$$\mathrm{Res}_{\mathrm{z}}((\mathrm{z}+\mathrm{w})^2)^L \iota_{\mathrm{z,w}} a(\mathrm{z}+\mathrm{w})b(\mathrm{w})c f(\mathrm{z}) = [\mathrm{Res}_{\mathrm{z}}((\mathrm{u}+\mathrm{z})^2)^L (a(\mathrm{z})b)(\mathrm{u})c f(\mathrm{z})]_{\mathrm{u}=\mathrm{w}}.$$

After the substitution $\mathrm{u}=\mathrm{w}$, this gives exactly Eq. (5.9) [cf. (5.16)]. □

Now we can prove the following statement, which shows that a vertex algebra can be defined in terms of Jacobi identity as in Ref. 19 for the $D=1$ case (see also Refs. 21 and 24).

Theorem 5.10: *Let V be a vector superspace endowed with an even vector $|0\rangle$ and with a parity preserving linear map $Y: V \mapsto Y(a,\mathrm{z}) \equiv a(\mathrm{z})$ to the space of fields on V. Assume that Jacobi identity* (5.11) *holds for every fixed $a,b,c \in V$ with parities p_a, p_b of a and b, respectively, for some $L \geqslant 0$ and for all $F(\mathrm{z},\mathrm{w}) \in \mathbb{C}[\![\mathrm{z},\mathrm{w}]\!]_{\mathrm{z}^2\mathrm{w}^2((\mathrm{z}-\mathrm{w})^2)\hat{\mathrm{z}}}$. Finally, let the following "partial vacuum axiom" be satisfied:*

$$Y(|0\rangle,\mathrm{z})a = a, \quad \mathrm{Res}_{\mathrm{z}}(\mathrm{z}^2)^{-D/2} Y(a,\mathrm{z})|0\rangle = a \quad \text{for all } a \in V.\tag{5.26}$$

Then there exist uniquely determined mutually commuting even endomorphisms $T_1,\ldots,T_D$ of V, which make V a vertex algebra over $\mathbb{C}^D$.

Proof: We have already pointed out that locality of $a(\mathrm{z})$ and $b(\mathrm{w})$ follows from Jacobi identity for $F(\mathrm{z},\mathrm{w})=((\mathrm{z}-\mathrm{w})^2)^N$ with $N \gg 0$. We will derive the rest of the axioms of vertex algebra (Definition 4.1) from Eqs. (5.9) and (5.26) (cf. Lemma 5.9).

Setting in Eq. (5.9) $b=|0\rangle$ and $L \gg 0$ such that $(\mathrm{z}^2)^L a(\mathrm{z})c \in V[\![\mathrm{z}]\!]$, we obtain that

$$((z+w)^2)^L(a(z)|0\rangle)(w)c \in V[[z,w]].$$

Since $(a(z)|0\rangle)(w)c \in V[[w]]_{w^2}[[z]]_{z^2}$, it makes sense to multiply the above equation by $\iota_{w,z}((z+w)^2)^{-L}$ and get

$$(a(z)|0\rangle)(w)c \in \iota_{w,z}V[[z,w]]_{(z+w)^2} \subset V[[w]]_{w^2}[[z]].$$

Then letting $c=|0\rangle$ and using the second equality in (5.26) (with respect to w), we deduce from here that $a(z)|0\rangle \in V[[z]]$ for all $a \in V$. Thus the second equality in (5.26) can be restated as $a(z)|0\rangle|_{z=0}=a$.

We define the translation endomorphisms $T_1, \ldots, T_D$ of V by the formula

$$T_\alpha a := \partial_{z^\alpha} a(z)|0\rangle\,|_{z=0}, \quad \alpha = 1, \ldots, D,$$

which should hold if V is a vertex algebra. Then setting $c=|0\rangle$ in Eq. (5.9), we deduce that

$$T_\alpha(a(z)b) - a(z)(T_\alpha b) = \partial_{z^\alpha} a(z)b,$$

while the substitution $b=|0\rangle$ in Eq. (5.9) implies $(T_\alpha a)(z)=\partial_{z^\alpha} a(z)$. The remaining axioms [Definition 4.1(a), (b)] are then immediate. □

Remark 5.2: With obvious modifications, Theorem 5.5 and Theorem 5.10 hold also for modules over vertex algebras (see Ref. 28, Sec. 6 for the definition of module).

The main subtlety of Jacobi identity (5.11) is that one cannot make the substitution u=w in each of the factors separately. However, in the next proposition we will show that this can be done if the field $a(z)$ has a special form. Recall that the regular and singular parts of a formal distribution were defined in Sec. III D.

Proposition 5.11: Let a,b be elements in a vertex algebra V, with parities p_a and p_b, respectively. Assume that for some $n \in \mathbb{Z}$ the singular part of $(z^2)^n a(z)b$ belongs to $V[z]_{z^2}$. Then we have:

$$\begin{aligned} &a(z)b(w)\iota_{z,w}((z-w)^2)^n - (-1)^{p_a p_b} b(w)a(z)\iota_{w,z}((z-w)^2)^n \\ &\quad = (\iota_{z,w} - \iota_{w,z})((a(z-w)b)(w)((z-w)^2)^n), \end{aligned} \tag{5.27}$$

and the right-hand side is well defined.

Proof: For an arbitrary fixed $c \in V$ and $L \gg 0$, set $F(z,w)=((z-w)^2)^n$ in Eq. (5.11). Because the regular part of $((z-w)^2)^n a(z-w)$ is killed by $\iota_{z,w}-\iota_{w,z}$, we can replace $((z-w)^2)^n a(z-w)$ by its singular part in the right-hand side of (5.11). But by assumption the coefficients of the singular part of $(z^2)^n a(z)b$ span a finite-dimensional subspace of V. Therefore, in (5.11) one can substitute u=w in each factor separately, and the right-hand side of (5.27) makes sense. After setting u=w in the other factor in (5.11) it cancels with $(z^2)^L$. □

Remark 5.3: When $D=1$, the assumption of Proposition 5.11 is satisfied for every pair of elements $a,b \in V$ and every $n \in \mathbb{Z}$. In this case, the collection of identities (5.27) is equivalent to the Jacobi identity of Ref. 19.

Let us note that for $D>1$ the assumption of Proposition 5.11 is in fact quite restrictive. For $n=0$ it holds for the scalar free field $\varphi(z)$ discussed in Sec. IV C [because $\varphi(z)$ is harmonic] but it does not hold for the Wick square $:\varphi(z)^2:$. Furthermore, it does not hold for $\varphi(z)$ itself when $n<0$. On the other hand, the assumption is satisfied for $n=0$ and any "generalized free field" (see Ref. 28, Sec. 5), thus providing a version of the *Wick theorem* (note that the element b is arbitrary).

E. Degree cutoffs and commutator formula

In this section, we derive a commutator formula, which shows in particular that the singular modes of fields close an algebraic structure under the commutator.

We have remarked at the end of the preceding section that the main difficulty for $D>1$ as opposed to $D=1$ is that the singular part of $a(z)b$ involves an infinite sum in general. To circumvent this problem we introduce "degree cutoffs" as follows. For a formal distribution $\phi(z)$, written as in (2.17), and for any $N \in \mathbb{R}$, we define the cutoff $\phi(z)^{\leqslant N}$ by restricting the sums over m and γ

in (2.17) to indices with $m+2\gamma \leqslant N$. In other words, we restrict the sum to terms with degrees in z less than or equal to N. We denote the remaining part of $\phi(z)$ by $\phi(z)^{>N} := \phi(z) - \phi(z)^{\leqslant N}$. In the same way, we define cutoffs $\phi(z)^{\leqslant N}_{s.p.}$ of the singular part of $\phi(z)$ [see (3.36)]. Note that all these operations are commuting projections on the space of formal distributions.

Even though the singular part $a(z)_{s.p.}b$ may involve infinitely many terms with arbitrarily high degrees in z, it is important that for fixed $N \in \mathbb{Z}$ the cutoff of the singular part $a(z)^{\leqslant N}_{s.p.}b$ is *finite*, i.e., it belongs to $V[z]_{z^2}$. Then the same argument as in the proof of Proposition 5.11 gives the following result.

Lemma 5.12: Let a,b,c be elements in a vertex algebra V, where a and b have parities p_a and p_b, respectively. Then for every $n,N \in \mathbb{Z}$ and every $L \geqslant N(a,c)$, we have

$$\begin{aligned} &a(z)b(w)\iota_{z,w}((z-w)^2)^n - (-1)^{p_a p_b} b(w)a(z)\iota_{w,z}((z-w)^2)^n \\ &\quad = (\iota_{z,w} - \iota_{w,z})((a(z-w)^{\leqslant N}b)(w)((z-w)^2)^n) \\ &\qquad + (z^2)^{-L}[((u+z-w)^2)^L(\iota_{z,w} - \iota_{w,z})(a(z-w)^{>N}b)(u)c((z-w)^2)^n]_{u=w}. \end{aligned}$$

We will now apply this lemma in the case $n=0$ when it reduces to a formula for the commutator of the fields $a(z)$, $b(w)$. Then, because of the presence of $\iota_{z,w} - \iota_{w,z}$, on the right-hand side of the above equation one can replace $a(z-w)^{\leqslant N}$ and $a(z-w)^{>N}$ by their singular parts and obtain

$$\begin{aligned} [a(z),b(w)]c = &(\iota_{z,w} - \iota_{w,z})(a(z-w)^{\leqslant N}_{s.p.}b)(w) \\ &+ [(z^2)^{-L}((u+z-w)^2)^L(\iota_{z,w} - \iota_{w,z})(a(z-w)^{>N}_{s.p.}b)(u)c]_{u=w}. \end{aligned} \tag{5.28}$$

The next result shows that the singular parts of fields themselves close a structure with respect to the commutator.

Proposition 5.13: For every three elements a,b,c in a vertex algebra V and for every $L \geqslant N(a,c)$, one has

$$[a(z)_{s.p.},b(w)_{s.p.}]c = ([(z^2)^{-L}((u+z-w)^2)^L(\iota_{z,w} - \iota_{w,z})(a(z-w)_{s.p.}b)(u)_{s.p.}c]_{u=w})_{s.p.}, \tag{5.29}$$

where the outer s.p. *on the right-hand side designates taking the singular part with respect to both* z *and* w.

Note that for $D>1$ a product of two singular terms may contain a regular part; that is why in (5.29) we must include the outer projection onto the singular parts.

Proof of Proposition 5.13: We will prove that (5.29) holds for all terms with total degree in z and w up to N, for every fixed $N \in \mathbb{Z}$. For this purpose, we consider all terms of total degree $\leqslant N$ in (5.28), and take the singular parts with respect to both z and w. We will consider separately the resulting two terms on the right-hand side.

In the first term, the expansion $\iota_{w,z}$ will not contribute because it produces terms regular in z. Since $\iota_{z,w}(a(z-w)^{\leqslant N}_{s.p.}b)(w)_+$ is regular in w, it will not contribute either, and we will obtain

$$(\iota_{z,w}(a(z-w)^{\leqslant N}_{s.p.}b)(w)_{s.p.}c)_{s.p.}.$$

Reversing the above reasoning, this expression can be rewritten as

$$((\iota_{z,w} - \iota_{w,z})(a(z-w)^{\leqslant N}_{s.p.}b)(w)_{s.p.}c)_{s.p.}.$$

Then, as in the derivation of Lemma 5.12, it is equal to

$$([(z^2)^{-L}((u+z-w)^2)^L(\iota_{z,w} - \iota_{w,z})(a(z-w)^{\leqslant N}_{s.p.}b)(u)_{s.p.}c]_{u=w})_{s.p.}.$$

It remains to prove that the second term resulting from the right-hand side of (5.28) is equal to

$$([(z^2)^{-L}((u+z-w)^2)^L(\iota_{z,w}-\iota_{w,z})(a(z-w)^{>N}_{s.p.}b)(u)_{s.p.}c]_{u=w})_{s.p.}.$$

This follows from the fact that

$$[(z^2)^{-L}((u+z-w)^2)^L(\iota_{z,w}-\iota_{w,z})(a(z-w)^{>N}_{s.p.}b)(u)_+c]_{u=w}$$

contains only terms with total degree in z and w strictly greater than N. □

VI. CONCLUDING REMARKS

In this paper we develop further the theory of vertex algebras in higher dimensions. We start by introducing useful formal calculus techniques including various spaces of formal series and a formal residue functional. This residue functional is uniquely determined (up to a multiplicative constant) by the property that it is translation invariant (Theorem 3.1), and so it plays the role of the integral. In addition, it satisfies an analog of the Cauchy formula [Eq. (3.24)]. The modes of fields can be obtained by integrating the fields (with respect to our residue functional) against certain test functions.

Our main goal was to understand the algebraic structure obeyed by the modes of local fields with respect to the commutator. For this purpose we derived an analog of the Jacobi identity for vertex algebras in higher dimensions (Theorem 5.5). Since the commutator of two local fields is expressed in terms of the singular part of their operator product expansion, a natural question arises whether the singular parts of fields close a structure under the commutator. Utilizing a certain degree cutoff technique we proved that this is indeed the case (Proposition 5.13).

Thus, if we denote by $a[z]b$ the singular part $a(z)_{s.p.}b$, we find that it closes the following structure. The map $a,b\mapsto a[z]b\in(V[\![z]\!]_{z^2})_{s.p.}$ is parity preserving and bilinear on a superspace V endowed with an action of mutually commuting even endomorphisms $T_1,\dots,T_D$, and the following axioms are satisfied:

(a) (*translation invariance*) $[T_\alpha,a[z]]b=(T_\alpha a)[z]b=\partial_{z^\alpha}a[z]b$;
(b) (*skew-symmetry*) $a[z]b=(-1)^{p_ap_b}(e^{z\cdot T}(b[-z]a))_{s.p.}$;
(c) (*Jacobi identity*)

$$[a[z],b[w]]c=((z^2)^{-L}[((u+z-w)^2)^L(\iota_{z,w}-\iota_{w,z})(a[z-w]b)[u]c]_{u=w})_{s.p.}$$

for $L\gg 0$, and the expression under the substitution on the right-hand side belongs to the space $(\iota_{z,w}-\iota_{w,z})V[\![z,w,u]\!]_{(z-w)^2u^2}$ where setting $u=w$ makes sense. It is expected that the obtained algebraic structure will play in higher dimensions the same role as vertex Lie algebras do in dimension one.

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APPENDIX: GEOMETRIC REALIZATION OF THE RESIDUE

In this appendix we will provide a geometric definition of the residue functional introduced in Sec. III A. We will suppose that the space–time dimension D is *even*.

Let us introduce the following one-parameter family $\{\bar{M}_r\}_{r>0}$ of D-dimensional real submanifolds of $\mathbb{C}^D$:

$$\bar{M}_r := \{\mathrm{z} \in \mathbb{C}^D | \mathrm{z} = \lambda \mathrm{u}, \quad \lambda \in \mathbb{C}, \quad |\lambda| = r, \quad \mathrm{u} \in \mathbb{S}^{D-1} \subset \mathbb{R}^D\}, \tag{A1}$$

where $\mathbb{S}^{D-1}$ denotes the unit sphere in $\mathbb{R}^D$. Note that $\bar{M}_1$ is exactly the *conformally compactified Minkowski space* (see Refs. 31 and 28).

We introduce a parametrization of $\bar{M}_r$,

$$\bar{M}_r \ni \mathrm{z} = re^{i\zeta}\mathrm{u} \quad \text{for } \zeta \in [0, \pi), \quad \mathrm{u} \in \mathbb{S}^{D-1}, \tag{A2}$$

which shows that $\bar{M}_r$ is diffeomorphic to $(\mathbb{S}^1 \times \mathbb{S}^{D-1})/\mathbb{Z}_2$, with the points $(e^{i\zeta}, \mathrm{u})$ and $(-e^{i\zeta}, -\mathrm{u})$ being identified. In particular, all $\bar{M}_r$ are orientable for even D. Thus, the volume form $\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D$ on $\mathbb{C}^D$ can be restricted to $\bar{M}_r$ and gives rise to a complex measure there. In parametrization (A2), we have

$$\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D \big|_{\bar{M}_r} = ir^D e^{iD\zeta}\, \mathrm{d}\zeta \wedge \mathrm{d}\sigma(\mathrm{u}), \tag{A3}$$

where $\mathrm{d}\sigma(\mathrm{u})$ is the $\mathrm{O}(D)$-invariant volume form $\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D|_{\mathbb{S}^{D-1}}$ on the unit sphere $\mathbb{S}^{D-1}$.

An important property of the family $\{\bar{M}_r\}$ is that if $\mathrm{z} \in \bar{M}_r$ and $\mathrm{w} \in \bar{M}_{r'}$ for $r \neq r'$ then $(\mathrm{z} - \mathrm{w})^2 \neq 0$. Indeed, writing

$$\mathrm{z} = re^{i\zeta}\mathrm{u}, \quad \mathrm{w} = r'e^{i\zeta'}\mathrm{u}', \quad \mathrm{u} \cdot \mathrm{u}' = \cos\alpha = (e^{i\alpha} + e^{-i\alpha})/2, \tag{A4}$$

we find that

$$(\mathrm{z} - \mathrm{w})^2 = (re^{i\zeta} - r'e^{i(\zeta'+\alpha)})(re^{i\zeta} - r'e^{i(\zeta'-\alpha)}). \tag{A5}$$

This shows that for $n \in \mathbb{Z}$ the formal Taylor expansion $\iota_{\mathrm{z},\mathrm{w}}((\mathrm{z}-\mathrm{w})^2)^n$ [see (2.26)] in the above parametrization corresponds to a geometric series expansion for $r > r'$. Note also that the conformal inversion $\mathrm{z} \mapsto \mathrm{z}/\mathrm{z}^2$ maps $\bar{M}_r$ onto $\bar{M}_{r^{-1}}$.

Proposition A.1: For $f(\mathrm{z}) \in \mathbb{C}[\mathrm{z}]_{\mathrm{z}^2}$ *and* $g(\mathrm{z},\mathrm{w}) \in \mathbb{C}[\mathrm{z},\mathrm{w}]_{\mathrm{z}^2\mathrm{w}^2(\mathrm{z}-\mathrm{w})^2}$, *we have*

$$\mathrm{Res}_{\mathrm{z}} f(\mathrm{z}) = (i\pi\mathcal{V}_{D-1})^{-1} \int_{\bar{M}_r} f(\mathrm{z})\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D, \tag{A6}$$

$$\mathrm{Res}_{\mathrm{z}}\, \iota_{\mathrm{z},\mathrm{w}} g(\mathrm{z},\mathrm{w}) = (i\pi\mathcal{V}_{D-1})^{-1} \int_{\bar{M}_r} g(\mathrm{z},\mathrm{w})\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D \quad \textit{for } \mathrm{w} \in \bar{M}_{r'}, \quad r' < r, \tag{A7}$$

$$\mathrm{Res}_{\mathrm{z}}\, \iota_{\mathrm{w},\mathrm{z}} g(\mathrm{z},\mathrm{w}) = (i\pi\mathcal{V}_{D-1})^{-1} \int_{\bar{M}_r} g(\mathrm{z},\mathrm{w})\mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^D \quad \textit{for } \mathrm{w} \in \bar{M}_{r'}, \quad r' > r, \tag{A8}$$

where $\mathcal{V}_{D-1} = \int_{\mathbb{S}^{D-1}} \mathrm{d}\sigma(\mathrm{u})$.

Proof: It is enough to check (A6) for the functions $(\mathrm{z}^2)^n h(\mathrm{z})$, where $n \in \mathbb{Z}$ and $h(\mathrm{z})$ is a harmonic homogeneous polynomial of degree m. Then (A6) follows from (A3) and the formulas

$$\int_{\mathbb{S}^{D-1}} h(\mathrm{u})\mathrm{d}\sigma(\mathrm{u}) = \delta_{m,0} h(0)\mathcal{V}_{D-1}, \quad \int_0^{\pi} e^{iD\zeta + 2in\zeta}\, \mathrm{d}\zeta = \pi\delta_{n,-(D/2)}.$$

Equation (A7) follows from (A6) because the expansion $\iota_{\mathrm{z},\mathrm{w}} g(\mathrm{z},\mathrm{w})$ converges uniformly to $g(\mathrm{z},\mathrm{w})$ for $\mathrm{z} \in \bar{M}_r$, $\mathrm{w} \in \bar{M}_{r'}$ and fixed $r > r'$ [see (A5)]. Finally, (A8) is proved in the same way as (A7) but for $r < r'$. □

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Finite dimensional representations of the Euclidean algebra $\mathfrak{e}(2)$ having two generators

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The Euclidean algebra $\mathfrak{e}(2)$ is the Lie algebra of the group E(2) of Euclidean transformations of the plane. This paper examines finite dimensional representations of $\mathfrak{e}(2)$ having two generators. To each representation with two generators we associate a graph. In term of graphs, we give a criterion for the indecomposability of such representations and describe an invariant for indecomposable representations. We also classify the indecomposable representations of dimensions 5 and 6, regardless of the number of generators (dimensions less than 5 have been classified). In each case there are finitely many such representations. Next, we show that for each dimension $\geqslant 8$ there are infinitely many nonequivalent indecomposable representations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2197688]

I. INTRODUCTION

The group E(2) of Euclidean motions of the plane is the noncompact semidirect product group $\mathbb{R}^2 \rtimes \mathrm{SO}(2)$. The complexification of its Lie algebra, $\mathfrak{e}(2)$, has basis $\{p_+, p_-, l\}$ with commutation relations given by

$$[p_+, p_-] = 0, \quad [l, p_\pm] = \pm p_\pm. \tag{1}$$

Let V be a complex representation of E(2); then V decomposes into weight spaces according to the action of $\mathfrak{so}(2)$,

$$V = \oplus V_k, \quad \text{where } V_k = \{v \in V : l \cdot v = kv\} \text{ and } k \in \mathbb{Z}. \tag{2}$$

Further, we have

$$p_+ V_k \subseteq V_{k+1}, \quad p_- V_k \subseteq V_{k-1}. \tag{3}$$

Henceforth, all representations will be over the complex numbers.

Since $\mathfrak{e}(2)$ is solvable, its finite dimensional, irreducible representations are all one dimensional (see Ref. 11), and thus of limited interest. Considerable research has been done investigating the infinite dimensional, unitary irreducible representations of $\mathfrak{e}(2)$ (see, for example, 1, 3, and 4). However, much less is known about the finite dimensional, indecomposable representations of $\mathfrak{e}(2)$. These representations play a significant role in the representation theory of the Poincaré group (see Refs. 2, 5, 8, and 9).

Given a finite dimensional representation V, a set of elements $v_1, \ldots, v_n \in V$ is defined to be a set of *generators* if each element is a weight vector, $V = \langle v_1, \ldots, v_n \rangle$, and fewer than n weight vectors will not generate V. A representation of $\mathfrak{e}(2)$ with one generator is necessarily indecomposable (see Ref. 6) and their classification is trivial. They are classified according to the dimensions of the weight spaces since $\langle v \rangle \cong \langle w \rangle$ if and only if $\dim(\langle v \rangle_k) = \dim(\langle w \rangle_k)$, for all k.

In this paper, we will investigate the finite dimensional representations of $\mathfrak{e}(2)$ with two generators. In Sec. II we describe how we may associate to a representation V with generators v_1 and v_2 a graph $\mathcal{G}(V, v_1, v_2)$. Section III contains necessary notation, terminology, and preliminaries.

The graph of a representation is dependent on the choice of generators. In Sec. IV we describe

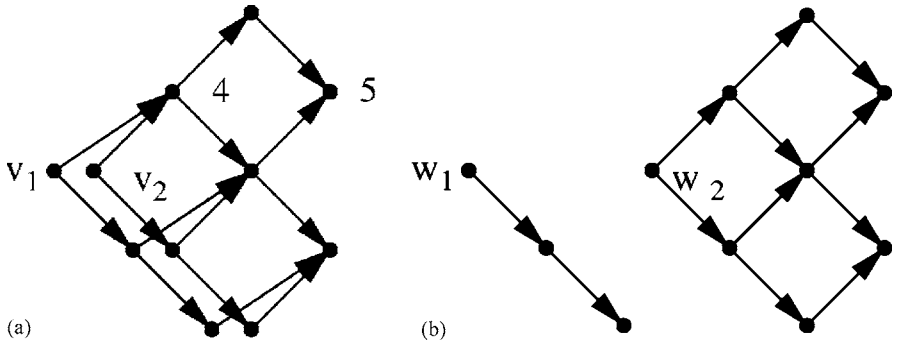

FIG. 1. Graphs (a) $\mathcal{G}(V,v_1,v_2)$, and (b) $\mathcal{G}(v,w_1,w_2)$.

an important type of graph of a representation called the *maximal form graph*. In Sec. V we present a criterion for the indecomposability of representations with two generators in terms of their maximal form graphs. In Sec. VI we derive a formula, the *generator change formula*, that describes how changing generators of a representation with two generators changes its graph. We then determine an invariant for indecomposable representations using the generator change formula and maximal form graphs.

In Sec. VII we classify the finite dimensional, indecomposable representations of dimensions 5 and 6 (regardless of the number of generators); in each case there are finitely many such representations (up to isomorphism). Those representations of dimension less than 5 were considered in Ref. 5. Next, we show that there are infinitely many nonequivalent indecomposable representations for all dimensions $\geqslant 8$.

II. THE GRAPH OF A REPRESENTATION OF $\mathfrak{e}(2)$

A representation of $\mathfrak{e}(2)$ may be completely described in term of generators and relations. Using this property, Repka and de Guise[10] introduced a method for graphically describing some finite dimensional representations of $\mathfrak{e}(2)$. According to this method, a finite dimensional representation is described by a graph with vertices and directed edges (or arrows); vertices at the same height form a basis of a weight space. Arrows pointing diagonally upwards represent the action of p_+ and arrows pointing diagonally downwards represent the action of p_-.

For example, the representation whose graph is in Fig. 1(a) has generators v_1 and v_2. We denote the graph $\mathcal{G}(V,v_1,v_2)$. The scalars, which can be any complex numbers, describe relations between v_1 and v_2. The relation in Fig. 1(a) is

$$p_+v_1 - 4p_+v_2 - 5p_+^2p_-v_2 = 0. \tag{4}$$

The scalars in the graph will always be associated with the generator with index 2.

Define $wt(v_i)$ to be the weight of v_i. Thus, in the case of Fig. 1(a), $wt(v_1)=wt(v_2)$.

Note that the graph of a representation is dependent on the choice of generators. For example, both Figs. 1(a) and 1(b) are graphs of the same representation. In Fig. 1(a) we have the graph $\mathcal{G}(V,v_1,v_2)$, and in Fig. 1(b) we have the graph $\mathcal{G}(V,w_1,w_2)$, where $w_1=v_1-4v_2-5p_+p_-v_2$, and $w_2=v_2$. $\mathcal{G}(V,w_1,w_2)$ is disconnected, reflecting the fact that the representation is decomposable with decomposition $\langle w_1\rangle \oplus \langle w_2\rangle$.

III. NOTATION, TERMINOLOGY AND PRELIMINARIES

Before we continue, we will introduce further notation and terminology and make preliminary remarks. Let V be a representation with generators v_1 and v_2. The generators will be indexed such that $wt(v_1) \geqslant wt(v_2)$. Define

$$H = wt(v_1) - wt(v_2). \tag{5}$$

Consider the relation

$$\sum_{i=0}^{N} p_+^{k+i} p_-^{l+i} W_i v_1 - \sum_{i=0}^{N} p_+^{m+i} p_-^{n+i} Z_i v_2 = 0, \tag{6}$$

where $Z_i, W_i \in \mathbb{C}$ and $Z_0, W_0 \neq 0$. Define invertible matrices

$$W = \begin{pmatrix} W_0 & W_1 & W_2 & \cdots & W_N \\ 0 & W_0 & W_1 & \cdots & W_{N-1} \\ 0 & 0 & W_0 & \cdots & W_{N-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & W_0 \end{pmatrix}, \quad Z = \begin{pmatrix} Z_0 & Z_1 & Z_2 & \cdots & Z_N \\ 0 & Z_0 & Z_1 & \cdots & Z_{N-1} \\ 0 & 0 & Z_0 & \cdots & Z_{N-2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & Z_0 \end{pmatrix}. \tag{7}$$

We shall write the relation in (6) as

$$p_+^k p_-^l W v_1 - p_+^m p_-^n Z v_2 = 0. \tag{8}$$

Writing relations in this form allows us to manipulate them easily. For example, multiplying both sides of (8) by W^{-1} gives

$$p_+^k p_-^l v_1 - p_+^m p_-^n W^{-1} Z v_2 = 0. \tag{9}$$

Let $\rho = gcd(p_+^k p_-^l, p_+^m p_-^n)$. Then Eq. (9) becomes

$$\rho(p_+^{k'} p_-^{l'} v_1 - p_+^{m'} p_-^{n'} W^{-1} Z v_2) = 0, \quad \text{for appropriate } k', m', l', n' \in \mathbb{N}. \tag{10}$$

Suppose we have a relation R of the form $\rho(p_+^{h_Z(1)} v_1 - p_+^{h_Z(0)} Z v_2) = 0$ where $h_Z(0), h_Z(1) \geqslant 0$ and by assumption $Z_0 \neq 0$. By a slight abuse of notation we shall often write the relation $\rho(p_-^{h_Z(1)} v_1 - p_+^{h_Z(0)} Z v_2) = 0$ as

$$R = \rho(p_-^{h_Z(1)} v_1 - p_+^{h_Z(0)} Z v_2). \tag{11}$$

The matrix Z of the relation is called a *relation matrix*. And, $h_Z(0)$ is called the *height* of the relation matrix Z. Of course, $h_Z(0)$ determines $h_Z(1)$ and vice versa since $H = h_Z(0) + h_Z(1)$.

Suppose $wt(v_1) > wt(v_2)$. Then, the relation in (11) is of *type 1* if $h_Z(1) > 0$ and $h_Z(0) > 0$; *type 2* if $h_Z(1) = 0$ and $h_Z(0) > 0$; *type 3* if $h_Z(1) > 0$ and $h_Z(0) = 0$.

Given relation matrices Z and W of the same height, define $\Delta(Z, W)$ to be the index of the first entries of Z and W that differ. The *gluing scalar* of a relation matrix is the leading entry (that is, the entry with index 0). A nonzero weight element $v \in V$ is *terminal* if $p_+ v = 0$ and $p_- v = 0$.

Given a matrix W as in (7), we will define a matrix $W[k]$ to be the matrix obtained by inserting k zero-columns on the left of W and removing the k rightmost columns of W. To illustrate this concept consider the following example:

$$\text{If } W = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \text{then } W[2] = \begin{pmatrix} 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{12}$$

Matrices of the form in (7) are called upper triangular Toeplitz matrices. For any such matrices W and Z, we have $(WZ)[k] = W[k]Z = WZ[k]$. Also note that $W[0] = W$.

IV. THE MAXIMAL FORM

As was mentioned above, the graph of a representation depends on the choice of generators. In this section we describe a particular choice of generators that will be used in the indecomposability criterion and for the invariant of indecomposable representations.

Let v_1 and v_2 be generators of a representation V such that $wt(v_1) \geqslant wt(v_2)$. Consider an arbitrary pair of generators w_1, w_2 of V such that $wt(v_1)=wt(w_1)$ and $wt(v_2)=wt(w_2)$. Recall $H=wt(v_1)-wt(v_2)$ and suppose

$$\dim(\langle v_1\rangle_k) \geqslant \max\{\dim(\langle w_1\rangle_k), \dim(\langle p_+^H w_2\rangle_k)\}, \tag{13}$$

$$\dim(\langle v_2\rangle_k) \geqslant \max\{\dim(\langle w_2\rangle_k), \dim(\langle p_-^H w_1\rangle_k)\}, \quad \forall\, k \in \mathbb{N}. \tag{14}$$

Then $\mathcal{G}(V, v_1, v_2)$ is in *maximal form*.

Note that every representation has a graph which is in maximal form; suppose that a representation V has generators v_1, v_2. Then, it is straightforward to show that $\mathcal{G}(V, v_1 - \lambda p_+^H v_2, p_-^H v_1 - \eta v_2)$ is in maximal form if λ and η are not zero, are not gluing scalars and $\lambda \neq \eta$.

The following lemma and Proposition 1 below establish several important properties of the maximal form that will be important in subsequent sections.

Lemma 1: Let V be a representation with generators v_1 and v_2 such that $wt(v_1) \geqslant wt(v_2)$. Suppose that $\mathcal{G}(V, v_1, v_2)$ is in maximal form. Then all relations are of type 1, 2, *or* 3.

Proof: Suppose there is a relation that is not of type 1, 2, or 3. We then have a relation

$$R_1 = \rho_1(v_1 - Z p_+^{H+l} p_-^l v_2), \tag{15}$$

or

$$R_2 = \rho_2(p_+^l p_-^{H+l} v_1 - Z v_2), \tag{16}$$

where $Z_0 \neq 0$ and $l > 0$. Assume there is a relation as in (15). Then

$$\langle \rho_1 v_1\rangle \cong \langle \rho_1 Z p_+^{H+l} p_-^l v_2\rangle. \tag{17}$$

Let

$$w_1 = v_1 - \lambda p_+^H v_2 \quad \text{and } w_2 = v_2, \tag{18}$$

where $\lambda \neq 0$ and if there are relation of the form $R=\rho(v_1 - W p_+^H v_2)$ such that $W_0 \neq 0$, then $\lambda \neq W_0$. Let $\rho_1 = p_+^s p_-^t$ and define $k = wt(v_1) + s - t$. Then, by (17) and (18),

$$\dim(\langle w_1\rangle_k) > \dim(\langle v_1\rangle_k). \tag{19}$$

This, however, contradicts the hypothesis that $\mathcal{G}(V, v_1, v_2)$ is maximal. Thus, we cannot have a relation as in (15) and we may show in a similar manner that we cannot have a relation as in (16). □

Consider graphs $\mathcal{G}(V, v_1, v_2)$ and $\mathcal{G}(U, u_1, u_2)$ in maximal form such that $wt(v_i)=wt(u_i)$ and $\langle v_i\rangle \cong \langle u_i\rangle$, for $i \in \{1,2\}$. A relation in $\mathcal{G}(U, u_1, u_2)$ is said to *correspond* to a relation in $\mathcal{G}(V, v_1, v_2)$ if they have the same weight.

Let the graphs $\mathcal{G}(V, v_1, v_2)$ and $\mathcal{G}(U, u_1, u_2)$ be in maximal form and $wt(v_i)=wt(u_i)$ for $i \in \{1,2\}$. Then, define

$$\mathcal{G}(V, v_1, v_2) \sim \mathcal{G}(U, u_1, u_2) \tag{20}$$

if

(1) $\langle v_i\rangle \cong \langle u_i\rangle$, for $i \in \{1,2\}$.
(2) There is a relation $R=\rho(p_-^{h_Z(1)} v_1 - Z p_+^{h_Z(0)} v_2)$ in $\mathcal{G}(V, v_1, v_2)$.

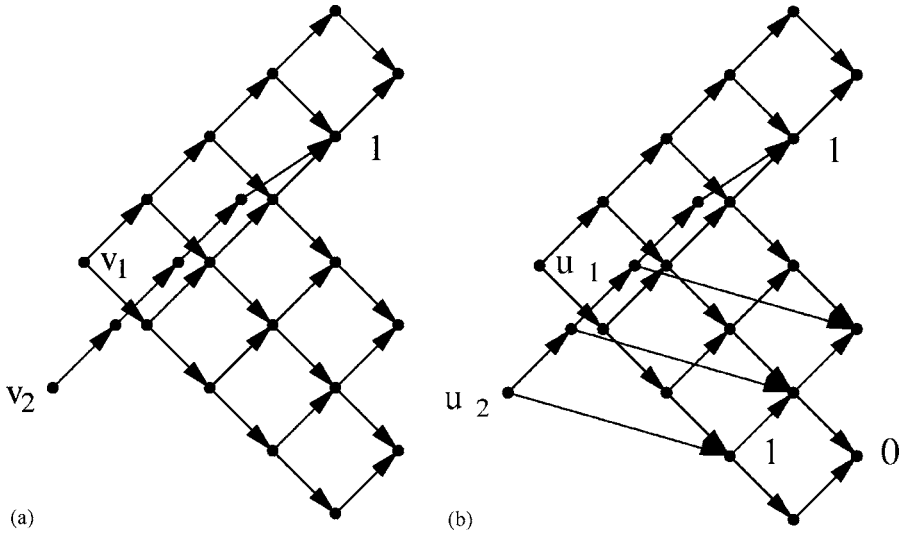

FIG. 2. Graphs of a representation (a) not in maximal form and (b) in maximal form.

($\Leftrightarrow$) There is a relation $S=\rho(p_-^{h_W(1)}u_1-Wp_+^{h_W(0)}u_2)$ in $\mathcal{G}(U,u_1,u_2)$, where R and S are corresponding relations.

Note that it is not necessary that $W=Z$, but if R and S correspond then necessarily $h_Z(0)=h_W(0)$ and $h_Z(1)=h_W(1)$ If $\mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(U,u_1,u_2)$, then these graphs are identical up to the scalar values in the relations.

Proposition 1: Let the graphs $\mathcal{G}(V,v_1,v_2)$ and $\mathcal{G}(U,u_1,u_2)$ be in maximal form. Then,

$$V\cong U\Rightarrow\mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(U,u_1,u_2). \tag{21}$$

Proof: Let $wt(v_1)=wt(u_1)\geqslant wt(u_2)=wt(v_2)$. Let w_1,w_2 be another set of generators of V such that $\mathcal{G}(V,w_1,w_2)$ is in maximal form, then we must have $\langle v_i\rangle_k=\langle w_i\rangle_k$ for $i=1,2$ and all $k\in\mathbb{N}$ by maximality. Hence, $\langle v_i\rangle\cong\langle w_i\rangle$ for $i=1,2$. It follows that

$$\langle v_i\rangle\cong\langle u_i\rangle,\quad i=1,2. \tag{22}$$

By Lemma 1, a relation of V must be of the form

$$R=\rho(p_-^{h_Z(1)}v_1-Zp_+^{h_Z(0)}v_2),\quad 0\leqslant h_Z(i)\leqslant H,\quad i\in\{1,2\}. \tag{23}$$

It suffices to show that if V has a relation as in (23) then U has a corresponding relation

$$S=\rho(p_-^{h_Z(1)}v_1-Wp_+^{h_Z(0)}v_2). \tag{24}$$

However, this follows from (22), consideration of dimensions and maximality. □

Unfortunately, if $\mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(U,u_1,u_2)$, then it is not necessarily true that $V\cong U$ (see Ref. 6). Further, if $V\cong U$ with $\mathcal{G}(V,v_1,v_2)$ and $\mathcal{G}(U,u_1,u_2)$ in maximal form then it is not necessarily true that $\mathcal{G}(V,v_1,v_2)=\mathcal{G}(U,u_1,u_2)$.

We end the section with an example of a maximal and a nonmaximal graph. Let V be a representation with generators v_1 and v_2 such that $wt(v_1)>wt(v_2)$ and graph as shown in Fig. 2(a). The graph is not in maximal form. But, if we let $u_1=v_1$ and $u_2=p_-^2v_1-v_2$ the graph is in maximal form [see Fig. 2(b)]. It will follow from the indecomposability criterion that V is indecomposable.

V. INDECOMPOSABILITY CRITERION

Let V be a representation with graph $\mathcal{G}(V,v_1,v_2)$ in maximal form. In this section we give a precise criterion under which V does or does not decompose. Equivalently, the criterion establishes when there exists a choice of generators u_1,u_2 for V such that $\mathcal{G}(V,u_1,u_2)$ is disconnected.

Let

$$w_1 = Av_1 + Bp_+^H v_2, \quad w_2 = Cp_-^H v_1 + Dv_2, \tag{25}$$

where $A=[a_i]$, $B=[b_i]$, $C=[c_i]$ and $D=[d_i]$ are upper triangular Toeplitz matrices. Then w_1 and w_2 generate V if and only if $a_0d_0 \neq b_{-H}c_{-H}$, where we define $b_i=0$, if $i<0$ (we similarly define a_i,c_i and d_i for $i<0$).

The indecomposability criterion is expressed in the following proposition.

Proposition 2: (a) *V is decomposable $\Leftrightarrow$ there is a generator change w_1,w_2 such that for each relation $\rho(p_-^{h(1)}v_1 - p_+^{h(0)}Zv_2)=0$ in the maximal graph $\mathcal{G}(V,v_1,v_2)$ either $\rho w_1=0$ or $\rho w_2=0$.*

(b) *Further, in the case of decomposability, $V=\langle w_1\rangle \oplus \langle w_2\rangle$.*

Proof: We first consider (a) ($\Leftarrow$) We will show that $V=\langle w_1\rangle \oplus \langle w_2\rangle$ [this will also establish (b)]. Consider the relation $\rho(p_-^{h(1)}v_1 - Zp_+^{h(0)}v_2)=0$. Since either $\rho w_1=0$ or $\rho w_2=0$ we have either $h(1)=0$ or $h(0)=0$, respectively.

Since $\mathcal{G}(V,v_1,v_2)$ is in maximal form, dimension considerations imply that no relations may be created as we change generators from v_1, v_2 to w_1, w_2; and no relation may be increased in length. Thus, it suffices to show that that for each relation of the form $\rho(v_1 - Zp_+^H v_2)=0$ or $\rho(p_-^H v_1 - Zv_2)=0$ we no longer have a relation between w_1 and w_2 of weight $wt(\rho w_1)$ or $wt(\rho w_2)$, respectively. This, however, follows from the fact that $\rho w_1=0$ or $\rho w_2=0$.

($\Rightarrow$) Suppose that V decomposes. Then for some generator change $w_1=Av_1+Bp_+^H v_2, w_2 = Cp_-^H v_1 + Dv_2$ we have $V=\langle w_1\rangle \oplus \langle w_2\rangle$. The generator change from v_1, v_2 to w_1, w_2 and the relation $\rho(p_-^{h(1)}v_1 - Zp_+^{h(0)}v_2)=0$ imply, via straightforward algebraic manipulation, that

$$\rho(C[h(0)]Z + D)p_-^{h(1)}w_1 = \rho(AZ + B[h(1)])p_+^{h(0)}w_2. \tag{26}$$

If both $C[h(0)]Z+D=0$ and $AZ+B[h(1)]=0$ then $a_0d_0=c_{-H}d_{-H}$ which is impossible since w_1,w_2 are generators. If both $C[h(0)]Z+D\neq 0$ and $AZ+B[h(1)]\neq 0$ then $\langle w_1\rangle \cap \langle w_2\rangle \neq 0$ which is impossible since $V=\langle w_1\rangle \oplus \langle w_2\rangle$.

Thus exactly one of $C[h(0)]Z+D=0$ or $AZ+B[h(1)]=0$. If $C[h(0)]Z+D=0$ then $h(0)=0$ and $a_0Z_0+b_{-H}\neq 0$ to satisfy $a_0d_0\neq c_{-H}d_{-H}$. Then $AZ+B[h(1)]$ is invertible so that (26) implies $\rho w_2=0$. Similarly if $AZ+B[h(1)]=0$ then $\rho w_1=0$ as required. □

Note that if a representation V is decomposable, its decomposition is unique up to isomorphism and permutation of components by the Krull-Schmidt theorem.[7]

The following corollaries express special cases of Proposition 2 which are often useful in practice.

Corollary 1: If $\mathcal{G}(V,v_1,v_2)$ has a type 1 relation then V is indecomposable.

Proof: Suppose that V were decomposable and let $\rho(p_-^{h(1)}v_1 - Zp_+^{h(0)}v_2)=0$ be a type 1 relation of $\mathcal{G}(V,v_1,v_2)$. Then, by Proposition 2, there would exist a generator change $w_1=Av_1 + Bp_+^H v_2, w_2=Cp_-^H v_1+Dv_2$ such that $\rho w_1=0$ or $\rho w_2=0$. However, since $h(0)>0$ and $h(1)>0$, this implies $a_0d_0=0=b_{-H}c_{-H}$, which contradicts the fact that w_1,w_2 is a set of generators. Hence, it must be the case that V is indecomposable. □

Corollary 2: If $H=0$ and $\mathcal{G}(V,v_1,v_2)$ has $\geqslant 3$ gluing scalars then V is indecomposable.

Proof: There are relations $R_i=\rho_i(v_1-\lambda_i v_2)$ for $i=1,2,3$ such that the λ_i are distinct. Suppose that V were to decompose. Then there would exist a generator change $w_1=Av_1+Bp_+^H v_2, w_2 = Cp_-^H v_1 + Dv_2$ as in Proposition 2. Then, by the above proposition, there must be two relations, say R_1 and R_2, such that either $\rho_1 w_1=0$ and $\rho_2 w_1=0$ or $\rho_1 w_2=0$ and $\rho_2 w_2=0$. Without loss of generality, assume the former. $\rho_1 w_1=0$ implies $\lambda_1=-b_0/a_0$ while $\rho_2 w_1=0$ implies $\lambda_2=-b_0/a_0$. This is impossible since then $\lambda_1\neq\lambda_2$. Hence it must be the case that V is indecomposable. □

Example: The graph in Fig. 3(a) is in maximal form. The relations in $\mathcal{G}(V,v_1,v_2)$ are

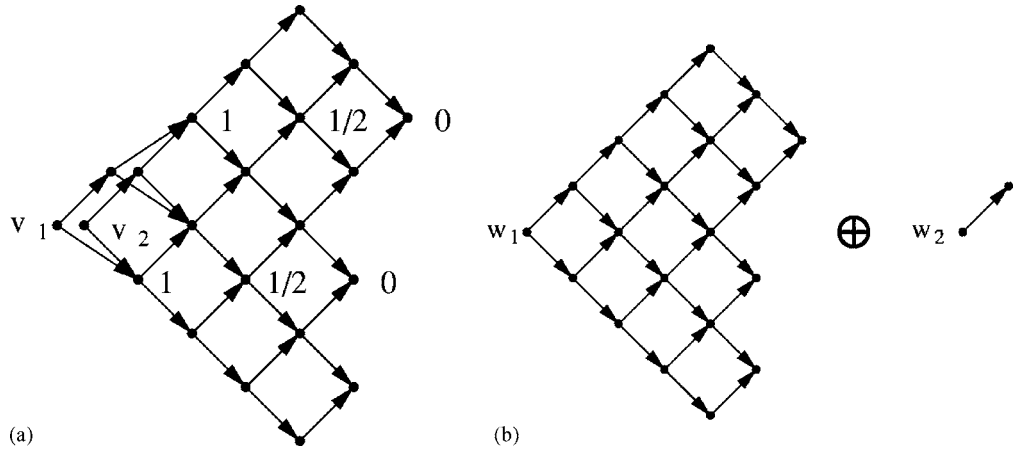

FIG. 3. (a) A decomposable graph and (b) its decomposition.

$$p_+^2\left(v_1-\begin{pmatrix}1 & \frac{1}{2}\\ 0 & 1\end{pmatrix}v_2\right)=0 \quad \text{and} \quad p_-\left(v_1-\begin{pmatrix}1 & \frac{1}{2}\\ 0 & 1\end{pmatrix}v_2\right)=0. \tag{27}$$

Consider the generator change $w_1=v_1$, and $w_2=v_1-v_2-\frac{1}{2}p_+p_-v_2$. Then $p_+^2w_2=0$ and $p_-w_2=0$. Thus, by Proposition 2, V decomposes as $\langle w_1\rangle\oplus\langle w_2\rangle$, as in Fig. 3(b).

Example: The graph $\mathcal{G}(V,v_1,v_2)$ in Fig. 4, which is in maximal form, has relations

$$\begin{gathered}p_+^5\left(v_1-\begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}p_+v_2\right)=0, \quad p_+^3p_-^2\left(v_1-\begin{pmatrix}1 & 2\\ 0 & 1\end{pmatrix}p_+v_2\right)=0,\\ p_-^5\left(p_-v_1-\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}v_2\right)=0.\end{gathered} \tag{28}$$

By Proposition 2, if V were to decompose there would be a generator change $w_1=Av_1+Bp_+v_2$, $w_2=Cp_-v_1+Dv_2$ such that $p_+^5w_1=0, p_+^3p_-^2w_1=0$ and $p_-^5w_2=0$. However, if $p_+^5w_1=0$, then $p_+^3p_-^2w_1=p_+^3p_-^2\left(v_1-\begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}p_+v_2\right)=p_+^5p_-^3v_2\neq 0$. Hence it must be the case that V is indecomposable.

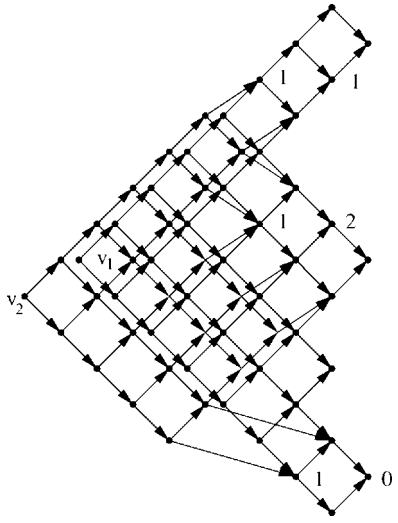

FIG. 4. An indecomposable graph.

VI. THE GENERATOR CHANGE TRANSFORMATION AND AN INVARIANT FOR INDECOMPOSABLE REPRESENTATIONS

In this section we describe an invariant for indecomposable representations. First we introduce a transformation on pairs of generators. Let

$$w_1 = Av_1 + Bp_+^H v_2, \quad w_2 = Cp_-^H v_1 + Dv_2 \tag{29}$$

be a generator change. The generator change from v_1, v_2 to w_1, w_2 induces a change of graphs from $\mathcal{G}(V, v_1, v_2)$ to $\mathcal{G}(V, w_1, w_2)$ which in turn induces a change in the relations and relation matrices. To this generator change we will also associate the transformation

$$\Gamma_{\{v_1,v_2\},\{w_1,w_2\}}(Z) = \frac{AZ + B[h(1)]}{C[h(0)]Z + D}, \tag{30}$$

where Z is an upper triangular Toeplitz matrix. In place of $\Gamma_{\{v_1,v_2\},\{w_1,w_2\}}$ we shall write Γ when no ambiguity arises. The transformation Γ is called the *generator change transformation*. After establishing preliminary results for generator change transformations we will construct an indecomposability criterion in Proposition 3 below.

Lemma 2: Suppose that V is an indecomposable representation with generators v_1, v_2 and $w_1 = Av_1 + Bp_+^H v_2, w_2 = Cp_-^H v_1 + Dv_2$ such that $\mathcal{G}(V, v_1, v_2)$ and $\mathcal{G}(V, w_1, w_2)$ are in maximal form. Then, $\mathcal{G}(V, v_1, v_2) \sim \mathcal{G}(V, w_1, w_2)$. Further, given a relation

$$\rho(p_-^{h(1)} v_1 - Z p_+^{h(0)} v_2) = 0 \tag{31}$$

in $\mathcal{G}(V, v_1, v_2)$, where $H = h(0) + h(1)$, the corresponding relation in $\mathcal{G}(V, w_1, w_2)$ is

$$\rho(p_-^{h(1)} w_1 - \Gamma(Z) p_+^{h(0)} w_2) = 0. \tag{32}$$

Note that by maximality, all relations are in the form of (31).

Proof: That $\mathcal{G}(V, v_1, v_2) \sim \mathcal{G}(V, w_1, w_2)$ follows from Proposition 1. And, as was mentioned above, the generator change $w_1 = Av_1 + Bp_+^H v_2, w_2 = Cp_-^H v_1 + Dv_2$ and the relation in (31), via straightforward algebraic manipulation, imply

$$\rho(C[h(0)]Z + D) p_-^{h(1)} w_1 = \rho(AZ + B[h(1)]) p_+^{h(0)} w_2. \tag{33}$$

If both $a_0 Z_0 + b_{-h(1)} = 0$ and $c_{-h(0)} Z_0 + d_0 = 0$ then we contradict $a_0 d_0 \neq c_{-H} d_{-H}$ which is a necessary condition for w_1, w_2 to be generators. If one of $a_0 Z_0 + b_{-h(1)} = 0$ or $c_{-h(0)} Z_0 + d_0 = 0$ then (33) contradicts Lemma 1. Thus $a_0 Z_0 + b_{-h(1)} \neq 0$ and $c_{-h(0)} Z_0 + d_0 \neq 0$, so that $C[h(0)]Z + D$ and $AZ + B[h(1)]$ are invertible, and

$$\rho p_-^{h(1)} w_1 = \rho \frac{AZ + B[h(1)]}{C[h(0)]Z + D} p_+^{h(0)} w_2 = \rho \Gamma(Z) p_+^{h(0)} w_2. \tag{34}$$

□

Lemma 3: Let v_1, v_2 and $w_1 = Av_1 + Bp_+^H v_2, w_2 = Cp_-^H v_1 + Dv_2$ be generators of a representation V. Further, let $\mathcal{G}(V, v_1, v_2)$ be in maximal form. If $a_0 Z_0 + b_{-h_Z(1)} \neq 0$ and $c_{-h_Z(0)} Z_0 + d_0 \neq 0$ for all relation matrices Z, then $\mathcal{G}(V, w_1, w_2)$ is also in maximal form.

Proof: Since $\mathcal{G}(V, v_1, v_2)$ is in maximal form, dimension considerations imply that no relations may be created as we change generators from v_1, v_2 to w_1, w_2. Hence to show that $\mathcal{G}(V, w_1, w_2)$ is in maximal form it suffices to show that no relations are shortened in length (they may not be lengthened by dimension considerations).

Consider the relation

$$\rho(p_-^{h(1)} v_1 - Z p_+^{h(0)} v_2) = 0. \tag{35}$$

As above we have,

$$\rho(C[h(0)]Z+D)p_-^{h(1)}w_1=\rho(AZ+B[h(1)])p_+^{h(0)}w_2. \tag{36}$$

Since $a_0Z_0+b_{-h_Z(1)}\neq 0$ and $c_{-h_Z(0)}Z_0+d_0\neq 0$, the matrices $C[h(0)]Z+D$ and $AZ+B[h(1)]$ are invertible thus the relation in (35) becomes

$$\rho p_-^{h(1)}w_1-\rho\frac{AZ+B[h(1)]}{C[h(0)]Z+D}p_+^{h(0)}w_2=0 \tag{37}$$

with the leading entry of $(AZ+B[h(1)])/(C[h(0)]Z+D)$ in $\mathbb{C}-\{0\}$, as required. □

The converse of Lemma 3 also holds, but will not be proved here. The next proposition determines an invariant for indecomposable representations.

Proposition 3: Let V and U be indecomposable representation with generators v_1,v_2 *and* u_1,u_2, *respectively, such that* $\mathcal{G}(V,v_1,v_2)$ *and* $\mathcal{G}(U,u_1,u_2)$ *are in maximal form. Then*

$$V\cong U\Leftrightarrow \mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(U,u_1,u_2), \tag{38}$$

and there exists a generator change Γ *such that* $\Gamma(Z)=W$ *for all corresponding relation matrices Z and W.*

Proof: ($\Rightarrow$) Suppose $V\cong U$, then Proposition 1 implies $\mathcal{G}(V,v_1,v_2),\sim\mathcal{G}(U,u_1,u_2)$. By equivalence, there must exist a generator change $w_1=Av_1+Bp_+^Hv_2, w_2=Cp_-^Hv_1+Dv_2$ such that $\mathcal{G}(V,w_1,w_2)=\mathcal{G}(U,u_1,u_2)$. Hence, by Lemma 2 we have a generator change transformation $\Gamma(Z)=(AZ+B[h(1)])/(C[h(0)]Z+D)=W$ for all corresponding relation matrices Z and W of $\mathcal{G}(V,v_1,v_2)$ and $\mathcal{G}(U,u_1,u_2)$, respectively.

($\Leftarrow$) Assume $\mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(U,u_1,u_2)$ and let Γ be a generator change such that $\Gamma(Z)=(AZ+B[h(1)])/(C[h(0)]Z+D)=W$, for all corresponding relation matrices Z and W.

Then, $w_1=Av_1+Bp_+^Hv_2, w_2=Cp_-^Hv_1+Dv_2$ are generators of V and the hypothesis of Lemma 3 is satisfied. Thus $\mathcal{G}(V,w_1,w_2)$ is in maximal form. Hence, by Proposition 1 $\mathcal{G}(V,v_1,v_2)\sim\mathcal{G}(V,w_1,w_2)$. It follows that $\mathcal{G}(V,w_1,w_2)\sim\mathcal{G}(U,u_1,u_2)$.

We have that $\Gamma(Z)=W$ is the relation in $\mathcal{G}(V,w_1,w_2)$ and in $\mathcal{G}(U,u_1,u_2)$ corresponding to Z in $\mathcal{G}(V,v_1,v_2)$. Hence $\mathcal{G}(V,w_1,w_2)\sim\mathcal{G}(U,u_1,u_2)$ with equal corresponding relations. That is, $\mathcal{G}(V,w_1,w_2)=\mathcal{G}(U,u_1,u_2)$. Thus $V\cong U$. □

Note that showing the existence of a generator change Γ such that $\Gamma(Z)=W$ for all corresponding relation matrices Z and W amounts to solving a system of linear equations in variables a_i,b_i,c_i, and d_i subject to the constraint $a_0d_0\neq b_{-H}c_{-H}$.

VII. CLASSIFICATION IN SMALL DIMENSION

In this section we classify the indecomposable representations of dimensions 5 and 6, regardless of the number of generators. In each case there are finitely many such representations (up to isomorphism). Next, we show that for all dimensions $\geqslant 8$ there are infinitely many nonequivalent indecomposable representations.

Any indecomposable representation V may be tensored with a character χ_r for $r\in\mathbb{Z}$ so that a weight space V_k with weight k becomes a weight space $V_k\otimes\chi_r$ of weight $k+r$. From here onward we shall assume that all indecomposable representations are renormalized so that their lowest weight is 0.

In Ref. 5, Cassinelli *et al.* describe a class $\mathcal{C}$ of indecomposable representations and classify the representations in this class of dimension $\leqslant 4$. The representations in $\mathcal{C}$ can be characterized as follows: $V\in\mathcal{C}$ if there exists a set of generators $v_1,v_2,\ldots,v_n$ such that $wt(v_i)>wt(v_{i+1})$ and $p_-^{\alpha_i}v_i=p_+^{\beta_i}v_{i+1}$ for $1\leqslant i\leqslant n-1$ and $\alpha_i,\beta_i\in\mathbb{N}_{>0}$.

The indecomposable representations in $\mathcal{C}$ of a given dimension are found by considering the connected graphs of the required dimension satisfying the characterization of the representations in $\mathcal{C}$ (and of course satisfying the requirement that $[p_-,p_+]=0$). These graphs are shown to be indecomposables and it is straightforward to show that two such representations are equivalent if and only if they have the same graph.[5]

Cassinelli *et al.* remark that they are uncertain whether or not all finite dimensional indecomposable representations are in $\mathcal{C}$. We illustrate below that there are indecomposable representations not in $\mathcal{C}$ for all dimensions $\geqslant 6$. In fact the most complicated representations (complicated in terms of creating an indecomposability criterion and classifying) are not contained in $\mathcal{C}$.

A. Classification in dimension 5

Figure 6 lists all five-dimensional representations in $\mathcal{C}$ and Proposition 4 below shows that all indecomposable representations of this dimension are contained in $\mathcal{C}$. In fact all indecomposable representation of dimension $\leqslant 5$ are in $\mathcal{C}$.

Figure 8 lists the indecomposable representations of dimension 6 in $\mathcal{C}$. There are two additional isomorphism classes which are not in $\mathcal{C}$; they are shown in Fig. 7. Figures 7 and 8 form a complete list of indecomposable, nonequivalent representations (Proposition 5 below).

The method described to assign graphs to representations with two generators may be generalized in a natural way to representations with an arbitrary number of generators, provided all relations among generators can be generated by pairwise relations between generators. We call such representations *graphical*. We will use the following lemma about graphical representations below.

Lemma 4: If V is indecomposable and dim$(V)\leqslant 6$ *then V is graphical.*

Proof: We consider just the case $\dim(V)=6$ and 3 generators since all other cases are similar and easier. Let v_1, v_2, and v_3 generate V with $wt(v_1)\geqslant wt(v_2)\geqslant wt(v_3)$.

Suppose that V is not graphical. Then we would have $\dim\{\rho_i v_i\}_{i=1,2,3}=2$ for some $\rho_i=p_+^{a_i}p_-^{b_i}$. It follows, by dimension considerations, that $p_+p_-v_i=0$ for all i. Hence, for each $i, \rho_i=p_+^{a_i}$ or $p_-^{b_i}$.

Suppose $a_i>0$ for all i. We would then have a relation $\Sigma_{i=1}^3\lambda_i p_+^{a_i}v_i=0$ with $\lambda_i\neq 0$ for all i. If this were the only relation required to describe all relations among the generators then $V=\langle v_3\rangle \oplus\langle v_1, \lambda_2 v_2+\lambda_3 p_+^{a_3-a_2}v_3\rangle$.

Suppose there is another relation among the generators. There is at most one other relation and it must be of the form $\eta_1 p_-^{c_1}v_1+\eta_2 p_-^{c_2}v_2+\eta_3 p_-^{c_3}v_3=0$ with exactly two of $\eta_i\neq 0$ (considering dimensions and $p_+p_-v_i=0$). Assume $\eta_1=0$ (other cases are similar). By dimension considerations, $wt(v_1)=wt(v_2)=wt(v_3)$ so that $a_1=a_2=a_3=1$. We have either $\dim\{p_+v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=1$ or 2. If $\dim\{p_+v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=1$ then $\langle \eta_2 v_2+\eta_3 v_3\rangle=\langle \lambda_2 v_2+\lambda_3 v_3\rangle$ and $V=\langle v_1, \eta_2 v_2+\eta_3 v_3\rangle\oplus\langle v_3\rangle$. If $\dim\{p_+v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=2$ then $V=\langle \eta_2 v_2+\eta_3 v_3\rangle\oplus\langle v_1, \lambda_2 v_2+\lambda_3 v_3\rangle$.

Similarly, if $b_i>0$ for all i then V would decompose. Now suppose that exactly two of $a_i>0$. Then we must have $b_1>0, a_2>0$ and $a_3>0$. Then we have a relation $\lambda_1 p_-^{b_1}v_1+\Sigma_{i=1}^2\lambda_i p_+^{a_i}v_i=0$ with $\lambda_i\neq 0$ for all i. If this is the only relation required to describe all relations among the generators then $V=\langle v_3\rangle\oplus\langle v_1, \lambda_2 v_2+\lambda_3 p_+^{a_3-a_2}v_3\rangle$.

Suppose there is another relation among the generators. There is at most one other relation and it must be of the form $\eta_2 p_-^{c_2}v_2+\eta_3 p_-^{c_3}v_3=0$ with $\eta_i\neq 0$ for all i (considering dimensions and $p_+p_-v_i=0$). By dimension considerations, $wt(v_2)=wt(v_3)$ and $a_1=b_2=b_3=1$. We have either $\dim\{p_-v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=1$ or 2. If $\dim\{p_-v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=1$ then $\langle \eta_2 v_2+\eta_3 v_3\rangle=\langle \lambda_2 v_2+\lambda_3 v_3\rangle$ and $V=\langle v_1, \eta_2 v_2+\eta_3 v_3\rangle\oplus\langle v_3\rangle$. If $\dim\{p_-v_1, \eta_2 p_+v_2+\eta_3 p_+v_3\}=2$ then $V=\langle \eta_2 v_2+\eta_3 v_3\rangle\oplus\langle v_1, \lambda_2 v_2+\lambda_3 v_3\rangle$.

Similarly, if exactly two of $b_i>0$ then V would decompose. Thus V, being indecomposable, is graphical. □

Proposition 4: Let V be an indecomposable representation with dim $(V)\leqslant 5$, *then* $V\in\mathcal{C}$.

Proof: Certainly there can be no more than five generators. If there were five generators, v_i for $i=1,2,3,\ldots,5$, then $\dim(V)=5$ and $V=\oplus_{i=1}^5\langle v_i\rangle$. If there is one generator then trivially $V\in\mathcal{C}$.

Suppose there were four generators. Let v_1, v_2, v_3, v_4 be a set of generators. If $\dim(V)=4$ then V would decompose as $V=\oplus_{i=1}^4\langle v_i\rangle$. Thus we must have $\dim(V)=5$.

By dimension considerations and indecomposability, for all i, $p_-v_i=0$, or $p_+v_i=0$; and p_-v_i, or p_+v_i is terminal. Thus, we must have $wt(v_i)=wt(v_j)$ for some $i\neq j$. Let $wt(v_1)=wt(v_2)$. We have either $p_+v_1-\lambda p_+v_2=0$ or $p_-v_1-\lambda p_-v_2=0$ for some $\lambda\in\mathbb{C}-\{0\}$. In either case, $V\cong\langle v_1-\lambda v_2\rangle \oplus\langle v_1, v_3, v_4\rangle$. Hence, V, being indecomposable, cannot have four generators.

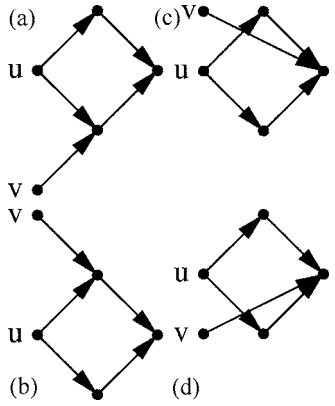

FIG. 5. The graphs $\mathcal{G}(V,u,v)$ of five dimensions such that $p_+p_-u\neq 0$.

Suppose that V has two generators. Let u and v generate V and suppose that $p_+p_-u\neq 0$. By dimension consideration we must then have $p_+p_-v=0, p_+^2p_-u=0$, and $p_+p_-^2u=0$. Then, V must be equivalent to one of the four graphs in Fig. 5.

The graphs in Figs. 5(a) and 5(b) are in $\mathcal{C}$. The graphs in Figs. 5(c) and 5(d) are decomposable; $V=\langle v-p_+u\rangle\oplus\langle u\rangle$ or $V=\langle v-p_-u\rangle\oplus\langle u\rangle$, respectively.

Now suppose that V has generators v_1,v_2 with $wt(v_1)\geqslant wt(v_2)$ such that $p_+p_-v_i=0$ for $i=1,2$. First let $wt(v_1)=wt(v_2)$. Then we may have relations of the form $p_+^av_1-\lambda p_+^av_2=0$ or $p_-^bv_1-\eta p_-^bv_2=0$.

If we have just the first relation then $V=\langle v_1-\lambda v_2\rangle\oplus\langle v_1\rangle$. If just the second then $V=\langle v_1-\eta v_2\rangle\oplus\langle v_1\rangle$. If we have both relations and $\lambda\neq\eta$ then $V=\langle v_1-\lambda v_2\rangle\oplus\langle v_1-\eta v_2\rangle$ while if $\lambda=\eta$ then $V=\langle v_1-\lambda v_2\rangle\oplus\langle v_2\rangle$.

Now suppose that $wt(v_1)>wt(v_2)$. If we have a relation $p_-^av_1-\lambda p_+^bv_2=0$ then we have no other relations and $V\in\mathcal{C}$. Otherwise we just have relations $p_-^av_1-\lambda p_-^bv_2=0$ or $p_+^cv_1-\eta p_+^dv_2=0$. If we have just the first relation then $V=\langle p_-^{a-b}v_1-\lambda v_2\rangle\oplus\langle v_1\rangle$. If just the second then $V=\langle v_1-\eta p_+^{d-c}v_1\rangle\oplus\langle v_2\rangle$. If both then $V=\langle v_1-\lambda p_+^{d-c}v_2\rangle\oplus\langle p_+^{a-b}v_1-\lambda v_2\rangle$.

Hence, if V has two generators than either $V\in\mathcal{C}$ or V is decomposable. The remaining case were V has three generators follows in an analogous manner to the two generator case and thus will not be considered. □

Figure 6 is a complete list of indecomposable, nonequivalent representations of dimension 5 in $\mathcal{C}$. Hence by Proposition 4 it is a complete list of all indecomposable, nonequivalent representations of this dimension.

B. Classification in dimension 6

Proposition 5: Let V be an indecomposable representation such that dim$(V)=6$ *then V is equivalent to one of the graphs in Fig.* 8 *or one of the six dimensional graphs in Fig.* 7 (*i.e.*, $k=0$ *in Fig.* 7).

Proof: Checking that $V\in\mathcal{C}$ if V does not have two generators follows as in the previous proof. Hence we will only show that if V has two generators then it is equivalent to one of the graphs in Fig. 8 or one of the six dimensional graphs in Fig. 7.

We first establish that we cannot have $wt(v_1)=wt(v_2)$. We may assume that $\mathcal{G}(V,v_1,v_2)$ is in maximal form so that $\langle v_1\rangle\cong\langle v_2\rangle$. Let T_i be the terminal space of $\langle v_i\rangle$ (i.e., $T_i=\{v\in\langle v_i\rangle : p_+v=0,\ p_-v=0\}$). By dimension considerations $\dim(T_i)\leqslant 2$ for $i=1,2$. Also by dimension considerations all relation matrices must be 1×1. Hence there can be at most two gluing scalars λ_1,λ_2 and all relations are in the form $\rho(v_1-\lambda_iv_2)=0$ for $i=1$ or 2. Hence, $V=\langle v_1\rangle\oplus\langle v_1-\lambda_1v_2\rangle$ in the case of one gluing scalar or $V=\langle v_1-\lambda_1v_2\rangle\oplus\langle v_1-\lambda_2v_2\rangle$ in the case of two gluing scalars.

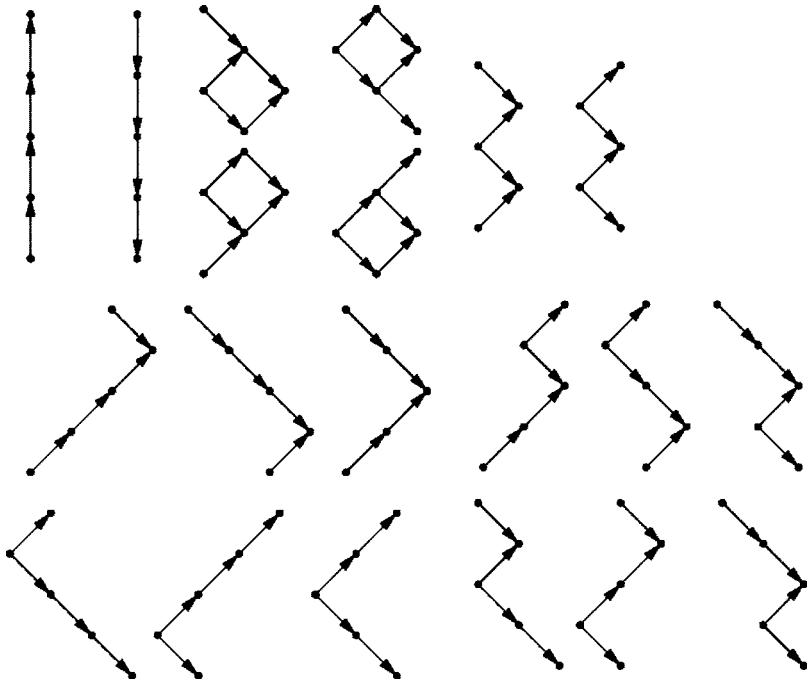

FIG. 6. The indecomposable representation of dimension 5.

Next we consider $wt(v_1) > wt(v_2)$. First suppose that $p_+p_-v_i=0$ for $i=1,2$. Then, we have only three possible relations; $p_+^{a_1}v_1-\lambda p_+^{a_2}v_2=0, p_-^{b_1}v_1-\lambda p_-^{b_2}v_2=0$ or $p_-^{c_1}v_1-\lambda p_+^{c_2}v_2=0$ for $\lambda \in \mathbb{C}-\{0\}$. If we have the last relation than we cannot have either of the other two and $V \in \mathcal{C}$. If we have one or both of $p_+^{a_1}v_1-\lambda_a p_+^{a_2}v_2=0, p_-^{b_1}v_1-\lambda_b p_-^{b_2}v_2=0$ then V decomposes. For instance if we have both then $V=\langle v_1-\lambda_a p_+^{a_2-a_1}v_2\rangle \oplus \langle p_-^{b_1-b_2}v_1-\lambda_b v_2\rangle$.

Now suppose that $p_+p_-v_1 \neq 0$. By dimension considerations $p_+^2p_-v_1=0$ and $p_+p_-^2v_1=0$. If V is not in $\mathcal{C}$ then the only possibility is that $p_+^2v_2-\lambda p_+p_-v_1=0$ for some $\lambda \in \mathbb{C}-\{0\}$ describes the relation between v_1 and v_2. We can always change generators to $w_1=v_1, w_2=\lambda v_2$ to get the first graph in Fig. 7. (By Corollary 1, it is indecomposable since it has a relation of type 1). The case where $p_+p_-v_2 \neq 0$ is similar. Hence we have shown that if $\dim(V)=6$ then either V decomposes or is equivalent to one of the graphs in Fig. 8 or one of the six-dimensional graphs in Fig. 7. □

The two graphs in Fig. 7 are clearly nonequivalent for any k. Figure 8 is a complete list of indecomposable, nonequivalent representations of dimension 6 in $\mathcal{C}$. Hence by Proposition 5, Figs. 8 and 7 form a complete list of all indecomposable, nonequivalent representations of this dimension.

Proposition 5 shows that not all indecomposable representations are in $\mathcal{C}$ for $\dim(V)=6$. In fact, for each dimension $\geqslant 6$ there are indecomposable representations not in $\mathcal{C}$. For example, the

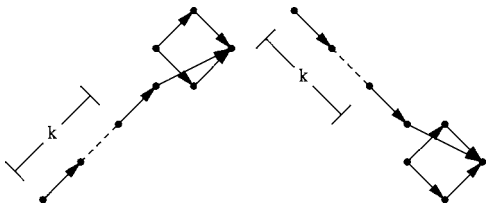

FIG. 7. Indecomposable representations of dimension $6+k$, for $k \in \mathbb{N}$, not in $\mathcal{C}$.

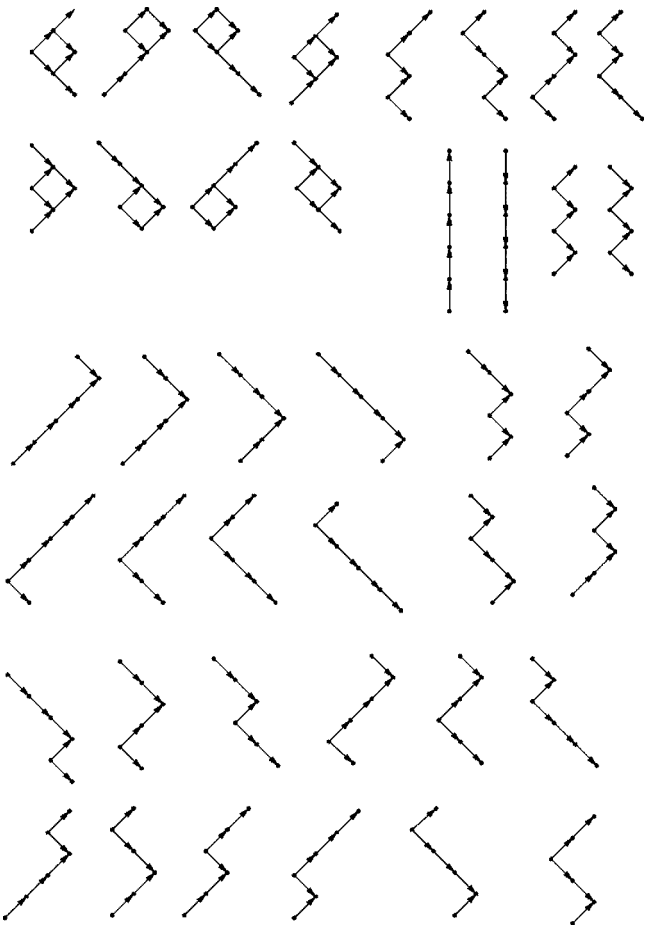

FIG. 8. The indecomposable representations of dimension 6 in $\mathcal{C}$.

representations in Fig. 7, which each have two generators, are $6+k$ dimensional for $k \in \mathbb{N}$. By Corollary 1, they are indecomposable since they have either a relation $p_+(p_-v_1 - p_+^{k+1}v_2)=0$ or $p_-(p_-^{k+1}v_1 - p_+v_2)=0$.

C. Higher dimensional representations

For each dimension $\geqslant 8$ there are infinitely many nonequivalent, indecomposable representations. The graph in Fig. 9 is from a representation V_z of dimension $8+k$ for $k \in \mathbb{N}$. The maximal graph $\mathcal{G}(V_z, v_1, v_2)$ has relations $p_+(p_-v_1 - p_+v_2)=0$ and $p_-(p_-v_1 - zp_+v_2)=0$. These relations are both type 1 and thus the representation is indecomposable (Corollary 1).

Proposition 6: $V_z \cong V_w \Leftrightarrow z=w$.

Proof: If $z=w$ then $\mathcal{G}(V_z, v_1, v_2)=\mathcal{G}(V_w, v_1, v_2)$ which implies $V_z \cong V_w$. Let $z \neq w$ and suppose that $V_z \cong V_w$. Then, by Proposition 3, we would have a generator change Γ such that $\Gamma(1)=1$ and $\Gamma(z)=w$. However, $\Gamma(1)=a_0 1/d_0=1$ thus $\Gamma(z)=a_0 z/d_0=z \neq w$; a contradiction. Hence, $z \neq w$ implies $V_z \ncong V_w$. □

Proposition 6 establishes that there are infinitely many nonequivalent indecomposable representations of dimension $8+k$ for $k \in \mathbb{N}$. We are uncertain if there are only finitely many indecomposable representations of dimension 7, but we conjecture that there are.

In a subsequent paper we will generalize the results of this paper pertaining to two generators to all graphical representations of $\mathfrak{e}(2)$. We will also classify all indecomposable representations having two generators.

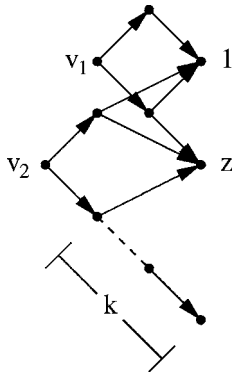

FIG. 9. The graph $\mathcal{G}(V_z, v_1, v_2)$ of dimension $8+k$ for $k \in \mathbb{N}$ and $z \in \mathbb{C}-\{0\}$.

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The exact correspondence between conserved quantities of a periodic box-ball system and string solutions of the Bethe ansatz equations

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We investigate the link between a periodic box-ball system (PBBS) and a solvable lattice model. Introducing a PBBS with an integer parameter corresponding to the dimensionality of the auxiliary space for the lattice model, we prove an important relationship between the conserved quantities of states of the PBBS and eigenvectors constructed through the string hypothesis. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A periodic box-ball system (PBBS) is a dynamical system of balls in a one-dimensional array of boxes with a periodic boundary condition. It can be obtained from the zero temperature limit of solvable lattice models which are generalizations of the six-vertex model.[1] In Ref. 2, we explained why the fundamental cycle of PBBS is obtained from the eigenvalues of the transfer matrix of the lattice model and conjectured an important relation between the string hypothesis of Bethe ansatz equation and the conserved quantities of PBBS. In this article, we prove this relation (Theorem 1.1) by introducing a positive integer parameter to the evolution rule of PBBS. As for the PBBS obeying this rule, we will shown the following properties: the time evolution rule is equivalent to an action of the transfer matrix of the solvable lattice model at the zero temperature limit (Theorem 2.1); the conserved quantities under the original time evolution rule of the PBBS are conserved under the new rule (Proposition 2.1).

In the rest of this section, we give definitions of the PBBS and the vertex models, and present the main theorem (Theorem 1.1). In Sec. II, we introduce yet another PBBS with the time evolution rule characterized by a positive integer, and we investigate its properties. In Sec. III, we prepare a proposition about eigenvalues of the transfer matrix in the zero temperature limit of the solvable lattice model, and prove Theorem 1.1. Section IV is devoted to the concluding remarks.

A. A periodic box-ball system

There may be many ways to describe the update rule of a periodic box-ball system.[1,3] Here we shall give yet another one. This is done in order that we may define a generalized model in Sec.

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II. We hope that the readers feel that things are clearly stated in the following description. The equivalent definition adopted in previous work is shown in the Appendix .

Let N and M be non-negative integers. Let $\Omega(N)$ be the set of all sequences of zeros and ones of length N, and let $\Omega_M(N)$ be the subset of $\Omega(N)$ consisting of sequences having exactly M 1's. That is,

$$\Omega(N) = \mathrm{Map}([N],\{0,1\}),$$

$$\Omega_M(N) = \{\boldsymbol{\alpha} | \boldsymbol{\alpha} \in \Omega(N), \# \boldsymbol{\alpha}^{-1}(\{1\}) = M\},$$

where $[N]=\{1,2,\ldots,N\}$, $\mathrm{Map}(A,B)$ denotes the set of all mappings of A into B, and $\#A$ the number of elements in a finite set A. We use $\boldsymbol{\alpha}$ to denote both the mapping $\boldsymbol{\alpha}:[N]\to\{0,1\}$ and a finite sequence $(\boldsymbol{\alpha}(1),\boldsymbol{\alpha}(2),\ldots,\boldsymbol{\alpha}(N))$.

In what follows, we always assume that $M<N/2$.

Let $\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\ldots,\alpha_N)\in\Omega_M(N)$. Let $\boldsymbol{\alpha}^{(0)}=\boldsymbol{\alpha}$, $N^{(0)}=N$, and $M^{(0)}=M$. For each $j=1,2,3,\ldots$, let $W^{(j)}$ be the set of all pairs of positions in $\boldsymbol{\alpha}^{(j-1)}$ where 0 follows 1. Because of the periodic boundary condition, this includes the case $\alpha_N=1$ and $\alpha_1=0$. By definition, $\#W^{(j)}$ is even; thus, define

$$p_j = \tfrac{1}{2}\# W^{(j)} \quad \text{and} \quad N^{(j)} = N^{(j-1)} - 2p_j;$$

let $n^{(j)}\in\mathrm{Map}([N^{(j)}],[N^{(j-1)}])$ be defined by

$$\{n^{(j)}(1),n^{(j)}(2),\ldots,n^{(j)}(N^{(j)})\} = [N^{(j-1)}]\setminus W^{(j)},$$

where $n^{(j)}(1)<n^{(j)}(2)<\cdots<n^{(j)}(N^{(j)})$; let $M^{(j)}=M^{(j-1)}-p_j$, and define a subsequence $\boldsymbol{\alpha}^j\in\Omega_{M^{(j)}}(N^{(j)})$ of $\boldsymbol{\alpha}^{(j-1)}$ by

$$\boldsymbol{\alpha}^{(j)} = \boldsymbol{\alpha}^{(j-1)}\circ n^{(j)}.$$

Let L be the integer uniquely determined by the condition

$$N^{(j-1)} > N^{(j)} \quad (j\le L) \quad \text{and} \quad N^{(j)} = N^{(L)} \quad (j\ge L).$$

Then we have

$$[N] = W^{(1)} \cup \left(\bigcup_{j=2}^{L} n^{(1)}(n^{(2)}(\cdots n^{(j-1)}(W^{(j)})\cdots)) \right)$$

$$\cup n^{(1)}(n^{(2)}(\cdots n^{(L-1)}(n^{(L)}([N^{(L)}]))\cdots)) \quad \text{(disjoint union)}.$$

For example, let $N=28$, $M=9$, and

$$\boldsymbol{\alpha} = (0,0,0,0,0,1,1,1,1,0,0,0,1,1,0,1,1,0,0,0,1,0,0,0,0,0,0,0).$$

Then we have

(1) $W^{(1)}=\{9,10,14,15,17,18,21,22\}$, $p_1=\frac{1}{2}\#W^{(1)}=4$,

$$N^{(1)} = N-2p_1 = 20, \quad M^{(1)} = M-p_1 = 5,$$

$$n^{(1)} = (1,2,3,4,5,6,7,8,11,12,13,16,19,20,23,24,25,26,27,28),$$

$$\boldsymbol{\alpha}^{(1)} = \boldsymbol{\alpha}\circ n^{(1)} = (0,0,0,0,0,1,1,1,0,0,1,1,0,0,0,0,0,0,0,0);$$

(2) $W^{(2)}=\{8,9,12,13\}$, $p_2=\frac{1}{2}\#W^{(2)}=2$,

$$N^{(2)} = N^{(1)}-2p_2 = 16, \quad M^{(2)} = M^{(1)}-p_2 = 3,$$

$$n^{(2)} = (1,2,3,4,5,6,7,10,11,14,15,16,17,18,19,20),$$

$$\boldsymbol{\alpha}^{(2)} = \boldsymbol{\alpha}^{(1)} \circ n^{(2)} = (0,0,0,0,0,1,1,0,1,0,0,0,0,0,0,0);$$

(3) $W^{(3)}=\{7,8,9,10\}$, $p_3=\frac{1}{2}\#W^{(3)}=2$,

$$N^{(3)} = N^{(2)} - 2p_3 = 12, \quad M^{(3)} = M^{(2)} - p_3 = 1,$$

$$n^{(3)} = (1,2,3,4,5,6,11,12,13,14,15,16),$$

$$\boldsymbol{\alpha}^{(3)} = \boldsymbol{\alpha}^{(2)} \circ n^{(3)} = (0,0,0,0,0,1,0,0,0,0,0,0);$$

(4) $W^{(4)}=\{6,7\}$, $p_4=\frac{1}{2}\#W^{(4)}=1$,

$$N^{(4)} = N^{(3)} - 2p_4 = 10, \quad M^{(4)} = M^{(3)} - p_4 = 0,$$

$$n^{(4)} = (1,2,3,4,5,8,9,10,11,12),$$

$$\boldsymbol{\alpha}^{(4)} = \boldsymbol{\alpha}^{(3)} \circ n^{(4)} = (0,0,0,0,0,0,0,0,0,0);$$

(5) For $k=5,6,7,\ldots$, $W^{(k)}=0$, $p_k=\frac{1}{2}\#W^{(k)}=0$,

$$N^{(k)} = N^{(k-1)} - 2p_k = 10, \quad M^{(k)} = M^{(k-1)} - p_k = 0,$$

$$n^{(k)} = (1,2,3,4,5,6,7,8,9,10),$$

$$\boldsymbol{\alpha}^{(k)} = \boldsymbol{\alpha}^{(k-1)} \circ n^{(k)} = (0,0,0,0,0,0,0,0,0,0);$$

hence, we obtain $L=4$ and the decomposition of $[28]=\{1,2,\ldots,28\}$

$$W^{(1)} \cup n^{(1)}(W^{(2)}) \cup n^{(1)}(n^{(2)}(W^{(3)}))$$

$$\cup n^{(1)}(n^{(2)}(n^{(3)}(W^{(4)}))) \cup n^{(1)}(n^{(2)}(n^{(3)}(n^{(4)}([N^{(4)}]))))$$

$$=\{9,10,14,15,17,18,21,22\} \cup \{8,11,16,19\} \cup \{7,12,13,20\}$$

$$\cup\{6,23\} \cup \{1,2,3,4,5,24,25,26,27,28\}.$$

Let $\bar{\mathbb{N}}=\mathbb{N}\cup\{\infty\}=\{1,2,3,\ldots\}\cup\{\infty\}$, and assume that $\infty > m$ for any number $m \in \mathbb{N}$. Define $\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\ldots,\lambda_N) \in \mathrm{Map}([N],\bar{\mathbb{N}})$ as follows:

$$\lambda_k = \begin{cases} 1 & \text{for } k \in W^{(1)} \\ j & \text{for } k \in n^{(1)}(n^{(2)}(\cdots n^{(j-1)}(W^{(j)})\cdots)) \quad (j=2,3,\ldots,L) \\ \infty & \text{otherwise.} \end{cases}$$

A *periodic box-ball system* (PBBS) is defined by the set $\Omega_M(N)$ whose elements are called *states* and a mapping T of $\Omega_M(N)$ into (in fact, onto) itself, which is called *time evolution*. For $\boldsymbol{\alpha} \in \Omega_M(N)$ and $k \in [N]$, we define

$$T(\boldsymbol{\alpha}) = (\alpha'_1, \alpha'_2, \ldots, \alpha'_N)$$

where

$$\alpha'_k = \begin{cases} 1-\alpha_k & \text{if } \lambda_k < \infty \\ \alpha_k & \text{if } \lambda_k = \infty \end{cases}.$$

For the above example,

$$\boldsymbol{\lambda} = (\infty, \infty, \infty, \infty, \infty, 4,3,2,1,1,2,3,3,1,1,2,1,1,2,3,1,1,4, \infty, \infty, \infty, \infty, \infty),$$

$$T(\boldsymbol{\alpha}) = (0,0,0,0,0,0,0,0,0,0,1,1,1,0,0,1,0,0,1,1,1,0,1,1,0,0,0,0,0).$$

Thus, the PBBS is a type of discrete dynamical system. The number N is called the number of boxes (or length of the system), and M is called the number of balls. We shall say that a state $\boldsymbol{\alpha} \in \Omega_M(N)$ has (or consists of) M balls.

It is convenient to write $\boldsymbol{\alpha}=(\alpha_1, \alpha_2, \ldots, \alpha_N) \in \Omega_M(N)$ as

$$\alpha_1 \alpha_2 \cdots \alpha_N;$$

for example

$$0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 1\ \ 1\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 0\ \ 1\ \ 1\ \ 0\ \ 0\ \ 0\ \ 1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0.$$

In a similar manner, we shall express $(\boldsymbol{\alpha}, \boldsymbol{\lambda})=(\alpha_1, \lambda_1), (\alpha_2, \lambda_2), \ldots, (\alpha_N, \lambda_N))$ as

$$\alpha_1^{\lambda_1}\ \alpha_2^{\lambda_2} \cdots \alpha_N^{\lambda_N};$$

for example

$$0^{\infty}0^{\infty}0^{\infty}0^{\infty}0^{\infty}1^4 1^3 1^2 1^1 0^1 0^2 0^3 1^3 1^1 0^1 1^2 1^1 0^1 0^2 0^3 1^1 0^1 0^4 0^{\infty}0^{\infty}0^{\infty}0^{\infty}0^{\infty},$$

or more simply

$$0\ 0\ 0\ 0\ 0\ 1^4 1^3 1^2 1^1 0^1 0^2 0^3 1^3 1^1 0^1 1^2 1^1 0^1 0^2 0^3 1^1 0^1 0^4 0\ 0\ 0\ 0\ 0$$

where ∞'s in the upper suffix are omitted.

The numbers p_j determined for a state $\boldsymbol{\alpha}$ by the above-noted procedure are conserved quantities of the PBBS;[3] that is, if we write $p_j(\boldsymbol{\alpha})$ for these numbers for a state $\boldsymbol{\alpha}$, then

$$p_j(T(\boldsymbol{\alpha})) = p_j(\boldsymbol{\alpha}) \quad \text{for } j = 1,2,3, \ldots, \text{ and for any } \boldsymbol{\alpha} \in \Omega_M(N).$$

Since, by definition,

$$p_1 \geq p_2 \geq p_3 \geq \ldots, \quad \text{and} \quad \sum_j p_j = M,$$

the sequence of conserved quantities $\boldsymbol{p}=(p_1, p_2, p_3, \ldots)$ is a partition of the integer M.

We shall not distinguish a partition $\boldsymbol{p}$ and a Young diagram, the array of squares left justified in decreasing order (p_1 squares in the top row, p_2 in the second row, and so on). The *conjugate* of a partition $\boldsymbol{p}$ is the partition $\boldsymbol{p}'=(p'_1, p'_2, p'_3, \ldots)$ defined by

$$p'_j = \#\{i | i \geq 1 \text{ and } p_i \geq j\};$$

or equivalently, in terms of Young diagrams, $\boldsymbol{p}'$ is the transpose of the diagram $\boldsymbol{p}$. An example is shown in Fig. 1.

Let Y be a Young diagram; we define a subset $\Omega_M^Y(N)$ of $\Omega_M(N)$ by

$$\Omega_M^Y(N) = \{\boldsymbol{\alpha} \in \Omega_M(N) | \boldsymbol{p}(\boldsymbol{\alpha}) \text{ is the conjugate of } Y\}.$$

In what follows, we shall often write $\Omega_M, \Omega_M^Y, \ldots$ for $\Omega_M(N), \Omega_M^Y(N), \ldots$, respectively, when their N-dependence is apparent.

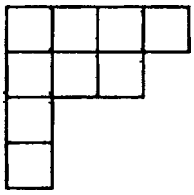

FIG. 1. Young diagram whose conjugate corresponds to the partition (4,2,2,1).

B. The vertex models

The six-vertex model and its higher spin generalizations are defined by the so-called R-matrices $R^{(\ell,\ell')}:\mathbb{C}^{\ell+1}\otimes\mathbb{C}^{\ell'+1}\to\mathbb{C}^{\ell+1}\otimes\mathbb{C}^{\ell'+1}$,

$$R^{(\ell,\ell')}(|i'\rangle\otimes|j'\rangle)=\sum_{i=0}^{\ell}\sum_{j=0}^{\ell'}\langle i,j|R^{(\ell,\ell')}|i',j'\rangle(|i\rangle\otimes|j\rangle),$$

where $\{|i\rangle|i=0,1,\ldots,\ell\}$ and $\{|j\rangle|j=0,1,\ldots,\ell'\}$ are bases of $\mathbb{C}^{\ell+1}$ and $\mathbb{C}^{\ell'+1}$, respectively. The R-matrices are parametrized by two parameters, x and q. We follow the parametrization given in Ref. 4. For $\ell'=1$, the parametrization of $R^{(\ell,1)}=R^{(\ell,1)}[x;q]$ we need is given by

(i) for $k=0,1,\ldots,\ell$,

$$\langle k,1|R^{(\ell,1)}[x;q]|k,1\rangle=\frac{q^{\ell-k}x-q^{k+1}x^{-1}}{x-q^{\ell+1}x^{-1}},$$

$$\langle k,0|R^{(\ell,1)}[x;q]|k,0\rangle=\frac{q^{k}x-q^{\ell-k+1}x^{-1}}{x-q^{\ell+1}x^{-1}};$$

(ii) for $k=1,2,\ldots,\ell$,

$$\langle k-1,1|R^{(\ell,1)}[x;q]|k,0\rangle=\langle k,0|R^{(\ell,1)}[x;q]|k-1,1\rangle$$

$$=\frac{\sqrt{(1-q^{2k})(1-q^{2(\ell-k+1)})}}{x-q^{\ell+1}x^{-1}};$$

(iii) otherwise, $\langle i,j|R^{(\ell,1)}[x;q]|i',j'\rangle=0$,

where x and q are called the spectral parameter and the deformation parameter, respectively. The matrix $R^{(1,\ell)}[x;q]$ is related to $R^{(\ell,1)}[x;q]$ by

$$R^{(1,\ell)}[x;q]=P^{(\ell,1)}R^{(\ell,1)}[x;q]P^{(1,\ell)},$$

where $p^{(m,n)}:\mathbb{C}^{m+1}\otimes\mathbb{C}^{n+1}\to\mathbb{C}^{n+1}\otimes\mathbb{C}^{m+1}$ is the permutation

$$P^{(m,n)}(|i\rangle\otimes|j\rangle)=|j\rangle\otimes|i\rangle.$$

For $\ell=1,2,3,\ldots$, we define the transfer matrix $\hat{t}_\ell[x;q]:V\to V(V:=\underbrace{\mathbb{C}^2\otimes\mathbb{C}^2\otimes\ldots\otimes\mathbb{C}^2}_{N})$ by

$$\hat{t}_\ell[x;q](|i_1'\rangle\otimes|i_2'\rangle\otimes\ \ldots\ \otimes|i_N'\rangle)$$

$$=\sum_{i_1,i_2,\ldots,i_N\in\{0,1\}}\langle i_1,i_2,\ldots,i_N|\hat{t}_\ell[x;q]|i_1',i_2',\ldots,i_N'\rangle(|i_1\rangle\otimes|i_2\rangle\otimes\ \ldots\ \otimes|i_N\rangle),$$

$$\langle i_1, i_2, \ldots, i_N | \hat{t}_\ell[x;q] | i'_1, i'_2, \ldots, i'_N \rangle$$

$$:= \sum_{j_1, j_2, \ldots, j_N = 0}^{\ell} \langle i_N, j_1 | R^{(1,\ell)}[x;q] | i'_N, j_N \rangle \langle i_{N-1}, j_N | R^{(1,\ell)}[x;q] | i'_{N-1}, j_{N-1} \rangle$$

$$\ldots \langle i_2, j_3 | R^{(1,\ell)}[x;q] | i'_2, j_2 \rangle \cdot \langle i_1, j_2 | R^{(1,\ell)}[x;q] | i'_1, j_1 \rangle .$$

The transfer matrices for different x's and ℓ's commute with each other by virtue of the Yang-Baxter relation which the R matrices obeys; that is,

$$\hat{t}_\ell[x;q]\hat{t}_{\ell'}[x';q] = \hat{t}_{\ell'}[x';q]\hat{t}_\ell[x;q] \quad \text{for any } \ell, \ell', x, \text{ and } x' .$$

Let $V_M := \mathrm{span}\{|i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle \in V \,|\, i_1 + i_2 + \ldots i_N = M\}$. Since the R-matrix obeys the so-called ice condition

$$\langle i, j | R^{(1,\ell)} | i', j' \rangle = 0 \quad \text{unless } i + j = i' + j' ,$$

$\hat{t}_\ell[x;q]$ maps V_M into itself.

Let $|\varphi\rangle$ be a vector in V of the form

$$|\varphi\rangle = |\varphi; \{x_j\}_{j=1}^M\rangle = C[x_1;q]C[x_2;q]\cdots C[x_M;q](|0\rangle \otimes |0\rangle \otimes \cdots \otimes |0\rangle),$$

where $C[x;q]: V \to V$ is a creation operator in the algebraic Bethe ansatz method.[5] Assume that the additional parameters $x_1, x_2, \ldots, x_M$ are mutually distinct and satisfy the so-called Bethe ansatz equation (BAE),

$$\left(\frac{q^{-1}x_k - q x_k^{-1}}{x_k - x_k^{-1}} \right)^N = \prod_{\substack{j=1 \\ j \neq k}}^{M} \frac{q^{-1}x_k x_j^{-1} - q x_k^{-1} x_j}{q x_k x_j^{-1} - q^{-1} x_k^{-1} x_j} \quad (k = 1, 2, \ldots, M). \tag{1}$$

Then it follows that $\hat{t}_\ell[x;q]|\varphi\rangle = \Lambda_\ell[x;\{x_j\};q]|\varphi\rangle$, where

$$\Lambda_\ell[x;\{x_j\};q] = \sum_{k=0}^{\ell} \left(\frac{q^k x - q^{\ell-k+1}x^{-1}}{x - q^{\ell+1}x^{-1}} \right)^N \prod_{j=1}^{M} \frac{(q^{-1}x_j^2)x^{-2} - q^{-\ell-2} - q^\ell + q^{-2}(q^{-1}x_j^2)^{-1}x^2}{q^{\ell-2k}(q^{-1}x_j^2)x^{-2} - 1 - q^{-2} + q^{2k-\ell-2}(q^{-1}x_j^2)^{-1}x^2}. \tag{2}$$

We are interested in these solutions at $q = 0$. We make use of the string hypothesis:[6]

Definition 1.1: *Let Y be the Young diagram, which represents a partition of M*

$$(\underbrace{m_1, m_1, \ldots, m_1}_{K_1}, \underbrace{m_2, m_2, \ldots, m_2}_{K_2}, \ldots, \underbrace{m_s, m_s, \ldots, m_s}_{K_s}), \tag{3}$$

where $m_1 < m_2 < \cdots < m_s$ and $K_i > 0 (i = 1, 2, \ldots, s)$ (Fig. 2). Then, the string hypothesis is the assumption that any solution $\{x_j\}_{j=1}^M$ to the BAE (1) is expressed as $\{x_{i\alpha k}\}$ of the form

$$(x_{i\alpha k}(q))^2 = q^{m_i - 2k + 2}(z_{i\alpha}^0 + O(q))$$

$$(i = 1, 2, \ldots, s;\ \alpha = 1, 2, \ldots, K_i;\ k = 1, 2, \ldots, m_i).$$

If all the eigenvectors can be obtained by the string hypothesis, the space V_M decomposes into subspaces $V_M^Y(q)$:

$$V_M = \bigoplus_Y V_M^Y(q),$$

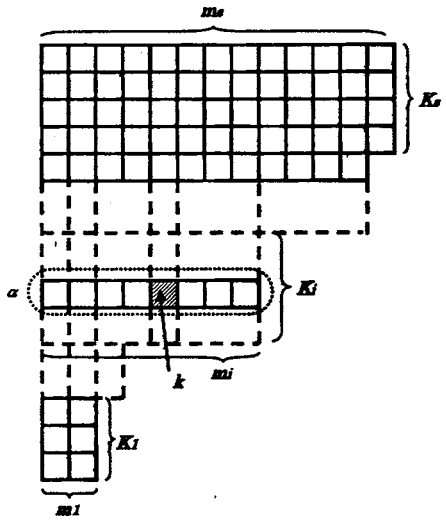

FIG. 2. The Young diagram corresponding to (3).

$$V_M^Y(q) = \mathrm{span}\{|\varphi;\{x_{i\alpha k}\}\rangle | \{x_{i\alpha k}\} \in S_Y\},$$

where S_Y is the set of all solutions to the BAE under the string hypothesis for a given Young diagram Y.

C. A statement of the main theorem

Let $V_M^Y := \lim_{q\to 0} V_M^Y(q)$. A 0,1 sequence $\boldsymbol{\alpha} \in \Omega_M$ corresponds to a monomial in V_M by the mapping $\iota: \Omega_M \to V_M$ defined by

$$\iota(\boldsymbol{\alpha}) = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ \ldots \ \otimes |\alpha_N\rangle,$$

and so we can identify V_M with the space spanned by vectors in $\iota(\Omega_M)$:

$$V_M = \mathrm{span}\ \iota(\Omega_M).$$

In this article, we prove the following theorem concerning this identification.

Theorem 1.1: *If the string hypothesis in Definition 1.1 is true, then*

(i) $V_M^Y \subset \mathrm{span}\iota(\Omega_M^Y)$.
Furthermore, if all the eigenvectors can obtained by the string hypothesis, the stronger condition
(ii) $V_M^Y = \mathrm{span}\ \iota(\Omega_M^Y)$
holds.

The above statements were conjectured in Ref. 2.

II. A PBBS WITH CARRIER AND THE VERTEX MODEL

In this section, we consider a class of PBBSs which obey different time evolution rules characterized by a positive integer parameter.

Let ℓ be a positive integer. A *periodic box-ball system with carrier (PBBSC) of capacity* ℓ is defined again by the set $\Omega_M(N)$ and a mapping $T_\ell: \Omega_M(N) \to \Omega_M(N)$ whose definition is given in the following.

In Sec. I we defined a sequence $\mathbf{\lambda}$ in $\bar{\mathbb{N}}$ for each state $\boldsymbol{\alpha} \in \Omega(N)$ and in this section we will define another sequence $\bar{\mathbf{\lambda}}$ in $\bar{\mathbb{N}}$. Both $\mathbf{\lambda}$ and $\bar{\mathbf{\lambda}}$ will be necessary to define the time evolution T_ℓ.

Still we are assuming that $M<N/2$. Let $\boldsymbol{\alpha}\in\Omega_M(N)$. Let $\bar{\boldsymbol{\alpha}}^{(0)}=\boldsymbol{\alpha}$, $N^{(0)}=N$, and $M^{(0)}=M$. For each $j=1,2,3,\ldots$, let $\bar{W}^{(j)}$ be the set of all pairs of positions in $\bar{\boldsymbol{\alpha}}^{(j-1)}$ where 1 follows 0; note that $\#\bar{W}^{(j)}=\#W^{(j)}=2p_j$; let $N^{(j)}=N^{(j-1)}-2p_j$ as before; let $\bar{n}^{(j)}\in\mathrm{Map}(N^{(j)},N^{(j-1)})$ be defined by

$$\{\bar{n}^{(j)}(1),\bar{n}^{(j)}(2),\ldots,\bar{n}^{(j)}(N^{(j)})\}=[N^{(j-1)}]\setminus\bar{W}^{(j)},$$

where $\bar{n}^{(j)}(1)<\bar{n}^{(j)}(2)<\cdots<\bar{n}^{(j)}(N^{(j)})$; define a subsequence $\bar{\boldsymbol{\alpha}}^{(j)}\in\Omega_{M^{(j)}}(N^{(j)})$ of $\bar{\boldsymbol{\alpha}}^{(j-1)}$ by

$$\bar{\boldsymbol{\alpha}}^{(j)}=\bar{\boldsymbol{\alpha}}^{(j-1)}\circ\bar{n}^{(j)}.$$

We again have a decomposition of $[N]$ into a disjoint union

$$[N]=\bar{W}^{(1)}\cup\left(\bigcup_{j=2}^{L}\bar{n}^{(1)}(\bar{n}^{(2)}(\cdots\bar{n}^{(j-1)}(\bar{W}^{(j)})\cdots))\right)\cup\bar{n}^{(1)}(\bar{n}^{(2)}(\cdots\bar{n}^{(L-1)}(\bar{n}^{(L)}([N^{(L)}]))\cdots)).$$

Define $\bar{\boldsymbol{\lambda}}\in\mathrm{Map}([N],\bar{\mathbb{N}})$ by

$$\bar{\lambda}_k=\begin{cases}1 & \text{for } k\in\bar{W}^{(1)}\\ j & \text{for } k\in\bar{n}^{(1)}(\bar{n}^{(2)}(\cdots\bar{n}^{(j-1)}(\bar{W}^{(j)})\cdots)) \quad (j=2,3,\ldots,L)\\ \infty & \text{otherwise.}\end{cases}$$

Then the time evolution T_ℓ is defined by

$$T_\ell(\boldsymbol{\alpha})=(\alpha'_1,\alpha'_2,\ldots,\alpha'_N),$$

where

$$\alpha'_k=\begin{cases}1 & \text{if } \alpha_k=0 \text{ and } \lambda_k\le\ell\\ 0 & \text{if } \alpha_k=1 \text{ and } \bar{\lambda}_k\le\ell\\ \alpha_k & \text{otherwise}\end{cases}$$

for $\bar{\boldsymbol{\alpha}}\in\Omega_M(N)$ and $k\in[N]$.

As before, we shall express $(\boldsymbol{\alpha},\boldsymbol{\lambda},\bar{\boldsymbol{\lambda}})=((\alpha_1,\lambda_1,\bar{\lambda}_1),(\alpha_2,\lambda_2,\bar{\lambda}_2),\ldots,(\alpha_N,\lambda_N,\bar{\lambda}_N))$ as

$$\alpha_{1\,\bar{\lambda}_1}^{\lambda_1}\alpha_{2\,\bar{\lambda}_2}^{\lambda_2}\cdots\alpha_{N\,\bar{\lambda}_N}^{\lambda_N};$$

for example,

$$0_\infty^\infty 0_4^\infty 0_3^\infty 0_2^\infty 0_1^\infty 1_1^4 1_2^3 1_3^2 1_4^1 0_3^1 0_2^2 0_1^3 1_1^3 1_2^1 0_1^1 1_1^2 1_3^1 0_\infty^1 0_\infty^2 0_1^3 1_1^1 0_\infty^1 0_\infty^4 0_\infty^\infty 0_\infty^\infty 0_\infty^\infty 0_\infty^\infty, \tag{4}$$

or more simply

$$0\ 0\ 0\ 0\ 0\ 0\ 1_1 1_2 1_3 1_4 0^1 0^2 0^3 1_1 1_2 0^1 1_1 1_3 0^1 0^2 0^3 1_1 0^1 0^4 0\ 0\ 0\ 0\ 0,$$

where only upper suffices of 0's and lower suffices of 1's are indicated.

From the definition of $\hat{t}_\ell[x;q]$ in the previous section, the action of $\hat{t}_\ell[x]:=\lim_{q\to0}\hat{t}_\ell[x;q]$ ($\ell=1,2,3,\ldots$) on a monomial $|\psi\rangle:=|i_1\rangle\otimes|i_2\rangle\otimes\cdots\otimes|i_N\rangle$ is

$$\hat{t}_\ell[x]|\psi\rangle=\sum_{\substack{i'_1,i'_2,\ldots\\ \ldots,i'_N\in\{0,1\}}}\sum_{y_0=0}^{\ell}\sum_{y_1=0}^{\ell}\cdots\sum_{y_N=0}^{\ell}(R^{i_1 i'_1}_{y_0 y_1}[x]R^{i_2 i'_2}_{y_1 y_2}[x]\cdots R^{i_N i'_N}_{y_{N-1} y_N}[x])$$

$$\times \delta_{y_0,y_N}|i_1'\rangle \otimes |i_2'\rangle \otimes \cdots \otimes |i_N'\rangle,$$

where

$$R_{yy'}^{ii'}[x] = \begin{cases} 1 & (i,y;i',y') = (1,\ell\,;1,\ell\,) \text{ or } (0,0;0,0) \\ 1/x & (i,y;i',y') = (1,k;0,k+1\ell) \text{ or } (0,k+1;1,k) \\ & (k=0,1,\ldots,\ell-1) \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Hereafter, for simplicity, we write $\hat{t}_\ell := \hat{t}_\ell[1]$ and $R_{yy'}^{ii'} := R_{yy'}^{ii'}[1]$.

Proposition 2.1:

$$\iota(T_\ell(\boldsymbol{\alpha})) = \hat{t}_\ell(\iota(\boldsymbol{\alpha})) \quad (\boldsymbol{\alpha} \in \Omega_M).$$

The following lemma guarantees that the vector $\hat{t}_\ell(\iota(\boldsymbol{\alpha}))$ is a monomial.

Lemma 2.1: *If $|\psi\rangle \in V$ is a monomial, then $\hat{t}_\ell|\psi\rangle$ is a monomial.*

Proof. From (5), we find that, for given i and y, there is one and only one pair (i',y') which satisfies $R_{yy'}^{ii'}=1$. Hence, for a given $(N+1)-\text{tuple}(y_0;i_1,i_2,\ldots,i_N)$, there exists one and only one $2N$-tuple $(y_1,y_2,\ldots,y_N;i_1',i_2',\ldots,i_N')$ which satisfies

$$R_{y_0y_1}^{i_1i_1'} R_{y_1y_2}^{i_2i_2'} R_{y_2y_3}^{i_3i_3'} \cdots R_{y_{N-1}y_N}^{i_Ni_N'} = 1. \tag{6}$$

Thus $(y_N;i_1',i_2',\ldots,i_N')$ is determined uniquely from the condition (6). Denote the induced mapping $(y_0;i_1,i_2,\ldots,i_N) \mapsto (y_N;i_1',i_2',\ldots,i_N')$ by

$$(y_0;\boldsymbol{i}) \mapsto (\tilde{y}(y_0;\boldsymbol{i});\tilde{\boldsymbol{i}}(y_0;\boldsymbol{i})) \tag{7}$$

where $\boldsymbol{i}=(i_1,i_2,\ldots i_N)$. [Furthermore, from a symmetry property of $R: R_{yy'}^{ii'} = R_{y'y}^{i'i}$ (for any i,i',y and y'), we can show that (7) is one-to-one.] If $|\boldsymbol{i}\rangle$ denotes a monomial $|i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$ then we have

$$\hat{t}_\ell|\boldsymbol{i}\rangle = \sum_{y_0=0}^{\ell} \delta_{y_0\tilde{y}(y_0;\boldsymbol{i})}|\tilde{\boldsymbol{i}}(y_0;\boldsymbol{i})\rangle$$

where $|\tilde{\boldsymbol{i}}(y_0;\boldsymbol{i})\rangle = |i_1'\rangle \otimes |i_2'\rangle \otimes \cdots \otimes |i_N'\rangle$. Hence it is enough to show that there is one and only one $y_0 (0 \le y_0 \le \ell\,)$ which satisfies $y_0=\tilde{y}(y_0;\boldsymbol{i})$.

Noticing the fact that the condition (5) determines $y_1,y_2,\ldots,y_N$ successively from y_0, we can easily find that there exist integers $a,b,c (0 \le a < b \le c \le \ell\,)$ such that

$$\tilde{y}(y_0;\boldsymbol{i}) = \begin{cases} a & (0 \le y_0 \le b) \\ y_0 + a - b & (b \le y_0 \le c) \\ a - b + c & (c \le y_0 \le \ell\,); \end{cases}$$

see Figs. 3 and 4. Therefore $y_0=\tilde{y}(y_0;\boldsymbol{i})$ if and only if $y_0=a$, which completes the proof. □

Corollary 2.1: *The operator $\hat{t}_\ell$ is invertible.*

Proof: In this proof, $\tilde{y}$ and $\tilde{\boldsymbol{i}}$ are as defined (7). For a given $\boldsymbol{i}$, let $y_0=a^{[\boldsymbol{i}]}$ denote the unique solution of $y_0=\tilde{y}(y_0;\boldsymbol{i})$. Then, Lemma 2.1 says that $\hat{t}_\ell(|\boldsymbol{i}\rangle) = |\tilde{\boldsymbol{i}}(a^{[\boldsymbol{i}]};\boldsymbol{i})\rangle$. Since it is sufficient to show that the mapping $\hat{t}_\ell$ is one-to-one on the set of all monomial, what is to be proved is that

$$\boldsymbol{i} \neq \boldsymbol{j} \text{ means } \tilde{\boldsymbol{i}}(a^{[\boldsymbol{i}]};\boldsymbol{i}) \neq \tilde{\boldsymbol{i}}(a^{[\boldsymbol{j}]};\boldsymbol{j}).$$

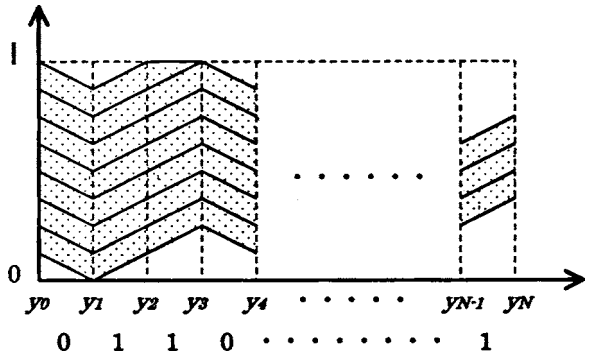

FIG. 3. Successive maps $y_i \mapsto y_{i+1} (i=0,1,2,\ldots,N-1)$.

So suppose that $\boldsymbol{i} \neq \boldsymbol{j}$. Since the mapping (7) is one-to-one, $(a^{[i]}; \tilde{\boldsymbol{i}}(a^{[i]}; \boldsymbol{i})) \neq (a^{[j]}; \tilde{\boldsymbol{i}}(a^{[j]}; \boldsymbol{j}))$. Hence, if $a^{[i]}=a^{[j]}$ then $\tilde{\boldsymbol{i}}(a^{[i]}; \boldsymbol{i}) \neq \tilde{\boldsymbol{i}}(a^{[j]}; \boldsymbol{j})$ follows. Now suppose that $a^{[i]} \neq a^{[j]}$ and assume that $\tilde{\boldsymbol{i}}(a^{[i]}; \boldsymbol{i}) \neq \tilde{\boldsymbol{i}}(a^{[j]}; \boldsymbol{j})$. Since R is symmetric ($R^{ii'}_{yy'} = R^{i'i}_{y'y}$), the mapping (7) gives

$$(a^{[i]}; \tilde{\boldsymbol{i}}(a^{[i]}; \boldsymbol{i})) \mapsto (a^{[i]}; \boldsymbol{i}) \quad \text{and} \quad (a^{[j]}; \tilde{\boldsymbol{i}}(a^{[i]}; \boldsymbol{i})) \mapsto (a^{[j]}; \boldsymbol{j});$$

then, as in the proof of Lemma 2.1, $a^{[i]}$ and $a^{[j]}$ must be equal, contrary to our assumption. □

Proof of Propostion 2.1: Let $\iota(\boldsymbol{\alpha}) = |a_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle$, and $\hat{t}_\ell(\iota(\boldsymbol{\alpha})) = |\alpha'_1\rangle \otimes |\alpha'_2\rangle \otimes \cdots \otimes |\alpha'_N\rangle$. From Lemma 2.1, there exists one and only one y_0 $(N+1)$-tuple $(y_0, y_1, \ldots, y_{N-1}, y_N = y_0)$ which satisfies (6) for $\iota(\boldsymbol{\alpha})$ and $\hat{t}_\ell(\iota(\boldsymbol{\alpha}))$.

When $\alpha_n = 0$, from (5), it holds that

$$\alpha'_n = \begin{cases} 0 & (y_{n-1} = 0) \\ 1 & (y_{n-1} \geq 1). \end{cases}$$

Suppose that $\lambda_n = j$, that is, ${\alpha_n}^{\lambda_n} = 0^j$. From the definition of $\boldsymbol{\lambda}$, there is a subsequence

$${\alpha_m}^{\lambda m} {\alpha_{m+1}}^{\lambda m+1} \cdots {\alpha_n}^{\lambda n} (\subset {\alpha_1}^{\lambda 1} {\alpha_2}^{\lambda 2} \cdots {\alpha_N}^{\lambda N})$$

where ${\alpha_m}^{\lambda m} = 1^j$ and $1 \leq \lambda_{m+1}, \lambda_{m+2}, \ldots, \lambda_{n-1} \leq j-1$. Among the subsequence, there exists at least one pair ${\alpha_s}^{\lambda s} {\alpha_{s+1}}^{\lambda s+1}$ which satisfies ${\alpha_s}^{\lambda s} {\alpha_{s+1}}^{\lambda s+1} = 1^1 0^1$ and

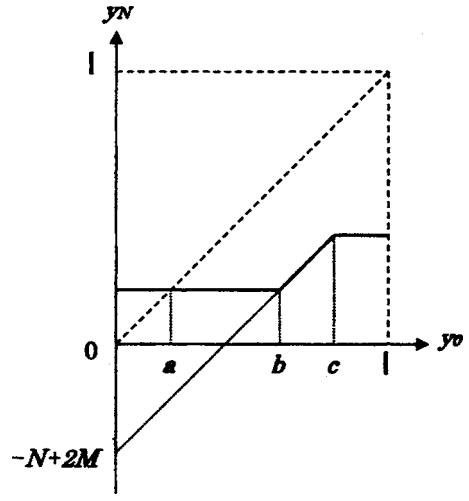

FIG. 4. A graph of $y_0 \mapsto y_N$.

$$\begin{cases} 1^k \in \{\alpha_{m+1}{}^{\lambda m+1}, \alpha_{m+2}{}^{\lambda m+2}, \ldots, \alpha_{s-1}{}^{\lambda s-1}\} \\ 0^k \in \{\alpha_{s+2}{}^{\lambda s+2}, \alpha_{s+3}{}^{\lambda s+3}, \ldots, \alpha_{n-1}{}^{\lambda n-1}\} \end{cases} \quad (k = 2,3,\ldots,j-1).$$

Note that the number of 1's in $\alpha_m\alpha_{m+1}\ldots\alpha_s$ is larger than that of 0's by j. Similarly the number of 0's in $\alpha_{s+1}\alpha_{s+2}\ldots\alpha_n$ is larger than that of 1's by j. Hence, using the action of R matrix, it holds that

$$\begin{aligned} &y_s = \ell \quad (j > \ell) \\ &j \le y_s \le \ell \quad (j \le \ell), \end{aligned} \tag{8}$$

and

$$y_{n-1} = \max[y_s - (j-1), 0]. \tag{9}$$

From (8) and (9), we find that

$$\begin{aligned} &y_{n-1} = 0 \qquad (j > \ell), \\ &y_{n-1} \ge 1 \qquad (j \le \ell), \end{aligned}$$

which implies

$$\alpha_n' = \begin{cases} 0 & (j > \ell) \\ 1 & (j \le \ell). \end{cases}$$

Furthermore, for 0^∞, it is immediately seen that $y_{n-1}=0$. Therefore the action of $\hat{t}_\ell$ is equivalent to the time evolution rule of T_ℓ for 0's.

The proof for 1's is carried out in a similar manner. □

Hereafter we fix a partition $\boldsymbol{p}=(p_1,p_2,p_3,\ldots)$ of M, that is, an integer sequence which satisfies $p_1,p_2,p_3,\ldots$ which satisfies $p_1 \ge p_2 \ge p_3 \ge \cdots \ge 0$ and $\Sigma_{j\ge 1} p_j = M$. Let Y be the Young diagram whose conjugate corresponds to the partition $\boldsymbol{p}$. Then we have the following corollary.

Corollary 2.2

$$\boldsymbol{\alpha} \in \Omega_M^Y \Leftrightarrow \hat{t}_\ell([\iota(\boldsymbol{\alpha})]) = x^{-2\Sigma_{i=1}^{\ell} p_i} \hat{t}_\ell(\iota(\boldsymbol{\alpha})) \quad (\ell = 1,2,3,\ldots).$$

Proof: In the proof of Lemma 2.1, we see

$$R^{i_1 i_1'}_{a y_1}[x] R^{i_2 i_2'}_{y_1 y_2}[x] R^{i_3 i_3'}_{y_2 y_3}[x] \cdots R^{i_N i_N'}_{y_{N-1} a}[x] = x^{-K(a)}$$

with a non-negative integer $K(a)$. Hence we have

$$\hat{t}_\ell[x](\iota(\boldsymbol{\alpha})) = x^{-K(a)} \hat{t}_\ell(\iota(\boldsymbol{\alpha})).$$

From (5) and Propostion 2.1, $K(a)$ is equal to the number of 0^j's and 1_j's $(1 \le j \le \ell)$.

Therefore,

$$K(a) = 2\sum_{i=1}^{\ell} p_i.$$

On the other hand, when $\boldsymbol{\alpha} \notin \Omega_M^Y$, clearly there exist ℓ_0 such that

$$\hat{t}_{\ell_0}[x](\iota(\boldsymbol{\alpha})) \ne x^{-2\Sigma_{i=1}^{\ell_0} p_i} \hat{t}_{\ell_0}(\iota(\boldsymbol{\alpha})),$$

which completes the proof. □

Next we show that the vector space spanned by the vectors in $\iota(\Omega_M^Y)$ is invariant under the action $\hat{t}_\ell$. For a monomial $|\psi\rangle \in \iota(\Omega_M^Y)$, we define

$$\pi_\ell(|\psi\rangle) := -2\sum_{i=1}^{\ell} p_i \quad (\ell = 1,2,3,\dots).$$

Lemma 2.2: *For an arbitrary monomial* $|\psi\rangle$ *and* $\ell=1,2,3,\dots,$

(a) $\pi_\ell(|\psi\rangle)=\pi_\ell(\hat{t}_1|\psi\rangle)$
and
(b) $\pi_1(|\psi\rangle)=\pi_1(\hat{t}_\ell|\psi\rangle)$.

Proof:

(a) For a state $\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\alpha_3\dots,\alpha_N)\in\Omega_M$, it holds that

$$T_1(\boldsymbol{\alpha})=(\alpha_N,\alpha_1,\alpha_2,\dots,\alpha_{N-1}),$$

and each conserved quantity does not change. Hence, from Proposition 2.1, we have $\pi_\ell(|\psi\rangle)=\pi_\ell(\hat{t}_1|\psi\rangle)$.

(b) From Corollary 2.2,

$$\hat{t}_1[x](\hat{t}_\ell[x]|\psi\rangle)=x^{\pi_\ell(|\psi\rangle)}\hat{t}_1[x](\hat{t}_\ell|\psi\rangle)=x^{\pi_\ell(|\psi\rangle)+\pi_1(\hat{t}_\ell|\psi\rangle)}\hat{t}_1\hat{t}_\ell|\psi\rangle\,,$$

$$\hat{t}_\ell[x](\hat{t}_1[x]|\psi\rangle)=x^{\pi_1(|\psi\rangle)}\hat{t}_\ell[x](\hat{t}_1|\psi\rangle)=x^{\pi_1(|\psi\rangle)+\pi_\ell(\hat{t}_1|\psi\rangle)}\hat{t}_\ell\hat{t}_1|\psi\rangle\,.$$

Since transfer matrices are commutative $\hat{t}_1[x]\hat{t}_\ell[x]=\hat{t}_\ell[x]\hat{t}_1[x]$, we obtain

$$\pi_\ell(|\psi\rangle)+\pi_1(\hat{t}_\ell|\psi\rangle)=\pi_1(|\psi\rangle)+\pi_\ell(\hat{t}_1|\psi\rangle).$$

Thus, from (a), $\pi_1(\hat{t}_\ell|\psi\rangle)=\pi_1(|\psi\rangle)$. □

For $\boldsymbol{\alpha}=(\alpha_1,\alpha_2,\dots,\alpha_N)\in\Omega_M$ and $\boldsymbol{\beta}=(\beta_1,\beta_2,\dots,\beta_N)\in\Omega_M$, we write $\boldsymbol{\alpha}\simeq\boldsymbol{\beta}$ when $\boldsymbol{\alpha}$ coincides with $\boldsymbol{\beta}$ up to shift, that is, $^{\exists}k\in\mathbb{Z},(\beta_1,\beta_2,\dots,\beta_N)=(\alpha_k,\alpha_{k+1},\dots,\alpha_N,\alpha_1,\alpha_2\dots,\alpha_{k-1})$. We also define $\hat{E}_{10}(\boldsymbol{\alpha})$ as the reduced 0,1 sequence with length $N-2p_1$ which is obtained by eliminating 1_1's and 0^1's from $(\boldsymbol{\alpha},\boldsymbol{\lambda},\bar{\boldsymbol{\lambda}})$.

Proposition 2.2: *For a state* $\boldsymbol{\alpha}\in\Omega_M$,

$$T_{\ell-1}\circ\hat{E}_{10}(\boldsymbol{\alpha})\simeq\hat{E}_{10}\circ T_\ell(\boldsymbol{\alpha})\quad(\ell=2,3,4,\dots).$$

Proof: A state consists of alternating sequences of consecutive 1's and of consecutive 0's. We call these sequences *domains of* 1's and *domains of* 0's. Note that the action of $\hat{E}_{10}$ is equivalent to removing one element from each domain.

By the definition of $T_{\ell-1}$ and $\hat{E}_{10}$, the operator $T_{\ell-1}\circ\hat{E}_{10}$ acts on a state as follows: Eliminate 1_1's and 0^1's, and replace $1_2,1_3,1_4,\dots$ and $0^2,0^3,0^4,\dots$ with $1_1,1_2,1_3,\dots$ and $0^1,0^2,0^3,\dots$ respectively; then replace 1_i and 0^i $(i=1,2,\dots,\ell-1)$ with 0 and 1, respectively. For example, in case of $\ell=2$,

$$0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1_1 1_2 1_3 1_4 0^1 0^2 0^3 1_1 1_2 0^1 1_1 1_3 0^1 0^2 0^3 1_1 0^1 0^4\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0$$

$$\overset{\hat{E}_{10}}{\mapsto}\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1_1 1_2 1_3 0^1 0^2 1_1 1_2 0^1 0^2 0^3 0\ \ 0\ \ 0\ \ 0\ \ 0$$

$$\overset{T_{\ell-1}}{\mapsto}\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 1\ \ 0\ \ 0\ \ 1\ \ 1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0.$$

It is equivalent to the action: Replace 1_i and 0^i $(i=1,2,\dots,\ell)$ with 0 and 1, respectively, and eliminate 0's and 1's corresponding to 1_1 and 0^1. For example, in case of $\ell=2$,

$$0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1_1 1_2 1_3 1_4 0^1 0^2 0^3 1_1 1_2 0^1 1_1 1_3 0^1 0^2 0^3 1_1 0^1 0^4 0\ \ 0\ \ 0\ \ 0\ \ 0$$

$$\overset{\text{Replacement}}{\mapsto}\ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 1\ \ 1\ \ 0\ \ 0\ \ 0\ \ 1\ \ 0\ \ 1\ \ 1\ \ 1\ \ 0\ \ 0\ \ 1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0$$

$$\overset{\text{Elimination}}{\mapsto}\ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 1\ \ 1\ \ 1\ \ 0\ \ 0\ \ 1\ \ 1\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0.$$

In this process, we eliminate p_1 0's and the same number of 1's which are arranged alternately in the sequence. Since from Lemma 2.2(b), the number of each domain does not change in the time evolution, we eliminate an element in each domain. Thus this action is equivalent to the action of $\hat{E}_{10} \circ T_\ell$. Therefore, we find

$$T_{\ell-1} \circ \hat{E}_{10}(\boldsymbol{\alpha}) \simeq \hat{E}_{10} \circ T_\ell(\boldsymbol{\alpha}).$$

Theorem 2.1: If $\alpha \in \Omega_M^Y$, *then* $T_\ell(\boldsymbol{\alpha}) \in \Omega_M^Y (\ell = 1,2,3,\ldots)$.

Proof: By the definition of $\hat{E}_{10}$, we have

$$\pi_{\ell-1}(\iota(\hat{E}_{10}(\boldsymbol{\alpha}))) = \pi_\ell(\iota(\boldsymbol{\alpha})) - \pi_1(\iota(\boldsymbol{\alpha})). \tag{10}$$

From Proposition II.1 and Lemma II.2(b),

$$\pi_1(\iota(\boldsymbol{\alpha})) = \pi_1(\iota(T_\ell(\boldsymbol{\alpha}))). \tag{11}$$

Hence, from (10), (11) and Proposition 2.2, it follows that

$$\begin{aligned}\pi_2(\iota(\boldsymbol{\alpha})) &= \pi_1(\iota(\hat{E}_{10}(\boldsymbol{\alpha}))) + \pi_1(\iota(\boldsymbol{\alpha})) \\ &= \pi_1(\iota(T_{\ell-1} \circ \hat{E}_{10}(\boldsymbol{\alpha}))) + \pi_1(\iota(T_\ell(\boldsymbol{\alpha}))) \\ &= \pi_1(\iota(\hat{E}_{10} \circ T_\ell(\boldsymbol{\alpha}))) + \pi_1(\iota(T_\ell(\boldsymbol{\alpha}))) \\ &= \pi_2(\iota(T_\ell(\boldsymbol{\alpha}))).\end{aligned}$$

Repeating a similar procedure for $\pi_3(\iota(\boldsymbol{\alpha})), \pi_4(\iota(\boldsymbol{\alpha})), \pi_5(\iota(\boldsymbol{\alpha})), \ldots$, we obtain

$$\pi_m(\iota(\boldsymbol{\alpha})) = \pi_m(\iota(T_\ell(\boldsymbol{\alpha}))) \quad (m = 1,2,3,\ldots).$$

Therefore the conserved quantities of $T_\ell(\boldsymbol{\alpha})$ are $p_1, p_2, p_3, \ldots$.

Corollary 2.3: *If* $|\varphi\rangle \in$ span $\iota(\Omega_M^Y)$, *then* $\hat{t}_\ell |\varphi\rangle \in$ span $\iota(\Omega_M^Y) (\ell = 1,2,3,\ldots)$.

Proof: This is a direct consequence of Proposition 2.1 and Theorem 2.1. □

III. PROOF OF THEOREM 1.1

In this section, we prove Theorem 1.1. we fix a Young diagram Y with M squares as in the previous section. The corresponding partition of M is given in Definition 1.1. We also denote by $p_j = (j = 1,2,3,\ldots)$ the jth column length of Y. Note that the following relation holds:

$$\sum_{i=1}^{s} \min[m_i, \ell\,] K_i = \sum_{i=1}^{\ell} p_i \quad (\ell = 1,2,3,\ldots). \tag{12}$$

In order to consider the eigenvalues $\Lambda_\ell[x;\{x_j\};q]$ of $\hat{t}_\ell[x]$ in (2), we put

$$\tilde{\Lambda}_\ell^{\langle k\rangle}[x;\{z_{i\alpha}^0\};q] := (q^k x^2 - q^{\ell-k+1})^N x^{-2N} \prod_{i=1}^{s} \prod_{\alpha=1}^{K_i} \prod_{h=1}^{m_i} Q_\ell^{\langle k\rangle}[x, z_{i\alpha}^0, r_{ih}; q]$$

where $r_{ih} := m_i - 2h + 1$ and

$$Q_\ell^{\langle k\rangle}[x,z,r;q] := \frac{q^{\ell+2r+2z^2} - q^r z x^2 + q^\ell x^4}{q^{2\ell-2k+2r+2z^2} - q^{\ell+r} z x^2 + q^{2k} x^4}.$$

By direct calculation, we see that

$$\Lambda_\ell[x] := \lim_{q\to 0} \Lambda_\ell[x;\{x_j\};q] = \lim_{q\to 0} \sum_{k=0}^{\ell} \tilde{\Lambda}_\ell^{\langle k\rangle}[x;\{z_{i\alpha}^0\};q].$$

When a function $f(q)$ is expressed as $f(q) = q^a(f_0 + f_1 q + f_2 q^2 + \cdots)(f_0 \neq 0)$, we write $\mathrm{ord}_q(f) = a$ and $f \sim q^a f_0$.

Lemma 3.1: *For* $k \neq 0$,

$$\mathrm{ord}_q(\tilde{\Lambda}_\ell^{\langle k\rangle}[x;\{z_{i\alpha}^0\};q]) \geq N - 2M.$$

Proof: For each $k (k = 1, 2, \ldots, \ell)$, we put

$$\eta_\ell^{\langle k\rangle}(r) := \mathrm{ord}_q(Q_\ell^{\langle k\rangle}[x, z_{i\alpha}^0; r; q]).$$

Then we have

$$\eta_\ell^{\langle k\rangle}(r) = \begin{cases} \ell - 2k & (\ell \leq r) \\ r - 2k & (2k - \ell \leq r \leq \ell) \\ -\ell & (2k - \ell - 2 \leq r \leq 2k - \ell) \\ -r - 2(\ell - k) - 2 & (-\ell - 2 \leq r \leq 2k - \ell - 2) \\ 2k - \ell & (r \leq -\ell - 2). \end{cases}$$

Since

$$\mathrm{ord}_q((q^k x^2 - q^{\ell-k+1})^N) = N \min[k, \ell - k + 1],$$
$$q^{N \min[k,\ell-k+1]} = q^{(N-2M)\min[k,\ell-k+1]} \cdot q^{2M \min[k,\ell-k+1]}$$

and $M = \sum_{i=1}^{s} m_i K_i$, we get

$$\mathrm{ord}_q(\tilde{\Lambda}_\ell^{\langle k\rangle}[x;\{z_{i\alpha}^0\};q]) = (N - 2M)\min[k, \ell - k + 1] + \sum_{i=1}^{s} \sum_{\alpha=1}^{Ki} \sum_{h=1}^{m_i} (\eta_\ell^{\langle k\rangle}(r_{ih}) + 2 \min[k, \ell - k + 1]).$$

Furthermore we obtain the following inequality immediately:

$$\eta_\ell^{\langle k\rangle}(r) + \eta_\ell^{\langle k\rangle}(-r) + 4 \min[k, \ell - k + 1] \geq 0 \quad (r \in \mathbb{Z}_{\geq 0}).$$

Therefore, for each $k (k = 1, 2, \ldots, \ell)$, we have

$$\mathrm{ord}_q(\tilde{\Lambda}_\ell^{\langle k\rangle}[x;\{z_{i\alpha}^0\};q]) \geq (N - 2M)\min[k, \ell - k + 1]$$
$$\geq N - 2M.$$

Proposition 3.1: *For* $\ell = 1, 2, 3, \ldots,$

$$\Lambda_\ell[x] = x^{-2\Sigma_{k=1}^{s}\min[m_k,\ell]K_k}\prod_{i=1}^{s}\prod_{\alpha=1}^{K_i}(-z_{i\alpha}^0)^{\min[m_i,\ell]}.$$

Proof: From Lemma 3.1, terms $\tilde{\Lambda}_\ell^{\langle k\rangle}$ for $k\geq 1$ would not contribute to $\Lambda_\ell[x]$ since we have assumed $N-2M>0$. For $Q_\ell^{\langle 0\rangle}[x,z_{i\alpha}^0,r;q]$, we have

$$Q_\ell^{\langle 0\rangle}[x,z_{i\alpha}^0,r;q]\sim\begin{cases} q^\ell & (\ell<r)\\ q^\ell(-z_{i\alpha}^0x^{-2}+1) & (r=\ell)\\ -q^r z_{i\alpha}^0x^{-2} & (-\ell<r<\ell)\\ \dfrac{-q^{-\ell}z_{i\alpha}^0}{-z_{i\alpha}^0+x^2} & (r=-\ell)\\ q^{-\ell} & (r<-\ell). \end{cases}$$

(i) If $m_i\equiv \ell \bmod 2$, then

$$Q_\ell^{\langle 0\rangle}[x,z_{i\alpha}^0,r;q]\sim\begin{cases} q^\ell & (r=\ell+1,\ell+3,\ell+5,\dots)\\ -q^r z_{i\alpha}^0x^{-2} & (r=-\ell+1,-\ell+3,\dots,\ell-1)\\ -q^{-\ell} & (r=-\ell-1,-\ell-3,-\ell-5,\dots). \end{cases}$$

(ii) If $m_i\not\equiv \ell \bmod 2$, then

$$Q_\ell^{\langle 0\rangle}[x,z_{i\alpha}^0,r;q]\sim\begin{cases} q^\ell & (r=\ell+2,\ell+4,\ell+6,\dots)\\ q^\ell(-z_{i\alpha}^0x^{-2}+1) & (r=\ell)\\ -q^r z_{i\alpha}^0x^{-2} & (r=-\ell+2,-\ell+4,\dots,\ell-2)\\ \dfrac{-q^{-\ell}z_{i\alpha}^0}{-z_{i\alpha}^0+x^2} & (r=-\ell)\\ q^{-\ell} & (r=-\ell-2,-\ell-4,-\ell-6,\dots). \end{cases}$$

Hence we obtain

$$\lim_{q\to 0}\prod_{h=1}^{m_i}Q_\ell^{\langle 0\rangle}[x,z_{i\alpha}^0,r_{ih};q] = x^{-2\,\min[m_i,\ell]}(-z_{i\alpha}^0)^{\min[m_i,\ell]},$$

which completes the proof.

Proof of Theorem 1.1(i): For an eigenvector $|\varphi\rangle\in V_M^Y$ of $\hat{t}_\ell[x]$ $(\ell=1,2,3,\dots)$, from Proposition 3.1 and (12), we have

$$\begin{aligned}\hat{t}_\ell[x]|\varphi\rangle &= x^{-2\Sigma_{k=1}^{s}\min[m_k,\ell]K_k}\prod_{i=1}^{s}\prod_{\alpha=1}^{K_i}(-z_{i\alpha}^0)^{\min[m_i,\ell]}|\varphi\rangle\\ &= x^{-2\Sigma_{k=1}^{s}\min[m_k,\ell]K_k}\hat{t}_\ell|\varphi\rangle\\ &= x^{-2\Sigma_{k=1}^{\ell}pk}\hat{t}_\ell|\varphi\rangle. \end{aligned}\tag{13}$$

On the other hand, $|\varphi\rangle$ can be expanded as

$$|\varphi\rangle=\sum_j C_j|\psi_j\rangle,$$

where $|\psi_j\rangle$ are monomials in V_M^Y and $C_j(\neq 0)$ are coefficients. Let $|\psi_j\rangle=\iota(\boldsymbol{\alpha}_j)(\boldsymbol{\alpha}_j\in\Omega_M)$.

Then, from Corollary 2.2,

$$\hat{t}_\ell[x]|\varphi\rangle = \hat{t}_\ell[x]\sum_j C_j|\psi_j\rangle = \sum_j C_j\hat{t}_\ell[x]|\psi_j\rangle$$
$$= \sum_j C_j\hat{t}_\ell[x](\iota(\boldsymbol{\alpha}_j)) = \sum_j C_j x^{-2\Sigma_{k=1}^{\ell} p_k^{\langle j\rangle}}\hat{t}_j(\iota(\boldsymbol{\alpha}_j)) = \sum_j C_j x^{2\Sigma_{k=1}^{\ell} p_k^{\langle j\rangle}}\hat{t}_\ell|\psi_j\rangle\,, \tag{14}$$

where $p_k^{\langle j\rangle}(k=1,2,\ldots,\ell)$ are conserved quantities of $\boldsymbol{\alpha}_j$. Since $|\psi_j\rangle$'s are linearly independent and $\hat{t}_\ell$ is invertible on V_M (Corollary 2.1), the vectors $\hat{t}_\ell|\psi_j\rangle$ are also linearly independent. Hence, from (13) and (14), we have

$$x^{-2\Sigma_{k=1}^{\ell} p_k^{\langle j\rangle}}\hat{t}_\ell|\psi_j\rangle = x^{-2\Sigma_{k=1}^{\ell} pk}\hat{t}_\ell|\psi_j\rangle\,,$$

that is,

$$\hat{t}_\ell[x]|\psi_j\rangle = x^{-2\Sigma_{k=1}^{\ell} pk}\hat{t}_\ell|\psi_j\rangle\,.$$

Thus, from Corollary 2.2, it follows that $|\psi_j\rangle \in \iota(\Omega_M^Y)$ for each j and $|\varphi\rangle \in \mathrm{span}\iota(\Omega_M^Y)$.

Therefore, if $|\psi\rangle$ is a vector in V_M^Y then it is also a vector in span $\iota(\Omega_M^Y)$. □

Proof of Theorem 1.1(ii): The completeness implies that

$$\bigoplus_Y V_M^Y = V_M.$$

On the other hand

$$\bigoplus_Y \mathrm{span}\iota(\Omega_M^Y) = V_M.$$

Therefore, it must be that

$$V_M^Y = \mathrm{span}\iota(\Omega_M^Y).$$

□

IV. CONCLUDING REMARKS

In this paper, we have showed an important relationship between the string hypothesis of BAE and the conserved quantities of PBBS (Theorem 1.1). In the limit that $q\to 0$, for a given Young diagram one may obtain eigenvectors from string hypothesis in terms of monomials. These monomials correspond exactly with the states of PBBS whose conserved quantities are given by exactly the same Young diagram. Although our result elucidates an aspect of the string solutions, it does not justify the string hypothesis or prove the completeness of Bethe vectors. However, we hope that our approach with PBBS may give some pieces of information about these problems.

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APPENDIX: EQUIVALENT DEFINITION OF PBBS

In this appendix, we give the equivalent definition of PBBS in previous work.[2,3] Consider a one-dimensional array of boxes each with a capacity of one ball. A periodic boundary condition is imposed by assuming that the last box is adjacent to the first one. We denote the number of boxes by N and the number of balls by M and we assume $M<N/2$. An arrangement of M balls in N boxes is called a state of the PBBS.

Denoting a vacant box by 0 and a filled box by 1, a state of the PBBS is represented as a 0,1 sequence of length N. For example, in a case of $N=8$ and $M=3$,

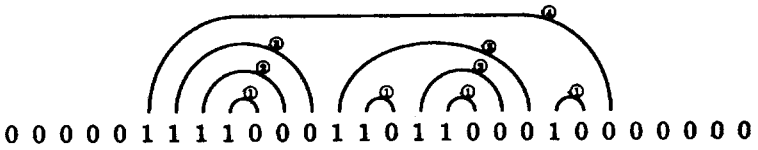
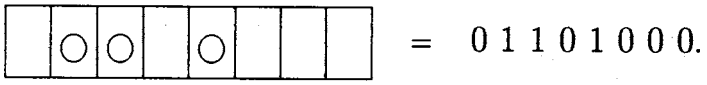


FIG. 5. A state of PBBS with $j^{\cap}$ arc lines.



If we think of this state at time t, the mapping T described in Sec. I A corresponds to incrementing time t to $t+1$. The time evolution rule from time step t to $t+1$ is also described as follows:

1. For a given state, connect all 10 pairs in the sequence with arc lines. We call them "$1^{\cap}$ arc lines."
2. Neglecting the 10 pairs which are connected in the first step, connect all the remaining 10's with arc lines. We call them "$2^{\cap}$ arc lines."
3. Repeat the above procedure until all 1's are connected to 0's with arc lines.
4. Exchange all the 1's and 0's which are connected with arc lines.

If we denote by $p_j(t)$ the number of $j^{\cap}$arc lines, we obtain a nonincreasing sequence of integers, $p_j(t)(j=1,2,3,\ldots)$. Then, this sequence is conserved in time, that is,

$$p_j(t) = p_j(t+1) \equiv p_j \quad (j = 1,2,3, \ldots).$$

For example, for the state considered in Sec. I A

$$0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 0\ 0\ 0\ 1\ 1\ 0\ 1\ 1\ 0\ 0\ 0\ 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0,$$

we draw arc lines as shown in Fig. 5 and evolve it by one time step according to the above procedure; then we obtain a new state

$$0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 0\ 0\ 1\ 0\ 0\ 1\ 1\ 1\ 0\ 1\ 1\ 0\ 0\ 0\ 0\ 0.$$

In this case, the conserved quantities are $p_1=4$, $p_2=2$, $p_3=2$, $p_4=1$, $p_j=0$ $(j=5,6,7,\ldots)$. These results are in agreement with those obtained by the other definition.

Next, we consider a class of PBBSs which obey different time evolution rules characterized by a positive integer parameter. Let ℓ be a positive integer.

1. For a given state, draw the arc lines in the same way as in the original time evolution rule of the PBBS.
2. For 01 pairs, we also draw arc lines by a similar procedure to that for 10 pairs. We call the arc lines drawn at jth step by "$j_{\cup}$ arc lines."
3. Replace with 0's all the 1's connected by $i_{\cup}$ arc lines $(i=1,2,\ldots,\ell)$ and replace with 1's all the 0's connected by $j^{\cap}$arc lines $(j=1,2,\ldots,\ell)$.

For example, for $\ell=2$, the state given in Fig. 6 evolves into

$$0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 0\ 0\ 0\ 1\ 0\ 1\ 1\ 1\ 0\ 0\ 1\ 0\ 0\ 0\ 0\ 0\ 0$$

at the next time step. When the system size is infinite and the number of 1's is finite, this rule coincides with the rule of a BBS with carrier of capacity ℓ introduced in Ref. 7. So we call the PBBS with the above rule a PBBS with carrier (PBBSC).

To see the state at the next time step, it is convenient to express a state as a 0,1 sequence with subscripts, where 1 and 0 connected by $i_{\cup}$ and $j^{\cap}$ arc lines are replaced 1_i and 0^j, respectively. For example, the state in Fig. 6 is expressed as

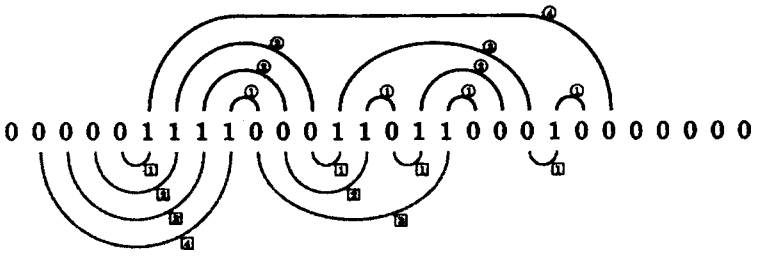


FIG. 6. A configuration with $j^{\cap}$ and $i^{\cup}$ arc lines.

$$0\ 0\ 0\ 0\ 0\ 1_1\ 1_2\ 1_3\ 1_4\ 0^1\ 0^2\ 0^3\ 1_1\ 1_2\ 0^1\ 1_1\ 1_3\ 0^1\ 0^2\ 0^3\ 1_1\ 0^1\ 0^4\ 0\ 0\ 0\ 0\ 0,$$

which coincides with (4). The time evolution rule of PBBSC of capacity ℓ is given as follows: replace 1_i and 0^i $(i=1,2,\ldots,\ell)$ with 0 and 1, respectively.

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Nested sequence of projectors. II. Multiparameter multistate statistical models, Hamiltonians, *S*-matrices

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Our starting point is a class of braid matrices, presented in a previous paper, constructed on a basis of a nested sequence of projectors. Statistical models associated to such $N^2\times N^2$ matrices for odd N are studied here. Presence of $\frac{1}{2}(N+3)\times(N-1)$ free parameters is the crucial feature of our models, setting them apart from other well-known ones. There are N possible states at each site. The trace of the transfer matrix is shown to depend on $\frac{1}{2}(N-1)$ parameters. For order r, N eigenvalues constitute the trace and the remaining (N^r-N) eigenvalues involving the full range of parameters come in zero-sum multiplets formed by the rth roots of unity, or lower dimensional multiplets corresponding to factors of the order r when r is not a prime number. The modulus of any eigenvalue is of the form $e^{\mu\theta}$, where μ is a linear combination of the free parameters, θ being the spectral parameter. For r a prime number an amusing relation of the number of multiplets with a theorem of Fermat is pointed out. Chain Hamiltonians and potentials corresponding to factorizable S-matrices are constructed starting from our braid matrices. Perspectives are discussed. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The most salient feature of the class of braid matrices presented in Ref. 1, setting it apart from other known examples, is the number of free parameters. This class was obtained for $N^2\times N^2$ braid matrices for *odd*

$$N=(2p-1)\quad (p=1,2,\ldots). \tag{1.1}$$

Such matrices, depending on a spectral parameter θ and satisfying the braid equation

$$\hat{R}_{12}(\theta-\theta')\hat{R}_{23}(\theta)\hat{R}_{12}(\theta')=\hat{R}_{23}(\theta')\hat{R}_{12}(\theta)\hat{R}_{23}(\theta-\theta') \tag{1.2}$$

have $\frac{1}{2}(N+3)(N-1)$ free parameters when the overall normalization is fixed. Thus for $N=3,5,7,\ldots$, the respective number of parameters are $6,16,30,\ldots$. These parameters appear in the coefficients of the N^2 projectors (the "*nested sequence*" defined in Ref. 1) providing the basis of $\hat{R}(\theta)$.

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The projectors are defined as follows. Let (ij) be the $N\times N$ matrix with a single nonzero element 1 on row i and column j. Then N^2 projectors are defined, with $\epsilon=\pm$ and $\bar{i}=N-i+1$, as

$$P_{pp}=(pp)\otimes(pp),$$

$$2P_{pi(\epsilon)}=(pp)\otimes[(ii)+(\bar{i}\bar{i})+\epsilon((i\bar{i})+(\bar{i}i))],$$

$$2P_{ip(\epsilon)}=[(ii)+(\bar{i}\bar{i})+\epsilon((i\bar{i})+(\bar{i}i))]\otimes(pp), \tag{1.3}$$

$$2P_{ij(\epsilon)}=(ii)\otimes(jj)+(\bar{i}\bar{i})\otimes(\bar{j}\bar{j})+\epsilon[(i\bar{i})\otimes(j\bar{j})+(\bar{i}i)\otimes(\bar{j}j)],$$

$$2P_{i\bar{j}(\epsilon)}=(ii)\otimes(\bar{j}\bar{j})+(\bar{i}\bar{i})\otimes(jj)+\epsilon[(i\bar{i})\otimes(\bar{j}j)+(\bar{i}i)\otimes(j\bar{j})],$$

where, from (1.1),

$$i=1,2,\ldots,p-1,\quad \bar{i}=N-i+1=2p-1,2p-2\ldots,p+1,\quad p=\tfrac{1}{2}(N+1). \tag{1.4}$$

The projectors satisfy [with α, β standing for triplets (i,j,ϵ)]

$$P_\alpha P_\beta=\delta_{\alpha\beta}P_\alpha,\quad \sum_\alpha P_\alpha^2=I_{N^2\times N^2}. \tag{1.5}$$

Their total number is

$$1+4(p-1)+4(p-1)^2=(2p-1)^2=N^2. \tag{1.6}$$

For our class of solutions, normalizing to 1 the coefficient of P_{pp},

$$\hat{R}(\theta)=P_{pp}+\sum_{i,\epsilon}(e^{m_{pi}^{(\epsilon)}\theta}P_{pi(\epsilon)}+e^{m_{ip}^{(\epsilon)}\theta}P_{ip(\epsilon)})+\sum_{i,j,\epsilon}(e^{m_{ij}^{(\epsilon)}\theta}P_{ij(\epsilon)}+e^{m_{i\bar{j}}^{(\epsilon)}\theta}P_{i\bar{j}(\epsilon)}), \tag{1.7}$$

with the crucial constraint,

$$m_{ij}^{(\epsilon)}=m_{i\bar{j}}^{(\epsilon)},\quad (\bar{j}=N-j+1=2p-j). \tag{1.8}$$

This sufficient and necessary constraint concerning the coefficient of θ in the exponents, leaves

$$\tfrac{1}{2}(N+3)(N-1) \tag{1.9}$$

free parameters. For $N=3$ one thus obtains, with six free parameters,

$$\hat{R}(\theta)=\begin{vmatrix} a_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_- \\ 0 & b_+ & 0 & 0 & 0 & 0 & 0 & b_- & 0 \\ 0 & 0 & a_+ & 0 & 0 & 0 & a_- & 0 & 0 \\ 0 & 0 & 0 & c_+ & 0 & c_- & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_- & 0 & c_+ & 0 & 0 & 0 \\ 0 & 0 & a_- & 0 & 0 & 0 & a_+ & 0 & 0 \\ 0 & b_- & 0 & 0 & 0 & 0 & 0 & b_+ & 0 \\ a_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_+ \end{vmatrix}, \tag{1.10}$$

where

$$a_{\pm} = \tfrac{1}{2}(e^{m_{11}^{(+)}\theta} \pm e^{m_{11}^{(-)}\theta}), \quad b_{\pm} = \tfrac{1}{2}(e^{m_{12}^{(+)}\theta} \pm e^{m_{12}^{(-)}\theta}), \quad c_{\pm} = \tfrac{1}{2}(e^{m_{21}^{(+)}\theta} \pm e^{m_{21}^{(-)}\theta}). \tag{1.11}$$

The parameters $a_{\pm}$ are each repeated in (1.10) according to (1.8), since

$$m_{1\bar{1}}^{(\pm)} = m_{11}^{(\pm)} \quad (\bar{1} = 3). \tag{1.12}$$

This is the case we will study mostly in the following sections. The corresponding results for $N > 3$ will be indicated briefly. For example, the generalization of the considerations below in this section for $N > 3$ is entirely straightforward. To explore the statistical model associated to (1.10) one starts by constructing explicit representations of the monodromy matrices $t_{ij}^{(r)}(\theta)$ of successive orders ($r = 1, 2, 3, \ldots$) obtained by taking coproducts of the fundamental 3×3 blocks (with the same θ for each factor)

$$t_{ij}^{(r)} = \sum_{j_1, \ldots, j_{r-1}} t_{ij_1} \otimes t_{j_1 j_2} \otimes \cdots \otimes t_{j_{r-1} j}. \tag{1.13}$$

For $N = 3$,

$$t^{(r)} = \begin{vmatrix} t_{11}^{(r)} & t_{12}^{(r)} & t_{1\bar{1}}^{(r)} \\ t_{21}^{(r)} & t_{22}^{(r)} & t_{2\bar{1}}^{(r)} \\ t_{\bar{1}1}^{(r)} & t_{\bar{1}2}^{(r)} & t_{\bar{1}\bar{1}}^{(r)} \end{vmatrix}. \tag{1.14}$$

If the $\hat{R}tt$ equation for the blocks $t_{ij}^{(r)}$ (Appendix C),

$$\hat{R}(\theta - \theta')(t^{(r)}(\theta) \otimes t^{(r)}(\theta')) = (t^{(r)}(\theta') \otimes t^{(r)}(\theta))\hat{R}(\theta - \theta') \tag{1.15}$$

is satisfied for $r = 1$, then the coproduct construction (1.13) ensures that (1.15) is satisfied for all higher values $r = 2, 3, \ldots$. The solution for $r = 1$ is given by

$$t^{(1)}(\theta) \equiv t(\theta) = P\hat{R}(\theta) = R(\theta), \tag{1.16}$$

where P is the permutation matrix

$$p = \sum_{ij} (ij) \otimes (ji) \tag{1.17}$$

and $R(\theta)$ is the Yang-Baxter (YB) matrix. This is a standard result valid generally for solutions of (1.2). (See Appendix B of Ref. 1 for sources cited.)

The transfer matrix, for each order r, is defined to be the trace (with argument θ)

$$T^{(r)} = t_{11}^{(r)} + t_{22}^{(r)} + t_{\bar{1}\bar{1}}^{(r)}. \tag{1.18}$$

The properties of the model depend crucially on the eigenvalues of $T^{(r)}$. References 2–4 provide ample information citing numerous basic sources.

So our basic task will be to construct the eigenstates and eigenvalues of $T^{(r)}(\theta)$. Remarkable feature following from (1.10) [and more generally from (1.7)] will be presented in the following sections and appendixes.

We will also construct chain Hamiltonians and potentials leading to factorizable S-matrices starting from our class of $\hat{R}(\theta)$.

Concerning each aspect we will try to display the role of our multiple parameters. For all

$$m_{ij}^{(+)}\theta \geqslant m_{ij}^{(-)}\theta \tag{1.19}$$

the elements of $\hat{R}(\theta)$ and hence the Boltzmann weights are non-negative, consistent with physical interpretations. For *definiteness* we consider the sector, say

$$m_{11}^{(+)} > m_{11}^{(-)} > m_{12}^{(+)} > m_{12}^{(-)} > m_{21}^{(+)} > m_{21}^{(-)}, \quad \theta \geqslant 0. \tag{1.20}$$

of (1.10). The eigenvalues will be ordered differently for other sectors. They can be considered separately.

II. TRANSFER MATRIX, EIGENVECTORS, EIGENVALUES ($N=3$): CRUCIAL FEATURES

We start by signalling some crucial features to be encountered below in the explicit constructions restricted (in this section) to $N=3$.

(1) The trace of the transfer matrix (1.17) of order r will turn out to be

$$\mathrm{tr}(T^{(r)}(\theta)) = 2e^{rm_{11}^{(+)}\theta} + 1. \tag{2.1}$$

Of the six parameters $(m_{11}^{(\pm)}, m_{12}^{(\pm)}, m_{21}^{(\pm)})$ of (1.11) *only* $m_{11}^{(+)}$ appears in the trace. A simple explanation of this fact will be given after discussing the generalization for $N>3$.

(2) The eigenvalue $e^{rm_{11}^{(+)}\theta}$ is obtained exactly *twice* for each r and the value 1 only *once*.

(3) The remaining (3^r-3) eigenvalues occur in multiplets of *zero sum* due to the presence of *roots of unity*. Hence they do not contribute to the trace. For r a prime number there will be "r-plets" (and possibly "nr-plets," n being an integer)

$$e^{\mu\theta}(1, e^{(2\pi i/r)}, e^{(2\pi i/r)\cdot 2}, \ldots, e^{(2\pi i/r)\cdot(r-1)}), \tag{2.2}$$

where μ is a *linear* combination of the parameters $m_{ij}^{(\pm)}$. When r is factorizable lower order multiplets can be present corresponding to the factors. Thus for $r=4$ one obtains both doublets and quadruplets

$$e^{\mu_2\theta}(1,-1), \quad e^{\mu_4\theta}(1, i, -1, -i), \tag{2.3}$$

with appropriate linear combinations μ_2, μ_4 to be displayed below.

(4) Apart from possible roots of unity phase factors the modulus of each eigenvalue is a simple exponential of the type $e^{\mu\theta}$ of (2.2). For $r=3$, for example, one obtains for μ the values (Appendix A)

$$\begin{gathered} 3m_{11}^{(+)}, \quad (m_{11}^{(+)} + 2m_{11}^{(-)}), \\ (m_{11}^{(+)} + m_{12}^{(+)} + m_{21}^{(+)}), \quad (m_{11}^{(+)} + m_{12}^{(-)} + m_{21}^{(-)}), \\ (m_{11}^{(-)} + m_{12}^{(+)} + m_{21}^{(-)}), \quad (m_{11}^{(-)} + m_{12}^{(-)} + m_{21}^{(+)}), \\ (m_{12}^{(+)} + m_{21}^{(+)}), \quad (m_{12}^{(-)} + m_{21}^{(-)}), \\ 0. \end{gathered} \tag{2.4}$$

Along with roots of unity factors these provide all the 27 eigenvalues as will be shown below.

(5) The values of μ depend crucially on the subspaces, to be introduced below, which are invariant under the action of $T^{(r)}(\theta)$, the transfer matrix.

A. Construction of $T^{(r)}(\theta)$ for $N=3$

The standard construction of the fundamental 3×3 block matrices $t_{ij}(\theta)$ implementing (1.15), (1.16), (1.10), (1.11), leads to [for $t^{(1)}(\theta) \equiv t(\theta)$ with $\bar{1}=3$]

$$t_{11}(\theta)=\begin{vmatrix} a_+ & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a_- \end{vmatrix},\quad t_{12}(\theta)=\begin{vmatrix} 0 & 0 & 0 \\ c_+ & 0 & c_- \\ 0 & 0 & 0 \end{vmatrix},\quad t_{1\bar{1}}(\theta)=\begin{vmatrix} 0 & 0 & a_- \\ 0 & 0 & 0 \\ a_+ & 0 & 0 \end{vmatrix},$$

$$t_{21}(\theta)=\begin{vmatrix} 0 & b_+ & 0 \\ 0 & 0 & 0 \\ 0 & b_- & 0 \end{vmatrix},\quad t_{22}(\theta)=\begin{vmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{vmatrix},\quad t_{2\bar{1}}(\theta)=\begin{vmatrix} 0 & b_- & 0 \\ 0 & 0 & 0 \\ 0 & b_+ & 0 \end{vmatrix}, \tag{2.5}$$

$$t_{\bar{1}1}(\theta)=\begin{vmatrix} 0 & 0 & a_+ \\ 0 & 0 & 0 \\ a_- & 0 & 0 \end{vmatrix},\quad t_{\bar{1}2}(\theta)=\begin{vmatrix} 0 & 0 & 0 \\ c_- & 0 & c_+ \\ 0 & 0 & 0 \end{vmatrix},\quad t_{\bar{1}\bar{1}}(\theta)=\begin{vmatrix} a_- & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & a_+ \end{vmatrix},$$

where, from (1.11),

$$(a_+ \pm a_-)=e^{m_{11}^{(\pm)}\theta},\quad (b_+ \pm b_-)=e^{m_{12}^{(\pm)}\theta},\quad (c_+ \pm c_-)=e^{m_{21}^{(\pm)}\theta}. \tag{2.6}$$

One now must implement these in (1.13), (1.14), and (1.18) to obtain $T^{(r)}(\theta)$. Then one proceeds to construct eigenvalues of $T^{(r)}(\theta)$.

B. Subspaces invariant under the action of $T^{(r)}(\theta)$

We start by introducing convenient, compact notations. The state vectors of the fundamental representation (2.5) are denoted as

$$\left(\begin{vmatrix} 1 \\ 0 \\ 0 \end{vmatrix}\right\rangle, \begin{vmatrix} 0 \\ 1 \\ 0 \end{vmatrix}\right\rangle, \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix}\right\rangle) \equiv (|1\rangle,|2\rangle,|\bar{1}\rangle). \tag{2.7}$$

Tensor products for higher orders are constructed as

$$(|1\rangle\otimes|1\rangle,|1\rangle\otimes|2\rangle,|1\rangle\otimes|\bar{1}\rangle,\dots) \equiv (|11\rangle,|12\rangle,|1\bar{1}\rangle,\dots) \tag{2.8}$$

and so on in evident continuation. The *order* of the labels $(1,2,\bar{1})$ will indicate the tensor product structure. Thus, for example,

$$|1\rangle\otimes|1\rangle\otimes|2\rangle\otimes|\bar{1}\rangle\otimes|1\rangle \equiv |112\bar{1}1\rangle. \tag{2.9}$$

Corresponding to the rth order coproduct, $T^{(r)}(\theta)$ acts on a space spanned by 3^r states (for $N=3$). Let

$$S(r,k)\quad (k=0,1,\dots,r) \tag{2.10}$$

denote the subspaces labeled by k, the *multiplicity* of the index 2. The coefficients of different power of x in the expansion

$$(x+2)^r = 1\cdot x^r + 2rx^{r-1} + \cdots + 2^{r-k}\binom{r}{r-k}x^k + \cdots + 2^r \tag{2.11}$$

give the number of states in the respective subspaces. Setting $x=1$ one obtains the total number

$$(1+2)^r = 3^r. \tag{2.12}$$

For example, for $r=3$, one obtains the subspaces,

$$
\begin{aligned}
S(3,3):&\quad |222\rangle;\\
S(3,2):&\quad |221\rangle,|22\bar{1}\rangle,|212\rangle,|2\bar{1}2\rangle,|122\rangle,|\bar{1}22\rangle;\\
S(3,1):&\quad |211\rangle,|21\bar{1}\rangle,|2\bar{1}1\rangle,|2\overline{11}\rangle,\\
&\quad |121\rangle,|12\bar{1}\rangle,|\bar{1}21\rangle,|\bar{1}2\bar{1}\rangle,\\
&\quad |112\rangle,|1\bar{1}2\rangle,|\bar{1}12\rangle,|\overline{11}2\rangle;\\
S(3,0):&\quad |111\rangle,|11\bar{1}\rangle,|1\bar{1}1\rangle,|\bar{1}11\rangle,\\
&\quad |\overline{111}\rangle,|\overline{11}1\rangle,|\bar{1}1\bar{1}\rangle,|1\overline{11}\rangle.
\end{aligned}
\tag{2.13}
$$

A striking and most helpful consequence of the structure of the matrices (2.5) and their coproducts is *each subspace $S(r,k)$ is invariant under the action of $T^{(r)}(\theta)$*. This facilitates considerably the construction of eigenstates. One works on lower dimensional spaces.

One possible approach is as follows: One selects any one state from the $2^{r-k}\binom{r}{r-k}$ states of $S(r,k)$ and computes the action of $T^{(r)}(\theta)$ on it. One gets on the right-hand side (rhs) a linear combination of states belonging to $S(r,k)$. Thus, for example,

$$
\begin{aligned}
T^{(4)}(\theta)|1111\rangle &= (a_+^4 + a_-^4)|1111\rangle + 2a_+^2a_-^2(|\overline{1111}\rangle + |1\bar{1}1\bar{1}\rangle + |\bar{1}1\bar{1}1\rangle)\\
&\quad + (a_+^2 + a_-^2)a_+a_-(|1\overline{11}\rangle + |\overline{11}1\rangle + |\bar{1}11\bar{1}\rangle + |1\overline{11}\rangle),
\end{aligned}
\tag{2.14}
$$

where $a_\pm = \frac{1}{2}(e^{m_{11}^{(+)}\theta} \pm e^{m_{11}^{(-)}\theta})$ as noted before. Next, one computes the action of $T^{(4)}$ successively on the other states appearing on the right-hand side. This continues until one obtains the coefficients for a closed subsystem. Then one searches for linear combinations such that under $T^{(4)}$ it is reproduced to within a factor. Thus one systematically obtains all eigenvectors and eigenvalues, for the subspace $S(r,k)$. For our class one must solve systems of *linear* equations with fairly simple coefficient. Even the 81 eigenstates and eigenvalues for $r=4$ were obtained directly without using a computer program and without any real difficulties.

We have thus obtained exhaustive solutions for $r=1,2,3,4$. The corresponding 3, 9, 27, and 81 eigenvalues are presented in Appendix A. We have also obtained explicitly all the corresponding eigenstates. For brevity they are not presented here. The eigenvalues of Appendix A fully illustrate the crucial properties (1)–(5) signalled at the start of this section. In the following section we indicate a related but somewhat differently formulated approach for various comparisons.

III. LINEAR CONSTRAINTS FOR EIGENVECTORS FOR $N=3$ AND COMPARISION WITH ALGEBRAIC BETHE ANSATZ

In Sec. II we have noted how, exploiting the invariance of the subspaces $S(r,k)$ defined by (2.10) one can construct step by step all the eigenstates. The comments following (2.14) indicate how the relevant linear equations are obtained. We formulate below the approach in a systematic, explicit fashion.

Starting with (2.5) and (2.6) for $t_{ij}^{(1)}(\theta)=t_{ij}(\theta)$ we define the operators

$$
U = b_+(-\theta)t_{21}(\theta) + b_-(-\theta)t_{2\bar{1}}(\theta) = \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0 \end{pmatrix},
$$

$$
A = t_{22}(\theta) = \begin{pmatrix} 0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0 \end{pmatrix},
\tag{3.1}
$$

$$D = b_-(-\theta)t_{21}(\theta) + b_+(-\theta)t_{2\bar{1}}(\theta) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Then (suppressing arguments θ of t_{ij})

$$\begin{aligned}
t_{11}(A,U,D) &= (0,a_+U,a_-D),\\
t_{12}(A,U,D) &= (0,c_+A,c_-A),\\
t_{1\bar{1}}(A,U,D) &= (0,a_+D,a_-U),\\
t_{21}(A,U,D) &= (b_+U + b_-D,0,0),\\
t_{22}(A,U,D) &= (A,0,0),\\
t_{2\bar{1}}(A,U,D) &= (b_-U + b_+D,0,0),\\
t_{\bar{1}1}(A,U,D) &= (0,a_-D,a_+U),\\
t_{\bar{1}2}(A,U,D) &= (0,c_-A,c_+A),\\
t_{\bar{1}\bar{1}}(A,U,D) &= (0,a_-U,a_+D).
\end{aligned} \tag{3.2}$$

Also from (2.7) and (3.1)

$$U|2\rangle = |1\rangle, \quad A|2\rangle = |2\rangle, \quad D|2\rangle = |\bar{1}\rangle. \tag{3.3}$$

For any r, starting with $S(r,r)$ one obtains the basic eigenstate [trivially since $S(r,r)$ is of dimension 1],

$$T^{(r)}(\theta)|22\cdots 2\rangle = 1|22\cdots 2\rangle. \tag{3.4}$$

Now one moves up in $(r-k)$ stepwise.

$S(r,r-1)(\dim 2r)$: With $2r$ coefficients $(u_i,d_i)(i=1,\ldots,r)$ one can label the states as

$$\begin{pmatrix} (u_1U + d_1D)\otimes A\otimes\cdots\otimes A \\ +A\otimes(u_2U+d_2D)\otimes A\otimes\cdots\otimes A \\ \vdots \\ +A\otimes A\otimes\cdots\otimes A\otimes(u_rU+d_rD) \end{pmatrix}|22\cdots 2\rangle. \tag{3.5}$$

The action of $T^{(r)}(\theta)$ on these leads to a linear system of equations in (u_i,d_i) corresponding to eigenstates. For $S(r,r-1)$ the solution is particularly simple. Define

$$|\omega,\epsilon\rangle = \begin{pmatrix} A\otimes A\otimes\cdots\otimes A\otimes(U+\epsilon D) \\ +\omega A\otimes A\otimes\cdots\otimes(U+\epsilon D)\otimes A \\ +\omega^2 A\otimes A\otimes\cdots\otimes(U+\epsilon D)\otimes A\otimes A \\ \vdots \\ +\omega^{r-1}(U+\epsilon D)\otimes A\otimes A\otimes\cdots\otimes A \end{pmatrix}|22\cdots 2\rangle, \tag{3.6}$$

where $\epsilon=\pm$ and ω can have r values (as a rth root of unity)

$$\omega = (1, e^{i2\pi/r}, \ldots, e^{(i2\pi/r)\cdot(r-1)}). \tag{3.7}$$

One obtains

$$T^{(r)}(\theta)|\omega, \epsilon\rangle = \omega^{r-1} e^{(m_{12}^{(\epsilon)} + m_{21}^{(\epsilon)})\theta} |\omega, \epsilon\rangle. \tag{3.8}$$

The $2r$ eigenvalues are

$$e^{(m_{12}^{(\epsilon)} + m_{21}^{(\epsilon)})\theta} (1, e^{i2\pi/r}, \ldots, e^{(i2\pi/r)(r-1)}). \tag{3.9}$$

The next step is $k=r-2$.

$S(r, r-2)$ $(\dim 2r(r-1))$: A set of states spanning this subspace is given by

$$\sum_{i \neq j} (A \otimes \cdots \otimes A \otimes (u_i U + d_i D) \otimes A \otimes \cdots \otimes (u_j U + d_j D) \otimes A \otimes \cdots \otimes A) |22 \cdots 2\rangle. \tag{3.10}$$

The parameters (u, d) must be constrained to obtain eigenstates. At each step one obtains sets of linear constraints. The pattern is now evident. At each step one inserts, as in (3.10), $(r-k)$ factors of the type $(u_i U + d_i D)$ excluding their coincidence.

Finally for $k=0$, one has $S(r,0)$ of dimension 2^r. Here a basis spanning the subspace can be labeled as

$$\left(\sum_i (u_1^{(i)} U + d_1^{(i)} D) \otimes (u_2^{(i)} U + d_2^{(i)} D) \otimes \cdots \otimes (u_r^{(i)} U + d_r^{(i)} D) \right) |22 \cdots 2\rangle. \tag{3.11}$$

Since there are no label $|2\rangle$ left, it can be shown from (3.2) that $T^{(r)}(\theta)$, acting on $S(r,0)$ simplifies to

$$T^{(r)} \approx t_{11}^{(r)} + t_{\bar{1}\bar{1}}^{(r)} \approx t_{11} \otimes t_{11}^{(r-1)} + t_{1\bar{1}} \otimes t_{\bar{1}1}^{(r-1)} + t_{\bar{1}1} \otimes t_{1\bar{1}}^{(r-1)} + t_{\bar{1}\bar{1}} \otimes t_{\bar{1}\bar{1}}^{(r-1)}. \tag{3.12}$$

In successive steps ($t^{(r-1)} \to t \otimes t^{(r-2)}$ and so on) only the indices $(1, \bar{1})$ need be retained. They only give nonzero contributions. From (3.2),

$$\begin{aligned}
t_{11}(u_s^{(i)} U + d_s^{(i)} D) &= (a_+ u_s^{(i)} U + a_- d_s^{(i)} D) \equiv X_{11}^{(i)}(s), \\
t_{1\bar{1}}(u_s^{(i)} U + d_s^{(i)} D) &= (a_- d_s^{(i)} U + a_+ u_s^{(i)} D) \equiv X_{1\bar{1}}^{(i)}(s), \\
t_{\bar{1}1}(u_s^{(i)} U + d_s^{(i)} D) &= (a_+ d_s^{(i)} U + a_- u_s^{(i)} D) \equiv X_{\bar{1}1}^{(i)}(s), \\
t_{\bar{1}\bar{1}}(u_s^{(i)} U + d_s^{(i)} D) &= (a_- u_s^{(i)} U + a_+ d_s^{(i)} D) \equiv X_{\bar{1}\bar{1}}^{(i)}(s).
\end{aligned} \tag{3.13}$$

Define, with indices taking values $(1, \bar{1})$ only,

$$X_{ab}^{(i)}(1,2,\ldots,r) = \sum_{b_1,\ldots,b_{r-1}} X_{ab_1}^{(i)}(1) \otimes X_{b_1 b_2}^{(i)}(2) \otimes \cdots \otimes X_{b_{r-1} b}^{(i)}(r). \tag{3.14}$$

The action of $T^{(r)}(\theta)$ on the generic state (3.11) finally reduces to

$$\left(\sum_{i=1}^{r} (X_{11}^{(i)}(1,2,\ldots,r) + X_{\bar{1}\bar{1}}^{(i)}(1,2,\ldots,r)) \right) |22 \cdots 2\rangle. \tag{3.15}$$

It is of particular interest to see what parametrizations in (3.11) corresponds to the *two* eigenstates (and two only for any r) that contribute to the trace.

For $r=2$,

$$T^{(2)}(\theta)(|11\rangle + |\overline{11}\rangle) = e^{2m_{11}^{(+)}\theta}(|11\rangle + |\overline{11}\rangle),$$
$$T^{(2)}(\theta)(|1\bar{1}\rangle + |\bar{1}1\rangle) = e^{2m_{11}^{(+)}\theta}(|1\bar{1}\rangle + |\bar{1}1\rangle). \tag{3.16}$$

Along with

$$T^{(2)}(\theta)|22\rangle = |22\rangle \tag{3.17}$$

the two states of (3.16) yield

$$\mathrm{tr}(T^{(2)}(\theta)) = 2e^{2m_{11}^{(+)}\theta} + 1. \tag{3.18}$$

For other six states provide the three zero sum doublets of (A4), (A5), (A6).

For $r=3$. Apart from eight zero sum triplets of eigenvalues (see Appendix A) and the corresponding eigenstates one obtains for

$$V_1 = |111\rangle + |1\overline{11}\rangle + |\bar{1}1\bar{1}\rangle + |\overline{1}\overline{1}1\rangle, \tag{3.19}$$

$$V_2 = |\overline{111}\rangle + |\bar{1}11\rangle + |1\bar{1}1\rangle + |11\bar{1}\rangle, \tag{3.20}$$

$$T^{(3)}(\theta)(V_1, V_2) = e^{3m_{11}^{(+)}\theta}(V_1, V_2). \tag{3.21}$$

Along with $|222\rangle$ these assure

$$\mathrm{tr}(T^{(3)}(\theta)) = 2e^{3m_{11}^{(+)}\theta} + 1. \tag{3.22}$$

For $r=4$, the two corresponding combinations are

$$V_1 = |1111\rangle + |11\overline{11}\rangle + |1\overline{11}1\rangle + |1\bar{1}1\bar{1}\rangle + |\overline{1111}\rangle + |\overline{11}11\rangle + |\bar{1}1\bar{1}1\rangle + |\bar{1}11\bar{1}\rangle,$$
$$V_2 = |111\bar{1}\rangle + |11\bar{1}1\rangle + |1\bar{1}11\rangle + |\bar{1}111\rangle + |\overline{111}1\rangle + |\overline{11}1\bar{1}\rangle + |\bar{1}1\overline{11}\rangle + |1\overline{111}\rangle, \tag{3.23}$$

with

$$T^{(4)}(\theta)(V_1, V_2) = e^{4m_{11}^{(+)}\theta}(V_1, V_2). \tag{3.24}$$

Along with $|2222\rangle$ these assure

$$\mathrm{tr}(T^{(4)}(\theta)) = 2e^{4m_{11}^{(+)}\theta} + 1. \tag{3.25}$$

The general pattern is now visible. Indeed the general result is that (with relative coefficients in the sums below being all unity as in the example above)

$$V_e = (\text{sum of states with } \textit{even} \text{ number of } |1\rangle),$$
$$V_0 = (\text{sum of states with } \textit{odd} \text{ number of } |1\rangle), \tag{3.26}$$

give

$$T^{(r)}(\theta)(V_e, V_0) = e^{rm_{11}^{(+)}\theta}(V_e, V_0). \tag{3.27}$$

Along with $|22\cdots2\rangle$ they assure

$$\mathrm{tr}(T^{(r)}(\theta)) = 2e^{rm_{11}^{(+)}\theta} + 1. \tag{3.28}$$

All the reaming (3^r-3) states are grouped unto subsets giving "zero-trace" multiplets of eigenvalues involving roots of unity.

This is as far as we propose to go in explicitly constructing the eigenstates. We repeat that, as mentioned in Appendix A, we could obtain the complete sets for $r=1,2,3,4$ the $3,3^2,3^3,3^4$ eigenstates exhaustively.

Let us now compare our approach with that via algebraic Bethe ansatz (Refs. 3, 5, and 6 provide a considerable number of references). For ready comparison we recapitulate the essential results for the relatively simple and well studied case of 6-vertex models. We follow the notation of Ref. 3 for the *ferroelectric regime* in particular. Starting with the 4×4 6-vertex braid matrix and denoting the Nth order transfer matrix blocks as (N, r having *different* significance here as compared to our notations)

$$T^{(N)}(\theta) = \begin{pmatrix} A(\theta) & B(\theta) \\ C(\theta) & D(\theta) \end{pmatrix} \tag{3.29}$$

with

$$\mathrm{tr}(T^{(N)}(\theta)) = A(\theta) + D(\theta). \tag{3.30}$$

The eigenvalues of this trace are extracted from the ansatz

$$\psi(\theta_1,\theta_2,\ldots,\theta_r) = B(\theta_1)B(\theta_2)\cdots B(\theta_r)\left(\left|\begin{matrix}1\\0\end{matrix}\right\rangle_1 \otimes \left|\begin{matrix}1\\0\end{matrix}\right\rangle_2 \otimes \cdots \otimes \left|\begin{matrix}1\\0\end{matrix}\right\rangle_N\right). \tag{3.31}$$

For the chosen regime, denoting

$$\lambda_j = i\left(\theta_j + \frac{\gamma}{2}\right) \tag{3.32}$$

(where γ is the single free parameter of $\hat{R}$) the constraints on the parameters $(\theta_1,\ldots,\theta_r)$ for (3.31) to give eigenstates reduce (due to the Rtt algebra) to

$$\left[\frac{\sin(\lambda_j + i\gamma/2)}{\sin(\lambda_j - i\gamma/2)}\right]^N = -\prod_{k=1}^{r}\frac{\sin(\lambda_j - \lambda_k + i\gamma)}{\sin(\lambda_j - \lambda_k - i\gamma)}. \tag{3.33}$$

One must find the solutions (in general complex) for $(\theta_1,\ldots,\theta_r)$ from these set of nonlinear constraints.

For our case the invariance of the subspaces $S(r,k)$ defined in (2.10) under the action of $T^{(r)}(\theta)$ [our r being N of (3.29)] clearly indicates the choice of

$$|22\cdots 2\rangle = \left|\begin{matrix}0\\1\\0\end{matrix}\right\rangle \otimes \left|\begin{matrix}0\\1\\0\end{matrix}\right\rangle \otimes \cdots \otimes \left|\begin{matrix}0\\1\\0\end{matrix}\right\rangle \tag{3.34}$$

with eigenvalue 1 (for all successive orders r) as the starting point. This is the subspace $S(r,r)$ with only one state.

From (3.1) to (3.28) we have defined and implemented operators which acting on (3.34) moves stepwise through the subspaces

$$S(r,r), S(r,r-1), \ldots, S(r,1), S(r,0). \tag{3.35}$$

For our class of higher dimensional structures, already for $N=3$, the state-labels $(1,2,\bar{1})$ necessitate different types of actions on the index 2. Instead of a single complex θ-dependent matrix [like $B(\theta)$ of (3.31)] we have chosen and systematically implemented the operators (U,A,D) to move

through the sequence (3.35). At each step our formalism leads to relatively simple *linear* constraints, (3.6) giving the complete results for $S(r,r-1)$ being the simplest example. The results (3.26)–(3.28) give the complete trace. The results in Appendix A (for $r=1,2,3,4$ for spaces of 3,9,27,81 dimensions, respectively) give a fair idea of the structure of the eigenvalues.

The fact that one finally solves only sets of linear equations with simple constant coefficients is not evident directly from (3.13)–(3.15), for example. But the fact that one ends up only with eigenvalues of the form $e^{\mu\theta}$ (where, as in Appendix A, μ is a linear function of the parameters $m_{ij}^{(\pm)}$) leads finally to such constraints. For the 3^r-3 eigenvalues of zero total trace one searches for multiplets formed by roots unity and hence summing to zero. This also is very helpful in constructing eigenstates. The eigenvalues, for each r, are known to a certain extent (through certainly not entirely) beforehand.

IV. HAMILTONIANS AND CONSERVED QUANTITIES ($N=3$)

We study here the role of our parameters in the sequence of conserved quantities, the first one in the sequence being chain Hamiltonian.[3,4] (Many source are cited in Ref. 3.) Define

$$H_n = \left.\frac{\partial^n}{\partial\theta^n}\ln T^{(r)}(\theta)\right|_{\theta=0}. \tag{4.1}$$

The commutativity of the transfer matrices $T(\theta)$, $T(\theta')$ implies

$$[H_n,H_m]=0. \tag{4.2}$$

If H_1 is regarded as the Hamiltonian of the system, there is infinite set of conserved quantities.

Using standard results[3,4] and taking account of our normalization and the regularity, i.e.,

$$\hat{R}(0)=PR(0)=I, \tag{4.3}$$

one obtains [since $(P\hat{R}(0))^{-1}(P\partial_\theta\hat{R}(\theta))_{\theta=0}=(\partial_\theta\hat{R}(\theta))_{\theta=0}$]

$$H_1 = (T^{(r)}(0))^{-1}\frac{\partial}{\partial\theta}T^{(r)}(\theta)\bigg|_{\theta=0} = \sum_{k=1}^{r} I\otimes\cdots\otimes\dot{\hat{R}}(0)_{k,k+1}\otimes\cdots\otimes I. \tag{4.4}$$

Note that due to the trace (circular boundary) constraint $k+1=r+1\approx 1$. Indeed starting with $r=2$, evaluating directly and explicitly

$$(T^{(2)}(0))^{-1}\frac{\partial}{\partial\theta}T^{(2)}(\theta)\bigg|_{\theta=0} \tag{4.5}$$

and setting

$$x_\pm=\tfrac{1}{2}(m_{11}^{(+)}\pm m_{11}^{(-)}),\quad y_\pm=\tfrac{1}{2}(m_{12}^{(+)}\pm m_{12}^{(-)}),\quad z_\pm=\tfrac{1}{2}(m_{21}^{(+)}\pm m_{21}^{(-)}), \tag{4.6}$$

one obtains (writing H for H_1 when $r=2$)

$$H = \begin{pmatrix} 2x_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2x_- \\ 0 & y_+ + z_+ & 0 & 0 & 0 & 0 & 0 & y_- + z_- & 0 \\ 0 & 0 & 2x_+ & 0 & 0 & 0 & 2x_- & 0 & 0 \\ 0 & 0 & 0 & y_+ + z_+ & 0 & y_- + z_- & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_- + z_- & 0 & y_+ + z_+ & 0 & 0 & 0 \\ 0 & 0 & 2x_- & 0 & 0 & 0 & 2x_+ & 0 & 0 \\ 0 & y_- + z_- & 0 & 0 & 0 & 0 & 0 & y_+ + z_+ & 0 \\ 2x_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2x_+ \end{pmatrix}$$

$$= \dot{\hat{R}}(0) + P\dot{\hat{R}}(0)P = \dot{\hat{R}}(0)_{12} + \dot{\hat{R}}(0)_{21}, \tag{4.7}$$

where, in evident notations,

$$\dot{\hat{R}}(0)_{12} = (x_+, y_+, x_+, z_+, 0, z_+, x_+, y_+, x_+)_{\text{diag}} + (x_-, y_-, x_-, z_-, 0, z_-, x_-, y_-, x_-)_{\text{antidiag}} \tag{4.8}$$

and

$$\dot{\hat{R}}(0)_{21} = (x_+, z_+, x_+, y_+, 0, y_+, x_+, z_+, x_+)_{\text{diag}} + (x_-, z_-, x_-, y_-, 0, y_-, x_-, z_-, x_-)_{\text{antidiag}}. \tag{4.9}$$

The expressions for (12) and (21) are related through the interchanges

$$(y_\pm, z_\pm) \to (z_\pm, y_\pm). \tag{4.10}$$

The appearance of (21) in (4.7) is consistent with the remark below (4.4).

For higher derivatives one has

$$\frac{d^l}{\mathrm{d}\theta^l}\hat{R}(\theta)\bigg|_{\theta=0} = (x_+^l, y_+^l, x_+^l, z_+^l, 0, z_+^l, x_+^l, y_+^l, x_+^l)_{\text{diag}} + (x_-^l, y_-^l, x_-^l, z_-^l, 0, z_-^l, x_-^l, y_-^l, x_-^l)_{\text{antidiag}}. \tag{4.11}$$

For H_2 one now obtains, as compared to (4.4),

$$H_2 = \sum_{j\neq k} I \otimes \cdots \otimes I \otimes \dot{\hat{R}}(0)_{jj+1} \otimes I \cdots \otimes I \otimes \dot{\hat{R}}(0)_{k,k+1} \otimes I \cdots \otimes I$$

$$+ \sum_k I \cdots \otimes I \otimes \ddot{\hat{R}}(0)_{k,k+1} \otimes I \cdots \otimes I. \tag{4.12}$$

Generalization to higher orders are carried out in evident fashion.

In Sec. 5 of Ref. 1 in constructing θ-expansions the H defined in (5.1) is *precisely* $\dot{\hat{R}}(0)$ of (4.8) above generalized to all odd N, namely $N=3,5,7,\ldots$. There it was noted [Eq. 5.9 of Ref. 1],

$$[H_{12} + H_{23}, [H_{12}, H_{23}]] = 0, \tag{4.13}$$

where $H_{12}=H\otimes I$ and $H_{23}=I\otimes H$. This vanishing double commutator is the simplest version of the Reshetikhin condition given in Eqs. 3.20 of Ref. 2 as

$$[H_{12} + H_{23}, [H_{12}, H_{23}]] = X_{12} - X_{23}, \tag{4.14}$$

the rhs being the difference of two two-point-quantities. In (4.13) the rhs is simply zero.

V. POTENTIAL FOR FACTORIZABLE *S*-MATRICES AND CAYLEY TRANSFORMS (*N*=3)

Potentials for scattering of bosons or fermions with quadratic interaction terms (Sec. 3 of Ref. 2 and Sec. 1 of Ref. 3 provide more references) can correspond to factorizable *S*-matrices (factorizable into two particle scatterings, independently of the chosen order of the latter ones) provided that such potentials are inverse Cayley transforms of Yang-Baxter matrices of appropriate dimensions, i.e., V being the potential (for a chosen helicity fixing the sign of θ)

$$-iV=(R(\theta)-\lambda(\theta)I)^{-1}(R(\theta)+\lambda(\theta)I). \tag{5.1}$$

As compared to Refs. 2 and 3 we display explicitly a free normalization factor

$$(\lambda(\theta))^{-1}R(\theta). \tag{5.2}$$

Our multiparametric case shows clearly that though the normalization (if well-defined) trivially cancels in the YB or the braid equation it must be compatible with the existence of the inverse of

$$(\lambda^{-1}(\theta)R(\theta)-I). \tag{5.3}$$

We will find that

$$\lambda(\theta)\neq(1,e^{m_{11}^{(\pm)}\theta},\pm e^{m_{11}^{(-)}\theta},\pm e^{(1/2)(m_{12}^{(\pm)}+m_{21}^{(\pm)})\theta}). \tag{5.4}$$

The inverse [when $\hat{R}(\theta)$ is given by (1.10)]

$$(\hat{R}(\theta)-\lambda'(\theta)I)^{-1} \tag{5.5}$$

can be shown to exist for

$$\lambda'(\theta)\neq(1,e^{m_{11}^{(\pm)}\theta},e^{m_{12}^{(\pm)}\theta},e^{m_{21}^{(\pm)}\theta}). \tag{5.6}$$

The significance of (5.6) is simple, the rhs exhibiting simply the coefficients of the projectors

$$(P_{22},P_{11}^{(\pm)},P_{12}^{(\pm)},P_{21}^{(\pm)}) \tag{5.7}$$

in (1.10).

Diagonalizing $\hat{R}(\theta)$ the situation becomes particularly transparent [Eqs. (3.4), (3.5) of Ref. 1]. M being given by (3.5) of Ref. 1,

$$M(\hat{R}(\theta)-\lambda'(\theta)I)M^{-1}=(e^{m_{11}^{(+)}\theta},e^{m_{12}^{(+)}\theta},e^{m_{11}^{(+)}\theta},e^{m_{21}^{(+)}\theta},1,e^{m_{21}^{(-)}\theta},e^{m_{11}^{(-)}\theta},e^{m_{12}^{(-)}\theta},e^{m_{11}^{(-)}\theta})_{\mathrm{diag}}-\lambda'(\theta)I. \tag{5.8}$$

When $\lambda'(\theta)$ is equal to any one of the eigenvalues (including 1) the determinant of $[\hat{R}(\theta)-\lambda'(\theta)I]$ vanishes. Hence (5.6).

For (5.1) one requires invertibility of

$$P\hat{R}(\theta)-\lambda(\theta)I. \tag{5.9}$$

The action of P finally leads to (5.4) rather than (5.6).

Defining X through

$$(R(\theta)-\lambda(\theta)I)X=I, \tag{5.10}$$

we present below the explicit form of X for our $N=3$ case,

$$X=\begin{pmatrix} x_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_8 \\ 0 & x_2 & 0 & x_6 & 0 & x_7 & 0 & x_4 & 0 \\ 0 & 0 & x_3 & 0 & 0 & 0 & x_9 & 0 & 0 \\ 0 & x_{10} & 0 & x_2 & 0 & x_4 & 0 & x_{11} & 0 \\ 0 & 0 & 0 & 0 & x_5 & 0 & 0 & 0 & 0 \\ 0 & x_{11} & 0 & x_4 & 0 & x_2 & 0 & x_{10} & 0 \\ 0 & 0 & x_9 & 0 & 0 & 0 & x_3 & 0 & 0 \\ 0 & x_4 & 0 & x_7 & 0 & x_6 & 0 & x_2 & 0 \\ x_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_1 \end{pmatrix}, \tag{5.11}$$

where [writing λ for $\lambda(\theta)$]

$$x_1=\frac{1}{2}\left(\frac{1}{e^{m_{11}^{(+)}\theta}-\lambda}+\frac{1}{e^{m_{11}^{(-)}\theta}-\lambda}\right),\quad x_8=\frac{1}{2}\left(\frac{1}{e^{m_{11}^{(+)}\theta}-\lambda}-\frac{1}{e^{m_{11}^{(-)}\theta}-\lambda}\right),$$

$$x_2=\frac{\lambda}{2}\left(\frac{1}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}+\frac{1}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right),$$

$$x_4=\frac{\lambda}{2}\left(\frac{1}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}-\frac{1}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right),$$

$$x_3=\frac{1}{2}\left(\frac{1}{e^{m_{11}^{(+)}\theta}-\lambda}-\frac{1}{e^{m_{11}^{(-)}\theta}+\lambda}\right),\quad x_9=\frac{1}{2}\left(\frac{1}{e^{m_{11}^{(+)}\theta}-\lambda}+\frac{1}{e^{m_{11}^{(-)}\theta}+\lambda}\right),$$

$$x_5=\frac{1}{1-\lambda}, \tag{5.12}$$

$$x_6=\frac{1}{2}\left(\frac{e^{m_{21}^{(+)}\theta}}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}+\frac{e^{m_{21}^{(-)}\theta}}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right),$$

$$x_7=\frac{1}{2}\left(\frac{e^{m_{21}^{(+)}\theta}}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}-\frac{e^{m_{21}^{(-)}\theta}}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right),$$

$$x_{10}=\frac{1}{2}\left(\frac{e^{m_{12}^{(+)}\theta}}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}+\frac{e^{m_{12}^{(-)}\theta}}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right),$$

$$x_{11}=\frac{1}{2}\left(\frac{e^{m_{12}^{(+)}\theta}}{e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}-\lambda^2}-\frac{e^{m_{12}^{(-)}\theta}}{e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}-\lambda^2}\right).$$

Now, from (5.1), (5.10), and (5.11),

$$\begin{aligned} -iV &= (R(\theta)-\lambda(\theta)I)^{-1}(R(\theta)+\lambda(\theta)I) \\ &= (R(\theta)-\lambda(\theta)I)^{-1}(R(\theta)-\lambda(\theta)I+2\lambda(\theta)I) \\ &= X(X^{-1}+2\lambda(\theta)I), \end{aligned}$$

$$-iV = I + 2\lambda(\theta)X. \tag{5.13}$$

From (5.12) it is evident that X is well-defined only when (5.4) is satisfied. We have thus obtained explicitly, for $N=3$, the potential leading to a factorizable S-matrix. The role played by our parameters is now displayed.

Note that any $\lambda(\theta)$ satisfying (5.4) can be implemented. One many choose to display this dependence on λ by denoting the potential as $V(\lambda)$. With our $V(\lambda)$ one now considers the fermionic Lagrangian

$$\mathcal{L} = \int \mathrm{d}x(i\bar{\psi}_a\gamma_v\partial_v\psi_a - g(\bar{\psi}_a\gamma_v\psi_c)V_{ab,cd}(\bar{\psi}_b\gamma_v\psi_d)), \tag{5.14}$$

where

$$V = \sum_{ab,cd}(V_{ab,cd})(ab)\otimes(cd). \tag{5.15}$$

There is an analogous, simpler, formulation for bosons. We will not further analyze the consequences of our V. But it should be compared to the detailed studies of the solutions obtained in Refs. 7 and 8.

VI. $N>3$

So far we have studied the case $N=3$ in detail. Now we indicate briefly the crucial new features arising for $N>3$. Many aspects are conserved also, as will be pointed out.

The first major feature is the generalization of (2.1). For $N=2p-1$, one obtains

$$\mathrm{tr}(T^{(r)}(\theta)) = 2(e^{rm_{11}^{(+)}\theta} + e^{rm_{22}^{(+)}\theta} + \cdots + e^{rm_{p-1,p-1}^{(+)}\theta}) + 1, \quad p = 2,3,4,\ldots. \tag{6.1}$$

There are

$$2(p-1)+1 = 2p-1 = N \tag{6.2}$$

terms. An explanation, promised below (2.1), is as follows. *Only the diagonal blocks $t_{ii}(\theta)$ have diagonal terms*. Thus in (2.5) only $t_{11}(\theta)$, $t_{22}(\theta)$, $t_{\bar{1}\bar{1}}(\theta)$, has nonzero elements on the diagonal, their sum being

$$\mathrm{tr}(T^{(1)}(\theta)) = 2(a_+ + a_-) + 1 = 2e^{m_{11}^{(+)}\theta} + 1 \quad (r=1). \tag{6.3}$$

For $r=2$ (and $N=3$) one obtains from the coproduct structure

$$\begin{aligned}\mathrm{tr}(T^{(2)}(\theta)) &= \mathrm{tr}((a_+a_+,0,a_+a_-)_{\mathrm{diag}} + (0,1,0)_{\mathrm{diag}} + (a_-a_-,0,a_-a_+)_{\mathrm{diag}} + (a_-a_+,0,a_-a_-)_{\mathrm{diag}} \\ &\quad + (a_+a_-,0,a_+a_+)_{\mathrm{diag}}) + \mathrm{tr}(\text{blocks with nondiagonal terms only}) = 2(a_+ + a_-)^2 + 1, \\ &\mathrm{tr}(T^{(2)}(\theta)) = 2e^{2m_{11}^{(+)}\theta} + 1,\end{aligned} \tag{6.4}$$

and so on.

For $N>3$ the basic features persist. Along with the crucial constraint (1.8)

$$m_{ij}^{(\epsilon)} = m_{\bar{i}\bar{j}}^{(\epsilon)} \quad (\bar{j} = 2p-j) \tag{6.5}$$

which symmetrizes the blocks on the diagonal [generalizing (1.10)], the final result is

$$\mathrm{tr}(T^{(r)}(\theta)) = 2\sum_{i=1}^{p-1}(a_{ii}^{(+)} + a_{ii}^{(-)})^r + 1 \tag{6.6}$$

$$=2\sum_{i=1}^{p-1} e^{rm_{ii}^{(+)}\theta}+1. \tag{6.7}$$

The result is obtained directly by looking closely at the structure of the matrices concerned, *without constructing eigenstates and their eigenvalues*. We have checked (6.7) directly and explicitly for arbitrary p (Appendix A). But this result has profound consequence on the spectrum of the eigenvalues for each r. Given (N,r) and the coproduct rule,

(1) the number of eigenvalues for $T^{(r)}(\theta)=N^r$,
(2) the number of eigenvalues contributing in the trace$=N$,
(3) the remaining (N^r-N) eigenvalues must sum to give zero contribution in the trace.

For $N=3$ we have shown (Appendix A) how this constraint is satisfied via the multiplet structures

$$e^{\mu\theta}(1,\omega_{(l)},\omega_{(l)}^{(2)},\ldots,\omega_{(l)}^{l-1}),\quad \omega_{(l)}=e^{2\pi i/l},$$
$$1+\omega_{(l)}+\omega_{(l)}^2+\cdots+\omega_{(l)}^{(l-1)}=0, \tag{6.8}$$

where μ is linear in $m_{ij}^{(\pm)}$ and for

$$r=2,\quad l=2,$$
$$r=3,\quad l=3, \tag{6.9}$$
$$r=4,\quad l=2,4,$$

and so on.

This multiplet structure involving roots of unity can also be shown to be carried over for $N>3$ explicitly. But apart from the fact that the number of eigenstates and the number of states in the linear combinations giving eigenstates increase very fast there are no other basic difficulties.

For $N=5$, for example, generalizing the basis (2.7), for $p=3$, to

$$\left\langle \begin{pmatrix}1\\0\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\0\\1\end{pmatrix} \right\rangle \equiv (|1\rangle,|2\rangle,|3\rangle,|\bar{2}\rangle,|\bar{1}\rangle,) \tag{6.10}$$

one again obtains subspaces stable under the action of $T^{(r)}(\theta)$,

$$S(r,k)\quad (k=0,1,\ldots,r), \tag{6.11}$$

where k is now the multiplicity of the index 3. The operator structures (3.1), (3.2), (3.3) are now generalized, in terms of operators $(t_{31}(\theta),t_{3\bar{1}}(\theta))$, $(t_{32}(\theta),t_{3\bar{2}}(\theta))$, $t_{33}(\theta)$ to construct

$$U_1|3\rangle=|1\rangle,\quad U_2|3\rangle=|2\rangle,$$
$$D_1|3\rangle=|\bar{1}\rangle,\quad D_2|3\rangle=|\bar{2}\rangle, \tag{6.12}$$
$$A|3\rangle=|3\rangle.$$

The subspace $S(r,r)$ is still given by a single state

$$T^{(r)}(\theta)|33\cdots3\rangle = |33\cdots3\rangle. \tag{6.13}$$

The subspace $S(r,r-1)$ is now spanned by $4r$ (instead of $2r$ for $N=3$) states and is easily diagonalized.

The stepwise generalization for $N=7,9,\ldots$ is now fairly evident. The dimensions of $S(r,k)$ is given by a generalization of (2.11) by the successive coefficients in

$$(x+2(p-1))^r = 1\cdot x^r + 2r(p-1)x^{r-1} + \cdots + (2(p-1))^{r-k}\binom{r}{r-k}x^k + \cdots + (2(p-k))^r. \tag{6.14}$$

For $x=1$, one gets the total dimension

$$(2p-1)^r = N^r. \tag{6.15}$$

The generalization of (3.26) is also fairly direct. When the order r of $T^r(\theta)$ is a prime number there is an amusing encounter with a theorem of Fermat in considering our multiplet structures. This is discussed in Appendix B.

The generalization of the structure of the Hamiltonian of Sec. IV involving $\dot{\hat{R}}(0)$ of (4.8) is particulary straightforward. But even for $N=5$ we have 24 nonzero terms on the diagonal and as many on the antidiagonal.

The potential (5.1) for $N=5,7,\ldots$ now involve inversions of N^2 dimensional matrices $(R(\theta)-\lambda(\theta)I)$. This is again straightforward, given our specific structure of $\hat{R}(\theta)$, but evidently lengthly.

Apart from such general indications as presented above systematic studies for cases $N>3$ are beyond the scope of this work. In particular possible substructures in each subspace $S(r,k)$ corresponding to multiplicities of different indices [say $(1,\bar{1})$ and $(2,\bar{2})$ for $N=5$] should be formulated with care.

VII. GENERALIZATION OF THE NESTED SEQUENCE OF PROJECTORS

The sequence of projectors (1.3), forming a complete orthonormalized basis admits the more general parametrization displayed below (for odd N)

$$P_{pp} = (pp)\otimes(pp),$$

$$(u_{pi}+u_{pi}^{-1})P_{pi(\pm)} = (pp)\otimes[u_{pi}^{\pm1}(ii)+u_{pi}^{\mp1}(\bar{i}\bar{i})\pm(v_{pi}(i\bar{i})+v_{pi}^{-1}(\bar{i}i))],$$

$$(u_{ip}+u_{ip}^{-1})P_{ip(\pm)} = [u_{ip}^{\pm1}(ii)+u_{ip}^{\mp1}(\bar{i}\bar{i})\pm(v_{ip}(i\bar{i})+v_{ip}^{-1}(\bar{i}i))]\otimes(pp), \tag{7.1}$$

$$(u_{ij}+u_{ij}^{-1})P_{ij(\epsilon)} = u_{ij}^{\pm1}(ii)\otimes(jj)+u_{ij}^{\mp1}(\bar{i}\bar{i})\otimes(\bar{j}\bar{j})\pm[v_{ij}(i\bar{i})\otimes(j\bar{j})+v_{ij}^{-1}(\bar{i}i)\otimes(\bar{j}j)],$$

$$(u_{i\bar{j}}+u_{i\bar{j}}^{-1})P_{i\bar{j}(\epsilon)} = u_{i\bar{j}}^{\pm1}(ii)\otimes(\bar{j}\bar{j})+u_{i\bar{j}}^{\mp1}(\bar{i}\bar{i})\otimes(jj)\pm[v_{i\bar{j}}(i\bar{i})\otimes(\bar{j}j)+v_{i\bar{j}}^{-1}(\bar{i}i)\otimes(j\bar{j})],$$

where the supplementary parameters introduced are compatible with the orthonormality and completeness conditions (1.5). For even N also an analogues pammetrization can be introduced. Thus 6-vertex and 8-vertex projector basis [given in (6.1) of Ref. 1] can be generalized to

$$(u_{11}+u_{11}^{-1})P_{11(\pm)}=\begin{pmatrix} u_{11}^{\pm 1} & 0 & 0 & \pm v_{11} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \pm v_{11}^{-1} & 0 & 0 & u_{11}^{\mp 1} \end{pmatrix},$$

$$(u_{1\bar{1}}+u_{1\bar{1}}^{-1})P_{1\bar{1}(\pm)}=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & u_{1\bar{1}}^{\pm 1} & \pm v_{1\bar{1}} & 0 \\ 0 & \pm v_{1\bar{1}}^{-1} & u_{1\bar{1}}^{\mp 1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{7.2}$$

Braid matrices on such bases of projectors and associated statistical models can be studied systematically. Such a study will be presented elsewhere with suitable restrictions on parameters for specific solutions. Setting $u_{ab}=v_{ab}=1$ for all values of the indices one recovers the projectors of (1.3).

VIII. DISCUSSION

Our results presented above, are limited to formal study of the transfer matrix, construction of chain Hamiltonians and potentials corresponding to factorizable S-matrices. Adequate study of the, consequences of the features obtained, of their deeper significance remains to be done. The role of our parameters should be analyzed in various domains for comparison with corresponding features of well-known statistical models.[3,9–11] Our braid matrices encode star-triangle relations.

Certain features are, of course, immediately available for our case. Thus the free energy (defined with the opposite sign in Ref. 10), is given by the maximum eigenvalue ($\theta>0$) as

$$f=-\lim_{r\to\infty}\frac{1}{r}\ln e^{rm_{11}^{(+)}\theta}=-m_{11}^{(+)}\theta \tag{8.1}$$

if we choose, say, the order

$$m_{11}^{(+)}>m_{22}^{(+)}>\cdots>m_{p-1,p-1}^{(+)}. \tag{8.2}$$

In our case results depend on the sector of the parameters selected (their ordering). The second largest eigenvalue, also of particular interest, is again directly obtained once the ordering is fixed.

Correlation functions are of major interest and a domain of intense activity.[12,13] Here our model can have quite interesting consequences. This aspect also remains to be explored.

We intend to continue our study elsewhere. But we consider the series of remarkable features presented here to be sufficiently rich in content. They open up a significantly different domain, as compared to standard, well known cases.

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APPENDIX A: EIGENVALUES OF $T^{(r)}(\theta)$ FOR $N=3$, $r=1,2,3,4$ AND DIRECT CONSTRUCTION OF TRACE FOR $N>3$

For each r, the eigenvalues of $T^{(r)}(\theta)$ are given systematically for the subspaces $S(r,k)$ defined in (2.10), for $k=0,1,\ldots,r$.

$r=1$(dim 3):

$$S(1,0)(\dim 2): \quad \begin{matrix} \text{eigenvalues} \\ e^{m_{11}^{(+)}\theta}(1,1), \end{matrix} \tag{A1}$$

$$S(1,1)(\dim 1): \quad 1, \tag{A2}$$

$$\mathrm{tr}(T^{(1)}(\theta)) = 2e^{m_{11}^{(+)}\theta} + 1. \tag{A3}$$

r=2(dim 9):

$$S(2,0)(\dim 4): \quad \begin{matrix} e^{2m_{11}^{(+)}\theta}(1,1), \\ e^{2m_{11}^{(-)}\theta}(1,-1); \end{matrix} \tag{A4}$$

$$S(2,1)(\dim 4): \quad \begin{matrix} e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}(1,-1), \\ e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta}(1,-1); \end{matrix} \tag{A5}$$

$$S(2,2)(\dim 1): \quad 1; \tag{A6}$$

$$\mathrm{tr}(T^{(2)}(\theta)) = 2e^{2m_{11}^{(+)}\theta} + 1. \tag{A7}$$

r=3(dim 27):

$$S(3,0)(\dim 8): \quad \begin{matrix} e^{3m_{11}^{(+)}\theta}(1,1), \\ e^{(m_{11}^{(+)}+2m_{11}^{(-)})\theta}(1,e^{2\pi i/3},e^{(2\pi i/3)2}) \quad [2 \text{ times}]; \end{matrix} \tag{A8}$$

$$S(3,1)(\dim 12): \quad \begin{pmatrix} e^{(m_{11}^{(+)}+m_{12}^{(+)}+m_{21}^{(+)})\theta} \\ e^{(m_{11}^{(+)}+m_{12}^{(-)}+m_{21}^{(-)})\theta} \\ e^{(m_{11}^{(-)}+m_{12}^{(+)}+m_{21}^{(-)})\theta} \\ e^{(m_{11}^{(-)}+m_{12}^{(-)}+m_{21}^{(+)})\theta} \end{pmatrix} (1,e^{2\pi i/3},e^{(2\pi i/3)2}); \tag{A9}$$

$$S(3,2)(\dim 6): \quad \begin{pmatrix} e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta} \\ e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta} \end{pmatrix} (1,e^{2\pi i/3},e^{(2\pi i/3)2}); \tag{A10}$$

$$S(3,3)(\dim 1): \quad 1; \tag{A11}$$

$$\mathrm{tr}(T^{(3)}(\theta)) = 2e^{3m_{11}^{(+)}\theta} + 1. \tag{A12}$$

r=4(dim 81):

$$S(4,0)(\dim 16): \quad \begin{matrix} e^{4m_{11}^{(+)}\theta}(1,1), \\ e^{2(m_{11}^{(+)}+m_{11}^{(-)})\theta}(1,e^{2\pi i/4},e^{(2\pi i/4)\cdot 2},e^{(2\pi i/4)\cdot 3}) \quad [3 \text{ times}]; \\ e^{4m_{11}^{(-)}\theta}(1,-1), \end{matrix} \tag{A13}$$

$$
\begin{aligned}
S(4,1)(\dim 32): \quad & e^{(m_{11}^{(+)}+m_{11}^{(-)}+m_{12}^{(+)}+m_{21}^{(-)})\theta}(1,e^{2\pi i/4},e^{(2\pi i/4)\cdot 2},e^{(2\pi i/4)\cdot 3},) \quad [2 \text{ times}],\\
& e^{(m_{11}^{(+)}+m_{11}^{(-)}+m_{12}^{(-)}+m_{21}^{(+)})\theta}(1,e^{2\pi i/4},e^{(2\pi i/4)\cdot 2},e^{(2\pi i/4)\cdot 3},) \quad [2 \text{ times}];\\
& \begin{pmatrix} e^{(2m_{11}^{(+)}+m_{12}^{(+)}+m_{21}^{(+)})\theta}\\ e^{(2m_{11}^{(+)}+m_{12}^{(-)}+m_{21}^{(-)})\theta}\\ e^{(2m_{11}^{(-)}+m_{12}^{(+)}+m_{21}^{(+)})\theta}\\ e^{(2m_{11}^{(-)}+m_{12}^{(-)}+m_{21}^{(+)})\theta} \end{pmatrix}(1,e^{2\pi i/4},e^{(2\pi i/4)\cdot 2},e^{(2\pi i/4)\cdot 3},),
\end{aligned} \tag{A14}
$$

$$
\begin{aligned}
S(4,2)(\dim 24): \quad & \begin{pmatrix} e^{2(m_{12}^{(+)}+m_{21}^{(+)})\theta}\\ e^{2(m_{12}^{(-)}+m_{21}^{(-)})\theta} \end{pmatrix}(1,-1),\\
& e^{(m_{12}^{(+)}+m_{12}^{(-)}+m_{21}^{(+)}+m_{21}^{(-)})\theta}(1,e^{2\pi i/4},e^{(2\pi i/4)\cdot 2},e^{(2\pi i/4)\cdot 3}),\\
& \begin{pmatrix} e^{(m_{11}^{(+)}+m_{12}^{(+)}+m_{21}^{(+)})\theta}\\ e^{(m_{11}^{(+)}+m_{12}^{(-)}+m_{21}^{(-)})\theta}\\ e^{(m_{11}^{(-)}+m_{12}^{(+)}+m_{21}^{(-)})\theta}\\ e^{(m_{11}^{(-)}+m_{12}^{(-)}+m_{21}^{(+)})\theta} \end{pmatrix}(1,e^{2\pi i/4},e^{2\pi i/4\cdot 2},e^{2\pi i/4\cdot 3});
\end{aligned} \tag{A15}
$$

$$
S(4,3)(\dim 8): \quad \begin{pmatrix} e^{(m_{12}^{(+)}+m_{21}^{(+)})\theta}\\ e^{(m_{12}^{(-)}+m_{21}^{(-)})\theta} \end{pmatrix}(1,e^{2\pi i/4},e^{2\pi i/4\cdot 2},e^{2\pi i/4\cdot 3}); \tag{A16}
$$

$$
S(4,4)(\dim 1): \quad 1; \tag{A17}
$$

$$
\operatorname{tr}(T^{(4)}(\theta)) = 2e^{4m_{11}^{(+)}\theta} + 1. \tag{A18}
$$

Now we indicate briefly the direct construction of trace for all N, without constructing the full set of eigenvalues explicitly.

Set, for the coefficients on the diagonal and the antidiagonal, respectively,

$$
d_{ij} = \tfrac{1}{2}(e^{m_{ij}^{(+)}\theta} + e^{m_{ij}^{(-)}\theta}) = d_{i\bar{j}}, \quad a_{ij} = \tfrac{1}{2}(e^{m_{ij}^{(+)}\theta} + e^{m_{ij}^{(-)}\theta}) = a_{i\bar{j}}, \tag{A19}
$$

where

$$
i = 1,2,\ldots,p-1, \quad \bar{i} = (2p-1),\ldots,(p+1), \quad p = \tfrac{1}{2}(N+1). \tag{A20}
$$

From (1.7) and (1.15)

$$
\begin{aligned}
t(\theta) = & \sum_i ((pi)\otimes(d_{ip}(ip)+a_{ip}(\bar{i}\bar{p})) + (p\bar{i})\otimes(a_{ip}(ip)+d_{ip}(\bar{i}\bar{p})) + (ip)\otimes(d_{pi}(pi)+a_{pi}(p\bar{i}))\\
& + (\bar{i}\bar{p})\otimes(a_{pi}(pi)+d_{pi}(p\bar{i}))) + \sum_{ij}((ji)\otimes(d_{ij}(ij)+a_{ij}(\bar{i}\bar{j})) + (\bar{j}\bar{i})\otimes(a_{ij}(ij)+d_{ij}(\bar{i}\bar{j})) + (j\bar{i})\\
& \otimes(d_{ij}(\bar{i}j)+a_{ij}(i\bar{j})) + (\bar{j}i)\otimes(d_{ij}(\bar{i}j)+a_{ij}(i\bar{j}))) + \sum_i((i\bar{i})\otimes(d_{ii}(\bar{i}\bar{i})+a_{ii}(ii)) + (\bar{i}\bar{i})\otimes(a_{ii}(\bar{i}\bar{i})\\
& + d_{ii}(i\bar{i}))) + \sum_i((ii)\otimes(d_{ii}(ii)+a_{ii}(\bar{i}\bar{i})) + (\bar{i}\bar{i})\otimes(a_{ii}(ii)+d_{ii}(\bar{i}\bar{i}))) + (pp)\otimes(pp).
\end{aligned} \tag{A21}
$$

Crucial features to be noted are the following:

(1) Only the diagonal blocks have nonzero terms on the diagonal.
(2) In each such block there are only two nonzero terms (with only one for the pth).

(3) These features are iterated under successive coproducts.

Thus

$$\mathrm{tr}(T(\theta)) = \mathrm{tr}\left(\sum_i (t_{ii}(\theta) + t_{\bar{i}\bar{i}}(\theta)) + t_{pp}(\theta)\right) = 2\sum_i (d_{ii} + a_{ii}) + 1 = 2\sum_i e^{m_{ii}^{(+)}\theta} + 1, \tag{A22}$$

$$\mathrm{tr}(T^{(2)}(\theta)) = 2\sum_i (d_{ii}(d_{ii} + a_{ii}) + a_{ii}(d_{ii} + a_{ii})) + 1 = 2\sum_i (d_{ii} + a_{ii})^2 + 1 = 2\sum_i e^{2m_{ii}^{(+)}\theta} + 1, \tag{A23}$$

and continuing stepwise

$$\mathrm{tr}(T^{(r)}(\theta)) = 2\sum_{i=1}^{p-1} (d_{ii} + a_{ii})^r + 1 = 2\sum_{i=1}^{p-1} e^{rm_{ii}^{(+)}\theta} + 1. \tag{A24}$$

This is how the structure of our projector basis leads to a direct evaluation of $\mathrm{tr}(T^{(r)}(\theta))$ for the general case without the full list of eigenvalues. The trace is given by $2(p-1)+1=2p-1=N$ eigenvalues. The remaining (N^r-N) eigenvalues give zero trace, as we have seen, due to multiplet structures corresponding to roots of unity.

APPENDIX B: ENCOUNTER WITH A THEOREM OF FERMAT

A well-known theorem of Fermat states

$$N^r = N \bmod r, \tag{B1}$$

where (N, r) are positive integers and r is a prime number. Writing it as

$$N^r - N = rM, \tag{B2}$$

we try to obtain the integer M explicitly with the following purpose.

In Sec. VI we noted that out of N^r eigenvalues of the transfer matrix $T^{(r)}(\theta)$ of order $r(N^r - N)$ eigenvalues must give zero trace when summed. We have also seen how such a zero trace constraint is implemented in our case through multiplets corresponding to roots of unity as explained in (6.8)–(6.10). When r is a prime number the minimal multiplets can be consistently "r-plets" (or "nr-plets") only if (B2) is satisfied. But precisely this is guaranteed by (B1). This is the link of our multiplet structure with (B1). When r is factorizable one can have lower multiplets $(r_1, r_2, \ldots)$ for, say, $r = r_1 \cdot r_2 \cdots r_n$. This is already seen for $r=4$ in (6.10). We are interested here in odd integers N, but (B2) holds also for even N. We now construct M giving the number of r-plets.

Different constructions of M are certainly possible. The one particularly suitable for our purpose is as follow. One has for $r = 1, 3, 5, 7, 11, \ldots$, respectively,

$$N - N = 0,$$

$$N^3 - N = (N-1)N(N+1),$$

$$N^5 - N = (N-2)(N-1)N(N+1)(N+2) + 5(N-1)N(N+1),$$

$$N^7 - N = (N-3)(N-2)(N-1)N(N+1)(N+2)(N+3)$$

$$+ 7(2(N-2)(N-1)N(N+1)(N+2) + 3(N-1)N(N+1)).$$

Continuing thus with product of consecutive factors

$$N^{11}-N=(N-5)\cdots N\cdots(N+5)+11[5(N-4)\cdots N\cdots(N+4)+57(N-3)\ldots N\ldots(N+3)$$
$$+128(N-2)\cdots N\cdots(N+2)+31(N-1N(N+1))]. \tag{B3}$$

Thus for $N=3$, $r=3,5,7,\ldots$, one has, respectively, eight triplets, 48 5-plets, 312 7-plets, and so on (unless 10-plets, 14-plets, and so on are also obtained).

The first term is

$$\left(N-\frac{r-1}{2}\right)\cdots\left(N+\frac{r-1}{2}\right) \tag{B4}$$

and being a product of r consecutive integers, evidently divisible by r. The lower order products all have r as a factor. Hence the result. When $N\leqslant(r-1)/2$ one or more higher order products vanish. Although now N^r is not directly, visibly present on the right-hand side, the results still hold. Thus though $(N-3)$ vanishes in the leading term,

$$3^7-3=0+7\times(312). \tag{B5}$$

For completeness we give the general result below

$$N^r-N=\sum_{p=1}^{(r-1)/2}A_p(r)\prod_{k=-p}^{p}(N+k)\equiv\sum_{p=0}^{(r-1)/2}A_p(r)B(N,p), \tag{B6}$$

where

$$A_{(r-1)/2}(r)=1,$$

$$A_{(r-2k+1)/2}(r)=\sum_{m_1=1}^{k-1}\sum_{m_2=1}^{m_1-1}\cdots\sum_{m_{k-1}=1}^{m_{k-2}-1}\left[-\frac{H_{m_1}^{2k-2m_1}(r)}{(2k-2m_1)!}\right]\times\left[-\frac{H_{m_2}^{2m_1-2m_2}(r)}{(2m_1-2m_2)!}\right]\times\cdots$$

$$\times\left[-\frac{H_{m_{k-1}}^{2m_{k-2}-2m_{k-1}}(r)}{(2m_{k-2}-2m_{k-1})!}\right],\quad k=2,3,\ldots,\frac{r-1}{2}. \tag{B7}$$

The elements H_k^m are given by

$$H_k^m(r)=\left(\sum_{p_1=-(r-2k+1)/2}^{(r-2k+1)/2}p_1\right)\left(\sum_{\substack{p_2=-(r-2k+1)/2\\ p_2\neq p_1}}^{(r-2k+1)/2}p_2\right)\cdots\left(\sum_{\substack{p_m=-(r-2k+1)/2\\ p_m\neq p_1,\ldots,p_{m-1}}}^{(r-2k+1)/2}p_m\right),\quad m\neq 0,$$
$$H_k^0(r)=1. \tag{B8}$$

For example,

$$H_k^2(r)=-\tfrac{1}{12}(r-2k+1)(r-2k+2)(r-2k+3),$$

$$H_k^4(r)=\tfrac{1}{240}(5r+17-10k)(r+3-2k)(r-2k+2)(r-2k+1)(r-2k)(r-1-2k),$$

$$H_{(r-2k+1)/2}^{2k}(r)=(-1)^k(2k)!\,(k!)^2,\quad k=0,\ldots,\frac{r-1}{2},$$

$$H_{(r-2p+1)/2}^{2p+2k-r-1}(r)=(2p+2k-r-1)!\left.\frac{d^{r-2k+2}B(N,p)}{dN^{r-2k+2}}\right|_{N=0},\quad p=\frac{r-2k+1}{2},\ldots,\frac{r-1}{2},$$

$$H_{m_1}^{2k-2m_1}(r) = (2k-2m_1)!\ \left.\frac{d^{2m_1+1}B\left(N,\frac{r-2m_1+1}{2}\right)}{\mathrm{d}N^{2m_1+1}}\right|_{N=0}, \quad m_1 = k, \ldots, \frac{r-1}{2}. \tag{B9}$$

The above formula gives the general expression for the coefficients. But, as A. Lascoux has pointed out, the symmetric form of Newton's interpolation formula relevant for our case leads to complete functions as coefficients. These can be obtained systematically and conveniently. Thus one obtains, for example

$$\begin{aligned} N^{11} - N = {} & (N-5)\cdots N\cdots(N+5) \\ & + (N-4)\cdots N\cdots(N+4)(1^2+2^2+3^2+4^2+5^2) \\ & + (N-3)\cdots N\cdots(N+3)(1^4+2^4+3^4+4^4+1^2\times 2^2+1^2\times 3^2 \\ & + 1^2\times 4^2+2^2\times 3^2+2^2\times 4^2+3^2\times 4^2) \\ & + (N-2)\cdots N\cdots(N+2)(1^6+2^6+3^6+1^4\times 3^2+2^4\times 3^2 \\ & + 2^4\times 1^2+3^4\times 1^2+3^4\times 2^2+1^4\times 2^2+1^2\times 2^2\times 3^2) \\ & + (N-1)N(N+1)(1^8+2^8+1^6\times 2^2+2^6\times 1^2+1^4\times 2^4). \end{aligned} \tag{B10}$$

This gives (B3) in which 11 is already factorized.

APPENDIX C: $\hat{R}tt$-ALGEBRA

We present below a canonical formulation of the $\hat{R}tt$ algebra[14] specifically adapted to our case. The Baxterized form with N^2 blocks of $N\times N$ matrices $t_{ij}(\theta)$ must satisfy

$$\hat{R}(\theta-\theta')(t(\theta)\otimes t(\theta')) = (t(\theta')\otimes t(\theta))\hat{R}(\theta-\theta'), \tag{C1}$$

where (since $P^2=I$)

$$t(\theta)\otimes t(\theta') = (t(\theta)\otimes I)(I\otimes t(\theta)) \equiv t_1(\theta)t_2(\theta) = (t_1(\theta)P)(Pt_2(\theta)). \tag{C2}$$

But $t_1(\theta)=Pt_2(\theta)P$, hence

$$t_1(\theta)P = t_2(\theta)P \equiv \hat{t}(\theta). \tag{C3}$$

Thus

$$\hat{R}(\theta-\theta')\hat{t}(\theta)\hat{t}(\theta') = \hat{t}(\theta')\hat{t}(\theta)\hat{R}(\theta-\theta'), \tag{C4}$$

where one has just matrix multiplication of the same matrix $\hat{t}$ with arguments (θ,θ').

Now suppose that one has obtained explicitly the diagonalizer M of $\hat{R}(\theta)$. When

$$\hat{R}(\theta) = \sum_{\alpha,\beta} f_{\alpha,\beta}(\theta)P_{\alpha,\beta}, \tag{C5}$$

where $P_{\alpha\beta}$ form a complete basis of θ-independent projectors (and the minimal polynomial equation satisfied by $\hat{R}(\theta)$ has no multiple roots for consistency) one can construct a θ-independent M to diagonalize each $P_{\alpha\beta}$ simultaneously. For our nested sequence of projectors (1.3) the diagonalizer is given in Sec. III of Ref. 1 as

$$\begin{aligned}\sqrt{2}M = \sqrt{2}M^{-1} &= \sqrt{2}(pp)\otimes(pp)\\ &+ (pp)\otimes\left(\sum_i ((ii)-(\bar{i}\bar{i})+(i\bar{i})+(\bar{i}i))\right)\\ &+ \left(\sum_i ((ii)-(\bar{i}\bar{i})+(i\bar{i})+(\bar{i}i))\right)\otimes(pp)\\ &+ \sum_{ij}(((ii)-(\bar{i}\bar{i}))\otimes((jj)+(\bar{j}\bar{j}))+((i\bar{i})+(\bar{i}i))\otimes((j\bar{j})+(\bar{j}j))),\end{aligned} \tag{C6}$$

where

$$i = 1,2,\ldots,p-1,\quad \bar{i} = 2p-1,\ldots,p+1,\quad N = 2p-1. \tag{C7}$$

For $N=3$ ($p=2$), one obtains [see (3.5) of Ref. 1]

$$\sqrt{2}M = \sqrt{2}M^{-1} = (1,1,1,1,\sqrt{2},-1,-1,-1,-1)_{\text{diag}} + (1,1,1,1,\sqrt{2},1,1,1,1)_{\text{antidiag}} \tag{C8}$$

($\sqrt{2}$ being the common element of diag and antidiag).

The general case is now evident. Defining

$$M\hat{R}(\theta)M^{-1} = D(\theta) \tag{C9}$$

a diagonal matrix and

$$M\hat{t}(\theta)M^{-1} = K(\theta) \tag{C10}$$

quite generally

$$D(\theta-\theta')K(\theta)K(\theta') = K(\theta')K(\theta)D(\theta-\theta'). \tag{C11}$$

This is our canonical formulation.[15] For our present case (3.3), (3.4) of Ref. 1,

$$D(\theta) = \left(e^{m_{11}^{(+)}\theta}, e^{m_{12}^{(+)}\theta}, \ldots, e^{m_{11}^{(-)}\theta}\right). \tag{C12}$$

From (C11)

$$D_{aa}(\theta-\theta')K_{ac}(\theta)K_{cb}(\theta') = K_{ac}(\theta')K_{cb}(\theta)D_{bb}(\theta-\theta'). \tag{C13}$$

For $N=3$, for our case, defining the 3×3 diagonal blocks

$$\begin{aligned} d_{11}(\theta) &= (e^{m_{11}^{(+)}\theta}, e^{m_{12}^{(+)}\theta}, e^{m_{11}^{(+)}\theta})_{\text{diag}},\\ d_{22}(\theta) &= (e^{m_{21}^{(+)}\theta}, 1, e^{m_{21}^{(-)}\theta})_{\text{diag}},\\ d_{\bar{1}\bar{1}}(\theta) &= (e^{m_{11}^{(-)}\theta}, e^{m_{12}^{(-)}\theta}, e^{m_{11}^{(-)}\theta})_{\text{diag}},\end{aligned} \tag{C14}$$

and denoting $(K(\theta),K(\theta'),D(\theta-\theta'))\equiv(K,K',D'')$ when $d_{11}(\theta-\theta')\equiv d''_{11}$ and so on

$$\begin{pmatrix} d''_{11}(KK')_{11} & d''_{11}(KK')_{12} & d''_{11}(KK')_{1\bar{1}} \\ d''_{22}(KK')_{21} & d''_{22}(KK')_{22} & d''_{22}(KK')_{2\bar{1}} \\ d''_{\bar{1}\bar{1}}(KK')_{\bar{1}1} & d''_{\bar{1}\bar{1}}(KK')_{\bar{1}2} & d''_{\bar{1}\bar{1}}(KK')_{\bar{1}\bar{1}} \end{pmatrix} = \begin{pmatrix} (K'K)_{11}d''_{11} & (K'K)_{12}d''_{22} & (K'K)_{1\bar{1}}d''_{\bar{1}\bar{1}} \\ (K'K)_{21}d''_{11} & (K'K)_{22}d''_{22} & (K'K)_{2\bar{1}}d''_{\bar{1}\bar{1}} \\ (K'K)_{\bar{1}1}d''_{11} & (K'K)_{\bar{1}2}d''_{22} & (K'K)_{\bar{1}\bar{1}}d''_{\bar{1}\bar{1}} \end{pmatrix}. \tag{C15}$$

Substituting the explicit form of $(KK')_{ij}$ one obtains the full set of 81 relations (for $N=3$) of the $\hat{R}tt$-algebra. Each K_{ij} is a 3×3 block whose elements are the blocks of t_{ij}. Thus

$$2K_{11}=\begin{pmatrix} t_{11}+t_{\bar{1}\bar{1}} & t_{12}+t_{\bar{1}2} & t_{1\bar{1}}+t_{\bar{1}1} \\ 0 & 0 & 0 \\ t_{1\bar{1}}+t_{\bar{1}1} & t_{12}+t_{\bar{1}2} & t_{11}+t_{\bar{1}\bar{1}} \end{pmatrix} = (t_{11}+t_{\bar{1}\bar{1}})((11)+(\bar{1}\bar{1}))+(t_{12}+t_{\bar{1}2})((12)+(\bar{1}2))+(t_{1\bar{1}}+t_{\bar{1}1}) \times((1\bar{1})+(\bar{1}1)). \tag{C16}$$

In such a notation

$$2K_{\bar{1}\bar{1}}=(t_{11}+t_{\bar{1}\bar{1}})(-(11)+(\bar{1}\bar{1}))+(t_{12}+t_{\bar{1}2})(-(12)+(\bar{1}2))+(t_{1\bar{1}}+t_{\bar{1}1})(-(1\bar{1})+(\bar{1}1)), \tag{C17}$$

$$2K_{1\bar{1}}=(t_{11}-t_{\bar{1}1})((11)-(\bar{1}\bar{1}))+(t_{12}-t_{\bar{1}2})((12)-(\bar{1}2))+(t_{11}-t_{\bar{1}\bar{1}})((1\bar{1})-(\bar{1}1)), \tag{C18}$$

$$2K_{\bar{1}1}=(t_{1\bar{1}}-t_{\bar{1}1})((11)+(\bar{1}\bar{1}))+(t_{12}-t_{\bar{1}2})((12)+(\bar{1}2))+(t_{11}-t_{\bar{1}\bar{1}})((1\bar{1})+(\bar{1}1)), \tag{C19}$$

$$2K_{12}=(t_{11}+t_{1\bar{1}}+t_{\bar{1}1}+t_{\bar{1}\bar{1}})(21)+\sqrt{2}(t_{12}+t_{\bar{1}2})(22)+(t_{11}-t_{\bar{1}\bar{1}}+t_{\bar{1}1}-t_{\bar{1}\bar{1}})(2\bar{1}), \tag{C20}$$

$$2K_{\bar{1}2}=(t_{11}+t_{1\bar{1}}-t_{\bar{1}1}-t_{\bar{1}\bar{1}})(21)+\sqrt{2}(t_{12}-t_{\bar{1}2})(22)+(t_{11}-t_{\bar{1}\bar{1}}-t_{\bar{1}1}+t_{\bar{1}\bar{1}})(2\bar{1}), \tag{C21}$$

$$2K_{21}=(t_{21}+t_{2\bar{1}})((11)+(\bar{1}\bar{1}))+2t_{22}(12)+(t_{21}-t_{2\bar{1}})((\bar{1}1)-(\bar{1}\bar{1})), \tag{C22}$$

$$2K_{2\bar{1}}=(t_{21}-t_{2\bar{1}})(-(11)+(1\bar{1}))+2t_{22}(\bar{1}2)+(t_{21}+t_{2\bar{1}})((\bar{1}1)+(\bar{1}\bar{1})), \tag{C23}$$

$$2K_{22}=\sqrt{2}(t_{21}+t_{2\bar{1}})(21)+2t_{22}(22)+\sqrt{2}(t_{21}-t_{2\bar{1}})(2\bar{1}). \tag{C24}$$

We have not directly utilized the $\hat{R}tt$ constraints in constructing eigenstates. But since (C1) is the basic equation providing the starting point we present here the most compact approach to the full set of 81 constraints for $N=3$.

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Time minimal trajectories for a spin 1/2 particle in a magnetic field

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In this paper we consider the minimum time population transfer problem for the z component of the spin of a (spin 1/2) particle, driven by a magnetic field, that is constant along the z axis and controlled along the x axis, with bounded amplitude. On the Bloch sphere (i.e., after a suitable Hopf projection), this problem can be attacked with techniques of optimal syntheses on two-dimensional (2-D) manifolds. Let $(-E,E)$ be the two energy levels, and $|\Omega(t)| \leq M$ the bound on the field amplitude. For each couple of values E and M, we determine the time optimal synthesis starting from the level $-E$, and we provide the explicit expression of the time optimal trajectories, steering the state one to the state two, in terms of a parameter that can be computed solving numerically a suitable equation. For $M/E \ll 1$, every time optimal trajectory is bang-bang and, in particular, the corresponding control is periodic with frequency of the order of the resonance frequency $\omega_R = 2E$. On the other side, for $M/E > 1$, the time optimal trajectory steering the state one to the state two is bang-bang with exactly one switching. For fixed E, we also prove that for $M \to \infty$ the time needed to reach the state two tends to zero. In the case $M/E > 1$ there are time optimal trajectories containing a singular arc. Finally, we compare these results with some known results of Khaneja, Brockett, and Glaser and with those obtained by controlling the magnetic field both on the x and y directions (or with one external field, but in the rotating wave approximation). As a byproduct we prove that the qualitative shape of the time optimal synthesis presents different patterns that cyclically alternate as $M/E \to 0$, giving a partial proof of a conjecture formulated in a previous paper. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A. Preliminaries

The issue of designing an efficient transfer of population between different atomic or molecular levels is crucial in atomic and molecular physics (see, e.g., Refs. 1–4). In the experiments, excitation and ionization are often induced by means of a sequence of laser pulses. The transfer should be as efficient as possible in order to minimize the effects of relaxation or decoherence that are always present. In the recent past years, people started to approach the design of laser pulses by using Geometric Control Techniques (see, for instance, Refs. 5–9). Finite-dimensional closed quantum systems are in fact left (or right) invariant control systems on $SU(n)$, or on the corresponding Hilbert sphere $S^{2n-1} \subset \mathbb{C}^n$, where n is the number of atomic or molecular levels. For these kinds of systems very powerful techniques were developed, both for what concerns controllability[10–13] and optimal control.[14–16]

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The dynamics of an n-level quantum system is governed by the time dependent Schrödinger equation (in a system of units such that $\hbar=1$),

$$i\dot{x}(t)=\left(H_0+\sum_{j=1}^{m}\Omega_j(t)H_j\right)x(t), \tag{1}$$

where $x(\cdot)$, defined on $[0,T]$, is a function taking values on the *state space* that is $SU(n)$ (if we formulate the problem for a time evolution operator) or the sphere S^{2n-1} (if we formulate the problem for the wave function). The quantity H_0 called the *drift Hamiltonian* is a Hermitian matrix, that is natural to assume diagonalized, i.e., $H_0=\mathrm{diag}(E_1,\ldots,E_n)$, where $E_1,\ldots,E_n$ are real numbers representing the *energy levels*. With no loss of generality we can assume $\Sigma_{j=1}^{n}E_j=0$. The real valued *controls* $\Omega_1(.),\ldots,\Omega_m(.)$, represent the *external pulsed field*, while the matrices H_j $(j=1,\ldots,m)$ are Hermitian matrices describing the coupling between the external fields and the system. The time dependent Hamiltonian $H(t):=H_0+\Sigma_{j=1}^{m}\Omega_j(t)H_j$ is called the *controlled Hamiltonian*.

The first problem that usually one would like to solve is the *controllability problem*, i.e., proving that for every couple of points in the state space one can find controls steering the system from one point to the other. For applications, the most interesting initial and final states are of course the *eigenstates of* H_0.

If $x\in SU(n)$, thanks to the fact that the control system (1) is a left invariant control system on the compact Lie group $SU(n)$, this occurs if and only if

$$\mathrm{Lie}\{iH_0,iH_1,\ldots,iH_m\}=su(n), \tag{2}$$

(see, for instance, Ref. 13). If the problem is formulated for the wave function, i.e., $x\in S^{2n-1}$, one can have controllability, with less restrictive conditions on the Lie algebra $\mathrm{Lie}\{iH_0,iH_1,\ldots,iH_m\}$, see Ref. 17. The problem of finding easily verifiable conditions under which (2) is satisfied has been deeply studied in the literature (see, for instance, Refs. 18 and 13). Here we just recall that the condition (2) is generic in the space of Hermitian matrices.

Once that controllability is proved, one would like to steer the system between two fixed points in the state space, in the most efficient way. Typical costs that are interesting to minimize for applications are as follows.

- Energy transferred by the controls to the system. $\int_0^T\Sigma_{j=1}^{m}\Omega_j^2(t)dt$,
- Time of transfer. In this case one can attack two different problems: one with *bounded* and one with *unbounded* controls.

The problem of minimizing time with unbounded controls has been deeply investigated in Refs. 19 and 8. The problems of minimizing time or energy with bounded controls are very difficult in general, and one can hope to find a complete solution in low dimension only.

In Refs. 5 and 20–22 a special class of systems, for which the analysis can be pushed much further, was studied, namely systems such that the drift term H_0 disappear in the interaction picture (by a unitary change of coordinates and a change of controls). For these systems the controlled Hamiltonian reads as

$$H(t)=\begin{pmatrix} E_1 & \mu_1\mathbf{\Omega}_1(t) & 0 & \cdots & 0 \\ \mu_1\mathbf{\Omega}_1^*(t) & E_2 & \mu_2\mathbf{\Omega}_2(t) & \ddots & \vdots \\ 0 & \mu_2\mathbf{\Omega}_2^*(t) & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & E_{n-1} & \mu_{n-1}\mathbf{\Omega}_{n-1}(t) \\ 0 & \cdots & 0 & \mu_{n-1}\mathbf{\Omega}_{n-1}^*(t) & E_n \end{pmatrix}. \tag{3}$$

Here $(^*)$ denotes the complex conjugation involution. The controls $\mathbf{\Omega}_1,\ldots,\mathbf{\Omega}_{n-1}$ are complex [they play the role of the real controls $\Omega_1,\ldots,\Omega_m$ in (1) with $m=2(n-1)$] and $\mu_j>0$ $(j$

$=1,\ldots,n-1$) are real constants describing the couplings (intrinsic to the quantum system) that we have restricted to couple only levels j and $j+1$ by pairs.

For $n=2$ the dynamics (3) describes the evolution of the z component of the spin of a (spin 1/2) particle driven by a magnetic field that is constant along the z axis and controlled both along the x and y axes, while for $n\geq 2$ it represents the first n levels of the spectrum of a molecule in the *rotating wave approximation* (see, for instance, Ref. 23), and assuming that each external fields couples only close levels. The complete solution to the optimal control problem between eigenstates of $H_0=\mathrm{diag}(E_1,\ldots,E_n)$ has been constructed for $n=2$ and $n=3$, for the minimum time problem with bounded controls (i.e., $|\mathbf{\Omega}_j|\leq M_j$) and for the minimum energy problem $\int_0^T\sum_{j=1}^{n-1}|\mathbf{\Omega}_j(t)|^2\,dt$ (with a fixed final time).

Remark 1: For the simplest case $n=2$ (studied in Refs. 5 and 7), the minimum time problem with bounded control and the minimum energy problem actually coincide. In this case the controlled Hamiltonian is

$$H(t)=\begin{pmatrix} -E & \mathbf{\Omega}(t) \\ \mathbf{\Omega}^*(t) & E \end{pmatrix}, \quad |\mathbf{\Omega}|\leq M, \tag{4}$$

and the optimal trajectories, steering the system from the first to the second eigenstate of $H_0=\mathrm{diag}(-E,E)$, correspond to controls in *resonance* with the energy gap $2E$, and with maximal amplitude, i.e., $\mathbf{\Omega}(t)=Me^{i[(2E)t+\phi]}$, where $\phi\in[0,2\pi[$ is an arbitrary phase. The quantity $\omega_R=2E$ is called the *resonance frequency*. In this case, the time of transfer T_C is proportional to the inverse of the laser amplitude. More precisely (see, for instance, Ref. 5), $T_C=\pi/(2M)$.

For $n=3$ the problem has been studied in Refs. 20 and 22, and it is much more complicated (in particular, when the coupling constants μ_1 and μ_2 are different). In the case of minimum time with bounded controls, it requires some nontrivial technical tools of 2-D syntheses theory for distributional systems that have been developed in Ref. 22.

For $n\geq 4$ the problem is very hard and still unsolved, but in Ref. 21, it has been proved that the optimal controls steering the system from any couple of eigenstates of H_0 are in *resonance*, i.e., they oscillate with a frequency equal to the difference of energy between the levels that the control is coupling. More precisely,

$$\mathbf{\Omega}_j=A_j(t)e^{i[(E_{j+1}-E_j)t+\phi_j]}, \quad j=1,\ldots,n-1, \tag{5}$$

where $A_j(.)$ are real functions describing the amplitude of the external fields and ϕ_j are arbitrary phases. Actually, this result holds for more general systems, initial and final conditions, and costs (see Ref. 21).

The problem of minimizing time with bounded controls or energy is even more difficult if it is not possible to eliminate the drift H_0. This occurs, for instance, in a system in the form (3) with real controls $\mathbf{\Omega}_j(t)=\mathbf{\Omega}_j^*(t)$, $j=1,\ldots,n-1$, as we are going to discuss now. (For more details on the elimination of the drift see Refs. 5, 20, and 21.)

B. A spin 1/2 particle in a magnetic field

In this paper we attack the simplest quantum mechanical model interesting for applications for which it is not possible to eliminate the drift, namely a *two-level quantum system* driven by a *real control*. This system describes the evolution of the z-component of the spin of a (spin 1/2) particle driven by a magnetic field, which is constant along the z axis and controlled along the x axis. Equivalently, it describes the first two levels of a molecule driven by an external field without the rotating wave approximation. The dynamics is governed by the time dependent Schrödinger equation (in a system of units such that $\hbar=1$):

$$i\frac{d\psi(t)}{dt} = H(t)\psi(t), \tag{6}$$

where $\psi(.)=[\psi_1(.),\psi_2(.)]^T:[0,T]\to\mathbb{C}^2$, $\Sigma_{j=1}^2|\psi_j(t)|^2=1$ [i.e., $\psi(t)$ belongs to the sphere $S^3\subset\mathbb{C}^2$], and

$$H(t)=\begin{pmatrix}-E & \Omega(t)\\ \Omega(t) & E\end{pmatrix}, \tag{7}$$

where $E>0$ and the control $\Omega(.)$, is assumed to be a real function. With the notation of formula (1), the drift Hamiltonian is

$$H_0=\begin{pmatrix}-E & 0\\ 0 & E\end{pmatrix},$$

while

$$H_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$$

and the controllability condition (2) is satisfied.

Notice that for a spin 1/2 system, it is equivalent to treat the problem for the wave function or for the time evolution operator since S^3 is diffeomorphic to $SU(2)$. The aim is to induce a transition from the first eigenstate of H_0 (i.e., $|\psi_1|^2=1$) to any other *physical state*. We recall that two states $\psi,\psi'\in S^3$ are physically equivalent if they differ by a factor of phase. More precisely, by the physical state we mean a point of the two dimensional sphere (called the *Bloch sphere*) $\mathbf{S}_B:=S^3/\sim$ where the equivalence relation $\sim$ is defined as follows: $\psi\sim\psi'$ (where $\psi,\psi'\in S^3$) if and only if $\psi=\exp(i\Phi)\psi'$, for some $\Phi\in[0,2\pi[$. The projection from S^3 to $\mathbf{S}_B$ is called the *Hopf projection*, and it is given explicitly in the next section. A particularly interesting transition is of course from the first to the second eigenstates of H_0 (i.e., from $|\psi_1|^2=1$ to $|\psi_2|^2=1$).

Due to the presence of the drift, in this case the minimum time problem with bounded control and the minimum energy problem are different. In Ref. 7 the authors studied the minimum energy problem (in that case, optimal solutions can be expressed in terms of elliptic functions), while here we minimize the time of transfer, with a bounded field amplitude:

$$|\Omega(t)|\le M, \quad \text{for every } t\in[0,T], \tag{8}$$

where T is the time of the transition and $M>0$ represents the maximum amplitude available. This problem requires completely different techniques with respect to those used in Ref. 7.

Thanks to the reduction to a two dimensional problem (on the Bloch sphere), this problem can be attacked with the techniques of optimal syntheses on 2-D manifolds developed by Sussmann, Bressan, Piccoli, and the first author; see, for instance, Refs. 24–27 and recently rewritten in Ref. 15. We make a brief recall of these techniques in Appendix A.

C. The control problem on the Bloch sphere $\mathbf{S_B}$

An explicit Hopf projection from S^3 to $\mathbf{S}_\mathrm{B}$ is given by

$$\Pi:\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\in S^3\subset\mathbb{C}^2\mapsto y=\begin{pmatrix}y_1\\ y_2\\ y_3\end{pmatrix}=\begin{pmatrix}-2\,\mathrm{Re}(\psi_1^*\psi_2)\\ 2\,\mathrm{Im}(\psi_1^*\psi_2)\\ |\psi_1|^2-|\psi_2|^2\end{pmatrix}\in\mathbf{S}_\mathrm{B}\subset\mathbb{R}^3. \tag{9}$$

Notice that Π maps the first eigenstate of H_0 (i.e., $|\psi_1|^2=1$) to the *North Pole* $P_N:=(0,0,1)^T$ of $\mathbf{S}_\mathrm{B}$, and the second eigenstate (i.e., $|\psi_2|^2=1$) to the *South Pole* $P_S:=(0,0,-1)^T$.

After setting $u(t)=\Omega(t)/M$, the Schrödinger equation (6), (7) projects to the following single input affine system (clarified below, after normalizations),

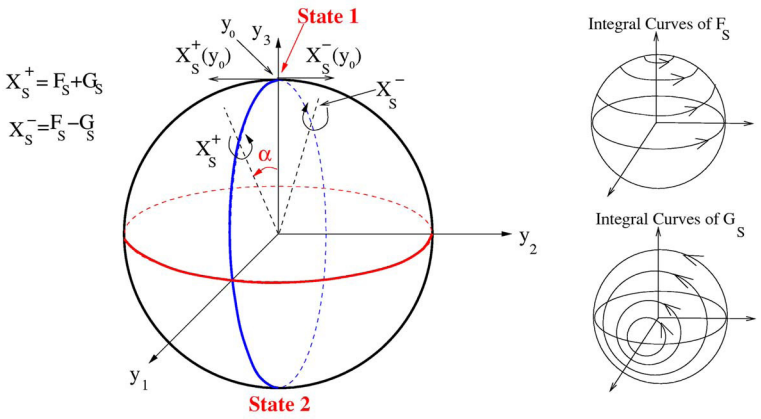

FIG. 1. (Color online) The Bloch sphere.

$$\dot{y} = F_S(y) + uG_S(y), \quad |u| \leq 1, \tag{10}$$

where

$$y \in \mathbf{S}_B := \left\{ (y_1, y_2, y_3) \in \mathbb{R}^3, \sum_{j=1}^{3} y_j^2 = 1 \right\}, \tag{11}$$

$$F_S(y) := k\cos(\alpha)\begin{pmatrix} -y_2 \\ y_1 \\ 0 \end{pmatrix}, \quad G_S(y) := k\sin(\alpha)\begin{pmatrix} 0 \\ -y_3 \\ y_2 \end{pmatrix}, \tag{12}$$

$$\alpha := \arctan\left(\frac{M}{E}\right) \in \left]0, \pi/2\right[, \quad k := 2E/\cos(\alpha) = 2\sqrt{M^2 + E^2}. \tag{13}$$

Remark 2 (**normalizations**)*:* In the following, to simplify the notations, we normalize $k=1$. This normalization corresponds to a reparametrization of the time. More precisely, if T is the minimum time to steer the state $\tilde{y}$ to the state $\bar{y}$ for the system with $k=1$, the corresponding minimum time for the original system is $T/(2\sqrt{M^2+E^2})$. Sometimes we need also the original system (6), (7) on S^3, with the normalization made in this remark, i.e., the system

$$i\frac{d\psi(t)}{dt} = \tilde{H}(t)\psi(t), \quad \text{where } \tilde{H}(t) = \frac{1}{2}\sin\alpha\begin{pmatrix} -\cot\alpha & u(t) \\ u(t) & \cot\alpha \end{pmatrix}. \tag{14}$$

We come back to the original value of k only in Sec. III C, where we compare our results with those of other authors.

We refer to Fig. 1. The vector fields $F_S(y)$ and $G_S(y)$ (that play the role, respectively, of H_0 and H_1) describe rotations, respectively, around the axes y_3 and y_1. Let us define the vector fields corresponding to constant control ± 1,

$$X_S^{\pm}(y) := F_S(y) \pm G_S(y). \tag{15}$$

The parameter $\alpha \in \left]0, \pi/2\right[$ (that is the only parameter of the problem) is the angle between the axes of rotations of F_S and X_S^+. The case $\alpha \geq \pi/4$ (resp., $\alpha < \pi/4$) corresponds to $M \geq E$ (resp., $M < E$).

Definition 1: An admissible control $u(.)$ *for the system* (10)–(13) *is a measurable function* $u(.):[a,b]\to[-1,1]$, *while an admissible trajectory is a Lipschitz functions* $y(.):[a,b]\to\mathbf{S}_B$ *sat-*

isfying (10), *a.e., for some admissible control* $u(.)$. *If* $y(.)$ *is an admissible trajectory and* $u(.)$ *the corresponding control, we say that* $[y(.),u(.)]$ *is an admissible pair.*

For every $\bar{y} \in \mathbf{S}_B$, our minimization problem is then to find the admissible pair steering the North Pole to $\bar{y}$ in minimum time. More precisely, we have the following.

Problem (P): *Consider the control system* (10)–(13). *For every* $\bar{y} \in \mathbf{S}_B$, *find an admissible pair* $[y(.),u(.)]$ *defined on* $[0,T]$ *such that* $y(0)=P_N$, $y(T)=\bar{y}$, *and* $y(.)$ *is time optimal.*

For us an optimal synthesis is the collection of all the solutions to the problem (**P**). More precisely we have the following.

Definition 2 (*optimal synthesis*)*: An optimal synthesis for the problem* (**P**) *is the collection of all time optimal trajectories* $\Gamma=\{y_{\bar{y}}(.):[0,b_{\bar{y}}]\mapsto \mathbf{S}_B,\ \bar{y} \in \mathbf{S}_B : y_{\bar{y}}(0)=P_N,\ y_{\bar{y}}(b_{\bar{y}})=\bar{y}\}$.

For more elaborated definitions of optimal synthesis see Refs. 15 and 28 and references therein.

Definition 3 [bang, singular for the problem (10)–(13)]: A control $u(.):[a,b]\to[-1,1]$ *is said to be a bang control if* $u(t)=+1$, *a.e., in* $[a,b]$ *or* $u(t)=-1$, *a.e., in* $[a,b]$. *A control* $u(.):[a,b]\to[-1,1]$ *is said to be a singular control if* $u(t)=0$, *a.e., in* $[a,b]$. *A finite concatenation of bang controls is called a bang-bang control. A switching time of* $u(.)$ *is a time* $\bar{t} \in [a,b]$ *such that, for every* $\varepsilon>0$, u *is not bang or singular on* $(\bar{t}-\varepsilon,\bar{t}+\varepsilon)\cap[a,b]$. *A trajectory of the control system (A4) is said a bang trajectory (or arc), singular trajectory (or arc), bang-bang trajectory, if it corresponds, respectively, to a bang control, singular control, bang-bang control. If* $\bar{t}$ *is a switching time, the corresponding point on the trajectory* $y(\bar{t})$ *is called a switching point.*

Remark 3: The definitions of singular trajectory and control, given above are very specific to our problem (10)–(13). For the definition of singular trajectories for more general systems see Definition 8, Appendix A.1.

In Ref. 29 it was proved that, for the same problem (10)–(13), but in which $y \in \mathbb{R}P^2$, for every couple of points there exists a time optimal trajectory joining them. Moreover it was proved that every time optimal trajectory is a finite concatenation of bang and singular trajectories. Repeating exactly the same arguments and recalling that S^2 is a double covering of $\mathbb{R}P^2$, one easily gets the same result on $\mathbf{S}_B$. More precisely we have the following.

Proposition 1: For the problem (10)–(13), *for each pair of points* p *and* q *belonging to* $\mathbf{S}_B$, *there exists a time optimal trajectory joining* p *to* q. *Moreover, every time the optimal trajectory for the problem* (10)–(13) *is a finite concatenation of bang and singular trajectories.*

Notice that the previous proposition does not apply if $\alpha=0$ or $\alpha=\pi/2$, since in these cases the controllability property is lost.

D. Purpose of the paper

Our aim is to study problem (**P**) for every possible value of the parameter α, giving a particular relief to the case in which $\bar{y}=P_S$ (i.e., to the optimal trajectory steering the North to the South Pole).

We will not be able to give a complete solution to the problem (**P**), without the help of numerical simulations. However, thanks to the theory developed in Ref. 15 we give a satisfactory description of the optimal trajectories. In the following we describe the main results and the structure of the paper.

For $\alpha<\pi/4$, every time optimal trajectory is bang-bang and, in particular, the corresponding control is periodic, in the sense that for every fixed optimal trajectory the time between two consecutive switchings is constant. Moreover, it tends to π as α goes to 0. For the original non-normalized problem this means that for $M/E \ll 1$, the optimal control oscillates with frequency of the order of the resonance frequency $\omega_R=2E$. In this case it is possible to give a satisfactory description of the optimal synthesis, excluding a neighborhood of the South Pole, in which we are able to find the optimal synthesis only numerically (such results were already given in Ref. 29, as we see later).

On the other side, if $\alpha \geq \pi/4$ the computation of the optimal trajectories is simpler since the number of switchings needed to cover the whole sphere is small (less than or equal than 2). In this

case, for α big enough, we are also able to give the exact value of the time needed to cover the whole sphere. However, there is a new difficulty, namely, the presence of singular arcs. Moreover, the qualitative shape of the optimal synthesis is rather different if α is close to $\pi/4$ or to $\pi/2$. A relevant fact is that this synthesis contains a singularity (the so called $(S,K)_3$) that is predicted by the general theory (see Ref. 15, pp. 61 and 82), and was never observed out from *ad hoc* examples.

The problem of finding explicitly the optimal trajectories from the North Pole P_N to the South Pole P_S, can be easily solved in the case $\alpha \geq \pi/4$ as a consequence of the construction of the time optimal synthesis. (Coming back to the original non-normalized problem, we also prove that at fixed E, for $M \to \infty$, the time of transfer from P_N to P_S tends to zero.)

For $\alpha < \pi/4$ the problem is more complicated. However, we are able to prove that if $u(t)$ is an optimal control steering the North Pole P_N to the South Pole P_S in time T, then $u(T-t)$ is as well (see Lemma 4 in Appendix B). Thanks to this fact, we can prove that the optimal trajectories steering the North to the South Pole belong to a set Ξ, containing, at most eight trajectories (half starting with control $+1$ and half starting with control -1, and switching exactly at the same times). These trajectories are determined in terms of a parameter (the first switching time) that can be easily computed numerically solving suitable equations. Once these trajectories are identified, one can check by hands which are the optimal ones.

The analysis can be pushed much forward. We also prove that the cardinality of Ξ depends on the so called *normalized remainder*,

$$\mathsf{R} := \frac{\pi}{2\alpha} - \left[\frac{\pi}{2\alpha}\right] \in [0,1[, \tag{16}$$

where $[.]$ denotes the integer part. In particular, for α small, we prove that if R is close to zero then Ξ contains exactly eight trajectories (and, in particular, there are four optimal trajectories), while if R is close to 1 then Ξ contains only four trajectories (two of them are optimal). The precise description of these facts is contained in Proposition 6, Sec. III B. As a consequence, the qualitative shape of the time optimal synthesis presents different patterns, that cyclically alternate, in the noncontrollability limit $\alpha \to 0$, giving a partial proof of a conjecture formulated in a previous paper (Ref. 29), that was supported by numerical simulations; see Remark 11. This is probably the most interesting byproduct of this paper.

Finally, we compare these results with some known results of Khaneja, Brockett, and Glaser and with those obtained by controlling the magnetic field both on the x and y directions.

The structure of the paper is as follows. In Sec. II we briefly resume the results of paper[29] that are connected to our problem and the conjectures formulated therein. The main results of the paper are described in Sec. III, while the proofs are postponed to Appendix B. In Appendix A we recall the main tools of the theory of optimal synthesis. In Appendix C we determine the last point reached by trajectories starting at P_N and the time needed to cover the whole sphere.

II. HISTORY OF THE PROBLEM AND KNOWN FACTS

The problem (**P**) (although with different purposes) was already partially studied in Ref. 29, in the case $\alpha < \pi/4$. In that paper the aim was to give an estimate on the maximum number of switchings for time optimal trajectories on $SO(3)$ (this problem was first studied by Agrachev and Gamkrelidze in Ref. 30, using index theory).

In Ref. 29 it has been proved that, for the problem (**P**) in the case $\alpha < \pi/4$, every optimal trajectory is bang-bang. More precisely, it was proved that in the case $\alpha < \pi/4$, if $y(.)$ is a time optimal trajectory starting at the North Pole, then it should satisfy the following properties.

(i) $y(.)$ is bang bang.
(ii) The duration s_i of the first bang arc satisfies $s_i \in [0, \pi]$.
(iii) The time duration between two consecutive switchings is the same for all *interior bang arcs* (i.e., excluding the first and the last bang), and it is the following function of s_i defined in the interval $[0, \pi]$,

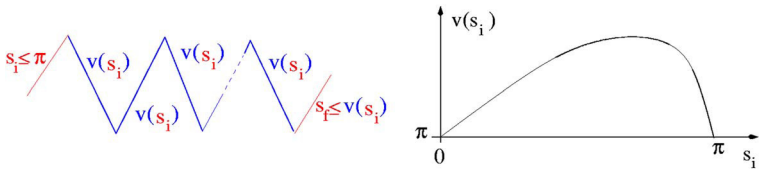

FIG. 2. (Color online) Time optimal trajectories for $\alpha < \pi/4$.

$$v(s_i) = \pi + 2\arctan\left(\frac{\sin(s_i)}{\cos(s_i) + \cot^2(\alpha)}\right). \tag{17}$$

One can immediately check that this function satisfies $v(0)=v(\pi)=\pi$ and $v(s_i)>\pi$ for every $s_i \in]0,\pi[$,

(iv) The time duration of the last arc is $s_f \in [0, v(s_i)]$.

Properties (i)–(iv) are illustrated in Fig. 2. Moreover, thanks to the analysis given in Ref. 29, one easily gets (always in the case $\alpha < \pi/4$).

(v) The number of switchings N_y of $y(.)$ satisfies the following inequality:

$$N_y \leq N_M := \left[\frac{\pi}{2\alpha}\right] + 1. \tag{18}$$

Conditions (i)–(v) define a set of candidate optimal trajectories. Notice that conditions (i)–(v) are just necessary conditions for optimality and one is faced with the problem of selecting, among them, those that are really optimal. In particular, given a trajectory satisfying conditions (i)–(v), one would like to find the time after which it is no more optimal. In the following we say that at this time the trajectory loses optimality.

The way in which these candidate optimal trajectories cover the whole sphere is shown in the top of Fig. 3.

Consider the following curves, made by points where the control switches from +1 to −1 or *vice versa*, called *switching curves*, defined by induction,

$$C_1^\varepsilon(s) = e^{X_S^\varepsilon v(s)} e^{X_S^{-\varepsilon} s} P_N, \quad C_k^\varepsilon(s) = e^{X_S^\varepsilon v(s)} C_{k-1}^{-\varepsilon}(s) \quad (\text{where } \varepsilon = \pm 1 \text{ and } k = 2, \ldots, N_M - 1). \tag{19}$$

See the top of Fig. 3.

Even if the analysis made in Ref. 29 was sufficient for the purpose of giving a bound on the maximum number of switchings for time optimal trajectories on $SO(3)$, some questions remained unsolved, in particular, questions about *local optimality* of the switching curves. Roughly speaking, we say that a switching curve is locally optimal if it never "reflects" the trajectories [see Fig. 4(A)]. [More precisely, consider a smooth switching curve C between two smooth vector field Y_1 and Y_2 on a smooth two-dimensional manifold. Let $C(s)$ be a smooth parametrization of C. We say that C is *locally optimal* if, for every $s \in \mathrm{Dom}(C)$, we have $\dot{C}(s) \neq \alpha_1 Y_1(C(s)) + \alpha_2 Y_2(C(s))$, for every α_1, α_2 s.t. $\alpha_1 \alpha_2 \geq 0$. The points of a switching curve on which this relation is not satisfied are usually called "conjugate points." See Fig. 4. The terminology "conjugate points" and "cut locus" comes from Riemannian Geometry.] When a family of trajectories is reflected by a switching curve, then local optimality is lost and some *cut locus* appear in the optimal synthesis.

Definition 4: A cut locus for the problem (**P**) *is a set of points reached at the same time by two* (*or more*) *optimal trajectories. A subset of a cut locus that is a connected* $\mathcal{C}^1$ *manifold is called the overlap curve*.

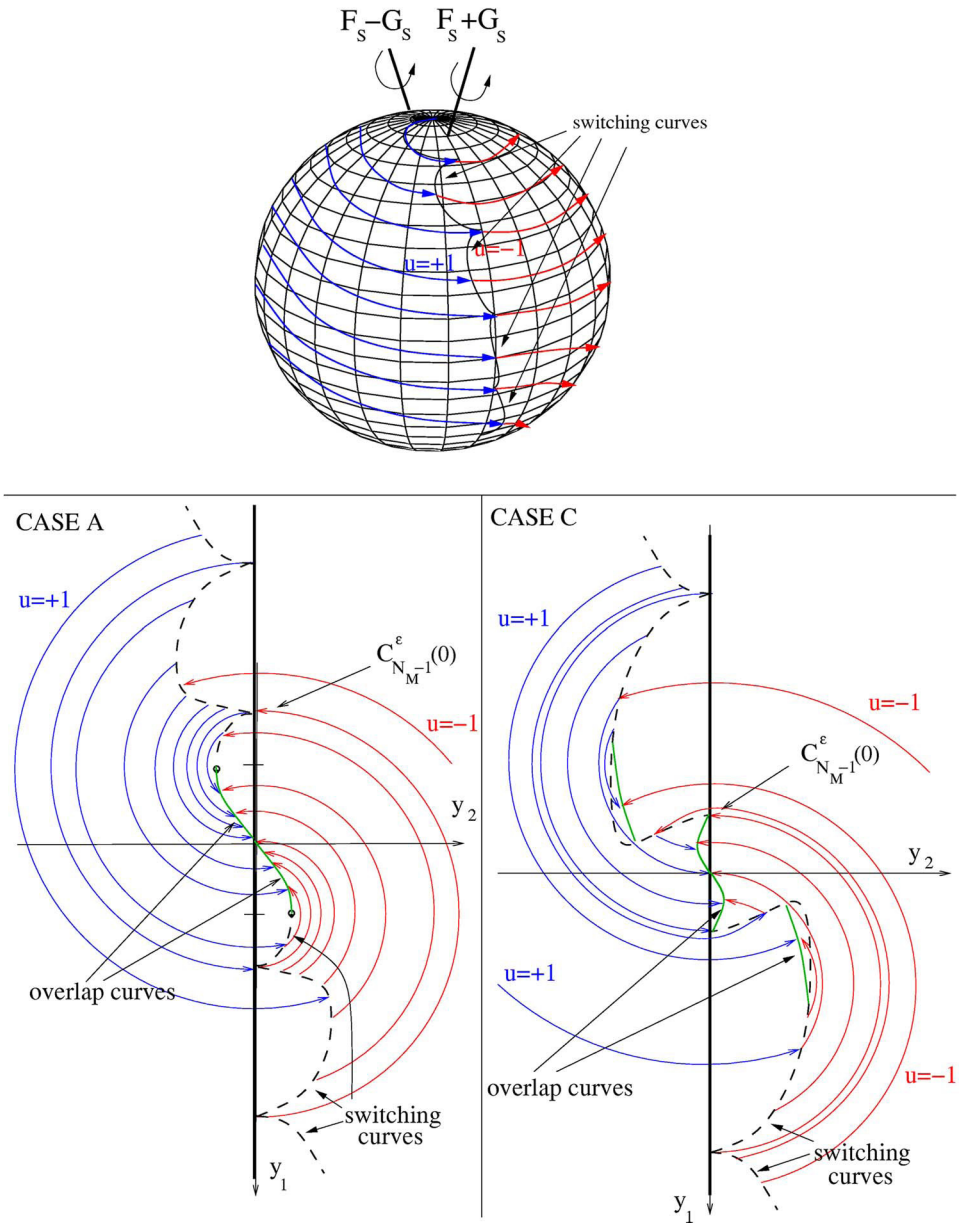

FIG. 3. (Color online) Synthesis on the sphere for $\alpha < \pi/4$ and a conjectured shape in a neighborhood of the South Pole.

An example showing how a "reflection" on a switching curves generate a cut locus is portrayed in Figs. 4(B) and 4(C). More details are given later. In Ref. 29, the following questions remain unsolved.

Question 1: Are the switching curves C_k^ε, $k=1,\ldots,N_M-1$, locally optimal? More precisely, one would like to understand how the candidate optimal trajectories previously described are going to lose optimality.

Question 2: What is the shape of the optimal synthesis in a neighborhood of the South Pole?

Numerical simulations suggested some conjectures regarding the previous questions. More precisely, we have the following

C1: Define $k_{\text{last}}=[(\pi-\alpha)/2\alpha]-1$. Then the curves $C_k^\varepsilon(s)$, $(k=1,\ldots,N_M-1)$ are locally optimal if and only if $k \leq k_{\text{last}}$. Notice that $k_{\text{last}} \in \{N_M-3, N_M-2\}$.

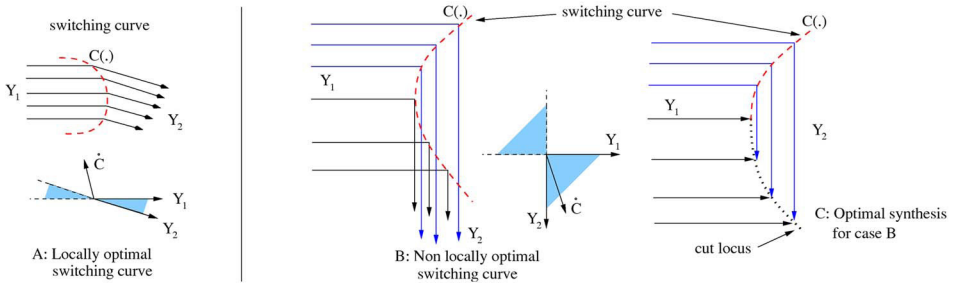

FIG. 4. (Color online) Locally optimal switching curves and nonlocally optimal switching curves with the corresponding synthesis.

Analyzing the evolution of the minimum time wave front in a neighborhood of the South Pole, it is reasonable to conjecture the following.

C2: The shape of the optimal synthesis in a neighborhood of the South Pole depends on the so called *remainder* $r := \pi - 2\alpha[\pi/2\alpha]$. [Notice that $r = 2\alpha\mathsf{R}$, where R has been defined in formula (16). In conjecture **C2**, we use the remainder r to keep the same notation of Ref. 29.] Notice that r belongs to the interval $[0, 2\alpha[$. More precisely, we conjecture that for $\alpha \in]0, \pi/4[$, there exist two positive numbers α_1 and α_2 such that $0 < \alpha_1 < \alpha < \alpha_2 < 2\alpha$ and the following:

CASE A: $r \in]\alpha_2, 2\alpha[$. The switching curve $C^{\varepsilon}_{N_M-1}$ glues to an overlap curve that passes through the origin (Fig. 3, Case A).

CASE B: $r \in [\alpha_1, \alpha_2]$. The switching curve $C^{\varepsilon}_{N_M-1}$ is not reached by optimal trajectories in the interval $]0, \pi]$. At the point $C^{\varepsilon}_{N_M-1}(0)$ an overlap curve starts and passes through the origin.

CASE C: $r \in]0, \alpha_1[$. The situation is more complicated and it is depicted in the bottom of Fig. 3, Case C.

For $r = 0$, the situation is the same as in CASE A, but for the switching curve starting at $C^{\varepsilon}_{N_M-2}(0)$.

III. MAIN RESULTS

We give here a brief description of the main results of the paper. The corresponding proofs are given in Appendix B. From now on we use the following conventions.

Remark 4 (*notation*)*:* Recall Definition 3. The letter B refers to a bang trajectory and the letter S refers to a singular trajectory. A concatenation of bang and singular trajectories is labeled by the corresponding letter sequence, written in order from left to right. Sometimes, we use a subscript to indicate the time duration of a trajectory so that we use B_t to refer to a bang trajectory defined on an interval of length t and, similarly, S_t for a singular trajectory defined on an interval of length t. Moreover, we indicate by γ^+ (resp., γ^-) the trajectory of (10)–(13) starting at the North Pole at time zero and corresponding to control $u \equiv 1$ (resp., $u \equiv -1$). Notice that $\gamma^{\pm}$ are defined for every time, and are periodic. Finally, we use the following subsets of $\mathbf{S}_{\mathrm{B}}$: the circle of equation $y_3 = 0$ called the *equator*, the set $y_3 > 0$, called *northern hemisphere* and the set $y_3 < 0$, called *southern hemisphere*.

From Sec. II, recall the definitions of switching curves, cut loci, and overlap curves.

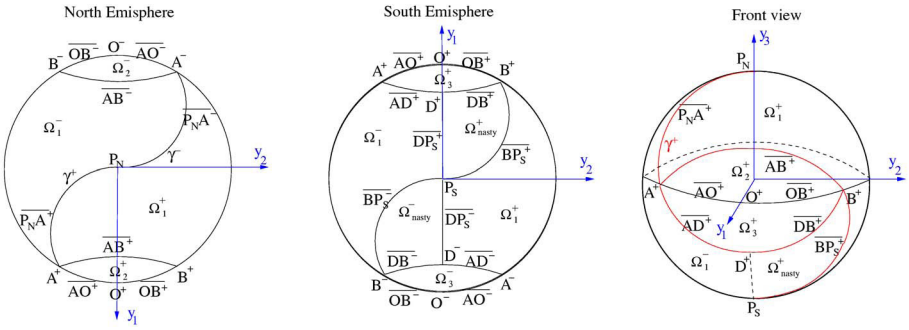

FIG. 5. (Color online) Definition 5.

A. Optimal synthesis for $\alpha \geq \pi/4$

In this section we describe the time optimal synthesis for $\alpha \geq \pi/4$. We divide $\mathbf{S}_B$ in 8 open regions called $\Omega_1^{\pm}, \ldots, \Omega_3^{\pm}$, $\Omega_{\text{nasty}}^{\pm}$ and in 16 arcs (see Definition 5, and Fig. 5). For every point $\bar{y} \in \mathbf{S}_B \setminus (\Omega_{\text{nasty}}^{+} \cup \Omega_{\text{nasty}}^{-})$, Theorem 1 gives the optimal trajectories reaching $\bar{y}$.

Unlike the $\alpha < \pi/4$ case, here it is possible to detect the presence of singular trajectories that are optimal, and also of cut loci (even not only in a neighborhood of the South Pole).

The region $\Omega_{\text{nasty}}^{+}$ (and similarly $\Omega_{\text{nasty}}^{-}$) is more difficult to analyze. It contains a cut locus that should be determined numerically. Even if we are not able to provide an analytic characterization of this locus, we are able to prove the following.

(i) $\alpha = \arcsin(1/\sqrt[4]{2})$ is a bifurcation point for the optimal synthesis, i.e., the qualitative shape is different if $\alpha \in [\pi/4, \arcsin(1/\sqrt[4]{2})[$ (called **Case 1**) or $\alpha \in [\arcsin(1/\sqrt[4]{2}), \pi/2[$ (called **Case 2**). More precisely, from the point $D^+ := \gamma^+(\pi)$, in **Case 1** it starts an optimal switching curve, while in **Case 2** it starts an overlap curve (see Proposition 3). The situation in $\Omega_{\text{nasty}}^{-}$ is symmetric.

(ii) The South Pole belongs to the cut locus and it is reached exactly by four optimal trajectories (see Proposition 2).

Numerical computations show that in **Case 2** the cut locus in $\Omega_{\text{nasty}}^{+}$ is an overlap curve connecting D^+ with the South Pole, while in **Case 1**, the switching curve starting from D^+ loses local optimality at a point of $\Omega_{\text{nasty}}^{+}$ and connects to an overlap curve that reaches the South Pole (see Fig. 6). Remark 9 explains that in **Case 2** it is not necessary to compute the cut locus lying

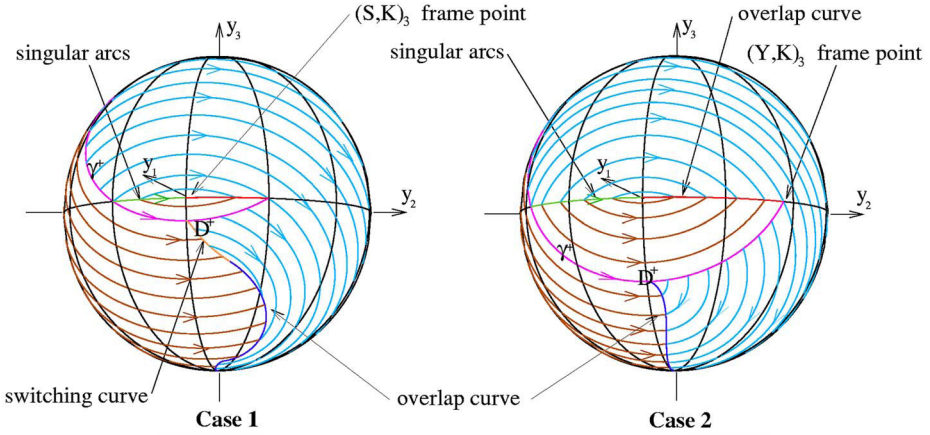

FIG. 6. (Color online) Optimal synthesis for $\alpha = \pi/3$ and α slightly larger than $\pi/4$.

in Ω^+_{nasty} to get the expression of the optimal trajectory connecting P_N to a point of Ω^+_{nasty}. The situation in Ω^-_{nasty} is symmetric.

Let us start with the description of the optimal synthesis in $\mathbf{S}_{\mathrm{B}}\backslash(\Omega^+_{\text{nasty}}\cup\Omega^-_{\text{nasty}})$. Even if Definition 5 and Theorem 1 look complicated, the shape of the optimal synthesis is quite simple, as it is shown in Fig. 6.

Definition 5: *According to Fig.* 5, *let us define the following curves on* $\mathbf{S}_{\mathrm{B}}$.

- *Let* t_1 *be the first time at which* γ^+ *intersects the equator and let* $A^+ := \gamma^+(t_1)$ [*notice that* $t_1=\pi-\arccos(\cot^2(\alpha))$]. *Define* $\overline{P_NA^+}=Supp(\gamma^+|_{[0,t_1]})$.
- *Let* ξ^- *be the trajectory corresponding to control* -1, *starting at time zero from* A^+. *Let* t_2 *be the first positive time at which* ξ^- *intersects the equator* [*notice that* $t_2=2\arccos(\cot^2(\alpha))$]. *Define* $B^+ := \xi^-(t_2)$ *and* $\overline{AB^+}=Supp(\xi^-|_{[0,t_2]})$.
- *Let* $O^+=(1,0,0)$. *Define* $\overline{AO^+}$ (*resp.*, $\overline{OB^+}$) *as the support of the trajectory corresponding to control zero, starting at* A^+ (*resp.*, O^+) *and ending at* O^+ (*resp.*, B^+).
- *Recall that* $D^+=\gamma^+(\pi)$, *and define* $\overline{AD^+}=Supp(\gamma^+|_{[t_1,\pi]})$, $\overline{DB^+}=Supp(\gamma^+|_{[\pi,t_3]})$, *where* t_3 *is the second intersection time of* γ^+ *with the equator* [*notice that* $t_3=\pi+\arccos(\cot^2(\alpha))=t_1+t_2$].
- *Let* $\overline{BP^+_S}$ *the support of the trajectory corresponding to control* -1, *starting at* B^+ *and ending at the South Pole*.
- *Let* $\overline{DP^+_S}$ *the connected subset of the meridian* $y_2=0$, *lying in the southern hemisphere and connecting the point* D^+ *to the South Pole*.

Similarly, define A^-, B^-, O^-, D^-, $\overline{P_NA^-}$, $\overline{AB^-}$, $\overline{AO^-}$, $\overline{OB^-}$, $\overline{AD^-}$, $\overline{DB^-}$, $\overline{BP^-_S}$, $\overline{DP^-_S}$.

According to Fig. 5, *define* $\Omega^\pm_1,\dots,\Omega^\pm_4,\Omega^\pm_{\text{nasty}}$ *as the open connected components of the open set obtained subtracting from* $\mathbf{S}_{\mathrm{B}}$ *all the arcs previously defined.*

The following theorem holds for every $\alpha\in\,]\pi/4,\pi/2[$. For the particular value $\alpha=\pi/4$, the claims of the theorem must be modified. Such changes are reported in Remark 5.

Theorem 1: *Let* $\gamma_{\bar y}$ *be the set of time optimal trajectories steering the North Pole to* $\bar y$. *We have the following*:

T1. *If* $\bar y\in\overline{P_NA^+}$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory corresponding to control* $+1$ *of the form* B_t, *with* $t\le t_1$.
T2. *If* $\bar y\in\overline{AB^+}\backslash B^+$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory of the form* $B_{t_1}B_t$ (*with the first bang corresponding to control* $+1$).
T3. *If* $\bar y\in\overline{AO^+}$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory of the form* $B_{t_1}S_s$ (*with the first bang corresponding to control* $+1$).
T4. *If* $\bar y\in\overline{OB^+}\backslash O^+$, *then* $\gamma_{\bar y}$ *is made by two trajectories of the form* $B_{t_1}S_sB_t$, *both starting with control* $+1$ *and ending, respectively, with control* $+1$ *and* -1. *These two trajectories have the same values of* $s\ge 0$ *and* $t>0$.
T5. *If* $\bar y\in\overline{AD^+}$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory corresponding to control* $+1$ *of the form* B_t, *with* $t\in[t_1,\pi]$.
T6. *If* $\bar y\in\overline{DB^+}\backslash B^+$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory corresponding to control* $+1$ *of the form* B_t, *with* $t\in[\pi,t_3[$.
T7. *If* $\bar y\in\overline{BP^+_S}$ *then* $\gamma_{\bar y}$ *is made by two trajectories, respectively, of the form* $B_{t_1}B_t$ *and* $B_{t_3}B_{t-t_2}$ *and starting with control* $+1$.
T8. *If* $\bar y\in\Omega^+_1\cup(\overline{DP^-_S}\backslash P_S)$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory of the form* $B_tB_{t'}$, *with* $0\le t<t_1$ *and the first bang corresponding to control* $+1$.
T9. *If* $\bar y\in\Omega^+_2$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory of the form* $B_{t_1}S_sB_t$, *with* $s>0$, *the first bang arc and the last bang arc corresponding respectively to control* $+1$ *and* -1.
T10. *If* $\bar y\in\Omega^+_3$, *then* $\gamma_{\bar y}$ *is made by a unique trajectory of the form* $B_{t_1}S_sB_t$, *with* $s>0$ *and both bang arcs corresponding to control* $+1$.
T11. *If* $\bar y=P_S$ *then* $\gamma_{\bar y}$ *is made by the four trajectories of the form* $B_{t_1}B_{t_3}$ *and* $B_{t_3}B_{t_1}$.
T12. *If* $\bar y\in\Omega^+_{\text{nasty}}$ *then every trajectory of* $\gamma_{\bar y}$ *is bang-bang with, at most, two switchings.*

If $\bar y$ *belongs to one of the remaining sets defined previously, the description of the optimal*

strategy is analogous, by symmetry.

Remark 5: In the case $\alpha=\pi/4$, some changes in the previous statement are required. In particular, the points A^+, B^+, O^+, and D^+ coincide (also the points A^-, B^-, O^-, and D^- coincide) and, consequently, there are no optimal trajectories containing singular arcs. Another immediate consequence of this fact is that there are only two optimal trajectories reaching the South Pole, of the form $B_\pi B_\pi$.

Remark 6: Notice that every point of $\overline{OB^+}\backslash O^+$, $\overline{OB^-}\backslash O^-$, $\overline{BP_S^+}$, $\overline{BP_S^-}$ is reached by more than one optimal trajectory, i.e., it belongs to the cut locus. Other points of the cut locus can be identified numerically in Ω^+_{nasty} and Ω^-_{nasty}, as explained in the next section.

Remark 7: In Theorem 1 we do not specify all the durations of the bang arcs. However, the missing ones can be obtained simply by following the switching strategy backward.

Remark 8: Note that the region reached by optimal trajectories containing a singular arc $\Omega_2^\pm\cup\Omega_3^\pm\cup\overline{AO^\pm}\cup\overline{OB^\pm}$ become bigger and bigger as α tends to $\pi/2$. Moreover, in this limit, since the modulus of the drift F_S becomes smaller and smaller, the time needed to cover such a region tends to infinity. Notice, however, that the time needed to reach P_S is always 2π. The time needed to reach every point of the sphere for α big enough, and the last point reached by an optimal trajectory containing a singular arc, can be computed explicitly. This is done in Appendix C.

Since the case $\bar{y}=P_S$ is important also for the determination of the cut locus in $\Omega^+_{\text{nasty}}\cup\Omega^-_{\text{nasty}}$, it is reported in the next section as a separate proposition (see Proposition 2).

1. The time optimal synthesis in $\Omega^\pm_{\text{nasty}}$ and optimal trajectories reaching P_S for $\alpha\geq\pi/4$

From the next proposition, T11 of Theorem 1 follows. More precisely, Proposition 2 shows that in the case $\alpha\geq\pi/4$, there are exactly four optimal trajectories steering P_N to P_S, and it characterizes them. As a consequence, the South Pole belongs to the cut locus.

Proposition 2: Consider the control system (10)–(13), *and assume* $\alpha\geq\pi/4$. *Then the optimal trajectories steering the North Pole to the South Pole are bang-bang with only one switching. More precisely, they are the four trajectories corresponding to the four controls*:

$$u^{(1)}=\begin{cases} u=1,\ t\in[0,t_1],\\ u=-1,\ t\in\,]\,t_1,T],\end{cases}\qquad u^{(2)}=\begin{cases} 1,\ t\in[0,t_3],\\ -1,\ t\in\,]\,t_3,T],\end{cases}$$

$$u^{(3)}=\begin{cases} -1,\ t\in[0,t_1],\\ 1,\ t\in\,]\,t_1,T],\end{cases}\qquad u^{(4)}=\begin{cases} -1,\ t\in[0,t_3],\\ 1,\ t\in\,]\,t_3,T],\end{cases}$$

where t_1 *and* t_3 *are defined in Definition 5, and* $T=2\pi$.

One can easily check that the switchings described in Proposition 2 occur on the equator ($y_3=0$).

The following proposition describes the optimal synthesis in $\Omega^\pm_{\text{nasty}}$, in a neighborhood of the points $D^\pm$ and the bifurcation occurring at $\alpha=\arcsin(1/\sqrt[4]{2})$.

Proposition 3: Let $\alpha\geq\pi/4$. *In a neighborhood of the point* D^+ *in* Ω^+_{nasty}, *there exists a switching curve starting at* D^+ *of the form* $e^{v(s)X_S^+}e^{sX_S^-}P_N$. *If* $\alpha>\pi/4$, *this curve is tangent to the equator at* D^+. *Moreover, if* $\alpha<\arcsin(1/\sqrt[4]{2})$ (*called* **Case 1**), *then the switching curve is optimal near* D^+, *while if* $\alpha\geq\arcsin(1/\sqrt[4]{2})$ (*called* **Case 2**) *then the switching curve is not locally optimal near* D^+ *and an overlap curve starts at the point* D^+. *A symmetric result holds in a neighborhood of* D^- *in* Ω^-_{nasty}.

The region Ω^+_{nasty} contains a cut locus that should be determined numerically. In **Case 2**, numerical simulations show that the switching curve starting at D^+ is never optimal, i.e., every point of Ω^+_{nasty} is reached by an optimal trajectory of the form $e^{tX_+}e^{sX_-}P_N$, with $s\in\,]0,t_1[$ or an optimal trajectory of the form $e^{tX_-}e^{sX_+}P_N$, with $s\in\,]\pi,t_3[$.

Remark 9: Notice, however, that, in **Case 2**, given a point $\bar{y}\in\Omega^+_{\text{nasty}}$, to find the time optimal trajectory reaching $\bar{y}$, it is not necessary to compute the cut locus. Indeed it is sufficient to compare

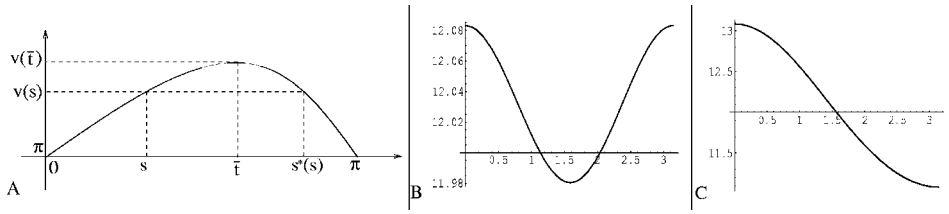

FIG. 7. Graph of $v(.)$ when $\alpha=\pi/6$ (A). Graph of the functions $\mathcal{F}$ and $\mathcal{G}$ when $\alpha=0.13$ (B) and (C).

the final times, corresponding to the two switching strategies given previously, and to chose the quickest one. The situation in Ω^-_{nasty} is symmetric.

In **Case 1**, the situation is more complicated. The switching curve described by Proposition 3 has the expression $C_1^+(s)=e^{X_S^+v(s)}e^{X_S^-s}P_N$, $s\in]0,t_1[$ where the function $v(.)$ is given by the same formula of the $\alpha<\pi/4$ case, i.e. $v(s)=\pi+2\arctan[(\sin s)/(\cos s+\cot^2\alpha)]$. (To verify such a formula, it is enough to repeat the computations done in Ref. 29.) As described by Proposition 3, this switching curve is optimal near D^+ and numerical simulations show that there exists $\bar{s}\in]0,t_1[$ such that there is an optimal trajectory switching on $C_1^+(s)$ if and only if $s\in[0,\bar{s}[$, and an overlap curve connecting $C_1^+(\bar{s})$ to the South Pole appears. The optimal synthesis for **Case 1** and **Case 2** is depicted in Fig. 6.

B. Optimal trajectories reaching the South Pole for $\alpha<\pi/4$

In this section we characterize the time optimal trajectories reaching the South Pole, in the case $\alpha<\pi/4$. This characterization is more complicated with respect to the case $\alpha\geq\pi/4$, due to the fact that the optimal trajectories have many switchings. The time optimal synthesis for $\alpha<\pi/4$ was already (partially) studied in Ref. 29, and it has been described in Sec. II.

From conditions (i)–(iv) in Sec. II, we know that every optimal trajectory starting at the North Pole has the form $B_{s_i}B_{v(s_i)}\cdots B_{v(s_i)}B_{s_f}$, where the function $v(s_i)$ is given by formula (17). [In the following we do not specify if the first bang corresponds to control $+1$ or -1, since, as a consequence of the symmetries of the problem, if $u(t)$ is an optimal control steering the North Pole to the South Pole, $-u(t)$ steers the North Pole to the South Pole as well.] It remains to identify one or more values of s_i,s_f and the corresponding number of switchings n for this trajectory to reach the South Pole.

Notice that $\bar{t}=\arccos(-\tan^2(\alpha))$ is the maximum of the function $v(.)$ on the interval $[0,\pi]$, $v(.)$ is increasing on $[0,\bar{t}]$ and decreasing on $[\bar{t},\pi]$ and $v(0)=v(\pi)=\pi$. Then, given $s\in[0,\pi]$ such that $s\neq\bar{t}$, there is a unique solution $s^*(s)\in[0,\pi]$, $s^*(s)\neq s$, to the equation $v(s^*)=v(s)$. The function $s^*(.)$ is extended to the whole interval $[0,\pi]$, setting $s^*(\bar{t})=\bar{t}$ [see Fig. 7(A)]. Thanks to the symmetries of the problem, we prove that if $\alpha<\pi/4$, s_f is equal either to s_i or to $s^*(s_i)$. This fact is described by Lemma 4 stated and proved in Appendix B.

The following two propositions describe how to identify candidate triples (s_i,s_f,n) for which the corresponding trajectory steers the North Pole to the South Pole in minimum time. From now on, all along the paper, we say that a bang-bang trajectory, solution of the system (10)–(13), is a *candidate optimal trajectory* if it is an extremal trajectory for problem (**P**) reaching the South Pole and it has a number n of switchings satisfying $n\leq N_M$ [defined in Formula (18)]. From Lemma 4, there are two kinds of candidate optimal trajectories:

- $s_f=s^*(s_i)$, called TYPE-1-candidate optimal trajectories
- $s_f=s_i$ called TYPE-2-candidate optimal trajectories

Define the following functions, whose geometric meaning is clarified in Appendix B.2:

$$\theta(s)=2\arccos\left(\sin^2\left(\frac{v(s)}{2}\right)\cos(2\alpha)-\cos^2\left(\frac{v(s)}{2}\right)\right), \tag{20}$$

$$\beta(s) = 2\arccos(\sin(\alpha)\cos(\alpha)(1-\cos(s))). \tag{21}$$

Proposition 4 (TYPE-1-trajectories): Fixed $\alpha < \pi/4$, *the equation for the couple* $(s,n) \in [0,\pi]\times\mathbb{N}$:

$$\mathcal{F}(s) := \frac{2\pi}{\theta(s)} = n, \tag{22}$$

has either two or zero solutions. More precisely, if (s,n) *is a solution to Eq.* (22), *then* $(s^*(s),n)$ *is the second one. The trajectories* $B_s\underbrace{B_{v(s)}\cdots B_{v(s)}}_{n-1}B_{s^*(s)}$ *and* $B_{s^*(s)}\underbrace{B_{v(s)}\cdots B_{v(s)}}_{n-1}B_s$ *are the TYPE-1-candidate optimal trajectories.*

Proposition 5 (TYPE-2-trajectories): Fixed $\alpha < \pi/4$, *the equation for the couple* $(s,n) \in [0,\pi]\times\mathbb{N}$:

$$\mathcal{G}(s) := \frac{2\beta(s)}{\theta(s)} + 1 = n, \tag{23}$$

has exactly two solutions. More precisely these solutions have the form (s_1,n), $(s_2,n+1)$. *The trajectories* $B_{s_1}\underbrace{B_{v(s_1)}\cdots B_{v(s_1)}}_{n-1}B_{s_1}$ *and* $B_{s_2}\underbrace{B_{v(s_2)}\cdots B_{v(s_2)}}_{n}B_{s_2}$ *are the TYPE-2-candidate optimal trajectories.*

In Figs. 7(B) and 7(C), the graphs of the functions (22) and (23) are drawn for a particular value of α, namely $\alpha=0.13$. Propositions 4 and 5 select a set of (possibly coinciding) four or eight candidate optimal trajectories (half of them starting with control +1 and the other half with control −1) corresponding to triples (s_i,s_f,n). Such triples can be easily computed numerically solving Eqs. (22) and (23). Then the optimal trajectories can be selected by comparing the times needed to reach the South Pole for each of the candidate optimal trajectory. Notice that there are at least two optimal trajectories steering the North to the South Pole (one starting with control +1 and the other with control −1).

If $\pi/(2\alpha)$ is an integer number $\bar{n}$, then TYPE-1 candidate optimal trajectories coincide with the TYPE-2 candidate optimal trajectories of the form $B_\pi\underbrace{B_\pi\ldots B_\pi}_{\bar{n}-2}B_\pi$. The remaining trajectories of TYPE-2 are of the form $B_s\underbrace{B_{v(s)}\ldots B_{v(s)}}_{\bar{n}-1}B_s$ for some $s\in]0,\pi[$. Otherwise, if $\pi/(2\alpha)$ is not an integer number, define the following:

$$m := \left[\frac{\pi}{2\alpha}\right], \quad \text{and the normalized remainder} \quad \mathsf{R} := \frac{\pi}{2\alpha} - \left[\frac{\pi}{2\alpha}\right] \in [0,1[.$$

where $[.]$ denotes the integer part. The following proposition determines precisely the time optimal trajectories for particular values of the parameter R:

Proposition 6: *For m large enough, there exist* $r_1(m) \le r_2(m) \in]0,1[$ *such that the following occurs*

A. *If* $\mathsf{R}\in]0,r_1(m)]$, *then Eq.* (22) *admits exactly two solutions that are both optimal, while TYPE-2 candidate optimal trajectories are not.*
B. *If* $\mathsf{R}\in]r_1(m),r_2(m)[$, *then Eq.* (22) *admits two solutions that are not optimal.*
C. *If* $\mathsf{R}\in]r_2(m),1[$ *then Eq.* (22) *does not admit any solution. Moreover,* $r_2(m)\to 0$ *for* $m\to\infty$.

Remark 10: The function $r_2(m)$ can be determined explicitly (see Appendix B2.1), while for $r_1(m)$ we are just able to prove the existence, and we conjecture that it can be taken equal to $r_2(m)$.

Remark 11: An important consequence of Proposition 6 is that for α small, the number of optimal trajectories reaching the South Pole is not fixed with respect to α. Indeed, such a number

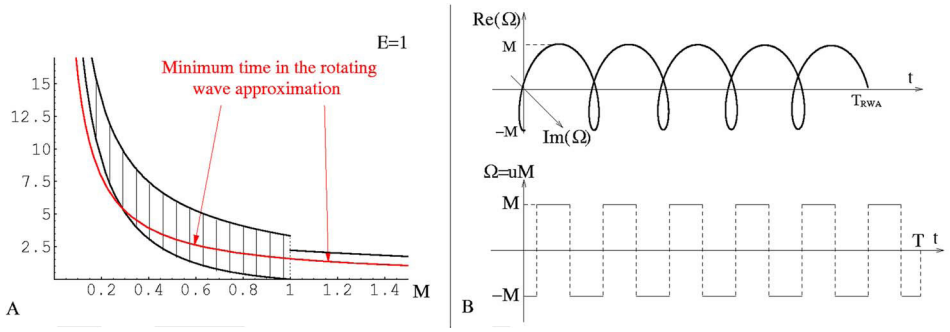

FIG. 8. (Color online) (A) Estimate of the minimum time to reach the state two and comparison with the time needed with two controls or in the rotating wave approximation (B) A comparison between the optimal strategy for our system and in the rotating wave approximation.

alternates as $\alpha \to 0$, according to Proposition 6: in particular, it is equal to 4 if $\mathsf{R} \in]0, r_1(m)]$ and it is equal to 2 if $\mathsf{R} \in]r_2(m), 1[\cup \{0\}$. This is enough to conclude that also the qualitative shape of the optimal synthesis in a neighborhood of the South Pole alternates, giving a partial proof to conjecture **C2** of Sec. II (originally stated in Ref. 29). In particular, it is a proof of the first assertion (on the dependence of the synthesis on the remainder $r=2\alpha\mathsf{R}$). Moreover, notice that the results of Proposition 6 perfectly fit with all the other statements of conjecture **C2**, with $r_2(m)$ playing the role of $\alpha_1/(2\alpha)$. One can apply the definition of locally equivalent syntheses given in Ref. 15 (see Definition 32, p. 59), to make rigorous the statement that the qualitative shape of the optimal synthesis changes with α.

Using the previous analysis one can easily show the following result (of which we skip the proof).

Proposition 7: If N is the number of switchings of an optimal trajectory joining the North to the South Pole, then

$$\frac{\pi}{2\alpha} - 1 \leq N < \frac{\pi}{2\alpha} + 1.$$

Using these inequalities and the fact that, for $\alpha < \pi/6$, the function $2s + (\pi/2\alpha - 1)v(s)$ is increasing on $[0, \pi]$, one can give a rough estimate of the time needed to reach the South Pole:

Proposition 8: The total time T of an optimal trajectory joining the North to the South Pole satisfies the inequalities:

$$\frac{\pi^2}{2\alpha} - 2\pi < T < \frac{\pi^2}{2\alpha} + \pi.$$

C. Comparison with results in the rotating wave approximation and with Ref. 8

In this section we come back to the original value of k, i.e., $k = 2E/\cos(\alpha) = 2\sqrt{M^2+E^2}$, and we compare the time necessary to steer the state one to the state two for our model and the model (4), described in Remark 1, in which we control the magnetic field both along the x and y directions, or we consider a two-level molecule in the rotating wave approximation. We recall that $-E, E$ are the energy levels and M is the bound on the control. For our model, the time of transfer T satisfies the following:

- for $\alpha \geq \pi/4$ (i.e., for $M \geq E$) then $T = 2\pi/k = \pi/\sqrt{M^2+E^2}$;
- for $\alpha < \pi/4$ (i.e., for $M < E$) then T is estimated by $1/k(\pi^2/2\alpha - 2\pi) < T < \frac{1}{k}(\pi^2/2\alpha + \pi)$.

On the other hand, for the model (4), the time of transfer is $T_C = \pi/(2M)$ (cf. Remark 1).

Fixed $E=1$, in Fig. 8(A) the times T and T_C as function of M are compared. Notice that

although T_C is bigger than the lower estimate of T in some interval, we always have $T_C \leq T$. This is due to the fact that the admissible velocities of our model are a subset of the admissible velocities of the model (4).

Notice that, fixed $E=1$, for $M \to 0$ we have $T \sim \pi^2/(4M) = (\pi/2)T_C$, while for $M \to \infty$, we have $T \sim \pi/M = 2T_C$.

Remark 12: For $M \ll E$ (i.e., for α small) the difference between two switching times is $v(s)/k \sim \pi/(2E)$. It follows that a time optimal trajectory connecting the North to the South Pole (in the interval between the first and the last bang) is periodic with period $P \sim \pi/E$, i.e., with a frequency of the order of the resonance frequency $\omega_R = 2E$ [see Fig. 8(B)]. On the other side, if $M > E$, then the time optimal trajectory connecting the North with the South Pole is the concatenation of two pulses. Notice that if $M \gg E$, the time of transfer is of the order of π/M and therefore tends to zero as $M \to \infty$. It is interesting to compare this result with a result of Khaneja, Brockett, and Glaser, for a two level system, but with no bound on controls (see Ref. 8). They estimate the infimum time to reach every point of the whole group $SU(2)$ in π/E. On the other side, in Appendix C it is proved that the time needed to cover the whole sphere $\mathbf{S}_B = SU(2)/S^1$ goes to $\pi/(4E)$ as M goes to infinity (however, this does not contradict the fact that the state two can be reached in an arbitrary small time, as we previously discussed).

Notice that our optimal control has the same "qualitative form" of the control computed in Ref. 8, i.e., a pulse (bang) followed by an evolution with the drift (singular) followed by a pulse (bang).

D. Some possible extensions

It is very easy to see that if $\{u_{\bar{y}}\}_{\bar{y} \in \mathbf{S}_B}$ is the collection of all time optimal controls steering the North Pole to all the points of $\mathbf{S}_B$, then the same set is also the collection of all time optimal controls starting from the South Pole.

Notice that nothing is changing if the controlled magnetic field is in any direction in the x-y plane. If this is not the case, the problem is different. However, the same techniques of this paper could be used to deal with this case, but the solution is probably more complicated.

Another interesting problem could be the variant of (**P**) in which one considers a different initial condition. In this case, generically, one loses the local controllability property (i.e., for small time, the trajectories do not cover a neighborhood of the starting point), but the structure of extremal trajectories (i.e., trajectories satisfying the Pontryagin Maximum Principle; cf. Appendix A) is very similar.

APPENDIX A: AN OVERVIEW ON OPTIMAL SYNTHESIS ON 2-D MANIFOLDS

In this section we briefly recall the theory of optimal syntheses on 2-D manifolds for a system of the kind $\dot{y} = F(y) + uG(y)$, $|u| \leq 1$, developed by Sussmann, Bressan, Piccoli, and the first author in Refs. 24–27 and recently rewritten in15. This appendix is written to be as much self-consistent as possible.

For every coordinate chart on the manifold it is possible to introduce the following three functions:

$$\Delta_A(y) := \mathrm{Det}(F(y), G(y)) = F_1(y)G_2(y) - F_2(y)G_1(y), \tag{A1}$$

$$\Delta_B(y) := \mathrm{Det}(G(y), [F,G](y)) = G_1(y)[F,G]_2(y) - G_2(y)[F,G]_1(y), \tag{A2}$$

$$f_S(y) := -\Delta_B(y)/\Delta_A(y). \tag{A3}$$

The sets $\Delta_A^{-1}(0), \Delta_B^{-1}(0)$ of zeros of Δ_A, Δ_B are, respectively, the set of points where F and G are parallel, and the set of points where G is parallel to $[F,G]$. These loci are fundamental in the construction of the optimal synthesis. In fact, assuming that they are a smooth embedded one-dimensional submanifold of M, we have the following:

- In each connected region of $M\backslash(\Delta_A^{-1}(0)\cup\Delta_B^{-1}(0))$, every extremal trajectory is bang-bang with, at most, one switching. Moreover, for every switching of the extremal trajectory, the value of the control passes from -1 to $+1$ if $f_S>0$ and from $+1$ to -1 if $f_S<0$.
- The support of singular trajectories (that are trajectories for which the switching function identically vanishes; see Definition 7) is always contained in the set $\Delta_B^{-1}(0)$.
- A trajectory not switching on the set of zeros of G is an abnormal extremal (i.e., a trajectory for which the Hamiltonian given by the Pontryagin Maximum Principle vanishes; see later) if and only if it switches on the locus $\Delta_A^{-1}(0)$.

Then the synthesis is built recursively on the number of switchings of extremal trajectories, canceling at each step the nonoptimal trajectories (see Ref. 15, Chap. 1).

Remark 13: Notice that, although the functions Δ_A and Δ_B depend on the coordinate chart, the sets $\Delta_A^{-1}(0)$, $\Delta_B^{-1}(0)$ and the function f_S do not, i.e., they are intrinsic objects of the control equation $\dot{y}=F(y)+uG(y)$.

1. Basic definitions and Pontryagin Maximum Principle on an *n*-dimensional manifold

In this section we define our optimization problem, we state the Pontryagin Maximum Principle (that is a key tool to compute optimal trajectories) and we give some basic definitions in the more general case of a n-dimensional manifold. We do this, since in Appendix B1 we stated some result for the original problem (14), on $S^3\sim SU(2)$.

Problem (Q): Consider the control system:

$$\dot{y}=F(y)+uG(y),\quad y\in M,\quad |u|\leq 1, \tag{A4}$$

where the following occurs.

(**H0**) *M is a smooth n-dimensional manifold. The vector fields $F(y)$ and $G(y)$ are $\mathcal{C}^\infty$.*

We are interested in the problem of reaching every point of M in minimum time from a point $y_0\in M$.

Definition 6: An admissible control $u(.)$ for the system (A4) *is a measurable function $u(.):[a,b]\to[-1,1]$, while an admissible trajectory is a Lipschitz functions $y(.):[a,b]\to M$ satisfying $\dot{y}(t)=F(y(t))+u(t)G(y(t))$, a.e., for some admissible control $u(.)$*

In the following we assume that the control system is *complete*, i.e., for every measurable control function $u(.):[a,b]\to[-1,1]$ and every initial state $\bar{y}$, there exists a trajectory $y(.)$ corresponding to $u(.)$, which is defined on the whole interval $[a,b]$ and satisfies $y(a)=\bar{y}$.

The main tool to compute time optimal trajectories is the Pontryagin Maximum Principle (PMP for short; see Refs. 14–16).

Theorem [Pontryagin maximum principle for the problem (Q)]: *Consider the control system* (A4) *subject to* (**H0**). *Define for every $(y,\lambda,u)\in T^*M\times[-1,1]$ the function*

$$\mathcal{H}(y,\lambda,u):=\langle\lambda,F(y)\rangle+u\langle\lambda,G(y)\rangle.$$

If the couple $(y(.),u(.)):[0,T]\to M\times[-1,1]$ is time optimal then there exist a never vanishing Lipschitz continuous covector $\lambda(.):t\in[0,T]\mapsto\lambda(t)\in T^*_{y(t)}M$ and a constant $\lambda_0\leq 0$ such that for, a.e., $t\in[0,T]$:

(i) $\dot{y}(t)=\frac{\partial\mathcal{H}}{\partial\lambda}(y(t),\lambda(t),u(t))$,
(ii) $\dot{\lambda}(t)=-\frac{\partial\mathcal{H}}{\partial y}(y(t),\lambda(t),u(t))=-\lambda(t)(\nabla F(y(t))+u(t)\nabla G(y(t)))$,
(iii) $\mathcal{H}(y(t),\lambda(t),u(t))=\mathcal{H}_M(y(t),\lambda(t))$ *where* $\mathcal{H}_M(y,\lambda):=\max\{\mathcal{H}(y,\lambda,u):u\in[-1,1]\}$,
(iiii) $\mathcal{H}_M(y(t),\lambda(t))+\lambda_0=0$.

Remark 14: The PMP is just a necessary condition for optimality. A trajectory $y(.)$ [resp., a couple $(y(.),\lambda(.))$] satisfying the conditions given by the PMP is said to be an *extremal* (resp., an *extremal pair*). An extremal corresponding to $\lambda_0=0$ is said to be an *abnormal extremal*, otherwise we call it a *normal extremal*.

We are now interested in determining the extremal trajectories satisfying the conditions given by the PMP. A key role is played by the following.

Definition 7 (switching function): Let $(y(.),\lambda(.))$ *be an extremal pair. The corresponding switching function is defined as* $\phi(t) := \langle \lambda(t), G(y(t)) \rangle$.

Notice that $\phi(.)$ is continuously differentiable [indeed $\dot{\phi}(t) = \langle \lambda(t), [F,G](y(t)) \rangle$, which is continuous].

Definition 8 (bang, singular): Let γ, *defined in* $[a,b]$, *be an extremal trajectory and* $u(.):[a,b] \to [-1,1]$ *the corresponding control. We say that* $u(.)$ *is a bang control if* $u(t) = +1$, *a.e., in* $[a,b]$ *or* $u(t) = -1$, *a.e., in* $[a,b]$. *We say that* $u(.)$ *is singular if the corresponding switching function* $\phi(t) = 0$ *in* $[a,b]$. *A finite concatenation of bang controls is called a bang-bang control. A switching time of* $u(.)$ *is a time* $\bar{t} \in [a,b]$ *such that, for every* $\varepsilon > 0$, u *is not bang or singular on* $(\bar{t}-\varepsilon, \bar{t}+\varepsilon) \cap [a,b]$. *An extremal trajectory of the control system* (A4) *is said abang extremal, singular extremal, bang-bang extremal, respectively, if it corresponds to a bang control, singular control, bang-bang control, respectively. If* $\bar{t}$ *is a switching time, the corresponding point on the trajectory* $y(\bar{t})$ *is called a switching point.*

The switching function is important because it determines where the controls may switch. In fact, using the PMP, one easily gets the following.

Proposition 9: A necessary condition for a time t to be a switching is that $\phi(t) = 0$. *Therefore, on any interval where* ϕ *has no zeroes* (*respectively, finitely many zeros*), *the corresponding control is bang* (*respectively, bang-bang*). *In particular,* $\phi > 0$ (*resp,* $\phi < 0$) *on* $[a,b]$ *implies* $u = 1$ (*resp.*, $u = -1$) *a.e. on* $[a,b]$. *On the other hand, if* ϕ *has a zero at t and* $\dot{\phi}(t)$ *is different from zero, then t is an isolated switching.*

2. More on singular extremals and predicting switchings for 2-D systems

Now we come back to the case in which M is two dimensional. In this section we compute the control corresponding to singular extremals and we would like to predict which kind of switchings can occur, using properties of the vector fields F and G. The following two lemmas illustrate the role of the functions $\Delta_A^{-1}(0)$, $\Delta_B^{-1}(0)$ in relation with singular and abnormal extremals. The proofs can be found in Refs. 24, 15, and 26.

Lemma 1: Let $y(.)$ *be an extremal trajectory that is singular in* $[a,b] \subset Dom(y(.))$. *Then* $y(.)|_{[a,b]}$ *corresponds to the so called singular control* $\varphi(y(t))$, *where*

$$\varphi(y) = -\frac{\nabla \Delta_B(y) \cdot F(y)}{\nabla \Delta_B(y) \cdot G(y)}, \tag{A5}$$

with Δ_A *and* Δ_B *defined in Eqs.* (A1) and (A2). *Moreover, on* $Supp(y(.))$, $\varphi(y)$ *is always well defined and its absolute value is less than or equal to one. Finally,* $Supp(y(.)|_{[a,b]}) \subset \Delta_B^{-1}(0)$.

Lemma 2: Let $y(.)$ *be a bang-bang extremal for the control problem* (A4), $t_0 \in Dom(y(.))$ *be a time such that* $\phi(t_0) = 0$ *and* $G(y(t_0)) \neq 0$. *Then, the following conditions are equivalent:* (i) $y(.)$ *is an abnormal extremal*; (ii) $y(t_0) \in \Delta_A^{-1}(0)$; and (iii) $y(t) \in \Delta_A^{-1}(0)$, *for every time* $t \in Dom(y(.))$, *such that* $\phi(t) = 0$.

The following lemma describes what happens when Δ_A and Δ_B are different from zero.

Lemma 3: Let $\Omega \subset M$ *be an open set such that* $\Omega \cap (\Delta_A^{-1}(0) \cup \Delta_B^{-1}(0)) = \emptyset$. *Then all connected components of* $Supp(y(.)) \cap \Omega$, *where* $y(.)$ *is an extremal trajectory of* (A4), *are bang-bang with, at most, one switching. Moreover, if* $f_S > 0$ *throughout* Ω, *then* $y(.)|_\Omega$ *is associated to a constant control equal to* $+1$ *or* -1 *or has a switching from* -1 *to* $+1$. *If* $f_S < 0$ *throughout* Ω, *then* $y(.)|_\Omega$ *is associated to a constant control equal to* $+1$ *or* -1 *or has a switching from* $+1$ *to* -1.

Remark 15: For the problem **(Q)**, under generic conditions on the vector fields F and G, one can make the complete classification of synthesis singularities, stable synthesis, singularities of the minimum time wave fronts. We refer to Ref. 15 for the general theory. For some extensions to higher dimension, see Refs. 31 and 32.

APPENDIX B: PROOF OF THE MAIN RESULTS

In this section we give the proof of our main results. We start with a lemma, stating a property of optimal trajectories, that is a consequence of the symmetries of the problem. It is used to identify the time optimal trajectories steering the North to the South Pole both for $\alpha \geq \pi/4$ and $\alpha < \pi/4$.

Lemma 4: Let $\alpha \in]0, \pi/2[$. *Every optimal bang-bang trajectory, connecting the North to the South Pole, with more than one switching is such that* $v(s_i)=v(s_f)$ *where* s_i *is the first switching time,* s_f *is the time needed to steer the last switching point to the South Pole and* $v(s_i)$ *is the time between two consecutive switchings.*

Proof of Lemma 4: Consider the problem of connecting P_S with P_N in minimum time for the system $\dot{z}=F'_S(z)+uG'_S(z)$, where $z \in S^2$ and $F'_S(z)=-F_S(z)$, $G'_S(z)=-G_S(z)$. The trajectories of this system coincide with those of the system (10)–(13), but the velocity is reversed. Therefore the optimal trajectories for the new problem coincide with the optimal ones for the system (10)–(13) connecting P_N to P_S, and the time between two switchings is the same. Since performing the change of coordinates $(z_1, z_2, z_3) \to (y_1, y_2, y_3)=(-z_1, z_2, -z_3)$, the new problem becomes exactly the original problem, we deduce that, if we have more than one switching, it must be $v(s_i)=v(s_f)$. ■

1. Time optimal synthesis for the two level quantum system for $\alpha \geq \pi/4$

In this section, we apply the theory of optimal syntheses on 2-D manifolds recalled in Appendix A, to the system (10)–(13). Our aim is to describe the time optimal synthesis for $\alpha \geq \pi/4$, i.e., to prove Theorem 1 and Propositions 2 and 3. First, we state some general results, holding for $\alpha \in]0, \pi/2[$, regarding time optimal trajectories of the system (14), on $S^3 \sim SU(2)$, analogous to those obtained in Ref. 29 for $SO(3)$ (in particular, the proofs can be repeated using the same arguments).

A. General results on S^3

In this section $\alpha \in]0, \pi/2[$. The first proposition states that singular extremals, defined as extremals for which the switching function vanishes (see Definitions 7 and 8) correspond to zero control. This fact is very specific for our problem.

Proposition 10: For the normalized minimum time problem on S^3 (14), *singular extremals are integral curves of the drift, i.e., they must correspond to a control almost everywhere vanishing.*

Since for a fixed $u \in [-1, 1]$ every trajectory of (14) is periodic with period $4\pi/\sqrt{u^2 \sin^2 \alpha + \cos^2 \alpha}$, we have the following.

Proposition 11: Given an extremal trajectory γ *of type* B_t (*resp.*, S_t), *then* $t < 4\pi$ (*resp.*, $t < 4\pi/\cos \alpha$).

The following proposition describes the switching behavior of abnormal and bang-bang normal extremals (see Sec. A 1 for the definition).

Proposition 12: Let γ *be an abnormal extremal of* (14). *Then it is bang-bang and the time duration between two consecutive switchings is always equal to* π. *In other words,* γ *is of kind* $B_s B_\pi \ldots B_\pi B_t$ *with* $s, t \leq \pi$.

On the other hand, if γ *is a bang-bang normal extremal, then the time duration* $\mathcal{T}$ *along an interior bang arc is the same for all interior bang arcs and verifies* $\pi < \mathcal{T} < 2\pi$ (*i.e.,* γ *is of kind* $B_s B_\mathcal{T} \ldots B_\mathcal{T} B_t$ *with* $s, t \leq \mathcal{T}$).

For the optimal trajectories containing a singular arc we have the following.

Proposition 13: Let γ *be a time optimal trajectory containing a singular arc. Then* γ *is of the type* $B_t S_s B_{t'}$, *with* $s \leq 2\pi/\cos \alpha$ *if* $t > 0$ *or* $t' > 0$ *and* $s < 4\pi/\cos \alpha$ *otherwise.*

These results on $S^3 \sim SU(2)$ are useful to determine the optimal synthesis on $\mathbf{S}_\mathrm{B}$, since every optimal trajectory on $\mathbf{S}_\mathrm{B}$ is the projection of an optimal trajectory on S^3. This is a simple consequence of the fact that $\mathbf{S}_\mathrm{B}$ is a homogeneous space of $SU(2)$.

Proposition 14: A time optimal trajectory γ *for the system* (10)–(13) *on* $\mathbf{S}_\mathrm{B}$ *starting at* P_N *is*

the projection of a time optimal trajectory of (14), *starting from a point satisfying* $|\psi_1|^2=1$ [*recall that* $\psi=(\psi_1,\psi_2)^T\in S^3\subset\mathbb{C}^2$].

Remark 16: Notice that, since two opposite points on S^3 project on the same point on $\mathbf{S}_\mathrm{B}$, it is easy to see from Proposition 11 that the projection on $\mathbf{S}_\mathrm{B}$ of an optimal trajectory of (14) of type B_t (resp., S_t), must be such that $t<2\pi$ (resp., $t<2\pi/\cos\alpha$). More precisely, for a fixed $u\in[-1,1]$ every trajectory of (10)–(13) is periodic with period $2\pi/\sqrt{u^2\sin^2\alpha+\cos^2\alpha}$ (the period divides by two after projection).

B. Construction of the synthesis on $\mathbf{S}_\mathrm{B}$

In this section we assume $\alpha\geq\pi/4$. Following Appendix A, we first need to determine the sets $\Delta_A^{-1}(0)$, $\Delta_B^{-1}(0)$, and the function f_S. Checking where F_S is parallel to G_S and where G_S is parallel to $[F_S,G_S]$, one gets $\Delta_A^{-1}(0)=\{y\in\mathbf{S}_\mathrm{B}:y_2=0\}$ and $\Delta_B^{-1}(0)=\{y\in\mathbf{S}_\mathrm{B}:y_3=0\}$. To find the function f_S we can choose for instance, the coordinate chart defined on each hemisphere by the projection on the plain $\{(y_1,y_2)\in\mathbb{R}^2\}$, obtaining $f_S=(\sin\alpha)y_3/y_2$. Then Lemma 3 says that every optimal trajectory belonging to one of the regions $\{y\in\mathbf{S}_\mathrm{B}:y_3>0,y_2>0\}$, $\{y\in\mathbf{S}_\mathrm{B}:y_3<0,y_2<0\}$ is bang-bang with, at most, one switching. Moreover only the switching from control -1 to control $+1$ is allowed. On the contrary, on the regions $\{y\in\mathbf{S}_\mathrm{B}:y_3>0,y_2<0\}$, $\{y\in\mathbf{S}_\mathrm{B}:y_3<0,y_2>0\}$, the control can switch only from $+1$ to -1. Moreover, thanks to Lemma 1, every singular extremal must lie on the equator. The following lemma characterizes the structure of the bang-bang extremals for the problem (**P**).

Lemma 5: Recall that $t_1=\pi-\arccos(\cot^2\alpha)$ *and* $t_3=\pi+\arccos(\cot^2\alpha)$ *and consider a bang-bang extremal for the problem* (**P**). *Then it is of the form* $B_sB_{v(s)}B_{v(s)}\ldots$ *with* $s\in[0,t_1]\cup[\pi,t_3]$, *where, on the set* $[0,t_1[\cup[\pi,t_3[$, $v(.)$ *is defined as follows:*

$$v(s):=\pi+2\arctan\left(\frac{\sin s}{\cos s+\cot^2\alpha}\right).$$

If $\alpha=\pi/4$ *then* $t_1=t_3=\pi$ *and* $v(\pi):=\pi$, *while if* $\alpha>\pi/4$ *we set* $v(t_1):=v(t_3):=2\pi$.

Notice that the function $v(.)$ has the same expression (17) obtained in the case $\alpha<\pi/4$ (excepted at the points t_1 and t_3). However, its interval of definition is different.

Proof of Lemma 5: As shown previously, the meridian $\Delta_A^{-1}(0)$ and the equator $\Delta_B^{-1}(0)$ divide the sphere in four parts and in each of them the sign of the function f_S is constant and changes when passing through $\Delta_A^{-1}(0)$ or $\Delta_B^{-1}(0)$. In particular, following γ^+ or γ^- (cf. Remark 4) in the case in which $\alpha>\pi/4$ this happens at the times t_1 (where the equator is crossed), at time π (where $\Delta_A^{-1}(0)$ is crossed) and at time t_3 (again is the equator to be crossed). Applying Lemma 3, we obtain that for an extremal trajectory the first switching may occur only on the intervals $[0,t_1]$ and $[\pi,t_3]$. Exactly as in,[29] one shows that the extremal must have the form $B_sB_{v(s)}B_{v(s)}\ldots$ with $s\in[0,t_1]\cup[\pi,t_3]$. The case $\alpha=\pi/4$ is similar. ■

Remark 17: One can also show that every trajectory starting from P_N, of the form $B_sB_{v(s)}B_{v(s)}\ldots$ with $s\in[0,t_1]\cup[\pi,t_3]$, is extremal, i.e., for every s in such a set, there exists an initial value of the covector λ such that the switching function $\phi(.)$ vanishes for the first time at time s.

Unlike the case in which $\alpha<\pi/4$, in the case $\alpha>\pi/4$ it is possible to establish the presence of optimal trajectories containing a singular arc, whose switching behavior is described by the following proposition, illustrated in Fig. 9(A).

Proposition 15: Let $\alpha\geq\pi/4$. *A trajectory* γ *of* (10)–(13) *starting with control* $u=1$ *and containing a singular arc is a solution of* (**P**) *if and only if it is of the form* $B_tS_sB_{t'}$ *and satisfies the following conditions.*

- $t=t_1=\pi-\arccos(\cot^2\alpha)$, *i.e., γ coincides with* γ^+ *until it reaches the equator.*
- $s\leq\arccos(\cot\alpha)/\cos\alpha$, *i.e., the singular arc is optimal until it reaches the point* $O^+=(1,0,0)^T$.
- *If* $s=\arccos(\cot\alpha)/\cos\alpha$, *then the trajectory is of type* B_tS_s, (*i.e., the time duration of the*

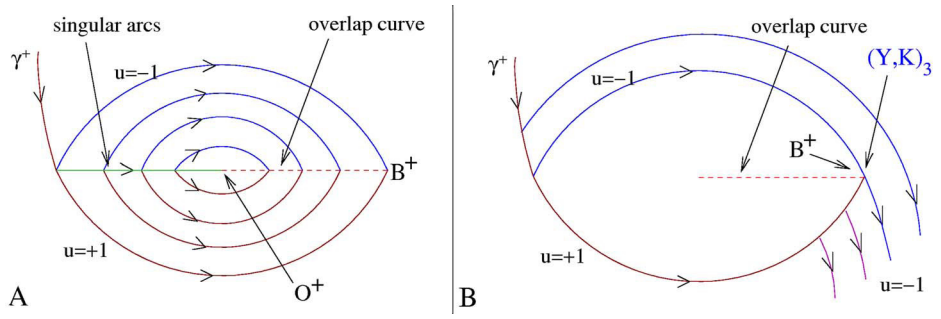

FIG. 9. (Color online) The region covered by optimal trajectories with singular arcs and the $(Y,K)_3$ frame point.

last bang arc reduces to zero). *If* $s<\arccos(\cot\alpha)/\cos\alpha$, *then* γ *is optimal until the last bang arc reaches the equator* [*i.e., it does not exist* $\bar{t}\in]0,t'[$ *such that* $\gamma(t+s+\bar{t})$ *is contained in the equator*].

An analogous result holds for trajectories, starting with control -1.

Remark 18: Notice that in the case $\alpha=\pi/4$, Proposition 15 provides a singular trajectory degenerated to a point. In other words, for $\alpha=\pi/4$ there are no singular trajectories that are optimal.

Remark 19: Notice that the previous result completely characterizes the optimal synthesis in some neighborhoods of the points $O^{\pm}=(\pm1,0,0)^T$, namely $\Omega_2^{\pm}\cup\Omega_3^{\pm}$, and moreover it determines the presence of two symmetric overlap curves contained inside the equator. The synthesis around the point O^+ is represented in Fig. 9(A).

Proof of Proposition 15: Consider a trajectory, solution of (**P**), starting with $u=+1$ and containing a singular arc. Using Propositions 13 and 14, this trajectory must be of the form $B_tS_sB_{t'}$, and, since the singular arc is contained inside the equator, we have $t=t_1$ (the case $t=t_3$ can be easily excluded). Consider a singular arc containing in its interior the point O^+. This arc contains two points of the form $(y_1^0,-y_2^0,0)^T$ and $(y_1^0,y_2^0,0)^T$, with both y_1^0, y_2^0 positive, that can be connected by a bang arc. Using classical comparison theorems for second order ODEs, one can easily compare the time needed to follow such a trajectory with the time needed to steer the two points along the singular arc finding that the bang arc is quicker than the singular arc. Therefore a singular arc containing O^+ cannot be optimal. By symmetry, the extremal trajectories that have the same singular arc, but the last bang arc corresponding to opposite control, must meet on a point of the equator. Therefore the arc of the equator that is comprised between the point O^+ (resp., O^-) and the second intersection point with γ^+ (resp., γ^-) is an overlap curve. It remains now to verify that the trajectories previously described are optimal (until the last bang arc reaches the equator). This is a straightforward consequence of the fact that the quickest bang-bang trajectories that enter the region spanned by such trajectories (i.e., the closure of the regions $\Omega_2^{\pm}\cup\Omega_3^{\pm}$) are not extremal because of Lemma 3 (see also Lemma 5). ■

Remark 20: Notice the trivial fact that, if a trajectory γ defined on the interval $[a,b]$ is optimal between $\gamma(a)$ and $\gamma(b)$, then the restriction of γ in $[c,d]$, $c,d\in[a,b]$, $c<d$, is optimal between $\gamma(c)$ and $\gamma(d)$.

Using Remark 20, we have that Proposition 15 characterizes completely the time optimal synthesis on $\overline{P_NA^{\pm}}$, and in the closure of $\Omega_2^{\pm}\cup\Omega_3^{\pm}$, i.e., it proves items **T1**–**T6**, **T9**, and **T10**, of Theorem 1.

Remark 21: From Lemma 5 we obtain that there are four families of bang-bang trajectories. In particular, the families starting with control $+1$ and switching, respectively, in $[0,t_1]$ and $[\pi,t_3]$ join at the point B^+, generating an amazing $(Y,K)_3$ frame point, in the framework of the classification of Ref. 15. See Fig. 9(B).

Next we give the proof of Proposition 2, from which it follows **T11** of Theorem 1, and, using again Remark 20, also **T7**.

Proof of Proposition 2: By Proposition 15, there are no optimal trajectories containing a singular arc joining P_N with P_S. One can easily see that the only possible trajectories steering P_N to P_S with only one switching are those described in the statement of the proposition, that we have to compare with trajectories having more than one switching. Trajectories having two switchings with the first or the last bang longer than π and trajectories with more than two switchings are excluded, since from Lemma 5 their total time is larger than 2π. Trajectories having two switchings and the length of the first arc s_i and the length of the last arc s_f satisfying $s_i, s_f < \pi$ are excluded, since by Lemma 4 they must satisfy $s_i = s_f$. For these trajectories the total time can be easily computed and it is $2\pi + 2\arcsin(1/2\sin(\alpha)) > 2\pi$. ■

Item **T8** is proved by the following.

Proposition 16: If $\bar{y} \in \Omega_1^+ \cup (\overline{DP_S^-} \backslash P_S)$, *then* $\gamma_{\bar{y}}$ *is made by a unique trajectory of the form* $B_t B_{t'}$, *with* $0 \le t < t_1$ *and the first bang corresponding to control* $+1$. *A similar result holds if* $\bar{y} \in \Omega_1^- \cup (\overline{DP_S^+} \backslash P_S)$. *As a consequence there is not a cut locus in the region,* $\Omega_1^+ \cup \Omega_1^-$. *On the other hand,* $\Omega_{\text{nasty}}^+ \cup \Omega_{\text{nasty}}^-$ *contains a cut locus.*

Proof of Proposition 16: Define the following three families of extremal trajectories:

$$\gamma_s^A(t) := e^{tX_S^+} e^{sX_S^-} P_N, \quad \text{with } s \in \,]0, t_1[\text{ and } t \le v(s),$$

$$\gamma_s^B(t) := e^{tX_S^-} e^{sX_S^+} P_N, \quad \text{with } s \in [\pi, t_3[\text{ and } t \le v(s),$$

$$\gamma_s^C(t) := e^{tX_S^-} e^{v(s)X_S^+} e^{sX_S^-} P_N, \quad \text{with } s \in \,]0, t_1[\text{ and } t \le v(s).$$

First, notice that from Proposition 2 that there are no optimal trajectories of kind γ_s^A reaching the arc $\overline{BP_S^+}$. Now for every point $x \in \overline{DP_S^+}$ the following occurs: (i) there exist s_A, t_A such that $x = \gamma_{s_A}^A(t_A)$, and they are unique; (ii) if there exist s_B, t_B (resp., s_C, t_C) such that $x = \gamma_{s_B}^B(t_B)$, [resp., $x = \gamma_{s_C}^C(t_C)$], then they are unique. By direct computation, one can compare the times the three trajectories need to reach x, i.e. $s_A + t_A, s_B + t_B, s_C + v(s_C) + t_C$, finding that the optimal trajectory is of kind γ^A (these computations are long, not very instructive, and we omit them). From this fact, the first part of the claim immediately follows. Moreover, it implies that there is not a cut locus in Ω_1^+, since the only trajectories entering such a region are those of the form γ^A. The existence of a cut locus in Ω_{nasty}^+ is evident, since no optimal trajectories belonging to the families γ^A, γ^B, γ^C leave Ω_{nasty}^+. The reasoning in Ω_1^- and in Ω_{nasty}^- is similar. ■

End of the proof of Theorem 1: To conclude the proof of Theorem 1, it remains to prove **T12**. Consider by contradiction an optimal bang-bang trajectory γ defined in $[0, t_\gamma]$ steering P_N to a point of Ω_{nasty}^+, with at least three switchings. Define $\bar{t} = \max\{t \in [0, t_\gamma] : \gamma(t) \notin \Omega_{\text{nasty}}^+\}$. Then, by Remark 20, $\gamma|_{[0,\bar{t}]}$ must be optimal between P_N and $\gamma(\bar{t})$. Then, from the results proved previously, we deduce that $\gamma|_{[0,\bar{t}]}$ can have, at most, one switching. Therefore γ switches at least two times in Ω_{nasty}^+, and the arc between them must be completely contained in Ω_{nasty}^+, and this leads to a contradiction since the sign of f_S is constant in Ω_{nasty}^+ (see Lemma 3). ■

Before proving Proposition 3, notice that the point D^+, which is obtained following the trajectory γ^+ for a time π (see Fig. 6), belongs to two different families of bang-bang trajectories at time π, one given by trajectories starting with control -1 and switching at time $s \le t_1$, the other one given by trajectories that start with control 1 and switching at time $s \in [\pi, t_3]$. Moreover, since $v(0) = \pi$, there must be a switching curve starting at D^+ and therefore we deduce that there are two possible behaviors of the optimal synthesis around this point: either this switching curve is optimal or the two fronts continue to intersect generating an overlap curve.

Observe that if $\alpha \ge \pi/3$ the trajectories of the type $B_s B_{v(s)} B_t$ with s small cannot be optimal since the vector fields X_S^+ and X_S^- point to opposite sides on the switching curve (i.e., the switching curve "reflects the trajectories," and therefore it is not locally optimal, by the definition given in Sec. II). In this case the two families of bang-bang trajectories described previously must intersect, giving rise to an overlap curve. Therefore to prove Proposition 3 we assume $\alpha < \pi/3$.

Proof of Proposition 3: First we parametrize the switching curve with respect to the first switching time (assuming without loss of generality that this curve starts with $u=-1$):

$$C(s) = e^{v(s)X_S^+} e^{sX_S^-} P_N.$$

We consider the functions $\xi_1(s)=\det(C(s), C'(s), X_S^+(C(s)))$ (here the superscript $'$ denotes the derivative with respect to s) and $\xi_2(s)=\det(C(s), C'(s), X_S^-(C(s)))$. It is easy to see that the optimality of $C(.)$, for s small, depends on the signs of such functions. Indeed $C(.)$ is locally optimal near the point $D^+=C(0)$ if and only if for every positive and small enough s, and given a neighborhood of $C(s)$ that is divided in two connected components U_1, U_2 by the trajectory $C(.)$, both $X_S^-(C(s))$ and $X_S^+(C(s))$ point toward U_1 or toward U_2. It is easy to see that this occurs if $\xi_1(s)$ and $\xi_2(s)$ have the same sign. Notice that $\xi_1(0)=\xi_2(0)=0$ and that $\xi_1(s) = \det(P_N, X_S^-(P_N), e^{-sX_S^-} X_S^+(e^{sX_S^-} P_N)) = 2\cos\alpha \sin^2\alpha \sin s$, which is positive for every $\alpha < \pi/2$ and $s \in]0, \pi[$. To determine the sign of $\xi_2(s)$ near 0, it is enough to look at the sign of the derivative $\xi_2'(0)$ that can be computed directly: $\xi_2'(0) = 4\cos\alpha \sin^2\alpha(1-2\sin^4\alpha)$. We deduce that, if $\alpha < \arcsin(1/\sqrt[4]{2})$, the switching curve $C(.)$ is optimal for s small enough. For the particular value $\alpha = \arcsin(1/\sqrt[4]{2})$, one can easily check that the function $\xi_2(.)$ is negative for $s>0$ small, and then $C(.)$ is no more optimal for $\alpha \geq \arcsin(1/\sqrt[4]{2})$. The tangency of the switching curve starting at D^+ if $\alpha > \pi/4$, is a consequence of the fact that, in this case, the bang-bang trajectory switching at D^+ is an abnormal extremal (see Proposition 2 and Ref. 15, Proposition 23, pp. 177). ■

2. Time optimal trajectories reaching the South Pole for $\alpha < \pi/4$

Our purpose of this section is to characterize the optimal trajectories steering P_N to P_S in the case $\alpha < \pi/4$, i.e., to prove Propositions 4 and 5. A key tool is Lemma 4. Recall the shape of the function $v(s)$, in the case $\alpha < \pi/4$ [see Fig. 7(A)]. Given $\alpha < \pi/4$ and $s \in [0, \pi]$ with $s \neq \arccos(-\tan^2\alpha)$, there exists one and only one time $s^*(s) \in [0, \pi]$ different from s, such that $v(s) = v(s^*(s))$. From Sec. III B, recall the following definition of candidate optimal trajectories:

- $s_f = s^*(s_i)$ (i.e., TYPE-1-candidate optimal trajectories),
- $s_f = s_i$ (i.e., TYPE-2-candidate optimal trajectories).

A useful relation between s and $s^*(s)$ is given by the following.

Lemma 6: For $\alpha < \pi/4$ and $s \in [0, \pi]$, it holds that $s + s^*(s) = v(s)$.

Proof of Lemma 6: Both s and $s^*(s)$ satisfy the following equation in $t \in [0, \pi]$:

$$\cot\left(\frac{1}{2}v(s)\right) = -\frac{\sin(t)}{\cos(t)+\cot^2(\alpha)} \Rightarrow \cos\left(\frac{1}{2}v(s)-t\right) = -\cos\left(\frac{1}{2}v(s)\right)\cot^2(\alpha).$$

Therefore, since $\frac{1}{2}v(s) - t \in [-\pi, \pi]$, $\forall s, t \in [0, \pi]$ and $s^*(s) \neq s$, it must be $s^*(s) - \frac{1}{2}v(s) = \frac{1}{2}v(s) - s \Rightarrow s + s^*(s) = v(s)$. ■

The description of candidate optimal trajectories is simplified by the following lemma, of which we skip the proof.

Lemma 7: Set

$$Z(s) = \frac{1}{\rho}\begin{pmatrix} 0 & \cot\left(\frac{1}{2}v(s)\right) & -\sin(\alpha) \\ -\cot\left(\frac{1}{2}v(s)\right) & 0 & 0 \\ \sin(\alpha) & 0 & 0 \end{pmatrix},$$

where $\rho = \sqrt{\cot^2\left(\frac{1}{2}v(s)\right) + \sin^2(\alpha)}$. *Then, if* $\theta(s)$ *is defined as in* (20), *we have* $e^{\theta(s)Z(s)} = e^{v(s)X_S^-} e^{v(s)X_S^+}$. Notice that the matrix $Z(s) \in so(3)$ is normalized in such a way that the map $t \mapsto e^{tZ(s)} \in SO(3)$ represents a rotation around the axes $R(s) = \left(0, \sin(\alpha), \cot\left(\frac{1}{2}v(s)\right)\right)^T$ with angular velocity equal to one.

To prove the results stated in Sec. III B we study separately the two possible cases previously listed.

Proof of Proposition 4: In this case we consider TYPE-1-candidate optimal trajectories. Assume that the optimal trajectory starts with $u=-1$ (the case $u=1$ is symmetric) and has an even number n of switchings. Then it must be

$$P_S = e^{s_f X_S^-} \underbrace{e^{v(s_i)X_S^+} \dots e^{v(s_i)X_S^+}}_{n-1 \text{ times}} e^{s_i X_S^-} P_N \tag{B1}$$

where P_N and P_S denote, respectively, the North and the South Pole, and we have that

$$e^{s_i X_S^-} P_S = e^{v(s_i)X_S^-} e^{v(s_i)X_S^+} \dots e^{v(s_i)X_S^+} e^{s_i X_S^-} P_N = e^{(1/2)n\theta(s_i)Z(s_i)} e^{s_i X_S^-} P_N,$$

from which we deduce that s_i must satisfy

$$\frac{1}{2} n\theta(s_i) = \pi + 2p\pi, \quad \text{for some integer} p.$$

It is easy to see that a value of s_i that satisfies a previous equation with $p>0$ does not give rise to a candidate optimal trajectory since the corresponding number of switchings is larger than N_M. Therefore in a previous equation it must be $p=0$. If n is odd, instead than (B1) we have

$$P_S = e^{s_f X_S^+} \underbrace{e^{v(s_i)X_S^-} \dots \dots e^{v(s_i)X_S^+}}_{n-1 \text{ times}} e^{s_i X_S^-} P_N \tag{B2}$$

and, moreover, by symmetry,

$$P_N = e^{s_f X_S^-} e^{v(s_i)X_S^+} \dots \dots e^{v(s_i)X_S^-} e^{s_i X_S^+} P_S.$$

Then, combining with (B2) and using the relation Lemma 6, we find

$$P_N = e^{-s_i X_S^-} \underbrace{e^{v(s_i)X_S^-} \dots \dots e^{v(s_i)X_S^+}}_{2n \text{ times}} e^{s_i X_S^-} P_N = e^{-s_i X_S^-} e^{n\theta(s_i)Z(s_i)} e^{s_i X_S^-} P_N.$$

Since $e^{s_i X_S^-} P_N$ is orthogonal to the rotation axis $R(s_i)$ corresponding to $Z(s_i)$, the previous identity is satisfied if and only if $n\theta(s_i)=2m\pi$ with m a positive integer. As in the previous case, for a candidate optimal trajectory, it must be $m=1$. ■

Proof of Proposition 5: Here we consider TYPE-2-candidate optimal trajectories. For simplicity call $s_i=s_f=s$. Assume, as before, that the optimal trajectory starts with $u=-1$. If this trajectory has $n=2q+1$ switchings then it must be

$$P_S = e^{sX_S^+} e^{q\theta(s)Z(s)} e^{sX_S^-} P_N.$$

In particular, the points $e^{-sX_S^+} P_S$ and $e^{sX_S^-} P_N$ must belong to a plane invariant with respect to rotations generated by $Z(s)$, and therefore the difference $e^{sX_S^-} P_N - e^{-sX_S^+} P_S$ must be orthogonal to the rotation axis $R(s)$. Actually it is easy to see that this is true for every value $s \in [0, \pi]$, since both $e^{-sX_S^+} P_S$ and $e^{sX_S^-} P_N$ are orthogonal to $R(s)$. Since the integral curve of $Z(s)$ passing through $e^{sX_S^-} P_N$ and $e^{-sX_S^+} P_S$ is a circle of radius 1, it is easy to compute the angle $\beta(s)$ between these points. In particular, the distance between $e^{sX_S^-} P_N$ and $e^{-sX_S^+} P_S$ coincides with $2\sin(\beta(s)/2)$, and so one easily gets the expression $\beta(s)=2\arccos(\sin(\alpha)\cos(\alpha))(1-\cos(s))$. Then Proposition 5 is proved when n is odd.

Assume now that the optimal trajectory has $n=2q+2$ switchings; then we can assume without loss of generality that $P_S = e^{sX_S^-} e^{v(s)X_S^+} e^{q\theta(s)Z(s)} e^{sX_S^-} P_N$. First of all, it is possible to see that $e^{-v(s)X_S^+} e^{-sX_S^-} P_S$ is orthogonal to $R(s)$. So it remains to compute the angle $\tilde{\beta}(s)$ between the point $e^{sX_S^-} P_N$ and the point $e^{-v(s)X_S^+} e^{-sX_S^-} P_S$ on the plane orthogonal to $R(s)$. As before, the distance

between these points coincides with $2\sin(\tilde{\beta}(s)/2)$. Instead of computing directly $\tilde{\beta}(s)$, we compute the difference between the angle $\tilde{\beta}(s)$ and the angle $\beta(s)$ previously defined above. We know that

$$2\sin\left(\frac{\beta(s)}{2}-\tilde{\beta}(s)\right)=\left|e^{-v(s)X_S^+}e^{-sX_S^-}P_S-e^{-sX_S^+}P_S\right|=\left|e^{-sX_S^-}P_S-e^{v(s)X_S^+}e^{-sX_S^+}P_S\right|=\left|e^{-sX_S^-}P_S-e^{s^*(s)X_S^+}P_S\right|.$$

Using the fact that s and $s^*(s)$ satisfy the relation $v(s)=v(s^*(s))$, one can easily find that

$$\left|e^{-sX_S^-}P_S-e^{s^*(s)X_S^+}P_S\right|=2\sqrt{1-\cos^2(\alpha)\sin^2\left(\frac{1}{2}v(s)\right)}.$$

Therefore $\beta(s)=\tilde{\beta}(s)+2\arccos\left(\cos(\alpha)\sin\left(\frac{1}{2}v(s)\right)\right)$. This leads to $\beta(s)-\tilde{\beta}(s)=\theta(s)/2$, and the proposition is proved also in the case n is even. ■

A. Proof of Proposition 6, on the alternating behavior of the optimal synthesis

In this section we need to consider also the dependence on α of the functions $v(s),\theta(s),\beta(s),\mathcal{F}(s),\mathcal{G}(s)$. Therefore we switch to the notation $v(s,\alpha),\theta(s,\alpha),\beta(s,\alpha),\mathcal{F}(s,\alpha),\mathcal{G}(s,\alpha)$.

The claims about the existence of solutions in Proposition 6 come from the fact that $\mathcal{F}(0)=\mathcal{F}(\pi)=\pi/2\alpha$ and the only minimum point of $\mathcal{F}$ occurs at $\bar{s}=\pi-\arccos(\tan^2(\alpha))$. It turns out that the image of $\mathcal{F}$ is a small interval whose length is of order α and therefore equation (22) has a solution only if α is close enough to $\pi/2m$ for some integer number m. This proves **C** with $r_2(m)$ satisfying $r_2(m)=O(1/m)$.

On the other hand, it is possible to estimate the derivative of $\mathcal{G}$ with respect to s, showing that it is negative in the open interval $]0,\pi[$. Therefore, since $\mathcal{G}(0)=\pi/2\alpha+1$ and $\mathcal{G}(\pi)=\pi/2\alpha-1$, Eq. (23) has always two positive solutions.

For the particular values $\alpha=\pi/2m$, where $m>1$ is an integer number, the solutions to Eqs. (22) and (23) give rise to two candidate optimal trajectories: the first one has exactly m bang arcs, all of length π (TYPE-1 and TYPE-2 candidate optimal trajectory at the same time), while the second one has one more switching and is a TYPE-2 candidate optimal trajectory. We want to see that the optimal trajectory is the first one. For this purpose, we need to estimate the time needed to reach the South Pole by the second candidate optimal trajectory, showing that it is greater than $m\pi=\pi^2/2\alpha$.

First, using the Taylor expansions with respect to α and centered at 0 of $\beta(\pi/2,\alpha)$ and $\theta(\pi/2,\alpha)$, one obtains

$$\mathcal{G}\left(\frac{\pi}{2},\alpha\right)=\frac{\pi}{2\alpha}-\alpha\frac{\pi}{4}+o(\alpha). \tag{B3}$$

We want now to estimate the solution $s(\alpha)$ of the equation $\mathcal{G}(s,\alpha)=\pi/2\alpha$. This can be done using (B3) and the following estimate on the derivative of $\mathcal{G}(.)$, with respect to s, near $s=\pi/2$:

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{G}(s,\alpha)=-1+o\left(|\alpha|+\left|\frac{\pi}{2}-s\right|\right).$$

Then it is easy to find that $s(\alpha)=\pi/2-\alpha(\pi/4)+o(\alpha)$, and, consequently, $v(s(\alpha),\alpha)=\pi+2\alpha^2+o(\alpha^2)$. Therefore $2s(\alpha)+(\pi/2\alpha-1)v(s(\alpha),\alpha)=\pi^2/2\alpha+\alpha(\pi/2)+o(\alpha)$. In particular, for $\alpha=\pi/2m$ this expression gives the time needed to reach the South Pole by the candidate optimal trajectory, and, since for m large enough it is larger than $m\pi=\pi^2/2\alpha$, we conclude that this trajectory cannot be optimal. Since the solutions to the equations (22), (23) change continuously with respect to α for each fixed number of switchings n, we easily deduce that, if we slightly decrease α starting from the value $\pi/2m$, the solution of (22) for $n=m$ does not give rise to an optimal trajectory.

For α slightly smaller than $\bar{\alpha} := \pi/2m$ there is a TYPE-2 candidate optimal trajectory corresponding to a solution $(s_1(\alpha), m+1)$ of (23), where $s_1(.)$ is continuous (on $[\bar{\alpha}-\varepsilon, \bar{\alpha}]$) and $s_1(\bar{\alpha}) = 0$, and there is also a TYPE-1 candidate optimal trajectory corresponding to a solution $(s_2(\alpha), m)$ of (22), where $s_2(.)$ is continuous (on $[\bar{\alpha}-\varepsilon, \bar{\alpha}]$) and $s_2(\bar{\alpha})=0$. Clearly for $\alpha=\bar{\alpha}$ these trajectories coincide. So we have to compare the time to reach the South Pole for such trajectories with α close to $\bar{\alpha}$.

We start with the TYPE-1 candidate optimal trajectory. From Eq. (22) we have that $(\mathrm{d}/\mathrm{d}\alpha)\theta(s_2(\alpha), \alpha)=0$. We use a subscript s, α to denote the partial differentiation with respect to such variables. Since $\theta_s(0, \alpha)=0$ we cannot apply directly the implicit function theorem near $(0, \bar{\alpha})$. However, if we set $\tilde{s}_2(\alpha)=s_2^2(\alpha)$ we find that $\tilde{s}_2'(\alpha)=2s_2(\alpha)\theta_\alpha(s_2(\alpha), \alpha))/\theta_s(s_2(\alpha), \alpha))$ (the superscript $'$ denotes differentiation with respect to α), and then, passing to the limit as $(s_2(\alpha), \alpha)$tends to $(0, \bar{\alpha})$, one easily finds that $\tilde{s}_2'(\bar{\alpha})=-2/\sin(\bar{\alpha})^3 \cos(\bar{\alpha})$.

Now we want to determine the way in which the total time $T_2(\alpha)=mv(s_2(\alpha), \alpha)$ changes. It is easy to see that $T_2(\alpha)$ is not differentiable at $\bar{\alpha}$, therefore we introduce the function $F(\alpha) = (T_2(\alpha)-T_2(\bar{\alpha}))^2 = m^2(v(s_2(\alpha), \alpha)-\pi)^2$.

Then $F'(\alpha)=2m^2(\mathrm{d}/\mathrm{d}\alpha)v(s_2(\alpha), \alpha)(v(s_2(\alpha), \alpha)-\pi)=2m^2(v_s(s_2(\alpha), \alpha)s_2'(\alpha)+v_\alpha(s_2(\alpha), \alpha))$ and, after the substitution $s_2'(\alpha)=\tilde{s}_2'(\alpha)/2s_2(\alpha)$ we can pass to the limit as α converges to $\bar{\alpha}$ obtaining

$$F'(\bar{\alpha}) = m^2 v_s^2(0, \bar{\alpha})\tilde{s}_2'(\bar{\alpha}) = -8m^2 \tan \bar{\alpha}.$$

Now we consider the TYPE-2 candidate optimal trajectory and we want to estimate $s_1(\alpha)$. From Eq. (23) we have that $s_1(.)$ is implicitly defined by the equation $\Phi(s_1(\alpha), \alpha) := 2\beta(s_1(\alpha), \alpha)-m\theta(s_1(\alpha), \alpha)=0$. As before, it is easy to see that $s_1(.)$ is not differentiable at $\bar{\alpha}$, and therefore we introduce the parameter $\tilde{s}_1(\alpha)=s_1^2(\alpha)$. As before, it is possible to compute the derivative $\tilde{s}_1'(\alpha)$:

$$\tilde{s}_1'(\bar{\alpha}) = -\lim_{\alpha\to\bar{\alpha}} \frac{2s_1(\alpha)\Phi_\alpha(s_1(\alpha), \alpha)}{\Phi_s(s_1(\alpha), \alpha)} = -\frac{2m}{\sin\bar{\alpha}\cos\bar{\alpha}(1+m\sin^2\bar{\alpha})}.$$

We have now to estimate the total time $T_1(\alpha)=2s_2(\alpha)+mv(s_2(\alpha), \alpha)$ for α close to $\bar{\alpha}$. After defining

$$G(\alpha) = (T_1(\alpha) - T_1(\bar{\alpha}))^2 = (2s_2(\alpha) + m(v(s_2(\alpha), \alpha) - \pi))^2,$$

we can compute the derivative of $G(.)$ as follows:

$$G'(\bar{\alpha}) = \lim_{\alpha\to\bar{\alpha}}\left[2(2s_2(\alpha) + m(v(s_2(\alpha), \alpha) - \pi))\left(\frac{\tilde{s}_2'(\alpha)}{s_2(\alpha)} + m\left(\frac{v_s(s_2(\alpha), \alpha)\tilde{s}_2'(\alpha)}{2s_2(\alpha)} + v_\alpha(s_2(\alpha), \alpha)\right)\right)\right]$$

$$= \lim_{\alpha\to\bar{\alpha}}\left[2\left(2 + m\frac{v(s_2(\alpha), \alpha) - v(0, \alpha)}{s_2(\alpha)}\right)\right]\lim_{\alpha\to\bar{\alpha}}\left[\tilde{s}_2'(\alpha) + m\left(\frac{1}{2}v_s(s_2(\alpha), \alpha)\tilde{s}_2'(\alpha) + v_\alpha(s_2(\alpha), \alpha)s_2(\alpha)\right)\right]$$

$$= (2 + mv_s(0, \bar{\alpha}))^2 s_2'(\bar{\alpha}) = -(2 + 2m\sin^2\bar{\alpha})^2 \frac{2m}{\sin\bar{\alpha}\cos\bar{\alpha}(1+m\sin^2\bar{\alpha})} = -\frac{8m(1+m\sin^2\bar{\alpha})}{\sin\bar{\alpha}\cos\bar{\alpha}}.$$

Since

$$\frac{8m(1+m\sin^2\bar{\alpha})}{\sin\bar{\alpha}\cos\bar{\alpha}} > m\tan\bar{\alpha},$$

we deduce that $G(\alpha)$ decreases faster than $F(\alpha)$ as α goes to $\bar{\alpha}$ and, since $T_1(\alpha)$ and $T_2(\alpha)$ are decreasing for α close to $\bar{\alpha}$, we have that $T_2(\alpha) > T_1(\alpha)$, i.e., the TYPE-1 trajectory is optimal for $\alpha \in [\bar{\alpha}-\varepsilon, \bar{\alpha}]$.

APPENDIX C: THE TIME NEEDED TO REACH EVERY POINT OF THE BLOCH SPHERE STARTING FROM THE NORTH POLE IN THE CASE $\alpha \in [\pi/4, \pi/2[$

In this section we assume $\alpha \in [\pi/4, \pi/2[$. If α is close to $\pi/4$, it is easy to verify that the South Pole is not the last point reached by bang-bang trajectories (the last point reached belongs to the cut locus present in the region $\Omega^{\pm}_{\text{nasty}}$), and the time needed to cover the whole sphere is slightly larger than 2π.

On the other hand, if α is large enough then the velocity along a singular arc is small and therefore the time needed to move along trajectories containing singular arcs is larger than 2π. The following proposition gives the asymptotic behavior of the total time needed to reach every point from the North Pole and determines the last point reached by the optimal synthesis for α large enough.

Proposition 17: Let $T(\alpha)$ the time needed to cover the whole sphere. Then, if α is large enough

$$T(\alpha) = \frac{\pi}{2\cos\alpha} + \pi - \frac{2\arcsin(\cot\alpha)}{\cos\alpha} + 2\arcsin(\cot^2\alpha) = \frac{\pi}{2\cos\alpha} + \pi - 2 + O\left(\frac{\pi}{2} - \alpha\right), \tag{C1}$$

and the last points reached for a fixed value of α are $\pm(\sqrt{1-\cot^2\alpha}, \cot\alpha, 0)^T$.

Proof of Proposition 17: From Proposition 2 the last points reached by optimal trajectories of the form $B_t S_s B_{t'}$ must lie on overlap curves that are subsets of the equator. Therefore it is enough to estimate the maximum time to reach these overlap curves. Assume that the first bang arc corresponds to the control $u=1$ and denote by β the angle corresponding to the arc of the equator between the last point of the singular arc and the point $O^+=(1,0,0)^T$. Notice that $\beta \in]0, \arccos(\cot\alpha)[$. Then it is easy to find the expression $T(\alpha,\beta)$ of the time needed to reach the overlap curve along that optimal trajectory:

$$T(\alpha,\beta) = \pi - \arccos(\cot^2\alpha) + \frac{\arccos(\cot\alpha)}{\cos\alpha} - \frac{\beta}{\cos\alpha} + \arccos\left(\frac{\cos^2\alpha - \tan^2\beta}{\cos^2\alpha + \tan^2\beta}\right).$$

The conclusion follows finding the maximum with respect to β of the previous quantity, which corresponds to the value $\bar{\beta} = \arcsin(\cot\alpha)$. Notice that $\bar{\beta}$ belongs to the interval of definition of β only if $\alpha > \operatorname{arccot}(\sqrt{2}/2)$. ■

Remark 22: Notice that, if $\alpha > \operatorname{arccot}(\sqrt{2}/2)$, then the set of points of the sphere reached within time t, with t in a left neighborhood of $T(\alpha)$, is not simply connected. More precisely there are two symmetric neighborhoods of the points $\pm(\sqrt{1-\cot^2\alpha}, \cot\alpha, 0)^T$ that are not reached in time less than or equal than t.

Remark 23: Recall that for system (6) the time needed to cover the whole sphere for α close enough to $\pi/2$ is obtained dividing by $k = 2E/\cos\alpha$ the expression (C1). Therefore, if we fix E it turns out that this quantity converges to $\pi/4E$ as M goes to infinity.

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Absence of reflection as a function of the coupling constant

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We consider solutions of the one-dimensional equation $-u''+(Q+\lambda V)u=0$ where $Q:\mathbb{R}\to\mathbb{R}$ is locally integrable, $V:\mathbb{R}\to\mathbb{R}$ is integrable with $\mathrm{supp}(V)\subset[0,1]$, and $\lambda\in\mathbb{R}$ is a coupling constant. Given a family of solutions $\{u_\lambda\}_{\lambda\in\mathbb{R}}$ which satisfy $u_\lambda(x)=u_0(x)$ for all $x<0$, we prove that the zeros of $b(\lambda):=W[u_0,u_\lambda]$, the Wronskian of u_0 and u_λ, form a discrete set unless $V\equiv 0$. Setting $Q(x):=-E$, one sees that a particular consequence of this result may be stated as: if the fixed energy scattering experiment $-u''+\lambda Vu=Eu$ gives rise to a reflection coefficient which vanishes on a set of couplings with an accumulation point, then $V\equiv 0$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2206691]

I. INTRODUCTION

The purpose of this paper is to prove a result concerning perturbations of one-dimensional Schrödinger-type equations. Let $Q:\mathbb{R}\to\mathbb{R}$ be locally integrable and let $u_0:\mathbb{R}\to\mathbb{C}$ be a solution of

$$-u_0''(x)+Q(x)u_0(x)=0 \tag{1}$$

that is not identically zero. The perturbation is a second (real-valued) potential, $V\in L^1(\mathbb{R})$ of compact support which, for simplicity, we assume satisfies $\mathrm{supp}(V)\subseteq[0,1]$. Define u_λ as the solution of

$$-u_\lambda''(x)+Q(x)u_\lambda(x)+\lambda V(x)u_\lambda(x)=0 \tag{2}$$

that obeys $u_\lambda(x)=u_0(x)$ for all $x<0$. The parameter λ is known as the coupling constant. In the problems of interest to us, it is real; however, we will allow it to vary over the complex plane as this does not affect our results.

The question we wish to discuss is the following: for how many values of λ is it possible that $u_\lambda(x)$ is a multiple of $u_0(x)$ in the region $x>1$? An equivalent formulation is to study the zeros of the Wronskian between u_0 and u_λ,

$$b(\lambda):=W[u_0,u_\lambda](x)=u_0'(x)u_\lambda(x)-u_0(x)u_\lambda'(x) \tag{3}$$

for any $x>1$.

Theorem 1.1: *The zeros of $b(\lambda)$ form a discrete set unless $V\equiv 0$.*

Furthermore, if b has infinitely many zeros, they must approach infinity rather rapidly.

Theorem 1.2: *If $V\not\equiv 0$, then the number of roots of $b(\lambda)=0$ in the disk $|\lambda|\le r$ (counted by multiplicity) is $O(r^{1/2})$ as $r\to\infty$.*

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When V is sign definite and $Q \equiv 0$, Chadan has shown that the zeros of $b(\lambda)$ determine V precisely in a slightly different scenario; see Ref. 2. A Liouville transformation is used to reduce the problem to the well-known uniqueness problem in the energy parameter.

The proof of Theorems 1 and 2 consist of using some classical analysis to reduce the problem to one treated by Stolz.[13] (We repeat his solution for the convenience of the reader.) As with this paper, Stolz was interested in such matters for their relation to localization for the Anderson model. Before elaborating this point, let us first explain the connection of our results to scattering theory.

Consider the time-independent Schrödinger equation with potential $q(x)$:

$$-\psi''(x) + q(x)\psi(x) = E\psi(x), \tag{4}$$

which describes the wave function of a quantum particle with energy E. For certain choices of q and E, this equation admits a solution, u_0, that corresponds to the particle travelling from right to left (the complex conjugate solution represents left-to-right motion). For example, when $q \equiv 0$ and $E = k^2$ with $k > 0$, we have $\psi(x) = e^{-ikx}$. The Floquet-Bloch waves form another example when q is periodic.

If a perturbation λV is introduced, this may cause the particle to be reflected back with nonzero probability. This situation can be analyzed by looking at the solution u_λ of (2) with $Q(x) = q(x) - E$. For $x > 1$, we may write $u_\lambda(x) = \alpha u_0(x) + \beta \overline{u_0}(x)$ for some complex numbers α and β. In this way, we obtain a formula for the probability of reflection, $|\beta/\alpha|^2$. We also see that there will be no reflection if and only if u_λ and u_0 are linearly dependent on the interval $[0,1]$. That is, there will be no reflection if and only if $b(\lambda) = 0$.

Our interest in this question stems from its relevance to the one-dimensional Anderson model. Consider solutions of (2) in the situation where the coupling constant λ is a random variable. As was first observed in the context of the random dimer model,[6,7] it is possible for the localization length to diverge (i.e., Lyapunov exponent vanish) at a fixed energy. In particular, this happens at positive energies when the reflection coefficient associated to the single site potential vanishes almost surely for a particular choice of random coupling constant. The presence of these exceptional energies leads to interesting transport phenomena (see Refs. 3 and 8 and references therein), while away from them one may prove exponential and dynamical localization (see Refs. 4 and 5). A consequence of Theorem 1.1 is that these divergences cannot occur unless the distribution of the couplings is purely discrete.

We assumed from the very beginning that V was an L^1 function. The theorems above are false if V is permitted to be a measure as the following example shows: see Ref. 5 for an analogous example in the discrete setting.

Example 1.3: Consider $Q(x) = -k^2$ and $u_0(x) = e^{ikx}$. For $V(x) = \delta(x) - \delta(x-1)$, a simple calculation reveals

$$b(\lambda) = \lambda\left(1 + \tfrac{\lambda}{2ik}\right)(e^{2ik} - 1). \tag{5}$$

Thus we see that $b \equiv 0$ whenever $k = n\pi$, $n \in \mathbb{Z}$. (The case $k = 0$ follows by a limiting argument.) The same is true for any other choice of u_0. This is particularly evident when $u_0 = \sin(n\pi x)$ for in this case, $u_\lambda(x) = \sin(n\pi x)$, which vanishes on the support of V.

One may ask for analogues of the theorems given above when V is not of compact support. In this case, one would define $u_\lambda(x)$ by the constraint $u_\lambda(x) - u_0(x) \to 0$ as $x \to -\infty$ and define $b(\lambda)$ as the limit of $W[u_0, u_\lambda](x)$ as $x \to +\infty$. Naturally, one would need to ensure that V decays fast enough so that these limits exist; moreover the choice of decay rate cannot be made without knowledge of the behavior of Q at infinity. We haven chosen not to pursue this matter.

II. PROOFS

Let us choose a solution v_0 of (1), linearly independent of u_0, normalized by the requirement $W[u_0,v_0]\equiv 1$. As $u_\lambda(x)$ is also a solution of (1) in the region $x>1$, we may write

$$u_\lambda(x) = a(\lambda)u_0(x) + b(\lambda)v_0(x) \quad \text{for all } x > 1;$$

moreover, by computing Wronskians, we see that $b(\lambda)$ is the same function defined in (3).

First we show that $a(\lambda)$ and $b(\lambda)$ are analytic functions of order one-half. This allows us to deduce Theorem 1.2 from Theorem 1.1. Moreover, it shows that if the zeros of b are not discrete, then b must vanish identically. These two applications require us only to treat b; however when u_0 is complex valued, we will need to invoke properties of a when we prove Theorem 1.1.

Proposition 2.1: The functions $a(\lambda)$ and $b(\lambda)$ are entire and obey

$$|a(\lambda)| \le C\exp\{c|\lambda|^{1/2}\}, \quad |b(\lambda)| \le C\exp\{c|\lambda|^{1/2}\} \tag{6}$$

for some positive constants c and C, which depend on u_0 and $\|V\|_{L^1}$.

Proof: As in the preceding paragraphs, let v_0 be a solution of (1) which satisfies $W[u_0,v_0]\equiv 1$. We define

$$K(x,t) = [u_0(x)v_0(t) - v_0(x)u_0(t)]V(t)$$

so $u_\lambda(x)$ can be constructed as the solution of the Volterra integral equation

$$u_\lambda(x) = u_0(x) + \lambda\int_0^x K(x,t)u_\lambda(t)\mathrm{d}t \tag{7}$$

acting on $C^0([0,\infty))$. While this equation arises naturally from variation of parameters, it is quicker to check it by differentiating both sides twice. The key observations are

$$K(x,x) = 0, \quad \frac{\partial K}{\partial x}(x,x) = V(x), \quad \text{and } \frac{\partial^2 K}{\partial x^2}(x,t) = Q(x)K(x,t).$$

One can solve (7) by repeated substitution, which gives rise to an infinite series for u_λ,

$$u_\lambda(x) = u_0(x) + \sum_{n=1}^{\infty}\lambda^n\int\cdots\int K(x,t_1)\cdots K(t_{n-1},t_n)u_0(t_n)\mathrm{d}t_1\cdots\mathrm{d}t_n, \tag{8}$$

where integration takes place over the region $0<t_n<\cdots<t_1<x$. Convergence of this series is a well-known property of Volterra operators (cf. Ref. 14, Sec. 36) and can be deduced from the estimates below.

From (8) we obtain power series for a and b,

$$a(\lambda) = 1 + \sum_{n=1}^{\infty}\lambda^n\int\cdots\int_{\Delta_n} v_0(t_1)V(t_1)K(t_1,t_2)\cdots K(t_{n-1},t_n)u_0(t_n)\mathrm{d}t_1\cdots\mathrm{d}t_n,$$

$$b(\lambda) = -\sum_{n=1}^{\infty}\lambda^n\int\cdots\int_{\Delta_n} u_0(t_1)V(t_1)K(t_1,t_2)\cdots K(t_{n-1},t_n)u_0(t_n)\mathrm{d}t_1\cdots\mathrm{d}t_n,$$

where Δ_n is the simplex $0<t_n<\cdots<t_1<1$. Our bound on the size of these functions will follow by estimating the individual terms in these series. We only give details for $b(\lambda)$ because the argument for $a(\lambda)$ is almost identical.

As u_0 and v_0 are C^1, one may choose a constant M so that

$$|u_0(t)| \le M \quad \text{and } |K(s,t)| \le M|s-t||V(t)| \quad \forall\, t,s \in [0,1].$$

Second, by the arithmetic/geometric mean inequality,

$$\prod_{j=1}^{n-1} |t_j - t_{j+1}| \le (n-1)^{-(n-1)}.$$

Combining these two observations, we can deduce

$$\begin{aligned} |b(\lambda)| &\le \sum_{n=1}^{\infty} \frac{|\lambda|^n M^{n+1}}{(n-1)^{n-1}} \int \cdots \int_{\Delta_n} |V(t_1)| \cdots |V(t_n)| \mathrm{d}t_1 \cdots \mathrm{d}t_n \\ &\le \sum_{n=1}^{\infty} \frac{|\lambda|^n M^{n+1}}{n\,!\,(n-1)^{n-1}} \|V\|_{L^1}^n. \end{aligned}$$

The resulting bound on $|b(\lambda)|$ can now be deduced either through the properties of the Bessel function

$$\sum_{n=0}^{\infty} \frac{r^{2n}}{(n\,!\,)^2} = I_0(2r) = \frac{1}{\pi} \int_0^{\pi} e^{2r\cos\theta}\, \mathrm{d}\theta \le e^{2|r|},$$

or by brute force. □

The one-half power appearing in (6) is the smallest possible; see Example 2.3 below.

In the proof of Theorem 1.1 will specifically consider only $\lambda \in \mathbb{R}$ in order to be able to use some facts about self-adjoint operators. When u_0 is real-valued, Theorem 1.1 follows by the argument presented in Lemma 3 of Ref. 13. Of course the problem is unchanged if u_0 is a complex multiple of a real solution. However, when $\operatorname{Re} u_0$ and $\operatorname{Im} u_0$ are linearly independent solutions, one needs to make some modifications. The approach we take is to show that one may replace u_0 by $\operatorname{Re} u_0$.

Proposition 2.2: Suppose $\operatorname{Re} u_0$ *and* $\operatorname{Im} u_0$ *are linearly independent and* $b(\lambda) \equiv 0$. *Then* $W[\operatorname{Re} u_0, \operatorname{Re} u_\lambda](x) = 0$ *for all* $x > 1$ *and all* $\lambda \in \mathbb{R}$.

Proof: By assumption, $u_\lambda(x) = a(\lambda) u_0(x)$ for all $x > 1$. For $\lambda \in \mathbb{R}$, both u_λ and $\overline{u_\lambda}$ are solutions of (2). Therefore,

$$W[u_0, \overline{u_0}] = W[u_\lambda, \overline{u_\lambda}] = |a(\lambda)|^2 W[u_0, \overline{u_0}],$$

which is nonzero because we assumed linear independence. Thus it follows that $a(\lambda)$ is unimodular for $\lambda \in \mathbb{R}$.

By the Schwarz reflection principle, the complex conjugate of any zero of a must be a pole; however, a is an entire function so we may conclude that it is zero-free. This means that $\log[a(\lambda)]$ is an entire function, but then by the estimate in Proposition 2.1, it must be constant. By taking $\lambda = 0$, we learn that $a(\lambda) \equiv 1$.

We have just seen that for all λ (real or complex) and all $x > 1$, $u_\lambda(x) = u_0(x)$. By taking real parts, we immediately obtain the conclusion sought. □

Proof of Theorem 1.1: In light of Proposition 2.2 we may assume that u_0 is real-valued. We now essentially repeat the argument from Lemma 3 of Ref. 13. Let us choose θ_0 and θ_1 so that

$$\cos(\theta_0) u_0(0) + \sin(\theta_0) u_0'(0) = 0 = \cos(\theta_1) u_0(1) + \sin(\theta_1) u_0'(1)$$

and consider the self-adjoint operators $H_\lambda u = -u'' + Qu + \lambda V u$ on $[0,1]$ with the boundary conditions

$$\cos(\theta_x) u(x) + \sin(\theta_x) u'(x) = 0 \quad \text{for } x \in \{0,1\}.$$

Suppose $V \neq 0$ and the set of λ for which $b(\lambda)=0$ has an accumulation point. In this case, $b(\lambda) \equiv 0$, and in particular, 0 is an eigenvalue of H_λ for every $\lambda \in \mathbb{R}$. As the spectrum of H_λ is simple, discrete, and bounded from below, this implies that the number of negative eigenvalues of H_λ is finite and independent of λ. We will derive a contradiction by using a very weak form of Weyl's law. (When Q and V obey some mild regularity hypotheses, full Weyl-law asymptotics are known, cf. Ref. 10 Theorem XIII.79.)

As $V \neq 0$, it must happen that either V is positive on a set of positive measure, or V is negative on a set of positive measure. We will treat the former case, the latter follows with obvious modifications.

For each $\epsilon > 0$, let us define

$$\phi_\epsilon(x) = \begin{cases} \sqrt{\frac{3}{2}}\epsilon^{-3/2}(\epsilon - |x|) & |x| < \epsilon, \\ 0 & |x| \geq \epsilon. \end{cases}$$

By the Lebesgue differentiation theorem, $\int \phi(x-t)^2 V(t) \mathrm{d}t \to V(x)$ as $\epsilon \downarrow 0$ for a.e. $x \in \mathbb{R}$. Therefore, given any integer $N > 0$, one can find N distinct points $x_1, \ldots, x_N \in (0,1)$ and ϵ sufficiently small, so that $\phi_\epsilon(x-x_j)$ are supported in disjoint subsets of $(0,1)$ and obey $\int V(x)\phi_\epsilon(x-x_j)\mathrm{d}x > \epsilon$. Thus, by the minimax principle (cf. Ref. 10, Sec. XIII.1) one can see that H_λ has at least N negative eigenvalues when λ is a sufficiently large negative number. □

An alternate approach to proving that $a(\lambda) \equiv 1$ implies $V \equiv 0$, is through recent work on the large-λ asymptotics of the spectral shift function $\arg[a(\lambda)]$; see Refs. 9 and 11, for example. The authors thank Pushnitski for explaining some of this material to us.

Proof of Theorem 1.2: The conclusion of this theorem holds for any nonzero entire function of order one-half and finite type; see Ref. 1, Theorem 2.5.13 or Ref. 12, Theorem 5.2.1. □

Theorem 1.2 is optimal with regard to the power of r. This is to be expected from Weyl's law and can be seen with an elementary example.

Example 2.3: Consider $Q \equiv -\pi^2$, $u_0(x) = \sin(\pi x)$, and $V = -\chi_{[0,1]}$. In this case,

$$b(\lambda) = -\cos(\sqrt{\lambda + \pi^2}).$$

As cosine is an even function, both branches of the square root lead to the same answer.

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Complex periodic potentials with a finite number of band gaps

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We obtain several new results for the complex generalized associated Lamé potential $V(x)=a(a+1)m\,\mathrm{sn}^2(y,m)+b(b+1)m\,\mathrm{sn}^2(y+K(m),m)+f(f+1)m\,\mathrm{sn}^2(y+K(m)+iK'(m),m)+g(g+1)m\,\mathrm{sn}^2(y+iK'(m),m)$, where $y\equiv x-K(m)/2-iK'(m)/2$, $\mathrm{sn}(y,m)$ is the Jacobi elliptic function with modulus parameter m, and there are four real parameters a,b,f,g. First, we derive two new duality relations which, when coupled with a previously obtained duality relation, permit us to relate the band edge eigenstates of the 24 potentials obtained by permutations of the parameters a,b,f,g. Second, we pose and answer the question: how many independent potentials are there with a finite number "a" of band gaps when a,b,f,g are integers and $a\geqslant b\geqslant f\geqslant g\geqslant 0$? For these potentials, we clarify the nature of the band edge eigenfunctions. We also obtain several analytic results when at least one of the four parameters is a half-integer. As a by-product, we also obtain new solutions of Heun's differential equation. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In a recent paper,[1] hereafter referred to as paper I, we discussed the generalized associated Lamé (GAL) potential given by

$$\begin{aligned}\hat{V}(x) &= a(a+1)m\,\mathrm{sn}^2(x,m)+b(b+1)m\,\mathrm{sn}^2(x+K(m),m)\\ &\quad+f(f+1)m\,\mathrm{sn}^2(x+K(m)+iK'(m),m)+g(g+1)m\,\mathrm{sn}^2(x+iK'(m),m)\\ &= a(a+1)m\,\mathrm{sn}^2(x,m)+b(b+1)m\frac{\mathrm{cn}^2(x,m)}{\mathrm{dn}^2(x,m)}+f(f+1)\frac{\mathrm{dn}^2(x,m)}{\mathrm{cn}^2(x,m)}+g(g+1)\frac{1}{\mathrm{sn}^2(x,m)},\end{aligned} \tag{1}$$

which involves four real parameters a,b,f,g. Here, sn (x,m), cn (x,m), dn (x,m) are Jacobi elliptic functions with elliptic modulus parameter $m(0\leqslant m\leqslant 1)$. They are doubly periodic functions with periods $[4K(m),i2K'(m)]$, $[4K(m),2K(m)+i2K'(m)]$, $[2K(m),i4K'(m)]$ respectively,[2] where $K(m)\equiv\int_0^{\pi/2}d\theta[1-m\sin^2\theta]^{-1/2}$ denotes the complete elliptic integral of the first kind, and $K'(m)\equiv K(1-m)$. From now on, unless essential, we will not explicitly display the modulus parameter m as an argument of Jacobi elliptic functions. It may be noted here that the four terms in the GAL potential (1) correspond to complex translations of the independent variable x by 0, $K(m),K(m)+iK'(m),iK'(m)$. Although the GAL potential is real, it does have singularities on the real axis coming from the zeros of the Jacobi elliptic functions sn (x) and cn (x) in the last two terms. One way to avoid these singularities is to make a complex change of variables $y=ix+\beta$,

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with β being an arbitrary real, nonzero constant, chosen so as to avoid the singularities arising from the zeros of Jacobi elliptic functions on the real axis.[3] This procedure was used in paper I, and we studied many of the properties of the resulting PT-invariant complex periodic potential.[4] However, consistent with the practice in the mathematics literature, in this paper we use an alternative approach of avoiding singularities by simply translating the independent variable x by an arbitrary nonzero amount in the complex plane. In fact, for simplicity, from symmetry considerations, we take the translated variable to be $x-K(m)/2-iK'(m)/2$. Note that the potential still is a PT-invariant complex periodic potential. One very important consequence of this choice is that the energy eigenvalues which we shall obtain here will be opposite in sign from the values obtained in paper I. This point should be kept in mind while comparing the results from the two papers. Thus explicitly, we consider the potential

$$\begin{aligned} V(x) &= \hat{V}(y) \\ &= a(a+1)m\,\mathrm{sn}^2(y,m) + b(b+1)m\,\mathrm{sn}^2(y+K(m),m) + f(f+1)m\,\mathrm{sn}^2(y+K(m)+iK'(m),m) \\ &\quad + g(g+1)m\,\mathrm{sn}^2(y+iK'(m),m) \\ &= a(a+1)m\,\mathrm{sn}^2(y,m) + b(b+1)m\frac{\mathrm{cn}^2(y,m)}{\mathrm{dn}^2(y,m)} + f(f+1)\frac{\mathrm{dn}^2(y,m)}{\mathrm{cn}^2(y,m)} \\ &\quad + g(g+1)\frac{1}{\mathrm{sn}^2(y,m)} \equiv [a,b,f,g], \end{aligned} \tag{2}$$

where

$$y = x - \frac{K(m)}{2} - \frac{iK'(m)}{2}. \tag{3}$$

It may be noted here that in paper I we used the notation $[a(a+1),b(b+1),f(f+1),g(g+1)]$ to denote this potential. However, for consistency with the prevailing practice in the mathematics literature, in this paper we use the notation $[a,b,f,g]$. In this notation, ordinary Lamé potentials are denoted by $[a, 0, 0, 0]$, and associated Lamé (AL) potentials are denoted by $[a,b, 0, 0]$. Note that the potential (2) remains unchanged when any one or more of the parameters a,b,f,g change to $-a-1,-b-1,-f-1,-g-1$ respectively.

There is one important observation which permits us to construct many supersymmetric partner potentials corresponding to a given potential.[5] Although this point was previously made in paper I, it is worth restating here. Normally, in supersymmetric quantum mechanics,[6] given a potential $V_-(x)$, the ground state wave function $\psi_0(x)$ is used to construct the superpotential $W(x)=-\psi_0'(x)/\psi_0(x)$, which then yields the supersymmetric (SUSY) partner potential $V_+(x)=W^2+W'$. If one uses any excited state wave function $\psi(x)$ of $V_-(x)$ to construct a superpotential $W(x)$, then the original potential $V_-(x)$ is recovered correctly (by construction), but the corresponding partner potential $V_+(x)$ turns out to be singular on the real x axis due to the zeros of the excited state wave function $\psi(x)$. However, for the complex potential (2), the singularities are not on the real axis.[7] Thus in this case one could also use any of the excited state wave functions to obtain the superpotential $W(x)$ and hence discover several supersymmetric partner potentials with the same energy spectrum.

In paper I we showed that several GAL potentials with specific integer values of a,b,f,g have a finite number of band gaps. Further, looking at the symmetry of these potentials, we conjectured that all GAL potentials with integer values of a,b,f,g also have a finite number of band gaps. Some results of this type are available in the mathematics literature, and it is worthwhile to present a brief review of what is already known about the GAL potential.

The GAL potential (2), expressed in terms of Weierstrass functions, was discussed in a brief note by Darboux in 1882,[8] as well as in two subsequent articles in 1914 and 1915. He mentioned that some results had already been presented by Hermite in 1872 in unpublished lectures at Ecole Polytechnique. In 1883, Sparre[9] wrote two long papers on the GAL potential expressed in terms of

Jacobi elliptic functions. Unfortunately, the mathematics community was largely unaware of these papers, and the GAL potential was "rediscovered" by Treibich and Verdier in 1990.[10] Nowadays, the GAL potential, expressed in terms of Weierstrass functions, is known as the Treibich-Verdier potential. Several investigators have shown that when a,b,f,g are integers, these potentials have a finite number of band gaps. In particular, the number of band gaps p is given by[11]

$$p = \tfrac{1}{2}\max\Big[2\max[a,b,f,g], 1+N-\{1+(-1)^N\}\Big\{\min[a,b,f,g]+\tfrac{1}{2}\Big\}\Big], \tag{4}$$

where $N=a+b+f+g$. It was also shown that finite band gap potentials are solutions of higher order KdV equations.[12] In recent times, several people have also discussed the connection between Heun's equation and the Treibich-Verdier potential.[13] Finally, some authors have studied other general potentials (different from GAL potentials) which have a finite number of band gaps.[14]

In paper I using supersymmetry we showed that the band edge eigenvalues of the Lamé and the AL potentials [2, 0, 0, 0], [3, 0, 0, 0], $[a,(a-3),0,0]$ are the same as those of the GAL potentials [1, 1, 1, 0], [2, 1, 1, 1], $[a,a-1,1,0]$, respectively. We had also conjectured in paper I that for integer a,b, Lamé and AL potentials have the same band edge eigenvalues as some GAL potentials—the explicit relationship being

$$\begin{aligned}
[a,0,0,0] &\equiv \left[\frac{a}{2},\frac{a}{2},\frac{a}{2},\frac{a-2}{2}\right], \quad a=\text{even integer},\\
[a,0,0,0] &\equiv \left[\frac{a+1}{2},\frac{a-1}{2},\frac{a-1}{2},\frac{a-1}{2}\right], \quad a=\text{odd integer},\\
[a,b,0,0] &\equiv \left[\frac{a+b}{2},\frac{a+b}{2},\frac{a-b}{2},\frac{a-b-2}{2}\right], \quad a+b=\text{even integer},\\
[a,b,0,0] &\equiv \left[\frac{a+b+1}{2},\frac{a+b-1}{2},\frac{a-b-1}{2},\frac{a-b-1}{2}\right], \quad a+b=\text{odd integer}.
\end{aligned} \tag{5}$$

Note that we are using the notation "≡" to denote "same band edge eigenvalues," but not identical potentials. It is interesting to note that recently, Takemura[15] has verified the conjectures expressed in (5). Further, more generally, he has proved that the GAL potential $[a,b,f,g]$ for integer a,b,f,g has the same band edge eigenvalues as another GAL potential, with the explicit relationship depending on whether $N\equiv a+b+f+g$ is an even or an odd integer. If N is an even integer, the relationship is

$$[a,b,f,g] \equiv \left[\frac{a+b+f-g}{2},\frac{a+b+g-f}{2},\frac{a+f+g-b}{2},\frac{b+f+g-a}{2}\right], \tag{6}$$

while if N is an odd integer, then the relationship is

$$[a,b,f,g] \equiv \left[\frac{a+b+f+g+1}{2},\frac{a+b-f-g-1}{2},\frac{a+f-b-g-1}{2},\frac{a+g-b-f-1}{2}\right]. \tag{7}$$

He has also shown that if a,b,f,g are all half-integers and their sum is an even integer, then the band edge energy eigenvalues of the potential $[a,b,f,g]$ are the same as two other GAL potentials where also all four parameters are half-integers with their sum being an even integer. In particular, the explicit relationships are

$$\left[a=k+\frac{1}{2},b=l+\frac{1}{2},f=n+\frac{1}{2},g=p+\frac{1}{2}\right]$$
$$\equiv\left[\frac{k+l+n+p+3}{2},\frac{k+l-n-p-1}{2},\frac{k+n-l-p-1}{2},\frac{k+p-n-l-1}{2}\right]$$
$$\equiv\left[\frac{k+l+n-p+1}{2},\frac{k+l+p-n+1}{2},\frac{k+n+p-l+1}{2},\frac{l+n+p-k+1}{2}\right]. \quad (8)$$

The above-mentioned results, when combined with our work in paper I, raise several questions. For example, while it is clear from relation (4) that all 24 potentials obtained by permutation of the four parameters a,b,f,g have the same number of band gaps, what is the precise relationship between the band edge eigenstates of these 24 potentials? Second, a very interesting question is to ask how many independent GAL potentials there are with say a band gaps. Third, is it possible to further generalize the results of Takemura?[15] Besides, what is the nature of the band edge eigenfunctions for a general GAL potential in case a,b,f,g are all integers? Finally, in view of the connection between the GAL potentials and Heun's equation,[9,13] it is worth inquiring about the implications of these results in the context of solutions to Heun's equation.

In this paper, we address all the above-raised issues. Further, we also consider GAL potentials in which at least one of the four parameters is a half-integer while the other parameters are arbitrary numbers and show that both relations (6) and (7) are valid in all these cases. As a consequence, we conjecture that relations (6) and (7) are in fact simultaneously valid even when all four parameters a,b,f,g are integers with their band edge eigenvalues being the same as the quasi-exactly solvable (QES) eigenvalues of potentials where all four parameters are half-integers (with their sum being an odd integer). Further, knowing the QES eigenvalues of the GAL potentials $[a,1/2,f,g]$, $[a,b,1/2,g]$, $[a,b,f,1/2]$ (where a,b,f,g are arbitrary numbers), and using the connection between the Schrödinger equation for the GAL potentials and Heun's equation, we show that the corresponding eigenfunctions can be obtained by directly solving the algebraic form of Heun's equation.

The plan of this paper is as follows. In Sec. II, we derive new duality relations and examine some consequences. In particular, using these duality relations we obtain the precise connection between the energy eigenvalues and eigenfunctions of the 24 potentials obtained by permuting the four parameters a,b,f,g. In Sec. III, we discuss the GAL potential (2) in some detail when the four parameters a,b,f,g are all integers. First, we find various GAL potentials which are related to each other in the sense that they have identical band edge energy eigenvalues. We also find a large number of self-isospectral potentials as well as self-dual but non-self-isospectral potentials. Using all these results, we obtain the number of independent potentials with say a band gaps. We also clarify the nature of the band edge eigenfunctions for these potentials. In Sec. IV we discuss the GAL potential when either one or more of the four parameters take half-integer values while the remaining parameters are arbitrary. In this case, in general one expects to obtain QES mid-band states, by which we mean any energy state lying inside an energy band and thus not a band edge. Quite remarkably, by generalizing Takemura's results[15] we obtain GAL potentials which have the same band edge eigenvalues as the mid-band energy values of the potentials with one or more of the parameters being half-integers. In Sec. V we discuss the GAL potential in case the parameters a,b,f,g take arbitrary values and obtain the corresponding GAL potentials with the same band edge and mid-band energy values when $a+b+f+g$ [or any other combination obtained by replacing one or more of these parameters by $-a-1,-b-1,-f-1,-g-1$, respectively] is an even integer. In Sec. VI we discuss the implications of all these results in the context of Heun's equation. In particular, we show that in view of the connection between the different GAL potentials, given a periodic solution of Heun's equation, one immediately obtains four periodic and three quasi-periodic solutions of the same equation. We also show that in many cases, knowing the QES energy values of a GAL potential, it is much easier to solve the algebraic form of Heun's equation and obtain the corresponding eigenfunctions of the GAL potential. Finally, in Sec. VII we summarize the results obtained in this paper and spell out some open problems.

II. DUALITY RELATIONS FOR GAL POTENTIALS

In this paper our main focus is on the Schrödinger equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x)+\hat{V}(x)\psi(x)=E\psi(x), \tag{9}$$

where $\hat{V}(x)$ is the GAL potential given by Eq. (1), and we have chosen units with $\hbar=2m=1$. Displaying parameters more explicitly, Eq. (9) states that the potential $\hat{V}(a,b,f,g,m;x)$ has band edge eigenvalues $E(a,b,f,g,m)$ and eigenfunctions $\psi(a,b,f,g,m;x)$. Of course, this means that the translated potential $V(x)\equiv V(a,b,f,g,m;x)=\hat{V}(a,b,f,g,m;x-K(m)/2-iK'(m)/2)$ given in Eq. (2) has the same eigenvalues $E(a,b,f,g,m)$ and eigenfunctions $\psi(a,b,f,g,m;x-K(m)/2-iK'(m)/2)$.

First we want to show that the band edge eigenstates of the 24 potentials [obtained via permutations of the 4 parameters, a,b,f,g in $V(x)$] are all related, so that once the band edge eigenstates of any one permutation are known, the complete band edge eigenstates of all 24 potentials are also known. Actually, these relations are valid for both band edges as well as mid-band states.

The first relation is simple—in view of the invariance of the Schrödinger Eq. (9) under the translation $x\to x+K(m)$ followed by the interchanges $a\leftrightarrow b$ and $f\leftrightarrow g$, one gets[1]

$$E(b,a,g,f,m)=E(a,b,f,g,m),\quad \psi(b,a,g,f,m;x)\propto\psi(a,b,f,g,m;x+K(m)). \tag{10}$$

Similarly, the translations $x\to x+iK'(m)$ and $x\to x+K(m)+iK'(m)$ followed by suitable interchanges of parameters yield

$$E(g,f,b,a,m)=E(a,b,f,g,m),\quad \psi(g,f,b,a,m;x)\propto\psi(a,b,f,g,m;x+iK'(m)), \tag{11}$$

$$E(f,g,a,b,m)=E(a,b,f,g,m),\quad \psi(f,g,a,b,m;x)\propto\psi(a,b,f,g,m;x+K(m)+iK'(m)). \tag{12}$$

Thus, once we obtain the eigenvalues and eigenfunctions of a given potential $[a,b,f,g]$, then we immediately know the eigenvalues and eigenfunctions of three other potentials: $[b,a,g,f]$, $[g,f,b,a]$, and $[f,g,a,b]$. Note that relations (10)–(12) all involve the same modulus parameter m.

We now derive three remarkable duality relations, which connect the energy states of different GAL potentials, and involve changes in the modulus parameter from m to $1-m$, $1/m$ and $-m/(1-m)$.

Duality Relation I: This was already derived in paper I and is given by

$$\begin{gathered}E(a,b,f,g,m)=[a(a+1)+b(b+1)+f(f+1)+g(g+1)]-E(a,g,f,b,1-m),\\ \psi(a,b,f,g,m;x)\propto\psi(a,g,f,b,1-m;x+K'(m)+iK(m)).\end{gathered} \tag{13}$$

Duality Relation II: Using the formulas[2]

$$\mathrm{sn}(x,m)=\frac{1}{k}\mathrm{sn}\left(kx,\frac{1}{m}\right),\quad \mathrm{cn}(x,m)=\mathrm{dn}\left(kx,\frac{1}{m}\right),\quad \mathrm{dn}(x,m)=\mathrm{cn}\left(kx,\frac{1}{m}\right),\quad k^2\equiv m, \tag{14}$$

and redefining a new variable $z=kx$, the Schrödinger equation (9) takes the form

$$-\frac{\mathrm{d}^2}{\mathrm{d}z^2}\psi(z)+\left[\frac{a(a+1)}{m}\mathrm{sn}^2\left(z,\frac{1}{m}\right)+\frac{f(f+1)}{m}\frac{\mathrm{cn}^2\left(z,\frac{1}{m}\right)}{\mathrm{dn}^2\left(z,\frac{1}{m}\right)}+b(b+1)\frac{\mathrm{dn}^2\left(z,\frac{1}{m}\right)}{\mathrm{cn}^2\left(z,\frac{1}{m}\right)}+g(g+1)\frac{1}{\mathrm{sn}^2\left(z,\frac{1}{m}\right)}\right]\psi(z)=\frac{E(m)}{m}\psi(z). \tag{15}$$

On comparing Eqs. (9) and (15) we then have the duality relation

$$E(a,b,f,g,m)=mE\left(a,f,b,g,\frac{1}{m}\right),\quad \psi(a,b,f,g,m;x)\propto\psi\left(a,f,b,g,\frac{1}{m};kx\right). \tag{16}$$

Duality Relation III: We again start from the Schrödinger equation (9) and now use the formulas[2]

$$\mathrm{sn}(x,m)=\frac{\mathrm{sn}[\sqrt{1-m}x,-m/(1-m)]}{\sqrt{1-m}\,\mathrm{dn}[\sqrt{1-m}x,-m/(1-m)]},$$

$$\mathrm{cn}(x,m)=\frac{\mathrm{cn}[\sqrt{1-m}x,-m/(1-m)]}{\mathrm{dn}[\sqrt{1-m}x,-m/(1-m)]}, \tag{17}$$

$$\mathrm{dn}(x,m)=\frac{1}{\mathrm{dn}[\sqrt{1-m}x,-m/(1-m)]}.$$

On defining a new variable $z=\sqrt{1-m}x$, the Schrödinger equation (9) takes the form

$$-\frac{d^2}{dz^2}\psi(z)+\left[-\frac{mb(b+1)}{1-m}\mathrm{sn}^2\left(z,\frac{-m}{1-m}\right)-\frac{ma(a+1)}{1-m}\frac{\mathrm{cn}^2\left(z,\frac{-m}{1-m}\right)}{\mathrm{dn}^2\left(z,\frac{-m}{1-m}\right)}+f(f+1)\frac{\mathrm{dn}^2\left(z,\frac{-m}{1-m}\right)}{\mathrm{cn}^2\left(z,\frac{-m}{1-m}\right)}+g(g+1)\frac{1}{\mathrm{sn}^2\left(z,\frac{-m}{1-m}\right)}\right]\psi(z)$$

$$=\frac{1}{1-m}E\psi(z)-\frac{m}{1-m}[a(a+1)+b(b+1)+f(f+1)+g(g+1)]\psi(z). \tag{18}$$

On comparing Eqs. (9) and (18) one gets the duality relation

$$E(a,b,f,g,m)=(1-m)E\left(b,a,f,g,\frac{-m}{1-m}\right)+m[a(a+1)+b(b+1)+f(f+1)+g(g+1)],$$

$$\psi(a,b,f,g,m;x)\propto\psi\left(b,a,f,g,\frac{-m}{1-m};\sqrt{1-m}x\right). \tag{19}$$

Using the three duality relations [Eqs. (13), (16), and (19)] along with the translation results [Eqs. (10)–(12)], it is easily shown that once the eigenstates of a given potential are known, we

can immediately obtain the energy eigenstates of all 24 potentials obtained by permuting the 4 parameters a,b,f,g. Hence, out of these 24 potentials, there is only one independent potential and without loss of any generality, throughout this paper we only consider the potential $[a,b,f,g]$ with $a \geqslant b \geqslant f \geqslant g$ (unless stated otherwise).

The duality relations are very powerful and have many interesting consequences. For example, we find that for arbitrary integer values of a,f, the potential $[a,0,f,0]$ has only a finite number of band gaps. This follows because Eq. (16) gives

$$E(a,0,f,0,m) = mE\left(a,f,0,0,\frac{1}{m}\right), \tag{20}$$

so that both the potentials $[a,f,0,0]$ and $[a,0,f,0]$ must have the same number of band edges. Since one knows[16] that the AL potential $[a,f,0,0]$ has a finite number of band gaps, the same statement holds for the potential $[a,0,f,0]$.

III. INDEPENDENT GAL POTENTIALS WITH *a* BAND GAPS [*a*,*b*,*f*,*g*=integers]

In this section, we want to answer the following interesting question: given a potential of the form $[a,b,f,g]$ with $a \geqslant b \geqslant f \geqslant g \geqslant 0$, how many independent GAL potentials are there with exactly a band gaps?

To begin, for a given integer a, let us calculate the total number of possible GAL potentials with $a \geqslant b \geqslant f \geqslant g \geqslant 0$. The number of such potentials is

$$\sum_{b=0}^{a}\sum_{f=0}^{b}\sum_{g=0}^{f} 1 = (a+1)(a+2)(a+3)/6. \tag{21}$$

Now due to the Landen transformations,[2,17] potentials of the form $[a,a,b,b]$ with $a \neq b$ are essentially the same as the potentials $[a,b,0,0]$ and hence are not really distinct. There are a such potentials (for any given value of a). Similarly, it is easy to show that the potential $[a,a,a,a]$ is related to the potential $[a,0,0,0]$ and hence not distinct. In particular, on using the relations[2]

$$\mathrm{sn}^2(x,m) = \frac{1-\mathrm{cn}(2x,m)}{1+\mathrm{dn}(2x,m)}, \quad m\,\mathrm{sn}^2(x+iK'(m),m) = \frac{1}{\mathrm{sn}^2(x,m)}, \tag{22}$$

one obtains

$$\mathrm{sn}^2(x,m) + \mathrm{sn}^2(x+K(m),m) + \mathrm{sn}^2(x+iK'(m),m) + \mathrm{sn}^2(x+K(m)+iK'(m),m) = 4\mathrm{sn}^2(2x+iK'(m),m). \tag{23}$$

Thus the number of distinct GAL potentials of the form $[a,b,f,g]$ with $a \geqslant b \geqslant f \geqslant g \geqslant 0$ is given by

$$N_{\mathrm{dist}} = a(a+1)(a+5)/6. \tag{24}$$

In view of formula (4) for the number of band gaps, it is obvious that these distinct potentials are of two types—there are those with exactly a band gaps and those with more than a band gaps. Using Eqs. (6) and (4) and (4) it follows that in case $a+b+f+g$ is an even integer and if $a+g \geqslant b+f$ then the potential has a band gaps while if $a+g<b+f$ then it has $(a+b+f-g)/2$ band gaps. Similarly, using Eqs. (7) and (4) it follows that in case $a+b+f+g$ is an odd integer and if $a \geqslant b+f+g$ then the potential has a band gaps while if $a<b+g+f$ then it has $(a+b+f+g+1)/2$ band gaps.

It is now straightforward to count the number of independent GAL potentials $[a,b,f,g]$ with a band gaps and show that

$$N_a = \frac{1}{18}[a^3+9a^2+6a+2], \quad a = 1(\mathrm{mod}\ 3),$$

$$N_a = \frac{1}{18}[a^3 + 9a^2 + 6a - 2], \quad a = 2(\text{mod } 3),$$

$$N_a = \frac{a}{18}[a^2 + 9a + 6], \quad a = 0(\text{mod } 3). \tag{25}$$

Several comments are in order at this stage.

1. There is only one independent potential with one band gap but there are three independent potentials with two band gaps and seven independent potentials with three band gaps. This then implies[12] that while there is only one independent KdV equation of third order, there should be three such equations of fifth order and seven such equations of seventh order. It is worth pointing out that indeed there are three such independent KdV equations of fifth order already known in the literature, called standard, Sawada-Kotera, and Kupershmidt (fifth-order) KdV equations. It may be interesting to explicitly obtain all seven independent KdV equations of seventh order.

2. On subtracting the number of independent potentials with a band gaps [as given by Eq. (25)] from the total number of allowed potentials as given by Eq. (24), we immediately find that the number of independent potentials of the form $[a,b,f,g]$ having more than a band gaps is given by

$$N_{>a} = \tfrac{1}{18}(a+2)(2a^2 + 5a - 1), \quad a = 1(\text{mod } 3),$$

$$N_{>a} = \tfrac{1}{18}(a+1)(2a^2 + 7a + 2), \quad a = 2(\text{mod } 3), \tag{26}$$

$$N_{>a} = \tfrac{1}{18}a(a+3)(2a+3), \quad a = 0(\text{mod } 3).$$

For example there are four potentials of the form $[a,b,f,g]$ with $a=2$ having more than two band gaps given by

$$N_{>2} = [2,2,2,0],[2,2,2,1],[2,2,1,0],[2,1,1,1], \tag{27}$$

while for $a=3$ there are nine such potentials with more than three band gaps, given by

$$N_{>3} = [3,3,3,0],[3,3,3,1],[3,3,3,2],[3,3,2,0],[3,3,2,1],[3,3,1,0],[3,2,1,1],[3,2,2,0],[3,2,2,2]. \tag{28}$$

3. If $a+b+f+g$ is an even integer and further if $a+g=b+f$, then both sides of Eq. (6) are identical and the corresponding potential is self-dual. Similarly, if $a+b+f+g$ is an odd integer and $a=b+f+g+1$, then both sides of Eq. (7) are identical, and one has a self-dual potential. As an illustration, the AL potential $[a,a-1,0,0]$ is self-dual, a fact we already knew from Ref. 18 But we now get a large number of additional self-dual GAL potentials, like [2,1,1,0], [4,2,2,0], and [4,2,1,0], for example.

4. A related question is, out of the above self-dual potentials how many are also self-isospectral?[18,19] It is easy to see that the most general form of (at least one of) the eigenfunction for the self-isospectral potentials is

$$\psi = \frac{\text{dn}^a(x,m)\text{sn}^b(x,m)}{\text{cn}^b(x,m)} \tag{29}$$

and that the corresponding self-isospectral potential has the form

$$[a,a-1,b,b-1], \quad b > 0, \quad [a,a-1,0,0], \quad b = 0. \tag{30}$$

The fact that the AL potentials of the form $[a,a-1,0,0]$ are self-isospectral was established many years ago.[18] However, what is new is the realization that the potentials $[a,a-1,b,b-1]$ are also self-isospectral potentials. Note that here a,b can be any integers. Some examples of self-

isospectral potentials are [1,0,0,0], [2,1,0,0], [3,2,2,0], [3,2,1,1], and [3,2,0,0]. Thus out of all the self-dual potentials, those which are of form (30) are also self-isospectral while the rest are self-dual but not self-isospectral. One can show that the number of self-dual potentials N_{sd} which are not self-isospectral is given by

$$N_{\mathrm{sd}} = \tfrac{1}{3}(a-1)^2, \quad a = 1,4,7,\ldots,$$
$$N_{\mathrm{sd}} = \tfrac{1}{3}a(a-2), \quad a = 2,3,5,6,\ldots. \tag{31}$$

On the other hand, it is easy to see that the number of self-isospectral potentials is $N_{\mathrm{si}}=a$. As an illustration, the self-isospectral potentials with two band gaps are [2,1,0,0] and [2,1,1,0] while there are no self-dual (but non-self-isospectral) potentials with two band gaps. On the other hand, the self-isospectral potentials with three band gaps are [3,2,2,1], [3,2,1,0], and [3,2,0,0], while the only self-dual (but non-self-isospectral) potential with three band gaps is [3,1,1,0].

5. Clearly all potentials with $a+g>b+f$ or $a>b+f+g+1$ depending on if $a+b+f+g$ is an odd or an even integer, have partner potentials as given by Eq. (6) or (7), respectively. Now out of these, some are SUSY partner potentials while the rest are merely partner potentials. So let us count both types of potentials. Now if two GAL potentials are SUSY partners, then one of their eigenfunctions must be related to each other by $\psi_{\mathrm{II}}=\psi_{\mathrm{I}}^{-1}$. Further, these two eigenfunctions must have the form

$$\mathrm{dn}^{\alpha}(x)\mathrm{cn}^{\beta}(x)\mathrm{sn}^{\gamma}(x). \tag{32}$$

Besides, from paper I we know that if the QES eigenfunction is of the form (32), then $b=-\alpha$, $f=-\beta$, $g=-\gamma$, and $a+b+f+g=0$. From here it is easy to show that the potential $[a,b,f,g]$ with a band gaps has a SUSY GAL partner provided either $a+g=b+f+2$ or $a=b+f+g+3$ depending on if $a+b+f+g$ is an even or an odd integer, respectively. Hence, all potentials of the form $[a,b,f,g]$ with a band gaps and satisfying $a+g>b+f+2$ or $a>b+g+f+3$ have merely partner potentials of the form (6) and (7), respectively. It is worth emphasizing that while these partner potentials have the same band edge eigenvalues, none of them are SUSY partner potentials. For example, [2,0,0,0] and [1,1,1,0] are SUSY partner GAL potentials with two band gaps. Similarly [3,1,0,0] and [2,2,1,0] are SUSY partner GAL potentials with three band gaps. On the other hand, [4,0,0,0] and [2,2,2,1] are merely partner potentials with four band gaps.

6. One can count the number of potentials (N_{su}) of the form $[a,b,f,g]$ with a band gaps having another GAL potential as its SUSY partner and it is easy to show that

$$N_{\mathrm{su}} = \tfrac{1}{3}[a^2-1], \quad a \neq 0(\mathrm{mod}\ 3),$$
$$N_{\mathrm{su}} = \tfrac{1}{3}a^2, \quad a = 0(\mathrm{mod}\ 3). \tag{33}$$

Finally, it is not difficult to show that the number of potentials of the form $[a,b,f,g]$ with a band gaps and having merely a (non-SUSY) partner potential of the form as given by Eqs. (6) and (7), respectively, is given by

$$N_{\mathrm{nsu}} = \tfrac{1}{18}(a-1)(a^2-2a-2), \quad a = 1(\mathrm{mod}\ 3),$$
$$N_{\mathrm{nsu}} = \tfrac{1}{18}(a-2)(a^2-a-2), \quad a = 2(\mathrm{mod}\ 3), \tag{34}$$
$$N_{\mathrm{nsu}} = \tfrac{1}{18}a^2(a-3), \quad a = 0(\mathrm{mod}\ 3).$$

7. On adding the number of self-dual (but non-self-isospectral), self-isospectral, SUSY partner and (non-SUSY) merely partner potentials as given by Eqs. (30)–(34) respectively, as expected, we find that the number of independent potentials with a band gaps is as given by Eq. (25).

8. One obvious interesting question is whether there are non-GAL potentials with a finite number of band gaps. The answer to this question is yes. In particular, since the general form of the eigenfunction for any GAL potential is of the form[1]

$$\psi_{\mathrm{GAL}}(x) = \mathrm{dn}^{-b}(x)\mathrm{cn}^{-f}(x)\mathrm{sn}^{-g}(x)\sum_{k=0}^{N} A_k \mathrm{sn}^{2k}(x), \tag{35}$$

it follows that non-GAL potentials of the form

$$V_+(x) = V_{\mathrm{GAL}}(x) - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln \psi_{\mathrm{GAL}}(x) \tag{36}$$

are also finite gap potentials. In this context it is worth mentioning that some people[14] have recently obtained potentials with a finite number of band gaps which are more general than the GAL potentials. It is not clear if those potentials and the potentials (36) have any overlap.

The nature of band edge eigenstates. In paper I we showed that if $a+b+f+g=2n$, then $n+1$ QES states can be obtained for GAL potentials (2) and they are of the form given in Eq. (35). On using this key result as well as the fact that the GAL potential $[a,b,f,g]$ remains unchanged when any one (or more) of the four parameters a,b,f,g is changed to $-a-1$, $-b-1$, $-f-1$, $-g-1$, respectively, it is easy to specify the nature of the band edge eigenfunctions for any potential $[a,b,f,g]$ with a band gaps. The nature as well as the number of eigenstates crucially depend on whether $a+b+f+g$ is an even or an odd integer—so we will discuss these situations separately.

$a+b+f+g=$*even integer:* In this case it is easy to show that one has $(a+b+f+g+2)/2$ eigenstates of the form

$$\mathrm{sn}^{-g}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{-b}(x)F_{(a+b+f+g)/2}[\mathrm{sn}^2(x)], \tag{37}$$

$(a+b-f-g)/2$ eigenstates of the form

$$\mathrm{sn}^{g+1}(x)\mathrm{cn}^{f+1}(x)\mathrm{dn}^{-b}(x)F_{(a+b-f-g-2)/2}[\mathrm{sn}^2(x)], \tag{38}$$

$(a+f-b-g)/2$ eigenstates of the form

$$\mathrm{sn}^{g+1}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{b+1}(x)F_{(a+f-b-g-2)/2}[\mathrm{sn}^2(x)], \tag{39}$$

and $(a+g-b-f)/2$ eigenstates of the form

$$\mathrm{sn}^{-g}(x)\mathrm{cn}^{f+1}(x)\mathrm{dn}^{b+1}(x)F_{(a+g-b-f-2)/2}[\mathrm{sn}^2(x)]. \tag{40}$$

If instead $b+g>a+f$, then one has $(b+f-a-g)/2$ eigenstates of the form

$$\mathrm{sn}^{g+1}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{-b}(x)F_{(b+f-a-g-2)/2}[\mathrm{sn}^2(x)]. \tag{41}$$

$a+b+f+g=$*odd integer:* In this case it is easy to show that one has $(a+b+f-g+1)/2$ eigenstates of the form

$$\mathrm{sn}^{g+1}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{-b}(x)F_{(a+b+f-g-1)/2}[\mathrm{sn}^2(x)], \tag{42}$$

$(a+b+g-f+1)/2$ eigenstates of the form

$$\mathrm{sn}^{-g}(x)\mathrm{cn}^{f+1}(x)\mathrm{dn}^{-b}(x)F_{(a+b+g-f-1)/2}[\mathrm{sn}^2(x)], \tag{43}$$

$(a+f+g-b+1)/2$ eigenstates of the form

$$\mathrm{sn}^{-g}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{b+1}(x)F_{(a+f+g-b-1)/2}[\mathrm{sn}^2(x)], \tag{44}$$

$(a-b-f-g-1)/2$ eigenstates of the form

$$\mathrm{sn}^{g+1}(x)\mathrm{cn}^{f+1}(x)\mathrm{dn}^{b+1}(x)F_{(a-b-f-g-3)/2}[\mathrm{sn}^2(x)]. \tag{45}$$

If instead $b+f+g>a-1$ then one has $(b+f+g-a+1)/2$ eigenstates of the form

$$\mathrm{sn}^{-g}(x)\mathrm{cn}^{-f}(x)\mathrm{dn}^{-b}(x)F_{(b+f+g-a-1)/2}[\mathrm{sn}^2(x)]. \tag{46}$$

Here $F_n[\mathrm{sn}^2(x)]$ denotes a polynomial of order n in $\mathrm{sn}^2(x)$. It is worth pointing out that not only the QES band edge eigenvalues are identical for the two partner potentials as given either by Eq. (6) or by (7), even the nature of the band edge eigenfunctions in the two cases is also similar. For example, the potential $[(a+b+f-g)/2,(a+b+g-f)/2,(a+f+g-b)/2,(b+f+g-a)/2]$ as given by Eq. (6) has the same band edge eigenvalues and further the corresponding eigenfunction is simply obtained from Eqs. (37)–(41) by replacing a,b,f,g with $(a+b+f-g)/2,(a+b+g-f)/2,(a+f+g-b)/2,(b+f+g-a)/2$, respectively. Exactly the same is also true about the equivalent potential given by Eq. (7) in case $a+b+f+g$ is an odd integer and the corresponding eigenfunctions are exactly as given by Eqs. (42)–(46) but with the replacement of a,b,f,g by $(a+b+f+g+1)/2,(a+b-f-g-1)/2,(a+f-b-g-1)/2,(a+g-b-f-1)/2$, respectively. It follows from here that irrespective of whether $a+b+f+g$ is an odd or an even integer, there are precisely a bound bands, same a number of band gaps and $2a+1$ number of band edges all of which are analytically known in principle, beyond which there is a continuum band extending up to $E=\infty$. Further, irrespective of whether $a+b+f+g$ is an odd or an even integer, if $a+b$ is an even (odd) integer, then there are $a+b+1$ band edges of period $2K(4K)$ and $a-b$ band edges of period $4K(2K)$.

Thus in general the band structure of the GAL potentials is unusual in that if $a+b$ is an even (odd) integer, then b band gaps of period $4K(2K)$ must be of zero width, i.e., there must be b doubly degenerate states of period $4K(2K)$. Unfortunately, till today we do not know either the eigenvalue or the nature of the eigenfunction of even one of these doubly degenerate states. One exception is the case of pure Lamé (and their GAL partners) potentials, i.e., when $b=f=g=0$, as in that case depending on if a is even or odd integer, one has $a+1$ band edges of period $2K(4K)$ and a band edges of period $4K(2K)$ and the band structure is normal one, with no doubly degenerate states.

As an illustration, consider the GAL potentials with two band gaps. As seen earlier, there are three distinct potentials with two band gaps out of which we have already discussed the band structure of the two potentials [2, 0, 0, 0] and [2, 1, 0, 0].[16,18] Thus it would be interesting to know the band edges and the band structure of the remaining potential with two band gaps, i.e., [2, 1, 1, 0]. Since $a+b=3$, it follows from the above discussion that in this case there must be four band edges of period $4K$ and 1 band edge of period $2K$. Using Table 4 of paper I it is easily seen that the eigenstate with period $2K$ is given by

$$\psi=\mathrm{dn}^2(x)\mathrm{sn}(x)\mathrm{cn}^{-1}(x),\quad E=9m, \tag{47}$$

while out of the four band edges of period $4K$, one eigenstate has the form

$$\psi=\mathrm{dn}^{-1}(x)\mathrm{sn}(x)\mathrm{cn}^2(x),\quad E=9. \tag{48}$$

The three other eigenstates of period $4K$ have the form

$$\psi=\mathrm{dn}^{-1}(x)\mathrm{cn}^{-1}(x)[A+B\,\mathrm{sn}^2(x)+D\,\mathrm{sn}^4(x)], \tag{49}$$

and the corresponding three eigenvalues satisfy the cubic equation

$$r^3+8(1+m)r^2+80mr+64m(1+m)=0,\quad E=-r+1+m. \tag{50}$$

Further, it is clear that there must be one doubly degenerate state of period $2K$ whose eigenvalue and eigenfunctions are not known analytically.

IV. GAL POTENTIALS [WITH AT LEAST ONE PARAMETER a,b,f,g=HALF-INTEGER]

So far, we have discussed GAL potentials when all four parameters a,b,f,g take integer values. We have seen that these are problems with a finite number of band gaps. We now consider the case when at least one of the parameters a,b,f,g is a half-integer. In general, all such problems have an infinite number of band gaps and one has only a few QES states.

A. a=half-integer

As mentioned in Sec. I, we conjecture that the relations (6) and (7) are simultaneously valid when at least one of the four parameters a,b,f,g is a half-integer. In particular, in case $a=k+\frac{1}{2}$ and b,f,g are arbitrary numbers, we assert that $k+1$ QES energy values are identical for three GAL potentials, that is

$$\begin{aligned}&\left[a=k+\frac{1}{2},b,f,g\right]\\&\equiv\left[\frac{2(k+b+f+g)+3}{4},\frac{2(k+b-f-g)-1}{4},\frac{2(k+f-b-g)-1}{4},\frac{2(k+g-b-f)-1}{4}\right]\\&\equiv\left[\frac{2(k+b+f-g)+1}{4},\frac{2(k+b+g-f)+1}{4},\frac{2(k+f+g-b)+1}{4},\frac{2(b+f+g-k)-1}{4}\right].\end{aligned}\tag{51}$$

This relation needs some clarification. What is being conjectured here is that there are $k+1$ QES mid-band energy values of the potential with $a=k+1/2$ and b,f,g being arbitrary numbers, which are the same as the band edge energy eigenvalues of the two other potentials given in (51). For these two potentials, we can always obtain $k+1$ QES band edges, since for both of them the sum of the four parameters characterizing the potentials is $2k$.[1]

We have explicitly verified our conjecture in the following cases: (i) Lamé potentials with $a=1/2,3/2$ (and $b=f=g=0$); (ii) AL potentials[16] with $a=1/2,3/2$, $b=1,2,3$ (and $f=g=0$); (iii) GAL potentials with $a=1/2,3/2$, and either b or f or g is arbitrary while the remaining two parameters take any integer values. For example, we know that the mid-band state of the $a=1/2$ Lamé potential is at $(1+m)/4$. Using Eq. (51), we predict that both the potentials $[\frac{3}{4},-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}]$ and $[\frac{1}{4},\frac{1}{4},\frac{1}{4},-\frac{3}{4}]$ must have a QES band edge eigenvalue at $E=(1+m)/4$. Using Table 4 of paper I it is easily checked that this is indeed so, with the corresponding band edge eigenfunctions being $\psi=[\mathrm{dn}(x)\mathrm{cn}(x)\mathrm{sn}(x)]^{1/4}$ and $\psi=\mathrm{dn}^{-1/4}(x)\mathrm{cn}^{-1/4}(x)\mathrm{sn}^{3/4}(x)$, respectively. Similarly, it is well known that the QES mid-band states of the $a=3/2$ Lamé potential are at

$$E=\frac{5(1+m)}{4}\pm\sqrt{1-m+m^2}.\tag{52}$$

Using Eq. (51) we then predict that both the potentials $[\frac{5}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4}]$ and $[\frac{3}{4},\frac{3}{4},\frac{3}{4},\frac{-1}{4}]$ must have QES band-edge eigenvalues as given by Eq. (52). Using Table 4 of paper I it is easily checked that this is indeed so, with the corresponding band edge eigenfunctions being respectively given by

$$\psi=[\mathrm{dn}(x)\mathrm{cn}(x)\mathrm{sn}(x)]^{-1/4}(1+[-(1+m)\pm\sqrt{1-m+m^2}]\mathrm{sn}^2(x)),\tag{53}$$

$$\psi=[\mathrm{dn}^{-3/4}(x)\mathrm{cn}^{-3/4}(x)\mathrm{sn}^{1/4}(x)](3+[-(1+m)\pm\sqrt{1-m+m^2}]\mathrm{sn}^2(x)).\tag{54}$$

We have similarly checked the equivalence in all the above-mentioned cases. For example, using the results[16] for the AL potential [3/2, 1, 0, 0], we find (and verify using Table 4 of paper I) that the GAL potentials $[7/4,3/4,-1/4,-1/4]$ and $[5/4,5/4,1/4,-1/4]$ have QES band edges at $E=(13+5m)/4\pm\sqrt{9-9m+m^2}$. The corresponding band edge eigenfunctions are

$$\psi = [\mathrm{dn}^{-3}(x)\mathrm{cn}(x)\mathrm{sn}(x)]^{-1/4}(3 + [-(3+m) \pm \sqrt{9 - 9m + m^2}]\mathrm{sn}^2(x)), \tag{55}$$

$$\psi = [\mathrm{dn}^{-5/4}(x)\mathrm{cn}^{-1/4}(x)\mathrm{sn}^{3/4}(x)](5 + [-(3+m) \pm \sqrt{9 - 9m + m^2}]\mathrm{sn}^2(x)), \tag{56}$$

respectively. Similarly, using the results in paper I for the mid-band states of the GAL potential $[\frac{1}{2}, t-\frac{1}{2}, 1, 0]$ we verify that the potentials $[t/2+1, t/2-1, (1-t)/2, -(1+t)/2]$ and $[(1+t)/2, -(1-t)/2, 1-t/2, t/2]$ indeed have a QES band edge eigenvalue $E=t^2+9m/4$, for any noninteger t and the corresponding eigenfunctions are $\psi = \mathrm{dn}^{(2-t)/2}(x)\mathrm{cn}^{(t-1)/2}(x)\mathrm{sn}^{(1+t)/2}(x)$ and $\psi = \mathrm{dn}^{(1-t)/2}(x)\mathrm{cn}^{(t-2)/2}(x)\mathrm{sn}^{(2+t)/2}(x)$.

Thus one is fairly confident that the remarkable relationship (51) is indeed valid. We now turn around and use (51) to predict new results for the mid-band states of GAL potentials with half-integer values of a in case b, f, g take arbitrary values. As an illustration, we predict that the potential $[1/2, b, f, g]$, where b, f, g are arbitrary numbers must have a QES state at energy

$$E = (b + 1/2)^2 + (f + 1/2)^2 m, \tag{57}$$

while the potential $[3/2, b, f, g]$ with b, f, g being arbitrary numbers must have two QES states with energies

$$E = [(b + 1/2)^2 + 1] + [1 + (f + 1/2)^2]m \pm 2\sqrt{[(b + 1/2) + (f + 1/2)m]^2 - (b + f + g + 3/2)(b + f - g + 1/2)m}. \tag{58}$$

Perhaps some clarification is required as to when the QES state is a band edge and when it is a mid-band state. We believe that only those states correspond to band edges for which $a+b+f+g$ [or any other combination obtained by changing one or more of these parameters to $-a-1$, $-b-1, -f-1, -g-1$, respectively] is equal to an even integer (including zero). All other QES states should correspond to mid-band states. We thus believe that the QES energy values as given above for the potentials $[1/2, b, f, g]$ and $[3/2, b, f, g]$ with arbitrary b, f, g are in most cases the energies for the mid-band states of these potentials. In Sec. VI we shall obtain the QES eigenstates corresponding to some of these QES eigenvalues by using the connection of the GAL potential problem and Heun's equation.

We can also predict the QES energy values when $a=5/2$ and b, f, g are arbitrary numbers, by computing the band edges of either of the two potentials given in (51). In this way, we predict that the mid-band energy values for the three QES states of the GAL potential $[5/2, b, f, g]$ are solutions of the cubic equation

$$r^3 + 2[1 + 6b + (1 + 6f)m]r^2 + 4[2(4b^2 - 1) + 2(4f^2 - 1)m^2 + (4b^2 + 4f^2 - 4g^2 + 24bf + 8b + 8f - 2g + 3)m]r + 8m[2b + 1 + (2f + 1)m][4(b + f)^2 - (2g + 1)^2] = 0, \tag{59}$$

where $r = -E + (3/2 - b)^2 + (3/2 - f)^2 m$. For the special cases (i) $b=f=g=0$ as well as (ii) $b=1, f=g=0$, it is easily checked that Eq. (59) agrees with well-known results,[16] thereby providing a powerful check on our calculations. Generalization to higher half-integer values is straightforward (in principle) and it is easy to see that energy values for $a+1/2$ QES mid-band states can be predicted (at least in principle) when b, f, g are arbitrary numbers and a is a half-integer.

B. a, b = half-integers

Let us now discuss the case when both a and b are half-integers while f and g are arbitrary numbers using our conjecture that Eqs. (6) and (7) are both simultaneously valid. In particular, for $a = k + \frac{1}{2}$, $b = l + \frac{1}{2}$ while f, g are any numbers, we assert that the three potentials

$$\left[a=k+\frac{1}{2},b=l+\frac{1}{2},f,g\right]$$
$$\equiv\left[\frac{k+l+f+g+2}{2},\frac{k+l-f-g}{2},\frac{k+f-l-g-1}{2},\frac{k+g-l-f-1}{2}\right]$$
$$\equiv\left[\frac{k+l+f-g+1}{2},\frac{k+l+g-f+1}{2},\frac{k+f+g-l}{2},\frac{l+f+g-k}{2}\right], \tag{60}$$

have the same $k+l+2$ QES energy values. This means that the QES mid-band energy values of the potential with $a=k+1/2$, $b=l+1/2$ are the same as the band edge eigenvalues of the two other potentials in (60). For these two potentials, we can obtain $k+l+2=a+b+1$ QES states since, for both of them, the sum of the four numbers characterizing the potentials is either $2k$ or $2l$. This is possible because the GAL potential $[a,b,f,g]$ remains unchanged when any one (or more) of the four parameters a,b,f,g changes to $[-a-1,-b-1,-f-1,-g-1]$, respectively.

As an illustration, consider the potential $[3/2,1/2,f,g]$ with f,g being arbitrary numbers. It is then easily shown that this potential must have three QES mid-band states at

$$E_1=4+(g+1/2)^2m, \tag{61}$$

$$E_{2,3}=2+[(f+1/2)^2+1]m\pm\sqrt{[2-(2f+1)m]^2+[(2g+1)^2-(2f-1)^2m]}. \tag{62}$$

The point is, from Eq. (60) it follows that the potential $[3/2,1/2,f,g]$ has the same QES mid-band states as the potentials

$$\left[\frac{3+f+g}{2},\frac{1-f-g}{2},\frac{f-g}{2},\frac{g-f}{2}\right] \text{ and } \left[\frac{2+f-g}{2},\frac{2+g-f}{2},\frac{1+f+g}{2},-\frac{1+f+g}{2}\right].$$

Now, using Table 4 of paper I, it is easily shown that these potentials indeed have these three QES eigenvalues. Further, corresponding to the eigenvalue E_1 in Eq. (61) the corresponding eigenfunctions for these two potentials, respectively, are

$$\mathrm{dn}^{(g+f-1)/2}(x)\mathrm{cn}^{(2+f-g)/2}(x)\mathrm{sn}^{(2+g-f)/2}(x),\quad \mathrm{dn}^{(f-2-g)/2}(x)\mathrm{cn}^{(3+f+g)/2}(x)\mathrm{sn}^{(1-f-g)/2}(x). \tag{63}$$

The eigenfunctions corresponding to the eigenvalues $E_{2,3}$ in Eq. (62) can similarly be written down using Table 4 of paper I.

Note that out of the $k+l+2$ QES states, the energies for the $k+1$ states can also be obtained by considering the previous case of $a=k+1/2$ and b,f,g arbitrary and putting $b=l+1/2$ at the end of the calculation. As an illustration, consider the case $[3/2,b,f,g]$ where b is any arbitrary number. As shown in the last section, there are two QES energies given by Eq. (58). On putting $b=1/2$ we find that the two QES energy values of the potential $[3/2,1/2,f,g]$ are precisely as given by Eq. (62). For the special case $f=g=0$, these eigenvalues agree with well-known results for the AL potential.[16] Similarly, consider the case $[5/2,b,0,0]$. As shown in Sec. IV A, there are three QES energy values as given by Eq. (59). On putting $b=1/2$, it is easily seen that the three eigenvalues are $E=(1+9m/4),(1+25m/4),(9+m/4)$, in agreement with the eigenvalues obtained by us previously.[16]

C. a,b,f=half-integers

We shall now discuss the case when three out of the four parameters (say a,b,f) are half-integers while g is any number (not a half-integer), and obtain the energies of the QES mid-band states. Our argument is again based on the assertion that relations (6) and (7) are simultaneously valid. In particular, we assert that for $a=k+\frac{1}{2}$, $b=l+\frac{1}{2}$, $f=n+\frac{1}{2}$ the three potentials

$$\left[a=k+\frac{1}{2},b=l+\frac{1}{2},f=n+\frac{1}{2},g\right]$$
$$\equiv\left[\frac{2(k+l+n+g)+5}{4},\frac{2(k+l-n-g)-1}{4},\frac{2(k+n-l-g)-1}{4},\frac{2(l+n-k-g)-1}{4}\right]$$
$$\equiv\left[\frac{2(k+l+n-g)+3}{4},\frac{2(k+l+g-n)+1}{4},\frac{2(k+n+g-l)+1}{4},\frac{2(l+n+g-k)+1}{4}\right] \tag{64}$$

have identical $k+l+n+3$ QES energy values. What is being asserted here is that the $k+l+n+3$ QES mid-band energies of the potential with half-integer values of a,b,f and arbitrary g are the same as the band edge energy eigenvalues of the two other potentials in (64). This happens because for arbitrary values of g, for the two potentials

$$\left[\frac{2(k+l+n+g)+5}{4},\frac{2(k+l-n-g)-1}{4},\frac{2(k+n-l-g)-1}{4},\frac{2(l+n-k-g)-1}{4}\right], \tag{65}$$

$$\left[\frac{2(k+l+n-g)+3}{4},\frac{2(k+l+g-n)+1}{4},\frac{2(k+n+g-l)+1}{4},\frac{2(l+n+g-k)+1}{4}\right], \tag{66}$$

we can always obtain $k+l+n+3=a+b+f+3/2$ QES band edges, since for both potentials the sum of the four numbers characterizing the potentials is either $2k$ or $2l$ or $2n$. This is possible because the GAL potential $[a,b,f,g]$ remains unchanged when any one (or more) of the four parameters a,b,f,g change to $-a-1,-b-1,-f-1,-g-1$, respectively. Thus we conjecture that the potential $[k+1/2,l+1/2,n+1/2,g]$, for arbitrary g has $k+l+n+3$ QES mid-band states. As an illustration, consider the case $k=l=n=0$ with g arbitrary. We assert that the potential $\left[\frac{1}{2},\frac{1}{2},\frac{1}{2},g\right]$ must have three QES states, being a partner of the potentials

$$\left[\frac{2g+5}{4},-\frac{(2g+1)}{4},-\frac{(2g+1)}{4},-\frac{(2g+1)}{4}\right]$$

and

$$\left[\frac{3-2g}{4},\frac{(2g+1)}{4},\frac{(2g+1)}{4},\frac{(2g+1)}{4}\right].$$

Using Table 4 of paper I it is easily checked that these two potentials have three QES energy eigenstates which are:
(i) $E=1+m$ with the two corresponding eigenfunctions respectively being

$$\psi=[\mathrm{cn}(x)\mathrm{dn}(x)]^{(2g+1)/4}\mathrm{sn}^{(3-2g)/4}(x),\quad \psi=[\mathrm{cn}(x)\mathrm{dn}(x)]^{-(2g+1)/4}\mathrm{sn}^{(2g+5)/4}(x). \tag{67}$$

(ii) $E=1+\left(g+\frac{1}{2}\right)^2 m$ with the two corresponding eigenfunctions being

$$\psi=[\mathrm{sn}(x)\mathrm{dn}(x)]^{(2g+1)/4}\mathrm{cn}^{(3-2g)/4}(x),\quad \psi=[\mathrm{sn}(x)\mathrm{dn}(x)]^{-(2g+1)/4}\mathrm{cn}^{(2g+5)/4}(x). \tag{68}$$

(iii) $E=\left(g+\frac{1}{2}\right)^2+m$ with the two corresponding eigenfunctions being

$$\psi=[\mathrm{sn}(x)\mathrm{cn}(x)]^{(2g+1)/4}\mathrm{dn}^{(3-2g)/4}(x),\quad \psi=[\mathrm{sn}(x)\mathrm{cn}(x)]^{-(2g+1)/4}\mathrm{dn}^{(2g+5)/4}(x). \tag{69}$$

We now make a number of predictions for the energy eigenvalues of the mid-band states for GAL potentials of the form $[k+1/2,l+1/2,n+1/2,g]$.

1. We predict that the potential $[1/2,1/2,1/2,g]$ has three QES mid-band states with energy values

$$E_1=(1+m),\quad E_2=1+(g+1/2)^2 m,\quad E_3=(g+1/2)^2+m. \tag{70}$$

2. The potential $[3/2,1/2,1/2,g]$ has four QES mid-band states with energy values

$$E_1=(4+m),\quad E_2=(g+1/2)^2+4m,\quad E_{3,4}=2(1+m)\pm\sqrt{4(1-m)^2+(2g+1)^2m}. \tag{71}$$

3. The potential $[3/2,3/2,1/2,g]$ has five QES mid-band states with energy values

$$\begin{gathered}E_1=(g+1/2)^2+4m,\quad E_{2,3}=5+2m\pm\sqrt{4(2-m)^2+(2g+1)^2m-4m},\\ E_{4,5}=5+[(g+1/2)^2+1]m\pm\sqrt{[4-(2g+1)m]^2-(2g-3)^2m+4m}.\end{gathered} \tag{72}$$

4. The potential $[3/2,3/2,3/2,g]$ has six QES mid-band states with energy values

$$\begin{gathered}E_{1,2}=(5+m)\pm\sqrt{16(1-m)^2+(2g+1)^2m},\\ E_{3,4}=5+[(g+1/2)^2+1]m\pm\sqrt{16-(2g+1)^2m(1-m)},\\ E_{5,6}=[(g+1/2)^2+1]+5m\pm\sqrt{16m^2+(2g+1)^2(1-m)}.\end{gathered} \tag{73}$$

5. One can readily obtain some QES mid-band energy values when (i) k is an arbitrary integer while l and/or n are either 0 or 1; (ii) k,l are arbitrary integers with $n=0$ or 1 and g being any arbitrary number. It would be nice to prove (or disprove) these conjectures and more importantly, try to obtain the corresponding energy eigenfunctions. We shall have something to say about this point when we discuss the implications of these results in the context of Heun's equation.

6. Note that out of the $k+l+n+3$ QES states, the energy values for $k+l+2$ states can also be obtained by considering the previous case $[a=k+1/2,\ b=l+1/2,f,\ g=\text{arbitrary}]$ and putting $f=n+1/2$ at the end of the calculation. As an illustration, consider the case $[3/2,1/2,f,g]$ where f,g are arbitrary numbers. As shown in Sec. IV B, there are three QES energy values and they are given by Eqs. (61) and (62). On putting $f=1/2$ in these equations, we find that three (out of four) QES eigenvalues of $[3/2,1/2,1/2,g]$ as given by Eq. (72) are correctly obtained.

D. a,b,f,g=half-integers

Finally, let us consider the case when all four parameters are half-integers. The potential is of the form $[k+1/2,l+1/2,n+1/2,p+1/2]$, where k,l,n,p are integers and we take $k\geqslant l\geqslant n\geqslant p$. We shall discuss the two cases when the sum $k+l+n+p$ is an even or an odd integer separately.

1. $k+l+n+p$=even-integer

As shown in paper I, for the GAL potential (2), QES energies are obtained when the sum of the four parameters is an even integer including zero. In this case, as already shown by Takemura,[15] both the relations (6) and (7) are simultaneously valid. We would like to assert here that in this case, in general there should be $k+n+l+p+4$ QES states, since the sum of the four numbers characterizing the potentials is either $2k$ or $2l$ or $2n$ or $2p$. This is possible because the GAL potential $[a,b,f,g]$ remains unchanged when any one (or more) of the four parameters a,b,f,g change to $-a-1,-b-1,-f-1,-g-1$, respectively. Unfortunately, in the several specific cases that we have examined, we find that some of the eigenvalues simply get repeated. Thus the true number of QES states may be much less than $k+l+n+p+4$. For example, consider the case of $[5/2,\ 1,\ 2,\ 1/2,1/2]$. Using Eqs. (6) and (7) it follows that this potential must have the same QES eigenvalues as the potential $[3/2,3/2,3/2,-1/2]$. While naively we expect six QES states for these potentials, we only find three QES levels. The three QES energy eigenstates for the two potentials are:

(i) $E=1+m$ with the two corresponding eigenfunctions being

$$\psi=[\mathrm{cn}(x)\mathrm{dn}(x)]^{-3/2}\mathrm{sn}^{1/2}(x),\quad \psi=[\mathrm{cn}(x)\mathrm{dn}(x)]^{3/2}\mathrm{sn}^{-1/2}(x). \tag{74}$$

(ii) $E=9+m$ with the two corresponding eigenfunctions being

$$\psi = \mathrm{dn}^{-3/2}(x)\mathrm{cn}^{5/2}(x)\mathrm{sn}^{1/2}(x), \quad \psi = [\mathrm{sn}(x)\mathrm{cn}(x)]^{3/2}\mathrm{dn}^{-1/2}(x). \tag{75}$$

(iii) $E=1+9m$ with the two corresponding eigenfunctions being

$$\psi = \mathrm{dn}^{5/2}(x)\mathrm{cn}^{-3/2}(x)\mathrm{sn}^{1/2}(x), \quad \psi = [\mathrm{sn}(x)\mathrm{dn}(x)]^{3/2}\mathrm{cn}^{-1/2}(x). \tag{76}$$

Similarly, for the potential $[9/2,1/2,1/2,1/2]$, while naively we expect eight QES states, we only find four QES levels at $E=(1+m)$, $(1+25m)$, $(25+m)$, $9(1+m)$.

2. $k+l+n+p$=odd integer

Let us now discuss perhaps the most intriguing case when all four parameters are half-integers and their sum is an odd integer. While it is clear from paper I that no QES band edges can be obtained when $k+l+n+p$ is an odd integer, it is not obvious whether mid-band states can be obtained in this case. In fact we shall now obtain energy values for several QES mid-band states for these potentials. As argued in Sec. I, while Takemura has shown that relations (6) or (7) are valid when $a+b+f+g$ is an even or an odd integer, respectively (and all are integers), we conjecture that irrespective of whether $a+b+f+g$ is an odd or an even integer, both relations are always valid. Using Eqs. (6) and (7), it then follows that irrespective of whether $a+b+f+g$ is an even or an odd integer, they always have a partner potential of the form $[k+1/2,l+1/2,n+1/2,p+1/2]$ where k,l,n,p are all integers and their sum is an odd integer. We thus conjecture that when $a+b+f+g$ is an even integer, then the QES mid-band energy values of the potential $[(a+b+f+g+1)/2, (a+b-f-g-1)/2, (a+f-b-g-1)/2, (a+g-b-f-1)/2]$ are the same as the band edge eigenvalues of the potential $[a,b,f,g]$. Similarly, when $a+b+f+g$ is an odd integer, then we conjecture that the QES mid-band energy values of the potential $[(a+b+f-g)/2, (a+b+g-f)/2, (a+f+g-b)/2, (b+f+g-a)/2]$ are the same as the band edge eigenvalues of the potential $[a,b,f,g]$. This is rather remarkable. Since the band edges of the GAL potentials $[a,b,f,g]$ with integer a,b,f,g are all known (at least in principle), hence one has a prediction for $k+l+n+p+4$ QES mid-band states of the GAL potentials of the type $[k+1/2,l+1/2,n+1/2,p+1/2]$ when $k+l+n+p$ is an odd integer. To be precise, we predict that the potential $[k+1/2,l+1/2,n+1/2,p+1/2]$ has $k+l+n+p+4$ QES mid-band states in case $k+l+n+p$ is an odd integer and these eigenvalues are identical to the band edges of the potential $[(k+l+n+p+3)/2, (k+l-n-p-1)/2, (k+n-l-p-1)/2, (k+p-l-n-1)/2]$. As an illustration, knowing the band edges of the Lamé potential $2m\mathrm{sn}^2(x)$ we predict that the three QES mid-band state energy values of the potential $[1/2,1/2,1/2,-1/2]$ must be at $E=m,1,1+m$. Similarly, we predict that the five mid-band QES energies of the potential $[3/2,1/2,1/2,1/2]$ are at

$$E_2 = 1+m, \quad E_3 = (1+4m), \quad E_4 = (4+m), \quad E_{1,5} = 2(1+m) \pm 2\sqrt{1-m+m^2}. \tag{77}$$

The validity of our conjecture and in a way the consistency of our whole approach can be checked by extrapolating the results obtained in the previous subsection. In particular, in the last subsection we have discussed the case when the potential is of the form $[k+1/2,l+1/2,n+1/2,g]$ where g is any arbitrary number and we have seen that in that case one obtains energies for $k+l+n+3$ QES mid-band states. On choosing $g=p+1/2$ and choosing k,l,n,p such that their sum is an odd integer, we have verified in many cases the validity of our conjectures.

We thus predict that the potentials $[3/2,1/2,1/2,1/2]$, $[5/2,1/2,1/2,-1/2]$ and $[3/2,3/2,1/2,-1/2]$ have exactly the same (five) QES mid-band energies as the band edge energy eigenvalues of the potentials [2, 0, 0, 0], [2, 1, 1, 0], [2, 1, 0, 0], respectively. It is worth observing that there are exactly three ways of obtaining $k+l+n+p=1$ given that $k\geqslant l\geqslant n\geqslant p$ and that while k,l,n are non-negative integers, p is $\geqslant -1$. It may be noted here that in case n is also -1 then the corresponding partner potentials as given by Eqs. (6) and (7) are potentials of the type $[a,a,b.b]$ and similarly if both $n=l=-1$ then the partner potentials are of type $[a,a,a,a]$ which, as explained in Sec. II, are not included in our analysis. Thus, put another way, the problem of finding the number of independent potentials with say a band gaps reduces to finding four integers k,l,n,p with $k\geqslant l\geqslant n\geqslant p$ (with $n\geqslant 0, p\geqslant -1$) such that their sum equals $2a-3$.

V. GAL POTENTIALS [a,b,f,g=ARBITRARY NUMBERS]

So far, we have discussed the cases when the four parameters a,b,f,g take integer values or at least one of them is half-integer. Now we want to extend this discussion to the general case when a,b,f,g take arbitrary values.

As seen in Sec. IV, when either one, two, or three of the parameters are half-integer while the remaining parameters are arbitrary, then clearly the corresponding partners indeed correspond to the case where a,b,f,g are arbitrary numbers. We therefore conjecture that the relations (6) and (7) are valid even when the four parameters a,b,f,g take any arbitrary values, the only restriction being that either $a+b+f+g$ or any other combination obtained by replacing one or more of these parameters by $-a-1,-b-1,-f-1,-g-1$, respectively, is a non-negative even integer. Further, in that case the two partner potentials have the same band-edge eigenvalues as the QES mid-band energies of the potentials where either one, two, or three of the parameters are half-integers.

A few illustrative examples are in order here. Consider the potential $[4/5,2/5,2/5,2/5]$. In this case while $a+b+f+g=2$, no other combination characterizing relations (38)–(46) gives an even integer. Using Eq. (6) we find that this potential has a GAL partner $[3/5,3/5,3/5,1/5]$. Using Table 4 of paper I it is easily shown that both these potentials have two (identical) QES band edge energy eigenvalues

$$E=\tfrac{26}{25}(1+m)\pm\tfrac{2}{5}\sqrt{1-m+m^2}. \tag{78}$$

If instead we consider the potential $[17/5,8/5,7/5,6/5]$, then only $a+f-b-g$ is an integer and the corresponding GAL partner potential is $[13/5,12/5,11/5,2/5]$ and both have one (identical) QES energy. Of course it can happen that a,b,f,g are such that more than one of the relations (37)–(46) are satisfied. In that case one has more QES band edge eigenvalues. For example, if the potential parameters are such that $a+b-g-f-1,a+f-b-g-1$ as well as $a+g-f-b-1$ are non-negative integers, then using Eqs. (38)–(40) it is easily seen that the number of QES energy eigenvalues is equal to $(3a-b-f-g)/2$. One illustration of this is the potential $[11/5,1/5,1/5,1/5]$ which has three QES energies $(1+m)$, $144/25+m$, $1+(144/25)m$. We might add here that the above-presented discussion is valid even if the numbers a,b,f,g are irrational numbers but such that $a+b+f+g$ or any other combination obtained by replacing one or more of a,b,f,g to $-a-1,-b-1,-f-1,-g-1$, respectively, is an even integer (including zero).

We would like to restate here that when all four parameters a,b,f,g are integers, one has a finite number of band gaps. In all other cases one expects to have an infinite number of bands and band gaps out of which only a few are QES states.

VI. IMPLICATIONS FOR HEUN'S EQUATION

Heun's equation, a second-order linear differential equation with four regular singular points has been extensively discussed in the mathematics literature.[20–22] The intimate connection between Heun's equation and GAL potentials is well known.[9] In recent years, this equation has also proven very useful in the context of a number of physical problems, like quasi-exactly solvable systems,[23] sphaleron stability,[24] Calogero-Sutherland models,[25] higher dimensional correlated systems,[26] Kerr-de Sitter black holes,[27] and finite lattice Bethe ansatz systems.[28]

The canonical form of Heun's equation is given by[20]

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\left(\frac{\gamma}{x}+\frac{\delta}{x-1}+\frac{\epsilon}{x-c}\right)\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\alpha\beta x-q}{x(x-1)(x-c)}\right]G(x)=0, \tag{79}$$

where $\alpha,\beta,\gamma,\delta,\epsilon,q,c$ are parameters, except that $c\neq 0,1$ and the first five parameters are related by

$$\gamma+\delta+\epsilon=\alpha+\beta+1. \tag{80}$$

The four regular singular points of Eq. (79) are located at $x=0,1,c$ and the point at infinity.

If we make the transformation $x=\mathrm{sn}^2(y,m)$, then Heun's equation takes the form[20]

$$F''(y)+\left[(1-2\epsilon)m\frac{\mathrm{sn}(y,m)\mathrm{cn}(y,m)}{\mathrm{dn}(y,m)}+(1-2\delta)\frac{\mathrm{sn}(y,m)\mathrm{dn}(y,m)}{\mathrm{cn}(y,m)}+(2\gamma-1)\frac{\mathrm{cn}(y,m)\mathrm{dn}(y,m)}{\mathrm{sn}(y,m)}\right]F'(y)$$
$$-[4mq-4\alpha\beta m\mathrm{sn}^2(y,m)]F(y)=0, \tag{81}$$

where $c=1/m$, $G(x)\equiv F(y)$. The periodic solutions of Eq. (81) correspond to the polynomial solutions of Eq. (79) while the quasiperiodic solutions correspond to nonpolynomial solutions of (79).

The interesting point is that after a transformation, the Schrödinger equation (9) for the GAL potential (2) is in fact Heun's Eq. (81). In particular, let us start from the Schrödinger equation (9) for the GAL potential (2). On substituting

$$\psi(y)=\mathrm{dn}^{-b}(y)\mathrm{cn}^{-f}(y)\mathrm{sn}^{-g}(y)\phi(y), \tag{82}$$

one can show that $\phi(y)$ satisfies the differential equation

$$\phi''(y)+2\left[mb\frac{\mathrm{sn}(y,m)\mathrm{cn}(y,m)}{\mathrm{dn}(y,m)}+f\frac{\mathrm{sn}(y,m)\mathrm{dn}(y,m)}{\mathrm{cn}(y,m)}-g\frac{\mathrm{cn}(y,m)\mathrm{dn}(y,m)}{\mathrm{sn}(y,m)}\right]\phi'(y)$$
$$-[R-Qm\mathrm{sn}^2(y,m)]\phi(y)=0, \tag{83}$$

where

$$R=-E+m(g+b)^2+(f+g)^2,\quad Q=(b+f+g)(b+f+g-1)-a(a+1). \tag{84}$$

Thus once we obtain solutions of the Schrödinger equation for the GAL potential (2), then we can immediately write the solutions for the periodic form of Heun's Eq. (81) and the solutions of the original Heun's Eq. (79) with the identification

$$\gamma=\tfrac{1}{2}-g,\quad \delta=\tfrac{1}{2}-f,\quad \epsilon=\tfrac{1}{2}-b,$$
$$\alpha+\beta=\tfrac{1}{2}-(b+f+g),\quad 4\alpha\beta=Q,\quad 4mq=R, F(y)\equiv\phi(y). \tag{85}$$

We now make a crucial observation. From Eq. (84), it follows that if under any transformation, the parameters b_1,f_1,g_1 change to b_2,f_2,g_2 and the energy E remains invariant, then the corresponding values of R are related by

$$R_1-m(b_1+g_1)^2-(f_1+g_1)^2=R_2-m(b_2+g_2)^2-(f_2+g_2)^2. \tag{86}$$

Making use of Eq. (86) and the connection between GAL potentials as given by Eqs. (6) and (7), we can obtain interesting relations for Heun's equation. Using the fact that the two GAL potentials given by Eq. (6) have the same band edge energy eigenvalues and the eigenfunctions for both the partners as are given by Eqs. (37)–(41), one can obtain the connection between the two corresponding solutions of Heun's equation. For example, consider the solution (37) and the corresponding solution of the GAL partner obtained by the above-noted substitution. Using Eq. (86) it then follows that corresponding to a given periodic (i.e., polynomial) solution of Heun's equation with parameter set (α, β, δ, ϵ, γ, q) there always exists another periodic solution with the *same* q provided the other parameters change as follows:

$$\gamma\to\alpha,\quad \alpha\to\gamma,\quad \beta\to\beta,\quad \epsilon\to 1+\beta-\delta,\quad \delta\to 1+\beta-\epsilon. \tag{87}$$

Similarly, on considering the other three periodic solutions as given by Eqs. (38)–(40) and the corresponding solutions of the GAL partner potential with the same energy, we find that corresponding to a given periodic solution of Heun's equation, there exist the following three (periodic) solutions with the change of parameters given by (note that $R=4mq$ and $c=1/m$)

$$\gamma\to 1+\beta-\epsilon,\quad \alpha\to\delta,\quad \beta\to\beta,\quad \epsilon\to 1+\beta-\gamma,\quad \delta\to\alpha,\quad q\to q-\beta(\delta-\alpha), \tag{88}$$

$$\epsilon \to \alpha, \quad \alpha \to \epsilon, \quad \beta \to \beta, \quad \gamma \to 1+\beta-\delta, \quad \delta \to 1+\beta-\gamma, \quad q \to q-\beta(\epsilon-\alpha)c, \tag{89}$$

$$\gamma \to 1+\beta-\gamma, \quad \alpha \to 1+\beta-\alpha, \quad \beta \to \beta, \quad \epsilon \to 1+\beta-\epsilon, \quad \delta \to 1+\beta-\delta,$$
$$q \to q+\beta[(\alpha-\delta)+(\alpha-\epsilon)c]. \tag{90}$$

Thus given a periodic solution of Heun's equation, one immediately has four other periodic solutions as given by Eqs. (87)–(90). We have checked that if instead we consider the two partner GAL potentials given by Eq. (7) and consider the corresponding eigenfunctions given by Eqs. (42)–(46) (and those of the corresponding GAL partner potentials with the same energy), then we again obtain the *same* relations [Eqs. (87)–(90)]. As an additional check, we have looked at the partner GAL potentials as given by Eqs. (51), (65), (66), (60), and (8) and in all these cases we get back the relations (87)–(90), which to the best of our knowledge, are new results. Several comments are in order:

1. In Sec. IV we have shown that the QES mid-band energy values of the GAL potential $[a=k+1/2, b, f, g]$ are the same as the QES energies of the two GAL potentials given in (51). What does this imply in the context of Heun's equation? It is easily shown that as a consequence of the discussion in Sec. IV, ven a periodic solution of Heun's equation with the set of parameters α, β, γ, δ, ϵ, q, one has a corresponding quasiperiodic solution with changed parameters:

$$\gamma \to 2-\alpha, \quad \alpha \to 1+\gamma-\alpha, \quad \beta \to 1+\beta-\alpha, \quad \epsilon \to 1+\beta-\delta, \quad \delta \to 1+\beta-\epsilon,$$
$$q \to q+(\alpha-1)[(1+\beta-\delta)+(1+\beta-\epsilon)c]. \tag{91}$$

An additional check on this relation is obtained by using the connection between the mid-band states of the GAL potentials $[a=k+1/2,\ b=l+1/2,\ f,\ g]$ and $[a=k+1/2,\ b=l+1/2,\ f=n+1/2,\ g]$ and the QES energies of the potentials (60), (65), and (66) and we again obtain the *same* connection between the periodic and quasiperiodic solutions of Heun's equation.

2. Using the results in Sec. IV regarding the case when three of the four parameters a, b, f, g are half-integers, we also obtain two more relations connecting the periodic and quasiperiodic solutions of Heun's equation. In particular, given a periodic solution of Heun's equation with the set of parameters α, β, γ, δ, ϵ, q, it implies the following two quasiperiodic solutions of Heun's equation:

$$\gamma \to \alpha, \quad \alpha \to 1+\alpha-\epsilon, \quad \beta \to \delta, \quad \epsilon \to 1+\delta-\beta, \quad \delta \to 1+\beta-\epsilon, \quad q \to q+\alpha(\beta-\delta), \tag{92}$$

$$\gamma \to \alpha, \quad \alpha \to 1+\alpha-\delta, \quad \beta \to \epsilon, \quad \epsilon \to 1+\beta-\delta, \quad \delta \to 1+\epsilon-\beta, \quad q \to q+4\alpha(\beta-\epsilon)c. \tag{93}$$

3. Needless to say that if instead, a quasiperiodic solution of Heun's equation is given, then by inverting Eqs. (91)–(93), we immediately obtain three periodic solutions of Heun's equation.

So far we have discussed how the connections between different GAL potentials can help in finding new solutions of Heun's equation. It may happen that in some cases it may be simpler to solve the algebraic Heun's equation (79) rather than its periodic variant. We now show that this is indeed so in the case of several quasiperiodic mid-band eigenfunctions. Consider for example the GAL potentials when either b or f or g is $1/2$ while the other three parameters are arbitrary. Using arguments of Sec. IV, we can easily obtain the eigenvalues for mid-band states for these potentials. We shall now show that using these eigenvalues we can easily solve the algebraic form of Heun's equation (79) and hence using the connection as explained earlier, obtain the eigenfunctions for the mid-band states of these GAL potentials.

Consider the GAL potential $[a, 1/2, f, g]$ where a, f, g are arbitrary numbers, Note that using the relations (6) and (7) and Table 4 of I, it is easily shown that the QES mid-band eigenvalue of

the GAL potential $[a,1/2,f,g]$ is at $E=(a+1/2)^2+m(g+1/2)^2$. On using the connection formulas (84) and (85) it is easily shown that the corresponding parameters for Heun's equation (79) are

$$\gamma = 1/2 - g, \quad \delta = 1/2 - f, \quad \epsilon = 0, \quad \alpha = (a - f - g + 1/2)/2,$$

$$\beta = -(a + f + g + 1/2)/2, \quad q = (a + f + g + 1/2)(f + g - a - 1/2)(c/4). \tag{94}$$

Remarkably, for these parameters, it is straightforward to obtain the solution of the algebraic Heun's equation (79) and show that

$$G(x) = F[(a - f - g + 1/2)/2, -(a + f + g + 1/2)/2, 1/2 - g; x], \tag{95}$$

where $F(a,b,c;x)$ is the hypergeometric function. The corresponding mid-band state eigenfunction for the GAL potential $[a,1/2,f,g]$ is then immediately written down. We have verified that this is indeed the correct eigenfunction in the following cases (i) $a=f=g=0$, (ii) a integral, $f=g=0$, (iii) a arbitrary while f, g are integral.

Similarly, for the GAL potential $[a,b,1/2,g]$, with arbitrary a, b, g, the QES mid-band energy eigenvalue is $E=(g+1/2)^2+(a+1/2)^2m$ and proceeding as above, it is easily shown that the solution of the algebraic Heun's equation (79) is given by

$$G(x) = F[(a - b - g + 1/2)/2, -(a + b + g + 1/2)/2, 1/2 - g; mx]. \tag{96}$$

Finally, for the GAL potential $[a,b,f,1/2]$, with arbitrary a, b, f, the QES energy is $E=(f+1/2)^2+(b+1/2)^2m$ and proceeding as above, it is easily shown that the solution of the algebraic Heun's equation (79) is given by

$$G(x) = F[(a - b - f + 1/2)/2, -(a + b + f + 1/2)/2, 1/2 - b; (1 - mx)/(1 - m)]. \tag{97}$$

On using the solutions (95)–(97) it follows that for the potential $[a,1/2,1/2,1/2]$ one knows three QES mid-band energy eigenstates. In the special case when $a=2k+3/2$ these eigenstates are the mid-band QES eigenstates for the potential $[2k+3/2,1/2,1/2,1/2]$ where the sum of the four parameters characterizing the potential is an odd integer.

VII. SUMMARY AND OPEN QUESTIONS

In this paper, we have addressed many issues regarding GAL potentials with a number of choices for the parameters a, b, f, g. The most interesting case is when all four parameters are integers. This is a potential with a finite number of band gaps. We have been able to count the number of independent GAL potentials with a given number of band gaps and completely specify the nature of the band edge eigenfunctions. We have introduced the new concept of self-dual potentials which are not self-isospectral. We are also able to specify how many of the independent potentials with a given number of band gaps have supersymmetric partner potentials and how many have nonsupersymmetric partner potentials. Finally, using the results for the GAL potentials, we have shown that given any one periodic solution of Heun's equation, one can obtain four more periodic solutions.

We have also discussed several issues related with GAL potentials when one or more of the parameters take half-integer values. In particular, while nothing is known so far about GAL potentials when three of the parameters take half-integer values, we have been able to obtain the QES energy values for several of these potentials. Further, using these eigenvalues and the algebraic form of Heun's equation, we have also been able to obtain the corresponding eigenfunctions for potentials of the form $[a,1/2,f,g]$, $[a,b,1/2,g]$, $[a,b,f,1/2]$ where a, b, f, g are arbitrary numbers. The key point to make while addressing these questions is that the relations (6) and (7) are not only valid when the four parameters a, b, f, g are integers but also when one or more of these parameters take half-integer values. This in turn immediately implies that these relations are also valid when the four parameters a, b, f, g take arbitrary values so long as either their sum $a+b+f+g$ [or one or more of the combinations obtained by changing one or more of the param-

eters to $-a-1$, $-b-1$, $-f-1$, $-g-1$, respectively] is a nonnegative even integer. We have also conjectured that both relations (6) and (7) are simultaneously valid when a, b, f, g are integers and that the energy eigenvalues for the band edges of these potentials are the same as mid-band QES energy values of GAL potentials in which all four parameters are half-integers and their sum is an odd integer. Finally, using these results we have also shown that given a periodic solution of Heun's equation, one can immediately obtain three quasiperiodic solutions of the same equation.

This work raises several issues which we have not been able to address satisfactorily:

1. Can one explicitly write down all seven KdV equations of seventh order?
2. What are the QES eigenfunctions for GAL potentials when one or more of the parameters is half-integral ($\geqslant 3/2$) while the remaining parameters are arbitrary?
3. The problem when two of the four parameters are half-integers needs further study. In particular, it is still not clear how many QES energy eigenvalues can be obtained, in general, in that case.
4. When the sum of all the four parameters is an even integer, it is clear that the QES states correspond to band edges. However, a complete understanding is still lacking regarding the number of QES states for various values of a, b, f, g. Further, when the sum of the four parameters is an odd integer, the form of the QES eigenfunctions is not clear when the half-integer parameters are $>1/2$.

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A geometrical characterization of commutative positive operator valued measures

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We show that a POV measure F on the Borel σ-algebra of the reals $\mathcal{B}(\mathbb{R})$ is commutative if and only if there exists a PV measure E on $\mathcal{B}(\mathbb{R})$ and, for every λ in the spectrum of E, a probability measure $\gamma_{(\cdot)}(\lambda)$ on $\mathcal{B}(\mathbb{R})$ such that the effect $F(\Delta)$ coincides with $\gamma_\Delta(A)$, where A is the self-adjoint operator associated to E. The relevance of this result to the theory of the sharp reconstruction is analyzed.
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I. INTRODUCTION

POV (positive operator valued) measures have been used to define generalized observables in quantum mechanics,[1–8] and are a consequence of the probabilistic structure of quantum mechanics. Their introduction can also be justified by the analysis of some ideal experiments which show that there are physical events which cannot be described by projection operators.[6] POV measures were also used to generalize Mackey's imprimitivity theorem[8] and to study the problem of the joint measurement of incompatible observables.[9,10]

As shown in Refs. 1–3 there exists a one-to-one correspondence between POV measures and affine maps $S\mapsto\mu_S^F(\cdot)$ from the set of states $\mathcal{S}$ into the set of probability measures on $\mathcal{B}(\mathbb{R})$. Moreover, this correspondence is determined by the relation $\mu_S^F(\Delta)=\mathrm{Tr}[SF(\Delta)]$. This allows one to interpret the number

$$\mu_S^F(\Delta)=\mathrm{Tr}[SF(\Delta)]$$

as the probability that the outcomes of a measurement of the observable F (corresponding to a POV measure F) is in Δ when the physical system is in the state $S\in\mathcal{S}$. We recall that an analogous relation holds for standard observables $E:\mathcal{B}(\mathbb{R})\to\mathcal{E}(\mathcal{H})$, that is:

$$\mu_S^E(\Delta)=\mathrm{Tr}[SE(\Delta)].$$

Therefore POV measures are a generalization of the standard quantum observables and the problem of giving them a clear physical meaning should be dealt with. In order to address this problem several characterizations of commutative POV measures were found.[11–16]

In Ref. 13 it is proved that for each commutative POV measure F, there exists a unique Baire probability measure $\mu:\mathcal{P}(\mathbb{R},\mathcal{A}(F))\to[0,1]$ [defined on the space of all the PV measures with values in the commutative von Neumann algebra $\mathcal{A}(F)$ generated by the set $\{F(\Delta)\}_{\Delta\in\mathcal{B}(\mathbb{R})}$] such that $F(\Delta)=\int_{\mathcal{P}(X,\mathcal{A}(F))}E(\Delta)\mathrm{d}\mu(E)$.

Naimark theorem[16] establishes that every POV measure F in a Hilbert space $\mathcal{H}$ can be dilated to a PV measure E^+ in an extended Hilbert space $\mathcal{H}^+$ such that F is the projection of E^+ on $\mathcal{H}$.

In Refs. 11 and 12 it is shown that: if $F:\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ is a commutative POV measure, then there exists a unique PV measure $E:\mathcal{P}_\mathbb{R}\to\mathcal{E}(\mathcal{H})$, where $\mathcal{P}_\mathbb{R}$ is the space of the probability measures on $\mathcal{B}(\mathbb{R})$, such that

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$$F(\Delta) = \int_{\mathcal{P}_{\mathbb{R}}} p(\Delta) E(\mathrm{d}p). \tag{1}$$

Here we follow a different approach, which stems from Refs. 14 and 15. In these papers, the outcomes of the measurement of a commutative POV measure are interpreted as deriving from a stochastic diffusion of the outcomes of the measurement of a particular PV measure. The starting point of this approach is a theorem due to von Neumann, which states that for any given set $\{F_i\}_{i\in I}$ of commuting self-adjoint operators there exists a self-adjoint operator A and a family of measurable functions $f_i(\lambda)$ such that $f_i(A)=F_i$ (see Theorem 1 below). von Neumann's theorem implies that a POV measure F is commutative if and only if there exists a self-adjoint operator A (corresponding to a PV measure E) and a family of functions $\{\mu_\Delta\}_{\Delta\in\mathcal{B}(\mathbb{R})}$ such that $F(\Delta)=\mu_\Delta(A)$.

In Ref. 14, starting from a commutative POV measure with spectrum in $[0, 1]$, the authors constructed explicitly a self-adjoint operator A with spectrum $\sigma(A)\subset[0,1]$ and, for every set $\Delta \in \mathcal{B}([0,1])$, a measurable function $\omega_\Delta(\lambda):\sigma(A)\to[0,1]$ such that $F(\Delta)=\omega_\Delta(A)$. Their construction uses a procedure analogous to the one used by Riesz and Nagy to prove von Neumann's theorem (see Ref. 21, Sec. 130).

In Ref. 15 it was shown that, for every real number λ, the application $\omega_{(\cdot)}(\lambda):\mathcal{B}([0,1]) \to[0,1]$, corresponding to the family of functions $\{\omega_\Delta(\lambda)\}_{\Delta\in\mathcal{B}([0,1])}$, defines an *additive* set function on a particular ring $\mathcal{R}(\mathcal{S})$ which generates $\mathcal{B}([0,1])$.

This result suggests to interpret the outcomes of the measurement of F as deriving from a randomization of the outcomes of the measurement of E. Indeed let us consider a pure state $S=P_\psi$. From $F(\Delta)=\omega_\Delta(A)$ we get

$$\mu_S^F(\Delta) = \int w_\Delta(\lambda)\|E((\lambda-\mathrm{d}\lambda,\lambda])\psi\|^2 = \int w_\Delta(\lambda)\mathrm{d}\mu_S^E, \tag{2}$$

where E is the PV measure corresponding to the operator A.

This relation shows that $w_\Delta(\lambda)$ could be interpreted, quoting from Ref. 15, "*as the probability that the outcome* λ *of* E *turns into an outcome in* Δ *for* F." The physical source of randomization could be the imprecision of the measuring apparatus, or some other cause.

The above interpretation is satisfactory if the application $\omega_{(\cdot)}(\lambda)$ is σ-additive on $\mathcal{B}([0,1])$. However, the problem of the σ-additivity of $\omega_{(\cdot)}(\lambda)$ was left open by the authors.

In this paper we follow a novel approach and give a general geometrical characterization of POV measures, without using constructive procedures. Specifically, we show that a POV measure $F:\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ is commutative if and only if there exists a PV measure $E:\mathcal{B}(\mathbb{R})\to\mathcal{E}(\mathcal{H})$ (corresponding to a self-adjoint operator A) and, for every $\lambda\in\sigma(A)$, a *probability measure* $\gamma_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ such that $F(\Delta)=\gamma_\Delta(A)$ (see Theorem 2). This result is founded on the ground of von Neumann's theorem. Its relevance to the interpretation of the commutative POV measures proposed in Refs. 14 and 15 is that, repeating the reasoning used to get Eq. (2), we get

$$\mu_S^F(\Delta) = \int \gamma_\Delta(\lambda)\mathrm{d}\mu_S^E$$

so that the sharp reconstruction E and the POV measure F are related by a probability measure.

It is worth mentioning that this result is close to the one obtained by Holevo[11,12] but, at variance with Theorem 2, the PV measure in (1) is not defined on $\mathcal{B}(\mathbb{R})$ but on the space of the probability measures on $\mathcal{B}(\mathbb{R})$. It would be interesting to check if there are relationships between the two characterizations.

The paper is organized as follows. In Sec. II we give some basic definitions and state the classical von Neumann's theorem. Then, in Sec. III, we prove the main result of the paper, Theorem 2. In Sec. IV we prove Proposition 2 which will be used in the last section where we discuss the relevance of Theorem 2 to the theory of the sharp reconstruction. In the appendices we give some technical results which are used in the paper.

II. PRELIMINARIES

In this section we fix the basic notation and terminology, and state von Neumann's theorem, which will be the starting point of the paper.

We denote by $\mathcal{B}(\mathbb{R})$ the Borel σ-algebra of $\mathbb{R}$, and by $\mathcal{F}(\mathcal{H})$ the space of bounded, positive self-adjoint operators acting on the Hilbert space $\mathcal{H}$. A POV measure is defined as follows:

Definition 1: A POV (positive operator valued) measure is a mapping $F:\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ *such that:*

1. $F(\Delta)\geqslant 0$ *for all* $\Delta\in\mathcal{B}(\mathbb{R})$*;*
2. *if* $\{\Delta_n\}$ *is a countable family of disjoint sets in* $\mathcal{B}(\mathbb{R})$ *then*

$$F\left(\bigcup_{n=1}^{\infty}\Delta_n\right)=\sum_{n=1}^{\infty}F(\Delta_n),$$

where the series converges in the weak operator topology;
The POV measure is said to be normalized if one has also

3. $F(\mathbb{R})=1$.

Definition 2: A PV (projection valued) measure is a normalized POV measure which is orthogonal, that is, such that

4. $F(\Delta_1)F(\Delta_2)=0$ *if* $\Delta_1\cap\Delta_2=\emptyset$.

If this is the case we have $F(\Delta)=F(\Delta)^2$. Then, $F(\Delta)$ is a projection operator for every $\Delta\in\mathcal{B}(\mathbb{R})$ and the PV measure is denoted by $E:\mathcal{B}(\mathbb{R})\to\mathcal{E}(\mathcal{H})$, where $\mathcal{E}(\mathcal{H})$ is the space of all the projection operators of the Hilbert space $\mathcal{H}$. We recall that to each PV measure it is possible to associate a measure $\langle E(\Delta)x,x\rangle$ for every $x\in\mathcal{H}$.

Definition 3: A POV measure F is said to be commutative if the following relations are valid:

$$[F(\Delta_1),F(\Delta_2)]=0;\quad \forall\,\Delta_1,\Delta_2\in\mathcal{B}(\mathbb{R}).$$

We recall that PV measures are also named *sharp* or *standard* observables and, by the spectral theorem,[17] they are in a one to one correspondence with the self-adjoint operators, while nonorthogonal normalized POV measures are also named *unsharp* observables.

In what follows we shall always refer to normalized POV measures defined on $\mathcal{B}(\mathbb{R})$.

Next we proceed to define the spectrum of a POV measure.

Definition 4, see Ref. 18: Given a POV measure F we define the co-spectrum of F as the open set

$$\rho(F)=\cup\{\Delta:\Delta\ \textit{is open},\ F(\Delta)=0\}$$

and the spectrum $\sigma(F)$ *of F as the complement of* $\rho(F)$.

The spectrum of a POV measure is characterized by the following proposition:

Proposition 1: The spectrum $\sigma(F)$ of *F is closed and coincides with the set* $\{\lambda\in\mathbb{R}:\forall\,\delta>0,F((\lambda-\delta,\lambda+\delta))\neq 0\}$.

Proof: Let us suppose $\lambda\in\sigma(F)$. Then, $\lambda\notin\rho(F)$ and $F(\Delta)\neq\mathbf{0}$ for every open set Δ. In particular,

$$F((\lambda-\delta,\lambda+\delta))\neq 0$$

for every $\delta>0$. On the converse, let us suppose that λ is so that $F((\lambda-\delta,\lambda+\delta))\neq 0$ for every $\delta>0$. For every open set Δ containing λ it must exist a number $\delta>0$ such that the open interval $(\lambda-\delta,\lambda+\delta)$ is contained in Δ. By items 1 and 2 of definition 1 we get

$$0<F((\lambda-\delta,\lambda+\delta))\leqslant F(\Delta)$$

then, $\lambda\notin\rho(F)$, hence $\lambda\in\sigma(F)$. □

We shall use the term "measurable" for the Borel measurable functions and consider the class $\mathcal{M}([0,1])$ of measurable functions defined on $[0, 1]$ which are bounded or are equal almost everywhere (a.e.), with respect to a PV measure E, to a bounded measurable function. Thus $\mathcal{M}([0,1])$ is the set of functions such that

$$E\text{-ess}\sup_{t\in[0,1]}|f(t)| = \inf_{E(\Delta)=I_{t\in\Delta}}\sup|f(t)| < +\infty.$$

The norm in $\mathcal{M}([0,1])$ is $\|f\|=E-\text{ess}\sup_{t\in[0,1]}|f(t)|$. Moreover we shall always consider equivalence classes of measurable functions. We say that two functions f and g are equivalent if $f=g$ a.e. with respect to a PV measure E, that is a.e. with respect to all the measures $\langle E(\Delta)x,x\rangle$, where x runs through all the vectors of the space $\mathcal{H}$.

As it is well known,[17,22] if a measurable function f is defined on the spectrum $\sigma(A)$ of a self-adjoint operator A, one has $f(A)=\int f(\lambda)E((\lambda-\mathrm{d}\lambda,\lambda])$ where E is the PV measure corresponding to A.

We shall denote by **0** and **1** the null and the identity operators, respectively.

Theorem 1 (von Neumann[19–21]): *For any family $\{F_i\}_{i\in\mathcal{I}}$ of self-adjoint operators acting on a Hilbert space $\mathcal{H}$ such that $[F_i,F_j]=\mathbf{0}$ for all $i,j\in\mathcal{I}$, there exist*

a) a bounded self-adjoint operator A;
b) a family of measurable functions $\{f_i:\mathbb{R}\to R\}_{i\in\mathcal{I}}$ such that for every $i\in\mathcal{I}$,

$$F_i = f_i(A) = \int_{-\infty}^{\infty} f_i(\lambda)E((\lambda - d\lambda,\lambda]) = \int_{-\infty}^{\infty} f_i(\lambda)\mathrm{d}E_\lambda$$

where E is the PV measure corresponding to A.

It follows that an unsharp observable $F:\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ is commutative if and only if there exist:[14]

- *a sharp observable $E:\mathcal{B}(\mathbb{R})\to\mathcal{E}(\mathcal{H})$ (which corresponds to a self-adjoint operator $\mathbf{0}<A<\mathbf{1}$),*
- *a family of set functions*

$$\omega_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1],\quad \Delta\mapsto\omega_\Delta(\lambda),\quad \lambda\in\sigma(A)$$

such that $F(\Delta)=\omega_\Delta(A)$.

Indeed the family $\{F(\Delta),\Delta\in\mathcal{B}(\mathbb{R})\}$ is a commutative family of bounded positive operators and von Neumann's theorem can be applied. Conversely, if a self-adjoint operator A exists such that all the operators $F(\Delta)$ are functions of A, then the family $\{F(\Delta),\Delta\in\mathcal{B}(\mathbb{R})\}$ is commutative (see Ref. 19, theorem 2, Sec. 75).

In what follows whenever a POV measure F, a self-adjoint operator A and an application $\mu_{(\cdot)}(\lambda)$ are such that $F(\Delta)=\mu_\Delta(A)$ we shall say that the triple $(F,A,\mu_{(\cdot)}(\lambda))$ satisfies the thesis of von Neumann's theorem.

III. A CHARACTERIZATION OF COMMUTATIVE POV MEASURES

Let us consider a family of functions $\mathcal{F}=\{\mu_\Delta(\lambda):[0,1]\to[0,1]\}_{\Delta\in\mathcal{B}(\mathbb{R})}$ and the corresponding family of set functions $\mathcal{F}_S=\{\mu_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1],\lambda\in\sigma(A)\}$ and assume that the triple $(F,A,\mu_{(\cdot)}(\lambda))$ satisfies the thesis of von Neumann's theorem. The aim of the present section is to show that the family of functions $\{\mu_\Delta(\lambda):[0,1]\to[0,1]\}_{\Delta\in\mathcal{B}(\mathbb{R})}$ can always be chosen in such a way that the corresponding set functions $\mu_{(\cdot)}(\lambda)\in\mathcal{F}_S$ are probability measures.

Theorem 2 (Main result): *A normalized POV measure $F:\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ is commutative if and only if there exist an application $\mu_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ and a PV measure $E:\mathcal{B}(\mathbb{R})\to\mathcal{E}(\mathcal{H})$ such that:*

1. *the application* $\mu_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\rightarrow[0,1]$ *is a probability measure for every* $\lambda\in\sigma(A)$*;*
2. $F(\Delta)=\mu_{\Delta}(A)=\int\mu_{\Delta}(\lambda)E((\lambda-\mathrm{d}\lambda,\lambda])$*,*

where A is the self-adjoint operator associated to the PV measure E.

To prove this theorem we need two lemmas:

Lemma 1: For any commutative POV measure F, it is possible to find a couple $(A,\omega_{(\cdot)}(\lambda))$ *such that the triple* $(F,A,\omega_{(\cdot)}(\lambda))$ *satisfies the thesis of von Neumann theorem and* $\omega_{(\cdot)}(\lambda)$ *is additive on an appropriate ring which generates the Borel* σ*-algebra* $\mathcal{B}(\mathbb{R})$.

Proof: Following Ref. 14 we shall consider, without loss of generality, POV measures with a bounded spectrum contained in [0, 1] so that $\Delta\in\mathcal{B}([0,1])$ (see Appendix A). To prove the lemma let us consider a family of set functions

$$\gamma_{(\cdot)}(\lambda):\mathcal{B}([0,1])\rightarrow[0,1],\quad \Delta\mapsto\mu_{\Delta}(\lambda),\quad \lambda\in\sigma(A)$$

such that the triple $(F,A,\gamma_{(\cdot)}(\lambda))$ satisfies the thesis of von Neumann's theorem. We have that $\gamma_{[0,1]}(A)=\mathbf{1}$. Moreover the function $\omega_{[0,1]}(\lambda):=1$ is such that $\omega_{[0,1]}(A)=F([0,1])$ so that we can replace $\gamma_{[0,1]}(\lambda)$ with $\omega_{[0,1]}(\lambda)$.

We proceed by showing that it is possible to replace the functions $\gamma_{[0,1/2]}(\lambda)$ and $\gamma_{(1/2,1]}(\lambda)$ with two measurable functions $\omega_{[0,1/2]}(\lambda)$ and $\omega_{(1/2,1]}(\lambda)$ such that:

1) $\omega_{[0,1/2]}(\lambda)+\omega_{(1/2,1]}(\lambda)=\omega_{[0,1]}(\lambda)$ for all λ;
2) $\omega_{[0,1/2]}(A)=F([0,1/2])$ and $\omega_{(1/2,1]}(A)=F((1/2,1])$.

We have

$$\int\omega_{[0,1]}(\lambda)\mathrm{d}E_{\lambda}=F([0,1])=F([0,1/2])+F((1/2,1])$$

$$=\int\gamma_{[0,1/2]}(\lambda)\mathrm{d}E_{\lambda}+\int\gamma_{(1/2,1]}(\lambda)\mathrm{d}E_{\lambda}=\int[\gamma_{[0,1/2]}(\lambda)+\gamma_{(1/2,1]}(\lambda)]\mathrm{d}E_{\lambda}$$

so that, by Ref. 22, Corollary 9 (see also Ref. 21, Chap. IX),

$$\gamma_{[0,1/2]}(\lambda)+\gamma_{(1/2,1]}(\lambda)=\omega_{[0,1]}(\lambda)\ \text{a.e. with respect to } E.$$

By setting

$$\omega_{(1/2,1]}(\lambda)=\omega_{[0,1]}(\lambda)-\gamma_{[0,1/2]}(\lambda)$$

$$\omega_{[0,1/2]}(\lambda)=\gamma_{[0,1/2]}(\lambda)$$

we get two measurable functions $\omega_{[0,1/2]}(\lambda)$ and $\omega_{(1/2,1]}(\lambda)$ such that items 1) and 2) are satisfied and which differ from functions $\gamma_{[0,1/2]}(\lambda)$ and $\gamma_{(1/2,1]}(\lambda)$ only in a set of zero E-measure.

We proceed by showing that it is possible to replace the functions $\gamma_{[0,1/4]}(\lambda)$ and $\gamma_{(1/4,1/2]}(\lambda)$ with two measurable functions $\omega_{[0,1/4]}(\lambda)$ and $\omega_{(1/4,1/2]}(\lambda)$ such that:

1′) $\omega_{[0,1/4]}(\lambda)+\omega_{(1/4,1/2]}(\lambda)=\omega_{[0,1/2]}(\lambda)$ for all λ;
2′) $\omega_{[0,1/4]}(A)=F([0,1/4])$ and $\omega_{(1/4,1/2]}(A)=F((1/4,1/2])$.

We have

$$\int \omega_{[0,1/2]}(\lambda)\mathrm{d}E_\lambda = F([0,1/2]) = F([0,1/4]) + F((1/4,1/2])$$

$$= \int \gamma_{[0,1/4]}(\lambda)\mathrm{d}E_\lambda + \int \gamma_{(1/4,1/2]}(\lambda)\mathrm{d}E_\lambda = \int [\gamma_{[0,1/4]}(\lambda) + \gamma_{(1/4,1/2]}(\lambda)]\mathrm{d}E_\lambda,$$

so that

$$\gamma_{[0,1/4]}(\lambda) + \gamma_{(1/4,1/2]}(\lambda) = \omega_{[0,1/2]}(\lambda) \text{ a.e. with respect to } E.$$

Let us consider the set $N \subset [0,1]$ such that $\gamma_{[0,1/4]}(\lambda) > \omega_{[0,1/2]}(\lambda)$. Since N is a null set, there exists a Borel set $\bar{\Delta}$ such that $N \subset \bar{\Delta}$ and $E(\bar{\Delta})=0$. Now we define the function

$$\bar{\gamma}_{[0,1/4]}(\lambda) := \begin{cases} \gamma_{[0,1/4]}(\lambda) & \text{if } \lambda \notin \bar{\Delta} \\ 0 & \text{if } \lambda \in \bar{\Delta}, \end{cases}$$

which is less than or equal to $\omega_{[0,1/2]}(\lambda)$. Moreover $\bar{\gamma}_{[0,1/4]}(\lambda)$ is measurable. Indeed by the measurability of $\gamma_{[0,1/4]}(\lambda)$ we have that, for every $x \in [0,1]$,

$$\{\lambda \in [0,1] | \bar{\gamma}_{[0,1/4]}(\lambda) \leqslant x\} = \{\lambda \in [0,1] \setminus \bar{\Delta} | \gamma_{[0,1/4]}(\lambda) \leqslant x\} \cup \bar{\Delta}$$

$$= [\{\lambda \in [0,1] | \gamma_{[0,1/4]}(\lambda) \leqslant x\} \cap \{[0,1] \setminus \bar{\Delta}\}] \cup \bar{\Delta} \in \mathcal{B}([0,1]).$$

By setting

$$\omega_{[0,1/4]}(\lambda) = \bar{\gamma}_{[0,1/4]}(\lambda),$$

$$\omega_{(1/4,1/2]}(\lambda) = \omega_{[0,1/2]}(\lambda) - \bar{\gamma}_{[0,1/4]}(\lambda),$$

we get two functions such that items 1′) and 2′) are satisfied and which differ from the functions $\gamma_{[0,1/4]}(\lambda)$ and $\gamma_{(1/4,1/2]}(\lambda)$ only in a set of zero E-measure.

Analogously, starting from the functions $\gamma_{(1/2,3/4]}(\lambda)$ and $\gamma_{(3/4,1]}(\lambda)$, we can define two measurable functions $\omega_{(1/2,3/4]}(\lambda)$ and $\omega_{(3/4,1]}(\lambda)$ such that

1″) $\omega_{(1/2,3/4]}(\lambda) + \omega_{(3/4,1]}(\lambda) = \omega_{(1/2,1]}(\lambda)$;

2″) $\omega_{(1/2,3/4]}(A) = F((1/2,3/4])$, and $\omega_{(3/4,1]}(A) = F((3/4,1])$.

Iterating the procedure we shall finally obtain a family of functions $\{\omega_\Delta(\lambda):[0,1] \to [0,1]\}_{\Delta \in \mathcal{S}}$ where $\mathcal{S}$ is the semi-ring:

$$\mathcal{S} = \{[0,1/2^{n-1}], (k/2^{n-1}, k+1/2^{n-1}]], k = 1,2,\ldots,2^{n-1}-1, n \in \mathbb{N}\}.$$

Moreover, for every given λ, the set function $\omega_{(\cdot)}(\lambda):\mathcal{S} \to [0,1]$ is additive on the semi-ring $\mathcal{S}$.

Now, for any λ, it is possible to extend $\omega_{(\cdot)}(\lambda):\mathcal{S} \to [0,1]$ to the ring $\mathcal{R}(\mathcal{S})$ generated by $\mathcal{S}$. The extension $\omega_{(\cdot)}(\lambda):\mathcal{R}(\mathcal{S}) \to [0,1]$ is an additive set function on $\mathcal{R}(\mathcal{S})$ such that $\omega_\Delta(A) = F(\Delta)$ (see Ref. 24). □

The following lemma concerns the definition and the monotonicity property of $\omega_{[0,t)}(\lambda)$ as a function of t. In particular it will be proved that $\omega_{[0,t)}(\lambda)$ is nondecreasing with respect to t and such that $\omega_{[0,t)}(A) = F[0,t)$.

In order to define $\omega_{[0,t)}(\lambda)$ we use the fact that it is always possible to decompose $[0,t)$ into the union of a disjoint sequence of intervals from $\mathcal{S}$.

Definition 5: For every $t \in (0,1]$ *we define* $\omega_{[0,t)}(\lambda) = \Sigma_{j=1}^{\infty} \omega_{\Delta_j}(\lambda)$ *where* $\{\Delta_j : \Delta_j \in \mathcal{S}\}_{j \in \mathbb{N}}$ *is a decomposition of the interval* $[0,t)$ *with the following property: for every* $x \in (0,t)$ *there is a closed interval* $[0,a]$: $a \geqslant x$ *such that* $[0,a] = \cup_{j=1}^{n} \Delta_j$. *The set of the decompositions so defined is denoted by* $\mathcal{D}$.

The series $\Sigma_{j=1}^{\infty}\omega_{\Delta_j}(\lambda)$ used to define the function $\omega_{[0,t)}(\lambda)$ is convergent. Indeed for every $p \in \mathbb{N}$, $\cup_{j=1}^{p}\Delta_j \subset [0,t) \subset [0,1]$ and then, using the additivity of the measure on $\mathcal{R}(\mathcal{S})$, $\Sigma_{j=1}^{p}\omega_{\Delta_j}(\lambda) \leqslant \omega_{[0,1]}$. Moreover, as shown in Appendix B, $\omega_{[0,t)}(\lambda)$ is well defined.

Lemma 2. The set function $\omega_{[0,t)}(\lambda)$, *is nondecreasing with respect to* t *and* $\omega_{[0,t)}(A) = F([0,t))$.

Proof. Let us consider the two intervals $[0,t)$ and $[0,t')$ where $t<t'$ and let us decompose them as $\{\Delta_k;\Delta_k \in \mathcal{S}\}_{k\in\mathbb{N}}$ and $\{\Delta'_k;\Delta'_k \in \mathcal{S}\}_{k\in\mathbb{N}}$, respectively. Following Definition 5 it is possible to find $m \in \mathbb{N}$ so that

$$[0,t) \subset [0,b] = \bigcup_{k=1}^{m}\Delta'_k \subset [0,t'),$$

with $[0,b] \in \mathcal{R}(\mathcal{S})$. We can write:

$$[0,t') = \left[\bigcup_{k=1}^{m}\Delta'_k\right] \cup \left[\bigcup_{k=m+1}^{\infty}\Delta'_k\right].$$

By the additivity of $\omega_{(\cdot)}(\lambda)$ on $\mathcal{R}(\mathcal{S})$ we get:

$$\omega_{[0,t')}(\lambda) = \sum_{k=1}^{m}\omega_{\Delta'_k}(\lambda) + \sum_{k=m+1}^{\infty}\omega_{\Delta'_k}(\lambda) = \omega_{[0,b]}(\lambda) + \sum_{k=m+1}^{\infty}\omega_{\Delta'_k}(\lambda) \geqslant \omega_{[0,b)}(\lambda).$$

Using again the additivity of the measure and the relation

$$\bigcup_{k=1}^{p}\Delta_k \subset \bigcup_{k=1}^{\infty}\Delta_k = [0,t) \subset [0,b]; \quad \forall\, p \in \mathbb{N},$$

we finally have

$$\omega_{(\cup_{k=1}^{p}\Delta_k)}(\lambda) \leqslant \omega_{[0,b]}(\lambda), \quad \forall\, p \in \mathbb{N},$$

$$\omega_{[0,b]}(\lambda) \geqslant \omega_{[0,t)}(\lambda),$$

which ends the proof of the first part of the proposition. The second assertion is proved as follows: $F([0,t)) = F(\cup_j\Delta_j) = \Sigma_j F(\Delta_j) = \Sigma_j \int \omega_{\Delta_j}(\lambda)dE_\lambda$ and, by Theorem VII.2.d in Ref. 17, we get

$$F([0,t)) = \int \sum_j \omega_{\Delta_j}(\lambda)\mathrm{d}E_\lambda = \omega_{[0,t)}(A).$$

□

Now we are ready to prove the main theorem of this paper.

Proof of Theorem 2. Let $(F,A,\omega_{(\cdot)}(\lambda))$ satisfy the thesis of von Neumann's theorem. By Lemma 1, the family of set functions $\{\omega_{(\cdot)}(\lambda), \lambda \in \sigma(A)\}$ can be chosen in such a way that, for each $\lambda \in \sigma(A)$, $\omega_{(\cdot)}(\lambda)$ is an additive set function. Moreover, Lemma 2 allows us to define a function $\omega_{[0,t)}(\lambda)$ which is nondecreasing with respect to t and such that $\omega_{[0,t)}(A) = F([0,t))$.

Now, starting from $\omega_t := \omega_{[0,t)}(\lambda)$, it is possible to define a distribution function $\mu_t(\lambda)$ continuous from the left as follows:

$$\mu_t(\lambda) = \begin{cases} \omega_{t^-}(\lambda) & \text{if } 0 < t \leqslant 1 \\ 0 & \text{if } t \leqslant 0 \\ 1 & \text{if } t > 1, \end{cases}$$

where $\omega_{t^-}(\lambda) = \lim_{x\to t^-}\omega_{[0,t)}(\lambda)$.

In its turn, for every λ, starting from the left continuous function $\mu_t(\lambda)$ it is possible to define the set function $\mu_{[a,b)}(\lambda)=\mu_b-\mu_a$, $[a,b)\subset(-\infty,\infty)$ which can be extended to a σ-additive probability measure (see Ref. 23, p. 97) $\mu_{(.)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ such that

$$\mu_\Delta(\lambda)=0 \quad \text{if } \Delta\cap[0,1]=\emptyset.$$

We want to prove that:

$$\mu_t(A)=F([0,1]\cap(-\infty,t)) \tag{3}$$

and that the probability measure $\mu_{(.)}(\lambda):\mathcal{B}([0,1])\to[0,1]$, which is the restriction of $\mu_{(.)}\times(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ to $\mathcal{B}([0,1])$, is such that

$$\mu_\Delta(A)=F(\Delta), \quad \Delta\in\mathcal{B}([0,1]). \tag{4}$$

First we prove (3). If $t\in(0,1]$, we have:

$$\mu_t(A)=\int\mu_t(\lambda)\mathrm{d}E_\lambda=\int[\lim_{x\to t^-}\omega_x(\lambda)]\mathrm{d}E_\lambda.$$

Notice that the integral exists thanks to the measurability of $\mu_t(\lambda)$ as a function of λ (see Remark 2 below). Let us consider a sequence $\{x_n\}$ such that $x_n\to t$ from the left. We have $\mu_t(A)=\int[\lim_{x\to t^-}\omega_x(\lambda)]\mathrm{d}E_\lambda=\int[\lim_{n\to\infty}\omega_{x_n}(\lambda)]\mathrm{d}E_\lambda$. By the continuity of F and theorem 11 in Ref. 18 we get

$$\mu_t(A)=\int[\lim_{n\to\infty}\omega_{x_n}(\lambda)]\mathrm{d}E_\lambda=\lim_{n\to\infty}\int\omega_{x_n}(\lambda)\mathrm{d}E_\lambda=\lim_{n\to\infty}F([0,x_n))=F([0,t))=F([0,1]\cap(-\infty,t)).$$

Moreover, if $t\leqslant 0$ then $\mu_t(A)=\mathbf{0}=F(\emptyset)=F([0,1]\cap(-\infty,t))$, while, if $t>1$ then $\mu_t(A)=\mathbf{1}=F([0,1])=F([0,1]\cap(-\infty,t))$.

It remains to prove that the probability measure $\mu_{(.)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ generated by $\mu_t(\lambda)$ is such that $\mu_\Delta(A)=F(\Delta)$, $\Delta\in\mathcal{B}([0,1])$. Let us consider the POV measure $F':\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ such that $F'(\Delta)=F(\Delta\cap[0,1])$. Notice that F is the restriction of F' to $\mathcal{B}([0,1])$ and $F'(\Delta)=\mathbf{0}$ if $\Delta\cap[0,1]=\emptyset$.

As a consequence of (3),

$$\begin{aligned}F'([t,\bar{t}))&=F'((-\infty,\bar{t}))-F'((-\infty,t))=F([0,1]\cap(-\infty,\bar{t}))-F([0,1]\cap(-\infty,t))\\&=\mu_{\bar{t}}(A)-\mu_t(A)=\mu_{[t,\bar{t})}(A)\end{aligned}$$

so that $F'(\Delta)=\mu_\Delta(A)$ for every set Δ in the ring $\mathcal{P}$ generated by sets of the kind $[t,\bar{t})\subset(-\infty,\infty)$. Moreover by the uniqueness of the extensions of $F':\mathcal{P}\to\mathcal{F}(\mathcal{H})$ to the σ-algebra $\mathcal{B}(\mathbb{R})$ (see Ref. 18, theorem 7), it follows that the probability measure $\mu_{(.)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ generated by the distribution function $\mu_t(\lambda)$ and the POV measure $F':\mathcal{B}(\mathbb{R})\to\mathcal{F}(\mathcal{H})$ are such that $F'(\Delta)=\mu_\Delta(A)$ for every $\Delta\in\mathcal{B}(\mathbb{R})$, hence $\mu_\Delta(A)=F(\Delta)$ for every $\Delta\in\mathcal{B}([0,1])$. □

Remark 1: The argument used to prove Theorem 2, applies to every pair $(B,\omega^B_{(.)}(\lambda))$ *such that the triple* $(F,B,\omega^B_{(.)}(\lambda))$ *satisfies the thesis of von Neumann's theorem. Therefore we can state the following corollary:*

Corollary 1: If the triple $(F,B,\omega^B_{(.)}(\lambda))$ *satisfies the thesis of von Neumann theorem then there exists a probability measure* $\mu^B_{(.)}(\lambda)$, *equivalent to* $\omega^B_{(.)}(\lambda)$ (*that is, for every* $\Delta\in\mathcal{B}([0,1])$, $\mu^B_\Delta(\lambda)=\omega^B_\Delta(\lambda)$ *a.e.*), *such that the triple* $(F,B,\mu^B_{(.)}(\lambda))$ *satisfies the thesis of von Neumann's theorem.*

Remark 2: The function $\mu_t(\cdot)$ *defined in the proof of Theorem 2 is measurable because it is the limit of a monotone sequence of measurable functions.*[17,23–25] *Indeed, for each* λ, *the function* $\omega_x(\lambda)$ *is bounded and nondecreasing with respect to* x, *then the limit* $\omega_{t^-}(\lambda)$ *exists and we have*

$\mu_t(\lambda)=\omega_{t^-}(\lambda)=\lim_{x\to t^-}\omega_x(\lambda)=\lim_{n\to\infty}\omega_{x_n}(\lambda)$ *where* $\{x_n\}$ *is an increasing sequence of numbers such that* $x_n\to t$ *from the left.*

IV. A NECESSARY AND SUFFICIENT CONDITION FOR THE σ-ADDITIVITY OF $\omega_{(\cdot)}(\lambda)$

In the proof of Theorem 2 we started from the *additive* set function $\omega_{(\cdot)}(\lambda):\mathcal{R}(\mathcal{S})\to[0,1]$ such that $\omega_\Delta(A)=F(\Delta)$, $\Delta\in\mathcal{R}(\mathcal{S})$ and proved the existence of a probability measure $\mu_{(\cdot)}(\lambda):\mathcal{B}([0,1])\to[0,1]$ such that the triple $(F,A,\mu_{(\cdot)}(\lambda))$ satisfies the thesis of von Neumann's theorem. Clearly, if $\omega_{(\cdot)}(\lambda):\mathcal{R}(\mathcal{S})\to[0,1]$ were σ-additive on $\mathcal{R}(\mathcal{S})$ it could be directly extended to a probability measure $\mu_{(\cdot)}(\lambda)$ on $\mathcal{B}([0,1])$ such that $\mu_\Delta(A)=F(\Delta)$. Now we want to show that the additive set function $\omega_{(\cdot)}(\lambda):\mathcal{R}(\mathcal{S})\to[0,1]$ is σ-additive if and only if $\omega_\Delta(\lambda)=\mu_\Delta(\lambda)$ for every $\Delta\in\mathcal{R}(\mathcal{S})$.

Proposition 2: The additive set function $\omega_{(\cdot)}(\lambda):\mathcal{R}(\mathcal{S})\to[0,1]$ *is* σ*-additive on* $\mathcal{R}(\mathcal{S})$ *if and only if* $\omega_\Delta(\lambda)=\mu_\Delta(\lambda)$ *for every* $\Delta\in\mathcal{R}(\mathcal{S})$, *where* $\mu_{(\cdot)}(\lambda)$ *is the probability measure introduced in the proof of Theorem 2.*

Proof: Let us assume that, for any λ, $\omega_{(\cdot)}(\lambda)$ is σ-additive on the ring $\mathcal{R}(\mathcal{S})$. Then, by Caratheodory theorem (see Ref. 24 p. 88, and Ref. 25), it can be uniquely extended to a σ-additive measure $\nu_{(\cdot)}(\lambda)$ on $\mathcal{B}([0,1])$. Now, we can define (see Theorem 4.8 of Ref. 24 and p. 88 of Ref. 23), a distribution function continuous from the left (see Definition 9 in Appendix D) as follows:

$$\nu_t(\lambda)=\begin{cases}\nu_{([0,t))}(\lambda) & t\in(0,1]\\ 1 & t>1\\ 0 & t\leqslant 0.\end{cases}$$

By Theorem 4 in Appendix D, it follows that the measure $\nu_{(\cdot)}(\lambda):\mathcal{B}(\mathbb{R})\to[0,1]$ generated by $\nu_t(\lambda)$ coincides with $\nu_{(\cdot)}(\lambda):\mathcal{B}([0,1])\to[0,1]$ on $\mathcal{B}([0,1])$ so that it is an extension of $\omega_{(\cdot)}(\lambda)$ to $\mathcal{B}(\mathbb{R})$. Moreover $\nu_\Delta(\lambda)=0$ if $\Delta\cap[0,1]=\emptyset$. Therefore, by the σ-additivity of the measure and by Definition 5, we have

$$\nu_{[0,t)}(\lambda)=\sum_{k=1}^{\infty}\nu_{\Delta_k}(\lambda)=\sum_{k=1}^{\infty}\omega_{\Delta_k}(\lambda)$$

for every decomposition

$$\cup_k\Delta_k=[0,t),\quad \Delta_k\in\mathcal{S}.$$

Hence,

$$\omega_{[0,t)}(\lambda)=\nu_{[0,t)}(\lambda),\quad t\in(0,1]$$

and $\omega_{[0,t)}(\lambda)$ is continuous from the left in (0,1]. Therefore we get

$$\nu_t(\lambda)=\mu_t(\lambda)=\begin{cases}\omega_{([0,t))}(\lambda) & t\in(0,1]\\ 1 & t>1\\ 0 & t\leqslant 0,\end{cases}\tag{5}$$

which means that the probability measure $\mu_{(\cdot)}(\lambda)$ corresponding to $\mu_t(\lambda)$ coincides with the probability measure $\nu_{(\cdot)}(\lambda)$ corresponding to $\nu_t(\lambda)$. Hence, $\mu_\Delta(\lambda)=\nu_\Delta(\lambda)=\omega_\Delta(\lambda)$ on $\mathcal{R}(\mathcal{S})$. The converse is obvious because if it were $\mu_\Delta(\lambda)=\omega_\Delta(\lambda)$ for every $\Delta\in\mathcal{R}(\mathcal{S})$, then $\omega_{(\cdot)}(\lambda)$ would be σ-additive on $\mathcal{R}(\mathcal{S})$. □

V. SHARP RECONSTRUCTION AND UNIQUENESS OF THE CHARACTERIZATION

This section is devoted to the analysis of the implications of Theorem 2 to the theory of the sharp reconstruction. Moreover we show (Theorem 3) that the result obtained in Ref. 15 implies the uniqueness (in a sense specified below) of the characterization in Theorem 2.

In Ref. 14, starting from a commutative POV measure F, the authors constructed a PV measure E (corresponding to a self-adjoint operator A) called the sharp reconstruction of F, and an application $\omega_{(.)}(\lambda):\mathcal{B}([0,1])\rightarrow[0,1]$ which connects A and F by means of relation $\omega_{\Delta}(A)=F(\Delta)$, proving that the triple $(F,A,\omega_{(.)}(\lambda))$ satisfies the thesis of von Neumann's theorem. In Ref. 15 it was proven that for every given $\lambda\in\sigma(A)$ the set function $\omega_{(.)}(\lambda)$ is *additive* on $\mathcal{R}(S)$. By Corollary 1 it follows that, for every given $\lambda\in\sigma(A)$, there exists a probability measure $\mu_{(.)}(\lambda):\mathcal{B}([0,1])\rightarrow[0,1]$ such that the triple $(F,A,\mu_{(.)}(\lambda))$ satisfies the thesis of von Neumann's theorem. Indeed, thanks to the additivity of $\omega_{(.)}(\lambda)$ on $\mathcal{R}(S)$, it is sufficient to apply the reasoning in the proof of Theorem 2 to the functions $\omega_{\Delta}(\lambda)$, $\Delta\in\mathcal{R}(S)$.

Moreover, by proposition 2, $\omega_{(.)}(\lambda)$ is σ-additive on $\mathcal{R}(S)$ if and only if $\omega_{\Delta}(\lambda)=\mu_{\Delta}(\lambda)$ for every $\Delta\in\mathcal{R}(S)$ so that if $\omega_{(.)}(\lambda)$ is not σ-additive on $\mathcal{R}(S)$ it would be interesting to check whether there are conditions, on the construction of the functions $\omega_{\Delta}(\lambda)$, $\Delta\in\mathcal{R}(S)$, which, added to conditions C and D in Ref. 14, imply the σ-additivity of $\omega_{(.)}(\lambda)$ on $\mathcal{R}(S)$. In Ref. 15 it was proven that the sharp reconstruction A is unique in the following sense: if the triples $(F,A,\omega_{(.)}\times(\lambda))$ and $(F,B,\omega^{B}_{(.)}(\lambda))$ satisfy the thesis of von Neumann's theorem then there exists a function $g:[0,1]\rightarrow[0,1]$ such that $A=g(B)$, so that, among the set of all sharp observables which satisfy the thesis of von Neumann's theorem, the sharp reconstruction A is the only one (modulo a bijection) which is related to the others by means of a relation of the kind $A=g(B)$. Due to the last relation, the operators A and B commute. This allowed the authors to consistently interpret the outcomes of measurements of the unsharp observable F as deriving from a randomization of the outcomes of measurements of the sharp reconstruction A (see Ref. 15). By Theorem 2 of the present work and by the main result of Ref. 15 we get the following theorem:

Theorem 3: *A POV measure $F:\mathcal{B}(\mathbb{R})\rightarrow\mathcal{F}(\mathcal{H})$ is commutative if and only if there exist a PV measure $E^{B}:\mathcal{B}(\mathbb{R})\rightarrow\mathcal{E}(\mathcal{H})$ (corresponding to a self-adjoint operator B) and, for every $\lambda\in\sigma(B)$, a probability measure $\mu^{B}_{(.)}(\lambda):\mathcal{B}(R)\rightarrow[0,1]$ such that the triple $(F,B,\mu^{B}_{(.)}(\lambda))$ satisfies the thesis of von Neumann's theorem. The sharp reconstruction A is the only one (modulo a bijection) which is related to the others as follows:*

for every triple $(F,B,\mu^{B}_{(.)}(\lambda))$ satisfying the thesis of von Neumann's theorem there exists a function $g:[0,1]\rightarrow[0,1]$ such that $A=g(B)$.

APPENDIX A: POV MEASURES WITH SPECTRUM IN [0, 1]

In this appendix we show[14] that, without loss of generality, we can restrict ourselves to POV measures with spectrum in [0, 1].

Definition 6: Given the POV measure F, the application $\omega_{(.)}(\lambda):\mathcal{B}(\mathbb{R})\rightarrow[0,1]$ and a bijective function $f:(0,1)\rightarrow\mathbb{R}$ we denote by $\bar{F}$ the POV measure $\Delta\in\mathcal{B}([0,1])\rightarrow F(f(\Delta))$ and by $\bar{\omega}_{(.)}(\lambda)$ the application $\Delta\in\mathcal{B}([0,1])\rightarrow\omega_{f(\Delta)}(\lambda)$.

Notice that the POV measure $\bar{F}$ has spectrum in [0, 1].

Proposition 3: Given a POV measure F and a self-adjoint operator A, the triple $(F,A,\omega_{(.)}\times(\lambda))$ satisfies the thesis of von Neumann's theorem if and only if the triple $(\bar{F},A,\bar{\omega}_{(.)}(\lambda))$ satisfies the thesis of von Neumann's theorem too.

Proof: If $(F,A,\omega_{(.)}(\lambda))$ satisfies the thesis of von Neumann's theorem then $\bar{F}(f^{-1}(\Delta))=F(\Delta)=\omega_{(\Delta)}(A)=\bar{\omega}_{f^{-1}(\Delta)}(A)$ for every $\Delta\in\mathcal{B}(\mathbb{R})$. Notice that f establishes a one to one correspondence between Borel sets in $\mathcal{B}([0,1])$ and Borel set in $\mathcal{B}(\mathbb{R})$. Therefore the triple $(\bar{F},A,\bar{\omega}_{(.)}(\lambda))$ satisfies the thesis of von Neumann theorem. Now let us suppose that the triple $(\bar{F},A,\bar{\omega}_{(.)}(\lambda))$ satisfies the thesis

of von Neumann theorem. Then we have $F(f(\Delta))=\bar{F}(\Delta)=\bar{\omega}_{(\Delta)}(A)=\omega_{f(\Delta)}(A)$ for every $\Delta \in \mathcal{B}([0,1])$ which means that $(F,A,\omega_{(\cdot)}(\lambda))$ satisfies the thesis of von Neumann's theorem. □

APPENDIX B: THE NONDECREASING REAL FUNCTION $\omega_{[0,t)}(\lambda)$

In this appendix we prove the following lemma:

Lemma 3: The sum in Definition 5 does not depend on the decomposition of the interval $[0,t)$.

In order to prove Lemma 3 the following simple facts will be used:

1) if the interval $((k'-1)/2^{q-1},k'/2^{q-1}=b]$ is an element of the decomposition $\{\Delta_j\}_{j\in\mathbb{N}}$ of $[0,t)$ it is not possible that intervals of the kind $((j-1)/2^{p-1},j/2^{p-1}=b]$ with $p\neq q$ be elements of the decomposition too. Otherwise $\{\Delta_j\}_{j\in\mathbb{N}}$ would not be a disjoint family of sets;
2) the extrema of the sets $\Delta \in \mathcal{S}$ define the set of points:

$$A=\left\{\frac{k}{2^{n-1}}k,n \in \mathbb{N}:k \leqslant 2^{n-1}\right\};$$

if $a \in A$ and $a \in ((i-1)/2^{n-1},i/2^{n-1}] \in \mathcal{S}$ it follows that $a=r/2^{l-1}$ for some $r,l \in \mathbb{N}$ such that $r \leqslant 2^{l-1}$ and $n \leqslant l$. Therefore every set $\Delta \in \mathcal{S}$ having $a=r/2^{l-1}$ as one of its extrema must be contained in $((i-1)/2^{n-1},i/2^{n-1}]$;
3) every point $a \in A$, with the exception of 0, is contained in [0, 1] as the right extreme of one interval $\Delta \in \mathcal{S}$

Definition 7: For any decomposition $d_t=\{\Delta_j\}_{j\in\mathbb{N}} \in \mathcal{D}$ *of* $[0,t)$ *and for any* $x \in (0,t)$ *we define the set*

$$\mathcal{M}_{d_t}(x)=\left\{b|x \in [0,b]=\bigcup_{l=1}^{m}\Delta_l,\Delta_l \in d_t\right\}.$$

Proposition 4: Let us consider two decompositions $d_t=\{\Delta_l\}_{l\in\mathbb{N}}$, $\tilde{d}_t=\{\tilde{\Delta}_k\}_{k\in\mathbb{N}} \in \mathcal{D}$ *of* $[0,t)$. *If for any* $0<x<t$ *it is* $\mathcal{M}_{d_t}(x)\cap\mathcal{M}_{\tilde{d}_t}(x)\neq\emptyset$ *then sequences* $\{\Sigma_{l=1}^{n}\omega_{\Delta_l}(\lambda)\}_{n\in\mathbb{N}}$ *and* $\{\Sigma_{k=1}^{n}\omega_{\tilde{\Delta}_k}(\lambda)\}_{n\in\mathbb{N}}$ *converge to the same limit*.

Proof: Let us choose a sequence of numbers $\{x_i;0\leqslant x_i<t\}$ such that $x_i\to t$. For every x_i there exists a number $b_i \in \mathcal{M}_{d_t}(x_i)\cap\mathcal{M}_{\tilde{d}_t}(x_i)$ such that $x_i\leqslant b_i<t$, hence a sequence $\{b_i\}$ such that $b_i \to t$ is defined. We have

$$\lim_{i\to\infty} b_i = t,$$

$$\lim_{i\to\infty} n(i) = \lim_{i\to\infty} m(i) = \infty,$$

$$[0,b_i]=\bigcup_{l=1}^{m_i}\Delta_l=\bigcup_{k=1}^{n_i}\tilde{\Delta}_k,$$

$$\sum_{l=1}^{m_i}\omega_{\Delta_l}(\lambda)=\sum_{k=1}^{n_i}\omega_{\tilde{\Delta}_k}(\lambda)\ \forall\, i,$$

hence

$$\lim_{i\to\infty}\sum_{l=1}^{m_i}\omega_{\Delta_l}(\lambda)=\lim_{i\to\infty}\sum_{k=1}^{n_i}\omega_{\tilde{\Delta}_k}(\lambda)$$

which proves the existence of two subsequences $\{\Sigma_{l=1}^{m_i}\omega_{\Delta_l}(\lambda)\}_{m_i\in\mathbb{N}}$ and $\{\Sigma_{k=1}^{n_i}\omega_{\tilde{\Delta}_k}(\lambda)\}_{n_i\in\mathbb{N}}$ of sequences $\{\Sigma_{l=1}^{n}\omega_{\Delta_l}(\lambda)\}_{n\in\mathbb{N}}$ and $\{\Sigma_{k=1}^{n}\omega_{\tilde{\Delta}_k}(\lambda)\}_{n\in\mathbb{N}}$, respectively, converging to the same limit. □

Now we are ready to prove Lemma 3.

Proof of Lemma 3: Let us consider two decompositions $\{\Delta_l\}_{l\in\mathbb{N}},\{\tilde{\Delta}_k\}_{k\in\mathbb{N}}\in\mathcal{D}$ of $[0,t)$. The proposition is proved if we prove that for every $0<x<1$ it is $\mathcal{M}_{d_t}(x)\cap\mathcal{M}_{\tilde{d}_t}(x)\neq\emptyset$.

For any x, with $0<x<t$, we denote by b the minimum of $\mathcal{M}_{d_t}(x)$ and by $\tilde{b}$ the minimum of $\mathcal{M}_{\tilde{d}_t}(x)$. The existence of the minimum comes from the definition of the class $\mathcal{D}$. If $b\neq\tilde{b}$ we suppose (without loss of generality) $b<\tilde{b}$.

Let $((k'-1)/2^{q-1},k'/2^{q-1}=\tilde{b}]\in\{\tilde{\Delta}_k\}_{k\in\mathbb{N}}$ be the interval of decomposition $\{\tilde{\Delta}_k\}_{k\in\mathbb{N}}$ having $\tilde{b}$ as the right extreme. Then, considering that $\tilde{b}$ is the minimum of set $\mathcal{M}_{\tilde{d}_t}(x)$ and that sets $\tilde{\Delta}_k$ are disjoint, we get $x\in((k'-1)/2^{q-1},k'/2^{q-1}=\tilde{b}]$. Let us consider the number $\bar{a}=\max\{a\in\mathcal{M}_{d_t}(x):[0,a]\subset[0,\tilde{b}]\}$. We have $x\leqslant\bar{a}<\tilde{b}$ and then $\bar{a}\in((k'-1)/2^{q-1},k'/2^{q-1}=\tilde{b}]$. Following item 2), we have that every interval of decomposition $\{\Delta_l\}_{l\in\mathbb{N}}$ having $\bar{a}$ as the left extreme is contained in $((k'-1)/2^{q-1},k'/2^{q-1}=\tilde{b}]$. In other words for every $\Delta_l\in\{\Delta_l\}_{l\in\mathbb{N}}\subset\mathcal{S}$ such that $\Delta_l=(\bar{a},y]$ $(y\in[0,1))$ it must be $y\leqslant\tilde{b}$. Considering that $\bar{a}$ is the maximum of $\mathcal{M}_{d_t}(x)$, that $\tilde{b}\in[0,1]$ and by item 3), we get $y=\tilde{b}$. This proves that $\mathcal{M}_{d_t}(x)\cap\mathcal{M}_{\tilde{d}_t}(x)\neq\emptyset$. The thesis derives from Proposition 4. □

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Spectral geometry of κ-Minkowski space

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After recalling Snyder's idea [Phys. Rev. **71**, 38 (1947)] of using vector fields over a smooth manifold as "coordinates on a noncommutative space," we discuss a two-dimensional toy-model whose "dual" noncommutative coordinates form a Lie algebra: this is the well-known κ-Minkowski space [Phys. Lett. B **334**, 348 (1994)]. We show how to improve Snyder's idea using the tools of quantum groups and noncommutative geometry. We find a natural representation of the coordinate algebra of κ-Minkowski as linear operators on an Hilbert space (a major problem in the construction of a physical theory), study its "spectral properties," and discuss how to obtain a Dirac operator for this space. We describe two Dirac operators. The first is associated with a spectral triple. We prove that the cyclic integral of Dimitrijevic *et al.* [Eur. Phys. J. C **31**, 129 (2003)] can be obtained as Dixmier trace associated to this triple. The second Dirac operator is equivariant for the action of the quantum Euclidean group, but it has unbounded commutators with the algebra. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In classical mechanics, Legendre transformation in the Hamiltonian formalism exhibits an evident symmetry between coordinate space and momentum space.

The same holds in quantum mechanics on a flat space ($\mathbb{R}^n$ or a quotient by a discrete subgroup), with Fourier transform/series replacing the Legendre transformation.

Dealing with quantum mechanics on a curved space M (a smooth manifold), the situation changes. While coordinate functions on M are elements of a commutative algebra, "momenta" (we mean, vector fields over M) no longer commute. A basic example is the 3-sphere, whose vector fields generate $su(2)$, the algebra of angular momenta of quantum mechanics.

Snyder's idea was to use momenta, i.e., vector fields over a smooth manifold M, as "coordinates on a noncommutative space" dual to M.

He applied this idea to the four-dimensional deSitter space, and was led to study the algebra generated by ten operators $\{x_\mu, J_{\mu\nu}\}$ satisfying the commutation rules (Greek letters run over $0,1,2,3$):

$$[x_\mu, x_\nu] = i\lambda^2 J_{\mu\nu}, \tag{1}$$

where $J_{\mu\nu}$ is an element of $so(3,1)$ with suitable commutators with the "coordinates" x_μ. One can notice that this algebra [isomorphic to $so(3,2)$] has too many generators to represent a four-dimensional "noncommutative space," while the elements x_μ alone are correct in number, but do not close an algebra.

A characteristic feature is the presence in (1) of an invariant length λ, whose role is to provide the correct physical dimensions and to allow us to recover $\mathbb{R}^4$ as λ goes to zero ("long distance" or "low energy" limit).

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The purpose of this article is to show how to modify Snyder's idea in such a way as to obtain an algebra that can be studied with noncommutative-geometric tools.

In Sec. II, we discuss Snyder's model in full detail in the two-dimensional version, and realize that Snyder's coordinates do not close an algebra, either in two dimensions, or in four.

In Sec. III, we retry in three dimensions, and realize a fundamental difference from the original Snyder example: in the three-dimensional case the "dual" of the deSitter space is an algebra. This is a basic property, if we want to study noncommutative geometry.[1–3]

The geometrical reason at the base of the difference between Snyder's model in three and in $n \neq 3$ dimensions is clear: the deSitter space in three dimensions is a Lie group, hence the tangent bundle trivialize and vector fields form a Lie algebra isomorphic to the Lie algebra of the group.

In Sec. IV, we search for a two-dimensional example and realize that there is only one, the spacetime studied in literature under the name of κ-Minkowski,[4] whose coordinate algebra is isomorphic to $U(sb(2,\mathbb{R}))$.

As a by-product of this section, we find a natural representation of the algebra as linear operators on a Hilbert space (the choice of a representation on a Hilbert space is a major problem in the construction of a physical theory). Another main point of this section is the realization of Poincaré as a symmetry of κ-Minkowski, in the spirit of Snyder's idea.

In Sec. V we adopt a different point of view and, applying Weyl quantization, construct a C^*-algebra encoding information on the "topology" of the underlying κ-Minkowski space.

We then focus attention on the construction of a spectral triple over κ-Minkowski space. A proposal for a Dirac operator on κ-Minkowski has already appeared in Ref. 5, although the Dirac operator they found does not satisfy Connes' axioms for a spectral triple (the same holds for the one in Ref. 6, as well as the one parametric family of Dirac operators in Ref. 7). For the generalization of such axioms to the noncompact case we refer to the original paper of Connes[2] (see also Refs. 8 and 9 for a comprehensive presentation).

In Sec. V C, we construct a Dirac operator that fulfills all axioms of a spectral triple, and prove that the Dixmier trace associated with the spectral triple is just the cyclic integral discussed in Ref. 10.

Then, we compute a Dirac operator imposing equivariance for the action of the quantum Euclidean group. This turns out to be very similar to the one in Refs. 5 and 6, and has not bounded commutators with the algebra.

II. THE TWO-DIMENSIONAL ANALOGUE OF SNYDER'S SPACETIME

In his original article, Snyder considers the deSitter space $SO(3,2)/SO(3,1)$ and identifies the spacetime "coordinate functions" with a basis of the vector subspace of $so(3,2)$ orthogonal to $so(3,1)$. The (connected component of the) $SO(3,1)$ subgroup provides the Lorentz symmetries and, with a suitable choice of the momenta, it can be extended to a Poincaré symmetry. For the sake of simplicity, we will study, in full detail, the two-dimensional version. Interested readers can find the four-dimensional model discussed in Snyder's original article.[11]

In the two-dimensional version, the deSitter space is $SO(2,1)/SO(1,1)$. If η_0, η_1, η_2 are coordinates of $\mathbb{R}^3$, the deSitter spacetime is the $SO(2,1)$-orbit with equation

$$\eta_0^2 - \eta_1^2 - \eta_2^2 = -1. \tag{2}$$

The (three-dimensional Lorentz) Lie algebra $so(2,1)$ has generators $\{J, K_1, K_2\}$ (a rotation and two boosts) given by

$$J = i(\eta_2 \partial_1 - \eta_1 \partial_2),$$

$$K_1 = i(\eta_0 \partial_1 + \eta_1 \partial_0),$$

$$K_2 = i(\eta_0\partial_2 + \eta_2\partial_0),$$

where $\partial_\mu = \partial/\partial\eta_\mu$. So, the commutation rules are

$$[J,K_1] = iK_2, \quad [J,K_2] = -iK_1, \quad [K_1,K_2] = -iJ. \tag{3}$$

Emulating Snyder, we call $N=K_2$ the generator of the $so(1,1)$ subalgebra (the one-dimensional Lorentz Lie-algebra, isomorphic to $\mathbb{R}$) that leaves fixed the point $m_0=(0,0,1)$, and $x=\lambda J$, $t=\lambda K_1$ the remaining generators [whose span is the subspace of vector fields over $SO(2,1)$ that are tangent to M at m_0]. The length λ provides the correct physical dimensions. By (3), the coordinates satisfy the commutation rule

$$[x,t] = i\lambda^2 N,$$

and clearly do not form a subalgebra of $so(2,1)$.

The higher-dimensional analogue is the commutator $[x_\mu,x_\nu]=i\lambda^2 J_{\mu\nu}$ anticipated in Sec. I.

The action of the Lorentz algebra $so(1,1)$ on the coordinates is via commutator, and by (3) is undeformed:

$$N \triangleright x = it, \quad N \triangleright t = ix.$$

Since the action is undeformed, the invariant is the classical quadratic element x^2-t^2.

We still need to introduce translations.

Let us recall the idea of Snyder: to start with a commutative spacetime, in which translations do not commute, and define a noncommutative spacetime with commutative momenta. Half of this idea was already applied, to find the noncommutative spacetime "dual" to deSitter.

To complete the picture, following Snyder, we define momenta as $P=\lambda^{-1}\eta_1$ and $E=\lambda^{-1}\eta_0$ (the presence of λ ensures the correct physical dimensions). Together with N they form the classical Poincaré algebra:

$$[E,P] = 0, \quad [N,P] = -iE, \quad [N,E] = -iP.$$

The momenta act on the coordinates via commutators. For example:

$$P \triangleright x = [P,x] = -i\lambda(\eta_2\partial_1 - \eta_1\partial_2)\lambda^{-1}\eta_1 = -i\eta_2 = -i\sqrt{\lambda^2(E^2-P^2)-1}.$$

In the last step we used Eq. (2), defining the deSitter space.

With a straightforward calculation we derive the (deformed) action of momenta on coordinates

$$P \triangleright x = -i\sqrt{\lambda^2(E^2-P^2)-1} = E \triangleright t, \quad P \triangleright t = E \triangleright x = 0,$$

while the associated phase-space is defined by

$$[x,P] = i\sqrt{\lambda^2(E^2-P^2)-1} = [t,E], \quad [t,P] = [x,E] = 0.$$

In the $\lambda \to 0$ limit, the spacetime reduces to a commutative one, phase space becomes the Heisenberg algebra, and the action of the Poincaré algebra reduces to the standard one; so for $\lambda=0$ we recover the classical scenario.

III. THE THREE-DIMENSIONAL ANALOGUE OF SNYDER'S SPACETIME

In two dimensions, we have just seen that "Snyder's coordinates" do not form a complete set of generators for an algebra. Let us try in three dimensions.

The space we consider here is the $SO(2,2)$-orbit $M \subset \mathbb{R}^4$ with equation

$$\eta_0^2+\eta_1^2-\eta_2^2-\eta_3^2=-1, \quad \eta_\mu\in\mathbb{R}^4. \tag{4}$$

The stability group of the point $m_0=(0,0,0,1)$ is $SO(2,1)$, so the orbit is the quotient $M\simeq SO(2,2)/SO(2,1)$. Being an homogeneous $SO(2,2)$-space, elements of the Lie algebra $so(2,2)$ [i.e., vector fields over $SO(2,2)$] correspond to derivatives of $C^\infty(M)$. Vectors of the subspace $so(2,1)\subset so(2,2)$ are orthogonal to M, so the "naive" approach would be to take a basis of $so(2,1)^\perp$, the orthogonal of $so(2,1)$ in $so(2,2)$, as coordinates of the noncommutative spacetime dual to M. But $so(2,1)^\perp$ is not a subalgebra of $so(2,2)$, this because M is not a group with the quotient structure [$SO(2,1)$ is not a *normal* subgroup of $SO(2,2)$].

Despite this, we can put a Lie group structure on M. Writing

$$g=\begin{pmatrix}\eta_0+\eta_3 & \eta_1+\eta_2\\ \eta_1-\eta_2 & -\eta_0+\eta_3\end{pmatrix}, \quad \eta_\mu\in\mathbb{R}^4, \tag{5}$$

we have the obvious (smooth manifold) isomorphism $M\simeq SL(2,\mathbb{R})$, the equation $\det g=1$ [that identifies $SL(2,\mathbb{R})$ inside $\mathrm{Mat}(2,\mathbb{R})$] being equivalent to (4). Thus, M is a double cover of the Lorentz group $SO(2,1)$.

This is the pseudo-Euclidean analogue of the fibration $SO(4)\overset{SO(3)}{\longrightarrow}S^3\simeq SU(2)$, i.e. $SO(2,2)\overset{SO(2,1)}{\longrightarrow}SL(2,\mathbb{R})$.

Since M is a Lie group, its tangent bundle is trivial. The Lie algebra of global vector fields on M, isomorphic to $sl(2,\mathbb{R})$, will be identified with the algebra "coordinate functions on the noncommutative spacetime," three-dimensional analogue of the Snyder's spacetime. Let us compute it explicitly.

We take $\widetilde{L}\in sl(2,\mathbb{R})$ (real traceless matrices) and call L the associated vector field on M, defined by

$$(Lf)(g)=\left.\frac{\mathrm{d}}{\mathrm{d}\tau}\right|_{\tau=0} f(\exp\{\tau L\}\cdot g), \tag{6}$$

for all $f\in C^\infty(M)$, $g\in SL(2,\mathbb{R})$. We fix a basis for $sl(2,\mathbb{R})$:

$$\widetilde{t}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \widetilde{x}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \widetilde{y}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},$$

compute the exponentials

$$\exp\{\tau\widetilde{t}\}=\begin{pmatrix}e^\tau & 0\\ 0 & e^{-\tau}\end{pmatrix},$$

$$\exp\{\tau\widetilde{x}\}=\begin{pmatrix}\cosh\tau & \sinh\tau\\ \sinh\tau & \cosh\tau\end{pmatrix},$$

$$\exp\{\tau\widetilde{y}\}\begin{pmatrix}\cos\tau & \sin\tau\\ -\sin\tau & \cos\tau,\end{pmatrix},$$

and their action via left multiplication on (5), the generic element of $SL(2,\mathbb{R})$. Then, through (6), we determine the associated vector fields. For example:

$$\exp\{\tau\widetilde{t}\}g=\begin{pmatrix}(\eta_0+\eta_3)e^\tau & (\eta_1+\eta_2)e^\tau\\ (\eta_1-\eta_2)e^{-\tau} & (-\eta_0+\eta_3)e^{-\tau}\end{pmatrix}.$$

So $\exp\{\tau\widetilde{t}\}$ maps η to the point $\eta^{(\tau)}$, with coordinates

$$\begin{pmatrix} \eta_0^{(\tau)} \\ \eta_1^{(\tau)} \\ \eta_2^{(\tau)} \\ \eta_3^{(\tau)} \end{pmatrix} = \begin{pmatrix} \eta_0 \cosh \tau + \eta_3 \sinh \tau \\ \eta_1 \cosh \tau + \eta_2 \sinh \tau \\ \eta_1 \sinh \tau + \eta_2 \cosh \tau \\ \eta_0 \sinh \tau + \eta_3 \cosh \tau \end{pmatrix},$$

and by (6):

$$(-i\lambda^{-1} t \cdot f)(\eta) = \left. \frac{\mathrm{d}}{\mathrm{d}\tau} \right|_{\tau=0} f(\eta^{(\tau)}),$$

where λ is a parameter with the dimensions of a length.

We have called $-i\lambda^{-1}t$ the derivation associated with $\tilde{\tau}$ because we like to work with symmetric operators, and we want a t with the dimension of a length.

Thus,

$$-i\lambda^{-1} t = \sum_{\mu} \left. \frac{\mathrm{d}\eta_\mu^{(\tau)}}{\mathrm{d}\tau} \right|_{\tau=0} \frac{\partial}{\partial \eta_\mu} = \eta_3 \partial_0 + \eta_2 \partial_1 + \eta_1 \partial_2 + \eta_0 \partial_3.$$

On the same line, one can compute x and y. The full list of vector fields is

$$t = i\lambda(\eta_3 \partial_0 + \eta_2 \partial_1 + \eta_1 \partial_2 + \eta_0 \partial_3),$$

$$x = i\lambda(-\eta_2 \partial_0 + \eta_3 \partial_1 - \eta_0 \partial_2 + \eta_1 \partial_3),$$

$$y = i\lambda(\eta_1 \partial_0 - \eta_0 \partial_1 + \eta_3 \partial_2 - \eta_2 \partial_3),$$

and the commutation rules are those of "$i \cdot sl(2,\mathbb{R})$:"

$$[t,x] = 2i\lambda y, \quad [t,y] = 2i\lambda x, \quad [x,y] = -2i\lambda t.$$

In contrast with the two-dimensional Snyder's model, now $\{t,x,y\}$ is the basis of a Lie algebra. Furthermore, this algebra has the correct number of generators to represent a three-dimensional noncommutative space, dual to the three-dimensional deSitter space.

This idea can easily be generalized: starting with a Lie group M, one can consider $U(\mathrm{Lie}\, M)$ as noncommutative space dual to M, and eventually study it with tools of noncommutative geometry.

A celebrated (compact, Riemannian) example is the *fuzzy sphere*,[12] quotient of $U(su(2))$ for the ideal generated by $J^2 - c$, with J^2 the Casimir and c a suitable constant.

In the next section we consider a simple, two-dimensional example.

IV. A TWO-DIMENSIONAL MODEL: κ-MINKOWSKI

In two dimensions, the unique (real connected) non-Abelian Lie group is the matrix group of elements (Ref. 13, Sec. 10.1)

$$\begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix}, \quad (a,b) \in \mathbb{R}^+ \times \mathbb{R}.$$

That is (the connected component of) the group of affine transformations of the real line:

$$\begin{pmatrix} y \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y \\ 1 \end{pmatrix} = \begin{pmatrix} ay + b \\ 1 \end{pmatrix}, \quad y \in \mathbb{R}.$$

The map

$$\begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix} \mapsto \begin{pmatrix} a & a^{-1}b \\ 0 & a^{-1} \end{pmatrix}$$

gives an isomorphism with $Sb(2,\mathbb{R})$, the group of special upper-triangular real matrices, so the variety $M \simeq Sb(2,\mathbb{R})$ is the starting point.

We want to compute the vector fields and identify them with noncommutative coordinates. Let $L=\left(\begin{smallmatrix} a & b \\ 0 & 0 \end{smallmatrix}\right)$ be the generic element of the Lie algebra, $a,b \in \mathbb{R}$, and $-i\tilde{L}$ the associated vector field:

$$(-i\tilde{L}f)(m) = \left.\frac{\mathrm{d}}{\mathrm{d}\tau}\right|_{\tau=0} f(\exp\{\tau L\}m), \quad f \in C^\infty(M).$$

We use physicists' habit of working with self-adjoint operators. Since

$$L^n = \begin{pmatrix} a^n & a^{n-1}b \\ 0 & 1 \end{pmatrix}, \quad \exp\{\tau L\} = \begin{pmatrix} e^{\tau a} & \dfrac{e^{\tau a}-1}{a}b \\ 0 & 1 \end{pmatrix},$$

if we indicate with $m=\begin{pmatrix} \eta_0 & \eta_1 \\ 0 & 1 \end{pmatrix}$ the generic point of M, $(\eta_0,\eta_1) \in \mathbb{R}^+ \times \mathbb{R}$, it is easy to compute

$$(\tilde{L}f)(\eta_0,\eta_1) = i(a\eta_0\partial_0 + (a\eta_1 + b)\partial_1)f(\eta_0,\eta_1),$$

with $\partial_\mu = \partial/\partial\eta_\mu$. We fix the basis

$$x = i\lambda\partial_1, \quad t = i\lambda(\eta_0\partial_0 + \eta_1\partial_1),$$

for vector fields on M, and define the algebra of "functions on the noncommutative spacetime" to be the algebra of polynomials generated by x and t. The presence of the length λ guarantees the correct physical dimensions, and enables us to recover $\mathbb{R}^2$ as $\lambda \to 0$ limit.

Thus, the algebra is generated by x and t modulo

$$[x,t] = i\lambda x. \tag{7}$$

This is just $U(sb(2,\mathbb{R}))$, the two-dimensional version of the so-called κ-Minkowski, introduced in Ref. 4 as homogeneous space for κ-Poincaré.[14]

The same Lie algebra, but with different real structure, emerges in the Weyl quantization of $S^1 \times \mathbb{R}$. In that case x is unitary, thus the space is "compact" in the x direction.

Now, let μ be the (left) Haar measure on M. Explicitly, for an integrable function f on M:

$$\int_M f\mathrm{d}\mu = \int_{\mathbb{R}^+\times\mathbb{R}} f(\eta_0,\eta_1)\,\eta_0^{-1}\mathrm{d}\eta_0\mathrm{d}\eta_1.$$

You can easily verify the invariance with respect to the left regular action, i.e., $\int_M f\mathrm{d}\mu = \int_M f'\mathrm{d}\mu$ with $f'(\eta_0,\eta_1) = f(a\eta_0, a\eta_1 + b)$ and for all $(a,b) \in \mathbb{R}^+ \times \mathbb{R}$.

With this measure, we can define the Hilbert space $\mathcal{H} = \mathcal{L}^2(M,\mu)$ with inner product $\langle\varphi,\psi\rangle = \int_M \varphi^* \psi \mathrm{d}\mu$.

The measure being invariant, it means that finite transformations of the group M act as isometries on the associated Hilbert space, i.e., as unitary operators. Thus, the vector fields x and t, the generators of these transformations, are represented by (unbounded) self-adjoint linear operators. I mean:

$$\langle x^*\varphi,\psi\rangle := \langle\varphi, x\psi\rangle \equiv \langle x\varphi,\psi\rangle,$$

$$\langle t^{*}\varphi,\psi\rangle := \langle \varphi, t\psi\rangle \equiv \langle t\varphi,\psi\rangle,$$

for all $\varphi,\psi\in\mathcal{H}$ and in the domain of x, respectively, t (it is an easy check to verify these equations). The self-adjointness of x and t allows us to interpret them as quantum-mechanical observables.

A. κ-Minkowski more in depth

Following Snyder's idea, we interpret vector fields on M as "coordinates," and define momenta as the following functions in $C(M)$:

$$P=\lambda^{-1}\eta_1, \quad E=\lambda^{-1}\log\ \eta_0.$$

Again, the presence of λ is for dimensional reasons and we choose E as a logarithm because we want it in $\mathbb{R}$, and not in $\mathbb{R}^{+}$.

The commutators defining phase-space are

$$[x,E]=0, \quad [x,P]=i=[t,E], \quad [t,P]=i\lambda P, \tag{8}$$

and reduce to the classical Heisenberg algebra for $\lambda=0$ (physically, this can be interpreted as a "low-energy limit," i.e., as an approximation for $|\lambda E|,|\lambda P|\ll 1$).

To complete the picture, we want to define the analogue of a boost generator: the generator of a transformation of M with a fixed point [of course, we choose the unit element $(\eta_0,\eta_1)=(1,0)$ as fixed point].

If we define

$$iN=E\partial_P+P\partial_E\equiv\ \eta_0\eta_1\partial_0+\log\ \eta_0\partial_1,$$

N acts on E and P as a classical boost, and $\{E,P,N\}$ generate the (undeformed) Poincaré algebra:

$$[N,E]=-iP, \quad [N,P]=-iE.$$

Since $N\equiv -Pt-(E-\lambda P^2)x$, the action on coordinates is

$$[N,x]=i(t-\lambda Px), \quad [N,t]=i(1-\lambda E-\lambda^2P^2)x+i\lambda Pt.$$

Thus, the action on coordinates is nonlinear and reduces to a classical boost for $\lambda\to 0$.

Like in Snyder's case, we have deformed $\mathbb{R}^2$ into a noncommutative space without breaking the Poincaré symmetry.

In the Snyder case, the coordinates are vector fields on $SO(2,1)$ orthogonal to the submanifold $SO(1,1)$, they are a G-algebra module for Poincaré and do not close an algebra.

In the κ-Minkowski case, the Lie group associated with $\{E,P,N\}$ is Poincaré, isomorphic to $SO(1,1)\ltimes Sb(2,\mathbb{R})$, where $SO(1,1)\simeq\mathbb{R}$ is the subgroup generated by N. Coordinates are vector fields on $M=Sb(2,\mathbb{R})\simeq\{SO(1,1)\ltimes Sb(2,\mathbb{R})\}/SO(1,1)$, and close a Lie algebra isomorphic to "$i\cdot sb(2,\mathbb{R})$." The boosts $SO(1,1)$ are the isotropy transformations of M, which we identify with momentum space. The Poincaré symmetry of spacetime is obtained by dualizing the action of $SO(1,1)$ and taking the cross-product with momenta.

All that has been done in this section can be generalized to $n+1$ dimensions. Just substitute M with the matrix group of elements

$$\begin{pmatrix} e^{a} & b \\ 0 & \mathbb{1} \end{pmatrix}$$

$$\text{with } a\in\mathbb{R}, b\in\mathbb{R}^n, \quad \text{and} \quad \mathbb{1} \text{ the } n\times n \text{ identity matrix.}$$

The associated Lie algebra is again called κ-Minkowski[4] and arises in quantum group theory as a quantum homogeneous space.

B. Quantum group of symmetries for κ-Minkowski

One could object that the action of the boost N on κ-Minkowski coordinates depends on momenta. In more mathematical terms: spacetime is not an algebra module for Poincaré, although phase-space is.

It is obvious that a noncommutative space cannot be a quantum homogeneous space for a Lie group (I mean "embeddable," see, e.g., Ref. 15 for the definition of homogeneous space in a noncommutative framework). Or, in other words, that the algebra of functions on a Lie group has only commutative subalgebras.

It results that κ-Minkowski is embeddable in a quantum group, κ-Poincaré, whose $\lambda \to 0$ limit is the classical Poincaré group. Or, from a dual point of view, it carries a covariant action of an Hopf algebra whose $\lambda \to 0$ limit is the universal enveloping algebra (UEA) of the classical Poincaré Lie algebra.

By using the tools of Hopf algebras,[16] it is not difficult to produce such a deformation. As algebra of momenta one takes the dual of κ-Minkowski Lie algebra, and as covariant action the left canonical one. Then, one adds a "boost" generator and determines the full Hopf algebra of symmetries and its action on coordinates using a bi-cross-product.[16]

The result is the Hopf algebra generated by three real elements $\{N,E,P\}$ (for notational convenience we continue to use the same symbols as in Sec. IV A, but we remark that the Hopf algebra is different) with commutation relations:

$$[E,P]=0, \quad [N,P]=\tfrac{i}{2\lambda}(1-e^{2\lambda E})-\tfrac{i\lambda}{2}P^2, \quad [N,E]=-iP,$$

coproduct:

$$\Delta E = E\otimes 1 + 1\otimes E, \tag{9a}$$

$$\Delta P = P\otimes 1 + e^{\lambda E}\otimes P, \tag{9b}$$

$$\Delta N = N\otimes 1 + e^{\lambda E}\otimes N, \tag{9c}$$

and counit/antipode:

$$\epsilon(E)=\epsilon(P)=\epsilon(N)=0, \quad S(E)=-E, \quad S(P)=-Pe^{-\lambda E}, \quad S(N)=-Ne^{-\lambda E}. \tag{9d}$$

This is the two-dimensional version of κ-Poincaré algebra, obtained for the first time in Ref. 14 by contraction of $U_q(so(3,2))$.

The action on coordinates is undeformed:

$$\begin{aligned} &N\triangleright x = it, \qquad P\triangleright x = -i, \qquad E\triangleright x = 0,\\ &N\triangleright t = ix, \qquad P\triangleright t = 0, \qquad E\triangleright t = -i. \end{aligned}$$

On the other hand, the coproduct is deformed. For this reason, one can calculate, for example:

$$N\triangleright x^2 = (N\triangleright x)x + x(N\triangleright x) = i(tx+xt),$$

$$N\triangleright t^2 = (N\triangleright t)t + (e^{\lambda E}\triangleright t)(N\triangleright t) = i(tx+xt)+\lambda x = N\triangleright x^2 - i\lambda N\triangleright t,$$

and prove that the quadratic invariant is deformed into $x^2-t(t+i\lambda)$, that is:

$$N\triangleright\{x^2 - t(t+i\lambda)\}=0.$$

Finally, a phase space can be obtained as a cross product of momenta and coordinates. The relations defining the phase space are

$$fg = (f_{(1)} \triangleright g) f_{(2)},$$

for f a generic function of the momenta, g a function of the coordinates, and $\Delta T = T_{(1)} \otimes T_{(2)}$ the Sweedler notation.[16] Thus:

$$[x,P] = [t,E] = i, \quad [t,P] = i\lambda P, \quad [x,E] = 0.$$

This is the same algebra defined by Eq. (8).

A second (different) phase space can be constructed via a cross product using the right canonical action of momenta on coordinates, instead of the left one.

The construction of phase space as a cross product (in 3+1 dimensions) was performed in Refs. 17 and 18, an analysis of physical consequences is in Ref. 19.

V. SPECTRAL GEOMETRY OF κ-MINKOWSKI

Let us quote from Ref. 2 the definition of spectral triple, noncommutative generalization of the notion of Riemannian spin^c manifold.

Definition 1: *A spectral triple* $(\mathcal{A},\mathcal{H},D)$ *is given by an involutive algebra* $\mathcal{A}$, *a representation* $\pi:\mathcal{A}\to\mathcal{B}(\mathcal{H})$ *by bounded operators on a Hilbert space* $\mathcal{H}$, *and a self-adjoint operator* $D=D^*$ *with dense domain in* $\mathcal{H}$, *such that*:

(S1) $\pi(a)(D^2+1)^{-1/2}$ *is a compact operator for all* $a\in\mathcal{A}$;
(S2) $[D,\pi(a)]$ *is a bounded operator for all* $a\in\mathcal{A}$.

A commutative example is the canonical spectral triple associated with the spin structure of $\mathbb{R}^2$: $(C_0^\infty(\mathbb{R}^2),\mathcal{H},\not{D})$, with $C_0^\infty(\mathbb{R}^2)$ smooth functions vanishing at infinity on $\mathbb{R}^2$, $\mathcal{H}=L^2(\mathbb{R}^2)\otimes\mathbb{C}^2$ the Hilbert space of L^2-spinors and $\not{D}$ the Dirac operator:

$$\not{D} = i(\sigma_1\partial_0 + \sigma_2\partial_1) = \begin{pmatrix} 0 & i\partial_0+\partial_1 \\ i\partial_0-\partial_1 & 0 \end{pmatrix}.$$

Here σ_j are the Pauli matrices, η_μ coordinates in $\mathbb{R}^2$ and $\partial_\mu := \partial/\partial\eta_\mu$ the corresponding derivatives. Greek letters run over 0,1. We define also $\vec{\eta}=(\eta_0,\eta_1)$.

$C_0^\infty(\mathbb{R}^2)$ is a Frechét pre-C^*-algebra. The supremum norm is equivalent to the operator norm on $\mathcal{H}$, and the C^*-algebra completion is $C_0(\mathbb{R}^2)$, the algebra of continuous functions vanishing at infinity.

Definition 2: *A spectral triple* $(\mathcal{A},\mathcal{H},D)$ *is even if there exists a grading* $\gamma\in\mathcal{B}(\mathcal{H})$, $\gamma=\gamma^*$ *and* $\gamma^2=1$, *such that* $\gamma D=-D\gamma$ *and* $a\gamma=\gamma a\ \forall\ a\in\mathcal{A}$.

The operator:

$$\gamma := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{10}$$

is a grading for the canonical spectral triple on $\mathbb{R}^2$.

We quote also the notion of equivariance with respect to the action of a Lie group.

Definition 3: *Let* H *be Lie group*, $\rho:H\to\mathcal{B}(\mathcal{H})$ *a representation and* $\triangleright:H\times\mathcal{A}\to\mathcal{A}$ *a covariant action. An even spectral triple* $(\mathcal{A},\mathcal{H},D,\gamma)$ *is H-equivariant if*:

(E1) $\rho(h)\pi(a)\rho(h)^{-1}=\pi(h\triangleright a)$ *for all* $a\in\mathcal{A}$, $h\in H$;
(E2) $\rho(h)D\rho(h)^{-1}=D$ *and* $\rho(h)\gamma\rho(h)^{-1}=\gamma$ *for all* $h\in H$.

The spin structure of $\mathbb{R}^2$ is equivariant with respect to the spin representation of $H:=ISO(2)\simeq SO(2)\ltimes\mathbb{R}^2$, the group of isometries of the Euclidean plane $\mathbb{R}^2$.

If $(R,\vec{v}),(R',\vec{v}')\in SO(2)\times\mathbb{R}^2$, the multiplication law of $ISO(2)$ is

$$(R,\vec{v})\cdot(R',\vec{v}')=(RR',\vec{v}+R\vec{v}'),$$

and the spin representation $\rho: H\to\mathcal{B}(\mathcal{H})$ is defined by

$$\{\rho(R,\vec{v})\psi\}(\vec{\eta}):=R\cdot\psi(R^{-1}(\vec{\eta}-\vec{v})),\quad \forall\,\psi\in\mathcal{H}. \tag{11}$$

The representation π of the algebra satisfies (E1) if we define $\triangleright$ to be the pull-back of the natural action on $\mathbb{R}^3$:

$$\{(R,\vec{v})\triangleright f\}(\vec{\eta})=f(R^{-1}(\vec{\eta}-\vec{v})),\quad \forall\, f\in C_0^\infty(\mathbb{R}^2).$$

Differentiating the action of the group, we arrive at the equivalent notion of $U(\mathrm{Lie}\,H)$-equivariance. This notion can be generalized to a generic Hopf-algebra.

Definition 4: *Let $\mathcal{U}$ be an Hopf-algebra, $\rho:\mathcal{U}\to\mathcal{B}(\mathcal{H})$ a representation and $\triangleright:\mathcal{U}\times\mathcal{A}\to\mathcal{A}$ a covariant action. An even spectral triple $(\mathcal{A},\mathcal{H},D,\gamma)$ is $\mathcal{U}$-equivariant if*:

(E1′) $\rho(u_{(1)})\pi(a)\rho(Su_{(2)})=\pi(u\triangleright a)$ *for all* $a\in\mathcal{A}$, $u\in\mathcal{U}$,
(E2′) $\rho(u)D=D\rho(u)$ *and* $\rho(u)\gamma=\gamma\rho(u)$ *for all* $u\in\mathcal{U}$.

In the following we construct the algebras replacing continuous and smooth functions vanishing at infinity associated with κ-Minkowski, and describe the spinor representation.

Since the metric properties of the space depend on the Dirac operator, at this point there is no difference between Euclidean and Lorenzian version.

We then analyze the problem of constructing an Euclidean Dirac operator. We exhibit an operator that is essentially the Dirac operator on the commutative subspace $\mathbb{R}$ of κ-Minkowski, and prove that it defines a spectral triple. We search also for an equivariant Dirac operator and find that there is just one, and does not satisfy the axioms of a spectral triple.

A. The algebra of polynomials of the "noncommutative coordinates"

Let us recall the construction of the algebra of coordinates on κ-Minkowski.

We call $G:=(\mathbb{R}^2,\dot{+})$ the space $\mathbb{R}^2$ with deformed sum:

$$(p_0,p_1)\dot{+}(p_0',p_1')=(p_0+p_0',p_1+p_1'e^{\lambda p_0}),\quad \forall\,(p_0,p_1),(p_0',p_1')\in\mathbb{R}^2.$$

The map:

$$(p_0,p_1)\mapsto g:=\begin{pmatrix}e^{\lambda p_0} & p_1\\ 0 & 1\end{pmatrix}$$

is an isomorphism between G and $\mathrm{Aff}_0(\mathbb{R})$, (the connected component of) the group of affine transformation of $\mathbb{R}$. We will identify G and $\mathrm{Aff}_0(\mathbb{R})$.

There is only one unitary irreducible infinite-dimensional representation of the group $\mathrm{Aff}(\mathbb{R})$, defined on the Hilbert space $L^2(\mathbb{R}^*,\mathrm{d}\eta_1/|\eta_1|)$ by:[20]

$$\{g\cdot\varphi\}(\eta_1):=e^{ib\eta_1}\varphi(a\eta_1),\quad \varphi\in L^2(\mathbb{R}^*,\mathrm{d}\eta_1/|\eta_1|),\quad g=\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix}\in\mathrm{Aff}(\mathbb{R}).$$

We take the tensor product of this representation with the trivial representation $g\mapsto e^{i\eta_0 p_0}$ of the Abelian subgroup $\mathbb{R}$. Then we take the direct integral on $\eta_0\in\mathbb{R}$ with an arbitrary measure $\mathrm{d}\mu(\eta_0)$ on $\mathbb{R}$.

The result is a unitary representation of G on the space:

$$\mathcal{H}_\mu:=L^2(\mathbb{R}\times\mathbb{R}^*,\mathrm{d}\mu(\eta_0)|\eta_1|^{-1}\mathrm{d}\eta_1)\otimes\mathbb{C}^2, \tag{12}$$

defined by

$$\pi: G \to \mathcal{B}(\mathcal{H}_\mu), \quad \vec{p} \mapsto \pi(\vec{p}),$$

$$\{\pi(\vec{p})\psi\}(\vec{\eta}) = e^{i\vec{p}\cdot\vec{\eta}}\psi(\eta_0, \eta_1 e^{\lambda p_0}), \tag{13}$$

where $\psi \in \mathcal{H}_\mu$. One can explicitly check that it is an homomorphism:

$$\pi(\vec{p})\pi(\vec{p}') = \pi(p_0 + p_0', p_1 + p_1' e^{\lambda p_0}).$$

We indicate with $\mathcal{H}_0$ the Hilbert space obtained taking as $\mathrm{d}\mu(\eta_0)$ the Lebesgue measure $\mathrm{d}\eta_0$.

In the previous section, we defined the noncommutative coordinates on κ-Minkowski as the vector fields associated with the generators of $U(\mathfrak{g})$:

$$\begin{pmatrix} \lambda & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

where $\mathfrak{g}$ is the Lie algebra of G.

We can obtain a representation of these coordinates on $\mathcal{H}_\mu$ using the differential of π:

$$\hat{x}_0 = i\mathrm{d}\pi\begin{pmatrix} \lambda & 0 \\ 0 & 0 \end{pmatrix} = \eta_0 - i\lambda\,\eta_1\partial_1,$$

$$\hat{x}_1 = i\mathrm{d}\pi\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \eta_1.$$

The operators $(\hat{x}_0, \hat{x}_1)$ generate an algebra isomorphic to the κ-Minkowski algebra:

$$[\hat{x}_0, \hat{x}_1] = -i\lambda\hat{x}_1. \tag{14}$$

We indicate with $\mathbb{R}^2_\lambda$ the virtual "quantum space" associated with the algebra $U(\mathfrak{g})$, and call elements of $U(\mathfrak{g})$ the "polynomial functions" on κ-Minkowski space.

When $\lambda = 0$, the representation $\mathrm{d}\pi$ reduces to the ordinary (unbounded) representation of polynomial functions on $\mathbb{R}^2$ via pointwise multiplication on $\mathcal{H}_\mu$.

B. Continuous and smooth "functions" on κ-Minkowski space

To construct a spectral triple with the polynomial algebra $U(\mathfrak{g})$ is problematic, since $\hat{x}_\mu$ cannot be represented by bounded operators, and (14) can be satisfied only on a dense domain in $\mathcal{H}_\mu$. It is the same problem one encounters in the canonical quantization of phase-space in quantum mechanics. A possible solution is to shift the attention from $\hat{x}_\mu$ to complex exponentials, that is, from the Lie algebra $\mathfrak{g}$ to the Lie group G. This is Weyl quantization, defined as a map associating complex exponentials on $\mathbb{R}^2$ to elements of G, represented by unitary operators on $\mathcal{H}_\mu$. The quantization map can be extended to an involutive subalgebra of $C_0(\mathbb{R}^2)$ using Fourier transform.

We call $\mathrm{Fun}(\mathbb{R}^2)$ the following class of functions:

$$\mathrm{Fun}(\mathbb{R}^2) := C_0(\mathbb{R}^2) \cap \mathcal{H}_0,$$

and define the following quantization map:

$$\Omega: \mathrm{Fun}(\mathbb{R}^2) \to \mathcal{B}(\mathcal{H}_\mu),$$

$$f \mapsto \Omega(f) = \int_{\mathbb{R}^2} \mathrm{d}^2 p \tilde{f}(\vec{p})\,\pi(\vec{p}),$$

where π is the representation (13) and $\tilde{f}$ is the Fourier transform of f:

$$\widetilde{f}(\vec{p}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} f(\vec{\eta})e^{-i\vec{p}\vec{\eta}}\mathrm{d}^2\eta.$$

Although $f = e^{i\vec{p}\vec{\eta}} \notin C_0(\mathbb{R}^2)$, one can formally verify taking $\widetilde{f}(\vec{p}\,') = \delta^{(2)}(\vec{p}-\vec{p}\,')$ that

$$\Omega(e^{i\vec{p}\vec{\eta}}) = \pi(\vec{p}),$$

and since

$$\eta_\mu = -i\ \frac{\partial}{\partial p_\mu}\bigg|_{\vec{p}=0} e^{i\vec{p}\vec{\eta}},$$

$$\Omega(\eta_\mu) = -i\frac{\partial}{\partial p_\mu}\big|_{\vec{p}=0}\pi(\vec{p}) \equiv \hat{x}_\mu.$$

The explicit expression of the quantization map is

$$\{\Omega(f)\psi\}(\vec{\eta}) = \int_{\mathbb{R}^2}\widetilde{f}(\vec{p})e^{i\vec{p}\vec{\eta}}\psi(\eta_0, \eta_1 e^{\lambda p_0})\mathrm{d}^2p, \quad f \in \mathrm{Fun}(\mathbb{R}^2), \quad \psi \in \mathcal{H}_\mu, \tag{15}$$

and we need to verify that it defines a bounded operator.

Proposition 5: *The quantization map* Ω, *defined by* (15), *sends* $\mathrm{Fun}(\mathbb{R}^2)$ *into bounded operators* $\mathcal{B}(\mathcal{H}_\mu)$. *For this class of functions*, *the operator norm is bounded by*

$$\|\Omega(f)\|^2 := \sup_{\psi\in\mathcal{H}_\mu,\psi\neq 0}\frac{\|\Omega(f)\psi\|^2_{\mathcal{H}_\mu}}{\|\psi\|^2_{\mathcal{H}_\mu}} \leq \frac{1}{2\pi}\|f\|^2_{\mathcal{H}_0}, \tag{16}$$

where $\|_{\mathcal{H}_\mu}$ *indicate the norm in the Hilbert space* $\mathcal{H}_\mu$.

Proof: Let $a = e^{\lambda p_0}$ and call:

$$F(\vec{\eta}, a) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\eta_0' f(\eta_0', \eta_1)e^{ip_0(\eta_0-\eta_0')} = \int_{\mathbb{R}}\mathrm{d}\eta_1\widetilde{f}(\vec{p})e^{i\vec{p}\vec{\eta}}.$$

Then:

$$\{\Omega(f)\psi\}(\vec{\eta}) = \int_{\mathbb{R}}\mathrm{d}p_0 F(\vec{\eta}, a)\psi(\eta_0, a\eta_1) = \int_{\mathbb{R}^+}\frac{\mathrm{d}a}{\lambda a}F(\vec{\eta}, a)\psi(\eta_0, a\eta_1).$$

Since (partial) Fourier transform is an isometry of L^2, then $F \in L^2(\mathbb{R}, \mathrm{d}p_0) = L^2(\mathbb{R}^+, \mathrm{d}a/\lambda a)$ for each fixed $\vec{\eta}$. Using Schwartz inequality:

$$|\Omega(f)\psi(\vec{\eta})|^2 \leq \left(\int_{\mathbb{R}^+}\frac{\mathrm{d}a}{\lambda a}\left|F(\vec{\eta}, a)\psi(\eta_0, a\eta_1)\right|\right)^2 \leq \left(\int_{\mathbb{R}^+}\frac{\mathrm{d}a}{\lambda a}|F(\vec{\eta}, a)|^2\right)\left(\int_{\mathbb{R}^+}\frac{\mathrm{d}a}{a}|\psi(\eta_0, a\eta_1)|^2\right). \tag{17}$$

Now:

$$\begin{aligned}\int_{\mathbb{R}^+}\frac{\mathrm{d}a}{\lambda a}|F(\vec{\eta}, a)|^2 &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}^+}\frac{\mathrm{d}a}{\lambda a}\left|\int_{\mathbb{R}}\mathrm{d}\eta_0' f(\eta_0', \eta_1)e^{ip_0(\eta_0-\eta_0')}\right|^2 \\ &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}p_0\int_{\mathbb{R}^2}\mathrm{d}\eta_0'\mathrm{d}\eta_0''\overline{f(\eta_0', \eta_1)}f(\eta_0'', \eta_1)e^{ip_0(\eta_0'-\eta_0'')} = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\eta_0'|f(\eta_0', \eta_1)|^2,\end{aligned} \tag{18a}$$

$$\int_{\mathbb{R}^+} \frac{\mathrm{d}a}{a} |\psi(\eta_0, a\eta_1)|^2 \leq \int_{\mathbb{R}^*} \frac{\mathrm{d}a}{|a|} |\psi(\eta_0, a\eta_1)|^2 = \int_{\mathbb{R}^*} \frac{\mathrm{d}\eta_1'}{|\eta_1'|} |\psi(\eta_0, \eta_1')|^2, \tag{18b}$$

where $\eta_1' = a\eta_1$ and in the last step we used dilatation invariance of the measure. Using the inequalities (17) and (18) we arrive at

$$\|\Omega(f)\psi\|_{\mathcal{H}_\mu}^2 = \int_{\mathbb{R}\times\mathbb{R}^*} \frac{\mathrm{d}\mu(\eta_0)\mathrm{d}\eta_1}{|\eta_1|} |\Omega(f)\psi(\vec{\eta})|^2 \leq \frac{1}{2\pi} \left(\int_{\mathbb{R}\times\mathbb{R}^*} \frac{\mathrm{d}\eta_0'\mathrm{d}\eta_1}{|\eta_1|} |f(\eta_0', \eta_1)|^2 \right)$$
$$\times \left(\int_{\mathbb{R}\times\mathbb{R}^*} \frac{\mathrm{d}\mu(\eta_0)\mathrm{d}\eta_1'}{|\eta_1'|} |\psi(\eta_0, \eta_1')|^2 \right) = \frac{1}{2\pi} \|f\|_{\mathcal{H}_0}^2 \cdot \|\psi\|_{\mathcal{H}_\mu}^2.$$

Using the last inequality, we find the upper bound (16) for the operator norm. □

We define the following $*$-product on $\mathrm{Fun}(\mathbb{R}^2)$:

$$f_1 * f_2 := \Omega(f_1) f_2, \quad \forall f_{1,2} \in \mathrm{Fun}(\mathbb{R}^2). \tag{19}$$

Let $\mathrm{Fun}^\infty(\mathbb{R}^2)$ be the subspace of smooth functions of $\mathrm{Fun}(\mathbb{R}^2)$.

Proposition 6: $\mathcal{A} := (\mathrm{Fun}(\mathbb{R}^2), *)$ *and* $\mathcal{A}^\infty := (\mathrm{Fun}^\infty(\mathbb{R}^2), *) \subset \mathcal{A}$ *are involutive algebras* (*associative without unit*). $\Omega : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\mu)$ *is a unitary representation*.

Proof: Since $\Omega(f_1)$ is a bounded operator on $\mathcal{H}_\mu$, for all μ, and $f_2 \in \mathcal{H}_0$, the product $f_1 * f_2$ is in $\mathcal{H}_0$. Moreover, $f_1 * f_2 \in C_0(\mathbb{R}^2)$ and is smooth if f_1 and f_2 are.

By construction:

$$\Omega(f_1 * f_2) = \Omega(f_1)\Omega(f_2).$$

This guarantees associativity of the product, and proves that Ω is a representation.

Finally, $\Omega(\bar{f}_1) = \Omega(f_1)^+$ is the adjoint of $\Omega(f_1)$, since the representation π of the group $\mathrm{Aff}_0(\mathbb{R})$ is unitary. So we have a unitary representation of $\mathcal{A}$. □

We call $\mathcal{A}$ the algebra of continuous functions on κ-Minkowski space, and $\mathcal{A}^\infty$ the subalgebra of "smooth functions." Since $1 \notin \mathcal{A}$, the space is not compact.

From (15), using Leibniz rule and the property $ip_\mu \widetilde{f} = \widetilde{\partial_\mu f}$, we deduce the following "deformed" Leibniz rule:

$$\partial_0\{\Omega(f_1)f_2\} = \Omega(\partial_0 f_1) f_2 + \Omega(f_1)\partial_0 f_2, \tag{20a}$$

$$\partial_1\{\Omega(f_1)f_2\} = \Omega(\partial_1 f_1) f_2 + \Omega(e^{-i\lambda\partial_0} f_1)\partial_1 f_2, \tag{20b}$$

or equivalently:

$$\partial_0(f_1 * f_2) = (\partial_0 f_1) * f_2 + f_1 * (\partial_0 f_2),$$

$$\partial_1(f_1 * f_2) = (\partial_1 f_1) * f_2 + (e^{-i\lambda\partial_0} f_1) * (\partial_1 f_2),$$

for all $f_1, f_2 \in \mathrm{Fun}^\infty(\mathbb{R}^2)$.

C. A Dirac operator for κ-Minkowski space

The first attempt to define a Dirac operator would be to use the classical one $\not{D}$.

Properties (20) means that $\not{D}$ has not bounded commutator with the algebra. Indeed:

$$[\partial_0, \Omega(f)] = \Omega(\partial_0 f), \quad f \in \mathcal{A}^\infty$$

is bounded, but $[\partial_1, \Omega(f)]$ is not, due to the presence of the unbounded operator $e^{-i\lambda\partial_0}$.

$D := i\partial_0$ has nontrivial sign (it is not positive), has dense domain in $\mathcal{H}$ and bounded commutators with $\mathcal{A}$. Geometrically, the evaluation at $\eta_1 = 0$:

$$\Omega(f) \mapsto f(\eta_0, 0)$$

is an algebra morphism $\mathcal{A} \to C_0(\mathbb{R})$, and tells us that $\mathbb{R}$ is a commutative subspace. D is just the Dirac operator on this subspace.

Let $\Delta := -\partial_0^2 + 1$. Intuitively, one would expect that the axiom (S1) in the definition of spectral triple is not satisfied. For $\lambda = 0$, $f \cdot \Delta^{-1/2}$ is not a compact operator on $L^2(\mathbb{R}^2)$. Surprisingly if $\lambda \neq 0$, $\Omega(f)\Delta^{-1/2}$ is a compact operator on $\mathcal{H}_\mu$, if μ is a finite measure on $\mathbb{R}$ [i.e., $\int_{\mathbb{R}} \mathrm{d}\mu(\eta_0) < \infty$] and absolutely continuous with respect to the Lebesgue measure.

Proposition 7: *Let μ be a finite measure on $\mathbb{R}$, absolutely continuous with respect to the Lebesgue measure, and let $\lambda \neq 0$. Then, $(\mathcal{A}^\infty, \mathcal{H}_\mu, i\partial_0)$ is a 1^+-summable spectral triple. The associated Dixmier trace is just the cyclic integral of*[10]

$$\fint \Omega(f)\Delta^{-1/2} := \mathrm{Res}_{z=1}\mathrm{Trace}_{\mathcal{H}_\mu}\Omega(f)\Delta^{-z/2} \propto \int_{\mathbb{R}\times\mathbb{R}^*} f(\vec{x})\frac{\mathrm{d}x_0\mathrm{d}x_1}{|x_1|}, \tag{21}$$

where $\Delta := -\partial_0^2 + 1$.

Proof: We decompose $\mathcal{H}_\mu = \mathcal{V}_0 \otimes \mathcal{V}_1$, with $\mathcal{V}_0 := L^2(\mathbb{R}, \mathrm{d}\mu(\eta_0))$ and $\mathcal{V}_1 := L^2(\mathbb{R}^*, \mathrm{d}\eta_1/|\eta_1|)$.

Let us recall some facts from Ref. 21 (see also Ref. 22 for a pedagogical presentation and Ref. 9 for considerations on the noncompact case).

Let $\mu'(\eta_0) = \mathrm{d}\mu(\eta_0)/\mathrm{d}\eta_0$. By hypothesis $\mu' \in C_0(\mathbb{R}^2)$.

$i\partial_0$ being the Dirac operator on $\mathbb{R}$, $f\Delta^{-1/2}$ is compact on $L^2(\mathbb{R}, \mathrm{d}\eta_0)$ for all $f \in C_0(\mathbb{R}^2)$. In particular, taking $f = \mu'$, we prove that $\Delta^{-1/2}$ is compact on $\mathcal{V}_0$.

From the formula:

$$\mathrm{Res}_{z=1}\mathrm{Trace}_{L^2(\mathbb{R},\mathrm{d}\eta_0)} f\Delta^{-z/2} \propto \int_{\mathbb{R}} f(\eta_0)\mathrm{d}\eta_0$$

(we do not care about the proportionality constant, which is independent on f) we deduce

$$\mathrm{Res}_{z=1}\mathrm{Trace}_{\mathcal{V}_0}\Delta^{-z/2} = \mathrm{Res}_{z=1}\mathrm{Trace}_{L^2(\mathbb{R},\mathrm{d}\eta_0)}\mu'\Delta^{-z/2} \propto \int_{\mathbb{R}} \mathrm{d}\mu(\eta_0) < \infty .$$

The operator $\Delta^{-z/2}$ is traceclass on $\mathcal{V}_0$ if $z > 1$, and in the Dixmier class $\mathcal{L}^{1+}(\mathcal{V}_0)$ if $z = 1$.

On $\mathcal{H}_\mu$, if $f \in \mathcal{A}$, the kernel of the operator $\Omega(f)\Delta^{-z/2}$ is the distribution:

$$K_f(\vec{\eta}, \vec{\eta}') = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{d}^2 p \tilde{f}(\vec{p}) e^{i\vec{p}\vec{\eta}} \delta(\eta_1' - \eta_1 e^{\lambda p_0}) \int_{\mathbb{R}} \mathrm{d}\xi (1+\xi^2)^{-z/2} e^{i\xi(\eta_0 - \eta_0')},$$

where the integral in $\mathrm{d}\xi$ is the resolvent of $\Delta^{z/2}$.

We consider first the case in which f is integrable ($f \in L^1(\mathbb{R}^*, \mathrm{d}\eta_0 \mathrm{d}\eta_1/|\eta_1|)$).

The partial trace of $\Omega(f)\Delta^{-z/2}$ on $\mathcal{V}_1$ is the operator with kernel:

$$\begin{aligned}\hat{K}_f(\vec{\eta}, \vec{\eta}') &= \int_{\mathbb{R}^*} \frac{\mathrm{d}\eta_1}{|\eta_1|} K_f(\eta_0, \eta_1; \eta_0', \eta_1) = \frac{\lambda^{-1}}{2\pi}\int_{\mathbb{R}^*}\frac{\mathrm{d}\eta_1}{|\eta_1|}\int_{\mathbb{R}} \mathrm{d}p_1 \tilde{f}(0, p_1) e^{ip_1\eta_1} \int_{\mathbb{R}} \mathrm{d}\xi (1+\xi^2)^{-z/2} e^{i\xi(\eta_0 - \eta_0')} \\ &= \frac{\lambda^{-1}}{2\pi}\left(\int_{\mathbb{R}\times\mathbb{R}^*} \frac{\mathrm{d}x_0\mathrm{d}x_1}{|x_1|} f(\vec{x})\right)\int_{\mathbb{R}} \mathrm{d}\xi (1+\xi^2)^{-z/2} e^{i\xi(\eta_0 - \eta_0')}.\end{aligned}$$

Then, as operators on $\mathcal{V}_0$:

$$\mathrm{Trace}_{\mathcal{V}_1}\{\Omega(f)\Delta^{-z/2}\} = \frac{\lambda^{-1}}{2\pi}\left(\int_{\mathbb{R}\times\mathbb{R}^*} f(\vec{x})\frac{\mathrm{d}x_0\mathrm{d}x_1}{|x_1|}\right)\Delta^{-z/2}. \tag{22}$$

From what was said above about $\Delta^{-z/2}$, we see that $\Omega(f)\Delta^{-z/2}$ is traceclass on $\mathcal{H}_\mu$ if $z > 1$, and in the Dixmier class $\mathcal{L}^{1+}(\mathcal{H}_\mu)$ if $z = 1$.

Taking the trace on $\mathcal{V}_0$ of (22) and then the residue in $z=1$ we prove (21).

Now, since $\mathrm{Fun}(\mathbb{R}^2)\subset L^2$, integrable functions are dense in the algebra $\mathcal{A}$. So, $\Omega(f)\Delta^{-1/2}$ is in the closure of $\mathcal{L}^{1+}(\mathcal{H}_\mu)$ for all $f\in\mathcal{A}$. The closure of the Dixmier class are the compact operators $\mathcal{K}$, and this concludes the proof. □

Remark: The spectral triple constructed in this section does not have a commutative analogue. Axiom (S1) is not satisfied for $\lambda=0$.

D. Equivariance properties of the representation

Let $\mathcal{A}$ be the involutive algebra defined in Proposition 6, $\mathcal{H}$ the Hilbert space:

$$\mathcal{H}:=\mathcal{H}_0\otimes\mathbb{C}^2=L^2(\mathbb{R}\times\mathbb{R}^*,|\eta_1|^{-1}\mathrm{d}\eta_0\mathrm{d}\eta_1)\otimes\mathbb{C}^2,$$

and γ the grading in (10). We lift trivially the representation (15) of $\mathcal{A}$ from $\mathcal{H}_0$ to $\mathcal{H}$.

We postpone the problem of constructing an equivariant Dirac operator and study the equivariance properties of the data $(\mathcal{A},\mathcal{H},\gamma)$. Clearly $\mathcal{A}$ commutes with γ, and so γ is a natural candidate for the grading.

The space $\mathcal{H}_0$ carries a representation of an Hopf-algebra, which we indicate with $U_\kappa(iso(2))$, that is the Euclidean analogue of κ-Poincaré. It is generated by three real operators, which we continue to denote with E,P,N, with commutation relations:

$$[E,P]=0,\quad [N,P]=\tfrac{i}{2\lambda}(1-e^{2\lambda E})+\tfrac{i\lambda}{2}P^2,\quad [N,E]=iP,$$

while coproduct, counit, and antipode are defined by (9), as for κ-Poincaré algebra.

Notice that in the basis

$$P_x=E,\quad P_y=Pe^{-\lambda E/2},\quad J=Ne^{-\lambda E/2},$$

the Hopf-algebra is just the *quantum Euclidean group* derived in Ref. 23 by contraction of $U_q(su(2))$.

There is a natural representation of the (E,P) sub-Hopf-algebra of $U_\kappa(iso(2))$ on a space dense in $\mathcal{H}_0$, defined by

$$\rho(E)=-i\partial_0,\quad \rho(P)=-i\partial_1.$$

This extends to a representation of the full Hopf-algebra if we define:

$$\rho(N)=\eta_0\rho(P)+\eta_1\rho\left(\frac{1-e^{2\lambda E}}{2\lambda}+\frac{\lambda}{2}P^2\right)=-i\eta_0\partial_1+\frac{1}{2\lambda}\eta_1(1-e^{-2i\lambda\partial_0})-\frac{\lambda}{2}\eta_1\partial_1^2. \tag{23}$$

On the space $\mathbb{C}^2$, we call σ the representation of the commutative $\mathbb{R}$ subalgebra, defined by

$$\sigma(N):=\frac{1}{2}\gamma=\frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad \sigma(E)=\sigma(P)=0.$$

On the space $\mathcal{H}=\mathcal{H}_0\otimes\mathbb{C}^2$ we consider the representation $\rho\otimes\sigma$ defined through the (opposite) coproduct:

$$(\rho\otimes\sigma)(h)=\rho(h_{(2)})\otimes\sigma(h_{(1)}),\quad \forall\, h\in U_\kappa(iso(2)).$$

This representation commutes with the grading γ, since the image through σ of the algebra is in the subspace of $\mathrm{Mat}_2(\mathbb{C})$ spanned by 1 and γ.

Before discussing the $U_\kappa(iso(2))$-equivariance of $(\mathcal{A},\mathcal{H},\gamma)$ we need to define a covariant action of the Hopf algebra on $\mathcal{A}$. If we define:

$$h\triangleright\Omega(f):=\Omega(\rho(h)f),\quad \forall\, h\in U_\kappa(iso(2)),\quad \Omega(f)\in\mathcal{A},$$

this is a representation of the Hopf-algebra. We want to prove that it is covariant, that is:

$$h \triangleright \Omega(f_1)\Omega(f_2) = \{h_{(1)} \triangleright \Omega(f_1)\}\{h_{(2)} \triangleright \Omega(f_2)\},$$

or equivalently using the $*$-product:

$$\rho(h)(f_1 * f_2) = \{\rho(h_{(1)})f_1\} * \{\rho(h_{(2)})f_2\}.$$

Proposition 8: *The action* $\triangleright$ *of* $U_\kappa(iso(2))$ *on* $\mathcal{A}$ *is covariant. Moreover*:

$$h \triangleright a = \rho(h_{(1)})a\rho(Sh_{(2)}),$$

for all $h \in U_\kappa(iso(2))$ *and* $a \in \mathcal{A}$ (*on a subspace dense in* $\mathcal{H}_0$).

Proof: Using (19), we deduce that the covariance condition is equivalent to

$$\rho(h)\Omega(f_1)f_2 = \Omega(\rho(h_{(1)})f_1) \cdot \{\rho(h_{(2)})f_2\}. \tag{24}$$

Since on both sides appear representations of $U_\kappa(iso(2))$, it is sufficient to do the check for the generators E, P, N.

We can rewrite (20a) as

$$\rho(E)\Omega(f_1)f_2 = \Omega(\rho(E)f_1)f_2 + \Omega(f_1)\{\rho(E)f_2\},$$

$$\rho(P)\Omega(f_1)f_2 = \Omega(\rho(P)f_1)f_2 + \Omega(\rho(e^{\lambda E})f_1)\{\rho(P)f_2\},$$

and then the action of E and P is covariant.

In the same way, using (20) and (23), it is a straightforward computation to prove the covariance of the action of N.

If in Eq. (24) we replace h with $h_{(1)}$, call $a=\Omega(f_1) \in \mathcal{A}$, $f_2=\rho(Sh_{(2)})\psi$, and recall that $\Omega(\rho(h_{(1)})f_1)=h_{(1)} \triangleright a$, we obtain

$$\rho(h_{(1)})a\rho(Sh_{(2)})\psi = (h_{(1)} \triangleright a)\rho(h_{(2)}S(h_{(3)}))\psi = \{\epsilon(h_{(2)})h_{(1)} \triangleright a\}\psi = (h \triangleright a)\psi.$$

This concludes the proof. □

Since the representation of $\mathcal{A}$ is lifted diagonally from $\mathcal{H}_0$ to $\mathcal{H}=\mathcal{H}_0 \otimes \mathbb{C}^2$, $\sigma(h)a=a\sigma(h)$ for all $h \in U_\kappa(iso(2))$ and $a \in \mathcal{A}$. Then, as a corollary:

$$h \triangleright a = (\rho \otimes \sigma)(h_{(1)})a(\rho \otimes \sigma)(Sh_{(2)}).$$

This means that:

Corollary 9: $(\mathcal{A}, \mathcal{H}, \gamma)$ *is* $U_\kappa(iso(2))$*-equivariant.*

E. An $U_\kappa(iso(2))$-equivariant Dirac operator

To have an equivariant spectral triple on κ-Minkowski space, it remains to find a Dirac operator D that is equivariant for the action of the quantum Euclidean group.

We write D as a formal pseudo-differential operator:

$$D\psi(\vec{\eta}) = \int_{\mathbb{R}^2} e^{i\vec{p}\vec{\eta}} \begin{pmatrix} 0 & T(\vec{\eta},\vec{p}) \\ T(\vec{\eta},\vec{p})^* & 0 \end{pmatrix} \tilde{\psi}(\vec{p}) \mathrm{d}^2p, \quad \psi \in \mathcal{H},$$

and determine the symbol T imposing equivariance. The matrix form of the symbol is a consequence of the grading and formal self-adjointness.

Since $(\rho\otimes\sigma)(E)=\rho(E)$, $(\rho\otimes\sigma)(P)=\rho(P)$ and $(\rho\otimes\sigma)(N)=\sigma(N)+\rho(N)\sigma(e^{\lambda E})=\rho(N)+\frac{1}{2}\gamma$, the equivariance conditions become

$$[\rho(E),D]=0, \quad [\rho(P),D]=0, \quad [\rho(N),D]=-\tfrac{1}{2}[\gamma,D] \equiv -\gamma D.$$

The first two conditions are equivalent to

$$\partial_0 T(\vec{\eta},\vec{p}) = \partial_1 T(\vec{\eta},\vec{p}) = 0.$$

Then, $T(\vec{\eta},\vec{p}) = T(\vec{p})$. The last condition can be written as

$$[\chi(N), T(\vec{p})] = -T(\vec{p}), \quad [\chi(N), T(\vec{p})^*] = T(\vec{p})^*, \tag{25}$$

where

$$\chi(N) := ip_1 \frac{\partial}{\partial p_0} + i\left(\frac{1-e^{2\lambda p_0}}{2\lambda} + \frac{\lambda}{2}p_1^2\right)\frac{\partial}{\partial p_1}.$$

If we define $\chi(E)=p_0$ and $\chi(P)=p_1$, then the map χ extends to a representation of the $U_\kappa(iso(2))$ Hopf algebra.

In Ref. 24 it was constructed for the first time a (formal) isomorphism between κ-Poincaré and the Poincaré algebra. The Euclidean counterpart is the change of coordinates:

$$e^{-\lambda p_0} p_1 =: r \sin\theta, \quad \frac{1}{\lambda}\sinh(\lambda p_0) + \frac{\lambda}{2}p_1^2 e^{-\lambda p_0} =: r\cos\theta,$$

with $r \in \mathbb{R}_0^+$ and $\theta \in S^1$. The Casimir of the quantum Euclidean group is:

$$m^2 := \left(\frac{2}{\lambda}\sinh\frac{\lambda E}{2}\right)^2 + e^{-\lambda E}P^2.$$

It is related to r^2 by

$$r^2 = \chi\left(m^2\left(1+\frac{\lambda^2 m^2}{4}\right)\right), \tag{26}$$

and then r^2 is central and $[\chi(N), r^2]=0$. So, $\chi(N)=\tilde{N}(r,\theta)\partial_\theta$ is a derivation in the θ direction, with $\tilde{N}$ defined by $\tilde{N}(r,\theta)re^{i\theta} = -i[\chi(N), re^{i\theta}]$.

With a straightforward computation we arrive at $[\chi(N), re^{i\theta}] = re^{i\theta}$, and prove that

$$\chi(N) = -i\frac{\partial}{\partial\theta}.$$

The general solution of (25) is $T(\vec{p}) = R(r)e^{-i\theta}$, with R an arbitrary function. If we want the classical Dirac operator as $\lambda=0$ limit, we are forced to choose $R(r)=-r$, and the final solution is

$$\begin{aligned} D &= -\rho\begin{pmatrix} 0 & \frac{1}{\lambda}\sinh(\lambda E) + e^{-\lambda E}P\left(\frac{\lambda}{2}P - i\right) \\ \frac{1}{\lambda}\sinh(\lambda E) + e^{-\lambda E}P\left(\frac{\lambda}{2}P + i\right) & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \frac{1}{\lambda}\sinh(i\lambda\partial_0) + e^{i\lambda\partial_0}\left(1+\frac{\lambda}{2}\partial_1\right)\partial_1 \\ \frac{1}{\lambda}\sinh(i\lambda\partial_0) - e^{i\lambda\partial_0}\left(1-\frac{\lambda}{2}\partial_1\right)\partial_1 & 0 \end{pmatrix}. \end{aligned} \tag{27}$$

This Dirac operator is very similar to the one constructed in Refs. 5–7, but for Euclidean signature instead of Lorentzian one, and $1+1$ dimension instead of $3+1$.

A deformed Leibniz rule for D comes from the coproduct of E, P, and tells us that commutators with the algebra are not bounded, due to the presence of the $e^{\lambda E}$ factor.

Using Eq. (2.5) of Ref. 7 one can reach the same conclusion for the Dirac operators in Refs. 5–7.

From (26) we derive the following relation:

$$D^2 = \rho\left(m^2\left(1 + \frac{\lambda^2 m^2}{4} \right) \right),$$

that is the same as Eq. (12) in Ref. 5.

VI. CONCLUSION

In quantum mechanics over $\mathbb{R}^n$, it is usual to work in momentum space by means of Fourier transform. If the physical system under consideration lives in a curved manifold, with trivial tangent bundle, momenta are globally defined as vector fields on the manifold, and in general do not commute. We have illustrated this situation with an example that is recurrent in physics, the deSitter space in three dimensions. In such a situation, if we want to work in "momentum space," we need the tools of noncommutative geometry.

In these notes, we have studied the lowest dimensional nontrivial (i.e., noncommutative) example, when the manifold M is the connected component of the group of affine transformations of the real line, and found that the "dual" space is κ-Minkowski. This is the unique two-dimensional noncommutative example coming from a Lie group.

We have found a natural representation of κ-Minkowski on $L^2(M,\mu)$, with μ the (left) Haar measure on the group M.

Usually this spacetime is studied from an Hopf-algebra point of view, considering $U(\mathrm{Lie}\, M)$ as the polynomial algebra of coordinates on some virtual space.[4] We have argued how, using Weyl quantization, it is possible to define the associated C^*-algebra. The definition of the C^*-algebra allows one to study the topology of the space, following the general philosophical viewpoint that C^*-algebra theory may be regarded as a kind of noncommutative topology.

In the last section, we have constructed a spectral triple associated with the cyclic integral of Ref. 10, and an $U_\kappa(iso(2))$-equivariant Dirac operator which does not satisfy the axioms for a spectral triple.

About the Dirac operator $i\partial_0$, it could be interesting to construct pure states of the algebra and investigate the properties of the distance defined by the celebrated Connes formula (see, e.g., Refs. 2 and 3). Since it only involves time derivatives, it is natural to expect that, in some way, it provides information only about the time distance between two events.

Apart from its intrinsic interest, κ-Minkowski is a simple nontrivial example in which to compare Connes' approach to noncommutative geometry with the Hopf-algebraic one.

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GHZ extraction yield for multipartite stabilizer states

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Let $|\Psi\rangle$ be an arbitrary stabilizer state distributed between three remote parties, such that each party holds several qubits. Let S be a stabilizer group of $|\Psi\rangle$. We show that $|\Psi\rangle$ can be converted by local unitaries into a collection of singlets, GHZ states, and local one-qubit states. The numbers of singlets and GHZs are determined by dimensions of certain subgroups of S. For an arbitrary number of parties m we find a formula for the maximal number of m-partite GHZ states that can be extracted from $|\Psi\rangle$ by local unitaries. A connection with earlier introduced measures of multipartite correlations is made. An example of an undecomposable four-party stabilizer state with more than one qubit per party is given. These results are derived from a general theoretical framework that allows one to study interconversion of multipartite stabilizer states by local Clifford group operators. As a simple application, we study three-party entanglement in two-dimensional lattice models that can be exactly solved by the stabilizer formalism. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2203431]

I. INTRODUCTION

Many quantum cryptographic protocols such as quantum key distribution,[1] coin flipping,[2] or other quantum games[3] operate with a single copy of a pure quantum state shared by three or more parties. Each party has complete control of its subsystem, so the states which can be converted to each other by local unitary (LU) operators may be regarded as equivalent. Unfortunately, in general, LU-equivalence classes lack any known concise analytical description. For tripartite pure states (or, equivalently, bipartite mixed states), substantial progress has been achieved only for Gaussian states of fermions[4] and bosons[5] with some additional symmetry properties.

In the present paper we study LU-equivalence classes of *stabilizer states*. A stabilizer state of n qubits can be thought of as an irreducible representation of an Abelian *stabilizer group* generated by n pairwise commuting operators in the Pauli group (i.e., tensor products of the identity I and the Pauli matrices σ^x, σ^y, σ^z). Important applications of stabilizer states include measurement-based schemes of quantum computation[6] and quantum error correction using ancillas.[7] They also provide exactly solvable models of condensed-matter systems.[8]

In the special case when each party holds exactly one qubit (so that a local operator means a one-qubit operator), LU-equivalence classes of stabilizer states have been already studied by Van den Nest, Dehaene, and De Moor in Refs. 9–11.

We assume that n qubits are distributed between a finite set of parties M. Each party may hold an arbitrary number of qubits. Our main results are summarized below.

Result 1: Three-party entanglement.

We prove that an arbitrary stabilizer state shared by three parties A,B,C is LU equivalent to a collection (tensor product) of states from a set $E_3=\{|0\rangle,|\Psi^+\rangle,|\Psi_3^+\rangle\}$, where

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|0,0\rangle + |1,1\rangle),$$
$$|\Psi_3^+\rangle = \frac{1}{\sqrt{2}}(|0,0,0\rangle + |1,1,1\rangle) \tag{1}$$

are the EPR state and the GHZ state. The set E_3 thus can be called an entanglement generating set (EGS) for three-party systems, as far as stabilizer states are concerned. LU-equivalence classes are completely specified by four integers (a,b,c,p), where a,b,c are the numbers of EPR states $|\Psi^+\rangle$ shared by BC, AC, and AB, respectively, while p is the number of GHZ states $|\Psi_3^+\rangle$ shared by all three parties. A prerequisite to this result is the work in Ref. 12, where a set $E_2=\{|0\rangle,|\Psi^+\rangle\}$ was shown to be an EGS for bipartite systems. It should be emphasized that the set E_3 is not an EGS for arbitrary tripartite states, even if one allows arbitrary local manipulation and classical communication (see Ref. 13).

Result 2: Multipartite entanglement.

Let $|\Psi\rangle$ be an n-qubit stabilizer state shared by a set of parties M, $|M|=m\geq 3$, and let S be its stabilizer group. We are interested in the maximal number of m-party GHZ states

$$|\Psi_m^+\rangle = \frac{1}{\sqrt{2}}(|0^{\otimes m}\rangle + |1^{\otimes m}\rangle)$$

that can be extracted from $|\Psi\rangle$ by local unitaries. Denote this number by p. We prove that

$$p = \dim(S) - \dim(S_{\mathrm{loc}}), \tag{2}$$

where S_{loc} is a subgroup of S generated by all stabilizer operators that act trivially on at least one party. [For bipartite systems the answer is slightly different, $p=(1/2)(\dim(S)-\dim(S_{loc}))$, see Ref. 12.]

In particular, p can be computed in polynomial time in the number of qubits. Interestingly, we will give below a constructive proof of Eq. (2), which translates naturally into an efficient algorithm to perform the GHZ extraction. An implementation of this algorithm will be available online soon.

It should be mentioned that Eq. (2) provides a simple upper bound on p. Indeed, if one can find l independent generators of S, such that each of them acts trivially on at least one party, then $\dim(S_{\mathrm{loc}})\geq l$ and thus $p\leq \dim(S)-l$.

Also, we show that the GHZ extraction yield p, considered as a functional of $|\Psi\rangle$, coincides with an entanglement measure introduced by Linden, Popescu, and Wootters in Ref. 14 to quantify irreducible multipartite correlations.

To illustrate the usefulness of Results 1 and 2, we consider two-dimensional lattice models that can be exactly solved by the stabilizer formalism. Well-known examples of such models include the cluster state used in one-way quantum computation[6] and Kitaev's toric code state.[8,15] In general, the ground state of such models can be specified as an eigenvector of local stabilizer operators. We study tripartite entanglement of the ground state with respect to a partition of the lattice into three angular segments with a common junction point (see Fig. 1 in Sec. VII). We show that the number of GHZ states extractable from the ground state is bounded from above by a constant that depends only upon the structure of stabilizers near the junction point (and does not depend upon the size of the lattice). This is a natural generalization of the entanglement saturation phenomenon found for 1D spin chains (see Ref. 16 and references therein).

The rest of the paper is organized as follows. Section II introduces notation and terminology. Our main technical theorems are proved in Sec. III. In Sec. IV we consider multipartite stabilizer states and prove Eq. (2). Section V establishes a connection between GHZ extraction yield and measures of multipartite correlations. LU-equivalence classes of tripartite states are discussed in

Sec. VI. We apply the developed technique to spin lattices in Sec. VII. The goal of Sec. VIII is to convince the reader that four-party stabilizer states are likely to lack a simple entanglement generating set.

II. PRELIMINARIES AND NOTATION

A. Stabilizer states

The goal of this section is to introduce convenient terminology. Whenever it is possible, we use the notation of Ref. 17, Chap. 15.

The Pauli operators σ^x, σ^y, σ^z, and the identity operator I will be labeled by elements of two-dimensional binary linear space $G=\{00,01,10,11\}$, such that

$$\sigma_{00}=I, \quad \sigma_{10}=\sigma^x, \quad \sigma_{01}=\sigma^z, \quad \sigma_{11}=\sigma^y.$$

For any integer n and $f=(\alpha_1,\beta_1,\ldots,\alpha_n,\beta_n)\in G^n$, define a *σ-operator*

$$\sigma(f)=\sigma_{\alpha_1\beta_1}\otimes\cdots\otimes\sigma_{\alpha_n\beta_n}.$$

For all $f,g\in G^n$, one has $\sigma(f)\sigma(g)=e^{i\theta}\sigma(f+g)$ for some phase factor $e^{i\theta}$. The commutation rules for σ-operators can be written as

$$\sigma(f)\sigma(g)=(-1)^{\omega(f,g)}\sigma(g)\sigma(f).$$

Here $\omega: G^n\otimes G^n\to\{0,1\}$ is a symplectic form,

$$\omega(f,f')=\sum_{j=1}^{n}\alpha_j\beta_j'+\beta_j\alpha_j' \bmod 2.$$

For any subspace $S\subseteq G^n$ define a dual subspace $S^\perp$ as

$$S^\perp=\{f\in G^n:\omega(f,g)=0 \text{ for all } g\in S\}.$$

A subspace S is called *isotropic* iff $S\subseteq S^\perp$, i.e., $\omega(f,g)=0$ for any $f,g\in S$. A subspace S is called self-dual iff $S^\perp=S$. For any isotropic (self-dual) subspace $S\subset G^n$ one has $\dim(S)\leq n$ ($\dim(S)=n$).

The Hilbert space of n qubits will be denoted $\mathcal{B}^n$. A unitary operator $U:\mathcal{B}^n\to\mathcal{B}^n$ belongs to the *Clifford group*, $U\in\mathrm{Cl}(n)$, iff it maps σ-operators to σ-operators (up to a sign) under the conjugation. In other words, $U\in\mathrm{Cl}(n)$ iff there exists a map $u:G^n\to G^n$ and a function $\epsilon:G^n\to\{+1,-1\}$, such that

$$U\sigma(f)U^\dagger=\epsilon(f)\sigma(u(f)) \tag{3}$$

for any $f\in G^n$. Unitarity of U implies that u is a linear invertible map preserving the inner product ω, i.e.,

$$\omega(f,g)=\omega(u(f),u(g))$$

for all $f,g\in G^n$. Such linear maps constitute a binary symplectic group $\mathrm{Sp}_2(n)$. In fact, all $u\in\mathrm{Sp}_2(n)$ can be realized through an appropriate choice of $U\in\mathrm{Cl}(n)$.

A *stabilizer state* $|\Psi\rangle\in\mathcal{B}^n$ is an irreducible representation of a group $\{\epsilon(f)\sigma(f):f\in S\}$, where $S\subset G^n$ is a self-dual subspace and $\epsilon:S\to\{+1,-1\}$ is a function that accounts for a phase in a product of σ operators. In other words,

$$\sigma(f)|\Psi\rangle=\epsilon(f)|\Psi\rangle, \quad f\in S. \tag{4}$$

The state $|\Psi\rangle$ is uniquely specified by Eq. (4). The subspace S is referred to as a *stabilizer group* of $|\Psi\rangle$. Two stabilizer states have the same stabilizer group iff they can be mapped to each other

by a σ operator, see Ref. 17. Any stabilizer state can be represented as $|\Psi\rangle = U|0^{\otimes n}\rangle$ for some operator $U \in \mathrm{Cl}(n)$.

B. Local Clifford equivalence

A state $|\Psi\rangle \in \mathcal{B}^n$ is called *M-partite* iff the n qubits are distributed between a finite set of parties M, i.e.,

$$n = \sum_{\alpha \in M} n_\alpha, \quad n_\alpha \geq 0. \tag{5}$$

We shall be interested in equivalence classes (orbits) of stabilizer states under local Clifford unitary (LCU) operators.

Definition 1: M-partite stabilizer states $|\Psi\rangle, |\Psi'\rangle \in \mathcal{B}^n$ *are called LCU-equivalent iff there exist Clifford unitaries* $\{U_\alpha \in \mathrm{Cl}(n_\alpha)\}_{\alpha \in M}$ *such that*

$$|\Psi'\rangle = \bigotimes_{\alpha \in M} U_\alpha |\Psi\rangle .$$

For any vector $f \in G^n$ and party α denote by $f_\alpha \in G^{n_\alpha}$ a projection of f onto the party α (if one regards f as a binary string, f_α is a substring that includes all qubits owned by a party α). In particular, $f_\alpha = 0$ iff $\sigma(f)$ acts trivially on the party α.

Definition 2: Suppose n qubits are distributed among a set of parties M. Let $S \subseteq G^n$ *be a linear subspace. For each* $\alpha \in M$ *define a local subspace* $S_\alpha \subseteq S$ *and a colocal subspace* $S_{\hat{\alpha}} \subseteq S$ *as*

$$S_\alpha = \{g \in S : g_\beta = 0 \text{ for all } \beta \in M \setminus \alpha\},$$

and

$$S_{\hat{\alpha}} = \{g \in S : g_\alpha = 0\}.$$

In other words, $f \in S_{\hat{\alpha}}$ iff $\sigma(f)$ acts as the identity on the party α; $f \in S_\alpha$ iff $\sigma(f)$ acts as the identity on all parties $\beta \neq \alpha$. In the case $n_\alpha = 0$ we shall use a convention $S_\alpha = 0$ and $S_{\hat{\alpha}} = S$. If S is a stabilizer group of some state, we shall use the terms local (colocal) subspace and local (colocal) subgroup interchangeably.

Consider an M-party stabilizer state $|\Psi\rangle$. Let ρ_α be the reduced state of the party α. To simplify the discussion we shall assume that $\mathrm{Rk}(\rho_\alpha) = 2^{n_\alpha}$ for all $\alpha \in M$, that is, that all states under consideration have the maximal possible local ranks. Let S be a stabilizer group of $|\Psi\rangle$. One can easily check that the requirement $\mathrm{Rk}(\rho_\alpha) = 2^{n_\alpha}$ is equivalent to the local subgroup S_α being trivial.

Definition 3: An M-party stabilizer state $|\Psi\rangle$ *with a stabilizer group S has full local ranks iff all local subgroups of S are trivial*:

$$S_\alpha = 0 \quad \text{for all } \alpha \in M.$$

In general case, if $\mathrm{Rk}(\rho_\alpha) = 2^k$, one has $\dim(S_\alpha) = n_\alpha - k$. Equivalently, $n_\alpha - k$ copies of the one-qubit state $|0\rangle$ can be extracted from $|\Psi\rangle$ for each $\alpha \in M$ by local Clifford unitaries (this will follow from Theorem 2 with $S' = S_\alpha$). After such local extractions we arrive at a state with full local ranks. A necessary and sufficient criterion for LCU equivalence is given below.

Theorem 1: *Let* $|\Psi\rangle, |\Psi'\rangle \in \mathcal{B}^n$ *be M-party stabilizer states with full local ranks. Let* $S, S' \subset G^n$ *be their stabilizer groups. The state* $|\Psi\rangle$ *is LCU equivalent to* $|\Psi'\rangle$ *iff there exists a linear invertible map* $T : S \to S'$ *such that*

$$\omega(T(f)_\alpha, T(g)_\alpha) = \omega(f_\alpha, g_\alpha) \quad \text{for all } f, g \in S, \alpha \in M.$$

We shall prove Theorem 1 in the next section.

III. LOCAL EXTRACTION

Let $|\Psi\rangle \in \mathcal{B}^n$ be an M-party stabilizer state. The most interesting stabilizer states are *LCU-irreducible* ones (which in this paper we simply refer to as *irreducible*), which are not LCU equivalent to a collection of stabilizer states of smaller dimension. For example, if one considers the finest partition, $M=\{1,2,\ldots,n\}$, a state $|\Psi\rangle$ is irreducible iff it is entangled with respect to any bipartition. On the other hand, we shall see that for bipartite and tripartite systems ($|M|=2$ or $|M|=3$), the only irreducible states are the EPR and GHZ states. If $|\Psi\rangle$ is not irreducible, one can *extract* some simpler stabilizer state from it by LCU operators. Given two M-party states $|\Psi\rangle$ and $|\Psi'\rangle$, one can ask under what circumstances $|\Psi'\rangle$ is extractable from $|\Psi\rangle$. The goal of this section is to answer this question. Note that LCU-equivalence of states is just a special case of extraction, when $|\Psi'\rangle$ and $|\Psi\rangle$ are composed from the same number of qubits.

Definition 4: Let $|\Psi\rangle \in \mathcal{B}^n$ and $|\Psi'\rangle \in \mathcal{B}^k$ be M-party stabilizer states, such that

$$n=\sum_{\alpha\in M} n_\alpha, \quad k=\sum_{\alpha\in M} k_\alpha, \quad 0\le k_\alpha \le n_\alpha.$$

The state $|\Psi'\rangle$ is extractable from $|\Psi\rangle$ iff $|\Psi\rangle$ is LCU-equivalent to $|\Psi'\otimes\Psi''\rangle$ for some M-party stabilizer state $|\Psi''\rangle$.

Remark: An equality $k_\alpha=0$ means that the party α owns no qubits of the state $|\Psi'\rangle$. Analogously, $k_\alpha=n_\alpha$ implies that the party α owns no qubits of the state $|\Psi''\rangle$.

A necessary and sufficient criterion for a state $|\Psi'\rangle$ to be extractable from $|\Psi\rangle$ is given below.

Theorem 2: *Let $|\Psi\rangle \in \mathcal{B}^n$ and $|\Psi'\rangle \in \mathcal{B}^k$ be M-party stabilizer states with stabilizer groups $S\subset G^n$ and $S'\subset G^k$. The state $|\Psi'\rangle$ is extractable from $|\Psi\rangle$ iff there exists a linear injective map $T:S'\to S$ such that*

(i) $\omega(T(f)_\alpha, T(g)_\alpha)=\omega(f_\alpha,g_\alpha)$ *for all* $f,g\in S'$ *and* $\alpha\in M$;
(ii) $(T\cdot S')_{\hat{\alpha}}=T\cdot(S'_{\hat{\alpha}})$ *for all* $\alpha\in M$.

This theorem is a simple consequence of the following lemma.

Lemma 1: Suppose n qubits are distributed among a set of parties M. Let $S,S'\subset G^n$ be linear subspaces. The following statements are equivalent:

(1) *There exist local operators $\{u_\alpha\in \mathrm{Sp}_2(n_\alpha)\}_{\alpha\in M}$ such that*

$$S'=\left(\bigoplus_{\alpha\in M} u_\alpha\right)\cdot S,$$

(2) *There exists a linear invertible map $T:S\to S'$ such that*

(i) $\omega(T(f)_\alpha, T(g)_\alpha)=\omega(f_\alpha,g_\alpha)$ *for all* $f,g\in S$ *and* $\alpha\in M$;
(ii) $T\cdot S_{\hat{\alpha}}=S'_{\hat{\alpha}}$ *for all* $\alpha\in M$.

Here the direct sum $\oplus_{\alpha\in M}u_\alpha$ corresponds to a decomposition of G^n into its local subspaces, i.e., $G^n=\oplus_{\alpha\in M}G^n_\alpha$. A proof of the lemma is presented in Appendix B.

Proof of Theorem 2: The nontrivial part is to prove that existence of T with the properties (i), (ii) implies that $|\Psi'\rangle$ is extractable from $|\Psi\rangle$. Let us split the n_α qubits owned by the party $\alpha\in M$ into two subsets

$$\{1,2,\ldots,n_\alpha\}=A_\alpha\cup B_\alpha,$$

such that $|A_\alpha|=k_\alpha$. We shall refer to a qubit as an A-qubit (B-qubit) if it belongs to one of the subsets A_α (B_α). Any vector $f\in G^n$ can be represented as a direct sum $f=f_A\oplus f_B$, where f_A and f_B are projections of f onto A-qubits and B-qubits, respectively.

Let us define a linear subspace $R'\subset G^n$ that is equal to a direct sum of S' on A-qubits and the zero space on B-qubits, i.e.,

$$R' = \{f \in G^n : f_B = 0 \text{ and } f_A \in S'\}.$$

Define also a subspace $R = T \cdot S' \subseteq S$, i.e.,

$$R = \{f \in G^n : f = T(g) \text{ for some } g \in S'\}. \tag{6}$$

The map T regarded as a map from R' to R obviously satisfies condition (2) of Lemma 1. We conclude that there exists a linear symplectic operator $u : G^n \to G^n$ such that

$$R' = u \cdot R, \quad u = \bigoplus_{\alpha \in M} u_\alpha, \tag{7}$$

where $u_\alpha \in \mathrm{Sp}_2(n_\alpha)$.

Consider a linear subspace

$$Q = u \cdot S \subset G^n. \tag{8}$$

The fact that $u \in \mathrm{Sp}_2(n)$ implies that Q is self-dual. Let $|\Phi\rangle \in \mathcal{B}^n$ be a stabilizer state with the stabilizer group Q. ($|\Phi\rangle$ is unique up to multiplication by a σ operator.) Since u is a direct sum of local symplectic operators, $|\Phi\rangle$ is LCU equivalent to $|\Psi\rangle$.

We still must show that $|\Phi\rangle$ is a tensor product of two stabilizer states, $|\Phi\rangle = |\Phi_A \otimes \Phi_B\rangle$, that live on the A-qubits and B-qubits, respectively. Indeed, since R is a subgroup of S, it follows from Eqs. (7) and (8) that

$$R' \subseteq Q.$$

Thus the state $|\Phi\rangle$ satisfies stabilizer equations

$$\sigma(f)|\Phi\rangle = \epsilon(f)|\Phi\rangle, \quad f \in R', \tag{9}$$

for some function $\epsilon : R' \to \{+1, -1\}$. By the definition of R', any operator $\sigma(f)$, $f \in R'$ acts trivially on B-qubits. If we restrict our attention to A-qubits only, R' is a self-dual subspace (since $R \cong S'$). Thus the stabilizer equations (9) completely specify the state of the A-qubits [see the remarks following Eq. (4)]. Denote this state $|\Phi_A\rangle$. Since the states $|\Phi_A\rangle$ and $|\Psi'\rangle$ have the same stabilizer group, they coincide up to a σ operator. Thus $|\Phi\rangle$ is LCU equivalent to $|\Psi' \otimes \Phi_B\rangle$ for some stabilizer state $|\Phi_B\rangle$. On the other hand, $|\Phi\rangle$ is LCU equivalent to $|\Psi\rangle$. We have proved that $|\Psi'\rangle$ is extractable from $|\Psi\rangle$.

Conversely, suppose $|\Psi\rangle$ is LCU equivalent to $|\Psi' \otimes \Psi''\rangle$. This means that $S = u \cdot (S' \oplus S'')$, where S'' is a self-dual subspace, $u = \oplus_{\alpha \in M} u_\alpha$ is a local symplectic operator, and the direct sum corresponds to the bipartition of all qubits in the state $|\Psi' \otimes \Psi''\rangle$. One can easily check that a map

$$T(f) = u \cdot (f \oplus 0)$$

from S' to S satisfies conditions (i) and (ii). The theorem is proved. □

Remark: Condition (ii) in Theorem 2 cannot be dropped. Indeed, consider as an example three-party states, $M = \{A, B, C\}$. Let $|\Psi\rangle = |\Psi_3^+\rangle$ be the GHZ state and $|\Psi'\rangle = |\Psi^+\rangle$ be the EPR state shared by A and B. Obviously, $|\Psi'\rangle$ cannot be extracted from $|\Psi\rangle$ without classical communication. However, the linear injective map T satisfying condition (i) exists. Indeed, consider a mapping

$$\sigma^x \otimes \sigma^x \to \sigma^x \otimes \sigma^x \otimes \sigma^x,$$

$$\sigma^z \otimes \sigma^z \to \sigma^z \otimes \sigma^z \otimes I$$

between stabilizer generators of $|\Psi'\rangle$ and $|\Psi\rangle$. It can be easily converted to a map $T : S' \to S$ between the stabilizer groups. This map preserves local commutation rules, so condition (i) is satisfied.

Proof of Theorem 1: Consider a special case of Theorem 2 with $k_\alpha = n_\alpha$ for all $\alpha \in M$, i.e., with

the state $|\Psi''\rangle$ being a complex number. In this case $S,S' \subset G^n$ are self-dual subspaces, so that $\dim(S)=\dim(S')=n$. Thus T is a linear invertible map and $T\cdot S'=S$. On the other hand, the statement "$|\Psi'\rangle$ is extractable from $|\Psi\rangle$" translates into "$|\Psi'\rangle$ is LCU equivalent to $|\Psi\rangle$." What we obtain is exactly Theorem 1 with T replaced by T^{-1} and with the extra condition (ii). We will show now that (ii) can be derived from (i), the equality $T\cdot S'=S$, and the maximal local rank assumption.

Indeed, consider some particular α and take any vector $f \in S'_{\hat{\alpha}}$, so $f_\alpha=0$. Denote $h=T(f) \in S$. Condition (i) tells us that

$$\omega(h_\alpha, g_\alpha) = \omega(f_\alpha, (T^{-1}(g))_\alpha) = 0 \quad \text{for any } g \in S.$$

Consider a vector $\tilde{h} \in G^n_\alpha$ such that $\tilde{h}_\alpha=h_\alpha$. Then $\omega(\tilde{h},g)=0$ for any $g \in S$, that is $\tilde{h} \in S^\perp$. Since $S^\perp=S$ we have $\tilde{h} \in S \cap G^n_\alpha=S_\alpha=0$. We conclude that $h_\alpha=0$, that is $h \in S_{\hat{\alpha}}$. This proves that

$$T \cdot S'_{\hat{\alpha}} \subseteq S_{\hat{\alpha}}.$$

Applying the same arguments to the map $T^{-1}: S \to S'$ [which, of course, also satisfies condition (i)] one gets

$$T^{-1} \cdot S_{\hat{\alpha}} \subseteq S'_{\hat{\alpha}}.$$

Therefore $S'_{\hat{\alpha}}$ and $S_{\hat{\alpha}}$ have the same dimension, and thus $T\cdot S'_{\hat{\alpha}}=S_{\hat{\alpha}}$. □

Remark: In fact, a little bit more work shows that the full local ranks assumption in Theorem 1 can be dropped. We sacrifice some generality for the sake of readability.

IV. GHZ-EXTRACTION FORMULA

Given a set of parties M, $|M|=m$, consider an M-party analogue of the GHZ state

$$|\Psi^+_m\rangle = \frac{1}{\sqrt{2}}(|0^{\otimes m}\rangle + |1^{\otimes m}\rangle) \in \mathcal{B}^m.$$

It is a stabilizer state with a stabilizer group generated by a vector $\bar{f} \in G^m$ such that

$$\sigma(\bar{f}) = \sigma^x_1 \otimes \sigma^x_2 \otimes \cdots \otimes \sigma^x_m, \tag{10}$$

and vectors $\{f_{\alpha\beta} \in G^m\}_{\alpha,\beta \in M}$ such that

$$\sigma(f_{\alpha\beta}) = \sigma^z_\alpha \otimes \sigma^z_\beta \tag{11}$$

(the identity factors are suppressed). The vectors $\bar{f}$, $f_{\alpha\beta}$ constitute an overcomplete basis of the stabilizer group.

Given an M-party stabilizer state $|\Psi\rangle \in \mathcal{B}^n$, one can ask how many copies of $|\Psi^+_m\rangle$ can be extracted from $|\Psi\rangle$ by local Clifford unitaries. The goal of this section is to answer this question. Let S be a stabilizer group of $|\Psi\rangle$, and $S_{\hat{\alpha}} \subseteq S$, $\alpha \in M$, be its colocal subgroups (see Definition 2). Define a subgroup

$$S_{\text{loc}} = \sum_{\alpha \in M} S_{\hat{\alpha}} \tag{12}$$

generated by all colocal subgroups. The sum above is generally not a direct one, since the colocal subgroups may overlap. By definition, $S_{\text{loc}} \subseteq S$, and, in general, $S_{\text{loc}} \subset S$. In the latter case one has a deficit of local stabilizer elements, meaning that for any choice of a basis in S there will be at least $n-\dim(S_{\text{loc}})$ basis vectors having support on all m parties $\alpha \in M$. We will see that each of these nonlocal basis vectors can be identified with the $\bar{f}$ element of the stabilizer of a state $|\Psi^+_m\rangle$ [see Eq. (10)].

It was pointed out in Ref. 12 that a functional

$$\Delta(\Psi) = n - \dim(S_{\mathrm{loc}}) = \dim(S) - \dim(S_{\mathrm{loc}}) \tag{13}$$

can be used as an entanglement measure that quantifies truly multipartite correlations in $|\Psi\rangle$. In the present paper we go further and prove the following theorem.

Theorem 3: *Let $|\Psi\rangle \in \mathcal{B}^n$ be an M-party stabilizer state with a stabilizer group S. Suppose that $m=|M| \geq 3$. The maximal number of states $|\Psi_m^+\rangle$ extractable from $|\Psi\rangle$ by local Clifford unitaries is equal to $\Delta(\Psi)$.*

Remarks: (1) Note that the functional $\Delta(\Psi)$ is invariant under extraction of local $|0\rangle$ states. Thus we can safely assume that $|\Psi\rangle$ has full local ranks. (2) The generalization of the theorem to arbitrary LU operators is discussed in Sec. V. (3) A shorter but less constructive proof of the theorem is given in Appendix A.

Proof: For each $\alpha \in M$ define a subspace $\mathcal{L}_\alpha \in G^n$ as

$$\mathcal{L}_\alpha = \{f \in G_\alpha^n : \omega(f,g) = 0 \text{ for all } g \in S_{\mathrm{loc}}\}.$$

Here G_α^n is the local subspace of G^n corresponding to the party α (see Definition 2). To illustrate the usefulness of this definition, consider as an example $|\Psi\rangle = |\Psi_m^+\rangle$. Then the subgroup S_{loc} is generated by vectors $\{f_{\alpha\beta}\}$ [see Eq. (11)], while $\mathcal{L}_\alpha$ is a one-dimensional subspace generated by σ_α^z. The remaining stabilizer generator of the GHZ state $\bar{f}$ anticommutes with σ_α^z for any $\alpha \in M$. Thus any product $\sigma_\alpha^z \otimes \sigma_\beta^z$ commutes with both $\bar{f}$ and stabilizer elements from S_{loc}. Therefore, $\sigma_\alpha^z \otimes \sigma_\beta^z$ is in the stabilizer of $|\Psi\rangle$. Similarly, in the general case, we shall use the subspaces $\mathcal{L}_\alpha$ to construct 2-local stabilizer elements of $|\Psi\rangle$ that are analogous to $\sigma_\alpha^z \otimes \sigma_\beta^z$ stabilizer elements of the GHZ state.

Our first goal is to prove that

$$\dim(\mathcal{L}_\alpha) = \Delta(\Psi) \quad \text{for any } \alpha \in M. \tag{14}$$

Choose an arbitrary subgroup $S_{\mathrm{ent}} \subseteq S$ such that

$$S = S_{\mathrm{loc}} \oplus S_{\mathrm{ent}}. \tag{15}$$

By definition of S_{loc}, any nonzero vector $f \in S_{\mathrm{ent}}$ has support on all parties, i.e., $f_\alpha \neq 0$ for all $\alpha \in M$. Define a bilinear form

$$\eta_\alpha : \mathcal{L}_\alpha \otimes S_{\mathrm{ent}} \to \{0,1\}, \quad \eta_\alpha(f,g) = \omega(f_\alpha, g_\alpha).$$

We claim that the form η_α is nonsingular, that is

$$\eta_\alpha(f,g) = 0 \quad \text{for all } g \in S_{\mathrm{ent}} \text{ iff } f = 0, \tag{16}$$

and

$$\eta_\alpha(f,g) = 0 \quad \text{for all } f \in \mathcal{L}_\alpha \quad \text{iff } g = 0. \tag{17}$$

Indeed, suppose $f \in \mathcal{L}_\alpha$ and $\omega(f,g)=0$ for all $g \in S_{\mathrm{ent}}$. By definition of $\mathcal{L}_\alpha$, we have $\omega(f,g)=0$ for all $g \in S_{\mathrm{loc}}$. Thus the decomposition Eq. (15) implies that $f \in S^\perp$. But since $S^\perp = S$, one has $f \in S$. Since the state $|\Psi\rangle$ has full local ranks (see the remark after the theorem), $\mathcal{L}_\alpha \cap S \subseteq S_\alpha = 0$, that is $f=0$. The property Eq. (16) is proved.

Suppose $g \in S_{\mathrm{ent}}$ and $\omega(f,g)=0$ for all $f \in \mathcal{L}_\alpha$ (for some particular $\alpha \in M$), that is $g \in \mathcal{L}_\alpha^\perp$. The definition of $\mathcal{L}_\alpha$ implies that

$$g \in \mathcal{L}_\alpha^\perp \text{ iff } g_\alpha = h_\alpha \quad \text{for some } h \in S_{\mathrm{loc}}.$$

[Here we use the fact that $(\mathcal{L}^\perp)^\perp = \mathcal{L}$ for any binary subspace $\mathcal{L}$.] Thus there exists a vector $h \in S_{\mathrm{loc}}$ such that $(h+g)_\alpha = 0$, i.e., $h+g \in S_{\mathrm{loc}}$. But this means that $g \in S_{\mathrm{loc}}$. Since decomposition Eq. (15) is a direct sum, the inclusion $g \in S_{\mathrm{ent}} \cap S_{\mathrm{loc}}$ implies $g=0$. The property Eq. (17) is proved.

The fact that η_α is nonsingular implies that the subspaces $\mathcal{L}_\alpha$ and S_{ent} have the same dimension. But from Eq. (15) we infer that $\dim(S_{\text{ent}})=\Delta(\Psi)$. The formula Eq. (14) is proved.

Denote $p=\Delta(\Psi)$ and choose an arbitrary basis $\bar{g}_1,\bar{g}_2,\ldots,\bar{g}_p$ in the subspace S_{ent}. For each $\alpha\in M$ choose the dual basis $g_{\alpha 1},g_{\alpha 2},\ldots,g_{\alpha p}$ in the subspace $\mathcal{L}_\alpha$ with respect to the form η_α. That is, the set of vectors $\{g_{\alpha j}\}_j$ must satisfy equations

$$\eta_\alpha(g_{\alpha j},\bar{g}_k)=\delta_{jk} \quad \text{for all } 1\le j,k\le p \quad \text{and } \alpha\in M. \tag{18}$$

Define vectors $g_{\alpha\beta j}\in G^n$ by

$$g_{\alpha\beta j}=g_{\alpha j}+g_{\beta j}, \quad j=1,\ldots,p.$$

It follows from Eq. (18) that

$$\omega(g_{\alpha\beta j},\bar{g}_k)=\eta_\alpha(g_{\alpha j},\bar{g}_k)+\eta_\beta(g_{\beta j},\bar{g}_k)=\delta_{jk}+\delta_{jk}=0.$$

Thus $g_{\alpha\beta j}\in S_{\text{ent}}^{\perp}$. On the other hand, by definition of the subspaces $\mathcal{L}_\alpha$, one has $\mathcal{L}_\alpha\subseteq S_{\text{loc}}^{\perp}$ for all $\alpha\in M$, that is $g_{\alpha\beta j}\in S_{\text{loc}}^{\perp}$. We infer from Eq. (15) that $g_{\alpha\beta j}\in S^{\perp}$. Since S is self-dual, we conclude that $g_{\alpha\beta j}\in S$.

All arguments above apply equally well to $m=2$ and $m\ge 3$. From now on we shall focus on the case $m\ge 3$.

We would like to show that the subspaces $\mathcal{L}_\alpha$ are isotropic, i.e.,

$$\omega(f,g)=0 \quad \text{for all } f,g\in\mathcal{L}_\alpha, \quad \alpha\in M. \tag{19}$$

Indeed, it suffices to show that $\omega(g_{\alpha j},g_{\alpha k})=0$ for any j,k. Assuming that $m\ge 3$, choose an arbitrary triple $\alpha,\beta,\gamma\in M$, such that $\alpha\ne\beta\ne\gamma$. Taking into account that $g_{\alpha\beta j}\in S$, $g_{\alpha\gamma k}\in S$, we obtain that

$$0=\omega(g_{\alpha\beta j},g_{\alpha\gamma k})=\omega(g_{\alpha j},g_{\alpha k}).$$

The property Eq. (19) is proved.

By definition, a vector $g_{\alpha\beta j}$ has a support only on two parties. If $m\ge 3$ it means that

$$g_{\alpha\beta j}\in S_{\text{loc}} \tag{20}$$

for all pairs of parties $\alpha,\beta\in M$ and $j=1,\ldots,p$.

Our next goal is to adjust the subspace S_{ent} to make it "locally isotropic," i.e., to fulfill the following property:

$$\omega(f_\alpha,g_\alpha)=0 \quad \text{for all } f,g\in S_{\text{ent}}, \quad \alpha\in M.$$

This adjustment can be achieved by adding a proper "local shift" taken from the subspaces $\mathcal{L}_\alpha$. Namely, the basis vectors $\bar{g}_j\in S_{\text{ent}}$ must be replaced by new basis vectors according to

$$\bar{g}_j\to\bar{g}_j+\sum_{\alpha\in M}\sum_{l=1}^{j-1}\Gamma_{jl}^{\alpha}g_{\alpha l}, \quad j=1,\ldots,p, \tag{21}$$

where

$$\Gamma_{jl}^{\alpha}=\omega((\bar{g}_j)_\alpha,(\bar{g}_l)_\alpha).$$

One can easily check that after this replacement we end up with

$$\omega((\bar{g}_j)_\alpha,(\bar{g}_k)_\alpha)=0$$

for all $\alpha\in M$ and all j,k. In addition, the fact that S_{ent} is an isotropic subspace, i.e., $\omega(\bar{g}_j,\bar{g}_k)=0$, implies that

$$\sum_{\alpha\in M}\Gamma^{\alpha}_{jl}=0$$

for any fixed j,l. This means that the vector added to $\bar{g}_j$ in Eq. (21) belongs to the stabilizer group S. Accordingly, the adjusted $S_{\rm ent}$ is still a subspace of S. Moreover, Eq. (20) implies that the added vector belongs to $S_{\rm loc}$, so the decomposition $S=S_{\rm loc}\oplus S_{\rm ent}$ remains a direct sum.

Summarizing, after the adjustment described above we can assume that

$$\omega(g_{\alpha j},g_{\alpha k})=0,\quad \omega((\bar{g}_j)_\alpha,(\bar{g}_k)_\alpha)=0,\quad \omega(g_{\alpha j},\bar{g}_k)=\delta_{jk}, \tag{22}$$

for all $\alpha\in M$. Here j and k are arbitrary integers in the range $1,\ldots,p$.

Denote by $S_{\rm ghz}\subset G^{m\cdot p}$ a stabilizer group of p copies of the GHZ state $|\Psi^+_m\rangle$. As generators of $S_{\rm ghz}$ let us choose p copies of the canonical GHZ generators [see Eqs. (10) and (11)]. Denote them as $\bar{f}_j$ and $f_{\alpha\beta j}$, where $j=1,\ldots,p$ refers to different copies of $|\Psi^+_m\rangle$. Define a linear map $T:S_{\rm ghz}\to S$ such that its action on the generators is as follows:

$$T(\bar{f}_j)=\bar{g}_j,\quad T(f_{\alpha\beta j})=g_{\alpha\beta j},$$

where $j=1,\ldots,p$ and $\alpha,\beta\in M$. We would like to prove that T satisfies all conditions of Theorem 2.

Using the fact that the vectors $\{\bar{g}_j,g_{\alpha k}\}$, $j,k=1,\ldots,p$, $\alpha\in M$ are linearly independent, one can easily show that T is a linear injection. Taking into account that $\bar{g}_1,\ldots,\bar{g}_p$ span the subspace $S_{\rm ent}$ that has no intersection with $S_{\rm loc}$, we conclude that $(T\cdot S_{\rm ghz})_{\hat{\alpha}}=T\cdot(S_{\rm ghz})_{\hat{\alpha}}$. Condition (i) of Theorem 2 follows from the local commutation relations Eq. (22). Thus one can extract *at least* p copies of the state $|\Psi^+_m\rangle$ from $|\Psi\rangle$.

Conversely, to prove the upper bound, assume that one can extract q copies of $|\Psi^+_m\rangle$ from $|\Psi\rangle$. Denote by $S_{\rm ghz}$ the stabilizer group of $|q\cdot\Psi^+_m\rangle$ and let $\bar{f}_1,\ldots,\bar{f}_q$ be the canonical σ^x-type stabilizers [see Eq. (10)]. Let $T:S_{\rm ghz}\to S$ be the linear injective map whose existence is guaranteed by Theorem 2. Clearly, a linear span of $\bar{f}_1,\ldots,\bar{f}_q$ has no intersection with colocal subspaces $(S_{\rm ghz})_{\hat{\alpha}}$. According to Theorem 2, vectors $T(\bar{f}_1),\ldots,T(\bar{f}_q)$ are linearly independent and their linear span has no intersection with $S_{\rm loc}$. This means that $\dim(S_{\rm loc})\le n-q$. Therefore $p\ge q$, i.e., one can extract *at most* p copies of $|\Psi^+_m\rangle$. □

V. BEYOND STABILIZER STATES

In this section we argue that the functional $\Delta(\Psi)$ defined in Eq. (13) for stabilizer states can be naturally extended to arbitrary multipartite states. Namely, it coincides with a measure of multipartite correlations introduced by Linden, Popescu, and Wootters in Ref. 14. A similar measure has been introduced also for multipartite probability distributions in Ref. 18. It will allow us to show that $\Delta(\Psi)$ is equal to the number of GHZ states extractable from $|\Psi\rangle$ by *arbitrary* local unitaries.

Denote by $D(\mathcal{B}^n)$ a set of all mixed n-qubit states. Assume that n qubits are distributed between a set of parties M. Let $|\Psi\rangle\in\mathcal{B}^n$ be an arbitrary M-party state. Define a set

$$\Gamma(\Psi)=\{\rho\in D(\mathcal{B}^n):{\rm Tr}_\alpha(\rho)={\rm Tr}_\alpha(|\Psi\rangle\langle\Psi|)\ \alpha\in M\},$$

where Tr_α is the partial trace. In other words, $\rho\in\Gamma(\Psi)$ iff ρ agrees with $|\Psi\rangle$ on any subset of $|M|-1$ parties. Following Ref. 14, define a functional

$$\Omega(\Psi)=\max_{\rho\in\Gamma(\Psi)}S(\rho), \tag{23}$$

where $S(\rho)=-{\rm Tr}\,\rho\log(\rho)$ is the von Neumann entropy. For bipartite states $\Omega(\Psi)$ coincides with the entanglement entropy (except for a factor 2) (see Ref. 14). The main result of this section is the following.

Theorem 4: *For any M-party stabilizer state $|\Psi\rangle$ with a stabilizer group S one has*

$$\Omega(\Psi) = \dim(S) - \dim(S_{\mathrm{loc}}),$$

where $S_{\mathrm{loc}} = \Sigma_{\alpha \in M} S_{\hat{\alpha}}$.

The proof is based on the following observation.

Lemma 2: *Let* $|\Psi\rangle$ *be an M-party stabilizer state with a stabilizer group S. If S is generated by its colocal subgroups*, $S = S_{\mathrm{loc}}$, *then* $|\Psi\rangle\langle\Psi|$ *is the only state that belongs to the set* $\Gamma(\Psi)$.

In other words a state $|\Psi\rangle$ with $S = S_{\mathrm{loc}}$ is the unique (mixed) state compatible with partial traces of $|\Psi\rangle$.

Proof: We shall use stabilizer equations $\sigma(f)|\Psi\rangle = \epsilon(f)|\Psi\rangle$, $f \in S$, uniquely specifying $|\Psi\rangle$ [see Eq. (4)]. Take any state $\rho \in \Gamma(\Psi)$. For any $f \in S_{\hat{\alpha}}$ one has

$$\mathrm{Tr}(\sigma(f)\rho) = \langle\Psi|\sigma(f)|\Psi\rangle = \epsilon(f).$$

Now consider a projector $\Pi = (1/2)(I + \epsilon(f)\sigma(f))$. Then $\mathrm{Tr}(\Pi\rho) = 1$. This is possible only if the range of ρ coincides with the range of Π. Thus, $\Pi\rho = \rho$, i.e.,

$$\sigma(f)\rho = \rho\sigma(f) = \epsilon(f)\rho \quad \text{for any } f \in S_{\hat{\alpha}}, \quad \alpha \in M. \tag{24}$$

Since S is generated by the subgroups $S_{\hat{\alpha}}$, the equalities Eq. (24) actually hold for any $f \in S$. But equations $\sigma(f)\rho = \epsilon(f)\rho$, $f \in S$, mean that ρ has support on the subspace stabilized by S, that is $\rho = |\Psi\rangle\langle\Psi|$. □

Corollary 1: *Let* $|\Psi\rangle = |\Psi' \otimes \Phi\rangle$ *be a collection of two M-party stabilizer states*, *such that* $|\Phi\rangle$ *satisfies the conditions of Lemma 2. Then*

$$\Gamma(\Psi) = \Gamma(\Psi') \otimes |\Phi\rangle\langle\Phi|. \tag{25}$$

To prove the corollary, take any state $\rho \in \Gamma(\Psi)$ and apply Lemma 2 to the partial trace of ρ over the first subsystem. Now we are ready to prove Theorem 4.

Proof: Let $p = \dim(S) - \dim(S_{\mathrm{loc}})$ and $m = |M|$. Obviously, $\Omega(\Psi)$ is invariant under local unitaries. As we know from Theorem 3, $|\Psi\rangle$ is LCU equivalent to a collection of p M-party GHZ states, $|p \cdot \Psi_m^+\rangle$, and some M-party stabilizer state $|\Phi\rangle$ satisfying the conditions of Lemma 2. Taking into account the factorization property Eq. (25), we obtain

$$\Omega(\Psi) = \Omega(p \cdot \Psi_m^+).$$

It remains to be shown that

$$\Omega(p \cdot \Psi_m^+) = p. \tag{26}$$

First of all, consider a mixed version of the GHZ state,

$$\rho = (1/2)|0^{\otimes m}\rangle\langle 0^{\otimes m}| + (1/2)|1^{\otimes m}\rangle\langle 1^{\otimes m}|. \tag{27}$$

It is clear that $\rho \in \Gamma(\Psi_m^+)$. Thus

$$\Omega(p \cdot \Psi_m^+) \geq S(\rho^{\otimes p}) = pS(\rho) = p. \tag{28}$$

To get an upper bound, take any $\rho \in \Gamma(\Psi)$. Divide M into three nonempty subsets by an arbitrary way: $M = M_1 \cup M_2 \cup M_3$. Let ρ_j and ρ_{jk} be the reduced states of the subset M_j and $M_j \cup M_k$ (with respect to ρ). The strong subadditivity inequality shows that

$$S(\rho) + S(\rho_1) \leq S(\rho_{12}) + S(\rho_{13}).$$

But the condition $\rho \in \Gamma(p \cdot \Psi_m^+)$ implies that all the states ρ_1, ρ_{12}, and ρ_{13} are the mixed versions of the GHZ state [Eq. (27)], that is $S(\rho_1) = S(\rho_{12}) = S(\rho_{13}) = p$. Thus we get $S(\rho) \leq p$. Combining it with the lower bound Eq. (28) we get Eq. (26). □

Corollary 2: *Theorem 3 gives the GHZ extraction yield from a stabilizer state for arbitrary local unitary operators*.

Proof: Let $p = \Delta(\Psi)$ and q be the number of GHZ states extractable from $|\Psi\rangle$ by local

unitaries. Obviously, $q \geq p$. Since the functional $\Omega(\Psi)$ is LU invariant, we infer from Eq. (26) that $\Omega(\Psi) \geq \Omega(q \cdot \Psi_m^+) = q$. It follows from Theorem 4 that $p \geq q$. Thus $p = q$. □

VI. TRIPARTITE STABILIZER STATES

As a simple application of Theorem 3 let us show that any tripartite stabilizer state is LCU equivalent to a collection of states from the set $E_3 = \{|0\rangle, |\Psi^+\rangle, |\Psi_3^+\rangle\}$. After extraction of all local $|0\rangle$ states one can consider only states with full local ranks.

Theorem 5: *Let $|\Psi\rangle \in \mathcal{B}^n$ be a stabilizer state with full local ranks shared by a set of parties $M = \{A, B, C\}$. Let S be a stabilizer group of $|\Psi\rangle$ and $S_{\mathrm{loc}} = \Sigma_{\alpha \in M} S_{\hat{\alpha}}$. Denote $p = \dim(S) - \dim(S_{\mathrm{loc}})$ and $d(\alpha) = \dim(S_{\hat{\alpha}})$. The state $|\Psi\rangle$ is LCU equivalent to a collection of*

(i) $(d(A) - p)/2$ *copies of* $|\Psi^+\rangle$ *shared by B and C*,
(ii) $(d(B) - p)/2$ *copies of* $|\Psi^+\rangle$ *shared by C and A*,
(iii) $(d(C) - p)/2$ *copies of* $|\Psi^+\rangle$ *shared by A and B*,
(iv) p *copies of the GHZ state* $|\Psi_3^+\rangle$.

Proof: As we already know from Theorem 3, one can extract p copies of $|\Psi_3^+\rangle$ from $|\Psi\rangle$. This allows us to consider only the case $p = 0$. Equivalently, we can assume that S is equal to the sum of its colocal subgroups, $S = S_{\mathrm{loc}}$. The full local ranks assumption means that the colocal subgroups do not overlap, i.e., $S_{\hat{\alpha}} \cap S_{\hat{\beta}} = 0$ for $\alpha \neq \beta$. Thus S can be represented as a direct sum,

$$S = S_{\hat{A}} \oplus S_{\hat{B}} \oplus S_{\hat{C}}. \tag{29}$$

Let us prove that $|\Psi\rangle$ is LCU equivalent to a collection of EPR states $|\Psi^+\rangle$. The proof consists of applying the same arguments to each pair of parties, so let us focus on the pair AB.

Denote $R \equiv S_{\hat{C}}$ and consider a bilinear form

$$\eta : R \otimes R \to \{0,1\}, \quad \eta(f,g) = \omega(f_A, g_A),$$

for any $f, g \in R$. We claim that η is a nonsingular form. Indeed, suppose that

$$\eta(f,g) = 0 \quad \text{for all } g \in R \tag{30}$$

and prove that $f = 0$. Indeed, Eq. (30) and decomposition Eq. (29) imply that $\omega(f_A, h_A) = 0$ for any $h \in S$. We can rewrite this as $\omega(\tilde{f}, h) = 0$ for any $h \in S$, where $\tilde{f} \in G_A^n$ is chosen such that $\tilde{f}_A = f_A$. It means that $\tilde{f} \in S^{\perp}$, that is $\tilde{f} \in S \cap G_A^n = S_A = 0$. Therefore, $f_A = 0$ and so $f \in S_B = 0$. We conclude that $f = 0$ and η is nonsingular.

Applying the Gram-Schmidt orthogonalization procedure, one can check that R must have an even dimension, $\dim(R) = 2l$, and that there exists a symplectic basis $\{g_j, \bar{g}_j\}_{j=1,\ldots,l}$ of R such that

$$\eta(g_j, g_k) = 0, \quad \eta(\bar{g}_j, \bar{g}_k) = 0, \quad \eta(g_j, \bar{g}_k) = \delta_{jk}. \tag{31}$$

(For a proof see Dickson's theorem in Ref. 19, Chap. 15.)

Denote by $S_{\mathrm{EPR}} \subset G^{2l}$ a stabilizer group of l copies of the EPR state, $|l \cdot \Psi^+\rangle$. We consider $|l \cdot \Psi^+\rangle$ as a tripartite state, such that C holds no qubits at all, and there are l EPR states shared by A and B. The group S_{EPR} has independent generators $\{f_j, \bar{f}_j\}_{j=1,\ldots,l}$ such that

$$\sigma(f_j) = \sigma_j^z \otimes \sigma_j^z, \quad \sigma(\bar{f}_j) = \sigma_j^x \otimes \sigma_j^x,$$

where j labels the copies of $|\Psi^+\rangle$, i.e., $j = 1, \ldots, l$. Define a linear map $T : S_{\mathrm{EPR}} \to S$ such that

$$T(f_j) = g_j, \quad T(\bar{f}_j) = \bar{g}_j, \quad j = 1, \ldots, l.$$

Obviously, $T(S_{\mathrm{EPR}}) = R$. We would like to check that T satisfies all the conditions of Theorem 2. Indeed, it is a linear injection because the images of the basis vectors of S_{EPR} are linearly independent. Condition (i) follows directly from Eq. (31). Condition (i) holds because S_{EPR} has trivial

colocal subgroup and so does R. Thus l copies of $|\Psi^+\rangle$ shared between A and B can be extracted from $|\Psi\rangle$.

Applying the same arguments to other pairs of parties, we conclude that AB, BC, and AC can extract $d(C)/2$, $d(A)/2$, and $d(B)/2$ EPR states, respectively. The total number of qubits in the extracted EPR states is $d(A)+d(B)+d(C)$ which coincides with $\dim(S)=n$, see Eq. (29). Thus no qubits are left after the extraction.

To conclude the proof it is sufficient to note that extraction of a single GHZ state $|\Psi_3^+\rangle$ reduces each of the dimensions $\dim(S_{\hat{\alpha}})$ by one. □

A simple corollary of Theorem 5 is that two tripartite stabilizer states $|\Psi\rangle, |\Psi'\rangle$ are LU-equivalent iff their decompositions into $|\Psi^+\rangle$, $|\Psi_3^+\rangle$, and local $|0\rangle$ states coincide. Indeed, make use of the fact that a partial trace of $|\Psi_3^+\rangle$ over any qubit is a separable state. LU equivalence of $|\Psi\rangle$ and $|\Psi'\rangle$ implies that all partial traces of $|\Psi\rangle$ and $|\Psi'\rangle$ are LU equivalent; that is, the number of singlets $|\Psi^+\rangle$ extractable by each pair of parties is the same for $|\Psi\rangle$ and $|\Psi'\rangle$. By counting the remaining dimensions we conclude that the numbers of GHZ's $|\Psi_3^+\rangle$ extractable from $|\Psi\rangle$ and $|\Psi'\rangle$ are the same. Thus LU-equivalence classes of tripartite stabilizer states are completely specified by the numbers of $|\Psi^+\rangle$ and $|\Psi_3^+\rangle$ in the decomposition of Theorem 5.

Remark: One could prove Theorem 5 by making use of mixed stabilizer states. A mixed stabilizer state is a maximally mixed state encoded by some stabilizer code. Bipartite mixed stabilizer states can be classified using the techniques of the paper.[12] It turns out that any bipartite mixed stabilizer state is LCU equivalent to a collection of (i) local pure states; (ii) local maximally mixed states; (iii) EPR states; (iv) two-qubit mixed states $(1/2)|0,0\rangle\langle 0,0|+(1/2)|1,1\rangle\langle 1,1|$. Combining this fact with the purification theorem one immediately gets Theorem 5. We refrain from pushing this approach further, because it is less symmetric than the one presented above.

VII. SATURATION OF MULTIPARTITE ENTANGLEMENT ENTROPY IN SPIN LATTICES

As was mentioned in the introduction, characterization of multipartite entangled states might be useful for quantum cryptography and quantum game theory. Another natural area to look for applications is condensed matter physics. It has been realized recently that ground states of d-dimensional spin lattices with spatially uniform short-range interactions are distinguished among all other states by obeying the *entropic area law* (see Ref. 16 and references therein). According to this law, entanglement entropy of a block of spins with a spatial size L (thus containing about L^d spins) scales as $E(L)=b\cdot L^{d-1}+o(L^{d-1})$, where b is a constant (critical systems are set aside). This law can be understood, at least very roughly, if one regards the ground state as a collection of short-range EPR states. Then $E(L)$ is equal to the number of EPR states that stretch between the interior and exterior of the block. It is obviously proportional to the area of the boundary. From this standpoint (which is of course only a rude approximation) $E(L)$ can be regarded as the maximal number of EPR states extractable from the ground state by local unitaries.

To get more insight into the structure of entanglement of the ground state, one can consider a partition of the lattice into several blocks of spins (which may or may not have junction points), and ask how many multipartite GHZ states can be extracted from the ground state by local unitaries. In this section we shall try to follow this program.

Let us first set the problem more strictly. We shall focus on the two-dimensional case (a generalization to an arbitrary d is trivial). Suppose that the system under consideration consists of n qubits that are assigned to sites of a 2D regular lattice. Let $|\Psi_0\rangle \in \mathcal{B}^n$ be the ground state of the system. Consider a partition of the lattice into three segments A, B, and C which have a common junction point O, while pairwise intersections are one-dimensional rays incident to O (see Fig. 1). The problem is to compute the quantity

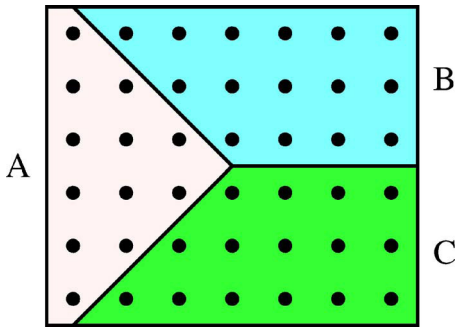

FIG. 1. (Color online) A junction point.

$$E_3(n) = \Omega(\Psi_0),$$

defined by Eq. (23). As was argued in Sec. V, the quantity $\Omega(\Psi_0)$ is a natural generalization of the GHZ extraction yield beyond stabilizer states. We are particularly interested in the asymptotic behavior of $E_3(n)$ when n goes to infinity (the thermodynamic limit).

It is natural to expect that $E_3(n)$ does not diverge as $n \to \infty$, since tripartite correlations must be formed by interactions acting on spins near the junction point O. As long as the Hamiltonian of the system is short ranged, there is only a finite number of such interactions. In other words, a natural conjecture is that

$$\sup_n E_3(n) < \infty . \tag{32}$$

This inequality says that $E_3(n)$ can be bounded from above by a constant that does not depend on the size of the system (this constant may depend upon the details of the system's Hamiltonian, however). The conjecture Eq. (32), if it is true, would generalize the entanglement saturation phenomenon found for one-dimensional spin chains[16] to higher dimensions.

In the rest of this section we prove Eq. (32) for a special case when (i) $|\Psi_0\rangle$ is a stabilizer state; (ii) the stabilizer group of $|\Psi_0\rangle$ has a set of geometrically local generators. Well-known examples of such states are the 2D cluster state[6] or the planar analogue of Kitaev's toric code state.[15]

Let $|\Psi_0\rangle \in \mathcal{B}^n$ be a stabilizer state and $S \subset G^n$ be its stabilizer group. Let us say that S has an *interaction length* l, iff there exists a family of vectors $f_1, \ldots, f_p \in S$, such that (i) S is generated by $f_1, \ldots, f_p$; (ii) for any j, the support of the vector f_j can be covered by a $l \times l$ rectangular block. We do not assume that the f_j are linearly independent, so in general $p > n$. However we assume that any vector $u \in G^n$ appears in the list $f_1, \ldots, f_p$ with multiplicity at most one (which, of course, is not a restriction at all). For example, one can easily check that the 2D cluster state and Kitaev's state have interaction length $l=3$ and $l=2$, respectively.

Consider a subgroup $S' \subseteq S$ generated by vectors f_j that have support on all three parties A, B, and C. Obviously, f_j is supported on all three parties only if the $l \times l$ block representing the support of f_j covers the junction point O. Since there are only l^2 different blocks that cover O and each block can represent at most l^2 independent vectors f_j, we conclude that

$$\dim(S') \leq l^4.$$

Consider now a subgroup $S_{\mathrm{loc}} \subseteq S$ generated by colocal subgroups of S [see Eq. (12)]. Since each f_j belongs to at least one of the subgroups S', S_{loc}, we infer that

$$S = S_{\mathrm{loc}} + S' \quad \text{and} \quad \dim(S_{\mathrm{loc}}) \geq \dim(S) - \dim(S').$$

Taking into account Theorem 4, one gets

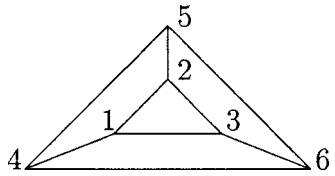

FIG. 2. Graph $\mathcal{G}$ used in the definition of $|\mathcal{G}\rangle$.

$$\Omega(\Psi_0) = \dim(S) - \dim(S_{\text{loc}}) \leq \dim(S') \leq l^4$$

which gives us an upper bound on the number of GHZ states $|\Psi_3^+\rangle$ that can be extracted from $|\Psi_0\rangle$. This bound does not depend upon n—only upon the interaction length l. Therefore Eq. (32) is proved.

Remark: Since the state $|\Psi_0\rangle$ is uniquely specified by stabilizer equations $\sigma(f)|\Psi_0\rangle = \epsilon(f)|\Psi_0\rangle$, $f \in S$ [see Eq. (4)], it can be regarded as the nondegenerate ground state of a Hamiltonian

$$H = -\sum_{j=1}^{p} \epsilon(f_j)\sigma(f_j).$$

This Hamiltonian is a sum of local interactions each of which affects the qubits inside some $l \times l$ block.

VIII. FOUR-PARTY STABILIZER STATES

As we learned from Sec. VI, there exists essentially one irreducible tripartite stabilizer state—the GHZ state $|\Psi_3^+\rangle$. What about four-party states? As the simplest example, consider a system of four qubits distributed between four parties. As was pointed out in Ref. 20, there exist only two irreducible four-qubit stabilizer states: the GHZ state $|\Psi_4^+\rangle$ and a state

$$|C_4\rangle = (1/2)(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle),$$

such that $|C_4\rangle = \Lambda(\sigma^z)[2,3]|\Psi^+ \otimes \Psi^+\rangle$ (one can check that $|C_4\rangle$ is LCU equivalent to the cluster state of a four-qubit linear chain).

Is it true that a set $E_4 = \{|0\rangle, |\Psi^+\rangle, |\Psi_3^+\rangle, |\Psi_4^+\rangle, |C_4\rangle\}$ is an entanglement generating set for four-party stabilizer states? In this section we give an example of a state that is not LCU equivalent to any collection of states from E_4, thus answering this question in the negative.

Consider a graph $\mathcal{G} = (V,E)$ with six vertices shown in Fig. 2. For each vertex $u \in V$ define a stabilizer $f_u \in G^6$ such that

$$\sigma(f_u) = \sigma_u^x \bigotimes_{(u,v)\in E} \sigma_v^z. \tag{33}$$

The vectors $\{f_u\}_{u\in V}$ generate a self-dual subspace $S \subset G^6$. Let $|\mathcal{G}\rangle \in \mathcal{B}^6$ be the corresponding stabilizer state [it is known as a *graph state* associated with the graph $\mathcal{G}$; one can also define $|G\rangle$ using a classical GF(4)-linear code known as *hexacode*, see Ref. 21]. This state has the following curious property.

Proposition: A partial trace of $|\mathcal{G}\rangle$ over any triple of qubits is maximally mixed:

$$\text{Tr}_{uvw}\big(|\mathcal{G}\rangle\langle\mathcal{G}|\big) = \tfrac{1}{8}I, \quad \text{for any } u \neq v \neq w. \tag{34}$$

For a proof see Ref. 22.

Suppose now that $|\mathcal{G}\rangle$ is shared by a set of parties $M = \{A,B,C,D\}$ such that

$$A = \{1,4\}, \quad B = \{3,6\}, \quad C = \{2\}, \quad D = \{5\}.$$

Lemma 3: *If* $|\mathcal{G}\rangle$ *is shared by the set of parties* $M=\{A,B,C,D\}$ *as above*, *it is irreducible*, *i.e.*, *no stabilizer state can be extracted from* $|\mathcal{G}\rangle$.

(Here we talk about extraction in the sense of Definition 4 and ignore the trivial possibility of extracting $|\mathcal{G}\rangle$ from itself.)

Proof: We shall first show that neither of the states $|\Psi^+\rangle$, $|\Psi_3^+\rangle$ can be extracted from $|\mathcal{G}\rangle$.

(a) $|\Psi_3^+\rangle$ *extraction*: Suppose one can extract one copy of $|\Psi_3^+\rangle$ which is shared by a subset of parties $M' \subset M$, $|M'|=3$. Obviously, M' contains at least one of A, B, and at least one of C, D. By the symmetry, assume that $A \in M'$ and $D \in M'$. Then the reduced state of the qubits $1,4,5$ has a rank at most 4, contradicting Eq. (34).

(b) $|\Psi^+\rangle$ *extraction*: Obviously, $|\Psi^+\rangle$ cannot be shared by C and D (the reduced state of any pair of qubits is maximally mixed). Thus there are only two possibilities: (i) $|\Psi^+\rangle$ is shared by one of $\{A,B\}$ and one of $\{C,D\}$. Then one of the triple of qubits AC, AD, BC, BD has a rank at most 2, contradicting Eq. (34). (ii) $|\Psi^+\rangle$ is shared by A and B. Then there must be two vectors $f,\bar{f} \in S$ such that

$$f_C = f_D = \bar{f}_C = \bar{f}_D = 0, \tag{35}$$

$$\omega(f_A,\bar{f}_A) = \omega(f_B,\bar{f}_B) = 1. \tag{36}$$

Taking into account the explicit form of the stabilizer generators Eq. (33), one can check that the only nontrivial stabilizer elements having a support on A and B are the following:

$$\sigma_1^y \otimes \sigma_4^z \otimes \sigma_3^y \otimes \sigma_6^z, \quad \sigma_1^z \otimes \sigma_4^y \otimes \sigma_3^z \otimes \sigma_6^y, \quad \sigma_1^x \otimes \sigma_4^x \otimes \sigma_3^x \otimes \sigma_6^x.$$

(All identity factors are suppressed.) Any pair of them commute locally on A and B. Thus the equations Eqs. (35) and (36) have no solutions and we get a contradiction.

Extraction of a four-party state from $|\mathcal{G}\rangle$ is impossible, since it leaves a bipartite (or a local pure state) which would also be extractable from $|\mathcal{G}\rangle$. As we already know, this would lead to a contradiction. □

This observation means that we must add the state $|\mathcal{G}\rangle$ to the entanglement generating set E_4. It raises a question: Is there a *finite* EGS for four-party stabilizer states? (Note that we allow an arbitrary number of qubits per party, so the total number of stabilizer states is infinite.) To the authors' best knowledge, the answer is unknown.

A closely related problem is to find LCU-equivalence classes of *bipartite* unitary operators from the Clifford group (it suffices to take two copies of a maximally entangled state and apply a unitary operator to one-half of each state, see Ref. 23 for more details).

Another open question is the relation between LU equivalence and LCU equivalence of stabilizer states. To the authors' best knowledge, there are no known examples of LU-equivalent stabilizer states which are not LCU equivalent. On the other hand, it was shown by Van den Nest, Dehaene, and De Moor in Ref. 11, extending the work of Rains,[24] that for a large class of stabilizer states, including the states specified by GF(4) linear codes, LCU equivalence coincides with LU equivalence (this statement applies only to one-qubit-per-party partitions).

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APPENDIX A

In this section we give a shorter (but less constructive) proof of the GHZ extraction formula, see Theorem 3.

Denote p the maximal number of states $|\Psi_m^+\rangle$ extractable from $|\Psi\rangle$. Clearly, $p>0$ implies $S \neq S_{\mathrm{loc}}$, and thus $\Delta(\Psi)>0$. Since $\Delta(\Psi)$ is additive under a tensor product of states, and $\Delta(\Psi_m^+)=1$ (for $m\geq 3$), it suffices to prove that $\Delta(\Psi)>0$ implies $p>0$.

(1) Consider a linear map $\Pi_\alpha: S\to G^{n_\alpha}$ that sends $f\in S$ to f_α (a projection onto party α). By definition of a colocal subspace, $\mathrm{Ker}(\Pi_\alpha)=S_{\hat{\alpha}}$. The fact that $|\Psi\rangle$ has full local ranks (see the remark after the statement of Theorem 3) implies that $\mathrm{Im}(\Pi_\alpha)=G^{n_\alpha}$. Therefore $\dim(S)=n_\alpha+\dim(S_{\hat{\alpha}})$ for any $\alpha\in M$. Thus any linear function $\lambda: S\to\{0,1\}$ such that $\lambda(S_{\hat{\alpha}})=0$ can be uniquely represented as $\lambda(f)=\omega(x_\alpha,f)$for some $x_\alpha\in G_\alpha^n$.

(2) Choose a nonzero linear function $\lambda: S\to\{0,1\}$ such that $\lambda(S_{\mathrm{loc}})=0$. As shown above, for any $\alpha\in M$ we can choose $x_\alpha\in G_\alpha^n$ such that $\lambda(f)=\omega(x_\alpha,f)$ for all $f\in S$. Then $\omega(x_\alpha+x_\beta,f)=0$ for all $f\in S$ and thus $x_\alpha+x_\beta\in S$ (recall that S is self-dual).

(3) Choose $\bar{g}\in S$ such that $\lambda(\bar{g})=1$. Define a linear subspace $V\subseteq S$, such that V is spanned by vectors $g_{\alpha,\beta}=x_\alpha+x_\beta$, $\alpha,\beta\in M$, and $\bar{g}$. From $\lambda(\bar{g})=1$ we infer that $\bar{g}\notin S_{\mathrm{loc}}$, and thus that $\bar{g}_\alpha\neq 0$ for all $\alpha\in M$. Besides, the fact that $\omega(x_\alpha,g)=\lambda(g)=1$ implies that x_α and g_α are linearly independent. Thus a colocal subspace $V_{\mathrm{loc}}\subset V$ is spanned by vectors $g_{\alpha,\beta}$.

(4) Let $S_{\mathrm{ghz}}\subset G^m$ be a stabilizer group of $|\Psi_m^+\rangle$ with canonical generators $f_{\alpha,\beta}$ and $\bar{f}$, see Eqs. (10) and (11). Define a linear map $T: S_{\mathrm{ghz}}\to S$ according to $T(f_{\alpha,\beta})=g_{\alpha,\beta}$ and $T(\bar{f})=\bar{g}$. Let us verify that T obeys conditions of Theorem 2. Indeed, T is the injective map since x_α and g_α are linearly independent. The property (i) follows from equality $\omega(x_\alpha,g_\alpha)=\lambda(g)=1$. The property (ii) follows from equality $T((S_{\mathrm{ghz}})_{\mathrm{loc}})=V_{\mathrm{loc}}$. Thus$|\Psi_m^+\rangle$ is extractable from $|\Psi\rangle$, i.e., $p>0$.

APPENDIX B

The goal of this section is to prove Lemma 1. We start by stating one more lemma.

Lemma 4: *Let $f_1,\ldots,f_p$ and $f_1',\ldots,f_p'$ be two families of vectors in G^n satisfying the following conditions*:

$$\omega(f_j,f_k)=\omega(f_j',f_k') \quad \textit{for all } 1\leq j,k\leq p, \tag{B1}$$

$$\sum_{j=1}^{p} x_j f_j=0 \quad \textit{iff} \sum_{j=1}^{p} x_j f_j'=0. \tag{B2}$$

Here $x_1,\ldots,x_p\in\{0,1\}$ are arbitrary binary coefficients. Then there exists a symplectic operator $u\in \mathrm{Sp}_2(n)$ such that

$$f_j'=u(f_j) \quad \textit{for all } j=1,\ldots,p.$$

Proof: Let us call a basis $e_1,\bar{e}_1,\ldots,e_n,\bar{e}_n$ of the space G^n canonical iff the following relations hold:

$$\omega(e_j,e_k)=0, \quad \omega(\bar{e}_j,\bar{e}_k)=0, \quad \omega(e_j,\bar{e}_k)=\delta_{jk}. \tag{B3}$$

One can extend the family $f_1,\ldots,f_p$ to a canonical basis $\{e_j,\bar{e}_j\}$ using the Gram-Schmidt orthogonalization algorithm. After that one can write

$$f_j = \sum_{k=1}^{n} F_{jk} e_k + \bar{F}_{jk} \bar{e}_k, \quad j = 1, \ldots, p,$$

where F and $\bar{F}$ are some binary $p \times n$ matrices. It is a property of the Gram-Schmidt algorithm that the coefficients F_{jk} and $\bar{F}_{jk}$ depend only upon the inner products Eq. (B1) and upon the set of linear dependencies Eq. (B2). Thus if we apply the same algorithm in parallel to the family $f'_1, \ldots, f'_p$, we shall end up with a canonical basis $\{e'_1, \bar{e}'_1, \ldots, e'_n, \bar{e}'_n\}$ such that

$$f'_j = \sum_{k=1}^{n} F_{jk} e'_k + \bar{F}_{jk} \bar{e}'_k, \quad j = 1, \ldots, p.$$

The symplectic group $\mathrm{Sp}_2(n)$ acts transitively on the set of canonical bases. Thus

$$e'_j = u(e_j), \quad \bar{e}'_j = u(\bar{e}_j), \quad j = 1, \ldots, n,$$

for some $u \in \mathrm{Sp}_2(n)$. This implies that $f'_j = u(f_j)$ for all $j = 1, \ldots, p$. □

Now we are ready to prove Lemma 1. The nontrivial part is to prove that statement 1 follows from statement 2. Choose an arbitrary basis $f_1, \ldots, f_p$ of the subspace S. Denote $f'_j = T(f_j) \in S'$. The condition that T is an invertible map implies that $f'_1, \ldots, f'_p$ is a basis of S'. For each $\alpha \in M$, consider projections $f_{\alpha j} = (f_j)_\alpha$ and $f'_{\alpha j} = (f'_j)_\alpha$. The condition (2-i) is equivalent to

$$\omega(f_{\alpha j}, f_{\alpha k}) = \omega(f'_{\alpha j}, f'_{\alpha k}) \quad \text{for all } \alpha \in M \tag{B4}$$

and any j, k in the range $1, \ldots, p$.

In addition, we have the following chain of implications: $\Sigma_{j=1}^{p} x_j f_{\alpha j} = 0$ iff $\Sigma_{j=1}^{p} x_j f_j \in S_{\hat{\alpha}}$ iff $T(\Sigma_{j=1}^{p} x_j f_j) \in S'_{\hat{\alpha}}$ iff $\Sigma_{j=1}^{p} x_j f'_{\alpha j} = 0$. The second implication is the condition (2-ii) of the lemma, while all others follow from the definition of the colocal subspace. Summarizing, we have

$$\sum_{j=1}^{p} x_j f_{\alpha j} = 0 \quad \text{iff} \sum_{j=1}^{p} x_j f'_{\alpha j} = 0. \tag{B5}$$

Now, for each $\alpha \in M$, let us apply Lemma 4 to the families of vectors $f_{\alpha 1}, \ldots, f_{\alpha p} \in G^{n_\alpha}$ and $f'_{\alpha 1}, \ldots, f'_{\alpha p} \in G^{n_\alpha}$. The conditions of Lemma 4 are equivalent to Eqs. (B4) and (B5). Thus there exist operators $u_\alpha \in \mathrm{Sp}_2(n_\alpha)$ such that

$$f'_{\alpha j} = u_\alpha(f_{\alpha j}), \quad \alpha \in M, \quad j = 1, \ldots, p.$$

This means that

$$f'_j = \left(\bigoplus_{\alpha \in M} u_\alpha \right)(f_j), \quad j = 1, \ldots, p.$$

This is equivalent to statement 1 of Lemma 1.

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Probability and Quantum Symmetries. II. The Theorem of Nœther in quantum mechanics

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For the largest class of physical systems having a classical analog, a new rigorous, but not probabilistic, Lagrangian version of nonrelativistic quantum mechanics is given, in terms of a notion of regularized action function. As a consequence of the study of the symmetries of this action, an associated Nœther theorem is obtained. All the quantum symmetries resulting from the canonical quantization procedure follow in this way, as well as a number of symmetries which are new even for the case of the simplest systems. The method is based on the study of a corresponding Lie algebra and an analytical continuation in the time parameter of the probabilistic construction given in paper I of this work. Generically, the associated quantum first integrals are time dependent and the probabilistic model provides a natural interpretation of the new symmetries. Various examples illustrate the physical relevance of our results. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2199087]

I. INTRODUCTION

This paper is the continuation of the one, referred hereafter simply as paper I, whose subtitle was the "Theorem of Nœther in Schrödinger's Euclidean quantum mechanics."[1] There, a probabilistic (i.e., "Euclidean") generalization of Nœther's theorem of classical mechanics was presented, for a class of Lagrangians quadratic in the velocities, and involving a special family of time-symmetric $\mathbb{R}^3$-valued diffusion processes. At the end of paper I, our physical motivation was indicated: after an appropriate analytic continuation in the time parameters, the main conclusion of the construction was preserved as a theorem on quantum symmetries, in the Heisenberg picture. In other words, although the probabilistic content of the theorem of Nœther was destroyed by this continuation in time, its geometrical one survived.

The purpose of this second paper is to describe in a detailed way the reason of this apparently surprising conclusion. This will provide us with a new Lagrangian version of the quantum theory of such a class of systems. The symmetries of the associated new concept of regularized action functional will be expressed as a quantum version of the theorem of Nœther. All the unusual regularizations introduced on the quantum side will correspond to the ones given for free with the underlying diffusion process, whose probability measures make sense only in the Euclidean setting. In point of fact, it will be shown that the corresponding symbolic "quantum diffusions" in real time have all the properties of the heuristic ones manipulated by Feynman in his famous path integral method.[2] In this sense, our indirect method is very much along the line of Feynman's space–time approach. It will be shown that we obtain many more quantum symmetries in this way than using the usual theorems on quantum symmetries, even for the simplest class of elementary integrable systems. Those "new" quantum symmetries are the keys of basic relations with stochastic analysis. A general argument of Lie group theory assures us, in fact, that all quantum symmetries arise in this way.

The organization of this work is as follows.

Section II introduces the notions (implicit in Feyman's approach) of (complex-valued) space–time observables associated with a family of regular quantum observables and of quantum derivatives along a state. Although these quantum derivatives are not observables in the sense of Von Neumann, they constitute a key tool of our construction. Under the quantum expectation, such differential operators behave like derivations.

Then, we define the concept of quantum conditional expectation in a state, given a space–time point. In spite of the fact that this concept shares a number of properties with its counterpart in probability theory, we show why it is not a conditional expectation in the probabilistic sense. The associated "quantum diffusions" are precisely the ones introduced by Feynman in time discretized manner.

Section III is devoted to the definition of the regularized action function for this class of systems and its relations with quantum dynamics.

The study of the symmetries of this quantum action is the subject of Sec. IV. In particular, the definition of the invariance of the action corresponds to a natural regularization of the classical notion. The symmetry group of the underlying Schrödinger equation is used in an essential way here, and the regular concept of constant observable of the motion is adapted to our calculus on space–time observable (or *quantum calculus*, for short).

In Sec. V the construction is specialized to the case of Hamiltonians which are polynomials of degrees ≤ 2 in the position and momentum observables. This is the case where all the calculations are explicit. Although this class is supposed to be completely known, our method provides, even for the most elementary systems, more symmetries than the traditional approach. For general Hamiltonians the main results hold true; but no explicit basis of the symmetry algebra can be found, in general and, therefore, the method is more indirect.

Section VI is devoted to the analysis of the content of our Nœther theorem in a Riemannian manifold.

In Sec. VII we come back to the relation of what we did with the ideas of Feynman and show in what sense the content of the present paper is a natural counterpart of paper I, where stochastic analysis is involved in an essential way.

Finally, the last section is devoted to a short collection of explicit examples of quantum symmetries with some emphasis on those not directly accessible to regular methods. Of course, as soon as we know it, the theorem of Nœther in quantum mechanics can be verified without any use of our detour via probability theory and stochastic analysis. However, it is argued in favor of this detour for the intuition it provides, in the same sense as Feynman's path integral approach has proved to be very useful for the discovery of many new aspects of quantum theory. A short Errata for paper I will conclude the present work.

II. THE CONCEPT OF QUANTUM MECHANICAL CONDITIONAL EXPECTATION

Let H be a self-adjoint, lower bounded Hamiltonian operator in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n, \mathrm{d}x)$ of square integrable complex-valued function over $\mathbb{R}^n$. Consider the one-parameter, strongly continuous groups of unitary operators $U_t: \mathcal{H} \to \mathcal{H}, t \in \mathbb{R}$,

$$U_t = e^{-(i/\hbar)tH},$$

with the reduced Planck constant $\hbar$. Then for any ψ in the definition domain $\mathcal{D}_H \subset \mathcal{H}$ of H,

$$\psi_t = U_t \psi, \tag{2.1}$$

solves the Schrödinger equation with the initial condition ψ:

$$\begin{aligned} i\hbar \frac{\partial \psi_t}{\partial t} &= H\psi_t, \\ \psi_0 &= \psi. \end{aligned} \tag{2.2}$$

Let consider a one-parameter family $A(t), t \in \mathbb{R}$, of self-adjoint operators in $\mathcal{H}$. Assume that $\mathcal{D}_{A(t)} \supset H\mathcal{D}_H$ and $A(t)\mathcal{D}_H \subset \mathcal{D}_H$, so that the commutators $[A(t),H]=A(t)H-HA(t)$ are well defined on $\mathcal{D}_H$. Let $0<T\leq\infty$ and define $\mathcal{D}_T^A(t) \equiv \mathcal{D}^A(t)$ by $\mathcal{D}^A(t)=\cap_{T\geq\Delta t\geq 0}\mathcal{D}_{A(t+\Delta t)}$. In particular we have $\mathcal{D}^A(t) \subset \mathcal{D}_{A(t)}$. If $A(t)$ is weakly differentiable on $\mathcal{D}^A(t)$ with respect to the time parameter $t \in [0,T)$,then we can compute

$$\lim_{\Delta t \downarrow 0}\left(\psi, \frac{A(t+\Delta t)-A(t)}{\Delta t}\varphi\right) \equiv \dot{\varepsilon_t^A}(\psi,\varphi).$$

It exists for any $\psi \in \mathcal{H}, \varphi \in \mathcal{D}^A(t)$, where $(\cdot,\cdot)$ denotes the scalar product in $\mathcal{H}$, and is linear in the second vector. Provided that $\mathcal{D}^{\dot{A}}(t)$ is dense in $\mathcal{H}, \dot{\varepsilon_t^A}: \mathcal{H}\times\mathcal{D}^A(t) \to \mathbb{C}$ is a densely defined sesquilinear form.

Now let us define, for $\psi_t \in \mathcal{H}$ and $\varphi_t \in \mathcal{D}_{A(t)}, I_{\psi,\varphi}(t)=(\psi_t,A(t)\varphi_t)$.

When $\varphi_t \in \mathcal{D}^A(t)$ and ψ_t is the solution of (2.2) with $\psi_t \in D_{A(t)}, T>t\geq 0$ and $\Delta t>0$, we can compute the relative time increment of $I_{\psi,\varphi}(t)$ as follows:

$$\begin{aligned} I_{\psi,\varphi}(t,\Delta t) &\equiv \frac{I_{\psi,\varphi}(t+\Delta t)-I_{\psi,\varphi}(t)}{\Delta t} \\ &= \frac{1}{\Delta t}[(\psi_{t+\Delta t},A(t+\Delta t)\varphi_{t+\Delta t})-(\psi_t,A(t+\Delta t)\varphi_{t+\Delta t}) \\ &\quad +(\psi_t,A(t+\Delta t)\varphi_{t+\Delta t})-(\psi_t,A(t)\varphi_{t+\Delta t}) \\ &\quad +(\psi_t,A(t)\varphi_{t+\Delta t})-(\psi_t,A(t)\varphi_t)]. \end{aligned}$$

If, in addition, $\varphi_t=U_t\varphi$ with $\varphi_0 \equiv \varphi \in \mathcal{D}(H)$ then the strong derivative $\dot{\varphi}_t$ of φ_t with respect to t exists and $\dot{\varphi_t}=(1/i\hbar)H\varphi_t$. But, by assumption, $H\varphi_t \in D_{A(t)}$. This, inserted in the above relative increment of $I_{\psi,\varphi}(t)$ gives, when $\Delta t \downarrow 0$, using the strong differentiability of ψ_t, φ_t, the strong continuity of $A(t)\varphi_t$ on $\mathcal{D}^A(t)$, the fact that $\varphi_{t+\Delta t} \in \mathcal{D}^A(t)$ and that $A(t)$ is weakly differentiable on $\mathcal{D}^A(t)$,

$$\lim_{\Delta t\downarrow 0} I_{\psi,\varphi}(t,\Delta t) = (\dot{\psi}_t,A(t)\varphi_t)+\dot{\varepsilon_t^A}(\psi_t,\varphi_t)+(\psi_t,A(t)\dot{\varphi}_t).$$

By (2.2), the corresponding equation for φ_t and the further assumption $\mathcal{D}^A(t) \supset H\mathcal{D}_H$, we see that the latter relation can be rewritten as

$$\lim_{\Delta t\downarrow 0} I_{\psi,\varphi}(t,\Delta t) = \left(\frac{1}{i\hbar}H\psi_t,A(t)\varphi_t\right)+\dot{\varepsilon_t^A}(\psi_t,\varphi_t)+\left(\psi_t,\frac{1}{i\hbar}A(t)H\varphi_t\right).$$

Since $A(t)\mathcal{D}_H \subset \mathcal{D}_H$ by assumption, and so $A(t)\varphi_t \in \mathcal{D}_H$, this reduces, by the self-adjointness of H, to

$$\frac{1}{i\hbar}(\psi_t,[A(t),H]\varphi_t)+\dot{\epsilon_t^A}(\psi_t,\varphi t)=\frac{d}{dt}(\psi_t,A(t)\varphi_t), \tag{2.3}$$

where we used the definitions of $I_{\psi,\varphi}(t,\Delta t)$, $I_{\psi,\varphi}(t)$, and $\dot{\epsilon_t^A}(\psi_t,\varphi_t)$.

We shall denote by $\varepsilon_D(\psi_t,\varphi_t)$ the sesquilinear form on left-hand side (lhs) of (2.3). So

$$\varepsilon_D(\psi_t,\varphi_t)=\frac{d}{dt}(\psi_t,A(t)\varphi_t). \tag{2.4}$$

We recall that for $T>t\geq 0$, $\varepsilon_D(\psi_t,\varphi_t)$ is well defined if $\varphi_t \in \mathcal{D}^A(t)$ and $A(t)\mathcal{D}_H \subset \mathcal{D}_H$.

Definition II.1: Let φ be in $\mathcal{H}$ and such that $\varphi_t \in \mathcal{D}_{A(t)}$. The complex-valued space–time observable $a_{\varphi_t}^A(x,t)$ associated with the family of quantum observable $A(t)$ in the state φ_t is defined

for all $x \in \mathbb{R}^n, t \in \mathbb{R}, s.t. \varphi_t(x) \neq 0$, *by*

$$a^A_{\varphi_t}(x,t) \equiv \frac{(A(t)\varphi_t)(x)}{\varphi_t(x)}. \tag{2.5}$$

We shall consider, for any x,t, versions of $\varphi_t(x)$ jointly measurable in $t \in \mathbb{R}$, $x \in \mathbb{R}^n$, and denote them again by $\varphi_t(x)$. For x,t such that $\varphi_t(x)=0$ we set $a^A_{\varphi_t}(x,t) \equiv 0$. Therefore, for any ψ_t in $\mathcal{H}$ and φ_t in $\mathcal{D}_{A(t)}$ we have

$$(\psi_t, A(t)\varphi_t) = \int_{(N_t^\varphi)^c} \bar{\psi}_t A(t)\varphi_t \, \mathrm{d}x + \int_{N_t^\varphi} \bar{\psi}_t A(t)\varphi_t \, \mathrm{d}x = \int_{(N_t^{\dot{\varphi}})^c} \bar{\psi}_t A(t)\varphi_t \, \mathrm{d}x,$$

where $\mathcal{N}_t^\varphi = \{x \in \mathbb{R}^n \,|\, \varphi_t(x)=0\}, (N_t^\varphi)^c = \mathbb{R}^n - N_t^\varphi$.

Using (2.5), it is clear that, by construction,

$$(\psi_t, A(t)\varphi_t) = \int \bar{\psi}_t \varphi_t a^A_{\varphi_t} \, \mathrm{d}x. \tag{2.6}$$

Assumption on the zeroes of the wave function

We shall need that $\mathcal{N}_t^\varphi$ has zero Lebesgue measure. Sufficient conditions for this are known in terms of assumption on H. See Sec. V.

Using (2.3) and (2.4) and our assumption that $\mathcal{N}_t^\varphi$ has zero Lebesgue measure, we get

$$\varepsilon_D(\psi_t,\varphi_t) = \frac{1}{i\hbar}(\psi_t,[A(t),H]\varphi_t) + \varepsilon_t^{\dot{A}}(\psi_t,\varphi_t) = \frac{1}{i\hbar}\int_{(N_t^\varphi)^c} \bar{\psi}_t \varphi_t \frac{1}{\varphi_t}[A(t),H]\varphi_t \, \mathrm{d}x + \varepsilon_t^{\dot{A}/\varphi_t}(\psi_t\bar{\varphi}_t, \varphi_t), \tag{2.7}$$

where we have defined $\varepsilon_t^{\dot{A}/\varphi_t}$, for $f/\bar{\varphi}_t \in \mathcal{H}$ and $g \in \mathcal{D}^A(t)$, by

$$\varepsilon_t^{\dot{A}/\varphi_t}(f,g) \equiv \lim_{\Delta t \downarrow 0}\left(f, \frac{1}{\varphi_t}\left[\frac{A(t+\Delta t)-A(t)}{\Delta t}\right]g\right).$$

Now suppose that, in the strong sense on $\mathcal{D}^A(t)$, there exist a linear operator $\partial A(t)/\partial t$ such that

$$\lim_{\Delta t \downarrow 0} \frac{A(t+\Delta t)-A(t)}{\Delta t}\varphi_t = \frac{\partial A}{\partial t}(t)\varphi_t, \quad 0 \leq t < T.$$

Then, for $\psi \in \mathcal{H}, \varphi_t \in \mathcal{D}^A(t)$, using the definition of $\varepsilon_t^{\dot{A}}(\psi_t,\varphi_t)$,

$$\left(\psi_t, \frac{\partial A}{\partial t}(t)\varphi_t\right) = \varepsilon_t^{\dot{A}}(\psi_t,\varphi_t).$$

Also, for any $\varphi_t \in \mathcal{D}^A(t)$,

$$\left(\frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t),H]\right)\varphi_t$$

is well defined [recall that we have assumed $H\mathcal{D}_H \subset \mathcal{D}_{A(t)}$ and $A(t)\mathcal{D}_H \subset \mathcal{D}_H$]. According to the definition (2.5), $a^A_{\varphi_t}.\varphi_t = A(t)\varphi_t$ is also well defined. Therefore in the sense of the identification of the corresponding Bochner integrals,

$$\frac{\partial}{\partial t}(a^A_{\varphi t}\cdot\varphi_t)=\frac{\partial A}{\partial t}(t)\varphi_t+\frac{1}{i\hbar}A(t)H\varphi_t,$$

for any $\varphi_t\in\mathcal{D}^A(t)$ and Lebesgue a.e. $t\in[0,T)$ [recalling our assumption that $\mathcal{D}^A(t)\supset H\mathcal{D}_H$]. From this it follows that

$$\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(a^A_{\varphi_t}\cdot\varphi_t)$$

is well defined and coincides, for Lebesgue a.e. t, with

$$\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t.$$

Now for any $x\in(\mathcal{N}^\varphi_t)^c$ we defined $D_t a^A_{\varphi_t}$ by

$$(D_t a^A_{\varphi_t})(x)=\frac{1}{\varphi_t}\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(a^A_{\varphi_t}\cdot\varphi_t)(x). \tag{2.8}$$

Using the relation above, we get first on $(N^\varphi_t)^c$ but then in the $L^2(\mathbb{R}^n)$-sense

$$D_t a^A_{\varphi_t}=\frac{1}{\varphi_t}\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t. \tag{2.9}$$

From this, for all $\psi_0=\psi\in D_H$ we obtain

$$(\psi_t,(D_t a^A_{\varphi_t})\varphi_t)=\left(\psi_t,\left(\frac{\partial A}{\partial t}+\frac{1}{i\hbar}[A(t),H]\right)\varphi_t\right)=\frac{d}{dt}(\psi_t,A(t)\varphi_t),$$

where (2.7) and (2.9) have been used. All equalities hold first for Lebesgue a.e. t but can be extended to all t if both sides of the equalities are continuous in t.

In summary, we have proved the following:

Proposition II.2:

Let H be a self-adjoint operator in $\mathcal{H}=L^2(\mathbb{R}^n,dx)$ and $A(t)$ a one-parameter family of self-adjoint operators in $\mathcal{H}$ with $A(t)\mathcal{D}_H\subset\mathcal{D}_H$ and $\mathcal{D}^A(t)\supset H\mathcal{D}_H$. For $\varphi\in\mathcal{D}_H$, consider $\varphi_t=e^{-(i/\hbar)tH}\varphi$ and assume that $\mathcal{N}^\varphi_t$ has a zero Lebesgue measure. Suppose that $\partial A(t)/\partial t$ exists in the strong sense on $\mathcal{D}^A(t)$. Define $\mathcal{D}_t a^A_{\varphi_t}$ by equations (2.8) and (2.9). *Then, for any $\varphi\in\mathcal{D}_H$ and $\psi_t\in\mathcal{D}_{A(t)}$, with ψ_t satisfying* (2.2), *we have*

$$\frac{d}{dt}(\psi_t,A(t)\varphi_t)=(\psi_t,(D_t a^A_{\varphi_t})\varphi_t), \tag{2.10}$$

for Lebesgue a.e. $t\in\mathbb{R}$. If both sides of (2.10) *are continuous in t, then* (2.10) *holds for all $t\in\mathbb{R}$.*

Corollary II.3:

If $A(t)$ is a quantum constant of motion *of the system with Hamiltonian H, defined on a dense domain $\mathcal{D}\subset\mathcal{H}$, in the sense that*

$$\left(\frac{\partial A}{\partial t}(t)+\frac{1}{i\hbar}[A(t),H]\right)\mathcal{X}=0\quad\text{for any }\mathcal{X}\in\mathcal{D},$$

then the space–time observable associated with $A(t)$ satisfies

$$D_t a^A_{\varphi_t}=0,$$

for all $\varphi_t\in\mathcal{D}^A(t)$.

Proof: By (2.9) we have $D_t a^A_{\varphi_t} = (1/\varphi_t)\dot{A}(t)\varphi_t = 0$, for

$$\dot{A}(t) \equiv \frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t), H].$$

$\dot{A}(t)$ is a closable operator since $A(t)$, $(\partial A/\partial t)(t)$ and H are all symmetric, defined on a common domain.

By approximation of $\varphi_t \in \mathcal{D}^A(t)$ through vectors in $\mathcal{D}$, and since $A(t)$ is a quantum constant of motion, we see that $\bar{\dot{A}}(t)\varphi_t = 0$, where the overbar denotes the closure. Since φ_t is in the domain of $\dot{A}(t)$, the conclusion follows. □

Remarks:

(1) If we call *quantum space–time observable* any operator-valued map $(x,t) \to g(x,t)$ measurable in the sense that $(x,t) \to (\phi, g(x,t)\varphi)$ is measurable for $\phi \in \mathcal{H}, \varphi \in \mathcal{D}$ a dense domain and $g(x,t)$ self-adjoint in $\mathcal{H}$, we can define D_t, $t \in \mathbb{R}$, on the set of such observables g by

$$D_t g \equiv \frac{1}{\varphi_t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar}H\right)(g\varphi_t), \tag{2.11}$$

whenever the right-hand side (rhs) makes sense [with $(g\varphi_t)(x) \equiv (g(x,t)\varphi_t)(x)$]. Then, for $g = a^A_{\varphi_t}$, $D_t a^A_{\varphi_t}$ coincides with (2.9). If $g\varphi_t \in \mathcal{D}_H$, $\partial g/\partial t$ exists in the strong sense on $\mathcal{D}_H$ and $\mathcal{D}_{\partial g/\partial t} \supset \mathcal{D}_H$, then the rhs of (2.11) is well defined (for $\varphi_t \in \mathcal{D}_H$). However, we are going to show that there is a more natural definition of D_t regarded as differential operator densely defined in an associated Hilbert space.

(2) D_t, acting on space–time functions $a^A_{\varphi_t}$, for example, should not be confused with the familiar Heisenberg derivative D acting on the family of self-adjoint operators $A(t)$ and defined heuristically by

$$DA(t) = \frac{\partial A}{\partial t}(t) + \frac{1}{i\hbar}[A(t), H].$$

Indeed, according to (2.9), the relation between these two derivatives is $D_t a^A_{\varphi_t} = (1/\varphi_t)(DA(t)\varphi_t)$. In particular, Heisenberg's derivative D does not depend on the state φ_t. In order to avoid any confusion, from now on we shall call D_t the *quantum derivative* along φ_t.

(3) Consider two arbitrary observables A and H, time independent and with $\mathcal{D}_A = \mathcal{D}_H = \mathcal{D}$, a common dense domain in $\mathcal{H}$, invariant under A and H. We say that A and H commute, and write $[A,H]=0$ whenever for any f, g bounded and Borel measurable one has $f(A)g(H) - g(H)f(A) = 0$.

A necessary and sufficient condition for this property is, for example, that

$$[e^{i(\alpha/\hbar)A}, e^{i(t/\hbar)H}] = 0 \quad \forall\ \alpha,\ t \in \mathbb{R}.$$

(cf., for example, Ref. 3). If A is essentially self-adjoint on a domain $\mathcal{D}$, invariant under $e^{i(t/\hbar)H}$, $\forall t \in \mathbb{R}$, then A and H commute if

$$A(t)\chi \equiv e^{i(t/\hbar)H} A e^{-i(t/\hbar)H}\chi = A\chi, \quad \forall\ \chi \in \mathcal{D} \text{ and } t \in \mathbb{R}.$$

So it suffices indeed to show that

$$\frac{d}{dt}(\phi, e^{i(t/\hbar)H}Ae^{-i(t/\hbar)H}\chi) = \frac{d}{dt}(\phi_t, A\chi_t)$$
$$= \left(\phi_t, \frac{1}{i\hbar}[A(t), H]\chi_t\right)$$
$$= 0$$

with

$$\phi_t \equiv e^{-i(t/\hbar)H}\phi, \quad \mathcal{X}_t \equiv e^{-i(t/\hbar)H}\chi, \quad \text{and } \forall\, \chi, \phi \text{ in } \mathcal{D} = \mathcal{D}_H \cap \mathcal{D}_A,$$

in order to prove that A and H commute (in the sense of the above-mentioned sufficient condition) and therefore that $A(t)$ is a constant of motion. According to the Corollary II.3, when this holds, we have $D_t a^A_{\varphi_t} = 0$.

Lemma II.4:

Let φ_t be the solution of the Schrödinger equation (2.2) *with initial condition φ in $L^2(\mathbb{R}^n)$ and let $\mathcal{N}_t^\varphi$ be a zero Lebesgue measure set. Then the quantum derivative D_t along the solution φ_t of the Schrödinger equation* (2.2) *with initial condition φ is a densely defined differential operator in $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx)$.*

Proof: Let φ_t be the solution of the Schrödinger equation (2.2) with the initial condition $\varphi \in L^2(\mathbb{R}^n, dx) \equiv \mathcal{H}$ and consider the weighted Hilbert space $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx)$. Since, by assumption, $\mathcal{N}_t^\varphi$ has zero Lebesgue measure, the two Hilbert spaces are unitarily equivalent through the transformation

$$U_{\varphi_t}: \quad L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx) \to L^2(\mathbb{R}^n, dx),$$
$$g \mapsto g\varphi_t.$$

Let $\mathcal{K}$ be the space of $\mathbb{R}$-indexed families of functions $f = (f^{(t)})_{t\in\mathbb{R}}$ with each $f^{(t)}$ strongly continuously differentiable from $\mathbb{R}$ into $\mathcal{H}$, such that

$$\frac{\partial}{\partial t} f^{(t)} \equiv \lim_{\Delta t \downarrow 0} \frac{f^{(t+\Delta t)} - f^{(t)}}{\Delta t} \in \mathcal{H},$$

where the limit is taken in the strong $\mathcal{H}$ sense. Let us define the partial differential operator

$$\mathcal{Q} = \frac{\partial}{\partial t} - \frac{1}{i\hbar}H$$

on the subset $\mathcal{K}_H$ of $\mathcal{K}$ consisting of those $(f^{(t)})_{t\in\mathbb{R}}$ such that the mapping $x \in \mathbb{R}^n \mapsto f^{(t)}(x)$ belongs to $\mathcal{D}_H$ for all $t \in \mathbb{R}$. We can also define the Hilbert space $W_1^2(\mathbb{R}, \mathcal{H})$, consisting of the functions $f = (f^{(t)})_{t\in\mathbb{R}}$, with $f \in \mathcal{K}$ such that $f^{(t)}(x), (\partial/\partial t) f^{(t)}(x) \in L^2(\mathbb{R}, dt)$ for dx a.e., $x \in \mathbb{R}^n$. The operator $i\mathcal{Q}$ is well defined on $\mathcal{K}_H^0 \equiv \{f^{(t)} \in \mathcal{K}_H, t \mapsto f^{(t)} \in C_0^1(\mathbb{R})\}$. This operator is symmetric in $W_1^2(\mathbb{R}^n, \mathcal{H})$, on a dense domain $\mathcal{K}_H^S \equiv \mathcal{D}_S$ (S for "Schrödinger"), independent of time.

Let $\mathcal{K}_t$ be the "tth copy" of $L^2(\mathbb{R}^n, dx)$ so that $f^{(t)} \in \mathcal{K}_t$ for any $t \in \mathbb{R}$. Let us consider the image under $U_{\varphi_t}^{-1}$ of $\mathcal{K}_t$. $U_{\varphi_t}^{-1}\mathcal{K}_t$ is made of all functions of the form $f^{(t)}(x)/\varphi_t(x)$, with $f^{(t)} \in \mathcal{K}_t$ and $(x, t) \notin \mathcal{N}_t^\varphi$.

$U_{\varphi_t}^{-1}$ can be extended to an operator $\tilde{U}_{\varphi_t}^{-1}$ from $\mathcal{K}$ into $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx)$, defined by

$$(\tilde{U}_{\varphi_t}^{-1} f^{(s)})(x) = \frac{f^{(s)}(x)}{\varphi_t(x)}, \quad (x,t) \notin \mathcal{N}_t^\varphi, \quad s \in \mathbb{R}.$$

Restricted to $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx)$, $\tilde{U}_{\varphi_t}^{-1}$ is unitary from $L^2(\mathbb{R}^n, |\varphi_t(x)|^2\, dx)$ to $L^2(\mathbb{R}^n, dx)$, since

$$\|\tilde{U}_{\varphi_t}^{-1} f^{(s)}\|_{L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)} = \|f^{(s)}\|_{L^2(\mathbb{R}^n,\mathrm{d}x)}, \quad \forall\, s,t \in \mathbb{R},$$

and its inverse is $\tilde{U}_{\varphi_t} f^{(s)} = \varphi_t f^{(s)}$.

We can look at the image of the operator $\mathcal{Q}_t$ in $\mathcal{K}$ under $\tilde{U}_{\varphi_t}^{-1}$ as an operator $\hat{\mathcal{Q}}_t$ whose action on elements of $L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$ is given by $\tilde{U}_{\varphi_t}^{-1}\mathcal{Q}_t\tilde{U}_{\varphi_t} = \hat{\mathcal{Q}}_t$ on $D \subset L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x), D$ being such that $\tilde{U}_{\varphi_t} D \in \mathcal{D}_{\mathcal{Q}t}$. Since $i\mathcal{Q}_t = i\partial/\partial t - (1/\hbar)H$ is symmetric on the dense domain $\mathcal{D}_S$ of $W_1^2(\mathbb{R},\mathcal{H})$, this means that $i\mathcal{Q}_t$ is symmetric on the dense domain $\tilde{U}_{\varphi_t}^{-1}\mathcal{D}_S$ in $L^2(\mathbb{R}^n \times \mathbb{R}, \mathrm{d}x\,\mathrm{d}t)$. On this domain, $\hat{\mathcal{Q}}_t$ is given by

$$\hat{\mathcal{Q}}_t \tilde{U}_{\varphi_t}^{-1} f = \frac{1}{\varphi_t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar}H\right) f,$$

with $f = (f^{(t)})_{t\in\mathbb{R}} \in \mathcal{D}_S$.

$\mathcal{D}_S$ contains, for example, the subset $\mathcal{D}_S^0$ consisting of all families $f = (f^{(t)})_{t\in\mathbb{R}}$ such that $f^{(t)}(\cdot)$ as well as $(\partial/\partial t) f^{(t)}(\cdot)$ are both in $C_0^\infty(\mathbb{R}^n)$ [if $\mathcal{D}_H \supset C_0^\infty(\mathbb{R}^n)$].

Setting $h = \tilde{U}_{\varphi_t}^{-1} f$ for $f \in \mathcal{D}_S^0$ we see that

$$\hat{\mathcal{Q}}_t h = \frac{1}{\varphi t}\left(\frac{\partial}{\partial t} - \frac{1}{i\hbar}H\right)(\varphi_t h).$$

Comparing with (2.11), this means that, on $\tilde{U}_{\varphi_t}^{-1}\mathcal{D}_S^0$ we have indeed

$$\hat{\mathcal{Q}}_t = D_t. \tag{2.12}$$

□

Remarks:

(1) Suppose that H is the Hamiltonian for a unit mass and charged particle in an electromagnetic field, i.e., $H = -(\hbar^2/2)[\nabla - (i/\hbar)A]^2 + V$ on $C_0^\infty(\mathbb{R}^n)$ or

$$H = -\frac{\hbar^2}{2}\Delta + i\hbar\, A\cdot\nabla + \frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}\|A\|^2 + V, \tag{2.13}$$

where $A:\mathbb{R}^n \mapsto \mathbb{R}^n$ is the vector potential and $V:\mathbb{R}^n \mapsto \mathbb{R}$ the scalar potential, both continuous, A being C^1, and such that H has a unique self-adjoint extension, also denoted by H (cf., for example, Ref. 4 for sufficient conditions such that this holds). In this case, using (2.11), we obtain explicitly a quantum derivative along φ_t (in the sense of Lemma II.4) given by

$$D_t = \frac{\partial}{\partial t} + \left(-i\hbar\,\frac{\nabla\varphi_t}{\varphi_t} - A\right)\cdot\nabla - \frac{i\hbar}{2}\Delta \tag{2.14}$$

on the domain of functions of the form $\varphi\cdot\mathcal{D}_S$, which is dense in $L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$. According to our Remark 1 after Corollary II.3, D_t is also defined on a larger set of functions in $L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$. For example, denoting by q the function

$$\begin{aligned}\mathbb{R}^n \times \mathbb{R} &\to \mathbb{R}^n, \quad \forall\, t, \quad \text{we have } D_t q = i\hbar\,\frac{\nabla\varphi_t}{\varphi_t} - A\\ (x,t) &\mapsto x\end{aligned}$$

which is well defined, provided

$$\int \bar{\varphi}_t(x)x(H\varphi_t)(x)\mathrm{d}x < \infty\,.$$

This is the case under weak restrictions on the vector and scalar potentials A and V.

(2) We shall also need the complex conjugate of the operator D_t, denoted by $\bar{D}_t$. On complex space–time observables of the form $a^A_{\varphi_t}$, one has, by definition,

$$\bar{D}_t a^A_{\bar{\varphi}_t} = \frac{1}{\bar{\varphi}_t}\left(\frac{\partial}{\partial t} + \frac{1}{i\hbar}H\right)(\bar{\varphi}_t a^A_{\bar{\varphi}_t}).$$

Proceeding as before in connection with (2.12), i.e., considering vectors h of the form $\tilde{U}^{-1}_{\bar{\varphi}_t} f$, with $f \in \mathcal{D}^0_S$, we have

$$\bar{D}_t h = \frac{1}{\bar{\varphi}_t}\left(\frac{\partial}{\partial t} + \frac{1}{i\hbar}H\right)(\bar{\varphi}_t h). \tag{2.15}$$

In particular, when the Hamiltonian H is of the form (2.13), $\bar{D}_t$ reduces on $\tilde{U}^{-1}_{\bar{\varphi}_t}\mathcal{D}^0_S$ to the differential operator

$$\bar{D}_t = \frac{\partial}{\partial t} + \left(i\hbar\frac{\nabla\bar{\varphi}_t}{\bar{\varphi}_t} - A\right)\cdot\nabla + \frac{i\hbar}{2}\Delta \tag{2.16}$$

defined on the elements $\{\tilde{U}^{-1}_{\bar{\varphi}_t}\mathcal{D}^0_S\}_{t\in\mathbb{R}}$ of $W^2_1(\mathbb{R}^n,\mathcal{H})$. These elements form a dense domain of $W^2_1(\mathbb{R}^n,\mathcal{H})$, as discussed in the proof of the Lemma II.4. Using the terminology introduced there, $\bar{D}_t$ will simply be called the *quantum derivative along* $\bar{\varphi}_t$.

(3) It follows clearly from (2.11) and (2.15) that

$$\overline{D_t g} = \bar{D}_t \bar{g},$$

where the lhs denotes the complex conjugate of $D_t g$.

Motivated by Born's probabilistic interpretation of the wave function, let us introduce the natural definition.

Definition II.5: Let $f=(f^{(t)})_{t\in\mathbb{R}}$, *with* $f^{(t)}(\cdot)$ *in* $L^1(\mathbb{R}^n,|\varphi_t(x)|^2\,\mathrm{d}x)$ *and* $f^{(t)}$ *measurable in* t. *The* quantum (absolute) expectation of f in the state φ_t *solving* (2.1), *denoted by* $\langle f\rangle_{\varphi_t}$, *is the integral*

$$\langle f\rangle_{\varphi_t} = \int f^{(t)}(x)|\varphi_t(x)|^2\,\mathrm{d}x \tag{2.17}$$

and we shall refer to $|\varphi_t(x)|^2$ *as the density* (*with respect to* $\mathrm{d}x$) *of the quantum probability in the state* φ_t.

The terminology chosen for D_t and $\bar{D}_t$ is due to the crucial observation that, under this quantum expectation, these differential operators behave like derivations.

Proposition II.6:

Let $f=(f^{(t)})_{t\in\mathbb{R}}$, $g=(g^{(t)})_{t\in\mathbb{R}}$ *be in the domains of the quantum derivatives* D_t *and* $\bar{D}_t$ *and with compact support in the space variables. Then* $\langle f\cdot g\rangle_{\varphi_t}$ *is differentiable with respect to the time variable and the following Leibniz rule holds:*

$$\frac{d}{\mathrm{d}t}\langle f\cdot g\rangle_{\varphi_t} = \langle D_t f\cdot g + f\cdot\bar{D}_t g\rangle_{\varphi_t}. \tag{2.18}$$

In particular,

$$\frac{d}{\mathrm{d}t}\langle f\rangle_{\varphi_t} = \langle D_t f\rangle_{\varphi_t} = \langle \bar{D}_t f\rangle_{\varphi_t}. \tag{2.19}$$

Corollary II.7:

If f, g *have supports with respect to the time variable strictly contained in the interior of an interval* $[t_0,t_1]$ *for some* $t_0,t_1\in\mathbb{R}$, *then* $\mathcal{D}^+_t=-\bar{D}_t$ *where* $^+$ *denotes the adjoint with respect to* $|\varphi_t(x)|^2\,\mathrm{d}x\,\mathrm{d}t$ *on* $\mathbb{R}^n\times[t_0,t_1]$.

Proof: Integrating (2.18), we obtain

$$\int_{t_0}^{t_1} \langle D_t f \cdot g \rangle_{\varphi_t} \, \mathrm{d}t = - \int_{t_0}^{t_1} \langle f \cdot \bar{D}_t g \rangle_{\varphi_t} \, \mathrm{d}t.$$

□

Proof of Proposition II.6: By definition, $(d/\mathrm{d}t)\langle f \cdot g \rangle_{\varphi_t}$ denotes

$$\lim_{\Delta t \downarrow 0} \frac{\langle f^{(t+\Delta t)} g^{(t+\Delta t)} \rangle_{\varphi_{t+\Delta t}} - \langle f^{(t)} g^{(t)} \rangle_{\varphi_t}}{\Delta t}.$$

The term under $\lim_{\Delta t \downarrow 0}$ means explicitly

$$\begin{aligned}
&\frac{1}{\Delta t}\left[\int f^{(t+\Delta t)} g^{(t+\Delta t)} |\varphi_{t+\Delta t}(x)|^2 \, \mathrm{d}x - \int f^{(t)} g^{(t)} |\varphi_t(x)|^2 \, \mathrm{d}x \right] \\
&\quad = \frac{1}{\Delta t}\left[\int (f^{(t+\Delta t)} - f^{(t)}) g^{(t+\Delta t)} |\varphi_{t+\Delta t}(x)|^2 \, \mathrm{d}x \right. \\
&\qquad + \int f^{(t)} (g^{(t+\Delta t)} - g^{(t)}) |\varphi(x)_{t+\Delta t}|^2 \, \mathrm{d}x \\
&\qquad \left. + \int f^{(t)} g^{(t)} (|\varphi_{t+\Delta t}(x)|^2 - |\varphi_t(x)|^2) \mathrm{d}x \right].
\end{aligned}$$

The first term on the rhs converges, when $\Delta t \downarrow 0$, to $\int (\dot{f}^{(t)} g^{(t)})(x) \, |\varphi_t(x)|^2 \, \mathrm{d}x$ by the dominated convergence theorem and the hypothesis that $f^{(t)}$ is strongly differentiable in $L^2(\mathbb{R}^n, \mathrm{d}x)$ [here we denote $(\partial/\partial t) f^{(t)}$ by $\dot{f}^{(t)}$ for simplicity]. Similarly we see that the second term of the rhs converges to $\int f^{(t)} \dot{g}^{(t)} |\varphi_t(x)|^2 \, \mathrm{d}x$.

For the third term we use again the dominated convergence theorem and the fact that, in the strong $L^2(\mathbb{R}^n, \mathrm{d}x)$ sense,

$$\frac{d}{\mathrm{d}t} |\varphi_t|^2 = \frac{d}{\mathrm{d}t} \bar{\varphi}_t \cdot \varphi_t = - \frac{1}{i\hbar} H \bar{\varphi}_t \cdot \varphi_t + \dot{\bar{\varphi}}_t \frac{1}{i\hbar} H \varphi_t,$$

where the Schrödinger equation has been used, together with the fact that $\dot{\bar{\varphi}}_t \cdot H\varphi_t$ as well as $H\bar{\varphi}_t \cdot \varphi_t$ are in $L^1(\mathbb{R}^n, \mathrm{d}x)$ and $f^{(t)}, g^{(t)}$ have compact support as functions of the space variable. In other words the rhs above becomes

$$\begin{aligned}
&\int \left\{ \dot{f}^{(t)} g^{(t)} + f^{(t)} \dot{g}^{(t)} + f^{(t)} g^{(t)} \left(\frac{1}{i\hbar} \frac{H\varphi_t}{\varphi_t} - \frac{1}{i\hbar} \frac{H\bar{\varphi}_t}{\bar{\varphi}_t} \right) \right\} (x) |\varphi_t(x)|^2 \, \mathrm{d}x \\
&\quad = \int (D_t f^{(t)} \cdot g^{(t)} + f^{(t)} \bar{D}_t g^{(t)})(x) |\varphi_t(x)|^2 \, \mathrm{d}x,
\end{aligned}$$

where the definition of $D_t, \bar{D}_t$ have been used together with the self-adjointness of H, in order to simplify the term involving $H(f^{(t)}\varphi_t)$.

The second part of the calculation follows from the first one by approaching in the $L^2(\mathbb{R}^n, |\varphi_t(x)|^2 \, \mathrm{d}x)$-norm $f^{(t)} = 1$, respectively, $g^{(t)} = 1$ through $C_0^\infty(\mathbb{R}^n)$ functions. □

Remarks:

(1) When the Hamiltonian H is of the explicit form (2.13), the relation (2.18) can be given a more illuminating form if we use exclusively one of the quantum derivatives,

$$\frac{d}{dt}\langle f\cdot g\rangle_{\varphi_t}=\langle (D_tf)\cdot g+f(D_tg)\rangle_{\varphi_t}-i\hbar\,\langle \nabla f\cdot\nabla g\rangle_{\varphi_t} \tag{2.20}$$

$$=\langle (\bar{D}_tf)\cdot g+f(\bar{D}_tg)\rangle_{\varphi_t}+i\hbar\,\langle \nabla f\cdot\nabla g\rangle_{\varphi_t}. \tag{2.21}$$

Proof: This follows directly from Proposition II.6, using the explicit expressions (2.14) and (2.16) of D_t and $\bar{D}_t$ available for the Hamiltonian (2.13). □

(2) Relations like (2.20) and (2.21) hold, in fact, also without integration with respect to $|\varphi_t(x)|^2\,dx$.

Proposition II.8:

For f,g in a dense domain of the form $\varphi_t\cdot\mathcal{D}_S\subset L^2(\mathbb{R}^n,|\varphi_t(x)|^2\,dx)$ (cf. Lemma II.4) and an Hamiltonian of the form (2.13), *one has*

$$D_t(f\cdot g)=(D_tf)\cdot g+f(D_tg)-i\hbar\,\nabla f\cdot\nabla g, \tag{2.20′}$$

$$\bar{D}_t(f\cdot g)=(\bar{D}_tf)\cdot g+f(\bar{D}_tg)+i\hbar\,\nabla f\cdot\nabla g, \tag{2.21′}$$

for any (t,x) such that $\varphi_t(x)\neq 0$.

Proof: Equations (2.20) and (2.21) can be written, for any $\varphi_t=U_t\varphi$, and any (t,x) s.t. $\varphi(t,x)\neq 0, \int A(x,t)|\varphi_t(x)|^2\,dx=0$ with $A(x,t)=\bar{D}(f\cdot g)-(\bar{D}_tf)g-f(\bar{D}_tg)-i\hbar\nabla f\cdot\nabla g$, and so equations (2.20′) and (2.21′) hold a.e. with respect to dx. Alternatively, one can use directly the definitions (2.14) and (2.16) to show that the conclusion holds. □

Equations (2.20′) and (2.21′) show that the quantum derivatives behave, in fact, like quantum *deformations* of derivatives in the (commutative) algebra of families of functions $f=(f^{(t)})_{t\in\mathbb{R}}$ with $f^{(t)}\in C_0(\mathbb{R}^n)$. To regard D_t and $\bar{D}_t$ as quantum deformations of derivations will prove, later on, to be a very natural interpretation.

Now we are going to introduce the quantum counterpart of the probabilistic concept of conditional expectation given a space point $x\in\mathbb{R}^n$ in the past time $t\geq 0$.

Definition II.9:

Let $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ be complex valued, measurable functions defined on $\mathbb{R}^n$ and such that $g^{(\tau)}\times(\cdot)\psi_\tau(\cdot)\in L^2(\mathbb{R}^n,dx)$ where, as before, $\psi_\tau=U_\tau\psi$. For $0\leq t\leq\tau$ and (t,x) such that $\psi_t(x)\neq 0$ [or, for short, (t,x) "ψ-admissible"] let us define the quantum conditional expectation $M^{\psi}_{t,x}$ in the state ψ, given (t,x) and evaluated at $g^{(\tau)}$ *by*

$$M^{\bar{\psi}}_{t,x}[g^{(\tau)}]=(\bar{\psi}_t(x))^{-1}(U_{\tau-t}(g^{(\tau)}\bar{\psi}_\tau))(x). \tag{2.22}$$

Let us first assume that the Hamiltonian H is time-independent and that the evolution group $U_{\tau-t}$ has an integral kernel, denoted by

$$k(x,\tau-t,q)=(e^{-(i/\hbar)(\tau-t)H})(x,q),\quad x,q\in\mathbb{R}^n,\ \tau>t.$$

Then the definition (2.22) means

$$M^{\bar{\psi}}_{t,x}[g^{(\tau)}]=(\bar{\psi}_t(x))^{-1}\int k(x,\tau-t,q)g^{(\tau)}(q)\bar{\psi}_\tau(q)dq, \tag{2.22′}$$

which is well defined for any ψ-admissible $(t,x)\in\mathbb{R}^+\times\mathbb{R}^n$. We shall denote by

$$\hat{p}(t,x,\tau,dq)=(\bar{\psi}_t(x))^{-1}k(x,\tau-t,q)\bar{\psi}_\tau(q)dq,\quad t\leq\tau,\ x,q\in\mathbb{R}^n, \tag{2.23}$$

the integral kernel associated with (2.22′) and refer to it as the *forward quantum transition* kernel ["forward" because the conditioning x is in the past $t\leq\tau$ and also because the initial quantum

probability density $|\psi_t(x)|^2$ is propagated towards the future by $\hat{p}$]. More precisely since, for $\tau > t$ the kernel $k(x,\tau-t,q)$ coincides with the retarded (or "casual") propagator

$$k_+(x,\tau-t,q) = \theta(\tau-t)(e^{-(i/\hbar)(\tau-t)H})(x,q),$$

(where θ is Heaviside's distribution) i.e., the distribution solving

$$\left(-i\hbar\frac{\partial}{\partial\tau}+H\right)k_+(x,\tau-t,q) = -i\hbar\,\delta(q-x)\delta(\tau-t),$$

Eq. (2.23) means that

$$\hat{p}(t,x,\tau,\mathrm{d}q) = (\bar{\psi}_t(x))^{-1}k_+(x,\tau-t,q)\bar{\psi}_\tau(q)\mathrm{d}q. \tag{2.23′}$$

Let us observe that sufficient conditions for the existence of k and therefore $\hat{p}$ as continuous functions in all the variable are known; cf., e.g., Refs. 5, 6, and 60.

We remark that when H is time dependent, Eq. (2.23) still holds with k replaced by the integral kernel of the two-parameter family of unitary operators $U(t,\tau)$, $t,\tau\in\mathbb{R}$ defining the corresponding time evolution.

The main properties of the quantum conditional expectation of Definition 2.9 are expressed by the following:

Proposition II.10:

For all ψ-admissible $(t,x)\in\mathbb{R}\times\mathbb{R}^n$ and $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ as in (2.22′), *with $\tau\geq t$,*

(1) *the quantum mechanical conditional expectation is linear*: *if $\alpha_i\in\mathbb{C}$ and $g_i=(g_i^{(\tau)})_{\tau\in\mathbb{R}}$, $i=1,2$ as above*,

$$M^{\bar{\psi}}_{t,x}[\alpha_1 g_1^{(\tau)}+\alpha_2 g_2^{(\tau)}] = \alpha_1 M^{\bar{\psi}}_{t,x}[g_1^{(\tau)}]+\alpha_2 M^{\bar{\psi}}_{t,x}[g_2^{(\tau)}];$$

(2) $M^{\bar{\psi}}_{t,x}[\alpha]=\alpha,\ \alpha\in\mathbb{C}$;

(3) $M^{\bar{\psi}}_{t,x}[g^{(\tau)}]=g^{(t)}(x),\ \tau\geq t$;

(4) $\langle M^{\bar{\psi}}_t[g^{(\tau)}]\rangle_{\psi_\tau}=\langle g^{(\tau)}\rangle_{\psi_\tau},\ \tau\geq t$;

(5) *when $M^{\bar{\psi}}_{s,x}[g_1^{(s)}g_2^{(t)}]$, $s\leq t$, is well defined, then*

$$M^{\bar{\psi}}_{s,x}[g_1^{(s)}g_2^{(t)}] = g_1^{(s)}(x)M^{\bar{\psi}}_{s,x}[g_2^{(t)}].$$

Proof: This follows from direct computations using the definitions (2.17) and (2.22). □

Remarks:

(1) We shall also need, for the same class of $g=(g^{(\tau)})_{\tau\in\mathbb{R}}$ as in Proposition II.10, and any ψ-admissible $(t,x)\in\mathbb{R}\times\mathbb{R}^n$, the definition (2.22) with ψ replaced by $\bar{\psi}$ and $U_{\tau-t}$ replaced by $U_{\tau-t}$, $0<\tau\leq t$, i.e.,

$$M^{t,x}_{\psi}[g^{(\tau)}] = (\psi_t(x))^{-1}(U_{t-\tau}(g^{(\tau)}\psi_\tau))(x). \tag{2.24}$$

The properties of $M^{t,x}_{\psi}$ are, of course, similar to the ones of $M^{\bar{\psi}}_{t,x}$.

Let us stress that, for the latter quantum conditional expectation in the state ψ, the conditioning x is lying in the future of the time interval under consideration [i.e., $t\geq\tau$; this justifies our alteration of notation with respect to (2.22)]. For this reason, we shall occasionally call backward (respectively, forward) the conditional expectation (2.24) [respectively (2.22)] when a confusion is possible between these two concepts. When needed, we shall denote by $p(\tau,\mathrm{d}q,t,x)$ the *backward quantum transition* kernel associated with (2.24), i.e.,

$$p(\tau,\mathrm{d}q,t,x) = \psi_\tau(q)k_-(q,t-\tau,x)(\psi_\tau(x))^{-1}\,\mathrm{d}q,\quad \tau\leq t, \tag{2.25}$$

for any (t,x) ψ-admissible. Here, we denote by k_- the advanced propagator defined in terms of the causal one by

$$k_-(x_1,s-u,x_2)=\overline{k_+(x_2,u-s,x_1)}. \tag{2.26}$$

(2) Comparing the definitions (2.23′) and (2.25), it is clear that the relation between the forward and backward quantum transition kernels can be expressed as

$$\overline{\hat{p}(t,x,s,y)}=p(s,y,t,x), \quad s\le t,\ x,y\in\mathbb{R}^n. \tag{2.27}$$

Definition II.11:

Let $f=(f^{(t)})_{t\in\mathbb{R}}$, $(g^{(s)})_{s\in\mathbb{R}}$ *as in the definitions* (2.22′) and (2.23). *The* quantum (absolute) expectation of their product $f^{(t)}\cdot g^{(s)}$ *in the state* ψ, *for* $t\ge s$, *is defined by*

$$\langle f^{(t)}g^{(s)}\rangle_\psi=\langle M^{\bar{\psi}}_{s,\cdot}[f^{(t)}]\cdot g^{(s)}\rangle_{\psi_s} \tag{2.28}$$

$$=\langle f^{(t)}M^{t,\cdot}_{\psi}[g^{(s)}]\rangle_{\psi_t}, \tag{2.28′}$$

when $M^{\bar{\psi}}_{s,\cdot}[f^{(t)}]\cdot g^{(s)}\in L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ *and* $f^{(t)}M^{t,\cdot}_{\psi}[g^{(s)}]\in L^2(|\psi_t(q)|^2\,\mathrm{d}q)$.

The consistency of this definition is verified by observing that equation (2.28) reduces, after simplification, to

$$\int\int \psi_s(x)g^{(s)}(x)k(x,t-s,q)f^{(t)}(q)\bar{\psi}_t(q)\mathrm{d}q\,\mathrm{d}x,$$

when the integral kernel (2.23′) exists (since $t\ge s$). On the other hand, using the forward conditional expectation of (2.28′), this absolute expectation in the state ψ_t reduces to

$$\int\int \psi_s(x)g^{(s)}(x)k_-(x,t-s,q)f^{(t)}(q)\bar{\psi}_t(q)\mathrm{d}q\,\mathrm{d}x,$$

i.e., to the same expression as before, by definition of the advanced propagator k_- when $t\ge s$.

This duality with respect to the time parameter suggests to introduce the following two-parameters family of operators $P^*_{s,t}, s\le t$ associated with quantum conditional expectations:

$$\begin{aligned} &P^*_{s,t}:L^2(|\psi_s(x)|^2\,\mathrm{d}x)\to L^2(|\psi_t(q)|^2\,\mathrm{d}q)\\ &g^{(s)}(\cdot)\mapsto\int g^{(s)}(x)p(s,\mathrm{d}x,t,q)\equiv M^{t,q}_{\psi}[g^{(s)}], \end{aligned} \tag{2.29}$$

where the backward transition kernel (2.25) has been introduced and its "time reversed" family $P_{t,s}$, $s\le t$,

$$\begin{aligned} &P_{t,s}:L^2(|\psi_t(q)|^2\,\mathrm{d}q)\to L^2(|\psi_s(x)|^2\,\mathrm{d}x),\\ &f^{(t)}(\cdot)\mapsto\int f^{(t)}(q)\hat{p}(s,x,t,\mathrm{d}q)\equiv M^{\bar{\psi}}_{s,x}[f^{(t)}], \end{aligned} \tag{2.29′}$$

so that the equality between (2.28) and (2.28′) can be rewritten as

$$\langle(P_{t,s}f^{(t)})\cdot g^{(s)}\rangle_{\psi_s}=\langle f^{(t)}\cdot(P^*_{s,t}g^{(s)})\rangle_{\psi_t}. \tag{2.30}$$

The properties of the operators $P^*_{s,t}$ (or $P_{t,s}$) for $s\le t$ are as follows:

(a) $P^*_{s,t}$ are linear operators; as a map from $\mathbb{R}_+\times\mathbb{R}_+$ into densely defined, bounded operators from $L^2(|\psi_s(x)|^2\,\mathrm{d}x)$ into $L^2(|\psi_t(q)|^2\,\mathrm{d}q)$, $(s,t)\mapsto P^*_{s,t}$ is continuous;

(b) $\|P^*_{s,t}g^{(s)}\|_{L^2(|\psi_t(q)|^2\,dq)}=\|g^{(s)}\|_{L^2(|\psi_s(x)|^2\,dx)}$;
(c) $P^*_{s,t}1_{(s)}=1_{(t)}$ where $1_{(s)}$ is the function identically 1 in $L^2(|\psi_s(x)|^2\,dx)$ [with $1_{(t)}$ the same in $L^2(|\psi_t(q)|^2\,dq)$] and $P_{t,s}1_{(t)}=1_{(s)}$;
(d) $P^*_{s,s}=\mathrm{Id}$, the identity operator from $L^2(|\psi_s(x)|^2\,dx)$ into $L^2(|\psi_s(x)|^2\,dx)$;
(e) $P^*_{t,u}\cdot P^*_{s,t}=P^*_{s,u}$, $\quad s\le t\le u$;
(f) $P^*_{s,t}\cdot P_{t,s}=1_{(t)}$ and $P_{t,s}\cdot P^*_{s,t}=1_{(s)}$.

We may summarize the situation as follows:

Proposition II.12:

The two-parameters family of bounded operators $P^*_{s,t}$ and $P_{t,s}$ are dual from $L^2(|\psi_s(x)|^2\,dx)$ into $L^2(|\psi_t(q)|^2\,dq)$ in the sense that for any $f^{(t)}\in\mathcal{D}_{P_{t,s}}$ and $g^{(s)}\in\mathcal{D}_{P^*_{s,t}}$, the relation (2.30) *holds. Moreover, the properties* (*a*) *to* (*f*) *are satisfied* [*where* (*a*) *to* (*e*) *have their natural counterparts for $P_{t,s}$*].

The proof follows directly from the definitions (2.23′) and (2.25) of the forward and backward quantum transition kernels.

Remarks:

(1) Let $f^{(s)}(\cdot)$ be non-negative in $L^2(|\psi_s(x)|^2\,dx)$. Then, clearly $P^*_{s,t}$ does not, in general, transform $f^{(s)}(\cdot)$ into a non-negative element of $L^2(|\psi_t(q)|^2\,dq)$ since the backward quantum transition kernel p is not even real. In particular, $p(s,\cdot,t,q)$ is not a measure, although it shares manifestly a number of properties with probability measures.
(2) The equality between (2.28) and (2.28′) can be rewritten infinitesimally using the quantum derivatives D_t and $\bar{D}_t$. To do this, we need another property of these derivatives, which will be the first result of the next section.

Let $P^*_{s,t}$ and $P_{t,s}$ a pair of 2-parameters family of operators satisfying the properties of Proposition II.12 and $p,\bar{p}$, respectively, their associated quantum transition kernels.

Definition II.13:

The two dual kernels define a quantum diffusion if $\forall s<t, x\in\mathbb{R}^n, \varepsilon>0$, we have

(1) $\hat{p}(s,x,t,S_\varepsilon(x)^c)=o(t-s)$, *where $S_\varepsilon(x)^c$ is the complement of the sphere $S_\varepsilon(x)$ of radius ε and center x.*
(2) *There is a $\mathbb{C}^n$-valued function $\hat{B}(x,s)$ s.t.,*

$$\int_{S_\varepsilon(x)}(q-x)\hat{p}(s,x,t,dq)=\hat{B}(x,s)(t-s)+o(t-s).$$

There is an $n\times n$ complex-valued function $\hat{C}(x,s)$ s.t.

$$\int_{S_\varepsilon(x)}(q-x)(q-x)^T\hat{p}(s,x,t,dq)=\hat{C}(x,s)(t-s)+o(t-s).$$

$\hat{C}$ will be called the quantum diffusion matrix *and $\hat{B}$ the* (forward) drift of the quantum diffusion.

(3) *There is a $\mathbb{C}^n$-valued function $B(x,t)$ s.t.*

$$\int_{S_\varepsilon(x)}(q-x)p(s,dx,t,q)=B(q,t)(t-s)+o(t-s),$$

and an $n\times n$ complex-valued function $C(x,s)$ s.t.

$$\int_{S_\varepsilon(x)}(q-x)(q-x)^Tp(s,dx,t,q)=C(q,t)(t-s)+o(t-s).$$

These properties are satisfied, e.g., for the kernels associated with the Hamiltonians (2.13) Compare also Refs. 5 and 6. Indeed we have the following.

Proposition II.14:

Let H be of the form (2.13) *and its associated kernel k be such that*

$$\lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int (q-x) R(q,x,\Delta s) k(x,\Delta s,q) \mathrm{d}q = 0,$$

where $R(q,x,\Delta s)=0((q-x)^2)+0(\Delta s)^2$ *is a term in the Taylor expansion of the integrand of* $\hat{B}(x,s)$ *in the proof below. Let* $(q,t) \in \mathbb{R}^n \times \mathbb{R}$ *be* ψ*-admissible, where* ψ_t *is a regular solution of the Schrödinger equation for H, admitting a Taylor expansion in powers of the space and time variables around* $\psi_t(q)$. *Then a quantum diffusion corresponds to this solution, whose drifts and diffusion matrix are, respectively, given by*

$$\hat{B}(q,t) = i\hbar \frac{\nabla \bar{\psi}_t}{\bar{\psi}_t}(q) - A(q),$$

$$B(q,t) = -i\hbar \frac{\nabla \psi_t}{\psi_t}(q) - A(q), \tag{2.31}$$

$$C(q,t) = \hat{C}(q,t) = i\hbar \mathbb{1},$$

where $\mathbb{1}$ *denotes the* $n \times n$ *identity matrix.*

Proof: By (3) and (2.23),

$$\begin{aligned}
\hat{B}(x,s) &= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) \hat{p}(s,x,s+\Delta s,q) \mathrm{d}q \\
&= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) (\bar{\psi}_s(x))^{-1} k(x,\Delta s,q) \bar{\psi}_{s+\Delta s}(q) \mathrm{d}q \\
&= \lim_{\Delta s \downarrow 0} \frac{1}{\Delta s} \int_{s_\varepsilon(x)} (q-x) \left[1 + \frac{\nabla \bar{\psi}_s}{\bar{\psi}_s}(x)(q-x) + \frac{\dot{\bar{\psi}}_s}{\bar{\psi}_s}(x)\Delta s + O((q-x)^2) + O(\Delta s^2) \right] k(x,\Delta s,q) \mathrm{d}q.
\end{aligned}$$

We can easily verify the following properties of the integral kernel $k(x,\tau,q)$ of the evolution group U_τ for the Hamiltonian (2.13):

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \left[1 - \int_{\mathbb{R}^n} k(x,\tau,q) \mathrm{d}q \right] = \frac{1}{2} \nabla \cdot A(x) + \frac{i}{2\hbar} \|A(x)\|^2 + \frac{i}{\hbar} V(x),$$

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \int_{\mathbb{R}^n} (q-x) k(x,\tau,q) \mathrm{d}q = A(x),$$

$$\lim_{\tau \downarrow 0} \frac{1}{\tau} \int_{\mathbb{R}^n} (q-x)(q-x)^T k(x,\tau,q) \mathrm{d}q = i\hbar \mathbb{1}.$$

Using these in the above rhs of the expression of $\hat{B}(x,s)$ we obtain the expected result. The other results follow in a similar way. □

Proposition II.15:

Let $\nabla \psi_t / \psi_t$ *and* $A(q)$ *be given and continuous, for a Hamiltonian of the form* (2.13). *Assume*

that, in the representations (2.29) and (2.29′), *the partial derivatives with respect to* (t,q) [*respectively* (s,x)] *of the quantum conditional expectations are well defined and continuous, and can be exchanged with the integrals. Then the quantum equation of Kolmogorov for the transition kernel* $\hat{p}$ *for* $s \leq t \in \mathbb{R}$, $x,y \in \mathbb{R}^n$, *is given by*

(a)

$$-\frac{\partial \hat{p}}{\partial s}(s,x,t,q) = \frac{i\hbar}{2}\frac{\partial^2 \hat{p}}{\partial x^j\, \partial x^j}(s,x,t,q) + \left(i\hbar\, \frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t}(q) - A^j(q) \right) \frac{\partial}{\partial x^j}\hat{p}(s,x,t,q) \tag{2.32}$$

(*with the usual summation convention over the indices j*). *Equivalently, regarded as a function of the past variable,* $\hat{p}$ *is the fundamental solution of*

$$\bar{D}_s u = 0, \quad for \quad u \in \mathcal{D}_{\bar{D}_s}, \tag{2.33}$$

with $\bar{D}_s$ *defined in* (2.16).

(b) *If all the involved partial derivatives exist and are continuous,* $\hat{p}$, *regarded as a function of the future variables, solves the quantum Fokker-Planck equation*

$$\frac{\partial \hat{p}}{\partial t}(s,x,t,q) = \frac{i\hbar}{2}\frac{\partial^2 \hat{p}}{\partial q^j\, \partial q^j}(s,x,t,q) - \frac{\partial}{\partial q^j}\left[\left(i\hbar\, \frac{\nabla^j \bar{\psi}_t}{\bar{\psi}_t}(q) - A^j(q) \right) \hat{p}(s,x,t,q) \right]. \tag{2.34}$$

Similarly, the transition kernel $p(s,x,t,q)$ *solves*

(c)

$$-\frac{\partial p}{\partial s}(s,x,t,q) = -\frac{i\hbar}{2}\frac{\partial^2 p}{\partial x^j\, \partial x^j}(s,x,t,q) + \left(-i\hbar\, \frac{\nabla^j \psi_t}{\psi_t}(q) - A^j(q) \right) \frac{\partial}{\partial x^j} p(s,x,t,q). \tag{2.35}$$

So that p *is the fundamental solution of*

$$D_s v = 0 \quad for \quad v \in \mathcal{D}_{D_s}, \tag{2.36}$$

with D_s *given by* (2.14) *and the following backward quantum Fokker-Planck equation holds*:

(d)

$$\frac{\partial p}{\partial t}(s,x,t,y) = -\frac{i\hbar}{2}\frac{\partial^2 p}{\partial q^j\, \partial q^j}(s,x,t,y) - \frac{\partial}{\partial q^j}\left[\left(-i\hbar\, \frac{\nabla^j \psi_t}{\psi_t}(q) - A^j(q) \right) p(s,x,t,y) \right]. \tag{2.37}$$

Proof: (*a*) Let us consider (2.29′)

$$(P_{t,s} f^{(t)})(x) = \int f^{(t)}(q)\hat{p}(s,x,t,\mathrm{d}q) \equiv u(s,x), \quad s < t,$$

for any $f^{(t)}$ of compact support in the class used to define (2.22). By hypothesis, we can differentiate with respect to (s,x) under the integral sign. Using Proposition II.12 (c) and the properties of the quantum transition kernels before Proposition II.14,

$$
\begin{aligned}
u(s_1,x)-u(s_2,x) &= \int_{S_\varepsilon(x)} [u(s_2,q)-u(s_2,x)]\hat{p}(s_1,x,s_2,q)\mathrm{d}q + o(s_2-s_1) \\
&= \int_{S_\varepsilon(x)} \left\{ (q-x)\,\nabla\, u(s_2,x) + (q-x)(q-x)^T \frac{1}{2}\nabla^2 u(s_2,x) + R \right\} \hat{p}\,\mathrm{d}q + o(s_2-s_1) \\
&= \left[\nabla u(s_2,x) \int_{S_\varepsilon(x)} (q-x)\hat{p}(s_1,x,s_2,q)\mathrm{d}q \right. \\
&\quad \left. + \frac{1}{2}\nabla^2 u(s_2,x) \int_{S_\varepsilon(x)} (q-x)(q-x)^T \hat{p}(s_1,x,s_2,q)\,\mathrm{d}q + R \right] (s_2-s_1) + o(s_2-s_1) \\
&= \left[\hat{B}(x,s_2)\,\nabla\, u(s_2,x) + \frac{1}{2}\hat{C}(s_2,x)\nabla^2 u(s_2,x) + R \right] (s_2-s_1) + o(s_2-s_1),
\end{aligned}
$$

where $\hat{B}$ and $\hat{C}$ have been computed in Proposition II.14 and $R \equiv R(s_1,s_2,q,x)$ is a remainder $O(|q-x|^2)$. Dividing by (s_2-s_1) and taking $\lim_{s_2\downarrow s}$, $\lim_{s_1\uparrow s}$ one verifies that $u(s,x)$ solves the quantum Fokker-Planck equation (2.34).

According to (2.29′), the boundary condition of this equation is provided by

$$
u(s,x) - f^{(s)}(x) = \int_{S_\varepsilon(x)} [f^{(t)}(q) - f^{(s)}(x)]\hat{p}(s,x,t,q)\mathrm{d}q + o(t-s).
$$

So

$$
\lim_{s\uparrow t} u(s,x) \equiv \lim_{s\uparrow t} M^{\bar{\psi}}_{s,x}[f^{(t)}] = f^{(t)}(x). \tag{2.33′}
$$

(b) Let $f^{(t)}$ be of compact support, twice continuously differentiable in the class used to define (2.22). As before, one verifies that

$$
\lim_{s_1\uparrow s, s_2\downarrow s} \frac{1}{s_2-s_1} \left[\int f^{(s_2)}(q)\hat{p}(s_1,x,s_2,q)\mathrm{d}q - f^{(s)}(x) \right] = \hat{B}(x,s)\,\nabla\, f^{(s)}(x) + \frac{1}{2}\hat{C}(x,s)\nabla^2 f^{(s)}(x). \tag{2.38}
$$

Now let us write

$$
\begin{aligned}
\frac{\partial}{\partial t}\int f^{(t)}(q)\hat{p}(s,x,t,q)\mathrm{d}q &= \lim_{s_1\uparrow t, s_2\downarrow t} \frac{1}{s_2-s_1} \int [\hat{p}(s,x,s_2,q) - \hat{p}(s,x,s_1,q)] f^{(t)}(q)\mathrm{d}q \\
&= \lim_{s_1\uparrow t, s_2\downarrow t} \int \hat{p}(s,x,s_1,q) \left[\frac{1}{s_2-s_1} \int f^{(s_2)}(z)\hat{p}(s_1,q,s_2,z)\mathrm{d}z - f^{(s_2)}(q) \right] \mathrm{d}q.
\end{aligned}
$$

Using (2.38) this reduces to

$$
\int \hat{p}(s,x,t,q) \left[\hat{B}(q,t)\,\nabla\, f^{(t)}(q) + \frac{1}{2}\hat{C}(q,t)\nabla^2 f^{(t)}(q) \right] \mathrm{d}q.
$$

After integration by parts, we get

$$
\int \frac{\partial}{\partial t}\hat{p}(s,x,t,q)\cdot f^{(t)}(q)\mathrm{d}q = \int \mathrm{d}q\, f^{(t)}(q) \left[-\nabla_q \left(\hat{p}(s,x,t,q)\hat{B}(q,t) - \frac{1}{2}\nabla_q \left(\hat{C}(q,t)\hat{p}(s,x,t,q) \right) \right) \right].
$$

□

Introducing $\hat{B}$, $\hat{C}$ of Proposition II.14, (2.34) holds since $f^{(t)}$ is arbitrary in the chosen dense class.

Starting from (2.29), one proves (c) and (d) in the same way.

Proposition II.16:

Under the same conditions as in Proposition II. 15, the density of the quantum probability in the state $\psi_t, \rho(x,t)\,\mathrm{d}x=|\psi_t(x)|^2\,\mathrm{d}x$, *solves the continuity equation*

$$\frac{\partial \rho}{\partial t}+\nabla_j\left[\frac{i\hbar}{2}(\psi_t\nabla^j\bar{\psi}_t-\bar{\psi}_t\nabla^j\psi_t)-A^j\rho\right]=0,$$

or

$$\frac{\partial \rho}{\partial t}+\nabla_j\left[\frac{i\hbar}{2}\left(\frac{\nabla^j\bar{\psi}_t}{\bar{\psi}_t}-\frac{\nabla^j\psi_t}{\psi_t}-A^j\right)\rho\right]=0. \tag{2.39}$$

Proof: It follows from the definition (2.23′) of the forward quantum transition kernel $\hat{p}(s,x,t,q)$ that, if $\rho^{(s)}(\mathrm{d}x)$ denotes the quantum probability density at time $s<t$, then

$$\rho(q,t)=\int \rho^{(s)}(\mathrm{d}x)\hat{p}(s,x,t,q). \tag{2.40}$$

Applying the integration with respect to $\rho^{(s)}(\mathrm{d}x)$ to the quantum Fokker-Planck equation (2.34) one can see that $\rho(q,t)$ satisfies the same equation, namely

$$\frac{\partial \rho}{\partial t}=-\nabla_j\left[\left(i\hbar\frac{\nabla^j\bar{\psi}_t}{\bar{\psi}_t}-A\right)\rho\right]+\frac{i\hbar}{2}\Delta\rho. \tag{2.41}$$

But the quantum probability density ρ is also propagated backward in time by the transition kernel p solving (2.37). This means that ρ solves as well

$$\frac{\partial \rho}{\partial t}=-\nabla_j\left[\left(-i\hbar\frac{\nabla^j\psi_t}{\psi_t}-A\right)\rho\right]-\frac{i\hbar}{2}\Delta\rho. \tag{2.42}$$

It follows that ρ also solves the average of (2.41) and (2.42), i.e., the usual quantum continuity equation (2.39), as claimed. □

III. THE QUANTUM ACTION FUNCTION AND ITS DYNAMICAL CONTENT

Let us show first why, in relation with the quantum conditional expectation in a given state, it is legitimate to call $\bar{D}_\tau$ a quantum (time) derivative. The next proposition can be regarded as a quantum version of the fundamental theorem of calculus.

Proposition III.1: Let $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ *be any function continuous in the time variable* τ, *and in the domain of* $\bar{D}_\tau$. *Then, for any* $t\leq u$ *we have*

$$M^{\bar{\psi}}_{t,x}\left[\int_t^u \bar{D}_\tau f^{(\tau)}\,\mathrm{d}\tau\right]=M^{\bar{\psi}}_{t,x}[f^{(u)}]-f^{(t)}(x), \tag{3.1}$$

where $\bar{D}_\tau$ *is defined by* (2.15), *for* φ *replaced by* ψ.

Proof: By the definition (2.22) of $M^{\bar{\psi}}_{t,x}$, the lhs of (3.1), for (t,x) ψ-admissible, is

$$(\bar{\psi}_t(x))^{-1}\left(\int_t^u U_{\tau-t}[\bar{D}_\tau f^{(\tau)}\cdot\bar{\psi}_\tau]\mathrm{d}\tau\right)(x).$$

Introducing the definition (2.15) of $\bar{D}_\tau$, this means

$$(\bar{\psi}_t(x))^{-1}\left(\int_t^u U_{\tau-t}\cdot\left[\frac{1}{\bar{\psi}}\left(\frac{\partial}{\partial\tau}+\frac{1}{i\hbar}H\right)(\bar{\psi}_\tau f^{(\tau)})\cdot\bar{\psi}_\tau\right]\mathrm{d}\tau\right)(x)$$
$$=[\bar{\psi}_t(x)]^{-1}\left(\int_t^u U_{\tau-t}\left[\left(\frac{\partial}{\partial\tau}+\frac{1}{i\hbar}H\right)(\bar{\psi}_\tau\cdot f^{(\tau)})\right]\mathrm{d}\tau\right](x).$$

By an integration by parts with respect to $\mathrm{d}\tau$ and using the self-adjointness of H in $L^2(\mathbb{R}^n,\mathrm{d}x)$ we obtain

$$(\bar{\psi}_t(x))^{-1}\left\{-\int_t^u\left(\frac{\partial}{\partial\tau}U_{\tau-t}\right)(\bar{\psi}_\tau f^{(\tau)})\mathrm{d}\tau+U_{\tau-t}(\bar{\psi}_\tau f^{(\tau)})\Big|_t^u(x)+\frac{1}{i\hbar}\int_t^u(HU_{\tau-t})(\bar{\psi}_\tau f^{(\tau)})\mathrm{d}\tau\right\}.$$

Since $U_{\tau-t}$ solves, for $\tau>t$, $(\partial/\partial\tau)U_{\tau-t}\chi=(1/i\hbar)HU_{\tau-t}\chi$ for all χ in $\mathcal{D}_H$, this reduces to

$$(\bar{\psi}_t(x))^{-1}U_{\tau-t}(\bar{\psi}_\tau f^{(\tau)})\Big|_t^u=(\bar{\psi}_t(x))^{-1}\{U_{u-t}(\bar{\psi}_u f^{(t)})(x)-\bar{\psi}_t(x)f^{(t)}(x)\}.$$

By definition of the quantum conditional expectation, this is the rhs of Eq. (3.1). □

Remark:

When U_τ admits an integral kernel k, as in Sec. II, then the lhs of Eq. (3.1) becomes

$$(\bar{\psi}_t(x))^{-1}\int_t^T\int k(x,\tau-t,q)\bar{D}_\tau f^{(\tau)}(q)\bar{\psi}_\tau(q)\mathrm{d}q\,\mathrm{d}\tau.$$

The integration by parts with respect to $\mathrm{d}\tau$ mentioned in Proposition III.1 is done using the fact that k coincides with the retarded (or causal) distribution k_+ solving, for $\tau\geq t$, in the sense of distributions

$$\left(-i\hbar\frac{\partial}{\partial\tau}+H\right)k_+(x,\tau-t,q)=-i\hbar\,\delta(q-x)\delta(\tau-t).$$

□

Corollary III.2:

Let $f=(f^{(t)})_{t\in\mathbb{R}}$ strongly continuously differentiable from $\mathbb{R}$ into $L^2(\mathbb{R}^n,\mathrm{d}x)$, with $f^{(t)}(\cdot)\in\mathcal{D}_H$, $\forall t$. Assume that $(Hf^{(t)})_{t\in\mathbb{R}}$ is continuous in the time variable t. Then

$$\bar{D}_t f^{(t)}(x)=\lim_{\Delta t\downarrow 0}M^{\bar{\psi}}_{t,x}\left[\frac{f^{(t+\Delta t)}(\cdot)-f^{(t)}(x)}{\Delta t}\right]. \tag{3.2}$$

Proof: By Proposition III.1 for $u=t+\Delta t$ and property (3) of Proposition II.10,

$$\Delta t M^{\bar{\psi}}_{t,x}[\bar{D}_{t^*}f^{(t^*)}]=M^{\bar{\psi}}_{t,x}[f^{(t+\Delta t)}(\cdot)-f^{(t)}(x)], \tag{3.3}$$

for some $t^*\geq t$. The lhs is

$$\Delta t(\bar{\psi}_t(x))^{-1}U_{t^*-t}\left[\left(\frac{\partial}{\partial t^*}+\frac{1}{i\hbar}H\right)(\bar{\psi}_{t^*}f^{(t^*)})\right].$$

Now $f^{(t^*)}\in\mathcal{D}_H$ and $H(\bar{\psi}_{t^*}f^{(t^*)})=\bar{\psi}_{t^*}Hf^{(t^*)}\to_{t^*\to t}\bar{\psi}_tHf^{(t)}=H(\bar{\psi}_tf^{(t)})$. By Lemma II.4 $(\partial/\partial t^*)f^{(t^*)}$ is continuous in time, thus $\lim_{t^*\to t}M^{\bar{\psi}}_{t,x}[\bar{D}_{t^*}f^{(t^*)}]$ exists. After division by Δt, the rhs limit of (3.3) is the rhs of (3.2).

Corollary III.2 provides another proof of Proposition II.14 regarding the forward quantum transition kernel $\hat{p}$.

Corollary III.3:

Let us assume that $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ is as before and, moreover, admits a Taylor expansion up to the second order around a ψ-admissible $(t,x)\in\mathbb{R}\times\mathbb{R}^n$. Then if the Hamiltonian H is of the form

(2.13), *equation* (3.2) *implies, for* $f^{(t)}(x)=x$,

$$\bar{D}_t x = \lim_{\Delta t \downarrow 0} M^{\bar{\psi}}_{t,x}\left[\frac{f^{(t+\Delta t)}(\cdot)-x}{\Delta t}\right] = i\hbar\,\frac{\nabla\bar{\psi}_t}{\bar{\psi}_t}(x) - A(x), \tag{3.4}$$

and

$$\lim_{\Delta t \downarrow 0} M^{\bar{\psi}}_{t,x}\left[\frac{(f^{(t+\Delta t)}(\cdot)-x)^2}{\Delta t}\right] = i\hbar\,\mathbb{1}, \tag{3.5}$$

where $(f^{(t+\Delta t)}(\cdot)-x)^2$ *refers to the tensor product* $(f^{(t+\Delta t)}(\cdot)-x)\otimes(f^{(t+\Delta t)}(\cdot)-x)$ *and* $\mathbb{1}$ *is the* $n\times n$ *identity matrix.*

In equations (3.4) and (3.5) *the dummy variable* $(\cdot)$ *is the one denoted by* q *in* (2.23′). *All such "quantum moments" of order higher than 2 vanish.*

Proof: Let us consider the Taylor expansion up to the second order,

$$M^{\bar{\psi}}_{t,x}[f^{(t+\Delta t)}(q)-f^{(t)}(x)] = M^{\bar{\psi}}_{t,x}\left[\frac{\partial f}{\partial t}(x,t)\,\nabla t + (q-x)\cdot\Delta f(x,t) + \frac{1}{2}\sum_{i,j}((q_i-x_i)(q_j-x_j))\frac{\partial^2 f}{\partial x^i\,\partial x^j}(x,t) + o(\Delta t)\right].$$

Using the linearity of the quantum conditional expectation, as well as the properties (3) and (5) of Proposition II.15, the conclusion follows from the comparison with the explicit form (2.16) of $\bar{D}_t$ (with ψ replacing φ) for the Hamiltonian (2.13). □

In a similar way one proves the following.

Proposition III.4:

Let $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ *be continuous in the time variable* τ *and in the domain of* D_τ. *Then,* $\forall t\geq s$,

$$M^{t,x}_{\psi}\left[\int_s^t D_\tau f^{(\tau)}\,\mathrm{d}\tau\right] = f^{(t)}(x) - M^{t,x}_{\psi}[f^{(s)}], \tag{3.6}$$

where D_τ *is defined by* (2.11), *with* φ *replaced by* ψ.

Corollary III.5:

Under the same conditions as in Corollary III.2 we have

$$D_t f^{(t)}(x) = \lim_{\Delta t\downarrow 0} M^{t,x}_{\psi}\left[\frac{f^{(t)}(x)-f^{(t-\Delta t)}(\cdot)}{\Delta t}\right]. \tag{3.7}$$

If f *admits a Taylor expansion up to the second order around a* ψ*-admissible* $(t,x)\in\mathbb{R}\times\mathbb{R}^n$, *with* H *as in* (2.13) *we have, for* $f^{(t)}(x)=x$,

$$D_t x = \lim_{\Delta t\downarrow 0} M^{t,x}_{\psi}\left[\frac{x-f^{(t-\Delta t)}(\cdot)}{\Delta t}\right] = -\,i\hbar\,\frac{\nabla\psi_t}{\psi_t}(x) - A(x), \tag{3.8}$$

and

$$\lim_{\Delta t\downarrow 0} M^{t,x}_{\psi}\left[\frac{(x-f^{(t-\Delta t)}(\cdot))^2}{\Delta t}\right] = i\hbar\,\mathbb{1}, \tag{3.9}$$

where $(\cdot)$ *is the dummy space variable of the definition* (2.24). *As before, all such moments of order higher than 2 vanish.*

As mentioned in Remark 2 after Proposition II.12, in the conditions of Propositions III.1 and III.4, the definitions of the quantum (absolute) expectation of $f^{(t)}\cdot g^{(s)}$ in the state ψ, $t\geq s$, given in (2.28) and (2.28′) can be reexpressed in terms of the quantum derivatives D_t and $\bar{D}_t$ as follows.

Corollary III.6:

$$\langle f^{(t)}g^{(s)}\rangle_\psi = \left\langle M^{\bar{\psi}}_{s,\cdot}\left[\int_s^t \bar{D}_\tau f^{(\tau)}\,\mathrm{d}\tau\right]\cdot g^{(s)} + f^{(s)}g^{(s)}\right\rangle_{\psi_s}$$
$$= \left\langle f^{(t)}g^{(t)} - f^{(t)}M^{t,\cdot}_{\psi}\left[\int_s^t D_\tau g^{(\tau)}\,\mathrm{d}\tau\right]\right\rangle_{\psi_t}, \quad t \geq s.$$

This relation could define, actually, the proper concept of time-dependent Dirichlet form relevant to quantum dynamics (or its Euclidean counterpart—cf. Ref. 7).

Let us apply the Proposition III.1 to a $f=(f^{(\tau)})_{\tau\in\mathbb{R}}$ in the domain of $\bar{D}_\tau$ which is, in fact, time independent and of the form $f^{(\tau)}(\cdot)=F(\cdot)$ for some regular F. Then the lhs of (3.1) can be made explicit using (2.16) for the Hamiltonian (2.13), as well as (3.4),

$$M^{\bar{\psi}}_{t,x}\int_t^T \bar{D}_\tau F\,\mathrm{d}\tau = M^{\bar{\psi}}_{t,x}\int_t^T \left(\bar{D}_\tau q\cdot\nabla F + \frac{i\hbar}{2}\Delta F\right)\mathrm{d}\tau = M^{\bar{\psi}}_{t,x}[F(\cdot)] - F(x). \tag{3.10}$$

This relation clearly displays a quantum deformation of the fundamental theorem of calculus for line integrals along C^1 trajectories

$$\gamma:[t,T]\subset\mathbb{R}\to\mathbb{R}^n$$
$$\tau\mapsto q(\tau).$$

We shall henceforth denote the lhs of (3.10) by

$$M^{\bar{\psi}}_{t,x}\int_t^T \nabla F\circ \mathrm{d}q \tag{3.11}$$

in order to remind ourselves that it coincides simply with the rhs of (3.10) but involves the mentioned deformation of the classical calculus.

Using (3.6) instead of (3.1), we shall write as well, when $s\leq t$,

$$M^{t,x}_{\psi}\int_s^t \nabla F\circ \mathrm{d}q = F(x) - M^{t,x}_{\psi}[F(\cdot)], \tag{3.11$'$}$$

understanding now the lhs as

$$M^{t,x}_{\psi}\int_s^t \left(D_\tau q\cdot\nabla F - \frac{i\hbar}{2}\Delta F\right)\mathrm{d}\tau. \tag{3.10$'$}$$

More generally, for any $A:\mathbb{R}^n\to\mathbb{R}^n$ regular such that

$$M^{\bar{\psi}}_{t,x}\int_t^T \left(\bar{D}_\tau q\cdot A + \frac{i\hbar}{2}\nabla A\right)\mathrm{d}\tau \tag{3.12}$$

makes sense, we shall denote the expression (3.12) simply by

$$M^{\bar{\psi}}_{t,x}\int_t^T A\circ \mathrm{d}q. \tag{3.13}$$

We preserve, however, the boundary value in the time variable, in order to stress that (3.13) is only a short notation for (3.12) and that, in particular, *no* assumption on the existence of some underlying continuous trajectories $\tau\mapsto q(\tau)$ is made. The same remark applies to

$$M_{\psi}^{t,x}\left[\int_s^t A\circ \mathrm{d}q\right] = M_{\psi}^{t,x}\int_s^t \left(D_\tau q\cdot A - \frac{i\hbar}{2}\nabla\cdot A\right)\mathrm{d}\tau, \tag{3.13$'$}$$

so, with the conventions (3.13) and (3.13′), this "quantum calculus" satisfies the rules of the classical (Riemann-Stieltjes) calculus.

Let us come back to the special Lagrangian system whose quantum Hamiltonian is (2.13), i.e., a unit mass and charge particle in an electromagnetic field. Its associated classical action S_L with initial condition $S^{(s)}$ is defined by

$$S_L(x,t) = S^{(s)}(q(s)) + \int_\gamma \left(\frac{1}{2}|\dot{q}|^2 + \dot{q}\cdot A - V(q)\right)\mathrm{d}\tau, \tag{3.14}$$

for $s<t$. It is a real valued function of $x\in\mathbb{R}^n$, $t\in\mathbb{R}$ and a functional along a bundle of solutions γ in $C^2([s,t];\mathbb{R}^n):\tau\mapsto q(\tau)$ of the classical Lagrangian equations of motion, with the mixed boundary conditions on $[s,t]$,

$$\dot{q}(s) = \left.\frac{\partial S^{(s)}}{\partial q}\right|_{q(s)} \quad \text{and} \quad q(t)=x.$$

It is well known (cf., e.g., Ref. 8) that for $|t-s|$ small enough [and A and V as in (2.13)], S_L is a well-defined function. Notice that the Lagrangian L of S_L [i.e., the integrand of (3.14)] can be rewritten as

$$\int_\gamma L\,\mathrm{d}\tau = \int_\gamma \left(\frac{1}{2}|\dot{q}|^2 - V(q)\right)\mathrm{d}\tau + \int_\gamma A\,\mathrm{d}q. \tag{3.15}$$

We are going to show that, using various regularizations provided by the quantum mechanical conditional expectation, we can define a quantization of the above classical action functional S_L which will prove to be natural later on.

For any $(\tau,q)\psi$-admissible, let us define

$$S(q,\tau) = -i\hbar\,\ln\psi_\tau(q), \tag{3.16}$$

where ψ_τ is a regular solution of the Schrödinger equation (2.2) with Hamiltonian (2.1), such that $S=(S^{(\tau)})_{\tau\in\mathbb{R}}$ is continuous in the domain of D_τ. [We may choose the principal determination of the logarithm in the definition (3.16).]

According to (3.8), we observe that

$$D_\tau q = \nabla S(q,\tau) - A(q) \tag{3.17}$$

is an element of $L^2(\mathbb{R}^n,|\psi_\tau(q)|^2\,\mathrm{d}q)$ when $\int|\nabla\psi_\tau|^2\,\mathrm{d}q<\infty$ as well as $\int A^2(q)\,|\psi_\tau(q)|^2\,\mathrm{d}q<\infty$. Using the definition (2.14) for our situation, we compute

$$D_\tau S(q,\tau) = \frac{\partial S}{\partial\tau} + \left(-i\hbar\,\frac{\nabla\psi_\tau}{\psi_\tau} - A\right)\cdot\nabla S - \frac{i\hbar}{2}\Delta S = \frac{1}{2}(D_\tau q)^2 - \frac{i\hbar}{2}\nabla\cdot A + A\cdot D_\tau q - V(q), \tag{3.18}$$

where the relation (3.16) and the fact ψ_i solves the Schrödinger equation with H as in (2.13) have been used. The rhs of (3.18) is interpreted as the Lagrangian $L(D_\tau q,q)$ of our quantum system. Then, by Proposition III.4,

$$M_{\psi}^{t,x}\left[\int_s^t\left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_s^t\left(A\cdot D_\tau q - \frac{i\hbar}{2}\nabla\cdot A\right)\mathrm{d}\tau\right] = S(x,t) - M_{\psi}^{t,x}[S^{(s)}(\cdot)].$$

With the convention (3.13), this means that we have defined a regularized action function by

$$S(x,t) = M_{\psi}^{t,x}[S^{(s)}(\cdot)] + M_{\psi}^{t,x}\left[\int_s^t \left(\frac{1}{2}(D_\tau q)^2 - V(q)\right) \mathrm{d}\tau\right] + M_{\psi}^{t,x}\left[\int_s^t A \circ \mathrm{d}q\right], \tag{3.19}$$

to be compared with the corresponding classical action (3.14) and (3.15). The relation (3.19) provides us with an exact representation of the solution ψ_t of the Schrödinger equation.

Theorem III.7:

Let ψ_t be the solution of the Cauchy problem in $L^2(\mathbb{R}^n, \mathrm{d}x), t \geq s$,

$$i\hbar \frac{\partial \psi_t}{\partial t} = H\psi_t,$$

$$\psi_s(x) = e^{(i/\hbar)S^{(s)}(x)} \in \mathcal{D}_H, \quad \textit{with } S^{(s)} \textit{ such that } S^{(s)} = -i\hbar \ \ln \psi_s(x) \textit{ exists},$$

for $H = -(\hbar^2/2)[\nabla - (i\hbar)A]^2 + V$, with A,V continuous as in Remark 1 after Lemma II.4. We also assume that $\int |\nabla \psi_\tau(q)|^2 \, \mathrm{d}q < \infty$ and $\int A^2 |\psi_\tau(q)|^2 \, \mathrm{d}q < \infty$, $\forall \tau \geq s$. Then the following exact integral representation of the solution ψ_t holds:

$$\psi_t(x) = \exp\left(\frac{i}{\hbar} M_{\psi}^{t,x}\left[\int_s^t \left(\frac{1}{2}(D_\tau q)^2 - V(q)\right) \mathrm{d}\tau + \int_s^t A \circ \mathrm{d}q + S^{(s)}(\cdot)\right]\right) = e^{(i/\hbar)S(x,t)}, \tag{3.20}$$

$\forall (t,x)$ ψ-admissible, where S is the (complex-valued) solution of the quantum Hamilton Jacobi equation on $\mathbb{R}^n \times [s, \infty[$

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - A)^2 + V + \frac{i\hbar}{2} \nabla \cdot A - \frac{i\hbar}{2}\Delta S = 0,$$

$$S^{(s)}(x) = -i\hbar \ \ln \psi_s(x). \tag{3.21}$$

Remark: The kinetic energy term in (3.20) (i.e., the term with $V=0, A=0$) involves the scalar product of real vectors and not an Hermitian product. So, since $D_\tau q$ is a complex function, the kinetic energy term is, in general, a complex function, denoted here by $(D_\tau q)^2$.

Proof: When $t=s$ the representation (3.20) holds trivially, according to the property (3) of Proposition II.10 of the quantum mechanical conditional expectation. When $t>s$, using the relation (3.17), Eq. (3.18) means

$$\frac{\partial S}{\partial t} + (\nabla S - A) \cdot \nabla S - \frac{i\hbar}{2}\Delta S = \frac{1}{2}(\nabla S - A)^2 - \frac{i\hbar}{2} \nabla \cdot A + A \cdot (\nabla S - A) - V.$$

After simplification, this reduces to (3.21). The integral representation (3.20) follows from the definition (3.16) and the relation (3.19).

Remarks: We shall interpret (3.20) as a rigorous substitute for Feynman's path integral representation of the wave function ψ_t.[2] Like this one, (3.20) is built in term of the Lagrangian of the underlying classical system. We are going to need this for our study of quantum symmetries. However, the mathematical status of (3.20) is quite distinct from Feynman's heuristic (and, in some cases, rigorous[9,10] sum over a path space, as it involves in an essential way the regularizations provided by the quantum conditional expectation and no underlying path space whatsoever (cf. Sec. VII).

Corollary III.8:

Let $\bar{\psi}_t$ be the solution of the boundary problem in $L^2(\mathbb{R}^n, \mathrm{d}x)$ which is complex conjugate to the one of Theorem III.7,

$$\begin{cases} -i\hbar\,\dfrac{\partial\bar{\psi}_t}{\partial t} = H\bar{\psi}_t, \quad 0 \le t \le T, H \text{ as in Theorem III.7}, \\ \bar{\psi}_T(x) = e^{(i/\hbar)S^{(T)}(x)}. \end{cases}$$

Then the following representation holds under the same assumptions as Theorem III.7:

$$\bar{\psi}_t(x) = \exp\left(\frac{i}{\hbar}M^{\bar{\psi}}_{(t,x)}\left[\int_t^T\left(\frac{1}{2}(\bar{D}_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_t^T A\circ \mathrm{d}q + S^{(T)}(\cdot)\right]\right) = e^{(i/\hbar)\hat{S}(x,t)}, \tag{3.22}$$

where $\hat{S}$ *solves the equation adjoint to* (3.21) *on* $\mathbb{R}^m\times[-\infty, T]$,

$$\begin{gathered} -\frac{\partial\hat{S}}{\partial t} + \frac{1}{2}(-\nabla\hat{S} - A)^2 + V - \frac{i\hbar}{2}\nabla\cdot A - \frac{i\hbar}{2}\Delta\hat{S} = 0, \\ \hat{S}(x,T) = \hat{S}^{(T)}(x) = -i\hbar\,\ln\bar{\psi}_T(x). \end{gathered} \tag{3.23}$$

Proof: Starting from the logarithmic transformation of (3.22), Eq. (2.16) shows that $\bar{D}_\tau q = -\nabla\hat{S} - A$. Also $\bar{D}_i\hat{S}(q,\tau) = -(1/2)(\bar{D}_\tau q)^2 + V(q) - \bar{D}_\tau q\cdot A - (i\hbar/2)\nabla$. A reduces to (3.23). The conclusion follows from the definition (3.10) and Proposition III.1. □

Notice the change of signs in the two Hamilton-Jacobi equation (3.21) and (3.23). In the heuristic classical limit $\hbar = 0$, this is a well-known observation when the action is computed as a function of the future or past configurations (Ref. 11). This limit could be computed rigorously using, e.g., the methods of Ref. 12.

Also notice that, up to the convention (3.10) and (3.11) and the fact that the classical norm $|\dot{q}|^2$ of (3.14) is replaced by the square of a complex-valued quantum derivative, the Lagrangian of (3.22) is indeed the classical one, but evaluated on regularized variables.

The regularized action (3.19) used in our integral representation (3.20) satisfies the following additivity property along an admissible family of states ψ_τ, $s \le \tau \le u$.

Corollary III.9:

For any $t \in [s,u]$ *and under the conditions of Theorem III.7*,

$$M^{u,z}_\psi\left[\int_s^t L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right] + M^{u,z}_\psi\left[\int_t^u L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right] = M^{u,z}_\psi\left[\int_s^t L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right].$$

Proof: According to the property (c) of the operator P^* defined by (2.29), using (3.19), and for $S^{(s)}$ like in the definition (3.21),

$$\begin{aligned} P^*_{t,u}\cdot P^*_{s,t}[S^{(s)}] &= M^{u,z}_\psi[M^{t,\cdot}_\psi[S^{(s)}]] \\ &= M^{u,z}_\psi\left[S^{(t)}(\cdot) - M^{t,\cdot}_\psi\left[\int_s^t L\mathrm{d}\tau + A\circ\mathrm{d}q\right]\right] \\ &= M^{u,z}_\psi[S^{(t)}(\cdot)] - M^{u,z}_\psi\left[M^{t,\cdot}_\psi\left[\int_s^t L\mathrm{d}\tau + A\circ\mathrm{d}q\right]\right] \\ &= S^{(u)}(z) - M^{u,z}_\psi\left[\int_t^u L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right] - M^{u,z}_\psi\left[\int_s^t L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right] \\ &= P^*_{s,u}[S^{(s)}] \\ &= S^{(u)}(z) - M^{u,z}_\psi\left[\int_s^u L\,\mathrm{d}\tau + A\circ\mathrm{d}q\right]. \end{aligned}$$

□

Let us see what the fundamental gauge invariance of quantum mechanics means in the context of our integral representation (3.20).

Proposition III.10:

Let ψ_t be the solution of the Cauchy problem of Theorem III.7. Let $\chi=(\chi^{(\tau)})_{\tau\in\mathbb{R}}$ be real continuous and differentiable in the domain of D_τ. Then the gauge transformation

$$A \mapsto A' = A + \nabla\chi,$$
$$V \mapsto V' = V - \frac{\partial\chi}{\partial\tau} \tag{3.24}$$

leaves the form of the Schrödinger equation invariant provided that the integral representation (3.20) *becomes*

$$\psi_t(x) \mapsto \psi'_t(x) = \exp\left(\frac{i}{\hbar}M_\psi^{t,x}\left[\int_s^t\left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}\tau + \int_s^t A\circ\mathrm{d}q + \int_s^t D_\tau\chi^{(\tau)}\mathrm{d}\tau + (S^{(s)}+\chi^{(s)})(\cdot)\right]\right). \tag{3.25}$$

Proof: According to (2.14), for φ_t replaced by ϕ_t, and (3.11),

$$M_\psi^{t,x}\left[\int_s^t D_\tau\chi^{(\tau)}\,\mathrm{d}\tau\right] = M_\psi^{t,x}\left[\int_s^t \nabla\chi\circ\mathrm{d}q + \int_s^t\frac{\partial\chi}{\partial\tau}\,\mathrm{d}\tau\right] = \chi^{(t)}(x) - M_\psi^{t,x}[\chi^{(t)}(\cdot)]. \tag{3.26}$$

Using the representation of $\psi_t(x)$ in Theorem III.7 and (3.26), the representation (3.25) reduces to

$$\psi'_t(x) = \psi_t(x)e^{(i/\hbar)\chi^{(t)}(x)}. \tag{3.27}$$

When the starting wave function ψ_t is subject to the phase transformation (3.27), it is well know that the Schrödinger equation is form invariant under the gauge transformation (3.24). And indeed, (3.25) coincides with the representation (3.20) of $\psi'_t(x)$ in term of V' and A' defined by (3.24). □

We shall need, later on, a dynamical characterization of what plays, for our regularized action (3.19), the role of the critical points of the classical action (3.15), regarded as a functional of the C^2 path $\gamma\colon\tau\mapsto q(\tau)$.

Proposition III.11:

For the action (3.19), *the regularized equations of motion and conservation of energy in the admissible state ψ_τ solving the Schrödinger equation* (2.2) *with Hamiltonian H* (2.13) *in $L^2(\mathbb{R}^3,\mathrm{d}q)$ are, respectively, when $D_\tau q$ is in the domain of D_τ,*

$$D_\tau D_\tau q = -\operatorname{rot}A\wedge D_\tau Z - \frac{i\hbar}{2}\operatorname{rot}(\operatorname{rot}A) - \nabla V, \tag{3.28}$$

when $\wedge$ denotes the exterior product in $\mathbb{R}^n$ and

$$D_\tau h^H_{\psi_\tau}(q,\tau) = \frac{\partial h^H_{\psi_\tau}}{\partial\tau}, \tag{3.29}$$

where $h^H_{\psi_\tau}$ is the space–time observable associated by (2.5) *with the Hamiltonian* (2.13), *i.e.,*

$$h^H_{\psi_\tau} = \frac{1}{2}p^2 - p\cdot A + \frac{i\hbar}{2}\nabla\cdot(A-p) + \frac{1}{2}A^2 + V$$

for p the vector $p^j=-i\hbar(\nabla^j\psi_\tau/\psi_\tau)=B^j-A^j, j=1,2,3$ and $B(q,\tau)=D_\tau q$. In (3.29), *$\partial h^H_{\psi_\tau}/\partial\tau$ denotes the space–time observable associated with $\partial H/\partial\tau$, i.e., here, $\partial V/\partial\tau$. In particular, for V time independent, $h^H_{\psi_\tau}$ is a quantum martingale along ψ_τ, i.e., $D_\tau h^H_{\psi_\tau}=0$.*

Proof: According to (2.14), we have $D_\tau q=-i\hbar(\nabla\psi_\tau/\psi_\tau)-A$. If $D_\tau q$ is in the domain of $\mathcal{D}_\tau$ we can compute $D_\tau D_\tau q$. Using the fact that ψ_τ solves the Schrödinger equation of Theorem III.7 one gets, after some simplification, the rhs of (3.28). Alternatively, taking the gradient ∇ of the quantum Hamilton-Jacobi equation (3.21) and, by (3.17),

$$D_\tau q=\nabla S(q,\tau)-A(q)\equiv B(q,\tau),$$

where we introduced the notation $B=-i\hbar(\nabla\psi_\tau/\psi_\tau)-A$ for the space–time observable $a_{\psi_\tau}^{P-A}$ associated by (2.5) with the quantum velocity observable $P-A(Q)$ (P being the momentum and Q the position observable). We verify that the resulting equation coincides with (3.28). The additional "quantum" deformation on the rhs of (3.28) comes from the vector identity in $\mathbb{R}^3$: $\nabla(\nabla\cdot A)=\mathrm{rot}(\mathrm{rot}\,A)+\Delta A$ for the potential vector A. Besides this extra term, the rhs of (3.28) is the quantum regularization of the classical Lorentz force acting, at the singular limit $\hbar=0$, on the system with Hamiltonian (2.13) (cf. remark below). Concerning (3.29), the space–time energy function h associated with the Hamiltonian (2.13) is, by (2.5), $(H\psi_\tau/\psi_\tau)$ for $\psi_\tau\in\mathcal{D}_H$. After substitution in (2.11) and using the fact that $i\hbar(\partial\psi_\tau/\partial\tau)=H\psi_\tau$, we obtain the conclusion. □

Remark: Using $\bar{D}_\tau$, as defined in (3.2), instead of D_τ, we would find that

$$\bar{D}_\tau\bar{D}_\tau q=\bar{D}_\tau q\wedge\mathrm{rot}\,A+\frac{i\hbar}{2}\mathrm{rot}(\mathrm{rot}\,A)-\nabla V, \tag{3.30}$$

instead of (3.28). In particular, only the average of $D_\tau D_\tau q$ and $\bar{D}_\tau\bar{D}_\tau q$ can provide a regularization of the classical Lorentz force free of quantum corrections but involving, instead, the symmetric velocity $(1/2)(D_\tau q+\bar{D}_\tau q)$, namely

$$\tfrac{1}{2}(D_\tau D_\tau q+\bar{D}_\tau\bar{D}_\tau q)=\tfrac{1}{2}(D_\tau q+\bar{D}_\tau q)\wedge\mathrm{rot}\,A-\nabla V. \tag{3.31}$$

Let us stress that our quantum calculus over space–time observables is perfectly commutative. For example, $-\mathrm{rot}\,A\wedge D_\tau q=D_\tau q\wedge\mathrm{rot}\,A$ in contrast with its operator counterpart,

$$-\mathrm{rot}\,A\wedge(P-A)=(P-A)\wedge\mathrm{rot}\,A+i\hbar\ \mathrm{rot}(\mathrm{rot}\,A), \tag{3.32}$$

but the quantum correction associated with the noncommutativity of the operators reappears now in (3.28) as a consequence of the definition (2.14) of D_τ. Also we remark that the use of both $\bar{D}_\tau$ and D_τ is really necessary for our quantum calculus. For example, as expressed by (3.32), $-\mathrm{rot}\,A\wedge q$ and $q\wedge\mathrm{rot}\,A$ differ after canonical quantization and, in fact, they do not even define, individually, symmetric operators. So our symmetrization leading to (3.31) is the space–time counterpart of the canonical (symmetrized) Lorentz equations of motion[13]

$$\frac{d^2Q}{\mathrm{d}\tau^2}=\frac{1}{2}[(P-A)\wedge\mathrm{rot}\,A-\mathrm{rot}\,A\wedge(P-A)]-\nabla V, \tag{3.33}$$

for Q and P, respectively, the position and momentum quantum observables in the sense of Heisenberg.

IV. SYMMETRIES OF THE QUANTUM ACTION FUNCTION AND THE THEOREM OF NŒTHER

Let $\mathbb{R}^n$ be the configuration manifold of the classical system associated with the quantum Hamiltonian H of (2.2). The corresponding Lagrangian is

$$\begin{gathered}L:\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}\to\mathbb{R}\\(q,\dot{q},t)\mapsto L(q,\dot{q},t).\end{gathered} \tag{4.1}$$

Let us consider a one-parameter local Lie group of transformations of the extended configuration space $\mathbb{R}^n \times \mathbb{R}$, of the form

$$U_\alpha : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n \times \mathbb{R}$$

$$(q,t) \mapsto (Q,\tau),$$

where

$$Q = q + \alpha X(q,t) + o(\alpha); \quad \tau = t + \alpha T(t) + o(\alpha); \tag{4.2}$$

the generators $X : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and $T : \mathbb{R} \to \mathbb{R}$ are real analytical functions and α is a real parameter.

Let us write the action function (3.19) associated with the special Hamiltonian H of Theorem III.7. With an appropriate choice of the gauge $\chi^{(t)}(x)$ (Proposition III.10), we can get rid of the initial condition in the representation (3.19) for, say, $s = t_0$ and $t = t_1$,

$$S_L(x,t_1) = M_\psi^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right] \tag{4.3}$$

where ψ denotes the underlying solution of the associated Cauchy problem of Theorem III.7.

In analogy with the concept of invariance of the action involved in the classical Theorem of Nœther[14] we want to use the change of space–time variables, defined by (4.2), for defining the invariance of our regularized action (4.3).

Let us assume the existence of a further, complex analytic, generator $\varphi^{(t)}$ in the domain of D_τ, called the "divergence."

Definition IV.1: The action (4.3) *is divergence invariant under the one-parameter group of transformations* (4.2) *if, any interval* $[t_0, t_1]$, *we have*

$$M_\psi^{t_1,x_1}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_\tau q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right] + \alpha M_\psi^{t_1,x_1}\left[\int_{t_0}^{t_1} D_\tau \varphi^{(t)} \mathrm{d}t\right]$$
$$= M_{\tilde{\psi}}^{\tau_1,Q_1}\left[\int_{\tau_0}^{\tau_1}\left(\frac{1}{2}(D_\tau Q)^2 - V(Q)\right)\mathrm{d}\tau + \int_{\tau_0}^{\tau_1} A \circ dQ\right] + o(\alpha), \tag{4.4}$$

where $\tilde{\psi}$ *denotes the associated solution of the same Cauchy problem as in Theorem III.7 but for the new space–time variables* (Q,τ) *resulting from the transformation* U_α.

We remark that the definition (4.2) implies, up to the first order in α,

$$q + \alpha X(q,t) = Q, \tag{4.5}$$

where Q refers to the new configuration at the new time τ (we do not denote Q by Q_τ only to avoid the suggestion that paths $\tau \mapsto Q_\tau$ are involved).

Clearly, the invariance condition (4.4) can only hold under severe restrictions on the generations X, T, and φ. These conditions are easier to find in terms of the two solutions ψ and $\tilde{\psi}$ of the underlying Cauchy problem.

First, Proposition III.10 suggests that the addition in (4.4) of the divergence term $D_t \varphi^{(t)}$ to the given Lagrangian should correspond to a relation similar to (3.27) between ψ and $\tilde{\psi}$. So, to the first order in the parameter α, it should hold that

$$\tilde{\psi} = \psi - \alpha \frac{i}{\hbar} \varphi \cdot \psi. \tag{4.6}$$

Now let us consider (4.2) and (4.6) together with the linear generator of the associated local group of transformations of the Schrödinger equation (2.2) (as before, Einstein's sum convention is used)

$$\mathcal{L} = X^j \frac{\partial}{\partial x^j} + T\frac{\partial}{\partial t} + \frac{i}{\hbar}\varphi, \quad j = 1, \ldots, n.$$

For further purposes, it will be more natural to consider, instead, the formal symmetry generator

$$\hat{N}(t) = -i\hbar\,\mathcal{L} = X^j(x,t)\left(-i\hbar\,\frac{\partial}{\partial x^j}\right) - T(t)\left(i\hbar\,\frac{\partial}{\partial t}\right) + \varphi(x,t), \tag{4.7}$$

as well as the Schrödinger partial differential operator [cf. (2.2)], already used in Lemma II.4 (up to a factor i),

$$\mathbb{Q} = i\frac{\partial}{\partial t} - \frac{1}{\hbar}H. \tag{4.8}$$

Definition IV.2: $\hat{N}(t)$ *is a symmetry operator for the Schrödinger* equation (2.2) *provided*

$$[\hat{N}(t), \mathbb{Q}] = \lambda_{\hat{N}}(x,t)\mathbb{Q}, \tag{4.9}$$

where the complex analytic function $\lambda_{\hat{N}}(x,t)$ *will depend, in general, on* $\hat{N}(t)$ *and is s.t.* $\lambda_{\hat{N}}\mathbb{Q}D_{\mathbb{Q}} \subset L^2(\mathbb{R}^n \times \mathbb{R}, \mathrm{d}x\,\mathrm{d}t)$.

The domain $\mathcal{D}_{\mathbb{Q}}$ of $\mathbb{Q}$ has been defined in Lemma II.4. For the time being, we assume that $\mathcal{D}_{\mathbb{Q}} \supset \mathbb{Q}\mathcal{D}_{\mathbb{Q}}$ and $\hat{N}(t)\mathcal{D}_{\mathbb{Q}} \subset \mathcal{D}_{\mathbb{Q}}$ so that the lhs commutator of (4.9) is well defined on $\mathcal{D}_{\mathbb{Q}}$. We shall be more specific about $\mathcal{D}_{\hat{N}}$ in Sec. V.

In Refs. 15 and 67 it was shown that, in the algebraic sense, we have the following:

A symmetry operator $\hat{N}(t)$ generates a group, mapping solutions of the Schrödinger equation (2.2) into other solutions. The collection $\mathfrak{g}$ of such symmetry operators $\hat{N}(t)$ is a complex Lie algebra, i.e., if $\hat{N}_1, \hat{N}_2 \in \mathfrak{g}$, then (1) $\beta_1\hat{N}_1 + \beta_2\hat{N}_2 \in \mathfrak{g}$, $\forall\,\beta_1,\ \beta_2 \in \mathbb{C}$, (2) $[\hat{N}_1, \hat{N}_2] \in \mathfrak{g}$.

The formal symmetry group $G \equiv \exp\mathfrak{g}$ of Eq. (2.2) results from products of formal exponentials of symmetry operators; it is a local Lie group.

Let us stress that, in order to make this claim analytical rigorous, we have first to define the symmetrization $N(t)$ of such a formal generator $\hat{N}(t)$ then a self-adjoint extension $\hat{N}(t)$ and finally the unitary group generated by $\hat{N}(t)$. This will be done in Sec. V.

For a given Hamiltonian H, the property (4.9) implies the explicit conditions on the coefficients X, T, and φ that we are looking for.

Proposition IV.3:

$\hat{N}(t)$ *is a symmetry operator for the Schrödinger equation in* $L^2(\mathbb{R}^n)$, *with Hamiltonian* (2.13) *(where V may depend on time), if and only if*

(1)

$$\frac{\mathrm{d}T}{\mathrm{d}t}\delta^{jk} = \frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^k}, \quad 1 \le j, \quad k \le n,$$

(2)

$$\frac{\partial X^j}{\partial t} = -\frac{\partial \varphi}{\partial x^j} - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k\frac{\partial A^j}{\partial x^k},$$

(3)

$$\frac{\partial \varphi}{\partial t} - A^j\frac{\partial \varphi}{\partial x^j} - \frac{i\hbar}{2}\Delta\varphi = X^j\frac{\partial}{\partial x^j}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + T\frac{\partial V}{\partial t},$$

where Einstein's sum convention has been used, $\nabla\cdot A$ *denotes the divergence of the vector field A*

and n is the dimension of the configuration space of the underlying classical system.

Remark: If we allow space–dependent time transformation $\tau=t+\alpha T(q,t)+o(\alpha)$ in (4.2) then, for the associated $\hat{N}(t)$ to be a symmetry operator it is necessary, in addition to (1), (2), (3), that

$$\frac{\partial T}{\partial x^j}=0, \quad j=1,\ldots,n.$$

In other words, our initial choice of $T=T(t)$ was not a restriction.

Proof: Using the definitions (4.7) and (4.8), the conclusion follows from (4.9), after a laborious computation. One verifies that the coefficient $\lambda_{\hat{N}}(x,t)$ in (4.9) is

$$\lambda_{\hat{N}}(x,t)=-\frac{\mathrm{d}T}{\mathrm{d}t}(t). \tag{4.10}$$

In particular $\lambda_{\hat{N}}$ is not space dependent. □

Notice that the "determining equations" (1)–(4) (Ref. 16) for the coefficients X^j, T, and φ of the symmetry operator (4.7) are linear. We shall come back later to discuss their integrability conditions.

According to Theorem III.7, when $\hat{N}$ is a symmetry operator for (2.2) with Hamiltonian H of the form (2.13), $\tilde{\psi}$ solves the same Schrödinger equation but in the new variables (Q,τ). Therefore it follows from (3.16) and (3.19) that

$$-i\hbar\ \ln\tilde{\psi}(Q,\tau)=M_{\tilde{\psi}}^{\tau,Q}\left[\int_{\tau_0}^{\tau}\left(\frac{1}{2}(D_sQ)^2-V(Q)\right)\mathrm{d}s+\int_{\tau_0}^{\tau}A\circ\mathrm{d}Q\right].$$

On the other hand, taken together, the relations (4.2) and (4.6) defining the Lie groups of transformation around the identity $\alpha=0$ mean that ψ and $\tilde{\psi}$ are related, up to the first order in α, by

$$\psi(q,t)\exp\left(-\frac{i\alpha}{\hbar}\varphi(q,t)\right)=\tilde{\psi}(q+\alpha X(q,t),t+\alpha T(t)).$$

By considering $(-i\hbar\ \ln)$ of this equality for the principal determination of ln, taking into account the relation (4.5), valid for α small enough, as well as the representations (3.20) and (3.26), we verify that the invariance condition (4.4) of the action (4.3) is satisfied. In other words, the following proposition holds.

Proposition IV.4:

When the determining equations (1)–(3) *are satisfied for the Schrödinger equation with Hamiltonian* (2.13) *i.e., when the operator* $\hat{N}$ *of* (4.7) *is a symmetry operator for this equation, the associated action* (4.3) *is divergence invariant under the Lie groups of transformations defined by* (4.2) *and* (4.6).

We shall need:

Proposition IV.5:

Let us denote by $L=L(D_tq,q,t)$ *the Lagrangian involved in* (3.18)–(3.20). *Then, a necessary condition for the divergence invariance* (4.4) *of the action is that*

$$\frac{\partial L}{\partial t}T+\frac{\partial L}{\partial q^j}X^j+\frac{\partial L}{\partial(D_tq)^j}\left(D_tX^j-(D_tq)^j\frac{\mathrm{d}T}{\mathrm{d}t}\right)+L\frac{\mathrm{d}T}{\mathrm{d}t}=-D_t\varphi. \tag{4.11}$$

Proof: For the Hamiltonian of Theorem III.7 we have, according to the definition (2.14) of D_t, densely defined in $L^2(\mathbb{R}^n,|\psi_t(x)|^2\,\mathrm{d}x)$,

$$D_t X^j = \frac{\partial X^j}{\partial t} + B^k \frac{\partial X^j}{\partial q^k} - \frac{i\hbar}{2}\Delta X^j, \tag{4.12}$$

where

$$B^k = -i\hbar \frac{\nabla^k \psi_t}{\psi_t} - A^k, \quad k = 1, \ldots, n.$$

By (1) and (2) of Proposition IV.3,

$$D_t X^j = -\frac{\partial \varphi}{\partial q^j} - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k \frac{\partial A^j}{\partial q^k} + B^k \frac{\partial X^j}{\partial q^k}.$$

In particular,

$$D_t X^j = -(D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t} = i\hbar \frac{\nabla^j \psi_t}{\psi_t} \cdot \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{\partial \varphi}{\partial q^j} - X^k \frac{\partial A^j}{\partial q^k} + \frac{1}{2} B^k \left(\frac{\partial X^j}{\partial q^k} - \frac{\partial X^k}{\partial q^j} \right).$$

After substitution of $L(D_t q, q, t) = (1/2)(D_t q)^2 + A \cdot D_t q - (i\hbar/2)\nabla \cdot A - V$ in (4.11) we verify that this relation reduces to the condition (3) of Proposition IV.3 and therefore to one of the conditions ensuring that the generator $\hat{N}$ of (4.7) is a symmetry operator for the Schrödinger equation of Theorem III.7. □

Proposition IV.6:

When the generator $\hat{N}(t)$ is a symmetry operator for the Schrödinger equation (2.2) *s.t.* $(\varphi_t, \hat{N}(t)\varphi_t)$ *is well defined and the assumption for* (4.9) *is satisfied, then we have* $\forall \varphi_t \in \mathcal{D}_{\hat{N}(t)}$,

$$\frac{d}{\mathrm{d}t}(\varphi_t, \hat{N}(t)\varphi_t) = 0.$$

Proof: The equation (2.3) for $A(t) = \hat{N}(t)$ holds even when the members of the one-parameter family of operators $\hat{N}(t)$ are not self-adjoint as long as H is, and if the $\hat{N}(t)$ are densely defined and such that $(\varphi_t, \hat{N}(t)\varphi_t)$ makes sense.

Then, for any $\varphi_t \in D_{\hat{N}(t)}$, using (2.3) for $\psi_t = \varphi_t$,

$$\begin{aligned} \frac{d}{\mathrm{d}t}(\varphi_t, \hat{N}(t)\varphi_t) &= \int \bar{\varphi}_t \left(\frac{\partial \hat{N}(t)}{\partial t} + \frac{i}{\hbar}[H, \hat{N}(t)] \right) \varphi_t \, \mathrm{d}x \\ &= -i \int \bar{\varphi}_t \{ \mathbb{Q}(\hat{N}(t)\varphi_t) - \hat{N}(t)\mathbb{Q}\varphi_t \} \mathrm{d}x, \end{aligned}$$

where the operator $-i\mathbb{Q} = [(\partial/\partial t) - (1/i\hbar)H]$ of Lemma II.4 has been introduced.

On the other hand, it follows from the definition (4.9) that when $\hat{N}$ is a symmetry operator for (2.2) then $\mathbb{Q}\varphi_t = 0 \Rightarrow \mathbb{Q}(\hat{N}(t)\varphi_t) = 0$. So the conclusion follows. □

Let us prove a stronger version of Proposition IV.6 (without expectation) in terms of space–time observables.

Theorem IV.7 (Theorem of Nœther):

When $\hat{N}(t)$ is a symmetry operator for the Schrödinger equation (2.2) *with Hamiltonian* (2.13), *and when the action* (4.3) *is divergence invariant under the Lie group of transformations generated by $\hat{N}(t)$, the associated space–time observable $n^{\hat{N}}_{\psi_t}$ in the state ψ_t satisfies $D_t n^{\hat{N}}_{\psi_t} = 0$,* for all *$\psi_t$-admissible elements in $\mathcal{D}_{\hat{N}(t)}$. In this case we shall say that $n^{\hat{N}}_{\psi_t}$ is a* quantum martingale *for this Schrödinger equation.*

Proof: According to the definition (4.7), writing n instead of $n^{\hat{N}}_{\psi_t}$ for simplicity, we have

$$D_t n(x,t) = D_t(X^j p_j - Th + \varphi)(x,t), \tag{4.13}$$

where the space–time functions associated with $\hat{N}$, the momentum observable P_j and the Hamiltonian observable H of (2.13) have been introduced.

Using the relation (4.12) and Proposition II.8, the derivative of the scalar product in (4.13) can be written as

$$D_t(X^j p_j) = (D_t X^j)p_j + X^j(D_t p_j) - i\hbar \frac{\partial X^j}{\partial x^k}\frac{\partial p_j}{\partial x^k}, \tag{4.14}$$

where we notice the quantum deformation of Leibniz rule. Since $p_j = -i\hbar(\nabla_j \psi_t/\psi_t)$, $\partial p_j/\partial x^k$ is symmetric in j and k, so

$$\begin{aligned} D_t(X^j p_j) &= (D_t X^j)p_j + X^j(D_t p_j) - i\hbar \frac{1}{2}\left(\frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^j}\right)\frac{\partial p^j}{\partial x^k} \\ &= (D_t X^j)p_j + X^j(D_t p_j) - \frac{\hbar^2}{2}\frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{\Delta\psi_t}{\psi_t} - \left(\frac{\nabla\psi_t}{\psi_t}\right)^2\right), \end{aligned}$$

since, by (1) of Proposition IV.3,

$$\frac{\partial X^k}{\partial x^j} + \frac{\partial X^j}{\partial x^k} = \frac{\mathrm{d}T}{\mathrm{d}t}\delta^{jk}. \tag{4.15}$$

On the other hand, coming back to (4.13), we have

$$h = -\frac{\hbar^2}{2}\frac{\Delta\psi_t}{\psi_t} + i\hbar\frac{\nabla\psi}{\psi}\cdot A + \frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V. \tag{4.16}$$

Using (2.11) it is easy to verify (cf. also Proposition III.11) that

$$D_t h = \frac{\partial V}{\partial t}. \tag{4.17}$$

We have already found, in Proposition IV.5, that

$$D_t X^j = (D_t q)^i \frac{\mathrm{d}T}{\mathrm{d}t} + i\hbar\frac{\nabla^j\psi_t}{\psi_t}\cdot\frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{\partial\varphi}{\partial x^j} - X^k\frac{\partial A^j}{\partial x^k}.$$

Also, by (3) of Proposition IV.3,

$$\begin{aligned} D_t\varphi &= \left(\frac{\partial\varphi}{\partial t} - A^j\frac{\partial\varphi}{\partial x^j} - \frac{i\hbar}{2}\Delta\varphi\right) - i\hbar\frac{\nabla^j\psi_t}{\psi_t}\frac{\partial\varphi}{\partial x^j} \\ &= X^j\frac{\partial}{\partial x^j}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla\cdot A + \frac{1}{2}|A|^2 + V\right) + T\frac{\partial V}{\partial t} - i\hbar\frac{\nabla^j\psi_t}{\psi_t}\frac{\partial\varphi}{\partial x^j}. \end{aligned}$$

By (3.28), we also have, since $p_j = (D_t q)_j + A_j$,

$$D_t p_j = (D_t q \wedge \mathrm{rot}\, A)_j - \frac{i\hbar}{2}\mathrm{rot}(\mathrm{rot}\, A)_j - \nabla_j V + D_t A_j,$$

where

$$D_t A_j = \left(-i\hbar\frac{\nabla\psi_t}{\psi_t}\cdot\nabla\right)A_j - (A\cdot\nabla)A_j - \frac{i\hbar}{2}\Delta A_j.$$

After substitution of all this in

$$D_t n = (D_t X^j) p_j + X^j (D_t p_j) - \frac{\hbar^2}{2}\left[\frac{\Delta\psi_t}{\psi_t} - \left(\frac{\nabla\psi_t}{\psi_t}\right)^2\right] - hD_t T - D_t h \cdot T + D_t\varphi,$$

we obtain, indeed, zero. □

Let us come back to the explicit definition (4.7) of a symmetry operator $\hat{N}(t)$ for the Schrödinger equation (2.2). Introducing the definitions of the momentum and energy quantum observables P and H (in Heisenberg's picture) we observe that

$$\hat{N}(t) = X^j P_j - TH + \varphi, \tag{4.18}$$

where the coefficients X^j, T, and φ solve the partial differential equations of Proposition IV.3.

Let us denote by $Q(t)$ the time (Heisenberg) evolution of the position observable under an Hamiltonian H of the form (2.13). Then we define the following symmetrization of $\hat{N}(t)$:

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t), \tag{4.19}$$

where $\circ$ denotes Jordan's multiplication of operators, i.e., $C \circ B = (1/2)(CB+BC)$. Then the phase φ should be redefined by

$$\hat{\varphi} = \varphi + \frac{i\hbar}{2}\nabla \cdot X. \tag{4.20}$$

Proceeding heuristically, without worrying about domains (cf. Sec. V for precise definitions), we see that by the Corollary II.3 and Theorem IV.7, $n_{\varphi_t}^{\hat{N}}$ satisfies

$$D_t n_{\varphi_t}^{\hat{N}} = \frac{1}{\varphi_t}\left(\frac{\partial\hat{N}}{\partial t} + \frac{1}{i\hbar}[\hat{N},H]\right)\varphi_t = 0, \tag{4.21}$$

or, equivalently, for $n_{\varphi_t}^{N}$. So we can also verify, using the definition (4.19) of $N(t)$, the following Heisenberg equations of motion for the Hamiltonian (2.13):

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = P - A(Q),$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} = [P,H] = \frac{1}{2}\{(P-A)\wedge \mathrm{rot}\,A - \mathrm{rot}\,A \wedge (P-A)\} - \nabla V + \frac{1}{i\hbar}[A,H], \tag{4.22}$$

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t},$$

and the equations (1), (2), and (3) of Proposition IV.3, that $N(t)$ is indeed a constant of motion, i.e., satisfies

$$\frac{\partial N(t)}{\partial t} + \frac{1}{i\hbar}[N(t),H] = 0. \tag{4.23}$$

So we have heuristically checked that the family of operators $N(t)$ defined by (4.19) in terms of any solution $\{X^j, T, \varphi_s\}$ of the system of determining equations of Proposition IV.3 are constants of motion of the system with Hamiltonian H (2.13), associated with the Lie groups of space–time transformations generated by $\hat{N}(t)$.

From now on, we shall refer to $N(t)$ as above as a Nœtherian operator. We must now prove that any Nœtherian operator is indeed a respectable quantum observable, in the sense of Von Neumann.

V. STUDY OF THE NŒTHERIAN OPERATORS

A. Quadratic Hamiltonians

We shall start from the special class of Hamiltonian observables used in Theorem III.7, i.e., of the form

$$H(Q,P,t) = \tfrac{1}{2}[P - A(Q)]^2 + V(Q,t) \quad \text{on } C_0^\infty(\mathbb{R}^n) \tag{5.1}$$

but where, in addition, H is a real-valued polynomial of degree ≤ 2 in Q and P, which may be time dependent.

Let us denote by H_c the classical observable (or symbol) on the phase space $\mathbb{R}^{2n}\times\mathbb{R}$ to which $H \equiv H^W$ is associated by the Weyl calculus[17] of pseudodifferential operators. The set of quadratic inhomogeneous polynomials in q,p on $\mathbb{R}^{2n}$, denoted by $IQ(2n)$, constitutes a Lie algebra under the classical Poisson bracket of observables

$$\{F_c, G_c\} = \sum_{j=1}^{n} \frac{\partial F_c}{\partial q^j}\frac{\partial G_c}{\partial p_j} - \frac{\partial F_c}{\partial p_j}\frac{\partial G_c}{\partial q^j}. \tag{5.2}$$

Since the algebra generated under (5.2) by $IQ(2n)$ and any additional polynomial of order >2 is the set of all polynomials, $IQ(2n)$ will be maximal for our purpose.

Let us consider a smooth family of initial conditions $\psi^\alpha \in \mathcal{D}_H \subset L^2(\mathbb{R}^n, dx)$, $\alpha \in \mathbb{R}$, for the Schrödinger equation of a quadratic Hamiltonian (5.1), such that $\psi^0 = \psi$. The infinitesimal generator $\mathcal{N}$ of the associated one-parameter group in $\mathcal{D}_H$ is defined formally by

$$\mathcal{N}\psi = \frac{d}{d\alpha}\psi^\alpha\bigg|_{\alpha=0}. \tag{5.3}$$

Using the notation (4.7) for the symmetry operator $\hat{N}(t)$ of this Schrödinger equation, we consider the family of transformations $\mathcal{N}$ of the initial conditions ψ such that, under the quantum evolution generated by the quadratic Hamiltonian H,

$$(\mathcal{N}\psi)_t(x) = \hat{N}(t)\psi_t(x), \tag{5.4}$$

where, as before, ψ_t denotes the solution of the above-mentioned Cauchy problem of Schrödinger with initial condition $\psi \in \mathcal{D}_H$.

On the other hand, the ("Weyl") quantization $(-i/\hbar)F^W(Q,P)$ of any observable $F(q,p) \in IQ(2n)$ provides a linear map between Lie algebras, preserving the Lie bracket operation, i.e., a *representation* of such quadratic polynomials by skew-symmetric operators, such that Dirac's correspondence holds,

$$[F^W(Q,P), G^W(Q,P)] = \frac{i}{\hbar}\{F_c, G_c\}^W(Q,P) \tag{5.5}$$

for Q and P the quantum position and momentum observables, respectively. We consider first the simplest quadratic Hamiltonian (5.1), i.e., the free case $A=V=0$. This will prove to be sufficient for any quadratic case (cf. Proposition V.4).

Proposition V.1:

The above (faithful) representation of $IQ(2n)$ can be exponentiated to a representation of a Lie group, called the inhomogeneous (or extended) metaplectic group and denoted $iMp(n)$, which is the semidirect product of $Mp(n)$, the ("metaplectic") group generated by the quadratic observables and W_n, the Heisenberg group generated by the linear and constant observables. In particular, any generator $\mathcal{N}$ satisfying (5.4) *belongs to the inhomogeneous metaplectic algebra, denoted by $imp(n)$.*

Proof: Let us denote by $k_0(q,t,x)$ the propagator of the free Schrödinger equation (2.2) [i.e.,

with $H=H_0$ in (5.1), where $A=V=0$]. Using the definition (4.7) of $\hat{N}(t)$, the rhs of Eq. (5.4) can be written as

$$\int_{\mathbb{R}^n} \psi(q)\left\{X^j(x,t)\left(-i\hbar\frac{\partial k_0}{\partial x^j}\right)-T(t)i\hbar\frac{\partial k_0}{\partial t}+\varphi(x,t)k_0\right\}(q,t,x)\mathrm{d}q$$
$$=\int_{\mathbb{R}^n}\left\{i\hbar X^j(x,t)\frac{\partial\psi(q)}{\partial q^j}+T(t)\frac{\hbar^2}{2}\frac{\partial^2\psi(q)}{\partial(q^j)^2}+\varphi(x,t)\right\}k_0(q,t,x)\mathrm{d}q,$$

where the space translation invariance of k_0 has been used. Taking $\lim_{t\downarrow 0}$, this provides the following explicit form of $\mathcal{N}$ defined on $C_0^\infty(\mathbb{R}^n)$ by (5.4):

$$\mathcal{N}=-X^j(Q,0)P_j-\tfrac{1}{2}T(0)P_j^2+\varphi(Q,0). \tag{5.6}$$

□

Clearly, the maximal Lie algebra generated by such infinitesimal operators is a subalgebra, denoted by $\mathcal{G}_s(n)$, of the above-mentioned Weyl quantization of $IQ(2n)$.

Equivalently, each $X^j(x,0)$ can be an inhomogeneous polynomial of degree 1, $T(0)$ is a constant and $\varphi(x,0)$ an inhomogeneous polynomial of degree 2. Taking into account the restrictions imposed by (5.4) and the special form of our free Schrödinger equation, one computes that the dimension of this ("symmetry") Lie algebra $\mathcal{G}_s(n)$ of skew-symmetric operators is $(n/2)(n+3)+4=l$.

Here is a basis of $\mathcal{G}_s(n)$, for $j,k=1,2,\ldots,n$:

$$B_s(n)=\left\{i, iq^k, \hbar\frac{\partial}{\partial q^k}, i\sum_k (q^k)^2, i\frac{\hbar^2}{2}\sum_k\frac{\partial^2}{\partial(q^k)^2}\quad,\quad \hbar\sum_k q^k\frac{\partial}{\partial q^k}+\frac{\hbar}{2}n,\ \hbar\left(q^j\frac{\partial}{\partial q^k}-q^k\frac{\partial}{\partial q^j}\right)\right\}. \tag{5.7}$$

We shall denote by $\mathcal{N}_j, j=1,2,\ldots,(n/2)(n+3)+4\equiv l$, the skew-Hermitian operators of $B_s(n)$ on $L^2(R^n)$. A necessary condition for exponentiating this representation of the Lie algebra $\mathcal{G}_s(n)$ is that all the generators $\mathcal{N}_j$ should be essentially skew-adjoint on a common domain in the Hilbert spaces. We shall use the following general result of Nelson[18] (cf. also Ref. 19):

Let G be a simply connected Lie group with an ℓ-dimensional Lie algebra $\mathcal{G}$, and a given representation of $\mathcal{G}$ by unbounded skew-Hermitian operators $\mathcal{N}_j, j=1,\ldots,\ell$, on a Hilbert space $\mathcal{H}$. Then this representation of $\mathcal{G}$ arises by differentiation of a unique unitary representation of $\mathcal{G}$ if there is dense set vectors ψ in the domain of any product $\mathcal{N}_{j_1},\ldots,\mathcal{N}_{j_m}$ and such that

$$\frac{\|\mathcal{N}_{j_1}\cdots\mathcal{N}_{j_m}\psi\|_{\mathcal{H}}}{m!}\le CK^m, \tag{5.8}$$

$\forall m\in\mathbb{N}$ and $\forall j_i\in\{1,\ldots,\ell\}$, for C,K two positive constants. Such a $\psi\in\mathcal{H}$ is called "analytic for $\{\mathcal{N}_j\}_{j=1}^{\ell}$."

In our case we have the following.

Lemma V.2:

The finite linear combinations of the Hermite functions on $\mathbb{R}^n$ (i.e., the products of one-dimensional Hermite functions) are analytic vectors for any products $\mathcal{N}_{j_1}\ldots\mathcal{N}_{j_m}$ of the generators listed in the basis (5.7) *of $\mathcal{G}_s(n)$.*

Proof: Since the set of finite linear combinations of Hermite functions is dense in $L^2(\mathbb{R}^n)$, one needs only to show that each Hermite function is an analytic vector for any $\mathcal{N}_{j1}\cdots\mathcal{N}_{jm}$. Instead of the standard basic $\{i, iq^k, \hbar\partial/\partial q^k\}, k=1,\ldots,n$, used in (5.7) for the Heisenberg algebra (of constant and linear observables in q and p), consider the linear combinations called creation and annihilation operators:

$$\left\{ i, A_k \equiv \frac{1}{\sqrt{2}}\left(q^k + \hbar \frac{\partial}{\partial q^k} \right), \quad A_k^+ \equiv \frac{1}{\sqrt{2}}\left(q^k - \hbar \frac{\partial}{\partial q^k} \right) \right\}. \tag{5.9}$$

Expressing the Hermite function in terms of A_k^+, one shows that those functions are analytical vectors for q^k and $-i\hbar(\partial/\partial q^k)$ (see, e.g., Ref. 4, p. 204). On the other hand, the operators of $B_s(n)$ quadratic in q and p are generated by all possible double products of creation and annihilation operators and it is known that the Hermite functions are analytic vectors as well for such quadratic observables (Ref. 19, p. 190). □

So there is indeed a unique representation of a Lie group $G_s(n)$ whose infinitesimal version (or differential) is the symmetry algebra $\mathcal{G}_s(n)$. The representation is included in the so-called extended metaplectic representation[19] which is the semidirect product of the $n(2n+1)$-dimensional metaplectic group $Mp(n)$, generated by all quadratic observables, and the $(2n+1)$-dimensional Heisenberg group W_n generated by the constant and liner observable.

In particular, let us consider matrices D in the symplectic Lie algebra $\mathcal{S}p(2n)$, i.e., of the form

$$D = \begin{pmatrix} W^T & Z \\ Y & -W \end{pmatrix}, \tag{5.10}$$

where Y and Z are $n \times n$ real matrices of the form $Y = \gamma \mathbb{1}, Z = \beta \mathbb{1}$, with γ, β two real constants, $\mathbb{1}$ the $n \times n$ identity matrix, and W is a $n \times n$ real matrix of the form

$$W = \begin{pmatrix} \delta & -W_{21} & -W_{31} & \cdots & \cdots & -W_{n1} \\ W_{21} & \delta & -W_{32} & \cdots & \cdots & -W_{n2} \\ W_{32} & W_{32} & \delta & \cdots & \cdots & -W_{n3} \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & -W_{nn-1} \\ W_{n1} & W_{n2} & \cdots & \cdots & W_{nn-1} & \delta \end{pmatrix} \tag{5.11}$$

for δ a constant. Then we use the faithful representation of $\mathcal{S}p(2n)$ by skew-Hermitian quadratic operators associated with the names of Segal, Shale, and Weil,[20]

$$D \mapsto -iP_D^W(Q,P) \equiv \beta \frac{i\hbar^2}{2} \frac{\partial^2}{\partial q_k^2} - \hbar\, q_k W_{jk} \frac{\partial}{\partial q^j} - \frac{\hbar}{2} n\delta + \gamma \frac{i}{2} q_k^2, \tag{5.12}$$

which is the infinitesimal version of the representation of some elements M_α of the symplectic groups $\mathcal{S}p(2n)$ by unitary groups $U_\alpha, \alpha \in R$, on $L^2(R^n)$,

$$M_\alpha = e^{\alpha D} \mapsto U_\alpha = e^{\alpha P_D^W(Q,P)}.$$

On the classical side, each M_α is a one-parameter group of linear difeomorphisms of the classical phase space $\mathbb{R}^{2n}$, whose associated quadratic Hamiltonian vector field v_D is defined by

$$\begin{aligned} v_D(F_c) &= \frac{\mathrm{d}}{\mathrm{d}\alpha} F_c(M_\alpha(q,p))\big|_{\alpha=0} = (W^T q + \beta p)\nabla_q F_c + (\gamma q - Wp)\nabla_p F_c \\ &= \nabla_p P_D^c \cdot \nabla_q F_c - \nabla_q P_D^c \cdot \nabla_p F_c \\ &= \{F_c, P_D^c\} \end{aligned} \tag{5.13}$$

on any F^c in the Schwartz space of smooth and rapidly decreasing functions, which are C^∞ vectors for the metaplectic representation. Equation (5.13) holds since the classical observable P_D^c in $IQ(2n)$ associated with $D \in \mathcal{S}p(2n)$ is

$$P_D^c(q,p) = \frac{\beta}{2}p^2 + qWp - \frac{\gamma}{2}q^2. \tag{5.14}$$

Notice that the only additional constant term in the representation (5.12) with respect to (5.14) is due to the Weyl (Jordan) symmetrization of the classical qWp term in (5.14).

The relation $D \in \mathcal{S}p(2n) \mapsto v_D$ preserves the respective Lie parentheses, i.e., is a Lie algebra homomorphism. As mentioned before, the Heisenberg algebra W_n adds to the previous picture the representation of the linear observable on $\mathbb{R}^{2n}$,

$$ap - bq + c \mapsto -i\hbar\, a_k \frac{\partial}{\partial qk} - b_k q^k + c, \tag{5.15}$$

where $a, b \in \mathbb{R}^n$ and $c \in \mathbb{R}$, so that, finally, the classical quadratic observable

$$P_D^c(q,p) = \frac{\beta}{2}p^2 + qWp - \frac{\gamma}{2}q^2 + ap - bq + c \tag{5.16}$$

of Hamiltonian vector field v_P associated with the (affine) equation of Hamilton,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \nabla_p P^c \\ -\nabla_q P^c \end{pmatrix} = \begin{pmatrix} W^T & \beta\mathbb{1} \\ \gamma\mathbb{1} & -W \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix},$$

is quantized, according to Weyl, by

$$P_D^W(Q,P) = -\frac{\beta}{2}\hbar^2 \frac{\partial^2}{\partial q_k^2} - i\hbar\, q_k W_{jk} \frac{\partial}{\partial q_j} - \frac{\gamma}{2} q_k^2 - i\hbar\, a_k \frac{\partial}{\partial q_k} - b_k q^k + \left(c - \frac{i\hbar}{2} n\delta \right) \tag{5.17}$$

(with the usual convention of summing over repeated indices). We can now be more specific about the comments at the beginning of this section: The Lie algebra $IQ(2n)$ associated with the semidirect product of the metaplectic group $Mp(n)$ and the Heisenberg group W_n is isomorphic to the algebra of all polynomial observables of degree ≤ 2 on $\mathbb{R}^{2n}$ equipped with the Poisson bracket (5.2) and the representation of the classical observables is Weyl quantization procedure.

Let us observe that some subgroups of $S_p(2n)$ have, under this representation, explicit integral formulations. We will not need them here. See Ref. 19 for some particular cases.

In particular, let us consider $D = \begin{pmatrix} 0 & \mathbb{1} \\ 0 & 0 \end{pmatrix} \in \mathcal{S}p(2n)$, i.e., the case $\beta = 1, \gamma = 0, W = 0$ in (5.14). So the associated classical observable reduces to our free Hamiltonian

$$P_A^c(q,p) = \tfrac{1}{2}p^2 \equiv H_0(p),$$

and its Weyl quantization is, of course,

$$P_A^W(Q,P) = -\frac{i}{\hbar} H_0(P)$$

or $i\mathcal{N}_{(2n+3)}$ in term of the $(2n+3)$th element of the basis $B_s(n)$ (5.7). Denoting the associated parameter α by t, let us consider

$$U_t = e^{tP_A^W} = e^{-(i/\hbar)tH_0}, \quad t \in \mathrm{R},$$

i.e., the strongly continuous unitary group evolution in $L^2(\mathbb{R}^n)$, solving the free Schrödinger equation, and defined on $\mathcal{D}_{H_0}$. This groups acts on the symmetry algebra $\mathcal{G}_s(n)$ generated by the symmetry operators $\mathcal{N}_j, j = 1, \cdots (n/2)(n+3)+4$ via the adjoint representation

$$\mathcal{N} \mapsto U_t \mathcal{N} U_t \equiv \hat{N}(t). \tag{5.18}$$

Since this representation sends analytic vectors into analytic vectors, the domains are preserved, $\mathcal{D}_{\mathcal{N}} = \mathcal{D}_{\hat{N}(t)}$. In other words, although H_0 and the operators $-i\mathcal{N}$ are unbounded symmetric operators, they are essentially self-adjoint and defined on a common dense invariant domain of analytic vectors in $L^2(\mathbb{R}^n)$. By a variant of the commutator theorem,[4] the Baker-Campbell-Hausdorff formula still holds. The image of the basis $B_s(n)$ under (5.18) is, therefore, computed as follows:

$$\left\{ i, iq^k - t\hbar \frac{\partial}{\partial q^k}, \hbar \frac{\partial}{\partial q^k}, i\sum_k (q^k)^2 - 2t\left(\sum_k q^k \hbar \frac{\partial}{\partial q^k} + \frac{\hbar}{2} n \right) - 2t^2 \hbar \frac{\partial}{\partial t}, \hbar \frac{\partial}{\partial t}, \right.$$
$$\left. \hbar \sum_k q^k \frac{\partial}{\partial q^k} + \frac{\hbar}{2} n + 2t\hbar \frac{\partial}{\partial t}, \hbar \left(q^j \frac{\partial}{\partial q^k} - q^k \frac{\partial}{\partial q^j} \right) \right\}, \tag{5.19}$$

where $j,k = 1, \cdots, n$. We shall denote by $\hat{N}_j(t), j = 1, \cdots, \ell$, any of those $\ell = (n/2)(n+3)+4$ resulting skew-symmetric operators.

Theorem V.3:

For fixed $t \in \mathbb{R}$, let us define by $U_t V_0^j(\alpha) U_{-t} = V_t^j(\alpha)$, $\alpha \in \mathbb{R}$, a one-parameter family of operators in $L^2(\mathbb{R}^n)$, with $V_0^j(\alpha) = e^{(\alpha/\hbar)\mathcal{N}_j}$ and $V_t^j(\alpha) = e^{(\alpha/\hbar)\hat{N}_j(t)}$, $\hat{N}_j(t)$ being any of the skew-symmetric operators of (5.19), *image under the adjoint representation* (5.18) *of the one-parameter group of operators $V_0^j(\alpha)$, $j = 1, \ldots, \ell$, generated by the basis* (5.7) *of the symmetry algebra $\mathcal{G}_s(n)$. Then, the $V_t^j(\alpha)$ are symmetry operators of the free, Schrödinger equation $i\hbar(\partial/\partial t)\psi_t = H_0\psi_t$ in $L^2(\mathbb{R}^n)$, i.e., they map any regular solution ψ_t of this equation in another solution of the same equation $\tilde{\psi}_t = V_t^j(\alpha)\psi_t$, and the $i\hat{N}_j(t)$ are constant observables of the free quantum system.*

Proof: Let us consider $\psi_t = U_t\psi$, $\psi \in \mathcal{D}_H$ for $U_t = e^{-(i/\hbar)tH_0}$, $t \in \mathbb{R}$. Then $V_t^j(\alpha)\psi_t \equiv e^{-(i/\hbar)tH_0}\psi^\alpha$, $\alpha \in \mathbb{R}$, is, by construction, solution of the same free Schrödinger equation, for the one-parameter family of initial conditions in $\mathcal{D}_H \subset L^2(\mathbb{R}^n)$ defined by $\psi^\alpha \equiv e^{(\alpha/\hbar)\mathcal{N}_j}\psi$.

It follows from the definition of $V_t^j(\alpha)$ and the computation of $(\partial/\partial\alpha)|_{\alpha=0}$ in the relation above that

$$(\mathcal{N}_j\psi)_t(x) = \hat{N}_j(t)\psi_t(x), \quad j = 1, \ldots, \frac{n}{2}(n+3)+4, \tag{5.20}$$

is the infinitesimal version of this relation, as required by the definition (5.4) of a symmetry operator.

Now by (5.18), $U_t \mathcal{N}_j U_t^{-1} = \hat{N}_j(t)$. Proceeding like in Sec. II (or observing, as before, that the Baker-Campbell-Hausdorff formula holds here), we see that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\psi_t, \hat{N}_j(t)\varphi_t) = \left(\psi_t, \left(\frac{\partial \hat{N}_j}{\partial t} + \frac{1}{i\hbar}[\hat{N}_j, H_0] \right) \varphi_t \right).$$

But, by definition (4.9) of a symmetry operator $\hat{N}(t)$ for the free Schrödinger operator

$$\mathbb{Q}\varphi_t \equiv \left(i\frac{\partial}{\partial t} - \frac{1}{\hbar}H_0 \right)\varphi_t, \tag{5.21}$$

we had

$$[\hat{N}(t), \mathbb{Q}]\varphi_t = \lambda_N \mathbb{Q}\varphi_t = 0 \tag{5.22}$$

for any $\varphi_t \in \mathcal{D}^{\hat{N}}(t)$ (in the notations of Proposition II.2). In particular, for any $\hat{N}_j(t)$ as before we find, by Proposition IV.6,

$$i\frac{\mathrm{d}}{\mathrm{d}t}(\varphi_t,\hat{N}_j(t)\varphi_t)=0, \tag{5.23}$$

i.e., that $i\hat{N}_j(t)$ is a constant observable of the free Schrödinger equation. □

Any quadratic Hamiltonian H of the form (5.1) can, in fact, be handled in the same way since the infinitesimal generators of $B_s(n)$ [cf. (5.7)] form a vector space. Let us see how, in the special case $n=2$ for the simplicity of the illustration (and notations).

Proposition V.4:

All Schrödinger equations in $L^2(\mathbb{R}^2)$, *of the form*

$$i\hbar\frac{\partial}{\partial t}\psi_t=\left[-\frac{\hbar^2}{2}\Delta+c_1((x^1)^2+(x^2)^2)+c_2\left(-i\hbar\frac{\partial}{\partial x^1}\right)+c_3\left(-i\hbar\frac{\partial}{\partial x^2}\right)+c_4\left(-i\hbar\left(x^1\frac{\partial}{\partial x^2}-x^2\frac{\partial}{\partial x^1}\right)\right)\right.$$
$$\left.+c_5x^1+c_6x^2+c_7\left(-i\hbar\left(x^1\frac{\partial}{\partial x^1}+x^2\frac{\partial}{\partial x^2}\right)\right)+c_8\right]\psi_t, \tag{5.24}$$

with $c_k\in\mathbb{R}$ *such that the Hamiltonian is essentially self-adjoint on* $C_0^\infty(\mathbb{R}^2)$, *have isomorphic symmetry algebras and are equivalent to the free equation*

$$i\hbar\frac{\partial}{\partial t}\psi_t=H_0\psi_t, \tag{5.25}$$

where H_0 *is the two-dimensional free Hamiltonian*

$$H_0=-\frac{\hbar^2}{2}\left(\frac{\partial^2}{\partial(x^1)^2}+\frac{\partial^2}{\partial(x^2)^2}\right).$$

Proof: Given in Ref. 15. □

In order to illustrate this isomorphism, let us consider the following linear combination of elements of $\mathcal{G}_s(2)$ [using the notations of (5.7)]:

$$\mathcal{N}=-\mathcal{N}_6+\frac{1}{2}\mathcal{N}_7=i\left(-\frac{\hbar^2}{2}\Delta+\frac{1}{2}((x^1)^2+(x^2)^2)\right)\equiv iH_{0s}. \tag{5.26}$$

H_{0s} is the Hamiltonian observable of the isotropic two-dimensional harmonic oscillator. So, for any $\psi\in\mathcal{D}_{H_{0s}}$,

$$\psi_t(x)=\left(e^{-(i/\hbar)tH_{0s}}\psi\right)(x) \tag{5.27}$$

solves in $L^2(\mathbb{R}^2)$

$$i\hbar\frac{\partial\psi_t}{\partial t}=H_{0s}\psi_t,$$
$$\psi_0(x)=\psi(x). \tag{5.28}$$

Now pick any $\mathcal{N}_j$, $j=1,\ldots,9$ in $B_s(2)$, the basis (5.7) of the free symmetry algebra $\mathcal{G}_s(2)$. Then, according to (5.18), but now for $U_t^{0s}=\exp(-(i/\hbar)tH_{0s})$,

$$\hat{N}_j^{0s}(t)=U_t^{0s}\mathcal{N}_j(U_t^{0s})^{-1} \tag{5.29}$$

is a symmetry generator of the harmonic oscillator, for the same reason as in Theorem V.3. Therefore $i\hat{N}_j^{0s}(t)$ is a constant observable of the quantum harmonic oscillator (5.28). All such harmonic symmetry operators $\hat{N}_j^{0s}(t)$, $j=1,\ldots,9$, are linear combinations of the $\mathcal{N}_j$ in $B_s(2)$, with time-dependent coefficients denoted by $X^k(x,t)$, $k=1,2,T(t)$ and $\varphi(x,t)$ in (4.7).

By Proposition IV.3, we already know the system of partial differential equations solved by these coefficients X^k, T, and φ regarded as functions. In our case, since $V(q)=\frac{1}{2}((x^1)^2+(x^2)^2)$ and the vector field A in (5.26) vanishes, they reduce to

$$\frac{\partial X^1}{\partial x^2}+\frac{\partial X^2}{\partial x^1}=0, \quad \frac{\partial X^1}{\partial x^1}+\frac{\partial X^2}{\partial x^2}=\frac{\mathrm{d}T}{\mathrm{d}t},$$
$$\frac{\partial X^j}{\partial t}=-\frac{\partial \varphi}{\partial x^j}, \quad j=1,2, \tag{5.30}$$
$$\frac{\partial \varphi}{\partial t}-\frac{i\hbar}{2}\Delta\varphi=X^1x^1+X^2x^2+\frac{\mathrm{d}T}{\mathrm{d}t}\cdot\frac{1}{2}((x^1)^2+(x^2)^2).$$

In particular, instead of solving (5.30), we could use the Baker-Campbell-Hausdorff formula in (5.29), for $\mathcal{N}_j$ any explicit element of the free basis $B_s(2)$ of (5.7). Let us take, for example, $\mathcal{N}_4=\hbar\,\partial/\partial x^1$. According to (5.19) this generator is invariant under (5.18), i.e., $\hat{N}_4(t)=\hbar\,\partial/\partial x^1$. On the other hand, under (5.29) we obtain, on $C_0^\infty(\mathbb{R}^2)$,

$$\hat{N}_4^{0s}(t)=\exp\left(-\frac{i}{\hbar}tH_{0s}\right)\mathcal{N}_4\exp\left(\frac{i}{\hbar}tH_{0s}\right)=\left(1-\frac{t^2}{2!}+\frac{t^4}{4!}-\cdots\right)\left(\hbar\frac{\partial}{\partial x^1}\right)-x^1\left(t-\frac{t^3}{3!}+\frac{t^5}{5!}-\cdots\right).$$

Comparing with the general form (4.7), this means that the coefficients of $\hat{N}_4^{0s}(t)$ are, respectively,

$$X^1(x,t)=\cos t, \quad X^2(x,t)=0, \quad T(t)=0, \quad \varphi(x,t)=x^1\sin t. \tag{5.31}$$

One verifies easily that (5.31) makes up a solution of the system (5.30). In other words,

$$\cos t\cdot P_1(t)+\sin t\cdot Q^1(t) \tag{5.32}$$

is a constant of motion of the quantum harmonic oscillator. This can also be easily verified otherwise: Consider the solution of the equation of motion of this system, in the Heisenberg picture. Those (linear) equations are, for $j=1,2$,

$$\begin{pmatrix}Q^j(t)\\P_j(t)\end{pmatrix}=\Omega(t)\begin{pmatrix}Q^j\\P_j\end{pmatrix}, \quad \text{with } \Omega(t)=\begin{pmatrix}\cos t & \sin t\\ -\sin t & \cos t\end{pmatrix}\in \mathrm{SO}(2). \tag{5.33}$$

In particular, the (constant) operators which are initial conditions of this solution are given by

$$\begin{pmatrix}Q^j\\P_j\end{pmatrix}=\begin{pmatrix}\cos t & -\sin t\\ \sin t & \cos t\end{pmatrix}\begin{pmatrix}Q^j(t)\\P_j(t)\end{pmatrix}, \quad j=1,2. \tag{5.34}$$

So the constant of motion (5.32) provided by Nœther's theorem coincides, in this elementary case, with the initial momentum P_1 of the solution (5.33). Another trivial example of symmetry generator is

$$\cos tQ^2(t)-\sin tP_2(t)\equiv Q^2, \tag{5.35}$$

associated with the following solution of the system (5.30)

$$X^1(x,t)=0, \quad X^2(x,t)=-\sin t, \quad T(t)=0, \quad \varphi(x,t)=x^2\cos t.$$

Fortunately, many nontrivial examples follow as well from this constructions (cf. Sec. VIII). In this way, the free basis $B_s(2)$ allows us to compute the basis of the symmetry Lie algebra of any quadratic Hamiltonian of the form (5.24) and then their associated symmetry operators $\hat{N}(t)$. We summarize this result (in two dimensions, for simplicity) as follows.

Proposition V.5:

Let us consider any essentially self-adjoint quadratic Hamiltonian H_Q in $L^2(\mathbb{R}^2)$, as in the rhs of equation (5.24), *i.e., resulting from a linear combination of elements of $\mathcal{G}_s(2)$. For any ψ*

$\in \mathcal{D}_{H_Q}$, $\psi_t = (e^{-(i/\hbar)tH_Q}\psi)(x)$ *solves the Cauchy problem for the associated Schrödinger equation. If* $\mathcal{N}_j$, $j=1,\ldots,9$, *denotes any element of the basis* $B_s(2)$ *of the free symmetry algebra* $\mathcal{G}_s(2)$ *then, on the dense invariant domain of analytic vectors of Lemma V.2*,

$$\hat{N}_j^{H_Q}(t) = U_t^Q \mathcal{N}_j (U_t^Q)^{-1} \tag{5.36}$$

is a symmetry generator of the H_Q*-system, where* U_t^Q, $t \in \mathbb{R}$, *denotes the one-parameter strongly continuous group of unitary operators*

$$U_t^Q = e^{-(i/\hbar)tH_Q} : L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2).$$

In particular, $i\hat{N}_j^{H_Q}(t)$ *is a constant of the motion of the* H_Q*-system. By construction, the time-dependent coefficients* $X^j(x,t), T(t)$ *and* $\varphi(x,t)$ *of this constant observable solve the system of equations of Proposition IV.3, for the quadratic Hamiltonian* H_Q.

Moreover, if W_t *denotes the one-parameter, strongly continuous, group of unitary operators in* $L^2(\mathbb{R}^2)$ *defined by*

$$W_t = U_t^Q \cdot e^{(i/\hbar)tH_0} \tag{5.37}$$

on the invariant domain of Lemma V.2, and for H_0 *as in* (5.25), *then* W_t *provides the time-dependent canonical transformation from the free system* (5.25) *to the one of Hamiltonian* H_Q. *In particular, we have*

$$H_Q = W_t H_0 W_t^{-1} + i\hbar \frac{\mathrm{d}W_t}{\mathrm{d}t} W_t^{-1}. \tag{5.38}$$

Proof: The Hamiltonian defined by the rhs of (5.24) is of the general quadratic form (5.18) with

$$\begin{gathered} \beta = 1, \quad W_{21} = -c_4, \quad \gamma = -2c_1, \quad a_1 = c_2, \quad a_2 = c_3, \\ b_1 = -c_5, \quad b_2 = -c_6, \quad \delta = c_7, \quad c - i\hbar\, c_7 = c_8 \end{gathered} \tag{5.39}$$

and results indeed from a linear combination of elements of $\mathcal{G}_s(2)$. Let H_Q denote a self-adjoint extension of this (lower-bounded) operator in $L^2(\mathbb{R}^2)$. By Stone's theorem, $U_t^Q = e^{-(i/\hbar)tH_Q}$ is a strongly continuous unitary group of evolution in $L^2(\mathbb{R}^n)$ solving the associated Schrödinger equation. Using (5.36), any $\mathcal{N}_j \in B_s(2), j=1,\ldots,9$, evolves into a symmetry generator $\hat{N}_j^{H_Q}(t)$ of the H_Q-system, as in the above-mentioned example.

Let us define a time-dependent unitary operator W_t on the invariant domain of Lemma V.2 by

$$W_t = U_t^Q e^{(i/\hbar)tH_0}.$$

Clearly, if ψ_t is a solution of the free Schrödinger equation (5.25) with initial condition $\psi_0 = \psi \in \mathcal{D}_{H_0}$ then $\phi_t = W_t\psi_t$ solves the Schrödinger equation with quadratic potential H_Q and the same initial condition. Equivalently, an H_Q-solution ϕ_t is given by a quadrature from a solution ψ_t of the free equation. (One could also introduce an extra unitary generator M acting as well on the initial condition ψ, so that

$$W_t' = U_t^Q M e^{(i/\hbar)tH_0}$$

is unitary.)

Then, it is well known that such a time-dependent unitary transformation W_t the Hamiltonian H_0 is transformed into H_Q given by (5.38). Precisely, this goes as follows.

Let us write $H_Q = H_0 + (H_Q - H_0)$ and denoted by $\mathcal{D}_Q$ the above-mentioned common dense domain of analytic vectors of H_0 and H_Q. Then $H_Q = U_t^Q H_0 (U_t^Q)^{-1} + U_t^Q (H_Q - H_0)(U_t^Q)^{-1}$ on $\mathcal{D}_Q$. By the definition (5.37) of W_t this is also $H_Q = W_t H_0 W_t^{-1} + U_t^Q (H_Q - H_0)(U_t^Q)^{-1}$ on $\mathcal{D}_Q$. Now on $\mathcal{D}_Q$ [in the strong $L^2(\mathbb{R}^n)$ sense]

$$
\begin{aligned}
i\hbar\frac{dW_t}{dt}\cdot W_t^{-1} &= ih\frac{d}{dt}(U_t^Q e^{(i/\hbar)tH_0})e^{-(i/\hbar)tH_0}(U_t^Q)^{-1}\\
&= H_Q - U_t^Q H_0 (U_t^Q)^{-1}\\
&= U_t^Q (H_Q - H_0)(U_t^Q)^{-1},
\end{aligned}
$$

so $H_Q = W_t H_0 W_t^{-1} + i\hbar(dW_t/dt)W_t^{-1}$ on $\mathcal{D}_Q$.

Since $\mathcal{D}_Q$ is a domain of essential self-adjointness, this implies (5.38). □

Let us make a remark on the problem of the zeroes set $\mathcal{N}_t^\psi = \{x \in \mathbb{R}^n \,|\, \psi_t(x) = 0\}$.

As mentioned in Sec. II, our construction [see the definitions (2.5) and (2.14), for example] requires to consider (t,x)-admissible states ψ, i.e., such that $\psi_t(x) \neq 0$.

The study of the zeroes of $\psi_t(x)$ amounts to investigate the wave front set WF of the integral kernel of Schrödinger,

$$k(x,t,y) = \text{kernel}(e^{-(i/\hbar)tH})(x,y)$$

for fixed initial configuration x and time t. This problem has been considered by Zelditch[21] and Weinstein[22] for H slight perturbations of a quadratic Hamiltonian H_Q.

For example, in the case of the classical harmonic oscillator Hamiltonian $P_A^c(q,p) = (1/2)p^2 + (\omega^2/2)q^2$ [i.e., the case $\beta = 1$, $\gamma = -\omega^2$ and $W = 0$ in (5.14)] the initial zero (cf. Mehler formula) of the associated ψ_t reappears at times $k\pi/\omega$ and positions $(-1)^k x = y, k \in \mathbb{Z}$.

For more about this, see also Fujiwara (Ref. 23).

Under bounded perturbations with bounded derivative, the singularities of ψ_t behave as if H was the harmonic Hamiltonian, i.e., the wave front sets are stable under these weak perturbations.

The study of these singularities is made using the geometry of the underlying Hamiltonian flow on the classical phase space.

B. General Hamiltonians

When the Hamiltonian H of our given quantum system is not of the quadratic form H_Q considered in Sec. V A (cf., for example, Proposition V.5), the symmetry operators $N(t)$ defined formally in (4.19) with coefficients X, T, φ solving the PDE of Proposition IV.3 are still quantum constants of motion.

However, Dirac's correspondence (5.5) does not hold anymore and the metaplectic representation used in Sec. V B is of no help. In general, no explicit basis of the associated symmetry algebra can be found. But since, by hypothesis, the coefficients X, T, and φ of the symmetry operator $N(t)$ are analytic functions, it is easy to show that $N(t)$ is well defined for a large class of Hamiltonians H.

Proposition V.6: *Let us consider* $H = -(\hbar^2/2)\Delta + V$, *with* $V: \mathbb{R}^n \to \mathbb{R}$ *as in the Kato-Rellich theorem, so that* H *is self-adjoint in* $L^2(\mathbb{R}^2)$. *Let* $X: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n, \varphi: \mathbb{R}^n \times \mathbb{R} \to \mathbb{C}$ *and* $T: \mathbb{R} \to \mathbb{R}$ *be analytic functions, respectively, of the form* $X(q,t) = \sum_{n=0}^\infty \alpha_n(t) q^n$, *with* α_n *real-valued smooth functions,* $\varphi(q,t) = \sum_{n=0}^\infty \gamma_n(t) q^n$ *with* γ_n *complex-valued and smooth. If* $\sum_{n=0}^\infty |\alpha_n(t)| \|Q^n P \varphi\| < \infty$ *and* $\sum_{n=0}^\infty |\gamma_n(t)| \, \|Q^n \varphi\| < \infty$, $\forall \varphi \in \mathcal{A}(H)$, *the set of analytic vectors for* H, *then the Nœtherian symmetry operator*

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t) \tag{5.40}$$

is a densely defined operator in $L^2(\mathbb{R}^n)$.

VI. THE QUANTUM THEOREM OF NŒTHER IN A RIEMANNIAN MANIFOLD

Let us consider now a classical system like the one of Sec. IV but with a configuration space which is, instead of $\mathbb{R}^n$, any n-dimensional smooth Riemannian manifold M, with positive-definite metric tensor $g_{i,j}$.

The state ψ of the associated quantum system evolves in $L^2(M,\mathrm{d}\mathcal{M})$, with volume element $\mathrm{d}\mathcal{M}(q)=\sqrt{g}\,\mathrm{d}q$, where $g=\det(g_{ij})$, according to

$$i\hbar\frac{\partial\psi_t}{\partial t}=H\psi_t \tag{6.1}$$

for the Hamiltonian of the form (2.13)

$$H=-\frac{\hbar^2}{2}\nabla^j\nabla_j+i\hbar A^j\nabla_j+\frac{i\hbar}{2}\nabla_k A^k+\frac{1}{2}\|A\|^2+V, \tag{6.2}$$

where $\|\cdot\|$ denotes the Riemannian norm and ∇_j is the covariant derivative with respect to the Levi-Civita connection. Let us recall that for this connection, the Christoffel symbols are symmetric: $\Gamma^i_{jk}=\Gamma^i_{kj}$, i.e., we are in the torsion-free case.

Conditions on the vector and scalar potentials V and A ensuring the self-adjointness of H on a dense domain of $L^2(M,\sqrt{g}\mathrm{d}q)$ are known; see, e.g., Refs. 24–27.

The relevant one-parameter group $U_\alpha, \alpha\in\mathbb{R}$, of transformations of the extended configuration space will be denoted, like in the flat case, by

$$U_\alpha: M\times\mathbb{R},(q^i,t)\mapsto(Q^i_\alpha=q^i+\alpha X^i(q,t)+o(\alpha),\tau_\alpha=t+\alpha T(t)+o(\alpha)), \tag{6.3}$$

where q^i are local configuration coordinates and

$$X: M\times\mathbb{R}\to M,\quad T:\mathbb{R}\to\mathbb{R},$$

are real analytic. For g any scalar field on $M\times\mathbb{R}$ such that $g\psi_t\in\mathcal{D}_H$ and such that $\dot{g}$ exists, let us define, like in (2.11), the quantum derivative along ψ_t by

$$D_t g=\frac{1}{\psi_t}\left(\frac{\partial}{\partial t}-\frac{1}{i\hbar}H\right)(g\psi_t). \tag{6.4}$$

Introducing (6.1) and (6.2), this means that

$$D_t g=\left(\frac{\partial}{\partial t}+\left(-i\hbar\frac{\nabla^j\psi_t}{\psi_t}-A^j\right)\nabla_j-\frac{i\hbar}{2}\nabla^j\nabla_j\right)g. \tag{6.5}$$

Since this can be interpreted as a quantum deformation of the classical "absolute" (or "intrinsic") derivative of the scalar g along a smooth continuous curve $q^j=q^j(t)$, we shall define $D_t q^j$ by the vector

$$D_t q^j=-i\hbar\frac{\nabla^j\psi_t(q)}{\psi_t(q)}-A^j(q)\equiv B^j(q,t), \tag{6.6}$$

in analogy with what we have done in the proof of Theorem III.7 of Sec. III. Choosing, like in Eq. (3.16), $g(q,\tau)=S(q,\tau)$, with

$$S(q,\tau)=-i\hbar\,\ln\psi_\tau(q) \tag{6.7}$$

for any τ,q ψ-admissible solution of the Schrödinger equation (6.1), we can compute

$$D_\tau S(q,\tau)=\frac{1}{2}D_\tau q^j D_\tau q_j-\frac{i\hbar}{2}\nabla_j A^j+A_j D_\tau q^j-V(q). \tag{6.8}$$

The rhs of (6.8) defines the Lagrangian $L(D_\tau q,q)$ associated with the quantum system (6.1). Defining, for any $g=(g^{(s)})_{s\in\mathbb{R}}$ complex-valued, measurable and such that $g^{(s)}(\cdot)\psi_s(\cdot)\in L^2(M,\mathrm{d}\mathcal{M})$, the (forward) quantum conditional expectation in the state ψ by

$$E_{\psi}^{t,x}[g^{(s)}] = \int g^{(s)}(\xi)p(s,\xi,t,x)\mathrm{d}\mathcal{M}(\xi), \tag{6.9}$$

where, for any (t,x) ψ-admissible, $s \leq t$,

$$p(s,\xi,t,x)\mathrm{d}\mathcal{M}(\xi) = \psi_s(\xi)k_-(\rho,t-s,x)(\psi_t(x))^{-1}\,\mathrm{d}\mathcal{M}(\xi) \tag{6.10}$$

with k_- the advanced propagator of the Schrödinger equation (6.1), one verifies that Theorem III.7 still holds. So, canceling the boundary term without loss of generality, the regularized action functional (6.3) becomes

$$\begin{aligned} S_L(x,t_1) &= M_{\psi}^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1}\left(A_j Dq^j - \frac{i\hbar}{2}\nabla_j A^j\right)\mathrm{d}t\right] \\ &= M_{\psi}^{t_1,x}\left[\int_{t_0}^{t_1}\left(\frac{1}{2}(D_t q)^2 - V(q)\right)\mathrm{d}t + \int_{t_0}^{t_1} A \circ \mathrm{d}q\right], \end{aligned} \tag{6.11}$$

where we have used on M the same notations as in the Euclidean case of equations (3.10) and (3.11).

Given an additional analytic generator $\varphi: M \times \mathbb{R} \to \mathcal{C}$, called the divergence, the invariance of the action (6.11) (up to this divergence term) is defined as in (4.4).

The formal symmetry operator on M becomes, instead of (4.7),

$$\hat{N}(t) = X^j(x,t)(-i\,\hbar\,\nabla_j) - T(t)\left(i\,\hbar\,\frac{\partial}{\partial t}\right) + \varphi(x,t), \tag{6.12}$$

and it is defined by the same commutation property (4.9) with the Schrödinger equation as in the Euclidean case. This property implies the following conditions on X, T, and φ.

Proposition VI.1:

$\hat{N}(t)$ is a symmetry operator for the Schrödinger equation (6.1) *in* $L^2(M,\mathrm{d}\mathcal{M})$, *with Hamiltonian* (6.2) (*where V may depend smoothly on time*) *if and only if the following determining equations hold*:

(1)

$$\frac{\mathrm{d}T}{\mathrm{d}t}g^{jk} = \nabla^j X^k + \nabla^k X^j,$$

(2)

$$\frac{\partial X^j}{\partial t} = -\nabla^j\varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t}A^j - X^k\nabla_k A^j,$$

(3)

$$\begin{aligned} \frac{\partial\varphi}{\partial t} - A^j\nabla_j\varphi - \frac{i\hbar}{2}\nabla_j\nabla^j\varphi &= X^j\nabla_j\left(\frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}\|A\|^2 + V\right) \\ &\quad + \frac{\mathrm{d}T}{\mathrm{d}t}\left(\frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}\|A\|^2 + V\right) + T\frac{\partial V}{\partial t}. \end{aligned}$$

Proof: This is based on a simple computation of $[\hat{N}(t),\mathbb{Q}] = \lambda_{\hat{N}}(x,t)\mathbb{Q}$, where $\mathbb{Q} = (\partial/\partial t) - (i/\hbar)H$ with the Hamiltonian (6.2). Like in the flat Euclidean case, one finds that

$$\lambda_{\hat{N}}(x,t) = -\frac{\mathrm{d}T}{\mathrm{d}t}(t). \tag{6.13}$$

□

Remark: As in the flat Euclidean case, if we allow space-dependent time transformations in (6.3), a further condition is needed for $\hat{N}(t)$ to be a symmetry operator for (6.1). This is

$$\nabla_j T = 0. \tag{6.14}$$

In other words (6.3) is indeed the most general space–time transformation for our purpose.

The integrability conditions of the determining equations (1)–(3) are not as obvious as in the flat Euclidean case, but they have already been investigated.[28]

When the determining equations (1)–(3) hold, the divergence invariance of the action (6.11) [in the sense of the relation (4.4)] is guaranteed by construction.

In order to obtain the general form of the invariance of the Lagrangian under our groups of transformations (Proposition IV.5) we need first to define the quantum derivative along ψ_t of a vector field Y^j on $M \times \mathbb{R}$.

In classical mechanics on a Riemannian manifold M, it is well known that the time derivative of the velocity field is, in general, not a tensor. In consequence, the acceleration is defined as the "absolute" (or "intrinsic") derivative of the velocity.[29] The result is indeed a contravariant tensor of rank one.

Definition VI.2: *Let R^j_k be the Ricci tensor of the Riemannian manifold M. Then the quantum ("absolute") derivative of the complex-valued vector field Y, on $M \times \mathbb{R}$ is defined by*

$$D_t Y^j = \frac{\partial Y^j}{\partial t} + B^k \nabla_k Y^j - \frac{i\hbar}{2}(\nabla^k \nabla_k Y^j + R^j_k Y^k), \tag{6.15}$$

where B^k is given by (6.6).

To be short, we shall denote simply by Δ the operator $\nabla^k \nabla_k + R$, so that

$$D_t Y^j = \frac{\partial Y^j}{\partial t} + B^k \nabla_k Y^j - \frac{i\hbar}{2} \triangle Y^j. \tag{6.15'}$$

On scalars and covariant vectors, the Laplacian $\triangle$ coincides with the Laplace-Kodaira-de Rham operator.[30] One easily shows that this Laplacian commutes with the gradient and the divergence, i.e., for g a scalar field as before,

$$\nabla_j \triangle g = \triangle \nabla_j g,$$

and for Y a vector field,

$$\nabla_j \triangle Y^j = \triangle \nabla_j Y^j.$$

Notice, in contrast, that $[\nabla^j \nabla_j, \nabla_i]$ is not zero, in general.

Proposition VI.3:

Let $L(D_t q, q, t)$ be the Lagrangian, defined by the rhs of (6.8), *of the quantum system, when the potential V is allowed to be a smooth function of the time. A necessary condition for the divergence invariance of the action functional* (6.11) *is*

$$\frac{\partial L}{\partial t} T + \frac{\partial L}{\partial q^j} X^j + \frac{\partial L}{\partial (D_t q)^j} \left(D_t X^j - (D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t} \right) + L \frac{\mathrm{d}T}{\mathrm{d}t} = -D_t \varphi. \tag{6.16}$$

Proof:

$$D_t X^j = \frac{\partial X^j}{\partial t} + B^k \nabla_k X^j - \frac{i\hbar}{2}(\nabla^k \nabla_k X^j + R^j_k X^k). \tag{6.17}$$

From the determining equation (1) (Proposition VI.1) and $(\mathrm{d}T/\mathrm{d}t) = (2/n)\nabla_j X^j$ (where $n = \dim M$) we have

$$\nabla_l \nabla_k X_j + \nabla_l \nabla_j X_k = 0.$$

Using this in the Ricci identity we get

$$\nabla_l \nabla_k X_j = R^m_{kjl} X_m, \tag{6.18}$$

where R^m_{kjl} denotes the Riemannian-Christoffel curvature tensor. The rhs of (6.18) coincides with $R_{kn,jl}X^n$, so

$$\nabla^n \nabla_k X_j = g^{n,l} R_{kn,jl} X^n$$

and

$$\nabla^k \nabla_k X^j = -R^j_k X^k. \tag{6.19}$$

After introduction of the determining equation (2) (Proposition VI.1) and of (6.19) in the definition (6.17) we obtain

$$D_t X^j = -\nabla^j \varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} \cdot A^j - X^k \nabla_k A^j + B^j \nabla_k X^j.$$

In particular,

$$D_t X^j - (D_t q)^j \frac{\mathrm{d}T}{\mathrm{d}t} = -\nabla^j \varphi - \frac{1}{2}\frac{\mathrm{d}T}{\mathrm{d}t} \cdot A^j - X^k \nabla_k A^j - \frac{1}{2} B^j \frac{\mathrm{d}T}{\mathrm{d}t} + \frac{1}{2} B^k (\nabla_k X^j - \nabla^j X_k). \tag{6.20}$$

Now consider the invariance condition (6.16). Using the rhs of (6.8) as a definition of the Lagrangian (for V smoothly time dependent) this condition means explicitly, after simplification,

$$\frac{\partial \varphi}{\partial t} - A^j \nabla_j \varphi - \frac{i\hbar}{2} \nabla_j \nabla^j \varphi = X^j \nabla_j \left[\frac{i\hbar}{2} \nabla_k A^k + \frac{1}{2}\|A\|^2 + V \right] + \frac{\mathrm{d}T}{\mathrm{d}t} \left(\frac{i\hbar}{2} \nabla_k A^k + \frac{1}{2}\|A\|^2 + V \right) + T \frac{\partial V}{\partial t}.$$

This is the determining equation (3) of Proposition VI.1 and, therefore, the invariance condition (6.16) constitutes indeed a necessary condition for the divergence invariance of the action (6.11) under the Lie group of transformations (6.13). □

The main results of the flat case are, now, easily generalized. Using the definition of the quantum derivative along ψ_t of the scalar field $\boldsymbol{S}$ defined by (6.7), one verifies that S solves the quantum Hamilton-Jacobi equation on $M \times \mathbb{R}$,

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - A)^2 + V + \frac{i\hbar}{2} \nabla_j A^j - \frac{i\hbar}{2} \nabla^j \nabla_j S = 0, \tag{6.21}$$

where the same remark as after (3.21) applies, as far as our notations are concerned. The quantum Hamilton-Jacobi equation (6.21) provides us with a direct derivation of the regularized equation of motion generalizing (3.28) and the Riemannian version of conservation of energy (3.29).

Let us compute

$$\nabla_j S = B_j + A_j. \tag{6.22}$$

We first notice that

$$\nabla_j \tfrac{1}{2}(\nabla S - A)^2 = \tfrac{1}{2}\nabla_j(B^k B_k) = B^k \nabla_k B_j + (\nabla_j B_k - \nabla_k B_j)B^k.$$

Since, for the Levi-Civita connection, there is no torsion, $\nabla_j B_k - \nabla_k B_j$ is the exterior derivative of B_k, generalizing the curl operator of Proposition III.11. By (6.22) this coincides with $-(\nabla_j A_k - \nabla_k A_j)$ so

$$\nabla_j \tfrac{1}{2}(\nabla S - A)^2 = B^k \nabla_k B_j - (\nabla_j A_k - \nabla_k A_j)B^k. \tag{6.23}$$

On the other hand, as observed after (6.15′), $[\Delta, \nabla_j]S = 0$ implies that

$$\nabla_j \nabla^k \nabla_k S = \nabla^k \nabla_k \nabla_j S + R^k_j \nabla_k S.$$

Finally, using (6.15) and (6.22), the covariant derivative of the quantum Hamilton-Jacobi equation (6.21) reduces to

$$D_t D_t q_j = -(\nabla_j A_k - \nabla_k A_j)B^k - \frac{i\hbar}{2}(\nabla_j \nabla_k A^k - \nabla A_j) - \nabla_j V. \tag{6.24}$$

Now let us consider the space–time observable of energy $h^H_{\psi_t}$ associated with (6.2), namely

$$h^H_{\psi_t} = \frac{H\psi_t}{\psi_t} = -\frac{\hbar^2}{2}\frac{\nabla^j \psi_t}{\psi_t}\frac{\nabla_j \psi_t}{\psi_t} - \frac{\hbar^2}{2}\nabla^j\left(\frac{\nabla_j \psi_t}{\psi_t}\right) + i\hbar A^j \frac{\nabla_j \psi_t}{\psi_t} + \frac{i\hbar}{2}\nabla_k A^k + \frac{1}{2}||A||^2 + V. \tag{6.25}$$

According to (6.6), it is consistent to denote the space–time momentum by

$$p^j = B^j + A^j, \tag{6.26}$$

so that the energy becomes

$$h^H_{\psi_t} = \frac{1}{2}p^2 - A^j p_j + \frac{i\hbar}{2}\nabla^j A_j - \frac{i\hbar}{2}\nabla^j p_j + \frac{1}{2}A^2 + V. \tag{6.25′}$$

Associated with the quantum Hamilton-Jacobi equation (6.21) we notice the following integrability condition:

$$\nabla_j h^H_{\psi_t} = -\frac{\partial B_j}{\partial t}. \tag{6.27}$$

Indeed, from the definition (2.5) and Schrödinger equation (6.1), $h^H_{\psi_t} = -(\partial/\partial t)S$, where the relation (6.7) has been used. In other words, according to (6.6), the relation (6.27) holds. Since the energy space–time observable is a scalar, its quantum derivative along ψ_t is given by (6.5),

$$D_t h^H_{\psi_t} = \frac{\partial h}{\partial t} - B^j \frac{\partial B_j}{\partial t} + \frac{i\hbar}{2}\nabla^j \frac{\partial B_j}{\partial t}, \tag{6.28}$$

where the integrability condition (6.27) was used. On the other hand, by the definition (6.25′) of $h^H_{\psi_t}$,

$$\frac{\partial H^H_{\psi_t}}{\partial t} = B^j \frac{\partial B_j}{\partial t} - \frac{i\hbar}{2}\nabla^j \frac{\partial B_j}{\partial t} + \frac{\partial V}{\partial t}.$$

After substitution in (6.28) we obtain the conservation of the energy

$$D_t h^H_{\psi_t} = \frac{\partial V}{\partial t}. \tag{6.29}$$

Let us collect this information in the

Proposition VI.4:

For the action functional S_L defined by (6.11), *the regularized equation of motion and conservation of energy in an admissible state ψ_t, solution of the Schrödinger equation* (6.1) *in* $L^2(M,\sqrt{g}\mathrm{d}q)$, *are given respectively by*

$$D_t D_t q_j = -(\nabla_j A_k - \nabla_k A_j)B^k - \frac{i\hbar}{2}(\nabla_j \nabla_k A^k - \triangle A_j) - \nabla_j V \tag{6.30}$$

and

$$D_t h^H_{\psi_t} = \frac{\partial V}{\partial t}. \tag{6.31}$$

In particular, when the scalar potential V is time independent, the energy space–time observable is a quantum martingale.

More generally, one shows, like in the flat case (cf. Ref. 31 and 32 for the probabilistic case), the following.

Theorem VI.5 (Theorem of Nœther):

Let us consider the Jordan symmetrization of the formal symmetry operator $\hat{N}(t)$ in $L^2(M,d\mathcal{M})$ defined in (6.12), *i.e., the Nœtherian operator*

$$N(t) = X^j(Q(t),t) \circ P_j(t) - T(t)H(t) + \hat{\varphi}(Q(t),t), \tag{6.32}$$

where $\circ$ denotes Jordan's multiplication of operators,

$$\hat{\varphi} = \varphi + \frac{i\hbar}{2}\nabla_j X^j \tag{6.33}$$

and X, T, and φ are solutions of the determining equations (1), (2), *and* (3) *of Proposition VI.1, for the symmetry groups of the Schrödinger equation* (6.1). *In* (6.32) *P_j and H are, respectively, the momentum and Hamiltonian observable in Heisenberg's picture [cf.* (6.26) *and* (6.2)*].*

Then $N(t)$ is a quantum constant observable, densely defined on $\mathcal{D}_{N(t)} \subset L^2(M,\mathrm{d}\mathcal{M})$ and the associated space–time (scalar) observable $n^N_{\psi_t}$ is a quantum martingale, i.e., $D_t n^N_{\psi_t} = 0$, $\forall\, \psi_t$ admissible.

VII. QUANTUM PHYSICS, FEYNMAN PATH INTEGRAL AND STOCHASTIC ANALYSIS

Von Neumann axiomatization of quantum mechanics in Hilbert space is the mathematical form of the original version of this theory.[33] It can be regarded as a generalization of classical Hamiltonian mechanics, where the commutative algebra of the (real) observables in phase space is replaced by a noncommutative one.

It is well known that there is no mathematically rigorous Lagrangian version of quantum theory. To construct such a framework was precisely one of Feynman's original motivations.[2] But, in spite of its success (founded on its extraordinary heuristic power), Feynman's path integral theory still cannot be regarded as such a satisfactory framework, from the mathematical point of view. Let us recall that Feynman represents the solution of the initial value problem (2.2) by the symbolic expression

$$\psi_t(x) = \int_{\Omega^{t,x}} \psi(\omega(0)) e^{(i/\hbar)S[\omega;t]} \mathcal{D}\omega, \tag{7.1}$$

where $\Omega^{t,x}$ denotes the path space $\{\omega \in C([0,t],\mathbb{R}^n) \,|\, \omega(t)=x\}$. $S[\omega;t]$ is the action functional of the underlying classical Lagrangian system. For example, when H is as in (2.13), with $A=0$,

$$S[\omega;t] = \int_0^t \left(\frac{1}{2}|\dot{\omega}(\tau)|^2 - V(\omega(\tau))\right)\mathrm{d}\tau \equiv S_0[\omega;t] - \int_0^t V(\omega(\tau))\mathrm{d}\tau, \tag{7.2}$$

$\mathcal{D}\omega$ is the heuristic "flat measure" on the path space $\Omega^{t,x}$ (used as a Lebesgue measure)

$$\mathcal{D}\omega = \prod_{0\le\tau\le t} \mathrm{d}\omega(\tau),$$

and

$$e^{(i/\hbar)S[\omega;t]} \equiv e^{-(i/\hbar)\int_0^t V(\omega(\tau))\mathrm{d}\tau} e^{(i/\hbar)S_0[\omega;t]}$$

is a complex weight.

Note that to make sense of the kinetic energy term in S_0 one should *a priori* assume that the paths $\tau \mapsto \omega(\tau)$ are absolutely continuous and in the Cameron-Martin Hilbert space $\mathcal{H}_{\mathrm{CM}}$ with (finite) norm

$$(\omega,\omega)_{\mathcal{H}} = \int_0^t |\dot{\omega}(\tau)|^2 \mathrm{d}\tau. \tag{7.3}$$

Using Lie-Trotter's formula, Nelson has shown that the rhs of (7.1) can be reinterpreted as the strong limit $j\to\infty$ in $L^2(\mathbb{R}^n)$ of a discretization of the time interval $0<t_1<t_2<\cdots<t_j=t$ along polygonal paths interpolating linearly between the corresponding configurations $\omega(t_k)=x_k$, $k=1,\ldots,j,\omega(t)=x$. But the heuristic expression for the limit of

$$e^{(i/\hbar)S_0[\omega,t]} \prod_{\tau\in\{t_1,\ldots,t_j=t\}} \mathrm{d}\omega(\tau) \tag{7.4}$$

is not σ-additive (cf. Ref. 18) and therefore cannot be used for the construction of a basic complex measure on $\Omega^{t,x}$. However, it is possible, but very hard, to construct a rigorous (nonprobabilistic) functional calculus on path space, using the time discretization approximation (cf. Ref. 34). For various other approaches, cf. also Ref. 35. Let us see (in the free case, for simplicity) how the lack of complex measure is reinterpreted in our distinct construction.

We consider a finite product of complex-valued functions like the ones used in our definition (2.28),

$$F = f_n^{(t)} \cdot f_{n-1}^{(t_j-1)} \cdots f_1^{(t_1)}, \quad n\in\mathbb{N}, \quad t > t_{j-1} > t_{j-2} > \cdots > t_1. \tag{7.5}$$

By iteration of the argument used there for only two such functions, the quantum (absolute) expectation of F in the state ψ becomes

$$\langle f_j^{(t)} \cdots f_1^{(t_1)}\rangle_\psi = \int \psi_{t_1}(x_1) f_1^{(t_1)}(x_1) k_0(x_1,t_2-t_1,x_2) f_2^{(t_2)}(x_2) k_0(x_2,t_3-t_2,x_3)\cdots k_0(x_{j-1},t-t_{j-1},x_j)$$
$$f_j^{(t)}(x_j)\bar{\psi}_t(x_j)\mathrm{d}x_1\cdots\mathrm{d}x_j, \tag{7.6}$$

where $k_0(x,t-s,y)$ denotes the integral kernel of the evolution group U_{t-s} when $V=0$.

The rhs of (7.6) is a multilinear functional of $f_1^{(t_1)},\ldots,f_j^{(t)}$ which is well defined. But the corresponding finite additive measure is not σ-additive (the proof goes back to Cameron.[36] See also Ref. 37) and, therefore, there is no way to look at such an additive measure as the path space measure of some diffusion process, i.e., a Markovian stochastic process with continuous sample paths $\tau\to\omega(\tau)$.

What we have called the forward quantum transition kernel $\hat{p}$ in (2.23), for example, is not positive in contrast with a crucial requirement of the existence proof of such a probability measure.[38] However, regarded only as defining a continuous complex-valued functional on a

reasonable domain of integrable functions and satisfying some basic properties needed otherwise for quantum theory, the limit of (7.4) makes sense and allows to obtain a number of results (see Refs. 39, 40, 37, 41, 42, and 61).

If we are insistent about interpreting Feynman's type of formula (7.1) as an integral over a space of continuous paths, the traditional way, in mathematical physics, is to appeal to Kac's approach (but cf. also Refs. 62–66). First one replaces Schrödinger's initial value problem (2.2) by its "Euclidean" (or "imaginary time") counterpart, say

$$-\hbar \frac{\partial \eta^*}{\partial t} = H\eta^* \tag{7.7}$$

with a bounded continuous initial condition χ in $L^2(\mathbb{R}^n)$. Then the counterpart of (7.4), i.e.,

$$e^{-(1/\hbar)\mathcal{S}_0[\omega;t]} \prod_{\tau\in\{t_1,\cdots,t_j=t\}} \mathrm{d}\omega(\tau), \tag{7.8}$$

converges to the Wiener measure with diffusion coefficient $\hbar$, denoted by $\mathrm{d}\mathcal{M}_W^\hbar$, on the path space $\Omega^{t,x}$ (cf., e.g., Ref. 38). The measure $\mathcal{M}_W^\hbar$ has support on continuous but not differentiable paths [in particular $\mathcal{M}_W^\hbar(\mathcal{H}_{\mathrm{CM}})=0$] so neither the first factor in (7.8) nor the second one are well defined but their product is. After a discrete absorption of the a.s. singular kinetic energy term in the measure, the probabilistic counterpart of (7.1) is Feynman-Kac formula,[43]

$$\eta_t^*(x) = \int_{\Omega^{t,x}} \chi(\omega(0)) e^{-(1/\hbar)\int_0^t V(\omega(\tau))\mathrm{d}\tau} \mathrm{d}\mathcal{M}_W(\omega) = E^{t,x}\left[\chi(W(0)) e^{-(1/\hbar)\int_0^t V(W(\tau))\mathrm{d}\tau}\right], \tag{7.9}$$

where the last expression adopts the probabilities notation for the conditional expectation given that the Wiener process satisfies $W(t)=x$ (our superscript t,x indicates that the condition lies in the future of the time interval of integration), as well as another notation η_χ^* for the solution of (7.7) stressing its dependence on the initial condition χ.

The process $W(\tau)$ is used exclusively as a technical tool in (7.9). We shall not insist here on the fact, underlined time and time again[44,45] that its (irreversible) dynamical properties have little to do with the (reversible) ones of free quantum dynamics. There is no surprise here: the way probability theory enters in (7.7)–(7.9) has nothing to do with the way it enters in quantum dynamics, where, in particular, no direct probabilistic concept of conditional expectation is defined but Born interpretation of ψ_t is fundamental to the absolute expectation.

The above-mentioned support of $\mathcal{M}_W^\hbar$ makes rather tricky the construction of any "stochastic (Euclidean) Lagrangian calculus" along the line suggested by Feynman in Ref. 2, since the irregularities of the "quantum paths" turn any classical action functional into a divergent one.

Any quantum observable should be defined as a function of the basic underlying "stochastic process." It is easy to check (see Chap. 7 of Ref. 2) that Feynman's implicit relation between self-adjoint operators in Hilbert space and associated "random variables" is precisely of our form (2.5) (although formulated by the authors in the time discretized context, i.e., before taking $\lim_{j\to\infty}$ in the above-mentioned construction, in order to avoid flagrant singularities). But the specific rules for handling these "random variables" are not established at all in Ref. 2. Their calculus seems to be plagued by the same kind of singularities as in naive computations along the paths of diffusion processes before the advent of Itô's calculus.

The first problem is, of course, that the precise nature of the underlying formal stochastic process itself (for a given H) is never specified. This may be due to the fact that, after the above-mentioned nonexistence proof of the "Feynman's process," the specific properties it should have were not, understandably, investigated. Is it clear, for example, that this process should be the one associated with the real time version of the Wiener measure or, instead, of the counterpart of some measure absolutely continuous with respect to the Wiener measure?

Also even if, given a quantum observable A, one admits (2.5) as a rule for the associated space–time observable, there are, of course, many other candidates providing the same quantum mechanical expectation $\langle\psi_t, A(t)\psi_t\rangle$. For example, Feynman gives two distinct space–time observ-

ables for the Hamiltonian H of the form (2.13) with zero vector potential (Ref. 2, p. 194). He does not indicate any way to choose which of those is more natural, for instance as defining the proper space–time counterpart of the quantum constant of motion. It is also worthwhile to observe here that Feynman's path integral approach does not provide, curiously, any Nœther Theorem although its whole point is to be a Lagrangian approach.

Nevertheless, Feynman's formal computations suggest that the abelian nature of the classical algebra of observables should be preserved under quantization but that other basic rules of Newtonian calculus should be "deformed in $\hbar$" so as to preserve the compatibility with regular (noncommutative) quantum mechanics in Hilbert space.

The point of our present work has been to investigate systematically the properties of the above-mentioned "process," beyond what Feynman did, without ever using what it certainly cannot provide, a well-defined probability measure on the path space, compatible with Born interpretation of the wave function ψ_t and all quantum mechanical predictions.

Our main improvement with respect to Feynman's original framework is the introduction of the quantum version(s) of conditional expectation(s) for his heuristic process. Indeed, this supplies us with a natural regularization of the many divergent terms in his formal computation, for example the kinetic energy term [cf. (3.20)] of the classical action function.

Introducing the quantum derivatives along an L^2-state associated with this quantum conditional expectation, our calculus of space–time observables follows directly, as well as the definition of quantum martingale, underlying Nœther theorem.

The key deformations of the rules of the classical calculus are, therefore, the ones of the derivations, given by Proposition II.8.

With this procedure, we have embedded regular quantum mechanics (more precisely, the class of elementary systems considered here) into a framework which, we claim, is much closer to probability theory and stochastic analysis than Feynman's path integral approach and, a fortiori, than quantum theory in Hilbert space.

Let us now recall why this claim is justified.

A solution of the Cauchy problems for Schrödinger's equation can be regarded as the value on the imaginary axis of a solution of the heat equation (7.7). This is the famous "Euclidean" relation (or "Wick rotation")

$$\psi_\chi(x,-it) = \eta^*_\chi(x,t) \tag{7.10}$$

for any $\chi \in \mathcal{D}_H \subset L^2(\mathbb{R}^n)$.

Let us restrict ourselves, for a fixed $T>0$, to χ in the dense set of vectors in $L^2(\mathbb{R}^n)$, denoted by $\mathcal{D}(e^{(T/2)H})$, such that

$$\sum_{n=0}^{\infty} \frac{1}{n!} \|H^n \chi\|_2 |t|^n < \infty, \quad \forall\, t \in I = \left[-\frac{T}{2}, \frac{T}{2}\right].$$

Then, together with the solution of (7.7), we can consider the solution, in the strong L^2-sense of the adjoint equation with respect to the time parameter

$$\begin{aligned} \hbar \frac{\partial \eta_{\bar\chi}}{\partial t} &= H \eta_{\bar\chi}, \quad t \in I \\ \eta_{\bar\chi}(\cdot,0) &= \bar\chi(\cdot), \end{aligned} \tag{7.11}$$

where the overbar denotes, now, the complex conjugate.

Clearly we have

$$\int_{\mathbb{R}^n} \eta_{\bar{\chi}} \eta_{\chi}^*(x,t)\mathrm{d}x = \|\chi\|_2^2, \tag{7.12}$$

in a striking analogy with Born's "probabilistic" interpretation of the associated wave function ψ_t [cf. definition (2.17)]. This observation is due to Schrödinger (cf. Refs. 44 and 45) and lies at the foundations of Euclidean quantum mechanics.

The identity (7.12) suggests the introduction of various Hilbert spaces associated with the pair of heat equations (7.7)–(7.11) and allowing to mimic what happens in regular quantum mechanics. For each $t \in I$, consider the solution space of (7.7), namely

$$\widetilde{\vartheta}_t^* \equiv \widetilde{\vartheta}_t^*(\mathbb{R}^n) = \left\{ \eta_{\chi}^*(t), \chi \in \mathcal{D}(e^{(T/2)H}) \right\},$$

and define

$$\begin{aligned} U_t^{-1} &: \widetilde{\vartheta}_t^* \to \mathcal{D}(e^{(T/2)H}), \\ \eta_{\chi}^*(t) &\mapsto \chi. \end{aligned} \tag{7.13}$$

Equation (7.12) suggests as well the definition of the following scalar product in $\widetilde{\vartheta}_t^*$:

$$(\eta_{\chi_1}^*(t)|\eta_{\chi_2}^*(t))_t = \langle U_t^{-1}\eta_{\chi_1}^*(t)|U_t^{-1}\eta_{\chi_2}^*(t)\rangle_2 = \langle \chi_1|\chi_2\rangle_2, \tag{7.14}$$

and to complete $\widetilde{\vartheta}_t^*$ with respect to $(\cdot|\cdot)_t$. The resulting space, denoted by ϑ_t^*, is called forward Hilbert space. As a matter of fact, $(\vartheta_t^*, (\cdot|\cdot)_t)$ is unitarily equivalent to $(L^2, \langle\cdot|\cdot\rangle_2)$ since U_t^{-1} can be extended unitarily from ϑ_t^* onto L^2. Using U_t, the Euclidean version of Heisenberg time evolution of observables will be, for any densely defined A,

$$A_{-t}^F = U_t A U_t^{-1}, \quad t \in I, \tag{7.15}$$

where F stands for forward (space).

So the familiar (Heisenberg's) quantum formulas will be valid, but without the factor $i = \sqrt{-1}$. For the same reason, the observables, in this framework, are densely defined normal operators (not necessarily self-adjoint). For example, the momentum observable in $\vartheta_0^*(\mathbb{R}^n) = L^2(\mathbb{R}^n)$ is defined as $-\hbar\nabla$ on its usual domain. A symmetric construction for equation (7.11) would introduce another one-parameter family of ("backward") Hilbert space, ϑ_t.

Before continuing, it is worth stressing that the "reciprocal" analytical continuation in time of the above construction adds nothing to regular quantum theory. Since the analytical vectors are dense in $L^2(\mathbb{R}^n)$ and $e^{-(i/\hbar)tH}(L^2(\mathbb{R}^n)) = L^2(\mathbb{R}^n)$ $\forall t$, the real time version of the key restriction $\chi \in \mathcal{D}(e^{(T/2)H})$ disappears since

$$\mathcal{D}(e^{i(T/2)H}) = L^2(\mathbb{R}^n), \quad \forall T \in \mathbb{R}.$$

Let us see that the probabilistic interpretation suggested by (7.12) and (7.14) is indeed fully justified on positive vectors in ϑ_t^*, if $e^{-(t/\hbar)H}$ is positively preserving. For H as in Theorem III.7, with $A=0$, this is the case when V belongs to a subset of a class of potentials introduced by Kato (cf. Ref. 45). The integral kernel of $e^{-(1/\hbar)(t-s)H}$ in $L^2(\mathbb{R}^n)$, denoted by

$$h(x, t-s, q), \tag{7.16}$$

is, then, known to be jointly continuous and strictly positive.

For $\chi > 0$ fixed as before, and $\eta_s^*(\cdot) = \eta_{\chi}^*(\cdot, s)$, the Euclidean counterpart of the quantum transition kernel (2.25) becomes

$$q^*(\tau, \mathrm{d}q, t, x) = \eta_{\tau}^*(q) h(q, t-\tau, x)(\eta_t^*(x))^{-1}\,\mathrm{d}q, \quad \tau \le t \text{ in } I. \tag{7.17}$$

In contrast with (2.25), q^* satisfies all the properties of the backward transition probability of a real-valued Markov process in I, for a given final probability distribution $p_{T/2}(y)\mathrm{d}y$.

For another fixed $\chi' > 0$, and $\eta_t(\cdot) = \eta_{\chi'}(\cdot, t)$ in $\vartheta_t(\mathbb{R}^n)$ one gets the Euclidean version of the quantum transition kernel (2.23), i.e.,

$$q(t,x,\tau,\mathrm{d}q) = \eta_t^{-1}(x) h(x,\tau-t,q)\,\eta_\tau(q)\mathrm{d}q, \quad t \le \tau \text{ in I}, \tag{7.18}$$

namely the (forward) transition probability of a Markov process for a given initial probability distribution $p_{-T/2}(x)\mathrm{d}x$. The existence of this Markov process $Z_t, t \in I$, introduced in 1984–1985 under the name of Bernstein diffusion[45] has been proved since then in more general settings (see Ref. 46 for a recent review, using the tools of statistical physics).

Notice that the quantum problem of the zeroes of the wave function disappears here since, by hypothesis on the potential V, $\exp(-(1/\hbar)(t-s)H)$ is positivity preserving. Using (7.17) and (7.18), one verifies easily that Z_t, $t \in I$, is a real valued inhomogeneous diffusion process whose drifts and diffusion matrix are given by the Euclidean version of Proposition II.14, i.e.,

$$B^*(q,t) = -\,\hbar\,\frac{\nabla \eta_t^*}{\eta_t^*}(q),$$

$$B(q,t) = \hbar\,\frac{\nabla \eta_t}{\eta_t}(q), \tag{7.19}$$

$$C(q,t) = C^*(q,t) = \hbar\,\mathbb{1},$$

with $\mathbb{1}$ the $n \times n$ identity matrix.

The particularity of such diffusions is that, in contrast with the traditional one-sided notion of Markov processes, they take seriously the fact that the Markov property itself is invariant under time reversal. If $\mathcal{P}_t$ denotes the σ-algebra generated by the past of Z_t, i.e., $\mathcal{P}_t = \sigma\{Z_s, s \in I, s \le t\}$ and $\mathcal{F}_t$ the future, $\mathcal{F}_t = \{Z_u, u \epsilon I, u \ge t\}$, then, for any events $A \in \mathcal{P}_t$ and $B \in \mathcal{F}_t$,[38]

$$P(AB|\mathcal{N}_t) = P(A|\mathcal{N}_t) \cdot P(B|\mathcal{N}_t) \tag{7.20}$$

almost surely, where $\mathcal{N}_t$ denotes the present $\sigma\{Z_t\}$ and $P(\cdot|\mathcal{N}_t)$ is the conditional probability given $\mathcal{N}_t$.

The time symmetry of $Z_t, t \in I$, shows up in the multiplicative aspect of the integrand of (7.12), for a pair of positive analytic vectors χ, χ', since Eqs. (7.7) and (7.11) are formally time reversed of each other.

The Euclidean version of the relation (2.5) between operators in Hilbert space and space–time observables provides us with well-defined random variables, functions of Z_t. For example, the above-mentioned momentum observable at time t corresponds to $-\hbar(\nabla \eta_t^* / \eta_t^*)(Z_t)$, i.e., the drift $B_*(z_k, t)$ already known by (7.19).

It follows that the Euclidean counterparts of the quantum derivatives (2.14) and (2.16) along the quantum state ψ_t and $\bar{\psi}_t$ are given, respectively, by

$$D_t^* = \frac{\partial}{\partial t} + \mathcal{L}^*, \tag{7.21}$$

$$D_t = \frac{\partial}{\partial t} + \mathcal{L}, \tag{7.22}$$

where $\mathcal{L}^*$ and $\mathcal{L}$ are backward and forward generators of $Z_t, t \in I$, namely the elliptic operators

$$\mathcal{L}^* = -\,\hbar\,\frac{\nabla \eta_t^*}{\eta_t^*} \cdot \nabla - \frac{\hbar}{2}\Delta, \tag{7.21$'$}$$

and

$$\mathcal{L} = \hbar \frac{\nabla \eta_t}{\eta_t} \cdot \nabla + \frac{\hbar}{2} \Delta. \tag{7.22'}$$

The derivatives (7.21) and (7.22) are better defined as limits (whenever they exist) of conditional expectations, for f smooth real valued with compact support on $\mathbb{R}^{n+1}$, namely

$$D_t^* f(Z_t,t) = \lim_{\Delta t \downarrow 0} E_t \left[\frac{f(Z_t,t) - f(Z_{t-\Delta t}, t-\Delta t)}{\Delta t} \right] \tag{7.23}$$

and

$$D_t f(Z_t,t) = \lim_{\Delta t \downarrow 0} E_t \left[\frac{f(Z_{t+\Delta t}, t+\Delta t) - f(Z_t,t)}{\Delta t} \right], \tag{7.24}$$

where E_t denotes the conditional expectation given Z_t in the future or in the past of the time interval, computed in terms of the kernels (7.17) or (7.18), respectively. These conditional expectations make sense from the probabilistic viewpoint, since the process Z_t does, in contrast with our quantum definitions (2.24) and (2.22).

Let us stress that, although the definitions (7.23) and (7.24) coincide with Nelson's ones in Ref. 47, the processes Z_t have little in common with the ones introduced by him in order to interpret probabilistically (2.2) (cf. Ref. 44 for more about that).

By definition of D_t^* and D_t, notice that $f(Z_t,t)$ is an $\mathcal{F}_t$ (respectively, $\mathcal{P}_t$) martingale if and only if $D_t^* f(Z_t,t)=0$ [respectively, $D_t f(Z_t,t)=0$].

The probabilistic counterpart of Proposition III.1, involving the derivative (7.24), is generally known in stochastic analysis, as Dynkin's formula (cf., e.g., Ref. 48). The fact that the counterpart of (3.4), using (7.23), holds as well is due to the time symmetry of Bernstein measures.

The infinitesimal operators D_t and D_t^* are keystones of Itô's stochastic calculus.[49,68] Although it is not as widely known in mathematical physics as it should, this calculus can indeed be formulated in a time-symmetric way as well as with respect to the usual increasing filtration $\mathcal{P}_t$. This requires the introduction of the time-reversed filtration $\mathcal{F}_t$, (Refs. 45, 47, and 50), used here. The quantum deformations (2.20′) and (2.21′) of Leibniz rule (for our class of Hamiltonians) become, respectively, in stochastic analysis, for f,g smooth and real valued,

$$D_t(f \cdot g) = (D_t f) \cdot g + f(D_t g) + \hbar \nabla f \cdot \nabla g, \tag{7.25}$$

$$D_t^*(f \cdot g) = (D_t^* f) \cdot g + f(D_t^* g) - \hbar \nabla f \cdot \nabla g, \tag{7.26}$$

The relations (3.13) and (3.13′) are the quantum counterparts of the relations between Itô and Stratonovich stochastic integrals [also denoted by $\circ$ (Ref. 50)] with respect to $\mathcal{P}_t$ and $\mathcal{F}_t$. It is well known that the latter relation had already been discovered by Feynman in his path integral approach to quantum theory.[2,44]

Using this, one shows that positive solutions of the two adjoint heat equations (7.7) and (7.11) admit two path integral representations in terms of $Z_t, t \in I$. These are the probabilistic counterparts of the integral representations (3.20) and (3.22).

The study of the symmetries of the action functionals involved in these path integrals results in the probabilistic version of the quantum theorem of Nœther, proved in paper I, which is in fact the origin of the present Lagrangian formulation of quantum theory for elementary systems.

One can further develop Feynman's ideas using the rigorous tools of stochastic analysis.[69] For example, his functional calculus[2] is well defined for the class of Bernstein diffusions and allows to prove the Euclidean version of his heuristic results.[51] The aim of Euclidean quantum mechanics, in the sense of Refs. 44 and 45 and for the present paper, is to transfer along this line, as much as possible of mathematical structures from stochastic analysis to regular quantum theory. The point of this indirect approach is to make the best of the irreducible probabilistic content of this theory

and discover more easily new conceptual and technical aspects of quantum dynamics which have been muddled along the years by the superficial role of probability in the traditional Hilbert space framework.

VIII. SOME CONCRETE EXAMPLES

A. One-dimensional free fall

Let the configuration manifold M of Sec. VI be simply $\mathbb{R}$ and consider the free fall Hamiltonian,

$$H = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2} + gq, \tag{8.1}$$

where g is a real constant. This is the (one dimensional) case $A=0, V(q,t)=gq$ of (6.2). In particular, H belongs to the quadratic class (5.1) and it follows from Sec. V that it is sufficient to compute the free case $V=0$. The basis $\mathcal{B}_s(1)$ of the symmetry Lie algebra $\mathfrak{g}_s(1)$ is six dimensional and, according to (5.7), given by

$$\mathcal{B}_s(1) = \left\{ i, iq, \hbar\frac{\partial}{\partial q}, iq^2, i\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2}, \hbar\, q\frac{\partial}{\partial q} + \frac{\hbar}{2} \right\} \equiv \{\mathcal{N}_j, j = 1, \ldots, 6\}. \tag{8.2}$$

We observe that the free fall Hamiltonian (8.1) results from a linear combination of elements of $\mathcal{B}_s(1)$.

By (5.19) we know that the constant observables of the one-dimensional free system are

$$\left\{ i, i\left(q + i\hbar\, t\frac{\partial}{\partial q}\right), \hbar\frac{\partial}{\partial q}, iq^2 - 2t\left[iq\left(-i\hbar\frac{\partial}{\partial q}\right) + \frac{\hbar}{2}\right] + 2it^2\left(i\hbar\frac{\partial}{\partial t}\right), \right.$$
$$\left. \hbar\frac{\partial}{\partial t}, q\hbar\frac{\partial}{\partial q} + \frac{\hbar}{2} - 2it\left(i\hbar\frac{\partial}{\partial t}\right) \right\} \tag{8.3}$$

Equivalently the coefficients of the symmetry generator defined in (4.18) for the one-dimensional free case are

X	T	φ
0	0	1
$-t$	0	q
1	0	0
$-qt$	$-t^2$	$\frac{1}{2}(i\hbar\, t + q^2)$
0	1	0
q	$2t$	$-\frac{i\hbar}{2}$.

(8.4)

According to the method of Proposition V,5 each of these generators is unitarily equivalent to one generator of the free fall Hamiltonian H via the strongly continuous one parameter groups of unitary operators in $L^2(\mathbb{R})$ defined by

$$W_t = e^{-(i/\hbar)tH} \cdot e^{(i/\hbar)tH_0}. \tag{8.5}$$

Using this, one computes the corresponding coefficients for the free fall symmetry generators. The results are

$$\begin{array}{ccc} X & T & \varphi \\ \hline 0 & 0 & 1 \\ -t & 0 & q-\frac{g}{2}t^2 \\ 1 & 0 & gt \\ -qt+\frac{g}{2}t^3 & -t^2 & \frac{1}{2}(i\hbar\, t+q^2)-\frac{3g}{2}t^2q+\frac{g^2}{8}t^4 \\ 0 & 1 & 0 \\ q-\frac{3g}{2}t^2 & 2t & -\frac{i\hbar}{2}+3gtq-\frac{g^2}{2}t^3. \end{array} \tag{8.6}$$

As they should, the constant observables of the free fall system reduce clearly to the ones of the pure free case (8.4) when the constant g vanishes.

We also observe that the second and third of those constants are "trivial" (although consistently forgotten) since they correspond to the initial position and momentum observables expressed, in the Heisenberg picture, in terms of $Q(t)$ and $P(t)$. On the other hand, the fourth and last observables are nontrivial constants for this elementary system with purely continuous spectrum σ_H.

B. The free particle on the sphere $S^2 \subset \mathbb{R}^3$

Now take for the configuration manifold M of Sec. VI the sphere S^2 of radius R in $\mathbb{R}^3$.

It is natural to introduce the spherical coordinates $(q^j)=(\theta,\phi)$ in $]0,\pi[\times[0,2\pi]$. Then, since $A=V=0$ here, the Lagrangian of the classical system reduces to the kinetic part

$$L(\dot\theta,\dot\phi,\theta,\phi)=\frac{R^2}{2}(\dot\theta^2+\sin^2\theta\dot\phi^2), \tag{8.7}$$

since the metric of S^2 is of the form

$$\mathrm{d}s^2=R^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\phi^2), \tag{8.8}$$

or, equivalently,

$$g_{ij}=\begin{pmatrix} R^2 & 0 \\ 0 & R^2\sin^2\theta \end{pmatrix}. \tag{8.9}$$

The associated Christoffel symbols and covariant derivatives are easily computed,

$$\begin{gathered} \Gamma^1_{11}=\Gamma^1_{12}=\Gamma^1_{21}=\Gamma^2_{11}=\Gamma^2_{22}=0, \\ \Gamma^2_{12}=\Gamma^2_{21}=\operatorname{cotg}\theta, \\ \Gamma^1_{22}=-\sin\theta\cos\phi, \end{gathered} \tag{8.10}$$

and

$$\begin{gathered} \nabla_\theta=\frac{\partial}{\partial\theta},\quad \nabla_\phi=\frac{\partial}{\partial\phi}, \\ \nabla^\theta=\frac{1}{R^2}\frac{\partial}{\partial\theta},\quad \nabla^\phi=\frac{1}{R^2\sin^2\theta}\frac{\partial}{\partial\phi}. \end{gathered} \tag{8.11}$$

The quantum momentum observables in $L^2(S^2,R^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi)$ are

$$P_\theta = -i\hbar\nabla_\theta - i\hbar\ \cot g\,\theta,$$
$$P_\phi = -i\hbar\nabla_\phi, \tag{8.12}$$

and the Hamiltonian observable is

$$H = -\frac{\hbar^2}{2R^2}\left[\left(\frac{\partial^2}{\partial\theta^2} + \text{cotg}\ \theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \tag{8.13}$$

It is known that for this case with constant curvature $K=R^{-2}>0$ and potentials $A=V=0$ the dimension of the symmetry algebra is maximal; here this is five. The table of the coefficients of the symmetry generator $\hat{N}(t)$ for the Schrödinger equation with Hamiltonian (8.13) is the following:

$X=(X^\theta,X^\phi)$	T	φ
$(0,0)$	1	0
$(0,0)$	0	1
$\left(\sin\phi,\frac{\cos\phi}{tg\ \theta}\right)$	0	0
$\left(-\cos\phi,\frac{\sin\phi}{tg\ \theta}\right)$	0	0
$(0,-1)$	0	0.

(8.14)

Given the definition (6.12) of the symmetry generator $\hat{N}(t)$, it is clear that the first symmetry corresponds to the conservation of the energy observable. The three last ones are interesting, but also of a purely classical origin.

$(X_j^\theta,X_j^\phi), j=1,2,3$ form a basis of the Killing vector field Lie algebra for S^2, an homogeneous manifold. Those vectors X_j are proportionals to the quantum angular momenta, known to be a basis of SO(3), the group of isometries (rotations) of S^2:

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\text{tg}\ \theta}\frac{\partial}{\partial\phi}\right) \equiv i\hbar\left(\sin\phi,\frac{\cos\phi}{\text{tg}\ \theta}\right) \equiv i\hbar X_1, \tag{8.15}$$

and correspondingly for L_y, L_z. The three vectors X_j solve the determining equation (1) of Proposition VI.1 which reduces here to Killing's equation

$$\nabla^\theta X_j^\phi + \nabla^\phi X_j^\theta = 0, \quad j=1,2,3. \tag{8.16}$$

The last symmetry of the table (8.14) corresponds to the conservation of the angular momentum P_ϕ.

The integrability of the underlying classical system is built on the existence of the two constants of motion H and P_ϕ allowing to foliate the data space by a two parameter family of two-dimensional tori.

C. An example of Goldstein

In Goldstein's *Classical Mechanics* (1980), (p. 430), the problem 2a) consists in showing that, for a one-dimensional classical system with Hamiltonian

$$H(q,p) = \frac{p^2}{2} - \frac{1}{2}q^{-2}, \tag{8.17}$$

there is a time-dependent constant of motion of the form

$$n = \frac{q}{2}p - tH. \tag{8.18}$$

This is the case where $M=\mathbb{R}, A(q)=0$, $V(q)=-\frac{1}{2}q^{-2}$and (8.18) shows that

$$X(q,t) = \frac{q}{2}, \quad T(t) = t, \quad \varphi(q,t) = 0.$$

The determining equations (1) and (2) of Proposition IV.3 are trivially satisfied and the "classical limit $\hbar=0$" of (3) holds as well, so n is indeed a (classical) constant of motion. Let us recall that there is nothing exotic about time-dependent classical first integrals, as shown by the ones associated with Galilean boosts.

D. Lewis and Riesenfeld invariant

This is a quantum invariant, discovered in 1969 (Ref. 52) for the harmonic oscillator with time-dependent frequency, i.e., with classical Hamiltonian ($M=\mathbb{R}$)

$$H(q,p,t) = \frac{1}{2}p^2 + \frac{\omega^2(t)}{2}q^2. \tag{8.19}$$

It can be shown that this invariant is of the form (6.32), with

$$X(q,t) = \frac{\dot{T}}{2}q, \quad \hat{\varphi}(q,t) = -\frac{\ddot{T}}{4}q^2, \quad T(t) = \rho^2(t),$$

where $\rho(t)$ solves the nonlinear equation

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{\rho^3} = 0.$$

Details can be found in Ref. 53.

IX. CONCLUSIONS

Our framework is founded on a dynamic reinterpretation of the symmetry group of the Schrödinger equation, itself very close to the one of the associated heat equation.

Given the fact that this group was computed by Lie around 1890, a number of the tools we used here are, indeed, quite old. The free Lie algebra can be found in most of the textbooks on Lie groups analysis of PDE published since 1970 (for example Refs. 15, 16, and 54), often with commentaries about the obscure physical interpretation of most explicitly time-dependent transformations, notably those presented as trivial in our Section V. Kuwabara's result[28] (1984) (discovered by us after the redaction of the present work was almost finished) is especially relevant, as it shows that the Lie algebraic structure for quantum (and classical) symmetries is time-dependent. He found, in particular, the form (6.12) of the symmetry operator, without regarding it as a consequence of a Nœther theorem or trying to relate it with a Lagrangian framework. Although we could not find a clear statement that the associated quantum first integrals should be understood in the sense of the Heisenberg picture of quantum dynamics, such a statement may well already exist in the vast literature on the subject, but is certainly not common knowledge in mathematical or theoretical physics.

The specific contribution of our indirect Euclidean approach lies, curiously, in the physical interpretation it provides of many time-dependent symmetries, through their elementary meaning in stochastic analysis.[69]

The simplest illustration is provided by the one-dimensional ($n=1$) free case ($A=V=0$) and the symmetry associated with the coefficients $X=-t, T=0, \varphi=x$ of the symmetric generator $\hat{N}(t)$ in (4.7), corresponding to a simple solution of the system of equations of Proposition IV.3. This symmetry corresponds to the one-parameter family of solutions

$$\psi_\alpha(x,t) = e^{(i/\hbar)(\alpha x-(\alpha^2/2)t)}\psi(x-\alpha t,t), \quad \alpha \in \mathbb{R} \tag{9.1}$$

of the free equation $i\hbar(\partial\psi/\partial t)=-(\hbar^2/2)\Delta\psi$, quite familiar in the context of the Galilean invariance of this equation.[55]

Let us rewrite (9.1) as

$$\psi_\alpha(x,t) = (e^{\alpha\hat{N}(t)}\psi)(x,t), \tag{9.2}$$

and expand in α this expression when ψ is the trivial (unnormalizable) free solution if $\psi_t=1$. On this "state," the space–time observables of momentum and energy vanish and the one associated with $\hat{N}(t)$ reduces to the phase φ [cf. (4.18)]. We find

$$\psi_\alpha(x,t) = 1 + \alpha x + \frac{\alpha^2}{2!}(x^2 + i\hbar t) - \frac{\alpha^3}{3!}(x^3 + 3i\hbar tx) + \cdots. \tag{9.3}$$

By successive taking of $(\partial/\partial\alpha)$ at $\alpha=0$ we obtain a collection of constant space–time observables $n_1^{\hat{N}^n}(x,t)\equiv\varphi_n(x,t), n\in\mathbb{N}$, each, indeed, solution of $D_t\varphi_n=0$.

Now $\hat{N}(t)=(-tP(t)+Q(t))$ itself is certainly a trivial quantum first integral, namely the initial position observable [since $Q(t)$ and $P(t)$ are solutions of the free Heisenberg equation of motion] and the $\hat{N}^n(t), n\in\mathbb{N}$, reduce to the successive powers of this trivial dynamical information on the free quantum system.

On the Euclidean side, we are dealing instead of (9.1) with the one parameter family

$$\eta_\alpha(q,t) = e^{(1/\hbar)(\alpha q-(\alpha^2/2)t)}\eta(q-\alpha t,t), \quad \alpha \in \mathbb{R} \tag{9.4}$$

of (positive) solutions of the free heat equation (7.11). It corresponds to the Euclidean counterpart (cf. paper I)

$$N_E(t) = t\frac{\partial}{\partial q} - q \tag{9.5}$$

of the real time symmetry generator $\hat{N}(t)$. The above unphysical state ψ_t turns into the trivial solution $\eta_t=1$ of the free equation (7.11) whose probabilistic role becomes fundamental. Indeed, according to (7.19) and (7.22′) the associated well-defined diffusion Z_t reduces to the one-dimensional Wiener process with diffusion coefficient $\hbar$. Notice that the corresponding solution of the free adjoint heat equation (7.7) is, then, the integral kernel $\eta_t^*=h_0(x,t,q)$ of this equation. Since the relation between η_t and η_t^* is manifestly not the Euclidean counterpart of a complex conjugacy, this means that for the Wiener process itself, the time invariance of the lhs of (7.12) (with an appropriate pair of positive boundary conditions) is the basis of our probabilistic interpretation of a complex quantum probability amplitude.

Now let us consider

$$h_\alpha(q,t) = \frac{\eta_\alpha}{\eta}(q,t). \tag{9.6}$$

If Z_t is the diffusion, of law P, built from η using (7.19), it is easy to show that h_α is a strictly positive $\mathcal{P}_t$-martingale of Z_t, i.e., satisfies $D_t h_\alpha(Z_t,t)=0$. Denoting by Z_t^α the new diffusion, of law P_α, built from η_α, one shows easily that P_α is absolutely continuous with respect to P, with Radon-Nikodym derivative $\mathrm{d}P_\alpha/\mathrm{d}P=h_\alpha$. In the case of the Wiener process, h_α is the exponential martingale of this process, a basic tool dating[44,49] back to the foundations of stochastic analysis.

The family of $\mathcal{P}_t$-martingales resulting from the successive taking of derivatives $\partial/\partial\alpha$ at $\alpha=0$, namely $\{1,q,q^2-\hbar t,q^3-3\hbar tq,\ldots\}$, coincides with the familiar Wick product of the Brownian motion[56] which is, therefore, reinterpreted as the probabilistic counterpart of the above-mentioned trivial dynamical information on the free quantum system provided by Nœther's theorem.

Thus stochastic analysis may help, indeed, to understand some conventional aspects of quantum dynamics.

The version of Euclidean quantum mechanics advocated in paper I is known to be valid for a class of Hamiltonians much larger than the one considered here (cf. Ref. 57) and it is expected that many ideas expressed here will survive in more general contexts (cf. Refs. 70 and 71).

Although, as shown here, the Riemannian formulation of our results is quite natural, the proper geometrical framework of this method is distinct. It should be regarded, in fact, as deformation of classical contact geometry.[58] This viewpoint also has serious computational advantages when adopted in the Euclidean context where the probability measures make sense, and quantum symmetries are reinterpreted as symmetries of families of diffusion processes.

X. ERRATA FOR PAPER I

(1) In Proposition 3.6 of Ref. 1 (cf. also Ref. 59), the term $\nabla\phi - X_q\cdot B$, i.e., the variation of the drift, is ambiguous. It should be understood as

$$\frac{\partial\phi}{\partial q^i}-\frac{\partial X^k}{\partial q^i}B^k$$

(where the summation convention is used).

(2) The "illustration of the central role of time symmetry," mentioned in p. 331 of Ref. 1 is wrong: the function $n(q,t)$ [respectively $n_*(q,t)$] solves our heat equation (7.11) [respectively, (7.7)] and so are $\mathcal{P}_t$ (respectively, $\mathcal{F}_t$) martingales of the starting process Z_t, $t\in I$. But they are not strictly positive and so cannot be used as h-functions, in the sense of Doob's h-transform. However, when the Nœtherian symmetry operator $\hat{N}$ is positivity preserving, $\eta_\alpha(q,t)=e^{-\alpha\hat{N}}\eta(q,t)$, where η is the positive solution of (7.11) associated with Z_t, is a one-parameter family of solutions of the same equation. Then $h_\alpha(q,t)=(\eta_\alpha/\eta)(q,t)$ is, indeed, the positive martingale needed for the h-transform producing the family of Bernstein diffusions Z_t^α associated with this symmetry (cf. Conclusion here, Sec. 6, Part 2 of Ref. 44, and Refs. 31, 32, and 58 for much more).

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The weak Hopf algebras related to generalized Kac-Moody algebra

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We define a kind of quantized enveloping algebra of a generalized Kac-Moody algebra $\mathcal{G}$ by adding a generator J satisfying $J^m=J^{m-1}$ for some integer m. We denote this algebra by $wU_q^\tau(\mathcal{G})$. This algebra is a weak Hopf algebra if and only if $m=2$. In general, it is a bialgebra, and contains a Hopf subalgebra. This Hopf subalgebra is isomorphic to the usually quantum envelope algebra $U_q(\mathcal{G})$ of a generalized Kac-Moody algebra $\mathcal{G}$. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In his study of Monstrous moonshine,[3–5] Borcherds introduced a new class of infinite dimensional Lie algebras called generalized Kac-Moody algebras. These generalized Kac-Moody algebra have a contravariant bilinear form which is almost positive definite. The fixed point algebra of any Kac-Moody algebra under a diagram automorphism is a generalized Kac-Moody algebra. A generalized Kac-Moody algebra can be regarded as a Kac-Moody algebra with imaginary simple roots. More explicitly, a generated Kac-Moody algebra is determined by a Borcherds-Cartan matrix $A=(a_{ij})_{(i,j)\in I\times I}$, where either $a_{ii}=2$, or $a_{ii}\leq 0$. If $a_{ii}\leq 0$, then the index i is called imaginary, and the corresponding simple root α_i is called imaginary root. In this paper, the set $\{i\in I|a_{ii}=2\}$ is denoted by I^+. Set $I^{im}=I\backslash I^+$. The structure and the representation theory of generalized Kac-Moody algebras are very similar to those of Kac-Moody algebras, and many basic facts about Kac-Moody algebras can be extended to generalized Kac-Moody algebras. For example, the Kac-Weyl formula about an irreducible representation over a Kac-Moody algebra is generalized to a formula about an irreducible representation over a generalized Kac-Moody algebra as follows:

$$chV(\lambda)=\frac{\sum_{w\in W}\sum_{F\subseteq T,F\perp\lambda}(-1)^{l(w)+|F|}e^{w(\lambda+\rho-s(F))}}{\sum_{w\in W,F\subseteq T}(-1)^{l(w)+|F|}e^{w(\rho-s(F))}},$$

where T is the set of all imaginary simple roots, F runs all over finite subsets of T such that any two elements in F are mutually perpendicular. We denote by $s(F)$ the sum of the roots in F. We call the above formula Borcherds-Kac-Weyl formula.

On the other hand, many mathematicians are interested in generalization of Hopf algebras, of which importance has been recognized in both mathematics and physics. One way to do this is to introduce a kind of weak coproduct such that $\Delta(1)\neq 1\otimes 1$ in Ref. 1. The face algebras[7] and generalized Kac algebras[14] are examples of this class of weak Hopf algebras. Li and Duplij have defined and studied another kind of weak Hopf algebras.[11] A bialgebra $(H,\mu,\eta,\Delta,\varepsilon)$ is called a weak Hopf algebra if there is an antiautomorphism T such that $T*\mathrm{id}_H*T=\mathrm{id}_H$ and $\mathrm{id}_H*T*\mathrm{id}_H=T$, where id_H is the identity map and * is the convolution product. Hopf algebras, and left or right Hopf[12,13] algebras are weak Hopf algebras in this sense. In the presented paper a weak Hopf

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algebra is always a mean weak Hopf algebra in this sense. The weak quantized enveloping algebras of semisimple Lie algebras are also weak Hopf algebras.[15] Our aim is to give more nontrivial examples of weak Hopf algebras. Thanks to the definition of quantized enveloping algebra $U_q(\mathcal{G})$ associated a generalized Kac-Moody algebra $\mathcal{G}$ defined in Ref. 7, we can also replace the group $G(U_q(\mathcal{G}))$of grouplike elements by some regular monoid as in Ref. 15, we use a generator J instead of the projector in Ref. 13. Our generator J satisfies $J^m=J^{m-1}$ for some integer $m\geq 2$. By this way, we obtain a subclass of bialgebra $wU_q(\mathcal{G})$. This bialgebra contains a subbialgebra $U^\tau(\mathcal{G})$, which is a weak Hopf algebra in the sense of Ref. 11. Moreover, the quotient algebra $wU_q(\mathcal{G})/(1-J^m)$ is isomorphic to a sub-Hopf algebra of the quantized enveloping algebra $U_q(\mathcal{G})$ as Hopf algebras. As in the case of the classic quantum group $U_q(\mathcal{G})$, we try to determine irreducible representation of $wU_q(\mathcal{G})$.

Finally, let us outline the structure of this paper. In Sec. II, we recall some basic facts related to the quantized enveloping algebra of a generalized Kac-Moody algebra. In Sec. III, we give the definition of $wU_q(\mathcal{G})$. We study the bialgebra structure of $wU_q(\mathcal{G})$ in Sec. IV. In the final section, we study the irreducible representation of $wU_q(\mathcal{G})$.

II. NOTATIONS AND PRELIMINARIES

In this section, we fix notations and recall fundamental results about generalized Kac-Moody algebras.

Let $I=\{1,\ldots,n\}$ or the set of positive integers, and $A=(a_{ij})_{I\times I}$, a Borcherds-Cartan matrix, i.e., it satisfies

(1) $a_{ii}=2$ or $a_{ii}\leq 0$ for all $i\in I$,
(2) $a_{ij}\leq 0$ for all $i\neq j$,
(3) $a_{ij}\in \mathbf{Z}$,
(4) $a_{ij}=0$ if only if $a_{ji}=0$.

We say that an index i is real if $a_{ii}=2$ and imaginary if $a_{ii}\leq 0$. We denote $I^+=\{i\in I\,|\,a_{ii}=2\}$ and $I^{im}=I-I^+$. Kang considered the generalized Kac-Moody algebras associated with Borcherds-Cartan matrices with charge[10]

$$\mathbf{m}=\{(m_i\in \mathbf{Z}_{\geq 0})\,|\,i\in I, m_i=1 \text{ for } i\in I\}.$$

The charge m_i is the multiplicity of the simple root corresponding to $i\in I$. In this paper, we follow Ref. 9, and assume that $m_i=1$ for all $i\in I$. However, we do not lose generality by this hypothesis. Indeed, if we take Borcherds-Cartan matrices with some of the rows and columns identical, then the generalized Kac-Moody algebras with charge introduced in Ref. 10 can be recovered from the ones in the present paper by identifying the h_i's and d_i's (and hence the α_i's) corresponding to these identical rows and columns.

Moreover, we also assume that A is symmetrizable; that is, there is a diagonal matrix $D=\mathrm{diag}\{s_i>0\,|\,i\in I\}$ such that DA is a symmetric matrix.

Let $P=(\oplus_{i\in I}\mathbf{Z}h_i)\oplus(\oplus_{i\in I}\mathbf{Z}d_i)$ be a free Abelian group generated by the set $\{h_i,d_i\,|\,i\in I\}$. This free Abelian group is called the coweight lattice of A. The element h_i in $\Pi^\vee=\{h_i\,|\,i\in I\}$ is called a simple coweight. We call $\Pi^\vee$ the set of all simple coweights. The space $\mathcal{H}=\mathbf{Q}\otimes_{\mathbf{Z}}P^\vee$ over the rational number field $\mathbf{Q}$ is said to be a Cartan subalgebra. The weight lattice is defined to be $P:=\{\lambda\in\mathcal{H}^*\,|\,\lambda(P^\vee)\subseteq\mathbf{Z}\}$, where $\mathcal{H}^*$ is the dual space of the Cartan subalgebra $\mathcal{H}=\mathbf{Q}\otimes_{\mathbf{Z}}P^\vee$. We denote by P^+ the set $\{\lambda\in P\,|\,\lambda(h_i)\geq 0,\ \textit{for every } i\in I\}$ of dominant integral weights.

Define $\alpha_i,\Lambda_i\in\mathcal{H}^*$ by

$$\alpha_i(h_j)=a_{ji},\quad \alpha_i(d_j)=\delta_{ij},$$

$$\Lambda_i(h_j)=\delta_{ij},\quad \Lambda_i(d_j)=0.$$

Then $\alpha_i, i\in I$ are called simple roots of A. Let $\Pi=\{\alpha_i\,|\,i\in I\}\subset P$ be the set of simple roots. The free Abelian group $Q=\oplus_{i\in I}\mathbf{Z}\alpha_i$ is called the root lattice. Set $Q_+=\Sigma_{i\in I}\mathbf{Z}_{\geq 0}\alpha_i$ and $Q_-=-Q_+$. For any

$\alpha \in Q_+$, we can write $\alpha = \Sigma_{k=1}^{n} \alpha_{i_k}$ for $i_1, i_2, \ldots, i_n \in I$. We set $ht(\alpha) = n$ and call it the height of α.

Let $(.|.)$ be the bilinear form on $(\oplus_i(\mathbf{Q}\alpha_i \oplus \mathbf{Q}\Lambda_i)) \times \mathcal{H}^*$ defined by

$$(\alpha_i|\lambda) = s_i\lambda(h_i), (\Lambda_i|\lambda) = s_i\lambda(d_i).$$

Since it is symmetric on $(\oplus_i(\mathbf{Q}\alpha_i \oplus \mathbf{Q}\Lambda_i)) \times (\oplus_i(\mathbf{Q}\alpha_i \oplus \mathbf{Q}\Lambda_i))$, one can extend this to a symmetric bilinear form on $\mathcal{H}^*$. Then such a form is nondegenerated.

We always assume that $\mathbf{K}$ is a field of characteristic 0. Let $q \in \mathbf{K}$ and $q_i = q^{d_i}$. It is assumed that $q_i \neq \pm 1, 0$ for all $i \in i$. For an indeterminant ν and an integer m, let

$$[m]_\nu = \frac{\nu^m - \nu^{-m}}{\nu - \nu^{-1}}, \quad [m]!_\nu = [m]_\nu \cdots [1]_\nu, \quad [0]_\nu = 1,$$

and

$$\begin{bmatrix} m \\ s \end{bmatrix}_\nu = \frac{[m]!_\nu}{[s]!_\nu [m-s]!_\nu}.$$

Definition: The quantized enveloping generalized Kac-Moody algebra $U_q(\mathcal{G})$ associated with a Borcherds-Cartan datum $(A, P^\vee, P, \Pi^\vee, \Pi)$ is the associated algebra with unit 1 over a field $\mathbf{K}$ *of characteristic* 0, *generated by the symbols e_i, f_i $(i \in I)$ and $P^\vee$ subject to the following defining relations:*

$$q^0 = 1, q^h q^{h'} = q^{h+h'} \quad \forall\, h, h' \in P^\vee,$$

$$q^h e_i q^{-h} = q^{\alpha_i(h)} e_i, \quad q^h f_i q^{-h} = q^{-\alpha_i(h)} f_i,$$

$$e_i f_j - f_j e_i = \delta_{ij} \frac{k_i - k_i^{-1}}{q_i - q_i^{-1}}, \quad \text{where } k_i = q^{s_i h_i},$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i e_i^{1-a_{ij}-r} e_j e_i^r = 0 \quad \text{if } a_{ii} = 2,\ i \neq j,$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i f_i^{1-a_{ij}-r} f_j f_i^r = 0 \quad \text{if } a_{ii} = 2,\ i \neq j,$$

$$e_i e_j - e_j e_i = f_i f_j - f_j f_i = 0 \quad \text{if } a_{ij} = 0.$$

The quantum generalized Kac-Moody algebra $U_q(\mathcal{G})$ has a Hopf algebra structure with the comultiplication Δ, the counit ε, and antipode S defined by

$$\Delta(q^h) = q^h \otimes q^h,$$

$$\Delta(e_i) = e_i \otimes k_i^{-1} + 1 \otimes e_i,$$

$$\Delta(f_i) = k_i \otimes f_i + f_i \otimes 1,$$

$$\varepsilon(q^h) = 1, \quad \varepsilon(e_i) = \varepsilon(f_i) = 0,$$

$$S(q^h) = q^{-h}, \quad S(e_i) = -e_i k_i, \quad S(f_i) = -k_i^{-1} f_i$$

for all $h \in P^\vee$ and $i \in I$.

Let $U_q^+(\mathcal{G})$ and $U_q^-(\mathcal{G})$ be the subalgebras of $U_q(\mathcal{G})$ generated by elements e_i and f_i, respectively, for $i \in I$, and let $U_q^0(\mathcal{G})$ be the subalgebra of $U_q(\mathcal{G})$ generated by $q^h (h \in P^\vee)$. Then we have the triangular decomposition[1,8]

$$U_q(\mathcal{G}) = U_q^-(\mathcal{G}) \otimes U_q^0(\mathcal{G}) \otimes U_q^+(\mathcal{G}).$$

Finally, let us use $U_q'(\mathcal{G})$ to denote a subalgebra of $U_q(\mathcal{G})$ generated by e_i, f_i, q^h, where $h \in \oplus_{i\in I}\mathbf{Z}s_i h_i \oplus \oplus_{i\in I}\mathbf{Z}d_i$. It is obvious that $U_q'(\mathcal{G})$ is a Hopf algebra.

III. WEAK QUANTUM ALGEBRAS $wU_q^T(\mathcal{G})$

Let m be a fixed positive integer. To generalize the invertibility condition $k_i k_i^{-1} = 1$ in $U_q(\mathcal{G})$, let us introduce some generators J, K_i, and $\bar{K}_i$, which subject the following relations:

$$J^m = J^{m-1} = K_i\bar{K}_i = \bar{K}_i K_i = D_i\bar{D}_i = \bar{D}_i D_i. \tag{3.1}$$

Moreover, we assume that $J^r \neq J^{r-1}$ for any $r < m$. Suppose K_i and $\bar{K}_i$ are not zero divisors. Then

$$K_i J = JK_i = K_i, \quad \bar{K}_i J = J\bar{K}_i = \bar{K}_i. \tag{3.2}$$

$$D_i J = JD_i = D_i, \quad \bar{D}_i J = J\bar{D}_i = \bar{D}_i. \tag{3.3}$$

In this paper we always assume that (3.2) and (3.3) hold. We call an element E_i of type one if it satisfies

$$K_j E_i = q_i^{a_{ij}} E_i K_j, \quad \bar{K}_j E_i = q_i^{-a_{ij}} E_i \bar{K}_j. \tag{3.4}$$

Similarly, if

$$K_j F_i = q_i^{-a_{ij}} F_i K_j, \quad \bar{K}_j F_i = q_i^{-a_{ij}} F_i \bar{K}_j, \tag{3.5}$$

then F_i is said to be type one. Suppose

$$K_j E_i \bar{K}_j = q^{a_{ij}} E_i. \tag{3.6}$$

Then we say that E_i is type zero. Similarly, F_i is type zero if it satisfies the following:

$$K_j F_i \bar{K}_j = q^{-a_{ij}} F_i. \tag{3.7}$$

Proposition III.1: E_i (*respectively,* F_i) *is type zero if and only if* E_i *is type one and* $E_i J^{m-1} = J^{m-1} E_i = E_i$ (*respectively*, $F_i J^{m-1} = J^{m-1} F_i = F_i$).

Proof: If E_i is type zero, then we obtain from (3.6),

$$K_j E_i \bar{K}_j K_j = K_j E_i J^m = q_i^{a_{ij}} E_i K_j.$$

On the other hand, since $J^m K_j = K_j$,

$$K_j E_i \bar{K}_j = K_j E_i J^m \bar{K}_j = q_i^{a_{ij}} E_i K_j \bar{K}_j = q_i^{a_{ij}} E_i J^{m-1}.$$

So $E_i = E_i J^{m-1}$. Similarly, we can prove that $E_i = J^{m-1} E_i$. Then

$$K_j E_i = K_j E_i J^m = q_i^{a_{ij}} E_i K_j$$

and

$$E_i \bar{K}_j = J^m E_i \bar{K}_j = q_i^{a_{ij}} \bar{K}_j E_i.$$

That is, E_i is type one. On the other hand, if E_i is type one, and $E_i J^m = J^m E_i = E_i$, then

$$q_i^{a_{ij}}E_i = q_i^{a_{ij}}E_iK_j\bar{K}_j = K_jE_i\bar{K}_j.$$

Similarly,we can prove the statement about F_i is true. By now, we complete the proof.

The types of E_i and F_i are denoted by κ_i, κ', respectively. Let $\tau=(\{\kappa_i\}_{i\in I}|\{\kappa_i'\}_{i\in I})$. By now, we can give the definition for the weak quantum algebra of type τ as follows.

Definition: The type τ weak quantum algebra $wU_q^\tau(\mathcal{G})$ associated with the generalized Kac-Moody algebra $\mathcal{G}$ is an associated algebra with unit 1 *over a field* **K** *of characteristic* 0, *generated by* J, $E_i,F_i(i\in I)$ *and* $K_i,D_i(i\in I)$ *subjecting with the following defining relations*:

$$J^m = J^{m-1} = K_i\bar{K}_i = D_i\bar{D}_i, \tag{3.8}$$

$$K_i\bar{K}_j = \bar{K}_jK_i, \quad K_iK_j = K_jK_i, \quad \bar{K}_i\bar{K}_j = \bar{K}_j\bar{K}_i, \tag{3.9}$$

$$D_i\bar{D}_j = \bar{D}_jD_i, \quad D_iD_j = D_jD_i, \quad \bar{D}_i\bar{D}_j = \bar{D}_j\bar{D}_i, \tag{3.10}$$

$$D_i\bar{K}_j = \bar{K}_jD_i, \quad K_iD_j = D_jK_i, \quad \bar{D}_iK_j = K_j\bar{D}_i, \quad \bar{D}_i\bar{K}_j = \bar{K}_j\bar{D}_i, \tag{3.11}$$

$$D_iJ = JD_i = D_i, \quad K_iJ = JK_i = K_i, \tag{3.12}$$

$$J\bar{D}_i = \bar{D}_iJ = D_i, \quad J\bar{K}_i = \bar{K}_iJ = \bar{K}_i, \tag{3.13}$$

$$E_i \quad F_i \quad \textit{are type } \tau, \tag{3.14}$$

$$E_iF_j - F_jE_i = \delta_{ij}\frac{K_i - \bar{K}_i}{q_i - q_i^{-1}}, \tag{3.15}$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i E_i^{1-a_{ij}-r}E_jE_i^r = 0 \quad \textit{if } a_{ii}=2, i\neq j, \tag{3.16}$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i F_i^{1-a_{ij}-r}F_jF_i^r = 0 \quad \textit{if } a_{ii}=2, i\neq j, \tag{3.17}$$

$$E_iE_j - E_jE_i = F_iF_j - F_jF_i = 0, \quad \textit{if } a_{ij}=0. \tag{3.18}$$

If $m=1$, and the Borcherds-Cartan matrix A is symmetric, then $wU_q^T(\mathcal{G})=U_q(\mathcal{G})$ provided that we identify K_i with q^{h_i}, $\bar{K}_i$ with q^{-h_i}, D_i with q^{d_i} and $\bar{D}_i$ with q^{-d_i}. If $m=2$ and $\mathcal{G}$ is a semisimple Lie algebra, then $wU_q^T(\mathcal{G})$ has been defined and studied by Yang in Ref. 14. Notice that the type zero was called type two by Yang.

Lemma III.1: J^m is a center idempotent element of $wU_q^\tau(\mathcal{G})$.

Proof: If E_i is type one, then $J^mE_i=K_j\bar{K}_jE_i=E_iK_j\bar{K}_j=E_iJ^m$. Similarly, we can prove that $F_iJ^m=J^mF_i$ provided F_i is type one. Hence this lemma follows from Proposition III.1.

In the following corollary, the subalgebra of $U_q(\mathcal{G})$ generated by $E_i,F_i,s_ih_i,d_i(i\in I)$ is denoted by $U_q'(\mathcal{G})$. It is a Hopf subalgebra of $U_q(\mathcal{G})$.

Corollary III.1:

(1) $wU_q^\tau(\mathcal{G})=wU_q^\tau(\mathcal{G})J^m\oplus wU_q^\tau(\mathcal{G})(1-J^m)$ *is a direct sum of algebras.*
(2) $wU_q^\tau(\mathcal{G})/(1-J)$ *is isomorphic to the algebra* $U_q'(\mathcal{G})$.
(3) $wU_q^\tau(\mathcal{G})J^m$ *is isomorphic to the algebra* $U_q'(\mathcal{G})$.

Proof: The proof of (1) and (2) is easy. To prove (3), let us define a map ψ from $U_q'(\mathcal{G})$ to $wU_q^\tau(\mathcal{G})J^m$ as follows.

$$\psi(q^{s_i h_i}) = K_i, \quad \psi(q^{d_i}) = D_i, \quad \psi(e_i) = E_i J^m, \quad \psi(f_i) = F_i J^m, \quad \psi(1) = J^m.$$

Then one can show that ψ is an algebra homomorphism. Similarly we can define an algebra homomorphism a map φ from $wU_q^\tau(\mathcal{G})J^m$ to $U_q'(\mathcal{G})$ as follows:

$$\varphi(K_i) = q^{s_i h_i}, \quad \varphi(D_i) = q^{d_i}, \quad \varphi(E_i J^m) = e_i, \quad \varphi(F_i J^m) = f_i, \quad \varphi(J^m) = 1.$$

It is easy to check that $\varphi\psi$=id and $\psi\varphi$=id. This proves (3).

Remark 1: *By Proposition III.1*, $wU_q^\tau(\mathcal{G})(1-J^m)$ *is generated by* $J^r - J^{m-1}$ *for* $0 \le r \le m-2$, $E_i(1-J^m)$ *and* $F_i(1-J^m)$, *where* E_i *and* F_i *are type one*. *Since* (3.15) *holds in* $wU_q^\tau(\mathcal{G})$, $E_i(1-J^m)F_j(1-J^m) = F_j(1-J^m)E_i(1-J^m)$. *If all* $\kappa_i = \bar{\kappa}_i = 0$, *then* $wU_q^\tau(\mathcal{G})(1-J^m)$ *is isomorphic to the group algebra* $\mathbf{K}[\mathbf{Z}_{m-2}]$.

IV. THE BIALGEBRA STRUCTURE OF $wU_q^\tau(\mathcal{G})$

The algebras $wU_q^\tau(\mathcal{G})J^m$ and $wU_q^\tau(\mathcal{G})(1-J^m)$ are denoted by w and $\bar{w}$, respectively, in the following. By Corollary III.1, w is isomorphic to the quantum group $U_q(\mathcal{G})$ provided $s_i = 1$. Thus the comultiplication and counit of $U_q(\mathcal{G})$ transplant to the algebra $wU_q^\tau(\mathcal{G})J^m$, and $wU_q^\tau(\mathcal{G})J^m$ becomes a Hopf algebra. Moreover, we can define three maps:

$$\Delta: wU_q^\tau(\mathcal{G}) \to wU_q^\tau(\mathcal{G}) \otimes wU_q^\tau(\mathcal{G}),$$

$$\varepsilon: wU_q^\tau(\mathcal{G}) \to \mathbf{K},$$

$$T: wU_q^\tau(\mathcal{G}) \to wU_q^\tau(\mathcal{G}),$$

as follows:

$$\Delta(K_i) = K_i \otimes K_i, \quad \Delta(\bar{K}_i) = \bar{K}_i \otimes \bar{K}_i, \tag{4.1}$$

$$\Delta(D_i) = D_i \otimes D_i, \quad \Delta(\bar{D}_i) = \bar{D}_i \otimes \bar{D}_i, \tag{4.2}$$

$$\Delta(J) = J \otimes J, \tag{4.3}$$

$$\Delta(E_i) = \begin{cases} 1 \otimes E_i + E_i \otimes K_i, & E_i \text{ is type one}, \\ J^{m-1} \otimes E_i + E_i \otimes K_i, & E_i \text{ is type zero}, \end{cases} \tag{4.4}$$

$$\Delta(F_i) = \begin{cases} F_i \otimes 1 + \bar{K}_i \otimes F_i, & F_i \text{ is type one}, \\ F_i \otimes J^{m-1} + \bar{K}_i \otimes F_i, & F_i \text{ is type zero}, \end{cases} \tag{4.5}$$

$$\varepsilon(K_i) = \varepsilon(\bar{K}_i) = 1, \quad \varepsilon(D_i) = \varepsilon(\bar{D}_i) = 1, \quad \varepsilon(J) = 1, \tag{4.6}$$

$$\varepsilon(E_i) = \varepsilon(F_i) = 0, \tag{4.7}$$

while the map T is defined as follows:

$$T(1) = 1, \quad T(K_i) = \bar{K}_i, \quad T(\bar{K}_i) = K_i, \tag{4.8}$$

$$T(J) = J, \quad T(D_i) = \bar{D}_i, \quad T(\bar{D}_i) = D_i, \tag{4.9}$$

$$T(E_i) = -E_i\bar{K}_i, \quad T(F_i) = -K_iF_i. \tag{4.10}$$

Then we extend them to the whole $wU_q^\tau(\mathcal{G})$. Thus we obtain the following lemma.

Lemma IV.1: *$wU_q^\tau(\mathcal{G})$ is a bialgebra with comultiplication Δ and counit ε.*

Proof: It can be shown by direct calculation that the following relations hold:

$$\Delta(K_i)\Delta(\bar{K}_j) = \Delta(\bar{K}_j)\Delta(K_i), \quad \Delta(D_i)\Delta(\bar{D}_j) = \Delta(\bar{D}_j)\Delta(D_i),$$

$$\Delta(J^{m-1}) = \Delta(K_i)\Delta(\bar{K}_i) = \Delta(D_i)\Delta(\bar{D}_i),$$

$$\Delta(JK_i) = \Delta(K_i), \quad \Delta(J\bar{K}_i) = \Delta(\bar{K}_i),$$

$$\Delta(JD_i) = \Delta(D_i), \quad \Delta(J\bar{D}_i) = \Delta(\bar{D}_i),$$

$$\varepsilon(K_i\bar{K}_j) = \varepsilon(K_i)\varepsilon(\bar{K}_j), \quad \varepsilon(D_i\bar{D}_j) = \varepsilon(D_i)\varepsilon(\bar{D}_j),$$

$$\varepsilon(JK_i) = \varepsilon(K_i), \quad \varepsilon(J\bar{K}_j) = \varepsilon(\bar{K}_j),$$

$$\varepsilon(J\bar{D}_i) = \varepsilon(D_i), \quad \varepsilon(J\bar{D}_j) = \varepsilon(\bar{D}_j),$$

$$\varepsilon(K_j)\varepsilon(E_i) = q_i^{a_{ij}}\varepsilon(E_i)\varepsilon(K_j), \quad \varepsilon(F_i)\varepsilon(\bar{K}_j) = q_i^{a_{ij}}\varepsilon(F_j)\varepsilon(\bar{K}_j),$$

$$\varepsilon(E_i)\varepsilon(F_j) - \varepsilon(F_j)\varepsilon(E_i) = \delta_{ij}\frac{\varepsilon(K_i) - \varepsilon(\bar{K}_i)}{q_i - q_i^{-1}}.$$

If E_i is type one, then

$$\Delta(K_j)\Delta(E_i) = (K_j \otimes K_j)((1 \otimes E_i + E_i \otimes K_i) = K_j \otimes K_jE_i + K_jE_i \otimes K_jK_i = q_i^{a_{ij}}\Delta(E_i)\Delta(K_j).$$

If E_i is type zero, then

$$\begin{aligned}\Delta(K_j)\Delta(E_i)\Delta(\bar{K}_j) &= (K_j \otimes K_j)(J^{m-1} \otimes E_i + E_i \otimes K_i)(\bar{K}_j \otimes \bar{K}_j) = K_j\bar{K}_j \otimes K_jE_i\bar{K}_j + K_jE_i\bar{K}_j \otimes K_jK_i\bar{K}_j \\ &= q_i^{a_{ij}}\Delta(E_i).\end{aligned}$$

Next we prove that

$$\Delta(E_i)\Delta(F_j) - \Delta(F_j)\Delta(E_i) = \delta_{ij}\frac{\Delta(K_i) - \Delta(\bar{K}_i)}{q_i - q_i^{-1}}. \tag{4.11}$$

For any integers $0 \le r, s \le m$, if $J^{m-r}F_j = F_jJ^{m-r}$ and $J^{m-s}E_i = E_iJ^{m-s}$, then

$$(J^{m-r} \otimes E_i + E_i \otimes K_i)(F_j \otimes J^{m-s} + \bar{K}_j \otimes F_j)$$

$$-(F_j \otimes J^{m-s} + \bar{K}_j \otimes F_j)(J^{m-r} \otimes E_i + E_i \otimes K_i)$$

$$= J^{m-r}F_j \otimes E_iJ^{m-s} + \bar{K}_j \otimes E_iF_j + E_iF_j \otimes K_i + E_i\bar{K}_j \otimes K_iF_j$$

$$
\begin{aligned}
&- F_j J^{m-r} \otimes J^{m-s} E_i - F_j E_i \otimes K_i - \bar{K}_j \otimes F_j E_i - \bar{K}_j E_i \otimes F_j K_i \\
&= \bar{K}_j \otimes (E_i F_j - F_j E_i) + (E_i F_j - F_j E_i) \otimes K_i \\
&= \delta_{ij} \frac{\Delta(K_i) - \Delta(\bar{K}_i)}{q_i - q_i^{-1}}.
\end{aligned}
$$

Thus (4.11) holds for all i, j.

Finally, we prove that Δ satisfies the quantum Serre relations, i.e., the relations from (3.16) to (3.18).

From $a_{ij}=0$, we obtain $E_iE_j=E_jE_i$, and $K_iE_j=q_j^{a_{ji}}E_jK_i=E_jK_i$. Hence

$$
\begin{aligned}
&(J^{m-r} \otimes E_i + E_i \otimes K_i)(J^{m-s} \otimes E_j + E_j \otimes K_j) \\
&- (J^{m-s} \otimes E_j + E_j \otimes K_j)(J^{m-r} \otimes E_i + E_i \otimes K_i) \\
&= J^{2m-r-s} \otimes E_iE_j + J^{m-r}E_j \otimes E_iK_j + E_iJ^{m-s} \otimes K_iE_j + E_iE_j \otimes K_iK_j \\
&- J^{2m-r-s} \otimes E_jE_i - J^{m-s}E_i \otimes E_jK_i - E_jJ^{m-r} \otimes K_jE_i - E_jE_i \otimes K_jK_i \\
&= J^{m-r}E_j \otimes E_iK_j + E_iJ^{m-s} \otimes K_iE_j - J^{m-s}E_i \otimes E_jK_i - E_jJ^{m-r} \otimes K_jE_i = 0,
\end{aligned}
$$

for any $1 \le r, s \le m$. So

$$\Delta(E_i)\Delta(E_j) - \Delta(E_j)\Delta(E_i) = 0.$$

Similarly, we can prove

$$\Delta(F_i)\Delta(F_j) - \Delta(F_j)\Delta(F_i) = 0.$$

By now we have proven that Δ satisfies the relation (3.18).

To prove that Δ satisfies the relation (3.16), we must consider the following cases:

(1) Both E_i and E_j are type one.
(2) Only one of the E_i and E_j is type one.
(3) Both E_i and E_j are type zero.

For the case (3). Since E_i is type zero,

$$\Delta(E_i) = J^m \otimes E_i + E_i \otimes K_i = (J^m \otimes 1)(1 \otimes E_i + E_i \otimes K_i) = (1 \otimes E_i + E_i \otimes K_i)(J^m \otimes 1).$$

Let us introduce notations. $(1 \otimes E_i + E_i \otimes K_i)$ is denoted by $\Delta'(E_i)$. Set $s = 1 - a_{ij}$. Then

$$
\begin{aligned}
&\sum_{r=0}^{s} (-1)^r \begin{bmatrix} s \\ r \end{bmatrix} \Delta(E_i)^{s-r} \Delta(E_j) \Delta(E_i)^r \\
&= (J^m \otimes 1)^{(s+1)} \sum_{r=0}^{s} (-1)^r \begin{bmatrix} s \\ r \end{bmatrix} \Delta'(E_i)^{s-r} \Delta'(E_j) \Delta'(E_i)^r = 0,
\end{aligned}
$$

by the discussion in Ref. 8, pp. 67 and 68. Hence Δ satisfies (3.16) in this case. For the other cases, the argument is more or less the same as case (3).

Similarly, we can prove that Δ satisfies (3.17). Therefore Δ and ε can be extended to an algebra morphism from $wU_q^\tau(\mathcal{G})$ to $wU_q^\tau(\mathcal{G}) \otimes wU_q^\tau(\mathcal{G})$, and from $wU_q^\tau(\mathcal{G})$ to $\mathbf{K}$, respectively.

It is easy to prove that

$$(\Delta \otimes 1)\Delta(X) = (1 \otimes \Delta)\Delta(X), \tag{4.12}$$

$$(\varepsilon \otimes 1)\Delta(X) = (1 \otimes \varepsilon)\Delta(X) \tag{4.13}$$

for any $X = E_i, F_i, K_i\bar{K}_i, D_i\bar{D}_i, J$. Since Δ, ε are algebra morphisms, (4.12) and (4.13) hold for any $X \in wU_q^\tau(\mathcal{G})$. By now we have completed the proof.

Next we prove that the map T, defined by (4.8), (4.9), (4.10), is a weak antipode of the subalgebra of a subbialgebra of the bialgebra $wU_q^\tau(\mathcal{G})$ generated by $E_i, F_i, K_i, \bar{K}_i, D_i, \bar{D}_i, J^m$. First we prove that T can be extended to an antiautomorphism of $wU_q^\tau(\mathcal{G})$. It is easy to prove the following relations are true:

$$T(K_i)T(\bar{K}_j) = T(\bar{K}_j)T(K_i), \quad T(D_i)T(\bar{D}_j) = T(\bar{D}_j)T(D_i),$$

$$T(D_i)T(\bar{K}_j) = T(\bar{K}_j)T(D_i), \quad T(K_i)T(\bar{D}_j) = T(\bar{D}_j)T(K_i),$$

$$T(\bar{D}_i)T(\bar{K}_j) = T(\bar{K}_j)T(\bar{D}_i), \quad T(J)T(\bar{K}_i) = T(\bar{K}_i), \quad T(J)T(K_i) = T(K_i)$$

$$T(J)T(\bar{D}_i) = T(\bar{D}_i), \quad T(J)T(D_i) = T(D_i),$$

$$T(E_i)T(E_j) = T(E_j)T(E_i), \quad T(F_i)T(F_j) = T(F_j)T(F_i) \quad \text{if } a_{ij} = 0.$$

If E_i is type one, then

$$T(E_i)T(K_j) = -E_i\bar{K}_i\bar{K}_j = -q_i^{a_{ij}}\bar{K}_jE_i\bar{K}_i = q_i^{a_{ij}}T(K_j)T(E_i).$$

If E_i is type zero, then

$$T(\bar{K}_j)T(E_i)T(K_j) = -K_jE_iK_i\bar{K}_j = -q_i^{a_{ij}}E_iK_i = q_i^{a_{ij}}T(E_i).$$

Similarly, we can prove

$$T(F_i)T(K_j) = q_i^{-a_{ij}}T(K_j)T(F_i)$$

if F_i is type one, and

$$T(\bar{K}_j)T(F_i)T(K_j) = q_i^{-a_{ij}}T(F_i)$$

if F_i is type zero. Moreover,

$$T(F_j)T(E_i) - T(E_i)T(F_j) = K_j(F_jE_i)\bar{K}_i - E_i\bar{K}_iK_jF_j = q_j^{-a_{jj}}q_i^{a_{ij}}F_jE_iK_j\bar{K}_i - q_j^{-a_{jj}}q_j^{a_{ji}}F_jE_iK_j\bar{K}_i$$
$$= \delta_{ij}\frac{\bar{K}_i - K_i}{q_i - q_i^{-1}}K_j\bar{K}_i = \delta_{ij}\frac{T(K_i) - T(\bar{K}_i)}{q_i - q_i^{-1}}.$$

Similarly to Ref. 15, p. 8, we can prove the following antirelations to the quantum Serre relations hold:

$$\sum_{r=0}^{s}(-1)^r\begin{bmatrix} s \\ r \end{bmatrix}T(E_i)^rT(E_j)T(E_i)^{s-r} = 0 \quad \text{if } a_{ii} = 2,$$

$$\sum_{r=0}^{s}(-1)^r\begin{bmatrix}s\\r\end{bmatrix}T(F_i)^rT(F_j)T(F_i)^{s-r}=0 \quad \text{if } a_{ii}=2,$$

where $s=1-a_{ij}$.

From the above discussion, we get that T is an antiautomorphism of $wU_q^\tau(\mathcal{G})$. Let U^τ be a subalgebra of $wU_q^\tau(\mathcal{G})$ generated by $K_i,\bar{K}_i,D_i,\bar{D}_i,E_i,F_i,J^m$.

Theorem IV.2: *T is a weak antipode of $U^\tau(\mathcal{G})$ and $U^\tau(\mathcal{G})$ is a weak Hopf algebra.*

Proof: It is easy to verify that the following relations hold:

$$(\mathrm{id} * T * \mathrm{id})(X) = X,$$

$$(T * \mathrm{id} * T)(X) = T(X),$$

for $X=K_i,\bar{K}_i,D_i,\bar{D}_i,E_i,F_i,J^m$.

Since

$$\mathrm{id} * T * \mathrm{id} = (\mu\otimes 1)\mu(\mathrm{id}\otimes T\otimes \mathrm{id})(\Delta\otimes 1)\Delta,$$

$\mathrm{id}*T*\mathrm{id}$ is a linear automorphism of $wU_q^\tau(\mathcal{G})$. To prove $(\mathrm{id}*T*\mathrm{id})(X)=X$, for any $X\in U^\tau(\mathcal{G})$, we only need to prove that

$$(\mathrm{id} * T * \mathrm{id})(xy) = xy \tag{4.14}$$

provided that $(\mathrm{id}*T*\mathrm{id})(x)=x$, and y is one of the generators $K_i,\bar{K}_i,D_i,\bar{D}_i,E_i,F_i,J^m$. Suppose $(\Delta\otimes 1)\Delta(x)=\Sigma x_{(1)}\otimes x_{(2)}\otimes x_{(3)}$. Then $(\Delta\otimes 1)\Delta(xJ^m)=\Sigma x_{(1)}J^m\otimes x_{(2)}J^m\otimes x_{(3)}J^m$ and hence

$$\mathrm{id} * T * \mathrm{id}(xJ^m) = \sum x_{(1)}T(x_{(2)})x_{(3)}J^m = xJ^m.$$

Similarly

$$\begin{aligned}\mathrm{id} * T * \mathrm{id}(xE_i) &= \sum x_{(1)}J^mT(x_{(2)}J^m)x_{(3)}E_i + \sum x_{(1)}J^mT(x_{(2)}E_i)x_{(3)}K_i + \sum x_{(1)}E_iT(x_{(2)}K_i)x_{(3)}K_i\\ &= \sum x_{(1)}T(x_{(2)})x_{(3)}E_i - \sum x_{(1)}E_i\bar{K}_iT(x_{(2)})x_{(3)}K_i + \sum x_{(1)}E_i\bar{K}_iT(x_{(2)})x_{(3)}K_i = xE_i,\end{aligned}$$

if E_i is type zero. We can prove (4.14) is true for other generators of $U^\tau(\mathcal{G})$. So $\mathrm{id}*T*\mathrm{id}(x)=x$ for any $x\in U^\tau(\mathcal{G})$ by induction.

Similarly, we can prove $T*\mathrm{id}*T(x)=T(x)$ for any $x\in U^\tau(\mathcal{G})$. So T is a weak antipode of $U^\tau(\mathcal{G})$, and $U^\tau(\mathcal{G})$ is a weak Hopf algebra.

Corollary IV.1: *$wU_q^\tau(\mathcal{G})$ is a weak Hopf algebra if and only if $m=2$. Moreover, if $m=2$, then $wU_q^\tau(\mathcal{G})$ is a noncommutative and noncocommutative weak Hopf algebra with the weak antipode T, but not a Hopf algebra.*

Proof: Since $m=2$, $J^{m-1}=J^m=J$. Thus $U^\tau(\mathcal{G})=wU_q^\tau(\mathcal{G})$. So it is a weak Hopf algebra. Suppose it is a Hopf algebra with antipode S. Then $J^m=S(J^m)J^m=1$. On the other hand, since $J^m=J^{m-1}$, $J^{m-1}(J-1)=0$ implies that $J=1$. This is impossible. So $wU_q^\tau(\mathcal{G})$ is not a Hopf algebra.

If $wU_q^\tau(\mathcal{G})$ is a weak Hopf algebra, then $\mathrm{id}*T*\mathrm{id}(J)=J^3=J$. From this and $J^m=J^{m-1}$, we can obtain $J^2=J$. Thus $m=2$ by our assumption.

Corollary IV.2: *$U^\tau(\mathcal{G})$ is a noncommutative and noncocommutative weak Hopf algebra with the weak antipode T, but not a Hopf algebra. Moreover, $wU_q^\tau(\mathcal{G})J^m=U^\tau(\mathcal{G})J^m$ is isomorphic to $U_q'(\mathcal{G})$ as Hopf algebras.*

Proof: It follows from Corollary III.1, Theorem IV.2.

Let H be a coalgebra. The set of grouplike elements of H is denoted by $G(H)$ in the next proposition.

Proposition IV.1: $G(U^\tau(\mathcal{G}))=G(U^\tau(\mathcal{G})J^m)\cup\{1\}$.

Proof: If $g\in G(U^\tau(\mathcal{G}))$, then $g=gJ^m+g(1-J^m)$. Let $g_1=gJ^m, g_2=g(1-J^m)$. Then $g\otimes g=\Delta(g)$

$=g_1\otimes g_1+g_1\otimes g_2+g_2\otimes g_1+g_2\otimes g_2$. Since $\Delta(g_1)=g_1\otimes g_1$ is a grouplike element, $\Delta(g_2)=g_1\otimes g_2+g_2\otimes g_1+g_2\otimes g_2$. So

$$(1\otimes\Delta)\Delta(g_2)=g_1\otimes g_1\otimes g_2+g_1\otimes g_2\otimes g_1+g_1\otimes g_2\otimes g_2+g_2\otimes g_1\otimes g_1+g_2\otimes g_1\otimes g_2+g_2\otimes g_2\otimes g_1+g_2\otimes g_2\otimes g_2.$$

Then

$$(T*\mathrm{id}*T)(g_2)=T(g_2)g_2T(g_2)=T(g_2),$$

$$(\mathrm{id}*T*\mathrm{id})(g_2)=g_2T(g_2)g_2=g_2. \tag{4.15}$$

Because $U^\tau(\mathcal{G})(1-J^m)$ is generated by $E_i(1-J^m),F_j(1-J^m),1-J^m$ and $T(E_i(1-J^m))=T(F_j(1-J^m))=0$, $T(g_2)=k(1-J^m)$ for some $k\in\mathbf{K}$. From (4.15), we obtain the following:

$$k^2g_2=k^2(1-J^m)^2g_2=k(1-J^m),$$

$$kg_2^2(1-J^m)=kg_2^2=g_2. \tag{4.16}$$

If $k=0$, then $g=g_1\in G(U^\tau(\mathcal{G}))$. If $k\neq 0$, then $g_2=(1/k)(1-J^m)$. Thus

$$\frac{1}{k}(1\otimes 1-J^m\otimes J^m)=\frac{1}{k}g_1\otimes(1-J^m)+\frac{1}{k}(1-J^m)\otimes g_1+\frac{1}{k^2}(1-J^m)\otimes(1-J^m).$$

Multiplying by $k(J^m\otimes 1)$ on both sides of the above equation, we get

$$J^m\otimes 1-J^m\otimes J^m=g_1\otimes(1-J^m).$$

Similarly, we have

$$1\otimes J^m-J^m\otimes J^m=(1-J^m)\otimes g_1.$$

Then

$$1\otimes 1-J^m\otimes J^m=J^m\otimes 1+1\otimes J^m-2J^m\otimes J^m+\frac{1}{k}(1-J^m)\otimes(1-J^m).$$

Hence

$$(1-J^m)\otimes(1-J^m)=\frac{1}{k}(1-J^m)\otimes(1-J^m).$$

Consequently, $k=1$. Notice that the set of grouplike elements of $U^\tau(\mathcal{G})J^m$ is a monoid generated by $K_i,\bar{K}_i,D_i,\bar{D}_i$ and J^m, and the elements from this monoid are linearly independent over $\mathbf{K}$. So we get $g_1=J^m$ from $1\otimes J^m-J^m\otimes J^m=(1-J^m)\otimes J^m=(1-J^m)\otimes g_1$. Hence $g=1$.

Proposition IV.2: Suppose φ is an automorphism of the bialgebra $wU_q^\tau(\mathcal{G})$. Then $\varphi(J)=J$ and the restriction of φ on w (respectively, $\bar{w}$) is an isomorphism of w (respectively, $\bar{w}$).

Proof: From $J^m=J^{m-1}$, we obtain $\varphi(J)^m=\varphi(J)^{m-1}$. Thus $\varphi(J)^mJ^m=\varphi(J)^{m-1}J^m$ is a grouplike element in $wU_q^\tau(\mathcal{G})\subseteq U_q(\mathcal{G})$. Hence $\varphi(J)J^m=J^m$. Suppose $\varphi(J)=J^m+x$, where $x=\varphi(J)(1-J^m)\in\bar{w}$. Since $T\varphi(J)=\varphi(T(J))=\varphi(J)$, $Tx=x$. Consequently, $x=\sum_{i=0}^{m-2}k_i(J^i-J^m)$. Then

$$\Delta(\varphi(J))=(J^m+x)\otimes(J^m+x)=J^m\otimes J^m+\sum_{i=0}^{m-2}k_i(J^i\otimes J^i)-\sum_{i=0}^{m-2}k_i(J^m\otimes J^m)$$

$$=J^m\otimes J^m+\sum_{i=0}^{m-2}k_i(J^i\otimes J^m)+\sum_{i=0}^{m-2}k_i(J^m\otimes J^i)+\sum_{i=0}^{m-2}k_iJ^i\otimes\sum_{j=0}^{m-2}k_jJ^j. \tag{4.17}$$

From (4.17), we obtain that $\varphi(J)=J^m+(J^r-J^m)=J^r$ for some $0\leq r\leq m-2$. If $r\geq 2$, then $\varphi(J^{m-2}-J^{m-1})=J^{r(m-2)}-J^{r(m-1)}=0$. This is a contradiction to the fact that φ is an isomorphism. So $r=1$.

Since $\varphi(J)=J$, $\varphi(w)=\varphi(wJ^m)=\varphi(w)J^m=w$. Consequently, the restriction of φ on w is a Hopf algebra isomorphism of w. Similarly, we can prove the restriction of φ on $\bar{w}$ is an algebra isomorphism of $\bar{w}$.

Similarly to Ref. 15, we can prove the following:

Corollary IV.3: Suppose $\mathcal{G}$ is a semisimple Lie algebra. Then the automorphism group of the bialgebra of $wU_q^\tau(\mathcal{G})$ is the semidirect product of N and H, where H is the group of diagram automorphism, and N is the group of diagonal automorphism and it is a normal subgroup of the automorphism group of $wU_q^\tau(\mathcal{G})$.

Remark: If $\mathcal{G}$ is a semisimple Lie algebra, then $U^\tau(\mathcal{G})$ is isomorphic to the weak quantum algebra defined by Yang in Ref 15.

V. THE REPRESENTATIONS OF $wU_q^\tau(\mathcal{G})$

In this section, we try to determine the irreducible representations of $wU_q^\tau(\mathcal{G})$. Suppose V is a simple module over the bialgebra $wU_q^\tau(\mathcal{G})$. Then $V=J^mV\oplus(1-J^m)V$. Since both J^mV and $(1-J^m)V$ are modules over $wU_q^\tau(\mathcal{G})$, either $V=J^mV$ or $V=(1-J^m)V$.

If $V=J^mV$, then $Jv=v$ for any $v\in V$. Suppose $v\in V$ satisfying $K_iv=\lambda_iv$, then $\lambda_i\neq 0$. In this case, $K_i\bar{K}_iK_iv=\lambda_i^2\bar{K}_iv=\lambda_iv$. So $\bar{K}_iv=(1/\lambda_i)v$.

If $V=(1-J^m)V$, then $J^mv=0$ $v\in V$, $K_iv=K_iJ^mv=0$ and $\bar{K}_iv=\bar{K}_iJ^mv=0$ for any $v\in V$.

By now we have completed the proof of the following proposition.

Proposition V.1: Let V be simple $wU_q^\tau(\mathcal{G})$-module. Then either $Jv=v$ for all $v\in V$, or $J^mv=0$ for any $v\in V$. Suppose there exists an $i\in I$ such that $K_iv=\lambda_iv$ for some nonzero vector v. Then $\bar{K}_iv=\bar{\lambda}_iv$ for λ_i, where

$$\bar{\lambda}_i=\begin{cases}\lambda_i^{-1} & \text{if } \lambda_i\neq 0,\\ 0 & \text{if } \lambda_i=0.\end{cases}$$

Moreover, $\lambda_i\neq 0$ *if and only if* $Jv=v$.

Suppose $V=J^mV$. Then V can be viewed as a module over $wU_q^\tau(\mathcal{G})/(1-J)$ by Proposition V.1. Notice that $wU_q^\tau(\mathcal{G})/(1-J)$ is isomorphic to $U_q'(\mathcal{G})$ by Corollary III.1(2). In this case, V has been studied by Kang.[10] For example, the limit of highest weight simple module is a highest weight simple module over the generalized Kac-Moody algebra $\mathcal{G}$ with the same weight λ. Then this simple module is unique determined by its formally Borcherd-Kac-Weyl character formula (see Sec. I).

Suppose $V=(1-J^m)V$. Then $J^mV=0$ and $K_iV=\bar{K}_iV=0$ for any $i\in I$ by Proposition V.1. Similarly, we can prove that $D_iV=\bar{D}_iV=0$ for all $i\in I$. Hence $E_iF_jV=F_jE_iV$ for all $i,j\in I$. Moreover, V can be viewed as a module over $\bar{w}$. Recall that $\bar{w}$ is generated by $J^r-J^m(0\leq r\leq m-2)$, $E_i(1-J^m)$, and $F_j(1-J^m)$, where E_i,F_j are type one. Hence $E_i(1-J^m)F_j(1-J^m)V=F_j(1-J^m)E_i(1-J^m)V$ for all $i,j\in I$. In the following, we try to determine the structure of V in some special case.

Proposition V.2: For any $wU_q^\tau(\mathcal{G})$ module V, if $V=(1-J^m)V$, then $JV=0$.

Proof: Consider the subalgebra B of $\bar{w}$ generated by J^i-J^m for $0\leq r\leq m-2$. Since $(J^i-J^m)\times(J^j-J^m)=J^r-J^m$, where $r\equiv i+j \bmod(m-2)$, B is isomorphic to $\mathbf{K}[\mathbf{Z}_{m-2}]$. Because char $\mathbf{K}=0$, B is a semisimple algebra. Hence V is a semisimple module over B. Let S be a simple B-module contained in V and v be a nonzero element of S. Then there exists r such that $J^rv=0$ and $J^{r-1}v\neq 0$. So S is equal to a vector space spanned by $v,Jv,\ldots,J^{r-1}v$ over $\mathbf{K}$. Since $\mathbf{K}J^{r-1}v$ is a nonzero module of S, $S=\mathbf{K}J^{r-1}v$ and $JS=0$. Consequently $JV=0$.

The above proposition also characterizes the simple $\bar{w}$ module when all E_i,F_j are type zero. In the general case, let $X_i=E_i(1-J^m),Y_i=F_i(1-J^m)$. Then every simple module V over $\bar{w}$ is a module over the algebra generated by $\{X_i,Y_j|$ for $i\in I_1,J\in I_2\}$, where $I_1=\{i\in I|E_i$ is type one$\}$, $I_2=\{j\in I|F_j$ is type one$\}$. The generators X_i,Y_j satisfy the following relation:

$$X_iY_j=Y_jX_i,$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i X_i^{1-a_{ij}-r} X_j X_i^r = 0 \quad \text{if} \quad a_{ii} = 2,\ i \neq j,$$

$$\sum_{r=0}^{1-a_{ij}} (-1)^r \begin{bmatrix} 1-a_{ij} \\ r \end{bmatrix}_i Y_i^{1-a_{ij}-r} Y_j Y_i^r = 0 \quad \text{if } a_{ii} = 2,\ i \neq j,$$

$$X_i X_j - X_j X_i = Y_i Y_j - Y_j Y_i = 0, \quad \text{if } a_{ij} = 0.$$

This simple module V satisfies $JV=0$. From the above discussion, we obtain the following result.

Corollary V.1: If $a_{ij}=0$ for any $i \in (I_1 \cup I_2) \cap I^+$, then every simple module over $\bar{w}$ is isomorphic to $\bar{w}/M$, where M is a maximal ideal of $\bar{w}$.

By Corollary V.1, the only simple over $\bar{w}$ is $\mathbf{K}[x]/(p(x))$ if $|I_1 \cup I_2| = 1$, where $p(x)$ is an irreducible polynomial in $\mathbf{K}[x]$. Suppose $\mathbf{K}$ is an algebraically closed field. If $a_{ij}=0$ for any $i \in (I_1 \cup I_2) \cap I^+$, and $|I_1 \cup I_2| = n$, then the simple module V over $\bar{w}$ is isomorphic to $\mathbf{K}[X_i, Y_j | i \in I_1, J_j \in I_2]/(\{X_i - a_i, Y_j - b_j | i \in I_1, j \in I_2\})$ for some $((a_i)_{i \in I_1}, (b_j)_{j \in I_2}) \in \mathbf{K}^n$. (See Refs. 2, 6, and 10.)

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Analytic calculation of energies and wave functions of the quartic and pure quartic oscillators

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Ground state energies and wave functions of quartic and pure quartic oscillators are calculated by first casting the Schrödinger equation into a nonlinear Riccati form and then solving that nonlinear equation analytically in the first iteration of the quasilinearization method (QLM). In the QLM the nonlinear differential equation is solved by approximating the nonlinear terms by a sequence of linear expressions. The QLM is iterative but not perturbative and gives stable solutions to nonlinear problems without depending on the existence of a smallness parameter. Our explicit analytic results are then compared with exact numerical and also with WKB solutions and it is found that our ground state wave functions, using a range of small to large coupling constants, yield a precision of between 0.1 and 1 percent and are more accurate than WKB solutions by two to three orders of magnitude. In addition, our QLM wave functions are devoid of unphysical turning point singularities and thus allow one to make analytical estimates of how variation of the oscillator parameters affects physical systems that can be described by the quartic and pure quartic oscillators. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A basic nonrelativistic quantum mechanics problem is to solve the Schrödinger equation with a potential $V(x)$ that governs motion of a given physical system. The first two terms of the power expansion of a one-dimensional, even potential around an equilibrium position are

$$\frac{g^2x^2}{2}+\lambda x^4, \tag{1}$$

where x is the deviation from an equilibrium position. The above potential describes the dynamics of a great many systems that deviate from the idealized picture of pure harmonic motion. When both g and λ are nonzero, we call this potential a "quartic" or quartic anharmonic oscillator; whereas, when $g=0$ with nonzero λ it is dubbed a "pure quartic" oscillator. In addition to providing an excellent description of spectroscopic molecular vibrational data (see Ref. 1 and references therein), the quartic anharmonic oscillator (1) also serves as a basic tool for checking various approximate and perturbative methods in quantum mechanics. Such an application appears in several recent field theoretical model studies.[2–14]

It is well known[15,16] that for the quartic anharmonic oscillator the perturbation expansion diverges even for small couplings and becomes completely useless for strong coupling. In view of this divergence of perturbation theory, we have adopted[17,18] the general and very powerful quasilinearization method (QLM),[19–23] which although iterative is not a perturbative method. In QLM the pth order solution of a nonlinear differential equation with N variables is obtained by first approximating the nonlinear aspect by a sequence of linear terms and then iteratively solving the

associated linear equations. This iterative process converges to a solution without requiring the existence of a smallness parameter. Properties and applications of the quasilinearization method were reviewed recently in Ref. 24.

To apply the quasilinearization method, one first casts the Schrödinger equation into the nonlinear Riccati form and then solves that nonlinear equation by the QLM iterations. In a series of presentations,[17,18,25–27] we have shown that for a range of anharmonic and other physical potentials (with both weak and strong couplings), the QLM iterates display very fast quadratic convergence. Indeed, after just a few QLM iterations, energies and wave functions are obtained with extremely high accuracy, reaching 20 significant figures for the energy of the sixth iterate even in the case of very large coupling constants.

Although numerical solutions using either the QLM or direct numerical solution of the differential equations can be very accurate, it is important to also provide analytic solutions. Analytic solutions allow one to gauge the role of different potential parameters, and explore the influence of such variations on the properties of the quantum system under study. However, in contrast to the harmonic oscillator, the anharmonic oscillator cannot be solved analytically, and thus one usually has to resort to approximations.

The goal of this paper is to obtain and test approximate analytic solutions for the quartic and pure quartic oscillators using the explicit analytic equation for the first QLM iterate. We will show that both energies and wave functions will be represented by closed analytic expressions with the accuracy of the wave functions being between 0.1 and 1 percent for both small and large coupling constants. Various accurate analytic expressions for the *energies* have already appeared in the literature based on using convergent, strong coupling expansions generated by rearrangement of the usual divergent weak coupling expansion[28] or by some variational requirement.[29] Variational anharmonic oscillator wave functions have also been obtained.[30,31] However, accurate nonvariational analytic expressions representing *wave functions* have not hitherto been known. That result is provided here.

II. MAIN FORMULAS

The usual WKB substitution $y(x)=\psi'(x)/\psi(x)$ converts the Schrödinger equation to the nonlinear Riccati form

$$\frac{dy(x)}{dx}+[k^2(x)+y^2(x)]=0. \tag{2}$$

Here $k^2(x)=2[E-V(x)]$, where we use $m=1$, $\hbar=1$ units. The quasilinearization[21–24] of Eq. (2) leads to the recurrence differential equation

$$\frac{dy_p(x)}{dx}+(2y_{p-1}(x))y_p(x)=y_{p-1}^2(x)-k^2(x), \tag{3}$$

where $y_p(x)$ is the subsequent pth QLM iterate, which have the same boundary condition as $y(x)$ of Eq. (2). Note that Eq. (3) is a linear equation of the form $dy_p(x)/dx+f(x)y_p(x)=q(x)$, with $f(x)=2y_{p-1}(x)$ and $q(x)=y_{p-1}^2(x)-k^2(x)$.

Let us use Eq. (3) to estimate the ground state wave function and energy of the quartic oscillator. Excited states will be considered elsewhere.

The ground state wave function is nodeless and for an even potential (1) should therefore be an even function. Its logarithmic derivative is necessarily odd, and therefore the boundary condition obviously is $y(0)=0$ and correspondingly $y_p(0)=0$.

TABLE I. Exact, WKB and linear guess QLM ground state energies.

λ	E_{exact}	E_{WKB}	ΔE_{WKB}	$E^{(1)}$ $y_0=-gx$	$\Delta E^{(1)}$ (%)	$E^{(2)};y_0=-gx$ second iteration	$\Delta E^{(2)}$ (%)
0	1/2	1/2	0	1/2	0	1/2	0
0.1	0.559 15	0.533 28	4.6	0.575	2.8	0.559 83	0.1
0.3	0.637 99	0.584 66	8.3	0.725	13.6	0.648 69	1.7
0.5	0.696 18	0.625 38	10.2	0.875	25.7	0.727 28	4.4
1	0.803 77	0.704 20	12.4	1.25	55.5	0.914 23	13.7
2	0.951 57	0.816 67	14.2	2	110	1.2829	34.8
10	1.504 97	1.254 12	16.7	8		4.2628	183
100	3.131 38	2.571 81	17.9	75.5			
1000	6.694 22	5.479 55	18.1	750.5			

A. Linear initial condition

The zero iterate should be based on physical considerations. Let us consider first an initial guess $y_0(x)=-gx$. This linear initial condition completely neglects the anharmonic term containing λ compared with the harmonic term and thus this initial guess is expected to be reasonable only for relatively small values of λ.

Solution of the first order linear differential Eq. (3) with the above zero boundary condition at the origin can always be found analytically. For $p=1$ the solution is

$$y_1(x) = 2e^{gx^2}\int_0^x e^{-gs^2}(g^2s^2 + \lambda s^4 - E_1)\mathrm{d}s. \tag{4}$$

Integration by parts, yields an expression for $y_1(x)$ that involves the error function $\mathrm{Erf}(x) \equiv (2/\sqrt{\pi})\int_0^x e^{-t^2}\,\mathrm{d}t$,

$$y_1(x) = \frac{1}{4g^{5/2}}\{-2x\sqrt{g}(2g^3 + 3\lambda + 2g\lambda x^2) + e^{gx^2}\sqrt{\pi}\,\mathrm{Erf}(x\sqrt{g})[2g^2(g-2E_1)+3\lambda]\}. \tag{5}$$

The asymptotic expression $\mathrm{Erf}(x) \simeq [1-(e^{-x^2}/\sqrt{\pi}x)]$ for $|x|\to\infty$, indicates that $y_1(x)$ will be exponentially large for very large x unless the second term in Eq. (5) is made zero. Correspondingly, invoking the condition $2g^2(g-2E_1)+3\lambda=0$ yields the energy and the logarithmic derivative in the first iteration: $E_1=a/2$ and $y_1(x)=-ax-bx^3$, where $a=g+3\lambda/2g^2$; $b=\lambda/g$. This leads to the first QLM iteration wave function $\psi(x)=C\exp\left[-\frac{gx^2}{2}-\lambda\left(\frac{3x^2}{4g^2}+\frac{x^4}{4g}\right)\right]$. This QLM result for the energy coincides with the perturbative result, as well as with the result obtained by Friedberg, Lee, and Zhao[32] who used their recently developed iterative method for solving the Schrödinger equation.

The wave functions we obtained above obviously have incorrect asymptotic behavior. Also, the energies E_1 calculated for different λ, as displayed in Table I ($g=1$), are far from being precise. Therefore, to improve the result one is tempted to go to the second QLM iteration, using $y_1(x)$ as an input.

Equation (3) then yields the second iterate

$$y_2(x) = e^{ax^2+(b/2)x^4}\int_0^x \{[a^2+g^2+2(ab+\lambda)t^2+b^2t^4]t^2 - 2E_2\}e^{-at^2-(b/2)t^4}\,\mathrm{d}t. \tag{6}$$

Since $y_2(x)e^{-[ax^2+(b/2)x^4]}$ approaches a constant when x goes to infinity, $y_2(x)$ and consequently the corresponding wave function grows exponentially at infinity, unless the integral in Eq. (6) equals zero when its upper limit equals infinity. This condition yields the following expression for the energy E_2 in the second iteration:

$$E_2 = \frac{\int_0^\infty [a^2 + g^2 + 2(ab + \lambda)t^2 + b^2 t^4] t^2 e^{-at^2 - (b/2)t^4}\, dt}{2\int_0^\infty e^{-at^2 - (b/2)t^4}\, dt}. \tag{7}$$

Values of E_2, for this initial linear form, are compared to exact values E calculated numerically in Table I (g=1). It is seen that E_2 approximates the exact E reasonably well only for small λ, as we anticipated would result from using an initial linear condition. We now turn to another choice for the initial form.

B. Quadratic initial condition

To ensure a proper wave function asymptotically, one needs an adequate initial guess. Our second condition is based on the asymptotic behavior of the quartic potential. The zeroth iterate of the logarithmic derivative, $y_0(x)$, is for example, now obtained by taking an initial iterate of quadratic form $y_0(x) = -\sqrt{2\lambda}x^2$. This choice for the first iterate automatically satisfies the asymptotic and $x=0$ boundary conditions, but is based on neglecting the harmonic term compare with the anharmonic one.

With this quadratic initial condition, the solution $y_1(x)$ of Eq. (3) satisfying $y_1(0)=0$ is then given by

$$y_1(x) = e^{(2/3)\sqrt{2\lambda}x^3} \int_0^x e^{-(2/3)\sqrt{2\lambda}s^3} [4\lambda s^4 + g^2 s^2 - 2E_1] ds. \tag{8}$$

Note, that $y_1(x)e^{-(2/3)\sqrt{2\lambda}x^3}$ approaches a constant, C_∞, as x goes to infinity, and consequently $y_1(x)$ grows exponentially at infinity unless the above limit C_∞, is set to zero. The latter condition yields another expression for the energy based on the quadratic initial condition:

$$E_1 = \frac{\int_0^\infty e^{-(2/3)\sqrt{2\lambda}s^3} \left[2\lambda s^4 + \frac{g^2 s^2}{2} \right] ds}{\int_0^\infty e^{-(2/3)\sqrt{2\lambda}s^3}\, ds}. \tag{9}$$

The integrals in Eq. (9) can be expressed in terms of the Euler gamma function $\Gamma(x)$.[33] The final expression for the first iterate energy based on a quadratic initial condition reads

$$E_1 = \frac{\lambda^{1/6}}{3^{1/3}\Gamma\left(\frac{1}{3}\right)} \left[\frac{3g^2}{4\sqrt{\lambda}} + \lambda^{1/6} 3^{2/3} \Gamma\left(\frac{2}{3}\right) \right]. \tag{10}$$

This result should be proper for large λ when the second term of the quartic potential $(g^2x^2/2) + \lambda x^4$ dominates over the harmonic term and thus a term containing g in initial guess $y_0(x)$ could be neglected. The above expression for the energy is not expected to be suitable for small λ. Indeed, one can see that for the $\lambda \to 0$, the energy in Eq. (10) diverges.

C. Linear plus quadratic initial condition

To obtain a result accommodating arbitrary values of both g and λ, one must start from an initial choice $y_0(x)$ that takes into account the asymptotic behavior of both the harmonic and the anharmonic parts of the potential. Let us choose, for example, $y_0(x) = -gx - \sqrt{2\lambda}x^2$ which is a linear combination of our two previous initial guesses. This yields

$$y_1(x) = 2e^{gx^2 + (2\sqrt{2\lambda}/3)x^3} \int_0^x [t^2(g^2 + g\sqrt{2\lambda}t + 2\lambda t^2) - E_1] e^{-gt^2 - (2\sqrt{2\lambda}/3)t^3}\, dt, \tag{11}$$

with

$$E_1 = \frac{\int_0^\infty t^2(g^2 + g\sqrt{2\lambda}t + 2\lambda t^2)e^{-gt^2-(2\sqrt{2\lambda}/3)t^3}\,dt}{\int_0^\infty e^{-gt^2-(2\sqrt{2\lambda}/3)t^3}\,dt}. \tag{12}$$

Another possible initial guess, which also accounts for the asymptotic behavior of both harmonic and anharmonic parts of the potential is $y_0(x) = -\sqrt{g^2x^2 + 2\lambda x^4}$. This guess is easy to justify by assuming that $y'(x)$ in Eq. (2) at large x becomes negligible compared with $y^2(x)$ and therefore $y^2(x)$ can be set equal to $k^2(x) = g^2x^2 + 2\lambda x^4 - 2E \approx g^2x^2 + 2\lambda x^4$ since in this expression we can neglect E for sufficiently large x.

The solution of Eq. (3) using the initial condition $y_0(x) = -\sqrt{g^2x^2 + 2\lambda x^4}$, is only slightly more complicated than in when one uses the initial guess $y_0(x) = -gx - \sqrt{2\lambda}x^2$, and is given by the expression

$$y_1(x) = 2e^{(g^2 + 2\lambda x^2)^{3/2}/3\lambda} \int_0^x e^{-(g^2 + 2\lambda t^2)^{3/2}/3\lambda}[g^2t^2 + 2\lambda t^4 - E_1]dt. \tag{13}$$

The condition to avoid exponential behavior of the logarithmic derivative at infinity now yields the following expression for the ground state energy:

$$E_1 = \frac{\int_0^\infty t^2(g^2 + 2\lambda t^2)e^{-(g^2 + 2\lambda t^2)^{3/2}/3\lambda}\,dt}{\int_0^\infty e^{-(g^2 + 2\lambda t^2)^{3/2}/3\lambda}\,dt}. \tag{14}$$

For a pure quartic oscillator with $g=0$, both Eqs. (11) and (13) reduce to

$$y_1(x) = 2e^{2\sqrt{2\lambda}x^3/3} \int_0^x e^{-2\sqrt{2\lambda}t^3/3}[2\lambda t^4 - E_1]dt \tag{15}$$

with E_1 given by

$$E_1 = \frac{2\lambda\int_0^\infty e^{-(2\sqrt{2\lambda}/3)s^3}s^4\,ds}{\int_0^\infty e^{-(2\sqrt{2\lambda}/3)s^3}\,ds} = \lambda^{1/3}3^{1/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{1}{3}\right)} \simeq 0.729\,011\lambda^{1/3}. \tag{16}$$

In view of Eq. (16) $y_1(x)$ of Eq. (15) can be expressed in terms of a special function, namely, the exponential integral[33] $\mathbf{EI}_\mu(z) = \int_1^\infty e^{-zt}t^{-\mu}\,dt$,

$$y_1(x) = -\sqrt{2\lambda}x^2 + \frac{2}{3}e^{(2\sqrt{2\lambda}/3)x^3}\left\{-\sqrt{2\lambda}x^2\mathbf{EI}_{1/3}\left(\frac{2\sqrt{2\lambda}}{3}x^3\right) + \lambda^{1/3}3^{1/3}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{1}{3}\right)}x\mathbf{EI}_{2/3}\left(\frac{2\sqrt{2\lambda}}{3}x^3\right)\right\}. \tag{17}$$

This expression for the log derivative yields a first iterate QLM wave function, based on the initial condition $y_0(x) = -\sqrt{g^2x^2 + 2\lambda x^4}$, that is the main result of our paper.

The exact dependence of E_1 on λ for the pure quartic oscillator has the same form, but with a factor of 0.667 986 259 before $\lambda^{1/3}$,[28] so that the accuracy of the QLM prediction for the energy is about 9.1 percent. The WKB energy can be easily estimated and gives $E_{\mathrm{WKB}} \simeq 0.546\,267\lambda^{1/3}$, an accuracy of 18.2 percent.

III. RESULTS AND DISCUSSION

The ground state energies for the quartic oscillator in the first QLM approximation for different initial guesses and for values of $g=1$ and λ between zero and 1000 and their comparison with the numerically calculated exact and WKB values are given in Tables I and II ($g=1$). One can see that the values computed using explicit equations (12) and (14) for the QLM energy are significantly more accurate than the WKB values or than values obtained in the first and second QLM iterations with the initial guess $y_0(x) = -gx$. They have a precision of 0.4 to 9 percent for values of λ varying between 0.1 and 1000, respectively.

TABLE II. Ground state QLM energies for the quadratic and linear plus quadratic guesses.

λ	$E^{(3)}$ $y_0=-x^2\sqrt{2\lambda}$	$\Delta E^{(3)}$ (%)	$E^{(4)};y_0=$ $-gx-x^2\sqrt{2\lambda}$	$\Delta E^{(4)}$ (%)	$E^{(5)};y_0=$ $-\sqrt{g^2x^2+2\lambda x^4}$	$\Delta E^{(5)}$ (%)
0			1/2	0	1/2	0
0.1	0.756 58	35	0.569 40	1.8	0.561 49	0.4
0.3	0.777 99	21.9	0.648 38	1.6	0.647 05	1.4
0.5	0.823 19	18.2	0.705 52	1.3	0.711 26	2.2
1	0.923 13	14.8	0.811 38	0.95	0.830 90	3.4
2	1.072 57	12.7	0.958 53	0.73	0.995 77	4.6
10	1.6607	10.3	1.5259	1.4	1.610 85	7.0
100	3.4256	9.4	3.2564	4.0	3.400 39	8.5
1000	7.3095	9.2	7.1171	6.3	7.297 44	9.0

However, the main results of our work, are not the expressions for the energy. As mentioned in the introduction, such expressions were already given in different forms by others. Our major results are the analytic expressions for the wave functions given by Eqs. (11) and (13), which are based on using the first QLM iterate with the initial conditions $y_0=-gx-\sqrt{2\lambda}x^2$ and $y_0=-\sqrt{g^2x^2+2\lambda x^4}$, respectively.

The graphs of the wave functions for the quartic oscillator with $g=1$ and for different λ together with the correspondent exact and WKB wave functions, are presented in Figs. 1, 3 and 5, while Figs. 2, 4, and 6 display the logarithm of the absolute value of the differences between the WKB or QLM wave functions and the exact solution for λ being equal to 0.1, 1, and 10, respectively. The same graphs for the pure quartic oscillator ($g=0$) are presented in Figs. 7, 9, 11 and in Figs. 8, 10, 12, respectively. One can see that in Figs. 1–12 the differences between the exact and QLM solutions are two to three orders of magnitude smaller than the differences between the exact and the WKB solutions and that the QLM wave functions expressed analytically by Eqs. (11), (13) have an accuracy of between 0.1 and 1 percent. The order of magnitude better accuracy of the wave function compared to the poorer accuracy of the energies is explained by the fact that the general theorems[19–24] for the QLM iterates show that the solutions converge quadratically with each iteration, while no such convergence theorem has been proven for the energy iterates. Note, that the dips in the figures are artifacts of the logarithmic scale, since the logarithm of the absolute

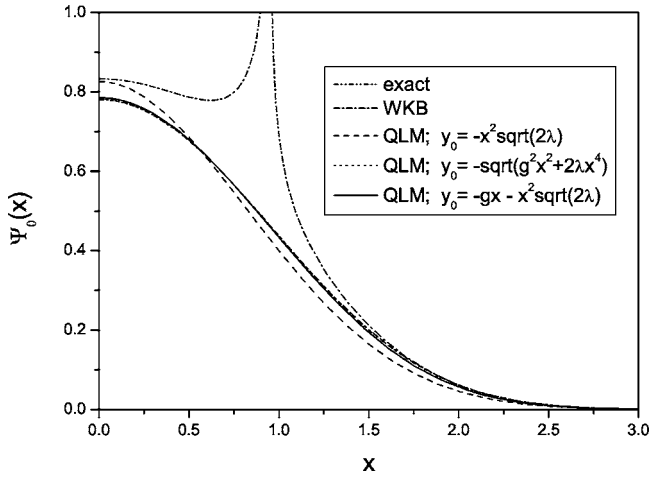

FIG. 1. Comparison of the WKB, QLM and exact wave functions for the ground state of the quartic oscillator for $g=1$, $\lambda=0.1$.

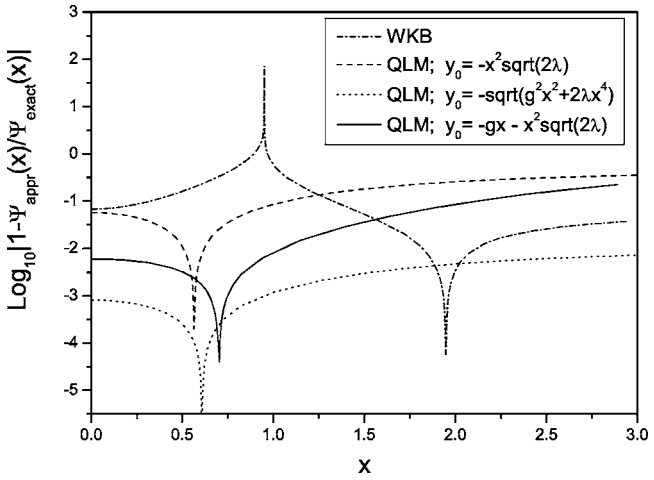

FIG. 2. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the quartic oscillator for $g=1$, $\lambda=0.1$.

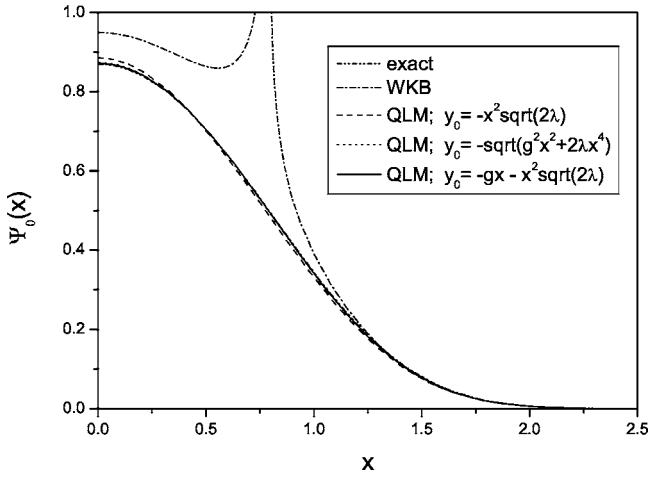

FIG. 3. Comparison of the WKB, QLM and exact wave functions for the ground state of the quartic oscillator for $g=1$, $\lambda=1$.

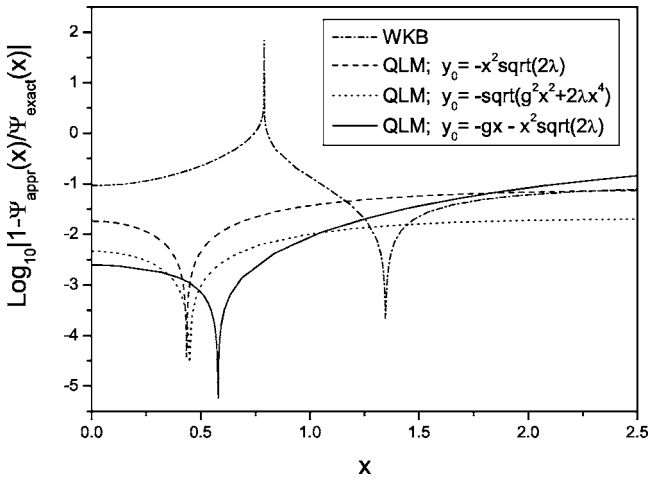

FIG. 4. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the quartic oscillator for $g=1$, $\lambda=1$.

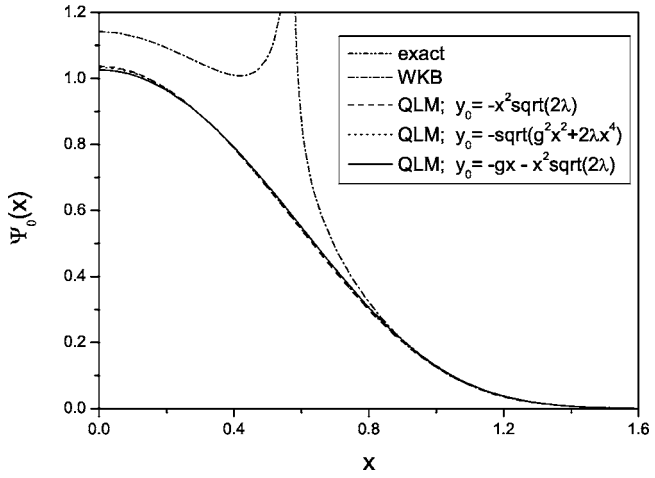

FIG. 5. Comparison of the WKB, QLM and exact wave functions for the ground state of the quartic oscillator for $g=1$, $\lambda=10$.

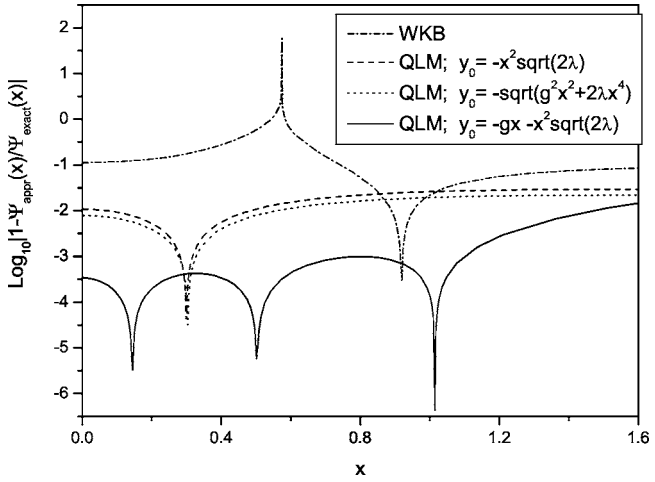

FIG. 6. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the quartic oscillator for $g=1$, $\lambda=10$.

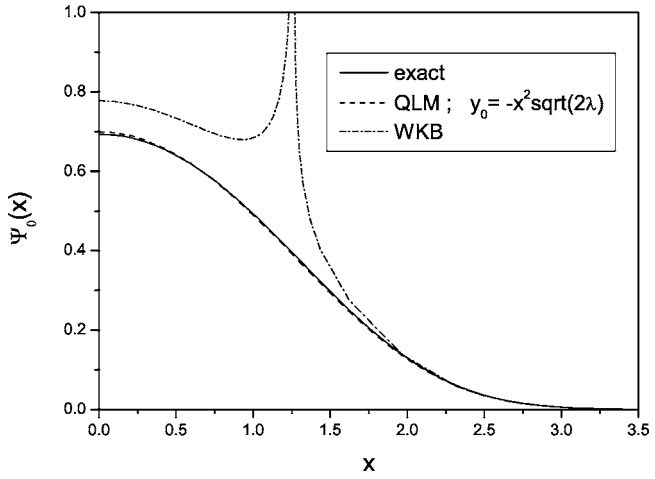

FIG. 7. Comparison of the WKB, QLM and exact wave functions for the ground state of the pure quartic oscillator for $g=0$, $\lambda=0.1$.

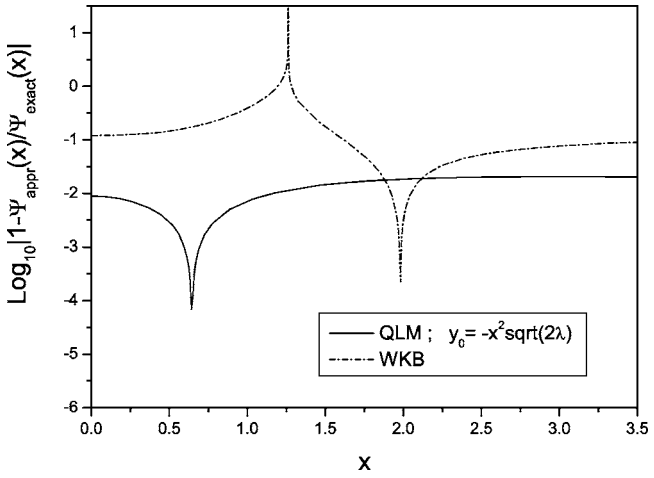

FIG. 8. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the pure quartic oscillator for $g=0$, $\lambda=0.1$.

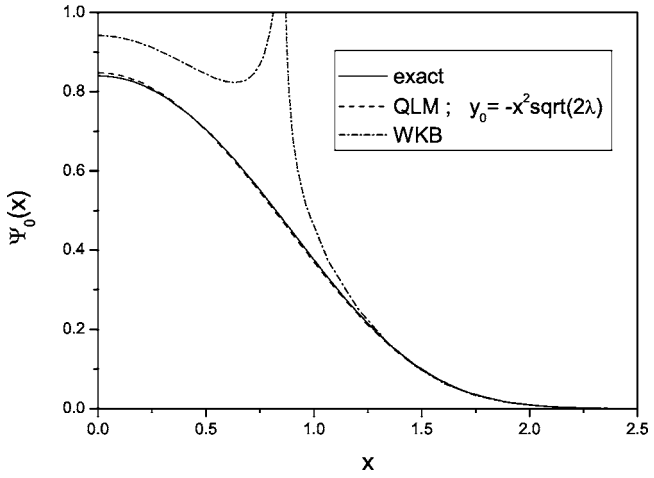

FIG. 9. Comparison of the WKB, QLM and exact wave functions for the ground state of the pure quartic oscillator for $g=0$, $\lambda=1$.

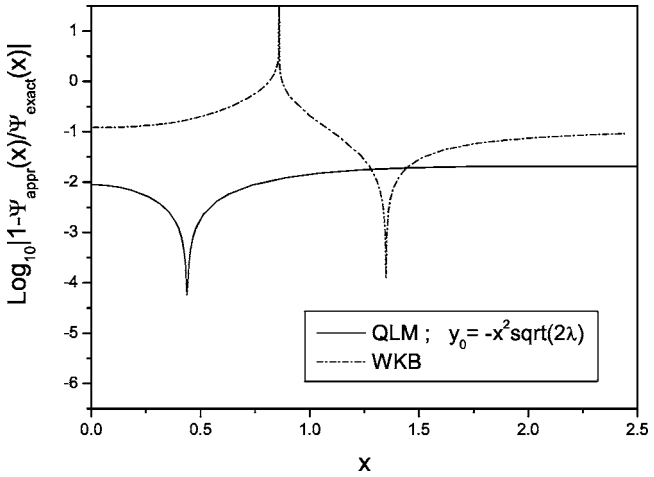

FIG. 10. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the pure quartic oscillator for $g=0$, $\lambda=1$.

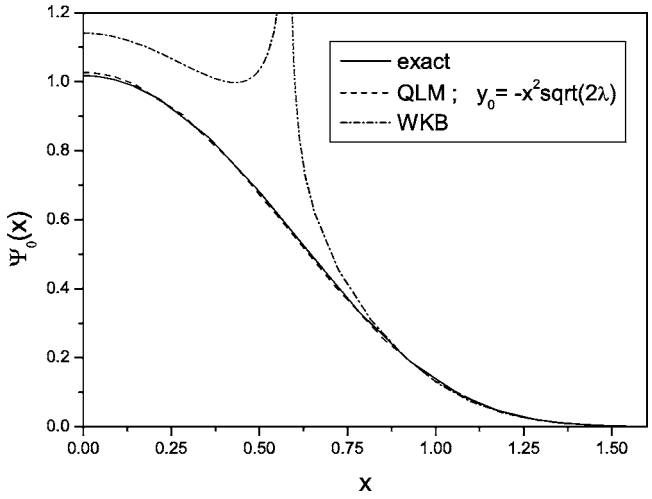

FIG. 11. Comparison of the WKB, QLM and exact wave functions for the ground state of the pure quartic oscillator for $g=0$, $\lambda=10$.

value of the difference of two solutions goes to $-\infty$ at points where the difference changes sign. The overall accuracy of the solution can therefore be inferred only at x values not too close to the dips.

IV. CONCLUSION

We calculated analytically the ground state energy and wave function of the quartic and pure quartic oscillators by casting the Schrödinger equation into the nonlinear Riccati form, which is then solved in the first iteration of the quasilinearization method (QLM), which approaches the solution of the nonlinear differential equation by approximating nonlinear terms with a sequence of linear ones and does not rely on the existence of a smallness parameter. Comparison of our results with exact numerical solutions and the WKB solutions shows that the explicit analytic expressions we obtain (12) and (14) for the ground state energy have a precision of only a few percent while the analytically expressed wave functions (11) and (13) have an accuracy of between 0.1 and 1 percent and are more accurate by two to three orders of magnitude than those

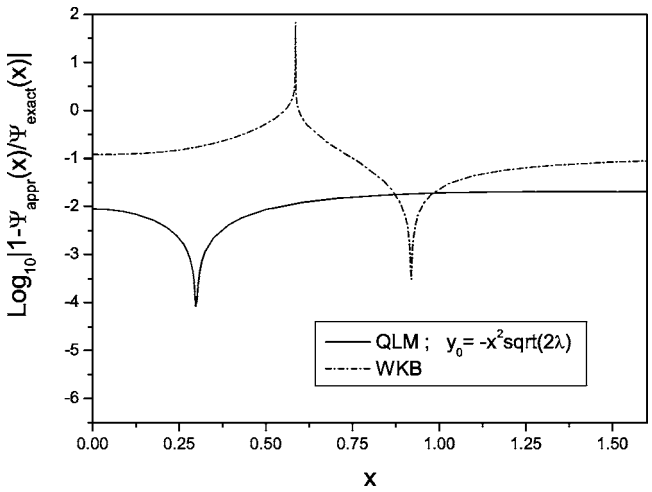

FIG. 12. Logarithm of the differences of the WKB and QLM wave functions with exact wave function for the ground state of the pure quartic oscillator for $g=0$, $\lambda=10$.

given in the WKB approximation. The QLM wave function in addition possess no unphysical turning point singularities which allows one to use these wave functions to make analytical estimates of the effects of variation of the oscillator parameters on the properties of systems described by quartic and pure quartic oscillators.

The next QLM iterations could be evaluated numerically.[17,18,25–27] These further QLM iterates for the different anharmonic and other physical potentials with both strong and weak couplings also display very fast quadratic convergence so that the accuracy of energies and wave functions obtained after a few iterations is extremely high, reaching 20 significant figures for the energy of the sixth iterate even in the case of very large coupling constants.

Extension of this approach to excited states and to other potentials is underway.

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The Bargmann transform and regularization of the 2, 3, 5-dimensional Kepler problem

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We introduce a Bargmann transform for the space $L^2(S^n)$ of square integrable functions on the $n=2,3,5$ dimensional unit sphere S^n inmersed in $\mathbb{R}^{n+1}$. This is done on base of the Hopf fibration for the spheres $S^k \mapsto S^d$ with $(k,d)=(1,1),(3,2),(7,4)$ and a suitable canonical transformation relating two different ways to regularize the $n=2,3,5$ dimensional Kepler problem (with fixed negative energy) involving the null complex quadric Q^n inmersed in $\mathbb{C}^{n+1}$. We prove the unitarity of the Bargmann transform onto a suitable space of analytical functions. We give reproducing kernels for these spaces of analytical functions which, for the cases $n=3,5$, are defined as the kernel of quantizations of restrictions for regularizations of the classical Kepler problem. We give an inversion formula for our Bargmann transform. We also give a set of coherent states for $L^2(S^n)$, $n=2,3,5$ and their semiclassical asymptotics $(\hbar \to 0)$. Our Bargmann transform is actually a coherent states transform. Additionally, we use the moment map technique in order to construct a map with values in Q^n that gives the base to define our canonical transformation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209556]

I. INTRODUCTION

In 1961, Bargmann[4] introduced the so called Bargmann transform as a unitary operator from $L^2(\mathbb{R}^n)$ onto a Hilbert space $\mathcal{B}_n$ of analytical functions which are square integrable with respect to a Gaussian measure on $\mathbb{C}^n$. This alternative representation of quantum mechanics through operators acting on spaces of analytical functions has shown to be very useful in semiclassical analysis (see Refs. 29, 23, and 26).

The main goal of this paper is to introduce and study a Bargmann transform when the configuration space is the unit n-sphere S^n (the set of all vectors of unit length in $\mathbb{R}^{n+1}$) in the special cases $n=2,3,5$. The reason to study this particular sphere is motivated by the physical fact that it is in this special dimension that the duality between the Kepler problem and harmonic oscillators holds: for fixed negative energy, the $n=2,3,5$ dimensional Kepler problem is transformed into $m=2,4,8$ harmonic oscillators with the same frequency, respectively. Here we are regarding the $n=2,3,5$ dimensional Kepler problem as the Hamiltonian system with phase space $T^*(\mathbb{R}^n-\{0\})$, symplectic form $d\mathbf{p}\wedge d\mathbf{x}$ (where $\mathbf{p}$ and $\mathbf{x}$ denote the momentum and position vectors of the particle, respectively) and Hamiltonian

$$H=\frac{|\mathbf{p}|^2}{2}-\frac{1}{|\mathbf{x}|}. \tag{1}$$

The duality between the Kepler problem and harmonic oscillators in the dimensions specified above has its roots, from the mathematical viewpoint, in the Hopf fibration between the spheres $S^k \mapsto S^d$ with $(k,d)=(1,1),(3,2),(7,4)$. By extending the Hopf fibrations $S^1 \mapsto S^1$ and $S^3 \mapsto S^2$ one

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obtains maps of the type used by Levi-Civita[25] and Kustaanheimo-Stiefel[19] to regularize the Kepler problem. Namely we can find new position variables where, for fixed negative energy E and after a time reparametrization, $[d/\mathrm{d}s=|\mathbf{x}|(d/\mathrm{d}t)$ with t and s the old and new time parameters, respectively] the equation of motion for the $n=2,3$ Kepler problem (1) appears as the equation of motion for $m=2,4$ harmonic oscillators, respectively, without any singularity. The oscillators have the same frequency which depends on the energy E. The same can be done for the case of the Hopf fibration $S^7\mapsto S^4$ and the $n=5$ dimensional Kepler problem obtaining $m=8$ harmonic oscillators. For this last case, the first reference we are aware of is Ref. 7. We will refer to these maps as Kustaanheimo-Stiefel-type maps and denote them by $\mathcal{H}_{(n,m)}$. Here and in the sequel, whenever we write (n,m) we mean the three possible cases $(n,m)=(2,2),(3,4),(5,8)$ unless a particular value of (n,m) is specified.

There is another way to regularize the Kepler problem which works for any dimension $n\geqslant 1$. This regularization was introduce by Moser.[22] The main idea here lies on the physical fact that the orbits of the Kepler problem for fixed negative energy and nonzero angular momentum when projected into the momentum space are circles. By a standard stereographic projection, those circles correspond to great circles on the n-sphere S^n not passing through the north pole. Moser extended this stereographic projection to a canonical transformation $\mathcal{M}_n$ from the phase space of the Kepler problem onto the cotangent bundle of S^n with the north pole removed in order that the one form $\mathbf{x}\cdot\mathrm{d}\mathbf{p}$ transforms into the one form $\xi\cdot\mathrm{d}\mathbf{w}$ with $\mathbf{w}\in S^n$ and ξ in the cotangent space of S^n at $\mathbf{w}$. Thus Moser shows, after the same time reparametrization $d/\mathrm{d}s=|\mathbf{x}|(d/\mathrm{d}t)$ considered above for the other type of regularization and for fixed negative energy $E=-1/2$, the equivalence between the Hamiltonian flow of the n-dimensional Kepler problem with the geodesic flow of the punctured n-sphere. The regularization of the Kepler problem is achieved when we add the north pole. This allows us to include the collision states (negative energy orbits with zero angular momentum) corresponding to geodesics passing through the north pole of S^n.

The relationship between the two different ways to regularize the Kepler problem mentioned above plays a crucial role in our definition of the Bargmann transform for the spaces $L^2(S^2)$, $L^2(S^3)$, and $L^2(S^5)$. We are denoting by $L^2(S^n)$, $n\geqslant 1$, the Hilbert space of square-integrable functions with respect to the normalized surface measure $\mathrm{d}S$ on the n-sphere S^n and endowed with the inner product

$$\langle\boldsymbol{\Psi}_1,\boldsymbol{\Psi}_2,\rangle_{L^2(S^n)}=\int_{\mathbf{w}\in S^n}\boldsymbol{\Psi}_1(\mathbf{w})\overline{\boldsymbol{\Psi}_2}(\mathbf{w})\mathrm{d}S(\mathbf{w}). \tag{2}$$

Kummer[18] showed how to relate the two regularizations in the case $n=3$ by using the moment map for the group SU(2,2). In Ref. 28 it is shown how a canonical transformation (denoted here by $\mathcal{C}_{(3,4)}$) between a suitable reduction of the space $\mathbb{C}^4-\{0\}$ and the cotangent bundle of the 3-sphere with the zero section removed $T^*S^3-\{0\}$ also links the two regularizations for $n=3$. This canonical transformation was actually obtained from the integral kernel of a Bargmann transform that we introduced in Ref. 27 for $L^2(S^3)$ by following the symmetries of the negative energy hydrogen atom problem given by the rotations group SO(4). The canonical transformation we are mentioning is actually the composition of two maps involving the null complex quadric $Q^3-\{0\}$ of four complex variables (for $n\geqslant 1$, a vector belongs to the null complex quadric Q^n if and only if the addition of the squares of the components of the vector is zero). Namely, the composition of a map $\rho_{(3,4)}$ from $\mathbb{C}^4-\{0\}$ onto the null complex quadric $Q^3-\{0\}$ and a map σ_3 from $Q^3-\{0\}$ onto $T^*S^3-\{0\}$. It is also shown that the function given by the inner product $(\rho_{(3,4)}(\mathbf{z})\cdot\mathbf{w})$ is a generating function of the canonical transformation $\mathcal{C}_{(3,4)}$ with $\mathbf{z}\in\mathbb{C}^4$ and $\mathbf{w}\in S^3$.

In order to build the Bargmann transform for $L^2(S^5)$, the key point for our approach is to consider a canonical transformation $\mathcal{C}_{(5,8)}$ from a reduced phase space of eight complex variables $\mathbb{C}^8-\{0\}$ onto the cotangent bundle of the 5-sphere $T^*S^5-\{0\}$ (with the zero section removed) and involving the null complex quadric Q^5. We take this canonical transformation as the composition of two maps $\rho_{(5,8)}$ and σ_5 involving the null complex quadric $Q^5-\{0\}$. Again, the function

$(\rho_{(5,8)}(\mathbf{z})\cdot\mathbf{w})$ (with $\mathbf{z}\in\mathbb{C}^8$ and $\mathbf{w}\in S^5$) is a generating function of the canonical transformation $\mathcal{C}_{(5,8)}$. More precisely, for the three cases we are considering we define a canonical transformation $\mathcal{C}_{(n,m)}$ as

$$\begin{array}{ccc} & \overset{\mathcal{C}_{(n,m)}}{\longrightarrow} & \\ \mathbb{C}^m-\{0\} & & T^*S^n-\{0\} \\ \Big\downarrow{\scriptstyle \rho_{(n,m)}} & \nearrow{\scriptstyle \sigma_n} & \\ Q^n-\{0\} & & \end{array}$$

and the following diagram holds:

$$\begin{array}{ccc} K_m & \xrightarrow{\mathcal{C}_{(n,m)}} & T^*S_0^n-\{0\} \\ \Big\downarrow{\scriptstyle \mathcal{T}_m^{-1}} & & \Big\downarrow{\scriptstyle \mathcal{M}_n^{-1}} \\ J_m & \xrightarrow{\mathcal{H}_{(n,m)}} & T^*(\mathbb{R}^n-\{0\}) \end{array}$$

where S_0^n denotes the n-sphere S^n with the north pole removed, $\mathcal{T}_m: T^*\mathbb{R}^m\mapsto\mathbb{C}_m$ is a complexification of $T^*\mathbb{R}^m$. For the cases $m=4,8$, the manifolds K_m and J_m are obtained from the inverse image of the zero value of moment maps $\mathcal{K}_m$ and $\mathcal{J}_m$ acting on $\mathbb{C}^m$ and $T^*(\mathbb{R}^m-\{0\})$ and related to the action of the groups S^1 and SU(2) for $m=2$ and $m=8$, respectively. In both cases we remove the inverse image of the cotangent space of S^n at the north pole under the map $\mathcal{C}_{(n,m)}$ and the origin from $\mathbb{C}^m$. In the case $m=2$, $J_2=T^*(\mathbb{R}^2-\{0\})$ and $K_2=\mathbb{C}^2-\{0\}$ (see Sec. V for details).

We remark that even though the map $\mathcal{C}_{(n,m)}$ is not injective, we still call it a canonical transformation as people in the physics literature do. In order to get an injective map, we need to consider the quotient (symplectic reduction in the cases $m=4,8$) of J_m and K_m by the action of the groups $\mathbb{Z}_2$, S^1 or SU(2) corresponding to the cases $m=2,4,8$, respectively.

For $m=4,8$, the map $\rho_{(n,m)}$ appearing in the first diagram is obtained by considering the moment map $\mathcal{I}$ of the action on $\mathbb{C}^m$ of the group F of matrices that leave invariant the moment map $\mathcal{K}_m$. Thus the map $\rho_{(n,m)}$ is invariant under the action of the groups S^1 and SU(2) for $m=4,8$, respectively. The map $\rho_{(2,2)}$ is obtained by considering a basis of the vector space of homogeneous polynomials in two complex variables of degree two (and then invariant under the action of the group $\mathbb{Z}_2$). The map σ_n appearing in the same diagram identifies $Q^n-\{0\}$ and $T^*S^n-\{0\}$ in a natural way (see Secs. V and VI for details).

Thus based on our experience on Bargmann transforms for $L^2(S^2)$ and $L^2(S^3)$ (see Refs. 27 and 28), we define a Bargmann transform for $L^2(S^n)$, $n=2,3,5$, as a suitable power series in the generating function $(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})$ of the canonical transformation $\mathcal{C}_{(n,m)}$. We choose the coefficients of the power series in such a way that our transform is an isometry and then we prove that our Bargmann transform is unitary. The Bargmann transform that we define in the present paper for the cases $n=2,3$ is actually the same as the one introduced in Ref. 27 (with the exception of nonrelevant changes in the definition of the map $\rho_{(n,m)}$). However the Bargmann transform in Ref. 27 is introduced as the linear extension of an assignment between corresponding orthonormal basis of its domain and range. This idea is hard to implement in the case $n=5$ since an explicit description of a basis of the range is quite complicated. So we present in this paper the three cases $n=2,3,5$ all together in the same framework. The nontrivial part for our present approach is now to prove that our Bargmann transform is well defined and unitary. We show those facts by following the method of Bargmann in his original paper.[4]

We show in detail that our Bargmann transform for $L^2(S^2)$, $L^2(S^3)$, and $L^2(S^5)$ is a unitary

operator and give a reproducing kernel for the corresponding range. This reproducing kernel is obtained by averaging the usual reproducing kernel for the Bargmann spaces over the groups $\mathbb{Z}_2$, S^1 and SU(2) appearing in the corresponding Hopf fibrations. The range of our Bargmann transforms for $L^2(S^3)$ and $L^2(S^5)$ is actually given by the kernel of suitable operators which are quantizations of restrictions appearing in the Kepler problem. We also give an inversion formula for our Bargmann transform.

We finally show that our Bargmann transform is actually a coherent states transform, i.e., when applied to a function $\Psi \in L^2(S^n)$ we obtain the inner product of Ψ with a coherent state labeled by a point in the cotangent bundle of S^n. Our coherent states for $L^2(S^n)$ have the property that their Bargmann transform give us the reproducing kernel of the range of the Bargmann transform. Moreover, our set of coherent states gives a resolution of the identity for $L^2(S^n)$, i.e., any element of $L^2(S^n)$ can be written as the limit (in the norm sense) of integrals involving projections of $\boldsymbol{\Psi}$ onto each coherent state with respect to a measure on the null complex quadric Q^n (the cotangent bundle $T^*S^n - \{0\}$ with the zero section removed can be identified with $Q^n - \{0\}$ through the map σ_n). Our coherent states are infinite linear combinations of states that concentrate on great circles of S^n in the large quantum numbers regime. In order to study the semiclassical behavior of our coherent states, we introduce the Planck's constant $\hbar$ in the definition of our Bargmann transforms. Based on the work of Thomas and Wassell,[26] we provide an asymptotic expression for our coherent states showing that they concentrate at points of the sphere S^n for $\hbar$ small.

We remark that the $n=5$ dimensional Kepler problem has been studied before in the classical mechanics setting (see Refs. 7 and 14) and its quantization (see Refs. 7 and 20). The work of Mladenov[20] about geometric quantization of the $n=5$ dimensional Kepler problem is quite relevant and connected with our work. The definition of the range of our Bargmann transform for $L^2(S^5)$ is actually described in Mladenov's paper. However, our Bargmann transform is not mentioned there.

We finally mention that other Bargmann-type transforms for spheres have been introduced in the literature before. We comment on this point in the discussion section of this paper.

The paper is organized as follows. Section II is devoted to describe the Hopf fibration and to obtain its explicit equations. We also show the action of the groups $\mathbb{Z}_2$, S^1 and SU(2) in the corresponding fibers. In Sec. III we extend the Hopf fibration and obtain a regularization of the $n=2,3,5$ dimensional Kepler problem of the type obtained by Levi-Civita and Kustaanheimo-Stiefel for the $n=2$ and $n=3$ dimensional problems, respectively. The restrictions appearing in the cases $n=3,5$ are introduced via a moment map. In Sec. III we describe the Moser regularization of the $n \geqslant 1$ dimensional Kepler problem. Despite the fact that the content of Secs. II–IV is known in the literature, we include these sections in the present paper in order to introduce notation and to try to make it as self-contained as possible. In Sec. V and following Kummer[18] in his work about the $n=3$ dimensional Kepler problem, we obtain the maps $\rho_{(n,m)}$ appearing in the diagram above through the moment map of the group of linear transformations which leave the moment map $\mathcal{K}_m$ invariant. Then in Sec. VI we present our canonical transformation $\mathcal{C}_{(n,m)}$ linking the two regularizations mentioned above and explain the second diagram above.

In Sec. VII we introduce and study our Bargmann transform for $L^2(S^n)$, $n=2,3,5$ and prove its unitarity. We also show the reproducing kernel for the range of our Bargmann transform and show that our Bargmann transform is actually a coherent states transform providing $L^2(S^n)$ with a set of coherent states. Then we introduce the parameter $\hbar$ into the definition of both the Bargmann transform and coherent states and show the localization property of our coherent states for $\hbar$ small. We conclude in Sec. VIII with a discussion concerning the possible use of our coherent states for $L^2(S^n)$ to define coherent states for the hydrogen atom problem (with negative energy) in dimensions $n=2,3,5$. We also include Appendix A about representations in $\mathbb{C}^m$, $m=2,4,8$, of the covering groups of rotations in $\mathrm{SO}(n+1)$, $n=2,3,5$ and Appendix B about an explicit expression for orthogonal projectors on eigenspaces of the Laplacian on S^n. Appendix A is used in Appendix B and to show the invariance of certain measures on the null complex quadric Q^n with respect to

rotations in SO($n+1$). However, we think that Appendix A is interesting on its own because it provides a nontrivial and specific representation of the covering group of SO(6) on the space $\mathbb{C}^8$.

II. THE HOPF FIBRATION

In this section we define the Hopf fibration $S^1 \mapsto S^1$, $S^3 \mapsto S^2$, $S^7 \mapsto S^4$ by following Ref. 24. We give explicit equations of these maps. We also describe the action of the corresponding group on the fibers.

A. Stereographic projection

In this section we give the equations of the stereographic projection $\mathbf{T}_k$ from $\mathbb{R}^k \cup \{\infty\}$, $k \geqslant 1$, onto the k-sphere,

$$S^k = \left\{ (x_1, \ldots, x_{k+1}) \in \mathbb{R}^{k+1} \Big| \sum_{i=1}^{k+1} x_i^2 = 1 \right\}. \tag{3}$$

Let us consider a point $\mathbf{x}=(x_1,\ldots,x_k) \in \mathbb{R}^k$ and the straight line joining this point with the north pole of S^k. This line intersects S^k at the point $\mathbf{w}=(w_1,\ldots,w_{k+1})$ given by

$$w_i = \frac{2x_i}{|\mathbf{x}|^2+1}, \quad i=1,\ldots,k,$$

$$w_{k+1} = \frac{|\mathbf{x}|^2-1}{|\mathbf{x}|^2+1}, \quad |\mathbf{x}|^2 = \sum_{i=1}^{k} x_i^2.$$

Then we can assign the north pole of S^k to ∞ if we need to.

B. The Hopf fibration $S^1 \mapsto S^1$, $S^3 \mapsto S^2$, $S^7 \mapsto S^4$

Our presentation of the definition of the Hopf fibration follows.[24] Let $\mathbb{F}$ denote either the field of real $\mathbb{R}$, complex $\mathbb{C}$ or quaternion $\mathbb{H}$ numbers. Let us define $\mathbb{F}^2=\mathbb{F}\times\mathbb{F}$ (the Cartesian product of $\mathbb{F}$ with itself). Let $\mathbb{F}P_1$ be the $\mathbb{F}$-projective space defined as the set of equivalence classes of $\mathbb{F}^2 - \{(0,0)\}$ (i.e., $\mathbb{F}^2$ with the origin removed) under the following equivalence relation: $(q_1',q_2') \sim (q_1,q_2)$ if and only if there exists $\lambda \in \mathbb{F}-\{0\}$ such that $(q_1',q_2')=(q_1,q_2)\lambda$.

For $k=1,3,7$, let us regard the k-sphere S^k as the set of points (q_1,q_2) where $q_1,q_2 \in \mathbb{F}$ and $|q_1|^2+|q_2|^2=1$, with $\mathbb{F}=\mathbb{R},\mathbb{C},\mathbb{H}$, respectively. Then consider the map D_k from S^k onto $\mathbb{F}P_1$ which assigns to (q_1,q_2) its equivalence class $[(q_1,q_2)]$ in $\mathbb{F}P_1$. Notice that elements of S^k of the form $(q,0)$ with $q \in \mathbb{F}-\{0\}$ are sent to the same equivalence class $[(q,0)]$. Any other element of S^k of the form (q_1,q_2) with $q_2 \neq 0$ (and $q_1 \in \mathbb{F}$ arbitrary) is equivalent to $(q_1 q_2^{-1},1)$. Thus, if we identify the equivalence class $[(q,0)]$ with ∞, then the map D_k can be seen as a map from S^k onto $\mathbb{F}\cup\{\infty\}$ under the identification of $\mathbb{F}P_1$ with $\mathbb{F}\cup\{\infty\}$.

The Hopf fibration $\mathbf{H}_{(k,d)}$ is the map from S^k onto S^d, with $(k,d)=(1,1),(3,2),(7,4)$, defined as the composition of the map D_k and the stereographic projection from the field $\mathbb{F}\cup\{\infty\}$ (with $\mathbb{F}$ identified with $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$) onto the sphere S^1,S^2,S^4, respectively.

Let us give the equations of the Hopf fibration for the cases we are considering. Let us regard the domain and range of the Hopf fibration as the sets $\{(u_1,\ldots,u_{k+1}) \in \mathbb{R}^{k+1} | u_1^2+\cdots+u_{k+1}^2=1\}$ and $\{(x_1,\ldots,x_{d+1}) \in \mathbb{R}^{d+1} | x_1^2+\cdots+x_{d+1}^2=1\}$ (with $k=1,3,7$ and $d=1,2,4$), respectively.

(i) *Case* $S^1 \mapsto S^1$:

$$x_1 = 2u_1u_2,$$

$$x_2 = u_1^2 - u_2^2. \tag{4}$$

(ii) *Case* $S^3 \mapsto S^2$: Here we regard a point $(u_1,\ldots,u_4) \in S^3$ as $(u_1+\imath u_2, u_3+\imath u_4)$.

$$x_1 = 2(u_1u_3 + u_2u_4),$$

$$x_2 = 2(u_2u_3 - u_1u_4), \tag{5}$$

$$x_3 = u_1^2 + u_2^2 - u_3^2 - u_4^2.$$

(iii) *Case* $S^7 \mapsto S^4$: Here we regard a point $(u_1,\ldots,u_8) \in S^7$ as (a_1,a_2) with a_1,a_2 quaternions given by the 2×2 matrices

$$a_1 = \begin{pmatrix} u_1 + \imath u_2 & u_3 + \imath u_4 \\ -u_3 + \imath u_4 & u_1 - \imath u_2 \end{pmatrix}, \quad a_2 = \begin{pmatrix} u_5 + \imath u_6 & u_7 + \imath u_8 \\ -u_7 + \imath u_8 & u_5 - \imath u_6 \end{pmatrix}. \tag{6}$$

Then the equations for the Hopf fibration are

$$x_1 = 2(u_1u_5 + u_2u_6 + u_3u_7 + u_4u_8),$$

$$x_2 = 2(-u_1u_6 + u_2u_5 - u_3u_8 + u_4u_7),$$

$$x_3 = 2(-u_1u_7 + u_2u_8 + u_3u_5 - u_4u_6), \tag{7}$$

$$x_4 = 2(-u_1u_8 - u_2u_7 + u_3u_6 + u_4u_5),$$

$$x_5 = u_1^2 + u_2^2 + u_3^2 + u_4^2 - u_5^2 - u_6^2 - u_7^2 - u_8^2.$$

The Hopf fibration map $\mathbf{H}_{(k,d)}$ that we have defined in the three cases above is onto but not one to one. The inverse image of a point $\mathbf{x}$ in the range of the Hopf fibration (the fiber of the Hopf fibration map at $\mathbf{x}$) is the set of points $(q_1,q_2) \in \mathbb{F}^2 - \{(0,0)\}$ (with $|q_1|^2+|q_2|^2=1$) such that $q_2q_1^{-1}$ is equal to the inverse image of $\mathbf{x}$ under the corresponding stereographic projection. The points $(q_1,q_2),(q_1',q_2') \in (\mathbb{F}^2-\{0,0\})$ such that $q_2q_1^{-1}=q_2'q_1'^{-1}$ are related to each other by the action of an element of the group $G=\mathbb{Z}^2$, S^1 or SU(2) for the Hopf fibration $S^1 \mapsto S^1$, $S^3 \mapsto S^2$ or $S^7 \mapsto S^4$, respectively. More explicitly, let us introduce the following equivalence relations in the spheres S^1, S^3 and S^7 given by $\mathbf{u}' \sim \mathbf{u},\mathbf{v}$ iff $\mathbf{u}' = \mathbf{T}(g)\mathbf{u}$ for some g in $\mathbb{Z}^2$, S^1 or SU(2), respectively, and $\mathbf{T}(g)$ defined in the following way.

(i) *Case* S^1:

$$\mathbf{T}(g) = \pm 1. \tag{8}$$

(ii) *Case* S^3. For $g=\exp(\imath\psi) \in S^1$,

$$\mathbf{T}(g) = \mathbf{C}^\dagger \mathbf{U} \mathbf{C}, \tag{9}$$

where $\mathbf{C}^\dagger$ denotes the adjoint of the following unitary matrix:

$$\mathbf{C} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\imath & -1 & 0 & 0 \\ 0 & 0 & 1 & -\imath \\ 0 & 0 & 1 & \imath \\ -\imath & 1 & 0 & 0 \end{pmatrix} \tag{10}$$

and

$$\mathbf{U}=\begin{pmatrix}\exp(-\imath\psi) & 0 & 0 & 0\\ 0 & \exp(-\imath\psi) & 0 & 0\\ 0 & 0 & \exp(\imath\psi) & 0\\ 0 & 0 & 0 & \exp(\imath\psi)\end{pmatrix}. \tag{11}$$

(iii) *Case* S^7: For $g\in \mathrm{SU}(2)$,

$$\mathbf{T}(g)=\mathbf{D}^{\dagger}\mathbf{V}\mathbf{D}, \tag{12}$$

where $\mathbf{D}$ is the following unitary matrix:

$$\mathbf{D}=\frac{1}{\sqrt{2}}\begin{pmatrix}-\imath & -1 & 0 & 0 & 0 & 0 & 0 & 0(25)\\ 0 & 0 & 1 & -\imath & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & -\imath & -1 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\imath\\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & -\imath\\ 0 & 0 & 0 & 0 & \imath & -1 & 0 & 0\\ 0 & 0 & 1 & \imath & 0 & 0 & 0 & 0\\ -\imath & 1 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix} \tag{13}$$

and

$$\mathbf{V}=\begin{pmatrix}g & 0 & 0 & 0\\ 0 & g & 0 & 0\\ 0 & 0 & g & 0\\ 0 & 0 & 0 & g\end{pmatrix}. \tag{14}$$

Thus the fibers of the Hopf fibration are the equivalence classes described above with the group $G=\mathbb{Z}^2$, S^1 or SU(2) (respectively) acting on them.

III. REGULARIZATION OF THE KEPLER PROBLEM IN $n=2,3,5$ DIMENSIONS

In this section we extend the Hopf fibration maps introduced above in order to get a regularization of the Kepler problem in $n=2,3,5$ dimensions.

First, let us extend the domain and range of the Hopf fibration maps. We do this by considering Eqs. (4), (5), and (7) and then regarding (u_1,u_2), $(u_1,\ldots,u_4)$ or $(u_1,\ldots,u_8)$ in $\mathbb{R}^2$, $\mathbb{R}^4$ or $\mathbb{R}^8$, respectively. Thus we obtain maps $\mathbb{R}^2\mapsto\mathbb{R}^2$, $\mathbb{R}^4\mapsto\mathbb{R}^3$, and $\mathbb{R}^8\mapsto\mathbb{R}^5$. All of these maps can be written as

$$\mathbf{x}=\mathbf{A}\mathbf{u} \tag{15}$$

in the following way (for each case that we are considering):

$$\begin{pmatrix}x_1\\ x_2\end{pmatrix}=\begin{pmatrix}u_2 & u_1\\ u_1 & -u_2\end{pmatrix}\begin{pmatrix}u_1\\ u_2\end{pmatrix}, \tag{16}$$

$$\begin{pmatrix}x_1\\ x_2\\ x_3\\ 0\end{pmatrix}=\begin{pmatrix}u_3 & u_4 & u_1 & u_2\\ -u_4 & u_3 & u_2 & -u_1\\ u_1 & u_2 & -u_3 & -u_4\\ u_2 & -u_1 & u_4 & -u_3\end{pmatrix}\begin{pmatrix}u_1\\ u_2\\ u_3\\ u_4\end{pmatrix}, \tag{17}$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} u_5 & u_6 & u_7 & u_8 & u_1 & u_2 & u_3 & u_4 \\ -u_6 & u_5 & -u_8 & u_7 & u_2 & -u_1 & u_4 & -u_3 \\ -u_7 & u_8 & u_5 & -u_6 & u_3 & -u_4 & -u_1 & u_2 \\ -u_8 & -u_7 & u_6 & u_5 & u_4 & u_3 & -u_2 & -u_1 \\ u_1 & u_2 & u_3 & u_4 & -u_5 & -u_6 & -u_7 & -u_8 \\ u_2 & -u_1 & -u_4 & u_3 & u_6 & -u_5 & -u_8 & u_7 \\ u_3 & u_4 & -u_1 & -u_2 & u_7 & u_8 & -u_5 & -u_6 \\ u_4 & -u_3 & u_2 & -u_1 & u_8 & -u_7 & u_6 & -u_5 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{pmatrix}, \tag{18}$$

where in the last two cases we have completed the matrix $\mathbf{A}$ such that the Eqs. (17) and (18) hold.

Notice that the rows of the matrix $\mathbf{A}$ are orthogonal among them (the same happens with the columns). It is here where the special dimensions $(n,m)=(2,2),(3,4),(5,8)$ appear. The rows of the matrix $\mathbf{A}$ give a frame for the spheres S^1, S^3, and S^7 that changes smoothly (notice that first row vector is actually the position vector in the corresponding sphere). This is possible because the k-sphere S^k is a parallelizable manifold only when $k=1,3,7$.

Since the matrix $\mathbf{A}$ satisfies the relation

$$\mathbf{A}^t\mathbf{A} = |\mathbf{u}|^2\mathbf{I} \tag{19}$$

(with $\mathbf{A}^t$ the transpose matrix of $\mathbf{A}$ and $\mathbf{I}$ the identity matrix) then $\mathbf{A}$ is invertible with inverse $\mathbf{A}^{-1}=\mathbf{A}^t/|\mathbf{u}|^2$ when $|\mathbf{u}|\neq 0$.

We will consider the Kepler problem in dimensions 2, 3, 5 by regarding the vector $\mathbf{x}$ [appearing on the left-hand side of Eqs. (16)–(18)] as a vector describing the position of a particle in $\mathbb{R}^2$, $\mathbb{R}^3$ or $\mathbb{R}^5$, respectively, under the influence of the gravitational force

$$\mathbf{F} = -\frac{\mathbf{x}}{|\mathbf{x}|^3} \tag{20}$$

and obeying the Newton's law $\mathbf{F}=-d^2\mathbf{x}/d^2t$.

The singularity of the force vector $\mathbf{F}$ at the origin $\mathbf{x}=0$ has been studied and regularized before. Two different ways to achieve this regularization are the following.

(a) By considering maps of the type appearing in Eqs. (16)–(18), Levi-Civita studied the first case $n=2$, Kustaanheimo and Stiefel[19] considered the second case $n=3$ and the third case $n=5$ can be solved via a Hurwitz transformation, Refs. 7 and 20. See Ref. 25 for a nice description of the first two cases.

(b) By considering an extension of the stereographic projection between $\mathbb{R}^n$ and the n-sphere S^n, Moser[22] regularized the Kepler problem for any dimension $n\geqslant 1$. This regularization will be presented in Sec. IV.

The two regularizations mentioned above use as a key idea to consider a reparametrization of time t in the following way: when the particle moves in a straight line towards the origin (a collision orbit) the speed of the particle goes to infinity. However the product $|\mathbf{x}|(d\mathbf{x}/dt)$ tends to a finite limit (zero) when $|\mathbf{x}|$ approaches the origin [this is a consequence of the conservation of energy $E=\frac{1}{2}|(d\mathbf{x}/dt)|^2-(1/|\mathbf{x}|)$]. Thus a new time parameter s is introduced via the following equation:

$$\frac{d}{\mathrm{d}s} = |\mathbf{x}|\frac{d}{\mathrm{d}t}. \tag{21}$$

In this way, the speed of the particle when it reaches the origin is finite and equal to zero with respect to time s.

In order to show the regularization indicated in (a), let us consider the symplectic spaces $N=(T^*(\mathbb{R}^n-\{0\}),\omega)$ and $M=(T^*(\mathbb{R}^m-\{0\}),\nu)$ with symplectic forms $\omega=\mathrm{d}\mathbf{p}\wedge\mathrm{d}\mathbf{x}$ and $\nu=4\,\mathrm{d}\mathbf{v}\wedge\mathrm{d}\mathbf{u}$,

respectively. We will show a canonical transformation that transforms the Hamiltonian system of the $n=2,3,5$ dimensional Kepler problem $\left[N, H=\frac{1}{2}|\mathbf{p}|^2-(1/|\mathbf{x}|)\right]$ into a suitable reduction of the Hamiltonian system $[M, H'=(1/|\mathbf{u}|^2)(2|\mathbf{v}|^2-1)]$ with $m=2,4,8$, respectively. Moreover, we will show that, for fixed negative energy $H=E$ and after the time reparametrization Eq. (21), the Hamiltonian flow of H is transformed into the Hamiltonian flow of the reduction of an isotropic harmonic oscillator $K=\frac{1}{2}(|\mathbf{v}|^2+k|\mathbf{u}|^2)$ with strength $k=-E/2$ and obtained from the Hamiltonian flow of H'. Since the Hamiltonian flow of K does not have any singularity, we will say that we have achieved a regularization of the $n=2,3,5$ dimensional Kepler problem.

Let us consider the following action of the group G on the symplectic manifold M: given $g \in G$ we define $(\mathbf{u}', \mathbf{v}')=(\mathbf{T}(g)\mathbf{u}, \mathbf{T}(g)\mathbf{v})$ where $\mathbf{T}(g)$ is defined by Eqs. (8)–(14). Since $\mathbf{T}(g)$ is an orthogonal matrix for all $g \in G$, then the action we are defining is symplectic.

In order to find the reduction of the symplectic manifold M under the action of the group G defined above, we need to find the moment map for the cases $m=4$ and $m=8$. First we introduce some notation.

Let $\mathcal{G}$ denote the Lie algebra of the group G. That is, $\mathcal{G}$ is the vector space $\mathbb{R}$ when $m=4$ or the real vector space su(2) of 2×2 self-adjoint and traceless complex matrices when $m=8$.

Let Υ denote the representation of the Lie algebra $\mathcal{G}$ obtained from the representation of G given by the matrices $\mathbf{T}(g)$. Let us denote the elements of Υ by $\mathcal{T}(\xi)$ with $\xi \in \mathcal{G}$. More specifically, for the case $m=4$,

$$\mathcal{T}(\xi) = \mathbf{C}^{\dagger}\mathcal{U}\mathbf{C}, \tag{22}$$

where $\mathbf{C}$ is given by Eq. (10) and

$$\mathcal{U} = \begin{pmatrix} -\psi & 0 & 0 & 0 \\ 0 & -\psi & 0 & 0 \\ 0 & 0 & \psi & 0 \\ 0 & 0 & 0 & \psi \end{pmatrix} \tag{23}$$

(for some $\xi=\psi \in \mathbb{R}$) and for the case $m=8$,

$$\mathcal{T}(\xi) = \mathbf{D}^{\dagger}\mathcal{V}\mathbf{D}, \tag{24}$$

where $\mathbf{D}$ is given by Eq. (13) and

$$\mathcal{V} = \begin{pmatrix} \xi & 0 & 0 & 0 \\ 0 & \xi & 0 & 0 \\ 0 & 0 & \xi & 0 \\ 0 & 0 & 0 & \xi \end{pmatrix} \tag{25}$$

with $\xi \in \mathrm{su}(2)$.

Let us introduce the following inner product in the Lie algebra $\mathbf{\Upsilon}$: for $\mathcal{T}(\xi_1)$ and $\mathcal{T}(\xi_2)$ in $\mathbf{\Upsilon}$, let us define

$$\langle \mathcal{T}(\xi_1), \mathcal{T}(\xi_2) \rangle = \tfrac{1}{8}\mathrm{tr}(\mathcal{T}(\xi_1)\mathcal{T}(\xi_2)) = \tfrac{1}{2}\mathrm{tr}(\xi_1\xi_2) \tag{26}$$

Let $\widetilde{\mathbf{\Upsilon}}$ be the representation of the Lie algebra $\mathcal{G}$ given by matrices of the form

$$\widetilde{\mathcal{T}}(\xi) = \begin{pmatrix} \mathcal{T}(\xi) & 0 \\ 0 & \mathcal{T}(\xi) \end{pmatrix} \tag{27}$$

with $\mathcal{T}(\xi) \in \mathbf{\Upsilon}$.

The moment map is defined as the function $\mathcal{J}_m: M \mapsto \tilde{\mathbf{Y}}^*$, where $\tilde{\mathbf{Y}}^*$ denotes the dual vector space of $\tilde{\mathbf{Y}}$, such that $\mathcal{J}_m(\mathbf{u},\mathbf{v})$ evaluated at $\tilde{\mathcal{T}}(\xi) \in \tilde{\mathbf{Y}}$ is equal to the infinitesimal generator of the action corresponding to $\tilde{\mathcal{T}}(\xi)$ at the point $(\mathbf{u},\mathbf{v})$. Namely, we want the following equation to hold:

$$\langle \mathcal{J}_m(\mathbf{u},\mathbf{v}), \tilde{\mathcal{T}}(\xi) \rangle = \left. \frac{d}{\mathrm{d}s} \right|_{s=0} \exp(is\tilde{\mathcal{T}}(\xi)) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \tag{28}$$

where we have used the Riez representation theorem and denoted the element of $\tilde{\mathbf{Y}}$ which represents $\mathcal{J}_m(\mathbf{u},\mathbf{v})$ by the same symbol.

The result is that the element $\xi(\mathbf{u},\mathbf{v}) \in \mathcal{G}$ determining $\mathcal{J}_m(\mathbf{u},\mathbf{v})$ is the following.

For the case $m=4$,

$$\xi(\mathbf{u},\mathbf{v}) = -u_2v_1 + u_1v_2 - u_4v_3 + u_3v_4. \tag{29}$$

For the case $m=8$,

$$\xi(\mathbf{u},\mathbf{v}) = \begin{pmatrix} \lambda & \alpha + i\beta \\ \alpha - i\beta & -\lambda \end{pmatrix} \tag{30}$$

with

$$\alpha(\mathbf{u},\mathbf{v}) = -u_3v_1 - u_4v_2 + u_1v_3 + u_2v_4 - u_7v_5 - u_8v_6 + u_5v_7 + u_6v_8,$$

$$\beta(\mathbf{u},\mathbf{v}) = u_4v_1 - u_3v_2 + u_2v_3 - u_1v_4 + u_8v_5 - u_7v_6 + u_6v_7 - u_5v_8,$$

$$\lambda(\mathbf{u},\mathbf{v}) = u_2v_1 - u_1v_2 - u_4v_3 + u_3v_4 + u_6v_5 - u_5v_6 - u_8v_7 + u_7v_8. \tag{31}$$

The equations $\lambda=0$ and $\alpha=\beta=\lambda=0$ are known in the physics literature as the restrictions of the Kepler problem in the variables $\mathbf{u}$ and $\mathbf{v}$ for the $n=3$ (see Ref. 19) and $n=5$ (see Ref. 7) dimensional Kepler problem, respectively. The geometrical meaning of them is that the momentum vector $\mathbf{v}$ is orthogonal to the fiber of the point $\mathbf{u}$ at the point $\mathbf{u}$ (see Ref. 25 for the $n=3$ dimensional case).

Thus we want to restrict ourselves to the submanifold $\mathcal{J}_m^{-1}(0)$ of M given by the inverse image of the zero element 0 of $\tilde{\mathbf{Y}}^*$. Since 0 is a regular value of $\mathcal{J}_m$, The Marsden-Weinstein reduction method (see Ref. 1) implies that we can take the reduction of M by the action of the Lie group G and consider the symplectic manifold $\mathcal{J}_m^{-1}(0)/G$ with a well-defined symplectic form $\tilde{\nu}$ acting on it and coming from the initial symplectic form $\nu = 4\,\mathrm{d}\mathbf{v} \wedge \mathrm{d}\mathbf{u}$.

Let us consider the map $\mathcal{H}_{(n,m)}: \mathcal{J}_m^{-1}(0) \mapsto N$ given by

$$\mathbf{x} = \mathbf{A}(\mathbf{u})\mathbf{u}, \quad \mathbf{p} = \frac{2}{|\mathbf{u}|^2}\mathbf{A}(\mathbf{u})\mathbf{v}, \tag{32}$$

where $\mathbf{A}(\mathbf{u})$ denotes the matrix $\mathbf{A}$ as a function of $\mathbf{u}$ as it appears in Eqs. (17) and (18). Notice that if $(\mathbf{u},\mathbf{v}) \in \mathcal{J}_m^{-1}(0)$ then $(\mathbf{v},\mathbf{u}) \in \mathcal{J}_m^{-1}(0)$, and the matrix $\mathbf{A}$ has the following property:

$$\mathbf{A}(\mathbf{u})\mathbf{v} = \mathbf{A}(\mathbf{u})\mathbf{v}, \tag{33}$$

where $\mathbf{A}(\mathbf{v})$ is the matrix $\mathbf{A}$ with entries for the components of the vector $\mathbf{v}$ instead of $\mathbf{u}$ (the importance of having this equation is emphasized in Ref. 25 for $m=2,4$). This property in particular implies that $\mathrm{d}\mathbf{x} = 2\mathbf{A}(\mathbf{u})\mathrm{d}\mathbf{u}$.

Since $\mathbf{A}^t(\mathbf{u})\mathbf{A}(\mathbf{u}) = |\mathbf{u}|^2\mathbf{I}$, then $\mathbf{p}\,\mathrm{d}\mathbf{x} = 4\mathbf{v}\,\mathrm{d}\mathbf{u}$, which in turn implies that $\mathcal{H}_{(n,m)}{}^*\omega = \nu$. Thus we can obtain a canonical transformation $\tilde{\mathcal{H}}_{(n,m)}$ from the symplectic manifold $(\mathcal{J}_m^{-1}(0)/G, \tilde{\nu})$ onto the symplectic manifold (N,ω).

The analog of the situation described in the last paragraph holds in the case $m=2$ as well. In this case the canonical transformation $\tilde{\mathcal{H}}_{(2,2)}$ goes from $T^*(\mathbb{R}^2-\{0\})/\mathbb{Z}_2$ onto $T^*(\mathbb{R}^2-\{0\})$ with corresponding symplectic forms $\tilde{\nu}$ and ω.

Since the Hamiltonian system $(\mathcal{J}_m^{-1}(0),\nu,H'=(1/|\mathbf{u}|^2)(2|\mathbf{v}|^2-1))$ is invariant under the action of G, the equations of motion of the corresponding reduced Hamiltonian system associated to $(\mathcal{J}_m^{-1}(0)/G,\tilde{\nu},\tilde{H})$ [with $\tilde{H}$ being the Hamiltonian H' acting on the reduced manifold $\mathcal{J}_m^{-1}(0)/G$] are determined by the equations of motion of $(\mathcal{J}_m^{-1}(0),\nu,H')$ which in turn are

$$\frac{d\mathbf{u}}{dt}=\frac{1}{4}\frac{\partial H'}{\partial \mathbf{v}}=\frac{\mathbf{v}}{|\mathbf{u}|^2},$$
$$\frac{d\mathbf{v}}{dt}=-\frac{1}{4}\frac{\partial H'}{\partial \mathbf{u}}=\frac{\mathbf{u}}{2|\mathbf{u}|^4}(2|\mathbf{v}|^2-1). \tag{34}$$

Thus on each surface of constant negative energy $H'=E$, and after the time reparametrization $d/dt=(1/|\mathbf{x}|)(d/ds)$, we obtain the equations of motion of an isotropic harmonic oscillator (with strength $k=-E/2$),

$$\frac{d\mathbf{u}}{ds}=\mathbf{v},$$
$$\frac{d\mathbf{v}}{ds}=\frac{E}{2}\mathbf{u}. \tag{35}$$

The Hamiltonian H' is mapped to the Hamiltonian of the Kepler problem $H=\frac{1}{2}|\mathbf{p}|^2-(1/|\mathbf{x}|)$ through the transformation $\mathcal{H}_{(n,m)}$ defined in Eq. (32) (i.e., $H'=H\circ\mathcal{H}_{(n,m)}$). Since $\mathcal{H}_{(n,m)}^*\omega=\nu$, the Hamilton equations of H' indicated in Eqs. (34) are mapped to the Hamilton equations of the Kepler problem:

$$\frac{d\mathbf{x}}{dt}=\frac{\partial H}{\partial \mathbf{p}}=\mathbf{p},$$
$$\frac{d\mathbf{p}}{dt}=-\frac{\partial H}{\partial \mathbf{x}}=-\frac{\mathbf{x}}{|\mathbf{x}|^3}. \tag{36}$$

We conclude that, for fixed negative energy $H=H'=E$, the Hamiltonian flow of the Kepler problem given by Eqs. (36) is equivalent, after a time reparametrization, to the reduction of the Hamiltonian flow of an isotropic harmonic oscillator $K=\frac{1}{2}(|\mathbf{v}|^2+k|\mathbf{u}|^2)$ with strength $k=-E/2$ under the corresponding action of $\mathbb{Z}_2$, S^1 or SU(2).

We remark that the study of the above moment map $\mathcal{J}_m$ has already been considered by Iwai[14] and Mladenov.[20]

IV. THE MOSER REGULARIZATION

Moser[22] introduced a different way to regularize the Kepler problem for fixed negative energy than the one described in the preceding section. The Moser regularization actually works for any dimension and not only for $n=2,3,5$. The Moser map that we describe below is usually associated to the fixed energy $E=-1/2$. Other negative values of the energy can be considered by taking the corresponding dilations (see Ref. 22).

In this section we briefly present the Moser regularization. The main idea goes as follows: The orbits corresponding to nonzero angular momentum (where the initial position and momentum vectors are linearly independent) are circles when projected into the momentum space. These circles correspond, under a stereographic projection $\mathbf{T}_n:\mathbb{R}^n\mapsto S_o^n$ and fixed energy $E=-1/2$, to

great circles on the punctured n-sphere S_o^n. The idea is to consider an extension of this stereographic projection $\mathbf{T}_n$ from the phase space $T^*\mathbb{R}^n$ onto the tangent bundle $T^*S_o^n$ of the punctured n-sphere S^n under the restriction: $\mathbf{T}_n^*\xi\cdot d\mathbf{w}=\mathbf{x}\cdot d\mathbf{p}$ where $(\mathbf{w},\xi)\in T^*S_o^n$, $\mathbf{w}\in S_o^n$. Thus we obtain a map $\mathcal{M}_n: T^*\mathbb{R}^n \mapsto T^*S_o^n$. The explicit equations are the following:

$$w_j = \frac{2}{|p|^2+1}p_j, \quad j=1,2,\ldots,n,$$

$$w_{n+1} = \frac{|p|^2-1}{|p|^2+1}, \tag{37}$$

$$\xi_j = \frac{|p|^2+1}{2}x_j - (\mathbf{x}\cdot\mathbf{p})p_j, \quad j=1,2,\ldots,n,$$

$$\xi_4 = \mathbf{x}\cdot\mathbf{p} = \sum_{j=1}^{n} x_j p_j. \tag{38}$$

The equations for the inverse transformation are

$$p_j = \frac{w_j}{1-w_4}, \quad j=1,2,\ldots,n,$$

$$x_j = (1-w_4)\xi_j + \xi_4 w_j, \quad j=1,2,\ldots,n. \tag{39}$$

The Moser map $\mathcal{M}_n$ is actually a symplectomorphism from the phase space $T^*\mathbb{R}^n$ endowed with its canonical symplectic form $\omega=d\mathbf{p}\wedge d\mathbf{x}$ onto $T^*S_o^n$ endowed with the symplectic form $\kappa=d\mathbf{w}\wedge d\xi$ obtained from the restriction to $T^*S_o^n$ of the canonical symplectic form of the ambient $T^*\mathbb{R}^{n+1}$. Moreover, for fixed negative energy $E=-1/2$, the Moser map $\mathcal{M}_n$ and the time reparametrization Eq. (21) transform the Hamiltonian flow of the n-dimensional Kepler problem $[(\mathbb{R}^n-\{0\})\times\mathbb{R}^n, d\mathbf{p}\wedge d\mathbf{x}, H=(|p|^2/2)-(1/|\mathbf{x}|)]$ onto the geodesic flow of the punctured n-sphere with the zero section of $T^*S_o^n$ removed [note that $|\xi|=[(|\mathbf{p}|^2+1)/2]|\mathbf{x}|$ which implies $\xi=0$ iff $\mathbf{x}=0$]. The collision orbits (orbits with zero angular momentum) are sent to geodesics passing through the north pole but not including the north pole itself.

The north pole can be included into the picture in the following way: it can be shown that, after the time reparametrization, a collision orbit of the n-dimensional Kepler problem corresponds to a particle moving on a segment with one of its ends at the origin and reaching the origin with zero speed. Thus, if we make the convention that after the collision with the center of attraction the particle goes back to its motion on the segment, then we have an oscillatory motion with respect to the time s. Note that we are now including the point $\mathbf{x}=0$. Moreover, since the total energy is conserved then $|\mathbf{x}|\to 0$ iff $|\mathbf{p}|\to\infty$ then we include the case $|\mathbf{p}|=\infty$ in the stereographic projection by assigning to $|\mathbf{p}|=\infty$ the north pole of S^n. The oscillatory motion corresponds to motion on a geodesic passing through the north pole including this point. Thus we say that, for fixed negative energy $E=-1/2$, the Hamiltonian flow of the n-dimensional Kepler problem is regularized by the geodesic flow of the whole n-sphere S^n after the time reparametrization. We will refer to this fact as the Moser regularization of the n-dimensional Kepler problem.

V. MAPPING A COMPLEXIFICATION OF $T^*\mathbb{R}^m$ ONTO A NULL QUADRIC THROUGH A MOMENT MAP

In this section we set up a map $\rho_{n,m}(\mathbf{z})$ from a complexification of $T^*\mathbb{R}^m$ onto a quadric Q^n that will play a key role when we define the Bargmann transform acting on $L^2(S^n)$. In the case of $m=4$ and $m=8$, such a map will be obtained through a moment map $\mathcal{I}$ of a suitable defined group

F acting on a related space to the above-mentioned complexification. The group F is defined as the set of $m\times m$ complex matrices that leave the moment map $\mathcal{K}_m$ [defined in (29)–(31)] invariant. This section is motivated by the work of Kummer[20] where he considers the case $m=4$.

Let us introduce the following complexification of $T^*\mathbb{R}^m$ (similar to the one considered by Mladenov[20]) $\mathcal{T}_m: T^*\mathbb{R}^m \mapsto \mathbb{C}^m$,

$$\mathbf{z} = \mathbf{M}\mathbf{u} + 2\imath\mathbf{M}\mathbf{v}, \tag{40}$$

where we take the following particular expression for the unitary matrix $\mathbf{M}$.

(i) *The case* $m=2$:

$$\mathbf{M} = \frac{1}{\sqrt{2}}\begin{pmatrix} -\imath & -1 \\ -\imath & 1 \end{pmatrix}. \tag{41}$$

(ii) *The case* $m=4$:

$$\mathbf{M} = \frac{1}{\sqrt{2}}\begin{pmatrix} -\imath & -1 & 0 & 0 \\ 0 & 0 & 1 & -\imath \\ 0 & 0 & 1 & \imath \\ -\imath & 1 & 0 & 0 \end{pmatrix}. \tag{42}$$

(iii) *The case* $m=8$:

$$\mathbf{M} = \frac{1}{\sqrt{2}}\begin{pmatrix} -\imath & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -\imath & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\imath & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & \imath \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\imath \\ 0 & 0 & 0 & 0 & \imath & -1 & 0 & 0 \\ 0 & 0 & 1 & -\imath & 0 & 0 & 0 & 0 \\ -\imath & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{43}$$

Since $\mathbf{M}$ is unitary, we have

$$\theta := -\imath\, d\mathbf{z}\wedge d\underline{\mathbf{z}} = 4\, d\mathbf{v}\wedge d\mathbf{u}. \tag{44}$$

Given k a positive integer number, we define the null quadric by

$$Q^k = \{\boldsymbol{\alpha}\in\mathbb{C}^{k+1} \mid \alpha_1^2 + \cdots + \alpha_{k+1}^2 = 0\}. \tag{45}$$

Let us first define the map $\rho(\mathbf{z})$ in the case $m=2$. In this case we have the action $\mathbf{z}'\mapsto\pm\mathbf{z}$ of the group $\mathbb{Z}_2$ on the complex manifold $\mathbb{C}^2$. The set of monomials $\{z_1^2, z_2, z_1z_2\}$ give a basis of the vector space V of all the homogeneous polynomials of degree 2 (all the elements of V are invariant under the $\mathbb{Z}_2$ action). Thus, we define the map $\rho(\mathbf{z})_{(2,2)}=(\rho_1(\mathbf{z}),\rho_2(\mathbf{z}),\rho_3(\mathbf{z}))$ by

$$\rho_1 = (z_2^2 - z_1^2)/2, \quad \rho_2 = \imath(z_1^2 + z_2^2)/2, \quad \rho_3 = z_1z_2. \tag{46}$$

The map $\rho(\mathbf{z})$ defined by Eq. (46) has values in the null quadric Q^2.

In order to consider the cases $m=4,8$, let us introduce the variable $\boldsymbol{\eta}\in\mathbb{C}^m$ and write it as $\boldsymbol{\eta}=(\boldsymbol{\eta}_{\mathrm{I}},\boldsymbol{\eta}_{\mathrm{II}})$ with $\boldsymbol{\eta}_{\mathrm{I}},\boldsymbol{\eta}_{\mathrm{II}}\in\mathbb{C}^{m/2}$. Let us consider the following change of variables from the variable $\mathbf{z}$ to the variable $\boldsymbol{\eta}$:

$$\boldsymbol{\eta}_{\mathrm{I}} = \mathbf{z}_{\mathrm{I}}, \quad \boldsymbol{\eta}_{\mathrm{II}} = \overline{\mathbf{z}}_{\mathrm{II}}. \tag{47}$$

Thus the symplectic form θ written in terms of $\boldsymbol{\eta}$ is

$$\theta = -\imath(\mathrm{d}\boldsymbol{\eta}_{\mathrm{I}} \wedge \mathrm{d}\overline{\boldsymbol{\eta}}_{\mathrm{I}} - \mathrm{d}\boldsymbol{\eta}_{\mathrm{II}} \wedge \mathrm{d}\overline{\boldsymbol{\eta}}_{\mathrm{II}}). \tag{48}$$

Let us denote by $\mathcal{K}_m$ the moment map associated to the action of the group G on the space $\mathbb{C}^m$ in terms of the variable $\boldsymbol{\eta}$.

The moment map $\mathcal{K}_m$ written in terms of $\boldsymbol{\eta}$ and $\overline{\boldsymbol{\eta}}$ is determined by the following equations [see Eqs. (29)–(31) and the definition of the complexification $\mathcal{T}_m$ in Eqs. (40)–(43))].

For the case $m=4$,

$$\xi(\boldsymbol{\eta}, \overline{\boldsymbol{\eta}}) = \frac{1}{4}\boldsymbol{\eta}^{\dagger}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\boldsymbol{\eta}, \tag{49}$$

where I denotes the 2×2 unit matrix and $\boldsymbol{\eta}^{\dagger}$ the adjoint of $\boldsymbol{\eta}$.

For the case $m=8$,

$$\alpha(\boldsymbol{\eta}, \overline{\boldsymbol{\eta}}) = -\frac{1}{4}\Re\left[\boldsymbol{\eta}^{t}\begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}\boldsymbol{\eta}\right],$$

$$\beta(\boldsymbol{\eta}, \overline{\boldsymbol{\eta}}) = \frac{1}{4}\Im\left[\boldsymbol{\eta}^{t}\begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}\boldsymbol{\eta}\right],$$

$$\lambda(\boldsymbol{\eta}, \overline{\boldsymbol{\eta}}) = -\frac{1}{4}\boldsymbol{\eta}^{\dagger}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\boldsymbol{\eta}, \tag{50}$$

where I denotes the 4×4 unit matrix and J is

$$J = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{51}$$

Let us define the group F as the group of linear transformations which leave the moment map $\mathcal{K}_m$ invariant. Namely, F is the Lie group of $m\times m$ matrices $\mathbf{S}$ which satisfy the condition

$$\mathbf{S}^{\dagger}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\mathbf{S} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{52}$$

and additionally the following condition for the case $m=8$:

$$\mathbf{S}^{t}\begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}\mathbf{S} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}, \tag{53}$$

where $\mathbf{S}^t$ denotes the transpose matrix of $\mathbf{S}$.

We will also require the condition that the elements of F have unit determinant in both cases. Notice that $F=\mathrm{SU}(2,2)$ for $m=4$ and F is a subgroup of $\mathrm{SU}(4,4)$ for $m=8$.

From the definition of the group F [Eq. (52)] and the expression of the symplectic form θ in terms of the variables $\boldsymbol{\eta}$ and $\overline{\boldsymbol{\eta}}$ [Eq. (48)], we have that the action of F on $\mathbb{C}^8$ is symplectic. Therefore we can consider the moment map $\mathcal{I}$ of the action of F on $\mathbb{C}^8$. We will obtain from this moment map a map $\rho(\mathbf{z})$ from $\mathbb{C}^8$ to T^*S^n which is invariant under the following action [obtained from the action of the group G in the last section and acting on the variables $(\mathbf{u},\mathbf{v})$].

Case $m=4$,

$$\mathbf{z}' = \begin{pmatrix} \exp(-\imath\psi) & 0 & 0 & 0 \\ 0 & \exp(-\imath\psi) & 0 & 0 \\ 0 & 0 & \exp(\imath\psi) & 0 \\ 0 & 0 & 0 & \exp(\imath\psi) \end{pmatrix}\mathbf{z}. \tag{54}$$

Case $m=8$,

$$\mathbf{z}' = \mathbf{L}^{\dagger}\mathbf{V}\mathbf{L}\mathbf{z}, \tag{55}$$

where $\mathbf{V}$ has the form indicated in Eq. (14) and

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{56}$$

The Lie algebra $\mathcal{F}$ of F is the real vector space of $m \times m$ traceless complex matrices ζ which have the following form.

Case $m=4$,

$$\begin{pmatrix} \mathbf{a} & \mathbf{b} \\ -\mathbf{b}^{\dagger} & \mathbf{d} \end{pmatrix} \tag{57}$$

with the 2×2 matrices $\mathbf{a}$ and $\mathbf{d}$ restricted to be self-adjoint.

Case $m=8$,

$$\zeta = \begin{pmatrix} \mathbf{a} & \mathbf{b} \\ -\mathbf{b}^{\dagger} & -J\mathbf{a}^{t}J \end{pmatrix}, \tag{58}$$

where the 4×4 matrices $\mathbf{a}$ and $\mathbf{b}$ satisfy

$$\mathbf{a}^{\dagger} = \mathbf{a}, \quad J\mathbf{b}^{t} = -\mathbf{b}J \tag{59}$$

or, equivalently, the matrix $\mathbf{b}$ must have the form

$$\mathbf{b} = \begin{pmatrix} \mathbf{b}_{11} & \mathbf{b}_{12} \\ \mathbf{b}_{21} & -\boldsymbol{\sigma}_3\mathbf{b}_{11}^{t}\boldsymbol{\sigma}_3 \end{pmatrix} \tag{60}$$

with $\mathbf{b}_{11}$ any 2×2 complex matrix, $\mathbf{b}_{12}$ and $\mathbf{b}_{21}$ any two complex multiples of the 2×2 matrix $\boldsymbol{\sigma}_3$ defined in Eq. (51).

Notice that the dimension of $\mathcal{F}$ is 15 and 28 when $m=4$ and $m=8$, respectively.

Let us introduce the following real valued inner product in $\mathcal{F}$:

$$\langle \zeta_1, \zeta_2 \rangle = \mathrm{tr}\left(\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \zeta_1 \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \zeta_2 \right). \tag{61}$$

Given a Hamiltonian system (H, ω), with $H=H(\boldsymbol{\eta}, \overline{\boldsymbol{\eta}})$, the associated Hamiltonian vector field X_H is

$$X_H = \imath \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \frac{\partial}{\partial \overline{\boldsymbol{\eta}}} H. \tag{62}$$

The infinitesimal generator $\zeta_{\boldsymbol{\eta}}$ associated to a given element ζ of the Lie algebra $\mathcal{F}$ at the point $\boldsymbol{\eta}$ is equal to $\imath\zeta\boldsymbol{\eta}$. Thus we want the moment map $\mathcal{I}$ to satisfy the following equation for all $\zeta \in \mathcal{F}$:

$$\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\zeta\boldsymbol{\eta} = \frac{\partial}{\partial\bar{\boldsymbol{\eta}}}\mathrm{tr}\left(\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\mathcal{I}(\boldsymbol{\eta},\bar{\boldsymbol{\eta}})\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\zeta\right). \tag{63}$$

The solution to Eq. (63) is the following.

Case $m=4$,

$$\mathcal{I}(\boldsymbol{\eta},\bar{\boldsymbol{\eta}}) = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\boldsymbol{\eta}\boldsymbol{\eta}^{\dagger}. \tag{64}$$

Case $m=8$,

$$\mathcal{I}(\boldsymbol{\eta},\bar{\boldsymbol{\eta}}) = \frac{1}{2}\left[\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\boldsymbol{\eta}\boldsymbol{\eta}^{\dagger} + \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}(\boldsymbol{\eta}\boldsymbol{\eta}^{\dagger})^{t}\begin{pmatrix} 0 & -J \\ J & 0 \end{pmatrix}\right]. \tag{65}$$

We are now ready to introduce the map $\rho(\mathbf{z})=(\rho_1,\ldots,\rho_{n+1})$. The real and imaginary parts of the components of $\rho(\mathbf{z})$ are defined as the Hamiltonians $\langle\mathcal{I}(\boldsymbol{\eta},\bar{\boldsymbol{\eta}}),\zeta\rangle$ written in terms of $\mathbf{z}$ with the following particular choices for $\zeta\in\mathcal{F}$.

Case $m=4$: Denote the elements of $\mathcal{F}$ by $\zeta=\zeta(\mathbf{a},\mathbf{b},\mathbf{d})$ as indicated in Eq. (57). Let us define

$$\begin{gathered}
\Re\rho_1 = \langle\mathcal{I},\zeta(0,\boldsymbol{\sigma}_0,0)\rangle, \quad \Im\rho_1 = \langle\mathcal{I},\zeta(0,\imath\boldsymbol{\sigma}_0,0)\rangle, \\
\Re\rho_2 = \langle\mathcal{I},\zeta(0,-\imath\boldsymbol{\sigma}_3,0)\rangle, \quad \Im\rho_2 = \langle\mathcal{I},\zeta(0,\boldsymbol{\sigma}_3,0)\rangle, \\
\Re\rho_3 = \langle\mathcal{I},\zeta(0,-\imath\boldsymbol{\sigma}_1,0)\rangle, \quad \Im\rho_3 = \langle\mathcal{I},\zeta(0,\boldsymbol{\sigma}_1,0)\rangle, \\
\Re\rho_4 = \langle\mathcal{I},\zeta(0,\imath\boldsymbol{\sigma}_2,0)\rangle, \quad \Im\rho_4 = \langle\mathcal{I},\zeta(0,\boldsymbol{\sigma}_2,0)\rangle,
\end{gathered} \tag{66}$$

where the matrix $\boldsymbol{\sigma}_0$ is the 2×2 identity matrix and $\boldsymbol{\sigma}_j$, $j=1,2,3$, are the Pauli matrices given by

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{67}$$

More explicitly, we define the components of $\rho_{(3,4)}$ by

$$\begin{gathered}
\rho_1(\mathbf{z}) = z_1z_3 + z_2z_4, \quad \rho_2(\mathbf{z}) = \imath(z_1z_3 - z_2z_4), \\
\rho_3(\mathbf{z}) = \imath(z_1z_4 + z_2z_3), \quad \rho_4(\mathbf{z}) = z_1z_4 - z_2z_3.
\end{gathered} \tag{68}$$

Case $m=8$: Denote the elements of $\mathcal{F}$ by $\zeta=\zeta(\mathbf{a},\mathbf{b}_{11},\mathbf{b}_{12},\mathbf{b}_{21})$ as indicated in Eqs. (58)–(60). Let us define then

$$\begin{gathered}
\Re\rho_1 = \langle\mathcal{I},\zeta(0,-\boldsymbol{\sigma}_2,0,0)\rangle, \quad \Im\rho_1 = \langle\mathcal{I},\zeta(0,-\imath\boldsymbol{\sigma}_2,0,0)\rangle, \\
\Re\rho_2 = \langle\mathcal{I},\zeta(0,\boldsymbol{\sigma}_1,0,0)\rangle, \quad \Im\rho_2 = \langle\mathcal{I},\zeta(0,\imath\boldsymbol{\sigma}_1,0,0)\rangle, \\
\Re\rho_3 = \langle\mathcal{I},\zeta(0,-\boldsymbol{\sigma}_3,0,0)\rangle, \quad \Im\rho_3 = \langle\mathcal{I},\zeta(0,-\imath\boldsymbol{\sigma}_3,0,0)\rangle, \\
\Re\rho_4 = \langle\mathcal{I},\zeta(0,\imath\boldsymbol{\sigma}_0,0,0)\rangle, \quad \Im\rho_4 = \langle\mathcal{I},\zeta(0,-\boldsymbol{\sigma}_0,0,0)\rangle, \\
\Re\rho_5 = \langle\mathcal{I},\zeta(0,0,\imath\boldsymbol{\sigma}_1,\imath\boldsymbol{\sigma}_1)\rangle, \quad \Im\rho_5 = \langle\mathcal{I},\zeta(0,0,-\boldsymbol{\sigma}_1,-\boldsymbol{\sigma}_1)\rangle, \\
\Re\rho_6 = \langle\mathcal{I},\zeta(0,0,\boldsymbol{\sigma}_1,-\boldsymbol{\sigma}_1)\rangle, \quad \Im\rho_6 = \langle\mathcal{I},\zeta(0,0,\imath\boldsymbol{\sigma}_1,-\imath\boldsymbol{\sigma}_1)\rangle.
\end{gathered} \tag{69}$$

More explicitly, we define the components of $\rho_{5,8}$ by

$$\begin{aligned}
\rho_1(\mathbf{z}) &= \imath(-z_1z_6 + z_3z_8 + z_2z_5 - z_4z_7),\\
\rho_2(\mathbf{z}) &= z_1z_6 + z_3z_8 + z_2z_5 + z_4z_7,\\
\rho_3(\mathbf{z}) &= z_2z_6 + z_3z_7 - z_1z_5 - z_4z_8,\\
\rho_4(\mathbf{z}) &= \imath(-z_1z_5 + z_4z_8 - z_2z_6 + z_3z_7),\\
\rho_5(\mathbf{z}) &= \imath(-z_1z_8 - z_2z_7 - z_3z_6 - z_4z_5),\\
\rho_6(\mathbf{z}) &= z_1z_8 + z_2z_7 - z_3z_6 - z_4z_5.
\end{aligned} \tag{70}$$

We remark that in each case ($m=4$ and $m=8$) the particular matrices $\zeta \in \mathcal{F}$ that we have chosen are orthogonal among them. Moreover, we can extend this particular subset of $\mathcal{F}$ to an orthonormal basis (as shown by Kummer[20] in the case $m=4$) obtaining Hamiltonians $\langle \mathcal{I}(\boldsymbol{\eta}, \bar{\boldsymbol{\eta}}), \zeta \rangle$ which give the six generators of the SO(4) group and the 15 generators of the SO(6) group for $m=4$ and $m=8$, respectively. Moreover, in both cases we can choose one of the basis elements such that we obtain the Hamiltonian $H=\sum_{k=1}^{k=m}|z_k|^2$. Thus we can obtain $8+6+1=15$ and $12+15+1=28$ elements of the basis of $\mathcal{F}$ when $m=4$ and $m=8$, respectively. Note that in both cases $m=4,8$ the moment map $\mathcal{I}$ is invariant under the action of G defined by Eqs. (54)–(56). Therefore, the map $\rho_{(n,m)}(\mathbf{z})$ enjoys that invariance property too and it is well defined on the reduced symplectic manifold $\mathcal{K}_m^{-1}(0)/G$. Moreover, the map $\rho(\mathbf{z})$ is onto and takes values in the null quadric Q^3 or Q^5 corresponding to the cases $m=4$ or $m=8$.

VI. CANONICAL TRANSFORMATION

In this section we provide a canonical transformation $\tilde{\mathcal{C}}_{(n,m)}$ from $(\mathcal{K}_m^{-1}(0)-\{0\})/G$ (with $\{0\}$ denoting the origin of $\mathbb{C}^m$) onto $T^*S^n-\{0\}$ (here $\{0\}$ denotes the zero section of T^*S^n). This transformation comes from a map $\mathcal{C}_{(n,m)}$ defined as the composition of the map $\rho_{(n,m)}$ defined in the preceding section (and restricted to $\mathbb{C}^m-\{0\}$) and a map σ which identifies the null quadric $Q^n-\{0\}$ with $T^*S^n-\{0\}$. The map $\tilde{\mathcal{C}}_{(n,m)}$ has the remarkable property that relates the two different ways to regularize the Kepler problem that we have explained in the preceding sections (the Moser and $\mathcal{H}_{(n,m)}$ maps). Moreover, the Bargmann transform for $L^2(S^n)$, $n=2,3,5$, that we will define in the next section can be regarded as the quantization of the canonical transformation $\mathcal{C}_{(n,m)}$.

Let us define the map σ_n in the following way. Since $\boldsymbol{\alpha} \in Q^n$ if and only if the real and imaginary parts of $\boldsymbol{\alpha}$ are orthogonal and have the same norm (as vectors in $\mathbb{R}^{n+1}$), then we can identify $Q^n-\{0\}$ with $T^*S^n-\{0\}$ through the map

$$\begin{aligned}
&\sigma_n: Q^n - \{0\} \mapsto T^*S^n - \{0\},\\
&\sigma_n(\boldsymbol{\alpha}) = \left(\frac{\Re\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|}, -\Im\boldsymbol{\alpha}\right).
\end{aligned} \tag{71}$$

Thus we define the map $\mathcal{C}_{(n,m)}$ as composition of the maps $\rho_{(n,m)}$ and σ_n,

$$\begin{aligned}
&\mathcal{C}_{(n,m)}: \mathbb{C}^m - \{0\} \mapsto T^*S^n - \{0\},\\
&\mathcal{C}_{(n,m)} = \rho_{(n,m)} \circ \sigma_n.
\end{aligned} \tag{72}$$

The map $\mathcal{C}_{(n,m)}$ makes the following diagram commute:

$$\begin{array}{ccc} \mathcal{K}_m^{-1}(0)-(\{0\}\cup P) & \xrightarrow{\mathcal{C}_{(n,m)}} & T^*S_0^n-\{0\} \\ \Big\downarrow \mathcal{T}_m^{-1} & & \Big\downarrow \mathcal{M}_n^{-1} \\ \mathcal{J}_m^{-1}(0) & \xrightarrow{\mathcal{H}_{(n,m)}} & T^*(\mathbb{R}^n-\{0\}) \end{array}$$

where the set P denotes the inverse image of the cotangent space of S^n at the north pole under the map $\mathcal{C}_{(n,m)}$ and $\mathcal{T}_m: T^*\mathbb{R}^m \mapsto \mathbb{C}_m$ denotes the complexification indicated in Eq. (40). Note that the set P is actually given by the inverse image of the real number one under the function $\Re\rho_{n+1}$ which is invariant under the action of the group G and therefore we can consider the quotient $\widetilde{P} := P/G$.

To check that the last diagram holds, we can make use of the relations $|\Re\rho_{(n,m)}| = |\rho_{(n,m)}|/\sqrt{2}$, $|\rho_{(n,m)}| = |\mathbf{z}|^2/\sqrt{2}$ and the equations

$$\begin{aligned} p_j &= \frac{\Re\rho_j(\mathbf{z})}{|\Re\rho_{(n,m)}(\mathbf{z})| - \Re\rho_{n+1}(\mathbf{z})}, \\ x_j &= \frac{-|\Re\rho_{(n,m)}(\mathbf{z})|\Im\rho_j(\mathbf{z}) + \Im\{\overline{\rho_{n+1}(\mathbf{z})}\rho_j(\mathbf{z})\}}{|\Re\rho_{(n,m)}(\mathbf{z})|}, \quad j=1,\ldots,n. \end{aligned} \tag{73}$$

where the components of $\rho_{(n,m)}$ are denoted by $\rho_j(\mathbf{z})$ as above. Then a long computation follows.

Moreover, when $\mathcal{C}_{(n,m)}$ is considered as in the last diagram, we can check through a direct computation that $\mathbf{w}\,\mathrm{d}\boldsymbol{\xi} = \Im\{\overline{\mathbf{z}}\,\mathrm{d}\mathbf{z}\}$, which in turn implies that $\mathcal{C}^*_{(n,m)}\kappa = \theta$.

Since $\mathcal{C}_{(n,m)}$ is invariant under the action of the group G, we can define our canonical transformation $\widetilde{\mathcal{C}}_{(n,m)}$ as the reduction of $\mathcal{C}_{(n,m)}$ and with domain $(\mathcal{K}_m^{-1}(0)-\{0\})/G-\widetilde{P}$. As indicated in the introduction of this paper, we still call $\mathcal{C}_{(n,m)}$ a canonical transformation even though it is not injective.

VII. BARGMANN TRANSFORM

In this section we define a Bargmann transform for the space $L^2(S^n)$ with $n=2,3,5$. We do this by following the ideas in Refs. 27 and 28. Namely, we regard the Bargmann transform as an integral operator from $L^2(S^n)$ onto a suitable Hilbert space of analytical functions of the complex variable $\mathbf{z}\in\mathbb{C}^m$ ($m=2,4,8$) with an integral kernel given as a power series of a function which in turn is the inner product of $\rho_{(n,m)}(\mathbf{z})$ with the variable $\mathbf{w}$ in S^n.

In order to define the range of the Bargmann transform for $L^2(S^n)$, let us recall the usual Bargmann spaces $\mathcal{B}_k$ introduced by Bargmann in Ref. 4.

A. Bargmann transform for $L^2(\mathbb{R}^k)$

For $k\in\mathbb{N}$, let $\mathcal{B}_k$ be the space of analytical functions in k complex variables [denoted by $\mathbf{z}=(z_1,z_2,\ldots,z_k)$] which are square integrable with respect to the Gaussian measure

$$\mathrm{d}\nu_k(\mathbf{z}) = \frac{1}{\pi^k}\exp(-|\mathbf{z}|^2)\prod_{j=1}^{k}\mathrm{d}x_j\,\mathrm{d}y_j, \tag{74}$$

where $|\mathbf{z}|^2 = |z_1|^2+|z_2|^2+\cdots+|z_k|^2$ and $z_j = x_j+\imath y_j$, $x_j,y_j\in\mathbf{R}$, with $j=1,2,\ldots,k$.

The space $\mathcal{B}_k$ is a Hilbert space endowed with the inner product

$$\langle F,G\rangle_{\mathcal{B}_k} = \int_{\mathbb{C}^k} F(\mathbf{z})\bar{G}(\mathbf{z})\mathrm{d}\nu_k(\mathbf{z}). \tag{75}$$

The norm of a function $F \in \mathcal{B}_k$ will be denoted by $\|F\|_{\mathcal{B}_k} = \sqrt{\langle F, F\rangle_{\mathcal{B}_k}}$.

The set of all monomials $z_1^{a_1} z_2^{a_2} \cdots z_k^{a_k} / \sqrt{a_1! a_2! \cdots a_k!}$, with $a_1, a_2, \ldots, a_k$ non-negative integers, is an orthonormal basis of $\mathcal{B}_k$.

The space $\mathcal{B}_k$ has a reproducing kernel. Let us denote by

$$\mathbf{\Psi}_{\mathbf{a}}(\mathbf{z}) = \exp(\bar{\mathbf{a}}\mathbf{z}), \quad \text{with } \mathbf{a} \in \mathbb{C}^k. \tag{76}$$

Then for all $\mathbf{\Phi} \in \mathcal{B}_k$ the following equation holds:

$$\mathbf{\Phi}(\mathbf{z}) = \langle \mathbf{\Phi}, \mathbf{\Psi}_{\mathbf{z}} \rangle_{\mathcal{B}_k} = \int_{\mathbb{C}^k} \exp(\mathbf{z}\bar{\eta}) \mathbf{\Phi}(\eta) \mathrm{d}\nu_k(\eta). \tag{77}$$

The Bargmann transform for $\mathrm{L}^2(\mathbb{R}^k)$ is defined as the operator $\mathbf{B}_{\mathbb{R}^k}: L^2(\mathbb{R}^k) \mapsto \mathcal{B}_k$ given by

$$\mathbf{B}_{\mathbb{R}^k} \mathbf{\Psi}(\mathbf{z}) = \frac{1}{\pi^{k/4}} \int_{\mathbb{R}^k} A(\mathbf{x}, \mathbf{z}) \Psi(\mathbf{x}) \mathrm{d}\mathbf{x}, \quad \mathbf{\Psi} \in L^2(\mathbb{R}^k), \tag{78}$$

where $\mathrm{d}\mathbf{x}$ is the usual Lebesgue measure on $\mathbb{R}^k$ and

$$A(\mathbf{x}, \mathbf{z}) = \exp\left(-\tfrac{1}{2}(\mathbf{z}^2 + \mathbf{x}^2) + \sqrt{2}\mathbf{z} \cdot \mathbf{x}\right), \tag{79}$$

with $\mathbf{z}^2 = z_1^2 + z_2^2 + \cdots + z_k^2$, $\mathbf{x} = (x_1, x_2, \ldots, x_k)$, $\mathbf{x}^2 = x_1^2 + x_2^2 + \cdots + x_k^2$ and $\mathbf{z} \cdot \mathbf{x} = z_1 x_1 + z_2 x_2 + \cdots + z_k x_k$. The Bargmann transform $\mathbf{B}_{R^k}$ is a unitary operator with $\mathrm{L}^2(\mathbb{R}^k)$ endowed with the usual inner product,

$$\langle \mathbf{\Psi}_1, \mathbf{\Psi}_2 \rangle_{L^2(\mathbb{R}^k)} = \int_{\mathbf{x} \in \mathbb{R}^k} \mathbf{\Psi}_1(\mathbf{x}) \overline{\mathbf{\Psi}_2}(\mathbf{x}) \mathrm{d}\mathbf{x}. \tag{80}$$

The inverse $\mathbf{B}_{\mathbb{R}^k}^{-1}$ is given by

$$\mathbf{B}_{\mathbb{R}^k}^{-1} F(\mathbf{x}) = \lim_{M \mapsto \infty} \int_{|\mathbf{z}| \leq M} \overline{A(\mathbf{x}, \mathbf{z})} F(\mathbf{z}) \mathrm{d}\nu_k(\mathbf{z}). \tag{81}$$

Here we need to take the limit because the integral over all the space $\mathbf{C}^k$ might not exist [note that, for fixed $\mathbf{x}$, $A(\mathbf{x}, \mathbf{z}) \notin \mathcal{B}_k$].

B. Bargmann transform for $L^2(S^n)$ with $n = 2, 3, 5$

The range of the Bargmann transform for $L^2(S^n)$ with $n = 2$, 3 or 5 will be defined as a closed subspace of the Bargmann space $\mathcal{B}_2$, $\mathcal{B}_4$ or $\mathcal{B}_8$, respectively.

(i) *Case* $L^2(S^2)$: Let us define the space $\mathcal{F}_2$ as the closed subspace of the Bargmann space $\mathcal{B}_2$ generated by the monomials $z_1^{a_1} z_2^{a_2}$ with $a_1 + a_2$ an even non-negative integer number.

(ii) *Case* $L^2(S^3)$: Let $\mathcal{F}_4 \subset \mathcal{B}_4$ be the kernel of the following operator:

$$\mathcal{L} \equiv z_1 \frac{\partial}{\partial z_1} + z_2 \frac{\partial}{\partial z_2} - z_3 \frac{\partial}{\partial z_3} - z_4 \frac{\partial}{\partial z_4}. \tag{82}$$

The domain of $\mathcal{L}$ is defined as $\{f \in \mathcal{B}_4 \,|\, \mathcal{L}f \in \mathcal{B}_4\}$.

(iii) *Case* $L^2(S^5)$: Let $\mathcal{F}_8 \subset \mathcal{B}_8$ be the intersection of the kernel of the following three operators:

$$\mathcal{R}_1 \equiv z_1 \frac{\partial}{\partial z_1} + z_2 \frac{\partial}{\partial z_2} + z_3 \frac{\partial}{\partial z_3} + z_4 \frac{\partial}{\partial z_4} - z_5 \frac{\partial}{\partial z_5} - z_6 \frac{\partial}{\partial z_6} - z_7 \frac{\partial}{\partial z_7} - z_8 \frac{\partial}{\partial z_8},$$

$$\mathcal{R}_2 \equiv z_7 \frac{\partial}{\partial z_1} - z_8 \frac{\partial}{\partial z_2} + z_5 \frac{\partial}{\partial z_3} - z_6 \frac{\partial}{\partial z_4} - z_1 \frac{\partial}{\partial z_7} + z_2 \frac{\partial}{\partial z_8} - z_3 \frac{\partial}{\partial z_5} + z_4 \frac{\partial}{\partial z_6},$$

$$\mathcal{R}_3 \equiv z_7\frac{\partial}{\partial z_1} - z_8\frac{\partial}{\partial z_2} + z_5\frac{\partial}{\partial z_3} - z_6\frac{\partial}{\partial z_4} + z_1\frac{\partial}{\partial z_7} - z_2\frac{\partial}{\partial z_8} + z_3\frac{\partial}{\partial z_5} - z_4\frac{\partial}{\partial z_6}. \tag{83}$$

The domains of $\mathcal{R}_q, q=1,2,3$ are defined in a similar way as the domain of $\mathcal{L}$. The definition of the operators $\mathcal{L}$ and $\mathcal{R}_q$ is motivated by the quantization of the restrictions given by $\mathcal{K}_m^{-1}\{0\}$ [see Eqs. (49) and (50) with the change of variables (47)] taking z_j and $\bar{z}_j$ to the operators of multiplication by the complex variable z_j and to partial derivation with respect to z_j, respectively, with $j=1,\ldots,m$.

Notice that, since the operators $\mathcal{L}$, $\mathcal{R}_1$, and $\mathcal{R}_2$ are closed (see Sec. 3d of Ref. 4), the spaces $\mathcal{F}_4$ and $\mathcal{F}_8$ are actually Hilbert spaces.

Following Refs. 27 and 28, we define the Bargmann transform in the three cases we are considering, initially in a formal way, as the following integral operator: For $\Psi \in L^2(S^n)$,

$$\mathbf{B}_{S^n}\boldsymbol{\Psi}(\mathbf{z}) = \int_{S^n}\left(\sum_{k=0}^{\infty} c_k(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right)\boldsymbol{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}), \quad \mathbf{z}\in\mathbb{C}^m, \tag{84}$$

where the inner product of two vectors in $\mathbb{C}^{n+1}$ is given by $\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=\Sigma_{j=1}^{n+1}\alpha_j\bar{\beta}_j$.

The coefficients c_k appearing in Eq. (84) are determined in such a way that $\mathbf{B}_{S^n}$ is an isometry. Thus let us consider the function $\boldsymbol{\Psi}_\ell(\mathbf{w})=d_\ell((\mathbf{e}_1+\imath\mathbf{e}_2)\cdot\mathbf{w})^\ell$ where ℓ is a non-negative integer, $\mathbf{e}_1=(1,0,\ldots,0)$ and $\mathbf{e}_2=(0,1,0,\ldots,0)$ are two unit vectors in $\mathbb{R}^{n+1}$ and d_ℓ is a normalization constant such that $\|\boldsymbol{\Psi}_\ell\|_{L^2(S^n)}=1$. Since the integral

$$\begin{aligned}\int_{S^n}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k((\mathbf{e}_1+\imath\mathbf{e}_2)\cdot\mathbf{w})^\ell\,\mathrm{d}S(\mathbf{w}) = \delta_{k,\ell}\Bigg\{&\frac{(2k)!!}{(2k+1)!!}\left(\frac{\alpha_1(\mathbf{z})+\imath\alpha_2(\mathbf{z})}{2}\right)^k \quad \text{for } n=2,\\ &\times\frac{1}{k}\left(\frac{\alpha_1(\mathbf{z})+\imath\alpha_2(\mathbf{z})}{2}\right)^k \quad \text{for } n=3,\\ &\times\frac{2}{(k+2)(k+1)}\left(\frac{\alpha_1(\mathbf{z})+\imath\alpha_2(\mathbf{z})}{2}\right)^k \quad \text{for } n=5\Bigg\},\end{aligned} \tag{85}$$

where $(2k)!!$ is the product of all positive even numbers lesser or equal than $2k$ [a similar definition for $(2k+1)!!$].

Then by demanding Ψ_ℓ to be sent to the function $\Phi_\ell=b_\ell([\alpha_1(\mathbf{z})+\imath\alpha_2(\mathbf{z})]/2)^\ell$ (with b_ℓ a normalization constant such that $\|\Phi_\ell\|_{\mathcal{B}_m}=1$) we can evaluate the constant c_k obtaining

$$c_k = \left\{\frac{\sqrt{2k+1}}{k!} \quad \text{for } n=2, \quad \frac{\sqrt{k+1}}{k!} \quad \text{for } n=3, \quad \sqrt{\frac{k+2}{2}}\frac{1}{k!} \quad \text{for } n=5\right\}. \tag{86}$$

Since the series $\Sigma_{k=0}^{\infty}c_k(\eta)^k$ is an analytic function in the complex variable η on the whole complex plane, and $|(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})|\leqslant|\rho_{(n,m)}(\mathbf{z})|$ then the integral appearing in Eq. (84) is well defined for $\boldsymbol{\Psi}\in L^2(S^n)$ [and therefore in $L^1(S^n)$] and $\mathbf{z}\in\mathbb{C}^m$. Moreover, $\mathbf{B}_{S^n}\boldsymbol{\Psi}$ has the following properties.

Proposition 1: Let $\boldsymbol{\Psi}\in L^2(S^n)$.

(i) *The function* $\mathbf{B}_{S^n}\boldsymbol{\Psi}$ *[defined by Eq. (84)] is an analytical function on the whole complex space* $\mathbb{C}^m$.
(ii) *The Bargmann transform* $\mathbf{B}_{S^n}$ *is an isometry,* $\|\mathbf{B}_{S^n}\boldsymbol{\Psi}\|_{\mathcal{B}_m}=\|\boldsymbol{\Psi}\|_{L^2(S^n)}$.
(iii) *The function* $\mathbf{B}_{S^n}\boldsymbol{\Psi}$ *is in the space* $\mathcal{F}_m$.

Note that from (ii) we have that the Bargmann transform $\mathbf{B}_{S^n}$ is one-to-one and that the function $\mathbf{B}_{S^n}\boldsymbol{\Psi}$ belongs to the space $\mathcal{B}_m$.

Proof:(i) Let $\mathbf{z}$ be a fixed element of $\mathbb{C}^m$. We will show that $(\partial/\partial z_j)\mathbf{B}_{S^n}\boldsymbol{\Psi}(\mathbf{z})$ exist for any j

$=1,2,\ldots,m$. Let $\mathbf{q}=(0,\ldots,h,\ldots,0)\in\mathbb{C}^m$ with the complex variable h in the jth entry and $|h|<\delta$ (for some positive number δ). Since

$$\frac{1}{h}[\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z}+\mathbf{q})-\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})]=\int_{S^n}\sum_{k=0}^{\infty}c_k\left[\frac{(\rho_{(n,m)}(\mathbf{z}+\mathbf{q})\cdot\mathbf{w})^k-(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k}{h}\right]\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}) \tag{87}$$

then, on base of the dominated convergence theorem, it will be enough to prove that the sequence of functions

$$f_h(\mathbf{w})\equiv\sum_{k=0}^{\infty}c_k\left[\frac{(\rho_{(n,m)}(\mathbf{z}+\mathbf{q})\cdot\mathbf{w})^k-(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k}{h}\right],\quad \mathbf{w}\in S^n \tag{88}$$

is uniformly bounded by a constant. Namely, from the Cauchy's integral formula we have

$$\left|\frac{(\rho_{(n,m)}(\mathbf{z}+\mathbf{q})\cdot\mathbf{w})^k-(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k}{h}\right|\leqslant\frac{1}{2\pi}\oint_{\mathcal{C}}\frac{|(\rho_{(n,m)}(\eta)\cdot\mathbf{w})^k|}{|(\eta-(\mathbf{z}+\mathbf{q}))||(\eta-\mathbf{z})|}d|\eta| \tag{89}$$

with $\mathcal{C}=\{(z_1,\ldots,z_j+r\exp(\imath 2\pi\theta),\ldots,z_m)\,|\,0\leqslant\theta\leqslant 1\}$ and $\delta<r$. Therefore,

$$|f_h(\mathbf{w})|\leqslant\frac{1}{r(r-\delta)}\sum_{k=0}^{\infty}c_k(\max\{|\rho_{(n,m)}(\eta)||\,\eta\in\mathcal{C}\})^k. \tag{90}$$

Thus we conclude that $\partial/\partial z_j\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})$ exist and

$$\begin{aligned}\frac{\partial}{\partial z_j}\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})&=\int_{S^n}\frac{\partial}{\partial z_j}\left(\sum_{k=0}^{\infty}c_k(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right)\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w})\\&=\int_{S^n}\left(\sum_{k=0}^{\infty}c_k\frac{\partial}{\partial z_j}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right)\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}).\end{aligned} \tag{91}$$

(ii) We will use the following criterion (see Sec. 1g of Ref. 4): an analytical function F on $\mathbb{C}^m$ is in the Bargmann space $\mathcal{B}_m$ if and only if for $0<\lambda<1$ the functions F_λ defined as $F_\lambda(\mathbf{z})=F(\lambda\mathbf{z})$ belong to $\mathcal{B}_m$ and their norms $\|F_\lambda\|_{\mathcal{B}_m}$ are uniformly bounded. Moreover, if $F\in\mathcal{B}_m$ then $F_\lambda\to F$ as $\lambda\to 1$ in the norm of $\mathcal{B}_m$.

Thus let us consider the functions $\mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})$. The main point in the following calculations is that $0<\lambda<1$ and then we can use Fubini's theorem.

Let us define

$$\begin{aligned}I=&\int_{\mathbb{C}^m}\int_{S^n\times S^n}\left(\sum_{k=0}^{\infty}c_k\lambda^{2k}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right)\\&\times\left(\sum_{\ell=0}^{\infty}c_\ell\lambda^{2\ell}\overline{(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{v})}^{\ell}\right)\mathbf{\Psi}(\mathbf{w})\overline{\mathbf{\Psi}(\mathbf{v})}\mathrm{d}S(\mathbf{w})\mathrm{d}S(\mathbf{v})\mathrm{d}\nu_m(\mathbf{z}).\end{aligned} \tag{92}$$

Let us define the following function:

$$f(\mathbf{z},(\mathbf{w},\mathbf{v}))=\left(\sum_{k=0}^{\infty}c_k\lambda^{2k}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right)\left(\sum_{\ell=0}^{\infty}c_\ell\lambda^{2\ell}\overline{(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{v})}^{\ell}\right). \tag{93}$$

Since $|\Re\rho_{(n,m)}(\mathbf{z})|=|\Im\rho_{(n,m)}(\mathbf{z})|$ and $|\Re\rho_{(n,m)}(\mathbf{z})|=(1/\sqrt{2})|\rho_{(n,m)}(\mathbf{z})|=\frac{1}{2}|\mathbf{z}|^2$ in all of the cases we are considering, then

$$\left|\sum_{k=0}^{\infty} c_k\lambda^{2k}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\right| \leqslant \sum_{k=0}^{\infty} c_k\lambda^{2k}\left|\frac{\Re\rho_{(n,m)}(\mathbf{z})}{|\Re\rho_{(n,m)}(\mathbf{z})|}\cdot\mathbf{w}+\imath\frac{\Im\rho_{(n,m)}(\mathbf{z})}{|\Im\rho_{(n,m)}(\mathbf{z})|}\cdot\mathbf{w}\right|^k|\Re\rho_{(n,m)}(\mathbf{z})|^k$$
$$\leqslant \sum_{k=0}^{\infty} c_k\lambda^{2k}|\mathbf{w}|^k\left(\frac{|\mathbf{z}|^2}{2}\right)^k \leqslant \sum_{k=0}^{\infty} d_k\lambda^k\frac{1}{k!}\left(\frac{\lambda|\mathbf{z}|^2}{2}\right)^k \tag{94}$$

with $d_k=c_k k!$

Now notice that given $0<\lambda<1$, there exist N_λ such that $d_k\lambda^k<1$ for $k\geqslant N_\lambda$. Therefore,

$$\sum_{k=0}^{\infty} d_k\lambda^k\frac{1}{k!}\left(\frac{\lambda|\mathbf{z}|^2}{2}\right)^k \leqslant P(|\mathbf{z}|^2)+\exp\left(\frac{\lambda|\mathbf{z}|^2}{2}\right) \tag{95}$$

for some polynomial P which degree depends on λ. Since a polynomial times $\exp(\lambda|\mathbf{z}|^2)$ is integrable with respect to the Gaussian measure $\mathrm{d}\nu_m(\mathbf{z})$, then the integral of $|f(\mathbf{z},(\mathbf{w},\mathbf{v}))|$ is finite with respect to $\mathrm{d}\nu_m(\mathbf{z})$. Moreover, since $\mathbf{\Psi}\in L^2(S^n)$ and then $\mathbf{\Psi}\in L^1(S^n)$, we can use Fubini's theorem in order to interchange the two integrals appearing in Eq. (92). Thus we have

$$I=\int_{S^n}\sum_{k=0}^{\infty}\int_{S^n}\int_{\mathbb{C}^m} c_k^2\lambda^{4k}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\overline{(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{v})}^k\,\mathrm{d}\nu_m(\mathbf{z})\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w})\overline{\mathbf{\Psi}(\mathbf{v})}\mathrm{d}S(\mathbf{v}), \tag{96}$$

where we have used the orthogonality of two given homogeneous polynomials of different degree in the Bargmann space $\mathcal{B}_m$.

Let us denote by P_k the projector onto the kth eigenspace of the Laplacian. In Appendix B we prove that the first two integrals in Eq. (96) give an expression of P_k acting on Ψ. Namely,

$$P_k\mathbf{\Psi}(\mathbf{v})=\int_{S^n} J_k(\mathbf{w},\mathbf{v})\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}) \tag{97}$$

with

$$J_k(\mathbf{w},\mathbf{v})=c_k^2\int_{\mathbb{C}^m}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k\overline{(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{v})}^k\,\mathrm{d}\nu_m(\mathbf{z}). \tag{98}$$

Thus we have

$$\int_{\mathbb{C}^m}\mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})\overline{\mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})}\mathrm{d}\nu_m(\mathbf{z})=\int_{S^n}\sum_{k=0}^{\infty}\lambda^{4k}P_k\mathbf{\Psi}(\mathbf{v})\overline{\mathbf{\Psi}(\mathbf{v})}\mathrm{d}S(\mathbf{v}). \tag{99}$$

Let

$$f_\lambda(\mathbf{v})=\sum_{k=0}^{\infty}\lambda^{4k}P_k\mathbf{\Psi}(\mathbf{v})\overline{\mathbf{\Psi}(\mathbf{v})} \tag{100}$$

By following the same procedure as in Eq. (94) we obtain

$$|J_k(\mathbf{w},\mathbf{v})|\leqslant\frac{c_k^2}{2^{2k}}\int_{\mathbb{C}^m}(|\mathbf{z}|^2)^{2k}\,\mathrm{d}\nu_m(\mathbf{z}). \tag{101}$$

Since $c_k^2\lambda^{2k}(2k)!/2^{2k+1}$ is bounded, then we obtain from the bounded dominated convergence theorem

$$|f_\lambda(\mathbf{v})| \leqslant C|\mathbf{\Psi}(\mathbf{v})| \int_{\mathbb{C}^m} (\exp(\lambda|\mathbf{z}|^2) + \exp(-\lambda|\mathbf{z}|^2)) \mathrm{d}\nu_m(\mathbf{z}) \tag{102}$$

for some constant involving the integral of $|\mathbf{\Psi}|$ on S^n.

Since $0<\lambda<1$ then $|f_\lambda(\mathbf{v})| \leqslant C|\mathbf{\Psi}(\mathbf{v})|$ (for some other finite constant C) which allows us to use the dominated convergence theorem in Eq. (99) to obtain

$$\int_{\mathbb{C}^m} \mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})\overline{\mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})}\mathrm{d}\nu_m(\mathbf{z}) = \sum_{k=0}^{\infty} \lambda^{4k}\langle P_k\mathbf{\Psi}, \mathbf{\Psi}\rangle = \sum_{k=0}^{\infty} \lambda^{4k}\|P_k\mathbf{\Psi}\|^2. \tag{103}$$

Since the right-hand side is finite then we have proved that, for $0<\lambda<1$, $\mathbf{B}_{S^n}\mathbf{\Psi}(\lambda\mathbf{z})$ are in $\mathcal{B}_m$ and their norms are uniformly bounded, therefore $\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})$ is in $\mathcal{B}_m$. Moreover,

$$\|\mathbf{B}_{S^n}\mathbf{\Psi}\|^2 = \lim_{\lambda\to 1} \sum_{k=0}^{\infty} \lambda^{4k}\|P_k\mathbf{\Psi}\|^2 = \sum_{k=0}^{\infty} \|P_k\mathbf{\Psi}\|^2 = \|\mathbf{\Psi}\|^2 \tag{104}$$

which proves that $\mathbf{B}_{S^n}$ is an isometry.

(iii) The case $(n,m)=(2,2)$ is immediate because the function $\rho_{(2,2)}$ is homogeneous of degree 2 in the variables (z_1,z_2). The cases $(n,m)=(3,4)$ and $(n,m)=(5,8)$, are consequence of Eq. (91) and the fact that each entry of the function $\rho_{(n,m)}(\mathbf{z})$ is in the kernel of the corresponding operators defining $\mathcal{F}_m$. □

C. Reproducing kernel for the spaces $\mathcal{F}_m$

by following Ref. 5 we will find the reproducing kernel of the spaces $\mathcal{F}_m$ by taking the average of the reproducing kernel of the corresponding Bargmann space (where $\mathcal{F}_m$ is contained) with respect to the action and Haar measures of the groups $\mathbb{Z}_2, S^1$, SU(2) for the cases $m=2,4,8$, respectively.

Let us consider the action of the group $G=\mathbb{Z}_2$, S^1, SU(2) on the space $\mathbb{C}^m$ for $m=2,4,8$, respectively, given by Eqs. (54)–(56).

Proposition 2. For $m=2,4,8$, the elements of the Hilbert spaces $\mathcal{F}_m$ are given by the invariant functions in $\mathcal{B}_m$ under the group actions of $\mathbb{Z}_2$, S^1, SU(2) described above. Namely, $\mathcal{F}_2=\{f \in \mathcal{B}_2 | f(T_g(z))=f(z)\ \forall\, g\in\mathbb{Z}_2\}$, $\mathcal{F}_4=\{f\in\mathcal{B}_4|f(T_g(z))=f(z)\ \forall\, g\in S^1\}$ and $\mathcal{F}_8=\{f\in\mathcal{B}_8|f(T_g(z))=f(z)\ \forall\, g\in \mathrm{SU}(2)$.

Proof: Since the set of monomials $z_1^{a_1}z_2^{a_2}/a_1!a_2!$ (with a_1 and a_2 non-negative integer numbers) is an orthonormal basis of $\mathcal{B}_2$, then the case $m=2$ is immediate.

Let us now consider a similar basis of monomials for the Bargmann space $\mathcal{B}_4$. One can show that $f\in\mathcal{B}_4$ is in $\mathcal{F}_4$ if and only if f is a linear combination of monomials of the type $z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}$ with $a_1+a_2-a_3-a_4=0$ (see the proof of Proposition 2.1 of Ref. 27). Thus if $f\in\mathcal{F}_4$ then f is clearly invariant under the action of S^1 described above. Conversely, if $f\in\mathcal{B}_4$ is invariant, then by considering the expansion of f in terms of all of the monomials $z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}$ (i.e., with $a_j, j=1,2,3,4$ arbitrary non-negative integer numbers) we conclude that $\exp(\imath(-a_1-a_2+a_3+a_4)\psi)=1\ \forall\,\psi\in\mathbb{R}$ which it is possible only if $a_1+a_2-a_3-a_4=0$. Thus f must belong to $\mathcal{F}_4$.

Let us assume that $f\in\mathcal{B}_8$ is invariant under the action of SU(2), that is

$$f(T_g(z)) = f(z)\ \forall\ g\in \mathrm{SU}(2). \tag{105}$$

Let us consider the following parametrization of $g\in\mathrm{SU}(2)$:

$$g = \begin{pmatrix} \cos(\theta)\exp(\imath\alpha) & \sin(\theta)\exp(\imath\beta) \\ -\sin(\theta)\exp(-\imath\beta) & \cos(\theta)\exp(-\imath\alpha) \end{pmatrix} \tag{106}$$

with $\theta\in[0,\pi/2]$ and $\alpha,\beta\in[-\pi,\pi]$

By considering the partial derivative of both sides in Eq. (105) with respect to α and evaluating the resulting equation at the point $(\theta,\beta,\alpha)=(0,0,0)$, we obtain that f must belong to the

kernel of the operator $\mathcal{R}_1$. In a similar way, we can prove that f is in the kernel of the operators $\mathcal{R}_2$ and $\mathcal{R}_3$ by considering the partial derivatives with respect to θ and β, respectively, and then evaluating at the point $(\theta,\beta,\alpha)=(0,0,0)$ (we actually need to take the limit $\theta\to 0$ in the last case).

Conversely, let us assume $\mathcal{R}_1 f=\mathcal{R}_2 f=\mathcal{R}_3 f=0$ and consider the function $h(\theta,\beta,\alpha)=f(T_g(\mathbf{z}))-f(\mathbf{z})$ regarding $\mathbf{z}\in\mathbb{C}^8$ as fixed. By considering the inverse transformation of Eq. (55), it is possible to show that the gradient of h with respect to the variables θ,β,α must be equal to zero. Since $h(0,0,0)=0$, then $h(\theta,\beta,\alpha)=0$ for all θ,β,α and then f must be invariant under the SU(2) action. □

Theorem 3: *The Hilbert space $\mathcal{F}_m$, $m=2,4,8$, has the following reproducing kernel (respectively):*

$$\mathbf{Q}_2(\mathbf{z},\mathbf{w})=\frac{1}{2}(\exp(z_1\bar{w}_1+z_2\bar{w}_2)+\exp(-z_1\bar{w}_1-z_2\bar{w}_2)),$$

$$\mathbf{Q}_4(\mathbf{z},\mathbf{w})=\frac{1}{2\pi}\int_{\psi=0}^{2\pi}\exp(z_1\bar{w}_1\exp(\imath\psi)+z_2\bar{w}_2\exp(\imath\psi)+z_3\bar{w}_3\exp(-\imath\psi)+z_4\bar{w}_4\exp(-\imath\psi))\mathrm{d}\psi,$$

$$\mathbf{Q}_8(\mathbf{z},\mathbf{w})=\frac{1}{2\pi^2}\int_{\theta=0}^{\pi/2}\int_{\alpha=0}^{2\pi}\int_{\beta=0}^{2\pi}\exp(z_1'\bar{w}_1+\cdots+z_8'\bar{w}_8)\mathrm{d}m(\theta,\alpha,\beta), \tag{107}$$

where $\mathbf{z}'=T_g(\mathbf{z})$ is given by the action of SU(2) defined in Eq. (55) and $\mathrm{d}m(\theta,\alpha,\beta)=(1/2\pi^2)\sin(\theta)\cos(\theta)\mathrm{d}\theta\,\mathrm{d}\alpha\,\mathrm{d}\beta$ is the Haar measure of SU(2).

Proof: We just need to use the previous Proposition and the fact that $\exp(z_1\bar{w}_1+\cdots+z_m\bar{w}_m)$ is the reproducing kernel of the Bargmann space $\mathcal{B}_m$. □

D. The reproducing kernel for $\mathcal{F}_m$ and the Bargmann transform $\mathbf{B}_{S^n}$

The purpose of this section is to introduce a set of states $\{\mathbf{\Phi}_{\boldsymbol{\alpha}}|\,\boldsymbol{\alpha}\in Q^n-\{0\}\}$ in $L^2(S^n)$, $n=2,3,5$ with the property that their Bargmann transform give us the reproducing kernel $\mathbf{Q}_m$ of the space $\mathcal{F}_m$ when we take $\boldsymbol{\alpha}=\rho_{(n,m)}(\mathbf{w})$, with $m=2,4,8$, respectively.

Following Refs. 27 and 28, let us define the following functions in $L^2(S^n)$, $n=2,3,5$:

$$\mathbf{\Phi}_{\bar{\boldsymbol{\alpha}}}(\mathbf{x})=\sum_{k=0}^{\infty}c_k(\bar{\boldsymbol{\alpha}}\cdot\mathbf{x})^k,\quad \bar{\boldsymbol{\alpha}}\in Q^n-\{0\} \tag{108}$$

with c_k given by Eq. (86).

Our first goal is to obtain an explicit expression for the Bargmann transform of $\mathbf{\Phi}_{\alpha}$. Let R be a rotation in $\mathrm{SO}(n+1)$ such that, for some $\mu>0$, $R\boldsymbol{\alpha}=\mu(\mathbf{e_1}+\imath\mathbf{e_2})$ with $\mathbf{e_1}=(1,0,\ldots,0)$ and $\mathbf{e_2}=(0,1,0,\ldots,0)$ two unit vectors in $\mathbb{R}^{n+1}$. Since $|(\mathbf{x}\cdot\boldsymbol{\alpha})|\leqslant|\Re\boldsymbol{\alpha}|$ for all $\mathbf{x}\in S^n$ and $\boldsymbol{\alpha}\in Q^n$ we obtain the following equation by using the dominated convergence theorem:

$$\begin{aligned}\mathbf{B}_{S^n}\mathbf{\Phi}_{\boldsymbol{\alpha}}(\mathbf{z})&=\sum_{k=0}^{\infty}\sum_{\ell=0}^{\infty}c_kc_\ell\int_{S^n}(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{x})^k(\mathbf{x}\cdot\boldsymbol{\alpha})^\ell\,\mathrm{d}S(\mathbf{x})\\&=\sum_{k=0}^{\infty}\sum_{\ell=0}^{\infty}\mu^\ell c_kc_\ell\int_{S^n}(R\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{y})^k(\mathbf{y}\cdot(\mathbf{e_1}+\imath\mathbf{e_2}))^\ell\,\mathrm{d}S(\mathbf{w}),\end{aligned} \tag{109}$$

where we have made the change of variable $\mathbf{y}=R\mathbf{x}$ and made use of the orthogonality of the rotation R.

The integral appearing in the last equation is equal to zero when $k \neq \ell$ because $(R\rho_{(n,m)} \times(\mathbf{z})\cdot\mathbf{y})^k$ and $(\mathbf{y}\cdot(\mathbf{e_1}+\imath\mathbf{e_2}))^\ell$ are eigenfunctions of the spherical Laplacian on S^n and therefore they are orthogonal (they are harmonic homogeneous polynomials of degree k and ℓ, respectively, in the components of the vector $\mathbf{y} \in \mathbb{R}^{n+1}$).

In order to evaluate the integral in Eq. (109) when $k=\ell$, let us introduce spherical coordinates $(\theta_1, \ldots, \theta_n)$ for the variable $\mathbf{y}=(y_1, \ldots, y_{n+1}) \in S^n$:

$$\begin{aligned} y_1 &= \sin(\theta_n)\cdots\sin(\theta_2)\sin(\theta_1), \\ y_2 &= \sin(\theta_n)\cdots\sin(\theta_2)\cos(\theta_1), \\ &\cdots, \\ y_n &= \sin(\theta_n)\cos(\theta_{n-1}), \\ y_{n+1} &= \cos(\theta_n). \end{aligned} \tag{110}$$

Since $\int_0^{2\pi} \exp(\_k\theta_1)\mathrm{d}\theta_1$ is equal to zero when $k \neq 0$ then we find after some computation,

$$\mathbf{B}_{S^n}\mathbf{\Phi}_{\boldsymbol{\alpha}}(\mathbf{z}) = \sum_{k=0}^{\infty} \mu^k f_k (R\rho_{(n,m)}(\mathbf{z})\cdot(\mathbf{e_1}+\imath\mathbf{e_2}))^k = 2\pi\sum_{k=0}^{\infty} f_k(\rho_{(n,m)}(\mathbf{z})\cdot\boldsymbol{\alpha})^k, \tag{111}$$

where

$$f_k = \left\{ \frac{1}{k!(2k-1)!!} \quad \text{for } n=2 \quad \frac{1}{2^k(k!)^2} \quad \text{for } n=3 \quad \frac{1}{2^k k!(k+1)!} \quad \text{for } n=5 \right\}. \tag{112}$$

By using the explicit expressions for the map $\rho_{(n,m)}$ [see Eqs. (46), (68), and (70)] in the expression $\rho_{(n,m)}(\mathbf{z})\cdot\boldsymbol{\alpha}$ with $\boldsymbol{\alpha}=\rho_{(n,m)}(\mathbf{w})$ we get the following equations:

$$\mathbf{B}_{S^2}\mathbf{\Phi}_{\rho_{(2,2)}(\mathbf{w})}(\mathbf{z}) = \sum_{k=0}^{\infty} \frac{1}{(2k)!}(z_1\bar{w}_1 + z_2\bar{w}_2)^{2k},$$

$$\mathbf{B}_{S^3}\mathbf{\Phi}_{\rho_{(3,4)}(\mathbf{w})}(\mathbf{z}) = \sum_{k=0}^{\infty} \frac{1}{(k!)^2}(z_1\bar{w}_1 + z_2\bar{w}_2)^k(z_3\bar{w}_3 + z_4\bar{w}_4)^k,$$

$$\begin{aligned} \mathbf{B}_{S^5}\mathbf{\Phi}_{\rho_{(5,8)}(\mathbf{w})}(\mathbf{z}) = \sum_{k=0}^{\infty} \frac{1}{k!(k+1)!}&([z_1\bar{w}_1 + z_2\bar{w}_2 + z_3\bar{w}_3 + z_4\bar{w}_4][z_5\bar{w}_5 + z_6\bar{w}_6 + z_7\bar{w}_7 + z_8\bar{w}_8] \\ &+ [z_7\bar{w}_1 - z_8\bar{w}_2 + z_5\bar{w}_3 - z_6\bar{w}_4][-z_3\bar{w}_5 + z_4\bar{w}_6 - z_1\bar{w}_7 + z_2\bar{w}_8])^k. \end{aligned} \tag{113}$$

We now establish the relation between the Bargmann transform of the functions $\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{w})}$ with the reproducing kernel of $\mathcal{F}_m$ in the following.

Theorem 4: *The Bargmann transform* $\mathbf{B}_{S^n}$ *of the functions* $\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{w})}$ *coincides with the reproducing kernel of the spaces* $\mathcal{F}_m$,

$$\mathbf{B}_{S^n}\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{w})}(\mathbf{z}) = \mathbf{Q}_m(\mathbf{z},\mathbf{w}). \tag{114}$$

Proof: Use the Taylor series expansion for the exponential function in the expression for $\mathbf{Q}_m(\mathbf{z},\mathbf{w})$ [see Eqs. (107)]. The last case $(n,m)=(5,8)$ requires a more elaborated calculation. For this case, integrate first with respect to α and then with respect to β. To perform the integration with respect

to θ use the identity $\int_0^{\pi/2} \sin^{2(k-\ell)+1}\cos^{2\ell+1} d(\theta)=(k-\ell)!\ell!/2(k+1)!$. □

In addition to having the property indicated in the last proposition, the set of functions $\{\mathbf{\Phi}_{\boldsymbol{\alpha}}|\,\boldsymbol{\alpha}\in Q^n-\{0\}\}$ provides a resolution of the identity which will be explained in the next section of this paper. Moreover, we will introduce in Section VII H the Planck's constant $\hbar$ into the definition of the states $\mathbf{\Phi}_{\boldsymbol{\alpha}}$ showing that they have a concentration property in the semi-classical limit $\hbar\to 0$. Thus, in analogy with some of the properties in the definition of coherent states for the harmonic oscillator (see Ref. 15 and Ref. 2 for different types of definitions of coherent states existing in the literature depending on the property to be emphasized), we will refer to $\{\mathbf{\Phi}_{\boldsymbol{\alpha}}|\,\boldsymbol{\alpha}\in Q^n-\{0\}\}$ as a set of coherent states for $L^2(S^n)$, $n=2,3,5$.

E. Unitarity of the Bargmann transform $\mathbf{B}_{S^n}$

In this section we show the following.

Theorem 5: *The Bargmann transform* $\mathbf{B}_{S^n}$, $n=2,3,5$, *is a unitary operator from* $L^2(S^n)$ *onto* $\mathcal{F}_m$, $m=2,4,8$.

Proof: We already have shown that $\mathbf{B}_{S^n}$ is an isometry [see Eq. (104)] which implies that $\mathbf{B}_{S^n}$ is a one-to-one operator and preserves the inner product (as a consequence of the polarization identity). Thus we only need to show that $\mathbf{B}_{S^n}$ is onto, i.e., that the range of $\mathbf{B}_{S^n}$ is the whole space $\mathcal{F}_m$.

From the preceding section we know that the reproducing kernel $\mathbf{Q}_m(\mathbf{z},\mathbf{w})$ is in the range of the Bargmann transform [think of $\mathbf{Q}_m(\mathbf{z},\mathbf{w})$ as a function of $\mathbf{z}$ for $\mathbf{w}$ fixed]. Therefore, the orthogonal complement in $\mathcal{F}_m$ of the range of $\mathbf{B}_{S^n}$ is the trivial vector space. Since $\mathcal{F}_m$ is a Hilbert space, then the range of $\mathbf{B}_{S^n}$ is dense in $\mathcal{F}_m$. Thus $\mathbf{B}_{S^n}$ is an isometry with dense range, which implies that it is onto. □

F. The inverse of the Bargmann transform $\mathbf{B}_{S^n}$

In this section we give an inversion formula for the Bargmann transform $\mathbf{B}_{S^n}$. Motivated by the expression for the inverse Segal-Bargmann transform introduced in Ref. 8 for $L^2(K)$ with K a compact Lie group, we state the following.

Theorem 6: *Let* $\{E_q|\,q\in\mathbb{N}\}$ *be an increasing sequence of bounded measurable sets in* $\mathbb{C}^m$ *such that* $\cup_{q=1}^{\infty}E_q=\mathbb{C}^m$. *Let* $f\in\mathcal{F}_m$. *Then the inverse Bargmann transform of* f *is given by*

$$\mathbf{B}_{S^n}^{-1}f(\mathbf{x})=\lim_{q\to\infty}\int_{E_q}\sum_{k=0}^{\infty}c_k\overline{(\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{x})^k}f(\mathbf{z})\mathrm{d}\nu_m(\mathbf{z}). \tag{115}$$

The proof of this proposition follows a standard procedure as in Ref. 8.

G. Coherent states for $L^2(S^n)$, $n=2,3,5$

In this section we show that the set of coherent states $\{\mathbf{\Phi}_{\boldsymbol{\alpha}}|\,\boldsymbol{\alpha}\in Q^n-\{0\}\}$ provides a resolution of the identity for the space $L^2(S^n)$. This resolution of the identity will be a consequence of the expression for the inverse of the Bargmann transform $\mathbf{B}_{S^n}$ that we obtained in the preceding section. We also include a description of the resolution of the identity for the eigenspaces of the Laplacian on S^n given by great-circle states that we define below.

Let $\mathbf{\Psi}\in L^2(S^n)$. From the inversion formula for the Bargmann transform obtained in the preceding section we have

$$\mathbf{\Psi}(x)=\lim_{q\mapsto\infty}\int_{E_q}\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{z})}\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})\mathrm{d}\nu_m(\mathbf{z}). \tag{116}$$

Notice that $\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})$ is equal to the inner product in $L^2(S^n)$ of $\mathbf{\Psi}$ with the coherent state $\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{z})}$:

$$\mathbf{B}_{S^n}\mathbf{\Psi}(\mathbf{z})=\langle\mathbf{\Psi},\mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{z})}\rangle. \tag{117}$$

Thus we conclude from Eq. (117) that

$$\mathbf{\Psi}(x) = \lim_{q\mapsto\infty} \int_{E_q} \langle \mathbf{\Psi}, \mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{z})} \rangle \mathbf{\Phi}_{\rho_{(n,m)}(\mathbf{z})} \, \mathrm{d}\nu_m(\mathbf{z}). \tag{118}$$

Let us now consider the map $\rho_{(n,m)}$ from $\mathbb{C}^m$ onto the null quadric Q^n. Let us denote by $\mathrm{d}\mu(\alpha)$ the measure on Q^n obtained from the measure $\mathrm{d}\nu_m(\mathbf{z})$ through the map $\rho_{(n,m)}$. Thus we can rewrite Eq. (118) as

$$\mathbf{\Psi}(\mathbf{x}) = \lim_{q\to\infty} \int_{E_q} \langle \mathbf{\Psi}, \mathbf{\Phi}_{\boldsymbol{\alpha}} \rangle \mathbf{\Phi}_{\boldsymbol{\alpha}} \, \mathrm{d}\mu_m(\boldsymbol{\alpha}). \tag{119}$$

We will refer to Eq. (119) as the resolution of the identity for $L^2(S^n)$.

Remark 7: *From Appendix A, it follows that the measure* $\mathrm{d}\mu_m$ *is* $\mathrm{SO}(n+1)$ *invariant. Namely, for all* $f \in L^1(\mathrm{d}\mu_m)$ *and* $R \in \mathrm{SO}(n+1)$ *we have*

$$\begin{aligned} \int f(R\boldsymbol{\alpha})\mathrm{d}\mu_m(\boldsymbol{\alpha}) &= \int f(R\rho_{(n,m)}(\mathbf{z}))\mathrm{d}\nu_m(\mathbf{z}) \\ &= \int f(\rho_{(n,m)}(U\mathbf{z}))\mathrm{d}\nu_m(\mathbf{z}) = \int f(\rho_{(n,m)}(\mathbf{z}'))\mathrm{d}\nu_m(\mathbf{z}') = \int f(\boldsymbol{\alpha})\mathrm{d}\mu_m(\boldsymbol{\alpha}), \end{aligned} \tag{120}$$

where we made the change of variables $\mathbf{z}' = U\mathbf{z}$ *and used the invariance of the Gaussian measure* $\mathrm{d}\nu_m$ *with respect to the action of* U.

Notice that the coherent states $\mathbf{\Phi}_{\boldsymbol{\alpha}}$ [see Eq. (108)] are infinite linear combinations of the states $\mathbf{\Phi}_{\boldsymbol{\alpha},k}(\mathbf{x}) \equiv (\boldsymbol{\alpha}\cdot\mathbf{x})^k$. These states $\mathbf{\Phi}_{\boldsymbol{\alpha},k}$ have in turn the following interesting properties (see Ref. 27).

Proposition 8: (i) The states $\mathbf{\Phi}_{\boldsymbol{\alpha},k}$ *are eigenfunctions of the Laplacian on* S^n, *i.e., for each* k, *the state* $\mathbf{\Phi}_{\boldsymbol{\alpha},k}$ *belongs to the eigenspace* $\mathcal{E}_k$ *of the Laplacian on* S^n.

(ii) For $|\Re\boldsymbol{\alpha}| = 1$ *and* k *large, the state* $\mathbf{\Phi}_{\alpha,k}$ *concentrates around the great circle in* S^n *generated by the two orthogonal unit vectors* $\Re\boldsymbol{\alpha}$ and $\Im\boldsymbol{\alpha}$.

(iii) For each k, *the set of states* $\mathbf{\Phi}_{\boldsymbol{\alpha},k}$ *provides a resolution of the identity in the eigenspace* $\mathcal{E}_k$. *Namely, for* $\mathbf{\Psi} \in \mathcal{E}_k$ we have

$$\mathbf{\Psi}(\mathbf{x}) = c_k^2 \int_{\mathbf{z}\in\mathbb{C}^m} \langle \mathbf{\Psi}, \mathbf{\Phi}_{\boldsymbol{\alpha},k} \rangle \mathbf{\Phi}_{\boldsymbol{\alpha},k}(\mathbf{x}) \mathrm{d}\nu_m(\mathbf{z}) = c_k^2 \int_{\boldsymbol{\alpha}\in Q^n} \langle \mathbf{\Psi}, \mathbf{\Phi}_{\boldsymbol{\alpha},k} \rangle \mathbf{\Phi}_{\boldsymbol{\alpha},k}(\mathbf{x}) \mathrm{d}\mu(\boldsymbol{\alpha}). \tag{121}$$

Since property (ii) of the previous proposition is satisfied, we will refer to the functions $\mathbf{\Phi}_{\boldsymbol{\alpha},k}$ as great-circle states (as suggested to us by Hall). Since these states provide a resolution of the identity for the space $\mathcal{E}_k$, we can also think of the great-circle states as coherent states for the space $\mathcal{E}_k$.

We end this section by giving an explicit expression for the inner product of two great-circle states.

Proposition 9:

$$\langle \mathbf{\Phi}_{\boldsymbol{\alpha},k}, \mathbf{\Phi}_{\beta,k} \rangle = \mathrm{d}_k \langle \boldsymbol{\alpha}, \beta \rangle \tag{122}$$

with

$$d_k = \left\{ \frac{k!}{(2k+1)!!} \quad \text{for } n=2, \quad \frac{1}{2^k(k+1)} \quad \text{for } n=3, \quad \frac{1}{2^{k-1}(k+2)(k+1)} \quad \text{for } n=5 \right\}. \tag{123}$$

Proof: Since the surface measure on S^n is $\mathrm{SO}(n+1)$ invariant we only need to show Eq. (122) when $\boldsymbol{\alpha} = (\mathbf{e}_1 + \imath\mathbf{e}_2)$. To that end, introduce spherical coordinates on S^n [see Eq. (110)] to evaluate

the inner product. □

Notice that the Bargmann transform $\mathbf{B}_{S^n}$ of the great-circle states can be easily obtained from the preceding equation,

$$\mathbf{B}_{S^n}\mathbf{\Phi}_{\boldsymbol{\alpha},k}(\mathbf{z}) = d_k\langle\rho_{(n,m)}(\mathbf{z}),\boldsymbol{\alpha}\rangle. \tag{124}$$

H. Asymptotic behavior of coherent states

In this section we introduce the Planck's constant $\hbar$ in the definition of the Bargmann transform and provide an asymptotic expression for the coherent states for $L^2(S^n)$, $n=2,3,5$ that we have introduced above.

By scaling the expression for the Bargmann transform in Eq. (84) and using Theorem 5 we obtain that the operator

$$\mathbf{B}^{\hbar}_{S^n}\mathbf{\Psi}(\mathbf{z}) = \int_{S^n}\left(\sum_{k=0}^{\infty} c_k\left(\frac{\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w}}{\hbar}\right)^k\right)\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}), \quad \mathbf{z}\in\mathbb{C}^m \tag{125}$$

is a unitary transformation from $L^2(S^n)$ onto the Hilbert space $\mathcal{F}^{\hbar}_m$ with the space $\mathcal{F}^{\hbar}_m$ having the same elements as $\mathcal{F}_m$ but endowed with the inner product

$$\langle f,g\rangle = \int_{\mathbb{C}^m} f(\mathbf{z})\bar{g}(\mathbf{z})\mathrm{d}\nu^{\hbar}_m(\mathbf{z}) \tag{126}$$

with the measure

$$\mathrm{d}\nu^{\hbar}_m(\mathbf{z}) := \frac{1}{(\pi\hbar)^n}\exp\left(-\frac{|\mathbf{z}|^2}{\hbar}\right)\prod_{j=1}^{k}\mathrm{d}x_j\,\mathrm{d}y_j. \tag{127}$$

Let us denote the coefficients c_k given by Eq. (86) as $c_k=\sqrt{ak+b}/k!$. Define the analytical function $g(z)=\Sigma_{k=0}^{\infty}c_kz^k$ with domain $\mathbb{C}$. Thomas and Wassel[26] have described an asymptotic expansion for $g(z)$ in the case $m=2$. Their proof can be adapted easily to the other cases $m=4,8$. Thus we have the following.

Proposition 10: For $\Re z\mapsto\infty$ and $|\Im z|\leqslant C\Re z$ and C a positive constant,

$$g(z) = \frac{2z^{1/2}}{\sqrt{a}}\exp(z)\left(1+\frac{a_1}{z}+\frac{a_2}{z^2}+\cdots\right). \tag{128}$$

Therefore we obtain an asymptotic expansion for the coherent states (with $\hbar$ included)

$$\mathbf{\Phi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{w}) = \sum_{k=0}^{\infty} c_k\left(\frac{\boldsymbol{\alpha}\cdot\mathbf{x}}{\hbar}\right)^k, \quad \boldsymbol{\alpha}\in Q^n-\{0\} \tag{129}$$

in the following way.

Proposition 11: Let $\boldsymbol{\alpha}\in\mathbf{Q}^n-\{0\}$. Then for $\hbar\mapsto 0$ and $|\mathbf{x}\cdot\Im\boldsymbol{\alpha}|\leqslant C\mathbf{x}\cdot\Re\alpha$ we have

$$\mathbf{\Phi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x}) = \frac{2(\mathbf{x}\cdot\boldsymbol{\alpha})^{1/2}}{\sqrt{a\hbar}}\exp\left(\frac{\mathbf{x}\cdot\boldsymbol{\alpha}}{\hbar}\right)\left(1+\frac{a_1\hbar}{\mathbf{x}\cdot\boldsymbol{\alpha}}+\frac{a_2\hbar^2}{(\mathbf{x}\cdot\boldsymbol{\alpha})^2}+\cdots\right). \tag{130}$$

This proposition describes asymptotically the coherent state $\mathbf{\Phi}^{\hbar}_{\boldsymbol{\alpha}}$ on a neighborhood around the point $\mathbf{a}=\Re\boldsymbol{\alpha}/|\Re\boldsymbol{\alpha}|$ in the sphere S^n when $\hbar$ is very small. In particular, it indicates concentration of the coherent states $\mathbf{\Phi}^{\hbar}_{\boldsymbol{\alpha}}$ around $\mathbf{a}$ for $\hbar$ small in the sense that the magnitude of the function $\mathbf{\Psi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x})\equiv[2(\mathbf{x}\cdot\boldsymbol{\alpha})^{1/2}/\sqrt{a\hbar}]\exp(\mathbf{x}\cdot\boldsymbol{\alpha}/\hbar)$ achieves its maximum value at $\mathbf{x}=\mathbf{a}$ and the relative quotient $|\mathbf{\Psi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x})/\mathbf{\Psi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{a})|$ goes to zero (with $\mathbf{x}\neq\mathbf{a}$ fixed) as a constant times $\exp((\mathbf{x}\cdot\Re\boldsymbol{\alpha}-|\Re\boldsymbol{\alpha}|)/\hbar)$.

The phase of the function $\mathbf{\Psi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x})$ contains information too. To see that, let us write the function

$$\mathbf{\Psi}^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x}) = \frac{2}{\sqrt{a}} \sqrt{\frac{\mathbf{x}\cdot\Re\boldsymbol{\alpha}}{\hbar}} \exp\left(\frac{\mathbf{x}\cdot\Re\boldsymbol{\alpha}}{\hbar}\right) \sqrt{1+\imath\frac{\mathbf{x}\cdot\Im\boldsymbol{\alpha}}{\mathbf{x}\cdot\Re\boldsymbol{\alpha}}} \exp\left(\frac{\imath\mathbf{x}\cdot\Im\boldsymbol{\alpha}}{\hbar}\right). \tag{131}$$

Thus for $\mathbf{x}\in S^n$ in a small neighborhood around the point $\mathbf{a}$ (and therefore the quotient $\mathbf{x}\cdot\Im\boldsymbol{\alpha}/\mathbf{x}\cdot\Re\boldsymbol{\alpha}$ a small number) the phase of $\Psi^{\hbar}_{\boldsymbol{\alpha}}(\mathbf{x})$ is mainly determined by the factor $\exp(\imath\mathbf{x}\cdot\Im\boldsymbol{\alpha}/\hbar)$. This is similar to what occurs in the case of the canonical coherent states [labeled by $\mathbf{z}=(\mathbf{q}-\imath\mathbf{p})/\sqrt{2}$] of the n-dimensional harmonic oscillator [see Eq. (5.1) of Ref. 28 for instance] having as a consequence in this last case that the Fourier transform of the coherent state is concentrated around $\mathbf{p}$ in momentum space. We remind the reader that a point $\boldsymbol{\alpha}$ in $Q^n-\{0\}$ corresponds under the map σ_n to a point in T^*S^n with momentum $\Im\boldsymbol{\alpha}$.

VIII. DISCUSSION

We have introduced a Bargmann transform $\mathbf{B}_{S^n}$ for $L^2(S^n)$, $n=2,3,5$, i.e., a unitary transformation from $L^2(S^n)$ onto a suitable Hilbert space of analytical functions $\mathcal{F}_m$, $m=2,4,8$, inmersed in the usual Bargmann space $\mathcal{B}_m$. The key point to build such a Bargmann transform is to consider the function $(\rho_{(n,m)}\cdot\mathbf{w})$ in its integral kernel. The relevant property of the function $(\rho_{(n,m)}\cdot\mathbf{w})$ is that it is a generating function of a canonical transformation which links the Moser map and the map $\mathcal{H}_{(n,m)}$ concerning the regularization of the $n=2,3,5$ dimensional Kepler problem. Thus our Bargmann transform can be regarded as the quantization of such a canonical transformation. We have proved in detail the unitarity of $\mathbf{B}_{S^n}$ and provided its range with an explicit reproducing kernel. We have also provided the inversion formula for $\mathbf{B}_{S^n}$ and given a set of coherent states for $L^2(S^n)$ including their semiclassical asymptotics. We also point out that the map $\rho_{(n,m)}$ is constructed via a moment map for a suitable defined group F [this construction has been done just in the case $(n,m)=(3,4)$ by Kummer[18]].

We comment that other Bargmann-type transforms have been introduced by Hall and Mitchell[10] for the n-sphere (with $n\geqslant 1$) and by Kowalski and Rembielínski[17] for the circle and the 2-sphere. However, theses Bargmann-type transforms are different than ours. The work of Hall and Mitchell is based on properties of heat kernel functions whereas the work of Kowalski and Rembielínski is based on the construction of certain types of coherent states defined as eigenstates of a vector operator whose addition of the squares of its components is one. In both of the cases the non-null complex quadric appears.

We also comment on the interesting work of Mladenov[20] on the geometric quantization of the $n=5$ dimensional Kepler problem. By following the technique of geometric quantization, Mladenov builds a Hilbert space $\widetilde{\mathcal{K}}$ of analytical functions called physically admissible states. The space $\widetilde{\mathcal{K}}$ is determined by considering the Hilbert space generated by the bound states of eight harmonic oscillators (with the same frequency) subject to the restrictions $\mathcal{R}_1\Psi=0$, $\mathcal{R}_2\Psi=0$, and $\mathcal{R}_3\Psi=0$ [see Eqs. (83)]. This is the same space $\mathcal{F}_8$ that we are considering and that we defined motivated by our previous work on the Bargmann transform for $L^2(S^3)$ (see Ref. 28). The Hilbert space $\widetilde{\mathcal{K}}$ is seen as quantization of the phase space $(\mathbb{C}^m-\{0\},-\imath\,\mathrm{d}\mathbf{z}\wedge\mathrm{d}\overline{\mathbf{z}})$ and then imposing the aforementioned conditions. The phase space $(\mathbb{C}^m-\{0\},-\imath\,\mathrm{d}\mathbf{z}\wedge\mathrm{d}\overline{\mathbf{z}})$ comes out from a complexification of $((\mathbb{R}^m-\{0\})\times\mathbb{R}^m,4\,\mathrm{d}\mathbf{v}\wedge\mathrm{d}\mathbf{u})$ considered by Mladenov. We remark that Mladenov's way to consider such a complexification was very inspiring for our present paper and useful in order to construct our canonical transformation. Mladenov uses the Hilbert space $\widetilde{\mathcal{K}}$ representation as an alternative method to the canonical quantization in order to find the eigenvalues and their multiplicities of the $n=5$ dimensional hydrogen atom.

On the other hand, the coherent states for $L^2(S^n)$, $n=2,3,5$, that we have introduced can be used to construct coherent states for the $n=2,3,5$ hydrogen atom problem. This can be done via a known unitary transformation between $L^2(S^n)$ and the Hilbert space generated by the bound states of the $n=2,3,5$ hydrogen atom problem (see Ref. 3). The development of this work and the

comparison of the coherent states obtained in this way with already known and proposed sets of coherent states for the hydrogen atom (like the coherent states of Klauder,[16] and the ones proposed by Horowski and Odzijewicz[13]) is part of future work.

We finally remark that Hilbert spaces of analytical functions on the null complex quadric Q^n endowed with the measure $d\mu_m(\boldsymbol{\alpha})$ can also be considered in the framework of our work. These Hilbert spaces are related with the ones introduced by Bargmann and Todorov.[5]

For the case $L^2(S^2)$, Thomas and Wassell have used the Bargmann transform presented in this paper in order to obtain approximations of eigenvalues of Schrödinger operators on the 2-sphere S^2. Our work could be also useful in semiclassical analysis like in the work done by Helffer *et al.* (see Refs. 11 and 12) about Schrödinger operators with a Coulomb type singularity where the Kustaanheimo-Stiefel regularization was implemented in the quantum mechanical setting.

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APPENDIX A: SO($n+1$) AND ITS COVERING GROUP ACTING ON THE QUADRIC Q^n AND $\mathbb{C}^m$, RESPECTIVELY

In this appendix we give the explicit relation between the SO($n+1$) action of rotations on the quadric Q^n and the corresponding action of its universal covering group on $\mathbb{C}^m$. Namely, we give representations of the groups SU(2), SU(2)$\times$SU(2) and SU(4) acting on $\mathbb{C}^2$, $\mathbb{C}^4$, and $\mathbb{C}^8$, respectively, and then, by using the maps $\rho_{(n,m)}$ [see Eqs. (46), (68), and (70)], we map these representations through a map Φ into the representations of the rotation groups SO(3), SO(4), and SO(6) acting on the quadric Q^2, Q^3, and Q^5, respectively. We show that the map $\boldsymbol{\Phi}$ is onto, two-to-one, and a homomorphism between the corresponding Lie groups.

We remark that the universal covering group of SO($n+1$) is also known as the spin group spin ($n+1$) (see Ref. 6).

The action of SO($n+1$) on the quadric Q^n is defined as follows: let R be a rotation in SO($n+1$) and $\boldsymbol{\alpha}$ in Q^n. Then we define

$$R\boldsymbol{\alpha} = R\Re\boldsymbol{\alpha} + \imath R\Im\boldsymbol{\alpha}, \tag{A1}$$

where $R\Re\boldsymbol{\alpha}$ and $R\Im\boldsymbol{\alpha}$ denote the usual action of R on the real and imaginary parts of $\boldsymbol{\alpha}$, respectively (regarded as elements of $\mathbb{R}^{n+1}$).

Let us consider the map $\rho_{(n,m)}$ [see Eqs. (46), (68), and (70)]. This map will give us the relation between the action defined in Eq. (A1) and the corresponding action of the covering group of SO($n+1$) on $\mathbb{C}^m$. The main idea is the same for the three cases $n=2,3,5$. We describe in detail the most complicated case $n=5$. The cases $n=2,3$ follow in a similar way and we do not include their description in order not to make this appendix too long.

The case $n=5$: let us write the map $\rho_{(5,8)}(\mathbf{z})=(\alpha_1(\mathbf{z}),\ldots,\alpha_6(\mathbf{z}))$ in matrix form

$$\alpha_j = (z_1,z_2,z_3,z_4)A_j\begin{pmatrix} z_5 \\ z_6 \\ z_7 \\ z_8 \end{pmatrix}, \quad j=1,\ldots,6, \tag{A2}$$

where the matrices A_j, $j=1,\ldots,6$ are defined as follows:

$$A_1 = \begin{pmatrix} 0 & -\imath & 0 & 0 \\ \imath & 0 & 0 & 0 \\ 0 & 0 & 0 & \imath \\ 0 & 0 & -\imath & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$A_3 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad A_4 = \begin{pmatrix} -\imath & 0 & 0 & 0 \\ 0 & -\imath & 0 & 0 \\ 0 & 0 & \imath & 0 \\ 0 & 0 & 0 & \imath \end{pmatrix}, \tag{A3}$$

$$A_5 = \begin{pmatrix} 0 & 0 & 0 & -\imath \\ 0 & 0 & -\imath & 0 \\ 0 & -\imath & 0 & 0 \\ -\imath & 0 & 0 & 0 \end{pmatrix}, \quad A_6 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

In order to find the action of SU(4) on $\mathbb{C}^8$, the key point is to consider the following transformation: let $U \in \mathrm{SU}(4)$ and define

$$\begin{pmatrix} z_1' \\ z_2' \\ z_3' \\ z_4' \end{pmatrix} = U \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}, \quad \begin{pmatrix} z_5' \\ z_6' \\ z_7' \\ z_8' \end{pmatrix} = EUE \begin{pmatrix} z_5 \\ z_6 \\ z_7 \\ z_8 \end{pmatrix}, \tag{A4}$$

where the matrix E is defined by

$$E = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{A5}$$

Let us denote by α_j', $j=1,\ldots,6$, the components of the vector $\rho_{(8,5)}(\mathbf{z}')$. Then

$$\alpha_j' = (z_1, z_2, z_3, z_4) U^t A_j EUE \begin{pmatrix} z_5 \\ z_6 \\ z_7 \\ z_8 \end{pmatrix}, \tag{A6}$$

where U^t denotes the transpose matrix of U.

Let V denote the real vector space generated by the matrices A_j, $j=1,\ldots,6$. The vector space V is the set of complex matrices of the form

$$A = \begin{pmatrix} -\mu & \bar{\delta} & 0 & \gamma \\ \delta & \bar{\mu} & \gamma & 0 \\ 0 & -\bar{\gamma} & \mu & \delta \\ -\bar{\gamma} & 0 & \bar{\delta} & -\bar{\mu} \end{pmatrix}, \tag{A7}$$

with $\mu, \delta, \gamma \in \mathbb{C}$.

We now claim that, for $U \in \mathrm{SU}(4)$, the matrix $U^t A_j EUE$ is in the vector space V. To prove this fact, let us denote by $U_{j,k}$ the matrix elements of U. Since $U^\dagger = U^{-1}$ and $\det(U)=1$ then by considering the explicit expression for the inverse matrix U^{-1} we find that the matrix elements of U must satisfy the following six relations:

$$\bar{U}_{11}\bar{U}_{33} - \bar{U}_{31}\bar{U}_{13} = U_{22}U_{44} - U_{42}U_{24}, \bar{U}_{21}\bar{U}_{43} - \bar{U}_{41}\bar{U}_{23} = U_{12}U_{34} - U_{32}U_{14},$$

$$\bar{U}_{31}\bar{U}_{23} - \bar{U}_{21}\bar{U}_{33} = U_{12}U_{44} - U_{42}U_{14}, \bar{U}_{11}\bar{U}_{43} - \bar{U}_{41}\bar{U}_{13} = U_{32}U_{24} - U_{22}U_{34}, \tag{A8}$$

$$\bar{U}_{11}\bar{U}_{23} - \bar{U}_{21}\bar{U}_{13} = U_{42}U_{34} - U_{32}U_{44}, \bar{U}_{41}\bar{U}_{33} - \bar{U}_{31}\bar{U}_{43} = U_{12}U_{24} - U_{22}U_{14}.$$

Then by using Eqs. (A8) and computing the explicit expression for the matrix $U^t A_j EUE$, we find that $U^t A_j EUE$ has the form indicated in Eq. (A7).

The vector space V is endowed with the real valued inner product

$$\langle A, B\rangle_V = \tfrac{1}{2}(\mathrm{trace}(AB^\dagger) + \mathrm{trace}(BA^\dagger)). \tag{A9}$$

The set of matrices $\{\frac{1}{2}A_j \,|\, j=1,\ldots,6\}$ gives an orthonormal basis for the space V. Thus $U^t A_j EUE$ must be the following linear combination of the basis elements (summation over repeated indexes):

$$U^t A_j EUE = \tfrac{1}{4}\langle U^t A_j EUE, A_k\rangle_V A_k, \quad j=1,\ldots,6. \tag{A10}$$

Therefore we have

$$\alpha'_j = (z_1, z_2, z_3, z_4) R_{jk} A_k \begin{pmatrix} z_5 \\ z_6 \\ z_7 \\ z_8 \end{pmatrix} = R_{jk}\alpha_k \tag{A11}$$

with the real numbers R_{jk}, $j,k=1,2,3$, given by

$$R_{jk} = \tfrac{1}{4}\langle U^t A_j EUE, A_k\rangle_V. \tag{A12}$$

Thus to each element $U \in \mathrm{SU}(4)$ we associate a 6×6 matrix R whose matrix elements are R_{jk} given by Eq. (A12). Since the matrix R satisfies the relation $R_{jk}R_{sk} = \delta_{js}$ (thus R must be an orthogonal matrix) then we have a continuous map $U \mapsto R$ from SU(4) into O(6). Since SU(4) is a connected manifold, then its image under the map we are considering must be the connected component of the identity matrix in O(6) [notice that from Eq. (A12) the identity element of SU(4) goes to the identity element of O(6)]. Thus the assignment $U \mapsto R$ gives us a map $\mathbf{\Phi}$ from SU(4) into SO(6). Moreover, since the set $\{\frac{1}{2}A_j \,|\, j=1,\ldots,6\}$ is an orthonormal basis for the space V, we obtain from Eq. (A12) that $\mathbf{\Phi}$ is a Lie group homomorphism.

We now claim that the map $\mathbf{\Phi}$ is onto. Let us consider an element $U \in \mathrm{SU}(4)$. Since SU(4) is a compact connected Lie group, the exponential map is onto and therefore there is a matrix σ in the Lie algebra of SU(4) [denoted by su(4)] such that $U = \exp(\imath\sigma)$. Consider the one-parameter group $U(s) = \exp(\imath s\sigma)$ with parameter $s \in \mathbb{R}$.

Let $\{\sigma_\ell \,|\, \ell = 1,\ldots,15\}$ be an orthonormal basis of SU(4) under the inner product $\langle A, B\rangle_{\mathrm{su}(4)} = \mathrm{trace}(AB)$. Thus we obtain a one-parameter group of rotations $R(s)$ whose matrix elements are given by

$$R(s)_{jk} = \tfrac{1}{4}\langle U^t(s)A_jEU(s)E, A_k\rangle_V, \quad j,k = 1, \ldots, 6 \tag{A13}$$

with $U(s)=\exp(\imath s h_j \sigma_j)$ and $h_\ell = \langle \sigma, \sigma_\ell\rangle_{\mathrm{su}(4)}$, $\ell = 1, \ldots, 15$. Let us now consider the element $\mathcal{A}$ of so(3) [the Lie algebra of SO(3)] obtained by taking the $-\imath$ times the derivative of $R(s)$ at $s=0$. Thus we have

$$\mathcal{A}_{jk} = \frac{1}{8}\left.\frac{d}{\mathrm{d}s}\right|_{s=0} \mathrm{trace}(U^t(s)A_jEU(s)EA_k + A_k(U^t(s)A_jEU(s)E)^\dagger) = h_\ell(\beta_\ell)_{jk}, \quad j,k = 1, \ldots, 6, \tag{A14}$$

where $(\beta_\ell)_{jk}$ denotes the (j,k) matrix element of the matrix β_ℓ defined by

$$(\beta_\ell)_{jk} = \tfrac{1}{8}\,\mathrm{trace}(\sigma_\ell^t(A_jA_k^\dagger - A_kA_j^\dagger) + \sigma_\ell E(A_k^\dagger A_j - A_j^\dagger A_k)E), \tag{A15}$$

where we have used the property $\sigma_\ell^\dagger = \sigma_\ell$.

Since the matrices A_j, $j=1, \ldots, 6$ satisfy the following equation:

$$E(A_k^\dagger A_j - A_j^\dagger A_k)E = -\overline{(A_jA_k^\dagger - A_kA_j^\dagger)}, \quad j,k = 1, \ldots, 6 \tag{A16}$$

and the matrices $\imath(A_jA_k^\dagger - A_kA_j^\dagger)$ are in su(4) (they are self-adjoint and traceless) then we find after some computation

$$(\beta_\ell)_{jk} = \frac{-\imath}{4}\langle \sigma_\ell, \imath(A_jA_k^\dagger - A_kA_j^\dagger)\rangle_{\mathrm{su}(4)}. \tag{A17}$$

From the last equation we see that the matrices $(1/\sqrt{2})\beta_\ell$ are in so(6) (they are of the form $\imath$ times an antisymmetric matrix with real entries) and they actually give an orthonormal set of so(6) under the inner product $\langle A, B\rangle_{\mathrm{so}(6)} = \mathrm{trace}(AB)$ because the set of matrices $\{(\imath/4)(A_jA_k^\dagger - A_kA_j^\dagger) \,|\, j,k = 1, \ldots, 6, j<k\}$ is an orthonormal set of SU(4).

Let $S \in \mathrm{SO}(6)$. Since $S \in \mathrm{SO}(6)$ is a compact connected group, there exist $\mathcal{D} \in \mathrm{so}(6)$ such that $S=\exp(\imath\mathcal{D})$. Since $\{(1/\sqrt{2})\beta_\ell\}$ is an orthonormal basis of so(6), then $\mathcal{D} = c_\ell(1/\sqrt{2})\beta_\ell$ with $c_\ell = \langle \mathcal{D}, (1/\sqrt{2})\beta_\ell\rangle_{\mathrm{so}(6)}$. Consider the matrix $U=\exp[\imath(c_\ell/\sqrt{2})\sigma_\ell[$ in SU(4). From Eq. (A14) we find that $\mathbf{\Phi}(U)=S$ and therefore Φ is onto.

Let us denote by $\phi: \mathrm{su}(4) \mapsto \mathrm{so}(6)$ the associated Lie algebra homomorphism of $\mathbf{\Phi}$. From Eq. (A14) we obtain that $\phi(\sigma) = \langle \sigma, \sigma_\ell\rangle_{\mathrm{su}(4)}\beta_\ell$ for all $\sigma \in \mathrm{su}(4)$. It is easy to check that ϕ is a linear bijection. Moreover ϕ is a Lie algebra isomorphism because of the way it is defined and Theorem 2.21 of Ref. 9.

Finally, $\mathbf{\Phi}$ is two-to-one. Since $\mathbf{\Phi}$ is an homomorphism, it is enough to show that the only two solutions of the equation $\mathbf{\Phi}(U)=I$ are the matrices $U=I$ or $U=-I$. Thus suppose that $\mathbf{\Phi}(U)=I$. From Eq. (A14) we must have that $U^tA_kEUE = A_k$ for all $k=1, \ldots, 6$. By performing the analysis of these equations we find that $U=I$ or $U=-I$ are the only two solutions.

APPENDIX B: ORTHOGONAL PROJECTORS ON EIGENSPACES OF THE LAPLACIAN

Let P_k denote the orthogonal projector onto the kth eigenspace $\mathcal{E}_k$ of the Laplacian on S^n ($n=2,3,5$). The finite dimensional vector space $\mathcal{E}_k$ is the space of restrictions of harmonic homogeneous polynomials of degree k in $n+1$ variables. The Hilbert space $L^2(S^n)$ is equal to the direct sum of all the spaces $\mathcal{E}_k$ (k a non-negative integer number). In particular, two elements of different eigenspaces of the Laplacian are orthogonal with respect to the usual inner product of $L^2(S^n)$.

Let us define the operator $S_k: L^2(S^n) \mapsto L^2(S^n)$ by the following expression:

$$S_k\mathbf{\Psi}(\mathbf{v}) = \int_{S^n} J_k(\mathbf{w}, \mathbf{v})\mathbf{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}) \tag{B1}$$

with

$$J_k(\mathbf{w},\mathbf{v}) = c_k^2 \int_{\mathbb{C}^m} (\rho_{(m,n)}(\mathbf{z})\cdot\mathbf{w})^k \overline{(\rho_{(m,n)}(\mathbf{z})\cdot\mathbf{v})}^k \, \mathrm{d}\nu_m(\mathbf{z}). \tag{B2}$$

Proposition 12: The operator S_k is equal to the orthogonal projector P_k.

Proof: Since, $\overline{J_k(\mathbf{w},\mathbf{v})}$ is in the space $\mathcal{E}_k$ as a function of $\mathbf{w}$ and $\mathbf{v}$ fixed, then $S_k\Psi=0$ for $\boldsymbol{\Psi}$ in the orthogonal complement of $\mathcal{E}_k$. Thus we only need to show that S_k is the identity operator when acting on the eigenspace $\mathcal{E}_k$. We will use the Schur's lemma for that purpose.

Let us define the following representation of the rotation group $\mathrm{SO}(n+1)$ on the eigenspace $\mathcal{E}_k$. Given $R\in\mathrm{SO}(n+1)$, define the operator $T_R:\mathcal{E}_k\mapsto\mathcal{E}_k$ by $T_R\boldsymbol{\Psi}(\mathbf{w})=\boldsymbol{\Psi}(R^{-1}\mathbf{w})$. The set of operators $\{T_R|R\in\mathrm{SO}(n+1)\}$ gives an irreducible representation of the group $\mathrm{SO}(n+1)$. By Schur's lemma we just need to prove that the operator S_k restricted to $\mathcal{E}_k$ commutes with T_R for all $R\in\mathrm{SO}(n+1)$ and that $S_k\boldsymbol{\Psi}=\boldsymbol{\Psi}$ for a particular nontrivial function in $\mathcal{E}_k$.

Notice that for $\boldsymbol{\Psi}$ in $\mathcal{E}_k$,

$$S_kT_R\boldsymbol{\Psi}(\mathbf{v}) = \int_{S^n} J_k(\mathbf{w},\mathbf{v})\boldsymbol{\Psi}(R^{-1}\mathbf{w})\mathrm{d}S(\mathbf{w}). \tag{B3}$$

On the other hand, we have

$$T_RS_k\boldsymbol{\Psi}(\mathbf{v}) = S_k\boldsymbol{\Psi}(R^{-1}\mathbf{v}) = \int_{S^n} J_k(\mathbf{w},R^{-1}\mathbf{v})\boldsymbol{\Psi}(\mathbf{w})\mathrm{d}S(\mathbf{w}) = \int_{S^n} J_k(R^{-1}\mathbf{w},R^{-1}\mathbf{v})\boldsymbol{\Psi}(R^{-1}\mathbf{w})\mathrm{d}S(\mathbf{w}), \tag{B4}$$

where we have made the change of variable $\mathbf{w}\mapsto R\mathbf{w}$ and used the invariance of the $\mathrm{SO}(n+1)$ surface measure $\mathrm{d}S(\mathbf{w})$. We now claim that $J_k(R^{-1}\mathbf{w},R^{-1}\mathbf{v})=J_k(\mathbf{w},\mathbf{v})$:

$$\begin{aligned} J_k(R^{-1}\mathbf{w},R^{-1}\mathbf{v}) &= c_k^2 \int_{\mathbb{C}^m} (\rho_{(n,m)}(\mathbf{z})\cdot R^{-1}\mathbf{w})^k \overline{(\rho_{(n,m)}(\mathbf{z})\cdot R^{-1}\mathbf{v})}^k \, \mathrm{d}\nu_m(\mathbf{z}) \\ &= c_k^2 \int_{\mathbb{C}^m} (R\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{w})^k \overline{(R\rho_{(n,m)}(\mathbf{z})\cdot\mathbf{v})}^k \, \mathrm{d}\nu_m(\mathbf{z}), \end{aligned} \tag{B5}$$

where we have used the orthogonality of the matrix $R\in\mathrm{SO}(n+1)$.

From Appendix A, we know that, given $R\in\mathrm{SO}(n+1)$, there exist a transformation U acting on $\mathbb{C}^m$ such that $R\rho_{(n,m)}(\mathbf{z})=\rho_{(n,m)}(U\mathbf{z})$ and $\mathrm{d}\nu_m(\mathbf{z})$ is invariant under the action of the matrix U. By considering the change of variables $\mathbf{z}\mapsto U\mathbf{z}$ we conclude that $J_k(R^{-1}\mathbf{w},R^{-1}\mathbf{v})=J_k(\mathbf{w},\mathbf{v})$ Using this fact in Eq. (B3) we obtain $S_kT_R\boldsymbol{\Psi}(\mathbf{v})=T_RS_k\boldsymbol{\Psi}(\mathbf{v})$ and therefore the operator S_k commutes with all of the operators T_R.

Now consider the particular function $\boldsymbol{\Upsilon}(\mathbf{w})=(\,(\mathbf{e}_1+\imath\mathbf{e}_2)\cdot\mathbf{w})^k$ in the eigenspace $\mathcal{E}_k$. From the expression for the inner product of two coherent states Eq. (122) and Fubini's theorem we conclude that $S_k\boldsymbol{\Upsilon}(\mathbf{z})=\boldsymbol{\Upsilon}(\mathbf{z})$.

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Asymptotic iteration method solutions to the relativistic Duffin-Kemmer-Petiau equation

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A simple exact analytical solution of the relativistic Duffin-Kemmer-Petiau equation within the framework of the asymptotic iteration method is presented. Exact bound state energy eigenvalues and corresponding eigenfunctions are determined for the relativistic harmonic oscillator as well as the Coulomb potentials. As a nontrivial example, the anharmonic oscillator is solved and the energy eigenvalues are obtained within the perturbation theory using the asymptotic iteration method. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2203429]

I. INTRODUCTION

Exact analytical solutions to relativistic wave equations are important in relativistic quantum mechanics since the wave function contains all the necessary information to describe a quantum system fully. There are only a few potentials for which the relativistic Dirac, Klein-Gordon, and Duffin-Kemmer-Petiau (DKP) equations can be solved analytically. So far, many methods such as the supersymmetric (SUSY),[1] shape invariance,[2,3] factorization and path integral,[4–7] etc., have been developed to solve the relativistic wave equations exactly, or quasiexactly, for potentials like Coulomb, harmonic oscillator, Pösch Teller and exponential type ones. In recent years, an asymptotic iteration method for solving second-order homogeneous linear differential equations has been proposed by Ciftci *et al.*[8–10] This method has been applied to solve the nonrelativistic radial Schrödinger and Dirac equations for various potentials.[10]

Since the DKP equation is being increasingly used to describe the interactions of relativistic spin-0 and spin-1 bosons,[11–19] it would be interesting to probe whether the DKP equation is amenable to exact solutions in the framework of the asymptotic iteration method (AIM). This is precisely the aim of this paper.

In the next section, we explain the AIM briefly and show how to solve a second-order homogeneous differential equation. Then, we introduce the DKP oscillator and Coulomb problems and obtain their exact eigenvalues and eigenfunctions. In Sec. V, we present the solution of the anharmonic oscillator as a nontrivial example within the perturbation theory. Finally, in the last section, we provide our summary and conclusion.

II. BASIC EQUATIONS OF THE ASYMPTOTIC ITERATION METHOD (AIM)

We briefly outline the asymptotic iteration method here; the details can be found in Refs. 8–10. The asymptotic iteration method was proposed to solve second-order differential equations of the form

$$y'' = \lambda_0(x)y' + s_0(x)y, \tag{1}$$

where $\lambda_0(x) \neq 0$ and $s_0(x)$, $\lambda_0(x)$ are in $C_\infty(a,b)$. The variables, $s_0(x)$ and $\lambda_0(x)$, are sufficiently differentiable. The differential equation (1) has a general solution[8]

$$y(x) = \exp\left(-\int^{x} \alpha \mathrm{d}x'\right)\left[C_2 + C_1 \int^{x} \exp\left(\int^{x'} \lambda_0(x'') + 2\alpha(x'')\mathrm{d}x''\right)\mathrm{d}x'\right] \tag{2}$$

if $n>0$, for sufficiently large n,

$$\frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} = \alpha, \tag{3}$$

where

$$\lambda_n = \lambda_n' + s_{n-1} + \lambda_0\lambda_{n-1} \quad \text{and } s_n = s_{n-1}' + s_0\lambda_{n-1}. \tag{4}$$

The quantization condition of the method together with Eq. (4) can also be written as follows:

$$\delta(x) = \lambda_{n+1}(x)s_n(x) - \lambda_n(x)s_{n+1}(x) = 0. \tag{5}$$

For a given potential, the idea is to convert the relativistic wave equation to the form of Eq. (1). Then, s_0 and λ_0 are determined and s_n and λ_n parameters are calculated. The energy eigenvalues are then obtained by the condition given by Eq. (5). However, the wave functions are determined by using the wave function generator, namely $\exp(-\int^x \alpha\, dx')$.

In this study, we seek the exact solution of DKP equation for which the relevant second-order homogeneous linear differential equation takes the following general form:

$$y'' = 2\left(\frac{ax^{N+1}}{1-bx^{N+2}} - \frac{(m+1)}{x}\right)y' - \frac{wx^N}{1-bx^{N+2}}y. \tag{6}$$

If this equation is compared to Eq. (1), it entails the following expressions:

$$\lambda_0 = 2\left(\frac{ax^{N+1}}{1-bx^{N+2}} - \frac{(m+1)}{x}\right), \quad s_0(x) = -\frac{wx^N}{1-bx^{N+2}} \tag{7}$$

while the condition (3) yields for $N=-1,0,1,2,3,\ldots$,

$$w_n^m(-1) = n(2a + 2bm + (n+1)b), \tag{8}$$

$$w_n^m(0) = 2n(2a + 2bm + (2n+1)b), \tag{9}$$

$$w_n^m(1) = 3n(2a + 2bm + (3n+1)b), \tag{10}$$

$$w_n^m(2) = 4n(2a + 2bm + (4n+1)b), \tag{11}$$

$$w_n^m(3) = 5n(2a + 2bm + (5n+1)b), \tag{12}$$

etc. Hence, these formulas are easily generalized as

$$w_n^m(N) = b(N+2)^2 n\left(n + \frac{(2m+1)b + 2a}{(N+2)b}\right). \tag{13}$$

The exact eigenfunctions can be derived from the following generator:

$$y_n(x) = C_2 \exp\left(-\int^{x} \alpha_k \mathrm{d}x'\right). \tag{14}$$

Using Eq. (3) and Eq. (7), the eigenfunctions are obtained as follows:

$$y_0(x) = 1,$$

$$y_1(x) = -C_2(N+2)\sigma\left(1 - \frac{b(\rho+1)}{\sigma}x^{N+2}\right),$$

$$y_2(x) = C_2(N+2)^2\sigma(\sigma+1)\left(1 - \frac{2b(\rho+2)}{\sigma}x^{N+2} + \frac{b^2(\rho+2)(\rho+3)}{\sigma(\sigma+1)}x^{2(N+2)}\right),$$

$$y_3(x) = -C_2\frac{\sigma(\sigma+1)(\sigma+2)}{(N+2)^{-3}}\left(1 - \frac{3b(\rho+3)}{\sigma}x^{N+2} + \frac{3b^2(\rho+3)(\rho+4)}{\sigma(\sigma+1)}x^{2(N+2)} - \frac{b^3(\rho+3)(\rho+4)(\rho+5)}{\rho(\rho+1)(\rho+2)}x^{3(N+2)}\right),$$

etc. Finally, the following general formula for the exact solutions $y_n(x)$ is acquired as:

$$y_n(x) = (-1)^n C_2(N+2)^n(\sigma)_{n2}F_1(-n,\rho+n;\sigma;bx^{N+2}), \tag{15}$$

where

$$(\sigma)_n = \frac{\Gamma(\sigma+n)}{\Gamma(\sigma)}, \quad \sigma = \frac{2m+N+3}{N+2}, \quad \text{and } \rho = \frac{(2m+1)b+2a}{(N+2)b}.$$

.

III. DKP HARMONIC OSCILLATOR

In this section, the Duffin-Kemmer-Petiau formalism[11,13] is briefly sketched and the DKP oscillator is solved using AIM. Generally, the first-order relativistic Duffin-Kemmer-Petiau equation for a free spin zero or spin one particle of mass m is

$$(c\beta\,.\,\mathbf{p} + mc^2)\psi = i\hbar\beta^0\frac{\mathrm{d}\psi}{\mathrm{d}t}, \tag{16}$$

where $\beta^\mu(\mu=0,1,2,3)$ matrices satisfy the commutation relation

$$\beta^\mu\beta^\nu\beta^\lambda + \beta^\lambda\beta^\nu\beta^\mu = g^{\mu\nu}\beta^\lambda + g^{\nu\lambda}\beta^\mu \tag{17}$$

which defines the so-called Duffin-Kemmer-Petiau algebra. The algebra generated by the four β matrices has three irreducible representations: a 10-dimensional one that is related to $S=1$, a five-dimensional one relevant for $S=0$ (spinless particles), and a one-dimensional one which is trivial.

In the spin-0 representation, β^μ are 5×5 matrices defined as $(i=1,2,3)$

$$\beta^0 = \begin{pmatrix} \theta & \tilde{0} \\ \overline{0}_T & \mathbf{0} \end{pmatrix}, \quad \beta^i = \begin{pmatrix} \tilde{0} & \rho^i \\ -\rho^i_T & \mathbf{0} \end{pmatrix} \tag{18}$$

with $\tilde{0}$, $\overline{0}$, $\mathbf{0}$ as 2×2, 2×3, 3×3 zero matrices, respectively, and

$$\theta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \rho^1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \rho^2 = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \rho^3 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}. \tag{19}$$

For spin one particles, β^μ are 10×10 matrices given by

$$\beta^0 = \begin{pmatrix} 0 & \overline{0} & \overline{0} & \overline{0} \\ \overline{0}^T & \mathbf{0} & \mathbf{I} & \mathbf{I} \\ \overline{0}^T & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \overline{0}^T & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \beta^i = \begin{pmatrix} 0 & \overline{0} & e_i & \overline{0} \\ \overline{0}^T & \mathbf{0} & \mathbf{0} & -is_i \\ e_i^T & \mathbf{0} & \mathbf{0} & 0 \\ \overline{0}^T & -is_i & \mathbf{0} & 0 \end{pmatrix}, \tag{20}$$

where s_i are the usual 3×3 spin one matrices

$$\overline{0} = (0\ 0\ 0), \quad e_1 = (1\ 0\ 0), \quad e_2 = (0\ 1\ 0), \quad e_3 = (0\ 0\ 1). \tag{21}$$

I and **0** are the identity and zero matrices, respectively. While the dynamical state ψ_{DKP} is a five component spinor for spin zero particles, it has 10 component spinors for $S=1$ particles.

For the external potential introduced with the nonminimal substitution

$$\mathbf{p} \to \mathbf{p} - im\omega\eta^0\mathbf{r}, \tag{22}$$

where ω is the oscillator frequency and $\eta^0 = 2\beta^{0^2} - 1$, the DKP equation for the system is

$$[c\beta\cdot(\mathbf{p} - im\omega\eta^0\mathbf{r}) + mc^2]\psi = i\hbar\beta^0\frac{\mathrm{d}\psi}{\mathrm{d}t}. \tag{23}$$

In the spin zero representation, the five component DKP spinor

$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_{\mathrm{upper}} \\ i\psi_{\mathrm{lower}} \end{pmatrix} \quad \text{with } \psi_{\mathrm{upper}} \equiv \begin{pmatrix} \phi \\ \varphi \end{pmatrix} \quad \text{and } \psi_{\mathrm{lower}} \equiv \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix}, \tag{24}$$

so that for stationary states the DKP equation can be written as

$$mc^2\phi = E\varphi + ic(\mathbf{p} + im\omega\mathbf{r})\cdot\mathbf{A},$$

$$mc^2\varphi = E\phi,$$

$$mc^2\mathbf{A} = ic(\mathbf{p} - im\omega\mathbf{r})\phi, \tag{25}$$

where **A** is the vector (A_1, A_2, A_3).

The five-component wave function ψ is simultaneously an eigenfunction of J^2 and J_3,

$$J^2\begin{pmatrix} \psi_{\mathrm{upper}} \\ \psi_{\mathrm{lower}} \end{pmatrix} = \begin{pmatrix} L^2\psi_{\mathrm{upper}} \\ (L+S)^2\psi_{\mathrm{lower}} \end{pmatrix} = J(J+1)\begin{pmatrix} \psi_{\mathrm{upper}} \\ \psi_{\mathrm{lower}} \end{pmatrix}, \tag{26}$$

$$J_3\begin{pmatrix} \psi_{\mathrm{upper}} \\ \psi_{\mathrm{lower}} \end{pmatrix} = \begin{pmatrix} L_3\psi_{\mathrm{upper}} \\ (L_3+s_3)\psi_{\mathrm{lower}} \end{pmatrix} = M\begin{pmatrix} \psi_{\mathrm{upper}} \\ \psi_{\mathrm{lower}} \end{pmatrix}, \tag{27}$$

where the total angular momentum $J=L+S$ which commutes with β^0, is a constant of the motion.

For $S=0$ DKP oscillator eigenstates problem, the most general solution for a central problem[11] is presented as follows:

$$\psi_{JM}(r) = \begin{pmatrix} F_{nJ}(r)Y_{JM}(\Omega) \\ G_{nJ}(r)Y_{JM}(\Omega) \\ i\sum\limits_L H_{nJL}(r)Y^M_{JL1}(\Omega) \end{pmatrix}, \tag{28}$$

where

$$\alpha_J = \sqrt{(J+1)/(2J+1)}, \quad \zeta_J = \sqrt{J/(2J+1)}, \tag{29}$$

$$F_{nJ}(r) = F(r), \quad G_{nJ} = G(r), \quad H_{n,J,J\pm1}(r) = H_{\pm1}(r), \tag{30}$$

ψ_{JM} of parity $(-1)^J$ is inserted into Eq. (23) and the following equations are found:

$$EF = mc^2 G, \tag{31}$$

$$\hbar c\left(\frac{d}{\mathrm{d}r} - \frac{J+1}{r} + \frac{m\omega r}{\hbar}\right)F = -\frac{1}{\alpha_J} mc^2 H_1, \tag{32}$$

$$\hbar c\left(\frac{d}{\mathrm{d}r} - \frac{J}{r} + \frac{m\omega r}{\hbar}\right)F = -\frac{1}{\zeta_J} mc^2 H_{-1}, \tag{33}$$

$$-\alpha_J\left(\frac{d}{\mathrm{d}r} + \frac{J+1}{r} - \frac{m\omega r}{\hbar}\right)H_1 + \zeta_J\left(\frac{d}{\mathrm{d}r} - \frac{J}{r} - \frac{m\omega r}{\hbar}\right)H_{-1} = \frac{1}{\hbar c}(mc^2 F - EG). \tag{34}$$

From the above equations, if Eqs. (31)–(33) are inserted into Eq. (34), the homogeneous second-order differential equation for the DKP harmonic oscillator[11] is obtained as

$$\left(\frac{d^2}{\mathrm{d}r^2} + \frac{(E^2 - m^2c^4)}{(\hbar c)^2} + \frac{3m\omega}{\hbar} - \frac{m^2\omega^2 r^2}{\hbar^2} - \frac{J(J+1)}{r^2}\right)F(r) = 0. \tag{35}$$

If we define $E_{\mathrm{eff}}=[(E^2-m^2c^4)/(\hbar c)^2]+(3m\omega/\hbar)$ and $k=m\omega/\hbar$, Eq. (35) becomes

$$\left(\frac{d^2}{\mathrm{d}r^2} + E_{\mathrm{eff}} - k^2 r^2 - \frac{J(J+1)}{r^2}\right)F(r) = 0. \tag{36}$$

The asymptotic iteration method requires selecting the wave function as follows:

$$F(r) = r^{J+1} e^{(-1/2)kr^2} f(r) \tag{37}$$

equating it into Eq. (36) leads to

$$\frac{d^2 f(r)}{\mathrm{d}r^2} - 2\left(kr - \frac{J+1}{r}\right)\frac{\mathrm{d}f(r)}{\mathrm{d}r} + (E_{\mathrm{eff}} - 3k - 2kJ)f(r) = 0, \tag{38}$$

where $\lambda_0=2\{kr-[(J+1)/r]\}$ and $s_0=3k+2kJ-E_{\mathrm{eff}}$. By means of Eq. (4), we may calculate $\lambda_n(r)$ and $s_n(r)$. This gives

$$\lambda_0 = 2\left(kr - \frac{J+1}{r}\right),$$

$$s_0 = 3k + 2kJ - E_{\mathrm{eff}},$$

$$\lambda_1 = 5k + 2\frac{J+1}{r^2} + 2kJ - E_{\mathrm{eff}} + 4\left(kr - \frac{J+1}{r}\right)^2,$$

$$s_1 = 2(3k + 2kJ - E_{\mathrm{eff}})\left(kr - \frac{J+1}{r}\right),$$

$$\lambda_2 = -4\frac{J+1}{r^3} + 2\left(kr - \frac{J+1}{r}\right)\left[4\left(k + \frac{J+1}{r^2}\right) + (3k - 2kJ - E_{\text{eff}}) + 2\left(kr - \frac{J+1}{r}\right)\right],$$

$$s_2 = (3k + 2kJ - E_{\text{eff}})\left[7k + 4\frac{J+1}{r^2} + 2kJ - E_{\text{eff}} + 4\left(kr - \frac{J+1}{r}\right)^2\right], \tag{39}$$

etc. Combining these results with the quantization condition given by Eq. (5) yields

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \Rightarrow (E_{\text{eff}})_0 = 3k + 2kJ, \tag{40}$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \Rightarrow (E_{\text{eff}})_1 = 7k + 2kJ, \tag{41}$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \Rightarrow (E_{\text{eff}})_2 = 11k + 2kJ, \tag{42}$$

etc.

When the above expressions are generalized, the DKP oscillator eigenvalues turn out as

$$(E_{\text{eff}})_n = k(4n + 3 + 2J). \tag{43}$$

If one inserts the values of k and E_{eff} into Eq. (43), the relativistic energy spectrum of DKP oscillator becomes

$$\frac{1}{2mc^2}(E_{NJ}^2 - m^2c^4) = N\hbar\omega, \tag{44}$$

where N is the principal quantum number defined as $N=2n+J$. Our result is in agreement with the result of Ref. 11 for the same potential.

As indicated in Sec. II, we can construct the corresponding eigenfunctions by using the wave function generator given by Eq. (14) and Eq. (39) where we obtain λ and s values. Therefore, similar to Eq. (15), the wave function $f_n(r)$ can be written

$$f_n(r) = (-1)^n C_2 2^n (\sigma)_n \, {}_1F_1(-n, \sigma; kr^2). \tag{45}$$

$F(r)$ ensues right away in the following form:

$$F(r) = r^{J+1} e^{-(1/2)kr^2}[(-1)^n C_2 2^n (\sigma)_n \, {}_1F_1(-n, \sigma; kr^2)], \tag{46}$$

where

$$\sigma = \frac{2J+3}{2} \quad \text{and } (\sigma)_n = \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)}. \tag{47}$$

Using the wave function $F(r)$, the wave functions $G(r)$, $H_1(r)$, and $H_{-1}(r)$ can be easily obtained by using Eqs. (31)–(34).

IV. DKP COULOMB POTENTIAL

We now apply the AIM method to the bound state problem of a spinless charged pion (π^-) in the Coulomb field of a nucleus. If we use the following *ansatz*:

$$a_{\pm}=\frac{mc^2\pm E}{\hbar c},\quad \gamma=\alpha Z,\quad \lambda_{\pi}=\frac{\hbar}{mc},\quad \kappa=\frac{2}{\hbar c}\sqrt{m^2c^4-E^2},\quad \xi=\frac{2\gamma E}{\kappa\hbar c},\quad \rho=\kappa r \tag{48}$$

the system of coupled equations for the Coulomb potential becomes

$$\alpha_J\left(\frac{\mathrm{d}F}{\mathrm{d}\rho}-\frac{J+1}{\rho}F\right)=-\frac{1}{\kappa\lambda_{\pi}}H_1, \tag{49}$$

$$\zeta_J\left(\frac{\mathrm{d}F}{\mathrm{d}\rho}+\frac{J}{\rho}F\right)=\frac{1}{\kappa\lambda_{\pi}}H_{-1}, \tag{50}$$

$$-\alpha_J\left(\frac{\mathrm{d}H_1}{\mathrm{d}\rho}+\frac{J+1}{\rho}H_1\right)+\zeta_J\left(\frac{\mathrm{d}H_{-1}}{\mathrm{d}\rho}-\frac{J}{\rho}H_{-1}\right)=\kappa\lambda_{\pi}\left(\frac{a_+}{\kappa}+\frac{\gamma}{\rho}\right)\left(\frac{a_-}{\kappa}-\frac{\gamma}{\rho}\right)F. \tag{51}$$

Eliminating H_1 and H_{-1} in favor of F, the second-order differential equation for the Coulomb potential becomes

$$\frac{d^2F(\rho)}{\mathrm{d}\rho^2}+\left(\frac{\xi}{\rho}-\frac{1}{4}-\frac{J(J+1)-\gamma^2}{\rho^2}\right)F(\rho)=0. \tag{52}$$

Let the radial wave function be factorized as

$$F(\rho)=\rho^{\Lambda+1}e^{-(1/2)\rho}f(\rho), \tag{53}$$

where

$$\Lambda=-\tfrac{1}{2}+\sqrt{\left(J+\tfrac{1}{2}\right)^2-\gamma^2}. \tag{54}$$

Equation (52) becomes

$$\frac{d^2f(\rho)}{\mathrm{d}\rho^2}-\frac{(\rho-2\Lambda-2)}{\rho}\frac{\mathrm{d}f(\rho)}{\mathrm{d}\rho}-\frac{(\Lambda+1-\xi)}{\rho}f(\rho)=0 \tag{55}$$

which is now amenable to an AIM solution. In order to find the exact energy eigenvalues, we define λ_0 and s_0 as

$$\lambda_0=-\frac{(\rho-2\Lambda-2)}{\rho},\quad s_0=-\frac{(\Lambda+1-\xi)}{\rho}. \tag{56}$$

Using the quantization condition given by Eq. (5), the ξ values take the form

$$\xi_1=\Lambda+1,\quad \xi_2=\Lambda+2,\quad \xi_3=\Lambda+3,\quad \text{etc.}, \tag{57}$$

which can be generalized as

$$\xi_n=\Lambda+n'. \tag{58}$$

Inserting ξ and Λ in Eq. (48) and defining the principal quantum number as $n=n'+J$, we obtain the exact bound state eigenenergies,

$$E_{nJ}=mc^2\left[1+\frac{(\alpha Z)^2}{\left(n-J-\frac{1}{2}+\sqrt{\left(J+\frac{1}{2}\right)^2-(\alpha Z)^2}\right)^2}\right]^{-1/2}, \tag{59}$$

which is in agreement with the results of Refs. 12 and 13 for the same potential. The binding energy B_{nJ} can be calculated from $B_{nJ}=mc^2-E_{nJ}$.

We can also construct the corresponding eigenfunctions using AIM as

$$f_n(\rho) = (-1)^n C_2(\sigma)_n \, {}_1F_1(-n, \sigma; \rho) \tag{60}$$

which gives

$$F(\rho) = \rho^{\Lambda+1} e^{-(1/2)\rho} [(-1)^n C_2(\sigma)_n \, {}_1F_1(-n, \sigma; \rho)], \tag{61}$$

where

$$\sigma = 2\Lambda + 2 \quad \text{and} \quad (\sigma)_n = \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)}. \tag{62}$$

Other components of the the wave functions $[G(\rho)$, $H_1(\rho)$, and $H_{-1}(\rho)]$ can be obtained through Eqs. (49) and (50) using $F(\rho)$.

V. ANHARMONIC OSCILLATOR

In this section, we present the application of the asymptotic iteration method to nontrivial problems. We have thus chosen a vector potential of the type

$$U_V = r^{2\xi}, \quad \xi = 2, 3, \ldots . \tag{63}$$

Taking $\xi=2$, the second-order DKP equation becomes as follows:

$$\frac{d^2}{dr^2} F(r) + \left(\frac{E^2 - 2Er^4 + r^8 - m^2c^4}{h^2c^2} - \frac{J(J+1)}{r^2} \right) F(r) = 0. \tag{64}$$

In order to solve this equation with AIM, we propose the following wave function to transform it to an equation similar to Eq. (1):

$$F(r) = e^{-1/2\beta r^2} f(r), \tag{65}$$

where β is an arbitrarily introduced constant to improve the convergence speed of the method. We take $\beta=5$ as in Ref. 20 to compare with their nonrelativistic results for a similar problem. By taking $\hbar=c=m=1$ and $J=0$ (s state) for simplicity and inserting this wave function into Eq. (64), we obtain

$$\frac{d^2}{dr^2} f(r) = (-E^2 + 2Er^4 + \beta + 1 - \beta^2 r^2 - r^8) f(r) + 2\beta r \frac{d}{dr} f(r) \tag{66}$$

which can be now solved by AIM. Here, the $s_0(r)$ and $\lambda_0(r)$ are as follows:

$$s_0(r) = (-E^2 + 2Er^4 + \beta + 1 - \beta^2 r^2 - r^8), \quad \lambda_0(r) = 2\beta r. \tag{67}$$

In order to obtain the energy eigenvalues from Eq. (66), using Eq. (4), we obtain the $s_k(r)$ and $\lambda_k(r)$ in terms of $s_0(r)$ and $\lambda_0(r)$. Then, using the quantization condition of the method given by Eq. (5), we obtain the energy eigenvalues. This straightforward application of AIM gives us the energy eigenvalues, however, we have observed that the energy eigenvalues oscillate and do not converge within a reasonable number of iterations. The sequence appears to converge when the number of iterations $k \leqslant \simeq 30$, but then it begins to oscillate as the iteration number k increases. This result violates the principle behind the AIM; as the number of iteration increases, the method should converge and should not oscillate. We have noticed that the first reason for the oscillatory behavior is the r^8 term and the second but less serious reason is the E^2 term.

Therefore, in order to overcome this problem, we have used a perturbation approach within the framework of the AIM, similar to Ref. 21. In order to apply the perturbation, we introduce a parameter γ for $s_0(r)$ in Eq. (67),

TABLE I. Ground state energy of the anharmonic oscillator where k is the iteration number [$n=0$, $\hbar=c=m=1$, and $J=0$ (s state)].

k	E_0^0	E_0^1	E_0^2	E_0^3	E_0^4	E_0^5	E_0	E_0 (Ref. 20)
5	2.478 891	−0.481 521	−0.171 317	−0.087 565	−0.038 408	−0.030 214	1.669 866	
10	2.477 792	−0.485 884	−0.158 642	−0.080 739	−0.054 255	−0.036 055	1.662 217	1.325 073 435
15	2.477 837	−0.485 459	−0.159 187	−0.082 888	−0.052 218	−0.035 973	1.662 112	1.147 766 154
20	2.477 839	−0.485 450	−0.159 249	−0.083 021	−0.051 830	−0.035 991	1.662 298	1.072 223 000
25	2.477 838	−0.485 452	−0.159 247	−0.082 987	−0.051 875	−0.036 052	1.662 225	1.062 711 298
30			−0.159 246	−0.082 983	−0.051 885	−0.036 069	1.662 203	1.060 482 716
35			−0.159 246	−0.082 984	−0.051 885	−0.036 062	1.662 209	1.060 372 025
40					−0.051 884	−0.036 060	1.662 212	1.060 362 059
45						−0.036 061	1.662 211	1.060 362 077
50								1.060 362 091
55								1.060 362 091
60								1.060 362 090
65								
70								

$$s_0(r) = (-E^2 + 2Er^4 + \beta + 1 + \gamma(-\beta^2 r^2 - r^8)), \tag{68}$$

γ is an artificially introduced perturbation expansion parameter and at the end of the calculations, it will be seen that it is equal to 1. After this, Eq. (5) becomes

$$\delta_k(x,\gamma) = \lambda_{k+1}(x,\gamma)s_k(x,\gamma) - \lambda_k(x,\gamma)s_{k+1}(x,\gamma) = 0. \tag{69}$$

If we expand $\delta(x,\gamma)$ near $\gamma=0$, we obtain the following series:

$$\delta_k(x,\gamma) = \delta_k(x,0) + \frac{\gamma}{1!}\left.\frac{\partial\delta_k(x,\gamma)}{\partial\gamma}\right|_{\gamma=0} + \frac{\gamma^2}{2!}\left.\frac{\partial^2\delta_k(x,\gamma)}{\partial\gamma^2}\right|_{\gamma=0} + \frac{\gamma^3}{3!}\left.\frac{\partial^3\delta_k(x,\gamma)}{\partial\gamma^3}\right|_{\gamma=0} + \cdots . \tag{70}$$

According to AIM, the quantization condition $\delta_k(x,\gamma)$ must be equal to zero,

$$\delta_k^{(j)}(x,\gamma) = \frac{\gamma^j}{j!}\left.\frac{\partial^j\delta_k(x,\gamma)}{\partial\gamma^j}\right|_{\gamma=0}, \quad j = 0,1,2,\ldots . \tag{71}$$

It is also suitable to expand the energy eigenvalue E,

$$E_n = E_n^0 + \gamma E_n^1 + \gamma^2 E_n^2 + \gamma^3 E_n^3 + \gamma^4 E_n^4 + \cdots . \tag{72}$$

E_n expansion terms can be obtained by comparing the terms with the same order of γ in Eqs. (71) and (72). Hence, it is clear that the roots of $\delta_k^{(0)}(x,0)=0$ give us the main contribution energy terms E_n^0 and the roots of $\delta_k^{(1)}(x,0)=0$ give us the first correction E_n^1 and so on.

After we apply this perturbation approach, we have obtained the ground and the first even excited state energy eigenvalues. The results are presented in Tables I and II, respectively, for the ground and the first even excited state eigenvalues. In the first column of Table I, we present the E_0^0 (unperturbed), the second column E_0^1 which is the first correction and so on. We have used the perturbation up to fifth term, but one can use higher terms to improve the results. However, the effect becomes smaller as it can be seen from tables. In the last column of Table I, we show the nonrelativistic results of Fernandez[20] for the same potential to compare with our results. For these calculations, we have observed that the first term (E_0^0) in the expansion (72) converges around $k=30$ iterations, however, the correction terms require higher iterations and start to converge around $k=50$.

TABLE II. First even excited state energy of the anharmonic oscillator where k is the iteration number [$n=2$, $\hbar=c=m=1$, and $J=0$ (s state)].

k	E_2^0	E_2^1	E_2^2	E_2^3	E_2^4	E_2^5	E_2
5	5.698 344	−1.478 344	0.027 555	−2.574 579	−1.656 472	3.568 314	3.584 818
10	5.370 588	−0.911 718	−0.040 349	−0.433 823	−0.040 637	−0.068 883	3.875 178
15	5.413 951	−0.974 055	−0.267 240	−0.202 274	−0.037 847	−0.001 956	3.930 579
20	5.415 995	−0.992 837	−0.286 535	−0.104 029	−0.066 451	−0.078 990	3.887 153
25	5.415 458	−0.991 076	−0.277 803	−0.121 674	−0.072 980	−0.054 753	3.897 172
30	5.415 453	−0.990 550	−0.276 740	−0.127 545	−0.073 126	−0.040 145	3.907 347
35	5.415 460	−0.990 604	−0.277 153	−0.126 693	−0.071 566	−0.043 842	3.905 602
40	5.415 460	−0.990 626	−0.277 226	−0.126 297	−0.071 080	−0.046 266	3.903 965
45	5.415 460	−0.990 623	−0.277 201	−0.126 333	−0.071 315	−0.045 760	3.904 228
50	5.415 460	−0.990 622	−0.277 194	−0.126 358	−0.071 409	−0.045 369	3.904 508

In Table II, we show the first even excited state energy eigenvalues. Again, the perturbation is calculated up to fifth and the first term (E_0^0) converges around $k=35$ iterations, however, the correction terms require higher iterations and we have run them up to $k=50$ iteration.

VI. CONCLUSION

This paper has presented a different approach, the asymptotic iteration method, to the calculation of the nonzero angular momentum solutions of the relativistic Duffin-Kemmer-Petiau equation. Exact eigenvalues and eigenfunction for the relativistic Duffin-Kemmer-Petiau oscillator and Coulomb problems are derived easily. The advantage of the asymptotic iteration method is that it gives the eigenvalues directly by transforming the second-order differential equation into a form of $y''=\lambda_0(r)y'+s_0(r)y$. The exact wave functions are easily constructed by iterating the values of s_0 and λ_0. We have also shown how to solve the nontrivial problems with the help of the perturbation theory within the framework of the asymptotic iteration method. The method presented in this study is general and worth extending to the solution of other interaction problems.

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More anomaly free models of six-dimensional gauged supergravity

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We construct a huge number of anomaly free models of six-dimensional $\mathcal{N}=(1,0)$ gauged supergravity. The gauge groups are products of U(1) and SU(2), and every hyperino is charged under some of the gauge groups. It is also found that the potential may have flat directions when the *R*-symmetry is diagonally gauged together with another gauge group. In an Appendix, we determine the contribution to the global SU(2) anomaly from symplectic Majorana Weyl fermions in six dimensions. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209767]

I. INTRODUCTION

Six-dimensional $\mathcal{N}=(1,0)$ supergravity[1,2] has many interesting features. The ungauged version has been useful in uncovering the interesting dynamics of string theory in six dimensions. The gauged one is particularly interesting, because it does not allow the flat six-dimensional Minkowski space-time as a solution. Their solutions typically describe space–times which are spontaneously compactified to lower dimensions.[3,4] They can also be used to build various higher-dimensional models of particle phenomenology and cosmology. See e.g., Refs. 5 and 6.

Any higher dimensional theory of gravity should be considered as a low energy approximation of some unknown quantized theory, and there are several consistency conditions that any low energy approximation should satisfy. Anomaly freedom is one of the most important criteria. The search for anomaly free models in six dimensions is more difficult and at the same time richer than in 10 dimensions. It is because in six dimensions we can include hypermultiplets, which contribute to perturbative anomalies.[7]

The $d=6$, $\mathcal{N}=(1,0)$ ungauged supergravity can be obtained from heterotic strings on *K*3, and many anomaly free models are known,[8–12] with the help of the Green-Schwarz mechanism[13] in six dimensions. For $d=6$, $\mathcal{N}=(1,0)$ gauged supergravity, however, only a handful of consistent models have been found so far. Furthermore, if we impose the constraint that all hyperini should be charged under some of the gauge groups, the number of consistent models is very small.[14–16]

In $d=10$, $\mathcal{N}=1$ supergravity the anomaly cancels only for a few models, namely SO(32), $E_8\times E_8$, $E_8\times \mathrm{U}(1)^{248}$ and $\mathrm{U}(1)^{496}$. Moreover, the discovery of anomaly freedom of $E_8\times E_8$ inspired the construction of heterotic string theories. It is thus quite interesting to study how many anomaly free models there are in $d=6$, $\mathcal{N}=(1,0)$ gauged supergravity, and it might suggest the existence of some totally novel quantum completion of those theories within superstring theory or outside of it. No consistent way to derive it from the compactification of string or *M* theory is not known yet, although some progress is being made.[17,18] This is also interesting from the point of view of its phenomenological or cosmological applications.

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In this paper, we investigate the models whose gauge groups are products of U(1) and SU(2). This choice makes the condition for anomaly cancellation relatively simple. It will be shown that there are enormously many models which are free of both perturbative and global anomaly.

The paper is organized as follows. First we recall basic knowledge on $d=6$, $\mathcal{N}=(1,0)$ gauged supergravity in Sec. II. In Sec. III, we describe the general form of both perturbative and global anomaly free conditions, and we carry out the search and give our results in Sec. IV. Section V is the summary and discussion. In Appendix A we collect our notations concerning the group representations. Appendix B discusses the global gauge anomaly from the symplectic Majorana-Weyl fermion charged under SU(2) gauge group.

II. GAUGED $\mathcal{N}=(1,0)$ SUPERGRAVITY IN SIX DIMENSIONS

A. The spectrum

$\mathcal{N}=(1,0)$ supergravity in six dimensions contains the following multiplets:

$$\begin{aligned} &\text{supergravity multiplet,} && (e_\mu{}^m,\ B^-_{\mu\nu},\ \psi_\mu{}^{A-});\\ &\text{tensor multiplet,} && (B^+_{\mu\nu},\ \chi^{A+},\ \varphi);\\ &\text{vector multiplet,} && (A_\mu,\ \lambda^{A-});\\ &\text{hypermultiplet,} && (4\phi,\ \psi^+); \end{aligned}$$

where $\mu,\nu=0,\ldots,5$ label space–time, $m=0,\ldots,5$ labels tangent space, $A=1,2$ labels the fundamental representation of $\mathrm{Sp}(1)_R$, and $\pm$ denotes the chirality of Weyl spinors or the self-duality of the field strength of antisymmetric two-forms.

Weyl spinors of SO(1,5) and the fundamental representation of $\mathrm{Sp}(1)_R$ are both pseudoreal. By combining two antilinear involutions, we can impose a reality condition to get symplectic Majorana-Weyl spinors. Gravitini, tensorini, and gaugini are symplectic Majorana-Weyl under $\mathrm{Sp}(1)_R$. Hyperini are inert under $\mathrm{Sp}(1)_R$ and are Weyl spinors in general. If some of the hypermultiplets form a pseudoreal representation under the gauge groups, then we can impose the symplectic reality condition on them. Such a hypermultiplet is called a half-hypermultiplet.

Hereafter we assume the number of tensor multiplet n_T is one. This is because only in this case Lorentz- and gauge-covariant Lagrangian exist at the classical level.

B. Gauging hyperscalar manifold

The $d=6,\mathcal{N}=(1,0)$ rigid supersymmetry requires the scalar fields in the hypermultiplets to parametrize a hyperkähler manifold. If we couple hypermultiplets to gravity, then it must be a quaternionic manifold with negative curvature. For simplicity we assume the target space of the hyperscalars to be the manifold

$$\mathcal{M}_H := \frac{\mathrm{Sp}(1,n_H)}{\mathrm{Sp}(1)_R \times \mathrm{Sp}(n_H)}, \tag{2.1}$$

where n_H is the number of hypermultiplets.

We introduce vector multiplets which gauge some part of the isometry group $\mathrm{Sp}(1)_R \times \mathrm{Sp}(n_H)$ of $\mathcal{M}_H$. Arbitrary subgroups of $\mathrm{Sp}(1)_R \times \mathrm{Sp}(n_H)$ can be gauged. Let us write the gauge groups as $G_R \times G_H \subset \mathrm{Sp}(1)_R \times \mathrm{Sp}(n_H)$, where $G_R \subset \mathrm{Sp}(1)_R \times \mathrm{Sp}(n_H)$ gauges some part of the R-symmetry and $G_H \subset \mathrm{Sp}(n_H)$ acts only on the hypermultiplets. The closure of Lie algebra requires that G_R be one of the following possibilities: $\mathrm{U}(1)_R$, $\mathrm{Sp}(1)_R$, $\mathrm{U}(1)_{R+}$, and $\mathrm{Sp}(1)_{R+}$, where in the latter two cases we take U(1) or Sp(1) subgroup of $\mathrm{Sp}(n_H)$ and gauge the diagonal combination of them with $\mathrm{U}(1)_R$ or $\mathrm{Sp}(1)_R$, respectively. We call these latter two choices as diagonal gaugings. When G_H is made out of several factors $G_{H1} \times G_{H2} \times \cdots$, we use the label $z=1,2,\ldots$ to distinguish different factors.

Gauging hyperscalar manifold brings an additional potential term to the Lagrangian, which is required by supersymmetry. Here we will write the general form of the potential, citing the results

of Refs. 1 and 2. We denote hyperscalars parametrizing the manifold $\mathcal{M}_H$ by ϕ^α, $\alpha=1,\ldots,4n_H$. Since $\mathcal{M}_H$ is a symmetric space, its tangent space is spanned by the coset of the Lie algebras. Let $L(\phi)$ be a representative of the coset $\mathrm{Sp}(1,n_H)/[\mathrm{Sp}(1)_R\times\mathrm{Sp}(n_H)]$ so that $L(\phi)=\mathbf{1}_{\mathrm{Sp}(1,n_H)}+\mathcal{O}(\phi)$, and define C-functions as (the C-function is known under various names: P function, Killing prepotential, triholomorphic moment map, etc.)

$$C^{AB}{}_{CD} := (L^{-1}T^{AB}L)_{CD}, \quad C_z{}^{ab}{}_{CD} := (L^{-1}T_z^{ab}L)_{CD}, \tag{2.2}$$

where T^{AB} and T_z^{ab} are the generators of G_R and G_{Hz}, respectively. Then, the potential is given by

$$V(\phi)=\frac{1}{4}e^{-\varphi}\left(g_R^2 C^{AB}{}_{CD}C^{ABCD}+\sum_z g_{Hz}^2 C_z{}^{ab}{}_{CD}C_z{}^{abCD}\right), \tag{2.3}$$

where g_R, g_{Hz} are the coupling constants [we normalize the gauge kinetic term as $-(e^{\pm\varphi}/4g_k^2)\mathrm{tr}_k F_{\mu\nu}F^{\mu\nu}$, with $k=R,H_z$] of G_R, G_{Hz}.

The potential (2.3) is non-negative, because it is the sum of the squares of C-functions. One important feature is that $C^{AB}{}_{CD}=T^{AB}{}_{DC}+\mathcal{O}(\phi)$ and $C_z{}^{ab}{}_{CD}=\mathcal{O}(\phi)$, hence the potential is positive at $\phi^\alpha=0$ if we gauge R-symmetry. It provides a positive cosmological constant in a six-dimensional sense. For a nondiagonal gauging, explicit calculations of Refs. 1, 15, and 19 show that $\phi^\alpha=0$ is the minimum of the potential and there is no possibility of Higgsing. If we take a diagonal gauging, however, the potential may have flat or tachyonic directions. In this case, one can spontaneously break R-symmetry and possibly it leads to ungauged supergravity theories. The physics of models with diagonal gauging is relatively unexplored, and we hope to revisit this problem in the future.

Another important feature is that in the examples discussed so far, quadratic terms of $V(\phi)$ are only from the R coupling. Thus, the mass of hyperscalars is determined by their R charges.

The way how hyperini acquire four-dimensional mass depends on the details of compactification. Consider, for example, a space–time $\mathbb{R}^{1,3}\times S^2$ with monopoles in the internal S^2. If we embed the field strength of the monopole in $G_R=\mathrm{U}(1)_R$, $d=4$, $\mathcal{N}=1$ supersymmetry can remain unbroken.[3] Other choices of monopole charges generically break all the supersymmetry and many of them induce instability. [See Ref. 20 for the models with monopoles sitting in the U(1) factor, and Ref. 21 for those with monopoles sitting in the non-Abelian factor.]

III. GENERAL ANOMALY FREE CONDITIONS

Any six-dimensional gauge theory must satisfy two constraints concerning its gauge groups and representations. They are the freedom from the local and the global gravitational, gauge and mixed anomaly. The local or the global anomaly measures the change in the fermion determinant, induced by a gauge transformation which can or cannot be continuously deformed to identity. One must choose the gauge groups and the representations carefully so that both kinds of anomaly will cancel.

A. Local anomaly

It is well known that the Green-Schwarz mechanism can cancel the local gravitational, gauge and mixed anomaly if anomaly polynomial factorizes. (Note that in six dimensions the consistency of the Green-Schwarz mechanism is rather subtle, because we need to modify the lowest-derivative terms in the Lagrangian in order to introduce the Green-Schwarz counterterm. More details can be found in Refs. 2 and 22, including the generalization to $n_T>1$.)

Anomaly polynomial can be explicitly calculated by summing up the contributions from fermions and (anti-) self-dual tensors. Fermions of positive chirality or antisymmetric tensor with self-dual field strength contribute to it positively, while fermions of negative chirality or antisymmetric tensor with anti-self-dual field strength do negatively. Hence in our case, the total anomaly polynomial P_{total} is of the form

$$P_{\text{total}} = -(I_{3/2} + I_A) + \sum_{\text{tensor}} (I_A + I_{1/2}) - \sum_{\text{vector}} I_{1/2} + \sum_{\text{hyper}} I_{1/2}, \tag{3.1}$$

where each term comes from the supergravity multiplet, tensor multiplets, vector multiplets, and hypermultiplets, respectively.

In six dimensions, the anomaly polynomials for spin 3/2 fermions and spin 1/2 fermions in the representation r are known to be[7,23]

$$I_{3/2} = \left(\tfrac{245}{360}\text{tr}\, R^4 - \tfrac{43}{288}(\text{tr}\, R^2)^2\right)\text{tr}_r\, 1 + \tfrac{19}{6}\,\text{tr}\, R^2\,\text{tr}_r\, F^2 + \tfrac{10}{3}\,\text{tr}_r\, F^4, \tag{3.2}$$

$$I_{1/2} = \left(\tfrac{1}{360}\,\text{tr}\, R^4 + \tfrac{1}{288}(\text{tr}\, R^2)^2\right)\text{tr}_r\, 1 - \tfrac{1}{6}\,\text{tr}\, R^2\,\text{tr}_r\, F^2 + \frac{2}{3}\,\text{tr}_r\, F^4, \tag{3.3}$$

and that for a real self-dual antisymmetric tensor to be

$$I_A = \tfrac{28}{360}\,\text{tr}\, R^4 - \tfrac{8}{288}(\text{tr}\, R^2)^2. \tag{3.4}$$

We will study what conditions are necessary for (3.1) to factorize into the product of four-forms.

First of all, the coefficients of $\text{tr}\, R^4$ and $\text{tr}_r\, F^4$ must vanish. Using (3.2) and (3.3), the $\text{tr}\, R^4$ condition gives

$$n_H = 273 - 29n_T + n_V. \tag{3.5}$$

To satisfy the $\text{tr}_r\, F^4$ condition, we restrict our analysis to particular representations for which $\text{tr}\, F^4$ is a multiple of $(\text{tr}\, F^2)^2$. We call such representations exceptional type. All finite dimensional irreducible representations of A_1, A_2, E_6, E_7, E_8, F_4, and G_2 are of exceptional type, which we call Lie algebras of exceptional type. Further studies on exceptional-type representations can be found in Refs. 24 and 25. Casimir invariants of exceptional-type Lie algebras are summarized in Appendix A.

When $\text{tr}\, R^4$ and $\text{tr}_r\, F^4$ vanish, we can rewrite the total anomaly polynomial as

$$P_{\text{total}} = \sum_{jk} \beta_{jk} K^j K^k, \tag{3.6}$$

where K^k is

$$\vec{K} := (\text{tr}\, R^2, \text{tr}_f\, F_{G_R}^2, \text{tr}_f\, F_{G_1}^2, \text{tr}_f\, F_{G_2}^2, \ldots, \text{tr}_f\, F_{G_n}^2), \tag{3.7}$$

where G_i is shorthand notation for G_{Hi} and f is the smallest nontrivial irreducible representation of G_i.

It is convenient to regard β_{ij} as a $(n+1)\times(n+1)$ matrix. We call β_{ij} as anomaly matrix of the model. The condition for factorization of P_{total} is equivalent to $\beta_{ij} = (\alpha_i\gamma_j + \alpha_j\gamma_i)/2$ for some α_i, γ_j. It is clear that the columns of β are linear combination of $\vec{\alpha}$ and $\vec{\gamma}$, so we must have

$$\text{rank}\, \beta \leq 2. \tag{3.8}$$

Besides, the two vectors $\vec{\alpha}$ and $\vec{\gamma}$ must be real, because they enter into Lagrangian through the Green-Schwarz counterterm. Elementary calculation shows that β has two real nonzero eigenvectors (and thus real $\vec{\alpha}$ and $\vec{\gamma}$) if and only if

$$\lambda^+\lambda^- \leq 0. \tag{3.9}$$

We call (3.8) and (3.9) the first and the second factorization condition, respectively.

As a preparation for the actual search for anomaly free models in the next section, we describe the anomaly matrix more explicitly in each case of $G_R=\mathrm{U}(1)_{R(+)}$ and $\mathrm{Sp}(1)_{R(+)}$. Throughout the paper, we write the representation of hyperini as ρ^H and use tr_H as the abbreviation for the trace over ρ^H.

For $G_R=\mathrm{U}(1)_R$, the gravitini, tensorini, and gaugini all have charge one under $\mathrm{U}(1)_R$. The gaugini are the adjoints of the gauge groups. The anomaly polynomial is given by (we normalize the total anomaly polynomial so that $\alpha_1=\gamma_1=1$)

$$P=(\mathrm{tr}\,R^2)^2+\frac{\mathrm{tr}\,R^2}{6}\left((-20+n_V)F_{\mathrm{U}(1)R}^2+\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^2-\mathrm{tr}_H\,F^2\right)$$
$$+\frac{2}{3}\left\{-(4+n_V)F_{\mathrm{U}(1)R}^4-\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^4-6F_{\mathrm{U}(1)R}^2\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^2+\mathrm{tr}_H\,F^4\right\}. \tag{3.10}$$

For $G_R=\mathrm{U}(1)_{R+}$, the anomaly polynomial is almost the same as (3.10), except that hyperini are charged under $\mathrm{U}(1)_{R+}$ in this case.

For $G_R=\mathrm{Sp}(1)_R$, recall that the symplectic Majorana-Weyl condition is imposed on gravitini, tensorini, and gaugini. Another important point to notice is that the gaugini of the $\mathrm{Sp}(1)_R$ symmetry transforms in the $\mathbf{2}\otimes\mathbf{3}$ representation. The anomaly polynomial is given by

$$P=(\mathrm{tr}\,R^2)^2+\frac{\mathrm{tr}\,R^2}{6}\left(\left(\frac{-12+n_V}{2}\right)\mathrm{tr}_2\,F_{\mathrm{Sp}(1)}^2+\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^2-\mathrm{tr}_H\,F^2\right)$$
$$+\frac{2}{3}\left\{-\left(\frac{84+n_V}{4}\right)(\mathrm{tr}_2\,F_{\mathrm{Sp}(1)R}^2)^2-\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^4-3\,\mathrm{tr}_2\,F_{\mathrm{Sp}(1)R}^2\sum_{i=1}^{n}\mathrm{tr}_{\mathrm{ad}}\,F_{G_i}^2+\mathrm{tr}_H\,F^4\right\}. \tag{3.11}$$

For $G_R=\mathrm{Sp}(1)_{R+}$, we need to take it into account that hyperini are charged under $\mathrm{Sp}(1)_{R+}$.

B. Global anomaly

Once one finds a perturbatively anomaly free model, one needs to check whether the global anomaly vanishes. Global gauge anomaly in six dimensions may appear if the gauge group G has the nonvanishing sixth homotopy group, $\pi_6(G)\neq 0$.[26] There are three simple Lie groups with $\pi_6(G)\neq 0$, namely $\pi_6(\mathrm{SU}(2))=\mathbb{Z}_{12}$, $\pi_6(\mathrm{SU}(3))=\mathbb{Z}_6$, and $\pi_6(\mathsf{G}_2)=\mathbb{Z}_3$. Abelian gauge groups do not cause global anomaly because $\pi_6(\mathrm{U}(1))=0$.

The conditions for the cancellation of global gauge anomaly have been investigated through the works of Refs. 27–31 for the case of Weyl spinors. The conditions with symplectic Majorana-Weyl spinors in six dimensions seem to be absent in the literature, so we will give the derivation in Appendix B. The results are

$$1-4C_4(\rho^H;\mathsf{G}_2)\equiv 0 \pmod 3 \quad \text{for } \mathsf{G}_2, \tag{3.12}$$

$$8-D_4(\rho^H;\mathrm{SU}(2))\equiv 0 \pmod{12} \quad \text{for } \mathrm{SU}(2), \tag{3.13}$$

$$-2C_4(\rho^H;\mathrm{SU}(3))\equiv 0 \pmod 6 \quad \text{for } \mathrm{SU}(3), \tag{3.14}$$

$$n_V-D_4(\rho^H;\mathrm{Sp}(1))\equiv 0 \pmod{12} \quad \text{for } \mathrm{Sp}(1)_{R(+)}, \tag{3.15}$$

where the quantity C_4 is defined in Appendix A and the quantity D_4 for $\mathrm{SU}(2)\simeq\mathrm{Sp}(1)$ is defined in Appendix B. If there are no half-hypermultiplets, the relation $D_4\equiv 4C_4 (\mathrm{mod}\ 12)$ holds. Then the condition (3.13) reduces to

$$4 - 2C_4(\rho^H;\mathrm{SU}(2)) \equiv 0 \pmod 6, \tag{3.16}$$

which is precisely the condition found in Ref. 31.

Assuming the vanishing of global gauge anomaly, one can show that there is no global gravitational anomaly in six dimensions if the space–time is S^6, by slightly generalizing the argument in Ref. 32. Furthermore, it means that any six-dimensional theory is free of global anomaly on a coordinate patch, because any large diffeomorphism or large gauge transformation on a small patch can be done likewise on S^6. There might be other global anomalies coming from the nontrivial topology of space–time, but it is beyond the scope of our present work.

IV. EXAMPLES OF MODELS

We performed an extensive computer-aided search of anomaly free models whose gauge groups are of the form $G_{R(+)} \times G_H$ where $G_{R(+)}$ and G_H are U(1) or SU(2). And then we discovered enormously many anomaly free models. In what follows, we describe the details of our search and show several examples of the models.

A. Abelian gauge groups

Let $\{h_i\}$ be the basis of Cartan subalgebra $\mathrm{u}(1)^{n_H}$ of $\mathrm{sp}(n_H)$, then the generator of a $\mathrm{u}(1) \subset \mathrm{u}(1)^{n_H}$ is written as

$$T := \sum_{i=1}^{n_H} q^i h_i. \tag{4.1}$$

We assume q^i's to be quantized in integers.

When there are more than one Abelian factor within the gauge groups under which hyperini are charged, the anomaly polynomial, in general, contains terms of the form

$$\mathrm{tr}\, F_{\mathrm{U}(1)_1} \mathrm{tr}\, F^3_{\mathrm{U}(1)_2}, \quad \mathrm{tr}\, F_{\mathrm{U}(1)_1} \mathrm{tr}\, F_{\mathrm{U}(1)_2} \mathrm{tr}\, F^2_{\mathrm{U}(1)_3}, \quad \mathrm{tr}\, F_{\mathrm{U}(1)_1} \mathrm{tr}\, F_{\mathrm{U}(1)_2} \mathrm{tr}\, F_{\mathrm{U}(1)_3} \mathrm{tr}\, F_{\mathrm{U}(1)_4}.$$

The presence of traces of odd powers of F necessitates the generalization of the procedure outlined in the preceding sections. Therefore, in such situations we assume the presence of a symmetry among U(1) charges which forbids the appearances of the trace of odd powers of $F_{\mathrm{U}(1)_i}$'s.

Before giving our calculation and results, let us explain what kind of solutions we seek. First, if one finds an anomaly free model, one can rescale the unit charge of any U(1) and obtain another solution. This operation is rather trivial, so we regard two charge vectors related in this way as the same solution.

Second, in the literature, solutions with so-called drones are considered to be unrealistic and uninteresting, and thus we search for anomaly free models without drones. By drones we mean hypermultiplets which are not charged under $G_R \times G_H$, and U(1) vector multiplets with no charged scalars or fermions.

$\mathrm{U}(1)_R$: One needs $n_H = 245$ neutral hypermultiplets to cancel $\mathrm{tr}\, R^4$ terms. Then the anomaly polynomial automatically factorizes into

$$(\mathrm{tr}\, R^2 - 4F^2_{\mathrm{U}(1)R})\left(\mathrm{tr}\, R^2 + \tfrac{5}{6}F^2_{\mathrm{U}(1)R}\right). \tag{4.2}$$

Thus, there is one anomaly free model, albeit lots of singlet hyperini entering into it.

$\mathrm{U}(1)_R \times \mathrm{U}(1)$: We have found more than 40 million solutions to (3.8), (3.9) without drones. Some of them are listed as follows:

$$(n_1,n_2,n_3,n_4) = (243,0,3,0), \quad (173,70,3,0), \quad (138,96,12,0), \quad (123,102,21,0),$$
$$(112,109,24,1), \quad (108,96,42,0), \quad (108,54,84,0), \quad (123,0,123,0),$$

where n_q is the number of hypermultiplets with charge q. We set $n_q = 0$ for $q > 4$.

We also found some infinite series of anomaly free solutions with drone U(1) vector multiplets. For example, if $n_V=2+n_{\text{drone}}$ and $n_H=246+n_{\text{drone}}$, the combinations

$$(n_1,n_2,n_3,n_4)=(243,0,3+n_{\text{drone}},0), \tag{4.3}$$

$$(n_1,n_2,n_3,n_4)=(173,70,3,n_{\text{drone}}) \tag{4.4}$$

solve the factorization conditions for any $n_{\text{drone}}\geq 1$. There might be a deeper reason why such infinite series exist.

$U(1)_{R+}$: In this case, β_{jk} is a two-by-two matrix and the anomaly polynomial immediately factorizes. We also need to check the constraint (3.9), of which one can easily find an enormous amount of solutions with no singlet hypers.

$U(1)_{R+}\times U(1)_H$: Now hyperini can have charges under two Abelian groups, so the term $\operatorname{tr} F_{U(1)_{R+}}\operatorname{tr} F^3_{U(1)_H}$ may appear. Let us denote by n_{ab} the number of hyperini whose $U(1)_{R+}$ charge is $\pm a$ and whose $U(1)_H$ charge is $\pm b$. We restrict n_{ab} to be even so that one-half of them have charge (a,b) and the other one-half $(a,-b)$. Then the terms containing $\operatorname{tr} F_{U(1)}$, $\operatorname{tr} F^3_{U(1)}$ are removed.

We have found thousands of anomaly free choices of n_{ab}, some of which are

$$\begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 114 & 12 & 2 \\ 22 & 66 & 30 \end{pmatrix}, \quad \begin{pmatrix} 2 & 4 & 6 \\ 150 & 4 & 2 \\ 6 & 62 & 10 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 190 & 14 & 30 \\ 10 & 2 & 0 \end{pmatrix},$$

where other n_{ab} are all zero.

B. Non-Abelian gauge groups

In addition to (3.8), (3.9), one must also check the vanishing of global gauge anomaly for $\mathrm{Sp}(1)_R$ and SU(2) when dealing with non-Abelian gauge groups. These conditions altogether are quite lengthy and therefore it becomes far rarer to find the solutions than in Abelian cases. Still, we are able to discover hundreds or thousands of anomaly free models. To be concrete, we will describe some of them in this section.

As explained in Sec. II A, we can impose symplectic Majorana-Weyl condition to the fermions which transform in a pseudoreal representation. A half-hypermultiplet contributes to the anomaly polynomial (3.3) half as much as a hypermultiplet. Thus, once half-hypermultiplets are taken into account, n_H should be decomposed as

$$n_H=\sum_r n_r \dim r, \tag{4.5}$$

where n_r is the number of hypermultiplets in the representation r, and we allow n_r to be half-integers if r is pseudoreal. The group-theoretical constants defined in Appendix A then become

$$C_2(\rho^H;G)=\sum_r n_r C_2(r;G), \quad C_4(\rho^H;G)=\sum_r n_r C_4(r;G), \tag{4.6}$$

where G is a non-Abelian simple Lie group.

$U(1)_R\times \mathrm{SU}(2)$: Anomaly free choices of ρ^H are listed as follows:

$$\begin{aligned}(n_2,n_3,n_4,n_5,n_6,n_7,n_8) = {} & (0,4,1,11,26,3,0), \quad (0,7,0,2,0,31,0), \\ & (1,0,12,0,33,0,0), \quad (1,3,1,3,7,24,1), \\ & (2,1,29,25,0,0,0), \quad (3,0,0,0,11,0,22), \\ & (5,0,0,0,37,0,2), \quad (124,0,0,0,0,0,0).\end{aligned}$$

$U(1)_{R+}\times SU(2)$: Let $n_{i,r}$ be the number of hypermultiplets with $U(1)_{R+}$ charge i and in the $SU(2)$ representation r. Let us list some solutions of anomaly free conditions,

$$\begin{pmatrix} n_{1,2} & n_{1,3} & n_{1,4} \\ n_{2,2} & n_{2,3} & n_{2,4} \\ n_{3,2} & n_{3,3} & n_{3,4} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 12 \\ 66 & 0 & 9 \\ 9 & 0 & 3 \end{pmatrix}, \quad \begin{pmatrix} 2 & 6 & 9 \\ 46 & 4 & 5 \\ 28 & 2 & 1 \end{pmatrix}, \quad \begin{pmatrix} 3 & 1 & 5 \\ 28 & 6 & 1 \\ 65 & 1 & 2 \end{pmatrix}, \quad \begin{pmatrix} 4 & 5 & 8 \\ 59 & 1 & 8 \\ 15 & 2 & 1 \end{pmatrix}.$$

$Sp(1)_R$, $Sp(1)_R\times U(1)$ and $Sp(1)_R\times SU(2)$: There are no consistent models, because the $Sp(1)_R$ part has global gauge anomaly.

$Sp(1)_{R+}$: A few examples of anomaly free spectrum are

$$\begin{aligned}(n_2,n_3,n_4,n_5) &= (107+1/2,0,8,0), \quad (109+1/2,8,1,0), \\ &\quad (117+1/2,1,1,1), \quad (119+1/2,0,2,0).\end{aligned}$$

$Sp(1)_{R+}\times U(1)$: Let us denote by $n_{r,i}$ the number of hypermultiplets with $U(1)$ charge i and in $Sp(1)_R$ representation r. Hypermultiplets like

$$\begin{pmatrix} n_{2,1} & n_{2,2} & n_{2,3} \\ n_{3,1} & n_{3,2} & n_{3,3} \\ n_{4,1} & n_{4,3} & n_{4,3} \end{pmatrix} = \begin{pmatrix} 0 & 22 & 56 \\ 0 & 0 & 0 \\ 0 & 4 & 19 \end{pmatrix}, \quad \begin{pmatrix} 15 & 28 & 11 \\ 0 & 0 & 0 \\ 5 & 11 & 19 \end{pmatrix}, \quad \begin{pmatrix} 23 & 0 & 9 \\ 23 & 8 & 1 \\ 0 & 18 & 4 \end{pmatrix}, \quad \begin{pmatrix} 32 & 24 & 0 \\ 28 & 0 & 4 \\ 6 & 2 & 2 \end{pmatrix}$$

give anomaly free models.

$Sp(1)_{R+}\times SU(2)$: Let us denote by $n_{r,s}$ the number of hypermultiplets in the representation (r,s) of $Sp(1)_R\times SU(2)$. Examples of solutions are

$$\begin{pmatrix} n_{1,1} & n_{1,2} & n_{1,3} \\ n_{2,1} & n_{2,2} & n_{2,3} \\ n_{3,1} & n_{3,2} & n_{3,3} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 2 & 6 & 5 \\ 26 & 16 & 2 \end{pmatrix}, \quad \begin{pmatrix} 0 & 35 & 0 \\ 49 & 7 & 0 \\ 9 & 3 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 56 & 1 \\ 3 & 0 & 2 \\ 12 & 12 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 92 & 5 \\ 9 & 6 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We set $n_{1,1}=0$ to exclude singlet hyperini.

Before closing this section, we would like to mention an extra anomaly free model with the gauge groups $U(1)_R\times SU(3)$. The hypermultiplets behave as a totally symmetric tensor of $SU(3)$ with 21 indices. And this model is free from the global $SU(3)$ anomaly.

V. SUMMARY AND DISCUSSION

We discussed consistency conditions of six-dimensional gauged supergravity coming from anomaly cancellation. By performing a computer-aided search for consistent models, we found an enormous number of anomaly free models where the one-loop anomaly from the fermions is cancelled via the Green-Schwarz mechanism.

In the literature, it has often been considered that anomaly free models of six-dimensional gauged supergravity are quite rare. Our results suggest that there are a huge number of other perturbatively anomaly free models in six-dimensional gauged supergravity. However, our search was limited to the cases where the gauge group is a product of $U(1)$ and/or $SU(2)$. In fact, it is still very hard to find consistent models whenever the gauge groups consist of more than two simple Lie groups. Thus, the existence of $E_7\times E_6\times U(1)_R$, $E_7\times G_2\times U(1)_R$, and $F_4\times Sp(9)\times U(1)_R$ models found in Refs. 14–16 is indeed miraculous.

If one incorporates several tensor multiplets at the cost of covariant Lagrangian formulation, one can employ the generalized Green-Schwarz mechanism. Then, if rank $\beta\leq n_T+1$, one can successfully cancel the local anomaly. Thus, we might be able to find enormously many consistent models with the gauge groups like $G_R\times G_1\times\cdots\times G_{n_H}$ in a similar manner. The need for the quantum formulation is much more pressing with $n_T>1$, since in this case we cannot tell anything about the effective action in a strict sense.

We would like to comment on possible applications of our results. We have shown several examples of anomaly free models of $d=6,\mathcal{N}=(1,0)$ gauge supergravity. And some of them look very simple compared to the consistent models known so far. We hope that they will help to study various aspects of six-dimensional supergravity.

For example, when one wants to derive six-dimensional gauged supergravity from the compactifications of type II theory on a smooth space, we often have only Abelian gauge groups except for R-symmetry, as well as lots of drone U(1)'s. If such compactification is consistent as type II string theory, then it should be automatically anomaly free. Thus, our solutions with local R-symmetry $\times$ Abelian factors seem to be a good step in this direction. However, how to obtain a large number of charged hypermultiplets from string theory and how to make gravitini charged still remain as big problems.

Compactification to four dimensions is worth a further investigation. Our models might find a use in constructing higher-dimensional models of phenomenology and cosmology.[5,6,33–35] Moreover, if we compactify the theory down to four dimensions with branes,[34] new anomaly possibly arises on the branes. Then one should take care of anomaly inflow[36,37] in that framework.

Furthermore, our results may also be interesting in building solutions of $d=6,\mathcal{N}=(1,0)$ gauged supergravity. For example, see the recent paper.[38]

Finally, the physics of diagonally gauged models can be studied more thoroughly. We may find interesting generalization of the aforementioned applications. We hope to revisit this problem in the future.

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APPENDIX A: REPRESENTATION THEORETICAL CONSTANTS

Let $F_G=F_G^i T_r^i$ be the field strength of gauge group G, acting on fermions in the representation r. When G is a simple non-Abelian gauge group, we define group-theoretical constants $C_2(R;G)$, $A(R;G)$, and $B(R;G)$ as

$$\mathrm{tr}_R F_G^2 \coloneqq C_2(R;G)\mathrm{tr}_f F_G^2, \quad \mathrm{tr}_R F_G^4 \coloneqq A(R;G)\mathrm{tr}_f F_G^4 + B(R;G)(\mathrm{tr}_R F_G^2)^2, \tag{A1}$$

where f is the smallest nontrivial irreducible representation of G. For exceptional-type representations which has no fourth-order Casimir invariants, we also define $C_4(R;G)$ as

$$\mathrm{tr}_R F_G^4 \coloneqq C_4(R;G)(\mathrm{tr}_f F_G^2)^2 = B(R;G)C_2(R;G)^2(\mathrm{tr}_f F_G^2)^2. \tag{A2}$$

We will omit G if it causes no ambiguity.

Some comments on the group-theoretical constants defined here: First, the ratio $\mathrm{tr}_r(F_G)^n/\mathrm{tr}_{r'}(F_G)^n$ is independent of the normalization of T_r^i. Thus the quantities $A(R;G)$, $B(R;G)$, and $C_i(R;G)$ are determined only by the representation R of G. Second, when R is the direct sum of irreducible representations $R=\oplus_i R_i$, then $C_2(R)$ and $C_4(R)$ are equal to the sums $\Sigma_i C_2(R_i)$ and $\Sigma_i C_4(R_i)$, respectively. Third, for an irreducible exceptional-type representation R, we have a formula[24]

$$C_4(R;G) = \frac{\dim G}{2\dim R(2+\dim G)}\left(6 - \frac{C_2(\mathrm{ad})}{\dim G}\cdot\frac{\dim R}{C_2(R)}\right)C_2(R;G)^2. \tag{A3}$$

APPENDIX B: GLOBAL GAUGE ANOMALY FOR MAJORANA-WEYL FERMIONS

If $\pi_6(H)=\mathbb{Z}_p$ for some gauge group H, global anomaly may exist. Then we must check whether the global gauge anomaly cancels.

1. Weyl fermions

First let us review the calculation for Weyl fermions.[27–31] The basic strategy is to embed H into G such that $\pi_7(G)=\mathbb{Z}$ and $\pi_6(G)=0$. Then, because the gauge group G has no global gauge anomaly in six dimensions, the global gauge transformation in H can be deformed continuously to identity in G. In this way we can reduce the calculation of global anomaly for H to that of perturbative anomaly for G.

The embedding

$$0 \to H \overset{\iota}{\to} G \overset{p}{\to} G/H \to 0 \tag{B1}$$

induces the homotopy exact sequence

$$\cdots \overset{\iota_*}{\to} \pi_7(G) \overset{p_*}{\to} \pi_7(G/H) \overset{\partial_*}{\to} \pi_6(H) \to \pi_6(G) = 0. \tag{B2}$$

Let us denote by g, g' the generators of $\pi_7(G)$ and $\pi_7(G/H)$, respectively. Then, $\tilde{g} \equiv \partial_* g'$ is a generator of $\pi_6(H)$ and there is an integer s such that $p_*(g)=(g')^s$ in our cases.

Let us embed the fermion in the representation r_L of H in the representation $R_L \ominus R_R$ of G (here the subscripts L and R denote the chirality), so that $R_L \ominus R_R$ decompose under H to r_L plus some fermions which can be massive. Then, following the argument of Ref. 27, the H gauge transformation corresponding to $\tilde{g}$ produces a phase $e^{i\theta(r)}$, with $\theta(r)$ given by

$$\theta(r) = \frac{1}{s}\int_{S^7} \gamma(g,A,F;R_L \ominus R_R), \tag{B3}$$

where $\gamma(g,A,F;R)$ is the change under g of the non-Abelian Chern-Simons terms in the representation R. We can easily show that $\int_{S^7}\gamma(g,A,F;R)=2\pi A(R;G)$ if $G=\mathrm{SU}(n)$. Thus we have

$$\theta(r) = 2\pi A(R;G)/s. \tag{B4}$$

For $H=\mathrm{SU}(2)$, $\mathrm{SU}(3)$, and G_2, we can choose G as $\mathrm{SU}(4)$, $\mathrm{SU}(4)$, $\mathrm{SU}(7)$, respectively.[28] We claim that, for the representation R of $\mathrm{SU}(4)$ or $\mathrm{SU}(7)$, $A(R;G)$ is given by

$$A(R;\mathrm{SU}(4)) \equiv 2\sum_i C_4(r_i;H) \pmod 6 \quad \text{for } H=\mathrm{SU}(2) \text{ or } \mathrm{SU}(3), \tag{B5}$$

$$A(R;\mathrm{SU}(7)) \equiv 4\sum_i C_4(r_i;H) \pmod 3 \quad \text{for } H=\mathsf{G}_2, \tag{B6}$$

provided that the representation R decomposes as $R=\oplus_i r_i$ under H.

To prove them, we evaluate $\mathrm{tr}_G F_R^4$ in two ways. Using (A1), it can be rewritten as

$$\mathrm{tr}_G F_R^4|_{\mathrm{on}\ H} = A(R;G)\mathrm{tr}_G F_f^4|_{\mathrm{on}\ H} + B(R;G)(\mathrm{tr}_G F_f^2|_{\mathrm{on}\ H})^2 = \{B(f;H)A(R;G) + B(R;G)\}(\mathrm{tr}_G F_f^2|_{\mathrm{on}\ H})^2, \tag{B7}$$

where f is the fundamental representation of G, and in the last line we evaluate the trace after restricting it on H. Using the direct product decomposition $R=\oplus_i r_i$, the trace is

$$\mathrm{tr}_G F_R^4|_{\mathrm{on}\ H} = \mathrm{tr}_H\left(\sum_i F_{r_i}\right)^4 = \sum_i \mathrm{tr}_H F_{r_i}^4 = \sum_i C_4(r_i;H)(\mathrm{tr}_H F_f^2)^2. \tag{B8}$$

By comparing the two, we get

$$B(f;H)A(R;G) + B(R;G) = \sum_i C_4(r_i;H). \tag{B9}$$

We have $B(f;H)=1/2$ for $H=\mathsf{A}_1,\mathsf{A}_2$ and $1/4$ for $H=\mathsf{G}_2$. Furthermore, one can show that $B(R;G)\equiv 0 \pmod 3$ by mathematical induction,[39] and the claims (B5) and (B6) immediately follow. It is easy to derive the equations (3.12), (3.14), and (3.16) from these results.

2. Majorana-Weyl fermions

Let us now move on to the case with Majorana-Weyl fermions. As discussed in Sec. II A, in six dimensions we can halve the degrees of freedom of Weyl spinors when they form a pseudoreal representation of the gauge groups. Such Majorana-Weyl fermions are more specifically called symplectic Majorana-Weyl fermions, though we use the two words interchangeably.

If we carry out this procedure for a hypermultiplet, the resulting multiplet is called a half-hypermultiplet. The gravitini, tensorini, and gaugini of $d=6,\mathcal{N}=(1,0)$ supergravity are all Majorana-Weyl, where we use the fact the **2** of $\mathrm{Sp}(1)_R$ is pseudoreal.

Of the gauge groups which have global anomaly in $d=6$, only SU(2) has pseudoreal irreducible representations. So hereafter we restrict our attention to global SU(2) [or Sp(1)] anomaly. We assume that the perturbative anomaly is already canceled by the Green-Schwarz mechanism. As we saw in the preceding section, the Weyl fermions in **2** produces the phase $e^{2\pi i/6}$ under the generator of $\pi_6(\mathrm{SU}(2))$. Let α be the phase produced by Majorana-Weyl fermions in **2**. Because $\alpha^2=e^{2\pi i/6}$, α must be either $e^{2\pi i/12}$ or $e^{2\pi i 7/12}$. Now we are going to determine which is the case.

To do it, we need to embed a symplectic Majorana-Weyl fermion in **2** of SU(2) in a Majorana-Weyl fermion in a larger gauge group without global anomaly. Thus **4** in Sp(2) is a good choice. Let it decompose into $\mathbf{2}\oplus\mathbf{1}\oplus\mathbf{1}$ under SU(2). We write the change of the Chern-Simons seven-form by $\gamma(g,A,F)$, as in the preceding section.

The phase change for Weyl fermions in the fundamental of SU(4) is $\int\gamma(g,A,F)=2\pi$ under the generator g of $\pi_7(\mathrm{SU}(4))$. Consider the homotopy exact sequence

$$\begin{aligned}\pi_8(S^5) = \mathbb{Z}_{24} \xrightarrow{\partial_*} \pi_7(\mathrm{Sp}(2)) = \mathbb{Z} \xrightarrow{\iota_*} \\ \pi_7(\mathrm{SU}(4)) = \mathbb{Z} \xrightarrow{p_*} \pi_7(S^5) = \mathbb{Z}_2 \xrightarrow{\partial_*} \pi_6(\mathrm{Sp}(2)) = 0.\end{aligned} \tag{B10}$$

[A considerable knowledge of algebraic topology is required for the actual calculation of homotopy groups. A concise table for the higher homotopy groups of the compact Lie groups can be found in the Appendix A of Ref. 40. Interested readers can consult the textbooks (Refs. 41 and 42) and references therein.]

It implies that the generator g' of $\pi_7(\mathrm{Sp}(2))$ is mapped to g^2. Thus, the phase change for Weyl fermions in **4** of Sp(2) under g' is 4π. Therefore it is 2π for Majorana-Weyl fermions in **4**.

Now consider another sequence

$$\begin{aligned}\pi_7(\mathrm{Sp}(1)) = \mathbb{Z}_2 \xrightarrow{\iota_*} \pi_7(\mathrm{Sp}(2)) \\ = \mathbb{Z} \xrightarrow{p_*} \pi_7(\mathrm{Sp}(2)/\mathrm{Sp}(1)) = \mathbb{Z} \xrightarrow{\partial_*} \pi_6(\mathrm{Sp}(1)) = \mathbb{Z}_{12} \xrightarrow{\iota_*} \pi_6(\mathrm{Sp}(2)) = 0.\end{aligned} \tag{B11}$$

Denote the generator of $\pi_7(\mathrm{Sp}(2)/\mathrm{Sp}(1))$ by h'. Then h' satisfies $p_*(g')=(h')^{12}$, and $\tilde{h}:=\partial_* h'$ is one of the generators of $\pi_6(\mathrm{Sp}(1))$. Thus, the phase change under $\tilde{h}$ for Majorana-Weyl fermions in **2** is $e^{2\pi i/12}$.

Let us go on to other representations. Let $[k]$ be the k-index symmetric tensor representation of Sp(1) or Sp(2). Let us bear in mind that $\mathbf{k}=[k-1]$ in Sp(1). Then, for Sp(2),

$$\mathrm{tr}_{[k]} F^4 = A(k)\mathrm{tr}_{[1]} F^4 + \cdots, \tag{B12}$$

where $A(k)=k(k+1)(k+2)(k+3)(k+4)(k^2+4k+2)/840$. Furthermore,

$$[k] \to [k] + 2[k-1] + 3[k-2] + 4[k-3] + \cdots . \tag{B13}$$

under the restriction of groups from Sp(2) to Sp(1). Thus, $[k-1]_L - 2[k-2]_R + [k-3]_L$ of Sp(2) reduces to $\mathbf{k}_L$ of Sp(1), and hence the phases under the global gauge transformation $\tilde{h}$ for Majorana-Weyl $\mathbf{k}$ is $2\pi D_4(\mathbf{k})/12$, where

$$D_4(\mathbf{k}) = A(k-1) - 2A(k-2) + A(k-3). \tag{B14}$$

Specifically, Majorana-Weyl fermions in **4** contribute $e^{-\pi i/3}$, and Weyl fermions in **3** contribute $e^{4\pi i/3}$ to the global anomaly phase.

Finally, by considering

$$I_{3/2} = \cdots + \tfrac{10}{3}\,\mathrm{tr}\,F^4, \quad I_{1/2} = \cdots + \tfrac{2}{3}\,\mathrm{tr}\,F^4,$$

and the embedding of gravitini into **4** of Sp(2) with the symplectic Majorana-Weyl condition, we see that a gravitino contributes five times as much as that of a spin 1/2 fermion.

Suppose we gauge the Sp(1) *R*-symmetry, then the contributions from various fermions are summarized as

$$\begin{aligned} &\text{gravitini in a supergravity multiplet,} && 5 \bmod 12;\\ &\text{tensorini in a tensor multiplet,} && -1 \bmod 12;\\ &\text{the } \mathrm{Sp}(1)_R \text{ gaugini,} && -1 \bmod 12;\\ &\text{other gaugini in a vector multiplet,} && 1 \bmod 12. \end{aligned} \tag{B15}$$

Thus, the condition for the cancellation of global $\mathrm{Sp}(1)_{R(+)}$ anomaly is

$$n_V - D_4(\rho^H; \mathrm{Sp}(1)) \equiv 0 \pmod{12}. \tag{B16}$$

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Character formulas and partition functions in higher dimensional conformal field theory

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A discussion of character formulas for positive energy, unitary irreducible representations of the conformal group is given, employing Verma modules and Weyl group reflections. Product formulas for various conformal group representations are found. These include generalizations of those found by Flato and Fronsdal for SO(3,2). In even dimensions the products for free representations split into two types depending on whether the dimension is divisible by four or not. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196241]

I. INTRODUCTION

Motivated by the AdS/CFT correspondence, which relates string theory in an AdS space to a conformal field theory on the boundary character formulas for groups associated with conformal symmetry have received greater attention recently.[1–4] In Refs. 1, 2, and 4 the way in which character formulas encode the spectrum of operators allowed in a conformal Yang-Mills theory has been their main use. We hope that the present discussion might be similarly useful for conformal Yang-Mills theories in higher dimensions.

It is well known that character formulas provide an elegant way of decomposing tensor products of Lie algebra representations—the Racah-Speiser algorithm for decomposing tensor products of finite dimensional irreducible representations of simple Lie algebras may be easily proved in terms of Weyl characters, see Ref. 5 for a summary. In conformal field theories the method of characters was used by Flato and Fronsdal[6] to decompose products of certain massless representations, called "Di" and "Rac," in three dimensions. Oscillator and other methods have been used by various authors to generalize this to higher dimensions.[7–10] Here we follow a more direct approach using character formulas for the conformal group to decompose products of positive energy unitary irreducible representations of the conformal group which *inter alia* provides a generalization of the Flato-Fronsdal results. These formulas may also be relevant to operator product expansions.

The layout of the paper is as follows. We rewrite the conformal algebra in terms of the orthonormal basis of $SO^*(d+2)$, the complexification of the conformal group in d dimensions, in Sec. II.

In Sec. III we construct the characters of any positive energy unitary irreducible representation of the conformal group. The problem is related to finding characters of certain infinite dimensional representations of $SO^*(d+2)$ and we make use of a result in Ref. 11, employing Verma module characters, for solving it. The main part of the task consists, in this approach, of finding sub-Verma modules of an original one. This is more straightforward in the orthonormal basis of $SO^*(d+2)$ due to simplifications in the Weyl group action on weights in this basis. In this section we also show how these formulas are equivalent to ones obtained as follows. The basis for the original $SO^*(d+2)$ Verma module is reduced in a way determined by Appendix C which discusses unitary representations of the conformal group. We write down the character of the reduced $SO^*(d+2)$

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Verma module and then simply act on it with the Weyl symmetry operator of SO(d). The formula obtained agrees with the character formula for the corresponding irreducible representation of $SO^*(d+2)$. We also give the three- and four-dimensional results explicitly and these match known results.[4,6,24,25]

In Sec. IV we discuss products of the unitary irreducible representations. As a simple example we first discuss the case of $d=4$. This is made simpler by the fact that the SO(4) character may be rewritten as a product of two SO(3) characters. We then go on to discuss higher dimensional cases which correspond to products of free representations. Crucial in this approach are expansion formulas of the characters in the following form, namely,

$$\sum_N s^{\Delta+N} F_N(x), \tag{1.1}$$

where Δ denotes the canonical conformal dimension, $F_N(x)$ is some linear combination of the SO(d) characters and with s and $\underline{x}=(x_1,\ldots,x_r)$, $r=\left[\frac{1}{2}d\right]$ being some variables. We give expansion formulas of the type (1.1) for all character formulas of interest.

In even dimensions the product formulas obtained divide into two forms depending on whether the dimension d is divisible by 4 or not.

While we do not find all such product formulas, we feel that the method presented generalizes easily when used in conjunction with expansion formulas of the type (1.1).

Expansions of the form (1.1) are used in Sec. V then to correlate our results for character formulas with one-particle partition functions which have been found by various authors[12–14] for the free scalar, Weyl fermion and $(d/2)$-form field strengths. We also discuss an expansion formula given for the character for conserved symmetric traceless tensor currents in the main text. A simple argument is given which explains the behavior of the character formula [in the form (1.1)] when $\underline{x}=(1,\ldots,1)$. Also it is found that the character for the free scalar obtained here matches the one particle partition function for a scalar field on the boundary of AdS in Ref. 15 when the spin of descendants is taken into account.

Various useful formulas and proofs are left in the remaining appendixes. In Appendix A results for character formulas for infinite dimensional representations of semisimple Lie groups are discussed. In Appendix B standard formulas for SO(d) Weyl characters are given. In Appendix C unitarity bounds are discussed. While unitarity bounds have been discussed in great detail by other authors, see, for example, Refs. 16–18, we feel that this attention is merited in that it determines which combination of generators are to be omitted from the full Verma module for $SO^*(d+2)$ when character formulas for unitary irreducible representations of the conformal group are analyzed. Appendix D contains proofs of certain product and expansion formulas for conformal group characters.

II. THE CONFORMAL ALGEBRA IN THE ORTHONORMAL BASIS

Starting from the Lie algebra for SO($d,2$),

$$[M_{AB},M_{CD}]=i(g_{AC}M_{BD}-g_{AD}M_{BD}-g_{BC}M_{AD}+g_{BD}M_{AC}), \tag{2.1}$$

for $A,B=1,\ldots,d+2$, $g_{AB}=\text{diag}\,(1,\ldots,1,-1,-1)$ and where $M_{AB}=-M_{BA}$ are Hermitian, then (2.1) may be related to the standard form of the conformal algebra by defining $M_{ab},\mathcal{P}_a,\mathcal{K}_a,H$, for $a,b=1,\ldots,d$ through

$$[M_{AB}]=\begin{pmatrix} M_{ab} & -M_{at} \\ M_{sb} & \epsilon_{st}H \end{pmatrix}, \tag{2.2}$$

where $s,t=d+1,d+2$, $\epsilon_{dd+1}=1$, $\epsilon_{st}=-\epsilon_{ts}$, and

$$\mathcal{P}_a=M_{ad+1}+iM_{ad+2}, \quad \mathcal{K}_a=M_{ad+1}-iM_{ad+2}. \tag{2.3}$$

Then

$$[M_{ab},M_{cd}] = i(\delta_{ac}M_{bd} - \delta_{ad}M_{bc} - \delta_{bc}M_{ad} + \delta_{bd}M_{ac}),$$

$$[M_{ab},\mathcal{P}_c] = i(\delta_{ac}\mathcal{P}_b - \delta_{bc}\mathcal{P}_a), \quad [M_{ab},\mathcal{K}_c] = i(\delta_{ac}\mathcal{K}_b - \delta_{bc}\mathcal{K}_a), \tag{2.4}$$

$$[H,\mathcal{P}_a] = \mathcal{P}_a, \quad [H,\mathcal{K}_a] = -\mathcal{K}_a, \quad [\mathcal{K}_a,\mathcal{P}_b] = -2iM_{ab} + 2\delta_{ab}H,$$

with all other commutators not mentioned in (2.4) vanishing. As usual, $M_{ab}=-M_{ba}$ are Hermitian generators of SO(d) rotations. Here H, the conformal Hamiltonian, is required to have a positive definite spectrum of eigenvalues for positive energy representations.

In (2.4) M_{ab} of course satisfy the Lie algebra of SO(d). For what follows we will use the orthonormal basis for SO(d) whereby the Cartan subalgebra is defined by

$$H_i = M_{2i-12i}, \quad i = 1,\ldots,r, \quad [H_i,H_j] = 0, \tag{2.5}$$

with raising and lowering operators formed from

$$E_{ij}^{\varepsilon\eta} = -E_{ji}^{\eta\varepsilon} = M_{2i-12j-1} + i\varepsilon M_{2i2j-1} + i\eta M_{2i-12j} - \varepsilon\eta M_{2i2j}, \quad i \neq j, \quad \varepsilon,\eta = \pm, \tag{2.6}$$

augmented by

$$E_i^{\pm} = M_{2i-12r+1} \pm iM_{2i2r+1}, \tag{2.7}$$

for SO($2r+1$).

In $2r$ dimensions the commutation relations among the SO($2r$) generators in the orthonormal basis are given by

$$[H_i,E_{jk}^{\varepsilon\eta}] = (\varepsilon\delta_{ij} + \eta\delta_{ik})E_{jk}^{\varepsilon\eta},$$

$$[E_{ij}^{\varepsilon\eta},E_{ij}^{\varepsilon'\eta'}] = (\varepsilon - \varepsilon')(1 - \eta\eta')H_i + (\eta - \eta')(1 - \varepsilon\varepsilon')H_j, \tag{2.8}$$

$$[E_{ij}^{\varepsilon\eta},E_{jk}^{\varepsilon'\eta'}] = i(\varepsilon'\eta - 1)E_{ik}^{\varepsilon\eta'}, \quad i \neq k,$$

where $i,j,k=1,\ldots,r$ and $\varepsilon,\varepsilon',\eta,\eta'=\pm$ with other commutators, that cannot be obtained through the symmetry $E_{ij}^{\varepsilon\eta}=-E_{ji}^{\eta\varepsilon}$, vanishing.

Using standard orthogonal unit vectors $e_i \in \mathbb{R}^r$ then E_{ij}^{++} for $1 \leqslant i < j \leqslant r$ correspond to the set of positive roots $e_i \pm e_j$ while E_{ij}^{--} correspond to the set of negative roots $-e_i \pm e_j$. The simple roots $e_i - e_{i+1}, e_{r-1} + e_r$ for $1 \leqslant i \leqslant r-1$ correspond to the linearly independent set of raising operators $E_{ii+1}^{+-}, E_{r-1r}^{++}$. Similarly the linearly independent set of lowering operators is $E_{ii+1}^{-+}, 1 \leqslant i \leqslant r-1, E_{r-1r}^{--}$.

In $2r+1$ dimensions we have additionally the following commutation relations involving the extra generators (2.7), namely,

$$[H_i,E_j^{\pm}] = \pm\delta_{ij}E_j^{\pm},$$

$$[E_i^{\varepsilon},E_i^{\eta}] = (\varepsilon - \eta)H_i, \quad [E_i^{\varepsilon},E_j^{\eta}] = iE_{ij}^{\varepsilon\eta}, \quad i \neq j, \tag{2.9}$$

$$[E_{ij}^{\varepsilon\eta},E_j^{\varepsilon'}] = -[E_{ji}^{\eta\varepsilon},E_j^{\varepsilon'}] = i(\varepsilon'\eta - 1)E_i^{\varepsilon},$$

for $i,j=1,\ldots,r$ with all other such vanishing.

For SO($2r+1$) E_i^+ corresponds to the extra positive roots e_i while E_i^- corresponds to the extra negative roots $-e_i$. The simple roots $e_i - e_{i+1}, 1 \leqslant i \leqslant r-1$ and e_r correspond to the linearly independent set of raising operators E_{ii+1}^{+-}, E_r^+. The linearly independent set of lowering operators is $E_{ii+1}^{-+}, 1 \leqslant i \leqslant r-1$ along with E_r^-.

In the orthonormal basis of SO($2r$), the $2r$ dimensional vector representation has highest weight e_1 and all other weights in the weight system are given by $\pm e_i, 1 \leqslant i \leqslant r$. The weight system may be represented diagrammatically by

$$\begin{array}{ccccccccccccccc} & & & & & & & & \mathrm{e}_r & & & & & & \\ & & & & & & & E^{-+}_{r-1\,r} \nearrow & & \searrow E^{--}_{r-1\,r} & & & & & \\ \mathrm{e}_1 & \xrightarrow{E^{-+}_{12}} & \mathrm{e}_2 & \cdots & \mathrm{e}_{r-2} & \xrightarrow{E^{-+}_{r-2\,r-1}} & \mathrm{e}_{r-1} & & & & -\,\mathrm{e}_{r-1} & \xrightarrow{E^{-+}_{r-2\,r-1}} & -\,\mathrm{e}_{r-2} & \cdots & -\,\mathrm{e}_2 \xrightarrow{E^{-+}_{1\,2}} -\,\mathrm{e}_1 \\ & & & & & & & E^{--}_{r-1\,r} \searrow & & \nearrow E^{-+}_{r-1\,r} & & & & & \\ & & & & & & & & -\mathrm{e}_r & & & & & & \end{array} \tag{2.10}$$

which also indicates the action of the lowering operators $E^{-+}_{ii+1}, 1 \leqslant i \leqslant r, E^{--}_{r-1r}$. As a convenient basis for the $\mathcal{P}_a, \mathcal{K}_a$ operators, which of course transform in the vector representation, we define

$$\mathcal{P}_{i\pm} = \mathcal{P}_{2i-1} \pm i\mathcal{P}_{2i}, \quad \mathcal{K}_{i\pm} = \mathcal{K}_{2i-1} \pm i\mathcal{K}_{2i}, \tag{2.11}$$

for which $[E^{+-}_{ii+1}, \mathcal{P}_{1+}] = [E^{++}_{r-1r}, \mathcal{P}_{1+}] = [E^{+-}_{ii+1}, \mathcal{K}_{1+}] = [E^{++}_{r-1r}, \mathcal{K}_{1+}] = 0$ and

$$[H_i, \mathcal{P}_{j\pm}] = \pm\,\delta_{ij}\mathcal{P}_{j\pm}, \quad [H_i, \mathcal{K}_{j\pm}] = \pm\,\delta_{ij}\mathcal{K}_{j\pm}, \tag{2.12}$$

so that $\mathcal{P}_{i\pm}, \mathcal{K}_{i\pm}$ correspond to the weights $\pm e_i$. In terms of explicit action of lowering operators, we have that

$$\begin{aligned} \mathcal{P}_{i\pm} &= -\frac{i}{2}[E^{-\pm}_{1i}, \mathcal{P}_{1+}], \quad i = 2, \ldots, r-1, \quad \mathcal{P}_{1-} = \tfrac{1}{4}[E^{-+}_{12}, [E^{--}_{12}, \mathcal{P}_{1+}]], \\ \mathcal{K}_{i\pm} &= -\frac{i}{2}[E^{-\pm}_{1i}, \mathcal{K}_{1+}], \quad i = 2, \ldots, r-1, \quad \mathcal{K}_{1-} = \tfrac{1}{4}[E^{-+}_{12}, [E^{--}_{12}, \mathcal{K}_{1+}]], \end{aligned} \tag{2.13}$$

which may be easily unravelled in terms of the action of the linearly independent set of lowering operators $E^{-+}_{ii+1}, 1 \leqslant i \leqslant r, E^{--}_{r-1r}$.

In fact the entire conformal algebra in this basis may be written in terms of the orthonormal basis of the SO$^*(2r+2)$ algebra. Making the definitions

$$H_0 = -H, \quad E^{-\pm}_{0i} = -E^{\pm-}_{i0} = \mathcal{P}_{i\pm}, \quad E^{\pm+}_{i0} = -E^{+\pm}_{0i} = \mathcal{K}_{i\pm}, \quad i = 1, \ldots, r \tag{2.14}$$

(so that $-H$ is the extra Cartan subalgebra element and $\mathcal{K}_{i\pm}/\mathcal{P}_{i\pm}$ form the extra raising/lowering operators) then the conformal algebra may be shown to be equivalent to (2.8) for the range of the indices i, j, k being extended to $0, 1, \ldots, r$. The linearly independent set of raising/lowering operators in this case is extended to include $\mathcal{K}_{1-}/\mathcal{P}_{1+}$.

The $2r+1$ dimensional vector representation of SO($2r+1$) has highest weight e_1 and the weight system is $\pm e_i$ and 0. Diagrammatically the weight system is given by

$$\begin{array}{ccccccccccccc} & E^{-+}_{12} & & & & E^{-+}_{r-1r} & E^{-}_{r} & E^{-}_{r} & & E^{-+}_{r-1r} & & & E^{-+}_{12} \\ e_1 \rightarrow & e_2 & \cdots & e_{r-1} & \rightarrow & e_r & \rightarrow 0 \rightarrow & -\,e_r & \rightarrow & -\,e_{r-1} & \cdots & -\,e_2 \rightarrow & -\,e_1, \end{array} \tag{2.15}$$

where we have indicated the action of lowering operators. In addition to (2.11) we may also choose

$$\mathcal{P}_0 = \mathcal{P}_{2r+1}, \quad \mathcal{K}_0 = \mathcal{K}_{2r+1}, \tag{2.16}$$

as extra elements of the basis for $\mathcal{P}_a, \mathcal{K}_a$ operators and these commute with $H_i, 1 \leqslant i \leqslant r$, so that they have weight 0.

Again, in this basis the conformal algebra may be written in terms of the orthonormal basis of SO$^*(2r+3)$. In addition to (2.14) in this case we define

$$E_0^- = \mathcal{P}_0, \quad -E_0^+ = \mathcal{K}_0, \tag{2.17}$$

and along with (2.8) the extra commutation relations are given by (2.9) for the range of the indices i,j being extended to $0,1,\ldots,r$. Again, the linearly independent set of raising/lowering operators in this case is extended to include $\mathcal{K}_{1-}/\mathcal{P}_{1+}$.

In terms of the orthonormal basis, unitarity requires that

$$H^\dagger = H, \quad H_i^\dagger = H_i, \quad E_{ij}^{\varepsilon\eta\dagger} = E_{ij}^{-\varepsilon-\eta}, \quad E_i^{\varepsilon\dagger} = E_i^{-\varepsilon}, \quad \mathcal{P}_{i\varepsilon}^\dagger = \mathcal{K}_{i-\varepsilon}, \quad \mathcal{P}_0^\dagger = \mathcal{K}_0. \tag{2.18}$$

III. CHARACTER FORMULAS FOR POSITIVE ENERGY UNITARY IRREDUCIBLE REPRESENTATIONS

Essential in our approach to finding the character formulas for positive energy irreducible representations of the conformal group are $\mathrm{SO}^*(d+2)$ Verma modules. These have basis generated by the arbitrary action of lowering operators on the conformal highest weight state $|\Delta,\ell\rangle^{\mathrm{hw}}$ corresponding to the $\mathrm{SO}^*(d+2)$ weight $\underline{\Lambda}=(-\Delta,\ell_1,\ldots,\ell_r)$, $r=\left[\frac{1}{2}d\right]$ (where for $a=0,1,\ldots,r$ then Λ_a are $H_a=-H,H_i$ eigenvalues). In what follows we assume that ℓ is a dominant integral highest weight with respect to $\mathrm{SO}(d)$, so that in the orthonormal basis $\ell_i=\ell\cdot e_i\in\frac{1}{2}\mathbb{Z}$ and (the Dynkin labels for even d are given by $\Lambda_i'=\ell_i-\ell_{i+1}, 1\leqslant i\leqslant r-2$ and $\Lambda_{r-1}'=\ell_{r-1}+\ell_r, \Lambda_r'=\ell_{r-1}-\ell_r$ while for odd d they are $\Lambda_i'=\ell_i-\ell_{i+1}, 1\leqslant i\leqslant r-1$ and $\Lambda_r'=2\ell_r$ and these are the conditions for them to be non-negative integers)

$$\ell_1 \geqslant \cdots \geqslant \ell_{r-1} \geqslant |\ell_r|, \tag{3.1}$$

for $\mathrm{SO}(2r)$ while for $\mathrm{SO}(2r+1)$

$$\ell_1 \geqslant \cdots \geqslant \ell_r \geqslant 0, \tag{3.2}$$

these being the respective dominant Weyl chambers (or boundaries thereof).

The highest weight state $|\Delta,\ell\rangle^{\mathrm{hw}}$ satisfies

$$H_a|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}} = \Lambda_a|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}}, \quad \mathcal{K}_{1-}|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}} = E_\alpha|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}} = 0, \tag{3.3}$$

for α being the simple roots of $\mathrm{SO}(d)$ so that

$$\{E_\alpha\} \to \{E_{ii+1}^{++}, 1\leqslant i\leqslant r-1, E_{r-1r}^{++}\}, \tag{3.4}$$

for $\mathrm{SO}(2r)$ while

$$\{E_\alpha\} \to \{E_{ii+1}^{++}, 1\leqslant i\leqslant r-1, E_r^{+}\}, \tag{3.5}$$

for $\mathrm{SO}(2r+1)$.

The Verma module $\mathcal{V}_\Lambda$ with highest weight Λ therefore has basis

$$\prod_{\substack{v=i\varepsilon,0\\ 1\leqslant i\leqslant r,\varepsilon=\pm}} \mathcal{P}_v^{n_v} \prod_{\alpha\in\Phi_-} E_\alpha^{n_\alpha}|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}}, \tag{3.6}$$

for Φ_- denoting the set of negative roots of $\mathrm{SO}(d)$ and with n_v,n_α all positive or zero integers, with $n_0=0$ for $\mathrm{SO}(2r)$. As mentioned before, for $\mathrm{SO}(2r)$ then $\{E_\alpha\}\to\{E_{ij}^{-\pm}\}$ while for $\mathrm{SO}(2r+1)$ then $\{E_\alpha\}\to\{E_{ij}^{-\pm},E_i^-\}$. Corresponding to the basis (3.6) the weights Λ' in the Verma module are given by

$$\Lambda_0' = -\Delta - \sum_{\substack{v=i\varepsilon,0 \\ 1\leqslant i\leqslant r,\varepsilon=\pm}} n_v, \quad \ell' = \ell - \sum_{\alpha\in\Phi_-} n_\alpha \alpha + \sum_{i=1}^{r} (n_{i+} - n_{i-}) e_i. \tag{3.7}$$

In (3.6) we assume some fixed ordering of $\mathcal{P}_v$, E_α. This ordering may be arbitrarily chosen since if a different ordering is assumed then the resulting Verma module basis can be expressed in terms of that in (3.6) due to $\mathcal{P}_v, E_\alpha$ having commutators which are closed among themselves.

In Appendix C we will use the form of the algebra in the last section, in terms of the orthonormal basis, to derive conditions necessary for conformal group representations to be unitary. These results are summarized by

$$\begin{gathered} \Delta \geqslant \Delta_p = \ell_1 + d - p - 1, \quad p = 1, \ldots, \left[\tfrac{1}{2}d\right] \quad \text{for } \ell_1 = \ell_2 = \cdots = \ell_p > \ell_{p+1}, \\ \Delta \geqslant \tfrac{1}{2}d - 1 \quad \text{or } \Delta = 0 \quad \text{for } \underline{\ell} = 0, \end{gathered} \tag{3.8}$$

while for odd d we have in addition that

$$\Delta \geqslant \left[\tfrac{1}{2}d\right] \quad \text{for } \ell_1 = \cdots = \ell_{\left[\frac{1}{2}d\right]} = \tfrac{1}{2}. \tag{3.9}$$

It has been proven elsewhere that these conditions are sufficient[16] (in order for states in irreducible representations of the conformal group to have strictly positive norm). We impose these conditions on the representations we are interested in.

Along with the highest weight Λ the weight system for $\mathcal{V}_\Lambda$ may contain other highest weights Λ^w being, for certain w in the relevant Weyl group $\mathcal{W}$, shifted (or affine) Weyl reflections given by

$$\Lambda^w = w(\Lambda + \rho) - \rho, \tag{3.10}$$

for ρ being the Weyl vector, $\rho = -\frac{1}{2}\Sigma_{\alpha\in\Phi_-}\alpha$. (A simple example is for the $\mathcal{V}_\ell$ Verma module of SO(d) whereby the state $|\underline{\ell}^{\sigma_{12}}\rangle = (E_{12}^{-+})^{\ell_1-\ell_{2+1}}|\underline{\ell}\rangle^{\text{hw}}$, for $\sigma_{12}(\ell_1,\ell_2,\ldots) = (\ell_2,\ell_1,\ldots)$, characterizes a sub-Verma-module $\mathcal{V}_{\ell^{\sigma_{12}}}$, for $|\underline{\ell}\rangle^{\text{hw}}$ being annihilated by all SO(d) raising operators. To see this it suffices to use that $[E_{12}^{+-},(E_{12}^{-+})^n] = 4n(H_1 - H_2 + n - 1)(E_{12}^{-+})^{n-1}$. For unitary representations $E_{ij}^{\varepsilon\eta\dagger} = E_{ij}^{-\varepsilon-\eta}$ and $|\underline{\ell}^{\sigma_{12}}\rangle$ is null.) As described more in Appendix A, $\mathcal{V}_{\Lambda^w}$ is a sub-Verma module if and only if the w can be made to satisfy condition (A9). A necessary conditions is that $\Lambda - \Lambda^w$ be expressible as a linear combination of positive roots with non-negative integer coefficients. This is equivalent to demanding that the state with weight Λ^w can be reached by applying lowering operators on the highest weight state with weight Λ. If the highest weight Λ is dominant integral then all $\mathcal{V}_\Lambda w$ are sub-Verma modules of $\mathcal{V}_\Lambda$.

As described in Appendix A, in order to find the character of $\mathcal{I}_\Lambda$ the first step is to find all Λ^w which are highest weights of sub-Verma modules. Below we give necessary conditions for SO$^*(d+2)$ weights to satisfy this for the highest weight having orthonormal basis labels $\underline{\Lambda} = (-\Delta, \ell_1, \ldots, \ell_r)$. We show how each such weight may be written as Λ'^w where $w \in \mathcal{W}_d$, the Weyl group of SO(d), and $\underline{\Lambda}' = (-\Delta', \underline{\ell}')$ has $\underline{\ell}'$ satisfying (3.1) and (3.2), so that ℓ' is a dominant integral weight of SO(d), or else such that the weight ℓ' has a Dynkin label equal to -1 in which case such contributions vanish in χ_Λ. Using the results of Appendix A we may then write the character as

$$\chi_\Lambda = \sum_{w\in\mathcal{W}_d} \operatorname{sgn}(w) \mathcal{C}_{\Lambda^w} + \sum_{w\in\mathcal{W}_d,\Lambda'} \gamma_{\Lambda'} \operatorname{sgn}(w) \mathcal{C}_{\Lambda' w}, \tag{3.11}$$

where $\mathcal{C}_{\Lambda'}$ are SO$^*(d+2)$ Verma module characters and $\gamma_{\Lambda'}$ is determined by a recurrence relation. To solve this recurrence relation requires knowing in more detail which submodules are contained in which and so condition (A9) applies here.

The Weyl group $\mathcal{W}_{d+2}$ acts in a particularly simple way on weights of the Verma module $\mathcal{V}_\Lambda$ of SO$^*(d+2)$ in the orthonormal basis. Choosing any $w \in \mathcal{W}_{d+2}$ then we may write

$$w(\Lambda_0, \ldots, \Lambda_r) = (\varepsilon_0 \Lambda_{\sigma(0)}, \ldots, \varepsilon_r \Lambda_{\sigma(r)}), \tag{3.12}$$

for $\sigma \in \mathcal{S}_{r+1}$ and $\varepsilon_a = \pm 1$ with $\Pi_a \varepsilon_a = 1$ for $d = 2r$. In the present case the relevant-Weyl vector has components

$$\rho_a = \tfrac{1}{2}d - a, \quad a = 0, \ldots, r, \tag{3.13}$$

in the orthonormal basis of $\mathrm{SO}^*(d+2)$. Notice that the last r components are the components of the Weyl vector for $\mathrm{SO}(d)$. From (3.10) we have that the components of Λ^w in the orthonormal basis are

$$\Lambda^w_a = \varepsilon_a \Lambda_{\sigma(a)} + (\varepsilon_a - 1)\tfrac{1}{2}d - \varepsilon_a \sigma(a) + a. \tag{3.14}$$

Now for $\mathrm{SO}^*(d+2)$ the weights $\underline{\Lambda} = (-\Delta, \ell_1, \ldots, \ell_r)$ are clearly not dominant integral unless $\Delta = \ell_i = 0$ which corresponds to the trivial representation. Sub-Verma-module weights must satisfy (3.7). Thus, for any Λ^w to be the highest weight of a sub-Verma-module then $\Lambda^w_0 = -\Delta - n$, $n \in \mathbb{N}$. Also the minimum value of Λ^w_0 is that for $\varepsilon_0 = -1$, $\sigma(0) = 1$ so that sub-Verma-modules exist for

$$-\ell_1 - d + 1 \leqslant \Lambda^w_0 = -\Delta - n. \tag{3.15}$$

Notice that for $\varepsilon_0 = 1$, $\sigma(0) = 0$ so that $\Lambda^w_0 = -\Delta$ then all $\mathcal{V}_{\Lambda^w}$, $w \in \mathcal{W}_d$ are sub-Verma-modules as ℓ is a dominant integral highest weight with respect to the $\mathrm{SO}(d)$ subgroup. For any other $\varepsilon_0, \sigma(0)$ then this corresponds to a definite action of $\mathcal{P}_v$ on the highest weight state so that for these cases $n \geqslant 1$.

Using the formula (3.11) and the results of Appendix A with condition (3.15) we now discuss the even and odd dimension character formulas separately.

A. Character formulas: even dimensions

For application of the results of Appendix A we need to specify what condition (A9) demands for $\mathrm{SO}^*(d+2)$ Weyl group elements in $d = 2r$ dimensions. For $S_{ab}, T_{(ab)}$ being the $\mathcal{W}_d$ element for the respective positive roots $e_a + e_b$, $e_a - e_b$, $0 \leqslant a < b \leqslant r$ then clearly

$$\begin{aligned} S_{ab}(\Lambda_0, \ldots, \Lambda_a, \ldots, \Lambda_b, \ldots, \Lambda_r) &= (\Lambda_0, \ldots, -\Lambda_b, \ldots, -\Lambda_a, \ldots, \Lambda_r), \\ T_{(ab)}(\Lambda_0, \ldots, \Lambda_a, \ldots, \Lambda_b, \ldots, \Lambda_r) &= (\Lambda_0, \ldots, \Lambda_b, \ldots, \Lambda_a, \ldots, \Lambda_r). \end{aligned} \tag{3.16}$$

$T_{(ab)}$ corresponds to the transposition (ab) and below we use the short-hand notation $T_\sigma = T_{(a_1 b_1)} \ldots T_{(a_j b_j)}$ for $\sigma = (a_1 b_1) \ldots (a_j b_j)$. Applying S_{ab}, respectively, $T_{(ab)}$, to some weight $\underline{\Lambda}' = (\Lambda'_0, \ldots, \Lambda'_r)$ then clearly condition (A9) allows only those S_{ab}, respectively, $T_{(ab)}$, for which $\Lambda'_a + \Lambda'_b \in \mathbb{N}$, respectively, $\Lambda'_a - \Lambda'_b \in \mathbb{N}$.

We may easily write the character formula for the $\mathrm{SO}^*(2r+2)$ Verma module with highest weight Λ, for $\underline{\Lambda} = (-\Delta, \underline{\ell})$, and weights Λ' given by (3.7) as

$$C^{(2r+2)}_{\underline{\Lambda}}(s,x) = \sum_{\Lambda'} e^{\Lambda'}(\mu) = s^\Delta C^{(2r)}_{\underline{\ell}}(x) P^{(2r)}(s,x), \tag{3.17}$$

where, for some general $\mathrm{SO}^*(d+2)$ weight μ,

$$s = e^{-e_0}(\mu) = e^{-\mu_0}, \quad x_i = e^{e_i}(\mu) = e^{\mu_i}, \tag{3.18}$$

$C^{(2r)}_{\underline{\ell}}(x)$ denotes the character of the $\mathrm{SO}(2r)$ Verma module with highest weight ℓ (given in Appendix B) and

$$P^{(2r)}(s,x)=\prod_{1\leqslant i\leqslant r}(1-sx_i)^{-1}(1-sx_i^{-1})^{-1}. \tag{3.19}$$

[$P^{(2r)}(s,x)$ comes from the summation over $n_{i\pm}$ implicit in (3.17).]

For $\Delta>\ell_1+d-2$ or Δ lying between two any of Δ_p and Δ_{p+1} in (3.8) then (3.15) implies that the only sub-Verma-modules are at most those having highest weights for $\varepsilon_0=1$, $\sigma(0)=0$ in (3.14). However, since ℓ is a dominant integral weight of SO(d) then all $\mathcal{V}_{\Lambda^w}$, $w\in\mathcal{W}_d$ are sub-Verma-modules of $\mathcal{V}_\Lambda$ in this case. Thus from (3.11) the corresponding character is

$$\mathcal{A}^{(2r)}_{[\Delta;\underline{\ell}]}(s,x)=\sum_{w\in\mathcal{W}_{2r}}\operatorname{sgn}(w)C^{(2r+2)}_{\underline{\Lambda}^w}(s,x)=s^\Delta\chi^{(2r)}_{\underline{\ell}}(x)P^{(2r)}(s,x). \tag{3.20}$$

Let us assume that $\ell_1=\ell_2=\cdots=\ell_p>|\ell_{p+1}|$, $p\leqslant r-1$, $\Delta=\Delta_p$. In this case only Λ_0^w for $\varepsilon_0=1,\sigma(0)=0$ and $\varepsilon_0=-1$, $\sigma(0)=1,\ldots,p$ in (3.14) satisfy (3.15). For $\varepsilon_0=1$, $\sigma(0)=0$ then all $\mathcal{V}_{\Lambda^w}$, $w\in\mathcal{W}_d$ are sub-Verma-modules. Let us assume $\varepsilon_0=-1$, $\sigma(0)=j$, $1\leqslant j\leqslant p$ for which $\Lambda_0^w=-\ell_1-d+j$ then it is not difficult to show that the rest of the components may be written as

$$(\ell_1,\ldots,\ell_1,\ell_{p+1},\ldots)^w=(\ell_1,\ldots,\ell_1,\underset{\substack{\uparrow\\ j\text{th position}}}{\ell_1-1},\ldots,\ell_1-1,\ell_{p+1},\ldots)^{w'},\quad w'\in\mathcal{W}_d; \tag{3.21}$$

whereby if in the original $w\in\mathcal{W}_{d+2}$ then $\sigma(k_a)=a,k_a\neq 0$, $a\neq j$ then w' is defined in terms of w by

$$\varepsilon_0'=-\varepsilon_0=1,\quad \varepsilon_{k_0}'=-\varepsilon_{k_0},\quad \varepsilon_{k_i}'=\varepsilon_{k_i},\quad \sigma'=(0pp-1\cdots j)\sigma, \tag{3.22}$$

so that $\sigma'(0)=0$ and σ' exhausts all members of $\mathcal{S}_r$. Thus we have shown that all weights for the case of $w\in\mathcal{W}_{d+2}$ having $\varepsilon_0=-1$, $\sigma(0)=j$ in (3.14) may be written as $\Lambda^{(j,p)w'}$, $w'\in\mathcal{W}_d$ with

$$\underline{\Lambda}^{(j,p)}=(-\ell_1-d+j,\ell_1,\ldots,\ell_1,\underset{\substack{\uparrow\\ (j+1)\text{th position}}}{\ell_1-1},\ldots,\ell_1-1,\ell_{p+1},\ldots). \tag{3.23}$$

[Also $\Pi_a\varepsilon_a'=\Pi_a\varepsilon_a$ and $\operatorname{sgn}(w')=(-1)^{p+j+1}\operatorname{sgn}(w)$. During the course of this work we noticed that, at this point, simply using the following formula:

$$\chi_\Lambda=\mathcal{C}_\Lambda+\sum_{\substack{w\in\mathcal{W},w\neq 1\\ \Lambda^w<\Lambda}}\operatorname{sgn}(w)\mathcal{C}_{\Lambda^w},$$

where the sum runs over all w satisfying condition (A9), gives exactly the same result for the character as we find here by a more laborious procedure. It would be interesting to know whether or not this formula holds for more general Lie algebras and highest weights. We have not been able to find such a simple formula in the literature.]

We may now easily show that $\Lambda^{(j,p)w'}$, $w'\in\mathcal{W}_d$ exhaust all other highest weights of sub-Verma-modules of $\mathcal{V}_\Lambda$ in this case. To see this notice that if condition (A9) of Appendix A is satisfied for the weight $\Lambda^{(j,p)}$ then it is satisfied for $\Lambda^{(j,p)w'}$, $w'\in\mathcal{W}_d$ since the $(\ell_1,\ldots,\ell_1,\ell_1-1,\ldots,\ell_1-1,\ell_{p+1},\ldots)$ corresponds to a dominant integral weight of SO(d). For $\Lambda^{(j,p)}$ itself we may show that $\Lambda^{(j,p)}=\Lambda^w$ where $w=S_{0p}T_\sigma$ for $\sigma=(pp-1\ldots j)$ satisfies condition (A9). We see this as $(pp-1\cdots j)=(pp-1)(p-1p-2)\cdots(j+1j)$ and $T_{(i+1i)}T_{(ii-1)}\cdots T_{(j+1j)}(\underline{\Lambda}+\rho)\cdot(\underline{e}_{i+2}-\underline{e}_{i+1})\in\mathbb{N}$ for $i<p$ and $T_\sigma(\underline{\Lambda}+\underline{\rho})\cdot(\underline{e}_0+\underline{e}_p)\in\mathbb{N}$.

It now remains to determine $\gamma_{\Lambda^{(j,p)}}\to\gamma_{j,p}$ in (3.11) for the weight $\Lambda^{(j,p)}$ by the recurrence relation in Appendix A. The first observation which is not difficult to show (in a similar fashion as above) is that among $\mathcal{V}_{\Lambda^{(k,p)}}$ the only such modules which contain $\mathcal{V}_{\Lambda^{(j,p)}}$ as a submodule are those for $j<k\leqslant p$ or none such if $j=p$. In fact it is possible to show that no proper submodule of $\mathcal{V}_\Lambda$ contains $\mathcal{V}_{\Lambda^{(p,p)}}$ so that in this case $\gamma_{p,p}=-1$.

To describe which submodules contain other $\mathcal{V}_{\Lambda^{(j,p)}}$ we first define a subset of the permutation group $\mathcal{T}_n \subset \mathcal{S}_n$ so that every $\tau \in \mathcal{T}_n$ has $1 \leqslant c \leqslant n$ cycles, where the first cycle consists of the first n_1 of the integers $n, n-1, \ldots, 2, 1$, preserving this ordering, the second consists of the next n_2 such integers, again preserving this ordering, and so on and where $n_1, \ldots, n_c \geqslant 1$ satisfy $\Sigma_{i=1}^{c} n_i = n$. For example, for $n=3$ then $\mathcal{T}_n = \{(321), (32)(1) = (32), (3)(21) = (21), (3)(2)(1) = 1\}$. It is not difficult to see that the number of such permutations with c cycles (counting trivial one cycles) is $\binom{n-1}{c-1}$ so that the total number of such permutations is 2^{n-1}. Further we have that for $n > 1$ there are 2^{n-2} of these permutations with signature 1 or -1 so that $\Sigma_{\tau \in \mathcal{T}_n} \operatorname{sgn}(\tau) = 0$.

With the above definition of $\mathcal{T}_n$ we have found that the submodules $\mathcal{V}_{\Lambda^{w'}}$, $w' \in \mathcal{W}_d, w' \neq 1$ contain $\mathcal{V}_{\Lambda^{(j,p)}}$ as a submodule only for $w' \in \mathcal{T}_{p+1-j}$ so that for $j > p$ then $\Sigma_{w'} \operatorname{sgn}(w') = -1$ is the contribution to $\gamma_{j,p}$ coming from these. Also we have found that the submodules $\mathcal{V}_{\Lambda^{(k,p)w'}}, j < k \leqslant p, w' \in \mathcal{W}_d$ containing $\mathcal{V}_{\Lambda^{(j,p)}}$ have $w' \in \mathcal{T}_{k-j}$ so that for $j+1 < k \leqslant p$ then $\Sigma_{w'} \operatorname{sgn}(w') = 0$ so that the contribution to $\gamma_{j,p}$ coming from these vanishes while for $k = j+1$ then $w' = 1$ and this contributes $\gamma_{j+1,p} \operatorname{sgn}(w') = \gamma_{j+1,p}$ to $\gamma_{j,p}$. With these results we may then easily find that

$$\gamma_{j,p} = (-1)^{p+j+1}, \tag{3.24}$$

solves the recurrence relation $\gamma_{j,p} = -\gamma_{j+1,p}, \gamma_{p,p} = -1$.

It is possible to show that for such w' as described above (essentially belonging to $\mathcal{T}_n$ for various n) then for $w \in \mathcal{W}_{d+2}$ so that $\Lambda^{(j,p)} = \Lambda^{ww'}$ or $\Lambda^{(j,p)} = \Lambda^{(k,p)ww'}$ the only w which satisfy condition (A9) are expressible as products of $S_{0l}, T_{(mn)}, 1 \leqslant l, m, n \leqslant p$.

Now applying (3.11) and the Weyl character formula for SO($2r$) in terms of (3.17) (Appendix B) we find that the corresponding character is

$$\begin{aligned} &\mathcal{D}^{(2r)}_{[\ell_1+2r-p-1;\ell_1,\ell_{p+1},\ldots,\ell_r]}(s,x) \\ &\quad = s^{\ell_1+2r-p-1}\left(\chi^{(2r)}_{\underline{\ell}}(x) + \sum_{1 \leqslant j \leqslant p} (-s)^{p+1-j} \chi^{(2r)}_{\underline{\ell}-\underline{e}_p-\cdots-\underline{e}_j}(x)\right) P^{(2r)}(s,x) \end{aligned} \tag{3.25}$$

for $\underline{\ell} = (\ell_1, \ldots, \ell_1, \ell_{p+1}, \ldots, \ell_r)$.

Notice that for even dimensions we also have the possibility of $\ell_1 = \cdots = \ell_{r-1} = \pm \ell_r, \Delta = \ell_1 + \frac{1}{2}d - 1$. Here the Λ_0^w satisfying (3.15) are those for $\varepsilon_0 = 1$, $\sigma(0) = 0$, $\varepsilon_0 = \mp 1$, $\sigma(0) = r$ along with $\varepsilon_0 = -1$, $\sigma(0) = 1, \ldots, r-1$. By an argument very similar to the previous we find that, for $\underline{\ell} = (\ell, \ldots, \ell, \pm \ell)$,

$$\begin{aligned} &\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_\pm}(s,x) \\ &\quad = s^{\ell+r-1}\left(\chi^{(2r)}_{\underline{\ell}}(x) + \sum_{1 \leqslant j \leqslant r} (-s)^{r+1-j} \chi^{(2r)}_{\underline{\ell}\mp\underline{e}_r-\cdots-\underline{e}_j}(x)\right) P^{(2r)}(s,x), \end{aligned} \tag{3.26}$$

is the corresponding character in this case.

The free scalar case, for which $\underline{\Lambda} = (-r+1, 0, \ldots, 0)$ is the highest SO($2r+2$) weight, is accounted for by (3.26) for $\ell = 0$ and has character

$$\mathcal{D}^{(2r)}_{[r-1;0]}(s,x) \equiv \mathcal{D}^{(2r)}_{[r-1;0]_\pm}(s,x) = s^{r-1}(1-s^2)P^{(2r)}(s,x), \tag{3.27}$$

since the SO($2r$) characters obey $\chi_{(0,\ldots,0,-1,\pm 1)}(x) = -1$ with $\chi_{(0,\ldots,0\pm 1)}(x) = 0$ and $\chi_{(0,\ldots,0,-1,\ldots,-1,\pm 1)} \times (x) = 0$ otherwise.

B. Character formulas: odd dimensions

Considerations for odd $d = 2r+1$ dimensions are very similar to those above for even $d = 2r$ dimensions and we will not go into as much detail here. Along with (3.16) $\mathcal{W}_{2r+1}$ has extra elements corresponding to the extra positive roots $e_i, 1 \leqslant i \leqslant r$ given by

$$S_a(\Lambda_0,\ldots,\Lambda_a,\ldots,\Lambda_r)=(\Lambda_0,\ldots,-\Lambda_a,\ldots,\Lambda_r). \tag{3.28}$$

Acting on some weight $\underline{\Lambda}'=(\Lambda_0',\ldots,\Lambda_r')$ then condition (A9) only allows those S_a for which $\Lambda_a'\in\frac{1}{2}\mathbb{N}$.

We may easily write the character formula for the $SO^*(2r+3)$ Verma module with highest weight Λ and weights Λ' given by (3.7) as

$$C_{\underline{\Lambda}}^{(2r+3)}(s,x)=\sum_{\Lambda'}e^{\Lambda'}(\mu)=s^{\Delta}C_{\underline{\ell}}^{(2r+1)}(x)P^{(2r+1)}(s,x), \tag{3.29}$$

where $C_{\underline{\ell}}^{(2r+1)}(x)$ denotes the character of the $SO(2r+1)$ Verma module with highest weight ℓ (given in Appendix B) and

$$P^{(2r+1)}(s,x)=(1-s)^{-1}\prod_{1\leqslant i\leqslant r}(1-sx_i)^{-1}(1-sx_i^{-1})^{-1}. \tag{3.30}$$

[$P^{(2r+1)}(s,x)$ comes from the summation over $n_{i\pm},n_0$ implicit in (3.29).]

For $\Delta>\ell_1+d-2$ or Δ lying between two any of Δ_p and Δ_{p+1} in (3.8) then character for positive energy unitary irreducible representations is

$$\mathcal{A}_{[\Delta;\underline{\ell}]}^{(2r+1)}(s,x)=\sum_{w\in\mathcal{W}_{2r+1}}\mathrm{sgn}(w)C_{\underline{\Lambda}^w}^{(2r+3)}(s,x)=s^{\Delta}\chi_{\underline{\ell}}^{(2r+1)}(x)P^{(2r+1)}(s,x), \tag{3.31}$$

where $\chi_{\underline{\ell}}^{(2r+1)}(x)$ is the character of the $SO(2r+1)$ irreducible representation with highest weight ℓ.

For $\bar{\Delta}=\Delta_p$ in (3.8) we may go through the same procedure as for the even dimensional case and find that the extra Weyl reflections (3.28) lead to nothing new as far as condition (A9) is concerned. Thus for odd d and with $\underline{\ell}=(\ell_1,\ldots,\ell_1,\ell_{p+1},\ldots,\ell_r)$ corresponding character for these representations is

$$\begin{aligned}&\mathcal{D}_{[\ell_1+2r-p;\ell_1,\ell_{p+1},\ldots,\ell_r]}^{(2r+1)}(s,x)\\&\quad=s^{\ell_1+2r-p}\left(\chi_{\underline{\ell}}^{(2r+1)}(x)+\sum_{1\leqslant j\leqslant p}(-s)^{p+1-j}\chi_{\underline{\ell}-\underline{e}_p-\cdots-\underline{e}_j}^{(2r+1)}(x)\right)P^{(2r+1)}(s,x).\end{aligned} \tag{3.32}$$

For the free scalar case, for which $\underline{\Lambda}=\left(-r+\frac{1}{2},0,\ldots,0\right)$ is the highest $SO(2r+3)$ weight, we have that the corresponding character is given by

$$\mathcal{D}_{[r-\frac{1}{2};0]}^{(2r+1)}(s,x)=s^{r-\frac{1}{2}}(1-s^2)P^{(2r+1)}(s,x). \tag{3.33}$$

For odd dimensions we also have the possibility of the highest weight Λ having components $\underline{\Lambda}=\left(-r,\frac{1}{2},\ldots,\frac{1}{2}\right)$. This time the Λ_0^w satisfying (3.15) are those for $\varepsilon_0=\pm1$, $\sigma(0)=0$, $\varepsilon_0=-1$, $\sigma(0)=j$, $1\leqslant j\leqslant r$. For $\varepsilon_0=-1$, $\sigma(0)=0$ then $\Lambda_0^w=-r-1$ and the remaining components may be rewritten as $\ell^w=\ell^{w'}$ where $w'\in\mathcal{W}_{2r+1}$ is identical to w save for $\varepsilon_0'=-\varepsilon_0=1$ so that $\Pi_a\varepsilon_a'=-\Pi_a\varepsilon_a$ and $\mathrm{sgn}(w')=-\mathrm{sgn}(w)$. The cases of $\varepsilon_0=-1$, $\sigma(0)=j$, $1\leqslant j\leqslant r$ are accounted for similarly as for even dimensions for $p=r$. However these cases have highest weights which are shifted $\mathcal{W}_{2r+1}$ Weyl group reflections of $(-\Delta',\underline{\ell}')=\left(-2r-1+j,-\frac{1}{2},\ldots,-\frac{1}{2},\frac{1}{2},\ldots\right)$. For these weights at least one of the Dynkin labels $\ell_{i+1}'-\ell_i'$ is equal to -1 so that contributions from all these Verma modules vanish from the character formula (by a result of Appendix A).

The only cases we must consider are for the Verma modules $\mathcal{V}_{\Lambda'w'},w'\in\mathcal{W}_{2r+1}$ for $\underline{\Lambda}'=\left(-r-1,\frac{1}{2},\ldots,\frac{1}{2}\right)$. By similar arguments as before all $\mathcal{V}_{\Lambda'w'}$ for $w'\neq1$ are submodules of $\mathcal{V}_{\Lambda'}$. Due to $\underline{\Lambda}'+\underline{\rho}=S_0(\underline{\Lambda}+\underline{\rho})$, where S_a is defined in (3.28) then condition (A9) [which is satisfied due to $e_0\cdot(\underline{\Lambda}+\underline{\rho})=\frac{1}{2}$] implies that all $\mathcal{V}_{\Lambda'w'},w'\in\mathcal{W}_{2r+1}$ are submodules of $\mathcal{V}_{\Lambda}$]. Further we may show that $\mathcal{V}_{\Lambda'}$ is contained only in $\mathcal{V}_{\Lambda}$, and no submodules of $\mathcal{V}_{\Lambda}$, and so $\gamma_{\Lambda'}=-1$.

Taking into account these considerations, we have that the character is, from (3.11),

$$\mathcal{D}^{(2r+1)}_{[r;\frac{1}{2}]}(s,x)=\sum_{w\in\mathcal{W}_{2r+1}}\mathrm{sgn}(w)(\mathcal{C}_{\Lambda^w}-\mathcal{C}_{\Lambda' w})=s^r(x_1^{1/2}+x_1^{-1/2})\cdots(x_r^{1/2}+x_r^{-1/2})(1-s)P^{(2r+1)}(s,x), \tag{3.34}$$

and where we have used that

$$\chi^{(2r+1)}_{(1/2,\ldots,1/2)}(x)=(x_1^{1/2}+x_1^{-1/2})\cdots(x_r^{1/2}+x_r^{-1/2}). \tag{3.35}$$

C. Relation with reduced Verma module bases

We wish to show here that omitting certain of $\mathcal{P}_v$ from the original Verma module basis (3.6) leads to formulas for characters which are equivalent to those obtained in the last sections.

Descendant states (i.e., those obtained by definite action of $\mathcal{P}_v$ on the highest weight state) are SO(d) representations belonging to the decomposition of $\mathbf{e}_1\otimes\cdots\otimes\mathbf{e}_1\otimes\ell$ in terms of irreducible representations. From Appendix C, these states are null for either of two reasons. One reason is that ℓ may lie on the boundary of the dominant Weyl chamber (3.1) (i.e., that some $\ell_1=\ell_2=\cdots$) so that certain descendant states are null with respect to the SO(d) subgroup. The other reason is that Δ may lie on a unitarity bound. By omitting the correct $\mathcal{P}_v$ from (3.6) we effectively discard states in the original Verma module which are null due to the value of Δ. Acting with the Weyl symmetry operator on the character of the reduced Verma module is equivalent to projecting out of the reduced module states which are null by virtue of which SO(d) representation they belong to. We may show that this prescription gives the same formulas for characters as found earlier.

For definiteness we consider the case where $\ell_1=\cdots=\ell_p>|\ell_{p+1}|$, $\Delta\geqslant\ell_1+d-p-1$, in even dimensions, $d=2r$, although the other cases of interest are similar.

For this case and in the notation of Appendix C, consider the SO($2r$) highest weight state $|\Delta+1,\underline{\ell}-\underline{e}_p\rangle$. The construction of such a state is nontrivial and in Appendix C only the simplest such states have been constructed. Nevertheless we may write down the state in principle as

$$|\Delta+1,\underline{\ell}-\underline{e}_p\rangle=\mathcal{A}_{\underline{\ell}}\mathcal{P}_{p-}|\Delta,\underline{\ell}\,\rangle^{\mathrm{hw}}+\sum_{v',\underline{\ell}'}\mathcal{B}_{v',\underline{\ell}'}\mathcal{P}_{v'}|\Delta,\underline{\ell}'\,\rangle\,, \tag{3.36}$$

where $\mathcal{P}_{v'}\leftrightarrow v'\in\{\pm e_i\}$ is the subset of $\mathcal{P}_{i\pm}$ which may be reached by applying SO($2r$) raising operators to $\mathcal{P}_{p-}$ and $\underline{\ell}'+\underline{v}'=\underline{\ell}-\underline{e}_p$. The subset $\mathcal{P}_{v'}$ may be easily determined from (2.10) to be given by $\mathcal{P}_{i+},\mathcal{P}_{j-}$ for $1\leqslant i\leqslant r$ and $p+1\leqslant j\leqslant r$. The complex numbers $\mathcal{A}_{\underline{\ell}},\mathcal{B}_{v',\underline{\ell}'}$ are determined by the condition that (3.36) be a highest weight state with respect to SO($2r$), i.e., that all SO($2r$) raising operators annihilate it. By the results of Appendix C, for Δ above the unitarity bound this state is not null however when $\Delta=\ell_1+d-p-1$ then $|\Delta+1,\underline{\ell}-\underline{e}_p\rangle=0$. This is equivalent to a conservation equation for the highest weight state $|\Delta,\underline{\ell}\rangle^{\mathrm{hw}}$.

Now the modulus of $\mathcal{A}_{\underline{\ell}}$ is nonzero despite $\ell_1=\cdots=\ell_p>|\ell_{p+1}|$. When $\Delta=\ell_1+d-p-1$, so that (3.36) vanishes, then $\mathcal{P}_{p-}|\bar{\Delta},\underline{\ell}\rangle^{\mathrm{hw}}$ may be expressed in terms of $\mathcal{P}_{i+}|\Delta,\ell'\rangle$, $\mathcal{P}_{j-}|\Delta,\ell'\rangle$ for $1\leqslant i\leqslant r$ and $p+1\leqslant j\leqslant r$. Also, as

$$E^{-+}_{ii+1}|\Delta,\ell_1,\ldots,\ell_1,\ell_{p+1},\ldots,\ell_r\rangle^{\mathrm{hw}}=0,\quad i=1,\ldots,p-1, \tag{3.37}$$

then applying such E^{-+}_{ii+1} to (3.36) and using (2.10), we have that for Δ on the unitarity bound then $\mathcal{P}_{i-}|\Delta,\underline{\ell}\rangle^{\mathrm{hw}}$, $1\leqslant i\leqslant p-1$ may be similarly expressed in terms of $\mathcal{P}_{i+}|\Delta,\ell'\rangle$, $\mathcal{P}_{j-}|\Delta,\ell'\rangle$ for $1\leqslant i\leqslant r$ and $p+1\leqslant j\leqslant r$. Thus, effectively the Verma module basis (3.6) becomes reduced so as to exclude $\mathcal{P}_{i-}$, $1\leqslant i\leqslant p$.

Acting with the SO(d) Weyl symmetry operator $\mathfrak{W}_d$ (see Appendixes A and B) on the character for the reduced Verma module yields the following formula:

$$\sum_{\Lambda',w\in\mathcal{W}_{2r}} e^{w(\Lambda')}(\mu) = s^{\ell_1+2r-p-1}\mathfrak{W}_d(C^{(2r)}_{\underline{\ell}}(x)(1-sx_1^{-1})\cdots(1-sx_p^{-1}))P^{(2r)}(s,x)$$
$$= s^{\ell_1+2r-p-1}\left(\chi^{(2r)}_{\underline{\ell}}(x) + \sum_{\substack{1\leqslant n\leqslant p\\ i_j\in(1,\ldots,p),i_j\neq i_k}} (-s)^n \chi^{(2r)}_{\underline{\ell}-\underline{e}_{i_1}-\cdots-\underline{e}_{i_n}}(x)\right)P^{(2r)}(s,x), \tag{3.38}$$

for $\underline{\ell}=(\ell_1,\ldots,\ell_1,\ell_{p+1},\ldots,\ell_r)$ and where now $\Lambda'=(-\Lambda'_0,\underline{\ell}')$ are specified by

$$\Lambda'_0 = -\Delta' = -\ell_1 - d + p + 1 - \sum_{1\leqslant i\leqslant r} n_{i+} - \sum_{p+1\leqslant j\leqslant r} n_{j-},$$
$$\ell' = \ell - \sum_{\alpha\in\Phi_-}\alpha + \sum_{1\leqslant i\leqslant r} n_{i+}e_i - \sum_{p+1\leqslant j\leqslant r} n_j - e_j. \tag{3.39}$$

It is easy to see that (3.38) reduces to (3.25). To see this note that $\chi_{\underline{\ell}'}(x)$ in (3.38) is nonzero only for $\underline{\ell}'=(\ell_1,\ldots,\ell_1,\ell_1-1,\ldots,\ell_1-1,\ell_{p+1},\ldots,\ell_r)$, i.e., for $i_j=k,k+1,\ldots,p$ for some $1\leqslant k\leqslant p$.

To summarize: when the conformal dimension Δ saturates a unitarity bound the Verma module basis is reduced so as to exclude certain of the $\mathcal{P}_{i\pm}$, $\mathcal{P}_0$ from (3.6). This is equivalent to conservation equations constraining the highest weight state. This subset may be determined in terms of the results of Appendix C. Acting with the SO(d) Weyl symmetry operator on the character of the reduced Verma module then leads to the characters for the corresponding unitary irreducible representation. Explicitly, for (3.25) and (3.32) the subset to be omitted from (3.6) is $\mathcal{P}_{i-}, 1\leqslant i\leqslant p$, for (3.26) the subset is $\mathcal{P}_{i-}, 1\leqslant i\leqslant r-1$ along with $\mathcal{P}_{r-}$ for $\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_+}$ or $\mathcal{P}_{r+}$ for $\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_-}$ while for (3.34) the subset is $\mathcal{P}_{i-}, 1\leqslant i\leqslant r$ along with $\mathcal{P}_0$.

D. Special cases

We here illustrate these character formulas for the simplest cases of the SO(3,2) and SO(4,2) conformal groups and mention how special cases relate to conformal field representations.

We have that,

$$C_\ell(x) \equiv C^{(3)}_\ell(x) = \frac{x^\ell}{1-x^{-1}}, \tag{3.40}$$

is the character of SO(3) Verma modules and

$$\chi_\ell(x) \equiv \chi^{(3)}_\ell(x) = C_\ell(x) + C_\ell(x^{-1}) = \frac{x^{\ell+(1/2)} - x^{-\ell-(1/2)}}{x^{1/2}-x^{-1/2}}, \tag{3.41}$$

is the usual character for SO(3) irreducible representations. We have therefore that,

$$\mathcal{A}^{(3)}_{[\Delta;\ell]}(s,x) = s^\Delta \chi_\ell(x)P^{(3)}(s,x),$$
$$\mathcal{D}^{(3)}_{[\ell+1;\ell]}(s,x) = s^{\ell+1}(\chi_\ell(x) - s\chi_{\ell-1}(x))P^{(3)}(s,x),$$
$$\mathcal{D}^{(3)}_{[1;1/2]}(s,x) = s(x^{1/2}+x^{-1/2})(1-sx)^{-1}(1-sx^{-1})^{-1}, \tag{3.42}$$
$$\mathcal{D}^{(3)}_{[1/2;0]}(s,x) = s^{1/2}(1+s)(1-sx)^{-1}(1-sx^{-1})^{-1},$$

exhaust all characters of the unitary irreducible representations of SO(3,2). (In terms of the notation employed in Ref. 6 these character formulas agree for $x\to\beta^2$, $s\to\alpha^2$. In the nomenclature

of Ref. 6, the representations $\mathcal{D}^{(3)}_{[1;1/2]}$ and $\mathcal{D}^{(3)}_{[1/2;0]}$ correspond to the "Di" and "Rac" singleton representations, respectively.)

For $SO(4)\simeq SU(2)\otimes SU(2)$ we have that

$$C^{(4)}_{(\ell_1,\ell_2)}(x_1,x_2)=C_j(x)C_{\bar{J}}(y) \quad \text{for } \ell_1=j+\bar{J}, \quad \ell_2=j-\bar{J}, \quad x_1=x^{1/2}y^{1/2}, \quad x_2=x^{1/2}y^{-1/2} \tag{3.43}$$

i.e., the Verma module character with dominant highest weight (ℓ_1,ℓ_2) may be expressed as a product of two SU(2) Verma module characters with highest weights $j,\bar{J}$. The characters of unitary irreducible representations of $SO(4,2)$ are given by

$$\mathcal{A}^{(4)}_{[\Delta;j,\bar{J}]}(s,x,y)=s^{\Delta}\chi_{\bar{J}}(x)\chi_{\bar{J}}(y)P^{(4)}(s,x,y),$$

$$\begin{aligned}
\mathcal{D}^{(4)}_{[j+\bar{J}+2;j,\bar{J}]}(s,x,y)&=s^{j+\bar{J}+2}(\chi_j(x)\chi_{\bar{J}}(y)-s\chi_{j-(1/2)}(x)\chi_{\bar{J}-(1/2)}(y))P^{(4)}(s,x,y),\\
\mathcal{D}^{(4)}_{[j+1;j]_+}(s,x,y)&=s^{j+1}(\chi_j(x)-s\chi_{j-(1/2)}(x)\chi_{1/2}(y)+s^2\chi_{j-1}(x))P^{(4)}(s,x,y),\\
\mathcal{D}^{(4)}_{[\bar{J}+1;\bar{J}]_-}(s,x,y)&=s^{\bar{J}+1}(\chi_{\bar{J}}(y)-s\chi_{\bar{J}-(1/2)}(y)\chi_{1/2}(x)+s^2\chi_{\bar{J}-1}(y))P^{(4)}(s,x,y).
\end{aligned} \tag{3.44}$$

Here we have written $P^{(4)}(s,x_1,x_2)\to P^{(4)}(s,x,y)$ for x_1,x_2 as in (3.43). This reproduces the results for character formulas in four dimensions found in Ref. 4.

Free fields have conformal dimension $\ell+\frac{1}{2}d-1$ and belong to the $(\ell,\ldots,\ell,\pm\ell)$ representation of $SO(2r)$ for any $\ell\in\frac{1}{2}\mathbb{N}$ in $d=2r$, dimensions and the $(\ell,\ldots,\ell,\ell)$ representation of $SO(2r+1)$ for $\ell=0,\frac{1}{2}$ in $d=2r+1$ dimensions.[19] The corresponding characters for even dimensions are $\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_\pm}(s,x)$ in (3.26) along with $\mathcal{D}^{(2r)}_{[r-1;0]}(s,x)$ in (3.27) for the scalar case. For odd dimensions the corresponding characters are $\mathcal{D}^{(2r+1)}_{[r;1/2]}(s,x)$of (3.34) and $\mathcal{D}^{(2r+1)}_{[r-(1/2);0]}(s,x)$ in (3.33).

The characters (3.25), (3.32) for the special case of $p=1$ and $\ell_1\equiv\ell,\ell_2=\cdots=\ell_r=0$ correspond to conserved symmetric traceless tensor-field representations of the conformal group, $T_{\mu_1\cdots\mu_\ell}=T_{(\mu_1\cdots\mu_\ell)}$, $T^{\mu}_{\mu\mu_2\cdots\mu_\ell}=\partial^{\mu_1}T_{\mu_1\cdots\mu_\ell}=0$. These have conformal dimension $d+\ell-2$ in d dimensions and examples are the conserved vector current for $\ell=1$ and energy momentum tensor for $\ell=2$.

IV. PRODUCT FORMULAS

We now turn to the determination of the decomposition of products of unitary irreducible representations of the conformal group into other unitary irreducible representations.

A. Product formulas: four dimensions

We illustrate for the $SO(4,2)$ case first. For these purposes we first note a useful identity, namely,

$$P^{(4)}(s,x,y)=\sum_{p,q=0}^{\infty}s^{2p+q}\chi_{(1/2)q}(x)\chi_{(1/2)q}(y). \tag{4.1}$$

With (4.1) we may now easily determine the products of unitary irreducible representations of the conformal group. Using the usual decomposition of products of SU(2) characters,

$$\chi_{j\otimes j'}(x)\equiv\chi_j(x)\chi_{j'}(x)=\sum_{q=|j-j'|}^{j+j'}\chi_q(x), \tag{4.2}$$

and (4.1), we notice that

$$\mathcal{D}^{(4)}_{[j+1;j]+}(s,x,y)=\sum_{q=0}^{\infty}s^{q+j+1}\chi_{j+(1/2)q}(x)\chi_{(1/2)q}(y). \tag{4.3}$$

Thus we may straightforwardly, determine that

$$\begin{aligned}&\mathcal{D}^{(4)}_{[j+1,j]+}(s,x,y)\mathcal{D}^{(4)}_{[j'+1;j']+}(s,x,y)\\&\quad=s^{j+j'+2}P(s,x,y)\left(\chi_{j\otimes j'}(x)+\sum_{q=1}^{\infty}s^q(\chi_{j+j'+(1/2)q}(x)\chi_{(1/2)q}(y)-s\chi_{j+j'+(1/2)q-(1/2)}(x)\chi_{(1/2)q-(1/2)}(y))\right)\\&\quad=\mathcal{A}^{(4)}_{[j+j'+2;j\otimes j',0]}(s,x,y)+\sum_{q=1}^{\infty}\mathcal{D}^{(4)}_{[j+j'+q+2;j+j'+(1/2)q,(1/2)q]}(s,x,y).\end{aligned} \tag{4.4}$$

Similarly, using (4.2), (4.3), we may easily determine that

$$\begin{aligned}&\mathcal{D}^{(4)}_{[j+1,j]+}(s,x,y)\mathcal{D}^{(4)}_{[\bar{J}+1;\bar{j}]-}(s,x,y)\\&\quad=s^{j+\bar{J}+2}P(s,x,y)\sum_{q=0}^{\infty}s^q(\chi_{j+(1/2)q}(x)\chi^{-}_{\bar{J}+(1/2)q}(y)-s\chi_{j+(1/2)q-(1/2)}(x)\chi^{-}_{\bar{J}+(1/2)q-(1/2)}(y))\\&\quad=\sum_{q=0}^{\infty}\mathcal{D}^{(4)}_{[j+\bar{J}+q+2;j+(1/2)q,\bar{J}+(1/2)q]}(s,x,y).\end{aligned} \tag{4.5}$$

Using (4.2), (4.3), we may also find that

$$\begin{aligned}&\mathcal{D}^{(4)}_{[j+\bar{J}+2;j,\bar{J}]+}(s,x,y)\mathcal{D}^{(4)}_{[j'+1,j']+}(s,x,y)\\&\quad=\sum_{q=0}^{\infty}(\mathcal{A}^{(4)}_{[\Delta_q,j+j'+(1/2)q,\bar{J}+(1/2)q]}(s,x,y)+\mathcal{A}_{[\Delta_q,[j-(1/2)]\otimes[j'+(1/2)q-(1/2)],\bar{J}+(1/2)q]}(s,x,y)\\&\qquad+\mathcal{A}^{(4)}_{[\Delta_q,j+j'+(1/2)q,(\bar{J}-(1/2))\otimes[(1/2)q-(1/2)]]}(s,x,y)),\quad \Delta_q=j+j'+\bar{J}+q+3,\end{aligned} \tag{4.6}$$

and

$$\mathcal{A}^{(4)}_{[\Delta;j,\bar{J}]}(s,x,y)\mathcal{D}^{(4)}_{[j'+1,j']+}(s,x,y)=\sum_{q=0}^{\infty}\mathcal{A}^{(4)}_{[\Delta+j'+q+1;j\otimes[j'+(1/2)q],\bar{J}\otimes 1/2q]}(s,x,y), \tag{4.7}$$

which exhausts all products involving $\mathcal{D}^{(4)}_{[j+1;j]+}(s,x,y)$. Those involving $\mathcal{D}^{(4)}_{[\bar{J}+1;J]-}(s,x,y)$ may be obtained by the exchange $x\leftrightarrow y$ above noting

$$\begin{gathered}\mathcal{D}^{(4)}_{[\bar{J}+1;\bar{j}]-}(s,x,y)=\mathcal{D}^{(4)}_{[\bar{J}+1;\bar{j}]+}(s,y,x),\quad \mathcal{D}^{(4)}_{[j+\bar{J}+2;j,\bar{J}]}(s,x,y)=\mathcal{D}^{(4)}_{[j+\bar{J}+2;\bar{J},j]}(s,y,x),\\ \mathcal{A}^{4}_{[\Delta;j,\bar{J}]}(s,x,y)=\mathcal{A}^{(4)}_{[\Delta;\bar{J},j]}(s,y,x).\end{gathered} \tag{4.8}$$

Similarly, using (4.1) directly, we have that

$$\mathcal{A}^{(4)}_{[\Delta;j,\bar{J}]}(s,y,x)\mathcal{A}_{[\Delta';j',\bar{J}']}(s,y,x)=\sum_{p,q=0}^{\infty}\mathcal{A}^{(4)}_{[\Delta+\Delta'+2p+q;j\otimes j'\otimes(1/2)q,\bar{J}\otimes\bar{J}'\otimes(1/2)q]}(s,x,y). \tag{4.9}$$

We may note that each of these product formulas is compatible with the blind partition functions,

$$\mathcal{A}^{(4)}_{[\Delta;j,\bar{J}]}(s,1,1)=\frac{s^{\Delta}}{(s-1)^4}(2j+1)(2\bar{J}+1),$$

$$\mathcal{D}^{(4)}_{[j+\bar{J}+2;j,\bar{J}]}(s,1,1)=\frac{s^{j+\bar{J}+2}}{(s-1)^4}((2j+1)(2\bar{J}+1)-4sj\bar{J}), \tag{4.10}$$

$$\mathcal{D}^{(4)}_{[j+1;j]_+}(s,1,1)=\mathcal{D}^{(4)}_{[j+1;j]_-}(s,1,1)=\frac{s^{j+1}}{(s-1)^3}(-(2j+1)+s(2j-1)).$$

As we see, the $d=4$ cases are relatively simple when we use expansion formulas of the type (4.1), (4.3) to expand one of the characters in the product of two. The general cases which we consider now are also made simpler with analogous expansion formulas.

B. Product formulas: even dimensions

Useful for finding product formulas for the $\mathrm{SO}(2r,2)$ conformal group is the following expansion of $P(s,x)$ in terms of $\mathrm{SO}(2r)$ characters, namely,

$$P^{(2r)}(s,x)=\sum_{p,q=0}^{\infty}s^{2p+q}\chi^{(2r)}_{(q,0,\ldots,0)}(x), \tag{4.11}$$

where

$$\chi^{2r}_{(q,0,\ldots,0)}(x)=\tfrac{1}{2}\det[x_i^{k_j}+x_i^{-k_j}]\Delta(x_1+x_1^{-1},\ldots,x_r+x_r^{-1})^{-1}, \tag{4.12}$$

with $k_1=q+r-1$, $k_j=r-j$, $j>1$, for $\Delta(x)$ being the Vandermonde determinant,

$$\Delta(x_1,\ldots,x_n)=\prod_{1\leqslant i<j\leqslant n}(x_j-x_i). \tag{4.13}$$

The latter expression for the character comes from Appendix B where also expressions for more general characters of $\mathrm{SO}(d)$ in even and odd dimensions are given.

Analogously to (4.3) we have for (3.26) that

$$\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_\pm}(s,x)=\sum_{q=0}^{\infty}s^{\ell+r+q-1}\chi^{(2r)}_{(\ell+q,\ell,\ldots,\ell,\pm\ell)}(x), \tag{4.14}$$

which we prove in Appendix D.

More generally for the $p=r-j$ case of (3.25) [note that (4.14) encapsulates the $p=r$ case] we have, for $\ell>\ell_1>\cdots>|\ell_j|$,

$$\begin{aligned}&\mathcal{D}^{(2r)}_{[\ell+r+j-1;\ell,\ell_1,\ldots,\ell_j]}(s,x)\\&\quad=\sum_{p_1,\ldots,p_j,q=0}^{\infty}\sum_{i_1=-\frac{1}{2}p_1}^{\frac{1}{2}p_1}\cdots\sum_{i_j=-\frac{1}{2}p_j}^{\frac{1}{2}p_j}s^{\ell+r+j+q+p_1+\cdots+p_j-1}\chi^{(2r)}_{(\ell+q,\ell,\ldots,\ell,\ell_1+2i_1,\ldots,\ell_j+2i_j)}(x),\end{aligned} \tag{4.15}$$

which we also prove in Appendix D. Note that the weights $(\ell+q,\ell,\ldots,\ell,\ell_1,+2i_1,\ldots,\ell_j+2i_j)$ may lie outside the dominant Weyl chamber, i.e., not satisfy (3.1) for particular ℓ,ℓ_i. However for such weights we may use that $\chi^{(2r)}_{\ell'}(x)=\mathrm{sgn}(w)\chi^{(2r)}_{\ell' w}(x)$, for some $w\in\mathcal{W}_{2r}$, to relate such characters to the character with dominant integral highest weight $\ell' w$.

A notable simplification to (4.15) occurs for the $p=1$ case of (3.25) for $\ell_1\equiv\ell,\ell_2=\cdots=\ell_r=0$ which corresponds to conserved symmetric traceless tensor representations of the conformal group. In this case we obtain that, for $d>4$,

$$\mathcal{D}^{(2r)}_{[\ell+2r-2;\ell,0\ldots,0]}(s,x)=\sum_{p,q=0}^{\infty}\sum_{k=0}^{\ell}s^{\ell+2r+2p+q-2}\chi^{(2r)}_{(q+k,\ell-k,0,\ldots,0)}(x). \tag{4.16}$$

We now discuss products involving the representations in (4.14) which contain the truncated representations in (3.25) for $p=1$ namely, $\mathcal{D}^{(2r)}_{[\ell_1+2r-2,\ell_1,\ldots,\ell_r]}$.

For $d=6$, for example, we may find using (4.14), (3.25) for $p=1$ and (3.26) that

$$\begin{aligned}&\mathcal{D}^{(6)}_{[\ell+2;\ell]_+}(s,x)\mathcal{D}^{(6)}_{[\ell'+2;\ell']_-}(s,x)\\&\quad=\mathcal{A}^{(6)}_{[\ell+\ell'+4;(\ell,\ell,\ell)\otimes(\ell',\ell',-\ell')]}(s,x)+\sum_{q=1}^{\infty}\mathcal{D}^{(6)}_{[\ell+\ell'+q+4;\ell+\ell'+q,\ell+\ell',\ell-\ell']}(s,x),\end{aligned} \tag{4.17}$$

and that

$$\mathcal{D}^{(6)}_{[\ell+2;\ell]_\pm}(s,x)\mathcal{D}^{(6)}_{[\ell'+2;\ell']_\pm}(s,x)=\sum_{q=0}^{\infty}\sum_{t=|\ell-\ell'|}^{\ell+\ell'}\mathcal{D}^{(6)}_{[\ell+\ell'+q+4;\ell+\ell'+q,t,\pm t]}(s,x). \tag{4.18}$$

Here and in the following we are using the short-hand notation, for $r=\left[\frac{1}{2}d\right]$,

$$\chi^{(d)}_{(\ell_1,\ldots,\ell_r)\otimes(\ell'_1,\ldots,\ell'_r)}(x)\equiv\chi^{(d)}_{(\ell_1,\ldots,\ell_r)}(x)\chi^{(d)}_{(\ell'_1,\ldots,\ell'_r)}(x), \tag{4.19}$$

in $\mathcal{A}_{[\Delta;\ell]}(s,x)$. Of course (4.19) may be decomposed in terms of SO(d) characters once we know how $\ell\otimes\ell'$ decomposes into irreducible representations.

More generally there is a distinction in such product formulas between the cases where the dimension is divisible by four or not so.

Explicitly, we have for $d=4m$ that

$$\begin{aligned}&\mathcal{D}^{(4m)}_{[\ell+2m-1;\ell]_+}(s,x)\mathcal{D}^{(4m)}_{[\ell'+2m-1;\ell']_-}(s,x)\\&\quad=\sum_{q=0}^{\infty}\sum_{\substack{t_i\geqslant t-\ell'\\ t_i\geqslant t_{i+1}}}\mathcal{D}^{(4m)}_{[\ell+\ell'+q+4m-2;\ell+\ell'+q,t_1,t_1,t_2,t_2,\ldots,t_{m-1},t_{m-1},\ell-\ell']}(s,x)\end{aligned} \tag{4.20}$$

and

$$\begin{aligned}&\mathcal{D}^{(4m)}_{[\ell+2m-1;\ell]_\pm}(s,x)\mathcal{D}^{(4m)}_{[\ell'+2m-1;\ell']_\pm}(s,x)\\&\quad=\mathcal{A}^{(4m)}_{[\ell+\ell'+4m-2;(\ell,\ldots,\pm\ell)\otimes(\ell',\ldots,\pm\ell')]}(s,x)\\&\qquad+\sum_{q=1}^{\infty}\sum_{\substack{t_i\geqslant|\ell-\ell'|\\ t_i\geqslant t_{i+1}}}^{\ell+\ell'}\mathcal{D}^{(4m)}_{[\ell+\ell'+q+4m-2;\ell+\ell'+q,\ell+\ell',t_1,t_1,t_2,t_2,\ldots,t_{m-1},\pm t_{m-1}]}(s,x),\end{aligned} \tag{4.21}$$

while for $d=4m+2$ we have that

$$\mathcal{D}^{(4m+2)}_{[\ell+2m;\ell]_+}(s,x)\mathcal{D}^{(4m+2)}_{[\ell'+2m;\ell']_-}(s,x)$$
$$=\mathcal{A}^{(4m+2)}_{[\ell+\ell'+4m;(\ell,\ldots,\ell)\otimes(\ell',\ldots,-\ell')]}(s,x)$$
$$+\sum_{q=1}^{\infty}\sum_{\substack{t_i\geqslant|\ell-\ell'|\\ t_i\geqslant t_{i+1}}}^{\ell+\ell'}\mathcal{D}^{(4m+2)}_{[\ell+\ell'+q+4m;\ell+\ell'+q,\ell+\ell',t_1,t_1,t_2,t_2,\ldots,t_{m-1},t_{m-1},\ell-\ell']}(s,x), \tag{4.22}$$

and

$$\mathcal{D}^{(4m+2)}_{[\ell+2m;\ell]_\pm}(s,x)\mathcal{D}^{(4m+2)}_{[\ell'+2m;\ell']_\pm}(s,x)=\sum_{q=0}^{\infty}\sum_{\substack{t_i\geqslant|\ell-\ell'|\\ t_i\geqslant t_{i+1}}}^{\ell+\ell'}\mathcal{D}^{(4m+2)}_{[\ell+\ell'+q+4m;\ell+\ell'+q,t_1,t_1,t_2,t_2,\ldots,t_m,\pm t_m]}(s,x). \tag{4.23}$$

A special case of the previous is the product involving the character $\mathcal{D}^{(2r)}_{[r-1;0]}$ in (3.27), corresponding to a free scalar field, for which we have

$$\mathcal{D}^{(2r)}_{[r-1;0]}(s,x)\mathcal{D}^{(2r)}_{[\ell+r-1;\ell]_\pm}(s,x)=\sum_{q=0}^{\infty}\mathcal{D}^{2r}_{[\ell+q+2r-2;\ell+q,\ell,\ldots,\pm\ell]}(s,x). \tag{4.24}$$

Another special case of the above contains a result first found by Vasiliev[10] which generalizes a well-known result by Flato and Fronsdal[6] in three dimensions to even dimensions $d=2r$. This result involves products of the representation corresponding to the free Dirac spinor,

$$Di^{(2r)}(s,x)\equiv\mathcal{D}^{(2r)}_{[r-(1/2),(1/2)]_+}(s,x)+\mathcal{D}^{(2r)}_{[r-(1/2),(1/2)]_-}(s,x)$$
$$=s^{r-(1/2)}(1-s)(\chi^{(2r)}_{(1/2,\ldots,1/2,1/2)}(x)+\chi^{(2r)}_{(1/2,\ldots,1/2,-1/2)}(x))P(s,x)$$
$$=s^{r-(1/2)}(1-s)(x_1^{(1/2)}+x_1^{-(1/2)})\cdots(x_r^{(1/2)}+x_r^{-(1/2)})P(s,x). \tag{4.25}$$

Using the above product formulas we may show that

$$Di^{(2r)}(s,x)Di^{(2r)}(s,x)=2\mathcal{A}^{(2r)}_{[2r-1,0,\ldots,0]}+2\sum_{q=0}^{\infty}(\mathcal{D}^{(2r)}_{[2r+q-1,q+1,1,1,\ldots,1,0]}(s,x)+\mathcal{D}_{[2r+q-1,q+1,1,1,\ldots,1,0,0]}(s,x)$$
$$+\cdots+\mathcal{D}^{(2r)}_{[2r+q-1,q+1,1,0,\ldots,0,0]}(s,x)+\mathcal{D}^{(2r)}_{[2r+q-1,q+1,0,0,\ldots,0,0]}(s,x))$$
$$+\sum_{q=0}^{\infty}(\mathcal{D}^{(2r)}_{[2r+q-1,q+1,11,\ldots,1,1]}(s,x)+\mathcal{D}^{(2r)}_{[2r+q-1,q+1,1,1,\ldots,1,-1]}(s,x)), \tag{4.26}$$

regardless of whether $d=2r$ is divisible by 4 or not so. The latter matches Vasiliev's result.

C. Product formulas: odd dimensions

For SO$(2r+1,2)$ we have that

$$P^{(2r+1)}(s,x)=\sum_{p,q=0}^{\infty}s^{2p+q}\chi^{(2r+1)}_{(q,0,\ldots,0)}(x), \tag{4.27}$$

where

$$\chi^{(2r+1)}_{(q,0,\ldots,0)}(x)=\tfrac{1}{2}\det[x_i^{k_j}-x_i^{-k_j}]\Delta(x_1+x_1^{-1},\ldots,x_r+x_r^{-1})^{-1}(x_1^{(1/2)}-x_1^{-(1/2)})^{-1}\cdots(x_r^{1/2}-x_r^{-(1/2)})^{-1}, \tag{4.28}$$

with $k_1=q+\frac{1}{2}+r-1$, $k_j=\frac{1}{2}+r-j$, $j>1$.

From the results of Appendix D, we have the following expansions for the free spinor case of (3.34) and the free scalar case of (3.33), namely,

$$\mathcal{D}^{(2r+1)}_{[r;1/2]}(s,x)=\sum_{q=0}^{\infty}s^{r+q}\chi^{(2r+1)}_{((1/2)+q,(1/2),\ldots,(1/2))}(x), \tag{4.29}$$

for the free spinor case and

$$\mathcal{D}^{(2r+1)}_{[r-(1/2);0]}(s,x)=\sum_{q=0}^{\infty}s^{r+q-(1/2)}\chi^{(2r+1)}_{(q,0,\ldots,0)}(x), \tag{4.30}$$

for the free scalar case.

For (3.32) and $p=r-j$ we have that, for $\ell>\ell_1>\cdots>\ell_j$,

$$\mathcal{D}^{(2r+1)}_{[\ell+r+j;\ell,\ell_1,\ldots,\ell_j]}(s,x)=\sum_{p_1,\ldots,p_j,q,t=0}^{\infty}\sum_{i_1=-\frac{1}{2}p_1}^{\frac{1}{2}p_1}\cdots\sum_{i_j=-\frac{1}{2}p_j}^{\frac{1}{2}p_j}s^{\ell+r+j+q+t+p_1+\cdots+p_j}\chi^{(2r+1)}_{(\ell+q,\ell,\ldots,\ell,\ell_1+2i_1,\ldots,\ell_j+2i_j)}(x), \tag{4.31}$$

which we show in Appendix D. Again, the weights $(\ell+q,\ell,\ldots,\ell,\ell_1+2i_1,\ldots,\ell_j,+2i_j)$ may lie outside the dominant Weyl chamber, i.e., not satisfy (3.2), for particular ℓ,ℓ_i. For such weights we may use that $\chi^{(2r+1)}_{\ell'}(x)=\mathrm{sgn}(w)\chi^{(2r+1)}_{\ell' w}(x)$, some $w\in\mathcal{W}_{2r+1}$, to relate such characters to those with dominant integral highest weights $\ell' w$.

Just as for even dimensions in (4.16) a simplification to (4.31) occurs for the $p=1$ case of (3.32) for $\ell_1\equiv\ell,\ell_2=\cdots=\ell_r=0$ for which,

$$\mathcal{D}^{(2r+1)}_{[\ell+2r-1;\ell,0,\ldots,0]}(s,x)=\sum_{p,q=0}^{\infty}\sum_{k=0}^{\ell}s^{\ell+2r+2p+q-1}\chi^{(2r+1)}_{(q+k,\ell-k,0,\ldots,0)}(x). \tag{4.32}$$

Regarding products of free representations, we may determine that, using (3.32) for $p=1$,

$$\begin{aligned}\mathcal{D}^{(2r+1)}_{[r;1/2]}(s,x)\mathcal{D}^{(2r+1)}_{[r;1/2]}(s,x)=\mathcal{A}_{[2r;0,\ldots,0]}(s,x)+\sum_{q=0}^{\infty}(&\mathcal{D}^{(2r+1)}_{[2r+q;q+1,1,\ldots,1]}(s,x)+\mathcal{D}^{(2r+1)}_{[2r+q;q+1,1,\ldots,1,0]}(s,x)\\&+\cdots+\mathcal{D}^{(2r+1)}_{[2r+q;q+1,0,\ldots,0]}(s,x)),\end{aligned} \tag{4.33}$$

and

$$\mathcal{D}^{(2r+1)}_{[r;1/2]}(s,x)\mathcal{D}^{(2r+1)}_{[r-(1/2);0]}(s,x)=\sum_{q=0}^{\infty}\mathcal{D}^{(2r+1)}_{[2r+q-(1/2);q+(1/2),(1/2),\ldots,(1/2)]}(s,x), \tag{4.34}$$

along with

$$\mathcal{D}^{(2r+1)}_{[r-(1/2);0]}(s,x)\mathcal{D}^{(2r+1)}_{[r-(1/2);0]}(s,x)=\sum_{q=0}^{\infty}\mathcal{D}^{(2r+1)}_{[2r+q-1;q,0,\ldots,0]}(s,x), \tag{4.35}$$

which generalize similar formulas obtained in Ref. 6 to odd dimensions.

V. PARTITION FUNCTIONS

As a partial check of the character formulas corresponding to free fields, we will compare them to partition functions which have been obtained by various authors in conformally invariant theories on $S^1 \times S^{d-1}$. For these cases, the single particle partition function for a local free operator F may expressed by

$$Y_F^{(d)}(s) = \sum_{q=0}^{\infty} n_{F,q}^{(d)} s^{\Delta_0+q}, \tag{5.1}$$

where $n_{F,q}^{(d)}$ enumerates the descendants of F in the flat background $\mathbb{R}^d$. For even d, the form (4.14) for the character formula corresponding to such free fields allows us to obtain $Y_F^{(d)}(s)$ directly when we set $x_1, \ldots, x_{(1/2)d}=1$. Thus we easily find that

$$Y_{F_\pm}^{(d)}(s) = \sum_{q=0}^{\infty} n_{F_\pm,q}^{(d)} s^{\ell+(1/2)d+q-1}, \tag{5.2}$$

where for $\ell \neq 0$ (from Appendix B)

$$\begin{aligned} n_{F_\pm,q}^{(d)} = \chi_{(\ell+q,\ell,\ldots,\ell+\pm\ell)}^{(d)}(1,\ldots,1) &= \dim(\mathcal{I}_{(\ell+q,\ell,\ldots,\ell)}^{(d)}) \\ &= 2^{(1/2)d-1} \prod_{i=1}^{\frac{1}{2}d-1} \frac{1}{(d-2i)!}(q+i)(2\ell+q+d-2-i) \\ &\quad \times \prod_{2\leqslant k<j\leqslant \frac{1}{2}d} (j-k)(2\ell+d-j-k), \end{aligned} \tag{5.3}$$

while for the scalar field

$$n_{S,q}^{(d)} = \chi_{(q,0,\ldots,0)}^{(d)}(1,\ldots,1) = \frac{2q+d-2}{q+d-2}\binom{q+d-2}{q}, \tag{5.4}$$

which is the dimension of the rank-q symmetric traceless tensor representation of SO(d). (This agrees with a similar formula in Ref. 12.) For chiral Weyl fermions we find, from (5.3) for $\ell=\frac{1}{2}$.

$$n_{f_{\pm},q}^{(d)} = 2^{(1/2)d}\frac{1}{q!}(q+1)(q+2)\cdots(q+d-2). \tag{5.5}$$

Similarly for the $\frac{1}{2}d$-form field strength, from (5.3) for $\ell=1$,

$$n_{V_{\pm},q}^{(d)} = \frac{d}{2(2q+d)}\binom{d}{\frac{1}{2}d}\binom{q+d-1}{q}. \tag{5.6}$$

Note that it may be easily checked that these occupancy numbers agree with those obtained in Ref. 13. For $d=4,6$ [where for $d=4$ then $Y_{V^+}^{(4)}(s)+Y_{V^-}^{(4)}(s)$ is the single particle partition function of the Maxwell field].

For bosonic F the multiparticle partition function is given by

$$Z_F^{(d)}(s) = \exp\left(\sum_{n=1}^{\infty}\frac{1}{n}Y_F^{(d)}(s^n)\right) = \prod_{q=0}^{\infty}(1-s^{\Delta_0+q})^{-n_{F,q}^{(d)}}, \tag{5.7}$$

while for fermionic F it is given by

$$Z_F^{(d)}(s) = \exp\left(\sum_{n=1}^{\infty} \frac{1}{n}(-1)^{n+1} Y_F^{(d)}(s^n)\right) = \prod_{q=0}^{\infty} (1+s^{\Delta_0+q})^{n_{F,q}^{(d)}}. \tag{5.8}$$

It is easy to check that (5.7), (5.8) for the scalar, Weyl fermion and field strength cases above match the results Ref. 13 for $d=4,6$.

Performing the summation in (5.2) for the scalar, Weyl fermion and $\frac{1}{2}d$-form field-strength cases we find

$$Y_S^{(d)}(s) = (s+1)\frac{s^{(1/2)d-1}}{(1-s)^{d-1}},$$

$$Y_{f\pm}^{(d)}(s) = 2^{(1/2)d}\frac{s^{(1/2)(d-1)}}{(1-s)^{d-1}}, \tag{5.9}$$

$$Y_{V_\pm}^{(d)}(s) = \frac{d!}{2\left(\frac{1}{2}d\right)!^2}\frac{s^{(1/2)d}}{(1-s)^{d-1}}F\left(1,-\tfrac{1}{2}d+1;\tfrac{1}{2}d+1;s\right),$$

[where $F(a,b;c;x)$ is the usual hypergeometric function] which may be read off directly from (3.26), (3.27) for $x_i=1$. This form may be directly compared to similar results in Ref. 14 whereby the formulas agree for the scalar and Weyl fermion cases.

It is not difficult to compute the first couple of numbers (5.6) for the self-dual $r=\frac{1}{2}d$ form field strength which we denote by $F_{\mu_1\cdots\mu_r}=*F_{\mu_1\cdots\mu_r}$. For $q=0$ this number just counts the number of independent components in $F_{\mu_1\cdots,\mu_r}$. Antisymmetry in the indices implies $\binom{2r}{r}$ independent components which is reduced by a factor of one-half due to self-duality. For $q=1$ (5.6) counts the number of first-order descendants, $\partial_\mu F_{\mu_1\cdots\mu_r}$. This will be $r\binom{2r}{r}$ less the number of constraint equations $\partial^{\mu_1}F_{\mu_1\cdots\mu_r}=0$ which is $\binom{2r}{r-1}$.

As a further example and check of our formulas, we consider the single particle partition function for rank-ℓ symmetric traceless tensor fields $T_{\mu_1\cdots\mu_\ell}$ satisfying the constraint equation $\partial^{\mu_1}T_{\mu_1\cdots\mu_\ell}=0$. The appropriate character formula in this case is given by (4.16). The corresponding occupation numbers, for $n_{F,q}^{(d)}\to N_{q,\ell}$ in (5.2), are given by

$$N_{q,\ell} = (q(d-2)(2\ell+d-3)+(d-1)(\ell+d-3)(2\ell+d-2)) \times\frac{1}{(d-1)(d-2)(d-3)}\binom{\ell+d-4}{\ell}\binom{q+d-2}{q}. \tag{5.10}$$

To see this we may use (4.16) to write

$$N_{q,\ell} = \sum_{i=0}^{\left[\frac{1}{2}q\right]} t_{q-2i,\ell} \quad \text{for } t_{q,\ell} = \sum_{k=0}^{\ell} \dim(\mathcal{I}^{(d)}_{(q+k,\ell-k,0,\ldots,0)}). \tag{5.11}$$

Using the dimension formula in Appendix B we may find that

$$t_{q,\ell} = (\ell+q+d-3)(4\ell q+(d-3)(2\ell+2q+d-2))\frac{1}{(d-2)(d-3)^2}\binom{\ell+d-4}{\ell}\binom{q+d-4}{q}, \tag{5.12}$$

and thence obtain (5.10) from (5.11).

Again it is not difficult to check that the first couple of numbers agree with expectations. We may easily show that $N_{\ell,0}=\dim(\mathcal{I}^{(d)}_{(\ell,0,\ldots,0)})$ given in (5.4) as expected. Also we may easily show that $N_{\ell,1}=d\,\dim(\mathcal{I}^{(d)}_{(\ell,0,\ldots,0)})-\dim(\mathcal{I}^{(d)}_{(\ell-1,0,\ldots,0)})$ which is the number of first-order descendants $\partial_\mu T_{\mu_1\cdots\mu_\ell}$ reduced by the number of constraint equations coming from the conservation condition. More generally

$$N_{\ell,q}=\binom{q+d-1}{q}\dim(\mathcal{I}^{(d)}_{(\ell,0,\ldots,0)})-\binom{q+d-2}{q-1}\dim(\mathcal{I}^{(d)}_{(\ell-1,0,\ldots,0)}), \tag{5.13}$$

which may be easily seen as the descendants at level q are given by $\partial_{\nu_1}\partial_{\nu_2}\cdots\partial_{\nu_q}T_{\mu_1\cdots\mu_\ell}$ whose number of independent components, is given by the first term in (5.13) which is reduced by the number of independent components in $\partial_{\nu_1}\partial_{\nu_2}\cdots\partial_{\nu_{q-1}}\partial^{\mu_1}T_{\mu_1\cdots\mu_\ell}$ which vanishes by conservation.

More generally, we may use (4.15) in even dimensions and (4.29), (4.30), (4.31) in odd dimensions for $x_i=1$ to determine the occupation numbers in the single particle partition function corresponding to fields whose conformal dimension saturates the unitarity bounds (3.8), (3.9). As mentioned before these are fields which satisfy certain conservation conditions which determines the particular unitarity bound.

Rotating quantum fields in an AdS_{d+1} background have been considered in Ref. 15. Here the modes of a quantum field are supposed to have energies E and angular momenta j_i where $i=1,\ldots,\lfloor\frac{1}{2}d\rfloor$. For the boundary conformal field theory on $\mathbb{R}\times S^{d-1}$ the energies are related to the conformal dimension of conformal fields and their descendants via $E=\Delta$ assuming that the sphere has unit radius while j_i correspond to $\mathrm{SO}(d)$ eigenvalues. Making the identification

$$s=e^{-\beta},\quad x_i=e^{\beta\Omega_i}, \tag{5.14}$$

where $\beta=T^{-1}$ for T being the temperature and Ω_i denote chemical potentials for angular momenta, then it can be shown that the one particle boundary partition function $\Sigma_{E,j_i}e^{-\beta(E-\Omega_i j_i)}$ and character formula for the conformal field coincide. For instance, for a free scalar field, the character formula (3.27) obtained here agrees with the corresponding single particle partition function for the boundary conformal field theory obtained in Ref. 15 when we make the identification (5.14).

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APPENDIX A: CHARACTER FORMULAS FOR INFINITE DIMENSIONAL IRREDUCIBLE MODULES OF SEMISIMPLE LIE ALGEBRAS

In this appendix we outline some results on character formulas of relevance for the main text. First we give basic definitions and notation.

The Weyl group $\mathcal{W}$ is generated by mappings w_α, for α being a root, which on weight space give

$$w_\alpha(\Lambda)=\Lambda-(\alpha^\vee,\Lambda)\alpha,\quad \alpha^\vee=2\alpha/(\alpha,\alpha). \tag{A1}$$

For $\Lambda=\beta$, another root, then $w_\alpha(\beta)$ is a reflection of β with respect to the hyperplane through the origin and perpendicular to α. Here (λ,μ) denotes the usual inner product on weight space between λ and μ. [In the Dynkin basis this is given by $(\lambda,\mu)=\Sigma_{i,j}\lambda_i G_{ij}\mu_j$ where λ_i,μ_i are Dynkin labels and $[G_{ij}]$ is the quadratic form matrix]. Any $w\in\mathcal{W}$ may be decomposed in terms of simple Weyl reflections $w_i\equiv w_{\alpha_i}$, for α_i being the simple roots, as $w=w_{i_1}\cdots w_{i_n}$ for some n which is generally not unique. However the signature of w defined, in the present case, by $\mathrm{sgn}(w)=(-1)^n$ is uniquely defined. We denote by $\ell(w)$ the minimum number of w_i in the composition of w. Clearly $\mathrm{sgn}(w)=(-1)^{\ell(w)}$.

The Weyl group divides the weight space into a family of open sets called Weyl chambers. These are simplicial cones defined by

$$\mathcal{H}_w = \{\lambda : (\alpha_i^\vee, w(\lambda)) > 0, \quad 1 \leqslant i \leqslant r\}, \tag{A2}$$

for $w \in \mathcal{W}$. The number of such equals the order of $\mathcal{W}$, $|\mathcal{W}|$. The weights lying on the boundary of the Weyl chambers are the points on the hyperplanes perpendicular to the roots $(\alpha_i^\vee, w(\lambda))=0$. In terms of Dynkin labels these are the weights having at least one vanishing Dynkin label.

The Weyl chamber corresponding to the identity of the Weyl group $\mathcal{H}_1$ is the fundamental or dominant Weyl chamber. In terms of Dynkin labels the weights in this chamber have strictly positive Dynkin labels. If all the Dynkin labels are non-negative and/or integers then we say the weight is dominant and/or integral.

Suppose we have some Lie algebra module V_Λ having highest weight Λ. The definition of the corresponding character we use is[5]

$$\mathrm{Char}_\Lambda \equiv \sum_{\lambda \in V_\Lambda} \mathrm{mult}_{V_\Lambda}(\lambda) e^\lambda, \tag{A3}$$

where $\mathrm{mult}_{V_\Lambda}(\lambda)$, $\mathrm{mult}_{V_\Lambda}(\Lambda)=1$, denotes the multiplicity of the weight λ in the weight system of V_Λ. This is to be interpreted as a function on weight space satisfying

$$e^\lambda e^\mu = e^{\lambda+\mu}, \quad e^\lambda(\mu) = e^{(\lambda,\mu)}. \tag{A4}$$

Under the action of the Weyl group, for $w \in \mathcal{W}$,

$$w(e^\lambda) = e^{w(\lambda)}. \tag{A5}$$

For a unitary group and with $\mathrm{mult}_{V_\Lambda}(\lambda)$ always finite we may recover a trace formula for the character by normalizing each vector $v_\lambda \in V_\Lambda$ corresponding to the weight λ so that $\langle v_\lambda | v_\lambda \rangle = 1$. Then we may write,

$$\mathrm{Char}_\Lambda(\mu) = \sum_{v_\lambda \in \tilde{V}_\Lambda} \langle v_\lambda | v_\lambda \rangle e^{(\lambda,\mu)} = \mathrm{Tr}(e^{(H,\mu)}), \tag{A6}$$

where $(H,\mu)=\Sigma_{i,j} H_i G_{ij} \mu_j$ in the Dynkin basis, for example, for H_i being Cartan subalgebra elements with $H_i|v_\lambda\rangle = \lambda_i |v_\lambda\rangle$.

As an example, consider a Verma module $\mathcal{V}_\Lambda$ with basis $\Pi_{\alpha\in\Phi_-} E_\alpha^{n_\alpha} |\underline{\Lambda}\rangle^{\mathrm{hw}}$ for Φ_- being negative roots and n_α being non-negative integers. For fixed n_α then the corresponding weight $\lambda_{(n_\alpha)} = \Lambda + \Sigma_{\alpha\in\Phi_-} n_\alpha \alpha$ has unit multiplicity in the weight system of $\mathcal{V}_\Lambda$. Thus we may write the character for the Verma module as

$$\mathcal{C}_\Lambda = \sum_{n_\alpha \geqslant 0} e^{\lambda(n_\alpha)} = e^\Lambda \prod_{\alpha\in\Phi_-} (1 - e^\alpha)^{-1}. \tag{A7}$$

Note that a given weight λ has multiplicity given by $\mathcal{P}(\Lambda - \lambda)$ where $\mathcal{P}(\mu)$ counts the number of ways in which the weight μ may be written as a linear combination of positive roots with non-negative integer coefficients.

We may easily also show that

$$w(\mathcal{C}_\Lambda) = \mathrm{sgn}(w) \mathcal{C}_{\Lambda^w}, \quad \Lambda^w = w(\Lambda + \rho) - \rho, \tag{A8}$$

for any $w \in \mathcal{W}$.

The character χ_Λ of an infinite dimensional irreducible module $\mathcal{I}_\Lambda$ of a semisimple Lie algebra has been written down long ago.[11] For the highest weight Λ not being dominant integral then $\mathcal{I}_\Lambda$ is infinite dimensional. Otherwise $\mathcal{I}_\Lambda$ is finite dimensional and the character is given by the well-known Weyl character formula. Before we give the result of Ref. 11 we quote a number of results which give insight into the structure of infinite dimensional irreducible modules.

Concerning Verma modules (which in Ref. 11 are called elementary representations), the first result we recount is that if Λ^w, $w \in \mathcal{W}$ is not a weight of $\mathcal{V}_\Lambda$ then $\mathcal{V}_\Lambda$ itself is irreducible. This is the simplest case and an example is $\mathcal{V}_\ell$ for SO(3) with ℓ being a negative half integer. We now give the conditions for $\mathcal{V}_\Lambda$ to contain submodules $\mathcal{V}_{\Lambda'}$ and so to be reducible.

We define a partial ordering on weights so that $\Lambda' \prec \Lambda$ if and only if $\Lambda - \Lambda' = \Pi$ for some $\Pi = \Sigma_{\alpha \in \Phi_+} p_\alpha \alpha$ for p_α being non-negative integers, not all zero. A necessary condition for a Verma module $\mathcal{V}_\Lambda$ to contain a submodule $\mathcal{V}_{\Lambda'}$ is that $\Lambda' = \Lambda^w \prec \Lambda$ for some $w \in \mathcal{W}$, $w \neq 1$. A crucial result is a theorem in Ref. 20 which proves that a necessary and sufficient condition for $\mathcal{V}_{\Lambda^w}$ to be a submodule of $\mathcal{V}_\Lambda$ is that there exist a sequence of positive roots $\beta_1, \ldots, \beta_K$ such that

$$w = w_{\beta_1} w_{\beta_2} \cdots w_{\beta_k}, \quad (w^\vee_{\beta_k}, w_{\beta_{k+1}} w_{\beta_{k+2}} \cdots w_{\beta_K}(\Lambda + \rho)) \in \mathbb{N}, \quad k = 1, \cdots, K, \tag{A9}$$

where we define $w_{\beta_{K+1}} \equiv 1$. For Λ being a dominant integral weight then condition (A9) holds for all Λ^w, $w \in \mathcal{W}$. This justifies the claim made in this paper that for Λ being dominant integral then Λ^w is a highest weight in $\mathcal{V}_\Lambda$ for every $w \in \mathcal{W}$.

A key result proved by Verma[21] and recounted in Ref. 11 is the following. A Verma module contains those and only those irreducible representations $\mathcal{I}_{\Lambda'}$ for which $\mathcal{V}_{\Lambda'}$ is a submodule of $\mathcal{V}_\Lambda$. Furthermore it contains $\mathcal{I}_{\Lambda'}$ at most once.

This results in the following formula for characters:

$$\mathcal{C}_\Lambda = \chi_\Lambda + \sum_{\substack{w \in \mathcal{W} \\ \Lambda^w \prec \Lambda}} \chi_{\Lambda^w}, \tag{A10}$$

where the sum runs over all w for which (A9) holds.

Using these results and formulas for multiplicities of weights determined for Verma modules in terms of the function $\mathcal{P}(\mu)$ above a formula has been given for χ_Λ in Ref. 11. This may be rewritten in the equivalent form

$$\chi_\Lambda = \mathcal{C}_\Lambda + \sum_{\substack{w \in \mathcal{W} \\ \Lambda^w \prec \Lambda}} \gamma_{\Lambda^w} \mathcal{C}_{\Lambda^w}, \tag{A11}$$

where each w satisfies condition (A9) and where the integers γ_{Λ^w} are determined by a recurrence relation as follows.

Consider a submodule $\mathcal{V}_{\Lambda^w}$ of $\mathcal{V}_\Lambda$ so that there is no other submodule $\mathcal{V}_{\Lambda^{w'}}$ of $\mathcal{V}_\Lambda$ containing $\mathcal{V}_{\Lambda^w}$ in turn as a submodule. Then in this case $\gamma_{\Lambda^w} = -1$.

For a submodule $\mathcal{V}_{\Lambda^w}$ of $\mathcal{V}_\Lambda$ which is in turn contained in the submodules $\mathcal{V}_{\Lambda^{w'}}$ of $\mathcal{V}_\Lambda$, then in this case

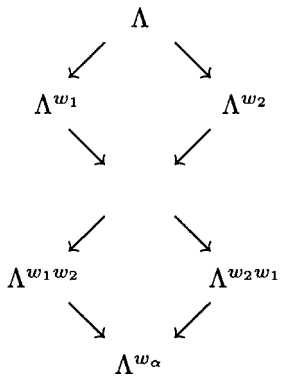
$$\gamma_{\Lambda^w} = -\sum_{w'} \gamma_{\Lambda^{w'}} - 1, \tag{A12}$$

which determines γ_{Λ^w} in (A11) recursively.

A simple example illustrates this formula. Consider Sl_3 whereby, for a weight $\Lambda = [a, b]$ with Dynkin labels a, b, the simple Weyl reflections are given by

$$w_1([a,b]) = [-a, a+b], \quad w_2([a,b]) = [a+b, -b]. \tag{A13}$$

The $\mathcal{S}_3$ Weyl group elements consist of $\{1, w_1, w_2, w_1 w_2, w_2 w_1, w_\alpha\}$ where $w_\alpha = w_1 w_2 w_1 = w_2 w_1 w_2$ is the Weyl reflection corresponding to the root $\alpha = \alpha_1 + \alpha_2$. The shifted Weyl reflections are given by $\Lambda^1 = \Lambda$, $\Lambda^{w_1} = \Lambda - (a+1)\alpha_1$, $\Lambda^{w_2} = \Lambda - (b+1)\alpha_2$, $\Lambda^{w_2 w_1} = \Lambda - (a+1)\alpha_1 - (a+b+2)\alpha_2$, $\Lambda^{w_1 w_2} = \Lambda - (a+b+2)\alpha_1 - (b+1)\alpha_2$, $\Lambda^{w_\alpha} = \Lambda - (a+b+2)\alpha$. For $\swarrow$ denoting a vector in the $-\alpha_1$ direction of length $a+1$ and $\searrow$ denoting such in the $-\alpha_2$ direction of length $b+1$ then we may represent the weight system of the Verma module $\mathcal{V}_\Lambda$ diagrammatically as follows:



(A14)

assuming Λ is dominant integral and where we have omitted any other weights occurring. In computing $\chi_{\Lambda^{w_1}}$, for example, we have that $\mathcal{V}_{\Lambda^{w_1 w_2}}$ and $\mathcal{V}_{\Lambda^{w_2 w_1}}$ are both sub-Verma modules of $\mathcal{V}_{\Lambda^{w_1}}$ with $\gamma_{\Lambda^{w_1 w_2}}=\gamma_{\Lambda^{w_2 w_1}}=-1$. Also $\mathcal{V}_{\Lambda^{w_\alpha}}$ is a sub-verma-module of both the latter and so $\gamma_{\Lambda^{w_\alpha}}=-(\gamma_{\Lambda^{w_1 w_2}}+\gamma_{\Lambda^{w_2 w_1}})-1=1$. Thus $\chi_{\Lambda^{w_1}}=\mathcal{C}_{\Lambda^{w_1}}-\mathcal{C}_{\Lambda^{w_2 w_1}}-\mathcal{C}_{\Lambda^{w_1 w_2}}+C_{\Lambda^{w_\alpha}}$ In fact for all $\Lambda'=\Lambda^{w'}$ it is easy to check that $\chi_{\Lambda'}=\mathcal{C}_{\Lambda'}+\sum_{\substack{w\in\mathcal{S}_3\\ \Lambda' w<\Lambda'}}\mathrm{sgn}(w)=\mathcal{C}_{\Lambda' w}$.

Other properties of $\mathcal{I}_\Lambda$ which are useful for what follows concern symmetry under Weyl group reflections. For all Dynkin labels Λ_i of the weight Λ which are non-negative integers then the subgroup $\mathcal{W}'$ generated by the corresponding simple Weyl reflections w_i is the maximal symmetry group of the weight system of $\mathcal{I}_\Lambda$. Furthermore $\mathcal{V}_{\Lambda^{w'}}$ is a submodule of $\mathcal{V}_\Lambda$ for all $w'\in\mathcal{W}', w'\neq 1$ [since all w' satisfy condition (A9)]. In terms of characters we have that $w'(\chi_\Lambda)=\chi_\Lambda$ for every $w'\in\mathcal{W}'$.

For Λ being dominant integral then this symmetry group is of course the Weyl group itsetf and $\mathcal{W}'=\mathcal{W}$. In this case we from (A11) that

$$\chi_\Lambda=\sum_{w\in\mathcal{W}}\mathrm{sgn}(w)\mathcal{C}_{\Lambda^w}=\prod_{\alpha\in\Phi_-}(1-e^\alpha)^{-1}\sum_{w\in\mathcal{W}}\mathrm{sgn}(w)e^{w(\Lambda+\rho)-\rho}, \tag{A15}$$

the usual Weyl character formula. This follows as symmetry under $\mathcal{W}$ determines $\gamma_{\Lambda^w}=\mathrm{sgn}(w)$ in this case. Using (A8) we may find that the Weyl character may be rewritten as

$$\chi_\Lambda=\sum_{w\in\mathcal{W}}w(\mathcal{C}_\Lambda)\equiv\mathfrak{W}(\mathcal{C}_\Lambda). \tag{A16}$$

Due to the invariance of $\mathcal{I}_\Lambda$ under the action of any $w\in\mathcal{W}$ then the Weyl symmetry operator $\mathfrak{W}$ defined by (A16) is obviously linear and idempotent on the vector space spanned by the characters of the Verma modules, $\mathfrak{W}^2=|\mathcal{W}|\mathfrak{W}$.

Denoting by I the subset of labels for which Λ_i, $i\in I$, are non-negative integers, supposing we find that every sub-Verma-module highest weight $\Lambda^{w''}$, $w''\in\mathcal{W}$ may be written in the form $\Lambda^{w''}=\Lambda^{w'w}$, $w\in\mathcal{W}$, $w'\in\mathcal{W}'$ for Λ_i^w, $i\in I$ being non-negative integers or $\Lambda_i^w=-1$ for some $i\in I$. We claim that the weights $\Lambda^{w''}<\Lambda$ are given by the disjoint union of the weights $\Lambda^{w'w}$ for every $w'\in\mathcal{W}'$. For the cases of $\Lambda_i^w=-1$ then the $\mathcal{C}_{\Lambda^{w'w}}$, $w'\in\mathcal{W}'$ cancel among themselves in χ_Λ.

Under this assumption (which holds in the cases considered in this paper) then using (A11) we may write for the character

$$\chi_\Lambda=\mathcal{C}_\Lambda+\sum_{\substack{w'\in\mathcal{W}'\\ w'\neq 1}}\gamma_{\Lambda^{w'}}\mathcal{C}_{\Lambda^{w'}}+\sum_{\substack{w'\in\mathcal{W}'\\ w\in\mathcal{W},w\neq 1}}\gamma_{\Lambda^{w'w}}\mathcal{C}_{\Lambda^{w'w}}, \tag{A17}$$

where the sum runs over only those $w\in\mathcal{W}$ which satisfy (A9) and for which Λ_i^w, $i\in I$, is a non-negative integer or -1. Using (A8) and $w'(\chi_\Lambda)=\chi_\Lambda$, $w'\in\mathcal{W}'$ and the claims proved below we may show that $\gamma_{\Lambda^{w'}}=\mathrm{sgn}(w')$, $\gamma_{\Lambda^{w'w}}=\gamma_{\Lambda^w}\mathrm{sgn}(w')$ and that the $\mathcal{C}_{\Lambda^{w'w}}$ for which $\Lambda_j^w=-1$ for some $j\in I$ cancel among themselves. It is then left to determine the remaining γ_{Λ^w} by the recurrence relation mentioned earlier.

We now show that for some arbitrary weight Λ which has Λ_i, $i \in I$ being non-negative integers that this is the unique weight among $\Lambda^{w'}$, $w' \in \mathcal{W}'$ having this property. Clearly under these assumptions $(\Lambda^{w_i})_i = (\alpha_i^\vee, \Lambda^{w_i}) = -\Lambda_i - 2$ is negative for $i \in I$. Since $\mathcal{W}'$ is generated by all w_i, $i \in I$, then we may consider all $w' = w_{i_1} \cdots w_{i_n}$, $i_j \in I$ such that $\ell(w') = n$. Denoting by Φ'_+ all those positive roots formed from linear combinations of the subset of simple roots α_i, $i \in I$, then we have the result that $\ell(w_i w') = \ell(w') + 1$ if and only if $w'^{-1}(\alpha_i) \in \Phi'_+$. (The argument for this is similar to one given in Ref. 22.) In this case we have that $(\Lambda^{w_i w'})_i = -(\alpha^\vee, \Lambda + \rho) - 1$ where $\alpha = w'^{-1}(\alpha_i) \in \Phi'_+$. Since $(\alpha^\vee, \Lambda + \rho) \geqslant 0$ then $(\Lambda^{w_j w'})_i$ must be negative. Hence all $\Lambda^{w'}$, $w' \in \mathcal{W}'$, $w' \neq 1$, have at least on of $\Lambda_i^{w'}$, $i \in I$ which is negative.

If some $\Lambda^{w'w} = \Lambda^{u'u}$ for some w', $u' \in \mathcal{W}'$ and with Λ_i^w, $\Lambda_i^u \geqslant 0$, $i \in I$, then clearly we may write $\Lambda^u = \Lambda^{u'^{-1}w'w}$ which contradicts the above unless $u = w$, $u' = w'$. Thus any two sets of such weights $\{\Lambda^{w'w}, w' \in \mathcal{W}'\}$ and $\{\Lambda^{w'u}, w' \in \mathcal{W}'\}$ for $w \neq u$ are disjoint.

If for some weight $\Lambda_j = -1$ for some $j \in I$ then $\Lambda^{w_j} = \Lambda$ since $(\alpha_j^\vee, \Lambda^w + \rho) = 0$. We claim that the only $\Lambda^{w'}$ for $w' \in \mathcal{W}'$ which equal Λ in this case are those for which w' is composed of the w_j. For simplicity we consider the case when $\Lambda_j = -1$ and otherwise Λ_i is non-negative for $i \in I$. In this case if $\Lambda^{w'} = \Lambda$ then clearly $\Lambda^{w_j w'} = \Lambda$ so that, for $\alpha = w^{-1}(\alpha_j)$, $(\Lambda^{w_j w'})_j = -(\alpha^\vee, \Lambda + \rho) - 1 = -1$ by assumption. Thus $(\alpha^\vee, \Lambda + \rho) = 0$ which is only the case if $\alpha \propto \alpha_j$. The only roots with this property are $\pm\alpha_i$ so that $w' = 1, w_j$. Also this implies that, for w', $u' \in \mathcal{W}'$, $\Lambda^{w'} = \Lambda^{u'}$ if and only if $u' = w'$ or $u' = w'w_j$. The generalization is clear.

APPENDIX B: WEYL CHARACTER FORMULAS FOR SO(*d*)

We now consider SO(d) character formulas. We define the variables $x_i = e^{e_i}(\mu) = e^{\mu_i}$ for some arbitrary SO(d) weight $\mu = \Sigma_{i=1}^r \mu_i e_i$.

For SO($2r$) the action of the Weyl group, $\mathcal{W}_{2r} = \mathcal{S}_r \ltimes \mathbb{Z}^{r-1}$, on weights in the orthonormal basis is given by $\mathcal{S}_r$ permutations on the labels followed by reflections involving an even number of sign flips in the labels. This means that for $\varrho = \rho_i \cdots \rho_j \in \mathbb{Z}^{r-1}$ where $\rho_i(\ell_1, \ldots, \ell_i, \ldots, r) = (\ell_1, \ldots, -\ell_i, \ldots \ell_r)$, $\rho_i^2 = 1$ then the number of ρ_i in the composition of ϱ is even and $\mathrm{sgn}(\varrho) = 1$. Using that

$$\sum_{\sigma \in \mathcal{S}_r} \mathrm{sgn}(\sigma) x_{\sigma(1)}^{\ell_1} \cdots x_{\sigma(r)}^{\ell_r} = \det[x_i^{\ell_j}], \tag{B1}$$

and the restriction mentioned on $\varrho \in \mathbb{Z}^{r-1}$ then[23]

$$\mathfrak{W}_{2r}\left(\prod_{i=1}^r x_i^{\ell_i}\right) = \frac{1}{2}\det[x_i^{\ell_j} + x_i^{-\ell_j}] + \frac{1}{2}\det[x_i^{\ell_j} - x_i^{-\ell_j}], \tag{B2}$$

for $\mathfrak{W}_{2r}$ denoting the SO($2r$) Weyl symmetry operator. For some highest weight $\ell = \Sigma_{i=1}^r \ell_i e_i$ corresponding Verma module character is given by

$$C_{\underline{\ell}}^{(2r)}(x) \equiv C_{\underline{\ell}}^{(2r)}(\mu) = \prod_{i=1}^r x_i^{\ell_i} \prod_{1 \leqslant j < k \leqslant r, \varepsilon = \pm} (1 - e^{(\alpha_{jk,\varepsilon}, \mu)})^{-1} = \prod_{i=1}^r x_i^{\ell_i + r - i} \Delta(x_1 + x_1^{-1}, \ldots, x_r + x_r^{-1})^{-1}, \tag{B3}$$

where $\alpha_{ij,\pm} = -e_i \pm e_j$, $1 \leqslant i < j \leqslant r$ are the negative roots and $\Delta(x)$ is the Vandermonde determinant (4.13). Using the fact that $\Delta(x_1 + x_1^{-1}, \ldots, x_r + x_r^{-1})$ is left alone by any $\varrho\sigma \in \mathcal{S}_r \ltimes \mathbb{Z}^{r-1}$ then we have quite simply that the Weyl character of the irreducible representation with dominant integral highest weight ℓ [given by $\chi_{\underline{\ell}}^{(2r)}(x) = \mathfrak{W}_{2r}(C_{\underline{\ell}}^{(2r)}(x))$] reduces to

$$\chi_{\underline{\ell}}^{(2r)}(x) = \tfrac{1}{2}(\det[x_i^{k_j} + x_i^{-k_j}] + \det[x_i^{k_j} - x_i^{-k_j}])\Delta(x_1 + x_1^{-1}, \ldots, x_r + x_r^{-1})^{-1}, \tag{B4}$$

for $k_i = \ell_i + r - i$. The dimension of the irreducible representation is given by

$$\dim(\mathcal{I}_{\underline{\ell}}^{(2r)}) = 2^{r-1}\prod_{i=1}^{r}\frac{1}{(2r-2i)!}\prod_{1\leqslant i<j\leqslant r}(\ell_i-\ell_j+j-i)(\ell_i+\ell_j+2r-i-j). \tag{B5}$$

For SO($2r+1$) the action of the Weyl group, $\mathcal{W}_{2r+1}=\mathcal{S}_r\ltimes\mathbb{Z}^r$, on weights in the orthonormal basis is given by $\mathcal{S}_r$ permutations on the labels followed by reflections involving any number of sign flips in the labels. Using (B1) we therefore have that[23]

$$\mathfrak{W}_{2r+1}\left(\prod_{i\neq 1}^{r}x_i^{\ell_i}\right) = \det[x_i^{\ell_j}-x_i^{-\ell_j}], \tag{B6}$$

for $\mathfrak{W}_{2r+1}$ denoting the SO($2r+1$) Weyl symmetry operator. This time for some highest weight $\ell=\Sigma_{i=1}^{r}\ell_i e_i$ the corresponding Verma module character is given by

$$\begin{aligned}C_{\underline{\ell}}^{(2r+1)}(x) \equiv C_{\underline{\ell}}^{(2r+1)}(\mu) &= \prod_{i=1}^{r}x_i^{\ell_i}\prod_{1\leqslant j<k\leqslant r,\varepsilon=\pm}(1-e^{(\alpha_{jk,\varepsilon},\mu)})^{-1}\prod_{1\leqslant l\leqslant r}(1-e^{(e_l,\mu)})^{-1}\\ &= \prod_{i=1}^{r}x_i^{\ell_i+(1/2)+r-i}\Delta(x_1+x_1^{-1},\ldots,x_r+x_r^{-1})^{-1}(x_1^{1/2}-x_1^{-1/2})^{-1}\cdots(x_r^{1/2}-x_r^{-1/2})^{-1},\end{aligned} \tag{B7}$$

since $-e_i$, $1\leqslant i\leqslant r$ are the weights of the extra negative roots in this case. Using that $\Delta(x_1+x_1^{-1},\ldots,x_r+x_r^{-1})^{-1}(x_1^{1/2}-x_1^{-1/2})^{-1}\cdots(x_r^{1/2}-x_r^{-1/2})^{-1}$ is left alone by any $\varrho\sigma\in\mathcal{S}_r\ltimes\mathbb{Z}^r$ then the Weyl character of the irreducible representation with dominant integral highest weight ℓ is given by, using (B6) and (B7),

$$\chi_{\underline{\ell}}^{(2r+1)}(x) = \det[x_i^{k_j}-x_i^{-k_j}]\Delta(x_1+x_1^{-1},\ldots,x_r+x_r^{-1})^{-1}(x_1^{1/2}-x_1^{(-1/2)})^{-1}\cdots(x_r^{1/2}-x_r^{-1/2})^{-1}, \tag{B8}$$

where $k_i=\ell_i+\frac{1}{2}+r-i$. The dimension of the irreducible representation is given by

$$\dim(\mathcal{I}_{\underline{\ell}}^{(2r+1)}) = \prod_{i=1}^{r}\frac{1}{(2r+1-2i)!}(2\ell_i+2r+1-2i)\prod_{1\leqslant i<j\leqslant r}(\ell_i-\ell_j+j-i)(\ell_i+\ell_j+2r+1-i-j). \tag{B9}$$

APPENDIX C: UNITARITY BOUNDS

Descendant states have bases, for $p=0,1,\ldots$,

$$\mathcal{B}^{(p)} = \left\{\prod_{\substack{v=i\varepsilon,0\\1\leqslant i\leqslant r,\varepsilon=\pm}}\mathcal{P}_v^{n_v}|\Delta;\underline{\ell}'\rangle, \sum_v n_v = p\right\}, \tag{C1}$$

for n_v being positive integers [with $n_0=0$ for SO($2r$)] and ℓ' being a weight in the weight system of the module of SO(d) with highest weight ℓ. For $p=0$ the norms of corresponding states are strictly positive for ℓ' being weights in the SO(d) irreducible representation with dominant integral highest weight ℓ and $\||\Delta;\ell'\rangle\|^2=\langle\Delta,\overline{\underline{\ell}'}\,|\,\Delta,\underline{\ell}'\rangle>0$.

Examining the simplest descendant states with basis $\mathcal{B}^{(1)}$ then these have SO(d) highest weight states

$$\mathcal{H}_d = \{|\Delta+1;\underline{\ell}+\underline{v}\rangle\}, \tag{C2}$$

where $v=\varepsilon e_i$, along with $v=0$ for $d=2r+1$, these of course occurring in the decomposition of the product between the vector representation and the representation with highest weight ℓ into irreducible representations, $e_1\otimes\ell=\oplus_v\ell\oplus v$. Remarkably, most of the restrictions necessary for the

states in $\mathcal{H}_d$ to have positive definite norm are sufficient for the unitarity constraints to be satisfied for all descendant states in $\mathcal{B}^{(p)}$—also conjectured in Ref. 18.

The simplest states in $\mathcal{H}_d$ may be constructed explicitly and are

$$|\Delta+1;\underline{\ell}+\underline{e}_1\rangle = \mathcal{P}_{1+}|\Delta;\underline{\ell}\rangle^{\mathrm{hw}},$$

$$|\Delta+1;\underline{\ell}+\underline{e}_2\rangle = (-2i(\ell_1-\ell_2)\mathcal{P}_{2+}+\mathcal{P}_{1+}E_{12}^{-+})|\Delta;\underline{\ell}\rangle^{\mathrm{hw}}, \tag{C3}$$

$$\begin{aligned}|\Delta+1;\underline{\ell}+\underline{e}_3\rangle = (&-4(\ell_1-\ell_3+1)(\ell_2-\ell_3)\mathcal{P}_{3+}-2i(\ell_1-\ell_3+1)\mathcal{P}_{2+}E_{23}^{-+}\\ &+(\ell_2-\ell_3+1)\mathcal{P}_{1+}E_{12}^{-+}E_{23}^{-+}-(\ell_2-\ell_3)\mathcal{P}_{1+}E_{23}^{-+}E_{12}^{-+})|\Delta;\underline{\ell}\rangle^{\mathrm{hw}},\end{aligned}$$

which are all annihilated by SO(d) raising operators. Using the conformal algebra and the unitarity conditions, the norms of these three states are given by

$$\|\|\Delta+1;\underline{\ell}+\underline{e}_1\rangle\|^2 = 4(\Delta+\ell_1)\|\|\Delta;\underline{\ell}\rangle\|^2,$$

$$\|\|\Delta+1;\underline{\ell}+\underline{e}_2\rangle\|^2 = 16(\Delta+\ell_2-1)(\ell_1-\ell_2)(\ell_1-\ell_2+1)\|\|\Delta;\underline{\ell}\rangle\|^2, \tag{C4}$$

$$\begin{aligned}\|\|\Delta+1;\underline{\ell}+\underline{e}_3\rangle\|^2 = &64(\Delta+\ell_3-2)(\ell_1-\ell_3+1)(\ell_1-\ell_3+2)\\ &\times(\ell_2-\ell_3)(\ell_2-\ell_3+1)\|\|\Delta;\underline{\ell}\rangle\|^2,\end{aligned}$$

and for these to be strictly positive this places obvious restrictions on Δ. Other examples which may be readily achieved are, for SO(3,2),

$$\begin{aligned}&|\Delta+1;\,\ell\,+1\rangle = \mathcal{P}_{1+}|\Delta;\,\ell\,\rangle^{\mathrm{hw}},\quad |\Delta+1;\,\ell\,\rangle = (-2i\,\ell\,\mathcal{P}_0+\mathcal{P}_{1+}E_1^-)|\Delta;\,\ell\,\rangle^{\mathrm{hw}},\\ &|\Delta+1;\,\ell-1\rangle = (2\,\ell\,(2\,\ell-1)\mathcal{P}_{1-}-2i(2\,\ell-1)\mathcal{P}_0E_1^-+\mathcal{P}_{1+}(E_1^-)^2)|\Delta;\,\ell\,\rangle^{\mathrm{hw}},\end{aligned} \tag{C5}$$

for which the norms are

$$\begin{aligned}&\|\|\Delta+1;\,\ell\,+1\rangle\|^2 = 4(\Delta+\,\ell\,)\|\|\Delta;\,\ell\,\rangle\|^2,\quad \|\|\Delta+1;\,\ell\,\rangle\|^2 = 8(\Delta-1)\,\ell\,(\ell+1)\|\|\Delta;\,\ell\,\rangle\|^2,\\ &\|\|\Delta+1;\,\ell-1\rangle\|^2 = 16(\Delta-\,\ell-1)\ell^2(4\ell^2-1)\|\|\Delta;\,\ell\,\rangle\|^2.\end{aligned} \tag{C6}$$

Another important example is for SO(4,2) whereby along with (C3), for $\underline{\ell}=(\ell_1,\ell_2)$, we also have

$$\begin{aligned}&|\Delta+1;\ell_1,\ell_2-1\rangle = (-2i(\ell_1+\ell_2)\mathcal{P}_{2-}+\mathcal{P}_{1+}E_{12}^{--})|\Delta;\underline{\ell}\rangle^{\mathrm{hw}},\\ &|\Delta+1;\ell_1-1,\ell_2\rangle = (-4(\ell_1^2-\ell_2^2)\mathcal{P}_{1-}-2i(\ell_1-\ell_2)\mathcal{P}_{2+}E_{12}^{--}-2_i(\ell_1+\ell_2)\mathcal{P}_{2-}E_{12}^{-+}+\mathcal{P}_{1+}E_{12}^{-+}E_{12}^{--})\\ &\qquad\times|\Delta;\underline{\ell}\rangle^{\mathrm{hw}},\end{aligned} \tag{C7}$$

for which the norms are

$$\begin{aligned}&\|\|\Delta+1;\ell_1,\ell_2-1\rangle\|^2 = 16(\Delta-\ell_2-1)(\ell_1+\ell_2)(\ell_1+\ell_2+1)\|\|\Delta;\underline{\ell}\rangle\|^2,\\ &\|\|\Delta+1;\ell_1-1,\ell_2\rangle\|^2 = 64(\Delta-\ell_1-2)(\ell_1^2-\ell_2^2)(\ell_1-\ell_1+1)(\ell_1+\ell_2+1)\|\|\Delta;\underline{\ell}\rangle\|^2.\end{aligned} \tag{C8}$$

Constructing other such elements of $\mathcal{H}_d$ is cumbersome. We here outline a simpler procedure for finding the unitarity constraints for $B^{(1)}$. The norms of the highest weight states in $\mathcal{H}_d$ are more generally given by

$$\|\|\Delta+1;\underline{\ell}+\underline{v}\rangle\|^2=(\Delta+g_{\underline{\ell}}^{(v)})f_{\ell}^{(v)}, \tag{C9}$$

where the functions $f_{\ell}^{(v)}$ are strictly positive for ℓ being strictly inside the dominant Weyl chamber, (3.1) or (3.2). We have that, assuming that ℓ is strictly inside the dominant Weyl chamber,

$$\mathcal{K}_{1-}|\Delta+1;\underline{\ell}+\underline{v}\rangle=0\Rightarrow\Delta+g_{\underline{\ell}}^{(v)}=0, \tag{C10}$$

which is in turn implied by the state $|\Delta+1;\underline{\ell}+\underline{v}\rangle$ being null. As an aid to solving (C10) we extend the definition of $\mathcal{B}^{(1)}$ in (C1) and consider $\ell'\in\mathcal{V}_{\ell}$ (the Verma module with dominant integral highest weight ℓ). Consider the following highest weight states with respect to SO(d), namely,

$$|\Delta+1;\underline{\ell}^{w_v}+\underline{e}_1\rangle=\mathcal{P}_{1+}|\Delta;\underline{\ell}^{w_v}\rangle,\quad \mathcal{K}_{1-}|\Delta+1;\underline{\ell}^{w_v}+\underline{e}_1\rangle=0\Rightarrow\Delta+\ell_1^{w_v}=0, \tag{C11}$$

where w_v are such members of the Weyl group $\mathcal{W}_r$ for which

$$\ell^{w_v}+e_1=(\ell+w_v^{-1}(e_1))^{w_v}=(\ell+v)^{w_v}, \tag{C12}$$

for some $v=\varepsilon e_j$ for $\varepsilon=\pm$. [Note that for SO($2r+1$) the vector $v=0$ is not on the Weyl orbit of e_1—we need a different approach to deal with this.] Thus the states (C11) are related to those in $\mathcal{H}_d$ by the action of SO(d) lowering operators on $|\Delta+1;\underline{\ell}+\underline{v}\rangle$. [For instance, we have that $|\Delta+1;\underline{\ell}^{\sigma_{12}}+\underline{e}_1\rangle=(E_{12}^{-+})^{\ell_1-\ell_2}|\Delta+1;\underline{\ell}+\underline{e}_2\rangle$ for $\sigma_{12}(\ell_1,\ell_2,\ldots)=(\underline{\ell}_2,\ell_1,\ldots)$ and with $|\Delta+1,\underline{\ell}+\underline{e}_2\rangle$ given in (C7).] Also, $\mathcal{K}_{1-}$ commutes with all such lowering operators so that the conditions (C10) and (C11) should be identical. Thus, using (3.14) [for $\varepsilon_1=\varepsilon,\sigma(1)=j$],

$$g_{\underline{\ell}}^{(\varepsilon e_j)}=\ell_1^{w_{\varepsilon e_j}}=\varepsilon\ell_j+(\varepsilon-1)\tfrac{1}{2}d-\varepsilon j+1, \tag{C13}$$

determining $g_{\ell}^{(v)}$, $v\neq0$ in (C9) for the states in $\mathcal{H}_d$.

To deal with the state $|\Delta+1;\ell\rangle\in\mathcal{H}_{2r+1}$ for SO($2r+1,2$) we first note an interesting observation. Consider the state $|\Delta+1;\underline{\ell}+\underline{e}_{r+1}\rangle\in\mathcal{H}_{2r+2}$ which is given by

$$|\Delta+1;\underline{\ell}+\underline{e}_{r+1}\rangle=\left(A_{\underline{\ell}}\mathcal{P}_{r+1+}+\sum_{1\leqslant i\leqslant r,\sigma}B_{\underline{\ell},i,\sigma}\mathcal{P}_{i+}E_{\sigma(ii+1)}^{-+}E_{\sigma(i+1i+2)}^{-+}\cdots E_{\sigma(rr+1)}^{-+}\right)|\Delta,\underline{\ell}\rangle^{\mathrm{hw}}, \tag{C14}$$

where σ permutes $(ii+1),\ldots,(rr+1)$ and $A_{\underline{\ell}}$, $B_{\underline{\ell},i,\sigma}$ are determined from the requirement that $E_{12}^{+-},\ldots,E_{rr+1}^{+-}$ annihilate the state (E_{rr+1}^{++} automatically annihilates it). Defining $\widetilde{A}_{(\ell_1,\ldots,\ell_r)}=A_{(\ell_1,\ldots,\ell_r,0)},\widetilde{B}_{(\ell_1,\ldots,\ell_r),i,\sigma}=B_{(\ell_1,\ldots,\ell_r,0),i,\sigma}$, then we claim that $|\Delta+1;\ell\rangle\in\mathcal{H}_{2r+1}$ is given by

$$|\Delta+1;\underline{\ell}\rangle=\left(\widetilde{A}_{\underline{\ell}}\mathcal{P}_0+\sum_{1\leqslant i\leqslant r,\sigma}\widetilde{B}_{\underline{\ell},i,\sigma}\mathcal{P}_i^{+}E_{\sigma(ii+1)}^{-+}E_{\sigma(i+1i+2)}^{-+}\cdots E_{\sigma(r)}^{-}\right)|\Delta,\underline{\ell}\rangle^{\mathrm{hw}}, \tag{C15}$$

where now σ permutes $(ii+1),\ldots,(r)$. This follows when we show that the conditions on $\widetilde{A}_{\ell},\widetilde{B}_{\underline{\ell},i,\sigma}$ arising from $E_{ii+1}^{+-},E_r^{+},1\leqslant i\leqslant r-1$ annihilating (C15) are exactly equivalent to those on $\bar{A}_{\underline{\ell}}B_{\underline{\ell},i,\sigma}$ arising from $E_{ii+1}^{+-},E_{rr+1}^{+-},1\leqslant i\leqslant r-1$ annihilating (C14) for $\ell_{r+1}=0$ if we identify $\mathcal{P}_0$ with $\mathcal{P}_{r+1}$ and $E_r^{-}$with E_{rr+1}^{-+}. We have that $[\mathcal{K}_{1-},\mathcal{P}_{r+1+}]=-2iE_{1r+1}^{-+}=(-2i)^{1-r}[E_{12}^{-+},\ldots,[E_{r-1r}^{-+},E_{rr+1}^{-+}]\cdots]$ and $[\mathcal{K}_{1-},\mathcal{P}_0]=-2iE_1^{-}=(-2i)^{1-r}[E_{12}^{-+},\ldots,[E_{r-1r}^{-+},E_r^{-}]\cdots]$. Due to this and as $\widetilde{A}_{(\ell_1,\ldots,\ell_r)}=A_{(\ell_1,\ldots,\ell_r,0)},\widetilde{B}_{(\ell_1,\ldots,\ell_r),i,\sigma}=B_{(\ell_1,\ldots,\ell_r,0),i,\sigma}$ then $\mathcal{K}_{1-}$ annihilating (C14) for $\ell_{r+1}=0$ results in the same equations for Δ as for $\mathcal{K}_{1-}$ annihilating (C15) if we identify E_{rr+1}^{-+} with E_r^{-}. Thus, from (C13) for $j=r+1,\varepsilon=+,\ell_{r+1}=0$,

$$\mathcal{K}_{1-}|\Delta+1,\underline{\ell}\rangle=0\Rightarrow g_{\underline{\ell}}^{(0)}=-r. \tag{C16}$$

Now that we have determined $g_{\ell}^{(v)}$ in (C9) to be given by (C13) and (C16), we may determine the unitarity bounds for states in $\mathcal{B}^{(\mathrm{T})}$, the simplest descendants. For $\mathcal{H}_d$ and $\ell_1=\cdots=\ell_p>|\ell_{p+1}|$,

$p \leqslant r-1$ then we have that $f^{(v)}_{\underline{\ell}}=0$ in (C9) for $v=-e_1, \varepsilon e_j, e_p$, $j=2,\ldots,p-1$ [here and in the following, this is because the corresponding states $|\Delta+1;\underline{\ell}+\underline{v}\rangle$ for ℓ being on the boundary of the dominant Weyl chamber are null as SO(d) representations] and that

$$\begin{aligned}\Delta &\geqslant \max\{-g^{(e_1)}_{\underline{\ell}}, -g^{(-e_p)}_{\underline{\ell}}, -g^{(e_j)}_{\underline{\ell}}, -g^{(-e_j)}_{\underline{\ell}}, p+1 \leqslant j \leqslant r\} \cup \{-g^{(0)}_{\underline{\ell}} \text{ for } d=2r+1\} \\ &= -g^{(-e_p)}_{\underline{\ell}} = \ell_1 + d - p - 1, \end{aligned} \tag{C17}$$

which matches the first requirement in (3.8). At the unitarity bound $\Delta=\ell_1+d-p-1$ then all the states $|\Delta+1;\underline{\ell}+\underline{v}\rangle$ for $v=-e_1, \varepsilon e_j, 2 \leqslant j \leqslant p$ in $\mathcal{H}_d$ are null.

In even dimensions, for $\ell_1=\cdots=\pm\ell_r$ for $\mathcal{H}_{2r}$ then we have that $f^{(v)}_{\underline{\ell}}=0$ in (C9) for $v=-e_1, \varepsilon e_j, \pm e_r$, $j=2,\ldots,r-1$,

$$\Delta \geqslant \max\{-g^{(e_1)}_{\underline{\ell}}, -g^{(\mp e_r)}_{\underline{\ell}}\} = \ell_1 + r - 1, \tag{C18}$$

with in addition the state $|\Delta+1;\underline{\ell} \mp \underline{e}_r\rangle$ being null at the unitarity bound.

In odd dimensions, for $\ell_1=\cdots=\ell_r>\frac{1}{2}$ for $\mathcal{H}_{2r+1}$ then $f^{(v)}_{\underline{\ell}}=0$ in (C9) for $v=-e_1, \varepsilon e_j, e_r$, $j=2,\ldots,r-1$ and

$$\Delta \geqslant \max\{-g^{(e_1)}_{\underline{\ell}}, -g^{(-e_r)}_{\underline{\ell}}, -g^{(0)}_{\underline{\ell}}\} = \ell_1 + r, \tag{C19}$$

with in addition the state $|\Delta+1, \underline{\ell}-\underline{e}_r\rangle$ being null at the unitarity bound. For $\ell_1=\cdots=\ell_r=\frac{1}{2}$ then $f^{(v)}_{\underline{\ell}}=0$ in (C9) for $v=-e_1, \varepsilon e_j$, $j=2,\ldots,r$ and

$$\Delta \geqslant \max\{-g^{(e_1)}_{\underline{\ell}}, -g^{(0)}_{\underline{\ell}}\} = r = \left[\tfrac{1}{2}d\right], \tag{C20}$$

with the state $|\Delta+1, \underline{\ell}\rangle$ being null at the unitarity bound.

APPENDIX D: EXPANSION AND PRODUCT FORMULAS

In this appendix various formulas from Sec. IV are proven. We make use of a simple property of the function $P^{(d)}(s,x)$ defined for $d=2r$ in (3.19) and $d=2r+1$ in (3.30). Under the action of the Weyl symmetry operator $\mathfrak{W}_d$ (defined in Appendixes A and B) it obeys

$$\mathfrak{W}_d(f(s,x)P^{(d)}(s,x)) = \mathfrak{W}_d(f(s,x))P^{(d)}(s,x), \tag{D1}$$

for any $f(s,x)$, as $P^{(d)}(s,x)$ is invariant under the action of any element of the SO(d) Weyl group, $\mathcal{W}_d$. Note also that $\mathcal{W}_d$ has no effect on the variable s.

We discuss the even dimensional cases of (4.11), (4.14), (4.15) first. For (4.14) we have that

$$\sum_{q=0}^{\infty} s^{\ell+r+q-1}\chi^{(2r)}_{(\ell+q,\ell,\ldots,\pm\ell)}(x) = s^{\ell+r-1}\mathfrak{W}_{2r}\left(\sum_{q=0}^{\infty}(sx_1)^q C^{(2r)}_{(\ell,\ldots,\pm\ell)}(x)\right) = s^{\ell+r-1}\mathfrak{W}_{2r}\left(\frac{1}{1-sx_1}C^{(2r)}_{(\ell,\ldots,\pm\ell)}(x)\right), \tag{D2}$$

which follows just by the definition of the character of the irreducible representation (B4) in terms of the Verma module character (B3). Using (D1) then (D2) may be rewritten as

$$\begin{aligned} &s^{\ell+r-1}P^{(2r)}(s,x)\mathfrak{W}_{2r}\left((1-sx_1^{-1})\prod_{i=2}^{r}(1-sx_i)(1-sx_i^{-1})C^{(2r)}_{(\ell,\ldots,\pm\ell)}(x)\right) \\ &\quad = s^{\ell+r-1}P^{(2r)}(s,x)\sum_{\substack{n_{i-},n_{j+}=0,1 \\ 0\leqslant n=\sum n_{i\varepsilon}\leqslant 2r-2}}(-s)^n\chi^{(2r)}_{(\ell-n_{1-},\ell+n_{2+}-n_{2-},\ldots,\pm\ell+n_{r+}-n_{r-})}(x). \end{aligned} \tag{D3}$$

For $n>0$ in (D3) we may use

$$\chi^{(d)}_{(\ell_1,\ldots,\ell_j,\ell-1,\ell+1,\ell_{j+3},\ldots,\ell_r)}(x) = -\chi^{(d)}_{(\ell_1,\ldots,\ell_j,\ell,\ell,\ell_{j+3},\ldots,\ell_r)}(x), \tag{D4}$$

to show that the contributions for given n reduce to a single one from

$$\begin{gathered}\chi^{(2r)}_{(\ell,\ldots,\ell,\ell-1,\ldots,\ell-1,\pm\ell\mp1)}(x),\\ \uparrow\\ n\text{th position}\end{gathered} \tag{D5}$$

with all contributions for $n>r$ vanishing. Hence we have that (D2) reduces to $\mathcal{D}^{(2r)}_{[\ell+r-1,\ell]_\pm}(s,x)$ defined in (3.26) thus proving (4.14). Notice that (4.11) is a special case of (4.14) when we take $\ell=0$ in the latter [whereby, as mentioned before, $\mathcal{D}^{(2r)}_{[\ell+r-1,\ell]_\pm}(s,x)\to s^{r-1}(1-s^2)P^{(2r)}(s,x)$].

We may prove (4.15) in a very similar way. The sum on the right-hand side of (4.15) may be reduced to

$$s^{\ell+r+j-1}\mathfrak{W}_{2r}\left((1-sx_1)^{-1}\prod_{i=r-j+1}^{r}(1-sx_i)^{-1}(1-sx_i^{-1})^{-1}C^{(2r)}_{(\ell,\ldots,\ell,\ell_1,\ldots,\ell_j)}(x)\right), \tag{D6}$$

in a similar fashion as (D2), when we perform the sums over $p_1,\ldots,p_j,q$. This may be rewritten using (D1) as

$$\begin{aligned}&s^{\ell+r+j-1}P^{(2r)}(s,x)\mathfrak{W}_{2r}\left((1-sx_1)\prod_{i=2}^{r-j}(1-sx_i)(1-sx_i^{-1})C^{(2r)}_{(\ell,\ldots,\ell,\ell_1,\ldots,\ell_j)}(x)\right)\\ &\quad= s^{\ell+r+j-1}P^{(2r)}(s,x)\sum_{\substack{n_{i-},n_{j+}=0,1\\ 0\leqslant n=\sum n_{i\varepsilon}\leqslant 2r-2j-2}}(-s)^n\chi^{(2r)}_{(\ell-n_{1-},\ell+n_{2+}-n_{2-},\ldots,\ell+n_{r-j+}-n_{r-j-},\ell_1,\ldots,\ell_r)}(x).\end{aligned} \tag{D7}$$

For similar reasons as before, for $n>0$ the contributions for given n reduce to a single one from

$$\begin{gathered}\chi^{(2r)}_{(\ell,\ldots,\ell,\ell-1,\ldots,\ell-1,\ell_1,\ldots,\ell_j)}(x),\\ \uparrow\\ n\text{th position}\end{gathered} \tag{D8}$$

so that (D7) equals $\mathcal{D}^{(2r)}_{[\ell+r+j-1,\ell,\ell_1,\ldots,\ell_j]}(s,x)$ in (3.25) for $p=r-j$.

Turning to the odd dimensional cases of (4.27), (4.29), (4.30), (4.31) these may be proven in a very similar way as for the even dimensional cases when we use (D1). Note that we may use the definition of the irreducible character (B8) in terms of the Verma module character (B7) and (3.30) to rewrite the sum on the right-hand side of (4.30) as

$$\begin{aligned}&s^rP^{(2r+1)}(s,x)(1-s)\mathfrak{W}_{2r+1}\left((1-sx_1^{-1})\prod_{i=2}^{r}(1-sx_i)(1-sx_i^{-1})C^{(2r+1)}_{(1/2,\ldots,1/2)}(x)\right)\\ &\quad= s^rP^{(2r+1)}(s,x)(1-s)\chi^{(2r+1)}_{(1/2,\ldots,1/2)}(x),\end{aligned} \tag{D9}$$

which matches (3.34). The free scalar case of (4.29) follows in a similar fashion. The identity (4.27) is in fact equivalent to (4.29). The sum on the right-hand side of (4.31) may be rewritten as

$$s^{\ell+r+j}\mathfrak{W}_{2r+1}\left((1-s)^{-1}(1-sx_1)^{-1}\prod_{i=r-j+1}^{r}(1-sx_i)^{-1}(1-sx_i^{-1})^{-1}C^{(2r+1)}_{(\ell,\ldots,\ell,\ell_1,\ldots,\ell_j)}(x)\right), \tag{D10}$$

when we perform the sums over p_i,q,t. This may be rewritten as

$$s^{\ell+r+j}P^{(2r+1)}(s,x)\mathfrak{W}_{2r+1}\left((1-sx_1)\prod_{i=2}^{r-j}(1-sx_i)(1-sx_i^{-1})C^{(2r+1)}_{(\ell,\ldots,\ell,\ell_1,\ldots,\ell_j)}(x)\right)$$
$$= s^{\ell+r+j}P^{(2r+1)}(s,x)\sum_{\substack{n_{i-},n_{j+}=0,1\\ 0\leqslant n=\sum n_{i\varepsilon}\leqslant 2r-2j-2}}(-s)^n\chi^{(2r+1)}_{(\ell-n_{1-},\ell+n_{2+}-n_{2-},\ldots,\ell+n_{r-j+}-n_{r-j-},\ell_1,\ldots,\ell_r)}(x). \tag{D11}$$

Using (D4), for $n>0$ the contributions for given n reduce to a single one from

$$\chi^{(2r+1)}_{(\ell,\ldots,\ell,\underset{\uparrow}{\ell-1},\ldots,\ell-1,\ell_1,\ldots,\ell_j)}(x), \qquad \begin{matrix}\\ n\text{th position}\end{matrix} \tag{D12}$$

so that (D11) equals $\mathcal{D}^{(2r+1)}_{[\ell+r+j,\ell,\ell_1,\ldots,\ell_j]}(s,x)$ in (3.32) for $p=r-j$.

To prove some product formulas we will use the expansions above and the following:

$$\mathfrak{W}_d(f(x)\chi^{(d)}_\ell(x))=\mathfrak{W}_d(f(x))\chi^{(d)}_\ell(x), \tag{D13}$$

for any $f(x)$.

For even dimensions we now prove (4.22) and (4.23) for $\ell'=\frac{1}{2}$. In this case we have that

$$\mathcal{D}^{(4m+2)}_{[(1/2)+2m;(1/2)]\pm}(s,x)=s^{(1/2)+2m}(\chi^{(4m+2)}_{(1/2,\ldots,1/2,\pm 1/2)}(x)-s\chi^{(4m+2)}_{(1/2,\ldots,1/2,\mp 1/2)}(x)), \tag{D14}$$

where we may determine from (B4) that

$$\chi^{(4m+2)}_{(1/2,\ldots,1/2)}(x)=\prod_{i=1}^{2m+1}x_i^{-1/2}\sum_{\substack{m\geqslant t\geqslant 0\\ 2m+1\geqslant j_1>\cdots>j_{2t+1}\geqslant 1}}x_{j_1}\cdots x_{j_{2t+1}},$$
$$\chi^{(4m+2)}_{(1/2,\ldots,-1/2)}(x)=\prod_{i=1}^{2m+1}x_i^{-1/2}\left(1+\sum_{\substack{m\geqslant t\geqslant 1\\ 2m+1\geqslant j_1>\cdots>j_{2t}\geqslant 1}}x_{j_1}\cdots x_{j_{2t}}\right). \tag{D15}$$

We use (D14) and (4.14) to expand $\mathcal{D}^{(4m+2)}_{[\ell+2m,\ell]\pm}(s,x)$ in (4.22) and then match powers of s on both sides. Clearly the O(1) terms on both sides of (4.22) agree. At O(s^q) for $q\geqslant 1$ we must show that

$$\chi^{(4m+2)}_{(\ell+q,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,-1/2)}(x)-\chi^{(4m+2)}_{(\ell+q-1,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,1/2)}(x)$$
$$=\sum_{\substack{t_i=\ell\pm(1/2)\\ t_i\geqslant t_{i+1}}}\chi^{(4m+2)}_{[\ell+(1/2)+q,\ell+(1/2),t_1,t_1,\ldots,t_{m-1},t_{m-1},\ell-(1/2)]}(x)-\chi^{(4m+2)}_{[\ell+(1/2)+q-2,\ell+(1/2),t_1,t_1,\ldots,t_{m-1},t_{m-1},\ell-(1/2)]}(x). \tag{D16}$$

Using (D13) and (D15) we may rewrite the left-hand side of (D16) as

$$\mathfrak{W}_{(4m+2)}(C^{(4m+2)}_{(\ell+q,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,-1/2)}(x)-C^{(4m+2)}_{(\ell+q-1,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,1/2)}(x))$$
$$=\mathfrak{W}_{4m+2}\left(C^{(4m+2)}_{[\ell+q-(3/2),\ell-(1/2),\ldots,\ell-(1/2)]}(x)(x_1^2-1)\sum_{\substack{m\geqslant t\geqslant 1\\ 2m+1\geqslant j_1>\cdots>j_{2t-1}\geqslant 2}}x_{j_1}\cdots x_{j_{2t-1}}\right). \tag{D17}$$

For $q\geqslant 1$ most of the terms in (D17) vanish under the action of the Weyl symmetry operator and it reduces to

$$\mathfrak{W}_{4m+2}\left(C^{(4m+2)}_{[\ell+q-(3/2),\ell-(1/2),\ldots,\ell-(1/2)]}(x)(x_1^2-1)\sum_{t=1}^{m}x_2x_3\cdots x_{2t}\right), \tag{D18}$$

and from here it is easy to show that this agrees with the right-hand side of (D16).

Similarly, using (D14) and (4.14) to expand $\mathcal{D}^{(4m+2)}_{[\ell+2m,\ell]_\pm}(s,x)$ in (4.23), then matching powers of s on both sides of the equation (4.23) we must show that for $q\geqslant 0$,

$$\begin{aligned}&\chi^{(4m+2)}_{(\ell+q,\ell,\ldots,\varepsilon\ell)}(x)\chi^{(4m+2)}_{[1/2,\ldots,\varepsilon(1/2)]}(x)-\chi^{(4m+2)}_{(\ell+q-1,\ell,\ldots,\varepsilon\ell)}(x)\chi^{(4m+2)}_{[1/2,\ldots,-\varepsilon(1/2)]}(x)\\&\quad=\sum_{\substack{t_i=\ell\pm(1/2)\\ t_i\geqslant t_i+1}}\chi^{(4m+2)}_{[\ell+(1/2)+q,t_1,t_1,\ldots,t_m,\varepsilon t_m]}(x)-\chi^{(4m+2)}_{[\ell+(1/2)+q-2,t_1,t_1,\ldots,t_m,\varepsilon t_m]}(x),\end{aligned} \tag{D19}$$

for $\varepsilon=\pm$. Using (D13) and (D15) we may rewrite the left-hand side of (D19) for $\varepsilon=+$ as

$$\begin{aligned}&\mathfrak{W}_{4m+2}(C^{(4m+2)}_{(\ell+q,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,1/2)}(x)-C^{(4m+2)}_{(\ell+q-1,\ell,\ldots,\ell)}(x)\chi^{(4m+2)}_{(1/2,\ldots,-1/2)}(x))\\&\quad=\mathfrak{W}_{4m+2}\left(C^{(4m+2)}_{[\ell+q-(3/2),\ell-(1/2),\ldots,\ell-(1/2)]}(x)(x_1^2-1)\left(1+\sum_{\substack{m\geqslant t\geqslant 1\\ 2m+1\geqslant j_1>\ldots>j_{2t}\geqslant 2}}x_{j_1}\cdots x_{j_{2t}}\right)\right).\end{aligned} \tag{D20}$$

For $q\geqslant 0$ most of the terms in (D20) vanish under the action of the Weyl symmetry operator and it reduces to

$$\mathfrak{W}_{4m+2}\left(C^{(4m+2)}_{[\ell+q-(3/2)\ell-(1/2),\ldots,\ell-(1/2)]}(x)(x_1^2-1)\left(1+\sum_{t=1}^{m}x_2x_3\cdots x_{2t+1}\right)\right), \tag{D21}$$

and from here it is easy to show that this agrees with the right-hand side of (D19) for $\varepsilon=+$.

We also have that

$$\mathcal{D}^{(4m)}_{[(1/2)+2m-1;(1/2)]_\pm}(s,x)=s^{(1/2)+2m-1}\left(\chi^{(4m)}_{(1/2,\ldots,1/2,\pm 1/2)}(x)-s\chi^{(4m)}_{(1/2,\ldots,1/2,\mp 1/2)}(x)\right), \tag{D22}$$

where,

$$\begin{aligned}\chi^{(4m)}_{(1/2,\ldots,-1/2)}(x)&=\prod_{i=1}^{2m}x_i^{-1/2}\sum_{\substack{m-1\geqslant t\geqslant 0\\ 2m\geqslant j_1>\ldots>j_{2t+1}\geqslant 1}}x_{j_1}\cdots x_{j_{2t+1}},\\ \chi^{(4m)}_{(1/2,\ldots,1/2)}(x)&=\prod_{i=1}^{2m}x_i^{-1/2}\left(1+\sum_{\substack{m\geqslant t\geqslant 1\\ 2m\geqslant j_1>\ldots>j_{2t}\geqslant 1}}x_{j_1}\cdots x_{j_{2t}}\right),\end{aligned} \tag{D23}$$

and this allows similar product formulas in $d=4m$ dimensions to be derived straightforwardly in an analogous fashion as above.

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Optical geometry analysis of the electromagnetic self-force

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We present an analysis of the behavior of the electromagnetic self-force for charged particles in a conformally static spacetime, interpreting the results with the help of optical geometry. Some conditions for the vanishing of the local terms in the self-force are derived and discussed. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The motion of a point particle with mass m, electric charge e, and four-velocity v^a is described by

$$ma_a = K_a + F_a, \tag{1.1}$$

where $a_a := v^b \nabla_b v_a$ is the particle four-acceleration, K_a is the sum of the external four-forces acting on the particle, and F_a accounts for the backreaction of the particle's own electromagnetic field on its motion. [We use latin indices a, b,… from the beginning of the alphabet as abstract indices,[1] while greek letters μ, ν,… denote components in some chart and run from 0 to 3. We work in units in which $G=c=1$, and choose the positive signature for the metric. We follow the conventions of Ref. 1 for the curvature tensors; the Ricci tensor R_{ab} has then the opposite sign than in Refs. 2 and 3.] In contrast to a well-established tradition, we shall avoid referring to F_a as the *radiation reaction*, because such terminology is somehow improper and can be misleading;[4,5] we shall use the term *self-force* instead. According to the classic analysis of DeWitt-Brehme-Hobbs,[2,3] F_a can be written as the sum of two contributions, $F_a = F_a^{(\mathrm{l})} + F_a^{(\mathrm{nl})}$, where

$$F_a^{(\mathrm{l})} = \tfrac{2}{3} e^2 k_a{}^b v^c \nabla_c a_b + \tfrac{1}{3} e^2 k_a{}^b R_{bc} v^c \tag{1.2}$$

and

$$F_a^{(\mathrm{nl})} = e^2 v^b \int_{-\infty}^{\tau} \mathrm{d}\tau' f_{aba'} v^{a'}. \tag{1.3}$$

[The equation of motion obtained putting together (1.1)–(1.3) contains third derivatives of the particle coordinates, and hence leads to unphysical conclusions such as preacceleration and runaway solutions, as it happens for the Lorentz-Dirac equation in flat spacetime.[4] These pathologies can be removed by a reduction-of-order technique.[6] Nevertheless, in the following we shall consider the standard expression (1.2) for $F_a^{(\mathrm{l})}$, that differs from the one so obtained only to higher orders, and is therefore equivalent to it as long as one limits oneself to the classical domain, in

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which the theory is defined.] Here v^a and τ are the four-velocity and proper time of the particle, $k_a{}^b=\delta_a{}^b+v_a v^b$ is the projector onto the three-space orthogonal to v^a, R_{ab} is the Ricci tensor, and $f_{aba'}$ is a bi-tensor associated with the presence of "tails" in the electromagnetic field.[2,7] The term $F_a^{(\mathrm{l})}$ is the relativistic generalization to a curved spacetime of the noncovariant expression $(2/3)e^2\ddot{\mathbf{v}}$ for the self-force,[4,5] and can be regarded as purely local, as it depends only on quantities evaluated at the actual position of the particle. On the contrary, the contribution $F_a^{(\mathrm{nl})}$ depends on the entire past history of the particle and on the property of spacetime of being able to backscatter electromagnetic waves,[2,7] encapsulated in the quantity $f_{aba'}$, and represents therefore an essentially nonlocal contribution. The two terms on the right-hand side of (1.2) are known as the von Laue[4,5] and the Hobbs[3] forces, respectively. We shall denote them as

$$F_a^{(\mathrm{vL})} := \tfrac{2}{3}e^2 k_a{}^b v^c \nabla_c a_b \tag{1.4}$$

and

$$F_a^{(\mathrm{H})} := \tfrac{1}{3}e^2 k_a{}^b R_{bc} v^c, \tag{1.5}$$

so (1.2) can be rewritten as $F_a^{(\mathrm{l})}=F_a^{(\mathrm{vL})}+F_a^{(\mathrm{H})}$. [Noteworthy, the von Laue force can also be written as $F_a^{(\mathrm{vL})}=\frac{2}{3}e^2\nabla_{(v)}^{(\mathrm{FW})}a_a$, where $\nabla_{(v)}^{(\mathrm{FW})}$ is the Fermi-Walker derivative along v^a, which for a generic field of one-forms u_a is[8] $\nabla_{(v)}^{(\mathrm{FW})}u_a := v^b\nabla_b u_a+(a_a v^b - v_a a^b)u_b$. Hence, the von Laue term $F_a^{(\mathrm{vL})}$ vanishes iff the acceleration a_a is Fermi-Walker transported along the particle worldline.] It should be clear from the outset that all this, as well as the treatment that follows, applies to classical point particles—an unrealistic model which presents pathologies, given that the size of a classical object cannot be smaller than its Compton wavelength. The extension to particles of a finite size has been discussed recently.[9]

In the last decade there has been a renewed interest in calculations of self-forces of different nature. The main motivation for such a revival is the possibility to go beyond the test particle approximation when studying motion in a gravitational field, which is important for investigations about the generation of gravitational waves. (For recent reviews, see Ref. 10, and references therein.) However, due to the complexity of the calculations in the gravitational case, several authors have considered simpler models involving the scalar and electromagnetic self-interactions, which are also interesting by themselves. In particular, much attention has been paid to the nonlocal contribution. In this article we shall instead focus on the behavior of the local term $F_a^{(\mathrm{l})}$ for the electromagnetic case, arguing that it can be understood more easily in terms of the so-called optical geometry, rather than of the usual geometry of spacetime. A similar analysis could be carried out for scalar and gravitational self-forces, but we shall not cover such cases here. Also, we leave for further investigation the issue of whether optical geometry could be successfully applied to the challenging problem of computing the nonlocal term (see, however, the end of Sec. V for a brief discussion of this point).

We begin by considering, in the next section, a situation in which the charge moves uniformly on a circular orbit in a static, spherically symmetric spacetime, comparing the results in the special cases of Einstein's universe and Schwarzschild spacetime. For the latter, we shall see that $F_a^{(\mathrm{l})}=0$ at the closed photon orbit $r=3M$. This property will be interpreted in Sec. III by introducing the notion of optical geometry, in which light paths on $t=$const hypersurfaces are geodesics. In Sec. IV we generalize the analysis to an arbitrary conformally static spacetime, showing that if a charge moves with constant speed along a possible light path, the self-force is the one associated with optical geometry (apart from an obvious conformal rescaling), and providing other conditions for the different parts of the self-force to vanish. Section V contains a brief summary of the results.

II. UNIFORM CIRCULAR MOTION IN STATIC SPHERICALLY SYMMETRIC SPACETIMES

Let us begin by discussing a rather special, but highly significant case. Consider a charge moving on a circular orbit $r=\text{const}$ in the plane $\theta=\pi/2$ of a static, spherically symmetric spacetime, with metric

$$g=-e^{2\Phi(r)}\mathrm{d}t^2+\alpha(r)\mathrm{d}r^2+r^2(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\varphi^2), \tag{2.1}$$

where Φ and α are known functions, with α positive. The components of the four-velocity are

$$v^\mu=\Gamma(\delta^\mu_t+\Omega\delta^\mu_\varphi), \tag{2.2}$$

where Ω is a parameter and $\Gamma=(e^{2\Phi}-\Omega^2r^2)^{-1/2}$ is fixed by the normalization $v_\mu v^\mu=-1$. It is convenient to introduce the velocity $v=e^{-\Phi}\Omega r$ measured by static observers, and the corresponding Lorentz factor $\gamma:=(1-v^2)^{-1/2}=e^{\Phi}\Gamma$.

If the motion is uniform, i.e., $\Omega=\text{const}$, the only nonvanishing component of the acceleration is

$$a_r=\Gamma^2\left(e^{2\Phi}\frac{\mathrm{d}\Phi}{\mathrm{d}r}-\Omega^2r\right), \tag{2.3}$$

and the von Laue force is given by

$$F^{(\mathrm{vL})}_\mu=\frac{2}{3}e^2\gamma^5\Omega r\frac{e^{-\Phi}}{\alpha}\left(1-r\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right)\left(e^{2\Phi}\frac{\mathrm{d}\Phi}{\mathrm{d}r}-\Omega^2r\right)(-\Omega\delta^t_\mu+\delta^\varphi_\mu). \tag{2.4}$$

The Hobbs term is

$$F^{(\mathrm{H})}_\mu=\tfrac{1}{3}e^2\gamma^3\Omega e^{-\Phi}(e^{-2\Phi}r^2R_{tt}+R_{\varphi\varphi})(-\Omega\delta^t_\mu+\delta^\varphi_\mu), \tag{2.5}$$

where

$$R_{tt}=\frac{e^{2\Phi}}{\alpha}\left(\frac{\mathrm{d}^2\Phi}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}\Phi}{\mathrm{d}r}+\left(\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right)^2-\frac{1}{2\alpha}\frac{\mathrm{d}\Phi}{\mathrm{d}r}\frac{\mathrm{d}\alpha}{\mathrm{d}r}\right) \tag{2.6}$$

and

$$R_{\varphi\varphi}=1-\frac{1}{\alpha}+\frac{r}{\alpha}\left(\frac{1}{2\alpha}\frac{\mathrm{d}\alpha}{\mathrm{d}r}-\frac{\mathrm{d}\Phi}{\mathrm{d}r}\right) \tag{2.7}$$

are the only relevant nonvanishing components of the Ricci tensor. [The component $R_{\varphi\varphi}$ in (2.7) is evaluated at $\theta=\pi/2$. The general expression for $R_{\varphi\varphi}$ contains an overall extra coefficient $\sin^2\theta$.] Because of the rather complicated dependence on Φ, α, and their derivatives, it is more instructive to focus on two particular cases.

A. Einstein's universe

The metric of Einstein's static universe corresponds to $\Phi=0$ and $\alpha(r)=(1-r^2/R^2)^{-1}$, where R is a positive parameter (the "radius" of the three-dimensional spherical space). The coordinate $r\in[0,R[$, however, does not cover the whole manifold, so it is convenient to introduce a new variable $\chi\in[0,\pi]$ defined through $r=R\sin\chi$. The metric then takes the form

$$g=-\mathrm{d}t^2+R^2\mathrm{d}\chi^2+R^2\sin^2\chi(\mathrm{d}\theta^2+\sin^2\theta\,\mathrm{d}\varphi^2), \tag{2.8}$$

showing that $R\chi$ measures the proper distance from the point $\chi=0$. The function α becomes $\alpha(\chi)=1/\cos^2\chi$, and the only nonvanishing component of the acceleration is

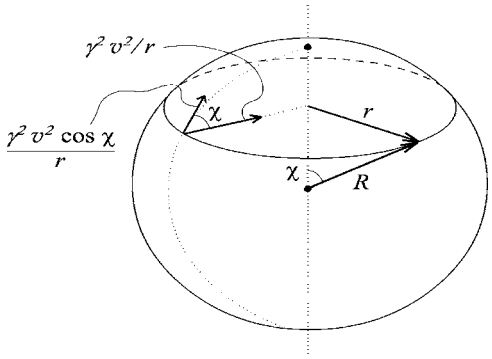

FIG. 1. Embedding diagram for the surface $t=$const, $\theta=\pi/2$ in Einstein's universe, showing the geometrical meaning of the quantities R, r, and χ. The centripetal acceleration of a particle moving at $r=$const is given by the tangential component of the acceleration in the fictitious three-dimensional Euclidean space. For $\chi<\pi/2$ the centripetal acceleration points in the direction of decreasing r, while for $\pi/2<\chi<\pi$ it points in the direction of increasing r.

$$a_\chi = \frac{\partial r}{\partial \chi} a_r = -\frac{\Omega^2 R^2 \sin\chi\cos\chi}{1-\Omega^2 R^2 \sin^2\chi}. \tag{2.9}$$

The magnitude (with sign) of the acceleration is $\gamma^2(v^2/r)\cos\chi$, so the acceleration differs from the special relativistic expression $\gamma^2 v^2/r$ only by the factor $\cos\chi$, whose origin can be easily understood by looking at Fig. 1. Note that the acceleration for orbits with $\chi\in\,]\pi/2,\pi[$ has the opposite sign than for those with $\chi\in\,]0,\pi/2[$, and vanishes when $\chi=\pi/2$.

The von Laue force is

$$F_\mu^{(\mathrm{vL})} = \tfrac{2}{3} e^2 \gamma^5 \Omega^3 R^2 \sin^2\chi\cos^2\chi(-\Omega\delta_\mu^t + \delta_\mu^\varphi). \tag{2.10}$$

It also vanishes for $\chi=\pi/2$, but does not exhibit any change in sign.

Finally, let us compute the Hobbs force. The components of the Ricci tensor can be evaluated directly from expressions (2.6) and (2.7), or simply remembering that the symmetries of Einstein's universe imply $R_{\mu\nu}=(2/R^2)h_{\mu\nu}$, where

$$h = (1-r^2/R^2)^{-1}\mathrm{d}r^2 + r^2(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2) = R^2\mathrm{d}\chi^2 + R^2\sin^2\chi(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2) \tag{2.11}$$

is the metric tensor on the $t=$const hypersurfaces.[11] Thus, we have

$$F_\mu^{(\mathrm{H})} = \tfrac{2}{3} e^2 \gamma^3 \Omega \sin^2\chi(-\Omega\delta_\mu^t + \delta_\mu^\varphi). \tag{2.12}$$

This expression is nonvanishing for all nontrivial values of χ. Therefore, the local part of the self-force,

$$F_\mu^{(\mathrm{l})} = \tfrac{2}{3} e^2 \gamma^5 \Omega \sin^2\chi(1+\Omega^2 R^2\cos 2\chi)(-\Omega\delta_\mu^t + \delta_\mu^\varphi), \tag{2.13}$$

never vanishes, in spite of the fact that when the motion takes place on the spatial geodesic $\chi=\pi/2$, the von Laue force does.

B. Schwarzschild spacetime

In Schwarzschild spacetime,

$$\Phi = \frac{1}{2}\ln\left(1-\frac{2M}{r}\right) \tag{2.14}$$

and $\alpha=e^{-2\Phi}$. Then, from Eq. (2.3) we obtain

$$a_r = \Gamma^2\left(\frac{M}{r^2} - \Omega^2 r\right) = \frac{M - \Omega^2 r^3}{r(r - 2M - \Omega^2 r^3)} \tag{2.15}$$

and, from (2.4),

$$F_\mu^{(\mathrm{vL})} = \frac{2}{3}e^2\gamma^5\Omega r\left(1 - \frac{2M}{r}\right)^{-3/2}\left(1 - \frac{3M}{r}\right)\left(\frac{M}{r^2} - \Omega^2 r\right)(-\Omega\delta_\mu^t + \delta_\mu^\varphi). \tag{2.16}$$

Since $R_{ab}=0$, the Hobbs force vanishes identically, so $F_\mu^{(\mathrm{l})}=F_\mu^{(\mathrm{vL})}$.

Let us now study the behavior of a_r and $F_\mu^{(\mathrm{l})}$ for different values of r. When r/M is very large (Newtonian gravity), Eq. (2.15) can be approximated as

$$a_r \approx \gamma^2\left(\frac{M}{r^2} - \Omega^2 r\right). \tag{2.17}$$

Apart from the factor γ^2, which represents only special-relativistic corrections, the norm of a_a is just the difference between the gravitational and the centripetal accelerations in Newtonian mechanics. This agrees with the physical interpretation of a_a, which represents the thrust per unit mass that must be applied to the particle in order to keep it at the fixed value of r with angular velocity Ω. In particular, $a_a=0$ for a Keplerian motion, $\Omega^2=\Omega_K(r)^2 := M/r^3$ or $r=r_K(\Omega) := (M/\Omega^2)^{1/3}$. In the same approximation,

$$F_\mu^{(\mathrm{l})} \approx \frac{2}{3}e^2\Omega r\gamma^5\left(\frac{M}{r^2} - \Omega^2 r\right)(-\Omega\delta_\mu^t + \delta_\mu^\varphi). \tag{2.18}$$

The local part of the self-force behaves then in the following way: When the motion is Keplerian it vanishes, consistent with the fact that $a_a=0$; in the super-Keplerian regime $[\Omega^2>\Omega_K(r)^2$ or $r>r_K(\Omega)]$ it points backward with respect to the direction of motion; finally, in the sub-Keplerian regime $[\Omega^2<\Omega_K(r)^2$ or $r<r_K(\Omega)]$ it points forward with respect to the direction of motion. In the particular case of a static charge, $\Omega=0$ and $F_\mu^{(\mathrm{l})}=0$.

It is interesting to note that this behavior is peculiar to gravity and has no counterpart for motion in other central fields such as, e.g., a Coulomb one. This is easily seen by computing the self-force associated with circular motion in Minkowski spacetime,

$$F_\mu \equiv F_\mu^{(\mathrm{l})} = -\tfrac{2}{3}e^2\Omega^3 r^2\gamma^5(-\Omega\delta_\mu^t + \delta_\mu^\varphi), \tag{2.19}$$

where the second equality follows immediately from (2.16) with $M=0$ (see also Ref. 12, where this expression is derived explicitly for the case of synchrotron radiation). Now, the self-force always points backward with respect to the direction of motion, regardless of the magnitude of Ω. This is related to the fact that the right-hand side of Eq. (2.19) does not contain any indication about the central force responsible for keeping the charge on circular motion, contrary to what happens in the gravitational case, where a term M/r^2 appears together with $\Omega^2 r$. The combination $M/r^2-\Omega^2 r$ is the same that appears in a_r—see Eq. (2.15)—and is ultimately linked to the association between gravity and curvature. Thus, although for most purposes one can think of Newtonian gravity as a field on a flat background, the present analysis shows that this picture would lead to incorrect conclusions as far as the self-force is concerned. [Apparently, this point is not appreciated in the extant literature. See, e.g., Ref. 4, p. 183, for an explicit statement that the Newtonian and Coulomb problems are alike.]

Let us come back to the analysis of a_r and $F_\mu^{(\mathrm{l})}$. For $r>3M$ the qualitative behavior of these quantities at different values of r is like in the Newtonian limit examined above, even when r/M is not large. However, it is easily seen from Eqs. (2.15) and (2.16) that when $r=3M$, $a_r=(3M)^{-1}$ and $F_\mu^{(\mathrm{l})}=0$. Thus, the thrust needed in order to keep a particle on the closed photon orbit does not depend on the particle speed.[13] Furthermore, if the particle is charged, the local part of the self-force vanishes, in spite of the fact that motion takes place on a circle and is not geodesic. [This point is related to earlier results.[14]] Finally, for orbits with $2M<r<3M$, it follows from

(2.16) that the local part of the self-force always points backward with respect to the direction of motion. Since such orbits are necessarily sub-Keplerian, as follows from the inequality

$$(\Omega^2 - \Omega_K(r)^2)r^2 < 1 - 3M/r, \tag{2.20}$$

this behavior is the opposite than for $r > 3M$. [Proof of (2.20): Consider the condition $2M/r + \Omega^2 r^2 < 1$, which guarantees that Γ be real or, equivalently, that the particle worldline be timelike; subtract $\Omega_K(r)^2 r^2$ from both sides, and use the definition $\Omega_K(r)^2 := M/r^3$.]

III. OPTICAL GEOMETRY

The behavior of a_r can be understood in the following way. The component a_r of the acceleration, given by expression (2.15), is proportional to the thrust necessary to keep the particle on its orbit, and can be written as the difference between a gravitational part $a_r^{(g)}$, independent of Ω, and a centripetal part $a_r^{(c)}$:

$$a_r^{(g)} = \frac{M}{r^2(1 - 2M/r)}, \tag{3.1}$$

$$a_r^{(c)} = \Omega^2 r \, \frac{r - 3M}{(1 - 2M/r)(r - 2M - \Omega^2 r^3)}. \tag{3.2}$$

(Of course, $a_r^{(g)}$ and $a_r^{(c)}$ have signs opposite to those of the gravitational and centripetal forces. Alternatively, one can identify $a_r^{(c)}$ with the centrifugal field acting on the particle in the comoving frame.) It is then evident from (3.2) that the centripetal force vanishes at $r = 3M$, for which $a_r = a_r^{(g)} = (3M)^{-1}$. In addition, (3.2) predicts that $a_r^{(c)}$ has an opposite sign in the regions $r > 3M$ and $r < 3M$.

These properties admit a simple explanation if one imagines that the particle motion takes place in the so-called optical spacetime,[15] with a metric $\tilde{g} = (1 - 2M/r)^{-1} g$, under the action of a "gravitational potential" Φ given by (2.14), which produces a "gravitational field"[16]

$$\tilde{\mathrm{g}}_\mu = - k_\mu{}^\nu \nabla_\nu \Phi = - \left(1 - \frac{2M}{r}\right)^{-1} \frac{M}{r^2} \delta^r_\mu. \tag{3.3}$$

We have then $a_r^{(g)} = -\tilde{\mathrm{g}}_r$ and, in the optical spacetime, the magnitude of the gravitational field is given by the simple Newtonian expression $(\tilde{g}^{\mu\nu} \tilde{\mathrm{g}}_\mu \tilde{\mathrm{g}}_\nu)^{1/2} = M/r^2$. Also, defining $\tilde{v}^\mu := (1 - 2M/r)^{1/2} v^\mu$, so that $\tilde{g}_{\mu\nu} \tilde{v}^\mu \tilde{v}^\nu = -1$, one gets

$$\tilde{a}_\mu = \tilde{g}_{\mu\sigma} \tilde{v}^\nu \tilde{\nabla}_\nu \tilde{v}^\sigma = - \frac{\Gamma^2 \Omega^2 (r - 3M)}{1 - 2M/r} \delta^r_\mu, \tag{3.4}$$

and $a_r^{(c)} = \tilde{a}_r$. The magnitude of the acceleration in optical spacetime is

$$(\tilde{g}^{\mu\nu} \tilde{a}_\mu \tilde{a}_\nu)^{1/2} = \Gamma^2 \Omega^2 |r - 3M|. \tag{3.5}$$

The presence of the factor $(r - 3M)$ in $a_r^{(c)}$ can be understood intuitively[17] considering an embedding diagram[18] of the section $\theta = \pi/2$ of the optical space $(\mathcal{S}, \tilde{h}_{ab})$, where $\mathcal{S}$ is any $t = \text{const}$ hypersurface of the Schwarzschild spacetime, and the metric $\tilde{h}_{ab}$ has the coordinate representation[15]

$$\tilde{h} = \left(1 - \frac{2M}{r}\right)^{-2} \mathrm{d}r^2 + \left(1 - \frac{2M}{r}\right)^{-1} r^2 (\mathrm{d}\theta^2 + \sin^2 \theta \, \mathrm{d}\varphi^2) \tag{3.6}$$

(see Fig. 2 and the Appendix).

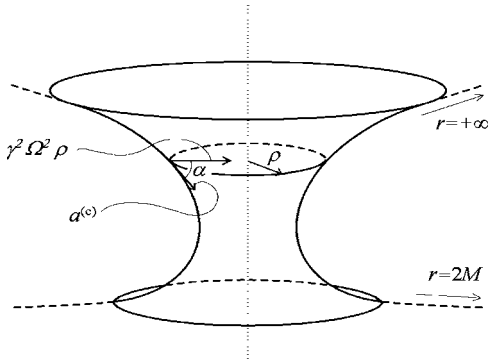

FIG. 2. Embedding diagram for part of the surface $t=\text{const}$, $\theta=\pi/2$ in Schwarzschild spacetime, with the optical geometry. The throat corresponds to $r=3M$. The centripetal acceleration of a particle moving at $r=\text{const}$ is given by the tangential component of the acceleration in the fictitious three-dimensional Euclidean space. Notice that for $r>3M$ the centripetal acceleration points in the direction of decreasing r, while for $2M<r<3M$ it points in the direction of increasing r.

Let us now consider the self-force. The von Laue term associated with the optical quantities has the components

$$\tilde{F}_\mu^{(\mathrm{vL})}=-\frac{2}{3}e^2\gamma^5\Omega^3r^2\left(1-\frac{2M}{r}\right)^{-2}\left(1-\frac{3M}{r}\right)^2(-\Omega\delta_\mu^t+\delta_\mu^\varphi), \tag{3.7}$$

so it always points backward with respect to the direction of motion, vanishes only at $r=3M$, and reduces to (2.19) in the region $r\gg M$. The Hobbs force in the optical space can be computed either directly, or by using the transformation formula (2.11) of Ref. 19. Its components are

$$\tilde{F}_\mu^{(\mathrm{H})}=\frac{2}{3}e^2\gamma^3\Omega\frac{M}{r}\left(1-\frac{2M}{r}\right)^{-1}\left(1-\frac{3M}{r}\right)(-\Omega\delta_\mu^t+\delta_\mu^\varphi). \tag{3.8}$$

For $r\gg M$, this becomes

$$\tilde{F}_\mu^{(\mathrm{H})}\approx\frac{2}{3}e^2\gamma^3\Omega\frac{M}{r}(-\Omega\delta_\mu^t+\delta_\mu^\varphi). \tag{3.9}$$

Note that the magnitude of the von Laue force is proportional to Ω^3r, like in Minkowski space, while the magnitude of the Hobbs force is proportional to $M\Omega/r^2$, which can be rewritten as M/r^3 times the speed Ωr. Thus, from the perspective offered by optical geometry, the coefficient

$$\frac{M}{r^2}-\Omega^2r$$

that appears in Eq. (2.18) should not be regarded as representing the difference between the gravitational and the centripetal forces, because the first term actually arises from the *curvature* of $(\mathcal{S},\tilde{h}_{ab})$. The same coefficient is present for uniform circular motion at $r=\text{const}$ on $(\mathcal{S},\tilde{h}_{ab})$, regardless of the nature (gravitational or other) of the "central" force. Therefore, when the local part of the self-force is analyzed in optical geometry, the puzzling peculiarity of gravity that was noticed in Sec. II B disappears.

It is worth pointing out that $F_\mu^{(\mathrm{l})}$, $\tilde{F}_\mu^{(\mathrm{vL})}$, and $\tilde{F}_\mu^{(\mathrm{H})}$ all vanish at $r=3M$, as it follows from Eqs. (2.16), (3.7), and (3.8). However, while the property $\tilde{F}_\mu^{(\mathrm{vL})}(3M)=0$ is natural from the point of view of optical geometry, because the circle $r=3M$ is a geodesic of $(\mathcal{S},\tilde{h}_{ab})$ and the charge motion is uniform, the fact that also $\tilde{F}_\mu^{(\mathrm{H})}(3M)=0$—hence $F_\mu^{(\mathrm{l})}(3M)=0$—is due to the algebraic properties

of the optical Ricci tensor at $r=3M$ rather than to the geodesic character in $(\mathcal{S},\tilde{h}_{ab})$ of the closed photon orbit (see Sec. IV B). Therefore, the change of sign of $F^{(\mathrm{l})}_{\mu}$ at $r=3M$ has a different origin than for other phenomena in which a similar "reversal" takes place.[20]

IV. GENERAL RESULTS

If $(\mathcal{M},g_{ab})$ and $(\mathcal{M},\tilde{g}_{ab})$ are two conformally related spacetimes, with

$$\tilde{g}_{ab}=e^{-2\Phi}g_{ab}, \tag{4.1}$$

the local and nonlocal parts of the corresponding self forces are related as $F^{(\mathrm{l})}_a=e^{-\Phi}\tilde{F}^{(\mathrm{l})}_a$ and $F^{(\mathrm{nl})}_a=e^{-\Phi}\tilde{F}^{(\mathrm{nl})}_a$.[19] Then, in order to compute $F^{(\mathrm{l})}_a$ or $F^{(\mathrm{nl})}_a$, one can work in a conformally related spacetime $(\mathcal{M},\tilde{g}_{ab})$ rather than in the physical one $(\mathcal{M},g_{ab})$. We now use this remark to put the results of Sec. II into a more general context extending the line of reasoning outlined in Sec. III, and to establish some extra necessary and/or sufficient conditions for the different parts of $F^{(\mathrm{l})}_a$ to vanish.

Let us consider a charge with four-velocity v^a in an arbitrary conformally static spacetime $(\mathcal{M},g_{ab})$. [This restriction is motivated mainly by simplicity. Optical geometry can be straightforwardly defined also for conformally stationary spacetimes,[21] and has been extended even to cases where no global time symmetry exists, as it happens in gravitational collapse.[22] For recent results concerning generalizations of optical geometry, see Ref. 23.] By definition, such a spacetime admits a hypersurface-orthogonal timelike conformal Killing vector field $\eta=\partial/\partial t$, corresponding to a conformal Killing time t. One can then define the scalar function

$$\Phi:=\tfrac{1}{2}\ln(-g_{ab}\eta^a\eta^b) \tag{4.2}$$

and consider the ultrastatic spacetime $(\mathcal{M},\tilde{g}_{ab})$ with $\tilde{g}_{ab}$ given by (4.1), in which η^a is a Killing vector field with unit norm, $\pounds_\eta\tilde{g}_{ab}=0$ and $\tilde{g}_{ab}\eta^a\eta^b=-1$.[24] It is not difficult to check that the projection, along the integral curves of η^a, of null geodesics of $(\mathcal{M},g_{ab})$ onto the spatial hypersurfaces $\mathcal{S}$ defined by the condition $t=$const, are geodesics of $(\mathcal{S},\tilde{h}_{ab})$, where $\tilde{h}_{ab}:=\tilde{g}_{ab}+\eta_a\eta_b$ and $\eta_a:=\tilde{g}_{ab}\eta^b$. Hence, generalizing what we have done in Sec. III, all quantities pertaining to the spacetime $(\mathcal{M},\tilde{g}_{ab})$ will be denoted as "optical." Instead of $F^{(\mathrm{l})}_a$, we can then consider $\tilde{F}^{(\mathrm{l})}_a$, computed in the optical spacetime $(\mathcal{M},\tilde{g}_{ab})$ starting from the rescaled four-velocity $\tilde{v}^a=e^{\Phi}v^a$.

At any point on the particle worldline, $\tilde{v}^a$ can be decomposed in a unique way as

$$\tilde{v}^a=\gamma(\eta^a+v\tilde{\tau}^a), \tag{4.3}$$

where $v\in\,]-1,1[$ is the speed of the particle according to an observer with four-velocity parallel to η^a, the coefficient $\gamma:=(1-v^2)^{-1/2}$ is the corresponding Lorentz factor, and $\tilde{\tau}^a$ is a spacelike vector orthogonal to η^a, such that $\tilde{g}_{ab}\tilde{\tau}^a\tilde{\tau}^b=1$. The four-acceleration $\tilde{a}_a:=\tilde{v}^b\tilde{\nabla}_b\tilde{v}_a$ of the particle in the optical spacetime $(\mathcal{M},\tilde{g}_{ab})$ is then

$$\tilde{a}_a=\gamma^2\tilde{T}_a\tilde{v}^b\tilde{\nabla}_b v+\gamma^2v^2\tilde{\tau}^b\tilde{\nabla}_b\tilde{\tau}_a+\gamma^2v\,\eta^b\tilde{\nabla}_b\tilde{\tau}_a, \tag{4.4}$$

where

$$\tilde{T}^a:=\frac{\tilde{k}^a{}_b\tilde{\tau}^b}{\sqrt{\tilde{k}_{cd}\tilde{\tau}^c\tilde{\tau}^d}}=\gamma(\tilde{\tau}^a+v\,\eta^a) \tag{4.5}$$

is a unit vector in $(\mathcal{M},\tilde{g}_{ab})$, orthogonal to $\tilde{v}^a$. Using now the orthogonality condition $\eta^a\tilde{\tau}_a=0$, and the property $\tilde{\nabla}_b\eta_a=0$ that follows from the fact that $(\mathcal{M},\tilde{g}_{ab})$ is ultrastatic, we have

$$\tilde{\nabla}_b\tilde{\tau}_a=\tilde{\mathrm{D}}_b\tilde{\tau}_a-\eta_b\eta^c\tilde{\nabla}_c\tilde{\tau}_a, \tag{4.6}$$

where $\tilde{\mathrm{D}}_b$ is the covariant derivative along directions orthogonal to η^a, hence on $(\mathcal{S},\tilde{h}_{ab})$. In order for both Eqs. (4.4) and (4.6) to make sense, one needs to know $\tilde{\tau}^a$ off the particle worldline. The

natural extension of $\tilde{\tau}^a$ is such that its integral curves (located on $t=$const hypersurfaces) coincide with the projection on $\mathcal{S}$ of the particle worldline along the integral curves of η^a. This is equivalent to requiring that $\pounds_\eta \tilde{\tau}^a = 0$, i.e., that $\eta^b \tilde{\nabla}_b \tilde{\tau}^a = \tilde{\tau}^b \tilde{\nabla}_b \eta^a$, and the latter quantity vanishes in an ultrastatic spacetime. Hence, $\eta^b \tilde{\nabla}_b \tilde{\tau}_a = 0$, and the particle acceleration in optical spacetime takes the very simple form

$$\tilde{a}_a = \gamma^2 \tilde{T}_a \tilde{v}^b \tilde{\nabla}_b v + \gamma^2 v^2 \tilde{\tau}^b \tilde{\mathrm{D}}_b \tilde{\tau}_a, \tag{4.7}$$

in which one can identify a tangential and an orthogonal (centripetal) component.[16]

The relationship[19]

$$\tilde{a}_a = a_a - k_a{}^b \nabla_b \Phi \tag{4.8}$$

generalizes the result, already obtained in Sec. III for the special case of Schwarzschild spacetime, according to which one can write the particle acceleration in optical spacetime, $\tilde{a}_a$, as the sum between the nongravitational thrust per unit mass, a_a, and a gravitational force per unit mass, $\tilde{\mathrm{g}}_a = -k_a{}^b \nabla_b \Phi$:

$$\tilde{a}_a = a_a + \tilde{\mathrm{g}}_a. \tag{4.9}$$

Equation (4.9) contains a precise formulation of the equivalence principle, because the quantity that is physically measurable at the particle location—the thrust, proportional to a_a—allows one only to determine the difference $\tilde{a}_a - \tilde{\mathrm{g}}_a$ between $\tilde{a}_a$ and $\tilde{\mathrm{g}}_a$, but not $\tilde{a}_a$ and $\tilde{\mathrm{g}}_a$ separately (unless one possesses extra knowledge, of a nonlocal nature, about the structure of the spacetime under consideration). [In particular, the two situations with $\tilde{a}_a = a_a$ and $\tilde{\mathrm{g}}_a = 0$, or with $\tilde{a}_a = 0$ and $\tilde{\mathrm{g}}_a = -a_a$, cannot be distinguished by a measurement of the thrust.] Inserting (4.7) into (4.9), and identifying $-\gamma^2 \tilde{T}_a \tilde{v}^b \tilde{\nabla}_b v$ and $-\gamma^2 v^2 \tilde{\tau}^b \tilde{\mathrm{D}}_b \tilde{\tau}_a$ with suitable inertial forces per unit mass,[16,25] one finds a general relativistic version of the statement, commonly expressed within the framework of Newtonian mechanics, that in a frame comoving with the particle there is perfect balance between the nongravitational thrust, the gravitational force, and the inertial forces acting on the particle.

On replacing (4.7) into the definition of $\tilde{F}_a^{(1)}$ one can find the local part of the self-force expressed in terms of v and $\tilde{\tau}^a$, that characterize the motion in optical spacetime $(\mathcal{M}, \tilde{g}_{ab})$. However, since the general expression is not particularly illuminating, let us focus instead on the most interesting particular cases.

A. Uniform motion along optical geodesics

It is obvious from Eq. (4.7) that a particle which moves uniformly (i.e., with $\tilde{v}^b \tilde{\nabla}_b v = 0$) along optical geodesics of space (so that $\tilde{\tau}^b \tilde{\mathrm{D}}_b \tilde{\tau}_a = 0$) has vanishing acceleration in $(\mathcal{M}, \tilde{g}_{ab})$, that is, $\tilde{a}_a = 0$. Then $\tilde{F}_a^{(1)}$ consists only of the Hobbs term and we can write

$$F_a = e^{-\Phi} \left(\frac{1}{3} e^2 k_a{}^b \tilde{R}_{bc} \tilde{v}^c + e^2 \tilde{v}^b \int_{-\infty}^{\tilde{\tau}} \mathrm{d}\tilde{\tau}' \tilde{f}_{aba'} \tilde{v}^{a'} \right). \tag{4.10}$$

Thus, the particle is indeed subjected to a self-force, but just to the one that is associated with the geometric properties of the optical space. In a sense, the charge "feels" the geometry of $(\mathcal{M}, \tilde{g}_{ab})$ rather than the one of the physical spacetime $(\mathcal{M}, g_{ab})$.

It may be interesting to note that, with the only exception of ultrastatic spacetimes, for which the ordinary and the optical geometries simply coincide, there are no lines in the ordinary space $(\mathcal{S}, h_{ab})$ such that the von Laue term vanishes identically for a charge that moves uniformly along them. On the contrary, in $(\mathcal{S}, \tilde{h}_{ab})$ the conditions that $v=$const and $\tilde{F}_a^{(\mathrm{vL})} = 0$ uniquely select optical geodesics.

B. Special metrics

If $k_a{}^b\widetilde{R}_{bc}\tilde{v}^c=0$, then expression (4.10) implies that $F_a=F_a^{(\mathrm{nl})}$, because $F_a^{(\mathrm{l})}$ and $F_a^{(\mathrm{nl})}$ do not mix under a conformal transformation.[19] [For a more general, nonuniform motion, one finds $\widetilde{F}_a^{(\mathrm{l})}=\widetilde{F}_a^{(\mathrm{vL})}$.] This can happen iff $\widetilde{R}_a{}^b\tilde{v}_b=\lambda\tilde{v}_a$ for some λ, and it is easy to see, by contracting this equation with η^a and noting that $\eta^a\widetilde{R}_a{}^b=0$ in an ultrastatic spacetime, that it must be $\lambda=0$. Using again the decomposition (4.3) and the property $\widetilde{R}_{ab}\eta^b=0$, one finally finds that the Hobbs term vanishes iff $v\widetilde{R}_a{}^b\tilde{\tau}_b=0$. Thus, excluding the trivial case $v=0$, there is no local self-force for uniform motion along optical geodesics whose directions are eigenvectors of $\widetilde{R}_a{}^b$ with zero eigenvalue. Such directions exist iff the determinant of the matrix made by the components $\widetilde{R}_i^j$ with $i,j=1,2,3$ is zero, i.e., iff such matrix is degenerate.

Let us reconsider the examples of Sec. II in the light of this conclusion. For the Einstein universe, $\widetilde{R}_i^j=R_i^j=(2/R^2)\delta_i^j$, which is always nondegenerate. For Schwarzschild spacetime,

$$\widetilde{R}_{\varphi i}=\frac{2M}{r}\left(1-\frac{2M}{r}\right)^{-1}\left(1-\frac{M}{r}(2+\sin^2\theta)\right)\delta_i^{\varphi} \tag{4.11}$$

and, for $\theta=\pi/2$, $\widetilde{R}_i^j$ becomes degenerate at $r=3M$. Hence, $F_a^{(\mathrm{l})}$ vanishes at $r=3M$ for uniform motion in an equatorial plane along *any* optical geodesic, not only for the circular orbit considered in Sec. II B. This result is far from trivial, but its derivation is rather straightforward working in the optical space.

C. Geodesic motion

For charges following a geodesic in $(\mathcal{M},g_{ab})$ the four-acceleration a_a vanishes, so the von Laue term $F_a^{(\mathrm{vL})}$ is identically zero. [We avoid referring to this situation as "free fall," because the latter would be appropriately identified by the vanishing of the external force in Eq. (1.1), $K_a=0$, whereas geodesic motion corresponds to $K_a+F_a=0$.] In optical geometry this result is not obvious, because it follows from a compensation between contributions coming from the "optical" von Laue and Hobbs terms. More precisely, applying (4.8) to this case one immediately finds $\tilde{a}_a=-k_a{}^b\nabla_b\Phi$. Then, the von Laue term $\widetilde{F}_a^{(\mathrm{vL})}$ in optical space contains first and second derivatives of Φ, that are canceled by identical contributions coming from the Hobbs term $\widetilde{F}_a^{(\mathrm{H})}$, because of the way the Ricci tensor changes under a conformal transformation.[19]

Thus, from the perspective of optical geometry, the fact that $F_a^{(\mathrm{vL})}=0$ just when $\tilde{a}_a=-k_a{}^b\nabla_b\Phi$ is somewhat surprising. For example, it is not evident that $\widetilde{F}_a^{(\mathrm{l})}=0$ for the Keplerian motions of Sec. II B because in optical geometry, where gravity is described by the physical field Φ, Keplerian motions have nothing qualitatively different from, say, orbits in a Coulomb field. In fact, it turns out that it is only thanks to a cancellation between the von Laue and the Hobbs terms in the optical geometry that $\widetilde{F}_a^{(\mathrm{l})}=0$. However, if one thinks that for a Keplerian motion in Schwarzschild spacetime $F_a^{(\mathrm{vL})}=F_a^{(\mathrm{H})}=0$, and that $\widetilde{F}_a^{(\mathrm{l})}=\mathrm{e}^{\Phi}F_a^{(\mathrm{l})}$, then such a compensation is only expected. Geodesics in $(\mathcal{M},g_{ab})$ are not geodesics in $(\mathcal{M},\tilde{g}_{ab})$, so $\widetilde{F}_a^{(\mathrm{vL})}$ does not vanish in general, and since $\widetilde{R}_{ab}\neq 0$, the Hobbs force $\widetilde{F}_a^{(\mathrm{H})}$ also does not vanish. Nevertheless, $\widetilde{F}_a^{(\mathrm{vL})}$ and $\widetilde{F}_a^{(\mathrm{H})}$ combine to form a vanishing local self-force, $\widetilde{F}_a^{(\mathrm{l})}=0$.

This remark should not be regarded as a drawback of the description based on optical geometry, though. Indeed, the fact that $F_a^{(\mathrm{vL})}$ does, or does not, vanish is not particularly important, because the physically interesting quantity is not $F_a^{(\mathrm{vL})}$, but $F_a^{(\mathrm{l})}$. And whether $F_a^{(\mathrm{l})}=0$ (or, equivalently, $\widetilde{F}_a^{(\mathrm{l})}=0$) cannot be established simply by looking at $F_a^{(\mathrm{vL})}$ (or $\widetilde{F}_a^{(\mathrm{vL})}$), unless one is in a situation for which $F_a^{(\mathrm{H})}=0$ (or $\widetilde{F}_a^{(\mathrm{H})}=0$). Thus, in the case of Schwarzschild spacetime the evaluation of $F_a^{(\mathrm{vL})}$ turns out to be convenient only because, since $R_{ab}=0$ there, the Hobbs force vanishes

identically, so $F_a^{(\mathrm{vL})}$ coincides with $F_a^{(\mathrm{l})}$. However, in a spacetime for which it is $\tilde{R}_{ab}$ that vanishes, one has $\tilde{F}_a^{(\mathrm{H})}=0$. Consequently, it is now $\tilde{F}_a^{(\mathrm{vL})}$ that one should inspect, in order to get information about the behavior of $F_a^{(\mathrm{l})}=0$.

D. Conformally static charge

In order to further illustrate the point made in the last paragraph of Sec. IV C, let us consider a conformally static charge, i.e., one with four-velocity $v^a=n^a$, where

$$n^a := e^{-\Phi}\eta^a = (-g_{bc}\eta^b\eta^c)^{-1/2}\eta^a \tag{4.12}$$

is the unit vector field parallel to η^a. This is obviously a subcase of the situations covered in Sec. IV A and since $\tilde{R}_{ab}\eta^b=0$, it is evident in optical geometry that $\tilde{F}_a^{(\mathrm{vL})}=\tilde{F}_a^{(\mathrm{H})}=0$, so also $\tilde{F}_a^{(\mathrm{l})}=0$ and $F_a^{(\mathrm{l})}=0$. On the other hand, this conclusion is not obvious at all if one works in the spacetime $(\mathcal{M},g_{ab})$, because in order to establish it, one must use highly nontrivial properties of the vector field n^a, that lead to cancelations between terms coming from $F_a^{(\mathrm{vL})}$ and $F_a^{(\mathrm{H})}$ (none of which, however, vanishes separately). Hence, in this case it is optical geometry that allows one to establish that $F_a^{(\mathrm{l})}=0$ in a simple way, by using the decomposition $\tilde{F}_a^{(\mathrm{l})}=\tilde{F}_a^{(\mathrm{vL})}+\tilde{F}_a^{(\mathrm{H})}$. The alternative split, $F_a^{(\mathrm{l})}=F_a^{(\mathrm{vL})}+F_a^{(\mathrm{H})}$, leads instead to rather cumbersome calculations.

V. CONCLUSIONS

Let us summarize the results of Secs. II–IV. We have seen that, for uniform motion along a spatial geodesic $\chi=\pi/2$ in Einstein's static universe, the von Laue force vanishes, whereas the Hobbs force does not (hence, the local part of the self-force also does not vanish). In Schwarzschild spacetime, for uniform motion along a circle at $r=3M$, the von Laue force vanishes; since the Hobbs force is identically zero (Schwarzschild spacetime is Ricci-flat), this implies that $F_a^{(\mathrm{l})}(3M)=0$. Similarly, in the optical Schwarzschild spacetime, $\tilde{F}_a^{(\mathrm{vL})}(3M)=\tilde{F}_a^{(\mathrm{H})}(3M)=\tilde{F}_a^{(\mathrm{l})}(3M)=0$. All these are instances of the following general results, valid in an arbitrary conformally static spacetime: (i) for geodesic motion in optical spacetime $(\mathcal{M},\tilde{g}_{ab})$—uniform motion along optical geodesics—, $\tilde{F}_a^{(\mathrm{vL})}=0$; (ii) for geodesic motion in the spacetime $(\mathcal{M},g_{ab})$, $F_a^{(\mathrm{vL})}=0$. Note that, however, the physically interesting result does not concern $F_a^{(\mathrm{vL})}$ or $\tilde{F}_a^{(\mathrm{vL})}$, but the entire local part of the self-force. Whether this vanishes in cases (i) and (ii) depends on the additional feature that the matrix $\tilde{R}_i^{\ j}$ or $R_\mu^{\ \nu}$, respectively, be degenerate. Also, note that the particular case of (i), that for a conformally static charge $F_a^{(\mathrm{l})}=\tilde{F}_a^{(\mathrm{l})}=0$, although nontrivial, is straightforward when regarded from the perspective offered by optical geometry. Hence, the latter appears to be a useful tool in calculations of self-force and related effects, as it happens already in several other circumstances.[15–17,20–22,25–28]. Indeed, although in this paper we deliberately avoided dealing with the nonlocal part of the self-force $F_a^{(\mathrm{nl})}$, there are good reasons to believe that working in the optical spacetime might also simplify its evaluation—a rather challenging task, in general. This is suggested by the fact that computing $F_a^{(\mathrm{nl})}$ amounts, basically, to finding the bi-tensor $f_{aba'}$ in Eq. (1.3). In turn, this amounts to the determination of a particular electromagnetic field in spacetime, and we know already from Ref. 28 that this is sometimes easier to do using optical geometry. We leave the development of this subject for future investigations.

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APPENDIX: CENTRIPETAL ACCELERATION IN OPTICAL GEOMETRY

We present a derivation of Eq. (3.5) based on the embedding diagram of Fig. 2. In the fictitious three-dimensional Euclidean space, the centripetal acceleration of a particle that moves uniformly on the orbit $r=\text{const}$ is $a_E^{(c)}=\gamma^2\Omega^2\rho$, where $\rho=(1-2M/r)^{-1/2}r$ is the distance from the axis[18]—also called "radius of gyration"[26] because $v=(1-2M/r)^{-1/2}\Omega r=\Omega\rho$. The centripetal acceleration in the optical space is given by the tangential component of a_{E}, namely

$$a^{(c)}=\gamma^2\Omega^2\rho\cos\alpha, \tag{A1}$$

where α is the angle indicated in Fig. 2. Let $z=f(\rho)$ be the equation of the surface in Fig. 2. The surface is isometric to the section $\theta=\pi/2$ of the optical space if[18]

$$\left(1+\left(\frac{\mathrm{d}f}{\mathrm{d}\rho}\right)^2\right)\mathrm{d}\rho^2=\left(1-\frac{2M}{r}\right)^{-2}\mathrm{d}r^2. \tag{A2}$$

But we have also $\mathrm{d}f/\mathrm{d}\rho=\tan\alpha$, so

$$\cos\alpha=\left(1-\frac{2M}{r}\right)\left|\frac{\mathrm{d}\rho}{\mathrm{d}r}\right|=\left(1-\frac{2M}{r}\right)^{-1/2}\left|1-\frac{3M}{r}\right|. \tag{A3}$$

Substituting into (A1) we recover Eq. (3.5).

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Parametrization of solutions of the Lewis metric by a Painlevé transcendent III

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Without making use of the Ernst formalism we look directly for particular solutions of field equations describing stationary axisymmetric vacuum space–time using Weyl coordinates. The solutions that we obtain, by simple separation of variables, are parametrized in the general case by a III transcendent of Painlevé with two arbitrary constants. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Here we study the stationary axisymmetric vacuum metric presented by Lewis.[1] This metric depends on four potentials and we present it in Weyl coordinates. We know that the solutions can be expressed in three distinct classes for the cylindrical case[2] and for the general case.[3] We have shown[3] that the solutions of Lewis metric implies a functional relation between the three principal potentials.

To find new solutions of Lewis metric here we use the method of separation of variables ρ and z. Through this procedure the solutions are parametrized by the III transcendental of Painlevé with two arbitrary constants,[4–6] one structure constant a and one constant of integration C.

Wils presented a very interesting review[7] of solutions of Einstein's field equations producing transcendents of Painlevé. Persides and Xanthopoulos[8] and Calvert and Woodhouse,[9] in the axisymmetric case, found solutions parametrized by Painlevé transcendents III and V, using different methods.

Section II presents the field equations, Sec. III gives the transcendent solutions and the paper finishes with a short conclusion.

II. FIELD EQUATIONS

The general line element for a stationary axisymmetric space–time can be written in the Lewis form[1]

$$ds^2 = -f\,dt^2 + 2k\,dt\,d\phi + e^{\mu}(d\rho^2 + dz^2) + l\,d\phi^2, \tag{1}$$

where f, k, μ, and l are only functions of the Weyl coordinates ρ and z. For convenience[3] we assume

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$$f = \rho\mathcal{F}(\rho,z), \quad k = \rho\mathcal{K}(\rho,z), \quad l = \rho\mathcal{L}(\rho,z). \tag{2}$$

Following the procedure of Ref. 3 with

$$\mathcal{F}\mathcal{L} + \mathcal{K}^2 = 1, \tag{3}$$

we obtain the vacuum field equations in the symmetric form

$$\mathcal{K}\Delta\mathcal{F} = \mathcal{F}\Delta\mathcal{K}, \tag{4}$$

$$\mathcal{L}\Delta\mathcal{K} = \mathcal{K}\Delta\mathcal{L}, \tag{5}$$

$$\mathcal{F}\Delta\mathcal{L} = \mathcal{L}\Delta\mathcal{F}, \tag{6}$$

where the Laplacian Δ is defined by

$$\Delta \equiv \partial_{\rho\rho} + \frac{1}{\rho}\partial_\rho + \partial_{zz}, \tag{7}$$

with the indexes standing for differentiation.

III. TRANSCENDENT SOLUTION

We look for solutions of the system (4)–(6) of the form

$$\mathcal{F} = F(\rho)H_1(z), \tag{8}$$

$$\mathcal{K} = K(\rho)H_2(z), \tag{9}$$

$$\mathcal{L} = L(\rho)H_3(z), \tag{10}$$

satisfying (3). Substituting (8)–(10) into (3) and differentiating twice with respect to ρ and z we obtain

$$H_1H_3 = 1, \quad H_2 = 1, \tag{11}$$

and with the field equations (4)–(6) we find

$$H_1 = e^{-az}, \quad H_2 = 1, \quad H_3 = e^{az}, \tag{12}$$

where $a \neq 0$ is an arbitrary constant. When $a=0$ we find again the cylindrically symmetric case.[2] Therefore the field equations (4)–(6) can be written

$$K\left(F_{\rho\rho} + \frac{1}{\rho}F_\rho + a^2F\right) = F\left(K_{\rho\rho} + \frac{1}{\rho}K_\rho\right), \tag{13}$$

$$L\left(K_{\rho\rho} + \frac{1}{\rho}K_\rho\right) = K\left(L_{\rho\rho} + \frac{1}{\rho}L_\rho + a^2L\right), \tag{14}$$

$$F\left(L_{\rho\rho} + \frac{1}{\rho}L_\rho\right) = L\left(F_{\rho\rho} + \frac{1}{\rho}F_\rho\right), \tag{15}$$

respectively, and we see that (13) is a consequence of (14) and (15). We can integrate (15) and obtain

$$\frac{F_\rho}{F} - \frac{L_\rho}{L} = \frac{C}{\rho FL}, \tag{16}$$

where C is an integration constant and from (3) and (11),

$$FL + K^2 = 1. \tag{17}$$

Finally we find

$$\frac{L_\rho}{L} = \frac{1}{K^2 - 1}\left(KK_\rho + \frac{C}{2\rho}\right). \tag{18}$$

We can rewrite (14) as

$$\frac{1}{K}\left(K_{\rho\rho} + \frac{1}{\rho}K_\rho\right) = \left(\frac{L_\rho}{L}\right)_\rho + \left(\frac{L_\rho}{L}\right)^2 + \frac{1}{\rho}\frac{L_\rho}{L} + a^2, \tag{19}$$

and with (18) it becomes a second-order differential equation for $K(\rho)$, or $\mathcal{K}$,

$$(1 - K^2)\left(K_{\rho\rho} + \frac{1}{\rho}K_\rho\right) + KK_\rho^2 - K\left(\frac{C^2}{4\rho^2} + a^2(1 - K^2)^2\right) = 0. \tag{20}$$

Considering the transformation

$$\rho = \sqrt{x}, \quad K = \left(\frac{R}{R-1}\right)^{1/2}, \tag{21}$$

where R is a function of ρ and ranging $R \in]-\infty, 0]$ and $R \in]1, \infty[$, then (20) becomes

$$R_{xx} + \frac{1}{x}R_x - \left(\frac{1}{2R} + \frac{1}{R-1}\right)R_x^2 - \frac{C^2R}{8x^2}(R-1)^2 - \frac{a^2R}{2x} = 0. \tag{22}$$

The second-order differential equation (22) is a canonical particular type of the V transcendent of Painlevé depending on two parameters.[4,6,10] We observe that (22) is the same that appears in Ref. 6 [see Eq. (2.16)] obtained from the field equation using the Ernst potential. Furthermore, (22) corresponds to the standard form of the V transcendent of Painlevé as proposed by Okamoto[11] with the parameter $\beta=0$, i.e., $v_1+v_2=0$ and $t=x$.

We can use a differential transformation between the III transcendent of Painlevé and the V transcendent (20).[12] Setting

$$r = 1 - K^2, \tag{23}$$

in (20), we obtain

$$r_{\rho\rho} - \frac{1}{2}\left(\frac{1}{r} + \frac{1}{r-1}\right)r_\rho^2 + \frac{1}{\rho}r_\rho - \frac{C^2}{2\rho}\left(1 - \frac{1}{r}\right) - 2a^2(r-1)r\rho = 0. \tag{24}$$

Now let us consider the system

$$y_\rho = 2y^2(2r-1) + \frac{C-1}{\rho}y - \frac{a^2}{2}, \tag{25}$$

$$r_\rho = \left(4yr + \frac{C}{\rho}\right)(1-r). \tag{26}$$

Eliminating y in this system we obtain (24), while eliminating r, we obtain a particular form of the III transcendent of Painlevé,

$$y_{\rho\rho} - \frac{1}{y}y_\rho^2 + \frac{1}{\rho}y_\rho - \frac{1}{\rho}(\alpha y^2 + \beta) - \gamma y^3 - \frac{\delta}{y} = 0, \tag{27}$$

with

$$\alpha = 2C, \quad \beta = \frac{a^2}{2}(C-2), \quad \gamma = 4, \quad \delta = -\frac{a^4}{4}, \tag{28}$$

where we can rescale, $\rho \to \rho/a$ and choose $a=1$. The link between r, of the V transcendent of Painlevé, and y, of the III transcendent, given by (25) and (26), is differential, and we observe that if in (20) we substitute

$$y = \frac{1}{2(K^2-1)}\left(\frac{K_\rho}{K} + \frac{C}{2\rho}\right), \tag{29}$$

with $K = \sqrt{1-r}$ we reobtain (26).

Finally, we find from (12), (17), (18), (21), and (22),

$$F = -(R-1)^{-1/2} \exp\left(\frac{C}{2}\int_{\rho_0}^{\rho} \frac{1-R}{\rho} \mathrm{d}\rho\right), \tag{30}$$

$$K = \left(\frac{R}{R-1}\right)^{1/2}, \tag{31}$$

$$L = (R-1)^{-1/2} \exp\left(\frac{C}{2}\int_{\rho_0}^{\rho} \frac{R-1}{\rho} \mathrm{d}\rho\right), \tag{32}$$

where $R(\rho^2)$ is a solution of (22), and from (2) and (8)–(10),

$$f = \rho e^{-az} F(\rho), \tag{33}$$

$$k = \rho K(\rho), \tag{34}$$

$$l = \rho e^{az} L(\rho). \tag{35}$$

Hence (33)–(35) are solutions of the potentials f, k, and l for an axisymmetric vacuum field (1) parametrized by a III transcendent of Painlevé with $C \neq 0$ in place of the usual harmonic functions like in the three classes of Lewis space–time.[3]

IV. CONCLUSION

Departing from a formulation of the stationary axisymmetric space–time given originally by Lewis, we consider a solution of the field equations where the potentials are parametrized in a particular reducible to a Painlevé III transcendent with two non-null constants, and not by a harmonic function which are known as Lewis solutions which suppose, not only the relation (17) but also a functional relation between the potentials.[3] This method presents a particular advantage since the calculations are straightforward and clear.

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On the geometry of Killing and conformal tensors

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The second order Killing and conformal tensors are analyzed in terms of their spectral decomposition, and some properties of the eigenvalues and the eigenspaces are shown. When the tensor is of type I with only two different eigenvalues, the condition to be a Killing or a conformal tensor is characterized in terms of its underlying almost-product structure. A canonical expression for the metrics admitting these kinds of symmetries is also presented. The space–time cases 1+3 and 2+2 are analyzed in more detail. Starting from this approach to Killing and conformal tensors a geometric interpretation of some results on quadratic first integrals of the geodesic equation in vacuum Petrov-Bel type D solutions is offered. A generalization of these results to a wider family of type D space–times is also obtained. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2207717]

I. INTRODUCTION

Killing tensors are associated with first integrals to the geodesic equation. In the second order case, they define quadratic first integrals and they play a central role in the theory of separability of the Hamilton-Jacobi equation. The relationship between separability and Killing tensors was shown by Eisenhart[1] and abundant literature exists regarding this property (for example, see Ref. 2 and references therein).

Within the relativistic framework the study of Killing tensors grew when Walker and Penrose[3] showed how the existence of a Killing tensor explains the Carter results[4] on the integrability by variable separation of the geodesic equation in the Kerr solution. Since then a lot of studies have been devoted to determining and classifying the space–times admitting Killing tensors and also to obtaining the Killing tensors of a given metric. A summary of known results on this subject can be found in Ref. 5.

The problem of finding the metrics admitting a quadratic integral of the geodesic equation was established by Eisenhart.[1] He wrote the *intrinsic Killing tensor equations*, i.e., the Killing equations in terms of the eigenvectors e_i and the eigenvalues ρ_i of a Killing tensor, and he pointed out that (see Ref. 1, p. 129): "the problem of finding all V_n admitting a quadratic integral consists in finding a tensor g and an orthogonal ennuple e_i that satisfy the conditions obtained by the elimination of the ρ's from the intrinsic Killing tensor equations. The general solution has not been obtained, but we shall consider two particular solutions of the problem." Later, he considered the

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trivial case when all the ρ's are equal, and the case with different eigenvalues and normal principal congruences, a case which led to the Stäckel form of the metric.[6,1]

The general solution to the problem set by Eisenhart is far from being solved, although a number of results are known for some classes of Einstein-Maxwell solutions or algebraically special space–times, as well as those for flat metrics.[5] Nevertheless, the usual way in which this subject is tackled differs from the Eisenhart conception. Indeed, the common approach consists of studying the integrability conditions of the Killing tensor equations, whereas the Eisenhart method involves the following: (i) to write the intrinsic Killing tensor equations, (ii) to determine the equivalent equations involving exclusively the eigenspaces and the metric tensor (the eigenvalues having been removed), and (iii) to study the integrability conditions of the aforementioned equations. Both procedures, the usual one and Eisenhart's, may be suitable depending on the different situations. In this work we adopt the Eisenhart approach and we will show how useful it is by considering the case of Killing tensors with two complementary eigenspaces.

The conformal extension of the Killing tensor equation determines the conformal tensors which define first integrals to the null geodesic equation. Here we also analyze the Eisenhart problem for the class of conformal tensors with two complementary eigenspaces.

In the problem of finding the Riemannian spaces admitting a Killing or a conformal tensor two different aspects can be considered. On the one hand, we can look for a general canonical expression for the metric tensors with these kinds of first integrals. In this case, we must also obtain the expression of the Killing or conformal tensors in terms of the elements appearing in this canonical form. This approach may be useful in working in spaces with these symmetries, the adapted coordinates allowing calculations to be simplified and throwing light on the geometric interpretation of the expressions we can find.

On the other hand, we can give explicit and intrinsic conditions that characterize the metric tensors, and then we must offer the expression of the Killing or conformal tensors in terms of metric concomitants (namely, the Riemann tensor and its covariant derivatives). This approach is helpful in analyzing when a metric, which is known in an arbitrary coordinate system, has these kinds of symmetries. Moreover, we can obtain these tensorial symmetries without solving the Killing or conformal equations.

In this work we analyze both viewpoints. Regarding the first one, we can quote several results previously obtained in the relativistic framework. Thus, canonical forms for the four-dimensional space–time metrics admitting a Killing or a conformal tensor of type $2+2$ have been proposed in literature.[7,8] In this case the Killing or conformal tensor admits two complementary eigenplanes. Here we generalize these results by considering a general $p+q$ tensor (with two complementary eigenspaces of dimensions p and q, respectively) in a generic Riemannian space with arbitrary signature and dimension.

The second approach, the intrinsic characterization of the metrics admitting Killing and conformal tensors, has also been partially considered in relativity. Thus, it is known that every Petrov-Bel type D vacuum solution admits a conformal tensor of type $2+2$ which may be obtained form the Weyl tensor.[5] Here we extend this result by characterizing all the Petrov-Bel type D metrics with conformal tensors. Moreover we also identify the type D solutions admitting a Killing tensor, thus generalizing some results that are known for the vacuum case.[5]

It is worth remarking that the Eisenhart approach used here allows the intrinsic and explicit labeling of the metrics to be obtained easily. Indeed, in this approach we give conditions for the underlying $2+2$ structure of the Killing or conformal tensors. Moreover, for the Petrov-Bel type D metrics, this is the principal structure one of the Weyl tensor, and it is explicitly known in terms of the metric tensor.[9] The reason why it is of interest to obtain an explicit and intrinsic characterization of a space–time metric has been pointed out elsewhere[10] and the method used here has been useful in labeling the Schwarszchild[10] and Reissner-Nordström[11] solutions, the static Petrov type I space–times[9] and the Petrov type I space–times admitting isotropic radiation.[12]

Here we show that the eigenspaces of a Killing or a conformal tensor are umbilical planes. Moreover they are totally geodesic for a conformal metric. This geometric interpretation could be useful in clarifying the role played by the Killing tensor in the separability theory.

The paper is organized as follows. Some notation, definitions and properties related to regular Riemannian p planes are introduced in Sec. II. In Sec. III we study some properties of the eigenvectors and eigenvalues of a Killing or a conformal tensor. The type I case (when the tensor admits an orthonormal basis of eigenvectors) is analyzed in detail in Sec. IV and we write the Eisenhart intrinsic Killing tensor equations in a form that is more useful to our purposes. In Sec. V we use this new form for the Killing tensor equations to analyze the Eisenhart problem when the Killing or the conformal tensor has two complementary eigenspaces. A canonical form for the metrics admitting these kinds of first integrals is presented in Sec. VI. In Sec. VII we study the $1+(n-1)$ case and outline when these Killing or conformal tensors are not reducible. In the last two sections some results concerning the usual four-dimensional space–time are obtained. The $2+2$ space–time structures associated to a Killing or conformal tensor are analyzed in detail in Sec. VIII. Finally, Sec. IX is devoted to obtaining an intrinsic and explicit characterization of the Petrov-Bel type D metrics admitting Killing or conformal tensors attached to its principal structure, and we also present an algorithm to obtain these quadratic first integrals in a given type D space–time.

II. SOME NOTATION AND USEFUL CONCEPTS

On an n-dimensional Riemannian manifold (M,g) we shall refer to a (regular) p-dimensional distribution V as a p plane. Let v be the projector on V and $h=g-v$ the projector on the plane orthogonal to V. The generalized second fundamental form of V is defined as the (2,1)-tensor Q_v given by

$$Q_v(x,y) = h(\nabla_{v(x)}v(y)) \tag{1}$$

for every pair of vector fields x, y. We can consider the decomposition of Q_v into its antisymmetric part A_v and its symmetric part $S_v \equiv S_v^T + (1/p)v \otimes \mathrm{Tr}\, S_v$, where S_v^T is a traceless tensor:

$$Q_v = A_v + \frac{1}{p} v \otimes \mathrm{Tr}\, S_v + S_v^T. \tag{2}$$

The plane V is a foliation if, and only if, $A_v=0$. In this case $Q_v=S_v$ and it coincides with the second fundamental form of the integral manifolds of the foliation V.[13] Moreover V is minimal, umbilical or geodesic if, and only if, $\mathrm{Tr}\, S_v=0$, $S_v^T=0$ or $S_v=0$, respectively. Then one can generalize these geometric concepts for plane fields which are not necessarily a foliation.

Definition 1: A plane field V is said to be geodesic, umbilical or minimal if the symmetric part S_v of its (generalized) second fundamental form Q_v satisfies $S_v=0$, $S_v^T=0$ or $\mathrm{Tr}\, S_v=0$, respectively.

From these definitions, and defining $\{x,y\}=\nabla_x y+\nabla_y x$, a lemma easily follows.

Lemma 1: A plane field V is umbilical for the metric g if, and only if, a vector field $\boldsymbol{a}$ *exists such that $h(\{x,y\})=g(x,y)\,\boldsymbol{a}$ for every $x,y \in V$, h being the projector on the plane orthogonal to V.*

On a n-dimensional Riemannian manifold (M,g) an almost-product structure is defined by a p-plane field V and its orthogonal complement H. The almost-product structures can be classified taking into account the invariant decomposition of the covariant derivative of the *structure tensor* $\Pi=v-h$. Likewise, they can be classified according to the foliation, minimal, umbilical or geodesic character of each plane.[14,15] We will say that a structure (V,H) is integrable when both planes are foliations and we will say that it is minimal, umbilical or geodesic if both of the planes are so.

In an oriented four-dimensional space–time (V_4,g) of signature $(-\ +\ +\ +)$ a more accurate classification for the almost-product structures follows taking into account the causal character of the planes.[16] Elsewhere[11] we have classified the Petrov-Bel type D space–times in accordance with the class of the $2+2$ principal structure of the Weyl tensor.

III. SECOND ORDER KILLING AND CONFORMAL TENSORS

The quadratic first integrals of the geodesic equation are associated with second rank *Killing tensors*.[1] Indeed, if K is a solution to the generalized *Killing equation*

$$[K,g]=0 \quad ([K,g]_{abc}=\nabla_{(a}K_{bc)}), \tag{3}$$

then the scalar $K(v,v)$ is constant along an affine parametrized geodesic with tangent vector v.

It is known[5] that if K is a Killing tensor, its traceless part $P=K-(1/n)\mathrm{Tr}\,Kg$ is a *conformal tensor*, i.e., it satisfies the *conformal equation*

$$[P,g]=\mathcal{S}\{g\otimes t\}, \tag{4}$$

where t is, up to a factor, the divergence of P, $t=[2/(n+2)]\nabla\cdot P$, and $\mathcal{S}\{B\}$ denotes the total symmetrization of a tensor B. Then, the scalar $P(v,v)$ is constant along an affinely parametrized null geodesic with tangent vector v. Moreover, Killing equation (3) implies

$$2n\,\nabla\cdot P+(n+2)\mathrm{d}\,\mathrm{Tr}\,K=0. \tag{5}$$

Then, we have the following.

Lemma 2: If K is a second rank Killing tensor [solution to (3)] then its traceless part $P=K-(1/n)\mathrm{Tr}\,Kg$ *is a conformal tensor [solutions to (4)] and it satisfies*

$$\mathrm{d}\nabla\cdot P=0. \tag{6}$$

Conversely if a traceless conformal tensor P satisfies (6), a scalar π *exists such that* $\mathrm{d}\pi=\nabla\cdot P$. *Then,* $K=P-[2/(n+2)]\pi g$ *is a Killing tensor.*

In this work we analyze some properties of the eigenvalues and eigenspaces of Killing and conformal tensors and we present some of their properties. We proceed by studying both classes of tensors simultaneously and we will comment on the differences when they exist. So, if we consider a second rank tensor T solution to (4) the consequences on its eigenspaces and eigenvalues apply to both, Killing and conformal tensors. We particularize the conformal case by taking T as a traceless tensor. If we add condition (6), then T is the traceless part of a Killing tensor. But we can also recover the Killing tensor case by taking the vector t to be zero. It is worth pointing out that if P is a traceless conformal tensor, then $P+\Phi g$ is a conformal tensor, and both define the same first integrals of the null geodesic equation. Nevertheless, here we will always work with the traceless representative.

We denote E_ρ the eigenspace of T corresponding to the eigenvalue ρ. Then, if $x,y\in E_\rho$, a straightforward calculation leads to

$$[T,g](x,y,\cdot)=x(\rho)y+y(\rho)x+g(x,y)\mathrm{d}\rho-(T-\rho g)\{x,y\}. \tag{7}$$

On the other hand,

$$\mathcal{S}\{g\otimes t\}(x,y,\cdot)=g(x,y)t+g(t,x)y+g(t,y)x. \tag{8}$$

So, for two eigenvectors $x,y\in E_\rho$, the conformal condition (4) implies

$$(T-\rho g)\{x,y\}=g(x,y)s+g(s,x)y+g(s,y)x, \quad s\equiv\mathrm{d}\rho-t. \tag{9}$$

On the other hand, if we consider three eigenvectors x,y,z corresponding to three different eigenvalues, a similar calculation leads to

$$T(x,\{y,z\})+T(z,\{x,y\})+T(y,\{z,x\})=0. \tag{10}$$

Thus, we can state the following.

Lemma 3: Let T be a Killing (*respectively, conformal*) *tensor. Then we have the following.*

(i) *If* $x,y\in E_\rho$ *are eigenvectors associated with the eigenvalue* ρ, *Eq. (9) holds, where the*

vector t is zero (*respectively*, $t=[2/(n+2)]\nabla\cdot T$).

(ii) *If* x,y,z *are eigenvectors corresponding to three different eigenvalues, Eq. (10) holds.*

A consequence of Lemma 3 follows by taking $x=y$ in Eq. (9). Indeed, if one makes a new product with x one obtains

$$x^2 g(\mathrm{d}\rho - t, x) = 0 \tag{11}$$

and so, if x,y are non-null vectors, Eq. (9) becomes

$$(T-\rho g)\{x,y\} = g(x,y)(\mathrm{d}\rho - t). \tag{12}$$

If E_ρ is a regular eigenspace of T, then a basis of E_ρ formed with non-null eigenvectors exists and, consequently, (12) holds even for the null eigenvectors. Moreover, taking into account (11) we have the following.

Lemma 4: Let E_ρ *be a regular eigenspace of a Killing (respectively, conformal) tensor* T. *Then* (12) *with* $t=0$ (*respectively*, $t=[2/(n+2)]\nabla\cdot T$) *holds for every* $x,y\in E_\rho$.

Moreover, $\mathrm{d}\rho\in E_\rho^\perp$ *[respectively*, $2\nabla\cdot T-(n+2)\mathrm{d}\rho\in E_\rho^\perp$*]*.

IV. EIGENVALUES AND EIGENVECTORS OF SECOND ORDER KILLING AND CONFORMAL TENSORS OF TYPE I

Let us now go to type I Killing and conformal tensors, that is, those admitting an orthonormal basis of eigenvectors. In this case every eigenspace is regular and then the Killing (or conformal) equation implies (10) and (12). Moreover a basis of eigenvectors exists and, consequently, these restrictions are also sufficient conditions for T to be a Killing (or conformal) tensor. Thus, we have the following.

Proposition 1: Let T *be a symmetric 2-tensor of type I and let* E_i *be the eigenspaces corresponding to the eigenvalues* ρ_i. *Then,* T *is a Killing* (*respectively, conformal*) *tensor if, and only if*

(i) $(T-\rho_i g)\{x,y\}=g(x,y)(\mathrm{d}\rho_i - t)$, *for every* $x,y\in E_i$, *where the vector* t *is zero* (*respectively*, $t=[2/(n+2)]\nabla\cdot T$).

(ii) $T(x,\{y,z\})+T(z,\{x,y\})+T(y,\{z,x\})=0$, *for* x, y, z, *eigenvectors with different eigenvalue*.

Let K be a Killing tensor of type I and let $\{e_a\}$ and $\{\rho_a\}$ be an orthonormal basis of eigenvectors and the corresponding eigenvalues. A straightforward calculation allows us to write the two conditions in Proposition 1 in terms of $\{e_a\}$ and $\{\rho_a\}$ obtaining, in this way

$$\rho_a s_{bca} + \rho_b s_{cab} + \rho_c s_{abc} = 0, \quad a,b,c \neq , \tag{13}$$

$$e_a^2 e_b(\rho_a) - (\rho_b - \rho_a) s_{aab} = 0, \quad a \neq b, \tag{14}$$

$$e_b(\rho_b) = 0, \tag{15}$$

where s_{abc} are the symmetrized rotation coefficients, $s_{abc}=g(e_c,\{e_a,e_b\})$. If we set Eqs. (13)–(15) in terms of the rotation coefficients we easily recover the *intrinsic Killing tensor equations* obtained by Eisenhart.[1] In order to study the metrics which admit a second order Killing tensor, Eisenhart[1] started from these intrinsic equations and he looked for a set of equivalent conditions involving the eigenvectors exclusively. He considered the case when all the eigenvalues are equal and the case with different eigenvalues and normal principal congruences.[1] In this work we solve this Eisenhart problem for both the Killing and conformal tensors, when the second order tensor admits two complementary eigenspaces. We could also start from Eqs. (13)–(15) and similar conditions for the conformal case, but we will choose an alternative approach that makes the geometric properties of the eigenspaces of the Killing and conformal tensors more evident.

Let ρ_i and h_i be the eigenvalue and the projector associated with the eigenspace E_i, and let p_i be its dimension. Then

$$T = \sum \rho_i h_i, \quad g = \sum h_i, \quad \mathrm{Tr}\, h_i = p_i. \tag{16}$$

With this notation, the second statement of Lemma 4 becomes $h_i(\mathrm{d}\rho_i - t) = 0$ and, consequently,

$$t = \sum h_i(\mathrm{d}\rho_i). \tag{17}$$

On the other hand, by projecting condition (i) in Proposition 1 on every eigenspace E_j one obtains

$$(\rho_j - \rho_i) h_j(\{x,y\}) = g(x,y) h_j(\mathrm{d}\rho_i - t). \tag{18}$$

So, if v_i denotes the projection on the orthogonal space $E_i^{\perp}$, one has

$$v_i(\{x,y\}) = g(x,y) \sum_{j \neq i} \frac{1}{\rho_j - \rho_i} h_j(\mathrm{d}\rho_i - t) \tag{19}$$

for every $x, y \in E_i$. Then, according to Lemma 1 and taking into account that t is zero for a Killing tensor and it can be written as (17) for a conformal one, we arrive to the following:

Theorem 1: *Let T be a symmetric 2-tensor of type I and let h_i be the projector corresponding to the eigenvalue ρ_i. Then, T is a Killing or a conformal tensor if, and only if,*

(i) *The eigenspaces are umbilical subspaces, that is, their second fundamental form can be written as $S_i = \frac{1}{2} h_i \otimes \boldsymbol{a}_i$.*

(ii) *For every eigenspace the trace of its second fundamental form $\mathrm{Tr}\, S_i = (p_i/2)\boldsymbol{a}_i$ satisfies*

$$\boldsymbol{a}_i = \sum_{j \neq i} \frac{1}{\rho_j - \rho_i} h_j(\mathrm{d}\rho_i), \quad h_i(\mathrm{d}\rho_i) = 0, \quad \textit{for a Killing tensor}, \tag{20}$$

$$\boldsymbol{a}_i = -\sum_{j \neq i} h_j(\mathrm{d}\ln|\rho_i - \rho_j|), \quad \sum p_i \rho_i = 0, \quad \textit{for a conformal tensor}. \tag{21}$$

(iii) $T(x,\{y,z\}) + T(z,\{x,y\}) + T(y,\{z,x\}) = 0$, *for x, y, z, eigenvectors with different eigenvalues.*

The first condition of this theorem gives a geometric property involving the eigenvectors exclusively: every eigenspace is an umbilical subspace. Thus, it offers a decoupled equation that partially solves the Eisenhart problem. In the next section we will analyze the other two conditions in Theorem 1 for the case of two complementary eigenspaces. The last condition makes no sense in this case and we will see that the second one can be easily decoupled.

V. GEOMETRY OF KILLING AND CONFORMAL TENSORS OF TYPE $p+q$

A particular case of type I second order tensors are those having two complementary eigenspaces of dimensions p and $q = n - p$. So, a $p+q$ almost-product structure (V,H) is associated with these tensors, and we say that they are of type $p+q$. If v and h are the projectors onto the eigenspaces and α and β are the eigenvalues, such a tensor takes the form $T = \alpha v + \beta h$. In this case the previous theorem can be stated concisely in terms of the canonical elements $(v,h;\alpha,\beta)$ as

Proposition 2: A symmetric 2-tensor $K = \alpha v + \beta h$ of type $p+q$ is a Killing tensor if, and only if, the following conditions hold:

(i) *The eigenstructure (V,H) is umbilical, that is, the second fundamental forms can be written as*

$$S_v = \tfrac{1}{2} v \otimes \boldsymbol{a}, \quad S_h = \tfrac{1}{2} h \otimes \boldsymbol{b}. \tag{22}$$

(ii) *The traces of the second fundamental forms, $\mathrm{Tr}\, S_v = (p/2)\boldsymbol{a}$ and $\mathrm{Tr}\, S_h = (q/2)\boldsymbol{b}$, and the eigenvalues α, β are related by*

$$\boldsymbol{a} = \frac{1}{\beta - \alpha} \mathrm{d}\alpha, \quad \boldsymbol{b} = \frac{1}{\alpha - \beta} \mathrm{d}\beta. \tag{23}$$

A similar result takes place for conformal tensors as the following proposition says.

Proposition 3: A traceless symmetric 2-tensor $P=\alpha(qv-ph)$ of type $p+q$ is a conformal tensor if, and only if, the following conditions hold:

(i) *The eigenstructure (V,H) is umbilical, that is, the second fundamental forms can be written as*

$$S_v = \tfrac{1}{2} v \otimes \boldsymbol{a}, \quad S_h = \tfrac{1}{2} h \otimes \boldsymbol{b}. \tag{24}$$

(ii) *The traces of the second fundamental forms,* $\mathrm{Tr}\, S_v = (p/2)\boldsymbol{a}$ *and* $\mathrm{Tr}\, S_h = (q/2)\boldsymbol{b}$, *and the scalar α are related by*

$$\boldsymbol{a} + \boldsymbol{b} = -\,\mathrm{d}\ln|\alpha|. \tag{25}$$

It is worth remembering that, for the space-time 2+2 case, the umbilical nature of the structure is equivalent to the geodesic and shear-free character of its two null principal directions.[11] Consequently, the above propositions generalize some results for the space–time Killing and conformal tensors of type 2+2 (see Ref. 5, theorem 35.4) to an arbitrary dimension n and an arbitrary type $p+q$. Now we want to remark that the covariant formalism used here allows us to accomplish the second step in the Eisenhart method: the characterization of the Killing and conformal tensors in terms of their eigenspaces.

The characterization of a $p+q$ Killing or conformal tensor presented in the propositions above involves the structure tensor [conditions (i) and (ii)] and the eigenvalues [condition (ii)]. The next step consists of removing the eigenvalues in order to obtain the conditions that an almost product structure must satisfy in order to be the eigenstructure of a Killing or a conformal tensor. Condition (ii) of Proposition 2 can be written as

$$(\alpha - \beta)\boldsymbol{a} = -\,\mathrm{d}\alpha, \quad (\alpha - \beta)\boldsymbol{b} = \mathrm{d}\beta. \tag{26}$$

Then we have $(\beta-\alpha)(\boldsymbol{a}+\boldsymbol{b})=\mathrm{d}(\alpha-\beta)$. If we differentiate (26) and make the substitution of $\mathrm{d}(\alpha-\beta)$ we get

$$\mathrm{d}\boldsymbol{a} + \boldsymbol{a} \wedge \boldsymbol{b} = 0, \quad \mathrm{d}\boldsymbol{b} + \boldsymbol{b} \wedge \boldsymbol{a} = 0. \tag{27}$$

Conversely, if $\boldsymbol{a}$, $\boldsymbol{b}$ satisfy Eqs. (27), two functions x, y exist such that

$$\boldsymbol{a} + \boldsymbol{b} = \mathrm{d}x, \quad \boldsymbol{a} - \boldsymbol{b} = e^{x}\mathrm{d}y.$$

Then, taking $\alpha=e^{-x}-y$ and $\beta=-e^{-x}-y$, Eq. (26) is satisfied and $K=\alpha v+\beta h$ is a Killing tensor provided that (22) holds. The freedom in choosing x and y leads to the family of Killing tensors $CK+Dg$, C and D being arbitrary constants.

In the same way, condition (25) for a conformal tensor implies that $\mathrm{d}(\boldsymbol{a}+\boldsymbol{b})=0$. Conversely, if $\mathrm{d}(\boldsymbol{a}+\boldsymbol{b})=0$, a function x exists such that $\boldsymbol{a}+\boldsymbol{b}=\mathrm{d}x$. Then, the traceless tensor $P=e^{-x}(qv-ph)$ is a conformal Killing tensor provided that (24) holds. The freedom in choosing x leads to the family CP, C being an arbitrary constant. Thus, we have obtained the following.

Theorem 2: *The necessary and sufficient conditions for a $p+q$ almost-product structure (V,H) to be the eigenstructure of a Killing or a conformal tensor are the following.*

(i) *(V,H) is umbilical, that is, the second fundamental forms take the expression*

$$S_v = \tfrac{1}{2} v \otimes \boldsymbol{a}, \quad S_h = \tfrac{1}{2} h \otimes \boldsymbol{b}. \tag{28}$$

(ii) *The traces,* $\mathrm{Tr}\, S_v = (p/2)\boldsymbol{a}$ and $\mathrm{Tr}\, S_h = (q/2)\boldsymbol{b}$, *of the second fundamental forms satisfy*

$$\mathrm{d}\boldsymbol{a} + \boldsymbol{a} \wedge \boldsymbol{b} = 0, \quad \mathrm{d}\boldsymbol{b} + \boldsymbol{b} \wedge \boldsymbol{a} = 0 \quad \textit{for Killing tensors}, \tag{29}$$

$$\mathrm{d}(\boldsymbol{a}+\boldsymbol{b})=0 \quad \textit{for conformal tensors}. \tag{30}$$

If (28) *and* (29) *hold, two functions* x, y *exist such that* $\boldsymbol{a}+\boldsymbol{b}=\mathrm{d}x$, $\boldsymbol{a}-\boldsymbol{b}=e^{x}\,\mathrm{d}y$. *Then taking* $\alpha=e^{-x}-y$, $\beta=-e^{-x}-y$, $K=C(\alpha v+\beta h)+Dg$ *is a Killing tensor*, C *and* D *being two arbitrary constants*.

If (28) *and* (30) *hold, a function* x *exists such that* $\mathrm{d}x=\boldsymbol{a}+\boldsymbol{b}$. *Then*, $P=Ce^{-x}(qv-ph)$ *is a conformal Killing tensor*, C *being an arbitrary constant*.

This theorem offers the second step in solving the Eisenhart problem for Killing or conformal tensors with two complementary eigenspaces. In fact, once the eigenvalues have been removed, we have obtained necessary and sufficient conditions involving the sole eigenspaces. In Sec. VIII we will see that, for the space–time 2+2 case, these conditions can be written as tensorial conditions on the structure tensor (or on the canonical 2-form associated with the structure). This fact allows us to give an intrinsic and explicit characterization of the four-dimensional Petrov-Bel type D space–times admitting a Killing or a conformal tensor in Sec. IX.

VI. METRICS ADMITTING A KILLING OR A CONFORMAL TENSOR OF TYPE $p+q$

In this section we show that a metric admitting a Killing or a conformal tensor of type $p+q$ admits a canonical expression in terms of a particular conformal metric and a specific conformal factor. First we state a corollary which trivially follows on from Propositions 2 and 3.

Corollary 1: Let (V,H) *be a* $p+q$ *almost-product structure for the metric tensor* g. *The following statements are equivalent:*

(i) (V,H) *is a* $p+q$ *totally geodesic almost-product structure*.
(ii) $Cv+Dh$ *is a Killing tensor*, C *and* D *being arbitrary constants*.
(iii) $C(qv-ph)$ *is a conformal tensor*, C *being an arbitrary constant*.

This corollary states that the Riemannian spaces admitting a second order Killing tensor with constant eigenvalues are those admitting a $p+q$ totally geodesic structure (V,H). We will show now that these Riemannian spaces generate all the spaces admitting Killing or conformal tensors by using an adequate conformal transformation.

The umbilical property is known to be a conformal invariant.[15,11] Moreover, if we take into account the change of the second fundamental form through a conformal transformation,[11] condition (25) for a conformal tensor states that the eigenstructure (V,H) is minimal for the conformal metric $\tilde{g}=|\alpha|^{-1}g$. Consequently, the family of metrics that admit a $p+q$ conformal tensor are those that are conformal to a metric which admits a totally geodesic $p+q$ structure. More precisely, we have the following.

Proposition 4. The metrics g *that admit a* $p+q$ *conformal tensor are those that may be written as* $g=|\alpha|\tilde{g}$, *where* $\tilde{g}$ *is a metric admitting a totally geodesic* $p+q$ *structure* (V,H).

Then the conformal tensor for g *is* $P=C\alpha(qv-ph)$, C *being an arbitrary constant*.

This proposition and Corollary 1 generalize to an arbitrary dimension n and an arbitrary type $p+q$ a result by Hauser and Malhiot[8] concerning the 2+2 space–time case. Moreover we also recover another known result easily:[17] a (contravariant) conformal tensor for a metric is a conformal tensor for every conformally related metric.

A similar result holds for Killing tensors. In fact, the sum of expressions (29) says that $\mathrm{d}(a+b)=0$, which is exactly the condition necessary for (V,H) to be the eigenstructure of a conformal tensor, and so the metric is conformal to a metric admitting a $p+p$ totally geodesic structure. But now, the conformal factor is not arbitrary because it must satisfy the two equations in (29). A detailed analysis of these conditions leads to the following.

Proposition 5: The metrics g *that admit a* $p+q$ *Killing tensor are those that may be written as* $g=|\alpha-\beta|\tilde{g}$, *where* $\tilde{g}$ *is a metric admitting a totally geodesic* $p+q$ *structure* (V,H), *and* α *and* β *are functions such that* $v(\mathrm{d}\alpha)=0$, $h(\mathrm{d}\beta)=0$.

Moreover, the Killing tensor for g *is* $K=C(\alpha v+\beta h)+Dg$, C *and* D *being arbitrary constants*.

The two propositions above imply that the study of the Riemannian spaces admitting a Killing

or a conformal tensor reduces to the study of the metrics $\tilde{g}$ admitting a totally geodesic $p+q$ structure. As Proposition 4 states, for every metric $\tilde{g}$ of this type we obtain a metric g admitting a conformal tensor by using an arbitrary conformal factor, $g=\Omega^2\tilde{g}$.

Nevertheless, Proposition 5 states that the richness of metrics admitting a Killing tensor conformally related to a $\tilde{g}$ of this type depends on the quantity of normal directions aligned with one of the planes of the structure. This fact induces a classification of the metrics admitting a totally geodesic $p+q$ structure.

In the more regular metrics no aligned normal direction exists and only constant conformal factors can be considered, the Killing tensor then have constant eigenvalues.

The more degenerate class corresponds to the product metrics $\tilde{g}=\tilde{v}+\tilde{h}$, $\tilde{v}_{AB}(x^C)$ and $\tilde{h}_{ij}(x^k)$ being two arbitrary p and q dimensional metrics, respectively; then, the available conformal factors are $\Omega^2=|\alpha-\beta|$, $\alpha(x^k)$ and $\beta(x^C)$ being arbitrary functions depending on the product coordinates and they coincide with the Killing tensor eigenvalues.

An intermediate situation occurs when, for example, only one normal aligned direction exists on each plane. Then, through the adequate conformal transformation we can obtain a metric admitting a Killing tensor with nonconstant eigenvalues. In dealing with $2+2$ space–time Killing tensors this case leads to the Hauser and Malhiot[7,8] canonical form for the metric.

VII. KILLING AND CONFORMAL TENSORS OF TYPE $1+(n-1)$

Let us consider the case of a $1+(n-1)$ structure (V,H) defined by the unitary direction u ($u^2=\epsilon=\pm 1$) and its orthogonal complement. Then $g=v+h$ where $v=\epsilon u\otimes u$ and $h=g-\epsilon u\otimes u$. In terms of the usual kinematic coefficients of u ($\nabla u=\epsilon u\otimes\dot{u}+[1/(n-1)]\theta h+\sigma+\Omega$) the (generalized) second fundamental forms are

$$Q_v=u\otimes u\otimes\dot{u},\quad Q_h=-\epsilon\left(\frac{1}{n-1}\theta h+\sigma+\Omega\right)\otimes u. \tag{31}$$

The condition for (V,H) to be an umbilical structure just states $\sigma=0$, and then

$$S_v=u\otimes u\otimes\dot{u},\quad S_h=-\epsilon\frac{1}{n-1}\theta h\otimes u. \tag{32}$$

Thus taking into account Theorem 2, we find that the necessary and sufficient condition for u to define the eigenstructure of a conformal tensor is

$$\sigma=0,\quad \mathrm{d}\left(\dot{u}-\frac{\theta}{n-1}u\right)=0. \tag{33}$$

But these conditions state that u defines the direction of a conformal Killing vector.[18] Thus, we have the following.

Proposition 6: A $1+(n-1)$ *structure defined by the unitary direction u is the eigenstructure of a conformal Killing tensor if, and only if, u defines the direction of a conformal Killing vector, that is, it satisfies (33).*

This proposition implies that every traceless conformal tensor of type $1+(n-1)$ is the traceless part of $\xi\otimes\xi$, ξ being a Killing conformal vector. In other words, *every* $1+(n-1)$ *conformal tensor is reducible*

A similar procedure allows us to characterize the fact that u defines the eigenstructure of a $1+(n-1)$ Killing tensor. But in this case we find that it is not, necessarily, reducible. Indeed, taking into account (32) the condition (29) of Theorem 2 is equivalent to

$$\mathrm{d}\left(\dot{u}-\frac{\theta}{n-1}u\right)=0, \quad \theta\,\mathrm{d}u+\mathrm{d}\theta\wedge u+2\epsilon\theta u\wedge\dot{u}=0.$$

When $\theta=0$ these equations hold if $\mathrm{d}\dot{u}=0$, that is, if u defines the direction of a Killing vector. On the contrary, if $\theta\neq 0$, the second equation implies $\mathrm{d}u\wedge u=0$, and so $\mathrm{d}u=\epsilon u\wedge\dot{u}$. In this case, u defines the direction of a normal conformal Killing vector and the second equation can be written as

$$\mathrm{d}(\theta^{1/3}u)=0. \tag{34}$$

These results are summarized in the following.

Proposition 7: The $1+(n-1)$ *structure defined by the unitary direction u is the eigenstructure of a Killing tensor if, and only if, one of the following conditions hold*:

(i) *u defines the direction of a Killing vector, that is, it satisfies* $\sigma=0=\theta$, $\mathrm{d}\dot{u}=0$.
(ii) *u defines the direction of a normal conformal Killing vector with integrant factor* $\theta^{1/3}$, *that is, it satisfies equations (33) and (34).*

This proposition shows that we can distinguish two classes of Killing tensors of type $1+(n-1)$. On the one hand, we have the reducible ones, that is, those that can be written as $\xi\otimes\xi+Bg$, ξ being a Killing vector and B an arbitrary constant. On the other hand, a class of irreducible Killing tensors that can be obtained from normal conformal Killing vectors. This last class has been considered by Koutras[19] and Rani *et al.*[17]

The results in the preceding section allow us to give the canonical form for the metric tensors admitting irreducible Killing tensors of type $1+(n-1)$. Indeed, as the eigenstructure is integrable, the metric will be conformally related to a $1+(n-1)$ product metric. Moreover Proposition 5 gives the conformal factor. Finally, we can state the following

Proposition 8: The metrics admitting an irreducible Killing tensor of type $1+(n-1)$ *are those that may be written as*

$$g=|\alpha(x^i)-\beta(x^0)|[\epsilon\,\mathrm{d}x^0\otimes\mathrm{d}x^0+\gamma(x^i)], \tag{35}$$

where $\gamma(x^i)$ *is an arbitrary* $(n-1)$*-dimensional metric.*

The Killing tensor is then given by $C|\alpha-\beta|[\epsilon\alpha\,\mathrm{d}x^0\otimes\mathrm{d}x^0+\beta\gamma(x^i)]+Dg$, *C and D being arbitrary constants.*

VIII. SPACE–TIME KILLING AND CONFORMAL TENSORS OF TYPE [(11) (11)]

Let T be a Killing or a conformal tensor of type [(11) (11)] in an oriented four-dimensional space–time (V_4,g) of signature $(-+++)$. Then T has two eigenspaces: a timelike two-plane V and its spacelike orthogonal complement H. The almost-product eigenstructure (V,H) is determined by the *canonical* unitary 2-form U, volume element of the timelike plane V. Then, the respective projectors are $v=U^2$ and $h=-(*U)^2$, where $U^2=U\times U=\mathrm{Tr}_{23}\,U\otimes U$ and $*$ is the Hodge dual operator.

In order to study the geometric properties of a 2+2 structure it is useful to introduce the self-dual unitary 2-form $\mathcal{U}\equiv(1/\sqrt{2})(U-i*U)$ associated with U. The metric on the self-dual 2-forms space is $\mathcal{G}=\frac{1}{2}(G-i\eta)$, where η is the metric volume element of the space–time, $G=\frac{1}{2}g\wedge g$ is the metric on the 2-forms space, and $\wedge$ denotes the double-forms exterior product, $(A\wedge B)_{\alpha\beta\mu\nu}=A_{\alpha\mu}B_{\beta\nu}+A_{\beta\nu}B_{\alpha\mu}-A_{\alpha\nu}B_{\beta\mu}-A_{\beta\mu}B_{\alpha\nu}$. Then, we can consider some first order differential concomitants of U that determine the geometric properties of the structure. Indeed, if $i(\cdot)$ denotes the interior product and δ the exterior codifferential, $\delta=*d*$, we have the following lemma.[11]

Lemma 5: Let us consider the 2+2 *structure defined by* $\mathcal{U}=(1/\sqrt{2})(U-i*U)$. Then

(i) *The traces of the second fundamental forms take the expression*

$$\mathrm{Tr}\,Q_v=\boldsymbol{a}[U]\equiv-i(\delta*U)*U, \quad \mathrm{Tr}\,Q_h=\boldsymbol{b}[U]\equiv i(\delta U)U. \tag{36}$$

(ii) *The structure is umbilical, if, and only if,*

$$\Sigma[U] \equiv \nabla\mathcal{U} - i(\delta\mathcal{U})\mathcal{U}\otimes\mathcal{U} - i(\delta\mathcal{U})\mathcal{G} = 0. \tag{37}$$

With this notation, we can write the intrinsic equations in Propositions 2 and 3 for the case of Killing or conformal tensors of type [(11) (11)] by using the eigenvalues and the canonical 2-form U exclusively.

Proposition 9: The traceless symmetric tensor $P=\alpha[U^2+(*U)^2]$ *is a conformal tensor if, and only if, the canonical elements* $\{\alpha, U\}$ *satisfy (37) and*

$$-\mathrm{d}\ln|\alpha| = \Phi[U] \equiv i(\delta U)U - i(\delta * U) * U. \tag{38}$$

Proposition 10: The symmetric tensor $K=\alpha U^2+\beta(*U)^2$ *is a Killing tensor if, and only if, the canonical elements* $\{\alpha, \beta, U\}$ *satisfy (37) and (38) and*

$$\mathrm{d}\alpha = (\alpha-\beta)i(\delta * U) * U. \tag{39}$$

This last proposition is the tensorial version of the intrinsic equations for a Killing tensor that are known in Newmann-Penrose formalism (Ref. 5, Theorem 35.4). Now we can easily write the conditions in Theorem 2 in terms of the canonical 2-form U, that is, we obtain the characterization of the Killing and conformal tensor in the sole variable U.

Theorem 3: The 2+2 *structure defined by the unitary simple 2-form U is the eigenstructure of a conformal tensor if, and only if, U satisfies*

$$\Sigma[U] \equiv \nabla\mathcal{U} - i(\delta\mathcal{U})\mathcal{U}\otimes\mathcal{U} - i(\delta\mathcal{U})\mathcal{G} = 0, \tag{40}$$

$$\mathrm{d}\Phi[U] \equiv \mathrm{d}[i(\delta U)U - i(\delta * U) * U] = 0. \tag{41}$$

If these conditions hold, a function α *exists such that* $\Phi[U]=-\mathrm{d}\ln|\alpha|$. *Then, the conformal tensor is* $P=C\alpha[U^2+(*U)^2]$, C *being an arbitrary constant.*

Theorem 4: *The* 2+2 *structure defined by the unitary simple 2-form U is the eigenstructure of a Killing tensor if, and only if, U satisfies*

$$\Sigma[U] \equiv \nabla\mathcal{U} - i(\delta\mathcal{U})\mathcal{U}\otimes\mathcal{U} - i(\delta\mathcal{U})\mathcal{G} = 0, \tag{42}$$

$$\mathrm{d}\Phi[U] \equiv \mathrm{d}[i(\delta U)U - i(\delta * U) * U] = 0, \tag{43}$$

$$\mathrm{d}i(\delta U)U = i(\delta U)U \wedge i(\delta * U) * U. \tag{44}$$

If these conditions hold, two functions α *and* β *exist such that* $\Phi[U]=-\mathrm{d}\ln|\alpha-\beta|$ *and* $\mathrm{d}(\alpha+\beta)=2(\alpha-\beta)[i(\delta U)U+i(\delta * U) * U]$. *Then, the Killing tensor is* $K=C[\alpha U^2-\beta(*U)^2]+Dg$, C *and* D *being two arbitrary constants*

It is worth pointing out that the first order differential properties of a 2+2 structure admit a kinematical interpretation[16] and, in particular, the umbilical conditions (40) and (42) equivalently imply that the two principal null directions of the structure are geodesic and shear-free congruences.[11] Thus, we recover a known result obtained independently by Hauser and Malhiot[7] and by Collinson.[20]

On the other hand, condition (41) states that the structure is pre-Maxwellian.[21,22] Then, taking into account the study of these structures given in Ref. 22 we have the following.

Corollary 2: The 2+2 *traceless tensor* $P=\alpha(v-h)$ *is a conformal tensor if, and only if,* $T=\alpha^{-2}(v-h)$ *is a conservative Maxwell-Minkowski energy tensor and the principal directions of the associated electromagnetic field are geodesic and shear-free congruences.*

IX. PETROV-BEL TYPE D SPACE–TIMES ADMITTING KILLING OR CONFORMAL TENSORS

The results in the preceding sections help us to characterize intrinsically and explicitly some families of metrics. More precisely, in this section: (i) we obtain necessary and sufficient conditions on the metric concomitants for a four-dimensional space–time to be a Petrov-Bel type D solution admitting a 2+2 Killing or conformal tensor and, when they hold, (ii) we give an algorithm to determine these tensors.

In the preceding section we have characterized the 2+2 Killing and conformal tensors in terms of the volume element U of their timelike eigenplane. Moreover, for the case of Petrov-Bel type D metrics, this 2-plane determines the Weyl principal structure and, consequently, U can be obtained from the Weyl tensor. The intrinsic and explicit characterization of type D solutions and the covariant obtaining of the Weyl canonical bivector have been given in Ref. 9. Consequently we can state the following invariant characterizations.

Proposition 11: A Petrov-Bel type D metric admits a conformal tensor if, and only if, the Weyl principal null directions define geodesic shear-free congruences and the Weyl canonical 2-form satisfies (43).

A Petrov-Bel type D metric admits a Killing tensor if, and only if, the Weyl principal null directions define geodesic shear-free congruences and the Weyl canonical 2-form satisfies (43) and (44).

Finally, taking into account the algebraic results for Petrov-Bel type D metrics quoted above (see Ref. 9), we obtain from Theorems 3 and 4 the explicit expression of the conditions in Proposition 11 and the algorithm for obtaining the conformal or Killing tensors.

Theorem 5: Let $\mathcal{W}\equiv\mathcal{W}(g)=\frac{1}{2}(W(g)-\mathrm{i}*W(g))$ *and* $\mathcal{G}\equiv\mathcal{G}(g)=\frac{1}{2}\left(\frac{1}{2}g\wedge g-\mathrm{i}\,\eta(g)\right)$ *the self-dual Weyl tensor and self-dual metric associated with a space–time metric* g, *and let us take the metric concomitants*

$$\rho\equiv-\frac{\mathrm{Tr}\mathcal{W}^3}{\mathrm{Tr}\mathcal{W}^2},\quad \mathcal{S}\equiv\frac{1}{3\rho}(\mathcal{W}-\rho\mathcal{G}),\quad \mathcal{U}\equiv\frac{\mathcal{S}(\mathcal{X})}{\sqrt{\mathcal{S}(\mathcal{X},\mathcal{X})}},\tag{45}$$

$$\Sigma\equiv\nabla\mathcal{U}-i(\delta\mathcal{U})\mathcal{U}\otimes\mathcal{U}-i(\delta\mathcal{U})\mathcal{G},\tag{46}$$

$$U\equiv\sqrt{2}\,\mathrm{Re}\{\mathcal{U}\},\quad \boldsymbol{a}\equiv-i(\delta*U)*U,\quad \boldsymbol{b}\equiv i(\delta U)U,\tag{47}$$

where $\mathcal{X}$ *is an arbitrary self-dual bivector.*

The necessary and sufficient conditions for g *to be a Petrov-Bel type D solution admitting a* 2+2 *conformal tensor are*

$$\rho\neq0,\quad \mathcal{S}^2+\mathcal{S}=0,\quad \Sigma=0,\quad \mathrm{d}(\boldsymbol{a}+\boldsymbol{b})=0.\tag{48}$$

When (48) hold, a function α *exists such that* $-\mathrm{d}\ln|\alpha|=\boldsymbol{a}+\boldsymbol{b}$. *Then, the conformal tensor is* $P=C\alpha[U^2+(*U)^2]$, C *being an arbitrary constant.*

The necessary and sufficient conditions for g *to be a type D solution admitting a* 2+2 *Killing tensor are* 48 *and*

$$\mathrm{d}\boldsymbol{b}+\boldsymbol{b}\wedge\boldsymbol{a}=0.\tag{49}$$

When (48) and (49) hold, two functions α *and* β *exist such that* $-\mathrm{d}\ln|\alpha-\beta|=\boldsymbol{a}+\boldsymbol{b}$ *and* $\mathrm{d}(\alpha+\beta)=2(\alpha-\beta)[\boldsymbol{b}-\boldsymbol{a}]$. *Then, the Killing tensor is* $K=C[\alpha U^2-\beta(*U)^2]+Dg$, C *and* D *being two arbitrary constants.*

For Petrov-Bel type D solutions with a vanishing Cotton tensor (the Weyl tensor is divergence-free) the Bianchi identities take the expression[11]

$$\nabla\mathcal{U} = i(\mathcal{U})[\mathcal{U}\otimes\mathcal{U}+\mathcal{G}], \quad i(\mathcal{U})\mathcal{U} = \tfrac{1}{3}\mathrm{d}\ln\rho, \tag{50}$$

where $\mathcal{U}$ is the Weyl canonical bivector and ρ the double Weyl eigenvalue. The real part of the second equation in (50) states

$$\tfrac{2}{3}\mathrm{d}\ln|\rho| = \Phi[U] \equiv i(\delta U)U - i(\delta * U) * U. \tag{51}$$

Thus, the principal structure of a type D divergence-free Weyl tensor is umbilical and pre-Maxwellian and, as a consequence of Theorem 3, it is the structure of a conformal tensor. Moreover, in this case the eigenvalue of the conformal tensor can be obtained algebraically from the Weyl eigenvalues if we take into account Proposition 9. Thus, we have the following.

Theorem 6: *Every Petrov-Bel type D solution with vanishing Cotton tensor admits a conformal tensor. Let* ρ, $\mathcal{S}$, *and* $\mathcal{U}$ *be the Weyl concomitants given in* (45). *Then we have the following*.

(i) *These space–times are characterized by the conditions*

$$\rho \neq 0, \quad \mathcal{S}^2 + \mathcal{S} = 0, \quad \delta W = 0. \tag{52}$$

(ii) *The conformal tensor is given by*

$$P = C|\rho|^{-2/3}\mathcal{U}\times\tilde{\mathcal{U}}. \tag{53}$$

This theorem generalizes the result about the existence of conformal tensors in Petrov-Bel type D vacuum solutions (see Ref. 5, Theorem 35.2).

We finish with two comments. The characterization of the Killing or conformal tensors in terms of their underlying structure has allowed us to give an explicit and intrinsic labeling of the Petrov-Bel type D space–times admitting Killing or conformal tensors, as well as to generalize some known results on the existence of these symmetries. Furthermore, our Eisenhart-type approach to the Killing and conformal tensor may also be useful in analyzing and extending other properties. For example, it is known that all type D vacuum solutions that admit a Killing tensor, also admit a Killing-Yano tensor.[20,23] Our result here and those given in Ref. 22 allow us to generalize this property. This question and other related topics will be considered elsewhere.[24]

Our study of the geometry of the Killing and conformal tensors and the canonical expressions of the metric tensor in terms of this geometry can be applied, in particular, to n-dimensional Lorentzian metrics. We know that, for four-dimensional Petrov-Bel type D space–times, this underlying geometry is closely related with the Weyl tensor and, this fact allows us to determine the $2+2$ Killing and conformal tensors (see Theorems 5 and 6). The generalization of these results to higher dimensions is an open problem that could be fruitful in some classes of the Weyl tensor. But this study will require a further analysis of the Weyl classification in higher dimensions.[25,26]

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Walker's theorem without coordinates

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We provide a coordinate-free version of the local classification, due to Walker [Q. J. Math. **1**, 69 (1950)], of null parallel distributions on pseudo-Riemannian manifolds. The underlying manifold is realized, locally, as the total space of a fiber bundle, each fiber of which is an affine principal bundle over a pseudo-Riemannian manifold. All structures just named are naturally determined by the distribution and the metric, in contrast with the noncanonical choice of coordinates in the usual formulation of Walker's theorem. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In 1950, Walker[1] described the local structure of all pseudo-Riemannian manifolds with null parallel distributions. The present paper provides a coordinate-free version of Walker's theorem.

Many authors, beginning with Walker himself,[2] have invoked Walker's 1950 result, often to generalize it or derive other theorems from it. In our bibliography, which is by no means complete, Refs. 3–16 all belong to this category. They invariably cite Walker's result in its original, local-coordinate form (reproduced in the Appendix).

Such an approach, perfectly suited for the applications just mentioned, tends nevertheless to obscure the geometric meaning of Walker's theorem. In fact, Walker coordinates are far from unique; choosing them results in making noncanonical objects a part of the structure.

To keep the picture canonical, some authors[3,5] replace a single Walker coordinate system by a whole maximal atlas of them. What we propose here, instead, is to use only ingredients such as fiber bundles, widely seen as more directly "geometric" than a coordinate atlas (even though one may ultimately need atlases to define them).

In our description, the coordinate-independent content of Walker's theorem amounts to realizing the underlying manifold, locally, as a fiber bundle whose fibers are also bundles, namely, affine principal bundles over pseudo-Riemannian manifolds. The bundle structures are all naturally associated with the original null parallel distribution; the distribution and the metric can in turn be reconstructed from them.

II. PRELIMINARIES

Throughout this paper, all manifolds, bundles, sections, subbundles, connections, and mappings, including bundle morphisms, are assumed to be of class C^∞. A bundle morphism may operate only between two bundles with the same base manifold, and acts by identity on the base.

A bundle always means a C^∞ locally trivial bundle and the same symbol, such as M, is used both for a given bundle and for its total space; the bundle projection $M \to \Sigma$ onto the base manifold

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Σ is denoted by π (or, sometimes, p). We let M_y stand for the fiber $\pi^{-1}(y)$ over any $y \in \Sigma$, while $\mathrm{Ker}\, \mathrm{d}\pi$ is the vertical distribution treated as a vector bundle (namely, a subbundle of the tangent bundle TM).

For real vector bundles $\mathcal{X}, \mathcal{Y}$ over a manifold Σ and a real vector space V with $\dim V < \infty$, we denote by $\mathrm{Hom}(\mathcal{X}, \mathcal{Y})$ the vector bundle over Σ whose sections are vector-bundle morphisms $\mathcal{X} \to \mathcal{Y}$, and by $\Sigma \times V$ the product bundle with the fiber V, the sections of which are functions $\Sigma \to V$. Thus, $\mathcal{X}^* = \mathrm{Hom}(\mathcal{X}, \Sigma \times \mathbf{R})$ is the dual of $\mathcal{X}$.

We will say that a given fiberwise structure in a bundle M over a manifold Σ *depends C^∞-differentiably on $y \in \Sigma$*, or *varies C^∞-differentiably with y*, if suitable C^∞ local trivializations of M make the structure appear as constant (the same in each fiber).

The symbol ∇ will be used for various connections in vector bundles. Our sign convention about the curvature tensor $R = R^\nabla$ of a connection ∇ in a vector bundle $\mathcal{X}$ over a manifold Σ is

$$R(u,v)\psi = \nabla_v \nabla_u \psi - \nabla_u \nabla_v \psi + \nabla_{[u,v]} \psi, \tag{1}$$

for sections ψ of $\mathcal{X}$ and vector fields u, v tangent to Σ. By the Leibniz rule, when ∇ is the Levi-Civita connection of a pseudo-Riemannian metric g and u, v, w are tangent vector fields, $2\langle \nabla_w v, u \rangle$ equals[17]

$$d_w\langle v,u\rangle + d_v\langle w,u\rangle - d_u\langle w,v\rangle + \langle v,[u,w]\rangle + \langle u,[w,v]\rangle - \langle w,[v,u]\rangle, \tag{2}$$

where d_v is the directional derivative and $\langle , \rangle$ stands for $g(,)$.

Remark 2.1: Let $\pi: M \to \Sigma$ be a bundle projection. A vector field w on the total space M is π-projectable onto the base manifold Σ if and only if, for every vertical vector field u on M, the Lie bracket $[w,u]$ is also vertical. This well-known fact is easily verified in local coordinates for M which make π appear as a standard Euclidean projection.

III. AFFINE PRINCIPAL BUNDLES

All principal bundles discussed below have Abelian structure groups G, so one need not decide whether G acts from the left or right.

Let N be a G-principal bundle over a base manifold L, where G is an Abelian Lie group. By the *N-prolongation* of the tangent bundle TL we mean the vector bundle $\mathcal{F}$ over L whose fiber $\mathcal{F}_c$ over $c \in L$ is the space of all G-invariant vector fields tangent to N along N_c (and defined just on N_c), with N_c denoting, as usual, the fiber of N over c. A vector subbundle $\mathcal{G} \subset \mathcal{F}$ now can be defined by requiring $\mathcal{G}_c$, for any $c \in L$, to consist of all G-invariant vector fields defined just on N_c which are vertical (i.e., tangent to N_c). Since each $\mathcal{G}_c$ is canonically isomorphic to the Lie algebra $\mathfrak{g}$ of G, the vector bundle $\mathcal{G}$ is naturally trivialized, that is, identified with the product bundle $L \times \mathfrak{g}$. Therefore

$$L \times \mathfrak{g} = \mathcal{G} \subset \mathcal{F}. \tag{3}$$

The quotient bundle $\mathcal{F}/\mathcal{G}$ is in turn naturally isomorphic to TL, via the differential of the bundle projection $N \to L$.

An *affine space* is a set A with a simply transitive action on A of the additive group of a vector space V. One calls V the *vector space of translations* of the affine space A.

An *affine bundle M* over a manifold Σ is a bundle with fibres M_y, $y \in \Sigma$, carrying the structures of affine spaces whose vector spaces $\mathcal{X}_y$ of translations form a vector bundle $\mathcal{X}$ over Σ, called the *associated vector bundle* of M. We also require the affine-space structure of M_y to vary C^∞-differentiably with $y \in \Sigma$, in the sense of Sec. II.

If, in addition, $\mathcal{X} = \Sigma \times V$, that is, the associated vector bundle of M happens to be a product bundle, then M is also a V-principal bundle, with the obvious action of the additive group of the vector space V. Such *affine principal bundles* are distinguished from arbitrary affine bundles by having a structure group that, instead of general affine transformations of a model fiber, contains only translations.

IV. PARTIAL METRICS AND EXTENSIONS

Let $\mathcal{C}$, $\mathcal{D}$, and $\mathcal{E}$ be real vector bundles over a manifold Q. By an $\mathcal{E}$-valued *pairing* of $\mathcal{C}$ and $\mathcal{D}$ we mean any vector-bundle morphism $\beta:\mathcal{C}\otimes\mathcal{D}\to\mathcal{E}$. This amounts to a C^∞ assignment of a bilinear mapping $\beta(z):\mathcal{C}_z\times\mathcal{D}_z\to\mathcal{E}_z$ to every $z\in Q$. An $\mathcal{E}$-valued *partial pairing* of $\mathcal{C}$ and $\mathcal{D}$ consists, by definition, of two vector subbundles $\mathcal{C}'\subset\mathcal{C}$ and $\mathcal{D}'\subset\mathcal{D}$, of some codimensions k and l, along with pairings $\gamma:\mathcal{C}\otimes\mathcal{D}'\to\mathcal{E}$ and $\gamma:\mathcal{C}'\otimes\mathcal{D}\to\mathcal{E}$ which coincide on the subbundle $\mathcal{C}'\otimes\mathcal{D}'$ (and so may be represented by the same symbol γ without risk of ambiguity). One can obviously restrict a given pairing $\beta:\mathcal{C}\otimes\mathcal{D}\to\mathcal{E}$ to $\mathcal{C}\otimes\mathcal{D}'$ and $\mathcal{C}'\otimes\mathcal{D}$, so that a partial pairing γ is obtained; we will then say that β is a *total-pairing extension* of γ.

Lemma 4.1: *For any fixed partial pairing* γ, *with* $\mathcal{C}$, $\mathcal{D}$, $\mathcal{E}$, $\mathcal{C}'$, $\mathcal{D}'$, k, l, *and* Q *as above*, *and with* m *denoting the fiber dimension of* $\mathcal{E}$, *the total-pairing extensions of* γ *coincide with sections of a specific affine bundle of fiber dimension klm over* Q, *whose associated vector bundle is* $\mathrm{Hom}(\mathcal{C}/\mathcal{C}'\otimes\mathcal{D}/\mathcal{D}',\mathcal{E})$.

Proof: Our γ is nothing else than a vector-bundle morphism $\mathcal{X}\to\mathcal{E}$, where $\mathcal{X}\subset\mathcal{C}\otimes\mathcal{D}$ is the subbundle spanned by $\mathcal{C}\otimes\mathcal{D}'$ and $\mathcal{C}'\otimes\mathcal{D}$. The affine bundle in question is the preimage of the section γ under the (surjective) restriction morphism $\mathrm{Hom}(\mathcal{C}\otimes\mathcal{D},\mathcal{E})\to\mathrm{Hom}(\mathcal{X},\mathcal{E})$. □

As usual,[5] by a *pseudo-Riemannian fiber metric* g in a vector bundle $\mathcal{T}$ over a manifold M we mean any family of nondegenerate symmetric bilinear forms $g(x)$ in the fibers $\mathcal{T}_x$ that constitutes a C^∞ section of the symmetric power $(\mathcal{T}^*)^{\odot 2}$. Equivalently, such g is a pairing of $\mathcal{T}$ and $\mathcal{T}$ valued in the product bundle $M\times\mathbf{R}$, symmetric and nondegenerate at every point of M.

Let $\mathcal{T}$ again be a vector bundle over a manifold M. We define a *partial fiber metric* in $\mathcal{T}$ to be a triple $(\mathcal{P},\mathcal{P}',\alpha)$ formed by vector subbundles $\mathcal{P}$ and $\mathcal{P}'$ of $\mathcal{T}$ along with a pairing $\alpha:\mathcal{P}'\otimes\mathcal{T}\to M\times\mathbf{R}$, valued in the product bundle $M\times\mathbf{R}$, such that

(i) $\mathcal{T},\mathcal{P}$, and $\mathcal{P}'$ are of fiber dimensions n,r and, respectively, $n-r$ for some n,r with $0\le r\le n/2$, while $\mathcal{P}\subset\mathcal{P}'$,
(ii) at every $x\in M$ the bilinear mapping $\alpha(x):\mathcal{P}'_x\times\mathcal{T}_x\to\mathbf{R}$ has the rank $n-r$, its restriction to $\mathcal{P}'_x\times\mathcal{P}'_x$ is symmetric, and its restriction to $\mathcal{P}'_x\times\mathcal{P}_x$ equals 0.

By a *total-metric extension* of $(\mathcal{P},\mathcal{P}',\alpha)$ we then mean any pseudo-Riemannian fiber metric in $\mathcal{T}$ whose restriction to $\mathcal{P}'\otimes\mathcal{T}$ is α.

Lemma 4.2: *The total-metric extensions* g *of any partial fiber metric* $(\mathcal{P},\mathcal{P}',\alpha)$, *with* r,M *as above*, *coincide with the sections of a specific affine bundle of fiber dimension* $r(r+1)/2$ *over* M. *For every such* g *the subbundle* $\mathcal{P}$ *is* g*-null and* $\mathcal{P}'$ *is its* g*-orthogonal complement*.

Proof: For any fixed point $x\in M$, let us choose a basis $e_1,\ldots,e_n$ of $\mathcal{T}_x$ such that $e_1,\ldots,e_r\in\mathcal{P}_x$ and $e_1,\ldots,e_{n-r}\in\mathcal{P}'_x$. The matrix of $g(x)$, for any total-metric extension g of our partial fiber metric, then is the matrix appearing in Walker's original theorem (see the Appendix), with $\det A\neq 0$, and with the two occurrences of I replaced by some nonsingular $r\times r$ matrix C and its transpose C'. The submatrices A,H,C (and H',C') are prescribed, while the freedom in choosing $g(x)$ is represented by an arbitrary symmetric $r\times r$ matrix B. □

V. WALKER'S THEOREM

Suppose that the following data are given:

(a) Integers n and r with $0\le r\le n/2$.
(b) An r-dimensional manifold Σ.
(c) A bundle over Σ with some total space M, whose every fiber M_y, $y\in\Sigma$, is a $T^*_y\Sigma$-principal bundle over a $(n-2r)$-dimensional manifold Q_y (cf. the last paragraph of Sec. III).
(d) A pseudo-Riemannian metric h_y on each $Q_y, y\in\Sigma$.

We assume that all y-dependent objects in (c) and (d), including the principal-bundle structure,

vary C^∞-differentiably with $y \in \Sigma$ (in the sense of Sec. II) and, in particular, the Q_y are the fibers of a bundle over Σ with a total space Q of dimension $n-r$. When $r=n/2$, each h_y is the "zero metric" on the discrete space Q_y, cf. Sec. VIII.

Let $\mathcal{F}$ be the vector bundle over Q whose restriction to Q_y, for each $y \in \Sigma$, is the M_y-prolongation of the tangent bundle TQ_y (see Sec. III) for the $T^*_y\Sigma$-principal bundle M_y over Q_y. Relation (3) now yields $\mathrm{p}^*(T^*\Sigma) \subset \mathcal{F}$, where $\mathrm{p}: Q \to \Sigma$ denotes the bundle projection. In other words, $\mathrm{p}^*(T^*\Sigma)$ may be treated as a vector subbundle of $\mathcal{F}$.

Furthermore, the quotient-bundle identification following formula (3) yields $\mathcal{F}/\mathrm{p}^*(T^*\Sigma) = \mathrm{Ker}\, \mathrm{dp}$ (the vertical subbundle of TQ, for the projection $\mathrm{p}: Q \to \Sigma$).

We define a partial pairing γ of $\mathcal{F}$ and TQ valued in the product bundle $Q \times \mathbf{R}$, as in Sec. IV, for our Q along with $\mathcal{C}=\mathcal{F}$, $\mathcal{D}=TQ$, $\mathcal{E}=Q\times\mathbf{R}$, $\mathcal{C}'=\mathrm{p}^*(T^*\Sigma)$ and $\mathcal{D}'=\mathrm{Ker}\, \mathrm{dp}$. Namely, given $z \in Q$, we set $\gamma(\xi,\zeta)=\xi(\mathrm{dp}_z\zeta)$ for $\xi \in T^*_y\Sigma=[\mathrm{p}^*(T^*\Sigma)]_z$ and $\zeta \in T_zQ$, with $y=\mathrm{p}(z) \in \Sigma$, as well as $\gamma(u,\psi)=h_y([u],\psi)$ for $u \in \mathcal{F}_z$ and $\psi \in \mathrm{Ker}\, \mathrm{dp}_z$, where $u \mapsto [u]$ denotes the surjective vector-bundle morphism $\mathcal{F} \to \mathrm{Ker}\, \mathrm{dp}$ with the kernel $\mathrm{p}^*(T^*\Sigma)$.

Our construction has two steps involving arbitrary choices.

Step 1: We choose $\beta: \mathcal{F} \otimes TQ \to Q \times \mathbf{R}$ to be any total-pairing extension of γ.

According to Lemma 4.1, such β is just an arbitrary section of an affine bundle of fiber dimension $(n-2r)r$ over Q. For the meaning of the above discussion in Walker's original language, see the Appendix.

The remainder of our construction proceeds as follows. Using β, we define a partial metric $(\mathcal{P},\mathcal{P}',\alpha)$ in the tangent bundle TM. Specifically, $\mathcal{T},\mathcal{P},\mathcal{P}'$ and n,r with the properties listed in (i) and (ii) of Sec. IV are chosen so that $\mathcal{T}=TM$, while n,r are the integers in (a) above, $\mathcal{P}$ is the subbundle of TM whose restriction to $M_y \subset M$, for each $y \in \Sigma$, is the vertical distribution on the $T^*_y\Sigma$-principal bundle M_y over Q_y, and $\mathcal{P}'=\mathrm{Ker}\, \mathrm{d}\pi$ is the vertical distribution of the bundle projection $\pi: M \to \Sigma$. We also set $\alpha(u',w)=\beta(u,\zeta)$ for any $x \in M$ and any vectors $w \in T_xM$, $u' \in \mathcal{P}'_x=T_xM_y$ with $y=\pi(x) \in \Sigma$, where u is the $T^*_y\Sigma$-invariant vector field tangent to M_y along the $T^*_y\Sigma$-orbit of x and having the value u' at x, while ζ is the image of w under the differential at x of the bundle projection $M \to Q$.

Step 2: We select an arbitrary total-metric extension g of $(\mathcal{P},\mathcal{P}',\alpha)$ restricted to U, where U is any fixed nonempty open subset of M.

The construction just described gives a null distribution $\mathcal{P}$ of dimension r on the n-dimensional pseudo-Riemannian manifold (U,g). This is clear from Lemma 4.2, which also implies that such metrics g are just arbitrary sections of some affine bundle over U.

The reader is again referred to the Appendix for a description of what the above steps correspond to in Walker's formulation.

We can now state a coordinate-free version of Walker's theorem.

Theorem 5.1: *If g and $\mathcal{P}$ are obtained as above from any prescribed data* (a)–(d), *then g is a pseudo-Riemannian metric on the n-dimensional manifold U, and $\mathcal{P}$ is a g-null, g-parallel distribution of dimension r on U.*

Conversely, up to an isometry, every null parallel distribution $\mathcal{P}$ on a pseudo-Riemannian manifold (M,g) is, locally, the result of applying the above construction to some data (a)–(d). *The data themselves are naturally associated with g and $\mathcal{P}$.*

A proof of Theorem 5.1 is given in the next two sections.

VI. PROOF OF THE FIRST PART OF THEOREM 5.1

By Lemma 4.2, $\mathcal{P}$ is g-null and $\mathcal{P}'$ is its g-orthogonal complement. That $\mathcal{P}$ is g-parallel will be clear if we establish the relation $\langle \nabla_w v, u\rangle = 0$, where ∇ is the Levi-Civita connection of g and $\langle,\rangle$ stands for $g(,)$, while v,u,w are any vector fields tangent to M such that v is a section of $\mathcal{P}$ and u is a section of $\mathcal{P}'$. We may further require w to be projectable under both bundle projections $M \to Q$ and $\pi: M \to \Sigma$. Finally, we may also assume that v restricted to each $T^*_y\Sigma$-principal bundle space M_y is an infinitesimal generator of the action of $T^*_y\Sigma$, while u restricted to each M_y is $T^*_y\Sigma$-invariant, (Locally, such w,v,u span the vector bundles $TM,\mathcal{P}$ and $\mathcal{P}'$.)

First, $[w,v]$ is a section of $\mathcal{P}$ and $[u,w]$ is a section of $\mathcal{P}'$ (from Remark 2.1 applied to both bundle projections), while $[v,u]=0$ by $T_y^*\Sigma$-invariance of u. The last three terms in (2) thus all equal zero.

Our claim will follow if we show that the first three terms in (2) vanish as well. To this end, note that $d_w\langle v,u\rangle=0$ since $\langle v,u\rangle=0$. Next, $d_v\langle w,u\rangle=0$. Namely, $\langle w,u\rangle=\alpha(u,w)=\beta(u,\zeta)$, for α,β,ζ described in Sec. V, is constant in the direction of v (and, in fact, constant along each leaf of $\mathcal{P}$): at a point $x\in M_y\subset M$ we obtain ζ as the projection image of $w(x)$, while u is $T_y^*\Sigma$-invariant, so that, due to projectability of w, both u and ζ depend only on the image of x under the bundle projection $M\to Q$, rather than x itself. Finally, $d_u\langle w,v\rangle=0$ as $\langle w,v\rangle=\xi(\tilde{w})$ is a function $\Sigma\to\mathbf{R}$, that is, a function $M\to\mathbf{R}$ constant along $\mathcal{P}'$. Here ξ is the section of $T^*\Sigma$ corresponding to v under the inclusion $\mathrm{p}^*(T^*\Sigma)\subset\mathcal{F}$ of Sec. V, while $\tilde{w}$ is the vector field on Σ onto which w projects; therefore, $\langle w,v\rangle=\xi(\tilde{w})$, since in Sec. V we set $\gamma(\xi,\zeta)=\xi(\mathrm{dp}_z\zeta)$.

VII. PROOF OF THE SECOND PART OF THEOREM 5.1

For any null parallel distribution $\mathcal{P}$ of dimension r on an $n-$dimensional pseudo-Riemannian manifold (M,g), the g-orthogonal complement $\mathcal{P}^\perp$ is a parallel distribution of dimension $n-r$. If the sign pattern of g has i_- minuses and i_+ pluses, it follows that

$$r\le\min(i_-,i_+), \tag{4a}$$

$$\mathcal{P}\subset\mathcal{P}^\perp, \tag{4b}$$

$$r\le n/2. \tag{4c}$$

In fact, $\mathcal{P}$ is null, which gives (4b) and $r\le n-r$, that is (4c), while (4a) follows since, in a pseudo-Euclidean space with the sign pattern as above, i_- (or, i_+) is the maximum dimension of a subspace on which the inner product is negative (or, positive) semidefinite.

Every null parallel distribution $\mathcal{P}$ satisfies the curvature relations

$$R(\mathcal{P},\mathcal{P}^\perp,-,-)=0, \tag{5a}$$

$$R(\mathcal{P},\mathcal{P},-,-)=0, \tag{5b}$$

$$R(\mathcal{P}^\perp,\mathcal{P}^\perp,\mathcal{P},-)=0, \tag{5c}$$

(5a) meaning that $R(v,u,w,w')=0$ whenever v,u,w,w' are vector fields, v is a section of $\mathcal{P}$, and u is a section of $\mathcal{P}^\perp$. [Similarly for (5b) and (5c).] In fact, for such v,u,w,w', (1) implies that $R(w,w')v$ is a section of $\mathcal{P}$, and so it is orthogonal to u. This proves (5a); (5a) and (4b) yield (5b), while (5a) and the first Bianchi identity give (5c).

We now show how a null parallel distribution $\mathcal{P}$ on a pseudo-Riemannian manifold (M,g) gives rise to objects (a)–(d) in Sec. V.

First, n and r are the dimensions of M and $\mathcal{P}$. By (4c), $r\le n/2$.

Being parallel, the distribution $\mathcal{P}^\perp$ is integrable. Since our discussion is local, we will assume, from now on, that M is the total space of a bundle over some r-dimensional base manifold Σ, whose fibers M_y, $y\in\Sigma$, are all contractible and coincide with the leaves of $\mathcal{P}^\perp$. As $\mathcal{P}$ is parallel, the Levi-Civita connection ∇ induces a connection in the vector bundle obtained by restricting $\mathcal{P}$ to any given submanifold N of M. In the case where $N=M_y$ is a leaf of $\mathcal{P}^\perp$, we have, for each $y\in\Sigma$, the following conclusion.

$$\begin{aligned}&T_y^*\Sigma \text{ is naturally isomorphic to the space } V_y \text{ of those sections of the restriction}\\&\text{of } \mathcal{P} \text{ to } M_y \text{ which are parallel (along } M_y).\end{aligned} \tag{6}$$

Instead of establishing (6) directly, we will show that *sections of $T^*\Sigma$ can be naturally identified with sections of $\mathcal{P}$ parallel along $\mathcal{P}^\perp$*, using an identification which is clearly valuewise, i.e., consists of operators $V_y \to T^*_y\Sigma, y \in \Sigma$. To this end, we denote by π the bundle projection $M \to \Sigma$. Every vector field on Σ is the π-image $(\mathrm{d}\pi)w$ of some π-projectable vector field w on M. Let v now be a section of the vector bundle $\mathcal{P}$ over M, parallel in the direction of $\mathcal{P}^\perp$. Our identification associates with v the cotangent vector field ξ on Σ that sends each vector field $(\mathrm{d}\pi)w$ to $g(v,w)$ treated as a function $\Sigma \to \mathbf{R}$. Note that ξ is well defined: two π-projectable vector fields w on M with the same π-image $(\mathrm{d}\pi)w$ differ by a section of $\mathcal{P}^\perp = \mathrm{Ker}\,\mathrm{d}\pi$, necessarily orthogonal to v, so that $g(v,w)$ is the same for both choices of w. Also, $g(v,w): M \to \mathbf{R}$ actually descends to a function $\Sigma \to \mathbf{R}$, i.e., is constant along the fibers M_y (leaves of $\mathcal{P}^\perp$). In fact, $d_u[g(v,w)]=0$ for any section u of $\mathcal{P}^\perp$, as $\nabla_u v = 0$ in view of the assumption about v, and $\nabla_u w = [u,w] + \nabla_w u$, while $[u,w]$ (or $\nabla_w u$) is a section of $\mathcal{P}^\perp$ by Remark 2.1 (or, since $\mathcal{P}^\perp$ is parallel).

Injectivity of the above assignment $v \mapsto \xi$ is obvious, since π-projectable vector fields w span TM. Surjectivity of the resulting operators $V_y \to T^*_y\Sigma$ now follows: both spaces have the same dimension, as the connections induced by ∇ in the restrictions of $\mathcal{P}$ to the leaves M_y are flat in view of (5c) [cf. (1)]. This proves (6).

Flatness of the induced connections also implies that the leaves of $\mathcal{P}$ contained in any given leaf M_y of $\mathcal{P}^\perp$ are the fibers of a V_y-principal bundle with the total space M_y over some base manifold Q_y. (Here M should be replaced with an open subset, if necessary.) Since each $T^*_y\Sigma$ is identified with V_y by (6), we thus obtain the data (c) of Sec. V.

Next, we define the metric h_y on each Q_y, required by (d) in Sec. V, so that it assigns the function $g(u,u')$ to two vector fields on Q_y which are images, under the $T^*_y\Sigma$-principal bundle projection $M_y \to Q_y$, of $T^*_y\Sigma$-invariant vector fields u, u' on M_y. Constancy of $g(u,u')$ along the $T^*_y\Sigma$-orbits, meaning that $d_v[g(u,u')]=0$ for any section v of $\mathcal{P}$ defined on M_y and parallel along $\mathcal{P}^\perp$, now follows: as v is $\mathcal{P}^\perp$-parallel and u is $T^*_y\Sigma$-invariant, we have $\nabla_u v = [v,u] = 0$, cf. (6), so that $\nabla_v u = 0$. For the same reason, $\nabla_v u' = 0$.

Finally, a suitable version of the construction in Sec. V, applied to the data (a)–(d) defined above, leads to the original g and $\mathcal{P}$, which is a consequence of how the identification (6) and the definition of h_y use g. The choices of the total-pairing and total-metric extensions, required in Sec. V, are provided by g as well. For instance, β in Step 1 is given by $\beta(u,\zeta) = g(u,w)$, where u is a section of $\mathcal{P}^\perp$ commuting with every section v of $\mathcal{P}$ that is parallel along $\mathcal{P}^\perp$, and ζ is a vector field on Q (the union of all Q_y), while w is any vector field on M projectable onto ζ under the bundle projection $M \to Q$. That $g(u,w)$ depends just on u and ζ (but not on w) is clear: two choices of w differ by a section of $\mathcal{P}$. Also, $g(u,w)$ is constant in the direction of $\mathcal{P}$ (and so it may be treated as a function $Q \to M$). Namely, $d_v[g(u,w)]=0$ for any section v of $\mathcal{P}$ parallel along $\mathcal{P}^\perp$, which follows as $\nabla_v u = \nabla_u v = 0$ (note that $[u,v]=0$), while $\nabla_v w = [v,w] + \nabla_w v$, and $[v,w]$ (or $\nabla_w v$) is a section of $\mathcal{P}$ by Remark 2.1 (or, respectively since $\mathcal{P}$ is parallel). This completes the proof of Theorem 5.1.

VIII. THE MID-DIMENSIONAL CASE

For an r-dimensional null parallel distribution $\mathcal{P}$ on a pseudo-Riemannian manifold (M,g) of dimension $n=2r$, the discussion in Sec. V amounts to nothing new: implicitly at least, it is already present in Sec. (6) of Walker's original paper.[1] See also Sec. 9 in Ref. 3. (A related global result is Theorem 5 in Ref. 5.) In this section we point out how the construction may be simplified when $n=2r$.

Let $\mathcal{P}$ and (M,g) be as above, with $n=2r\geq 2$. The relations $i_- + i_+ = n$ and (4a) imply that g has the *neutral* sign pattern: $i_- = i_+ = r = n/2$. In (c) and (d) of Sec. V, each Q_y is a 0-dimensional (discrete) manifold, and h_y is the "zero metric" on Q_y. Also, the choice of a total-pairing extension β in Step 1 of Sec. V is now unique: the affine bundle having β as a section is of fiber dimension 0. The construction in Sec. V can therefore be rephrased as follows. Given

(a) an even integer $n \geq 2$,
(b) a manifold Σ of dimension $r = n/2$,

(c) an affine bundle over Σ with some total space M, for which $T^*\Sigma$ is the associated vector bundle (Sec. III),

we define a partial metric $(\mathcal{P},\mathcal{P}',\alpha)$ in the tangent bundle TM by choosing $\mathcal{P}=\mathcal{P}'$ to be the vertical distribution $\operatorname{Ker} \mathrm{d}\pi$ for the bundle projection $\pi: M\to\Sigma$, and setting $\alpha(\xi,w)=\xi(\mathrm{d}\pi_x w)$ for any $x \in M, \xi\in\mathcal{P}_x=T^*_y\Sigma$, where $y=\pi(x)$, and $w\in T_xM$. Selecting any total-metric extension g of $(\mathcal{P},\mathcal{P}',\alpha)$ on a fixed nonempty open set $U\subset M$, we now obtain an n-dimensional pseudo-Riemannian manifold (U,g) on which $\mathcal{P}$ is a g-null, g-parallel distribution of dimension $r=n/2$.

Conversely, up to an isometry, every null parallel distribution $\mathcal{P}$ of dimension $r\geq 1$ on a pseudo-Riemannian manifold (M,g) with $\dim M=2r$ arises, locally, from the above construction applied to some data (a)–(c), themselves naturally determined by g and $\mathcal{P}$.

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APPENDIX: WALKER'S ORIGINAL STATEMENT

Walker stated his classification result as follows.[1]

Theorem 1: *A canonical form for the general V_n of class C^∞ (or C^ω) admitting a parallel null r-plane is given by the fundamental tensor*

$$(g_{ij})=\begin{pmatrix} O & O & I \\ O & A & H \\ I & H' & B \end{pmatrix},$$

where I is the unit $r\times r$ matrix and A,B,H,H' are matrix functions of the coordinates, of the same class as V_n, satisfying the following conditions but otherwise arbitrary:

(i) *A and B are symmetric, A is of order $(n-2r)\times(n-2r)$ and nonsingular, B is of order $r\times r$, H is of order $(n-2r)\times r$, and H' is the transpose of H.*

(ii) *A and H (and therefore H') are independent of the coordinates $x^1,\ldots,x^r$.*

A basis for the parallel null r-plane is the set of vectors $\delta^i_1,\delta^i_2,\ldots,\delta^i_r$.

Here is how the coordinates and matrix functions appearing above correspond to the objects used for the construction in Sec. V. Walker's coordinates $x^i, i=1,\ldots,n$, serve as a coordinate system for the manifold M of Sec. V. Coordinates for other manifolds appearing in Sec. V are obtained from x^i by restricting the range of the index i, to $i>n-r$ (for Σ), $i>r$ (for Q), $i\leq n-r$ (for each M_y) and $r<i\leq n-r$ (for each Q_y). The center submatrix A in Walker's matrix corresponds to the family $h_y, y\in\Sigma$, of pseudo-Riemannian metrics [(d) in Sec. V] and, consequently, also to the formula for $\gamma(u,\psi)$, while the last two matrices $O\ I$ in the first row represent the definition of $\gamma(\xi,\zeta)$. The Walker-matrix counterpart of the extension β chosen in Step 1 is the $(n-r)\times(n-r)$ submatrix with the rows $O\ I$ and $A\ H$, so that the freedom in choosing β amounts to arbitrariness in the selection of H (and H is independent of the coordinates $x^i, i=1,\ldots,r$, which translates into the fact that β is a morphism of vector bundles over the manifold Q with the coordinates $x^i, i>r$). Once chosen, β is used in Sec. V to define $\mathcal{P},\mathcal{P}'$ and α. In terms of Walker's coordinates and matrix functions, $\mathcal{P}$ (or, $\mathcal{P}'$) is spanned by the x^i coordinate directions with $i\leq r$ (or, respectively, $i\leq n-r$), while the analog of α is the $(n-r)\times n$ submatrix with the rows $O\ O\ I$ and $O\ A\ H$. Finally, the extension in Step 2 is nothing else than augmenting this last submatrix by a third row, $I\ H'B$, in which B is completely arbitrary.

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Two-component cosmological fluids with gravitational instabilities

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A survey of linearized cosmological fluid equations with a number of different matter components is made. To begin with, the one-component case is reconsidered to illustrate some important mathematical and physical points rarely discussed in the literature. The work of some previous studies of two-component systems are examined and reanalyzed to point out some deficiencies of solutions, and further solutions and physical interpretation are then presented. This leads into a general two-component model with variable velocity dispersion parameters and mass density fractions of each component. The equations, applicable to both hot dark matter (HDM) and cold dark matter (CDM) universes are solved in the long wavelength limit. This region is of interest, because some modes in this range of wave numbers are Jeans unstable. The mixture Jeans wave number of the two-component system is introduced and interpreted, and the solutions are discussed, particularly in comparison to analogous solutions previously derived for plasma modes. This work is applicable to that region in the early Universe ($20<z<140$), where large scale structure formation is thought to have occurred. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209172]

I. INTRODUCTION

The theory of structure formation in the Universe has become one of the most popular and intensely studied topics in modern cosmology. Throughout the past century there has been an accumulating volume of work on the analytic investigation of the cosmological structure formation equations. The various approaches include both fluid and kinetic theory formulations. They principally consider the gravitational interaction of components of the cosmological medium, though sometimes other forms of interaction such as magnetic fields are also included (for some standard examples see, e.g., Refs. 1 and 2). The analysis of these equations has employed ever more diverse and complicated techniques and approximation schemes to model increasingly realistic physical situations. This has been comprehensively supported and now superseded by large *N*-body simulations. The algorithms which govern these large numerical studies have grown progressively more refined and subtle, and are now producing very accurate and realistic results, which can be directly compared with observations (e.g., Ref. 3).

Despite the current trends in modern cosmological structure formation theory, much can still be learned from relatively simple analytic models. We consider such models, in the face of modern computing power, to analyze at a fundamental level some of the basic physical processes which cause the clustering observed in the Universe. This helps to isolate physical mechanisms difficult to discern numerically. In this paper our interest will focus on the linearized cosmological fluid equations. These equations have been used to build up the components of the cosmological density perturbation power spectrum, and must be evolved through the various stages of cosmological

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evolution, and over a large range of physical scales. There are several reasons for taking such an approach. The equations may be solved numerically to give detailed power spectra for the various cosmological models currently viable. The power spectra may then be used as initial data to evolve the large *N*-body simulations, which are ultimately compared to observations. The equations may also be used to build up a semiquantitative picture of the evolution of the power spectrum. This can show how the various sized perturbations scale with respect to the Friedmann expansion parameter a during different epochs of the Universe, and give a direct insight into some of the fundamental physical processes operating to produce structure in the Universe (see, e.g., Ref. 1).

The evolution of perturbation modes with wavelength greater than the Hubble radius may be studied through a relativistic formulation of the perturbation equations, whereas for modes with wavelengths smaller than this radius, a Newtonian formalism suffices. There is a range of physical parameters and variety of differential equations describing the evolution processes of density fluctuations in the early Universe. This involves such elements as equations of state for energy constituents, and specification of the expansion parameter a by the Friedmann cosmological equations. As a consequence, there is a large wealth of literature on this subject, and most of the currently important techniques and results have been collected in some well-known textbooks.[1,2,4] Some of the relatively complicated systems of equations have also been studied in the literature, and it is our goal to both review many of these studies, and to extend them in new directions, achieving some new unique results.

In this paper we will only study the Newtonian limit of the linearized cosmological perturbation equations, valid for density fluctuations on scales well within the Hubble radius. Our main concern is with some mathematically more complicated multicomponent models, which although not usually considered in standard power spectrum analysis, have realistic and interesting physical meaning. The primary concept of the Jeans gravitational instability[5] has been investigated in a static universe for multicomponent models, to reveal the more complicated structure of modes possible.[6,7] This provides some interesting qualitative ideas about the possible mechanisms for structure formation, but the lack of an expanding background space–time in the models leads to unrealistic solutions, exponential in form. The inclusion of cosmological expansion in the equations leads to the more realistic power law and logarithmic solutions, familiar from the standard power spectrum analysis. Previous work in this area has focused both on some particular models,[8] and on a more general classification of the equations and solutions for a range of parameter values (some of them only of mathematical interest) and physical contexts.[9–11] Analytic solutions for some of the most general cases of the equations considered above, which often have significant physical interest, have not been achieved. It is our aim here to rectify this situation and investigate a system of equations modeling a two-component fluid in the matter dominated post-recombination era of an Einstein-deSitter universe. One of these components consists of baryons, and the other some form of nonrelativistic dark matter particles. Through this work we will amend what appear to be some errors in the previous general studies of Haubold and Mathai.[11]

This paper makes a comprehensive study of the linear perturbation equations for cosmological fluids with gravitational instabilities with application to large scale structure formation. For a historical perspective we note that Lifshitz[12] concluded that gravitational instability could not be responsible for the formation of structure in the Universe. The correct conclusion, that gravitational instability suffices, was pointed out by Novikov.[13] As our work details the mathematical structure of the appropriate equations describing cosmological structure formation, we note the nice series of papers by Ratra and Peebles[14] directed to understanding the applications of special functions to the problem of gravitational instability in cosmological models. We further note the nice series by Buchert *et al.*[15] concerning analytic results and their relevance to observational cosmology.

We will also make a comparison with work done in cosmological plasma physics in an Einstein-deSitter background.[16–18] This is interesting due to the mathematically very similar form of fluid equations for both types of systems. This similarity is largely due to the similarity of the electromagnetic and gravitational forces. In this paper we will analyze the long wavelength region

of the solutions. This corresponds to the Jeans unstable region of parameter space, and requires use of Frobenius methods of expansion of the differential equations. In a follow-up paper[19] we will investigate the short wavelength region of the solutions, which will require a WKB approximation scheme to be developed.

In these papers we take explictly the temperature relationship $T \sim 1/a(t)^2$, where $a(t)$ is the radius of the Universe. We give here the explanation why this is so. Following standard textbook material in Padmanabhan[1] [as summarized in equation (3.118)] and Peebles (1993, p. 179) we find that the baryons follow this relationship when

$$1 + z = 142(\Omega_b h^2/0.024)^{2/5}.$$

Here Ω_b has been scaled to the WMAP best fit value. Thus for redshifts below $z \sim 140$ the baryon temperature drops as $1/a^2$ down to $z \sim 20$, where the Universe reionizes (probably in a patchy fashion) and the $1/a^2$ scaling no longer holds. This $20 < z < 140$ redshift region is important, as it is where early large scale structure formation is thought to have occurred.

The paper is to be organized as follows. In Sec. II we introduce the most general cosmological density perturbation equations in the Newtonian approximation. We review and classify previous work on these equations to put our current work into context, showing what has been achieved, what needs amendment, and where we will seek to expand current knowledge. In Sec. III we revert to the one-component equations, to illustrate some of the basic principles which will be important later in our analysis, and to reveal some apparently new results. This will enable us to begin to tackle the two-component problem in Sec. IV. In this section the CDM two-component model in an expanding universe will be investigated. This has ties with the previous work cited, and we will demonstrate the limitations of the existing formalism here. We present new results apparently overlooked in the work of Haubold and Mathai.[11] After this, we are ready to study the most general baryonic and dark matter equations in Sec. V, where we will consider the long wavelength approximation, applicable to either HDM or CDM. This is followed by our conclusions in Sec. VI.

II. A CLASSIFICATION OF COSMOLOGICAL DENSITY PERTURBATION EQUATIONS

As discussed in Sec. I, there are a vast spectrum of equations describing cosmological density perturbations in different physical regimes. We begin directly with the linearized Newtonian approach. The equations for an n-component system of nonrelativistic species is derived in all the standard texts. Given a density perturbation δ_i in the ith component of the mass density ρ_i,

$$\delta_i(\mathbf{r},t) = \frac{\delta\rho_i}{\rho_i}, \tag{2.1}$$

it may be decomposed into its Fourier plane wave modes with wave vector $\mathbf{k}$,

$$\delta_i(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int \delta_{\mathbf{k}i}(t)\exp(-i\mathbf{k}\cdot\mathbf{r})d^3r. \tag{2.2}$$

Here $\mathbf{r}$ is the physical spatial coordinate, and t is cosmic time.

To be able to solve the equations, the implicit time dependence of the physical variables needs to be removed. We will adopt the convention that barred variables will denote comoving quantities, independent of time. Thus we define the comoving wave number $\bar{\mathbf{k}} = a\mathbf{k}$. Using the Eulerian equations of motion describing a perfect fluid, a set of coupled second order equations for the Fourier modes $\delta_i(t)$ (where we now drop the subscript $\mathbf{k}$) are achieved:

$$\frac{d^2\delta_i}{\mathrm{d}t^2} + 2\frac{\dot{a}}{a}\frac{\mathrm{d}\delta_i}{\mathrm{d}t} + \frac{v_i^2\bar{k}^2}{a^2}\delta_i = 4\pi G\sum_{i=1}^{n}\rho_i\delta_i, \quad i = 1,2,\ldots,n. \tag{2.3}$$

Overdots will denote derivatives with respect to t. The above equations contain the sound velocity

$$v_i^2 = \frac{\mathrm{d}p_i}{\mathrm{d}\rho_i} \propto \rho_i^{\gamma_i - 1}. \tag{2.4}$$

The sound velocity depends on the equation of state of the medium, and is in general dependent on time. We have introduced the specific heat ratio γ_i, and assumed an equation of state of the form $p_i \propto \rho_i^{\gamma_i}$.

The introduction of a sound velocity implicitly assumes that the fluids involved are collisional. This means that there are considerable interactions between the particles comprising each matter component. It is in fact generally assumed that dark matter is *collisionless*, in which case a fluid equation is not strictly correct. The dark matter component would better be modeled by a distribution function satisfying the Vlasov equation. "Fluid-like" equations can still be derived in this case by taking velocity moments of the Vlasov equation, and identifying the velocity dispersion with the above parameter v_i. Thus although in the present paper we will refer to "sound velocities," this should be taken as a generic expression for a velocity dispersion parameter. Such an approach should work fine for CDM, but may neglect an important damping term found in HDM models. The complete analogous equation to (2.3) for HDM gives a fluid equation perspective on free-streaming, the phenomenon found in HDM models of neutrinolike matter. An approximate equation has been derived for a hot neutrinolike component by Setayeshgar,[20] which tends to wipe out perturbations below a certain scale (see also the lecture notes by Bertschinger[21]). In this work the exact Vlasov equation kinetic treatment was considered, and the usual Fermi-Dirac distribution function was replaced by a carefully chosen approximate form, allowing the conversion of the integro-differential equation into the following pure differential equation:

$$\ddot{\delta}_\nu + \left(\frac{2\dot{a}}{a} + \frac{2\bar{k}v_\nu}{a^2} \right) \dot{\delta}_\nu + \frac{v_\nu^2 \bar{k}^2}{a^2} \delta_\nu = 4\pi G \sum_{i=1}^{n} \rho_i \delta_i. \tag{2.5}$$

Here the damping term $2\bar{k}v_\nu$ gives rise to nonoscillating solutions heavily damped at short wavelengths. Thus an equation of the form (2.3) is not correct for HDM of a neutrinolike nature. We examine the general equations for both CDM and HDM, without specifying too carefully the exact nature of the dark component involved. This allows comparison of the results in this paper with previous work in the literature, which has also neglected this point. If some aspects of HDM models are poorly described by (2.3), the equations are still applicable to other two-component cosmological systems such as a hydrogen-helium gas not in equilibrium, where the lighter hydrogen component has a greater sound speed.

At present (2.3) has been displayed in a quite general form, with an unspecified scale factor a, given by the Friedmann cosmological equation

$$\frac{\dot{a}^2}{a^2} = \frac{8\pi G}{3}\rho + \frac{\Lambda}{3} - \frac{k_c}{a^2}. \tag{2.6}$$

General parameters describing the nature of the Universe in this equation are $k_c = 0, \pm 1$, the spatial curvature, and Λ, the cosmological constant. It is difficult to make much progress without first becoming more specific about the energy content of the Universe. All the studies cited previously[8–11] have only examined the Einstein-deSitter, matter dominated case, with various physical components and equations of state possible. The studies,[10,11] all of which are equivalent, make the pretense to study the radiation dominated era as well, but this is incorrect for the equations presented. It was explicitly assumed that $a \propto t^{2/3}$ in the scaling of the energy densities $\rho_i = \Omega_i/(6\pi G t^2)$ and the velocity parameters, yet an allowance was made for a general Hubble expansion $H = \eta t^{-1}$. The general parameter η can only be equal to $\frac{2}{3}$ for the equations presented to be physically correct. The fluid equations were formulated to allow for general equations of state, by writing the sound velocities such that both their magnitudes and time dependences were freely parametrized. A range of solutions were obtained for different cases of the parameters, and were generally classified by Meijer G functions.[22,23] We will show that the solutions found for a CDM

and baryon model have been evaluated incorrectly, and will proceed to find their general exact representation. We will also proceed to investigate a more general dark matter and baryon problem than considered in any of the above. In Ref. 9, several subcases of the above-mentioned studies were considered in some detail, and given a range of physical interpretations. The solutions were of a mathematically simpler nature, involving either Bessel functions or simple power law behavior. The investigations in Ref. 8 concentrated on a three-component medium, involving baryons, CDM and photons. They incorrectly used the nonrelativistic Newtonian cosmological equations to model the photon component, so that the solutions, expressed in terms of Meijer G functions, cannot be considered as physically relevant.

Let us now make the choice of the matter dominated era of cosmological evolution in which to set (2.3), and in particular the post-recombination era, where baryons had decoupled from photons. This allows us to determine how the energy density and sound velocity scale with respect to a, and consequently exhibit all explicit time dependences in the equations. We therefore introduce the comoving total background density $\bar{\rho}_0 \equiv a^3 \rho_0$, and the constant $\epsilon_i \equiv \rho_i / \rho_0$, the fraction of the total mass density contributed by species i. This is distinct from the in general time-dependent quantity $\Omega_i(t) \equiv \rho_i / \rho_c$, where ρ_c is the critical density of the Universe

$$\rho_c = \frac{3H^2}{8\pi G}. \tag{2.7}$$

We will consider a two-component fluid comprised of baryons (subscripted by B) and dark matter (subscripted by D). In the post-recombination era, the adiabatic speed of sound of species i assumes the following behavior:

$$v_i^2 \propto T_i \propto a^{-2}, \tag{2.8}$$

where T_i is the temperature of the component. This prompts us to define the time-independent quantity $\bar{v}_i^2 \equiv a^2 v_i^2$. With these definitions, the linearized cosmological perturbation equations may be written as

$$\frac{d^2\delta_B}{\mathrm{d}t^2} + 2\frac{\dot{a}}{a}\frac{\mathrm{d}\delta_B}{dt} + \frac{\bar{v}_B^2 \bar{k}^2}{a^4}\delta_B = \frac{4\pi G\bar{\rho}_0}{a^3}(\epsilon_B\delta_B + \epsilon_D\delta_D), \tag{2.9}$$

$$\frac{d^2\delta_D}{\mathrm{d}t^2} + 2\frac{\dot{a}}{a}\frac{\mathrm{d}\delta_D}{\mathrm{d}t} + \frac{\bar{v}_D^2 \bar{k}^2}{a^4}\delta_D = \frac{4\pi G\bar{\rho}_0}{a^3}(\epsilon_B\delta_B + \epsilon_D\delta_D). \tag{2.10}$$

The equations currently still represent a fairly general cosmological setting. The curvature parameter k_c and cosmological constant Λ have not been specified, and control the behavior of a through the Friedmann equation (2.6). To see how these influence the evolution of the density perturbations, we transform the dependent variable from t to a. We also use (2.6) and another cosmological dynamics equation for the acceleration of a:

$$\ddot{a} = \frac{4}{3}\pi G\frac{\bar{\rho}_0}{a^2} + \frac{\Lambda}{3}a. \tag{2.11}$$

This equation is derived in conjunction with the Friedmann equation by taking the spatial components of the Einstein equation. The cosmological perturbation equations are now able to be written in a form purely dependent on a, and parametrized explicitly by the cosmological dynamical constants:

$$\left(\frac{8}{3}\pi G\bar{\rho}_0 + \frac{\Lambda}{3}a^3 - k_c a\right)\delta_B'' + a^{-1}(4\pi G\bar{\rho}_0 + \Lambda a^3 - 2k_c a)\delta_B' + \frac{\bar{v}_B^2\bar{k}^2}{a^3}\delta_B - \frac{4\pi G\bar{\rho}_0}{a^2}(\epsilon_B\delta_B + \epsilon_D\delta_D) = 0, \tag{2.12}$$

$$\left(\frac{8}{3}\pi G\bar{\rho}_0+\frac{\Lambda}{3}a^3-k_c a\right)\delta_D''+a^{-1}(4\pi G\bar{\rho}_0+\Lambda a^3-2k_c a)\delta_D'+\frac{\bar{v}_D^2\bar{k}^2}{a^3}\delta_D-\frac{4\pi G\bar{\rho}_0}{a^2}(\epsilon_B\delta_B+\epsilon_D\delta_D)=0. \tag{2.13}$$

In the above, a prime denotes differentiation with respect to a.

A general analysis of (2.12) and (2.13) has not been attempted previously. To begin with, we can test for exactness of the equations (see Ref. 24, pp. 92, 93), to determine whether a first integral exists. In general, a second order ordinary differential equation of the form

$$A_0(x)y''+A_1(x)y'+A_2(x)y=0 \tag{2.14}$$

[arbitrary functions $A_i(x)$] is exact if

$$A_0''-A_1'+A_2=0. \tag{2.15}$$

Let us first consider the one-component example. This is the uncoupled case of (2.12) ($\epsilon_D=0$, $\epsilon_B=1$), which gives

$$A_0''-A_1'+A_2=\frac{\bar{v}_B^2\bar{k}^2}{a^3}. \tag{2.16}$$

Thus the one-component equation is only exact for a pressureless gas $\bar{v}_B=0$. This means that no closed form solution is possible, and approximations need to be made. We note that the pressureless one-component case has been studied extensively (e.g., Ref. 2) for various values of the parameters.

To make progress with the perturbation equations, and also to make contact with previous work in the literature, we need to make some assumptions about k_c and Λ. The $k_c\neq 0$ cases tend to be more complicated mathematically, as generally only parametric solutions can be found, where a is represented by hyperbolic functions ($k_c=-1$ open universe) or trigonometric functions ($k_c=1$ closed universe). Current observations, and the weight of theoretical tendencies in cosmology (e.g., $\Omega=1$ as demanded by inflation) make the choice of flat universe $k_c=0$ seem the most favorable. Ω contains a contribution from Λ as well as matter components. The large amount of observational data now being analyzed, increasingly points to the existence of a cosmological constant comprising a major fraction of the energy density (see, e.g., Ref. 25–27), with a value of $\Omega_\Lambda\simeq 0.7$. The Einstein-deSitter ($\Lambda=0$, $\Omega=1$) model is generally not the model of choice anymore for detailed numerical studies in cosmology, however we do not make a claim that the solutions presented here are of an exact quantitative nature. Many other factors must also be taken into account when attempting to build up an exact, numerical model of structure formation. We wish to correct and extend some previous results, as well as perform some semiquantitative analysis. Our intent is to keep work analytically tractable at this stage.

We set $k_c=\Lambda=0$ in (2.12) and (2.13). In the Einstein-deSitter model, the critical density can be written explicitly as

$$\rho_c=\frac{\bar{\rho}_0}{a^3}=\frac{1}{6\pi G t^2}, \tag{2.17}$$

and the relation $\epsilon_B+\epsilon_D=1$ holds. We also introduce quantities resembling the comoving Jeans wave numbers for each component taken separately,

$$\bar{k}_B^2=\frac{4\pi G\bar{\rho}_0}{\bar{v}_B^2},\quad \bar{k}_D^2=\frac{4\pi G\bar{\rho}_0}{\bar{v}_D^2}. \tag{2.18}$$

The difference with the true comoving Jeans wave number for a one-component fluid is the inclusion of the total mass density $\bar{\rho}_0$, rather than just the mass density of the component in question $\bar{\rho}_i$. Equations (2.12) and (2.13) now become

$$\delta_B'' + \frac{3}{2a}\delta_B' + \frac{3}{2a^3}\left(\frac{\bar{k}}{\bar{k}_B}\right)^2 \delta_B = \frac{3}{2a^2}(\epsilon_B\delta_B + \epsilon_D\delta_D), \tag{2.19}$$

$$\delta_D'' + \frac{3}{2a}\delta_D' + \frac{3}{2a^3}\left(\frac{\bar{k}}{\bar{k}_D}\right)^2 \delta_D = \frac{3}{2a^2}(\epsilon_B\delta_B + \epsilon_D\delta_D). \tag{2.20}$$

The effects of the various physical processes are now clearly evident. The expansion of the Universe produces a damping term $3\delta_i'/(2a)$, causing the solutions to be in power law form rather than exponential. The relation of the mode wave number to the Jeans wave number is expressed as a ratio, transparently showing in which region of physical scales the mode lies. This ratio can be compared to the fractions ϵ_B and ϵ_D to decide whether gravity or pressure dominates the dynamics. The true Jeans instability scale for a two-component medium is not given by either $\bar{k}_B$ or $\bar{k}_D$, but by a combination of the two, as demonstrated in Refs. 6 and 7. This scale will be introduced in due course.

We finally perform a couple more manipulations, to cast the equations in their simplest form. We define the dimensionless parameters

$$K_B = \frac{\bar{k}}{\bar{k}_B}, \quad K_D = \frac{\bar{k}}{\bar{k}_D}. \tag{2.21}$$

Then $K_i < 1$ corresponds to the Jeans unstable region in the one-component analog of the equations, and $K_i > 1$ to the acoustic region. We also make the variable transformation $\chi = a^{-1/2}$. This gives the final form of the system of differential equations to be studied in the ensuing sections,

$$\delta_B'' + 6\left(K_B^2 - \frac{\epsilon_B}{\chi^2}\right)\delta_B - \frac{6\epsilon_D}{\chi^2}\delta_D = 0, \tag{2.22}$$

$$\delta_D'' + 6\left(K_D^2 - \frac{\epsilon_D}{\chi^2}\right)\delta_D - \frac{6\epsilon_B}{\chi^2}\delta_B = 0. \tag{2.23}$$

A prime now denotes differentiation with respect to χ. These equations bear a strong resemblance to the equations of an electron-proton cosmological plasma studied in Ref. 18 [Eqs. (4.8) and (4.9) of that paper]. As is well known from the analogy between the simple Jeans instability and Langmuir modes, this resemblance is not surprising when the mathematical similarity between the electromagnetic and gravitational forces is considered. The techniques employed in Ref. 18 will be useful in our current analysis. In this paper we will employ the Frobenius method in obtaining long wavelength solutions. In a related paper,[19] some general WKB techniques are developed further than previously. Apart from facilitating some short wavelength solutions to the current problem, these techniques will also indicate further results possible in cosmological plasma physics.

Before we proceed to a general analysis of (2.22) and (2.23), we wish to digress to the simpler case of a one-component system. Surprisingly, we will derive some apparently new results, which provide a conceptually useful introduction to the ensuing analysis.

III. THE ONE-COMPONENT EQUATION REVISITED

The Einstein-deSitter one-component equation for a baryonic or dark matter fluid in the post-recombination era is a canonical example studied in all textbooks for linearized cosmological perturbation theory. It gives the familiar Jeans unstable power law solutions $\delta \propto t^{2/3}$, t^{-1} in the limit of large scales, and acoustic oscillations in the limit of small scales. Despite this, we have not found the full exact solutions completely displayed and analyzed in any textbooks or review articles in the current literature. Although a full analysis will not bring any startling new physical

revelations, the mathematical techniques required are of some interest in their relation to the physics, and as an introduction to the more complicated analysis we will require later. This section may be seen as a useful orientation to the further work carried out in the bulk of this paper.

We begin with the one-component version of (2.19), i.e., with $\epsilon_B=1$ and $\epsilon_D=0$ [or vice versa for (2.20)]. Analogous to the definitions of K_B and K_D, we define the one-component comoving Jeans ratio for the fluid, which has comoving Jeans wave number $\bar{k}_J$, as $K_J=\bar{k}/\bar{k}_J$. The one-component density perturbation equation then becomes

$$\delta'' + \frac{3}{2a}\delta' + \left(\frac{3}{2a^3}K_J^2 - \frac{3}{2a^2}\right)\delta = 0. \tag{3.1}$$

The solution of this equation is a Bessel function of order 5/2. A Bessel function of half odd-integer order can be recast in terms of a spherical Bessel function. To begin with, we will choose the spherical Bessel functions of the first and second kind, j_ν and y_ν, respectively. The solution may be rewritten as

$$\delta(a) = c_1 a^{-1/2} j_2\left(\sqrt{\frac{6}{a}}K_J\right) + c_2 a^{-1/2} y_2\left(\sqrt{\frac{6}{a}}K_J\right), \tag{3.2}$$

with arbitrary constants of integration c_1 and c_2. For this case the fortuitous circumstance arises that the solutions may be represented in terms of elementary trigonometric functions (see, e.g., Ref. 28). The solutions as shown are exact mathematical representations, containing all the information of the modes over all scales. As is usually the case with such solutions, a simple inspection does not reveal all the physical properties of the modes in an obvious manner. For example, it is a little difficult to interpret the time dependence of the modes through the argument of the Bessel functions $\sqrt{6/a}K_J$. We will require various approximations and numerical plotting to extract more physical meaning out of the solutions.

To begin with, we seek to place the solutions into a canonical form, for easy comparison with other examples. The most useful such form comprises, to leading order, a product of a power law time factor and complex exponential factor. This approach was adopted in the studies of cosmological plasmas[16–18] for one- and two-component systems. As mentioned previously, due to the similarity between the gravitational and electromagnetic forces, the corresponding modes display many similarities.

The most useful Bessel function solutions for our purposes are the Hankel functions, due to the fact that their leading order terms contain complex exponentials. We use the spherical Hankel functions $h_2^{(1)}$ and $h_2^{(2)}$, given by the expressions

$$h_2^{(1)}(z) = \frac{1}{z}\exp\left[i\left(z - \frac{3\pi}{2}\right)\right]\left(1 - \frac{3}{z^2} - \frac{3}{iz}\right), \tag{3.3}$$

$$h_2^{(2)}(z) = \frac{1}{z}\exp\left[-i\left(z - \frac{3\pi}{2}\right)\right]\left(1 - \frac{3}{z^2} + \frac{3}{iz}\right). \tag{3.4}$$

We may make the comparison here to plasma results, where analogous series were obtained for large z. Contrary to this paper, where the series has a finite number of terms, the series for plasma modes were only asymptotic.

We write the explicit one-component solution via Hankel functions as

$$\delta(a) = \left(1 + \frac{a}{2K_j^2} + \frac{a^2}{4K_J^4}\right)^{1/2} \exp\left\{\pm i\left[\frac{\sqrt{6}K_J}{a^{1/2}} + \arctan\left(\frac{\sqrt{6}K_J a^{-1/2}}{2K_J^2 a^{-1} - 1}\right)\right]\right\}. \tag{3.5}$$

It must be stressed that unlike the plasma solutions, this is an exact result. The modulus of the solution grows with respect to time to leading order as $\delta \propto a$ if $K_J \ll 1$, or else if $K_J \gg 1$ the modulus is approximately constant, with a first order time correction proportional to a. There is also a

complex exponential portion to the solution, which usually gives a dispersion relation. The dispersion relation may be extracted by differentiating the phase with respect to t. This follows from the general fact that given an observed frequency ω, a solution of the form

$$\delta \propto \exp\left[\pm i \int^t \omega(t)\mathrm{d}t\right] \tag{3.6}$$

is expected. This is assuming, of course, that the solution oscillates—if not, some other form of real valued solution must be available. Using the matter dominated time dependence of a, namely

$$a = \left(\frac{t}{t_i}\right)^{2/3}, \tag{3.7}$$

where t_i is an arbitrary constant, we find the frequency to be

$$\omega = \frac{\bar{v}_s \bar{k} a^{-2}}{1 + \frac{1}{2}K_J^{-2}a + \frac{1}{4}K_J^{-4}a^2} \approx \frac{\bar{v}_s \bar{k}}{a^2}\left(1 - \frac{1}{2}\frac{a}{K_J^2} + \frac{1}{8}\frac{a^3}{K_J^6} - \frac{1}{16}\frac{a^4}{K_J^8} + \cdots\right), \quad K_J > 1. \tag{3.8}$$

The result has been expanded for $K_J > 1$, as we may suspect that due to the Jeans instability, acoustic waves only exist in this region, and thus we can only attach physical meaning to ω for $K_J > 1$. This assertion will be derived rigorously in what ensues.

The result of (3.8) may come as a surprise. How does it relate to the well-known Jeans dispersion relation derived for a static space–time

$$\omega^2 = v_s^2 k^2 - 4\pi G\rho_0 \ ? \tag{3.9}$$

In a cosmological setting, we may expect the dispersion relation to follow a similar form, with appropriate time factors included. For plasma modes, it was demonstrated in Ref. 18 that the dispersion relations could be written down to leading order in exactly the same form as their static space–time counterparts in terms of physical (nonbarred) variables, and then converted to comoving variables by inserting the correct time factors. Thus we may expect

$$\omega \approx \frac{\bar{v}_s \bar{k}}{a^2}\left(1 - \frac{a}{K_J^2}\right)^{1/2} \tag{3.10}$$

at least in the form of a binomial expansion, namely

$$\omega \sim \frac{\bar{v}_s \bar{k}}{a^2}\left(1 - \frac{1}{2}\frac{a}{K_J^2} - \frac{1}{8}\frac{a^2}{K_J^4} - \frac{1}{16}\frac{a^3}{K_J^6} + \cdots\right). \tag{3.11}$$

This form for ω may also be expected to contain some other time dependent terms, as was demonstrated for a number of plasma modes. Comparing the expansions in (3.8) and (3.11), we see in fact that they only agree to first order. This still indicates some form of Jeans instability, but the dispersion relations are quite different. This difference in behavior between the linearized gravitational modes and plasma modes may be attributed to the special role the density plays in the gravitational perturbation equations. Equation (3.1) contains only one free parameter, the Jeans ratio K_J, whereas the plasma equations contain both the sound velocity and plasma frequency, which cannot be reduced to one parameter. This implies that the relation between the gravitational source and the Friedmann equation, which fixes the background space–time, means that the same form for the dispersion relation as found in static space–time need not necessarily be expected in the expanding Einstein-deSitter model.

We have a general solution in terms of a modulus and complex exponential, which is exact and thus contains all the information of the problem. How do we infer the usual Jeans instability behavior from this? Let us examine plots of the solutions to gain a pictorial idea of what is

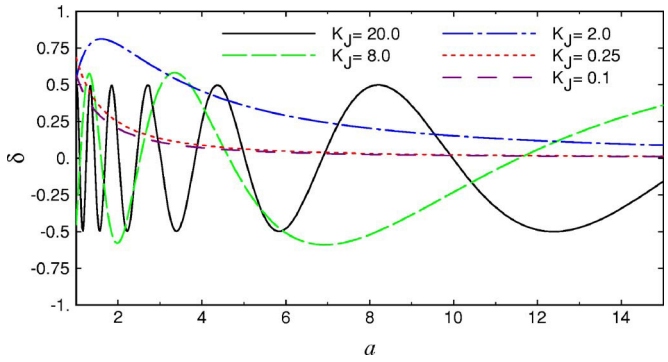

FIG. 1. (Color online) The transition of the decaying one-component modes as K_J varies through the Jeans instability.

happening. In Figs. 1 and 2 we see the transition from acoustic oscillations to growing and decaying modes as K_J is decreased—we are examining ever larger scales, and passing through the instability. To all fit on the same set of axes, the plots have been approximately normalized. The dependent variable a is rather arbitrary [as can be deduced from (3.7)]. An appropriate starting time t_i may be chosen to normalize a to 1 at the beginning of the chosen epoch of evolution, and the solutions may then be propagated forward in time. The tendency for the period of the acoustic oscillations to grow longer in time is evident from the plots, and the approximate constancy of the amplitude predicted previously from (3.5) is evident. In the extreme case, the oscillation period becomes so long that a perturbation cannot complete one full oscillation, and then the instability arises. This behavior can clearly be seen in Figs. 1 and 2 for the K_J=2.0, 8.0 plots.

We now perform some approximations to make contact with some better known results of the one-component problem. Let us begin with a small K_J^2/a expansion. For the spherical Hankel solutions (3.5), we find

$$\delta \sim \frac{a}{2K_J^2}\left[1+\frac{K_J^2}{a}+O\left(\frac{K_J^4}{a^2}\right)\right]\exp\left\{\mp i\sqrt{6}\frac{K_J}{a^{1/2}}\left[1-\frac{4}{5}\frac{K_J^4}{a^2}+O\left(\frac{K_J^6}{a^3}\right)\right]\right\}. \tag{3.12}$$

The above expansion explains what happens to acoustic oscillations when $K_J \lesssim 1$. In this region, the leading order factor $K_J a^{-1/2}$ in the exponential must always lie between 1 and 0 numerically, and decreases with increasing time. This is because $a \geqslant 1$ and increases monotonically for all time. Thus the solution lies within one period of oscillation for all time, and only the growing or decaying modes may be observed. When K_J becomes larger than 1, more than one period of oscillation may be spanned by the $K_J a^{-1/2}$ factor, and the solution will begin to develop acoustic waves. The expansion (3.12) shows $\delta \propto a$, which only gives the familiar growing mode, discussed in all texts. The decaying mode has not been found in the current analysis, because spherical

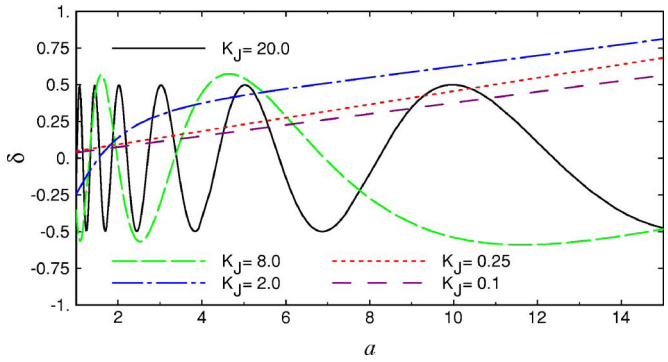

FIG. 2. (Color online) The transition of the growing one-component modes as K_J varies through the Jeans instability.

Hankel functions have been chosen to represent the Bessel function solutions. The spherical Hankel functions are linear combinations of the original j_2 and y_2 solutions, which contain both modes. The decaying mode has been "asymptotically swamped" by the growing mode in this linear combination. The decaying mode may be liberated by a direct small variable expansion of (3.2) for each spherical Bessel function. We find the j_2 component gives the decaying mode

$$\delta \sim a^{-3/2}\left[1 - \frac{3}{7}\frac{K_J^2}{a} + O\left(\frac{K_J^4}{a^2}\right)\right], \tag{3.13}$$

and the y_2 component gives the same growing mode as (3.12) in the slightly different form

$$\delta \sim a\left[1 + \frac{K_J^2}{a} + O\left(\frac{K_J^4}{a^2}\right)\right] \tag{3.14}$$

without the exponential phase factor. These solutions clearly correspond to the usual textbook modes found when pressure is ignored. They have included the pressure corrections, given as a series in the Jeans ratio, with matching time factors to all orders in the expansion.

We now turn to the large parameter expansion, from which we expect to liberate the acoustic oscillations. Equation (3.5) is in fact already in the form of a large parameter expansion, only that it has a finite number of terms, and is consequently exact. The phase of the exponential does not seem to show the structure of the familiar Jeans dispersion relation. This was discussed above, where it was indicated that this is not necessarily to be expected. It is possible to see why this is so in a lucid fashion by applying the WKB method to the original equation (3.1). Through this method we will derive a dispersion relation displaying very similar characteristics to the familiar textbook one, that shows the presence of the Jeans instability. A more complicated WKB approximation scheme was developed in Ref. 18 to deal with plasma modes of a more intricate form, involving larger numbers of coupled equations. This method is used in Ref. 19 to handle the two-component cosmological density perturbation equations in the short wavelength approximation. For the present simple second order equation, the standard textbook approach suffices (for a good explanation of WKB methods, see Ref. 29).

To see the physics most clearly, we transform (3.1) to depend on t. Using the variable transformation given by (3.7), the equation

$$\ddot{\delta} + \frac{4}{3t}\dot{\delta} + \left(\frac{2}{3}K_J^2\frac{t_i^{2/3}}{t^{8/3}} - \frac{2}{3t^2}\right)\delta = 0 \tag{3.15}$$

results. The usual Jeans dispersion relation can be directly seen in this equation. Consider the factor $2/(3t^2)$, arising from the gravitational source term. This term may be transformed to explicitly see the source parameters emerge. We consider the physical (time-dependent) value of the total energy density

$$4\pi G\rho_0 = 4\pi G\rho_c = \frac{4\pi G}{6\pi G t^2} = \frac{2}{3t^2}, \tag{3.16}$$

and the relation

$$K_J^2 = \tfrac{3}{2}\bar{v}_s^2\bar{k}^2 t_i^2. \tag{3.17}$$

Then the Jeans dispersion relation can be directly seen in (3.15),

$$\bar{v}_s^2\bar{k}^2\left(\frac{t_i}{t}\right)^{8/3} - \frac{2}{3t^2} = v_s^2k^2 - 4\pi G\rho_0. \tag{3.18}$$

In the static space–time case the physical variables would of course not depend on time, and the first derivative term $4\dot{\delta}/(3t)$ in (3.15) would not exist. This leads to the exact exponential solutions

and the familiar dispersion relation given by (3.18), as originally found by Jeans.

The most straightforward way to effect a WKB approximation in the present situation is to remove the first derivative from the equation. One way to do this is by the variable change $\chi = a^{-1/2}$. We then find the equation

$$\frac{d^2\delta}{d\chi^2} + \left(6K_J^2 - \frac{6}{\chi^2}\right)\delta = 0. \tag{3.19}$$

Now we suggestively define

$$\tilde{\omega}(\chi) = \left(6K_J^2 - \frac{6}{\chi^2}\right)^{1/2}. \tag{3.20}$$

Applying the WKB approximation to (3.19) gives the leading order solution

$$\delta(\chi) \sim \tilde{\omega}^{-1/2} \exp\left[\pm i \int \tilde{\omega}(\chi) d\chi\right]. \tag{3.21}$$

A dispersion relation has indeed been derived, and is given by $\tilde{\omega}$ as defined in (3.20). If we consider

$$\int \tilde{\omega}(\chi) d\chi = -\int \left(\frac{2}{3}K_J^2 \frac{t^{2/3}}{t_i^{8/3}} - \frac{2}{3t^2}\right)^{1/2} dt = -\int \left(\frac{t}{t_i}\right)^{-4/3}\left[\bar{v}_s^2\bar{k}^2 - \frac{2}{3t_i^2}\left(\frac{t}{t_i}\right)^{2/3}\right]^{1/2} dt, \tag{3.22}$$

then a physical frequency $\omega(t)$ can be identified by use of (3.18) and the relation $t_i^2 = 1/(6\pi G\bar{\rho}_0)$. Thus

$$\int \tilde{\omega}(\chi) d\chi = \int \omega(t) dt = \int (v_s^2 k^2 - 4\pi G\rho_0)^{1/2}\, dt, \tag{3.23}$$

and the physical connection has been made. Another point to note is that the amplitude $\tilde{\omega}(\chi)^{-1/2}$ is time independent to leading order (because $K_J \gg 1$). Thus the amplitude is approximately constant, as noted previously.

To make a direct comparison of (3.21) and (3.5), we now evaluate the integral in the phase of the WKB solutions. A change of integration variable from χ back to a sets the integral into a form which has been tabulated,[30] and we find

$$\int \tilde{\omega}(\chi) d\chi = \left(\frac{6K_J^2}{a} - 6\right)^{1/2} - \frac{\sqrt{6}}{2}\arcsin\left(1 - \frac{2a}{K_J^2}\right). \tag{3.24}$$

The solution generated by the WKB method may be compared to the exact one given by (3.5). The amplitudes and phases need to be expanded for large K_J,

$$\text{WKB phase,} \quad \left(\frac{6K_J^2}{a} - 6\right)^{1/2} - \frac{\sqrt{6}}{2}\arcsin\left(1 - \frac{2a}{K_J^2}\right) = \sqrt{6}\frac{K_J}{a^{1/2}}\left[1 - \frac{\pi}{4}\frac{a^{1/2}}{K_J} + O\left(\frac{a}{K_J^2}\right)\right], \tag{3.25}$$

$$\text{exact phase,} \quad \frac{\sqrt{6}K_J}{a^{1/2}} + \arctan\left(\frac{\sqrt{6}K_J a^{-1/2}}{2K_J^2 a^{-1} - 1}\right) = \sqrt{6}\frac{K_J}{a^{1/2}}\left[1 + \frac{a}{2K_J^2} + O\left(\frac{a}{K_J^2}\right)\right], \tag{3.26}$$

$$\text{WKB amplitude,} \quad (6K_J^2 - 6a)^{-1/4}\frac{1}{6^{1/4}K_J^{1/2}}\left[1 + \frac{a}{4K_J^2} + O\left(\frac{a^2}{K_J^4}\right)\right], \tag{3.27}$$

$$\text{exact amplitude,} \quad \left(1+\frac{a}{2K_J^2}+\frac{a^2}{4K_J^4}\right)^{1/2}\left[1+\frac{a}{4K_J^2}+O\left(\frac{a^2}{K_J^4}\right)\right]. \tag{3.28}$$

It can be seen that the two solutions only agree to leading order (modulo time independent constant factors). Given that the WKB method only gives a leading order solution to the problem, no more can be expected. This discussion has highlighted the difference between the expected dispersion relations of static space–time to those derived in an expanding universe context. WKB can reproduce the same form as the static space–time dispersion relations, but this may only agree to leading order to the true dispersion relation found in an expanding universe scenario.

IV. IMPROVEMENTS ON PREVIOUS CDM PERTURBATION RESULTS

We now return to the two-component equations and consider the case of CDM perturbations characterized by strictly zero temperature. If the velocity dispersion is considered to be an adiabatic sound velocity as given by (2.8), then $T_i=0$ corresponds to $K_D=0$ in (2.23). Such an approximation facilitates an exact analytic solution to the problem, which is otherwise impossible. The resulting system of equations was one of the main cases investigated in the general analysis of Ref. 11. In this section we will point out what appears to be an error in the analysis of that paper, which leads to some markedly different solutions, derived in what ensues.

Before we proceed with this, it is pertinent to point out a general problem with taking $K_D=0$ in Eqs. (2.22) and (2.23). For simplicity, it is possible to neglect space–time expansion, as the qualitative behavior will be the same. Thus the static space–time cosmological equations studied in Ref. 7 are sufficient for this discussion. These equations are also examined in Ref. 19, and using the notation employed there we have

$$\ddot{\delta}_D+(v_D^2k^2-W_D)\delta_D-W_B\delta_B=0, \tag{4.1}$$

$$\ddot{\delta}_B+(v_B^2k^2-W_B)\delta_B-W_D\delta_D=0, \tag{4.2}$$

with $W_i=4\pi G\rho_i$. This system of equations can be reduced to a first order linear autonomous dynamical system describing a state vector

$$\mathbf{x}=(x_1,x_2,x_3,x_4)^T\equiv(\dot{\delta}_D,\delta_D,\dot{\delta}_B,\delta_B)^T, \tag{4.3}$$

where T denotes the transpose of a vector. The dynamical system has a k-dependent critical point found by solving the equation $\dot{\mathbf{x}}=0$. This critical point happens to give the Jeans wave number of the mixture, and is given by

$$k^2=k_M^2\equiv k_B^2+k_D^2=\frac{W_B}{v_B^2}+\frac{W_D}{v_D^2}. \tag{4.4}$$

Note the slight difference in this definition of k_i in comparison to $\bar{k}_i$ defined in (2.18). It is already evident that a problem arises if we take $v_D\to 0$ in (4.4), and this will be physically elucidated by studying the four independent modes of the system, given by the eigenvalues of the dynamical system.

The eigenvalues give the structure of the modes (see Ref. 7 or Ref. 19 for the details). They are found to be of the general form

$$\lambda_1=-\lambda_2=\frac{1}{\sqrt{2}}\sqrt{f+\sqrt{f^2+4g}}, \tag{4.5}$$

$$\lambda_3 = -\lambda_4 = \frac{1}{\sqrt{2}}\sqrt{f - \sqrt{f^2 + 4g}}.$$

For the case of CDM currently under consideration, where $v_D = 0$, the k-dependent functions f and g are given by

$$f(k) = W_B + W_D - k^2 v_B^2, \tag{4.6}$$

$$g(k) = k^2 W_D^2 v_B^2. \tag{4.7}$$

It was previously found that the eigenvalues λ_1 and λ_2 described the Jeans unstable modes, whereas λ_3 and λ_4 described acoustic oscillations at all wave numbers. An examination of λ_1 in the current context will show this not to be the case for CDM. If we define (analogously to the one-component scenario)

$$K_J = \frac{v_B^2 k^2}{W_B + W_D}, \tag{4.8}$$

λ_1 may be written as follows:

$$\lambda_1 = \frac{1}{\sqrt{2}}(W_B + W_D)^{1/2}\{1 - K_J^2 + [(1 - K_J^2)^2 + 4\epsilon_D K_J^2]^{1/2}\}^{1/2}. \tag{4.9}$$

This does not equal zero for $K_J = 1$, and it is straightforward to show that it has no zeros for all $k \neq 0$. Thus a CDM perturbation would collapse for *all* scales, clearly a physical impossibility.

If we examine Eqs. (4.1) and (4.2), it can be seen that with the removal of the pressure term $v_D k^2$, there is no mechanism to counter the remaining gravitational source terms $-W_D \delta_D$ and $-W_B \delta_B$, whose sign indicate an attractive forcing, initiating gravitational collapse. This is the case no matter how small the fraction of dark matter compared to baryons, thus no amount of baryonic pressure support can prevent a collapse at any scale. This physically absurd situation is the root of the problem of taking $v_D \to 0$ in the fluid models. A physically correct equation must include some sort of velocity dispersion term, even if the matter is totally collisionless and an adiabatic speed of sound cannot be defined.

With these thoughts in mind, we must view the current section as more of a mathematical digression, than a physically realistic model. It nevertheless serves a purpose. We can make contact with the work of Ref. 11, and uncover some interesting mathematical properties associated with these cosmological perturbation equations in general. We find mathematical subtleties overlooked in Ref. 11, which also indicate the nature of the general solutions to follow in the next section. They allow an interesting comparison with cosmological plasma modes discussed in Ref. 18, where the limit $T_D \to 0$ is valid. The special nature of gravity, and the extra complications it entails are revealed by this comparison.

We now proceed to obtain a solution of Eqs. (2.22) and (2.23) (with $K_D = 0$) in the long wavelength (small k) limit. A short wavelength solution is trivially obtained by setting $K_D = 0$ everywhere in the results presented in Ref. 19. To align ourselves with earlier notation, and to stress the fact that there is only one Jeans related scale now occurring, we will rename K_B to K_J. Rather than directly reducing Eqs. (2.22) and (2.23) into a single equation, we attempt a solution by the Frobenius method. This is useful as a precursor to the general solution derived in the following section in a similar manner.

To begin with, we assume an arbitrary expansion of the solutions in the form

$$\delta_B(\rho, \chi) = \chi^\rho \sum_{n=0}^{\infty} a_n \chi^n, \tag{4.10}$$

$$\delta_D(\rho,\chi) = \chi^\rho \sum_{n=0}^{\infty} b_n \chi^n. \tag{4.11}$$

Here ρ is an arbitrary exponent to be determined, and a_n and b_n are series coefficients also to be determined by the Frobenius method. We substitute these series into (2.22) and (2.23) to obtain a set of algebraic relations between the undetermined coefficients. Then all coefficients of like power of χ are collected and equated to zero.

Arising out of this procedure are a pair of indicial equations for ρ, with one of a_0 or b_0 remaining an arbitrary constant,

$$\rho(\rho-1)a_0 - 6\epsilon_B a_0 - 6\epsilon_D b_0 = 0, \tag{4.12}$$

$$\rho(\rho-1)b_0 - 6\epsilon_D b_0 - 6\epsilon_B a_0 = 0. \tag{4.13}$$

A set of recursion relations also arise for all higher order coefficients:

$$6K_J^2 a_n + [(\rho+n+2)(\rho+n+1) - 6\epsilon_B]a_{n+2} - 6\epsilon_D b_{n+2} = 0, \tag{4.14}$$

$$[(\rho+n+2)(\rho+n+1) - 6\epsilon_D]b_{n+2} - 6\epsilon_B a_{n+2} = 0. \tag{4.15}$$

In retaining the arbitrary constant a_0 or b_0, it is assumed that all odd indexed terms vanish from propagation of the initial values $a_1 = b_1 = 0$ through the recursion relations.

If we solve (4.12) and (4.13) for ρ, we find four possible values,

$$\rho = 0, 1, 3, -2. \tag{4.16}$$

A comparison with the analogous case for cosmological plasma modes[18] immediately shows a difference in the nature of the exponents. In the preceding case the exponents are exactly determined integers, whereas for plasmas the exponents depended on the plasma frequency. When the one-component solutions were discussed in the preceding section, an analogous difference was observed between the spherical Bessel function solutions of the gravitational perturbation modes, and the general order Bessel function solutions of the plasma modes. Whereas in the one-component study the solutions were simplified by this property of gravity, in the present case they are in fact complicated. The plasma solutions were representable in terms of ${}_2F_3$ generalized hypergeometric functions, but a similar representation is not well-defined here. This is because the exponents differ by integers—a fact which necessitates a modification of the basic Frobenius method. This modification is borne out in the solutions by the fact that parameters appearing in the denominator of generalized hypergeometric function expansions cannot differ by integers. In such situations the generalized hypergeometric functions are not definable, and one must resort to classifying solutions of the equation by Meijer G-functions.

To apply the Frobenius method to indices differing by integers, the recursion relations must first be solved for general ρ. This is achieved by employing (4.12) and (4.13), and writing the system of differential equations as

$$\mathbf{L}\begin{bmatrix} \delta_B(\rho,\chi) \\ \delta_D(\rho,\chi) \end{bmatrix} = \begin{bmatrix} \rho(\rho-1)a_0 - 6\epsilon_B a_0 - 6\epsilon_D b_0 \\ \rho(\rho-1)b_0 - 6\epsilon_D b_0 - 6\epsilon_B a_0 \end{bmatrix} \chi^{\rho-2}, \tag{4.17}$$

where the operator $\mathbf{L}$ is defined by

$$\mathbf{L} = \begin{bmatrix} \frac{\partial^2}{\partial\chi^2} + 6\left(K_J^2 - \frac{\epsilon_B}{\chi^2}\right) & -\frac{6\epsilon_D}{\chi^2} \\ -\frac{6\epsilon_B}{\chi^2} & \frac{\partial^2}{\partial\chi^2} - \frac{6\epsilon_D}{\chi^2} \end{bmatrix}. \tag{4.18}$$

At present there is no relation between a_0 and b_0, but the recursion relations will provide one. A lengthy algebraic exercise is needed to solve the recursion relations. The result is

$$a_{2n} = a_0 \frac{\left(\frac{1}{2}\rho - \frac{1}{2}\nu_D + \frac{3}{4}\right)_n \left(\frac{1}{2}\rho + \frac{1}{2}\nu_D + \frac{3}{4}\right)_n}{\left(\frac{1}{2}\rho - \frac{1}{2}\right)_n \left(\frac{1}{2}\rho + \frac{1}{2}\right)_n \left(\frac{1}{2}\rho + 1\right)_n \left(\frac{1}{2}\rho + 2\right)_n} \left(-\frac{3}{2}K_J^2\right)^n, \tag{4.19}$$

$$b_{2n} = \frac{6a_0\epsilon_B}{\rho(\rho-1) - 6\epsilon_D} \frac{\left(\frac{1}{2}\rho - \frac{1}{2}\nu_D - \frac{1}{4}\right)_n \left(\frac{1}{2}\rho + \frac{1}{2}\nu_D - \frac{1}{4}\right)_n}{\left(\frac{1}{2}\rho - \frac{1}{2}\right)_n \left(\frac{1}{2}\rho + \frac{1}{2}\right)_n \left(\frac{1}{2}\rho + 1\right)_n \left(\frac{1}{2}\rho + 2\right)_n} \left(-\frac{3}{2}K_J^2\right)^n. \tag{4.20}$$

In the above, the parameter ν_D has been introduced as a shorthand,

$$\nu_D \equiv \sqrt{\tfrac{1}{4} + 6\epsilon_D}, \tag{4.21}$$

and the notation $(\,)_n$ is the Pochhammer symbol. It is clear that the coefficients as derived will not exist for $\rho = 1, -2$. This is the basis for requiring a modification to the straightforward method of substituting in the four calculated values of ρ (4.16) into (4.19) and (4.20) to generate four independent solutions.

To proceed, we extract from (4.19) and (4.20) the relation

$$b_0 = \frac{6a_0\epsilon_B}{\rho(\rho-1) - 6\epsilon_D}, \tag{4.22}$$

which allows (4.17) to be rewritten as

$$\mathbf{L}\begin{bmatrix} \delta_B(\rho,\chi) \\ \delta_D(\rho,\chi) \end{bmatrix} = a_0 \begin{bmatrix} \frac{1}{\epsilon_B} \frac{\rho(\rho-1)(\rho+2)(\rho-3)}{\rho(\rho-1) - 6\epsilon_D} \\ 0 \end{bmatrix} \chi^{\rho-2}. \tag{4.23}$$

For $\rho = 0, 3$, direct substitution is permissible to obtain two independent solutions, which turn out to be generalized hypergeometric ${}_2F_3$ functions, analogously to the plasma results. For $\rho = 1, -2$, we take advantage of the fact that a_0 is arbitrary, and set it, respectively, equal to $\rho - 1$ and $\rho + 2$. After differentiation with respect to ρ and evaluation at the respective points $\rho = 1$ and $\rho = -2$, we obtain the result

$$\mathbf{L} \begin{bmatrix} \frac{\partial}{\partial\rho}\delta_B(\rho,\chi) \\ \frac{\partial}{\partial\rho}\delta_D(\rho,\chi) \end{bmatrix} \Bigg|_{\rho=1,-2} = 0. \tag{4.24}$$

This gives two more solutions.

The above discussion has defined an algorithm for finding small k expansions of the solutions of the cosmological density perturbation equations. This algorithm is readily implemented into a symbolic manipulation computer code. We will write such a code to find the solutions to the general equations in the next section. The solutions for the CDM case under consideration may

now be written down. The need to differentiate with respect to ρ for the $\rho=1,-2$ cases result in solutions involving digamma functions ψ and logarithmic terms—quite a complication to the ${}_2F_3$ functions derived for the plasma perturbations in Ref. 18. To display the modes in their simplest form, linear combinations of the modes derived directly by the above algorithm need to be taken, and the use of various mathematical identities involving digamma functions employed. The final set of four CDM modes are given as follows:

$$\delta_{B1}(\chi)=\frac{c_1}{\epsilon_B}\sum_{n=0}^{\infty}\frac{\left(\frac{3}{4}-\frac{1}{2}\nu_D\right)_n\left(\frac{3}{4}+\frac{1}{2}\nu_D\right)_n}{\left(-\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n(2)_n n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n$$
$$=\frac{c_1}{\epsilon_B}{}_2F_3\left(\frac{3}{4}-\frac{1}{2}\nu_D,\frac{3}{4}+\frac{1}{2}\nu_D;-\frac{1}{2},\frac{1}{2},2;-\frac{3}{2}K_J^2\chi^2\right), \tag{4.25}$$

$$\delta_{D1}(\chi)=\frac{c_1}{\epsilon_D}\sum_{n=0}^{\infty}\frac{\left(-\frac{1}{4}-\frac{1}{2}\nu_D\right)_n\left(-\frac{1}{4}+\frac{1}{2}\nu_D\right)_n}{\left(-\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n(2)_n n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n$$
$$=\frac{c_1}{\epsilon_D}{}_2F_3\left(-\frac{1}{4}-\frac{1}{2}\nu_D,-\frac{1}{4}+\frac{1}{2}\nu_D;-\frac{1}{2},\frac{1}{2},2;-\frac{3}{2}K_J^2\chi^2\right), \tag{4.26}$$

$$\delta_{B2}(\chi)=c_2\frac{\chi}{\epsilon_B}+c_2\frac{\chi}{\epsilon_B}\sum_{n=1}^{\infty}\frac{\left(\frac{5}{4}-\frac{1}{2}\nu_D\right)_n\left(\frac{5}{4}+\frac{1}{2}\nu_D\right)_n}{\left(\frac{3}{2}\right)_n\left(\frac{5}{2}\right)_n(n-1)!n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n\left[\psi\left(\frac{5}{4}-\frac{1}{2}\nu_D+n\right)\right.$$
$$\left.+\psi\left(\frac{5}{4}+\frac{1}{2}\nu_D+n\right)-\psi(n)-\psi(n+1)-\psi\left(n+\frac{3}{2}\right)-\psi\left(n+\frac{5}{2}\right)+\log\chi^2\right], \tag{4.27}$$

$$\delta_{D2}(\chi)=-c_2\frac{\chi}{\epsilon_D}-c_2\frac{\chi}{\epsilon_D}\sum_{n=1}^{\infty}\frac{\left(\frac{1}{4}-\frac{1}{2}\nu_D\right)_n\left(\frac{1}{4}+\frac{1}{2}\nu_D\right)_n}{\left(\frac{3}{2}\right)_n\left(\frac{5}{2}\right)_n(n-1)!n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n\left[\psi\left(\frac{1}{4}-\frac{1}{2}\nu_D+n\right)\right.$$
$$\left.+\psi\left(\frac{1}{4}+\frac{1}{2}\nu_D+n\right)-\psi(n)-\psi(n+1)-\psi\left(n+\frac{3}{2}\right)-\psi\left(n+\frac{5}{2}\right)+\log\chi^2\right], \tag{4.28}$$

$$\delta_{B3}(\chi)=c_3\chi^3{}_2F_3\left(\frac{9}{4}-\frac{1}{2}\nu_D,\frac{9}{4}+\frac{1}{2}\nu_D;\frac{5}{2},\frac{7}{2},2;-\frac{3}{2}K_J^2\chi^2\right), \tag{4.29}$$

$$\delta_{D3}(\chi)=c_3\chi^3{}_2F_3\left(\frac{5}{4}-\frac{1}{2}\nu_D,\frac{5}{4}+\frac{1}{2}\nu_D;\frac{5}{2},\frac{7}{2},2;-\frac{3}{2}K_J^2\chi^2\right), \tag{4.30}$$

$$\delta_{B4}(\chi) = c_4\left(\frac{3}{2}K_J^2\chi^2\right)^{-1} + 2c_4\epsilon_D\sum_{n=1}^{\infty}\frac{\left(\frac{3}{4}-\frac{1}{2}\nu_D\right)_n\left(\frac{3}{4}+\frac{1}{2}\nu_D\right)_n}{\left(-\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n(2)_n n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n\left[\psi\left(\frac{3}{4}-\frac{1}{2}\nu_D+n\right)\right.$$
$$\left.+\psi\left(\frac{3}{4}+\frac{1}{2}\nu_D+n\right)-\psi(n+2)-\psi(n+1)-\psi\left(n-\frac{1}{2}\right)-\psi\left(n+\frac{1}{2}\right)+\log\chi^2\right], \quad (4.31)$$

$$\delta_{D4}(\chi) = c_4\left(\frac{3}{2}K_J^2\chi^2\right)^{-1} - 2c_4\epsilon_B\sum_{n=1}^{\infty}\frac{\left(-\frac{1}{4}-\frac{1}{2}\nu_D\right)_n\left(-\frac{1}{4}+\frac{1}{2}\nu_D\right)_n}{\left(-\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n(2)_n n!}\left(-\frac{3}{2}K_J^2\chi^2\right)^n\left[\psi\left(-\frac{1}{4}-\frac{1}{2}\nu_D+n\right)\right.$$
$$\left.+\psi\left(-\frac{1}{4}+\frac{1}{2}\nu_D+n\right)-\psi(n+2)-\psi(n+1)-\psi\left(n-\frac{1}{2}\right)-\psi\left(n+\frac{1}{2}\right)+\log\chi^2\right]. \quad (4.32)$$

The same solutions may be obtained by considering Meijer *G*-function solutions to the original differential equations. The procedure for determining solutions to generalized hypergeometriclike equations which contain parameters differing by integers is discussed in detail by Luke,[23] pp.138–143. The study outlined a method for developing Meijer *G*-function solutions from the equations, which involved the differentiation of generalized hypergeometric functions with respect to their parameters—a procedure analogous to the differentiation of ρ indices in the above. The analysis involved is lengthy and tedious, but leads to the solutions obtained above. We refrain from a physical interpretation of the above gravitational modes for now, and take that up in the next section when we discuss the more general solutions. The one obvious difference will be the fact that no Jeans instability is apparent for any of the above modes, with two modes always collapsing and two modes always acoustic, whereas for the general modes a Jeans instability will be apparent.

We now compare the solutions obtained to those of Refs. 10 and 11. In these studies general solutions were written as

$$\phi_1 \equiv t^{-\alpha}\delta_B = c_1G_1 + c_2G_2 + c_3G_3 + c_4G_4. \quad (4.33)$$

Here c_i are constants, and the functions G_i denote Meijer *G* functions,

$$G_h = G_{2,4}^{m,n}\left(x\Big|\begin{matrix}a_1^*+1, a_2^*+1\\ b_h^*, b_1^*\cdots\#\cdots b_4^*\end{matrix}\right), \quad h=1,2,3,4. \quad (4.34)$$

The notation # signifies that b_h is to be omitted in its usual place. The *G* function is defined so that $0\leqslant m\leqslant 4$ and $0\leqslant n\leqslant 2$. The parameters a_i^*, b_j^* depend on ϵ_B, ϵ_D, the adiabatic index γ_B, and the exponent η of t in the Hubble expansion parameter (which we pointed out earlier *must* be equal to $\frac{2}{3}$ for the equations as formulated to be physically correct—even though Refs. 10 and 11 used a greater range of values). The time parameter $x=\frac{3}{2}K_J^2\chi^2$ in our notation. A particular set of solutions is given by m and n being given specific values. In general, $m=1$, $n=2$ will give such a set of solutions for small x in the above example. The *G* functions can then normally be expressed in terms of ${}_2F_3$ functions (for example, the plasma solutions), but in the particular case under discussion, since some of the b_j^* differ by integers, this is not possible. It is this point that Haubold and Mathai missed in Ref. 11.

Let us give specifics to illustrate the point. Under the general classification scheme, the CDM case under consideration corresponds to $\eta=\frac{2}{3}$, $\gamma_i=\frac{5}{3}$, in the notation of Ref. 11. This implies that the parameters take the following values:

$$a_1^*, a_2^* = -1 \pm \tfrac{1}{2}\nu_D,$$

$$b_1^*, b_2^* = \pm \tfrac{1}{4}, \quad b_3^*, b_4^* = \pm \tfrac{5}{4}.$$

To evaluate the G functions in this special case, where some parameters differ by integers, the integral representation of the G functions was considered in Ref. 11:

$$G_1 = \frac{1}{2\pi i}\int_L \frac{\Gamma\left(\frac{1}{4}+s\right)\Gamma(-a_1^*-s)\Gamma(-a_2^*-s)}{\Gamma\left(\frac{5}{4}-s\right)\Gamma\left(-\frac{1}{4}-s\right)\Gamma\left(\frac{9}{4}-s\right)} x^{-s}\,\mathrm{d}s. \tag{4.35}$$

Using the fact that

$$\frac{\Gamma\left(\frac{1}{4}+s\right)}{\Gamma\left(-\frac{1}{4}-s\right)} - \frac{\Gamma\left(\frac{5}{4}+s\right)}{\Gamma\left(\frac{3}{4}-s\right)}, \tag{4.36}$$

it was found that

$$G_1 = -x^{5/4}\frac{\Gamma\left(-a_1^*+\frac{5}{4}\right)\Gamma\left(-a_2^*+\frac{5}{4}\right)}{\Gamma\left(\frac{5}{2}\right)\Gamma(2)\Gamma\left(\frac{7}{2}\right)}\,{}_2F_3\left(-a_1^*+\frac{5}{4},-a_2^*+\frac{5}{4};\frac{5}{2},2,\frac{7}{2};-x\right), \tag{4.37}$$

which agrees with δ_{B3} in (4.29). Performing the same analysis as above for G_3 however, it is found that G_1 and G_3 are exactly the same function. It appears as though this was never checked in Ref. 11. The same applies to G_2 and G_4,

$$G_2 = G_4 = -x^{-1/4}\frac{\Gamma\left(-a_1^*-\frac{1}{4}\right)\Gamma\left(-a_2^*-\frac{1}{4}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma(2)\Gamma\left(-\frac{1}{2}\right)}\,{}_2F_3\left(-a_1^*-\frac{1}{4},-a_2^*-\frac{1}{4};\frac{1}{2},2,-\frac{1}{2};-x\right), \tag{4.38}$$

which agrees with δ_{B1} in (4.25). Thus the solutions degenerate by employing this method, and two of the solutions, namely δ_{B2} and δ_{B4} which contain logarithmic terms, are totally missed. The correct way to evaluate the G functions when some parameters differ by integers is given by Luke,[23] pp. 143–147. A careful study of this rather complicated procedure will show that the logarithmic solutions δ_{B2} and δ_{B4} are found in this way.

It is interesting to note that a linear combination of the solutions δ_{B2} and δ_{B4} are in fact found in Ref. 11 in the large x limit. In this case the function $G_{2,4}^{4,1}$ was evaluated from the contour integral representation to achieve some analogous series to (4.27) and (4.31). Although the solutions (4.25)–(4.32) are valid for all x, such a representation does not seem very useful for x large, as the solutions are comprised of an infinite ascending series in x. Thus very many terms would be required to represent the solutions accurately in this limit through δ_{B2} and δ_{B4}. In Ref. 19 we develop a much better method for evaluating the solutions for large x using a WKB approximation scheme.

We have now thoroughly investigated the CDM two-component model using the $K_D=0$ limit, and tidied up previous work in this area. As discussed earlier, although this work is of dubious physical relevance, it has been an interesting mathematical investigation, and has allowed comparisons with the previous work in cosmological perturbation theory and cosmological plasma physics. We now turn to the more general two-component model, which has a firmer physical basis.

V. THE GENERAL TWO-COMPONENT SOLUTIONS

We finally investigate the most general set of equations, those with both K_B and K_D nonzero. The equations thus posed can model both CDM and HDM, though the discussion initiated earlier about the lack of a free streaming damping term for neutrinolike HDM should be heeded.

The algorithm needed to solve the equations was developed in the preceding section for $K_D=0$, and can be used here. Thus if (4.10) and (4.11) are substituted into (2.22) and (2.23), we obtain the same indicial equations (4.12) and (4.13) as previously, and the following set of coupled recursion relations:

$$(\rho+n+2)(\rho+n+1)(\rho+n+4)(\rho+n-1)a_{n+2}+6K_B^2\left(\rho+n+\tfrac{3}{2}-\nu_D\right)\left(\rho+n+\tfrac{3}{2}+\nu_D\right)a_n + 36\epsilon_D K_D^2 b_n=0, \tag{5.1}$$

$$(\rho+n+2)(\rho+n+1)(\rho+n+4)(\rho+n-1)b_{n+2}+6K_D^2\left(\rho+n+\tfrac{3}{2}-\nu_B\right)\left(\rho+n+\tfrac{3}{2}+\nu_B\right)b_n + 36\epsilon_B K_B^2 a_n=0. \tag{5.2}$$

Here $\nu_B^2=\frac{1}{4}+6\epsilon_B$ in analogy with the previous definition of ν_D. A closed solution for this set of recursion relations cannot be obtained for all n, so that solutions to (2.22) and (2.23) can only be generated iteratively, to whatever order desired. Lacking the ability to generate an infinite series representation for the solutions means that they cannot be classified by known analytic functions. To handle the complicated algebra involved in finding successive terms iteratively, we have developed a symbolic computation code using the functional programming language Mathematica. The algorithm described in the preceding section can be used to generate a solution up to a certain power in χ.

The coefficients increase in complexity very quickly for increasing n. Although the code can generate solutions up to arbitrary order, we find it sufficient to present only the first two orders for each solution here. We express the results in terms of the original parameters K_B and K_D, rather than in terms of ν_B and ν_D, as no simplification is gained in using the latter. The solutions, corresponding to $\rho=0,1,3,-2$, respectively, are

$$\delta_{B1}(\chi)=1+\tfrac{3}{2}(K_B^2-3\epsilon_D K_B^2-3\epsilon_B K_D^2)\chi^2+O(\chi^4), \tag{5.3}$$

$$\delta_{D1}(\chi)=-\frac{\epsilon_B}{\epsilon_D}\left[1+\frac{3}{2}(K_D^2-3\epsilon_D K_B^2-3\epsilon_B K_D^2)\chi^2+O(\chi^4)\right], \tag{5.4}$$

$$\delta_{B2}(\chi)=\chi+\frac{1}{25}\left(6K_B^2-31\epsilon_D K_B^2-31\epsilon_B K_D^2+5\frac{\epsilon_B}{\epsilon_D}K_D^2\right)\chi^3+\frac{6}{5}\epsilon_B(K_D^2-K_B^2)\chi^3\log\chi+O(\chi^5), \tag{5.5}$$

$$\delta_{D2}(\chi)=-\frac{\epsilon_B}{\epsilon_D}\left[\chi-\frac{1}{25}(31\epsilon_D K_B^2+31\epsilon_B K_D^2-K_D^2)\chi^3-\frac{6}{5}\epsilon_D(K_D^2-K_B^2)\chi^3\log\chi+O(\chi^5)\right], \tag{5.6}$$

$$\delta_{B3}(\chi)=\chi^3+\tfrac{3}{70}(3\epsilon_D K_B^2-3\epsilon_D K_D^2-10K_B^2)\chi^5+O(\chi^7), \tag{5.7}$$

$$\delta_{D3}(\chi)=\chi^3+\tfrac{3}{70}(3\epsilon_B K_D^2-3\epsilon_B K_B^2-10K_D^2)\chi^5+O(\chi^7), \tag{5.8}$$

$$\delta_{B4}(\chi)=\chi^{-2}+\left(K_B^2-5\frac{\epsilon_B}{\epsilon_D}K_D^2+5\epsilon_D K_B^2-5\epsilon_D K_D^2\right)+6\epsilon_D(K_B^2-K_D^2)\log\chi+O(\chi^2), \tag{5.9}$$

TABLE I. A comparison of gravitational and plasma linear perturbation modes

Gravitational modes	Plasma modes
$\delta_1 \sim \chi^0 \sim t^0$	$y_1 \sim \eta^0 \sim t^0$
$\frac{\delta_B}{\delta_D} \sim -\frac{\epsilon_D}{\epsilon_B}$	$\frac{n_e}{n_i} \sim 1$
Lower ${}_2F_3$ parameters: $-\frac{1}{2}, \frac{1}{2}, 2$	$\frac{1}{2}, \frac{3}{4}-\frac{1}{2}\nu, \frac{3}{4}+\frac{1}{2}\nu$
Acoustic mode	Ion-sound mode
$\delta_2 \sim \chi \sim a^{-1/2} \sim t^{-1/3}$	$y_2 \sim \eta^{-1} \sim a^{-1/2} \sim t^{-1/3}$
$\frac{\delta_B}{\delta_D} \sim -\frac{\epsilon_D}{\epsilon_B}$	$\frac{n_e}{n_i} \sim 1$
Logarithmic solutions	Parameters do not correspond
Acoustic mode	Ion-sound mode
$\delta_3 \sim \chi^3 \sim a^{-3/2} \sim t^{-1}$	$y_3 \sim \eta^{-1/2-\nu} \sim a^{-1/4-(1/2)\nu} \sim t^{-1/6-(1/3)\nu}$
$\frac{\delta_B}{\delta_D} \sim 1$	$\frac{n_e}{n_i} \sim -\frac{P_e^2}{P_i^2}$
Lower ${}_2F_3$ parameters: $-\frac{5}{2}, \frac{7}{2}$ 2	$1+\nu, \frac{3}{4}+\frac{1}{2}\nu,, \frac{5}{4}+\frac{1}{2}\nu$
Collapsing mode	Langmuir mode
$\delta_4 \sim \chi^{-2} \sim a \sim t^{2/3}$	$y_4 \sim \eta^{-1/2+\nu} \sim a^{-1/4+(1/2)\nu} \sim t^{-1/3+(1/3)\nu}$
$\frac{\delta_B}{\delta_D} \sim 1$	$\frac{n_e}{n_i} \sim -\frac{P_e^2}{P_i^2}$
Logarithmic solutions	Parameters do not correspond
Collapsing mode	Langmuir mode

$$\delta_{D4}(\chi) = \chi^{-2} + (6K_D^2 - 5\epsilon_B K_B^2 + 5\epsilon_B K_D^2) + 6\epsilon_D(K_D^2 - K_B^2)\log\chi + O(\chi^2). \tag{5.10}$$

It remains now to make a physical interpretation of these solutions. This is most usefully achieved by constructing a table comparing different properties of the modes, and comparing the solutions to the corresponding cosmological plasma modes. The results are summarized in Table I, which uses notation defined in Ref. 18. Both the $K_D=0$ modes of the preceding section and the modes of this current section are included in each category under the table. The plasma modes $y_1, \ldots, y_4$ of Ref. 18, Eq. (4.16) correspond to the $K_D=0$ modes (4.25)–(4.32). The current gravitational modes (5.3)–(5.10) (that is $\delta_1, \ldots, \delta_4$) correspond to the more general expansions Eqs. (4.20), (4.21), (4.29)–(4.32) of Ref. 18.

In Table I, the power of χ gives the corresponding exponent ρ. The parameter $\nu \equiv \sqrt{\frac{1}{4} - P_i^2 - P_e^2}$ found in the plasma modes depends on the plasma frequencies of the electron and ion components. For the gravitational modes, the signs of P_i and P_e must be reversed since (as opposed to the electromagnetic force) gravity is always attractive. In addition $P_i^2 + P_e^2$ corresponds to $\epsilon_B + \epsilon_D = 1$ (once again the special nature of gravity in cosmology is apparent). This implies that the general parameter ν in the plasma modes should be replaced with $\frac{5}{2}$ for the gravitational modes—the reason why many of the parameters in the ${}_2F_3$ and Meijer G functions were pure rational numbers not depending on physical constants. Notice that the ratio of the amplitudes of baryonic/dark matter modes and electron/ion modes differ. This is because the couplings in the differential equations are different. For the gravitational modes the couplings involve terms such as $\epsilon_D\delta_D$ and $\epsilon_B\delta_B$, whereas for the plasma modes the couplings involve terms such as $P_i^2\bar{n}_{e1}$ and $P_e^2\bar{n}_{i1}$.

We have indicated the corresponding collapsing and acoustic modes for the gravitational density perturbations. It is difficult to show this rigorously for the series solutions as presented. We

can make comparisons to the one-component results, and identify the leading order powers of the expansion parameter a. This yields the classification as stated. We can also make an analogy to the ion-sound modes of plasma physics, which are of a similar nature to acoustic oscillations. They show a collective behavior of both components oscillating approximately in phase.

We are finally left with the question of how the Jeans scale enters into the solutions. In Sec. IV the mixture wave number k_M, Eq. (4.4) was briefly introduced as being the only physically meaningful scale for instabilities in a two-component fluid. To make this quantity dimensionless, it would be appropriate to make the definition

$$K_M^2 = \frac{k^2}{W_B/v_B^2 + W_D/v_D^2}. \tag{5.11}$$

This quantity is only of relevance to a static spacetime scenario. To place it in the context of the expanding Universe, the substitutions

$$W_B \to \frac{6\epsilon_B}{\chi^2}, \quad v_B^2 k^2 \to 6K_B^2,$$

$$W_D \to \frac{6\epsilon_D}{\chi^2}, \quad v_D^2 k^2 \to 6K_D^2$$

are required. Then K_M takes on the revised definition

$$K_M^2 = \frac{\chi^2}{\epsilon_B/K_B^2 + \epsilon_D/K_D^2} = \frac{\chi^2}{\chi_c^2}. \tag{5.12}$$

We have introduced the quantity $\chi_c(k)$, which can be thought of as a critical time. For $\chi > \chi_c$, $K_M > 1$ and acoustic oscillations would only be expected to exist for all modes. For $\chi < \chi_c$, $K_M < 1$ and two of the modes become unstable and undergo gravitational collapse. Since the precise magnitude of the scale factor a is not determined by cosmology [see Eq. (3.7), which contains an arbitrary initial time t_i], we may arbitrarily assign an initial time $a_0 = 1$, so that $\chi_0 = 1$ and decreases with increasing time. Then we may interpret the Jeans instability in two ways by considering the critical time χ_c. Initially we may study all k-dependent modes at a particular time χ, where a subset will be unstable for values of k for which $\chi_c(k) > \chi$ (we stress that χ_c is a function of k). We may then consider what occurs as the modes evolve through time from this particular instant. The critical time χ_c is fixed for any particular mode, so that a subset of modes that were originally acoustic will become unstable as $\chi \to \chi_c^+$ (those modes corresponding to the solutions δ_3 and δ_4 in Table I). Consequently more and more modes pass through the instability as the Universe evolves. The physical wave number k is of course dependent on time, thus the dependence of the instability on a time χ_c shows the inextricable link between the wave number and time.

It is illuminating at this stage to refer back to the one-component modes discussed in Sec. III. For the one-component case, solutions were found in terms of the combination $K_J a^{-1/2}$. With the identification $\chi = a^{-1/2}$, the quantity χ_c is seen to be the two-component analog of K_J.

It would be useful to convert the expansions (5.3)–(5.10) to depend on K_M or χ_c, to see how the Jeans scale enters. This is achieved by the following relations:

$$K_B^2 = \frac{1}{\chi_c^2}(\epsilon_B + \epsilon_D V^2), \quad K_D^2 = \frac{1}{\chi_c^2}\left(\epsilon_D + \frac{\epsilon_B}{V^2}\right). \tag{5.13}$$

Here $V = v_B/v_D$ is the ratio of sound velocities. We then find that the expansions are all in terms of increasing powers of χ/χ_c, with coefficients in terms of ϵ_B, ϵ_D, and V:

$$\delta_{B1}(\chi) = 1 + \frac{3}{2}\left(\epsilon_B + \epsilon_D V^2 - 6\epsilon_B\epsilon_D - 3\epsilon_D^2 V^2 - \frac{3\epsilon_B^2}{V^2}\right)\frac{\chi^2}{\chi_c^2} + O\left(\frac{\chi^4}{\chi_c^4}\right), \tag{5.14}$$

$$\delta_{D1}(\chi) = -\frac{\epsilon_B}{\epsilon_D}\left[1 + \frac{3}{2}\left(\epsilon_D + \frac{\epsilon_B}{V^2} - 6\epsilon_B\epsilon_D - 3\epsilon_D^2V^2 - \frac{3\epsilon_B^2}{V^2}\right)\frac{\chi^2}{\chi_c^2} + O\left(\frac{\chi^4}{\chi_c^4}\right)\right], \tag{5.15}$$

$$\delta_{B2}(\chi) = \chi\left\{1 + \frac{1}{25}\left[5 + \epsilon_D + \frac{6\epsilon_B}{V^2} + \frac{5\epsilon_B^2}{\epsilon_D V^2} - 31\left(\epsilon_D V + \frac{\epsilon_B}{V}\right)^2\right]\frac{\chi^2}{\chi_c^2} + \frac{6}{5}\epsilon_B\left(\epsilon_D - \epsilon_B - \epsilon_D V^2 + \frac{\epsilon_B}{V^2}\right)\frac{\chi^2}{\chi_c^2}\log\chi + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}, \tag{5.16}$$

$$\delta_{D2}(\chi) = -\frac{\epsilon_B}{\epsilon_D}\chi\left\{1 - \frac{1}{25}\left[\epsilon_D - \frac{\epsilon_B}{V^2} + 31\left(\epsilon_D V + \frac{\epsilon_B}{V}\right)^2\right]\frac{\chi^2}{\chi_c^2} - \frac{6}{5}\epsilon_D\left(\epsilon_D - \epsilon_B - \epsilon_D V^2 + \frac{\epsilon_B}{V^2}\right)\frac{\chi^2}{\chi_c^2}\log\chi + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}, \tag{5.17}$$

$$\delta_{B3}(\chi) = \chi^3\left\{1 + \frac{3}{70}\left[3\epsilon_D\left(\epsilon_B - \epsilon_D + \epsilon_D V^2 - \frac{\epsilon_B}{V^2}\right) - 10(\epsilon_B + \epsilon_D V^2)\right]\frac{\chi^2}{\chi_c^2} + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}, \tag{5.18}$$

$$\delta_{D3}(\chi) = \chi^3\left\{1 + \frac{3}{70}\left[3\epsilon_B\left(\epsilon_D - \epsilon_B - \epsilon_D V^2 + \frac{\epsilon_B}{V^2}\right) - 10\left(\epsilon_D + \frac{\epsilon_B}{V^2}\right)\right]\frac{\chi^2}{\chi_c^2} + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}, \tag{5.19}$$

$$\delta_{B4}(\chi) = \chi^{-2}\left\{1 + \left[-4\epsilon_B + \epsilon_D V^2 + 5\epsilon_B\epsilon_D + 5\epsilon_D^2(V^2 - 1) - 5\left(\frac{\epsilon_B}{\epsilon_D} + \epsilon_D\right)\frac{\epsilon_B}{V^2}\right]\frac{\chi^2}{\chi_c^2} + 6\epsilon_D\left(\epsilon_B - \epsilon_D + \epsilon_D V^2 - \frac{\epsilon_B}{V^2}\right)\frac{\chi^2}{\chi_c^2}\log\chi + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}, \tag{5.20}$$

$$\delta_{D4}(\chi) = \chi^{-2}\left\{1 + \left[6\epsilon_D - 5\epsilon_B^2 + 5\epsilon_B\epsilon_D(1 - V^2) + \frac{5\epsilon_B^2}{V^2}\right]\frac{\chi^2}{\chi_c^2} - 6\epsilon_B\left(\epsilon_B - \epsilon_D + \epsilon_D V^2 - \frac{\epsilon_B}{V^2}\right)\frac{\chi^2}{\chi_c^2}\log\chi + O\left(\frac{\chi^4}{\chi_c^4}\right)\right\}. \tag{5.21}$$

This is a convenient parametrization of the solutions. The scale of the modes are chosen by χ_c, the nature of the matter involved is determined by V, and the proportions are determined by ϵ_B and ϵ_D. A complete solution to the problem has thus been achieved up to whatever order desired.

VI. CONCLUSIONS AND FURTHER WORK

A method for determining the small k solutions of a general two-component cosmological density perturbation model has been expounded in this paper. We have only displayed the solutions to first order, but it is possible to derive them up to any order by the method in principle. We have explored the mathematical properties and peculiarities of density perturbations influenced by gravitational interaction, particularly contrasting them to plasma modes, and correcting a number of previous misconceptions in the literature. The expanding Universe introduces new features not predictable from simple static space–time considerations. In particular, totally new structures to the dispersion relations are found, even in the one-component example. We have shown how the mixture Jeans wave number enters the solutions, and clarified its role in an expanding universe context.

More work is required to investigate the solutions around the critical scale defined by k_M. Although the expansions as derived in this paper are applicable to this region, they are not

particularly useful, as many terms in the equations need to be retained when the expansion parameter χ/χ_c is of $O(1)$. It is unclear how an analytical investigation of this region could proceed at present. We have performed some preliminary studies which involved producing a large number of terms in the expansions (5.3)–(5.10) using the Mathematica program described, and then substituting in numerical values for the various physical parameters to obtain numerical coefficients with an ascending series in χ. At present the plots of these expansions over a range of values of χ do not yield reliable results—it is possible that many more terms than are practically calculable will be required, and a very high order of numerical precision will have to be maintained. Other methods of analyzing the modes in this interesting region probably need to be investigated.

Of ultimate interest is exploring how these type of modes contribute to the power spectrum. More physical effects may need to be introduced, such as a cosmological constant, or the addition of more matter components. To determine the actual density contrast at a given scale $1/k$, the Fourier modes of the density contrast as derived in this paper would also need to be integrated over the whole range $0<k<1/k$. It would be of considerable interest to compare the power spectra calculated by such a method with the well-known power spectra of the various cosmological models in existence today.

In concluding, we remark that a similar analysis could be carried out in the postrecombination region $140<z<1150$, where now the baryons follow the $T\sim 1/a$ relationship. The differential equations in Sec. II will now be different, as will be their solutions; but we expect that the ensuing analysis would yield qualitatively similar results but quantitatively different scaling. This would be a useful future study.

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Short wavelength analysis of the evolution of perturbations in a two-component cosmological fluid

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The equations describing a two-component cosmological fluid with linearized density perturbations are investigated in the small wavelength or large k limit. The equations are formulated to include a baryonic component, as well as either a hot dark matter (HDM) or cold dark matter (CDM) component. Previous work done on such a system in static space–time is extended to reveal some interesting physical properties, such as the Jeans wave number of the mixture, and resonant mode amplitudes. A WKB technique is then developed to study the expanding universe equations in detail, and to see whether such physical properties are also of relevance in this more realistic scenario. The Jeans wave number of the mixture is reinterpreted for the case of an expanding background space–time. The various modes are obtained to leading order, and the amplitudes of the modes are examined in detail to compare to the resonances observed in the static space–time results. It is found that some conclusions made in the literature about static space–time results cannot be carried over to an expanding cosmology. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209551]

I. INTRODUCTION

The analysis of cosmological perturbations in the Newtonian limit is a well studied problem in theories of structure formation, and it may be supposed that there is little left to learn from this theory. Most of the effort has gone into the study of the one-component cosmological fluid equations, and the results have been well expounded in many standard texts.[1–5] There is, however, still a wealth of problems remaining in the detailed analysis of two-component cosmological fluids and their linearized gravitational perturbation modes. In particular, if pressure effects are included so that the Jeans instability becomes an issue, the equations present a considerable analytic challenge, and a range of new physical effects become apparent. Some of these effects have been studied in the contrived case of a static space–time background.[6,7] In this scenario there is no expansion, so that the mathematics is considerably simplified, and solutions can easily be found. This is useful to gain some qualitative idea about physical phenomena observable, but to gain a true picture in a cosmological context, the expanding background space–time given by the Friedmann-Robertson-Walker cosmologies is required.

There have been a variety of studies of the multicomponent cosmological fluid equations, ranging from some relatively specific applications under certain cosmological scenarios,[8,9] to a broad mathematical study and classification.[10] A discussion of the application and validity of some of the equations mentioned in these previous studies, together with the solution of an unsolved set of two-component post-recombination equations, has recently been undertaken by the authors.[11] The system of equations described the interaction between a dark matter and baryonic component in the Newtonian regime (density fluctuations on scales well within the Hubble radius). A series

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expansion of the solutions for small wave number k (large scales) was presented. This allowed comparison with some of the previous work, in particular with the Meijer G-function classifications given by Ref. 10. This region of k-space is also interesting because it is the region in which the Jeans instability is known to occur.

In this paper we wish to complete this study by examining the large k asymptotic region of the solutions. Such a study is worthwhile, in order to make contact with the static space–time results of Ref. 7. Although not realistic as cosmological solutions, these results displayed a number of little known physical phenomena associated with the linearized modes, which we wish to expand on here. The techniques required to analyze the expanding universe solutions are also of interest in their own right mathematically, where a generalized WKB method will be expounded. It is possible to make a comparison with the work done in cosmological plasma physics in an Einstein-deSitter background.[12–14] This is interesting because of the mathematically very similar form of fluid equations for both type of systems, which is due to the similarity of the electromagnetic and gravitational forces. Thus mathematical techniques employed in the analysis of plasma equations will be useful in this paper, and give clues as to how to proceed with some challenging mathematical analysis of gravitational density perturbation modes.

The paper is to be organized as follows. The relevant equations will be introduced in Sec. II. The discussion will then be focused in Sec. III, by reconsidering the two-component modes in a static space–time. This investigation is by necessity of a qualitative nature, but gives a useful introduction to the concepts and interesting physical effects not found in the standard one-component analysis. The work of Ref. 7 will also be extended. The expanding universe baryonic and dark matter equations will then be considered in Sec. IV. The short wavelength (WKB) approximation will be utilized to complete the study of these equations initiated in Ref. 11. The relevance of the previous work on static space–time systems is revealed through this analysis. This will allow meaningful conclusions to be drawn about this whole area of study, and point to where promising future work may lie. These aspects are discussed in Sec. V.

II. THE GOVERNING EQUATIONS

A broad survey of the Newtonian cosmological perturbation equations under various cosmological scenarios was given in Ref. 11. This paper also gave a detailed derivation of the equations of interest for present analysis. We will not repeat such a detailed discussion here, but directly introduce the relevant equations.

The starting point is the equations for an n-component system of nonrelativistic species, as derived in all the standard texts. Given a density perturbation δ_i of the ith component of the mass density ρ_i,

$$\delta_i(\mathbf{r},t) = \frac{\delta\rho_i}{\rho_i}, \tag{2.1}$$

it may be decomposed into its Fourier plane wave modes with wave vector $\mathbf{k}$,

$$\delta_i(\mathbf{r},t) = \frac{1}{(2\pi)^3}\int \delta_{\mathbf{k}i}(t)\exp(-i\mathbf{k}\cdot\mathbf{r})d^3r. \tag{2.2}$$

Here $\mathbf{r}$ is the physical spatial coordinate, and t is cosmic time. Using the Eulerian equations of motion describing a perfect fluid, a set of coupled second order equations for the Fourier modes $\delta_i(t)$ (where we now drop the subscript $\mathbf{k}$) are achieved,

$$\frac{d^2\delta_i}{\mathrm{d}t^2} + 2\frac{\dot{a}}{a}\frac{\mathrm{d}\delta_i}{\mathrm{d}t} + v_i^2k^2\delta_i = 4\pi G\sum_{i=1}^{n}\rho_i\delta_i, \quad i = 1,2,\ldots,n. \tag{2.3}$$

Overdots will denote derivatives with respect to t.

The above equations contain the universe expansion factor a and sound velocities v_i. We use the expression "sound velocity" fairly loosely. The parameters v_i could also denote a general

velocity dispersion for a collisionless fluid. To be able to solve the equations, the time dependence of the physical variables needs to be made explicit. We will adopt the convention that barred variables will denote comoving quantities, independent of time. Thus the definition of comoving wave number $\bar{\mathbf{k}}=a\mathbf{k}$ arises naturally. An assumption must also be made about the scaling of the sound velocities v_i. In the post-recombination era, the adiabatic speed of sound follows the behavior $v \propto a^{-1}$, so we will introduce the time independent quantities $\bar{v}_i \equiv a v_i$. The total background energy density ρ_0 can also be made independent of time by the definition $\bar{\rho}_0 \equiv a^3 \rho_0$. This enables us to introduce the useful parameter $\epsilon_i = \rho_i / \rho_0$, the fraction of mass density contributed by species i.

We will not go into detail on how the equations are transformed into their simplest form here (instead see Ref. 11), but briefly describe the important points. The equations are first transformed so that a is the only explicit temporal variable. This allows parameters specifying particular large scale cosmological dynamics to enter the equations, namely the cosmological constant Λ and spatial curvature k_c. In this paper, a background Einstein-deSitter cosmology will be employed ($k_c=0$, $\Lambda=0$). Although this model has been ruled out with high confidence by current observations, it is sufficient for our purposes. We wish to study some important physical process without additional complications.

It is found that the following important parameters arise:

$$\bar{k}_B^2 = \frac{4\pi G \bar{\rho}_0}{\bar{v}_B^2}, \quad \bar{k}_D^2 = \frac{4\pi G \bar{\rho}_0}{\bar{v}_D^2}. \tag{2.4}$$

They resemble the comoving Jeans wave numbers for each component taken separately. The strict Jeans one-component wave numbers are given by replacing ρ_0 with ρ_i in (2.4) (see next section). The wavelength parameters defined above indicate whether gravity $\bar{k}_i > \bar{k}$ or pressure support $\bar{k}_i < \bar{k}$ dominate the dynamics, and thus whether the region of k-space under consideration is Jeans unstable. It may also be noted that the relation $\epsilon_B + \epsilon_D = 1$ holds.

It is useful to define the parameters

$$K_B = \frac{\bar{k}}{\bar{k}_B}, \quad K_D = \frac{\bar{k}}{\bar{k}_D}, \tag{2.5}$$

for a clear dimensionless partitioning of parameter space. $K_i < 1$ corresponds to the Jeans unstable region in the single component analog of the equations, and $K_i > 1$ to the acoustic region. The cosmological fluid equations are finally written in terms of the variable $\chi = a^{-1/2}$, to give the canonical form of the system of differential equations to be studied in this paper,

$$\delta_B'' + 6\left(K_B^2 - \frac{\epsilon_B}{\chi^2}\right)\delta_B - \frac{6\epsilon_D}{\chi^2}\delta_D = 0, \tag{2.6}$$

$$\delta_D'' + 6\left(K_D^2 - \frac{\epsilon_D}{\chi^2}\right)\delta_D - \frac{6\epsilon_B}{\chi^2}\delta_B = 0. \tag{2.7}$$

The prime denotes differentiation with respect to χ.

These equations bear a strong resemblance to the equations of an electron-proton cosmological plasma studied in Ref. 14 [Eqs. (4.8) and (4.9) of that paper]. Considering the mathematical similarity between the electromagnetic and gravitational forces, this was to be expected. A manifestation of this fact is the close resemblance between the dispersion relation for the simple one-component Jeans instability and Langmuir modes. The techniques employed in Ref. 14 will be adopted and developed further to the current problem. In particular, some general WKB techniques will be extended. This will also indicate further results obtainable in cosmological plasma physics.

We now digress to an analysis of the static space–time perturbation equations to introduce some new physical phenomena, which are to be scrutinized for their applicability in an expanding universe.

III. THE STATIC TWO-COMPONENT PROBLEM

A. Eigenvalues and eigenvectors

The static space–time results for a two-component fluid are well understood, though receive little attention in standard linearized structure formation theory, which aims to produce the power spectrum of density perturbations. We will extend the current results to facilitate understanding the general expanding universe scenario later. This section aims to develop some concepts in a relatively simple setting. Previous work on the static problem has been done in Refs. 6 and 7. We will in particular rely quite heavily on the notation and results of Ref. 7 in this section. Although the solutions are unrealistic as an application to cosmology, they display some similar qualitative features, and allow an exposition of the basic physical ideas without the complication of space–time expansion being introduced. The static nature of the space–time simplifies the mathematics greatly, and is thus useful in understanding the general problem.

In this section, there is no need to refer to barred (comoving) physical quantities, and all physical variables may be assumed to be constant in time, unless otherwise specified. With the expansion parameter a set equal to unity, the general fluid equations (2.3) may be written as

$$\ddot{\delta}_D + (v_D^2 k^2 - W_D)\delta_D - W_B\delta_B = 0, \tag{3.1}$$

$$\ddot{\delta}_B + (v_B^2 k^2 - W_B)\delta_B - W_D\delta_D = 0, \tag{3.2}$$

with an overdot denoting differentiation with respect to t, and $W_i = 4\pi G\rho_i$. A study of the behavior of the solutions to these equations is most readily undertaken by reducing the system to a first order autonomous dynamical system, undertaken in Ref. 7. To analyze the dynamical system, a solution needs to be found for the state vector

$$\mathbf{x} = (x_1, x_2, x_3, x_4)^T \equiv (\dot{\delta}_D, \delta_D, \dot{\delta}_B, \delta_B)^T. \tag{3.3}$$

We just state the results here.

The most important feature discovered in Ref. 7 was the existence of a parameter dependent critical point of the dynamical system given by

$$k^2 = k_M^2 \equiv k_B^2 + k_D^2 = \frac{W_B}{v_B^2} + \frac{W_D}{v_D^2}, \tag{3.4}$$

where k_B and k_D have been defined in terms of the density and velocity parameters of each matter component, and are slightly different from $\bar{k}_B$ and $\bar{k}_D$ defined in (2.4). The special value of the wave number k_M, may be thought of as the Jeans wave number of a two-component fluid (the mixture wave number). It comprises the Jeans wave numbers of each fluid taken separately, but it is possible to show that $k=k_M$ is the only physical quantity which indicates an instability—both $k=k_D$ and $k=k_B$ have no such interpretation for the coupled two-component case.

With solutions of the form

$$\mathbf{x}(t) = \sum_{i=1}^{4} \alpha_i \exp(\lambda_i t)\boldsymbol{\xi}_i, \tag{3.5}$$

where the α_i are amplitude functions dependent on k and determined by initial conditions, the solutions for the eigenvalues λ_i and eigenvectors $\boldsymbol{\xi}_i$ of the dynamical system are, respectively,

$$\lambda_1 = -\lambda_2 = \tfrac{1}{\sqrt{2}}\sqrt{f + \sqrt{f^2 + 4g}},$$

$$\lambda_3 = -\lambda_4 = \tfrac{1}{\sqrt{2}}\sqrt{f - \sqrt{f^2 + 4g}}, \tag{3.6}$$

with

$$f(k) = W_B + W_D - k^2(v_B^2 + v_D^2), \tag{3.7}$$

$$g(k) = k^2(W_B v_D^2 + W_D v_B^2) - k^2 v_B^2 v_D^2, \tag{3.8}$$

and

$$\boldsymbol{\xi}_i = (\beta_i \lambda_i, \beta_i, \lambda_i, 1)^T, \quad i = 1,2,3,4, \tag{3.9}$$

with

$$\beta_1 = \beta_2 = \tfrac{1}{2W_D}(h + \sqrt{h^2 + 4W_B W_D}),$$

$$\beta_3 = \beta_4 = \tfrac{1}{2W_D}(h - \sqrt{h^2 + 4W_B W_D}), \tag{3.10}$$

and

$$h(k) = W_D - W_B + k^2(v_B^2 - v_D^2). \tag{3.11}$$

For calculational purposes, we note that

$$h^2 + 4W_B W_D = f^2 + 4g. \tag{3.12}$$

An examination of the real and imaginary parts of the λ_i will show that the λ_1 and λ_2 modes represent acoustic oscillations for $k > k_M$ and growing and decaying modes for $k < k_M$. The λ_3 and λ_4 modes however always represent acoustic oscillations. The exponential nature of the solutions indicate that the growing and decaying modes do not have the typical power law behavior exhibited by expanding universe solutions, however the solutions exhibit the correct qualitative behavior in the regions below and above the critical point given by $k = k_M$.

To gain a feel for the properties of the above eigenvalues and eigenvectors, which allows us to make direct contact with the physics of the solutions, we study the quantities in various asymptotic regimes, and examine some plots. This will be effectively facilitated if the quantities are reparametrized in terms of some dimensionless variables. We need only consider the eigenvalues λ_1 and λ_3. To indicate the nature of the dark matter, the sound velocities may be coalesced into the single variable

$$V^2 = \frac{v_B^2}{v_D^2}. \tag{3.13}$$

Then $V \ll 1$ corresponds to HDM while $V \gg 1$ corresponds to CDM. We also introduce the quantities ϵ_D and ϵ_B as used elsewhere in the paper. In this context, they may be defined as

$$\epsilon_D = \frac{W_D}{W_B + W_D}, \quad \epsilon_B = \frac{W_B}{W_B + W_D}. \tag{3.14}$$

We also parametrize the wave-number dependence in units of the mixed Jeans wave number; thus we define

$$K_M = \frac{k}{k_M}. \tag{3.15}$$

It then follows that the eigenvalues may be written as

$$\lambda_{1,3} = \frac{1}{\sqrt{2}}(W_B + W_D)^{1/2}\left\{1 - K_M^2 - \left(\epsilon_D V^2 + \frac{\epsilon_B}{V^2}\right)K_M^2 \pm \left[\left(1 - K_M^2 - \left(\epsilon_D V^2 + \frac{\epsilon_B}{V^2}\right)K_M^2\right)^2 + 4\left(\frac{\epsilon_B}{V} + \epsilon_D V\right)^2 K_M^2(1 - K_M^2)\right]^{1/2}\right\}^{1/2}. \tag{3.16}$$

These expressions may be expanded for small and large K_M. The results are

$$\lambda_1 \sim (W_B + W_D)^{1/2}\left[1 + \frac{1}{2V^2}(-\epsilon_B + \epsilon_B^2 - V^2 + 2\epsilon_B\epsilon_D V^2 - \epsilon_D V^4 + \epsilon_D^2 V^4)K_M^2 + \cdots\right], \quad K_M \ll 1, \tag{3.17}$$

$$\lambda_1 \sim iK_M\frac{1}{\sqrt{2}}(W_B + W_D)^{1/2}\{1 + \epsilon_B/V^2 + \epsilon_D V^2 - [(1 + \epsilon_B/V^2 + \epsilon_D V^2)^2 - 4(\epsilon_B/V + \epsilon_D V)^2]^{1/2}\}^{1/2}, \quad K_M \gg 1, \tag{3.18}$$

$$\lambda_3 \sim iK_M(W_B + W_D)^{1/2}(\epsilon_B/V^2 + \epsilon_D V^2), \quad K_M \ll 1, \tag{3.19}$$

$$\lambda_3 \sim iK_M\frac{1}{\sqrt{2}}(W_B + W_D)^{1/2}\{1 + \epsilon_B/V^2 + \epsilon_D V^2 + [(1 + \epsilon_B/V^2 + \epsilon_D V^2)^2 - 4(\epsilon_B/V + \epsilon_D V)^2]^{1/2}\}^{1/2}, \quad K_M \gg 1. \tag{3.20}$$

These expansions confirm the earlier statement, whereby the λ_3 (and equivalently λ_4) modes display acoustic oscillations at all wavelengths, whereas the λ_1 (and equivalently λ_2) modes undergo a Jeans instability to growing (decaying) modes for $K_M < 1$. It is also evident that at very large wave numbers (small scales) the acoustic oscillations have a very large frequency, growing in proportion to the wave number, whereas for very low wave numbers the λ_3 modes behave in a very slowly varying oscillatory manner, the frequency again being proportional to the wave number. In this regime the λ_1 and λ_2 modes comprise exponentially growing or decaying perturbations over an almost wave number independent timescale, approximately equal to $(W_B + W_D)^{1/2}$. These properties are illustrated in Fig. 1, where the absolute values of the eigenvalues are plotted as a function of K_M for a variety of H/CDM scenarios. The values $\epsilon_B = 0.1$ and $\epsilon_D = 0.9$ have been used in the plots, which is a fairly typical proportion of baryonic and dark matter mass density expected in the Universe.

B. Interesting scales

It is evident that at certain scales the eigenvalues undergo some qualitatively interesting changes, which have been marked on the plots by some arrows. For wave numbers around $K_M = 1$, the λ_1 eigenvalue drops very quickly to zero, indicating the Jeans instability, but the λ_3 eigenvalue displays uniform behavior in this region. There is another interesting scale in the $K_M < 1$ region for small V. The physical motivation for this scale was discussed in Ref. 7. It corresponds to a critical wave number k_C, defined to be when the frequencies of each component taken separately coincide, i.e., when

$$v_B^2 k^2 - W_B = v_D^2 k^2 - W_D. \tag{3.21}$$

The wave number $k = k_C$ is consequently given by

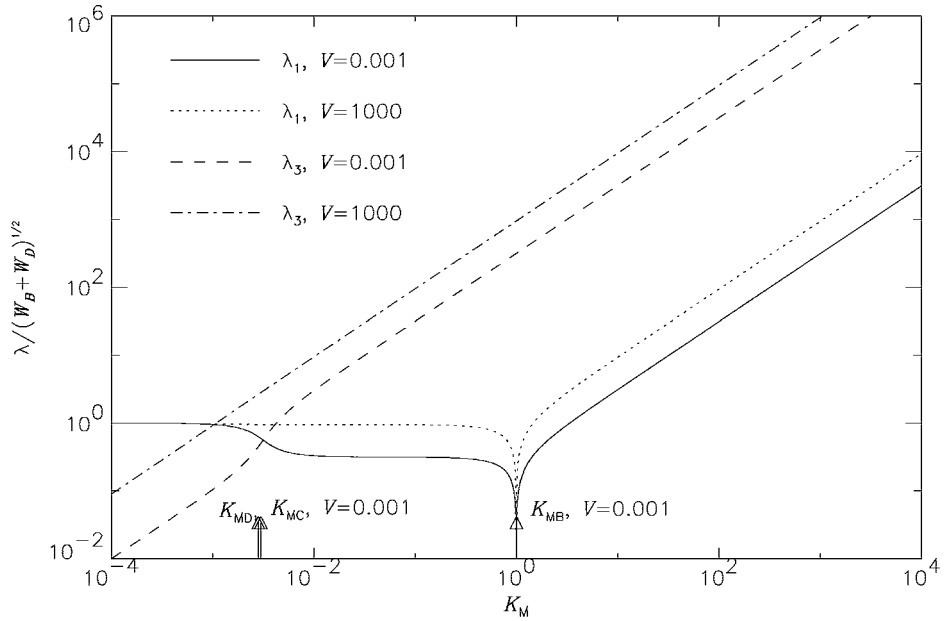

FIG. 1. The eigenvalues for HDM and CDM in the static universe scenario with ϵ_B=0.1, ϵ_D=0.9.

$$k_C = \left(\frac{W_D - W_B}{v_D^2 - v_B^2} \right)^{1/2}. \tag{3.22}$$

It is interesting that the importance of this scale is only apparent for small V, where a sudden increase in the magnitude of λ_3 and decrease in the magnitude of λ_1 is apparent. For all $V \gtrsim 1$, the plots would be almost identical to the displayed plots of $V=1000$ in Fig. 1.

To gain a better understanding of this behavior, it is useful to convert k_C into units of k_M, which are the plotting units of all the figures. Thus

$$K_{MC} \equiv \frac{k_C}{k_M} = \left(\frac{\epsilon_D - \epsilon_B}{\epsilon_D - \epsilon_B - \epsilon_D V^2 + \epsilon_B / V^2} \right)^{1/2}. \tag{3.23}$$

It is interesting to compare this quantity to the individual Jeans instability scales for each fluid taken separately,

$$K_{MD} \equiv \frac{k_D}{k_M} = \left(\frac{\epsilon_D}{\epsilon_B / V^2 + \epsilon_D} \right)^{1/2}, \tag{3.24}$$

$$K_{MB} \equiv \frac{k_D}{k_M} = \left(\frac{\epsilon_B}{\epsilon_B + \epsilon_D V^2} \right)^{1/2}. \tag{3.25}$$

A better qualitative feel for these scales is facilitated by considering their expansions in the HDM and CDM regimes. For HDM, with $V \ll 1$ we find

$$K_{MC}^2 = V^2 \left(\frac{\epsilon_D}{\epsilon_B} - 1 \right) \left[1 - \left(\frac{\epsilon_D}{\epsilon_B} - 1 \right) V^2 + O(V^4) \right], \tag{3.26}$$

$$K_{MD}^2 = V^2 \frac{\epsilon_D}{\epsilon_B} \left[1 - \frac{\epsilon_D}{\epsilon_B} V^2 + O(V^4) \right], \tag{3.27}$$

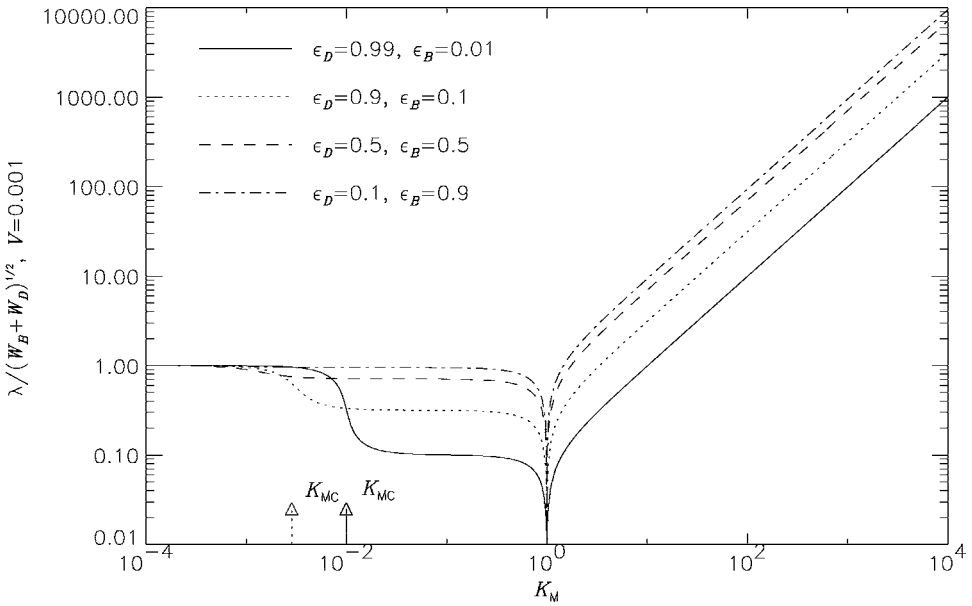

FIG. 2. The eigenvalue λ_1 for a range of ϵ_D and ϵ_B, with $V=0.001$ in the static universe scenario.

$$K_{MB}^2 = 1 - \frac{\epsilon_D}{\epsilon_B} V^2 + O(V^4). \tag{3.28}$$

From this it may be concluded that if

(1) $\epsilon_D \gg \epsilon_B$, then $K_{MC} \sim K_{MD}$,
(2) $\epsilon_D \gtrsim \epsilon_B$, then $K_{MC} \ll 1$,
(3) $\epsilon_B > \epsilon_D$, then K_{MC} is imaginary (no physical significance).

This last point is also borne out by the original definition (3.22), where it is seen that for k_C to be real, the dominant component must also be the hotter component. For CDM, with $V \gg 1$ the corresponding relations are given by

$$K_{MC}^2 = V^{-2}\left(\frac{\epsilon_B}{\epsilon_D} - 1\right)\left[1 - \left(\frac{\epsilon_B}{\epsilon_D} - 1\right)V^{-2} + O(V^{-4})\right], \tag{3.29}$$

$$K_{MD}^2 = 1 - \frac{\epsilon_B}{\epsilon_D} V^{-2} + O(V^{-4}), \tag{3.30}$$

$$K_{MB}^2 = V^{-2}\frac{\epsilon_B}{\epsilon_D}\left[1 - \frac{\epsilon_B}{\epsilon_D} V^{-2} + O(V^{-4})\right]. \tag{3.31}$$

This shows that if

(1) $\epsilon_B \gg \epsilon_D$, then $K_{MC} \sim K_{MB}$,
(2) $\epsilon_B \gtrsim \epsilon_D$, then $K_{MC} \ll 1$,
(3) $\epsilon_D > \epsilon_B$, then K_{MC} is imaginary (no physical significance).

The position of the arrows in Fig. 1 bear out the above relations, as do the arrows in Fig. 2 and 3 to be discussed more below.

In conclusion, the fact that all eigenvalues have been plotted for the values $\epsilon_B=0.1$ and $\epsilon_D=0.9$ means that the scale k_C is only physically relevant for HDM. This is why all plots for $V \gtrsim 1$ (CDM) are so similar. Given that the real Universe is now considered almost certainly CDM

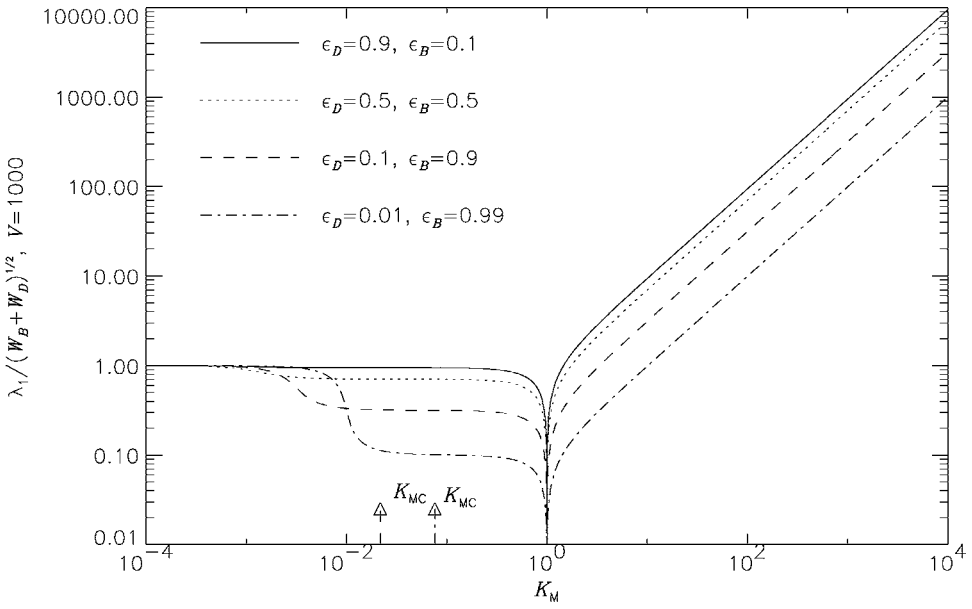

FIG. 3. The eigenvalue λ_1 for a range of ϵ_D and ϵ_B, with $V=1000$ in the static universe scenario.

dominated, it is doubtful as to whether this potentially interesting physical effect given by the equations has any discernible effect on structure formation scenarios in pure CDM models. A H +CDM model may give similar interesting results as discussed here. This however is a three-component problem beyond the scope of this paper, but may be considered a worthwhile topic of research for future work in this area.

C. Other qualitative behavior

We briefly consider some other features of the solutions, to help better understand the mathematical properties. The qualitative features we wish to explore are the same for both the λ_1 and λ_3 modes, so we will concentrate only on the λ_1 modes here. The eigenvalue λ_1 is plotted for different values of ϵ_B and ϵ_D in Fig. 2 and 3. An interesting feature of these figures is that there is a one-to-one correspondence between each of the four plots in one figure to a particular plot in the other figure, yet each plot corresponds to different physical parameters in each figure. This property highlights the symmetry of the eigenvalues. If the original analytic expression (3.16) for λ_1 is examined, it is clear that the expression retains an identical form if ϵ_D and ϵ_B are interchanged together with V and $1/V$. Real values of K_{MC} have also been marked in. They indicate when the critical scale k_C is physically relevant. Related to this property is the fact that in Fig. 2 all plots for $\epsilon_D \lesssim 0.1$ and $\epsilon_B \gtrsim 0.9$ are almost identical to the values of $\epsilon_D=0.1$ and $\epsilon_B=0.9$. Analogously, in Fig. 3 the same may be said for all plots $\epsilon_D \gtrsim 0.9$ and $\epsilon_B \lesssim 0.1$.

We now turn to study the behavior of β_1 and β_3, which give an indication of the relative proportion of baryonic and dark matter in each of the modes [see, for example, the x_2 and x_4 components of the eigenvectors in Eq. (3.9)]. In dimensionless variables, β_1 and β_3 may be written as

$$\beta_{1,3}=\frac{1}{2}\left\{1-\frac{\epsilon_B}{\epsilon_D}+\left(\frac{\epsilon_B}{\epsilon_D}-\frac{\epsilon_B}{\epsilon_D V^2}+V^2-1\right)K_M^2 \pm\left[\frac{1}{\epsilon_D^2}+2\left(1-\frac{\epsilon_B}{\epsilon_D}\right)\left(\frac{\epsilon_B}{\epsilon_D}-\frac{\epsilon_B}{\epsilon_D V^2}+V^2-1\right)K_M^2\right.\right.$$
$$\left.\left.+\left(\frac{\epsilon_B}{\epsilon_D}-\frac{\epsilon_B}{\epsilon_D V^2}+V^2-1\right)^2 K_M^4\right]^{1/2}\right\}. \tag{3.32}$$

It is obvious from inspection that for all wave numbers β_1 and β_3 are real valued and $\beta_1>0$,

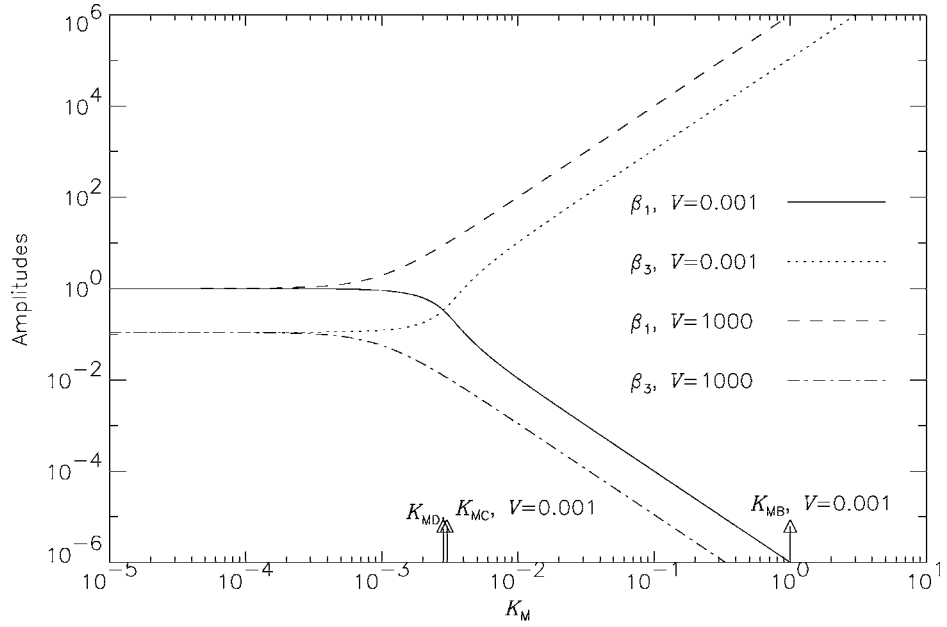

FIG. 4. The eigenvector amplitude functions β_1 and β_3 for HDM and CDM in the static universe scenario.

$\beta_3 < 0$. The almost symmetrical nature of the quantities are well illustrated in Fig. 4 for the opposing cases of H/CDM. Of interest here again is the scale K_{MC}, around which all the β_i undergo an abrupt change. Figure 4 shows that either β_1 or β_3 will dominate very rapidly for increasing wave number, depending on the value of V. Stated more specifically, for the HDM scenario ($V \ll 1$), baryons will dominate the λ_1 modes and dark matter will dominate the λ_3 modes, and vice versa for the CDM scenario ($V \gg 1$). We refrain from examining the asymptotics of β_1 and β_3 now, and leave that task to when we derive analogous expressions in the expanding universe scenario. The asymptotics will confirm the present qualitative discussion.

D. Initial conditions and amplitudes

Having completed a study of the behavior of the general solutions, we now turn to consider the effect of initial conditions. The study of the amplitudes of the various modes was studied with particular interest in Ref. 7, where the presence of a resonance was discovered at the scale k_C. We extend that work here to consider the amplitude functions at a wider range of scales, and for CDM as well. This will be of relevance when the expanding universe scenario is analyzed in the next section, where the $K_M > 1$ range of scales needs to be considered. It is also of course of relevance from the fact that the Universe is believed to be CDM dominated.

The amplitudes are k-dependent functions, which also depend on the various constants in the problem. Consider the initial conditions at some time t_0 given by the constants $x_i(t_0) = x_{i0}$. Here and henceforth, any variable subscripted with a 0 (possibly together with other subscripts) denotes that quantity evaluated at $t = t_0$. As a reasonable simplifying assumption, the perturbations are assumed to start from rest, so that $x_{10} = x_{30} = 0$. The matter density perturbations may then be written in the form

$$\delta_D(\tau) = x_{20}[\zeta_1(e^{\lambda_1 \tau} + e^{-\lambda_1 \tau}) + \zeta_2 \cos(i\lambda_3 \tau)], \tag{3.33}$$

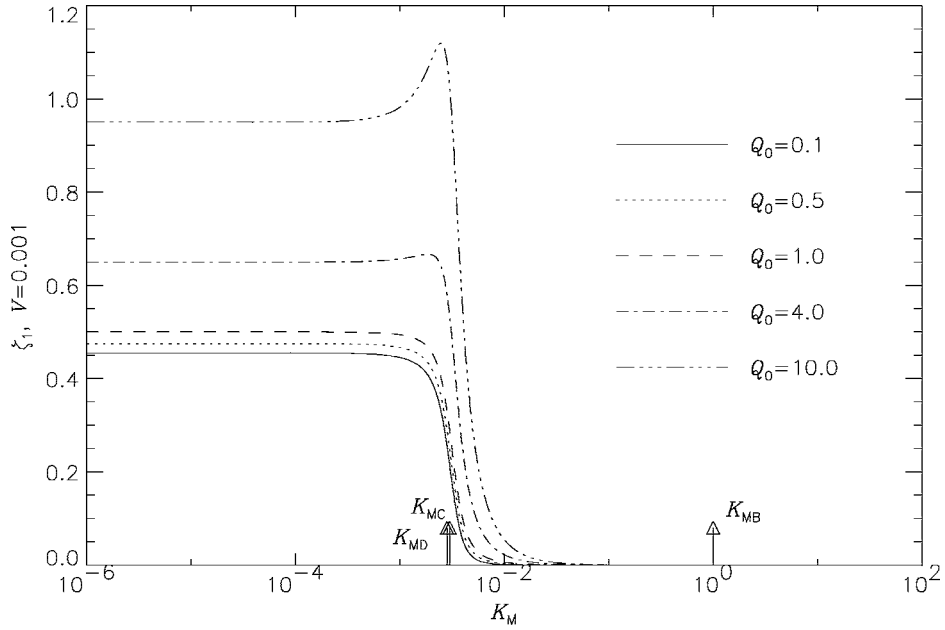

FIG. 5. The k-dependent amplitudes of the λ_1 dark matter modes in a HDM universe for a range of initial conditions $Q_0=x_{40}/x_{20}$.

$$\delta_B(\tau) = x_{40}[\zeta_3(e^{\lambda_1\tau} + e^{-\lambda_1\tau}) + \zeta_4 \cos(i\lambda_3\tau)], \tag{3.34}$$

where the time origin has been shifted by the definition $\tau=t-t_0$. The amplitude functions ζ_i are constructed out of the mode eigenvector functions β_i, as well as the ratio of initial densities $Q_0 = x_{40}/x_{20}$. They are

$$\zeta_1 = \frac{\beta_1}{2}\frac{1-Q_0\beta_3}{\beta_1-\beta_3}, \quad \zeta_2 = \beta_3\frac{Q_0\beta_1-1}{\beta_1-\beta_3}, \tag{3.35}$$

$$\zeta_3 = \frac{1}{2}\frac{Q_0^{-1}-\beta_3}{\beta_1-\beta_3}, \quad \zeta_4 = \frac{\beta_1-Q_0^{-1}}{\beta_1-\beta_3}. \tag{3.36}$$

Of particular interest is the fact that some of the ζ_i display a resonance around the scale k_C. This scale has of course previously shown its significance in the behavior of the eigenvalues and the β_i. The fact that k_C defines the scale at which the collapse times of the components taken separately coincide indicates that a resonance may well be expected to occur at this scale. The behavior of the various amplitudes over a wide range of scales, and in both the HDM and CDM scenarios are illustrated in Figs. 5–12. The distinguishing feature of all the plots of HDM amplitudes is the rapid change of the functions around the scale k_C.

The analytic properties of ζ_1 and in particular ζ_3 are discussed at some length in Ref. 7. Under some restrictive conditions (only HDM and certain initial values of Q_0) it was shown that ζ_1 would not obtain a resonance, whereas ζ_3 would for

$$Q_0 < \frac{1}{2}\left(\frac{v_D^2}{v_B^2} - \frac{W_D}{W_B}\frac{v_B^2}{v_D^2}\right). \tag{3.37}$$

In contrast no resonances are observed in the CDM scenario, but the amplitudes still undergo a rapid change around the scale K_{MB}. Both $K_M=K_{MB}$ and $K_M=K_{MD}$ are always less than $K_M=1$, so that no significant behavior occurs in the long wavelength limit, a fact of some importance in later work.

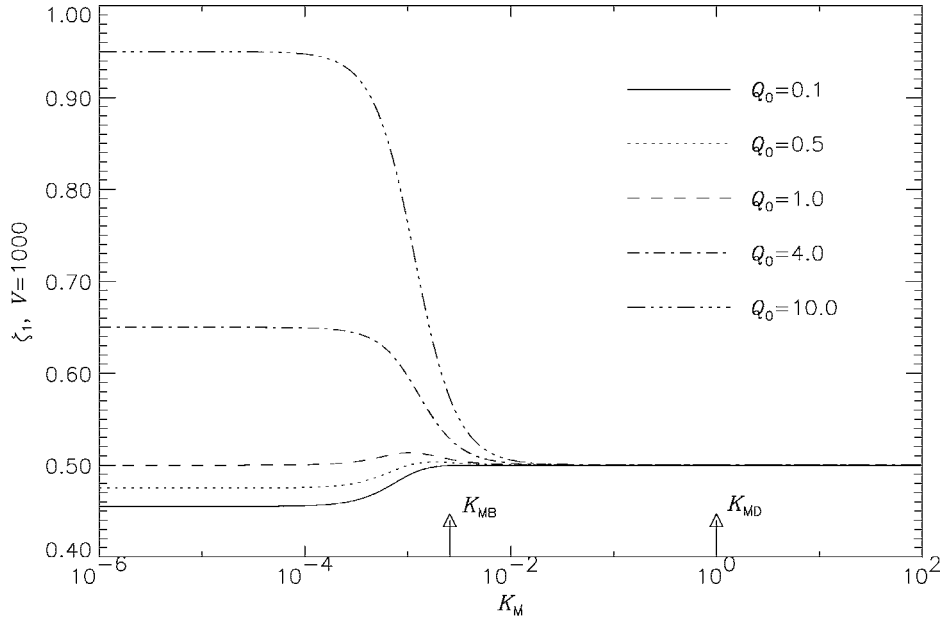

FIG. 6. The k-dependent amplitudes of the λ_1 dark matter modes in a CDM universe for a range of initial conditions $Q_0=x_{40}/x_{20}$.

IV. THE SHORT WAVELENGTH APPROXIMATION IN THE EXPANDING UNIVERSE

A. Matrix formulation

We are now prepared to tackle the most general equations formulated for the current problem, given by (2.6) and (2.7). The solution to this system of equations cannot be classified by known analytic functions, so approximation schemes need to be implemented. This paper investigates a short wavelength approximation, which would be expected to probe the acoustic regime of the

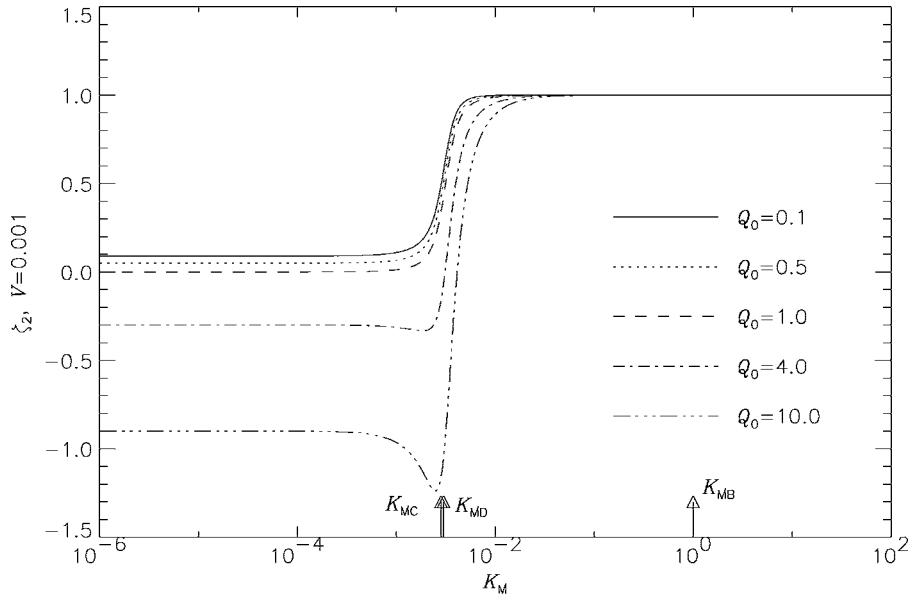

FIG. 7. The k-dependent amplitudes of the λ_3 dark matter modes in a HDM universe for a range of initial conditions $Q_0=x_{40}/x_{20}$.

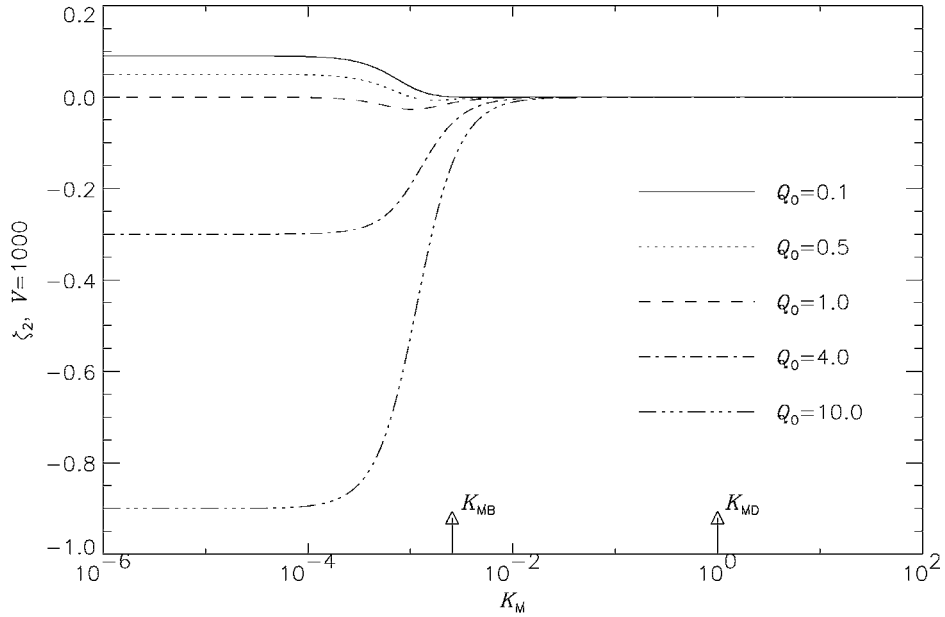

FIG. 8. The k-dependent amplitudes of the λ_3 dark matter modes in a CDM universe for a range of initial conditions $Q_0=x_{40}/x_{20}$.

modes. A WKB-type method may be employed for this. This is interesting, because through the derivation the explicit physical approximations required and type of solutions obtainable will naturally arise as a consequence of the method. A WKB method for coupled systems of equations in a cosmological plasma setting was expounded in Ref. 14. We will further develop that method here for the current system, which is more complicated than anything considered previously.

To begin with, the equations must be reduced to a first order system. Thus as in the static case (3.3), we define

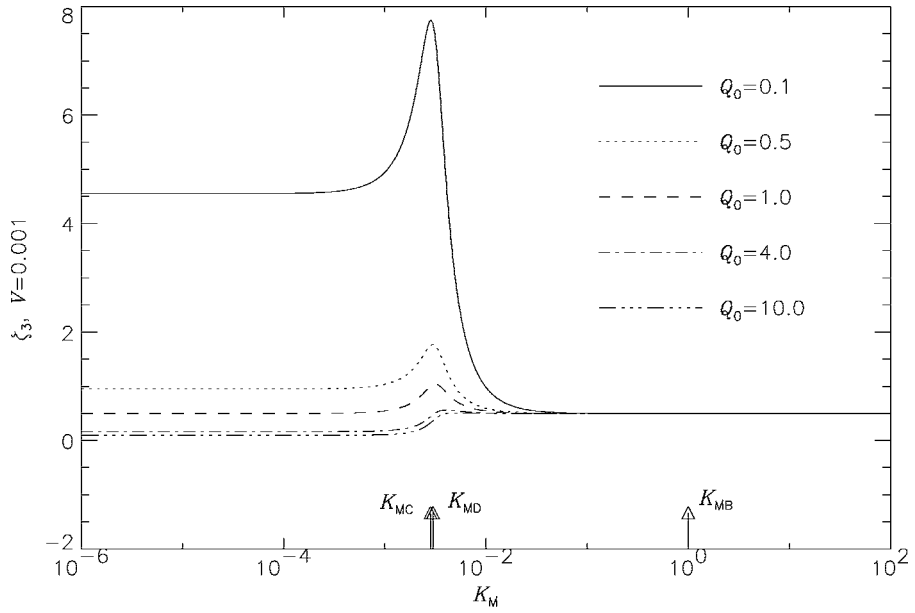

FIG. 9. The k-dependent amplitudes of the λ_1 baryonic modes in a HDM universe for a range of initial conditions $Q_0=x_{40}/x_{20}$.

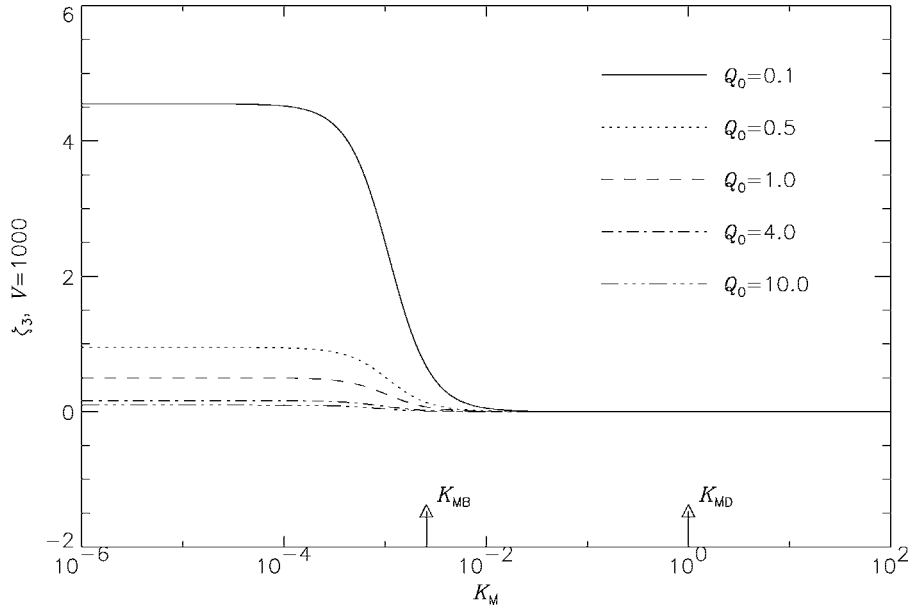

FIG. 10. The k-dependent amplitudes of the λ_1 baryonic modes in a CDM universe for a range of initial conditions $Q_0 = x_{40}/x_{20}$.

$$\mathbf{x} = (x_1, x_2, x_3, x_4)^T \equiv (\delta_D', \delta_D, \delta_B', \delta_B)^T. \tag{4.1}$$

The system may be written in matrix form

$$\mathbf{x}' = \mathbf{T}\mathbf{x}, \tag{4.2}$$

with the definition

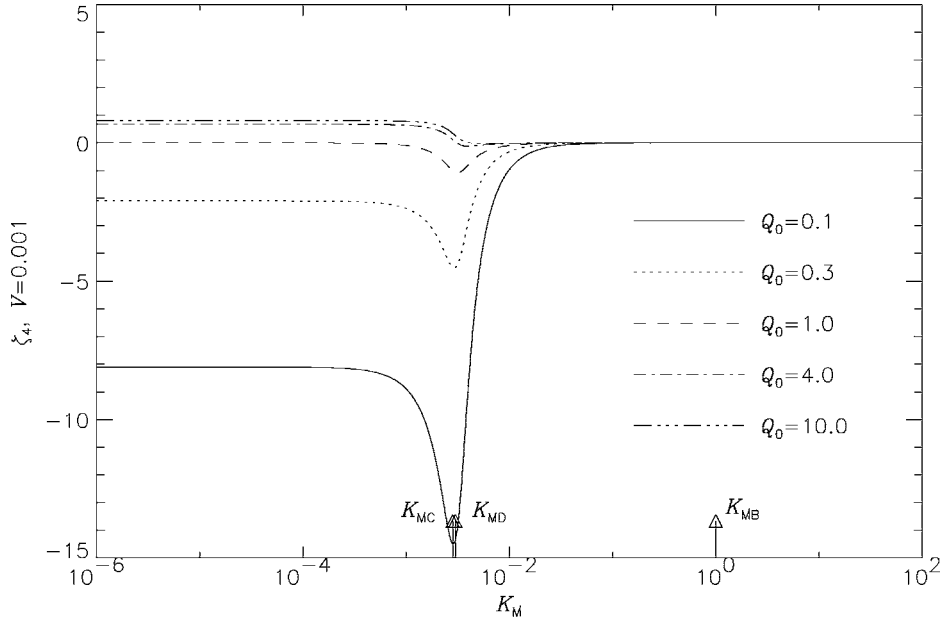

FIG. 11. The k-dependent amplitudes of the λ_3 baryonic modes in a HDM universe for a range of initial conditions $Q_0 = x_{40}/x_{20}$.

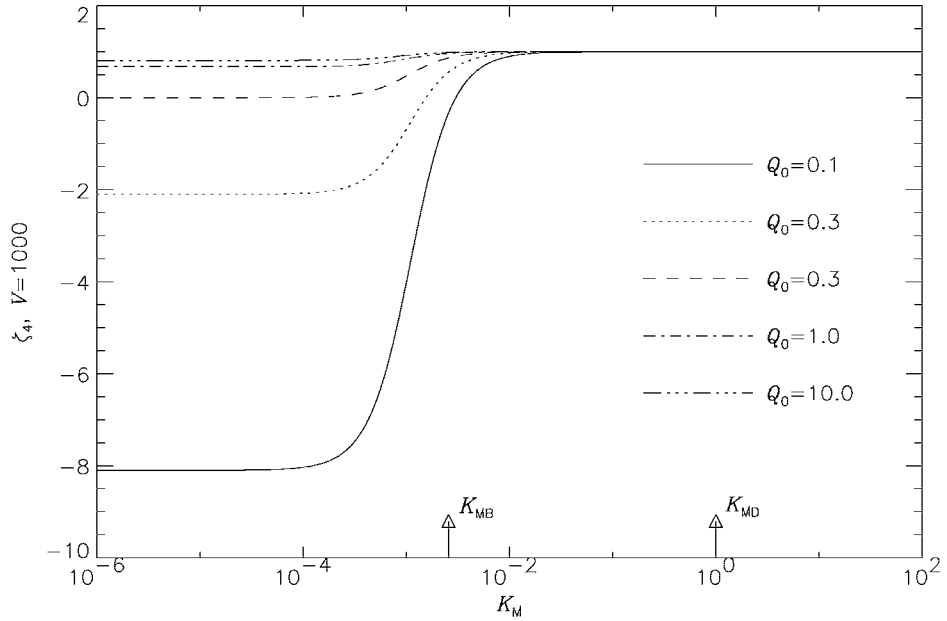

FIG. 12. The k-dependent amplitudes of the λ_3 baryonic modes in a CDM universe for a range of initial conditions $Q_0 = x_{40}/x_{20}$.

$$\mathbf{T} = \begin{bmatrix} 0 & -6K_D^2 + \dfrac{6\epsilon_D}{\chi^2} & 0 & \dfrac{6\epsilon_B}{\chi^2} \\ 1 & 0 & 0 & 0 \\ 0 & \dfrac{6\epsilon_D}{\chi^2} & 0 & -6K_B^2 + \dfrac{6\epsilon_B}{\chi^2} \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{4.3}$$

The idea behind the method is to attempt to remove the coupling between equations as much as possible, hopefully relegating it to some lower order, which can then be dealt with by a suitable approximation. To this end we define the matrices **A** and **f** such that

$$\mathbf{x} = \mathbf{A}\mathbf{f}. \tag{4.4}$$

A is chosen appropriately in order to diagonalize **T**. Then (4.2) may formally be written as

$$\mathbf{f}' = \mathbf{A}^{-1}\mathbf{T}\mathbf{A}\mathbf{f} - \mathbf{A}^{-1}\mathbf{A}'\mathbf{f}, \quad \det \mathbf{A} \neq 0. \tag{4.5}$$

To diagonalize **T**, we must first find its eigenvalues and eigenvectors. The structure of **T** is very similar to its static space–time counterpart, so the four eigenvalues also have the form given by (3.6). In the present case however, f and g are functions of χ and $\bar{k}$, defined as

$$f(\chi,\bar{k}) = \frac{6}{\chi^2} - 6(K_B^2 + K_D^2), \tag{4.6}$$

$$g(\chi,\bar{k}) = \frac{36}{\chi^2}(K_D^2\epsilon_B + K_B^2\epsilon_D) - 36K_B^2K_D^2. \tag{4.7}$$

Note that unlike the static space–time results, where f contained an expression of the form $W_B + W_D$, no analogous expression exists here due to the physical constraint of the Einstein-deSitter universe, $\epsilon_B + \epsilon_D = 1$. The eigenvectors $\boldsymbol{\xi}_i$ corresponding the eigenvalues λ_i are also identical in

structure to their static space–time counterparts (3.9). In this case the functions β_i are given by

$$\beta_1 = \beta_2 = \frac{1}{2}\frac{\chi^2}{6\epsilon_D}\left(h + \sqrt{h^2 + 4\frac{36\epsilon_B\epsilon_D}{\chi^4}}\right), \tag{4.8}$$

$$\beta_3 = \beta_4 = \frac{1}{2}\frac{\chi^2}{6\epsilon_D}\left(h - \sqrt{h^2 + 4\frac{36\epsilon_B\epsilon_D}{\chi^4}}\right), \tag{4.9}$$

with

$$h(\chi,\bar{k}) = \frac{6}{\chi^2}(\epsilon_D - \epsilon_B) + 6(K_B^2 - K_D^2). \tag{4.10}$$

It is worthwhile to point out here for the sake of calculations that

$$S \equiv \sqrt{h^2 + 4\frac{36\epsilon_B\epsilon_D}{\chi^4}} = \sqrt{f^2 + 4g}. \tag{4.11}$$

The eigenvectors may be used to form the diagonalizing matrix

$$\mathbf{A} = (\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \boldsymbol{\xi}_3, \boldsymbol{\xi}_4), \tag{4.12}$$

whose inverse exists. This enables the formal equation (4.5) to be written explicitly

$$\begin{bmatrix} f_1' \\ f_2' \\ f_3' \\ f_4' \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 \\ 0 & 0 & 0 & -\lambda_3 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} - \begin{bmatrix} \epsilon_1 & \epsilon_2 & \epsilon_3 & \epsilon_4 \\ \epsilon_2 & \epsilon_1 & \epsilon_4 & \epsilon_3 \\ \epsilon_5 & \epsilon_6 & \epsilon_7 & \epsilon_8 \\ \epsilon_6 & \epsilon_5 & \epsilon_8 & \epsilon_7 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}. \tag{4.13}$$

We have introduced eight new parameters here, all of which can be written in terms of λ_1, λ_3, β_1, and β_3. In what follows, let us use the shorthand

$$\beta_{13} \equiv \beta_1 - \beta_3 = \frac{\chi^2}{6\epsilon_D}S = \frac{1}{\epsilon_D}\sqrt{1 + 2\chi^2(\epsilon_D - \epsilon_B)(K_B^2 - K_D^2) + \chi^4(K_B^2 - K_D^2)^2}. \tag{4.14}$$

The parameters are defined by

$$\epsilon_1 = \frac{\beta_1'}{\beta_{13}} + \frac{\lambda_1'}{2\lambda_1}, \tag{4.15}$$

$$\epsilon_2 = -\frac{\lambda_1'}{2\lambda_1}, \tag{4.16}$$

$$\epsilon_3 = \frac{\beta_3'}{2\beta_{13}}\left(1 + \frac{\lambda_3}{\lambda_1}\right), \tag{4.17}$$

$$\epsilon_4 = \frac{\beta_3'}{2\beta_{13}}\left(1 - \frac{\lambda_3}{\lambda_1}\right), \tag{4.18}$$

$$\epsilon_5 = -\frac{\beta_1'}{2\beta_{13}}\left(1 + \frac{\lambda_1}{\lambda_3}\right), \tag{4.19}$$

$$\epsilon_6 = -\frac{\beta_1'}{2\beta_{13}}\left(1 - \frac{\lambda_1}{\lambda_3}\right), \tag{4.20}$$

$$\epsilon_7 = -\frac{\beta_3'}{\beta_{13}} + \frac{\lambda_3'}{2\lambda_3}, \tag{4.21}$$

$$\epsilon_8 = -\frac{\lambda_3'}{2\lambda_3}. \tag{4.22}$$

Let us consider the meaning of (4.13) more closely. Using the terminology of WKB theory, the first matrix on the right-hand side will give us the leading order "control factor"—the fastest varying part of the solution, typically an exponential factor. This factor may indicate rapid oscillations for imaginary λ_i, or rapid growth or decay for real λ_i. The second matrix contains a collection of parameters, which determine further slowly varying behavior. For this to be true, the condition $\epsilon_i \ll \lambda_j$, $\forall i, j$ must hold. It is then possible to show that the four equations all decouple to leading order, and WKB solutions may be written down. The proof of this is quite involved, but it is worthwhile to pursue. A bonus of the proof is that through a careful consideration of the approximations required, some instructive physics is learned along the way.

B. The WKB approximation criteria

In an attempt to decouple the equations, we need to consider more carefully the various criteria which constitute the condition $\epsilon_i \ll \lambda_j$, $\forall i, j$, which allow the WKB method to work. To begin with, we will assume the λ_i's are of about the same order. Although their magnitude varies greatly over various scales, an examination of Fig. 1 shows this assumption to hold fairly well in general. When we find, through the reasoning which follows, the precise scales of interest for a WKB approximation, we will see that this assumption is justified *post facto*. The essence of the WKB approximation is to assume

$$\left|\frac{\lambda_i'}{\lambda_i}\right| \ll |\lambda_i|, \tag{4.23}$$

that is, the eigenvalues vary slowly over the time scale which they define. In the current context, this corresponds physically to many oscillations in a universe expansion time for the acoustic region of k-space, or a far shorter collapse time than a universe expansion time for perturbations in the region where modes are Jeans unstable. In what follows, exactly which type of modes (acoustic or collapse) do fall into the category defined by (4.23) will become apparent.

From the results of static space–time, we suspect that a Jeans instability must exist, and in such a region, it should follow that one of the λ_i be zero, rendering (4.23) false. Consequently, we need to find the critical points of the λ_i, dependent on the wave number k. A consideration of the equation $\lambda_1^2(\chi)=0$ gives a solution for a "critical time" $\chi=\chi_c$,

$$\chi_c^2 \equiv \frac{\epsilon_B}{K_B^2} + \frac{\epsilon_D}{K_D^2}. \tag{4.24}$$

It turns out that λ_3 however has no such time.

Let us examine the behavior of $\lambda_1(\chi)$ around $\chi \sim \chi_c$ more closely. We set $\chi^2=\chi_c^2(1+\epsilon)$ for a small parameter ϵ, and expand λ_1 in powers of ϵ. It turns out that

$$f + \sqrt{f^2 + 4g} = -12\epsilon K_B^2 K_D^2 \frac{K_D^2\epsilon_B + K_B^2\epsilon_D}{K_D^4\epsilon_B + K_B^4\epsilon_D} + O(\epsilon^2), \tag{4.25}$$

so that $\lambda_1 \propto \sqrt{-\epsilon}$ for $\chi \sim \chi_c$. This dependence of λ_1 on ϵ gives a clear picture of how λ_1 changes around the critical point. For $\chi > \chi_c$, $\epsilon > 0$ and λ_1 is imaginary. This corresponds to acoustic

oscillations, in the stable part of k-space. For $\chi<\chi_c$, $\epsilon<0$ and λ_1 is real. This corresponds to an unstable part of k-space, so that χ_c is an indication of the transition through the Jeans instability. The time parameters may be defined so that initial time corresponds to $a_0=1$. This is because the explicit magnitude of a_0 is not determined by cosmology. By the definition $\chi=a^{-1/2}$, it is clear that χ begins at 1 and decreases with increasing time. This gives us two ways of looking at the Jeans instability. One way is to consider the instability at a particular instant in time. For a particular time χ, a subset of modes will be unstable for values of k for which $\chi_c(k)>\chi$ (we stress that χ_c is a function of k). We may then consider what occurs as these modes evolve through time from this particular instant. The critical time χ_c is fixed for any one mode, so that the modes which were originally acoustic will become unstable as $\chi\to\chi_c^+$. Consequently more and more modes pass through the instability as the Universe evolves. The physical wave number k is of course dependent on time, thus the dependence of the instability on a time χ_c shows the inextricable link between the wave number and time.

We wish to relate these concepts back to the result discussed for static space–time, and so must ask how the critical time χ_c is related to the critical wave number k_M of the mixture of components. In static space–time we defined

$$K_M^2=\frac{k^2}{W_B/v_B^2+W_D/v_D^2} \tag{4.26}$$

as the dimensionless parameter, indicating the relation of a mode to the instability at $K_M=1$. To place this quantity in an expanding universe context, the substitutions

$$W_B\to\frac{6\epsilon_B}{\chi^2},\quad v_B^2k^2\to 6K_B^2,$$

$$W_D\to\frac{6\epsilon_D}{\chi^2},\quad v_D^2k^2\to 6K_D^2$$

are required. This gives K_M the following form:

$$K_M^2=\frac{\chi^2}{\epsilon_B/K_B^2+\epsilon_D/K_D^2}=\frac{\chi^2}{\chi_c^2}. \tag{4.27}$$

It is explicitly seen here that the scale of instability changes with time, as was explained above. The analogy with the one-component case discussed in Ref. 11 may be made here, where solutions were found in terms of the one-component Jeans wave number $K_Ja^{-1/2}$. With $\chi=a^{-1/2}$, we see that the quantity χ_c^{-1} in the two-component case is the exact analogy of K_J for the one-component case.

Now that we have determined that λ_1 approaches zero in a particular region, it becomes clear that the WKB approximation will not be valid in this region $\chi\sim\chi_c$, from the condition (4.23). Let us examine λ_1'/λ_1^2 in more detail, to determine its behavior over the whole of k-space. An explicit evaluation using the definitions of f and g from (4.6) and (4.7) gives

$$\frac{\lambda_1'}{\lambda_1^2}=-\frac{3}{(\lambda_1\chi)^3}(1+F), \tag{4.28}$$

where

$$F=\frac{1+(\epsilon_D-\epsilon_B)(K_B^2-K_D^2)\chi^2}{\epsilon_D\beta_{13}}. \tag{4.29}$$

In the ensuing discussion we use the quantity $\bar{k}$ to describe the comoving wave-number dependence of the quantities involved. If we denote the numerator of (4.29) by N, it is simple to see that $N^2<\epsilon_D^2\beta_{13}^2$ for all $\bar{k}$ [see (4.14)], so that $|F|\leq 1$. We also consider the limits of F for large and

small $\bar{k}$. For $\bar{k}\to 0$, $F\to 1$ and for $\bar{k}\to\infty$, $F\to\epsilon_D-\epsilon_B$ if $K_B>K_D$, and $F\to\epsilon_B-\epsilon_D$ if $K_D>K_B$. This means that asymptotically F is independent of $\bar{k}$, and since $|F|\leq 1$ for all $\bar{k}$, λ_1'/λ_1^2 does not change sign. It now becomes clear that the magnitude of λ_1'/λ_1^2 is mainly dependent on the factor $(\lambda_1\chi)^{-3}$. We already know that as $\bar{k}\to\bar{k}_M$, $\lambda_1\to 0$ so that in this region it has been confirmed that $\lambda_1'/\lambda_1^2\gg 1$. Suitable regions where WKB might be valid must be sought far from the neighborhood $\bar{k}\sim\bar{k}_M$. The dependence of λ_1'/λ_1^2 on $\lambda_1\chi$ leads us to suggest the WKB criterion in the amended form $\lambda_1\chi\gg 1$. This makes good physical sense, because if λ_1 is considered a frequency/inverse of a dynamical collapse time, the WKB criteria requires that a large number of oscillations/significant change in δ_i occurs during an expansion time.

A similar analysis needs to be performed for λ_3. We find

$$\frac{\lambda_3'}{\lambda_3^2}=-\frac{3}{(\lambda_3\chi)^3}(1-F). \tag{4.30}$$

This too demands the criterion $\lambda_3\chi\gg 1$. To find how λ_3 behaves, consider first the $\bar{k}\to 0$ limit. This limit gives $\lambda_3\to 0$, so this region of k-space is clearly inappropriate for WKB analysis. We note, however, that since $\lambda_3\neq 0$ at $\bar{k}=\bar{k}_M$, this region should be checked more closely. After a careful examination of λ_3,

$$\lambda_3\chi=\sqrt{3}\sqrt{1-(K_B^2+K_D^2)\chi^2-\epsilon_D\beta_{13}}, \tag{4.31}$$

it becomes apparent that $\lambda_3\chi\gg 1$ only when both $K_B\gg 1$ and $K_D\gg 1$. This corresponds to the region $\bar{k}\gg\bar{k}_M$, and so the region $\bar{k}\sim\bar{k}_M$ must be excluded from consideration as well. For λ_3, we are only left with the region $\bar{k}\gg\bar{k}_M$ as fulfilling the WKB criterion. For completeness, the same reasoning should also be applied to λ_1. The $\bar{k}\to 0$ limit applied to λ_1 gives

$$\frac{3}{(\lambda_1\chi)^3}\to\frac{1}{2\sqrt{6}}, \tag{4.32}$$

which is not much less than 1, as is required to define it as a region amenable to WKB analysis. Thus the $\bar{k}\ll\bar{k}_M$ region is inappropriate for λ_1 as well.

In conclusion, $\bar{k}\gg\bar{k}_M$ is the *only* region for which the WKB approximation holds. We may summarize the methods available to analyze the two-component problem in various regions of k-space by the following classification.

$\bar{k}\gg\bar{k}_M$: The WKB method will give acoustic oscillations for all modes, with the rapidly varying part of the solution taking the form $\exp(\pm i|\lambda_i|\chi)$.

$\bar{k}\ll\bar{k}_M$: A Frobenius expansion (small parameter expansion) of the solutions needs to be developed. Some growing and decaying modes following a power law behavior may be expected for solutions corresponding to λ_1, while some low frequency acoustic oscillations may be expected for solutions corresponding to λ_3.

$\bar{k}\sim\bar{k}_M$: This region of parameter space is not accessible to analytic solution. Some numerics will be required to investigate this interesting region.

We will continue with the WKB analysis in this paper, and show how the equations (4.13) decouple. An investigation of the other regions of k-space are taken up in Ref. 11.

We still need to check how β_1 and β_3 vary, to ensure that all the ϵ_i are small. In particular, we need to consider whether relations of the form

$$\frac{\beta_i'}{\beta_{13}}\ll\lambda_j,\quad i,j=1,3 \tag{4.33}$$

are true. The analysis proceeds very similarly to that described above for the derivatives of λ_1 and λ_3, and a full description will not be given here. As a brief example, it can be shown that

$$\frac{\beta_1'}{\beta_{13}\lambda_1} \sim \frac{1}{\lambda_1 \chi} \tag{4.34}$$

for $\bar{k} \gg \bar{k}_M$, once again fulfilling the criterion $\lambda_1 \chi \gg 1$. Other cases follow similarly. Given that the relations (4.33) do hold, we can finally make the important statement that $\epsilon_i \ll \lambda_j$, $\forall i, j$ if $\bar{k} \gg \bar{k}_M$.

C. The solutions

Now that we have worked out the region of k-space in which the WKB method produces valid leading order solutions, we proceed to derive these solutions by decoupling the equations. To illustrate how the equations (4.13) decouple, we begin with an example. Taking the top row of the matrix equation, the following suggestive equation for f_1 may be written

$$f_1' - (\lambda_1 - \epsilon_1) f_1 = -\epsilon_2 f_2 - \epsilon_3 f_3 - \epsilon_4 f_4. \tag{4.35}$$

This may be treated as a first order inhomogeneous ordinary differential equation (ODE) for f_1. The homogeneous portion has a simple solution

$$f_1 \sim c_1 \exp\left[\int_{\chi_0}^{\chi} (\lambda_1 - \epsilon_1) \mathrm{d}\chi \right], \tag{4.36}$$

with a constant of integration c_1. This may be considered to be a first approximation to the solution, though it remains to be shown that it is the full leading order result. To evaluate the inhomogeneous portion of the solution of (4.35), we require the first approximations for the other f_i as well. A corresponding analysis to that illustrated for f_1 yields

$$f_2 \sim c_2 \exp\left[-\int_{\chi_0}^{\chi} (\lambda_1 + \epsilon_1) \mathrm{d}\chi \right], \tag{4.37}$$

$$f_3 \sim c_3 \exp\left[\int_{\chi_0}^{\chi} (\lambda_3 - \epsilon_7) \mathrm{d}\chi \right], \tag{4.38}$$

$$f_4 \sim c_4 \exp\left[-\int_{\chi_0}^{\chi} (\lambda_3 + \epsilon_7) \mathrm{d}\chi \right]. \tag{4.39}$$

When these are substituted into (4.35), we achieve the rather complicated result

$$\begin{aligned} f_1 \sim \exp\left[\int_{\chi_0}^{\chi} (\lambda_1 - \epsilon_1) \mathrm{d}\chi \right] \Bigg\{ & c_{11} + c_{12} \int_{\chi_0}^{\chi} \mathrm{d}\chi \epsilon_2 \exp\left[-2 \int_{\chi_0}^{\chi} \lambda_1 \mathrm{d}\chi \right] \\ & + c_{13} \int_{\chi_0}^{\chi} \mathrm{d}\chi\, \epsilon_3 \exp\left[\int_{\chi_0}^{\chi} (-\lambda_1 + \lambda_3 + \epsilon_1 - \epsilon_7) \mathrm{d}\chi \right] \\ & + c_{14} \int_{\chi_0}^{\chi} \mathrm{d}\chi\, \epsilon_4 \exp\left[\int_{\chi_0}^{\chi} (-\lambda_1 - \lambda_3 + \epsilon_1 - \epsilon_7) \mathrm{d}\chi \right] \Bigg\}. \end{aligned} \tag{4.40}$$

There are a number of integrals present here which need to be estimated to determine how the approximation is to proceed.

As an example of a generic type of integral to evaluate, consider

$$I = \int_{\chi_0}^{\chi} \mathrm{d}\chi\, \epsilon_2 \exp\left[-2\int_{\chi_0}^{\chi} \lambda_1\, \mathrm{d}\chi \right]. \tag{4.41}$$

Since the region of interest is $\bar{k} \gg \bar{k}_M$, λ_1 is imaginary, and consequently the definition of the real function $\psi(\chi) \equiv -i\lambda(\chi)$ is useful. We integrate I by parts to obtain

$$I = \left. \frac{\lambda_1'}{4\lambda_1^2} \exp\left[-2i\int_{\chi_0}^{\chi} \psi(\chi)\mathrm{d}\chi \right] \right|_{\chi_0}^{\chi} - \frac{1}{4}\int_{\chi_0}^{\chi} \mathrm{d}\chi \left(\frac{d}{\mathrm{d}\chi}\frac{\lambda_1'}{\lambda_1^2} \right) \exp\left[-2i\int_{\chi_0}^{\chi} \psi(\chi)\mathrm{d}\chi \right]. \tag{4.42}$$

It is our aim to show that all corrections to the leading order results (4.36)–(4.39) are of $O(\epsilon)$, where ϵ generically denotes any of the small quantities ϵ_i, $i=1,2,\ldots,8$. It is already obvious that the first term in (4.42) is of $O(\epsilon)$, because it consists of a λ_1'/λ_1^2 term multiplied by a phase factor. We may constrain the second term by

$$\left| \int_{\chi_0}^{\chi} \mathrm{d}\chi \left(\frac{d}{\mathrm{d}\chi}\frac{\lambda_1'}{\lambda_1^2} \right) \exp\left[-2i\int_{\chi_0}^{\chi} \psi(\chi)\mathrm{d}\chi \right] \right| \leq \int_{\chi_0}^{\chi} \mathrm{d}\chi \left| \left(\frac{d}{d\chi}\frac{\lambda_1'}{\lambda_1^2} \right) \right| \left| \left. \frac{\lambda_1'}{\lambda_1^2} \right|_{\chi_0}^{\chi} \right|. \tag{4.43}$$

This shows that indeed $I \sim O(\epsilon)$.

The same type of analysis may be performed for the other more complicated integrals. In general, integration by parts is involved, and the terms may be shown to be bounded by some expressions of the form λ_i'/λ_j^2, or $\beta_i'/(\beta_{13}\lambda_j)$. It is found that in the WKB approximation, (4.36) is the correct leading order term, and the integrals arising from considering the inhomogeneous portion of the ODE (4.35) are all of $O(\epsilon)$ below this leading order term. Similar correction integrals to those found in (4.40) may be written down for f_2, f_3, and f_4, all of which take the same generic form as those evaluated in the f_1 case. A lengthy analysis will show that all the corrections are of $O(\epsilon)$, so we have shown that to leading order we may effectively neglect the off-diagonal ϵ_i in (4.13). In conclusion, the full leading order WKB solution to $\mathbf{f}$ is given by (4.36)–(4.39).

These solutions contain two important terms in the integrals. The λ_1 and λ_3 terms represent the rapidly varying oscillatory portion of the solutions, i.e., the control factor mentioned earlier. To obtain the true frequencies, these integrals need to be converted to integrals over t. We expect the ϵ_1 and ϵ_7 terms to represent some slowly varying time-dependent amplitude. To reveal the time-dependent structure of the solutions more explicitly, the integrals of ϵ_1 and ϵ_7 need to be evaluated. This is facilitated greatly by the relation

$$\beta_1\beta_3 = -\frac{\epsilon_B}{\epsilon_D}. \tag{4.44}$$

For ϵ_1 consider the integral

$$\int_{\chi_0}^{\chi} \frac{\beta_1'}{\beta_1 - \beta_3}\mathrm{d}\chi = \int_{\chi_0}^{\chi} \frac{\beta_1\beta_1'}{\beta_1^2 + \epsilon_B/\epsilon_D}\mathrm{d}\chi = \left. \frac{1}{2}\log\left(\beta_1^2 + \frac{\epsilon_B}{\epsilon_D} \right) \right|_{\chi_0}^{\chi}. \tag{4.45}$$

Using (4.44) once more we find

$$\int_{\chi_0}^{\chi} \frac{\beta_1'}{\beta_1 - \beta_3} d\chi = \frac{1}{2}\log\left[\frac{\beta_1(\chi)}{\beta_1(\chi) - \beta_3(\chi)} \right] - \frac{1}{2}\log\left[\frac{\beta_1(\chi_0)}{\beta_1(\chi_0) - \beta_3(\chi_0)} \right]. \tag{4.46}$$

For notational expedience, we define the tilde quantities

$$\tilde{\beta}_i(\chi) = \frac{\beta_i(\chi)}{\beta_i(\chi_0)}, \quad i = 1,3, \tag{4.47}$$

$$\tilde{\beta}_{13}(\chi) = \frac{\beta_1(\chi) - \beta_3(\chi)}{\beta_1(\chi_0) - \beta_3(\chi_0)}, \tag{4.48}$$

$$\tilde{\lambda}_i(\chi) = \frac{\lambda_i(\chi)}{\lambda_i(\chi_0)}, \quad i = 1,3, \tag{4.49}$$

with the obvious property that $\tilde{f}(\chi_0)=1$, for any quantity $f(\chi)$. This allows us to write the integrals as follows:

$$-\int_{\chi_0}^{\chi} \epsilon_1 \, \mathrm{d}\chi = \frac{1}{2} \log\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1 \tilde{\lambda}_1} \right), \tag{4.50}$$

$$-\int_{\chi_0}^{\chi} \epsilon_7 \, \mathrm{d}\chi = \frac{1}{2} \log\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3 \tilde{\lambda}_3} \right). \tag{4.51}$$

Here the integral involving ϵ_7 was calculated using identical techniques as just illustrated for ϵ_1.

At last the final form of leading order solution for **f** may be written down, with the explicit time-dependent amplitude and rapidly varying oscillatory part,

$$f_{1,2} \sim c_{1,2} \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1 \tilde{\lambda}_1} \right)^{1/2} \exp\left(\pm \int_{\chi_0}^{\chi} \lambda_1 \, \mathrm{d}\chi \right), \tag{4.52}$$

$$f_{3,4} \sim c_{3,4} \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3 \tilde{\lambda}_3} \right)^{1/2} \exp\left(\pm \int_{\chi_0}^{\chi} \lambda_3 \, \mathrm{d}\chi \right). \tag{4.53}$$

We are now in a position to recover the original physical state vector **x** by multiplying these auxiliary functions by the matrix **A**, as given in the original definition (4.4). The matrix **A** contains λ's and β's, which are *not* tilde quantities. The full general solution to (2.6) and (2.7) is finally given by

$$\begin{bmatrix} \delta_D' \\ \delta_D \\ \delta_B' \\ \delta_B \end{bmatrix} \sim c_1 \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1 \tilde{\lambda}_1} \right)^{1/2} \boldsymbol{\xi}_1 \exp\left(i \int_{\chi_0}^{\chi} |\lambda_1| \mathrm{d}\chi \right) + c_2 \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1 \tilde{\lambda}_1} \right)^{1/2} \boldsymbol{\xi}_2 \exp\left(-i \int_{\chi_0}^{\chi} |\lambda_1| \mathrm{d}\chi \right)$$
$$+ c_3 \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3 \tilde{\lambda}_3} \right)^{1/2} \boldsymbol{\xi}_3 \exp\left(i \int_{\chi_0}^{\chi} |\lambda_3| \mathrm{d}\chi \right) + c_4 \left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3 \tilde{\lambda}_3} \right)^{1/2} \boldsymbol{\xi}_4 \exp\left(-i \int_{\chi_0}^{\chi} |\lambda_3| \mathrm{d}\chi \right). \tag{4.54}$$

Here the $\boldsymbol{\xi}_i$ are the eigenvectors defined by (3.9). In summary, this leading order solution represents acoustic oscillations in the short wavelength limit, defined as

$$k^2 \gg k_M^2 = \frac{4\pi G \rho_B}{v_B^2} + \frac{4\pi G \rho_D}{v_D^2}, \tag{4.55}$$

which is a time-dependent quantity. Equivalently, we may view the limit as given by

$$\frac{\epsilon_B}{K_B^2} + \frac{\epsilon_D}{K_D^2} \gg \chi^2. \tag{4.56}$$

A Jeans instability will not be evident for the solutions in this region of k-space, but the time dependence will mean that the period of oscillation becomes longer until a point is reached at which the WKB approximation is no longer accurate, and the solutions as displayed are not realistic representations of the underlying physics. Then different approximations need to be considered. The methods involved are discussed in detail in Ref. 11.

D. Relative amplitudes of the solutions

The slowly varying time-dependent amplitudes of the solutions (4.54) show how either dark matter or baryons dominate various modes, depending on whether HDM or CDM is being considered. This feature was noticed in the static case, and we now demonstrate it more fully through asymptotic analysis in the expanding universe scenario. The information is contained in the eigenvectors $\boldsymbol{\xi}_i$, which give the relative amplitudes. It can be seen directly from (3.9) that

$$\frac{\delta_B}{\delta_D} \propto \frac{1}{\beta_1} = -\frac{\epsilon_D}{\epsilon_B}\beta_3 \tag{4.57}$$

for the λ_1 modes, and

$$\frac{\delta_B}{\delta_D} \propto \frac{1}{\beta_3} = -\frac{\epsilon_D}{\epsilon_B}\beta_1 \tag{4.58}$$

for the λ_3 modes. At first glance this may appear a little surprising, as there seems to be an asymmetry in the solutions. If the indices are interchanged $D \leftrightarrow B$, the amplitudes do not appear to be the same, yet all such an interchange is doing is swapping the order the equations are written down in.

As an illustration for the λ_1 modes

$$\begin{bmatrix} \delta_D \\ \delta_B \end{bmatrix} \propto \begin{bmatrix} \beta_1 \\ 1 \end{bmatrix}, \quad \text{with } \beta_1 = \frac{\chi^2}{12\epsilon_D}(h+S), \tag{4.59}$$

whereas after the interchange $D \leftrightarrow B$,

$$\begin{bmatrix} \delta_B \\ \delta_D \end{bmatrix} \propto \begin{bmatrix} \beta_1^* \\ 1 \end{bmatrix}, \quad \text{with } \beta_1^* = \frac{\chi^2}{12\epsilon_B}(-h+S). \tag{4.60}$$

The quantity β_1^* is defined as being the form of β_1 after the interchange has been made. The square root term S, defined in (4.11) is invariant under the interchange, whereas an examination of (4.10) shows that under the interchange $h \to -h$. It is however simple to show that $\beta_1\beta_1^* = 1$, which is to be expected from the symmetry of the differential equations. The same result holds for the λ_3 mode, where it can be shown that $\beta_3\beta_3^* = 1$ for the quantities

$$\beta_3 = \frac{\chi^2}{12\epsilon_D}(h-S), \quad \beta_3^* = \frac{\chi^2}{12\epsilon_B}(-h-S)\,. \tag{4.61}$$

We now examine the behavior of the amplitudes more carefully, to find the dominant components of matter. A useful large expansion parameter in the analysis will be the quantity $y \equiv |K_B^2 - K_D^2|\chi^2$. Let us also introduce the notation $\sigma = \text{sign}(K_B^2 - K_D^2) = \pm 1$, and expand the eigenvalues in y. For the λ_1 modes we may write

$$\beta_1 = \frac{y}{2\epsilon_D}\left[\sigma + \frac{\epsilon_D - \epsilon_B}{y} + \sqrt{1 + 2\sigma(\epsilon_D - \epsilon_B)y^{-1} + y^{-2}}\right], \tag{4.62}$$

from which the following results may be deduced:

$$\beta_1 = \begin{cases} \dfrac{y}{\epsilon_D}\left[1 + \dfrac{\epsilon_D - \epsilon_B}{y} + O(y^{-2})\right], & K_B > K_D, \quad (\sigma = 1), \\ \dfrac{1 - (\epsilon_D - \epsilon_B)^2}{4\epsilon_D y}\left[1 + \dfrac{\epsilon_D - \epsilon_B}{y} + O(y^{-2})\right], & K_D > K_B, \quad (\sigma = -1). \end{cases} \tag{4.63}$$

This indicates that for CDM ($K_B > K_D$)

$$\beta_1 \propto (K_B^2 - K_D^2)\chi^2,$$

and the dark matter oscillations are dominant in the λ_1 modes, although as time increases they become less so. On the other hand, for HDM ($K_D > K_B$)

$$\beta_1 \propto \frac{1}{(K_D^2 - K_B^2)\chi^2},$$

and the baryon oscillations dominate, and their dominance increases with time. The λ_3 modes display complementary behavior,

$$\beta_3 = \begin{cases} \dfrac{-1 + (\epsilon_D - \epsilon_B)^2}{4\epsilon_D y}\left[1 + \dfrac{\epsilon_B - \epsilon_D}{y} + O(y^{-2})\right], & K_B > K_D, \quad (\sigma = 1), \\ -\dfrac{y}{\epsilon_D}\left[1 - \dfrac{\epsilon_B - \epsilon_D}{y} + O(y^{-2})\right], & K_D > K_B, \quad (\sigma = -1). \end{cases} \tag{4.64}$$

In this case for CDM,

$$\beta_3 \propto -\frac{1}{(K_B^2 - K_D^2)\chi^2},$$

so that the baryon oscillations dominate, and the dominance increases with time, while for HDM,

$$\beta_3 \propto -(K_D^2 - K_B^2)\chi^2,$$

which shows that dark matter oscillations dominate, but the dominance decreases with time. In summary, in a CDM scenario ($K_D > K_B$) baryons dominate the λ_3 mode and dark matter dominates the λ_1 mode, whereas the situation is opposite for HDM.

The apparent asymmetry of these results with respect to interchange of subscripts $B \leftrightarrow D$ can be easily explained by taking into account the relations (4.59)–(4.61). It was shown that after an interchange $B \leftrightarrow D$, the β's are given by

$$\beta_1^* = -\beta_3 \quad \text{and} \quad \beta_3^* = -\beta_1. \tag{4.65}$$

This is the correct way to view the asymptotic forms for the β's after an interchange, rather than by a direct swapping of subscripts. By deriving the asymptotic results, information has been lost and direct swapping is no longer valid. As an example, for $K_B > K_D$,

$$\beta_1 \sim (K_B^2 - K_D^2)\chi^2 \rightarrow \beta_1^* = -\beta_3 \sim \frac{1}{(K_B^2 - K_D^2)\chi^2}, \tag{4.66}$$

and the expected result $\beta_1\beta_1^* = 1$ holds.

Now that we have gained some insight into the behavior of the modes in a generic sense, let us be a little more specific and investigate the full leading order solutions under some tighter physical constraints to see some more physical effects emerge.

E. Initial conditions and resonances

We attempt to reproduce the resonances described in the static space–time case by imposing some initial conditions on our solutions, and eliminating the arbitrary constants of integration c_i, $i=1,\ldots,4$, using a similar procedure to that employed previously. In the static space–time scenario we just stated the results, but here we explicitly go through the derivation. The general solution may be expediently written in the form

$$x_i(\chi)=\sum_{j=1}^{4} c_j v_{(j)i}(\chi)\exp\left(\int_{\chi_0}^{\chi}\lambda_j\,\mathrm{d}\chi\right). \tag{4.67}$$

The amplitudes are given by the vectors

$$\mathbf{v}_{(1),(2)}=\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1\tilde{\lambda}_1}\right)^{1/2}\boldsymbol{\xi}_{1,2},\quad \mathbf{v}_{(3),(4)}=\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3\tilde{\lambda}_3}\right)^{1/2}\boldsymbol{\xi}_{3,4}. \tag{4.68}$$

At $\chi=\chi_0$, $v_{(j)}(\chi_0)=\boldsymbol{\xi}_j(\chi_0)$, and an equation for the initial conditions x_{i0} is obtained,

$$x_{i0}=\sum_{j=1}^{4} c_j\xi_{(j)i}(\chi_0). \tag{4.69}$$

Note that henceforth any variable subscripted with a 0 (possibly together with other subscripts) denotes that quantity evaluated at $\chi=\chi_0$. As a reasonable simplifying assumption, we once again take $x_{10}=x_{30}=0$, i.e., the perturbations start from rest. This gives a simple algebraic system for the c_i, with the solution

$$\begin{bmatrix} c_1\\ c_2\\ c_3\\ c_4\end{bmatrix}=\frac{x_{20}}{2\beta_{130}}\begin{bmatrix} 1-Q_0\beta_{30}\\ 1-Q_0\beta_{30}\\ Q_0\beta_{10}-1\\ Q_0\beta_{10}-1\end{bmatrix}, \tag{4.70}$$

where the ratio of initial conditions $Q_0=x_{40}/x_{20}$ is used once more.

When the above expressions for the c_i are substituted back into the general solution (4.54), a simplified result follows:

$$\begin{bmatrix}\delta_D'\\ \delta_D\\ \delta_B'\\ \delta_B\end{bmatrix}\sim\frac{x_{20}}{\beta_{130}}(1-Q_0\beta_{30})\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1\tilde{\lambda}_1}\right)^{1/2}\begin{bmatrix} i\beta_1\lambda_1\sin\\ \beta_1\cos\\ i\lambda_1\sin\\ \cos\end{bmatrix}\left(\int_{\chi_0}^{\chi}|\lambda_1|\mathrm{d}\chi\right)+\frac{x_{20}}{\beta_{130}}(Q_0\beta_{10}-1)$$
$$\times\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3\tilde{\lambda}_3}\right)^{1/2}\begin{bmatrix} i\beta_3\lambda_3\sin\\ \beta_3\cos\\ i\lambda_3\sin\\ \cos\end{bmatrix}\left(\int_{\chi_0}^{\chi}|\lambda_3|\mathrm{d}\chi\right). \tag{4.71}$$

Let us concentrate in particular on the x_2 and x_4 components, which describe the actual matter content of the Universe, and may have some interesting implications for structure formation results. We may write the solutions in a form analogous to the static space–time results,

$$\delta_D(\chi) = x_{20}\left[\zeta_1 \cos\left(\int_{\chi_0}^{\chi} |\lambda_1| d\chi\right) + \zeta_2 \cos\left(\int_{\chi_0}^{\chi} |\lambda_3| d\chi\right)\right], \tag{4.72}$$

$$\delta_B(\chi) = x_{40}\left[\zeta_3 \cos\left(\int_{\chi_0}^{\chi} |\lambda_1| d\chi\right) + \zeta_4 \cos\left(\int_{\chi_0}^{\chi} |\lambda_3| d\chi\right)\right]. \tag{4.73}$$

The amplitudes are given by the expressions

$$\zeta_1 = \beta_1 \frac{1 - Q_0\beta_{30}}{\beta_{130}}\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1\tilde{\lambda}_1}\right)^{1/2}, \tag{4.74}$$

$$\zeta_2 = \beta_3 \frac{Q_0\beta_{10} - 1}{\beta_{130}}\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3\tilde{\lambda}_3}\right)^{1/2}, \tag{4.75}$$

$$\zeta_3 = \frac{Q_0^{-1} - \beta_{30}}{\beta_{130}}\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_1\tilde{\lambda}_1}\right)^{1/2}, \tag{4.76}$$

$$\zeta_4 = \frac{\beta_{10} - Q_0^{-1}}{\beta_{130}}\left(\frac{\tilde{\beta}_{13}}{\tilde{\beta}_3\tilde{\lambda}_3}\right)^{1/2}. \tag{4.77}$$

The immediate obvious differences for these amplitudes with the static space–time results are the following.

(1) Missing factors of $\frac{1}{2}$ for ζ_1 and ζ_3, because the solutions are now all of a cosine form, rather than real exponentials (which is due to the fact that we are considering the $\bar{k} \gg \bar{k}_M$ region).
(2) The amplitudes are all time varying.
(3) The amplitudes contain extra tilde factors which equal one at the initial time, but in general contain other time-dependent terms not present even as constant factors in the static space–time amplitudes.

For $\chi = \chi_0$ the amplitudes correspond exactly to those of the static space–time amplitudes, and Figs. 5–12 are accurate representations of the amplitudes over a wide range of k. As time increases, the amplitudes tend to grow, but retain the same qualitative shape with the most marked features still occurring around the scale $K_M = K_{MC}$. Since the WKB solutions are only valid for $k \gg k_M$, this interesting region of k-space does not apply, and the ζ_i as presently defined should not be extrapolated to have any meaning around $K_M = K_{MC}$. In the $K_M \gg 1$ region the ζ_i show no significant behavior, just tending to constant values close to zero or one. In particular no resonances are apparent. Thus the potentially interesting resonant features discovered by de Carvalho and Macedo[7] do not apply in the physically more realistic expanding universe scenario. Any significant effects would have to be sought from the small k solutions presented in Ref. 11.

In addition to these statements, it must be added that the λ_i eigenvalues characterizing the modes in the large k region do not have any physical significance in the small k region either. This was already apparent in the small k expansions for the one-component solutions discussed in Ref. 11. The characteristic Jeans dispersion relation

$$\omega = \sqrt{v_s^2 k^2 - 4\pi G\rho_0} \tag{4.78}$$

is not apparent in the small K_J expansions presented in Ref. 11, and likewise, the λ_i found in the present paper are not apparent in the general solutions given by Eqs. (5.3)–(5.10) of Ref. 11. With

these facts in mind, the discussion of the physical information we are able to extract from the WKB solutions at present is complete.

V. CONCLUSIONS AND FURTHER WORK

The structure and behavior of the eigenvalues and eigenvectors of two-component cosmological density perturbations have been studied in great detail in this paper. We have reviewed the previous work done in a static space–time background, and produced further results in this simple context. This has enabled the far more difficult expanding universe problem to be tackled.

The WKB method employed has produced the full leading order behavior of all the modes in the Einstein-deSitter expanding universe scenario. These solutions represent acoustic oscillations for wavelengths much smaller than the Jeans scale. The Jeans scale of the mixture has arisen in a natural way out of the analysis of the eigenvalues obtained through the WKB method, with some interesting interpretation. It is now a straightforward task to adapt the methods developed here to study a variety of further cosmological plasma modes. The ion-sound and two-component Langmuir oscillations would follow directly from the results presented here, and more complicated modes involving magnetic fields could also be obtained by similar procedures.

We have also obtained the time- and k-dependent amplitudes of the modes in a fairly general setting (the one restriction being initial perturbations beginning from rest). These results have shown that the amplitudes are very constant in the region of interest. The existence of resonances in the amplitudes found for static space–time results do not apply here, as all resonances occurred for wave numbers far smaller than k_M. Thus a resonant amplitude cannot be viewed as a mechanism for producing structures of a preferred scale in a two-component model. The eigenvalues derived in this paper also do not have any direct physical interpretation around the Jeans scale, or for small k expansions of the solutions of Eqs. (2.6) and (2.7). Thus the results obtained in this paper must be considered to be restricted to the parameter regions considered here.

It may be interesting to investigate different models such as a three-component HDM +CDM+baryon fluid, or models involving a cosmological constant (especially given the weight of current observations[15–17]). The analytics would become considerably more complicated, but some other interesting resonant scales may be found with a direct implication for structure formation.

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Eigenvalues of zero energy in the linearized NLS problem

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We study a pair of neutrally stable eigenvalues of zero energy in the linearized NLS equation. We prove that the pair of isolated eigenvalues, where each eigenvalue has geometric multiplicity one and algebraic multiplicity N, is associated with $2P$ negative eigenvalues of the energy operator, where $P=N/2$ if N is even and $P=(N-1)/2$ or $P=(N+1)/2$ if N is odd. When the potential of the linearized NLS problem is perturbed due to parameter continuations, we compute the exact number of unstable eigenvalues that bifurcate from the neutrally stable eigenvalues of zero energy. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2203233]

I. INTRODUCTION

Spectral stability of solitary waves is defined by the number of unstable eigenvalues in a linearized problem associated with the underlying nonlinear equation. Unstable eigenvalues for solitary waves of the nonlinear Schrödinger (NLS) equation have been recently studied within the inertia law,[1] the constrained variational problems and wave operators,[2] and the Grillakis projection method.[3]

The count of unstable eigenvalues is simplified in Refs. 1 and 2, with the technical assumption that the unstable and potentially unstable eigenvalues are structurally stable to parameter continuations. In particular, the count of eigenvalues is modified if the linearized problem admits an isolated eigenvalue of zero Krein signature (see Ref. 3 for definitions), which we refer to here as *an eigenvalue of zero energy*. The simplest instability bifurcation, called *the Hamiltonian-Hopf bifurcation*, occurs when the eigenvalue of zero Krein signature arises due to coalescence of two simple eigenvalues with positive and negative Krein signatures.[4,5]

In our present paper, we focus on a general Hamiltonian-Hopf bifurcation within the framework of a scalar NLS equation. We study properties of this general bifurcation and the number of unstable eigenvalues that are generated due to parameter continuations. Specifically, we use the notations from Ref. 2 and consider the linearized operator $\sigma_3\mathcal{H}$, where $\mathcal{H}$ is the energy operator,

$$\mathcal{H}=\begin{pmatrix} -\Delta+\omega+f(x) & g(x) \\ g(x) & -\Delta+\omega+f(x) \end{pmatrix}, \tag{1.1}$$

the standard Pauli matrices are used,

$$\sigma_1=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.2}$$

$x\in\mathbb{R}^n$, $n\geq 1$, $\omega>0$, and $f,g:\mathbb{R}^n\to\mathbb{R}$ are exponentially decaying C^∞ functions. The spectral problem for the operator $\sigma_3\mathcal{H}$ is considered on $L^2(\mathbb{R}^n,\mathbb{C}^2)$:

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$$\sigma_3 \mathcal{H} \boldsymbol{\psi} = z \boldsymbol{\psi}, \tag{1.3}$$

where $\boldsymbol{\psi}=(\psi_1,\psi_2)^T$. Eigenvalues z of the spectral problem (1.3) are called *unstable* if $\mathrm{Im}(z)>0$, *neutrally stable* if $\mathrm{Im}(z)=0$ and *stable* if $\mathrm{Im}(z)<0$ (see Ref. 2). The following notations are used for inner products: $\langle \mathbf{c},\mathbf{d}\rangle_{\mathbb{C}^N}$ for $\mathbf{c},\mathbf{d}\in\mathbb{C}^N$, $\langle \mathbf{f},\mathbf{g}\rangle$ for $\mathbf{f},\mathbf{g}\in L^2(\mathbb{R}^n,\mathbb{C}^2)$ and (f,g) for $f,g\in L^2(\mathbb{R}^n)$.

It is shown in the previous paper[2] that the spectrum of the linearized operator $\sigma_3\mathcal{H}$ is defined in part by the sign of the energy quadratic form in $H^1(\mathbb{R}^3,\mathbb{C}^2)$:

$$h = \langle \boldsymbol{\psi}, \mathcal{H}\boldsymbol{\psi}\rangle. \tag{1.4}$$

In particular, the number of unstable eigenvalues in the point spectrum of $\sigma_3\mathcal{H}$ in the upper half-plane is bounded by the number of negative eigenvalues of $\mathcal{H}$, while the energy quadratic form (1.4) is positive definite on the nonsingular part of the essential spectrum of $\sigma_3\mathcal{H}$. The singular part of the essential spectrum of $\sigma_3\mathcal{H}$ (which only includes the embedded eigenvalues but not the embedded resonances) is studied with the Fermi Golden rule, from which it follows that the embedded eigenvalue z of positive energy $h>0$ disappears under generic perturbation, while that of negative energy $h<0$ bifurcates into isolated complex eigenvalues of the point spectrum of $\sigma_3\mathcal{H}$.[2,5]

One of the technical assumptions in Ref. 2 postulates that the real eigenvalues z of the point spectrum of $\sigma_3\mathcal{H}$ have nonzero energy $h\neq 0$. In the present work we remove this assumption and study the case when there exists a pair of isolated eigenvalues $z=\pm z_0$, where $0<z_0<\omega$, which corresponds to the zero energy $h=0$. We show that a pair of isolated eigenvalues of zero energy has a higher algebraic multiplicity in the spectrum of $\sigma_3\mathcal{H}$. Our precise result is formulated as follows.

Theorem 1: *Let $z=\pm z_0$ be a pair of isolated eigenvalues of $\sigma_3\mathcal{H}$, where each eigenvalue has geometric multiplicity one and algebraic multiplicity N. Let $\mathcal{X}_g$ be a subspace spanned by a set of generalized eigenvectors $\{\boldsymbol{\psi}_j,\sigma_1\boldsymbol{\psi}_j\}_{j=0}^{N-1}$, such that $s_0=\frac{1}{2}\langle\sigma_3\boldsymbol{\psi}_{N-1},\boldsymbol{\psi}_0\rangle\neq 0$. Then,*

$$n(\mathcal{H})\big|_{\mathcal{X}_g} = 2P,$$

where $P=N/2$, when N is even, $P=(N-1)/2$, when N is odd, and $s_0>0$, and $P=(N+1)/2$, when N is odd, and $s_0<0$. Therefore, $n(\mathcal{H})\geq 2P$.

When the potentials of the linearized operator $\sigma_3\mathcal{H}$ are perturbed by a continuous deformation, we compute the exact number of unstable eigenvalues with $\mathrm{Im}(z)>0$ that bifurcate from the eigenvalue z_0 of zero energy $h=0$. In particular, we study the perturbed spectral problem:

$$\sigma_3(\mathcal{H}+\varepsilon\mathcal{V}_p(x))\boldsymbol{\psi} = z\boldsymbol{\psi}, \tag{1.5}$$

where the perturbation matrix $\mathcal{V}_p(x)$ is C^∞, real-valued and bounded, such that $\mathcal{V}_p\in L^\infty(\mathbb{R}^n)$. We assume that the perturbation matrix $\mathcal{V}_p$ is *generic* in the sense that $\langle\boldsymbol{\psi}_0,\mathcal{V}_p\boldsymbol{\psi}_0\rangle\neq 0$, where $\boldsymbol{\psi}_0$ is the eigenvector of $\sigma_3\mathcal{H}$ for the eigenvalue $z=z_0$. Our precise result is formulated as follows.

Theorem 2: *Let z_0 be an isolated eigenvalue of $\sigma_3\mathcal{H}$ with geometric multiplicity one and algebraic multiplicity N. Let $\boldsymbol{\psi}_0$ be the corresponding eigenvector of $\sigma_3\mathcal{H}$, such that $s_0=\frac{1}{2}\langle\sigma_3\boldsymbol{\psi}_{N-1},\boldsymbol{\psi}_0\rangle\neq 0$. Then, there exists a small $\varepsilon_0>0$, such that the problem (1.5) with $0<|\varepsilon|<\varepsilon_0$ has N simple eigenvalues near $z=z_0$, which are approximated to the leading order by roots of*

$$(z_k-z_0)^N = \frac{\varepsilon}{2s_0}\langle\boldsymbol{\psi}_0,\mathcal{V}_p\boldsymbol{\psi}_0\rangle + O(\varepsilon^{(N+1)/N}), \quad k=1,\ldots,N. \tag{1.6}$$

We note that results of Theorems 1 and 2 are no longer restricted to the case $n=3$, unlike the previous work.[2] Theorem 1 is proved in Sec. II, while Theorem 2 is proved in Sec. III.

A typical example of the spectral problem (1.3) with operators (1.1)–(1.2) arises in the linearization of the nonlinear Schrödinger (NLS) equation,

$$i\psi_t = -\Delta\psi + U(x)\psi + F(|\psi|^2)\psi, \tag{1.7}$$

where $F(0)=0$ and $U(x)$ decays to zero, at the solitary wave solution $\psi=\phi(x)e^{i\omega t}$, where $\phi(x)$ is a real-valued function and $\omega>0$ is a parameter. Linearization of the NLS equation (1.7) with the ansatz,

$$\psi = (\phi(x) + \varphi(x)e^{-izt} + \bar{\theta}(x)e^{i\bar{z}t})e^{i\omega t}, \tag{1.8}$$

leads to the spectral problem (1.3) with $\boldsymbol{\psi}=(\varphi,\theta)^T$, $f(x)=U(x)+F(\phi^2)+F'(\phi^2)\phi^2$, and $g(x)=F'(\phi^2)\phi^2$. When $F(\phi^2)$ is C^∞ and $U(x)$ and $\phi(x)$ are exponentially decaying C^∞ functions, then the assumptions on $f(x)$, $g(x)$ are satisfied.

The Hamiltonian-Hopf bifurcation is typical with $N=2$ when the real isolated eigenvalue $z=z_0$ has a geometric multiplicity *one* and an algebraic multiplicity *two*.[3,4] If (ω,ϕ) is a pair for the solitary wave solution that corresponds to the bifurcation case and $\varepsilon=\delta\omega$ is a variation of parameter ω while $\varepsilon\ \delta\phi$ is a variation of the solution $\phi(x)$ along the solution family, then the perturbation matrix $\mathcal{V}_p(x)$ takes the form:

$$\mathcal{V}_p = \begin{pmatrix} 1+\delta f(x) & \delta g(x) \\ \delta g(x) & 1+\delta f(x) \end{pmatrix},$$

where

$$\varepsilon\ \delta f(x) \equiv F((\phi+\varepsilon\delta\phi)^2) - F(\phi^2) + F'((\phi+\varepsilon\delta\phi)^2)(\phi+\varepsilon\delta\phi)^2 - F'(\phi^2)\phi^2,$$

$$\varepsilon\ \delta g(x) \equiv F'((\phi+\varepsilon\delta\phi)^2)(\phi+\varepsilon\delta\phi)^2 - F'(\phi^2)\phi^2,$$

are variations of the potentials $f(x)$ and $g(x)$ along the solution family. The particular perturbation matrix $\mathcal{V}_p(x)$ satisfies the assumption that $\mathcal{V}_p(x)$ is C^∞ bounded matrix-valued function. An analysis of a general Hamiltonian–Hopf bifurcation is described in Sec. IV.

II. PROPERTIES OF AN EIGENVALUE OF ZERO ENERGY

We rewrite the system (1.3) in new variables $\boldsymbol{\psi}=(u+w,u-w)^T$:

$$\sigma_1 \mathrm{H}\mathbf{u} = z\mathbf{u}, \tag{2.1}$$

where $\mathbf{u}=(u,w)^T$ and H is the new energy operator:

$$H = \begin{pmatrix} L_+ & 0 \\ 0 & L_- \end{pmatrix}, \tag{2.2}$$

with $L_\pm=-\Delta+\omega+f(x)\pm g(x)$. Let $n(H)$ denote the negative index of the energy operator H, which is the number of negative eigenvalues of H in $L^2(\mathbb{R}^n,\mathbb{C}^2)$ counting their multiplicity. Let $n(H)|_X$ be the negative index of H restricted to some subspace $X\subset L^2(\mathbb{R}^n,\mathbb{C}^2)$. We assume that there exists an isolated eigenvalue $0<z_0<\omega$ and eigenvector $\mathbf{u}_0=(u_0,w_0)^T$ of the spectral problem (2.1), such that

$$\sigma_1 \mathrm{H}\mathbf{u}_0 = z_0\mathbf{u}_0. \tag{2.3}$$

The adjoint problem has then the same eigenvalue z_0 with the eigenvector $\mathbf{u}_{0,\mathbf{a}}$, such that

$$\mathrm{H}\sigma_1\mathbf{u}_{0,a} = z_0\mathbf{u}_{0,a}, \quad \mathbf{u}_{0,a} = \sigma_1\mathbf{u}_0. \tag{2.4}$$

We assume that the eigenvalue z_0 has zero energy $h=\langle\mathbf{u}_0,H\mathbf{u}_0\rangle=0$, such that the algebraic multiplicity of the eigenvalue z_0 exceeds its geometric multiplicity. We consider the situation when the geometric multiplicity of the eigenvalue z_0 is one, while its algebraic multiplicity is N, such that $\ker(\sigma_1 H-z_0)=\{\mathbf{u}_0\}$ and $N_g(\sigma_1 H-z_0)=\{\mathbf{u}_0,\mathbf{u}_1,\ldots,\mathbf{u}_{N-1}\}$. The generalized eigenvectors $\mathbf{u}_j=(u_j,w_j)^T$, $1\le j\le N-1$ are defined from the Jordan chain equations:

$$\sigma_1 H \mathbf{u}_j = z_0 \mathbf{u}_j + \mathbf{u}_{j-1}. \tag{2.5}$$

The adjoint problem has $N-1$ generalized eigenvectors $\mathbf{u}_{j,a}=\sigma_1\mathbf{u}_j$, $1\leq j\leq N-1$ that solve the inhomogeneous equations:

$$H\sigma_1 \mathbf{u}_{j,a} = z_0 \mathbf{u}_{j,a} + \mathbf{u}_{j-1,a}. \tag{2.6}$$

If z_0 is an eigenvalue of $\sigma_1 H$, then $-z_0$ is also an eigenvalue of both $\sigma_1 H$ and its adjoint $H\sigma_1$, such that $\dim(N_g(\sigma_1 \mathrm{H}+z_0))=\dim(N_g(\mathrm{H}\sigma_1+z_0))=N$. Explicitly, we have

$$\sigma_1 H \mathbf{u}_0^- = -z_0 \mathbf{u}_0^-, \tag{2.7}$$

$$\sigma_1 H \mathbf{u}_j^- = -z_0 \mathbf{u}_j^- + \mathbf{u}_{j-1}^-, \tag{2.8}$$

where $\mathbf{u}_0^-=\sigma_3\mathbf{u}_0$ and $\mathbf{u}_j^-=(-1)^j\sigma_3\mathbf{u}_j$ and similarly

$$\mathrm{H}\sigma_1 \mathbf{u}_{0,a}^- = -z_0 \mathbf{u}_{0,a}^-, \tag{2.9}$$

$$\mathrm{H}\sigma_1 \mathbf{u}_{j,a}^- = -z_0 \mathbf{u}_{j,a}^- + \mathbf{u}_{j-1,a}^-, \tag{2.10}$$

where $\mathbf{u}_{0,a}^-=\sigma_1\mathbf{u}_0^-$ and $\mathbf{u}_{j,a}^-=\sigma_1\mathbf{u}_j^-$. Let $X_g=N_g(\sigma_1 H-z_0)\oplus N_g(\sigma_1 H+z_0)$ be the subspace spanned by the generalized eigenvectors $\{\mathbf{u}_j,\sigma_3\mathbf{u}_j\}_{j=0}^{N-1}$. Let L_+ and L_- be diagonal compositions of $(L_+,0)$ and $(0,L_-)$. The exact number of negative eigenvalues of H restricted to the subspace X_g is given by Theorem 1 in notations of the equivalent system (1.3). In order to prove Theorem 1, we establish some useful relations between eigenvectors of the generalized subspace X_g.

Lemma 2.1: Let $2N=\dim(X_g)$, *where* $2\leq N<\infty$. *Then, it is true that*

$$\langle \sigma_1\mathbf{u}_0, \mathbf{u}_j\rangle = 0, \quad 0\leq j\leq N-2, \quad \langle \sigma_1\mathbf{u}_0, \mathbf{u}_{N-1}\rangle \neq 0. \tag{2.11}$$

Proof: By the Fredholm Alternative Theorem, it follows from (2.4) and (2.5) that $\langle \mathbf{u}_{j-1},\mathbf{u}_{0,a}\rangle=0$, $1\leq j\leq N-1$ and $\langle \mathbf{u}_{N-1},\mathbf{u}_{0,a}\rangle\neq 0$. Since $\mathbf{u}_{0,a}=\sigma_1\mathbf{u}_0$, these conditions are equivalent to the statement (2.11). ■

Let U be an auxiliary matrix with the elements:

$$U_{i,j} = \langle \sigma_1\mathbf{u}_{i-1}, \mathbf{u}_{j-1}\rangle, \quad 1\leq i, j\leq N. \tag{2.12}$$

We study the structure of the matrix U.

Definition 2.2: *Suppose* M *is a square matrix of size* N. *The subset of its elements* $M_{i,j}$, $1\leq i,j\leq N$, *such that* $i+j=k+1$ *is said to be the* k*th antidiagonal of the matrix* M, *where* $1\leq k\leq 2N-1$. *The* k*th antidiagonal of* M *is said to be constant if all its elements are equal.*

Lemma 2.3: *Each* k*th antidiagonal of* U *is constant. There exists a basis* $\{\hat{\mathbf{u}}_j,\sigma_3\hat{\mathbf{u}}_j\}_{j=0}^{N-1}$ *in the subspace* X_g, *such that*

$$U = s_0 \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & \dots & \dots & 0 \end{pmatrix}, \tag{2.13}$$

where $s_0=\langle \sigma_1\hat{\mathbf{u}}_{N-1},\hat{\mathbf{u}}_0\rangle$. *Moreover,*

$$\langle \sigma_1\sigma_3\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j\rangle = 0, \quad 0\leq i, j\leq N-1. \tag{2.14}$$

Proof: By Lemma 2.1, the first antidiagonal of U is zero. It follows from (2.5) and (2.6) that

$$\langle \mathbf{u}_{i-1,a}, \mathbf{u}_j \rangle = \langle \mathbf{u}_{i,a}, \mathbf{u}_{j-1} \rangle, \quad 1 \le i, j \le N-1. \tag{2.15}$$

Therefore, the relation $\langle \sigma_1 \mathbf{u}_i, \mathbf{u}_{j-1} \rangle = \langle \sigma_1 \mathbf{u}_{i-1}, \mathbf{u}_j \rangle$ holds for $2 \le i+j \le 2N-2$. Since $\langle \sigma_1 \mathbf{u}_0, \mathbf{u}_j \rangle = 0$ by Lemma 2.1 for any $0 \le j \le N-2$, then all antidiagonals of U are zero for $1 \le k \le N-1$, such that $\langle \sigma_1 \mathbf{u}_i, \mathbf{u}_j \rangle = 0$ for $0 \le i+j \le N-2$. We show that by a proper choice of the generalized eigenvectors all but the main antidiagonals of U are zero for $N \le k \le 2N-1$. We introduce a sequence of transformations for $1 \le j \le N-1$:

$$\hat{\mathbf{u}}_k = \mathbf{u}_k, \quad 0 \le k \le j-1,$$

$$\hat{\mathbf{u}}_k = \mathbf{u}_k - \alpha_j \mathbf{u}_{k-j}, \quad j \le k \le N-1, \tag{2.16}$$

where the constants α_j are chosen from the condition that

$$\langle \sigma_1 \hat{\mathbf{u}}_j, \hat{\mathbf{u}}_{N-1} \rangle = 0, \quad 1 \le j \le N-1. \tag{2.17}$$

It is clear from (2.5) that the modified generalized eigenvectors $\{\hat{\mathbf{u}}_k\}_{k=0}^{N-1}$ satisfy the same inhomogeneous problems for any $1 \le j \le N-1$. By using recurrently the relations (2.16), we find that

$$\langle \sigma_1 \hat{\mathbf{u}}_j, \hat{\mathbf{u}}_{N-1} \rangle = \langle \sigma_1 \mathbf{u}_j, \mathbf{u}_{N-1} \rangle - 2\alpha_j \langle \sigma_1 \mathbf{u}_0, \mathbf{u}_{N-1} \rangle,$$

such that

$$\alpha_j = \frac{\langle \sigma_1 \mathbf{u}_j, \mathbf{u}_{N-1} \rangle}{2\langle \sigma_1 \mathbf{u}_0, \mathbf{u}_{N-1} \rangle}.$$

Since all antidiagonals of U are constants, the previous orthogonalization implies that $\langle \sigma_1 \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j \rangle = 0$, $N \le i+j \le 2N-2$. Furthermore, we have the normalization $\langle \sigma_1 \hat{\mathbf{u}}_{N-1}, \hat{\mathbf{u}}_0 \rangle = s_0$ on the main antidiagonal. It follows from (2.5) and (2.10) that

$$2z_0 \langle \mathbf{u}_{i,a}^-, \mathbf{u}_j \rangle + \langle \mathbf{u}_{i,a}^-, \mathbf{u}_{j-1} \rangle - \langle \mathbf{u}_{i-1,a}^-, \mathbf{u}_j \rangle = 0, \quad 1 \le i, j \le N-1. \tag{2.18}$$

Using the relation (2.18), we prove (2.14) by induction. ■

Corollary 2.4: *There exists a basis of generalized eigenvectors* $\{\hat{\mathbf{u}}_j, \sigma_3 \hat{\mathbf{u}}_j\}_{j=0}^{N-1}$ *in the subspace* X_g, *such that it satisfies the skew-orthogonality relations*,

$$\langle \sigma_1 \hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j \rangle = s_0 \delta_{i,N-1-j}, \quad 0 \le i, j \le N-1, \tag{2.19}$$

and any $\mathbf{f} \in L^2(\mathbb{R}^n, \mathbb{C}^2)$ *can be decomposed as follows:*

$$\mathbf{f} = \sum_{j=0}^{N-1} (c_j \hat{\mathbf{u}}_j + d_j \sigma_3 \hat{\mathbf{u}}_j) + \mathbf{f}_c, \tag{2.20}$$

where

$$c_j = \frac{1}{s_0} \langle \sigma_1 \hat{\mathbf{u}}_{N-1-j}, \mathbf{f} \rangle, \quad d_j = -\frac{1}{s_0} \langle \sigma_1 \sigma_3 \hat{\mathbf{u}}_{N-1-j}, \mathbf{f} \rangle, \quad 0 \le j \le N-1$$

and

$$\langle \sigma_1 \hat{\mathbf{u}}_j, \mathbf{f}_c \rangle = \langle \sigma_1 \sigma_3 \hat{\mathbf{u}}_j, \mathbf{f}_c \rangle = 0, \quad 0 \le j \le N-1.$$

Remark 2.5: Let P_g be the skew-orthogonal projection operator to the subspace X_g. We have $P_g^2 = P_g$ and $(I-P_g)^2 = I-P_g$ on $L^2(\mathbb{R}^n, \mathbb{C}^2)$. Operators P_g and $(I-P_g)$ are bounded, such that

$$\|P_g\| \leq \frac{2}{|s_0|} \sum_{k=0}^{N-1} \|\hat{\mathbf{u}}_{N-1-k}\|_{L^2} \|\hat{\mathbf{u}}_k\|_{L^2}, \quad \|I - P_g\| \leq 1 + \|P_g\|,$$

where the operator norm $\|\cdot\|_{L^2 \to L^2}$ is denoted as $\|\cdot\|$.

Remark 2.6: In what follows, the hats over the basis elements of the subspace X_g will be omitted for the simplicity of notations. Let $H|_{X_g} = P_g^* H P_g$ be the restriction of the energy operator to the generalized subspace X_g. The restriction of the energy operator is defined in terms of the matrices M_+ and M_-, where

$$(M_+)_{i,j} = (L_+ u_{i-1}, u_{j-1}), \quad 1 \leq i, j \leq N,$$

$$(M_-)_{i,j} = (L_- w_{i-1}, w_{j-1}), \quad 1 \leq i, j \leq N. \tag{2.21}$$

The structure of the matrices M_+ and M_- follows from that of the matrix U.

Lemma 2.7: *The matrices M_+ and M_- are equal and have the structure*:

$$M_+ = M_- = \frac{s_0}{2} \begin{pmatrix} 0 & 0 & \dots & 0 & z_0 \\ 0 & 0 & \dots & z_0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ z_0 & 1 & \dots & \dots & 0 \end{pmatrix}. \tag{2.22}$$

Proof: Using the definitions (2.12) and (2.21), the systems (2.3) and (2.5), and the identity (2.14), we derive the relations

$$2(M_+)_{1,j} = z_0 U_{j,1}, \quad 2(M_-)_{1,j} = z_0 U_{1,j}, \quad 1 \leq j \leq N,$$

and

$$2(M_+)_{i,j} = z_0 U_{j,i} + U_{j,i-1}, \quad 2(M_-)_{i,j} = z_0 U_{i,j} + U_{i-1,j}, \quad 2 \leq i \leq N, \quad 1 \leq j \leq N.$$

By Lemma 2.3, these formulas imply the representation (2.22). ■

Remark 2.8: The structure of matrices U and $M_\pm$ enables us to estimate the number of their positive and negative eigenvalues. Since $s_0 \neq 0$ and $z_0 \neq 0$, the main anti-diagonal of the matrices is nonzero, such that their determinant is nonzero and no zero eigenvalue exists. We denote the number of positive and negative eigenvalues of an abstract symmetric non-singular matrix M by $p(M)$ and $n(M)$ respectively, such that $p(M)+n(M)=N$.

Lemma 2.9: *Let M be a symmetric N-by-N matrix, such that each kth antidiagonal of M is zero for $1 \leq k \leq N-1$ and the Nth antidiagonal of M is $a \neq 0$. If N is even, then $n(M)=p(M)=N/2$. If N is odd, then $n(M)=(N-1)/2$ and $p(M)=(N+1)/2$ for $a>0$ and $n(M)=(N+1)/2$ and $p(M)=(N-1)/2$ for $a<0$.*

Proof: Let $\{\lambda_k\}_{k=0}^{N-1}$ be eigenvalues of M ordered by $\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{N-1}$. It follows from the structure of M that $\det M = (-1)^{N(N-1)/2} a^N$. We introduce the auxiliary subspace $V_d \subset \mathbb{R}^N$ spanned by the unit vectors $\{\mathbf{e}_k\}_{k=1}^d$ in $\mathbb{R}^N$, where $d=N/2$ when N is even and $d=(N-1)/2$ when N is odd. Let P_d be the orthogonal projection from $\mathbb{R}^N$ onto V_d, such that P_d has the matrix elements:

$$(P_d)_{i,j} = \begin{cases} 1, & 1 \leq i = j \leq d, \\ 0, & d+1 \leq i = j \leq N, \\ 0, & i \neq j. \end{cases} \tag{2.23}$$

A trivial computation gives that the elements of $M|_{V_d}$ are

$$(P_d M P_d)_{i,j} = (P_d)_{i,i} M_{i,j} (P_d)_{j,j}, \quad 1 \leq i,j \leq N,$$

which are nonzero only if $i,j \leq d$ and $i+j \geq N+1$. However, the intersection of these two sets is empty due to the definition of d. Therefore, the matrix $P_d M P_d = 0$ and all d eigenvalues of $M|_{V_d}$ are

zero. By the Rayleigh-Ritz theorem (see Theorem XIII.3 in Ref. 6), d eigenvalues of M are nonpositive due to the upper bound by the eigenvalues of $M|_{V_d}$. Therefore, $n(M) \geq d$. The same argument for $-M$ shows that $p(M) \geq d$. This proves that $n(M)=p(M)=N/2$ if N is even. If N is odd, there are two possibilities: either $n(M)=(N-1)/2$ and $p(M)=(N+1)/2$ or $n(M)=(N+1)/2$ and $p(M)=(N-1)/2$. Since

$$\text{sign}(\det(M)) = (-1)^{N(N-1)/2}(\text{sign}(a))^N = (-1)^{n(M)},$$

we find that the first case occurs for $a>0$ and the second case occurs for $a<0$. ■

Proof of Theorem 1: We recall that $\mathrm{H}|_{X_g} = P_g^* H P_g$ denotes the restriction of the energy operator to the generalized subspace X_g. By Lemma 2.7, a trivial calculation shows that the quadratic form of $H|_{X_g}$ can be rewritten as

$$\left\langle H\big|_{X_g}\mathbf{u},\mathbf{u}\right\rangle = 2\langle M_+\mathbf{c},\mathbf{c}\rangle_{\mathbb{C}^N} + 2\langle M_+\mathbf{d},\mathbf{d}\rangle_{\mathbb{C}^N}, \tag{2.24}$$

where $\mathbf{c}=(c_0,c_1,\ldots,c_{N-1})^T \in \mathbb{C}^N$, $\mathbf{d}=(d_0,d_1,\ldots,d_{N-1})^T \in \mathbb{C}^N$, and the matrices $M_\pm$ are defined by (2.21). Let $\{\mathbf{v}_s\}_{s=1}^{n(M_+)}$ be an orthonormal set of eigenvectors corresponding to negative eigenvalues of the matrix M_+. Then we can construct a subspace of X_g, spanned by the vectors $\tilde{\mathbf{u}}_s = \Sigma_{k=0}^{N-1}(\mathbf{v}_s)_k \mathbf{u}_\mathbf{k}$ and $\sigma_3\tilde{\mathbf{u}}_s$ for $1 \leq s \leq n(M_+)$. It follows from (2.24) that the operator $H|_{X_g}$ is negative definite on this subspace, i.e., via the Rayleigh-Ritz theorem $n(H)|_{X_g} \geq 2n(M_+)$. Let $\mathcal{M}_+ = M_+ \otimes M_+$ be the block matrix on $\mathbb{C}^{2N}$. To obtain the inequality reverse to the one above we consider the orthonormal set of eigenvectors $\{\mathbf{w}_s\}_{s=1}^{n(H)|_{X_g}}$, which spans the negative subspace of $H|_{X_g}$. Applying the projection operator, we have $P_g\mathbf{w}_\mathbf{s} = \Sigma_{k=0}^{N-1}(\boldsymbol{\alpha}_s)_k\mathbf{u}_k + \Sigma_{k=0}^{N-1}(\boldsymbol{\beta}_s)_k\sigma_3\mathbf{u}_\mathbf{k}$. Therefore, there is a subspace of $\mathbb{C}^{2N}$ spanned by the vectors $(\boldsymbol{\alpha}_s,\boldsymbol{\beta}_s)^T$, $1 \leq s \leq n(H)|_{X_g}$. It follows from (2.24) that the matrix $\mathcal{M}_+$ is negative definite on this subspace, which yields $n(\mathcal{M}_+)=2n(M_+) \geq n(H)|_{X_g}$. We have $a=\frac{1}{2}z_0 s_0$ and $z_0>0$, such that it follows by Lemmas 2.7 and 2.9 that $n(H)|_{X_g}=2n(M_+)=2P$. By the Rayleigh–Ritz Theorem,[6] we then have $n(H) \geq n(H)|_{X_g}$. ■

III. SPLITTING OF AN EIGENVALUE OF ZERO ENERGY

When the perturbation is applied to the spectral problem (2.1), one can expect that the multiple isolated eigenvalue $z=z_0$ is destroyed and N simple eigenvalues bifurcate in the neighborhood of $z=z_0$. This splitting of the multiple eigenvalue $z=z_0$ may result in the instability bifurcations if $\text{Im}(z)>0$ for some of the simple eigenvalues. The location of N simple eigenvalues in the neighborhood of $z=z_0$ for small nonzero ε is given by Theorem 2 in notations of the perturbed spectral problem (1.5). For convenience, we rewrite (1.5) in the equivalent form

$$\sigma_1(H+\varepsilon V_p)\mathbf{u} = z\mathbf{u}, \tag{3.1}$$

where $V_p(x)$ is C^∞, real-valued, and a bounded perturbation matrix given by $V_p = U^{-1}\mathcal{V}_p U$, with

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = U^{-1}.$$

In order to prove Theorem 2, we use the resolvent $R(z)=(\sigma_1\mathrm{H}-z)^{-1}$ defined for the values of z away from the spectrum of $\sigma_1 H$. The perturbed problem (3.1) is rewritten in the resolvent form

$$(I+\varepsilon R(z)\sigma_1 V_p)\mathbf{u} = 0. \tag{3.2}$$

We shall consider the subspace $X_g^+ = N_g(\sigma_1\mathrm{H}-z_0)$ with the projection operator P_g^+ onto this subspace. In what follows, the superscript for the subspace X_g^+ and the projection operator P_g^+ will be omitted for the simplicity of notations. Our plan is to use the projection operator P_g and to reduce the perturbed problem (3.1) to the finite-dimensional equations on the subspace X_g, where a regular perturbation theory can be applied.[7] For this purpose, we study properties of the resolvent $R(z)$ and the related projection operator onto X_g.

Lemma 3.1: Let the subspace X_g be spanned by the set $\{\mathbf{u}_j\}_{j=0}^{N-1}$. Then,

$$R(z)\mathbf{u}_j = \sum_{k=0}^{j} \frac{(-1)}{(z-z_0)^{j-k+1}}\mathbf{u}_k, \tag{3.3}$$

for $z \neq z_0$ and $0 \leq j \leq N-1$.

Proof: The formula (3.3) with $j=0$ follows from the problem (2.3). We use the induction method and assume that the formula (3.3) holds for some $j=s$ for $0 \leq s \leq N-2$. It follows from (2.5) that

$$R(z)\mathbf{u}_{s+1} = \frac{1}{z-z_0}R(z)\mathbf{u}_s - \frac{1}{z-z_0}\mathbf{u}_{s+1},$$

such that

$$R(z)\mathbf{u}_{s+1} = \sum_{k=0}^{s+1} \frac{(-1)}{(z-z_0)^{s-k+2}}\mathbf{u}_k,$$

and the formula (3.3) remains true for $j=s+1$. ■

Corollary 3.2: Let z be not in the spectrum of $\sigma_1 H$. Then,

$$(I-P_g)R(z)P_g = 0, \quad P_g R(z)(I-P_g) = 0.$$

Proof: Let $\mathbf{f}$ be an arbitrary function in $L^2(\mathbb{R}^n, \mathbb{C}^2)$. By Lemma 3.1, we have $R(z)P_g\mathbf{f} \in X_g$ for $z \neq z_0$, and therefore $(I-P_g)R(z)P_g\mathbf{f}=0$. On the other hand, for any $k=0, \ldots, N-1$ we have

$$\langle R(z)(I-P_g)\mathbf{f}, \sigma_1\mathbf{u}_k\rangle = \langle (I-P_g)\mathbf{f}, (H\sigma_1 - \bar{z})^{-1}\sigma_1\mathbf{u}_k\rangle = \langle (I-P_g)\mathbf{f}, \sigma_1 R(\bar{z})\mathbf{u}_k\rangle = 0$$

such that $P_g R(z)(I-P_g)\mathbf{f}=0$. ■

Remark 3.3: Let $\bar{D}(z_0,\delta)=\{z \in \mathbb{C}: |z-z_0| \leq \delta\}$ be a closed disk that contains no eigenvalues of the operator $\sigma_1 H$ other than $z=z_0$. The resolvent $R(z)$ has the only singularity in $\bar{D}(z_0,\delta)$ at $z=z_0$.

Lemma 3.4: Let $T(z)=(I-P_g)R(z)(I-P_g)\sigma_1 V_p$. The operator $T(z)$ is uniformly bounded in $\bar{D}(z_0,r) \subseteq \bar{D}(z_0,\delta)$, such that

$$\|T(z)\| \leq C < \infty, \tag{3.4}$$

where $r>0$ and $C>0$.

Proof: The proof is a standard argument, which uses the analyticity of the resolvent outside the spectrum, the Corollary 3.3, the boundedness of the operator $I-P_g$, and the fact that $V_p \in L^\infty$. ■

Lemma 3.5: The problem (3.2) *projected onto the subspace X_g is equivalent to the problem:*

$$[I + \varepsilon R(z)P_g\sigma_1 V_p(I+S(\varepsilon,z))]P_g\mathbf{u} = 0, \tag{3.5}$$

where the operator $S(\varepsilon,z)$ is analytic in ε and $\|S(\varepsilon,z)\| \leq 2C|\varepsilon|$, while C is defined in (3.4), *$z \in \bar{D}(z_0,r)$, and $\varepsilon \neq 0$ is small, such that $|\varepsilon| \leq 1/2C$.*

Proof: Applying P_g and $(I-P_g)$ to the problem (3.2), we obtain

$$P_g\mathbf{u} + \varepsilon P_g R(z)\sigma_1 V_p P_g\mathbf{u} + \varepsilon P_g R(z)\sigma_1 V_p(I-P_g)\mathbf{u} = 0$$

and

$$[I + \varepsilon(I-P_g)R(z)\sigma_1 V_p](I-P_g)\mathbf{u} = -\varepsilon(I-P_g)R(z)\sigma_1 V_p P_g\mathbf{u}.$$

By Corollary 3.2, we have

$$[I+\varepsilon P_g R(z) P_g \sigma_1 V_p] P_g \mathbf{u} + \varepsilon P_g R(z) P_g \sigma_1 V_p (I-P_g)\mathbf{u} = 0 \tag{3.6}$$

and

$$[I+\varepsilon T(z)](I-P_g)\mathbf{u} = -\varepsilon T(z) P_g \mathbf{u}. \tag{3.7}$$

By Lemma 3.1, we have $P_g R(z) P_g = R(z) P_g$ for $z \neq z_0$, such that we need to derive the equation expressing $(I-P_g)\mathbf{u}$ via $P_g\mathbf{u}$. It follows from (3.7) that

$$(I-P_g)\mathbf{u} = [(I+\varepsilon T(z))^{-1} - I] P_g \mathbf{u}, \tag{3.8}$$

such that the equation (3.6) yields

$$[I+\varepsilon R(z) P_g \sigma_1 V_p [I+\varepsilon T(z)]^{-1}] P_g \mathbf{u} = 0.$$

The operator $[I+\varepsilon T(z)]^{-1}$ can be written as $I+S(\varepsilon,z)$, where

$$S(\varepsilon,z) = \sum_{k=1}^{\infty} [-\varepsilon T(z)]^k. \tag{3.9}$$

By Lemma 3.4 and a comparison with the geometric series, the series (3.9) converges absolutely in the $\|.\|$ norm for $z \in \bar{D}(z_0,r)$. When $|\varepsilon| \leq 1/2C$, we have $\|S(\varepsilon,z)\| \leq 2C|\varepsilon|$. ■

Remark 3.6: By Lemma 3.5, the finite-rank operator on the left-hand side of the projection equations (3.5) is analytic in ε for small ε. The determinant of the left-hand side is the Weinstein–Aronszajn determinant, properties of which and its relation to the spectrum of the perturbed operator are rigorously derived in Ref. 7, pp. 244–250. We truncate the projection equations (3.5) by linear terms in ε and obtain the finite rank operator $W(\varepsilon,z) = I + \varepsilon R(z) P_g \sigma_1 V_p$ on the subspace X_g. The matrix elements of $W(\varepsilon,z)$ are expressed in terms of the elements $\{\mathbf{u}_j\}_{j=0}^{N-1}$ of the subspace X_g.

Lemma 3.7: For all $i,j=1,\ldots,N$, we have

$$W_{i,j}(\varepsilon,z) = \delta_{i,j} - \frac{\varepsilon}{s_0} \sum_{s=i-1}^{N-1} \frac{\langle \mathbf{u}_{N-1-s}, V_p \mathbf{u}_{j-1} \rangle}{(z-z_0)^{s-i+2}}. \tag{3.10}$$

Proof: Due to the orthogonality relations (2.19), the matrix elements of the finite rank operator W are equal to

$$W_{i,j}(\varepsilon,z) = \frac{1}{s_0} \langle \sigma_1 \mathbf{u}_{N-i}, W \mathbf{u}_{j-1} \rangle, \quad 1 \leq i,j \leq N. \tag{3.11}$$

Corollary 2.4 and Lemma 3.1 yield

$$\varepsilon R(z) P_g \sigma_1 V_p \mathbf{u}_j = -\frac{\varepsilon}{s_0} \sum_{s=0}^{N-1} \sum_{q=0}^{s} \frac{\langle \mathbf{u}_{N-1-s}, V_p \mathbf{u}_j \rangle}{(z-z_0)^{s-q+1}} \mathbf{u}_q.$$

Substituting this relation into the representation (3.11) and using the orthogonality conditions (2.19) we derive the identity (3.10). ■

Proof of Theorem 2: According to Ref. 7, the Weinstein-Aronszajn determinant is a meromorphic function, which has the pole of the Nth order at $z=z_0$. The eigenvalues of the perturbed problem (3.1) are given by the zeros $z=z_k$ of the Weinstein–Aronszajn determinant. We define the operator $F(\varepsilon,z) = (z-z_0)W(\varepsilon,z)$, such that $\det F(\varepsilon,z)$ is a polynomial in $z-z_0$ and ε. By Lemma 3.7, the matrix elements of $F(\varepsilon,z)$ are equal to

$$F_{i,j}(\varepsilon,z)=(z-z_0)\,\delta_{i,j}-\frac{\varepsilon}{s_0}\sum_{s=i-1}^{N-1}\frac{\langle \mathbf{u}_{N-1-s},V_p\mathbf{u}_{j-1}\rangle}{(z-z_0)^{s-i+1}},\quad i,j=1,\ldots,N.$$

Since $\det F(\varepsilon,z)$ is a polynomial in ε, we have the expansion:

$$\det F(\varepsilon,z)=\det F(0,z)+\varepsilon\frac{\partial}{\partial\varepsilon}\det F(0,z)+O(\varepsilon^2,z-z_0),\tag{3.12}$$

where $O(\varepsilon^2,z-z_0)$ is a polynomial in ε and $z-z_0$. The expansion (3.12) allows us to obtain the estimate on the zeros $z=z_k$ of the Weinstein–Aronszajn determinant. We find that

$$\det F(0,z)=(z-z_0)^N$$

and

$$\frac{\partial}{\partial\varepsilon}\det F(0,z)=\sum_{i=1}^{N}\det D^i(z),$$

where

$$D^i_{q,j}(z)=\begin{cases}(z-z_0)\,\delta_{q,j}, & q\neq i,\\ D^i_{i,j}(z), & q=i,\end{cases}$$

such that

$$D^i_{i,j}(z)=-\frac{1}{s_0}\sum_{s=i-1}^{N-1}\frac{\langle \mathbf{u}_{N-1-s},V_p\mathbf{u}_{j-1}\rangle}{(z-z_0)^{s-i+1}},$$

or explicitly

$$D^i(z)=\begin{pmatrix} z-z_0 & 0 & 0 & \ldots & 0 & 0 & 0\\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & \ldots & z-z_0 & 0 & 0 & \ldots & 0\\ D^i_{i,1}(z) & D^i_{i,2}(z) & \ldots & D^i_{i,i}(z) & \ldots & \ldots & D^i_{i,N}(z)\\ 0 & \ldots & 0 & 0 & z-z_0 & \ldots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & 0 & \ldots & 0 & z-z_0 \end{pmatrix}.$$

A straightforward computation shows that

$$\det D^i(z)=(z-z_0)^{N-1}D^i_{i,i}(z)=-\frac{1}{s_0}\sum_{s=i-1}^{N-1}(z-z_0)^{N-2-(s-i)}\langle \mathbf{u}_{N-1-s},V_p\mathbf{u}_{i-1}\rangle.$$

The expansion (3.12) implies that the zeros of the Weinstein–Aronszajn determinant are given by the algebraic equation

$$(z-z_0)^N-\frac{\varepsilon}{s_0}\sum_{i=1}^{N}\sum_{s=i-1}^{N-1}(z-z_0)^{N-2-(s-i)}\langle \mathbf{u}_{N-1-s},V_p\mathbf{u}_{i-1}\rangle+\varepsilon^2F_2(z-z_0,\varepsilon)=0,\tag{3.13}$$

where $\lim_{\varepsilon\to0}F_2(z-z_0,\varepsilon)$ exists. By the Implicit Function Theorem, roots of the algebraic equation (3.13) exist and satisfy the estimate $z-z_0=O(\varepsilon^{1/N})$. Therefore, the zero energy eigenvalue of the unperturbed problem splits into N simple eigenvalues, which are given asymptotically by roots of

$$(z_k - z_0)^N = \frac{\varepsilon}{s_0}\langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle + O(\varepsilon^{(N+1)/N}), \quad k = 1, \ldots, N. \tag{3.14}$$

Equation (3.14) coincides with (1.6) in notations of (1.5). ■

IV. A GENERAL HAMILTONIAN–HOPF INSTABILITY BIFURCATION

The pair of eigenvalues of zero energy $z = \pm z_0$ is neutrally stable in the linearized spectral problem (2.1), since $\mathrm{Im}(z_0) = 0$. If there are no other isolated eigenvalues with $\mathrm{Im}(z) > 0$, it would imply that the spectral problem (2.1) is weakly spectrally stable. However, the multiple eigenvalue of zero energy is structurally unstable and splits into simple eigenvalues, when the spectral problem (2.1) is perturbed with a bounded potential V_p in the form (3.1). When simple eigenvalues from the roots of (3.14) satisfy $\mathrm{Im}(z_k) > 0$ for some k, the spectral problem (3.1) undertakes an instability bifurcation, referred to as the *general Hamiltonian–Hopf bifurcation*. We show that there is only one bifurcation that gives a transition to instability, such that neutrally stable eigenvalues for one sign of ε split into stable and unstable eigenvalues for the other sign of ε. This bifurcation occurs for $N = 2$. Other bifurcations with $N \geq 3$ lead to unstable eigenvalues for either sign of $\varepsilon \neq 0$. We compute the exact number of unstable eigenvalues for each N, considering separately the cases $N = 2$ and $N \geq 3$.

Proposition 4.1: Let $\langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle \neq 0$ *and* $0 < |\varepsilon| < \varepsilon_0$. *When* $N = 2$, *there exist two neutrally stable eigenvalues of the spectral problem* (3.1) *in a local neighborhood of* $z = z_0$ *for* $\mathrm{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle) = 1$, *one of positive and the other one of negative energy*, *and two (stable and unstable) eigenvalues for* $\mathrm{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle) = -1$.

Proof: It follows from (3.14) with $N = 2$ that

$$z_{1,2}^+ = z_0 \pm \sqrt{\frac{\varepsilon}{s_0}\langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle} + O(\varepsilon), \tag{4.1}$$

when $\mathrm{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle) = 1$ and

$$z_{1,2}^- = z_0 \pm i\sqrt{\left|\frac{\varepsilon}{s_0}\langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle\right|} + O(\varepsilon),$$

when $\mathrm{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0\rangle) = -1$. Since the total multiplicity of eigenvalues near $z = z_0$ is continuous in ε and complex eigenvalues occur in pairs, the eigenvalues $z_{1,2}^+$ are real and neutrally stable. The eigenvalues $z_{1,2}^-$ are complex, such that z_1^+ is stable and z_1^- is unstable. Let $\mathbf{v}_{1,2}^+$ be the eigenvectors of the problem (3.1) that correspond to $z_{1,2}^+$. We need to show that the energy operator is positive on one of the eigenvectors and negative on the other eigenvector. It follows from (3.1) that

$$\langle (H + \varepsilon V_p)\mathbf{v}_j^+, \mathbf{v}_j^+\rangle = z_j^+ \langle \sigma_1 \mathbf{v}_j^+, \mathbf{v}_j^+\rangle, \quad j = 1, 2. \tag{4.2}$$

Using the projection onto the subspace X_g, we rewrite (4.2) as follows:

$$\langle \sigma_1 \mathbf{v}_j^+, \mathbf{v}_j^+\rangle = \langle \sigma_1 P_g \mathbf{v}_j^+, P_g \mathbf{v}_j^+\rangle + \langle \sigma_1 (I - P_g)\mathbf{v}_j^+, (I - P_g)\mathbf{v}_j^+\rangle + 2\langle \sigma_1 P_g \mathbf{v}_j^+, (I - P_g)\mathbf{v}_j^+\rangle. \tag{4.3}$$

Let us estimate each of these three terms and show that only the first one plays the leading role. We have

$$P_g \mathbf{v}_j^+ = c_0^+ \mathbf{u}_0 + c_1^+ \mathbf{u}_1, \tag{4.4}$$

where the constants c_0^+ and c_1^+ satisfy

$$W_{2,1}(\varepsilon, z_j^+)c_0^+ + W_{2,2}(\varepsilon, z_j^+)c_1^+ + O(\varepsilon^2) = 0. \tag{4.5}$$

Using the explicit expression (3.10), we have

$$W_{2,1}(\varepsilon,z_j^+)=-\frac{\varepsilon}{s_0}\frac{\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}{z_j^+-z_0},\quad W_{2,2}(\varepsilon,z_j^+)=1-\frac{\varepsilon}{s_0}\frac{\langle \mathbf{u}_0,V_p\mathbf{u}_1\rangle}{z_j^+-z_0}. \tag{4.6}$$

This expression can be rewritten by using (4.1), or, explicitly,

$$\frac{|\varepsilon|}{z_j^+-z_0}=(-1)^{j+1}\sqrt{\frac{s_0\varepsilon}{\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}}+O(\varepsilon),$$

such that

$$W_{2,1}(\varepsilon,z_j^+)=(-1)^j\sqrt{\frac{\varepsilon}{s_0}\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}+O(\varepsilon)$$

and

$$W_{2,2}(\varepsilon,z_j^+)=1+(-1)^j\,\mathrm{sign}(\varepsilon s_0)\sqrt{\frac{\varepsilon}{s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}}\langle \mathbf{u}_0,V_p\mathbf{u}_1\rangle+O(\varepsilon).$$

We let $c_0^+=1$ by scaling and obtain from (4.5) that

$$c_1^+=(-1)^{j+1}\sqrt{\frac{\varepsilon}{s_0}\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}+O(\varepsilon).$$

By the triangle inequality applied to (4.4), we have the norm estimate

$$\|P_g\mathbf{v}_j^+\|_{L^2}\le\|\mathbf{u}_0\|_{L^2}+O(\sqrt{\varepsilon})\|\mathbf{u}_1\|_{L^2}. \tag{4.7}$$

For the first term on the right side of (4.3) using (4.4), we derive

$$\langle\sigma_1P_g\mathbf{v}_j^+,P_g\mathbf{v}_j^+\rangle=2(-1)^{j+1}\,\mathrm{sign}(s_0)\sqrt{\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}+O(\varepsilon). \tag{4.8}$$

For the second and the third terms on the right side of (4.3), we get bounds via the identity (3.8), the Schwarz inequality, the estimate on the norm of the operator $S(\varepsilon,z)$ given in Lemma 3.5, and the bound (4.7). Thus

$$|\langle\sigma_1(I-P_g)\mathbf{v}_j^+,(I-P_g)\mathbf{v}_j^+\rangle|\le\|S(\varepsilon,z_j^+)P_g\mathbf{v}_j^+\|_{L^2}^2\le\widetilde{C}^2\varepsilon^2(\|\mathbf{u}_0\|_{L^2}+O(\sqrt{\varepsilon})\|\mathbf{u}_1\|_{L^2})^2$$

and

$$|2\langle\sigma_1P_g\mathbf{v}_j^+,(I-P_g)\mathbf{v}_j^+\rangle|\le2\|P_g\mathbf{v}_j^+\|_{L^2}\|S(\varepsilon,z_j^+)P_g\mathbf{v}_j^+\|_{L^2}\le2\widetilde{C}|\varepsilon|(\|\mathbf{u}_0\|_{L^2}+O(\sqrt{\varepsilon})\|\mathbf{u}_1\|_{L^2})^2.$$

Using the inequalities above along with (4.8) in the identity (4.3) and substituting into (4.2), we arrive at

$$\langle(H+\varepsilon V_p)\mathbf{v}_1^+,\mathbf{v}_1^+\rangle=2z_0\,\mathrm{sign}(s_0)\sqrt{\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}+O(\varepsilon), \tag{4.9}$$

$$\langle(H+\varepsilon V_p)\mathbf{v}_2^+,\mathbf{v}_2^+\rangle=-2z_0\,\mathrm{sign}(s_0)\sqrt{\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle}+O(\varepsilon), \tag{4.10}$$

for ε sufficiently small and $\mathrm{sign}(\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle)=1$. Thus, the quadratic forms (4.9) and (4.10) have opposite signs. ■

Proposition 4.2: Let $\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle\neq0$ *and* $0<|\varepsilon|<\varepsilon_0$. *When* $N\ge3$, *there exist unstable eigenvalues of the spectral problem* (3.1) *in a local neighborhood of* $z=z_0$ *for either sign of* $\varepsilon\neq0$. *When N is odd, there are* $(N-1)/2$ *unstable eigenvalues. When N is even, there are* $N/2-1$ *unstable eigenvalues for* $\mathrm{sign}(\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle)=1$ *and* $N/2$ *unstable eigenvalues for* $\mathrm{sign}(\varepsilon s_0\langle \mathbf{u}_0,V_p\mathbf{u}_0\rangle)=-1$.

Proof: We have

$$z_k^+ = z_0 + \sqrt[N]{\frac{\varepsilon}{s_0}\langle \mathbf{u}_0, V_p \mathbf{u}_0 \rangle} e^{i[2\pi(k-1)/N]} + O(\varepsilon^{2/N}), \quad k = 1, \ldots, N, \tag{4.11}$$

for $\text{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0 \rangle) = 1$ and

$$z_k^- = z_0 + \sqrt[N]{\left|\frac{\varepsilon}{s_0}\langle \mathbf{u}_0, V_p \mathbf{u}_0 \rangle\right|} e^{i[(-\pi+2\pi k)/N]} + O(\varepsilon^{2/N}), \quad k = 1, \ldots, N, \tag{4.12}$$

for $\text{sign}(\varepsilon s_0 \langle \mathbf{u}_0, V_p \mathbf{u}_0 \rangle) = -1$. Unstable eigenvalues with $\text{Im}(z_k) > 0$ exist among both $\{z_k^+\}_{k=1}^N$ and $\{z_k^-\}_{k=1}^N$, e.g., $\text{Im}(z_2^+) > 0$ and $\text{Im}(z_1^-) > 0$. The count of unstable eigenvalues follows from the explicit expressions (4.11) and (4.12). ■

Remark 4.3: In practical situations, the NLS equation (1.7) has limits when the eigenvalues of the spectral problem (1.3) are all neutrally stable. When the NLS equation (1.7) deviates from the stable limit due to parameter continuations, real eigenvalues z start to move, which may lead to coalescence. The practical outcome of the above analysis shows that the coalescence of N neutrally stable eigenvalues with $N \geq 3$ cannot lead to a multiple eigenvalue $z = z_0$ of geometric multiplicity one and algebraic multiplicity N. If the resulting eigenvalue $z = z_0$ has zero energy, then it corresponds to several Jordan blocks, where each block splits according to our analysis in Propositions 4.1 and 4.2.

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Non-Laplacian growth, algebraic domains, and finite reflection groups

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Dynamics of planar domains with moving boundaries driven by the gradient of a scalar field that satisfies an elliptic PDE is studied. We consider the question: For which kind of PDEs are the domains algebraic, provided the field has singularities at a fixed point inside the domain? The construction reveals a direct connection with the theory of the Calogero-Moser systems related to finite reflection groups and their integrable deformations. © *2006 American Institute of Physics.*
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I. NONHOMOGENEOUS POROUS MEDIUM FLOWS

Laplacian growth is a process that governs the dynamics of the boundary $\partial\Omega=\partial\Omega(t)$ in the plane separating two disjoint, open regions (Ω and $\mathbb{C}\backslash\bar{\Omega}$) in which harmonic (scalar) fields are defined. These may be interpreted as the pressure fields for incompressible fluids (porous-medium flows, Hele-Shaw flows, etc. See, e.g., Ref. 14, and references therein). In the recent literature there have appeared several new formulations of the Laplacian growth related with the theory of integrable systems and random matrices, quantum Hall effect, and Dirichlet boundary problem in two dimensions (see, e.g., Refs. 8, 9, and 15, and references therein).

In the present paper, we consider a new connection with the theory of quantum integrable systems. To be more precise, we study an integrable generalization of the Laplacian growth, when the boundary is driven by a field satisfying an elliptic PDE, that is not generally reduced to a Beltrami-Laplace equation ("non-Laplacian" growth). To be specific, we use the porous medium fluid dynamics interpretation.

We find variable-coefficient elliptic PDEs for which the boundary dynamics can be described explicitly and the moving fluid occupies evolving algebraic domains (see the following). These, turn out to be PDEs of the Calogero-Moser type, related to finite reflection (Coxeter) groups as well as their integrable deformations (see Secs. VII–IX), that possibly complete the list of all second-order PDEs connected with the algebraic domains (our main conjecture).

In this section we set the problem in terms of the porous medium fluid dynamics. Formulation of the problem in terms of quadrature domains is given in the next section.

Consider a flow of an incompressible liquid in a thin nonplanar layer of nonhomogeneous porous medium. The layer can be viewed as a two-dimensional surface embedded in the three-dimensional Euclidean space. We let the layer curvature, permeability, porosity, and thickness depend on the surface spatial coordinates x,y. We can choose x,y such that locally

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$$dl^2 = G(x,y)(dx^2 + dy^2),$$

where dl is the surface length element. The surface area element is $d\Sigma = G dx dy$, and the volume of the liquid that can be absorbed in the range $x+dx, y+dy$ equals

$$dV = \eta h d\Sigma = \eta h G dx dy,$$

where $\eta = \eta(x,y), h = h(x,y)$ are the medium porosity and the layer thickness, respectively.

In the porous medium, the flow velocity $v = (dx/dt, dy/dt)$ is proportional to the gradient $\nabla = (\partial/\partial x, \partial/\partial y)$ of the pressure P,

$$v = -\frac{\kappa}{\sqrt{G}} \nabla P,$$

where $\kappa = \kappa(x,y)$ is the medium permeability.

It is seen from the above that only the two combinations of variable coefficients, namely

$$\eta h G, \quad \frac{\kappa}{\sqrt{G}}$$

enter the flow equation of motion, and it is convenient to absorb h and G into definitions of the other coefficients. Therefore, without loss of generality, we can consider the flow in the plane parametrized by the complex coordinates $z = x+iy, \bar{z} = x-iy$, choosing η and κ to depend on $z, \bar{z}$ and setting remaining coefficients to unity. The liquid volume conservation leads to the continuity equation

$$(\nabla \cdot \eta v) = 0, \tag{1}$$

while the dynamical law of motion rewrites as

$$v = -\kappa \nabla P. \tag{2}$$

We consider a situation where the liquid occupies bounded, simply connected open region Ω of the plane, whose time evolution $\Omega = \Omega(t)$ is induced by the flow.

At fixed time t, the pressure is constant along the boundary

$$P(\partial\Omega(t)) = P_0(t). \tag{3}$$

Note that dynamics of simply connected domains is independent of $P_0(t)$, and the latter is often set to zero.

The normal velocity of the boundary v_n and that of the flow coincide at $\partial\Omega$,

$$v_n = n \cdot v \quad \text{if } z \in \partial\Omega. \tag{4}$$

The flow is singularity driven. For instance

$$P \to \frac{-q(t)}{2\kappa(z_1,\bar{z}_1)\eta(z_1,\bar{z}_1)} \log|z - z_1| + \sum_{j=1}^{k} \left(\frac{\mu_j(t)}{(z-z_1)^j} + \frac{\bar{\mu}_j(t)}{(\bar{z}-\bar{z}_1)^j} \right) \quad \text{as } z \to z_1, \tag{5}$$

when a multipole source of order $k+1$ is located at $z = z_1$. Equations (1)–(5) constitute the free boundary problem where the evolution of the boundary $\partial\Omega(t)$ is completely determined by the initial condition $\partial\Omega(0)$ and strengths $q(t) = \bar{q}(t), \mu_j(t), \bar{\mu}_j(t), j = 1, \ldots, k$ as well as position z_1 of the sources.

II. CONSERVATION LAWS AND QUADRATURE DOMAINS

From (1), (2), (5) it follows that the pressure satisfies the elliptic PDE

$$\nabla \kappa \eta \nabla P = -\pi \hat{q}[\delta(x-x_1)\delta(y-y_1)], \tag{6}$$

where $\hat{q}=\hat{q}(t)$ is the differential operator of order k,

$$\hat{q} = q(t) + \sum_{j=1}^{k} (-1)^j \left(q_j(t) \frac{\partial^j}{\partial z^j} + \bar{q}_j(t) \frac{\partial^j}{\partial \bar{z}^j} \right), \quad \bar{q} = q. \tag{7}$$

Let $\phi(z,\bar{z})$ be a time-independent function satisfying

$$\nabla \kappa \eta \nabla \phi = 0, \quad z \in \Omega \tag{8}$$

in the whole region Ω, including point $z=z_1$.

Let us now estimate the time derivatives of the following quantities:

$$M[\phi] = \int_{\Omega(t)} \eta \phi \mathrm{d}x\mathrm{d}y.$$

Considering an infinitesimal variation of the fluid domain $\Omega(t) \to \Omega(t+dt)$, we get

$$\frac{\mathrm{d}M[\phi]}{\mathrm{d}t} = \oint_{\partial\Omega(t)} v_n \eta \phi \mathrm{d}l,$$

where $\mathrm{d}l$ is the boundary arclength. From (2), (2), (4) it follows

$$\frac{\mathrm{d}M[\phi]}{\mathrm{d}t} = \oint_{\partial\Omega(t)} (P\kappa\eta\nabla\phi - \phi\kappa\eta\nabla P)\cdot n dl.$$

Applying the Stokes theorem and remembering that P and ϕ satisfy (6), (8), we obtain

$$\frac{\mathrm{d}M[\phi]}{dt} = \pi \hat{q}^*[\phi](z_1,\bar{z}_1), \quad \hat{q}^* = q(t) + \sum_{j=1}^{k} \left(q_j(t) \frac{\partial^j}{\partial z^j} + \bar{q}_j(t) \frac{\partial^j}{\partial \bar{z}^j} \right). \tag{9}$$

Note that mixed derivatives are absent in $\hat{q}$ [cf. (7)], for by (8), $\partial^2\phi/\partial z\,\partial\bar{z}$ is expressed through first derivatives of ϕ. $\bar{q}_j$ is the complex conjugate of q_j, since both $\phi(z,\bar{z})$ and $\bar{\phi}(\bar{z},z)$ satisfy (8).

It follows that $M[\phi]$ is conserved for any solution of (8), such that $\hat{q}^*[\phi](z_1,\bar{z}_1)=0$.

The conservation laws have been first obtained for the homogeneous medium flows in Ref. 12, the variable-coefficient generalization seems to have been first presented in Ref. 7. A wider class of conservation laws was considered in Ref. 10.

The flow in the homogeneous medium

$$\kappa = 1, \quad \eta = 1 \tag{10}$$

is the simplest example, where the conservation laws can be written down explicitly.[12] In this example, any (anti)analytic in Ω function satisfies (8),

$$\phi(z,\bar{z}) = f(z) + g(\bar{z}), \quad \text{for } \kappa = 1, \quad \eta = 1, \tag{11}$$

where f,g are univalent in Ω and the quantities

$$\int_{\Omega(t)} (f(z)(z-z_1)^k + g(\bar{z})(\bar{z}-\bar{z}_1)^k)\mathrm{d}x\mathrm{d}y$$

are integrals of motion for the free-boundary flows driven by a multipole source of order $k+1$ located at $z=z_1$ in homogeneous medium.

Returning to the general case, we integrate (9)

$$M[\phi](t) = M[\phi](0) + \pi\hat{Q}[\phi](z_1,\bar{z}_1),$$

where

$$\hat{Q} = \int_0^t \hat{q}^*(t')\mathrm{d}t' = Q + \sum_{j=1}^{k}\left(Q_j\frac{\partial^j}{\partial z^j} + \bar{Q}_j\frac{\partial^j}{\partial \bar{z}^j}\right). \tag{12}$$

Therefore, $M[\phi](t)$ and, consequently, form of the domain, does not depend on the history of the sources and is a function of "multipole fluxes"

$$Q = \int_0^t q(t')\mathrm{d}t', \quad Q_j = \int_0^t q_j(t')\mathrm{d}t', \quad \bar{Q}_j = \int_0^t \bar{q}_j(t')\mathrm{d}t', \; j = 1, \ldots, k$$

injected by time t.

Now consider the special case when $M[\phi](0)=0$ that describes the injection of the fluid to an initially empty medium. In such a case

$$\int_\Omega \eta(z,\bar{z})\phi(z,\bar{z})\mathrm{d}x\mathrm{d}y = \pi\hat{Q}[\phi](z_1,\bar{z}_1). \tag{13}$$

Equation (13) is a generalization of quadrature identities (those expressing integrals over Ω through evaluation of integrands and a finite number of their derivatives at a finite number of points inside Ω) appearing in the theory of harmonic functions[13] to the case of elliptic equations with variable coefficients. Special domains for which the quadrature identities hold are called quadrature domains in the theory of harmonic functions. We extend this definition to solutions of any elliptic PDE with regular in Ω coefficients.

To construct quadrature domains (or equivalently domains resulted from injection of fluid into an initially empty medium), one needs an explicit form of a general solution of (8). Such explicit solutions are available for a class of the second-order differential equations that are related to the Schrödinger operators of integrable systems on the plane. We, however, postpone construction of these solution to Sec. IV and present our main result in the next section.

III. THE MAIN RESULT

Let us start with the simplest possible example, where the liquid is injected into initially empty homogeneous porous medium through the single monopole source at $z=z_1=x_1+iy_1$. By symmetry, the solution is a circular disc of the radius $r(t)$, centered at $z=z_1$,

$$|z-z_1| < r(t). \tag{14}$$

The pressure satisfies

$$\Delta P = -\pi\tilde{q}(t)\delta(x-x_1)\delta(y-y_1),$$

where the source strength and the total flux are

$$\tilde{q}(t) = \frac{\mathrm{d}r(t)^2}{\mathrm{d}t}, \quad \tilde{Q} = r^2,$$

respectively.

The remarkable fact is that the variable-coefficient problem for a medium with constant porosity and permeability that varies as an inverse square of one Cartesian coordinate

$$\kappa = \frac{1}{x^2}, \quad \eta = 1 \tag{15}$$

admits the same circular solution (14) if the flow is driven by a combination of the same monopole source of strength $q=\tilde{q}(t)$ and a dipole source of strength $q_1=-\tilde{q}\tilde{Q}/2x_1$, both located at the point $z=z_1$,

$$\nabla \frac{1}{x^2} \nabla P = -\pi \hat{q}[\delta(x-x_1)\delta(y-y_1)], \quad \hat{q} = \frac{\mathrm{d}r^2}{\mathrm{d}t}\left(1 - \frac{r^2}{2x_1}\frac{\partial}{\partial x}\right). \tag{16}$$

Indeed, it is not difficult to check that

$$P = r\frac{\mathrm{d}r}{\mathrm{d}t}\left((2x_1x + \rho^2 + r^2)\log\rho - \frac{r^2x(x-x_1)}{\rho^2} - \rho^2 + x(x-x_1) - (2x_1x+\rho^2)\log(r)\right), \tag{17}$$

where $\rho=|z-z_1|$, satisfies (16), and the boundary conditions (2), (15),

$$\frac{\mathrm{d}r}{\mathrm{d}t} = -\frac{1}{x^2}\left(\frac{\partial P}{\partial n}\right)_{\rho=r},$$

as well as (6) holds at the disc boundary.

Also the following quadrature identity holds:

$$\int_{|z-z_1|<r} \phi \mathrm{d}x\mathrm{d}y = \pi r^2 \phi(z_1,\bar{z}_1) + \frac{\pi r^4}{4x_1}\left(\frac{\partial \phi}{\partial x}\right)_{z=z_1},$$

which is a simplest nontrivial generalization of the mean value theorem for harmonic functions to the case of regular in (14) solutions of the elliptic PDE

$$\nabla \frac{1}{x^2} \nabla \phi = 0.$$

The above example is a special case of the main result presented in the following.

Let $\Omega(t)$ be a domain, resulted from the injection of the fluxes $\tilde{Q},\tilde{Q}_j, j=1,\ldots,\tilde{k}$ into a homogeneous medium through a multipole source of order $\tilde{k}+1$ located at $z=z_1$. Then the same domain can be formed by an injection of a special combination of fluxes $Q,Q_j, j=1,\ldots,k$ through a multipole source of order $k+1$, where $k=(\tilde{k}+1)(s(n+l)+1)-1$ located at $z=z_1$ into an initially empty nonhomogeneous medium with permeability

$$\kappa = \frac{1}{(z^s+\bar{z}^s)^{2n}(z^s-\bar{z}^s)^{2l}}, \quad n > l \geqslant 0, \quad s > 0, \quad \eta = 1 \tag{18}$$

and constant porosity, where s,n,l are integers.

In more details, the multipole fluxes of nonhomogeneous medium problem must be fixed functions of fluxes of its homogeneous medium counterpart

$$Q=\tilde{Q},\quad Q_j=Q_j(\tilde{Q},\tilde{Q}_1,\ldots,\tilde{Q}_{\tilde{k}},\bar{\tilde{Q}}_1,\ldots,\bar{\tilde{Q}}_{\tilde{k}},z_1,\bar{z}_1),\quad j=1\ldots(\tilde{k}+1)(s(n+l)+1)-1.$$

For instance, in the above example of circular $\tilde{k}=0$ solution in a medium with permeability (15) [that is the special case $n=1,l=0,s=1$ of (18)]

$$k=(0+1)(1(1+0)+1)-1=1,\quad Q=\tilde{Q},\quad Q_1=\frac{\tilde{Q}^2}{4x_1}.$$

Note that (18) can be rewritten in the form

$$\kappa=\frac{1}{\zeta(x,y)^2},\quad \zeta(x,y)=\prod_{\alpha\in\mathcal{R}_+}(\alpha\cdot z)^{m_\alpha},\quad (a\cdot b):=\mathrm{Re}(\bar{a}b),$$

where $\mathcal{R}=\{\alpha\}$ is a set of root vectors of a finite reflection (Coxeter) group on the plane (Dihedral group). $\mathcal{R}$ is invariant under reflections

$$z\to z-2\frac{(\alpha\cdot z)}{(\alpha\cdot\alpha)}\alpha$$

in a mirror (line), normal to any root vector $\alpha\in\mathcal{R}$, and $\mathcal{R}_+$ denotes "positive" subset of $\mathcal{R}$, containing a half of all root vectors [i.e., $\mathcal{R}=(-\mathcal{R}_+)\cup\mathcal{R}_+$]. The multiplicities m_α must be non-negative integers that are functions on the group orbits. If $l=0$, the reflection group has one orbit and $m_\alpha=n$. Otherwise, the group has two orbits and multiplicities m_α take values n and l on each orbit respectively. The permeability (18) is therefore an invariant of the group of symmetries of a regular $4s$-polygon ($2s$-polygon if $l=0$) and its singular locus [i.e., union of all points z, such that $1/\kappa(z,\bar{z})=0$] coincides with the union of mirrors.

The pressure satisfies the elliptic PDE

$$\nabla\zeta(x,y)^{-2}\nabla P=\zeta(x,y)^{-1}H\zeta(x,y)^{-1}P=-\pi\hat{q}[\delta(x-x_k)\delta(y-y_k)]$$

$$\mathrm{order}(\hat{q})=(\tilde{k}+1)(\deg(\zeta(x,y))+1)-1=(\tilde{k}+1)\left(1+\sum_{\alpha\in\mathcal{R}_+}m_\alpha\right)-1,$$

where H is the Schrödinger operator of the Calogero-Moser system related to the dihedral group[3,6,11]

$$H=\Delta-\sum_{\alpha\in\mathcal{R}_+}(\alpha\cdot\alpha)\frac{m_\alpha(m_\alpha+1)}{(\alpha\cdot z)^2}.$$

Also, regular in Ω solutions $\phi(z,\bar{z})$ of the elliptic PDEs $\nabla\zeta(x,y)^{-2}\nabla\phi=0$ satisfy the quadrature identities

$$\int_\Omega\phi dxdy=\hat{Q}[\phi](z_1,\bar{z}_1),\quad \mathrm{order}(\hat{Q})=(\tilde{k}+1)(\deg(\zeta(x,y))+1)-1$$

that are generalization of the mean value theorem for harmonic functions to the case of solutions of the variable-coefficient elliptic PDEs in (generally) non-circular domains.

Before proving the main result we need to construct a complete set of solutions to (8) for the medium with κ,η given by (18).

IV. NONHOMOGENEOUS POROUS MEDIUM FLOWS AND INTEGRABLE SYSTEMS RELATED TO THE FINITE REFLECTION GROUPS

In this section we show how to obtain a general solution $\phi(z,\bar{z})$ to (8), (18). It is instructive to consider the special case $s=1,l=0$ of (18)

$$\kappa = \frac{1}{x^{2n}}, \quad \eta = 1, \tag{19}$$

when permeability depends on one Cartesian coordinate only. Construction of solutions in the general case (18) is conceptually similar.

Consider the simplest nontrivial example $n=1$ in (19) and start with factorizing the differential operator ∂_x^2 as

$$\frac{\partial^2}{\partial x^2} = \left(\frac{1}{x}\frac{\partial}{\partial x}\right)\left(x\frac{\partial}{\partial x} - 1\right).$$

By associativity of differential operators

$$\left(x\frac{\partial}{\partial x} - 1\right)\underbrace{\left(\frac{1}{x}\frac{\partial}{\partial x}\right)\left(x\frac{\partial}{\partial x} - 1\right)}_{\partial_x^2} = \underbrace{\left(x\frac{\partial}{\partial x} - 1\right)\left(\frac{1}{x}\frac{\partial}{\partial x}\right)}_{x^2\partial_x\frac{1}{x^2}\partial_x}\left(x\frac{\partial}{\partial x} - 1\right).$$

Therefore,

$$T_1\Delta = L_1T_1, \quad T_1 = x\frac{\partial}{\partial x} - 1, \quad L_1 = x^2\,\nabla\,\frac{1}{x^2}\nabla \tag{20}$$

and the elliptic equation (8) is nontrivially related to the Laplace equation when $\kappa\eta = 1/x^2$. In general, the identity

$$T\Delta = LT$$

that relates two differential operators (e.g., Δ and L above) through a differential operator T is called an intertwining identity and T is an intertwining operator.

A differential operator that is related to Δ through the intertwining identity equals, modulo a gauge transformation, a Schrödinger operators of an integrable system. Indeed,

$$T(\Delta - \lambda) = (L - \lambda)T$$

and when ν is an eigenfunction of Δ with the eigenvalue λ, $T[\nu]$ is an eigenfunction of L with the same eigenvalue or zero.

The factorization approach leading to the simplest nontrivial intertwining identity (20) can be now applied to L_1, etc. By induction we get the intertwining identity for an arbitrary nonnegative integer n in (19),

$$T_n\Delta = L_nT_n, \quad L_n = x^{2n}\,\nabla\,\frac{1}{x^{2n}}\,\nabla\,, \tag{21}$$

where

$$T_n = x^n\left(\frac{\partial}{\partial x} - \frac{n}{x}\right)\left(\frac{\partial}{\partial x} - \frac{n-1}{x}\right)\cdots\left(\frac{\partial}{\partial x} - \frac{1}{x}\right) = \sum_{i=0}^{n} a_{i;n}x^i\frac{\partial^i}{\partial x^i}. \tag{22}$$

Any solution ϕ to (8), (19) in Ω can be represented in the form

$$\phi = T_n[f], \quad \Delta f = 0, \quad z \in \Omega. \tag{23}$$

Let us show this for $n=1$, where T_1 is given by (20). Introduce f satisfying

$$x\frac{\partial f}{\partial x} - f = \phi,$$

where $L_1[\phi]=0$ in Ω and $\phi=0$ for $z \notin \Omega$. It is not difficult to see that

$$f(z,\bar{z}) = x\int_{-\infty}^{x} \frac{\phi(x'+iy,x'-iy)}{(x')^2}\mathrm{d}x' + xF(y),$$

where $F(y)$ is an arbitrary regular function of y. Therefore, for any ϕ regular in Ω (which is the case) there exists a regular in Ω function f, such that $T_1[f]=\phi$. From the intertwining identity (20) it follows that $T_1\Delta f=0$ and $\Delta f \in \mathrm{Ker}(T_1)$, if $z \in \Omega$, i.e.,

$$\Delta[f] = xC(y), \quad z = x+iy \in \Omega,$$

where $C(y)$ is an arbitrary function of y. It follows that

$$\Delta[f+xF(y)] = 0, \quad \frac{\mathrm{d}^2F(y)}{\mathrm{d}y^2} = C(y).$$

Since f is defined modulo $xF(y)$, we can set $F=0$ and any solution of $L_1[\phi]=0$ can be represented as $\phi=T_1[f]$, where $\Delta[f]=0$. Similar proof applies to the arbitrary n case (23).

In the general case (18)

$$T_{n,l;s}\Delta = L_{n,l;s}T_{n,l;s}, \quad L_{n,l;s} = (z^s+\bar{z}^s)^{2n}(z^s-\bar{z}^s)^{2l}\,\nabla\,\frac{1}{(z^s+\bar{z}^s)^{2n}(z^s-\bar{z}^s)^{2l}}\,\nabla\,,$$

where the intertwining operator can be expressed in the form of a Wronskian[3]

$$T_{n,l;s}[f] = \rho^{s(n+l)}\frac{W[\sin(\theta_1),\sin(\theta_2),\ldots,\sin(\theta_n),f]}{\cos(s\theta)^{n(n-1)/2}\sin(s\theta)^{l(l-1)/2}}, \quad W[f_1,\ldots,f_k] := \det\left[\frac{\partial^{j-1}f_i}{\partial\theta^{j-1}}\right]_{1\leqslant i,j\leqslant k} \tag{24}$$

with

$$z=\rho e^{i\theta}, \quad \theta_k = \begin{cases} k\left(s\theta+\dfrac{\pi}{2}\right), & k=1,2,\ldots n-l \\ (2k+l-n)\left(s\theta+\dfrac{\pi}{2}\right), & n-l<k\leqslant n \end{cases}.$$

It is important that the intertwining operator $T_{n,l;s}$ is a homogeneous differential polynomial in $z,\bar{z},\partial_z,\partial_{\bar{z}}$. This fact allows one to construct the quadrature domains for solutions ϕ of $L_{n,l;s}[\phi]=0$.

Note that, in general, there exist several independent operators intertwining Δ and another second-order differential operator (forming a linear space of intertwining operators). For instance, T_n in (21) that intertwines Δ with $L_n=L_{n,0;1}$ is not the special case $T_{n,0;1}$ of (24). However, any nonzero linear combination of them can be used to obtain solutions to the corresponding elliptic equations $L_{n,0;1}[\phi]=0$.

V. PROOF OF THE MAIN RESULT

The zero-initial condition solution of the homogeneous-porous medium flow that is driven by a multipole source of order $\tilde{k}+1$ is described by the polynomial conformal map of degree $\tilde{k}+1$ from the unit disc in the parametric $|w|$-plane into the fluid region Ω,

$$z(w) = z_1 + rw + \sum_{i=1}^{\tilde{k}} u_i w^{i+1}, \quad |w| < 1. \tag{25}$$

The map is analytic in $|w|<1$, and the unit circle $|w|=1$ is mapped to the boundary $\partial\Omega$. As shown above such regions are also quadrature domains. They are special (polynomial) cases of (rational) algebraic domains.[14] The map coefficients $r, u_i, i=1,\ldots,\tilde{k}$ are functions of $\tilde{Q}, \tilde{Q}_i, \bar{\tilde{Q}}_i, i=1,\ldots,\tilde{k}$. The "conformal radius" r can be chosen to be real.

The main idea of the proof is to show that the quadrature identity (13) for solutions of (8), (18) holds in domains defined by (25).

Consider illustrative examples of the problem (19) with permeability changing in one direction. As shown in the previous section any solution of the elliptic equation $L_n[\phi]=0$ can be represented as

$$T_n[f(z) + g(\bar{z})], \tag{26}$$

where $f(z), g(\bar{z})$ are holomorphic and anti-holomorphic, respectively.

According to (13) we have to show that

$$\int_\Omega T_n[f(z)]\mathrm{d}x\mathrm{d}y = \pi\hat{Q}T_n[f(z)]_{z=z_1}$$

holds for any analytic in Ω function $f(z)$ when Ω is defined by the conformal map (25). Using the Green theorem and taking (22) into account we rewrite the last equation as

$$\sum_{j=0}^{n} \frac{a_{j;n}}{2^j(j+1)} \frac{1}{2\pi i} \oint_{\partial\Omega} (z+\bar{z})^{j+1} \frac{\partial^j f(z)}{\partial z^j} \mathrm{d}z = \hat{Q}T_n[f(z)]_{z=z_1}. \tag{27}$$

Since $\bar{w}=1/w$ if $|w|=1$, $\bar{z}(\bar{w})=\bar{z}(1/w)$ along the boundary, we can rewrite the left-hand side of the last equation as

$$\sum_{j=0}^{n} \frac{a_{j;n}}{2^j(j+1)} \frac{1}{2\pi i} \oint_{|w|=1} \left((z(w)+\bar{z}(1/w))^{j+1} \left(\frac{1}{\frac{\partial z(w)}{\partial w}} \frac{\partial}{\partial w} \right)^j [f(z(w))] \right) \frac{\partial z(w)}{\partial w} \mathrm{d}w.$$

Since $z(w)$ is analytic in $|w|<1$, $\bar{z}(1/w)$ has poles only at $w=0$, and the above integral is a pure sum of residues

$$\sum_{j=0}^{(\tilde{k}+2)(n+1)-2} V_j \left(\frac{\partial^j f(z)}{\partial z^j} \right)_{z=z_1}, \tag{28}$$

where $V_j, j=0\ldots(\tilde{k}+2)(n+1)-2$ are functions of the parameters $z_1, \bar{z}_1, r, u_j, \bar{u}_j, j=1\ldots\tilde{k}$ of the conformal map (25). Equating it with the right-hand side of (27), we see that $\hat{Q}_k$ must be (differential operators) of order $(\tilde{k}+1)(n+1)-1$ and

$$\hat{Q}T_n[f(z)]_{z=z_1} = \sum_{j=0}^{(\tilde{k}+2)(n+1)-2} U_j \left(\frac{\partial^j f(z)}{\partial z^j} \right)_{z=z_1}, \tag{29}$$

where $U_j, j=0\ldots(\tilde{k}+2)(n+1)-2$ are linear functions of $Q, Q_j, \bar{Q}_j, j=1\ldots(\tilde{k}+1)(n+1)-1$. Therefore, the quadrature identity (27) is satisfied if the following system of $2(\tilde{k}+2)(n+1)-1$ linear equations

$$V_j - U_j = 0, \quad \bar{V}_j - \bar{U}_j = 0, \quad j = 0 \ldots (\tilde{k}+2)(n+1) - 2 \tag{30}$$

for $2(\tilde{k}+1)(n+1)$ unknowns

$$Q, \bar{Q}, Q_j, \bar{Q}_j, \quad j = 1 \ldots (\tilde{k}+1)(n+1) - 1 \tag{31}$$

has solutions.

Note that the condition $\bar{Q}=Q$ is satisfied automatically, since, as is easily seen from (27), (25), (12), the $j=0$ subset of (30)

$$V_0 - U_0 = 0, \quad \bar{V}_0 - \bar{U}_0 = 0$$

are equations for $Q, \bar{Q}$ that have the same form for any $n \geqslant 0$ in (22). They have real solution

$$Q = \tilde{Q} = r^2 + \sum_{i=1}^{\tilde{k}} (i+1) u_i \bar{u}_i.$$

The number of equations in (30) exceeds the number of unknowns (31) by $2n$ and the system of equations (30) is overdermined for the nonhomogeneous medium problem $n > 0$.

For instance, for the circular domain $\tilde{k}=0$,

$$z(w) = z_1 + rw$$

in a medium with permeability $1/x^2$, that has been considered in Sec. III, the system of equations (30) consists of six equations

$$\begin{aligned}
&Q - r^2 = 0, \quad \bar{Q} - r^2 = 0, \\
&2Qx_1 - Q_1 + \bar{Q}_1 - 2x_1 r^2 = 0, \quad 2\bar{Q}x_1 - \bar{Q}_1 + Q_1 - 2x_1 r^2 = 0, \\
&4Q_1 x_1 - r^4 = 0, \quad 4\bar{Q}_1 x_1 - r^4 = 0
\end{aligned}$$

for four unknowns $Q, \bar{Q}, Q_1, \bar{Q}_1$. It has the following solution:

$$Q = \bar{Q} = r^2, \quad Q_1 = \bar{Q}_1 = r^4/4x_1.$$

Returning to the general case, we are going to show that not all equations in (30) are independent, the system is compatible and has a unique solution, which proves our main result.

To prove the compatibility, we introduce the basis

$$\phi_j(z,\bar{z}) = c_j T_n[(z-z_1)^{j+n}], \quad \bar{\phi}_j(\bar{z},z) = c_j T_n[(\bar{z}-\bar{z}_1)^{j+n}], \quad j = 0,1,2, \ldots, \tag{32}$$

where $c_j = j!/(j+n)!\, x_1^n$, in the space of solutions $\phi(z,\bar{z})$ of $L_n[\phi]=0$ that are regular in neighborhood of $z=z_1$, and then show that the quadrature identity (13) holds for any element of this basis.

Indeed, according to (22), (32) is a set of solutions of $L_n[\phi]=0$ that continuously tends to the basis of functions analytic in a neighborhood of $z=z_1$,

$$\phi_j(z,\bar{z}) \to (z-z_1)^j, \quad j = 0,1,2, \ldots, \quad x_1 \to \infty$$

as the position of the source $z_1 = x_1 + iy_1$ goes to infinity. On the other hand, $L_n[\phi(z,\bar{z})]=0, z \in \Omega$ continuously tends to the Laplace equation when region Ω is moved to infinity. Therefore, set (32) is homotopically equivalent to $(z-z_1)^j, (\bar{z}-\bar{z}_1)^j, j=0,1,2,\ldots$ under a continuous deformation of the Laplace operator and thus contains a basis of solutions of $L_n[\phi]=0$ that is regular in a neighborhood of $z=z_1$.

It then follows from (28) and (29) that the quadrature identity holds if

$$(V_j - U_j)\left(\frac{d^j f(z)}{dz^j}\right)_{z=z_1} = 0, \quad (\bar{V}_j - \bar{U}_j)\left(\frac{d^j f(\bar{z})}{d\bar{z}^j}\right)_{z=z_1} = 0, \quad j = 0 \ldots (\tilde{k}+2)(n+1) - 2 \tag{33}$$

for

$$f(z) \in \{(z - z_1)^j, j \geqslant n\}.$$

Since $j \geqslant n$, the left-hand sides of the first n equations in (33) vanish, and there remains $2(\tilde{k}+1) \times (n+1)$ independent equations and the equal number of unknowns (31).

We now have to prove the compatibility of remaining equations. (30) is a nonhomogeneous system of linear equations for unknowns $Q, \bar{Q}, Q_j, \bar{Q}_j, j = 1 \ldots (\tilde{k}+1)(n+1) - 1$, that fixes dependence of these unknowns on parameters $z_1, \bar{z}_1, r, u_1, \ldots, u_{\tilde{k}}, \bar{u}_1, \ldots, \bar{u}_{\tilde{k}}$. The system is compatible if its homogeneous part does not have nontrivial solutions. Let us suppose that it does. Recall that the homogeneous part of the system has been obtained by action of the operator $\hat{Q}$ to an arbitrary solution of $L_n[\phi] = 0$ at point $z = z_1$. So, if the homogeneous part of the system had nontrivial solutions, then operator $\hat{Q}$ would annihilate any solution ϕ of $L_n[\phi] = 0$ at $z = z_1$, i.e.,

$$\hat{Q} T_n[f(z)] = 0 \quad \text{at } z = z_1, \tag{34}$$

where $f(z)$ is any analytic in Ω function. If the above were true, then changing continuously the position $z = z_1$ of the source, we could construct such operator $\hat{Q}$, with coefficients depending on z, that $\hat{Q} T_n[f(z)] = 0$ in some region of the plane for an arbitrary $f(z)$. But this is evidently impossible, since the highest symbols of $\hat{Q}$ and T_n contain pure derivatives in z, so does their composition.

Therefore, (30) has a unique solution and quadrature identity holds in the polynomial algebraic domains, that leads to our main result (see Sec. III).

Similar result can be analogously proved for the general system with permeability given by (18).

VI. GENERALIZATION TO HIGHER DIMENSIONS

Our study can be extended to PDEs in more than two dimensions, since the derivation of the conservation laws in Sec. II is not restricted to the two-dimensional flows.

For instance, if we take solution $\phi(\xi)$ of $\nabla \xi_1^{-2} \nabla \phi = 0$, where $\xi := (\xi_1, \ldots, \xi_d)$ and $\nabla := (\partial/\partial\xi_1, \ldots, \partial/\partial\xi_d)$, then the following quadrature identity holds:

$$\int_{|\xi - \xi'| < r} \phi(\xi) \mathrm{d}\xi_1 \ldots \mathrm{d}\xi_d = v_d \left(\phi(\xi) + \frac{r^2}{(d+2)\xi_1} \frac{\partial \phi(\xi)}{\partial \xi_1} \right)_{\xi = \xi'} \tag{35}$$

in the d-dimensional ball of radius r with center at $\xi = \xi'$, where $v_d = \int_{|\xi - \xi'| < r} \mathrm{d}\xi_1 \ldots \mathrm{d}\xi_d$ is the volume of the ball. Since the Hadamard expansion of the fundamental solution of the Calogero-Moser type operators truncates (see, e.g., Refs. 4 and 6), the pressure distribution in the corresponding free-boundary flow can be written down explicitly for any d [e.g., we have used the technique of Ref. 4 for derivation of (17)].

VII. GENERALIZATIONS TO NON-COXETER ARRANGEMENTS

According to works on algebraic integrability,[6] it is likely that the second-order elliptic operators related to the Coxeter root systems as well as their special deformations exhaust all possible operators that can be related to the Laplace operators through intertwining operators with rational coefficients. These are elliptic operators for which a rational Baker-Akhieser function exists. We call all such operators the algebraic Calogero-Moser operators. For instance, the algebraic Calogero-Moser equations[6] related to the porous medium problems (8) with the permeability

$$\kappa = x^{-2m}((2m+1)y^2 - x^2)^{-2}, \quad \eta = 1, \tag{36}$$

where $m=2,3,4,\ldots$, are the simplest examples that extend the main result of the present paper to non-Coxeter arrangements of mirrors.

A more general class of such algebraic Calogero-Moser systems was found in Ref. 3, and it was shown in Ref. 2 that they exhaust all algebraically integrable systems with linear arrangements of mirrors in two dimensions. Such systems are labeled by a sequence of integer positive numbers $0 \leqslant k_1 < k_2 < \ldots < k_n$ and a sequence $\omega_1, \ldots, \omega_n$ of complex parameters ("phases"). The corresponding algebraically integrable elliptic operator is

$$L = \zeta^2 \nabla \zeta^{-2} \nabla \tag{37}$$

where rational function $\zeta = \zeta(x,y)$ is the ratio of Wronskians

$$\zeta(x,y) = \rho^{k_n} \frac{W[\sin(\theta_1), \ldots \sin(\theta_{n-1}), \sin(\theta_n)]}{W[\sin(\theta_1), \ldots \sin(\theta_{n-1})]}, \quad \theta_j = k_j\theta + \omega_j, \quad z = \rho e^{i\theta}. \tag{38}$$

The corresponding intertwining operator is of the order n and can be rewritten in the form of a Wronskian

$$T[f] = \rho^{k_n} \frac{W[\sin(\theta_1), \ldots \sin(\theta_n), f]}{W[\sin(\theta_1), \ldots \sin(\theta_{n-1})]}$$

with (24) being a special case. The results of the present paper, e.g., algebraicity of quadrature domains, etc., also hold for systems with

$$\kappa = 1/\zeta(x,y)^2, \quad \eta = 1$$

where ζ is given by (38), with such $k_1, \ldots k_n$ and $\omega_1, \ldots \omega_n$ that the Wronskian in the denominator of (38) divides that in the numerator and ζ is a polynomial in x, y [these include systems with Coxeter arrangements of mirrors, deformed systems of type (36), and many others]. For these kinds of systems, the intertwining operator has polynomial coefficients and the corresponding Baker-Akhieser function is polynomial in the spectral parameter.

More generally, one can consider a situation where the porosity $\eta(x,y)$ is not constant, and is such that the quadrature identities (13) hold in domains determined by the conformal maps (25) not only when $\zeta(x,y)$ is a polynomial, but also when it is a rational function (38) of x,y. We consider related examples in the next section.

VIII. SYSTEMS WITH AFFINE SINGULAR LOCI

We considered systems with mirrors arranged linearly, i.e., all mirrors passing through the same point (origin). There, however, exist generalizations of the above construction with affine arrangement of mirrors. In the present section we give examples of such systems that are nonhomogeneous in one direction. These are related to rational solutions of the Korteveg-de-Vries equation. The permeability and porosity are expressed in terms of the Adler-Moser[1] polynomials $p_n(x)$ (first introduced by Burcnhall and Chaundy in Ref. 5) as follows:

$$\kappa\eta = \zeta(x)^{-2}, \quad \zeta(x) = \frac{p_n(x)}{p_{n-1}(x)}, \quad \eta = p_{n-1}(x)S(x) \tag{39}$$

where $S(x)$ is an arbitrary polynomial of x. The Adler-Moser polynomial p_n can be represented as the Wronskian

$$p_0 = 1, \quad p_n(x;t_3, \ldots, t_n) = W[\psi_1(x), \psi_2(x), \ldots, \psi_n(x)], \quad \psi_1 = x, \quad \partial_x^2 \psi_n = \psi_{n-1}.$$

The nth Adler-Moser polynomial depends on $n-1$ parameters $t_3, \ldots t_{2n-1}$ [that can be viewed as integration constants for $\psi_k(x), k=2\ldots n$) and is of degree $n(n+1)/2$ in x. $t_3, t_5, \ldots$ are the KdV

hierarchy flow parameters ("times"), while $p_n, n=0,1,2,\ldots$ are τ-functions of the hierarchy. Examples of several first Adler-Moser polynomials are

$$p_0 = 1, \quad p_1 = x, \quad p_2 = x^3 + t_3, \ldots .$$

Elliptic operator (37) is related to the Laplace operator by the intertwining operator that can be written in terms of the Wronskians

$$T[f] = \frac{W[\psi_1, \ldots, \psi_n, f]}{W[\psi_1, \ldots \psi_{n-1}]}.$$

It is a differential operator of order n with rational coefficients.

Note that expression (39) for κ, η is given for generic values of $t_3, t_5, \ldots$, when the greatest common divisor of p_n and p_{n-1} is a constant. For instance, (19), (21) correspond to a special case of Adler-Moser polynomials, when all times $t_{2i-1}, i>1$ are set to zero and $p_n = x^{n(n+1)/2}$ is divisible by $p_{n-1} = x^{n(n-1)/2}$. In this case the intertwining operator has polynomial coefficients and one can choose η to be a constant, rather than a polynomial of nonzero degree in x [cf. (37)].

The quadrature identities (13) hold in algebraic domains determined by (25). In generic case, the order of $\hat{Q}$ in the right-hand side of (13) is

$$\operatorname{order}(\hat{Q}) = \left(\deg(S(x)) + \frac{n(n+1)}{2} + 1 \right) \deg(z(w)) - 1 .$$

For example, in circular domain (14) with $S(x)=1$ and $n=2$ in (39)

$$\int_{|z-z_1|<r} x\phi \mathrm{d}x\mathrm{d}y = \pi \sum_{i=0}^{3} Q_i \left(\frac{\partial^i \phi}{\partial x^i} \right)_{z=z_1}, \tag{40}$$

where ϕ is any solution of

$$\nabla \frac{x^2}{(x^3 + t_3)^2} \nabla \phi = 0$$

regular in (14), and

$$Q_0 = x_1 r^2, \quad Q_1 = \frac{x_1 r^4 (6x_1^2 + r^2)}{8(x_1^3 + t_3)}, \quad Q_2 = \frac{r^6 (16x_1^5 + 16x_1^2 t_3 + r^2 t_3)}{128(x_1^3 + t_3)^2}, \quad Q_3 = \frac{x_1 r^8}{192(t_3 + x_1^3)}.$$

IX. CONCLUSION, MAIN CONJECTURE

In this article we have found examples of nonhomogeneous porous medium flows, driven by multipole source located at a fixed point, whose boundaries obey the same dynamics as those of the homogeneous-medium flows also driven by a multipole source located at the same point. Namely, in the main set of examples, the medium permeability is a homogeneous rational function of x, y, and an invariant of the dihedral group. We also considered examples with permeability that is a homogeneous rational function of x, y, which is not generally dihedral-invariant, as well as examples with affine arrangements of singular loci. For the latter examples, the medium permeability as well as its porosity are nonhomogeneous rational functions of x, y. The multipole fluxes of the nonhomogeneous medium problem must be fixed functions of those of its homogeneous medium counterpart. Related variable-coefficient elliptic PDEs for the pressure distribution are of the algebraic Calogero-Moser type[6] and the quadrature identities for solutions of such equations hold in algebraic domains determined by polynomial conformal maps of unit disc.

In conclusion, one may pose the classification problem: *Find the complete list of all PDEs whose solutions satisfy quadrature identities in polynomial algebraic domains*. In view of the above it is reasonable to expect that it has the following solution:

Conjecture: The algebraic Calogero-Moser equations exhaust, up to a gauge equivalence, all possible second-order elliptic PDEs whose solutions satisfy quadrature identities in polynomial algebraic domains.

As mentioned in Sec. VI, our study can be extended to PDEs in more than two dimensions. Although we cannot use conformal maps to parametrize algebraic domains in higher dimensions, we can still pose the classification problem for domains with spherical boundaries, looking for a complete list of elliptic equations for which generalized mean value theorem holds. More precisely, one can look for equations in d-dimensions whose solutions possess the following property: *There exists such d-dimensional measure that the integral of an arbitrary solution taken over an arbitrary d-dimensional ball equals a linear combination of the value of the solution and those of a finite number of its derivatives at the ball center. Coefficients of the linear combination may depend on the ball position and radius, while the measure is determined by coefficients of the elliptic PDE only*. Typical examples of this property are (35) (where the measure is simply $d\xi_1 \ldots d\xi_d$) and (40) (with measure $x\mathrm{d}x\mathrm{d}y$).

Extending our conjecture to higher dimensions we may expect that algebraic Calogero-Moser equations complete the above list. Note, that our classification problem seems to be equivalent to classical Hadamard's problem of classification of Huygens' operators. As in our case, all known examples of such Huygens' operators are related to algebraic Calogero-Moser systems.[6]

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On scattering trajectories of dynamical systems

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Dynamical systems on $\mathbb{R}^n$ presenting geometric chaos, i.e., open domains where bounded and unbounded orbits are intermingled, have been constructed. The opposite situation (open scattering) has been studied for integrable Hamiltonian and non-Hamiltonian vector fields and for equations of type $\ddot{\mathbf{x}}=-\nabla V(\mathbf{x})$ when the potential has the form $V=a(r)+b(r)F(\theta)$ in spherical coordinates. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2206880]

I. INTRODUCTION

Let $\mathbf{X}$ be a smooth dynamical system on $\mathbb{R}^n$. The solution $\mathbf{x}(\mathbf{x}_0;t)$ through $\mathbf{x}_0$ is called a *scattering orbit* if

$$\lim_{t\to\omega,\omega'} \|\mathbf{x}(\mathbf{x}_0;t)\| = +\infty,$$

$$\omega \in \mathbb{R}^+ \cup \{+\infty\}, \quad \omega' \in \mathbb{R}^- \cup \{-\infty\}, \tag{1}$$

(ω',ω) being the maximal interval around $t_0=0$ on which $\mathbf{x}(\mathbf{x}_0;t)$ is defined.

Orbits of this kind often appear in Mechanics concerning the vector field (vf)

$$\mathbf{X} = (\dot{\mathbf{x}}, -\nabla V(\mathbf{x})),$$

$$\mathbf{x} \in \mathbb{R}^m \tag{2}$$

associated with the Newtonian equation

$$\ddot{\mathbf{x}} = -\nabla V(\mathbf{x}) \tag{3}$$

ruling the motion of a particle in the potential $V(\mathbf{x})$, cf. Ref. 1.

In this paper we study the robustness of scattering trajectories, i.e., if we consider orbits through initial conditions close to $\mathbf{x}_0$, are all these orbits also of scattering type? A negative answer could yield a nonuniform behavior which would make predictability impossible due to the practical small uncertainties in initial conditions. The nonuniformity would be reflected by the existence of bounded solutions arbitrarily near scattering ones.

It is important to note that in this work we are interested in analyzing whether the orbits near a given scattering trajectory are bounded or not. In this sense our approach is closer to the concept of uniform behavior of a dynamical system[2] than to the well-known concept of chaotic scattering.

Recall that, via numerical experiments, it has been suggested that chaotic scattering can appear in vf of type (2) when there exist multiple exit modes for the solutions. Chaotic scattering

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usually refers to the fractality of the boundaries separating the basins of different exits, the appearance of the Wada phenomenon being the most typical situation. There is a vast literature on chaotic scattering, the interested reader can consult, e.g., Refs. 3–8 although we will not focus on this phenomenon.

Although chaotic scattering usually gives rise to complex phase portraits we are not interested in complexity arising from the existence of multiple exit modes but in unpredictability associated with the concept of geometric chaos.[9] We say that there exists *geometric chaos* in $\mathcal{R}$ when the set $\mathcal{K}\subset\mathcal{R}$, $\mathcal{R}$ standing for an open set of $\mathbb{R}^n$, formed by the initial conditions $\mathbf{x}_0$ supporting a scattering solution $\mathbf{x}(\mathbf{x}_0,t)$, and its complement $\mathcal{K}^c$ in $\mathcal{R}$, formed by nonscattering trajectories, are both dense in $\mathcal{R}$. Rigorous mathematical examples of chaotic scattering are given in Sec. II for vf in $\mathbb{R}^n$ with first integrals. As far as we know these are the first examples in the literature of integrable vf presenting geometric chaos.

Conditions in order that geometric chaos does not arise are also given in Sec. II.

We warn the reader that a similar phenomenon (that is, Arnold's diffusion[10]) appears when a completely integrable Hamiltonian system with m $(m>2)$ degrees of freedom is perturbed in the form

$$\mathbf{X}_H \to \mathbf{X}_H + \epsilon \mathbf{X}_{H_1},$$

$$\epsilon \in \mathbb{R};\ \epsilon \neq 0 \text{ and small}. \tag{4}$$

The only difference being that geometric chaos appears without needing to perturb another vf. On the other hand, geometric chaos can appear for $\mathbb{R}^n$ vf for any value of n $(n\geqslant 3)$ while Arnold's diffusion only appears when $n\geqslant 4$ $(n=2m)$. Note also that Arnold's diffusion has been observed, cf. Refs. 11 and 12, in many physical systems: motion of a charge in the focusing magnetic field of an accelerator, motion of electrons in a magnetic bottle, interactions of colliding electron-positrons beams, etc.

The opposite situation to geometric chaos is *open scattering*, in which there exists a neighborhood $\mathcal{N}(\gamma)$ of a scattering trajectory γ such that all the orbits of $\mathbf{X}$ with initial conditions in $\mathcal{N}(\gamma)$ are scattering trajectories. This situation is studied in Sec. III for Liouville integrable systems and for Newtonian vector fields verifying certain assumptions.

It becomes evident that open scattering gives rise to uniformity in the sense that all trajectories near certain scattering trajectory are of scattering type, although the behavior of the system could be nonuniform in the sense of chaotic scattering (but we will not focus here on this issue). Open scattering is desirable from the physical viewpoint because the presence of geometric chaos makes it impossible to predict whether the evolution of an initial condition will remain in some compact set or on the contrary it will tend to infinity. One of the most relevant results that we obtain is that, even when $2n-2$ conserved quantities exist (n is the number of degrees of freedom), geometric chaos may arise, thus extending the results of nonuniformity obtained in Ref. 2. This phenomenon is not as well known as chaotic scattering and hence it complements the literature on chaos in Hamiltonian systems. Furthermore we provide criteria in order to avoid geometric chaos in physically relevant Newtonian systems, thus justifying the interest of our study both in Physics and Applied Mathematics.

II. GEOMETRIC CHAOS

Smooth $\mathbb{R}^3$ vf with a first integral whose level sets are tori are constructed, see Sec. II A, exhibiting geometric chaos over an open domain $\mathcal{R}\subset\mathbb{R}^3$. The set $\mathcal{K}^c$, which is the complement of the set $\mathcal{K}=\cup$ (scattering orbits), is formed by S^1 orbits of $\mathbf{X}$. This construction is generalized to $\mathbb{R}^n$ vf with r $(1\leqslant r\leqslant n-2)$ first integrals whose level sets are diffeomorphic to $(S^1)^{n-r}$. When $\mathbf{X}$ has $n-1$ first integrals it is proved that geometric chaos is not possible.

Examples are also given of $\mathbb{R}^3$ vf with a first integral whose level sets are cylinders, see Sec.

II B, for which geometric chaos is impossible. For $\mathbb{R}^3$ vf with a first integral whose level sets are different from tori or cylinders the discussion of geometric chaos is given at the end of Secs. II A and II B.

A. Geometric chaos in integrable systems

Let $\mathbf{X}$ be any C^∞ vf in $\mathbb{R}^3$ with a differentiable first integral $I(\mathbf{x})$ such that:

$$\begin{aligned} &\text{(a) } I(\mathbf{x}) = I(\mathbf{x}_0) = I_0 \text{ are tori if } \mathbf{x}_0 \notin z-\text{axis}.\\ &\text{(b) The orbits of the vf } \mathbf{X}|_{I=I_0} \text{ are either dense in } I_0 \text{ (irrational orbits) or are,}\\ &\quad \text{all of them, topological circles.}\\ &\text{(c) Both } S^1 \text{ tori (i.e., rational tori) and irrational tori are dense in an open domain.} \end{aligned} \tag{5}$$

A physical example for which these conditions are fulfilled is

$$\mathbf{X} = \mathbf{B} + \partial_\phi, \tag{6}$$

$\mathbf{B}$ standing for the magnetic vf created by a circular wire of center (0, 0, 0) lying on the (x,y) plane,[13] and ∂_ϕ being the vf $-y\partial_x + x\partial_y$ representing rotations around the z axis. It can be proved[13] that the magnetic field has the form $\mathbf{B}=A_1(r,z)\partial_r + A_2(r,z)\partial_z$ in cylindrical coordinates (r,ϕ,z). The orbits of $\mathbf{B}$ on the (r,z) planes consist of the z axis and topological circles around the point of intersection between the wire and these planes. This gives rise to a global first integral $I(r,z)$ on $\mathbb{R}^3$ whose level sets are tori around the circular wire. The frequency of $\mathbf{B}$ on these tori is a nonconstant function $\omega(I)$, and hence the tori on which $\omega(I)/2\pi \in \mathbb{Q}$ are filled by periodic orbits of $\mathbf{X}$, otherwise we have irrational tori. $\mathbf{X}$ becomes globally smooth after multiplication of any function which goes to zero fast enough on the wire.

Note that assumption (4)-(5b) is automatically fulfilled when $\mathbf{X}$ is divergence-free and has no zeros on $\mathcal{R}$.[1]

Consider now the set

$$\mathbb{R}^3 \setminus \mathfrak{s}, \tag{7}$$

$\mathfrak{s}$ being any C^1, properly embedded, unbounded curve starting at (1, 1, 1) and transversal to the level sets of I lying on the domain $\mathcal{R}$ ($\mathcal{R}$ being the complement in $\mathbb{R}^3\setminus$ (z axis) of the domain bounded by the torus $I=I(1,1,1)$). Assume that $\mathfrak{s}$ intersects each level set of I in $\mathcal{R}$ only once.

It can be seen that $\mathbb{R}^3\setminus\mathfrak{s}$ is diffeomorphic to $\mathbb{R}^3$ via a smooth diffeomorphism D. Indeed, consider that $\mathfrak{s}$ is a half straight-line starting at (1, 1, 1) and take a foliation of $\mathbb{R}^3\setminus(1,1,1)$ by spheres S_r of centers (1, 1, 1) and radii $r>0$, becoming topological planes after removing in S_r the point $S_r \cap \mathfrak{s}$.

Now, any torus T ($T \subset \mathcal{R}$) becomes a horned torus after deletion of the point $T \cap \mathfrak{s}$ and the vf $\mathbf{X^D}$ transformed of $\mathbf{X}|_{\mathbb{R}^3\setminus\mathfrak{s}}$ under D is again an $\mathbb{R}^3$ smooth vector field. $\mathbf{X^D}$ exhibits geometric chaos because the horns of $T\setminus(T\cap\mathfrak{s})$ blow-up to infinity under the action of D, while the S^1 orbits on the tori are preserved (except for the S^1 orbits passing through $T\cap\mathfrak{s}$, which are transformed in unbounded orbits of $\mathbf{X^D}$). Dense orbits in tori become scattering dense orbits in the horned tori $D(T\setminus(T\cap\mathfrak{s}))$.

The above conclusion holds for $\mathbb{R}^n$ vf $\mathbf{X}$ ($n>3$) when r C^1 first integrals of $\mathbf{X}$ are given, the (regular) level sets of them are codimension r tori $(S^1)^{n-r}$ and (5b), (5c) hold. The only modification is that (7) becomes

$$\mathbb{R}^n \setminus L_r, \tag{8}$$

L_r being a half-linear space of dimension r ($L_1=\mathfrak{s}$, $L_2=$a half plane,…) transversal to the tori $(S^1)^{n-r}$, which guarantees a unique intersection among each of these tori and L_r. Note that $\mathbb{R}^n\setminus L_r$

is smooth diffeomorphic to $\mathbb{R}^n$ (this follows from a well-known theorem by Stallings[14]). In fact, this diffeomorphism can be taken as a symplectomorphism, ensuring that $\mathbf{X_D}$ remains Hamiltonian if $\mathbf{X}$ is ($n=2m$, the symplectic structure in $\mathbb{R}^{2m}$ possibly being nonglobally equivalent to the standard one[15,16]).

For example, when $n=4$ and $r=2$ (consider an $\mathbb{R}^2$ foliation similar to the one introduced for $n=3$, $r=1$), take $\mathbf{X}$ as the vf associated with the uncoupled differential equations

$$\ddot{x} = -x,$$

$$\ddot{y} = -y^3. \tag{9}$$

The explicit expression of the vf $\mathbf{X^D}$ associated with Eq. (9) can be immediately obtained from the expression of the diffeomorphism D, which in this case is given by

$$D = D_1 \times D_2,$$

$$R^4 \setminus L_2 = (R^2 \setminus L_1)^1 \times (R^2 \setminus L_1)^2,$$

$$D_i = \Psi_i \circ \Phi_i,$$

$$(R^2 \setminus L_1)^i = R^2 \setminus \{x_i \leqslant 0, y_i = 0\},$$

$$i = 1,2, \tag{10}$$

Ψ_i and Φ_i being defined by

$$(r_i, \Theta_i) \in (R^2 \setminus L_1)^i \xrightarrow{\Phi_i} (r_i, \Theta_i/2) \xrightarrow{\Psi_i} (\log x_i, y_i),$$

$$r_i > 0, \quad -\pi < \Theta_i < \pi \tag{11}$$

(r_i, Θ_i) being polar coordinates in the splitted planes $(R^2 \setminus L_1)^i$, around (0, 0) with $(L_1)=\{\Theta_i = \pi\}$.

Note that the effect of Φ_i is that of transforming $(R^2 \setminus L_1)^i$ in the half-plane $x_i > 0$, and the effect of Ψ_i that of transforming this half-plane into $\mathbb{R}^2$.

Once D has been defined, $\mathbf{X^D}$ is obtained by just transforming the $\mathbb{R}^4$ vf $\mathbf{X}$ associated with Eq. (9):

$$\mathbf{X} = (\dot{\mathbf{x}}, -\mathbf{x}, \dot{\mathbf{y}}, -\mathbf{y}^3), \tag{12}$$

under D. This gives rise to a very involved expression for $\mathbf{X^D}$ which for brevity is omitted.

The tori foliating open sets of $\mathbb{R}^4$ are given by

$$(\dot{x}^2/2 + x^2/2 = c_1) \times (\dot{y}^2/2 + y^4/4 = c_2), \tag{13}$$

and $L_r = L_2$ (a half plane in phase-space). Assumptions (5b) and (5c) are satisfied since the ratio of the frequencies of the orbits in the uncoupled equations is a C^ω nonconstant function.

Let us now prove that when $r=n-1$ (i.e., the vector field $\mathbf{X}$ is completely integrable) and the first integrals are independent of ϑ (a periodic orbit of $\mathbf{X}$) then geometric chaos cannot arise. Let $(I_1, \ldots, I_{n-1})$ be the first integrals of $\mathbf{X}$. Indeed let us construct $n-1$ vector fields $\mathbf{S_i}$ in a neighborhood $N(\vartheta)$ of ϑ as

$$\mathbf{S_i} = \sum_{j=1}^{n-1} a_{ij} \nabla I_j \tag{14}$$

such that

$$\mathbf{S_i}(I_j) = \delta_{ij}, \tag{15}$$

δ_{ij} standing for the Kronecker delta. Note that in Eq. (15) $\mathbf{S_i}(I_j)$ denotes the Lie derivative of the function I_j along the streamlines of $\mathbf{S_i}$. Therefore, $\mathbf{S_i}(I_j)=\mathbf{S_i}\cdot\nabla I_j$, the dot standing for the standard Euclidean scalar product in $\mathbb{R}^3$.

The Lie derivative of I_j is, of course, defined by,

$$\mathbf{S_i}(I_j) = \left.\frac{dI_j(\alpha_i(t;\mathbf{x}))}{dt}\right|_{t=0}, \tag{16}$$

$\alpha_i(t;\mathbf{x})$ begin the flow induced by $\mathbf{S_i}$.

It is straightforward to see that the coefficients a_{ij} in (14) are smooth functions and are uniquely defined by Eq. (15) in $N(\vartheta)$. $\mathbf{S_i}$ are obviously [by (15)] $n-1$ independent symmetries of $\mathbf{X}$, thus implying, on account of the compactness of ϑ, that $N(\vartheta)$ is covered by periodic orbits of $\mathbf{X}$. This rules out the existence of geometric chaos. The reader can have a look at Ref. 9 where some criteria for the existence of open scattering in completely integrable vector fields are given.

The generalization of the results of this section to $r<n-1$ first integrals foliating an open subset of $\mathbb{R}^n$ with fiber F ($\dim F=n-r$), $F\neq(S^1)^{n-r}$ is problematic since, except for tori, we are not aware of foliations of open domains of $\mathbb{R}^n$ satisfying assumptions (5b) and (5c).

B. A topological obstruction to the existence of geometric chaos

We now give examples of $\mathbb{R}^3$ analytic vf with a first integral I whose (regular) level sets are cylinders for which geometric chaos is impossible. The analyticity of I is a key property in the construction.

Consider the vf $\mathbf{X}$ defied by

$$\mathbf{X} = \mathbf{X}_2(x,y) + a(x,y,z)\partial_z, \tag{17}$$

$\mathbf{X}_2, a \in C^\omega$, satisfying

$$I = I(x,y), \quad \mathbf{X}(I) = 0,$$

$$I(x,y) = c \text{ are circular cylinders (in } \mathbb{R}^3),$$

$$\text{rank } (\nabla I)|_{(x,y)\neq(0,0)} = 1,$$

$$\text{periods } T(c) \text{ of } \mathbf{X}_2 \text{ on } I=c \text{ cover (as } c \text{ varies in } \mathbb{R}) \text{ an open interval of } \mathbb{R},$$

where $\mathbf{X}(\mathbf{I})$ denotes the Lie derivative of I along the streamlines of $\mathbf{X}$. Calling $(x(t),y(t))$ the periodic solution of $\dot{\mathbf{x}}=\mathbf{X}_2(\mathbf{x})$ with initial condition $(x_0,y_0)\in\mathbb{R}^2$, its period T_0 is an analytic function of $c_0=I(x_0,y_0)$.

We get $z(t)$ along this solution via

$$\frac{\mathrm{d}z}{\mathrm{d}t} = a(x,y,z)|_{(x(t),y(t))} = F_0(t;z), \tag{18}$$

F_0 being C^ω and periodic in t (of period T_0).

Any periodic solution $\mathbf{p}$ of $\mathbf{X}$ lying on the cylinder $I(x,y)=c_0$ satisfies, see Ref. 17,

$$\Pi^n(z;T_0) = z,$$

$$z \in \mathbf{p}; n(z,T_0) \in \mathbb{N}, \tag{19}$$

Π being the Poincaré map

$$\Pi(z;T_0) = \phi(t = T_0; z_0 = z) \tag{20}$$

associated with Eq. (18) and $\phi(t;z_0)$ the general solution of Eq. (18). Remember[17] that Π is an analytic function of z and T_0 (since $\mathbf{X}$ is analytic).

Let $\mathcal{R}$ be an open $\mathbb{R}^3$-domain and assume the existence of a periodic orbit $\Theta(P)$ through a point $P \in \mathcal{R}$ (on the cylinder $I=c_0$). The analyticity of the Poincaré map Π of $\mathbf{X}|_{I=c_0}$ near $\Theta(P)$ implies[17] that in a neighborhood $N(\Theta(P))$ either all the orbits of $\mathbf{X}|_{I=I_0}$ are of type S^1 or none, but $\Theta(P)$, is of type S^1 (limit cycle). In the second case the cylinders $I=c$ (for c running on an interval of $\mathbb{R}$ centered at c_0) would hold a one-parameter family of S^1 orbits of $\mathbf{X}$ (possibly with only one element), whose closure can never be an open subset of $\mathbb{R}^3$.

In the first case (taking into account the topology of $I=c_0$) it follows that the period $n(z,T_0)$ of Π is independent of z and T_0, and is in fact equal to 1. Therefore we get [see Eq. (19)]

$$\Pi(z;T_0) = z,$$

$$\forall T_0 \text{s.t.} N(\Theta(P)) \cap (I = c_0) \text{ is foliated by } S^1 \text{ orbits}. \tag{21}$$

Summarizing, any cylinder $I=c$ on which a S^1 orbit lies is either foliated with S^1 orbits or contains a countable number $m(c)$ of isolated S^1 orbits ($m(c)=0$ not being excluded).

When geometric chaos is present, the closure of the values of T_0 for which Eq. (21) holds must contain an interval J of $\mathbb{R}$. Since $\Pi(z;T_0)-z$ is C^ω, its zeros z_i on J are either a finite set or otherwise $\Pi(z;T_0)-z \equiv 0$ on J, and hence we can write

$$\Pi(z;T_0) \equiv z,$$

$$\forall T_0 \in J, \tag{22}$$

thus implying that the cylinders through $\mathcal{R}$ are foliated by S^1 orbits. Therefore geometric chaos is also impossible. Note that the key points in the proof are the analyticity of $\mathbf{X}$ and that the topology of $I=I_0$ is $S^1 \times \mathbb{R}$, which implies that the period n in Eq. (19) is constant ($n=1$). For example, if $I=I_0$ were a torus $S^1 \times S^1$ the period would not be constant in general and the proof would fail (rational and irrational tori are generally intermingled).

In ending this section let us observe that when the level sets of the first integral of $\mathbf{X}$ are neither tori nor cylinders the problem of knowing whether or not an S^1 orbit of $\mathbf{X}$ belongs to a chaotic region $\mathcal{R}$ is a global one and therefore it cannot generally be solved by using local techniques, like considerations concerning the local Poincaré map.

III. OPEN SCATTERING

Section III A deals with open-scattering for $\mathbb{R}^{2n}$ Hamiltonian vf $\mathbf{X}_H$ with n first integrals in involution (Liouville-integrability). In Sec. III B open-scattering in the presence of ignorable coordinates is studied. Finally, in Sec. III C, some analytical conditions based on inequalities are given ensuring open-scattering for positive values of the energy.

Let us first show some examples of vf with and without *open scattering orbits*. Recall that a scattering solution of a vf $\mathbf{X}$ [see Eq. (1)] is called open if Eq. (1) is satisfied not only at the point $\mathbf{x}_0$, but for every $\mathbf{y}_0$ in an open neighborhood $N(\mathbf{x}_0)$ of $\mathbf{x}_0$.

It is well known that the $\mathbb{R}^4$ vf associated with the Newton equations

$$\ddot{\mathbf{x}} = -\nabla V(r),$$

$$\mathbf{x} \in \mathbb{R}^2,$$

$$\lim_{r\to\infty} V(r) = 0, \tag{23}$$

where $r=\|\mathbf{x}\|$, do certainly possess open scattering orbits (see, e.g., Arnold in Ref. 1).

An example of $\mathbb{R}^2$ Hamiltonian vf without open scattering orbits (because its only unbounded orbit is isolated) is

$$\mathbf{X_H} = \left(\frac{\partial H}{\partial y}, -\frac{\partial H}{\partial x}\right), \tag{24}$$

$H(x,y)$ being the Newtonian potential created by the charge dipole $(-q,q)$ lying on $((-1,0),(1,0))$, that is

$$H = -\frac{q}{\sqrt{(x+1)^2+y^2}} + \frac{q}{\sqrt{(x-1)^2+y^2}}. \tag{25}$$

The vf $\mathbf{X_H}$ defined by (24) and (25) has the y axis as a scattering orbit which is surrounded by S^1 orbits of $\mathbf{X_H}$ centered at $(-1,0)$ and $(1,0)$ (i.e., the level sets $H(x,y)=c$ of H, $c\neq 0$).

Note that this vf can be globalized either by multiplication by a suitable smooth function $\lambda(x,y)$ vanishing at $(-1,0)$ and $(1,0)$ or by constructing a vf $\mathbf{Y}_{\tilde{\mathbf{H}}}$, with $\tilde{H}$ an adequate function of H.

Can a similar example (of isolated scattering orbit) be found for vf of type $(\dot{\mathbf{x}}, -\nabla V(\mathbf{x}))$, $\mathbf{x}\in\mathbb{R}^n$?

A. Open scattering and Liouville integrability

For the sake of simplicity let us assume that $n=2$ (the case $n>2$ can be treated in a similar way). Consider that the Hamiltonian vf $\mathbf{X_H}$ in $\mathbb{R}^4$ is Liouville integrable;[1] that is, in addition to the Hamiltonian H, a second first integral I is known such that

1. rank $(\nabla I, \nabla H)=2$ either globally or at least in the open domain $\mathcal{D}$ where we are working.
2. (H,I) Poisson-commute.
3. $\mathbf{X_H}$ and $\mathbf{X_I}$ are complete vf globally or at least in $\mathcal{D}$.
4. The topology of the level sets $(H=C_1, I=C_2)$ near the level set $L_0=(H=C_{10}, I=C_{20})$ does not vary with (C_1,C_2). Assume that $\mathcal{D}$ contains L_0 and it is saturated by level sets of (H,I).

We are now given a scattering orbit S lying on the level set L_0. Call L any level set $(H=C_1, I=C_2)$ near L_0. Note that L_0 must be diffeomorphic to $\mathbb{R}^2$ or $S^1\times\mathbb{R}$ (tori being excluded by the presence of S, which is unbounded), by the well-known Arnold-Liouville's theorem.[1] In what follows $\mathcal{D}$ will be an open neighborhood of L_0.

Open scattering does certainly appear when $L_0\cong\mathbb{R}^2$. Indeed, since $\nabla H\neq 0$ on L then $\mathbf{X_H}|_L \neq 0$ and hence (by Poincaré-Bendixon theorem[17]) the orbits of $\mathbf{X_H}|_L$ must be of type $\mathbb{R}$.

When $L_0\cong S^1\times\mathbb{R}$ the action of $\mathbf{X_I}$ on S (remember that $\mathbf{X_I}$ is complete on $\mathcal{D}$) defines a foliation on L_0 whose leaves are diffeomorphic to $\mathbb{R}$. In fact $\mathbf{X_H}|_{L_0}$ is conjugate to a helicoidal vector field, i.e., there exists coordinates $(\phi,z)\in S^1\times\mathbb{R}$ on L_0 such that[10]

$$\mathbf{X_H}|_{L_0} = a\partial_\phi + b\partial_z, \tag{26}$$

$a,b\in\mathbb{R}$ and $b\neq 0$ because of the presence of S in L_0.

Equation (26) implies that all the orbits of $\mathbf{X_H}|_{L_0}$ go from one end of L_0 to the other, thus proving that $\mathbf{X_H}|_{L_0}$ is structurally stable.[18] Therefore L is foliated by $\mathbb{R}$ orbits and hence there is open scattering in $\mathcal{D}$.

When the level sets L near L_0 do not keep a fixed topological type, e.g., there are bifurcations from $\mathbb{R}^2$ to $S^1\times\mathbb{R}$ or from $S^1\times\mathbb{R}$ to $S^1\times S^1$ we cannot conclude anything on open scattering. An illustrative example is the Kepler problem when L_0 is the level set $(H=C_{10}, I=C_{20}\neq 0)$ of the first integrals

$$H = \frac{\dot{x}^2 + \dot{y}^2}{2} - \frac{1}{\sqrt{x^2 + y^2}}, \quad I = x\dot{y} - y\dot{x}.$$

Assumptions (1)–(4) are fulfilled if $C_{10} > 0$, thus implying open scattering. If $C_{10} = 0$ then only assumptions (1)–(3) hold because the level sets ($H < 0$, $I = C_{20}$) are tori. In this case open scattering does not occur.

B. Open scattering and ignorable coordinates

We now study the effect on open scattering of the existence of $n-1$ ignorable coordinates (call them $y_2, \ldots, y_n$) in the n first integrals ($I_1, \ldots, I_n$) of the second order differential equation (not necessarily Hamiltonian)

$$\ddot{\mathbf{y}} = C(\mathbf{y}, \dot{\mathbf{y}}),$$

$$\mathbf{y} = (y_1, \ldots, y_n) \in \mathbb{R}^n. \tag{27}$$

System (27) is assumed to have the n first integrals:

$$I_1(y_1, \dot{y}_1, \ldots, \dot{y}_n),$$

$$\vdots$$

$$I_n(y_1, \dot{y}_1, \ldots, \dot{y}_n). \tag{28}$$

Assume that $\dot{y}_2, \ldots, \dot{y}_n$ can be globally eliminated in

$$I_1(y_1, \dot{y}_1, \ldots, \dot{y}_n) = C_1,$$

$$\vdots$$

$$I_n(y_1, \dot{y}_1, \ldots, \dot{y}_n) = C_n. \tag{29}$$

We get in this way

$$\Lambda(y_1, \dot{y}_1; C_1, \ldots, C_n) = 0, \tag{30}$$

Λ being called the eliminant (sometimes also called resultant, particularly when $I_1, \ldots, I_n$ are polynomials in $\dot{y}_2, \ldots, \dot{y}_n$).

If $y_1 \in \mathbb{R}$ ($y_2, \ldots, y_n$ can vary either on $\mathbb{R}$ or S^1) and Eq. (27) possesses a scattering solution S on the level set $(C_{10}, \ldots, C_{n0})$, $y_1(t)$ being unbounded, then the curve ϑ_0 on the $(y_1, \dot{y}_1)$ plane defined by $\Lambda(y_1, \dot{y}_1; C_{10}, \ldots, C_{n0}) = 0$ has some connected component which is also unbounded. If the values $(C_1, \ldots, C_n)$ of the first integrals are close to $(C_{10}, \ldots, C_{n0})$, does the curve ϑ defined by $\Lambda(y_1, \dot{y}_1; C_1, \ldots, C_n) = 0$ remain unbounded? In the next paragraph we give a sufficient condition ensuring that if $(C_1, \ldots, C_n)$ are near $(C_{10}, \ldots, C_{n0})$ then ϑ is close to ϑ_0, thus proving that open scattering around S occurs.

If $\|\nabla\Lambda\,(y_1, \dot{y}_1; C_{10}, \ldots, C_{n0})|_{\vartheta_0}\| \geqslant c > 0$ then the curves ϑ for $(C_1, \ldots, C_n)$ close enough to $(C_{10}, \ldots, C_{n0})$ are diffeomorphic to ϑ_0. Indeed, this assumption on $\nabla\Lambda$ is a particular case of Malgrange condition and hence it implies the nonexistence of asymptotic critical values.[19] Although ϑ_0 is noncompact the fact that $\|\nabla\Lambda\|$ is bounded below implies that Thom's isotopy theorem[20] holds, thus showing that a small perturbation of Λ gives rise to a curve ϑ which is diffeomorphic (via a smooth diffeotopy arbitrarily close to the identity) to ϑ_0. If $(C_1, \ldots, C_n)$ are near $(C_{10}, \ldots, C_{n0})$ then, on account of the continuous dependence, $\Lambda(y_1, \dot{y}_1; C_1, \ldots, C_n)$ is a small perturbation of $\Lambda(y_1, \dot{y}_1; C_{10}, \ldots, C_{n0})$, and the result follows.

Newton equations for central potentials satisfy Eq. (28) in the polar chart $(y_1=r, y_2=\theta)$. In this case the first integrals take the form $I_1=\frac{1}{2}\dot{y}_1^2+\frac{1}{2}y_1^2\dot{y}_2^2+V(y_1)$, $I_2=y_1^2\dot{y}_2$.

Let us illustrate the main result of this section with a classical example: the Kepler problem. In this case it is easy to check that the eliminant is given by

$$\Lambda(y_1,\dot{y}_1;C_1,C_2)=\frac{1}{2}\dot{y}_1^2+\frac{C_2^2}{2y_1^2}-\frac{1}{y_1}-C_1=0. \tag{31}$$

The critical points of Λ are $p_1(y_1=C_2^2,\dot{y}_1=0)$ and $p_2(y_1\to\infty,\dot{y}_1=0)$. Since

$$\Lambda(p_1)=-\frac{1}{C_2^2}-C_1 \text{ and } \Lambda(p_2)=-C_1$$

it follows, on account of the previous discussion, that when $C_1=C_{10}>0$ and $C_2=C_{20}\neq 0$ there exists open scattering (hyperbolic orbits). If $C_1=C_{10}=0$ (parabolic orbits) then the curve ϑ_0 has an asymptotic critical value and the criterion does not work, in fact in this case there is no open scattering because the orbits with $C_1<0$ are periodic.

A particularly relevant situation in which equations of type (30) arise is for Stackel's separable systems.[21] In this case it is not difficult to reach the following expression

$$\Lambda_i(y_i,\dot{y}_i;C_1,\ldots,C_n)=\tfrac{1}{2}\dot{y}_i^2+\phi_i(y_i;C_1,\ldots,C_n)=0 \tag{32}$$

for each $i=1,\ldots,n$. If the (type $\mathbb{R}$) coordinate y_k is unbounded for the scattering orbit S then our criterion applied to Λ_k implies open scattering.

C. Potentials with open scattering for positive energy

In the Kepler problem all the trajectories with energy $E>0$ (and nonvanishing angular momentum) are scattering orbits, thus exhibiting the open scattering phenomenon when $E>0$. We now give a procedure in order to get open scattering in Newtonian systems $\ddot{\mathbf{x}}=-\nabla V(\mathbf{x})$, $\mathbf{x}\in\mathbb{R}^n$, when $V(\mathbf{x})$ is of type $a(r)+b(r)F(\theta)$, $(r,\theta)\in\mathbb{R}^+\times S^{n-1}$ being spherical coordinates in $\mathbb{R}^n$, and the energy $E>0$.

The method is based on the inequalities

$$\ddot{r}\geqslant -a'(r)-b'(r)F(\theta),$$

$$a(r)+b(r)F(\theta)\leqslant E \tag{33}$$

obtained from the equation $\ddot{\mathbf{x}}=-\nabla V(\mathbf{x})$ written in spherical coordinates and the energy conservation law

$$\frac{\dot{\mathbf{x}}^2}{2}+V(\mathbf{x})=E. \tag{34}$$

Assume that $b(r)<0, b'(r)<0$ or $b(r)>0, b'(r)>0$ (if r is large enough), in these cases, by eliminating $F(\theta)$ in Eq. (33), we get the following inequality:

$$\ddot{r}\geqslant\frac{\mathrm{d}W(r)}{\mathrm{d}r}, \tag{35}$$

where $W(r)=a(r)+E\ln|b(r)|-\int b'(r)a(r)/b(r)\mathrm{d}r$.

Inequalities of type (35) have been studied in Refs. 22 and 23 in order to prove the existence of scattering solutions. The arguments developed in these works yield that open scattering occurs when $W(r)<c$ $(c\in\mathbb{R})$ and $W''(r)<0$ for large values of r.

For example, if $a(r)=-1/r^k$ $(k>1)$ and $b(r)$ satisfies $0<b(r)<k$, $b'(r)>0$, $b''(r)<0$ if $r>R$ then open scattering exists for positive energy. Indeed $W(r)$ is given by

$$W = -\frac{1}{r^k} + E \ln b(r) + \int \frac{b'(r)}{r^k b(r)} \mathrm{d}r. \tag{36}$$

It is not difficult to check that $W(r)$ is bounded above when $r > R$ and furthermore

$$W''(r) = -\frac{k(1+k)}{r^{k+2}} + \left(E + \frac{1}{r^k}\right) \frac{b''(r)b(r) - b'(r)^2}{b(r)^2} - \frac{b'(r)}{r^{k+1}b(r)}. \tag{37}$$

Equation (37) implies that $W''(r) < 0$ (r large) when $E > 0$ and therefore open scattering is guaranteed for positive energy.

The criterion of this section is analytical and very easy to check in specific examples. Other potentials that can be studied with this technique are of type $V(r) = a(r)G(\theta) + b(r)F(\theta)$, $G(\theta) \geqslant c > 0$.

IV. CONCLUSION

In this paper we have studied the robustness of scattering type trajectories when the initial condition is perturbed. We have shown that geometric chaos is possible even for integrable vector fields, thus obtaining a new chaotic phenomenon different from the well-known chaotic scattering. In the phenomenon that we have reported the complexity and nonuniformity of the trajectories is manifested in the (practical) impossibility of determining whether a given solution is bounded or not because scattering and nonscattering orbits are intermingled. We have also found some topological obstructions to the presence of geometric chaos.

The opposite situation to geometric chaos is open scattering. In this case all the orbits through some open set are of scattering type. This situation is desirable from the physical viewpoint because it guarantees that all the orbits will escape to infinity, i.e., there is no uncertainty in the boundedness of the trajectories. We have provided criteria for ensuring open scattering in some particularly relevant situations, like Liouville integrable systems, Stackel separable systems and potential systems with positive energy.

It remains open to ascertain how often is the presence of geometric chaos in Hamiltonian systems (e.g., is geometric chaos robust under small perturbations of the vector field?), and to provide more criteria guaranteeing open scattering.

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Point interactions in acoustics: One-dimensional models

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A one-dimensional system made up of a compressible fluid and several mechanical oscillators, coupled to the acoustic field in the fluid, is analyzed for different settings of the oscillator array. The dynamical models are formulated in terms of singular perturbations of the decoupled dynamics of the acoustic field and the mechanical oscillators. Detailed spectral properties of the generators of the dynamics are given for each model we consider. In the case of a periodic array of mechanical oscillators it is shown that the energy spectrum presents a band structure. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209553]

INTRODUCTION

In this paper we study the dynamics of a system consisting of one or more mechanical oscillators (the sources) coupled with the acoustic field they produce in the compressible fluid surrounding them.

Classical electromagnetism is perhaps the most well-known case in theoretical physics where all attempts to construct a complete, covariant, causal, divergence-free theory for the evolution of the fields together with their sources were unsuccessful up to now (in fact, it is hard to say that there is a single case in classical or in quantum physics in which this problem was completely solved).

Whereas theories with extended rigid charges are quite well understood both at the classical and the quantum level [see, e.g., a recent book (Spohn, 2004) for a systematic introduction to the subject and for a long list of references], there is no mathematically consistent theory of point charges interacting with their own electromagnetic field. Indeed, Newton equations with a Lorentz force require the fields to be evaluated at the particle positions, and this produces infinities due to the presence of the pointlike sources. These difficulties directly lead to the need of mass renormalization. In his seminal paper, Dirac (1938) [see also Infeld and Wallace (1940), Kijowski (1994), and Marino (2002)], without using a Lorentz force but exploiting the conservation of energy and momentum and considering their flow through a thin tube of radius r, derived an equation for the motion of a charged point particle (the Lorentz-Dirac equation). As Dirac himself pointed out, the equation obtained in the limit $r \downarrow 0$, together with the mass renormalization, leads to the presence of runaway solutions, i.e., solutions for which the acceleration increases beyond any bound even in the absence of external fields.

An approach based on the theory of singular perturbations of the free dynamics was initiated in Noja and Posilicano (1998, 1999) for the case of classical electrodynamics of a point particle in the dipole (or linearized) case. Here the generator of the limit dynamics of both the field and the particle appears to be a singular perturbation of the generator of the free dynamics. The phenom-

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enological mass plays the role of the parameter describing a suitable family of self-adjoint extensions and the boundary condition naturally appearing in the domain of the generator results to be nothing else that a regularized (and linearized) version of the usual velocity-momentum relation in the presence of an electromagnetic field. In this framework runaway solutions are unavoidable because a negative eigenvalue appears in the spectrum of the generator after mass renormalization.

Our interest in a similar problem in acoustics was prompted by the appearance in 1999 of a paper by Templin (1999). In that paper the author analyzed the dynamics of a simple model of a spherical oscillator interacting with the acoustic field it generates. The existence of a spherically symmetric radiation field (the *acoustic monopole*) makes the acoustic case significantly different from the electromagnetic one. Moreover, the pressure field at the surface of the sphere completely characterizes the contact forces responsible for the interaction between the source and field in the acoustic case.

Templin performed a detailed analysis of the field emitted by the acoustic monopole, explicitly computing both its radiation and near-field components. He noticed that a deduction of the *reaction field* obtained from the emitted radiation power, therefore neglecting the near field component, brings to an equation for the radius of the oscillating sphere showing *runaway solutions*.

In analogy with what was done for the electromagnetic case in Noja and Posilicano (1998), we want to provide a formalization of the problem of a finite or infinite number of oscillators coupled with their acoustic field in terms of singular perturbations of the generator of the free dynamics.

In this paper we will consider only the one-dimensional case. In the abstract setting we will work in the physical model of interaction between the sources and the field will appear as the only possible extension of the free dynamics. The generalization to three dimensions is not straightforward. On the one hand, a model of a physically relevant, symmetric, mechanical oscillator with finite degrees of freedom is lacking. On the other hand, point perturbations of the free dynamics are much more singular in higher dimensions. We plan to discuss the three-dimensional case in future work.

We want to stress an aspect of the dynamical system we analyze here that was extensively studied in different contexts. As an immediate consequence of the third Newton's law and of the assumption of persistent contact between the fluid and the surface of the oscillators, the total energy, sum of the (positive) energy of the acoustic field E_{ac} and the (positive) energy of the oscillators E_{osc}, is a constant of motion. As an immediate consequence, one can exclude the existence of runaway solutions in this case. Moreover, lacking a mechanism of reflection of the acoustic waves at some exterior boundary, the motion of the oscillators should be damped and the energy should finally diffuse over the field degrees of freedom for almost every initial condition. The situation is reminiscent of the one investigated in Soffer and Weinstein (1998a, 1998b, 1999) that concerned the diffusion of energy from bound states to continuous states triggered by time-dependent perturbations in quantum and classical systems. In our system there is no external potential, the interaction being given by internal forces.

This paper is organized as follows. In Sec. I we introduce a list of notations and we briefly recall the equations for the acoustic field. Afterwards we exemplify the problem of the interaction between the field and a source in the completely solvable case of a single wall attracted toward the origin by a linear restoring force.

In Sec. II we analyze the case of a finite number of sources in the framework of the possible extensions of the free dynamics outside the points where the sources are placed. In Sec. III we generalize the construction to the case of infinitely many sources and study the case of sources periodically placed on the real line. We give detailed results on the characteristic band structure of the spectrum of the generator of the dynamics.

To the best of our knowledge, these kinds of systems of oscillators coupled with the acoustic field was never proposed and solved. A remark on the band structure of a similar model is in Griffiths and Steinke (2001).

I. THE ACOUSTIC MONOPOLE IN ONE DIMENSION

We give a detailed description of our model in the simplest case of one oscillator coupled with the acoustic field.

Consider an infinite pipe filled with a nonviscous, compressible fluid. We suppose that there is no friction between the fluid and the pipe, and we choose a coordinate system with the x axis parallel to the axis of the pipe. The mechanical oscillator is made up of a very thin wall of mass M positioned in the pipe perpendicularly to the axis in $x=0$. The thin wall is connected to a spring of elastic constant K. We analyze only one-dimensional cases, hence the acoustic field is described by the pressure field $p(x,t)$ and the velocity field $v(x,t)$. The motion of the mechanical oscillator is described through the position and the velocity of the thin wall.

The field $p(x,t)$ represents deviations of the pressure in point x at time t with respect to an equilibrium pressure P_0. In the linearized acoustics regime the continuity equation, the Newton's second law, and the adiabatic equation of state read

$$\frac{\partial \rho}{\partial t} + \rho_0 \frac{\partial v}{\partial x} = 0, \quad \rho_0 \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x}, \quad p = a^2 \rho, \tag{1.1}$$

where $\rho(x,t)$ is the deviation of the density in point x at time t with respect to the equilibrium density ρ_0 and a is the velocity of sound in the fluid.

Then we have for $p(x,t)$ and $v(x,t)$ the following coupled differential equations:

$$\frac{\partial p}{\partial t} = -a^2 \rho_0 \frac{\partial v}{\partial x}, \quad \frac{\partial v}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x}. \tag{1.2}$$

We consider only small oscillations of the thin wall around its equilibrium position $x=0$, we indicate with $y(t)$ the displacement of the wall from its equilibrium position at time t, and we suppose that the wall always remains in contact with the fluid:

$$v(y(t),t) = \frac{dy(t)}{dt} \quad \forall\, t \geqslant 0. \tag{1.3}$$

Notice that we consider a wall of zero thickness. We make the approximation $v(y(t),t) \simeq v(0,t)$ and condition (1.3) becomes

$$v(0,t) = \frac{dy(t)}{dt} \quad \forall\, t \geqslant 0. \tag{1.4}$$

The equation of motion for the position of the thin wall $y(t)$ is

$$M\ddot{y}(t) = -Ky(t) - S(p(0^+,t) - p(0^-,t)), \tag{1.5}$$

where S is the area of the transverse section of the pipe and we made the approximation $p(y^{\pm}(t),t) \simeq p(0^{\pm},t)$.

The total energy of the system is given by

$$E_{\text{tot}} = E_{\text{ac}} + E_{\text{osc}}, \tag{1.6}$$

with

$$E_{\text{ac}} = \frac{S}{2a^2\rho_0} \int_{-\infty}^{\infty} p(x)^2 dx + \frac{S\rho_0}{2} \int_{-\infty}^{\infty} v(x)^2 dx, \tag{1.7}$$

$$E_{\text{osc}} = \frac{K}{2} y^2 + \frac{M}{2} \dot{y}^2. \tag{1.8}$$

E_{ac} is the energy stored in the acoustic field while E_{osc} is the energy of the mechanical oscillator.

As the system is isolated, the energy is constant. The motion of the wall produces acoustic waves, thus transferring continuously energy from the oscillator to the acoustic field. One then expects that $y(t)$ decreases to zero when $t\to\infty$.

In spite of being a simple exercise, the exact computation of the solution of problems (1.2), (1.4), and (1.5) and, in turn, of the damping rate of the oscillations rarely appears in textbooks.

In the following we give the solution of the Cauchy problem of coupled ordinary and partial differential equations with time-dependent boundary conditions

$$\begin{aligned}
&\frac{\partial p}{\partial t} = -a^2\rho_0\frac{\partial v}{\partial x} \quad \forall\, t\geqslant 0 \ \ \forall\, x\in\mathbb{R}\setminus\{0\},\\
&\frac{\partial v}{\partial t} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x} \quad \forall\, t\geqslant 0 \ \ \forall\, x\in\mathbb{R}\setminus\{0\},\\
&\ddot{y}(t) = -\omega_0^2 y(t) - \frac{S}{M}(p(0^+,t)-p(0^-,t)) \quad \forall\, t\geqslant 0,\\
&p(x,0) = f(x) \quad \forall\, x\in\mathbb{R}\setminus\{0\},\\
&v(x,0) = g(x) \quad \forall\, x\in\mathbb{R}\setminus\{0\},\\
&y(0) = y_0,\\
&\dot{y}(0) = \dot{y}_0,\\
&v(0,t) = \dot{y}(t) \quad \forall\, t\geqslant 0,
\end{aligned} \tag{1.9}$$

where $f(x)$ and $g(x)$ are two real functions and $\omega_0^2 = K/M$.

Suppose that

$$f(x)\in C_0^2(\mathbb{R}); \quad g(x)\in C_0^2(\mathbb{R}) \quad \text{and} \quad y_0 = \frac{1}{\omega_0^2\rho_0}f'(0); \quad \dot{y}_0 = g(0), \tag{1.10}$$

then the solution of problem (1.9) reads

$$p(x,t) = p_f(x,t) + a\rho_0\,\mathrm{sgn}(x)\,Y\left(t-\frac{|x|}{a}\right), \tag{1.11}$$

$$v(x,t) = v_f(x,t) + Y\left(t-\frac{|x|}{a}\right), \tag{1.12}$$

$$y(t) = -\frac{\dot{v}_f(0,t)}{\omega_0^2} + \frac{\displaystyle\int_0^t \frac{F(t')}{\beta_+}e^{\beta_+(t-t')}dt' - \int_0^t \frac{F(t')}{\beta_-}e^{\beta_-(t-t')}dt'}{\beta_+-\beta_-}, \tag{1.13}$$

where $p_f(x,t)$ and $v_f(x,t)$ are solution of the wave equation in $(-\infty,+\infty)$ with initial conditions $f(x)$ and $g(x)$:

$$p_f(x,t) = \frac{f(x-at)+f(x+at)}{2} + \frac{a\rho_0}{2}(g(x-at)-g(x+at)), \tag{1.14}$$

$$v_f(x,t) = \frac{g(x-at)+g(x+at)}{2} + \frac{1}{2a\rho_0}(f(x-at)-f(x+at)),$$
$$F(t) = -\ddot{v}_f(0,t) - \omega_0^2 v_f(0,t), \tag{1.15}$$

and

$$Y(t) = \frac{\int_0^t F(t')e^{\beta_+(t-t')}dt' - \int_0^t F(t')e^{\beta_-(t-t')}dt'}{\beta_+ - \beta_-}, \tag{1.16}$$

with $\beta_\pm = (-\gamma \pm \sqrt{\gamma^2 - 4\omega_0^2})/2$ with $\gamma = 2a\rho_0 S/M$.

With conditions (1.10) one can easily obtain that $y(t)$ and $\dot{y}(t)$ are both continuous and decrease exponentially to zero with a decay constant $\tau = \gamma/2$.

II. SINGULAR PERTURBATIONS OF THE FREE DYNAMICS

In this section we present a generalization of problem (1.9) formulated in terms of a unitary flow on a space of finite energy.

Let us consider a system of n thin walls positioned in a pipe, perpendicular to its axis. Let $\mathcal{S} = \{s_1, \ldots, s_n\} \subset \mathbb{R}$ be the set of equilibrium positions of the thin walls. The ith thin wall, placed in s_i has mass M_i and is connected to a spring of elastic constant K_i. The acoustic field is described by the pressure field p and the velocity field v. The motion of the walls is described by the displacements y_j from their equilibrium positions and by the corresponding velocities z_j.

The generator of the dynamics, $\hat{A}$, will be defined as a singular perturbation of the skew-adjoint operator A generating the uncoupled evolution of the acoustic field and of the oscillators.

The system of first-order differential equations,

$$\frac{\partial p}{\partial t} = -a^2\rho_0 \frac{\partial v}{\partial x} \quad \forall\, x \in \mathbb{R}, \tag{2.1}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x} \quad \forall\, x \in \mathbb{R}, \tag{2.2}$$

$$\frac{dy_j}{dt} = z_j \quad 1 \leqslant j \leqslant n, \tag{2.3}$$

$$\frac{dz_j}{dt} = -\frac{K_j}{M_j} y_j \quad 1 \leqslant j \leqslant n, \tag{2.4}$$

describes, in the linear approximation, the independent evolution of n mechanical oscillators and of the acoustic field.

We want to show first how Eqs. (2.1)–(2.4) define an unitary flow in a complex Hilbert space. To this aim let us consider Eqs. (2.1)–(2.4) for complex functions v, p, y_j, z_j of position and time.

The set of all the displacements and velocities will be represented respectively by the vectors in $\mathbb{C}^n$:

$$\underline{y} = y_1\underline{e}_1 + \cdots + y_n\underline{e}_n, \quad \underline{z} = z_1\underline{e}_1 + \cdots + z_n\underline{e}_n, \tag{2.5}$$

where $\underline{e}_1, \cdots, \underline{e}_n$ is the canonical orthonormal basis in $\mathbb{C}^n$.

Let us denote by $L^2(\mathbb{R})$ the space of square-integrable functions on the real line. $\bar{H}^1(\mathbb{R})$ indicates the homogeneous Sobolev space of locally square-integrable functions with a square-integrable (distributional) derivative, and $H^1(\mathbb{R})$ is the usual Sobolev space $H^1(\mathbb{R}) := \bar{H}^1(\mathbb{R}) \cap L^2(\mathbb{R})$.

Therefore the linear operator A in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n$ generating the dynamics (2.1)–(2.4) is defined by

$$A: H^1(\mathbb{R}) \oplus H^1(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n, \tag{2.6}$$

$$A(p,v,\underline{y},\underline{z}) := \left(-a^2\rho_0 \frac{dv}{dx}, -\frac{1}{\rho_0}\frac{dp}{dx}, \underline{z}, -\sum_{1\leqslant j\leqslant n} \frac{K_j}{M_j} y_j \underline{e}_j \right), \tag{2.7}$$

where a, ρ_0, K_j, M_j, $1 \leqslant j \leqslant n$, are the positive real constants representing the physical parameters.

In the following, a capital Greek letter will indicate a generic vector $(p,v,\underline{y},\underline{z})$ in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n$.

A is a real operator, i.e., it preserves the (physical) linear subspace of real elements

$$\{(p,v,\underline{y},\underline{z}): p(x) \in \mathbb{R}, v(x) \in \mathbb{R}, \underline{y} \in \mathbb{R}^n, \underline{z} \in \mathbb{R}^n\}. \tag{2.8}$$

A is skew-symmetric with respect to the scalar product

$$\langle\langle \Psi_1, \Psi_2 \rangle\rangle \equiv \frac{1}{a^2\rho_0}\langle p_1, p_2\rangle + \rho_0 \langle v_1, v_2\rangle + \frac{1}{S}\sum_{1\leqslant j\leqslant n} K_j \bar{y}_{1j} y_{2j} + M_j \bar{z}_{1j} z_{2j}, \tag{2.9}$$

where $\langle\cdot,\cdot\rangle$ indicates the standard scalar product in $L^2(\mathbb{R})$, $\mathcal{S}$ is the area of the transverse section of the pipe, and denotes complex conjugation. $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n$ is a Hilbert space with the scalar product (2.9).

The square norm of a vector Ψ, $\|\Psi\|^2 = \langle\langle \Psi, \Psi\rangle\rangle$, defines the total energy of the system in the state Ψ,

$$E_{\text{tot}} = \frac{S}{2}\|\Psi\|^2 = E_{\text{ac}} + E_{\text{osc}}, \tag{2.10}$$

where E_{ac} is the energy stored in the acoustic field while E_{osc} is the energy of the oscillators:

$$E_{\text{ac}} = \frac{\mathcal{S}}{2a^2\rho_0}\langle p,p\rangle + \frac{\rho_0 \mathcal{S}}{2}\langle v,v\rangle; \quad E_{\text{osc}} = \frac{1}{2}\sum_{1\leqslant j\leqslant n} (K_j |y_j|^2 + M_j |z_j|^2). \tag{2.11}$$

For any $\zeta \in \mathbb{C}\backslash i\mathbb{R}$ the resolvent of A is

$$(-A+\zeta)^{-1}(p,v,\underline{y},\underline{z}) = \left(\rho_0 \left(-\frac{d^2}{dx^2} + \frac{\zeta^2}{a^2} \right)^{-1} \left(-\frac{dv}{dx} + \frac{\zeta}{a^2\rho_0} p \right), \right.$$

$$\frac{1}{a^2\rho_0}\left(-\frac{d^2}{dx^2} + \frac{\zeta^2}{a^2} \right)^{-1} \left(-\frac{dp}{dx} + \zeta\rho_0 v \right), \quad \sum_{1\leqslant j\leqslant n} \frac{M_j z_j + \zeta M_j y_j}{K_j + \zeta^2 M_j} \underline{e}_j, \tag{2.12}$$

$$\left. \sum_{1\leqslant j\leqslant n} \frac{-K_j y_j + \zeta M_j z_j}{K_j + \zeta^2 M_j} \underline{e}_j \right).$$

Since

$$\text{Ran}(-A \pm 1) = L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n, \tag{2.13}$$

A is skew-adjoint. Moreover, the essential spectrum of A is purely absolutely continuous and

$$\sigma_{\mathrm{ess}}(A)=\sigma_{\mathrm{ac}}(A)=i\mathbb{R},\quad \sigma_{\mathrm{pp}}(A)=\left\{\pm i\sqrt{\frac{K_j}{M_j}},1\leqslant j\leqslant n\right\}. \tag{2.14}$$

Being skew-adjoint, the operator A describes, by the Stone theorem, the uncoupled evolution of the acoustic field and of the oscillators through the unitary flow $\exp tA$ corresponding to the Cauchy problem for the first-order differential equation

$$\frac{d}{dt}\Psi(t)=A\Psi(t), \tag{2.15}$$

which is equivalent to the system written at the beginning of the section.

Now we consider the linear operator A_0 obtained by restricting A on the set of vectors in its domain satisfying

$$\{v(s_j)=z_j,\ 1\leqslant j\leqslant n\}, \tag{2.16}$$

which represents the kinematic constraint (1.4) at each thin wall. A_0 is a closed, densely defined, skew-symmetric linear operator with defect indices (n,n). We want to characterize the skew-adjoint extensions of A_0. The family of extensions of A_0 can be parameterized by relations $K\subset\mathbb{C}^n\oplus\mathbb{C}^n$, which are skew-symmetric, i.e., such that $K=(IK)^{\perp}$, where $I(\underline{z}_1,\underline{z}_2):=(\underline{z}_2,\underline{z}_1)$ [see, e.g., Gorbachuk and Gorbachuk (1991), Theorem 1.6, Chap. 3, for the analogous self-adjoint case]. A skew-symmetric relation in $\mathbb{C}^n\oplus\mathbb{C}^n$ extends the notion of the graph of a skew-symmetric operator $\Theta:\mathbb{C}^n\to\mathbb{C}^n$ through the relation $K=\{(\underline{z},\Theta\underline{z}),\underline{z}\in\mathbb{C}^n\}$. In order to be a candidate to describe the interacting dynamics of the system under analysis, a skew-adjoint extension of A_0 must be local and real, i.e., it must generate a coupling between the fields evaluated in s_j and the jth oscillator, $1\leqslant j\leqslant n$, and it must preserve the linear space of physical data defined in (2.8). The only admissible extension different from A itself will be the one corresponding to the graph of the zero operator, $\Theta=0$. The next theorem completely characterizes such an extension.

Theorem 2.1: *The only local, real, and skew-adjoint extension of A_0 is given by*

$$\hat{A}:D(\hat{A})\subset L^2(\mathbb{R})\oplus L^2(\mathbb{R})\oplus\mathbb{C}^n\oplus\mathbb{C}^n\to L^2(\mathbb{R})\oplus L^2(\mathbb{R})\oplus\mathbb{C}^n\oplus\mathbb{C}^n, \tag{2.17}$$

$$D(\hat{A})=\{\Psi\equiv(p,v,\underline{y},\underline{z}):p\in L^2(\mathbb{R})\cap H^1(\mathbb{R}\setminus\mathcal{S}),v\in H^1(\mathbb{R}),\underline{y}\in\mathbb{C}^n,\underline{z}\in\mathbb{C}^n,p(s_i^+)-p(s_i^-)=\sigma_i,v(s_j)=z_j,\underline{\sigma}\in\mathbb{C}^n\}, \tag{2.18}$$

$$\hat{A}(p,v,\underline{y},\underline{z}):=\left(-a^2\rho_0\frac{dv}{dx},-\frac{1}{\rho_0}\frac{dp_0}{dx},\underline{z},-\sum_{1\leqslant j\leqslant n}\left(\frac{K_j}{M_j}y_j+\frac{S}{M_j}\sigma_j\right)\underline{e}_j\right). \tag{2.19}$$

Here $p_0\in\bar{H}^1(\mathbb{R})$,

$$p_0(x):=p(x)-\frac{1}{2}\sum_{1\leqslant j\leqslant n}\sigma_j\,\mathrm{sgn}(x-s_j), \tag{2.20}$$

denotes the regular part of p. The resolvent of $\hat{A}$ is given by

$$(-\hat{A}+\zeta)^{-1}=(-A+\zeta)^{-1}+\sum_{1\leqslant i,j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}G^i_\zeta\otimes\breve{G}^j_{\bar{\zeta}},\quad \zeta\in\mathbb{C}\setminus i\mathbb{R}, \tag{2.21}$$

where

$$\Gamma(\zeta)_{ij}:=-\zeta\left(\pm\frac{e^{\mp\zeta|s_i-s_j|/a}}{2a\rho_0\zeta}+\frac{S\delta_{ij}}{K_j+\zeta^2M_j}\right),\quad \pm\,\mathrm{Re}\,\zeta>0 \tag{2.22}$$

and

$$\breve{G}^j_\zeta(x) = \left(\mathcal{G}'_\zeta(x-s_j), \frac{\zeta}{a^2\rho_0}\mathcal{G}_\zeta(x-s_j), \frac{S}{K_j+\zeta^2 M_j}\underline{e}_j, \frac{-\zeta S}{K_j+\zeta^2 M_j}\underline{e}_j \right), \tag{2.23}$$

$$G^j_\zeta(x) = \left(-\mathcal{G}'_\zeta(x-s_j), \frac{\zeta}{a^2\rho_0}\mathcal{G}_\zeta(x-s_j), \frac{-S}{K_j+\zeta^2 M_j}\underline{e}_j, \frac{-\zeta S}{K_j+\zeta^2 M_j}\underline{e}_j \right), \tag{2.24}$$

$$\mathcal{G}_\zeta(x) = \pm\frac{a}{2\zeta}e^{\mp\zeta|x|/a}, \quad \mathcal{G}'_\zeta(x) = -\frac{1}{2}\,\mathrm{sgn}(x)e^{\mp\zeta|x|/a}, \quad \pm\,\mathrm{Re}\,\zeta > 0. \tag{2.25}$$

Proof: Since iA_0 is a closed, densely defined, symmetric operator with defect indices (n,n), all its self-adjoint extensions can be obtained by the famed von Neumann theory on self-adjoint extensions [see, e.g., Theorem X.2 in Reed and Simon (1975)]. However, since A_0 is obtained by restricting the skew-adjoint operator A to the kernel of the continuous, surjective linear operator

$$\tau: H^1(\mathbb{R}) \oplus H^1(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \to \mathbb{C}^n, \tag{2.26}$$

$$\tau(p,v,\underline{y},\underline{z}) := \sum_{1\leqslant j\leqslant n} (v(s_j)-z_j)\underline{e}_j, \tag{2.27}$$

it is easier to make use of the (equivalent) procedure developed in Posilicano (2001) [also see the Appendix in Posilicano (in press) for a compact review]. Here below we provide the (almost) self-contained construction of the skew-adjoint extensions of A_0 by using such a procedure.

Given the map τ we can define the bounded linear operator

$$\breve{G}(\zeta) := \tau(-A+\zeta)^{-1}: L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \to \mathbb{C}^n. \tag{2.28}$$

By the relation

$$\breve{G}(\zeta)(p,v,\underline{y},\underline{z}) = \sum_{1\leqslant j\leqslant n} \langle\langle \breve{G}^j_{\overline{\zeta}}, (p,v,\underline{y},\underline{z})\rangle\rangle \underline{e}_j, \quad 1\leqslant j\leqslant n, \tag{2.29}$$

$\breve{G}(\zeta)$ is represented by the vector $\breve{G}^j_\zeta$. By $\breve{G}(\zeta)$ we define the bounded linear operator

$$G(\zeta) := -\breve{G}(-\overline{\zeta})^*: \mathbb{C}^n \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n, \tag{2.30}$$

where $\breve{G}(\zeta)^*$ indicates the adjoint of $\breve{G}(\zeta)$. The action of $G(\zeta)$ on $\mathbb{C}^n$ is given by

$$G(\zeta)\underline{e}_j = G^j_\zeta, \quad 1\leqslant j\leqslant n. \tag{2.31}$$

Let us notice that

$$\mathrm{Ran}(G(\zeta)) \cap H^1(\mathbb{R}) \oplus H^1(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n = \{0\}. \tag{2.32}$$

Now we consider the linear operator $\Gamma_\Theta(\zeta): \mathbb{C}^n \to \mathbb{C}^n$ represented by the matrix $\Theta_{ij} + \Gamma(\zeta)_{ij}$, where $\Theta: \mathbb{C}^n \to \mathbb{C}^n$ is skew-Hermitian. By noticing that

$$\Gamma_\Theta(\zeta) - \Gamma_\Theta(\xi) = \tau(G(\xi) - G(\zeta)) \tag{2.33}$$

and that, by the definition of $G(\zeta)$ and by the first resolvent identity,

$$(\zeta-\xi)(-A+\xi)^{-1}G(\zeta) = G(\xi) - G(\zeta), \tag{2.34}$$

one has that $\Gamma_\Theta(\zeta)$ satisfies the identity

$$\Gamma_\Theta(\zeta) - \Gamma_\Theta(\xi) = (\zeta - \xi)\breve{G}(\xi)G(\zeta). \tag{2.35}$$

By the definitions of $\breve{G}(\zeta)$ and $G(\zeta)$, by (2.35) and by $\Gamma_\Theta(\bar{\zeta})^* = -\Gamma_\Theta(-\zeta)$, it follows that $\det \Gamma_\Theta(\zeta) \neq 0$ for any $\zeta \in \mathbb{C}\backslash i\mathbb{R}$ and that

$$\hat{R}(\zeta) := (-A + \zeta)^{-1} + G(\zeta)\Gamma_\Theta(\zeta)^{-1}\breve{G}(\zeta) \tag{2.36}$$

satisfies the first resolvent identity

$$(\zeta - \xi)\hat{R}(\xi)\hat{R}(\zeta) = \hat{R}(\xi) - \hat{R}(\zeta) \tag{2.37}$$

and

$$\hat{R}(\bar{\zeta})^* = -\hat{R}(-\zeta) \tag{2.38}$$

[for details see Posilicano (2001)]. Moreover, $\hat{R}(\zeta)$ is injective by (2.32). Therefore

$$\hat{A} := -\hat{R}(\zeta)^{-1} + \zeta \tag{2.39}$$

is well defined on

$$D(\hat{A}) := \mathrm{Ran}(\hat{R}(\zeta)). \tag{2.40}$$

By (2.37) such a definition of $\hat{A}$ is ζ independent. $\hat{A}$ is skew-symmetric by (2.38) and is skew-adjoint since

$$\mathrm{Ran}(-\hat{A} \pm 1) = L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \tag{2.41}$$

by construction.

Since we require $\hat{A}$ to be real, i.e., to preserve the linear space (2.8), we have to restrict the choice of Θ to real, skew-symmetric matrices. Off-diagonal elements in the matrix Θ would correspond to nonlocal couplings between the pressure field and the oscillators. Since we are looking for local interactions the only admissible choice for the skew-symmetric matrix Θ is $\Theta = 0$.

By (2.40) $(p, v, \underline{y}, \underline{z}) \in D(\hat{A})$ if and only if

$$p(x) = p_\zeta(x) - \sum_{1 \leq i,j \leq n} (\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j) - z_{\zeta j})\mathcal{G}'_\zeta(x - s_i), \tag{2.42}$$

$$v(x) = v_\zeta(x) + \frac{\zeta}{a^2\rho_0} \sum_{1 \leq i,j \leq n} (\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j) - z_{\zeta j})\mathcal{G}'_\zeta(x - s_i), \tag{2.43}$$

$$\underline{y} = \underline{y}_\zeta - S \sum_{1 \leq i,j \leq n} (\Gamma(\zeta)^{-1})_{ij} \frac{v_\zeta(s_j) - z_{\zeta j}}{K_i + \zeta^2 M_i} \underline{e}_i, \tag{2.44}$$

$$\underline{z} = \underline{z}_\zeta - \zeta S \sum_{1 \leq i,j \leq n} (\Gamma(\zeta)^{-1})_{ij} \frac{v_\zeta(s_j) - z_{\zeta j}}{K_i + \zeta^2 M_i} \underline{e}_i, \tag{2.45}$$

with $(p_\zeta(x), v_\zeta(x), \underline{y}_\zeta, \underline{z}_\zeta) \in D(A)$. Posing

$$\hat{A}(p, v, \underline{y}, \underline{z}) \equiv (\hat{A}_1(p, v, \underline{y}, \underline{z}), \hat{A}_2(p, v, \underline{y}, \underline{z}), \hat{A}_3(p, v, \underline{y}, \underline{z}), \hat{A}_4(p, v, \underline{y}, \underline{z})), \tag{2.46}$$

the action of $\hat{A}$ on $(p, v, \underline{y}, \underline{z})$ is given by

$$[\hat{A}_1(p,v,\underline{y},\underline{z})](x) = -a^2\rho_0\frac{dv_\zeta}{dx}(x) - \zeta\sum_{1\leqslant i,j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j)-z_{\zeta j})\mathcal{G}'_\zeta(x-s_i), \tag{2.47}$$

$$[\hat{A}_2(p,v,\underline{y},\underline{z})](x) = -\frac{1}{\rho_0}\frac{dp_\zeta}{dx}(x) + \frac{\zeta^2}{a^2\rho_0}\sum_{1\leqslant i,j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j)-z_{\zeta j})\mathcal{G}'_\zeta(x-s_i), \tag{2.48}$$

$$\hat{A}_3(p,v,\underline{y},\underline{z}) = \underline{z}_\zeta - \zeta S\sum_{1\leqslant i,j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}\frac{v_\zeta(s_j)-z_{\zeta j}}{K_i+\zeta^2 M_i}\underline{e}_i, \tag{2.49}$$

$$\hat{A}_4(p,v,\underline{y},\underline{z}) = -\sum_{1\leqslant j\leqslant n}\frac{K_j}{M_j}y_{\zeta j}\underline{e}_j - \zeta^2 S\sum_{1\leqslant i,j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}\frac{v_\zeta(s_j)-z_{\zeta j}}{K_i+\zeta^2 M_i}\underline{e}_i. \tag{2.50}$$

By the definitions of $D(\hat{A})$ and $\Gamma(\zeta)$ one has

$$\hat{A}_1(p,v,\underline{y},\underline{z}) = -a^2\rho_0\frac{dv}{dx}, \tag{2.51}$$

$$\hat{A}_3(p,v,\underline{y},\underline{z}) = \underline{z}, \tag{2.52}$$

and, defining

$$\sigma_i := p(s_i^+) - p(s_i^-) = \sum_{1\leqslant j\leqslant n}(\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j)-z_{\zeta j}), \tag{2.53}$$

formula (2.50) becomes

$$\hat{A}_4(p,v,\underline{y},\underline{z}) = -\sum_{1\leqslant j\leqslant n}\frac{K_j}{M_j}y_{\zeta j}\underline{e}_j - \zeta^2 S\sum_{1\leqslant i\leqslant n}\frac{\sigma_i}{K_i+\zeta^2 M_i}\underline{e}_i \tag{2.54}$$

$$= -\sum_{1\leqslant j\leqslant n}\left(\frac{K_j}{M_j}y_j + \frac{S}{M_j}\sigma_j\right)\underline{e}_j. \tag{2.55}$$

Then, posing

$$p(x) = p_\zeta(x) - \sum_{1\leqslant j\leqslant n}\sigma_j\mathcal{G}'_\zeta(x-s_j) = p_0(x) + \frac{1}{2}\sum_{1\leqslant j\leqslant n}\sigma_j\,\mathrm{sgn}(x-s_j), \tag{2.56}$$

one obtains

$$[\hat{A}_2(p,v,\underline{y},\underline{z})](x) = -\frac{1}{\rho_0}\frac{dp_0}{dx}(x) - \sum_{1\leqslant j\leqslant n}\frac{\sigma_j}{\rho_0}\left(\frac{d}{dx}\frac{|x-s_j|}{2(x-s_j)} - \left(-\frac{d^2}{dx^2}+\frac{\zeta^2}{a^2}\right)\mathcal{G}_\zeta(x-y_j)\right) \tag{2.57}$$

$$= -\frac{1}{\rho_0}\frac{dp_0}{dx}. \tag{2.58}$$

Finally

$$v(s_k) = v_\zeta(s_k) + \frac{\zeta}{a^2\rho_0} \sum_{1\leqslant i,j\leqslant n} (\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j) - z_{\zeta j}) \frac{a}{\pm 2\zeta} e^{\mp\zeta|s_k - s_i|/a} \tag{2.59}$$

$$= v_\zeta(s_k) - \sum_{1\leqslant i,j\leqslant n} (\Gamma(\zeta)^{-1})_{ij}(v_\zeta(s_j) - z_{\zeta j}) \left((\Gamma(\zeta))_{ki} + \frac{\zeta S \delta_{ki}}{K_i + \zeta^2 M_i} \right) \tag{2.60}$$

$$= z_{\zeta k} - \zeta S \sum_{1\leqslant j\leqslant n} (\Gamma(\zeta)^{-1})_{kj} \frac{v_\zeta(s_k) - z_{\zeta k}}{K_k + \zeta^2 M_k} = z_k. \tag{2.61}$$

□

By the previous theorem the differential equation

$$\frac{d}{dt}\Psi(t) = \hat{A}\Psi(t) \tag{2.62}$$

is equivalent to the system of equations

$$\frac{\partial p}{\partial t} = -a^2\rho_0 \frac{\partial v}{\partial x}, \tag{2.63}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0}\frac{\partial p_0}{\partial x} \equiv -\frac{1}{\rho_0}\left(\frac{\partial p}{\partial x} - \sum_{1\leqslant j\leqslant n} \sigma_j \delta_{s_j} \right), \tag{2.64}$$

$$\frac{d\underline{y}}{dt} = \underline{z}, \tag{2.65}$$

$$\frac{d\underline{z}}{dt} = -\sum_{1\leqslant j\leqslant n} \left(\frac{K_j}{M_j} y_j + \frac{S}{M_j}\sigma_j \right) \underline{e}_j, \tag{2.66}$$

and the corresponding Cauchy problem generates the strongly continuous unitary group of evolution $\exp t\hat{A}$ on $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n$, which preserves $D(\hat{A})$. Here δ_{s_j} denotes the Dirac mass at the point s_j and σ_j [see (2.18)] is the pressure jump at s_j.

It is worth noting that the only real, skew-adjoint extension of the free operator A restricted to the space of the vectors $(p, v, \underline{y}, \underline{z})$ such that $v(s_i, t) = z_i$ corresponds to the relevant physical coupling between the pressure field and the oscillators.

The next result will be useful in the spectral analysis of $\hat{A}$.

Lemma 2.2: The matrix

$$\Gamma_\pm(\lambda)^{-1} := \lim_{\varepsilon \downarrow 0} \Gamma(\lambda \pm \varepsilon)^{-1} \tag{2.67}$$

is well defined for any $\lambda \in i\mathbb{R}\backslash\{0\}$.

Proof: We give the proof only for the matrix $\Gamma_+(\lambda)$. The proof for $\Gamma_-(\lambda)$ is analogous.

Let the matrix $\Gamma_+(\zeta)$ be the analytic continuation to $\mathbb{C}\backslash\cup_{j=1}^n\{\pm i\sqrt{K_j/M_j}\}$ of $\Gamma(\zeta)$ defined for $\mathrm{Re}\,\zeta > 0$ in (2.22). Suppose that $s_i > s_j$ if $i > j$, then

$$\Gamma_+(\zeta) = -\Pi(\zeta) - T(\zeta), \tag{2.68}$$

where Π is the operator

$$\Pi = (\underline{\phi}^-(\zeta) \otimes \underline{\phi}^+(\bar{\zeta})) \tag{2.69}$$

with $\underline{\phi}^{\pm}(\zeta) = \Sigma_i e^{\pm \zeta s_i/a}/\sqrt{2a\rho_0}\underline{e}_i$. While $T(\zeta)$ is the upper triangular matrix

$$T(\zeta)_{ij} = \begin{cases} \dfrac{\zeta S \delta_{ij}}{K_i + \zeta^2 M_i} + \dfrac{\sinh \zeta(s_i - s_j)}{a\rho_0} & i \leqslant j \\ 0 & i > j, \end{cases} \tag{2.70}$$

we use the formula

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{\Pi(\zeta) + T(\zeta)} = -\frac{1}{T(\zeta)} + \frac{1}{T(\zeta)}\Pi(\zeta)\frac{1}{\Pi(\zeta) + T(\zeta)} \tag{2.71}$$

$$= -\sum_{n=0}^{\infty} \frac{(-1)^n}{T(\zeta)}\left(\Pi(\zeta)\frac{1}{T(\zeta)}\right)^n, \tag{2.72}$$

valid for all ζ for which the series converges.

Matrix $T(\zeta)$ is invertible and its inverse $T(\zeta)^{-1}$ is a lower triangular matrix with $(T(\zeta)^{-1})_{ii} = 1/(T(\zeta))_{ii}$. The eigenvalues of $T(\zeta)^{-1}$ are $1/(T(\zeta))_{ii}$ and we can write

$$T(\zeta)^{-1} = D(\zeta)\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}, \tag{2.73}$$

where $D(\zeta)$ is a unitary matrix, analytic for $\zeta \in \mathbb{C}\backslash\{0\}$, and

$$(\tilde{T}(\zeta)^{-1})_{ij} = \frac{1}{(T(\zeta))_{ii}}\delta_{ij} = \frac{K_i + \zeta^2 M_i}{\zeta S}\delta_{ij}. \tag{2.74}$$

We obtain for $\Gamma_+(\zeta)^{-1}$ the expression

$$\Gamma_+(\zeta)^{-1} = -D(\zeta)\sum_{n=0}^{\infty}(-1)^n(\underline{\psi}(\zeta) \otimes \underline{\chi}(\zeta))^n\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}, \tag{2.75}$$

with

$$(\underline{\psi}(\zeta))_i = \frac{K_i + \zeta^2 M_i}{\zeta S}(D(\zeta)^{-1}\underline{\phi}^-(\zeta))_i, \tag{2.76}$$

$$(\underline{\chi}(\zeta))_i = (D(\zeta)^{-1}\underline{\phi}^+(\bar{\zeta}))_i. \tag{2.77}$$

Then

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{T(\zeta)} + \sum_{n=0}^{\infty}(-1)^n(\langle\underline{\chi}(\zeta), \underline{\psi}(\zeta)\rangle_{\mathbb{C}^n})^n D(\zeta)\underline{\psi}(\zeta) \otimes \underline{\chi}(\zeta)\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}. \tag{2.78}$$

For all ζ for which the series converges, one has

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{T(\zeta)} + \frac{D(\zeta)\underline{\psi}(\zeta) \otimes \underline{\chi}(\zeta)\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}}{1 + \langle\underline{\chi}(\zeta), \underline{\psi}(\zeta)\rangle_{\mathbb{C}^n}}. \tag{2.79}$$

Consider the scalar product in $\mathbb{C}^n$:

$$\langle \underline{\chi}(\zeta), \underline{\psi}(\zeta)\rangle_{\mathbb{C}^n} = \sum_{i=1}^{n} \overline{(D(\zeta)^{-1}\underline{\phi}^{+}(\bar{\zeta}))_i} \frac{K_i + \zeta^2 M_i}{\zeta S} (D(\zeta)^{-1}\underline{\phi}^{-}(\zeta))_i. \tag{2.80}$$

Notice that, for $\lambda \in i\mathbb{R}\backslash\{0\}$, $\langle \underline{\chi}(\lambda), \underline{\psi}(\lambda)\rangle_{\mathbb{C}^n} \in i\mathbb{R}$ and

$$-i\langle \underline{\chi}(\lambda), \underline{\psi}(\lambda)\rangle_{\mathbb{C}^n} \to +\infty \quad \text{for } \lambda \to +i\infty, \tag{2.81}$$

$$-i\langle \underline{\chi}(\lambda), \underline{\psi}(\lambda)\rangle_{\mathbb{C}^n} \to -\infty \quad \text{for } \lambda \to i0^{+}. \tag{2.82}$$

Then there exists at least one point $\lambda \in i\mathbb{R}$ in which $\langle \underline{\chi}(\lambda), \underline{\psi}(\lambda)\rangle_{\mathbb{C}^n} = 0$. In a neighborhood of this point the series converges and defines an analytic function. By (2.79) and (2.80) it is clear that $\Gamma_+(\zeta)^{-1}$ exists for any $\zeta \in \mathbb{C}\backslash\{0\}$. The same relations show that one can put $\Gamma_+(\zeta)^{-1} := 0$ if $\zeta = i\sqrt{K_j/M_j}$, $j = 1, \ldots, n$. □

The following theorem completely characterizes the spectrum of $\hat{A}$.

Theorem 2.3: *The essential spectrum of $\hat{A}$ is purely absolutely continuous and*

$$\sigma_{\mathrm{ess}}(\hat{A}) = \sigma_{\mathrm{ac}}(\hat{A}) = i\mathbb{R}, \quad \sigma_{pp}(\hat{A}) = \{0\}. \tag{2.83}$$

Any vector of the kind

$$\left(\frac{1}{2}\sum_{1\le j\le n} \sigma_j \operatorname{sgn}(x - s_j), 0, -\sum_{1\le j\le n} \frac{S}{K_j}\sigma_j \underline{e}_j, \underline{0}\right), \tag{2.84}$$

with

$$\sum_{1\le j\le n} \sigma_j = 0, \tag{2.85}$$

is an eigenvector corresponding to the $(n-1)$-fold degenerate eigenvalue $\lambda = 0$.

The generalized eigenfunctions $\hat{\Phi}^{\pm}(\lambda)$ corresponding to the point of the absolutely continuous spectrum relative to right $(+)$ and left $(-)$ incidence are given by

$$\hat{\Phi}^{\pm}(\lambda, x) = (\hat{\phi}_p^{\pm}(\lambda, x), \hat{\phi}_v^{\pm}(\lambda, x), \hat{\underline{\phi}}_{\underline{y}}^{\pm}(\lambda), \hat{\underline{\phi}}_{\underline{z}}^{\pm}(\lambda)), \quad \lambda \in i\mathbb{R}, \tag{2.86}$$

$$\hat{\phi}_p^{\pm}(\lambda, x) = Ce^{\pm\lambda x/a} \mp \frac{C}{2a\rho_0} \sum_{1\le i,j\le n} (\Gamma_+(\lambda)^{-1})_{ij} e^{\pm\lambda s_j/a} \operatorname{sgn}(x - s_i) e^{-\lambda|x - s_i|/a}, \tag{2.87}$$

$$\hat{\phi}_v^{\pm}(\lambda, x) = \mp C\frac{e^{\pm\lambda x/a}}{a\rho_0} \mp \frac{C}{2a^2\rho_0^2} \sum_{1\le i,j\le n} (\Gamma_+(\lambda)^{-1})_{ij} e^{\pm\lambda s_j/a} e^{-\lambda|x - s_i|/a}, \tag{2.88}$$

$$\hat{\underline{\phi}}_{\underline{y}}^{\pm}(\lambda) = \pm\frac{SC}{a\rho_0} \sum_{1\le i,j\le n} (\Gamma_+(\lambda)^{-1})_{ij} \frac{e^{\pm\lambda s_j/a}}{K_i + \lambda^2 M_i} \underline{e}_i, \tag{2.89}$$

$$\hat{\underline{\phi}}_{\underline{z}}^{\pm}(\lambda) = \pm\frac{\lambda SC}{a\rho_0} \sum_{1\le i,j\le n} (\Gamma_+(\lambda)^{-1})_{ij} \frac{e^{\pm\lambda s_j/a}}{K_i + \lambda^2 M_i} \underline{e}_i, \tag{2.90}$$

with $C = \sqrt{a\rho_0/(4\pi)}$.

Proof: For $\zeta \in \rho(A) \cap \rho(\hat{A})$, $(-\hat{A} + \zeta)^{-1} - (-A + \zeta)^{-1}$ is of finite rank; then from Weyl's criterion [see, e.g., Reed and Simon (1978) Theorem XIII.14] one has $\sigma_{\mathrm{ess}}(\hat{A}) = \sigma_{\mathrm{ess}}(A) = i\mathbb{R}$. Moreover, by the Birman-Kato invariance principle, the wave operators $\Omega_{\pm}(\hat{A}, A)$ exist and are complete [see,

e.g., Reed and Simon (1979), Corollary 2 to Theorem XI.11]. Thus $\sigma_{\mathrm{ac}}(\hat{A})=\sigma_{\mathrm{ac}}(A)$.

Let $\hat{\mu}_{\Psi}^{sc}$ be the singular continuous part of the spectral measure on $i\mathbb{R}$ corresponding to $\hat{A}$ and Ψ. Since $\|\breve{G}(\zeta)\Psi\|<\infty$ for all $\zeta\in\mathbb{C}\backslash\sigma_{pp}(A)$ and for all $\Psi\in D$,

$$D:=\{\Psi\equiv(p,v,\underline{y},\underline{z}):p\in L^1(\mathbb{R})\cap L^2(\mathbb{R}),\ v\in L^1(\mathbb{R})\cap L^2(\mathbb{R})\},\tag{2.91}$$

by Lemma 2 and Reed and Simon (1978), Theorem XIII.19, one has supp $\hat{\mu}_{\Psi}^{sc}\subseteq\{0\}\cup\sigma_{pp}(A)$, i.e., supp $\hat{\mu}_{\Psi}^{sc}=\emptyset$, since $\hat{\mu}_{\Psi}^{sc}$ has no atoms by its definition. Since D is dense this gives $\sigma_{sc}(\hat{A})=\emptyset$.

One can check that any vector Ψ of the kind (2.84) is in the domain of $\hat{A}$ and solves the equation $\hat{A}\Psi=0$. The degeneration of eigenvalue $\{0\}$ follows from condition (101).

Suppose now $\lambda\in i\mathbb{R}\backslash\{0\}$ and consider the equation $\hat{A}\Psi=\lambda\Psi$. This produces, if $\Psi\equiv(p,v,\underline{y},\underline{z})$, the equation

$$v''-\frac{\lambda^2}{a^2}v=-\frac{\lambda}{a^2\rho_0}\sum_{1\leqslant j\leqslant n}\sigma_j\delta_{s_j},\tag{2.92}$$

with $\sigma_i\in\mathbb{C}$, $i=1,\ldots,n$, which has no square integrable solution.

The expression for the generalized eigenfunctions is a consequence of the Stone's formula [see, e.g., Reed and Simon (1972), Theorem VII.13], which gives the generalized expansion formula

$$\Psi=\mathrm{s}-\lim_{a\downarrow-\infty,b\uparrow\infty}\mathrm{s}-\lim_{\varepsilon\downarrow0}\frac{1}{2\pi}\int_a^b[\hat{R}(\lambda+\varepsilon)-\hat{R}(\lambda-\varepsilon)]\Psi d\lambda.\tag{2.93}$$

□

In the following lemma the asymptotic behavior of the oscillations of the thin walls is characterized. It is proved that the oscillators relax (as $|t|\to\infty$) toward their equilibrium positions for any initial data orthogonal to the eigenspace relative to eigenvalue zero. For example, this is true for any initial datum of the kind $\Psi_0\equiv(p,v,\underline{0},\underline{z})$, where the support of p is outside the interval containing the points $s_1,\cdots,s_n$ which denote the equilibrium position of the walls.

Lemma 2.4: Given Ψ_0 orthogonal to the eigenspace relative to eigenvalue zero, let us denote by $(\underline{y}(t),\underline{z}(t))$ the projection onto $\mathbb{C}^n\oplus\mathbb{C}^n$ of $e^{t\hat{A}}\Psi_0$. Then

$$\lim_{|t|\to\infty}\|\underline{y}(t)\|_{\mathbb{C}^n}=0\quad\text{and}\quad\lim_{|t|\to\infty}\|\underline{z}(t)\|_{\mathbb{C}^n}=0.$$

Proof: Let $\hat{P}(dk)$ be the projection-valued measure corresponding to the self-adjoint operator $-i\hat{A}$. Since Ψ_0 is in the absolutely continuous subspace, for any Ψ the bounded complex measure $\langle\langle\Psi,\hat{P}(dk)\Psi_0\rangle\rangle$ is absolutely continuous with respect to the Lebesgue measure and hence its density belongs to $L^1(\mathbb{R})$. Thus by the spectral theorem and Riemann-Lebesgue lemma,

$$\lim_{|t|\to\infty}\langle\langle\Psi,e^{t\hat{A}}\Psi_0\rangle\rangle=\lim_{|t|\to\infty}\int_{\mathbb{R}}e^{-itk}\langle\langle\Psi,\hat{P}(dk)\Psi_0\rangle\rangle=0.\tag{2.94}$$

By taking $\Psi=(0,0,\underline{e}_i,\underline{0})$ and $\Psi=(0,0,\underline{0},\underline{e}_i)$, $i=1,\ldots,n$, one then obtains

$$\lim_{|t|\to\infty}y_i(t)=0\quad\text{and}\quad\lim_{|t|\to\infty}z_i(t)=0.\tag{2.95}$$

□

In order to obtain a more precise estimate on the asymptotic behavior of solutions of Eq. (2.62), for particular initial conditions, a detailed analysis of $\Gamma(\lambda)^{-1}$ is required. For example, in specific cases one can prove the existence of frequencies that are totally transmitted by the array of oscillators.

III. KRONIG-PENNEY MODEL IN ACOUSTICS

It is possible to extend the previous construction to the case of an array of infinitely many oscillators. We prove that in the case of a periodic array of identical oscillators the energy spectrum shows a band structure.

As a first step we define the operator $\hat{A}$ introduced in Sec. II when $\mathcal{S}=\{s_1,s_2,\ldots\}$ is a denumerable set such that

$$d := \inf_{i\neq j}|s_i - s_j| > 0 \quad i,j \in \mathbb{N}. \tag{3.1}$$

Defining the linear map

$$\tau(p,v,\underline{y},\underline{z}) := \sum_{j=1}^{\infty} (v(s_j) - z_j)\underline{e}_j, \tag{3.2}$$

where $\{\underline{e}_j\}_1^\infty$ is the usual complete orthonormal system for ℓ^2, one has the following.

Lemma 3.1: τ is bounded as a map on $H^1(\mathbb{R})\oplus H^1(\mathbb{R})\oplus \ell^2\oplus\ell^2$ to ℓ^2.

Proof: We will follow closely Albeverio *et al.* (2005). Let $\{I_j\}_1^\infty$ be a partition of $\mathbb{R}$ and let $K(x-y)$ be the kernel of $(-\Delta+1)^{-1/2}$. Since

$$v(x) = \sum_{j=1}^{\infty} \int_{I_j} K(x-y)[(-\Delta+1)^{1/2}v](y)dy, \tag{3.3}$$

to prove the lemma amounts to show that the infinite matrix

$$M_{ij} := \left(\int_{I_j} K(x-s_i)^2 dx\right)^{1/2} \tag{3.4}$$

corresponds to a bounded linear operator M on ℓ^2. By Lemma C.3 in Albeverio *et al.* (2005), one has

$$\|M\|^2_{\ell^2,\ell^2} \leqslant \sup_i \sum_{j=1}^{\infty} \left(\int_{I_j} K(x-s_i)^2 dx\right)^{1/2} \sup_j \sum_{i=1}^{\infty} \left(\int_{I_j} K(x-s_i)^2 dx\right)^{1/2}. \tag{3.5}$$

Since

$$\frac{1}{\sqrt{x}} = \frac{2}{\pi}\int_0^\infty \frac{d\mu}{x+\mu^2}, \quad x>0,$$

by functional calculus one has

$$K(x-y) = \frac{1}{\pi}\int_0^\infty \frac{e^{-\sqrt{1+\mu^2}|x-y}}{\sqrt{1+\mu^2}} d\mu. \tag{3.6}$$

By taking $I_j=[s_j-\varepsilon_j, s_j+\delta_j)$, where ε_j is one half the distance between s_j and the preceding point and δ_j is one half the distance between s_j and the successive point, a straightforward calculation leads to

$$\int_{I_j} K(x-s_i)^2 dx \leqslant \frac{2}{d^2\pi^2} e^{-|s_i-s_j|/\sqrt{2}}, \tag{3.7}$$

from where the estimate $\|M\|_{\ell^2,\ell^2}<+\infty$ follows immediately.

The construction proceeds now along the same lines as in the case of a finite set of points. We state the final result:

Theorem 3.2: *Let* $\{K_j\}_1^\infty$ $\{M_j\}_1^\infty$, $K_j>0$, $M_j>0$ *be in* ℓ^∞ *and suppose that* $\{K_j/M_j\}_1^\infty$ *and* $\{1/M_j\}_1^\infty$ *are in* ℓ^∞ *too. The linear operator*

$$\hat{A}:D(\hat{A}) \subset L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \ell^2 \oplus \ell^2 \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \ell^2 \oplus \ell^2, \tag{3.8}$$

$$\begin{aligned} D(\hat{A}) = \{(p,v,\underline{y},\underline{z}):& p \in L^2(\mathbb{R}) \cap H^1(\mathbb{R}\setminus\mathcal{S}), v \in H^1(\mathbb{R}), \underline{y} \in \ell^2, \underline{z} \in \ell^2, p(s_i^+) - p(s_i^-) = \sigma_i, v(s_j) \\ &= z_j, \underline{\sigma} \in \ell^2\}, \end{aligned} \tag{3.9}$$

$$\hat{A}(p,v,\underline{y},\underline{z}) := \left(-a^2\rho_0 \frac{dv}{dx}, -\frac{1}{\rho_0}\frac{dp_0}{dx}, \underline{z}, -\sum_{j=1}^{\infty}\left(\frac{K_j}{M_j}y_j + \frac{S}{M_j}\sigma_j\right)\underline{e}_j \right) \tag{3.10}$$

is real and skew-adjoint. Here $p_0 \in \bar{H}^1(\mathbb{R})$,

$$p_0(x) := p(x) - \frac{1}{2}\sum_{j=1}^{\infty}\sigma_j \operatorname{sgn}(x-s_j), \tag{3.11}$$

denotes the regular part of p. The resolvent of $\hat{A}$ *is given by*

$$(-\hat{A}+\zeta)^{-1} = (-A+\zeta)^{-1} + \sum_{i,j=1}^{\infty}(\Gamma(\zeta)^{-1})_{ij} G_\zeta^i \otimes \breve{G}_{\bar{\zeta}}^j, \quad \zeta \in C\setminus i\mathbb{R}. \tag{3.12}$$

Now we can proceed to the study of a periodic system. We use the same notation of Albeverio *et al.* (2005).

In this case $\mathcal{S}$ will be the "Bravais" lattice,

$$\mathcal{S} = \{nL : n \in \mathbb{Z}\}, \quad L>0, \tag{3.13}$$

and $\hat{\mathcal{S}}$ the "Brillouin" zone,

$$\hat{\mathcal{S}} = \left[-\frac{b}{2},\frac{b}{2}\right), \quad b = \frac{2\pi}{L}. \tag{3.14}$$

We consider a Hilbert space $\mathcal{H}$ on $L^2\oplus L^2\oplus\ell^2\oplus\ell^2$ in which the scalar product is defined by

$$\frac{1}{a^2\rho_0}\langle p_1,p_2\rangle + \rho_0\langle v_1,v_2\rangle + \frac{K}{S}\langle \underline{y}_1,\underline{y}_2\rangle + \frac{M}{S}\langle \underline{z}_1,\underline{z}_2\rangle \tag{3.15}$$

where $\langle\cdot,\cdot\rangle$ represents either the usual scalar product in L^2, when concerning pressure and velocity fields, or the usual scalar product in ℓ^2, for $\underline{y}$ and $\underline{z}$.

M, K, and S are positive constants representing the mass of oscillating walls, the elastic constant of the springs, and the area of the transverse section of the pipe.

The Hilbert space $\mathcal{H}$ can be decomposed as

$$\mathcal{H} = \tilde{W}^{-1}\hat{\mathcal{H}}(\hat{\mathcal{S}},b^{-1}d\theta;L^2([-L/2,L/2)) \oplus L^2([-L/2,L/2)) \oplus \mathbb{C}\oplus\mathbb{C}) \tag{3.16}$$

$$= \tilde{W}^{-1}\int_{[-b/2,b/2)}^{\oplus}\frac{d\theta}{b}(L^2([-L/2,L/2)) \oplus L^2([-L/2,L/2)) \oplus \mathbb{C}\oplus\mathbb{C}), \tag{3.17}$$

where

$$\tilde{W}:\mathcal{H} \to \hat{\mathcal{H}}(\hat{\mathcal{S}},b^{-1}d\theta;L^2([-L/2,L/2)) \oplus L^2([-L/2,L/2)) \oplus \mathbb{C}\oplus\mathbb{C}), \tag{3.18}$$

$$\tilde{W}(p,v,\underline{y},\underline{z}) \equiv ((\tilde{W}p)(\theta,\nu),(\tilde{W}v)(\theta,\nu),(\tilde{W}\underline{y})(\theta),(\tilde{W}\underline{z})(\theta)), \tag{3.19}$$

$$(\tilde{W}p)(\theta,\nu) \equiv \tilde{p}(\theta,\nu) = \sum_{n\in Z} e^{in\theta L} p(\nu+nL), \tag{3.20}$$

$$(\tilde{W}v)(\theta,\nu) \equiv \tilde{v}(\theta,\nu) = \sum_{n\in Z} e^{in\theta L} v(\nu+nL), \tag{3.21}$$

$$(\tilde{W}\underline{y})(\theta) \equiv \tilde{y}(\theta) = \sum_{n\in Z} e^{in\theta L} y_n, \tag{3.22}$$

$$(\tilde{W}\underline{z})(\theta) \equiv \tilde{z}(\theta) = \sum_{n\in Z} e^{in\theta L} z_n \quad \nu \in [-L/2,L/2), \quad \theta \in [-b/2,b/2), \tag{3.23}$$

and

$$\tilde{W}^{-1}:\hat{\mathcal{H}}(\hat{\mathcal{S}},b^{-1}d\theta;L^2([-L/2,L/2)) \oplus L^2([-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C}) \to \mathcal{H}, \tag{3.24}$$

$$\tilde{W}^{-1}(\tilde{p},\tilde{v},\underline{y},\underline{z}) \equiv ((\tilde{W}^{-1}\tilde{p})(\nu+nL),(\tilde{W}^{-1}\tilde{v})(\nu+nL),\{(\tilde{W}^{-1}\tilde{y})_n\},\{(\tilde{W}^{-1}\tilde{z})_n\}), \tag{3.25}$$

$$(\tilde{W}^{-1}\tilde{p})(\nu+nL) = b^{-1}\int_{-b/2}^{b/2} d\theta e^{-in\theta L}\tilde{p}(\theta,\nu), \tag{3.26}$$

$$(\tilde{W}^{-1}\tilde{v})(\nu+nL) = b^{-1}\int_{-b/2}^{b/2} d\theta e^{-in\theta L}\tilde{v}(\theta,\nu), \tag{3.27}$$

$$(\tilde{W}^{-1}\tilde{y})_n = b^{-1}\int_{-b/2}^{b/2} d\theta e^{-in\theta L}\tilde{y}(\theta), \tag{3.28}$$

$$(\tilde{W}^{-1}\tilde{z})_n = b^{-1}\int_{-b/2}^{b/2} d\theta e^{-in\theta L}\tilde{z}(\theta) \quad \nu \in [-L/2, \quad L/2), \quad n \in \mathbb{Z}. \tag{3.29}$$

The scalar product in $L^2([-L/2,L/2)) \oplus L^2([-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C}$ is defined by

$$\frac{1}{a^2\rho_0}\langle\tilde{p}_1,\tilde{p}_2\rangle_{L/2} + \rho_0\langle\tilde{v}_1,\tilde{v}_2\rangle_{L/2} + \frac{K}{S}\bar{\tilde{y}}_1\tilde{y}_2 + \frac{M}{S}\bar{\tilde{z}}_1\tilde{z}_2, \tag{3.30}$$

where $\langle\cdot,\cdot\rangle_{L/2}$ indicates the usual scalar product in $L^2([-L/2,L/2))$.

From Theorem 3.2 we obtain the following.

Corollary 3.3: The linear operator

$$\hat{A}:D(\hat{A}) \subset \mathcal{H} \to \mathcal{H}, \tag{3.31}$$

$$D(\hat{A}) = \{(p,v,\underline{y},\underline{z}):p \in L^2(\mathbb{R}) \cap H^1(\mathbb{R}\setminus\mathcal{S}), v \in H^1(\mathbb{R}), \underline{y} \in \ell^2, \underline{z} \in \ell^2, p(nL^+) - p(nL^-) = \sigma_n, v(nL) = z_n \ \forall\, n \in \mathbb{Z}, \underline{\sigma} \in \ell^2\}, \tag{3.32}$$

$$\hat{A}(p,v,\underline{y},\underline{z}) := \left(-a^2\rho_0\frac{dv}{dx},-\frac{1}{\rho_0}\frac{dp_0}{dx},\underline{z},-\frac{K}{M}\underline{y}-\frac{S}{M}\underline{\sigma}\right), \tag{3.33}$$

where the regular part of $p(x)$, *denoted with* $p_0 \in \bar{H}^1(\mathbb{R})$, is

$$p_0(x) = p(x) - \frac{1}{2}\sum_{n\in Z}\sigma_n \operatorname{sgn}(x-nL), \tag{3.34}$$

is real and skew-adjoint.

We want to study the spectral structure of $\hat{A}$. To this aim we introduce the family of operators $\hat{A}(\theta)$:

$$\hat{A}(\theta):D(\hat{A}(\theta)) \subset L^2((-L/2,L/2)) \oplus L^2((-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C} \to L^2((-L/2,L/2)) \oplus L^2((-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C}, \tag{3.35}$$

$$\begin{aligned} D(\hat{A}(\theta)) = \Bigg\{ & (\tilde{p}(\theta),\tilde{v}(\theta),\tilde{y}(\theta),\tilde{z}(\theta)):\tilde{p}(\theta) \in H^1((-L/2,L/2)\setminus\{0\}),\tilde{v}(\theta) \in H^1((-L/2,L/2)),\tilde{y}(\theta) \\ & \in \mathbb{C},\tilde{z}(\theta) \in \mathbb{C}\tilde{p}(\theta,0^+) - \tilde{p}(\theta,0^-) = \tilde{\sigma}(\theta),\tilde{v}(\theta,0) = \tilde{z}(\theta),\tilde{\sigma}(\theta) \in \mathbb{C},\tilde{p}\left(\theta,-\frac{L}{2}^+\right) \\ & = e^{i\theta L}\tilde{p}\left(\theta,\frac{L}{2}^-\right),\tilde{v}\left(\theta,-\frac{L}{2}^+\right) = e^{i\theta L}\tilde{v}\left(\theta,\frac{L}{2}^-\right)\Bigg\}; \quad \forall\ \theta \in \left[-\frac{b}{2},\frac{b}{2}\right) \end{aligned} \tag{3.36}$$

$$\hat{A}(\theta)(\tilde{p}(\theta),\tilde{v}(\theta),\tilde{y}(\theta),\tilde{z}(\theta)) := \left(-a^2\rho_0\frac{d\tilde{v}(\theta)}{d\nu},-\frac{1}{\rho_0}\frac{d\tilde{p}_0(\theta)}{d\nu},\tilde{z}(\theta),-\frac{K}{M}\tilde{y}(\theta)-\frac{S}{M}\tilde{\sigma}(\theta)\right), \tag{3.37}$$

where $\tilde{p}_0(\theta) \in H^1(\mathbb{R})$ is the regular part of $\tilde{p}(\theta)$,

$$\tilde{p}_0(\theta,\nu) = \tilde{p}(\theta,\nu) - \frac{1}{2}\tilde{\sigma}(\theta)\operatorname{sgn}(\nu). \tag{3.38}$$

Boundary conditions for $\tilde{p}(\theta,\nu)$ and $\tilde{v}(\theta,\nu)$ in $\nu=0$ and $\nu=\pm L/2$ are such that all operators in this family are skew-adjoint with respect to the scalar product (3.30).

The operator $\hat{A}$ is related to $\hat{A}(\theta)$ by the relation (see Albeverio *et al.* (2005))

$$\tilde{W}\hat{A}\tilde{W}^{-1} = \int_{[-b/2,b/2)}^{\oplus}\frac{d\theta}{b}\hat{A}(\theta). \tag{3.39}$$

The spectrum of $\hat{A}(\theta)$ is described by the following

Theorem 3.4: *Let* $\theta \in [-b/2,b/2)$, *then the spectrum of* $\hat{A}(\theta)$ *is purely discrete, in particular its eigenvalues* $E_n(\theta)$ are given by

$$E_n(\theta) = \lambda_n(\theta) = 2i\xi_n(\theta)\frac{a}{L}; \quad n \in \mathbb{Z}, \quad \xi_n(\theta) \in \mathbb{R}, \tag{3.40}$$

where $\xi_n(\theta)$ are the real solutions of

$$\sin\xi[\sin\xi - F(\xi)\cos\xi]\cos^2\frac{\theta L}{2} = \cos\xi[\cos\xi + F(\xi)\sin\xi]\sin^2\frac{\theta L}{2}, \tag{3.41}$$

$$F(\xi)=\frac{M}{M_g}\left(\pi^2\frac{\omega_o^2}{\omega_g^2}\frac{1}{\xi}-\xi\right);\quad M_g=\rho_0 SL,\quad \omega_o^2=\frac{K}{M},\quad \omega_g=2\pi\frac{a}{L}. \tag{3.42}$$

The corresponding eigenfunctions are

$$\Phi_n(\theta,x)=(\tilde{p}_n(\theta,\nu),\tilde{v}_n(\theta,\nu),\tilde{y}_n(\theta),\tilde{z}_n(\theta));\quad n\in\mathbb{Z},\quad \theta\in[-b/2,b/2), \tag{3.43}$$

$$\begin{aligned}\tilde{p}_n(\theta,\nu)=C_n\Bigg[&\left(\sin\left(\xi_n-\frac{\theta L}{2}\right)-F(\xi_n)\cos\left(\xi_n-\frac{\theta L}{2}\right)\right)\cos\frac{2\xi_n}{L}\nu+\\&-i\sin\left(\xi_n-\frac{\theta L}{2}\right)\left(\sin\frac{2\xi_n}{L}\nu-F(\xi_n)\frac{|\nu|}{\nu}\cos\frac{2\xi_n}{L}\nu\right)\Bigg],\end{aligned} \tag{3.44}$$

$$\begin{aligned}\tilde{v}_n(\theta,\nu)=-\frac{iC_n}{a\rho_0}\Bigg[&\left(\sin\left(\xi_n-\frac{\theta L}{2}\right)-F(\xi_n)\cos\left(\xi_n-\frac{\theta L}{2}\right)\right)\sin\frac{2\xi_n}{L}\nu\\&+i\sin\left(\xi_n-\frac{\theta L}{2}\right)\left(\cos\frac{2\xi_n}{L}\nu+F(\xi_n)\sin\frac{2\xi_n}{L}|\nu|\right)\Bigg],\end{aligned} \tag{3.45}$$

$$\tilde{y}_n(\theta)=-i\frac{C_nL}{a^2\rho_0\xi_n}\sin\left(\xi_n-\frac{\theta L}{2}\right), \tag{3.46}$$

$$\tilde{z}_n(\theta)=\frac{C_n}{a\rho_0}\sin\left(\xi_n-\frac{\theta L}{2}\right). \tag{3.47}$$

For $\theta\in[-b/2,b/2)$ *zero is an eigenvalue with eigenfunction*

$$\Psi_0=\left(C_0\left(\cos\frac{\theta L}{2}-i\sin\frac{\theta L}{2}\,\mathrm{sgn}(\nu)\right),0,2iC_0\frac{S}{K}\sin\frac{\theta L}{2},0\right). \tag{3.48}$$

Moreover, the following chain of inequalities holds:

$$\begin{aligned}&0<E_1(0)<E_1(-b/2)\leqslant E_2(-b/2)<E_2(0)\leqslant E_3(0)<E_3(-b/2)\leqslant E_4(-b/2)<E_4(0)\leqslant E_5(0)\\&<E_4(-b/2)\leqslant E_5(-b/2)<\cdots.\end{aligned} \tag{3.49}$$

In general, the eigenvalues $E_n(\theta)$ *are all distinct and nondegenerate. If* $\omega_o/\omega_g=n/2$ *with* $n\in\mathbb{N}$, *there is just one twofold degenerate eigenvalue equal to* $n\pi/2$; *such an eigenvalue corresponds to* $\theta=0$ *for n even and to* $|\theta|=b/2$ *for n odd.*

If $E(\theta)$ *is an eigenvalue then* $-E(\theta)$ *is an eigenvalue.*

Given $\theta\in[-b/2,b/2)$ *the following relation holds*:

$$E_n(-\theta)=E_n(\theta). \tag{3.50}$$

Proof: Eigenvalues and eigenfunctions (3.40)–(3.48) are given by direct computation. We solve the system of equations

$$\hat{A}(\theta)(\tilde{p}(\theta),\tilde{v}(\theta),\tilde{y}(\theta),\tilde{z}(\theta))=\lambda(\tilde{p}(\theta),\tilde{v}(\theta),\tilde{y}(\theta),\tilde{z}(\theta))\quad \lambda\in i\mathbb{R}; \tag{3.51}$$

with the condition $\tilde{v}(\theta,0)=\tilde{z}(\theta)$, the solution reads

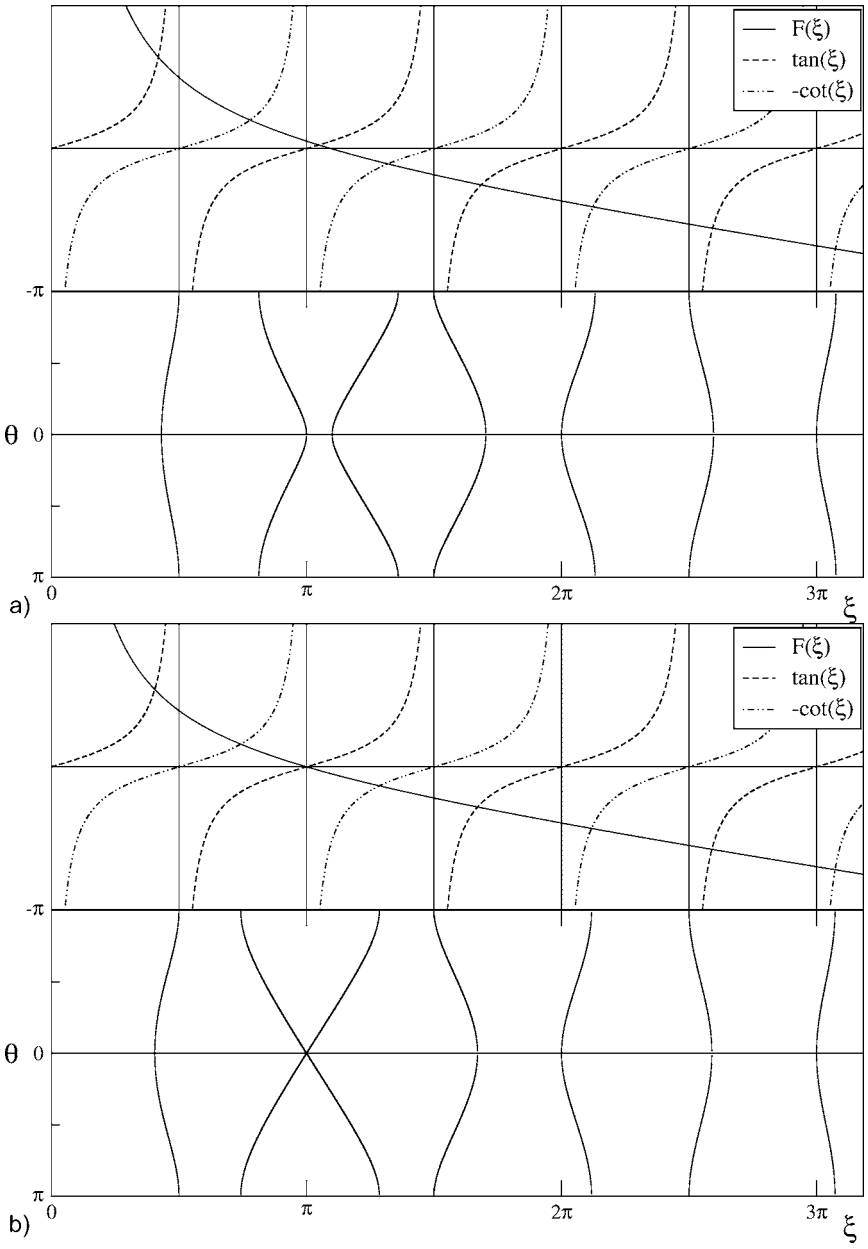

FIG. 1. Graphical solution of Eqs. (3.55) and (3.56). (b) and corresponding band structure for (a) a non-degenerate case (b) a degenerate case.

$$\tilde{p}(\theta,\nu) = C(\xi)\cos\frac{2\xi\nu}{L} + D(\xi)\left[\sin\frac{2\xi\nu}{L} - F(\xi)\mathrm{sgn}(\nu)\cos\frac{2\xi\nu}{L}\right], \tag{3.52}$$

$$\tilde{v}(\theta,\nu) = \frac{C(\xi)}{ia\rho_0}\sin\frac{2\xi\nu}{L} - \frac{D(\xi)}{ia\rho_0}\left[\cos\frac{2\xi\nu}{L} + F(\xi)\sin\frac{2\xi|\nu|}{L}\right], \tag{3.53}$$

where $\xi = -iL\lambda/(2a) \in \mathbb{R}$, and $C(\xi)$ and $D(\xi)$ are two unknown functions of ξ. To determine $C(\xi)$ and $D(\xi)$ we have to take into account the boundary conditions

$$\tilde{p}\left(\theta,-\frac{L}{2}^{+}\right)=e^{i\theta L}\tilde{p}\left(\theta,\frac{L}{2}^{-}\right),$$
$$\tilde{v}\left(\theta,-\frac{L}{2}^{+}\right)=e^{i\theta L}\tilde{v}\left(\theta,\frac{L}{2}^{-}\right). \tag{3.54}$$

This system has only the trivial solution $C(\xi)=0$ and $D(\xi)=0$ for the values of ξ for which the determinant of the matrix of the coefficients of the system is zero. The condition that the determinant is zero implies Eq. (3.41) for the eigenvalues. For ξ satisfying condition (3.41) the solutions of the system of dependent equations (3.54) give the eigenfunctions.

For $\theta=0$ and $\theta=-b/2$ relation (3.41) becomes

$$\tan\xi=0 \quad \text{or} \quad \tan\xi=F(\xi)=\frac{M}{M_g}\left(\pi^2\frac{\omega_o^2}{\omega_g^2}\frac{1}{\xi}-\xi\right); \quad \theta=0, \tag{3.55}$$

$$\cot\xi=0 \quad \text{or} \quad -\cot\xi=F(\xi)=\frac{M}{M_g}\left(\pi^2\frac{\omega_o^2}{\omega_g^2}\frac{1}{\xi}-\xi\right); \quad \theta=-b/2. \tag{3.56}$$

Graphic solutions of the transcendental equations (3.55) and (3.56) are given in the upper part of Figs. 1(a) and 1(b). The chain of inequalities (3.49) follows by the monotone behavior of $F(\xi)$.

Degeneration of eigenvalues for $\omega_o/\omega_g=n/2$, the fact that $-E(\theta)$ is an eigenvalue if $E(\theta)$ is an eigenvalue and relation (3.50) follow directly by Eq. (3.41) and by $F(\xi)=-F(-\xi)$. □

One can show that there is a band structure writing equation (3.41) as

$$\tan^2\frac{\theta L}{2}=\tan\xi\left[\frac{\tan\xi-F(\xi)}{1+F(\xi)\tan\xi}\right]. \tag{3.57}$$

It is possible to find solutions of Eq. (3.57) only for values of ξ such that the right-hand side is positive. In the lower part of Figs. 1(a) and 1(b) the resulting band structure is shown. The figures clearly show that the width of the gaps is connected to the structure of the spectrum. In particular, Fig. 1(b) shows that when there is a degenerate eigenvalue, $\omega_o/\omega_g=n\pi/2$ with $n\in\mathbb{N}$, a gap disappears because of the overlapping of two bands.

The bandwidth increases when the ratio M/M_g decreases.

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On inverse scattering for the multidimensional relativistic Newton equation at high energies

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Consider the Newton equation in the relativistic case (that is the Newton-Einstein equation) $\dot{p}=F(x)$, $F(x)=-\nabla V(x)$, $p=\dot{x}/\sqrt{1-(|\dot{x}|^2/c^2)}$, $p=\mathrm{d}p/\mathrm{d}t$, $\dot{x}=\mathrm{d}x/\mathrm{d}t$, $x \in C^1(\mathbb{R},\mathbb{R}^d)$, where $V \in C^2(\mathbb{R}^d,\mathbb{R})$, $|\partial_x^j V(x)| \leqslant \beta_{|j|}(1+|x|)^{-(\alpha+|j|)}$ for $|j| \leqslant 2$ and some $\alpha>1$. We give estimates and asymptotics for scattering solutions and scattering data for the equation for the case of small angle scattering. We show that at high energies the velocity valued component of the scattering operator uniquely determines the x-ray transform PF. Applying results on inversion of the x-ray transform P we obtain that for $d \geqslant 2$ the velocity valued component of the scattering operator at high energies uniquely determines F. In addition we show that our high energy asymptotics found for the configuration valued component of the scattering operator does not uniquely determine F. The results of the present work were obtained in the process of generalizing some results of Novikov to the relativistic case. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2206690]

I. INTRODUCTION

Consider the Newton equation in the relativistic case (that is the Newton-Einstein equation)

$$\dot{p} = F(x), \quad F(x) = -\nabla V(x),$$

$$p = \frac{\dot{x}}{\sqrt{1-\dfrac{|\dot{x}|^2}{c^2}}}, \quad \dot{p} = \frac{dp}{dt}, \quad \dot{x} = \frac{dx}{dt}, \quad x \in C^1(\mathbb{R},\mathbb{R}^d), \tag{1.1}$$

where

$$V \in C^2(\mathbb{R}^d,\mathbb{R}), \quad |\partial_x^j V(x)| \leqslant \beta_{|j|}(1+|x|)^{-(\alpha+|j|)} \tag{1.2}$$

for $|j| \leqslant 2$ and some $\alpha>1$ [here j is the multi-index $j \in (\mathbb{N} \cup \{0\})^d$, $|j|=\Sigma_{n=1}^d j_n$ and $\beta_{|j|}$ are positive real constants]. The equation (1.1) is an equation for $x=x(t)$ and is the equation of motion in $\mathbb{R}^d$ of a relativistic particle of mass $m=1$ and charge $e=1$ in an external electric field described by the scalar potential V (see Ref. 1 and, for example, Sec. 17 of Ref. 5). In this equation x is the position of the particle, p is its impulse, F is the force acting on the particle, t is the time and c is the speed of light.

For the equation (1.1) the energy

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$$E = c^2\sqrt{1+\frac{|p(t)|^2}{c^2}} + V(x(t))$$

is an integral of motion. We denote by B_c the Euclidean open ball whose radius is c and whose center is 0.

Yajima[10] studied in dimension 3 (without loss of generality for the case of dimension $d \geqslant 2$) the direct scattering of relativistic particle in an external electromagnetic field described by four vector $(V(x),\mathbf{A}(x))$ where the scalar potential V and the vector potential $\mathbf{A}$ are both rapidly decreasing. We recall the results of Yajima[10] in our case.

Under the conditions (1.2), the following is valid (see Ref. 10): for any $(v_-,x_-) \in B_c \times \mathbb{R}^d$, $v_- \neq 0$, the equation (1.1) has a unique solution $x \in C^2(\mathbb{R},\mathbb{R}^d)$ such that

$$x(t) = v_- t + x_- + y_-(t), \tag{1.3}$$

where $\dot{y}_-(t) \to 0$, $y_-(t) \to 0$, as $t \to -\infty$; in addition for almost any $(v_-,x_-) \in B_c \times \mathbb{R}^d$, $v_- \neq 0$,

$$x(t) = v_+ t + x_+ + y_+(t), \tag{1.4}$$

where $v_+ \neq 0$, $|v_+| < c$, $v_+ = a(v_-,x_-)$, $x_+ = b(v_-,x_-)$, $\dot{y}_+(t) \to 0$, $y_+(t) \to 0$, as $t \to +\infty$.

The map $S: B_c \times \mathbb{R}^d \to B_c \times \mathbb{R}^d$ given by the formulas

$$v_+ = a(v_-,x_-), \quad x_+ = b(v_-,x_-) \tag{1.5}$$

is called the scattering map for the equation (1.1); in addition, $a(v_-,x_-)$, $b(v_-,x_-)$ are called the scattering data for the equation (1.1).

By $\mathcal{D}(S)$ we denote the domain of definition of S; by $\mathcal{R}(S)$ we denote the range of S [by definition, if $(v_-,x_-) \in \mathcal{D}(S)$, then $v_- \neq 0$ and $a(v_-,x_-) \neq 0$].

Under the conditions (1.2), the map S has the following simple properties (see Ref. 10): for any $(v,x) \in B_c \times \mathbb{R}^d$, $(v,x) \in \mathcal{D}(S)$ if and only if $(-v,x) \in \mathcal{R}(S)$; $\mathcal{D}(S)$ is an open set of $B_c \times \mathbb{R}^d$ and $\mathrm{Mes}((B_c \times \mathbb{R}^d) \setminus \mathcal{D}(S)) = 0$ for the Lebesgue measure on $B_c \times \mathbb{R}^d$ induced by the Lebesgue measure on $\mathbb{R}^d \times \mathbb{R}^d$; the map $S: \mathcal{D}(S) \to \mathcal{R}(S)$ is continuous and preserves the element of volume, $a(v_-,x_-)^2 = v_-^2$.

If $V(x) \equiv 0$, then $a(v_-,x_-) = v_-$, $b(v_-,x_-) = x_-$, $(v_-,x_-) \in B_c \times \mathbb{R}^d$, $v_- \neq 0$. Therefore for $a(v_-,x_-)$, $b(v_-,x_-)$ we will use the following representation:

$$\begin{aligned} a(v_-,x_-) &= v_- + a_{sc}(v_-,x_-) \\ b(v_-,x_-) &= x_- + b_{sc}(v_-,x_-) \end{aligned} \quad (v_-,x_-) \in \mathcal{D}(S). \tag{1.6}$$

We will use the fact that, under the conditions (1.2), the map S is uniquely determined by its restriction to $\mathcal{M}(S) = \mathcal{D}(S) \cap \mathcal{M}$, where

$$\mathcal{M} = \{(v_-,x_-) \in B_c \times \mathbb{R}^d | v_- \neq 0, v_- x_- = 0\}.$$

Consider

$$T\mathbb{S}^{d-1} = \{(\theta,x) | \theta \in \mathbb{S}^{d-1}, \quad x \in \mathbb{R}^d, \theta x = 0\},$$

where $\mathbb{S}^{d-1}$ is the unit sphere in $\mathbb{R}^d$.

Consider the x-ray transform P which maps each function f with the properties

$$f \in C(\mathbb{R}^d,\mathbb{R}^m), \quad |f(x)| = O(|x|^{-\beta}), \quad \text{as } |x| \to \infty, \quad \text{for some } \beta > 1$$

into a function $Pf \in C(T\mathbb{S}^{d-1},\mathbb{R}^m)$, where Pf is defined by

$$Pf(\theta,x) = \int_{-\infty}^{+\infty} f(t\theta + x)\mathrm{d}t, \quad (\theta,x) \in T\mathbb{S}^{d-1}.$$

Concerning the theory of the x-ray transform, the reader is referred to Refs. 8, 2, 6, and 7.

Let

$$\mu(c,d,\tilde{\beta},\alpha,r_v,r_x,r)=\frac{1}{\sqrt{1+\dfrac{r_v^2}{4(c^2-r_v^2)}}}\frac{2^{2\alpha+6}(1+3\tilde{\beta}/c)d^2\sqrt{d}\tilde{\beta}(r_v/\sqrt{2}+1-r)^3}{r(\alpha-1)(r_v/\sqrt{2}-r)^4(1+r_x/\sqrt{2})^{\alpha-1}} \tag{1.7a}$$

and let $z=z(c,d,\tilde{\beta},\alpha,r_x,r)$, $z_1=z_1(c,d,\beta_1,\alpha,r_x,r)$, and $z_2=z_2(c,d,\beta_1,\alpha,r_x)$ be defined as the roots of the following equations:

$$\mu(c,d,\tilde{\beta},\alpha,z,r_x,r)=1, \quad z\in\,]\sqrt{2}r,c[, \tag{1.7b}$$

$$\frac{z_1}{\sqrt{1-\dfrac{z_1^2}{c^2}}}-\frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(z_1/\sqrt{2}-r)(r_x/\sqrt{2}+1)^{\alpha}}=0, \quad z_1\in\,]\sqrt{2}r,c[, \tag{1.7c}$$

$$\frac{z_2}{\sqrt{1-\dfrac{z_2^2}{c^2}}}-\frac{8\beta_1\sqrt{d}}{\alpha(z_2/\sqrt{2})(1+r_x/\sqrt{2})^{\alpha}}=0, \quad z_2\in\,]0,c[, \tag{1.7d}$$

where r_v, r_x, and r are some non-negative numbers such that $0<r\leqslant 1$, $r<c/\sqrt{2}$, $\sqrt{2}r<r_v<c$, and where $\tilde{\beta}=\max(\beta_1,\beta_2)$.

The main results of the present work consist in the small angle scattering asymptotics and estimates for the scattering data a_{sc} and b_{sc} (and scattering solutions) for the equation (1.1) and in application of these asymptotics and estimates to inverse scattering for the equation (1.1) at high energies. Our main results include, in particular, Theorem 1.1 and Proposition 1.1 given below.

Theorem 1.1: *Let the conditions* (1.2) *be valid*, $\tilde{\beta}=\max(\beta_1,\beta_2)$, $(\theta,x)\in T\mathbb{S}^{d-1}$, *and let r be a positive constant such that* $0<r\leqslant 1$, $r<c/\sqrt{2}$. *Then*

$$PF(\theta,x)=\lim_{\substack{s\to c\\ s<c}}\frac{s}{\sqrt{1-\dfrac{s^2}{c^2}}}a_{sc}(s\theta,x), \tag{1.8a}$$

and, in addition,

$$\left|PF(\theta,x)-\frac{s}{\sqrt{1-\dfrac{s^2}{c^2}}}a_{sc}(s\theta,x)\right|\leqslant\frac{d^2\tilde{\beta}^2 2^{2\alpha+5}s(s/\sqrt{2}+1-r)^2}{\sqrt{1+\dfrac{s^2}{4(c^2-s^2)}}\alpha(\alpha-1)(s/\sqrt{2}-r)^4(1+|x|/\sqrt{2})^{2\alpha-1}} \tag{1.8b}$$

for $s<c$, $s>z(c,d,\tilde{\beta},\alpha,|x|,r)$, $s\geqslant z_1(c,d,\beta_1,\alpha,|x|,r)$;

$$\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau-\int_{0}^{+\infty}\int_{\tau}^{+\infty}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau+PV(\theta,x)\theta=\lim_{\substack{s\to c\\ s<c}}\frac{s^2}{\sqrt{1-\dfrac{s^2}{c^2}}}b_{sc}(s\theta,x) \tag{1.9a}$$

and, in addition,

$$\left|\frac{b_{sc}(s\theta,x)}{\sqrt{1-\frac{s^2}{c^2}}}-\frac{1}{c^2}PV(\theta,x)\theta+\frac{1}{s^2}\int_0^{+\infty}\int_\tau^{+\infty}F(u\theta+x)\mathrm{d}u\,\mathrm{d}\tau-\frac{1}{s^2}\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\,\mathrm{d}\tau\right|$$
$$\leqslant\sqrt{1-\frac{s^2}{c^2}}\left[C+\frac{d^3\sqrt{d}\left(\beta_2+3\frac{\beta_1\beta_2}{c}\right)\beta_1 2^{3\alpha+8}\left(\frac{s}{\sqrt{2}}+1-r\right)^3}{\left(1-\frac{3}{4}\frac{s^2}{c^2}\right)\alpha(\alpha-1)^2\left(\frac{s}{\sqrt{2}}-r\right)^6\left(1+\frac{|x|}{\sqrt{2}}\right)^{2\alpha-2}}\right] \tag{1.9b}$$

for $s<c$, $s>z(c,d,\tilde{\beta},\alpha,|x|,r)$, $s\geqslant\max(z_1(c,d,\beta_1,\alpha,|x|,r),z_2(c,d,\beta_1,\alpha,|x|))$ *and some constant* $C=C(c,d,\beta_0,\beta_1,\alpha,|x|)$ *which can be given explicitly.*

Consider the vector function w of (θ,x) arising on the left-hand side of (1.9a),

$$w(V,\theta,x)=\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau-\int_0^{+\infty}\int_\tau^{+\infty}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau+PV(\theta,x)\theta,\quad(\theta,x)\in T\mathbb{S}^{d-1}.$$

Proposition 1.1: The vector w as a function of potential V satisfying the conditions (1.2) *and of* $(\theta,x)\in T\mathbb{S}^{d-1}$ *has the following simple properties:*

(1) *under the conditions* (1.2), *for any potential V the vector* $w(V,\theta,x)$ *is orthogonal to* θ,
(2) *there exists a potential V which satisfies the conditions* (1.2) *and for which* $w(V,\theta,x)$ *is not null for all* $(\theta,x)\in T\mathbb{S}^{d-1}$,
(3) *for any spherical symmetric potential V satisfying the conditions* (1.2) *we have* $w(V,\theta,x)=0$ *for all* $(\theta,x)\in T\mathbb{S}^{d-1}$.

From (1.8a) and inversion formulas for the x-ray transform for $d\geqslant 2$ (see Refs. 8, 2, 6, and 7) it follows that a_{sc} determines uniquely F at high energies. Moreover for $d\geqslant 2$ methods of reconstruction of f from Pf (see Refs. 8, 2, 6, and 7) permit to reconstruct F from the velocity valued component a of the scattering map at high energies. The formula (1.9a) and the item (3) of Proposition 1.1 show that the first term of the asymptotics of b_{sc} does not uniquely determine the potential V or the force F. The item (2) of Proposition 1.1 ensures us that the asymptotics which was found for b_{sc} is nontrivial. Note that Nicoleau paid our attention to the fact that, in addition of the item (3) of Proposition 1.1, $w(V,\theta,x)$, $(\theta,x)\in T\mathbb{S}^{d-1}$, uniquely determines V satisfying (1.2) modulo spherical symmetric potentials.

Inverse scattering for the classical multidimensional Newton equation was first studied by Novikov[7] (the existence of the scattering states, asymptotic completeness and scattering map for the classical Newton equation was studied by Simon[9]). Novikov proved two formulas which link scattering data at high energies to the x-ray transform of F and V. These formulas are generalized to the relativistic case by the formulas (1.8a) and (1.9a) of Theorem 1.1. Then applying results on inversion of the x-ray transform, Novikov obtains that at high energies the velocity valued component of the scattering data determines uniquely the x-ray transform of F whereas the configuration valued component of the scattering operator determines uniquely the x-ray transform of V. Note that in the relativistic case [due to the formula (1.9a) and Proposition 1.1] the asymptotics of b_{sc} does not determine uniquely F. We follow Novikov's framework[7] to obtain our results. Note also that for the classical multidimensional Newton equation in a bounded open strictly convex domain an inverse boundary value problem at high energies was first studied in Ref. 3.

Further our paper is organized as follows. In Sec. II we transform the differential equation (1.1) with initial conditions (1.3) in an integral equation which takes the form $y_-=A_{v_-,x_-}(y_-)$. Then we study A_{v_-,x_-} on a suitable space and we give estimates and contraction estimates about A_{v_-,x_-} (Lemmas 2.1, 2.2, 2.3). In Sec. III we give estimates and asymptotics for the deflection $y_-(t)$ from (1.3) and for scattering data $a_{sc}(v_-,x_-)$, $b_{sc}(v_-,x_-)$ from (1.6) (Theorem 3.1 and Theorem 3.2). From these estimates and asymptotics the formulas (1.8a) and (1.9a) will follow when the parameters c, β_m, α, d, $\hat{v}_-$, x_- are fixed and $|v_-|$ increases [where $\beta_{|j|}$, α, d are constants from (1.2),

$\beta_m=\max(\beta_0,\beta_1,\beta_2)$; $\hat{v}_-=v_-/|v_-|$]. In these cases $\sup_{t\in\mathbb{R}}|\theta(t)|$ decreases, where $\theta(t)$ denotes the angle between the vectors $\dot{x}(t)=v_-+\dot{y}_-(t)$ and v_-, and we deal with small angle scattering. Note that, under the conditions of Theorem 3.1, without additional assumptions, there is the estimate $\sup_{t\in\mathbb{R}}|\theta(t)|<\frac{1}{4}\pi$ and we deal with rather small angle scattering (concerning the term "small angle scattering" see Ref. 7 and Sec. 20 of Ref. 4). Theorem 1.1 follows from Theorem 3.1 and Theorem 3.2. Section IV, Sec. V, and Sec. VI are devoted to Proofs of our Theorems and Lemmas.

II. A CONTRACTION MAP

Let us transform the differential equation (1.1) in an integral equation. Consider the function $g:\mathbb{R}^d\to B_c$ defined by

$$g(x)=\frac{x}{\sqrt{1+\frac{|x|^2}{c^2}}},$$

where $x\in\mathbb{R}^d$. One can see that g has, in particular, the following simple properties:

$$|g(x)-g(y)|\leqslant\sqrt{d}|x-y| \quad \text{for } x,y\in\mathbb{R}^d, \tag{2.1}$$

g is an infinitely smooth diffeomorphism between $\mathbb{R}^d$ and B_c, and its inverse is given by

$$\gamma(x)=\frac{x}{\sqrt{1-\frac{|x|^2}{c^2}}}, \quad x\in B_c.$$

Now, if x satisfies the differential equation (1.1) and the initial conditions (1.3), then x satisfies the integral equation

$$x(t)=v_-t+x_-+\int_{-\infty}^{t}\left[g\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(x(s))\mathrm{d}s\right)-v_-\right]\mathrm{d}\tau, \tag{2.2}$$

where $F(x)=-\nabla V(x)$, $v_-\in B_c\backslash\{0\}$.

For $y_-(t)$ this equation takes the form

$$y_-(t)=A_{v_-,x_-}(y_-)(t), \tag{2.3}$$

where

$$A_{v_-,x_-}(f)(t)=\int_{-\infty}^{t}\left[g\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f(s))\mathrm{d}s\right)-v_-\right]\mathrm{d}\tau, \quad v_-\in B_c\backslash\{0\}.$$

From (2.2), (1.2), and (2.1) [applied on "x"$=\gamma(v_-)+\int_{-\infty}^{\tau}F(x(s))\mathrm{d}s$ and "y"$=\gamma(v_-)$], and $y_-(t)\in C(\mathbb{R},\mathbb{R}^d)$, $y_-(t)\to 0$, as $t\to-\infty$, it follows, in particular, that

$$y_-(t)\in C^1(\mathbb{R},\mathbb{R}^d) \quad \text{and } |\dot{y}_-(t)|=O(|t|^{-\alpha}), \quad |y_-(t)|=O(|t|^{-\alpha+1}), \quad \text{as } t\to-\infty, \tag{2.4}$$

where $v_-\in B_c\backslash\{0\}$ and x_- are fixed.

Consider the complete metric space

$$M_{T,r}=\{f\in C^1(]-\infty,T],\mathbb{R}^d)|\ \|f\|_T\leqslant r\},$$

where

$$\|f\|_T = \max\left(\sup_{t\in]-\infty,T]} |\dot{f}(t)|, \sup_{t\in]-\infty,T]} |f(t) - t\dot{f}(t)| \right) \tag{2.5}$$

(where for $T=+\infty$ we understand $]-\infty,T]$ as $]-\infty,+\infty[$). From (2.4) it follows that, at fixed $T<+\infty$,

$$y_-(t) \in M_{T,r} \text{ for some } r \text{ depending on } y_-(t) \text{ and } T. \tag{2.6}$$

Lemma 2.1: Under the conditions (1.2), *the following is valid: if* $f\in M_{T,r}$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$, *then*

$$\|A_{v_-,x_-}(f)\|_T \leqslant \rho_T(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)$$
$$= \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}} \frac{2^{\alpha+1} d\beta_1 (|v_-|/\sqrt{2}+1-r)}{(\alpha-1)(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)T)^{\alpha-1}} \tag{2.7a}$$

for $T\leqslant 0$,

$$\|A_{v_-,x_-}(f)\|_T \leqslant \rho(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)$$
$$= \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}} \frac{2^{\alpha+2} d\beta_1 (|v_-|/\sqrt{2}+1-r)}{(\alpha-1)(|v_-|\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha-1}} \tag{2.7b}$$

for $T\leqslant +\infty$; *if* $f_1, f_2 \in M_{T,r}$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$, *then*

$$\|A_{v_-,x_-}(f_2) - A_{v_-,x_-}(f_1)\|_T \leqslant \lambda_T(c,d,\beta_2,\alpha,|v_-|,|x_-|,r)\|f_2-f_1\|_T,$$

$$\lambda_T(c,d,\beta_2,\alpha,|v_-|,|x_-|,r) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}(\alpha-1)}$$
$$\times \frac{2^{\alpha+2} d\sqrt{d}\beta_2 (|v_-|/\sqrt{2}+1-r)^2}{(|v_-|/\sqrt{2}-r)^3(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)T)^{\alpha-1}} \tag{2.8a}$$

for $T\leqslant 0$,

$$\|A_{v_-,x_-}(f_2) - A_{v_-,x_-}(f_1)\|_T \leqslant \lambda(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r)\|f_2-f_1\|_T,$$

$$\lambda(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}} \frac{2^{2\alpha+6}(\beta_2+3\beta_1\beta_2/c) d^2\sqrt{d}(|v_-|/\sqrt{2}+1-r)^3}{(\alpha-1)(|v_-|/\sqrt{2}-r)^4(1+|x_-|/\sqrt{2})^{\alpha-1}} \tag{2.8b}$$

for $T\leqslant +\infty$.

Note that

$$\max\left(\frac{\rho_T(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)}{r}, \lambda_T(c,d,\beta_2,\alpha,|v_-|,|x_-|,r) \right) \leqslant \mu_T(c,d,\tilde{\beta},\alpha,|v_-|,|x_-|,r)$$
$$= \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}} \frac{2^{\alpha+2} d\sqrt{d}\tilde{\beta}(|v_-|/\sqrt{2}+1-r)^2}{r(\alpha-1)(|v_-|/\sqrt{2}-r)^3(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)T)^{\alpha-1}} \tag{2.9a}$$

for $T\leqslant 0$,

$$\max\left(\frac{\rho(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)}{r},\ \lambda(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r)\right)$$

$$\leqslant \mu(c,d,\tilde{\beta},\alpha,|v_-|,|x_-|,r) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}}$$

$$\times \frac{2^{2\alpha+6}(1+3\tilde{\beta}/c)d^2\sqrt{d}\tilde{\beta}(|v_-|/\sqrt{2}+1-r)^3}{r(\alpha-1)(|v_-|/\sqrt{2}-r)^4(1+|x_-|/\sqrt{2})^{\alpha-1}} \tag{2.9b}$$

for $T\leqslant+\infty$, where $\tilde{\beta}=\max(\beta_1,\beta_2)$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$.

From Lemma 2.1 and the estimates (2.9) we obtain the following result.

Corollary 2.1: Under the conditions (1.2), $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$, *the following result is valid:*

if $\mu_T(c,d,\tilde{\beta},\alpha,|v_-|,|x_-|,r)<1$, *then* $A_{v_-x_-}$ *is a contraction map in* $M_{T,r}$ *for* $T\leqslant 0$;

if $\mu(c,d,\tilde{\beta},\alpha,|v_-|,|x_-|,r)<1$, *then* $A_{v_-x_-}$ *is a contraction map in* $M_{T,r}$ *for* $T\leqslant+\infty$.

Taking into account (2.6) and using Lemma 2.1, Corollary 2.1 and the lemma about the contraction maps we will study the solution $y_-(t)$ of the equation (2.3) in $M_{T,r}$.

We will use also the following results.

Lemma 2.2: Under the conditions (1.2), $f\in M_{T,r}$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$, *the following is valid:*

$$|\dot{A}_{v_-x_-}(f)(t)| \leqslant \zeta_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}}$$

$$\times \frac{d\beta_1 2^{\alpha+1}}{\alpha(|v_-|/\sqrt{2}-r)(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha}}, \tag{2.10}$$

$$|A_{v_-x_-}(f)(t)| \leqslant \xi_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}}$$

$$\times \frac{d\beta_1 2^{\alpha+1}}{(\alpha-1)\alpha(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha-1}}, \tag{2.11}$$

for $t\leqslant T$, $T\leqslant 0$;

$$A_{v_-x_-}(f)(t) = k_{v_-x_-}(f)t + l_{v_-x_-}(f) + H_{v_-x_-}(f)(t), \tag{2.12}$$

where

$$k_{v_-x_-}(f) = g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s+x_-+f(s))\mathrm{d}s\right) - v_-, \tag{2.13a}$$

$$l_{v_-,x_-}(f) = \int_{-\infty}^{0} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_- s + x_- + f(s))\mathrm{d}s \right) - v_- \right] \mathrm{d}\tau + \int_{0}^{+\infty} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_- s + x_- + f(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_- s + x_- + f(s))\mathrm{d}s \right) \right] \mathrm{d}\tau, \tag{2.13b}$$

$$|k_{v_-,x_-}(f)| \leqslant 2\zeta_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,0), \tag{2.14a}$$

$$|l_{v_-,x_-}(f)| \leqslant 2\xi_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,0), \tag{2.14b}$$

$$|\dot{H}_{v_-,x_-}(f)(t)| \leqslant \zeta_+(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}\alpha(|v_-|/\sqrt{2}-r)} \times \frac{d\beta_1 2^{\alpha+1}}{(1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r)t)^{\alpha}}, \tag{2.15}$$

$$|H_{v_-,x_-}(f)(t)| \leqslant \xi_+(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t) = \frac{1}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^2} \times \frac{d\beta_1 2^{\alpha+1}}{(1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r)t)^{\alpha-1}}, \tag{2.16}$$

for $T=+\infty$, $t\geqslant 0$.

Lemma 2.3: Let the conditions (1.2) *be valid,* $y_-(t)\in M_{T,r}$ *be a solution of* (2.3), $T=+\infty$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$, *then*

$$|k_{v_-,x_-}(y_-) - k_{v_-,x_-}(0)| \leqslant \varepsilon'_a(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r) = \frac{d\sqrt{d}\beta_2 2^{\alpha+3}(|v_-|/\sqrt{2}+1-r)}{\alpha(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha}} \times \frac{\rho(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}}, \tag{2.17a}$$

$$\left| \frac{k_{v_-,x_-}(y_-)}{\sqrt{1-\dfrac{|v_-|^2}{c^2}}} - \int_{-\infty}^{+\infty} F(x_- + v_- s)\mathrm{d}s \right| \leqslant \varepsilon_a(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r) = \frac{d\beta_2 2^{\alpha+3}(1+|v_-|/\sqrt{2}-r)\rho(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)}{\alpha(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha}}, \tag{2.17b}$$

$$|l_{v_-,x_-}(y_-) - l_{v_-,x_-}(0)| \leqslant \varepsilon_b(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r) = \frac{d^2\sqrt{d}(\beta_2+3\beta_1\beta_2/c)2^{2\alpha+6}(|v_-|/\sqrt{2}+1-r)^2}{\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^4(1+|x_-|/\sqrt{2})^{\alpha-1}} \times \frac{\rho(c,d,\beta_1,\alpha,|v_-|,|x_-|,r)}{\sqrt{1+|v_-|^2/(4(c^2-|v_-|^2))}}. \tag{2.17c}$$

Proofs of Lemmas 2.1, 2.2, 2.3 are given in Sec. V.

III. SMALL ANGLE SCATTERING

Under the conditions (1.2), for any $(v_-,x_-)\in B_c\times\mathbb{R}^d$, $v_-\neq 0$, the equation (1.1) has a unique solution $x\in C^2(\mathbb{R},\mathbb{R}^d)$ with the initial conditions (1.3). Consider the function $y_-(t)$ from (1.3). This function describes deflection from free motion.

Using Corollary 2.1 the lemma about contraction maps, and Lemmas 2.2 and 2.3 we obtain the following result.

Theorem 3.1: *Let the conditions (1.2) be valid,* $\mu(c,d,\widetilde{\beta},\alpha,|v_-|,|x_-|,r)<1$, $\widetilde{\beta}=\max(\beta_1,\beta_2)$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|<c$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $v_-x_-=0$. *Then the deflection* $y_-(t)$ *has the following properties:*

$$y_-\in M_{T,r},\quad T=+\infty, \tag{3.1}$$

$$|\dot{y}_-(t)|\leqslant \zeta_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t), \tag{3.2}$$

$$|y_-(t)|\leqslant \xi_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t)\quad \textit{for } t\leqslant 0, \tag{3.3}$$

$$y_-(t)=a_{sc}(v_-,x_-)t+b_{sc}(v_-,x_-)+h(v_-,x_-,t), \tag{3.4}$$

where

$$\left|a_{sc}(v_-,x_-)-\left[\frac{\gamma(v_-)+\int_{-\infty}^{+\infty}F(v_-s+x_-)\mathrm{d}s}{\sqrt{1+\dfrac{|\gamma(v_-)+\int_{-\infty}^{+\infty}F(v_-s+x_-)\mathrm{d}s|^2}{c^2}}}-v_-\right]\right|\leqslant \varepsilon'_a(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r), \tag{3.5a}$$

$$\left|\frac{a_{sc}(v_-,x_-)}{\sqrt{1-\dfrac{|v_-|^2}{c^2}}}-\int_{-\infty}^{+\infty}F(v_-s+x_-)\mathrm{d}s\right|\leqslant \varepsilon_a(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r), \tag{3.5b}$$

$$|b_{sc}(v_-,x_-)-l_{v_-,x_-}(0)|\leqslant \varepsilon_b(c,d,\beta_1,\beta_2,\alpha,|v_-|,|x_-|,r), \tag{3.5c}$$

$$|a_{sc}(v_-,x_-)|\leqslant 2\zeta_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,0), \tag{3.6a}$$

$$|b_{sc}(v_-,x_-)|\leqslant 2\xi_-(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,0), \tag{3.6b}$$

$$|\dot{h}(v_-,x_-,t)|\leqslant \zeta_+(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t), \tag{3.7}$$

$$|h(v_-,x_-,t)|\leqslant \xi_+(c,d,\beta_1,\alpha,|v_-|,|x_-|,r,t) \tag{3.8}$$

for $t\geqslant 0$, *where* $l_{v_-,x_-}(0)$ (*respectively*, ε'_a, ε_a, ε_b, ζ_-, ζ_+, ξ_- *and* ξ_+) *is defined in* (2.13b) [*respectively*, (2.17a), (2.17b), (2.17c), (2.10), (2.15), (2.11), *and* (2.16)].

We will use the following observations.

(I) Let $0<r\leqslant 1$, $r<c/\sqrt{2}$, $0\leqslant u$,

$$\frac{s_1}{\sqrt{1-\frac{s_1^2}{c^2}}}-\frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(s_1/\sqrt{2}-r)(u/\sqrt{2}+1)^{\alpha}}>\frac{s_2}{\sqrt{1-\frac{s_2^2}{c^2}}}-\frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(s_2/\sqrt{2}-r)(u/\sqrt{2}+1)^{\alpha}}$$

for $\sqrt{2}r<s_2<s_1<c$.

(II) Let $0<r\leqslant 1$, $r<c/\sqrt{2}$, $u\in\,]\sqrt{2}r,c[$,

$$\frac{u}{\sqrt{1-\frac{u^2}{c^2}}}-\frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(u/\sqrt{2}-r)(s_1/\sqrt{2}+1)^{\alpha}}>\frac{u}{\sqrt{1-\frac{u^2}{c^2}}}-\frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(u/\sqrt{2}-r)(s_2/\sqrt{2}+1)^{\alpha}}$$

for $0\leqslant s_2<s_1$.

(III) Let $0<r\leqslant 1$, $r<c/\sqrt{2}$, x some real non-negative number, $\tilde{\beta}=\max(\beta_1,\beta_2)$ and $\sqrt{2}r<s<c$ then

$$\mu(c,d,\tilde{\beta},\alpha,s,|x|,r)<1\Leftrightarrow s>z(c,d,\tilde{\beta},\alpha,|x|,r).$$

Observations (I) and (II) imply that $z_1(c,d,\beta_1,\alpha,s_2,r)>z_1(c,d,\beta_1,\alpha,s_1,r)$ for $\sqrt{2}r<s_2<s_1<c$ when c, β_1, α, d, r are fixed.

Theorem 3.1 gives, in particular, estimates for the scattering process and asymptotics for the velocity valued component of the scattering map when c, β_1, β_2, α, d, $\hat{v}_-$, x_- are fixed (where $\hat{v}_-=v_-/|v_-|$) and $|v_-|$ increases or, e.g., c, β_1, β_2, α, d, v_-, $\hat{x}_-$ are fixed and $|x_-|$ increases. In these cases $\sup_{t\in\mathbb{R}}|\theta(t)|$ decreases, where $\theta(t)$ denotes the angle between the vectors $\dot{x}(t)=v_-+\dot{y}_-(t)$ and v_-, and we deal with small angle scattering. Note that already under the conditions of Theorem 3.1, without additional assumptions, there is the estimate $\sup_{t\in\mathbb{R}}|\theta(t)|<\frac{1}{4}\pi$ and we deal with a rather small angle scattering. Theorem 3.1 with (3.5c) will give the asymptotics of the configuration valued component $b(v_-,x_-)$ of the scattering map if we can study the asymptotics of $l_{v_-,x_-}(0)$. This is the subject of Theorem 3.2.

Theorem 3.2: *Let c, d, β_0, β_1, α, $|x|$ be fixed. Then there exists a constant $C_{c,d,\beta_0,\beta_1,\alpha,|x|}$ such that*

$$\left|\frac{l_{v,x}(0)}{\sqrt{1-\frac{|v|^2}{c^2}}}-\frac{1}{c^2}PV(\hat{v},x)\hat{v}+\frac{1}{|v|^2}\int_0^{+\infty}\int_{\tau}^{+\infty}F(u\hat{v}+x)\mathrm{d}u\,\mathrm{d}\tau-\frac{1}{|v|^2}\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(u\hat{v}+x)\mathrm{d}u\,\mathrm{d}\tau\right|$$
$$\leqslant C_{c,d,\beta_0,\beta_1,\alpha,|x|}\sqrt{1-\frac{|v|^2}{c^2}} \tag{3.9}$$

for any $v\in B_c$, $|v|\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, $vx=0$, and where $\hat{v}=v/|v|$.

The proof of Theorem 3.2 is given in Sec. VI. Using this proof one can compute $C_{c,d,\beta_0,\beta_1,\alpha,|x|}$ explicitly.

IV. PRELIMINARIES FOR THE MAIN PROOFS

A. Inequalities for *F*

Lemma 4.1: Under the conditions (1.2), *the following estimates are valid:*

$$|F(x)|=\left(\sum_{j=1}^{d}\left|\frac{\partial}{\partial x_j}V(x)\right|^2\right)^{1/2}\leqslant\beta_1\sqrt{d}(1+|x|)^{-(\alpha+1)}\quad \textit{for } x\in\mathbb{R}^d, \tag{4.1}$$

$$|F(x)-F(y)|\leqslant\beta_2 d\sup_{\varepsilon\in[0,1]}(1+|\varepsilon x+(1-\varepsilon)y|)^{-(\alpha+2)}|x-y|,\quad \textit{for } x,y\in\mathbb{R}^d. \tag{4.2}$$

Lemma 4.1 follows directly from the formula $F(x)=-\nabla V(x)$ and the conditions (1.2).

B. Infinitely smooth function $g:\mathbb{R}^d \to B_c$

Lemma 4.2: The following estimates hold:

$$|\nabla g_i(x)|^2 \leqslant \frac{1}{1+\dfrac{|x|^2}{c^2}} \quad \text{for } x \in \mathbb{R}^d, \quad i=1,\ldots,d, \tag{4.3}$$

$$|g(x)-g(y)| \leqslant \sqrt{d} \sup_{\varepsilon\in[0,1]} \frac{1}{\sqrt{1+\dfrac{|\varepsilon x+(1-\varepsilon)y|^2}{c^2}}} |x-y| \quad \text{for } x, \quad y \in \mathbb{R}^d, \tag{4.4}$$

$$|\nabla g_i(x)-\nabla g_i(y)| \leqslant \frac{3\sqrt{d}}{c} \sup_{\varepsilon\in[0,1]} \frac{1}{1+\dfrac{|\varepsilon x+(1-\varepsilon)y|^2}{c^2}} |x-y| \quad \text{for } x, \quad y \in \mathbb{R}^d, \tag{4.5}$$

where $g=(g_1,\ldots,g_d)$.

Lemma 4.2 follows from straightforward calculations.

Remark 4.1: Using the growth properties of $g(p)$ with respect to $|p|$ and following Novikov's framework,[7] we will easily generalize some of the results of Ref. 7 to the relativistic case. Note that $1/(1+|p|^2/c^2)\to 0$ when $p\in\mathbb{R}^d$, $|p|\to+\infty$.

C. Some estimates of integrals

We will use the following estimates. For $a>0$, $b>0$, $\beta>1$,

$$\int_{-\infty}^{t} (a+b|s|)^{-\beta}\,\mathrm{d}s = \frac{1}{(\beta-1)b(a-bt)^{\beta-1}} \quad \text{for } t\leqslant 0, \tag{4.6}$$

$$\int_{-\infty}^{t} (a+b|s|)^{-\beta}\,\mathrm{d}s \leqslant \frac{2}{(\beta-1)ba^{\beta-1}} \quad \text{for } t\geqslant 0. \tag{4.7}$$

For $a>0$, $b>0$, $\beta>2$,

$$\int_{-\infty}^{t}\int_{-\infty}^{\tau} (a+b|s|)^{-\beta}\,\mathrm{d}s\,\mathrm{d}\tau = \frac{1}{(\beta-2)(\beta-1)b^2(a-bt)^{\beta-2}} \quad \text{for } t\leqslant 0, \tag{4.8}$$

$$\int_{0}^{t}\int_{\tau}^{t} (a+bs)^{-\beta}\,\mathrm{d}s\,\mathrm{d}\tau \leqslant \frac{1}{(\beta-2)(\beta-1)b^2a^{\beta-2}} \quad \text{for } t\geqslant 0. \tag{4.9}$$

For $a\geqslant 1$, $b>0$, $\beta>2$,

$$\int_{-\infty}^{t} (a+b|s|)^{-\beta}(1+|s|)\mathrm{d}s \leqslant \frac{b+1}{(\beta-2)b^2(a-bt)^{\beta-2}} \quad \text{for } t\leqslant 0, \tag{4.10}$$

$$\int_{-\infty}^{t} (a+b|s|)^{-\beta}(1+|s|)\mathrm{d}s \leqslant 2\frac{b+1}{(\beta-2)b^2a^{\beta-2}} \quad \text{for } t\geqslant 0. \tag{4.11}$$

For $a\geqslant 1$, $b>0$, $\beta>3$,

$$\int_0^t \int_\tau^t (a+bs)^{-\beta}(1+s)\mathrm{d}s\,\mathrm{d}\tau \leqslant \frac{b+1}{(\beta-3)(\beta-2)b^3a^{\beta-3}} \quad \text{for } t \geqslant 0. \tag{4.12}$$

For the proof of (4.6)–(4.12), see Ref. 7.

D. About $z_1(c,d,\beta_1,\alpha,|x_-|,r)$

Let c, d, β_1, α, $|x_-|$, $0<r\leqslant 1$, $r<c/\sqrt{2}$, be fixed. We consider the one-dimensional infinitely smooth function $\sigma:]\sqrt{2}r,c[\to\mathbb{R}$ defined by

$$\sigma(s) = \frac{s}{\sqrt{1-\frac{s^2}{c^2}}} - \frac{2^{\alpha+4}\beta_1\sqrt{d}}{\alpha(s/\sqrt{2}-r)(|x_-|/\sqrt{2}+1)^\alpha}.$$

σ is an increasing function (its derivative is a positive function) and as a consequence $z_1(c,d,\beta_1,\alpha,|x_-|,r)$ is well defined in the Introduction and the observation (I) of Sec. III holds.

E. About $M_{T,r}$, $0<r\leqslant 1$, $r<c/\sqrt{2}$

Lemma 4.3: Let $f,f_1,f_2\in M_{T,r}$, $v_-\in B_c\backslash\{0\}$, $v_-x_-=0$, $|v_-|>\sqrt{2}r$, then

$$\varepsilon f_1 + (1-\varepsilon)f_2 \in M_{T,r} \quad \textit{for } 0\leqslant\varepsilon\leqslant 1, \tag{4.13}$$

$$2(1+|x_- + v_-s + f(s)|) \geqslant (1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r)|s|) \quad \textit{for } s\leqslant T, \tag{4.14}$$

$$\left|\int_{-\infty}^t F(v_-s+x_-+f(s))\mathrm{d}s\right| \leqslant \frac{\beta_1\sqrt{d}2^{\alpha+2}}{\alpha(|v_-|/\sqrt{2}-r)(|x_-|/\sqrt{2}+1)^\alpha} \quad \textit{for } t\in\,]-\infty,+\infty], \tag{4.15}$$

$$\left(1+\frac{1}{c^2}\left|\gamma(v_-)+\varepsilon_1\int_{-\infty}^t F(v_-s+x_-+f_1(s))\mathrm{d}s+\varepsilon_2\int_w^u F(v_-s+x_-+f_2(s))\mathrm{d}s\right|^2\right)^{-\beta}$$
$$\leqslant \left(1+\frac{|v_-|^2}{4(c^2-|v_-|^2)}\right)^{-\beta}, \tag{4.16}$$

for u, $t\in\,]-\infty,T]$, $w\in[-\infty,u]$, $\beta>0$, $-1\leqslant\varepsilon_1$, $\varepsilon_2\leqslant 1$, f_1, $f_2\in M_{T,r}$ and if $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $|v_-|<c$, where γ is defined by

$$\gamma(v) = \frac{v}{\sqrt{1-|v|^2/c^2}},$$

for $v\in B_c$.

Proof of Lemma 4.3: For the proof of (4.14) see Ref. 7. Inequality (4.1) with (4.14) and (4.7) proves (4.15). (4.13) follows from the definition of $M_{T,r}$. Inequality (4.15) gives in particular for u, $t\in\,]-\infty,T]$, $w\in[-\infty,u]$, $\beta>0$, $-1\leqslant\varepsilon_1$, $\varepsilon_2\leqslant 1$, f_1, $f_2\in M_{T,r}$,

$$\left|\gamma(v_-)+\varepsilon_1\int_{-\infty}^t F(v_-s+x_-+f_1(s))\mathrm{d}s+\varepsilon_2\int_w^u F(v_-s+x_-+f_2(s))\mathrm{d}s\right|$$
$$\geqslant |\gamma(v_-)| - \frac{\beta_1\sqrt{d}2^{\alpha+3}}{\alpha(|v_-|/\sqrt{2}-r)(|x_-|/\sqrt{2}+1)^\alpha}$$

$$= \frac{|v_-|}{\sqrt{1-|v_-|^2/c^2}} - \frac{\beta_1\sqrt{d}2^{\alpha+3}}{\alpha(|v_-|/\sqrt{2}-r)(|x_-|/\sqrt{2}+1)^\alpha}$$

$$\geqslant \frac{c|v_-|}{2\sqrt{c^2-|v_-|^2}} \quad \text{if } |v_-| \geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r), \quad |v_-|<c,$$

which implies (4.16).

V. PROOFS OF LEMMAS 2.1, 2.2, 2.3

Proof of Lemma 2.1: The property

$$A_{v_-x_-}(f) \in C^1(]-\infty,T],\mathbb{R}^d) \quad \text{for } f \in M_{T,r} \quad (0<r\leqslant 1,\ r<|v_-|/\sqrt{2}) \tag{5.1}$$

follows from (1.2) and (2.1) [applied on "x" $=\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f(s))\mathrm{d}s$ and "y" $=\gamma(v_-)$] and the definition of $A_{v_-x_-}(f)$.

Now we always suppose that $0<r\leqslant 1$, $r<c/\sqrt{2}$, $|v_-|\geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)$, $|v_-|<c$, $v_-x_-=0$. Consider

$$\begin{aligned} A_{v_-x_-}(f)(t) &= \int_{-\infty}^{t}\left[g\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f(s))\mathrm{d}s\right)-v_-\right]\mathrm{d}\tau \\ \frac{\mathrm{d}}{\mathrm{d}t}A_{v_-x_-}(f)(t) &= g\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f(s))\mathrm{d}s\right)-v_-. \end{aligned} \quad \text{for } f\in M_{T,r}, \tag{5.2}$$

First we shall prove some estimates about $(\mathrm{d}/\mathrm{d}t)A_{v_-x_-}(f)$.

Note that $g(\gamma(v_-))=v_-$. From (5.2) and (4.4) [applied on "x" $=\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f(s))\mathrm{d}s$ and "y" $=\gamma(v_-)$], (4.1), (4.14), and (4.16) it follows that

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-x_-}(f)(t)\right| \leqslant \frac{d\beta_1 2^{\alpha+1}}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}}\int_{-\infty}^{t}(1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r)|s|))^{-(\alpha+1)}\,\mathrm{d}s. \tag{5.3}$$

Our next purpose is to prove estimates (5.5) and (5.9) given below.

From (5.3), (4.8), and (4.6) it follows that

$$|A_{v_-x_-}(f)(t)| \leqslant \frac{d\beta_1\,2^{\alpha+1}}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}\alpha(\alpha-1)\left(\dfrac{|v_-|}{\sqrt{2}}-r\right)^2\left(1+\dfrac{|x_-|}{\sqrt{2}}-\left(\dfrac{|v_-|}{\sqrt{2}}-r\right)t\right)^{\alpha-1}}, \tag{5.4a}$$

$$\left|t\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-x_-}(f)(t)\right| \leqslant \frac{d\beta_1\,2^{\alpha+1}}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}\alpha\left(\dfrac{|v_-|}{\sqrt{2}}-r\right)^2\left(1+\dfrac{|x_-|}{\sqrt{2}}-\left(\dfrac{|v_-|}{\sqrt{2}}-r\right)t\right)^{\alpha-1}}, \tag{5.4b}$$

for $t\leqslant T$, $t\leqslant 0$. From (5.4) it follows that

$$\left| A_{v_-,x_-}(f)(t) - t\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f)(t) \right| \leqslant \frac{d\beta_1 2^{\alpha+1}}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}(\alpha-1)(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha-1}}, \tag{5.5}$$

for $t \leqslant T$, $t \leqslant 0$.

For $t \leqslant T$, $t \geqslant 0$, note that

$$A_{v_-,x_-}(f)(t) - t\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f)(t) = A_{v_-,x_-}(f)(0) + \int_0^t \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + f(s))\mathrm{d}s \right) \right] \mathrm{d}\tau. \tag{5.6}$$

For $A_{v_-,x_-}(f)(0)$ we use the estimate (5.4a), i.e.,

$$|A_{v_-,x_-}(f)(0)| \leqslant \frac{d\beta_1 2^{\alpha+1}}{\sqrt{1+(|v_-|^2/(4(c^2-|v_-|^2)))}\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha-1}}. \tag{5.7}$$

We estimate the second term on the right-hand side of (5.6) in the following way: from (4.4), (4.16), (4.1), (4.14), and (4.9), it follows that

$$\begin{aligned} &\left| \int_0^t \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + f(s))\mathrm{d}s \right) \right] \mathrm{d}\tau \right| \\ &\leqslant \frac{\sqrt{d}}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}} \int_0^t \left| \int_t^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s \right| \mathrm{d}\tau \\ &\leqslant \frac{d\beta_1 2^{\alpha+1}}{\sqrt{1+(|v_-|^2/(4(c^2-|v_-|^2)))}\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha-1}}, \end{aligned} \tag{5.8}$$

for $0 \leqslant t \leqslant T$. From (5.6)–(5.8) it follows that

$$\left| A_{v_-,x_-}(f)(t) - t\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f)(t) \right| \leqslant \frac{d\beta_1 2^{\alpha+2}}{\sqrt{1+\dfrac{|v_-|^2}{(4(c^2-|v_-|^2))}}\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^2(1+|x_-|/\sqrt{2})^{\alpha-1}} \tag{5.9}$$

for $0 \leqslant t \leqslant T$. Using (5.3) and (4.6) and using (5.5) we obtain (2.7a). Using (5.3) and (4.7) and using (5.9) we obtain (2.7b).

Our next purpose is to prove estimate (5.14) given below. Consider $(\mathrm{d}/\mathrm{d}t)(A_{v_-,x_-}(f_2)(t) - A_{v_-,x_-}(f_1)(t))$ for $f_1, f_2 \in M_{T,r}$ $[0 < r \leqslant 1,\ r < c/\sqrt{2},\ |v_-| < c,\ v_-x_- = 0,\ |v_-| \geqslant z_1(c,d,\beta_1,\alpha,|x_-|,r)]$. First

$$\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_2)(t) - \frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_1)(t) = g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + f_2(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + f_1(s))\mathrm{d}s \right) \tag{5.10}$$

for $t \leqslant T$. From (5.10), (4.4), and (4.16) it follows that

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_2)(t)-\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_1)(t)\right| \leqslant \frac{\sqrt{d}}{\sqrt{1+(|v_-|^2/(4(c^2-|v_-|^2)))}}\int_{-\infty}^{t}|F(v_-s+x_-+f_2(s)) - F(v_-s+x_-+f_1(s))|\mathrm{d}s, \tag{5.11}$$

for $t\leqslant T$. From (4.13), (4.14), and (4.2), it follows that

$$|F(v_-s+x_-+f_2(s))-F(v_-s+x_-+f_1(s))| \leqslant d\beta_2 2^{\alpha+2}(1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r)|s|)^{-(\alpha+2)}|f_2(s) - f_1(s)| \quad \text{for } s\leqslant T. \tag{5.12}$$

Moreover

$$|f_2(s)-f_1(s)| \leqslant (1+|s|)\|f_2-f_1\|_T \quad \text{for } s\leqslant T. \tag{5.13}$$

Thus, from (5.11)–(5.13) it follows that

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_2)(t)-\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_1)(t)\right| \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}\|f_2-f_1\|_T}{\sqrt{1+(|v_-|^2/(4(c^2-|v_-|^2)))}}\int_{-\infty}^{t}(1+|x_-|/\sqrt{2}+(|v_-|/\sqrt{2}-r) \times|s|)^{-(\alpha+2)}(1+|s|)\mathrm{d}s. \tag{5.14}$$

Our next purpose is to prove estimates (5.17) and (5.31) given below. From (5.14), (4.10), and (4.6) it follows that

$$|A_{v_-,x_-}(f_2)(t)-A_{v_-,x_-}(f_1)(t)| \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}(|v_-|/\sqrt{2}+1-r)\|f_2-f_1\|_T}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}\alpha(\alpha-1)(|v_-|/\sqrt{2}-r)^3(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha-1}} \tag{5.15}$$

for $t\leqslant T$, $t\leqslant 0$. From (5.14) and (4.10) it also follows that

$$|t|\left|\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_2)(t)-\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_1)(t)\right| \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}(|v_-|/\sqrt{2}+1-r)\|f_2-f_1\|_T}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}\alpha(|v_-|/\sqrt{2}-r)^3(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha-1}} \tag{5.16}$$

for $t\leqslant T$, $t\leqslant 0$. Hence from (5.15) and (5.16) it follows that

$$\left|A_{v_-,x_-}(f_2)(t)-A_{v_-,x_-}(f_1)(t)-t\frac{\mathrm{d}}{\mathrm{d}t}(A_{v_-,x_-}(f_2)(t)-A_{v_-,x_-}(f_1)(t))\right| \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}(|v_-|/\sqrt{2}+1-r)\|f_2-f_1\|_T}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}(\alpha-1)(|v_-|/\sqrt{2}-r)^3(1+|x_-|/\sqrt{2}-(|v_-|/\sqrt{2}-r)t)^{\alpha-1}} \tag{5.17}$$

for $t\leqslant T$, $t\leqslant 0$.

For $0\leqslant t\leqslant T$, using (5.6) we obtain

$$\left|A_{v_-,x_-}(f_2)(t)-A_{v_-,x_-}(f_1)(t)-t\left(\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_2)(t)-\frac{\mathrm{d}}{\mathrm{d}t}A_{v_-,x_-}(f_1)(t)\right)\right| \leqslant |A_{v_-,x_-}(f_2)(0)-A_{v_-,x_-}(f_1)(0)|$$
$$+\left|\int_0^t\left[g\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)-g\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)\right.\right.$$
$$\left.\left.-g\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)+g\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)\right]\mathrm{d}\tau\right|. \tag{5.18}$$

From (5.15) it follows that

$$|A_{v_-,x_-}(f_2)(0)-A_{v_-,x_-}(f_1)(0)| \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}(|v_-|/\sqrt{2}+1-r)\|f_2-f_1\|_T}{\sqrt{1+\dfrac{|v_-|^2}{4(c^2-|v_-|^2)}}\alpha(\alpha-1)\left(\dfrac{|v_-|}{\sqrt{2}}-r\right)^3\left(1+\dfrac{|x_-|}{\sqrt{2}}\right)^{\alpha-1}}. \tag{5.19}$$

In order to estimate the second term of the right-hand side of (5.18), we will estimate

$$\int_0^t\left[g_j\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)-g_j\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)\right.$$
$$\left.-g_j\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)+g_j\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)\right]\mathrm{d}\tau \tag{5.20}$$

for $1\leqslant j\leqslant d$ and $0\leqslant t\leqslant T$.

Let $1\leqslant j\leqslant d$ and $0\leqslant t\leqslant T$, $0\leqslant\tau\leqslant t$. Note that

$$g_j\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)-g_j\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)$$
$$-\left(g_j\left(\gamma(v_-)+\int_{-\infty}^{\tau}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)-g_j\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_1(s))\mathrm{d}s\right)\right)$$
$$=\Delta^1_{j,t}(\tau)+\Delta^2_{j,t}(\tau), \tag{5.21}$$

where

$$\Delta^1_{j,t}(\tau)=\int_t^{\tau}(F(v_-s+x_-+f_2(s))-F(v_-s+x_-+f_1(s)))ds$$
$$\bigstar\int_0^1\nabla g_j\left(\gamma(v_-)+\int_{-\infty}^{t}F(v_-s+x_-+f_2(s))\mathrm{d}s+\varepsilon\int_t^{\tau}F(v_-s+x_-+f_2(s))\mathrm{d}s\right)\mathrm{d}\varepsilon, \tag{5.22a}$$

$$\Delta_{j,t}^2(\tau) = \int_t^\tau F(v_-s + x_- + f_1(s))\mathrm{d}s$$
$$\star \int_0^1 \left[\nabla g_j\left(\gamma(v_-) + \int_{-\infty}^t F(v_-s + x_- + f_2(s))\mathrm{d}s + \varepsilon \int_t^\tau F(v_-s + x_- + f_2(s))\mathrm{d}s \right) \right.$$
$$\left. - \nabla g_j\left(\gamma(v_-) + \int_{-\infty}^t F(v_-s + x_- + f_1(s))\mathrm{d}s + \varepsilon \int_t^\tau F(v_-s + x_- + f_1(s))\mathrm{d}s \right) \right] \mathrm{d}\varepsilon, \tag{5.22b}$$

where ★ denotes the usual scalar product on $\mathbb{R}^d$.

Using (5.22a), (4.3), (4.2), (4.16), (4.14), and (5.13), we obtain

$$|\Delta_{j,t}^1(\tau)| \leqslant \frac{d\beta_2\, 2^{\alpha+2}}{\sqrt{1 + \dfrac{|v_-|^2}{4(c^2 - |v_-|^2)}}} \int_\tau^t (1 + |x_-|/\sqrt{2} + (|v_-|/\sqrt{2} - r)s)^{-(\alpha+2)}(1+s)\mathrm{d}s \|f_2 - f_1\|_T. \tag{5.23}$$

Thus from (4.12) it follows that

$$\int_0^t |\Delta_{j,t}^1(\tau)|\mathrm{d}\tau \leqslant \frac{d\beta_2\, 2^{\alpha+2}(|v_-|/\sqrt{2} + 1 - r)}{\sqrt{1 + \dfrac{|v_-|^2}{4(c^2 - |v_-|^2)}}\, \alpha(\alpha-1)(|v_-|/\sqrt{2} - r)^3(1 + |x_-|/\sqrt{2})^{\alpha-1}} \|f_2 - f_1\|_T. \tag{5.24}$$

Using (5.22b), (4.5), and (4.16), we obtain

$$|\Delta_{j,t}^2(\tau)| \leqslant \int_\tau^t |F(v_-s + x_- + f_1(s))|\mathrm{d}s \left[\frac{3\sqrt{d}}{c(1 + (|v_-|^2/(4(c^2 - |v_-|^2))))} \right.$$
$$\times \int_0^1 \left| \int_{-\infty}^t (F(v_-s + x_- + f_2(s)) - F(v_-s + x_- + f_1(s)))\mathrm{d}s \right.$$
$$\left. \left. + \varepsilon \int_t^\tau (F(v_-s + x_- + f_2(s)) - F(v_-s + x_- + f_1(s)))\mathrm{d}s \right| \mathrm{d}\varepsilon \right]. \tag{5.25}$$

We shall use

$$\left| \int_{-\infty}^t (F(v_-s + x_- + f_2(s)) - F(v_-s + x_- + f_1(s)))\mathrm{d}s \right.$$
$$\left. + \varepsilon \int_t^\tau (F(v_-s + x_- + f_2(s)) - F(v_-s + x_- + f_1(s)))\mathrm{d}s \right|$$
$$\leqslant 2 \int_{-\infty}^t |(F(v_-s + x_- + f_2(s)) - F(v_-s + x_- + f_1(s)))|\mathrm{d}s, \tag{5.26}$$

for all $0 \leqslant \varepsilon \leqslant 1$ (we remind that $\tau \leqslant t$).

From (5.25) and (5.26) it follows that

$$|\Delta_{j,t}^2(\tau)| \leqslant \int_\tau^t |F(v_- s + x_- + f_1(s))| \mathrm{d}s \times \frac{6\sqrt{d}}{c\left(1 + \dfrac{|v_-|^2}{4(c^2 - |v_-|^2)}\right)} \int_{-\infty}^t |(F(v_- s + x_- + f_2(s)) - F(v_- s + x_- + f_1(s)))| \mathrm{d}s. \tag{5.27}$$

Using (4.2), (4.14), (5.13), and (4.11) we obtain

$$\int_{-\infty}^t |F(v_- s + x_- + f_2(s)) - F(v_- s + x_- + f_1(s))| \mathrm{d}s \leqslant \frac{d\beta_2\, 2^{\alpha+3}(|v_-|/\sqrt{2} + 1 - r)}{\alpha(|v_-|/\sqrt{2} - r)^2(1 + |x_-|/\sqrt{2})^\alpha} \|f_2 - f_1\|_T. \tag{5.28}$$

Using (4.1), (4.14), and (4.9) we obtain

$$\int_0^t \int_\tau^t |F(v_- s + x_- + f_1(s))| \mathrm{d}s\, \mathrm{d}\tau \leqslant \frac{\sqrt{d}\beta_1 2^{\alpha+1}}{\alpha(\alpha-1)(|v_-|/\sqrt{2} - r)^2(1 + |x_-|/\sqrt{2})^{\alpha-1}}. \tag{5.29}$$

From (5.27)–(5.29) it follows that

$$\int_0^t |\Delta_{j,t}^2(\tau)| \mathrm{d}\tau \leqslant \frac{3}{c(1 + (|v_-|^2/(4(c^2 - |v_-|^2))))} \frac{d^2\beta_1\beta_2 2^{2\alpha+5}(|v_-|/\sqrt{2} + 1 - r)}{\alpha^2(\alpha-1)(|v_-|/\sqrt{2} - r)^4(1 + |x_-|/\sqrt{2})^{2\alpha-1}} \|f_2 - f_1\|_T. \tag{5.30}$$

From (5.18), (5.19), (5.21), (5.24), and (5.30), it follows that

$$\begin{aligned} &\left| A_{v_-,x_-}(f_2)(t) - A_{v_-,x_-}(f_1)(t) - t\left(\frac{\mathrm{d}}{\mathrm{d}t} A_{v_-,x_-}(f_2)(t) - \frac{\mathrm{d}}{\mathrm{d}t} A_{v_-,x_-}(f_1)(t)\right)\right| \\ &\quad \leqslant \frac{d\sqrt{d}\beta_2 2^{\alpha+2}(|v_-|/\sqrt{2} + 1 - r)}{\sqrt{1 + (|v_-|^2/(4(c^2 - |v_-|^2)))}\,\alpha(\alpha-1)(|v_-|/\sqrt{2} - r)^3(1 + |x_-|/\sqrt{2})^{\alpha-1}} \\ &\qquad \times \left[2 + \frac{3}{c\sqrt{(1 + (|v_-|^2/(4(c^2 - |v_-|^2))))}} \frac{d\beta_1\, 2^{\alpha+3}}{\alpha(|v_-|/\sqrt{2} - r)(1 + |x_-|/\sqrt{2})^\alpha}\right] \\ &\qquad \times \|f_1 - f_2\|_T. \end{aligned} \tag{5.31}$$

Using (5.14), (4.10), and (5.17) we obtain (2.8a). Using (5.14), (4.11), and (5.31) we obtain (2.8b). Lemma 2.1 is proved.

Proof of Lemma 2.2: The estimates (2.10) and (2.11) follow immediately from (5.3), (4.6), and (5.4a). From (4.1), (4.14), and (4.7) it follows that

$$\int_{-\infty}^{+\infty} F(v_- s + x_- + f(s)) \mathrm{d}s$$

converges absolutely for any $f \in M_{T,r}$. Moreover, using (4.4) and (4.16) and then (4.1), (4.14), and (4.8) we obtain for $u > 0$,

$$\int_u^{+\infty} \left| g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right) - g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right)\right| \mathrm{d}\tau$$
$$\leqslant \frac{d\beta_1\, 2^{\alpha+1}}{\sqrt{1 + \dfrac{|v_-|^2}{4(c^2 - |v_-|^2)}}} \int_u^{+\infty} \int_{\tau}^{+\infty} (1 + |x_-|/\sqrt{2} + (|v_-|/\sqrt{2} - r)s)^{-(\alpha+1)}\, \mathrm{d}s\, \mathrm{d}\tau$$
$$\leqslant \frac{d\beta_1\, 2^{\alpha+1}(1 + |x_-|/\sqrt{2} + (|v_-|/\sqrt{2} - r)u)^{-(\alpha-1)}}{\sqrt{1 + \dfrac{|v_-|^2}{4(c^2 - |v_-|^2)}}\, \alpha(\alpha-1)(|v_-|/\sqrt{2} - r)^2} \tag{5.32}$$

As a consequence we can write

$$A_{v_-,x_-}(f)(t) = t\left[g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right) - v_-\right] + \int_{-\infty}^{0} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right) - v_-\right]\mathrm{d}\tau + \int_0^{+\infty} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right) - g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right)\right]\mathrm{d}\tau - \int_t^{+\infty} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right) - g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right)\right]\mathrm{d}\tau \tag{5.33}$$

and (2.12) and (2.13) follow, where

$$H_{v_-,x_-}(f)(t) = \int_t^{+\infty} \left[g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right) - g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right)\right]\mathrm{d}\tau. \tag{5.34}$$

The formulas (5.34) and (5.32) prove (2.16). Using (5.34), (4.4), (4.16), (4.1), (4.14), and (4.6), we obtain (2.15).

Using (2.13a), (4.4), (4.16), (4.1), (4.14), and (4.7) we obtain (2.14a).

We write

$$l_{v_-,x_-}(f) = A_{v_-,x_-}(f)(0) + \int_0^{+\infty} \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + f(s))\mathrm{d}s\right) - g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s\right)\right]\mathrm{d}\tau. \tag{5.35}$$

Using (5.35), (5.7), and (5.32), we obtain (2.14b).

Thus Lemma 2.2 is proved.

Proof of Lemma 2.3: Using (2.3) and (2.7b) we obtain

$$\|y_- - 0\|_T = \|y_-\|_T \leqslant \rho(c, d, \beta_1, \alpha, |v_-|, |x_-|, r), \quad T = +\infty.$$

Using (2.13a) and (5.10) with (5.14) and (4.11) ($T = +\infty$ and $t \to +\infty$), we obtain (2.17a).

From (5.35) it follows that

$$
\begin{aligned}
&|l_{v_-,x_-}(y_-) - l_{v_-,x_-}(0)| \\
&\quad \leqslant |A_{v_-,x_-}(y_-)(0) - A_{v_-,x_-}(0)(0)| \\
&\quad + \left| \lim_{t\to+\infty} \left\{ \int_0^t \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) \right.\right. \\
&\quad - g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_-)\mathrm{d}s \right) + g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_-)\mathrm{d}s \right) \\
&\quad - \left(g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) \right) \\
&\quad \left.\left. + \left(g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_-)\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_-)\mathrm{d}s \right) \right) \right] \mathrm{d}\tau \right\} \right|. \qquad (5.36)
\end{aligned}
$$

Using (4.4), (4.16), (4.1), (4.14), and (4.6) we obtain

$$
t \left| g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + f(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + f(s))\mathrm{d}s \right) \right| \to 0 \text{ as } t \to +\infty \qquad (5.37)
$$

for $f \in M_{T,r}$.

From (5.36) and (5.37) it follows that

$$
\begin{aligned}
&|l_{v_-,x_-}(y_-) - l_{v_-,x_-}(0)| \\
&\quad \leqslant |A_{v_-,x_-}(y_-)(0) - A_{v_-,x_-}(0)(0)| \\
&\quad + \left| \lim_{t\to+\infty} \left\{ \int_0^t \left[g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) - g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_- + y_-(s))\mathrm{d}s \right) \right.\right. \\
&\quad \left.\left. - g\left(\gamma(v_-) + \int_{-\infty}^{\tau} F(v_-s + x_-)\mathrm{d}s \right) + g\left(\gamma(v_-) + \int_{-\infty}^{t} F(v_-s + x_-)\mathrm{d}s \right) \right] \mathrm{d}\tau \right\} \right|. \qquad (5.38)
\end{aligned}
$$

Using (5.19)–(5.21), (5.24), and (5.30), $\|y_-\|_T \leqslant \rho(c, d, \beta_1, \alpha, |v_-|, |x_-|, r)$, $T = +\infty$, and (5.38) we obtain (2.17c).

We shall prove (2.17b). First

$$
v_- + k_{v_-,x_-}(y_-) = g\left(\gamma(v_-) + \int_{-\infty}^{+\infty} F(v_-s + x_- + y_-(s))\mathrm{d}s \right). \qquad (5.39)
$$

Using the integral of motion E, we have $|v_-| = |v_- + k_{v_-,x_-}(y_-)|$ and applying γ to (5.39) we obtain

$$
\frac{k_{v_-,x_-}(y_-)}{\sqrt{1 - |v_-|^2/c^2}} = \int_{-\infty}^{+\infty} F(v_-s + x_- + y_-(s))\mathrm{d}s. \qquad (5.40)
$$

From (5.40), (5.12), (5.13), and (4.11) and $\|y_-\|_T \leqslant \rho(c, d, \beta_1, \alpha, |v_-|, |x_-|, r)$, $T = +\infty$, we obtain (2.17b).

Lemma 2.3 is proved.

VI. PROOFS OF THEOREM 3.2 AND PROPOSITION 1.1

Let $(\theta,x)\in T\mathbb{S}^{d-1}$, α, d, c, β_1, β_2 be fixed.

We shall use

$$\left|\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|\leqslant\frac{\beta_1\sqrt{d}}{\alpha(s/\sqrt{2})(1+|x|/\sqrt{2})^{\alpha}} \tag{6.1a}$$

for $s\in]0,c[$ and $u\in]-\infty,0]$; replacing θ by $-\theta$ in (6.1a), we obtain

$$\left|\frac{1}{s}\int_{u}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|\leqslant\frac{\beta_1\sqrt{d}}{\alpha(s/\sqrt{2})(1+|x|/\sqrt{2})^{\alpha}} \tag{6.1b}$$

for $s\in]0,c[$ and $u\in[0,+\infty[$.

We prove (6.1a). As $\theta x=0$, the following formula is valid:

$$|x+w\theta|\geqslant|x|/\sqrt{2}+|w|/\sqrt{2}, \tag{6.2}$$

for any $w\in\mathbb{R}$. Then estimate (6.1a) follows from (4.1), (6.2), and (4.6).

Before proving Theorem 3.2, we need to introduce three lemmas and prove them.

Lemma 6.1: There exists integrable $\tilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}:]-\infty,0]\to[0,+\infty[$ *such that*

$$\left|(1+\delta_1(c,\theta,x,s,u))^{-1/2}-1-\frac{V(x+u\theta)\sqrt{1-\frac{s^2}{c^2}}}{c^2}\right|\leqslant\tilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}(u)(1-s^2/c^2), \tag{6.3}$$

for $u\in]-\infty,0]$ *and* $s<c$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, *and where*

$$\delta_1(c,\theta,x,s,u)=\frac{-2V(x+u\theta)\sqrt{1-\frac{s^2}{c^2}}+\left(\frac{1}{s^2}-\frac{1}{c^2}\right)\left|\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2}{c^2}\geqslant-\frac{3}{4}, \tag{6.4}$$

for $u\in]-\infty,0]$ *and* $s<c$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$.

Proof of Lemma 6.1.

Let $s\in]0,c[$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$ and $u\in]-\infty,0]$.

From (6.1a) and the definition of $z_2(c,d,\beta_1,\alpha,|x|)$ [see (1.7d)] it follows that

$$\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|\geqslant\frac{s}{2\sqrt{1-s^2/c^2}}. \tag{6.5}$$

Expanding the square of the norm we obtain

$$\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2=\frac{s^2}{1-s^2/c^2}-\frac{2V(x+u\theta)}{\sqrt{1-s^2/c^2}}+\left|\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2. \tag{6.6}$$

Using (6.5) and (6.6), we obtain

$$\delta_1(c,\theta,x,s,u)=\frac{1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2}{1+\frac{s^2}{c^2-s^2}}-1\geqslant\frac{1+\frac{s^2}{4(c^2-s^2)}}{1+\frac{s^2}{c^2-s^2}}-1\geqslant-3/4. \tag{6.7}$$

Moreover, from the definition of $\delta_1(c,\theta,x,s,u)$, (1.2) and (6.1a) and the hypothesis $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, $s<c$, it follows that

$$|\delta_1(c,\theta,x,s,u)|\leqslant\sqrt{1-s^2/c^2}\left[\frac{\beta_0 2(1+|x|/\sqrt{2}-u/\sqrt{2})^{-\alpha}}{c^2}+\frac{\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}\beta_1^2 d2(1+|x|/\sqrt{2}-u/\sqrt{2})^{-2\alpha}}{z_2(c,d,\beta_1,\alpha,|x|)^2c^2\alpha^2}\right]. \tag{6.8}$$

Using Taylor expansion of the map $]-1,+\infty[\to\mathbb{R}$, $\delta\mapsto(1+\delta)^{-1/2}$ at $\delta=0$, we obtain that

$$(1+\delta_1(c,\theta,x,s,u))^{-1/2}-1-\frac{V(x+u\theta)\sqrt{1-\frac{s^2}{c^2}}}{c^2}=-\frac{1-s^2/c^2}{2s^2c^2}\left|\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2+\frac{3}{4}\int_0^1(1-w)\times(1+w\delta_1(c,\theta,x,s,u))^{-5/2}\,\mathrm{d}w\;\delta_1(c,\theta,x,s,u)^2. \tag{6.9}$$

We estimate the first term on the right-hand side of (6.9) with the help of (6.1a). We estimate the second term on the right-hand side of (6.9) with the help of (6.7) and (6.8). Using also the inequality $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, we finally obtain

$$\left|(1+\delta_1(c,\theta,x,s,u))^{-1/2}-1-\frac{V(x+u\theta)\sqrt{1-\frac{s^2}{c^2}}}{c^2}\right|\leqslant\widetilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}(u),$$

where

$$\widetilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}(u)=\frac{d\beta_1^2}{c^2z_2(c,d,\beta_1,\alpha,|x|)^2\alpha^2(1+|x|/\sqrt{2}-u/\sqrt{2})^{2\alpha}}+4^{5/2}\frac{3}{2c^4}\left[\beta_0(1+|x|/\sqrt{2}-u/\sqrt{2})^{-\alpha}+\frac{\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}\beta_1^2 d(1+|x|/\sqrt{2}-u/\sqrt{2})^{-2\alpha}}{z_2(c,d,\beta_1,\alpha,|x|)^2\alpha^2}\right]^2.$$

Lemma 6.1 is proved.

Lemma 6.2: Let $\beta>0$, $s\in]0,c[$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$. *Then there exists a positive real number* $k_{\beta,c,d,\beta_1,\alpha,|x|}$ *such that*

$$\left|\left(1+\frac{1-s^2/c^2}{s^2c^2}\left|\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2\right)^{-\beta}-1\right|\leqslant(1-s^2/c^2)k_{\beta,c,d,\beta_1,\alpha,|x|}.$$

Proof of Lemma 6.2: We define

$$\delta_2(c,\theta,x,s)=\frac{1-s^2/c^2}{s^2c^2}\left|\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2\geqslant 0. \tag{6.10}$$

Using (6.1) and $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, we obtain

$$\delta_2(c,\theta,x,s) \leqslant (1-s^2/c^2)\frac{d\beta_1^2 8}{c^2 z_2(c,d,\beta_1,\alpha,|x|)^2\alpha^2(1+|x|/\sqrt{2})^{2\alpha}}. \tag{6.11}$$

Using the Taylor expansion of the map $]-1,+\infty[\to\mathbb{R}$, $\delta\mapsto(1+\delta)^{-\beta}$ at $\delta=0$ and using (6.10), we obtain

$$(1+\delta_2(c,\theta,x,s))^{-\beta}-1=-\beta\delta_2(c,\theta,x,s)\int_0^1(1+w\delta_2(c,\theta,x,s))^{-(\beta+1)}\,\mathrm{d}w. \tag{6.12}$$

From (6.10)–(6.12) it follows that

$$\left|(1+\delta_2(c,\theta,x,s))^{-\beta}-1\right| \leqslant \beta\delta_2(c,\theta,x,s) \leqslant (1-s^2/c^2)k_{\beta,c,d,\beta_1,\alpha,|x|},$$

where

$$k_{\beta,c,d,\beta_1,\alpha,|x|}=\frac{\beta\, d\beta_1^2\, 8}{c^2 z_2(c,d,\beta_1,\alpha,|x|)^2\alpha^2(1+|x|/\sqrt{2})^{2\alpha}}.$$

Lemma 6.2 is proved.

We always suppose that $(\theta,x)\in T\mathbb{S}^{d-1}$, α, d, c, β_1, β_2 are fixed. Let $s\in]0,c[$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, $u\in[0,+\infty[$, we define

$$A(c,\theta,x,s,u)=(1+t(c,\theta,x,s,u))^{-1/2}, \tag{6.13}$$

where

$$t(c,\theta,x,s,u)=\frac{1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|^2}{1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2}-1. \tag{6.14}$$

Expanding the square of the norms in the numerator and denominator of the fraction of the right-hand side of (6.14), we obtain that

$$\begin{aligned}t(c,\theta,x,s,u)=&\frac{-2V(x+u\theta)\sqrt{1-s^2/c^2}+\frac{1-s^2/c^2}{s^2}\left|\int_u^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2}{\left(1+\frac{(1-s^2/c^2)}{s^2c^2}\left|\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2\right)c^2}\\&-\frac{\frac{2(1-s^2/c^2)}{s^2}\int_u^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\,.\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau}{\left(1+\frac{(1-s^2/c^2)}{s^2c^2}\left|\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2\right)c^2}.\end{aligned} \tag{6.15}$$

Lemma 6.3: There exists $h_{c,d,\beta_0,\beta_1,\alpha,|x|}:[0,+\infty[\to[0,+\infty[$ *an integrable function such that for* $s\in]0,c[$, $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, $u\in[0,+\infty[$,

$$\left|A(c,\theta,x,s,u)-1-V(x+u\theta)\frac{\sqrt{1-s^2/c^2}}{c^2}\right| \leqslant (1-s^2/c^2)h_{c,d,\beta_0,\beta_1,\alpha,|x|}(u).$$

Proof of Lemma 6.3: We first look for a lower bound for $t(c,\theta,x,s,u)$. The following estimate is valid

$$\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|\geqslant\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|-\left|\frac{1}{s}\int_{u}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|. \tag{6.16}$$

From (6.1) it follows that

$$\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|\geqslant\frac{s}{\sqrt{1-s^2/c^2}}-\frac{2\beta_1\sqrt{d}}{\alpha(s/\sqrt{2})(1+|x|/\sqrt{2})^{\alpha}}. \tag{6.17}$$

Using first (6.1b) and then $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$ and (6.17) we obtain

$$\begin{aligned}\left|\frac{1}{s}\int_{u}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|&\leqslant\frac{\beta_1\sqrt{d}}{(s/\sqrt{2})\alpha(1+|x|/\sqrt{2})^{\alpha}}\leqslant\frac{1}{6}\left(\frac{s}{\sqrt{1-s^2/c^2}}-\frac{2\beta_1\sqrt{d}}{\alpha(s/\sqrt{2})(1+|x|/\sqrt{2})^{\alpha}}\right)\\&\leqslant\frac{1}{6}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|.\end{aligned} \tag{6.18}$$

From (6.16) and (6.18) it follows that

$$\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{u}F(x+\tau\theta)\mathrm{d}\tau\right|\geqslant\frac{5}{6}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|. \tag{6.19}$$

Using (6.14) and (6.19) we obtain

$$t(c,\theta,x,s,u)\geqslant\tfrac{25}{36}-1=-\tfrac{11}{36}. \tag{6.20}$$

Now we look for an upper bound for $t(c,\theta,x,s,u)$. The right-hand side of (6.15) consists of a subtraction of two fractions whose denominator is greater than c^2 and this implies

$$\begin{aligned}|t(c,\theta,x,s,u)|\leqslant c^{-2}\Bigg|&-2V(x+u\theta)\sqrt{1-s^2/c^2}+\frac{1-s^2/c^2}{s^2}\left|\int_{u}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\right|^2\\&-\frac{2(1-s^2/c^2)}{s^2}\int_{u}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\bigstar\int_{-\infty}^{+\infty}F(x+\tau\theta)\mathrm{d}\tau\Bigg|,\end{aligned} \tag{6.21}$$

where $\bigstar$ denotes the usual scalar product on $\mathbb{R}^d$. Thus, using (1.2), (6.1), (4.7) and the fact that $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, we obtain

$$\begin{aligned}|t(c,\theta,x,s,u)|\leqslant c^{-2}\sqrt{1-s^2/c^2}\Bigg[&2\beta_0(1+|x|/\sqrt{2}+u/\sqrt{2})^{-\alpha}\\&+\frac{\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{z_2(c,d,\beta_1,\alpha,|x|)^2}\frac{d\beta_1^2 2}{\alpha^2(1+|x|/\sqrt{2}+u/\sqrt{2})^{2\alpha}}\\&+\frac{\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{z_2(c,d,\beta_1,\alpha,|x|)^2}\frac{d\beta_1^2 8}{\alpha^2(1+|x|/\sqrt{2}+u/\sqrt{2})^{\alpha}(1+|x|/\sqrt{2})^{\alpha}}\Bigg].\end{aligned} \tag{6.22}$$

Using (6.13) and (6.20), the Taylor expansion of the map $]-1,+\infty[\mapsto\mathbb{R}$, $\delta\mapsto(1+\delta)^{-1/2}$ at $\delta=0$ and (6.15), we obtain

$$
\begin{aligned}
&\left| A(c,\theta,x,s,u) - 1 - \frac{V(x+u\theta)\sqrt{1-s^2/c^2}}{c^2} \right| \\
&= \left| \frac{1}{2} t(c,\theta,x,s,u) + \frac{3}{4}\int_0^1 (1-w)(1+wt(c,\theta,x,s,u))^{-5/2}\,\mathrm{d}w\; t(c,\theta,x,s,u)^2 \right. \\
&\quad \left. - \frac{V(x+u\theta)\sqrt{1-s^2/c^2}}{c^2} \right| \\
&\leqslant \left| \frac{V(x+u\theta)\sqrt{1-s^2/c^2}}{c^2} \left[1 - \left(1 + \frac{1-s^2/c^2}{c^2 s^2} \left| \int_{-\infty}^{+\infty} F(x+\tau\theta)\mathrm{d}\tau \right|^2 \right)^{-1} \right] \right| \\
&\quad + \frac{1}{2} \frac{\dfrac{1-s^2/c^2}{s^2} \left| \displaystyle\int_u^{+\infty} F(x+\tau\theta)\mathrm{d}\tau \right|^2 + \dfrac{2(1-s^2/c^2)}{s^2} \displaystyle\int_u^{+\infty} |F(x+\tau\theta)|\mathrm{d}\tau \int_{-\infty}^{+\infty} |F(x+\tau\theta)|\mathrm{d}\tau}{\left(1 + \dfrac{(1-s^2/c^2)}{s^2 c^2} \left| \displaystyle\int_{-\infty}^{+\infty} F(x+\tau\theta)\mathrm{d}\tau \right|^2 \right) c^2} \\
&\quad + \frac{3}{8}\left(\frac{25}{36}\right)^{-5/2} t(c,\theta,x,s,u)^2. \qquad (6.23)
\end{aligned}
$$

We use Lemma 6.2, conditions (1.2) and the fact that $s \geqslant z_2(c,d,\beta_1,\alpha,|x|)$ to estimate the first term on the right-hand side of the inequality (6.23). In order to estimate the second term on the right-hand side of the inequality (6.23), we use the fact that the denominator is greater than c^2, and we also use (6.1), (4.7), the fact that $s \geqslant z_2(c,d,\beta_1,\alpha,|x|)$. We estimate the third term on the right-hand side of the inequality with (6.22). Thus we obtain

$$
\left| A(c,\theta,x,s,u) - 1 - \frac{V(x+u\theta)\sqrt{1-s^2/c^2}}{c^2} \right| \leqslant (1-s^2/c^2) h_{c,d,\beta_0,\beta_1,\alpha,|x|}(u),
$$

where

$$
\begin{aligned}
h_{c,d,\beta_0,\beta_1,\alpha,|x|}(u) = \frac{1}{c^2}(1+|x|/\sqrt{2}+u/\sqrt{2})^{-\alpha} \Bigg\{ & \beta_0 k_{1,c,d,\beta_1,\alpha,|x|} \sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2} \\
& + \frac{\beta_1^2 d}{\alpha^2 z_2(c,d,\beta_1,\alpha,|x|)^2} ((1+|x|/\sqrt{2}+u/\sqrt{2})^{-\alpha} + 4(1+|x|/\sqrt{2})^{-\alpha}) \\
& + \frac{3}{2c^2}\left(\frac{25}{36}\right)^{-5/2} \Bigg[\beta_0 (1+|x|/\sqrt{2}+u/\sqrt{2})^{-\alpha/2} \\
& + \frac{d\beta_1^2 \sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{z_2(c,d,\beta_1,\alpha,|x|)^2 \alpha^2 (1+|x|/\sqrt{2}+u/\sqrt{2})^{\alpha/2}} \\
& \times ((1+|x|/\sqrt{2}+u/\sqrt{2})^{-\alpha} + 4(1+|x|/\sqrt{2})^{-\alpha}) \Bigg]^2 \Bigg\}.
\end{aligned}
$$

Lemma 6.3 is proved.

Proof of Theorem 3.2: Let $(\theta,x) \in T\mathbb{S}^{d-1}$, α, d, c, β_1, β_2, $s \in]0,c[$, $s \geqslant z_2(c,d,\beta_1,\alpha,|x|)$ be fixed. We shall study the asymptotics of $l_{s\theta,x}(0)$ which is defined by formula (2.13b).

First we look for the asymptotics of

$$\int_{-\infty}^{0}\left[g\left(\gamma(s\theta)+\int_{-\infty}^{\tau}F(us\theta+x)\mathrm{d}u\right)-s\theta\right]\mathrm{d}\tau.$$

By changes of variables, we obtain

$$\begin{aligned}&\int_{-\infty}^{0}\left[g\left(\gamma(s\theta)+\int_{-\infty}^{\tau}F(us\theta+x)\mathrm{d}u\right)-s\theta\right]\mathrm{d}\tau\\&=\int_{-\infty}^{0}\left[\frac{\dfrac{\theta}{\sqrt{1-s^2/c^2}}+\dfrac{1}{s^2}\displaystyle\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u}{\sqrt{1+c^{-2}\left|\dfrac{s\theta}{\sqrt{1-s^2/c^2}}+\dfrac{1}{s}\displaystyle\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|^2}}-\theta\right]\mathrm{d}\tau.\end{aligned}\tag{6.24}$$

Expanding the square of the norm in the denominator of the fraction under the integral in (6.24), the denominator becomes

$$\left(1+c^{-2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}=(1+\delta_1(c,\theta,x,s,\tau))^{-1/2}(1-s^2/c^2)^{1/2},\tag{6.25}$$

where δ_1 is defined by formula (6.4). We define

$$\begin{aligned}\Lambda_1(\theta,x,s)=\Bigg|&(1-s^2/c^2)^{-1/2}\int_{-\infty}^{0}\left[g\left(\gamma(s\theta)+\int_{-\infty}^{\tau}F(us\theta+x)\mathrm{d}u\right)-s\theta\right]\mathrm{d}\tau-c^{-2}\int_{-\infty}^{0}V(\tau\theta+x)\mathrm{d}\tau\,\theta\\&-s^{-2}\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\,\mathrm{d}\tau\Bigg|.\end{aligned}\tag{6.26}$$

From (6.26), (6.24), and (6.25), it follows that

$$\begin{aligned}\Lambda_1(\theta,x,s)\leqslant&\int_{-\infty}^{0}|(1+\delta_1(c,\theta,x,s,\tau))^{-1/2}-1-c^{-2}V(\tau\theta+x)\sqrt{1-s^2/c^2}|\\&\times\left(\frac{1}{\sqrt{1-s^2/c^2}}+s^{-2}\int_{-\infty}^{\tau}|F(u\theta+x)|\mathrm{d}u\right)\mathrm{d}\tau\\&+\int_{-\infty}^{0}\left|(1+c^{-2}V(\tau\theta+x)\sqrt{1-s^2/c^2})\left(\frac{\theta}{\sqrt{1-s^2/c^2}}+s^{-2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right)\right.\\&\left.-\frac{\theta}{\sqrt{1-s^2/c^2}}-c^{-2}V(\tau\theta+x)\theta-s^{-2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|\mathrm{d}\tau.\end{aligned}\tag{6.27}$$

We estimate the first integral on the right-hand side of (6.27) by the use of Lemma 6.1. Therefore expanding the first product under the second integral of the form $\int_{-\infty}^{0}$ on the right-hand side of (6.27), we obtain

$$\begin{aligned}\Lambda_1(\theta,x,s)\leqslant&\sqrt{1-s^2/c^2}\int_{-\infty}^{0}\left[\widetilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}(\tau)\left(1+s^{-2}\sqrt{1-s^2/c^2}\int_{-\infty}^{\tau}|F(u\theta+x)|\mathrm{d}u\right)\right.\\&\left.+\left|\frac{V(\tau\theta+x)}{s^2c^2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|\right]\mathrm{d}\tau.\end{aligned}\tag{6.28}$$

We define $|V|_\infty=\sup_{y\in\mathbb{R}^d}|V(y)|$. Using (6.28), (1.2), (6.1a), and (4.8) and the fact that $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, we obtain

$$\Lambda_1(\theta,x,s) \leqslant \sqrt{1-s^2/c^2}\left[\left(1+\frac{\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{z_2(c,d,\beta_1,\alpha,|x|)^2}\frac{\beta_1\sqrt{d}\sqrt{2}}{\alpha(1+|x|/\sqrt{2})^{\alpha}}\right)\int_{-\infty}^{0}\tilde{g}_{c,d,\beta_0,\beta_1,\alpha,|x|}(\tau)\mathrm{d}\tau + \frac{\beta_1\sqrt{d}2|V|_{\infty}}{z_2(c,d,\beta_1,\alpha,|x|)^2c^2\alpha(\alpha-1)(1+|x|/\sqrt{2})^{\alpha-1}}\right]. \tag{6.29}$$

Now we look for the asymptotics of

$$\int_0^{+\infty}\left[g\left(\gamma(s\theta)+\int_{-\infty}^{\tau}F(us\theta+x)\mathrm{d}u\right)-g\left(\gamma(s\theta)+\int_{-\infty}^{+\infty}F(us\theta+x)\mathrm{d}u\right)\right]\mathrm{d}\tau.$$

By changes of variables, we obtain

$$\begin{aligned}&\int_0^{+\infty}\left[g\left(\gamma(s\theta)+\int_{-\infty}^{\tau}F(us\theta+x)\mathrm{d}u\right)-g\left(\gamma(s\theta)+\int_{-\infty}^{+\infty}F(us\theta+x)\mathrm{d}u\right)\right]\mathrm{d}\tau\\ &=\int_0^{+\infty}\left[\frac{\frac{\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s^2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u}{\sqrt{1+c^{-2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|^2}}\right.\\ &\left.-\frac{\frac{\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s^2}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u}{\sqrt{1+c^{-2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2}}\right]\mathrm{d}\tau.\end{aligned} \tag{6.30}$$

First we study the denominator of the first fraction under the integral of (6.30). From (6.14) and (6.13) it follows that

$$\begin{aligned}&\left(1+c^{-2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\\ &\quad=\left(1+c^{-2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}A(c,\theta,x,s,\tau).\end{aligned} \tag{6.31}$$

We define

$$\begin{aligned}\Lambda_2(c,\theta,x,s)=\Bigg|&(1-s^2/c^2)^{-1/2}\int_0^{+\infty}\left[g\left(\gamma(s\theta)+\int_{\tau}^{+\infty}F(us\theta+x)\mathrm{d}u\right)\right.\\ &\left.-g\left(\gamma(s\theta)+\int_{-\infty}^{+\infty}F(us\theta+x)\mathrm{d}u\right)\right]\mathrm{d}\tau-c^{-2}\int_0^{+\infty}V(\tau\theta+x)\mathrm{d}\tau\,\theta\\ &+s^{-2}\int_0^{+\infty}\int_{\tau}^{+\infty}F(u\theta+x)\mathrm{d}u\,\mathrm{d}\tau\Bigg|.\end{aligned} \tag{6.32}$$

From (6.30)–(6.32) it follows that

$$\Lambda_2(c,\theta,x,s)\leqslant\Lambda_{2,1}(c,\theta,x,s)+\Lambda_{2,2}(c,\theta,x,s), \tag{6.33}$$

where

$$\Lambda_{2,1}(c,\theta,x,s)=\int_0^{+\infty}\left|(1-s^2/c^2)^{-1/2}\left(1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\right.$$
$$\left.\times\left(A(c,\theta,x,s,\tau)-1-V(\tau\theta+x)\frac{\sqrt{1-\frac{s^2}{c^2}}}{c^2}\right)\left(\frac{\theta}{\sqrt{1-\frac{s^2}{c^2}}}+\frac{1}{s^2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right)\right|\mathrm{d}\tau, \tag{6.34a}$$

$$\begin{aligned}\Lambda_{2,2}(c,\theta,x,s)=&\int_0^{+\infty}\left|(1-s^2/c^2)^{-1/2}\left(1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\right.\\&\times\left[\left(1+V(\tau\theta+x)\frac{\sqrt{1-s^2/c^2}}{c^2}\right)\left(\frac{\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s^2}\int_{-\infty}^{\tau}F(u\theta+x)\mathrm{d}u\right)\right.\\&\left.\left.-\left(\frac{\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s^2}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right)\right]\right.\\&\left.-\frac{V(\tau\theta+x)}{c^2}\theta+\frac{1}{s^2}\int_{\tau}^{+\infty}F(u\theta+x)\mathrm{d}u\right|\mathrm{d}\tau.\end{aligned} \tag{6.34b}$$

Let us estimate $\Lambda_{2,1}(c,\theta,x,s)$.

From Lemma 6.3 and (6.34a) it follows that

$$\begin{aligned}\Lambda_{2,1}(c,\theta,x,s)\leqslant&\sqrt{1-s^2/c^2}\left(1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\\&\times\left(\frac{1}{\sqrt{1-s^2/c^2}}+\frac{1}{s^2}\int_{-\infty}^{+\infty}|F(u\theta+x)|\mathrm{d}u\right)\int_0^{+\infty}h_{c,d,\beta_0,\beta_1,\alpha,|x|}(\tau)\mathrm{d}\tau.\end{aligned} \tag{6.35}$$

In addition, expanding the square of the norm, we obtain

$$\begin{aligned}&\left(1+\frac{1}{c^2}\left|\frac{s\theta}{\sqrt{1-s^2/c^2}}+\frac{1}{s}\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\\&\quad=\sqrt{1-s^2/c^2}\left(1+\frac{1-s^2/c^2}{s^2c^2}\left|\int_{-\infty}^{+\infty}F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2}\end{aligned} \tag{6.36a}$$

$$\leqslant\sqrt{1-s^2/c^2}. \tag{6.36b}$$

Using (6.35), (6.36), (4.1), (6.2), and (4.7) and the fact that $s\geqslant z_2(c,d,\beta_1,\alpha,|x|)$, we obtain

$$\Lambda_{2,1}(c,\theta,x,s)\leqslant\sqrt{1-s^2/c^2}\left(1+\frac{\beta_1\sqrt{d}\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}2\sqrt{2}}{z_2(c,d,\beta_1,\alpha,|x|)^2\alpha(1+|x|/\sqrt{2})^{\alpha}}\right)\int_0^{+\infty}h_{c,d,\beta_0,\beta_1,\alpha,|x|}(\tau)\mathrm{d}\tau. \tag{6.37}$$

Let us estimate $\Lambda_{2,2}(c,\theta,x,s)$.

From (6.34b) and (6.36a) it follows that

$$\Lambda_{2,2}(c,\theta,x,s) \leqslant \int_0^{+\infty} \left| \left(1+\frac{1-s^2/c^2}{s^2c^2}\left|\int_{-\infty}^{+\infty} F(u\theta+x)\mathrm{d}u\right|^2\right)^{-1/2} - 1 \right|$$
$$\times \left| -\frac{1}{s^2}\int_\tau^{+\infty} F(u\theta+x)\mathrm{d}u + \frac{V(\tau\theta+x)}{c^2}\theta + \frac{\sqrt{1-s^2/c^2}}{s^2c^2}V(\tau\theta+x) \right.$$
$$\left. \times \int_{-\infty}^{\tau} F(u\theta+x)\mathrm{d}u \right| \mathrm{d}\tau + \int_0^{+\infty} \left| \frac{\sqrt{1-s^2/c^2}}{s^2c^2}V(\tau\theta+x)\int_{-\infty}^{\tau} F(u\theta+x)\mathrm{d}u \right| \mathrm{d}\tau. \tag{6.38}$$

Thus using Lemma 6.2, conditions (1.2), (4.1), (6.2), (4.6), and (4.7) and the fact that $s \geqslant z_2(c,d,\beta_1,\alpha,|x|)$, it follows that

$$\Lambda_{2,2}(c,\theta,x,s) \leqslant \sqrt{1-s^2/c^2}\left[\frac{k_{1/2,c,d,\beta_1,\alpha,|x|}\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{(\alpha-1)(1+|x|/\sqrt{2})^{\alpha-1}} \right.$$
$$\times \left(\frac{\sqrt{d}\beta_1 2}{z_2(c,d,\beta_1,\alpha,|x|)^2\alpha} + \frac{\beta_0\sqrt{2}}{c^2} + \frac{\sqrt{d}\beta_0\beta_1 4\sqrt{1-z_2(c,d,\beta_1,\alpha,|x|)^2/c^2}}{z_2(c,d,\beta_1,\alpha,|x|)^2c^2\alpha(1+|x|/\sqrt{2})^{\alpha}} \right)$$
$$\left. + \frac{\sqrt{d}\beta_0\beta_1 4}{z_2(c,d,\beta_1,\alpha,|x|)^2c^2\alpha(\alpha-1)(1+|x|/\sqrt{2})^{2\alpha-1}} \right]. \tag{6.39}$$

From (2.13b), (6.26), (6.29), (6.32), (6.34), (6.35), and (6.39) it follows that there exists $C_{c,d,\beta_0,\beta_1,\alpha,|x|}$ such that

$$\left| \frac{l_{s\theta,x}(0)}{\sqrt{1-s^2/c^2}} - \frac{1}{c^2}PV(\theta,x)\theta + \frac{1}{s^2}\int_0^{+\infty}\int_\tau^{+\infty} F(x+u\theta)\mathrm{d}u\,\mathrm{d}\tau - \frac{1}{s^2}\int_{-\infty}^{0}\int_{-\infty}^{\tau} F(x+u\theta)\mathrm{d}u\,\mathrm{d}\tau \right|$$
$$\leqslant \Lambda_1(c,\theta,x,s) + \Lambda_2(c,\theta,x,s) \leqslant C_{c,d,\beta_0,\beta_1,\alpha,|x|}\sqrt{1-s^2/c^2}. \tag{6.40}$$

The estimate (3.9) follows from (6.40).

Theorem 3.2 is proved.

Proof of Proposition 1.1: The item (1) follows immediately from

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t\theta+x) = \nabla V(t\theta+x)\theta \quad \text{for all } (\theta,x) \in T\mathbb{S}^{d-1}, \quad t \in \mathbb{R}.$$

Proof of item (2). Take

$$V(x) = \frac{x_1}{(1+|x|^2)^\beta} \quad \text{for } x=(x_1,\ldots,x_d) \in \mathbb{R}^d, \beta > 1.$$

and take $(\theta,x) \in T\mathbb{S}^{d-1}$. By a straightforward calculation and using $\theta x = 0$, we obtain

$$\left(\int_{-\infty}^{0}\int_{-\infty}^{\tau} F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau - \int_0^{+\infty}\int_\tau^{+\infty} F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau + PV(\theta,x)\theta \right) \star x$$
$$= -4\beta\theta_1|x|^2\int_0^{+\infty}\int_\tau^{+\infty} \frac{s}{(1+s^2+|x|^2)^{\beta+1}}\mathrm{d}s\,\mathrm{d}\tau \neq 0 \text{ if and only if } x \neq 0 \text{ and } \theta_1 \neq 0,$$

where $\star$ denotes the scalar product.

Proof of item (3): Let V be a spherical symmetric potential [i.e., V takes the form $m(|x|)$] that satisfies the conditions (1.2) [e.g., $V(x)=(1+|x|^2)^{-\beta}$ where $\beta > \frac{1}{2}$]. Then $m \in C^1(]0,+\infty[,\mathbb{R})$ and

$\nabla V(x)=m'(|x|)(x/|x|)$. Let $(\theta,x)\in T\mathbb{S}^{d-1}$ and let $\theta^{\perp}$ be an orthogonal vector to θ. A straighforward calculation gives

$$F(s\theta+x)\theta^{\perp}=m'(\sqrt{s^2+|x|^2})\frac{x\star\theta^{\perp}}{\sqrt{s^2+|x|^2}}$$

for any $s\in\mathbb{R}$. Hence

$$\left(\int_{-\infty}^{0}\int_{-\infty}^{\tau}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau-\int_{0}^{+\infty}\int_{\tau}^{+\infty}F(s\theta+x)\mathrm{d}s\,\mathrm{d}\tau+PV(\theta,x)\theta\right)\star\theta^{\perp}=0. \tag{6.41}$$

Item (3) follows from item (1) and formula (6.41).

Proposition 1.1 is proved.

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Classification of infinitesimal symmetries in covariant classical mechanics

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In the framework of general relativistic classical mechanics on a spacetime with absolute time, we classify the infinitesimal symmetries of the classical structure by means of distinguished Lie subalgebras of the Lie algebra of "special phase function." These subalgebras are crucial also for the classification of infinitesimal quantum symmetries, which will be analyzed in a forthcoming paper. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2199068]

I. INTRODUCTION

This paper is the first part of a sequence of two papers. They are aimed at classifying systematically the symmetries of classical and quantum mechanics within the geometric framework of "covariant classical and quantum mechanics."

This framework is a geometric formulation of classical and quantum mechanics on a curved spacetime with absolute time and spacelike Riemannian metric, expressed in a manifestly coordinate free and observer independent way. We assume minimal axioms describing just the fundamental classical interactions, namely the gravitational and electromagnetic fields. The goal of this theory is to combine the standard quantum mechanics with those ideas and methods of Einstein's general relativity that are not related to the Lorentz metric and the speed of light, in order to understand quantum mechanics in a general relativistic observer independent way, as far as possible.

This approach requires methods based on fibered manifolds, jets, connections, and the Lie algebra of special phase functions. On the other hand, in the flat case the theory yields just the standard Schrödinger equation and the quantum operators for all usual examples. This approach has some analogies with other well-known geometric formulations of quantum mechanics, in particular, with geometric quantization (see, for instance, Refs. 1, 29, and 68). But, it presents several methodological novelties and results as well, by overcoming several typical difficulties in the theory of geometric quantization.

This approach was proposed in Refs. 33 and 34 and further developed by several authors (see, for instance, Refs. 38, 36, 61, and 62, and references therein). On the other hand, several authors have been involved with a formulation of classical and quantum mechanics in the framework of a curved Galileian background (see, for instance, Refs. 11, 18–24, 32, 40–44, 46, 54, and 65–67). One of the typical features of covariant classical mechanics is the role played by a cosymplectic

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two-form. This is a concept more general than that of contact two-form and appropriate to account for the covariance of the theory. Actually, the literature on symplectic geometry is much wider and better known than that on cosymplectic geometry; however, several authors have analyzed the second one (see, for instance, Refs. 2, 8, 14, 17, 35, and 48, and references therein).

In the present paper, we start by introducing the basic objects of the theory, namely the spacetime fibered over absolute time, the spacelike Riemannian metric, the spacetime gravitational connection, and the electromagnetic field.

Then, we introduce the classical phase space and the main geometric objects induced by the spacetime structure, namely the contact maps, the phase connection, the second-order phase connection, the phase two-form and the phase two-vector. An important role is played by the phase two-form, which encodes all other objects and turns out to be cosymplectic. This set up allows us to introduce in a natural way the distinguished Lie algebra of special phase functions and their various lifts. The special Lie bracket is linked to the Poisson bracket and allows us to deal with spacetime functions, momentum, and energy on the same footing. An essential feature of special phase functions is that they admit a lift to the tangent space of spacetime.

Eventually, we classify systematically the infinitesimal symmetries of the above classical objects and show, step by step, that they are generated by distinguished subalgebras of the Lie algebra of special phase functions.

We observe that the classical Lagrangian formalism, Nöther's theorem, and the momentum map[1,10,15,16,27,28,30,45,58,57,60,64] arise naturally in the present scheme ruled by a cosymplectic two-form and by the Lie algebra of special phase functions. The literature dealing with Lie algebras associated with geometric structures of analytical mechanics from different perspectives is very wide (see, for instance, Refs. 3–7, 9, 12, 13, 25, 26, 31, 47, 49–51, 53, 52, and 56). On the other hand, the present paper is devoted to the specific setting of covariant classical mechanics of a particle effected by the fundamental classical fields.

This paper extends considerably the results obtained in Refs. 62 and 38, mainly by classifying the distinguished subalgebras of the Lie algebra of special phase functions and its relation to infinitesimal symmetries.

The above results will play an essential role in the subsequent paper devoted to infinitesimal quantum symmetries, where we achieve analogous results by a similar approach. In particular, we will prove in this forthcoming paper that the Lie algebra of special phase functions yields a Lie algebra of quantum currents; the conserved probability current is just a particular case of this construction.

Thus, throughout the two papers, a crucial role is played by the Lie algebra of special phase functions, which turn out to be the generators of the infinitesimal symmetries both of the classical and quantum theories. The special phase functions are the functions of the phase space whose second order vertical differential (with respect to the fibering of the phase space over spacetime) is proportional to the metric.

For each manifold $\boldsymbol{M}$, $\boldsymbol{N}$ and each fibered manifolds $\boldsymbol{F}\to\boldsymbol{B},\boldsymbol{G}\to\boldsymbol{B}$, we denote the sheaf of local maps $f:\boldsymbol{M}\to\boldsymbol{N}$ by map $(\boldsymbol{M},\boldsymbol{N})$, the sheaf of local sections $s:\boldsymbol{B}\to\boldsymbol{F}$ by $\mathrm{sec}(\boldsymbol{B},\boldsymbol{F})$ and the sheaf of local fibered morphisms $f:\boldsymbol{F}\to\mathbf{G}$ over $\boldsymbol{B}$ by $\mathrm{fib}(\boldsymbol{F},\boldsymbol{G})$.

II. COVARIANT CLASSICAL MECHANICS

A. Spacetime and its structure

1. Scale spaces

In the covariant formulation of physical theories the independence from the choice of coordinates and of units of measurements appear on the same footing. Thus, a rigorous treatment of units of measurement is necessary.

We introduce the fundamental *scale spaces* $\mathbb{U}$ as "positive 1-dimensional semi-vector spaces" over $\mathbb{R}^+$. A detailed account for this notion can be found in Refs. 34 and 37. Roughly speaking, they have the same algebraic structure as $\mathbb{R}^+$, but no distinguished generator over $\mathbb{R}^+$. We can naturally define the tensor product between scale spaces and ordinary vector spaces. Moreover, we

can naturally define the rational powers $\mathbb{U}^{p/q}$ of a scale space $\mathbb{U}$. Rules analogous to those of real numbers hold for scale spaces; accordingly, we adopt analogous notation. In particular, we shall write $\mathbb{U}^0 := \mathbb{U}, \mathbb{U}^{-1} := \mathbb{U}^*, \mathbb{U}^p := \otimes^p \mathbb{U}$.

These spaces will appear in the theory tensorialized with spacetime tensors. The scale spaces appearing in tensor products are not effected by differential operators, hence their elements can be treated as constants.

We introduce the space $\mathbb{T}$ of *future oriented time intervals*, the space $\mathbb{L}$ of *lengths*, and the space $\mathbb{M}$ of *masses*.

We shall refer to particles of mass $m \in \mathbb{M}$ and charge $q \in \mathbb{T}^{-1} \otimes \mathbb{L}^{3/2} \otimes \mathbb{M}^{1/2}$.

Moreover, we will consider time units $u_0 \in \mathbb{T}$, or their duals $u^0 \in \mathbb{T}^*$.

In order to unscale some objects of the theory, we will need a scale with scale dimensions of the *Planck constant* $\hbar : \mathbb{T}^{-1} \otimes \mathbb{L}^2 \otimes \mathbb{M}$. Actually, in the classical theory any such scale would do; on the other hand, in the quantum theory, we have to assume just the actual value of this scale.

2. Spacetime

Our basic framework is spacetime with its fibering over absolute time.[34,37]

We assume *time* to be an affine space $\boldsymbol{T}$ associated with the vector space $\overline{\mathbb{T}} := \mathbb{T} \otimes \mathbb{R}$ and *spacetime* to be an oriented four-dimensional manifold $\boldsymbol{E}$ fibered over time by the *absolute time map* $t : \boldsymbol{E} \to \boldsymbol{T}$.

We shall refer to *spacetime charts* $(x^\lambda) = (x^0, x^i)$ adapted to the time fibering, to the affine structure of time, to a time unit of measurement $u_0 \in \overline{\mathbb{T}}$ and to the orientation of spacetime.

We shall be concerned with the *tangent space* $T\boldsymbol{E}$ of spacetime and its *vertical tangent* subspace $J : V\boldsymbol{E} \subset T\boldsymbol{E}$, consisting of the vectors tangent to the fibers, which are called *spacelike*. Moreover, we shall be concerned with the *cotangent space* $T^*\boldsymbol{E}$ of spacetime and its *horizontal subspace* $H^*\boldsymbol{E} := \boldsymbol{E} \times \overline{\mathbb{T}}^* \subset T^*\boldsymbol{E}$, consisting of forms vanishing on vertical vectors, which are called *timelike*. Furthermore, we shall be concerned with the *horizontal space* $H\boldsymbol{E} := \boldsymbol{E} \times \overline{\mathbb{T}}$ and the *cotangent vertical* space $V^*\boldsymbol{E}$. The local coordinate bases of $T\boldsymbol{E}$, $V\boldsymbol{E}$, $T^*\boldsymbol{E}$, $H\boldsymbol{E}$, and $V^*\boldsymbol{E}$ are denoted by

$$\partial_\lambda \in \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E}), \quad \partial_i \in \mathrm{sec}(\boldsymbol{E}, V\boldsymbol{E}), \quad d^\lambda \in \mathrm{sec}(\boldsymbol{E}, T^*\boldsymbol{E}), \quad d^0 \in \mathrm{sec}(\boldsymbol{E}, H^*\boldsymbol{E})$$

$$u_0 \in \mathrm{sec}(\boldsymbol{E}, H\boldsymbol{E}), \quad \check{d}^i \in \mathrm{sec}(\boldsymbol{E}, V^*\boldsymbol{E}).$$

We have the distinguished scaled *time form* $dt : \boldsymbol{E} \to \mathbb{T} \otimes T^*\boldsymbol{E}$, with coordinate expression $dt = u_0 \otimes d^0$. It generates the horizontal subbundle $H^*\boldsymbol{E} \subset T^*\boldsymbol{E}$. We shall often make the natural identification $u^0 \simeq d^0$ via pullback.

We have the natural *timelike projection* and *spacelike projection*

$$dt : T\boldsymbol{E} \to H\boldsymbol{E} : X \mapsto dt(X) \quad \text{and} \quad J^* : T^*\boldsymbol{E} \to V^*\boldsymbol{E} : \alpha \mapsto \check{\alpha} := \alpha \circ J,$$

with coordinate expressions $dt(X) = X^0 u_0$ and $\check{\alpha} = \alpha_i \check{d}^i$.

In general, the inverted caret "$\check{}$" will denote the vertical restriction of spacetime forms. We stress that we *do not* have natural inclusions and projections of the following type

$$V^*\boldsymbol{E} \subset T^*\boldsymbol{E}, \quad H\boldsymbol{E} \subset T\boldsymbol{E} \quad \text{and} \quad T\boldsymbol{E} \to V\boldsymbol{E}, \quad T^*\boldsymbol{E} \to H^*\boldsymbol{E}.$$

This is an important feature of our relativistic model; indeed, we need the choice of an "observer" in order to achieve such inclusions and projections.

We shall be involved with the Lie subalgebras

$$\mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E}) \subset \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E}) \quad \text{and} \quad \mathrm{fine}(\boldsymbol{E}, T\boldsymbol{E}) \subset \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E})$$

of spacetime vector fields which are projectable on $\boldsymbol{T}$ and whose time component is constant, respectively. Their coordinate expressions are of the type

$$X = X^0\partial_0 + X^i\partial_i \in \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E}) \quad \text{with} \quad X^0 \in \mathrm{map}(\boldsymbol{T}, \mathbb{R}), X^i \in \mathrm{map}(\boldsymbol{E}, \mathbb{R}),$$

$$X = X^0\partial_0 + X^i\partial_i \in \mathrm{fine}(\boldsymbol{E}, T\boldsymbol{E}) \quad \text{with} \quad X^0 \in \mathbb{R} \quad X^i \in \mathrm{map}(\boldsymbol{E}, \mathbb{R}).$$

3. Observers

Observers are essential tools for performing physical measurements. In the standard literature, the measurements are usually described by coordinates. But what is essentially necessary is the observer underlying a system of coordinates.

Our relativistic model does not exhibit any distinguished observer.

The choice of an observer yields the observed inclusions and projections which are not provided by the time fibering.

An *observer* is defined to be a (local) section $o:\boldsymbol{E}\to\mathbb{T}^*\otimes T\boldsymbol{E}$, which projects on $\mathbf{1}\in\mathbb{T}^*\otimes\mathbb{T}$, i.e., a (local) section $o:\boldsymbol{E}\to J_1\boldsymbol{E}$, where $J_1\boldsymbol{E}$ denotes the first jet space of spacetime. Thus, an observer is just a connection of the spacetime fibering.

The coordinate expression of an observer o is of the type $o=u^0\otimes(\partial_0+o_0^i\partial_i)$, where $o_0^i \in \mathrm{map}(\boldsymbol{E},\mathbb{R})$. The charts (x^λ) for which $o_0^i=0$ are said to be *adapted* to o. Conversely, each chart (x^λ) is adapted to a unique observer, whose coordinate expression turns out to be $o:=u^0\otimes\partial_0$.

Each observer o yields the *observed spacelike projection* $\nu[o]:T\boldsymbol{E}\to V\boldsymbol{E}:X\mapsto X-o(dt(X))$ and the *observed timelike projection* $o^*:T^*\boldsymbol{E}\to H^*\boldsymbol{E}:\alpha\circ o\simeq o\rfloor\alpha$, whose coordinate expressions are $\nu[o]=(d^i-o_0^id^0)\otimes\partial_i$ and $o^*=d^0\otimes(\partial_0+o_0^i\partial_i)$.

Moreover, an observer o yields the *observed spacelike inclusion* $\nu^*[o]:V^*\boldsymbol{E}\hookrightarrow T^*\boldsymbol{E}:\alpha\mapsto\alpha\circ\nu[o]$ and the *observed timelike inclusion* $o:H\boldsymbol{E}\hookrightarrow T\boldsymbol{E}:X\mapsto o(X)$, whose coordinate expressions are $\nu^*[o](\alpha)=\alpha_i(d^i-o_0^id^0)$ and $o(X)=X^0(\partial_0+o_0^i\partial_i)$.

Thus, an observer o yields the *observed splittings* of the tangent and cotangent spaces of spacetime into the direct sum of their timelike and spacelike components

$$T\boldsymbol{E}=H\boldsymbol{E}\oplus V\boldsymbol{E}:X\mapsto dt(X)+\nu[o](X),\quad T^*\boldsymbol{E}=H^*\boldsymbol{E}\oplus V^*\boldsymbol{E}:\alpha\mapsto o^*(\alpha)+\jmath^*(\alpha).$$

4. Metric field

The fibers of spacetime are equipped with a given Riemannian metric.[34,37]

We assume spacetime to be equipped with a scaled Riemannian metric of the fibers $g:\boldsymbol{E}\to\mathbb{L}^2\otimes(V^*\boldsymbol{E}\otimes V^*\boldsymbol{E})$.

With reference to a particle of mass m, it is useful to define the *rescaled spacelike metric* $G:=(m/\hbar)g:\boldsymbol{E}\to\mathbb{T}\otimes(V^*\boldsymbol{E}\otimes V^*\boldsymbol{E})$.

We denote the contravariant spacelike metric and the contravariant rescaled spacelike metric by $\bar g:\boldsymbol{E}\to\mathbb{L}^{*2}\otimes(V\boldsymbol{E}\otimes V\boldsymbol{E})$ and $\bar G:=(\hbar/m)\bar g:\boldsymbol{E}\to\mathbb{T}^*\otimes(V\boldsymbol{E}\otimes V\boldsymbol{E})$.

The spacelike metric g and the spacetime orientation naturally yield the scaled *spacelike volume form* $\eta:\boldsymbol{E}\to\mathbb{L}^3\otimes\Lambda^3V^*\boldsymbol{E}$, with coordinate expression $\eta=\sqrt{|g|}\check d^1\wedge\check d^2\wedge\check d^3$.

Moreover, the time form and the spacelike volume form yield the scaled *spacetime volume form* $v:=dt\wedge\eta:\boldsymbol{E}\to(\mathbb{T}\otimes\mathbb{L}^3)\otimes\wedge^4T^*\boldsymbol{E}$, with coordinate expression $v=\sqrt{|g|}u_0\otimes d^0\wedge d^1\wedge d^2\wedge d^3$.

For each $X\in\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$, the Lie derivative $L[X]\bar G\in\mathrm{sec}(\boldsymbol{E},\mathbb{T}^*\otimes(V\boldsymbol{E}\otimes V\boldsymbol{E}))$ has the coordinate expression $L[X]\bar G=(X^\lambda\partial_\lambda G_0^{ij}-G_0^{hj}\partial_hX^i-G_0^{ih}\partial_hX^j)u^0\otimes\partial_i\otimes\partial_j$.

For each $X\in\mathrm{proj}(\boldsymbol{E},T\boldsymbol{E})$, the Lie derivative $L[X]G\in\mathrm{sec}(\boldsymbol{E},\mathbb{T}\otimes(V^*\boldsymbol{E}\otimes V^*\boldsymbol{E}))$, has the coordinate expression $L[X]G=(X^\lambda\partial_\lambda G_{ij}^0+G_{hj}^0\partial_iX^h+G_{ih}^0\partial_jX^h)u_0\otimes\check d^i\otimes\check d^j$.

For each $X\in\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$, the *spacetime divergence* $\mathrm{div}_vX\in\mathrm{map}(\boldsymbol{E},\mathbb{R})$ is well defined by the equality $L[X]v=(\mathrm{div}_vX)v$.

For each $X\in\mathrm{proj}(\boldsymbol{E},T\boldsymbol{E})$, the *spacelike divergence* $\mathrm{div}_\eta X\in\mathrm{map}(\boldsymbol{E},\mathbb{R})$ and the *timelike divergence* $\mathrm{div}_{dt}X\in\mathrm{map}(\boldsymbol{E},\mathbb{R})$ are well defined, respectively, by the equalities $L[X]\eta=(\mathrm{div}_\eta,X)\eta$ and $L[X]dt=(\mathrm{div}_{dt}X)dt$.

We have the coordinate expressions

$$\mathrm{div}_v X = \frac{\partial_\lambda(X^\lambda\sqrt{|g|})}{\sqrt{|g|}}, \quad \mathrm{div}_\eta X = X^0\frac{\partial_0\sqrt{|g|}}{\sqrt{|g|}} + \frac{\partial_j(X^j\sqrt{|g|})}{\sqrt{|g|}}, \quad \mathrm{div}_{dt} X = \partial_0 X^0.$$

Hence, for each $X \in \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E})$, we obtain $\mathrm{div}_v X = \mathrm{div}_{dt} X + \mathrm{div}_\eta X$ and, for each $X \in \mathrm{fine}(\boldsymbol{E}, T\boldsymbol{E})$, we obtain $\mathrm{div}_v X = \mathrm{div}_\eta X$.

Moreover, for each $X \in \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E})$, we obtain $\mathrm{div}_\eta X = \frac{1}{2}\langle \bar{G}, L[X]G\rangle$.

5. Gravitational and electromagnetic fields

Spacetime is equipped with given gravitational and electromagnetic fields.[34]

We assume spacetime to be equipped with a *gravitational field*, i.e., with a linear connection $K^\natural : T\boldsymbol{E} \to T^*\boldsymbol{E} \otimes TT\boldsymbol{E}$, such that $\nabla^\natural dt = 0$ and $\nabla^\natural g = 0$, and such that its curvature tensor $R[K^\natural]$ fulfills the symmetry condition $R^\natural{}_{i\lambda j\mu} = R^\natural{}_{.j\mu i\lambda}$.

Proposition 2.1: The coordinate expression of the gravitational field is of the type

$$K^\natural{}_\lambda{}^0{}_\mu = 0,$$

$$K^\natural{}_0{}^i{}_0 = -G_0^{ij} 2\Phi_{0j},$$

$$K^\natural{}_0{}^i{}_h = K^\natural{}_h{}^i{}_0 = -\tfrac{1}{2} G_0^{ij}(\partial_0 G^0_{jh} + 2\Phi_{hj}),$$

$$K^\natural{}_k{}^i{}_h = K^\natural{}_h{}^i{}_k = -\tfrac{1}{2} G_0^{ij}(\partial_h G^0_{jk} - \partial_j G^0_{hk} + \partial_k G^0_{jh}),$$

where $\Phi^\natural[o] = \Phi^\natural{}_{\lambda\mu} d^\lambda \wedge d^\mu \in \mathrm{sec}(\boldsymbol{E}, \Lambda^2 T^*\boldsymbol{E})$ is a closed two-form, which depends on the chosen chart only through the associated observer o. QED

We shall denote by $A^\natural[o]$ the local potentials of $\Phi^\natural[o]$, according to $2dA^\natural[o] = \Phi^\natural[o]$.

We assume spacetime to be equipped with an *electromagnetic field*, i.e., with a closed scaled two-form $F : \boldsymbol{E} \to (\mathbb{L}^{1/2} \otimes \mathbb{M}^{1/2}) \otimes \Lambda^2 T^*\boldsymbol{E}$ (see also Ref. 46).

Given a particle with mass $m \in \mathbb{M}$ and charge $q \in \mathbb{T}^{-1} \otimes \mathbb{L}^{3/2} \otimes \mathbb{M}^{1/2}$, it is convenient to consider, respectively, the unscaled field and the rescaled field

$$\tfrac{q}{\hbar} F : \boldsymbol{E} \to \Lambda^2 T^*\boldsymbol{E} \quad \text{and} \quad \tfrac{q}{m}\hat{F} : \boldsymbol{E} \to \mathbb{T}^{-1} \otimes (V\boldsymbol{E} \otimes T^*\boldsymbol{E}),$$

where $\hat{F} = g^{\sharp 2}(F) = g^{ih} F_{\lambda h} \partial_i \otimes d^\lambda$.

The electromagnetic field F can be "joined," in a covariant way, to the gravitational field yielding the *"joined" spacetime connection* $K = K^\natural - dt \otimes (q/2m)\hat{F} - (q/2m)\hat{F} \otimes dt$.

The joined K still fulfills the properties that we have assumed for $K^\natural$. Moreover, all objects derived from the joined connection split into components related to the gravitational and the electromagnetic fields.

In particular, the observed potential $A[o]$ of the joined connection splits into the sum of the gravitational and electromagnetic potentials as $A[o] = A^\natural[o] + (q/\hbar)A^e$, where $A^e \in \mathrm{sec}(\boldsymbol{E}, (\mathbb{L}^{1/2} \otimes \mathbb{M}^{1/2}) \otimes T^*\boldsymbol{E})$ is a local (observer independent) potential of F, according to $2dA^e = F$.

Thus, from now on, with reference to a particle of mass m and charge q, we shall refer to the spacetime structure constituted by the 4-plet $(\boldsymbol{E}, t, G, K)$, whose elements fulfill the properties mentioned above.

6. Basic model of spacetime

The present paper deals with a curved spacetime. However, this model includes flat or partially flat spacetimes, as well.[34] Thus, the standard mechanics can be recovered as a particular case of our theory.

The simplest model of spacetime is given by the following construction.

We consider an oriented affine space $\boldsymbol{E}$ that is associated with the vector space $\bar{\boldsymbol{E}}$ and equipped with an affine map $t:\boldsymbol{E}\to\boldsymbol{T}$ of rank 1.

Let us consider the vector subspace $\boldsymbol{S}:=\ker Dt\subset\bar{\boldsymbol{E}}$. We can easily see that all fibers of the fibering $t:\boldsymbol{E}\to\boldsymbol{T}$ are affine subspaces of $\boldsymbol{E}$ associated with the same vector space $\boldsymbol{S}$. Hence, the spacetime fibered space turns out to be an Abelian principal bundle with structural group $\boldsymbol{S}$.

We assume as spacelike metric a constant Euclidean metric on $\boldsymbol{S}$.

Moreover, we assume as gravitational connection the connection induced by the affine structure of spacetime. Eventually, we assume a vanishing electromagnetic field.

Clearly, the above objects fulfill our axioms. We call such a spacetime a *special Newtonian spacetime*. In this model we can easily define the standard inertial motions and inertial observers.

We could consider also a little more complex model, which assumes the previous structure for background and adds a gravitational connection which is Ricci flat. This model accounts for the standard notions of classical mechanics, including Newton's law of gravitation.

The rigid body provides a further nontrivial example of our model.[59]

B. Phase space and the induced structure

1. Classical phase space

We assume as phase space of a classical particle the first jet space of sections of spacetime.[34,37]

The first jet space (Refs. 39 and 63) $J_1\boldsymbol{E}$ of $t:\boldsymbol{E}\to\boldsymbol{T}$ is a fibered manifold $t^1:J_1\boldsymbol{E}\to\boldsymbol{T}$ over $\boldsymbol{T}$ and an affine bundle $t^1_0:J_1\boldsymbol{E}\to\boldsymbol{E}$ over $\boldsymbol{E}$, associated with the vector bundle $\mathbb{T}^*\otimes V\boldsymbol{E}$. Hence, the vertical space of $J_1\boldsymbol{E}$ with respect to $\boldsymbol{E}$ turns out to be $V_0J_1\boldsymbol{E}=\mathbb{T}^*\otimes V\boldsymbol{E}$.

We denote the fibered charts of the phase space by (x^0,x^i,x^i_0).

The above affine structure yields the natural tensor $\nu:J_1\boldsymbol{E}\to\mathbb{T}\otimes(V^*\boldsymbol{E}\otimes VJ_1\boldsymbol{E})$, with $\nu=u_0\otimes\check{d}^i\otimes\partial^0_i$.

We recall the natural *contact maps* $\mathit{\Pi}:J_1\boldsymbol{E}\to\mathbb{T}^*\boldsymbol{E}\otimes T\boldsymbol{E}$ and $\theta:J_1\boldsymbol{E}\to\mathbb{T}^*\otimes V\boldsymbol{E}$, with $\mathit{\Pi}=u^0\otimes(\partial_0+x^i_0\partial_i)$ and $\theta=\partial_i\otimes(d^i-x^i_0d^0)$. From now on, $J_1\boldsymbol{E}$ is considered as a subspace of $\mathbb{T}^*\otimes T\boldsymbol{E}$, according to the natural embedding $\mathit{\Pi}$.

We shall be involved with the Lie subalgebras

$$\mathrm{proj}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})\subset\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})\quad\text{and}\quad\mathrm{fine}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})\subset\mathrm{proj}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$$

of vector fields of $J_1\boldsymbol{E}$, which are projectable on $\boldsymbol{E}$ and $\boldsymbol{T}$, and additionally whose time components are constant, respectively.

2. Holonomic prolongation of spacetime vector fields

We have a natural prolongation of spacetime vector fields to phase vector fields.

Proposition 2.2:[37,55] There is a natural fibered morphism $r_1:J_1T\boldsymbol{E}\to TJ_1\boldsymbol{E}$ over $J_1\boldsymbol{E}\underset{\boldsymbol{T}}{\times}J_1T\boldsymbol{T}$, with $(x^0,x^i,x^i_0;\dot{x}^0\dot{x}^i,\dot{x}^i_0)\circ r_1=(x^0,x^i,x^i_0;\dot{x}^0,\dot{x}^i,\dot{x}^i_0-\dot{x}^i_0\dot{x}^0_0)$.

Then, for each $X\in\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$, we obtain the vector field, called *first holonomic prolongation* of X, $X_{(1)}:=r_1\circ J_1X\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$, which projects on X. Its coordinate expression is $X_{(1)}=X^0\partial_0+X^i\partial_i+(\partial_0X^i+\partial_jX^ix^j_0-\partial_0X^0x^i_0-\partial_jX^0x^j_0x^i_0)\partial^0_i$.

The map $r_1\circ J_1:\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})\to\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E}):X\mapsto X_{(1)}$ turns out to be an injective $\mathbb{R}$-linear morphism of Lie algebras. QED

In the particular case when the vector field X is projectable on $\boldsymbol{T}$, we recover the standard holonomic prolongation obtained through the first jet prolongation of the fibered flow of X. In fact, the above map restricts to the injective $\mathbb{R}$-linear map

$$\mathrm{proj}(\boldsymbol{E},T\boldsymbol{E})\to\mathrm{proj}(J_1\boldsymbol{E},TJ_1\boldsymbol{E}):X\mapsto X_{(1)},$$

with coordinate expression $X_{(1)}=X^0\partial_0+=X^i\partial_i+(\partial_0X^i+\partial_jX^ix^j_0-\partial_0X^0x^i_0)\partial^0_i$.

Later, we shall use the following technical results.

Lemma 2.3:[37] For each $X \in \sec(\boldsymbol{E}, T\boldsymbol{E})$, we have the equalities

$$L[X_{(1)}]\theta = (\text{Д} \,.\, (dt(X)))\,\theta \quad \text{and} \quad L[X_{(1)}]\,\text{Д} = -\,(\text{Д} \,.\, (dt(X)))\,\text{Д}\,,$$

with coordinate expressions

$$L[X_{(1)}]\theta = (\partial_0 X^0 + \partial_j X^0 x_0^j)(d^i - x_0^i d^0) \otimes \partial_i^0\,,$$

$$L[X_{(1)}]\,\text{Д} = -\,(\partial_0 X^0 + x_0^j \partial_j X^0)(\partial_0 + x_0^i \partial_i)\,.$$

QED

For each $X^{\uparrow} \in \text{proj}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ which projects on $X \in \text{proj}(\boldsymbol{E}, T\boldsymbol{E})$, the *spacelike divergence* $\text{div}_{\eta} X^{\uparrow} \in \text{map}(J_1\boldsymbol{E}, \mathbb{R})$ is well defined by the equality $L[X^{\uparrow}]\eta = (\text{div}_{\eta} X^{\uparrow})\,\eta$ and we obtain $\text{div}_{\eta} X^{\uparrow} = \text{div}_{\eta} X$.

3. Distinguished phase fields

The spacetime connection and the rescaled metric yield in a covariant way further objects on the phase space.[34,37]

The spacetime connection K yields a torsion free affine connection of the affine bundle $J_1\boldsymbol{E} \to \boldsymbol{E}$, called *phase connection*, $\Gamma[K]: J_1\boldsymbol{E} \to T^*\boldsymbol{E} \otimes TJ_1\boldsymbol{E}$, with coordinate expression $\Gamma_{\lambda 0}^{\ i} := \Gamma_{\lambda 0 j}^{\ i 0} x_0^j + \Gamma_{\lambda 00}^{\ i 0}$, where $\Gamma_{\lambda 0 \mu}^{\ i 0} = K_{\lambda}^{\ i}{}_{\mu}$ Conversely, Γ characterizes K.

The phase connection Γ splits into the gravitational and electromagnetic components as $\Gamma = \Gamma^{\natural} + \Gamma^e$ where $\Gamma^e = -(g/2m)(\hat{F} + \text{Д} \lrcorner \hat{F}) \in \sec(J_1\boldsymbol{E}, \mathbb{T}^* \otimes (T^*\boldsymbol{E} \otimes V\boldsymbol{E}))$.

We have $\Gamma_{00}^{i\,j} - \Gamma_{00}^{j\,i} = -G_0^{ih} G_0^{jk}((\partial_h G_{kl}^0 - \partial_k G_{hl}^0) x_0^l + \partial_h A_k - \partial_k A_h)$, with $\Gamma_{00}^{hk} := G_0^{hl} \Gamma_{l0}^k$.

Then, Γ yields the *second-order connection* $\gamma[\Gamma] := \text{Д} \lrcorner \Gamma : J_1\boldsymbol{E} \to J_2\boldsymbol{E} \subset \mathbb{T}^* \otimes TJ_1\boldsymbol{E}$, with $\gamma = u^0 \otimes (\partial_0 + x_0^i \partial_i + \gamma_{00}^{\ i} \partial_i^0)$, where

$$\begin{aligned}\gamma_{00}^{\ i} &= K_h^{\ i}{}_k x_0^h x_0^k + 2K_h^{\ i}{}_0 x_0^h + K_0^{\ i}{}_0 \\ &= -\,G_0^{ij}\Big(\Big(\partial_h G_{jk}^0 - \tfrac{1}{2}\partial_j G_{hk}^0\Big) x_0^h x_0^k + (\partial_0 G_{hj}^0 + \partial_h A_j - \partial_j A_h) x_0^h + \partial_0 A_j - \partial_j A_0\Big).\end{aligned}$$

Conversely, γ characterizes Γ.

The second-order connection γ splits into the gravitational and electromagnetic components as $\gamma^{\natural} + \gamma^e$, where $\gamma^e = -(q/m)\,\text{Д} \lrcorner \hat{F} : J_1\boldsymbol{E} \to (\mathbb{T}^* \otimes \mathbb{T}^*) \otimes V\boldsymbol{E}$ equals the Lorentz force.

Then, Γ and G yield the *phase two-form* $\Omega[G, \Gamma] := G \lrcorner (\nu[\Gamma] \wedge \theta) : J_1\boldsymbol{E} \to \Lambda^2 J_1 T\boldsymbol{E}$, with $\Omega = G_{ij}^0 (d_0^i - \gamma_{00}^{\ i} d^0 - \Gamma_{h0}^{\ i} \theta^h) \wedge \theta^j$, and where $\nu[\Gamma]$ is the vertical valued form associated with Γ. Conversely, Ω characterizes Γ and G.[62]

The two-form Ω splits into the gravitational and electromagnetic components as $\Omega = \Omega^{\natural} + \Omega^e$, where $\Omega^e = (q/2\hbar)F$.

Then, Γ and G yield the two-vector $\Lambda[G, \Gamma] := \bar{G} \lrcorner (\check{\Gamma} \wedge \nu) : J_1\boldsymbol{E} \to \Lambda^2 V J_1\boldsymbol{E}$, with $\Lambda = G_0^{ij}(\partial_i + \Gamma_{i0}^{\ h}) \wedge \partial_j^0$, where $\check{\Gamma} : J_1\boldsymbol{E} \to V^*\boldsymbol{E} \otimes V J_1\boldsymbol{E}$ is the vertical restriction of Γ.

The two-vector Λ splits into the gravitational and electromagnetic components as $\Lambda = \Lambda^{\natural} + \Lambda^e$, where $\Lambda^e = (q/2\hbar) G^{\sharp}(F) : J_1\boldsymbol{E} \to \Lambda^2 V J_1\boldsymbol{E}$.

We have the identities $i(\gamma)dt = 1$, $i(\gamma)\Omega = 0$, $L[\gamma]\Lambda = 0$, $[\Lambda, \Lambda] = 0$.

Therefore, $(J_1\boldsymbol{E}, dt, \Omega)$ turns out to be a scaled cosymplectic manifold, where γ is the associated scaled Reeb vector field and Λ is the associated two-vector.

We have the following results which will be used later.

Proposition 2.4:[62] For each $X \in \text{proj}(\boldsymbol{E}, T\boldsymbol{E})$, the following implications hold:

$$L[X_{(1)}]\Omega = 0 \Leftrightarrow L[X_{(1)}]\Gamma = 0, \quad L[X]G = 0\,,$$

$$L[X_{(1)}]\Omega = 0 \Rightarrow \text{div}_{\eta} X = 0\,.$$

QED

C. Classical mechanics

The spacetime structure and the joined connection allow us to formulate the dynamics of a classical particle under the action of the gravitational and electromagnetic fields.[34,37]

1. Classical kinematics

A *motion* is defined to be a section $s \in \mathrm{sec}(\boldsymbol{T},\boldsymbol{E})$ and its *absolute velocity* is defined to be the first jet prolongation $j_1 s \in \mathrm{sec}(\boldsymbol{T},J_1\boldsymbol{E})$.

An observer o yields the following objects:

- the affine fibered morphism $\nabla[o] := \mathbf{id} - (o \circ t_0^1) \in \mathrm{fib}(J_1\boldsymbol{E},\mathbb{T}^*\otimes V\boldsymbol{E})$ over $\boldsymbol{E}$,
- the observed *kinetic momentum* $\mathcal{Q}[o] := G^\flat \circ \nabla[o] : J_1\boldsymbol{E} \to V^*\boldsymbol{E}$ and the observed *kinetic energy* $\mathcal{K}[o] := \frac{1}{2} G \lrcorner (\nabla[o] \otimes \nabla[o]) : J_1\boldsymbol{E} \to \mathbb{T}^* \otimes \mathbb{R}$,
- for each motion s, the *observed velocity* $\nabla[o]s := j_1 s - o \circ s \in \mathrm{sec}(\boldsymbol{T},\mathbb{T}^*\otimes V\boldsymbol{E})$,

Their expressions, in adapted coordinates, are

$$\nabla[o] = x_0^i u^0 \otimes \partial_i, \quad \mathcal{Q}[o] = G^0_{ij} x_0^j \check{d}^i, \quad \mathcal{K}[o] = \tfrac{1}{2} G^0_{ij} x_0^i x_0^j u^0, \quad \nabla[o]s = \partial_0 s^i u^0 \otimes \partial_i.$$

In the special Newtonian spacetime, we can also define the usual *observed angular momentum* $\mathcal{M}[o,c] := r[c] \times \mathcal{Q}[o]$ with respect to an inertial motion c as reference center.

For each motion s, the absolute gravitational *acceleration* is defined to be the section $\nabla[\gamma^\natural] j_1 s := j_2 s - (\gamma^\natural \circ j_1 s) \in \mathrm{sec}(\boldsymbol{T},\mathbb{T}^*\otimes\mathbb{T}^*\otimes V\boldsymbol{E})$ and the absolute joined *acceleration* is defined to be the section $\nabla[\gamma] j_1 s := j_2 s - (\gamma \circ j_1 s) \in \mathrm{sec}(\boldsymbol{T},\mathbb{T}^*\otimes\mathbb{T}^*\otimes V\boldsymbol{E})$. Clearly, we have $\nabla[\gamma] j_1 s = \nabla[\gamma^\natural] j_1 s - \gamma^\mathscr{C} \circ j_1 s$. We have the coordinate expression

$$\nabla[\gamma] j_1 s = (\partial_{00} s^i - (K_h{}^i{}_k \circ s)\partial_0 s^h \partial_0 s^k - 2(K_0{}^i{}_h \circ s)\partial_0 s^h - (K_0{}^i{}_0 \circ s)) u^0 \otimes u^0 \otimes \partial_i.$$

2. Classical dynamics

We assume the *generalized Newton's law* as equation of motion for classical dynamics $\nabla[\gamma] j_1 s := j_2 s - \gamma \circ j_1 s = 0$.

A function $f \in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$ such that $\gamma \cdot f = 0$ is said to be *conserved*. We denote the subsheaf of conserved functions by $\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$.

We can also obtain the classical dynamics by a Lagrangian formalism according to a cohomological procedure in the following way.

The phase two-form Ω admits locally *horizontal potentials* $A^\uparrow \in \mathrm{sec}(J_1\boldsymbol{E},T^*\boldsymbol{E})$, which are defined up to a closed spacetime form $\alpha \in \mathrm{sec}(\boldsymbol{E},T^*\boldsymbol{E})$. Each horizontal potential $A^\uparrow$ splits, in a covariant way, as $A^\uparrow = \mathcal{L}[A^\uparrow] + \mathcal{P}[A^\uparrow]$, through the horizontal component $\mathcal{L}[A^\uparrow] := \Pi \lrcorner A^\uparrow$, called *Lagrangian*, and the Π-vertical component $\mathcal{P}[A^\uparrow] := \theta \lrcorner A^\uparrow$, called *momentum*. Moreover, we obtain $D\mathcal{L}[A^\uparrow] = \check{\mathcal{P}}[A^\uparrow]$. Hence, each horizontal potential $A^\uparrow$ turns out to be just the *Poincaré-Cartan form* Θ of the associated Lagrangian $\mathcal{L}[A^\uparrow]$.

Moreover, the horizontal component of Ω turns out to be the fibered morphism $\mathcal{E} = G^\flat(\nabla[\gamma]) : J_2\boldsymbol{E} \to \mathbb{T}^* \otimes V^*\boldsymbol{E}$. Indeed, $\mathcal{E}$ turns out to be just the Euler-Lagrange operator associated with the Lagrangian $\mathcal{L}(A^\uparrow)$, for each horizontal potential $A^\uparrow$.

Next, let us choose a horizontal potential $A^\uparrow$ and an observer o.

Then, we define the *observed potential* to be the spacetime one-form $A[o] := o^* A^\uparrow \in \mathrm{sec}(\boldsymbol{E},T^*\boldsymbol{E})$. This form turns out to be just an observed potential of the joined connection K. Moreover, we define the observed *Hamiltonian* to be the function $\mathcal{H}[o] := -o \lrcorner A^\uparrow$ and the observed *momentum* to be the form $\mathcal{P}[o] := \nu[o] \lrcorner A^\uparrow$.

We have the following expressions, in adapted coordinates,

$$A^{\uparrow} = -\tfrac{1}{2}G^0_{ij}x^i_0x^j_0d^0 + G^0_{ij}x^j_0d^i + A_\lambda d^\lambda,$$

$$\mathcal{L} = \mathcal{L}_0d^0 = \left(\tfrac{1}{2}G^0_{ij}x^i_0x^j_0 + A_ix^i_0 + A_0\right)d^0, \quad \mathcal{P} = (G^0_{ij}x^j_0 + A_i)(d^i - x^i_0d^0),$$

$$A[o] = A_\lambda d^\lambda, \quad \mathcal{H}[o] = \mathcal{H}_0d^0 = \left(\tfrac{1}{2}G^0_{ij}x^i_0x^j_0 - A_0\right)d^0, \quad \mathcal{P}[o] = (G^0_{ij}x^j_0 + A_i)d^i.$$

D. Hamiltonian methods

We devote the following to the basic recalls concerning the splitting of the tangent space of the phase space, the Hamiltonian lift of phase functions, and the Poisson bracket of phase functions.[34,37]

1. Hamiltonian splitting

The time fibering and the second-order connection yield in a covariant way a splitting of the tangent and cotangent spaces of the phase space.

We have the natural dual splittings over $J_1\boldsymbol{E}$,

$$TJ_1\boldsymbol{E} = H_\gamma J_1\boldsymbol{E} \oplus VJ_1\boldsymbol{E} \quad \text{and} \quad T^*J_1\boldsymbol{E} = H^*J_1\boldsymbol{E} \oplus V^*_\gamma J_1\boldsymbol{E},$$

given by $X^{\uparrow} = dt(X^{\uparrow})\gamma + (X^{\uparrow} - dt(X^{\uparrow})\gamma)$ and $\phi^{\uparrow} = \phi^{\uparrow}(\gamma)dt + (\phi^{\uparrow} - \phi^{\uparrow}(\gamma)dt)$, where

- $VJ_1\boldsymbol{E} \subset TJ_1\boldsymbol{E}$ is the vertical subbundle with respect to dt,
- $H^*J_1\boldsymbol{E} \subset T^*J_1\boldsymbol{E}$ is the horizontal subbundle generated by dt,
- $H_\gamma J_1\boldsymbol{E} \subset TJ_1\boldsymbol{E}$ is the horizontal subbundle generated by γ,
- $V^*_\gamma J_1\boldsymbol{E} \subset T^*J_1\boldsymbol{E}$ is the vertical subbundle of forms which annihilate γ.

We define the *musical morphisms* to be the linear maps

$$\Omega^\flat : \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, V^*_\gamma J_1\boldsymbol{E}) : X^{\uparrow} \mapsto i(X^{\uparrow})\Omega,$$

$$\Lambda^\sharp : \mathrm{sec}(J_1\boldsymbol{E}, T^*J_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, VJ_1\boldsymbol{E}) : \phi^{\uparrow} \mapsto i(\phi^{\uparrow})\Lambda.$$

The musical morphisms restrict to the mutually inverse linear maps

$$\Omega^\flat_0 : \mathrm{sec}(J_1\boldsymbol{E}, VJ_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, V^*_\gamma J_1\boldsymbol{E})$$

$$\Lambda^\sharp_0 : \mathrm{sec}(J_1\boldsymbol{E}, V^*_\gamma J_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, VJ_1\boldsymbol{E}).$$

For each $X^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ and $\phi^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, T^*J_1\boldsymbol{E})$, we obtain the equalities

$$(\Lambda^\sharp \circ \Omega^\flat)(X^{\uparrow}) = X^{\uparrow} - dt(X^{\uparrow})\gamma, \quad \Omega^\flat(X^{\uparrow}) = (\Lambda^\sharp{}_0)^{-1}(X^{\uparrow} - dt(X^{\uparrow})\gamma),$$

$$(\Omega^\flat \circ \Lambda^\sharp)(\phi^{\uparrow}) = \phi^{\uparrow} - \phi^{\uparrow}(\gamma)dt, \quad \Lambda^\sharp(\phi^{\uparrow}) = (\Omega^\flat{}_0)^{-1}(\phi^{\uparrow} - \phi^{\uparrow}(\gamma)dt).$$

Hence, we can write $X^{\uparrow} = dt(X^{\uparrow})\gamma + (\Lambda^\sharp \circ \Omega^\flat)(X^{\uparrow})$ and $\phi^{\uparrow} = \phi^{\uparrow}(\gamma)dt + (\Omega^\flat \circ \Lambda^\sharp)(\phi^{\uparrow})$.

Given a *time scale* $\tau \in \mathrm{map}(J_1\boldsymbol{E}, \overline{\mathbb{T}})$, we define the τ-horizontal subbundle $H_\tau J_1\boldsymbol{E} \subset TJ_1\boldsymbol{E}$ consisting of vectors whose time components are given by τ. Then, we obtain the mutually inverse affine maps

$$\Omega^\flat{}_\tau : \mathrm{sec}(J_1\boldsymbol{E}, H_\tau J_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, V^*_\gamma J_1\boldsymbol{E}) : X^{\uparrow} \mapsto i(X^{\uparrow})\Omega,$$

$$\Lambda^\sharp{}_\tau : \mathrm{sec}(J_1\boldsymbol{E}, V^*_\gamma J_1\boldsymbol{E}) \to \mathrm{sec}(J_1\boldsymbol{E}, H_\tau J_1\boldsymbol{E}) : \phi^{\uparrow} \mapsto \gamma(\tau) + i(\phi^{\uparrow})\Lambda.$$

For each $X^{\uparrow}, \bar{X}^{\uparrow} \in \sec(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ and $\phi^{\uparrow}, \bar{\phi}^{\uparrow} \in \sec(J_1\boldsymbol{E}, T^*J_1\boldsymbol{E})$, we have the following equivalences:

$$X^{\uparrow} = \bar{X}^{\uparrow} \Leftrightarrow dt(X^{\uparrow}) = dt(\bar{X}^{\uparrow}), \quad \Omega^{\flat}(X^{\uparrow}) = \Omega^{\flat}(\bar{X}^{\uparrow})$$

$$\phi^{\uparrow} = \bar{\phi}^{\uparrow} \Leftrightarrow \phi^{\uparrow}(\gamma) = \phi^{\uparrow}(\bar{\gamma}), \quad \Lambda^{\sharp}(\phi^{\uparrow}) = \Lambda^{\sharp}(\bar{\phi}^{\uparrow}).$$

2. Poisson bracket

We introduce the Poisson bracket in our cosymplectic framework by an approach which is rather analogous to that of symplectic manifolds[34,37]

We define the *Poisson bracket* on $\mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$ by $\{f,g\} := i(df \wedge dg)\Lambda$, which has the coordinate expression $\{f,g\} = G_0^{ij}(\partial_i f \partial_j^0 g - \partial_i g \partial_j^0 f) - (\Gamma_{00}^{ij} - \Gamma_{00}^{ji})\partial_i^0 f \partial_j^0 g$.

For each $f, g \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$, we have[37] $\gamma.\{f,g\} = \{\gamma.f, g\} + \{f, \gamma.g\}$. Hence, the subsheaf $\mathrm{cons}(J_1\boldsymbol{E}, \mathbb{R}) \subset \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$ is closed with respect to the Poisson bracket.

3. Hamiltonian lift of phase functions

In our cosymplectic framework we can introduce the vertical Hamiltonian lift, which partially resembles the usual Hamiltonian lift of symplectic manifolds. Moreover, we can introduce a further affine Hamiltonian lift which depends on an arbitrary choice of a time scale. Furthermore, we obtain a distinguished affine Hamiltonian lift through the distinguished time scale exhibited by each phase function.[34,37]

For each $f \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$, we define its *vertical Hamiltonian lift* to be the vertical vector field $\Lambda^{\sharp}(df) = (\Omega^{\flat}{}_0)^{-1}(df - \gamma.f) \in \sec(J_1\boldsymbol{E}, VJ_1\boldsymbol{E})$, with coordinate expression $\Lambda^{\sharp}(df) = -G_0^{ij}\partial_j^0 f \partial_i + (G_0^{ij}\partial_j f + (\Gamma_{00}^{ij} - \Gamma_{00}^{ji})\partial_j^0 f)\partial_i^0$.

For each $f, g \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$, we have $[\Lambda^{\sharp}(df), \Lambda^{\sharp}(dg)] = \Lambda^{\sharp}(d\{f,g\})$. Hence, the map $\mathrm{map}(J_1\boldsymbol{E}, \mathbb{R}) \to \sec(J_1\boldsymbol{E}, TJ_1\boldsymbol{E}) : f \mapsto \Lambda^{\sharp}(df)$ turns out to be a morphism of Lie algebras.

For each $f \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$, we define its *Hamiltonian lift*, with respect to the *time scale* $\tau \in \mathrm{map}(J_1\boldsymbol{E}, \bar{\mathbb{T}})$, to the vector field $X^{\uparrow}{}_{\mathrm{ham}}[\tau, f] := \gamma(\tau) + \Lambda^{\sharp}(df) \in \sec(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$, with coordinate expression

$$H^{\uparrow}{}_{\mathrm{ham}}[\tau, f] = \tau^0\partial_0 + (\tau^0 x_0^i - G_0^{ij}\partial_j^0 f)\partial_i + (\tau^0 \gamma_{00}^i + G_0^{ij}\partial_j f + (\Gamma_{00}^{ij} - \Gamma_{00}^{ji})\partial_j^0 f)\partial_i^0.$$

We stress that we need the choice of the time scale τ because γ is a scaled vector field. This fact is not a minor point of our theory; instead, it plays an essential role throughout the classical and quantum theories.

Actually, each $f \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$ yields the time scale $f'' := \frac{1}{3}\langle \bar{G}, D^2 f \rangle$, where $D^2 f \in \mathrm{fib}(J_1\boldsymbol{E}, \mathbb{T}^2 \otimes (V^*\boldsymbol{E} \otimes V^*\boldsymbol{E}))$ is the second fiber derivation of f with respect to the affine fiber of the bundle $J_1\boldsymbol{E} \to \boldsymbol{E}$. Thus, we have the coordinate expression $f'' = f^0 u_0 = \frac{1}{3} G_0^{ij}\partial_i^0 \partial_j^0 f u_0$. The map f'' is called the *time component of* f.

We define the *Hamiltonian lift* of each $f \in \mathrm{map}(J_1, \boldsymbol{E}, \mathbb{R})$ to be the vector field

$$X^{\uparrow}{}_{\mathrm{ham}}[f] := X^{\uparrow}_{\mathrm{ham}}[f'', f] = \gamma(f'') + \Lambda^{\sharp}(df) \in \sec(j_1\boldsymbol{E}, TJ_1\boldsymbol{E}).$$

E. Special phase functions

In the following we collect some basic facts on special phase functions, their Lie bracket and their tangent, Hamiltonian and holonomic lifts.[34,37]

1. The sheaf of special phase functions

A *special phase function* is defined to be a function $f \in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$, such that $D^2 f = \tau \otimes G$, with $\tau \in \mathrm{map}(\boldsymbol{E},\overline{\mathbb{T}})$. Clearly, if $f \in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$ is a special phase function, then we obtain $\tau = f''$, hence $D^2 f = f'' \otimes G$, with $f'' \in \mathrm{map}(\boldsymbol{E},\overline{\mathbb{T}})$.

The coordinate expression of a special phase function is of the type

$$f = f^0 \tfrac{1}{2} G^0_{ij} x^i_0 x^j_0 + f^i G^0_{ij} x^j_0 + \breve{f} \quad \text{with} \quad f^0, f^i, \breve{f} \in \mathrm{map}(\boldsymbol{E},\mathbb{R}).$$

Given an observer o, a special phase function f can be written as

$$f = f'' \lrcorner \mathcal{K}[o] + f'[o] \lrcorner \mathcal{Q}[o] + f[o],$$

where, in adapted coordinates,

$$f'' = \tfrac{1}{3}\langle \bar{G}, D^2 f\rangle = f^0 u_0 \in \mathrm{map}(\boldsymbol{E},\overline{\mathbb{T}}),$$

$$f'[o] = G^\sharp(Df) \circ o = f^i \partial_i \in \mathrm{sec}(\boldsymbol{E}, \mathbb{T}^* \otimes V\boldsymbol{E}),$$

$$f[o] = f \circ o = \breve{f} \in \mathrm{map}(\boldsymbol{E},\mathbb{R}).$$

Given a horizontal potential $A^\uparrow$ and an observer o, a special phase function f can be written as $f = f'' \lrcorner \mathcal{H}[A^\uparrow, o] + f'[o] \lrcorner \mathcal{P}[A^\uparrow, o] + (f[o] + f^0 A_0 - f^i A_i)$.

The subsheaf of special phase functions is denoted by $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$.

Moreover, we shall be involved with the distinguished subsheaves related to the affine structure of the bundle $J_1\boldsymbol{E} \to \boldsymbol{E}$. Thus, we define the following subsheaves:

- the sheaf $\mathrm{proj}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$ consisting of functions, called *projectable*, whose time component $f'' \in \mathrm{map}(\boldsymbol{T},\overline{\mathbb{T}})$ depends only on $\boldsymbol{T}$;
- the sheaf $\mathrm{fine}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{proj}(J_1\boldsymbol{E},\mathbb{R})$ consisting of projectable functions, called *fine*, whose time component $f'' \in \overline{\mathbb{T}}$ is constant;
- the sheaf $\mathrm{aff}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{fine}(J_1\boldsymbol{E},\mathbb{R})$ consisting of projectable functions, called *affine*, whose time component $f'' = 0$ vanishes, i.e., the subsheaf of affine functions with respect to the affine fibers of the bundle $J_1\boldsymbol{E} \to \boldsymbol{E}$;
- the sheaf $\mathrm{map}(\boldsymbol{E},\mathbb{R}) \subset \mathrm{aff}(J_1\boldsymbol{E},\mathbb{R})$ consisting of affine functions such that $Df = 0$, i.e., the subsheaf of affine functions which depend only on $\boldsymbol{E}$.

2. Lifts of special phase functions

Let us analyze three distinguished lifts of special phase functions into vector fields: the Hamiltonian lift, the tangent lift and the holonomic lift.

Let us start with the Hamiltonian lift. The special phase functions are characterized by the following property.

Theorem 2.5: *Let* $\tau \in \mathrm{map}(J_1\boldsymbol{E},\overline{\mathbb{T}})$ *and* $f \in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$. *Then, the following conditions are equivalent*:

1) $X^\uparrow_{\mathrm{ham}}[\tau, f] \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ *is projectable on a vector field* $X[\tau, f] \in \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E})$,

2) $f \in \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$ *and* $\tau = f''$.

If either of the above conditions is fulfilled, then we obtain

$$X^\uparrow_{\mathrm{ham}}[\tau, f] = X^\uparrow{}_{\mathrm{ham}}[f] := \gamma(f'') + \Lambda^\sharp(df).$$

QED

The *Hamiltonian lift* of special phase functions turns out to be the $\mathrm{map}(\boldsymbol{T},\mathbb{R})$-linear map $X^\uparrow{}_{\mathrm{ham}} : \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R}) \to \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E}) : f \mapsto X^\uparrow{}_{\mathrm{ham}}[f] = X^\uparrow{}_{\mathrm{ham}}[f'', f]$, with coordinate expression $X^\uparrow{}_{\mathrm{ham}}[f] = f^0\partial_0 - f^i\partial_i + X^i_0\partial^0_i$, where

$$X_0^i = G_0^{ij}\Big(\tfrac{1}{2}\partial_j f^0 G_{hk}^0 x_0^h x_0^k + (\partial_j f_h^0 + f^k(\partial_k G_{jh}^0 - \partial_j G_{kh}^0) - f^0\partial_0 G_{jh}^0)x_0^h + \partial_j \breve{f} + f^h(\partial_h A_j - \partial_j A_h) - f^0(\partial_0 A_j - \partial_j A_0)\Big).$$

Hence, the kernel of $X^{\uparrow}{}_{\mathrm{ham}}$ is the subsheaf $\mathrm{map}(\boldsymbol{T},\mathbb{R}) \subset \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$.

Then, let us analyze the tangent lift. We obtain the *tangent lift* of special phase functions defined as the map $X:\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R}) \to \mathrm{sec}(\boldsymbol{E},T\boldsymbol{E}):f \mapsto X[f] := X[f'',f]$, with coordinate expresssion $X[f]=f^0\partial_0 - f^i\partial_i$. As a consequence, X is surjective and its kernel is the subsheaf $\mathrm{map}(\boldsymbol{E},\mathbb{R}) \subset \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$. We also obtain the map $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})/\mathrm{map}(\boldsymbol{E},\mathbb{R}) \to \mathrm{sec}(\boldsymbol{E},T\boldsymbol{E}):[f] \mapsto X[f]$, whose inverse has Coordinate expression $X^0\partial_0 + X^i\partial_i \mapsto \big[X^0\frac{1}{2}G_{ij}^0 x_0^i x_0^j - G_{ij}^0 X^j x_0^i\big]$.

Eventually, let us introduce the holonomic lift.[61]

We define the *holonomic lift* of special phase functions to be the $\mathbb{R}$-linear map $X^{\uparrow}{}_{\mathrm{hol}}:\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R}) \to \mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E}):f \mapsto X^{\uparrow}{}_{\mathrm{hol}}[f] := (X[f])_{(1)}$, with coordinate expression $X^{\uparrow}{}_{\mathrm{hol}}[f] = f^0\partial_0 - f^i\partial_i - (\partial_0 f^i + \partial_j f^i x_0^j + \partial_0 f^0 x_0^i)\partial_i^0$.

The kernel of $X^{\uparrow}{}_{\mathrm{hol}}$ is the subsheaf $\mathrm{map}(\boldsymbol{E},\mathbb{R}) \subset \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$.

3. Special Lie bracket

The special phase functions are not closed under the Poisson bracket. Also for this reason, one introduces a nonstandard Lie bracket.[34,37]

We define the *special bracket* on $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$ by $[\![f,g]\!] := \{f,g\} + \gamma(f'')\cdot g - \gamma(g'')\cdot f$, with coordinate expression

$$[\![f,g]\!]^\lambda = f^0\partial_0 g^\lambda - g^0\partial_0 f^\lambda - f^h\partial_h g^\lambda + g^h\partial_h f^\lambda,$$

$$[\![f,\breve{g}]\!] = f^0\partial_0\breve{g} - g^0\partial_0\breve{f} - f^h\partial_h\breve{g} + g^h\partial_h\breve{f} - (f^0 g^h - g^0 f^h)\Phi_{0h} + f^h g^k \Phi_{hk}.$$

The sheaf $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$ is an $\mathbb{R}$-Lie algebra with respect to the special bracket.

The subsheaves

$$\mathrm{aff}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{fine}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{proj}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R}) \subset \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$$

are subsheaves of $\mathbb{R}$-Lie subalgebras with respect to the special bracket. Moreover, the subsheaf $\mathrm{map}(\boldsymbol{E},\mathbb{R}) \subset \mathrm{aff}(J_1\boldsymbol{E},\mathbb{R})$ is a subsheaf of ideals.

At a first insight, the special bracket resembles the Jacobi bracket.[48] However, these brackets have essential differences.

In fact, in our context, the Jacobi bracket would be $[f,g] := \{f,g\} + f\gamma\cdot g - g\gamma\cdot f$ and not $[\![f,g]\!] := \{f,g\} + \gamma(f'')\cdot g - \gamma(g'')\cdot f$. Indeed, the special phase functions are not closed with respect to the Jacobi bracket; moreover, in our context, the Jacobi bracket is not well defined with respect to scale dimensions, as it is not invariant with respect to time scales. Except for this trouble, the Jacobi bracket could be defined for all phase functions, while the special bracket can be defined only for special phase functions, as it involves their "time components." We stress that the Jacobi bracket depends on the first jets of the functions, while the special bracket depends on the second jet, because the time component of the special phase functions depends on the second jet.

Furthermore, we observe that in our context we have $[\Lambda,\Lambda]=0$ and not $[\Lambda,\Lambda]=2\gamma\wedge\Lambda$, but, still, the special bracket fulfills the Jacobi property of Lie brackets. These facts do not conflict with the Lichnerowicz theorem concerning the classification of Lie algebras of functions (see, for instance, Ref. 48, p. 336), because the special phase functions are not closed with respect to the real multiplication.

4. Morphisms of Lie algebras

Let us analyze the relation between the special bracket of special phase functions and the Lie bracket of their prolongations.

The map $X^{\uparrow}_{\mathrm{ham}}:\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})\to\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ is *not* a morphism of Lie algebras, with respect to the special bracket and the Lie bracket, respectively. On the other hand, we have the following result.

Proposition 2.6:[37] For each $f,g\in\mathrm{proj}(J_1\boldsymbol{E},\mathbb{R})$, we have

$$X^{\uparrow}_{\mathrm{ham}}[[\![f,g]\!]]=[X^{\uparrow}_{\mathrm{ham}}[f],X^{\uparrow}_{\mathrm{ham}}[g]].$$

Thus, the sheaf of Hamiltonian lifts of projectable special phase functions is closed with respect to the Lie bracket and the map $X^{\uparrow}_{\mathrm{ham}}:\mathrm{proj}(J_1\boldsymbol{E},\mathbb{R})\to\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ is a morphism of Lie algebras. QED

Proposition 2.7:[34] For each $f,g\in\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, we have

$$X[[\![f,g]\!]]=[X[f],X[g]].$$

Thus, the map $X:\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})\to\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$ is a morphism of Lie algebras. QED

Proposition 2.8: For each $f,g\in\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, we have

$$X^{\uparrow}_{\mathrm{hol}}[[\![f,g]\!]]=[X^{\uparrow}_{\mathrm{hol}}[f],X^{\uparrow}_{\mathrm{hol}}[g]].$$

Hence, the map $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})\to\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E}):f\mapsto X^{\uparrow}_{\mathrm{hol}}[f]$ is a morphism of Lie algebras. Its kernel equals map $(\boldsymbol{E},\mathbb{R})$.

Proof: If $f,g\in\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, then, by virtue of Proposition 2.7 and Proposition 2.2, we obtain

$$X^{\uparrow}_{\mathrm{hol}}[[\![f,g]\!]]:=(X[[\![f,g]\!]])_{(1)}=[X[f];X[g]]_{(1)}=[(X[f])_{(1)},(X[g])_{(1)}]:=[X^{\uparrow}_{\mathrm{hol}}[f],X^{\uparrow}_{\mathrm{hol}}[g]].$$

QED

III. CLASSICAL SYMMETRIES

The following deals with the main aim of the paper. It is devoted to the analysis of the distinguished subalgebras of the algebra of special phase functions and to the classification of classical infinitesimal symmetries.

A. Subalgebras of special phase functions

We have distinguished subsheaves of the sheaf of special phase functions, which are closed with respect to the special bracket. These subalgebras will play an important role with respect to the infinitesimal symmetries of the classical structure.

1. Subalgebra of conserved special phase functions

We define the sheaf $\mathrm{cons\,spec}(J_1\boldsymbol{E},\mathbb{R}):=\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})\cap\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, and, analogously, the subsheaves $\mathrm{cons\,proj}(J_1\boldsymbol{E},\mathbb{R})$, $\mathrm{cons\,fine}(J_1\boldsymbol{E},\mathbb{R})$, $\mathrm{cons\,aff}(J_1\boldsymbol{E},\mathbb{R})$, and $\mathrm{cons\,map}(\boldsymbol{E},\mathbb{R})$.

We stress that the special bracket reduces to the Poisson bracket on the sheaf $\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$, hence also on the above subsheaves.

Proposition 3.1: The sheaf $\mathrm{cons\,spec}(J_1\boldsymbol{E},\mathbb{R})$ is closed with respect to the special bracket.

Proof: If $f,g\in\mathrm{cons\,spec}(J_1\boldsymbol{E},\mathbb{R})$, then $\gamma\cdot[\![f,g]\!]=\gamma.\{f,g\}=\{\gamma.f,g\}+\{f,\gamma.g\}=0$. QED

Lemma 3.2: For each $\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, we have the coordinate expression

$$\begin{aligned}\gamma_0.f\equiv\gamma(u_0).f=&\tfrac{1}{6}(\partial_i f^0G^0_{hk}+\partial_k f^0G^0_{ih}+\partial_h f^0G^0_{ki})x^i_0x^h_0x^k_0+\tfrac{1}{2}(\partial_0 f^0G^0_{hk}\\&-f^0\partial_0G^0_{hk}+f^i\partial_iG^0_{hk}+\partial_h f^iG^0_{ik}+\partial_k f^iG^0_{ih})x^h_0x^k_0\\&-(f^0(\partial_0A_h-\partial_hA_0)+f^i(\partial_hA_i-\partial_iA_h)-\partial_0f^iG^0_{ih}-\partial_h\breve{f})x^h_0+\partial_h\breve{f}-f^i(\partial_0A_i-\partial_iA_0).\end{aligned}$$

Proof: The proof follows from a long computation in coordinates by using the coordinate expressions

$$\gamma_{00}^{\ i} = -G_0^{ij}\Big(\big(\partial_h G^0_{jk} - \tfrac{1}{2}\partial_j G^0_{hk}\big)x_0^h x_0^k + (\partial_0 G^0_{hj} + (\partial_h A_j - \partial_j A_h))x_0^h + \partial_0 A_j - \partial_j A_0\Big),$$

$$f = f^0 \tfrac{1}{2} G^0_{hk} x_0^h x_0^k + f^h G^0_{hk} x_0^k + \breve{f}.$$

QED

Proposition 3.3: The sheaf cons spec$(J_1\boldsymbol{E}, \mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_i f^0 G^0_{hk} + \partial_k f^0 G^0_{ih} + \partial_h f^0 G^0_{ki} = 0,$$

$$\partial_0 f^0 G^0_{hk} - f^0 \partial_0 G^0_{hk} + f^i \partial_i G^0_{hk} + \partial_h f^i G^0_{ik} + \partial_k f^i G^0_{ih} = 0,$$

$$f^0(\partial_0 A_h - \partial_h A_0) + f^i(\partial_h A_i - \partial_i A_h) - \partial_0 f^i G^0_{ih} - \partial_h \breve{f} = 0,$$

$$\partial_0 \breve{f} - f^i(\partial_0 A_i - \partial_i A_0) = 0.$$

QED

A general analysis of the above system is beyond the scope of the present paper. Here, we just discuss some equivalences and simple examples in the basic model of spacetime. A similar remark holds for the systems of differential equations, which will appear in the forthcoming sections.

Proposition 3.4: We have the useful identities $\gamma_0 . \mathcal{H}_0 = -\partial_0 \mathcal{L}_0$ and $\gamma_0 . \mathcal{P}_i = \partial_i \mathcal{L}_0$. Moreover, we have the following equivalences:

$$\gamma . x_0^i = 0 \Leftrightarrow K_\lambda{}^r{}_\mu = 0,$$

$$\gamma . \mathcal{K}_0 = 0 \Leftrightarrow \partial_0 G^0_{hk} = 0, \quad \partial_0 A_h - \partial_h A_0 = 0,$$

$$\gamma . \mathcal{H}_0 = 0 \Leftrightarrow \partial_0 G^0_{hk} = 0, \quad \partial_0 A_\lambda = 0,$$

$$\gamma . \mathcal{Q}_i = 0 \Leftrightarrow \partial_i G^0_{hk} = 0, \quad \partial_i A_\lambda - \partial_\lambda A_i = 0,$$

$$\gamma . \mathcal{P}_i = 0 \Leftrightarrow \partial_i G^0_{hk} = 0, \quad \partial_i A_\lambda = 0,$$

$$\gamma . \mathcal{L}_0 = 0 \Leftrightarrow \nabla_h A_k + \nabla_k A_h = \partial_0 G^0_{hk}, \quad \nabla_h A_0 = 0, \quad A_0^i(\partial_0 A_i - \partial_i A_0) = \partial_0 A_0.$$

QED

Example 3.5: In the special Newtonian spacetime, the sheaf cons spec$(J_1\boldsymbol{E}, \mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_i f^0 = 0,$$

$$\partial_0 f^0 = -2\partial_1 f^1 = -2\partial_2 f^2 = -2\partial_3 f^3,$$

$$\partial_1 f^2 = -\partial_2 f^1, \quad \partial_1 f^3 = -\partial_3 f^1, \quad \partial_2 f^3 = -\partial_3 f^2,$$

$$\partial_0 f^i = -\partial_i \breve{f},$$

$$\partial_0 \check{f} = 0.$$

A solution of this system is given by

$$f^0 = -a_0(x^0)^2 + d^0, \quad f^i = (a_0 x^i + b_0^i)x^0, \quad \check{f} = -\left(\tfrac{1}{2}a_0 \sum_i (x^i)^2 + \sum_i b_0^i x^i + c\right),$$

where $a_0, b_0^i, c, d^0 \in \mathbb{R}$. In particular, we obtain cons spec$(J_1\boldsymbol{E}, \mathbb{R}) \subset$ proj$(J_1\boldsymbol{E}, \mathbb{R})$.

For instance, the components of the kinetic energy, of the momentum, and of the angular momentum with respect to an inertial observer are conserved special phase functions. QED

2. Subalgebra of holonomic functions

We can compare the holonomic and Hamiltonian lifts of a special phase function. The special phase functions whose holonomic and Hamiltonian lifts coincide constitute a subalgebra with respect to the special bracket.

We call $f \in$ spec $(J_1\boldsymbol{E}, \mathbb{R})$ *holonomic* if $X^{\uparrow}{}_{\text{hol}}[f] = X^{\uparrow}{}_{\text{ham}}[f]$.

We denote the subsheaf of holonomic functions by hol$(J_1\boldsymbol{E}, \mathbb{R}) \subset$ spec$(J_1\boldsymbol{E}, \mathbb{R})$.

Accordingly, we set

$$\text{hol fine}(J_1\boldsymbol{E}, \mathbb{R}) := \text{hol}(J_1\boldsymbol{E}, \mathbb{R}) \cap \text{fine}(J_1\boldsymbol{E}, \mathbb{R}),$$

$$\text{hol aff}(J_1\boldsymbol{E}, \mathbb{R}) := \text{hol}(J_1\boldsymbol{E}, \mathbb{R}) \cap \text{aff}(J_1\boldsymbol{E}, \mathbb{R}),$$

$$\text{hol map}(\boldsymbol{E}, \mathbb{R}) := \text{hol}(J_1\boldsymbol{E}, \mathbb{R}) \cap \text{map}(\boldsymbol{E}, \mathbb{R}).$$

Proposition 3.6: The sheaf hol $(J_1\boldsymbol{E}, \mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_i f^0 = 0,$$

$$\partial_0 f^0 G_{ij}^0 - f^0 \partial_0 G_{ij}^0 + f^h \partial_h G_{ij}^0 + \partial_j f^h G_{ih}^0 + \partial_i f^h G_{jh}^0 = 0,$$

$$f^0(\partial_i A_0 - \partial_0 A_i) + \partial_0 f^h G_{ih}^0 + f^h(\partial_h A_i - \partial_i A_h) + \partial_i \check{f} = 0.$$

As a consequence, we obtain hol $(J_1\boldsymbol{E}, \mathbb{R}) \subset$ proj $(J_1\boldsymbol{E}, \mathbb{R})$.

Proof: By the coordinate expressions of the holonomic and Hamiltonian lifts of projectable special phase functions

$$X^{\uparrow}{}_{\text{hol}}[f] = f^0\partial_0 - f^i\partial_i - (\partial_0 f^i + \partial_j f^i x_0^j + \partial_0 f^0 x_0^i + \partial_j f^0 x_0^j x_0^i)\partial_i^0,$$

$$\begin{aligned} X^{\uparrow}{}_{\text{ham}}[f] = f^0\partial_0 - f^i\partial_i + G_0^{ij}\Big(\partial_j \check{f} + \partial_j f^0 \tfrac{1}{2} G_{hk}^0 x_0^h x_0^k + \partial_j f^h G_{hk}^0 x_0^k - f^0(\partial_0 G_{hj}^0 x_0^h \\ + (\partial_0 A_j - \partial_j A_0)) + f^h(\partial_h G_{jk}^0 x_0^k - (\partial_j A_h - \partial_h A_j))\partial_i^0, \end{aligned}$$

we obtain the following coordinate expression of the condition $X^{\uparrow}{}_{\text{hol}}[f] = X^{\uparrow}{}_{\text{ham}}[f]$:

$$\begin{aligned} -(\partial_0 f^i + \partial_j f^i x_0^j + \partial_0 f^0 x_0^i + \partial_j f^0 x_0^j x_0^i) = G_0^{ij}\Big(\partial_j \check{f} + \partial_j f^0 \tfrac{1}{2} G_{hk}^0 x_0^h x_0^k + \partial_j f^h G_{hk}^0 x_0^k - f^0(\partial_0 G_{hj}^0 x_0^h \\ + (\partial_0 A_j - \partial_j A_0)) + f^h(\partial_h G_{jk}^0 x_0^k - (\partial_j A_h - \partial_h A_j)). \end{aligned}$$

This is equivalent to the system

$$-\partial_h f^0 \delta_k^i = \partial_j f^0 \frac{1}{2} G_0^{ij} G_{hk}^0,$$

$$-(\partial_h f^i + \partial_0 f^0 \delta^i_h) = G_0^{ij}(\partial_j f^k G^0_{hk} - f^0 \partial_0 G^0_{hj} + f^k \partial_k G^0_{jh}),$$

$$-\partial_0 f^i = G_0^{ij}(\partial_j \breve{f} - f^0(\partial_0 A_j - \partial_j A_0) + f^h(\partial_h A_j - \partial_j A_h)).$$

By contracting the first equality with $G_0^{hk} G^0_{ir}$ and the second and third equalities with G^0_{ir}, we get

$$\partial_r f^0 = 0,$$

$$-(\partial_h f^i G^0_{ir} + \partial_0 f^0 G^0_{hr}) = \partial_r f^k G^0_{hk} - f^0 \partial_0 G^0_{hr} + f^k \partial_h G^0_{rk},$$

$$-\partial_0 f^i G^0_{ir} = \partial_r \breve{f} - f^0(\partial_0 A_r - \partial_r A_0) + f^h(\partial_h A_r - \partial_r A_h)$$

and thus

$$\partial_r f^0 = 0,$$

$$-(\partial_i f^h G^0_{hj} + \partial_0 f^0 G^0_{ij}) = \partial_j f^h G^0_{ih} - f^0 \partial_0 G^0_{ij} + f^h \partial_i G^0_{jh},$$

$$-\partial_0 f^h G^0_{hi} = \partial_i \breve{f} - f^0(\partial_0 A_i - \partial_i A_0) + f^h(\partial_h A_i - \partial_i A_h)$$

QED

Proposition 3.7: The sheaf hol $(J_1\boldsymbol{E}, \mathbb{R})$ is closed with respect to the special bracket.

Proof: If $f, g \in \mathrm{hol}(J_1\boldsymbol{E}, \mathbb{R})$, then, obtain

$$X^{\uparrow}{}_{\mathrm{ham}}[[\![f,g]\!]] = [X^{\uparrow}{}_{\mathrm{ham}}[f], X^{\uparrow}{}_{\mathrm{ham}}[g]] = [X^{\uparrow}{}_{\mathrm{hol}}[f], X^{\uparrow}{}_{\mathrm{hol}}[g]] = X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]].$$

QED

Example 3.8: In the special Newtonian spacetime, the sheaf $\mathrm{hol}(J_1\boldsymbol{E}, \mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_i f^0 = 0,$$

$$\partial_0 f^0 = -2\partial_1 f^1 = -2\partial_2 f^2 = -2\partial_3 f^3,$$

$$\partial_1 f^2 = -\partial_2 f^1, \quad \partial_1 f^3 = -\partial_3 f^1, \quad \partial_2 f^3 = -\partial_3 f^2,$$

$$\partial_0 f^i = -\partial_i \breve{f}.$$

A solution of this system is given by

$$f^0 = -2\int a d^0, \quad f^i = a x^i + b^i, \quad \breve{f} = -\left(\frac{1}{2}\partial_0 a \sum_i (x^i)^2 + \sum_i \partial_0 b^i x^i + c\right),$$

where $a, b^i c \in \mathrm{map}(\boldsymbol{T}, \mathbb{R})$. QED

3. Subalgebra of self-holonomic functions

Here, we consider special phase functions such that their holonomic prolongation is related to their differential through the cosymplectic two-form. These special phase functions turn out to be conserved and holonomic.

We call $f \in \mathrm{spec}(J_1\boldsymbol{E}, \mathbb{R})$ *self-holonomic* if $i(X^{\uparrow}{}_{\mathrm{hol}}[f])\Omega = df$.

We denote the subsheaf of self-holonomic functions by $\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\subset\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$. Accordingly, we set

$$\mathrm{self\ fine}(J_1\boldsymbol{E},\mathbb{R}) := \mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\cap\mathrm{fine}(J_1\boldsymbol{E},\mathbb{R}),$$

$$\mathrm{self\ aff}(J_1\boldsymbol{E},\mathbb{R}) := \mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\cap\mathrm{aff}(J_1\boldsymbol{E},\mathbb{R}),$$

$$\mathrm{self\ map}(\boldsymbol{E},\mathbb{R}) := \mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\cap\mathrm{map}(\boldsymbol{E},\mathbb{R}).$$

Lemma 3.9: If $f\in\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})$, then $\gamma.f=0$, hence

$$\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\subset\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R}).$$

Proof: We have $\gamma.f=i(\gamma)df=i(\gamma)i(X^{\uparrow}{}_{\mathrm{hol}}[f])\Omega=-i(X^{\uparrow}{}_{\mathrm{hol}}[f])i(\gamma)\Omega=0$. QED

Lemma 3.10: If $f\in\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})$, then $X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$, hence

$$\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\subset\mathrm{hol}(J_1\boldsymbol{E},\mathbb{R}).$$

Proof: The equality $i(X^{\uparrow}{}_{\mathrm{hol}}[f])\Omega=df$ yields

$$X^{\uparrow}{}_{\mathrm{ham}}[f] := \gamma(f'')+\Lambda^{\sharp}(df)=\gamma(f'')+\Lambda^{\sharp}(\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[f])).$$

Therefore, we have

$$X^{\uparrow}{}_{\mathrm{ham}}[f]=\gamma(f'')+X^{\uparrow}{}_{\mathrm{hol}}[f]-\gamma(X^{\uparrow}{}_{\mathrm{hol}}[f])=\gamma(f'')+X^{\uparrow}{}_{\mathrm{hol}}[f]-\gamma(X[f])$$

$$=\gamma(f'')+X^{\uparrow}{}_{\mathrm{hol}}[f]-\gamma(f'')=X^{\uparrow}{}_{\mathrm{hol}}[f].$$

QED

Proposition 3.11: For each $f,g\in\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})$, we obtain

$$\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]])=d[\![f,g]\!].$$

Hence, the subsheaf $\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})\subset\mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$ is closed with respect to the special bracket.

Proof: It sufficies to prove that

$$\Lambda^{\sharp}(\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]))=\Lambda^{\sharp}(d[\![f,g]\!]),$$

$$i(\gamma)(\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]))=i(\gamma)(d[\![f,g]\!]).$$

In fact, we have

$$\Lambda^{\sharp}(\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]))=X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]-\gamma(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]])$$

$$=X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]-\gamma(X[[\![f,g]\!]])$$

$$=X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]-\gamma([\![f,g]\!]'').$$

By Lemma 2.10 we have

$$\Lambda^{\sharp}(\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]]))=X^{\uparrow}{}_{\mathrm{ham}}[[\![f,g]\!]]-\gamma([\![f,g]\!]'')$$

$$=\Lambda^{\sharp}(d[\![f,g]\!]).$$

On the other hand, the identity $i(\gamma)\Omega=0$ yields $i(\gamma)\Omega^{\flat}(X^{\uparrow}{}_{\mathrm{hol}}[[\![f,g]\!]])=0$ and the definition of the special bracket and Lemma 3.9 yield

$$i(\gamma)d[\![f,g]\!] = i(\gamma)d(\{f,g\} + \gamma(f'') \,.\, g - \gamma(g'') \,.\, f)$$

$$= \{\gamma \,.\, f, g\} + \{f, \gamma \,.\, g\} + i(\gamma)d(\gamma(f'') \cdot g - \gamma(g'') \,.\, f) = 0.$$

Hence, $\Omega^\flat(X^\uparrow{}_{\mathrm{hol}}[[\![f,g]\!]]) = d[\![f,g]\!]$. QED

Now, we state the conditions aimed at classifying the self-holonomic functions.

Lemma 3.12: For each $f \in \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$, we obtain

$$\begin{aligned} i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = {} & G^0_{ij}(f^0 x^j_0 + f^j)d^i_0 + \Big(f^0\Big((\partial_0 A_j - \partial_j A_0) + \partial_0 G^0_{jh} x^h_0 + \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0\Big) \\ & - f^i((\partial_i A_j - \partial_j A_i) + (\partial_i G^0_{jh} - \partial_j G^0_{ih})x^h_0) - G^0_{ij}(\partial_0 f^i + \partial_h f^i x^h_0 + \partial_0 f^0 x^i_0)\Big)d^j \\ & + \Big(f^j\Big((\partial_0 A_j - \partial_j A_0) + \partial_0 G^0_{jh} x^h_0 + \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0\Big) + (\partial_0 f^i + \partial_k f^i x^k_0 + \partial_0 f^0 x^i_0) G^0_{ij} x^j_0\Big)d^0. \end{aligned}$$

Proof: The proof follows from a long computation in coordinates, by taking into account the coordinate expressions

$$X^\uparrow{}_{\mathrm{hol}}[f] = f^0\partial_0 - f^i\partial_i - (\partial_0 f^i + \partial_j f^i x^j_0 + \partial_0 f^0 x^i_0)\partial^0_i,$$

$$\begin{aligned} \Omega = {} & G^0_{ij} d^i_0 \wedge (d^j - x^j_0 d^0) + \Big((\partial_0 A_j - \partial_j A_0) + \partial_0 G^0_{jh} x^h_0 \\ & + \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0\Big)d^0 \wedge d^j + \tfrac{1}{2}((\partial_i A_j - \partial_j A_i) + (\partial_i G^0_{jh} - \partial_j G^0_{ih})x^h_0)d^i \wedge d^j. \end{aligned}$$

QED

Lemma 3.13: For each $f \in \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$, we obtain

$$\begin{aligned} df = {} & \Big(\partial_0 f^0 \tfrac{1}{2} G^0_{hk} x^h_0 x^k_0 + \partial_0 f^h G^0_{hk} x^k_0 + \partial_0 \breve{f} + f^0 \tfrac{1}{2}\partial_0 G^0_{hk} x^h_0 x^k_0 + f^h \partial_0 G^0_{hk} x^k_0\Big)d^0 \\ & + \Big(\partial_j f^h G^0_{hk} x^k_0 + \partial_j \breve{f} + f^0 \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0 + f^h \partial_j G^0_{hk} x^k_0\Big)d^j \\ & + (f^0 G^0_{ih} x^h_0 + f^h G^0_{ih})d^i_0. \end{aligned}$$

QED

Proposition 3.14: The sheaf $\mathrm{self}(J_1\boldsymbol{E}, \mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_i f^0 = 0,$$

$$f^0\partial_0 G^0_{ij} - \partial_0 f^0 G^0_{ij} - f^h \partial_h G^0_{ij} - \partial_j f^h G^0_{ih} - \partial_i f^h G^0_{jh} = 0,$$

$$f^0(\partial_0 A_j - \partial_j A_0) - f^i(\partial_i A_j - \partial_j A_i) - G^0_{ij}\partial_0 f^i - \partial_j \breve{f} = 0,$$

$$f^i(\partial_i A_0 - \partial_0 A_i) + \partial_0 \breve{f} = 0.$$

Proof: By virtue of Lemmas 3.12 and 3.13, for each $f \in \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$, we have $i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = df$ if and only if

$$\begin{aligned} & f^j\Big((\partial_0 A_j - \partial_j A_0) + \partial_0 G^0_{jh} x^h_0 + \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0\Big) + (\partial_0 f^i + \partial_h f^i x^h_0 + \partial_0 f^0 x^i_0) G^0_{ik} x^k_0 \\ & = \partial_0 f^0 \tfrac{1}{2} G^0_{hk} x^h_0 x^k_0 + \partial_0 f^h G^0_{hk} x^k_0 + \partial_0 \breve{f} + f^0 \tfrac{1}{2}\partial_0 G^0_{hk} x^h_0 x^k_0 + f^h \partial_0 G^0_{hk} x^k_0, \end{aligned}$$

$$\begin{aligned} & f^0\Big((\partial_0 A_j - \partial_j A_0) + \partial_0 G^0_{jh} x^h_0 + \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0\Big) - f^i((\partial_i A_j - \partial_j A_i) + (\partial_i G^0_{jh} - \partial_j G^0_{ih})x^h_0) \\ & - G^0_{ij}(\partial_0 f^i + \partial_h f^i x^h_0 + \partial_0 f^0 x^i_0) = \partial_j f^h G^0_{hk} x^k_0 + \partial_j \breve{f} + f^0 \tfrac{1}{2}\partial_j G^0_{hk} x^h_0 x^k_0 + f^h \partial_j G^0_{hk} x^k_0. \end{aligned}$$

By comparing the coefficients of the two above polynomial equalities, we obtain the following equivalent system:

$$f^j(\partial_0 A_j - \partial_j A_0) - \partial_0 \breve{f} = 0,$$

$$f^0(\partial_0 A_j - \partial_j A_0) - f^i(\partial_i A_j - \partial_j A_i) - G^0_{ij}\partial_0 f^i - \partial_j \breve{f} = 0,$$

$$f^0 \partial_0 G^0_{jh} - \partial_0 f^0 G^0_{hj} - f^i \partial_i G^0_{jh} - \partial_h f^i G^0_{ij} - \partial_j f^i G^0_{ih} = 0.$$

QED

The system of the previous Proposition can be reexpressed in terms of an observer and the tangent lift of the projectable special phase function.

Proposition 3.15: Let us consider an observer o. Then, the sheaf $\mathrm{self}(J_1\boldsymbol{E},\mathbb{R})$ is constituted by the projectable special phase functions f such that

$$L[X[f]]G = df'' \lrcorner G,$$

$$X[f] \lrcorner \Phi[o] + \nu^*[o](G^\flat(L[o]X[f])) = d(f[o]).$$

Proof: We can write the system which characterizes self-holonomic functions (Proposition 3.14) as

$$\partial_\mu G^0_{hk} X[f]^\mu + G^0_{ih}\partial_k(X[f]^i) + G^0_{ik}\partial_h(X[f]^i) = \partial_0 f^0 G^0_{hk},$$

$$X[f]^\mu(\partial_\mu A_j - \partial_j A_\mu) + G^0_{ij}\partial_0(X[f]^i) - \partial_j \breve{f} = 0,$$

$$X[f]^i(\partial_i A_0 - \partial_0 A_i) - \partial_0 \breve{f} = 0.$$

On the other hand, we have the coordinate expressions

$$L[X[f]]G = (\partial_\mu G^0_{hk} X[f]^\mu + G^0_{ih}\partial_k(X[f]^i) + G^0_{ik}\partial_h(X[f]^i))u_0 \otimes \breve{d}^h \otimes \breve{d}^k,$$

$$df'' \lrcorner G = \partial_0 f^0 G^0_{hk} u_0 \otimes \breve{d}^h \otimes \breve{d}^k,$$

$$X[f] \lrcorner \Phi[o] + \nu^*[o](G^\flat(L[o]X[f])) = X[f]^\mu \Phi_{\mu\nu} d^\nu + G^0_{ij}\partial_0(X[f]^i)d^j,$$

$$d(f[o]) = \partial_\mu \breve{f}.$$

QED

We have the following further intrinsic characterizations of self-holonomic special phase functions, which will play an important role in the classification of classical symmetries.

Theorem 3.16: *Let* $f \in \mathrm{proj}(J_1\boldsymbol{E},\mathbb{R})$. *Then, the following conditions are equivalent:*

1) $i[X^\uparrow{}_{\mathrm{hol}}[f]]\Omega = df$,
2) $L[X^\uparrow{}_{\mathrm{hol}}[f]]\Omega = 0$, *with* $f \in \mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$,
3) $X^\uparrow{}_{\mathrm{hol}}[f] = X^\uparrow{}_{\mathrm{ham}}[f]$, *with* $f \in \mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$.

Proof: 1)$\Rightarrow$2). Let $i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = df$. Then $L(X^\uparrow{}_{\mathrm{hol}}[f])\Omega := di(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = ddf = 0$.
On the other hand, the identity $i(\gamma)\Omega = 0$ yields $i(\gamma)df = 0$, i.e., $f \in \mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$.
2)$\Rightarrow$3). Let $L[X^\uparrow{}_{\mathrm{hol}}[f]]\Omega = 0$, i.e., $di(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = 0$.
Then, we have locally the equality $i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = dg$, with $g \in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$.
On the other hand, the identity $i(\gamma)\Omega = 0$ yields $i(\gamma)dg = 0$, i.e., $g \in \mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$.

As a consequence we obtain $(\Lambda^\sharp \circ \Omega^\flat)(X^\uparrow{}_{\mathrm{hol}}[f]) = \Lambda^\sharp(dg)$ and from this we can deduce that $X^\uparrow{}_{\mathrm{hol}}[f] - \gamma(X^\uparrow{}_{\mathrm{hol}}[f]) = X^\uparrow{}_{\mathrm{hol}}[f] - \gamma(f'') = \Lambda^\sharp(dg)$. Hence $X^\uparrow{}_{\mathrm{hol}}[f] = \gamma(f'') + \Lambda^\sharp(dg) := X^\uparrow{}_{\mathrm{ham}}[f'', g]$.

On the other hand, since $X^\uparrow{}_{\mathrm{hol}}[f]$ is projectable on $\boldsymbol{E}$, Theorem 2.5 implies $g \in \mathrm{spec}(J_1\boldsymbol{E}, \mathbb{R})$ and $g'' = f''$.

Hence, we obtain $X^\uparrow{}_{\mathrm{hol}}[f] = X^\uparrow{}_{\mathrm{ham}}[g]$, which yields $X[f] = X[g]$, hence $f = g + h$, with $h \in \mathrm{map}(\boldsymbol{E}, \mathbb{R})$.

On the other hand, $f, g \in \mathrm{cons}(J_1\boldsymbol{E}, \mathbb{R})$ implies $h \in \mathrm{cons\ map}(\boldsymbol{E}, \mathbb{R}) = \mathbb{R}$.

Therefore, we obtain $X^\uparrow{}_{\mathrm{hol}}[f] = X^\uparrow{}_{\mathrm{ham}}[f]$ in the domain of definition of g. But, if the above equality holds locally, then it holds in the domain of definition of f.

3) $\Rightarrow$ 1). Let $f \in \mathrm{cons}(J_1\boldsymbol{E}, \mathbb{R})$. Then, the identities concerning the linear musical isomorphisms and the identity $i(\gamma)\Omega = 0$ yield $i(X^\uparrow{}_{\mathrm{ham}}[f])\Omega := i(\gamma(f'') + \Lambda^\sharp(df))\Omega = (\Omega^\flat \circ \Lambda^\sharp)(df) = df - i(\gamma)df = df$.

Hence, $X^\uparrow{}_{\mathrm{hol}}[f] = X^\uparrow{}_{\mathrm{ham}}[f]$ implies $i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = df$ QED

Corollary 3.17: We have self $(J_1\boldsymbol{E}, \mathbb{R}) = \mathrm{cons}(J_1, \boldsymbol{E}\mathbb{R}) \cap \mathrm{hol}(J_1\boldsymbol{E}, \mathbb{R})$. QED

Indeed, an even stronger result holds.

Theorem 3.18: We have $\mathrm{self}(J_1\boldsymbol{E}, \mathbb{R}) = \mathrm{cons\ proj}(J_1\boldsymbol{E}, \mathbb{R})$.

Proof: The classifying systems of Proposition 3.14 and of Proposition 3.3 coincide.

Hence, $\mathrm{self}(J_1\boldsymbol{E}, \mathbb{R}) = \mathrm{cons\ proj}(J_1\boldsymbol{E}, \mathbb{R})$. QED

4. Subalgebra of unimodular functions

Next, we consider the subalgebras of the algebra of projectable special phase functions related to the divergence of the tangent lift.

A vector field $X \in \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E})$ is called *conformal unimodular, or unimodular*, if we have, respectively, $d(\mathrm{div}_\eta X) = 0$, or $\mathrm{div}_\eta X = 0$.

For each $X, \bar{X} \in \mathrm{proj}(\boldsymbol{E}, T\boldsymbol{E})$, we have $\mathrm{div}_\eta([X, \bar{X}]) = X.\mathrm{div}_\eta \bar{X} - \bar{X}.\mathrm{div}_\eta X$. Hence, the sheaves of conformal unimodular and unimodular vector fields of $T\boldsymbol{E}$ are closed with respect to the Lie bracket.

A function $f \in \mathrm{spec}(J_1\boldsymbol{E}, \mathbb{R})$ is said to be *unimodular*, or *conformal unimodular* if, respectively, $\mathrm{div}_\eta X[f] = 0$, or $d(\mathrm{div}_\eta X[f]) = 0$. The subsheaves of unimodular and conformal unimodular projectable special phase functions are denoted, respectively, by $\mathrm{unim}(J_1\boldsymbol{E}, \mathbb{R}) \subset \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$ and $\mathrm{c\text{-}unim}(J_1\boldsymbol{E}, \mathbb{R}) \subset \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$.

In the above definition, we need to consider projectable special phase functions, because $\mathrm{div}_\eta X$ is defined only for a projectable spacetime vector field X, due to the fact that η is a vertical form.

A vector field $X^\uparrow \in \mathrm{proj}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ is called *conformal unimodular*, or *unimodular*, if we have, respectively, $d(\mathrm{div}_\eta X^\uparrow) = 0$, or $\mathrm{div}_\eta X^\uparrow = 0$.

The sheaves of conformal unimodular and unimodular vector fields of $J_1\boldsymbol{E}$ are closed with respect to the Lie bracket.

Proposition 3.19: The sheaves of conformal unimodular and unimodular special phase functions are closed with respect to the special bracket.

Proof: If $f, g \in \mathrm{proj}(J_1\boldsymbol{E}, \mathbb{R})$, then we obtain

$$\mathrm{div}_\eta(X[[\![f, g]\!]]) = \mathrm{div}_\eta[X[f], X[g]] = X[g]\,.\,\mathrm{div}_\eta(X[f]) - X[f]\,.\,\mathrm{div}_\eta(X[g])\,.$$

QED

Proposition 3.20: If $f \in \mathrm{self\ fine}(J_1\boldsymbol{E}, \mathbb{R})$, then $\mathrm{div}_\eta(X[f]) = 0$, hence

$$\mathrm{self\ fine}(J_1\boldsymbol{E}, \mathbb{R}) = \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R}) \subset \mathrm{unim}(J_1\boldsymbol{E}, \mathbb{R})\,.$$

Proof: The equality $i(X^\uparrow{}_{\mathrm{hol}}[f])\Omega = df$ yields $L[X^\uparrow{}_{\mathrm{hol}}[f]]\Omega = 0$, hence, by virtue of Proposition 2.4, $\mathrm{div}_\eta(X[f]) = 0$. QED

5. Subalgebra of classic generators

Eventually, we consider the subalgebra of the algebra of special phase functions, which generates the infinitesimal symmetries of the full classical structure.

Each $f \in \text{cons fine}(J_1\boldsymbol{E},\mathbb{R})$ is called a *classical generator*. We denote the sheaf of classical generators by $\text{clas}(J_1\boldsymbol{E},\mathbb{R}) := \text{cons fine}(J_1\boldsymbol{E},\mathbb{R})$.

Theorem 3.21: We have $\text{clas}(J_1\boldsymbol{E},\mathbb{R}) = \text{self fine}(J_1\boldsymbol{E},\mathbb{R}) \subset \text{hol}(J_1\boldsymbol{E},\mathbb{R})$ and $\text{clas}(J_1\boldsymbol{E},\mathbb{R}) \subset \text{unim}(J_1\boldsymbol{E},\mathbb{R})$.

Proof: It follows immediately from Theorem 3.18, Lemma 3.10 and Proposition 3.20. QED

By reformulating a previous result, we have the following characterization of the classical generators.

Corollary 3.22: The sheaf $\text{clas}(J_1\boldsymbol{E},\mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_\lambda f^0 = 0,$$

$$f^0\partial_0 G^0_{ij} - f^h\partial_h G^0_{ij} - \partial_j f^h G^0_{ih} - \partial_i f^h G^0_{jh} = 0,$$

$$f^0(\partial_0 A_j - \partial_j A_0) - f^i(\partial_i A_j - \partial_j A_i) - G^0_{ij}\partial_0 f^i - \partial_j \breve{f} = 0,$$

$$f^i(\partial_i A_0 - \partial_0 A_i) + \partial_0 \breve{f} = 0.$$

QED

Example 3.23: In the special Newtonian spacetime, the sheaf $\text{clas}(J_1\boldsymbol{E},\mathbb{R})$ is constituted by the special phase functions f such that

$$\partial_\lambda f^0 = 0,$$

$$\partial_1 f^1 = \partial_2 f^2 = \partial_3 f^3 = 0,$$

$$\partial_1 f^2 = -\partial_2 f^1, \quad \partial_1 f^3 = -\partial_3 f^1, \quad \partial_2 f^3 = -\partial_3 f^2,$$
$$\partial_0 f^i = -\partial_i \breve{f},$$
$$\partial_0 \breve{f} = 0.$$

For instance, a solution of this system is given by

$$f^0 = a^0,$$

$$f^i = b^i_j x^j + c^i_0 x^0 + d^i,$$

$$\breve{f} = -\sum_{1\le i\le 3} c^i_0 x^i + e,$$

where $a^0, b^i_j, c^i_0, d^i, e \in \mathbb{R}$ and $b^i_j = -b^j_i$. QED

B. Classical infinitesimal symmetries

We classify the vector fields of the phase space which are infinitesimal symmetries of spacetime and its structures.

1. Infinitesimal symmetries of geometric structures

We start by defining the infinitesimal symmetries of some typical geometric structures. All concepts below are defined in such a way that the corresponding local group of diffeomeorphisms act on the geometric structure and preserve it.

We introduce the following general concepts.

1. We define an *infinitesimal symmetry* of a fibered manifold $p:\boldsymbol{F}\to\boldsymbol{B}$ to be a projectable vector field X of $\boldsymbol{F}$.
2. We define an *infinitesimal symmetry* of a bundle $q:\boldsymbol{G}\to\boldsymbol{M}$, which is a natural prolongation of a manifold $\boldsymbol{M}$, to be the projectable vector field Y obtained by the corresponding natural lift of a vector field X of $\boldsymbol{M}$.
3. We define an *infinitesimal symmetry* of a bundle $q:\boldsymbol{G}\to\boldsymbol{F}$, which is a natural prolongation of a fibered manifold $p:\boldsymbol{F}\to\boldsymbol{B}$ to be the projectable vector field Y obtained by the corresponding natural lift of a vector field X of $\boldsymbol{F}$.
3. We define an *infinitesimal symmetry* of a tensor σ of a manifold $\boldsymbol{M}$ to be a vector field X of $\boldsymbol{M}$ such that $L[X]\sigma=0$.
4. We define an *infinitesimal symmetry* of a covariant vertical tensor σ of a fibered manifold $p:\boldsymbol{F}\to\boldsymbol{B}$ to be a projectable vector field X of $\boldsymbol{F}$ such that $L[X]\sigma=0$.
5. We define an *infinitesimal symmetry* of an affine space $\boldsymbol{A}$ to be a constant vector field of $\boldsymbol{A}$.

2. Infinitesimal symmetries of spacetime and phase space

According to the above guideline, we introduce the infinitesimal symmetries of time, of spacetime, and of the phase space as the vector fields which preserve the affine structure of time, the time fibering of spacetime, and the natural first jet functor.

An *infinitesimal symmetry of time* is defined to be an infinitesimal symmetry of the affine structure of $\boldsymbol{T}$, which can be regarded just as an element $\underline{X}\in\overline{\mathbb{T}}$ (i.e., a constant vector field of $\boldsymbol{T}$).

An *infinitesimal symmetry of spacetime* is defined to be an infinitesimal symmetry of the time fibering t yielding also an infinitesimal symmetry of the affine structure of $\boldsymbol{T}$, i.e., a vector field $X\in\mathrm{fine}(\boldsymbol{E},T\boldsymbol{E})$.

An *infinitesimal symmetry of the phase space* is defined to be the infinitesimal symmetry of the first jet prolongation of spacetime yielding also an infinitesimal symmetry of the time fibering t and an infinitesimal symmetry of the affine structure of $\boldsymbol{T}$, i.e., the holonomic prolongation of an infinitesimal symmetry of spacetime $X_{(1)}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$, with $X\in\mathrm{fine}(\boldsymbol{E},T\boldsymbol{E})$.

We define, respectively, a spacetime *infinitesimal symmetry* of dt and a phase, *infinitesimal symmetry* of dt to be vector fields $X\in\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$ and $X^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$, such that $L[X]dt=0$ and $L[X^{\uparrow}]dt=0$.

Proposition 3.24: The infinitesimal symmetries of dt are the vector fields of the type $X\in\mathrm{fine}(\boldsymbol{E},T\boldsymbol{E})$ and $X^{\uparrow}\in\mathrm{fine}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$.

Proof: In fact, we have $L[X]dt=di(X)dt$ and $L[X^{\uparrow}]dt=di(X^{\uparrow})dt$. QED

Corollary 3.25: A vector field $X\in\mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$ is an infinitesimal symmetry of spacetime if and only if it is an infinitesimal symmetry of dt. QED

3. Infinitesimal symmetries of the cosymplectic two-form

We define an *infinitesimal symmetry* of Ω to be a vector field $X^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$, such that $L[X^{\uparrow}]\Omega=0$.

Theorem 3.26: *The infinitesimal symmetries* $X^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ *of* Ω *are of the local type* $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{ham}}[\tau,f]$, *with* $\tau\in\mathrm{map}(J_1\boldsymbol{E},\overline{\mathbb{T}})$ *and* $f\in\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$, *where* f *is determined up to a constant*.

Proof: Let us consider any $X^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ and set $\tau:=dt(X^{\uparrow})\in\mathrm{map}(J_1\boldsymbol{E},\overline{\mathbb{T}})$.

Then, $X^{\uparrow}$ can be uniquely written as $X^{\uparrow}=\gamma(\tau)+\bar{X}^{\uparrow}$, with $\bar{X}^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},VJ_1\boldsymbol{E})$.

Moreover, by recalling the identity $i(\gamma)\Omega=0$, we obtain $L[\gamma(\tau)]\Omega=0$.

Furthermore, by recalling the identity $d\Omega=0$, we have $L[\bar{X}^{\uparrow}]\Omega=0$ if and only if $di(\bar{X}^{\uparrow})\Omega=0$, i.e., if and only if locally $i(\bar{X}^{\uparrow})\Omega=df$, with $\gamma.f=0$, i.e., by virtue of the results of Sec. II D 1, if and only if locally $\bar{X}^{\uparrow}=\Lambda^{\sharp}(df)$, with $\gamma.f=0$. QED

Corollary 3.27: The infinitesimal symmetries $X^{\uparrow}\in\mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ of dt and Ω are of the local type $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{ham}}[\tau,f]$, with $\tau\in\overline{\mathbb{T}}$ and $f\in\mathrm{cons}(J_1\boldsymbol{E},\mathbb{R})$, where f is defined up to a constant. QED

4. Infinitesimal symmetries of the classical structure

Next, we classify the infinitesimal symmetries of dt and Ω, which are projectable on $\boldsymbol{E}$. Indeed, the projectability condition yields an important consequence: namely, it implies that the vector field is generated by a special phase function.

Corollary 3.28: The infinitesimal symmetries $X^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ of Ω, which are projectable on $\boldsymbol{E}$, are of the local type $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ spec}(J_1\boldsymbol{E}, \mathbb{R})$, where f is defined up to a constant.

Proof: It follows from Theorem 3.26 and Theorem 2.5. QED

Corollary 3.29: The infinitesimal symmetries $X^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ of dt and Ω, which are projectable on $\boldsymbol{E}$, are of the type $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})$, where f is determined up to a constant.

Proof: It follows from the above Corollary 3.28 and Proposition 3.24. QED

Corollary 3.30: Let us consider a vector field $X \in \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E})$.

If its holonomic prolongation $X_{(1)} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ is an infinitesimal symmetry of dt and Ω, then we obtain locally $X_{(1)}=X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})$ and $X=X[f]$.

Proof: By virtue of Corollary 3.29, we obtain $X_{(1)}=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})$.

On the other hand, by virtue of Proposition 2.2, $X_{(1)}$ projects on X and, by virtue of Theorem 2.5, $X^{\uparrow}{}_{\mathrm{ham}}[f]$ projects on $X[f]$. Hence, we obtain $X=X[f]$ and $X_{(1)}=X^{\uparrow}{}_{\mathrm{hol}}[f]$. QED

We can reformulate the above result in a slightly stronger way.

An *infinitesimal symmetry of the classical structure* is defined to be a vector field $X^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$, which is an infinitesimal symmetry of dt and Ω and which is projectable on $\boldsymbol{E}$.

Corollary 3.31: The infinitesimal symmetries $X^{\uparrow} \in \mathrm{sec}(J_1\boldsymbol{E}, TJ_1\boldsymbol{E})$ of the classical structure are of the local type $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})$.

Proof: By virtue of Corollary 3.29, we obtain $X^{\uparrow}=X^{\uparrow}{}_{\mathrm{ham}}[f]$, with $f \in \mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})$.

On the other hand, by virtue of Theorem 3.21, we have $\mathrm{cons\ fine}(J_1\boldsymbol{E}, \mathbb{R})=\mathrm{self\ fine}(J_1\boldsymbol{E}, \mathbb{R})$, hence $X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$. QED

Proposition 3.32: The subsheaf of infinitesimal symmetries of the classical structure is a sheaf of Lie subalgebras.

Proof: It follows from the fact that the holonomic lift of special phase functions is a morphism of Lie algebras and that the holonomic lift of projectable special phase functions is a morphism of Lie algebras. QED

Of course, we can analogously prove that also the other subsheaves of infinitesimal symmetries considered above are subalgebras.

C. Classical currents

We devote the following to the analysis of distinguished functions that are generated by symmetries of our structure.

1. Functions generated by a horizontal potential

Each pair consisting of a spacetime vector field X and a horizontal potential $A^{\uparrow}$ of Ω yield a special phase function. This construction turns out to be an important source of special phase functions in our classical and quantum theories. Indeed, the above simple definition encodes deep aspects relating the horizontal potentials of Ω and the classical and quantum symmetries.

Let us consider a spacetime vector field $X \in \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E})$ and a horizontal potential $A^{\uparrow} \in \mathrm{fib}(J_1\boldsymbol{E}, T^*\boldsymbol{E})$ of Ω.

We define the *function generated* by X and $A^{\uparrow}$ as $-X \rfloor A^{\uparrow} \in \mathrm{map}(J_1\boldsymbol{E}, \mathbb{R})$.

Proposition 3.33: The function $-X \rfloor A^{\uparrow}$ is a special phase function.

Its coordinate expression is $-X \rfloor A^{\uparrow}=X^0\frac{1}{2}G^0_{ij}x^i_0x^j_0-X^iG^0_{ij}x^j_0-X^{\lambda}A_{\lambda}$ and, with reference to an observer o, we have $-X \rfloor A^{\uparrow}=X \rfloor \mathcal{K}[o]-\nu[o](X) \rfloor \mathcal{Q}[o]-X \rfloor A[o]$.

Proof: It follows from the coordinate expression of $A^{\uparrow}$. QED

Now, as a particular case, let us consider an $f \in \mathrm{spec}(J_1\boldsymbol{E}, \mathbb{R})$ and its tangent prolongation $X[f] \in \mathrm{sec}(\boldsymbol{E}, T\boldsymbol{E})$.

Corollary 3.34: We obtain the special phase function $-X[f]\lrcorner A^{\uparrow}\in \mathrm{spec}(J_1\boldsymbol{E},\mathbb{R})$, with observed expression $-X[f]\lrcorner A^{\uparrow}=f\circ o-X[f]\lrcorner A[o]$. In an adapted chart, we get

$$-X[f]\lrcorner A^{\uparrow}=f^0\left(\tfrac{1}{2}G^0_{ij}x^i_0x^j_0-A_0\right)+f^i(G^0_{ij}x^j_0+A_i)=f-(\check{f}+f^0A_0-f^iA_i).$$

Indeed, we obtain $X[-X[f]\lrcorner A^{\uparrow}]=X[f]$. QED

Corollary 3.35: For each observer o, the function

$$\bar{f}:=f\circ o+X[f]\lrcorner A[o]=f+X[f]\lrcorner A^{\uparrow}\in \mathrm{map}(\boldsymbol{E},\mathbb{R}),$$

does not depend on the choice of the observer o. Therefore, the coordinate expression $\bar{f}=\check{f}+f^0A_0-f^iA_i$ does not depend on the adapted chart.

proof: In fact, f and $X[f]\lrcorner A^{\uparrow}$ do not depend on the choice of any observer. QED

For instance, we have $-X[\mathcal{L}_0]\lrcorner A^{\uparrow}=\mathcal{L}_0-2A_0+G^{ij}_0A_iA_j$, $-X[\mathcal{H}_0]\lrcorner A^{\uparrow}=\mathcal{H}_0$, and $-X[\mathcal{P}_i]\lrcorner A^{\uparrow}=\mathcal{P}_i$.

2. Nöther's theorem

The previous results on infinitesimal symmetries can be applied to the Lagrangian formalism. Here, we call in mind some of results already presented in Ref. 62 and add new results as well.

Let us consider a horizontal potential $A^{\uparrow}\in \mathrm{fib}(J_1\boldsymbol{E},T^*\boldsymbol{E})$ of Ω and the associated Lagrangian $\mathcal{L}\in \mathrm{sec}(J_1\boldsymbol{E},H^*J_1\boldsymbol{E})$ and momentum $\mathcal{P}\in \mathrm{sec}(J_1\boldsymbol{E},T^*J_1\boldsymbol{E})$.

We define an *infinitesimal symmetry* of $A^{\uparrow}$ to be a vector field $X^{\uparrow}\in \mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$, such that $L[X^{\uparrow}]A^{\uparrow}=0$.

Lemma 3.36: Each infinitesimal symmetry of $A^{\uparrow}$ is an infinitesimal symmetry of Ω. QED

We can formulate the following (Nöther) theorem which relates holonomic infinitesimal symmetries of $A^{\uparrow}$ to conserved functions. For this, let us consider an $X\in \mathrm{sec}(\boldsymbol{E},T\boldsymbol{E})$.

We say that X is a *holonomic infinitesimal symmetry* of a tensor ϕ of the phase space if its holonomic prolongation $X_{(1)}\in \mathrm{sec}(J_1\boldsymbol{E},TJ_1\boldsymbol{E})$ is an infinitesimal symmetry of ϕ, i.e., if $L[X_{(1)}]\phi=0$.

Theorem 3.37: *If* $L[X_{(1)}]A^{\uparrow}=0$, *then the one-form* $i(X_{(1)})\Omega\in \mathrm{sec}(J_1\boldsymbol{E},T^*J_1\boldsymbol{E})$ *is exact and the function* $f:=-X\lrcorner A^{\uparrow}\in \mathrm{map}(J_1\boldsymbol{E},\mathbb{R})$ *turns out to be a potential of* $i(X_{(1)})\Omega$. *Moreover, we obtain* $f\in \mathrm{cons\ self}(J_1\boldsymbol{E},\mathbb{R})$ *and* $X_{(1)}=X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$.

Proof: We have $i(X_{(1)})\Omega=i(X_{(1)})dA^{\uparrow}=L[X_{(1)}]A^{\uparrow}-di(X_{(1)})A^{\uparrow}=0-di(X)A^{\uparrow}=df$.

Hence, f is a potential $i(X_{(1)})\Omega$. Moreover, by virtue of Lemma 3.36 and Corollary 3.28, we obtain $f\in \mathrm{cons\ self}(J_1\boldsymbol{E},\mathbb{R})$ and $X_{(1)}=X^{\uparrow}{}_{\mathrm{hol}}[f]=X^{\uparrow}{}_{\mathrm{ham}}[f]$ in the whole domain of $A^{\uparrow}$. QED

Corollary 3.38: If X is an infinitesimal symmetry of dt and a holonomic infinitesimal symmetry of $A^{\uparrow}$, then the potential $f:=-X\lrcorner A^{\uparrow}=-(X\lrcorner\mathcal{P}+X\lrcorner\mathcal{L})$ of $i(X_{(1)})\Omega$ is a classical generator.

Proof: It follows from the above Theorem 3.37, Corollary 3.30, the definition of classical generators and Proposition 3.24. QED

Corollary 3.39: If an observer $o\in \mathrm{sec}(\boldsymbol{E},\mathbb{T}^*\otimes T\boldsymbol{E})$ is a (scaled) infinitesimal symmetry of $A^{\uparrow}$, then the associated (scaled) potential of $i(o_{(1)})\Omega$ is just the associated Hamiltonian $\mathcal{H}[A^{\uparrow},o]:=-o\lrcorner A^{\uparrow}\in \mathrm{map}(J_1\boldsymbol{E},\mathbb{T}^*\otimes\mathbb{R})$. In particular, $\mathcal{H}[A^{\uparrow},o]$ turns out to be a conserved (scaled) function. QED

Next, we prove that the holonomic infinitesimal symmetries of dt and of the horizontal potential are just the holonomic infinitesimal symmetries of dt and of the Lagrangian.

Lemma 3.40: For each $X\in \mathrm{fine}(\boldsymbol{E},T\boldsymbol{E})$, we have the coordinate expressions

$$L[X_{(1)}]\mathcal{L}=(X^{\mu}\partial_{\mu}\mathcal{L}_0+\partial_0X^j\partial^0_j\mathcal{L}_0+\partial_hX^jx^h_0\partial^0_j\mathcal{L}_0)d^0,$$

$$L[X_{(1)}]\mathcal{P}=\partial^0_i(X^{\mu}\partial_{\mu}\mathcal{L}_0+\partial_0X^j\partial^0_j\mathcal{L}_0+\partial_hX^jx^h_0\partial^0_j\mathcal{L}_0)d^i-\partial^0_i(X^{\mu}\partial_{\mu}\mathcal{L}_0+\partial_0X^j\partial^0_j\mathcal{L}_0+\partial_hX^jx^h_0\partial^0_j\mathcal{L}_0)x^i_0d^0.$$

Proof: We have

$$
\begin{aligned}
L[X_{(1)}]\mathcal{P} &= (X^\mu \partial_\mu \partial_i^0 \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_i X^j \partial_j^0 \mathcal{L}_0) d^i \\
&\quad - ((X^\mu \partial_\mu \partial_i^0 \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \partial_i^0 \mathcal{L}_0) x_0^i + \partial_0 X^i \partial_i^0 \mathcal{L}_0 + \partial_h X^i x_0^h \partial_i^0 \mathcal{L}_0 - \partial_0 X^j \partial_j^0 \mathcal{L}_0) d^0 \\
&= (X^\mu \partial_\mu \partial_i^0 \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_i X^j \partial_j^0 \mathcal{L}_0) d^i \\
&\quad - ((X^\mu \partial_\mu \partial_i^0 \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \partial_i^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \partial_i^0 \mathcal{L}_0) x_0^i + \partial_h X^i x_0^h \partial_i^0 \mathcal{L}_0) d^0 \\
&= \partial_i^0 (X^\mu \partial_\mu \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \mathcal{L}_0 - \partial_i X^j \partial_j^0 \mathcal{L}_0 + \partial_i X^j \partial_j^0 \mathcal{L}_0) d^i \\
&\quad - (\partial_i^0 (X^\mu \partial_\mu \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \mathcal{L}_0) x_i^0 \\
&\quad - \partial_i X^j x_0^i \partial_j^0 \mathcal{L}_0 + \partial_h X^i x_0^h \partial_i^0 \mathcal{L}_0) d^0 \\
&= \partial_i^0 (X^\mu \partial_\mu \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \mathcal{L}_0) d^i \\
&\quad - \partial_i^0 (X^\mu \partial_\mu \mathcal{L}_0 + \partial_0 X^j \partial_j^0 \mathcal{L}_0 + \partial_h X^j x_0^h \partial_j^0 \mathcal{L}_0) x_0^i d^0 .
\end{aligned}
$$

QED

Proposition 3.41: For each $X \in \mathrm{fine}(\boldsymbol{E}, T\boldsymbol{E})$, we have the following implication

$$L[X_{(1)}]\mathcal{L} = 0 \Rightarrow L[X_{(1)}]\mathcal{P} = 0 .$$

QED

Theorem 3.42:[62] *For each* $X \in \mathrm{fine}(\boldsymbol{E}, T\boldsymbol{E})$, *the following equivalence holds*

$$L[X_{(1)}]A^\uparrow = 0 \Leftrightarrow L[X_{(1)}]\mathcal{L} = 0 .$$

Proof: If $L[X_{(1)}]A^\uparrow = 0$, then, by virtue of Lemma 2.3, we have

$$L[X_{(1)}]\mathcal{L} := L[X_{(1)}] i(\Delta) A^\uparrow = -i(\Delta) L[X_{(1)}]A^\uparrow + i([X_{(1)}, \Delta])A^\uparrow = 0 + 0 .$$

If $L[X_{(1)}]\mathcal{L} = 0$, then, by virtue of Sec. II C 2, and Proposition 3.41

$$L[X_{(1)}]A^\uparrow = L[X_{(1)}](\mathcal{L} + P) = 0 + 0 .$$

QED

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Proof of the existence of the axial-to-planar channeling transition in a simple crystal model

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Consider a fast nonrelativistic, positively charged particle (ion) traversing a crystal, assumed to be simple cubic and monatomic for simplicity. Let the Cartesian coordinates X_1, X_2, X_3 be parallel to the crystal axes, and η_i be the initial value of the component of the particle's momentum vector along X_i. If $|\eta_3|$ is sufficiently large compared to $|\eta_1|, |\eta_2|$, then (under mild technical assumptions) the ion's motion is well approximated for a long time by a solution of the equations of motion (EOM) of the axial-continuum Hamiltonian $\bar{H}$, obtained from the ion's nonrelativistic Hamiltonian H by replacing the potential $V(X_1, X_2, X_3)$, describing its interaction with the atoms of the crystal, by its average $\bar{V}(X_1, X_2)$ over X_3. Furthermore, if $|\eta_2|, |\eta_3|$ are sufficiently large compared with $|\eta_1|, |\eta_2|$, respectively, then to a good approximation its motion is given, again for a long time, by a solution of the EOM of the planar continuum Hamiltonian $\bar{\bar{H}}$, obtained from $\bar{H}$ by replacing $\bar{V}(X_1, X_2)$ by its average $\bar{\bar{V}}(X_1)$ over X_2. We define motions of the first (respectively, second) type as axial (respectively, planar) channeling. In this paper, the transition from the first to the second kind of motion, occurring when the crystal is suitably rotated, is discussed in a mathematically rigorous way by using an improved version of first-order single-phase averaging theory. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The transition from axial to planar channeling in crystals has been investigated by many authors, both experimentally and theoretically (see, e.g., Refs. 1–3 and the references cited therein). Previous theoretical studies differ from the present one in two main respects. First, they were carried out by using numerical or partially formal analytical procedures. Second, they deal with all stages of the transition. Here we study the phenomenon in a mathematically rigorous way in a simple cubic crystal model by using an improved version of the first-order single-phase averaging theory of nonlinear dynamical systems.[4] The transition from axial to planar channeling which we study occurs for sufficiently large values of the components of the initial momentum along the X_2, X_3 crystal axes, keeping fixed its component along the X_1 axis, and is induced by rotating the crystal while immersed in the incident particle beam. The present paper deals with a relatively late stage of the phenomenon, when the transition is almost complete.

Consider such a crystal traversed by a fast nonrelativistic, positively charged particle (ion) in a direction almost, but not exactly, parallel to the X_3 cubic axis. We assume that the particle's motion is "governed" by the nonrelativistic Hamiltonian $H: (\mathbf{R}^3 \backslash \mathbf{Z}^3) \times \mathbf{R}^3 \to (0, \infty)$ defined by

$$H(X,P) = \frac{1}{2}\sum_{i=1}^{3} P_i^2 + V(X) \tag{1.1a}$$

in suitable units. Here $X=(X_1, X_2, X_3) \in \mathbf{R}^3 \backslash \mathbf{Z}^3$and $P=(P_1, P_2, P_3) \in \mathbf{R}^3$denote the coordinate and momentum vectors of the particle, and

$$V(X) = \sum_{k \in \mathbf{Z}^3} v(X-k) \tag{1.1b}$$

denotes the potential acting on the particle at $X \in \mathbf{R}^3 \backslash \mathbf{Z}^3$, due to the combined effect of the repulsive, shielded Coulomb potentials of the individual atoms of a single species, idealized as pointwise, which are located at the sites of a cubic lattice $\mathbf{Z}^3$. The potential at $X \in \mathbf{R}^3 \backslash \mathbf{Z}^3$ due to the presence of an atom at $k \in \mathbf{Z}^3$ is given by $v(X-k)$. We assume that $v \in C^2(\mathbf{R}^3 \backslash \{0\})$ and is strictly positive, and that $v(Y) = O(\|Y\|^{-1}), \|Y\| \to 0$.[5] Additionally, we assume that the series (1.1b) converges uniformly on compacts in $\mathbf{R}^3 \backslash \mathbf{Z}^3$, thus defining a strictly positive potential $V(X)$ of this same class which tends to infinity as $X \to k \in \mathbf{Z}^3$ and is 1-periodic in each coordinate $X_i (i = 1,2,3)$ in terms of the present units.

We will say that the particle is axially channeled along the X_3 direction if its motion is well approximated by a solution of the equations of motion (EOM) of the axial-continuum Hamiltonian $\bar{H}: (\mathbf{R}^3 \backslash \mathbf{Z}^3) \times \mathbf{R}^3 \to (0, \infty)$ for a long time, where

$$\bar{H}(X,P) = \frac{1}{2} \sum_{i=1}^{3} P_i^2 + \bar{V}(X_1, X_2), \tag{1.2a}$$

with

$$\bar{V}(X_1, X_2) = \int_{(0,1)} V(X_1, X_2, X_3') \mathrm{d}X_3'. \tag{1.2b}$$

By our assumptions on V, the integral in (1.2b) exists as a Riemann integral and defines a strictly positive function $\bar{V}$ of class $C^2(\mathbf{R}^2 \backslash \mathbf{Z}^2)$, which is *unbounded* from above in a neighborhood of each point of $\mathbf{Z}^2$. To say that the particle is channeled parallel to the X_2, X_3 plane will mean that its motion is well approximated by the solution of the EOM of the planar continuum Hamiltonian $\bar{\bar{H}}: (\mathbf{R}^3 \backslash \mathbf{Z}^3) \times \mathbf{R}^3 \to (0, \infty)$, again for a long time, where

$$\bar{\bar{H}}(X,P) = \frac{1}{2} \sum_{i=1}^{3} P_i^2 + \bar{\bar{V}}(X_1). \tag{1.3a}$$

Here

$$\bar{\bar{V}}(X_1) = \int_{(0,1)^2} V(X_1, X_2', X_3') \mathrm{d}X_2' \, \mathrm{d}X_3', \tag{1.3b}$$

where the double integral exists in the above sense for $X_1 \in \mathbf{R} \backslash \mathbf{Z}$, and defines a strictly positive function $\bar{\bar{V}}$ of class $C^1(\mathbf{R} \backslash \mathbf{Z})$, which is *bounded* from above in a neighborhood of each point of $\mathbf{Z}$, again by our hypotheses on V. More precise definitions of axial and planar channeling for the cases of interest will be given in the respective Secs. II and III.

For simplicity, we will confine ourselves to discussing channeling along the said axis and planes. A generalization to channeling along arbitrary axes and planes in simple cubic or more complicated crystals involves no essentially new ideas.

Let the initial values of the position and momentum vectors $X = (X_1, X_2, X_3)$, $P = (P_1, P_2, P_3)$ be denoted by $\xi = (\xi_1, \xi_2, \xi_3)$, $\eta = (\eta_1, \eta_2, \eta_3)$, respectively. Under the present hypotheses on V, one can show that if η is almost, but not exactly, parallel to the X_3 axis and $\|\eta\|$ is sufficiently large, the particle remains axially channeled along X_3 over distances of order $\sqrt{2E}$, where E is the total particle energy in the present units [Eq. (2.4b)]. If in addition $|\eta_2| \gg |\eta_1|$ and $|\eta_1|$ is small enough, it becomes planarly channeled between two adjacent atomic planes parallel to the X_2, X_3 plane over distances of order $\sqrt{2E_\perp}, E_\perp$ being the transverse particle energy in these units [Eq. (3.1b)].

In the usual terminology, the variation from the first situation to the second constitutes a transition from axial to planar channeling. A more precise characterization of the transition is given in Sec. III.

The organization of this paper is as follows. In Sec. II, we discuss axial channeling in simple cubic crystals using an improved version of single-phase first-order averaging theory. The main results of the discussion are summarized in Theorems 2.1 and 2.2, the former being used in the proof of the latter. The existence of an axial-to-planar transition in these crystals is asserted by Theorem 3.3 of Sec. III. This result is established there with the aid of Theorems 2.2 and 3.2, the proof of the latter being based on Theorem 3.1. In Appendix A we state Propositions A.1 and A.2 concerning certain inequalities needed in Secs. II and III. Finally in Appendix B we establish Theorem B.1, a basic result of first-order single-phase averaging theory which we use to prove Theorems 2.1 and 3.1 in Secs. II and III, respectively.

II. AXIAL CHANNELING (Ref. 6)

Consider the equations of motion (EOM)

$$\frac{\mathrm{d}X_i}{\mathrm{d}t} = P_i \quad (i=1,2,3), \tag{2.1a}$$

$$\frac{\mathrm{d}P_i}{\mathrm{d}t} = -D_i V(X) \quad (i=1,2,3),$$

corresponding to the Hamiltonian (1.1a), D_i being the partial derivative with respect to the ith entry in $V(.,.,.)$. Since V is strictly positive and of class $C^2(\mathbf{R}^3\backslash\mathbf{Z}^3)$, there exists[7] for all $t\in\mathbf{R}$ and all $\omega:=(\xi,\eta)\in(\mathbf{R}^3\backslash\mathbf{Z}^3)\times\mathbf{R}^3$ a unique solution $X_i(t,\omega),P_i(t,\omega)(i=1,2,3)$ of Eqs. (2.1a) satisfying the initial conditions

$$X_i(0,\omega)=\xi_i, \quad P_i(0,\omega)=\eta_i \quad (i=1,2,3). \tag{2.1b}$$

Henceforth we assume that $\zeta=(\xi_1,\xi_2,\eta_1,\eta_2)$ is in the multiply connected open set

$$U(K)=\left\{((x_1,x_2),(x_3,x_4))\in(\mathbf{R}^2\setminus\mathbf{Z}^2)\times\mathbf{R}^2:\tfrac{1}{2}(x_3^2+x_4^2)+\bar{V}(x_1,x_2)<K\right\}, \tag{2.2}$$

where K is a positive constant such that $K>\inf_{y\in\mathbf{R}^2\backslash\mathbf{Z}^2}\bar{V}(y)$. Hence $U(K)$ is a nonempty set which is invariant under the transverse Hamiltonian $\bar{H}_\perp:(\mathbf{R}^2\backslash\mathbf{Z}^2)\times\mathbf{R}^2\to(0,\infty)$ defined by

$$\bar{H}_\perp(X_\perp,P_\perp)=\frac{1}{2}\sum_{j=1,2}P_j^2+\bar{V}(X_\perp), \tag{2.3}$$

where $X_\perp=(X_1,X_2)$ and $P_\perp=(P_1,P_2)$. Typically, $\bar{V}(x_1,x_2)$ consists of a set of sharp, infinitely high peaks surrounding the atomic rows parallel to the X_3 axis. For sufficiently large K, the projection $U_p(K)=\{(x_1,x_2)\in\mathbf{R}^2\backslash\mathbf{Z}^2:((x_1,x_2),(x_3,x_4))\in U(K)\}$ of $U(K)$ into the X_1,X_2 plane is a multiply connected set reminiscent of Swiss cheese, the holes being deformed circular disks surrounding these rows.

The total energy E of the solution $X_i(t,\omega),P_i(t,\omega)(i=1,2,3)$ is defined by

$$E:=H(X(t,\omega),P(t,\omega))=H(X(0,\omega),P(0,\omega))=\frac{1}{2}\sum_{j=1}^{3}\eta_j^2+V(\xi), \tag{2.4a}$$

where $X(t,\omega)=(X_1(t,\omega),X_2(t,\omega),X_3(t,\omega))$ and $P(t,\omega)=(P_1(t,\omega),P_2(t,\omega),P_3(t,\omega))$, and where we have used (2.1) and conservation of energy. We define the positive parameter

$$\varepsilon =: 1/\sqrt{2E} = \left\{ \sum_{j=1}^{3} \eta_j^2 + 2V(\xi) \right\}^{-1/2}, \tag{2.4b}$$

with the range of values $(0, 1/\sqrt{2V_0}]$, where $V_0 = \inf_{x \in \mathbf{R}^3 \setminus \mathbf{Z}^3} V(x) = \min_{x \in \mathbf{R}^3 \setminus \mathbf{Z}^3} V(x) \in (0, \infty)$. This parameter will play an important role in the sequel.

For convenience we suppose henceforth that

$$\xi_1 \in (0,1), \quad \xi_j = 0 \quad (j = 2,3), \quad \eta_k > 0 \quad (k = 1,2,3), \tag{2.5}$$

in the absence of an explicit statement to the contrary. Moreover, in the present section we fix $\xi_1, \eta_k (k=1,2)$, leaving η_3 as the only free parameter. Because of (2.4b) and (2.5), we will view ε in this section as a function of η_3 alone, with $\varepsilon \sim 1/\eta_3$ for $\eta_3 \to \infty$.

In order to formulate the relevant equations of motion in a manner suitable for the application of averaging theory, we will isoenergetically reduce the sixth-order autonomous system (2.1a) to a fourth order nonautonomous one.[8] This will be done by changing t to an independent variable u, given by

$$u = X_3(t,\omega) = \int_0^t P_3(s,\omega)\mathrm{d}s = (1/\varepsilon) \int_0^t \{1 - 2\varepsilon^2 [V(X(s,\omega)) + (1/2)P_\perp^2(s,\omega)]\}^{1/2}\, \mathrm{d}s, \tag{2.6}$$

where we have used (1.1a), (2.1), and (2.4b); assumed that $P_3(s,\omega)$ does not change sign for $s \in [0,t]$; and written $P_\perp^2(s,\omega) = \Sigma_{i=1}^2 P_i^2(s,\omega)$.

Let

$$x_i(u,\varepsilon) = X_i(t,\omega) \quad (i = 1,2),$$

$$x_{i+2}(u,\varepsilon) = P_i(t,\omega) \quad (i = 1,2), \tag{2.7}$$

where the dependence of $x_j(u,\varepsilon)$ on ω is not exhibited explicitly. By (2.1), (2.6), and (2.7), at least formally, $x(u,\varepsilon) = (x_1(u,\varepsilon), \ldots, x_4(u,\varepsilon))$ solves the IVP (initial-value problem)

$$\frac{\mathrm{d}x}{\mathrm{d}u} = \varepsilon f(x,u) + \varepsilon^2 r(x,u,\varepsilon), \tag{2.8a}$$

$$x(0,\varepsilon) = \zeta \in U(K), \tag{2.8b}$$

where we use x in (2.8a) as shorthand for $x(\mathrm{u},\varepsilon)$. An analogous shorthand notation will be used to define other IVPs occurring in the paper. However, in order to define the functions f and r in (2.8a), we will let x stand for any point $(x_1,x_2,x_3,x_4) \in \mathbf{R}^4$. No confusion should arise from this usage in this section or from the analogous usage in Sec. III. With x understood in the latter sense, we write

$$f(x,u) = (x_3, x_4, -D_1 V(x_1,x_2,u), -D_2 V(x_1,x_2,u)), \tag{2.9a}$$

$$r(x,u,\varepsilon) = \varepsilon^{-1}\{[k(x,u,\varepsilon)]^{-1} - 1\} f(x,u), \tag{2.9b}$$

$$k(x,u,\varepsilon) = \left\{1 - 2\varepsilon^2 \left[V(x_1,x_2,u) + \tfrac{1}{2}(x_3^2 + x_4^2) \right] \right\}^{1/2}. \tag{2.9c}$$

Since $V(x_1,x_2,u)$ is C^2 for $(x_1,x_2) \in \mathbf{R}^2 \setminus \mathbf{Z}^2, u \in \mathbf{R}$ and since it is 1-periodic in u, (2.9a) defines $f(.,.)$ as a C^1-mapping from $U(\mathbf{K}) \times \mathbf{R}$ into $\mathbf{R}^4$, which is 1-periodic in the second entry. Moreover, at each $\varepsilon \in (0, \varepsilon^{(0)}), r(.,.,\varepsilon)$, defined by (2.9a), (2.9b), and (2.9c), is a *bounded* C^1 mapping from $U(K) \times \mathbf{R}$ into $\mathbf{R}^4$. Here $\varepsilon^{(0)} = \varepsilon^{(0)}(K)$ is a positive constant defined in Proposition A.1 of Appendix A. The boundedness property of this mapping is expressed by the estimate

$$\sup_{(x,u,\varepsilon)\in U(K)\times\mathbf{R}\times(0,\varepsilon^{(0)})}\|r(x,u,\varepsilon)\|<\infty \tag{2.10}$$

asserted by that proposition, and its C^1 property is implied by elementary arguments.

In order to determine rigorously a set of values of u,t where relations (2.7) between the IVPs (initial-value problems) (2.1) and (2.8) hold, we proceed in a reverse manner to that by which (2.8) was obtained heuristically from (2.1). We first define the mapping $u\mapsto t$ by

$$t=\varepsilon\int_0^u\{1-2\varepsilon^2[V(x_1(r,\varepsilon),x_2(r,\varepsilon),r)+(1/2)[x_3^2(r,\varepsilon)+x_4^2(r,\varepsilon)]]\}^{-1/2}\,\mathrm{d}r \tag{2.6$'$}$$

for $u\in J(\varepsilon,T),0<\varepsilon<\varepsilon^{(1)}$. Here $J(\varepsilon,T)=(-\alpha(\varepsilon,T),T/\varepsilon+\alpha(\varepsilon,T))$, where $\alpha(\varepsilon,T)>0$ is considered below, the constant $T\in(0,\infty)$ is defined in the paragraph containing (2.13), and both T and $\varepsilon^{(1)}=\varepsilon^{(1)}(K,\zeta,T)$ appear in Theorem 2.1. (If $u<0,\int_0^u=-\int_{-u}^0$.) By this theorem, the solution $x(u,\varepsilon)=(x_1(u,\varepsilon),\ldots,x_4(u,\varepsilon))$ of the IVP (2.8) exists uniquely and remains in $U(K)$ for $0\le u\le T/\varepsilon,0<\varepsilon<\varepsilon^{(1)}<\varepsilon^{(0)}$. Since $U(K)$ is open, $x(u,\varepsilon)$ also has these properties if $u\in J(\varepsilon,T),0<\varepsilon<\varepsilon^{(1)}$, provided that $\alpha(\varepsilon,T)$ is small enough at each such ε,T, by virtue of elementary existence and uniqueness theorems of ODEs. Since $x(r,\varepsilon)\in U(K)$ for $0\le r\le u\in J(\varepsilon,T)$ at all the latter ε,T, the quantity in curly brackets in (2.6$'$) is positive at these r,ε values by (A4) in Appendix A, and hence the mapping $u\mapsto t$ exists at the latter ε values. Indeed, one can show that at each $\varepsilon\in(0,\varepsilon^{(1)}),T\in(0,\infty)$the relation (2.6$'$) defines a C^1 diffeomorphism $u\mapsto t$ from $J(\varepsilon,T)$ onto a finite open interval $J'(\varepsilon,T)$ containing the point $t=0$, whose inverse $t\mapsto u$ is given by (2.6). Second, for $t\in J'(\varepsilon,T),\ \varepsilon\in(0,\varepsilon^{(1)})$ we define $X_i(t,\omega),\ P_i(t,\omega)(i=1,2)$ by (2.7), and set $X_3(t,\omega)=u,\ P_3(t,\omega)=\mathrm{d}u/\mathrm{d}t$. This can be shown to imply that $X_i(t,\omega),\ P_i(t,\omega)(i=1,2,3)$ satisfies the IVP (2.1) at each of the latter t,ε. Hence, this solution of (2.1) coincides locally, and therefore globally, with the global solution $X_i(t,\omega),\ P_i(t,\omega)(i=1,2,3)$ mentioned in the first paragraph of this section. We have thus justified (2.7) for $u\in J(\varepsilon,T),\ T\in(0,\infty)$. Hence (2.7) holds for $t\in[0,T],\ \varepsilon\in(0,\varepsilon^{(1)})$, since at each such ε,T the latter interval is contained in the image of $0\le u\le T/\varepsilon$ under the diffeomorphism $u\mapsto t$.

Define

$$\bar{f}(x)=(x_3,x_4,-D_1\bar{V}(x_1,x_2),-D_2\bar{V}(x_1,x_2)) \tag{2.11}$$

for $x=(x_1,x_2,x_3,x_4)\in\mathbf{R}^4$. Then the "averaged" IVP

$$\frac{\mathrm{d}\bar{x}}{\mathrm{d}u}=\varepsilon\bar{f}(\bar{x}), \tag{2.12a}$$

$$\bar{x}(0,\varepsilon)=\zeta, \tag{2.12b}$$

has a unique solution $\bar{x}(u,\varepsilon)=(\bar{x}_i(u,\varepsilon))(i=1,\ldots,4)$ for $u\in\mathbf{R},\varepsilon>0$. This follows from the strict positivity of $\bar{V}\in C^2(\mathbf{R}^2\backslash\mathbf{Z}^2)$ by arguments of the same type as ones adduced earlier in a similar connection.[7]

At each $\varepsilon>0$ the IVP (2.12) is equivalent to the IVP

$$\frac{\mathrm{d}y}{\mathrm{d}\tau}=\bar{f}(y), \tag{2.13a}$$

$$y(0)=\zeta, \tag{2.13b}$$

which has a unique solution $y(\tau)$, where $\tau:=\varepsilon u$. We have

$$\bar{x}(u,\varepsilon) = y(\tau) = (y_1(\tau), y_2(\tau), y_3(\tau), y_4(\tau)), \tag{2.14}$$

where we omit the dependence of the $y_k(\tau)$ on ζ. Note that system (2.13a) constitutes the EOM of the transverse Hamiltonian $H_\perp(y_1,y_2,y_3,y_4)=\frac{1}{2}(y_3^2+y_4^2)+\bar{V}(y_1,y_2)$ in terms of the time τ, where y_3, y_4 are the momenta canonically conjugate to the respective coordinates y_1, y_2. Since $H_\perp$ conserves transverse energy, and (2.14) and $\zeta \in U(K)$ hold, the unique solution $\bar{x}(u,\varepsilon)$ of the IVP (2.12) remains confined to $U(K)$ for all $u \in \mathbf{R}, \varepsilon > 0$. Let $[0, T_1(\zeta))$ be the maximum forward interval of existence of the solution of the IVP (2.13), and T a positive number *less* than $T_1(\zeta)$. Obviously, $T_1(\zeta)=\infty$, and hence $T \in (0,\infty)$.

Theorem 2.1: Let $T \in (0,\infty)$ be given. Then there exist positive constants $c = c(K,\zeta,T)$, $\varepsilon^{(1)}=\varepsilon^{(1)}(K,\zeta,T)$, independent of ε and hence of η_3, with $\varepsilon^{(1)} < \varepsilon^{(0)} = \varepsilon^{(0)}(K)$ and such that the IVP (2.8) has a unique solution $x(u,\varepsilon)$ which remains in $U(K)$ and is uniformly approximated therein by $\bar{x}(u,\varepsilon)$ according to

$$\|x(u,\varepsilon) - \bar{x}(u,\varepsilon)\| < c\varepsilon \tag{2.15}$$

for $0 \le u \le T/\varepsilon$, $0 < \varepsilon < \varepsilon^{(1)}$.

Proof: This theorem is a special case of Theorem B.1 in Appendix B. To show this, we first note the following correspondences between key symbols used in the former and latter theorems: $U \in \mathbf{R}^n \to U(K) \in \mathbf{R}^4$, $\alpha \in \mathbf{R}^n \to \zeta \in \mathbf{R}^4$, $T \to T$, $\varepsilon_0 \to \varepsilon^{(0)}$, $\varepsilon_1 \to \varepsilon^{(1)}$, $x(u,\varepsilon) \to x(u,\varepsilon)$, $y(u,\varepsilon) \to \bar{x}(u,\varepsilon)$, $C_1 \to c$, where we remark that $U(K)$ is uniquely determined by K. Second, we note that the IVP (2.8) [respectively, (2.12)] has the same form as the IVP (B1) [respectively, (B3)]. Third, we observe that the functions f, r in (2.8a) satisfy special cases of the conditions (B2) imposed on their respective generalizations in (B1) [see the paragraph containing (2.10)]. Keeping in mind these remarks, one readily sees that Theorem B.1 implies the present theorem. □

The solution $\bar{X}_i(t,\omega), \bar{P}_i(t,\omega)(i=1,2,3)$ of the EOM

$$\frac{d\bar{X}i}{dt} = \bar{P}_i \ (i=1,2,3), \tag{2.16a}$$

$$\frac{d\bar{P}_i}{dt} = -D_i\bar{V}(\bar{X}_1,\bar{X}_2) \quad (i=1,2,3),$$

corresponding to the averaged Hamiltonian $\bar{H}$ and satisfying the same initial conditions

$$\bar{X}_i(0,\omega) = \xi_i, \quad \bar{P}_i(0,\omega) = \eta_i \quad (i=1,2,3) \tag{2.16b}$$

as that of the EOM (2.1a) exists and is unique for all $t \in \mathbf{R}$ for reasons similar to those ensuring that the solution of the IVP (2.13) has these same properties. By (2.16b) and (2.5), the projection of the particle's motion along the X_3 axis is uniform and given by

$$\bar{X}_3(t,\omega) = \eta_3 t, \quad \bar{P}_3(t,\omega) = \eta_3. \tag{2.17}$$

Note that

$$(\bar{X}_1(t,\omega),\bar{X}_2(t,\omega),\bar{P}_1(t,\omega),\bar{P}_2(t,\omega)) = (y_1(t),y_2(t),y_3(t),y_4(t)) \tag{2.18}$$

for $t \in \mathbf{R}$. Indeed, the 4-vector on the lhs of (2.18) satisfies an IVP of the form

$$\frac{dy}{dt} = \bar{f}(y), \tag{2.19a}$$

$$y(0) = \zeta \tag{2.19b}$$

at each $t \in \mathbf{R}$, as follows from (2.16), the fact that the initial conditions satisfied by the components of the latter 4-vector are of the form (2.12b), and the uniqueness of solution of the IVP (2.19). These properties immediately imply (2.18).

Set $Z(t,\omega)=(X(t,\omega),P(t,\omega)) \in \mathbf{R}^6$ and define $\bar{X}(t,\omega)$, $\bar{P}(t,\omega)$, $\bar{Z}(t,\omega)$ similarly to $X(t,\omega)$, $P(t,\omega)$, $Z(t,\omega)$ in terms of barred quantities. We now use Theorem 2.1 to prove the next theorem, which is its analogue in terms of $Z(t,\omega)$ and $\bar{Z}(t,\omega)$.

Theorem 2.2: Let $T \in [0,\infty)$ be given. Then there exist positive constants $C = C(K,\zeta,T), \varepsilon^{(2)} = \varepsilon^{(2)}(K,\zeta,T)$, independent of η_3, with $\varepsilon^{(2)} < \varepsilon^{(1)}$, and such that $Z(t,\omega)$ is uniformly approximated by $\bar{Z}(t,\omega)$ according to

$$\|Z(t,\omega) - \bar{Z}(t,\omega)\| < C\varepsilon \tag{2.20}$$

for $0 \le t \le T, 0 < \varepsilon < \varepsilon^{(2)}$.

This theorem suggests the following definition.

Definition 2.1: For any $\delta > 0$, we say that a particle with Hamiltonian H [see (1.1a), (1.1b)] is δ-axially channeled for given parameters K,ω if for each of the t,ε values mentioned in Theorem 2.2 the inequality (2.20) holds with its right-hand side (rhs) replaced by δ.

Proof of Theorem 2.2: Fixing $i=1,2$ for the moment, we have

$$\begin{aligned} |Z_i(t,\omega) - \bar{Z}_i(t,\omega)| &= |X_i(t,\omega) - \bar{X}_i(t,\omega)| = |x_i(u,\varepsilon) - y_i(t)| \le |x_i(u,\varepsilon) - \bar{x}_i(u,\varepsilon)| + |y_i(t) - y_i(\tau)| \\ &< \text{const}\,\varepsilon + |y_i(t) - y_i(\tau)| \end{aligned} \tag{2.21}$$

by (2.7), (2.14), (2.18), and Theorem 2.1, for $0 \le u \le T/\varepsilon$, $0 < \varepsilon < \varepsilon^{(1)}$, and for the corresponding values of t determined by the diffeomorphism $u \mapsto t$, which include all $t \in [0,T]$, as mentioned above. In (2.21) and henceforth, "const" denotes a constant dependent on K,ζ, but independent of η_3. Recalling that $\tau = \varepsilon u$, and using arguments analogous to ones adduced to establish (3.56) in the proof of Theorem 3 of Ref. 5, we see that

$$\begin{aligned} |y_i(t) - y_i(\tau)| &\le |\eta_i| \,.\, |t-\tau| + \left| \int_\tau^t \mathrm{d}s \int_0^s \mathrm{d}r\, D_i \bar{V}(y_1(r), y_2(r)) \right| \\ &\le |\eta_i| \,.\, |t-\tau| + \tfrac{1}{2}|t^2 - \tau^2| \sup_{r \in \mathbf{R}} |D_i \bar{V}(y_1(r), y_2(r))| \\ &\le |\eta_i| \,.\, |t-\tau| + \tfrac{1}{2}|t^2 - \tau^2| \sup_{(y_1,y_2) \in [U_p(K)]^{\mathrm{cl}} \cap [0,1]^2} |D_i \bar{V}(y_1,y_2)| < \text{const}\,\varepsilon^2, \end{aligned} \tag{2.22}$$

at all $t \in [0,T]$, $0 < \varepsilon < \varepsilon^{(2)}$, where $\varepsilon^{(2)}$ is a constant sufficiently smaller than $\varepsilon^{(1)}$. The third inequality (2.22) follows because $(y_1(t), y_2(t)) \in U_p(K)$ at all such t,ε by Theorem 2.1 and because $D_i \bar{V}(y_1,y_2)$ is 1-periodic in its arguments. The fourth inequality (2.22) is implied by the facts that at the t,ε in question $t+\tau < 2T$ and $|t-\tau| < \text{const}\,\varepsilon^2$, and that the last sup in (2.22) is finite. Its finiteness follows by $\bar{V} \in C^2(\mathbf{R}^2 \backslash \mathbf{Z}^2)$ and because the distance between the closure $[U_p(K)]^{\mathrm{cl}}$ of $U_p(K)$ and the set $\mathbf{Z}^2$ of singular points of $D_i \bar{V}$ is positive. Thus, $D_i \bar{V}(y_1,y_2)$ is continuous, and therefore bounded on the compact subset $[U_p(K)]^{\mathrm{cl}} \cap [0,1]^2 \subset \mathbf{R}^2$. Only the second inequality in the penultimate sentence calls for comment. At the latter t,ε, it is directly implied by the fact that

$$t - \tau < \tau\{[K + V_1(K) - V_2]\varepsilon^2 + O(\varepsilon^4)\}$$

for $\varepsilon \downarrow 0$, uniformly with respect to the relevant variables, as one easily sees using (2.6) and (A4).

By (2.21) and (2.22),

$$|Z_i(t,\omega) - \bar{Z}_i(t,\omega)| < \text{const}\,\varepsilon \tag{2.23}$$

for $i=1,2$ when t,ε are as stated in the theorem, making $\varepsilon^{(2)}$ even smaller than above if necessary. Similar considerations show that (2.23) holds for $i=3,4$ at each such t,ε in terms of constants of the indicated type. For $i=5,6$ one can easily prove that (2.23) holds at such t,ε by using, in particular, conservation of energy and (A4). Therefore, (2.20) obtains in the stated sense. □

III. TRANSITION TO PLANAR CHANNELING

We begin with a few definitions and, for the moment, regard the components of the vector ω as freely choosable real parameters.

The transverse particle energy $E_\perp$ is defined as the energy of the solution $(X_\perp(t,\omega), P_\perp(t,\omega))$ of the EOM of the transverse Hamiltonian (2.3) by

$$E_\perp := H_\perp(X_\perp(t,\omega),P_\perp(t,\omega)) = H_\perp(X_\perp(0,\omega),P_\perp(0,\omega)) = \tfrac{1}{2}\sum_{j=1,2}\eta_j^2 + \bar{V}(\xi_1,\xi_2), \tag{3.1a}$$

where we have used (2.3), (2.16b), and conservation of energy. Analogously to before, we define the positive parameter

$$\varepsilon_\perp := 1/\sqrt{2E_\perp} = \left\{\sum_{j=1,2}\eta_j^2 + 2\bar{V}(\xi_1,\xi_2)\right\}^{-1/2}, \tag{3.1b}$$

having the range of values $(0, 1/\sqrt{2\bar{V}_0}]$, where $\bar{V}_0 = \inf_{x\in\mathbf{R}^2\setminus\mathbf{Z}^2}\bar{V}(y) = \min_{x\in\mathbf{R}^2\setminus\mathbf{Z}^2}\bar{V}(y) \in (0,\infty)$. This parameter plays a role in this section comparable to that of ε in the previous one.

From now on in this section, we fix $\xi=(\xi_1,\xi_2,\xi_3)$, η_1, leaving η_2,η_3 as the only free parameters. Moreover, henceforth ξ_j, $\eta_k(j,k=1,2,3)$ will be assumed to satisfy the conditions (2.5). The transition from axial to planar channneling occurs when η_2,η_3 are both sufficiently large, as explained in detail near the end of the section.

We proceed to isoenergetically reduce the fourth-order subsystem (2.16a) for $i=1,2$ to second order. We do this by introducing a new "time" v as the independent variable,

$$v = \bar{X}_2(t,\omega) = \int_0^t \bar{P}_2(s,\omega)\mathrm{d}s = (1/\varepsilon_\perp)\int_0^t \{1 - 2\varepsilon_\perp^2[\bar{V}(\bar{X}_\perp(s,\omega)) + (1/2)\bar{P}_1^2(s,\omega)]\}^{1/2}\,\mathrm{d}s, \tag{3.2}$$

where we have used (2.3), (2.16a), (2.16b), and (3.1); assumed that $\bar{P}_2(s,\omega)$ does not change sign for $s\in[0,t]$; and defined $\bar{X}_\perp(t,\omega)=(\bar{X}_1(t,\omega),\bar{X}_2(t,\omega))$. No confusion would arise from the different meanings of v in (3.2) and (1.1b).

Define

$$z_1(v,\varepsilon_\perp) = \bar{X}_1(t,\omega), \quad z_2(v,\varepsilon_\perp) = \bar{P}_1(t,\omega). \tag{3.3}$$

By (3.2) and (3.3), at least formally, the fourth-order system (2.16a) for $i=1,2$ and the corresponding initial conditions (2.16b) can be expressed as

$$\frac{\mathrm{d}z}{\mathrm{d}v} = \varepsilon_\perp g(z,v) + \varepsilon_\perp^2\rho(z,v,\varepsilon_\perp), \tag{3.4a}$$

$$z(0,\varepsilon_\perp) = \bar{\zeta}. \tag{3.4b}$$

Here $z=(z_1,z_2)\in(\mathbf{R}\setminus\mathbf{Z})\times\mathbf{R}$, $\bar{\zeta}=(\xi_1,\eta_1)$, and

$$g(z,v) = (z_2, -D_1\bar{V}(z_1,v)), \tag{3.5a}$$

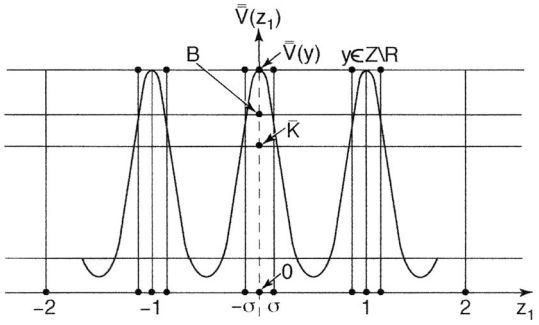

FIG. 1. Example of a function $\bar{\bar{V}}$ having the properties (1) and (2) stated in the paragraph containing (3.7).

$$\rho(z,v,\varepsilon_\perp)=\varepsilon_\perp^{-1}\{[\ell(z,v,\varepsilon_\perp)]^{-1}-1\}g(z,v), \tag{3.5b}$$

$$\ell(z,v,\varepsilon_\perp)=\{1-2\varepsilon_\perp^2[\bar{V}(z_1,v)+(1/2)z_2^2]\}^{1/2}. \tag{3.5c}$$

For the potential V defined in Sec. I, (3.5a) defines $g(.,.)$ as a C^1 mapping from $\bar{U}(\bar{K})\times\mathbf{R}$ into $\mathbf{R}^2$ which is 1-periodic in the second entry. Here $\bar{U}(\bar{K})$ is defined as the nonempty, multiply connected open set

$$\bar{U}(\bar{K})=\left\{(z_1,z_2)\in(\mathbf{R}\setminus\mathbf{Z})\times\mathbf{R}:\tfrac{1}{2}z_2^2+\bar{\bar{V}}(z_1)<\bar{K}\right\}, \tag{3.6}$$

where $\bar{K}$ is a positive constant such that $0<\inf_{y\in\mathbf{R}\backslash\mathbf{Z}}\bar{\bar{V}}(y)<\bar{K}<\sup_{y\in\mathbf{R}\backslash\mathbf{Z}}\bar{\bar{V}}(y)<\infty$. Moreover, if certain additional, physically reasonable conditions on $\bar{\bar{V}}$ and $\bar{K}$ stated below are satisfied, then Proposition A.2 in Appendix A guarantees that $\rho(.,.,\varepsilon_\perp)$, as defined by (3.5a), (3.5b), and (3.5c), is a bounded C^1 mapping from $\bar{U}(\bar{K})\times\mathbf{R}$ into $\mathbf{R}^2$ at each $\varepsilon_\perp\in(0,\varepsilon_\perp^{(0)})$. Here $\varepsilon_\perp^{(0)}=\varepsilon_\perp^{(0)}(\bar{K})$ is a positive constant defined by (A8), which is such that

$$\sup_{(z,v,\varepsilon_\perp)\in\bar{U}(\bar{K})\times\mathbf{R}\times(0,\varepsilon_\perp^{(0)})}\|\rho(z,v,\varepsilon_\perp)\|<\infty, \tag{3.7}$$

by virtue of that proposition. The latter holds if $\bar{\bar{V}}$ and $\bar{K}$ satisfy the following conditions: (1) there exist positive constants $\sigma<1/2$ and $B<\sup_{y\in\mathbf{R}\backslash\mathbf{Z}}\bar{\bar{V}}(y)$ such that $\bar{\bar{V}}(z_1)\geq B$ iff $z_1\in[n-\sigma,n+\sigma]$ $\forall n\in\mathbf{Z}$; and (2) $\bar{K}<B$ (see Fig. 1). To simplify the notation, we fix σ and B henceforth, which allows us to omit stating the dependence of the relevant quantities on them without fear of confusion. Defining $\bar{U}_p(\bar{K})=\{z_1\in\mathbf{R}\backslash\mathbf{Z}:(z_1,z_2)\in\bar{U}(\bar{K})\}$, it follows that $\operatorname{dist}\{\bar{U}_p(\bar{K}),\mathbf{Z}\}>0$ under the conditions stated in the penultimate sentence. The definition of the key constant $\varepsilon_\perp^{(0)}$ in (A8) makes sense because of the latter inequality. The boundedness of the mapping $\rho(.,.,\varepsilon_\perp)$ at each $\varepsilon_\perp\in(0,\varepsilon_\perp^{(0)})$ follows immediately from (3.7), and its asserted C^1 property is easily proved.

We now determine a set of v,t values for which (3.3) holds by arguments analogous to those adduced in the case of (2.7). Supposing that $0<\varepsilon_\perp<\varepsilon_\perp^{(1)}<\varepsilon_\perp^{(0)}$ and $T\in(0,\infty)$, we first define the mapping $v\mapsto t$ by

$$t=\varepsilon_\perp\int_0^v\{1-\varepsilon_\perp^2[\bar{V}(z_1(r,\varepsilon_\perp),r)+(1/2)z_2^2(r,\varepsilon_\perp)]\}^{-1/2}\,\mathrm{d}r \tag{3.2$'$}$$

for $v\in L(\varepsilon_\perp,T)$, a bounded open interval of the form $(-\beta(\varepsilon_\perp,T),T/\varepsilon_\perp+\beta(\varepsilon_\perp,T))$, where $\beta(\varepsilon_\perp,T)$ is a sufficiently small positive constant. Theorem 3.1, together with (A10), the openness of $\bar{U}(\bar{K})$, and elementary existence-uniqueness theorems of ODEs show that the quantity inside the curly brackets in (3.2$'$) exists and is positive for $0\leq r\leq v\in L(\varepsilon_\perp,T)$. It follows that for each $\varepsilon_\perp\in(0,\varepsilon_\perp^{(1)})$, $T\in(0,\infty)$ (3.2$'$) defines a C^1 diffeomorphism $v\mapsto t$ from $L(\varepsilon_\perp,T)$ onto a bounded

open interval $L'(\varepsilon_\perp,T)$ containing $t=0$, whose inverse $t\mapsto v$ is given by (3.2). In the second place, for $t\in L'(\varepsilon_\perp,T)$, $\varepsilon_\perp\in(0,\varepsilon_\perp^{(1)})$ we define $\bar{X}_1(t,\omega)$, $\bar{P}_1(t,\omega)$ by (3.7) and set $\bar{X}_2(t,\omega)=v$, $\bar{P}_2(t,\omega)=\mathrm{d}v/\mathrm{d}t$. Hence $\bar{X}_i(t,\omega)$, $\bar{P}_i(t,\omega)(i=1,2)$ satisfies the IVP (2.16) for $i=1,2$ if $t\in L'(\varepsilon_\perp,T)$, thus coinciding locally with the global solution with the same name defined earlier. This entails that (3.3) holds if $v\in L(\varepsilon_\perp,T)$, $\varepsilon_\perp\in(0,\varepsilon_\perp^{(1)})$, and hence if $t\in[0,T],\varepsilon_\perp\in(0,\varepsilon_\perp^{(1)})$.

The averaged IVP corresponding to (3.4) has the form

$$\frac{\mathrm{d}\bar{z}}{\mathrm{d}v}=\varepsilon_\perp\bar{g}(\bar{z})=\varepsilon_\perp(\bar{z}_2,-D_1\bar{\bar{V}}(\bar{z}_1)),\tag{3.8a}$$

$$\bar{z}(0,\varepsilon_\perp)=\bar{\zeta},\tag{3.8b}$$

where $\bar{z}=(\bar{z}_1,\bar{z}_2)\in(\mathbf{R}\backslash\mathbf{Z})\times\mathbf{R}$. In analogy with (2.14), we express the solution of the VIP (3.8) as

$$\bar{z}(v,\varepsilon_\perp)=w(\tau_\perp)=(w_1(\tau_\perp),w_2(\tau_\perp))\tag{3.9}$$

for $\varepsilon_\perp>0$. Here $\tau_\perp=\varepsilon_\perp v$, and $w(\tau_\perp)$, whose dependence and that of its components on $\bar{\zeta}$ has been omitted, is the unique solution of the IVP

$$\frac{\mathrm{d}w}{\mathrm{d}\tau_\perp}=\bar{g}(w),\tag{3.10a}$$

$$w(0)=\bar{\zeta},\tag{3.10b}$$

existing for all $\tau_\perp\in\mathbf{R}$.[7]

Analogously to the fact that (2.13a) are the EOM of the Hamiltonian $H_\perp(y_1,y_2,y_3,y_4)$ in terms of the time τ, (3.10a) are those of the Hamiltonian $h(w_1,w_2)=w_2^2/2+\bar{\bar{V}}(w_1)$ in terms of the time $\tau_\perp$, w_2 being the momentum canonically conjugate to the coordinate w_1. Note that $w(\tau_\perp)$ describes a particle bouncing periodically within the interval $(0,1)$ in the projection $\bar{U}_p(\bar{K})$ of $\bar{U}(\bar{K})$ into the X_1 axis. This follows from $0<\xi_1<1,\bar{\zeta}=(\xi_1,\eta_1)\in\bar{U}(\bar{K})$. Indeed, the last relation and our assumptions on $\bar{\bar{V}}$ and $\bar{K}$ entail that $(1/2)\eta_1^2+\bar{\bar{V}}(\xi_1)<\bar{K}<B<\sup_{y\in(0,1)}\bar{\bar{V}}(y)$. Hence the energy of the particle is too small for it to escape from the relevant potential well, and consequently it oscillates in (0,1) for all $\tau_\perp\in[0,\infty)$. In the next two theorems, T denotes a positive number less than $T_1(\bar{\zeta})$, where $[0,T_1(\bar{\zeta}))$ is the maximum forward interval of the solution of the IVP (3.10). Since $T_1(\bar{\zeta})=\infty$, T can be freely chosen in $(0,\infty)$.

Theorem 3.1: Let $T\in(0,\infty)$ be given. Then there exist positive constants $c_\perp=c_\perp(\bar{K},\bar{\zeta},T),\varepsilon_\perp^{(1)}=\varepsilon_\perp^{(1)}(\bar{K},\bar{\zeta},T)$, independent of η_2,η_3, with $\varepsilon_\perp^{(1)}<\varepsilon_\perp^{(0)}=\varepsilon_\perp^{(0)}(\bar{K})$, and such that the solution $\bar{z}(v,\varepsilon_\perp)$ remains in $\bar{U}(\bar{K})$ and uniformly approximates $z(v,\varepsilon_\perp)$ therein according to

$$\|z(v,\varepsilon_\perp)-\bar{z}(v,\varepsilon_\perp)\|<c_\perp\varepsilon_\perp\tag{3.11}$$

for $0\le v\le T/\varepsilon_\perp,0<\varepsilon_\perp<\varepsilon_\perp^{(1)}$.

Proof: By (3.4), (3.8), and the properties of $g(z,v),\rho(z,v,\varepsilon_\perp)$ in the paragraph containing (3.6), the theorem is directly implied by Theorem B.1, except for the assertion that $c_\perp,\varepsilon_\perp^{(1)}$ are independent of η_3. With this exception, the present theorem follows by reasoning analogous to that used to prove Theorem 2.1. The η_3-independence property is a trivial consequence of the fact that $\varepsilon_\perp$ does not depend on η_3. □

Let

$$(\bar{\bar{X}}_1(t,\omega),\bar{\bar{P}}_1(t,\omega))=(w_1(t),w_2(t)),\tag{3.12a}$$

$$\bar{\bar{X}}_i(t,\omega) = \eta_i t + \xi_i, \quad \bar{\bar{P}}_i(t,\omega) = \eta_i \quad (i=2,3), \tag{3.12b}$$

and define $\bar{\bar{X}}(t,\omega), \bar{\bar{P}}(t,\omega)$ analogously to the corresponding unbarred quantities. Arguments of the same type as those advanced above in a similar connection show that $\bar{\bar{Z}}(t,\omega)=(\bar{\bar{X}}(t,\omega), \bar{\bar{P}}(t,\omega)) \in \mathbf{R}^6$ is the solution of the EOM corresponding to the Hamiltonian $\bar{\bar{H}}$. By (3.12) and a previous remark, this solution describes a planarly channeled particle bouncing periodically in the X_1 direction between two adjacent atomic planes parallel to the X_2, X_3 plane which intersect the X_1 axis at $X_1=0,1$, and travelling at constant speed in the X_2 and X_3 directions.

The next theorem is analogous to Theorem 3.1 in terms of t.

Theorem 3.2: Let $T \in (0,\infty)$ be given. Then there exist positive constants $C_\perp = C_\perp(\bar{K},\bar{\zeta},T), \varepsilon_\perp^{(2)} = \varepsilon_\perp^{(2)}(\bar{K},\bar{\zeta},T)$, independent of η_2, η_3, with $\varepsilon_\perp^{(2)} < \varepsilon_\perp^{(1)}$, and such that $\bar{Z}(t,\omega)$ is uniformly approximated by $\bar{\bar{Z}}(t,\omega)$ according to

$$\|\bar{Z}(t,\omega) - \bar{\bar{Z}}(t,\omega)\| < C_\perp \varepsilon_\perp \tag{3.13}$$

for $0 \le t \le T, 0 < \varepsilon_\perp < \varepsilon_\perp^{(2)}$.

Proof: Follows by Theorem 3.1 and arguments similar to those invoked to prove Theorem 2.2. □

We will consider a single fixed $T \in (0,\infty)$ henceforth in this section. This is convenient in formulating the key estimate used to establish the existence of a transition from axial to planar channeling as well as for other purposes. This estimate, immediately implied by (2.20) and (3.13), is given by

$$\|Z(t,\omega) - \bar{\bar{Z}}(t,\omega)\| < C(K,\zeta)\varepsilon + C_\perp(\bar{K},\bar{\zeta})\varepsilon_\perp, \tag{3.14}$$

where $0 \le t \le T$, and where we have dropped the T symbols in the pertinent constants, as we will do from now on without fear of confusion. Intuitively, in order for the transition to occur, the rhs of (3.14) must be small, which entails that η_2, η_3 must be large.

Remark on nomenclature: Henceforth K, ω and its components, and ε will be modified by the addition of a superscript zero, e.g., $K^0, \omega^0 = (\xi_1^0, \xi_2^0, \xi_3^0, \eta_1^0, \eta_2^0, \eta_3^0)$ [with ξ_j^0, η_k^0 obeying (2.5) for $j,k=1,2,3$] when they refer to axial channeling, and $\varepsilon^{(2)}$ will be written as $\varepsilon^{(2)}(K^0,\zeta^0)$ when referring to this case. In the absence of such a superscript, the parameters mentioned below correspond to planar channeling. The words "particle P" will designate a particle where motion is "governed" by the Hamiltonian H in (1.1a).

Definition 3.1: For any $\delta > 0$, we say that particle P is δ-planarly channeled for given parameters $K, \bar{K}, \omega$ if the inequality

$$\|Z(t,\omega) - \bar{\bar{Z}}(t,\omega)\| < \delta \tag{3.15}$$

holds for all $t \in [0,T]$ for some $\varepsilon \in (0, \varepsilon^{(2)}(K,\zeta)), \varepsilon_\perp \in (0, \varepsilon_\perp^{(2)}(\bar{K},\bar{\zeta}))$.

Definition 3.2: For any $\delta^0, \delta > 0$, we say that particle P has made a (δ^0,δ) axial-to-planar transition [or simply a (δ^0,δ) transition] with initial parameters K^0, ω^0 and final parameters K, $\bar{K}, \omega$ if for all $t \in [0,T]$ the inequality

$$\|Z(t,\omega^0) - \bar{Z}(t,\omega^0)\| < \delta^0 \tag{3.16}$$

holds for some $\varepsilon^0 \in (0, \varepsilon^{(2)}(K^0,\zeta^0))$ and (3.15) holds for some $\varepsilon \in (0, \varepsilon^{(2)}(K,\zeta)), \varepsilon_\perp \in (0, \varepsilon_\perp^{(2)}(\bar{K},\bar{\zeta}))$.

Remarks: By Theorem 2.2, particle P is δ^0-axially channeled for fixed $\delta^0 > 0$, $\xi_j^0 (j=1,2,3), \eta_k^0 (k=1,2)$ at all $t \in [0,T]$ if η_3^0 is sufficiently large. Therefore, to prove that a (δ^0,δ) transition has occurred, it suffices to show that (3.15) holds at the stated $t, \varepsilon, \varepsilon_\perp$.This simple fact will be used in the proof of the next theorem.

Theorem 3.3 (Existence of the axial-to-planar transition): For arbitrary $\delta^0, \delta > 0$, particle P makes a (δ^0, δ) transition with initial parameters K^0, ω^0 and final parameters $K, \bar{K}, \omega$ as defined in the proof below.

Proof: It is important to keep in mind that $\varepsilon_\perp^{(2)}(\bar{K}, \bar{\zeta}), C_\perp(\bar{K}, \bar{\zeta})$ are independent of η_2, η_3, and that $\varepsilon^{(2)}(K, \zeta), C(K, \zeta)$ are independent of η_3. We remind the reader that $\bar{\zeta} = (\xi_1, \eta_1)$ is fixed, and we also fix $\delta > 0$. By the inequality $(1/2)(\eta_1^2 + \eta_2^2) + \bar{V}(\xi_1, \xi_2) < K$ and definition (3.1b), we may (and will) choose K and $\eta_2 > \eta_1 > 0$ so large that $K/2 < (1/2)(\eta_1^2 + \eta_2^2) + \bar{V}(\xi_1, \xi_2)$ and $1/\sqrt{K} < \varepsilon_\perp^{(2)}(\bar{K}, \bar{\zeta}, \xi_2)$, and hence so large that $\varepsilon_\perp$ satisfies

$$1/\sqrt{2K} < \varepsilon_\perp < 1/\sqrt{K} < \varepsilon_\perp^{(2)}(\bar{K}, \bar{\zeta}). \tag{3.17}$$

In addition, we may (and will) assume that K is so large that, because of the second inequality (3.17),

$$C_\perp(\bar{K}, \bar{\zeta})\varepsilon_\perp < \delta/2. \tag{3.18}$$

Recalling (2.4b), we next choose $\eta_3 > \eta_2$ so large that ε satisfies the inequalities

$$\varepsilon < \varepsilon^{(2)}(K, \zeta), \tag{3.19}$$

$$C(K, \zeta)\varepsilon < \delta/2. \tag{3.20}$$

By (3.17)–(3.20) and Theorems 2.2 and 3.2 it follows that (2.10) and (3.14) hold for all $t \in [0, T]$. Moreover, by (2.20), (3.14), (3.18), and (3.20) it follows that, for the chosen parameters, (3.15) holds at all such t, and we are done. □

The version of Theorem 3.3 stated next is important physically, and follows by arguments similar to those used to prove that theorem. Its importance stems from its assertion that if the total particle energy is large enough, then one can induce a transition from axial to planar channeling by appropriately rotating the crystal while keeping this energy fixed.

Theorem 3.4: For arbitrary $\delta_0 > 0$, let particle P be δ_0-axially channeled, with parameters K^0, ω^0, where η_3^0 is sufficiently large. Then for arbitrary $\delta > 0$ it makes a (δ_0, δ) transition from the initial parameters K^0, ω^0 to the final parameters $K, \bar{K}, \omega$ chosen as explained in the proof of Theorem 3.3, with $\xi_j = \xi_j^0 (j = 1, 2, 3)$ and $\eta = \mathbf{R}\eta^0$, where $\mathbf{R}$ denotes a (proper) rotation operator in $\mathbf{R}^3$. That is, $\|\eta\| = \|\eta^0\|$, and thus $\varepsilon = \varepsilon^0$.

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APPENDIX A: AUXILIARY PROPOSITIONS

In this appendix we state Propositions A.1 and A.2, which play important roles in Secs. II and III. The notation used in this appendix is in accord with that in those two sections.

Recall that K is a positive constant such that $K > \inf_{y \in \mathbf{R}^2 \setminus \mathbf{Z}^2} \bar{V}(y)$. We fix the value of K in this appendix and set

$$V_1(K) = \sup_{((x_1, x_2), u) \in U_p(K) \times \mathbf{R}} V(x_1, x_2, u),$$

$$V_2 = \inf_{(x_1, x_2) \in \mathbf{R}^2 \setminus \mathbf{Z}^2} \bar{V}(x_1, x_2), \tag{A1}$$

where $U_p(K) \subset \mathbf{R}^2$ is defined in the paragraph containing (2.3).

Proposition A.1: Let $\varepsilon^{(0)} = \varepsilon^{(0)}(K)$ be a positive constant given by

$$\varepsilon^{(0)} = \kappa/\sqrt{2[K + V_1(K) - V_2]}, \tag{A2}$$

where $\kappa \in (0,1)$ is a fixed numerical constant as close to unity as desired. Then

$$\sup_{(x,u,\varepsilon) \in U(K)\times\mathbf{R}\times(0,\varepsilon^{(0)})} \|r(x,u,\varepsilon)\| < \infty, \tag{A3}$$

where $U(K)$ and $r(x,u,\varepsilon)$ are given by (2.2) and (2.9b), respectively.

Remarks: Before proving this proposition, we make the following remarks to show that it makes sense. As to (A2), note that under the assumptions on V in Sec. I it follows that $0 < V_1(K) < \infty$, $V_2 > 0$, $K + V_1(K) - V_2 > 0$. Indeed, if $V_1(K) = \infty$, there would exist a sequence in $U_p(K)$ tending to some point in $\mathbf{Z}^2$, along which $\bar{V}(x_1,x_2) < \infty$, since $\bar{V}(x_1,x_2) < \infty$ on $(\mathbf{R}\backslash\mathbf{Z})^2$ and $\bar{V}(x_1,x_2) \to \infty$ along such a sequence. But this is impossible, since $\bar{V}(x_1,x_2) < K$ on $U_p(K)$. So (A2) is well defined. As to (A3), recall that $\varepsilon \in (0, 1/\sqrt{2V_0}]$, where V_0 is defined in the paragraph containing (2.4b). By this and the easily proved fact that $\varepsilon^{(0)} \in (0, 1/\sqrt{2V_0}]$, (A3) makes sense.

Proof of Proposition A.1: By (A1), (A2), and (2.2),

$$1 - 2\varepsilon^2\{(1/2)(x_3^2 + x_4^2) + V(x_1,x_2,u)\} > 1 - 2\varepsilon^2[K + V_1(K) - V_2] = 1 - \kappa^2 > 0 \tag{A4}$$

for $(x,u,\varepsilon) \in U(K)\times\mathbf{R}\times(0,\varepsilon^{(0)})$. Hence,

$$\inf_{(x,u,\varepsilon) \in U(K)\times\mathbf{R}\times(0,\varepsilon^{(0)})} k(x,u,\varepsilon) > 0 \tag{A5}$$

by (A4) and (2.9c).

We claim that

$$[1 - k(x,u,\varepsilon)]/\varepsilon = \mathrm{O}(\varepsilon) \tag{A6}$$

for $\varepsilon \downarrow 0$, uniformly with respect to (x,u) in $U(K)\times\mathbf{R}$. The boundedness property (A3) follows directly from (2.9b), the property of $f(.,.)$ in the paragraph containing (2.10), (A5), and the fact that (A6) holds in this uniform sense. This fact is an easy consequence of (2.9c), (A4), and elementary arguments. □

Henceforth in this appendix we assume that $B, \bar{K}$ are positive constants such that $\bar{K} < B < \sup_{y\in\mathbf{R}} \bar{\bar{V}}(y) < \infty$ and that the properties (1) and (2) stated in the fifth sentence of the paragraph containing (3.6) hold (see Fig. 1). Define

$$\bar{V}_1(\bar{K}) = \sup_{(x_1,u)\in\bar{U}_p(\bar{K})\times\mathbf{R}} \bar{V}(x_1,u),$$

$$\bar{V}_2 = \inf_{x_1\in\mathbf{R}\backslash\mathbf{Z}} \bar{\bar{V}}(x_1), \tag{A7}$$

where $\bar{U}_p(\bar{K})$ is defined in the last mentioned paragraph.

Proposition A.2: Let $\varepsilon_\perp^{(0)} = \varepsilon_\perp^{(0)}(\bar{K})$ be a positive constant given by

$$\varepsilon_\perp^{(0)} = \kappa/\sqrt{2[\bar{K} + \bar{V}_1(\bar{K}) - \bar{V}_2]}. \tag{A8}$$

Then,

$$\sup_{(z,v,\varepsilon_\perp)\in\bar{U}(\bar{K})\times\mathbf{R}\times(0,\varepsilon_\perp^{(0)})} \|\rho(z,v,\varepsilon_\perp)\| < \infty, \tag{A9}$$

where $\rho(z,v,\varepsilon_\perp)$ is defined by (3.5b).

Remarks: Their purpose is to show that Proposition A.2 makes sense under the hypotheses on $\bar{V}, \bar{\bar{V}}, \bar{K}$ in Secs. I and III. As to (A8), note that under these hypotheses $0 < \bar{V}_1(\bar{K}) < \infty$, $\bar{V}_2(\bar{K}) > 0$,

$\bar{K}+\bar{V}_1(\bar{K})-\bar{V}_2>0$. Only the finitess of $\bar{V}_1(\bar{K})$ merits comment. Suppose that $\bar{V}_1(\bar{K})=\infty$. Then, since $\bar{V}(x_1,u)<\infty\ \forall\,(x_1,u)\in(\mathbf{R}\backslash\mathbf{Z})\times\mathbf{R}$ and $\bar{V}(x_1,u)$ is unbounded from above in a neighborhood of each point of $\mathbf{Z}$ at every such u, there exists a sequence in $\bar{U}_p(\bar{K})$ converging to a point in $\mathbf{Z}$. This contradicts the inequality dist $\{\bar{U}_p(\bar{K}),\mathbf{Z}\}>0$ proved in the paragraph containing (3.7). As to (A9), recall that $\varepsilon_\perp\in(0,1/\sqrt{2\bar{V}_0}]$, where $\bar{V}_0$ is defined in the paragraph containing (3.1b). By this and the readily proved fact that $\varepsilon_\perp^{(0)}\in(0,1/\sqrt{2\bar{V}_0}]$, (A9) makes sense.

Proof of Proposition A.2: By (A7), (A8), and (3.7), we have

$$1-2\varepsilon_\perp^2\{(1/2)z_2^2+\bar{V}(z_1,v)\}>1-2\varepsilon_\perp^2[\bar{K}+\bar{V}_1(\bar{K})-\bar{V}_2]>1-\kappa^2>0 \tag{A10}$$

for $(z,v,\varepsilon_\perp)\in\bar{U}(\bar{K})\times\mathbf{R}\times(0,\varepsilon_\perp^{(0)})$. Hence

$$\inf_{(z,v,\varepsilon_\perp)\in\bar{U}(\bar{K})\times\mathbf{R}\times(0,\varepsilon_\perp^{(0)})}\ell\,(z,v,\varepsilon_\perp)>0, \tag{A11}$$

where $\ell(z,v,\varepsilon_\perp)$ is given by (3.5c).

One arrives at (A9) by using (A11) and arguments analogous to those adduced to establish (A3) in the proof of Lemma A.1. □

APPENDIX B: FIRST-ORDER AVERAGING THEOREM FOR A CLASS OF PERIODIC SYSTEMS

The main purpose of this appendix is to state and prove Theorem B.1, which underpins our results in Secs. II and III in an essential way. This theorem is a version of a very general existence, uniqueness, and approximation theorem in Ref. 4.

Consider the IVP

$$\frac{\mathrm{d}x}{\mathrm{d}u}=\varepsilon f(x,u)+\varepsilon^2 r(x,u,\varepsilon), \tag{B1a}$$

$$x(0,\varepsilon)=\alpha\in U. \tag{B1b}$$

Here $x\in\mathbf{R}^n(n\geq 1)$, $U\subset\mathbf{R}^n$ is a connected open set, $u\in\mathbf{R}$, and $\varepsilon\in(0,\infty)$. The functions f,r are assumed to have the following properties:

$$f(.,.)\in C^1(U\times\mathbf{R})\quad\text{and}\quad f(x,u)=f(x,u+1)\ \text{for}\ x\in U,\quad u\in\mathbf{R}; \tag{B2a}$$

$$r(.,.,\varepsilon)\in C^1(U\times\mathbf{R})\ \text{for}\ \varepsilon\in(0,\varepsilon_0), \tag{B2b}$$

where $\varepsilon_0=\varepsilon_0(U)$ is a positive constant such that

$$\sup_{(x,u,\varepsilon)\in U\times\mathbf{R}\times(0,\varepsilon_0)}\|r(x,u,\varepsilon)\|<\infty. \tag{B2c}$$

Under these hypotheses, one can approximate the solution of the IVP (B1) over a u interval of length of order $1/\varepsilon$ for sufficiently small $\varepsilon>0$ by the solution $y(u,\varepsilon)$ of the "averaged" VIP

$$\frac{\mathrm{d}y}{\mathrm{d}u}=\varepsilon\bar{f}(y), \tag{B3a}$$

$$y(0,\varepsilon)=\alpha\in U, \tag{B3b}$$

as stated precisely by Theorem B.1 below. Here $\bar{f}:U\to\mathbf{R}^n$ is defined by

$$\bar{f}(y) = \int_0^1 f(y,s)\mathrm{d}s. \tag{B4}$$

Via $\tau=\varepsilon u$, the IVP (B3) is equivalent to the IVP,

$$\frac{\mathrm{d}y_0}{\mathrm{d}\tau} = \bar{f}(y_0), \tag{B5a}$$

$$y_0(0) = \alpha \tag{B5b}$$

for $\varepsilon>0$,where $y(u,\varepsilon)=y_0(\tau)$.

By (B2a)–(B2c) and standard existence and uniqueness theorems, there exists a maximal forward interval $0\le\tau<T_1=T_1(\alpha)$ in which the IVP (B5) has a unique solution $y_0(\tau)$, where T_1 may be a finite positive real or $+\infty$. Let T be a positive constant *less* than T_1. Then the VIP (B3) has a unique solution $y(u,\varepsilon)=y_0(\varepsilon u)$ in U for $0\le u\le T/\varepsilon$ at each $\varepsilon>0$, which lies in the compact orbit $S\subset U$ "swept out" by $y_0(\tau)$ in the interval $0\le\tau\le T$. Hence S is at a *positive* distance from the boundary of U. Let $d>0$ be *less* than this distance.

Theorem B.1: Let the functions f,r in the IVP (B1) have the properties (B2a)–(B2c), and let such a constant T be given. Then there exist positive, ε-independent constants $\varepsilon_1=\varepsilon_1(U,\alpha,T)$, $C_1=C_1(U,\alpha,T)$, with $\varepsilon_1<\varepsilon_0=\varepsilon_0(U)$ and having the property that the IVP (B1) has a unique solution $x(u,\varepsilon)$ which remains in U and is uniformly approximated therein by the unique solution $y(u,\varepsilon)$ of the IVP (B3) in accordance with

$$\|x(u,\varepsilon) - y(u,\varepsilon)\| < C_1\varepsilon \tag{B6}$$

for $0\le u\le T/\varepsilon$, $0<\varepsilon<\varepsilon_1$.

Proof: By (B2a)–(B2c), the IVP (B1) has a unique solution $x(u,\varepsilon)$ in U on a maximal forward interval $[0,\beta(\varepsilon))$ for $0<\varepsilon<\varepsilon_0$. A key element of the present proof is to show that $[0,T/\varepsilon]\subset[0,\beta(\varepsilon))$ for small enough $\varepsilon>0$.

In integral form, the IVP (B1) and its averaged version (B3) become

$$x(u,\varepsilon) = \alpha + \varepsilon\int_0^u f(x(s,\varepsilon)\mathrm{d}s + \varepsilon^2\int_0^u r(x(s,\varepsilon),s,\varepsilon)\mathrm{d}s \tag{B7}$$

for $u\in[0,\beta(\varepsilon))$, $0<\varepsilon<\varepsilon_0$, and

$$y(u,\varepsilon) = \alpha + \varepsilon\int_0^u f(y(s,\varepsilon)\mathrm{d}s - \varepsilon\int_0^u \tilde{f}(y(s,\varepsilon),s)\mathrm{d}s \tag{B8}$$

for $u\in[0,T/\varepsilon]$, $\varepsilon>0$, where

$$\tilde{f}(y,u) = f(y,u) - \bar{f}(y). \tag{B9}$$

Subtracting (B8) from (B7), we obtain

$$\|x(u,\varepsilon) - y(u,\varepsilon)\| \le \varepsilon\int_0^u \|f(x(s,\varepsilon),\varepsilon) - f(y(s,\varepsilon),\varepsilon)\|\mathrm{d}s + \varepsilon\int_0^u \|\tilde{f}(y(s,\varepsilon),\varepsilon)\|\mathrm{d}s$$
$$+ \varepsilon^2\int_0^u \|r(x(s,\varepsilon),s,\varepsilon)\|\mathrm{d}s \tag{B10}$$

for $u\in[0,J(\beta(\varepsilon))$, $0<\varepsilon<\varepsilon_0$. Here $J(\beta(\varepsilon)) := [0,\beta(\varepsilon))\cap[0,T/\varepsilon]$.

We now estimate the three integrals on the rhs of (B10) at the latter values of u,ε. By our assumption that $f(.,.)\in C^1(U\times\mathbf{R})$, the following inequality holds for the first integral:

$$\int_0^u \|f(x(s,\varepsilon),\varepsilon) - f(y(s,\varepsilon),\varepsilon)\| \mathrm{d}s < L \int_0^u \|x(s,\varepsilon) - y(s,\varepsilon)\| \mathrm{d}s, \tag{B11a}$$

where L is an x-Lipschitz constant of $f(x,\varepsilon)$ in a compact $d/2$-neighborhood U_d of the orbit S in U, and hence depending solely on U_d. By Lemma 5 of Ref. 4, the second integral obeys the inequality[9]

$$\left\| \int_0^u \tilde{f}(y(s,\varepsilon),\varepsilon) \mathrm{d}s \right\| < \Gamma(\varepsilon t + 1), \tag{B11b}$$

where Γ is a constant which depends on α, U, but not T or ε. Finally, the third integral in (B10) satisfies the inequality

$$\int_0^u \|r(x(s,\varepsilon),\varepsilon)\| \mathrm{d}s \leq \Gamma_1 u, \tag{B11c}$$

where Γ_1 denotes the sup in (B2c).

By (B10) and (B11a)–(B11c), we immediately infer that

$$\|x(u,\varepsilon) - y(u,\varepsilon)\| < \varepsilon L \int_0^u \|x(s,\varepsilon) - y(s,\varepsilon)\| \mathrm{d}s + \Gamma\varepsilon(\varepsilon t + 1) + \Gamma_1 \varepsilon^2 u \tag{B12}$$

for $u \in [0, J(\beta(\varepsilon))$, $0 < \varepsilon < \varepsilon_0$. Using (B12) and Gronwall's inequality,[10] we find after a simple computation:

$$\|x(u,\varepsilon) - y(u,\varepsilon)\| < M\varepsilon(1 + \varepsilon u)\exp(L\varepsilon u) \tag{B13}$$

at the last mentioned u, ε values, where M is a constant depending on α, U, but not T or ε. Let $\varepsilon_1 < \varepsilon_0$ be a positive constant so small that $M\varepsilon_1(1+T)\exp(LT) < d/2$, and suppose that the inequality $\beta(\varepsilon) \leq T/\varepsilon$ holds at *some* positive $\varepsilon < \varepsilon_1$. Then the unique solution $x(u,\varepsilon)$ of the IVP (B1) corresponding to this ε and to the values of α, T under consideration keeps away from the boundary of U for $u \in [0, \beta(\varepsilon))$, thus contradicting maximality. Therefore, $\beta(\varepsilon) > T/\varepsilon$ at *all* positive $\varepsilon < \varepsilon_1$. It follows that (B6) holds in terms of the ε-independent constants ε_1 and $C_1 = M(1 + T)\exp(LT)$ at the values of u, ε stated in the theorem. □

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On entropy production for controlled Markovian evolution

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We consider thermodynamic systems with finitely many degrees of freedom and subject to an external control action. We derive some basic results on the dependence of the relative entropy production rate on the controlling force. Applications to macromolecular cooling and to controlling the convergence to equilibrium rate are sketched. Analogous results are derived for closed and open n-level quantum systems. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2207716]

I. INTRODUCTION

Advances in nanotechnology permit nowadays to implement feedback control actions on nanodevices. For instance, in surface topography, the deflection of a cantilever is captured by a photodetector that records the angle of reflection from a laser beam focused on the mirrored surface on the back side of the cantilever. Position feedback control is used to maintain the probe at a constant force or distance from the object surface. Position can also be differentiated, allowing us to apply a velocity-dependent external force. A velocity-dependent feedback control (VFC) has been recently implemented to reduce thermal noise of a cantilever in atomic force microscopy (AFM)[23] and in dynamic force microscopy.[41] A contribution to a rigorous thermodynamical foundation of macromolecules under VFC operating in nonequilibrium steady state is provided in Ref. 18. The entropy production rate there is decomposed into a *positive entropy production rate* (PEPR) and an *entropy pumping rate* (EPuR). The latter indicates how much entropy is pumped out or into the macromolecule by the control force. It may render the overall entropy production negative. This is at the basis of a macromolecular cooling mechanism.[4,23,41]

In this paper, we study entropy production in the presence of an external force in a more general situation. Our approach is new and complementary to Ref. 18 in that we study the free energy change rather than the total entropy change of the heat bath and of the Brownian particles as done in Ref. 18. As "distance" between two probability densities associated to the unperturbed and perturbed evolution we employ the information *relative entropy* (in the quantum case, the von Neumann relative entropy for density operators). We show that it is possible to derive some basic formulas on the entropy production rate that extend those of Ref. 18 whenever the evolution of the physical system is in some suitable sense *Markovian*. We study nonequilibrium thermodynamical systems with finitely many degrees of freedom. Corresponding results are also sketched for n-level closed and open quantum systems. The perturbation of the Hamiltonian is interpreted as a *control function* which is designed by the controller in order to obtain a desired behavior of the system (reduction of thermal noise, transfer to another state, etc.).

Among potential applications, we mention molecular kinetics,[8] macromolecular cooling,[4,18,23,41] and quantum computation.[31] As it is well known, relative entropy plays a central

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role in many areas of modern science besides physics such as mathematical statistics, information theory, probability, signal processing and quantum information processing; see, e.g., Refs. 3, 5–7, 11–13, 19, 20, 34, 35, and 37 , and Ref. 43 and references therein. Some of these results have been announced without proofs in our conference papers.[32,33]

The paper is outlined as follows. In the next section, we consider finite-dimensional, nonequilibrium thermodynamical systems. In Sec. III, we derive a basic formula on relative entropy evolution for probability densities satisfying a continuity-type equation. This result is then applied in the following section to controlled thermodynamic systems. Section V is devoted to the study of von Neumann entropy production for closed and open finite-dimensional quantum systems. In the Appendix, we show that the basic result may also be extended to *non-Markovian* finite-energy diffusions.

II. THERMODYNAMIC SYSTEMS

Consider an open thermodynamic system whose macroscopic evolution is modeled by an n-dimensional Markov diffusion process $\{x(t); t_0 \leq t\}$. The components of x form a *complete set*, i.e., all other variables have a much shorter relaxation time.[14] Let $\bar{\rho}(x)$ be the Maxwell-Boltzmann probability density corresponding to thermodynamical equilibrium

$$\bar{\rho}(x) = Z^{-1} \exp\left[-\frac{H(x)}{kT} \right]. \tag{1}$$

Here H is the (continuously differentiable) Hamiltonian function, and the (forward) Ito differential of x is

$$dx(t) = \left[-\frac{1}{2kT} \Sigma \Sigma^T \nabla H(x(t)) + u(x(t),t) \right] dt + \Sigma dW, \tag{2}$$

where W is a standard n-dimensional Wiener process. The probability density ρ_t of $x(t)$ satisfies the *Fokker-Planck equation*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left[\left(-\frac{1}{2kT} \Sigma \Sigma^T \nabla H + u \right) \rho \right] = \frac{1}{2} \sum_{i,j=1}^{n} (\Sigma \Sigma^T)_{ij} \frac{\partial^2 \rho}{\partial x_i \, \partial x_j}. \tag{3}$$

In the uncontrolled case $u=0$, under reasonable assumptions, see, e.g., Ref. 22, as $t \to \infty$, the density ρ_t of $x(t)$ tends to $\bar{\rho}$ in *relative entropy* and, consequently, in total variation.[21] For the ergodic properties of this class of diffusions, see, e.g., Ref. 40, Sec. 7.5.

Example II.1: In polymer dynamics,[9] the *macromolecule* is described by a Hamiltonian

$$H(x,y) = \tfrac{1}{2} \langle y, My \rangle + \varphi(x),$$

where M stands for the direct sum

$$M = M_1 \oplus \cdots \oplus M_N, \quad M_k = m_k I_3, \quad k = 1, \ldots, N.$$

Here x and y are $3N$-dimensional vectors, with x_i, y_i three-dimensional position and momentum of the ith hard building block of the macromolecule. Moreover, $\varphi(x)$ is the *internal potential* of macromolecule (in AFM experiment,[23] $\varphi(x) = Kx^2/2$, where K is the spring constant of the cantilever). Random collisions between solvent water molecules and building blocks of the macromolecule are modeled by the formal derivative of a Wiener process, namely *Gaussian white noise*. The six-dimensional stochastic process $(q_{i,x}, q_{i,y}, q_{i,z}, p_{i,x}, p_{i,y}, p_{i,z})$ associated with the ith block obeys the equation

$$dq_{i\alpha} = \partial_{p_{i\alpha}} H(q,p) dt, \tag{4}$$

$$dp_{i\alpha} = [-\partial_{q_{i\alpha}} H(q,p) + f_{i\alpha} + u_{i\alpha}(q,p)]dt + \Gamma_{i\alpha}^{j\beta} dW_{j\beta}(t), \tag{5}$$

where Einstein's convention has been used. Here f is a frictional force and u is a *position-velocity dependent control*. In the AFM experiment, $f=-\gamma V$, $u=-\alpha V$, $\gamma>0$, $\alpha>0$, with V a velocity. The control here acts *like* a frictional force on the macromolecule. Since the frictional coefficient has been increased, one can introduce an *effective* temperature T_{eff} which is lower than the thermostat temperature T. As is well known, different uncontrolled ($u=0$) versions of this model[16] play an important role also in other applications such as nonlinear circuits with noisy resistors.[42]

To simplify the writing, we shall assume henceforth that in (2) $\Sigma\Sigma^T=\sigma^2 I_n$. The results of this paper, however, extend in a straightforward way to the case where the diffusion matrix $\Sigma\Sigma^T$ is any symmetric, nonnegative definite [possibly singular as in (4) and (5)] matrix. Let us first recall a few basic concepts concerning the uncontrolled, nonequilibrium system (2). Let us introduce the *fluxes* $J(x,t)$ and *forces* $\Phi(x,t)$ by

$$J(x,t) = -\frac{1}{2}\sigma^2 \nabla \rho_t(x) - \frac{1}{2kT}\sigma^2 \nabla H(x)\rho_t(x),$$

$$\Phi(x,t) = -\nabla\mu(x,t),$$

where $\mu=H+kT\log\rho_t$ is the *electrochemical potential*. Notice the following:

(1) The Fokker-Plank equation (3) may be rewritten (see e.g., Ref. 14) as a continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot J = 0. \tag{6}$$

(2) Both fluxes and forces are zero in equilibrium. Moreover,

$$J(x,t) = \frac{\sigma^2}{2kT}\Phi(x,t)\rho_t(x), \tag{7}$$

which plays the role of *constitutive relations*.

(3) For ρ and σ non-negative measurable functions on $\mathbb{R}^n$, we define the information *relative entropy* (*divergence, Kullback-Leibler distance*) by

$$\mathbb{D}(\rho\|\sigma) = \int_{\mathbb{R}^n} \log\frac{\rho}{\sigma}\rho\, dx.$$

As it is well known,[19] when ρ and σ are integrable functions with

$$\int_{\mathbb{R}^n}\rho(x)\,dx = \int_{\mathbb{R}^n}\sigma(x)\,dx,$$

we have $\mathbb{D}(\rho||\sigma)\geq 0$. Moreover, $\mathbb{D}(\rho||\sigma)=0$ if and only if $\rho=\sigma$. Define the *free energy* functional

$$F(\rho_t) = kT\int_{\mathbb{R}^n}\log\frac{\rho_t}{\bar\rho}\rho_t\,dx = kT\mathbb{D}(\rho_t||\bar\rho).$$

The free energy decay may now be expressed as[14]

$$\frac{d}{dt}F(\rho_t) = -\frac{\sigma^2 kT}{2}\int_{\mathbb{R}^n}\left|\nabla \log\frac{\rho_t}{\bar{\rho}}\right|^2 \rho_t\, dx = -\int J(x,t)\Phi(x,t)\, dx. \tag{8}$$

Suppose now that, like in the AFM experiment, the thermodynamic system is subject to a feedback control action so that the macroscopic evolution is given by (2) with $u \neq 0$. The density ρ_t^u of the solution x_t^u satisfies the controlled Fokker-Planck equation (3). We are interested in the evolution of $\mathbb{D}(\rho_t^u||\rho_t^0)$, where $\{\rho_t^0, t \geq t_0\}$ is an uncontrolled evolution ($u \equiv 0$). We first need a simple but useful result.

III. A RELATIVE ENTROPY PRODUCTION FORMULA

Consider two families of non-negative functions on $\mathbb{R}^n$: $\{\rho_t; t_0 \leq t \leq t_1\}$ and $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$. We are interested in how the relative entropy $\mathbb{D}(\tilde{\rho}_t||\rho_t)$ evolves in time.

Assumptions A1: There exist measurable functions $f(x,t)$ and $\tilde{f}(x,t)$ such that $\{\rho_t; t_0 \leq t \leq t_1\}$ and $\{\tilde{\rho}_t; t_0 \leq t \leq t_1\}$ are everywhere positive C^1 solutions of

$$\frac{\partial \rho_t}{\partial t} + \nabla \cdot (f\rho_t) = 0, \tag{9}$$

$$\frac{\partial \tilde{\rho}_t}{\partial t} + \nabla \cdot (\tilde{f}\tilde{\rho}_t) = 0. \tag{10}$$

Assumption A2: For every $t \in [t_0, t_1]$

$$\lim_{|x|\to\infty} f(x,t)\tilde{\rho}_t(x) = 0,$$

$$\lim_{|x|\to\infty} \tilde{f}(x,t)\tilde{\rho}_t(x) = 0,$$

$$\lim_{|x|\to\infty} \tilde{f}(x,t)\tilde{\rho}_t(x) \log\frac{\tilde{\rho}_t}{\rho_t}(x) = 0.$$

Theorem III.1: *Suppose* $\mathbb{D}(\tilde{\rho}_t||\rho_t) < \infty, \forall t \geq 0$. *Assume moreover Assumptions A*1 *and A*2 *above. Then*

$$\frac{d}{dt}\mathbb{D}\left(\tilde{\rho}_t||\rho_t\right) = \int_{\mathbb{R}^n}\left[\nabla \log\frac{\tilde{\rho}_t}{\rho_t} \cdot (\tilde{f} - f)\right]\tilde{\rho}_t\, dx.$$

Proof:

$$\begin{aligned}
\frac{d}{dt}\mathbb{D}(\tilde{\rho}_t\|\rho_t) &= \int_{\mathbb{R}^n}\frac{d}{dt}[(\log\tilde{\rho}_t - \log\rho_t)\tilde{\rho}_t]\, dx = \int_{\mathbb{R}^n}\left\{\left[\frac{1}{\tilde{\rho}_t}\frac{\partial\tilde{\rho}_t}{\partial t} - \frac{1}{\rho_t}\frac{\partial\rho_t}{\partial t}\right]\tilde{\rho}_t + \log\frac{\tilde{\rho}_t}{\rho_t}\frac{\partial\tilde{\rho}_t}{\partial t}\right\} dx \\
&= \int_{\mathbb{R}^n}\left[-\nabla\cdot(\tilde{f}\tilde{\rho}_t) + \frac{\tilde{\rho}_t}{\rho_t}\nabla\cdot(f\rho_t) - \log\frac{\tilde{\rho}_t}{\rho_t}\nabla\cdot(\tilde{f}\tilde{\rho}_t)\right] dx \\
&= \int_{\mathbb{R}^n}\left[\nabla\log\frac{\tilde{\rho}_t}{\rho_t}\cdot\tilde{f}\tilde{\rho}_t - \nabla\frac{\tilde{\rho}_t}{\rho_t}\cdot f\frac{\rho_t}{\tilde{\rho}_t}\tilde{\rho}_t\right] dx \\
&= \int_{\mathbb{R}^n}\left[\nabla\log\frac{\tilde{\rho}_t}{\rho_t}\cdot(\tilde{f}-f)\right]\tilde{\rho}_t\, dx,
\end{aligned}$$

where we have used (9) and (10) and integration by parts (the boundary terms are zero because of

Assumption 2). □

For $\rho_t(x) \equiv 1$, we have that $-\mathbb{D}(\tilde{\rho}_t||\rho_t) = S(\tilde{\rho}_t)$ is the entropy. Taking $f(x,t) \equiv 0$, we see that the first condition in Assumption A2 is verified. Theorem III.1 then gives (exchanging ρ_t with $\tilde{\rho}_t$) the following:

Corollary III.2: Suppose $\{\rho_t; t_0 \leq t \leq t_1\}$ *is of class* C^1 *and*

$$\lim_{|x|\to\infty} v(x,t)\rho_t(x) = 0, \lim_{|x|\to\infty} v(x,t)\rho_t(x) \log \rho_t(x) = 0.$$

Suppose $S(\rho_t) < \infty$, $\forall\, t \in [t_0, t_1]$. *Then*

$$\frac{d}{dt} S(\rho_t) = -\int_{\mathbb{R}^n} [\nabla \log \rho_t \cdot f] \rho_t \, dx. \tag{11}$$

IV. ENTROPY PRODUCTION FOR CONTROLLED EVOLUTION

Consider now again the controlled thermodynamic system of Sec. II (2). Let ρ_t^u denote the density of the controlled process satisfying (3). We are interested in the evolution of $\mathbb{D}(\rho_t^u||\rho_t^0)$, where $\{\rho_t^0, t \geq t_0\}$ is an uncontrolled evolution ($u \equiv 0$). First of all, recall that the Fokker-Planck equations of the uncontrolled and controlled system may be written as continuity equations as in (6). Thus, we can apply Theorem III.1 with

$$f = -\frac{\sigma^2}{2kT} \nabla H(x) - \frac{\sigma^2}{2} \nabla \log \rho_t^0(x), \quad \tilde{f} = -\frac{\sigma^2}{2kT} \nabla H(x) + u(x,t) - \frac{\sigma^2}{2} \nabla \log \rho_t^u(x).$$

We get

$$\frac{d}{dt} \mathbb{D}\left(\rho_t^u||\rho_t^0\right) = \int_{\mathbb{R}^n} \left(\nabla \log \frac{\rho_t^u}{\rho_t^0} \cdot \left(u - \frac{\sigma^2}{2} \nabla \log \frac{\rho_t^u}{\rho_t^0} \right) \right) \rho_t^u \, dx. \tag{12}$$

Suppose now $\rho_t^0 \equiv \bar{\rho}$, where $\bar{\rho}$ is the Maxwell-Boltzmann distribution (1). We obtain the following:

*Theorem IV.1: Under assumptions A*1 *and A*2,

$$\frac{d}{dt} \mathbb{D}(\rho_t^u||\bar{\rho}) = -\frac{\sigma^2}{2} \int_{\mathbb{R}^n} \|\nabla \log \frac{\rho_t^u}{\bar{\rho}}\|^2 \rho_t^u \, dx + \int_{\mathbb{R}^n} \nabla \log \frac{\rho_t^u}{\bar{\rho}} \cdot u \rho_t^u \, dx. \tag{13}$$

Remark IV 2: Formula (13) generalizes the decomposition of the entropy production exhibited in Ref. 18 for the controlled Langevin equations. In Ref. 18, the total entropy change of the heat bath and of the Brownian macromolecules is studied. The entropy production rate (EPR) is decomposed into the sum of two terms. The first, named PEPR (*positive entropy production rate*), is an always positive term expressed as the product of the thermodynamic force and the corresponding flux as in (8). The second, named EPuR (*entropy pumping rate*), describes the amount of entropy pumped out of or into the macromolecule by the external agent. We recognize that (13) implies that $-(d/dt)\mathbb{D}(\rho_t^u||\bar{\rho})$ is also decomposed into an always positive term and into a term depending explicitly on the control function.

One can try to employ (13) to analyze macromolecular cooling.[4,18,23,41] Another direction of application is the following. Suppose we are interested in modifying the rate at which the solution ρ_t of (3) tends to the invariant density (1). Let

$$\alpha(t) > -\frac{\sigma^2}{2},$$

and consider in (2) the feedback control

$$u(x,t) = -\alpha(t)\,\nabla\,\log\frac{\rho_t^u}{\bar{\rho}}(x). \tag{14}$$

Then, ρ_t^u satisfies the Fokker-Planck equation

$$\frac{\partial\rho^u}{\partial t} - \nabla\cdot\left(\left(\frac{\sigma^2}{2}+\alpha(t)\right)\frac{1}{kT}\nabla H\rho^u\right) = \left(\frac{\sigma^2}{2}+\alpha(t)\right)\Delta\rho^u. \tag{15}$$

A few observations are now in order.

(1) Although the feedback control law is *nonlinear* in ρ_t^u, Eq. (15) is *linear*.
(2) The initial value problem for Eq. (15) is well posed since $\sigma^2/2+\alpha(t)>0$.
(3) Equation (15) still has as invariant density the Maxwell-Boltzmann distribution (1).
(4) It is conceivable to solve (15) off-line, and consequently compute the feedback law (14) beforehand.
(5) The flow of one-dimensional probability densities $\{\rho_t^u; t\geq 0\}$ of $x^u(t)$ satisfying (2) with the control given by (14) is the same as for the uncontrolled stochastic process ξ with differential

$$d\xi = -\left(\frac{\sigma^2}{2}+\alpha(t)\right)\frac{1}{kT}\nabla H(\xi)dt + \sqrt{\sigma^2+2\alpha(t)}dW, \tag{16}$$

provided $\xi(0)$ is distributed according to ρ_0^u.
(6) The friction and diffusion coefficients in (16), although time varying, still satisfy the Einstein fluctuation-dissipation relation (see, e.g., Ref. 28).

We now employ (13) to compute the relative entropy derivative. We get

$$\frac{d}{dt}\mathbb{D}(\rho_t^u\|\bar{\rho}) = -\left(\frac{\sigma^2}{2}+\alpha(t)\right)\int_{\mathbb{R}^n}|\nabla\log\frac{\rho_t^u}{\bar{\rho}}|^2\rho_t^u\,dx. \tag{17}$$

Hence, the controlled diffusion still tends to the Maxwell-Boltzmann distribution but at a different, "modulated" rate. In the linear Gauss-Markov case (i.e., when H is quadratic), the results assume a very concrete form. In particular, Eq. (15) may be replaced by a linear matricial equation (see Ref. 33 for details).

The results of this section may be readily extended to non-Markovian, finite-energy diffusions employing the Nelson-Föllmer kinematics[10,29] (see the Appendix). Notice that this family plays a central role in several branches of mathematical physics (see, e.g., Refs. 11 and 30). The results also extend without too much difficulty to a large class of diffusions with constant but singular diffusion coefficient such as in the case of the Orstein-Uhlenbeck model of physical Brownian motion[28] or, more generally, in the case of model (4) and (5). They may also be established for a large class of Markovian diffusion processes with local diffusion coefficient given the results in Refs. 15 and 25–28.

V. *n*-LEVEL QUANTUM SYSTEMS

It is apparent that Theorem III.1 can be applied to statistical mixtures in classical mechanics [Ref. 32, Sec. IV]. Indeed, Liouville's equation, expressing conservation of density in phase space, is just a continuity equation for the Hamiltonian evolution. One then gets the idea that it might be possible to establish a similar result in the quantum case, replacing the Liouville equation with the Landau-von Neumann equation for the density operator. First of all, we need to recall the basic formalism of statistical quantum mechanics.

A. Closed quantum systems

As in standard quantum mechanics,[36] to every physical system S is associated a complex Hilbert space $\mathcal{H}_S$. In the standard formulation, the state of the system is described by a unit vector $\psi \in \mathcal{H}_S$. For the sake of simplicity, here we will consider only finite-dimensional Hilbert spaces, but results hold in the general case.

We consider situations in which uncertainty on the system state affects our model. The quantum analog of a classical probability density is a density operator ρ in $\mathcal{H}_S$: A density operator is a positive semi-definite, unit trace operator on $\mathcal{H}_S$. They form a convex set $\mathcal{D}(\mathcal{H}_S)$ and the extremals of $\mathcal{D}(\mathcal{H}_S)$ are the one-dimensional orthogonal projections. These are called *pure states* and are equivalent to unit vectors in $\mathcal{H}_S$ up to an overall phase factor, by setting $\rho = \langle \psi, \cdot \rangle \psi$. Physical observables are represented by Hermitian operators on $\mathcal{H}_S$.

Let A be an observable: The expected value of A for a system described by a density operator ρ is defined as

$$\langle a \rangle_\rho := \mathrm{trace}(\rho \mathrm{A}). \tag{18}$$

Hence, the variance for an observable A given ρ is naturally defined as

$$\mathrm{Var}(A)_\rho := \langle (A - \langle a \rangle_\rho)^2 \rangle_\rho. \tag{19}$$

It is easy to see that if ρ_p is a pure state, then there exists an observable A such that the variance $\mathrm{Var}(A)_{\rho_p} = 0$, clarifying the definition and the analogy with the classical case. The time evolution for the density operator of an isolated quantum system is determined by the Hamiltonian, i.e., the energy observable. The dynamical equation is the *Landau-von Neumann equation*:

$$i\hbar \frac{d}{dt} \rho_t = [H, \rho_t], \tag{20}$$

where $[\cdot, \cdot]$ denotes the commutator

$$[A, B] := AB - BA,$$

and $\hbar$ is Planck's constant divided by 2π.

Quantum analogs of entropic functionals have been considered since the very beginning of the mathematical foundation of quantum mechanics.[44] Recently renewed interest came from quantum information applications.[31] We are interested here in the quantum relative entropy, which is defined as

$$\mathbb{D}(\rho \| \tilde{\rho}) := \mathrm{trace}(\rho(\log \rho - \log \tilde{\rho})). \tag{21}$$

We define $0 \log 0 = 0$. As in the classical case, quantum relative entropy has the property of a pseudo-distance (see, e.g., Refs. 31 and 37). We now consider the effect of a perturbation ΔH on the evolution of a quantum system originally driven by a free Hamiltonian H (we denote by $\tilde{H} = H + \Delta H$ the perturbed Hamiltonian).

Proposition V.1: Let ρ_t and $\tilde{\rho}_t$ be the solution of (20) *corresponding to the unperturbed and the perturbed Hamiltonians, respectively. The relative entropy production for the perturbed evolution is given by*

$$\frac{d}{dt} \mathbb{D}(\rho \| \tilde{\rho}) = \frac{i}{\hbar} \langle [\Delta H, \log \tilde{\rho}] \rangle_\rho. \tag{22}$$

Proof: Observing that $[\rho, \log \rho] = 0$ and, consequently,

$$\frac{d}{dt} \mathrm{trace}(\rho \log \rho) = 0$$

(i.e., the *von Neumann entropy* is time invariant under Hamiltonian evolution), and using the cyclic property of trace, we have

$$\frac{d}{dt}\mathbb{D}(\rho\|\tilde{\rho}) = \frac{d}{dt}\mathrm{trace}(\rho\log\rho) + \frac{i}{\hbar}\mathrm{trace}([H,\rho]\log\tilde{\rho} + \rho[\tilde{H},\log\tilde{\rho}])$$

$$= \frac{i}{\hbar}\mathrm{trace}([H,\rho\log\tilde{\rho}] + \rho[\Delta H,\log\tilde{\rho}]) = \frac{i}{\hbar}\mathrm{trace}(\rho[\Delta H,\log\tilde{\rho}]). \tag{23}$$

Q.E.D.

We remark that the initial conditions for the perturbed and the unperturbed evolution can be different, and we can easily exchange the role of perturbed and unperturbed evolution adding a minus sign on the right-hand side. The analogy with the corresponding relative entropy evolution formula in classical mechanics[32] is apparent. As in the classical case, the perturbation can be interpreted as an additive control Hamiltonian.

B. Open quantum systems

When we consider a quantum system interacting with the environment in some uncontrollable way, namely an *open quantum system*,[1,31] the situation changes significantly. The complete dynamical description of the situation should be done considering the tensor product space of both the system and the environment space. Usually, the environment has too many degrees of freedom to be modeled. Moreover, only partial information about environment initial state interactions may be available. In these cases, we can still obtain a dynamical equation for the system state by averaging over the environment degrees of freedom.[1] If the system evolution is assumed to be Markovian, strongly continuous in time, and completely positive,[31] a general form for the generator of the system density operator dynamics is the following:[24]

$$\frac{d}{dt}\rho_t = -\frac{i}{\hbar}[H,\rho_t] + \mathcal{L}[\rho_t], \tag{24}$$

where H is the effective Hamiltonian, in general different from the free drift Hamiltonian, and the generator for the dissipative evolution $\mathcal{L}$ has the form

$$\mathcal{L}[\rho] = \frac{1}{2}\sum_k ([L_k\rho,L_k^\dagger] + [L_k,\rho L_k^\dagger]). \tag{25}$$

The operators L_k can be derived under different assumptions on the couplings with the environment or on a phenomenological basis (see, e.g., Ref. 1 and reference therein). This equation can be seen as a quantum analog of a Fokker-Planck equation, since it describes the time evolution of the density operator in the absence of conditioning measurements. Assume that (24) admits a stationary state commuting with the effective Hamiltonian, and denote it with $\bar{\rho}$. Noting that

$$\mathrm{trace}\left(\rho\frac{d}{dt}\log\rho\right) = \mathrm{trace}\left(\frac{d}{dt}\rho\right) = 0,$$

since the generator (24) has zero trace, we obtain for the relative entropy production (see also Ref. 39)

$$\frac{d}{dt}\mathbb{D}(\rho||\bar{\rho}) = \mathrm{trace}(\mathcal{L}[\rho](\log\rho - \log\bar{\rho})) \leq 0. \tag{26}$$

The fact that $\mathbb{D}(\rho||\bar{\rho})$ is nonincreasing for the dynamical semigroup generated by (24) was established by Lindblad (see, e.g., Ref. 1). To extend this result to the case of a perturbed Hamiltonian, we consider now $\bar{\rho}$ as a *fixed target state*, since the introduction of perturbations could in general change the stationary states. In this setting, we get

$$\frac{d}{dt}\mathbb{D}(\rho\|\bar{\rho}) = \mathrm{trace}\left(\frac{\mathrm{i}}{\hbar}[\tilde{\mathrm{H}},\rho]\log\bar{\rho} + \mathcal{L}[\rho](\log\rho - \log\bar{\rho})\right)$$

$$= -\frac{i}{\hbar}\langle[\Delta H,\log\bar{\rho}]\rangle_{\rho} + \mathrm{trace}(\mathcal{L}[\rho](\log\rho - \log\bar{\rho})), \tag{27}$$

where now ρ is undergoing a *perturbed evolution* $\tilde{H}=H+\Delta H$ and $[\bar{\rho},H]=0$ as before. In the quantum case, however, the effectiveness of a control Hamiltonian is severely limited. For instance, in the closed system case, the density operator eigenvalues cannot be modified by a control Hamiltonian, precluding convergence in relative entropy if the target state has a different spectrum from the initial condition. A detailed analysis of the dissipative case from a control theoretic viewpoint can be found, e.g., in Refs. 2 and 38. Whether these formulas could be of help in designing or analyzing control strategies will be a matter of further work (see also comments on this issue in Ref. 33, Sec. VII).

Further analogies with the classical thermodynamics setting can be unravelled if we restrict our attention to Eq. (24) when it is derived from, e.g., a *weak coupling* limit.[1] This is essentially a constructive derivation of equations of the form (24) from the joint (tensor) description of the system and the environment, which is consistent with classical thermodynamics. In fact, the Gibbs state

$$\rho_G = Z^{-1}e^{-\beta H},$$

where Z is the *partition function* and H is the system Hamiltonian, is a stationary state for the resulting equation. Since, as we already recalled, relative entropy with respect to the stationary state is nonincreasing, for this class of dissipative Markovian evolutions we have a full correspondence with the classical mechanical case.[32]

VI. CONCLUSION AND OUTLOOK

We have derived explicit dependence of the *relative entropy production rate* on the control action for various uncertain physical systems exhibiting a *Markovian evolution*. Further work is needed to find other significant applications of the results as well as possible extension to other, more complex, systems with Markovian evolution such as interacting particle systems.

APPENDIX: FINITE-ENERGY DIFFUSIONS

Let $\Omega := \mathcal{C}([t_0,t_1],\mathbb{R}^n)$ denote the family of n-dimensional continuous functions, and let P and $\tilde{P}$ be two probability distributions on Ω. The *relative entropy* $H(\tilde{P},P)$ of $\tilde{P}$ with respect to P is defined by

$$H(\tilde{P},P) = \begin{cases} E_{\tilde{P}}\left[\log\dfrac{d\tilde{P}}{dP}\right] & \text{if } \tilde{P} \ll P, \\ +\infty & \text{otherwise.} \end{cases}$$

Let W_x denote Wiener measure on Ω starting at $x\in\mathbb{R}^n$, and let

$$W := \int W_x\, dx$$

be stationary Wiener measure. Let $\sigma>0$, and denote by $\mathbb{D}$ the family of distributions P on Ω such that $H(P,\sigma W)<\infty$. Let $\mathcal{F}_t$ and $\mathcal{G}_t$ denote the σ algebras of events observable up to time t and from time t on, respectively. It then follows from the Girsanov's theory[10,17] that $P\in\mathbb{D}$ possesses both a forward drift β^P and a backward drift γ^P, namely under P, the increments of the canonical coordinate process $x(t,\omega)=\omega(t)$ admit the representations

$$x(t) - x(s) = \int_s^t \beta^P(\tau)d\tau + \sigma[w_+(t) - w_+(s)], \quad t_0 \le s < t \le t_1, \tag{A1}$$

$$x(t) - x(s) = \int_s^t \gamma^P(\tau)d\tau + \sigma[w_-(t) - w_-(s)], \quad t_0 \le s < t \le t_1. \tag{A2}$$

$\beta^P(t)$ is at each time t $\mathcal{F}_t$-measurable and $w_+(\cdot)$ is a standard, n-dimensional Wiener process. Symmetrically, $\gamma^P(t)$ is $\mathcal{G}_t$-measurable and w_- is another standard Wiener process. Moreover, β^P and γ^P satisfy the finite-energy condition

$$E\left\{\int_{t_0}^{t_1} \beta^P(t)\cdot\beta^P(t)dt\right\} < \infty, \quad E\left\{\int_{t_0}^{t_1} \gamma^P(t)\cdot\gamma^P(t)dt\right\} < \infty. \tag{A3}$$

It was shown in Ref. 13 that the one-time probability density $p_t(\cdot)$ of $x(t)$ (which exists for every t) is absolutely continuous on $\mathbb{R}^n$ and the following relation holds a.s. $\forall t > 0$

$$E\{\beta^P(t) - \gamma^P(t)|x(t)\} = \sigma^2 \nabla \log p_t(x(t)). \tag{A4}$$

Let us introduce the *current drift* and the *current drift field* of P

$$v^P(t) = \frac{\beta^P(t) + \gamma^P(t)}{2}, \quad v^P(x,t) = E\{v^P(t)|x(t) = x\}. \tag{A5}$$

Then, the one-time density p_t satisfies weakly[32] a continuity-type equation

$$\frac{\partial p_t}{\partial t} + \nabla\cdot(v^P p_t) = 0. \tag{A6}$$

Hence, Theorem III.1 holds true for finite energy diffusions provided we define the v fields according to (A5).

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Global spectrum fluctuations for the β-Hermite and β-Laguerre ensembles via matrix models

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We study the global spectrum fluctuations for β-Hermite and β-Laguerre ensembles via the tridiagonal matrix models introduced previously by the present authors [J. Math. Phys. **43**, 5830 (2002)], and prove that the fluctuations describe a Gaussian process on polynomials. We extend our results to slightly larger classes of random matrices. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A. The semicircle law, deviations and fluctuations, numerically

The most celebrated theorem of random matrix theory, the Wigner semicircle law,[44,45] may be illustrated as in Fig. 1 by histogramming the eigenvalues of a single random symmetric matrix using the simple MATLAB code (normalization omitted)

```
A = randn(n); S = (A + A')/sqrt(8 * n); a = hist(eig(S),[-1:delta:1]);
bar([-1:delta:1],a/(n * delta))
```

Every time we run this experiment, we obtain deviations from the semicircle. The difference from theory is readily explained computationally:

- we use a finite matrix size n, while the semicircle law is a theorem about the $n=\infty$ limit;
- histograms bin eigenvalues into boxes of finite width, while the semicircle density is a continuous function.

There can also be numerical error in the experiments due to finite precision computations and truncation error, but in practice this does not appear to be significant.

It is worth noting that the above-noted algorithm is inefficient in two ways: first, it uses the full matrix A, rather than the equivalent tridiagonal matrix $H_{\beta,n}$ of Table II (with $\beta=1$), and it calculates the eigenvalues to obtain the histogram. For more on how to obtain the histogram plot efficiently and without calculating the eigenvalues, see Sec. V.

To study the next order behavior in the law, for large n, we can subtract away the semicircle and multiply by n. The next order *average* behavior is what we call the deviation and it was first computed by Johansson[21] to be

$$DEVIATION = \frac{1}{4}\delta_{-1}(x) + \frac{1}{4}\delta_1(x) - \frac{1}{2\pi}\sqrt{1-x^2}. \tag{1}$$

This expression for the deviation is the $\beta=1$ (corresponding to real matrices) instance of the more general $\beta>0$ case (which was also computed by Johansson, and will be explained in the next sections). The $\beta>0$ deviation contains a $(2/\beta-1)$ multiplicative factor in front of the expression on the right of (1), which notably disappears for $\beta=2$.

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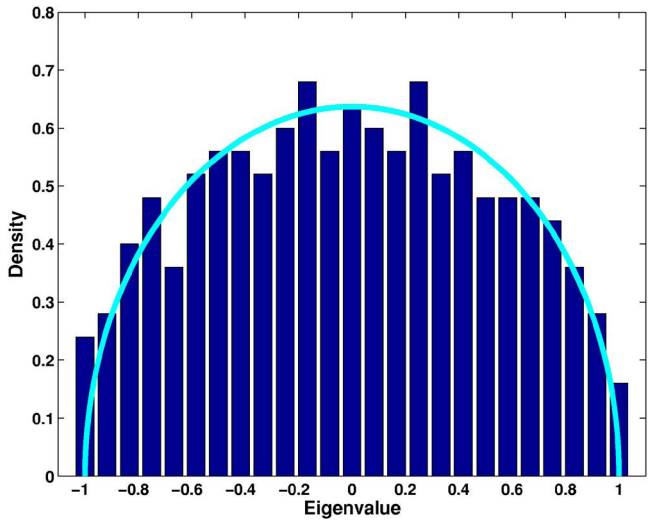

FIG. 1. (Color online) 25 bin-histogram of the eigenvalues of a 300×300 symmetric matrix from the real Gaussian distribution, vs the semicircle.

One can see this deviation result as stating that as $n\to\infty$ the eigenvalues are decremented in the interior at a rate that is fastest at the center, pulling the eigenvalues toward the endpoints.

Upon further examination of the next-order term, one can observe a phenomenon not appearing in the leading order term; there are fluctuations around the mean.

Each time we run a trial we can compute this fluctuation. For example, if we have 25 bins, the random fluctuation vector $v=(v_1,\ldots,v_{25})^T$ is the difference between the count in each bin and the number of eigenvalues predicted by the semicircle plus the deviation. The entries of v can vary quite wildly, but inner products with discretized smooth functions result in normal distributions in the continuous limit. Specifically, if f_k is the vector of size 25 consisting of the evaluations of $f(x)=x^k$ on the centers of the bins, then the dot products $f_k^T v$ are heading toward Gaussians with covariances $E[(f_{k_1}^T v)(f_{k_2}^T v)]$.

Precise statements require the size of the matrix to go to infinity and the histogram to melt into a smooth density function so that the v vector becomes a Gaussian process.

Denote by $FLUCTUATION(f(x))$ the random quantity representing the limit obtained of $f^T v$ where, as above, f is the vector of function values and v is the vector of histogram differences. For smooth functions, $FLUCTUATION(f(x))$ converges to a normal distribution; for example, in the limit as $n\to\infty$,

$$FLUCTUATION(x^k)\sim 2N(0,\sigma_k^2), \tag{2}$$

where

$$\sigma_k^2=\begin{cases}\dfrac{k}{2^{2k}}\left(\dfrac{k-1}{\frac{k-1}{2}}\right)^2 & \text{if } k=1 \bmod 2\\[2ex] \dfrac{k}{2^{2k+2}}\left(\dfrac{k}{\frac{k}{2}}\right)^2 & \text{if } k=0 \bmod 2.\end{cases}$$

For general β, the right side of (2) gains a multiplicative factor of $1/\beta$.

The limit of the entry (k_1,k_2) of the covariance matrix becomes the covariance between $FLUCTUATION(x^{k_1})$ and $FLUCTUATION(x^{k_2})$ (see Theorem 1.2 with $\beta=1$).

TABLE I. Random matrix ensembles with eigenvalue distribution proportional to $f(x_1,\ldots,x_n)\propto\Pi_{i<j}|x_i-x_j|^\beta\Pi_w(x_i)$ with w defined on an interval $I\subseteq\mathbb{R}$. MANOVA stands for Multivariate ANalysis Of Variance.

Name	Parameters	I	w	Historical name/constraints
Hermite	$\beta>0$	$\mathbb{R}$	$w(x)=e^{-x^2/2}$	Gaussian $\beta=1,2,4$
Laguerre	$\beta>0$ $a>(n-1)\beta/2$	$[0,\infty)$	$w(x)=x^p e^{-x/2}$ $p=a-(n-1)\beta/2-1$	Wishart $\beta=1,2$ $a=m\beta/2, m\in\mathbb{N}$
Jacobi	$\beta>0$ $a_1,a_2>(n-1)\beta/2$	$[0,1]$	$w(x)=x^{p_1}(1-x)^{p_2}$ $p_1=a_1-(n-1)\beta/2-1$ $p_2=a_2-(n-1)\beta/2-1$	MANOVA $\beta=1,2$ $a_1=m_1\beta/2, m_1\in\mathbb{N}$ $a_2=m_2\beta/2, m_2\in\mathbb{N}$

B. β-Hermite and β-Laguerre ensembles

This paper studies deviations and fluctuations in a wider context than real symmetric matrices with semicircular asymptotic density: We consider Hermite and Laguerre matrices with general parameter $\beta>0$. For a great reference for these ensembles, see Forrester's upcoming book.[16]

Classical finite random matrix theory considers the study of eigenvalue ensembles with joint density

$$f(x_1,\ldots,x_n)=c_{w,n}\prod_{i<j}|x_i-x_j|^\beta\prod_{i=1}^n w(x_i),$$

with w a scalar weight function on an interval I. This interval may be a subinterval of the real line, or the unit circle in the complex plane; other possibilities have been considered, too, and generalizations are easily conceived. A good reference for these formulas can be found in Lal Mehta's book.[27]

Some of the most studied eigenvalue ensembles have Hermite, Laguerre, and Jacobi weight functions on the real line, or uniform weight on the unit circle. In this paper we will be examining the ensembles with Hermite and Laguerre weights on the real line (respectively, half-line); see Table I.

For more references on Gaussian ensembles, see Ref. 27; for Wishart and MANOVA ensembles, see Ref. 30; for Hermite, Laguerre, and Jacobi ensembles, see Ref. 16.

For three particular values of β, namely 1, 2, and 4, these ensembles have been studied since the birth of the field, as the Gaussian real, complex, and quaternion ensembles (Hermite with $\beta=1,2,4$) of nuclear physics.[44,45,14,1] Similarly, the Wishart real and complex (Laguerre with $\beta=1,2$ and some restrictions on the Laguerre parameter) matrices emerged from the world of statistical multivariate analysis.[46,6,20,24]

The parameter β (making the connection to the Boltzmann factor of statistical physics) is seen by some communities (e.g., statistical mechanics) as an inverse temperature, or repulsion strength, of the ensemble of eigenvalues (the higher the β, the more separated the eigenvalues). It also has the advantage of the easy mnemonic of 1,2, and 4 corresponding to real, complex, and quaternion entries in the matrix models. However, some communities (like algebraic combinatorics) consider a different parameter, $\alpha=2/\beta$, which tends to simplify certain formulas.[28,36] In this paper we will use both notations, for convenience, and make sure that the reader is informed when changes take place.

The reason for the attractivity and success that the study of Gaussian orthogonal, unitary, and symplectic (Hermite with $\beta=1,2,4$), and the Wishart real and complex (Laguerre with $\beta=1,2$), ensembles have enjoyed lies in the existence of matrix models with real, complex, and quaternion

TABLE II. *Unscaled and scaled* tridiagonal matrix models for the β-Hermite and β-Laguerre ensembles with any $\beta>0$, $n\in\mathbb{N}$, $a\in\mathbb{R}$, and $a>(\beta/2)(n-1)$.

Hermite matrix, unscaled	$H_{\beta,n}\sim\frac{1}{\sqrt{2}}\begin{pmatrix} N(0,2) & \chi_{(n-1)\beta} & & & \\ \chi_{(n-1)\beta} & N(0,2) & \chi_{(n-2)\beta} & & \\ & \ddots & \ddots & \ddots & \\ & & \chi_{2\beta} & N(0,2) & \chi_{\beta} \\ & & & \chi_{\beta} & N(0,2) \end{pmatrix}$
Hermite matrix, scaled	$\tilde{H}_{\beta,n}=\frac{1}{\sqrt{2n\beta}}H_{\beta,n}$
Laguerre matrix, unscaled	$L^a_{\beta,n}=B^a_{\beta,n}(B^a_{\beta,n})^T$, where $B^a_{\beta,n}\sim\begin{pmatrix} \chi_{2a} & & & \\ \chi_{\beta(n-1)} & \chi_{2a-\beta} & & \\ & \ddots & \ddots & \\ & & \chi_{\beta} & \chi_{2a-\beta(n-1)} \end{pmatrix}$
Laguerre matrix, scaled	$\tilde{L}^a_{\beta,n}=\frac{\gamma}{n\beta}L^a_{\beta,n}$

entries (see Refs. 27 and 30). These models have not only originated the study, but have also allowed for a relatively thorough analysis of the finite and asymptotical eigenstatistics (statistical properties of the eigenvalues).

One of the developments in the study of arbitrary β-Hermite, -Laguerre, and -Jacobi ensembles is the introduction of general *real* matrix models (see Refs. 11, 25, and 38). For every β, there are simple *real tridiagonal matrices* which model the corresponding eigenvalue distributions given by Table I. For the β-Hermite and -Laguerre ensembles, we present these forms in Table II. These matrix forms allow for efficient Monte Carlo experiments and an alternative representation for the study of eigenstatistics in the general β case.

This paper contains one example of such analysis. With the help of these matrix models, we compute asymptotical global spectrum fluctuations for the β-Hermite and -Laguerre ensembles. For the latter, these results are new in the general β context; the global spectrum fluctuations of complex Wishart matrices (β-Laguerre with $\beta=2$) were studied by Speicher *et al.*,[26] and before by Cabanal-Duvillard.[5] Johansson's more extensive study[21] covers our results for the β-Hermite ensembles.

To prove our theorems, we use a very diverse set of methods and techniques from Jack polynomial theory, special functions, perturbation theory, and combinatorial pathcounting. Some of the techniques we used in studying the traces of powers of random matrices have been inspired by the work of Soshnikov and Sinai,[33,34] and by the study of traces of unitary random matrices by Diaconis and Shahshahani.[9]

C. Statements of results

Among the asymptotical eigenstatistics one may distinguish two classes of properties: local (like the scaled distributions and fluctuations of extremal eigenvalues, or like the level spacing distribution, i.e., the distance between neighboring eigenvalues) and global (like the limiting level density, i.e., the distribution of a random eigenvalue, and fluctuations thereof). The term global tends to refer to a property that involves all or a significant portion of the eigenvalues, while local tends to refer to a property that occurs near an individual or a constant number of eigenvalues. Among the more famous local properties we enumerate the level spacings for the Gaussian ensembles (see Refs. 27 and 39) and the extremal (largest, corresponding to "soft edge," smallest, to "hard edge") eigenvalue asymptotics (see Refs. 41, 40, 22, and 23). All these results relate to real, complex, or quaternion matrices; in the category of results relating to general β, we have to mention recent work by Desrosiers and Forrester,[8] where they analyze the asymptotical corrections to the eigenvalue density, and, for $\beta \in 2\mathbb{N}$, obtain the expected $O(n^{2/3})$ order in the fluctuation of the largest eigenvalue in the case of both β-Hermite and -Laguerre ensembles.

For n (the size of the ensembles) finite, the n eigenvalues may be considered as n fluctuating particles. Roughly speaking, the larger the β, the less fluctuation there is in the particles (hence β is seen as an inverse temperature). As $\beta \to \infty$ the particle positions behave like multivariate normals with variance $O(1/\beta)$ and means located at the roots of a Hermite (respectively, Laguerre) polynomial (see Ref. 12).

For a fixed β, as $n \to \infty$ and, in the case of Laguerre ensembles, $2a/(n\beta) \to \gamma$, the particles have an emerging (global) level density which obeys a simple law (Wigner's semicircle law[45] for the Hermite ensembles, respectively the Marčenko-Pastur laws[29] for the Laguerre ensembles). The roots of the Hermite, respectively Laguerre, polynomial have this same asymptotical density—the fluctuations do not change the asymptotics, as they are on a smaller scale.

In Ref. 10, we have proved convergence almost surely (as $n \to \infty$) of the asymptotical eigenvalue distribution of the β-Hermite ensemble to the semicircle distribution S with density $(2/\pi)\sqrt{1-x^2}$, and of the asymptotical eigenvalue distribution of the β, a-Laguerre ensemble (with $n\beta/(2a) \to \gamma \leqslant 1$) to the Marčenko-Pastur E_γ distribution with density $\frac{1}{2\pi\gamma}\frac{\sqrt{(x-(\sqrt{\gamma}-1)^2)((\sqrt{\gamma}+1)^2-x)}}{x}$. We recall that convergence almost surely is stronger (and implies) convergence in distribution, a.k.a. convergence of moments.

We examine here the distribution of the statistic $\Sigma_{i=1}^n f(\lambda_i)$, where f is a function of the *scaled* eigenvalues λ_i. The scaling is $\lambda \to \sqrt{2n\beta}\lambda$ for the β-Hermite ensembles and $\lambda \to n\beta/\gamma\lambda$ for the β-Laguerre ensembles (see Table II).

General β results for this kind of statistic can be found in Refs. 4 and 21; this or similar linear statistics have been considered also in Ref. 15 (for unitary matrices), Ref. 32 (for Wishart matrices), and, heuristically, in Ref. 31. Another path of interest is represented by asymptotical large deviations from the density (spectral measure); we mention the results of Refs. 5, 2, and 18 (which also covers global fluctuations for Wishart matrices), Refs. 19 and 7 (which covers moderate deviations).

For the linear statistic $\Sigma_{i=1}^n f(\lambda_i)$, the Wigner and Marčenko-Pastur laws for the β-Hermite and β-Laguerre ensembles state that for any "well-behaved" function f,

$$\frac{1}{n}\sum_{i=1}^{n} f(\lambda_i) \to \frac{2}{\pi}\int_{-1}^{1} f(t)\sqrt{1-t^2}\,dt, \quad \text{respectively,} \tag{3}$$

$$\frac{1}{n}\sum_{i=1}^{n} f(\lambda_i) \to \frac{1}{2\pi\gamma}\int_{(\sqrt{\gamma}-1)^2}^{(\sqrt{\gamma}+1)^2} f(t)\frac{\sqrt{(t-(\sqrt{\gamma}-1)^2)((\sqrt{\gamma}+1)^2-t)}}{t}\,dt, \tag{4}$$

where the convergence in the above is almost certain. (Such a result is sometimes given the name of "strong law of large numbers.")

Examining the fluctuations from these laws takes us one step further. For f a polynomial, we prove that once we subtract the expected average over the limiting level density [i.e., the right-hand sides of (3) and (4)], the rescaled resulting quantity tends asymptotically to a normal distribution with mean and variance depending on f. In other words, once the semicircle or Marčenko-Pastur distributions are subtracted, the fluctuations in the statistic $\Sigma_{i=1}^{n} f(\lambda_i)$ tend asymptotically to a Gaussian process on polynomials f.

How much more we can extend the class of functions that this process is well-defined on depends on the entries of the covariance matrix $C=\{C_{ij}\}$ (which can be expressed in any polynomial basis). One would be tempted to believe that a Gaussian process W defined on polynomials could, in principle, be extended to a class of continuous functions $h(x)$ with the property that, given a sequence of polynomials $p_n(x) \to h(x)$ in some norm, given $v_n = Var_W(p_n)$, $v_n \to \tilde{v} < \infty$, such that $\tilde{v} = Var_W(h)$.

Definition 1.1: Let $\gamma \in [0,1]$ be a real parameter, and let $a=(\sqrt{\gamma}-1)^2$, $b=(\sqrt{\gamma}+1)^2$. We define the following two measures:

$$\mu_H(x) := \begin{cases} \frac{1}{4}\delta_1(x) + \frac{1}{4}\delta_{-1}(x) - \frac{1}{2\pi}\frac{1}{\sqrt{1-x^2}} & \text{if } x \in [-1,1] \\ 0 & \text{otherwise}, \end{cases}$$

$$\mu_L^{\gamma}(x) := \begin{cases} \frac{1}{4}\delta_b(x) + \frac{1}{4}\delta_a(x) - \frac{1}{2\pi}\frac{1}{\sqrt{(x-a)(b-x)}} & \text{if } x \in [a,b] \\ 0 & \text{otherwise}. \end{cases}$$

Theorem 1.2: *Let $\tilde{H}_{\beta,n}$ be a scaled matrix from the β-Hermite ensemble of size n, with (scaled) eigenvalues $(\lambda_1, \ldots, \lambda_n)$, and let $k \geqslant 1$ be a positive integer. For all $i=1,\ldots,k$, let*

$$X_i = \operatorname{tr}((\tilde{H}_{\beta,n})^i) - n\frac{1}{4^{i/2}\left(\frac{i}{2}+1\right)}\binom{i}{\frac{i}{2}}\delta_{(i \bmod 2),0} - \left(\frac{2}{\beta}-1\right)\int_{-1}^{1} t^i \mu_H(t)\,\mathrm{d}t$$

$$\equiv \sum_{j=1}^{n} \lambda_j^i - n\frac{2}{\pi}\int_{-1}^{1} t^i\sqrt{1-t^2}\,\mathrm{d}t - \left(\frac{2}{\beta}-1\right)\int_{-1}^{1} t^i \mu_H(t)\,\mathrm{d}t.$$

Let $(Y_1, Y_2, \ldots, Y_k)$ be a centered multivariate Gaussian with covariance matrix

$$\operatorname{Cov}(Y_i, Y_j) = \begin{cases} \frac{1}{2^{i+j}}\frac{2ij}{i+j}\binom{i-1}{\frac{i-1}{2}}\binom{j-1}{\frac{j-1}{2}} & \text{if } i=j=1 \bmod 2 \\ \frac{1}{2^{i+j+2}}\frac{2ij}{i+j}\binom{i}{\frac{i}{2}}\binom{j}{\frac{j}{2}} & \text{if } i=j=0 \bmod 2 \\ 0 & \text{otherwise}. \end{cases} \tag{5}$$

Then, as $n \to \infty$,

$$(X_1, X_2, \ldots, X_k) \Rightarrow \sqrt{\frac{2}{\beta}}(Y_1, Y_2, \ldots, Y_k).$$

Remark 1.3: For any size k, if we add a first row and a first column of zeros to the covariance matrix (5), *the resulting* $(k+1)\times(k+1)$ *matrix* C_k *has a scaled Cholesky decomposition as* $C_k = T_k D_k T_k^T$, *where* D_k *is the diagonal matrix having on the diagonal the vector* $(0,1,2,3,\ldots,k)$, *and* T_k *has an interpretation as the change-of-base matrix in the space of univariate polynomials from monomials basis to the Chebyshev polynomials basis. One can also look at the infinite version* $C_\infty = T_\infty D_\infty T_\infty^T$.

Remark 1.4: This Gaussian process has been first described in a more general context (and extended to a larger class of continuous functions h) by Johansson in Ref. 21. *Johansson conjectured that the regularity conditions imposed on h were purely technical, and that in fact the correct condition should be that the function h admits a Fourier-like expansion in the Chebyshev basis. We restate this as follows: write h as an (infinite) vector* $\vec{h}$ *of coefficients in the Chebyshev basis; then* $V_C(h) := \vec{h}^T D_\infty \vec{h}$ *is the variance of h under the Gaussian process expressed in Chebyshev basis. Johansson's conjecture is equivalent to saying that the process could be extended to any class of functions h such that V(h) (or equivalently, the variance of h under the Gaussian process expressed in monomial basis,* $V_m(h) := (T_\infty \vec{h})^T C_\infty (T_\infty \vec{h})$ *is finite; note that* $T_\infty \vec{h}$ *is the vector of coefficients in monomial basis.*

Theorem 1.5: *Let* $\tilde{L}^a_{\beta,n}$ *be a scaled matrix from the* β*-Laguerre ensemble of parameter a and size n, with (scaled) eigenvalues* $(\lambda_1, \ldots, \lambda_n)$, *and let* $k \geqslant 1$ *be a positive integer. Assume that* $n\beta/(2a) \to \gamma \leqslant 1$, *and let* $\gamma_{min} = (\sqrt{\gamma}-1)^2$, $\gamma_{max} = (\sqrt{\gamma}+1)^2$. *For all* $i = 1, \ldots, k$, *let*

$$\begin{aligned} X_i &= \mathrm{tr}((\tilde{L}^a_{\beta,n})^i) - n\sum_{r=0}^{i-1} \frac{1}{r+1}\binom{k}{r}\binom{k-1}{r}\gamma^r - \left(\frac{2}{\beta}-1\right)\int_{\gamma_{\min}}^{\gamma_{\max}} t^i \mu_L^\gamma(t)\mathrm{d}t \\ &\equiv \sum_{j=1}^{n} \lambda_j^i - n\frac{1}{2\pi\gamma}\int_{\gamma_{\min}}^{\gamma_{\max}} t^i \sqrt{(t-\gamma_{\min})(\gamma_{\max}-t)}\mathrm{d}t - \left(\frac{2}{\beta}-1\right)\int_{\gamma_{\min}}^{\gamma_{\max}} t^i \mu_L^\gamma(t)\mathrm{d}t. \end{aligned}$$

Let $(Y_1, Y_2, \ldots, Y_k)$ *be a centered multivariate Gaussian with covariance matrix*

$$\mathrm{Cov}(Y_i, Y_j) = T_D(i,j) + T_S(i,j), \tag{6}$$

where

$$T_D(i,j) = \sum_{q=1}^{i+j-1} (-1)^{q+1}\gamma^{j+j-q}\frac{\binom{i+j}{q}}{i+j}\sum_{l=q+1}^{i+j}\frac{(-1)^l}{\binom{i+j-1}{l-1}}\sum_{\substack{r+s=l \\ 1\leqslant r\leqslant i \\ 1\leqslant s\leqslant j}} rs\binom{i}{r}^2\binom{j}{s}^2,$$

and

$$T_S(i,j) = \sum_{q=0}^{i+j-2} (-1)^q \gamma^{j+j-q}\frac{\binom{i+j}{q}}{i+j}\sum_{l=q}^{i+j-2}\frac{(-1)^l}{\binom{i+j-1}{l}}\sum_{\substack{r+s=1 \\ 0\leqslant r\leqslant i-1 \\ 0\leqslant s\leqslant j-1}} (i-r)(j-s)\binom{i}{r}^2\binom{j}{s}^2.$$

Then, as $n \to \infty$,

$$(X_1, X_2, \ldots, X_k) \Rightarrow \sqrt{\frac{2}{\beta}}(Y_1, Y_2, \ldots, Y_k).$$

Remark 1.6: For any size k, if we add a first row and a first column of zeros to the covariance matrix (6), the resulting matrix C should admit a scaled Cholesky decomposition of the form $C_k = T_k D_k T_k^T$, *with* D_k *being the diagonal matrix with diagonal entries* $\{j\gamma^{-j}\}_{0\leqslant j\leqslant k}$, *and* T_k *being the change-of-basis matrix in the space of polynomials from monomial basis to the shifted* Chebyshev *polynomials of the first kind (as defined by Cabanal-Duvillard*[5] *and used in Ref. 26). Note that the constant c in Ref. 26 is our* $1/\gamma$. *It may also be useful to look at* $C_\infty = T_\infty D_\infty T_\infty^T$.

Remark 1.7: It is worth noting that results like Theorems 1.2 and 1.5, where one averages over a set of quantities, then subtracts the mean and scales by the variance to obtain a limiting Gaussian, are sometimes called **central limit theorems** *(see, for example, Refs. 32 and 33). Free Probability uses this term as well, see, for example Ref. 35, in a different context, namely, to express the fact that averaging over random matrices creates an eigenvalue distribution that approaches the semicircular law. Both uses of the term "central limit theorem" draw different parallels to the classical case*.

Our approach to proving Theorems 1.2 and 1.5 consists of computing the first-order deviation from the mean (in Sec. II), showing that the centered process is Gaussian on monomials (by the method of moments), and computing the covariance matrices (in Sec. III).

Finally, in Sec. IV, we generalize our approach to two different classes of random matrices.

II. DEVIATION FROM THE SEMICIRCLE AND MARČENKO-PASTUR LAWS

A. Dependence on β: Symmetric functions and the "palindrome" effect

As stated in Sec. I, we are interested in computing the deviation to the semicircle and Marčenko-Pastur laws (denoted below by $LAW(\infty)$, as opposed to the $LAW(n)$, which is the level density for finite n). These deviations have the form

$$LAW(n) \sim LAW(\infty) + \frac{1}{n}\left(\frac{2}{\beta} - 1\right) DEVIATION + o\left(\frac{1}{n}\right),$$

as $n \to \infty$.

By integrating the above against x^k, we can write this in the moment form

$$moment_k(n) = moment_k(\infty) + \frac{1}{n}\left(\frac{2}{\beta} - 1\right) moment_k(DEVIATION) + o\left(\frac{1}{n}\right),$$

again as $n \to \infty$.

We mention two interesting points, the first of which we prove in this section:

1. The factor $2/\beta - 1$ in the first-order term in n and the fact that *DEVIATION* does not depend on β can be obtained from a symmetry principle alone. It is a direct consequence of Jack polynomial theory that the coefficient of $1/n^j$ in $moment_k(n)$ is a *palindromic* polynomial (we define "palindromic" below) in $-2/\beta$, and from the tridiagonal matrix models it follows that the degree of this polynomial is j; thus when $j=1$ this polynomial must be a multiple of $2/\beta - 1$. Mathematically, this is significant because in order to study the deviations, it is sufficient to then study the non-random case, $\beta = \infty$. In summary, the powerful Jack polynomial theory allows us to take a complicated random matrix problem and reduce it to an exercise on the properties of univariate Hermite and Laguerre polynomials.
2. With the Maple Library *MOPs*,[13] we can compute symbolically the exact values of $moment_k(n)$ for small values of k, *as a function of n and* β. In other words, while this paper concerns itself with the constant and $O(1/n)$ behavior, it is worth remembering that higher order terms are in principle available to us.

To make notation a bit clearer, we have used the $\alpha=2/\beta$ in the following; we also recall the scaled matrices $\widetilde{H}_{\beta,n}$ and $\widetilde{L}^{a}_{\beta,n}$, from Sec. I B. The following are the first three non-trivial moments for the traces of the scaled β-Hermite and β-Laguerre matrices with $a=n\beta/(2\gamma)=n/(\alpha\gamma)$. We omit the n and a in the notation for reasons of space,

$$\frac{1}{n}E[\mathrm{tr}(H_{2/\alpha}^2)]=\frac{1}{4}+\frac{\alpha-1}{4n},$$

$$\frac{1}{n}E[\mathrm{tr}(H_{2/\alpha}^4)]=\frac{2}{16}+\frac{5\alpha-5}{16n}+\frac{3\alpha^2-5\alpha+3}{16n^2},$$

$$\frac{1}{n}E[\mathrm{tr}(H_{2/\alpha}^6)]=\frac{5}{64}+\frac{11\alpha-11}{32n}+\frac{16\alpha^2-27\alpha+16}{32n^2}+\frac{15\alpha^3-32\alpha^2+32\alpha-15}{64n^3},$$

$$\frac{1}{n}E[\mathrm{tr}(L_{2/\alpha})]=1,$$

$$\frac{1}{n}E[\mathrm{tr}(L_{2/\alpha}^2)]=(1+\gamma)+\frac{\gamma(\alpha-1)}{n},$$

$$\frac{1}{n}E[\mathrm{tr}(L_{2/\alpha}^3)]=(1+3\gamma+\gamma^2)+\frac{3\gamma(\gamma+1)(\alpha-1)}{n}+\frac{\gamma^2(2\alpha^2-3\alpha+2)}{n^2}.$$

Note that the $O(1)$ terms in the above correspond to the second, fourth, and sixth moments of the semicircle, in the Hermite case, respectively, to the first, second, and third moments of the Marčenko-Pastur distributions in the Laguerre case; these are Catalan numbers (scaled down by powers of 4 because of the semicircle $[-1,1]$ normalization), respectively, Narayana polynomials in γ.

The $O(1/n)$ terms, the moments of the deviation, are always multiplied by $\alpha-1$, while the other coefficients of the negative powers of n in the above are "palindromic polynomials" of $(-\alpha)$; we recall the definition in the following.

Definition 2.1: A classical "palindromic polynomial" is defined by the fact that its list of coefficients is the same whether read from beginning to end or from end to beginning.

Remark 2.2: An odd-degree palindromic polynomial in x is a multiple of $(x+1)$.

To prove that the dependence of the first-order term in the deviation is indeed a multiple of $\alpha-1$, i.e., of $2/\beta-1$, we will use elements of Jack polynomial theory, and also a stronger form of a duality principle proved in Ref. 10.

We introduce in the following two notational conventions to be used throughout the rest of the paper.

Definition 2.3: We denote by $E_{\delta}^{H}[P(x_1,\ldots,x_s)]$, respectively, $E_{\delta,a}^{L}[P(x_1,\ldots,x_s)]$, the expectations of the polynomial P over the **scaled** *$2/\delta$-Hermite, respectively, $2/\delta$, a-Laguerre, ensembles of size s.*

We denote by $\mathcal{E}_{\delta}^{H}[P(x_1,\ldots,x_s)]$, respectively, *$\mathcal{E}_{\delta,a}^{L}[P(x_1,\ldots,x_s)]$, the expectations of the polynomial P over the unscaled $2/\delta$-Hermite, respectively, $2/\delta$, a-Laguerre, ensembles of size s.*

Let $\mathbb{R}[x_1,\ldots,x_n]$ be the space of symmetric polynomials in n variables (by symmetric we mean invariant under any permutation of the variables). A homogeneous basis for this vector space is a set of linearly independent, symmetric, and homogeneous polynomials which generate $\mathbb{R}[x_1,\ldots,x_n]$. One such basis is given by the power-sum functions, defined multiplicatively below. For reference, see Refs. 37 and 28.

Definition 2.4: Let $\lambda\equiv(\lambda_1,\lambda_2,\ldots,\lambda_n)$ denote an ordered partition $(\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_n)$. We define the power sum functions by

$$p_{\lambda_i}=\sum_{j=1}^{n}x_j^{\lambda_i},\quad \textit{and}$$

$$p_\lambda = p_{\lambda_1} p_{\lambda_2} \cdots p_{\lambda_n}.$$

The Jack polynomials J_λ^α constitute a parameter-dependent (the parameter being usually denoted by α) class of orthogonal multivariate polynomials; they are indexed by the powers of the highest-order term λ (in lexicographical ordering).

Throughout this section, we will think of the parameter α as a sort of inverse to β (recall that we have denoted $\alpha = 2/\beta$).

The Jack polynomials allow for several equivalent definition (up to certain normalization constraints). We will work here with definition 2.5, which arose in combinatorics. We follow Macdonald's book.[28]

Definition 2.5: The Jack polynomials J_λ^α are orthogonal with respect to the inner product defined in the following on power-sum functions

$$\langle p_\lambda, p_\mu \rangle_\alpha = \alpha^{l(\lambda)} z_\lambda \delta_{\lambda\mu},$$

where $z_\lambda = \Pi_{i=1}^{l(\lambda)} a_i! i^{a_i}$, a_i being the number of occurrences of i in λ. In addition, the coefficient of the lowest-order term in J_λ^α, which corresponds to the partition $[1^{|\lambda|}] \equiv (1,1,\ldots,1)$ (of length $|\lambda|$), is $|\lambda|!$.

From now on, we will use the notations I_n for the vector of n ones and we will refer to the quantity $J_\kappa^\alpha(x_1,\ldots,x_n)/J_\kappa^\alpha(I_n)$ as the *normalized* Jack polynomial.

To prove our results, we will need the two lemmas to follow, the first of which is a stronger variant of the duality principle proved in Ref. 10 as Theorem 8.5.3 (the proof is virtually the same as in Ref. 10 and we will not repeat it here). The second one is a rewrite of a particular case ($z_a = 0$ and formula (4.14a)) of formula (4.36b) in Ref. 3.

Lemma 2.6: Let κ' denote the conjugate partition to κ (obtained by transposing the rows and columns in the Young tableau). Then for any integers $m, n \geqslant 0$,

$$\mathcal{E}_\alpha^H \left[\frac{J_\kappa^\alpha(x_1,\ldots,x_n)}{J_\kappa^\alpha(I_n)} \right] = (-\alpha)^{-k/2} \mathcal{E}_{1/\alpha}^H \left[\frac{J_{\kappa'}^{1/\alpha}(y_1,\ldots,y_m)}{J_{\kappa'}^{1/\alpha}(I_m)} \right].$$

Lemma 2.7: The following identity is true:

$$\mathcal{E}_{\alpha,a}^L \left[\frac{J_\lambda^\alpha(x_1,\ldots,x_n)}{J_\kappa^\alpha(I_n)} \right] = 2^k \sum_{(x,y)\in\kappa} \left(a - \frac{x}{\alpha} + y \right).$$

In particular, for $a = n/(\alpha\gamma)$,

$$\mathcal{E}_{\alpha,n/\gamma\alpha}^L \left[\frac{J_\kappa^\alpha(x_1,\ldots,x_n)}{J_\kappa^\alpha(I_n)} \right] = 2^k \sum_{(x,y)\in\kappa} \left(\frac{n}{\alpha\gamma} - \frac{x}{\alpha} + y \right).$$

We can now prove the two main results of this section.

Theorem 2.8: *For k an even integer, let*

$$\mathcal{E}_\alpha^H [p_{[k]}(x_1,\ldots,x_n)] = \sum_{j=0}^{k/2} f(\alpha,j) n^{k/2+1-j},$$

with $p_{[k]}$ being the power-sum corresponding, to partition $[k]$. Then $f(\alpha,j)$ is an integer-coefficient polynomial in $1/\alpha$ of degree at most $k/2$ such that

$$f(\alpha,j) = (-\alpha)^{-k+j} f(1/\alpha, j).$$

Remark 2.9: When we scale the ensembles, we have to multiply the expectation by $(2n\beta)^{-k/2} = (\alpha/(4n))^{k/2}$, which means that

$$\frac{1}{n}E_{\alpha}^{H}[p_{[k]}(x_1,\ldots,x_n)]=\frac{1}{2^k}\sum_{j=0}^{k/2}\alpha^{k/2}f(\alpha,j)n^{-j}.$$

The corollary below follows.

Corollary 2.10: It follows that $g(\alpha,j):=\alpha^{k/2}f(\alpha,j)$ *is an integer-coefficient polynomial of* α *for which*

$$g(\alpha,j)=(-\alpha)^j g\left(\frac{1}{\alpha},j\right),$$

so the degree of $g(\alpha,j)$ *is at most* j*. This yields, in particular,* $g(\alpha,1)=c_k(\alpha-1)$*, with* c_k *a constant depending on* k*.*

Similarly, for the Laguerre ensembles, we have the following theorem.

Theorem 2.11: *Let* $a=n/\alpha\gamma$*, and*

$$\mathcal{E}_{\alpha,a}^{L}[p_{[k]}(x_1,\ldots,x_n)]=2^k\sum_{j=1}^{k+1}\sum_{r=0}^{j-1}f(\alpha,j,r)\frac{n^j}{\gamma^r},$$

with $p_{[k]}$ *being the power-sum corresponding to partition* $[k]$*. Then* $f(\alpha,j,r)$ *is a polynomial in* $1/\alpha$ *of degree at most* k *such that*

$$f(\alpha,j,r)=(-\alpha)^{-k-j+1}f(1/\alpha,j,r).$$

Remark 2.12: When we scale the ensembles, we have to multiply the expectation by $(\gamma/(n\beta))^k=(\gamma\alpha/(2n))^k$*, which means that*

$$\frac{1}{n}E_{\alpha,a}^{L}[p_{[k]}(x_1,\ldots,x_n)]=\sum_{j=1}^{k+1}\sum_{r=0}^{j-1}\alpha^k f(\alpha,j,r)n^{-k+j-1}\gamma^{k-r}.$$

The corollary below follows.

Corollary 2.13: It follows that $g(\alpha,j,r)=\alpha^k f(\alpha,j,r)$ *is an integer-coefficient polynomial of* α *for which*

$$g(\alpha,j,r)=(-\alpha)^{k-j+1}g(1/\alpha,j,r),$$

so that the degree of $g(\alpha,j,r)$ *is at most* $k-j+1$*. This yields, in particular,* $g(\alpha,k,r)=c_{k,r}(\alpha-1)$*.*

Proof of Theorem 2.8: Note that $1/\alpha=2/\beta$ and that $p_{[k]}(x_1,\ldots,x_n)=\mathrm{tr}(X^k)$, for any matrix X with eigenvalues $x_1,\ldots,x_n$. By using the unscaled matrix model $H_{\beta,n}$ for the β-Hermite ensembles found in Table II, one can obtain, as in Application 3 of Ref. 11 (more precisely, from Corollary 4.3), that $\mathcal{E}_{\alpha}^{H}[p_{[k]}(x_1,\ldots,x_n)]$ is an integer-coefficient polynomial in $1/\alpha$ of degree $k/2$, and a polynomial in n of degree $k/2+1$. Hence $f(\alpha,j)$ is an integer-coefficient polynomial in $1/\alpha$ of degree at most $k/2$.

Let us now express $p_{[k]}$ in Jack polynomial basis:

$$p_{[k]}=\sum_{\lambda\vdash k}c_{\lambda}(\alpha)J_{\lambda}^{\alpha}, \tag{7}$$

omitting the variables for simplicity.

Let $\mathbb{Q}(\alpha)$ be the field of all rational functions of α with rational coefficients.

Let $\Lambda\times\mathbb{Q}(\alpha)$ be the vector space of all symmetric polynomials of bounded degree with coefficients in $\mathbb{Q}(\alpha)$.

For every $0\neq\theta\in\mathbb{Q}(\alpha)$, define the $\mathbb{Q}(\alpha)$-algebra automorphism $\omega_\theta:\Lambda\times\mathbb{Q}(\alpha)\to\Lambda\times\mathbb{Q}(\alpha)$ by the condition $\omega_\theta(p_k)=(-1)^{k-1}\theta p_k$, for all $k\geqslant 1$. This family of automorphisms appears in [Ref. 28, Chap. 10], and similarly in Ref. 36. In particular, $\omega=\omega_1$ is known as the Macdonald involution (and can be found in [Ref. 28, Chap. 1]).

We will use the following formula due to Stanley,[36] which can also be found as formula (10.24) in Ref. 28:

$$\omega_\alpha J_\kappa^\alpha = \alpha^{|\kappa|} J_{\kappa'}^{1/\alpha}, \tag{8}$$

where κ' is the conjugate partition of κ (obtained from κ by transposing rows and columns in the Young tableau).

The first step of the proof is given by the following lemma.

Lemma 2.14: The coefficients in Eq. (7) satisfy

$$c_\lambda(\alpha) = (-\alpha)^{1-k} c_{\lambda'}(1/\alpha).$$

Proof: We apply ω_α to both sides of (7), and use (7) with parameters α and $1/\alpha$ to obtain

$$\omega_\alpha p_{[\kappa]} = (-1)^{k-1} \alpha p_{[k]} = (-1)^{k-1} \alpha \sum_{\lambda \vdash k} c_\lambda(1/\alpha) J_\lambda^{1/\alpha}.$$

On the other hand, since ω_α is linear, with the help of (8) we write

$$\omega_\alpha p_{[k]} = \sum_{\lambda \vdash k} c_\lambda(\alpha) \alpha^k J_{\lambda'}^{1/\alpha}.$$

Since there is a unique way of writing $\omega_\alpha p_{[k]}$ in Jack polynomial basis, it follows that

$$c_\lambda(\alpha) = (-\alpha)^{1-k} c_{\lambda'}(1/\alpha).$$

□

Remark 2.15: Note that Lemma 2.14 does not say anything about expectations.

We now write the expectation of $p_{[k]}$ over the unscaled Hermite ensemble using (7):

$$\mathcal{E}_\alpha^H[p_{[k]}(x_1, \ldots, x_n)] = \sum_{\lambda \vdash k} c_\lambda(\alpha) J_\lambda^\alpha(I_n) \mathcal{E}_\alpha^H \left[\frac{J_\lambda^\alpha(x_1, \ldots, x_n)}{J_\lambda^\alpha(I_n)} \right].$$

We know (for example, from Ref. 36, Theorem 5.4) that $J_\lambda^\alpha(I_n) = \Pi_{(x,y)\in\lambda}(n - x + \alpha y)$; hence

$$\mathcal{E}_\alpha^H[p_{[k]}(x_1, \ldots, x_n)] = \sum_{\lambda \vdash k} c_\lambda(\alpha) \mathcal{E}_\alpha^H \left[\frac{J_\lambda^\alpha(x_1, \ldots, x_n)}{J_\lambda^\alpha(I_n)} \right] \prod_{(x,y)\in\lambda} (n - x + \alpha y). \tag{9}$$

By Lemma 2.6,

$$\mathcal{E}_\alpha^H \left[\frac{J_\lambda^\alpha(x_1, \ldots, x_n)}{J_\lambda^\alpha(I_n)} \right]$$

does *not* depend on n. Write

$$\prod_{(x,y)\in\lambda} (n - x + \alpha y) = \sum_{j=0}^{|\lambda|} b_\lambda(j, \alpha) n^j,$$

we have

$$\prod_{(x,y)\in\lambda} (n - x + \alpha y) = \prod_{(y,x)\in\lambda'} \left(n + \alpha \left(y - \frac{x}{\alpha} \right) \right),$$

and consequently

$$b_\lambda(j, \alpha) = (-\alpha)^{k-j} b_{\lambda'}(j, 1/\alpha). \tag{10}$$

Using (9) and (10), Lemma 2.14, Lemma 2.6, and substituting $k/2+1-j$ for j (in the power index of n), we obtain the statement of Theorem 2.8. □

Proof of Theorem 2.11: The fact that $f(\alpha,j,r)$ is a polynomial in $1/\alpha$ of degree k follows similarly to Corollary 4.3 in Application 3 of Ref. 11.

We write

$$\mathcal{E}^L_{\alpha,a}[p_{[k]}(x_1,\ldots,x_n)] = \sum_{\lambda\vdash k} c_\lambda(\alpha)\mathcal{E}^L_{\alpha,a}\left[\frac{J^\alpha_\lambda(x_1,\ldots,x_n)}{J^\alpha_\lambda(I_n)}\right]\prod_{(x,y)\in\lambda}(n-x+\alpha y) \tag{11}$$

$$= 2^k\sum_{\lambda\vdash k} c_\lambda(\alpha)\prod_{(x,y)\in\lambda}\left(\frac{n}{\alpha\gamma}-\frac{x}{\alpha}+y\right)\prod_{(x,y)\in\lambda}(n-x+\alpha y). \tag{12}$$

If we write

$$\prod_{(x,y)\in\lambda}\left(\frac{n}{\alpha\gamma}-\frac{x}{\alpha}+y\right) = \sum_{j=0}^{|\lambda|}\tilde{b}_\lambda(j,\alpha)n^j\gamma^{-j},$$

it is not hard to see that

$$\tilde{b}_\lambda(j,\alpha) = (-\alpha)^{-k-j}\tilde{b}_{\lambda'}(j,1/\alpha). \tag{13}$$

Using (10) and (13), and Lemma 2.14, we obtain the statement of Theorem 2.11. □

B. Computing the β-independent part of the deviation

In this section we will examine the deviation at $\beta=\infty$ for the Hermite and Laguerre ensembles. In proving this we employ a simple differential equations trick that will allow us to compute the zero- and first-order terms in the mean of the eigenvalue distributions at $\beta=\infty$.

Given a function $y(x)$ which satisfies the second-order homogeneous differential equation

$$f(x)y''(x)+g(x)y'(x)+h(x)y(x)=0,$$

denote by $m(x)$ the function $m(x)=y'(x)/y(x)$ [with poles at the zeroes of $y(x)$].

Proposition 2.16: The function $m(x)$ satisfies the first-order differential algebraic equation

$$m^2(x)+\frac{g(x)}{f(x)}m(x)+\frac{h(x)}{f(x)}+m'(x)=0.$$

The proof is immediate.

Remark 2.17: If the function $y(x)$ is a polynomial with a finite number k of distinct roots, $m(x)$ is the generating function for the powers of y's roots.

Let $\tilde{H}_{\beta,n}$ and $\tilde{L}^a_{\beta,n}$ denote matrices from the β-Hermite, respectively, β-Laguerre ensembles. As in Ref. 10, to obtain the deviation, we once again will examine the averaged traces of powers of the matrices $\tilde{H}_{\beta,n}$ and $\tilde{L}^a_{\beta,n}$, this time looking at the first-order terms.

As a consequence of Corollaries 2.10 and 2.13, for k an even positive integer in the Hermite case, and k an arbitrary positive integer in the Laguerre case with parameter $a=(n\beta)/(2\gamma)$,

$$\frac{1}{n}E^H_\beta[p_{[k]}(x_1,\ldots,x_n)] = c_k + c^1_k\frac{\frac{2}{\beta}-1}{n}+O(n^{-2}),$$

while

$$\frac{1}{n}E_\beta^{L,a}[p_{[k]}(x_1,\ldots,x_n)] = c_k(\gamma) + c_k^1(\gamma)\frac{\frac{2}{\beta}-1}{n} + O(n^{-2}).$$

It follows that the deviation is given by the moments c_k^1, respectively, $c_k^1(\gamma)$, times the scaling factor $2/\beta-1$. Equivalently, if we examine the generating functions

$$m(n,\beta,x) = \frac{1}{n}E_\beta^H\left[\sum_{i=1}^{n}\frac{1}{x-\lambda_i}\right] = \frac{1}{n}\sum_{k=0}^{\infty}\frac{E_\beta^H[p_{[k]}(x_1,\ldots,x_n)]}{x^{k+1}} = \sum_{k=0}^{\infty}\left(\frac{c_k}{x^{k+1}} + \frac{1}{n}\left(\frac{2}{\beta}-1\right)\frac{c_k^1}{x^{k+1}} + \cdots\right)$$

and $(a=n/\alpha\gamma=n\beta/2\gamma)$

$$m(n,a,\beta,x) = \frac{1}{n}E_{\beta,a}^L\left[\sum_{i=1}^{n}\frac{1}{x-\lambda_i}\right] = \frac{1}{n}\sum_{k=0}^{\infty}\frac{E_{\beta,a}^L[p_{[k]}(x_1,\ldots,x_n)]}{x^{k+1}} = \sum_{k=0}^{\infty}\left(\frac{c_k}{x^{k+1}} + \frac{1}{n}\left(\frac{2}{\beta}-1\right)\frac{c_k^1(\gamma)}{x^{k+1}} + \cdots\right)$$

then in order to find the first-order asymptotics of $m(n,\beta,x)$ and $m(n,a,\beta,x)$, it is enough to compute $\Sigma_{k=0}^{\infty}(c_k^1/x^{k+1})$, respectively, $\Sigma_{k=0}^{\infty}[c_k^1(\gamma)/x^{k+1}]$.

We will do this by keeping n fixed, letting $\beta\to\infty$, and computing the zero- and first-order terms in $1/n$ in the generating function of the resulting matrix ensemble.

Remark 2.18: Knowing that the quantities $(1/n)E_\beta^H[p_{[k]}(x_1,\ldots,x_n)]$ *and* $(1/n)E_\beta^{L,a}[p_{[k]}(x_1,\ldots,x_n)]$ *are polynomial expressions in* $1/n$ *and* $2/\beta$ *(which follows immediately by recalling the results of Theorems 2.8 and 2.11) is the key factor in allowing us to let* $\beta\to\infty$ *while keeping in fixed.*

To aid us in our calculations, we will make use of a beautiful property of the χ_r distribution, which will allow us to replace our tridiagonal models with even simpler ones. We give this property as a Proposition.

Proposition 2.19: Let $\{X_n\}_{n\in\mathbb{N}}$ *be a set of random variables with distributions* χ_{r_n}, $n\in\mathbb{N}$, *such that* $r_n\to\infty$ *as* $n\to\infty$. *Then the sequence* $\{X_n-\sqrt{r_n}\}_{n\in\mathbb{N}}$ *converges in distributions to a centered normal of variance* $1/2$.

It follows then that, as we have already shown in Ref. 12, that given n and $\gamma\leqslant 1$ fixed, the entries of the scaled random matrices $\tilde{H}_{\beta,n}$ and $\tilde{L}_{\beta,n}^a=B_{\beta,n}^a(B_{\beta,n}^a)^T$ [with $a=(n\beta)/(2\gamma)$] converge as $\beta\to\infty$ to the following models:

$$\tilde{H}_{\beta,n}\to H = \frac{1}{2\sqrt{n}}\begin{pmatrix} 0 & \sqrt{n-1} & & & & \\ \sqrt{n-1} & 0 & \sqrt{n-2} & & & \\ & \sqrt{n-2} & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & \sqrt{1} \\ & & & & \sqrt{1} & 0 \end{pmatrix}, \tag{14}$$

respectively, to

$$\tilde{L}^a_{\beta,n} \to L_\gamma = \frac{\gamma}{n}\begin{pmatrix} \frac{n}{\gamma} & \sqrt{\frac{n}{\gamma}}\sqrt{n-1} & & & & \\ \sqrt{\frac{n}{\gamma}}\sqrt{n-1} & \frac{n}{\gamma}+n-2 & \sqrt{\frac{n}{\gamma}-1}\sqrt{n-2} & & & \\ & \sqrt{\frac{n}{\gamma}-1}\sqrt{n-2} & \frac{n}{\gamma}+n-3 & & & \\ & & \ddots & & & \\ & & & \sqrt{\frac{n}{\gamma}-n+2}\sqrt{2} & & \\ & & \sqrt{\frac{n}{\gamma}-n+2}\sqrt{2} & \frac{n}{\gamma}-n+4 & \sqrt{\frac{n}{\gamma}-n+1}\sqrt{1} & \\ & & & \sqrt{\frac{n}{\gamma}-n+1}\sqrt{1} & \frac{n}{\gamma}-n+2 & \end{pmatrix}. \tag{15}$$

Note also that if we denote by $\tilde{B}^a_{\beta,n}$ the matrix such that $\tilde{L}^a_{\beta,n}=\tilde{B}^a_{\beta,n}(\tilde{B}^a_{\beta,n})^T$, then

$$\tilde{B}^a_{\beta,n} \to B_\gamma = \sqrt{\frac{\gamma}{n}}\begin{pmatrix} \sqrt{\frac{n}{\gamma}} & & & & \\ \sqrt{n-1} & \sqrt{\frac{n}{\gamma}-1} & & & \\ & \sqrt{n-2} & \sqrt{\frac{n}{\gamma}-2} & & \\ & & \ddots & & \\ & & \sqrt{2} & \sqrt{\frac{n}{\gamma}-n+2} & \\ & & & \sqrt{1} & \sqrt{\frac{n}{\gamma}-n+1} \end{pmatrix} \tag{16}$$

and that $L_\gamma=B_\gamma B_\gamma^T$.

Since H, L_γ, and b_γ are *non-random* matrices, all expectations are exact.

1. $\beta=\infty$, Hermite case

The matrix H (see (14)) has as eigenvalues $h_1/\sqrt{2n},\ldots,h_n/\sqrt{2n}$, where $h_1,\ldots,h_n$ are the roots of the nth Hermite polynomial $H_n(x)$ (this can be easily deduced from the three-term recurrence for the Hermite polynomials, see, for example, Ref. 42). For a more detailed description of the properties of this matrix, see Ref. 12.

It follows that the generating function we need to compute is

$$\tilde{m}(n,x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{x - \frac{h_i}{\sqrt{2n}}}.$$

We use the well-known identity

$$\sum_{i=1}^{n} \frac{1}{x-x_i} = \frac{p'(x)}{p(x)}, \tag{17}$$

where x_i are distinct values, and $p(x)$ is the polynomial whose roots the x_i's are, to obtain that

$$\tilde{m}(n,x) = \sqrt{\frac{n}{2}}\frac{H_n'(x\sqrt{2n})}{H_n(x\sqrt{2n})},$$

and by applying Proposition 2.16 to the second-order differential equation satisfied by the Hermite polynomials (for a reference, see Ref. 42), we get that $\tilde{m}(n,x)$ satisfies the algebraic differential equation

$$(\tilde{m}(n,x))^2 - 4x\tilde{m}(n,x) + 4 + \frac{\tilde{m}'(n,x)}{n} = 0. \tag{18}$$

Writing $\tilde{m}(n,x) = m_0(x) - (1/n)m_1(x) + O(n^{-2})$, we obtain from (18) that

$$m_0(x) = 2(x - \sqrt{x^2-1}),$$

$$m_1(x) = \frac{(x - \sqrt{x^2-1})}{2(x^2-1)}.$$

Computing the inverse Cauchy transform for $m_0(x)$ and $m_1(x)$ yields the semicircle distribution and, respectively,

$$\mu_H(x) = \begin{cases} \frac{1}{4}(\delta_1(x) + \delta_{-1}(x)) - \frac{1}{2\pi}\frac{1}{\sqrt{1-x^2}} & \text{if } x \in [-1,1] \\ 0 & \text{otherwise.} \end{cases} \tag{19}$$

We have thus proved the following result.

Lemma 2.20: For any polynomial P,

$$E_\beta^H\left[\sum_{i=1}^n P(x_i)\right] - n\int_{-1}^1 P(x)s(x)\mathrm{d}x \to \left(\frac{2}{\beta} - 1\right)\int_{-1}^1 P(x)\mu_H(x)\mathrm{d}x,$$

as $n \to \infty$.

Remark 2.21: As a side note, in the computation above we have provided yet another way to obtain the semicircle law for all β.

2. $\beta = \infty$, Laguerre case

The matrix L_γ has as eigenvalues $\gamma l_1/n, \ldots, \gamma l_n/n$, where $l_1, \ldots, l_n$ are the roots of the nth Laguerre polynomial $L_n^{n(1/\gamma - 1)}(x)$ (see Ref. 43) (this can be easily deduced from one of the many recurrences for Laguerre polynomials, found for example as (26) in Ref. 43). To get a more detailed description of the properties of this matrix, refer to Ref. 12, substituting $n(1/\gamma) - 1$ for γ.

Since we need to rescale the eigenvalues by an additional n, it follows that the quantity of interest is

$$\tilde{m}(n,\gamma,x) = \frac{1}{n}\sum_{i=1}^n \frac{1}{x - \frac{\gamma l_i}{n}},$$

Once again we use identity 17 and obtain that

$$\tilde{m}(n,\gamma,x)=\frac{1}{n}\frac{(L_n^{n(1/\gamma-1)})'\left(\frac{xn}{\gamma}\right)}{L_n^{n(1/\gamma-1)}\left(\frac{xn}{\gamma}\right)},$$

and by applying Proposition 2.16 to the second-order differential equation satisfied by Laguerre polynomials (for a reference, see Ref. 43), we get that $\tilde{m}(n,\gamma,x)$ satisfies the algebraic differential equation

$$\gamma(\tilde{m}(n,\gamma,x))^2-\tilde{m}(n,\gamma,x)\left(1-\frac{1}{x}+\frac{\gamma}{x}\right)+\frac{1}{x}+\frac{\gamma\tilde{m}'(n,\gamma,x)+\frac{\gamma\tilde{m}(n,\gamma,x)}{x}}{n}=0. \tag{20}$$

Writing $\tilde{m}(n,\gamma,x)=m_0(x)-(1/n)m_1(x)+O(n^{-2})$, we obtain from (20) that

$$m_0(x)=\frac{x+\gamma-1-\sqrt{(x-(\sqrt{\gamma}-1)^2)(x-(\sqrt{\gamma}+1)^2)}}{2\gamma x},$$

$$m_1(x)=\frac{x-\gamma-1-\sqrt{(x-(\sqrt{\gamma}-1)^2)(x-(\sqrt{\gamma}+1)^2)}}{2(x-(\sqrt{\gamma}-1)^2)(x-(\sqrt{\gamma}+1)^2)}.$$

By calculating the inverse Cauchy transforms of $m_0(x)$ and $m_1(x)$, one obtains the Marčenko-Pastur distribution, respectively,

$$t_\gamma(x)=\begin{cases}\frac{1}{4}\delta_b(x)+\frac{1}{4}\delta_a(x)-\frac{1}{2\pi}\frac{1}{\sqrt{(x-a)(b-x)}} & \text{if } x\in[a,b]\\ 0 & \text{otherwise,}\end{cases} \tag{21}$$

with $a=(\sqrt{\gamma}-1)^2$, $b=(\sqrt{\gamma}+1)^2$.

We have thus proved the following result.

Lemma 2.22: For any polynomial P,

$$E_{\beta,a}^L\left[\sum_{i=1}^n P(x_i)\right]-n\int_a^b P(x)e_\gamma(x)\mathrm{d}x\to\left(\frac{2}{\beta}-1\right)\int_a^b P(x)t_\gamma(x)\mathrm{d}x,$$

as $n\to\infty$.

III. FLUCTUATION OF THE SEMICIRCLE AND MARČENKO-PASTUR LAWS

In this section we compute the fluctuations terms for the β-Hermite and β-Laguerre ensembles; we show that the fluctuation of the trace of any given power of the matrix corresponding to the ensemble approaches in distribution a normal variable.

The essence of the argument is simple. We will think of the random matrix as the sum between the non-random matrix of means (which we can also think about *roughly* as the $\beta=\infty$ non-random matrix) and a random matrix of the centered entries, and do some obvious computations of traces of powers. Much of the work goes into the technical carefulness to provide a complete argument, but the readers should not let the details draw them away from the simplicity of the idea, which is based on the matrix formula

$$\mathrm{tr}(T^k)=\sum_{i_1,\ldots,i_k}t_{i_1i_2}t_{i_2i_3}\cdots t_{i_ki_1},$$

with the proviso that the above-noted sum is especially simple when the matrix $T=(t_{ij})_{i,j}$ is symmetric and tridiagonal.

We provide here a heuristic explanation for the Hermite case, just for the purpose of emphasizing that the main idea is simple.

One can think of the random matrix, for all practical purposes, as

$$T \approx T_{\beta=\infty} + \frac{1}{\sqrt{\beta n}} G,$$

where G is a symmetric tridiagonal matrix of $O(1)$-variance Gaussians (similar to the decomposition we used in Ref. 12), with entries which are mutually independent, up to the symmetry condition.

Then for any polynomial h,

$$\mathrm{tr}(h(T)) \approx \mathrm{tr}(h(T_{\beta=\infty})) + \frac{1}{\sqrt{\beta n}} \mathrm{tr}(h'(T_{\beta=\infty})G),$$

the second term is clearly normally distributed, and all we have to do is compute the variance and show it is finite (which we can achieve by examining the cases when h is a monomial).

It is worth noting that, in principle, one should be able to do this computation for continuously differentiable functions h with some additional conditions imposed by the fact that the variance needs to be finite.

The technicalities arise because $n \to \infty$ and the above-mentioned equalities are just approximations, but this should not detract from the main idea. Using the method of moments, we will show that we do *not* need G's entries to be Gaussian (or even *approximately* Gaussian) in order for the *fluctuation* to monomials h to be Gaussian.

A. The β-Hermite case

We write the scaled matrix $\widetilde{H}_{\beta,n}$ as

$$\widetilde{H}_{\beta,n} = A + \frac{1}{\sqrt{n\beta}} Y, \tag{22}$$

where $A = E^H_\beta[\widetilde{H}_{\beta,n}]$ is the symmetric tridiagonal matrix of mean entries $(A(i,i+1) = (1/(2\sqrt{n\beta}))E[\chi_{(n-i)\beta}]$; all other entries are 0), and Y is symmetric tridiagonal matrix of centered variables (with a diagonal of independent Gaussians of variance 1/2). Technically, A and Y depend both on n and on β; we drop these indices from notation for the sake of simplicity.

Remark 3.1: From Proposition 2.19, we know that if $A = (a_{ij})_{1 \leq i,j \leq n}$, *then for any* $\epsilon > 0$, *there exists* $i_\epsilon \in \mathbb{N}$ *such that*

$$(2\sqrt{n\beta}a_{i,i+1} - \sqrt{(n-i)\beta}) < \epsilon \text{ for any } i \leq (n - i_\epsilon),$$

and that $Y_{i,i+1} \to N(0, 1/8)$ *in distribution as* $i \to \infty$, *while* $Y_{i,i} \sim N(0, 1/2)$ *for all* i.

Remark 3.2: (bounded moments) Note that the entries of A are **bounded**, *both from below and from above; we will think of them as* $O(1)$. *Similarly, for any* k *and* l *finite, we know from the above that there exists an* M *such that*

$$E\left[\prod_{i=1}^{kl} Y_{j_i j'_i}^{c_i}\right] \leq M,$$

for all $0 \leq c_i \leq kl$, *and for all* $j_1, \ldots, j_{kl}$ *and* $j'_1, \ldots, j'_{kl}$ *such that* $|j_i - j'_i| \leq 1$.

Given integers k and n, consider the random variable

$$\omega_k(n) = \mathrm{tr}(\widetilde{H}^k_{\beta,n}) - E^H_\beta[\mathrm{tr}(\widetilde{H}^k_{\beta,n})].$$

Claim 3.2.1: For any fixed integers k *and* l,

$$\lim_{n\to\infty} E[(\omega_k(n))^l] = \begin{cases} \left(\frac{2}{\beta}\right)^{l/2} \frac{(l-1)!!}{2^{(k+1)l}} k^{l/2} \left(\begin{matrix} k \\ \frac{k}{2} \end{matrix}\right)^l & \text{if } k, l \text{ are even} \\ \left(\frac{2}{\beta}\right)^{l/2} \frac{(l-1)!!}{2^{kl}} k^{l/2} \left(\begin{matrix} k-1 \\ \frac{k-1}{2} \end{matrix}\right)^l & \text{if } k \text{ is odd and } l \text{ is even} \\ 0 & \text{if } l \text{ is odd.} \end{cases}$$

Claim 3.2.2: For any fixed integers k_1 and k_2,

$$\lim_{n\to\infty} \mathrm{Cov}(\omega_{k_1}(n), \omega_{k_2}(n)) = \begin{cases} \frac{2}{\beta} \frac{1}{2^{k_1+k_2}} \frac{2k_1k_2}{k_1+k_2} \left(\begin{matrix} k_1-1 \\ \frac{k_1-1}{2} \end{matrix}\right) \left(\begin{matrix} k_2 \\ \frac{k_2-1}{2} \end{matrix}\right) & \text{if } k_1, k_2 \text{ are odd} \\ \frac{2}{\beta} \frac{1}{2^{k_1+k_2+2}} \frac{2k_1k_2}{k_1+k_2} \left(\begin{matrix} k_1 \\ \frac{k_1}{2} \end{matrix}\right) \left(\begin{matrix} k_2 \\ \frac{k_2}{2} \end{matrix}\right) & \text{if } k_1, k_2 \text{ are even} \\ 0 & \text{otherwise.} \end{cases}$$

Remark 3.3: Claims 3.2.1 and 3.2.2 show that the centered fluctuation of the β-Hermite ensembles describes the Gaussian process on monomials defined in Theorem 1.2.

For the remainder of this section, we will prove Claims 3.2.1 and 3.2.2. To give the reader a rough idea of where the calculations will lead, we provide in the following an intuition of what we will be doing.

Intuitive explanation: The first step is to note that $\mathrm{tr}(T^k)$ is a sum of products of k entries of T; for a tridiagonal matrix $T=(t_{i,j})_{1\leq i,j\leq n}$ with $t_{i,j}=0$ if $|i-j|>1$,

$$\mathrm{tr}(T^k) = \sum_{1\leq i_1,\ldots,i_k\leq n} t_{i_1,i_2} t_{i_2,i_3} \ldots t_{i_k,i_1},$$

where the sum needs to be taken only over the sequences $i_1,\ldots,i_k$ such that $|i_j-i_{j+1}|\leq 1$, for all $j=1,\ldots,k-1$, and also $|i_k-i_1|\leq 1$.

We have a sliding "window" of size k down the diagonal of the matrix T in which we take products of powers of the elements. In particular, for the matrix A, this is easy to visualize, because with the exception of a finite bottom right corner, the entries of A in any finite window look roughly the same.

The second step is to identify the significant terms, i.e., the terms that have non-zero asymptotical contributions. Roughly speaking, these will be the terms which will contain *precisely* one element of Y, and all the others from A. Nothing surprising here, as Y is scaled by $1/\sqrt{n\beta}$ (see (22)).

Finally, we will compute the contribution from the significant terms and show it agrees with the result of Claim 3.2.1. Then we will note that the same reasoning yields the result of Claim 3.2.2.

We now proceed to make the above-noted intuitive description rigorous. We need to introduce some notation.

Definition 3.4: For given n and p, we denote by $\mathcal{S}_{n,p}\subset\{1,\ldots,n\}^p$ the set of sequences of integers $i_1,\ldots,i_p$ such that $(i_1,\ldots,i_p)\in\{1,\ldots,n\}^p$ and $|i_j-i_{j+1}|\leq 1$ for all $j=1,\ldots,p-1$, and also $|i_p-i_1|\leq 1$.

We denote by $\mathcal{I}$ an element of $\mathcal{S}_{n,p}$, and we denote by

$$(T)_{\mathcal{I}} := t_{i_1,i_2} t_{i_2,i_3} \cdots t_{i_p,i_1},$$

where $(i_1,i_2,\ldots,i_p)=:\mathcal{I}$.

For a given $\mathcal{I} \in \mathcal{S}_{n,p}$, note that we can break up the sequence $(i_1, \ldots, i_p)$ into concatenations of sequences

$$J = ((i_{p_0}, \ldots, i_{p_1}), (i_{p_2}, \ldots, i_{p_3}), (i_{p_4}, \ldots, i_{p_5}), \ldots, (i_{p_{2q}}, \ldots, i_{p_{2q+1}})),$$

and

$$R = ((i_{p_1}, \ldots, i_{p_2}), (i_{p_3}, \ldots, i_{p_4}), \ldots, (i_{p_{2q-1}}, \ldots, i_{p_{2q}})),$$

such that in each of the sequences $i_{p_{2k}}, i_{p_{2k}}+1, \ldots, i_{p_{2k+1}}$ (for $k=0, \ldots, q$) which form J, consecutive indices differ by exactly 1, and in addition to this

$$(i_1, \ldots, i_p) = (i_{p_0}, \ldots, i_{p_1}, i_{p_1+1}, \ldots, i_{p_2}, i_{p_2+1}, \ldots, i_{p_3}, \ldots, i_{p_{2q+1}}).$$

We allow for the possibility of having empty sequences $i_{p_0}, \ldots, i_{p_1}$ in the beginning and/or $i_{p_{2q}}, \ldots, i_{p_{2q+1}}$ in the end of J.

Remark 3.5: To give an intuition for these sequences, note that any term in $\mathrm{tr}((H_{\beta,n})^k)$ *can be thought of in terms of products of entries from A and entries from Y*; *the sequences J and R will be overlapping "runs" recording the former, respectively, the latter.*

Also note that, given a fixed $\mathcal{I}$, *each J satisfying the requirements above has exactly one* $R = R(J)$ *corresponding to it, and that to different R's correspond different J's. Furthermore, since k is finite, a given R may be associated only to a finite number of sequences* $\mathcal{I}$ (*since all indices must be within k of each other*).

Definition 3.6: We define the set $\mathcal{J} = \mathcal{J}(\mathcal{I})$ *as the set of pairs* (J,R) *that corresponds to a given* $\mathcal{I}$. *For a tridiagonal matrix T, we define*

$$(T)_J = t_{i_{p_0}, i_{p_0}+1} \cdots t_{i_{p_1}-1, i_{p_1}} t_{i_{p_2} i_{p_2}+1} \cdots t_{i_{p_3}-1, i_{p_3}} \cdots t_{i_{2q}, i_{2q}+1} \cdots t_{i_{2p+1}-1, i_{2q+1}},$$

similarly,

$$(T)_R = t_{i_{p_1}, i_{p_1}+1} \cdots t_{i_{p_2}-1, i_{p_2}} t_{i_{p_3} i_{p_3}+1} \cdots t_{i_{p_4}-1, i_{p_4}} \cdots t_{i_{2q-1}, i_{2q-1}+1} \cdots t_{i_{2q}-1, i_{2q}}.$$

For any sequence $\mathcal{I} \in \mathcal{S}_{n,p}$, we can write

$$(\tilde{H}_{\beta,n})_{\mathcal{I}} = \left(A + \frac{1}{\sqrt{n\beta}} Y \right)_{\mathcal{I}} = \sum_{(J,R) \in \mathcal{J}} \frac{1}{(n\beta)^{P/2}} (A)_J (Y)_R, \tag{23}$$

with P being the total length of the "runs" in the sequence R (i.e., $P = (p_2 - p_1 + 1) + (p_4 - p_3 + 1) + \cdots + (p_{2q} - p_{2q-1} + 1)$).

We have now enough information to start the proof of Claim 3.2.1.

Proof of Claim 3.2.1: First we examine

$$E[(\omega_k(n))^l] = E[(\mathrm{tr}(\tilde{H}^k_{\beta,n}) - E^H_\beta[\mathrm{tr}(\tilde{H}^k_{\beta,n})])^l],$$

note that

$$E[(\omega_k(n))^l] = E\left[\sum_{\mathcal{I}_1, \ldots, \mathcal{I}_l \in \mathcal{S}_{n,k}} \prod_{j=1}^{l} ((\tilde{H}_{\beta,n})_{\mathcal{I}_j} - E[(\tilde{H}_{\beta,n})_{\mathcal{I}_j}]) \right].$$

Using (23), we write

$$E[(\omega_k(n))^l] = E\left[\sum_{\substack{\mathcal{I}_j \in \mathcal{S}_{n,k} \\ 1 \leqslant j \leqslant l}} \sum_{(J_j, R_j) \in \mathcal{J}_j} \frac{1}{(n\beta)^{P_j/2}} \prod_{j=1}^{l} ((A)_{J_j} (Y)_{R_j} - E[(A)_{J_j} (Y)_{R_j}]) \right]. \tag{24}$$

Since A is a non-random matrix, it follows that we can rewrite (24) as

$$E[(\omega_k(n))^l] = \sum_{\substack{\mathcal{I}_j \in \mathcal{S}_{n,k} \\ 1 \leqslant j \leqslant l}} \sum_{(J_j,R_j) \in \mathcal{J}_j} \left(\prod_{j=1}^{l} \frac{1}{(n\beta)^{P_j/2}} (A)_{J_j} \right) E\left[\prod_{j=1}^{l} ((Y)_{R_j} - E[(Y)_{R_j}]) \right]. \tag{25}$$

Denoting by $q = q(\mathcal{I}_1, \ldots, \mathcal{I}_l) := \Sigma_{j=1}^{l} P_j/2$, we obtain that

$$E[(\omega_k(n))^l] = \sum_{\substack{\mathcal{I}_j \in \mathcal{S}_{n,k} \\ 1 \leqslant j \leqslant l}} \sum_{(J_j,R_j) \in \mathcal{J}_j} \frac{1}{(n\beta)^q} \left(\prod_{j=1}^{l} (A)_{J_j} \right) E\left[\prod_{j=1}^{l} ((Y)_{R_j} - E[(Y)_{R_j}]) \right]. \tag{26}$$

Lemma 3.7: The non-zero terms in (26) have $q \geqslant l/2$.

Proof: If any of the l terms in the product $\Pi_{j=1}^{l}((Y)_{R_j} - E[(Y)_{R_j}])$ involves only variables that are independent from all other variables appearing in the remaining $l-1$ terms of the product, the expected value of the product is 0. This includes the case when at least one of the R_j's is empty. Hence, in all of the terms that have non-zero contribution to the expectation, each R_j must be non-empty, and thus $2q = \Sigma_{j=1}^{l} P_j \geqslant l$. □

Remark 3.8: Note that in fact something stronger follows, namely, that for each $1 \leqslant j_1 \leqslant l$, *there exists an* $1 \leqslant j_2 \leqslant n$, $j_2 \neq j_1$, *such that the some variable appearing in* $(Y)_{R_{j_1}}$ *also appears in* $(Y)_{R_{j_2}}$.

Since the entries of A are $O(1)$, and k and l are fixed, the factors $\Pi_{j=1}^{l}(A)_{J_j}$ are all $O(1)$. By Remark 3.8 and Lemma 3.7, it follows that every term with non-zero contribution in the double sum (26) corresponds to an l-tuple $(R_1, \ldots, R_l)$ with the property described in Remark 3.8. Each such l-tuple comes with a weight proportional to $1/n^q$.

To compute the asymptotics of the sum, we will do the following thought experiment: select a non-zero contribution term and draw the "correlation" graph with R_j as vertices, and an edge between R_{j_1} and R_{j_2} if and only if $(Y)_{R_{j_1}}$ and $(Y)_{R_{j_2}}$ are correlated (i.e., share variables). The resulting graph will have s connected components, with $1 \leqslant s \leqslant \lfloor l/2 \rfloor$.

Call these connected components $C_1, \ldots, C_s$. Consider now the set of variables $V_1, \ldots, V_s$, such that $v \in V_i$ if and only if there is an R_j in C_i such that v appears in $(Y)_{R_j}$. Select from each V_i a single variable; these variables will be independent. A variable corresponds to a choice of one index and three possibilities (since it will be of the form $Y_{i,i+1}$, $Y_{i+1,i}$, or $Y_{i,i}$).

If we were to choose a set of s independent variables from Y, roughly, to how many such l-tuples $(R_1, \ldots, R_l)$ would this choice correspond, and in turn, to how many sequences $\mathcal{I}_1, \ldots, \mathcal{I}_l$ do these correspond? In other words, to how many non-zero contribution terms in the sum (26) can a choice of s independent variables correspond?

The answer is $O(1)$.

Indeed, by the way we defined $\mathcal{I}$ and R, it follows that, once we have chosen a variable $v \in V_i$, for all other variables in V_i we have a finite number of corresponding indices to choose from. This happens because the correlation of R_j's induces a "clustering" of variables (since all indices must be within $|V_i| \times (k+1) \leqslant l(k+1)$ of each other).

Hence, for each of the possible $O(n^s)$ choices of s "representative" variables, we have only $O(1)$ possible non-zero contribution terms in the sum (26).

Going backwards, it follows that for any s, there are $O(n^s)$ terms for which the correlation graph has s components. Since each of these terms has weight at most $1/n^q \leqslant 1/n^{l/2}$, we have proved the following lemma.

Lemma 3.9: The contribution to the expectation sum (26) from all terms with $s < l/2$ *or* $q > l/2$ *is asymptotically negligible*.

Thus, the only terms of asymptotical significance are those for which $s = q = l/2$. If l is odd, this immediately implies

Lemma 3.10: With the notations above, for k and l fixed, l odd,

$$\lim_{n \to \infty} E[\omega_k(n)^l] = 0.$$

Let us examine what happens when l is even and $s=q=l/2$. Such terms are easy to understand: they correspond precisely to l-tuples $(R_1,\ldots,R_l)$ for which $|R_j|=1$ for all j, and for each $1\leqslant j_1\leqslant l$ there exists a unique $1\leqslant j_2\leqslant l$ such that $(Y)_{R_{j_1}}=(Y)_{R_{j_2}}$.

We make the following simple observation.

Lemma 3.11: The number of diagonal terms $Y_{i,i}$ contained in each $(Y)_{R_j}$, counting multiplicities, has to have the same parity as k.

Proof: Indeed, by the definition of any R, all the diagonal terms found in $(\tilde{H}_{\beta,n})_{\mathcal{I}}$ must be found in $(Y)_R$. The parity of these terms, counting multiplicities, has to be the same as the parity of k. This is easy to see; if $\mathcal{I}=(i_1,i_2,\ldots,i_k)$, then by Definition 3.6

$$i_1-i_2+i_2-i_3+\cdots+i_{k-1}-i_k+i_k-i_1=0,$$

and since each difference i_j-i_{j+1} above is either 0, 1, or −1, it follows that the number of differences equal to 0 has the same parity as k. The number of differences equal to 0 is the number of diagonal terms. □

It then follows that, for all l-tuples of $(R_1,\ldots,R_l)$ for which $s=q=l/2$,

- if k is odd, all variables present in the $(Y)_{R_j}$'s are diagonal variables, and
- if k is even, all variables present in the $(Y)_{R_j}$'s are off-diagonal variables.

We summarize here what we now know about the terms we need to study when l is even.

Lemma 3.12: The only asymptotically relevant terms have the property that there exist $l/2$ distinct indices $i_1,\ldots,i_{l/2}$ such that for each i_j there exist precisely two values $j_1<j_2$ for which

1. *if k is odd, $R_{j_1}=R_{j_2}=\{(i_j,i_j)\}$,*
2. *if k is even, either one of these four possibilities:*
   - $R_{j_1}=R_{j_2}=\{(i_j,i_j+1)\}$, *or*
   - $R_{j_1}=R_{j_2}=\{(i_j+1,i_j)\}$, *or*
   - $R_{j_1}=\{(i_j,i_j+1)\}$ *and* $R_{j_2}=\{(i_j+1,i_j)\}$, *or*
   - $R_{j_1}=\{(i_j+1,i_j)\}$ *and* $R_{j_2}=\{(i_j,i_j+1)\}$.

Note that in this case, $(Y)_{R_{j_1}}=(Y)_{R_{j_2}}$, because the matrix is symmetric. We call all such terms **significant**.

We will now need a stronger result than Remark 3.2.

Lemma 3.13: For any given $\epsilon>0$ and $k,l\in\mathbb{N}$, with l even, there exists some $i_\epsilon\in\mathbb{N}$ such that for any significant term $(\Pi_{j=1}^{l}(A)_{j_i})E[\Pi_{j=1}^{l}((Y)_{R_i}-E[(Y)_{R_i}])]$ and the corresponding $l/2$-tuplet $(i_1,\ldots,i_{l/2})$, if $k\leqslant i_1,\ldots,i_{l/2}\leqslant n-i_\epsilon$, then

- *if k is odd,*

$$\left|\left(\prod_{j=1}^{l}(A)_{J_j}\right)E\left[\prod_{j=1}^{l}((Y)_{R_j}-E[(Y)_{R_j}])\right]-\frac{1}{2^{(k-1)l+l/2}}\prod_{m=1}^{l/2}\left(1-\frac{i_m}{n}\right)^{k-1}\right|<\epsilon;$$

- *if k is even,*

$$\left|\left(\prod_{j=1}^{l}(A)_{J_j}\right)E\left[\prod_{j=1}^{l}((Y)_{R_j}-E[(Y)_{R_j}])\right]-\frac{1}{2^{(k-1)l+3l/2}}\prod_{m=1}^{l/2}\left(1-\frac{i_m}{n}\right)^{k-1}\right|<\epsilon.$$

Proof: The lemma follows easily from Proposition 2.19 and Remark 3.1, together with the fact that if R_j contains the index i, then all indices present in J_j are within k of i. □

We prove now that it is enough to look at the significant terms for which $n-i_\epsilon\geqslant i_1,\ldots,i_{l/2}\geqslant k$ (i.e., those covered by Lemma 3.13).

Lemma 3.14: The contribution of significant terms for which some $i_j>n-i_\epsilon$ or $i_j<k$ is asymptotically negligible, i.e., $o(1)$.

Proof: Each contribution from a significant term

$$\left(\prod_{j=1}^{l}(A)_{J_j}\right)E\left[\prod_{j=1}^{l}((Y_{R_j}-E[(Y)_{R_j}])\right]$$

is bounded by some constant $\tilde{M}$, by Lemmas 3.2 and 3.1. Since restricting a choice of i_j to be greater than $n-i_\epsilon$ or less than k yields a finite number of choices for that particular i_j, and since $j<l$ is finite, it follows that there are only $O(n^{l/2-1})$ such restricted terms. But since the contribution of any such term is weighted by $1/n^{l/2}$, the statement of the lemma follows. □

So we have reduced the computation to examining the contribution from the terms for which $n-i_\epsilon \geqslant 1,\ldots,i_{l/2}\geqslant k$. Assume w.l.o.g $i_\epsilon > k$ (we can always choose a smaller ϵ).

Given an ordered $l/2$-tuplet of distinct indices $n-i_\epsilon\geqslant 1,\ldots,i_{l/2}\geqslant k$, how many terms can correspond to them? First, there are $(l-1)!!$ ways of pairing these indices to the R_j's in this order. Second, once the pairing is given,

- for k odd, the corresponding $\mathcal{I}_j$ sequence must be a sequence where all but one consecutive difference are ± 1 (the one difference that is 0 corresponds to the insertion of the diagonal term). There are $\left(k\binom{k-1}{(k-1)/2}\right)$ such choices for each $\mathcal{I}_j$, for a total of $\left(k\binom{k-1}{(k-1)/2}\right)^l$ choices.
- for k even, the corresponding $\mathcal{I}_j$ sequence must be a sequence where all consecutive difference are ± 1, and one of these differences corresponding to the "marked" term that belongs to R_j. Taking into account all four possible cases, we obtain a total number of $k^2\binom{k}{k/2}^2$ for each pair of matched $\mathcal{I}_j$'s, and thus a total number of $\left(k\binom{k}{k/2}\right)^{l/2}$ choices.

Note that in either one of the two above-mentioned cases, all choices of sequences are valid, because the indices in each sequence will stay between 1 and n (this is where we need that all $k\leqslant i_j\leqslant n-i_\epsilon$).

Thus, the total number of significant terms which correspond to a given ordered $l/2$-tuplet of distinct indices $n-i_\epsilon\geqslant 1,\ldots,i_{l/2}\geqslant k)$ is

- $(l-1)!!\left(k\binom{k-1}{(k-1)/2}\right)^l$ if k is odd, and
- $(l-1)!!\left(k\binom{k}{k/2}\right)^l$ if k is even.

From Lemmas 3.9, 3.12, 3.13, and 3.14, we obtain that for any given ϵ, if k is odd,

$$E[(\omega_k(n))^l]=\sum_{\substack{\text{all significant terms}\\ \text{with } k\leqslant i_j\leqslant n-i_\epsilon\forall j}}\frac{1}{(n\beta)^q}\left(\prod_{j=1}^{l}(A)_{J_j}\right)E\left[\prod_{j=1}^{l}((Y)_{R_j}-E[(Y)_{R_j}])\right]+o(1),$$

and so

$$\left|E[(\omega_k(n))^l]-(l-1)!!\left(k\binom{k-1}{\frac{k-1}{2}}\right)^l\frac{1}{2^{kl-l/2}}\sum_{\substack{\text{all significant terms}\\ \text{with } k\leqslant i_j\leqslant n-i_\epsilon\forall j}}\frac{1}{(n\beta)^{l/2}}\prod_{j=1}^{l/2}\left(1-\frac{i_j}{n}\right)^{k-1}\right|$$

$$\leqslant(l-1)!!\left(k\binom{k-1}{\frac{k-1}{2}}\right)^l\frac{1}{2^{kl-l/2}}\sum_{\substack{n-i_\epsilon\geqslant i_1,\ldots,i_{l/2}\geqslant k\\ \text{all } i_j \text{ distinct}}}\frac{1}{(n\beta)^{l/2}}\epsilon+o(1)$$

$$=(l-1)!!\left(k\binom{k-1}{\frac{k-1}{2}}\right)^l\frac{1}{2^{kl-l/2}}\epsilon(1+o(1))+o(1)=(l-1)!!\left(k\binom{k-1}{\frac{k-1}{2}}\right)^l\frac{1}{2^{kl-l/2}}\epsilon(1+o(1)).$$

Since ϵ was arbitrarily small, it follows that if we can compute

$$S = (l-1)!!\left(k\binom{k-1}{\frac{k-1}{2}}\right)^l \frac{1}{2^{kl-l/2}} \sum_{\substack{n-i_\epsilon \geqslant i_1,\ldots,i_{l/2}\geqslant k \\ \text{all } i_j \text{ distinct}}} \frac{1}{(n\beta)^{l/2}} \prod_{j=1}^{l/2} \left(1-\frac{i_j}{n}\right)^{k-1},$$

we are done. But, since l and k are fixed, the sum in S is asymptotically the same as the value of the integral $((1/\beta)\int_0^1 (1-x)^{k-1}\mathrm{d}x)^{l/2}$, hence

$$\sum_{\substack{n-i_\epsilon \geqslant i_1,\ldots,i_{l/2}\geqslant k \\ \text{all } i_j \text{ distinct}}} \frac{1}{(n\beta)^{l/2}} \prod_{j=1}^{l/2} \left(1-\frac{i_j}{n}\right)^{k-1} \sim \frac{1}{\beta^{l/2}} \frac{1}{k^{l/2}},$$

hence

$$E[(\omega_k(n))^l] - \left(\frac{2}{\beta}\right)^{l/2} \frac{(l-1)!!}{2^{kl}} k^{l/2} \binom{k-1}{\frac{k-1}{2}}^l = O(\epsilon),$$

for arbitrarily small ϵ.

Similarly, for k even, we obtain through the same sort of calculation that

$$E[(\omega_k(n))^l] - \left(\frac{2}{\beta}\right)^{l/2} \frac{(l-1)!!}{2^{(k+1)l}} k^{l/2} \binom{k}{\frac{k}{2}}^l = O(\epsilon),$$

for arbitrarily small ϵ.

Claim 3.2.1 is thus proved. □

Proof of Claim 3.2.2: The proof is based on the same idea as the proof of Claim 3.2.1; the same reasoning applies to yield the asymptotical covariance result. □

Remark 3.15: Note that we never actually used the full power of the fact that the entries of the tridiagonal symmetric matrix Y tend to independent centered **normal** *variables. We only used the following three properties:*

- $E[Y_{i,i}] = E[Y_{i+1,i}] = 0$;
- $\mathrm{Var}[Y_{i,i}] = \frac{1}{2}$, *while* $\lim_{n\to\infty} \mathrm{Var}[Y_{i+1,i}] = \frac{1}{8}$;
- *for any k, there exists a number* $M_k > 0$ *such that* $|E[(Y_{i,j})^k]| < M_k$, *for all* $1 \leqslant i, j \leqslant n$ (*boundedness of moments*).

B. The β-Laguerre case

Given an integer k, consider the random variable

$$\eta_{k,\gamma}(n) = \mathrm{tr}((\tilde{L}^a_{\beta,n})^k) - E^L_{\beta,a}[\mathrm{tr}((\tilde{L}^a_{\beta,n})^k)].$$

The main results of this section are given in the Claims to follow.

Claim 3.15.1: For any fixed integers k and l,

$$\lim_{n\to\infty} E[(\eta_{k,\gamma}(n))^l] = \begin{cases} \left(\frac{2}{\beta}\right)^{l/2} (\mathrm{Sum}_1(k,\gamma) + \mathrm{Sum}_2(k,\gamma))^{l/2} (l-1)!! & \text{if } l \text{ is even} \\ 0, & \text{if } l \text{ is odd}, \end{cases}$$

where

$$\mathrm{Sum}_1(k,\gamma)=\sum_{q=1}^{2k-1}(-1)^{q+1}\gamma^{2k-q}\frac{\binom{2k}{q}}{2k}\sum_{j=q+1}^{2k}\frac{(-1)^j}{\binom{2k-1}{j-1}}\sum_{\substack{s_1+s_2=j\\1\leqslant s_1,s_2\leqslant k}}s_1s_2\binom{k}{s_1}^2\binom{k}{s_2}^2,$$

$$\mathrm{Sum}_2(k,\gamma)=\sum_{q=0}^{2k-2}(-1)^{q}\gamma^{2k-q}\frac{\binom{2k}{q}}{2k}\sum_{j=q}^{2k-2}\frac{(-1)^j}{\binom{2k-1}{j}}\sum_{\substack{s_1+s_2=j\\0\leqslant s_1,s_2\leqslant k-1}}(k-s_1)(k-s_2)\binom{k}{s_1}^2\binom{k}{s_2}^2.$$

Claim 3.15.2: For any fixed integers k and l,

$$\lim_{n\to\infty}\mathrm{Cov}(n_{i,\gamma}(n),\eta_{j,\gamma}(n))=\frac{2}{\beta}(\mathrm{Sum}_1(i,j,\gamma)+\mathrm{Sum}_2(i,j,\gamma)),$$

where

$$\mathrm{Sum}_1(i,j,\gamma)=\sum_{q=1}^{i+j-1}(-1)^{q+1}\gamma^{j+j-q}\frac{\binom{i+j}{q}}{i+j}\sum_{j=q+1}^{i+j}\frac{(-1)^j}{\binom{i+j-1}{j-1}}\sum_{\substack{r+s=j\\1\leqslant r\leqslant i\\1\leqslant s\leqslant j}}rs\binom{i}{r}^2\binom{j}{s}^2,$$

$$\mathrm{Sum}_2(i,j,\gamma)=\sum_{q=0}^{i+j-2}(-1)^{q}\gamma^{j+j-q}\frac{\binom{i+j}{q}}{i+j}\sum_{j=q}^{i+j-2}\frac{(-1)^j}{\binom{i+j-1}{j}}\sum_{\substack{r+s=j\\0\leqslant r\leqslant i-1\\0\leqslant s\leqslant j-1}}(i-r)(j-s)\binom{i}{r}^2\binom{j}{s}^2.$$

The method we employ for proving these claims is basically the same as in Sec. III A; the only things that change are the details of the sequences we will deal with. In the following we will point out where definitions and calculations differ from before, but we will not go over the reduction arguments again, for the sake of brevity.

We write the scaled matrix $\tilde{B}^a_{\beta,n}$ as

$$\tilde{B}^a_{\beta,n}=D+\frac{1}{\sqrt{\beta n}}Z,$$

where $D=E^L_{\beta,a}[\tilde{B}^a_{\beta,n}]$ is the bidiagonal matrix of mean entries $D(i,i)=(\sqrt{\gamma}/\sqrt{n\beta})E[\chi_{2a-i\beta}]$ and $D(i+1,i)=(\sqrt{\gamma}/\sqrt{n\beta})E[\chi_{(n-i)\beta}]$, and Z is the lower bidiagonal matrix of centered variables; we drop the dependence of D and Z on β, a, and n, for simplicity.

Remark 3.16: From Proposition 2.19, if $D=(d_{ij})_{1\leqslant i,j\leqslant n}$, given any $\varepsilon>0$, there is an $i_\epsilon\in\mathbb{N}$ such that

$$|\sqrt{n\beta/\gamma}\,d_{i,i}-\sqrt{n\beta/\gamma-i\beta}|\leqslant\epsilon,\quad \textit{and}$$

$$|\sqrt{n\beta/\gamma}\,d_{i+1,i}-\sqrt{(n-i)\beta}|\leqslant\epsilon,$$

for any $i\leqslant n-i_\epsilon$.

Here we also used the fact that $2a/(n\beta)\sim 1/\gamma$.

Similarly, again from Proposition 2.19, we know that $Z_{i,i} \to N(0, \gamma/2)$ *and* $Z_{i+1,i} \to N(0, \gamma/2)$ *in distribution*.

As in Sec. III A we start from the expression for $\mathrm{tr}((BB^T)^k)$, for B a lower bidiagonal matrix:

$$\mathrm{tr}((BB^T)^k) = \sum_{1 \leqslant i_1, i_2, \ldots, i_{2k} \leqslant n} b_{i_1,i_2} b_{i_2,i_3} \cdots b_{i_{2k-1},i_{2k}} b_{i_{2k},i_1},$$

where the sum is taken over sequences $(i_1, \ldots, i_{2k})$ with the property that $i_{2j-1} - i_{2j} \in \{0, 1\}$, for all $1 \leqslant j \leqslant k$, and $i_{2j} - i_{2j+1} \in \{0, -1\}$, for all $1 \leqslant j \leqslant k-1$, and also $i_{2k} - i_1 \in \{0, -1\}$.

Just as before, we will introduce a few notations (we "recycle" some of the notations we used before; note that the quantities change).

Definition 3.17: We denote by $S_{n,k} \in \{1, \ldots, n\}^{2k}$ *the set of sequences of integers* $i_1, \ldots, i_{2k}$ *such that* $i_{2j-1} - i_{2j} \in \{0, 1\}$, *for all* $1 \leqslant j \leqslant k$, *and* $i_{2j} - i_{2j+1} \in \{0, -1\}$, *for all* $1 \leqslant j \leqslant k-1$, *and also* $i_{2k} - i_1 \in \{0, -1\}$. *We denote by* $\mathcal{I}$ *an element in* $S_{n,k}$.

For each such $\mathcal{I}$, we consider all the ways in which we can "break up" $\mathcal{I} := (i_1, \ldots, i_{2k})$ into overlapping "runs" J and R, i.e.,

$$J = ((i_{p_0}, \ldots, i_{p_1}), (i_{p_2}, \ldots, i_{p_3}), (i_{p_4}, \ldots, i_{p_5}), \ldots, (i_{p_{2q}}, \ldots, i_{p_{2q+1}})),$$

and

$$R = ((i_{p_1}, \ldots, i_{p_2}), (i_{p_3}, \ldots, i_{p_4}), \ldots, (i_{p_{2q-1}}, \ldots, i_{p_{2q}})),$$

with

$$(i_1, \ldots, i_{2k}) = (i_{p_0}, \ldots, i_{p_1}, i_{p_1+1}, \ldots, i_{p_2}, i_{p_2+1}, \ldots, i_{p_3}, \ldots, i_{p_{2q+1}}).$$

Note that this preserves the requirement that $i_j - i_{j+1} \in \{0, (-1)^{1+j \bmod 2}\}$ for all j.

We allow for the possibility of having empty sequences $i_{p_0}, \ldots, i_{p_1}$ in the beginning and/or $i_{p_{2q}}, \ldots, i_{p_{2q+1}}$ in the end of J.

Definition 3.18: For any $\mathcal{I}$, *we introduce the set* $\mathcal{J} = \mathcal{J}(\mathcal{I})$ *of pairs* (J, R) *corresponding to the sequence* $\mathcal{I}$. *For a bidiagonal matrix* B, *we define*

$$(BB^T)_{\mathcal{I}} = b_{i_1,i_2} b_{i_2,i_3} \cdots b_{i_{2k-1},i_{2k}} b_{i_{2k},i_1},$$

$$(BB^T)_J = b_{i_{p_0},i_{p_0}+1} \cdots b_{i_{p_1}-1,i_{p_1}} b_{i_{p_2}b_{p_2}+1} \cdots b_{i_{p_3}-1,i_{p_3}} \cdots b_{i_{2q},i_{2q}+1} \cdots b_{i_{2q+1}-1,i_{2q+1}},$$

$$(BB^T)_R = b_{i_{p_1},i_{p_1}+1} \cdots b_{i_{p_2}-1,i_{p_2}} b_{i_{p_3}i_{p_3}+1} \cdots b_{i_{p_4}-1,i_{p_4}} \cdots b_{i_{2q-1},i_{2q-1}+1} \cdots b_{i_{2q}-1,i_{2q}}.$$

Remark 3.19: Note that any term in $\mathrm{tr}((L^{\alpha}_{\beta,n})^k)$ *will consist of terms in* D *and terms in* Z, *with a sequence of runs* J *recording the former, and a sequence of runs* R *recording the latter*.

Proof of Claim 3.15.2: As before, we note that

$$(\widetilde{L}^{a}_{\beta,n})_{\mathcal{I}} = \left(\left(D + \frac{1}{\sqrt{n\beta}} Z \right) \left(D + \frac{1}{\sqrt{n\beta}} Z \right)^T \right)_{\mathcal{I}} = \sum_{(J,R) \in \mathcal{J}} \frac{1}{(n\beta)^{P/2}} (D)_J (Z)_R, \tag{27}$$

with $P = p_2 - p_1 + 1 + \cdots + p_{2q} - p_{2q-1} + 1$.

Similarly with (26), write

$$E[(\eta_{k,\gamma}(n))^l] = \sum_{\substack{\mathcal{I}_j \in \mathcal{S}_{n,k} \\ 1 \leqslant j \leqslant l}} \sum_{(J_j,R_j) \in \mathcal{J}_j} \frac{1}{(n\beta)^q} \left(\prod_{j=1}^{l} (D)_{J_j} \right) E\left[\prod_{j=1}^{l} ((Z)_{R_j} - E[(Z)_{R_j}]) \right], \tag{28}$$

with $q=q(\mathcal{I}_1,\ldots,\mathcal{I}_l):=\Sigma_j P_j/2$.

The rest of the argument follows in the footsteps of the proof of Claim 3.2.1. Just as before, it can be shown that the only terms with significant contribution are those for which, for each j, $(Z)_{R_j}$ consists of a single term, and, in addition to that, the set of R_j's can be split in pairs (R_{j_1},R_{j_2}) such that $(Z)_{R_{j_1}}=(Z)_{R_{j_2}}$. This yields

$$\lim_{n\to\infty} E[(\eta_{k,\gamma}(n))^{2p+1}]=0.$$

Also, if l is even, the argument that we can consider only the terms for which there is an $l/2$-tuple $(i_1,\ldots,i_{l/2})$ which "avoids" the upper and lower corners of the matrix (like in Lemmas 3.13 and 3.14) still applies.

The one way in which this computation differs from the one we made for the proof of Claim 3.2.1 lies in the fact that approximating $(D)_J$, given an index i_1 present in J, becomes a little trickier, since the diagonal and off-diagonal elements will approximate, respectively, to $\sqrt{\gamma}\sqrt{1/\gamma-i/n}$ and $\sqrt{\gamma}\sqrt{1-i/n}$.

Thus, one more parameter will become important, namely, the number of off-diagonal terms in each $(D)_{J_j}$. Note that in each sequence $\mathcal{I}$ we must have an *even* number $2s$ of off-diagonal terms (either from D or from Z), since $i_1-i_2+\cdots+i_{2k}-i_1=0$, and this also implies that we have an even number $2(k-s)$ of diagonal terms.

1. Suppose we fix the term in Z_{R_j} to be the diagonal term $z_{i,i}$; to how many sequences $\mathcal{I}$ with a fixed number $2s$ of off-diagonal terms can this correspond? The answer is $2(k-s)\ \binom{k}{s}^2$; we have $\binom{k}{s}$ ways of picking the off-diagonal terms (because of the alternating property), and once those are picked we have $2(k-s)$ choices for the location of $z_{i,i}$ among the diagonal terms remaining; this determines the sequence uniquely.

Each such sequence will have asymptotical weight

$$(D)_J\sim\gamma^{k-1/2}\left(\frac{1}{\gamma}-\frac{i}{n}\right)^{k-s-1/2}\left(1-\frac{i}{n}\right)^{s}.$$

2. Suppose we now fix the term in Z_{R_j} to be the off-diagonal term $z_{i+1,i}$; to how many sequences $\mathcal{I}$ with a fixed number $2s$ of off-diagonal terms can this correspond? The answer is $2s\ \binom{k}{s}^2$; we have $\binom{k}{s}$ ways of picking the off-diagonal terms (because of the alternating property), and once those are picked we have $2s$ choices for the location of $z_{i+1,i}$ among them.

Each such sequence will have asymptotical weight

$$(D)_J\sim\gamma^{k-1/2}\left(\frac{1}{\gamma}-\frac{i}{n}\right)^{k-s}\left(1-\frac{i}{n}\right)^{s-1/2}.$$

Finally, using the binomial formula

$$\left(\frac{1}{\gamma}-\frac{t}{n}\right)^{s-1}=\sum_{i=0}^{s-1}(-1)^i\binom{s-1}{i}\gamma^{-s+1-i}\left(\frac{t}{n}\right)^i,$$

and after some processing and use of the Riemann-sum and Beta-function formula

$$\lim_{n\to\infty}\frac{1}{n}\sum_{t=0}^{n}\left(1-\frac{t}{n}\right)^{2k-r-s}\left(\frac{t}{n}\right)^{r+s-1}=\int_0^1(1-x)^{2k-r-s}x^{r+s-1}\mathrm{d}x=\frac{(2k-r-s)!(r+s-1)!}{(2k)!},$$

combined with all the possible pairings of the R_j's (which yields the necessary $(l-1)!!$), we obtain the result of claim 3.15.1. □

Claim 3.15.2 has a similar proof.

Remark 3.20: As in Sec. III A, we never actually use the full power of the fact that the entries of the bidiagonal matrix Z tend to independent centered ***normal*** *variables. We only used the following three properties:*

- $E[Z_{i,i}]=E[Z_{i+1,i}]=0$;
- $\lim_{n\to\infty} Var[Z_{i+1,i}]=\lim_{n\to\infty} Var[Z_{i,i}]=\frac{\gamma}{2}$;
- *for any* k, *there exists a number* $M_k>0$ *such that* $|E[(Z_{i,j})^k]|<M_k$, *for all* $1\leqslant i,j\leqslant n$ (*boundedness of moments*).

IV. A MORE GENERAL SETTING

We present here a way to generalize the "non-random matrix+small random fluctuation" decompositions we have used in Sec. III in order to analyze the deviation and fluctuation from the asymptotical law for the eigenvalue density in the case of the Hermite and Laguerre β-ensembles.

A. Tridiagonals

Let f and g be two integrable functions $f,g:[0,1]\to\mathbb{R}$ such that the integrals $\int_0^1 f^a(x)g^b(x)\mathrm{d}x$ exist for all $a,b\in\mathbb{N}$, and such that the quantities

$$m_k := \sum_{r=0}^{\lfloor k/2\rfloor} \binom{k}{r,r,k-2r} \int_0^1 f^{k-2r}(x)g^{2r}(x)\mathrm{d}x \tag{29}$$

are the moments of a (uniquely determined) distribution ρ, defined on a compact $[a,b]$.

For any $n\in\mathbb{R}$, we then consider the $n\times n$ matrix F_T:

$$F_T=\begin{pmatrix} f\left(\frac{n}{n}\right) & g\left(\frac{n-1}{n}\right) & & & & & \\ g\left(\frac{n-1}{n}\right) & f\left(\frac{n-1}{n}\right) & g\left(\frac{n-2}{n}\right) & & & & \\ & g\left(\frac{n-2}{n}\right) & \ddots & \ddots & & & \\ & & & \ddots & \ddots & g\left(\frac{1}{n}\right) & \\ & & & & g\left(\frac{1}{n}\right) & f\left(\frac{1}{n}\right) & \end{pmatrix},$$

so the diagonal of F_T is an equidiscretization of f with step $1/n$ (with the exception of the endpoint at 0, which is missing), and the off-diagonal is an equidiscretization of g with step $1/n$ (missing both the endpoint at 1 and the one at 0).

We consider the tridiagonal symmetric matrix

$$R_T=\begin{pmatrix} x_n & y_{n-1} & & & & & \\ y_{n-1} & x_{n-1} & y_{n-2} & & & & \\ & y_{n-2} & \ddots & \ddots & & & \\ & & \ddots & \ddots & y_2 & & \\ & & & y_2 & x_2 & y_1 & \\ & & & & y_1 & x_1 & \end{pmatrix},$$

with the variables x_i and y_j being mutually independent and satisfying the following three properties:

- $E[x_i]=E[y_j]=0$, for all $1\leqslant i\leqslant n$, $1\leqslant j\leqslant n-1$,
- $\mathrm{Var}[x_i]=\sigma^2$, for all $1\leqslant i\leqslant n$, and $\mathrm{Var}[y_j]=\eta^2$, for all $1\leqslant j\leqslant n-1$,

- for all k there exists a $M_k > 0$ such that $|E[(x_i)^k]| < M_k$ and $|E[(y_j)^k]| < M_k$, for all $1 \leqslant i \leqslant n$, $1 \leqslant j \leqslant n-1$.

Note that F_T is non-random matrix, while R_T is a random one.

Now we consider the matrix model

$$M_T = F_T + \frac{1}{\sqrt{n}} R_T. \tag{30}$$

We will compute the asymptotical eigenvalue distribution, the first-order deviation from it, and the first-order fluctuation for the random matrix M_T.

We need two more definitions.

Definition 4.1: Let P be a path on the lattice $\mathbb{Z}^2$, *starting at* $(0,0)$ *and ending at* $(k,0)$, *with up* $((x,y) \to (x+1,y+1))$, *down* $((x,y) \to (x+1,y-1))$, *and level* $((x,y) \to (x+1,y))$ *steps. For each level* $j \in \mathbb{Z}$, *we define the quantities* $a_j(P)$ *and* $b_j(P)$, *as follows:*

$$a_j(P) := \#\ \textit{of level steps from } j \textit{ to } j;$$

$$b_j(P) := \#\ \textit{of down steps from } j \textit{ to } j-1.$$

Note that, since the path P ends at $(k,0)$, *the number of up steps it takes must always equal the number of down steps it takes.*

Also let

$$\mathcal{P}_{r,k} := \{\textit{paths from } (0,0) \textit{ to } (k,0) \textit{ with exactly } r \textit{ down steps}\},$$

$$\mathcal{P}_{r,k,i} := \{\textit{paths in } \mathcal{P}_{r,k} \textit{ which descend to, but not below, } y = -i\},$$

$$p_{r,k,i} := |\mathcal{P}_{r,k,i}|,$$

$$\mathcal{P}_k := \cup_{r=0}^{\lfloor k/2 \rfloor} \mathcal{P}_{r,k}.$$

Theorem 4.2: *Let* M_T *be a matrix from the ensemble defined by* (30), *of size n, with eigenvalues* $(\lambda_1, \ldots, \lambda_n)$, *and let* $k \geqslant 1$ *be a positive integer. For all* $i = 1, \ldots, k$, *let*

$$\begin{aligned}
\mu_i = \sum_{r=0}^{\lfloor i/2 \rfloor} \Bigg(& f(1)^{i-2r} g(1)^{2r} \left(\sum_{j=0}^{r-1} (r-j) p_{k,j,r} - \frac{1}{2} \binom{i}{r,r,i-2r} \right) + f(0)^{i-2r} g(0)^{2r} \left(\sum_{j=0}^{r-1} (r-j) p_{i,j,r} \right. \\
& \left. - \frac{3}{2} \binom{i}{r,r,i-2r} \right) \Bigg) - \sum_{P \in \mathcal{P}_{r,i}} \sum_{j \in \mathbb{Z}} j a_j(P) \int_0^1 f^{i-2r-1}(t) g^{2r}(t) f'(t) \mathrm{d}t \\
& - 2 \sum_{P \in \mathcal{P}_{r,i}} \sum_{j \in \mathbb{Z}} j b_j(P) \int_0^1 f^{i-2r}(t) g^{2r-1}(t) g'(t) \mathrm{d}t + \sigma^2 \left(\sum_{P \in \mathcal{P}_{r,i}} \sum_{j \in \mathbb{Z}} \binom{a_j(P)}{2} \right) \int_0^1 f^{i-2r-2}(t) g^{2r}(t) \mathrm{d}t \\
& + \eta^2 \left(\sum_{P \in \mathcal{P}_{r,i}} \sum_{j \in \mathbb{Z}} \binom{2b_j(P)}{2} \right) \int_0^1 f^{i-2r}(t) g^{2r-2}(t) \mathrm{d}t.
\end{aligned}$$

Also, for any $1 \leqslant i \leqslant k$, *let*

$$X_i = \mathrm{tr}((M_T)^i) - n \int_a^b x^i \rho(x) \mathrm{d}x - \mu_i,$$

$$\equiv \sum_{j=1}^{n} \lambda_j^i - n \int_a^b x^i \rho(x) \mathrm{d}x - \mu_i$$

Let $(Y_1, Y_2, \ldots, Y_k)$ *be a centered multivariate Gaussian with covariance matrix*

$$\mathrm{Cov}(Y_i,Y_j)=\sigma^2\sum_{\substack{0\leqslant r\leqslant \lfloor i/2\rfloor -1\\ 0\leqslant s\leqslant \lfloor j/2\rfloor -1}}(i-2r)(j-2s)\binom{i}{r,r,i-2r}\binom{j}{s,s,j-2s}\int_0^1 f^{A(r,s)}(x)g^{B(r,s)}(x)\mathrm{d}x$$
$$+\eta^2\sum_{\substack{1\leqslant r\leqslant \lfloor i/2\rfloor \\ 1\leqslant s\leqslant \lfloor j/2\rfloor}}4rs\binom{i}{r,r,i-2r}\binom{j}{s,s,j-2s}\int_0^1 f^{C(r,s)}(x)g^{D(r,s)}(x)\mathrm{d}x,$$

where $A(r,s)=i-2r+j-2s-2$, $B(r,s)=2r+2s$, $C(r,s)=2r+2s-2$, *and* $D(r,s)=i-2r+j-2s$.

Then, as $n\to\infty$,

$$(X_1,X_2,\ldots,X_k)\Rightarrow(Y_1,Y_2,\ldots,Y_k).$$

Proof: A technical but simple calculation in the spirit of the ones performed in Sec. III A shows that m_k are the moments of the asymptotic level density, via the expansion of $\mathrm{tr}(M_T^k)$ as a sum of products of the entries of M_T and separation of the zero-order term. Furthermore, examining the first-order terms in this expansion yields the covariance result, using the same counting techniques as in Sec. III A.

Computing the first-order deviation from the mean is slightly more complicated, as first-order terms in the expansion come from four sources; we only enumerate these sources here and indicate how they play a part in the total sum.

We begin with expressing

$$E[\mathrm{tr}(M_T^k)]=E\left[\mathrm{tr}\left(\left(F_T+\frac{1}{\sqrt{n}}R_T\right)^k\right)\right]=E\left[\sum_{\mathcal{I}\in S_{n,k}}(M_T)_{\mathcal{I}}\right]=E\left[\sum_{\mathcal{I}\in S_{n,k}}\sum_{(J,R)\in\mathcal{J}}\frac{1}{n^{P/2}}(F_T)_J(R_T)_R\right],$$

where we have used the notation of Sec. III A.

It is easy to prove, like we did in Sec. III A, that the zero-order terms are given by the pairs (J,R) where $R=\emptyset$, that the terms $(R_T)_R$ which contain a single variable (at first power) are annihilated by the expectation (since all variables in R_T are centered), and that the terms where $(R_T)_R$ contains three or more variables (counting multiplicities) do not contribute to the first-order deviation.

To each sequence $\mathcal{I}$ (recall that $\mathcal{I}=(i_1,\ldots,i_k)$ with $|i_j-i_{j+1}|\in\{0,1\}$ for $1\leqslant i\leqslant k-1$ and $|i_k-i_1|\in\{0,1\}$) we associate in a one-to-one fashion, a path from (0,0) to $(k,0)$ taking steps up, down, or level (depending on the nest term being larger, smaller, or equal to the current one). The zero-order terms sum asymptotically to m_k (with the integral being obtained from the Riemann sum and with $\binom{k}{r,r,k-2r}=|\mathcal{P}_k|$).

Three of the first-order term sources come from those terms that have $|R|=\emptyset$, while the fourth comes from the terms for which $(R_T)_R$ contains a single variable, at the second power. Note also that the terms for which $(R_T)_R$ contains two different variables will be annihilated by the expection.

Source 1. In the zero-order count, we ignore the fact that at the "edges," i.e., upper left corner, corresponding to $i_1\in\{1,\ldots,\lfloor k/2\rfloor\}$, and lower right corner, corresponding to $i_1\in\{n-\lfloor k/2\rfloor,\ldots,n\}$, not all paths in $\mathcal{P}_{k,r}$ can appear in the sum. This approximation yields a first-order term which is asymptotically equal to

$$S_1:=\sum_{r=0}^{\lfloor k/2\rfloor}\left((f(1)^{k-2r}g(1)^{2r}+f(0)^{k-2r}g(0)^{2r})\left(\sum_{i=0}^{r-1}(r-i)p_{k,i,r}-\binom{k}{r,r,k-2r}\right)\right).$$

Source 2. In the zero-order approximation, we approximate the value of the integral $\int_0^1 f^{k-2r}(x)g^{2r}(x)\mathrm{d}x$ by the Riemann sum $(1/n)\Sigma_{i=0}^n f(i/n)^{k-2r}\,g(i/n)^{2r}$. Using the Euler-Maclauren formula, this yields a first-order term asymptotically equal to

$$S_2 := \sum_{r=0}^{\lfloor k/2 \rfloor} \frac{1}{2} \binom{k}{r,r,k-2r} (f(1)^{k-2r} g(1)^{2r} - f(0)^{k-2r} g(0)^{2r}).$$

Source 3. Finally, in the zero-order approximation, we replace $f((i-j)/n)$ and $g((i-j)/n)$ by $f(i/n)$, respectively $g(i/n)$ for each $j \in \{-k, \ldots, k\}$. A Taylor series approximation and the counting of terms shows that this way we need to subtract off haveing a first-order term which is asymptotically

$$S_3 := \sum_{r=0}^{\lfloor k/2 \rfloor} \sum_{P \in \mathcal{P}_{r,k}} \sum_{j \in \mathbb{Z}} \left(j a_j(P) \int_0^1 f^{k-2r-1}(t) g^{2r}(t) f'(t) \mathrm{d}t - 2 j b_j(P) \int_0^1 f^{k-2r}(t) g^{2r-1}(t) g'(t) \mathrm{d}t \right).$$

Source 4. The last source of first-order terms comes from the terms in which $(R_T)_R$ contains a single variable at the second power, and its contribution is asymptotically equal to

$$S_4 := \sigma^2 \left(\sum_{P \in \mathcal{P}_{r,k}} \sum_{j \in \mathbb{Z}} \binom{a_j(P)}{2} \right) \int_0^1 f^{k-2r-2}(t) g^{2r}(t) \mathrm{d}t + \eta^2 \left(\sum_{P \in \mathcal{P}_{r,k}} \sum_{j \in \mathbb{Z}} \binom{2b_j(P)}{2} \right) \int_0^1 f^{k-2r}(t) g^{2r-2}(t) \mathrm{d}t.$$

Finally, adding S_1, S_2, S_3, and S_4 yields the statement of Theorem 4.2. □

Remark 4.3: Note that when $f(x)=\sqrt{x}/2$, $g(x)=0$ *for all* $x \in [0,1]$, $\sigma^2 = 1/(2\beta)$, *and* $\eta^2 = 1/(8\beta)$, *both the level density asymptotics* **and** *the covariance matrix for the fluctuations are the same as for the* β*-Hermite ensemble of Sec. III A.*

Crucially, the deviation is **different**. *The reason is that in the approximation*

$$E\left[\tfrac{1}{2}\chi_{(n-i)\beta}\right] \sim \tfrac{1}{2}\sqrt{(n-i)\beta},$$

the next order term is of order $1/\sqrt{(n-i)\beta}$, *which plays a part in computing the deviation.*

We remind the reader that we computed the deviation for the β*-Hermite ensembles by using the palindromic property of expectations of trace, thus reducing the problem to computing the deviation for the "*$\beta=\infty$*" case, for which we used Hermite polynomials properties. This allowed us to find the distribution behind the moments of the deviation.*

B. Bidiagonals

Let f and g be two integrable functions, $f, g, : [0,1] \to \mathbb{R}$, such that the integrals $\int_0^1 f^a(x) g^b(x) \mathrm{d}x$ exist for all $a, b \in \mathbb{N}$, and such that the quantities

$$\tilde{m}_k := \sum_{r=0}^{k} \binom{k}{r}^2 \int_0^1 f^{2r}(x) g^{2(k-r)}(x) \mathrm{d}x$$

are the moments of a (uniquely determined) distribution ν defined on $[a,b]$.

For any $n \in \mathbb{N}$, we consider the $n \times n$ matrix F_B, defined in the following:

$$F_B = \begin{pmatrix} f\left(\frac{n}{n}\right) & & & \\ g\left(\frac{n-1}{n}\right) & f\left(\frac{n-1}{n}\right) & & \\ & \ddots & \ddots & \\ & & g\left(\frac{1}{n}\right) & f\left(\frac{1}{n}\right) \end{pmatrix},$$

in other words the diagonal of F_B is an equidiscretization of f with step $1/n$ (with the exception of the endpoint at 0, which is missing), and the subdiagonal is an equidiscretization of g with step $1/n$ (missing both the endpoint at 0 and the one at 1).

We next consider the random bidiagonal matrix

$$R_B = \begin{pmatrix} x_n & & & \\ y_{n-1} & x_{n-1} & & \\ & \ddots & \ddots & \\ & & y_1 & x_1 \end{pmatrix},$$

where the variables x_i, y_j are mutually independent and satisfying the following properties:

- $E[x_i]=E[y_j]=0$ for all $1\leqslant i\leqslant n$, $1\leqslant j\leqslant n-1$,
- $\mathrm{Var}[x_i]=\sigma^2$ for all $1\leqslant i\leqslant n$ and $\mathrm{Var}[y_j]=\eta^2$, for all $1\leqslant j\leqslant n-1$,
- for all k there is a constant $M_k>0$ such that $|E[(x_i)^k]|<M_k$ and $|E[(y_j)^k]|<M_k$ for all $1\leqslant i\leqslant n$ and $1\leqslant j\leqslant n-1$.

Finally, consider the matrix

$$M_L = M_B M_B^T, \tag{31}$$

with

$$M_B = F_B + \frac{1}{\sqrt{n}} R_B.$$

Note that while F_B is a non-random matrix, R_B, M_B, and M_L are random.

We will compute the asymptotical level density and the first-order deviation and fluctuation for the random matrix M_L.

We need to define the following quantities.

Definition 4.4: Let Q be a path on the lattice $\mathbb{Z}^2$, starting at $(0,0)$ and ending at $(2k,0)$, with up $((x,y)\to(x+1,y+1))$, down $((x,y)\to(x+1,y-1))$, and level $((x,y)\to(x+1,y))$ steps. In addition, we require that the path is alternating, i.e., on each odd-numbered step (first, third, etc.) the path is only allowed to go down or stay at the same level, whereas on each even-numbered step (second, fourth, etc.), the path is allowed only to go up or stay at the same level.

For each level $j\in\mathbb{Z}$, we define the quantities $c_j(Q)$ and $d_j(Q)$, as follows:

$$c_j(Q) := \#\text{ of level steps from } j \text{ to } j,$$
$$d_j(Q) := \#\text{ of down steps from } j \text{ to } j-1.$$

Note that, since the path Q ends at $(2k,0)$, the number of up steps it takes must always equal the number of down steps it takes.

Also let

$$\mathcal{Q}_{r,k} := \{\text{alternating paths from } (0,0) \text{ to } (2k,0) \text{ with exactly } r \text{ down steps}\},$$
$$\mathcal{Q}_{r,k,i} := \{\text{alternating paths in } \mathcal{Q}_{r,k} \text{ which descends to, but not below, } y=-i\},$$
$$q_{r,k,i} := |\mathcal{Q}_{r,k,i}|,$$
$$\mathcal{Q}_k := \cup_{r=0}^{k}\mathcal{Q}_{r,k}.$$

Theorem 4.5: *Let M_L be the matrix from the ensembles defined by* (31)*, of size n, with eigenvalues $(\lambda_1,\ldots,\lambda_n)$, and let $k\geqslant 1$ be a positive integer. For all $1\leqslant i\leqslant k$, let*

$$\begin{aligned}\tilde{\mu}_i = &\sum_{r=0}^{i}\left(f(1)^{2i-2r}g(1)^{2r}\left(\sum_{j=0}^{r-1}(r-i)q_{i,j,r}-\frac{1}{2}\binom{i}{r}^2\right)+f(0)^{2i-2r}g(0)^{2r}\left(\sum_{j=0}^{r-1}(r-j)q_{i,j,r}-\frac{3}{2}\binom{i}{r,r}^2\right)\right)\\ &-\sum_{Q\in\mathcal{Q}_{r,i}}\sum_{j\in\mathbb{Z}}jc_j(Q)\int_0^1 f^{2i-2r-1}(t)g^{2r}(t)f'(t)\mathrm{d}t-2\sum_{Q\in\mathcal{Q}_{r,i}}\sum_{j\in\mathbb{Z}}jd_j(Q)\int_0^1 f^{2i-2r}(t)g^{2r-1}(t)g'(t)\mathrm{d}t\\ &+\sigma^2\left(\sum_{Q\in\mathcal{Q}_{r,i}}\sum_{j\in\mathbb{Z}}\binom{c_j(Q)}{2}\right)\int_0^1 f^{2i-2r-2}(t)g^{2r}(t)\mathrm{d}t\end{aligned}$$

$$+\eta^2\left(\sum_{Q\in\mathcal{Q}_{r,i}}\sum_{j\in\mathbb{Z}}\binom{2d_j(Q)}{2}\right)\int_0^1 f^{2i-2r}(t)g^{2r-2}(t)\mathrm{d}t.$$

Also, for for any $1\leqslant i\leqslant k$, *let*

$$X_i=\mathrm{tr}((M_l)^i)-n\int_a^b x^i\nu(x)\mathrm{d}x-\tilde{\mu}_i,$$

$$\equiv\sum_{j=1}^{i}\lambda_j^i-n\int_a^b x^i\nu(x)\mathrm{d}x-\tilde{\mu}_i.$$

Let $(Y_1,Y_2,\ldots,Y_k)$ *be a centered multivariate Gaussian with covariance matrix*

$$\mathrm{Cov}(x^i,x^j)=4\sigma^2\sum_{\substack{1\leqslant r\leqslant i\\1\leqslant s\leqslant j}}rs\binom{i}{r}^2\binom{j}{s}^2\int_0^1 f^{A(r,s)}(x)g^{B(r,s)}(x)\mathrm{d}x+4\eta^2\sum_{\substack{0\leqslant r\leqslant i-1\\0\leqslant s\leqslant j-1}}(i-r)(j-s)$$
$$\times\binom{i}{r}^2\binom{j}{s}^2\int_0^1 f^{A(r,s)+2}(x)g^{B(r,s)-2}(x)\mathrm{d}x,$$

with $A(r,s)=2(r+s-1)$ *and* $B(r,s)=2(i+j-r-s)$.

Then, as $n\to n$,

$$(X_1,X_2,\ldots,X_k)\Rightarrow(Y_1,Y_2,\ldots,Y_k).$$

Proof: The proof of Theorem 4.5 is based on the same calculations as Theorem 4.2. The covariance can be computed using the same general principles as in Sec. III B, and the examination of the zero-order and first-order terms in the mean can be done as in Sec. IV B. Moreover, the sources of the first-order terms are the same as in Sec. IV B; it is only the type of path we are counting that changes (from paths of length k to alternating paths of length $2k$). □

Remark 4.6: Note that when $f=\sqrt{1/\gamma-1+x}$, $g=\sqrt{x}$, $\sigma^2=\eta^2=\gamma/(2\beta)$, *both the level density asymptotics* and *the covariance matrix for the fluctuations are the same as for the* β*-Laguerre ensemble of Sec. III B.*

Once again, the deviation is ***different****, for the same reason as in Sec. IV B: in the approximation* $E\left[\frac{1}{2}\chi_{(n-i)\beta}\right]\sim\frac{1}{2}\sqrt{(n-i)\beta}$ *the next order term is of order* $1/\sqrt{(n-i)\beta}$, *which plays a part in computing the deviation.*

We computed the deviation for the β*-Laguerre ensembles by using the palindromic property of expectations of trace, thus reducing the problem to computing the deviation for the "*$\beta=\infty$*" case, for which we used Laguerre polynomials properties. This allowed us to find the distribution behind the moments of the deviation.*

V. HISTOGRAMMING EIGENVALUES EFFICIENTLY

We propose a very effective numerical trick for counting the number of eigenvalues in an interval numerically. This method does not require the computation of eigenvalues and requires a number of operations that is $O(n)$, rather than $O(n^2)$, which allows for counts for matrices of a very large size. The method is the standard Sturm sequence method for tridiagonal symmetric matrices. We take as input D, a vector of length n, which is the diagonal of the matrix, and E, a vector of length $n-1$, the squares of the elements on the super or subdiagonal. This avoids unnecessary square roots in the formation of the matrix which can slow down computation.

The algorithm is remarkably simple. For a given value σ, which is not an eigenvalue of the matrix, compute

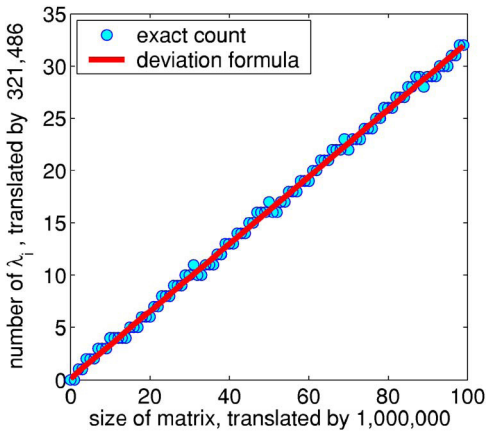

FIG. 2. (Color online) Calculating the deviation in the interval $I=[0.2,0.8]$ for the $\beta=\infty$ Hermite ensemble with sizes $10^6:1:(10^6+99)$; circles represent the eigenvalue count minus the area under the semicircle over I; the solid line is the theoretical deviation given in (33).

$$t_i := D_i - \sigma - E_{i-1}/t_{i-1}$$

for $t=1$ through n with $t_0=1$ and $E_0=0$.

From Sturm's theorem (see, for example Ref. 17, Theorem 13) we know that the number of eigenvalues of the tridiagonal matrix less than or equal to σ is the number of t_i's that are negative, with $1 \leqslant i \leqslant n$.

To histogram eigenvalues of β ensembles for n's into the millions or even the billions, one can simply compute E from a chi-square random number generator (implemented in MATLAB's Statistics Toolbox as `chi2rnd`), and D from a normal random number generator for the β-Hermite case (`randn`) or from another chi-square in the β-Laguerre case.

An interesting special case is the β-Hermite case with $\beta=\infty$, which computes the roots of the corresponding scaled Hermite polynomial. This may be performed by taking D to be the zero vector of length n and $E=(n-1,n-2,\ldots,2,1)/(4n)$.

When $\beta=\infty$, there is no fluctuation, but there are deviations for large n. The Sturm theorem roughly states that the number of eigenvalues in an interval I is linear of the form

$$(\#\ \text{eigenvalues}) = n(\text{area under the semicircle}) + DEVIATION, \tag{32}$$

where

$$DEVIATION = \frac{1}{2\pi}\arcsin(x)\Big|_I \tag{33}$$

and we subtract $1/4$ if I contains $+1$ and $1/4$ if I contains -1.

In one numerical experiment (see Fig. 2), we took $n=1\,000\,000+i$ for $i=0,1,\ldots,99$ and computed the deviation from the mean, i.e., the number of eigenvalues in the interval I minus the area

$$A = n\frac{1}{2\pi}\int_I \sqrt{1-x^2}\mathrm{d}x;$$

we did this arbitrarily for the interval $I=[0.2,0.8]$. Since this experiment is non-random it is repeatable without any reference to a random number generator. We found the experimental deviation of 0.1167 which is close to the theoretical deviation of 0.1155, given by (33).

Figure 2 plots the results of the experiment. The red line which contains the theoretical value of the intercept represents the best fit line to the data in the sense that the average vertical deviation is minimized.

VI. REMARKS AND OPEN PROBLEMS

There are many object-counting (combinatorial) approaches to the study of traces of powers of random matrices; they depend on the matrix model, and on the polynomial whose trace is being computed. For example, the counting approach of Ref. 34 uses full matrix models (all entries are non-zero variables), and traces of powers (thus using the monomial basis, like we have done here), and counts paths in the complete graph of size n. By contrast, in Ref. 26, the polynomials used are the shifted Chebyshev polynomials, and the objects counted are non-crossing annular partitions; the matrix models are still full. Here, we use tri/bidiagonal matrix models, consider the monomials, and count essentially paths with three types of steps (up, down, level) in the plane.

Though the objects we count here are simpler than in Ref. 26, our counting technique expresses the results in a less compact form than in Refs. 21 and 26. In the latter two papers, the covariance matrix is diagonalized by the choice of polynomial basis, whereas in our paper it is obtained as full because we work with the monomials. There seems to be a trade-off between the simplicity of the object to be counted and the simplicity of the form in which the covariance matrix is expressed.

We would like to conjecture that by using a hybrid way of counting, for example, using the tridiagonal matrices and some of the techniques of Ref. 26, both the counting process and the resulting format of the answer could be simplified. The development of such a technique would be of great interest.

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On the Birkhoff factorization problem for the Heisenberg magnet and nonlinear Schrödinger equations

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A geometrical description of the Heisenberg magnet (HM) equation with classical spins is given in terms of flows on the quotient space G/H_+, where G is an infinite dimensional Lie group and H_+ is a subgroup of G. It is shown that the HM flows are induced by an action of $\mathbb{R}^2$ on G/H_+, and that the HM equation can be integrated by solving a Birkhoff factorization problem for G. For the HM flows that are Laurent polynomials in the spectral variable, we derive an algebraic transformation between solutions of the nonlinear Schrödinger (NLS) and Heisenberg magnet equation. The Birkhoff factorization problem for G is treated in terms of the geometry of the Segal-Wilson Grassmannian $\mathrm{Gr}(H)$. The solution of the problem is given in terms of a pair of Baker functions for special subspaces in $\mathrm{Gr}(H)$. The Baker functions are constructed explicitly for subspaces that yield multisoliton solutions of NLS and HM equations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

From the work of Zakharov-Shabat[1] and Sato-Segal-Wilson,[2] it is known that completely integrable partial differential equations, such as the Korteweg-de Vries (KdV) or the nonlinear Schrödinger (NLS) equation, are related with loop groups and infinite dimensional Grassmannians. Our aim in this paper is to describe the Heisenberg magnet (HM) equation,

$$\frac{\partial \vec{S}}{\partial t} = \vec{S} \times \frac{\partial^2 \vec{S}}{\partial x^2}, \quad S_1^2 + S_2^2 + S_3^2 = 1, \tag{1}$$

in the context of loop groups, and to explore the construction of its solutions from the point of view that is close to that of Segal-Wilson's work on KdV. The HM equation is a completely integrable system for which integrability was proved in Ref. 3 and the inverse scattering transform was developed in Ref. 4. Equation (1) is the isotropic case of the Landau-Lifshitz (LL) equation, $\vec{S}_t = \vec{S} \times \vec{S}_{xx} + \vec{S} \times J\vec{S}$, when the interaction constants are given by $J = \mathrm{diag}(J_0, J_0, J_0)$. The LL model was studied by a number of authors. In Ref. 5, it was integrated by the Riemann factorization problem on a torus. Soliton solutions using the dressing procedure and real algebraic-geometric solutions using theta functions were found in Refs. 6 and 7. For a historical account of the HM and LL equations, see Ref. 8. For our consideration of particular interest is the work by Carrey *et al.*,[9] in which a spectral curve for the zero-curvature form of the LL hierarchy was introduced. The authors show that the LL flows are induced by a group action on an infinite dimensional homogeneous space, and that solutions of the LL hierarchy can be constructed by an analog of Birkhoff factorization for elliptic curves. However, the factorization problem is fairly difficult to solve explicitly which poses an obstacle in computing the flows. The motivation for the present work stems from the fact that the computation of the HM flows is reduced to solving a Birkhoff factorization for a subgroup of $\Lambda GL(2,\mathbb{C})$, $GL(2,\mathbb{C})$-valued loops defined on the unit circle. This has the consequence that the homogeneous space on which the HM flows are defined is closely

related to the Segal-Wilson Grassmannian. We study solutions of the HM equation in terms of the geometry of the Grassmannian, and explore its relation to solutions of the focusing NLS equation. We show that solutions of the NLS equation can be expressed in terms of the Baker functions for certain subspaces of the Grassmannian. By using the gauge transformation between the NLS and HM equations, one can associate these subspaces to solutions of the HM equation. We also exhibit subspaces that yield multisoliton solutions of NLS and find an algebraic transformation that maps these solutions to multisoliton solutions of HM.

The paper is organized as follows. In Sec. II we give a brief account of the group theoretic approach to integrable systems. We describe a general construction of partial differential equations that can be formulated as the zero-curvature condition on the Lie algebra of a Banach-Lie group G. The solutions of such equations are represented by flows induced by an action of $\mathbb{R}^n$ on an infinite dimensional homogeneous space. The flows can be integrated by solving a Birkhoff factorization problem for G. In Sec. III we discuss the HM equation within the framework of Sec. II. We define a loop group $G \subset \Lambda GL(2,\mathbb{C})$ and show that the HM flows are induced by an action of $\mathbb{R}^n$ on the homogeneous space G/H_+, where H_+ is a subgroup of "positive" loops in G. We also show that by choosing a different subgroup $G_+ \subset G$ the action induces the NLS flows on G/G_+ that are related with the HM flows by a gauge transformation. This transformation is interpreted as a map between the quotient spaces $\Gamma: G/G_+ \to G/H_+$. We show that if the NLS flows are Laurent polynomials in the spectral variable $z \in S^1$, then Γ is an algebraic transformation between the NLS and HM solutions. In Sec. IV we describe a method for solving the Birkhoff factorization problem for NLS by modeling the space G/G_+ as the Segal-Wilson Grassmannian $\mathrm{Gr}(H)$ of the Hilbert space $H=L^2(S^1,\mathbb{C}^2)$. We associate subspaces in $\mathrm{Gr}(H)$ to solutions of NLS and show that the NLS flows can be computed explicitly in terms of a pair of Baker functions for such subspaces. By modifying the ideas from Ref. 2 we construct subspaces that yield the multisoliton solutions of NLS. These solutions are then mapped to the multisoliton solutions of HM by the transformation Γ.

II. GROUP THEORETIC FORMULATION OF INTEGRABLE SYSTEMS

In this section we give a brief account of the group theoretic construction of integrable systems that admit the zero-curvature representation. A more detailed discussion of the subject can be found, for example, in Ref. 10.

Definition 1: Let G be a Banach Lie group. We say that G admits a Birkhoff factorization denoted (G,G_-,G_+) *if G contains closed subgroups* G_- *and* G_+ *such that* $G_- \cap G_+ = \{e\}$ *and the product* G_-G_+ *is open in G.*

Let $\mathfrak{g}$ be the Lie algebra of G with the Lie bracket $[\cdot,\cdot]$. The set G_-G_+ is open in G if and only if $\mathfrak{g}$ splits into a direct sum of subalgebras $\mathfrak{g}=\mathfrak{g}_- \oplus \mathfrak{g}_+$, where $\mathfrak{g}_\pm$ is the Lie algebra of $G_\pm$. The Birkhoff factorization is modeled to generalize the factorization of $GL(n,\mathbb{C})$ into upper and lower triangular matrices to infinite dimensions. Let $X_1, X_2, \ldots, X_n$ be pairwise commuting elements of $\mathfrak{g}_+$, $[X_i, X_j]=0$, and consider a differentiable action $\mathbb{R}^n \times G \to G$ defined by

$$\mathbf{t} * g = \exp\left(\sum_{i=1}^{n} t_i X_i\right) g, \tag{2}$$

where $\mathbf{t}=(t_1,t_2,\ldots,t_n)$. If $g \in G_-G_+$, then for $\mathbf{t}$ in a neighborhood of $0 \in \mathbb{R}^n$ we have $\mathbf{t}*g \in G_-G_+$ because G_-G_+ is open in G. Hence, $\mathbf{t}*g$ can be factored in a unique way as

$$\mathbf{t} * g = g_-(\mathbf{t}) g_+(\mathbf{t}), \tag{3}$$

where $g_\pm(\mathbf{t}) \in G_\pm$. We say that the action (2) induces the flow $g_\pm(\mathbf{t})$ on $G_\pm$. The element $X_i \in \mathfrak{g}_+$ is called the infinitesimal generator of the t_i flow. Note that the action (2) descends to an action on the quotient space G/G_+ by $\mathbf{t}*(gG_+)=(\mathbf{t}*g)G_+$, thus inducing the flow $g_-(\mathbf{t})G_+$ on G/G_+.

Next, we show that the flow $g_-(\mathbf{t})$ represents solutions to a hierarchy of partial differential equations (PDE) in zero-curvature form on the Lie algebra of $\mathfrak{g}_+$. Let $p_+:\mathfrak{g}\to\mathfrak{g}_+$ denote the orthogonal projection. Observe that Eqs. (2) and (3) imply

$$\mathrm{Ad}(g_-^{-1})X_i = g_-^{-1}\frac{\partial g_-}{\partial t_i} + \frac{\partial g_+}{\partial t_i}g_+^{-1}. \tag{4}$$

By projecting Eq. (4) onto $\mathfrak{g}_+$, we obtain the following system of differential equations:

$$\frac{\partial g_+}{\partial t_i} = M_i(\mathbf{t})g_+(\mathbf{t}), \quad \text{where } M_i(\mathbf{t}) = p_+(\mathrm{Ad}(g_-^{-1}(\mathbf{t}))X_i), \quad 1\le i\le n. \tag{5}$$

Since $[X_i,X_j]=0$, the t_i and t_j flows commute so the compatibility condition $\partial_i\partial_j g_+=\partial_j\partial_i g_+$ yields the zero-curvature equation[1]

$$\frac{\partial M_i}{\partial t_j} - \frac{\partial M_j}{\partial t_i} + [M_i,M_j] = 0, \quad i,j = 1,2,\ldots,n. \tag{6}$$

Equation (6) represents a hierarchy of partial differential equations for the vector fields $M_i(\mathbf{t})$. In concrete realizations of integrable systems, G is a Banach loop group, and Eq. (6) is equivalent with a system of differential equations for matrix elements $\{u(\mathbf{t})\}$ of M_i and M_j. The zero-curvature equation is an evolution equation for $u(x,t)$, where $x=t_1$ is the space variable and $t=t_k$, $k\ge 2$, is the time variable in the kth equation of the hierarchy. Since $u(\mathbf{t})$ can be calculated explicitly from $g_-(\mathbf{t})$, $u(\mathbf{t})$ is represented by the flow $g_-(\mathbf{t})G_+$ on the homogeneous space G/G_+. The group theoretic approach to integrable systems can be used to study explicit solutions, symmetries, and conservation laws in terms of these flows. Note that the map $g\mapsto g_-(\mathbf{t})$ is invariant under the right multiplication of g by an element of G_+. Hence, we may assume that $g=g_-(0)$, so g encodes initial data for Eq. (6). Clearly,

$$\exp\left(\sum_{i=1}^{n}\Delta t_i X_i\right)(g_-(\mathbf{t})G_+) = g_-(\mathbf{t}+\Delta\mathbf{t})G_+,$$

which means that the left multiplication of $g_-(\mathbf{t})G_+$ by $\exp(\Delta t_k X_k)$ pushes $u(\mathbf{t})$ in the t_k direction by the amount Δt_k. In this sense, the Birkhoff factorization linearizes the equation for $u(\mathbf{t})$; hence the map $g_-(\mathbf{t})\mapsto u(\mathbf{t})$ can be viewed as an abstract version of the inverse scattering transform for Eq. (6).

III. BIRKHOFF FACTORIZATION FOR THE HEINSENBERG MAGNET EQUATION

In this section we discuss the Heisenberg magnet equation from the geometrical viewpoint presented in Sec. II. We define a loop group G and show that the flows corresponding to the HM and NLS equations are induced by an action of $\mathbb{R}^n$ on the homogeneous spaces G/H_+ and G/G_+, where H_+ and G_+ are subgroups of "positive" loops in G. Furthermore, we show that the gauge transformation between the NLS and HM equations can be interpreted as a map between the quotient spaces on which the flows are defined. For loops that are Laurent polynomials in the spectral parameter $z\in S^1$ this leads to an algebraic transformation between solutions of the NLS and HM equations.

In order to provide G with a Banach structure we start by introducing the Wiener algebra (see Dorfmeister[11])

$$\mathcal{A} = \left\{ f:S^1\to\mathbb{C} \middle| f(z) = \sum_{n=-\infty}^{\infty} c_n z^n, \sum_{n=-\infty}^{\infty}|c_n| < \infty \right\}.$$

This is a Banach algebra relative to the norm $\|f\|_1=\Sigma_{n=-\infty}^{\infty}|c_n|$. The algebra $\mathcal{A}$ consists of continuous functions on S^1 that have an absolutely convergent Fourier series. Let $gl(n,\mathcal{A})$ denote the

Banach algebra of matrices with elements in $\mathcal{A}$ equipped with the commutator bracket and the norm $\|g\|=\Sigma_{i,j}\|g_{ij}\|_1$. In view of Wiener's lemma,[12] the matrix $g(z)$ is invertible if and only if $\det(g(z))\neq 0$ for all $z\in S^1$. Hence, the group of invertible elements $GL(n,\mathcal{A})=\{g \in gl(n,\mathcal{A})\,|\det(g(z))\neq 0\,\forall\, z\in S^1\}$ is a Banach-Lie group as an open submanifold of $gl(n,\mathcal{A})$. Let σ be a continuous automorphism of the algebra $gl(n,\mathcal{A})$and define the group

$$G=\{g \in GL(n,\mathcal{A})|\sigma(g)=g\}.$$

G is a closed submanifold of $gl(n,\mathcal{A})$, and hence a Banach-Lie group with Lie algebra,

$$\mathfrak{g}=\{g \in gl(n,\mathcal{A})|\sigma(g)=g\}.$$

We shall use the above construction of loop group G in order to derive the HM and NLS flows. We remark that in some cases it is more convenient to use an involution τ on $gl(n,\mathcal{A})$, $\tau^2=id$, and to consider the subgroup $\widetilde{G}=\{g\in GL(n,\mathcal{A})\,|\,\tau(g)g=I\}$. This construction includes twisted loop groups related to systems such as the modified KdV equation[13] and the Neumann oscillator.[14] For more examples of loop groups and integrable systems see Ref. 11.

In order to relate the HM equation with the loop group G define the automorphism $\sigma: gl(2,\mathcal{A})\to gl(2,\mathcal{A})$ by

$$\sigma(g(z))=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\overline{g(\bar{z})}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}.$$

Evaluating the condition $\sigma(g)=g$, we obtain

$$G=\left\{g \in GL(2,\mathcal{A})|g(z)=\begin{pmatrix}a(z) & b(z)\\ -\overline{b(\bar{z})} & \overline{a(\bar{z})}\end{pmatrix}\right\}. \tag{7}$$

Consider the subgroups

$$H_-=\left\{h \in G|h(z)=\sum_{n=0}^{\infty}A_n z^{-n}\right\} \quad \text{and} \quad H_+=\left\{h \in G|h(z)=I+\sum_{n=1}^{\infty}B_n z^{n}\right\}.$$

Clearly, H_- and H_+ are closed subgroups of G and $H_-\cap H_+=\{I\}$. Furthermore, the Lie algebras of H_- and H_+ decompose the Lie algebra of G into a direct sum $\mathfrak{g}=\mathfrak{h}_-\oplus\mathfrak{h}_+$, hence the set H_-H_+ is open in G. Thus (G,H_-,H_+) is a Birkhoff factorization for G. We will frequently use the Pauli spin matrices,

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \text{and}\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

Now consider the pairwise commuting elements $X_k(z)=\sigma z^k\in\mathfrak{h}_+$ where $\sigma=i\sigma_3$, and define a differentiable action of $\mathbb{R}^n$ on G by

$$\mathbf{t}*h=\exp\left(\sum_{k=1}^{n}t_k\sigma z^k\right)h. \tag{8}$$

For any $h\in H_-H_+$ we have a unique factorization $\mathbf{t}*h=h_-(\mathbf{t})h_+(\mathbf{t})$ for $h\in H_-H_+$ when $\mathbf{t}$ is near $0\in\mathbb{R}^n$ because H_-H_+ is open in G. Let $p_+:\mathfrak{g}\to\mathfrak{h}_+$ denote the orthogonal projection onto strictly positive powers of z, and consider the matrices

$$M_k(\mathbf{t})=p_+(h_-^{-1}(\mathbf{t})\sigma z^k h_-(\mathbf{t})),\quad 1\le k\le n. \tag{9}$$

Observe that M_k is a matrix polynomial of order k in the parameter z. According to the general scheme outlined in Sec. II, the matrices (9) satisfy the zero-curvature condition (6). The system of equations obtained in this way will be called the HM hierarchy. The following result shows that

the first equation in the HM hierarchy is Eq. (1), and that solutions of Eq. (1) are obtained from the factorization $(x,t)*h=h_-(x,t)h_+(x,t)$ for some $h\in H_-H_+$.

Lemma 1: Consider the Birkhoff factorization $(x,t)*h=h_-(x,t)h_+(x,t)$ *for some initial data* $h\in H_-H_+$, *and let* $h_-(x,t)=\Sigma_{k=0}^{\infty}A_k(x,t)z^{-k}$. *Then* $S(x,t)=A_0^{-1}(x,t)\sigma_3A_0(x,t)$ *is the matrix representation of a solution of the HM equation* (1).

Proof: Substituting $h_-(x,t)=\Sigma_{k=0}^{\infty}A_k(x,t)z^{-k}$ into Eq. (9) we obtain the matrix polynomials,

$$M_1=(A_0^{-1}\sigma A_0)z,\quad M_2=(A_0^{-1}\sigma A_0)z^2+[A_0^{-1}\sigma A_0,A_0^{-1}A_1]z.$$

We show that

$$\frac{M_1}{\partial t}-\frac{M_2}{\partial x}+[M_1,M_2]=0 \tag{10}$$

is the zero-curvature representation of Eq. (1). Define the matrices $S=A_0^{-1}\sigma_3A_0$ and $P=A_0^{-1}A_1$. Since

$$A_0=\begin{pmatrix} a_0 & b_0 \\ -\overline{b_0} & \overline{a_0}\end{pmatrix},$$

S is a Hermitian matrix of the form

$$S=\begin{pmatrix} S_3 & S_1-iS_2 \\ S_1+iS_2 & -S_3\end{pmatrix}=\sum_{k=1}^{3}S_k\sigma_k,$$

for some real-valued functions $S_k(x,t)$. Moreover, we have $S^2=I$, which implies $S_1^2+S_2^2+S_3^2=1$. From this, it follows that Eq. (10) is equivalent with the system of equations for S and P,

$$i\frac{\partial S}{\partial x}+[S,[S,P]]=0, \tag{11}$$

$$\frac{\partial S}{\partial t}-\frac{\partial}{\partial x}[S,P]=0. \tag{12}$$

By substituting the identity $[S,[S,P]]=2S[P,S]$ into Eq. (11), we obtain $[S,P]=(i/2)SS_x$. Then Eq. (12) yields

$$\frac{\partial S}{\partial t}=\frac{i}{2}\left[\frac{\partial^2S}{\partial x^2}S+\left(\frac{\partial S}{\partial x}\right)^2\right]. \tag{13}$$

Finally, we note that $2(S_x)^2=-S_{xx}S-SS_{xx}$, thus Eq. (13) becomes

$$\frac{\partial S}{\partial t}=\frac{1}{4i}\left[S,\frac{\partial^2S}{\partial x^2}\right]. \tag{14}$$

After dilating the time variable $t\mapsto t/2$ we conclude that Eq. (14) is equivalent with Eq. (1). ■

Thus, solutions of the HM equation are represented by the flows $h_-(x,t)H_+$ on the homogeneous space G/H_+.

Next, we discuss the gauge transformation between the focusing NLS and HM equations in the context of Birkhoff factorization for G. Recall that the gauge transformation $\gamma_g:\mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}\times\mathfrak{g}$ by an element $g(x,t)\in G$ is defined by

$$\gamma_g(U,V)=\left(\mathrm{Ad}(g)U+\frac{\partial g}{\partial x}g^{-1},\mathrm{Ad}(g)V+\frac{\partial g}{\partial t}g^{-1}\right).$$

This transformation preserves the zero-curvature condition, and two systems of equations are said to be gauge equivalent if their zero-curvature representations are related by a gauge transformation.

It is well known that Eq. (1) is gauge equivalent with the focusing NLS equation,

$$i\frac{\partial u}{\partial t}-\frac{1}{2}\frac{\partial^2 u}{\partial x^2}-4u|u|^2=0, \tag{15}$$

where $u(x,t)$ is a complex valued function.[3] We show that on the group level the gauge transformation $NLS\mapsto HM$ can be interpreted as a map between the quotient spaces $\Gamma: G/G_+\to G/H_+$, where (G,G_-,G_+) is the Birkhoff factorization for G defined by the subgroups

$$G_-=\left\{g\in G|g(z)=I+\sum_{n=1}^{\infty}A_n z^{-n}\right\},\quad G_+=\left\{g\in G|g(z)=\sum_{n=0}^{\infty}B_n z^n\right\}. \tag{16}$$

Clearly, $\mathfrak{g}=\mathfrak{g}_-\oplus\mathfrak{g}_+$ where $\mathfrak{g}_\pm$ is the Lie algebra of $G_\pm$. One can think of (G,H_-,H_+) and (G,G_-,G_+) as two factorizations that differ in the normalization conditions: $h_+(0)=I$ and $g_-(\infty)=I$.

The NLS equation can be written in zero-curvature form as follows. Suppose that the action of $\mathbb{R}^n$ on G is given by (8), and consider now the factorization $\mathbf{t}*g=g_-(\mathbf{t})g_+(\mathbf{t})$ for some $g\in G_-G_+$. Let $q_+:\mathfrak{g}\to\mathfrak{g}_+$ denote the orthogonal projection onto non-negative powers of z. Then the matrix polynomials defined by

$$\hat{M}_k(\mathbf{t})=q_+(g_-^{-1}(\mathbf{t})\sigma z^k g_-(\mathbf{t})),\quad k=1,2,\ldots,n, \tag{17}$$

satisfy the system of equations (6), which is called the NLS hierarchy. It is not difficult to see that Eq. (15) is the first equation in the hierarchy. Denoting $g_-(x,t)=I+\sum_{n=1}^{\infty}A_n(x,t)z^{-n}$ and evaluating Eq. (17), we obtain

$$\hat{M}_1=\sigma z+[\sigma,A_1],\quad \hat{M}_2=\sigma z^2+[\sigma,A_1]z+[\sigma,A_2]-A_1[\sigma,A_1].$$

Since

$$A_n=\begin{pmatrix}a_n & b_n\\ -\bar{b}_n & \bar{a}_n\end{pmatrix},$$

the matrices $\hat{M}_1$ and $\hat{M}_2$ have the form

$$\hat{M}_1=\sigma z+2\begin{pmatrix}0 & ib_1\\ -\overline{ib_1} & 0\end{pmatrix},\quad \hat{M}_2=\sigma z^2+2\begin{pmatrix}0 & ib_1\\ -\overline{ib_1} & 0\end{pmatrix}z+2\begin{pmatrix}-i|b_1|^2 & v\\ -\bar{v} & i|b_1|^2\end{pmatrix}, \tag{18}$$

where $v=i(b_2-a_1b_1)$. It is easily verified that the zero-curvature condition (6) for $\hat{M}_1$ and $\hat{M}_2$ is equivalent with Eq. (15) for $u=b_1$. The NLS equation can also be obtained by a reduction as a special case of the AKNS hierarchy.[15]

We have seen that the loop group G defined by Eq. (7) admits two factorizations: (G,G_-G_+) and (G,H_-H_+). In fact, the sets G_-G_+ and H_-H_+ are equal, so we may denote them by K. Since each $k\in K$ can be factored uniquely as $k=g_-g_+=h_-h_+$ we can define a map $\Gamma: K/G_+\to K/H_+$ by $\Gamma(g_-G_+)=h_-H_+$. The elements $h_\pm$ are related to $g_\pm$ simply by $h_-=g_-B_0$ and $h_+=B_0^{-1}g_+$, where B_0 is the zeroth-order Fourier coefficient of g_+. Note that if $k(x,t)=(x,t)*g$ is the flow in G based at $k(0,0)=g\in G_-$, then the cosets $k(x,t)G_+$ and $k(x,t)H_+$ represent the NLS and HM flows, respectively. Thus, on the group level Γ maps the NLS solutions to HM solutions. Moreover, since g_+

$=B_0 h_+$ and the vector fields (M_1, M_2) satisfy Eq. (5), we conclude that (M_1, M_2) and $(\hat{M}_1, \hat{M}_2)$ are related by $(M_1, M_2) = \gamma(\hat{M}_1, \hat{M}_2)$, where γ is the gauge transformation by B_0^{-1}.Thus, we have the following.

Lemma 2: Let $\tilde{K}$ be the set of flows $\{(x,t) * g \,|\, g \in G_-\}$. Then the diagram

$$\begin{array}{ccc} \mathfrak{g}_+ \times \mathfrak{g}_+ & \overset{\gamma}{\rightarrow} & \mathfrak{h}_+ \times \mathfrak{h}_+ \\ \hat{\pi} \uparrow & & \uparrow \pi \\ \tilde{K}/G_+ & \overset{\Gamma}{\rightarrow} & \tilde{K}/H_+ \end{array}$$

is commutative, where the maps $\hat{\pi}(g_- G_+) = (\hat{M}_1, \hat{M}_2)$ and $\pi(h_- H_+) = (M_1, M_2)$ are defined in terms of Eqs. (17) and (9), *respectively, and γ is the gauge transformation by B_0^{-1}.*

If $g_-(x,t)$ is a Laurent polynomial in the spectral parameter $z \in S^1$, then Γ leads to a simple algebraic transformation between the NLS and HM solutions. Suppose for the moment that $g_-(x,t)$ has a pole of order N at $z=0$, so that

$$(x,t) * g = \left(I + \sum_{k=1}^{N} A_k(x,t) z^{-k} \right) \left(\sum_{k=0}^{\infty} B_k(x,t) z^k \right), \tag{19}$$

where $g = I + \Sigma_{k=1}^{N} A_k(0,0) z^{-k}$. Comparing the coefficients with z^{-N} on both sides of Eq. (19), we conclude that $B_0(x,t) = A_N^{-1}(x,t) A_N(0,0)$. The solution of the HM equation is thus given by

$$S(x,t) = B_0^{-1}(x,t) \sigma_3 B_0(x,t)$$

$$= A_N^{-1}(0,0) A_N(x,t) \sigma_3 A_N^{-1}(x,t) A_N(0,0).$$

Denote

$$A_N(x,t) = \begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix}$$

and let $a(0,0) = a_0$, $b(0,0) = b_0$. A straightforward computation shows that the elements of S can be expressed as

$$S_3 = \frac{(|a|^2 - |b|^2)(|a_0|^2 - |b_0|^2) + 4\,\mathrm{Re}(ab\overline{a_0 b_0})}{(|a|^2 - |b|^2)(|a_0|^2 - |b_0|^2)},$$

$$S_1 + iS_2 = \frac{2[(|a|^2 - |b|^2) a_0 \bar{b}_0 + ab\bar{b}_0^2 - \overline{ab} a_0^2]}{(|a|^2 - |b|^2)(|a_0|^2 - |b_0|^2)}. \tag{20}$$

Hence, if $g_-(x,t)$ has a pole at $z=0$, then the transformation (20) completely determines the vector $\vec{S} = (S_1, S_2, S_3)$ from the lowest order Fourier coefficient of the NLS flow $g_-(x,t)$. We will show in the next section that factorization (19) leads to multisoliton solutions of NLS. In this case the transformation $\Gamma : \tilde{K}/G_+ \to \tilde{K}/H_+$ maps multisoliton solutions of NLS to multisoliton solutions of HM. Finally, we remark that the correct choice of the loop group is important for obtaining the desired classes of solutions. For example, the NLS equation can also be derived from the group $G \cap SL(2, \mathcal{A})$, but the subgroup $(G \cap SL(2, \mathcal{A}))_-$ no longer contains Laurent polynomials, and hence no soliton solutions.

As an example of transformation (20) consider the initial data

$$g(z) = I + \begin{pmatrix} 0 & -i\alpha \\ -i\alpha & 0 \end{pmatrix} z^{-1}.$$

The time evolution of $g(z)$ determined by Eq. (19) is given by

$$g_-(x,t) = I + \begin{pmatrix} -i\alpha \tanh(2\alpha x) & -i\alpha e^{-i\alpha^2 t} \operatorname{sech}(2\alpha x) \\ -i\alpha e^{i2\alpha^2 t} \operatorname{sech}(2\alpha x) & i\alpha \tanh(2\alpha x) \end{pmatrix} z^{-1}.$$

Then the transformation (20) yields

$$S_1(x,t) = 2\cos(2\alpha^2 t)\tanh(2\alpha x)\operatorname{sech}(2\alpha x),$$

$$S_2(x,t) = -2\sin(2\alpha^2 t)\tanh(2\alpha x)\operatorname{sech}(2\alpha x),$$

$$S_3(x,t) = 2\operatorname{sech}^2(2\alpha x) - 1.$$

This is a solution of the HM equation that represents the magnetization vector $\vec{S}$ of unit length that rotates about the z axis.

IV. EXPLICIT SOLUTION OF THE BIRKHOFF FACTORIZATION PROBLEM

In this section we describe a geometrical solution of the Birkhoff factorization problem for the focusing NLS equation in terms of an infinite dimensional Grassmannian $\mathrm{Gr}(H)$. Our approach is based on the ideas of Segal and Wilson[2] who obtained solutions of the KdV equation in terms of the Baker function for special subspaces in $\mathrm{Gr}(H)$. By a similar procedure we construct a pair of Baker functions that yield solutions of the NLS equation. The geometrical approach to the NLS equation has been studied by several authors. Guil and Mañas[15] have used the Grassmannian model in the study of self-similar solutions of the AKNS hierarchy. As a byproduct, they characterized points in the Segal-Wilson Grassmannian that correspond to Nakamura-Hirota rational solutions of the nonfocusing NLS equation.[16] In Ref. 17 Previato obtained solutions of the focusing and nonfocusing NLS in terms of theta functions for the corresponding hyperelliptic curve. Although the Grassmannian model for integrable systems has been well studied, the solution of the factorization problem for NLS given here does not seem to appear in the literature.

In the following we give a brief account of the Segal-Wilson Grassmannian of the Hilbert space $H=L^2(S^1,\mathbb{C}^2)$. More details can be found in Refs. 2 and 18. Let H be the Hilbert space of square integrable functions on S^1 with values in $\mathbb{C}^2$, $f(z)=\Sigma_{k\in\mathbb{Z}}a_k z^k$, $a_k\in\mathbb{C}^2$ and $|z|=1$. The space H has a natural decomposition $H=H_+\oplus H_-$ into closed subspaces $H_+=\{\Sigma_{k\geq 0}a_k z^k\}$ and $H_-=\{\Sigma_{k<0}a_k z^k\}$. The Grassmannian $\mathrm{Gr}(H)$ is the set of closed subspaces $W\subset H$ such that the orthogonal projection $p_+: W\to H_+$ is a Fredholm operator and $p_-: W\to H_-$ is a Hilbert-Schmidt operator. It is not difficult to see that $\mathrm{Gr}(H)$ is a Hilbert manifold modeled on the space of Hilbert-Schmidt operators $\mathcal{C}_2(H_+,H_-)$. A chart around $W\in\mathrm{Gr}(H)$ is the set $\mathcal{U}_W=\{G(T)\,|\,T\in\mathcal{C}_2(W,W^\perp)\}$, where $G(T)=\{x+Tx\,|\,x\in W\}$ is the graph of T, together with the map $\mathcal{U}_W\to\mathcal{C}_2(W,W^\perp)$ defined by $G(T)\mapsto T$. Since W and $W^\perp$ are both infinite dimensional, the Hilbert spaces $\mathcal{C}_2(W,W^\perp)$ and $\mathcal{C}_2(H_+,H_-)$ are isomorphic.

Recall that the index of a Fredholm operator T is defined by $\mathrm{ind}(T)=\dim(\ker(T))-\dim(\mathrm{coker}(T))$. If $W\in\mathrm{Gr}(H)$, then the index of $p_+: W\to H_+$ is called the virtual dimension of W, $v.\dim(W)$. The Grassmannian is not connected since the connected components are indexed by the integers $v.\dim(W)$. Only the component $\mathrm{Gr}_0(H)=\{W\in\mathrm{Gr}(H)\,|\,v.\dim(W)=0\}$ will play a role in applications to NLS. The set $\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$ is sometimes called the "big cell," and has the following important property.

Lemma 3: (i) $W\in\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$ *if and only if* $p_+: W\to H_+$ *is an isomorphism.* (ii) *If* $W\in\mathrm{Gr}_0(H)$, *then* $W\in\mathcal{U}_{H_+}$, *if and only if* $W\cap H_-=\{0\}$.

Proof: (i) Suppose that $W\in\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$. Then $p_+: W\to H_+$ has index zero and the subspace

W is of the form $W=\{x+Tx|x\in H_+\}$ for some Hilbert-Schmidt operator $T:H_+\to H_-$. If $p_+(x+Tx)=0$, then clearly $x=0$; hence p_+ is injective. Furthermore, $\mathrm{ind}(p_+)=0$ implies that $\dim(\mathrm{coker}(p_+))=0$. Thus, p_+ is both injective and surjective, and hence an isomorphism.

Now suppose that $p_+:W\to H_+$ is an isomorphism. Then clearly $\mathrm{ind}(p_+)=0$, and hence $W\in \mathrm{Gr}_0(H)$. Since the projection $p_-:W\to H_-$ is a Hilbert-Schmidt operator, so is the product $T=p_-p_+^{-1}:H_+\to H_-$. We note that $W=\{x+Tx|x\in H_+\}$, which proves that $W\in\mathcal{U}_{H_+}$. Thus, $W\in \mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$. Part (ii) is proved in a similar fashion. ■

The full group $\mathrm{GL}(H)$ of bounded invertible operators with bounded inverse does not act on $\mathrm{Gr}(H)$, as it does not preserve the properties of the projections $p_\pm:W\to H_\pm$. However, the restricted general linear group $\mathrm{GL}_{\mathrm{res}}(H)$ acts on $\mathrm{Gr}(H)$. $\mathrm{GL}_{\mathrm{res}}(H)$ is the subgroup of $\mathrm{GL}(H)$ consisting of operators whose block form $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with respect to the decomposition $H=H_+\oplus H_-$ has off-diagonal terms Hilbert-Schmidt: $b\in\mathcal{C}_2(H_-,H_+)$ and $c\in\mathcal{C}_2(H_+,H_-)$. The diagonal terms are then automatically Fredholm. The action of $\mathrm{GL}_{\mathrm{res}}(H)$ is transitive since the orbit through H_+ is $\mathrm{Gr}(H)$.

We shall be interested in the group Γ_+ of holomorphic maps on the unit disk $g:D_0\to GL(2,\mathbb{C})$, $D_0=\{|z|\le 1\}$. The elements of Γ_+ can be viewed as multiplication operators on H. A computation involving the expansion of $g(z)$ into the Taylor series around $z=0$ shows that if $g(z)$ is holomorphic, then the corresponding multiplication operator $M_g:H_+\oplus H_-\to H_+\oplus H_-$ has the block form $M_g=\begin{pmatrix} a & b \\ 0 & d \end{pmatrix}$, where a and d are invertible and b is Hilbert-Schmidt. Hence $M_g\in\mathrm{GL}_{\mathrm{res}}(H)$, and so Γ_+ acts on $\mathrm{Gr}(H)$. In fact, since a is invertible, Γ_+ acts on the connected component $\mathrm{Gr}_0(H)$. By a similar argument, it can be shown that the group Γ_- of based holomorphic maps $g:D_\infty\to GL(2,\mathbb{C})$, $D_\infty=\{|z|\ge 1\}$, where $g(\infty)=I$ also acts on $\mathrm{Gr}_0(H)$. Due to the analytical structure of the group G introduced in Sec. III, we have $G_\pm\subset\Gamma_\pm$ [see Eq. (16)]. In particular, the loop $\exp(\Sigma_{k=1}^n t_k\sigma z^k)\in\Gamma_+$ acts on $\mathrm{Gr}_0(H)$. For any $W\in\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$, define the subspace

$$W(\mathbf{t})=\exp\left(\sum_{k=1}^n t_k\sigma z^k\right)W.$$

Clearly, $W(\mathbf{t})\in Gr_0(H)\cap\mathcal{U}_{H_+}$ when $\mathbf{t}$ is near $0\in\mathbb{R}^n$ because $\mathcal{U}_{H_+}$ is open and Γ_+ acts on $\mathrm{Gr}_0(H)$. Hence, by Lemma 3(i) the orthogonal projection $p_+:W(\mathbf{t})\to H_+$ is an isomorphism.

Definition 2: Let $W\in\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$ and consider the isomorphism $p_+:W(\mathbf{t})\to H_+$. The Baker functions for the subspace W are the unique elements $\Psi_1(\mathbf{t},z)$, $\Psi_2(\mathbf{t},z)\in W$ such that

$$\exp\left(\sum_{k=1}^n t_k\sigma z^k\right)\Psi_1(\mathbf{t},z)=p_+^{-1}(e_1),\quad \exp\left(\sum_{k=1}^n t_k\sigma z^k\right)\Psi_2(\mathbf{t},z)=p_+^{-1}(e_2),\tag{21}$$

where $e_1=\begin{pmatrix}1\\0\end{pmatrix}$, $e_2=\begin{pmatrix}0\\1\end{pmatrix}$.

In the following we show that the flows of the NLS hierarchy can be expressed in terms of the Baker functions Ψ_1 and Ψ_2. For certain subspaces W this yields the multisoliton solutions of NLS. Let $g\in G_-$ and consider the subspace $gH_+\in\mathrm{Gr}(H)$. Suppose for the moment that gH_+ contains a subspace W such that $W\in\mathrm{Gr}_0(H)\cap\mathcal{U}_{H_+}$, and let Ψ_1, Ψ_2 be the Baker functions for W. The existence of such subspaces will be shown shortly. Since $W\subset gH_+$ we have $\Psi_1=gf_1$, $\Psi_2=gf_2$ for some $f_1,f_2\in H_+$, and

$$\exp\left(\sum_{k=1}^n t_k\sigma z^k\right)gf_1=p_+^{-1}(e_1),\quad \exp\left(\sum_{k=1}^n t_k\sigma z^k\right)gf_2=p_+^{-1}(e_2).$$

This can be combined into the matrix equation

$$\exp\left(\sum_{k=1}^{n} t_k \sigma z^k\right) g[f_1|f_2] = [p_+^{-1}(e_1)|p_+^{-1}(e_2)].$$

We note that the matrices involved here have the form

$$[f_1|f_2] = \sum_{k=0}^{\infty} B_k z^k, \quad [p_+^{-1}(e_1)|p_+^{-1}(e_2)] = I + \sum_{k=1}^{\infty} A_k z^{-k}.$$

If the matrix $[f_1|f_2]$ is invertible, then by uniqueness of the Birkhoff factorization (G, G_-, G_+), we have

$$\exp\left(\sum_{k=1}^{n} t_k \sigma z^k\right) g = g_-(\mathbf{t}) g_+(\mathbf{t}), \quad g_\pm \in G_\pm, \tag{22}$$

where $g_+(\mathbf{t}) = [f_1|f_2]^{-1}$ and $g_-(\mathbf{t}) = [p_+^{-1}(e_1)|p_+^{-1}(e_2)]$, which is precisely the factorization problem for NLS. The importance of the last relation is that in view of Eq. (21) the flow $g_-(\mathbf{t})$ can be expressed in terms of the Baker functions:

$$g_-(\mathbf{t}) = \exp\left(\sum_{k=1}^{n} t_k \sigma z^k\right) [\Psi_1|\Psi_2]. \tag{23}$$

This result can be formulated as the following theorem.

Theorem 1: *Let $g \in G_-$ and let W be a subspace of $gH_+ \in Gr(H)$ such that $W \in Gr_0(H) \cap \mathcal{U}_{H_+}$. Then the flow $g_-(\mathbf{t})$ given by Eq.* (23) *is the unique solution of the NLS factorization problem* (22), *where Ψ_1 and Ψ_2 are the Baker functions for W.*

Example 1 (one-soliton solution): Perhaps the simplest interesting example of a subspace in $\mathrm{Gr}_0(H) \cap \mathcal{U}_{H_+}$ is the one which yields the one-soliton solution of NLS. Its construction resembles the one-soliton space for the KdV equation given in Ref. 2. Consider the points in the unit disk $0 < |p_i| < 1$, $i = 1, 2$, and the parameters $\lambda, \mu \in \mathbb{C}^\times$, $\lambda \neq \mu$. Define W_1 to be the L^2 closure of the space of functions $f: S^1 \to \mathbb{C}^2$, $f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$, where f_1 and f_2 are holomorphic in D_0, except possibly for a simple pole at $z = 0$; and that satisfy the condition

$$f_1(p_1) = \lambda f_2(p_1), \quad f_1(p_2) = \mu f_2(p_2). \tag{24}$$

It is straightforward to verify that $W_1 \in \mathrm{Gr}_0(H)$ and $W_1 \cap H_- = \{0\}$. It follows from Lemma 3(ii) that $W_1 \in \mathrm{Gr}_0(H) \cap \mathcal{U}_{H_+}$, so $p_+: W_1(\mathbf{t}) \to H_+$ is an isomorphism. In order to obtain the Baker functions for the NLS equation let us write $x = t_1$, $t = t_2$, and suppress t_k for $k \geq 3$. Denote

$$p_+^{-1}(e_1) = \begin{pmatrix} az^{-1} + 1 \\ cz^{-1} \end{pmatrix}, \quad p_+^{-1}(e_2) = \begin{pmatrix} bz^{-1} \\ dz^{-1} + 1 \end{pmatrix}.$$

Then the Baker functions for W_1 have the form

$$\Psi_1(x,t,z) = \exp(-x\sigma z - t\sigma z^2) p_+^{-1}(e_1) = \begin{pmatrix} (1 + az^{-1}) e^{-ixz - itz^2} \\ cz^{-1} e^{ixz + itz^2} \end{pmatrix},$$

$$\Psi_2(x,t,z) = \exp(-x\sigma z - t\sigma z^2) p_+^{-1}(e_2) = \begin{pmatrix} bz^{-1} e^{-ixz - itz^2} \\ (1 + dz^{-1}) e^{ixz + itz^2} \end{pmatrix}.$$

Since Ψ_1 and Ψ_2 satisfy the condition (24), the coefficients a, b, c, d are given by

$$a = \frac{p_1 \mu e^{i\theta_2} - p_2 \lambda e^{i\theta_1}}{\lambda e^{i\theta_1} - \mu e^{i\theta_2}}, \quad b = -\frac{\lambda\mu(p_1 - p_2)}{\lambda e^{-i\theta_2} - \mu e^{-i\theta_1}}, \tag{25}$$

$$c = \frac{p_1 - p_2}{\lambda e^{i\theta_1} - \mu e^{i\theta_2}}, \qquad d = -\frac{p_1 \lambda e^{-i\theta_2} - p_2 \mu e^{-i\theta_1}}{\lambda e^{-i\theta_2} - \mu e^{-i\theta_1}}, \tag{26}$$

where $\theta_k = 2(xp_k + tp_k^2)$, $k = 1, 2$. In view of the relation

$$g_-(x,t) = \exp(x\sigma z + t\sigma z^2)[\Psi_1 | \Psi_2] = I + \begin{pmatrix} a & b \\ c & d \end{pmatrix} z^{-1},$$

for the Baker functions to generate solutions of the NLS equation we must have $g_-(x,t) \in G_-$, i.e., the matrix coefficients must satisfy $c = -\bar{b}$ and $d = \bar{a}$. These conditions are satisfied, provided $p_1 = \bar{p}_2$ and $\lambda\bar{\mu} = -1$. Let us write $p_1 = \alpha + i\beta$ and $\lambda = e^{-2\beta x_0} e^{i2\varphi}$ for some $\varphi, x_0 \in \mathbb{R}$. Then it follows from Eq. (25) that a and b have the particularly simple form

$$a(x,t) = -\alpha + i\beta \tanh[2\beta(x + \alpha t + x_0)],$$

$$b(x,t) = i\beta \exp[i2(\alpha x + (\alpha^2 - \beta^2)t + \varphi)] \operatorname{sech}[2\beta(x + \alpha t + x_0)].$$

According to the discussion in Sec. III [see Eq. (18)] the coefficient $b(x,t)$ is a solution of Eq. (15), which is the well-known one-soliton solution of NLS.

Example 2 (n-soliton solution): The n-soliton solution is obtained by a simple generalization of the above construction. Consider n points in the unit disk $0 < |p_i| < 1$, $1 \le i \le n$, and n parameters $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{C}^\times$. Let W_n the L^2 closure of the space of functions $f: S^1 \to \mathbb{C}^2$, where f_1 and f_2 are holomorphic in D_0 except possibly for a pole of order n at $z = 0$, and that satisfy the $2n$ conditions

$$f_1(p_j) = \lambda_j f_2(p_j), \quad f_1(\bar{p}_j) = \mu_j f_2(\bar{p}_j), \quad j = 1, 2, \ldots, n, \tag{27}$$

where $\lambda_j \bar{\mu}_j = -1$. The Baker functions for W_n are given by

$$\Psi_1(x,t,z) = \begin{pmatrix} (1 + \sum_{k=1}^n a_k z^{-k}) e^{-i(xz + tz^2)} \\ (\sum_{k=1}^n c_k z^{-k}) e^{i(xz + tz^2)} \end{pmatrix},$$

$$\Psi_2(x,t,z) = \begin{pmatrix} (\sum_{k=1}^n b_k z^{-k}) e^{-i(xz + tz^2)} \\ (1 + \sum_{k=1}^n d_k z^{-k}) e^{i(xz + tz^2)} \end{pmatrix}.$$

Conditions (27) yield the following system of equations for a_k, b_k, c_k, d_k:

$$\sum_{k=1}^n \left(\lambda_j e^{i\theta_j} \frac{1}{p_j^k} c_k - \frac{1}{p_j^k} a_k \right) = 1, \quad \sum_{k=1}^n \left(\mu_j e^{i\bar{\theta}_j} \frac{1}{\bar{p}_j^k} c_k - \frac{1}{\bar{p}_j^k} a_k \right) = 1, \tag{28}$$

$$\sum_{k=1}^n \left(\frac{1}{\lambda_j e^{i\theta_j}} \frac{1}{p_j^k} b_k - \frac{1}{p_j^k} d_k \right) = 1, \quad \sum_{k=1}^n \left(\frac{1}{\mu_j e^{i\bar{\theta}_j}} \frac{1}{\bar{p}_j^k} b_k - \frac{1}{\bar{p}_j^k} d_k \right) = 1, \tag{29}$$

where $\theta_j = 2(xp_j + tp_j^2)$, $1 \le j \le n$. The consistency condition $\lambda_j \bar{\mu}_j = -1$ ensures that $c_k = -\bar{b}_k$ and $d_k = \bar{a}_k$. The n-soliton solution of NLS is then given as the quotient of the determinants $b_1 = \Delta_1 / \Delta$, where

$$\Delta = \prod_{j=1}^{n} \frac{1}{\lambda_j \mu_j} \begin{vmatrix} q_1 e^{-i\theta_1} & q_1^2 e^{-i\theta_1} & \cdots & q_1^n e^{-i\theta_1} & -\lambda_1 q_1 & -\lambda_1 q_1^2 & \cdots & -\lambda_1 q_1^n \\ \vdots & & & & & & & \vdots \\ q_n e^{-i\theta_n} & q_n^2 e^{-i\theta_n} & \cdots & q_n^n e^{-i\theta_n} & -\lambda_n q_n & -\lambda_n q_n^2 & \cdots & -\lambda_n q_n^n \\ \bar{q}_1 e^{-i\bar{\theta}_1} & \bar{q}_1^2 e^{-i\bar{\theta}_1} & \cdots & \bar{q}_1^n e^{-i\bar{\theta}_1} & -\mu_1 \bar{q}_1 & -\mu_1 \bar{q}_1^2 & \cdots & -\mu_1 \bar{q}_1^n \\ \vdots & & & & & & & \vdots \\ \bar{q}_n e^{-i\bar{\theta}_n} & \bar{q}_n^2 e^{-i\bar{\theta}_n} & \cdots & \bar{q}_n^n e^{-i\bar{\theta}_n} & -\mu_n \bar{q}_n & -\mu \bar{q}_n^2 & \cdots & -\mu_n \bar{q}_n^n \end{vmatrix},$$

$q_j = 1/p_j$, and Δ_1 is obtained by replacing the first column of Δ by the vector $(\lambda_1 \ldots \lambda_n \mu_1 \ldots \mu_n)^T$. The explicit form of b_1 becomes fairly complicated as n increases. To conclude our discussion we remark that by solving system (28) and (29) for the lowest order coefficients a_n and b_n, and applying the transformation (20) to a_n and b_n we obtain the n-soliton solution of the HM equation. Hence, we can associate solutions of the HM equation to the subspaces $W_n \in \mathrm{Gr}(H)$ via the mappings $W_n \mapsto (a_n, b_n) \mapsto (S_1, S_2, S_3)$.

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Block-diagonalizability problem for hydrodynamic type systems

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The necessary and sufficient conditions are derived for the reducibility of a hydrodynamic type system into a block-diagonal form with k mutually interacting blocks. Applications to the perturbations of the Benney system and to the Hamiltonian systems of partial differential equations are presented. The algebraic identities connecting the Nijenhuis tensors $N_{B(A)}(u,v)$ and $N_A(u,v)$ and Haantjes tensors $H_{B(A)}(u,v)$ and $H_A(u,v)$ are discovered. © *2006 American Institute of Physics.*
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I. INTRODUCTION

As is known, the block diagonalizability of a hydrodynamic type system

$$\frac{\partial u^\ell}{\partial t}=\sum_{j=1}^{n} A_m^\ell(u^1,\ldots,u^n)\frac{\partial u^m}{\partial x} \tag{1.1}$$

drastically effects its properties and the computer time required for its numerical investigation. Until now no necessary and sufficient conditions for the block diagonalizability were known. The Courant problem on the block diagonalizability[1] is formulated as follows.

When a given system (1.1) can be transformed in some coordinates $v^1(u),\ldots,v^n(u)$ *into block-diagonal form*

$$\frac{\partial v^{m_j+i}}{\partial t}=\sum_{\ell=1}^{n_j}\tilde{A}_{m_j+\ell}^{m_j+i}(v^1,\ldots,v^n)\frac{\partial v^{m_j+\ell}}{\partial x} \tag{1.2}$$

with $n_j\times n_j$ *mutually interacting blocks where* $n_1+\cdots+n_k=n$*?* Here $j=1,\ldots,k$, $i=1,\ldots,n_j$ and $m_j=n_1+\cdots+n_{j-1}$; $u^1,\ldots,u^n$ and $v^1(u),\ldots,v^n(u)$ form systems of local coordinates in the Euclidean space R^n. The first result concerning the block-diagonalizability problem follows from the Haantjes theorem[2] on the X_m-forming sets of eigenvalues of a (1,1)-tensors $A_j^i(u^1,\ldots,u^n)$. The theorem is proved in Ref. 2 and is equivalent to the following statement.

The necessary and sufficient condition for the complete diagonalizability of the system (1.1) with real and distinct eigenvalues of $A_j^i(u)$ *is the vanishing of the corresponding Haantjes (1,2)-tensor*[2]

$$H_{Ajk}^i=A_\alpha^i A_\beta^\alpha N_{jk}^\beta+N_{\alpha\beta}^i A_j^\alpha A_k^\beta-A_\alpha^i N_{\beta k}^\alpha A_j^\beta-A_\alpha^i N_{j\beta}^\alpha A_k^\beta \tag{1.3}$$

that is defined in terms of the Nijenhuis tensor[3]

$$N_{Aik}^j=A_i^\alpha\frac{\partial A_k^j}{\partial u^\alpha}-A_k^\alpha\frac{\partial A_i^j}{\partial u^\alpha}+A_\alpha^j\frac{\partial A_i^\alpha}{\partial u^k}-A_\alpha^j\frac{\partial A_k^\alpha}{\partial u^i}. \tag{1.4}$$

The more general case of complex eigenvalues of $A_j^i(u)$ was not studied in Refs. 2 and 3. It is evident however that for a generic system of pde's (1.1) some of the eigenvalues of $A_j^i(u)$ are complex.

In this paper we prove Theorem 1 that gives the necessary and sufficient conditions for the block diagonalizability of systems (1.1). The proof of Theorem 1 presented in Sec. III is based on a new algebraic identity that connects the Nijenhuis tensor $N_{B(A)}(u,v)$ with the $N_A(u,v)$ where $B(A)$ is an arbitrary polynomial in A. The identity and its analog for the Haantjes tensor are proved in Sec. II. In Sec. IV we demonstrate applications to the perturbations of the Benney system[4] and to the Hamiltonian systems of partial differential equations in R^3.

The Nijenhuis tensor appears in many problems of mathematical physics and differential geometry, mostly as the vanishing condition $N_A(u,v)=0$: The Gelfand-Dorfman-Magri-Morosi theorem[5,6] states that the two Poisson structures P_1 and P_2 are compatible in Magri's sense[7] if and only if $N_A(u,v)=0$ where $A=P_1P_2^{-1}$. The Newlander-Nirenberg theorem[8] states that a quasicomplex structure $A(x)$, $A^2(x)=-1$, is complex if and only if the Nijenhuis tensor $N_A(u,v)$ vanishes. The condition $N_A(u,v)=0$ is used in Refs. 6, 9, and 10 as the definition of the Poisson-Nijenhuis structures and in Ref. 11 as the definition of the Nijenhuis G-manifolds with applications to the KP systems. The condition $N_A(u,v)=0$ is used in Refs. 12 and 13 as a sufficient condition for the existence of conservation laws for systems of pde's (1.1).

In Refs. 14 and 15 we applied the nonzero Nijenhuis and Haantjes tensors to study the necessary criteria for the existence of the Hamiltonian and bi-Hamiltonian structures for systems (1.1).

II. ALGEBRAIC IDENTITIES FOR THE NIJENHUIS AND HAANTJES TENSORS

(i) The Nijenhuis tensor is defined by the formula[3]

$$N_A(u,v)=A^2[\tilde{u},\tilde{v}]+[A\tilde{u},A\tilde{v}]-A[A\tilde{u},\tilde{v}]-A[\tilde{u},A\tilde{v}], \tag{2.1}$$

where u and v are tangent vectors at a point $x\in R^n$, $\tilde{u}$ and $\tilde{v}$ are arbitrary vector fields extending the vectors u and v, and $[\tilde{u},\tilde{v}]$ is the commutator of the vector fields. The expression (2.1) is independent of the extensions $\tilde{u}$ and $\tilde{v}$.

The Haantjes (1,2)-tensor $H_A(u,v)$ (Ref. 2) is defined in terms of the Nijenhuis tensor $N_A(u,v)$ (2.1),

$$H_A(u,v)=A^2N(u,v)+N(Au,Av)-AN(Au,v)-AN(u,Av) \tag{2.2}$$

and has components (1.3).

Let $B(A)$ be any polynomial in A with the variable coefficients

$$B(A)=\sum_{m=0}^{k} b_m(x)A^m(x). \tag{2.3}$$

In this section we derive the formulas that connect the Nijenhuis tensors $N_{B(A)}(u,v)$ and $N_A(u,v)$ and the Haantjes tensors $H_{B(A)}(u,v)$ and $H_A(u,v)$. The formulas give a complete solution to the problem on the interconnections between the tensors $N_{B(A)}(u,v)$ and $N_A(u,v)$ raised by Nijenhuis in Ref. 3.

(ii) *The (1,2)-tensors representation of the ring of polynomials* $P[z,\lambda,\mu]$. Let us consider the commutative ring $P_3=P[z,\lambda,\mu]$ of polynomials in three independent variables z,λ,μ with coefficients depending on a point x of a manifold M^n. Elements of the ring P_3 are polynomials

$$S(z,\lambda,\mu)=\sum_{i,j,k}^{N} a_{ijk}(x)z^i\lambda^j\mu^k, \quad x\in M^n, \tag{2.4}$$

where coefficients $a_{ijk}(x)$ are arbitrary smooth functions on M^n.

We introduce a representation T of the ring P_3 in the linear space of (1,2)-tensors $V(u,v)$ on M^n. The representation depends on an arbitrary (1,1)-tensor $A(x)$ on M^n and is defined for an arbitrary polynomial $S(z,\lambda,\mu)$ (2.4) by the formula

$$(T_S V)(u,v) = \sum_{i,j,k}^{N} a_{ijk}(x) A^i V(A^j u, A^k v). \tag{2.5}$$

Here the action of λ and μ is associated, respectively, with the first and the second entries of $V(u,v)$; the action of z is associated with the value of V. The representation (2.5) possesses the standard properties

$$T_{S_1+S_2} = T_{S_1} + T_{S_2}, \quad T_{S_1 \cdot S_2} = T_{S_2 \cdot S_1} = T_{S_1} \cdot T_{S_2}. \tag{2.6}$$

The first identity (2.6) is obvious; the second one is evidently true for any monomials $S_1 = a(x) z^i \lambda^j \mu^k$ and $S_2 = b(x) z^p \lambda^q \mu^r$; hence the general case follows by the bilinearity.

(iii) In terms of the representation T_S (2.5), formula (2.2) takes the form

$$H_A(u,v) = T_D N_A(u,v), \tag{2.7}$$

where D is the polynomial $D(z,\lambda,\mu) = (z-\lambda)(z-\mu)$. It is evident that any (1,2)-tensor $W(u,v)$ of the form

$$W(u,v) = \sum_{m=0}^{N} [u(g_m(x)) A^m v + v(h_m(x)) A^m u]$$

is annihilated by the operator T_D,

$$T_D W(u,v) = 0. \tag{2.8}$$

Let $B(z)$ be a polynomial, $B(z) = \sum_{m=0}^{k} b_m(x) z^m$. We will use the well-known Bezout identity

$$B(z) - B(\lambda) = (z-\lambda) Q_B(z,\lambda), \tag{2.9}$$

where $Q_B(z,\lambda)$ is the symmetric polynomial

$$Q_B(z,\lambda) = \sum_{m=1}^{k} b_m(x) \sum_{p+q=m-1} z^p \lambda^q. \tag{2.10}$$

Remark 1: All tensors $U(A)$ considered in this paper have the form

$$U\left(A^i_j, \frac{\partial^k A^i_j(x)}{\partial x_{\alpha_1} \cdots \partial x_{\alpha_k}} \right)$$

and are polynomials with respect to their arguments. Therefore the tensors $U(A)$ can be continued onto the complexifications of the tangent bundle $T(M^n)$ and the cotangent bundle $T^*(M^n)$. We will mean this continuation when the (1,1)-tensor $A^i_j(x)$ has complex eigenvalues and eigenvectors.

Remark 2: Let a (k,l)-tensor $U(A)$ analytically depend on the entries of the (1,1)-tensor $A^i_j(x)$ and their partial derivatives up to a finite order N. If tensor $U(A)$ is equal to zero for all (1,1) tensors $A^i_j(x)$ with distinct (complex) eigenvalues then $U(A) \equiv 0$ for any (1,1)-tensor $A^i_j(x)$. This evidently follows by continuation from the nondegenerate case $A^i_j(x)$ with distinct eigenvalues.

Let $\lambda_1(x), \ldots, \lambda_k(x)$ be the eigenvalues of an operator $A(x)$, corresponding to the eigenvectors $e_1(x), \ldots, e_k(x)$, $k \leqslant n$. The operator $B(A(x))$ (2.3) has the same eigenvectors $e_i(x)$ with the eigenvalues $B(\lambda_i(x))$.

For the Nijenhuis (1,2)-tensor $N_{B(A)}(u,v)$ (2.1), the formula holds

$$N_{B(A)}(e_i,e_j) = (B(A) - B(\lambda_i))(B(A) - B(\lambda_j))[e_i,e_j] + (B(\lambda_i) - B(\lambda_j))(e_i(B(\lambda_j))e_j + e_j(B(\lambda_i))e_i). \tag{2.11}$$

Indeed, formula (2.11) follows from the Nijenhuis formula[3]

$$N_A(e_i,e_j)=(A-\lambda_i)(A-\lambda_j)[e_i,e_j]+(\lambda_i-\lambda_j)(e_i(\lambda_j)e_j+e_j(\lambda_i)e_i). \tag{2.12}$$

Lemma 1: For any polynomial $B(A)$ (2.3), *the Nijenhuis tensor* $N_B(u,v)$ *is connected with* $N_A(u,v)$ *by the formula*

$$\begin{aligned} N_B(u,v)=&\sum_{m,l=1}^{k} b_m b_l \sum_{p<m,q<l} A^{m+l-p-q-2}N_A(A^p u,A^q v)\\ &+\sum_{m=0}^{k}[B(A)u(b_m)A^m v-B(A)v(b_m)A^m u-u(b_m)B(A)A^m v+v(b_m)B(A)A^m u]. \end{aligned} \tag{2.13}$$

Proof: We first assume that the operator $A(x)$ has distinct eigenvalues $\lambda_1(x),\dots,\lambda_n(x)$. Using the Bezout identity (2.9), we find

$$\begin{gathered} Q_B(\lambda,\lambda)=\frac{\partial B(\lambda)}{\partial\lambda},\\ e(B(\lambda))=\sum_{m=0}^{k}(b_m e(\lambda^m)+e(b_m)\lambda^m)=Q_B(\lambda,\lambda)e(\lambda)+\sum_{m=0}^{k}e(b_m)\lambda^m, \end{gathered} \tag{2.14}$$

where e is an arbitrary tangent vector, $e\in T_x(M^n)$. In view of the identities (2.9) and (2.14), formula (2.11) takes the form

$$\begin{aligned} N_B(e_i,e_j)=&Q_B(A,\lambda_i)Q_B(A,\lambda_j)(A-\lambda_i)(A-\lambda_j)[e_i,e_j]\\ &+Q_B(\lambda_i,\lambda_j)(\lambda_i-\lambda_j)[Q_B(\lambda_j,\lambda_j)e_i(\lambda_j)e_j+Q_B(\lambda_i,\lambda_i)e_j(\lambda_i)e_i]\\ &+\sum_{m=0}^{k}(B(\lambda_i)-B(\lambda_j))[e_i(b_m)\lambda_j^m e_j+e_j(b_m)\lambda_i^m e_i]. \end{aligned}$$

Applying the Nijenhuis formula (2.12), we obtain

$$\begin{aligned} N_B(e_i,e_j)=&Q_B(A,\lambda_i)Q_B(A,\lambda_j)N_A(e_i,e_j)+\sum_{m=0}^{k}[B(A)e_i(b_m)A^m e_j-B(A)e_j(b_m)A^m e_i-e_i(b_m)B(A)A^m e_j\\ &+e_j(b_m)B(A)A^m e_i]. \end{aligned} \tag{2.15}$$

In view of (2.5), the first term in (2.15) has the form

$$Q_B(A,\lambda_i)Q_B(A,\lambda_j)N_A(e_i,e_j)=T_{Q_B(z,\lambda)Q_B(z,\mu)}N_A(e_i,e_j).$$

Thus we get

$$\begin{aligned} N_B(u,v)=&T_{Q_B(z,\lambda)Q_B(z,\mu)}N_A(u,v)\\ &+\sum_{m=0}^{k}[B(A)u(b_m)A^m v-B(A)v(b_m)A^m u-u(b_m)B(A)A^m v+v(b_m)B(A)A^m u], \end{aligned} \tag{2.16}$$

where $u=e_i$ and $v=e_j$. Hence formula (2.16) follows by the bilinearity for arbitrary vectors u and v, for the case of distinct eigenvalues of $A(x)$. The formula (2.13) coincides with (2.16) in view of the definitions (2.5) and (2.10). Thus formula (2.13) is proven for any (1,1)-tensor $A^i_j(x)$ having distinct eigenvalues. Applying Remark 2, we obtain that formula (2.13) holds for an arbitrary (1,1)-tensor $A^i_j(x)$. □

Lemma 2: For any polynomial $B(A,x)$ with variable coefficients, the Haantjes tensor $H_B(u,v)$ is connected with $H_A(u,v)$ by the formula

$$H_B(u,v) = T_{Q_B^2(z,\lambda)Q_B^2(z,\mu)} H_A(u,v). \tag{2.17}$$

Proof: The Haantjes tensor $H_{B(A)}(u,v)$ is connected with the Nijenhuis tensor $N_{B(A)}(u,v)$ by the relation

$$H_B(u,v) = B^2 N_B(u,v) + N_B(Bu,Bv) - BN_B(Bu,v) - BN_B(u,Bv),$$

that is equivalent to the expression

$$H_{B(A)}(u,v) = T_{(B(z)-B(\lambda))(B(z)-B(\mu))} N_{B(A)}(u,v).$$

Using the Bezout identity (2.9), we obtain

$$H_{B(A)}(u,v) = T_{Q_B(z,\lambda)Q_B(z,\mu)} T_D N_{B(A)}(u,v),$$

where $D=(z-\lambda)(z-\mu)$. Substituting here formula (2.16) and using Eqs. (2.7) and (2.8), we obtain the identity (2.17). □

Proposition 1: The Nuijenhuis tensors $N_A(u,v)$ and $N_{B(A)}(u,v)$ are connected by the identity

$$\begin{aligned} &A^2 N_B(u,v) + N_B(Au,Av) - AN_B(Au,v) - AN_B(u,Av) \\ &\quad = B^2 N_A(u,v) + N_A(Bu,Bv) - BN_A(Bu,v) - BN_B(u,Bv). \end{aligned} \tag{2.18}$$

Indeed, applying operator T_D, $D=(z-\lambda)(z-\mu)$, to the identity (2.16) and using Bezout formula (2.9) and Eq. (2.8), we arrive at the identity (2.18). □

III. THE BLOCK-DIAGONALIZABILITY PROBLEM

For a generic hydrodynamic type system in the block-diagonal form (1.2), the eigenvalues corresponding to any two different blocks $\widetilde{A}^{m_j+i}_{m_j+\ell}(v^1,\dots,v^n)$ do not coincide with each other almost everywhere for $x \in R^n$ (while inside a given block some eigenvalues can coincide, for example, if its Jordan normal form is not diagonal).

Theorem 1: *For a system of hydrodynamic type (1.1) to be reducible to a block-diagonal form with k blocks of dimensions $n_j \times n_j$ with $n_1+\cdots+n_k=n$ it is necessary and sufficient that in the tangent spaces $T_x(R^n)$ there exist k smooth distributions $L_{1x},\dots,L_{kx}$ of dimensions $n_1,\dots,n_k$ such that $L_{1x}\oplus\cdots\oplus L_{kx}=T_x(R^n)$ and the conditions*

$$A(L_{ix}) \subset L_{ix}, \quad H_A(L_{ix},L_{ix}) \subset L_{ix}, \quad H_A(L_{ix},L_{jx}) \subset L_{ix}+L_{jx} \tag{3.1}$$

hold provided that the eigenvalues of the operator $A(x)$ in any two different subspaces L_{ix} and L_{jx} are different almost everywhere for $x \in R^n$. Here $i \neq j$; $i,j \in \{1,\dots,k\}$.

Proof: (i) The necessary condition. Suppose that in some coordinates $v^1,\dots,v^n$ system (1.1) has block-diagonal form (1.2) with the diagonal blocks in the subspaces $v^1,\dots,v^{n_1} \in L_1$, $v^{n_1+1},\dots,v^{n_1+n_2} \in L_2,\dots,v^{n-n_k+1},\dots,v^n \in L_k$ that form the distributions L_j, $L_1\oplus\cdots\oplus L_k=T(R^n)$. Then the (1,1)-tensor $\widetilde{A}^{\alpha}_{\beta}(v^1,\dots,v^n)$ has invariant subspaces L_i and L_i+L_j and the definition (2.1) yields $N(L_{ix},L_{ix}) \subset L_{ix}$ and $N(L_{ix},L_{jx}) \subset L_{ix}+L_{jx}$. Hence using Eq. (2.2) and $A(L_{ix}) \subset L_{ix}$ we get the necessary conditions (3.1).

(ii) The sufficient condition. Let $P(\lambda)=\det(A-\lambda)$ be the characteristic polynomial of the (1,1)-tensor A^{α}_{β}, all depend on a point $x \in R^n$. Let $A_i(x)$ be the restriction of the operator $A(x)$ onto the invariant subspace L_{ix} and $P_i(\lambda)=\det(A_i(x)-\lambda)$ be the corresponding characteristic polynomial. Since $L_{1x}\oplus\cdots\oplus L_{kx}=T_x(R^n)$, we obtain $P(\lambda)=P_1(\lambda)\cdots P_k(\lambda)$. Let us define the polynomials

$$B_j(\lambda) = P_1(\lambda)\cdots P_{j-1}(\lambda)P_{j+1}(\lambda)\cdots P_k(\lambda) = P(\lambda)/P_j(\lambda). \tag{3.2}$$

By the Cayley-Hamilton theorem we have $P_\ell(A_\ell)=0$. Hence we get $B_j(A_\ell)=0$ for $j\neq\ell$; $j,\ell \in \{1,\ldots,k\}$. The operator $B_j(A_j)$ is nondegenerate almost everywhere because the operators A_{jx} and $A_{\ell x}$ do not have coinciding eigenvalues for $j\neq\ell$ almost everywhere for $x\in R^n$. Hence the restriction of the operator $B_j(A)$ onto the invariant subspace $L_{jx}\subset T_x(R^n)$ is nondegenerate and is zero on all other subspaces $L_{\ell x}\subset T_x(R^n)$.

The polynomial $B_j(\lambda)$ has some form

$$B_j(\lambda) = \sum_{m=0}^{n-n_j} b_{jm}(x)\lambda^m, \tag{3.3}$$

where coefficients $b_{jm}(x)$ depend on point $x\in R^n$. Let $H_{B_j}(u,v)$ be the Haantjes (1,2)-tensor defined by the (1,1)-tensor

$$B_j(A) = \sum_{m=0}^{n-n_j} b_{jm}(x)A^m. \tag{3.4}$$

Applying Lemma 2, we obtain the formula

$$H_{B_j}(u,v) = T_{Q^2_{B_j}(z,\lambda)Q^2_{B_j}(z,\mu)}H_A(u,v).$$

Hence equations (3.1) yield

$$H_{B_j}(L_{ix},L_{mx}) \subset L_{ix}+L_{mx}, \quad i\neq m; \quad i,m\in\{1,\ldots,k\}. \tag{3.5}$$

Let us consider the $(n-n_j)$-dimensional distribution

$$M_{jx} = L_{1x}+\cdots+L_{(j-1)x}+L_{(j+1)x}+\cdots+L_{kx}. \tag{3.6}$$

Equations (3.5) and (3.6) yield

$$H_{B_j}(M_{jx},M_{jx}) \subset M_{jx}. \tag{3.7}$$

For any eigenvector fields $e_p(x)$, $e_q(x)$ corresponding to the eigenvalues $\lambda_p(x)$, $\lambda_q(x)$ of a (1,1)-tensor C, the formula[14]

$$H_C(e_p,e_q) = (C-\lambda_p)^2(C-\lambda_q)^2[e_p,e_q] \tag{3.8}$$

holds, where $[e_p,e_q]$ is the commutator of the vector fields. By the definition of the (1,1)-tensor $B_j(A)$, all vector fields $v(x)\in M_{jx}$ are zero eigenvector fields of the (1,1)-tensor $B_j(A)$, $B_j(A)v=0$, because the (1,1)-tensor $B_j(A)$ annihilates the distribution M_j. Applying formula (3.8) to the arbitrary vector fields $v,w\in M_j$, we obtain

$$H_{B_j}(v,w) = (B_j(A))^4[v,w]. \tag{3.9}$$

Since $L_{jx}\oplus M_{jx}=T_x(R^n)$ and the restriction of the operator $B_j(A)$ onto the invariant subspace L_{jx} is nondegenerate, the generalized zero eigenspace of the operator $B_j(A(x))$ is exactly the subspace M_{jx} (3.6). Hence Eqs. (3.7) and (3.9) yield $[v,w](x)\in M_{jx}$ for any vector fields $v(x),w(x)\in M_{jx}$ and almost everywhere for $x\in R^n$. Hence by the continuity $[v,w](x)\in M_{jx}$ everywhere and the distribution M_j is involutive. Equation (3.9) implies $H_{B_j}(M_{jx},M_{jx})=0$; Eq. (2.1) yields $N_{B_j}(M_{jx},M_{jx})=0$. Applying Frobenius theorem,[16] we obtain that each point $x\in R^n$ belongs to an $(n-n_j)$-dimensional integral submanifold that is tangent to the linear subspaces M_{jx}. Hence there exist n_j functionally independent functions $f_{j1}(x),\ldots,f_{jn_j}(x)$ such that

$$\mathrm{d}f_{jm}(L_i)=0, \quad i\neq j, \quad m=1,\ldots,n_j,$$

and differentials $\mathrm{d}f_{jm}$ form a basis of the dual space L_j^*. Hence all differentials $\mathrm{d}f_{jm}$ for $j=1,\ldots,k$ and $m=1,\ldots,n_j$ form a basis of the dual space $T^*(R^n)=L_1^*\oplus\cdots\oplus L_k^*$. Therefore the n functions $v_\ell=f_{im}(x)$, $\ell=1,\ldots,n$, form a system of local coordinates on the manifold R^n.

The integrability of the distributions M_j implies the integrability of each distribution L_j because L_j is the intersection of all distributions M_ℓ for $\ell\neq j$. The distribution L_j is defined by the equations

$$\mathrm{d}f_{im}(L_j)=0, \quad i\neq j; \quad i,j\in\{1,\ldots,k\}, \quad m=1,\ldots,n_i.$$

Hence in the coordinates $v_\ell=f_{im}(x)$ the integral submanifolds of the distribution L_j are n_j-dimensional planes defined by the equations

$$f_{im}(x)=c_{im}=\mathrm{const}, \quad i\neq j; \quad i,j\in\{1,\ldots,k\}, \quad m=1,\ldots,n_i.$$

Coordinates f_{jm}, $m=1,\ldots,n_j$, are arbitrary on L_j. Since the subspaces L_{jx} are A invariant, the (1,1)-tensor A_β^α has the block-diagonal form in the local coordinates $f_{im}(x)$ with $(n_j\times n_j)$-dimensional blocks. This gives the block diagonalization of the system (1.1) in the local coordinates $v_\ell=f_{im}$, $\ell=1,\ldots,n$. □

IV. CONCRETE APPLICATIONS

(i) Theorem 1 has the following equivalent form in terms of the Nijenhuis tensor (notations are the same).

Theorem 2: *The necessary and sufficient conditions for the block diagonalizability of system (1.1) are*

$$A(L_{ix})\subset L_{ix}, \quad N_A(L_{ix},L_{ix})\subset L_{ix}, \quad N_A(L_{ix},L_{jx})\subset L_{ix}+L_{jx}, \tag{4.1}$$

provided that the eigenvalues of the operator $A(x)$ in any two different subspaces L_{ix} and L_{jx} are different almost everywhere for $x\in R^n$. Here $i\neq j$; $i,j\in\{1,\ldots,k\}$.

Indeed, the necessity of conditions (4.1) is proved in Theorem 1. Their sufficiency follows from Theorem 1 because Eqs. (2.2) and (4.1) imply Eqs. (3.1). □

For the case of block diagonalization with only two diagonal blocks and $L_{1x}\oplus L_{2x}=T_x(R^n)$, the necessary and sufficient conditions (4.1) have the simple form $A(L_{ix})\subset L_{ix}$, $N_A(L_{ix},L_{ix})\subset L_{ix}$, $i=1,2$.

(ii) *Example 1:* Let us consider the hydrodynamic type system

$$u_{it}=-u_iu_{ix}-\sum_{j=1}^{k}f_j(\eta_j)\eta_{jx}, \quad \eta_{it}=-\eta_iu_{ix}-u_i\eta_{ix}, \tag{4.2}$$

where $i=1,\ldots,k$. The systems (4.2) with arbitrary functions $f_j(\eta_j)$ form perturbations of the Benney system[4] that corresponds to $f_j(\eta_j)=1$. Let $e_i=\partial/\partial u_i$, $h_i=\partial/\partial\eta_i$ be the basis tangent vectors. For system (4.2), the (1,1)-tensor A_j^i has the form

$$A(e_i)=-u_ie_i-\eta_ih_i, \quad A(h_i)=-f_iE-u_ih_i, \quad E=e_1+\cdots+e_k. \tag{4.3}$$

The corresponding Nijenhuis tensor is defined by the formulas

$$N(e_i,e_j)=0, \quad N(h_i,h_j)=f_ih_j-f_jh_i, \quad N(e_i,h_j)=-f_ie_i+\eta_if_j'\delta_j^iE, \tag{4.4}$$

where $f_j'=\mathrm{d}f_j/\mathrm{d}\eta_j$. Let v be a tangent vector $v=\Sigma_i(x_ie_i+y_ih_i)$. We define a 1-form $\psi(v)=f_1y_1+\cdots+f_ky_k$. For any tangent vector $w=\Sigma_i(\alpha_ie_i+\beta_ih_i)$, formulas (4.4) yield

$$N(v,w)=\psi(v)w-\psi(w)v+\varphi(v,w)E, \tag{4.5}$$

where $\varphi(v,w)$ is the 2-form,

$$\varphi(v,w)=\sum_{i=1}^{k}(x_i\beta_i-y_i\alpha_i)\,\eta_i f_i'(\eta_i). \tag{4.6}$$

For the Haantjes tensor (2.2) we find

$$H(v,w)=\varphi(v,w)A^2E+\varphi(Av,Aw)E-[\varphi(Av,w)+\varphi(v,Aw)]AE. \tag{4.7}$$

For the Benney system one has $f_j(\eta_j)=1$ and hence $\varphi(v,w)=0$. Hence the Benney system that is a hyperbolic one[4] can be transformed to a diagonal form because its Haantjes tensor (4.7) vanishes.

A generic perturbation (4.2) of the Benney system for $f_j'(\eta_j)\neq 0$ cannot be transformed into a block-diagonal form with three or more diagonal blocks. Indeed, for $f_j'(\eta_j)\neq 0$ the 2-form (4.6) is nondegenerate so its Lagrangian planes $\varphi(v,w)=0$ have dimension k. If a representation with three or more diagonal blocks existed then $T_x(R^n)=L_1\oplus L_2\oplus L_3$ where L_i are invariant subspaces satisfying (4.1). One subspace, say L_1, has dimension $m<k$. Let $L=L_2\oplus L_3$, then $k<\dim L=2k-m<2k$. Hence L is not a Lagrangian plane for the form $\varphi(v,w)$ (4.6) and there exist vectors v, $w\in L$ such that $\varphi(v,w)\neq 0$. Hence Eqs. (4.1) and (4.5) yield that vector $E\in L$. Vector E is a cyclic vector for the operator A_j^i (4.3): the vectors $E,AE,A^2E,\ldots,A^{2k-1}E$ form a basis. All these vectors in view of (4.1) belong to the subspace L. Hence $\dim L=2k$. The contradiction proves that the block-diagonalization with three or more blocks is impossible. □

(iii) The Haantjes theorem[2] on the X_m-forming sets of eigenvalues of a (1,1)-tensors $A_j^i(u)$ implies that for the complete diagonalizability of a system (1.1) with real and distinct eigenvalues of $A_j^i(u)$ it is necessary and sufficient that the Haantjes tensor (1.3) vanishes.

Proposition 2: If a (1,1)-tensor $A_j^i(u)$ (1.1) has complex and real distinct eigenvalues and its Haantjes tensor is zero then it has a block-diagonal representation with 2×2 and 1×1 blocks.

Proof: Since all eigenvalues of $A_j^i(u)$ are distinct, to each pair of complex conjugate eigenvalues it corresponds a two-dimensional invariant distribution L_j and to each real eigenvector it corresponds an invariant vector field L_k. Since $H_A(v,w)=0$, the conditions (3.1) of Theorem 1 are satisfied and we obtain the existence of the required block-diagonal form. □

Remark 3: Proposition 2 proves that condition $H_A(v,w)=0$ is sufficient for the 2×2 and 1×1 block diagonalization. However it is not necessary as the following example shows. Let us consider the simplest block-diagonal (1,1)-tensor

$$A_j^i=\begin{pmatrix}\alpha & -\beta & 0\\ \beta & \alpha & 0\\ 0 & 0 & \gamma\end{pmatrix}, \tag{4.8}$$

where α,β,γ are arbitrary smooth functions of x^1,x^2,x^3. Matrix (4.8) has eigenvalues $\lambda_{1,2}=\alpha\pm i\beta$, $\lambda_3=\gamma$. The corresponding Haantjes tensor (1.3) is nonzero:

$$H_{23}^1=2\beta^2\left((\alpha-\gamma)\frac{\partial\beta}{\partial x^3}-\beta\frac{\partial\alpha}{\partial x^3}\right).$$

(iv) A Hamiltonian system of n pde's (1.1) is called nondegenerate if the corresponding (2,0)-tensor $g^{ij}(u)$ is nondegenerate.

Proposition 3: A nondegenerate Hamiltonian system (1.1) in R^3 with $H_A(v,w)\neq 0$ does not have any block-diagonal representations.

Proof: For the three-dimensional case, the Haantjes tensor $H_A(v,w)$ defines a Lie algebra structure $\mathcal{G}_x$ in each tangent space $T_x(M^3)$.[14] For any nondegenerate Hamiltonian system (1.1) with $H_A(v,w)\neq 0$, the Lie algebras $\mathcal{G}_x$ are simple,[14] so the derivative Lie subalgebras $\mathcal{G}_x'=\mathcal{G}_x$. Suppose that in some coordinates u^1,u^2,u^3 the system has a block-diagonal form

$$A_j^i = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix}. \tag{4.9}$$

Then for the coordinate basis vectors e_1, e_2, e_3, the formulas (4.9), (2.1), and (2.2) imply $H_A(e_1, e_2)=0$. Hence the derivative Lie subalgebras $\mathcal{G}'_x$ are generated by two vectors $H_A(e_1, e_3)$ and $H_A(e_2, e_3)$ and $\mathcal{G}'_x \neq \mathcal{G}_x$. The contradiction proves that the block-diagonal representation (4.9) is impossible. □

Proposition 4: The following identities hold: for the Haantjes tensor

$$H_{f(x)A+g(x)I}(u,v) = f^4(x) H_A(u,v), \tag{4.10}$$

where I is the unit (1,1) tensor, $I_j^k = \delta_j^k$, $f(x)$ *and* $g(x)$ *are smooth functions; and for the Nijenhuis tensor*

$$N_{f(x)A+g(x)I}(u,v) = f^2(x) N_A(u,v) + f[(Au(f) - u(g))Av - (Av(f) - v(g))Au - u(f)A^2v + v(f)A^2u + Au(g)v - Av(g)u]. \tag{4.11}$$

Indeed, for the operator

$$B(A,x) = f(x)A(x) + g(x)I, \tag{4.12}$$

we have

$$b_1(x) = f(x), \quad b_0(x) = g(x), \quad Q_B(z,\lambda) = f(x). \tag{4.13}$$

Since $Q_B(z,\lambda)Q_B(z,\mu)=f^2(x)$, formula (2.17) implies identity (4.10). The identity (4.11) follows from formula (2.16) after substituting expressions (4.12) and (4.13). □

Remark 4: Formula (4.10) means that the Haantjes tensor $H_A(u,v)$ is invariant with respect to the gauge transformations (4.12). The gauge invariance of the Haantjes (1,2)-tensor was first discovered in Ref. 14. Formula (4.11) shows that the Nijenhuis tensor $N_A(u,v)$ is not gauge invariant.

Remark 5: In Ref. 17 we prove that the necessary and sufficient conditions for the reducibility of a system (1.1) into k noninteracting subsystems[1] have the form

$$A(L_{ix}) \subset L_{ix}, \quad N_A(L_{ix}, L_{ix}) \subset L_{ix}, \quad N_A(L_{ix}, L_{jx}) = 0,$$

where notations are the same as in Theorem 1.

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Nonlinear Schrödinger equation with harmonic potential

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I. INTRODUCTION

In this paper, we study the Cauchy problem for the nonlinear Schrödinger equation with harmonic potential

$$i\varphi_t = -\Delta\varphi + |x|^2\varphi - |\varphi|^{p-1}\varphi, \quad t > 0,\ x \in R^N,$$

$$\varphi(0,x) = \varphi_0(x), \tag{1}$$

where $\varphi=\varphi(t,x)$ denotes the complex-value wave function, $i=\sqrt{-1}$, Δ is the Laplace operator on R^N, $1<p<(N+2)/(N-2)^+$ [we use the convention $(N+2)/(N-2)^+=N-2$ when $N\geq 3$ and $(N+2)/(N-2)^+=\infty$ when $N=1,2$]. When $p=3$, (1) describes attractive Bose-Einstein condensation.[1–3]

For nonlinear Schrödinger equation without potential

$$i\varphi_t + \Delta\varphi + |\varphi|^{p-1}\varphi = 0, \quad t > 0,\ x \in R^N, \quad \varphi(0,x) = \varphi_0(x), \tag{2}$$

many results[4–7] have been achieved. In particular, Zhang[8,9] obtained a sharp criterion for blow-up and global existence of solutions by variational methods.

For (1), Cazenave[10] and Oh[11] established the local existence in corresponding energy space. Zhang[12,13] obtained blow-up and global existence of solutions, the stability of standing waves.

In this paper, we further exploit the sharp conditions of global existence which is attributed to Zhang.[9,14] By establishing a cross-constrained variational problem and the invariant sets under the flow generated by the Cauchy problem (1), we can derive some new blowup theorems and establish the sharp criterion for global existence and blowup of the solutions of (1). From viewpoint of physics, the sharp criterion is just a sharp stability threshold of attractive Bose-Einstein condensation.[1,12] These arguments originate in Pagne and Scattinger,[15] Levine,[16] Berestycki and Cazenave,[17] Weinstein.[18]

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This paper is organized as follows. In the second section, we give some preliminaries. In the third section, we construct two constrained variational problems. In the fourth section, we give some new theorems of blow-up and sharp sufficient conditions of global existence.

II. PRELIMINARIES

For (1), we define the energy space in the course of nature by

$$H := \{\psi \in H^1(\mathbb{R}^N), \int |x|^2|\psi|^2 \, dx < \infty\}. \tag{3}$$

Here and hereafter, for simplicity, we denote $\int_{\mathbb{R}^N} dx$ by $\int dx$, H becomes a Hilbert space, continuously embedded in $H^1(\mathbb{R}^N)$, when endowed with the inner product as follows:

$$\langle \psi, \phi \rangle_H := \int \nabla\psi \nabla \bar{\phi} + \psi\bar{\phi} + |x|^2\psi\bar{\phi} \, dx, \tag{4}$$

whose associated norm we denote by $\|\cdot\|_H$.

From Cazenave[10] and Oh,[11] we can get the local well-posedness for the Cauchy problem (1) in energy space H.

Proposition 2.1: Let $\varphi_0 \in H$. Then there exists a unique solution φ of the Cauchy problem (1) *in $C([0,T];H)$ for some $T \in (0,\infty]$ (maximal existence time), and either $T=\infty$ (global existence) or else $T<\infty$ and*

$$\lim_{t\to T} \|\varphi\|_H = \infty \text{ (blow-up)}.$$

First we have the following lemmas.[7,10,19]

Lemma 2.2: Let $\varphi_0 \in H$ and φ be a solution of the Cauchy problem (1) *in $C([0,T];H)$. Set the energy functional*

$$E(\varphi) = \frac{1}{2}\int \left(|\nabla\varphi|^2 + |x|^2|\varphi|^2 - \frac{2}{p+1}|\varphi|^{p+1} \right) dx.$$

Then one has

$$\int |\varphi|^2 \, dx = \int |\varphi_0|^2 \, dx, \tag{5}$$

$$E(\varphi) \equiv E(\varphi_0). \tag{6}$$

Lemma 2.3: Let $\varphi_0 \in H$ and $1<p<1+(4/N)$. Then the solution φ of the Cauchy problem (1) *exists globally.*

Lemma 2.4: Let $\varphi_0 \in H$ and $1+(4/N) \le p < (N+2)/(N-2)^+$. If $E(\varphi_0)<0$. Then the solution φ of the Cauchy problem (1) *blows up in a finite time.*

Remark 2.5: From the above two lemmas we see that $p=1+\frac{4}{N}$ is critical nonlinearity index for blow-up and global existence. In the following we call $p<1+(4/N), p=1+(4/N), p>1+(4/N)$ subcritical, critical, supercritical cases, respectively.

Lemma 2.6: Let $\varphi_0 \in H$ and φ be the solution of the Cauchy problem (1) *in $C([0,T];H)$, $|x|\varphi_0 \in L^2(R^N)$. Set $J(t)=\int |x|^2|\varphi|^2 \, dx$. Then one has*

$$J''(t) = 8\int \left(|\nabla\varphi|^2 - |x|^2|\varphi|^2 - \frac{N(p-1)}{2(p+1)}|\varphi|^{p+1} \right) \mathrm{d}x. \tag{7}$$

III. THE CROSS-CONSTRAINED VARIATIONAL PROBLEM

For $u \in H$ and $1 < p < (N+2)/(N-2)^+$, we define the following functionals:

$$I(u) = \frac{1}{2}\int \left(|\nabla u|^2 + |u|^2 + |x|^2|u|^2 - \frac{2}{p+1}|u|^{p+1} \right) \mathrm{d}x, \tag{8}$$

$$S(u) = \int \left(|\nabla u|^2 + |u|^2 - \frac{N(p-1)}{2(p+1)}|u|^{p+1} \right) \mathrm{d}x, \tag{9}$$

$$Q(u) = \int \left(|\nabla u|^2 + |x|^2|u|^2 - \frac{N(p-1)}{2(p+1)}|u|^{p+1} \right) \mathrm{d}x, \tag{10}$$

and define the manifold

$$M := \{u \in H \setminus \{0\}, S(u) < 0, Q(u) = 0\}.$$

Now we consider two constrained variational problems,

$$d_\omega = \inf_{\{u \in H\setminus\{0\}, S(u)=0\}} I(u), \tag{11}$$

$$d_M = \inf_{u \in M} I(u). \tag{12}$$

First we have the following.

Lemma 3.1: $d_\omega > 0$ *provided* $1 + (4/N) < p < (N+2)/(N-2)^+$.

Proof: From $S(u) = 0$, we have

$$I(u) = \int \left(\frac{1}{2} - \frac{2}{N(p-1)} \right) |\nabla u|^2 + \left(\frac{1}{2} - \frac{2}{N(p-1)} \right) |u|^2 + \frac{1}{2}|x|^2|u|^2 \, \mathrm{d}x. \tag{13}$$

Since $1 + (4/N) < p < (N+2)/(N-2)^+$, (13) and $u \neq 0$ implies that $I(u) > 0$. Thus from (11), we get $d_\omega \geq 0$. In the following we use the Sobolev embedding inequality:

$$\int |u|^{p+1} \, \mathrm{d}x \leq c\left(\int |\nabla u|^2 + |u|^2 \, \mathrm{d}x \right)^{(p+1)/2}. \tag{14}$$

Here and hereafter c denotes various positive constants. From $S(u) = 0$ it follows that

$$\int |\nabla u|^2 + |u|^2 \, \mathrm{d}x = \frac{N(p-1)}{2(p+1)} \int |u|^{p+1} \, \mathrm{d}x \leq c\left(\int |\nabla u|^2 + |u|^2 \, \mathrm{d}x \right)^{(p+1)/2}.$$

From $p > 1$ it follows that

$$\int |\nabla u|^2 + |u|^2 + |x|^2|u|^2 \, \mathrm{d}x > \int |\nabla u|^2 + |u|^2 \, \mathrm{d}x \geq c > 0. \tag{15}$$

Since $p > 1 + (4/N)$, (13) and (15) yields that

$$I(u) \geq c > 0, \quad \textit{for all } u \in M.$$

Thus (11) implies that $d_\omega > 0$ for $1 + (4/N) < p < (N+2)/(N-2)^+$. □

Next from (12) we have the following.

Lemma 3.2: $d_M>0$ *provided* $1+(4/N)<p<(N+2)/(N-2)^+$.

Proof: Let $u\in M$. From $S(u)<0$, we have $u\neq 0$. From $Q(u)=0$, we have

$$I(u)=\int\left(\frac{1}{2}-\frac{2}{N(p-1)}\right)|\nabla u|^2+\frac{1}{2}|u|^2+\left(\frac{1}{2}-\frac{2}{N(p-1)}\right)|x|^2|u|^2\,\mathrm{d}x. \tag{16}$$

Since $1+(4/N)<p<(N+2)/(N-2)^+$, (16) and $u\neq 0$ implies that $I(u)>0$ for all $u\in M$. Thus from (12), we get $d_M\geq 0$. Now we use the Sobolev embedding inequality

$$\int|u|^{p+1}\,\mathrm{d}x\leq c\left(\int|\nabla u|^2+|u|^2\,\mathrm{d}x\right)^{(p+1)/2}. \tag{17}$$

Here and hereafter c denotes various positive constants. From $S(u)<0$ it follows that

$$\int|\nabla u|^2+|u|^2\,\mathrm{d}x<\frac{N(p-1)}{2(p+1)}\int|u|^{p+1}\,\mathrm{d}x\leq c\left(\int|\nabla u|^2+|u|^2\,\mathrm{d}x\right)^{(p+1)/2}.$$

From $p>1$ it follows that

$$\int|\nabla u|^2+|u|^2+|x|^2|u|^2\,\mathrm{d}x>\int|\nabla u|^2+|u|^2\,\mathrm{d}x\geq c>0. \tag{18}$$

Since $p>1+(4/N)$, (16) and (18) yields that

$$I(u)\geq c>0,\quad \textit{for all } u\in M.$$

Thus (12) implies that $d_M>0$ for $1+(4/N)<p<(N+2)/(N-2)^+$. □

Now we define

$$d:=\min\{d_\omega,d_M\}. \tag{19}$$

Then from Lemma 3.1 and Lemma 3.2 it implies the following.

Theorem 3.3: $d>0$ *when* $1+(4/N)<p<(N+2)/(N-2)^+$.

Remark 3.4: We call the variational problem (12) *cross-constrained variational problem since there are two constrained conditions in* (12). *The following corresponding invariant manifold will be called cross-invariant manifold.*

Theorem 3.5: *Define*

$$K:=\{\phi\in H,I(\phi)<d,Q(\phi)<0,S(\phi)<0\}. \tag{20}$$

If $1+(4/N)<p<(N+2)/(N-2)^+$, *then K is an invariant manifold of* (1), *that is, if* $\varphi_0\in K$, *then the solution* $\varphi(t,x)$ *of the Cauchy problem* (1) *also satisfies* $\varphi(t,x)\in K$ *for any* $t\in[0,T)$.

Proof: Let $\varphi_0\in K$. By Proposition 2.1, there exists a unique $\varphi(t,x)\in C([0,T);H)$ with $T\leq\infty$ such that $\varphi(t,x)$ is a solution of the Cauchy problem (1). From (5), (6), we have

$$I(\varphi)=I(\varphi_0),\quad t\in[0,T). \tag{21}$$

Thus $I(\varphi_0)<d$ implies that $I(\varphi)<d$ for any $t\in[0,T)$.

Now we show $S(\varphi)<0$ for $t\in[0,T)$. If otherwise, from the continuity, there were a $t_0\in[0,T)$ such that $S(\varphi(t_0,.))=0$. By (21), $I(\varphi(t_0,.))=\int\left[\frac{1}{2}-[2/N(p-1)]\right]|\nabla\varphi(t_0,.)|^2+\frac{1}{2}|\varphi(t_0,.)|^2+\left[\frac{1}{2}-[2/N(p-1)]\right]|x|^2|\varphi(t_0,.)|^2\,\mathrm{d}x=I(\varphi_0)>0$, note that $1+(4/N)<p<(N+2)/(N-2)^+$, thus $\varphi(t_0,x)\neq 0$. From (11) and (19) it follows that $I(\varphi(t_0,.))\geq d$. This is contradictory with $I(\varphi(t,.))<d$ for $t\in[0,T)$. Therefore $S(\varphi(t,.))<0$ for all $t\in[0,T)$.

At last we show $Q(\varphi(t,.))<0$ for $t\in[0,T)$. If otherwise, from the continuity, there were a $t_1\in[0,T)$ such that $Q(\varphi(t_1,.))=0$. Because we have showed $S(\varphi(t_1,.))<0$, it follows that $\varphi(t_1,.)\in M$. Thus (12) and (19) implies $I(\varphi(t_1,.))\geq d_M\geq d$. This is contradictory with $I(\varphi(t,.))<d$ for $t\in[0,T)$. Therefore $Q(\varphi(t,.))<0$ for all $t\in[0,T)$.

From the above we proved $\varphi(t,x)\in K$ for any $t\in[0,T)$.

This completes the proof of this theorem. □

By the same argument as Theorem 3.5, we can get the following results.

Theorem 3.6: *Define*

$$K_+ := \{\phi\in H, I(\phi)<d, Q(\phi)>0, S(\phi)<0\},$$

$$R_- := \{\phi\in H, I(\phi)<d, S(\phi)<0\},$$

$$R_+ := \{\phi)\in H, I(\phi)<d, S(\phi)>0\}.$$

If $1+(4/N)<p<(N+2)/(N-2)^+$, *then* K_+, R_-, R_+ *are all invariant manifolds of* (1).

IV. SHARP CONDITIONS FOR GLOBAL EXISTENCE

Theorem 4.1: *Let* $1+(4/N)<p<(N+2)/(N-2)^+$. *If* $\varphi_0\in K_+\cup R_+$, *then the solution* φ *of the Cauchy problem* (1) *globally exists on* $t\in[0,\infty)$.

Proof: First we let $\varphi_0\in K_+$. Thus Theorem 3.6 implies that the solution φ of the Cauchy problem (1) satisfies that $\varphi(t,.)\in K_+$ for $t\in[0,T)$. For fixed $t\in[0,T)$, denote $\varphi(t,.)=\varphi$. Thus we have $I(\varphi)<d$, $Q(\varphi)>0$. It follows that from (8) and (10),

$$\int\left(\frac{1}{2}-\frac{2}{N(p-1)}\right)|\nabla\varphi|^2+\frac{1}{2}\omega|\varphi|^2\,dx+\left(\frac{1}{2}-\frac{2}{N(p-1)}\right)|x|^2|\varphi|^2\,dx<d. \tag{22}$$

For $1+(4/N)<p<(N+2)/(N-2)^+$, from (22), we always have

$$\int|\nabla\varphi|^2+|x|^2|\varphi|^2\,dx<c. \tag{23}$$

Therefore Proposition 2.1 implies that φ globally exists on $t\in[0,\infty)$.

Thus for $\varphi_0\in K_+$ we proved the solution φ of the Cauchy problem (1) globally exists on $t\in[0,\infty)$.

Now let $\varphi_0\in R_+$. Thus Theorem 3.6 implies that the solution φ of the Cauchy problem (1) satisfies that $(\varphi(t,.))\in R_+$ for $t\in[0,T)$. Thus we have $I(\varphi)<d$, $S(\varphi)>0$. It follows that

$$\left(\frac{1}{2}-\frac{2}{N(p-1)}\right)\int|\nabla\varphi|^2+\omega|\varphi|^2\,dx+\int\frac{1}{2}|x|^2|\varphi|^2\,dx<d. \tag{24}$$

Thus Proposition 2.1 implies that φ globally exists on $t\in[0,\infty)$.

This completes the proof of this theorem. □

Theorem 4.2: *Let* $1+(4/N)<p<(N+2)/(N-2)^+$. *If* $\varphi_0\in K$ *and* $|\cdot|\varphi_0\in L^2(R^N)$, *then the solution* φ *of the Cauchy problem* (1) *blows up in a finite time.*

Proof: From $\varphi_0\in K$, Theorem 3.5 implies that the solution φ of the Cauchy problem (1) satisfies that $\varphi(t,.)\in K$ for $t\in[0,T)$. For $J(t)=\int|x|^2|\varphi|^2\,dx$, (7) and (10) imply that

$$J''(t)<8Q(\varphi(t,.)),\quad t\in[0,T). \tag{25}$$

Fix $t\in[0,T)$, and denote $\varphi(t,.)=\varphi$. Since $\varphi\in K$, it follows that

$$J''(t) < 8Q(\varphi) < 0. \tag{26}$$

Obviously $J(t)$ cannot verify (26) for all time t.[19] Therefore from Proposition 2.1, it must be the case that $T<\infty$, which implies

$$\lim_{t\to T}\|\varphi\|_H = \infty .$$

This completes the proof of this theorem. □

Remark 4.3: It is clear that

$$\{\phi \in H, I(\phi) < d\} = R_+ \cup K_+ \cup K.$$

Thus Theorem 4.2 shows that Theorem 4.1 is sharp.

By the above remark, we immediately have the following.

Corollary 4.4: Let $1+(4/N)<p<(N+2)/(N-2)^+$ *and* φ_0 *satisfy* $I(\varphi)<d$, *then the solution* φ *of the Cauchy problem* (1) *blows up in a finite time if and only if* $\varphi_0 \in K$.

By Theorem 4.1 we also get another condition for global existence of the solution of (1).

Corollary 4.5: If $\varphi_0 \in H$ *and satisfy* $\|\varphi_0\|_H^2 < 2d$, *then the solution* φ *of the Cauchy problem* (1) *globally exists on* $t \in [0,\infty)$.

Proof: From $\|\varphi_0\|_H^2 < 2d$, we have $I(\varphi_0) < d$. Moreover we claim that $S(\varphi_0) > 0$. If otherwise, there were a $0<\lambda\leq 1$ such that $S(\lambda\varphi_0)=0$. Thus $I(\lambda\varphi_0)\geq d$. On the other hand,

$$\|\lambda\varphi_0\|_H^2 = \lambda^2\|\varphi_0\|_H^2 < 2\lambda^2 d < 2d.$$

It follows that $I(\lambda\varphi_0)<d$. This is a contradiction. Therefore we have $\varphi_0 \in R_+$. Thus Theorem 4.1 implies this corollary. □

Remark 4.6: It is clear that d_ω *and* d_M *in this paper is different from in Ref.* 14.

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Scale invariance in the spectral action

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The arbitrary mass scale in the spectral action for the Dirac operator is made dynamical by introducing a dilaton field. We evaluate all the low-energy terms in the spectral action and determine the dilaton couplings. These results are applied to the spectral action of the noncommutative space defined by the standard model. We show that the effective action for all matter couplings is scale invariant, except for the dilaton kinetic term and Einstein-Hilbert term. The resulting action is almost identical to the one proposed for making the standard model scale invariant as well as the model for extended inflation and has the same low-energy limit as the Randall-Sundrum model. Remarkably, all desirable features with correct signs for the relevant terms are obtained uniquely and without any fine tuning. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2196748]

I. INTRODUCTION

It is known that the standard model of strong and electroweak interactions is classically almost scale invariant, and that the only terms that break the dilatation symmetry are the mass terms in the Higgs sector. Scale invariance of the classical Lagrangian can be achieved by introducing a compensating dilaton field.[1–3] Breaking of scale invariance occurs after the electroweak symmetry is broken spontaneously through the generation of radiative corrections to the scalar potential. The dilaton mass scale is much larger than the weak scale and could be as large as the GUT scale or Planck scale. This leads naturally to consider the coupling of the dilaton to gravity. The dilaton is always part of the low energy spectrum in string theory. Historically it first appeared in the Jordan-Brans-Dicke theory of gravity which corresponds to one particular coupling of the dilaton to the metric.[2] The dilaton plays a fundamental role in models of inflation.[4] It also appears in the gravitational couplings of the noncommutative Connes-Lott formulation of the standard model,[5–8] where the dilaton is the scalar field that couples the two sheets of space time. The resulting matter interactions in this case are also scale invariant, and the gravitational couplings are different than the Jordan-Brans-Dicke theory. More recently, a scalar field, the radion field, appeared in the Randall-Sundrum (RS) scenario of compactification[9] which is related to the question of masses and scales in physics. The RS scenario was shown to be equivalent to the results derived from noncommutative geometry,[10] which is not too surprising, because both the Connes-Lott model and the RS model, describe a system with two branes.

At present, and within the noncommutative geometric picture, the spectral action gives the most elegant formulation of the standard model.[11,12] All details of the standard model as well as its unification with gravity are achieved by postulating the action

$$\text{Trace } F(D^2/m^2) + \langle \Psi | D | \Psi \rangle,$$

where D is the Dirac operator of a certain noncommutative space and Ψ is a spinor in the Hilbert space of the observed quarks and leptons. However, the dilaton field does not appear in the spectral action, which is to be contrasted with the Connes-Lott formulation of the noncommutative action where the dilaton field is part of the gravitational interactions. This suggests that the Dirac

operator used in the construction of the spectral action should be modified in order to take into account the presence of the dilaton.

The appearance of the dilaton field in physical models is related to the question of mass and scales. It is therefore natural to consider replacing the mass parameter in the ratio D^2/m^2 by a function of the dilaton, thus introducing a sliding scale, as the Dirac operator have the dimension of mass. This is also relevant when dealing with noncompact manifolds where D no longer has discrete spectrum and the counting of eigenvalues requires a localization. Let the dynamical scale factor ρ be written in the form

$$\rho = me^{\phi},$$

where we assume that ϕ is dimensionless. The dilaton can be related to a scalar field σ of dimension one by writing

$$\phi = \frac{1}{f}\sigma,$$

where f is the dilaton decay constant. The mass scale m can be absorbed by the redefinition

$$\phi \to \phi - \ln m,$$

and therefore we can assume, without any loss in generality, that $\rho = e^{\phi}$. One can always recover the scale m by performing the opposite transformation $\phi \to \phi + \ln m$. Now using ρ instead of the scalar m in the counting of eigenvalues:

$$N(m) = \mathrm{Dim}\{D^2 \leqslant m^2\} \to N(\rho) = \mathrm{Dim}\{D^2 \leqslant \rho^2\}$$

is equivalent to replacing the operator D^2/m^2 in Ref. 11 by

$$P = e^{-\phi} D^2 e^{-\phi}.$$

If we insist that the metric $g_{\mu\nu}$ be dimensionless to insure that its flat limit be the Minkowski metric, then the scale m will explicitly appear in the action after rescaling $e^{\phi} \to me^{\phi}$. Otherwise we can absorb this mass scale by assuming that the metric has the dimension of mass.

The aim of this article is to determine the interactions of the dilaton field ϕ with all other fields present in the spectral action formulation of the standard model. Because of the spectral character of the action, it is completely determined from the form of P and there is no room for fine tuning the results. It is then very reassuring to find that the resulting interactions are identical to those constructed in the literature by postulating a hidden scale invariance of the matter interactions.[3] These are also equivalent to the interactions of the radion field in the RS model.[9] All of these results now support the conclusion that space time at high energies reveals its discrete structure, and is governed by noncommutative geometry. The plan of this article is as follows. In Sec. II we briefly review the derivation of the spectral action and comment on the modifications needed to include the dilaton. In Sec. III we derive the Seeley-de Witt coefficients of the spectral action in presence of the dilaton. In Sec. IV we give the full low-energy spectral action including dilaton interactions specialized to the noncommutative space of the standard model. In Sec. V we compare our results with those obtained by imposing scale invariance on the standard model interactions, to the RS model and the model of extended inflation. Section six is the conclusion. The appendices contain detailed proofs of some identities used.

II. A SUMMARY OF SPECTRAL ACTION

We begin by summarizing the results of Ref. 11. The square of the Dirac operator appearing in the spectral triple of a noncommutative space is written in the following form suitable to apply the standard local formulas for the heat expansion (see Ref. 13 Sec. 4.8).

$$D^2 = -(g^{\mu\nu} I \partial_\mu \partial_\nu + A^\mu \partial_\mu + B), \tag{1}$$

where $g^{\mu\nu}$ plays the role of the inverse metric, I is the unit matrix, and A^μ and B are matrix functions computed from the Dirac operator. The bosonic part of the spectral action can be expanded in a power series as a function of the inverse scale m, and is given in dimension 4 by

$$\mathrm{Trace}(F(D^2/m^2)) \simeq \sum_{n \geqslant 0} f_n a_n(D^2/m^2),$$

where F is a positive function and

$$f_0 = \int_0^\infty F(u) u \, \mathrm{d}u, \quad f_2 = \int_0^\infty F(u) \mathrm{d}u, \quad f_{2n+4} = (-1)^n F^{(n)}(0), \quad n \geqslant 0. \tag{2}$$

The positivity of the function F will insure that the actions for gravity, Yang-Mills, Higgs couplings are all positive and the Higgs mass term is negative. We will comment on the positive sign of the cosmological constant at the end of the article.

The first few Seeley-deWitt coefficients $a_n(D^2/m^2)$ are given (see Ref. 13, Theorem 4.8) by [according to our notations the scalar curvature R is negative for spheres (see Ref. 13 Sec. 2.3) and the space is Euclidean]

$$a_0(D^2/m^2) = \frac{m^4}{16\pi^2} \int_M \mathrm{d}^4x \sqrt{g} \, \mathrm{Tr}(1), \tag{3}$$

$$a_2(D^2/m^2) = \frac{m^2}{16\pi^2} \int_M \mathrm{d}^4x \sqrt{g} \, \mathrm{Tr}\left(-\frac{R}{6} + E\right), \tag{4}$$

$$a_4(D^2/m^2) = \frac{1}{16\pi^2} \frac{1}{360} \int_M \mathrm{d}^4x \sqrt{g} \, \mathrm{Tr}(-12R^\mu_{;\mu} + 5R^2 - 2R_{\mu\nu}R^{\mu\nu} + 2R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} - 60RE + 180E^2 + 60E^\mu_{;\mu} + 30\Omega_{\mu\nu}\Omega^{\mu\nu}), \tag{5}$$

whereas the odd ones all vanish

$$a_{2n+1}(D^2/m^2) = 0.$$

The notations are as follows, one lets $\Gamma^\rho_{\mu\nu}(g)$ be the Christoffel symbols of the Levi-Civita connection of the metric g and lets

$$\Gamma^\rho(g) = g^{\mu\nu}\Gamma^\rho_{\mu\nu}(g).$$

The connection form $\overline{\omega}$, its curvature Ω, and the endomorphism E are then defined by (see Ref. 13 Sec. 4.8)

$$\overline{\omega}_\mu = \tfrac{1}{2} g_{\mu\nu}(A^\nu + \Gamma^\nu(g) I), \tag{6}$$

$$\Omega_{\mu\nu} = \partial_\mu \overline{\omega}_\nu - \partial_\nu \overline{\omega}_\mu + [\overline{\omega}_\mu, \overline{\omega}_\nu], \tag{7}$$

$$E = B - g^{\mu\nu}(\partial_\mu \overline{\omega}_\nu + \overline{\omega}_\mu \overline{\omega}_\nu - \Gamma^\rho_{\mu\nu}(g)\overline{\omega}_\rho). \tag{8}$$

To understand algebraically the dependence in the operator D it is convenient to express the previous coefficients as residues and this is done as follows in the generality that we need. One lets P be a second order elliptic operator with positive scalar principal symbol and defines a zeta function as

$$\zeta_P(s) = \mathrm{Trace}(P^{-s/2}).$$

One then gets in the required generality for our purpose the equality

$$\mathrm{Trace}(F(P/m^2)) \sim \frac{m^4}{2}\mathrm{Res}_{s=4}\zeta_P(s)f_0 + \frac{m^2}{2}\mathrm{Res}_{s=2}\zeta_P(s)f_2 + \zeta_P(0)f_4 + \cdots,$$

which, using the Wodzicki residue which is given independently of D by

$$⨍ T = \mathrm{Res}_{s=0}\,\mathrm{Trace}\,(T(D^2)^{-s/2}), \tag{9}$$

can be written as

$$\mathrm{Trace}\,(F(P/m^2)) \sim \frac{m^4}{2}f_0⨍ P^{-2} + \frac{m^2}{2}f_2⨍ P^{-1} + f_4\zeta_P(0) + \cdots. \tag{10}$$

We want to compute the spectral action associated with the operator $P=e^{-\phi}D^2e^{-\phi}$, i.e., to determine the dependence of the spectral action on the dilaton field ϕ. The first term $⨍P^{-2}$ is a Dixmier trace and one can permute the functions with the operators without altering the result since the Dixmier trace vanishes on operators of order <-4. One thus gets, for any test function h,

$$⨍ hP^{-2} = ⨍ he^{4\phi}D^{-4}$$

which shows that we get an overall factor of $e^{4\phi}$ multiplying $a_0(x,D^2)$. For the second term $⨍P^{-1}$ we have

$$⨍ hP^{-1} = ⨍ he^{\phi}D^{-2}e^{\phi} = ⨍ he^{2\phi}D^{-2}$$

using the trace property of the residue and again we get an overall factor of $e^{2\phi}$ multiplying $a_2(x,D^2)$. Note that the result remains valid when the test function h is taken with values in endomorphisms of the vector bundle on which P is acting. This suggests that the invariance of the a_2 term (up to the $e^{2\phi}$ scale factor) takes place before taking the fiberwise trace. The direct computation as follows in Eq. (18) will confirm this point.

The term $f_4\zeta_P(0)$ is more tricky to analyze and we shall only give now a heuristic argument explaining why it should be independent of ϕ. We shall then check it by a direct calculation. The formal argument proceeds as follows. First one lets

$$P(t) = e^{-t\phi}D^2e^{-t\phi}$$

so that $P(0)=D^2$ and $P(1)=P$ with the previous notations. Let then

$$Y(t) = \log P(t) - \log P(0).$$

Using the equality $(a>0)$

$$\log a = \int_0^\infty \left(\frac{1}{\lambda+1} - \frac{1}{\lambda+a}\right)\mathrm{d}\lambda,$$

applied to $P(t)$ one obtains the relation

$$\frac{\mathrm{d}}{\mathrm{d}t}Y(t) = -\int_0^\infty (P(t)+\lambda)^{-1}(\phi P(t) + P(t)\phi)(P(t)+\lambda)^{-1}\mathrm{d}\lambda. \tag{11}$$

One then shows that

$$\frac{\mathrm{d}}{\mathrm{d}t}Y(t) = -2\phi + [P(t), C(t)], \tag{12}$$

where $C(t)$ is a pseudodifferential operator (see Appendix A). Thus one gets a similar expression

$$Y = Y(1) = -2\phi + \int_0^1 [P(t), C(t)]\mathrm{d}t. \tag{13}$$

Next one uses the expansional formula

$$e^{A+B}e^{-A} = \sum_0^\infty \int_{0\leqslant t_1\leqslant\cdots\leqslant t_n\leqslant 1} B(t_1)B(t_2)\ldots B(t_n)\prod \mathrm{d}t_i,$$

where

$$B(t) = e^{tA}Be^{-tA}.$$

One lets $A=-s\log P(0)$ and $B=-sY$. This gives an equality of the form

$$P^{-s} = D^{-2s} - s\int_0^1 \sigma_{-st}(Y)\mathrm{d}t D^{-2s}$$
$$+ \sum_2^\infty (-s)^n \int_{0\leqslant t_1\leqslant\cdots\leqslant t_n\leqslant 1} \sigma_{-st_1}(Y)\sigma_{-st_2}(Y)\cdots\sigma_{-st_n}(Y)\prod \mathrm{d}t_i D^{-2s},$$

where

$$\sigma_u(T) = (D^2)^u T (D^2)^{-u}.$$

One infers from this equality and the absence of poles of order >1 in the zeta functions of the form $\mathrm{Tr}(QD^{-2s})$ that the terms of order $n>1$ in s will not contribute to the value at $s=0$. Thus the following should hold:

$$\zeta_P(0) - \zeta_{D^2}(0) = -\frac{1}{2}\fint Y$$

and using (13) one gets

$$\zeta_P(0) - \zeta_{D^2}(0) = \fint \phi = 0,$$

as the residue vanishes on differential operators. It would take a lot more care to really justify the previous manipulations. Instead, in the next section, we shall show by a brute force calculation that a_4 is independent of ϕ so that the above-mentioned identity is valid.

We thus see that in the first few terms of the spectral action, the only modification we expect when the operator D^2 is replaced by P is to get an overall factor of $e^{(4-n)\phi}$ multiplying $a_n(x, D^2)$:

$$\mathrm{Trace}(F(P)) \simeq \sum_{n=0}^6 f_n \int \mathrm{d}^4x\sqrt{g}e^{(4-n)\phi}a_n(x, D^2) + \cdots.$$

Also as will be shown in Appendix B, we have the identity

$$a_n(x, e^{-\phi}D^2e^{-\phi}) = a_n(x, D^2e^{-2\phi}) = a_n(x, e^{-2\phi}D^2).$$

It is easy to check that by applying the inverse transformation $\phi\to\phi+\ln m$ one recovers all the m scaling factors obtained in Ref. 11. In the next section, we shall confirm this result by directly evaluating the spectral action associated with the operator P and in particular the low-energy terms

a_0, a_2, and a_4. We will not attempt to evaluate higher order terms as these are not needed in our analysis.

III. DILATON AND SEELEY-deWITT COEFFICIENTS

We compare quite generally the Seeley-deWitt coefficients of an operator $P_0=D^2$ given by (1) and those of the rescaled operator $P=e^{-\phi}D^2e^{-\phi}$. We use the rescaled metric G in the Einstein frame, where the dilaton factor is absorbed in the metric. First we write

$$P = e^{-\phi}D^2e^{-\phi} = -(G^{\mu\nu}\partial_\mu\partial_\nu + \mathcal{A}^\mu\partial_\mu + \mathcal{B}), \tag{14}$$

where

$$G^{\mu\nu} = e^{-2\phi}g^{\mu\nu},$$

$$\mathcal{A}^\mu = e^{-2\phi}A^\mu - 2G^{\mu\nu}\partial_\nu\phi,$$

$$\mathcal{B} = e^{-2\phi}B + G^{\mu\nu}(\partial_\mu\phi\partial_\nu\phi - \partial_\mu\partial_\nu\phi) - e^{-2\phi}A^\mu\partial_\mu\phi.$$

The Seeley-deWitt coefficients for $a_n(P)$ are expressed in terms of $\mathcal{E}$ and $\mathbf{\Omega}_{\mu\nu}$ defined by (6) so that,

$$\mathcal{E} = \mathcal{B} - G^{\mu\nu}(\partial_\mu\overline{\omega'}_\nu + \overline{\omega'}_\mu\overline{\omega'}_\nu - \Gamma^\rho_{\mu\nu}(G)\overline{\omega'}_\rho),$$

$$\overline{\omega'}_\mu = \tfrac{1}{2}G_{\mu\nu}(\mathcal{A}^\nu + \Gamma^\nu(G)),$$

$$\mathbf{\Omega}_{\mu\nu} = \partial_\mu\overline{\omega'}_\nu - \partial_\nu\overline{\omega'}_\mu + [\overline{\omega'}_\mu, \overline{\omega'}_\nu].$$

These relations imply that

$$\overline{\omega'}_\mu = \tfrac{1}{2}g_{\mu\nu}A^\nu - \partial_\mu\phi + \tfrac{1}{2}G_{\mu\nu}\Gamma^\nu(G).$$

The conformal transformations of the Christoffel connection give

$$\Gamma^\mu_{\nu\rho}(G) = \Gamma^\mu_{\nu\rho}(g) + (\delta^\mu_\nu\partial_\rho\phi + \delta^\mu_\rho\partial_\nu\phi - g_{\nu\rho}g^{\mu\sigma}\partial_\sigma\phi),$$

$$\Gamma^\mu(G) = e^{-2\phi}\Gamma^\mu(g) - 2e^{-2\phi}g^{\mu\nu}\partial_\nu\phi.$$

Using these relations we finally get

$$\overline{\omega'}_\mu = \overline{\omega}_\mu - 2\partial_\mu\phi, \tag{15}$$

$$\mathcal{E} = e^{-2\phi}(E + g^{\mu\nu}(\nabla^g_\mu\nabla^g_\nu\phi + \partial_\mu\phi\partial_\nu\phi)), \tag{16}$$

where the covariant derivative ∇^g_μ is taken with respect to the metric g. It is quite striking that the perturbation is only a scalar multiple of the identity matrix and does not involve the endomorphisms A^μ at all.

The term a_0 only involves $\sqrt{G}\,\mathrm{Tr}(1)$ which, when expressed in terms of the metric g gives $\sqrt{g}e^{4\phi}\mathrm{Tr}(1)$.

The a_2 term is proportional to

$$\int \mathrm{d}^4x\sqrt{G}\,\mathrm{Tr}\left(\mathcal{E}-\frac{1}{6}R(G)\right),$$

where the curvature scalar is constructed as function of the metric G. We now use (16) and the relation

$$R(G)=e^{-2\phi}(R(g)+6g^{\mu\nu}(\nabla^g_\mu\nabla^g_\nu\phi+\partial_\mu\phi\partial_\nu\phi)) \tag{17}$$

to obtain at the level of endomorphisms (before taking the fiberwise trace)

$$\mathcal{E}-\tfrac{1}{6}R(G)=e^{-2\phi}\left(E-\tfrac{1}{6}R(g)\right). \tag{18}$$

This of course implies the required rescaling of the a_2 term in the required generality, but it is more precise since it holds before taking the trace. We shall use this more precise form in the proof of the invariance of the a_4 term.

The term $a_4(P)$ is given by

$$\frac{1}{16\pi^2}\frac{1}{360}\int d^4x\sqrt{G}\,\mathrm{Tr}\,[(5R^2(G)-2R_{\mu\nu}(G)R^{\mu\nu}(G)+2R_{\mu\nu\rho\sigma}(G)R^{\mu\nu\rho\sigma}(G))$$

$$-60R(G)\mathcal{E}+180\mathcal{E}^2+30\mathbf{\Omega}_{\mu\nu}\mathbf{\Omega}_{\rho\sigma}G^{\mu\rho}G^{\nu\sigma}\,],$$

where we have omitted the total derivative terms $12(-R(G)+5\mathcal{E})^{\mu}_{;\mu}$. As the modification from $\overline{\omega}_\mu$ to $\overline{\omega'}_\mu$ is Abelian (15) we get

$$\mathbf{\Omega}_{\mu\nu}=\Omega_{\mu\nu}$$

and

$$\mathbf{\Omega}_{\mu\nu}\mathbf{\Omega}_{\rho\sigma}G^{\mu\rho}G^{\nu\sigma}=e^{-4\phi}\Omega_{\mu\nu}\Omega_{\rho\sigma}g^{\mu\rho}g^{\nu\sigma}.$$

Next we group the terms

$$180\mathcal{E}^2-60\mathcal{E}R(G)+5R^2(G)=180\left(\mathcal{E}-\tfrac{1}{6}R(G)\right)^2,$$

which yields upon using Eq. (18)

$$180e^{-4\phi}\left(E-\tfrac{1}{6}R(g)\right)^2.$$

We are left with the terms

$$30\mathbf{\Omega}_{\mu\nu}\mathbf{\Omega}_{\rho\sigma}G^{\mu\rho}G^{\nu\sigma}-2R_{\mu\nu}(G)R^{\mu\nu}(G)+2R_{\mu\nu\rho\sigma}(G)R^{\mu\nu\rho\sigma}(G).$$

We now use

$$30\,\mathrm{Tr}(\mathbf{\Omega}_{\mu\nu}\mathbf{\Omega}_{\rho\sigma}G^{\mu\rho}G^{\nu\sigma})=30e^{-4\phi}\mathrm{Tr}(\Omega_{\mu\nu}\Omega_{\rho\sigma}g^{\mu\rho}g^{\nu\sigma}).$$

$$-2R_{\mu\nu}(G)R^{\mu\nu}(G)+2R_{\mu\nu\rho\sigma}(G)R^{\mu\nu\rho\sigma}(G)=-R(G)^*R^*(G)+3C_{\mu\nu\rho\sigma}(G)C^{\mu\nu\rho\sigma}(G).$$

In deriving the last relation we made use of the two identities

$$R^*R^*-R^2=R^2_{\mu\nu\rho\sigma}-4R^2_{\mu\nu},$$

$$C^2_{\mu\nu\rho\sigma}-\tfrac{1}{3}R^2=R^2_{\mu\nu\rho\sigma}-2R^2_{\mu\nu},$$

where $C_{\mu\nu\rho\sigma}$ is the conformal tensor and

$$R^*R^* = \frac{1}{4\sqrt{g}}\epsilon^{\mu\nu\rho\sigma}\epsilon_{\alpha\beta\gamma\delta}R^{\alpha\beta}_{\mu\nu}R^{\gamma\delta}_{\rho\sigma}.$$

These imply

$$R^2_{\mu\nu\rho\sigma} = 2C^2_{\mu\nu\rho\sigma} - R^*R^* + \tfrac{1}{3}R^2,$$

$$R^2_{\mu\nu} = \frac{1}{2}C^2_{\mu\nu\rho\sigma} - \frac{1}{2}R^*R^* + \tfrac{1}{3}R^2.$$

The square of the conformal tensor is known to be conformal invariant

$$\int d^4x\sqrt{G}C_{\mu\nu\rho\sigma}(G)C^{\mu\nu\rho\sigma}(G) = \int \mathrm{d}^4x\sqrt{g}C_{\mu\nu\rho\sigma}(g)C^{\mu\nu\rho\sigma}(g).$$

The topological Gauss-Bonnet term is metric independent and therefore conformal invariant

$$\int \mathrm{d}^4x\sqrt{G}R(G)^*R^*(G) = \int \mathrm{d}^4x\sqrt{g}R(g)^*R^*(g),$$

and this can be rewritten as

$$\frac{1}{4}\int \mathrm{d}^4x\frac{1}{\sqrt{g}}\epsilon^{\mu\nu\rho\sigma}\epsilon_{\alpha\beta\gamma\delta}R^{\alpha\beta}_{\mu\nu}R^{\gamma\delta}_{\rho\sigma}.$$

This shows that the a_4 term has the expected invariance under the rescaling of the operator $P_0 \to P = e^{-\phi}P_0e^{-\phi}$.

IV. SPECTRAL ACTION WITH DILATON

We now use the result of the previous section to compute the spectral action with dilaton as a function of the rescaled metric G in the Einstein frame, where the dilaton factor is absorbed in the metric.

The lowest term in the spectral action is given by

$$\frac{45}{4\pi^2}f_0\int \mathrm{d}^4x\sqrt{g}e^{4\phi} = \frac{45}{4\pi^2}f_0\int \mathrm{d}^4x\sqrt{G}.$$

(Note that the dimension of the bundle on which the operator is acting is $4\times3\times15$ where the 4 is the dimension of spinors, 3 the number of generations, and $15=4\times3+3$ is the content of each generation).

The next term in the spectral action with dilaton of the standard model is, in terms of the original metric g:

$$\frac{3}{4\pi^2}f_2\int \mathrm{d}^4x\sqrt{g}e^{2\phi}\left(\frac{5}{4}R(g) - 2y^2H^*H\right). \tag{19}$$

We can transform this back to the Einstein frame with metric $G_{\mu\nu}$ so that the curvature scalar term has no scale factors in front of it. Using Eq. (17) with $g\to G$ and $\phi\to-\phi$ the curvature $R(g)$ is

$$R(g) = e^{2\phi}(R(G) + 6G^{\mu\nu}(-\nabla^G_\mu\nabla^G_\nu\phi + \partial_\mu\phi\partial_\nu\phi)),$$

and we obtain

$$\int \mathrm{d}^4x\sqrt{g}e^{2\phi}R(g) = \int \mathrm{d}^4x\sqrt{G}(R(G) + 6G^{\mu\nu}(-\nabla^G_\mu\nabla^G_\nu\phi + \partial_\mu\phi\partial_\nu\phi))$$

$$= \int \mathrm{d}^4x\sqrt{G}(R(G) + 6G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi)$$

after integrating by parts. The a_2 term (19) thus becomes

$$\frac{3}{4\pi^2}f_2\int \mathrm{d}^4x\sqrt{G}\left(\frac{5}{4}R(G) + \frac{15}{2}G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - 2y^2H'^*H'\right), \tag{20}$$

where we have defined

$$H = e^\phi H',$$

so that the only appearance of the dilaton ϕ is through its kinetic energy.

Let us pause a bit and discuss signs at this point. For a positive test function F the coefficients f_0, f_2, f_4 are all positive. It is important that the Einstein term $\int \mathrm{d}^4x\sqrt{G}R(G)$ appears in (20) with the correct sign for the Euclidean functional integral, and that the kinetic term for ϕ namely $\int \mathrm{d}^4x\sqrt{G}G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$ appears with a positive coefficient in (20).

The next term coming from $a_4(x,P)$ is unchanged for the spectral action with dilaton, and thus given independently of ϕ by Ref. 11,

$$\frac{f_4}{4\pi^2}\int \mathrm{d}^4x\sqrt{g}\left(\frac{1}{32}(11R(g)^*R^*(g) - 18C_{\mu\nu\rho\sigma}(g)C_{\alpha\beta\gamma\delta}(g)g^{\mu\alpha}g^{\nu\beta}g^{\rho\gamma}g^{\sigma\delta})\right.$$
$$+ 3y^2\left(D_\mu H^*D_\nu H g^{\mu\nu} - \frac{1}{6}R(g)H^*H\right)$$
$$\left. + \left(g_3^2G^i_{\mu\nu}G^i_{\rho\sigma} + g_2^2F^\alpha_{\mu\nu}F^\alpha_{\rho\sigma} + \frac{5}{3}g_1^2B_{\mu\nu}B_{\rho\sigma}\right)g^{\mu\rho}g^{\nu\sigma} + 3z^2(H^*H)^2\right),$$

where we have omitted total derivatives as they only contribute to boundary terms. Let us show that we can rewrite this term in the following way as a function of the metric $G_{\mu\nu}$ by making use of the conformal invariance of a_4:

$$\frac{f_4}{4\pi^2}\int \mathrm{d}^4x\sqrt{G}\left(\frac{1}{32}(11R(G)^*R^*(G) - 18C_{\mu\nu\rho\sigma}(G)C_{\alpha\beta\gamma\delta}(G)G^{\mu\alpha}G^{\nu\beta}G^{\rho\gamma}G^{\sigma\delta})\right.$$
$$+ 3y^2\left(D_\mu H'^*D_\nu H' G^{\mu\nu} - \frac{1}{6}R(G)H'^*H'\right)$$
$$\left. + \left(g_3^2G^i_{\mu\nu}G^i_{\rho\sigma} + g_2^2F^\alpha_{\mu\nu}F^\alpha_{\rho\sigma} + \frac{5}{3}g_1^2B_{\mu\nu}B_{\rho\sigma}\right)G^{\mu\rho}G^{\nu\sigma} + 3z^2(H'^*H')^2\right).$$

The terms which only involve the metric are conformal by construction. The same holds for the terms which involve the gauge fields since the Yang-Mills action is conformal. Thus we need only to take care of the terms that involve the Higgs fields. We have to show that the following expression is unchanged by $g\to G$ and $H\to H'$;

$$\frac{3f_4y^2}{4\pi^2}\int \mathrm{d}^4x\sqrt{g}\left(g^{\mu\nu}D_\mu H^*D_\nu H - \frac{1}{6}R(g)H^*H\right).$$

To see this we first rescale the kinetic energy of the Higgs field

$$\sqrt{g}g^{\mu\nu}D_\mu H^* D_\nu H = \sqrt{G}G^{\mu\nu}e^{-2\phi}D_\mu(e^\phi H'^*)D_\nu(e^\phi H')$$
$$= \sqrt{G}G^{\mu\nu}(D_\mu H'^* D_\nu H' + \partial_\mu\phi H'^* D_\nu H'$$
$$+ D_\mu H'^* H'\partial_\nu\phi + H'^* H'\partial_\mu\phi\partial_\nu\phi).$$

The conformal coupling of the Higgs field to the scalar curvature transforms as

$$-\frac{1}{6}\sqrt{g}R(g)H^*H = -\frac{1}{6}\sqrt{G}H'^* H'(R(G) - 6G^{\mu\nu}((\nabla_\mu\nabla_\nu)^G\phi - \partial_\mu\phi\partial_\nu\phi)).$$

After integrating by parts the term

$$\int d^4x\sqrt{G}H'^* H'(\nabla_\mu\nabla_\nu)^G\phi G^{\mu\nu},$$

we find that all cross terms cancel, thus obtaining

$$\int d^4x\sqrt{g}\left(g^{\mu\nu}D_\mu H^* D_\nu H - \frac{1}{6}R(g)H^*H\right) = \int d^4x\sqrt{G}\left(G^{\mu\nu}D_\mu H'^* D_\nu H' - \frac{1}{6}R(G)H'^* H'\right).$$

The quartic Higgs interactions are evidently scale invariant

$$\int d^4x\sqrt{g}(H^*H)^2 = \int d^4x\sqrt{G}(H'^* H')^2.$$

Collecting all terms, the low-energy bosonic part of the spectral action with dilaton is given by

$$I_b = \frac{45}{4\pi^2}f_0\int d^4x\sqrt{G} + \frac{3}{4\pi^2}f_2\int d^4x\sqrt{G}\left(\frac{5}{4}R(G) + \frac{15}{2}G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - 2y^2H'^* H'\right)$$
$$+ \frac{f_4}{4\pi^2}\int d^4x\sqrt{G}\left(\frac{1}{32}(11R(G)^*R^*(G) - 18C_{\mu\nu\rho\sigma}(G)C^{\mu\nu\rho\sigma}(G)) + 3y^2\left(D_\mu H'^* D_\nu H' G^{\mu\nu}\right.\right.$$
$$\left.\left. - \frac{1}{6}R(G)H'^* H'\right) + \left(g_3^2 G^i_{\mu\nu}G^i_{\rho\sigma} + g_2^2 F^\alpha_{\mu\nu}F^\alpha_{\rho\sigma} + \frac{5}{3}g_1^2 B_{\mu\nu}B_{\rho\sigma}\right)G^{\mu\rho}G^{\nu\sigma} + 3z^2(H'^* H')^2\right). \tag{21}$$

For higher order terms one expects a scaling factor of the form $e^{(4-n)\phi}$ to be present, but derivatives of the dilaton field ϕ may also occur. Therefore in the Einstein frame, one does not expect the dilaton field ϕ to acquire a potential. As will be discussed later, this will change when quantum corrections are taken into account and the dilaton acquires a potential of the Coleman-Weinberg type.[14]

Fermionic interactions take the simple form

$$\langle\Psi|D|\Psi\rangle = \int d^4x\sqrt{g}\overline{\Psi}D\Psi,$$

where the metric $g_{\mu\nu}$ is used to insure hermiticity of D. We will now show that the fermions will not feel the dilaton. To see this we first redefine the spinors by

$$\Psi = e^{(3/2)\phi}\Psi',$$

then we have, for the parts not involving the Higgs or gauge fields,

$$\langle\Psi|D|\Psi\rangle = \int d^4x\sqrt{G}e^{-4\phi}e^{(3/2)\phi}\bar{\Psi}'\gamma^c e^{\phi}E_c^{\mu}\left(\partial_\mu + \frac{1}{4}\omega_\mu^{ab}(e)\gamma_{ab}\right)(e^{(3/2)\phi}\Psi'),$$

where the rescaled vierbein is $E_\mu^a = e^{\phi}e_\mu^a$. We have to express the spin connection $\omega_\mu^{ab}(e)$ in terms of the spin connection of the rescaled vierbein $\Omega_\mu^{ab}(E)$. To do this we use the equations

$$\partial_\mu e_\nu^a - \partial_\nu e_\mu^a - \omega_\mu^{ab}(e)e_{\nu b} + \omega_\nu^{ab}(e)e_{\mu b} = 0,$$

$$\partial_\mu E_\nu^a - \partial_\nu E_\mu^a - \Omega_\mu^{ab}(E)E_{\nu b} + \Omega_\nu^{ab}(E)E_{\mu b} = 0,$$

and these imply that

$$\omega_\mu^{ab}(e) = \Omega_\mu^{ab}(E) + (e_\mu^a e^{\nu b} - e_\mu^a e^{\nu b})\partial_\nu\phi.$$

Therefore

$$\gamma^c e_c^{\mu}\left(\tfrac{3}{2}\partial_\mu\phi + \tfrac{1}{4}\omega_\mu^{ab}(e)\gamma_{ab}\right) = \gamma^c e^{\phi}E_c^{\mu}\left(\tfrac{1}{4}\Omega_\mu^{ab}(E)\gamma_{ab}\right),$$

and the fermionic action reduces to the nice form

$$\int \mathrm{d}^4x\sqrt{G}\,\overline{\Psi'}\gamma^c E_c^{\mu}\left(\partial_\mu + \frac{1}{4}\Omega_\mu^{ab}(E)\gamma_{ab}\right)\Psi',$$

which is independent of the dilaton. Finally the parts involving interactions between the fermions and the Higgs or gauge fields could be written in the forms

$$\int \mathrm{d}^4x\sqrt{g}\overline{\Psi}\gamma_5 H\Psi = \int d^4x\sqrt{G}\,\overline{\Psi'}\gamma_5 H'\Psi',$$

$$\int \mathrm{d}^4x\sqrt{g}\overline{\Psi}\gamma^\rho e_a^{\mu}A_\mu\Psi = \int \mathrm{d}^4x\sqrt{G}\,\overline{\Psi'}\gamma^\rho E_a^{\mu}A_\mu\Psi'.$$

The fermionic interactions are

$$I_f = \langle Q|D_q|Q\rangle + \langle L|D_l|L\rangle,$$

where

$$Q = \begin{pmatrix} u_L \\ d_L \\ d_R \\ u_R \end{pmatrix}, \quad \begin{pmatrix} \nu_L \\ e_L \\ e_R \end{pmatrix}$$

and these take exactly the same form as those without dilaton when expressed in terms of the metric $G_{\mu\nu}$. Rewriting this in terms of the fermionic fields

$$Q' = e^{-(3/2)\phi}Q, \quad L' = e^{-(3/2)\phi}L,$$

and the Higgs field H' we obtain

$$I_f = \int \mathrm{d}^4x\sqrt{G}(\overline{L'}D_l'L' + \overline{Q'}D_q'Q'),$$

where[11]

$$D_l' = \begin{pmatrix} \gamma^\mu \otimes \left(D_\mu \otimes 1_2 - \frac{i}{2} g_2 A_\mu^\alpha \sigma^\alpha + \frac{i}{2} g_1 B_\mu \otimes 1_2\right) \otimes 1_3 & \gamma_5 \otimes k^e \otimes H' \\ \gamma_5 \otimes k^{*e} \otimes H^{*\prime} & \gamma^\mu \otimes (D_\mu + i g_1 B_\mu) \otimes 1_3 \end{pmatrix}$$

$$D_q' = \begin{pmatrix} \gamma^\mu \otimes \nabla_\mu^{(1,2)} \otimes 1_3 & \gamma_5 \otimes k^d \otimes H' & \gamma_5 \otimes k^u \otimes \widetilde{H'} \\ \gamma_5 \otimes k^{*d} \otimes H^{*\prime} & \gamma^\mu \otimes \left(D_\mu + \frac{i}{3} g_1 B_\mu\right) \otimes 1_3 & 0 \\ \gamma_5 \otimes k^{*u} \otimes \widetilde{H}'^* & 0 & \gamma^\mu \otimes \left(D_\mu - \frac{2i}{3} g_1 B_\mu\right) \otimes 1_3 \end{pmatrix}$$
$$+ \gamma^\mu \otimes 1_4 \otimes 1_3 \otimes \left(-\frac{i}{2} g_3 V_\mu^i \lambda^i\right),$$

and

$$\gamma^\mu = \gamma^a E_a^\mu,$$

$$D_\mu = \partial_\mu + \tfrac{1}{4} \Omega_\mu^{ab}(E) \gamma_{ab},$$

$$\nabla_\mu^{(1,2)} = D_\mu \otimes 1_2 - \frac{i}{2} g_2 A_\mu^\alpha \sigma^\alpha - \frac{i}{6} g_1 B_\mu \otimes 1_2.$$

From the previous considerations we deduce that the only effect of the dilaton on the low-energy terms of the spectral action is that the dilaton gets a kinetic term with no other interactions. This confirms that all matter interactions in the above-mentioned Lagrangian are scale invariant when expressed in the rescaled fields $G_{\mu\nu}$, H', and Ψ'. Only the Einstein term and the dilaton kinetic energy are not scale invariant.

Note that the invariance of the action for the Fermions, that is the equality

$$\langle \Psi | D | \Psi \rangle = \langle \Psi' | D' | \Psi' \rangle', \tag{22}$$

where D' corresponds to the metric G and the fields H', does not mean that the operators D and D' are the same. Indeed the transformation $\Psi \to \Psi'$ is not unitary and one has

$$\langle \Psi' | \Psi' \rangle' = \langle \Psi | e^\phi | \Psi \rangle, \tag{23}$$

which gives the unitary equivalence

$$D' \sim e^{-\phi/2} D e^{-\phi/2}. \tag{24}$$

One might then be tempted to conclude that the square of $e^{-\phi/2} D e^{-\phi/2}$ should be unitarily equivalent to $P = e^{-\phi} D^2 e^{-\phi}$ but this does not hold precisely because of the additional kinetic term in the spectral action with dilaton. Indeed one can prove (Appendix C) in the general framework of spectral triples, with a minimum amount of hypothesis, the identity

$$\int e^{2\phi} D^{-2} = \int (e^{-\phi/2} D e^{-\phi/2})^{-2} + \frac{1}{2} \int [D, e^\phi][D, e^\phi]^* D^{-4} \tag{25}$$

with $D' = e^{-\phi/2} D e^{-\phi/2}$ the last term gives the canonical kinetic energy of the dilaton

$$\frac{1}{2} \int [D' \phi][D', \phi]^* D'^{-4}$$

with the correct sign.

V. APPLICATIONS

We have shown that the dilaton interactions of the spectral action are almost the same as the ones proposed in the literature,[2,3] the difference lies in the derivative couplings of the dilaton field. These were obtained by requiring the standard model matter sector to be scale invariant by introducing a compensating dilaton field. The origin of the dilatational symmetry breaking are the mass terms of the Higgs potential, and these are scaled with the dilaton field to make them scale invariant. In a curved space time all fields couple to gravity, and the dilaton. The proposed action for the gravity-dilaton-Higgs sectors, in our notation, was derived to be (this expression is in the conventions of Ref. 4 and is in Minkowski space)[3,4]

$$I=\int \mathrm{d}^4x\sqrt{G}\left(-\frac{1}{2\kappa^2}R+\frac{1}{2}\left(1+\frac{6}{\kappa^2 f^2}\right)G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi+G^{\mu\nu}D_\mu H'^{*}D_\nu H'-V_0(H'^{*}H')\right).$$

There it was shown that in curved space-time this corresponds to the Jordan-Brans-Dicke theory of gravity. The only difference between this action and the spectral action is that the latter has the conformal coupling

$$\tfrac{1}{6}R(G)(H'^{*}H')^2,$$

which is necessary to make the matter couplings scale invariant. A slight modification was also proposed in the study of models of extended inflation, by also considering the possibility of modifying the Higgs sector by taking[4]

$$e^{(2/f)\phi}G^{\mu\nu}D_\mu H^{*}D_\nu H-e^{(4/f)\phi}V_0(H^{*}H).$$

This differs from the spectral action by the appearance of derivative couplings of the form

$$G^{\mu\nu}D_\mu H'^{*}H'\partial_\nu\phi.$$

It is amusing to note that this alternative proposed action is exactly the same action as the one derived for the Connes-Lott gravitational interactions.[6,10] Therefore the two models proposed in the literature for making the Higgs sector scale invariant are the same as the interactions obtained for the noncommutative standard model, either for the spectral action formulation, or the Connes-Lott formulation. We also note that scale invariance of the action is broken by the Einstein term and by the kinetic term for the dilaton. This is remarkable because it was shown that if the full action is scale invariant, then the couplings will not lead to a model with extended inflation. Quantum corrections and renormalization conditions break scale invariance in the matter sector of the standard model and lead to an exponentially large hierarchy between the mass scale f where $\phi=(1/f)\sigma$ and the electroweak scale without fine tuning. The scale f is normally of the order of the Planck scale. The dilaton mass obtained depends on the Higgs mass, but should be constrained to be smaller than 10^{-6} eV.

The noncommutative space of the standard model is obtained by taking the product of a four-dimensional Riemannian manifold times a discrete space dictated by the symmetries of the Hilbert space spanned by the quarks and leptons. The presence of left- and right-handed fermions provides the intuitive picture where these fermions are placed on different sheets. The gauge fields in the discrete dimensions are the Higgs fields, with the inverse of the distance between the sheets interpreted as the electroweak energy scale. This picture is similar to the RS scenario where the four-dimensional space is embedded into a five-dimensional space as a three-brane positioned at the points $x_5=0$ and $x_5=\pi r_c$, where r_c is the compactification radius. The action for the Higgs sector in the RS model[9] was obtained to be

$$\int d^4x\sqrt{g}(g^{\mu\nu}D_\mu H^* D_\nu H - \lambda(|H|^2 - v_0^2))$$

$$= \int d^4x\sqrt{\bar{g}}(\bar{g}^{\mu\nu}D_\mu H'^* D_\nu H' - \lambda(|H'|^2 - e^{-2kr_c\pi}v_0^2)),$$

where

$$g^{\mu\nu} = e^{-2kr_c\pi}\bar{g}^{\mu\nu},$$

$$H' = e^{2kr_c\phi}H,$$

in the visible sector located at $x_5 = \pi r_c$. The physical mass scales are set by the symmetry breaking scale $v = e^{-kr_c\pi}v_0$ so that $m = m_0 e^{-kr_c\pi}$. The bare symmetry breaking scale v_0 is taken to be of the order of the Planck scale at 10^{19} GeV and the scaling factor $e^{kr_c\pi}$ tuned to be of the order of 10^{15} so that the low-energy masses are of the order of TeV. The hierarchy problem is only partially solved in a technical sense because the tuning could not be maintained at the quantum level. A choice of $kr_c = 10$ can generate the large scale 10^{15} GeV. Comparing the Higgs sectors in the RS action with that in the spectral action we immediately see that they are identical provided we identify the expectation value of the dilaton field $\langle\phi\rangle$ with $kr_c\pi$.

VI. CONCLUSIONS

The Dirac operator being a differential operator has the dimensions of mass. The spectral action in noncommutative geometry is defined as a function of a dimensionless operator which is taken to be the Dirac operator divided by some arbitrary large mass scale. The arbitrariness of the mass scale naturally suggests to make this scale dynamical by introducing a dilaton field in the Dirac operator of the noncommutative space defined by the standard model. To understand the appearance of the mass scales of the spectral action, we evaluated all interactions of the dilaton with the matter sector in the standard model. We found the remarkable result that the low-energy action, when evaluated in the Einstein frame, is scale invariant except for the Einstein-Hilbert term and the dilaton kinetic term. The resulting model is almost identical to the one proposed in the literature.[2–4] The main motivation in these works is the observation that the standard model is classically almost scale invariant, with the symmetry only broken by the mass term in the Higgs potential. The symmetry is restored by the use of a dilaton field. When coupled to gravity, neither the dilaton kinetic energy nor the scalar curvature are scale invariant, leading to a Jordan-Brans-Dicke theory of gravity. The vacuum expectation value of the Higgs field is then dependent on the dilaton and is classically undetermined. Quantum corrections break the scale invariance of the scalar potential and change the vacuum expectation value of the Higgs field. The dilaton acquires a large negative expectation value given by $-m$ and a small mass. The hierarchy in mass scales is due to the large Yukawa coupling of the top quark. The dilaton expectation value can range between the GUT scale of 10^{15} GeV to the Planck scale of 2.4×10^{18} GeV. The hierarchy in mass scales is not possible if the dilaton kinetic energy and the gravitational action were scale invariant. It is remarkable that all the essential features of building a scale invariant standard model interactions to generate a mass hierarchy and predict the Higgs mass are naturally included in the spectral action without any fine tuning. It is worth mentioning that the scalar potential of exactly the same model considered here was shown to admit extended inflation and a metastable ground state. It also evades the problems of the original version of extended inflation.

The vacuum expectation value of the dilaton field is determined by getting contributions from classical and radiative corrections to the vacuum energy density. One does not obtain naturally a vanishing cosmological constant. There are two possibilities to cure this problem. The first is to determine the low-energy value of the cosmological constant as determined by the renormalization group equations and then fine tune this value to cancel the contributions of the Coleman-Weinberg

potential. The second possibility to cure this problem is to fix the total invariant volume. This restricts general relativity to the form considered in Ref. 15, where the volume form is held fixed. There it was shown that this picture is consistent both at the classical and quantum levels.[16–18] This fixes the total invariant volume and eliminates the scalar mode of the metric tensor $g_{\mu\nu}$. This is done at the expense of introducing the dilaton mode ϕ.[3] In noncommutative geometry the volume is fixed by a Hochschild cycle c whose compatibility with the Dirac operator D is a basic constraint on the Hilbert space representation giving the metric.[19] One applies the representation to monomials

$$\pi(f_0,f_1,f_2,f_3,f_4) = f_0[D,f_1][D,f_2][D,f_3][D,f_4],$$

and requires that when applied to the Hochschild cycle c it gives

$$\pi(c) = \gamma_5.$$

The cosmological constant becomes determined by the initial conditions of the theory.

To summarize, we have shown that the spectral action includes naturally a dilaton field which guarantees the scale invariance of the standard model interactions, and provides a mechanism to generate mass hierarchies. This is in addition to the advantages obtained previously in Ref. 11 which are now well known.[12] There it was shown that all the correct features of the standard model are obtained without any fine tuning, such as unification with gravity, unification of the three gauge coupling constants and relating the Higgs to the gauge couplings. These results should be taken to support the idea that all the geometric information about the physical space is captured by the knowledge of the Dirac operator of an appropriate noncommutative space.

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APPENDIX A

In this appendix we shall prove formula (12). Given an elliptic positive invertible second order operator Q and a differential operator T we use the notation $\nabla(T)=[Q,T]$ and the following identity (for $n\geqslant 0$):

$$Q^{-1}T = \sum_0^n (-1)^k \nabla^k(T) Q^{-k-1} + (-1)^{n+1} Q^{-1} \nabla^{n+1}(T) Q^{-n-1}. \tag{A1}$$

We apply this to $Q=P(t)+\lambda$, $T=\phi P(t)+P(t)\phi$. The operator $\nabla^k(T)$ is independent of λ and is a differential operator of order $\leqslant 2+k$ since $\nabla^k(\phi)$ is at most of order k. Thus the operator $\nabla^k(T)Q^{-k-1}$ is pseudodifferential of order at most $2+k-2(k+1)=-k$ and the remainder in (A1) is of order at most $-n-1$. This shows that when working modulo operators of order less than $-n$ we have

$$(P(t)+\lambda)^{-1}T \sim T(P(t)+\lambda)^{-1} + \sum_1^n (-1)^k \nabla^k(T)(P(t)+\lambda)^{-k-1}$$

so that

$$(P(t)+\lambda)^{-1}T(P(t)+\lambda)^{-1} \sim T(P(t)+\lambda)^{-2} + \sum_1^n (-1)^k \nabla^k(T)(P(t)+\lambda)^{-k-2}.$$

But one has

$$\sum_{1}^{n}(-1)^k\nabla^k(T)(P(t)+\lambda)^{-k-2}=[P(t),A(t,\lambda)],$$

where

$$A(t,\lambda)=\sum_{1}^{n}(-1)^k\nabla^{k-1}(T)(P(t)+\lambda)^{-k-2}.$$

Thus integrating from $\lambda=0$ to ∞ and using (11) we get that, modulo operators of order less than $-n$,

$$\frac{\mathrm{d}}{\mathrm{d}t}Y(t)\sim-\int_0^\infty(\phi P(t)+P(t)\phi)(P(t)+\lambda)^{-2}\mathrm{d}\lambda+[P(t),A(t)]$$

where

$$A(t)=-\int_0^\infty A(t,\lambda)\mathrm{d}\lambda.$$

This thus gives

$$\frac{\mathrm{d}}{\mathrm{d}t}Y(t)\sim-(\phi P(t)+P(t)\phi)P(t)^{-1}+[P(t),A(t)]=-2\phi+[P(t),C(t)],\quad C(t)=A(t)-\phi P(t)^{-1}.$$

It is important to note that all of the previous manipulations hold in the general context of spectral triples with simple dimension spectrum. Moreover one can prove fairly strong properties of the spectral action in this general context.

APPENDIX B

In this appendix we shall prove the identity

$$a_n(x,P)=a_n(x,P_1)=a_n(x,P_2),$$

where $P=e^{-\phi}D^2e^{-\phi}$ and $P_1=D^2e^{-2\phi}$, $P_2=e^{-2\phi}D^2$. It can then be used to simplify some of the computations of Sec. III.

One simply writes

$$P=e^{-\phi}P_1e^{\phi}$$

so that

$$\mathrm{Trace}\,(P^{-s})=\mathrm{Trace}\,(P_1^{-s}).$$

From this the identity $a_n(x,P)=a_n(x,P_1)$ immediately follows.

One can also do a direct check as follows, one first writes

$$P=-(G^{\mu\nu}I\partial_\mu\partial_\nu+\mathcal{A}^\mu\partial_\mu+\mathcal{B}),$$

$$P_1=-(G^{\mu\nu}I\,\partial_\mu\partial_\nu+\mathcal{A}_1^\mu\partial_\mu+\mathcal{B}_1),$$

where

$$G^{\mu\nu} = e^{-2\phi} g^{\mu\nu},$$

$$\mathcal{B} = e^{-2\phi} B + G^{\mu\nu}(\partial_\mu \phi \partial_\nu \phi - \partial_\mu \partial_\nu \phi) - e^{-2\phi} A^\mu \partial_\mu \phi,$$

$$\mathcal{A}^\mu = e^{-2\phi} A^\mu - 2G^{\mu\nu}\partial_\nu \phi,$$

$$\mathcal{A}_1^\mu = e^{-2\phi} A^\mu - 4G^{\mu\nu}\partial_\nu \phi,$$

$$\mathcal{B}_1 = e^{-2\phi} B + 2G^{\mu\nu}(2\partial_\mu \phi \partial_\nu \phi - \partial_\mu \partial_\nu \phi) - 2e^{-2\phi} A^\mu \partial_\mu \phi.$$

These relations imply

$$\mathcal{A}_1^\mu = \mathcal{A}^\mu - 2G^{\mu\nu}\partial_\nu \phi,$$

$$\mathcal{B}_1 = \mathcal{B} + G^{\mu\nu}(\partial_\mu \phi \partial_\nu \phi - \partial_\mu \partial_\nu \phi) - \mathcal{A}^\mu \partial_\mu \phi.$$

We also have

$$\begin{aligned} \overline{\omega'}_{1\mu} &= \tfrac{1}{2} G_{\mu\nu}(\mathcal{A}_1^\nu + \Gamma^\nu(G)) \\ &= \overline{\omega'}_\mu - \partial_\mu \phi, \end{aligned}$$

so that

$$\mathcal{E}_1 = \mathcal{B}_1 - G^{\mu\nu}(\partial_\mu \overline{\omega'}_{1\nu} + \overline{\omega'}_{1\mu}\overline{\omega'}_{1\nu} - \Gamma^\rho_{\mu\nu}(G)\overline{\omega'}_{1\rho}) = \mathcal{E}.$$

Similarly

$$\mathbf{\Omega}_{1\mu\nu} = \mathbf{\Omega}_{\mu\nu}$$

and the equality of the Seely-de Witt coefficients follow from the fact that these depend only on $\mathcal{E}$, $\mathbf{\Omega}_{\mu\nu}$ and the curvature tensors are functions of the same metric $G_{\mu\nu}$.

APPENDIX C

In this appendix we shall show (25) and the appearance of the kinetic term in the general framework of spectral triples using the following manipulations. One has

$$\fint (e^{-\phi/2} D e^{-\phi/2})^{-2} = \fint e^\phi D^{-1} e^\phi D^{-1}. \tag{C1}$$

Also

$$D^{-1} e^\phi = e^\phi D^{-1} - D^{-1}[D, e^\phi] D^{-1}, \tag{C2}$$

which allows to write (C1) as

$$\fint (e^{-\phi/2} D e^{-\phi/2})^{-2} = \fint e^{2\phi} D^{-2} - \fint e^\phi D^{-1}[D, e^\phi] D^{-2}, \tag{C3}$$

and using (C2) again,

$$-\fint e^\phi D^{-1}[D, e^\phi] D^{-2} = -\fint e^\phi [D, e^\phi] D^{-3} - \fint D^{-1}[D, e^\phi] D^{-1}[D, e^\phi] D^{-2}.$$

The first of the two terms vanishes since the residue is a trace. The second is given by

$$-\int D^{-1}[D,e^{\phi}]D^{-1}[D,e^{\phi}]D^{-2}=\int [D,e^{\phi}]^2D^{-4}+R, \tag{C4}$$

where R is the remainder

$$R=-\int D^{-2}[D^2,e^{\phi}]D^{-1}[D,e^{\phi}]D^{-2}.$$

Let us show that

$$R=-\frac{1}{2}\int [D^2,e^{\phi}]^2D^{-6}. \tag{C5}$$

To see this write

$$R=-\int D^{-2}[D^2,e^{\phi}]DD^{-2}[D,e^{\phi}]D^{-2}, \tag{C6}$$

and note that the commutator of D with $[D^2,e^{\phi}]$ is equal to $[D^2,[D,e^{\phi}]]$ and has order 1 so that

$$\int D^{-2}[D,[D^2,e^{\phi}]]D^{-2}[D,e^{\phi}]D^{-2}=0.$$

Thus moving D to the left and using the trace property of the residue one gets

$$R=-\frac{1}{2}\int [D^2,e^{\phi}]D^{-2}(D[D,e^{\phi}]+[D,e^{\phi}]D)D^{-4},$$

and one obtains (C5). Summarizing, we have shown the equality

$$\int (e^{-\phi/2}De^{-\phi/2})^{-2}=\int e^{2\phi}D^{-2}+\int [D,e^{\phi}]^2D^{-4}-\frac{1}{2}\int [D^2,e^{\phi}]^2D^{-6}.$$

Thus to obtain (C1) one just needs to prove the equality

$$\int [D,a]^2D^{-4}=\int [D^2,a]^2D^{-6}, \tag{C7}$$

and apply it to $a=e^{\phi}$. One can check (C7) directly in the Riemannian case by computing the residue as the integral of the principal symbols on the unit sphere bundle. The factor 2^2 from the Poisson brackets $[D^2,a]$ is compensated by the integral of ξ_{μ}^2 on the sphere which gives $\frac{1}{4}$. In the general framework of spectral triples one gets (C7) from the general hypothesis

$$\int a[D,b]D^{-3}=0, \quad \forall\, a,b\in\mathcal{A}.$$

Note that the commutator $[D,e^{\phi}]$ is skew adjoint and in particular $[D,e^{\phi}]^*=-[D,e^{\phi}]$. Thus we get the correct sign in

$$\int e^{2\phi}D^{-2}=\int (e^{-\phi/2}De^{-\phi/2})^{-2}+\frac{1}{2}\int [D,e^{\phi}][D,e^{\phi}]^*D^{-4}. \tag{C8}$$

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Clebsch-Gordan coefficients for U(8)⊃O(8)⊃SU(3)

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The group chain U(8)⊃O(8)⊃SU(3) plays an important role in many particle systems whenever the fundamental particles have eight degrees of freedom. As a particular example, the systems of many gluons and pairs of quark-antiquark are discussed, which can be coupled to a flavor octet. In order to determine the explicit structure of states and decay probabilities, the calculation of the Clebsch-Gordan coefficients (CGC) of this group chain is indispensable. In this contribution, the polynomial states of the U(8) chain are constructed and also the isoscalar factors of the CGC's. Tables of isoscalar factors are presented. The method shown serves as an example for higher rank groups. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Clebsch-Gordan coefficients (CGC) play an important role in physics. The group structure related to it depends on the particular problem to consider. For example, in the case of angular momentum, spin or total spin of a many particle system, the underlying structure is the group SU(2). Knowing the CGC serves to calculate matrix elements of tensors of SU(2), which are, for example, related to interactions in a Hamiltonian and/or to transition operators. The fundamental group involved [here the SU(2)] depends on the basic degrees of freedom of the lowest nontrivial irreducible spin representation (irrep), which is spin $\frac{1}{2}$. There are other types of CGC, which are related to different basic degrees of freedom. As a further example we mention the SU(3) group. It appears in nuclear physics as the symmetry group of the harmonic oscillator in three dimensions and it defines the fundamental structure of the shell model.[1] Much effort has been involved to obtain these CGC's. The culmination is the work presented in Refs. 2–4 where up to recoupling coefficients are given, equivalent to the 6-j and 9-j symbols of SU(2).[5] The SU(3) CGC's are also used in particle physics, where the meaning of SU(3) is different and rather related to flavor or color.

In order to obtain the CGC's, in the example of SU(2) and SU(3) the recursion relations, obtained from the algebraic properties of the Lie algebra, were exploited. The number of these recursion relations is given by the number of generators minus the rank of the group. For SU(2) it is 2 while for SU(3) it is 6, still a manageable number. However, for groups like U(8), of interest here, this number of recursion relations raises to 56. Thus, alternative procedures are called for.

Now, why to use an U(8) group? The group U(8) appears whenever eight degrees of freedom are involved. Of course, the main motivation is the current need of this group in a particular, though very important, area in physics, namely particle physics. The description of many particle state becomes more important since the recognition that a hadron state is not just a three-quark state (for baryons), a quark-antiquark state (for mesons) or a two gluon state (for low-lying glueballs), i.e., there is an additional background of pairs of quark-antiquark and gluons. The spin problem of the nucleon[6] is one hint in this direction. It implies the urgent need to obtain the CGC's in higher rank groups. Simple SU(3) coupling coefficients, related, for example, to color and/or flavor, will not suffice. The SU(3) CGC is expressed in terms of a product of an SU(2) CGC and an *isoscalar factor*. This will be similar for U(8)⊃O(8)⊃SU(3), i.e., the CGC will be expressed in terms of already known SU(3) CGC's and isoscalar factors. The U(8) group also appears in

many gluon systems. Gluons have eight color degrees of freedom[7] and thus the color part can be described by a U(8) group. Because the gluon has spin one it has three mathematical spin degrees of freedom (to distinguish them from the physical ones which only involve the transverse modes), i.e., a many gluon system can be described by $U(24) \supset U(8) \otimes U(3)$,[8] where the U(3) refers to the spin part and a many gluon state must be in the complete symmetric irreducible representation $[N]$ of U(24). Because $[N]$ is symmetric, the color and spin part are intimately connected due to complementarity.[9] The U(8) group can be reduced to the color SU(3) group and further the U(3) to the spin SO(3) group, with integer spins only. The group reduction is well known and given in Refs. 8 and 10. The construction of states is less known. For symmetric irreps, the first attempts are presented in Refs. 11 and 12, though, the SU(3) subgroup considered in Ref. 12 is not the color group.

The symmetric irreps play a particular important role in a system of many quark-antiquark pairs, as in the model presented in Refs. 13–15, where an effective model of QCD is proposed considering many quark and antiquark states. A general classification for many quark and antiquark states in the *s*-orbital level was given. In order to simplify calculations, pairs of quark-antiquark were mapped to bosons.[16] There are four different types of bosons corresponding to quark-antiquark pairs with flavor (λ,λ) $(\lambda=0,1)$ and spin S $(S=0,1)$ denoted by $[\lambda,S]$. The cases $[0,0]$ and $[0,1]$ correspond to a one- and three-dimension harmonic oscillator, known from textbooks. The case $[1,0]$ corresponds to the eight-dimensional harmonic oscillator, i.e., to the U(8) group with just a symmetric irrep. The last case $[1,1]$ is mathematically identical to the many gluon problem and allows up to three rows in the Young diagram of U(8). The same structure appears in any model whose basic ingredients are quark-antiquark and/or gluon pairs.

Restricting to symmetric irreps, coupling coefficients are still important in obtaining information on decay properties and for the coupling of two systems. Though, so far we mainly mentioned bosonic systems, the isoscalar factors, calculated in this contribution, also serve for the equivalent *fermion pairs*.

Another motivation is to decide whether the pentaquark[17–21] exists in the model or not. A first estimate within the schematic model, where we have information about the distribution of quark-antiquark pairs in the pentaquark and in the residual particles, indicates that the pentaquark is just the sum of a nucleon and a kaon or at most a molecule in these particles, i.e., the width of the state should be very large and a peak should not be seen, confirmed in part by other experiments and also criticized in Ref. 22 (and references therein). If this is the case, it can only be decided through an explicit calculation, using U(8) CGC's.

Of course, the immediate application to topics in particle physics is only one possible application, used here as an example.

Does one also need the explicit form of the states defined by the U(8) group? The answer is that they are necessary for the calculation of CGC's. In the calculation of CGC's one usually exploits the algebraic properties of a group obtaining recursion relations, as illustrated in Ref. 5 for the SU(2) group and in Refs. 2–4 for the SU(3) group. However, for higher rank groups these methods get more involved and unpractical. In Refs. 23 and 24 a more practical procedure was proposed for the $U(5) \supset SO(5) \supset SO(3)$, playing an important role in the geometric model of the nucleus.[1] There, the polynomial expressions of the U(5) states were constructed explicitly using elementary tensors in terms of boson creation operators. The Clebsch-Gordan coefficients were obtained by direct calculation of the integrals involving the polynomial states, with the help of algebraic routines. The basic idea for the construction of the polynomials were borrowed from Refs. 25 and 26. In conclusion, the explicit knowledge of the polynomial states is of great use.

Thus, a first and important step forward towards the construction of many particle states is the explicit construction of these states in the symmetric irrep of U(8). The CGC's are obtained as integrals over a product of three polynomials. The first steps of the procedure were presented in Ref. 27 where the basic ingredients are illustrated for the case of the well investigated group chain $SU(3) \supset SO(3)$.

In this contribution, explicit expressions of the polynomial states up to eight particles and tables of U(8) isoscalar factors are presented, which are useful for models treating, for example,

TABLE I. Content of SU(3) irreps for a given seniority. When a SU(3) irrep appears more than once (multiplicity larger than 1) it is indicated by an upper index.

ν	(λ,μ)
0	$(0,0)$
1	$(1,1)$
2	$(1,1)+(2,2)$
3	$(0,0)+(3,0)+(0,3)+(2,2)+(3,3)$
4	$(1,1)+(2,2)+(4,1)+(1,4)+(3,3)+(4,4)$
5	$(1,1)+(2,2)+(4,1)+(1,4)+(3,3)+(5,2)+(2,5)+(4,4)$ $+(5,5)$
6	$(0,0)+(3,0)+(0,3)+(2,2)+(3,3)^2+(6,0)+(0,6)+(5,2)$ $+(2,5)+(4,4)+$ $(6,3)+(3,6)+(5,5)+(6,6)$
7	$(1,1)+(2,2)+(4,1)+(1,4)+(3,3)+(5,2)+(2,5)+(4,4)^2$ $+(7,1)+(1,7)+$ $(6,3)+(3,6)+(5,5)+(7,4)+(4,7)+(6,6)+(7,7)$
8	$(1,1)+(2,2)+(4,1)+(1,4)+(3,3)+(5,2)+(2,5)+(4,4)^2$ $+(7,1)+(1,7)+$ $(6,3)+(3,6)+(5,5)^2+(8,2)+(2,8)+(7,4)+(4,7)+(6,6)$ $+(8,5)+(5,8)+$ $(7,7)+(8,8)$

many gluon and fermion pair systems, as outlined above. These tables are of great use in determining the structure and the decay properties of a many particle state, like hadrons or a system of many quarks, antiquarks and gluons, and the quark-gluon plasma.

The paper is structured as follows: In the second section we give the classification and the explicit expressions of the states up to eight particles in the symmetric representation of $U(8)\supset O(8)\supset SU(3)\supset SU(2)\otimes U(1)$ in terms of the polynomials in boson creation and annihilation operators. We show how to obtain states with good seniority. In Sec. III the isoscalar factors are calculated. In Sec. IV conclusions are drawn.

II. THE HIGHEST WEIGHT STATES IN SU(3) OF $U(8)\supset O(8)\supset SU(3)\supset SU(2)\otimes U(1)$

The particles under consideration have eight degrees of freedom and belong to the SU(3) irrep $(1,1)$.

For symmetric irreps, the relevant group chain is

$$\begin{array}{ccccccc} U(8) & \supset & O(8) & \supset & SU(3) & \supset & U(1)\otimes SU(2) \\ [N] & & (\nu 000) & & (\lambda,\mu) & & Y \quad T,\ T_z, \end{array} \tag{1}$$

where Y is the hypercharge, T the isospin, and T_z its third component. The N is the total number of bosons, ν the seniority [number of bosons *not coupled* in pairs with flavor $(0,0)$]. The CGC's of the chain $SU(3)\supset U(1)\otimes SU(2)$ are well known and available.[28,29]

The classification of the states, described by the group chain $U(8)\supset SU(3)$, is immediately obtained, using Ref. 10. The reduction of U(8) to O(8) is obtained recursively: For a given N the possible values of the seniority are $\nu=N,N-2,\ldots,0$ or 1. When the content up to a given seniority $\nu=N$ is known, the one for $\nu=(N+2)$ is obtained, determining the content of the irrep $[N+2]$ of U(8) and subtracting the SU(3) content of all seniorities up to $\nu=N$. The SU(3) content of O(8) for $\nu=0$ is (0,0) and for $\nu=1$ it is (1,1), which can be used as initial conditions. In Table I we give the list up to seniority eight.

The generators of U(8) are given by

TABLE II. Linearization of the index (YTT_z) to ξ.

ξ	Y	T	T_z
1	0	1	1
2	1	$\frac{1}{2}$	$\frac{1}{2}$
3	−1	$\frac{1}{2}$	$\frac{1}{2}$
4	0	1	0
5	0	0	0
6	1	$\frac{1}{2}$	$-\frac{1}{2}$
7	−1	$\frac{1}{2}$	$-\frac{1}{2}$
8	0	1	−1

$$\boldsymbol{C}^{\rho\Gamma}_{YTT_3} = [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{\rho\Gamma}_{YTT_z}, \tag{2}$$

where Γ is a short-hand notation for (λ,μ) and ρ is a multiplicity label which is 1 except for the irrep $\Gamma=(1,1)$ where it obtains values 1 and 2. For this case, the value $\rho=1$ refers to the antisymmetric coupling and $\rho=2$ to the symmetric coupling.[30] The possible values of Γ are (0,0), (2,2), and $(1,1)_2$ for the symmetric and (3,0), (0,3), and $(1,1)_1$ for the antisymmetric coupling. The index (YTT_z) can be linearized to ξ as defined in Table II, which is of use in the further discussion.

The generators of O(8) are given by the coupling to the antisymmetric irreps Γ, implying 28 generators for the algebra of O(8). The generators of the SU(3) subgroup are obtained, restricting the Γ to $(1,1)_1$.

The Lie algebra for the generators (2) is given by

$$\begin{aligned}[\boldsymbol{C}^{\rho\Gamma'}_{\xi'}, \boldsymbol{C}^{\rho\Gamma}_{\xi}] = {} & (-1)^{\mathrm{sign}(\lambda_0,\mu_0)+\mathrm{sign}(\lambda,\mu)+\rho^{(\lambda,\mu)}_{\max}+\lambda+\mu-\rho}\left(1-(-1)^{\mathrm{sign}(\lambda,\mu)+\mathrm{sign}(\lambda',\mu')+\mathrm{sign}(\lambda_0,\mu_0)}\right) \\ & \times \sum_{\rho_{\max}}^{\rho^{(\lambda_0,\mu_0)}_{\max}} \sum_{(\lambda_0,\mu_0)\xi_0} (-1)^{\rho^{(\lambda_0,\mu_0)}_{\max}-\rho_0} \sum_{\rho''=1}^{\rho_{\max}} (-1)^{\rho_{\max}-\rho''} \sqrt{\frac{\dim(\lambda,\mu)}{8}} \\ & \times \langle(\lambda,\mu)\xi,(\lambda',\mu')\xi'|(\lambda_0,\mu_0)\xi_0\rangle_{\rho''} \\ & \times U[(\mu_0,\lambda_0)(1,1)(\mu,\lambda)(1,1);(1,1)\rho_0\rho(\lambda',\mu')\rho'\rho''][\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{\rho_0(\lambda_0,\mu_0)}_{\xi_0}. \end{aligned} \tag{3}$$

The $\rho^{(\lambda_0,\mu_0)}_{\max}$ refers to the multiplicity in the coupling $(1,1)\otimes(1,1)\to(\lambda_0,\mu_0)$, the $\rho^{(\lambda,\mu)}_{\max}$ to the multiplicity in the coupling $(1,1)\otimes(1,1)\to(\lambda,\mu)$, $\rho_{\max}$ to $(\lambda,\mu)\otimes(\lambda',\mu')\to(\lambda_0,\mu_0)$, $\mathrm{sign}(\lambda,\mu)$ to the symmetry property of the $(1,1)\otimes(1,1)\to(\lambda,\mu)$ under exchange of the first two irreps in the GCG (symmetric or antisymmetric) and $U[\cdots]$ is the U-coefficient, whose definition can be found in Ref. 30.

As a particular case, the algebra for the subgroup SU(3), which is a subgroup of O(8), is given by

$$[\boldsymbol{C}^{1(1,1)}_{\xi'}, \boldsymbol{C}^{1(1,1)}_{\xi}] = \sum_{\xi_0} \langle(1,1)\xi',(1,1)\xi|(1,1)\xi_0\rangle_1 [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{(1,1)_1}_{\xi_0}. \tag{4}$$

In terms of the standard notation of the SU(3) generators,[31] the relation to the $\boldsymbol{C}^{1(1,1)}_{\mu}$ of Eq. (2) is $(\boldsymbol{T}_0=\boldsymbol{T}_z)$

$$\begin{aligned} \boldsymbol{T}_\pm &= \pm\sqrt{6}[\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{1(1,1)}_{01\pm1}, \quad \boldsymbol{T}_0 = -\sqrt{3}[\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{1(1,1)}_{010}, \\ \boldsymbol{V}_\pm &= \pm\sqrt{6}[\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{1(1,1)}_{\pm1(1/2)\pm(1/2)}, \\ \boldsymbol{U}_\pm &= \sqrt{6}[\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{1(1,1)}_{\pm1(1/2)\mp(1/2)}, \end{aligned} \tag{5}$$

$$\boldsymbol{Y} = -2[\boldsymbol{b}^\dagger \otimes \boldsymbol{b}]^{1(1,1)}_{000}.$$

In the next step we express an arbitrary tensor of U(8) in terms of a product of powers of "elementary" tensors, which are called *elementary couplings* (epd's)[25,26] (sometimes also called *integrity basis*). The origin of this name is that any tensor of a given order can be expressed in terms of products of powers in these epd's. The epd's are basic tensors each coupled to the maximum weight in SU(3). Because these elementary tensors are of maximum weight in SU(3), any product of two or more of these tensors result again in a tensor of maximum weight in SU(3), in the same way two tensors with spin j_1 and j_2 with maximal projection, i.e., $m_1=j_1$ and $m_2=j_2$, result in a new tensor with spin $j=j_1+j_2$ and projection $m=j$. Products of powers in these epd's generate U(8) states with quantum numbers N and (λ,μ) in the maximum weight state of SU(3). One must take care that the list of epd's is complete, checking if all irreps of U(8) can be written in terms of them. If one state is missing, a further epd must be added.

In Ref. 11 a procedure is developed how to obtain these epd's using *generating functions*. Please consult this reference for more details and further references. This method was applied successfully to various areas of physics, like the geometric collective model[1,25,26] and in Ref. 11 more possible applications are given, like the problem we are interested in this contribution. In Ref. 11 the following epd's (sometimes denoted as *integrity basis*) where obtained using the method of generating functions [see Eq. (16) of Ref. 11]. The epd's are given by

$$\begin{aligned}
\boldsymbol{A} &= \boldsymbol{b}^\dagger_{011},\\
\boldsymbol{B} &= [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}^\dagger]^{(0,0)}_{000},\\
\boldsymbol{C} &= [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}^\dagger]^{(1,1)}_{011},\\
\boldsymbol{D} &= [\boldsymbol{b}^\dagger \otimes [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}^\dagger]^{(1,1)}]^{(0,0)}_{000},\\
\boldsymbol{E} &= [\boldsymbol{b}^\dagger \otimes [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}^\dagger]^{(1,1)}]^{(3,0)}_{1(3/2)(3/2)},\\
\boldsymbol{F} &= [\boldsymbol{b}^\dagger \otimes [\boldsymbol{b}^\dagger \otimes \boldsymbol{b}^\dagger]^{(1,1)}]^{(0,3)}_{-1(3/2)(3/2)},
\end{aligned} \tag{6}$$

where the coupling of two boson creation operators must be always symmetric, otherwise it would give zero due to the symmetry properties of the CGC. These are expressions obtained by coupling the definite SU(3) tensors $\boldsymbol{b}^\dagger_\xi$ to new tensors using the SU(3) CGC's.

A *pedestrian way* to look at it, is to ask: How many basic tensors one needs to construct all possible state polynomials which are in the maximum weight in SU(3)? Table I is here for assistance: For a given number of bosons N the SU(3) content is obtained by summing the seniority content for $\nu=N,N-2,\ldots,0$ or 1. For $N=1$ we need a tensor with the SU(3) structure (1,1), which is just $\boldsymbol{A}$. However, powers of the type $\boldsymbol{A}^{n_1}$ gives only polynomials with the SU(3) irrep labels (n_1,n_1). Inspecting Table I we see that for $N=2$ the SU(3) content is $(0,0)+(1,1)+(2,2)$, implying that we also need tensors with the SU(3) labels (0,0) and (1,1), which gives us the tensors $\boldsymbol{B}$ and $\boldsymbol{C}$. The irrep (2,2) is presented by $\boldsymbol{A}^2$. Powers and products of$\mathbf{A}$, $\boldsymbol{B}$, and $\boldsymbol{C}$ are still not sufficient: For $N=3$ the SU(3) content is given by $(0,0)+(3,0)+(0,3)+(1,1)+(2,2)+(3,3)$. The states with (3,3), (2,2), and (1,1) are, respectively, presented by $\boldsymbol{A}^3$, $\boldsymbol{AC}$, and $\boldsymbol{AB}$. We note the need of tensors with SU(3) labels (0,0), (3,0), and (0,3), which are just the $\boldsymbol{D}$, $\boldsymbol{E}$, and $\boldsymbol{F}$ tensors. Continuing to larger N one notes that all other polynomial states are obtained by the product of powers in these basic tensors. An ambiguity, however, arises when the product of the tensors $\boldsymbol{E}$ with $\boldsymbol{F}$ or powers of $\boldsymbol{C}^3$ are considered. For example, for $N=6$ and the SU(3) irrep (6,3) there are the following possible representations, namely $\boldsymbol{FA}^3$ and $\boldsymbol{EA}^3$, though, (6,3) appears only once. This will be discussed in what follows.

A maximum weight state [in SU(3)] is a monomial in these epd's, where according to Ref. 11 the epd $\boldsymbol{C}$ appears only in powers of 0, 1 or 2, i.e., the $\boldsymbol{C}^3$ can be expressed as a linear combination in the other epd's. Instead of choosing $\boldsymbol{C}^3$ as dependent, the $\boldsymbol{E}$ and $\boldsymbol{F}$ can be used as dependent epd's. These two epd's satisfy a relation which permits the appearance of powers in $\boldsymbol{E}$ or $\boldsymbol{F}$ only. The relation of the product $\boldsymbol{EF}$ to the other epd's is given by

$$\boldsymbol{EF} = -\frac{1}{6}\sqrt{\frac{15}{2}}\boldsymbol{C}^3 + \sqrt{\frac{3}{5}}\boldsymbol{A}^2\boldsymbol{BC} - \frac{2}{\sqrt{15}}\boldsymbol{A}^3\boldsymbol{D}, \tag{7}$$

i.e., any product of $\boldsymbol{EF}$ can be expressed in terms of the other epd's, implying that either only powers in $\boldsymbol{E}$ or $\boldsymbol{F}$ may appear. This relation can also be used to express third powers of $\boldsymbol{C}$ in terms of the other epd's, as is suggested in Ref. 11. We take the choice (7) as also was done in Ref. 12.

Choosing $\boldsymbol{E}$ and $\boldsymbol{F}$ as dependent epd's, there are two types of polynomials, one with $(\lambda+3k,\lambda)$ and the other with $(\lambda,\lambda+3k)$, respectively, i.e.,

$$\boldsymbol{E}^{n_5}\boldsymbol{D}^{n_4}\boldsymbol{C}^{n_3}\boldsymbol{B}^{n_2}\boldsymbol{A}^{n_1}|0\rangle, \quad \boldsymbol{F}^{n_5}\boldsymbol{D}^{n_4}\boldsymbol{C}^{n_3}\boldsymbol{B}^{n_2}\boldsymbol{A}^{n_1}|0\rangle, \tag{8}$$

which now covers all possible irreps of U(8), as proven in Ref. 11. Fixing the total number of quanta N, the λ and μ for the first case (only powers of $\boldsymbol{E}$ appear), we obtain the following relation between the powers of the monomial:

$$\begin{aligned} N &= n_1 + 2n_2 + 2n_3 + 3n_4 + 3n_5, \\ \lambda &= n_1 + n_3 + 3n_5, \\ \mu &= n_1 + n_3. \end{aligned} \tag{9}$$

These relations are obtained, applying the number operator to the polynomial state, taking into account the order of the tensors in the creation operators and by noting that the tensors $\boldsymbol{A}$, $\boldsymbol{C}$ are in the maximum weight and transform as $(1,1)$, while $\boldsymbol{E}$ transforms as $(3,0)$, which is also in the maximum SU(3) weight.

Similar relations hold when only powers of $\boldsymbol{F}$ appear

$$\begin{aligned} N &= n_1 + 2n_2 + 2n_3 + 3n_4 + 3n_5, \\ \lambda &= n_1 + n_3, \\ \mu &= n_1 + n_3 + 3n_5. \end{aligned} \tag{10}$$

Up to now, the polynomials have no definite seniority ν, the quantum number of the O(8) group. This is achieved requiring that the application of

$$\overline{\boldsymbol{B}} = [\boldsymbol{b}\otimes\boldsymbol{b}]^{(0,0)}_{000} \tag{11}$$

on a polynomial in terms of the monomials of Eq. (8), gives zero (no pairs are contained, see, e.g., Refs. 25 and 26). This leads to the polynomials which have a seniority $\nu=N$. Explicitly, the condition reads

$$\overline{\boldsymbol{B}}P_{N=\nu(\lambda,\mu)}(\boldsymbol{A},\boldsymbol{B},\boldsymbol{C},\boldsymbol{D},\boldsymbol{E}(\boldsymbol{F}))|0\rangle = 0, \tag{12}$$

where the polynomial has the following structure for the case when only powers of $\boldsymbol{E}$ appear

$$\boldsymbol{P}_1 = \boldsymbol{E}^{(\lambda-\mu)/3}\sum_{n_1 n_2} c_{n_1 n_2}\boldsymbol{A}^{n_1}\boldsymbol{B}^{n_2}\boldsymbol{C}^{\mu-n_1}\boldsymbol{D}^{(N-\lambda-\mu+n_1-2n_2)/3}, \tag{13}$$

and similar when only powers of $\boldsymbol{F}$ appear

TABLE III. List of the polynomial coefficients with definite seniority for $\nu=0$ until $\nu=4$. For the coefficients only numerical values are given. They can be expressed in terms of square roots of rational numbers. However, for larger N there are cases where this cannot be done (see comments in text), which is the reason for this presentation. The powers of all epd's can be deduced using Eqs. (13) and (14), the value of the SU(3) irrep and the numbers of n_1, n_2 listed.

ν	(λ,μ)	n_1	n_2	State No. k	$c_{n_1n_2}$
0	(0,0)	0	0	1	1
1	(1,1)	1	0	1	1
2	(2,2)	2	0	1	0.707 106 78
2	(1,1)	0	0	1	0.707 106 78
3	(3,3)	3	0	1	0.408 248 29
3	(2,2)	1	0	1	0.597 614 31
3	(3,0)	0	0	1	0.527 046 28
3	(0,3)	0	0	1	0.527 046 28
3	(0,0)	0	0	1	0.223 606 80
4	(4,4)	4	0	1	0.204 124 15
4	(3,3)	2	0	1	0.372 678 00
4	(4,1)	1	0	1	0.372 678 00
4	(1,4)	1	0	1	0.372 678 00
4	(2,2)	0	0	1	0.289 318 78
4	(2,2)	2	1	1	−0.019 287 92
4	(1,1)	0	1	1	0.031 497 04
4	(1,1)	1	0	1	−0.195 180 02

$$\boldsymbol{P}_2 = \boldsymbol{F}^{(\mu-\lambda)/3} \sum_{n_1 n_2} c_{n_1 n_2} \boldsymbol{A}^{n_1} \boldsymbol{B}^{n_2} \boldsymbol{C}^{\lambda-n_1} \boldsymbol{D}^{(N-\mu-\lambda+n_1-2n_2)/3}. \tag{14}$$

Each of these polynomials we will abbreviate by

$$\boldsymbol{P} = \sum_{n_1 n_2} c_{n_1 n_2} |n_1 n_2\rangle, \tag{15}$$

where we omitted the labels (λ,μ) and applied the operators on the vacuum, resulting in a ket-state. Applying from the left $\langle n_1' n_2' | \overline{\boldsymbol{B}}$, with $n_1'+n_2'+1=n_1+n_2$ and the same (λ,μ) on both sides, we arrive at the defining equation for the coefficients $c_{n_1n_2}$,

$$\sum_{n_1 n_2} c_{n_1 n_2} \langle n_1' n_2' + 1 | n_1 n_2 \rangle = 0. \tag{16}$$

The overlaps $\langle n_1' n_2' + 1 \,|\, n_1 n_2 \rangle$ in the sum are calculated. How to determine the overlaps is described in more detail in Sec. III. Having obtained the overlaps, the above equation is solved numerically, leading in this way to maximal weight states in SU(3) with good seniority and $N=\nu$. The state with $N>\nu$ is depicted below in Eq. (32).

In Tables III–VIII we give a list of all polynomials up to eight bosons, with the additional restriction of $N=\nu$. In case there is more than one state, an additional multiplicity index is assigned, called k. Only numerical values are given, though, most of the numbers listed in the tables can be expressed as square roots of rational numbers. However, when more than one state for a given seniority and SU(3) irrep (λ,μ) appears, a Schmidt orthogonalization procedure is applied, yielding only simple numbers for the first state but in general real numbers for states with a higher index in k. In calculations within the models of Refs. 8, 13, and 14 no more than six bosons are needed.

Up to now, only highest weight states in SU(3) were considered. In the highest weight of the irrep (λ,μ) the value of the hypercharge and the third component of the isospin is given by

TABLE IV. The same as in Table III, but now for $\nu = 5$.

ν	(λ,μ)	n_1	n_2	State No.	$c_{n_1 n_2}$
5	(5,5)	5	0	1	0.091 287 09
5	(4,4)	3	0	1	0.194 624 74
5	(5,2)	2	0	1	0.204 124 15
5	(2,5)	2	0	1	0.204 124 15
5	(3,3)	1	0	1	0.220 479 28
5	(3,3)	3	1	1	−0.012 598 82
5	(4,1)	0	0	1	0.208 333 33
5	(1,4)	0	0	1	0.208 333 33
5	(2,2)	1	1	1	0.034 580 21
5	(2,2)	2	0	1	−0.125
5	(1,1)	0	0	1	0.109 108 95
5	(1,1)	1	2	1	−0.003 521 48

$(\lambda-\mu)/3$ and $(\lambda+\mu)/2$,[31] respectively. A state with a lower weight can be reached via the application of $\boldsymbol{T}_-^{\alpha}\boldsymbol{U}_+^{\beta}\boldsymbol{V}_-^{\gamma}$. When the weight of a state is given by (Y,T) and the difference to the highest weight is $-\Delta T_z$, for the third component of the isospin, and $+\Delta Y$ for the hypercharge, the exponents α, β, and γ fulfill the relations

$$\Delta T_z = \alpha + \tfrac{1}{2}(\beta+\gamma), \quad \Delta Y = \beta - \gamma. \tag{17}$$

As can be seen, there is in general more than one possibility. The final state reached has only a definite isospin when β or γ is zero. In general, the construction of the states with definite isospins, for a fixed weight Y and T_z must still be performed.

For the construction of states with a definite isospin, the overlap of the states

TABLE V. The same as in Table III, but now for $\nu = 6$.

ν	(λ,μ)	n_1	n_2	State No.	$c_{n_1 n_2}$
6	(6,6)	6	0	1	0.037 267 80
6	(5,5)	4	0	1	0.089 514 36
6	(6,3)	3	0	1	0.096 225 04
6	(3,6)	3	0	1	0.096 225 04
6	(4,4)	2	0	1	0.125 629 73
6	(4,4)	4	1	1	−0.006 281 49
6	(5,2)	1	0	1	0.144 337 57
6	(2,5)	1	0	1	0.144 337 57
6	(6,0)	0	0	1	0.107 582 87
6	(0,6)	0	0	1	0.107 582 87
6	(3,3)	0	0	1	0.070 812 72
6	(3,3)	2	1	1	0.
6	(3,3)	3	0	1	−0.029 254 03
6	(3,3)	0	0	2	0.044 592 127
6	(3,3)	2	1	2	−0.028 629 62
6	(3,3)	3	0	2	0.060 427 62
6	(2,2)	0	1	1	0.010 228 96
6	(2,2)	1	0	1	−0.084 515 43
6	(2,2)	2	2	1	0.002 045 79
6	(3,0)	0	0	1	0.070 429 52
6	(0,3)	0	0	1	0.070 429 52
6	(0,0)	0	0	1	0.024 397 50
6	(0,0)	0	3	1	−0.000 508 28

TABLE VI. The same as in Table III, for $\nu = 7$.

ν	(λ,μ)	n_1	n_2	State No.	$c_{n_1 n_2}$
7	(7,7)	7	0	1	0.014 085 90
7	(6,6)	5	0	1	0.037 267 80
7	(7,4)	4	0	1	0.040 662 50
7	(4,7)	4	0	1	0.040 662 50
7	(5,5)	3	0	1	0.060 657 70
7	(5,5)	5	1	1	−0.002 695 90
7	(6,3)	2	0	1	0.076 072 58
7	(3,6)	2	0	1	0.076 072 58
7	(7,1)	1	0	1	0.062 113 00
7	(1,7)	1	0	1	0.062 113 00
7	(4,4)	1	0	1	0.047 921 22
7	(4,4)	3	1	1	0.
7	(4,4)	4	0	1	−0.014 847 85
7	(4,4)	1	0	2	0.036 066 36
7	(4,4)	3	1	2	−0.016 830 97
7	(4,4)	4	0	2	0.027 936 88
7	(5,2)	0	0	1	0.055 170 93
7	(5,2)	2	1	1	−0.002 452 04
7	(2,5)	0	0	1	0.055 170 93
7	(2,5)	2	1	1	−0.002 452 04
7	(3,3)	1	1	1	0.010 594 03
7	(3,3)	2	0	1	−0.049 236 60
7	(3,3)	3	2	1	0.000 926 98
7	(4,1)	0	1	1	0.004 910 46
7	(1,4)	1	0	1	−0.045 643 55
7	(1,4)	0	1	1	0.004 910 46
7	(4,1)	1	0	1	−0.045 643 55
7	(2,2)	0	0	1	0.033 785 15
7	(2,2)	1	2	1	−0.001 453 88
7	(2,2)	2	1	1	−0.001 501 56
7	(1,1)	0	1	1	0.004 066 25
7	(1,1)	1	0	1	−0.018 898 22
7	(1,1)	1	3	1	0.000 262 48

$$|N\nu k(\lambda,\mu)\alpha\beta\gamma\rangle = \boldsymbol{T}_{-}^{\alpha}\boldsymbol{U}_{+}^{\beta}\boldsymbol{V}_{-}^{\gamma}|\mathrm{hw}\rangle = |\alpha\beta\gamma\rangle \tag{18}$$

must be determined, where hw is an abbreviation for "highest weight" and in the last line a short-hand notation for the state is given. This overlap is directly obtained using the commutation properties of the operators involved. The final result is

$$\begin{aligned}\langle\alpha'\beta'\gamma'|\alpha\beta\gamma\rangle &= \frac{\alpha!\,\alpha'!\,\gamma!\,\beta!\,\beta'!\lambda!\,(\lambda+\mu-\alpha-\beta-\gamma+\alpha')!\,(\gamma+\beta'-\beta)!}{(\lambda-\gamma)!\,(\mu+\gamma-\beta)!\,(\lambda-\gamma-\beta'+\beta)!} \\ &\times \sum_{k=\max(0,\beta-\beta')}^{\min(\alpha',\beta,\gamma)} \frac{(\lambda-\gamma+k)!\,(\mu+\gamma-k)!}{k!\,(\alpha'-k)!\,(\gamma-k)!\,(\lambda+\mu-\alpha-\beta-\gamma+k)!\,(\beta'-\beta+k)!\,(\beta-k)!}.\end{aligned} \tag{19}$$

TABLE VII. The same as in Table III. Partial list for $\nu = 8$.

ν	(λ,μ)	n_1	n_2	State No.	$c_{n_1 n_2}$
8	(8,8)	8	0	1	0.004 980 12
8	(7,7)	6	0	1	0.014 291 55
8	(8,5)	5	0	1	0.015 748 52
8	(5,8)	5	0	1	0.015 748 52
8	(6,6)	4	0	1	0.026 041 67
8	(6,6)	6	1	1	−0.001 041 67
8	(7,4)	3	0	1	0.034 366 09
8	(4,7)	3	0	1	0.034 366 09
8	(8,2)	2	0	1	0.028 752 73
8	(2,8)	2	0	1	0.028 752 73
8	(5,5)	2	0	1	0.025 227 06
8	(5,5)	4	1	1	0.
8	(5,5)	5	0	1	−0.006 253 05
8	(5,5)	2	0	2	0.019 911 16
8	(5,5)	4	1	2	−0.008 147 65
8	(5,5)	5	0	2	0.011 894 31
8	(6,3)	1	0	1	0.037 297 65
8	(6,3)	3	1	1	−0.001 491 91
8	(3,6)	1	0	1	0.037 297 65
8	(3,6)	3	1	1	−0.001 491 91
8	(7,1)	0	0	1	0.029 611 21
8	(1,7)	0	0	1	0.029 611 21
8	(4,4)	0	0	1	0.014 674 54
8	(4,4)	2	1	1	0.
8	(4,4)	3	0	1	−0.012 124 64
8	(4,4)	4	2	1	0.000 260 88

States with definite isospin are obtained by diagonalizing the operator $\boldsymbol{T}^2 = \boldsymbol{T}_+\boldsymbol{T}_- + \boldsymbol{T}_z(\boldsymbol{T}_z - 1)$ within the states given above. Note, however, that $|\alpha\beta\gamma>$ are not orthogonal with respect to different values of α, β, and γ. The overlap is given in (19). The most practical method is to solve numerically the equation

$$\sum_{\alpha'\beta'\gamma'} \frac{\langle \alpha'\beta'\gamma'|\boldsymbol{T}^2|\alpha\beta\gamma\rangle}{\sqrt{\langle \alpha'\beta'\gamma'|\alpha'\beta'\gamma'\rangle\langle\alpha\beta\gamma|\alpha\beta\gamma\rangle}} a_{\alpha'\beta'\gamma'} = T(T+1) \sum_{\alpha'\beta'\gamma'} \frac{\langle \alpha'\beta'\gamma'|\alpha\beta\gamma\rangle}{\sqrt{\langle \alpha'\beta'\gamma'|\alpha'\beta'\gamma'\rangle\langle\alpha\beta\gamma|\alpha\beta\gamma\rangle}} a_{\alpha'\beta'\gamma'}, \tag{20}$$

where the coefficients $a_{\alpha\beta\gamma}$ are the expansion coefficients in the basis $|\alpha\beta\gamma>$. The matrix elements of $\boldsymbol{T}_+\boldsymbol{T}_-$ are obtained through the overlaps

$$\frac{\langle \alpha'+1\beta'\gamma'|\alpha+1\beta\gamma\rangle}{\sqrt{\langle \alpha'\beta'\gamma'|\alpha'\beta'\gamma'\rangle\langle\alpha\beta\gamma|\alpha\beta\gamma\rangle}}, \tag{21}$$

while T_z is diagonal.

The state with definite isospin is then given by

$$|N\nu(\lambda,\mu)YTT_z\rangle = \sum_{\alpha\beta\gamma} a^{YTT_z}_{\alpha\beta\gamma} |N\nu(\lambda,\mu)\alpha\beta\gamma\rangle / \sqrt{\langle\alpha\beta\gamma|\alpha\beta\gamma\rangle}, \tag{22}$$

with the constriction on α, β, and γ given by $Y = [(\lambda+\mu)/3] + (\beta-\gamma)$ and $T_z = [(\lambda-\mu)/2] - \alpha - \frac{1}{2}(\beta+\gamma)$.

TABLE VIII. The same as in Table III. Partial list for $\nu = 8$.

ν	(λ,μ)	n_1	n_2	State No.	$c_{n_1 n_2}$
8	(4,4)	0	0	2	0.011 363 92
8	(4,4)	2	1	2	−0.008 933 20
8	(4,4)	3	0	2	0.021 364 60
8	(4,4)	4	2	2	−0.000 261 18
8	(5,2)	1	1	1	0.004 504 69
8	(5,2)	2	0	1	−0.023 262 11
8	(2,5)	1	1	1	0.004 504 69
8	(2,5)	2	0	1	−0.023 262 11
8	(3,3)	0	1	1	0.002 337 37
8	(3,3)	1	0	1	−0.024 140 23
8	(3,3)	2	2	1	0.000 727 18
8	(3,3)	3	1	1	0.000 965 61
8	(4,1)	0	0	1	0.021 759 71
8	(4,1)	1	2	1	−0.000 468 19
8	(1,4)	0	0	1	0.021 759 71
8	(1,4)	1	2	1	−0.000 468 19
8	(2,2)	0	2	1	0.000 229 88
8	(2,2)	1	1	1	−0.004 273 52
8	(2,2)	2	0	1	0.011 034 19
8	(2,2)	2	3	1	−0.000 107 28
8	(1,1)	0	0	1	0.009 009 37
8	(1,1)	0	3	1	−0.000 125 13
8	(1,1)	1	2	1	−0.000 387 70

Care must still be taken with respect to the phase. The lower weight states are obtained via the application of $\boldsymbol{T}_-$, $\boldsymbol{U}_+$, and $\boldsymbol{V}_-$. For example, when only a power of the $\boldsymbol{T}_-$ operator is applied to the maximal weight state, we arrive at $|\alpha 00\rangle$ *with a positive sign in front* and the same isospin as in the maximum weight state. Similar, parting from the highest weight state, the application of only U_+ or only V_- leads to a state with definite isospin $(\lambda+\mu-\beta)/2$ (for $\gamma=0$) or $(\lambda+\mu-\gamma)/2$ (for $\beta=0$). Posterior application of T_- leads to states with the same isospin. Therefore, we require that the component $|\alpha\beta\gamma\rangle$ with either β or γ equal to zero, within a state of definite isospin, has also a positive sign in front of $|\alpha\beta 0\rangle$ (for $\gamma=0$) or $|\alpha 0\gamma\rangle$ (for $\beta=0$). In case the numerical program produced states with an opposite sign, we corrected for it by multiplying all coefficients by (-1).

III. THE ISOSCALAR FACTORS AND CLEBSCH-GORDAN COEFFICIENTS

Once the states are obtained, we can proceed in the calculation of the CGC's. Before that, a general remark on the Wigner-Eckart theorem for a given group chain $G \supset H$ is due: When Γ represents the label of the group G and μ of its subgroup H and $\boldsymbol{T}^{\Gamma}_{\mu}$ is a tensor, then the matrix elements can be expressed as[9]

$$\langle \Gamma'\mu'|\boldsymbol{T}^{\Gamma_0}_{\mu_0}|\Gamma\mu\rangle = \sum_{\rho} \langle \Gamma\mu,\Gamma_0\mu_0|\Gamma'\mu'\rangle_{\rho}\langle \Gamma'\|T^{\Gamma_0}\|\Gamma\rangle_{\rho}, \tag{23}$$

where ρ is a multiplicity index in the coupling $\Gamma\otimes\Gamma_0\rightarrow\Gamma'$, the first factor in the sum over ρ is the CGC and the last one the reduced matrix element. In order to distinguish the reduced matrix element of a group G different from SU(2), often the notation of "multiple reduced" matrix element is used. Like in SU(3) (Ref. 30) where the reduced matrix element of SU(3) is called *triple reduced* matrix element. Here we will continue to use this notation for SU(3) and for the reduced matrix element of $U(8)\supset O(8)\supset SU(3)$ the name of *quadruple reduced matrix element* is

proposed. The sum over the multiplicity index is only applied when the multiplicity is larger than one.

Now we will return to the determination of the $U(8) \supset O(8) \supset SU(3)$ CGC's and its isoscalar factors.

In a first step we determine the triple reduced matrix elements with respect to the SU(3) group.[30] The equation to solve is

$$\begin{aligned}
&\langle N_3 \nu_3 k_3(\lambda_3,\mu_3) Y_3 T_3 T_{3z} | P_{N_1 \nu_1 k_1(\lambda_1,\mu_1) Y_1 T_1 T_{1z}}(\boldsymbol{b}^\dagger) | N_2 \nu_2 k_2(\lambda_2,\mu_2) Y_2 T_2 T_{2z} \rangle \\
&\quad = \sum_\rho \langle (\lambda_2,\mu_2) Y_2 T_2 T_{2z}; (\lambda_1,\mu_1) Y_1 T_1 T_{1z} | (\lambda_3,\mu_3) Y_3 T_3 T_{3z} \rangle_\rho \\
&\qquad \times \langle N_3 \nu_3 k_3(\lambda_3,\mu_3) ||| P_{N_1 \nu_1 k_1(\lambda_1,\mu_1)}(\boldsymbol{b}^\dagger) ||| N_2 \nu_2 k_2(\lambda_2,\mu_2) \rangle .
\end{aligned} \tag{24}$$

Let us suppose that we have the result concerning the first line in Eq. (24). How to obtain it will be explained further below. The SU(3) Clebsch-Gordan coefficients are well known[29] and, thus, (24) represents an equation to determine the triple reduced matrix elements. It suffices to use maximal weight states for the polynomial 1 and 3, while the weight of the second polynomial is given by the difference of the weight of the third with the first polynomial.

In the next step, the Wigner-Eckart theorem for the $U(8) \supset O(8) \supset SU(3)$ group chain is used, i.e.,

$$\begin{aligned}
&\langle N_3 \nu_3 k_3(\lambda_3,\mu_3) Y_3 T_3 T_{3z} | P_{N_1 \nu_1 k_1(\lambda_1,\mu_1) Y_1 T_1 T_{1z}}(\boldsymbol{b}^\dagger) | N_2 \nu_2 k_2(\lambda_2,\mu_2) Y_2 T_2 T_{2z} \rangle \\
&\quad = (N_2 \nu_2 k_2(\lambda_2,\mu_2) Y_2 T_2 T_{2z}; N_1 \nu_1 k_1(\lambda_1,\mu_1) Y_1 T_1 T_{1z} | N_3 \nu_3 k_3(\lambda_3,\mu_3) Y_3 T_3 T_{3z}) \langle N_3 |||| P_{N_1}(\boldsymbol{b}^\dagger) |||| N_2 \rangle .
\end{aligned} \tag{25}$$

There is no sum over a multiplicity index because the labels of the U(8) irrep is the number $[N]$, given here in the notation of a Young diagram, and the multiplication of two symmetric irreps is always free of multiplicities.

Comparing Eq. (25) with Eq. (24) we arrive at

$$\begin{aligned}
&(N_2 \nu_2 k_2(\lambda_2,\mu_2) Y_2 T_2 T_{2z}; N_1 \nu_1 k_1(\lambda_1,\mu_1) Y_1 T_1 T_{1z} | N_3 \nu_3 k_3(\lambda_3,\mu_3) Y_3 T_3 T_{3z}) \\
&\quad = \sum_\rho \langle (\lambda_2,\mu_2) Y_2 T_2 T_{2z}; (\lambda_1,\mu_1) Y_1 T_1 T_{1z} | (\lambda_3,\mu_3) Y_3 T_3 T_{3z} \rangle_\rho \\
&\qquad \times \frac{\langle N_3 \nu_3 k_3(\lambda_3,\mu_3) ||| P_{N_1 \nu_1 k_1(\lambda_1,\mu_1)}(\boldsymbol{b}^\dagger) ||| N_2 \nu_2 k_2(\lambda_2,\mu_2) \rangle_\rho}{\langle N_3 |||| P_{N_1}(\boldsymbol{b}^\dagger) |||| N_2 \rangle} .
\end{aligned} \tag{26}$$

The CGC of the SU(3) group are known, thus, it suffices to determine

$$\begin{aligned}
&\langle N_2 \nu_2 k_2(\lambda_2,\mu_2), N_1 \nu_1 k_1(\lambda_1,\mu_1) \| N_3 \nu_3 k_3(\lambda_3,\mu_3) \rangle_\rho \\
&\qquad = \frac{\langle N_3 \nu_3 k_3(\lambda_3,\mu_3) ||| P_{N_1 \nu_1 k_1(\lambda_1,\mu_1)}(\boldsymbol{b}^\dagger) ||| N_2 \nu_2 k_2(\lambda_2,\mu_2) \rangle_\rho}{\langle N_3 |||| P_{N_1}(\boldsymbol{b}^\dagger) |||| N_2 \rangle} ,
\end{aligned} \tag{27}$$

which we will denote as *isoscalar factors* of the group chain $U(8) \supset O(8) \supset SU(3)$.

Equation (27) implies that the triple reduced matrix element with respect to the group chain $SU(3) \supset SU(2) \otimes U(1)$ and the quadruple reduced matrix element of $U(8) \supset O(8)$ must be determined. The last is the simplest one. For that, the U(8) CGC's are calculated, assuming the seniority ν_k in all polynomials *equal to* N_k (then, the CGC is just 1). The polynomials have the form

$$P_k = \frac{1}{\sqrt{N_k!}} \boldsymbol{A}^{N_k} |0\rangle , \tag{28}$$

with $k=1,2,3$. The result is

$$\langle N_3 || || P^{[N_1]} || || N_2 \rangle = \left[\frac{N_3!}{N_1!\, N_2!} \right]^{1/2} . \tag{29}$$

The triple reduced matrix elements of the group chain $\mathrm{SU}(3) \supset \mathrm{SU}(2) \otimes \mathrm{U}(1)$ are obtained through the use of Eq. (24), as already explained.

The important part is the calculation of the left-hand side of Eq. (24). In a first step the overlaps $\langle n_1' n_2' | n_1 n_1 \rangle$, as defined in Eqs. (15) and (16), are determined. For that, we write the explicit form of the epd's in terms of the boson creation operators. To simplify notations, we rename a boson creation operator $\boldsymbol{b}_\xi^\dagger$ by a coordinate x_ξ and the corresponding annihilation operator $\boldsymbol{b}^\xi$ by a derivative $\partial/\partial x_\xi$. Both satisfy the same commutation relations (with this, it is easier to translate it to an algebraic routine, like MATEMATICA,[32] which assists in the evaluation of the overlaps). In terms of this new notation and using the association of the linear index ξ to (YTT_z) (see Table II), the epd's of U(8) have the following structure:

$$\begin{aligned}
\boldsymbol{A} &= x_1, \\
\boldsymbol{B} &= \frac{1}{\sqrt{8}}(x_4^2 - 2x_1x_8 + x_5^2 - 2x_2x_7 + 2x_3x_6), \\
\boldsymbol{C} &= 2\sqrt{\frac{3}{10}} x_3x_2 - \frac{2}{\sqrt{5}} x_1x_5, \\
\boldsymbol{D} &= \sqrt{\frac{3}{10}} \left(-\frac{3}{2}\sqrt{2} x_1x_6x_7 + \sqrt{3} x_1x_5x_8 + \frac{\sqrt{3}}{2} x_3x_5x_6 - \frac{\sqrt{3}}{2} x_2x_5x_7 \right. \\
&\quad \left. + \frac{3}{2} x_2x_4x_7 - \frac{3}{2}\sqrt{2} x_2x_3x_8 + \frac{3}{2} x_3x_4x_6 - \frac{\sqrt{3}}{2} x_4^2x_5 + \frac{1}{2\sqrt{3}} x_5^3 \right), \\
\boldsymbol{E} &= \sqrt{\frac{3}{5}} x_2^2x_3 - \frac{3}{\sqrt{10}} x_1x_2x_5 - \sqrt{\frac{3}{5}} x_1^2x_6 + \sqrt{\frac{3}{10}} x_1x_2x_4, \\
\boldsymbol{F} &= -\sqrt{\frac{3}{5}} x_1^2x_7 + \sqrt{\frac{3}{10}} x_1x_3x_4 - \sqrt{\frac{3}{5}} x_3^2x_2 + \frac{3}{\sqrt{10}} x_1x_3x_5 .
\end{aligned} \tag{30}$$

These expressions are obtained using the explicit values of the SU(3) CGS's, as obtained in Refs. 2–4. One can easily verify that they are in the maximum weight of the corresponding SU(3) label [see Eq. (6)]. The Hermitian conjugate expressions are obtained by changing x_ξ to $\partial/\partial x_\xi$.

What we also need is the explicit form of the lowering operators T_-, U_+, and V_-, in order to obtain a lower weight state in what we call the second polynomial. Starting from Eq. (5) and using the explicit form of the SU(3) CGC's, we obtain

$$\boldsymbol{T}_- = \sqrt{2} x_8 \frac{\partial}{\partial x_4} + \sqrt{2} x_4 \frac{\partial}{\partial x_1} + x_6 \frac{\partial}{\partial x_2} + x_7 \frac{\partial}{\partial x_3},$$

$$\boldsymbol{U}_+ = -\sqrt{\frac{3}{2}}x_5\frac{\partial}{\partial x_3} + \frac{1}{\sqrt{2}}x_4\frac{\partial}{\partial x_3} + x_8\frac{\partial}{\partial x_7} - \frac{1}{\sqrt{2}}x_6\frac{\partial}{\partial x_4} + \sqrt{\frac{3}{2}}x_6\frac{\partial}{\partial x_5} - x_2\frac{\partial}{\partial x_1}, \tag{31}$$

$$\boldsymbol{V}_- = \frac{1}{\sqrt{2}}x_4\frac{\partial}{\partial x_2} + \sqrt{\frac{3}{2}}x_5\frac{\partial}{\partial x_2} + x_8\frac{\partial}{\partial x_6} + x_3\frac{\partial}{\partial x_1} + \sqrt{\frac{3}{2}}x_7\frac{\partial}{\partial x_5} + \frac{1}{\sqrt{2}}x_7\frac{\partial}{\partial x_4}.$$

For the overlaps, we must apply these lowering operators to a highest weight state in SU(3) of what we called the second polynomial, as given in Eq. (18), using the norm depicted in Eq. (19) and multiply it with what we called the first polynomial in the highest weight state. That is, we must construct $P_{N_1\nu_1k_1(\lambda_1,\mu_1)Y_1^{\max}T_1^{\max}T_1^{\max}}(x)\ P_{N_2\nu_2k_2(\lambda_2,\mu_2)Y_2T_2T_{2z}}(x)$. This gives us an expression which depends on the x_ξ only. On that we must apply the conjugate expression of what we call the third polynomial, which is a pure function of derivatives, i.e. $P_{N_3\nu_3k_3(\lambda_3,\mu_3)Y_3^{\max}T_3^{\max}T_3^{\max}}(\partial/\partial x)$. In principle, this quite involved calculation can be done by hand. It is advisable to take the assistance of an algebraic routine like MATEMATICA,[32] considering that the number of overlaps to calculate is in the thousands. With this help, we finally obtain the overlap on the left-hand side of Eq. (24).

Not all possible matrix elements were calculated but only those with $N_1=\nu_1$, $N_2=\nu_2$ and, thus, $N_3=\nu_1+\nu_2$ and $N_3\geq\nu_3$. The corresponding isoscalar factors of Eq. (27) were determined. In order to obtain all other possible isoscalar factors, with $N_k>\nu_k$ $(k=1,2)$ and $N_3=N_1+N_2$, we note that the corresponding state can be written as

$$|N_k\nu_k\xi_k\rangle = \left[\frac{(\nu_k+3)!}{4^{(N_k-\nu_k)/2}\left(\frac{N_k-\nu_k}{2}\right)!\left(\frac{N_k+\nu_k+6}{2}\right)!}\right]^{1/2}(\boldsymbol{b}^\dagger\cdot\boldsymbol{b}^\dagger)^{(N_k-\nu_k)/2}|\nu_k\xi_k\rangle, \tag{32}$$

where now ξ_k denote all other quantum numbers $(\lambda_k,\mu_k)\ Y_kT_kT_{kz}$, $|\nu_k\xi_k\rangle$ is the state with $N_k=\nu_k$ and $(\boldsymbol{b}^\dagger\cdot\boldsymbol{b}^\dagger)$ is the scalar product between the boson creation operators.

Introducing this on the left-hand side of Eq. (25) leads to

$$\begin{aligned}&\langle N_3\nu_3\xi_3|P_{N_1\nu_1\xi_1}(\boldsymbol{b}^\dagger)|N_2\nu_2\xi_2\rangle\\ &=\left[\frac{(\nu_1+3)!\,(\nu_2+3)!\left(\frac{N_3-\nu_3}{2}\right)!\left(\frac{N_3+\nu_3+6}{2}\right)!}{\left(\frac{N_1-\nu_1}{2}\right)!\left(\frac{N_2-\nu_2}{2}\right)!\left(\frac{N_1+\nu_1+6}{2}\right)!\left(\frac{N_2+\nu_2+6}{2}\right)!\left(\frac{\nu_1+\nu_2-\nu_3}{2}\right)!\left(\frac{\nu_1+\nu_2+\nu_3+6}{2}\right)!}\right]^{1/2}\\ &\times\langle N_3=\nu_1+\nu_2,\nu_3\xi_3|P_{N_1=\nu_1\nu_1\xi_1}(\boldsymbol{b}^\dagger)|N_2=\nu_2,\nu_2\xi_2\rangle.\end{aligned} \tag{33}$$

Using (25), we arrive at the following relations of CGC's:

$$\begin{aligned}&\langle N_2\nu_2\xi_2,N_1\nu_1\xi_1|N_3\nu_3\xi_3\rangle\\ &=\left[\frac{(\nu_1+3)!\,N_1!}{\left(\frac{N_1-\nu_1}{2}\right)!\,\nu_1!\left(\frac{N_1+\nu_1+6}{2}\right)!}\frac{(\nu_2+3)!\,N_2!}{\left(\frac{N_2-\nu_2}{2}\right)!\,\nu_2!\left(\frac{N_2+\nu_2+6}{2}\right)!}\frac{\left(\frac{N_3-\nu_3}{2}\right)!\left(\frac{N_3+\nu_3+6}{2}\right)!}{N_3!}\right.\\ &\left.\times\frac{(\nu_1+\nu_2)!}{\left(\frac{\nu_1+\nu_2-\nu_3}{2}\right)!\left(\frac{\nu_1+\nu_2+\nu_3+6}{2}\right)!}\right]^{1/2}\\ &\times\langle N_2=\nu_2,\nu_2\xi_2,N_1=\nu_1,\nu_1\xi_1|N_3=(\nu_1+\nu_2),\nu_3\xi_3\rangle.\end{aligned} \tag{34}$$

The same holds for the isoscalar factors, which can be verified using Eq. (26).

Programs for all the steps mentioned are available and can be handed over on request.

In Table IX a partial list of the isoscalar factors for up to eight bosons is given, involving only the SU(3) irreps (0,0), (1,1), (3,0), (0,3) and restricting to $\nu_1\geq\nu_2$ (for $\nu_1<\nu_2$ we use the symmetric property of the isoscalar factors under permutation of the first two irreps). Irreps with a higher value were calculated, too, but are not tabulated. In total there are about 15 000 isoscalar factors calculated involving states up to eight particles. Here, we only give a partial list containing, as we think, the isoscalar factors of most interest. These involve the SU(3) irreps (0,0), (1,1), (3,0),

TABLE IX. Partial list of isoscalar factors (denoted by IF) for the group chain $U(8) \supset O(8) \supset SU(3)$. Only those are listed with $\nu_k = N_k$ $(k=1,2)$ and $\nu_1 > \nu_2$, thus, the $N_3 = \nu_1 + \nu_2$. For this reason, the value of N_3 is not listed. Equation (34) must be applied in order to obtain the isoscalar factors for $N_1 > \nu_1$, $N_2 > \nu_2$ and $N_3 = N_1 + N_2$.

ν_2	k_2 (λ_2,μ_2)	ν_1	k_1 (λ_1,μ_1)	ν_3	k_3 (λ_3,μ_3)	ρ	IF
0	1 (0,0)	0	1 (0,0)	0	1 (0,0)	1	1
0	1 (0,0)	1	1 (1,1)	1	1 (1,1)	1	1
1	1 (1,1)	1	1 (1,1)	2	1 (1,1)	1	0
1	1 (1,1)	1	1 (1,1)	2	1 (1,1)	2	1
1	1 (1,1)	1	1 (1,1)	0	1 (0,0)	1	1
0	1 (0,0)	2	1 (1,1)	2	1 (1,1)	1	1
1	1 (1,1)	2	1 (1,1)	3	1 (0,0)	1	1
1	1 (1,1)	2	1 (1,1)	3	1 (0,3)	1	−0.774 596 67
1	1 (1,1)	2	1 (1,1)	3	1 (3,0)	1	0.774 596 67
1	1 (1,1)	2	1 (1,1)	1	1 (1,1)	1	0
1	1 (1,1)	2	1 (1,1)	1	1 (1,1)	2	0.365 148 37
2	1 (1,1)	2	1 (1,1)	4	1 (1,1)	1	0
2	1 (1,1)	2	1(1,1)	4	1 (1,1)	2	−0.648 074 07
2	1 (1,1)	2	1 (1,1)	2	1 (1,1)	1	0
2	1 (1,1)	2	1 (1,1)	2	1 (1,1)	2	−0.141 421 36
2	1 (1,1)	2	1 (1,1)	0	1 (0,0)	1	0.365 148 37
0	1 (0,0)	3	1 (3,0)	3	1 (3,0)	1	1
0	1 (0,0)	3	1 (0,3)	3	1 (0,3)	1	1
0	1 (0,0)	3	1 (0,0)	3	1 (0,0)	1	1
1	1 (1,1)	3	1 (3,0)	4	1 (1,1)	1	0.467 707 18
1	1 (1,1)	3	1 (0,3)	4	1 (1,1)	1	−0.467 707 18
1	1 (1,1)	3	1 (0,0)	4	1 (1,1)	1	−0.572 821 96
1	1 (1,1)	3	1 (3,0)	2	1 (1,1)	1	0.306 186 22
1	1 (1,1)	3	1 (0,3)	2	1 (1,1)	1	−0.306 186 22
1	1 (1,1)	3	1 (0,0)	2	1 (1,1)	1	0.125
2	1 (1,1)	3	1 (3,0)	5	1 (1,1)	1	0.374 165 74
2	1 (1,1)	3	1 (0,3)	5	1 (1,1)	1	−0.374 165 74
2	1 (1,1)	3	1 (0,0)	5	1 (1,1)	1	0.458 257 57
2	1 (1,1)	3	1 (3,0)	3	1 (3,0)	1	0
2	1 (1,1)	3	1 (0,3)	3	1 (0,3)	1	0
2	1 (1,1)	3	1 (3,0)	1	1 (1,1)	1	−0.122 474 49
2	1 (1,1)	3	1 (0,3)	1	1 (1,1)	1	0.122 474 49
2	1 (1,1)	3	1 (0,0)	1	1 (1,1)	1	0.05
3	1 (3,0)	3	1 (3,0)	6	1 (0,3)	1	0
3	1 (0,3)	3	1 (3,0)	6	1 (0,0)	1	−0.483 045 89
3	1 (0,0)	3	1 (3,0)	6	1 (3,0)	1	0.374 165 74
3	1 (3,0)	3	1 (0,3)	6	1 (0,0)	1	−0.483 045 89
3	1 (0,3)	3	1 (0,3)	6	1 (3,0)	1	0
3	1 (0,0)	3	1 (0,3)	6	1 (0,3)	1	0.374 165 74
3	1 (3,0)	3	1 (0,0)	6	1 (3,0)	1	0.374 165 74
3	1 (0,3)	3	1 (0,0)	6	1 (0,3)	1	0.374 165 74
3	1 (0,0)	3	1 (0,0)	6	1 (0,0)	1	0.458 257 57
3	1 (0,3)	3	1 (3,0)	4	1 (1,1)	1	0
3	1 (3,0)	3	1 (0,3)	4	1 (1,1)	1	0
3	1 (0,3)	3	1 (3,0)	2	1 (1,1)	1	0
3	1 (3,0)	3	1 (0,3)	2	1 (1,1)	1	0
3	1 (0,3)	3	1 (3,0)	0	1 (0,0)	1	0.158 113 88
3	1 (3,0)	3	1 (0,3)	0	1 (0,0)	1	0.158 113 88
3	1 (0,0)	3	1 (0,0)	0	1 (0,0)	1	0.05
0	1 (0,0)	4	1 (1,1)	4	1 (1,1)	1	1

TABLE IX. (*Continued.*)

ν_2	$k_2\ (\lambda_2,\mu_2)$	ν_1	$k_1\ (\lambda_1,\mu_1)$	ν_3	$k_3\ (\lambda_3,\mu_3)$	ρ	IF
1	1 (1,1)	4	1 (1,1)	5	1 (1,1)	1	0
1	1 (1,1)	4	1 (1,1)	5	1 (1,1)	2	−0.8
1	1 (1,1)	4	1 (1,1)	3	1 (0,0)	1	−0.547 722 56
1	1 (1,1)	4	1 (1,1)	3	1 (0,3)	1	−0.141 421 36
1	1 (1,1)	4	1 (1,1)	3	1 (3,0)	1	0.141 421 36
2	1 (1,1)	4	1 (1,1)	6	1 (0,0)	1	−0.8
2	1 (1,1)	4	1 (1,1)	6	1 (0,3)	1	−0.505 964 43
2	1 (1,1)	4	1 (1,1)	6	1 (3,0)	1	0.505 964 43
2	1 (1,1)	4	1 (1,1)	4	1 (1,1)	1	0
2	1 (1,1)	4	1 (1,1)	4	1 (1,1)	2	0.103 279 56
2	1 (1,1)	4	1 (1,1)	2	1 (1,1)	1	0
2	1 (1,1)	4	1 (1,1)	2	1 (1,1)	2	−0.089 442 72
3	1 (3,0)	4	1 (1,1)	7	1 (1,1)	1	0.318 727 63
3	1 (0,3)	4	1 (1,1)	7	1 (1,1)	1	−0.318 727 63
3	1 (0,0)	4	1 (1,1)	7	1 (1,1)	1	0.390 360 03
3	1 (3,0)	4	1 (1,1)	5	1 (1,1)	1	0.089 087 08
3	1 (0,3)	4	1 (1,1)	5	1 (1,1)	1	−0.089 087 08
3	1 (0,0)	4	1 (1,1)	5	1 (1,1)	1	−0.021 821 79
3	1 (3,0)	4	1 (1,1)	3	1 (3,0)	1	0
3	1 (0,3)	4	1 (1,1)	3	1 (0,3)	1	0
3	1 (3,0)	4	1 (1,1)	1	1 (1,1)	1	0.026 726 12
3	1 (0,3)	4	1 (1,1)	1	1 (1,1)	1	−0.026 726 12
3	1 (0,0)	4	1 (1,1)	1	1 (1,1)	1	−0.032 732 68
4	1 (1,1)	4	1 (1,1)	8	1 (1,1)	1	0
4	1 (1,1)	4	1 (1,1)	8	1 (1,1)	2	0.505 390 45
4	1 (1,1)	4	1 (1,1)	6	1 (0,0)	1	0.208 656 21
4	1 (1,1)	4	1 (1,1)	6	1 (0,3)	1	0
4	1 (1,1)	4	1 (1,1)	6	1 (3,0)	1	0
4	1 (1,1)	4	1 (1,1)	4	1 (1,1)	1	0
4	1 (1,1)	4	1 (1,1)	4	1 (1,1)	2	0.006 023 39
4	1 (1,1)	4	1 (1,1)	2	1 (1,1)	1	0
4	1 (1,1)	4	1 (1,1)	2	1 (1,1)	2	0.018 070 16
4	1 (1,1)	4	1 (1,1)	0	1 (0,0)	1	0.057 142 86
0	1 (0,0)	5	1 (1,1)	5	1 (1,1)	1	1
1	1 (1,1)	5	1 (1,1)	6	1 (0,0)	1	1
1	1 (1,1)	5	1 (1,1)	6	1 (0,3)	1	−0.632 455 53
1	1 (1,1)	5	1 (1,1)	6	1 (3,0)	1	0.632 455 53
1	1 (1,1)	5	1 (1,1)	4	1 (1,1)	1	0
1	1 (1,1)	5	1 (1,1)	4	1 (1,1)	2	−0.258 198 89
2	1 (1,1)	5	1 (1,1)	7	1 (1,1)	1	0
2	1 (1,1)	5	1 (1,1)	7	1 (1,1)	2	−0.552 052 45
2	1 (1,1)	5	1 (1,1)	5	1 (1,1)	1	0
2	1 (1,1)	5	1 (1,1)	5	1 (1,1)	2	−0.061 721 34
2	1 (1,1)	5	1 (1,1)	3	1 (0,0)	1	0.169 030 85
2	1 (1,1)	5	1 (1,1)	3	1 (0,3)	1	−0.043 643 58
2	1 (1,1)	5	1 (1,1)	3	1 (3,0)	1	0.043 643 58
3	1 (3,0)	5	1 (1,1)	8	1 (1,1)	1	−0.295 468 42
3	1 (0,3)	5	1 (1,1)	8	1 (1,1)	1	0.295 468 42
3	1 (0,0)	5	1 (1,1)	8	1 (1,1)	1	0.361 873 43
3	1 (3,0)	5	1 (1,1)	6	1 (3,0)	1	0
3	1 (0,3)	5	1 (1,1)	6	1 (0,3)	1	0
3	1 (3,0)	5	1 (1,1)	4	1 (1,1)	1	−0.035 214 76
3	1 (0,3)	5	1 (1,1)	4	1 (1,1)	1	0.035 214 76
3	1 (0,0)	5	1 (1,1)	4	1 (1,1)	1	−0.008 625 82

TABLE IX. (*Continued.*)

ν_2	k_2 (λ_2,μ_2)	ν_1	k_1 (λ_1,μ_1)	ν_3	k_3 (λ_3,μ_3)	ρ	IF
3	1 (3,0)	5	1 (1,1)	2	1 (1,1)	1	0.021 128 86
3	1 (0,3)	5	1 (1,1)	2	1 (1,1)	1	−0.021 128 86
3	1 (0,0)	5	1 (1,1)	2	1 (1,1)	1	0.025 877 46
0	1 (0,0)	6	1 (3,0)	6	1 (3,0)	1	1
0	1 (0,0)	6	1 (0,3)	6	1 (0,3)	1	1
0	1 (0,0)	6	1 (0,0)	6	1 (0,0)	1	1
1	1 (1,1)	6	1 (3,0)	7	1 (1,1)	1	0.487 950 04
1	1 (1,1)	6	1 (0,3)	7	1 (1,1)	1	−0.487 950 04
1	1 (1,1)	6	1 (0,0)	7	1 (1,1)	1	−0.487 950 04
1	1 (1,1)	6	1 (3,0)	5	1 (1,1)	1	0.218 217 89
1	1 (1,1)	6	1 (0,3)	5	1 (1,1)	1	−0.218 217 89
1	1 (1,1)	6	1 (0,0)	5	1 (1,1)	1	0.109 108 95
2	1 (1,1)	6	1 (3,0)	8	1 (1,1)	1	0.361 873 43
2	1 (1,1)	6	1 (0,3)	8	1 (1,1)	1	−0.361 873 43
2	1 (1,1)	6	1 (0,0)	8	1 (1,1)	2	0.361 873 43
2	1 (1,1)	6	1 (3,0)	6	1 (3,0)	1	0
2	1 (1,1)	6	1 (0,3)	6	1 (0,3)	1	0
2	1 (1,1)	6	1 (3,0)	4	1 (1,1)	1	0.069 006 56
2	1 (1,1)	6	1 (0,3)	4	1 (1,1)	1	−0.069 006 56
2	1 (1,1)	6	1 (0,0)	4	1 (1,1)	1	−0.034 503 28
0	1 (0,0)	7	1 (1,1)	7	1 (1,1)	1	1
1	1 (1,1)	7	1 (1,1)	8	1 (1,1)	1	0
1	1 (1,1)	7	1 (1,1)	8	1 (1,1)	2	−0.741 619 85
1	1 (1,1)	7	1 (1,1)	6	1 (0,0)	1	−0.408 248 29
1	1 (1,1)	7	1 (1,1)	6	1 (0,3)	1	−0.129 099 45
1	1 (1,1)	7	1 (1,1)	6	1 (3,0)	1	0.129 099 45
0	1 (0,0)	8	1 (1,1)	8	1 (1,1)	1	1

and (0,3). For example, when a many quark-antiquark state with one additional gluon is considered, the quark state must be in a color (1,1) irrep as the gluon. Likewise, when one quark-antiquark pair is coupled to a color (or flavor) octet, the other pair must be in the same state (not necessarily for the flavor case). More complicated isoscalar factors are available on request.

Next we explain the tests performed in order to assure that the results are of confidence. First of all, we calculated by hand many of the overlap matrix elements of the polynomial No. 3 with the product of the polynomials with Nos. 2 and 1 and compared them to the values obtained via the MATEMATICA code. This we did up to eight bosons choosing arbitrarily the states. Then we checked if the isoscalar factors obtained satisfy the orthogonality condition. We use the orthogonality relation of the U(8) CGC's, i.e.,

$$\sum_{\nu_i k_i \xi_i} \langle N_2 \nu_2 k_2 \xi_2, N_1 \nu_2 k_1 \xi_1 | N_3 \nu_3 k_3 \xi_3 \rangle \langle N_2 \nu_2 k_2 \xi_2, N_1 \nu_2 k_1 \xi_1 | N_3' \nu_3' k_3' \xi_3' \rangle = \delta_{N_3, N_3'} \delta_{\nu_3, \nu_3'} \delta_{\xi_3, \xi_3'}, \quad (35)$$

where the index i is 1 or 2.

We arrive at the following condition for the isoscalar factors, given in (27),

$$\sum_{\nu_i k_i (\lambda_i, \mu_i) \rho} \langle N_2 \nu_2 k_2 (\lambda_2, \mu_2), N_1 \nu_1 k_1 (\lambda_1, \mu_1) \| N_3 \nu_3 k_3 (\lambda_3, \mu_3) \rangle_\rho \times \langle N_2 \nu_2 k_2 (\lambda_2, \mu_2), N_1 \nu_1 k_1 (\lambda_1, \mu_1) \| N_3' \nu_3' k_3' (\lambda_3, \mu_3) \rangle_\rho = \delta_{N_3 N_3'} \delta_{\nu_3 \nu_3'} \delta_{k_3 k_3'}. \quad (36)$$

This orthogonality relation we have checked throughout the range from zero to eight bosons. In total about 350 orthogonality relations, involving several thousand isoscalar factors, were checked.

IV. CONCLUSIONS

In this contribution we have constructed the isoscalar factors for the group chain $U(8) \supset O(8) \supset SU(3)$. Only the totally symmetric irreps $[N]$ of $U(8)$ were taken into account. This is of use in any model/theory which deals with quark-antiquark and/or gluon pairs, as in the model published in Refs. 13–15. The CGC's will be used to calculate transition probabilities and can be used in any other model involving quark-antiquark and/or gluon pairs, like the background in hadron states. The coefficients are also of importance for many gluon systems, restricting to the completely symmetric irreps of $U(8)$, which lie at lower energies.

The method presented is very practical for high rank groups when only few particular irreps are of interest and thus serves as an example. It is more powerful than traditional methods, which use the whole algebraic structure of the group and all recursion relations possible.

For many gluon systems, up to three rows in the Young diagrams are needed, i.e., $[h_1, h_2, h_3]$. Therefore, the next step is to consider two rowed Young diagrams. Steps in this direction are already taken by the authors.

We presented the procedure on how to obtain the Clebsch-Gordan coefficients of the chain $U(8) \supset O(8) \supset SU(3) \supset U(1) \otimes SU(2)$ for symmetric irreducible representations in $U(8)$, through the use of isoscalar factors.

The importance of the Clebsch-Gordan coefficients of the chain starting with $U(8)$ lies not only in the possibility to obtain, via their use, branching ratios of hadron decays involving gluons and quark-antiquark pairs, but it can also be used in any other problem related to a $U(8)$ group, i.e., eight degrees of freedom, not necessarily in particle physics, though this was the main motivation. Another area where the $U(8)$ group could play a role, though probably still far in the future, is in *quantum computing*,[33] related to cyclic networks of quantum gates with three-qubits as elementary structure. Trying to describe a system of many three-qubits will require $U(8)$ CGS's, though, one must still understand the basic three-qubit structure alone.

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Closed form of the generalized Green's function for the Helmholtz operator on the two-dimensional unit sphere

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The closed representation of the generalized (known also as reduced or modified) Green's function for the Helmholtz partial differential operator on the surface of the two-dimensional unit sphere is derived. In its compact form, the derived formula contains a Legendre polynomial and a derivative of the Legendre function of the first kind with respect to its index. An explicit expression for that derivative is found and used to obtain an expanded (and potentially more suitable in applications) form of the generalized Green's function for the operator in question. The related problem of constructing the closed form of the generalized Green's function for the Legendre ordinary differential operator on the segment $-1<x<1$, with the boundary conditions of finiteness at $x=\pm 1$, is also solved. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2203430]

I. INTRODUCTION

Let $\mathbb{S}^2$ be the surface of the unit sphere in $\mathbb{R}^3$, parametrized by the unit radius vector $\mathbf{n}$. The spatial orientation of the vector $\mathbf{n}$ (hence, also the location of a point on $\mathbb{S}^2$ for which $\mathbf{n}$ is the radius vector) is uniquely determined by fixing the polar angle $0\leqslant\theta\leqslant\pi$ and the azimuthal angle $0\leqslant\varphi<2\pi$ in some spherical system of coordinates, with the origin of the latter located at the center of $\mathbb{S}^2$.

Some models of propagation of time-harmonic waves on spherical surfaces used in mathematical geophysics (cf., e.g., the recent work of Yoshizawa and Kennett[29]) lead to the inhomogeneous scalar Helmholtz equation on $\mathbb{S}^2$:

$$[\boldsymbol{\nabla}_{\mathbf{n}}^2+\lambda(\lambda+1)]\Psi(\lambda;\mathbf{n})=\Phi(\mathbf{n}). \tag{1.1}$$

In this equation

$$\boldsymbol{\nabla}_{\mathbf{n}}^2=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{1.2}$$

is the angular part of the Laplace operator (the spherical Laplacian) and $\Phi(\mathbf{n})$ is a source term. For the sake of later convenience, the square of the (in general complex) propagation constant has been written in the form $\lambda(\lambda+1)$, where $\lambda\in\mathbb{C}$. Equation (1.1) is to be solved subject to some boundary and/or regularity conditions imposed on $\Psi(\lambda;\mathbf{n})$. If the wave described by Eq. (1.1) propagates over the entire spherical surface, which will be implicit throughout the rest of this paper, these conditions are the single valuedness and finiteness of $\Psi(\lambda;\mathbf{n})$.

With present-day computers and software (see, e.g., the paper by Adams and Swarztrauber[1]), Eq. (1.1), with the aforementioned regularity conditions, may be solved numerically on $\mathbb{S}^2$ for a

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practically arbitrary form of the source function $\Phi(\mathbf{n})$. On the other hand, it appears that the formal analytical solution to Eq. (1.1) is also available; except for the case when $\lambda(\lambda+1)$ is an eigenvalue of $-\boldsymbol{\nabla}_{\mathbf{n}}^2$ on $\mathbb{S}^2$, it is given by

$$\Psi(\lambda;\mathbf{n}) = \oint_{\mathbb{S}^2} \mathrm{d}^2\mathbf{n}'\, G(\lambda;\mathbf{n},\mathbf{n}')\Phi(\mathbf{n}'), \tag{1.3}$$

where $G(\lambda;\mathbf{n},\mathbf{n}')$ is the Green's function for the Helmholtz operator

$$\mathcal{H}(\lambda;\mathbf{n}) = \boldsymbol{\nabla}_{\mathbf{n}}^2 + \lambda(\lambda+1) \tag{1.4}$$

on $\mathbb{S}^2$. Following the general theory,[8,12,13,15,17,20,23,25,27,28] $G(\lambda;\mathbf{n},\mathbf{n}')$ is defined as a solution to the inhomogeneous partial differential equation (with $\mathbf{n}'$ fixed)

$$[\boldsymbol{\nabla}_{\mathbf{n}}^2 + \lambda(\lambda+1)]G(\lambda;\mathbf{n},\mathbf{n}') = \delta^{(2)}(\mathbf{n}-\mathbf{n}'), \tag{1.5}$$

subject to the constraints of single-valuedness and finiteness (with the latter relaxed at the point $\mathbf{n}=\mathbf{n}'$). In Eq. (1.5) the inhomogeneity $\delta^{(2)}(\mathbf{n}-\mathbf{n}')$ is the Dirac delta function on $\mathbb{S}^2$. The closed form of the Green's function $G(\lambda;\mathbf{n},\mathbf{n}')$ is known[2–7,9,10,24,26] to be

$$G(\lambda;\mathbf{n},\mathbf{n}') = \frac{1}{4\sin(\pi\lambda)} P_\lambda(-\mathbf{n}\cdot\mathbf{n}') \quad (\lambda \notin \mathbb{Z}), \tag{1.6}$$

where

$$P_\lambda(x) = {}_2F_1\left(-\lambda,\lambda+1;1;\frac{1-x}{2}\right) = \sum_{n=0}^{\infty} \frac{(-\lambda)_n(\lambda+1)_n}{(n!)^2}\left(\frac{1-x}{2}\right)^n \quad (-1 \leqslant x \leqslant 1) \tag{1.7}$$

is the Legendre function of the first kind,[16,22] with

$$(\zeta)_n = \frac{\Gamma(\zeta+n)}{\Gamma(\zeta)} \quad (n \in \mathbb{N}) \tag{1.8}$$

denoting the Pochhammer symbol.[22]

Equation (1.3) fails to represent a solution of Eq. (1.1) on $\mathbb{S}^2$ when $\lambda \in \mathbb{Z}$, i.e., if it holds that

$$\lambda(\lambda+1) = L(L+1) \quad (L \in \mathbb{N}). \tag{1.9}$$

This corresponds to the situation when the operator (1.4) has a null eigenvalue in its spectrum. It is known from the general theory of linear inhomogeneous equations[20] that in such a case a solution to Eq. (1.1) exists only if the source term is orthogonal to the null space of the operator $\mathcal{H}(L;\mathbf{n})$, spanned by $2L+1$ complex spherical harmonics

$$Y_{LM}(\mathbf{n}) = \frac{(-)^{L+M}}{2^L L!}\sqrt{\frac{2L+1}{4\pi}\frac{(L-M)!}{(L+M)!}}\sin^M\theta\frac{\mathrm{d}^{L+M}\sin^{2L}\theta}{\mathrm{d}\cos^{L+M}\theta}e^{iM\varphi}, \tag{1.10}$$

with $M \in \{0,\pm1,\ldots,\pm L\}$ [the phase choice in Eq. (1.10) conforms to the widely accepted Condon and Shortley[11] convention], i.e., when

$$\oint_{\mathbb{S}^2} \mathrm{d}^2\mathbf{n} Y_{LM}^*(\mathbf{n})\Phi(\mathbf{n}) = 0 \quad (M \in \{0,\pm1,\ldots,\pm L\}). \tag{1.11}$$

If the constraints (1.9) and (1.11) hold simultaneously, a (nonunique) solution to the spherical Helmholtz equation (1.1) is formally given by

$$\Psi_L(\mathbf{n}) = \sum_{M=-L}^{L} a_{LM} Y_{LM}(\mathbf{n}) + \oint_{\mathbb{S}^2} \mathrm{d}^2\mathbf{n}' \overline{G_L}(\mathbf{n},\mathbf{n}')\Phi(\mathbf{n}'), \tag{1.12}$$

where $\{a_{LM}\}$, $(M \in \{0, \pm 1, \ldots, \pm L\})$, are arbitrary constants, while $\overline{G_L}(\mathbf{n},\mathbf{n}')$ is a generalized (known also as reduced or modified) Green's function for the Helmholtz operator $\mathcal{H}(L;\mathbf{n})$. This function is defined as this particular solution to the inhomogeneous partial differential equation

$$[\boldsymbol{\nabla}_{\mathbf{n}}^2 + L(L+1)]\overline{G_L}(\mathbf{n},\mathbf{n}') = \delta^{(2)}(\mathbf{n}-\mathbf{n}') - \sum_{M=-L}^{L} Y_{LM}(\mathbf{n}) Y_{LM}^*(\mathbf{n}') \quad (L \in \mathbb{N}), \tag{1.13}$$

which is single-valued and finite on $\mathbb{S}^2$ (except at the point $\mathbf{n}=\mathbf{n}'$), being, in addition, orthogonal to the null space of the operator $\mathcal{H}(L;\mathbf{n})$:

$$\oint_{\mathbb{S}^2} \mathrm{d}^2\mathbf{n} Y_{LM}^*(\mathbf{n}) \overline{G_L}(\mathbf{n},\mathbf{n}') = 0 \quad (M \in \{0, \pm 1, \ldots, \pm L\}). \tag{1.14}$$

In contrary to the case of $G(\lambda;\mathbf{n},\mathbf{n}')$, despite performing the extensive search through the mathematical and physical literature, we have found no studies on the *closed* form of $\overline{G_L}(\mathbf{n},\mathbf{n}')$, except for the particular case $L=0$ (cf. Refs. 12, 14, 18, and 19). It is therefore the purpose of this work to fill in this gap by presenting the construction of the closed representation of the generalized Green's function for the Helmholtz operator (1.4), constrained by Eq. (1.9), on the unit sphere $\mathbb{S}^2$.

The structure of the paper is as follows. First, in Sec. II we show that $\overline{G_L}(\mathbf{n},\mathbf{n}')$ may be expressed compactly in terms of the derivative $[\partial P_\lambda(-\mathbf{n}\cdot\mathbf{n}')/\partial\lambda]_{\lambda=L}$. Then, in Sec. III we find the explicit representation of $[\partial P_\lambda(x)/\partial\lambda]_{\lambda=L}$, the result which, apart from being important in the context of the present work, seems to be also of interest for itself. Finally, in Sec. IV we combine the findings of Secs. II and III, arriving at the sought explicit closed form of $\overline{G_L}(\mathbf{n},\mathbf{n}')$. We also show that in the particular case $L=0$ the known result for the spherical Laplacian[14,19] is recovered. In addition, we provide the inhomogeneous three-term recurrence relation satisfied by $\overline{G_L}(\mathbf{n},\mathbf{n}')$. The intermediate result obtained in Sec. III is of wider applicability than the subject of this work might suggest. We illustrate this in the Appendix, where the closed form of the generalized Green's function for the one-dimensional Legendre operator

$$\mathcal{L}(L;x) = \frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x} + L(L+1) \quad (L \in \mathbb{N}) \tag{1.15}$$

on the interval $-1<x<1$, with the boundary conditions of finiteness at $x=\pm 1$, is constructed.

II. COMPACT CLOSED FORM OF THE GENERALIZED GREEN'S FUNCTION FOR THE HELMHOLTZ OPERATOR ON $\mathbb{S}^2$

From the general theory of Green's functions (cf. the relevant references cited in Sec. I) it follows that one may construct the generalized spherical Helmholtz Green's function $\overline{G_L}(\mathbf{n},\mathbf{n}')$ in the form of the so-called spectral series

$$\overline{G_L}(\mathbf{n},\mathbf{n}') = \sum_{\substack{l=0 \\ (l\neq L)}}^{\infty} \sum_{m=-l}^{l} \frac{Y_{lm}(\mathbf{n}) Y_{lm}^*(\mathbf{n}')}{L(L+1) - l(l+1)}. \tag{2.1}$$

Comparing this with the spectral series representation of the Green's function $G(\lambda;\mathbf{n},\mathbf{n}')$, known to be

$$G(\lambda;\mathbf{n},\mathbf{n}') = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{Y_{lm}(\mathbf{n})Y_{lm}^*(\mathbf{n}')}{\lambda(\lambda+1)-l(l+1)}, \tag{2.2}$$

it may be inferred that the functions $\overline{G}_L(\mathbf{n},\mathbf{n}')$ and $G(\lambda;\mathbf{n},\mathbf{n}')$ are related through

$$\overline{G}_L(\mathbf{n},\mathbf{n}') = \lim_{\lambda(\lambda+1)\to L(L+1)}\frac{\partial}{\partial[\lambda(\lambda+1)]}\{[\lambda(\lambda+1)-L(L+1)]G(\lambda;\mathbf{n},\mathbf{n}')\}. \tag{2.3}$$

This, after exploiting the result (1.6), may be rewritten as

$$\overline{G}_L(\mathbf{n},\mathbf{n}') = \frac{1}{4(2L+1)}\lim_{\lambda\to L}\frac{\partial}{\partial\lambda}\frac{(\lambda-L)(\lambda+L+1)}{\sin(\pi\lambda)}P_\lambda(-\mathbf{n}\cdot\mathbf{n}'). \tag{2.4}$$

The limit on the right-hand side of the above equation may be evaluated by using the l'Hospital rule. After exploiting the fact that for a non-negative integer index the Legendre function (1.7) degenerates to the Legendre polynomial

$$P_L(x) = \frac{1}{2^L L!}\frac{\mathrm{d}^L(x^2-1)^L}{\mathrm{d}x^L} \quad (L\in\mathbb{N}), \tag{2.5}$$

and making use of the following reflection property of the Legendre polynomials:

$$P_L(-x) = (-)^L P_L(x) \quad (L\in\mathbb{N}), \tag{2.6}$$

one eventually finds that the closed form of $\overline{G}_L(\mathbf{n},\mathbf{n}')$ is

$$\overline{G}_L(\mathbf{n},\mathbf{n}') = \frac{(-)^L}{4\pi}\frac{\partial P_\lambda(-\mathbf{n}\cdot\mathbf{n}')}{\partial\lambda}\bigg|_{\lambda=L} + \frac{1}{4\pi}\frac{P_L(\mathbf{n}\cdot\mathbf{n}')}{2L+1}. \tag{2.7}$$

From the purely theoretical point of view, arriving at Eq. (2.7) completes the task of determining the closed form of $\overline{G}_L(\mathbf{n},\mathbf{n}')$. However, in most of the actual applications formula (2.7) will be unhandy, if not useless. To find a representation of $\overline{G}_L(\mathbf{n},\mathbf{n}')$ which is suitable for practical purposes, the derivative $[\partial P_\lambda(x)/\partial\lambda]_{\lambda=L}$ must be evaluated explicitly. We shall be concerned with the latter problem in the following section.

III. EVALUATION OF $[\partial P_\lambda(x)/\partial\lambda]_{\lambda=L}$

Throughout the whole section, it will be implicit that L is an arbitrary non-negative integer and that $-1\leqslant x\leqslant 1$.

Consider the definition (1.7). Differentiating it with respect to λ, after making use of the following differential property of the Pochhammer symbol:

$$\frac{\mathrm{d}(\zeta)_n}{\mathrm{d}\zeta} = [\psi(\zeta+n)-\psi(\zeta)](\zeta)_n, \tag{3.1}$$

where

$$\psi(\zeta) = \frac{1}{\Gamma(\zeta)}\frac{\mathrm{d}\Gamma(\zeta)}{\mathrm{d}\zeta} \tag{3.2}$$

is the digamma function,[16,22] one obtains

$$\frac{\partial P_\lambda(x)}{\partial \lambda} = \sum_{n=1}^{\infty} \frac{(-\lambda)_n(\lambda+1)_n}{(n!)^2}[\psi(\lambda+1+n) - \psi(\lambda+1) + \psi(-\lambda) - \psi(-\lambda+n)]\left(\frac{1-x}{2}\right)^n. \tag{3.3}$$

It is evident from Eq. (3.3) that the function $\partial P_\lambda(x)/\partial\lambda$ obeys

$$\left.\frac{\partial P_{\lambda'}(x)}{\partial \lambda'}\right|_{\lambda'=-\lambda-1} = -\left.\frac{\partial P_{\lambda'}(x)}{\partial \lambda'}\right|_{\lambda'=\lambda}. \tag{3.4}$$

The right-hand side of Eq. (3.3) may be simplified. On exploiting the known relation[16,22]

$$\psi(\zeta) = \psi(1-\zeta) - \pi\cot(\pi\zeta) \tag{3.5}$$

one finds

$$-\psi(\lambda+1) + \psi(-\lambda) - \psi(-\lambda+n) = -\psi(\lambda+1-n). \tag{3.6}$$

Hence, it follows that

$$\frac{\partial P_\lambda(x)}{\partial \lambda} = \sum_{n=1}^{\infty} \frac{(-\lambda)_n(\lambda+1)_n}{(n!)^2}[\psi(\lambda+1+n) - \psi(\lambda+1-n)]\left(\frac{1-x}{2}\right)^n. \tag{3.7}$$

Equation (3.7) does not look simple. However, at this stage we may take advantage of the fact that for the purposes of the present work the derivative $\partial P_\lambda(x)/\partial\lambda$ is to be evaluated for $\lambda = L \in \mathbb{N}$ only.

At first, consider what happens if $\lambda = 0$. Since

$$\lim_{\lambda\to 0} \frac{\psi(\lambda+1+n)}{\Gamma(-\lambda)} = 0 \quad (n \in \mathbb{N}) \tag{3.8}$$

and

$$\lim_{\lambda\to 0} \frac{\psi(\lambda+1-n)}{\Gamma(-\lambda)} = 1 \quad (n \in \mathbb{N}\setminus\{0\}), \tag{3.9}$$

in this particular case we arrive at the known result[16,22]

$$\left.\frac{\partial P_\lambda(x)}{\partial \lambda}\right|_{\lambda=0} = -\sum_{n=1}^{\infty} \frac{1}{n}\left(\frac{1-x}{2}\right)^n = \ln\frac{1+x}{2}. \tag{3.10}$$

Next, the Legendre function (1.7) is known[16,22] to satisfy the three-term homogeneous recurrence relation

$$(\lambda+1)P_{\lambda+1}(x) - (2\lambda+1)xP_\lambda(x) + \lambda P_{\lambda-1}(x) = 0. \tag{3.11}$$

Differentiating this relation with respect to λ yields the three-term inhomogeneous recurrence relation for the function (3.7)

$$(\lambda+1)\frac{\partial P_{\lambda+1}(x)}{\partial\lambda} - (2\lambda+1)x\frac{\partial P_\lambda(x)}{\partial\lambda} + \lambda\frac{\partial P_{\lambda-1}(x)}{\partial\lambda} = -P_{\lambda+1}(x) + 2xP_\lambda(x) - P_{\lambda-1}(x), \tag{3.12}$$

which, upon exploiting again Eq. (3.11), may be rewritten in the form

$$(\lambda+1)\frac{\partial P_{\lambda+1}(x)}{\partial\lambda}-(2\lambda+1)x\frac{\partial P_\lambda(x)}{\partial\lambda}+\lambda\frac{\partial P_{\lambda-1}(x)}{\partial\lambda}=\frac{1}{2\lambda+1}[P_{\lambda+1}(x)-P_{\lambda-1}(x)]. \tag{3.13}$$

If $\lambda=L\in\mathbb{N}$, the recurrence (3.13) becomes

$$(L+1)\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=L+1}-(2L+1)x\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=L}+L\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=L-1}=\frac{1}{2L+1}[P_{L+1}(x)-P_{L-1}(x)]. \tag{3.14}$$

Equation (3.14) is to be solved with formula (3.10) taken as an initial condition. Now, it is known from the general theory of linear difference equations[21] that the solution to the problem (3.14) and (3.10) may be sought in the form

$$\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=L}=F_L(x)+W_L(x), \tag{3.15}$$

where $F_L(x)$ solves

$$(L+1)F_{L+1}(x)-(2L+1)xF_L(x)+LF_{L-1}(x)=0 \tag{3.16}$$

subject to the inhomogeneous initial condition

$$F_0(x)=\ln\frac{1+x}{2}, \tag{3.17}$$

while $W_L(x)$ satisfies

$$(L+1)W_{L+1}(x)-(2L+1)xW_L(x)+LW_{L-1}(x)=\frac{1}{2L+1}[P_{L+1}(x)-P_{L-1}(x)] \tag{3.18}$$

subject to the homogeneous initial condition

$$W_0(x)=0. \tag{3.19}$$

Equations (3.18) and (3.19) imply that $W_L(x)$ is a polynomial in x, of degree L, such that

$$W_L(1)=0. \tag{3.20}$$

We shall make use of this observation shortly.

The solution to the problem constituted by Eqs. (3.16) and (3.17) is immediately found to be

$$F_L(x)=P_L(x)\ln\frac{1+x}{2}. \tag{3.21}$$

To find $W_L(x)$, we observe that the derivative $\partial P_\lambda(x)/\partial\lambda$ satisfies the inhomogeneous differential equation

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}+\lambda(\lambda+1)\right]\frac{\partial P_\lambda(x)}{\partial\lambda}=-(2\lambda+1)P_\lambda(x), \tag{3.22}$$

obtainable from the Legendre identity

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}+\lambda(\lambda+1)\right]P_\lambda(x)=0 \tag{3.23}$$

by its differentiation with respect to λ. On combining Eqs. (3.22), (3.15), and (3.21), and after making use of the known relationship[22]

$$x\frac{\mathrm{d}P_L(x)}{\mathrm{d}x} - LP_L(x) = \frac{\mathrm{d}P_{L-1}(x)}{\mathrm{d}x}, \tag{3.24}$$

one deduces that $W_L(x)$ satisfies the inhomogeneous differential equation

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x} + L(L+1)\right]W_L(x) = 2\frac{\mathrm{d}P_{L-1}(x)}{\mathrm{d}x} - 2\frac{\mathrm{d}P_L(x)}{\mathrm{d}x}. \tag{3.25}$$

Since $W_L(x)$ is the polynomial, the pertinent boundary conditions supplementing Eq. (3.25) are

$$W_L(x) \text{ bounded for } x \to \pm 1. \tag{3.26}$$

It is evident that by solving the boundary value problem constituted by Eqs. (3.25) and (3.26) one is able to determine $W_L(x)$ only up to a multiple of the Legendre polynomial $P_L(x)$, since the latter solves the associated homogeneous boundary value problem. With this fact in mind, on applying the machinery of Green's functions, $W_L(x)$ is found to have the form

$$W_L(x) = c_L P_L(x) + 2\int_{-1}^{1} \mathrm{d}x'\, \overline{g_L}(x,x')\left[\frac{\mathrm{d}P_{L-1}(x')}{\mathrm{d}x'} - \frac{\mathrm{d}P_L(x')}{\mathrm{d}x'}\right], \tag{3.27}$$

where

$$\overline{g_L}(x,x') = \frac{1}{2}\sum_{\substack{l=0 \\ (l\neq L)}}^{\infty} \frac{2l+1}{(L-l)(L+l+1)}P_l(x)P_l(x') \tag{3.28}$$

is the generalized Green's function (in its spectral form, cf. the Appendix) for the Legendre operator (1.15), while c_L is a coefficient which remains to be determined. The integral on the right-hand side of Eq. (3.27) may be evaluated if one makes use of the known relationship[16]

$$\frac{\mathrm{d}P_L(x)}{\mathrm{d}x} = \sum_{l=0}^{\mathrm{int}[(L-1)/2]} (2L-4l-1)P_{L-2l-1}(x) \tag{3.29}$$

[in Eq. (3.29), and hereafter, it is implicit that if the upper limit of the summation is smaller than the lower one, than the sum is identically zero], which implies that it holds that

$$\frac{\mathrm{d}P_{L-1}(x)}{\mathrm{d}x} - \frac{\mathrm{d}P_L(x)}{\mathrm{d}x} = \sum_{l=0}^{L-1} (-)^{L+l}(2l+1)P_l(x). \tag{3.30}$$

On inserting Eqs. (3.28) and (3.30) into Eq. (3.27), after exploiting the orthogonality property[16,22]

$$\int_{-1}^{1} \mathrm{d}x\, P_L(x)P_{L'}(x) = \frac{2}{2L+1}\delta_{LL'}, \tag{3.31}$$

one obtains $W_L(x)$ in the form

$$W_L(x) = c_L P_L(x) + 2\sum_{l=0}^{L-1} (-)^{L+l}\frac{2l+1}{(L-l)(L+l+1)}P_l(x). \tag{3.32}$$

It remains to determine the coefficient c_L. To this end, in Eq. (3.32) one sets $x=1$ and then exploits the property

$$P_\lambda(1) = 1, \tag{3.33}$$

and also Eq. (3.20), obtaining

$$c_L = -2\sum_{l=0}^{L-1}(-)^{L+l}\frac{2l+1}{(L-l)(L+l+1)}. \tag{3.34}$$

This leads to the following representation of the polynomial $W_L(x)$:

$$W_L(x) = 2\sum_{l=0}^{L-1}(-)^{L+l}\frac{2l+1}{(L-l)(L+l+1)}[P_l(x)-P_L(x)]. \tag{3.35}$$

[Observe that, according to the convention introduced below Eq. (3.29), from Eq. (3.35) it follows that $W_0(x)=0$, which is in agreement with Eq. (3.19).]

The results obtained above may be summarized in the following formula for the sought derivative $[\partial P_\lambda(x)/\partial\lambda]_{\lambda=L}$:

$$\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=L} = P_L(x)\ln\frac{1+x}{2} + 2\sum_{l=0}^{L-1}(-)^{L+l}\frac{2l+1}{(L-l)(L+l+1)}[P_l(x)-P_L(x)]. \tag{3.36}$$

In particular, from Eq. (3.36) it follows that

$$\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=1} = x\ln\frac{1+x}{2} + (x-1), \tag{3.37}$$

$$\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=2} = \frac{1}{2}(3x^2-1)\ln\frac{1+x}{2} + \left(\frac{7}{4}x^2 - \frac{3}{2}x - \frac{1}{4}\right), \tag{3.38}$$

$$\left.\frac{\partial P_\lambda(x)}{\partial\lambda}\right|_{\lambda=3} = \frac{1}{2}(5x^3-3x)\ln\frac{1+x}{2} + \left(\frac{37}{12}x^3 - \frac{5}{2}x^2 - \frac{5}{4}x + \frac{2}{3}\right). \tag{3.39}$$

We parenthetically observe also that, if needed, the derivatives $[\partial P_\lambda(x)/\partial\lambda]_{\lambda=-L-1}$ may be deduced from Eqs. (3.4) and (3.36).

IV. DISCUSSION

From Eqs. (2.7), (3.36), and (2.6) one deduces that the explicit form of the generalized Green's function for the Helmholtz operator (1.4), with the constraint (1.9), is

$$\overline{G}_L(\mathbf{n},\mathbf{n}') = \frac{1}{4\pi}P_L(\mathbf{n}\cdot\mathbf{n}')\left[\ln\frac{1-\mathbf{n}\cdot\mathbf{n}'}{2} - 2\sum_{l=0}^{L-1}(-)^{L+l}\frac{2l+1}{(L-l)(L+l+1)} + \frac{1}{2L+1}\right] + \frac{1}{2\pi}\sum_{l=0}^{L-1}\frac{2l+1}{(L-l)(L+l+1)}P_l(\mathbf{n}\cdot\mathbf{n}'). \tag{4.1}$$

In the particular case $L=0$, when the spherical Helmholtz operator (1.4) reduces to the spherical Laplacian, Eq. (4.1) yields

$$\overline{G}_0(\mathbf{n},\mathbf{n}') = \frac{1}{4\pi}\left(\ln\frac{1-\mathbf{n}\cdot\mathbf{n}'}{2} + 1\right). \tag{4.2}$$

This result agrees with that of Kneser[19](see also the paper by Freeden[14]), after rescaling his formula to achieve the consistency with our defining Eq. (1.13), but at the first sight seems to contradict the finding of Courant and Hilbert,[12] whose result, again after due rescaling, in our notation is

$$\overline{G_0^{(\mathrm{CH})}}(\mathbf{n},\mathbf{n}') = \frac{1}{4\pi}\left(\ln\frac{1-\mathbf{n}\cdot\mathbf{n}'}{2} + 2\ln 2\right). \tag{4.3}$$

The reason for this discrepancy is that the latter authors did not impose the orthogonality constraint (1.14) on the solution to the inhomogeneous equation (1.13), specialized to the case $L=0$. Consequently, in their approach the generalized Green's function for the spherical Laplace operator is determined only up to a multiple of $Y_{00}(\mathbf{n})Y_{00}^{*}(\mathbf{n}')$, i.e., up to an additive constant. If this constant is added to $\overline{G_0^{(\mathrm{CH})}}(\mathbf{n},\mathbf{n}')$, and then chosen so that the result satisfies the constraint (1.14), our finding (4.2) is recovered.

Finally, we find it noteworthy that Eqs. (2.7), (3.11), and (3.14) imply that the function $\overline{G_L}(\mathbf{n},\mathbf{n}')$ satisfies the three-term inhomogeneous recurrence relation

$$\begin{aligned}(L+1)\overline{G_{L+1}}(\mathbf{n},\mathbf{n}') - (2L+1)\mathbf{n}\cdot\mathbf{n}'\overline{G_L}(\mathbf{n},\mathbf{n}') + L\overline{G_{L-1}}(\mathbf{n},\mathbf{n}') \\ = \frac{1}{4\pi}\left[\frac{P_{L+1}(\mathbf{n}\cdot\mathbf{n}')}{(2L+1)(2L+3)} + \frac{P_{L-1}(\mathbf{n}\cdot\mathbf{n}')}{|2L-1|(2L+1)}\right],\end{aligned} \tag{4.4}$$

subject to the initial condition constituted by Eq. (4.2).

APPENDIX: CLOSED FORM OF THE GENERALIZED GREEN'S FUNCTION FOR THE LEGENDRE OPERATOR (1.15)

The Legendre Green's function $g(\lambda;x,x')$ is defined as the solution to the inhomogeneous differential equation (with x' fixed)

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x} + \lambda(\lambda+1)\right]g(\lambda;x,x') = \delta(x-x') \quad (-1 < x,x' < 1) \tag{A1}$$

satisfying the boundary conditions

$$g(\lambda;x,x') \text{ bounded for } x \to \pm 1. \tag{A2}$$

In Eq. (A1), and hereafter, $\delta(x-x')$ is the one-dimensional Dirac delta distribution. The function $g(\lambda;x,x')$ has the spectral series representation

$$g(\lambda;x,x') = \frac{1}{2}\sum_{l=0}^{\infty}\frac{2l+1}{\lambda(\lambda+1)-l(l+1)}P_l(x)P_l(x') \quad (\lambda \notin \mathbb{Z}), \tag{A3}$$

while its closed form may be shown to be

$$g(\lambda;x,x') = \frac{\pi}{2\sin(\pi\lambda)}P_\lambda(-x_<)P_\lambda(x_>) \quad (\lambda \notin \mathbb{Z}), \tag{A4}$$

with

$$x_< = \min(x,x'), \quad x_> = \max(x,x'). \tag{A5}$$

Evidently, $g(\lambda;x,x')$ fails to exist if $\lambda \in \mathbb{Z}$, i.e., if the condition (1.9) is satisfied. In this appendix, with the help of the results of Sec. III, we shall find the closed form of the generalized Legendre Green's function $\overline{g_L}(x,x')$ for this case.

The function $\overline{g_L}(x,x')$ is defined as this particular solution to the inhomogeneous equation (with x' fixed)

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}+L(L+1)\right]\overline{g}_L(x,x')=\delta(x-x')-\frac{2L+1}{2}P_L(x)P_L(x')\quad(-1<x,x'<1),\tag{A6}$$

which satisfies the boundary conditions

$$\overline{g}_L(x,x')\text{ bounded for }x\to\pm 1\tag{A7}$$

and the orthogonality constraint

$$\int_{-1}^{1}\mathrm{d}x\,P_L(x)\overline{g}_L(x,x')=0.\tag{A8}$$

The spectral series representation of $\overline{g}_L(x,x')$ is

$$\overline{g}_L(x,x')=\frac{1}{2}\sum_{\substack{l=0\\(l\neq L)}}^{\infty}\frac{2l+1}{L(L+1)-l(l+1)}P_l(x)P_l(x')\tag{A9}$$

and this particular form of $\overline{g}_L(x,x')$ has been helpful in deriving Eq. (3.32).

To find the closed form of $\overline{g}_L(x,x')$, we observe that, as it follows from Eqs. (A3) and (A9), it is related to the Green's function $g(\lambda;x,x')$ through

$$\overline{g}_L(x,x')=\lim_{\lambda(\lambda+1)\to L(L+1)}\frac{\partial}{\partial[\lambda(\lambda+1)]}\{[\lambda(\lambda+1)-L(L+1)]g(\lambda;x,x')\}.\tag{A10}$$

In virtue of Eq. (A4), this relation may be rewritten as

$$\overline{g}_L(x,x')=\frac{\pi}{2}\frac{1}{2L+1}\lim_{\lambda\to L}\frac{\partial}{\partial\lambda}\frac{(\lambda-L)(\lambda+L+1)}{\sin(\pi\lambda)}P_\lambda(-x_<)P_\lambda(x_>).\tag{A11}$$

Performing the limiting passage with the aid of the l'Hospital rule gives

$$\overline{g}_L(x,x')=\frac{(-)^L}{2}\frac{\partial P_\lambda(-x_<)}{\partial\lambda}\bigg|_{\lambda=L}P_L(x_>)+\frac{(-)^L}{2}P_L(-x_<)\frac{\partial P_\lambda(x_>)}{\partial\lambda}\bigg|_{\lambda=L}+\frac{1}{2}\frac{P_L(x_<)P_L(x_>)}{2L+1},\tag{A12}$$

and transforming further Eq. (A12) with the help of Eqs. (3.15), (3.21), and (2.6) leads to the final result

$$\overline{g}_L(x,x')=\frac{1}{2}P_L(x_<)P_L(x_>)\ln\frac{(1-x_<)(1+x_>)}{4}+\frac{1}{2}W_L(-x_<)P_L(-x_>)+\frac{1}{2}P_L(x_<)W_L(x_>)+\frac{1}{2}\frac{P_L(x_<)P_L(x_>)}{2L+1},\tag{A13}$$

with $W_L(x)$ given explicitly by Eq. (3.35). In the particular case $L=0$, Eq. (A13) simplifies to the well-known formula[12,20]

$$\overline{g}_0(x,x')=\frac{1}{2}\ln\frac{(1-x_<)(1+x_>)}{4}+\frac{1}{2}.\tag{A14}$$

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Jacobi ϑ-functions and discrete Fourier transforms

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Properties of the Jacobi ϑ_3-function and its derivatives under discrete Fourier transforms are investigated, and several interesting results are obtained. The role of modulo N equivalence classes in the theory of ϑ-functions is stressed. An important conjecture is studied. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Methods in mathematical physics usually provide an interface between quite different areas of physics, and it is not unusual that such areas advance in parallel, mostly ignoring each other's steps. This is the case with finite dimensional inner product spaces (hereafter mentioned as the "discrete"), with its leading role in quantum mechanics (hence quantum information theory) and in finite signal analysis. References 1–3 provide some links between those theories.

Both quantum mechanics of finite dimensional Hilbert spaces and finite signal analysis rely heavily on the discrete Fourier transform (DFT, sometimes mentioned finite or fractional Fourier transform), and, regarding quantum mechanics, after the seminal work of Weyl on finite dimensional systems,[4] it was Schwinger who observed and explored the fact that two physical observables whose families of eigenstates are connected *via* DFT share a maximum degree of incompatibility.[5]

Although, at first glance, a finite system might look much simpler than anything defined on a nonenumerable infinite dimensional Hilbert space (hereafter referred to as the "continuum"), there is much more knowledge about the latter than the former. In one phrase, in the continuum we have one, and only one, harmonic oscillator, while in the discrete there are a lot of candidates for that role, each one surely with its virtues, but surely no undisputed champion.

The eigenstates associated to the harmonic oscillator, the Gaussian function and the Hermite polynomials, have a very distinguishable behavior under the action of the (usual) Fourier transform, so widely known that any comment on this regard is completely superfluous. Over such properties rests a huge amount of physical knowledge. On the other hand, however, although the discrete Fourier transform (DFT) is a well known tool, there is nothing on this context which could claim for itself a role analogous to that of the Gaussian function/Fourier transform "duo."

A decisive step in an attempt to "regain," in the discrete, all interpretative power derived from the qualitative behavior of the harmonic oscillator eigenfunctions, lost when one leaves the continuum realm, was given in Ref. 6, where the eigenstates of the DFT are obtained. The purpose of this paper is to further explore this path, showing results which closely parallel those of the continuum. Those results are obtained in a strikingly simple fashion, exploring the technique of breaking infinite sums in modulo N equivalence classes. Pertinent research on the eigenstates of the DFT can also be found in Ref. 7.

A remark must be made about the orthogonality of the DFT's eigenstates. Mehta has conjectured that those states are indeed orthogonal, what seems to be most reasonable. One may be led to believe that, just as in the continuum, the eigenstates of the DFT may be also (nondegenerate)

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eigenstates of some other (unitary or self-adjoint) operator, and thus orthogonal. Further evidence supporting such conjecture is that the continuous limit of the DFT eigenstates recovers, as expected, the Gaussian times the Hermite polynomials. However, as it will be shown, quite surprisingly, the conjecture *does not* hold, giving another fine example of the peculiarities of the finite dimensional context.

The eigenstates of the DFT are seen to be the Jacobi ϑ_3-function and its derivatives.[8] Interest in Jacobi ϑ-functions, by their own turn, may come from a variety of directions. First, its mathematical interest goes without saying (see, for example, Ref. 9 and references therein). To cite relatively recent examples in physics, in quantum physics it is deeply related to coherent states associated to both circle[10] and finite lattice topology.[11] Its modular properties have proven to be of fundamental importance in superstring theory, as it is shown by standard literature in this field.[12]

The basic notation adopted in this paper and some preliminary results are presented in the next section. Following, orthogonality of the DFT's eigenstates is discussed. Section IV contains the main results, for which a two variable generalization is verified in the subsequent section. Further relations among ϑ_3-functions are obtained in Sec. VI, which precedes the concluding section.

II. PRELIMINARY RESULTS

In Ref. 6 it is shown that there is a set of functions with the following remarkable property

$$f_n(j) = \frac{i^n}{\sqrt{N}} \sum_{k=0}^{N-1} f_n(k) \exp\left[\frac{2\pi i}{N} kj\right], \tag{1}$$

where N is a natural number. The functions

$$f_n(j) = \sum_{\alpha=-\infty}^{\infty} \exp\left[-\frac{\pi}{N}(\alpha N + j)^2\right] H_n\big(\epsilon(\alpha N + j)\big), \quad \epsilon = \sqrt{\frac{2\pi}{N}} \tag{2}$$

are defined making use of the Hermite polynomial H_n. Writing $H_n(x)$ in terms of its generating function, $H_n(x) = \frac{\partial^n}{\partial t^n} \exp[2xt - t^2]|_{t=0}$, it is possible to write this state (to use a quantum mechanical terminology) as[8]

$$f_n(j) = \frac{1}{\sqrt{N}} \frac{\partial^n}{\partial t^n} \vartheta_3\left(\frac{j}{N} - \frac{\epsilon}{\pi} t, \frac{i}{N}\right) \exp[t^2]\Big|_{t=0}, \tag{3}$$

where

$$\vartheta_3(z,\tau) = \sum_{\alpha=-\infty}^{\infty} \exp[i\pi\tau\alpha^2] \exp[2\pi i \alpha z], \quad \mathrm{Im}(\tau) > 0, \tag{4}$$

is the Jacobi ϑ_3-function, following Vilenkin's notation.[13] In this notation the basic properties of this even function read as

$$\vartheta_3(z + m + n\tau, \tau) = \exp[-i\pi\tau m^2] \exp[-2\pi i n z] \vartheta_3(z,\tau), \tag{5}$$

$$\vartheta_3(z, i\tau) = \tau^{-1/2} \exp\left[-\frac{\pi z^2}{\tau}\right] \vartheta_3\left(\frac{z}{i\tau}, \frac{i}{\tau}\right), \tag{6}$$

emphasizing its period 1 and quasiperiod τ. A beautiful consequence of (6) is that this function can be written as a sum of Gaussians,

$$\vartheta_3\left(\frac{z}{L},\frac{i}{\sigma^2}\right)=\sigma\sum_{\alpha=-\infty}^{\infty}\exp\left[-\pi\left(\frac{\sigma}{L}\right)^2(\alpha L+z)^2\right], \tag{7}$$

a form in which the width L/σ becomes apparent. Property (6) also provides an easy way to obtain the additional identity (also given by Ref. 6)

$$f_n(j)=\epsilon(-i)^n\sum_{\alpha=-\infty}^{\infty}\exp\left[-\frac{\pi}{N}\alpha^2+\frac{2\pi i}{N}j\alpha\right]H_n(\epsilon\alpha), \tag{8}$$

which is in fact a generalization of Eq. (7) (if one compares it to Eq. (2)).

III. ORTHOGONALITY OF THE f_n'S

According to Eq. (1), the functions $\{f_n(j)\}$ are eigenstates of the DFT with associated eigenvalue i^n. Mehta has conjectured that $\{f_n(j)\}_{n=0}^{N-1}$ is an orthogonal set, and thus complete, over a finite set of N points (for odd N. For even N one must replace $f_{N-1}(j)$ by $f_N(j)$). This reasonable conjecture, quite surprisingly indeed, does not hold for arbitrary N (it holds for large N). As, in the following, evidence will be collected *against* the original conjecture, details shall be kept to a level higher than usual.

Let (f_n,f_m) denote the inner product

$$(f_n,f_m)=\sum_{j=0}^{N-1}f_n^*(j)f_m(j)=\epsilon^2(-i)^{n+m}\sum_{j=0}^{N-1}\sum_{\alpha,\beta=-\infty}^{\infty}\exp\left[-\frac{\pi}{N}(\alpha^2+\beta^2)+\frac{2\pi i}{N}j(\alpha-\beta)\right]H_n(\epsilon\alpha)H_m(\epsilon\beta).$$

The sum over $\{j\}$ is a realization of the modulo N Kroenecker delta,

$$\delta_{\alpha,\beta}^{[N]}=\begin{cases}1 & \alpha=\beta\ (\mathrm{mod}\ N),\\ 0 & \alpha\neq\beta\ (\mathrm{mod}\ N),\end{cases}$$

thus

$$(f_n,f_m)=2\pi(-i)^{n+m}\sum_{\alpha,\beta=-\infty}^{\infty}\delta_{\alpha,\beta}^{[N]}\exp\left[-\frac{\pi}{N}(\alpha^2+\beta^2)\right]H_n(\epsilon\alpha)H_m(\epsilon\beta). \tag{9}$$

The well-known identity,

$$\exp\left[-\frac{1}{2}x^2\right]H_k(x)=\frac{i^k}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dy\exp\left[-\frac{1}{2}y^2+ixy\right]H_k(y),$$

together with the sum over $\{\beta\}$ leads to

$$(f_n,f_m)=\sum_{\alpha,\gamma=-\infty}^{\infty}\int_{-\infty}^{\infty}dy\,dz\exp\left[-\frac{1}{2}(y^2+z^2)+iy\epsilon\alpha+iz\epsilon(\alpha+\gamma N)\right]H_n(y)H_m(z),$$

where the infinite sum on $\{\gamma\}$ covers the equivalence class present in $\delta_{\alpha,\beta}^{[N]}$. Now, the sum over $\{\alpha\}$ by its turn is a realization of a modulo 2π Dirac delta, thus, with the integration over $\{z\}$ and convenient changes of variables,

$$(f_n,f_m)=2\pi\sum_{\gamma,\upsilon=-\infty}^{\infty}\int_{-\infty}^{\infty}dy\exp\left[-y^2-\frac{\pi^2\upsilon^2}{\epsilon^2}+i(y\epsilon N-\upsilon\pi N)\gamma\right]H_n\left(y-\frac{\pi\upsilon}{\epsilon}\right)H_m\left(y+\frac{\pi\upsilon}{\epsilon}\right),$$

where again an infinite sum is introduced due to the modulo 2π delta.

The above expression is rather elucidative. It is not hard to realize that the infinite sums over $\{\gamma,\upsilon\}$ are a direct consequence of the equivalence classes brought in by the modulo N Kroenecker

delta present in Eq. (9). For large N, the term corresponding to $\gamma=\upsilon=0$ becomes increasingly important, and a simple check shows that this term is exactly $\delta_{n,m}$. Thus, as expected, the limit $N\to\infty$ recovers the usual harmonic oscillator results. For finite (and small) N, however, all terms in the above summation must be taken into account.

Following then, the sum on γ is seen to be a realization of the modulo 2π Dirac delta, $\delta^{[2\pi]}(y\epsilon N-\upsilon\pi N)$, and after a change of variables one has

$$(f_n,f_m)=2\pi\epsilon\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}\left(\mu+\frac{N\upsilon}{2}\right)^2-\frac{N\pi\upsilon^2}{2}\right]H_n(\epsilon\mu)H_m\left(\frac{2\pi\upsilon}{\epsilon}+\epsilon\mu\right).$$

Again, summation over $\{\mu\}$ must be included to account for the 2π periodicity of the Dirac delta. Splitting the sum on ν in two sums, over the odd and even integers and shifting the sum on μ by νN results in

$$\begin{aligned}(f_n,f_m)=&\,2\pi\epsilon\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}\mu^2-2\pi N\upsilon^2\right]H_n(\epsilon\mu-\epsilon N\upsilon)H_m(\epsilon\mu+\epsilon N\upsilon)\\&+2\pi\epsilon\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}\left(\mu+\frac{N}{2}\right)^2-2\pi N(\upsilon+1/2)^2\right]H_n(\epsilon\mu-\epsilon N\upsilon)H_m(\epsilon(\mu+\upsilon N+N)).\end{aligned}$$

Denoting the second term above by $(f_n,f_m)_{\text{odd}}$, if $N=2h+k$, where the binary variable k controls the parity of N, then

$$(f_n,f_m)_{\text{odd}}=2\pi\epsilon\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}(\mu+h+k/2)^2-2\pi N(\upsilon+1/2)^2\right]H_n(\epsilon\mu-\epsilon N\upsilon)H_m(\epsilon(\mu+\upsilon N+N))$$

and yet again shifting the sum on μ by $h+k/2$ and the one on ν by $1/2$,

$$(f_n,f_m)_{\text{odd}}=2\pi\epsilon\sum_{\mu=-\infty}^{\infty}(k)\sum_{\upsilon=-\infty}^{\infty}(1)\exp\left[-\frac{2\pi}{N}\mu^2-2\pi N\upsilon^2\right]H_n(\epsilon(\mu-N\upsilon))H_m(\epsilon(\mu+\upsilon N)),$$

where now $\Sigma_{\mu=-\infty}^{\infty}(k)$ denotes a sum over the integers (half-integers) if $k=0$ ($k=1$), so that back to the general expression,

$$\begin{aligned}(f_n,f_m)=&\,2\pi\epsilon\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}\mu^2-2\pi N\upsilon^2\right]H_n(\epsilon(\mu-N\upsilon))H_m(\epsilon(\mu+\upsilon N))\\&+2\pi\epsilon\sum_{\mu=-\infty}^{\infty}(k)\sum_{\upsilon=-\infty}^{\infty}(1)\exp\left[-\frac{2\pi}{N}\mu^2-2\pi N\upsilon^2\right]H_n(\epsilon(\mu-N\upsilon))H_m(\epsilon(\mu+\upsilon N)).\end{aligned}$$

Now, recourse to the Hermite polynomial's generating function gives

$$\begin{aligned}(f_n,f_m)=2\pi\epsilon\frac{\partial^n}{\partial t^n}\frac{\partial^m}{\partial s^m}\Bigg\{&\sum_{\mu,\upsilon=-\infty}^{\infty}\exp\left[-\frac{2\pi}{N}\mu^2+2\mu\epsilon(t+s)-2\epsilon\nu N(t-s)-t^2-s^2\right]\\&+\sum_{\mu=-\infty}^{\infty}(k)\sum_{\upsilon=-\infty}^{\infty}(1)\exp\left[-\frac{2\pi}{N}\mu^2+2\mu\epsilon(t+s)-2\epsilon\nu N(t-s)-t^2-s^2\right]\Bigg\}_{t=s=0}.\end{aligned}$$

The sum on $\{\mu\}$ results in a ϑ_3-function in the first term, and a ϑ_3 for $k=0$ or a ϑ_2 for $k=1$ in the second. The sum on $\{\nu\}$, by its turn, gives ϑ_3-function in the first term, and a ϑ_2 in the second, as

$$(f_n,f_m)=2\pi\epsilon\frac{\partial^n}{\partial t^n}\frac{\partial^m}{\partial s^m}\left\{\left[\vartheta_3\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_3\left(\frac{i\epsilon N(t-s)}{\pi},2Ni\right)+\vartheta_{3-k}\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_2\left(\frac{i\epsilon N(t-s)}{\pi},2Ni\right)\right]\exp[-t^2-s^2]\right\}\Bigg|_{t=s=0}.$$

Using the basic properties,

$$\vartheta_3(z,i\tau)=\tau^{-1/2}\exp\left[-\frac{\pi z^2}{\tau}\right]\vartheta_3\left(\frac{z}{i\tau},\frac{i}{\tau}\right),$$

$$\theta_2(z,i\tau)=\tau^{-1/2}\exp\left[-\frac{\pi z^2}{\tau}\right]\vartheta_4\left(\frac{z}{i\tau},\frac{i}{\tau}\right),$$

one gets

$$(f_n,f_m)=\frac{2\pi^{3/2}}{N}\frac{\partial^n}{\partial t^n}\frac{\partial^m}{\partial s^m}\left\{\left[\vartheta_3\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_3\left(\frac{\epsilon(t-s)}{2\pi},\frac{i}{2N}\right)+\vartheta_{3-k}\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_4\left(\frac{\epsilon(t-s)}{2\pi},\frac{i}{2N}\right)\right]\exp[-2ts]\right\}_{t=s=0}.$$

Finally, compact expressions can be achieved with

$$\theta_3(z,\tau)=\frac{1}{2}\left[\theta_3\left(\frac{z}{2},\frac{\tau}{4}\right)+\theta_4\left(\frac{z}{2},\frac{\tau}{4}\right)\right],$$

$$\theta_2(z,\tau)=\frac{1}{2}\left[\theta_3\left(\frac{z}{2},\frac{\tau}{4}\right)-\theta_4\left(\frac{z}{2},\frac{\tau}{4}\right)\right],$$

thus for $k=0$

$$(f_n,f_m)=\frac{\pi^{3/2}}{N}\frac{\partial^n}{\partial t^n}\frac{\partial^m}{\partial s^m}\ \vartheta_3\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_3\left(\frac{\epsilon(t-s)}{\pi},\frac{2i}{N}\right)\exp[-2ts]\Bigg|_{t=s=0}$$

and for $k=1$

$$(f_n,f_m)=\frac{\pi^{3/2}}{N}\frac{\partial^n}{\partial t^n}\frac{\partial^m}{\partial s^m}\left\{\vartheta_3\left(\frac{i\epsilon(t+s)}{\pi},\frac{2i}{N}\right)\vartheta_3\left(\frac{\epsilon(t-s)}{\pi},\frac{2i}{N}\right)-2\vartheta_4\left(\frac{i\epsilon(t+s)}{2\pi},\frac{i}{2N}\right)\vartheta_4\left(\frac{\epsilon(t-s)}{2\pi},\frac{i}{2N}\right)\exp[-2ts]\right\}_{t=s=0}.$$

Again, the limit $N\to\infty$ easily recovers the usual results, as the i factor inside the ϑ-functions guarantees that, in this limit, only a term proportional to $(\partial^n/\partial t^n)(\partial^m/\partial s^m)\exp[-4ts]|_{t=s=0}$ survives. Anyhow, with the above expressions any term (f_n,f_m) can be calculated as a sum of ϑ-function derivatives evaluated at zero. The particular situation $m=0$, for example, for N even, is quite instructive. In this case

$$(f_n,f_0)=\frac{\pi^{3/2}}{N}\frac{\partial^n}{\partial t^n}\vartheta_3\left(\frac{i\epsilon t}{\pi},\frac{2i}{N}\right)\vartheta_3\left(\frac{\epsilon t}{\pi},\frac{2i}{N}\right)_{t=0},$$

$$(f_n,f_0)= \frac{\pi^{3/2}}{N}\sum_{j=0}^{n}\binom{n}{j}i^j\frac{\partial^j}{\partial t^j}\vartheta_3\left(\frac{\epsilon t}{\pi},\frac{2i}{N}\right)\Bigg|_{t=0}\left(\frac{\partial^{n-j}}{\partial t^{n-j}}\vartheta_3\left(\frac{\epsilon t}{\pi},\frac{2i}{N}\right)\Bigg|_{t=0}\right),$$

and it is immediate to see that all n=odd terms are zero. For $n=2$ (and for all even numbers not multipliers of 4), the symmetry of the binomial term and the multiplicity of the powers of i lead to a pairwise cancellation of all non-zero terms. For $n=4$ (and its multipliers), the situation is different. The simplest case is $n=4$,

$$(f_4,f_0)= \frac{\pi^{3/2}}{N}\sum_{j=0}^{4}\binom{4}{j}i^j\frac{\partial^j}{\partial t^j}\vartheta_3\left(\frac{\epsilon t}{\pi},\frac{2i}{N}\right)\Bigg|_{t=0}\left[\frac{\partial^{4-j}}{\partial t^{4-j}}\vartheta_3\left(\frac{\epsilon t}{\pi},\frac{2i}{N}\right)\Bigg|_{t=0}\right]$$

$$(f_4,f_0)=\frac{\pi^{3/2}}{N}\left\{2\vartheta_3\left(0,\frac{2i}{N}\right)\vartheta_3'''\left(0,\frac{2i}{N}\right)-6\left[\vartheta_3''\left(0,\frac{2i}{N}\right)\right]^2\right\}.$$

This term (with proper normalization) goes to zero quite fast with increasing N. In fact, for $N=10$ it is already of order of 10^{-6}. On the other hand, it is immaterial to discuss the case $N=4$ (or smaller), as in this situation the distinct eigenvalues of the Fourier operator are enough to guarantee orthogonality of the whole set. Considering all this, it comes down to, literally, one-half a dozen different values of the dimensionality N (the range $[5,10]$) for which a significant deviation from the "expected" results (that is, orthogonality) can be observed.

IV. DFT AND WIDTH INVERSION

Starting from the own definition of the ϑ_3-function, Eq. (4), with $\xi\in\mathbf{R}$, a fractional shift of the ϑ_3 function can be calculated,

$$\vartheta_3\left(z+\frac{k}{N},\frac{i\xi^2}{N}\right)=\sum_{\alpha=-\infty}^{\infty}\exp\left[-\frac{\pi}{N}\xi^2\alpha^2\right]\exp\left[2\pi i\alpha\left(z+\frac{k}{N}\right)\right],$$

where k is an integer. The sum over $\{\alpha\}$ can be broken into modulo N equivalence classes as

$$\vartheta_3\left(z+\frac{k}{N},\frac{i\xi^2}{N}\right)=\sum_{j=0}^{N-1}\sum_{\beta=-\infty}^{\infty}\exp\left[-\frac{\pi}{N}\xi^2(j+\beta N)^2\right]\exp\left[2\pi i(j+\beta N)\left(z+\frac{k}{N}\right)\right].$$

Conveniently regrouping the terms one gets

$$\vartheta_3\left(z+\frac{k}{N},\frac{i\xi^2}{N}\right)=\sum_{j=0}^{N-1}\left(\sum_{\beta=-\infty}^{\infty}\exp\left[-\pi N\xi^2\beta^2\right]\exp\left[2\pi i\beta(i\xi^2 j+Nz)\right]\right)\times\exp\left[-\frac{\pi}{N}\xi^2 j^2+2\pi ijz+\frac{2\pi i}{N}jk\right],$$

where the term inside the brackets can be identified as ϑ_3-function,

$$\vartheta_3\left(z+\frac{k}{N},\frac{i\xi^2}{N}\right)=\sum_{j=0}^{N-1}\vartheta_3(i\xi^2 j+Nz,iN\xi^2)\exp\left[-\frac{\pi}{N}\xi^2 j^2+2\pi ijz+\frac{2\pi i}{N}jk\right].$$

Use of property (6) leads to

$$\vartheta_3\left(z+\frac{k}{N},\frac{i\xi^2}{N}\right)=\frac{1}{\sqrt{N\xi^2}}\sum_{j=0}^{N-1}\vartheta_3\left(\frac{iz}{\xi^2}-\frac{j}{N},\frac{i}{N\xi^2}\right)\exp\left[-\frac{\pi N}{\xi^2}z^2+\frac{2\pi i}{N}jk\right] \tag{10}$$

and taking advantage of the Fourier coefficients $\exp\left[\frac{2\pi i}{N}jk\right]$ it is easy to obtain the inverse relation

$$\vartheta_3\left(\frac{iz}{\xi^2}-\frac{k}{N},\frac{i}{N\xi^2}\right)=\sqrt{\frac{N}{\xi^2}}\sum_{j=0}^{N-1}\vartheta_3\left(z+\frac{j}{N},\frac{i\xi^2}{N}\right)\exp\left[\frac{\pi N}{\xi^2}z^2-\frac{2\pi i}{N}jk\right]. \tag{11}$$

Particular cases of these equations are most interesting, and a lot of peculiar relations can be obtained with the different possible choices of z,k and ξ. Two straightforward examples are: First, setting $z=0$ in (10),

$$\vartheta_3\left(\frac{k}{N},\frac{i\xi^2}{N}\right)=\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\vartheta_3\left(\frac{j}{N},\frac{i}{N\xi^2}\right)\exp\left[\frac{2\pi i}{N}jk\right], \tag{12}$$

and, according to Eq. (7), the ϑ_3-function on the left-hand side has width ξ, while the one under the action of the DFT has width ξ^{-1}. This property is the obvious discrete counterpart of the well-known behavior of the Gaussian function under the usual Fourier transform.

The case $k=0$, by its turn, after some manipulation gives

$$\vartheta_3(Nz,iN\xi^2)=\sqrt{\frac{N}{\xi^2}}\sum_{j=0}^{N-1}\vartheta_3\left(z+\frac{j}{N},\frac{i\xi^2}{N}\right).$$

A. Application

With the above results it is possible to generalize the result of Ref. 6 in a straightforward way. Introducing

$$f_n(j,\xi)=\sqrt{\frac{N}{\xi}}\ \frac{\partial^n}{\partial t^n}\vartheta_3\left(\frac{j}{N}-\frac{\epsilon}{\pi}\xi t,\frac{i\xi^2}{N}\right)\exp[t^2]\Big|_{t=0},$$

its DFT can be directly calculated,

$$\overline{f_n}(k,\xi)=\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}\exp\left[\frac{2\pi i}{N}jk\right]f_n(j,\xi),$$

$$\overline{f_n}(k,\xi)=\frac{1}{\sqrt{\xi}}\frac{\partial^n}{\partial t^n}\sum_{j=0}^{N-1}\exp\left[\frac{2\pi i}{N}jk\right]\ \vartheta_3\left(\frac{j}{N}-\frac{\epsilon}{\pi}\xi t,\frac{i\xi^2}{N}\right)\exp[t^2]\Big|_{t=0},$$

and use of Eq. (11) together with change of variables from t to it leads to

$$\overline{f_n}(k,\xi)=\sqrt{N\xi}i^n\frac{\partial^n}{\partial t^n}\ \vartheta_3\left(\frac{k}{N}-\frac{\epsilon t}{\pi\xi},\frac{i}{N\xi^2}\right)\exp[t^2]\Big|_{t=0},$$

thus

$$f_n(k,\xi^{-1})=i^n\sum_{j=0}^{N-1}\exp\left[\frac{2\pi i}{N}jk\right]f_n(j,\xi), \tag{13}$$

which reproduces Eq. (1) for $\xi=1$. From this relation, most identities obtained in Ref. 6 may also be generalized.

V. TWO VARIABLE'S DFT

Yet another generalization of the main result of Ref. 6 regards a two variable DFT, which, for the sake of briefness, here it will be merely verified. Apart from the obvious product solution $f_m(j)f_n(l)$, if one considers the quantity

$$F_{m,n}(j,l)=\sum_{k=0}^{N-1} f_m(k)f_n(k-l)\exp\left[\frac{2\pi i}{N}jk\right],$$

which obeys

$$(F_{m,n}(j,l))^*=F_{m,n}(j,l)\exp\left[\frac{2\pi i}{N}jl\right],$$

use of Eq. (1), and some simple manipulations lead to the nontrivial result

$$|F_{m,n}(j,l)|^2=\frac{(-i)^{m+n}}{N}\sum_{a,b=0}^{N-1}|F_{m,n}(a,b)|^2\exp\left[\frac{2\pi i}{N}(ma+nb)\right].$$

As in the one variable case, these states obey

$$\sum_{j,l=0}^{N-1}|F_{m,n}(j,l)|^2|F_{m',n'}(j,l)|^2=\delta_{m,m'}\delta_{n,n'},\quad m+n\neq m'+n'(\mathrm{mod}\,4),$$

which imply a multitude of relations involving derivatives of the ϑ_3-functions (or the Hermite polynomials). Motivated by the preceding section, it should be investigated whether this relation holds for $m+n=m'+n'(\mathrm{mod}\,4)$.

VI. FURTHER RELATIONS INVOLVING THE WIDTH

So far it has been seen that to break up the infinite sum present in the definition of the Jacobi ϑ_3-function leads to interesting properties of this very function. In order to further explore this technique, from Eq. (7) it is straightforward to write

$$\vartheta_3\left(\frac{z}{L},\frac{i\xi^2}{L}\right)=\frac{\sqrt{L}}{\xi}\sum_{\alpha=-\infty}^{\infty}\exp\left[-L\pi\left(\frac{z}{\xi L}+\frac{\alpha}{\xi}\right)^2\right],\tag{14}$$

with L a positive real number. Choosing ξ integer, it is possible to break the sum over $\{\alpha\}$ into modulo ξ equivalence classes

$$\vartheta_3\left(\frac{z}{L},\frac{i\xi^2}{L}\right)=\frac{\sqrt{L}}{\xi}\sum_{j=0}^{\xi-1}\sum_{\mu=-\infty}^{\infty}\exp\left[-L\pi\left(\frac{z}{\xi L}+\frac{j+\mu\xi}{\xi}\right)^2\right],$$

$$\vartheta_3\left(\frac{z}{L},\frac{i\xi^2}{L}\right)=\frac{\sqrt{L}}{\xi}\sum_{j=0}^{\xi-1}\sum_{\mu=-\infty}^{\infty}\exp\left[-L\pi\left(\frac{z+jL}{\xi L}+\mu\right)^2\right],$$

and the infinite sum can be identified as a ϑ_3,

$$\vartheta_3\left(\frac{z}{L},\frac{i\xi^2}{L}\right)=\frac{1}{\xi}\sum_{j=0}^{\xi-1}\vartheta_3\left(\frac{z+jL}{\xi L},\frac{i}{L}\right).\tag{15}$$

It is quite interesting to set $z=z\xi$ above and observe that

$$\vartheta_3\left(\frac{z\xi}{L},\frac{i\xi^2}{L}\right)=\frac{1}{\xi}\sum_{j=0}^{\xi-1}\vartheta_3\left(\frac{z}{L}+\frac{j}{\xi},\frac{i}{L}\right),$$

which, for the particular case $\xi=2$ gives the well-known result

$$\vartheta_3\left(\frac{2z}{L},\frac{4i}{L}\right)=\frac{1}{2}\left[\vartheta_3\left(\frac{z}{L},\frac{i}{L}\right)+\vartheta_3\left(\frac{z}{L}+\frac{1}{2},\frac{i}{L}\right)\right],$$

$$\vartheta_3\left(\frac{2z}{L},\frac{4i}{L}\right)=\frac{1}{2}\left[\vartheta_3\left(\frac{z}{L},\frac{i}{L}\right)+\vartheta_4\left(\frac{z}{L},\frac{i}{L}\right)\right].$$

Similar reasoning would lead to the complementary relation

$$\vartheta_3\left(\frac{z}{L},\frac{i}{L}\right)=\frac{1}{\xi}\sum_{j=0}^{\xi-1}\vartheta_3\left(\frac{z}{\xi L}+\frac{j}{\xi},\frac{i}{L\xi^2}\right). \tag{16}$$

And again, the particular case $\xi=2$ gives

$$\vartheta_3\left(\frac{z}{L},\frac{i}{L}\right)=\frac{1}{2}\left[\vartheta_3\left(\frac{z}{2L},\frac{i}{4L}\right)+\vartheta_4\left(\frac{z}{2L},\frac{i}{4L}\right)\right].$$

Equations (15) and (16) can be combined to provide an alternative width inversion relation

$$\vartheta_3\left(\frac{z\xi}{L},\frac{i\xi^2}{L}\right)=\frac{1}{\xi^2}\sum_{j,j'=0}^{\xi-1}\vartheta_3\left(\frac{z}{\xi L}+\frac{j'}{\xi}+\frac{j}{\xi^2},\frac{i}{L\xi^2}\right).$$

VII. CONCLUSIONS

The results here presented seem to argue in favor of one basic point: The Jacobi ϑ_3-function, together with the DFT, plays, in finite dimensional spaces, the same role played by the Gaussian function in conjunction with the usual Fourier transform. Concerning quantum mechanics, Schwinger has already noted that, if the families of eigenstates of two different observables are connected *via* DFT, then those observables share a maximum degree of incompatibility.[5] In this connection, the width inversion relation obeyed by the $f_n(j,\xi)$ functions strongly suggests that one may be able to construct, for finite dimensional spaces, states which behavior resembles that of the continuous minimum uncertainty states.

However, such a reasoning meets an important hindrance if one considers that the orthogonality of the DFT's eigenstates ultimately fails. It is a fact, however, that with increasing N it becomes, in a numerical sense, true, and in this case the $N\to\infty$ limit is reached, as witty as it may sound, somewhere near one dozen. This fact may illustrate a true finite dimensional idiosyncrasy, or it might lead one to look for the possibility of finding different sets of DFT's eigenstates, an issue which is a matter of current research.

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Inverse scattering transform for the vector nonlinear Schrödinger equation with nonvanishing boundary conditions

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The inverse scattering transform for the vector defocusing nonlinear Schrödinger (NLS) equation with nonvanishing boundary values at infinity is constructed. The direct scattering problem is formulated on a two-sheeted covering of the complex plane. Two out of the six Jost eigenfunctions, however, do not admit an analytic extension on either sheet of the Riemann surface. Therefore, a suitable modification of both the direct and the inverse problem formulations is necessary. On the direct side, this is accomplished by constructing two additional analytic eigenfunctions which are expressed in terms of the adjoint eigenfunctions. The discrete spectrum, bound states and symmetries of the direct problem are then discussed. In the most general situation, a discrete eigenvalue corresponds to a quartet of zeros (poles) of certain scattering data. The inverse scattering problem is formulated in terms of a generalized Riemann-Hilbert (RH) problem in the upper/lower half planes of a suitable uniformization variable. Special soliton solutions are constructed from the poles in the RH problem, and include dark-dark soliton solutions, which have dark solitonic behavior in both components, as well as dark-bright soliton solutions, which have one dark and one bright component. The linear limit is obtained from the RH problem and is shown to correspond to the Fourier transform solution obtained from the linearized vector NLS system. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2209169]

I. INTRODUCTION

The inverse scattering transform (IST) for the scalar nonlinear Schrödinger (NLS) equation

$$iq_t = q_{xx} - 2\sigma|q|^2 q \tag{1.1}$$

(subscripts x and t denote partial differentiation throughout) has been extensively studied in the literature, both in the focusing ($\sigma=-1$) and in the defocusing ($\sigma=1$) cases.[1–3] In particular, the defocusing case with nonvanishing boundary conditions was first studied in 1973;[4] the problem was subsequently clarified and generalized in various works,[5–10] and a detailed study can be found in the monograph.[11] Equation (1.1) with $\sigma=1$ admits soliton solutions with nontrivial boundary conditions, the so-called dark/gray solitons, which have the form

$$q(x,t) = q_0 e^{2iq_0^2 t}[\cos\alpha + i\sin\alpha\tanh[\sin\alpha q_0(x - 2q_0\cos\alpha t - x_0)]] \tag{1.2}$$

with q_0, α and x_0 arbitrary real parameters. Such solutions satisfy the boundary conditions

$$q(x,t) \to q_{\pm}(t) = q_0 e^{2iq_0^2 t \pm i\alpha} \quad \text{as } x \to \pm\infty$$

and appear as localized dips of intensity $q_0^2 \sin^2 \alpha$ on the background field q_0.

While the IST for the scalar NLS equation was developed many years ago, both with vanishing and nonvanishing boundary conditions, the basic formulation of IST has not been fully developed for the vector nonlinear Schrödinger (VNLS) equation

$$i\mathbf{q}_t = \mathbf{q}_{xx} - 2\sigma\|\mathbf{q}\|^2\mathbf{q}, \tag{1.3}$$

where $\mathbf{q}=\mathbf{q}(x,t)$ is, in general, an M-component vector and $\|\cdot\|$ is the standard Euclidean norm. The focusing case ($\sigma=-1$) with vanishing boundary conditions in two components was developed by Manakov in 1974.[12] However, the IST for the VNLS with nonzero boundary conditions has been open for over 30 years (partial results can be found in Ref. 13). It is worth noting that Ref. 14 provides an elegant direct and inverse scattering theory for decaying potentials on the real line. The extension to nondecaying potentials, however, is not straightforward and therefore here we employ a different approach. We should also remark that direct methods have been applied to VNLS as a way to derive explicit bright and dark soliton solutions, see for instance Refs. 17–20 and the review article Ref. 21.

In this work we present the IST for the two-component defocusing VNLS equation [namely, Eq. (1.3) with $\sigma=1$ and $M=2$] with nonvanishing boundary conditions as $x\to\pm\infty$. In Sec. II we discuss the direct scattering problem. Section II A is devoted to the study of the analyticity of the scattering eigenfunctions. Similar to the scalar equation, the spectral parameter of the associated block-matrix scattering problem for the VNLS is an element of a two-sheeted Riemann surface. The vector problem however presents additional difficulties due, in part, to the fact that two out of the six scattering eigenfunctions, defined via their asymptotics at infinity, do not admit an analytic extension on either sheet of the surface. Therefore a suitable modification both of the direct and of the inverse problem is necessary. On the direct side, this is achieved by defining in Sec. II B an "adjoint" scattering problem, which provides two additional analytic solutions of the original scattering problem. In Sec. II C we study the symmetries, and in Sec. II D we introduce a uniformization variable. In Sec. II E we study the asymptotic behavior of the eigenfunctions for large values of the scattering parameter, and in Sec. II F we discuss the discrete spectrum. The inverse problem is formulated in Sec. III as a Riemann-Hilbert (RH) problem associated with analytic eigenfunctions. The RH problem is then transformed into a closed linear system of algebraic-integral equations. The time evolution of the scattering data and the conserved quantities are discussed in Sec. IV. Explicit solutions are obtained in Sec. V; they include vector generalization of the dark and gray soliton solutions of the scalar case as well as more exotic dark-bright soliton solutions. Finally, in Sec. VI the linearized solution of the VNLS equation is obtained and found to be consistent with that of the RH formulation, and in the Appendix we discuss the WKB expansion of the eigenfunctions at large values of the scattering parameter.

II. DIRECT PROBLEM

It is well-known[12] that the two-component defocusing VNLS equation (1.3) with $\sigma=1$ and $M=2$ is associated to the Lax pair

$$v_x = (ik\mathbf{J} + \mathbf{Q})v, \tag{2.1a}$$

$$v_t = \begin{pmatrix} 2ik^2 + i\mathbf{q}^T\mathbf{r} & -2k\mathbf{q}^T - i\mathbf{q}_x^T \\ -2k\mathbf{r} + i\mathbf{r}_x & -2ik^2\mathbf{I}_2 - i\mathbf{r}\mathbf{q}^T \end{pmatrix} v, \tag{2.1b}$$

where $v(x,t,k)=(v^{(1)}(x,t,k),v^{(2)}(x,t,k),v^{(3)}(x,t,k))^T$ is the scattering eigenfunction, k is the scattering parameter, $\mathbf{q}(x,t)=(q^{(1)}(x,t),q^{(2)}(x,t))^T$ and $\mathbf{r}(x,t)=(r^{(1)}(x,t),r^{(2)}(x,t))^T=\mathbf{q}^*(x,t)$ are the scattering potentials, $\mathbf{I}_N$ is the $N\times N$ identity matrix, the superscript T denotes matrix transpose, and where

$$\mathbf{J} = \mathrm{diag}(-1,1,1), \quad \mathbf{Q}(x,t) = \begin{pmatrix} 0 & \mathbf{q}^T \\ \mathbf{r} & 0_{2\times 2} \end{pmatrix}. \tag{2.2}$$

Explicitly, the compatibility of the system of equations (2.1) (i.e., the equality of the mixed derivatives of the 3-component vector v with respect to x and t), together with the constraint $\mathbf{r}=\mathbf{q}^*$, is equivalent to the requirement that $\mathbf{q}(x,t)$ satisfy Eq. (1.3) with $\sigma=1$. Throughout this work, we consider potentials with the same time-independent amplitudes at both space infinities, which we can write without loss of generality as

$$\mathbf{q}(x,t) \sim \mathbf{q}_\pm(t) = e^{i\Theta_\pm(t)}\mathbf{q}_0, \quad \mathbf{r}(x,t) \sim \mathbf{r}_\pm(t) = e^{-i\Theta_\pm(t)}\mathbf{q}_0, \quad x \to \pm\infty, \tag{2.3}$$

where $\Theta_\pm(t)=\mathrm{diag}(\theta_\pm^{(1)},\theta_\pm^{(2)})$ and $\mathbf{q}_0=(q_0^{(1)},q_0^{(2)})^T \in \mathbb{R}^+\times\mathbb{R}^+$, and where $\|\mathbf{q}_0\|=\sqrt{(q_0^{(1)})^2+(q_0^{(2)})^2}$ is assumed to be non-zero. For brevity, in the following we will use $q_0=\|\mathbf{q}_0\|$.

A. Eigenfunctions, integral equations and analyticity

The eigenfunctions for the scattering problem (2.1a) with boundary conditions (2.3) are introduced by fixing the large-x asymptotics for $k\in\mathbb{R}$ with $|k|\geqslant q_0$,

$$\phi_1(x,k) \sim w_1^-(k)e^{-i\lambda x}, \quad \phi_2(x,k) \sim w_2^-(k)e^{ikx}, \quad \phi_3(x,k) \sim w_3^-(k)e^{i\lambda x}, \quad x\to-\infty, \tag{2.4a}$$

$$\psi_1(x,k) \sim w_1^+(k)e^{-i\lambda x}, \quad \psi_2(x,k) \sim w_2^+(k)e^{ikx}, \quad \psi_3(x,k) \sim w_3^+(k)e^{i\lambda x}, \quad x\to+\infty, \tag{2.4b}$$

where $\lambda(k)=\sqrt{k^2-q_0^2}$, the eigenvectors $w_1^\pm(k), w_2^\pm(k), w_3^\pm(k)$ are given by

$$w_1^-(k) = \begin{pmatrix} \lambda+k \\ i\mathbf{r}_- \end{pmatrix}, \quad w_2^-(k) = \begin{pmatrix} 0 \\ -i\mathbf{q}_-^\perp \end{pmatrix}, \quad w_3^-(k) = \begin{pmatrix} \lambda-k \\ -i\mathbf{r}_- \end{pmatrix}, \tag{2.5a}$$

$$w_1^+(k) = \begin{pmatrix} \lambda+k \\ i\mathbf{r}_+ \end{pmatrix}, \quad w_2^+(k) = \begin{pmatrix} 0 \\ -i\mathbf{q}_+^\perp \end{pmatrix}, \quad w_3^+(k) = \begin{pmatrix} \lambda-k \\ -i\mathbf{r}_+ \end{pmatrix}, \tag{2.5b}$$

and where we introduced a notation which we will use throughout this work: for any two-component vector $\mathbf{p}=(p^{(1)},p^{(2)})^T$ we write $\mathbf{p}^\perp=(p^{(2)},-p^{(1)})^T$. Note that for brevity we will omit the time dependence of the potentials and eigenfunctions throughout the discussion of the direct problem.

The Wronskian of a set $\{v_1,v_2,v_3\}$ of solutions of the scattering problem (2.1a) is defined in the usual way as

$$\mathrm{Wr}(v_1,v_2,v_3) = \det(v_1,v_2,v_3),$$

and satisfies the equation $d[\mathrm{Wr}(v_1,v_2,v_3)]/dx = ik\,\mathrm{Wr}(v_1,v_2,v_3)$. Taking into account the asymptotic behavior of the solutions in Eq. (2.4) we then have

$$\mathrm{Wr}(\phi_1,\phi_2,\phi_3) = \mathrm{Wr}(\psi_1,\psi_2,\psi_3) = -2\lambda q_0^2 e^{ikx}. \tag{2.6}$$

Hence, for any nondecaying potential $\mathbf{q}(x,t)$, the two Wronskians in Eq. (2.6) are nonzero for all $x\in\mathbb{R}$ and all k such that $\lambda(k)\neq 0$ (i.e., everywhere except at the branch points of λ). We also introduce the solutions with fixed (with respect to x) boundary conditions

$$M_1(x,k) = e^{i\lambda x}\phi_1(x,k), \quad M_2(x,k) = e^{-ikx}\phi_2(x,k), \quad M_3(x,k) = e^{-i\lambda x}\phi_3(x,k), \tag{2.7a}$$

$$N_1(x,k) = e^{i\lambda x}\psi_1(x,k), \quad N_2(x,k) = e^{-ikx}\psi_2(x,k), \quad N_3(x,k) = e^{-i\lambda x}\psi_3(x,k), \tag{2.7b}$$

which can be represented in terms of the integral equations

$$M_j(x,k) = w_j^-(k) + \int_{-\infty}^{\infty} \mathbf{G}_j^-(x-x',k)(\mathbf{Q}(x') - \mathbf{Q}_-)M_j(x',k)\mathrm{d}x', \tag{2.8a}$$

$$N_j(x,k) = w_j^+(k) + \int_{-\infty}^{\infty} \mathbf{G}_j^+(x-x',k)(\mathbf{Q}(x') - \mathbf{Q}_+)N_j(x',k)\mathrm{d}x' \tag{2.8b}$$

for $j=1,2,3$, where

$$\mathbf{Q}_\pm = \begin{pmatrix} 0 & \mathbf{q}_\pm^T \\ \mathbf{r}_\pm & 0_{2\times 2} \end{pmatrix}, \tag{2.9}$$

and where the matrix Green's functions $\mathbf{G}_j^\pm(x,k)$ are defined below. The choice of Green's functions, together with the choice of the inhomogeneous terms in Eqs. (2.8), determine the analytic properties of the corresponding eigenfunctions. The superscripts $\pm$ in the Green's functions, like in the inhomogeneous terms, refer to the corresponding eigenfunctions being defined in terms of their asymptotics as $x \to \pm\infty$.

Using the Fourier transform technique, one can show that

$$\begin{aligned}\mathbf{G}_1^\mp(x,k) = \pm\,\theta(\pm x)\Bigg\{ & \frac{1}{2\lambda(\lambda+k)}[(\lambda+k)(\lambda\mathbf{I}_3 - k\mathbf{J}) + i(\lambda+k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{e^{2i\lambda x}}{2\lambda(\lambda-k)}[(\lambda-k)(\lambda\mathbf{I}_3 \\ & + k\mathbf{J}) - i(\lambda-k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{e^{i(\lambda+k)x}}{q_0^2}\widetilde{\mathbf{Q}}_\mp\Bigg\},\end{aligned} \tag{2.10a}$$

$$\begin{aligned}\mathbf{G}_3^\mp(x,k) = \pm\,\theta(\pm x)\Bigg\{ & \frac{1}{2\lambda(\lambda-k)}[(\lambda-k)(\lambda\mathbf{I}_3 + k\mathbf{J}) - i(\lambda-k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{e^{-2i\lambda x}}{2\lambda(\lambda+k)}[(\lambda+k)(\lambda\mathbf{I}_3 \\ & - k\mathbf{J}) + i(\lambda+k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{e^{-i(\lambda-k)x}}{q_0^2}\widetilde{\mathbf{Q}}_\mp\Bigg\},\end{aligned} \tag{2.10b}$$

$$\begin{aligned}\mathbf{G}_2^\mp(x,k) = \pm\,\theta(\pm x)\Bigg\{ & \frac{e^{-i(\lambda+k)x}}{2\lambda(\lambda+k)}[(\lambda+k)(\lambda\mathbf{I}_3 - k\mathbf{J}) + i(\lambda+k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{e^{i(\lambda-k)x}}{2\lambda(\lambda-k)}[(\lambda-k)(\lambda\mathbf{I}_3 \\ & + k\mathbf{J}) - i(\lambda-k)\mathbf{Q}_\mp + \widetilde{\mathbf{Q}}_\mp] + \frac{1}{q_0^2}\widetilde{\mathbf{Q}}_\mp\Bigg\},\end{aligned} \tag{2.10c}$$

where

$$\widetilde{\mathbf{Q}}_\pm = \begin{pmatrix} 0 & \mathbf{0}_{1\times 2} \\ \mathbf{0}_{2\times 1} & \mathbf{q}_\pm^\perp(\mathbf{r}_\pm^\perp)^T \end{pmatrix} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & q_\pm^{(2)} r_\pm^{(2)} & -r_\pm^{(1)} q_\pm^{(2)} \\ 0 & -r_\pm^{(2)} q_\pm^{(1)} & r_\pm^{(1)} q_\pm^{(1)} \end{pmatrix}. \tag{2.11}$$

Note that Eqs. (2.10) are significantly more complicated than the case of the vector system with zero boundary conditions (e.g., see Ref. 22).

So far, the integral equations and Green's functions are only defined for real k and λ. In order to extend the eigenfunctions to complex values of k, we note that, for instance, the Green's function $\mathbf{G}_1^-(x,k)$ does not grow exponentially as $|k| \to \infty$ if and only if

$$\mathrm{Im}\,\lambda \geqslant 0 \quad \text{and } \mathrm{Im}(\lambda+k) \geqslant 0. \tag{2.12a}$$

Similarly, $\mathbf{G}_1^+(x,k)$ does not grow exponentially as $|k| \to \infty$ if and only if

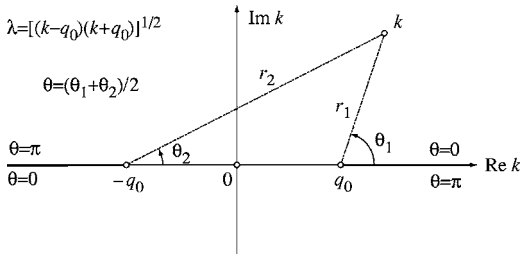

FIG. 1. The choice of branch cut for $\lambda=(k^2-q_0^2)^{1/2}$ in the complex k-plane. Here $\theta=(\theta_1+\theta_2)/2$.

$$\mathrm{Im}\,\lambda \leqslant 0 \quad \text{and } \mathrm{Im}(\lambda + k) \leqslant 0. \tag{2.12b}$$

It is therefore natural to introduce the Riemann surface of equation $\lambda^2=k^2-q_0^2$ obtained by gluing together two copies of the extended complex k-plane, which we will call $\mathbb{C}_1$ and $\mathbb{C}_2$, cut along the semilines $(-\infty,-q_0)$ and (q_0,∞).

On $\mathbb{C}_1$ one can introduce the local polar coordinates

$$k-q_0=r_1e^{i\theta_1}, \quad 0 \leqslant \theta_1 < 2\pi,$$

$$k+q_0=r_2e^{i\theta_2}, \quad -\pi \leqslant \theta_2 < \pi$$

with the magnitudes r_1 and r_2 uniquely fixed by the location of the point k: $r_1=|k-q_0|$ and $r_2=|k+q_0|$ (cf. Fig. 1). Then one can define

$$\lambda(k)=(r_1r_2)^{1/2}e^{i(\theta_1+\theta_2)/2}. \tag{2.13}$$

If $\theta=(\theta_1+\theta_2)/2$, then θ varies continuously between 0 and π both in the upper and in the lower k-planes, with a cut in the region $(-\infty,-q_0)\cup(q_0,\infty)$, and one has $\mathrm{Im}\,\lambda \geqslant 0$ and $\mathrm{Im}(\lambda \pm k) \geqslant 0$ for all $k \in \mathbb{C}_1$. Conversely, on $\mathbb{C}_2$ one defines

$$\lambda(k)=-(r_1r_2)^{1/2}e^{i(\theta_1+\theta_2)/2}, \tag{2.14}$$

which will give $\mathrm{Im}\,\lambda \leqslant 0$ and also $\mathrm{Im}(\lambda \pm k) \leqslant 0$, again with a cut in the region $(-\infty, -q_0)\cup(q_0,\infty)$. The upper branches of the cuts on sheet $\mathbb{C}_1$ are then glued with the lower branches on sheet $\mathbb{C}_2$ and vice versa as shown in Fig. 2(a).

With the above definitions, both conditions (2.12a) are satisfied if and only if k is on the upper sheet of the Riemann surface, and both conditions (2.12b) if and only if k is on the lower sheet. For potentials that rapidly approach $\mathbf{Q}_\pm$ as $x \to \pm\infty$, the Green's function $\mathbf{G}_1^-(x,k)$ then defines via Eq. (2.8a) an eigenfunction $M_1(x,k)$ which admits analytic extension on the entire upper sheet of the Riemann surface. Similarly, for suitable potentials the eigenfunction $N_1(x,k)$ defined by $\mathbf{G}_1^+(x,k)$ via Eq. (2.8b) admits analytic extension on the entire lower sheet. In a similar way one can investigate the properties of the remaining Green's functions. Overall we conclude that the eigenfunctions $M_1(x,k)=\phi_1(x,k)e^{i\lambda x}$ and $N_3(x,k)=\psi_3(x,k)e^{-i\lambda x}$ *are analytic on the upper sheet*, and $M_3(x,k)=\phi_3(x,k)e^{-i\lambda x}$ and $N_1(x,k)=\psi_1(x,k)e^{i\lambda x}$ *are analytic on the lower sheet*. Unlike the case of vanishing boundaries, however, the remaining two eigenfunctions, namely $M_2(x,k)$ and $N_2(x,k)$, in general are analytic neither on the upper nor on the lower sheet.

Equation (2.6) shows that for all real $k \neq \pm q_0$, the two matrices $\Phi(x,k)=(\phi_1,\phi_2,\phi_3)$ and $\Psi(x,k)=(\psi_1,\psi_2,\psi_3)$ each contain a set of three linearly independent solutions of the third-order scattering problem (2.4a). Thus it must be possible to express one set of solutions as a linear combination of the other, where the coefficients depend on k but are independent of x:

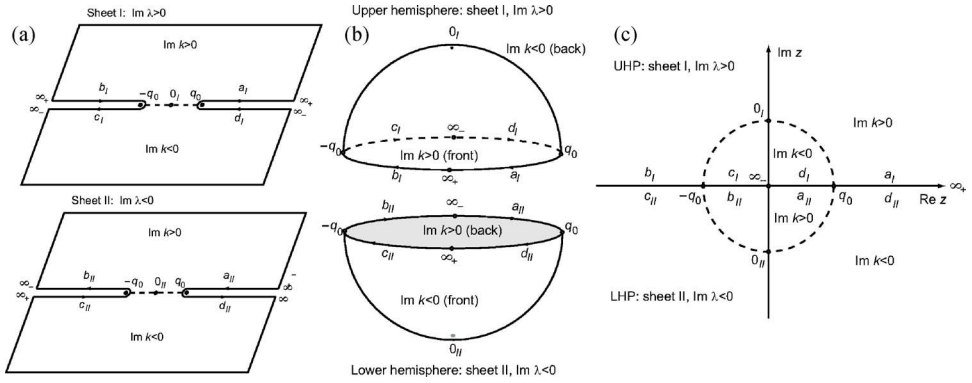

FIG. 2. (a) The two-sheeted covering of the complex plane defined by the scattering parameters (k,λ). (b) The topologically equivalent genus-0 Riemann sphere. (c) The corresponding complex plane for the uniformization variable $z=k+\lambda$ (which will be introduced in Sec. II D).

$$\Phi(x,k) = \Psi(x,k)\mathbf{A}^T(k), \tag{2.15a}$$

where $\mathbf{A}(k)=(a_{ij})$ is the 3×3 matrix of scattering coefficients. That is, $\phi_1(x,k)=a_{11}(k)\psi_1(x,k)+a_{12}(k)\psi_2(x,k)+a_{13}(k)\psi_3(x,k)$, with similar expressions for $\phi_2(x,k)$ and $\phi_3(x,k)$. Note that Eqs. (2.6) imply $\det(\mathbf{A})=1$. We can also express the "right" eigenfunctions in terms of the "left" ones,

$$\Psi(x,k) = \Phi(x,k)\mathbf{B}^T(k), \tag{2.15b}$$

where $\mathbf{B}(k)=(b_{ij})=\mathbf{A}^{-1}(k)$. Note that the scattering coefficients $a_{ij}(k)$ and $b_{ij}(k)$ are in general only defined where all of the eigenfunctions are, i.e., for $k\in\mathbb{R}$ and $|k|>q_0$, or, more precisely, on the oriented half-lines defined in Fig. 2, namely on $a_{\mathrm{I}}\equiv d_{\mathrm{II}}$, $b_{\mathrm{I}}\equiv c_{\mathrm{II}}$, $c_{\mathrm{I}}\equiv b_{\mathrm{II}}$, and $d_{\mathrm{I}}\equiv a_{\mathrm{II}}$. Note also that upper and lower banks of the cut are not equivalent, because both $\lambda(k)$ and the scattering eigenfunctions are discontinuous along the cut. These semilines define the contour $\mathcal{L}=a_{\mathrm{I}}\cup b_{\mathrm{I}}\cup c_{\mathrm{I}}\cup d_{\mathrm{I}}\equiv d_{\mathrm{II}}\cup c_{\mathrm{II}}\cup b_{\mathrm{II}}\cup a_{\mathrm{II}}$ namely $\mathcal{L}=(q_0+i0,\infty+i0)\cup(-\infty+i0,-q_0+i0)\cup-(-q_0-i0,-\infty-i0)\cup-(\infty-i0,q_0-i0)$ on the upper sheet.

Some of the scattering coefficients can be analytically extended off the real axis. From Eqs. (2.15) one can derive Wronskian representations for the scattering coefficients. Unlike the scalar case, however, such representations are not definitive in order to establish analyticity, since they all involve either $\phi_2(x,k)$ and/or $\psi_2(x,k)$, which do not admit analytic continuation. However, one can derive alternative representations for the scattering coefficients that provide the analytic extension sought for. For instance, using the first column of Eq. (2.15a) and the asymptotics (2.4b), one can check that

$$a_{11}(k) = \frac{1}{2\lambda(\lambda+k)} \lim_{x\to+\infty} e^{i\lambda x}[(\lambda+k)\phi_1^{(1)}(x,k) + iq_+^{(1)}\phi_1^{(2)}(x,k) + iq_+^{(2)}\phi_1^{(3)}(x,k)], \tag{2.16}$$

and since this expression for $a_{11}(k)$ only depends on the components of the vector $e^{i\lambda x}\phi_1(x,k)$, it indicates that for suitable potentials $a_{11}(k)$ can be analytically extended on the upper sheet of the Riemann surface. Similarly one finds that $a_{33}(k)$ and $b_{11}(k)$ can be analytically extended on the lower sheet of the Riemann surface, and $b_{33}(k)$ can be extended on the upper sheet of the Riemann surface. In general, however, the remaining scattering coefficients do not have any special analyticity properties.

The problem of determining the class of potentials for which a limit like (2.16) (with respect to a parameter, here x) of an analytic function of k is still an analytic function of k, is beyond the scope of this paper. We point out that this result is true for all the special solutions considered in this work.

B. Adjoint problem and auxiliary eigenfunctions

In order to formulate and solve the inverse scattering problem, one needs two independent sets of analytic eigenfunctions. The main issue at this stage is eliminating the nonanalytic eigenfunctions ϕ_2 and ψ_2. The approach introduced by Kaup in Ref. 15 for investigating the three-wave interaction is generalized here in order to obtain a representation of the nonanalytic eigenfunctions in terms of analytic eigenfunctions and scattering data. The key idea is to consider the "adjoint" eigenvalue problem

$$v_x^{\mathrm{ad}} = (-ik\mathbf{J} + \mathbf{Q}^T)v^{\mathrm{ad}} \tag{2.17}$$

where $\mathbf{Q}$ and $\mathbf{J}$ are defined in Eq. (2.2). One then recalls the well-known fact (see, for instance Ref. 16) that if $u^{\mathrm{ad}}(x,k)$ and $w^{\mathrm{ad}}(x,k)$ are two arbitrary solutions of the adjoint problem (2.17), then

$$v(x,k) = -\mathbf{J}(u^{\mathrm{ad}}(x,k) \wedge w^{\mathrm{ad}}(x,k))e^{ikx}, \tag{2.18}$$

where $\wedge$ denotes the vector product, is a solution of the original scattering problem (2.1a). As before, one defines two sets of solutions of Eq. (2.17), i.e., as $x \to -\infty$

$$\phi_1^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} \lambda + k \\ -i\mathbf{q}_- \end{pmatrix} e^{i\lambda x}, \quad \phi_2^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} 0 \\ i\mathbf{r}_-^{\perp} \end{pmatrix} e^{-ikx}, \quad \phi_3^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} \lambda - k \\ i\mathbf{q}_- \end{pmatrix} e^{-i\lambda x} \tag{2.19a}$$

and as $x \to +\infty$

$$\psi_1^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} \lambda + k \\ -i\mathbf{q}_+ \end{pmatrix} e^{i\lambda x}, \quad \psi_2^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} 0 \\ i\mathbf{r}_+^{\perp} \end{pmatrix} e^{-ikx}, \quad \psi_3^{\mathrm{ad}}(x,k) \sim \begin{pmatrix} \lambda - k \\ i\mathbf{q}_+ \end{pmatrix} e^{-i\lambda x}. \tag{2.19b}$$

With techniques identical to those used to derive the integral equations and the Green's functions associated to the eigenfunctions of the scattering problem (2.1a), one can then show that $e^{i\lambda x}\phi_3^{\mathrm{ad}}(x,k)$ and $e^{-i\lambda x}\psi_1^{\mathrm{ad}}(x,k)$ are analytic in the upper sheet of the Riemann surface, $e^{-i\lambda x}\phi_1^{\mathrm{ad}}(x,k)$ and $e^{i\lambda x}\psi_3^{\mathrm{ad}}(x,k)$ are analytic on the lower sheet and $e^{ikx}\phi_2^{\mathrm{ad}}(x,k)$ and $e^{ikx}\psi_2^{\mathrm{ad}}(x,k)$ on neither sheet. Analogues of Eqs. (2.15) also exist,

$$\Phi^{\mathrm{ad}}(x,k) = \Psi^{\mathrm{ad}}(x,k)\tilde{\mathbf{B}}^T(k), \quad \Psi^{\mathrm{ad}}(x,k) = \Phi^{\mathrm{ad}}(x,k)\tilde{\mathbf{A}}^T(k), \tag{2.20}$$

where $\Phi^{\mathrm{ad}}(x,k) = (\phi_1^{\mathrm{ad}}, \phi_2^{\mathrm{ad}}, \phi_3^{\mathrm{ad}})$ and $\Psi^{\mathrm{ad}}(x,k) = (\psi_1^{\mathrm{ad}}, \psi_2^{\mathrm{ad}}, \psi_3^{\mathrm{ad}})$, and where $\tilde{\mathbf{A}}(k) = (\tilde{a}_{ij})$ and $\tilde{\mathbf{B}}(k) = (\tilde{b}_{ij}) = \tilde{\mathbf{A}}^{-1}(k)$ are the adjoint scattering matrices.

From these adjoint states, we can now use Eqs. (2.19) to define via (2.18) two new solutions of the original scattering problem (2.1a), namely,

$$\bar{\chi}(x,k) = -e^{ikx}\mathbf{J}(\phi_1^{\mathrm{ad}}(x,k) \wedge \psi_3^{\mathrm{ad}}(x,k)), \tag{2.21a}$$

$$\chi(x,k) = -e^{ikx}\mathbf{J}(\phi_3^{\mathrm{ad}}(x,k) \wedge \psi_1^{\mathrm{ad}}(x,k)). \tag{2.21b}$$

By construction, $\bar{\chi}(x,k)e^{-ikx}$ is analytic in the lower sheet [where $\phi_1^{\mathrm{ad}}(x,k)e^{-i\lambda x}$ and $\psi_3^{\mathrm{ad}}(x,k)e^{i\lambda x}$ are], and $\chi(x,k)e^{-ikx}$ is analytic in the upper sheet [where $\phi_3^{\mathrm{ad}}(x,k)e^{i\lambda x}$ and $\psi_1^{\mathrm{ad}}(x,k)e^{-i\lambda x}$ are]. Moreover, by comparing the asymptotic behavior as $x \to \pm\infty$ of eigenfunctions and adjoint eigenfunctions, one can check that, for all cyclic indices j,l,m,

$$\phi_j(x,k) = -e^{ikx}\mathbf{J}(\phi_l^{\mathrm{ad}}(x,k) \wedge \phi_m^{\mathrm{ad}}(x,k))/\Gamma_j(k), \tag{2.22a}$$

$$\psi_j(x,k) = -e^{ikx}\mathbf{J}(\psi_l^{\mathrm{ad}}(x,k) \wedge \psi_m^{\mathrm{ad}}(x,k))/\Gamma_j(k), \tag{2.22b}$$

and reciprocally

$$\phi_j^{\mathrm{ad}}(x,k) = -e^{-ikx}\mathbf{J}(\phi_l(x,k) \wedge \phi_m(x,k))/\Gamma_j(k), \tag{2.22c}$$

$$\psi_j^{\mathrm{ad}}(x,k) = -e^{-ikx}\mathbf{J}(\psi_l(x,k)\wedge\psi_m(x,k))/\Gamma_j(k), \tag{2.22d}$$

where

$$\Gamma_1(k)=\lambda-k, \quad \Gamma_2(k)=2\lambda, \quad \Gamma_3(k)=\lambda+k. \tag{2.23}$$

From Eqs. (2.22) and (2.15), (2.20) it then follows that

$$\widetilde{\mathbf{A}}^T(k)=\Gamma(k)\mathbf{A}(k)\Gamma^{-1}(k), \quad \widetilde{\mathbf{B}}^T(k)=\Gamma(k)\mathbf{B}(k)\Gamma^{-1}(k), \tag{2.24}$$

where $\Gamma(k)=\mathrm{diag}(\Gamma_1(k),\Gamma_2(k),\Gamma_3(k))$. Substituting the first of Eq. (2.20) into Eq. (2.21) and using (2.22b) yields

$$\chi(x,k)=2\lambda[b_{33}(k)\psi_2(x,k)-b_{23}(k)\psi_3(x,k)], \tag{2.25a}$$

$$\bar{\chi}(x,k)=2\lambda[b_{21}(k)\psi_1(x,k)-b_{11}(k)\psi_2(x,k)]. \tag{2.25b}$$

Each of these two relations provides a decomposition of the nonanalytic eigenfunction $\psi_2(x,k)$,

$$\psi_2(x,k)=\frac{b_{21}(k)}{b_{11}(k)}\psi_1(x,k)-\frac{1}{2\lambda}\frac{\bar{\chi}(x,k)}{b_{11}(k)}=\frac{b_{23}(k)}{b_{33}(k)}\psi_3(x,k)+\frac{1}{2\lambda}\frac{\chi(x,k)}{b_{33}(k)}. \tag{2.26}$$

Similar relations hold for the eigenfunction $\phi_2(x,k)$, where now the scattering coefficients $a_{ij}(k)$ are involved. Precisely, one finds

$$\bar{\chi}(x,k)=2\lambda[a_{23}(k)\phi_3(x,k)-a_{33}(k)\phi_2(x,k)], \tag{2.27a}$$

$$\chi(x,k)=2\lambda[a_{11}(k)\phi_2(x,k)-a_{21}(k)\phi_1(x,k)] \tag{2.27b}$$

and consequently one obtains similar representations for $\phi_2(x,k)$:

$$\phi_2(x,k)=\frac{a_{23}(k)}{a_{33}(k)}\phi_3(x,k)-\frac{1}{2\lambda}\frac{\bar{\chi}(x,k)}{a_{33}(k)}=\frac{a_{21}(k)}{a_{11}(k)}\phi_1(x,k)+\frac{1}{2\lambda}\frac{\chi(x,k)}{a_{11}(k)}. \tag{2.28}$$

These expressions will be key to define the inverse scattering problem in Sec. III.

C. Symmetries

Importantly, the scattering problem admits two symmetries, which relate the value of the eigenfunctions on different sheets of the Riemann surface. These symmetries translate into compatibility conditions (constraints) on the scattering data, and will play a fundamental role in the formulation of the inverse problem.

First symmetry $(k,\lambda)\to(k^*,\lambda^*)$*:* When the potential satisfies the symmetry condition $\mathbf{r}=\mathbf{q}^*$, one has $\mathbf{Q}^H=\mathbf{Q}$, and therefore from Eq. (2.17) it follows that

$$\frac{\partial}{\partial x}[v^{\mathrm{ad}}(k^*)]^*=(ik\mathbf{J}+\mathbf{Q}^H)(v^{\mathrm{ad}}(k^*))^*=(ik\mathbf{J}+\mathbf{Q})(v^{\mathrm{ad}}(k^*))^*.$$

Hence, taking into account the boundary conditions (2.4) and (2.19), we have

$$\phi_j^{\mathrm{ad}}(k,\lambda)=(\phi_j(k^*,\lambda^*))^*, \quad \psi_j^{\mathrm{ad}}(k,\lambda)=(\psi_j(k^*,\lambda^*))^*, \quad j=1,2,3 \tag{2.29}$$

and, as a consequence of Eqs. (2.24), (2.15), and (2.20)

$$\Gamma(k,\lambda)\mathbf{B}(k,\lambda)\Gamma^{-1}(k,\lambda)=\mathbf{A}^H(k^*,\lambda^*), \tag{2.30}$$

where $\Gamma(k,\lambda)=\mathrm{diag}(\Gamma_1,\Gamma_2,\Gamma_3)$ as before. In particular, Eqs. (2.30) give

$$b_{11}(k,\lambda) = a_{11}^{*}(k^{*},\lambda^{*}), \quad b_{33}(k,\lambda) = a_{33}^{*}(k^{*},\lambda^{*}) \tag{2.31}$$

showing that $a_{11}(k,\lambda)$ [respectively, $b_{33}(k,\lambda)$] has a zero on the upper sheet of the Riemann surface at a point $(k_n,\lambda(k_n))$ if and only if $b_{11}(k,\lambda)$ [respectively, $a_{33}(k,\lambda)$] has a zero at the conjugate point $(k_n^{*},\lambda^{*}(k_n^{*}))$ on the lower sheet.

Second symmetry $(k,\lambda)\to(k,-\lambda)$*:* This involution relates the values of the eigenfunctions on the two sheets, and in particular across the cuts, for arbitrary fixed k on either sheet and $\lambda\to-\lambda$. Indeed, the scattering problem is clearly invariant with respect to the exchange $(k,\lambda)\to(k,-\lambda)$, and by looking at the boundary conditions (2.4) and (2.5) one can check that

$$\psi_1(x,k,-\lambda) = -\psi_3(x,k,\lambda), \quad \phi_1(x,k,-\lambda) = -\phi_3(x,k,\lambda) \tag{2.32a}$$

while ψ_2 and ϕ_2 are invariant with the respect to the symmetry $\lambda\leftrightarrow-\lambda$, i.e.,

$$\psi_2(x,k,-\lambda) = \psi_2(x,k,\lambda), \quad \phi_2(x,k,-\lambda) = \phi_2(x,k,\lambda). \tag{2.32b}$$

Therefore, from the equations (2.15a) defining the scattering coefficients one has

$$a_{11}(k,-\lambda) = a_{33}(k,\lambda), \quad a_{22}(k,-\lambda) = a_{22}(k,\lambda), \tag{2.33a}$$

$$a_{12}(k,-\lambda) = -a_{32}(k,\lambda), \quad a_{13}(k,-\lambda) = a_{31}(k,\lambda), \quad a_{21}(k,-\lambda) = -a_{23}(k,\lambda). \tag{2.33b}$$

The same symmetry relations hold for the coefficients $b_{ij}(k)$, i.e.,

$$b_{11}(k,-\lambda) = b_{33}(k,\lambda), \quad b_{12}(k,-\lambda) = -b_{32}(k,\lambda), \quad b_{13}(k,-\lambda) = b_{31}(k,\lambda) \tag{2.34a}$$

$$b_{22}(k,-\lambda) = b_{22}(k,\lambda), \quad b_{21}(k,-\lambda) = -b_{23}(k,\lambda). \tag{2.34b}$$

Note that Eq. (2.33a) implies that $(k_n,\lambda(k_n))$ is a zero of $a_{11}(k,\lambda)$ in the upper sheet if and only if $(k_n,-\lambda(k_n))$ is a zero for $a_{33}(k,\lambda)$ in the lower sheet, and the same for $b_{11}(k,\lambda)$ and $b_{33}(k,\lambda)$. Finally, note that, taking into account Eqs. (2.32) and (2.34), comparing Eqs. (2.25a) and (2.25b) yields

$$\chi(x,k,\lambda) = \bar{\chi}(x,k,-\lambda). \tag{2.35}$$

D. Uniformization coordinate

In a similar way as for the scalar problem (e.g., see Ref. 11), we can introduce a uniformization variable z (global uniformizing parameter) defined by the conformal mapping

$$z = k + \lambda(k). \tag{2.36a}$$

The inverse mapping is given by

$$k = \tfrac{1}{2}(z + \hat{z}^{*}), \quad \lambda = z - k = \tfrac{1}{2}(z - \hat{z}^{*}), \tag{2.36b}$$

where we have introduced the shorthand notation

$$\hat{z} = q_0^2/z^{*}, \tag{2.36c}$$

which we will use throughout the rest of this work. (Note $\lambda-k=-\hat{z}^{*}$, which will also be useful later on.) With regard to the mapping $(k,\lambda)\to z$, it should be observed that (cf. Fig. 2(a),(c)):

(i) The branch cuts on the two sheets of the Riemann surface are mapped onto the real z-axis.
(ii) The two sheets $\mathbb{C}_1$ and $\mathbb{C}_2$ of the Riemann surface are, respectively, mapped onto the upper and lower half-planes of the complex z-plane.
(iii) A neighborhood of $k=\infty$ on either sheet is mapped onto a neighborhood of $z=\infty$ or $z=0$ depending on the sign of k_{im} (cf. Sec. II E).

(iv) The symmetry $k-i0\to k+i0$ on the contours (giving the discontinuity of eigenfunctions and scattering data on the banks of the cut) transforms into $z\to\hat{z}^*=q_0^2/z$ on the real z-axis.

According to the discussion in Secs. I A and I B, the eigenfunctions $\phi_1(x,z)e^{i\lambda(z)x}$, $\psi_3(x,z)e^{-i\lambda(z)x}$ and $\chi(x,z)e^{-ik(z)x}$ are analytic in the upper half-plane of z, while $\phi_3(x,z)e^{-i\lambda(z)x}$, $\psi_1(x,z)e^{i\lambda(z)x}$ and $\bar{\chi}(x,z)e^{-ik(z)x}$ are analytic in the lower half-plane. Similarly, the scattering coefficients $a_{11}(z)$ and $b_{33}(z)$ are analytic in the upper half-plane of z, while $a_{33}(z)$ and $b_{11}(z)$ are analytic in the lower half-plane.

It should be noted that although the uniformization coordinate will be important in the inverse problem, it is not essential in our formulation of the direct problem. We introduce it here because it turns out to be convenient when discussing the location of the discrete eigenvalues, which is done in Sec. II F.

In terms of the global parameter z, the first symmetry becomes $z\to z^*$. Under this transformation, the symmetry relations (2.29) and (2.30) are then, respectively, written as

$$\phi_j^{\mathrm{ad}}(x,z)=(\phi_j(x,z^*))^*,\quad \psi_j^{\mathrm{ad}}(x,z)=(\psi_j(x,z^*))^*,\quad j=1,2,3, \tag{2.37}$$

$$b_{\ell j}^*(z^*)=\Gamma_j(z)a_{j\ell}(z)\Gamma_\ell^{-1}(z),\quad \ell,j=1,2,3, \tag{2.38}$$

where

$$\Gamma_1(z)=-\hat{z}^*,\quad \Gamma_2(z)=2\lambda(z),\quad \Gamma_3(z)=z. \tag{2.39}$$

Equation (2.38) can also be written compactly as

$$\Gamma(z)\mathbf{B}(z)\Gamma^{-1}(z)=\mathbf{A}^H(z^*), \tag{2.40}$$

where $\Gamma(z)=\mathrm{diag}(\Gamma_1,\Gamma_2,\Gamma_3)$ as before. Taking into account Eq. (2.22), the symmetries (2.37) can be written in terms of eigenfunctions as follows:

$$\phi_j^*(x,z^*)=-e^{-ik(z)x}\mathbf{J}(\phi_l(x,z)\wedge\phi_m(x,z))/\Gamma_j(z) \tag{2.41a}$$

and

$$\psi_j^*(x,z^*)=-e^{-ik(z)x}\mathbf{J}(\psi_l(x,z)\wedge\psi_m(x,z))/\Gamma_j(z) \tag{2.41b}$$

where j,l,m are cyclic indices.

The second symmetry relates values of eigenfunctions and scattering coefficients at points (k,λ) and $(k,-\lambda)$ on the two sheets or at the cuts. In terms of the uniformization variable z, the transformation then becomes $z\to\hat{z}^*=q_0^2/z$. Hence the symmetry relations (2.33) can be written as

$$a_{11}(\hat{z}^*)=a_{33}(z),\quad a_{12}(\hat{z}^*)=-a_{32}(z), \tag{2.42a}$$

$$a_{13}(\hat{z}^*)=a_{31}(z),\quad a_{21}(\hat{z}^*)=-a_{23}(z), \tag{2.42b}$$

and the same relations hold for the coefficients $b_{ij}(z)$. Also note that the symmetry relations (2.32) between the auxiliary eigenfunctions can be written as

$$\phi_1(x,z)=-\phi_3(x,\hat{z}^*),\quad \psi_1(x,z)=-\psi_3(x,\hat{z}^*), \tag{2.43a}$$

$$\chi(x,z)=\bar{\chi}(x,\hat{z}^*). \tag{2.43b}$$

Taking into account Eq. (2.30) and recalling that $\mathbf{B}(z)=\mathbf{A}^{-1}(z)$ and that both matrices have unit determinant, on either side of the real z-axis we find

$$|a_{11}(z)|^2 + |a_{12}(z)|^2 \frac{\Gamma_1(z)}{\Gamma_2(z)} + |a_{13}(z)|^2 \frac{\Gamma_1(z)}{\Gamma_3(z)} = 1,$$

where $z \in \mathbb{R}$. Combining this with Eq. (2.39) we then obtain

$$|a_{11}(z)|^2 = 1 + \frac{q_0^2}{z^2}|a_{13}(z)|^2 + \frac{q_0^2}{z^2 - q_0^2}|a_{12}(z)|^2 \quad \forall\, z \in \mathbb{R}. \tag{2.44}$$

The second term on the right-hand side is non-negative; the last term, however, can be either positive or negative and therefore one cannot *a priori* exclude real zeros of $a_{11}(z)$ if $z \in (-q_0, q_0)$. Similar results follow for zeros of $a_{33}(z)$, $b_{11}(z)$, and $b_{33}(z)$, taking into account the symmetry relations (2.38) and (2.42).

Note that both symmetry transformations relate values in the upper half z-plane to values in the lower half z-plane, since both z^* and $\hat{z}^*$ are in the opposite half-plane as z. In the following we will assume that the scattering coefficients $a_{11}(z)$, etc., have no zeros on the real z-axis.

E. Asymptotic behavior of eigenfunctions and scattering data

In order to determine the asymptotic behavior of the eigenfunctions for large values of the scattering parameter k, we first note the following: in the upper sheet of the Riemann surface (i.e., when $\lambda_{\text{im}} \geqslant 0$), one has, above the cut (i.e., when $k_{\text{im}} > 0$)

$$\lambda + k \sim 2k + O(1), \quad \lambda - k \sim -\frac{q_0^2}{2k} + o(1/k) \quad \text{as } |k| \to \infty, \tag{2.45a}$$

and below the cut (i.e., when $k_{\text{im}} < 0$)

$$\lambda + k \sim \frac{q_0^2}{2k} + o(1/k), \quad \lambda - k \sim -2k + O(1) \quad \text{as } |k| \to \infty. \tag{2.45b}$$

Similar relations hold in the lower sheet of the Riemann surface (i.e., when $\lambda_{\text{im}} \leqslant 0$). Using these relations we can obtain the large-k expansion of the eigenfunctions on each sheet. It is more convenient however to express this behavior in terms of the uniformization variable z, which will be used in the inverse problem. To this aim, we note that (cf. Fig. 2)

(i) $|k| \to \infty$ in the upper-half-plane of sheet I corresponds to $z \to \infty$ in the upper-half z-plane,
(ii) $|k| \to \infty$ in the lower-half-plane of sheet II corresponds to $z \to \infty$ in the lower-half z-plane,
(iii) $|k| \to \infty$ in the lower-half-plane of sheet I corresponds to $z \to 0$ in the upper-half z-plane,
(iv) $|k| \to \infty$ in the upper-half-plane of sheet II corresponds to $z \to 0$ in the lower-half z-plane.

It should be noted here that there is no conceptual distinction between the points $z=0$ and $z=\infty$ in the z-plane, and one can change one into the other by simply defining $z=k-\lambda$ instead of $z=k+\lambda$.

Taking Eqs. (2.45) into account and using both the integral equations (2.8) and the WKB expansions of the eigenfunctions (see the Appendix) we obtain that as $z \to \infty$ in the upper-half z-plane one has

$$\phi_1(x,z)e^{i\lambda x} \sim \begin{pmatrix} z \\ i\mathbf{r}(x) \end{pmatrix}, \quad \psi_3(x,z)e^{-i\lambda x} \sim -\begin{pmatrix} \mathbf{q}^T(x)\mathbf{r}_+/z \\ i\mathbf{r}_+ \end{pmatrix}, \tag{2.46a}$$

while as $z \to 0$ in the upper-half z-plane one has

$$\phi_1(x,z)e^{i\lambda x} \sim \begin{pmatrix} \mathbf{q}^T(x)\mathbf{r}_-/\hat{z}^* \\ i\mathbf{r}_- \end{pmatrix}, \quad \psi_3(x,z)e^{-i\lambda x} \sim -\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}(x) \end{pmatrix}. \tag{2.46b}$$

Similarly, as $z \to 0$ in the lower-half z-plane one has

$$\phi_3(x,z)e^{-i\lambda x} \sim -\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}(x) \end{pmatrix}, \quad \psi_1(x,z)e^{i\lambda x} \sim \begin{pmatrix} \mathbf{q}^T(x)\mathbf{r}_+/\hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix}, \tag{2.46c}$$

while as $z \to \infty$ in the lower-half z-plane one has

$$\phi_3(x,z)e^{-i\lambda x} \sim -\begin{pmatrix} \mathbf{q}^T(x)\mathbf{r}_-/z \\ i\mathbf{r}_- \end{pmatrix}, \quad \psi_1(x,z)e^{i\lambda x} \sim \begin{pmatrix} z \\ i\mathbf{r}(x) \end{pmatrix}. \tag{2.46d}$$

Asymptotic expansions for the adjoint eigenfunctions can also be obtained. Then, using the asymptotics of $\phi_j^{\mathrm{ad}}(x,z)$ and $\psi_j^{\mathrm{ad}}(x,z)$ as well as Eqs. (2.21), one can obtain the asymptotic expansions for the auxiliary eigenfunctions $\bar{\chi}(x,z)$ and $\chi(x,z)$. Explicitly, in the upper-half z-plane one has

$$\chi(x,z)e^{-ikx} \sim -\begin{pmatrix} \mathbf{q}^T(x)\mathbf{q}_-^\perp \\ i\mathbf{q}_-^\perp z \end{pmatrix} \quad \text{as } z \to \infty, \tag{2.47a}$$

$$\chi(x,z)e^{-ikx} \sim \begin{pmatrix} \mathbf{q}^T(x)\mathbf{q}_+^\perp \\ i\mathbf{q}_+^\perp \hat{z}^* \end{pmatrix} \quad \text{as } z \to 0, \tag{2.47b}$$

whereas in the lower-half z-plane

$$\bar{\chi}(x,z)e^{-ikx} \sim -\begin{pmatrix} \mathbf{q}^T(x)\mathbf{q}_- \\ i\mathbf{q}_-^\perp \hat{z}^* \end{pmatrix} \quad \text{as } z \to 0, \tag{2.47c}$$

$$\bar{\chi}(x,z)e^{-ikx} \sim \begin{pmatrix} \mathbf{q}^T(x)\mathbf{q}_+^\perp \\ i\mathbf{q}_+^\perp z \end{pmatrix} \quad \text{as } z \to \infty. \tag{2.47d}$$

Equations (2.16) and (2.46) also allow us to obtain the asymptotic behavior of the scattering coefficients. For example, in the upper-half z-plane, as $z \to \infty$ one has

$$a_{11}(z) \sim 1, \quad b_{33}(z) \sim \mathbf{q}_-^T\mathbf{r}_+/q_0^2, \tag{2.48a}$$

while as $z \to 0$ one has

$$a_{11}(z) \sim \mathbf{q}_+^T\mathbf{r}_-/q_0^2, \quad b_{33}(z) \sim 1. \tag{2.48b}$$

Similar expressions hold for $b_{11}(z)$ and $a_{33}(z)$ in the lower-half z-plane: namely, as $z \to 0$ one has

$$a_{33}(z) \sim 1, \quad b_{11}(z) \sim \mathbf{q}_-^T\mathbf{r}_+/q_0^2 \tag{2.48c}$$

while as $z \to \infty$ one has

$$a_{33}(z) \sim \mathbf{q}_+^T\mathbf{r}_-/q_0^2, \quad b_{11}(z) \sim 1. \tag{2.48d}$$

Note that $\mathbf{q}_+^T\mathbf{r}_- = (\mathbf{q}_-^T\mathbf{r}_+)^* = e^{i\Delta\theta^{(1)}}|q_0^{(1)}|^2 + e^{i\Delta\theta^{(2)}}|q_0^{(2)}|^2$, where we have introduced the asymptotic phase differences for the potentials, $\Delta\theta^{(1)} = \theta_+^{(1)} - \theta_-^{(1)}$ and $\Delta\theta^{(2)} = \theta_+^{(2)} - \theta_-^{(2)}$ (cf. Eq. (2.3)). Hereafter, we will assume that these asymptotic phase differences are the same in both components, namely

$$\Delta\theta^{(1)} = \Delta\theta^{(2)} =: \Delta\theta. \tag{2.49}$$

If Eqs. (2.49) are satisfied, then

$$\mathbf{q}_+^T\mathbf{r}_- = (\mathbf{q}_-^T\mathbf{q}_+)^* = e^{i\Delta\theta}q_0^2, \tag{2.50}$$

and the asymptotic behaviors of the scattering coefficients in Eqs. (2.48) simplify correspondingly.

F. Discrete eigenvalues and bound states

Recall that in the 2×2 scattering problem for the nondecaying scalar NLS equation there is a one-to-one correspondence between poles of the transmission coefficients [here, zeros of $a_{11}(z)$ etc] and eigenvalues, which, in turn, are related to bound states. Hence, the unitarity relation [i.e., the analog of Eq. (2.44)], together with the self-adjointness of the scattering problem, ensure that the transmission coefficients can only have poles at $k=k_n\in(-q_0,q_0)$, i.e., for $z=z_n$ on the circle C_0 of radius q_0 centered at the origin (e.g., see Ref. 11). As we will see in the following, in the case of vector NLS equation with nondecaying boundary conditions, the decay properties of the eigenfunctions at a pole of the transmission coefficients are not sufficient to give a bound state.

Importantly, when $\mathbf{r}=\mathbf{q}^*$ any solution $v(x,k)$ of the scattering problem (2.1a) satisfies the relation

$$-i(k-k^*)\|v(x,k)\|^2=\frac{\partial}{\partial x}[|v^{(1)}(x,k)|^2-|v^{(2)}(x,k)|^2-|v^{(3)}(x,k)|^2]. \tag{2.51}$$

Equation (2.51) shows that in order for $k=k_n$ to be an eigenvalue corresponding to a square integrable eigenfunction, k_n must be real (i.e., $k_n=k_n^*$). For $k_n\in\mathbb{R}$ with $|k_n|<q_0$ (i.e., for $z\in C_0$) one has $\lambda(k_n)=\pm i\sqrt{q_0^2-k_n^2}$ (with the upper/lower sign on sheet I/II of the Riemann surface, respectively). Correspondingly, $\phi_1(x,k_n,\lambda(k_n))$ and $\phi_3(x,k_n,\lambda(k_n))$ are exponentially decaying as $x\to-\infty$ while $\psi_1(x,k_n,\lambda(k_n))$ and $\psi_3(x,k_n,\lambda(k_n))$ are exponentially decaying as $x\to+\infty$. As we will see in Sec. II F 1, poles of the transmission coefficient at these points then give rise to bound states. It should be noted that, unlike the scalar case, the unitarity conditions [e.g., see Eq. (2.44)] are not enough to exclude poles of the transmission coefficients for $k\in\mathbb{R}$ with $|k|>q_0$ (i.e., for real values of z). In these cases, however, all eigenfunctions are oscillating as $x\to\pm\infty$. Hence, the only eigenvalues $k=k_n$ corresponding to square integrable eigenfunctions lie in the segment $(-q_0,q_0)$. In terms of the uniformization variable z, this means that *any* eigenfunctions belonging to $L_2(\mathbb{R})$ correspond to discrete eigenvalues on the circle C_0 of radius q_0. Therefore, if the scattering coefficients $a_{11}(z)$, etc., have a zero off the circle C_0, then the corresponding eigenfunctions cannot form a bound state, that is, either they are not decaying rapidly enough at both space infinities, or they are singular, which prevents the eigenfunction from being $L_2(\mathbb{R})$. We will see that both situations can in principle occur, the first case corresponding to zeros z_n of $a_{11}(z)$ inside the circle, while the second case to zeros outside the circle.

In order to locate discrete eigenvalues as it will apply to the inverse problem, it is convenient to introduce the 3×3 matrices

$$E_+(x,z)=(\phi_1,\chi,\psi_3),\quad E_-(x,z)=(\psi_1,\bar{\chi},\phi_3).$$

With this notation, $E_+(x,z)$ collects three eigenfunctions which are analytic in the upper-half z-plane, and $E_-(x,z)$ three eigenfunctions analytic in the lower-half-plane. Then we note that Eqs. (2.6), (2.25), and (2.27) together imply

$$\det(E_+(x,z))=\mathrm{Wr}(\phi_1(x,z),\chi(x,z),\psi_3(x,z))=-4q_0^2\lambda^2(z)a_{11}(z)b_{33}(z)e^{ik(z)x}, \tag{2.52a}$$

$$\det(E_-(x,z))=\mathrm{Wr}(\psi_1(x,z),\bar{\chi}(x,z),\phi_3(x,z))=4q_0^2\lambda^2(z)a_{33}(z)b_{11}(z)e^{ik(z)x}. \tag{2.52b}$$

Equation (2.52a) shows that the Wronskian vanishes (i.e., the three solutions which comprise E_+ become linearly dependent) at the zeros of $a_{11}(z)$ and $b_{33}(z)$. Due to the symmetries (2.38) and (2.42) among the scattering coefficients, however, we have

$$a_{11}(z_n)=0\Leftrightarrow b_{11}(z_n^*)=0\Leftrightarrow b_{33}(\hat{z}_n)=0\Leftrightarrow a_{33}(\hat{z}_n^*)=0 \tag{2.53}$$

[where as before we used the notation (2.36c), i.e., $\hat{z}=q_0^2/z^*$]. If the zero z_n of $a_{11}(z)$ is on the circle C_0 of radius q_0, then $\hat{z}_n\equiv z_n$, and therefore $a_{11}(z)$ and $b_{33}(z)$ vanish at the same point. Hence, the Wronskian (2.52a) will have a double zero at $z=z_n$ in this case. However, if $a_{11}(z)$ admits a simple zero at a point $z=z_n$ off the circle C_0 (i.e., $|z_n|\neq q_0$ and $\mathrm{Im}\,z_n>0$), then such zeros appear in

quartets (cf. Fig. 3), and the Wronskian (2.52a) will have a simple zero both at z_n and at $\hat{z}_n = q_0^2/z_n^*$ in the upper-half-plane. Similarly, with regard to Eq. (2.52b), $a_{33}(z)$ and $b_{11}(z)$ can either both vanish at the conjugate points $z_n^* \equiv \hat{z}_n^*$, on the lower-half circle, or vanish individually at two different points in the lower-half-plane ($\hat{z}_n^*$ and $z_n^* = q_0^2/z_n$, respectively). Hereafter we will use ζ_n to denote zeros of $a_{11}(z)$ *on the circle* C_0, and we will reserve the notation z_n for the zeros of $a_{11}(z)$ *off the circle* C_0.

1. Zeros on the circle

Let us first consider the case of zeros on the circle of radius q_0 and assume that $a_{11}(z)$ and $b_{33}(z)$ both have a simple zero at the point $z=\zeta_n=k_n+i\nu_n$, with $|k_n|<q_0$ and $\nu_n=\sqrt{q_0^2-k_n^2}>0$. As we noted earlier, in this case the Wronskians (2.52a) and (2.52b) each have a double zero, respectively, at $z=\zeta_n$ and at $z=\zeta_n^*$. In principle there are two possibilities: either $\chi(x,\zeta_n)=0$ or $\chi(x,\zeta_n)\neq 0$. If $\chi(x,\zeta_n)=0$, then also $\bar{\chi}(x,\zeta_n^*)=0$, due to the symmetry (2.43b) (since in this case $\zeta_n^* = q_0^2/\zeta_n$). If $\chi(x,\zeta_n)\neq 0$ instead, one also has $\bar{\chi}(x,\zeta_n^*)\neq 0$. In the following we show that in fact it is always the case that $\chi(x,\zeta_n)=\chi(x,\zeta_n^*)=0$.

Indeed, let ζ_n be a zero of $a_{11}(z)$ and $b_{33}(z)$ on the circle of radius q_0. Then, according to Eq. (2.21b), $\chi(x,\zeta_n)=0$ if and only if $\phi_3^{\mathrm{ad}}(x,\zeta_n)\wedge\psi_1^{\mathrm{ad}}(x,\zeta_n)=0$. Since $\phi_3^{\mathrm{ad}}(x,z)$ and $\psi_1^{\mathrm{ad}}(x,z)$ are eigenfunctions whose asymptotic behavior is fixed, they cannot vanish identically for all x. Hence for $\chi(x,\zeta_n)$ to be zero $\phi_3^{\mathrm{ad}}(x,\zeta_n)$ and $\psi_1^{\mathrm{ad}}(x,\zeta_n)$ must be proportional to each other. Then, due to the symmetry (2.29), it follows that $\phi_3(x,\zeta_n^*)\propto\psi_1(x,\zeta_n^*)$. Moreover, Eq. (2.43b) implies that $\chi(x,\zeta_n)=\bar{\chi}(x,\zeta_n^*)$, and therefore [recalling the definition (2.21a)] we conclude that

$$\chi(x,\zeta_n)=\bar{\chi}(x,\zeta_n^*)=0 \quad \text{iff } \phi_3(x,\zeta_n^*)\propto\psi_1(x,\zeta_n^*) \text{ and } \phi_1(x,\zeta_n)\propto\psi_3(x,\zeta_n). \tag{2.54}$$

Suppose now that $\chi(x,\zeta_n)\neq 0$ [and hence also $\bar{\chi}(x,\zeta_n^*)\neq 0$]. If Eqs. (2.25a) and (2.27b) can be continued off the real z-axis, then it follows that

$$\chi(x,\zeta_n)\propto\psi_3(x,\zeta_n), \quad \chi(x,\zeta_n)\propto\phi_1(x,\zeta_n)$$

[with nonzero proportionality coefficients because by assumption $\chi(x,\zeta_n)\neq 0$]. If this is the case, then $\phi_1(x,\zeta_n)\propto\psi_3(x,\zeta_n)$, and [due to the symmetry (2.29)] one also has $\phi_1^{\mathrm{ad}}(x,\zeta_n^*)\propto\psi_3^{\mathrm{ad}}(x,\zeta_n^*)$. But then it follows that $\bar{\chi}(x,\zeta_n^*)=0$, which contradicts the hypothesis. In conclusion, if ζ_n and ζ_n^* are a pair of zeros on the circle, then $\chi(x,\zeta_n)=\bar{\chi}(x,\zeta_n^*)=0$, Eq. (2.54) holds and one can write

$$\phi_1(x,\zeta_n)=b_n^{(1)}\psi_3(x,\zeta_n), \tag{2.55a}$$

$$\phi_3(x,\zeta_n^*)=\bar{b}_n^{(1)}\psi_1(x,\zeta_n^*), \tag{2.55b}$$

corresponding to a bound state. Note that due to the symmetry (2.32a) between the eigenfunctions, from Eqs. (2.55) it follows that

$$\bar{b}_n^{(1)}=b_n^{(1)}. \tag{2.56}$$

Since $\chi(x,\zeta_n)=\bar{\chi}(x,\zeta_n^*)=0$ for all zeros ζ_n of $a_{11}(z)$ and ζ_n^* of $a_{33}(z)$ on the circle of radius q_0, it is then natural in this case to rescale the Wronskians in Eq. (2.52a) as

$$\mathrm{Wr}\left(\phi_1(x,z),\frac{\chi(x,z)}{2\lambda(z)b_{33}(z)},\psi_3(x,z)\right)=-2q_0^2\lambda(z)a_{11}(z)e^{ik(z)x}, \tag{2.57a}$$

$$\mathrm{Wr}\left(\psi_1(x,z),\frac{\bar{\chi}(x,z)}{2\lambda(z)b_{11}(z)},\phi_3(x,z)\right)=2q_0^2\lambda(z)a_{33}(z)e^{ik(z)x}. \tag{2.57b}$$

The rescaled Wronskians will then have simple zeros at ζ_n and ζ_n^*.

2. Zeros off the circle

Suppose that $a_{11}(z)$, which is analytic in the upper-half z-plane, has a simple zero at a point $z=z_n=k_n+i\nu_n$, with $\nu_n>0$ and $|z_n|\neq q_0$. First of all, note that, according to (2.36b),

$$k(z_n)=\tfrac{1}{2}[k_n(1+|\hat{z}_n|^2/q_0^2)+i\nu_n(1-|\hat{z}_n|^2/q_0^2)],$$

$$\lambda(z_n)=\tfrac{1}{2}[k_n(1-|\hat{z}_n|^2/q_0^2)+i\nu_n(1+|\hat{z}_n|^2/q_0^2)].$$

Thus, the behavior of $e^{ik(z_n)x}$ at large x depends on whether $|z_n|\lessgtr q_0$ (recall that $\hat{z}=q_0^2/z^*$; hence, one has $|\hat{z}_n|\lessgtr q_0$ for $|z_n|\gtrless q_0$), and it will be exponentially decaying at one space infinity and exponentially growing at the other one. On the other hand, $\phi_1(x,z_n)\sim e^{-i\lambda(z_n)x}$ will be decaying as $x\to-\infty$ and $\psi_3(x,z_n)\sim e^{i\lambda(z_n)x}$ will be decaying as $x\to+\infty$ irrespective of whether z_n is inside or outside the circle.

If the zero z_n of $a_{11}(z)$ is off the circle C_0, then $b_{33}(z)$ will have a zero at point $\hat{z}_n=q_0^2/z_n^*\neq z_n$, but $b_{33}(z_n)\neq 0$ *in general*. Then from Eq. (2.52a) it follows that z_n is a simple zero of the Wronskian. In this case we assume that $\chi(x,z_n)$ does not vanish. Then from Eq. (2.25a) we deduce that

$$\chi(x,z_n)\sim -2i\lambda(z_n)b_{33}(z_n)\begin{pmatrix}0\\ \mathbf{q}_+^{\perp}\end{pmatrix}\exp\{\tfrac{1}{2}[ik_n(1+|z_n|^2/q_0^2)+\nu_n(1-|z_n|^2/q_0^2)]x\},\quad x\to+\infty, \tag{2.58}$$

where we note that the other contribution formally obtained from $b_{23}(z)\psi_3(x,z)$ in Eq. (2.25a) is exponentially small (and in any case, smaller than the contribution of the remaining term). On the other hand, from Eq. (2.27b) it follows that, at a zero z_n of $a_{11}(z)$, the eigenfunction $\chi(x,z_n)$ is proportional to $\phi_1(x,z_n)$:

$$\phi_1(x,z_n)=b_n^{(2)}\chi(x,z_n). \tag{2.59}$$

If $|z_n|>q_0$ (i.e., if the zero is *outside* the circle C_0), we would obtain a bound state, since the eigenfunctions $\chi(x,z_n)$ and $\phi_1(x,z_n)$ would be decaying at both space infinities. Therefore zeros of $a_{11}(z)$ outside the circle C_0 cannot occur for a smooth eigenfunction, since this would violate the eigenvalue relation (2.51). On the other hand, if $|z_n|<q_0$ (i.e., if the zero is *inside* C_0), the relation (2.59) still holds, but the eigenfunctions $\chi(x,z_n)$ and $\phi_1(x,z_n)$ will be exponentially growing as $x\to+\infty$, according to Eq. (2.58), and this does not contradict Eq. (2.51). Hence zeros z_n inside the circle C_0 are not forbidden.

Similarly, the Wronskian (2.52a) vanishes at the zero of $b_{33}(z)$ corresponding to z_n, that is [according to Eq. (2.53)], at the point $\hat{z}_n=q_0^2/z_n^*$. If z_n is inside the circle C_0 of radius q_0, then $\hat{z}_n$ will be outside the same circle, and *vice versa*. Also, in general $a_{11}(\hat{z}_n)\neq 0$, and consequently from Eq. (2.27b) it follows

$$\chi(x,\hat{z}_n)\sim -2i\lambda(\hat{z}_n)a_{11}(\hat{z}_n)\begin{pmatrix}0\\ \mathbf{q}_-^{\perp}\end{pmatrix}\exp\{\tfrac{1}{2}[ik_n(1+|z_n|^2/q_0^2)-\nu_n(1-|z_n|^2/q_0^2)]x\},\quad x\to-\infty. \tag{2.60}$$

From Eq. (2.25a), however, one deduces that $\chi(x,\hat{z}_n)$ is proportional to $\psi_3(x,\hat{z}_n)$,

$$\chi(x,\hat{z}_n)=\hat{b}_n^{(2)}\psi_3(x,\hat{z}_n). \tag{2.61}$$

Therefore, if $|z_n|>q_0$ (i.e., if $\hat{z}_n$ is *inside* C_0), this would be a bound state, since $\psi_3(x,\hat{z}_n)$ decays as $x\to+\infty$ and $\chi(x,\hat{z}_n)$ as $x\to-\infty$, according to Eq. (2.60). Hence, as before, this situation cannot occur for a smooth eigenfunction, in accordance with Eq. (2.51). On the other hand, if $|z_n|<q_0$ (i.e., if $\hat{z}_n$ is *outside* C_0), the eigenfunctions $\chi(x,z_n)$ and $\psi_3(x,z_n)$ are exponentially growing as $x\to+\infty$. Hence such situations do not contradict Eq. (2.51).

Finally, one has analogous results for the eigenfunctions in the lower-half-plane in correspondence to the points $z_n^*=k_n-i\nu_n$ [zeros of $b_{11}(z)$ off the circle C_0] and $\hat{z}_n^*=q_0^2/z_n$ [zeros of $a_{33}(z)$ off the circle C_0]. Specifically, at points z_n^*, where $b_{11}(z_n^*)=0$, one has

$$\bar{\chi}(x,z_n^*)=\bar{b}_n^{(2)}\psi_1(x,z_n^*). \tag{2.62}$$

Again, if $|z_n|>q_0$, this would correspond to a bound state. On the other hand, if $|z_n|<q_0$ the eigenfunctions in (2.62) will be growing as $x\to-\infty$. Also, at points $q_0^2/z_n\equiv\hat{z}_n^*$, where $a_{33}(\hat{z}_n^*)=0$, one has $\bar{\chi}(x,\hat{z}_n^*)$ proportional to $\phi_3(x,\hat{z}_n^*)$,

$$\phi_3(x,\hat{z}_n^*)=\check{b}_n^{(2)}\bar{\chi}(x,\hat{z}_n^*). \tag{2.63}$$

Summarizing, in the case of a pair of zeros z_n and $\hat{z}_n$ in the upper-half-plane such that $a_{11}(z_n)=0$ and $b_{33}(\hat{z}_n)=0$ (with z_n inside the circle C_0 of radius q_0 and $\hat{z}_n=q_0^2/z_n^*$ outside C_0), the eigenfunctions are related to each other as

$$\chi(x,\hat{z}_n)=\hat{b}_n^{(2)}\psi_3(x,\hat{z}_n), \tag{2.64a}$$

$$\phi_1(x,z_n)=b_n^{(2)}\chi(x,z_n)\equiv b_n^{(2)}\bar{\chi}(x,\hat{z}_n^*) \tag{2.64b}$$

[cf. Eqs. (2.61) and (2.59)], but neither $\chi(x,\hat{z}_n)$ nor $\phi_1(x,z_n)$ are bound states. In Eq. (2.64b) we used the symmetry (2.43b) to express $\chi(x,z)$ in terms of $\bar{\chi}(x,z)$. At the corresponding pair of zeros in the conjugate points in the lower half plane it is $a_{33}(\hat{z}_n^*)=0$ and $b_{11}(z_n^*)=0$, and one has the following relations:

$$\phi_3(x,\hat{z}_n^*)=\check{b}_n^{(2)}\bar{\chi}(x,\hat{z}_n^*)\equiv-b_n^{(2)}\bar{\chi}(x,\hat{z}_n^*), \tag{2.64c}$$

$$\bar{\chi}(x,z_n^*)=\bar{b}_n^{(2)}\psi_1(x,\hat{z}_n^*)\equiv-\hat{b}_n^{(2)}\psi_1(x,z_n^*) \tag{2.64d}$$

[cf. Eqs. (2.63) and (2.62)], where we have used the symmetries (2.43) for the eigenfunctions in order to express the proportionality constants in terms those appearing in Eqs. (2.64).

Finally, it should be noted that there is no conceptual difference between the interior and the exterior of the circle C_0. The reason why the z_n are only allowed to be inside C_0 is because they are defined as the zeros of $a_{11}(z)$. One could equivalently define z_n as the zeros of $b_{33}(z)$ (which amounts to switching $z_n\leftrightarrow\hat{z}_n$), in which case one would obtain that z_n are only allowed to be outside C_0.

G. Symmetries in the norming constants

Eigenvalues on the circle: We first consider a pair of zeros $\{\zeta_n,\zeta_n^*\}$ on the circle C_0 of radius q_0. At these points, Eqs. (2.55) hold, with $\bar{b}_n^{(1)}=b_n^{(1)}$, according to Eq. (2.56). Moreover, from symmetries Eqs. (2.41a) and (2.55) if follows

$$\psi_3^*(x,\zeta_n)=(1/b_n^{(1)})^*\phi_1^*(x,\zeta_n)=-(1/b_n^{(1)})^*e^{-ik(\zeta_n^*)x}\mathbf{J}(\phi_2(x,\zeta_n^*)\wedge\phi_3(x,\zeta_n^*))/\Gamma_1(\zeta_n^*)$$

and, on the other hand, Eq. (2.41b) implies

$$\psi_3^*(x,\zeta_n)=-e^{-ik(\zeta_n^*)x}\mathbf{J}(\psi_1(x,\zeta_n^*)\wedge\psi_2(x,\zeta_n^*))/\Gamma_3(\zeta_n^*).$$

Then observe that from Eqs. (2.26) and (2.28) it follows

$$\psi_1(x,\zeta_n^*)\wedge\psi_2(x,\zeta_n^*)=-\frac{1}{2\lambda(\zeta_n^*)}\psi_1(x,\zeta_n^*)\wedge\frac{\bar{\chi}(x,\zeta_n^*)}{b_{11}(\zeta_n^*)}, \tag{2.65a}$$

$$\phi_2(x,\zeta_n^*)\wedge\phi_3(x,\zeta_n^*)=-\frac{1}{2\lambda(\zeta_n^*)}\frac{\bar{\chi}(x,\zeta_n^*)}{a_{33}(\zeta_n^*)}\wedge\phi_3(x,\zeta_n^*), \tag{2.65b}$$

and from the discussion in Sec. II F 1 we have $\bar{\chi}(x,\zeta_n^*)/a_{33}(\zeta_n^*)\neq 0$. Back-substituting, we finally obtain

$$(b_n^{(1)})^*=-\frac{\Gamma_3(\zeta_n^*)}{\Gamma_1(\zeta_n^*)}\frac{b_{11}(\zeta_n^*)}{a_{33}(\zeta_n^*)}\bar{b}_n^{(1)}.$$

In order to simplify the above relation, first note that from Eq. (2.39) it follows $-\Gamma_1(\zeta_n^*)/\Gamma_3(\zeta_n^*)=\zeta_n/\zeta_n^*$. For the special case of reflectionless potential, with only one pair of eigenvalues (zeros) $\{\zeta_n,\zeta_n^*\}$ on the circle C_0 of radius q_0, one has

$$a_{11}(z)=\frac{z-\zeta_n}{z-\zeta_n^*},\quad a_{33}(z)=a_{11}(\hat{z}^*)=\frac{\zeta_n}{\zeta_n^*}\cdot\frac{z-\zeta_n^*}{z-\zeta_n},\quad b_{11}(z)=a_{11}^*(z^*)=\frac{z-\zeta_n^*}{z-\zeta_n}$$

so that $b_{11}(z)/a_{33}(z)\equiv\zeta_n^*/\zeta_n$. In conclusion, one has

$$(b_n^{(1)})^*=\left(\frac{\zeta_n^*}{\zeta_n}\right)^2\bar{b}_n^{(1)}\equiv\left(\frac{\zeta_n^*}{\zeta_n}\right)^2 b_n^{(1)} \tag{2.66}$$

which, in particular, implies that

$$\frac{\zeta_n^*}{\zeta_n}b_n^{(1)}\in\mathbb{R}.$$

Eigenvalues off the circle: We now consider the case of zeros off the circle C_0, and establish a relation between the norming constants $b_n^{(2)}$ and $\hat{b}_n^{(2)}$ in Eq. (2.64). Recall that

$$\chi(x,\hat{z}_n)=\hat{b}_n^{(2)}\psi_3(x,\hat{z}_n),\quad \phi_1(x,z_n)=b_n^{(2)}\chi(x,z_n)$$

and, instead of the second relation, we could as well make use of the symmetry relations (2.43) and consider

$$\phi_3(x,\hat{z}_n^*)=-b_n^{(2)}\bar{\chi}(x,\hat{z}_n^*). \tag{2.67}$$

Then we can write

$$\chi^*(x,\hat{z}_n)=(\hat{b}_n^{(2)})^*\psi_3^*(x,\hat{z}_n)=-\frac{1}{2\lambda(\hat{z}_n^*)\Gamma_3(\hat{z}_n^*)b_{11}(\hat{z}_n^*)}\frac{(\hat{b}_n^{(2)})^*}{b_n^{(2)}}\chi^*(x,\hat{z}_n)$$

[where Eqs. (2.41b), the first of Eqs. (2.26) and Eqs. (2.67), (2.37), and (2.21b) were used in turn]. As a result we obtain

$$(\hat{b}_n^{(2)})^*=-2\lambda(\hat{z}_n^*)\Gamma_3(\hat{z}_n^*)b_{11}(\hat{z}_n^*)b_n^{(2)}. \tag{2.68}$$

The previous relation can be simplified by taking into account that $-2\lambda(\hat{z}_n^*)=(z_n^2-q_0^2)/z_n$ and $\Gamma_3(\hat{z}_n^*)=q_0^2/z_n$, and that in the reflectionless case, with only one quartet of eigenvalues $\{z_n,z_n^*,\hat{z}_n,\hat{z}_n^*\}$ (cf. Fig. 3), one has

$$b_{11}(z)=\frac{z-z_n^*}{z-z_n},\quad b_{11}(\hat{z}_n^*)=\frac{q_0^2-|z_n|^2}{q_0^2-z_n^2}$$

(again recall $\hat{z}=q_0^2/z^*$), so that

$$(\hat{b}_n^{(2)})^* = \frac{q_0^2}{z_n^2}(|z_n|^2 - q_0^2) b_n^{(2)}. \tag{2.69}$$

III. INVERSE PROBLEM

In order to formulate the inverse scattering in terms of a Riemann-Hilbert (RH) problem, one needs a representation of eigenfunctions that are meromorphic in the upper-half z-plane in terms of a combination of eigenfunctions that are meromorphic in the lower-half-plane via suitably defined jump conditions. In this case one employs the two sets of analytic eigenfunctions $E_+(x,z) = (\phi_1, \chi, \psi_3)$ and $E_-(x,z) = (\psi_1, \bar{\chi}, \phi_3)$, which have already been used in Sec. II F. One then uses Eqs. (2.15a), which define the scattering coefficients, together with Eq. (2.25a) [which gives $\chi(x,z)$ in terms of $\psi_2(x,z)$ and $\psi_3(x,z)$] and Eqs. (2.26) [which give $\psi_2(x,z)$ in terms of $\psi_1(x,z)$ and $\bar{\chi}(x,z)$], to obtain for all $z \in \mathbb{R}$,

$$\frac{\phi_3(x,z)}{a_{33}(z)} e^{-i\lambda(z)x} = \psi_3(x,z) e^{-i\lambda(z)x} - \left[\frac{b_{31}(z)}{b_{11}(z)} \psi_1(x,z) + \frac{a_{32}(z)}{a_{33}(z)} \frac{\bar{\chi}(x,z)}{2\lambda(z) b_{11}(z)} \right] e^{-i\lambda(z)x}, \tag{3.1a}$$

$$\frac{\phi_1(x,z)}{a_{11}(z)} e^{i\lambda(z)x} = \psi_1(x,z) e^{i\lambda(z)x} + \left[\frac{a_{12}(z)}{a_{11}(z)} \frac{\chi(x,z)}{2\lambda(z) b_{33}(z)} - \frac{b_{13}(z)}{b_{33}(z)} \psi_3(x,z) \right] e^{i\lambda(z)x}, \tag{3.1b}$$

$$\frac{\chi(x,z)}{2\lambda(z) b_{33}(z)} e^{-ik(z)x} = -\frac{\bar{\chi}(x,z)}{2\lambda(z) b_{11}(z)} e^{-ik(z)x} + \left[\frac{b_{21}(z)}{b_{11}(z)} \psi_1(x,z) - \frac{b_{23}(z)}{b_{33}(z)} \psi_3(x,z) \right] e^{-ik(z)x}. \tag{3.1c}$$

Note that in the equations above we have used the relation $\mathbf{A}(z) = \mathbf{B}(z)^{-1}$ among the scattering coefficients. Recalling the symmetries (2.42) and (2.43b), the system of Eqs. (3.1) can be written as

$$\frac{\phi_3(x,z)}{a_{33}(z)} e^{-i\lambda(z)x} = \psi_3(x,z) e^{-i\lambda(z)x} - \left[\rho_1(z) \psi_1(x,z) - \rho_2(\hat{z}^*) \frac{\bar{\chi}(x,z)}{2\lambda(z) b_{11}(z)} \right] e^{-i\lambda(z)x}, \tag{3.2a}$$

$$\frac{\phi_1(x,z)}{a_{11}(z)} e^{i\lambda(z)x} = \psi_1(x,z) e^{i\lambda(z)x} - \left[\rho_1(\hat{z}^*) \psi_3(x,z) - \rho_2(z) \frac{\bar{\chi}(x,\hat{z}^*)}{2\lambda(z) b_{11}(\hat{z}^*)} \right] e^{i\lambda(z)x}, \tag{3.2b}$$

$$\frac{\chi(x,z)}{2\lambda(z) b_{33}(z)} e^{-ik(z)x} = -\frac{\bar{\chi}(x,z)}{2\lambda(z) b_{11}(z)} e^{-ik(z)x} + [\bar{\rho}_2(z) \psi_1(x,z) + \bar{\rho}_2(\hat{z}^*) \psi_3(x,z)] e^{-ik(z)x}, \tag{3.2c}$$

where again $\hat{z} = q_0^2/z^*$, and where we have introduced the analogs of reflection coefficients

$$\rho_1(z) = \frac{b_{31}(z)}{b_{11}(z)}, \quad \rho_2(z) = \frac{a_{12}(z)}{a_{11}(z)}, \quad \bar{\rho}_2(z) = \frac{b_{21}(z)}{b_{11}(z)}. \tag{3.3}$$

Note that only two of the above three coefficients are independent, since according to Eq. (2.40) one has

$$\bar{\rho}_2^*(z^*) = \frac{q_0^2}{q_0^2 - z^2} \rho_2(z). \tag{3.4}$$

A. Riemann-Hilbert problem

The system of Eqs. (3.2) can be considered as a generalized matrix Riemann-Hilbert problem on the real z-axis in the variables z, $\hat{z}^* \equiv q_0^2/z$, with poles in correspondence with the zeros of $a_{11}(z)$ and $b_{33}(z)$ in the upper-half-plane, as well as the zeros of $b_{11}(z)$ and $a_{33}(z)$ in the lower-half-plane. The next task is to solve the above RH problem by expressing the solutions in terms of a linear system of algebraic-integral equations.

Let us consider the first equation, namely Eq. (3.2a). From the asymptotic expansions (2.46) it follows

$$\frac{\phi_3(x,z)}{a_{33}(z)}e^{-i\lambda(z)x} \sim \psi_3(x,z)e^{-i\lambda(z)x} \sim \begin{pmatrix} 0 \\ -i\mathbf{r}_+ \end{pmatrix}, \quad z \to \infty, \tag{3.5a}$$

$$\frac{\phi_3(x,z)}{a_{33}(z)}e^{-i\lambda(z)x} \sim \psi_3(x,z)e^{-i\lambda(z)x} \sim \begin{pmatrix} -\hat{z}^* \\ -i\mathbf{r}(x) \end{pmatrix}, \quad z \to 0. \tag{3.5b}$$

Therefore, in Eq. (3.2a) we subtract from both sides the behavior at infinity and the pole at zero (which are the same for the left-hand side and the first term on the right-hand side). Also, note that the left-hand side is meromorphic in the lower-half-plane, with (simple) poles at the zeros of $a_{33}(z)$ (which we have denoted by $\zeta_n^*, \hat{z}_n^*$), while the first term on the right-hand side is analytic in the upper-half-plane. Hence, we also subtract from both sides of the equation the residues at the poles. We then introduce the Cauchy projectors,

$$P_\pm(f)(z) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{f(\zeta)}{\zeta - (z \pm i0)}\mathrm{d}\zeta, \tag{3.6}$$

which are well defined for any function $f(\zeta)$ that is integrable on the real line (e.g., see Ref. 23). Applying P_+ to Eq. (3.2a) after the above-mentioned subtractions, we then get

$$\begin{aligned}\psi_3(x,z)e^{-i\lambda(z)x} = &-\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix} + \sum_{\substack{n=1 \\ |\zeta_n|=q_0}}^{N_1} \frac{\phi_3(x,\zeta_n^*)e^{-i\lambda(\zeta_n^*)x}}{a_{33}'(\zeta_n^*)(z-\zeta_n^*)} + \sum_{\substack{n=1 \\ |z_n|<q_0}}^{N_2} \frac{\phi_3(x,\hat{z}_n^*)e^{-i\lambda(\hat{z}_n^*)x}}{a_{33}'(\hat{z}_n^*)(z-\hat{z}_n^*)} \\ &+ \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\mathrm{d}\zeta}{\zeta - (z+i0)}\left[\rho_1(\zeta)\psi_1(x,\zeta) - \rho_2(\hat{\zeta}^*)\frac{\bar{\chi}(x,\zeta)}{2\lambda(\zeta)b_{11}(\zeta)}\right]e^{-i\lambda(\zeta)x},\end{aligned} \tag{3.7}$$

where N_1 and N_2 are, respectively, the number of zeros ζ_n of $a_{11}(z)$ on the circle C_0 of radius q_0 and of zeros z_n inside the circle C_0 (cf. section II F 2). Regarding the contribution of the discrete spectrum we now take into account that for any zero ζ_n on the circle C_0, according to Eq. (2.55b) we can write $\phi_3(x,\zeta_n^*) = \bar{b}_n^{(1)}\psi_1(x,\zeta_n^*)$, while for any zero z_n off the circle C_0, Eq. (2.64c) gives $\phi_3(x,\hat{z}_n^*) = -b_n^{(2)}\bar{\chi}(x,\hat{z}_n^*)$. Therefore, from Eq. (3.7) we obtain

$$\begin{aligned}\psi_3(x,z)e^{-i\lambda(z)x} = &-\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix} + \sum_{\substack{n=1 \\ |\zeta_n|=q_0}}^{N_1} \bar{C}_n^{(1)}\frac{\psi_1(x,\zeta_n^*)e^{-i\lambda(\zeta_n^*)x}}{z-\zeta_n^*} + \sum_{\substack{n=1 \\ |\zeta_n|<q_0}}^{N_2} C_n^{(2)}\frac{\bar{\chi}(x,\hat{z}_n^*)e^{-i\lambda(\hat{z}_n^*)x}}{\hat{z}_n^*(z-\hat{z}_n^*)} \\ &+ \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{\mathrm{d}\zeta}{\zeta - (z+i0)}\left[\rho_1(\zeta)\psi_1(x,\zeta) - \rho_2(\hat{\zeta}^*)\frac{\bar{\chi}(x,\zeta)}{2\lambda(\zeta)b_{11}(\zeta)}\right]e^{-i\lambda(\zeta)x}.\end{aligned} \tag{3.8a}$$

In a similar way one can treat Eqs. (3.2b) and (3.2c). Applying a projector P_- and using (2.55a), (2.64b), and (2.64d) yields in these cases

$$\psi_1(x,z)e^{i\lambda(z)x} = \begin{pmatrix} z \\ i\mathbf{r}_+ \end{pmatrix} + \sum_{\substack{n=1 \\ |\zeta_n|=q_0}}^{N_1} \frac{z}{z-\zeta_n} C_n^{(1)} \psi_3(x,\zeta_n) e^{i\lambda(\zeta_n)x} + \sum_{\substack{n=1 \\ |\zeta_n|<q_0}}^{N_2} \frac{z}{z-z_n} C_n^{(2)} \bar{\chi}(x,\hat{z}_n^*) e^{i\lambda(z_n)x}$$
$$- \frac{z}{2\pi i} \int_{-\infty}^{\infty} \frac{d\zeta}{\zeta - (z-i0)} \left[\rho_1(\hat{\zeta}^*)\psi_3(x,\zeta) - \rho_2(\zeta) \frac{\bar{\chi}(x,\hat{\zeta}^*)}{2\lambda(\zeta) b_{11}(\hat{\zeta}^*)} \right] \frac{e^{i\lambda(\zeta)x}}{\zeta}, \tag{3.8b}$$

$$\frac{\bar{\chi}(x,z)e^{-ik(z)x}}{2\lambda(z)b_{11}(z)} = \begin{pmatrix} 0 \\ i\mathbf{q}_+^{\perp} \end{pmatrix} - \sum_{\substack{n=1 \\ |z_n|<q_0}}^{N_2} \bar{C}_n^{(2)} \psi_1(x,z_n^*) e^{-ik(z_n^*)x} \frac{z}{(z-\hat{z}_n)(z-z_n^*)}$$
$$- \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\zeta}{\zeta - (z-i0)} [\bar{\rho}_2(\zeta)\psi_1(x,\zeta) + \bar{\rho}_2(\hat{\zeta}^*)\psi_3(x,\zeta)] e^{-ik(\zeta)x}. \tag{3.8c}$$

Note that in Eqs. (3.8) we have introduced the norming constants

$$\bar{C}_n^{(1)} = \frac{\bar{b}_n^{(1)}}{a_{33}'(\zeta_n^*)}, \quad C_n^{(1)} = \frac{b_n^{(1)}}{\zeta_n a_{11}'(\zeta_n)}, \quad C_n^{(2)} = \frac{b_n^{(2)}}{z_n a_{11}'(z_n)}, \quad \bar{C}_n^{(2)} = -\frac{\bar{b}_n^{(2)}}{z_n^* b_{11}'(z_n^*)} \equiv \frac{\hat{b}_n^{(2)}}{z_n^* b_{11}'(z_n^*)}. \tag{3.9}$$

From the symmetry (2.42), whenever $|\zeta_n|=q_0$, it follows

$$a_{11}'(\zeta_n) = -\frac{q_0^2}{\zeta_n^2} a_{33}'(\zeta_n^*) = -\frac{\zeta_n^*}{\zeta_n} a_{33}'(\zeta_n^*). \tag{3.10}$$

Hence, recalling Eq. (3.9) and (2.56), one has

$$\bar{C}_n^{(1)} = \frac{\bar{b}_n^{(1)}}{a_{33}'(\zeta_n^*)} = -\frac{b_n^{(1)}\zeta_n^*}{\zeta_n a_{11}'(\zeta_n)} \equiv -\zeta_n^* C_n^{(1)}. \tag{3.11a}$$

Also, symmetry (2.38) implies $(b_{11}'(z_n^*))^* = a_{11}'(z_n)$ and therefore

$$(\bar{C}_n^{(2)})^* = \frac{q_0^2}{z_n^2}(|z_n|^2 - q_0^2) C_n^{(2)}. \tag{3.11b}$$

Equations (3.8) are the fundamental equations for the inverse scattering problem. They contain the N_1+N_2 independent (complex) norming constants $C_n^{(1)}$ and $C_n^{(2)}$. In the absence of discrete eigenvalues (that is, when $N_1=N_2=0$), Eqs. (3.8) are a linear system of three vector integral equations for the three eigenfunctions $\psi_1(x,z)$, $\psi_3(x,z)$, and $\bar{\chi}(x,z)$. In general (that is, when $N_1 \neq 0$ or $N_2 \neq 0$), the system is consistently closed by evaluating the first equation at $z=\zeta_n$, for $n=1,\ldots,N_1$, the second at $z=\zeta_n^*$ for $n=1,\ldots,N_1$ and $z=z_n^*$ for $n=1,\ldots,N_2$ and the last one at $z=\hat{z}_n^*$, $n=1,\ldots,N_2$.

It should be noted that, using the WKB expansions for the eigenfunctions (see the Appendix) and the Wronskian relations for the scattering coefficients, one can show that the reflection coefficients (3.3) decay as appropriate powers of z both as $z\to 0$ and as $z\to\infty$ so as to make the integrals in Eqs. (3.8) convergent.

B. Trace formula

From the definition of the reflection coefficients (3.3) and the symmetries (2.38), we can write Eq. (2.44) as

$$|a_{11}(z)|^{-2} = 1 - \frac{z^2}{q_0^2}|\rho_1(z)|^2 - \frac{q_0^2}{z^2 - q_0^2}|\rho_2(z)|^2. \tag{3.12}$$

Recall that $a_{11}(z)$ is analytic in the upper-half z-plane, with $a_{11}(z) \sim 1$ as $|z| \to \infty$, and that it has (simple) zeros at the points $\{\zeta_n\}_{n=1}^{N_1}$ on the circle C_0 of radius q_0, and $\{z_n\}_{n=1}^{N_2}$ off the circle C_0. Therefore, assuming that it does not vanish for any $z \in \mathbb{R}$, one can explicitly write

$$a_{11}(z) = \prod_{n=1}^{N_1} \frac{z - \zeta_n}{z - \zeta_n^*} \prod_{n=1}^{N_2} \frac{z - z_n}{z - z_n^*} \exp\left\{ - \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\log[1 - \zeta^2 |\rho_1(\zeta)|^2/q_0^2 - q_0^2|\rho_2(\zeta)|^2/(\zeta^2 - q_0^2)]}{\zeta - z} \mathrm{d}\zeta \right\}. \tag{3.13}$$

The scattering coefficients $a_{33}(z)$, $b_{11}(z)$, and $b_{33}(z)$ can obviously be obtained from $a_{11}(z)$ by symmetry [cf. Eqs. (2.38) and (2.42)]. In fact, it is worth noting that all other entries in the scattering matrix $\mathbf{A}(z) = (a_{ij}(z))$ and its inverse $\mathbf{B}(z) = (b_{ij}(z))$ can be reconstructed in terms of the reflection coefficients (3.3) and of the elements of the discrete spectrum, once the symmetries (2.38) and (2.42) are taken into account. In this sense, the reflection coefficients (3.3), together with the discrete eigenvalues and relative norming constants, constitute a minimal set of scattering data.

We also mention that from the asymptotic behavior (2.48b) of $a_{11}(z)$ as $z \to 0$, the following relation between the scattering data and the asymptotic phase differences $\Delta\theta = \theta_+^{(j)} - \theta_-^{(j)}$ in the potentials can be obtained:

$$e^{i\Delta\theta} = \prod_{n=1}^{N_1} \frac{\zeta_n}{\zeta_n^*} \prod_{n=1}^{N_2} \frac{z_n}{z_n^*} \exp\left\{ - \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\log[1 - \zeta^2 |\rho_1(\zeta)|^2/q_0^2 - q_0^2|\rho_2(\zeta)|^2/(\zeta^2 - q_0^2)]}{\zeta} \mathrm{d}\zeta \right\}. \tag{3.14}$$

Equation (3.14) is the analog of the Θ-condition that was obtained in Ref. 11 for the scalar NLS equation.

IV. TIME EVOLUTION

Equation (2.1b) fixes the time evolution of eigenfunctions and scattering data, as well as the asymptotic phases of the potential. Thus, asymptotically, the time dependence of the eigenfunctions is given by

$$\frac{\partial v}{\partial t} \sim \begin{pmatrix} 2ik^2 + iq_0^2 & -2k\mathbf{q}_\pm^T \\ -2k\mathbf{r}_\pm & -2ik^2\mathbf{I}_2 - i\mathbf{r}_\pm\mathbf{q}_\pm^T \end{pmatrix} v \quad \text{as } x \to \pm\infty. \tag{4.1}$$

The eigenfunctions $\phi_j(x,t,k)$ and $\psi_j(x,t,k)$ however are defined at all times t by the asymptotic behavior in Eqs. (2.4) as $x \to \pm\infty$. Those boundary conditions are not compatible with the time evolution prescribed by Eq. (2.1b). To determine the time evolution of $\phi_j(x,t,k)$ and $\psi_j(x,t,k)$, one can introduce modified eigenfunctions which are simultaneously solutions of the x and t part of the Lax pair. For instance, let $\tilde{\phi}_1(x,t,k) = e^{i\omega_\infty^{(1)} t}\phi_1(x,t,k)$, so that

$$\frac{\partial \widetilde{\phi}_1}{\partial t} = i\omega_\infty^{(1)} \widetilde{\phi}_1 + e^{i\omega_\infty^{(1)} t} \frac{\partial \phi_1}{\partial t}. \tag{4.2}$$

Requiring that $\widetilde{\phi}_1(x,t,k)$ be a solution of the time-differential Eq. (2.1b) [and hence, asymptotically as $x \to -\infty$, of Eq. (4.1) with the lower sign], and recalling that $r_-^{(j)}(t)$ depends on t via the phase $\theta_-^{(j)}(t)$ [cf. (2.3)], one then obtains from (2.4) and (2.5),

$$\phi_1 \sim \begin{pmatrix} \lambda + k \\ i\mathbf{r}_-(t) \end{pmatrix} e^{-i\lambda x}, \quad \frac{\partial \phi_1}{\partial t} \sim \begin{pmatrix} 0 \\ \dot{\Theta}_-(t) i\mathbf{r}_-(t) \end{pmatrix} e^{-i\lambda x}, \quad \frac{\partial \phi_1}{\partial x} \sim -i\lambda \begin{pmatrix} \lambda + k \\ i\mathbf{r}_-(t) \end{pmatrix} e^{-i\lambda x},$$

where $\dot{\Theta}_\pm(t) = \mathrm{diag}(\dot{\theta}_\pm^{(1)}(t), \dot{\theta}_\pm^{(2)}(t))$ and the dot denotes differentiation with respect to time. Substituting these into Eq. (4.1) and looking at each of the three components of $\widetilde{\phi}_1(x,t,k)$ we then obtain, respectively, from each component,

$$\omega_\infty^{(1)} = 2k\lambda + q_0^2 = \dot{\theta}_-^{(1)} - q_0^2 + 2k\lambda = \dot{\theta}_-^{(2)} - q_0^2 + 2k\lambda.$$

In order for these three expressions to be compatible, it is necessary that $\dot{\theta}_-^{(1)}(t) = \dot{\theta}_-^{(2)}(t) = 2q_0^2$, that is,

$$\theta_-^{(j)}(t) = \theta_-^{(j)} + 2q_0^2 t, \quad j = 1,2, \tag{4.3}$$

which completely fixes the time evolution of the asymptotic phases $\theta_-^{(j)}$ for the potential. In a similar way one can obtain the evolution of the asymptotic phases as $x \to +\infty$ to show that

$$\theta_+^{(j)}(t) = \theta_+^{(j)}(0) + 2q_0^2 t, \quad j = 1,2. \tag{4.4}$$

[Note that Eq. (4.4) can also be obtained directly from the asymptotics of the VNLS Eq. (1.3) as $x \to \pm\infty$.] Moreover, one finds that all of the eigenfunctions $\phi_j(x,t,k)$ and $\psi_j(x,t,k)$ satisfy a modified version of Eq. (2.1b),

$$\frac{\partial v_j}{\partial t} = \begin{pmatrix} 2ik^2 + i\mathbf{q}^T\mathbf{r} & -2k\mathbf{q}^T - i\mathbf{q}_x^T \\ -2k\mathbf{r} + i\mathbf{r}_x & -2ik^2\mathbf{I}_2 - i\mathbf{r}\mathbf{q}^T \end{pmatrix} v_j - i\omega_\infty^{(j)} v_j, \tag{4.5}$$

where $\omega_\infty = \mathrm{diag}(\omega_\infty^{(1)}, \omega_\infty^{(2)}, \omega_\infty^{(3)})$, and

$$(\omega_\infty^{(1)}, \omega_\infty^{(2)}, \omega_\infty^{(3)}) = (2k\lambda + q_0^2, -2k^2 - 2q_0^2, q_0^2 - 2k\lambda).$$

Differentiating the scattering equations (2.15a) with respect to t and taking into account Eq. (4.5), one then obtains the time evolution of the elements of the scattering matrix $\mathbf{A}$,

$$\frac{\partial a_{j\ell}}{\partial t} = i(\omega_\infty^{(\ell)} - \omega_\infty^{(j)}) a_{j\ell}, \quad j,\ell = 1,2,3. \tag{4.6}$$

From Eq. (4.6) it follows immediately that all the diagonal elements $a_{\ell\ell}(k)$ of the scattering matrix are time independent. Since $a_{11}(k)$ and $a_{33}(k)$ [as well as $b_{11}(k)$ and $b_{33}(k)$, which are related to the previous ones by symmetries (2.31)] are constants of the motion, the eigenvalues k_n, being the zeros of $a_{11}(k)$, are also time independent. The same holds for the zeros of $a_{33}(k)$. It is convenient to write explicitly the time dependence of the off-diagonal scattering coefficients

$$a_{13}(k,t) = e^{-4ik\lambda t} a_{13}(k,0), \quad a_{31}(k,t) = e^{4ik\lambda t} a_{31}(k,0), \tag{4.7a}$$

$$a_{23}(k,t) = e^{2i(k^2 - k\lambda + q_0^2)t + iq_0^2 t} a_{23}(k,0), \quad a_{32}(k,t) = e^{-2i(k^2 - k\lambda + q_0^2)t - iq_0^2 t} a_{32}(k,0), \tag{4.7b}$$

$$a_{12}(k,t) = e^{-2i(k^2+k\lambda+q_0^2)t-iq_0^2t}a_{12}(k,0), \quad a_{21}(k,t) = e^{2i(k^2+k\lambda+q_0^2)t+iq_0^2t}a_{21}(k,0). \tag{4.7c}$$

The evolution of the coefficient $b_{j\ell}(k,t)$ is the same as that of the $a_{j\ell}(k,t)$.

In a similar way one can determine the time dependence of the norming constants. Indeed, differentiating (2.55a) and (2.55b) and taking into account Eq. (4.5) we get for an eigenvalue $\zeta_n = k_n + i\nu_n$ with $|\zeta_n| = q_0$,

$$b_n^{(1)}(t) = b_n^{(1)}(0)e^{4k_n\nu_n t}, \quad \bar{b}_n^{(1)}(t) = \bar{b}_n^{(1)}(0)e^{4k_n\nu_n t}. \tag{4.8}$$

Therefore, according to the definitions (3.9)

$$\bar{C}_n^{(1)}(t) = \bar{C}_n^{(1)}(0)e^{4k_n\nu_n t}, \quad C_n^{(1)}(t) = C_n^{(1)}(0)e^{4k_n\nu_n t}, \quad n = 1, \ldots, N_1. \tag{4.9}$$

Similarly, for eigenvalues z_n and $\hat{z}_n$ off the circle (cf. Fig. 3), Eqs. (2.61) and (2.59) yield

$$b_n^{(2)}(t) = b_n^{(2)}(0)\exp[-i(z_n^2 + 4q_0^2)t], \quad \hat{b}_n^{(2)}(t) = \hat{b}_n^{(2)}(0)\exp[i((z_n^*)^2 + 4q_0^2)t], \quad n = 1, \ldots, N_2. \tag{4.10}$$

A. Conserved quantities

According to Eq. (4.6), the scattering coefficient $a_{11}(z)$ is time independent. Since $a_{11}(z)$ is analytic in the upper-half z-plane and $a_{11}(z) \to 1$ as $z \to \infty$, it admits an asymptotic Laurent series expansion whose coefficients are constants of motion. Similarly, the coefficients of the Taylor series expansion of $a_{11}(z)$ about $z=0$ are constant of the motion as well. Moreover, one can write the following expansions of the modified eigenfunction $M_1(x,z)$:

$$M_1^{(j)}(x,z) = zM_{1,\infty}^{(j,-1)}(x) + M_{1,\infty}^{(j,0)}(x) + \frac{1}{z}M_{1,\infty}^{(j,1)}(x) + \frac{1}{z^2}M_{1,\infty}^{(j,2)}(x) + \cdots, \quad j = 1,2,3 \tag{4.11}$$

as $z \to \infty$, and

$$M_1^{(j)}(x,z) = M_{1,0}^{(j,0)}(x) + zM_{1,0}^{(j,1)}(x) + z^2M_{1,0}^{(j,2)}(x) + \cdots, \quad j = 1,2,3 \tag{4.12}$$

as $z \to 0$. Substituting Eqs. (4.11) and (4.12) in Eq. (2.16), we can then obtain two infinite sets of conserved quantities:

$$I_m = M_{1,\infty}^{(1,m)}(+\infty) + iq_+^{(1)}M_{1,\infty}^{(2,m-1)}(+\infty) + iq_+^{(2)}M_{1,\infty}^{(3,m-1)}(+\infty), \quad m = 0,1,2,\ldots, \tag{4.13a}$$

$$K_m = M_{1,0}^{(1,m-2)}(+\infty) + iq_+^{(1)}M_{1,0}^{(2,m)}(+\infty) + iq_+^{(2)}M_{1,0}^{(3,m)}(+\infty), \quad m = 1,2,\ldots, \tag{4.13b}$$

where

$$M_{1,\infty}^{(j,m)}(+\infty) = \lim_{x\to+\infty} M_{1,\infty}^{(j,m)}(x), \quad M_{1,0}^{(j,m)}(+\infty) = \lim_{x\to+\infty} M_{1,0}^{(j,m)}(x), \quad j = 1,2,3$$

and where $M_{1,\infty}^{(2,-1)}(+\infty)$, $M_{1,\infty}^{(3,-1)}(+\infty)$ and $M_{1,0}^{(1,-1)}(+\infty)$, $M_{1,0}^{(1,-2)}(+\infty)$ are all assumed to be identically zero.

The first few coefficients of the asymptotic expansions (4.11) and (4.12) are computed in the Appendix, by means of a WKB expansion. Taking into account (1.2) and (1.3) and (1.10), (1.11), we can write explicitly the first few conserved quantities in (4.13). From Eq. (4.13a) we have

$$I_0 = \int_{-\infty}^{\infty} (\|\mathbf{q}(x,t)\|^2 - q_0^2)\mathrm{d}x, \quad I_1 = \int_{-\infty}^{\infty} \mathbf{q}^T(x,t)\mathbf{r}_x(x,t)\mathrm{d}x, \tag{4.14a}$$

$$I_2 = \int_{-\infty}^{\infty} [\mathbf{q}^T(x,t)\mathbf{r}_{xx}(x,t) - \|\mathbf{q}(x)\|^2(\|\mathbf{q}(x,t)\|^2 - q_0^2)]\mathrm{d}x, \tag{4.14b}$$

or equivalently

$$I_2 = -\int_{-\infty}^{\infty} [\|\mathbf{q}_x(x,t)\|^2 + (\|\mathbf{q}(x,t)\|^4 - q_0^4)]\mathrm{d}x,$$

etc. Note that I_2 is the Hamiltonian of the VNLS equation (1.3). Similarly, from Eq. (4.13b) one obtains

$$K_1 = \mathbf{q}_+^T\mathbf{r}_-, \quad K_2 = \int_{-\infty}^{\infty} \mathbf{q}_+^T(\mathbf{r}(x,t)\mathbf{q}^T(x,t)\mathbf{r}_- - q_0^2\mathbf{r}_-)\mathrm{d}x, \tag{4.15a}$$

and so on and so forth. Note that assuming the asymptotic phase differences are the same in both components [cf. Eq. (2.49)], Eq. (4.15a) becomes

$$K_1 = e^{i\Delta\theta}q_0^2, \quad K_2 = e^{i\Delta\theta}q_0^2 I_0,$$

etc., which show that the asymptotic phase difference is constant, in agreement with Eq. (4.4).

Finally, note that motion constants are also given in terms of the scattering data by the trace formula (3.13). In fact, recalling that $a_{11}(z)$, as well as its zeros z_n, ζ_n (discrete eigenvalues) are time independent, the coefficients of the expansions of $a_{11}(z)$ both as $z \to 0$ and as $z \to \infty$ in the upper-half-plane of z, i.e.,

$$J_n = \int_{-\infty}^{+\infty} \zeta^n \log[1 - \zeta^2|\rho_1(\zeta)|^2/q_0^2 - q_0^2|\rho_2(\zeta)|^2/(\zeta^2 - q_0^2)]\mathrm{d}\zeta, \quad n \in \mathbb{Z} \tag{4.16}$$

provide an infinite set of conserved quantities, assuming all of these integrals are convergent.

V. EXPLICIT SOLUTIONS

Let us discuss the special solutions obtained in the case where there is no continuum spectrum, that is, for reflectionless potentials, $\rho_j(z) = \bar{\rho}_j(z) \equiv 0$ for $j = 1, 2$ and all $z \in \mathbb{R}$.

A. Dark-dark soliton solutions

We first consider the case of a reflectionless potential with one single eigenvalue on the circle C_0 of radius q_0 (i.e., $N_1 = 1$ and $N_2 = 0$), and let $\zeta_1 = k_1 + i\nu_1$ with $-q_0 < k_1 < q_0$ and $\nu_1 = \sqrt{q_0^2 - k_1^2}$. In this case the first two equations of the inverse problem [namely Eqs. (3.8a) and (3.8b)] reduce to the closed system

$$\psi_3(x,z)e^{-i\lambda(z)x} = -\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix} + \bar{C}_1^{(1)} \frac{\psi_1(x,\zeta_1^*)e^{-\nu_1 x}}{z - \zeta_1^*}, \tag{5.1a}$$

$$\psi_1(x,z)e^{i\lambda(z)x} = \begin{pmatrix} z \\ i\mathbf{r}_+ \end{pmatrix} + \frac{z}{z - \zeta_1} C_1^{(1)} \psi_3(x,\zeta_1)e^{-\nu_1 x}. \tag{5.1b}$$

Evaluating Eq. (5.1a) at $z = \zeta_1$ and Eq. (5.1b) at $z = \zeta_1^*$, we get a linear system whose solution is given by

$$\psi_3(x,\zeta_1) = -\begin{pmatrix} \zeta_1^* \\ i\mathbf{r}_+ \end{pmatrix} e^{-\nu_1 x} \frac{1 + \dfrac{i\bar{C}_1^{(1)}}{2\nu_1} e^{-2\nu_1 x}}{1 - \dfrac{C_1^{(1)}\bar{C}_1^{(1)}}{(2\nu_1)^2}\zeta_1^* e^{-4\nu_1 x}}, \tag{5.2a}$$

$$\psi_1(x,\zeta_1^*) = \begin{pmatrix} \zeta_1^* \\ i\mathbf{r}_+ \end{pmatrix} e^{-\nu_1 x} \frac{1 - \dfrac{i\zeta_1^*\bar{C}_1^{(1)}}{2\nu_1} e^{-2\nu_1 x}}{1 - \dfrac{C_1^{(1)}\bar{C}_1^{(1)}}{(2\nu_1)^2}\zeta_1^* e^{-4\nu_1 x}}, \tag{5.2b}$$

where we used the fact that $|\zeta_1|^2 = q_0^2$. We write the common denominator of Eqs. (5.2) as

$$1 - \frac{C_1^{(1)}\bar{C}_1^{(1)}}{(2\nu_1)^2}\zeta_1^* e^{-4\nu_1 x} \equiv (1 + \gamma e^{-2\nu_1 x})(1 - \gamma e^{-2\nu_1 x})$$

with $(2\nu_1\gamma)^2 = C_1^{(1)}\bar{C}_1^{(1)}\zeta_1^*$. Then from (3.11a) it follows

$$\bar{C}_1^{(1)} = -\zeta_1^* C_1^{(1)} \tag{5.3}$$

and therefore

$$\frac{i\bar{C}_1^{(1)}}{2\nu_1} = \mp \frac{\sqrt{C_1^{(1)}\bar{C}_1^{(1)}\zeta_1^*}}{2\nu_1} \equiv \mp\,\gamma \tag{5.4}$$

so that the eigenfunctions (5.2a) and (5.2b) can be written as

$$\psi_1(x,\zeta_1^*) = -\psi_3(x,\zeta_1) = \begin{pmatrix} \zeta_1^* \\ i\mathbf{r}_+ \end{pmatrix} e^{-i\nu_1 x} \frac{1}{1 \pm \gamma e^{-2\nu_1 x}}. \tag{5.5}$$

Recalling the definitions (3.9) and the symmetry relation (3.10), we get

$$C_1^{(1)}\bar{C}_1^{(1)}\zeta_1^* = -\bar{b}_1^{(1)} b_1^{(1)} / (a_{33}'(\zeta_1^*))^2.$$

Furthermore, in the pure one-soliton case, one has $\zeta_1^* a_{33}'(\zeta_1^*) = \zeta_1/(\zeta_1^* - \zeta_1)$ and hence the previous relation becomes $C_1^{(1)}\bar{C}_1^{(1)}\zeta_1^* = (2\nu_1)^2 \bar{b}_1^{(1)} b_1^{(1)} (\zeta_1^*/\zeta_1)^2$ so that $\gamma^2 = \bar{b}_1^{(1)} b_1^{(1)} (\zeta_1^*/\zeta_1)^2$. Finally, using the symmetry (2.66) we have

$$\gamma^2 = |b_1^{(1)}|^2,$$

that is $\gamma = |b_1^{(1)}|$ assuming without loss of generality that $\gamma > 0$. Then, from Eq. (5.4) it follows that $\bar{C}_1^{(1)} = \pm i(2\nu_1\gamma)$ that is, $\bar{C}_1^{(1)}$ is purely imaginary. In the following, in order to exclude singular solutions from the IST procedure, we assume the imaginary part of $\bar{C}_1^{(1)}$ is positive, i.e., corresponding to the upper sign. Then from (5.1a) we obtain

$$\psi_3(x,z)e^{-i\lambda(z)x} = -\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix} + \frac{2i\nu_1\gamma}{z - \zeta_1^*}\begin{pmatrix} \zeta_1^* \\ i\mathbf{r}_+ \end{pmatrix} \frac{e^{-2\nu_1 x}}{1 + \gamma e^{-2\nu_1 x}}. \tag{5.6}$$

According to (2.46b), from the last two components of (5.6) in the limit $z \to 0$ it follows

$$\mathbf{r}(x) = \mathbf{r}_+ \left[1 + \frac{2i\nu_1\gamma}{\zeta_1^*} \frac{e^{-2\nu_1 x}}{1+\gamma e^{-2\nu_1 x}} \right]. \tag{5.7}$$

Taking into account the time dependence of the norming constant as given in Eq. (4.9) and then taking the complex conjugate to get $\mathbf{q}(x,t)$ one obtains a solution of the VNLS equation

$$\mathbf{q}(x,t) = \mathbf{q}_+(0) e^{2iq_0^2 t} \left[1 + (e^{2i\alpha} - 1) \frac{e^{2q_0 (\sin\alpha)(x - 2q_0 (\cos\alpha)t - x_0)}}{1 + e^{2q_0 (\sin\alpha)(x - 2q_0 (\cos\alpha)t - x_0)}} \right], \tag{5.8a}$$

$$\zeta_1 = k_1 + i\nu_1 = q_0 e^{-i\alpha}, \quad e^{2\nu_1 x_0} = \gamma(0) \equiv |b_1^{(1)}(0)| \tag{5.8b}$$

which is of the same type as Eq. (1.2) in both components, multiplied by the constant polarization (i.e., unit magnitude) vector $\mathbf{p}_+ = \mathbf{q}_+(0)/q_0$. Let us also mention that from Eq. (5.7) it follows that $\mathbf{r}(x) \to \mathbf{r}_+$ as $x \to +\infty$. Also, as $x \to -\infty$ one has

$$\mathbf{r}(x) \sim \left(1 + \frac{2i\nu_1}{\zeta_1^*} \right) \mathbf{r}_+ = \frac{\zeta_1}{\zeta_1^*} \mathbf{r}_+$$

therefore the asymptotic behavior satisfies the analog of the Θ-condition for the scalar NLS equation (cf. Ref. 11), that is,

$$\frac{r_-^{(j)}}{r_+^{(j)}} = \frac{\zeta_1}{\zeta_1^*}, \quad j = 1,2 \tag{5.9}$$

in agreement with Eq. (3.14) with $\rho_j = 0$, $N_1 = 1$ and $N_2 = 0$. Note that the right-hand side of Eq. (5.9) is independent of j, which is consistent with the assumption that the asymptotic phase difference is the same in both components.

B. Dark-bright soliton solutions

We now consider one quarter of eigenvalues off the circle C_0 of radius q_0 (cf. Fig. 3) and no continuous spectrum (i.e., $N_1 = 0$ and $N_2 = 1$). The system of equation (3.8) for the inverse problem then reduces to

$$\psi_3(x,z) e^{-i\lambda(z)x} = -\begin{pmatrix} \hat{z}^* \\ i\mathbf{r}_+ \end{pmatrix} + \frac{C_1^{(2)}}{\hat{z}_1^*} \frac{\bar{\chi}(x,\hat{z}_1^*) e^{-i\lambda(\hat{z}_1^*)x}}{z - \hat{z}_1^*}, \tag{5.10a}$$

$$\psi_1(x,z) e^{i\lambda(z)x} = \begin{pmatrix} z \\ i\mathbf{r}_+ \end{pmatrix} + \frac{z}{z - z_1} C_1^{(2)} \bar{\chi}(x,\hat{z}_1^*) e^{i\lambda(z_1)x}, \tag{5.10b}$$

$$\frac{\bar{\chi}(x,z) e^{-ik(z)x}}{2\lambda(z) b_{11}(z)} = \begin{pmatrix} 0 \\ i\mathbf{q}_+^\perp \end{pmatrix} - \bar{C}_1^{(2)} \frac{z}{(z - \hat{z}_1)(z - z_1^*)} \psi_1(x, z_1^*) e^{-ik(z_1^*)x}, \tag{5.10c}$$

where $\bar{C}_1^{(2)}$ and $C_1^{(2)}$ are given by Eqs. (3.9). To obtain a closed system, we evaluate the second equation at point $z = z_1^*$ and the third equation at $z = \hat{z}_1^*$, which gives a system of two equations for two unknowns, $\psi_1(x, z_1^*)$ and $\bar{\chi}(x, \hat{z}_1^*)$. Then, back-substituting, we obtain the expression of all the (z-dependent) eigenfunctions. Indeed, from Eqs. (5.10b) and (5.10c) one obtains

$$\bar{\chi}(x,\hat{z}_1^*) = \frac{e^{ik(\hat{z}_1^*)x}}{1 + \beta_1\gamma_1 e^{-2\nu_1 x}} \left[\alpha_1 \begin{pmatrix} 0 \\ i\mathbf{q}_+^\perp \end{pmatrix} - \beta_1 \begin{pmatrix} z_1^* \\ i\mathbf{r}_+ \end{pmatrix} e^{-i(k(z_1^*) + \lambda(z_1^*))x} \right],$$

where

$$\alpha_1 = 2\lambda(\hat{z}_1^*)b_{11}(\hat{z}_1^*), \quad \beta_1 = \alpha_1 \bar{C}_1^{(2)} \frac{\hat{z}_1^*}{(\hat{z}_1^* - \hat{z}_1)(\hat{z}_1^* - z_1^*)}, \quad \gamma_1 = C_1^{(2)} \frac{z_1^*}{z_1^* - z_1} \tag{5.11}$$

and, substituting into Eq. (5.10b),

$$\psi_1(x,z)e^{i\lambda(z)x} = \begin{pmatrix} z \\ i\mathbf{r}_+ \end{pmatrix} + \frac{z}{z - z_1} C_1^{(2)} \frac{e^{iz_1 x}}{1 + \beta_1 \gamma_1 e^{-2\nu_1 x}} \left[\alpha_1 \begin{pmatrix} 0 \\ i\mathbf{q}_+^{\perp} \end{pmatrix} - \beta_1 \begin{pmatrix} z_1^* \\ i\mathbf{r}_+ \end{pmatrix} e^{-iz_1^* x} \right].$$

To find a dark-bright soliton solution, we take $r_+^{(1)}=0$ (and consequently $q_+^{(1)}=0$) with $r_+^{(2)} = (q_+^{(2)})^* \neq 0$, and we look at the second and third components of $\psi_1(x,t)e^{i\lambda x}$, which, according to (2.46d), in the limit $z \to \infty$ reconstruct the potential $\mathbf{r}(x)$. Explicitly, we get

$$r^{(1)}(x) = \alpha_1 q_+^{(2)} C_1^{(2)} e^{ik_1 x} \frac{e^{-\nu_1 x}}{1 + \beta_1 \gamma_1 e^{-2\nu_1 x}}, \tag{5.12a}$$

$$r^{(2)}(x) = r_+^{(2)} \left[1 - C_1^{(2)} \beta_1 \frac{e^{-2\nu_1 x}}{1 + \beta_1 \gamma_1 e^{-2\nu_1 x}} \right]. \tag{5.12b}$$

In the pure one-soliton case, using the analyticity properties we can write explicitly the scattering coefficients $b_{11}(z)$ and $a_{11}(z)$ and their derivatives. Recalling that $a_{11}(z)$ is analytic in the upper-half-plane, that it goes to 1 as $z \to \infty$, and assuming that it has a single, simple zero at $z=z_1$ [cf. Eq. (2.53)], we get

$$a_{11}(z) = \frac{z - z_1}{z - z_1^*}, \quad a_{11}'(z_1) = \frac{1}{z_1 - z_1^*}.$$

Thus, recalling that $b_{11}(z)=a_{11}^*(z^*)$ and substituting into Eq. (5.11), we obtain

$$\alpha_1 = \frac{q_0^2 - |z_1|^2}{z_1}, \quad \beta_1 = \bar{C}_1^{(2)} \frac{z_1^*}{z_1^* - z_1}, \quad \gamma_1 = C_1^{(2)} \frac{z_1^*}{z_1^* - z_1}. \tag{5.13}$$

Note that α_1 vanishes if $|z_1|=q_0$ so that for zeros on the circle C_0 the bright component becomes trivial. Note also that from Eq. (3.11b) it follows that

$$\beta_1 \gamma_1 \equiv \frac{q_0^2}{4\nu_1^2}(q_0^2 - |z_1|^2)|C_1^{(2)}|^2$$

which is real and positive for any eigenvalue z_1 inside the circle C_0 of radius q_0. Note that having $|z_1| > q_0$ (i.e., an eigenvalue outside C_0) would produce a singular potential.

Inserting the time dependence (4.10) into the expressions for the potential (5.12), we finally obtain the dark-bright soliton solution of the VNLS equation (1.3),

$$r^{(1)}(x,t) = \nu_1 (q_0^2/|z_1|^2 - 1)^{1/2} e^{i\varphi_1 - 2iq_0^2 t + ik_1 x - i(k_1^2 - \nu_1^2)t} \operatorname{sech}[\nu_1(x - 2k_1 t) + x_0], \tag{5.14a}$$

$$r^{(2)}(x,t) = q_0 e^{i\varphi_2 - 2iq_0^2 t} \left[1 + \frac{2i\nu_1}{z_1^*} \frac{\exp[-2\nu_1 x + 4k_1\nu_1 t + 2x_0]}{1 + \exp[-2\nu_1 x + 4k_1\nu_1 t + 2x_0]} \right], \tag{5.14b}$$

where

$$e^{2x_0} = \frac{q_0^2}{4\nu_1^2}(q_0^2 - |z_1|^2)|C_1^{(2)}(0)|^2, \quad \varphi_1 = \arg C_1^{(2)}(0) + \theta_+^{(2)}(0), \quad \varphi_2 = -\theta_+^{(2)}(0). \tag{5.15}$$

As usual, the solution $\mathbf{q}(x,t)$ of Eq. (1.3) is obtained taking the complex conjugate of Eq. (5.14). The dark-bright solution (5.14) can be written in the more compact form

$$q^{(1)}(x,t) = -\nu_1 \sin\alpha \sqrt{q_0^2 - |z_1|^2}\, \mathrm{sech}[\nu_1(x-2k_1t)+x_0] e^{-ik_1x + i[2q_0^2 + (k_1^2 - \nu_1^2)]t - i\varphi_1}, \tag{5.16a}$$

$$q^{(2)}(x,t) = q_0\{\cos\alpha + i\sin\alpha \tanh[\nu_1(x-2k_1t)+x_0]\} e^{2iq_0^2 t - i\varphi_2}, \tag{5.16b}$$

where

$$k_1 = |z_1|\cos\alpha, \quad \nu_1 = -|z_1|\sin\alpha. \tag{5.17}$$

Again, note that the condition $k_1^2+\nu_1^2 \equiv |z_1|^2 < q_0^2$ (i.e., the requirement that the discrete eigenvalue z_1 is inside the circle C_0 of radius q_0) is necessary and sufficient to ensure the regularity of the solution at all times.

Equation (5.16) describes a two-component solution in which the second component $q^{(2)}(x,t)$ represents a dark soliton similar to that in Eq. (1.2) (but with a different relation between amplitude and velocity), while the first component $q^{(1)}(x,t)$ describes a bright soliton similar to that of the scalar focusing NLS (but with a different relation between amplitude and phase). The two components travel together at the same speed $2k_1$. Note that the amplitude of the bright soliton component and that of the intensity dip in the dark soliton component are related by the condition $k_1^2+\nu_1^2 < q_0^2$, and the amplitude of the bright component goes to zero as the eigenvalue approaches the circle (i.e., in the limit $|z_1| \to q_0$). With proper identification of the parameters, Eqs. (5.16) also coincide with the dark-bright soliton solution given in Ref. 19 in the case of x-independent asymptotic boundaries and with $x_0=0$.

VI. SMALL AMPLITUDE LIMIT

It is useful to consider the limit in which the solution $\mathbf{q}(x,t)$ of Eq. (1.3) is a small perturbation of the background field.

A. Linearization

Recall that $\mathbf{q}(x,t) \to \mathbf{q}_\pm(t) = e^{i\Theta_\pm(t)}\mathbf{q}_0$ as $x \to \pm\infty$, with $\Theta_\pm(t) = \mathrm{diag}(\theta_\pm^{(1)}, \theta_\pm^{(2)})$, and $\theta_\pm^{(j)}(t) = \theta_\pm^{(j)}(0) + 2iq_0^2 t$, and with $q_0 = \|\mathbf{q}_0\|$ as usual. We then consider the "normalized" vector NLS equation

$$i\tilde{\mathbf{q}}_t = \tilde{\mathbf{q}}_{xx} + 2(q_0^2 - \|\tilde{\mathbf{q}}\|^2)\tilde{\mathbf{q}}, \tag{6.1}$$

for the rescaled field $\tilde{\mathbf{q}}(x,t) = \mathbf{q}(x,t)e^{-2iq_0^2 t}$, and we define

$$\tilde{\mathbf{q}}(x,t) = e^{i\Theta_+(0)}(\mathbf{q}_0 + \mathbf{u}(x,t)), \tag{6.2}$$

with $\|\mathbf{u}(x,t)\| \ll q_0$, so that $\mathbf{u}(x,t)$ represents a small perturbation of the background field $\mathbf{q}_+(t)$. Inserting Eq. (6.2) into the rescaled VNLS equation (6.1) and neglecting higher powers of $\mathbf{u}$ we then obtain a linearization of the VNLS equation around the background solution,

$$i\mathbf{u}_t = \mathbf{u}_{xx} - 2\mathbf{q}_0\mathbf{q}_0^T(\mathbf{u} + \mathbf{u}^*). \tag{6.3}$$

We now look for solutions of Eq. (6.3) employing standard Fourier transforms, where for convenience we write the transform pair as follows:

$$\mathbf{u}(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{\mathbf{u}}(k,t)e^{2ikx}\,dk, \quad \hat{\mathbf{u}}(k,t) = 2\int_{-\infty}^{\infty} \mathbf{u}(x,t)e^{-2ikx}\,dx. \tag{6.4}$$

Inserting the first of Eqs. (6.4) into Eq. (6.3) with (6.2), one finds a system of four first-order differential equations in time for the functions $\hat{\mathbf{u}}(k,t) \equiv (\hat{u}_1(k,t), \hat{u}_2(k,t))$ and $\hat{\mathbf{u}}^*(-k,t)^T \equiv (\hat{u}_1^*(-k,t), \hat{u}_2^*(-k,t))^T$, which can then be solved to obtain

$$\hat{\mathbf{u}}(k,t) = A_1(k)e^{4ik^2t}\mathbf{q}_0^{\perp} + (k - \sqrt{k^2+q_0^2})A_2(k)e^{-4ik\sqrt{k^2+q_0^2}t}\mathbf{q}_0 + (k + \sqrt{k^2+q_0^2})A_3(k)e^{4ik\sqrt{k^2+q_0^2}t}\mathbf{q}_0, \tag{6.5}$$

where $\mathbf{q}_0^{\perp} = (q_0^{(2)}, -q_0^{(1)})^T \in \mathbb{R}^2$. The functions $A_1(k), A_2(k), A_3(k)$ satisfy the symmetry conditions

$$A_2^*(-k) = -A_2(k), \quad A_3^*(-k) = -A_3(k), \tag{6.6}$$

and can be written in terms of the Cauchy data as follows:

$$A_1(k) = \frac{\hat{\mathbf{u}}_0^T(k)\mathbf{q}_0^{\perp}}{q_0^2}, \tag{6.7a}$$

$$A_2(k) = \frac{1}{4kq_0^2\sqrt{k^2+q_0^2}}[(-k + \sqrt{k^2+q_0^2})\mathbf{q}_0^T\hat{\mathbf{u}}_0(k) + (k + \sqrt{k^2+q_0^2})\mathbf{q}_0^T\hat{\mathbf{u}}_0^*(-k)], \tag{6.7b}$$

$$A_3(k) = \frac{1}{4kq_0^2\sqrt{k^2+q_0^2}}[(-k + \sqrt{k^2+q_0^2})\mathbf{q}_0^T\hat{\mathbf{u}}_0^*(-k) + (k + \sqrt{k^2+q_0^2})\mathbf{q}_0^T\hat{\mathbf{u}}_0(k)], \tag{6.7c}$$

where $\hat{\mathbf{u}}_0(k) = \hat{\mathbf{u}}(k,0)$. Together, Eqs. (6.5) and (6.7) yield the solution of the linearized VNLS Eq. (6.3) in terms of given Cauchy data, which in turn provides an approximation of the solution $\mathbf{q}(x,t)$ of the VNLS equation (1.3) in the small amplitude limit.

B. Small amplitude limit from the inverse problem

If we consider the equations of the inverse problem (3.8a), (3.8b), and (3.8c) with no solitons, in the small amplitude limit we can approximate each term on the left-hand side with a series in powers of $\rho_j(z,t)$. Keeping only linear terms in $\rho_j(z,t)$, according to Eq. (2.46b), the expansion as $z \to 0$ of the last two components of $\psi_3(x,z)e^{-i\lambda(z)x}$ yields

$$\mathbf{q}(x,t) = \mathbf{q}_+(t)\left[1 + \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{d\zeta}{\zeta}\rho_1^*(\zeta,t)e^{2i\lambda(\zeta)x}\right] - \mathbf{r}_+^{\perp}(t)\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{d\zeta}{\zeta}\rho_2^*(\hat{\zeta}^*,t)e^{-i(k(\zeta)-\lambda(\zeta))x} \tag{6.8}$$

(with $\hat{\zeta} = q_0^2/\zeta^*$ as usual). In order to compare with the Fourier transform solutions obtained in the preceding sections, we recall that $\mathbf{q}_{\pm}(t) = e^{i\Theta_{\pm}(t)}\mathbf{q}_0$ and $\mathbf{r}_{\pm}(t) = \exp[-i\Theta_{\pm}(t)]\ \mathbf{q}_0$, and we consider again the normalization $\tilde{\mathbf{q}}(x,t) = \mathbf{q}(x,t)e^{-2iq_0^2t}$. Then, taking into account the time dependence of the scattering coefficients [cf. Eqs. (4.7)], from Eqs. (6.8) we get

$$\tilde{\mathbf{q}}(x,t) = \mathbf{q}_+\left[1 + \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{d\zeta}{\zeta}\rho_1^*(\zeta,0)e^{2i\lambda(\zeta)x - 4ik(\zeta)\lambda(\zeta)t}\right] - \mathbf{r}_+^{\perp}\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{d\zeta}{\zeta}\rho_2^*(\hat{\zeta}^*,0)e^{-i(q_0^2/\zeta)x + i(q_0^2/\zeta)^2t}, \tag{6.9}$$

where now $\mathbf{q}_+ \equiv \mathbf{q}_+(0)$ and $\mathbf{r}_+ \equiv \mathbf{r}_+(0)$. In order to compare with the results in the preceding section, we then perform appropriate changes of variables. Consider the term in square brackets in Eq. (6.9). First, we revert from ζ to the original coordinates $k, \lambda(k)$, so that k runs over the contour $\mathcal{L}$ given by the branch cuts in Fig. 1 and defined in Sec. II A. Then we introduce the variable

$$\xi = \sqrt{k^2 - q_0^2},$$

so that $\xi\, d\xi = k\, dk$, obtaining

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}\zeta}{\zeta}\rho_1^*(\zeta,0)e^{2i\lambda(\zeta)x}e^{-4ik(\zeta)\lambda(\zeta)t}=\int_{\mathcal{L}}\frac{\mathrm{d}k}{\lambda(k)}\rho_1^*(k,\lambda(k),0)e^{2i\lambda(k)x}e^{-4ik\lambda(k)t}$$
$$=\int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{\sqrt{\xi^2+q_0^2}}e^{2i\xi x}\big[\rho_1^*(\sqrt{\xi^2+q_0^2},\xi,0)e^{-4i\xi\sqrt{\xi^2+q_0^2}t}$$
$$-\rho_1^*(-\sqrt{\xi^2+q_0^2},\xi,0)e^{4i\xi\sqrt{\xi^2+q_0^2}t}\big]. \tag{6.10}$$

On the other hand, the second term in Eq. (6.9) can be written as an ordinary Fourier transform by simply performing the change of variable $2\xi=-q_0^2/\zeta$. By comparison, one can then show that Eq. (6.9), obtained solving the inverse problem in the limit of small amplitude, indeed coincides with the solution obtained via linearization, i.e., Eq. (6.2) with $\mathbf{u}(x,t)$ given by Eq. (6.4) and $\hat{\mathbf{u}}(k,t)$ by Eq. (6.5). More precisely, one has

$$A_1(\xi)=-\frac{1}{2k}e^{-i(\theta_+^{(1)}+\theta_+^{(2)})}\rho_2^*(-2\xi,\lambda(-2\xi),0), \tag{6.11a}$$

$$A_2(\xi)=\frac{i}{\sqrt{\xi^2+q_0^2}(\sqrt{\xi^2+q_0^2}-\xi)}\rho_1^*(\sqrt{\xi^2+q_0^2},\xi,0), \tag{6.11b}$$

$$A_3(\xi)=\frac{i}{\sqrt{\xi^2+q_0^2}(\sqrt{\xi^2+q_0^2}+\xi)}\rho_1^*(-\sqrt{\xi^2+q_0^2},\xi,0). \tag{6.11c}$$

Then, as a consequence of the symmetry conditions (6.6), it follows that

$$\rho_1(\sqrt{\xi^2+q_0^2},-\xi,0)=\frac{\sqrt{\xi^2+q_0^2}+\xi}{\sqrt{\xi^2+q_0^2}-\xi}\rho_1^*(\sqrt{\xi^2+q_0^2},\xi,0),$$

that is, in terms of the uniformization variable z,

$$\rho_1(\hat{z}^*)=\frac{z^2}{q_0^2}\rho_1^*(z),\quad z\in\mathbb{R}. \tag{6.12}$$

Note that Eq. (6.12) arises from the scattering data relations as well. Indeed, from the definitions (3.3) and symmetry (2.38) it follows

$$\rho_1^*(z)=\frac{b_{31}^*(z)}{b_{11}^*(z)}=\Gamma_1(z)\frac{a_{13}(z)}{a_{11}(z)}\Gamma_3^{-1}(z)\equiv-\frac{q_0^2}{z^2}\frac{a_{13}(z)}{a_{11}(z)} \tag{6.13a}$$

and the analog of symmetries (2.42) for the coefficients $b_{ij}(z)$ yields

$$\rho_1(z)=\frac{b_{31}(z)}{b_{11}(z)}=\frac{b_{13}(\hat{z}^*)}{b_{33}(\hat{z}^*)}. \tag{6.13b}$$

Recalling that $\mathbf{B}(z)=(b_{ij}(z))$ is the inverse matrix of $\mathbf{A}(z)=(a_{ij}(z))$, one can write

$$b_{13}(z)=a_{12}(z)a_{23}(z)-a_{13}(z)a_{22}(z),\quad b_{33}(z)=a_{11}(z)a_{22}(z)-a_{12}(z)a_{21}(z). \tag{6.14}$$

Then, since in the small amplitude limit terms $a_{ij}(z)$ with $i\neq j$ are $o(1)$ while $a_{jj}(z)=O(1)$, one has

$$\rho_1(z)=\frac{b_{13}(\hat{z}^*)}{b_{33}(\hat{z}^*)}\sim-\frac{a_{13}(\hat{z}^*)a_{22}(\hat{z}^*)}{a_{11}(\hat{z}^*)a_{22}(\hat{z}^*)},$$

and consequently Eq. (6.12) follows from Eq. (6.13).

VII. CONCLUSION

We have presented the inverse scattering transform (IST) for the defocusing VNLS equation (1.3) with nonvanishing boundary conditions as $|x|\to\infty$. The direct problem is constructed in terms of scattering eigenfunctions and adjoint eigenfunctions. The six scattering eigenfunctions provide four analytic functions, and the adjoint problem is used to construct two additional analytic functions. A global uniformizing parameter, z, is introduced in order to simplify and elucidate the analysis. The discrete eigenvalues are studied and it is found that one can have pairs of eigenvalues on a circle and/or quartets of eigenvalues symmetrically located inside and outside the circle. The inverse problem is formulated as a generalized Riemann-Hilbert (RH) problem for meromorphic functions in the complex plane of the uniformizing parameter z. The RH problem is transformed into a closed linear system of algebraic-integral equations. The trace formula, conservation laws, and explicit solutions (dark-dark and dark-bright solitons) are obtained. The solution in the small amplitude limit is studied by direct Fourier transform methods and it is shown to agree with the linearized reduction of the inverse problem.

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APPENDIX: WKB EXPANSION OF THE EIGENFUNCTIONS

Consider the following ansatz for the expansion of the eigenfunction $M_1(x,z)$ as $z\to\infty$:

$$M_1^{(1)}(x,z) = zM_{1,\infty}^{(1,-1)}(x) + M_{1,\infty}^{(1,0)}(x) + z^{-1}M_{1,\infty}^{(1,1)}(x) + z^{-2}M_{1,\infty}^{(1,2)}(x) + \cdots , \tag{A1a}$$

$$M_1^{(2)}(x,z) = M_{1,\infty}^{(2,0)}(x) + z^{-1}M_{1,\infty}^{(2,1)}(x) + z^{-2}M_{1,\infty}^{(2,2)}(x) + \cdots , \tag{A1b}$$

$$M_1^{(3)}(x,z) = M_{1,\infty}^{(3,0)}(x) + z^{-1}M_{1,\infty}^{(3,1)}(x) + z^{-2}M_{1,\infty}^{(3,2)}(x) + \cdots . \tag{A1c}$$

Substituting these expressions into the scattering problem (2.1) with $k=(z+q_0^2/z)/2$ and matching the terms with the same order in z^{-n} for $n=-1,0,1,2,\ldots$ yields $M_{1,\infty}^{(1,-1)}(x)=\text{const}$, and the integral equation (2.8a) allows one to fix this constant value to

$$M_{1,\infty}^{(1,-1)}(x) = 1. \tag{A2a}$$

Proceeding further gives

$$M_{1,\infty}^{(2,0)}(x) = ir^{(1)}(x), \quad M_{1,\infty}^{(3,0)}(x) = ir^{(2)}(x), \quad \partial_x M_{1,\infty}^{(1,0)}(x) = i(\|\mathbf{q}(x)\|^2 - q_0^2), \tag{A2b}$$

that is,

$$M_{1,\infty}^{(1,0)}(x) = i\int_{-\infty}^{x} (\|\mathbf{q}(x')\|^2 - q_0^2)\mathrm{d}x' . \tag{A2c}$$

Similarly, at higher orders one has

$$M_{1,\infty}^{(j,m+1)}(x) = ir^{(j-1)}(x)M_{1,\infty}^{(1,m)}(x) - i\partial_x M_{1,\infty}^{(j,m)}(x), \quad m=0,1,2,\ldots \tag{A3a}$$

for $j=2,3$, as well as

$$\partial_x M_{1,\infty}^{(1,m)}(x) = -iq_0^2 M_{1,\infty}^{(1,m-1)}(x) + q^{(1)}(x)M_{1,\infty}^{(2,m)}(x) + q^{(2)}(x)M_{1,\infty}^{(3,m)}(x), \quad m=1,2,\ldots \tag{A3b}$$

which allow one to calculate iteratively all coefficients of the asymptotic expansion, with the recurrence relations in Eqs. (A3) anchored by Eqs. (A2). For instance, from Eq. (A3a) with $m=0$ we obtain

$$M_{1,\infty}^{(1,1)}(x) = I_1(x) - \tfrac{1}{2}(I_0(x))^2, \tag{A4a}$$

$$M_{1,\infty}^{(2,1)}(x) = r_x^{(1)}(x) - r^{(1)}(x)I_0(x), \quad M_{1,\infty}^{(3,1)}(x) = r_x^{(2)}(x) - r^{(2)}(x)I_0(x), \tag{A4b}$$

where

$$I_0(x) = \int_{-\infty}^{x} (\|\mathbf{q}(x')\|^2 - q_0^2)\mathrm{d}x', \quad I_1(x) = \int_{-\infty}^{x} \mathbf{q}^T(x')\mathbf{r}_{x'}(x')\mathrm{d}x'. \tag{A4c}$$

Furthermore, from Eq. (A3a) with $m=1$ it follows that

$$M_{1,\infty}^{(2,2)}(x) = ir^{(1)}(x)\left[I_1(x) - \tfrac{1}{2}(I_0(x))^2\right] - ir_{xx}^{(1)}(x) + i(r^{(1)}(x)I_0(x))_x, \tag{A5}$$

$$M_{1,\infty}^{(3,2)}(x) = ir^{(2)}(x)\left[I_1(x) - \tfrac{1}{2}(I_0(x))^2\right] - ir_{xx}^{(2)}(x) + i(r^{(2)}(x)I_0(x))_x \tag{A6}$$

which can be substituted into Eq. (A3b) for $m=2$ to get

$$M_{1,\infty}^{(1,2)}(x) = iI_0(x)I_1(x) - \frac{i}{6}(I_0(x))^3 - iI_2(x), \tag{A7}$$

where

$$I_2(x) = \int_{-\infty}^{x} [\mathbf{q}^T(x')\partial_{x'}^2\mathbf{r}(x') - \|\mathbf{q}(x')\|^2(\|\mathbf{q}(x')\|^2 - q_0^2)]\mathrm{d}x' \tag{A8}$$

and so on and so forth.

Similarly, one can write a Taylor series expansion of the eigenfunction $M_1(x,z)$ as $z\to 0$ in the form

$$M_1^{(1)}(x,z) = zM_{1,0}^{(1,1)}(x) + z^2M_{1,0}^{(1,2)}(x) + z^3M_{1,0}^{(1,3)}(x) + \cdots, \tag{A9a}$$

$$M_1^{(2)}(x,z) = M_{1,0}^{(2,0)}(x) + zM_{1,0}^{(2,1)}(x) + z^2M_{1,0}^{(2,2)}(x) + \cdots, \tag{A9b}$$

$$M_1^{(3)}(x,z) = M_{1,0}^{(3,0)}(x) + zM_{1,0}^{(3,1)}(x) + z^2M_{1,0}^{(3,2)}(x) + \cdots. \tag{A9c}$$

Substituting this into Eq. (2.1) and matching terms with the same powers of z^n yields $M_{1,0}^{(2,0)}(x)$ $=$const and $M_{1,0}^{(3,0)}(x)=$const. As before, the value of such constants is fixed by the integral equation (2.8a) to give

$$M_{1,0}^{(2,0)}(x) = ir_-^{(1)}, \quad M_{1,0}^{(3,0)}(x) = ir_-^{(3)}. \tag{A10a}$$

In turn, these allow one to get

$$q_0^2M_{1,0}^{(1,1)}(x) = \mathbf{q}^T(x)\mathbf{r}_-. \tag{A10b}$$

Proceeding to higher orders, one obtains the recurrence relations

$$\partial_x M_{1,0}^{(j,m)}(x) = iM_{1,0}^{(j,m-1)}(x) + r^{(j-1)}(x)M_{1,0}^{(1,m)}(x), \quad m = 1,2,\ldots \tag{A11a}$$

for $j=2,3$, as well as

$$q_0^2M_{1,0}^{(1,m+1)}(x) = i\partial_x M_{1,0}^{(1,m)}(x) - iq^{(1)}(x)M_{1,0}^{(2,m)}(x) - iq^{(2)}(x)M_{1,0}^{(3,m)}(x), \quad m = 0,1,\ldots. \tag{A11b}$$

For instance, the first terms are

$$q_0^2 M_{1,0}^{(2,1)}(x) = \int_{-\infty}^{x} [r^{(1)}(x')\mathbf{q}^T(x')\mathbf{r}_- - q_0^2 r_-^{(1)}]\mathrm{d}x',$$

$$q_0^2 M_{1,0}^{(3,1)}(x) = \int_{-\infty}^{x} [r^{(2)}(x')\mathbf{q}^T(x')\mathbf{r}_- - q_0^2 r_-^{(2)}]\mathrm{d}x',$$

which in turn give

$$q_0^4 M_{1,0}^{(1,2)}(x) = i\mathbf{r}_-^T\mathbf{q}_x(x) - i\mathbf{q}^T(x)\int_{-\infty}^{x} [\mathbf{r}(x')\mathbf{q}^T(x')\mathbf{r}_- - q_0^2\mathbf{r}_-]\mathrm{d}x'$$

and so on and so forth.

In a similar way one can obtain the asymptotic expansions for the remaining analytic eigenfunctions and adjoint eigenfunctions.

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Modified non-Abelian Toda field equations and twisted quasigraded Lie algebras

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We construct a new family of quasigraded Lie algebras that admit the Kostant-Adler scheme. They coincide with special quasigraded deformations of twisted subalgebras of the loop algebras. Using them we obtain new hierarchies of integrable equations in partial derivatives which we call "modified" non-Abelian Toda field hierarchies. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2207719]

I. INTRODUCTION

Integrability of equations of 1+1 field theory and condensed matter physics is based on the possibility to represent them in the form of the so-called zero-curvature equations,[28,27]

$$\frac{\partial U(x,t,\lambda)}{\partial t} - \frac{\partial V(x,t,\lambda)}{\partial x} + [U(x,t,\lambda), V(x,t,\lambda)] = 0, \tag{1}$$

where $U(x,t,\lambda)$, $V(x,t,\lambda)$ are auxiliary matrices depending on dynamical variables (fields), their derivatives, and an additional complex parameter λ usually called "spectral."

The most productive interpretation of the zero-curvature equations is achieved (see Refs. 5, 7, and 15) if one treats them as a consistency condition for a set of commuting Hamiltonian flows on a dual space to some infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ of matrix-valued function of λ written in the Euler-Arnold (generalized Lax) form. In this case the corresponding U-V pairs coincide with the matrix gradients of mutually commuting Hamiltonians with respect to the natural Lie-Poisson bracket on $\tilde{\mathfrak{g}}^*$. The method that provides the needed set of the commuting Hamiltonian flows is the famous Kostant-Adler scheme.[18,15] The main ingredient of this scheme is an existence of the decomposition of the algebra $\tilde{\mathfrak{g}}$ into the sum of two subalgebras, $\tilde{\mathfrak{g}}=\tilde{\mathfrak{g}}_+ + \tilde{\mathfrak{g}}_-$. Although this approach was originally based on the graded loop algebras $L(\mathfrak{g})=\mathfrak{g}\otimes P(\lambda,\lambda^{-1})$ (Refs. 7 and 15) that possess decompositions into sums of two subalgebras, in Refs. 8 and 9 it was shown that a special Lie algebra $\mathfrak{g}_{\mathcal{E}}$, living on an elliptic curve $\mathcal{E}$, also possess the decomposition $\mathfrak{g}_{\mathcal{E}}=\mathfrak{g}^+_{\mathcal{E}}+\mathfrak{g}^-_{\mathcal{E}}$. In our papers (Refs. 10, 20, and 21) we have generalized results of Refs. 8 and 9 onto the case of special guasigraded Lie algebras $\mathfrak{g}_{\mathcal{H}}$ living on an algebraic curve $\mathcal{H}$. In papers Refs. 22 and 23 we gave a Lie algebraic explanation of this construction. We have constructed a family of quasigraded Lie algebras $\tilde{\mathfrak{g}}_A$ possessing the decomposition $\tilde{\mathfrak{g}}_A=\tilde{\mathfrak{g}}^+_A+\tilde{\mathfrak{g}}^-_A$ parametrized by some numerical matrices A, that may be viewed as a quasigraded deformations of loop algebras, such that loop algebras themselves correspond to the case $A\equiv 0$ and quasigraded Lie algebras $\mathfrak{g}_{\mathcal{H}}$ correspond to the case $A\in \mathrm{Diag}(n)$.

In our previous papers (Refs. 24 and 25), using the constructed quasigraded Lie algebras $\tilde{\mathfrak{g}}_A$ we have obtained new hierarchies of integrable equations that coincide with the various generalizations of Landau-Lifshitz and anisotropic chiral field hierarchies.

In the present paper we develop our approach to the hierarchies of the integrable equations based on the quasigraded Lie algebras. We combine our previous results,[22–25] ideas of Refs. 14, 4,

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and 3, and define new types of the quasigraded Lie algebras admitting Kostant-Adler scheme. They coincide with the "twisted" subalgebras of the Lie algebras $\tilde{\mathfrak{g}}_A$ defined with the help of a Z_p grading of a finite-dimensional Lie algebra $\mathfrak{g}: \mathfrak{g}=\sum_{k=0}^{p-1}\mathfrak{g}_{\bar{k}}$ or, equivalently, with some its automorphism σ of the order p. It turned out, that for a special choice of the matrices A (that depends on the chosen Z_p grading of $\mathfrak{g}$) it is possible to define twisted subalgebras $\tilde{\mathfrak{g}}_A^{\sigma}\subset\tilde{\mathfrak{g}}_A$ in the analogous way as for the case of ordinary loop algebras $L(\mathfrak{g})$.[11,3]

Using the technique of Refs. 5, 15, and 7 we develop a general scheme of obtaining nonlinear partial differential equations admitting the zero-curvature representation starting from the Lie algebras $\tilde{\mathfrak{g}}_A^{\sigma}$. For this purpose we explicitly construct the dual space, coadjoint action, its invariants and Lie-Poisson brackets for the case of the Lie algebra $\tilde{\mathfrak{g}}_A^{\sigma}$. In the result we obtain integrable hierarchies satisfying zero-curvature conditions associated with the Lie algebras $\tilde{\mathfrak{g}}_A^{\sigma}$.

We explicitly obtain the simplest equations of these hierarchies which we call "modified" non-Abelian Toda field equations. These are the system of the two sets of equations of the hyperbolic type that could be rewritten in the form of the one set of nonlinear equations in partial derivatives of the following form (compare with a standard non-Abelian Toda field equation[17,16]):

$$\frac{\partial}{\partial x_+}\left(g_0^{-1}\frac{\partial}{\partial x_-}g_0\right)=\left[g_0^{-1}\frac{\partial}{\partial x_-}g_0, g_0^{-1}C^{(-1)}g_0\right]_A, \tag{2}$$

where $g_0\in G_0$, G_0 is a group of the Lie subalgebra $\mathfrak{g}_{\bar{0}}$ stable under the action of the automorphism σ, $C^{(-1)}\in\mathfrak{g}_{-\bar{1}}$ is a constant element, $[X,Y]_A\equiv XAY-YAX$ is the so-called A-bracket.

In the case of the trivial automorphism σ the corresponding equations are equivalent to the chiral field type equations independently discovered in Refs. 6 and 23. In the case of the second-order automorphism and Lie algebra so(4) the equations (2) are equivalent to one more type of the so(3) anisotropic chiral field equations. In the case of the Coxeter automorphism (principal grading) equations (2) coincide with the Abelian modified Toda field equations introduced for the case of $\mathfrak{g}=\mathrm{gl}(n)$ in Ref. 19 and for the case of a general $\mathfrak{g}$ in Ref. 26. In the case of the general automorphism σ equations (2) are new.

The structure of the present paper is the following: in the second section we define the quasigraded Lie algebras $\tilde{\mathfrak{g}}_A$, their "twisted" subalgebras $\tilde{\mathfrak{g}}_A^{\sigma}$ and consider in details the case of "principal" twisted subalgebras. In the third section we define dual spaces, Lie-Poisson brackets, and Casimir functions on $\tilde{\mathfrak{g}}_A^{\sigma}$. In the fourth section we obtain the zero-curvature equations with the values in the twisted subalgebras $\tilde{\mathfrak{g}}_A^{\sigma}$ and consider the case of modified non-Abelian Toda field equations as the simplest equations they yield. We also consider several examples of the obtained equations, in particular, the case of the trivial automorphism σ, Coxeter automorphism and automorphism of the second order.

II. *K-A* ADMISSIBLE QUASIGRADED LIE ALGEBRAS

A. "Homogeneous" quasigraded Lie algebras $\tilde{\mathfrak{g}}_A$

Definition 2.1: The infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ *is called* $\mathbb{Z}$*-quasigraded of type* (p,q) (*Ref.* 13) *if it admits the decomposition*

$$\tilde{\mathfrak{g}}=\sum_{j\in\mathbb{Z}}\mathfrak{g}_j, \quad \textit{such that } [\mathfrak{g}_i,\mathfrak{g}_j]\subset\sum_{k=-p}^{q}\mathfrak{g}_{i+j+k}.$$

The following proposition holds true.[22]

Proposition 2.1: Let $\tilde{\mathfrak{g}}$ *be* $\mathbb{Z}$*-quasi-graded of type* $(0,1)$, *or* $(1,0)$. *Then* $\tilde{\mathfrak{g}}$ *admits the decomposition into the sum of its two subalgebras* $\tilde{\mathfrak{g}}=\tilde{\mathfrak{g}}_+ + \tilde{\mathfrak{g}}_-$.

In order to construct $\mathbb{Z}$-quasigraded algebras of type $(0,1)$ we will deform the Lie algebraic structure in loop algebras. We will introduce the new Lie bracket into $L(\mathfrak{g})=\mathfrak{g}\otimes Pol(\lambda,\lambda^{-1})$:

$$[X \otimes p(\lambda), Y \otimes q(\lambda)]_F = [X,Y] \otimes p(\lambda)q(\lambda) - F(X,Y) \otimes \lambda p(\lambda)q(\lambda), \tag{3}$$

where $X, Y \in \mathfrak{g}$, $p(\lambda), q(\lambda) \in Pol(\lambda, \lambda^{-1})$, $[\ ,\ ]$ on the right-hand side of this identity denotes an ordinary Lie bracket in $\mathfrak{g}$ and the map $F: \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ is skew. It is evident by the very construction that the Lie algebras with so defined bracket are $\mathbb{Z}$-quasi graded algebras of type $(0,1)$ with the quasigrading being defined in the standard way by degrees of the spectral parameter λ.

The next Propositions hold true.

Proposition 2.2: Let the cochain F satisfy the following two requirements:

$$(J1) \quad \sum_{c.p.\{i,j,k\}} (F([X_i,X_j],X_k) + [F(X_i,X_j),X_k]) = 0,$$

$$(J2) \quad \sum_{c.p.\{i,j,k\}} F(F(X_i,X_j),X_k) = 0.$$

Then bracket (3) *satisfies the Jacobi identity.*

In the case of classical matrix Lie algebras it is possible to give an explicit construction of a large (multiparametric) family of cochains F, that satisfy conditions (J1) and (J2).

Let $\mathfrak{g}$ be a classical matrix Lie algebra of the type $\mathrm{gl}(n)$, $\mathrm{so}(n)$, and $\mathrm{sp}(n)$ over the field of the complex or real numbers. We will realize algebra $\mathrm{so}(n)$ as follows: $\mathrm{so}(n) = \{X \in \mathrm{gl}(n) \,|\, X = -sX^{\mathrm{T}}s\}$, where s is the symmetric matrix and $s^2 = 1$, algebra $\mathrm{sp}(n)$ as the following matrix algebra: $\mathrm{sp}(n) = \{X \in \mathrm{gl}(n) \,|\, X = wX^{\mathrm{T}}w\}$, where n is an even number, $w \in \mathrm{so}(n)$ and $w^2 = -1$.

As it follows from the results of Ref. 2 (see also Ref. 1) the following Proposition holds true.

Proposition 2.3: Let $\mathfrak{g}$ *be a classical matrix Lie algebra over the field* $\mathbb{K}$ *of complex or real numbers. Let us define the numerical* ($\mathbb{K}$*-valued*) $n \times n$ *matrix A of the following type:*

(1) *A is arbitrary for* $\mathfrak{g} = \mathrm{gl}(n)$,
(2) $A = sA^{\mathrm{T}}s$ *for* $\mathfrak{g} = \mathrm{so}(n)$,
(3) $A = -wA^{\mathrm{T}}w$ *for* $\mathfrak{g} = \mathrm{sp}(n)$.

Then maps $F_A: \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ *of the form* $F_A(X,Y) = [X,Y]_A = XAY - YAX$ *are correctly defined skew symmetric maps that satisfy conditions (J1) and (J2).*

We will denote the infinite-dimensional Lie algebra with the Lie bracket, given by (3), by $\tilde{\mathfrak{g}}_A$ and the finite-dimensional vector space $\mathfrak{g}$ with the bracket $[\ ,\ ]_A$ by $\mathfrak{g}_A$.

Remark 1: The algebra $\tilde{\mathfrak{g}}_A$ could be realized also in the space of special matrix valued functions of λ with an ordinary Lie bracket $[\ ,\ ]$ (see Refs. 20–23). Nevertheless we consider realization in the space $\mathfrak{g} \otimes \mathrm{Pol}(\lambda, \lambda^{-1})$ with the "deformed" bracket to be more convenient.

B. "Twisted" quasigraded Lie algebras $\tilde{\mathfrak{g}}_A^{\sigma}$

In this section we will define another class of the quasigraded Lie algebras of the type $(0,1)$. They will coincide with the "twisted" subalgebras of the algebras $\tilde{\mathfrak{g}}_F$.

Let $\mathfrak{g} = \Sigma_{k=0}^{p-1} \mathfrak{g}_{\bar{k}}$ (where $\bar{j}$ denotes a class of equivalence of the elements $j \in \mathbb{Z} \bmod p\mathbb{Z}$) be a $\mathbb{Z}/p\mathbb{Z}$ grading of $\mathfrak{g}$. Let $X_{\alpha}^{\bar{j}}$ be a basic element of the subspace $\mathfrak{g}_{\bar{j}}$.

Let us consider the following subspace in $\tilde{\mathfrak{g}}_F$:

$$\tilde{\mathfrak{g}}_F^{\sigma} = \bigoplus_{j \in \mathbb{Z}} \mathfrak{g}_{\bar{j}} \otimes \lambda^j, \tag{4}$$

The next proposition holds true

Proposition 2.4: The subspace $\tilde{\mathfrak{g}}_F^{\sigma}$ *is the closed Lie subalgebra in* $\tilde{\mathfrak{g}}_F$ *if and only if:*

$$F(\mathfrak{g}_{\bar{i}}, \mathfrak{g}_{\bar{j}}) \subset \mathfrak{g}_{\overline{i+j+1}}. \tag{5}$$

Remark 2: It is known, that the $\mathbb{Z}/p\mathbb{Z}$ grading of $\mathfrak{g}$ may be defined with the help of some automorphism σ of the order p. If we extend the automorphism σ to the map $\hat{\sigma}$ of the whole

algebra $\tilde{\mathfrak{g}}_F$, defining its action on the space $\mathfrak{g}\otimes \mathrm{Pol}(\lambda,\lambda^{-1})$ in the standard way:[11] $\hat{\sigma}(X\otimes\lambda^k)=\sigma(X)\otimes e^{-2\pi ik/p}\lambda^k$, then subalgebra $\tilde{\mathfrak{g}}_F^{\sigma}$ can be defined as follows

$$\tilde{\mathfrak{g}}_F^{\sigma}=\{X\otimes p(\lambda)\in\tilde{\mathfrak{g}}_F|\sigma(X\otimes p(\lambda))=X\otimes p(\lambda)\,.\}.$$

Remark 3: From the very definition of $\tilde{\mathfrak{g}}_F^{\sigma}$ and the commutation relation in $\tilde{\mathfrak{g}}_F$ it follows that the algebra $\tilde{\mathfrak{g}}_F^{\sigma}$ is Z-quasigraded of type $(0,1)$.

From the above proposition it follows in particular, that the algebra $\tilde{\mathfrak{g}}_F^{\sigma}$ admits the direct sum decomposition $\tilde{\mathfrak{g}}_F^{\sigma}=\tilde{\mathfrak{g}}_F^{\sigma+}+\tilde{\mathfrak{g}}_F^{\sigma-}$, where

$$\tilde{\mathfrak{g}}_F^{\sigma+}=\bigoplus_{j\geq 0}\mathfrak{g}_{\bar{j}}\otimes\lambda^j,\quad \tilde{\mathfrak{g}}_F^{\sigma-}=\bigoplus_{j<0}\mathfrak{g}_{\bar{j}}\otimes\lambda^j \tag{6}$$

Now let us pass to the case of the matrix Lie algebras and the cochains F_A given by the proposition (2.3). In this case, condition (5) can be specialized.

The following Proposition holds true.

Proposition 2.5: Let us define the map $\mathcal{A}:\mathfrak{g}\to\mathfrak{g}$ *by the following formula:*

$$\mathcal{A}(X)=1/2(AX+XA).$$

Then condition (5) *is satisfied if and only if*

$$\mathcal{A}(\mathfrak{g}_{\bar{i}})\subset\mathfrak{g}_{\overline{i+1}}. \tag{7}$$

Proof: It is easy to show, that the cochain F_A can be rewritten in the following form:

$$F_A(X,Y)=[\mathcal{A}(X),Y]+[X,\mathcal{A}(Y)]-\mathcal{A}([X,Y]).$$

From this it immediately follows that condition (5) is satisfied if and only if $\mathcal{A}(\mathfrak{g}_{\bar{i}})\subset\mathfrak{g}_{\overline{i+1}}$.

That proves the proposition.

We will denote the Lie algebra $\tilde{\mathfrak{g}}_F^{\sigma}$ defined with the help of cocycle F_A by $\tilde{\mathfrak{g}}_A^{\sigma}$.

C. Example: "Principal" quasigraded Lie algebra

Let an algebra $\mathfrak{g}$ with the bracket $[\ ,\ ]$ be semisimple (reductive) classical Lie algebra of the rank r. Let $\mathfrak{h}\subset\mathfrak{g}$ be its Cartan subalgebra, $\Delta_{\pm}$ be its set of positive (negative) roots, Π—the set of simple roots, $H_i\in\mathfrak{h}$ basis of Cartan subalgebra E_{α}, $\alpha\in\Delta$ the corresponding root vectors.

Let us define the so-called "principal" grading of $\mathfrak{g}$,[11] setting

$$\deg H_i=0,\quad \deg E_{\alpha_i}=1,\quad \deg E_{-\alpha_i}=-1.$$

It is evident that in such a way we obtain the grading of $\mathfrak{g}$: $\mathfrak{g}=\Sigma_{k=0}^{h-1}\mathfrak{g}_{\bar{k}}$ with the graded subspaces $\mathfrak{g}_{\bar{k}}$ be defined as follows: $\mathfrak{g}_{\bar{k}}=\mathrm{Span}_C\{E_{\alpha}\}$, where α is the root of the length k, i.e., $\alpha=\Sigma_{i=1}^{r}k_iE_{\alpha_i}$ if $\alpha\in\Delta_+$, $\alpha=\Sigma_{i=1}^{r}k_iE_{-\alpha_i}$ if $\alpha\in\Delta_-$ and $k=\Sigma_{i=1}^{r}k_i$, h is a Coxeter number of $\mathfrak{g}$. In particular $\mathfrak{g}_{\bar{0}}=\mathfrak{h}$, $\mathfrak{g}_{\bar{1}}=\mathrm{Span}_C\{E_{\alpha_i},E_{-\theta}|a_i\in\Pi\}$, $\mathfrak{g}_{\overline{-1}}=\mathrm{Span}_C\{E_{-\alpha_i},E_{\theta}|a_i\in\Pi\}$ and θ is the longest root of the length $h-1$.

If the matrix A satisfies condition (7) we may define the corresponding "principal" quasigraded Lie algebra $\tilde{\mathfrak{g}}_A^{\sigma}$ in the following way:

$$\tilde{\mathfrak{g}}_A^{\sigma}=\sum_{m\in\mathbb{Z}}\sum_{j\in 0}^{h-1}\mathfrak{g}_{\bar{j}}^{(m)}\otimes\lambda^{j+mh},\quad \text{where } \mathfrak{g}_{\bar{j}}^{(m)}\simeq\mathfrak{g}_{\bar{j}}. \tag{8}$$

Remark 4: For all the classical Lie algebras $\mathfrak{g}$ and matrices A satisfying condition (7) it is possible to introduce (see Ref. 26) the following "pseudoroots" β_i^A ($\beta_i^A:\mathfrak{g}_{\overline{-1}}\to\mathbb{K}$):

$$[X,H_i]_A=\beta_i^A(X)H_i, \tag{9}$$

where $X\in\mathfrak{g}_{\overline{-1}}$ and H_i are basic elements in Cartan subalgebra.

III. DUAL SPACE, POISSON BRACKET AND ALGEBRA OF INTEGRALS

In order to describe an application of the Lie algebras $\tilde{\mathfrak{g}}_A^\sigma$ to the theory of finite-dimensional integrable Hamiltonian systems it is necessary to define a corresponding Lie-Poisson bracket on $(\tilde{\mathfrak{g}}_A^\sigma)^*$ and its central functions (Casimir functions) which will be used in order to produce the needed set of mutually commuting Hamiltonians on $(\tilde{\mathfrak{g}}_A^\sigma)^*$.

A. Coadjoint representation and Casimir functions of $\tilde{\mathfrak{g}}_A^\sigma$

In this section we will construct a dual space, a coadjoint representation and its invariants for the case of the twisted algebras $\tilde{\mathfrak{g}}_A^\sigma$. Due to the fact, that $\tilde{\mathfrak{g}}_A^\sigma$ is a subalgebra of $\tilde{\mathfrak{g}}_A$ we may consider $(\tilde{\mathfrak{g}}_A^\sigma)^*$ as a subspace of an σ-invariants in $\tilde{\mathfrak{g}}_A^*$. If p is the order of σ then from the properties of an invariant form on simple Lie algebras it follows[11] that $(\mathfrak{g}_i^-, \mathfrak{g}_{\bar{j}}^-)=0$ if $i+j\neq 0 \bmod p$. Hence defining a pairing between $\tilde{\mathfrak{g}}_A^\sigma$and $(\tilde{\mathfrak{g}}_A^\sigma)^*$ in the standard way,

$$\langle X,L\rangle = \mathrm{res}_{\lambda=0}\lambda^{-1}\,\mathrm{Tr}(X(\lambda)L(\lambda)). \tag{10}$$

we obtain that the generic element $L(\lambda)\in(\tilde{\mathfrak{g}}_A^\sigma)^*$ has the following form:

$$L(\lambda)=\sum_{j\in Z}\sum_{\alpha=1}^{\dim \mathfrak{g}_{\bar{j}}^-} l_\alpha^{(j)} X_\alpha^{\overline{-j}}\lambda^{-j},$$

where $X_\alpha^{\overline{-j}}$ is a basic element of subspace $\mathfrak{g}_{\overline{-j}}$.

The following proposition holds true.

Proposition 3.1: Let the functions $I^m(L)$ be the invariants of a coadjoint representation of $\mathfrak{g}$, $L(\lambda)\in(\tilde{\mathfrak{g}}_A^\sigma)^*$ *be defined as above*. Let $A(\lambda)=1-A\lambda$. *Then the functions*

$$I_k^m(L(\lambda))=\mathrm{res}_{\lambda=0}\lambda^{-k-1}I^m(L(\lambda)A(\lambda)^{-1}), \tag{11}$$

are the invariants of the coadjoint representation of the Lie algebra $\tilde{\mathfrak{g}}_A^\sigma$.

A proof of this proposition follows from the explicit form of the coadjoint action which, as it is easy to show, has the following form:

$$ad^*_{X(\lambda)}\circ L(\lambda)=A(\lambda)X(\lambda)L(\lambda)-L(\lambda)X(\lambda)A(\lambda), \tag{12}$$

where $X(\lambda), Y(\lambda)\in\tilde{\mathfrak{g}}_A^\sigma$, $L(\lambda)\in(\tilde{\mathfrak{g}}_A^\sigma)^*$.

Remark 5: The matrix $A(\lambda)^{-1}$ must be understood as a power series in λ in the neighborhood of 0 or ∞: $A(\lambda)^{-1}=(1+A\lambda+A^2\lambda^2+\cdots)$ or $A(\lambda)^{-1}=-(A^{-1}\lambda^{-1}+A^{-2}\lambda^{-2}+\cdots)$.

B. Lie-Poisson bracket

Let us define the Poisson structure in the space $(\tilde{\mathfrak{g}}_A^\sigma)^*$. Using pairing (10) described in the preceding section we can define the Lie-Poisson bracket on $P((\tilde{\mathfrak{g}}_A^\sigma)^*)$ in the standard way:

$$\{F_1(L(\lambda)),F_2(L(\lambda))\}=\langle L(\lambda),[\nabla F_1(L(\lambda)),\nabla F_2(L(\lambda))]_{A(\lambda)}\rangle, \tag{13}$$

here

$$\nabla F_i(L(\lambda))=\sum_{j\in Z}\sum_{\alpha=1}^{\dim \mathfrak{g}_{\bar{j}}^-}\frac{\partial F_i}{\partial l_\alpha^{(j)}}X_\alpha^{\bar{j}}\lambda^j$$

and

$$[\nabla F_1(L(\lambda)),\nabla F_2(L(\lambda))]_{A(\lambda)}=\nabla F_1(L(\lambda))A(\lambda)\,\nabla F_2(L(\lambda))-\nabla F_2(L(\lambda))A(\lambda)\,\nabla F_1(L(\lambda))$$

and $X_\alpha^{\bar{j}}$ is a basic element of the subspace $\mathfrak{g}_{\bar{j}}^-$.

Let us explicitly calculate Poisson bracket (13). It is easy to show, that for the coordinate functions $l_\alpha^{(i)}$, $l_\beta^{(j)}$, where $l_\alpha^{(i)} \in (\mathfrak{g}_{\bar{i}})^*$, $l_\beta^{(j)} \in (\mathfrak{g}_{\bar{j}})^*$, this bracket will have the following form:

$$\{l_\alpha^{(i)}, l_\beta^{(j)}\} = \sum_\gamma C_{\alpha,\beta}^\gamma l_\gamma^{(i+j)} - \sum_\delta C_{\alpha,\beta}^\delta(A) l_\delta^{(i+j+1)}, \tag{14}$$

where l_γ and l_δ are coordinate functions on $(\mathfrak{g}_{\overline{i+j}})^*$ and $(\mathfrak{g}_{\overline{i+j+1}})^*$.

This bracket determines in the space of linear functions $\{l_\alpha^{(i)}\}$ the Lie algebra structure isomorphic to $\tilde{\mathfrak{g}}_A^\sigma$ and, hence, the subspaces $((\tilde{\mathfrak{g}}_A^\sigma)^\pm)^*$ are Poisson.

C. Infinite-component Hamiltonian systems via $\tilde{\mathfrak{g}}_A^\sigma$

In this section we construct Hamiltonian systems on the infinite-dimensional space $(\tilde{\mathfrak{g}}_A^\sigma)^*$ possessing infinite number of independent, mutually commuting integrals of motion. Let

$$L^\mp(\lambda) = \sum_{j \in \mathbb{Z}_\pm} \sum_{\alpha=1}^{\dim \mathfrak{g}_j^-} l_\alpha^{(j)} \lambda^{-j} X_\alpha^{\overline{-j}}$$

be the generic elements of the spaces $(\tilde{\mathfrak{g}}_A^{\sigma\pm})^*$. Let us consider the polynomial functions on $(\tilde{\mathfrak{g}}_A^\sigma)^*$ of the form

$$I_k^{m\mp}(L(\lambda)) \equiv I_k^m(L^\mp(\lambda)), \tag{15}$$

where $\{I_k^m(L(\lambda))\}$ are the Casimir functions of $\tilde{\mathfrak{g}}_A^\sigma$. The Hmiltonian flows corresponding to the Hamiltonians $I_k^{m\mp}(L(\lambda))$ are written in a standard way,

$$\frac{\partial l_\alpha^{(j)}}{\partial t_k^{m\mp}} = \{l_\alpha^{(j)}, I_k^{m\mp}(L(\lambda))\}. \tag{16}$$

The following theorem is true.

Theorem 3.1: *(i) The time flows defined by the equations (16) mutually commute. (ii) Euler-Arnold equations* (16) *could be written in the deformed Lax form*

$$\frac{\partial L(\lambda)}{\partial t_k^{m\mp}} = A(\lambda) M_k^{m\pm}(\lambda) L(\lambda) - L(\lambda) M_k^{m\pm}(\lambda) A(\lambda). \tag{17}$$

where

$$M_k^{m\pm}(\lambda) = \nabla I_k^m(L^\mp(\lambda)) = \sum_{j \in \mathbb{Z}_\pm} \sum_{\alpha=1}^{\dim \mathfrak{g}_j^-} \frac{\partial I_k^m}{\partial l_\alpha^{(j)}} X_a^{\bar{j}} \lambda^j.$$

(iii) The functions $I_q^p(L^\pm)$ are constant along all times $t_k^{m\pm}$ and $t_l^{n\mp}$.

The proof of this theorem repeats the proof of the analogous theorem for the case of ordinary loop algebras (see Ref. 15 and references therein).]

IV. "MODIFIED" TODA FIELD EQUATIONS

A. Zero-curvature condition with the values in $\tilde{\mathfrak{g}}_A^\sigma$

In this section we will obtain zero-curvature-ype equations with the values in the Lie algebras $\tilde{\mathfrak{g}}_A^\sigma$.

The following theorem holds true.

Theorem 4.1: *Let the infinite-dimensional Lie algebras $\tilde{\mathfrak{g}}_A^\sigma$, $\tilde{\mathfrak{g}}_A^{\sigma\pm}$, their dual spaces and polynomial Hamiltonians $I_k^m(L^\pm(\lambda))$, $I_s^n(L^\pm(\lambda))$ on them be defined as in preceding sections. Then the algebra-valued gradients of these functions satisfy the "deformed" zero-curvature equations*

$$\frac{\partial \nabla I_k^m(L^{\pm}(\lambda))}{\partial t_l^{n\pm}} - \frac{\partial \nabla I_s^n(L^{\pm}(\lambda))}{\partial t_k^{m\pm}} + [\nabla I_k^m(L^{\pm}(\lambda)), \nabla I_s^n(L^{\pm}(\lambda))]_{A(\lambda)} = 0, \tag{18}$$

$$\frac{\partial \nabla I_k^m(L^{\pm}(\lambda))}{\partial t_l^{n\mp}} - \frac{\partial \nabla I_s^n(L^{\mp}(\lambda))}{\partial t_k^{m\pm}} + [\nabla I_k^m(L^{\pm}(\lambda)), \nabla I_s^n(L^{\mp}(\lambda))]_{A(\lambda)} = 0. \tag{19}$$

Idea of the Proof: The statement of the theorem, i.e., validity of the equations (18) and (19), follows from the commutativity of the "deformed" Lax flows (17) constructed in the preceding section.

Remark 6: Using the above-mentioned realizations of $\tilde{\mathfrak{g}}_A^{\sigma}$ the deformed zero-curvature equations can be rewritten in the form of the standard zero-curvature equations, but in this case the corresponding *U-V* pairs will be more complicated and we will work with the zero-curvature equations in the "deformed" form (18) and (19).

Theorem 4.1 provides us with an infinite number of $\tilde{\mathfrak{g}}_A^{\sigma}$-valued *U-V* pairs that satisfy zero-curvature-type equations. The latter are nonlinear equations in partial derivatives in the dynamical variables—matrix elements of the matrix $L(\lambda)$. In the terminology of Ref. 27 equations generated by the infinite set of *U-V* pairs are called "integrable in the kinematic sense." In the next sections we will consider the simplest examples of such integrable equations and their hierarchies.

B. Modified non-Abelian Toda-field equations

In this section we obtain concrete examples of integrable equations satisfying the "deformed" zero-curvature representations constructed in the preceding section. The most interesting of them will be "modified" non-Abelian Toda field equations.

Let us at first consider a general situation. Let the Lie algebra $\tilde{\mathfrak{g}}_A^{\sigma}$ and its decomposition $\tilde{\mathfrak{g}}_A^{\sigma} = \tilde{\mathfrak{g}}_A^{\sigma+} + \tilde{\mathfrak{g}}_A^{\sigma-}$ be defined as in Sec. II C. Generic elements $L^{\pm}(\lambda) \in (\tilde{\mathfrak{g}}_A^{\sigma\mp})^*$ of the dual spaces have the following form:

$$L^{+}(\lambda) = \lambda L^{(-1)} + \lambda^2 L^{(-2)} + \cdots, \quad L^{-}(\lambda) = L^{(0)} + \lambda^{-1} L^{(1)} + \lambda^{-2} L^{(2)} + \cdots,$$

where $L^{(k)} \in \mathfrak{g}_{\overline{-k}}$. Now we can formulate the following theorem.

Theorem 4.2: *Let* $\mathfrak{g}$ *be one of the classical matrix Lie algebras* $gl(n)$, $so(n)$, $sp(n)$. *Let* $\mathfrak{g} = \sum_{j=0}^{p-1} \mathfrak{g}_k$ *be* Z_p *grading of* $\mathfrak{g}$ *corresponding to some automorphism* σ *of order p. Let the "deformation" matrix A satisfy conditions* (7). *Then*

(i) *among the corresponding equations* (19) *there is the equation equivalent to the system of the following differential equations:*

$$\frac{\partial U^{(0)}}{\partial x_+} = [U^{(0)}, V^{(-1)}]_A, \tag{20a}$$

$$\frac{\partial V^{(-1)}}{\partial x_-} = -[V^{(-1)}, U^{(0)}]. \tag{20b}$$

The corresponding U-V pair for the "deformed" zero-curvature conditions is

$$U = U^{(0)} = \sum_{\alpha=1}^{\dim \mathfrak{g}_0} u_{\alpha}^{(0)} X_{\alpha}^{\bar{0}} \in \mathfrak{g}_{\bar{0}}, \quad V = \lambda^{-1} V^{(-1)} = \lambda^{-1} \sum_{\alpha=1}^{\dim \mathfrak{g}_0} v_{\alpha}^{(-1)} X_{\alpha}^{\overline{-1}} \in \mathfrak{g}_{\overline{-1}} \lambda^{-1}. \tag{21}$$

(ii) *System of equations* (20a) and (20b) *is written in the form of the "modified" non-Abelian Toda field equations*,

$$\frac{\partial}{\partial x_+}\left(g_0^{-1} \frac{\partial}{\partial x_-} g_0\right) = \left[g_0^{-1} \frac{\partial}{\partial x_-} g_0, g_0^{-1} C^{(-1)} g_0\right]_A, \tag{22}$$

where g_0 is an element of the subgroup G_0 and $C^{(-1)}$ is a fixed element of the subspace $\mathfrak{g}_{-1}$.

Proof: To prove item (i) of the theorem we will show, that among the integrals I_k^m, I_l^n there are such integrals $I_{k_0}^{m_0}, I_{l_0}^{n_0}$ that

$$I_{k_0}^{m_0}(L^+(\lambda)) \equiv I_{k_0}^{m_0}(L^{(-1)}), \quad I_{l_0}^{n_0}(L^-(\lambda)) \equiv I_{l_0}^{n_0}(L^{(0)}).$$

Indeed, let us consider the generating series $I_{k_0}^{m_0}(L^+(\lambda))$,

$$I_{k_0}^{m_0}(L^+(\lambda)) = I^{m_0}(A^{-1}(\lambda)L^+(\lambda)) = I^{m_0}((1 + A\lambda + A^2\lambda^2 + \dots)(\lambda L^{(-1)} + \lambda^2 L^{(-2)} + \dots)).$$

Taking into account that I^{m_0} is a homogeneous polynomial on $\mathfrak{g}^*$ we easily obtain that $I_{m_0}^{m_0}(L^+(\lambda)) = I_{m_0}^{m_0}(L^{(-1)})$. Now, for the role of I^{m_0} we must take any Casimir function on $\mathfrak{g}$ that has a nontrivial restriction onto $\mathfrak{g}_{\overline{1}}$. Such the Casimir function always exists because the generic element of the space $\mathfrak{g}_{\overline{1}}$ is never nilpotent.

Let us now consider the generating series $I^{n_0}(L^-(\lambda))$. It is evident that if we choose the generating Casimir function as follows: $I^{n_0}(L^-(\lambda)) = \det A(\lambda)\mathrm{Det}(L^-(\lambda)A(\lambda)^{-1})$, we obtain

$$I^{n_0}(L^-(\lambda)) = \mathrm{Det}(L^-(\lambda)), \quad D_0^{n_0}(L^-(\lambda)) = \mathrm{Det}(L^{(0)}).$$

Matrix gradients of these functions have the following form:

$$\nabla I_{m_0}^{m_0}(L^+(\lambda)) \equiv V = \lambda^{-1} \sum_{\beta=1}^{\dim \mathfrak{g}_0} v_\beta^{(-1)} X_\beta^{\overline{-1}}, \nabla I_0^{n_0}(L^-(\lambda)) \equiv U = \sum_{\alpha=1}^{\dim \mathfrak{g}_0} u_\alpha^{(0)} X_\alpha^{\overline{0}},$$

where $u_\alpha \equiv \partial I_0^{n_0} / \partial l_\alpha^{(0)}$, $v_\beta \equiv \partial I_{m_0}^{m_0} / \partial l_\beta^{(-1)}$. Substituting this into zero-curvature condition

$$\frac{\partial U}{\partial x_+} - \frac{\partial V}{\partial x_-} + [U, V]_{A(\lambda)} = 0$$

we obtain item (i) of the theorem.

It is easy to verify, that by the substitution of variables $U^{(0)} = -g_0^{-1}(\partial/\partial x_-)g_0$, $V^{(-1)} = g_0^{-1}C^{(-1)}g_0$, where g_0 is an element of the subgroup $G_0 \subset G$ corresponding to the subalgebra $\mathfrak{g}_{\overline{0}}$ and $C^{(-1)}$ is a fixed element of the subspace $\mathfrak{g}_{\overline{-1}}$, we solve Eq. (20b) and obtain Eq. (22). That proves item (ii).

Theorem is proved.

Remark 7: In general, having the cocycle F satisfying conditions (J1) and (J2) and (5) on an *arbitrary* semisimple or reductive Lie algebra $\mathfrak{g}$ it is possible to write more general form of the system: (20a) and (20b), namely,

$$\frac{\partial U^{(0)}}{\partial x_+} = F(U^{(0)}, V^{(-1)}), \quad \frac{\partial V^{(-1)}}{\partial x_-} = -[V^{(-1)}, U^{(0)}]. \tag{23}$$

The corresponding generalized "modified" non-Abelian Toda field equation has the form

$$\frac{\partial}{\partial x_+}\left(g_0^{-1}\frac{\partial}{\partial x_-}g_0\right) = F\left(g_0^{-1}\frac{\partial}{\partial x_-}g_0, g_0^{-1}C^{(-1)}g_0\right), \tag{24}$$

where g_0 is an element of the group G_0 and $C^{(-1)}$ is a fixed element of the subspace $\mathfrak{g}_{-1}$. Of course these equations coincide with the Eqs. (20a), (20b), and (22) if $F \equiv F_A$. But in the case of the general F it is not possible to write coadjoint invariants of $\widetilde{\mathfrak{g}}_F^\sigma$ without the detailization of the form of F. That is why in the general case it is difficult to give to equations (23) interpretation of the consistency condition of two Hmiltonian flows without such detailization, and we have considered the case $F \equiv F_A$ as our basic example.

C. Example: anisotropic chiral field-type equation

In this section we consider the case $\sigma=\mathrm{id}$ that corresponds to the homogeneous grading of $\mathfrak{g}$. We will show that anisotropic "chiral field-type" equations independently discovered in Refs. 6 and 22 is a particular case of the non-Abelian modified Toda field equations. In this case $p=1$ and $\mathfrak{g}_i^- \simeq \mathfrak{g}_{\overline{i+1}}$ and we may put $\mathfrak{g}_{\bar{0}}=\mathfrak{g}_{\overline{-1}}=\mathfrak{g}$. Taking into account that no requirements (5) and (7) are imposed in this case onto the cochain F_A and matrix A we may formulate the following corollary of the Theorem 4.2.

Corollary 4.1: Let $\sigma=\mathrm{id}$. *In this case equations* (20a) and (20b) *coincide with the anisotropic chiral field-type equations*

$$\frac{\partial U}{\partial x_+}=[U,V]_A, \quad \frac{\partial V}{\partial x_-}=-[V,U]. \tag{25}$$

The corresponding U-V pair for the "deformed" zero-curvature conditions is

$$U(\lambda)=U, \quad V(\lambda)=\lambda^{-1}V, \quad U,V\in\mathfrak{g}.$$

Let us consider the most interesting small rank example of equations (25).

Example 1: Let $\mathfrak{g}=\mathrm{so}(3)$, $A=\mathrm{diag}(a_1,a_2,a_3)$. In this case we can consider elements of $U,V \in \mathfrak{g}^* \simeq \mathrm{so}(3)$ as vectors $\vec{u},\vec{v}\in\mathbb{R}^3$ and rewrite equations (25) in the following form:

$$\frac{\partial \vec{u}}{\partial x_+}=A([\vec{u}\times\vec{v}]), \quad \frac{\partial \vec{v}}{\partial x_-}=[\vec{u}\times\vec{v}], \tag{26}$$

where matrix A acts on $\vec{u}=\Sigma_{i=1,3}u_kX_k$ as on a vector in $\mathbb{R}^3$: $A(\vec{u})=\Sigma_{i=1,3}a_ku_kX_k$. In this case it is possible to introduce the vector-potential $\vec{\phi}$ such that $\vec{u}=A(\partial\vec{\phi}/\partial x_-)$, $\vec{v}=\partial\vec{\phi}/\partial x_+$ and rewrite two equations (26) in the form of one equation in partial derivatives,

$$\frac{\partial^2\vec{\phi}}{\partial x_+\,\partial x_-}=-\left[\frac{\partial\vec{\phi}}{\partial x_+}\times A\left(\frac{\partial\vec{\phi}}{\partial x_-}\right)\right]. \tag{27}$$

Anisotropic chiral field-type equations (25) are in a certain sense maximally "non-Abelian" among all of the non-Abelian modified Toda-field equations and contain a maximal number of independent variables. All other non-Abelian (and Abelian) modified Toda-field equations may be viewed as their reductions with the help of some automorphism of the order p. Of course, each of these reductions is possible only in the case when matrix A satisfy additionally condition (7). In the next section we will consider such conditions and the corresponding reductions in the case $\sigma^2=\mathrm{id}$.

D. Example: "intermediate" modified Toda equation

In this section we consider "intermediate" modified Toda equation that corresponds to the involutive automorphism: $\sigma^2=\mathrm{id}$. In this case $p=2$, $\mathfrak{g}=\mathfrak{g}_{\bar{0}}+\mathfrak{g}_{\bar{1}}$ and we set $\mathfrak{g}_0\equiv\mathfrak{g}_+$, $\mathfrak{g}_1\equiv\mathfrak{g}_-$. Besides it is possible to simplify condition (7). The following Proposition holds.

Proposition 4.1: Let an involutive automorphism σ *of* $\mathfrak{g}\subset gl(n)$ *be lifted to the automorphism (minus antiautomorphism) of the algebra* $gl(n)$ *as an associative algebra. Then condition* (7) *is satisfied if and only if*

$$\sigma(A)=-A \quad [\sigma(A)=A]. \tag{28}$$

Now we can formulate the corollary of the Theorem 4.2 in the following way.

Corollary 4.2: Let $\sigma^2=id$ *and matrix A satisfies condition* (28). *In this case equations* (20a) and (20b) *acquire the following form:*

$$\frac{\partial U_+}{\partial x_+}=[U_+,V_-]_A, \quad \frac{\partial V_-}{\partial x_-}=-[V_-,U_+]. \tag{29}$$

The corresponding U-V pair for the "deformed" zero-curvature conditions is

$$U = U_+, \quad V = \lambda^{-1} V_-, \quad V_- \in \mathfrak{g}_-, \quad U_+ \in \mathfrak{g}_+. \tag{30}$$

Equations (29) may be viewed as a reduction of the equations (25). Let us consider the following low rank example.

Example 2: Let $\mathfrak{g}=\mathrm{so}(4)$. We introduce the following standard basis of so(4): $X_k \equiv \epsilon_{ijk} X_{ij}$, $Y_k \equiv X_{k4}$, $i,j,k \in 1,3$, $X_{ij}=-X_{ji}$ and consider Z_2 grading of so(n): $\mathrm{so}(4)=\mathrm{so}(4)_0+\mathrm{so}(4)_1 \equiv \mathrm{so}(3)+\mathbb{R}^3$, where $\mathrm{so}(3)=\mathrm{Span}_C\{X_i\}$, $\mathbb{R}^3=\mathrm{Span}_C\{Y_i\}$. In this case the corresponding automorphism σ has the form $\sigma(X)=wXw^{-1}$, where $w=\mathrm{diag}(1,1,1,-1)$, and, evidently is lifted to the (inner) automorphism of gl(4). Hence, according to the condition (28) the matrix A should belong to $\mathrm{gl}(4)_1$ and be symmetric in order to provide that bracket $[\ ,\ ]_A$ be closed on so(4).

U-V pair and matrix A has in this case the following form:

$$U_+ = \sum_{1\le k\le 3} u_k X_k, \quad V_- = \sum_{1\le k\le 3} v_k Y_k, \quad A = \sum_{1\le k\le 3} a_k Y_k^+,$$

where $Y_k^+ = E_{k4} + E_{4k}$ and E_{kl} is the standard matrix basis in gl(n), $(E_{kl})_{\alpha\beta} = \delta_{k\alpha}\delta_{l\beta}$. Introducing in the evident manner three-component vectors $\vec{u}$, $\vec{v}$, $\vec{a}$ and the following notation, $J_a(\vec{u}) \equiv [\vec{a}\times\vec{u}]$, we may rewrite corresponding equations (31) as follows:

$$\frac{\partial \vec{u}}{\partial x_+} = [\vec{v} \times J_a(\vec{u})], \quad \frac{\partial \vec{v}}{\partial x_-} = [\vec{u} \times \vec{v}]. \tag{31}$$

These equations are also *the anisotropic chiral field-type equations*, possessing very special "anisotropy tensor" J_a. Equations (31) seems to be new. Their possible generalization are equations

$$\frac{\partial \vec{u}}{\partial x_+} = F(\vec{u},\vec{v}), \quad \frac{\partial \vec{v}}{\partial x_-} = [\vec{u} \times \vec{v}], \tag{32}$$

where F is any other Lie bracket on so(4) compatible with the standard one and satisfying condition (5) for the described above Z_2 gradation of so(4).

E. Example: "Abelian" modified Toda-field equation

Let us consider the equations (20a) and (20b) in the case of the "principal" quasigrading that was described in Sec. II C. In this case G_0 coincides with the Cartan subgroup, $\mathfrak{g}_0$ is the Cartan subalgebra and the corresponding modified Toda system is Abelian.

By the direct verification one can prove the following corollary of the Theorem 4.2.

Corollary 4.3: (i) Let σ be Coxeter automorphism and the matrix A satisfies condition (7). *In this case equations* (20a) and (20b) *coincide with the following "Volterra coupled system:"*

$$\partial_t u_i = u_i \beta_i^A(v), \quad \partial_x v_i = v_i \alpha_i(u), \tag{33}$$

where β_i^A are the "pseudoroots" on $\mathfrak{g}_{\overline{-1}}$ defined by (9) *and depending on the "deformation" matrix A and the Lie algebra $\mathfrak{g}$, $\alpha_i \in \Pi \cup \{-\Theta\}$ are linear forms (roots) on $\mathfrak{h}$, H_i is the basis in $\mathfrak{h}$, $E_{-\alpha_i}, E_\Theta$ is the basis in $\mathfrak{g}_{\overline{-1}}$, and*

$$U = u = \sum_{i=1}^{\dim \mathfrak{h}} u_i H_i, \quad V = \lambda^{-1} v = \lambda^{-1}\left(\sum_{\alpha_i \in \Pi \cup -\Theta} v_i E_{-\alpha_i}\right) \tag{34}$$

is the corresponding U-V pair.

(ii) The Volterra coupled system (33) *is written in the form of the abelian "modified" Toda-field equations.*

$$\partial_{xt}^2\psi_i = \partial_x\psi_i\left(\sum_{\alpha_j\in\Pi\cup\{-\Theta\}}\beta_{i,j}^A e^{\alpha_j(\psi)}\right), \tag{35}$$

where $\psi=\Sigma_{i=1}^n\psi_i H_i$, $\beta_{i,j}^A=\beta_i^A(E_{-\alpha_j})$, *and* $u_i=\partial_x\psi_i$.

Remark 8: In the cases of all classical matrix Lie algebra equation (35) could be written explicitly. They are obtained and analyzed in Ref. 26. In the particular case $\mathfrak{g}=\mathrm{gl}(n)$ and special choice of the matrix A, $A=\Sigma_{i=1}^{n-1}X_{ii+1}+X_{n1}$, equation (35) has the form

$$\partial_{xt}^2\psi_i = \partial_x\psi_i(e^{\psi_{i+1}-\psi_i}-e^{\psi_i-\psi_{i-1}}), \quad \text{where } i=1,n,n+1\equiv 1.$$

They coincide with the periodic closure of the infinite "modified Toda chain" obtained by other methods in Ref. 19.

V. CONCLUSION AND DISCUSSION

In the present paper using special quasigraded Lie algebras "twisted" with the help of an automorphism σ of finite order we have obtained new hierarchies of integrable equations in partial derivatives. We considered the simplest equations of these hierarchies. We called them "modified" non-Abelian Toda-field equations. In the case of the automorphisms of the maximal order they coincide with the Abelian "modified" Toda-field equations obtained for the case $\mathfrak{g}=\mathrm{gl}(n)$ (Ref. 19) and generalized for the case of general $\mathfrak{g}$ in Ref. 26.

The interesting open problem is to find soliton solutions of the discovered integrable equations. It would be also very interesting to construct τ-functions for the obtained integrable hierarchies using the representation theory methods.[12]

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Erratum: "The equation for time-like extremal surfaces in Minkowski space $\mathbb{R}^{2+n}$" [J. Math. Phys. 47, 013503 (2006)]

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We would like to correct some inexactitudes in the statement of the last paragraph in page 013503–3 in our above cited paper and we apologize to the reader for this inconvenience.

The last paragraph in page 013503–3 and the first line in page 013503–4 in the above cited paper should be replaced by:

We next consider the Cauchy problem for Eq. (1.7) with the initial data

$$\phi(0,x) = f(x), \quad \phi_t(0,x) = g(x), \tag{1.13}$$

where f is a given C^2 vector-valued function, g is a given C^1 vector-valued function, and they satisfy

$$\Delta(f'(x), g(x)) > 0, \quad \forall\, x \in \mathbb{R}, \tag{1.13a}$$

here and hereafter the function $\Delta = \Delta(\cdot,\cdot)$ is defined by (1.11). Define

$$\Lambda_{\pm}(x) = \frac{1}{1+|f'(x)|^2}\left[-\langle f'(x), g(x)\rangle \pm \sqrt{\Delta(f'(x), g(x))}\,\right]. \tag{1.14}$$

We assume that, for every fixed $y \in \mathbb{R}$,

$$\Lambda_+(y) > \Lambda_-(x), \quad \forall\, x \in (-\infty, y). \tag{1.15}$$

Taking this opportunity, we also correct another inexactitude:
$\mathbb{R}^{2+n}$ in the title should be replaced by $\mathbb{R}^{1+(1+n)}$.

A Finslerian version of 't Hooft deterministic quantum models

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Using the Finsler structure living in the phase space associated to the tangent bundle of the configuration manifold, deterministic models at the Planck scale are obtained. The Hamiltonian functions are constructed directly from the geometric data and some assumptions concerning time inversion symmetry. The existence of a maximal acceleration and speed is proved for Finslerian deterministic models. We investigate the spontaneous symmetry breaking of the orthogonal symmetry $SO(6N)$ of the Hamiltonian of a deterministic system. This symmetry break implies the nonvalidity of the argument used to obtain Bell's inequalities for spin states. It is introduced and motivated in the context of Randers spaces, an example of a simple 't Hooft model with interactions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The possibility to use deterministic models at the Planck scale has been presented, for instance, in Refs. 1 and 2. Following these ideas, Hilbert space techniques are useful tools to deal with probabilistic predictions at atomic, nuclear, or standard model scale physics. Quantum mechanics is considered to be a powerful formalism to deal with the chaotic evolution of these systems. However, the behavior of physical systems at the Planck scale can be very different. Therefore deterministic models can be useful to describe the physical systems at this more fundamental level.

Particular motivations to investigate deterministic models at the Planck scale have been explained in Ref. 1. We recall briefly some of these reasons:

1. There is the feeling that fundamental concepts like locality, space, and time are becoming more and more obscure in contemporary physics and that this tendency will gradually grow in modern quantum theories. It seems that it is not a nice consequence of modern physics.
2. There are conceptual problems related with quantum cosmology. Let us suppose that the physical system being described is the entire universe through a master quantum wave function. The meaning of this wave function of the universe is problematic because we cannot make any experiment to test the correctness of it: we live in one universe only and we do not have an ensemble of identical universes to check the probabilistic predictions of the theory. It seems it is not possible to contrast a quantum model of the whole universe.
3. Black hole physics is problematic from the point of view of quantum mechanics. The research in this area has produced, among other results, the discovery of a fundamental principle as the holographic principle.[3] The interpretation of this principle is not intuitive from a field theory point of view; let us consider the fundamental area

$$A_p = 4 \ln 2 L_p^2,$$

where L_p is the Planck length. This principle can be stated in the following way:
The quantum degree of freedom of a quantum black hole are such that the total information

is distributed on a surface in such a way that a bit of information is contained in an area A_p. In a local quantum field theory the density of states is proportional to the volume of the system. Therefore, an interpretation of the holographic principle in the framework of a local quantum field theory becomes difficult.

4. Finally, physicists have found strong difficulties in their attempts to unify quantum mechanics with a theory of gravity. This unified theory should be important at short distances, where gravity become strong and comparable to other interactions. Usually the strategy consist of searching for the right laws of gravity at short distances, maintaining quantum mechanics as a complete theory. This persistent problem is a reason to reconsider the status of quantum mechanics as a fundamental theory at the scale where is gravity as strong as it is in other interactions.

The approach advocated in Ref. 1 is to investigate deterministic systems at the Planck scale as an alternative way to solve these problems. Due to a dissipative dynamics, after a long term evolution, different states evolve into the same one, reducing the dimensionality of the Hilbert space. All the ontological states evolving into the same state define an equivalence class. The equivalence classes can be nonlocally defined, and it is speculated that they are the states described by rays of a Hilbert space, as they are represented in quantum mechanics. In addition, it was shown that the use of Hilbert space theory in the description of these deterministic models is useful to find the connection with ordinary quantum mechanics.

The Hilbert space approach to deterministic systems has some problems. The main one is that the Hamiltonian of a deterministic system is linear in the momentum variables and therefore is not bounded from below. This implies the instability of the system. In addition, only few examples are known with a mechanism generating a Hamiltonian bounded from below, but these models do not involve interactions. Moreover, any deterministic description of quantum mechanics seems to be plagued by Bell's inequalities. It was conjectured in Ref. 1 that at the Planck scale physical systems do not meet the required symmetries used in the proof of Bell's inequalities for spin states. The reason is that at this level the system can be so complex that usual rotation symmetries do not hold.

The geometric nature or interpretation of important physical models are known. For instance, the point particle action is the length of a curve, the string action is a generalized area, and Yang-Mills actions are a function of connections on bundles. General relativity also has an interpretation in terms of the semi-Riemannian geometry. The objective nature of the geometric entities (that is, covariance respects a transformation group) implies the relevance of the geometric actions, making apparent the independence of the physical phenomenon from the particular way a description is adopted. We can say that the actions of important physical models are related to Riemannian or semi-Riemannian structures and generalized notions of distance metrics.

Finsler structures are actually natural and constitutes a branch from differential geometry and theoretical physics with a huge recent development (some general references for Finsler geometry and some of its applications are Refs. 3–9). Finsler structures are as natural as Riemannian structures but have less restrictions than Riemannian ones, and it sometimes seems strange why they have not appeared recently in field theory in a natural way. Nevertheless, recently considerable work has be done in some applications in string theory and general relativity (for instance in Ref. 6) and in the thermodynamics theory in curved spaces (Ref. 6 and references therein). Previous applications of Finsler geometry to physics were performed by the school of Miron at Rumania.[7–9]

However, our application of Finsler geometry to obtain deterministic models is completely different. It is based on the following general ideas:

1. In the construction of physical models, geometric structures are of extreme importance. Indeed, more of the main theories such as string and general relativity are formulated using metric theories, in particular structures existing in a pseudo-Riemannian manifold. Metric structures are usually required and natural.

2. If we are looking for a formalism that could be also applicable to the whole universe, it should contain an irreversible element. We live in one universe and the notion of reversible law is maybe not completely valid because it is not completely under experimental control when it is applied to a large portion of the universe or to the whole universe.

Finsler geometry has enough ingredients to address both points. It probably is not the only possibility, but we were able to use this sophisticated geometry to find some results that maybe can be useful for future research in this area. Finslerian distance (usually associated with the length of a curve using the Finsler metric) can be nonsymmetric, that is, the distance between point a and point b is not the same as the distance from b to a. We consider that nonsymmetric Finsler metrics (which means when the above asymmetry is possible) are useful to describe the behavior of irreversible evolutions at the fundamental scale. For example, the action of a particle moving in a Finsler space is not invariant under the inversion of the parameter of the curve. This asymmetry in the metric implies the possibility to describe an irreversible evolution from a geometric point of view. This is the main reason to use models in physics based on Finsler geometry (another idea of how to describe thermodynamics using Finsler structures can be found in Ref. 5. However, our application mainly differs from this one because we are concerned with the most basic level in the description of phenomena).

The aim of the present work is as follows. First, we investigate some general consequences of the 't Hooft theory. Second, in order to give a geometric basis for the theory, we explain the relation of 't Hooft's models with the Finsler structure of the cotangent bundle of the tangent bundle of the configuration manifold $\mathbf{M}$, $\mathbf{T}^*\mathbf{TM}$. Finslerian models are free of some problems of the initial 't Hooft's theory. In particular, they provide a geometric argument to obtain a lower bound for a Hamiltonian coming from a deterministic system.

The structure of this work is as follows. In Sec. II the basic notions and results of the 't Hooft theory are presented. Also, the main problems of this approach are explained.

In Sec. III the use of Finsler geometry to find deterministic models is presented. In addition, we develop some consequences of the Finslerian approach as the existence of a higher limit for generalized physical acceleration and speed. We describe the spontaneous symmetric breaking that can occur in the Finslerian deterministic model. The possible absence of Bell's inequalities for spin at the Planck scale is also argued, but the argument can be changed to a more general framework than Finslerian models, provided a geometric argument is possible.

In Sec. IV we to discuss our results in the context of the geometry of spaces of smooth Finsler structures. We describe a simple deterministic model where interactions are present. This model is based on some geometric construction and some additional physical requirements.

Finally, in the Appendix , the basic definitions and results of the Finsler geometry and other geometric objects mentioned in this work are given.

II. THE 't HOOFT THEORY

't Hooft has investigated the possibility to use deterministic models in order to describe physical systems at the Planck scale through a Hilbert space formulation[1,2] of these models. The physical system is described by an eigenstate $|x\rangle|$ of a set of commuting operators $\{\hat{X}_i(t)\}$,

$$[\hat{X}_i(t),\hat{X}_j(\tilde{t})]=0,\ \forall\ i,j,\quad \hat{X}_i(t)|x\rangle = x_i(t)|x\rangle\ ,$$

such that the eigenvalues $\{x_i(t)\}$ completely describe the state of the system. These states are called ontological. The parameter t is associated with a macroscopic phenomenon or device and used as the time parameter by an macroscopic observer, although we consider microscopic processes, which are at the level of the deterministic description. At each instant t, the physical system is in correspondence with a particular vector defined by the set of eigenvalues $\{x_i(t)\}$. This set of functions defines the real configuration of the system at any instant t. The Hilbert space is generated by the vectors representing the configurations of the physical system. A linear combination of elements of a basis of the Hilbert space produces a vector such that the square of the module of

each component is the probability of the system to be in this particular state.

The Hamiltonian of a deterministic system with $6N$ degrees of freedom in the phase space is

$$\mathbf{H} = \sum_{i=1}^{6N} p_i f^i(x) + g(x). \tag{2.1}$$

(x,p) are canonical variables, $\{x_i, p_j\} = \delta_{ij}$. After canonical quantization this Hamiltonian reproduces the evolution differential equations, which are the Heisenberg equations for the operators $\{X^i, i=1,\ldots,6N\}$,

$$\frac{d\hat{X}^i}{dt} = f^i(\hat{X}), \quad i = 1, \ldots, 6N. \tag{2.2}$$

When we take the average value of the Eq. (2.2) we obtain

$$|\tilde{x}\rangle\left(\frac{d\hat{X}^i}{dt} - f^i(\hat{X})\right)|x\rangle = 0, \quad i = 1, \ldots, 6N.$$

This implies the classical ordinary differential equations

$$\frac{dx^i}{dt} = f^i(x), \quad i = 1, \ldots, 6N \tag{2.3}$$

because the scalar product of the Hilbert space is positively defined. Any system whose evolution is given by Eqs. (2.3) and has a complete and defined set of initial conditions is called deterministic.

Let us consider the quantization of the Hamiltonian (2.1). It does not have a minimal eigenvalue because it is linear in momentum. However, the existence of a ground state is essential for the stability of the physical system. This parameter is a fundamental difficulty in the Hilbert space formulation of deterministic systems.

For this problem let us consider that a dissipative dynamics, a system with a rather turbulent or chaotic behavior at the beginning, can reach stability in a finite time. This kind of dissipation implies the possibility to define the physical states as equivalence classes at equilibrium. An equivalence class is defined by the set of ontological states that, after a long term in the parameter t, evolve to the same final state.

't Hooft has proposed the following solution to the problem of the missing of the lower bound of the Hamiltonian: *If dissipation of information it is possible*, *the final Hamiltonian could be bounded from below*. It was suggested in Refs. 1 and 2 that the actual quantum mechanics describes not the basic degrees of freedom of our universe, but the dynamics of equivalence classes reached by these basic states after a long term evolution with a dissipation of information: various states can evolve into the same equilibrium state. The ontological states follow a deterministic dynamics that is described by the set of first order, ordinary differential equations of type (2.3) (in addition with a complete set of initial conditions). These states are locally well defined. By contrast, the equivalence classes of states could not be locally well defined and their evolution is quantum mechanical.

This evolution onto equivalence classes can solve the problem of the ground state because their number is smaller than the number of ontological states. It could be that even with an infinite number of ontological states, we have a finite number of equivalence classes, a finite Hilbert space, and as a consequence the Hamiltonian has a defined ground state.[1] Several examples has been found by 't Hooft where there is a mechanism producing a Hamiltonian with a lower bound: the free bosonic system, the free Maxwell field, and the free massless neutrino system are deterministic systems. These examples at least prove the existence of deterministic models with a Hamiltonian bounded from below.

In this work we denote by a 't Hooft model a deterministic system with a mechanism producing a lower bound for the final Hamiltonian at equilibrium. By dissipative mechanism we mean an information loss mechanism.

III. FINSLERIAN DETERMINISTIC QUANTUM MODELS AT THE PLANCK SCALE

Let us denote by **M** the configuration manifold of all the degrees of freedom at the Planck scale. By configuration manifold we mean a submanifold **M** of a $2n$-manifold **N** such that $\mathbf{TM}=\mathbf{N}$. With this definition we adopt the formalism of Lagrange spaces[7] (indeed dual Lagrange spaces), instead of considering the formalism of higher order Lagrange spaces.[8]

The relation between Finsler structures and deterministic systems is based on the following points:

1. The ontological states at the Planck scale are described by points of the phase space $\mathbf{T}^*\mathbf{TM}$ and the tangent bundle **TM** is equipped with a dual Randers metric F^*.
2. The reduction of the ontological Hilbert space to the quantum mechanical Hilbert space is in correspondence with the reduction of the Randers structure $(\mathbf{TM},F^*)$ to the Riemannian structure $(\mathbf{TM},h)$. We postulate that this reduction corresponds to the average operation investigated in Ref. 10.
3. We assume that for each particle with a generalized velocity $y=dx^i/dt$ there is another particle associated such that it is evolving backwards in time t with velocity $-y$ and the separation between them is zero.

For the definition of a Finsler structure and Randers structures, basic notions in the present work, we refer to the Appendix or to Ref. 4. The term dual makes reference to the manifold $\mathbf{T}^*\mathbf{TM}$ where F^* lives in our formalism. These spaces are treated in the literature (see Ref. 6 and references therein) and are called Cartan spaces. Points 1 and 2 are the main link between geometry and physics in our proposal. Point 1 is a nominative axiom, relating notions from geometry and physics. Point 2 refers to the link between the geometric theory of Finsler geometry described in Ref. 10 with a reduction of the associated Hilbert space. This point is especially important to keep in mind when finding the link between quantum mechanics and deterministic models at the Planck scale. It is only explanatory; while point 1 is completely arbitrary, point 2 is just a consequence of point 1 and the theory developed in Ref. 10. Point 3 is a generalization of the particle-antiparticle creation in the context of a nonsymmetric geometry background. Due to this asymmetry, a nontrivial system arises with a defined fundamental time arrow.

In addition to the above statements, we note two other implicit facts in our construction:

1. There is a microscopic time arrow associated with the mechanism that produces the evolution from the Randers structure $(\mathbf{TM},F^*)$ to the actual Riemannian structure $(\mathbf{TM},h)$.
2. There is a Hamiltonian function obtained directly from the geometric data contained in the Randers structure $(\mathbf{TM},F^*)$.

Consider a Randers function F^* with the following form (see the Appendix for the definition of Randers space),

$$F^*(x,p)=\alpha(x,p)+\beta(x,p).$$

Then we perform the following identification between the Hamiltonian function and the nonsymmetric part of the Randers function,

$$\mathbf{H}=\sum_{i=1}^{n} p_i f^i(x) \rightarrow 2\sum_{i=1}^{n} \beta^i(x)p_i, \tag{3.1}$$

and if we identify component by component,

$$2\beta^i = f^i, \quad i = 1, \ldots, 6N. \tag{3.2}$$

The ordinary differential equations (2.3) are then

$$f^i = \beta^i = \frac{dx^i}{dt}, \quad i = 1, \ldots, 6N. \tag{3.3}$$

In order to quantize the model we use the canonical quantization through the prescription

$$x^i \to \hat{X}^i, \quad \beta^i(x) \to \beta^i(\hat{X}), \quad p_i \to -i\frac{\partial}{\partial x^i} = \hat{P}_i. \tag{3.4}$$

This representation holds the canonical quantization relation:

$$[\hat{X}_i, \hat{P}_j] = \delta_{ij}.$$

The reason why we choose the above Hamiltonian function (3.1) is as follows: the first term corresponds to a particle moving forward in time while the second term corresponds to a particle moving backward in time, both at the same position; there is a democracy in the choice of the macroscopic time arrow.

We would like to justify the Hamiltonian function (3.1) in more detail. Since we use phase space variables, we translate the above assumption from velocities to momentum variables. An example of a dual Finsler structure with Finsler function F^* living in the cotangent bundle $\mathbf{T}^*(\mathbf{TM})$ is defined using the following procedure: if $(\mathbf{TF}, F)$ is a Finsler structure, let us consider the dual Finsler structure defined by

$$F^*(x,p) := F(x,y_p) \text{ such that } y_p(\tilde{p}) := g_{y_p}(p,\tilde{p}),$$

$\vec{p} = p^i(\partial/\partial x^i) \in \mathbf{T}^*_u\mathbf{T}_x\mathbf{M}; y \in \mathbf{T}_u\mathbf{T}_x\mathbf{M}$. y_p is the dual vector of the 1-form p defined by the second relation. g_{y_p} is the fundamental tensor of the structure $(\mathbf{TM}, F)$ evaluated at the point y_p (for the definition, see the Appendix).

The classical Hamiltonian function (3.2) coincides with

$$\mathbf{H} = F^*(x,p) - F^*(\tau(x), \tau(p)) = 2\beta^i p_i. \tag{3.5}$$

The transformation τ is the time inversion operator with respect to the microscopic time t. The action of the time inversion operator in the canonical variables is defined such that the canonical relation $\{x_i, p_j\} = \delta_{ij}$ remains invariant.

The quantization of the above models is equivalent to the quantum mechanical description of a deterministic system. The quantized Hamiltonian is defined by

$$\hat{\mathbf{H}} = F^*(\hat{X}, \hat{P}) - F^*(\hat{T}\hat{X}\hat{T}^{-1}, \hat{T}\hat{P}\hat{T}^{-1}).$$

$\hat{T}$ is the time inversion operator. The Hamiltonian is

$$\hat{\mathbf{H}} = 2\beta^i(\hat{X})\hat{P}_i. \tag{3.6}$$

A simple calculation shows that for this Hamiltonian the relation $\hat{T}\hat{\mathbf{H}}\hat{T}^{-1} = -\hat{\mathbf{H}}$ holds and that the elementary evolution operator

$$\hat{\mathbf{U}}(t, t+\delta t) = \hat{I} - i\,\delta t\hat{\mathbf{H}}$$

is invariant under time inversion $\hat{T}$, producing a geometric time arrow (note that states are invariant by the time inversion operation).

Hamiltonian (3.6) is not bounded from below. In order to solve this problem we propose the following mechanism: Let us define the average classical Hamiltonian defined by

$$\langle \mathbf{H} \rangle := \int_{\mathbf{I}_x^*} \mathbf{H}(x,p) |\psi(x,p)|^2 d^{6N-1}p.$$

The manifold $\mathbf{I}_x^* \subset \mathbf{T}_\mathbf{x}^*(\mathbf{TM})$ is defined by $\mathbf{I}_x^* := \{p \in \mathbf{T}_\mathbf{x}^*(\mathbf{TM}) \,|\, F^*(x,p)=1\}$. $|\psi(x,p)|^2$ is a weight function on the indicatrix $\mathbf{I}_x^*$ and it is determined by the geometric data $(\mathbf{TM}, F^*)$.

The justification of this construction is as follows. In Ref. 10 the existence of a map from the Finsler category to the Riemannian category relating the most important geometric notions was proved. This map was basically interpreted as an "average" of the Finslerian objects (although in Ref. 10 we formulated our mathematical construction mainly related with the so-named Chern's connection. However, it was noted that a similar average operation is also applicable to other connection as the Cartan connection or in general to any linear connection in $\pi^*\mathbf{TM}$. We also think that the construction is also extendable to the nonlinear connection, a very important notion in Finsler geometry). Here we remark that this average operation is also applicable to the Hamiltonian operator after canonical quantization of the classical Hamiltonian because it is constructed using the Finsler function. This average is interpreted as a long term evolution of the initial Hamiltonian. Another more physical reason to integrate only over $\mathbf{I}_x^*$ is the "holographic principle in phase space": all the quantum information is contained in a submanifold of dimension $n-1$, in this case the indicatrix $\mathbf{I}_x^*$. This holographic principle is formulated in the phase space instead of the normal formulation in the configuration space and appears as a reinterpretation of the positive homogeneity requirement. It seems to be possible to translate this construction to the configuration space just through a generalized Fourier transformation.

The above average Hamiltonian function has an associated quantum operator (better a density operator) $\langle \hat{\mathbf{H}} \rangle$. This operator is defined by the action on an arbitrary element of the Hilbert space of the states of defined generalized coordinates:

$$\langle \mathbf{H} \rangle_x(\hat{X},\hat{P})|p\rangle := \int_{\mathbf{I}_x^*} \hat{\mathbf{H}}(\hat{X},\hat{P})|\psi(x,p)|^2|p\rangle d^{6N-1}p = \int_{\mathbf{I}_x^*} (\mathbf{H}(x,p)|\psi(x,p)|^2)|p+G(x)\rangle d^{6N-1}p,$$
$$\forall\, |p\rangle \in \mathcal{H}. \tag{3.7}$$

The average quantum Hamiltonian density operator $\langle \hat{\mathbf{H}} \rangle(\hat{X},\hat{P})$ is linear. $\{|p\rangle\}$ is the set of vectors such that the Finsler norm is 1: $\hat{P}^i|p\rangle = p^i|p\rangle$ with $F^*(x,p)=1$. The function $G(x)$ is the translation produced by the operators $\hat{X}^i$ on the momentum state $|p\rangle$, computable from the canonical conditions and the form of the operators $\beta^i(\hat{X})$.

The first property of the above Hamiltonian (3.7) comes from the definition of Randers space. All the terms are bounded and positively defined because the functions $\{\beta^i\}$ are bounded and also because we are integrating only over the indicatrix $\mathbf{I}_x^*$. Therefore we obtain the following result.

Theorem 1: *Let* $(\mathbf{TM}, F^*)$ *be a Randers space. Then there is a deterministic system with the average Hamiltonian density defined by relation (3.7) and with* $\hat{\mathbf{H}}$ *defined by Eq. (3.6). Then the average Hamiltonian* $\langle \mathbf{H} \rangle_x$ *is bounded.*

The local converse of this result also holds, proving the generality of the connection between deterministic systems and Randers geometry,

Theorem 2: *Let* $\hat{\mathbf{H}} = 2\beta^i(\hat{X})\hat{P}_i$ *be a quantum Hamiltonian operator describing a deterministic system. Suppose that the average Hamiltonian is bounded. Then there is a Randers structure that reproduces the above Hamiltonian, and the Randers function is defined locally at one point by the expression*

$$F(x,p) = \sqrt{\delta_{ij}p^i p^j} + f_i p^i.$$

Proof: We read from the Riemannian metric and the 1-form that characterizes the Randers structure from the Hamiltonian; the Hamiltonian of a deterministic system is of the form $\mathbf{H} = f^i(x)p$. We associated the following structure locally such that at the point x it is given by

$$a_{ij} = \delta_{ij}, \quad 2\beta^i(x) = f^i(x),$$

where the functions $f^i(x)$ characterize the deterministic system. That the final Hamiltonian is bounded implies that the functions $\beta^i(x)$ are also bounded, which is a fundamental requirement to obtain a Randers function.

It is important to note that the Randers structure of the thesis of Theorem 3.2 and the Randers structure of the hypothesis of Theorem 3.1 are not the same. The reason is because they describe different deterministic systems. In addition, let us note that the Riemannian structure $a_{ij}=\delta_{ij}$ is arbitrary: our choice was the simplest one, but it can be constrained because of the topology of the manifold **TM** (although locally the Finsler structure resembles the one in Theorem 3.2) and of the physical consistency, as we will see (β should be bounded by a_{ij}). When the metric a is given globally we can extend *beta*, defining a Randers space in the whole manifold **TM**, assuming that it is simply connected.

Another consequence of the geometric origin of the Hamiltonian is that because the requirements that F^* is a Randers function, the functions $\{\beta^i\}$ are bounded. This implies that generalized velocities and accelerations of the particles are bounded,

Corollary 3: *Consider a deterministic system associated with a Randers space. Then the generalized speed and acceleration of any physical subsystem are bounded.*

This consequence is interesting because it means the following for our model. From the geometric point of view, bounded means to respect the metric structure a_{ij} of the given Randers structure (α, β). Because both accelerations and velocities can become observables in some models, this also happens with the metric a_{ij}, which becomes not arbitrary and dynamical. The problem of finding the correct structure such that the 1-form β is bounded with the Riemannian metric a_{ij} implies some additional hypothesis concerning the dynamical behavior of both.

As consequence of the existence of a maximal physical acceleration, there is a limit for the strength of the gravitational field, if the strong equivalence principle holds. Therefore we are dealing with a theory that contains a finite gravitational interaction.

A simple mechanical model can give an estimation of the value of the maximal acceleration. Suppose that the universe has a limited energy content, there is a minimal distance L_p, the maximal speed is c, and the ontological degrees of freedom of the model describe the molecules of a classical gas. We can write the elementary work that the rest of the universe can make on a defined subsystem. Since this maximal work is equivalent to the energy of the particles involved, we obtain the relation

$$L_p m a_p \sim \delta m c^2.$$

The maximal exchange of energy is bounded by $\sim M_U c^2$, where M_U is the equivalent mass of the total energy of the universe, excluding the subsystem considered. The mass m appearing in the left side is just the mass of the particle, and if this mass is the Planck mass M_p, then

$$a_p \sim \frac{M_U}{M_p}\frac{c^2}{L_p}.$$

This acceleration is very huge when L_P is the Planck scale,

$$a_p \sim \frac{M_u}{M_p} 10^{52}\ \mathrm{m/s^2}.$$

If the change in the state of the subsystem is only produced by the neighborhood of the elementary particle, then instead of M_U there is a mass comparable to m. Therefore the maximal acceleration is

$$a_p \sim 10^{52}\ \mathrm{m/s^2}.$$

Note that this acceleration is independent of the mass of the particles. This implies that the equivalence principle for the maximal acceleration holds in this limit. In addition, this example

shows the equivalence between the maximal acceleration and a minimal length L_p, when there is a maximal speed c.

As another example of application of our geometric formalism, let us consider the Hamiltonian describing a deterministic system with 12 degrees of freedom associated with two pairs of particles living in a space **M** of dimension three. The symmetry group of the Hamiltonian is contained in the group $O(12)$ because it is the Euclidean product of two vectors of a 12-dimensional space (by associated particles we mean a pair of identical particles such that they are at the same position but one is moving forward and the other backward on the external time t). Let us consider a particular configuration describing a system of two correlated pairs of associated particles and their environment. The symmetry group for this special configuration contains the group $O(6)\times O(6)\times G$, where the first two terms $O(6)$ describe the symmetry related with the two separated pair of particles and G determines the symmetry of any other subsystem. This configuration implies a spontaneous symmetry break of the group $O(6N)$,

$$O(6N) \to O(6) \times O(6) \times G.$$

This symmetry break produces Goldstone's bosons that we consider part of the environment.

Consider the subsystem composed of two correlated pairs. The symmetry of this Hamiltonian is $O(6)\times O(6)$. The existence of an internal time t implies the existence of the time inversion transformation $\hat{T}$ defined by the action on the generalized canonical coordinates (let us recall that the velocity y is also considered as a coordinate in the Hilbert space approach to deterministic systems),

$$(x,y) \to (x,-y).$$

Invariance of the canonical quantization implies the transformation

$$(\hat{P}_x,\hat{P}_y) \to (-\hat{P}_x,\hat{P}_y),$$

because the time inversion is an antiunitary transformation on the Hilbert space.[11] A similar transformation for the classical momentum holds.

We remark that the consistency of this splitting of the cotangent space $\mathbf{T}^*\mathbf{TM}$ is based on the existence of an additional geometric structure associated with the time inversion $\hat{T}$. This additional structure again breaks the symmetry of the Hamiltonian,

$$O(6) \times O(6) \to O^2(3) \times O^2(3).$$

Because the physical system is deterministic and has a well defined momentum and generalized position values, it is in a particular defined state. The evolution of these states is in a one-to-one correspondence with the 1-form $(\beta^1_-(1),\beta^2_-(1),\beta^3_-(1),\beta^1_+(1),\beta^2_+(1),\beta^3_+(1))$ describing the evolution of the first pair and $(\beta^1_-(2),\beta^2_-(2),\beta^3_-(2),\beta^1_+(2),\beta^2_+(2),\beta^3_+(2))$ for the second (the notation $\pm$ corresponds to the splitting induced by time inversion in $\mathbf{T}_x\mathbf{M}$). But when the system follows the evolution guided by a particular value of the above forms, the symmetry is again broken,

$$O^2(3) \times O^2(3) \to O^2(2) \times O^2(2).$$

The final group $O^2(2)\times O^2(2)$ because it is the biggest group preserving a particular deterministic evolution.

Therefore it is not possible that the system could hold a nontrivial irreducible representation of the rotation group $SO(3)$ consistent with a deterministic evolution: the symmetry group for a defined system of two correlated pair of particles at the Planck scale is $O^2(2)\times O^2(2)$. This group is not enough to contain the rotation group $SO(3)$.

Theorem 4: *For a deterministic system composed by two correlated, identical pairs of associated particles with energies at the Planck scale, there is not a nontrivial irreducible representation of the rotation group leaving invariant the deterministic evolution defined by particular values of the beta function.*

One consequence of this fact is that the ordinary proof of Bell's inequalities for spin does not hold at the Planck scale for this system. The reason is that the proof uses the rotation symmetry and it does not hold for deterministic systems at this scale. Even the notion of spin is not truly defined in this context. Therefore the claim is that Bell's inequalities for spin does not hold for deterministic Finslerian models.

At ordinary energies the breaking $O^2(3)\times O^2(3)\rightarrow O^2(2)\times O^2(2)$ is not given. Only at high energies of order of the Planck scale can we expect this break because it means that the system cannot decouple from the ambient in a way that rotation transformations of the system make sense. However, at ordinary scales this decoupling indeed does make sense and the above symmetry break does not hold.

This possible absence was anticipated by 't Hooft and is independent of the nature of the model, Finslerian or not. Here we remark the geometric character of this phenomenon in the case of Finslerian deterministic models.

IV. DISCUSSION

The relations between the Finsler structure $(\mathbf{TM},F^*)$ and the Riemannian structure $(\mathbf{TM},h)$ are described in Ref. 10 (indeed the case of a general, smooth manifold $\mathbf{M}$ was considered). In addition, the existence of a map from the category of Finsler spaces to the category of Riemannian spaces mapping the Chern connection of F (generally, any linear connection living in $\pi^*\mathbf{M}$) to a linear connection on $\pi^*\mathbf{TM}$ and the hh curvature to the curvature of this linear connection was shown. These transformations can be interpreted as "average" operations of the Finsler structures and objects. The physical interpretation of these averages is that the Finsler structure living in the phase space manifold $\mathbf{T}^*\mathbf{TM}$ evolves after a long term to the equilibrium described by the Riemannian structure $(\mathbf{TM},h)$. This Riemannian structure describes the geometry of the phase space when the systems of all ontological states reach the equilibrium. However, the Hamiltonian describing the evolution of the averaged system when the system has evolved after a long term is not the Hamiltonian coming from the "average" Finsler structure $(\mathbf{TM},h)$ (that is indeed Riemannian). The reason is because these averaged physical systems are not systems of fundamental particles at the Planck scale, but could be composite objects like strings. Since they do not have times as small as the Planck time L_p/c, the Hamiltonian guiding their dynamics is the average Hamiltonian $\langle\hat{H}\rangle$, not the deterministic Hamiltonian based on the geometric structure, Finslerian or Riemannian.

When the system arrives into the equilibrium, the Finsler structure is just the Riemannian structure $(\mathbf{TM},h)$. From the definition of the fundamental or ontological Hamiltonian (3.6), we obtain in the equilibrium the condition

$$\hat{\mathbf{H}}=0.$$

The existence of macroscopic matter structures and gravity can be associated with the following decomposition:

$$\hat{\mathbf{H}}=\langle\hat{\mathbf{H}}\rangle+\delta\hat{\mathbf{H}}=\hat{\mathbf{H}}_{\text{matter}}+\delta\hat{\mathbf{H}}.$$

If we take the average of each member of this relation, one obtains at equilibrium

$$\langle\hat{\mathbf{H}}\rangle=\langle\langle\hat{\mathbf{H}}_U\rangle\rangle+\langle\delta\hat{\mathbf{H}}\rangle=\hat{\mathbf{H}}_{\text{matter}}+\langle\delta\hat{\mathbf{H}}\rangle=0.$$

We associate $\langle\hat{\mathbf{H}}_U\rangle=\hat{\mathbf{H}}_{\text{matter}}$, $\langle\delta\hat{H}\rangle=\hat{\mathbf{H}}_{\text{gravity}}$. Therefore in this model the distinction between matter and gravity appears as result of a long term evolution of the ontological states. Also it appears remarkable that while in equilibrium gravity appears to compensate matter, at nonequilibrium (that is when the structure is Finslerian) there is some kind of pregravity interaction, described by the Hamiltonian $\delta\hat{\mathbf{H}}$. The qualitative characteristic of this interaction should be study further. Matter seems identical (the particle content seems complete identical because the Hamiltonian for matter,

before and after average is the same $\langle \hat{\mathbf{H}} \rangle$. This fact implies the universality of our formalism in order to get any quantum system from a deterministic model.

Connecting with the 't Hooft theory, we describe in a geometric way the projection from an ontological state to an equivalence class as follows:

The projection after a long term evolution of a deterministic system to the equilibrium equivalence class is described by the transformation that averages the dual Finsler structures living in the manifold $\mathbf{T}^*\mathbf{TM}$.

It is a remarkable consequence of the Finslerian 't Hooft models that we obtain the prediction of the value of a maximal acceleration and speed for physical systems. This can be interpreted as the requirement of the existence of two natural constants by geometric consistency. In addition, the possible absence of Bell's inequalities for spin is a remarkable prediction for the general 't Hooft models: these inequalities are the main obstructions for the construction of hidden variables theories. In the present paper we have shown that the absence of Bell's inequalities is possible at the Planck scale, where not decoupling of the system with the ambient is taken and even the notion of three-dimensional rotations become unclear. This explanation is simultaneous with the prediction of the existence of pregravity interaction in a natural way. Therefore it is possible to construct the hidden variables theories at this energy without the introduction of nonlocal actions, and the mechanisms could be promoted by a pregravity interaction.

That all of the 't Hooft models have a local geometric interpretation in terms of Finsler geometry and the geometric origin of a microscopic time arrow obtained from the geometric data are the mayor goals of these models. In addition, we can motivate a deterministic model based in some construction of a Randers space containing interactions. Unfortunately, the model is not completely defined by the geometry and physical hypothesis should be introduced.

We start reviewing the treatment of 't Hooft of a deterministic system with a dissipative dynamics.[1] The quantum Hamiltonian i:

$$\hat{\mathbf{H}} = \vec{p} \cdot \vec{f}(\vec{g}).$$

Consider a scalar operator $\rho(\vec{q})$ such that $[\rho(\vec{q}), \hat{\mathbf{H}}]=0$. Then we can perform the following decomposition:

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_1 - \hat{\mathbf{H}}_2, \tag{4.1}$$

with

$$\hat{\mathbf{H}}_1 = \frac{1}{4\rho}(\rho^2 + \hat{\mathbf{H}})^2, \quad \hat{\mathbf{H}}_2 = \frac{1}{4\rho}(\rho^2 - \hat{\mathbf{H}})^2.$$

Both Hamiltonians commute, $[\hat{\mathbf{H}}_1, \hat{\mathbf{H}}_2]=0$.

In order to bound from below the complete Hamiltonian, one can introduce the constraint than on physical states the following condition holds:

$$\hat{\mathbf{H}}|\psi\rangle \to 0. \tag{4.2}$$

That should be understood as a long term evolution statement: the physical system evolves to states obeying condition (4.2). This constraint immediately implies the bound of the Hamiltonian:

$$\hat{\mathbf{H}} \to \hat{\mathbf{H}}_1 \to \rho^2 \geq 0.$$

These constraints can be motivated first if we mimic the system in terms of a nondissipative model and where the system corresponds to a quantum oscillator, where all the "orbits" are stable such that $\hat{\mathbf{H}}=\vec{p}\cdot\vec{f}(\vec{g})$ holds and such that $[H_s, \rho^2]=0$.

The stable orbits are restricted by the condition

$$e^{-\hat{\mathbf{H}}T}|\psi\rangle = |\psi\rangle, \tag{4.3}$$

where T is the period of the orbit $\rho=1$. This condition, equivalent to constraint (4.2), implies the limitation of trajectories to stable orbits at equilibrium.

Let us compare this construction with a parallel construction using Finslerian models. One starts directly with a classical Hamiltonian of the form

$$H = F(\vec{q},\vec{p}) - F(\vec{q},-\vec{p}).$$

After canonical quantization, we identify $\hat{\mathbf{H}}_1 = F(\vec{q},\vec{p}) = \alpha+\beta$, $\hat{\mathbf{H}}_2 = F(\vec{q},\vec{p}) = \alpha-\beta$.

We propose the constraint $\rho=1$ on physical states. It is equivalent to an average operation defined in the following way:

$$h_{ij} = \int_{\mathrm{S}} g_{ij}(x,y), \tag{4.4}$$

where the integration is done on the sphere $\mathbf{S}^{6\mathbf{N}-1} \subset \mathbf{T}_u^*\mathbf{T}_x\mathbf{M}$.

Taking this average in the underlying geometric structure corresponds to constrain the values of the quantum states: after a long term evolution, the physical states arrive to the submanifold $\mathbf{S}^{6\mathbf{N}-1}$.

Suppose now the system is composed of two identical elementary systems, with their dynamics described by a deterministic Hamiltonian of the form (4.1). Let us suppose they are modeled on Randers spaces, so their Hamiltonians are determined by (α_1,β_1) and (α_2,β_2). The 1-forms $\beta_i, i=1,2.$ have a norm of less than 1 by the corresponding Riemannian norms $\alpha_i, i=1,2$. There are at least two ways to produce a bigger Randers space using just the above geometric data:

1. The first way is valid for complete general structures

$$\alpha = \alpha_1 \oplus \alpha_2, \quad \beta = \beta_1 \oplus \beta_2.$$

   This construction does not produce interaction terms in the total Hamiltonian. There is *a priori* no relation $\alpha_1\alpha_2$.
2. The second form recovers the impossibility for an external observer to differentiate between identical particles:

$$\vec{p} = \vec{p}_1 \times \vec{0} + \vec{0} \times \vec{p}_2, \quad \vec{\beta} = \vec{\beta}_1 \times \vec{0} + \vec{0} \times \vec{\beta}_2,$$

$$\alpha = \alpha_1 \oplus \alpha_2, \quad \alpha_1 = \alpha_2.$$

   The quantum total Hamiltonian is given by

$$\vec{\beta}(\vec{p}) = \left(\frac{1}{2}\vec{\beta}_1(\vec{p}_1) + \vec{\beta}_1(\vec{p}_2) + \vec{\beta}_2(\vec{p}_1) + \vec{\beta}_2(\vec{p}_2)\right).$$

   The mixed terms produce the interaction. The condition $\alpha_1=\alpha_2$ ensures that the above construction is a Randers space.

In order to conclude the discussion we would like to discuss our idea with some recent applications of Finsler geometry in physics (see Ref. 6 and references therein). Our application of Finsler geometry and in particular, of Randers spaces, seems new even if it contains elements that have been already used in other contests. Considerable work was performed on higher order mechanics and generalized Finsler spaces (see Refs. 7–9 and also Ref. 6), but the bird of deterministic models at the Planck scale is very recent and the application of Finsler geometry presented in this paper is also new. In addition, we remark that we are not concerned at this stage with a field theory for these deterministic systems, but with the general formalism that we could use to describe them. Finsler geometry is rather intrincately complex with so many natural connections,

for instance, like Chern's or Cartan's connections. Also the notion of nonlinear connection is of fundamental importance. But we are not concern with these important topics in this paper because the construction proposed involves only notions at the metric level: our average is a universal procedure, valid for any linear connection $\pi^*\mathbf{TM}$. Further research can provide a mechanism to select a right d connection for a field theory of deterministic degrees of freedom. In addition, some additional research is needed to understand the extension of the average operation applied to the nonlinear connection.

APPENDIX: BASIC RESULTS ON FINSLER GEOMETRY FOR DETERMINISTIC SYSTEMS

In this Appendix we recall the basic notions of Finsler geometry used in the present work. The main reference for this Appendix is Ref. 4. We present the notions for an arbitrary smooth manifold $\mathbf{M}$.

Let $(x,\mathbf{U})$ be a local coordinate system over a point $x \in \mathbf{M}$, where $x \in \mathbf{U}$ have local coordinates $(x^1,\ldots,x^n)$, $\mathbf{U} \subset \mathbf{M}$ is an open set, and $\mathbf{TM}$ is the tangent bundle. We use Einstein's convention for up and down equal indices in this work.

A tangent vector at the point $x \in \mathbf{M}$ is denoted by $y^i(\partial/\partial x^i) \in \mathbf{T}_x\mathbf{M}$, $y^i \in \mathbf{R}$. We also denote by $\mathbf{TM}$ the set of sections of the tangent bundle. We can identify point x with its coordinates $(x^1,\cdots,x^n)$ and the tangent vector $y \in \mathbf{T}_x\mathbf{M}$ at x with its components $y=(y^1,\cdots,y^n)$. Then each local coordinate system $(x,\mathbf{U})$ induces a local coordinate system in $\mathbf{TM}$ denoted by $(x,y,\mathbf{U})$ such that $y=y^i(\partial/\partial x^i) \in \mathbf{T}_x\mathbf{M}$ has local natural coordinates $(x^1,\cdots,x^n, y^1,\cdots,y^n)$.

Let us denote by $\mathbf{N}=\mathbf{TM}\backslash\{0\}$. The notion of a Finsler structure is given through the following definition.

Definition 1: A Finsler structure F on the manifold $\mathbf{M}$ is a non-negative, real function $F:\mathbf{TM}\to[0,\infty[$ such that

1. *It is smooth in the split tangent bundle $\mathbf{N}$.*
2. *Positive homogeneity holds: $F(x,\lambda y)=\lambda F(x,y)$ for every $\lambda>0$.*
3. *Strong convexity holds: the Hessian matrix*

$$g_{ij}(x,y) := \frac{1}{2}\frac{\partial^2 F^2(x,y)}{\partial y^i\,\partial y^j} \tag{A1}$$

is positively definite in $\mathbf{N}$.

We also denote by a Finsler structure in $\mathbf{M}$ the pair $(\mathbf{M},F)$.

The minimal smoothness requirement for the Finsler structure is $\mathcal{C}^5$ in $\mathbf{N}$ when second Bianchi identities are used; more generally only, a $\mathcal{C}^4$ differentiable structure is required. The matrix $g_{ij}(x,y)$ is the matrix components of the fundamental tensor g. The homogeneity condition can be stronger: $F(x,\lambda y)=|\lambda|F(x,y)$. Then $(\mathbf{M},F)$ is called the absolutely homogeneous Finsler structure.

Example 2: A Randers space is characterized by a Finsler function of the form

$$F(x,y) = \alpha(x,y) + \beta(x,y), \tag{A2}$$

where $\alpha(x,y)=a_{ij}(x)y^iy^j$ is a Riemannian metric and $\beta(x,y)=\beta_i(x)y^i$. The requirement of being g_{ij} positively definite implies that the 1-form $(\beta_1,\cdots,\beta_n)$ is bounded, using the above Riemannian metric α. Examples of Randers spaces can be found, for instance, in Refs. 4 and 5.

Definition 3: (Ref. 4) *Let $(\mathbf{M},F)$ be a Finsler structure and $(x,y,\mathbf{U})$ a local coordinate system induced on $\mathbf{TM}$ from the coordinate system $(x,\mathbf{U})$ of $\mathbf{M}$. The Cartan tensor components are defined by the set of functions*

$$A_{ijk} = \frac{F}{2}\frac{\partial g_{ij}}{\partial y^k}, \quad i,j,k = 1,\ldots,n. \tag{A3}$$

These coefficients are homogeneous of degree zero in $(y^1,\ldots,y^n)$. In the Riemannian case A_{ijk} are zero and this fact characterizes Riemannian geometry from other types of Finsler geometries (Deicke's theorem).

Since the components of the fundamental and Cartan's tensors have a dependence on the tangent vector y, it is natural to use a manifold other than $\mathbf{M}$ to study Finsler geometry. One possible construction is the following: consider $\pi^*\mathbf{TM}$, the pullback bundle of $\mathbf{TM}$ by the projection

$$\pi:\mathbf{N}\to\mathbf{M}. \tag{A4}$$

The vector bundle $\pi^*\mathbf{TM}$ has as a base manifold $\mathbf{N}$, the fiber over the point $u=(x,y)\in\mathbf{N}$ is diffeomorphic to $\mathbf{T}_x\mathbf{M}$ for every point $u\in\mathbf{N}$ with $\pi(u)=x$, and the structure group is diffeomorphic to $\mathbf{GL}(n,\mathbf{R})$.

The vector bundle $\pi^*\mathbf{TM}\subset\mathbf{TM}\times\mathbf{N}$ and the projection on the first and second factors are given by

$$\pi_1:\pi^*\mathbf{TM}\to\mathbf{N}, \tag{A5}$$

$$\pi_2:\pi^*\mathbf{TM}\to\mathbf{TM}. \tag{A6}$$

$\pi^*\mathbf{TM}$ is completely determined as a subset of $\mathbf{TM}\times\mathbf{N}$ by the following relation; for every $u\in\mathbf{N}$ and $\xi\in\pi_1^{-1}(u)$,

$$(u,\xi)\in\pi^*\mathbf{TM}\quad\text{iff}\quad\pi\circ\pi_2(u,\xi)=\pi(u). \tag{A7}$$

A similar construction $\pi^*\mathbf{TM}$ can be performed over $\mathbf{SM}$, the sphere bundle over $\mathbf{N}$.

One essential notion in Finsler geometry is the nonlinear connection. We introduce the nonlinear connection coefficients, defined by the formula

$$\frac{N_j^i}{F}=\gamma_{jk}^i\frac{y^k}{F}-A_{jk}^i\gamma_{rs}^k\frac{y^r}{F}\frac{y^s}{F},\quad i,j,k,r,s=1,\ldots,n$$

where the *formal second kind Christoffel's symbols* γ_{jk}^i are defined in local coordinates by the formulas

$$\gamma_{jk}^i=\frac{1}{2}g^{is}\left(\frac{\partial g_{sj}}{\partial x^k}-\frac{\partial g_{jk}}{\partial x^s}+\frac{\partial g_{sk}}{\partial x^j}\right),\quad i,j,k=1,\ldots,n;$$

$A_{jk}^i=g^{il}A_{ljk}$, and $g^{il}g_{lj}=\delta_j^i$. Note that the coefficients N_j^i/F are invariant under the scaling $y\to\lambda y$, $\lambda\in\mathbf{R}^+$, $y\in\mathbf{T}_x\mathbf{M}$.

Let us consider the local coordinate system $(x,y,\mathbf{U})$ of the manifold $\mathbf{TM}$. A tangent basis for $\mathbf{T}_u\mathbf{N},u\in\mathbf{N}$ is defined by the distributions[4]

$$\left\{\left.\frac{\delta}{\delta x^1}\right|_u,\cdots\left.\frac{\delta}{\delta x^n}\right|_u,F\left.\frac{\partial}{\partial y^1}\right|_u,\ldots,F\left.\frac{\partial}{\partial y^n}\right|_u\right\},$$

$$\left.\frac{\delta}{\delta x^j}\right|_u=\frac{\delta}{\delta x^j}{}_u-\left.N_j^i\frac{\delta}{\delta y^i}\right|_u,\quad i,j=1,\ldots,n.$$

The set of local sections

$$\left\{\left.\frac{\delta}{\delta x^1}\right|_u,\ldots,\left.\frac{\delta}{\delta x^n}\right|_u,u\in\pi^{-1}(x),x\in\mathbf{U}\right\}$$

generates the local horizontal distribution $\mathcal{H}_U$ while

$$\left\{ \left.\frac{\partial}{\partial y^1}\right|_u, \ldots, \left.\frac{\partial}{\partial y^n}\right|_u, u \in \pi^{-1}(x), x \in \mathbf{U} \right\}$$

the vertical distribution $\mathcal{V}_U$. The subspaces $\mathcal{V}_u$ and $\mathcal{H}_u$ are such that the following splitting of $\mathbf{T}_u\mathbf{N}$ holds:

$$\mathbf{T}_u\mathbf{N} = \mathcal{V}_u \oplus \mathcal{H}_u, \quad \forall\, u \in \mathbf{N}.$$

This decomposition is invariant by the action of $\mathbf{GL}(n,\mathbf{R})$ and it defines a nonlinear connection (a connection in the sense of Ehresmann) on the principal fiber bundle $\mathbf{N}(\mathbf{M},\mathbf{GL}(n,\mathbf{R}))$.

Theorem 4: (*Chern's connection*, Ref. 4) *Let* $(\mathbf{M},F)$ *be a Finsler structure. The vector bundle* $\pi^*\mathbf{TM}$ *admits a unique linear connection characterized by the connection 1-forms* $\{\omega^i_j, i,j = 1,\ldots,n\}$ *such that the following structure equations hold:*

1. "*Torsion- free*" *condition*,

$$d(dx^i) - dx^j \wedge w^i_j = 0, \quad i,j = 1,\ldots,n. \tag{A8}$$

2. *Almost g-compatibility condition*,

$$dg_{ij} - g_{kj}w^k_i - g_{ik}w^k_j = 2A_{ijk}\frac{\delta y^k}{F}, \quad i,j,k = 1,\ldots,n. \tag{A9}$$

Chern's connection is nonmetric compatible but has null torsion. Cartan's connection is completely metric compatible, but has torsion. The relation between the Cartan connection 1-forms $(\omega_c)^k_i$ in relation with the Chern connection ω^k_i 1-forms are given by[4]

$$(\omega_c)^k_i = \omega^k_i + A^k_{ij}\frac{\delta y^j}{F}.$$

At this point we should stress the importance of the Cartan connection on physical applications and in general of the metric connections in field theory.[6] Chern's connection is not metric compatible, which is a bit problematic for physical applications; it is preferable to use Cartan's connection or d-connection, which is metric compatible.

The manifold $\mathbf{I}_x$ is called the indicatrix and is defined by

$$\mathbf{I}_x := \{y \in \mathbf{T}_x\mathbf{M} | F(x,y) = 1\}.$$

Let us denote by $\mathcal{F}(\mathbf{I}_x)$ the set of real, smooth functions on the indicatrix $\mathbf{I}_x$. Then the average operation is defined as follows.

Definition 5: Let $(\mathbf{M},F)$ *be a Finsler structure. Let* $f \in \mathcal{F}(\mathbf{I}_x)$ *be a real, smooth function defined on the indicatrix* $\mathbf{I}_x$ *and* $(\psi,\mathbf{I}_x)$ *the invariant measure. We define the map*

$$\begin{gathered} \langle\cdot\rangle_\psi : \mathcal{F}(\mathbf{I}_x) \to \mathbf{R} \\ f(x,y) \to \frac{1}{\mathrm{vol}(\mathbf{I}_x)} \int_{\mathbf{I}_x} d\,\mathrm{vol}\ \psi(x,y) f(x,y). \end{gathered} \tag{A10}$$

In the case of smooth Finsler structures the coefficients $\{h_{ij}, i,j = 1,\ldots,n\}$ are smooth in $\mathbf{M}$. They are the components of a Riemannian metric in $\mathbf{M}$.

Proposition 6: Let $(\mathbf{M},F)$ *be a Finsler structure. Then the functions*

$$h_{ij}(x) := \langle g_{ij}(x,y)\rangle, \quad \forall\, x \in \mathbf{M} \tag{A11}$$

are the components of a Riemannian metric in $\mathbf{M}$ *such that in a local basis* $(x,\mathbf{U})$ *is*

$$h(x) = h_{ij}dx^i \otimes dx^j. \tag{A12}$$

We should mention that the restriction on the indicatrix $\mathbf{I}_x$ in the integration is not necessary: we can perform similar averages procedures on any compact submanifold of codimension 1 and also of codimension 0 (see Ref. 10, Propositions 3.13 and 3.14). Indeed, Proposition 3.14 of Ref. 10 implies that we can take the limit of the whole tangent bundle, provided a convenient normalization is used.

The average operation can be extended to obtain average connections and average curvatures.[10] This fact can be used to introduce a field theory based on connections as fundamental variables for deterministic theories at the Planck scale.

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Quantum graphs as holonomic constraints

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We consider the dynamics on a quantum graph as the limit of the dynamics generated by a one-particle Hamiltonian in $\mathbb{R}^2$ with a potential having a deep strict minimum on the graph, when the width of the well shrinks to zero. For a generic graph we prove convergence outside the vertices to the free dynamics on the edges. For a simple model of a graph with two edges and one vertex, we prove convergence of the dynamics to the one generated by the Laplacian with Dirichlet boundary conditions in the vertex. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Several physical systems, like electronic nanostructures or periodic solids made up of aromatic molecules, display the common feature that the motion of the electrons can be thought of as being confined in one or more directions by a strong potential barrier, which prevents the particles from escaping from the structure and allows propagation in the remaining (free) directions.

In solid state physics, a concrete example of this phenomenon is given by quantum wires and carbon nanotubes, where the high purity achieved in fabrication techniques and the weakness of electron-phonon interaction give rise to ballistic transport. Therefore, using the strong-coupling method, one can in first approximation model the interaction of electrons with the crystal assuming that they move freely with an effective mass m [a more detailed discussion of the physical hypotheses on which this approximation is based can be found in Duclos and Exner (1995), Londergan *et al.* (1999)].

Taking into account the strong potential barrier which keeps them confined, their dynamics are then given by the one-particle Hamiltonian

$$\hat{H}_\varepsilon := -\frac{1}{2}\Delta + \frac{1}{2\varepsilon^2}W(q), \tag{1}$$

where we have chosen suitable units so that $\hbar$ and the effective mass are equal to 1.

The parameter ε is the natural small parameter of the problem and is linked to the ratio l/L, where L is the characteristic length of the wire along the free direction where the electrons can propagate and l is the analogous length in the confined directions.

In general, the function W is assumed to be zero on the quantum wire and strictly positive outside, so that when ε becomes small one expects the electron to be better and better confined to the wire. For this reason, W is called the *constraining potential*.

Our aim in this paper is to analyze the dynamics generated by (1) in the limit $\varepsilon \to 0$ for two-dimensional systems constrained to a singular one-dimensional manifold given by a graph Γ.

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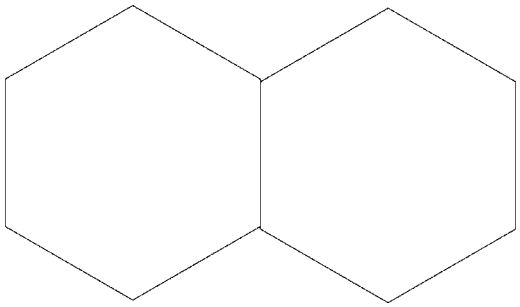


FIG. 1. Skeleton of naphthalene molecule.

We consider an explicit form of the constraining potential, i.e., the square of the distance of a point from the graph. This potential is obviously continuous, but does not belong to $C^1(\mathbb{R}^2)$, because of the vertices. Outside the vertices, the potential is a quadratic function of the coordinates, so it can be regarded as the first nonzero term of the Taylor expansion of more general functions which are zero on the graph, and whose gradient is zero on the edges. This is the natural class of constraining potentials considered in the literature to model holonomic constraints in classical and quantum mechanics [Bornemann (1998), Froese and Herbst (2001), and references therein]. We will argue that the results we find can be generalized to a wider class of potentials, whose Taylor expansion near the graph contains higher order terms.

As it is clear from the brief remarks given above, this case is relevant for solid state physics in order to determine the leading order behavior for the dynamics of electrons moving in a *branched* nanostructure, made up of several wires which meet in a crossing region represented by the vertices of the graph in the limit $\varepsilon \to 0$.

Another important field where Equation (1) can be applied is given by theoretical chemistry, in the so-called quantum network model (QNM) [for a recent review which contains also some comparison with experimental data see Amovilli *et al.* (2004) and references therein]. This model is used to study the motion of valence electrons (also called π-electrons) in aromatic molecules or periodic solids like graphene. In first approximation, they are thought to move freely through the skeleton of the molecule determined by σ-electrons, which create a potential keeping π-electrons confined to the molecular structure. The most famous example, described in Fig. 1, is probably naphthalene molecule, first studied by Ruedenberg and Scherr (1953).

The characteristic feature shared by the examples presented is that we always expect the limiting dynamics to take place on a graph, on which we must define a suitable Hamiltonian. The couple made up of the graph and a differential or pseudodifferential self-adjoint operator defined on it is usually called quantum graph [a detailed review on this topic is given in Kuchment (2002, 2004, 2005)].

The main problem one runs into if one wants to describe the physical systems mentioned above by a quantum graph is that there are a host of self-adjoint Hamiltonians which can be defined on it.

If, for example, one assumes that the dynamics outside the vertices is free, i.e., that the Hamiltonian is the Laplacian $-d^2/\mathrm{d}x^2$, where x is the natural arc length coordinate on the edges of the graph, and that the graph has one vertex and n edges, then the possible self-adjoint extensions are determined by n^2 parameters [Kostrykin and Schrader (1999)].

To eliminate this ambiguity, a natural procedure is to consider the quantum graph as a limit of a more realistic model. We call the method employing a strong constraining potential a *soft approximation* of the graph. As we have pointed out above, this is a physically reasonable approximation, which, for a smooth constraint, has been investigated, e.g., in Belov *et al.* (2004), Dell'Antonio and Tenuta (2004), Froese and Herbst (2001). As far as the authors' knowledge is concerned, the remark by Kuchment (2002) that "the graph case (i.e., in the presence of vertices) has not been explored" is still largely true.

Another appropriate choice, which we call *rigid approximation* of quantum graphs, is to consider a "thickened graph," composed in the simplest cases of thin tubes of radius ε, which has the same topology as the original graph and reduces to it when ε goes to zero. It is reasonable to suppose that the motion of the electron in this thickened structure is free, but one needs to specify boundary conditions to get a well-defined Laplacian. The most natural choice is to use Dirichlet boundary conditions, which correspond to an infinite constraining potential barrier. Some light on this case has been shed in two recent papers by Molchanov and Vainberg (unpublished) and Post (2005).

Post considers thickened graphs which near the vertices are strictly *smaller* than the ones defined by the distance function,

$$V_{\varepsilon,\Gamma} := \{(x,y) \in \mathbb{R}^2 : d_\Gamma(x,y) \leqslant \varepsilon\}, \tag{2}$$

and shows convergence to the Laplacian with Dirichlet boundary conditions at the vertices of the graph. This limitation on the size of the neighborhoods gives another reason why the study of a constraining potential equal to the square of the distance is interesting.

Molchanov and Vainberg analyze a somewhat less realistic model, where separation of variables is possible, and are interested in the asymptotic expansion of the solutions to the scattering problem on the thickened graph to the solutions of a problem on the quantum graph. Even though they are in a stationary setting, they conclude that, near the threshold of the absolutely continuous spectrum, one gets generically again Dirichlet boundary conditions at the vertices.

For technical reasons, however, much more attention has been devoted to the case of Neumann boundary conditions, which is by now well understood [Exner and Post (2005), Kuchment and Zeng (2001, 2003), Rubinstein and Schatzman (2001), Post (unpublished)].

We stress that, apart from Post (unpublished) and Molchanov and Vainberg (2006), all the papers we have quoted deal with the *convergence of the spectrum* of the Laplacian, defined on a thickened graph, to the spectrum of a self-adjoint operator, defined on a graph whose edges have finite length, while we are primarily interested in the convergence of the dynamics and eventually in scattering theory.

The dynamical problem for parabolic equations (diffusion processes) was studied by Freidlin (1996) and Freidlin and Wentzell (1993), who examined it in the context of the Neumann rigid approximation.

In the same setting, a weak form of resolvent convergence for the Laplacian was studied by Saitō [Saitō (2000, 2001)], but his results do not allow to infer the structure of time evolution.

In Post (unpublished) these results are improved, and norm resolvent convergence is established, under the hypotheses that the vertex neighborhoods are "small" (for the precise meaning of the term we refer to the original paper) and, for graphs embedded in $\mathbb{R}^2$, that the angle between two different edges has a global lower bound.

Another important difference in our paper is related to the class of initial conditions we consider. From a physical point of view, one expects that, when $\varepsilon \to 0$, the Hamiltonian (1) gives rise to fast oscillations of the electron in the directions orthogonal to the edges of the graph. To prove the results mentioned above, one projects, roughly speaking, on the ground state of this transverse oscillation. Nonetheless, in the spirit of adiabatic perturbation theory [Teufel (2003)] we expect to be able to get an effective dynamics inside every transverse subspace, because they become broadly separated in energy when ε goes to zero. For this reason, we consider initial wave functions which are localized inside one edge, and belong to an eigenspace of the transverse Hamiltonian (which will be defined more precisely in Sec. II).

We consider longitudinal initial conditions which are independent of ε. This corresponds to study longitudinal states which vary over a wavelength which is much bigger than the transverse one. As it has been stressed in Belov *et al.* (2004) however, longitudinal states are not homogeneous, and it would be interesting to consider also wave functions which vary on a scale of order $\varepsilon^{1/2}$, for example, analyzing in this way a semiclassical limit.

One should also remark that, in the Neumann case, the energy of the transverse ground state is independent of ε, because the Neumann Laplacian has always the eigenvalue zero correspond-

ing to the constant function, while in the Dirichlet and soft approximation cases, the energy of every transverse mode tends to infinity when $\varepsilon \to 0$. This makes it necessary to subtract a divergent phase to get a finite result.

We will now describe briefly the structure of this paper.

In Sec. II we study the convergence of the unitary group generated by (1) for an arbitrary graph (i.e., with an arbitrary number of vertices and edges). As we have already mentioned, we consider initial conditions which belong to a transverse eigenspace and are localized inside one edge of the graph and we choose a constraining potential given by the square of the distance of a point from the graph. Using weak convergence methods we study the limit flow on the graph outside the vertices. To describe completely the limit flow, we must study its structure in a neighborhood of the vertices.

This may be a difficult task; this can be seen from the exact treatment we give in Sec. III of a simpler system, in which the graph is a continuous curve in the plane.

In this example, the graph has one vertex and two straight edges at an angle $0 < \vartheta < \pi$. In this case we approximate the graph by a sequence of smooth curves converging to the graph when $\varepsilon \to 0$. We prove that generically (in particular if the curvature of the approximating curves is everywhere non-negative) the limit dynamics along the graph correspond to Dirichlet boundary conditions at the vertex.

The proof is achieved by reducing the problem to the study of the dynamics with Dirichlet boundary conditions on the boundary of narrow tubes containing the graph, using a refined version of a theorem due to Froese and Herbst (2001). This however is not possible for every smooth curve approximating the graph, and a condition on the curvature comes in. From this result, it seems that the constraining potential and Dirichlet boundary conditions are not always interchangeable, as one could naively think.

Even though the geometry of the graph is very simple, this model demonstrates a mechanism through which adiabatic decoupling among different transverse modes takes place. In particular, it shows that the bound states localized near the vertices that can arise [and indeed do arise if instead of the constraining potential one considers a narrow tube with Dirichlet boundary conditions, see Carini *et al.*(1992, 1993), Goldstone and Jaffe (1992)] do not interfere with the propagation of product states localized inside one of the edges *at the leading order*, because their spectral distance becomes infinite in the limit.

II. CONVERGENCE OUTSIDE THE VERTICES

In this section we consider a finite metric graph, denoted by Γ, whose edges can have infinite length. We assume that it is embedded in $\mathbb{R}^2$ and, for the sake of simplicity, that all the edges are straight lines.

We denote by $V=\{v_i\}_{i\in I}$ the (finite) set of vertices and by $E=\{e_j\}_{j\in J}$ the (finite) set of edges connecting them. We assume that there are no isolated vertices.

A graph is said to be a metric graph if to each edge e is assigned a length $l_e \in (0, +\infty]$. Edges of infinite length arise naturally if one considers scattering theory on graphs [see, e.g., Melnikov and Pavlov (1995) and references therein].

We can now identify each edge with a finite or infinite interval $[0, l_e]$, with the natural coordinate x_e along it. One can also define function spaces (e.g., L^p spaces, Sobolev spaces); in the case of Sobolev spaces, one must have some care at the vertices [see Kuchment (2004)].

As mentioned in the introduction, we approximate the dynamics on the graph using an Hamiltonian, acting on $L^2(\mathbb{R}^2)$, with a constraining potential given by the square of the distance from Γ,

$$\hat{H}(\varepsilon) = -\frac{1}{2}\Delta + \frac{1}{2\varepsilon^2} d_\Gamma^2,$$

$$d_\Gamma(q) := \inf_{\tilde{q}\in\Gamma}|q-\tilde{q}|, \quad q,\tilde{q}\in\mathbb{R}^2. \tag{3}$$

One could use a different potential, whose Taylor expansion away from the vertices contains higher order terms, but we make the important assumption that the Hessian is constant along the edges with the same value on all edges. This condition is reasonable in view of the analysis in Dell'Antonio and Tenuta (2004) and Froese and Herbst (2001) when the system is constrained to smooth submanifolds.

In this case, the energy of the transverse oscillation appears as a potential energy in the longitudinal motion, in the form $\omega(x)/\varepsilon$, where ω is the frequency of the oscillation. If ω does not depend on x, the resulting phase factor in the dynamics can be discarded. Otherwise, it originates a constraining potential along the edge, so that in the limit $\varepsilon\to 0$ we expect that the wave function concentrates along the minima of ω.

We denote by $\hat{U}_t(\varepsilon)$ the unitary evolution associated to Hamiltonian (3),

$$\hat{U}_t(\varepsilon) := \exp(-it\hat{H}(\varepsilon)), \tag{4}$$

and we take as initial a state which "lies in a subband," i.e., is in a fixed transverse mode and localized within one edge (see Fig. 2). These are the states which are thought to describe the propagation of particles in semiconductor structures.

We have then

$$\psi_0(x_{e_{j_0}}, y_{e_{j_0}}) = f(x_{e_{j_0}})\Phi_n^\varepsilon(y_{e_{j_0}}), \tag{5}$$

where $f\in C_0^\infty(0, l_{e_{j_0}})$ and Φ_n^ε is an eigenstate of the harmonic oscillator,

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2}+\frac{1}{2\varepsilon^2}y^2\right)\Phi_n^\varepsilon(y) = \frac{E_n}{\varepsilon}\Phi_n^\varepsilon(y),$$

$$E_n = n+\frac{1}{2}. \tag{6}$$

$x_{e_{j_0}}$ is the natural coordinate along the edge e_{j_0} and $y_{e_{j_0}}$ is the corresponding coordinate in the orthogonal direction. $x_{e_{j_0}}$ varies in the interval $[0, l_{e_{j_0}}]$ (or $[0,+\infty)$ if the edge has infinite length) and, since the edges are straight lines, $y_{e_{j_0}}$ is well defined and assumes values between $-\infty$ and $+\infty$ (to simplify the notation, from now we denote these coordinates just by x_j and y_j).

Applying $\hat{U}_t(\varepsilon)$ to ψ_0 we expect the appearance of a strongly oscillating factor, given by $\exp(-iE_nt/\varepsilon)$. To avoid this (irrelevant) phase, we consider the modified unitary group,

$$\tilde{H}(\varepsilon) := \hat{H}(\varepsilon) - \frac{E_n}{\varepsilon},$$

$$\psi_t^\varepsilon := \tilde{U}(\varepsilon)\psi_0 := \exp(-it\tilde{H}(\varepsilon))\psi_0. \tag{7}$$

To analyze the adiabatic decoupling, we split ψ_t^ε according to the different transverse components in each edge,

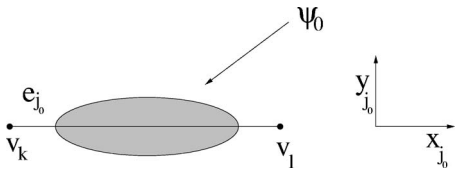


FIG. 2. Schematic representation of the initial state.

$$s_j^m(t,x_j;\varepsilon) := \int \mathrm{d}y_j\, \Phi_m^\varepsilon(y_j)^*\, \psi_t^\varepsilon(x_j,y_j),^1 \tag{8}$$

where x_j is the natural coordinate along e_j and y_j is orthogonal to it. (See Fig. 2)

Proposition 1: Let P_j^m be the operator from $\mathcal{S}(\mathbb{R}^2)$ to $H^k(\mathbb{R})$ defined by

$$P_j^m \psi(x_j) := \int_{\mathbb{R}} \mathrm{d}y_j\, \Phi_m^\varepsilon(y_j)^*\, \psi(x_j,y_j), \tag{9}$$

then P_j^m extends to a unique operator (of norm 1) from $H^k(\mathbb{R}^2)$ to $H^k(\mathbb{R})$, for every $k \in \mathbb{N}$, $k \geqslant 0$.

Proof. Given $\psi \in \mathcal{S}(\mathbb{R}^2)$ it is clear that

$$\begin{aligned}
\partial_x^l (P_j^m \psi)(x) &= \int_{\mathbb{R}} \mathrm{d}y \Phi_m(y)^* \partial_x^l \psi(x,y) = \langle \Phi_m, \partial_x^l \psi \rangle_{L^2(\mathbb{R}_y)} \Rightarrow |\partial_x^l (P_j^m \psi)(x)|^2 \\
&\leqslant \|\Phi_m\|^2_{L^2(\mathbb{R})} \cdot \int \mathrm{d}y |\partial_x^l \psi(x,y)|^2 \Rightarrow \int \mathrm{d}x |\partial_x^l (P_j^m \psi)(x)|^2 \\
&\leqslant \|\Phi_m\|^2_{L^2(\mathbb{R})} \cdot \|\partial_x^l \psi\|^2_{L^2(\mathbb{R}^2)} \Rightarrow \|P_j^m \psi\|^2_{H^k(\mathbb{R})} = \sum_{l=0}^{k} \|\partial_x^l P_j^m \psi\|^2_{L^2(\mathbb{R})} \leqslant \|\Phi_m\|^2 \sum_{l=0}^{k} \|\partial_x^l \psi(x,y)\|^2_{L^2(\mathbb{R}^2)}.
\end{aligned} \tag{10}$$

□

Corollary 1: The components $s_j^m(t,x_j;\varepsilon)$ are well defined, belong to $H^1(\mathbb{R})$ in the variable x_j and satisfy

$$\sup_{t\in[0,T]} \|s_j^m(t,\cdot\,;\varepsilon)\|_{L^2(\mathbb{R})} \leqslant \text{const.} \tag{11}$$

Proof: The domain of the quadratic form associated to $\widetilde{H}(\varepsilon)$ is given by

$$Q(\widetilde{H}(\varepsilon)) := H^1(\mathbb{R}^2) \cap Q(d^2), \tag{12}$$

where $Q(d^2) := \{\psi \in L^2(\mathbb{R}^2) : d_\Gamma(x,y)\psi \in L^2(\mathbb{R}^2)\}$. ψ_0 belongs to $Q(\widetilde{H}(\varepsilon))$, so ψ_t^ε is in $H^1(\mathbb{R}^2)$. □

Lemma 1:

$$\|\widetilde{H}(\varepsilon)\psi_0\| \leqslant C \quad \text{(independent of } \varepsilon\text{)}. \tag{13}$$

Proof: Since the Laplacian is invariant by rotations and translations, we have (for simplicity we drop the index j_0 in x and y)

[1]With an abuse of notation, we denote by $\psi_t^\varepsilon(x_j,y_j)$ the function ψ_t^ε written in coordinates (x_j,y_j). Since the different systems of coordinates associated to each edge are linked to one another by a rigid motion of the plane, this does not modify the differentiablity or integrability properties of ψ_t^ε. Note, instead, that $\Phi_m^\varepsilon(y_j)$ is an eigenfunction of the harmonic oscillator in the variable y_j.

$$\widetilde{H}(\varepsilon)\psi_0 = -\frac{1}{2}\partial_x^2 f\cdot\Phi_n - \frac{1}{2}f\cdot\partial_y^2\Phi_n + \frac{1}{2\varepsilon^2}d_\Gamma^2 f\cdot\Phi_n - \frac{E_n}{\varepsilon}f\cdot\Phi_n = -\frac{1}{2}\partial_x^2 f\cdot\Phi_n + \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)f\cdot\Phi_n$$
$$-\frac{1}{2}f\cdot\partial_y^2\Phi_n + f\frac{1}{2\varepsilon^2}y^2\cdot\Phi_n - \frac{E_n}{\varepsilon}f\cdot\Phi_n = -\frac{1}{2}\partial_x^2 f\cdot\Phi_n + \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)f\cdot\Phi_n.$$

Let a be the infimum of the support of f, and $b>a$ the supremum. Since f is supported inside the edge e_{j_0} and near each edge the distance from the graph is equal to $|y_j|$, the function $(1/2\varepsilon^2)(d_\Gamma^2-y^2)f\cdot\Phi_n$ will be zero when $|y|<D$, where D, depending on the support of f, can be small, but it is strictly positive. Therefore we have

$$\left\|\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)f\cdot\Phi_n\right\|^2 = \int_a^b \mathrm{d}x\int_{|y|>D}\mathrm{d}y\frac{1}{4\varepsilon^4}(d_\Gamma^2 - y^2)^2|f(x)\Phi_n^\varepsilon(y)|^2. \tag{14}$$

Now we use the following two properties:

(i) d_Γ^2 is equal to a polynomial of second order in the variables (x,y);
(ii) Φ_n^ε is equal to a polynomial in $y/\varepsilon^{1/2}$ times $\exp(-y^2/2\varepsilon)$.

The norm (14) contains then terms of the form (P and Q are polynomials)

$$\int_a^b \mathrm{d}x|f(x)|^2\int_{|y|>D}\mathrm{d}y\,P(x,y)Q(x,y/\varepsilon^{1/2})\exp\left(-\frac{y^2}{\varepsilon}\right)$$
$$= \int_a^b \mathrm{d}x|f(x)|^2\int_{|y|>D}\mathrm{d}y\,P(x,y)Q(x,y/\varepsilon^{1/2})\exp\left[-\left(\frac{1}{\varepsilon}-M\right)y^2\right]\exp(-My^2)$$
$$\leqslant \exp\left[-\left(\frac{1}{\varepsilon}-M\right)D^2\right]\int_a^b \mathrm{d}x|f(x)|^2\int_{|y|>D}\mathrm{d}y\,P(x,y)Q(x,y/\varepsilon^{1/2})\exp(-My^2) = O(e^{-c/\varepsilon}).$$

This implies that

$$\left\|\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)f\cdot\Phi_n\right\|^2 = O(e^{-c/\varepsilon}), \tag{15}$$

and therefore the thesis is proved. □

Corollary 2: For every system of coordinates (x_j,y_j) associated to an edge e_j we have

$$\frac{1}{2}\|\partial_{x_j}\psi_t^\varepsilon\|^2 + \frac{1}{2}\|\partial_{y_j}\psi_t^\varepsilon\|^2 + \frac{1}{2\varepsilon^2}\|d_\Gamma\psi_t^\varepsilon\|^2 \leqslant \frac{C}{\varepsilon}. \tag{16}$$

Corollary 3: Let $F_{d_\Gamma\geqslant\delta}$ be the characteristic function of the set $\{(x,y): d_\Gamma(x,y)\geqslant\delta\}$, where δ is any positive number, then

$$\sup_{t\in[0,T]}\|F_{d_\Gamma\geqslant\delta}\psi_t^\varepsilon\|_{L^2(\mathbb{R}^2)} = O(\varepsilon^{1/2}). \tag{17}$$

Proof: Last term in (16) gives

$$\tfrac{1}{2}\|d_\Gamma\psi_t^\varepsilon\|^2 \leqslant C\varepsilon.$$

Therefore we get

$$\delta^2\cdot\langle\psi_t^\varepsilon, F_{d_\Gamma\geqslant\delta}\psi_t^\varepsilon\rangle \leqslant \langle d_\Gamma\psi_t^\varepsilon, F_{d_\Gamma\geqslant\delta}d_\Gamma\psi_t^\varepsilon\rangle \leqslant 2C\varepsilon.$$

□

We are now ready to prove the following.

Theorem 1: *For $m\neq n$ and $j\in J$*

$$s_j^m(t,x_j;\varepsilon) \overset{*}{\rightharpoonup} 0, \quad \varepsilon \to 0, \tag{18}$$

where the convergence is in the weak topology of* $L^\infty((0,T),L^2(\mathbb{R}))$.

Proof: For convenience of the reader, we recall that a *bounded* sequence f_ε of functions in $L^\infty((0,T),L^2(\mathbb{R}))$ converges to a limit $f_0 \in L^\infty((0,T),L^2(\mathbb{R}))$ in the weak* topology if and only if

$$\int_0^T \mathrm{d}t\ \varphi(t)\langle \chi(\cdot), f_\varepsilon(t,\cdot)\rangle_{L^2(\mathbb{R})} \to \int_0^T \mathrm{d}t\ \varphi(t)\langle \chi(\cdot), f_0(t,\cdot)\rangle_{L^2(\mathbb{R})}$$

for every function $\varphi \in L^1(0,T)$ and every function $\chi \in L^2(\mathbb{R})$.

It is a standard fact about weak* topology that it is enough to consider only φ and χ in dense subsets of $L^1((0,T))$ and $L^2(\mathbb{R})$, respectively [see, e.g., Bornemann (1998), Appendix B or Rudin (1973), Theorems 3.15 and 3.16].

Let us then show first that

$$\sup_{t\in[0,T]} |\langle \chi(\cdot), s_j^m(t,\cdot;\varepsilon)\rangle_{L^2(\mathbb{R})}| \to 0, \quad \varepsilon \to 0, \tag{19}$$

for every function $\chi \in C_0^\infty(\mathbb{R}\backslash\{0,l_{e_j}\})$ if the edge e_j has finite length and for every $\chi \in C_0^\infty(\mathbb{R}\backslash\{0\})$ if e_j has infinite length. We consider explicitly only the latter case, the former being analogous.

If the support of χ is contained in $(-\infty,0)$ then

$$|\langle \chi, s_j^m\rangle_{L^2(\mathbb{R})}| = |\langle \chi\cdot\Phi_m^\varepsilon, \psi_t^\varepsilon\rangle_{L^2(\mathbb{R}^2)}| = |\langle \chi\cdot\Phi_m^\varepsilon, F_\chi\psi_t^\varepsilon\rangle| \leqslant \|\chi\cdot\Phi_m^\varepsilon\|\cdot\|F_\chi\psi_t^\varepsilon\| = O(\varepsilon^{1/2}),$$

where F_χ is the characteristic function of the support of χ and we have used Corollary 3.

If the support of χ in contained in $(0,+\infty)$, then, following the proof of Lemma 1 we can show that

$$\widetilde{H}(\varepsilon)[\chi(x_j)\Phi_m^\varepsilon(y_j)] = (\text{we drop the index } j) - \frac{1}{2}\partial_x^2\chi\cdot\Phi_m^\varepsilon + \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi\cdot\Phi_m^\varepsilon + \frac{E_m - E_n}{\varepsilon}\chi\cdot\Phi_m^\varepsilon.$$

Since χ is supported away from the vertex (located at x_j=0), an equation similar to (15) holds,

$$\left\| \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi\cdot\Phi_m^\varepsilon \right\|^2 = O(e^{-c/\varepsilon}).$$

Since $m \neq n$, we have then

$$\chi\Phi_m^\varepsilon = \frac{\varepsilon}{m-n}\left\{ \widetilde{H}(\varepsilon)[\chi(x_j)\Phi_m^\varepsilon(y_j)] + \frac{1}{2}\partial_x^2\chi\cdot\Phi_m^\varepsilon \right\} + O(e^{-c/\varepsilon}).$$

This implies

$$\begin{aligned}\langle \chi(\cdot), s_j^m(t,\cdot;\varepsilon)\rangle &= \langle \chi(\cdot)\Phi_m^\varepsilon, \psi_t^\varepsilon\rangle = \frac{\varepsilon}{m-n}\langle \chi(\cdot)\Phi_m^\varepsilon, \widetilde{H}(\varepsilon)\psi_t^\varepsilon\rangle + \frac{\varepsilon}{m-n}\left\langle \frac{1}{2}\partial_x^2\chi\cdot\Phi_m^\varepsilon, \psi_t^\varepsilon \right\rangle + O(e^{-c/\varepsilon}) \\ &= (\text{Lemma 1})O(\varepsilon).\end{aligned}$$

Now, if $\varphi \in L^1((0,T))$, we get

$$\left| \int_0^T \mathrm{d}t\ \varphi(t)\langle \chi(\cdot), s_j^m(t,\cdot;\varepsilon)\rangle_{L^2(\mathbb{R})} \right| \leqslant \|\varphi\|_{L^1}\cdot \sup_{t\in[0,T]} |\langle \chi(\cdot), s_j^m(t,\cdot;\varepsilon)\rangle|,$$

but we have just shown that the right-hand side goes to zero for $\chi \in C_0^\infty(\mathbb{R}\backslash\{0\})$ [or $C_0^\infty(\mathbb{R}\backslash\{0,l_{e_j}\})$ for an edge of finite length] which is dense in $L^2(\mathbb{R})$. □

Theorem 1 shows that, although in a weak sense, there is indeed adiabatic separation between the different transverse states even in the presence of vertices, if the initial state is localized in two

senses: first, it must be localized inside one edge to avoid mixing between the different transverse states associated to each edge and second, it must be in one (or a finite number of) transverse band(s).

Since the limit of s_j^m for $m \neq n$ is zero, to analyze in a complete way the (limit) evolution of ψ_0 we must determine the behavior of s_j^n, $j \in J$ as a function of time.

Theorem 2: *There exists a weak* convergent subsequence of* $s_j^n(t,x_j;\varepsilon)$ *in* $L^\infty((0,T),L^2(\mathbb{R}))$ *(denoted again by the same symbol), whose limit* $s_j^n(t,x_j;0) \in L^\infty((0,T),L^2(\mathbb{R}))$ *satisfies*

$$i\partial_t s_j^n(t,x_j;0) = -\frac{1}{2}\partial_x^2 s_j^n(t,x_j;0) \quad \text{in } \mathcal{D}'((0,T)\times(0,l_{e_j})). \tag{20}$$

Remark 1: By Corollary 1, $s_j^n(t,x_j;\varepsilon)$ is a bounded sequence in $L^\infty((0,T),L^2(\mathbb{R}))$. Since the balls in $L^\infty((0,T),L^2(\mathbb{R}))$ are compact metric spaces with respect to the weak* topology (see the theorems in the book of Rudin quoted above), a weak* convergent subsequence certainly exists.

Moreover, if one shows that all the weak* convergent subsequences converge to the same limit, then this implies that the sequence itself converges.

The equation satisfied by the limit in Theorem 2 is clearly independent of the subsequence, but it does not determine the behavior of the limit in the vertices, so we cannot conclude convergence of the sequence.

For this it would be necessary to control the behavior of the sequence in a neighborhood of the vertices. This difficulty [which is not present for smooth submanifolds, where the same strategy has been successfully applied by Bornemann (1998) in the classical case] is linked with the fact that the operator $-d^2/\mathrm{d}x^2$ defined for functions which vanish in a neighborhood of the origin has many self-adjoint extensions which define different dynamics.

We split the proof of the theorem into a number of lemmas.

Lemma 2: $s_j^n(t,x_j;\varepsilon)$ *belongs to* $C^1([0,T],L^2(\mathbb{R}))$ *and moreover it is an equicontinuous sequence of function from* $[0,T]$ *to* $L^2(\mathbb{R})$.

Proof: Let us denote by $\tilde{s}_j^n(t,x_j;\varepsilon) \in C^0([0,T],L^2(\mathbb{R}))$ the function

$$P_j^n[-i\tilde{H}(\varepsilon)\psi_t^\varepsilon].$$

Using Proposition 1 we have that

$$\left\| \frac{s_j^n(t+h,\cdot\,;\varepsilon)-s_j^n(t,\cdot\,;\varepsilon)}{h} - \tilde{s}_j^n(t,\cdot\,;\varepsilon) \right\|_{L^2(\mathbb{R})} = \left\| P_j^n\left[\frac{\tilde{U}_{t+h}(\varepsilon)-\tilde{U}_t(\varepsilon)}{h} + i\tilde{U}_t(\varepsilon)\tilde{H}(\varepsilon) \right]\psi_0 \right\|$$
$$\leqslant \left\| \left[\frac{\tilde{U}_{t+h}(\varepsilon)-\tilde{U}_t(\varepsilon)}{h} + i\tilde{U}_t(\varepsilon)\tilde{H}(\varepsilon) \right]\psi_0 \right\| \to 0.$$

This proves that

$$i\partial_t s_j^n(t,x_j;\varepsilon) = \tilde{s}_j^n(t,x_j;\varepsilon) = P_j^m[-i\tilde{U}_t(\varepsilon)\tilde{H}(\varepsilon)\psi_0]. \tag{21}$$

Since $\|\tilde{H}(\varepsilon)\psi_0\|$ is bounded (Lemma 1), $\|\tilde{s}_j^m(t,x_j;\varepsilon)\|$ is bounded, therefore

$$\|s_j^m(t,\cdot\,;\varepsilon)-s_j^m(t',\cdot\,;\varepsilon)\|_{L^2(\mathbb{R})} = \left\| \int_t^{t'} \mathrm{d}\tau\, \partial_\tau s_j^m(\tau,\cdot\,;\varepsilon) \right\| \leqslant \int_t^{t'} \mathrm{d}\tau \|\partial_\tau s_j^m(\tau,\cdot\,;\varepsilon)\| \leqslant C|t-t'|,$$

showing that $s_j^m(t,x_j;\varepsilon)$ is an equicontinuous sequence. □

Corollary 4: There exists a subsequence $s_j^m(t,x_j;\varepsilon)$ *which satisfies*

(1) $s_j^m(t,x_j;\varepsilon)$ *converges, in the weak topology of* $L^2(\mathbb{R})$, *uniformly in* t, *to a limit* $s_j^m(t,x_j;0) \in L^2(\mathbb{R})$. *Moreover, the limit is continuous in* t *in the weak topology of* L^2.

(2) $\partial_t s_j^m(t,x_j;\varepsilon) \overset{*}{\rightharpoonup} \partial_t s_j^m(t,x_j;0)$ *in* $L^\infty((0,T),L^2(\mathbb{R}))$, *where the derivative* $\partial_t s_j^m(t,x_j;0)$ *is to be interpreted as derivative in* $\mathcal{D}'((0,T)\times\mathbb{R}_x)$.

Proof: The sequence $s_j^m(t,x_j;\varepsilon)$ is contained in a ball in $L^2(\mathbb{R})$. This ball is a compact metric space with respect to the weak topology. Since the sequence is equicontinuous with respect to the strong topology, it will be equicontinuous with respect to the weak topology too. Therefore, the theorem of Ascoli-Arzelà [see, e.g., Royden (1988), Theorem 10.40] proves the first point.

Equation (21) implies that $\partial_t s_j^m(t,x_j;\varepsilon)$ is a bounded sequence in $L^\infty((0,T),L^2(\mathbb{R}))$, so, extracting possibly another subsequence, we have that there exists $g_j^m \in L^\infty((0,T),L^2(\mathbb{R}))$ such that (again, we denote the subsequence with the same symbol as the sequence itself)

$$\partial_t s_j^m(t,x_j;\varepsilon) \overset{*}{\rightharpoonup} g_j^m,$$

but this implies that $\forall\varphi\in C_0^\infty((0,T))$, $\forall\chi\in C_0^\infty(\mathbb{R})$,

$$\begin{aligned}\int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x\, g_j^m(t,x)\varphi(t)\chi(x) &= \int_0^T \mathrm{d}t\, \varphi(t)\langle\chi(\cdot), g_j^m(t,\cdot)\rangle_{L^2(\mathbb{R})} \leftarrow \int_0^T \mathrm{d}t\, \varphi(t)\langle\chi, \partial_t s_j^m(t,\cdot\,;\varepsilon)\rangle \\ &= \int_0^T \mathrm{d}t\, \varphi(t)\partial_t\langle\chi, s_j^m(t,\cdot\,;\varepsilon)\rangle = -\int_0^T \mathrm{d}t\, \partial_t\varphi\langle\chi, s_j^m(t,\cdot\,;\varepsilon)\rangle \\ &\to -\int_0^T \mathrm{d}t\, \partial_t\varphi\langle\chi, s_j^m(t,\cdot\,;0)\rangle = \int_0^T \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}x\, s_j^m(t,x;0)\partial_t\varphi(t)\chi(x), \\ &\Rightarrow g_j^m = \partial_t s_j^m(t,x_j;0) \quad \text{in } \mathcal{D}'((0,T)\times\mathbb{R}_x).\end{aligned}$$

□

We can now prove Theorem 2.

Proof: We suppose that edge e_j has infinite length. The proof for an edge of finite length is analogous.

Corollary 3, together with the proof of the first part of the proof of theorem 1 implies that

$$\sup_{t\in[0,T]} |\langle\chi, s_j^m(t,\cdot\,;\varepsilon)\rangle| = O(\varepsilon^{1/2}),$$

for all $j\in J$ and for all $\chi\in C_0^\infty(-\infty,0)$, but the first point of Corollary 4 gives

$$\langle\chi, s_j^m(t,\cdot\,;0)\rangle_{L^2(\mathbb{R})} = \lim_{\varepsilon\to 0}\langle\chi, s_j^m(t,\cdot\,;\varepsilon)\rangle = 0.$$

Equation (21) allows us to write, for all $\chi\in C_0^\infty(0,+\infty)$,

$$\begin{aligned}\langle\chi, i\partial_t s_j^m(t,\cdot\,;\varepsilon)\rangle_{L^2(\mathbb{R})} &= \langle\chi\cdot\Phi_n^\varepsilon, \widetilde{H}(\varepsilon)\psi_t^\varepsilon\rangle_{L^2(\mathbb{R}^2)} = \langle\widetilde{H}(\varepsilon)\chi\cdot\Phi_n^\varepsilon, \psi_t^\varepsilon\rangle \\ &= \left\langle -\frac{1}{2}\partial_x^2\chi\cdot\Phi_n^\varepsilon, \psi_t^\varepsilon\right\rangle + \left\langle \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi\cdot\Phi_n^\varepsilon, \psi_t^\varepsilon\right\rangle \\ &= \left\langle -\frac{1}{2}\partial_x^2\chi, s_j^m(t,\cdot\,;\varepsilon)\right\rangle_{L^2(\mathbb{R})} + \left\langle \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi\cdot\Phi_n^\varepsilon, \psi_t^\varepsilon\right\rangle.\end{aligned}$$

Since χ is supported in $(0,+\infty)$, Eq. (15) holds also in this case, therefore

$$\left\| \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi\cdot\Phi_n^\varepsilon \right\|^2 = O(e^{-c/\varepsilon}).$$

We have then, for all $\varphi \in C_0^\infty(0,T)$, and for all $\chi \in C_0^\infty(0,+\infty)$,

$$\int_0^T \mathrm{d}t\ \varphi(t)\langle \chi, i\partial_t s_j^n\ (t,\cdot\,;0))\rangle_{L^2(\mathbb{R})} \leftarrow \int_0^T \mathrm{d}t\ \varphi(t)\langle \chi, i\partial_t s_j^n(t,\cdot\,;\varepsilon)\rangle_{L^2(\mathbb{R})} = \int_0^T \mathrm{d}t\ \varphi(t)$$
$$\times \left\langle -\frac{1}{2}\partial_x^2\chi, s_j^n(t,\cdot\,;\varepsilon)\right\rangle_{L^2(\mathbb{R})} + O(e^{-c/\varepsilon})\|\varphi\|_{L^1(0,T)} \to \int_0^T \mathrm{d}t\ \varphi(t)$$
$$\times \left\langle -\frac{1}{2}\partial_x^2\chi, s_j^n(t,\cdot\,;0)\right\rangle_{L^2(\mathbb{R})},$$

$$\Rightarrow i\partial_t s_j^n(t,x_j;0) = -\tfrac{1}{2}\partial_x^2 s_j^n(t,x_j;0) \quad \text{in } \mathcal{D}'((0,T)\times(0,+\infty)). \tag{22}$$

□

III. A GRAPH WITH TWO EDGES

In this section, we are going to put forward a different kind of soft approximation for a graph with one vertex and two infinite edges. We denote it by Γ_ϑ, where ϑ is the angle made by the two edges, $0<\vartheta<\pi$.

As we have already said in the introduction, we do not consider directly Γ_ϑ, but we approximate it by smooth curves, $\Gamma_{\vartheta,\delta}$, whose curvature becomes bigger and bigger in a region whose width, given by δ, goes to zero and we consider a potential constraining to this family of curves.

More precisely, to specify the approximating curves we need only to specify their curvature, k_δ, because, as it is well known, this determines the curve up to rigid motions of the plane. Naturally, we want that, when δ goes to zero, the curves tend to the graph. This in particular implies that the turning angle must become equal to ϑ when $\delta\to 0$.

A simple choice which satisfies these requests is (s is the arc length parameter)

$$k_\delta(s) := \frac{\vartheta}{\delta}k\left(\frac{s}{\delta}\right), \quad \int_{\mathbb{R}} \mathrm{d}s\ k(s) = 1,$$

$$k \in C_0^\infty(-1,1), \quad \begin{matrix} k=1, & |s|<1/2 \\ k=0, & |s|>3/4, \end{matrix} \tag{23}$$

which amounts to deformate the graph in a neighborhood of the vertex replacing it with an arc of a circle. Note that the δ scaling is fixed by the request that the turning angle of the approximating curves be ϑ,

$$\int_{\mathbb{R}} \mathrm{d}s \frac{\vartheta}{\delta}k\left(\frac{s}{\delta}\right) = \vartheta.$$

Actually, our result does not depend on this specific choice we have made, because, from the proof, one can see that the only essential ingredient is the singularity $1/\delta$, which is forced by the requirement that the turning angle is ϑ.

We consider the Hamiltonian

$$\hat{H}(\varepsilon,\delta(\varepsilon)) = -\frac{1}{2}\Delta + \frac{1}{\varepsilon^2}W_{\delta(\varepsilon)}, \quad \delta(\varepsilon)\to 0 \text{ when } \varepsilon\to 0,$$

where, for simplicity, we suppose that

$$W_{\delta(\varepsilon)}(x,y) = \frac{1}{2}d^2_{\delta(\varepsilon)}(x,y) = \frac{1}{2}\mathrm{dist}[(x,y),\Gamma_{\vartheta,\delta(\varepsilon)}]^2.$$

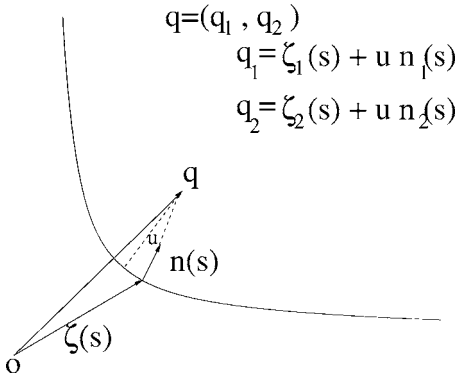
The remark we made above about the possibility to generalize the analysis to potentials with constant Hessian, applies here too. As in the preceding section, we are interested in the time evolution of a product state which is initially localized away from the vertex.

We expect that the particle oscillates very fast along the direction normal to the curve, so to analyze the motion we should use a suitable system of coordinates, adapted to the curve. A natural choice is given by *tubular coordinates*, which are a set of local coordinates suited to study tubular neighborhoods of embedded submanifolds [see, e.g., Lang (1995)]. If the submanifold one considers has codimension (and dimension) bigger than one, then the metric in tubular coordinates is in general not diagonal, and the Laplacian in these coordinates contains a gauge term which couples the longitudinal and the transverse motion [Mitchell (2001) and references therein].

In our case, since both the dimension and the codimension are equal to one, these problems do not appear.

Given a smooth curve C, with parametric equation $\zeta:\Omega\to\mathbb{R}^2$ such that $|\partial_s\zeta(s)|=1$, we can describe the position of points in a tubular neighborhood N of C via the curvilinear coordinates (s,u) defined by

$$q(s,u)=\zeta(s)+u\mathbf{n}(s), \tag{24}$$



where q is an arbitrary point of N, $\mathbf{n}(s)$ is the normal unit vector to the curve, and u is assumed to be smaller than the radius of curvature.

In the case we are dealing with, this means that curvilinear coordinates are defined only in the region

$$\{(x,y)\in\mathbb{R}^2: d_\delta(x,y)<\varrho\}, \tag{25}$$

where ϱ is the radius of curvature of $\Gamma_{\vartheta,\delta}$. When k_δ is different from zero, this quantity is proportional to δ itself, so, by hypothesis, it goes to zero when $\varepsilon\to 0$.

To get rid of the region $\{(x,y): d_\delta(x,y)>\delta\}$ we will use a theorem, proved first by Froese and Herbst in the more general context of a potential constraining to a submanifold [proposition 8.1 in Froese and Herbst (2001)], which basically says that if one starts from an initial state more and more localized near the constraint, then all that matters for the time evolution is a small region near the constraint itself. We repeat the proof of Froese and Herbst because we need to keep track of the dependence of all the constants in the estimates on δ, to apply them to the region $\{(x,y)\in\mathbb{R}^2: d_\delta(x,y)<\delta(\varepsilon)\}$.

Theorem 3: *Let* $\psi\in L^2(\mathbb{R}^2)$, $\|\psi\|=1$ *and* $\|\hat{H}(\varepsilon,\delta)\psi\|\leqslant C_1/\varepsilon$ (C_1 *independent of* δ). *Then*,

$$\|F_{d_\delta\geqslant\delta}e^{-it\hat{H}(\varepsilon,\delta)}\psi\|\leqslant(2C_1)^{1/2}\frac{\varepsilon^{1/2}}{\delta}. \tag{26}$$

F indicates the characteristic function of the region indicated.

Moreover, let $\hat{H}_D(\varepsilon,\delta)$ *be the Hamiltonian* $\hat{H}(\varepsilon,\delta)$ *with Dirichlet boundary conditions on the set* $\{(x,y)\in\mathbb{R}^2: d_\delta(x,y)=\delta\}$.

Let us suppose that $\delta=\delta(\varepsilon)$, $\lim_{\varepsilon\to 0}\delta(\varepsilon)=0$. *Taking into account* (26), *let us also assume that*

$$\lim_{\varepsilon\to 0}\frac{\varepsilon^{1/2}}{\delta(\varepsilon)}=0. \tag{27}$$

Then, for all $t\in[0,T]$, *we have*

$$\|F_{d_\delta<\delta}e^{-it\hat{H}(\varepsilon,\delta)}\psi-e^{-it\hat{H}_D(\varepsilon,\delta)}F_{d_\delta<\delta}\psi\|\leqslant C_2(C_1,T)\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}}+\frac{\varepsilon^{1/2}}{\delta^3}\right). \tag{28}$$

Remark 2: The theorem implies that if we choose a $\delta(\varepsilon)$ such that

$$\lim_{\varepsilon\to 0}\frac{\varepsilon^{1/10}}{\delta(\varepsilon)}=0 \tag{29}$$

then we can restrict ourselves to analyze the Dirichlet Hamiltonian $\hat{H}_D(\varepsilon,\delta(\varepsilon))$, which is localized inside the region where tubular coordinates are defined. This, however, means that we must consider a "tube" encircling the graph whose diameter is much bigger than the localization of the transverse states, which for an harmonic oscillator is $\varepsilon^{1/2}$.

Remark 3: As already observed in Froese and Herbst (2001), the estimate (28) is not optimal.

Proof: Let us first prove (26).

Since $\|\hat{H}(\varepsilon,\delta)\psi\|\leqslant C_1/\varepsilon$, we have from Schwarz inequality

$$\langle\psi,\hat{H}(\varepsilon,\delta)\psi\rangle\leqslant\frac{C_1}{\varepsilon}.$$

This implies immediately that

$$\frac{C_1}{\varepsilon}\geqslant\langle\hat{H}^{1/2}\psi,\hat{H}^{1/2}\psi\rangle=\frac{1}{2}\|\nabla\psi\|^2+\frac{1}{2\varepsilon^2}\|d_\delta\psi\|^2\Rightarrow\|d_\delta\psi\|^2\leqslant 2C_1\varepsilon. \tag{30}$$

It follows then

$$\delta^2\langle F_{d_\delta\geqslant\delta}\psi,F_{d_\delta\geqslant\delta}\psi\rangle\leqslant\langle d_\delta F_{d_\delta\geqslant\delta}\psi,d_\delta F_{d_\delta\geqslant\delta}\psi\rangle\leqslant\|d_\delta\psi\|^2\leqslant 2C_1\varepsilon. \tag{31}$$

The same argument can be applied also to $e^{-it\hat{H}(\varepsilon,\delta)}\psi$, so (26) is proved.

We need now to prove an estimate on the behavior of the gradient of ψ away from the graph.

Let $\tilde{\chi}\in C_0^\infty(\mathbb{R})$ be 1 when $1/4<|x|<3/4$ and 0 when $|x|\leqslant 1/8$ or $|x|\geqslant 7/8$, then the function

$$\chi(u):=\tilde{\chi}\left(\frac{1}{2(\alpha-\lambda_1)}|u|+\frac{1}{4}-\frac{\lambda_1}{2(\alpha-\lambda_1)}\right)$$

will be when $\lambda_1<|u|<\alpha$ and 0 for $|u|$ near zero. If we choose λ_1 and α such that $0<\lambda_1<\alpha<\delta$, then χ is well defined [and $\in C_0^\infty(\mathbb{R})$] when u is the coordinate along the direction normal to the curve $\Gamma_{\vartheta,\delta}$.

We have then

$$\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\|=\|F_{\lambda_1<d_a<\alpha}\nabla(\chi\psi)\|\leqslant\|\nabla(\chi\psi)\|.$$

Using again the Schwarz inequality and the fact that $\chi\psi\in\mathcal{D}(\Delta)$ (the potential is bounded on the support of χ) we get

$$\|\nabla(\chi\psi)\| \leqslant \|\Delta(\chi\psi)\|^{1/2}\|\chi\psi\|^{1/2},$$

so, to estimate $\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\|$ we need to get an estimate on $\|\Delta(\chi\psi)\|$. To obtain it, we use an energy estimate of second order, i.e., we calculate the quadratic form associated to $\hat{H}(\varepsilon,\delta)^2$.

$$\hat{H}(\varepsilon,\delta)^2 = \frac{1}{4}|p|^4 + \left(\frac{1}{2\varepsilon^2}d_\delta^2\right)^2 + \sum_j p_j \frac{1}{2\varepsilon^2}d_\delta^2 p_j - \frac{1}{2\varepsilon^2}\Delta d_\delta^2, \tag{32}$$

where $p=-i\nabla$. The first three terms are positive operators, while if we take the mean value of the last one with respect to the state $\chi\psi$ we get

$$\begin{aligned}\langle\chi\psi,\Delta d_\delta^2\chi\psi\rangle &= \int_{d_\delta<\delta} \mathrm{d}x\,\mathrm{d}y|\chi\psi|^2\Delta d_\delta^2 = \int_{|u|<\delta}\mathrm{d}s\,\mathrm{d}u[1+uk_\delta(s)]|\chi\psi|^2[1+uk_\delta(s)]^{-1}\\ &\times\partial_u\{[1+uk_\delta(s)]2u\} = \int_{|u|<\delta}\mathrm{d}s\,\mathrm{d}u[1+uk_\delta(s)]|\chi\psi|^2\cdot 2\\ &+\int_{|u|<\delta}\mathrm{d}s\,\mathrm{d}u|\chi\psi|^2 2uk_\delta(s) \leqslant C\|\chi\psi\|^2,\end{aligned}$$

where the Jacobian of the change to curvilinear coordinates is given by

$$\frac{\partial(q_1,q_2)}{\partial(s,u)} = 1 + k_\delta(s)u \tag{33}$$

and in the last step we have used the fact that

$$\sup_{|u|<\delta}|uk_\delta(s)| \leqslant \delta k_\delta(s) = \vartheta k\left(\frac{s}{\delta}\right) \leqslant \text{const (independent of } \delta).$$

Taking the mean value of (32) with respect to $\chi\psi$ we obtain then

$$\left\|\frac{1}{2}\Delta(\chi\psi)\right\|^2 \leqslant \|\hat{H}(\varepsilon,\delta)(\chi\psi)\|^2 + \frac{C}{\varepsilon^2},$$

which can be written equivalently as

$$\frac{1}{2}\|\Delta(\chi\psi)\| \leqslant \frac{C^{1/2}}{\varepsilon} + \|\hat{H}(\varepsilon,\delta)\psi\| + \frac{1}{2}\|[\Delta,\chi]\psi\|.$$

The last term is equal to

$$[\Delta,\chi]\psi = (\Delta\chi)\psi + \nabla\chi\cdot\nabla\psi,$$

and we can estimate its norm changing to curvilinear coordinates,

$$\nabla\chi = \partial_x\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)}\frac{u}{|u|}\boldsymbol{n}(s),$$

$$\begin{aligned}\Delta\chi &= (1+k_\delta u)^{-1}\partial_u[(1+k_\delta u)\partial_u\chi] = \partial_u^2\chi + (1+k_\delta u)^{-1}k_\delta\partial_u\chi = \partial_x^2\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)^2}\\ &+\partial_x\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)}\frac{u}{|u|}\frac{k_\delta}{1+k_\delta u}.\end{aligned}$$

Using (30) to estimate $\|\nabla\psi\|$, we have then

$$\|[\Delta,\chi]\psi\| \leqslant \frac{C}{\varepsilon^{1/2}(\alpha-\lambda_1)} + \frac{C}{(\alpha-\lambda_1)^2} + \frac{C}{\delta(\alpha-\lambda_1)}. \tag{34}$$

In what follows, we will need to choose α and λ_1 proportional to δ. Assumption (27) implies then that all terms in (34) are *at most* of order ε^{-1}.

To sum up, we have

$$\|\Delta(\chi\psi)\| \leqslant \frac{C}{\varepsilon}, \tag{35}$$

from which it follows that [assuming that α and λ_1 are proportional to δ and that $\delta(\varepsilon)$ satisfies (27)]

$$\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\| \leqslant C\varepsilon^{-1/2}\frac{\varepsilon^{1/4}}{\delta^{1/2}} = \frac{C}{\varepsilon^{1/4}\delta^{1/2}}. \tag{36}$$

Let now $\tilde{\xi}$ be a function in $C_0^\infty(\mathbb{R})$ such that $\tilde{\xi}(x)=1$ when $|x|<1/4$ and $\tilde{\xi}(x)=0$ when $|x|>1/2$. We define the function ξ by the equation $\xi(u):=\tilde{\xi}(u/\delta)$, where u is the curvilinear coordinate normal to the curve.

Because of (26), to prove (28) is enough to show that

$$\|e^{it\hat{H}_D(\varepsilon,\delta)}\xi e^{-it\hat{H}(\varepsilon,\delta)}\psi - \xi\psi\| \leqslant C_2(C_1,T)\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}} + \frac{\varepsilon^{1/2}}{\delta^3}\right)$$

for $t\in[0,T]$. Let

$$\phi_{t,\varepsilon,\delta} := e^{it\hat{H}_D(\varepsilon,\delta)}\xi e^{-it\hat{H}(\varepsilon,\delta)}\psi - \xi\psi.$$

Integrating the derivative we have

$$\begin{aligned}\phi_{t,\varepsilon,\delta} &= i\int_0^t \mathrm{d}s\, e^{is\hat{H}_D(\varepsilon,\delta)}[\hat{H}_D(\varepsilon,\delta)\xi - \xi\hat{H}(\varepsilon,\delta)]e^{-is\hat{H}(\varepsilon,\delta)}\psi \\ &= \int_0^t \mathrm{d}s\, e^{is\hat{H}_D(\varepsilon,\delta)}[\nabla\xi\cdot p - (i/2)\Delta\xi]e^{-is\hat{H}(\varepsilon,\delta)}\psi,\end{aligned}$$

therefore

$$\|\phi_{t,\varepsilon,\delta}\|^2 = \int_0^t \mathrm{d}s\langle e^{-is\hat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}, [\nabla\xi\cdot p - (i/2)\Delta\xi]e^{-is\hat{H}(\varepsilon,\delta)}\psi\rangle.$$

Let now $\tilde{\zeta}$ be a $C_0^\infty(\mathbb{R})$ function which is 1 on the support of $\partial_x\tilde{\xi}$ and 0 when $|x|$ is near zero. As above, we denote by $\zeta(u):=\tilde{\zeta}(u/\delta)$. We can then write

$$\begin{aligned}\|\phi_{t,\varepsilon,\delta}\|^2 &\leqslant \int_0^t \mathrm{d}s\|\zeta e^{-is\hat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\|(\|\nabla\xi\cdot p e^{-is\hat{H}(\varepsilon,\delta)}\psi\| + \|(1/2)\Delta\xi e^{-is\hat{H}(\varepsilon,\delta)}\psi) \\ &\leqslant C\left(\frac{1}{\delta^{3/2}\varepsilon^{1/4}} + \frac{1}{\delta^2}\right)\int_0^t \mathrm{d}s\|\zeta e^{-is\hat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\|,\end{aligned} \tag{37}$$

where we have used (36) and the definition of ξ.

Now

$$\begin{aligned}\langle \phi_{t,\varepsilon,\delta}, \hat{H}_D(\varepsilon,\delta)\phi_{t,\varepsilon,\delta}\rangle &\leqslant 2\langle \xi e^{-it\hat{H}(\varepsilon,\delta)}\psi, \hat{H}_D(\varepsilon,\delta)\xi e^{-it\hat{H}(\varepsilon,\delta)}\psi\rangle + 2\langle \xi\psi, \hat{H}_D(\varepsilon,\delta)\xi\psi\rangle \\ &= 2\left\langle \xi e^{-it\hat{H}(\varepsilon,\delta)}\psi, \left[-\tfrac{1}{2}\Delta\xi - i\nabla\xi\cdot p + \xi\hat{H}_D(\varepsilon,\delta)\right]e^{-it\hat{H}(\varepsilon,\delta)}\psi\right\rangle \\ &\quad + 2\left\langle \xi\psi, \left[-\tfrac{1}{2}\Delta\xi - i\nabla\xi\cdot p + \xi\hat{H}_D(\varepsilon,\delta)\right]\psi\right\rangle.\end{aligned}$$

Using again Equation (36) and the definition of ξ, we get

$$\left|\left\langle \xi\psi, -\frac{1}{2}\Delta\xi\psi\right\rangle\right| \leqslant \frac{C}{\delta^2},$$

$$|\langle \xi\psi, -i\nabla\xi\cdot p\psi\rangle| \leqslant \frac{C}{\varepsilon^{1/4}\delta^{3/2}},$$

$$|\langle \xi\psi, \xi\hat{H}_D(\varepsilon,\delta)\psi\rangle| \leqslant \frac{C}{\varepsilon},$$

and corresponding equations with $e^{-it\hat{H}(\varepsilon,\delta)}\psi$ instead of ψ. If we suppose that the sequence $\delta(\varepsilon)$ satisfies (27), then all the terms grow at most as ε^{-1}, so we obtain in the end

$$\langle \phi_{t,\varepsilon,\delta}, \hat{H}_D(\varepsilon,\delta)\phi_{t,\varepsilon,\delta}\rangle \leqslant \frac{C}{\varepsilon}.$$

Repeating the proof of (26), we can then show that

$$\|\zeta e^{-is\hat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\| \leqslant \frac{C\varepsilon^{1/2}}{\delta},$$

and substituting this back in (37) we get

$$\|\phi_{t,\varepsilon,\delta}\|^2 \leqslant C\left(\frac{1}{\delta^{3/2}\varepsilon^{1/4}} + \frac{1}{\delta^2}\right)\frac{\varepsilon^{1/2}}{\delta} = C\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}} + \frac{\varepsilon^{1/2}}{\delta^3}\right). \tag{38}$$

□

Now, let us fix a sequence $\delta(\varepsilon)$ satisfying (29). As in the preceding section, we consider the time evolution of a product state localized inside one of the two edges, away from the vertex,

$$\psi_t^\varepsilon = e^{-it\hat{H}(\varepsilon,\delta(\varepsilon))}\psi_0,$$

$$\psi_0(x,y) = f(x)\Phi_n^\varepsilon(y), \tag{39}$$

where (x,y) is the system of coordinates associated to one of the edges, $f \in C_0^\infty(\mathbb{R})$ and Φ_n^ε has been defined in (6). If we choose ε sufficiently small, the tubular coordinates associated to the curve $\Gamma_{\vartheta,\delta}$, (s_δ, u_δ), coincide with (x,y) apart from a small neighborhood of the vertex. The state ψ_0 is then well defined and independent of δ. The limit $\varepsilon \to 0$ gives us therefore the leading behavior of an initial state which propagates through a tube which curves slowly with respect to the transverse wavelength.

Equation (26) allows us to discard $F_{d_{\delta(\varepsilon)}>\delta(\varepsilon)}\psi_t^\varepsilon$, while (28) allows us to approximate $F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_t^\varepsilon$ with $e^{-it\hat{H}_D(\varepsilon,\delta(\varepsilon))}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0$.

We can now prove the following.

Proposition 2: Let ψ_t^ε *be given by* (39), *then, for* $t \in [0,T]$,

$$\|\exp[-it\hat{H}_D(\varepsilon,\delta(\varepsilon))]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0 - \exp[-it\hat{K}(\delta(\varepsilon)) - itE_n/\varepsilon](f)\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\Phi_n^{\varepsilon}(u_{\delta(\varepsilon)})\| \to 0,$$
$$\varepsilon \to 0, \tag{40}$$

where

$$\hat{K}(\delta(\varepsilon)) = -\frac{1}{2}\partial_s^2 - \frac{k_\delta(s)^2}{8}. \tag{41}$$

Proof: The proof is an application of the fundamental theorem of calculus (also called, in this context, Duhamel formula),

$$\begin{aligned}
&\|\exp[-it\hat{H}_D(\varepsilon,\delta(\varepsilon))]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0 - \exp[-it\hat{K}(\delta(\varepsilon)) - itE_n/\varepsilon](f)\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\Phi_n^{\varepsilon}(u_{\delta(\varepsilon)})\| \\
&= \|\{\exp[it\hat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\hat{K}(\delta(\varepsilon)) - itE_n/\varepsilon] - \mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_{\delta(\varepsilon)}) \\
&\quad + F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^{\varepsilon}(u_\delta) - F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^{\varepsilon}(y)\| \leqslant \|\{\exp[it\hat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\hat{K}(\delta(\varepsilon)) \\
&\quad - itE_n/\varepsilon] - \mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_\delta)\| + \|F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^{\varepsilon}(u_\delta) - F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^{\varepsilon}(y)\| \\
&= \|\{\exp[it\hat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\hat{K}(\delta(\varepsilon)) - itE_n/\varepsilon] - \mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_\delta)\|,
\end{aligned}$$

because the second term is zero if ε (and therefore δ) is sufficiently small.

Applying now Duhamel formula,[2] we have that

$$\|\{\exp[it\hat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\hat{K}(\delta(\varepsilon)) - itE_n/\varepsilon] - \mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_\delta)\| \leqslant \int_0^t \mathrm{d}s\|[\hat{H}_D(\varepsilon,\delta(\varepsilon))$$
$$-\hat{K}(\delta(\varepsilon)) - E_n/\varepsilon]\times\exp[-is\hat{K}(\delta(\varepsilon)) - isE_n/\varepsilon]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_\delta)\|. \tag{42}$$

The Hamiltonian $\hat{H}_D(\varepsilon,\delta(\varepsilon))$ in curvilinear coordinates, acting on $L^2(\mathbb{R}\times[0,\delta],\mathrm{d}s\,\mathrm{d}u)$, is given by

$$\hat{H}_D(\varepsilon,\delta(\varepsilon)) = -\frac{1}{2}\frac{1}{[1+uk_\delta(s)]^2}\frac{\partial^2}{\partial s^2} + \frac{1}{[1+uk_\delta(s)]^3}uk'_\delta(s)\frac{\partial}{\partial s} + V(s,u) - \frac{1}{2}\frac{\partial^2}{\partial u^2} + \frac{1}{2\varepsilon^2}u^2,$$

where V is the geometric potential,

$$V(s,u) = \frac{1}{2}\left\{-\frac{k_\delta^2}{4[1+uk_\delta]^2} + \frac{uk''_\delta}{2[1+uk_\delta]^2} - \frac{5}{4}\frac{u^2(k'_\delta)^2}{[1+uk_\delta]^2}\right\}. \tag{43}$$

Making a unitary dilation by the factor $\varepsilon^{1/2}$ along u, we get an operator acting on $L^2(\mathbb{R}\times[0,\delta(\varepsilon)/\varepsilon^{1/2}],\mathrm{d}s\,\mathrm{d}u)$, given by

$$\begin{aligned}
D_{\varepsilon^{1/2}}\hat{H}_D(\varepsilon,\delta(\varepsilon))D^{\dagger}_{\varepsilon^{1/2}} &= -\frac{1}{2}\frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^2}\frac{\partial^2}{\partial s^2} + \frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^3}\varepsilon^{1/2}uk'_\delta(s)\frac{\partial}{\partial s} + V(s,\varepsilon^{1/2}u) \\
&\quad - \frac{1}{2\varepsilon}\frac{\partial^2}{\partial u^2} + \frac{1}{2\varepsilon}u^2,
\end{aligned} \tag{44}$$

where

$$D_{\varepsilon^{1/2}}\psi(u) = \varepsilon^{1/4}\psi(\varepsilon^{1/2}u).$$

[2]For every fixed δ, the domain of $\hat{K}(\delta)$ is $H^2(\mathbb{R})$, so $\exp[-it\hat{K}(\delta)](f)\cdot F_{d_\delta<\delta}\Phi(u_\delta)$ is in the domain of $\hat{H}_D(\varepsilon,\delta)$.

Therefore, Eq. (42) becomes

$$\begin{aligned}&\|\{\exp[it\hat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\hat{K}(\delta(\varepsilon))-itE_n/\varepsilon]-\mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^{\varepsilon}(u_\delta)\|\\&\leqslant\int_0^t \mathrm{d}s\|[D_{\varepsilon^{1/2}}\hat{H}_D(\varepsilon,\delta(\varepsilon))D^{\dagger}_{\varepsilon^{1/2}}-\hat{K}(\delta(\varepsilon))-E_n/\varepsilon]\\&\quad\times\exp[-is\hat{K}(\delta(\varepsilon))-isE_n/\varepsilon]f\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\|.\end{aligned}$$

Therefore, it is clear from previous equations that

$$\|[V(s,\varepsilon^{1/2}u)+k_\delta^2/8]\exp[-is\hat{K}(\delta(\varepsilon))-isE_n/\varepsilon]f\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\|=O(\varepsilon^{1/2}/\delta^3)\to 0,\quad \varepsilon\to 0,$$

$$\left\|\left(-\frac{1}{2\varepsilon}\frac{\partial^2}{\partial u^2}+\frac{1}{2\varepsilon}u^2-\frac{E_n}{\varepsilon}\right)\exp[-is\hat{K}(\delta(\varepsilon))-isE_n/\varepsilon]f\times F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\right\|\to 0,\quad \varepsilon\to 0,$$

so we need to control only the terms containing the derivative with respect to s in (44).

Using Lemma 3, proved below, we have that

$$\begin{aligned}&\left\|\frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^3}\varepsilon^{1/2}uk'_\delta(s)\frac{\partial}{\partial s}\exp[-it\hat{K}(\delta(\varepsilon))-itE_n/\varepsilon]f(s)\times F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\right\|\\&\leqslant(\varepsilon^{1/2}\|k'_\delta\|_{L^\infty}\cdot\|\partial_s f\|_{L^2}+|t|\cdot\varepsilon^{1/2}\|k_\delta\|_{L^\infty}\|k'_\delta\|^2_{L^\infty}\|f\|_{L^2})\times\|u\Phi_n^{\varepsilon=1}(u)\|=O(\varepsilon^{1/2}/\delta^5)\to 0,\quad \varepsilon\to 0.\end{aligned}$$

In the same way we also have

$$\begin{aligned}&\left\|-\frac{1}{2}\left\{\frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^2}-1\right\}\frac{\partial^2}{\partial s^2}\exp[-it\hat{K}(\delta(\varepsilon))-itE_n/\varepsilon]f(s)\times F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\right\|\\&\leqslant C\varepsilon^{1/2}\|k_\delta\|_\infty[\|\partial_s^2 f\|+|t|\times(2\|k_\delta\|_\infty\cdot\|k'_\delta\|_\infty\|\partial_s f\|+\|k'_\delta\|^2_\infty\|f\|+\|k_\delta\|_\infty\|k''_\delta\|_\infty\|f\|)]=O(\varepsilon^{1/2}/\delta^5)\to 0,\\&\quad\varepsilon\to 0.\end{aligned}$$

□

Remark 4: As stressed above, in this model the dynamics under a strong constraining potential are well approximated by Dirichlet boundary conditions on a "large" tube surrounding the smooth curve. Proposition 2 says that this choice gives the same result as the procedure of constraining first the particle to the motion to the curve, and then taking the limit when the curve approaches the graph.

Lemma 3: Let $\hat{H}$ be the one-dimensional Hamiltonian $\hat{H}=-\frac{1}{2}\partial_x^2+V$, where V is a potential bounded together with its first two derivatives, then, given $\psi\in H^1(\mathbb{R})$, we have

$$\|\partial_x\exp(-it\hat{H})\psi\|_{L^2(\mathbb{R})}\leqslant\|\partial_x\psi\|_{L^2(\mathbb{R})}+|t|\cdot\|\partial_x V\|_{L^\infty}\cdot\|\psi\|_{L^2(\mathbb{R})},\tag{45}$$

and, given $\varphi\in H^2(\mathbb{R})$,

$$\|\partial_x^2\exp(-it\hat{H})\varphi\|_{L^2(\mathbb{R})}\leqslant\|\partial_x^2\varphi\|_{L^2(\mathbb{R})}+|t|(2\|\partial_x V\|_{L^\infty}\cdot\|\partial_x\varphi\|_{L^2(\mathbb{R})}+\|\partial_x^2 V\|_{L^\infty}\cdot\|\varphi\|_{L^2(\mathbb{R})}).\tag{46}$$

Proof: Since V is bounded, the domain of the quadratic form associated to $\hat{H}$ is $H^1(\mathbb{R})$, and the time evolution sends it into itself. It makes therefore sense to write, for $\psi\in H^1(\mathbb{R})$,

$$[-i\partial_x, e^{-it\hat{H}}]\psi = e^{-it\hat{H}}\int_0^t \mathrm{d}s\ \partial_s e^{is\hat{H}}(-i\partial_x)e^{-is\hat{H}}\psi = ie^{-it\hat{H}}\int_0^t \mathrm{d}s\ e^{is\hat{H}}[\hat{H}, -i\partial_x]e^{-is\hat{H}}\psi$$

$$= e^{-it\hat{H}}\int_0^t \mathrm{d}s\ e^{is\hat{H}}\partial_x V e^{-is\hat{H}}\psi,$$

but this implies immediately

$$-i\partial_x e^{-it\hat{H}}\psi = e^{-it\hat{H}}(-i\partial_x)\psi + [-i\partial_x, e^{-it\hat{H}}]\psi \Rightarrow \|-i\partial_x e^{-it\hat{H}}\psi\| \leqslant \|-i\partial_x\psi\| + \int_0^t \mathrm{d}s\|\partial_x V e^{-is\hat{H}}\psi\|,$$

which gives (45).

Following the same path and noticing that

$$[\hat{H}, -\partial_x^2] = -\partial_x^2 V - 2\partial_x V\cdot\partial_x \tag{47}$$

we get (46). □

To complete the analysis of this case we need to study the limit of the dynamics $\exp[-it\hat{K}(\delta(\varepsilon))]$ when $\varepsilon\to 0$.

The limit of one-dimensional Hamiltonians containing rescaled potentials has been studied in detail in the context of the approximation of singular interactions, like the delta coupling, by short range smooth potentials (Albeverio *et al.* (2005) and references therein). The scaling used by us in (41) however, is not covered in the results presented in Albeverio *et al.*, but it can be analyzed using exactly the same techniques.

The idea is to show convergence in norm of the resolvent of $\hat{K}(\delta(\varepsilon))$ to the resolvent of the Hamiltonian with Dirichlet boundary conditions in $s=0$. As it is well known [Reed and Simon (1972), Theorem VIII.21] this implies strong convergence of the corresponding unitary group.

One could expect convergence to Dirichlet boundary conditions because the potential $-k_\delta^2/8$ is a strongly attractive well, which becomes deeper and deeper, but whose range is shorter and shorter. As explained in Englisch and Šeba (1986) in a different context, we expect this to give rise to Dirichlet boundary conditions. This in particular says that the strong convergence of the unitary group (or the norm resolvent convergence) does not capture the behavior of the eigenvalues which go to $-\infty$ when $\delta\to 0$, because, even though the ground state of $\hat{K}(\delta(\varepsilon))$ tends to $-\infty$, its resolvent converges to that of a semibounded operator. This phenomenon has already been illustrated in Gesztesy (1980).

We can now prove the following.

Theorem 4: *Let* $[\hat{K}(\delta(\varepsilon))-z^2]^{-1}$ *be the resolvent of* $\hat{K}(\delta(\varepsilon))$, *where* $\Im z>0$, *then*

$$[\hat{K}(\delta(\varepsilon)) - z^2]^{-1} \to [\hat{K}_D - z^2]^{-1}, \quad \varepsilon\to 0, \tag{48}$$

in the norm of bounded operators on $L^2(\mathbb{R})$, *where* K_D *is the free Laplacian on* $L^2(\mathbb{R})$ *with Dirichlet boundary conditions in* $s=0$.

Proof: The potential $Q(s) := -k^2/8$ is in $L^1(\mathbb{R})\cap L^\infty(\mathbb{R})$, so we can apply the dilation technique described in Albeverio *et al.* (1984) [see also Albeverio *et al.* (2005)]. Applying lemma A.1 of Albeverio *et al.* (1984) we get

$$[\hat{K}(\delta(\varepsilon)) - z^2]^{-1} = G_z - A_\delta(z)[\delta + B_\delta(z)]^{-1}C_\delta(z), \quad \Im z>0, \tag{49}$$

where G_z is the free resolvent, with kernel $g_z(w)$,

$$G_z := (\hat{H}_0 - z^2)^{-1}, \quad g_z(w) := \frac{i}{2z}e^{iz|w|},$$

$$\hat{H}_0 := -\frac{\partial^2}{\partial s^2}, \quad D(\hat{H}_0) = H^2(\mathbb{R}), \tag{50}$$

while $A_\delta(z)$, $B_\delta(z)$, and $C_\delta(z)$ are Hilbert-Schmidt operators with kernels

$$A_\delta(z,s,r) = g_z(s-\delta r)|Q(r)|^{1/2},$$

$$B_\delta(z,s,r) = -|Q(s)|^{1/2} g_z[\delta(s-r)]|Q(r)|^{1/2},$$

$$C_\delta(z,s,r) = -|Q(s)|^{1/2} g_z(\delta s - r). \tag{51}$$

It is not difficult to see [Lemma 2.3, Albeverio *et al.* (1984)] that

$$A_\delta \to A_0,$$

$$B_\delta \to B_0,$$

$$C_\delta \to C_0, \tag{52}$$

in Hilbert-Schmidt norm, where A_0, B_0, and C_0 have kernels

$$A_0(z,s,r) = g_z(s)|Q(r)|^{1/2},$$

$$B_0(z,s,r) = -g_z(0)|Q(s)|^{1/2}|Q(r)|^{1/2},$$

$$C_0(z,s,r) = -|Q(s)|^{1/2} g_z(-r). \tag{53}$$

The operator B_0 is not invertible on the whole Hilbert space, but it is clear from the expression of the kernel that it actually acts on the one-dimensional subspace, denoted by $\mathcal{H}_Q$, generated by the vector φ_Q given by

$$\varphi_Q(s) := \frac{|Q(s)|^{1/2}}{\||Q(s)|^{1/2}\|_{L^2(\mathbb{R})}} = \frac{|Q(s)|^{1/2}}{\|Q(s)\|^{1/2}_{L^1(\mathbb{R})}}. \tag{54}$$

So we can write

$$B_0 = -g_z(0)\|Q(s)\|_{L^1(\mathbb{R})} \varphi_Q \langle \varphi_Q, \cdot \rangle. \tag{55}$$

On $\mathcal{H}_Q$, B_0 is invertible and the inverse is given by

$$B_0^{-1} = -\frac{1}{g_z(0)\|Q(s)\|_{L^1(\mathbb{R})}} \varphi_Q \langle \varphi_Q, \cdot \rangle. \tag{56}$$

Since the operator C_0 has range equal to $\mathcal{H}_Q$ and A_0 acts nontrivially only on $\mathcal{H}_Q$, we get that

$$[\hat{K}(\delta(\varepsilon)) - z^2]^{-1} \to G_z - A_0 B_0^{-1} C_0,$$

which has a kernel given by

$$g_z(s-r) - \frac{g_z(s) g_z(-r)}{g_z(0)}, \tag{57}$$

which is the kernel of the resolvent of the Dirichlet Hamiltonian. □

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Differential realization of pseudo-Hermiticity: A quantum mechanical analog of Einstein's field equation

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For a given pseudo-Hermitian Hamiltonian of the standard form: $H=p^2/2m+v(x)$, we reduce the problem of finding the most general (pseudo-)metric operator η satisfying $H^\dagger=\eta H \eta^{-1}$ to the solution of a differential equation. If the configuration space is $\mathbb{R}$, this is a Klein-Gordon equation with a nonconstant mass term. We obtain a general series solution of this equation that involves a pair of arbitrary functions. These characterize the arbitrariness in the choice of η. We apply our general results to calculate η for the $\mathcal{PT}$-symmetric square well, an imaginary scattering potential, and a class of imaginary delta-function potentials. For the first two systems, our method reproduces the known results in a straightforward and extremely efficient manner. For all these systems we obtain the most general η up to second-order terms in the coupling constants. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The key aspect of the general theory of relativity (GR) that distinguishes it from other well-established physical theories is that in GR the very geometry of the spacetime, which is the arena of physical reality in classical physics, is itself a dynamical quantity. In contrast, in quantum mechanics (QM), the geometry of the Hilbert space, which plays a similar role as the spacetime does in classical physics, is an absolute entity. This is to some extent dictated by the well-known mathematical fact that all separable Hilbert spaces are unitary equivalent. For the past 75 years or so, this equivalence has been used to justify the absolutism associated with the convention of fixing the (inner product of the) Hilbert space from the outset. This is actually quite surprising, for the existence of an equivalence relation in a theory is clearly an evidence of the presence of a freedom in its formulation. In the case of QM, this is the freedom to choose the inner product of the Hilbert space, a freedom that has been left unused until recently.[1,2]

In Ref. 2, we have investigated the consequences of promoting the inner product of the Hilbert space into a degree of freedom. This revealed certain similarities between QM and GR and led to some interesting observations such as a direct link between geometric phases and the geometry of the Hilbert space and a new root to a certain nonlinear generalization of QM. In the present paper, we derive and examine a differential equation that includes among its solutions all possible choices of the inner product for a given physical system. This is the quantum mechanical analog of Einstein's field equation. (The same way Einstein's equation does not generally restrict the metric tensor to have a particular signature, the above-mentioned equation does not restrict its solutions to correspond to positive-definite metric operators.) For a system having $\mathbb{R}$ as its configuration space we obtain a series solution of this equation that involves two functional degrees of freedom. These signify the arbitrariness in the choice of the (pseudo-)metric operator. Our approach allows a more direct way of addressing some of the basic practical problems arising in

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the application of quasi- and pseudo-Hermitian quantum mechanics.[1,3–13] In particular it provides an extremely powerful technical tool for the perturbative calculation of the (pseudo-)metric operators for various toy models.

II. DIFFERENTIAL REPRESENTATION OF PSEUDO-HERMITICITY

Consider a physical system described by a separable Hilbert space $\mathcal{H}$ and a pseudo-Hermitian Hamiltonian operator $H:\mathcal{H}\to\mathcal{H}$. Let $\mathcal{M}$ denote the set of all linear invertible Hermitian operators $\eta:\mathcal{H}\to\mathcal{H}$, then by definition[14] the pseudo-Hermiticity of H means that $\mathcal{M}_H:=\{\eta\in\mathcal{M}\,|\,H^\dagger=\eta H\eta^{-1}\}$ is a nonempty subset of $\mathcal{M}$. The elements of $\mathcal{M}$ are called pseudo-metric operators, for they may be used to define a pseudo-inner product (a nondegenerate sesquilinear form[15]) $\langle\cdot|\cdot\rangle_\eta:=\langle\cdot|\,\eta\cdot\rangle$ on $\mathcal{H}$, where $\langle\cdot|\cdot\rangle$ denotes the defining inner product of $\mathcal{H}$. (Strictly speaking, $\langle\cdot|\cdot\rangle_\eta$ is a nondegenerate sesquilinear form defined on the domain of η).

The Hamiltonian H is Hermitian with respect to $\langle\cdot|\cdot\rangle_\eta$ for all $\eta\in\mathcal{M}_H$.[14,16] If $\mathcal{M}_H$ includes a positive-definite element, i.e., a *metric operator*, η_+, then H is Hermitian with respect to the positive-definite inner product $\langle\cdot|\cdot\rangle_{\eta_+}$. This implies that H is diagonalizable and has a real spectrum. The converse of this statement holds true at least for the case that the spectrum of H is discrete, i.e., if H is diagonalizable and has a real spectrum then $\mathcal{M}_H$ includes a positive-definite element and equivalently H is Hermitian with respect to a positive-definite inner product.[17,18] Furthermore, in this case one can show that H is necessarily quasi-Hermitian, i.e., it may be mapped to a Hermitian Hamiltonian $h:\mathcal{H}\to\mathcal{H}$ via a similarity transformation, $H=\rho^{-1}h\rho$.[17,18] This and only this class of Hamiltonians are capable of supporting a unitary time evolution in an associated *physical Hilbert space*. The latter is defined by endowing $\mathcal{H}$ with the inner product $\langle\cdot|\cdot\rangle_{\eta_+}$ and will be denoted by $\mathcal{H}_{\eta_+}$.[4,5,7,9,19]

An important fact about this construction is that η_+ is not unique. Different choices for η_+ yield kinematically distinct quantum systems that nevertheless share the same dynamical structure. The quantum mechanical analog of the principle of general covariance of GR is the physical (unitary) equivalence of quantum systems $(\mathcal{H}_{\eta_+},H)$.[2] The metric operators η_+ and more generally pseudo-metric operators η are linked to and consequently determined by the Hamiltonian H via the pseudo-Hermiticity condition

$$H^\dagger=\eta H\eta^{-1}. \tag{1}$$

The same way Einstein's field equation links the metric tensor to the energy-momentum tensor, (1) links the pseudo-metric operator to the Hamiltonian. The resemblance may be made more pronounced for a Hamiltonian of the standard form,

$$H=\frac{\vec{p}^{\,2}}{2m}+v(\vec{x}), \tag{2}$$

that acts in $L^2(\mathbb{R}^n)$. Applying both sides of (1) on η, substituting (2), and representing the resulting equation in the $\vec{x}$-basis, we find

$$\left(-\nabla_x^2+\nabla_y^2+\frac{2m}{\hbar^2}[v(\vec{x})^*-v(\vec{y})]\right)\eta(\vec{x},\vec{y})=0, \tag{3}$$

where $\nabla_u^2:=\Sigma_{j=1}^n\partial^2/\partial u_j^2$ for $u=x,y$ and $\eta(\vec{x},\vec{y}):=\langle\vec{x}|\,\eta\,|\vec{y}\rangle$. For $n=1$, this is a Klein-Gordon equation with a variable mass term,

$$[-\partial_x^2+\partial_y^2+\mu^2(x,y)]\eta(x,y)=0,\quad \mu^2(x,y):=\frac{2m}{\hbar^2}[v(x)^*-v(y)]. \tag{4}$$

According to (3) if $\eta(\vec{x},\vec{y})$ is a solution, then so is $\eta(\vec{y},\vec{x})^*$. The pseudo-metric operators $\eta\in\mathcal{M}_H$ correspond to solutions that satisfy

$$\eta(\vec{x},\vec{y})^* = \eta(\vec{y},\vec{x}). \tag{5}$$

Note that even for non-pseudo-Hermitian Hamiltonians of the form (2), Eq. (3) admit solutions. However, these solutions fail to satisfy either the Hermiticity requirement (5) or the invertibility condition:

$$\int_{\mathbb{R}^n} \mathrm{d}^n\vec{y}\,\eta(\vec{x},\vec{y})\psi(\vec{y}) = 0 \text{ implies } \psi = 0. \tag{6}$$

If $\mathcal{M}_H$ happens to include positive-definite elements η_+, then these elements correspond to the solutions $\eta_+(\vec{x},\vec{y})$ of (3) that in addition to (5) satisfy

$$\int_{\mathbb{R}^n} \mathrm{d}^n\vec{x} \int_{\mathbb{R}^n} \mathrm{d}^n\vec{y}\,\psi(\vec{x})^* \eta_+(\vec{x},\vec{y})\psi(\vec{y}) > 0 \text{ for } \psi \neq 0. \tag{7}$$

The fact that for a diagonalizable Hamiltonian with a real and discrete spectrum such solutions exist is a consequence of the spectral theorems given in Refs. 17 and 18. Indeed if $\{\psi_n, \phi_n\}$ is a biorthonormal system associated with H, i.e., $H\psi_n = E_n\psi_n$, $H^\dagger\phi_n = E_n\phi_n$, $\langle\psi_n|\,\phi_m\rangle = \delta_{mn}$, then

$$\eta_+(\vec{x},\vec{y}) = \sum_n \phi_n(\vec{x})\phi_n(\vec{y})^* \tag{8}$$

is a solution of (3) that satisfies both (5) and (7). As shown in Refs. 20 and 21, in this case the most general (positive-definite) metric operator has the form $A^\dagger\eta_+A$, where A is invertible and commutes with H. The latter corresponds to a solution of (3) that is of the form

$$\eta'_+(\vec{x},\vec{y}) = \sum_n \int_{\mathbb{R}^n} \mathrm{d}^n\vec{u} \int_{\mathbb{R}^n} \mathrm{d}^n\vec{v} A(\vec{u},\vec{x})^* \phi_n(\vec{u})\phi_n(\vec{v})^* A(\vec{v},\vec{y}), \tag{9}$$

where $A(\vec{x},\vec{y})$ satisfies

$$\left(-\nabla_x^2 + \nabla_y^2 + \frac{2m}{\hbar^2}[v(\vec{x}) - v(\vec{y})]\right) A(\vec{x},\vec{y}) = 0, \tag{10}$$

and

$$\int_{\mathbb{R}^n} \mathrm{d}^n\vec{y} A(\vec{x},\vec{y})\psi(\vec{y}) = 0 \text{ implies } \psi = 0. \tag{11}$$

For a real-valued potential v, $\delta(\vec{x}-\vec{y})$ is a solution of (3). It corresponds to the choice $\eta = I$, where I is the identity operator acting in $\mathcal{H} = L^2(\mathbb{R})$. This is consistent with the Hermiticity of H. For a $\mathcal{PT}$-symmetric potential v that satisfies $v(-\vec{x}) = v(\vec{x})^*$, $\delta(\vec{x}+\vec{y})$ is a solution of (3). This is a manifestation of $\mathcal{P}$-pseudo-Hermiticity of the Hamiltonian,[14] for $\langle\vec{x}|\,\mathcal{P}\,|\vec{y}\rangle = \delta(\vec{x}+\vec{y})$.

For $n > 1$, (3) is an ultrahyperbolic equation with quite peculiar properties.[22] We will therefore focus our attention on the case $n = 1$. Our main purpose is to obtain the general solution of (3) without having to resort to its spectral decomposition (8). This is mainly because of the difficulties with summing the series in (8) or evaluating the integrals that replace the latter whenever the spectrum becomes continuous.[7]

In Ref. 9, we have pursued a similar approach to construct the most general η_+ for the imaginary cubic potential $v = i\varepsilon x^3$ in some low orders of perturbation theory. The approach of Ref. 9 applies to any (preferably imaginary) potential with a real spectrum. It yields an infinite system of iteratively decoupled partial differential equations whose solution provides the contributions to η_+ in various orders of the perturbation theory. Although these equations have the same structure, at each order one must compute their nonhomogeneous term and solve them separately. In contrast, in the present paper, we obtain a single differential equation satisfied by η, namely (4),

that applies for an arbitrary potential $v(x)$ rendering the Hamiltonian pseudo-Hermitian. An important advantage of the approach of the present paper over that of Ref. 9 is that in view of the simple structure of (4), we are able to offer (as discussed in Sec. III) a general scheme for constructing a series solution of this equation. This solution involves two arbitrary functions that provide an explicit characterization of the arbitrariness in the choice of η.

Another recent application of the powerful machinery of differential equations to compute (pseudo-)metric operators is due to Scholtz and Geyer.[10] These authors obtain a phase-space representation of the (pseudo-)metric operators η. They use the Moyal product techniques to deal with the difficult factor-ordering problems that arise in this representation. The following are the main differences between the method of Ref. 10 and the one presented in the present paper.

- The method of Ref. 10 leads to an equation for η that is a differential equation[11] provided that $v(x)$ is a polynomial potential. Even for a polynomial potential the general character and in particular the order of this differential equation depends on the structure of $v(x)$ and its degree. In contrast, in the present paper we offer a universal differential equation, namely (4), that applies for polynomial as well as nonpolynomial potentials, and has the same simple structure for all potentials. It is this appealing property that allows us to treat the well-known toy models of Sec. IV. The application of the method of Ref. 10 to these models yields pseudo-differential equations (differential equations of infinite order) whose solution is extremely difficult if not impossible.
- Suppose v is a polynomial potential, so that the method of Ref. 10 yields a differential equation, and suppose that one is able to solve this equation. Then one obtains an explicit expression for η in terms of the operators x and p that involves a number of arbitrary functions. The condition that η be Hermitian must be imposed to fix some of these functions. This is done by adopting a set of appropriate boundary conditions.[10](The author is unaware of a systematic method of selecting the boundary conditions that achieve this purpose.) In contrast, our method yields an expression for $\eta(x,y)$ that satisfies the Hermiticity condition $\eta(x,y)^*=\eta(y,x)$ manifestly and specifies a unique Hermitian η according to

$$(\eta\psi)(x)=\int_{\mathrm{R}} \mathrm{d}y\, \eta(x,y)\psi(y).$$

- It achieves this without making use of the Moyal product or having to select certain boundary conditions that ensures the Hermiticity of η. Its successful application, however, does not yield an explicit expression for η in terms of x and p. As explained in Ref. 9, the latter may be obtained by Fourier transforming $\eta(x,y)=\langle x|\eta|y\rangle$ over y to obtain $\langle x|\eta|p\rangle$ and arranging the terms in the expression for $\sqrt{2\pi\hbar}e^{-ixp/\hbar}\langle x|\eta|p\rangle$ in such a way that x's are placed to the left of p's. This is how the issue of ordering of factors is addressed in this construction.

A common feature of both methods is that solving the associated differential equations yields generally non-positive-definite pseudo-metric operators. The (positive-definite) metric operators η_+, if they exist, correspond to certain special solutions that are to be identified using different means. [The construction of η given here may be supplemented with the procedure proposed in Ref. 10 for selecting the positive-definite metric operators η_+ among η's. This is expected to be a difficult task in practice, and we will not pursue it here. We suffice to point out that given $\eta(x,y)$ we can obtain an expression for η in terms of x and p as outlined in Ref. 9. This allows for making direct contact with the approaches of Refs. 10 and 11].

III. SERIES EXPANSION FOR $\eta(x,y)$

We begin our analysis by expressing (4) in the form

$$(-\partial_x^2+\partial_y^2)\,\eta(x,y)=f(x,y)-f(y,x)^*, \tag{12}$$

where

$$f(x,y) := \frac{2m}{\hbar^2} v(y)\,\eta(x,y). \tag{13}$$

We note that for a Hermitian η, (12) is equivalent to

$$\eta(x,y) = \chi(x,y) + \chi(y,x)^*, \tag{14}$$

$$(-\partial_x^2 + \partial_y^2)\chi(x,y) = f(x,y). \tag{15}$$

Next, we recall that the general solution of the wave equation $(-\partial_x^2+\partial_y^2)u(x,y)=0$ is given by

$$u(x,y) = u_+(x-y) + u_-(x+y), \tag{16}$$

where $u_\pm:\mathbb{R}\to\mathbb{C}$ are a pair of arbitrary twice-differentiable functions (or distributions). Consequently, the general solution of (12) has the form

$$\eta(x,y) = u_+(x-y) + u_-(x+y) + \chi_p(x,y) + \chi_p(y,x)^*, \tag{17}$$

where $u_\pm$ satisfy $u_\pm(x)^* = u_\pm(\mp x)$ and $\chi_p(x,y)$ is a particular solution of (15). The latter is a nonhomogeneous wave equation in $1+1$ dimensions. It admits a particular solution that in view of (13) takes the form

$$\chi_p(x,y) = \frac{m}{\hbar^2}\int^y \mathrm{d}r \int_{x-y+r}^{x+y-r} \mathrm{d}s\; v(r)\,\eta(s,r). \tag{18}$$

Combining (16)–(18), we find

$$\eta(x,y) = u(x,y) + \mathcal{K}\eta(x,y), \tag{19}$$

where $\mathcal{K}$ is the integral operator defined by

$$\begin{aligned}\mathcal{K}\eta(x,y) &:= \frac{m}{\hbar^2}\left[\int^y \mathrm{d}r \int_{x-y+r}^{x+y-r} \mathrm{d}s\; v(r)\,\eta(s,r) + \int^x \mathrm{d}r \int_{-x+y+r}^{x+y-r} \mathrm{d}s\; v^*(r)\,\eta(s,r)^*\right]\\ &= \frac{m}{\hbar^2}\left[\int^y \mathrm{d}r \int_{x-y+r}^{x+y-r} \mathrm{d}s\; v(r)\,\eta(s,r) + \int^x \mathrm{d}s \int_{-x+y+s}^{x+y-s} \mathrm{d}r\; v(s)^*\,\eta(s,r)\right].\end{aligned} \tag{20}$$

In view of the analogy with the derivation of the Lippmann-Schwinger equation,[23] it is not difficult to see that (19) admits the following general series solution:

$$\eta(x,y) = [I-\mathcal{K}]^{-1}u(x,y) = \sum_{\ell=0}^{\infty} \mathcal{K}^\ell u(x,y). \tag{21}$$

Clearly, η is determined in terms of the arbitrary functions $u_\pm$.

For $v=0$, i.e., a free particle, $\eta(x,y)=u(x,y)$. As shown in Ref. 9, this is equivalent to

$$\eta = L(p) + K(p)\mathcal{P}, \tag{22}$$

where $L(p)^\dagger = L(p)$ and $K(p)^\dagger = \mathcal{P}K(p)\mathcal{P}$, equivalently L and K are respectively real-valued and $\mathcal{PT}$-invariant [this means $K(r)^* = K(-r)$ for all $r\in\mathbb{R}$] functions. (They may be further restricted to constants if one postulates the nonexistence of a hidden length scale for the problem. See Ref. 9 for details.) They are related to the Fourier transform [in our convention, the Fourier transform of a function φ is given by $\widetilde{\varphi}(k) := (2\pi)^{-1/2}\int_{-\infty}^{\infty}\mathrm{d}x e^{-ikx}\varphi(x)$] $\widetilde{u}_\pm$ of $u_\pm$ according to

$$L(p)=\sqrt{2\pi}\tilde{u}_+\left(\frac{p}{\hbar}\right),\quad K(p)=\sqrt{2\pi}\tilde{u}_-\left(-\frac{p}{\hbar}\right). \tag{23}$$

For a real-valued potential the ordinary choice for the metric operator that yields the L^2-inner product, i.e., $\eta=I$, corresponds to setting

$$u(x,y)=\delta(x-y)-\frac{m}{\hbar^2}\int^{x+y/2}\mathrm{d}r\, v(r). \tag{24}$$

To see this, we first calculate $K\delta(x-y)$ for an arbitrary (possibly complex-valued) potential v. Using the well-known properties of the step function

$$\theta(x):=\begin{cases}0 & \text{for } x<0\\ \frac{1}{2} & \text{for } x=0\\ 1 & \text{for } x>0,\end{cases} \tag{25}$$

we then find

$$\mathcal{K}\delta(x-y)=\frac{m}{\hbar^2}\left(\int^{x+y/2}\mathrm{d}r\Re[v(r)]+i\,\mathrm{sign}(y-x)\int^{x+y/2}\mathrm{d}r\Im[v(r)]\right), \tag{26}$$

where $\Re[v]$ and $\Im[v]$ respectively stand for the real and imaginary parts of v, and

$$\mathrm{sign}(x):=\theta(x)-\theta(-x)=\begin{cases}-1 & \text{for } x<0\\ 0 & \text{for } x=0\\ 1 & \text{for } x>0.\end{cases}$$

If v is a real potential, $\Re[v]=v$ and $\Im[v]=0$. In this case (26) together with (19) and $\eta(x-y)=\delta(x-y)$ yield (24).

For a purely imaginary potential, $\Re[v]=0$, $v=i\Im[v]$, and (26) takes the following form:

$$\mathcal{K}\delta(x-y)=\frac{m}{\hbar^2}\mathrm{sign}(y-x)\int^{x+y/2}\mathrm{d}r\, v(r). \tag{27}$$

IV. APPLICATIONS

A. $\mathcal{PT}$-symmetric square well

The $\mathcal{PT}$-symmetric square well potential,

$$v(x):=\begin{cases}-i\zeta\,\mathrm{sign}(x) & \text{for } |x|<\frac{L}{2}\\ \infty & \text{for } |x|>\frac{L}{2},\end{cases} \tag{28}$$

with $\zeta\in\mathbb{R}$ and $L\in\mathbb{R}^+$, defines one of the best-known exactly solvable toy models that captures the generic properties of pseudo-Hermitian quantum systems.[24,25] A thorough investigation of the physical content of this model is conducted in Ref. 4, where a particular perturbative calculation of a metric operator and the corresponding physical observables, localized states, probability density, and the underlying classical Hamiltonian is performed. This calculation makes use of the fact that the non-Hermiticity effects in this model diminish for energy states with larger spectral label N. More specifically, it is ζ/N^2 that plays the role of the perturbation parameter.

More recently, Bender and Tan[12] performed a more conventional perturbative calculation of a metric operator taking ζ as the perturbation parameter. This is the metric operator η_+ that is

associated with the $\mathcal{CPT}$-inner product $(\cdot,\cdot)_{\mathcal{CPT}}$,[26] that is $(\cdot,\cdot)_{\mathcal{CPT}}=\langle\cdot|\eta_+\cdot\rangle$.[21] Expressing η_+ in its exponential form, $\eta_+=e^{-Q}$, and noting that Bender and Tan set $\hbar=2m=L/\pi=1$, take $\epsilon=-\zeta$ for the coupling constant, and use "$\varepsilon(x)$" for "sign (x)," we can summarize their principal result [Eq. (11) of Ref. 12] as

$$\langle x|Q|y\rangle =: Q(x,y) = -\frac{i\zeta}{4}[x-y+\mathrm{sign}(x-y)(|x+y|-\pi)]+\mathcal{O}(\zeta^3), \tag{29}$$

where $\mathcal{O}(\zeta^n)$ stands for terms of order n and higher in powers of ζ. In particular, in view of the identity $x-y=|x-y|\mathrm{sign}(x-y)$, we have the following expression for the $\mathcal{CPT}$-metric operator η_+:

$$\eta_+(x,y)=\delta(x-y)+\frac{i\zeta}{4}(|x-y|+|x+y|-\pi)\mathrm{sign}(x-y)+\mathcal{O}(\zeta^2). \tag{30}$$

The perturbative calculation of the metric operator using the method developed in the preceding section is quite straightforward. Inserting (28) in (27) and performing the trivial integral in the resulting equation, we find

$$\mathcal{K}\delta(x-y)=\frac{im\zeta}{2\hbar^2}|x+y|\mathrm{sign}(x-y). \tag{31}$$

The most general metric operator η that reduces to the identity operator in the Hermitian limit $\zeta\to 0$ is obtained by setting

$$u(x,y)=\delta(x-y)+\zeta[w_+(x-y)+w_-(x+y)]+\mathcal{O}(\zeta^2) \tag{32}$$

in (21), where $w_\pm:[-L/2,L/2]\to\mathbb{C}$ are arbitrary functions satisfying $w_\pm(x)^*=w_\pm(\mp x)$ and $w_\pm(\pm L)=0$. [These conditions arise from the Hermiticity requirement on the metric operator and its spectral resolution (8).] This together with (31) yields

$$\eta(x,y)=\delta(x-y)+\zeta\left[w_+(x-y)+w_-(x+y)+\frac{im}{2\hbar^2}|x+y|\mathrm{sign}(x-y)\right]+\mathcal{O}(\zeta^2). \tag{33}$$

Setting $\hbar=2m=L/\pi=1$ in this equation, we find that the $\mathcal{CPT}$-metric operator (30) obtained by Bender and Tan[12] is a particular example of the metric operators (33). It corresponds to the choice $w_+(x)=(i/4)(|x|-\pi)\mathrm{sign}(x)$ and $w_-(x)=0$.

We can calculate higher-order terms in the expression for the metric operator using our iterative method. Each additional order will involve an arbitrary pair of functions that enter the expression for u in (21). This calculation is not only completely general (as it yields the most general metric operator), but it is also much simpler to perform. This is mainly because unlike its alternatives[4,12] it avoids approximating or summing complicated series.

B. An imaginary scattering potential

Consider the following variant of the $\mathcal{PT}$-symmetric square well potential:[27]

$$v(x) := \frac{i\zeta}{2}\left[\mathrm{sign}\left(x+\frac{L}{2}\right)+\mathrm{sign}\left(x-\frac{L}{2}\right)-2\,\mathrm{sign}(x)\right]=\begin{cases}-i\zeta\,\mathrm{sign}(x) & \text{for } |x|<\dfrac{L}{2}\\ 0 & \text{for } |x|>\dfrac{L}{2},\end{cases} \tag{34}$$

where $\zeta\in\mathbb{R}$ is a coupling constant and $L\in\mathbb{R}^+$ is a length scale.

In Ref. 7 we established the reality of the spectrum of this potential and used the spectral method of Refs. 14, 17, and 18 to obtain a perturbative expression for an associated metric operator η_+. This involved constructing an appropriate biorthonormal system for the model and performing a highly tedious calculation of the integrals appearing in the spectral resolution of η_+.

Indeed, this calculation could only be done after expanding all the relevant quantities in powers of ζ and restricting to the first-order terms. Although the results reported in Ref. 7 required performing extremely lengthy calculations partly done using Mathematica, the expression obtained for $\eta_+(x,y) := \langle x|\eta_+|y\rangle$ took a surprising simple form, namely

$$\eta_+(x,y) = \delta(x-y) + \frac{im\zeta}{4\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-L|)\mathrm{sign}(x-y) + \mathcal{O}(\zeta^2). \quad (35)$$

Here we wish to use the scheme developed in the preceding section to construct the most general metric operator η that reduces to the identity operator in the Hermitian limit $\zeta \to 0$. In order to do this first we insert (34) in (27) and perform the trivial integral in the resulting equation to obtain

$$\mathcal{K}\delta(x-y) = \frac{im\zeta}{4\hbar^2}(|x+y+L| + |x+y-L| - 2|x+y|)\mathrm{sign}(y-x). \quad (36)$$

Substituting (32) in (21) and using (36), we then find

$$\eta(x,y) = \delta(x-y) + \zeta\left[w_+(x-y) + w_-(x+y) + \frac{im}{4\hbar^2}(2|x+y| - |x+y+L| - |x+y-L|)\mathrm{sign}(x-y)\right] + \mathcal{O}(\zeta^2), \quad (37)$$

where $w_\pm : \mathbb{R} \to \mathbb{C}$ are arbitrary functions satisfying $w_\pm^*(x) = w_\pm(\pm x)$. Clearly, the positive-definite inner product (35) constructed in Ref. 7 corresponds to setting $w_+(x) = imL/2\hbar^2\,\mathrm{sign}(x)$ and $w_-(x) = 0$.

C. Imaginary δ-function potentials

Consider the potential

$$v(x) = i\zeta\delta(x-a), \quad (38)$$

where $\zeta, a \in \mathbb{R}$. (Clearly, we can choose the origin of the x-axis so that $a=0$. We retain a for future use where we consider the multi-delta-function potentials.) It is not difficult to solve the time-independent Schrödinger equation for this potential and show that $H = (p^2/2m) + v(x)$ has a real continuous spectrum. [H is not $\mathcal{PT}$-symmetric. But one may attempt to use the results of Ref. 21 to construct a generalized $\mathcal{PT}$-operator (an antilinear involution) that commutes with H.] This in turn suggests that one can construct an associated pseudo-metric operator using the spectral method of Refs. 17 and 18. This construction is similar to the one offered in Ref. 7 for the potential (34). An explicit calculation of η using this method is however quite involved. A much simpler construction that we will describe in the following is based on the method of Sec. III.

First, we substitute (38) in (20) to establish

$$\mathcal{K}F(x,y) = \mathcal{F}(x,y) + \mathcal{F}(y,x)^*, \quad \mathcal{F}(x,y) := \frac{iz}{2}\theta(y-a)\int_{x-y+a}^{x+y-a} \mathrm{d}s F(s,a), \quad (39)$$

where $z := 2m\zeta/\hbar^2$ and $F(x,y)$ is a test function. If we choose a z-independent u, the series expansion (21) becomes a power series in the coupling constant z. For definiteness we shall first choose $u(x,y) = \delta(x-y)$. Setting $F(x,y) = \delta(x-y)$ in (39) and using the properties of the step function (25), we then find

$$\mathcal{K}u(x,y) = \frac{iz}{2}\theta(x+y-2a)\mathrm{sign}(y-x) =: u_1(x,y). \quad (40)$$

Alternatively, we could directly use (27) to obtain (40).

Next, we compute $\mathcal{K}^2 u(x,y)$ by substituting u_1 for F in (39). This yields

$$\mathcal{K}^2u(x,y)=\frac{z^2}{4}[\theta(x-a)+\theta(y-a)][(x+y-2a)\,\theta(x+y-2a)-|x-y|]. \tag{41}$$

The higher-order terms in (21) can be similarly calculated. Moreover, because of the simple form of (39) and (40), we can actually obtain an upper bound on $|\mathcal{K}^\ell u(x,y)|$ and use it to find a lower bound on the radius of the convergence of the series (21).

First, we recall[28] that if a function $g:\mathbb{R}\to\mathbb{C}$ is bounded on an interval $[\alpha,\beta]$ by some $M\in\mathbb{R}^+$, i.e., $|g(r)|<M$ for all $r\in[\alpha,\beta]$, then $|\int_\alpha^\beta dr\, g(r)|\leqslant M(\beta-\alpha)$. Now, let $F(x,y)$ be a function such that $|F(s,a)|$ has an upper bound M_F as s takes values between $|x-y|+a$ and $x+y-a$. Then, according to (39),

$$|\mathcal{K}F(x,y)|\leqslant|z|(|x-a|+|y-a|)M_F. \tag{42}$$

In view of (40), for all $x,y\in\mathbb{R}$, $|\mathcal{K}u(x,y)|\leqslant|z|/2$. To obtain an upper bound on $|\mathcal{K}^2u(x,y)|$ we set $F(x,y)=\mathcal{K}u(x,y)$ in (42), which allows us to identify M_F with $|z|/2$ and yields for all $x,y\in\mathbb{R}$:

$$|\mathcal{K}^2u(x,y)|\leqslant\frac{z^2}{2}(|x-a|+|y-a|). \tag{43}$$

We can directly verify this relation using (41). Repeating the procedure that leads to (43), we find for all $\ell\geqslant1$ and all $x,y\in\mathbb{R}$: $|\mathcal{K}^\ell u(x,y)|\leqslant|z|^\ell(|x-a|+|y-a|)^{\ell-1}/2$. This in turn implies, in view of the elementary comparison tests, that the series (21) converges (absolutely) for $|z|(|x-a|+|y-a|)<1$. Hence, it converges in an open disc in the x-y plane that is centered at $(x=a,\ y=a)$ and has a radius $\varrho>(\sqrt{2}|z|)^{-1}$.

In summary, for every given value of z, truncation of the series (21) yields a reliable approximation for η provided that we keep a sufficiently large number of terms in the series and deal with wave functions $\psi(x)$ that decay sufficiently rapidly as $|x|\to\infty$. (Our analysis only yields a lower bound on ϱ. It does not imply that ϱ is finite.)

We can extend our treatment to a potential consisting of more than one delta function:

$$v(x)=i\sum_{n=1}^{N}\zeta_n\delta(x-a_n), \tag{44}$$

where $N\in\mathbb{Z}^+$ and $\zeta_n,a_n\in\mathbb{R}$. An example is the $\mathcal{PT}$-symmetric potentials[29–31] corresponding to the cases that N is even and $\zeta_{N/2+k}=-\zeta_k$, $a_{(N/2)+k}=-a_k$ for all $k=1,2,\cdots N/2$. [Here we assume that (ζ_n,a_n) are such that the Hamiltonian is pseudo-Hermitian. This is the generic case, for the values of (ζ_n,a_n) that render the spectrum of the Hamiltonian nonreal form a measure-zero subset of the set $\mathbb{R}^{2N}$ of all possible values of (ζ_n,a_n).]

For these multi-delta-function potentials the calculation of the first-order term in $z_n:=2m\zeta_n/\hbar^2$ in the series expansion (21) reduces to the case $N=1$ that we considered above. In view of (40),

$$\mathcal{K}\delta(x,y)=\frac{i}{2}\sum_{n=1}^{N}z_n\theta(x+y-2a_n)\mathrm{sign}(y-x). \tag{45}$$

The most general η that reduces to $\eta=I$ in the Hermitian limit $z_n\to0$ is obtained up to second-order terms in z_n by setting $u(x,y)=\delta(x-y)+\sum_{n=1}^{N}z_n[w_{n+}(x-y)+w_{n-}(x+y)]+\mathcal{O}(z_n^2)$, where $w_{n\pm}:\mathbb{R}\to\mathbb{C}$ are arbitrary functions satisfying $w_{n\pm}(x)^*=w_{n\pm}(\mp x)$. This together with (45) and (21) yields

$$\eta(x,y) = \delta(x-y) + \sum_{n=1}^{N} z_n \left[w_{n+}(x-y) + w_{n-}(x+y) + \frac{i}{2}\theta(x+y-2a_n)\mathrm{sign}(y-x) \right] + \mathcal{O}(z_n^2). \tag{46}$$

We close this section by the following general remarks. As we observe in the study of the above toy models, the series solution (21) may be used to obtain a perturbative expansion for the pseudo-metric operator η. In general, depending on the details of the model under study, one may or may not have access to a dimensionless perturbation parameter. Typical examples for which this occurs are the imaginary cubic potential and the single imaginary delta-function potential (38). In this case, as explained in Ref. 9, the truncation of the perturbative expansion of $\eta(x,y)$ generally yields a reliable result only within a sufficiently small region in the x-y plane. Furthermore, one expects that for sufficiently small values of the perturbation parameter (the coupling constant ζ or ζ_n in the above examples) the perturbative corrections to a positive-definite metric operator such as $\eta=I$ leave this property intact.

V. CONCLUDING REMARKS

In this article, we have outlined a differential realization of the pseudo-Hermiticity condition that plays a central role in devising a unitary quantum theory based on quasi-Hermitian Hamiltonians of the standard form. The integral kernel $\eta(x,y)$ for the corresponding pseudo-metric operators η satisfies a linear partial differential equation. For systems having $\mathbb{R}$ as their configuration space this is nothing but a particular variable-mass Klein-Gordon equation. We have obtained a general series solution for this equation and demonstrated its application in treating the $\mathcal{PT}$-symmetric square well potential, an imaginary $\mathcal{PT}$-symmetric scattering potential, and a class of imaginary delta-function potentials. In particular, for the former two potentials, the approach presented here is by far more practical than the alternative approaches that use the spectral resolution of the metric operator. Another advantage of the former approach is that it is capable of producing the most general pseudo-metric operator. In particular, imposing the positive-definiteness condition (7), it yields the general form of the metric operators.

Our method is not only practically advantageous but also conceptually appealing. It furthers the analogy between QM and GR, for the differential pseudo-Hermiticity relation plays a similar role in QM as the Einstein's field equation does in GR [not to mention the curious fact that the field theoretic extension of the pseudo-Hermiticity relation (3) is a functional differential equation that has the same structure as the Wheeler-DeWitt equation of the conventional canonical quantum gravity]. Another valuable outcome of our method is a concrete characterization of the arbitrariness of the metric operator. Each choice of a metric operator defines a separate quantum system. One can pursue the prescription used in the so-called quasi-Hermitian quantum mechanics[1] to select an irreducible set of compatible quasi-Hermitian operators O_α and fix the metric operator η_+ (up to scale) through the requirement that O_α be η_+-pseudo-Hermitian. Alternatively, one can follow the approach of the so-called pseudo-Hermitian quantum mechanics,[3] choose η_+ directly, and construct the Hilbert space and observables of the theory accordingly.[4,5,7,9]

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Phase space quantization and the operator moment problem

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We consider questions related to a quantization scheme in which a classical variable $f:\Omega\to\mathbb{R}$ on a phase space Ω is associated with a (preferably unique) semispectral measure E^f, such that the moment operators of E^f are required to be of the form $\Gamma(f^k)$, with Γ a suitable mapping from the set of classical variables to the set of (not necessarily bounded) operators in the Hilbert space of the quantum system. In particular, we investigate the situation where the map Γ is implemented by the operator integral with respect to some fixed positive operator measure. The phase space Ω is first taken to be an abstract measurable space, then a locally compact unimodular group, and finally $\mathbb{R}^2$, where we determine explicitly the relevant operators $\Gamma(f^k)$ for certain variables f, in the case where the quantization map Γ is implemented by a translation covariant positive operator measure. In addition, we consider the question under what conditions a positive operator measure is projection valued. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Quantization can be any procedure that associates a quantum mechanical observable to a given classical dynamical variable. The traditional way to realize a quantization is to assign to each classical variable a Hermitean (symmetric, or even essentially self-adjoint) operator that should describe the quantum observable. The question is how to modify the traditional scheme in order to fit it into the context of modern quantum mechanics.

We recall that, in this formulation, observables of a quantum system with a Hilbert space $\mathcal{H}$ are given as semispectral measures $E:\mathcal{B}(\mathbb{R})\to L(\mathcal{H})$ and states as positive trace one operators $T:\mathcal{H}\to\mathcal{H}$. The probability measure $X\mapsto \mathrm{Tr}[TE(X)]$ defined by a pair (E,T) is taken to describe the measurement outcome probabilities of the observable E in the state T. Here $\mathcal{B}(\mathbb{R})$ denotes the Borel σ-algebra of the real line $\mathbb{R}$, and $L(\mathcal{H})$ is the set of bounded operators on $\mathcal{H}$.

Classical variables can be represented by real valued measurable functions defined on some measurable space $(\Omega,\mathcal{A})$, which is the phase space of the classical system. The phase space can be taken to be, e.g., $\mathbb{R}^{2n}$, in which case the variables are Borel functions. In the conventional approach to quantization, we would have a map Γ from the set of real measurable functions to the set of all linear (not necessarily bounded) operators in a Hilbert space $\mathcal{H}$, and $\Gamma(f)$ would be the observable corresponding to the classical variable f (see, e.g., Refs. 9, 15, 28, 32, and 33).

We would like to modify this scheme so that we could assign a semispectral measure to the function f, instead of an operator. To do this, we still assume that we have a map Γ as above, but now we use all the operators $\Gamma(f^k)$, $k\in\mathbb{N}$, instead of just $\Gamma(f)$. (In this paper, $\mathbb{N}$ is the set of positive integers.) The idea is to consider the moment problem of finding the unique semispectral measure $E^f:\mathcal{B}(\mathbb{R})\to L(\mathcal{H})$ with the property that $\int x^k dE^f=\Gamma(f^k)$ for all $k\in\mathbb{N}$. Here $\int x^k dE^f$, the kth

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moment of E^f, is the operator integral $L(x^k, E^f)$ of the function $x \mapsto x^k$ with respect to E^f; see the next section for its definition. So if Γ and f are such that there exists a unique solution E^f of the described moment problem, then the collection of the operators $\{\Gamma(f^k) | k \in \mathbb{N}\}$ is eligible to represent a quantization E^f of f. The motivation for this approach lies in the fact that then the moments of the measurement outcome probabilities of a quantum observable E^f correspond to those of the original classical variable f, which are simply the powers of its values.

One way to obtain a quantization map Γ is to use the operator integral with respect to some given positive operator measure E, i.e., define Γ to be the map $f \mapsto L(f, E)$. In this case, if we define E^f on the Borel sets of the real line by $B \mapsto E(f^{-1}(B))$, we have simply $L(x^k, E^f) = L(f^k, E)$, as is easily seen by using the definition of the next section and the usual change of variables in the integral with respect to a complex measure. So then E^f is a solution to the moment problem described above, which leaves us with the uniqueness question. Note that if we choose E to be a projection operator measure, we end up getting only spectral measures as the quantized observables, with all the operators $L(f^k, E)$ mutually commuting. We also remark that, in any case, all the observables obtained via this type of quantization are *functionally coexistent*,[26] so that they can be measured together in the sense of Ludwig (see Ref. 29, D.3.1, p. 153).

We mention that the approach described above is used, for instance, in Ref. 14 in the description of a quantum measurement. In a typical measurement situation, where one aims to measure a (traditional) quantum observable represented by a self-adjoint operator, one is actually measuring a noisy or unsharp version of that observable. The noisy version, represented by a semispectral measure, may agree with the observable intended to be measured, on the statistical level of expectations. The unsharpness of the measurement is reflected in the fact that the dispersion of the measurement statistics is actually greater than what would be obtained in the noiseless case. The observable, as represented by a semispectral measure, cannot be described using a single operator. Accordingly, in the approach of Ref. 14, each moment of the measurement outcome distribution is considered to be an average of a certain operator, called an "operational observable," and the collection of these operators then represents the measured observable. We want to point out that these operational observables are nothing more but the moment operators of the semispectral measure representing the observable. Note that these moments need not determine the semispectral measure uniquely. In certain special cases, however, they do,[12,13] and sometimes even the first moment is enough.[8,25]

The structure of this paper is as follows. In the Sec. II we give some results on the theory of operator integrals and give a simple characterization of the quantization maps that can be represented by an operator integral with respect to a positive operator measure. In Sec. III, we consider the operator integral with respect to covariant positive operator measures on a locally compact to pological group. Section IV is devoted to the quantizations obtained by using the covariant phase space observables in $\mathbb{R}^2$, and in Sec. V, we discuss the "optimal" choice for such a covariant observable, in view of quantization. In Sec. VI, we consider the question under what conditions a positive operator measure is a spectral one.

II. THE OPERATOR INTEGRAL

The basic tool in our quantization procedure is the operator integral. It associates a linear (not necessarily bounded) operator in the Hilbert space $\mathcal{H}$ of a quantum system to each complex measurable function on the phase space Ω. In this section we review the basic results concerning the theory of operator integrals and give some additional remarks in relation to quantization.

Let Ω be a nonempty set and $\mathcal{A}$ a σ-algebra of subsets of Ω. Let $\mathcal{H}$ be a complex Hilbert space and $L(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$. Let $E: \mathcal{A} \to L(\mathcal{H})$ be a positive operator measure, i.e., a positive operator valued set function that is σ-additive with respect to weak operator topology. For each $\varphi, \psi \in \mathcal{H}$, let $E_{\psi,\varphi}$ denote the complex measure $B \mapsto \langle \psi | E(B) \varphi \rangle$. We recall that a normalized positive operator measure E is called a semispectral measure, and that a semispectral measure E is a spectral measure exactly when $E(A \cap B) = E(A)E(B)$ for all $A, B \in \mathcal{A}$. As mentioned in Sec. I, semispectral measures are also called observables.

Let $\mathcal{F}(\Omega,\mathcal{A})$, or $\mathcal{F}(\Omega)$ in brief, denote the set of all complex $\mathcal{A}$-measurable functions defined on Ω, and $\mathcal{O}(\mathcal{H})$ the set of all (not necessarily bounded) linear operators in $\mathcal{H}$. For $f\in\mathcal{F}(\Omega)$, define

$$D(f,E)=\{\varphi\in\mathcal{H}|f \text{ is } E_{\psi,\varphi}-\text{integrable for each } \psi\in\mathcal{H}\}$$

and

$$\tilde{D}(f,E)=\{\varphi\in\mathcal{H}||f|^2 \text{ is } E_{\varphi,\varphi}-\text{integrable}\}.$$

The following result was proved in Ref. 22. The operator $L(f,E)$ appearing in it is called *the operator integral of f with respect to E*.

Theorem 1:

(a) *The set $D(f,E)$ is a linear (not necessarily dense) subspace of $\mathcal{H}$, and there is a unique linear operator $L(f,E)=\int f dE$ on the domain $D(f,E)$ satisfying*

$$\langle\psi|L(f,E)\varphi\rangle=\int f dE_{\psi,\varphi}$$

for all $\psi\in\mathcal{H}$ and $\varphi\in D(f,E)$.

(b) *The set $\tilde{D}(f,E)$ is a subspace of $D(f,E)$.*

(c) *If f is real valued, $L(f,E)$ is a symmetric operator.*

(d) *While the inclusion $\tilde{D}(f,E)\subset D(f,E)$ may in general be proper, $\tilde{D}(f,E)=D(f,E)$ in the case where E is a spectral measure.*

Remark: Since the operator measure E is also strongly σ-additive, each set function $\mathcal{A}\ni B\mapsto E_\varphi:=E(B)\varphi\in\mathcal{H}$, for $\varphi\in\mathcal{H}$, is an $\mathcal{H}$-valued vector measure. The definition of the operator integral states that $D(f,E)$ is the set of those $\varphi\in\mathcal{H}$ for which f is integrable with respect to the vector measure E_φ in the sense of Ref. 20, p. 21, and $L(f,E)\varphi=\int f dE_\varphi$ for each $\varphi\in D(f,E)$. As pointed out in Ref. 20, p. 37, this definition of integrability is equivalent to that of Ref. 10, p. 323 (for proof, see Ref. 41, Corollary 3.6).

The vector measure approach provides an easy way to characterize the operator integral $L(f,E)$ by approximating f with bounded functions. For each $f\in\mathcal{F}(\Omega)$, and $n\in\mathbb{N}$, let $\tilde{f}_n$ be such that $\tilde{f}_n(x)=f(x)$ if $|f(x)|\leqslant n$, and $\tilde{f}_n(x)=0$ otherwise. It is a well-known fact that in the case where E is a spectral measure, we have

$$D(f,E)=\tilde{D}(f,E)=D^{f,E}:=\{\varphi\in\mathcal{H}|\lim_{n\to\infty}L(\tilde{f}_n,E)\varphi \text{ exists}\}.$$

In addition, $L(f,E)\varphi=\lim_{n\to\infty}L(\tilde{f}_n,E)\varphi$ for all $\varphi\in D^{f,E}$ (see, e.g., Ref. 11, p. 1196). In the case of a general positive operator measure E, this need not be true. For example, take a probability measure defined on the Borel sets of $\mathbb{R}$, such that it has a density that is an even function, and $\int_0^\infty x d\mu(x)=\infty$. Let E be the positive operator measure $B\mapsto\mu(B)I$, and $f(x)=x$. Now f is not μ-integrable, so $D(f,E)=\{0\}$. But if $\varphi\in\mathcal{H}$, we have $\langle\psi|L(\tilde{f}_n,E)\varphi\rangle=\langle\psi|\varphi\rangle\int_{-n}^{n}x d\mu(x)=0$ for all $n\in\mathbb{N}$ and $\psi\in\mathcal{H}$ because the density of μ is even, so that $D^{f,E}=\mathcal{H}$.

Thus in the general case, the existence of the limit $\lim_{n\to\infty}L(\tilde{f}_n,E)\varphi$ does not guarantee that $\varphi\in D(f,E)$. However, the following result holds.

Proposition 1: Let $E:\mathcal{A}\to L(\mathcal{H})$ be a positive operator measure, and $f\in\mathcal{F}(\Omega)$. Then

$$D(f,E)=\{\varphi\in H|\lim_{n\to\infty}L(\chi_B\tilde{f}_n,E)\varphi \text{ exists for each } B\in\mathcal{A}\},$$

and $L(f,E)\varphi=\lim_{n\to\infty}L(\tilde{f}_n,E)\varphi$ for all $\varphi\in D(f,E)$.

Proof: Denote by D the right-hand side of the set equality appearing in the statement. Let $\varphi\in D$, and let $B\in\mathcal{A}$, with $\eta_B=\lim_{n\to\infty}L(\chi_B\tilde{f}_n,E)\varphi$. Since each $\tilde{f}_n$ is bounded, we can choose a

sequence of $\mathcal{A}$-simple functions g_n, such that $|g_n(x)-\tilde{f}_n(x)|\leq 1/n$ for each $n\in\mathbb{N}$ and $x\in\Omega$. Clearly the sequence (g_n) converges to f pointwise. Now

$$\|L(\chi_B g_n-\chi_B\tilde{f}_n,E)\varphi\|=\sup_{\|\psi\|\leq 1}\left|\int_B (g_n-\tilde{f}_n)dE_{\psi,\varphi}\right|\leq\frac{1}{n}\sup_{\|\psi\|\leq 1}|E_{\psi,\varphi}|(\Omega)\leq\frac{4}{n}\|E(\Omega)\|\|\varphi\|,$$

so that

$$\left\|\int_B g_n dE_\varphi-\eta_B\right\|\leq\frac{4}{n}\|E(\Omega)\|\|\varphi\|+\|L(\chi_B f_n,E)\varphi-\eta_B\|.$$

It follows that the sequence $(\int_B g_n dE_\varphi)$ of vectors converges for each $B\in\mathcal{A}$ (to η_B), so by the definition of Ref. 10, p. 323, f is integrable with respect to the vector measure E_φ, i.e. $\varphi\in D(f,E)$ (see the Remark following Theorem 1). Conversely, let $\varphi\in D(f,E)$. Since $D(f,E)=D(|f|,E)$ by definition, and for each $B\in\mathcal{A}$ the sequence $(\chi_B\tilde{f}_n)$ converges to $\chi_B f$ pointwise, with $|\chi_B\tilde{f}_n|\leq|\chi_B f|$, it follows e.g. from the dominated convergence theorem for the vector measure E_φ (see Ref. 10, p. 328) that

$$L(\chi_B f,E)\varphi=\int\chi_B f dE_\varphi=\lim_{n\to\infty}\int\chi_B\tilde{f}_n dE_\varphi=\lim_{n\to\infty}L(\chi_B\tilde{f}_n,E)\varphi$$

for each $B\in\mathcal{A}$. Thus $\varphi\in D$, and $L(f,E)\varphi=\lim_{n\to\infty}L(\tilde{f}_n,E)\varphi$. □

Remark:

(a) We now have the subspace inclusions $\tilde{D}(f,E)\subset D(f,E)\subset D^{f,E}$, with each of them possibly proper. In the case where E is a spectral measure, both inclusions are equalities.

(b) It is well known that in the case where E is a spectral measure, the domain $D(f,E)$ is dense. As seen before in Proposition 1, this need not be the case in general, so a question arises what is required for E and f to make $D(f,E)$ dense.

(c) Another difference to the spectral case is that for real valued $f\in\mathcal{F}(\Omega)$, the symmetric operator $L(f,E)$ is not necessarily self-adjoint (the adjoint need not even exist), and it seems to be difficult, in general, to determine when $L(f,E)$ might have self-adjoint extensions. In the case where f is positive and $D(f,E)$ dense, the positive symmetric operator $L(f,E)$ of course has its self-adjoint Friedrichs extension.

As noted in Sec. I, the starting point of our quantization scheme is a map Γ from real valued measurable functions to the set $\mathcal{O}(\mathcal{H})$. The following theorem characterizes those maps $\Gamma:\mathcal{F}(\Omega)\to\mathcal{O}(\mathcal{H})$, which are implemented by an operator integral. The corresponding result involving bounded functions is well known. Here the functions $\tilde{f}_n$ are defined for each f as in Proposition 1.

Theorem 2: *A map $\Gamma:\mathcal{F}(\Omega)\to\mathcal{O}(\mathcal{H})$ coincides with the map $f\mapsto L(f,E)$ for a (clearly unique) positive operator measure E if and only if the following conditions are satisfied.*

(i) Γ *restricted to bounded functions is a positive linear map with values in* $L(\mathcal{H})$;

(ii) *if (f_n) is an increasing sequence of positive $\mathcal{A}$-measurable functions converging pointwise to a bounded $f\in\mathcal{F}(\Omega)$, then* $\sup_{n\in\mathbb{N}}\langle\varphi|\Gamma(f_n)\varphi\rangle=\langle\varphi|\Gamma(f)\varphi\rangle$ *for each* $\varphi\in\mathcal{H}$;

(iii) *for each $f\in\mathcal{F}(\Omega)$, the domain $D(\Gamma(f))$ of $\Gamma(f)$ consists of those vectors $\varphi\in\mathcal{H}$ for which the sequence $(\Gamma(\chi_B\tilde{f}_n)\varphi)$ of vectors converges for each $B\in\mathcal{A}$.*

(iv) *for each $\varphi\in D(\Gamma(f))$, the sequence $(\Gamma(\tilde{f}_n)\varphi)$ converges to $\Gamma(f)\varphi$.*

Proof: Assume first that there is a positive operator measure E, such that $\Gamma(f)=L(f,E)$ for each f. The above properties follow easily: Property (i) is well known (see, e.g., Ref. 2, pp. 22-28), and (ii) follows from the monotone convergence theorem. Proposition 1 gives (iii) and (iv). Next assume that (i)-(iii) hold for a map $\Gamma:\mathcal{F}(\Omega)\to\mathcal{O}(\mathcal{H})$. By (i) the map $\mathcal{A}\ni B\mapsto E^\Gamma(B):=\Gamma(\chi_B)\in\mathcal{O}(\mathcal{H})$ is a positive operator valued additive set function. Since Γ is positive for bounded functions by (i), $\sup_{n\in\mathbb{N}}$ in condition of (ii) can be replaced by $\lim_{n\to\infty}$. This implies that each set function $B\mapsto\langle\varphi|E^\Gamma(B)\varphi\rangle$ is a positive measure, so that E^Γ is a positive operator measure. If f

$\in \mathcal{F}(\Omega)$ is a bounded positive function, we have $\langle\varphi|\Gamma(f)\varphi\rangle = \langle\varphi|L(f,E^\Gamma)\varphi\rangle$ for all $\varphi \in \mathcal{H}$, as is seen by approximating f with an increasing sequence of simple functions and using linearity, (ii), and the monotone convergence theorem. Hence, if $f \in \mathcal{F}(\Omega)$ is bounded, it follows by linearity and polarization that $\Gamma(f) = L(f,E^\Gamma)$. Now let $f \in \mathcal{F}(\Omega)$ be arbitrary. It follows by (iii) and Proposition 1 that $D(\Gamma(f)) = D(f,E^\Gamma)$, and (since each $\widetilde{f}_n$ is bounded), also

$$L(f,E^\Gamma)\varphi = \lim_{n\to\infty} L(\widetilde{f}_n,E^\Gamma)\varphi = \lim_{n\to\infty} \Gamma(\widetilde{f}_n)\varphi = \Gamma(f)\varphi$$

for all $\varphi \in D(\Gamma(f))$ [where (iv) is used], so $L(f,E^\Gamma) = \Gamma(f)$. □

Remark: In the quantization scheme described in Sec. I the classical variables were thought to be real valued. Obviously, the preceding Theorem holds also with $\mathcal{F}(\Omega)$ replaced by the set of real $\mathcal{A}$-measurable functions.

We end this section by discussing briefly a simple way of obtaining quantization maps without the use of positive operator measures. This approach is essentially the one frequently used in the conventional quantization (e.g., Weyl quantization): the operator corresponding to a given classical variable $f:\mathbb{R}^{2n}\to\mathbb{R}$ is obtained by integrating the variable with respect to some operator valued function defined on the phase space. The quantization of the variable then becomes a continuous distribution valued operator defined on some dense subspace of $L^2(\mathbb{R})$, which does not depend on the variable itself. In the case of Weyl quantization, for example, all the quantized operators are defined on a common domain (see, e.g., Refs. 9 and 36). However, to make the situation similar to that of the operator integral map considered above, we define the quantization map in the following simple way. The proof is a direct adaptation of the proof of Theorem 1 (a) (see Ref. 22). Note that it follows from (i) that the integrand in (ii) is $\mathcal{A}$-measurable. This is so because $\|\varphi\| = \sup\{|\langle\psi|\varphi\rangle| \,|\, \psi\in\mathcal{M}, \|\psi\|=1\}$ for any vector $\varphi\in\mathcal{H}$, where $\mathcal{M}$ is a fixed countable dense set in the separable Hilbert space $\mathcal{H}$. Hence the integral in (ii) is well defined.

Proposition 2: Let $(\Omega,\mathcal{A},\mu)$ *be a measure space*, $\mathcal{H}$ *a separable Hilbert space, and* $\Lambda:\Omega\to L(\mathcal{H})$ *a map with the following properties:*

(i) $\omega\mapsto\langle\psi|\Lambda(\omega)\varphi\rangle$ *is* $\mathcal{A}$*-measurable for all* $\psi,\varphi\in\mathcal{H}$;
(ii) $\int_B \|\Lambda(\omega)\varphi\| d\mu(\omega) < \infty$ *for each* $\varphi\in\mathcal{H}$ *and* $B\in\mathcal{A}$ *with* $\mu(B)<\infty$.

Then for each $\mathcal{A}$*-measurable function* $f:\Omega\to\mathbb{C}$, *there exists a linear operator* $\Gamma_\Lambda(f)$ *in* $\mathcal{H}$, *such that*

$$D(\Gamma_\Lambda(f)) = \{\varphi\in\mathcal{H} | f\langle\psi|\Lambda(\cdot)\varphi\rangle \text{ is } \mu-\text{integrable for each } \psi\in\mathcal{H}\},$$

and

$$\langle\psi|\Gamma_\Lambda(f)\varphi\rangle = \int f(x)\langle\psi|\Lambda(\omega)\varphi\rangle d\mu(\omega)\psi\in\mathcal{H}, \quad \varphi\in D(\Gamma_\Lambda(f)).$$

Proof: It is clear that $D(\Gamma_\Lambda(f))\subset\mathcal{H}$ is a vector subspace. Let (f_n) be a sequence of simple functions converging pointwise to f, with $|f_n|\leqslant|f|$ for all $n\in\mathbb{N}$. Since $|\langle\psi|\Lambda(\omega)\varphi\rangle| \leqslant \|\psi\|\|\Lambda(\omega)\varphi\|$ for each $\psi,\varphi\in\mathcal{H},\omega\in\Omega$, it follows from (ii) and (i) that for each $n\in\mathbb{N}$, we have $D(\Gamma_\Lambda(f_n))=\mathcal{H}$ and the linear functional $\psi\mapsto\int\overline{f_n(\omega)}\langle\psi|\Lambda(\omega)\varphi\rangle d\mu(\omega)$ is continuous for each $\varphi\in\mathcal{H}$. Hence, for each $n\in\mathbb{N}$ and $\varphi\in\mathcal{H}$, there is $\eta_n^\varphi\in\mathcal{H}$, such that

$$\langle\psi|\eta_n^\varphi\rangle = \int f_n(\omega)\langle\psi|\Lambda(\omega)\varphi\rangle d\mu(\omega)$$

for all $\psi\in\mathcal{H}$. Now, let $\varphi\in D(\Gamma_\Lambda(f))$. Since $|f_n|\leqslant|f|$ for all n, the dominated convergence theorem implies that the sequence $\langle\psi|\eta_n^\varphi\rangle$ converges for each $\psi\in\mathcal{H}$ to $\int f(\omega)\langle\psi|\Lambda(\omega)\varphi\rangle d\mu(\omega)$, so by the uniform boundedness theorem and the reflexivity of $\mathcal{H}$, there is $\Gamma_\Lambda(f)\varphi\in\mathcal{H}$, such that

$$\langle\psi|\Gamma_\Lambda(f)\varphi\rangle = \int f(\omega)\langle\psi|\Lambda(\omega)\varphi\rangle d\mu(\omega)$$

for all $\psi \in \mathcal{H}$. Clearly, the map $D(\Gamma_\Lambda(f)) \ni \varphi \mapsto \Gamma_\Lambda(f)\varphi \in \mathcal{H}$ is linear, so the proof is complete. □

Remark: Consider the situation where we have a locally compact unimodular topological group G, with a left Haar measure μ, and a strongly continuous projective unitary representation $U: G \to \mathcal{U}(\mathcal{H})$. Then, for any $A \in L(\mathcal{H})$, the map $\Lambda: G \to L(\mathcal{H})$, defined by $\Lambda(g) = U(g)AU(g)^*$, satisfies the conditions of the preceding Proposition, so we get the corresponding quantization map Γ_Λ. Notice that in the case where the representation is square integrable and A positive, the quantization map Γ_Λ can be represented by an operator integral if and only if A has finite trace. Namely, the case $\mathrm{Tr}[A] = \infty$ gives $D(\Gamma_\Lambda(\chi_G)) = \{0\}$ (see, e.g., Ref. 19, Lemma 2), while the case $\mathrm{Tr}[A] < \infty$ leads to the usual quantization map given by the operator integral with respect to a covariant positive operator measure (multiplied by some constant).

Consider the case where $G = \mathbb{R}^2$, $U(g) = U((q,p))$ are the Weyl operators, and A is the parity operator $L^2(\mathbb{R}) \ni \psi \mapsto \psi(-\cdot) \in L^2(\mathbb{R})$ (multiplied by a suitable constant). Now Γ_Λ is the Weyl quantization map. It is well known that for $f \in L^1(\mathbb{R}^2) \cup L^2(\mathbb{R}^2)$, the operator $\Gamma_\Lambda(f)$ is bounded. Moreover, if $f \in L^2(\mathbb{R}^2)$, then $\Gamma_\Lambda(f)$ is a Hilbert-Schmidt operator, and if f is a Schwartz function, then $\Gamma_\Lambda(f)$ is a trace class operator (see, e.g., Ref. 36). It is a well-known fact that the Weyl quantizations of the classical position and momentum variables are the position and momentum operators Q and P, in the "distributional" sense. Note, however, that the actual domains of Q and P are not given by the formula of the preceding theorem. For example, the characteristic function $\chi_{[-1,1]}$ is in the domain of Q, but the function $(q,p) \mapsto q\langle\chi_{[-1,1]}|\Lambda(q,p)\chi_{[-1,1]}\rangle$ is not (Lebesgue)-integrable, as is easily seen by calculating the explicit form of the function.

III. COVARIANT QUANTIZATION

We now take the set Ω of the preceding section to be a locally compact second countable unimodular topological group, henceforth denoted as G, and let $\mathcal{B}(G)$ denote the Borel σ-algebra of G. Fix λ to be a Haar measure in G. Let $\mathcal{T}(\mathcal{H})$ denote the Banach space of trace class operators on the Hilbert space $\mathcal{H}$, and let $\mathrm{Aut}(\mathcal{T}(\mathcal{H}))$ denote the set of linear, positive, trace norm preserving bijections from $\mathcal{T}(\mathcal{H})$ onto itself. We consider it equipped with the topology given by the functionals $\mathrm{Aut}(\mathcal{T}(\mathcal{H})) \ni \beta \mapsto \mathrm{Tr}[A\beta(T)] \in \mathbb{C}$, where $A \in L(\mathcal{H})$ and $T \in \mathcal{T}(\mathcal{H})$.

Assume further that there is a continuous group homomorphism $\beta: G \to \mathrm{Aut}(\mathcal{T}(\mathcal{H}))$ and a constant $d > 0$, satisfying

$$\int \mathrm{Tr}[P_1\beta(g)(P_2)]d\lambda = d \text{ for all one-dimensional projections } P_1, P_2 \text{ on } \mathcal{H}. \tag{1}$$

We now consider quantizations connected to the structure of G given by the homomorphism β, in the following sense: A map $\Gamma: \mathcal{F}(G) \to \mathcal{O}(\mathcal{H})$ with the property that $\Gamma(f) \in L(\mathcal{H})$ for all bounded functions $f \in \mathcal{F}(G)$ is said to be *β-covariant*, if $\beta(g)^*(\Gamma(f)) = \Gamma(f(g\cdot))$ for all $g \in G$ and all bounded functions $f \in \mathcal{F}(G)$.

If Γ is such that it can be represented by the operator integral with respect to an observable E (i.e., Γ satisfies the conditions of Theorem 2), then it is straightforward to verify that Γ is β-covariant if and only if the observable E is β-covariant in the following sense: An observable $E: \mathcal{B}(G) \to L(\mathcal{H})$ is said to be β-covariant if $\beta(g)^*(E(B)) = E(g^{-1}B)$ for all $g \in G$, $B \in \mathcal{B}(G)$.

Covariant observables are essential in quantum mechanics, and hence they have been studied quite extensively. The canonical examples of covariant observables are constructed, e.g., in Ref. 7, and there are (at least) two completely different ways to obtain their characterization: a direct approach,[16,19,38] which uses the theory of integration with respect to vector measures, and a group theoretical approach.[6] The most general of these characterizations is in Ref. 6. In our context of a unimodular group, the characterization is given by the following theorem.

Theorem 3: *Let T be a positive operator of trace one. Then there is a β-covariant observable*

$E^T:\mathcal{B}(G)\to L(\mathcal{H})$, *such that*

$$E^T(B)=d^{-1}\int_B \beta(g)(T)d\lambda(g) \tag{2}$$

in the ultraweak sense for each $B\in\mathcal{B}(G)$. *Conversely, assume that* $E:\mathcal{B}(G)\to L(\mathcal{H})$ *is a* β*-covariant observable. Then there is a unique positive operator* T *of trace one, such that* $E=E^T$.

If E is a β-covariant observable, we call the corresponding trace-one positive operator T the *generating operator* for E. Thus, for a β-covariant observable E, we have

$$D(f,E)=\{\varphi\in\mathcal{H}|g\mapsto f(g)\langle\psi|\beta(g)(T)\varphi\rangle \text{ is } \lambda\text{ - integrable for each } \psi\in\mathcal{H}\}$$

and

$$\langle\psi|L(f,E)\varphi\rangle=d^{-1}\int f(g)\langle\psi|\beta(g)(T)\varphi\rangle d\lambda(g)$$

for all $\varphi\in D(f,E)$ and $\psi\in\mathcal{H}$, where T is the generating operator for E.

According to the Wigner theorem, each $\beta(g)$ has the form $\beta(g)(T)=U(g)TU(g)^*$ for some unitary or antiunitary operator $U(g)$, which is unique up to a phase factor, so that $\beta(g)$ corresponds to the associated equivalence class of unitary operators (see, e.g., Ref. 5, p. 19 or Ref. 16, p. 22). It follows that, in the case where G is connected, the map $g\mapsto U(g)$ is a weakly (Borel) measurable projective unitary representation of G, where each $U(g)$ is chosen from the equivalence class corresponding to $\beta(g)$ by means of some (measurable) section (see Ref. 16, p. 23 and Ref. 5, pp. 30 and 100). Relation (1) gives the so-called square integrability condition

$$\int|\langle\psi|U(g)\varphi\rangle|^2d\lambda(g)=d$$

for all unit vectors $\psi,\varphi\in\mathcal{H}$. Clearly, for each $\varphi,\psi\in\mathcal{H}$ there is a $g\in G$ such that $\langle\psi|U(g)\varphi\rangle\neq 0$. This implies that the closed linear span of $\{U(g)\varphi|g\in G\}$ is dense in $\mathcal{H}$ for each $\varphi\in\mathcal{H}$, which means that the projective representation $g\mapsto U(g)$ is irreducible. The β-covariance condition for an observable E takes the form $U(g)^*E(B)U(g)=E(g^{-1}B)$ for all $g\in G$, $B\in\mathcal{B}(G)$.

Hence, we know that each covariant quantization map $\Gamma:\mathcal{F}(G)\to\mathcal{O}(\mathcal{H})$, which can be represented by an operator integral, is of the form $\Gamma=\Gamma^T:=L(\cdot,E^T)$ for some generating operator T. It is worth noting that in certain cases the observables produced by the quantization scheme associated with a map Γ^T are never spectral measures. Namely, the irreducibility of U implies the following, perhaps well-known result.

Proposition 3: Assume that G *is connected, and that the projective representation* U *associated with* β *is strongly continuous. Let* $T\in\mathcal{T}(\mathcal{H})$ *be positive and of trace one. Then the only projections in the range of* E^T *are* O *and* I.

Proof: First we notice that if $E^T(X)$ is a projection for some $X\in\mathcal{B}(G)$ and positive operator T of trace one, then there is a nonzero $\varphi\in\mathcal{H}$, such that $E^{|\varphi\rangle\langle\varphi|}(X)$ is a projection. Indeed, let T be a positive operator of trace one, $\lambda>0$ an eigenvalue of T (so that $\lambda\leqslant 1$), and $\varphi\in\mathcal{H}$ an associated eigenvector. Then we can decompose T as $T=\lambda|\varphi\rangle\langle\varphi|+(1-\lambda)T'$, where $|\varphi\rangle\langle\varphi|$ and T' are positive and of trace one, so we can write $E^T(X)=\lambda E^{|\varphi\rangle\langle\varphi|}(X)+(1-\lambda)E^{T'}(X)$. Since any projection is an extreme point of the convex set $\{A\in L(\mathcal{H})|0\leqslant A\leqslant I\}$ (see, e.g., Ref. 7, p. 19), it follows that if $E^T(X)$ is a projection, then $E^T(X)=E^{|\varphi\rangle\langle\varphi|}(X)$.

Hence, it suffices to show that for each unit vector $\eta\in\mathcal{H}$, the only projections in the range of $E^{|\eta\rangle\langle\eta|}$ are O and I. Denote $T=|\eta\rangle\langle\eta|$, and assume that there is a projection P in the range of E^T. Then $PE^T(B)=E^T(B)P$ for all $B\in\mathcal{B}(G)$.[27] Let $\varphi\in\mathcal{H}$. Now

$$\int_B \langle\varphi|P\beta(g)(T)\varphi\rangle d\lambda(g) = \int_B \langle\varphi|\beta(g)(T)P\varphi\rangle d\lambda(g)$$

for all $B \in \mathcal{B}(G)$. Since $g \mapsto \langle\varphi|(P\beta(g)(T) - \beta(g)(T)P)\varphi\rangle$ is continuous, it is thus zero for all $g \in G$. Hence, $P\beta(g)(T) = \beta(g)(T)P$ for all $g \in G$.

Let U_η denote the map $g \mapsto U(g)\eta$. We then have

$$P|U_\eta(g)\rangle\langle U_\eta(g)| = |U_\eta(g)\rangle\langle U_\eta(g)|P$$

for all $g \in G$.

It follows that for each $g \in G$, either $U_\eta(g) \in P(\mathcal{H})$ or $U_\eta(g) \in P(\mathcal{H})^\perp$. Let $f: G \to \{0,1\}$ be the function such that $f(g) = 0$ if $U_\eta(g) \in P(\mathcal{H})$ and $f(g) = 1$ if $U_\eta(g) \in P(\mathcal{H})^\perp$. Then f is continuous, when the set $\{0,1\}$ is equipped with the discrete topology. Indeed, let $g_0 \in G$. Since U_η is continuous, $W = U_\eta^{-1}(\{\varphi \in \mathcal{H} \,|\, \|U_\eta(g_0) - \varphi\| < \sqrt{2}\})$ is an open set in G containing g_0. Assume first that $f(g_0) = 0$. Since all vectors $U_\eta(g)$ are of unit length, it follows that $\|U_\eta(g) - U_\eta(g_0)\| = \sqrt{2}$ whenever $f(g) = 1$. Hence, $f(W) \subset \{0\}$. Similarly, if we assume that $f(g_0) = 1$, it follows that $f(W) \subset \{1\}$. This implies that f is continuous. Since G is connected, f cannot be a surjection, so either $U_\eta(g) \in P(\mathcal{H})$ for all $g \in G$, or $U_\eta(g) \in P(\mathcal{H})^\perp$ for all $g \in G$. But, due to the irreducibility of the projective representation U, the closed linear span of the set $\{U_\eta(g) \,|\, g \in G\}$ is dense in $\mathcal{H}$. This is clearly possible only if either $P = I$ or $P = O$. The proof is complete. □

The following observation is another consequence of the irreducibility of the projective representation associated with β. It uses a calculation similar to that appearing e.g. in Ref. 40, p. 40 in a different context. Part (a) is mentioned also in Ref. 39.

Proposition 4: Assume that G is connected and let U be the projective representation associated with β. Let $E: \mathcal{B}(G) \to L(\mathcal{H})$ be a β -covariant observable.

(a) *Assume that $f \in \mathcal{F}(G)$ is such that $\widetilde{D}(f,E) \subset \widetilde{D}(f(g\cdot),E)$* for all $g \in G$. *Then $U(g)\widetilde{D}(f,E) = \widetilde{D}(f,E)$ for all $g \in G$, and either $\widetilde{D}(f,E) = \{0\}$ or $\widetilde{D}(f,E)$ is dense.*

(b) *Assume that $f \in \mathcal{F}(G)$ is such that $D(f,E) \subset D(f(g\cdot),E)$ for all $g \in G$. Then $U(g)D(f,E) = D(f,E)$ for all $g \in G$, and either $D(f,E) = \{0\}$ or $D(f,E)$ is dense. Moreover,*

$$U(g)^* L(f,E) U(g) \subset L(f(g\,\cdot),E) \tag{3}$$

for all $g \in G$.

Proof: Let T be the positive trace one operator associated with E, so that

$$\widetilde{D}(f,E) = \{\varphi \in \mathcal{H} | g \mapsto |f(g)|^2 \langle\varphi|U(g)TU(g)^*\varphi\rangle \text{ is } \lambda\text{-integrable}\},$$

$$D(f,E) = \{\varphi \in \mathcal{H} | g \mapsto |f(g)||\langle\psi|U(g)TU(g)^*\varphi\rangle| \text{ is } \lambda\text{-integrable for all } \psi \in \mathcal{H}\}.$$

For all $h, g \in G$, we have $U(h)^*U(g) = c(g,h)U(h^{-1}g)$, where $(h,g) \mapsto c(h,g)$ is some torus valued function, so that $U(g)^*U(h) = [U(h)^*U(g)]^* = c(g,h)^{-1}U(h^{-1}g)^*$, and hence

$$U(h)^*U(g)TU(g)^*U(h) = U(h^{-1}g)TU(h^{-1}g)^*. \tag{4}$$

(a) Let $\varphi \in \widetilde{D}(f,E)$, and $h \in G$. By the left invariance of the Haar measure and (4), we have

$$\begin{aligned}\int |f(g)|^2 \langle U(h)\varphi|U(g)TU(g)^*U(h)\varphi\rangle d\lambda(g) &= \int |f(g)|^2 \langle\varphi|U(h^{-1}g)TU(h^{-1}g)^*\varphi\rangle d\lambda(g) \\ &= \int |f(hg)|^2 \langle\varphi|U(g)TU(g)^*\varphi\rangle d\lambda(g),\end{aligned}$$

with all the integrands positive. Since $\varphi \in \widetilde{D}(f(h\cdot),E)$ by assumption, the last integral is finite, so $U(h)\varphi \in \widetilde{D}(f,E)$. Thus $\widetilde{D}(f,E)$ is an invariant subspace of the projective represen-

tation U, implying that the closure $\overline{\tilde{D}(f,E)}$ is a closed invariant subspace of U. It follows from the irreducibility of U that $\tilde{D}(f,E)$ is either trivial or dense. The fact that $U(h)\tilde{D}(f,E)=\tilde{D}(f,E)$ follows because we have $U(h^{-1})=c'(h)U(h)^*$ for some torus valued function c'. The proof of (a) is complete.

(b) Let $h\in G$, $\varphi\in D(f,E)$, and $\psi\in\mathcal{H}$. Then by using (4) and the assumption, we get

$$\begin{aligned}\int |f(g)||\langle\psi|U(g)TU(g)^*U(h)\varphi\rangle|d\lambda(g) &= \int |f(g)||\langle U(h)U(h)^*\psi|U(g)TU(g)^*U(h)\varphi\rangle|d\lambda(g)\\ &= \int |f(g)||\langle U(h)^*\psi|U(h^{-1}g)TU(h^{-1}g)^*\varphi\rangle|d\lambda(g)\\ &= \int |f(hg)||\langle U(h)^*\psi|U(g)TU(g)^*\varphi\rangle|d\lambda(g)<\infty,\end{aligned}$$

so that $U(h)\varphi\in D(f,E)$. Thus $D(f,E)$ is an invariant subspace for U, and hence $D(f,E)$ is either trivial or dense. The fact that $U(h)D(f,E)=D(f,E)$ follows for the same reason as the corresponding one in (a).

Let $h\in G$. By repeating the preceding calculation without the absolute value signs, we get

$$\langle\psi|L(f,E)U(h)\varphi\rangle=\langle U(h)^*\psi|L(f(h\cdot),E)\varphi\rangle=\langle\psi|U(h)L(f(h\cdot),E)\varphi\rangle$$

for each $\psi\in\mathcal{H}$ and $\varphi\in U(h)^*D(f,E)=D(f,E)\subset D(f(h\cdot),E)$, so that (3) holds. □

Remark:

(a) If we assume $D(f,E)=D(f(g\cdot),E)$ for all $g\in G$, then Proposition 4 (b) gives the strict operator equality $U(g)^*L(f,E)U(g)=L(f(g\cdot),E)$ for each $g\in G$, with dense domain $D(f,E)$. This resembles the covariance condition for the observable E.

(b) Since each $E_{\psi,\varphi}$ is a finite measure, it is clear that the conditions of Proposition 4 (a) and (b) are satisfied, e.g., by all functions $f\in\mathcal{F}(G)$ with the property that for each $h\in G$ there are nonnegative constants K_h and M_h, such that $|f(hg)|\leqslant K_h|f(g)|+M_h$ for almost all $g\in G$. In the case where $G=\mathbb{R}^{2n}$ (see the beginning of the next section), all polynomials of the form $\mathbb{R}^{2n}\ni(x_1,\ldots,x_{2n})\mapsto p(x_i)\in\mathbb{R}$, where $p:\mathbb{R}\to\mathbb{R}$ is a polynomial and $i=1,\ldots,2n$, are like this.

IV. PHASE SPACE QUANTIZATION ON $\mathbb{R}^2$

Consider the special case where $G=\mathbb{R}^2$, with λ the Lebesgue measure. Fix $\{|n\rangle|n\geq 0\}$ to be an orthonormal basis of $\mathcal{H}$, and let $U:L^2(\mathbb{R})\to\mathcal{H}$ be the unitary operator that maps the nth Hermite function h_n to $|n\rangle$. Define $W(q,p)=UW_0(q,p)U^{-1}$, where $(W_0(q,p)f)(t)=e^{i1/2qp}e^{ipt}f(t+q)$, and $\beta:\mathbb{R}^2\to\mathrm{Aut}(\mathcal{T}(\mathcal{H}))$ by $\beta(q,p)(T)=W(-q,p)TW(-q,p)^*$. Now β is a continuous group homomorphism, satisfying (1), with $d=2\pi$, and λ the Lebesgue measure of $\mathbb{R}^2$. Let $A_\pm$ be the ladder operators associated with the basis $\{|n\rangle\}$, and define Q and P to be the closures of the operators $1/\sqrt{2}(A_++A_-)$ and $1/\sqrt{2}i(A_+-A_-)$, respectively. Then $A_+=A_-^*$, and Q and P are unitarily equivalent to the position and momentum operators in $L^2(\mathbb{R})$ via U. Let N denote the self-adjoint operator A_+A_-.

According to the general result described above, each positive operator T of trace one generates the map $f\mapsto L(f,E^T)$, where

$$E^T(B)=d^{-1}\int_B\beta(q,p)(T)d\lambda(q,p).$$

The generating operators T of the form $T=\Sigma_n w_n|n\rangle\langle n|$, where $\Sigma_n w_n=1$, and $w_n\geqslant 0$ for each n, have a special significance, as they are the ones for which E^T is covariant with respect to the phase shifts also, i.e.,

$$e^{i\theta N}E^T([0,\infty)\times B)e^{-i\theta N}=E^T([0,\infty)\times(B+\theta))$$

for all $\theta\in[0,2\pi)$ and $B\in B([0,2\pi))$, where $\mathbb{R}^2=[0,\infty)\times[0,2\pi)$ and the sum $B+\theta$ is understood modulo 2π. (cf. Ref. 23).

Since $(q,p)\mapsto W(q,p)$ is a strongly continuous projective representation, and $\mathbb{R}^2$ is connected, Proposition 3 tells us that the range of E^T does not contain nontrivial projections. In particular, the corresponding quantization scheme cannot then produce spectral measures.

In this section, we inspect the possibility of applying the quantization scheme described earlier to the classical position and momentum variables, using the quantization map $\Gamma^T=L(\cdot,E^T)$ with various generating operators T. For each $k\in\mathbb{N}$, let x^k and y^k denote the functions $(q,p)\mapsto q^k$ and $(q,p)\mapsto p^k$.

The essential question is whether the operator measures $B\mapsto E^T(B\times\mathbb{R})$ and $B\mapsto E^T(\mathbb{R}\times B)$ are uniquely determined by their respective moment operator sets $\{\Gamma^T(x^k)\,|\,k\in\mathbb{N}\}$ and $\{\Gamma^T(y^k)\,|\,k\in\mathbb{N}\}$. It is known that this is indeed the case when T is a number state $|n\rangle\langle n|$, $n\geq 0$ (see Ref. 13). In that case, the operator sets $\{\Gamma^T(x^k)\,|\,k\in\mathbb{N}\}$ and $\{\Gamma^T(y^k)\,|\,k\in\mathbb{N}\}$ are eligible to represent the quantizations of x and y, respectively. As is well known, the associated quantum mechanical observables are unsharp position and momentum observables.

Our goal here is to explicitly determine the operators $\Gamma^T(x^k)$ and $\Gamma^T(y^k)$ for certain generating operators T.

To begin with, we consider the square integrability domains. According to Proposition 4 and the associated Remark, these sets are either dense or trivial. The following two Propositions specify them completely.

Proposition 5: Let $k\in\mathbb{N}$, let $\eta\in\mathcal{H}$ be a unit vector, and denote $u=U^{-1}\eta\in L^2(\mathbb{R})$.

(a) *$\widetilde{D}(x^k,E^{|\eta\rangle\langle\eta|})\neq\{0\}$ if and only if $\eta\in D(Q^k)$, and in this case, $\widetilde{D}(x^k,E^{|\eta\rangle\langle\eta|})=D(Q^k)$.*

(b) *The statement of (a) holds true, if "x" and "Q" are replaced by "y" and "P."*

Proof: Let $0\neq\varphi\in\mathcal{H}$ and $f=U^{-1}\varphi\in L^2(\mathbb{R})$. We get

$$\begin{aligned}\int_{\mathbb{R}^2}q^{2k}dE^{|\eta\rangle\langle\eta|}_{\varphi,\varphi}(q,p)&=\frac{1}{2\pi}\int q^{2k}\left(\int|\langle\varphi|W(-q,p)|\eta\rangle|^2dp\right)dq=\int q^{2k}\left(\int|F(\bar{u}(\cdot-q)f)(p)|^2dp\right)dq\\&=\int q^{2k}\left(\int|u(t-q)|^2|f(t)|^2dt\right)dq=\int\left(\int q^{2k}|u(t-q)|^2|f(t)|^2dq\right)dt\\&=\int\int(t-q)^{2k}|u(q)|^2|f(t)|^2dqdt,\end{aligned}$$

where Lemma 2 of Ref. 18, the unitarity of the Fourier-Plancherel operator, and Fubini's theorem have been used. (Since all the functions and measures involved are positive, the calculation is valid regardless of whether the integrals are finite or not.)

Now the last integral is finite if and only if φ and η are both in $D(Q^k)$. This is seen as follows.

Assume first that the last integral is finite. Then it follows from Fubini's theorem that $t\mapsto(t-q)^{2k}|f(t)|^2|u(q)|^2$ is integrable for almost all q, and $q\mapsto(t-q)^{2k}|u(q)|^2|f(t)|^2$ is integrable for almost all t. Thus $t\mapsto t^{2k}|f(t)|^2$ and $q\mapsto q^{2k}|u(q)|^2$ are integrable. (The fact that $t\mapsto t^{2k}|f(t)|^2$ is integrable is seen as follows: Take $q\in\mathbb{R}$, such that $|u(q)|^2>0$ and $t\mapsto(t-q)^{2k}|f(t)|^2|u(q)|^2$ is integrable. This is possible, since $\|\eta\|>0$, which implies that $|u(q)|^2>0$ in some non-null set. Then use the fact that there exist positive constants A,B,M, such that $At^{2k}\leq(t-q)^{2k}\leq Bt^{2k}$ for $|t|\geq M$. The fact that $q\mapsto q^{2k}|u(q)|^2$ is integrable follows similarly, since we assumed that also $\|\varphi\|>0$.) Thus f and u are in the domain of the kth power of the position operator in $L^2(\mathbb{R})$, so $\varphi,\eta\in D(Q^k)$.

Conversely, assume that $\varphi,\eta\in D(Q^k)$, so that $t\mapsto t^{2k}|f(t)|^2$ and $q\mapsto q^{2k}|u(q)|^2$ are integrable. Hence also $t\mapsto|t^l\|f(t)|^2$ and $q\mapsto|q^l\|u(q)|^2$ are integrable for all $l\leq 2k$, implying that $(t,q)\mapsto(t-q)^{2k}|u(q)|^2|f(t)|^2$ is integrable over $\mathbb{R}^2$. Thus the last integral of the above calculation is finite.

We conclude that $\widetilde{D}(x^k,E^{|\eta\rangle\langle\eta|})\neq\{0\}$ if and only if $\eta\in D(Q^k)$, and in this case, $\widetilde{D}(x^k,E^{|\eta\rangle\langle\eta|})=D(Q^k)$.

The result concerning $\widetilde{D}(y^k, E^{|\eta\rangle\langle\eta|})$ is obtained in an analogous manner by using the calculation

$$\begin{aligned}\int_{\mathbb{R}^2} p^{2k} dE^{|\eta\rangle\langle\eta|}_{\varphi,\varphi}(q,p) &= \frac{1}{2\pi}\int p^{2k}\left(\int |\langle\varphi|W(-q,p)|\eta\rangle|^2 dq\right)dp \\ &= \int p^{2k}\left(\int |F^{-1}(\overline{Fu}(\cdot - p)Ff)(q)|^2 dq\right)dp \\ &= \int p^{2k}\left(\int |Fu(t-p)|^2 |Ff(t)|^2 dx\right)dp \\ &= \int \left(\int p^{2k}|Fu(t-p)|^2 |Ff(t)|^2 dp\right)dt \\ &= \int\int (t-p)^{2k}|Fu(p)|^2|Ff(t)|^2 dp dt,\end{aligned}$$

as well as the fact that $P = UF^{-1}U^{-1}QUFU^{-1}$.

Now we consider the case of an arbitrary positive operator T of trace one. The following elementary fact is needed. The proof is included for the reader's convenience.

Lemma 1: Let T be a positive operator of trace one. Let (η_n) *be an orthonormal sequence and* (w_n) a sequence of nonnegative numbers, such that $T = \Sigma_n w_n |\eta_n\rangle\langle\eta_n|$. *Let A be a closed operator. Then*

$$\sum_{n=1}^{\infty} w_n \|A\eta_n\|^2 < \infty,$$

if and only if $A\sqrt{T}$ *is a Hilbert-Schmidt operator. [Here we have denoted* $\|A\eta_n\| = \infty$ *whenever* $\eta_n \notin D(A)$, *and used the convention* $0\cdot\infty = 0$.*] In particular, the convergence of the series is not dependent on the representation of T in terms of* (η_n) *and* (w_n).

Proof: Let $S = \Sigma_{n=1}^{\infty} w_n \|A\eta_n\|^2 (\leqslant \infty)$. Assume first that $S < \infty$, so that, in particular, $\eta_n \in D(A)$ for all those $n \in \mathbb{N}$ for which $w_n > 0$. Let $\varphi \in \mathcal{H}$. Since the series $\sqrt{T} = \Sigma_n \sqrt{w_n} |\eta_n\rangle\langle\eta_n|$ converges in the operator norm, the vector series $\Sigma_n \sqrt{w_n}\langle\eta_n|\varphi\rangle\eta_n$ converges to $\sqrt{T}\varphi$ in the norm of $\mathcal{H}$. Since (η_n) is orthonormal, the Cauchy-Schwartz inequality gives

$$\sum_n \sqrt{w_n}|\langle\eta_n|\varphi\rangle| \|A\eta_n\| \leqslant \sqrt{S}\|\varphi\| < \infty,$$

so also the series $\Sigma_n \sqrt{w_n}\langle\eta_n|\varphi\rangle A\eta_n$ converges in norm. Since A is closed, it follows that $\sqrt{T}\varphi \in D(A)$ and $A\sqrt{T}\varphi$ equals the sum of the latter series. In particular, $D(A\sqrt{T}) = \mathcal{H}$. Now the previous inequality shows that $\|A\sqrt{T}\varphi\| \leqslant \sqrt{S}\|\varphi\|$, so $A\sqrt{T}$ is bounded. Clearly $\Sigma_{\xi\in K}\|A\sqrt{T}\xi\|^2 = S < \infty$ if K is an orthonormal basis of H, which includes all the η_n, so $A\sqrt{T}$ is Hilbert-Schmidt.

Assume then that $A\sqrt{T}$ is a Hilbert-Schmidt operator. Now $\eta_n = w_n^{-1/2}\sqrt{T}\eta_n \in D(A)$ if $w_n > 0$, and $S = \Sigma_{\xi\in K}\|A\sqrt{T}\xi\|^2 < \infty$, where $\mathcal{K}$ is an orthonormal basis including all the η_n. □

Proposition 6:

(a) *Let* $k \in \mathbb{N}$. *Then* $\widetilde{D}(x^k, E^T) \neq \{0\}$ *if and only if* $Q^k\sqrt{T}$ *is a Hilbert-Schmidt operator, and in that case,* $\widetilde{D}(x^k, E^T) = D(Q^k)$.

(b) *The statement in* (*a*) *holds true, if* "*x*" *and* "*Q*" *are replaced by* "*y*" *and* "*P*."

Proof: Write T in the form $T = \Sigma_{n=1}^{\infty} w_n |\eta_n\rangle\langle\eta_n|$, where $\Sigma_n w_n = 1$, $t_n \geqslant 0$, and (η_n) is an orthonormal sequence in $\mathcal{H}$. The series converges in the trace norm, as well as in the operator norm.

For each $\varphi \in \mathcal{H}$, let $A^{\eta}_{\varphi,\varphi}$ be the density function of the positive measure $E^{|\eta\rangle\langle\eta|}_{\varphi,\varphi}$. Since the density function of the measure $E^T_{\varphi,\varphi}$ is $\Sigma_n w_n A^{\eta_n}_{\varphi,\varphi}$, we have $\varphi \in \widetilde{D}(x^k, E^T)$ if and only if the function

$x^{2k}\Sigma_n w_n A^{\eta_n}_{\varphi,\varphi}$ is integrable over $\mathbb{R}^2$. In view of the Proposition 5, it is therefore clear that $\tilde{D}(x^k,E^T)\neq\{0\}$ only if $\eta_n\in D(Q^k)$ for all those $n\in\mathbb{N}$ for which $w_n>0$, and that in any case, $\tilde{D}(x^k,E^T)\subset D(Q^k)$.

Assume now that $\eta_n\in D(Q^k)$ for all $n\in\mathbb{N}$ with $w_n>0$, and $0\neq\varphi\in D(Q^k)$. Let $u_n=U^{-1}\eta_n$ for each n. The monotone convergence theorem and the proof of Proposition 5 imply that

$$\int x^{2k}dE^T_{\varphi,\varphi}=\sum_n w_n\int x^{2k}dE^{|\eta_n\rangle\langle\eta_n|}_{\varphi,\varphi}=\int\int\sum_n (t-q)^{2k}w_n|u_n(q)|^2|(U^{-1}\varphi)(t)|^2dtdq$$

(regardless of whether the series converges or not). Now if the above integral is finite [i.e., $\varphi\in\tilde{D}(x^k,E^T)$], then Fubini's theorem gives that $q\mapsto(t-q)^{2k}|(U^{-1}\varphi)(t)|^2\Sigma_n w_n|u_n(q)|^2$ is integrable for almost all t, so by the argument similar to that used in the proof of the preceding Proposition, it follows that $\Sigma_n w_n\|Q^k\eta_n\|^2=\int\Sigma_n w_n q^{2k}|u_n(q)|^2dq<\infty$. On the other hand, if $\Sigma_n w_n\|Q^k\eta_n\|^2<\infty$, then each function $q\mapsto\Sigma_n w_n q^l|u_n(q)|^2$, with $l\leqslant 2k$ is integrable, so that $(q,t)\mapsto\Sigma_n(t-q)^{2k}w_n|u_n(q)|^2|(U^{-1}\varphi)(t)|^2$ is integrable over $\mathbb{R}^2$. [Note that since we assumed that $\varphi\in D(Q^k)$, the function $t\mapsto t^l|(U^{-1}\varphi)(t)|^2$ is integrable for each $l\leqslant 2k$.] Thus $\int x^{2k}dE^T_{\varphi,\varphi}<\infty$, so $\varphi\in\tilde{D}(x^k,E^T)$.

We have proved that $\tilde{D}(x^k,E^T)\neq\{0\}$ if and only if $\eta_n\in D(Q^k)$ for all $n\in\mathbb{N}$ with $w_n>0$, and

$$\sum_{n=1}^{\infty} w_n\|Q^k\eta_n\|^2<\infty$$

[where it is understood that $\|Q^k\eta_n\|=\infty$ if $\eta_n\notin D(Q^k)$ and we use the convention $0\cdot\infty=\infty$]. Since Q^k is closed, (a) follows from the preceding Lemma. The statement of (b) is proved similarly, since

$$\int x^{2k}dE^T_{\varphi,\varphi}=\int\int\sum_n w_n(t-p)^{2k}|Fu_n(p)|^2|FU^{-1}\varphi(t)|^2dpdt,$$

$P=UF^{-1}U^{-1}QUFU^{-1}$, and P^k is also closed. The proof is complete. □

Now we proceed to determine the operators $L(x^k,E^T)$ and $L(y^k,E^T)$ for $T=\Sigma_n w_n|\eta_n\rangle\langle\eta_n|$ satisfying the condition of the preceding Proposition.

Theorem 4:

(a) *Assume that T satisfies the condition of the previous Proposition* (*a*). *Then* $L(x^k,E^T)=\Sigma_{l=0}^k s^Q_{kl}Q^l$, *where* $s^Q_{kl}=\binom{k}{l}(-1)^{k-l}\operatorname{Tr}[Q^{k-l}T]$, *with each* $Q^{k-l}T$ *a trace class operator*.

(b) *The statement in* (*a*) *holds true, if* "(*a*)," "*x*," *and* "*Q*" *are replaced by* "(*b*)," "*y*," *and* "*P*."

Proof: Assume first that $T=|\eta\rangle\langle\eta|$ for $\eta\in D(Q^k)$. Denote $u=U^{-1}\eta\in L^2(\mathbb{R})$. Define a polynomial $p^\eta:\mathbb{R}\to\mathbb{R}$ by

$$p^\eta(t)=\langle\eta|(t-Q)^k\eta\rangle=\sum_{l=0}^{k}\binom{k}{l}(-1)^{k-l}\langle\eta|Q^{k-l}\eta\rangle t^l.$$

Since p^η is a polynomial of order k, the operator $p^\eta(Q)$ is self-adjoint, and has the domain $D(Q^k)$. Thus by Proposition 5 we have $D(p^\eta(Q))=D(Q^k)=\tilde{D}(x^k,E^{|\eta\rangle\langle\eta|})$.

Let $\varphi\in\tilde{D}(x^k,E^{|\eta\rangle\langle\eta|})\subset D(x^k,E^{|\eta\rangle\langle\eta|})$, and $\psi\in\mathcal{H}$. Let $f=U^{-1}\varphi$, $g=U^{-1}\psi$. Since the function

$$(q,p)\mapsto q^k\langle\psi|W(-q,p)|\eta\rangle\overline{\langle\varphi|W(-q,p)|\eta\rangle}$$

is integrable over $\mathbb{R}^2$ [by the definition of $D(x^k,E^{|\eta\rangle\langle\eta|})$], we get

$$\langle\psi|L(x^k,E^{|\eta\rangle\langle\eta|})\varphi\rangle = \int_{\mathbb{R}^2} q^k dE^{|\eta\rangle\langle\eta|}_{\psi,\varphi}(q,p) = \frac{1}{2\pi}\int q^k\left(\int \langle\psi|W(-q,p)|\eta\rangle\overline{\langle\varphi|W(-q,p)|\eta\rangle}dp\right)dq$$

$$= \int q^k\left(\int \overline{F(\bar{u}(\cdot-q)g)(p)}F(\bar{u}(\cdot-q)f)(p)dp\right)dq$$

$$= \int q^k\left(\int \overline{u(t-q)g(t)}u(t-q)f(t)dt\right)dq = \int\left(\int q^k|u(t-q)|^2dq\right)\overline{g(t)}f(t)dt$$

$$= \int\left(\int (t-q)^k|u(q)|^2dq\right)\overline{g(t)}f(t)dt,$$

$$= \int \langle\eta|(t-Q)^k|\eta\rangle\overline{g(t)}f(t)dt = \langle\psi|p^\eta(Q)\varphi\rangle.$$

The fifth equality follows from Fubini's theorem, since $(q,t)\mapsto q^k|u(t-q)|^2\overline{g(t)}f(t)$ is integrable [because of the Cauchy-Schwarz inequality and the square integrability of the maps $(q,t)\mapsto|u(t-q)g(t)|$ and $(q,t)\mapsto|q^ku(t-q)f(t)|$, the latter being a consequence of the proof of Proposition 5.] It follows that $p^\eta(Q)\subset L(x^k,E^{|\eta\rangle\langle\eta|})$.

The equality $p^\eta(Q)=L(x^k,E^{|\eta\rangle\langle\eta|})$ follows from the fact that being self-adjoint, the operator $p^\eta(Q)$ cannot have a proper symmetric extension.

Now we take $T=\Sigma_n w_n|\eta_n\rangle\langle\eta_n|$ under the condition of the preceding Proposition, so that $\tilde{D}(x^k,E^T)=D(Q^k)=\tilde{D}(x^k,E^{|\eta\rangle\langle\eta|})$ for each n. Let $\varphi\in D(Q^k)$ and $\psi\in\mathcal{H}$, and f,g be as before.

According to Proposition 1 of Ref. 18, we have

$$\langle\psi|L(x^k,E^T)\varphi\rangle = \sum_{n=1}^{\infty} w_n\langle\psi|L(x^k,E^{|\eta_n\rangle\langle\eta_n|})\varphi\rangle$$

$$= \sum_{n=1}^{\infty} w_n\langle\psi|p^{\eta_n}(Q)\varphi\rangle = \sum_{n=1}^{\infty} w_n\sum_{l=0}^{k}\binom{k}{l}(-1)^{k-l}\langle\eta_n|Q^{k-l}\eta_n\rangle\langle\psi|Q^l\varphi\rangle.$$

Since

$$\|Q^{k-l}\eta_n\|^2 = \int q^{2(k-l)}|(U^{-1}\eta_n)(q)|^2dq \leqslant 1+\int q^{2k}|(U^{-1}\eta_n)(q)|^2dq = 1+\|Q^k\eta_n\|,$$

it follows from the preceding Lemma that also each $Q^{k-l}\sqrt{T}$ is defined in all of $\mathcal{H}$ and is a Hilbert-Schmidt operator. Thus each $Q^{k-l}T=Q^{k-l}\sqrt{T}\sqrt{T}$ is defined in all of $\mathcal{H}$ and is a bounded operator of trace class. Thus the series $\Sigma_n w_n\langle\eta_n|Q^{k-l}\eta_n\rangle$ converges (clearly to $\mathrm{Tr}\,[Q^{k-l}T]$) for each l, so

$$\langle\psi|L(x^k,E^T)\varphi\rangle = \sum_{l=0}^{k} s^Q_{kl}\langle\psi|Q^l\varphi\rangle.$$

Since φ was arbitrarily chosen from the set $\tilde{D}(x^k,E^T)=D(Q^k)$ and the operator $\Sigma_{l=0}^k s^Q_{kl}Q^l$ is self-adjoint, we conclude that $L(x^k,E^T)=\Sigma_{l=0}^k s^Q_{kl}Q^l$, and the proof of (a) is complete.

Statement (b) is proved similarly by using the unitary equivalence of Q and P. □

Remark: As mentioned at the beginning of the section, the uniqueness of the operator measure that gives the moment operators of Theorem 4, is verified only in the case where $T=|n\rangle\langle n|$ for some n. The uniqueness question in the general case remains open.

We close this section with a remark on another application of our quantization scheme. Consider the function $h(q,p)=\frac{1}{2}(q^2+p^2)$, i.e., the classical oscillator energy variable. It is known that for each $n\in\mathbb{N}$, the operators $\Gamma^{|n\rangle\langle n|}(h^k)$, $k\in\mathbb{N}$, are the moment operators of the polar margin of the phase space observable $E^{|n\rangle\langle n|}$, and that the marginal observable is uniquely determined by

its moments.[12] Thus a quantization of h is given by the set $\{\Gamma^{|n\rangle\langle n|}(h^k)\,|\,k\in\mathbb{N}\}$ of operators. These operators were determined explicitly in Ref. 22; they are certain polynomials of the usual oscillator Hamiltonian $\frac{1}{2}(Q^2+P^2)$. The quantized oscillator energy observable is the unsharp number observable (see Ref. 4, p. 90).

V. OPTIMAL PHASE SPACE QUANTIZATION IN $\mathbb{R}^2$

Consider the situation of the previous section. At least in the case where $T=|n\rangle\langle n|$, the quantizations of the position and momentum variables x and y corresponding to the covariant quantization map $\Gamma^T=L(\cdot,E^T)$ are the Cartesian margins of E^T, or, equivalently, the sets of the operators $\{\Gamma^T(x^k)\,|\,k\in\mathbb{N}\}$ and $\{\Gamma^T(y^k)\,|\,k\in\mathbb{N}\}$. If the margins were projection valued, the quantization of, e.g., x would just be the spectral measure of $L(x,E^T)$, with each operator $L(x^k,E^T)$ equal to the corresponding power of $L(x,E^T)$. Although this is not the case, we can still try to find those generating operators T for which the situation would be in some sense close to this ideal situation, where only the first power of x is needed to determine its quantization.

First, we can find the generating operators T that give $L(x,E^T)=Q$ and $L(y,E^T)=P$, so as to make the operators $\Gamma^T(x)$ and $\Gamma^T(y)$ equal to the actual position and momentum operators. In view of Theorem 4, we know that the square integrability domains of $L(x,E^T)$ and $L(y,E^T)$ are nontrivial if and only if $Q\sqrt{T}$ and $P\sqrt{T}$ are Hilbert-Schmidt operators. In that case we have

$$L(x,E^T)=Q-\mathrm{Tr}\,[QT]I,$$

$$L(y,E^T)=P-\mathrm{Tr}\,[PT]I.$$

So if we assume that the square integrability domains of $L(x,E^T)$ and $L(y,E^T)$ are nontrivial, we have $L(x,E^T)=Q$ and $L(y,E^T)=P$ exactly when T is such that $\mathrm{Tr}\,[QT]=\mathrm{Tr}\,[PT]=0$. This occurs, for example, if we choose T to be a mixture of number states, i.e., $T=\Sigma_n w_n|n\rangle\langle n|$. Then the above Hilbert-Schmidt conditions take the form $\Sigma_n w_n n<\infty$.[18]

Consider next the operators $\Gamma^T(x^2)$ and $\Gamma^T(y^2)$. According to Theorem 4, they are given by

$$L(x^2,E^T)=Q^2-2\mathrm{Tr}\,[QT]Q+\mathrm{Tr}\,[Q^2T]I,$$

$$L(y^2,E^T)=P^2-2\mathrm{Tr}\,[PT]P+\mathrm{Tr}\,[P^2T]I,$$

provided that $Q^2\sqrt{T}$ and $P^2\sqrt{T}$ are Hilbert-Schmidt operators [or, equivalently, that $\tilde{D}(x^2,E^T)$ and $\tilde{D}(y^2,E^T)$ are nontrivial]. In order to make the situation close to the spectral measure case, we would like to minimize the "noise" operators $R^T(x)=L(x^2,E^T)^2-L(x,E^T)^2$ and $R^T(y)=L(y^2,E^T)^2-L(y,E^T)^2$. Now

$$R^T(x)=(\mathrm{Tr}\,[Q^2T]-\mathrm{Tr}\,[QT]^2)I=\mathrm{Var}(Q,T)I,$$

$$R^T(y)=(\mathrm{Tr}\,[P^2T]-\mathrm{Tr}\,[PT]^2)I=\mathrm{Var}(P,T)I,$$

on the domains $D(Q^2)$ and $D(P^2)$, respectively, where, e.g., $\mathrm{Var}(Q,T)$ denotes the variance of the probability measure $p_T^Q:=\mathrm{Tr}\,[TE^Q(\cdot)]$, with E^Q the spectral measure of Q. The last equalities are obtained as follows: Let $T=\Sigma_n w_n|\eta_n\rangle\langle\eta_n|$, $p_T^Q=\mathrm{Tr}\,[TE^Q(\cdot)]$, and $p_n^Q=\langle\eta_n|E^Q(\cdot)\,\eta_n\rangle$, where E^Q is the spectral measure of Q. Now $p_T^Q=\Sigma_n w_n p_n^Q$, with the series converging absolutely in the total variation norm, so we have (by, e.g., Lemma 1 of Ref. 18) that

$$\mathrm{Tr}\,[Q^2T]-\mathrm{Tr}\,[QT]^2=\sum_n w_n\langle\eta_n|Q^2\eta_n\rangle-\left(\sum_n w_n\langle\eta_n|Q\eta_n\rangle\right)^2$$
$$=\sum_n w_n\int x^2dp_n^Q-\left(\sum_n w_n\int xdp_n^Q\right)^2=\int x^2dp_T^Q-\left(\int xdp_T^Q\right)^2.$$

Therefore, $R^T(x)=\mathrm{Var}(Q,T)$. The result $R^T(y)=\mathrm{Var}(P,T)I$ follows similarly. Since $\mathrm{Var}(Q,T)$ and $\mathrm{Var}(P,T)$ are always positive, we see explicitly that $R^T(x)$ and $R^T(y)$ are never zero.

As is well known, the generating operator T can be chosen so that, e.g., $R^T(x)=\mathrm{Var}(Q,T)I$ is arbitrarily small [in the sense that $\|R^T(x)\|=\mathrm{Var}(Q,T)$ is such], but then $R^T(y)$ becomes large, because of the inequality $\mathrm{Var}(Q,T)\mathrm{Var}(P,T)\geqslant\frac{1}{4}$. The product $R^T(x)R^T(y)$ can reach its lower bound $\frac{1}{4}$ only in the case where T is a vector state of minimal uncertainty. If we assume that $\mathrm{Tr}\,[QT]=0=\mathrm{Tr}\,[PT]$ as discussed before, the operators T that give $R^T(x)R^T(y)=\frac{1}{4}$ are of the form $T=|\eta\rangle\langle\eta|$, with

$$(U^{-1}\eta)(t)=(\sqrt{\pi}\Delta q)^{-1/2}e^{-[t^2/4(\Delta q)^2]},$$

where $\Delta q>0$ [in fact, $(\Delta q)^2=\mathrm{Var}(Q,|\eta\rangle\langle\eta|)$ (Ref. 35, p. 92)]. Moreover, we could require that $R^T(x)=R^T(y)$, so as to make the situation symmetric between x and y. This leaves us with only one generating operator, namely $T=|0\rangle\langle 0|$. Note that this choice indeed gives a quantization of position and momentum, for the associated operator measure is uniquely determined by its moment operators (see Remark of Theorem 4).

VI. WHEN IS A POSITIVE OPERATOR MEASURE PROJECTION VALUED?

Let $E:\mathcal{B}(\mathbb{R})\to L(\mathcal{H})$ be a positive operator measure. If E is a spectral measure, the first moment $L(x,E)$ is always self-adjoint on the domain $\widetilde{D}(x,E)$, and $\int x^2dE_{\varphi,\varphi}=\|L(x,E)\varphi\|^2$ for all $\varphi\in\widetilde{D}(x,E)$. In the case of a general positive operator measure, this need not be true, as the above case of the Cartesian margins of the phase space observable E^T demonstrates. It turns out that this condition is sufficient for a positive operator E to be a spectral measure. This is explained in Ref. 1, p. 130, but the (sketch of) proof given there does not contain certain details, and so we give a (slightly different) proof here as part (b) of the following Proposition.

An adaptation of the steps leading to the result in Ref. 31, p. 466 gives part (a) of the following Proposition. For each $k\in\mathbb{N}$, we let $\widetilde{L}(x^k,E)$ denote the restriction of $L(x^k,E)$ to $\widetilde{D}(x^k,E)$.

Proposition 7: Let $E:\mathcal{B}(\mathbb{R})\to L(\mathcal{H})$ be a positive operator measure, such that

$$\int x^2dE_{\varphi,\varphi}=\|L(x,E)\varphi\|^2$$

for all $\varphi\in\widetilde{D}(x,E)$.

(a) $\widetilde{L}(x^n,E)=\widetilde{L}(x,E)^n$ *for all* $n\in\mathbb{N}$.

(b) If $\widetilde{L}(x,E)$ *is assumed to be self-adjoint, then E is projection valued.*

Proof: Let $P:\mathcal{B}(\mathbb{R})\to\mathcal{K}$ be a Naimark dilation of E into a spectral measure acting on a Hilbert space $\mathcal{K}$. Let $V:\mathcal{H}\to\mathcal{K}$ be the associated isometric map, so that $E(B)=V^*P(B)V$ for all $B\in\mathcal{B}(\mathbb{R})$. Denote by $P_{\mathcal{H}}$ the projection VV^*, acting on $\mathcal{K}$ with $\mathcal{V}\mathcal{H}$ as its range. (Note that V^*V is the identity operator of $\mathcal{H}$.) Now $\widetilde{L}(x^k,E)=V^*L(x^k,P)V$ for each $k\in\mathbb{N}$ (see Ref. 24). Since P is a spectral measure, we thus have

$$\widetilde{L}(x^k,E)=V^*A^kV \tag{5}$$

for all $k\in\mathbb{N}$, where $A=L(x,P)$. Denote $E_1=\widetilde{L}(x,E)$. We prove by induction that for each $n\in\mathbb{N}$,

$$\widetilde{D}(x^n,E) = D(E_1^n), \quad \text{and } A^n V\varphi = VE_1^n\varphi \text{ for all } \varphi \in \widetilde{D}(x^n,E). \tag{6}$$

Take first $n=1$, and let $\varphi \in \widetilde{D}(x,E)=D(E_1)=D(AV)$. Since the measures $E_{\varphi,\varphi}$ and $P_{V\varphi,V\varphi}$ are the same, and P is a spectral measure, the assumption implies that

$$\|AV\varphi\|^2 = \int x^2 dP_{V\varphi,V\varphi} = \int x^2 dE_{\varphi,\varphi} = \|E_1\varphi\|^2.$$

Using (5) and the fact that V is isometric, we thus get

$$\|AV\varphi\|^2 = \|E_1\varphi\|^2 = \|V^*AV\varphi\|^2 = \|P_H AV\varphi\|^2.$$

Since P_H is a projection, this means that

$$AV\varphi = P_{\mathcal{H}}AV\varphi = VE_1\varphi \text{ for all } \varphi \in \widetilde{D}(x,E) = D(E_1), \tag{7}$$

i.e., (6) holds for $n=1$. Now let $k \in \mathbb{N}$, $k>1$, and assume that (6) holds for $n=k-1$. Let $\varphi \in \widetilde{D}(x^k,E)$. By (5), this implies that $V\varphi \in D(A^k)$, so that $AV\varphi \in D(A^{k-1})$. Since $\varphi \in \widetilde{D}(x^k,E) \subset \widetilde{D}(x,E)$, it thus follows from (7) that $V(E_1\varphi)=AV\varphi \in D(A^{k-1})$, so (5) and the induction assumption give $E_1\varphi \in \widetilde{D}(x^{k-1},E)=D(E_1^{k-1})$. Hence, $\varphi \in D(E_1^k)$. Conversely, if $\varphi \in D(E_1^k)$, then $\varphi \in \widetilde{D}(x,E)=D(AV)$ and $E_1\varphi \in D(E_1^{k-1})=\widetilde{D}(x^{k-1},E)$, so $AV\varphi=V(E_1\varphi) \in D(A^{k-1})$ by (7) and (5), implying that $V\varphi \in D(A^k)$, i.e., $\varphi \in \widetilde{D}(x^k,E)$. Thus, $\widetilde{D}(x^k,E)=D(E_1^k)$. Let φ be in this set. Since now $E_1\varphi \in D(E_1^{k-1})$, the induction assumption [along with the fact that $AV\varphi=V(E_1\varphi)$] gives

$$A^k V\varphi = A^{k-1}(AV\varphi) = A^{k-1}V(E_1\varphi) = VE_1^{k-1}(E_1\varphi) = VE_1^k\varphi,$$

completing the induction proof of (6).

Let $n \in \mathbb{N}$. Now (5) and (6) give $\widetilde{L}(x^n,E)\varphi=V^*A^nV\varphi=V^*VE_1^n\varphi=E_1^n\varphi$ for all $\varphi \in \widetilde{D}(x^n,E) =D(E_1^n)$, so $\widetilde{L}(x^n,E)=\widetilde{L}(x,E)^n$. This proves (a).

If we assume that $\widetilde{L}(x,E)$ is selfadjoint, it follows from (7) that $P_{\mathcal{H}}D(A) \subset D(A)$. This fact is proved in Ref. 34, but we include the proof here for the reader's convenience. To that end, let $\psi \in D(A)$, and let $\varphi \in D(E_1)$ be arbitrary. Using (7), we get

$$\langle E_1\varphi | V^*\psi\rangle = \langle VE_1\varphi|\psi\rangle = \langle AV\varphi|\psi\rangle = \langle \varphi|V^*A\psi\rangle,$$

which implies that $V^*\psi \in D(E_1^*)$. Since E_1 is self-adjoint, $V^*\psi \in D(E_1)$, so $P_{\mathcal{H}}\psi=V(V^*\psi) \in VD(E_1)$. But $VD(E_1)$ is contained in $D(A)$, because $D(E_1)=D(AV)$. Thus $P_{\mathcal{H}}\psi \in D(A)$, proving the fact $P_{\mathcal{H}}D(A) \subset D(A)$. In addition, the above calculation shows that $V^*D(A) \subset D(E_1)$, and $E_1V^*\psi=E_1^*(V^*\psi)=V^*A\psi$ for all $\psi \in D(A)$. Combining this with (7), we get

$$P_{\mathcal{H}}A\psi = VV^*A\psi = V(E_1V^*\psi) = VE_1(V^*\psi) = AV(V^*\psi) = AP_{\mathcal{H}}\psi$$

for all $\psi \in D(A)$. Consequently, $P_{\mathcal{H}}A \subset AP_{\mathcal{H}}$. Since A is self-adjoint, this implies that $P_{\mathcal{H}}$ commutes with all the spectral projections $P(B)$ (Ref. 31, pp. 301 and 320). It follows that each $E(B)$ is a projection (Ref. 27, Corollary 2.2.2.), so the proof is complete. □

Remark: As mentioned before, the result appearing in part (b) of the above Proposition can be found in the classic book of Akhiezer and Glazman.[1] The result seems to be somewhat well known (see, e.g., Refs. 30 and 37 both of which refer to the works of Akhiezer and Glazman). However, the fact is given in a much later work[21] without reference to Ref. 1 (though we have not been able to convince ourselves of their argumentation), and Werner (Ref. 39, p. 796) only mentions that it holds for normalized compactly supported operator measures. Moreover, Ingarden (Ref. 17, p. 87) says that all the semispectral measures with the same self-adjoint first moment A have variances greater than or equal to that of the spectral measure of A. Part (b) of the above Proposition gives more—it asserts that the minimum variance occurs *only* in the case of the spectral measure of A.

We note also that the proof given in Ref. 17, p. 87 considers only compactly supported semispectral measures, and contains no reference to Ref. 1.

Now we get the following characterization for projection valued measures.

Theorem 5: *Let $E:\mathcal{B}(\mathbb{R})\to L(\mathcal{H})$ be a positive normalized operator measure, such that $\widetilde{L}(x,E)$ is self-adjoint. Then the following conditions are equivalent.*

(i) *E is a spectral measure*;
(ii) $L(x^2,E)=L(x,E)^2$;
(iii) $\int x^2 dE_{\varphi,\varphi}=\|L(x,E)\varphi\|^2$ *for all* $\varphi\in\widetilde{D}(x,E)$.

Proof. Since $\widetilde{L}(x,E)$ is self-adjoint, it coincides with its symmetric extension $L(x,E)$.

Assume that (i) holds. Then $\widetilde{L}(x^2,E)=\widetilde{L}(x,E)^2$ by a standard result of spectral theory. Since E is projection valued, we have also $\widetilde{L}(x^2,E)=L(x^2,E)$, so (ii) holds.

Assume (ii). Then we have

$$\int x^2 dE_{\varphi,\varphi}=\|L(x,E)\varphi\|^2 \tag{8}$$

for all $\varphi\in D(x^2,E)$. In order to get (iii), we have to establish this identity for vectors in the larger set $D(x,E)=\widetilde{D}(x,E)$. Let $\varphi\in\widetilde{D}(x,E)=D(x,E)$. Since $L(x,E)=\widetilde{L}(x,E)$ is self-adjoint, the closure of the restriction of $L(x,E)$ to the domain of $L(x,E)^2$ is $L(x,E)$ itself (Ref. 11, p. 1245). Therefore, by (ii), we can pick a sequence (φ_n) of vectors in $D(x^2,E)$, converging to φ, such that $(L(x,E)\varphi_n)$ converges to $L(x,E)\varphi$. Since $\varphi_n\in D(x^2,E)$ for each n, (8) gives that

$$\lim_n \int x^2 dE_{\varphi_n,\varphi_n}=\lim_n \|L(x,E)\varphi_n\|^2=\|L(x,E)\varphi\|^2.$$

Since $|E_{\varphi_n,\varphi_n}(B)-E_{\varphi,\varphi}(B)|\leqslant(\|\varphi_n\|+\|\varphi\|)\|E(\mathbb{R})\|\,\|\varphi_n-\varphi\|$ for all $n\in\mathbb{N}$ and $B\in\mathcal{B}(\mathbb{R})$, the sequence $(E_{\varphi,\varphi}(B))$ converges to $E_{\varphi,\varphi}(B)$ uniformly for $B\in\mathcal{B}(\mathbb{R})$, so the sequence $(E_{\varphi,\varphi})$ of positive measures converges to $E_{\varphi,\varphi}$ in the total variation norm (Ref. 10, p. 97). It follows by Ref. 22, Lemma A.5 that

$$\int x^2 dE_{\varphi,\varphi}\leqslant\|L(x,E)\varphi\|^2,\varphi\in D(x,E). \tag{9}$$

It follows, e.g., from the proof of Lemma A.2 of Ref. 22 (see Ref. 3, p. 65) that $\|L(x,E)\varphi\|^2\leqslant\int x^2 dE_{\varphi,\varphi}$ for all $\varphi\in D(x,E)$. Combining this with (9), we get (iii).

Because (iii) implies (i) by the preceding Proposition, the proof is complete. □

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Representation of state property systems

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A "state property system" is the mathematical structure which models an arbitrary physical system by means of its set of states, its set of properties, and a relation of "actuality of a certain property for a certain state." We work out a new axiomatization for standard quantum mechanics, starting with the basic notion of state property system, and making use of a generalization of the standard quantum mechanical notion of "superposition" for state property systems. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217807]

I. INTRODUCTION

In standard quantum mechanics a state $p_{\bar{c}}$ of a quantum entity S is represented by the one-dimensional subspace or the ray $\bar{c}$ of a separable complex Hilbert space $\mathcal{H}$. An experiment e_A testing an observable A is represented by a self-adjoint operator $\mathcal{A}$ on $\mathcal{H}$, and the set of outcomes of this experiment e_A is the spectrum $\mathrm{spec}(\mathcal{A})$ of this self-adjoint operator $\mathcal{A}$. Measurable subsets $B \subset \mathrm{spec}(\mathcal{A})$ represent the events (in the sense of probability theory) of outcomes. The interaction of the experiment e_A with the physical entity being in state $p_{\bar{c}}$ is described in the following way: (1) the probability for a specific event $B \subset \mathrm{spec}(\mathcal{A})$ to occur if the entity is in a specific state $p_{\bar{c}}$ is given by $\langle c, P_B(c)\rangle$, where P_B is the spectral projection corresponding to B, c is the unit vector in the ray $\bar{c}$ representing state $p_{\bar{c}}$, and $\langle,\rangle$ is the in-product in the Hilbert space $\mathcal{H}$; (2) if the outcome is contained in B, the state $p_{\bar{c}}$ is changed to $p_{\bar{d}}$ where $\bar{d}$ is the ray generated by $P_B(c)$.

Hence in standard quantum mechanics the states and experiments are represented by means of mathematical entities of a complex Hilbert space. The crucial role that is played by this complex Hilbert space is very much *ad hoc*, in the sense that there are no physically plausible reasons why the Hilbert space structure should be at the origin of both the structure of the state space, as well as the structure of the experiments.

This initiated the search for an axiomatic theory for quantum mechanics where the Hilbert space structure would be derived from more general and physically more plausible axioms. The area of forming physical models in the field of quantum mechanics is very large, and often involves philosophical problems of physics. Let us mention some of the most well known axiomatic approaches: the algebraic approach,[1–3] where the basic notions are observables, the convexity approach,[4–8] where the basic notion is the convex set of states, the empirical logic approach,[9–13] where the authors start with primitive notions of an operation or a test, and the quantum logic approach,[14–20] which starts with the set of experimental propositions.

Due to the original focus[14] on the collection of "experimental propositions" of a physical entity—with the conviction that such an experimental proposition would be a good basic concept—most of the later axiomatics were constructed taking as their basic concept the set $\mathcal{L}$ of experimental propositions concerning an entity S. The first breakthrough came with a theorem of

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Constantin Piron, who proved that if $\mathcal{L}$ is a complete [axiom 1], orthocomplemented [axiom 2] atomic [axiom 3] lattice, which is weakly modular [axiom 4] and satisfies the covering law [axiom 5], then each irreducible component of the lattice $\mathcal{L}$ can be represented as the lattice of all "biorthogonal" subspaces of a vector space V over a division ring K (with some other properties satisfied that we shall not explicitly address here).[17] Such a vector space is called an "orthomodular space" and also sometimes a "generalized Hilbert space." It can be proven that an infinite dimensional orthomodular space over a division ring which is the real or complex numbers, or the quaternions, is a Hilbert space. For a long time there did not even exist any other example of an infinite dimensional orthomodular space. The search for a further characterization of the real, complex, quaternionic Hilbert space started (see, e.g., Ref. 21). Then Hans Keller constructed a nonclassical orthomodular space,[22] and recently Maria Pia Solèr proved that any orthomodular space that contains an infinite orthonormal sequence is a real, complex, or quaternionic Hilbert space.[23,24] It is under investigation in which way this result of Solèr can be used to formulate new physically plausible axioms.[24–27]

The axiomatic approach, apart from delivering an axiomatic foundation for quantum mechanics, has been used fruitfully to study concrete problems in quantum mechanics. As an example we mention the problem of the description of joint quantum entities, and the problems of entanglement, nonlocality, and appearance of the complex numbers in quantum mechanics. Most recently this problem has been studied within the axiomatic approach with very interesting results.[28–34]

Next to the idea of finding axioms that introduce the Hilbert space structure step by step was the attempt to determine the basic notions for the axiomatics in a physically clear and operational way. "Operationality" means that the axioms should be introduced in such a way that they can be related to "real physical operations" that can be performed in the laboratory.

The approaches that have tried to formulate quantum mechanics operationally are the Geneva-Brussels approach,[17,18,35–41] the Amherst approach,[9–13] and the Marburg approach.[42,43] In the present article we elaborate further on the Geneva-Brussels approach. In the last versions of the formalism that were presented in this approach the power of making a good distinction between the mathematical aspects of the formalism and its physical foundations had been identified.[44,45] Let us explain more concretely what we mean. In the older founding papers of the Geneva-Brussels approach,[35–41] although the physical foundation of the formalism is defined in a clear way, and the resulting mathematical structures are treated rigorously, it is not always clear what are the "purely mathematical" properties of the structures that are at the origin of the results. That is the reason that in more recent work on the formalism we have made an attempt to divide up the physical foundation and the resulting mathematical structure as much as possible. We first explain in which way certain aspects of the mathematical structure arise from the physical foundation, but then, in a second step, define these aspects in a strictly mathematical way, such that propositions and theorems can be proven, "only" using the mathematical structure without physical interpretation. Afterwards, the results of these propositions and theorems can then be interpreted in a physical way again. This not only opens the way for mathematicians to start working on the structures, but also lends a greater axiomatic strength to the whole approach on the fundamental level. More concretely, it is the mathematical structure of a "state property system" that has been identified to be the proper mathematical structure of the Geneva-Brussels approach, i.e., the structure used to describe a physical entity by means of its states and properties.[44–46] This step turned out to be fruitful from the start, since we could prove that a state property system as a mathematical structure is isomorphic to a closure space.[44–46] This means that the mathematics of closure spaces can be translated to the mathematics of state property systems, and in this sense becomes relevant for the foundations of quantum mechanics. The step of dividing up the mathematics from the physics in a systematic way also led to a scheme to derive the morphisms for the structures that we consider from a covariance principle rooted in the relation of a subentity to the entity of which it is a subentity.[45,46] This paved the way to a categorical study of the mathematical structures involved.

Not only was it possible to connect with a state property system a closure space in an

isomorphic way, but, after we had introduced the morphisms starting from a merological covariance principle, it was possible to prove that the category of state property systems and their morphisms, that we have named **SP**, is equivalent to the category of closure spaces and continuous functions, denoted by **Cls**.[45,46] More specifically we could prove that SP is the amnestic modification of **Cls**.[47]

It could be proven that some of the axioms of axiomatic quantum mechanics[17,36,37] correspond to separation properties of the corresponding closure spaces.[48] More concretely, the axiom of state determination in a state property system[44] is equivalent to the T_0 separation axiom of the corresponding closure space,[48,49] and the axiom of atomicity in a state property system[44] is equivalent to the T_1 separation axiom of the corresponding closure space.[50,51] More recently it has been shown that "classical properties"[36,38,40,41] of the state property system correspond to clopen (open and closed) sets of the closure space,[52–54] and, explicitly making use of the categorical equivalence, a decomposition theorem for a state property system into its nonclassical components can be proved that corresponds to the decomposition of the corresponding closure space into its connected components.[52,53,57]

In the present article we put forward a new axiomatization for standard quantum mechanics, starting with the basic notion of "state property system," and founded on the concept of "superposition," that started in the quantum logic approach and was developed in Ref. 55. The general reason for introducing the new axiomatization is to put under one roof the Geneva-Brussels approach in its recent form and the quantum logic approach and to combine the algebraic approach and the probabilistic approach. We also wish to find out how the recent development in projective geometry (see Ref. 56) can be reflected in the axiomatization. A more specific reason for this new axiomatization is to take it as a mathematical basis for further research into the problem of the description of joint quantum systems. Both authors have done extensive research on the problem of the description of joint quantum systems.[57–60,37,61–65] One of the hard problems is that all types of product constructions on the level of the quantum logic structure give rise to a situation where the joint quantum entity only has product states of the subentities. On the level of the Hilbert space, the joint system of two quantum systems is described by means of the tensor product of the Hilbert spaces of the subsystems, and in this case there is an abundance of nonproduct states, giving rise to the well-known phenomenon of quantum entanglement. We plan to study the still open problem of coupled physical systems with entanglement, by investigating in which way we can introduce "superpositions between product states" by means of the notion of superposition which we introduced in this axiomatization on the level of the quantum logic.

The notion of a superposition of states was introduced by Varadarajan[66] for states as probability measures on quantum logics, i.e., orthomodular lattices. In the same sense it is also used in Ref. 55. In the present paper, we use a more general frame of a state property system to introduce the notion of superposition. We use superpositions to create two kinds of closure operations. The first one, together with a few simple additional axioms, enables us to associate the structure of a projective geometry with our state property system. A very useful tool here is the material presented in the recent book by Faure and Frölicher.[56] The first of our closure operations based on superposition leads to the formation of subspaces of a projective geometry. The second of our closure operations enables us to characterize closed subspaces of the projective geometry. Probabilities enter into play in order to introduce orthocomplementation on a subset $\mathcal{L}_0$ of the lattice $\mathcal{L}$, and we show that $\mathcal{L}_0$ can be organized into a σ- orthomodular poset with an order determining set of probability measures, which are supported by elements of the set Σ. The set $\mathcal{L}_0$ may be interpreted as a set of measurable properties, and may depend on the present state of knowledge and experimental techniques. In the following parts of the article, conditions are found under which the orthocomplementation can be extended to the whole $\mathcal{L}$, and $\mathcal{L}$ then becomes a complete, atomistic, orthocomplemented lattice. Moreover, $\mathcal{L}$ can be related with the closed subspaces of the projective geometry via the so-called Cartan map. The notion of "superposition principle" is introduced to obtain irreducibility of the projective geometry. More generally, sectors are introduced as the minimal subspaces in which the superposition principle holds, and their topological characterization as clopen subspaces is derived. In the following the classical properties (or the

superselection rules) are specified, and it is shown that they correspond exactly to the central elements of the lattice $\mathcal{L}$. In the following, we study conditions under which our projective geometry may admit some deeper properties, described in Ref. 56, such as the Mackey property or to become an orthogeometry. Although not all of our axioms have a physical meaning, we try to specify simple axioms which enable us to obtain different stages of the projective geometry. Eventually we find conditions under which a vector space can be associated with our state property system, and we finish with an analogue of the famous Piron theorem.

II. STATE PROPERTY SYSTEMS AND SUPERPOSITION

Definition 1:[44–46] *We say that* $(\Sigma,\mathcal{L},\xi)$ *is a state-property system if* $(\Sigma,<)$ *is a preordered set,* $(\mathcal{L},<,\wedge,\vee)$ *is a complete lattice with the greatest element I and the smallest element* 0, *and* ξ *is a function*

$$\xi:\Sigma\to\mathcal{P}(\mathcal{L}) \tag{1}$$

such that for $p\in\Sigma$ *and* $(a_i)_i\subseteq\mathcal{L}$, *we have*

$$I\in\xi(p), \tag{2}$$

$$0\notin\xi(p), \tag{3}$$

$$a_i\in\xi(p)\ \forall\, i\Leftrightarrow\wedge_i a_i\in\xi(p)\ (\textit{for an arbitrary set of indices}) \tag{4}$$

and for $p,q\in\Sigma$ *and* $a,b\in\mathcal{L}$ *we have*

$$p<q\Leftrightarrow\xi(q)\subseteq\xi(p), \tag{5}$$

$$a\leqslant b\Leftrightarrow\ \forall\, r\in\Sigma:a\in\xi(r)\Rightarrow b\in\xi(r). \tag{6}$$

Elements of Σ are called *states*, elements of $\mathcal{L}$ are called *properties*.

Let $(\Sigma,\mathcal{L},\xi)$ be a state-property system. For $S\subset\Sigma$ define $S\mapsto\lambda(S)$ as follows. First define, for any $p,q\in\Sigma$,

$$\lambda\{p,q\}:=\{s\in\Sigma:a\in\xi(p)\cap\xi(q)\Rightarrow a\in\xi(s)\}. \tag{7}$$

We will say that a subset $S\subseteq\Sigma$ is λ-*closed* if for any $p,q\in S$ we have $\lambda\{p,q\}\subset S$. Denote by $\mathcal{L}(\Sigma)$ the set of all λ-closed subsets. For any $P\subset\Sigma$, define

$$\lambda(P):=\ \cap\{G:G\in\mathcal{L}(\Sigma),P\subset G\}. \tag{8}$$

That is, $\lambda(P)$ is the intersection of all λ-closed subsets of Σ that contain P.

Lemma 1: (i) *For every subset* $P\subseteq\Sigma$, $\lambda(P)\in\mathcal{L}(\Sigma)$. (ii) *A subset* $S\subseteq\Sigma$ *is* λ-*closed if and only if* $S=\lambda(S)$.

Proof: (i) Let $p,q\in\lambda(P)$, then $p,q\in G$ for every $P\subseteq G\in\mathcal{L}(\Sigma)$. Therefore $\lambda\{p,q\}\subseteq G$ for every such G, and consequently $\lambda\{p,q\}\subseteq\lambda(P)$.

(ii) If $S=\lambda(S)$, then $S\in\mathcal{L}(\Sigma)$ by (i). If S is λ-closed, then clearly, S is the smallest λ-closed subset of Σ containing S, hence $\lambda(S)=S$. □

That is,

$$\mathcal{L}(\Sigma)=\{S\subset\Sigma:S=\lambda(S)\}. \tag{9}$$

Proof of the following statement is immediate.

Lemma 2: The mapping $\lambda:P\mapsto\lambda(P)$ *satisfies the following properties:*

(C1) $P\subseteq\lambda(P)$,
(C2) $P_1\subseteq\lambda(P_2)\Rightarrow\lambda(P_1)\subseteq\lambda(P_2)$.

We recall that a map $C:\mathcal{P}(X)\to\mathcal{P}(X)$ satisfying conditions (C1) and (C2) is a *closure operator* on the set X (Ref. 56, Definition 3.1.1). Consequently, λ is a closure operator on the set Σ.

According to Ref. 56, Remark 3.1.2, the following conditions are satisfied:

(1^0) $\lambda(A\cup B)=\lambda(\lambda(A)\cup B)=\lambda(\lambda(A)\cup\lambda(B))$,
(2^0) $\lambda(A\cap B)\subseteq\lambda(\lambda(A)\cap B)\subseteq\lambda(A)\cap\lambda(B)$.

More generally,

(3^0) $\lambda(\cup\mathcal{A})=\lambda(\cup\lambda(\mathcal{A}))$,
(4^0) $\lambda(\cap\mathcal{A})\subseteq\cap\lambda(\mathcal{A})$,

where $\mathcal{A}\subseteq\mathcal{P}(\Sigma)$ is an arbitrary subset and $\lambda(\mathcal{A})$ denotes the set $\{\lambda(A):A\in\mathcal{A}\}$.

Recall that a system $\mathcal{S}$ of sets is an *intersection system* if $\mathcal{A}\subseteq\mathcal{S}$ implies $\cap\mathcal{A}\in\mathcal{S}$. By [Ref. 56, Proposition 3.1.4], $\mathcal{L}(\Sigma)$ is an intersection system.

Definition 2: We say that a state-property system $(\Sigma,\mathcal{L},\xi)$ *satisfies property*

(A) *if there are at least two distinct states* $r,s\in\Sigma$ *and for all* $p,q\in\Sigma$, $\xi(p)\subset\xi(q)\Rightarrow p=q$.

Property (A) implies that $\xi:\Sigma\to\mathcal{P}(\mathcal{L})$ is injective. By Ref. 46, Proposition 14, the pre-order $<$ on Σ defined by (5) of Definition 1 is a partial order. Property (A) implies that Σ has only a trivial order $p<q$ iff $p=q$.

Recall that a closure operator C on a set X is called *simple* if it satisfies the additional axiom:

(C5) $C(\emptyset)=\emptyset$ and $C(x)=\{x\}$ for every $x\in X$.

(We write $C(x)$ instead of $C(\{x\})$). If X contains at least two different points, then the second property in (C5) implies the first one. Indeed, $\emptyset\subset\{x\},\emptyset\subset\{y\}$ implies $C(\emptyset)\subset C(x)\cap C(y)=\{x\}\cap\{y\}=\emptyset$.

Lemma 3: Let $(\Sigma,\mathcal{L},\xi)$ *be a state-property system such that there are at least two different states* $p,q\in\Sigma$. *Then the closure operator* λ *is simple if and only if property* (A) *of Definition 2 holds*.

Proof: If (A) holds, then for every $p\in\Sigma$,

$$\lambda\{p\}=\{s\in\Sigma:a\in\xi(p)\Rightarrow a\in\xi(s)\}=\{s\in\Sigma:\xi(p)\subset\xi(s)\}=\{p\}.$$

If $\lambda(\emptyset)$ contains r, then $\lambda(\emptyset)\subseteq\lambda(q)=\{q\}$ implies $r\in\{q\}$, hence $r=q$ for all q, a contradiction.

Conversely, if λ is simple and $\xi(p)\subseteq\xi(q)$ for $p\neq q$, then

$$\lambda(p)=\{s\in\Sigma:\xi(p)\subseteq\xi(s)\}\ni q$$

contradicting $\lambda(p)=\{p\}$. □

Proposition 1: Let $(\Sigma,\mathcal{L},\xi)$ *be a state property system satisfying* (A). *Then* $\mathcal{L}$ *is a complete atomistic lattice with the lattice operations*

$$\wedge S_\alpha=\cap S_\alpha,\quad \vee S_\alpha=\lambda(\cup S_\alpha).$$

Proof: Follows by Ref. 56, Proposition 3.1.4. □

In what follows, we introduce the notion of a superposition of states in analogy with Ref. 19.

Definition 3: A state $p\in\Sigma$ *is a superposition of a set of states* S, $S\subseteq\Sigma$, *if for each* $a\in\mathcal{L}$, $a\in\xi(s)$ *for all* $s\in S$ *implies* $a\in\xi(p)$, *i.e., if* $\cap_{s\in S}\xi(s)\subseteq\xi(p)$.

For $S\subseteq\Sigma$, *define*

$$\bar{S}=\left\{p\in\Sigma:\bigcap_{s\in S}\xi(s)\subseteq\xi(p)\right\}. \tag{10}$$

That is, $\bar{S}$ is the set of all superpositions of states in S. Obviously, for arbitrary $p,q\in\Sigma$,

$$\{p,q\}^-=\lambda\{p,q\}. \tag{11}$$

Definition 4: A state $p \in \Sigma$ is a minimal superposition of a subset $S \subseteq \Sigma$ if

(i) $p \in \bar{S}$,

(ii) $p \notin \bar{Q}$ *for any proper subset* $Q \subseteq S$.

For example, if (A) holds, then $s \in \{p,q\}^-$ is a minimal superposition iff $s \neq p$, $s \neq q$.

Definition 5: Let $(\Sigma, \mathcal{L}, \xi)$ be a state-property system.

(1) *We will say that a minimal superposition principle* (MSP) *holds for $(\Sigma, \mathcal{L}, \xi)$ if for every subset $S \subseteq \Sigma$ and for every minimal superposition p of S,*

$$\{S_1 \cup p\}^- \cap \bar{S}_2 \neq \emptyset \tag{12}$$

whenever S_1, S_2 are proper subsets of S such that $S_1 \cap S_2 = \emptyset$ and $S_1 \cup S_2 = S$.

(2) *We will say that a finite MSP* (f-MSP) *holds for $(\Sigma, \mathcal{L}, \xi)$ if* (12) *holds for every finite subset $S \subseteq \Sigma$.*

(3) *We will say that an n-MSP holds for $(\Sigma, \mathcal{L}, \xi)$ if* (12) *holds for every subset $S \subseteq \Sigma$ with the cardinality at most n.*

For example, the 3-MSP holds for a state-property system $(\Sigma, \mathcal{L}, \xi)$ iff for every $p,q,r,s \in \Sigma$ (not necessarily all different), if $p \in \{q,r,s\}^-$ is a minimal superposition, then $\{p,q\}^- \cap \{r,s\}^- \neq \emptyset$ and $\{p,q,r\}^- \cap \{s\}^- \neq \emptyset$. Clearly, MSP implies f-MSP, which in turn implies n-MSP for every $n \in \mathbb{N}$. Observe also that if (A) holds, then 2-MSP is the following exchange property: if $r \in \{p,q\}^-$ and $r \neq p,q$, then $p \in \{r,q\}^-$.

Theorem 1: *Let $(\Sigma, \mathcal{L}, \xi)$ be a state-property system with properties* (A) *and* 3-MSP. *Then the operator $*: \Sigma \times \Sigma \to \mathcal{P}(\Sigma)$ defined by $p*q = \lambda\{p,q\}$ has the following properties*:

(P1) $p*p = \{p\}$,

(P2) $p \in p*q$ *for all* $p,q \in \Sigma$,

(P3) $p \in q*r$ *and* $r \in s*t$ *and* $p \neq s$ *imply* $(p*s) \cap (q*t) \neq \emptyset$

That is, the system $(\Sigma, *)$ is a projective geometry.[56]

Proof: (P1) By (A), $\lambda\{p,p\} = \{p\}$.

(P2) Clearly, $p*q = \lambda\{p,q\} \supseteq \{p\}$.

(P3) From $p \in \{q,r\}^-$ and $r \in \{s,t\}^-$ we obtain $p \in \{q,s,t\}^-$. If $p \in q*s$, respectively, $p \in s*t$, then either $p = q$, respectively, $p = t$, or 2-MSP implies that $q \in p*s$, respectively, $t \in p*s$. In every case, (P3) is satisfied. It remains the case that either $p \in q*t$ or p is a minimal superposition of $\{q,s,t\}$. In the first case, $p \in (p*s) \cap (q*t)$ holds by (P2). In the second case the statement follows by 3-MSP. □

By Ref. 56, Definition 2.3.1, the λ-closed subsets of Σ coincide, under the suppositions of Theorem 1, with the subspaces of the projective geometry $(\Sigma, *)$ associated with $(\Sigma, \mathcal{L}, \xi)$. Consequently, we have the following.

Theorem 2: *Let $(\Sigma, \mathcal{L}, \xi)$ be a state-property system satisfying conditions* (A) *and* 3-MSP. *Then $\mathcal{L}(\Sigma)$ is a projective lattice, i.e., a complete atomistic meet-continuous modular lattice.*

Therefore we will call the elements of $\mathcal{L}(\Sigma)$ the *subspaces* of Σ. From the next theorem we can derive what properties satisfy the closure operator λ on the system $(\Sigma, *)$ with $p*q = \lambda\{p,q\}$. (We write $\lambda(x)$ instead of $\lambda(\{x\})$ and $\lambda(A \cup x)$ instead of $\lambda(A \cup \{x\})$.)

Theorem 3: *Let $(\Sigma, \mathcal{L}, \xi)$ be a state-property system such that $(\Sigma, *)$ with $p*q = \lambda\{p,q\}$ is a projective geometry, i.e., properties* (P1), (P2), *and* (P3) *are satisfied. Then the closure operator λ satisfies the following conditions*:

(C3) $x \in \lambda(A)$ *implies* $x \in \lambda(B)$ *for some finite subset* $B \subseteq A$, *i.e.*, λ *is finitary.*

(C4) $x \notin \lambda(A)$ *and* $x \in \lambda(A \cup y)$ *imply* $y \in \lambda(A \cup x)$, *i.e.*, λ *satisfies the exchange property.*

(C5) $\lambda(\emptyset) = \emptyset$ *and* $\lambda(x) = \{x\}$, *i.e.*, λ *is simple.*

(C6) $\lambda(A \cup B) = \cup\{\lambda\{x,y\} : x \in \lambda(A)$ *and* $y \in \lambda(B)\}$ *for every* $A, B \subseteq \Sigma$.

Proof: See Ref. 56, Theorem 3.3.4. □

Notice that (C6) is called a *projective law*. According to Ref. 56, Lemma 3.3.2, if a closure operator $C:\mathcal{P}(X)\to\mathcal{P}(X)$ satisfies the projective law, then for any nonempty subset $A\subseteq X$ and any $b\in X$ one has

(C7) $C(A\cup b)=\cup\{C(x,b):x\in C(A)\}$.

Moreover, the converse holds provided the closure operator C satisfies (C3), i.e., is finitary. The following proposition follows by Ref. 56, Proposition 3.3.4.

Proposition 2: Let the closure operator $\lambda:\mathcal{P}(\Sigma)\to\mathcal{P}(\Sigma)$ *satisfy properties* (C4), (C5), *and* (C7). *The couple* $(\Sigma,*)$ *where* $p*q=\lambda\{p,q\}$ *is a projective geometry*.

Now we will study connections between the mappings $A\mapsto\lambda(A)$ and $A\mapsto\bar{A}$, $A\subseteq\Sigma$. First we prove the following properties of $A\mapsto\bar{A}$.

Lemma 4: Let $(\Sigma,\mathcal{A},\xi)$ *be a state-property system. The operator* $A\mapsto\bar{A}$ *satisfies the following properties for every* $A,B\subseteq\Sigma$.

(i) $A\subseteq\bar{A}$.

(ii) $A\subseteq\bar{B}\Rightarrow\bar{A}\subseteq\bar{B}$.

(iii) $\bar{A}\in\mathcal{L}(\Sigma)$.

Proof: (i) Follows directly from the definition.

(ii) Let $p\in\bar{A}$, i.e., $\cap_{s\in A}\xi(s)\subseteq\xi(p)$. $A\subseteq\bar{B}$ implies that for every $s\in A$, $\cap_{q\in B}\xi(q)\subseteq\xi(s)$, so that $\cap_{q\in B}\xi(q)\subseteq\cap_{s\in A}\xi(s)\subseteq\xi(p)$. Hence $p\in\bar{B}$, and so $\bar{A}\subseteq\bar{B}$.

(iii) From $\lambda\{p,q\}=\{p,q\}^-\subseteq\bar{A}$ for every $p,q\in A$ we see that $\bar{A}$ is λ-closed, i.e., $\bar{A}=\lambda(\bar{A})$. □

Observe that (i) and (ii) in Lemma 4 coincide with the properties (C1) and (C2), respectively, so that $A\mapsto\bar{A}$ is a closure operator. Let us denote by $\mathcal{F}(\Sigma)$ the set of superposition-closed subsets of Σ, that is,

$$\mathcal{F}(\Sigma):=\{S\subset\Sigma:\bar{S}=S\}. \tag{13}$$

Proposition 3: Let $(\Sigma,\mathcal{L},\xi)$ *be a state property system satisfying condition* (A). *Then the set* $\mathcal{F}(\Sigma)$ *is a complete atomistic lattice. Moreover, if* $S_i\in\mathcal{F}(\Sigma),i\in I$, *for any index set* I, *then* $\wedge_{i\in I}S_i=\cap_{i\in I}S_i$, *and* $\vee_{i\in I}S_i=(\cup_{i\in I}S_i)^-$.

Proof: If $S\subset\Sigma$, $S=\emptyset$ or $S=\{s\}$, then $S=\bar{S}$ by condition (A). So one-element sets belong to $\mathcal{F}(\Sigma)$ which are atoms in $\mathcal{F}(\Sigma)$. From the properties of closure operators (Ref. 56, Proposition 3.1.4), we get $\wedge_{i\in I}S_i=\cap_{i\in I}S_i$, and $\vee_{i\in I}S_i=(\cup_{i\in I}S_i)^-$. □

Theorem 4: *Let* $(\Sigma,\mathcal{L},\xi)$ *be a state-property system such that condition* (A) *is satisfied.*

(i) *If* 3-MSP *holds, then for every* $p,q,s\in\Sigma$,

$$\{p,q,s\}^-=\lambda\{p,q,s\}. \tag{14}$$

(ii) *If* f-MSP *holds, then for every finite subset* $A=\{s_1,s_2,\ldots,s_n\}\subseteq\Sigma$,

$$\lambda(A)=\bar{A}. \tag{15}$$

Proof: (i) For every $p,q\in\Sigma$, $\lambda\{p,q\}=\{p,q\}^-$, and by Lemma 4(iii), $\lambda\{p,q,s\}\subseteq\{p,q,s\}^-$ for every $p,q,s\in\Sigma$. To prove the converse inclusion, let $t\in\{p,q,s\}^-$. If $t\in\{p,q\}^-$, then $t\in\lambda\{p,q\}\subseteq\lambda\{p,q,s\}$. Hence we may assume that t is a minimal superposition. Then by 3-MSP, there is $r\in\{p,t\}^-\cap\{q,s\}^-$. By 2-MSP, $t\in\lambda\{r,p\}\subseteq\lambda\{p,q,s\}$. This implies that $\{p,q,s\}^-\subseteq\lambda\{p,q,s\}$.

(ii) We will proceed by induction. For $n=2$, the statement holds. Assume that the statement holds for every $k\leqslant n$, $k,n\in\mathbb{N}$. Let $A=\{s_1,s_2\ldots,s_n,s_{n+1}\}$, and assume that $t\in\bar{A}$ is a minimal superposition. By f-MSP and induction hypothesis, there is $r\in\{t,s_{n+1}\}^-\cap\{s_1,\ldots,s_n\}^-\subseteq\lambda\{s_1,\ldots,s_n\}$. Now $t\in\lambda\{r,s_{n+1}\}\subseteq\lambda((\lambda\{s_1,\ldots,s_n\}\cup s_{n+1})\subseteq\lambda(A)$. If t is not a

minimal superposition, there is a subset $B \subseteq A$ such that $t \in \bar{B} = \lambda(B) \subseteq \lambda(A)$ by induction hypothesis. Hence $\bar{A} \subseteq \lambda(A)$. The converse holds by Lemma 4(iii). □

III. PROBABILITY MEASURES AND ORTHOCOMPLEMENTATION

Let $(\Sigma, \mathcal{L}, \xi)$ be a state-property system. Let there be a subset $\mathcal{L}_0 \subset \mathcal{L}$ such that $\mathcal{L}_0$ contains 0 and 1, and let there be a mapping $\mu: \Sigma \times \mathcal{L}_0 \to [0,1]$, $(p,a) \mapsto \mu_p(a)$, where $[0,1]$ is the unit interval of the reals, such that

(Oi) $\mu_p(a)=1$ iff $a \in \xi(p)$ $(a \in \mathcal{L}_0)$,
(Oii) $a \leqslant b$ implies $\mu_p(a) \leqslant \mu_p(b)$ $(a,b \in \mathcal{L}_0)$,
(Oiii) If $(a_i)_{i=1}^{\infty} \subset \mathcal{L}_0$ is a sequence such that for all i,j, and every $p \in \Sigma$,

$$\mu_p(a_i) + \mu_p(a_j) \leqslant 1,$$

then there is $b \in \mathcal{L}_0$ such that

$$\mu_p(b) + \sum_{i=1}^{\infty} \mu_p(a_i) = 1.$$

Clearly, $\mu_p(I)=1$ and $\mu_p(0)=0$ for all $p \in \Sigma$. Define a relation $\perp \subset \mathcal{L}_0 \times \mathcal{L}_0$ by setting $a \perp b$ iff $\mu_p(a)+\mu_p(b) \leqslant 1$ for all $p \in \Sigma$. We will say that a and b are *orthogonal* if $a \perp b$.

Lemma 5: Let $(\mathcal{L}, \Sigma, \xi)$ be a state-property system. Let $\mathcal{L}_0 \subset \mathcal{L}$ and $\mu: \Sigma \times \mathcal{L}_0 \to [0,1]$ satisfy the assumptions (Oi)–(Oiii). *Then*

(i) *$\mu_p(a) \leqslant \mu_p(b)$ for every $p \in \Sigma$ implies $a \leqslant b$.*
(ii) *$\mu_p(a) = \mu_p(b)$ for all $p \in \Sigma$ if and only if $a=b$.*
(iii) *For every $a \in \mathcal{L}_0$ there is a unique element $a' \in \mathcal{L}_0$ such that $\mu_p(a)+\mu_p(a')=1$ for all $p \in \Sigma$. Moreover, the mapping $a \mapsto a'$ is an orthocomplementation in $\mathcal{L}_0$, i.e.,* (1) *$a \leqslant b \Rightarrow b' \leqslant a'$,* (2) *$a'' := (a')' = a$,* (3) *$a \vee_0 a' = I$, $a \wedge_0 a' = 0$, where $\vee_0$ and $\wedge_0$ denote the supremum and infimum in $\mathcal{L}_0$, respectively.*
(iv) *For every sequence $(a_i)_{i=1}^{\infty}$ of mutually orthogonal elements in $\mathcal{L}_0$, their supremum $a = \vee_{0\, i=1}^{\infty} a_i$ exists in $\mathcal{L}_0$, and coincides with the supremum of $(a_i)_{i=1}^{\infty}$ in $\mathcal{L}$.*

Proof: (i) If $\mu_p(a) \leqslant \mu_p(b)$ for every $p \in \Sigma$, then $\mu_p(a)=1 \Rightarrow \mu_p(b)=1$, hence by (Oi), $a \in \xi(p) \Rightarrow b \in \xi(p)$, which implies $a \leqslant b$.

(ii) Follows by (Oii) and (i).

(iii) Let $a \in \mathcal{L}_0$, and consider the sequence $(a_i)_{i=1}^{\infty}$ where $a_1=a$, $a_i=0$, $i=2,3,\ldots$. By (Oiii), there is $b \in \mathcal{L}_0$ such that $\mu_p(b)+\mu_p(a)=1$ for all $p \in \Sigma$, i.e., $\mu_p(b)=1-\mu_p(a)$ for all $p \in \Sigma$. Hence we may put $a'=b$. By (ii), a' is uniquely defined. Now we prove that $a \mapsto a'$ is an orthocomplementation.

(1) $a \leqslant b \Rightarrow \mu_p(a) \leqslant \mu_p(b)$ for all $p \in \Sigma$, which implies $\mu_p(b')=1-\mu_p(b) \leqslant 1-\mu_p(a)=\mu_p(a')$ for all $p \in \Sigma$, which by (ii) entails $b' \leqslant a'$.

(2) $\mu_p((a')')=1-\mu_p(a')=1-(1-\mu_p(a))=\mu_p(a)$ for all $p \in \Sigma$, which entails $a''=a$.

(3) Let $c \in \mathcal{L}_0$ be such that $a \geqslant c, a' \geqslant c$. From $\mu_p(a)+\mu_p(a')=1$ and $\mu_p(a)=1$ iff $a \in \xi(p)$, it follows that $a \in \xi(p) \Rightarrow a' \notin \xi(p)$, and vice versa. Hence $a \in \xi(p)$ and $a' \in \xi(p)$ happen for no $p \in \Sigma$, which entails, by Definition 1, that $a \wedge a' = 0$ in $\mathcal{L}$. Since $0 \in \mathcal{L}_0$, the infimum of a and a' in $\mathcal{L}_0$ is 0.

Properties (1) and (2) imply de Morgan laws in $\mathcal{L}_0$: $a \vee_0 b$ exists, then $(a \vee_0 b)' = a' \wedge_0 b'$, and $(a \wedge_0 b)' = a' \vee_0 b'$ in the sense that if one side exists, so does the other, and they are equal. Therefore for every $a \in \mathcal{L}_0$, $a' \wedge_0 a'' = 0$ implies $(a' \wedge_0 a'')' = a \vee_0 a' = I$.

(iv) Let $(a_i)_{i=1}^{\infty}$ be a sequence of pairwise orthogonal elements of $\mathcal{L}_0$. Let b be the element from (Oiii). Put $a := b'$, then for every $p \in \Sigma$ we have $\mu_p(a) = \Sigma_{i=1}^{\infty} \mu_p(a_i)$. It follows that $\mu_p(a_i) \leqslant \mu_p(a)$ for all $i \in \mathbb{N}$, and for all $p \in \Sigma$. Hence a is an upper bound of $a_i, i=1,2,\ldots$. Let $c \in \mathcal{L}_0$ be

any other upper bound of $a_i, i=1,2,\ldots$. Then $a_i \leqslant c$ for all $i$implies that $c', a_1, a_2, \ldots$ are mutually orthogonal. By (Oiii), there is an element $d \in \mathcal{L}_0$ such that for every $p \in \Sigma$,

$$\mu_p(d) = \mu_p(c') + \sum_{i=1}^{\infty} \mu_p(a_i) = \mu_p(c') + \mu_p(a).$$

From this we obtain $\mu_p(c) = \mu_p(d') + \mu_p(a)$, which entails by (i) that $a \leqslant c$.

Let u be the supremum of $(a_i)_{i=1}^{\infty}$. The we have $\forall p \in \Sigma$, $u \in \xi(p)$ if and only if $a_i \in \xi(p)$ for some i. But then $u \in \xi(p)$ if and only if $a \in \xi(p)$, which entails that $u=a$. □

We will say that a set $\mathcal{F}$ of functions $f: L \to [0,1]$ defined on a partially ordered set L is *order determining* if $a \leqslant b \Leftrightarrow \forall f \in \mathcal{F}, f(a) \leqslant f(b)$.

Theorem 5: *Let* $(\mathcal{L}, \Sigma, \xi)$ *be a state-property system,* $\mathcal{L}_0 \subseteq \mathcal{L}$, *and let* $\mathcal{M} := \{\mu: \Sigma \times \mathcal{L}_0 \to [0,1]\}$ *satisfy conditions* (Oi)–(Oiii). *Then the set* L_0 *is a* σ*-orthomodular poset and the set* $\mathcal{M}$ *is order determining for* L_0. *Moreover, for every* $a \in L_0$, $a \neq 0$, *there is* $p \in \Sigma$ *such that* $\mu_p(a)=1$.

Proof: By definition, the set $\mathcal{L}_0$ with the ordering inherited from $\mathcal{L}$ is a partially ordered set. By Lemma 5, $\mathcal{L}_0$ is an orthocomplemented set such that the supremum of every pairwise orthogonal sequence exists in $\mathcal{L}_0$. Moreover, $\mathcal{M}$ is ordering for $\mathcal{L}_0$. Assume $a \leqslant b$, $a, b \in \mathcal{L}_0$. Then $\forall p \in \Sigma$, $\mu_p(a) \leqslant \mu_p(b)$ implies $\mu_p(a) + \mu_p(b') \leqslant 1$, so that $a \vee b'$ exists in $\mathcal{L}_0$ and $\mu_p(a \vee b') = \mu_p(a) + \mu_p(b')$ for all $p \in \Sigma$, which entails that $\mu_p(b) = \mu_p(a) + \mu_p(a' \wedge b)$ for all $p \in \Sigma$, hence $\mu_p(b) = \mu_p(a \vee (a' \wedge b))$ for all $p \in \Sigma$, so by Lemma 5(ii), $b = a \vee (a' \wedge b)$, which is the orthomodular law. Hence $\mathcal{L}_0$ is a σ-orthocomplete orthomodular poset.

Let $a \in \mathcal{L}$, $a \neq 0$, and assume that $\forall p \in \Sigma$, $a \notin \xi(p)$. Then the implication

$$\forall r \in \Sigma: a \in \xi(r) \Rightarrow 0 \in \xi(r)$$

holds, which by (5) of Definition 1 means that $a=0$, a contradiction. If $0 \neq a \in \mathcal{L}_0$, then $a \in \xi(p)$ for at least one $p \in \Sigma$ means that $\mu_p(a)=1$. □

From now on, we will write $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ to denote a state property system for which there is $\mathcal{L}_0 \subset \mathcal{L}$ with a system of functions $\mu_s, s \in \Sigma$ such that conditions (Oi), (Oii), and (Oiii) are satisfied.

Definition 6: Let $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be given. We will say that* μ_p *has a support* (*in* $\mathcal{L}_0$) *if there is an element* $b \in \mathcal{L}$ $(b \in \mathcal{L}_0)$ *such that* $\forall a \in \mathcal{L}_0$, $\mu_p(a)=1$ *iff* $b \leqslant a$.

Clearly, if a support exists, it is unique.

Proposition 4: Let $(\Sigma, \mathcal{L}, \xi)$ *be a state property system, satisfying condition* (A). *For* $p \in \Sigma$, *let* $a_p := \wedge\{a: a \in \xi(p)\}$. *Then* $a_p, p \in \Sigma$, *coincide with the atoms in* $\mathcal{L}$. *Moreover,* $a \in \xi(p)$ *if and only if* $a_p \leqslant a$.

Proof: Observe that condition (A) also implies condition

(A′) for all $p \in \Sigma$, the element $a_p = \wedge\{a: a \in \xi(p)\} \neq 0$.

Indeed, by Definition 1, $\wedge\{a: a \in \xi(p)\} \in \xi(p)$, and $0 \notin \xi(p)$. Hence $a_p \in \xi(p)$, and clearly, a_p is the smallest element in $\xi(p)$. Assume that $a_p \in \xi(r)$, $r \in \Sigma$. Now $a_p \leqslant a$ for all $a \in \xi(p)$ implies that $a \in \xi(r)$ for all $a \in \xi(p)$, hence $\xi(p) \subset \xi(r)$. By condition (A) then $p=r$.

Assume $b \leqslant a_p$, $b \neq 0$, then $\exists r, b \in \xi(r)$ and we have

$$\forall r \in \Sigma, b \in \xi(r) \Rightarrow a_p \in \xi(r) \Rightarrow a \in \xi(r) \; \forall \, a \in \xi(p),$$

$$\xi(p) \subset \xi(r) \Rightarrow p = r \Rightarrow b \in \xi(p) \Rightarrow a_p \leqslant b.$$

This proves that a_p is an atom in $\mathcal{L}$.

Now let a be an atom of $\mathcal{L}$. Then there is $r \in \Sigma$ with $a \in \xi(r)$, hence $a_r \leqslant a$. Since a_r is an atom, $a_r = a$. □

Notice that under conditions of Proposition 4, the element a_p is a support of μ_p.

Theorem 6: *Under the suppositions of* Proposition 4, $\mathcal{L}$ *is an atomistic lattice.*

Proof: Let $b \in \mathcal{L}$, put $c = \vee\{a_s: b \in \xi(s)\}$. Then clearly $c \leqslant b$, and if $b \in \xi(p)$, then $a_p \leqslant c$ im-

plies $c \in \xi(p)$, therefore $b=c$. □

Theorem 7: *Let* $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be a state property system satisfying condition* (A) *and*

(B) *For every* $s \in \Sigma$, a_s *belongs to* $\mathcal{L}_0$.
(C) *For every* $b \in \mathcal{L}$, $b = \wedge\{a'_s : b \leqslant a'_s\}$.

Then $\mathcal{L}$ *with the mapping* $b' := \vee\{a_s : b \leqslant a'_s\}$ *is a complete, atomistic, orthocomplemented lattice.*

Proof: Owing to Theorem 6, it suffices to prove that $\mathcal{L}$ is orthocomplemented. (i) If $b \leqslant c$, then $\{a_s : c \leqslant a'_s\} \subset \{a_s : b \leqslant a'_s\}$, which by (C) implies $c' \leqslant b'$. (ii) From $b' \leqslant a'_s$ iff $a_s \leqslant b$ we obtain that $(b')' = \vee\{a_s : b' \leqslant a'_s\} = \vee\{a_s : a_s \leqslant b\} = b$. It remains to prove that $b \wedge b' = 0$. Assume that $a_s \leqslant b, a_s \leqslant b'$. By (i) and (ii), $a_s \leqslant b \leqslant a'_s$, which contradicts (B), so $b \wedge b' = 0$. By duality we get $b \vee b' = I$. □

Definition 7: Let $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be given. We will say that* p *is orthogonal to* q, $p, q \in \Sigma$, *if there is* $a \in \mathcal{L}_0$ *such that* $\mu_p(a) = 1$ *and* $\mu_q(a) = 0$ (*equivalently*, $p \perp q$ *if* $a \in \xi(p)$, $a' \in \xi(q)$). *If* p *is orthogonal to* q *we will write* $p \perp q$.

It is obvious that the relation $\perp$ is symmetric and antireflexive. For $T \subset \Sigma$, we put $T' = \{p \in \Sigma : p \perp T\}$, where $p \perp T$ means that $p \perp t$ for all $t \in T$. Clearly, $\emptyset' = \Sigma$, $T \subseteq T''$ and $T_1 \subset T_2$ implies $T'_1 \supset T'_2 \forall T_1, T_2 \subset \Sigma$. If $s, p \in \Sigma$ have supports in $\mathcal{L}_0$, then $s \perp p$ if and only if their supports are orthogonal.

Denote by $\bar{T}^0$ the set of all $s \in \Sigma$ such that $\forall a \in \mathcal{L}_0$, $a \in \xi(t) \forall t \in T \Rightarrow a \in \xi(s)$. That is, $\bar{T}^0$ is the set of all superpositions of $T \subset \Sigma$ with respect to $\mathcal{L}_0$. Equivalently, $\bar{T}^0 = \{s \in \Sigma : \forall a \in \mathcal{L}_0, a_t \leqslant a \Rightarrow a_s \leqslant a\}$. Clearly, $\bar{T} \subset \bar{T}^0$.

Proposition 5: Let $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be a state property system satisfying conditions* (A), (B), (C). *Then for every* $T \subset \Sigma$, $\bar{T} = \bar{T}^0$.

Proof: It suffices to prove that $\bar{T}^0 \subset \bar{T}$. We have $s \in \bar{T}^0$ iff $\forall a \in \mathcal{L}_0$, $a_t \leqslant a \forall t \in T \Rightarrow a_s \leqslant a$. Let us take $b \in \mathcal{L}$, and assume that $a_t \leqslant b \forall t \in T$. By property (C), $b = \wedge\{a'_r : b \leqslant a'_r\}$, which yields $a_t \leqslant a'_r$ for all $t \in T$ and r such that $b \leqslant a'_r$. From $s \in \bar{T}^0$we obtain that $a_s \leqslant a'_r$ for all corresponding r, and therefore $a_s \leqslant \wedge\{a'_r : b \leqslant a'_r\} = b$. In other words, $\vee_{t \in T} \xi(t) \subset \xi(s)$, hence $s \in \bar{T}$. □

Proposition 6: Let $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$. *Suppose that* (A), (B) *are satisfied. Then for any* $T \subset \Sigma$ *we have* $T'' = \bar{T}^0$.

Proof: We follow the proof of Ref. 55, Proposition 3.3.15. We will identify μ_s with $s \in \Sigma$ and write $T(a) = k$ if $\mu_t(a) = k \forall t \in T$. First we show that $T' = \emptyset$ if and only if $\{a \in \mathcal{L}_0 : T(a) = 1\} = \{1\}$. Assume that $T' = \emptyset$ and let $a \in \mathcal{L}_0$ be such that $a \neq 1$ and $T(a) = 1$. Since $a' \neq 0$, there is $p \in \Sigma$ such that $p(a') = 1$. But then $p(a) = 0$, so that $a \in T'$, a contradiction. Now assume that $\{a \in \mathcal{L}_0 : T(a) = 1\} = \{1\}$ and also that $p \in T'$. Then for the supports we have $a_p \perp a_t \forall t \in T$. Hence $t(a'_p) = 1$ for all $t \in T$, which is again a contradiction.

To prove the equality $T'' = \bar{T}^0$, assume first that $T' = \emptyset$. We have already proved that then $\{a \in \mathcal{L}_0 : T(a) = 1\} = \{1\}$, which implies $\bar{T}^0 = \Sigma = T''$.

Assume that $T' \neq \emptyset$ and also that $p \in \bar{T}^0$. We will show that $p \in T''$. Assume that $q \in T'$, then $a_q \perp a_t \forall t \in T$, and hence $T(a'_q) = 1$. This implies $a'_q \in \cap_{t \in T} \xi(t)$, which implies that $a'_q \in \xi(p)$. This implies $q \perp p$, which implies that $\bar{T}^0 \subset T''$.

Assume that $p \in T''$ and also that $T(a) = 1$ for some $a \in \mathcal{L}_0$. Without loss of generality we may assume that $a \neq 1$. We have $a_q \leqslant a'$ iff $q(a') = 1$. But $q(a') = 1$ implies that $q \in T'$. This means that $q \perp p$, and so $a_p \perp a_q$ for all q such that $q(a') = 1$. Hence $a_q \leqslant a'$ implies $a_q \leqslant a'_p$, so that $a' \leqslant a'_p$, so that $p(a) = 1$. This shows that $p \in \bar{T}^0$ and this completes the proof. □

As a corollary of Propositions 5 and 6, we obtain the following.

Corollary 1: Let $(\Sigma, \mathcal{L}, \mathcal{L}_0 \xi)$ *be a state property system satisfying* (A), (B), (C). *Then for every* $T \subset \Sigma$, $\bar{T} = T''$.

Theorem 8: *Let* $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be a state property system satisfying* (A), (B). *Define* $\mathcal{F}^0(\Sigma) := \{S \subset \Sigma : S = \bar{S}^0\}$. *Then the mapping* $S \mapsto S'$ *is an orthocomplementation on* $\mathcal{F}^0(\Sigma)$. *Consequently,* $\mathcal{F}^0(\Sigma)$ *is a complete, atomistic, orthocomplemented lattice. If also* (C) *holds, then* $S \mapsto S'$ *is an orthocomplementation on* $\mathcal{F}(\Sigma)$, *and* $\mathcal{F}(\Sigma)$ *is a complete, atomistic, orthocomplemented lattice.*

Proof: It is easy to check that $S \mapsto \bar{S}^0$ is a closure operation, and hence $\mathcal{F}^0(\Sigma)$ is a complete lattice with lattice operations $S \wedge T = S \cap T$ and $S \vee T = (S \cup T)^{-0}$. Owing to property (A), $\mathcal{F}^0(\Sigma)$ is atomistic. To prove orthocomplementation, observe that $S \subset T \Rightarrow T' \subset S'$ and $S \wedge S' = \emptyset$ follow directly from the definition of the mapping $S \mapsto S'$. Property $S'' = S$ for $S \in \mathcal{F}^0(\Sigma)$ follows from Proposition 6. The remaining statement follows from Corollary 1. □

Definition 8: Suppose that $(\Sigma, \mathcal{L}, \xi)$ *is a state property system. The map* $\kappa: \mathcal{L} \to \mathcal{P}(\Sigma)$ *defined by*

$$\kappa(a) = \{p \in \Sigma : a \in \xi(p)\} \tag{16}$$

is called the Cartan map.

According to Ref. 46, Proposition 5, $\kappa: \mathcal{L} \to (\kappa(\mathcal{L}), \subset, \cap)$ has the following properties:

$$\kappa(1) = \Sigma, \tag{17}$$

$$\kappa(0) = \emptyset, \tag{18}$$

$$a \leqslant b \Leftrightarrow \kappa(a) \subset \kappa(b), \tag{19}$$

$$\kappa\left(\bigwedge_i a_i\right) = \bigcap_i \kappa(a_i). \tag{20}$$

That is, κ is an isomorphism of complete lattices. Moreover, by Ref. 46, Theorem 2, $\{\kappa(a) : a \in \mathcal{L}\}$ is an intersection system. Consequently, the operator $\mathrm{cl}: Y \mapsto \cap\{\kappa(a) : Y \subset \kappa(a)\}$ is a closure operator.[56]

The next lemma shows that $\kappa(a)$ is closed under superpositions.

Lemma 6: Let $(\Sigma, \mathcal{L}, \xi)$ *be a state property system. For all* $a \in \mathcal{L}$, $\kappa(a) \in \mathcal{F}(\Sigma)$.

Proof: For every $a \in \mathcal{L}$ we have $\kappa(a) \subset \kappa(a)^-$. Observe that $p \in \kappa(a) \Leftrightarrow a \in \xi(p)$. Let $s \in \bar{\kappa}(a)$, then $\cap_{p \in \kappa(a)} \xi(p) \subset \xi(s)$ implies $a \in \xi(s)$, which means that $s \in \kappa(a)$. □

Proposition 7: Let $(\Sigma, \mathcal{L}, \xi)$ *be a state property system such that condition* (A) *is satisfied. Then* $\kappa(\mathcal{L})$ *and* $\mathcal{F}(\Sigma)$ *are isomorphic as complete atomistic lattices*.

Proof: By Lemma 6, the range of κ is in $\mathcal{F}(\Sigma)$. By Ref. 46, Proposition 5, $\kappa(\mathcal{L})$ and $\mathcal{F}(\Sigma)$ are isomorphic as complete lattices. Let $a \in \mathcal{L}$ be an atom. By definition, $\kappa(a) = \{p \in \Sigma : a \in \xi(p)\}$. By (A), $a \in \xi(p)$ iff $a_p \leqslant a$, hence $a_p = a$ because a is an atom. By (A) we may conclude that $\kappa(a) = \{p\}$. □

Theorem 9: *Let* $(\Sigma, \mathcal{L}, \mathcal{L}_0, \xi)$ *be a state property system satisfying* (A), (B). *Then the mapping* $\kappa: \mathcal{L}_0 \to \mathcal{F}(\Sigma)$, $a \mapsto \kappa(a)$ *has the following properties*:

(i) *If* $a \wedge b$ *exists in* $\mathcal{L}_0$, *then* $\kappa(a \wedge b) = \kappa(a) \wedge \kappa(b)$.
(ii) *For all* $a \in \mathcal{L}_0$, $\kappa(a') = \kappa(a)'$.

Consequently, $\kappa(\mathcal{L}_0)$ *and* $\mathcal{L}_0$ *are isomorphic as atomistic* σ*-orthomodular posets*.

If also condition (C) *is satisfied*, *then* $\kappa(\mathcal{L})$ *and* $\mathcal{F}(\Sigma)$ *are isomorphic as complete*, *atomistic orthocomplemented lattices*.

Proof: (i) Suppose that $a \wedge b$ exists in $\mathcal{L}_0$. Obviously, $\kappa(a \wedge b) \leqslant \kappa(a) \wedge \kappa(b)$. Suppose that $s \in \kappa(a) \wedge \kappa(b) = \kappa(a) \cap \kappa(b)$. This gives $a, b \in \xi(s)$, hence $a_s \leqslant a, a_s \leqslant b$, consequently $a_s \leqslant a \wedge b$, i.e., $s \in \kappa(a \wedge b)$.

(ii) Assume that $p \in \kappa(a)'$, where $a \in \mathcal{L}_0$ with $0 < a < 1$. Then $p \perp q$ for all $q \in \kappa(a)$. It follows that $\forall q \in \kappa(a)$, $a_q \leqslant a'_p$. Hence $a_p \leqslant (\vee_{q \in \kappa(a)} a_q)' = a'$. This proves $\kappa(a)' \leqslant \kappa(a')$.

Now let $p \in \kappa(a')$, then $a_p \leqslant a' = (\vee\{a_q : a_q \leqslant a\})'$, hence $a_p \leqslant a'_q$ for all $q \in \kappa(a)$, which entails $p \in \kappa(a)'$.

The rest follows by Proposition 7. □

IV. SUPERPOSITION PRINCIPLE AND SECTORS

Let $(\mathcal{L},\Sigma,\xi)$ be a state property system such that property (A) and 3-MSP are satisfied. By Theorem 1, $(\Sigma,*)$, where $p*s=\lambda\{p,s\}=\{p,s\}^-$ is a projective geometry.

Definition 9: We will say that a superposition principle (SP, *for short*) *is satisfied in* $(\mathcal{L},\Sigma,\xi)$, *if for every* $p,q\in\Sigma$, $p\neq q$, *there is* $r\in\{p,q\}^-$ *such that* $r\neq p,r\neq q$.

The following statement is straightforward.

Theorem 10: *Let* $(\mathcal{L},\Sigma,\xi)$ *be a state property system such that* (A), 3-MSP *and* SP *are satisfied. The* $(\Sigma,*)$ *is an irreducible projective geometry*.

The notion of a sector was introduced in Ref. 67 (see also Ref. 55, Definition 3.2.7). Roughly speaking, a sector is a maximal λ-closed subset of Σ in which SP holds.

Definition 10: A nonempty subset $S\subset\Sigma$ *is called a sector if the following conditions hold*:

(i) $S\in\mathcal{L}(\Sigma)$;
(ii) *for any two different* $p,q\in S$ *we can find* $r\in\{p,q\}^-$ *distinct from* p *and* q;
(iii) *if* $q\in\Sigma\backslash S$, *then* $\{p,q\}^-=\{p,q\}$ *for every* $p\in S$.

A basic property of sectors is the following.

Lemma 7: If S,P *are sectors, then either* $S=P$ *or* $S\cap P=\emptyset$.

Proof: Assume that $S\neq P$. Then there is $q\in S\backslash P$ (or $q\in P\backslash S$), and by (ii) of Definition 10, $\{s,q\}^-\neq\{s,q\}$ whenever $s\in S\cap P$, while by (iii) of Definition 10, $\{s,q\}^-=\{s,q\}$. This contradiction implies that $S\cap P=\emptyset$. □

Theorem 11:[55] *Let* $(\mathcal{L},\Sigma,\xi)$ *be a state property system such that* (A) *and* 3-MSP *are satisfied. Then* Σ *can be written as a set theoretical union of sectors*.

Proof: Let us define a binary relation $\approx$ on Σ as follows: (i) for every $s\in\Sigma$, $s\approx s$, (ii) for distinct $s,t\in\Sigma$, $s\approx t$ if there is $r\in\{s,t\}^-$, $r\neq s,r\neq t$. We will prove that $\approx$ is an equivalence relation. Reflexivity and symmetry are clear from the definition. To prove transitivity, assume that $p\approx r$ and $r\approx s$. With no loss of generality, we may assume that p,r,s are mutually different. Let $x\in\{p,r\}^-\backslash\{p,r\}$, $y\in\{r,s\}^-\backslash\{r,s\}$. By 2-MSP we have $\{p,r\}^-=\{p,x\}^-=\{r,x\}^-$, $\{r,s\}^-=\{r,y\}^-=\{s,y\}^-$. Moreover, $r\in\{x,p\}^-$ implies $y\in\{x,p,s\}^-=\lambda\{x,p,s\}\subset S$ by 3-MSP. If $y\in\{p,s\}^-$ and $y\neq p$, then y is a minimal superposition of $\{p,s\}$, and hence $p\approx s$. If $y=p$, then $p\in\{r,s\}^-$ implies $r\in\{s,p\}^-$, hence $p\approx s$. If $y=x$, then $\{r,x\}^-=\{r,y\}^-$implies $\{p,r\}^-=\{r,s\}^-$, $p\in\{r,s\}^-$, hence $r\in\{s,p\}^-$ and $p\approx s$. Finally, if y is a minimal superposition, then $\{y,x\}^-\cap\{p,s\}^-\neq\emptyset$ implies that $p\approx s$.

Let $\hat{s}$ denote the equivalence class containing $s\in\Sigma$. We may write $\Sigma=\cup\{\hat{s}:s\in\Sigma\}$. It can be easily seen that $\hat{s}$ is a sector for every $s\in\Sigma$. □

Sectors can be characterized by the closure operator λ as follows.

Theorem 12: *Let* $(\mathcal{L},\Sigma,\xi)$ *be a state property system such that* (A) *and* 3-MSP *are satisfied. Let* $\Sigma=\cup_i S_i$, *where* $S_i\in\mathcal{L}(\Sigma)$ *and* (SP) *is satisfied on* S_i, $\forall i$. *Then* S_i *are sectors if and only if they are* λ*-clopen sets*.

Proof: By Theorem 11, Σ can covered by sectors, which are λ-closed. Let S be a sector. To prove that S is clopen, it suffices to prove that $\Sigma\backslash S$ is λ-closed. Assume that $p,q\in\Sigma\backslash S$ and let r be a minimal superposition of p,q. If $r\in S$, then by 2-MSP, $p\in\lambda\{r,q\}$. Since $r\in S$ and $q\notin S$, and S is a sector, we have $\lambda\{r,q\}=\{r,q\}$, which is a contradiction. Therefore $r\in\Sigma\backslash S$. This proves that sectors are λ-clopen sets.

Conversely, let S be a λ-clopen set such that SP is satisfied on S. Then conditions (i) and (ii) of Definition 10 are satisfied. To prove (iii), assume that $p\in S,q\notin S$, and $r\in\{p,q\}^-$, $r\neq p,q$, then either $r\in S$ or $r\notin S$. If $r\in S$, we get $q\in\{r,p\}^-$, which contradicts the supposition that S is λ-closed. If $r\notin S$, we get $p\in\{r,q\}^-$, which contradicts the supposition that S is open. It follows that $\{p,q\}^-=\{p,q\}$, hence S is a sector. □

Definition 11: We say that an element $a\in\mathcal{L}$ *is classical* (*or a superselection rule*) *if there is an element* $a'\in\mathcal{L}$ *such that for every* $s\in\Sigma$, $a\in\xi(s)\Leftrightarrow a'\notin\xi(s)$.

Clearly, 0 and 1 are classical elements.

Theorem 13: *Let $a \in \mathcal{L}$ be a classical element. Then $\kappa(a)=\{s \in \Sigma : a \in \xi(s)\}$ is a clopen set in $\mathcal{F}(\Sigma)$.*

Proof: We have $\Sigma=\{s:a \in \xi(s)\} \cup \{s:a' \in \xi(s)\}$. By symmetry, it suffices to prove that $S := \{s:a \in \xi(s)\}$ belongs to $\mathcal{F}(\Sigma)$. It easily follows from the fact that $r \in \bar{S}$ iff $\cap\{\xi(s):s \in S\} \subset \xi(r)$, which entails that if $a \in \xi(s)\, \forall\, s \in S$, then $a \in \xi(r)$, hence $r \in S$. □

From the fact that $\mathcal{F}(\Sigma) \subset \mathcal{L}(\Sigma)$, we obtain that $\kappa(a)$ is clopen also in $\mathcal{L}(\Sigma)$.

We recall that an element z in a lattice L with 0 and 1 is *central* when there exist two lattices L_1 and L_2 and an isomorphism between L and the direct product $L_1 \times L_2$ such that z corresponds to the element $(1_1, 0_2) \in L_1 \times L_2$. [cf., e.g., Ref. 68, Definition (4.12).] Evidently 0 and 1 are central elements.

Lemma 8: [Reference 68, Theorem (4.13)] *An element z of a lattice L with* 0 *and* 1 *is central if and only if there is an element z' in L such that*

$$a = (a \wedge z) \vee (a \wedge z') = (a \vee z) \wedge (a \vee z') \text{ for every } a \in L. \tag{21}$$

If L is orthocomplemented, then z is central if and only if the first equality in (21) *is satisfied for every $a \in L$* ([Ref. 68, Lemma (29.9)]).

Theorem 14: *Let $(\mathcal{L}, \mathcal{L}_0, \Sigma, \xi)$ be a state-property system such that conditions* (A), (B), (C) *are satisfied. Then an element $c \in \mathcal{L}$ is central if and only if c is classical.*

Proof: If properties (A), (B), (C) are satisfied, then $\mathcal{L}$ is a complete, atomistic, orthocomplemented lattice, and $\kappa: \mathcal{L} \to \mathcal{F}(\Sigma)$ is an isomorphism (Theorem 9).

Let c be a central element of L, then by (21), for every atom $a \in \mathcal{L}$, $a=(a \wedge c) \vee (a \wedge c')$, hence either $a=a \wedge c$, or $a=a \wedge c'$. By Proposition 7, $\kappa(a)=\{s\}$ for some $s \in \Sigma$. Moreover, $\kappa(a) = \kappa(a \wedge c) \vee \kappa(a \wedge c')$, hence either $\kappa(a \wedge c)=\{s\}$, or $\kappa(a \wedge c')=\{s\}$, that is, either $c \in \xi(s)$ or $c' \in \xi(s)$. This entails that c is classical.

Conversely, if c is classical, i.e., for every $s \in \Sigma$, either $s \in \kappa(c)$ or $s \in \kappa(c')$, then for every $a \in \mathcal{L}$,

$$\begin{aligned} a &= \vee\{a_s : s \in \kappa(a)\} = \vee\{a_s : s \in \kappa(a) \cap \kappa(c)\} \vee \vee\{a_s : s \in \kappa(a) \cap \kappa(c')\} \\ &= \vee\{a_s : s \in \kappa(a \wedge c)\} \vee \vee\{a_s : s \in \kappa(a \wedge c')\}, \end{aligned}$$

and consequently, $a=(a \wedge c) \vee (a \wedge c')$. By Lemma 8, c is central element of $\mathcal{L}$. □

V. CLOSED SUBSPACES AND MACKEY PROPERTY

Throughout this section we will use the following notations:

$$\text{For any } A, B \in \mathcal{L}(\Sigma), A \sqcup B := \lambda(A \cup B). \tag{22}$$

$$\text{For any } A, B \in \mathcal{F}(\Sigma), A \vee B := (A \cup B)^{-}. \tag{23}$$

For infima in both $\mathcal{L}(\Sigma)$, $\mathcal{F}(\Sigma)$ we use the same notation $A \wedge B (= A \cap B)$.

In Ref. 56, the following definitions were introduced, and the equivalence of the following three categories was proved.

Definition 12: A Mackey geometry is a projective geometry G together with a subset $\mathcal{S}$ of subspaces of G satisfying the following axioms:

(i) *$\mathcal{A} \subseteq \mathcal{S}$ implies $\cap \mathcal{A} \in \mathcal{S}$ (hence $\mathcal{S}$ is an intersection system)*,
(ii) *$\emptyset \in \mathcal{S}$*,
(iii) *if $E \in \mathcal{S}$, then $a \vee E \in \mathcal{S}$ for every $a \in G$.*

The elements of $\mathcal{S}$ are called the closed subspaces of G. An isomorphism of Mackey geometries is an isomorphism of projective geometries $g: G_1 \to G_2$ satisfying $S \in \mathcal{S}_1$ iff $g(E) \in \mathcal{S}_2$ (where E is any subspace of G_1).

Definition 13: A Mackey lattice is a projective lattice L together with an operator $x \to c(x)$

satisfying the following axioms:

(i) $x \leqslant c(x)$ *for every* $x \in L$,
(ii) $x \leqslant c(y)$ *implies* $c(x) \leqslant c(y)$,
(iii) $c(0)=0$,
(iv) *if* $x=c(x)$, *the* $a \vee x = c(a \vee x)$ *for every atom* a *in* L.

An element $x \in L$ *is closed if* $x=c(x)$. *An isomorphism of Mackey lattices is an isomorphism of* (*projective*) *lattices* $h: L_1 \to L_2$ *satisfying* $h(c_1(x))=c_2(h(x))$ *for every element* $x \in L_1$.

For any lattice L we shall denote by A_L the set of all atoms of L. We say that a lattice L has the *intersection property* (cf. [Ref. 56, Definition 2.5.1]) if one has

$$a,b \in A_L, a \neq b, x \in L \text{ and } a \leqslant b \vee x \Rightarrow \exists\, c \in A_L \text{ with } c \leqslant (a \vee b) \wedge x. \tag{24}$$

If L is an atomistic lattice, the following conditions are equivalent:

(1) L is upper and lower semimodular. A lattice L is called *upper semimodular* if $u \wedge v \lessdot v$ implies $u \lessdot u \vee v$, and L is *lower semimodular* if $u \lessdot u \vee v$ implies $u \wedge v \lessdot v$. Here $a \lessdot b$ means that b covers a.
(2) L has the covering property. A lattice L has the *covering property* if for $x \in L$ and any atom $a \in L$ one has, $a \wedge x = 0 \Rightarrow x \lessdot a \vee x$.
(3) L has the intersection property.

Moreover, the implications $1 \Rightarrow 2 \Rightarrow 3$ hold for any lattice.

Definition 14: An intersection lattice is a complete atomistic lattice C having the intersection property. (*Equivalently*, *C is both upper and lower semimodular.*)

Let L_1 and L_2 be Mackey lattices. We say that a morphism $f: L_1 \to L_2$ is *continuous* if

$$f(c_1(x)) \leqslant c_2(f(x)) \text{ for every } x \in L_1. \tag{25}$$

Theorem 15: [Reference 56, Theorem 13.3.8] *The categories of Mackey geometries*, *of Mackey lattices and of intersection lattices are equivalent. This means that one has a functor* $\mathcal{L}$ *from Mackey geometries to Mackey lattices*, *a functor* $\mathcal{C}$ *from Mackey lattices to intersection lattices*, *a functor* $\mathcal{G}$ *from intersection lattices to Mackey geometries*, *and natural isomorphisms* $G \cong \mathcal{G}(\mathcal{C}(\mathcal{L}(G)))$, $L \cong \mathcal{L}(\mathcal{G}(\mathcal{C}(L)))$ *and* $C \cong \mathcal{C}(\mathcal{L}(\mathcal{G}(C)))$.

In our setting, we obtain the following result.

Theorem 16: *Let* $(\mathcal{L}, \mathcal{L}_0, \Sigma, \xi)$ *satisfy properties* (A), (B), (C) *and* 3-MSP. *Then* $\mathcal{L}(\Sigma)$ *with the closure operation* $c(A)=\bar{A}$, $A \in \mathcal{L}(\Sigma)$, *is a Mackey lattice*.

Proof: (cf. Ref. 55, Proposition 3.3.18). Properties (i)–(iii) of Definition 13 are clear. We have to prove only property (iv).

By Theorem 8, $\mathcal{F}(\Sigma)$ is a complete, atomistic, orthocomplemented lattice with the orthocomplementation $S \mapsto S'$. We will use the fact that $\mathcal{L}(\Sigma) \supset \mathcal{F}(\Sigma)$, and $\mathcal{L}(\Sigma)$ is modular (Theorem 2). We must show that if $S \in \mathcal{F}(\Sigma)$ and $p \in \Sigma \backslash S$, $p \vee S = p \sqcup S$. Modularity of $\mathcal{L}(\Sigma)$ implies that $S \prec S \sqcup p$ (that is, $S \sqcup p$ covers S). Dually, $(S \sqcup p)' = S' \wedge \{p\}' \prec S'$. Then there is an atom $q \in \Sigma$ such that $(S \sqcup \{p\})' \sqcup \{q\} = S'$. Then $((S \sqcup \{p\})' \sqcup \{q\})' = S'' = S \prec (S \sqcup \{p\})''$. This entails $(S \sqcup \{p\})'' = S \vee \{p\} = S \sqcup \{p\}$. □

Corollary 2: If $(\mathcal{L}, \mathcal{L}_0, \Sigma, \xi)$ *satisfy properties* (A), (B), (C) *then for every* $S \in \mathcal{F}(\Sigma)$ *and a finite dimensional element* $P=\{p_1, \ldots, p_n\}^-$, *we have* $S \vee P = S \sqcup P$.

In accordance with Theorems 15 and 16, if a state property system $(\mathcal{L}, \Sigma, \xi)$ satisfies conditions (A), (B), (C) and 3-MSP, we may consider Σ with elements of $\mathcal{F}$ as closed subspaces as Mackey geometry, $\mathcal{L}(\Sigma)$ with the operator $S \to \bar{S}$ as a Mackey lattice, and $\mathcal{F}(\Sigma)$) as intersection lattice. Indeed, by Theorem 16, $\mathcal{L}(\Sigma)$ with the operation $S \mapsto \bar{S}$ is a Mackey lattice. By Ref. 56, Proposition 13.2.7, the set $\mathcal{F}(\Sigma)$ is an intersection lattice for the induced order. The infimum of any subset $\mathcal{A} \subset \mathcal{F}(\Sigma)$ is the element $\wedge \mathcal{A}$ and the supremum is $\vee \mathcal{A} = (\sqcup \mathcal{A})^-$. Moreover, the atoms of $\mathcal{F}(\Sigma)$are the atoms of $\mathcal{L}(\Sigma)$, that is, elements of Σ. Further, $\mathcal{F}(\Sigma)$ being an intersection lattice, the set of all atoms Σ of $\mathcal{F}(\Sigma)$ is a projective geometry (cf. Ref. 56, 2.5.7 and Theorem 1), and the set

of closure subspaces coincides with the sets $\{F \subset \Sigma : F \in \mathcal{F}(\Sigma)\}$ as closed subspaces. Owing the isomorphism between $\mathcal{F}(\Sigma)$ and $\mathcal{L}$, the lattice $\mathcal{L}$ can be considered as an intersection lattice with the atoms $\{a_s \in L : s \in \Sigma\}$.

In the sequel, we will need the following definition.

Definition 15: [Reference 56, Definition 13.4.6] *A Mackey lattice L is called regular if for every closed element $x \in L$ and every atom $a \not\leqslant x$, there exists a closed coatom $h \in L$ such that $x \leqslant h$ and $a \not\leqslant h$.*

VI. ORTHOGEOMETRIES, ORTHOLATTICES AND ORTHOSYSTEMS

Definition 16: [Reference 56, Definition 14.1.1] *An orthogeometry is a projective geometry with a relation $\perp$, called orthogonality, which satisfies the following axioms*:

(1) (O_1) *$a \perp b$ implies $b \perp a$,*
(2) (O_2) *if $a \perp p$, $b \perp p$ and $c \in a * b$, then $c \perp p$,*
(3) (O_3) *if $a, b, c \in G$ and $b \neq c$, then there is $p \in b * c$ with $p \perp a$,*
(4) (O_4) *for every $a \in G$ there exists $b \in G$ with $a \not\perp b$.*

An isomorphism of orthogeometries is an isomorphism of projective geometries $g : G_1 \to G_2$ satisfying $a \perp b$ iff $ga \perp gb$.

For any subset $A \subseteq G$ the *orthogonal set* $A^{\perp} := \{x \in G : x \perp a$ for every $a \in A\}$ is a subspace of G by condition (O_2). A point a of an orthogeometry G is called a *null point* if $a \in a^{\perp}$. The geometry is called *non-null* if it contains a non-null point and *pure* if every point is non-null [Ref. 56, Definition 14.1.7].

Definition 17: An ortholattice (please do not mistake it with orthocomplemented lattice, which is sometimes also called ortholattice) *is a projective lattice together with an operator $x \mapsto x^{\perp}$ which satisfies the following conditions*:

(1) $x \leqslant x^{\perp\perp}$ *for every* $x \in L$,
(2) $x \leqslant y$ *implies* $y^{\perp} \leqslant x^{\perp}$,
(3) $0^{\perp\perp} = 0$,
(4) *if* $x = x^{\perp\perp}$, *then* $a \vee x = (a \vee x)^{\perp\perp}$ *for every atom* $a \in L$.

An isomorphism of ortholattices is an isomorphism of lattices $f : L_1 \to L_2$ such that $f(x^{\perp}) = (fx)^{\perp}$ for every element $x \in L_1$.

Proposition 8: If L is an ortholattice, then L together with the operator $c(x) := x^{\perp\perp}$ is a regular Mackey lattice.

Definition 18: An orthosystem is an intersection lattice C together with an operator $x \mapsto x'$ satisfying the following conditions:

(1) $x = x''$ *for every* $x \in C$,
(2) $x \leqslant y$ *implies* $y' \leqslant x'$.

An isomorphism of orthosystems is an isomorphism of lattices $h : C_1 \to C_2$ such that $h(x') = (hx)'$ for every $x \in C_1$.

By Ref. 56, Remark 14.2.7, instead of an intersection lattice it is enough to require that C is a complete atomistic lattice satisfying the exchange property.

In Ref. 56, it is proved that there is a triple correspondence between orthogeometries and ortholattices and orthosystems [Ref. 56, Proposition 14.2.11]. We summarize the results in the next theorem.

Theorem 17:

(1) *If L is an orthogeometry, then the projective lattice $\mathcal{L}(G)$ together with the operator $E \mapsto E^{\perp}$ is an ortholattice* [Ref. 56, Proposition 14.2.5].
(2) *Let L be an ortholattice. Denote by $\mathcal{C}(L)$ the set of all closed element $x = x^{\perp\perp}$ of L. Then $\mathcal{C}(L)$ together with the operator $x \mapsto x^{\perp}$ is an orthosystem* (*for the induced order*) [Ref. 56, Proposition 14.2.8].

(3) *Let C be an orthosystem. Then the projective geometry* $\mathcal{G}(C)$ *consisting of the set* A_C *of all atoms of C and the operator* $*$, $a*b=\{c\in A_C: c\leqslant a\vee b\}$, *together with the relation* $a\perp b$ *iff* $a\leqslant b'$, *is an orthogeometry* [Ref. 56, Proposition 14.2.9].

Theorem 18: *Let* $(\mathcal{L},\mathcal{L}_0,\Sigma,\xi)$ *satisfy properties* (A), (B), (C) *and* 3-MSP. *Then* $\mathcal{F}(\Sigma)$ *is an orthosystem*.

Proof: By Theorems 16 and 15, $\mathcal{F}(\Sigma)$ is an intersection lattice. By Theorem 8, the mapping $S\mapsto S'$ is an orthocomplementation on $\mathcal{F}(\Sigma)$, which implies the desired result. □

Remark 1: If $(\mathcal{L},\mathcal{L}_0,\Sigma,\xi)$ *satisfies properties* (A), (B), (C) *and* 3-MSP *then, according to* Theorem 17, (Σ,λ) *is an orthogeometry and* $\mathcal{L}(\Sigma)$ *with the closed subspaces* $\mathcal{F}(\Sigma)$ *is an orthomodular lattice. Moreover, since* $\bar{S}=S''$, *in accordance with* Ref. 56, Proposition 14.2.4, $\mathcal{F}(\Sigma)$ *is a regular Mackey lattice*.

VII. REPRESENTATIONS IN VECTOR SPACES

Let V be any vector space over a field K. We emphasize that the dimension of V is arbitrary (possibly infinite) and K is allowed to be a skew field (often called division ring).

Proposition 9: [Reference 56, Proposition 2.1.6]. *Let V be any vector space. On* $V^*:=V\backslash\{0\}$ *one defines a binary relation as follows*: $x\sim y$ *iff* x,y *if* x,y *are linearly dependent. Since this is an equivalence relation, the quotient set* $\mathcal{P}(V):=V^*/\sim$ *is well defined and becomes a projective geometry if for any elements* $X,Y,Z\in\mathcal{P}(V)$ *one defines* $\ell(X,Y,Z)$ *iff* X,Y,Z *have linearly dependent representatives* x,y,z.

Theorem 19: *Let G be an irreducible projective geometry containing at least four independent points. Then there exists a (left) vector space V over a field K such that G is isomorphic to* $\mathcal{P}(V)$.

Definition 19: [Reference 56, Definition 14.1.5] *Let V be a vector space over K. A map*: $\Phi: V\times V\to K$ *is called a reflexive (or also symmetric) sesquilinear form if there exists an anti-isomorphism of fields* $\sigma: K\to K$ *such that the following axioms are satisfied:*

(1) $\Phi(x_1+x_2,y)=\Phi(x_1,y)+\Phi(x_2,y)$ *and* $\Phi(\lambda x,y)=\lambda.\Phi(x,y)$,
(2) $\Phi(x,y_1+y_2)=\Phi(x,y_1)+\Phi(x,y_2)$ *and* $\Phi(x,\mu y)=\Phi(x,y).\sigma(\mu)$;
(4) $\Phi(x,y)=0$ *iff* $\Phi(y,x)=0$.

A map $\Phi: V\times V\to K$ *is called a Hermitian form if there exists an involution* $\sigma: K\to K$, *i.e., an anti-isomorphism of order 2, such that the following axioms are satisfied*:

(1) $\Phi(x-1+x_2,y)=\Phi(x_1,y)+\phi(x_2,y)$ *and* $Phi(\lambda x,y)=\lambda.\Phi(x,y)$,
(4) $\Phi(x,y)=\sigma(\Phi(y,x))$ *for all* $x,y\in V$.

Obviously, these two axioms imply both (2) *and* (3). *Finally, we recall that the form* Φ *is nonsingular if* $\Phi(x,y)=0$ *for all* $y\in V$ *implies* $x=0$.

Proposition 10: [Ref. 56, Proposition 14.1.6] *If* $\Phi: V\times V\to K$ *is a nonsingular reflexive sesquilinear form, then the projective geometry* $\mathcal{P}(V)$ *together with the relation* $\perp$ *defined by* $[x]\perp[y]$ *iff* $\Phi(x,y)=0$ *is an orthogeometry.*

Definition 20: A point a of an orthogeometry G is called a null point if $a\in a^{\perp}$. *The orthogeometry is called non-null if it contains a non-null point and pure if every point is non-null.*

Let V be a pre-Hilbertian space over $\mathbb{R},\mathbb{C},\mathbb{H}$, then trivially the associated orthogeometry $\mathcal{P}(V)$ is pure.

Theorem 20: [Reference 56, Theorem 14.1.8] *Let V be a vector space of dimension* $\geqslant 3$ *over a field K, and suppose that* $\mathcal{P}(V)$ *together with the relation* $\perp$ *is an orthogeometry. Then there exists a nonsingular reflexive sesquilinear form* $\Phi: V\times V\to K$ *which induces the orthogonality* $\perp$ *in the sense of Proposition 10. Moreover, if* $\mathcal{P}(V)$ *is non-null, then* $\perp$ *can be induced by a (non-singular) Hermitian form.*

We call states $S:=\{s_1,\ldots,s_n\}$ in Σ *independent* if $\forall i$, $s_i\notin\lambda(S\backslash s_i)$.

Theorem 21: *Let* $(\mathcal{L},\Sigma,\xi)$ *be a state property system such that conditions* (A), SP, 3-MSP *are*

satisfied. Assume that there exist at least four independent states in Σ. *Then there is a field K and a vector space V over K such that the set* $\mathcal{L}(\Sigma)$ *of all linear subspaces of* Σ *is isomorphic to the lattice* $\mathcal{L}(V)$ *of all linear subspaces of V*.

Theorem 22: *Let* $(\mathcal{L},\Sigma,\xi)$ *be a state property system such that conditions* (A), (B),(C), SP, 3-MSP *are satisfied. Assume that there exist at least four independent states in* Σ. *Then there exists a field K, an involutive ant-automorphism* $^*:K\to K$, *a vector space V over K and a Hermitian form* $f:V\times V\to K$ *such that* $\mathcal{F}(\Sigma)$ *is orthoisomorphic to the set* $\mathcal{L}_f(V)$ *of all closed subspaces of V*.

(See Ref. 68 for the ideas of proof).

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On the ground state energy for a magnetic Schrödinger operator and the effect of the DeGennes boundary condition

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Motivated by the Ginzburg-Landau theory of superconductivity, we estimate in the semiclassical limit the ground state energy of a magnetic Schrödinger operator with De Gennes boundary condition and we study the localization of the ground states. We exhibit cases when the De Gennes boundary condition has strong effects on this localization. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218980]

I. INTRODUCTION

Let $\Omega \subset \mathbb{R}^2$ be an open bounded domain with regular boundary. Let us consider a cylindrical superconducting sample of cross section Ω. The superconducting properties are described by the minimizers (ψ,A) of the Ginzburg-Landau functional (cf. Refs. 1–3):

$$\mathcal{G}(\psi,A)=\int_{\Omega}\left\{|(\nabla-i\sigma\kappa A)\psi|^2+\sigma^2\kappa^2|\mathrm{curl}\,A-1|^2+\frac{\kappa^2}{2}(|\psi|^2-1)^2\right\}\mathrm{d}x+\int_{\partial\Omega}\tilde{\gamma}|\psi(x)|^2\mathrm{d}u_{|\partial\Omega}(x), \tag{1.1}$$

which is defined for pairs $(\psi,A)\in H^1(\Omega;\mathbb{C})\times H^1(\Omega;\mathbb{R}^2)$. The parameter κ is a characteristic of the material. A material is said to be of type I if κ is sufficiently small and it is said to be of type II when κ is large. The parameter σ is the intensity of the applied magnetic field which is supposed to be constant and perpendicular to Ω. For a minimizer (ψ,A) of the energy $\mathcal{G}$, the function ψ is called the order parameter and $|\psi|^2$ measures the density of superconducting Cooper electron pairs; the vector field A is called the magnetic potential and curl A is the induced magnetic field. Note that the order parameter ψ satisfies the following boundary condition proposed by De Gennes:[1]

$$\nu\cdot(\nabla-i\sigma\kappa A)\psi+\tilde{\gamma}\psi=0, \tag{1.2}$$

where ν is the unit outward normal of $\partial\Omega$ and $\tilde{\gamma}\in\mathbb{R}$ is called in the physical literature the De Gennes parameter. Note that the boundary condition (1.2) was initially introduced in the theory of PDE by Robin.

The physicist De Gennes[1] introduced the parameter $\tilde{\gamma}$ in order to model interfaces between superconductors and normal materials. In that context, $\tilde{\gamma}$ is taken to be a nonzero positive constant and $1/\tilde{\gamma}$ (called the extrapolation length) usually measures the penetration of the superconducting Cooper electron pairs in the normal material. The size of $\tilde{\gamma}$ depends on the nature of the material adjacent to the superconductor and it ranges from $\tilde{\gamma}=0$ (interfaces with insulators) to $\tilde{\gamma}=+\infty$ (interfaces with magnetic and ferromagnetic materials). Experiments show that for superconductors adjacent to ferromagnetic materials, the order parameter ψ vanishes at the boundary[4] and the boundary condition (1.2) is changed to the Dirichlet boundary condition. Negative values of $\tilde{\gamma}$

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were also considered in the physical literature.[5] It is suggested that negative values of $\tilde{\gamma}$ would be useful for modeling the situation when a superconductor is adjacent to another superconductor of higher transition temperature.

Suppose that we have a type II superconductor (i.e., κ is large). The functional $\mathcal{G}$ has a critical point of the type $(0,A)$. Such a critical point is called a normal state. It is then natural to study whether a normal state is a local minimum of $\mathcal{G}$ in the presence of a strong applied magnetic field. The Hessian of $\mathcal{G}$ near a normal state is given by

$$(\phi,B)\mapsto 2\left[\int_\Omega (|(\nabla-i\sigma\kappa A)\phi|^2-\kappa^2|\phi|^2)\mathrm{d}x+\int_{\partial\Omega}\tilde{\gamma}|\phi|^2\mathrm{d}\mu_{|_{\partial\Omega}}(x)+(\sigma\kappa)^2\int_\Omega|\mathrm{curl}\,B|^2\mathrm{d}x\right].$$

By defining the change of parameter $h=1/\sigma\kappa$, we then have to study as $h\to 0$ the positivity of the quadratic form:

$$H^1(\Omega)\ni u\mapsto\|(h\nabla-iA)u\|^2_{L^2(\Omega)}+h^2\int_{\partial\Omega}\tilde{\gamma}|u|^2\mathrm{d}\mu_{|_{\partial\Omega}}(x)-(\kappa h)^2\|u\|^2_{L^2(\Omega)}.$$

The semiclassical limit $h\to 0$ is now equivalent to a large field limit $\sigma\to+\infty$. In order to study the influence of the size of $\tilde{\gamma}$, it seems reasonable to suppose that $\tilde{\gamma}$ is depending on h. Also, due to the possibility of having different materials exterior to Ω together with possible lack of symmetry in the geometry of Ω, it seems also convenient to take $\tilde{\gamma}$ as a function of the boundary. Thus, given a vector field $A\in C^\infty(\bar{\Omega};\mathbb{R}^2)$, a regular real valued function $\gamma\in C^\infty(\partial\Omega;\mathbb{R})$, and a number $\alpha>0$, let us define the quadratic form:

$$H^1(\Omega)\ni u\mapsto q^{\alpha,\gamma}_{h,A,\Omega}(u)=\|(h\nabla-iA)u\|^2_{L^2(\Omega)}+h^{1+\alpha}\int_{\partial\Omega}\gamma(x)|u(x)|^2\mathrm{d}\mu_{|_{\partial\Omega}}(x). \tag{1.3}$$

Observing that $q^{\alpha,\gamma}_{h,A,\Omega}$ is semibounded, we consider the self-adjoint operator associated to $q^{\alpha,\gamma}_{h,A,\Omega}$ by Friedrich's theorem. This is the magnetic Schrödinger operator $P^{\alpha,\gamma}_{h,A,\Omega}$ with domain $D(P^{\alpha,\gamma}_{h,A,\Omega})$ defined by

$$P^{\alpha,\gamma}_{h,A,\Omega}=-(h\nabla-iA)^2,$$

$$D(P^{\alpha,\gamma}_{h,A,\Omega})=\{u\in H^2(\Omega);\ \nu\cdot(h\nabla-iA)u_{|_{\partial\Omega}}+h^\alpha\gamma u_{|_{\partial\Omega}}=0\}. \tag{1.4}$$

We denote by $\mu^{(1)}(\alpha,\gamma,h)$ the ground state energy of $P^{\alpha,\gamma}_{h,A,\Omega}$ which is defined using the min-max principle by

$$\mu^{(1)}(\alpha,\gamma,h):=\inf_{u\in H^1(\Omega),u\neq 0}\frac{q^{\alpha,\gamma}_{h,A,\Omega}(u)}{\|u\|^2_{L^2(\Omega)}}. \tag{1.5}$$

Let us also recall that this eigenvalue problem is gauge invariant.

In the case when $\gamma\equiv 0$ (which corresponds to a superconductor surrounded by the vacuum), a lot of papers are devoted to the estimate in a semiclassical regime of the ground state energy of $P^{\alpha,\gamma}_{h,A,\Omega}$. We would like to mention here the works of Baumann-Phillips-Tang,[6] Bernoff-Sternberg,[7] del Pino-Felmer-Sternberg,[8] Helffer-Mohamed,[9] Helffer-Morame,[10] and the recent work of Fournais-Helffer.[11] The special case when $\alpha=1$ and γ is a positive constant was considered by Lu-Pan.[12,13] It was shown that in this case the effect of the De Gennes parameter γ is weak in the sense that the limit $\lim_{h\to 0}[\mu^{(1)}(1,\gamma,h)]/h$ is the same as in the case $\gamma=0$. This regime is therefore not sufficient to recover all the physically interesting cases considered in Refs. 4 and 5. It is the object of this paper to establish the results announced in Ref. 14 and to analyze (for all values of α) the influence of the boundary term in (1.3) on the localization of the ground state energy of the operator $P^{\alpha,\gamma}_{h,A,\Omega}$.

Following the technique of Helffer-Morame,[10] we have to understand the model case of the half-plane when the magnetic field and the function γ are both constant. Consider the magnetic potential:

$$A_0(x_1,x_2)=\tfrac{1}{2}(-x_2,x_1),\quad \forall\,(x_1,x_2)\in\mathbb{R}\times\mathbb{R}_+. \tag{1.6}$$

Notice that $\operatorname{curl} A_0=1$. Let us define the function

$$\mathbb{R}\ni\gamma\mapsto\Theta(\gamma),$$

where

$$\Theta(\gamma):=\inf_{u\in H^1_{A_0}(\mathbb{R}\times\mathbb{R}_+),u\neq 0}\frac{\|(\nabla-iA_0)u\|^2_{L^2(\mathbb{R}\times\mathbb{R}_+)}+\gamma\displaystyle\int_{\mathbb{R}}|u(x_1,0)|^2\mathrm{d}x_1}{\|u\|^2_{L^2(\mathbb{R}\times\mathbb{R}_+)}}, \tag{1.7}$$

and

$$H^1_{A_0}(\mathbb{R}\times\mathbb{R}_+)=\{u\in L^2(\mathbb{R}\times\mathbb{R}_+);\ (\nabla-iA_0)u\in L^2(\mathbb{R}\times\mathbb{R}_+)\}. \tag{1.8}$$

Note that $\Theta(\gamma)$ is the bottom of the spectrum of the operator $P^{\alpha,\gamma}_{h,A_0,\Omega}$ with $h=1$ and $\Omega=\mathbb{R}\times\mathbb{R}_+$. We shall see that $\Theta(\gamma)<1$ (cf. Theorem II.2). If $\gamma=0$, we write:

$$\Theta_0:=\Theta(0). \tag{1.9}$$

It is Θ_0 which appears in the analysis for the Neumann problem.[6–13] Actually, we are interested in the bottom of the spectrum of the operator $P^{\alpha,\gamma}_{h,A_0,\mathbb{R}\times\mathbb{R}_+}$ but a scaling argument gives us

$$\forall h\in\mathbb{R}_+,\quad \forall\,\alpha,\gamma\in\mathbb{R},\quad \inf\operatorname{Sp}(P^{\alpha,\gamma}_{h,A_0,\mathbb{R}\times\mathbb{R}_+})=h\Theta(h^{\alpha-1/2}\gamma). \tag{1.10}$$

The semiclassical analysis of the half-plane model depends then on the sign of both $\alpha-\frac{1}{2}$ and γ. We have then to investigate the asymptotic behavior of $\Theta(\gamma)$ when $\gamma\to 0$ and when $\gamma\to\pm\infty$. This will be the object of study in Sec. II.

Now we state our main results.

Theorem I.1: *Suppose that $\Omega\subset\mathbb{R}^2$ is open, bounded, connected, and having a smooth boundary. Suppose moreover that the magnetic field is constant* $\operatorname{curl} A=1$. *Then, for $\alpha>0$ and $\gamma\in C^\infty(\partial\Omega;\mathbb{R})$, the ground state energy of the operator $P^{\alpha,\gamma}_{h,A,\Omega}$ satisfies*

$$\mu^{(1)}(\alpha,\gamma,h)=h\Theta(h^{\alpha-1/2}\gamma_0)(1+o(1))\quad (h\to 0), \tag{1.11}$$

where $\gamma_0:=\min_{x\in\partial\Omega}\gamma(x)$.

Theorem I.1 gives a first term approximation of $\mu^{(1)}(\alpha,\gamma,h)$. The asymptotics (1.11) is valid without the need for any nondegeneracy hypothesis on the set of minima of γ, and holds for the function γ being constant as well. Let us remark that the asymptotics (1.11) depends strongly on α. In particular, when $\alpha=\frac{1}{2}$, we get

$$\lim_{h\to 0}\frac{\mu^{(1)}(\alpha,\gamma,h)}{h}=\Theta(\gamma_0)<1,$$

and if $\gamma_0=0$ or if $\alpha>\frac{1}{2}$, then (cf. Proposition II.5):

$$\lim_{h\to 0}\frac{\mu^{(1)}(\alpha,\gamma,h)}{h}=\Theta_0<1.$$

When $\alpha<\frac{1}{2}$, it is the sign of γ_0 that affects the asymptotics. Actually, if $\gamma_0<0$ we have (cf. Proposition II.8)

$$\lim_{h\to 0}\frac{\mu^{(1)}(\alpha,\gamma,h)}{h^{2\alpha}}=-\gamma_0^2,$$

and if $\gamma_0>0$, we have (cf. (2.46))

$$\lim_{h\to 0}\frac{\mu^{(1)}(\alpha,\gamma,h)}{h}=1,$$

which is the same behavior as that for the Dirichlet problem.[10] This last regime ($0<\alpha<\frac{1}{2}$ and $\gamma_0>0$) is in accordance with the physical observations in Ref. 4.

In the next theorem, we give a two-term asymptotics of $\mu^{(1)}(\alpha,\gamma,h)$ when $\alpha\in]\frac{1}{2},1[$.

Theorem I.2: *Suppose in addition to the hypotheses of Theorem I.1 that* $\frac{1}{2}<\alpha<1$ *and that the function* γ *is nonconstant. Then we have the following asymptotic expansion as* h *tends to* 0:

$$\mu^{(1)}(\alpha,\gamma,h)=h\Theta_0+6M_3\gamma_0 h^{\alpha+1/2}+\mathcal{O}(h^{\inf(3/2,2\alpha)}),\tag{1.12}$$

where M_3 *is a strictly positive universal constant.*

The constant M_3 satisfies $\Theta'(0)=6M_3$ and it will be defined precisely in Sec. II, see however (2.25) and (2.27). Compared with the result obtained in Ref. 10, the second term in the two-term asymptotics of $\mu^{(1)}(\alpha,\gamma,h)$ when $\gamma=0$ is of order $h^{3/2}$, whereas it is of order $h^{\alpha+1/2}$ in the regime considered in Theorem I.2. Let us mention also that in Ref. 11, the authors obtain (when $\gamma=0$) a complete asymptotic expansion under a generic hypothesis on the scalar curvature of $\partial\Omega$. It seems that a complete asymptotic expansion could be obtained in the regime of Theorem I.2 but under the following generic hypothesis over γ:

(1) γ has a finite number of minima;
(2) all the minima of γ are nondegenerate.

We leave this point hoping to analyze it in a future work.

Next we turn to the question of the localization of the ground states. Let $u_{\alpha,\gamma,h}$ be a ground state of the operator $P_{h,A,\Omega}^{\alpha,\gamma}$. We say that $u_{\alpha,\gamma,h}$ is exponentially localized as h tends to 0 near a closed set $\mathcal{B}$ in $\bar{\Omega}$ if there exists $\beta>0$, and for each neighborhood $\mathcal{V}$ of $\mathcal{B}$, there exist positive constants h_0, δ and C such that

$$\|u_{\alpha,\gamma,h}\|_{L^2(\Omega\setminus\mathcal{V})}\leqslant C\exp\left(-\frac{\delta}{h^\beta}\right)\|u_{\alpha,\gamma,h}\|_{L^2(\Omega)},\quad\forall\, h\in]0,h_0].\tag{1.13}$$

In the next theorem we describe some effect of γ on the localization of the ground states of the operator $P_{h,A,\Omega}^{\alpha,\gamma}$.

Theorem I.3: *Under the hypotheses of Theorem I.1, if* $\gamma_0\leqslant 0$ *or* $\frac{1}{2}\leqslant\alpha<1$, *a ground state of the operator* $P_{h,A,\Omega}^{\alpha,\gamma}$ *is exponentially localized as* h *tends to* 0 *near the boundary points where* γ *is minimum.*

More precisely, (1.13) *is satisfied with* $\beta=1-\alpha$ *if* $\gamma_0<0$, $\beta=(1-\alpha)/2$ *if* $\frac{1}{2}<\alpha<1$, *and* $\beta=1/2$ *otherwise.*

In the special case $\alpha=1$, the scalar curvature κ_r and the function γ affects the asymptotic expansion of the ground state energy to the same order.

Theorem I.4: *Suppose in addition to the hypotheses of Theorem I.1 that* $\alpha=1$. *Then we have the following asymptotic expansion as* h *tends to* 0:

$$\mu^{(1)}(\alpha,\gamma,h)=h\Theta_0-2M_3(\kappa_r-3\gamma)_{\max}h^{3/2}+\mathcal{O}(h^{13/8}),\tag{1.14}$$

and a ground state $u_{\alpha,\gamma,h}$ *of the operator* $P_{h,A,\Omega}^{1,\gamma}$ *is localized near the boundary points where the function* $\kappa_r-3\gamma$ *is maximal.*

More precisely, (1.13) *is satisfied with* $\beta=1/4$.

If γ is constant, the remainder in (1.14) is better and of order $\mathcal{O}(h^{5/3})$. When $\gamma\equiv 0$ we recover in the above theorem the result of Helffer-Morame.[10] Let us mention that the expansion (1.14) is

announced by Pan[25] in the particular case when γ is a positive constant. As in Ref. 11, we believe that an asymptotic expansion with higher terms could be obtained under a generic hypothesis on the function $\kappa_r - 3\gamma$.

In the next theorem, we study the case when the function γ is constant and we find that only the scalar curvature plays a role.

Theorem I.5: *Suppose in addition to the hypotheses of Theorem I.1 that the function γ is constant and that $\alpha \geqslant \frac{1}{2}$. There exists a constant $M_3(\alpha,\gamma) > 0$ such that we have the following asymptotic expansion as h tends to* 0:

$$\mu^{(1)}(\alpha,\gamma,h) = h\Theta(h^{\alpha-1/2}\gamma) - 2M_3(\alpha,\gamma)(\kappa_r)_{\max}h^{3/2} + o(h^{3/2}). \tag{1.15}$$

Moreover, a ground state of the operator $P^{\alpha,\gamma}_{h,A,\Omega}$ is localized as h tends to 0 *near the boundary points where the scalar curvature is maximal, and* (1.13) *is satisfied with $\beta = 1/4$.*

When $\alpha > \frac{1}{2}$, the constant $M_3(\alpha,\gamma)$ is equal to the universal constant M_3. When $\alpha = \frac{1}{2}$, we have $M_3(\frac{1}{2},\gamma) = M_3(\gamma)$, where the constant $M_3(\gamma)$ will be defined in Sec. II cf. (2.24).

This paper is organized in the following way. In Sec. II, we link the analysis of the half-plane model operator to that of a one-dimensional operator. We get in particular the existence of a number $\xi(\gamma) > 0$ such that $\Theta(\gamma)$ is the lowest eigenvalue of the operator $-\partial_t^2 + (t-\xi(\gamma))^2$. Let φ_γ be an eigenfunction associated to $\Theta(\gamma)$. We establish the regularity of $\Theta(\gamma)$ and φ_γ as functions of γ, the asymptotic behavior of $\Theta(\gamma)$ as $\gamma \to \pm\infty$, and uniform estimates with respect to γ describing the exponential decay of φ_γ at infinity.

In Sec. III, we use the eigenfunction φ_γ to construct a test function inspired by Refs. 7 and 10 and we obtain an upper bound for $\mu^{(1)}(\alpha,\gamma,h)$. We then carry out a similar analysis to that in Ref. 10 and we use the results of Sec. II to prove Theorem I.1.

In Sec. IV, we show how to get the localization of the ground states using Agmon's technique.[15] Finally, in Sec. V, the analysis of a one-dimensional family of operators on a weighted L^2-space appears (cf. (5.21)). It is the same family of operators appearing in Ref. 10 (Sec. 11) but with a different boundary condition this time. This analysis permits us to derive two-term asymptotics of the ground state energy showing the influence of the scalar curvature. We finish then the proofs of Theorems I.2, I.3, I.4, and I.5.

II. THE MODEL OPERATOR

Given $\gamma \in \mathbb{R}$, let us consider the quadratic form:

$$H^1_{A_0}(\mathbb{R}\times\mathbb{R}_+) \ni u \mapsto q[\gamma](u) = \|(\nabla - iA_0)u\|^2_{L^2(\mathbb{R}\times\mathbb{R}_+)} + \gamma\int_{\mathbb{R}} |u(x_1,0)|^2 \mathrm{d}x_1. \tag{2.1}$$

The magnetic potential A_0 and the form domain $H^1_{A_0}(\mathbb{R}\times\mathbb{R}_+)$ are defined, respectively, in (1.6) and (1.8). Observing that the quadratic form $q[\gamma]$ is bounded from below, we can associate to $q[\gamma]$, by taking the Friedrichs extension, a unique self-adjoint operator $P[\gamma]$ on $L^2(\mathbb{R}\times\mathbb{R}_+)$. The min-max principle gives that the bottom of the spectrum of $P[\gamma]$ is equal to $\Theta(\gamma)$ (cf. (1.7)).

A. Link with a one-dimensional operator

By a change of gauge and a partial Fourier transformation with respect to the first variable, we obtain that the spectral analysis of the operator $P[\gamma]$ will be deduced from that of the ξ-family of one dimensional operators:

$$H[\gamma,\xi] = -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + (t-\xi)^2, \tag{2.2}$$

with domain

$$D(H[\gamma,\xi]) = \{u \in B^2(\mathbb{R}_+);\ u'(0) = \gamma u(0)\}, \tag{2.3}$$

where, for a given integer k, the space $B^k(\mathbb{R}_+)$ is defined by

$$B^k(\mathbb{R}_+) = \{u \in H^k(\mathbb{R}_+);\ t^k u \in L^2(\mathbb{R}_+)\}. \tag{2.4}$$

Note that the operator $H[\gamma,\xi]$ has compact resolvent and hence the spectrum is discrete. We denote by $\mu^{(1)}(\gamma,\xi)$ the first eigenvalue of $H[\gamma,\xi]$. The min-max principle gives

$$\mu^{(1)}(\gamma,\xi) = \inf_{u\in B^1(\mathbb{R}_+),u\neq 0} \frac{q[\gamma,\xi](u)}{\|u\|^2_{L^2(\mathbb{R}_+)}},$$

where $q[\gamma,\xi]$ is the quadratic form associated to $H[\gamma,\xi]$:

$$q[\gamma,\xi](u) = \int_{\mathbb{R}_+} (|u'(t)|^2 + |(t-\xi)u(t)|^2)\mathrm{d}t + \gamma|u(0)|^2. \tag{2.5}$$

A spectral analysis using the separation of variables (cf. Ref. 16) gives us

$$\Theta(\gamma) = \inf_{\xi\in R} \mu^{(1)}(\gamma,\xi). \tag{2.6}$$

In the following lemma, we collect some useful estimates of $\mu^{(1)}(\gamma,\xi)$.

Lemma II.1: Given $\epsilon \in]0,1[$, *we have*

$$\mu^{(1)}(\gamma,\xi) \geqslant (1-\epsilon)\mu^{(1)}(0,\xi) - \frac{(\gamma_-)^2}{\epsilon}, \quad \forall\ \gamma,\xi \in \mathbb{R}, \tag{2.7}$$

where $\gamma_- = \max(-\gamma,0)$.

Moreover, given $\gamma \in \mathbb{R}$, *we have*

$$\lim_{\xi\to-\infty} \mu^{(1)}(\gamma,\xi) = +\infty, \quad \lim_{\xi\to+\infty} \mu^{(1)}(\gamma,\xi) = 1. \tag{2.8}$$

Proof: Using the density of $C_0^\infty(\overline{\mathbb{R}_+})$ in $H^1(\mathbb{R}_+)$, we get for any $u \in H^1(\mathbb{R}_+)$:

$$|u(0)|^2 = -2\int_0^\infty u(t)u'(t)\mathrm{d}t. \tag{2.9}$$

By the Cauchy-Schwarz inequality, we get for any $\alpha>0$:

$$|u(0)|^2 \leqslant \alpha\|u\|^2_{L^2(\mathbb{R}_+)} + \frac{1}{\alpha}\|u'\|^2_{L^2(\mathbb{R}_+)}.$$

Taking $\alpha = \epsilon/\gamma$ (with $\gamma<0$), we get

$$q[\gamma,\xi](u) \geqslant (1-\epsilon)q[0,\xi](u) - \frac{(\gamma_-)^2}{\epsilon}\|u\|^2_{L^2(\mathbb{R}_+)}, \quad \forall\ u \in B^1(\mathbb{R}_+). \tag{2.10}$$

The min-max principle now gives (2.7).

Notice that (2.8) is valid for $\gamma=0$ (Ref. 10). So the limit as $\xi\to-\infty$ in (2.8) is now a consequence of the estimate (2.7). For the reader's convenience, let us give for nonzero γ a proof for the limit as $\xi\to+\infty$ in (2.8). Let us denote by $\mu^D(\xi)$ the first eigenvalue of the Dirichlet realization of the harmonic oscillator $-\partial_t^2+(t-\xi)^2$ on $\mathbb{R}_+$. We have by the min-max principle:

$$\mu^{(1)}(0,\xi) + \gamma|\varphi_{\gamma,\xi}(0)|^2 \leqslant \mu^{(1)}(\gamma,\xi) \leqslant \mu^D(\xi), \tag{2.11}$$

where $\varphi_{\gamma,\xi}$ is the L^2-normalized eigenfunction associated to $\mu^{(1)}(\gamma,\xi)$. Let us notice also that[10,16] $\lim_{\xi\to+\infty}\mu^D(\xi)=1$. So, if we know that $\lim_{\xi\to+\infty}|\varphi_{\gamma,\xi}(0)|^2=0$, then (2.11) is sufficient to deduce the

limit as $\xi \to +\infty$ in (2.8). Thus, it remains for us to prove the following claim:

Given $\epsilon \in \,]0,1[$ and $\gamma \in \mathbb{R}$, there exists a constant $C > 0$ such that

$$\forall\, \xi \in [C, +\infty[, \quad |\varphi_{\gamma,\xi}(0)|^2 \leqslant Ce^{-\epsilon\xi/2}. \tag{2.12}$$

Let us mention that the decay in (2.12) is not optimal.[17,18] We prove (2.12) using Agmon type estimates.[15] Let Φ be a regular function with compact support. An integration by parts gives the following identity:

$$q[\gamma,\xi](e^{\Phi}\varphi_{\gamma,\xi}) = \mu^{(1)}(\gamma,\xi)\|e^{\Phi}\varphi_{\gamma,\xi}\|^2_{L^2(\mathbb{R}_+)} + \|\Phi' e^{\Phi}\varphi_{\gamma,\xi}\|^2_{L^2(\mathbb{R}_+)}. \tag{2.13}$$

Using the estimate (2.10) (with $\epsilon = 1/2$) together with the fact that $\mu^D(\xi)$ is bounded for $\xi \in \mathbb{R}_+$, we can rewrite (2.13) in the form:

$$\tfrac{1}{2}(\|(e^{\Phi}\varphi_{\gamma,\xi})'\|^2_{L^2(\mathbb{R}_+)} + \|(t-\xi)e^{\Phi}\varphi_{\gamma,\xi}\|^2_{L^2(\mathbb{R}_+)}) \leqslant \widetilde{C}\|e^{\Phi}\varphi_{\gamma,\xi}\|^2_{L^2(\mathbb{R}_+)} + \|\Phi' e^{\Phi}\varphi_{\gamma,\xi}\|^2_{L^2(\mathbb{R}_+)}, \tag{2.14}$$

for some constant $\widetilde{C} > 0$. We choose now Φ as

$$\Phi(t) := \begin{cases} \epsilon\xi\dfrac{(t-1)^2}{2} & \text{if } 0 \leqslant t \leqslant 1 \\ 0 & \text{if } t \geqslant 1. \end{cases}$$

Under this choice of Φ, we can get a sufficiently large constant $C > 0$ such that, for $\xi \in [C, +\infty[$, we can rewrite (2.14) in the form:

$$\|e^{\Phi}\varphi_{\gamma,\xi}\|_{H^1(\Omega)} \leqslant C.$$

Using the Sobolev imbedding $H^1(\mathbb{R}_+) \hookrightarrow L^\infty(\mathbb{R}_+)$, this last estimate is sufficient to deduce (2.12). □

Following the analysis of Dauge-Helffer,[19] we have now the following result.

Theorem II.2: *For each* $\gamma \in \mathbb{R}$, $\Theta(\gamma) < 1$ *and the function* $\mathbb{R} \ni \xi \mapsto \mu^{(1)}(\gamma,\xi)$ *attains its minimum at a unique positive point* $\xi(\gamma)$ *that satisfies*

$$\xi(\gamma)^2 = \Theta(\gamma) + \gamma^2. \tag{2.15}$$

Proof: Let us notice that by Kato's theory (Ref. 20), the maps

$$\xi \mapsto \mu^{(1)}(\gamma,\xi), \quad \xi \mapsto \varphi_{\gamma,\xi} \in L^2(\mathbb{R}_+)$$

are analytic. Here we recall that $\varphi_{\gamma,\xi}$ is the unique strictly positive and L^2-normalized eigenfunction associated to $\mu^{(1)}(\gamma,\xi)$. Let us consider $\tau > 0$. Note that

$$\mu^{(1)}(\gamma,\xi+\tau)\varphi_{\gamma,\xi+\tau}(t+\tau) = H[\gamma,\xi](\varphi_{\gamma,\xi+\tau}(t+\tau)), \quad \forall\, t \in \mathbb{R}_+.$$

Taking the scalar product with $\varphi_{\gamma,\xi}$ and then integrating by parts, we get

$$(\mu^{(1)}(\gamma,\xi+\tau) - \mu^{(1)}(\gamma,\xi))\int_{\mathbb{R}_+} \varphi_{\gamma,\xi+\tau}(t+\tau)\varphi_{\gamma,\xi}(t)\mathrm{d}t = \varphi'_{\gamma,\xi+\tau}(\tau)\varphi_{\gamma,\xi}(0) - \gamma\varphi_{\gamma,\xi+\tau}(\tau)\varphi_{\gamma,\xi}(0). \tag{2.16}$$

Recall that we have the boundary conditions

$$\varphi'_{\gamma,\xi+\tau}(0) = \gamma\varphi_{\gamma,\xi+\tau}(0), \quad \varphi'_{\gamma,\xi}(0) = \gamma\varphi_{\gamma,\xi}(0).$$

Then we can rewrite (2.16) as

$$\frac{\mu^{(1)}(\gamma,\xi+\tau)-\mu^{(1)}(\gamma,\xi)}{\tau}\int_{\mathbb{R}_+}\varphi_{\gamma,\xi+\tau}(t+\tau)\varphi_{\gamma,\xi}(t)\mathrm{d}t$$
$$=\left[\frac{\varphi'_{\gamma,\xi+\tau}(\tau)-\varphi'_{\gamma,\xi+\tau}(0)}{\tau}-\gamma\frac{\varphi_{\gamma,\xi+\tau}(\tau)-\varphi_{\gamma,\xi+\tau}(0)}{\tau}\right]\cdot\varphi_{\gamma,\xi}(0).$$

By taking the limit as $\tau\to 0$, we get

$$\partial_\xi\mu^{(1)}(\gamma,\xi)=(\varphi''_{\gamma,\xi}(0)-\gamma\varphi'_{\gamma,\xi}(0))\varphi_{\gamma,\xi}(0).$$

Finally, we make the substitutions

$$\varphi''_{\gamma,\xi}(0)=(\xi^2-\mu^{(1)}(\gamma,\xi))\varphi_{\gamma,\xi}(0),\quad \varphi'_{\gamma,\xi}(0)=\gamma\varphi_{\gamma,\xi}(0),$$

and we get the following formula,

$$\partial_\xi\mu^{(1)}(\gamma,\xi)=(\xi^2-\mu^{(1)}(\gamma,\xi)-\gamma^2)|\varphi_{\gamma,\xi}(0)|^2, \tag{2.17}$$

called usually the *F*-formula (cf. Refs. 19 and 21). Using (2.7) and (2.8), we get

$$\partial_\xi\mu^{(1)}(\gamma,\xi)_{|_{\xi=0}}<0,\quad \partial_\xi\mu^{(1)}(\gamma,\xi)_{|_{\xi=\eta}}>0,$$

for a sufficiently large $\eta>0$. This gives the existence of a positive critical point of $\mu^{(1)}(\gamma,\xi)$. Let us notice now that for any critical point ξ_c of $\mu^{(1)}(\gamma,\xi)$, we have

$$\partial^2_\xi\mu^{(1)}(\gamma,\xi)_{|_{\xi=\xi_c}}=2\xi_c|\varphi_{\gamma,\xi}(0)|^2.$$

This shows that any negative critical point is a global maximum and any positive critical point is a global minimum of $\mu^{(1)}(\gamma,\xi)$. Coming back to (2.8), $\lim_{\xi\to-\infty}\mu^{(1)}(\gamma,\xi)=+\infty$, and thus there does not exist any negative critical points. Therefore, the minimum of $\xi\mapsto\mu^{(1)}(\gamma,\xi)$ is attained at a unique point $\xi(\gamma)>0$ and the function $\xi\mapsto\mu^{(1)}(\gamma,\xi)$ is strictly increasing on $[\xi(\gamma),+\infty[$. This proves in particular (recalling (2.6)):

$$\Theta(\gamma)=\mu^{(1)}(\gamma,\xi(\gamma))<1.$$

□

In the sequel, we denote by φ_γ the unique strictly positive and L^2-normalized eigenfunction associated to the eigenvalue $\Theta(\gamma)$, and by $H[\gamma]$ the operator $H[\gamma,\xi(\gamma)]$:

$$\varphi_\gamma=\varphi_{\gamma,\xi(\gamma)},\quad H[\gamma]=H[\gamma,\xi(\gamma)]. \tag{2.18}$$

In the next lemma, we collect various useful relations satisfied by the eigenfunction φ_γ. These relations are similar to those given in Appendix A of Ref. 10.

Lemma II.3: For each $\gamma\in\mathbb{R}$, *the following relations hold:*

$$\int_{\mathbb{R}_+}(t-\xi(\gamma))|\varphi_\gamma(t)|^2\mathrm{d}t=0, \tag{2.19}$$

$$\int_{\mathbb{R}_+}(t-\xi(\gamma))^2|\varphi_\gamma(t)|^2\mathrm{d}t=\frac{\Theta(\gamma)}{2}-\frac{\gamma}{4}|\varphi_\gamma(0)|^2, \tag{2.20}$$

$$\int_{\mathbb{R}_+}(t-\xi(\gamma))^3|\varphi_\gamma(t)|^2\mathrm{d}t=\frac{1}{6}[1-2(\gamma\xi(\gamma))^2]|\varphi_\gamma(0)|^2. \tag{2.21}$$

Proof: We follow the calculations done in Bernoff-Sternberg.[7] Let us consider the differential operator:

$$L = -\partial_t^2 + (t - \xi(\gamma))^2 - \Theta(\gamma).$$

Note that for any polynomial p, we have the following identity:

$$L(2p\varphi_\gamma - p'\varphi_\gamma) = (p^{(3)} - 4[(t - \xi(\gamma) - \Theta(\gamma)]p' - 4(t - \xi(\gamma))p)\varphi_\gamma. \tag{2.22}$$

Let $v = 2p\varphi_\gamma - p'\varphi'_\gamma$. Integrating by parts we obtain

$$\int_0^{+\infty} \varphi_\gamma(t)(Lv)(t)\mathrm{d}t = (v'(0) - \gamma v(0))\varphi_\gamma(0). \tag{2.23}$$

Taking $p=1$, we get

$$-4\int_0^{+\infty} (t - \xi(\gamma))|\varphi_\gamma(t)|^2\mathrm{d}t = 2(\xi(\gamma)^2 - \gamma^2 - \Theta(\gamma))|\varphi_\gamma(0)|^2.$$

Recalling (2.15), the above formula proves (2.19).

We prove (2.20) by taking $p=(t-\xi(\gamma))$. To prove (2.21), we take $p=(t-\xi(\gamma))^2$. Note that we have in this case

$$v'(0) - \gamma v(0) = 2(2(\gamma\xi(\gamma))^2 - 1)\varphi_\gamma(0).$$

We get now from (2.22) and (2.23)

$$-12\int_0^{+\infty} (t - \xi(\gamma))^3|\varphi_\gamma(t)|^2\mathrm{d}t = 2(2(\gamma\xi(\gamma))^2 - 1)|\varphi_\gamma(0)|^2.$$

This proves (2.21). □

For $\gamma \in \mathbb{R}$, let us define the parameter

$$M_3(\gamma) = \tfrac{1}{6}(1 + (\gamma\xi(\gamma))^2)|\varphi_\gamma(0)|^2, \tag{2.24}$$

and when $\gamma=0$, we write $M_3 := M_3(0)$. Note that (2.21) gives

$$M_3 = \int_{\mathbb{R}_+} (t - \xi_0)^3|\varphi_0(t)|^2\mathrm{d}t, \tag{2.25}$$

where $\xi_0 := \xi(0)$. The constant M_3 is the universal constant appearing in Theorems I.2, I.4, and the parameter $M_3(\gamma)$ appears as $M_3\left(\frac{1}{2}, \gamma\right)$ in Theorem I.5.

B. Regularity

We discuss now the regularity of the functions $\gamma \to \Theta(\gamma) \in \mathbb{R}$ and $\gamma \mapsto \varphi_\gamma \in L^2(\mathbb{R}_+)$. It seems for us that Kato's theory (cf. Ref. 20) does not apply in this context at least for the reason that we do not know *a priori* whether the expression of the operator

$$H[\gamma] = -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + (t - \xi(\gamma))^2$$

depends analytically on γ. Inspired by Bonnaillie,[22] we use a modification of Grushin's method[23] and we get the following proposition.

Proposition II.4. The functions $\mathbb{R} \ni \gamma \mapsto \Theta(\gamma) \in \mathbb{R}$ *and* $\mathbb{R} \ni \gamma \mapsto \varphi_\gamma \in L^2(\mathbb{R}_+)$ *are* C^∞.

Moreover, the function $\mathbb{R} \ni \gamma \mapsto \varphi_\gamma \in L^\infty(\mathbb{R}_+)$ *is locally Lipschitz.*

The specific difficulty in proving Proposition II.4 comes from the fact that both the expression and the domain of the operator $H[\gamma]$ depend on γ. To work with an operator with a fixed domain, we consider a cut-off χ that is equal to 1 on $[0, 1]$ and we apply the invertible transformation

$\varphi \mapsto \widetilde{\varphi} = e^{-\gamma t \chi(t)} \varphi$ that transforms the boundary condition $\varphi'(0) = \gamma \varphi(0)$ to the usual Neumann boundary condition $\widetilde{\varphi}'(0) = 0$ and leaves the spectrum invariant (cf. Proof of Proposition II.7).

In the next proposition we determine $\Theta'(\gamma)$. This is a first step in the proof of Proposition II.4.

Proposition II.5: The function $\gamma \mapsto \Theta(\gamma)$ is of class C^1 and satisfies

$$\Theta'(\gamma) = |\varphi_\gamma(0)|^2. \tag{2.26}$$

In particular, we have

$$\Theta'(0) = 6M_3. \tag{2.27}$$

Remark II.6: Using Formula (2.15) we get also that the function $\gamma \mapsto \xi(\gamma)$ is of class C^1.

Proof of Proposition II.5: Let τ be a real number. We shall define the following trial function:

$$u = e^{\pi t}(\varphi_\gamma + \tau u_1),$$

where

$$u_1 = (H[\gamma] - \Theta(\gamma))^{-1}\{|\varphi_\gamma(0)|^2 \varphi_\gamma + 2\varphi_\gamma' + 2(\xi(\gamma + \tau) - \xi(\gamma))(t - \xi(\gamma))\varphi_\gamma\}.$$

By standard Fredholm theory, the operator $(H[\gamma] - \Theta(\gamma))^{-1}$ is defined on the orthogonal space of φ_γ and has values in $D(H[\gamma])$. Hence, the function u_1 is well defined, thanks to (2.19), and the function u satisfies the boundary condition $u'(0) = (\gamma + \tau)u(0)$. When τ is sufficiently small, it is a result of the exponential decay of φ_γ at $+\infty$ (cf. Propositions II.9 and II.10) and standard elliptic estimates that $u \in B^2(\mathbb{R}_+)$. Therefore, $u \in D(H[\gamma + \tau])$, and we have

$$H[\gamma + \tau](u) = e^{\pi t}(-\partial_t^2 + (t - \xi(\gamma + \tau))^2 - 2\tau\partial_t - \tau^2)(\varphi_\gamma + \tau u_1). \tag{2.28}$$

Using the decomposition:

$$H[\gamma + \tau] = H[\gamma] - 2(\xi(\gamma + \tau) - \xi(\gamma))(t - \xi(\gamma)) + (\xi(\gamma + \tau) - \xi(\gamma))^2,$$

we can rewrite (2.28) as

$$(H[\gamma + \tau] - \Theta(\gamma) - |\varphi_\gamma(0)|^2 \tau)(u) = \tau^2 e^{\pi t}(\Theta(\gamma) + |\varphi_\gamma(0)|^2)u_1 + (\xi(\gamma + \tau) - \xi(\gamma))^2 u. \tag{2.29}$$

We make the following claim:

$$\forall\, \gamma \in \mathbb{R}, \quad \exists\, C > 0, \quad \forall\, \tau \in [-1, 1], \quad |\xi(\gamma + \tau) - \xi(\gamma)| \leqslant C|\tau|. \tag{2.30}$$

Therefore, thanks to (2.29) and (2.30), there exist constants $\widetilde{C}, \tau_0 > 0$ such that, for all $\tau \in [-\tau_0, \tau_0]$, we have

$$\|(H[\gamma + \tau] - \Theta(\gamma) - |\varphi_\gamma(0)|^2 \tau)u\|_{L^2(\mathbb{R}_+)} \leqslant \widetilde{C}\tau^2 \|u\|_{L^2(\mathbb{R}_+)}.$$

We now get by the spectral theorem the existence of an eigenvalue $\widetilde{\Theta}(\gamma + \tau)$ of the operator $H[\gamma + \tau]$ that satisfies the following estimate:

$$|\widetilde{\Theta}(\gamma + \tau) - \Theta(\gamma) - |\varphi_\gamma(0)|^2 \tau| \leqslant \widetilde{C}\tau^2, \quad \forall\, \tau \in [-\tau_0, \tau_0]. \tag{2.31}$$

We make now another claim:

$$\forall\, \gamma \in \mathbb{R}, \quad \exists\, C_1 > 0, \quad \forall\, \tau \in [-1, 1], \quad |\mu^{(2)}(\gamma + \tau, \xi(\gamma + \tau)) - \mu^{(2)}(\gamma, \xi(\gamma))| \leqslant C|\tau|, \tag{2.32}$$

where for $(\eta, \xi) \in \mathbb{R} \times \mathbb{R}$, $\mu^{(2)}(\eta, \xi)$ denotes the second eigenvalue of the operator $H[\eta, \xi]$. Under the above claim, the estimate (2.31) gives

$$\widetilde{\Theta}(\gamma+\tau)=\Theta(\gamma+\tau),\quad \forall\,\tau\in[-\tau_0,\tau_0].$$

Consequently, we get that $\Theta(\gamma)$ is differentiable and satisfies formula (2.26). We make now a final claim:

$$\text{The function } \gamma\mapsto|\varphi_\gamma(0)|^2 \text{ is locally Lipschitz.} \tag{2.33}$$

To achieve the proof of the theorem, we only need to prove (2.30), (2.32), and (2.33).

Proof of (2.30): As we have the formula (2.15), it is sufficient to prove

$$\forall\,\gamma\in\mathbb{R},\quad \exists\,C>0,\quad \forall\,\tau\in[-1,1],\quad |\Theta(\gamma+\tau)-\Theta(\gamma)|\leqslant C|\tau|. \tag{2.34}$$

The min-max principle gives

$$\mu^{(1)}(\gamma,\xi)+\tau|\varphi_{\gamma+\tau,\xi}(0)|^2\leqslant\mu^{(1)}(\gamma+\tau,\xi)\leqslant\mu^{(1)}(\gamma,\xi)+\tau|\varphi_{\gamma,\xi}(0)|^2,\quad \forall\,\xi\in\mathbb{R}. \tag{2.35}$$

Thus, given an eigenfunction φ of $H[\gamma,\xi]$, we need to estimate $|\varphi(0)|^2$. Let $u\in D(H[\gamma])$. Using (2.9) we get

$$|u(0)|^2\leqslant 2\|u\|_{L^2(\mathbb{R}_+)}\|u'\|_{L^2(\mathbb{R}_+)}. \tag{2.36}$$

We use now (2.10) (with $\epsilon=1/2$) to obtain

$$\|u'\|^2_{L^2(\mathbb{R}_+)}\leqslant 2q[\gamma,\xi](u)+(\gamma_-)^2\|u\|^2_{L^2(\mathbb{R}_+)}. \tag{2.37}$$

Combining (2.36) and (2.37), we get after an integration by parts and the application of the Cauchy-Schwarz inequality,

$$|u(0)|^2\leqslant 2\|H[\gamma,\xi]u\|_{L^2(\mathbb{R}_+)}\|u\|_{L^2(\mathbb{R}_+)}+(\gamma_-)^2\|u\|^2_{L^2(\mathbb{R}_+)},\quad \forall\,u\in D(H[\gamma]). \tag{2.38}$$

Let $M:=\sup_{\tau\in[-1,1]}\xi(\gamma+\tau)$. Let us show that $M<+\infty$. Actually, the min-max principle gives

$$\mu^{(1)}(\gamma-1,\xi)\leqslant\mu^{(1)}(\gamma+\tau,\xi)\leqslant\mu^{(1)}(\gamma+1,\xi),\quad \forall\,\tau\in[-1,1],\quad \forall\,\xi\in\mathbb{R}.$$

Recalling (2.6), we obtain $\Theta(\gamma-1)\leqslant\sup_{\tau\in[-1,1]}\Theta(\gamma+\tau)\leqslant\Theta(\gamma+1)$. Formula (2.15) now gives $M<+\infty$. Therefore, (2.38) gives

$$|\varphi_{\gamma,\xi}(0)|^2\leqslant C,\quad |\varphi_{\gamma+\tau,\xi}(0)|^2\leqslant C,\quad \forall\,\tau\in[-1,1],\quad \forall\,\xi\in[-M,M],$$

for some constant $C>0$. Consequently (2.35) yields the estimate

$$\mu^{(1)}(\gamma,\xi)-C\tau_-\leqslant\mu^{(1)}(\gamma+\tau,\xi)\leqslant\mu^{(1)}(\gamma,\xi)+C\tau_+,\quad \forall\,\xi\in[-M,M].$$

Minimizing with respect to ξ, we get (2.34), thanks to Theorem II.2.

Proof of (2.32): Let $u\in B^1(\mathbb{R}_+)$. We shall compare $q[\gamma+\tau,\xi(\gamma+\tau)](u)$ and $q[\gamma,\xi(\gamma)](u)$. In fact, we have

$$q[\gamma+\tau,\xi(\gamma+\tau)][u]=q[\gamma,\xi(\gamma)](u)-2(\xi(\gamma+\tau)-\xi(\gamma))\int_0^{+\infty}(t-\xi(\gamma))|u(t)|^2\mathrm{d}t+(\xi(\gamma+\tau)$$

$$-\xi(\gamma))^2\int_0^{+\infty}|u(t)|^2\mathrm{d}t+\tau|u(0)|^2,$$

where, combining (2.36) and (2.37),

$$|u(0)|^2\leqslant 2q[\gamma,\xi](u)+(\gamma_-)^2\|u\|^2_{L^2(\mathbb{R}_+)}.$$

The Cauchy-Schwarz inequality gives

$$2\left|\int_0^{+\infty}(t-\xi(\gamma))|u(t)|^2\mathrm{d}t\right| \leqslant \int_0^{+\infty}|(t-\xi(\gamma))u(t)|^2\mathrm{d}t+\int_0^{+\infty}|u(t)|^2\mathrm{d}t.$$

Using (2.30), we get a constant $C>0$ such that, for all $\tau\in[-1,1]$, we have

$$(1-C\tau_-)q[\gamma,\xi(\gamma)](u)-C\tau_-\|u\|^2_{L^2(\mathbb{R}_+)}\leqslant q[\gamma,\xi(\gamma+\tau)](u)\leqslant(1+C\tau_+)q[\gamma,\xi(\gamma)](u)+C\tau_+\|u\|^2_{L^2(\mathbb{R}_+)}.$$

The min-max principle now proves the claim.

Proof of (2.33): Let $u=\varphi_\gamma(t)-e^{-\pi}\varphi_{\gamma+\tau}(t)$. It is sufficient to prove that

$$|u(0)|^2\leqslant C|\tau|,\quad \forall\ \tau\in[-\tau_0,\tau_0], \tag{2.39}$$

for constants $C,\tau_0>0$. Using (2.38), we have to estimate $\|u\|_{L^2(\mathbb{R}_+)}$ and $\|H[\gamma,\xi]u\|_{L^2(\mathbb{R}_+)}$. Let $f=(H[\gamma]-\Theta(\gamma))u$. Then:

$$f=(\Theta(\gamma)-\Theta(\gamma+\tau))u+w,$$

where

$$w(t)=e^{-\pi}(-2\tau\partial_t+2(\xi(\gamma+\tau)-\xi(\gamma))(t-\xi(\gamma))-(\xi(\gamma+\tau)-\xi(\gamma))^2+\tau^2)\varphi_\gamma(t).$$

Therefore, thanks to (2.30) and (2.34), we have

$$\|f\|_{L^2(\mathbb{R}_+)}\leqslant C|\tau|,\quad \forall\ \tau\in[-\tau_0,\tau_0]. \tag{2.40}$$

Noticing that, after an integration by parts, $\langle f,\varphi_\gamma\rangle_{L^2(\mathbb{R}_+)}=0$, we write

$$u=(H[\gamma]-\Theta(\gamma))^{-1}f.$$

It is a standard result that the operator norm of $(H[\gamma]-\Theta(\gamma))^{-1}$ is bounded on the orthogonal space of φ_γ and is estimated by the inverse of the gap between the first two eigenvalues of $H[\gamma]$. Therefore, thanks to (2.40), we get that $\|u\|_{L^2(\mathbb{R}_+)}\leqslant\widetilde{C}|\tau|$ for some constant $\widetilde{C}>0$. Plugging this estimate together with (2.40) in (2.38), we get (2.39). □

In the next proposition we have a regularity result with respect to the two variables (γ,ξ).

Proposition II.7: The functions $(\gamma,\xi)\mapsto\mu^{(1)}(\gamma,\xi)$ *and* $(\gamma,\xi)\mapsto\varphi_{\gamma,\xi}$ *are of class* C^∞ *in* $\mathbb{R}^2$. *Moreover, we have*

$$\partial_\gamma\mu^{(1)}(\gamma,\xi)=|\varphi_{\gamma,\xi}(0)|^2. \tag{2.41}$$

Using Proposition II.5 and Remark II.6, Proposition II.7 is sufficient for achieving the proof of Proposition II.4.

Proof of Proposition II.7: In order to reduce the problem to a problem of an operator with a fixed domain, we define the bounded operator $V[\gamma]$ on $L^2(\mathbb{R}_+)$ by

$$V[\gamma]u=e^{\gamma\chi(t)t}u,\quad \forall\ u\in L^2(\mathbb{R}_+).$$

We then define the operator $\widetilde{H}[\gamma,\xi]$ by

$$D(\widetilde{H}[\gamma,\xi])=\{u\in B^2(\mathbb{R}_+);u'(0)=0\},$$

$$\widetilde{H}[\gamma,\xi]=V[-\gamma]H[\gamma,\xi]V[\gamma].$$

Note that the domain of $\widetilde{H}[\gamma,\xi]$ is independent of γ and ξ. Note also that $\widetilde{H}[\gamma,\xi]$ is not self-adjoint but it has the same spectrum as $H[\gamma,\xi]$. A fundamental state of $\widetilde{H}[\gamma,\xi]$ is given by

$$\tilde{\varphi}_{\gamma,\xi}(t) = V[-\gamma]\varphi_{\gamma,\xi}(t).$$

We denote by $\varphi^*_{\gamma,\xi}$ the orthogonal projector on $\varphi_{\gamma,\xi}$. Let us consider a point (γ_0, ξ_0). We define the operator $M_0 : D(\tilde{H}[\gamma,\xi]) \times \mathbb{C} \to L^2(\mathbb{R}_+) \times \mathbb{C}$ by

$$M_0 := \begin{pmatrix} \tilde{H}[\gamma_0,\xi_0] - \mu_0 & \tilde{\varphi}_0 \\ \varphi_0^* & 0 \end{pmatrix},$$

where $\mu_0 = \mu^{(1)}(\gamma_0, \xi_0)$ and $\varphi_0 = \varphi_{\gamma_0,\xi_0}$.

The operator M_0 is invertible and its inverse R_0 is given by

$$R_0 = \begin{pmatrix} E_0 & E_0^+ \\ E_0^- & E_0^{+-} \end{pmatrix},$$

where the coefficients of R_0 are

$$E_0 = V[-\gamma_0]\tilde{R}[\gamma_0,\xi_0]V[\gamma_0], \tag{2.42}$$

$$E_0^+ = V[-\gamma_0]\varphi_0, \tag{2.43}$$

$$E_0^- = \varphi_0^* V[\gamma_0], \tag{2.44}$$

$$E_0^{+-} = 0. \tag{2.45}$$

The operator $\tilde{R}[\gamma_0,\xi_0]$ is the regularized resolvent which is equal to 0 on $\mathbb{R}\cdot\varphi_0$ and to $(H[\gamma_0,\xi_0]-\mu_0)^{-1}$ on $\varphi_0^\perp$.

Now we define, in a neighborhood of (γ_0, ξ_0, μ_0), the operator $M(\gamma,\xi,\mu)$ by

$$M(\gamma,\xi,\mu) = \begin{pmatrix} \tilde{H}[\gamma,\xi] - \mu & \tilde{\varphi}_0 \\ \varphi_0^* & 0 \end{pmatrix}.$$

The operator $M(\gamma,\xi,\mu)$ is also invertible in a neighborhood of (γ_0,ξ_0,μ_0) and we denote its inverse by

$$R(\gamma,\xi,\mu) = \begin{pmatrix} E(\gamma,\xi,\mu) & E^+(\gamma,\xi,\mu) \\ E^-(\gamma,\xi,\mu) & E^{+-}(\gamma,\xi,\mu) \end{pmatrix}.$$

It is then standard to prove the following two points (cf. Ref. 18 for details):

- The coefficients of $R(\gamma,\xi,\mu)$ are C^∞ in a neighborhood of (γ_0,ξ_0,μ_0).
- A number μ is an eigenvalue of $H[\gamma,\xi]$ if and only if $E^{+-}(\gamma,\xi,\mu)=0$.

Moreover, in a neighborhood of (γ_0,ξ_0,μ_0), if μ is an eigenvalue of $H[\gamma,\xi]$, then $V[\gamma]E^+(\gamma,\xi,\mu)$ is a corresponding eigenfunction.

Thus, in a neighborhood of (γ_0,ξ_0), the eigenvalues of the operator $H[\gamma,\xi]$ are given by the solutions of the equation $E^{+-}(\gamma,\xi,\mu)=0$. By viewing the operator $M(\gamma,\xi,\mu)$ as a perturbation of M_0, we can calculate the coefficients of $R(\gamma,\xi,\mu)$ and we obtain that

$$\partial_\mu E^{+-}(\gamma_0,\xi_0,\mu_0) = 1.$$

As the function $E^{+-}(\gamma,\xi,\mu)$ is of class C^∞, we can apply the implicit function theorem and get the existence of a number $\eta>0$ and a function μ of class C^∞ such that

$$\forall (\gamma,\xi) \in]\gamma_0-\eta,\gamma_0+\eta[\times]\xi_0-\eta,\xi_0+\eta[, \quad \forall\, \mu \in]\mu_0-\eta,\mu_0+\eta[,$$

$$E^{+-}(\gamma,\xi,\mu)=0 \Leftrightarrow \mu=\mu(\gamma,\xi).$$

This proves that the functions $(\gamma,\xi)\mapsto\mu^{(1)}(\gamma,\xi)$ and $(\gamma,\xi)\mapsto\varphi_{\gamma,\xi}$ are of class C^∞. □

C. Asymptotic behavior

The asymptotic behavior at $\pm\infty$ of the eigenvalue $\Theta(\gamma)$ with respect to the parameter γ is given in the following proposition.

Proposition II.8: There exist constants $C_0,\gamma_0>0$ such that the eigenvalue $\Theta(\gamma)$ satisfies

$$1-C_0\gamma\exp(-\gamma^2)\leqslant\Theta(\gamma)<1,\quad\forall\ \gamma\in[\gamma_0,+\infty[, \tag{2.46}$$

and

$$-\gamma^2\leqslant\Theta(\gamma)\leqslant-\gamma^2+\frac{1}{4\gamma^2},\quad\forall\ \gamma\in]-\infty,0[. \tag{2.47}$$

Proof: We prove the estimate (2.46). Note that by the min-max principle and Theorem II.2 we get for any $\gamma>0$:

$$\mu^{(1)}(0,\xi(\gamma))\leqslant\Theta(\gamma)<1. \tag{2.48}$$

The following estimate for the Neumann problem is obtained by Bolley-Helffer[17] (formula (A18):

$$|\mu^{(1)}(0,\xi)-1|\leqslant C\xi\exp-\xi^2,\quad\forall\ \xi\in[A,+\infty[,$$

where $C,A>0$ are constants independent of ξ. Recalling (2.15), the last estimate gives

$$|\mu^{(1)}(0,\xi(\gamma))-1|\leqslant C_0\gamma\exp-\gamma^2,\quad\forall\ \gamma\in[\gamma_0,+\infty[,$$

where $\gamma_0=\max(\sqrt{A},1)$ and $C_0=2C$. Upon substitution in (2.48), we arrive at the estimate (2.46).

The relation (2.15) gives the lower bound $\Theta(\gamma)\geqslant-\gamma^2$. To get the upper bound in (2.47), we use the function $e^{\gamma t}$ (with $\gamma<0$) as a trial function for the quadratic form defining $H[\gamma,0]$, this which gives

$$\frac{q[\gamma,0](e^{\gamma t})}{\|e^{\gamma t}\|^2_{L^2(\mathbb{R}_+)}}\leqslant-\gamma^2+\frac{1}{4\gamma^2},\quad\forall\ \gamma\in]-\infty,0[.$$

Therefore, we get by the min-max principle that $\mu^{(1)}(\gamma,0)\leqslant-\gamma^2+1/4\gamma^2$. Recalling (2.6), we get the upper bound in(2.47).

D. Exponential decay of the ground state

Using Agmon's technique (cf. Ref. 15), we get the following decay result for the eigenfunction φ_γ.

Proposition II.9: For each $\epsilon\in]0,1[$ there is a positive constant C_ϵ such that, for all $\gamma\in\mathbb{R}$, we have the following estimate for the eigenfunction φ_γ:

$$\left\|\exp\left(\epsilon\frac{(t-\xi(\gamma))^2}{2}\right)\varphi_\gamma\right\|_{H^1(\{t\in\mathbb{R}_+;(t-\xi(\gamma))\geqslant C_\epsilon\})}\leqslant C_\epsilon(1+\gamma_-+\gamma_-^2), \tag{2.49}$$

where we use the notation $\gamma_-=\max(-\gamma,0)$.

Proof: Let us consider a function $\Phi\in H^1(\mathbb{R}_+)$. Given an integer $N\in\mathbb{N}$, an integration by parts gives the following identity:

$$\int_0^N [|(e^{\Phi}\varphi_\gamma)'|^2 + |(t-\xi(\gamma))e^{\Phi}\varphi_\gamma|^2]\mathrm{d}t + \gamma|e^{\Phi(0)}\varphi_\gamma(0)|^2 - \varphi'_\gamma(N)e^{2\Phi(N)}\varphi_\gamma(N) = \Theta(\gamma)\|e^{\Phi}\varphi_\gamma\|^2_{L^2([0,N])} + \|\Phi' e^{\Phi}\varphi_\gamma\|^2_{L^2([0,N])}. \tag{2.50}$$

Let us recall that the eigenfunction φ_γ is strictly positive. It results then from the eigenvalue equation satisfied by φ_γ:

$$\varphi''_\gamma(t) = ((t-\xi(\gamma))^2 - \Theta(\gamma))\varphi_\gamma(t) > 0, \quad \forall\, t \in]\sqrt{\Theta(\gamma)} + \xi(\gamma), +\infty[.$$

Therefore, the function φ'_γ is increasing on $]\sqrt{\Theta(\gamma)}+\xi(\gamma), +\infty[$. On the other hand, as $\varphi_\gamma \in H^2(\mathbb{R}_+)$, the Sobolev imbedding theorem gives $\lim_{t\to+\infty}\varphi'_\gamma(t)=0$. Thus, combining with the monotonicity of φ'_γ, we get finally that

$$\varphi'_\gamma(t) < 0, \quad \forall\, t \in \sqrt{\Theta(\gamma)} + \xi(\gamma), +\infty[.$$

Taking $N > \sqrt{\Theta(\gamma)}+\xi(\gamma)$ and recalling that $\Theta(\gamma)<1$, the identity (2.50) yields the estimate:

$$\int_0^N [|(e^{\Phi}\varphi_\gamma)'|^2 + |(t-\xi(\gamma))e^{\Phi}\varphi_\gamma|^2]\mathrm{d}t + \gamma|e^{\Phi(0)}\varphi_\gamma(0)|^2 \leqslant \|e^{\Phi}\varphi_\gamma\|^2_{L^2([0,N])} + \|\Phi' e^{\Phi}\varphi_\gamma\|^2_{L^2([0,N])}. \tag{2.51}$$

To estimate the boundary term in (2.51), we recall that (2.38) (with $u=\varphi_\gamma$ and $\xi=\xi(\gamma)$) gives

$$|\varphi_\gamma(0)|^2 \leqslant 2 + (\gamma_-)^2.$$

Therefore, the estimate (2.51) becomes

$$\int_0^N [|(e^{\Phi}\varphi_\gamma)'|^2 + ((t-\xi(\gamma))^2 - |\Phi'|^2 - 1)|e^{\Phi}\varphi_\gamma|^2]\mathrm{d}t \leqslant \gamma_-\sqrt{2+(\gamma_-)^2}e^{2\Phi(0)}. \tag{2.52}$$

Now we take Φ as

$$\Phi(t) = \epsilon\frac{(t-\xi(\gamma))^2}{2}.$$

We can then rewrite (2.52) as

$$\int_{t\in[0,N],(t-\xi(\gamma))\geqslant a_\epsilon} [|(e^{\Phi}\varphi_\gamma)'|^2 + |e^{\Phi}\varphi_\gamma|^2]\mathrm{d}t \leqslant \gamma_-\sqrt{2+(\gamma_-)^2}e^{\epsilon\xi(\gamma)} + e^{\epsilon a_\epsilon}, \tag{2.53}$$

where $a_\epsilon > 0$ satisfies

$$a_\epsilon^2 - \epsilon^2 a_\epsilon - 1 \geqslant 1.$$

Notice that the first term on the right hand side of (2.53) is effective only if $\gamma<0$. Coming back to the regularity of the function $\Theta(\gamma)$, the decay of $\Theta(\gamma)$ in (2.47) and the relation (2.15), we get that the function $\xi(\gamma)$ is bounded for $\gamma<0$. Let us now take

$$C_0 = \sup_{\gamma<0}\xi(\gamma), \quad C_\epsilon = \max(a_\epsilon, e^{\epsilon C_0}, e^{\epsilon a_\epsilon}).$$

The estimate (2.53) reads now as

$$\int_{t\in[0,N],(t-\xi(\gamma))\geqslant C_\epsilon} [|(e^{\Phi}\varphi_\gamma)'|^2+|e^{\Phi}\varphi_\gamma|^2]\mathrm{d}t \leqslant C_\epsilon(1+\gamma_-+(\gamma_-)^2).$$

Noticing that the above estimate is uniform with respect to N, we get (2.49) upon passing to the limit $N\to+\infty$.

Let us now recall that the regularized resolvent $\widetilde{R}[\gamma]$ is the bounded operator defined on $L^2(\mathbb{R}_+)$ by

$$\widetilde{R}[\gamma]\phi=\begin{cases}0, & \phi\|\varphi_\gamma,\\ (H[\gamma]-\Theta(\gamma))^{-1}\phi, & \phi\perp\varphi_\gamma,\end{cases} \tag{2.54}$$

and extended by linearity. Again, using the Agmon's technique, we get that this regularized resolvent is uniformly continuous in suitable weighted spaces.

Proposition II.10: For each $\delta\in]0,1[$ *and* $\eta_0>0$, *there exist positive constants* C_0,t_0 *such that*

$$\forall\,\gamma\in[-\eta_0,\eta_0],\quad \forall\,u\in L^2(\mathbb{R}_+;e^{\delta(t-\xi(\gamma))}\mathrm{d}t),\quad u\perp\varphi_\gamma,$$

we have

$$\|e^{\delta(t-\xi(\gamma))}\widetilde{R}[\gamma]u\|_{H^1([t_0,+\infty[)}\leqslant C_0\|e^{\delta(t-\xi(\gamma))}u\|_{L^2(\mathbb{R}_+)}. \tag{2.55}$$

III. PROOF OF THEOREM I.1

In this section we prove Theorem I.1 by comparing with the basic model introduced in the preceding section. We introduce a coordinate system (s,t) near the boundary $\partial\Omega$ where t measures the distance to $\partial\Omega$ and s measures the distance in $\partial\Omega$ (cf. the Appendix).

Proposition III.1 (Upper bound): Under the hypothesis of Theorem I.1, there exist positive constants C and h_0 *such that,* $\forall h\in]0,h_0]$, *we have*

$$\mu^{(1)}(\alpha,\gamma,h)\leqslant h\Theta(h^{\alpha-1/2}(\gamma_0+Ch^{1/2}))+Ch^{3/2}. \tag{3.1}$$

Proof: We start with the easy case when $\alpha<\frac{1}{2}$ and $\gamma_0>0$. Notice that in this case, given a constant $C>0$, formula (2.46) gives the existence of $h_0>0$ such that

$$|\Theta(h^{\alpha-1/2}(\gamma_0+Ch^{1/2}))-1|\leqslant\exp(-h^{2\alpha-1}),\quad \forall\,h\in]0,h_0]. \tag{3.2}$$

By comparing with the Dirichlet realization, the min-max principle gives

$$\mu^{(1)}(\alpha,\gamma,h)\leqslant\lambda^{(1)}(h),$$

where $\lambda^{(1)}(h)$ is the first eigenvalue of the Dirichlet realization (on Ω) of $-(h\nabla-iA)^2$. Using the following upper bound for $\lambda^{(1)}(h)$ (cf. Ref. 9):

$$\lambda^{(1)}(h)\leqslant h+Ch^{3/2},\quad \forall\,h\in]0,1],$$

together with (3.2), we get (3.1).

We suppose now that $\gamma_0\leqslant 0$ if $\alpha<\frac{1}{2}$. Consider a point $x_0\in\partial\Omega$ such that $\gamma(x_0)=\gamma_0$. We suppose that $x_0=0$ in the coordinate system (s,t) near the boundary (cf. the Appendix). Using this coordinate system we construct a trial function $u_{h,\alpha}$ supported in the rectangle $K_h=]-h^{1/4},h^{1/4}[\times[0,t_0[$ following the idea of Helffer-Morame[10] and Bernoff-Sternberg.[7] Since x_0 is a minimum of γ, Taylor's formula up to the first order gives the existence of positive constants C_1,h_0 such that

$$\forall\,h\in]0,h_0],\quad |\gamma(s)-\gamma_0|\leqslant C_1h^{1/2}\quad \text{in }]-h^{1/2},h^{1/2}[.$$

Thus, given a trial function u supported in K_h, we have the following estimate:

$$q^{\alpha,\gamma}_{h,A,\Omega}(u) \leqslant q^{\alpha,\tilde{\gamma}_0}_{h,A,\Omega}(u), \quad \forall\, h \in]0,h_0], \tag{3.3}$$

where $\tilde{\gamma}_0 = \gamma_0 + C_1 h^{1/2}$. So it is enough to work with $q^{\alpha,\tilde{\gamma}_0}_{h,A,\Omega}$.

We introduce $\eta = h^{\alpha-1/2}\tilde{\gamma}_0$ and we choose now the following trial function:

$$u_{h,\alpha} = a^{-1/2} \exp\left(-i\frac{\xi(\eta)s}{h^{1/2}}\right) v_{h,\alpha}, \tag{3.4}$$

where $a(s,t) = 1 - t\kappa_r(s)$ and

$$v_{h,\alpha} = h^{-3/8}\varphi_\eta(h^{-1/2}t)\chi(t) \times f(h^{-1/4}s). \tag{3.5}$$

The function χ is a cut-off equal to 1 in a compact interval $[0, t_0/2]$ and the function $f \in C_0^\infty(]-1/2, 1/2[;\mathbb{R})$ is chosen such that $\|f\|_{L^2(\mathbb{R})} = 1$.

Note that the decay of φ_η in Proposition II.9 gives:[1] For every $\delta > 0$ and $k \in \mathbb{N}$, there exist positive constants $C_{k,\delta}$ and h_0 such that,

$$\int_{\mathbb{R}_+} t^k |\varphi_\eta(t)|^2 \mathrm{d}t \leqslant C_{k,\delta} h^{-\delta k}, \quad \forall\, h \in]0,h_0]. \tag{3.6}$$

We work with the choice of gauge given in Proposition A2. Using formula (A3), we can write

$$\begin{aligned} q^{\alpha,\tilde{\gamma}_0}_{h,A,\Omega}(u_{h,\alpha}) = &\int_{-|\partial\Omega|/2}^{|\partial\Omega|/2} \int_0^{t_0} \left[|h\partial_t v_{h,\alpha}|^2 + a^{-2} \left| \left(h^{1/2}\xi(\eta) - t\left(1 - \frac{t}{2}\kappa_r(s)\right)\right) v_{h,\alpha} \right|^2 \right] \mathrm{d}s\mathrm{d}t \\ &+ h^{3/2}\eta \int_{-|\partial\Omega|/2}^{|\partial\Omega|/2} |v_{h,\alpha}(s,0)|^2 \mathrm{d}s + h^2 \int_{-|\partial\Omega|/2}^{|\partial\Omega|/2} \int_0^{t_0} [|(\partial_t a^{-1/2}) v_{h,\alpha}|^2 + 2a^{-1/2}(\partial_t a^{-1/2}) \\ &\times (\partial_t v_{h,\alpha}) v_{h,\alpha} + a^{-2} |\partial_s v_{h,\alpha}|^2] a \mathrm{d}s\mathrm{d}t. \end{aligned} \tag{3.7}$$

Recalling the expression of $v_{h,\alpha}$ (cf.(3.5)), we can replace the function χ by 1 getting an exponentially small error on the right-hand side of (3.7), thanks to the decay of φ_η in Proposition II.9. After a change of variables and using the decay of φ_η in (3.6), the leading order term on the right-hand side of (3.7) is equal to

$$h\left(\int_0^{+\infty} [|\varphi_\eta'(t)|^2 + |(t - \xi(\eta))\varphi_\eta|^2 \mathrm{d}t] \mathrm{d}t + \eta |\varphi_\eta(0)|^2 \right),$$

and the error is of order $\mathcal{O}(h^{3/2})$. Therefore, we get constants $C, h_0 > 0$ such that

$$|q^{\alpha,\tilde{\gamma}_0}_{h,A,\Omega}(u_{h,\alpha}) - h\Theta(\eta)| \leqslant Ch^{3/2}, \quad \forall\, h \in]0,h_0].$$

Using formula (A4) and the decay of φ_η (Proposition II. 9), we obtain that the L^2 norm of $u_{h,\alpha}$ is exponentially close to 1 as $h \to 0$. The application of the min-max principle permits one now to prove (3.1).

Remark III.2: In the regime $\alpha \in]\frac{1}{2}, 1[$, *we have, thanks to Proposition II.5:*

$$\Theta(h^{\alpha-1/2}\gamma_0) = \Theta_0 + 6M_3 h^{\alpha-1/2} + \mathcal{O}(h^{2\alpha-1}).$$

Substituting the above expansion in the upper bound (3.1), we get the following upper bound for the eigenvalue $\mu^{(1)}(\alpha,\gamma,h)$,

$$\mu^{(1)}(\alpha,\gamma,h) \leqslant h\Theta_0 + 6M_3\gamma_0 h^{\alpha+1/2} + \mathcal{O}(h^{\inf(3/2,2\alpha)}).$$

We shall prove that this upper bound is actually an asymptotic expansion of $\mu^{(1)}(\alpha,\gamma,h)$ *as* h

[1] Actually we shall need this decay only when $\alpha < 1/2$ and $\gamma_0 < 0$.

tends 0 (see Remark V.11).

Proposition III.3 (Lower bound): Under the hypothesis of Theorem I.1, there exist positive constants C, C' and h_0 such that, $\forall h \in]0, h_0]$, we have

$$\mu^{(1)}(\alpha, \gamma, h) \geqslant h\Theta(h^{\alpha-1/2}\gamma_0(1 + C'h^{1/4})) - Ch^{5/4}. \tag{3.8}$$

Proof: We follow the technique of Ref. 10 and we localize by means of a partition of unity to compare with the model operators in $\mathbb{R}^2$ and $\mathbb{R} \times \mathbb{R}_+$. Let us explain the heuristic idea. A partition of unity permits one to estimate the quadratic form $q^{\alpha,\gamma}_{h,A,\Omega}$ locally in small subsets of Ω. Near the boundary, we obtain after a transformation of coordinates that the expression of $q^{\alpha,\gamma}_{h,A,\Omega}$ is to leading order asymptotics as that of the half-plane model. In the interior of Ω, the expression of the quadratic form is actually like that of the entire-plane model.

Let us introduce a partition of unity (χ_j) of $\mathbb{R}^2$ that satisfies

$$\sum_j |\chi_j|^2 = 1, \quad \sum_j |\nabla \chi_j|^2 < +\infty, \quad \text{supp}\, \chi_j \subset D(z_j, 1),$$

where for $z \in \mathbb{R}^2$ and $r > 0$, we denote by $D(z, r)$ the disk of center z and radius r.

We introduce now the scaled partition of unity:

$$\chi^h_j(z) := \chi_j(\epsilon_0 h^\rho z), \quad \forall\, z \in \mathbb{R}^2,$$

where ϵ_0 and ρ are two positive numbers to be chosen suitably. Note that (χ^h_j) now satisfies

$$\sum_j |\chi^h_j|^2 = 1, \tag{3.9}$$

$$\sum_j |\nabla \chi^h_j|^2 \leqslant C\epsilon_0^{-2} h^{-2\rho}, \tag{3.10}$$

$$\text{supp}\, \chi^h_j \subset Q^h_j := D(z^h_j, \epsilon_0 h^\rho), \tag{3.11}$$

where C is a positive constant. We can also suppose that

$$\text{either supp}\, \chi^h_j \cap \partial\Omega = \emptyset \ \text{ or } z^h_j \in \partial\Omega. \tag{3.12}$$

Note that the alternative in (3.12) permits us to write the sum in (3.9) under the form:

$$\sum = \sum_{\text{int}} + \sum_{\text{bnd}},$$

where the summation over "int" means that the support of χ^h_j does not meet the boundary while that over "bnd" means the converse.

We have now the following decomposition formula:

$$q^{\alpha,\gamma}_{h,A}(u) = \sum_j q^{\alpha,\gamma}_{h,A}(\chi^h_j u) - h^2 \sum_j \| |\nabla \chi^h_j| u\|^2, \quad \forall\, u \in H^1(\Omega), \tag{3.13}$$

usually called the IMS formula (cf. Ref. 24). We have now to bound from below each of the terms on the right-hand side of (3.13). Note that (3.10) permits one to estimate the contribution of the last term in (3.13):

$$h^2 \sum_j \| |\nabla \chi^h_j| u\|^2 \leqslant C\epsilon_0^{-2} h^{2-2\rho} \|u\|^2, \quad \forall\, u \in H^1(\Omega). \tag{3.14}$$

If χ^h_j is supported in Ω, then we have

$$q_{h,A}^{\alpha,\gamma}(\chi_j^h u) = \int_{\mathbb{R}^2} |(h\nabla - iA)\chi_j^h u|^2 \mathrm{d}x.$$

Since the lowest eigenvalue of the Schrödinger operator with constant magnetic field in $\mathbb{R}^2$ is equal to h, we get

$$q_{h,A}^{\alpha,\gamma}(\chi_j^h u) \geqslant h\int_{\Omega} |\chi_j^h u|^2 \mathrm{d}x, \quad \forall\, u \in H^1(\Omega). \tag{3.15}$$

We now have to estimate $q_{h,A,\Omega}^{\alpha,\gamma}(\chi_j^h u)$ when χ_j^h meets the boundary. It is in this case that we see the effect of the boundary condition. We shall do that by writing $q_{h,A,\Omega}^{\alpha,\gamma}(\chi_j^h u)$ in the boundary coordinates. Note that, thanks to Proposition A.1, there exists a positive constant C_1 independent of h and j such that

$$\int_{\Omega} |(h\nabla - iA)\chi_j^h u|^2 \mathrm{d}x \geqslant (1 - C_1\epsilon_0 h^{\rho})\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - i\widetilde{A})\chi_j^h u|^2 \mathrm{d}s\mathrm{d}t, \quad \forall\, u \in H^1(\Omega), \tag{3.16}$$

where $\widetilde{A}$ is the vector field associated to A by (A2).

By a gauge transformation, we get a new magnetic potential $\widetilde{A}_{\mathrm{new},j}$ satisfying

$$\widetilde{A}_{\mathrm{new},j} = \widetilde{A} - \nabla\phi_j^h,$$

$$\widetilde{A}_{\mathrm{new},j}(z_j^h) = 0,$$

$$|\widetilde{A}_{\mathrm{new},j}(w) - \widetilde{A}_{\mathrm{lin}}^j(w)| \leqslant C|w|^2, \quad w = (s,t), \tag{3.17}$$

where $A_{\mathrm{lin}}^j := \frac{1}{2}(-t,s)$ is the linear magnetic potential and $C>0$ is a constant independent of h and j.

Given $\theta>0$ and any function v of support in $\mathbb{R}\times\mathbb{R}_+$, we get by the Cauchy-Schwarz inequality,

$$\left|\int_{\mathbb{R}\times\mathbb{R}_+} (h\nabla - i\widetilde{A}_{\mathrm{new},j})v \cdot \overline{(\widetilde{A}_{\mathrm{new},j} - \widetilde{A}_{\mathrm{lin}}^j)v}\mathrm{d}s\mathrm{d}t\right| \leqslant h^{2\theta}\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - i\widetilde{A}_{\mathrm{new},j})v|^2 + h^{-2\theta}\int_{\mathbb{R}\times\mathbb{R}_+} |(\widetilde{A}_{\mathrm{new},j} - \widetilde{A}_{\mathrm{lin}}^j)v|^2.$$

Writing $\widetilde{A}_{\mathrm{new},j} = \widetilde{A}_{\mathrm{lin}}^j + (\widetilde{A}_{\mathrm{new},j} - \widetilde{A}_{\mathrm{lin}}^j)$ and using (3.17), we get a positive constant $\widetilde{C}$ independent of h and j such that

$$\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - i\widetilde{A}_{\mathrm{new},j})v|^2 \mathrm{d}s\mathrm{d}t \geqslant (1 - h^{2\theta})\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - i\widetilde{A}_{\mathrm{lin}}^j)v|^2 \mathrm{d}s\mathrm{d}t - \widetilde{C}h^{-2\theta}\||w|^2\chi_j^h u\|^2. \tag{3.18}$$

Let us recall that $\chi_j^h u$ is supported in the disk $D(z_j^h, \epsilon_0 h^{\rho})$. Upon noticing that

$$\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - i\widetilde{A})\chi_j^h u|^2 \mathrm{d}s\mathrm{d}t = \int_{\mathbb{R}\times\mathbb{R}_+} \left|(h\nabla - i\widetilde{A}_{\mathrm{new},j})\exp\left(-i\frac{\phi_j^h}{h}\right)\chi_j^h u\right|^2 \mathrm{d}s\mathrm{d}t,$$

we get by combining (3.18) (with $v = \exp(-i(\phi_j^h/h))\chi_j^h u$) together with (3.16), a constant $C_2>0$ such that

$$\int_{\mathbb{R}\times\mathbb{R}_+} |(h\nabla - iA)\chi_j^h u|^2 \mathrm{d}x \geqslant (1 - C_2\epsilon_0 h^\rho - C_2 h^{2\theta}) \int_{\mathbb{R}\times\mathbb{R}_+} \left| (h\nabla - i\widetilde{A}_{\mathrm{lin}}^j)\exp\left(-i\frac{\phi_j^h}{h}\right)\chi_j^h u \right|^2 \mathrm{d}s\mathrm{d}t$$
$$- C_2\epsilon_0 h^{4\rho-2\theta} \int_{\mathbb{R}\times\mathbb{R}_+} |\chi_j^h u|^2 \mathrm{d}s\mathrm{d}t. \tag{3.19}$$

Notice also (possibly changing C_2) we have in $D(z_j^h, \epsilon_0 h^\rho)$,

$$\gamma(x) \geqslant \gamma(z_j^h) - C_2\epsilon_0 h^\rho.$$

Then, by putting,

$$\widetilde{\gamma}_j = \frac{\gamma(z_j^h) - C_2\epsilon_0 h^\rho}{1 - C_2 h^{2\theta} - C_2\epsilon_0 h^\rho},$$

the estimate (3.19) reads finally

$$q_{h,A,\Omega}^{\alpha,\gamma}(\chi_j^h u) \geqslant (1 - C_2\epsilon_0 h^\rho - C_2 h^{2\theta}) q_{h,\widetilde{A}_{\mathrm{lin}}^j,\mathbb{R}\times\mathbb{R}_+}^{\alpha,\widetilde{\gamma}_j}\left(\exp\left(-i\frac{\phi_j^h}{h}\right)\chi_j^h u\right) - C_2\epsilon_0^2 h^{4\rho-2\theta}\|\chi_j^h u\|^2. \tag{3.20}$$

Note that this permits one to compare with the half-plane model operator and to get finally the energy estimate (cf. (1.10)):

$$q_{h,A,\Omega}^{\alpha,\gamma}(\chi_j^h u) \geqslant \{(1 - C_2\epsilon_0 h^\rho - C_2 h^{2\theta})h\Theta(h^{\alpha-1/2}\widetilde{\gamma}_j) - C_2\epsilon_0^2 h^{4\rho-2\theta}\}\|\chi_j^h u\|_{L^2(\Omega)}^2. \tag{3.21}$$

We now substitute the estimates (3.8), (3.14), and (3.15), in (3.13) and get finally

$$q_{h,A,\Omega}^{\alpha,\gamma}(u) \geqslant h\sum_{\mathrm{int}} \int_\Omega |\chi_j^h u|^2 \mathrm{d}x + h\sum_{\mathrm{bnd}} \Theta(h^{\alpha-1/2}\widetilde{\gamma}_j) \int_\Omega |\chi_j^h u|^2 \mathrm{d}x - C(h^{4\rho-2\theta} + \epsilon_0^{-2}h^{2-2\rho} + h^{1+\rho} + h^{1+2\theta})$$
$$\times \|u\|^2, \quad \forall\, u \in H^1(\Omega). \tag{3.22}$$

As γ_0 is the minimum of γ, we can replace (3.20) by the estimate

$$q_{h,A,\Omega}^{\alpha,\gamma}(\chi_j^h u) \geqslant (1 - C_2\epsilon_0 h^\rho - C_2 h^{2\theta}) q_{h,\widetilde{A}_{\mathrm{lin}}^j,\mathbb{R}\times\mathbb{R}_+}^{\alpha,\widetilde{\gamma}_0}\left(\exp\left(-i\frac{\phi_j^h}{h}\right)\chi_j^h u\right) - C_2\epsilon_0^2 h^{4\rho-2\theta}\|\chi_j^h u\|^2, \tag{3.23}$$

where $\widetilde{\gamma}_0$ is defined by

$$\widetilde{\gamma}_0 := \frac{\gamma_0}{1 - C_2 h^{2\theta} - C_2\epsilon_0 h^\rho}.$$

We then get instead of (3.22):

$$q_{h,A,\Omega}^{\alpha,\gamma}(u) \geqslant h\sum_{\mathrm{int}} \int_\Omega |\chi_j^h u|^2 \mathrm{d}x + h\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0)\sum_{\mathrm{bnd}} \int_\Omega |\chi_j^h u|^2 \mathrm{d}x - C(h^{4\rho-2\theta} + \epsilon_0^{-2}h^{2-2\rho} + h^{1+\rho} + h^{1+2\theta})$$
$$\times \|u\|^2, \quad \forall\, u \in H^1(\Omega). \tag{3.24}$$

The advantage of (3.22) is that it gives a lower bound of the quadratic form $q_{h,A,\Omega}^{\alpha,\gamma}$ in terms of a potential, see however Sec. IV.

We choose now $\epsilon_0 = 1$, and we optimize by taking $2-2\rho = 1+\rho = 4\rho-2\theta$ (i.e., $\rho = 3/8$ and $\theta = 1/8$) in (3.24). We obtain then (3.8) by applying the min-max principle. □

Proof of Theorem I.1: The proof follows in principle from Propositions III.1 and III.3. Actually, in the regime $\alpha<\frac{1}{2}$, we use further Proposition II.8, while in the regime $\alpha\geqslant\frac{1}{2}$, we use the continuity of the function $\Theta(\gamma)$ (Proposition II.4). □

IV. LOCALIZATION OF THE GROUND STATE

We work in this section under the hypotheses of Theorem I.3. Due to Theorem I.1 we have in this case that

$$\lim_{h\to 0}\frac{\mu^{(1)}(\alpha,\gamma,h)}{h}<1. \tag{4.1}$$

Then this gives, by following the same lines of the proof of Theorem 6.3 in Ref. 10, the following proposition.

Theorem IV.1: *Under the hypotheses of Theorem I.3, there exist positive constants* δ, C, h_0 *such that, for all* $h\in\,]0,h_0]$, *a ground state* $u_{\alpha,\gamma,h}$ *of the operator* $P^{\alpha,\gamma}_{h,A,\Omega}$ *satisfies*

$$\left\|\exp\left(\frac{\delta d(x,\partial\Omega)}{h^{\beta}}\right)u_{\alpha,\gamma,h}\right\|_{L^2(\Omega)}\leqslant C\|u_{\alpha,\gamma,h}\|_{L^2(\Omega)}, \tag{4.2}$$

and

$$\left\|\exp\left(\frac{\delta d(x,\partial\Omega)}{h^{\beta}}\right)u_{\alpha,\gamma,h}\right\|_{H^1(\Omega)}\leqslant Ch^{-\min(1/2,\beta)}\|u_{\alpha,\gamma,h}\|_{L^2(\Omega)}, \tag{4.3}$$

where $\beta=1-\alpha$ *if* $\gamma_0<0$ *and* $\alpha<\frac{1}{2}$, *and* $\beta=1/2$ *otherwise.*

Proof: Integrating by parts, we get for any Lipschitz function Φ:

$$q^{\alpha,\gamma}_{h,A,\Omega}\left(\exp\left(\frac{\Phi}{h^{\beta}}\right)u_{\alpha,\gamma,h}\right)=\mu^{(1)}(\alpha,\gamma,h)\left\|\exp\left(\frac{\Phi}{h^{\beta}}\right)u_{\alpha,\gamma,h}\right\|^2_{L^2(\Omega)}+h^{2-2\beta}\left\||\nabla\Phi|\exp\left(\frac{\Phi}{h^{\beta}}\right)u_{\alpha,\gamma,h}\right\|^2_{L^2(\Omega)}. \tag{4.4}$$

Let $u=\exp(\Phi/h^{\beta})u_{\alpha,\gamma,h}$. Using the lower bound for $q^{\alpha,\gamma}_{h,A,\Omega}(u)$ in (3.24) together with the upper bound for $\mu^{(1)}(\alpha,\gamma,h)$ in (3.1), we get from (4.4):

$$\sum_{\text{int}}\int_{\Omega}(1-\Theta(h^{\alpha-1/2}(\gamma_0+Ch^{1/2}))-C\epsilon_0^{-2}h^{1-2\rho}-Ch^{4\rho-2\theta-1}-Ch^{\min(\rho,2\theta)}-h^{1-2\beta}|\nabla\Phi|^2)\times|\chi_j^h u|^2\mathrm{d}x$$

$$\leqslant\sum_{\text{bnd}}\int_{\Omega}(\Theta(h^{\alpha-1/2}\tilde{\gamma}_0)-\Theta(h^{\alpha-1/2}(\gamma_0+Ch^{1/2}))+h^{\min(4\rho-2\theta-1,1-2\rho)}+h^{1-2\beta}|\nabla\Phi|^2)\times|\chi_j^h u|^2\mathrm{d}x.$$

We choose $\rho=\beta$ so that each χ_j^h is supported in a disk of radius $\epsilon_0 h^{\beta}$. We choose also $\theta>0$ such that $4\rho-2\theta-1>0$ and we define the function Φ by

$$\Phi(x)=\delta\max(\mathrm{dist}(x,\partial\Omega);\epsilon_0 h^{\beta}),$$

where δ is a positive constant to be chosen appropriately. Note that $1-\Theta(h^{\alpha-1/2}\tilde{\gamma}_0)$ decays in the following way:

$$\exists\, C_0,h_0>0\text{s.t.},\quad \forall\, h\in\,]0,h_0],$$

$$1-\Theta(h^{\alpha-1/2}\tilde{\gamma}_0)\geqslant C_0h^{2\alpha-1}\quad\text{if }\gamma_0<0\text{ and }\alpha<\frac{1}{2},$$

$$1-\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0)\geqslant C_0 \quad \text{otherwise}.$$

Thus we can choose ϵ_0 and δ small enough, so that we get finally the following decay:

$$\sum_{\text{int}}\int_\Omega\left|\chi_j^h\exp\frac{\Phi}{h^\beta}u_{\alpha,\gamma,h}\right|^2\mathrm{d}x\leqslant C\int_\Omega|u_{\alpha,\gamma,h}|^2\mathrm{d}x.$$

This actually permits one to conclude (4.2) and, thanks to (4.4),

$$q_{h,A,\Omega}^{\alpha,\gamma}\left(\exp\frac{\delta d(x,\partial\Omega)}{h^\beta}u_{\alpha,\gamma,h}\right)\leqslant Ch^{\min(2-2\beta,1)}\left\|\exp\frac{\delta d(x,\partial\Omega)}{h^\beta}u_{\alpha,\gamma,h}\right\|^2_{L^2(\Omega)}. \tag{4.5}$$

For a function $u\in H^1(\Omega)$, let $\widetilde{u}(s,t)$ be defined by means of boundary coordinates (s,t) and equal to the restriction of u in Ω_{t_0} (cf. the Appendix). Notice that

$$|\widetilde{u}(s,0)|^2=-2\int_0^\infty\{\partial_t(\chi(t)\widetilde{u}(s,t))\}\chi(t)\widetilde{u}(s,t)\mathrm{d}t,$$

where χ is the same cut-off introduced in (3.5). Integrating the above identity with respect to the variable s then applying a Cauchy-Schwarz inequality, we get after a change of variables the following interpolation inequality:

$$\|u\|^2_{L^2(\partial\Omega)}\leqslant C\|u\|_{L^2(\Omega)}\times\|u\|_{H^1(\Omega)},$$

where C is a positive constant depending only on Ω.

Applying again a Cauchy-Schwarz inequality, the preceding estimate gives

$$\|(h\nabla-iA)u\|^2_{L^2(\Omega)}\leqslant 2q_{h,A,\Omega}^{\alpha,\gamma}(u)+Ch\|u\|^2_{L^2(\Omega)},\quad \forall\, u\in H^1(\Omega).$$

In particular, for $u=\exp\left(\frac{\delta d(x,\partial\Omega)}{h^\beta}\right)u_{\alpha,\gamma,h}$, we get (4.3), thanks to (4.2) and (4.5). □

We study now the decay near the boundary. Let us consider a number $\beta>0$ and a Lipschitz function Φ_0 defined in $\bar{\Omega}$. The function Φ_0 and the number β will be chosen later in an appropriate manner. Choosing $\rho=\frac{3}{8}$, $\theta=\frac{1}{8}$, and ϵ_0 large enough, the energy estimate (3.22) together with the upper bound (3.1) give the existence of a positive constant C such that

$$\begin{aligned}0\geqslant h\sum_{\text{int}}\int_\Omega&(1-\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0)-Ch^{1/4}-h^{1-2\beta}|\nabla\Phi_0|^2)\left|\exp\left(\frac{\Phi_0}{h^\beta}\right)\chi_j^h u_{\alpha,\gamma,h}\right|^2\mathrm{d}x\\&+h\sum_{\text{bnd}}\int_\Omega[(\Theta(h^{\alpha-1/2}\widetilde{\gamma}(x))-\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0))-Ch^{1/4}-h^{1-2\beta}|\nabla\Phi_0|^2]\left|\exp\left(\frac{\Phi_0}{h^\beta}\right)\chi_j^h u_{\alpha,\gamma,h}\right|^2\mathrm{d}x,\end{aligned}$$

where $\widetilde{\gamma}_0=\gamma_0+Ch^{1/2}$. The function γ is extended to a small boundary sheath by means of boundary coordinates in the following way:

$$\gamma(x)=\gamma(s(x)),\quad \forall\, x\in\Omega_{t_0}.$$

In the case $\alpha<\frac{1}{2}$ and $\gamma_0=0$, thanks to Proposition II.8, the difference between $\Theta(h^{\alpha-1/2}\widetilde{\gamma}(x))$ and $\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0)$ decays in the following way:

$$\forall\,\varepsilon>0,\quad \exists\, C_\varepsilon>0,\quad \forall\, x\in(\gamma-\gamma_0)^{-1}([\epsilon,+\infty[),\quad \Theta(h^{\alpha-1/2}\widetilde{\gamma}(x))-\Theta(h^{\alpha-1/2}\widetilde{\gamma}_0)>C_\varepsilon.$$

In the case $\alpha<\frac{1}{2}$ and $\gamma_0<0$, we have a stronger decay:

$$\forall\,\varepsilon>0,\quad \exists\, C_\varepsilon>0,\quad \forall\, x\in(\gamma-\gamma_0)^{-1}([\epsilon,+\infty[),$$

$$\Theta(h^{\alpha-1/2}\tilde{\gamma}(x)) - \Theta(h^{\alpha-1/2}\tilde{\gamma}_0) > C_\varepsilon h^{1-2\alpha}.$$

So by taking Φ_0 in the form:

$$\Phi_0(x) = \delta\chi(\mathrm{dist}(x,\partial\Omega))\mathrm{dist}(x,\{x \in \partial\Omega; \gamma(x) = \gamma_0\}),$$

with δ an appropriate positive constant and χ is the same as in (3.5), we get for each $\epsilon > 0$ the following decay near the boundary:

$$\int_{\mathrm{dist}(x,\partial\Omega)<t_0} \left| \exp \frac{\Phi_0}{h^\beta} u_{\alpha,\gamma,h} \right|^2 \mathrm{d}x \leqslant C_\epsilon \exp \frac{\epsilon}{h^\beta} \|u_{\alpha,\gamma,h}\|^2, \quad \forall\, h \in]0,h_\epsilon], \tag{4.6}$$

with $\beta = 1-\alpha$ if $\gamma_0 < 0$ and $\alpha < \frac{1}{2}$, and $\beta = \frac{1}{2}$ otherwise. This gives finally the decay in Theorem I.3.

For the critical case $\alpha = \frac{1}{2}$ and γ_0 arbitrary, we define the function Φ_0 by

$$\Phi_0(x) = \delta\chi(\mathrm{dist}(x,\partial\Omega))\mathrm{dist}_{\mathrm{agm}}(x,\{x \in \partial\Omega; \gamma(x) = \gamma_0\}),$$

where $\mathrm{dist}_{\mathrm{agm}}$ is the Agmon distance associated to the metric $(\Theta(\gamma(x)) - \Theta(\gamma_0))_+$. We obtain then a similar decay result to (4.6).

In the case when $\alpha > \frac{1}{2}$, we need a finer energy estimate than (3.22), see however Remark V.11.

V. TWO-TERM ASYMPTOTICS

In this section we suppose in addition to the hypotheses of Theorem II.1 that $\alpha \geqslant \frac{1}{2}$. We give two-term asymptotic expansions for the ground state energy showing the influence of the scalar curvature and we finish the proofs of the remaining theorems announced in Sec. I.

A. Upper bound

We construct a trial function defined by means of boundary coordinates (s,t) near a point $z_0 \in \partial\Omega$. We suppose that $z_0 = 0$ in the coordinate system (s,t) and we denote by $\kappa_0 = \kappa_r(0)$, $a_0 = 1 - t\kappa_0$ and $\eta(z_0) = h^{\alpha-1/2}\gamma(z_0)$. We then define the trial function:

$$u_h = \exp\left(-i\frac{\xi(\eta(z_0))s}{h^{1/2}}\right) v_h(s,t), \tag{5.1}$$

with

$$v_h(s,t) = h^{-5/16} a_0^{-1/2}(t) \varphi_{\eta(z_0)}(h^{-1/2}t)\chi(t) \cdot f(h^{-1/8}s), \tag{5.2}$$

and where the functions χ and f are as in (3.5).

We continue now to work in the spirit of Ref. 10. We work with the gauge given in Proposition A.2. An explicit calculation, thanks to the decay of $\varphi_{\eta(z_0)}$ (Proposition II.9), gives the following lemma.

Lemma V.1: With the above notations, for each $\alpha \in \left[\frac{1}{2}, 1\right]$ *and* $\gamma \in C^\infty(\partial\Omega;\mathbb{R})$, *there exist positive constants* C, h_0 *such that,* $\forall h \in]0,h_0]$, *we have the following estimate:*

$$\left| q_{h,A,\Omega}^{\alpha,\gamma(z_0)}(u_h) - \int_{\mathbb{R}_+} H^h(U^h\varphi_{\eta(z_0)}) \times (U^h\varphi_{\eta(z_0)})\mathrm{d}t \right| \leqslant Ch^{13/8}, \tag{5.3}$$

where the operators H^h *and* U^h *are defined, respectively, by*

$$H^h = a_0^{-2}\left(t\left(1 - t\frac{\kappa_0}{2}\right) - h^{1/2}\xi(\eta(z_0))\right)^2 - h^2 a_0^{-1}\partial_t(a_0\partial_t),$$

$$(U^h g)(t) = h^{-1/4} g(h^{-1/2}t), \quad \forall\, g \in L^2(\mathbb{R}_+).$$

Proof: Note that in the support of u_h we have[2]

$$a = a_0 + \mathcal{O}(h^{5/8}), \quad \widetilde{A}_1 = -t\left(1 - \frac{t}{2}\kappa_0\right) + \mathcal{O}(h^{9/8}).$$

Then, thanks to formula (A3) (also cf. (3.7)) and the decay of $\varphi_{\eta(z_0)}$ (Proposition II.9), we get modulo $\mathcal{O}(h^{13/8})$:

$$q^{\alpha,\gamma(z_0)}_{h,A,\Omega}(u_h) = \int_{\mathbb{R}\times\mathbb{R}_+} a_0\left\{|h\partial_t v_h|^2 + a_0^{-2}\left|\left(t\left(1-\frac{t}{2}\kappa_0\right) - h^{1/2}\xi(\eta(z_0))\right)v_h\right|^2\right\}\mathrm{d}s\mathrm{d}t$$
$$+ h^{3/2}\eta(z_0)\int_{\mathbb{R}} |v_h(s,0)|^2. \tag{5.4}$$

Integrating with respect to s, the right-hand side above is equal to

$$h^{-1/2}\int_{\mathbb{R}} a_0\left\{h^2|\partial_t(a_0^{-1/2}\varphi_{\eta(z_0)}(h^{-1/2}t)\chi(t))|^2 + a_0^{-3}\left|\left(t\left(1-\frac{t}{2}\kappa_0\right) - h^{1/2}\xi(\eta(z_0))\right)\varphi_{\eta(z_0)}\right.\right.$$
$$\left.\left.\times(h^{-1/2}t)\chi(t)\right|^2\right\}\mathrm{d}s\mathrm{d}t + h\,\eta(z_0)|\varphi_{\eta(z_0)}(0)|^2.$$

We can replace the function χ in the above expression by 1 getting an exponentially small error, thanks to Proposition II.9. Thus, modulo a small exponential error, we rewrite the above expression as

$$\int_{\mathbb{R}}\left\{h^2 a_0|\partial_t(U^h\varphi_{\eta(z_0)})|^2 + a_0^{-2}\left|\left(t\left(1-\frac{t}{2}\kappa_0\right) - h^{1/2}\xi(\eta(z_0))\right)(U^h\varphi_{\eta(z_0)})\right|^2\right\}\mathrm{d}s\mathrm{d}t$$
$$+ h^{3/2}\eta(z_0)|(U^h\varphi_{\eta(z_0)})(0)|^2.$$

Notice that we have the boundary condition $(U^h\varphi_{\eta(z_0)})'(0) = h^{-1/2}\eta(z_0)(U^h\varphi_{\eta(z_0)})(0)$. Therefore, integrating by parts, the above expression is equal to $\int_{\mathbb{R}_+} H^h(U^h\varphi_{\eta(z_0)})\times(U^h\varphi_{\eta(z_0)})\mathrm{d}t$. Upon substituting in (5.3), this finishes the proof of the lemma. □

Similar computations also give the following lemma.

Lemma V.2: Under the hypotheses of Lemma V.1, there exist positive constants C, h_0 such that, $\forall h \in]0, h_0]$, we have

$$\|(H^h - H_0^h - H_1^h)U^h\varphi_{\eta(z_0)}\|_{L^2(\mathbb{R}_+)} \leqslant Ch^2, \tag{5.5}$$

where the operators H_0^h and H_1^h are defined, respectively, by

$$H_0^h = -h^2\partial_t^2 + (t - h^{1/2}\xi(\eta(z_0)))^2,$$

$$H_1^h = 2t\kappa_0(t - h^{1/2}\xi(\eta(z_0)))^2 - \kappa_0 t^2(t - h^{1/2}\xi(\eta(z_0))) + h^2\kappa_0\partial_t.$$

Let us denote by (cf. (2.24) and (2.25)):

$$M_3\left(\tfrac{1}{2}, \gamma(z_0)\right) = M_3(\gamma(z_0)), \quad M_3(\alpha, \gamma(z_0)) = M_3 \quad \text{for } \alpha > \tfrac{1}{2}.$$

The next lemma permits us to conclude an upper bound for the eigenvalue $\mu^{(1)}(\alpha, \gamma, h)$.

Lemma V.3: Under the above notations, there exist positive constants C, h_0 such that, when $h \in]0, h_0]$, we have the following estimate:

[2]Actually, if z_0 is a point of maximum of κ_r, the remainder is better and of order $\mathcal{O}(h^{3/4})$ for the first term. Consequently, we obtain (5.4) modulo an error of order $\mathcal{O}(h^{7/4})$.

$$|q^{\alpha,\gamma}_{h,A,\Omega}(u_h) - \{\Theta(\eta(z_0)) - 2M_3(\alpha,\gamma(z_0))\kappa_0 h^{3/2}\}\|u_h\|^2_{L^2(\Omega)}| \leqslant Ch^{\epsilon_\alpha},$$

where $\epsilon_\alpha = \inf(13/8, 2\alpha + \frac{1}{2})$ *for* $\alpha > \frac{1}{2}$ *and* $\epsilon_{1/2} = 13/8$.

Proof: Notice that in the support of u_h we have $\gamma(z) = \gamma(z_0) + \mathcal{O}(h^{1/8})$. Then this gives

$$q^{\alpha,\gamma}_{h,A,\Omega}(u_h) - q^{\alpha,\gamma(z_0)}_{h,A,\Omega}(u_h) = \mathcal{O}(h^{9/8+\alpha}).$$

In view of Lemmas V.1 and V.2, we get the following estimate:

$$\left| q^{\alpha,\gamma}_{h,A,\Omega}(u_h) - \int_{\mathbb{R}_+} (H^h_1 + H^h_0)(U^h \varphi_{\eta(z_0)}) \times U^h \varphi_{\eta(z_0)} dt \right| \leqslant Ch^{13/8}. \tag{5.6}$$

We note also that we have the following relations:

$$(U^h)^\star H^h_0 U^h = h\{-\partial_t^2 + (t - \xi(\eta(z_0)))^2\}, \tag{5.7}$$

$$(U^h)^\star H^h_1 U^h = \kappa_0 h^{3/2} H_1, \tag{5.8}$$

where the operator H_1 is defined by

$$H_1 = (t - \xi(\eta(z_0)))^3 - \xi(\eta(z_0))^2 (t - \xi(\eta(z_0))) + \partial_t.$$

By defining $K_3(\alpha,h) := \int_{\mathbb{R}_+} H_1 \varphi_{\eta(z_0)} \cdot \varphi_{\eta(z_0)} \mathrm{d}t$, the estimate (5.6) reads as

$$|q^{\alpha,\gamma}_{h,A,\Omega}(u_h) - \{h\Theta(\eta(z_0)) + K_3(\alpha,h)\kappa_0 h^{3/2}\}| \leqslant Ch^{13/8}. \tag{5.9}$$

Now, for $\alpha = \frac{1}{2}$, we get by using (2.3) that $K_3(\frac{1}{2},h) = -2M_3(\frac{1}{2},\gamma(z_0))$. For $\alpha > \frac{1}{2}$, thanks to Propositions II.4 and II.5, we get that

$$K_3(\alpha,h) = -2M_3 + \mathcal{O}(h^{2\alpha-1}).$$

Finally, the decay of $\varphi_{\eta(z_0)}$ in Proposition II.9 gives that $\|u_h\|_{L^2(\Omega)}$ is exponentially close to 1. This achieves the proof of the lemma. □

The min-max principle gives now, thanks to Lemma V.3, an upper bound for $\mu^{(1)}(\alpha,\gamma,h)$. Under the hypothesis of Theorem I.4, we take z_0 such that

$$(\kappa_r - 3\gamma)(z_0) = (\kappa_r - 3\gamma)_{\max}$$

and we use the expansion (cf. (2.27)):

$$\Theta(\eta(z_0)) = \Theta_0 + 6M_3\gamma(z_0)h^{1/2} + \mathcal{O}(h).$$

Therefore, (5.9) gives the following upper bound:

$$\mu^{(1)}(1,\gamma,h) \leqslant h\Theta_0 - 2M_3(\kappa_r - 3\gamma)_{\max} h^{3/2} + \mathcal{O}(h^{13/8}). \tag{5.10}$$

Under the hypothesis of Theorem 1.5, we choose z_0 such that $\kappa_r(z_0) = (\kappa_r)_{\max}$.

B. Lower bound

As in the proof of Proposition III.3, we consider a standard scaled partition of unity[3] $(\chi_{j,h^{1/6}})_{j\in\mathbb{Z}^2}$ of $\mathbb{R}^2$ that satisfies

$$\sum_{j\in J} |\chi_{j,h^{1/6}}(z)|^2 = 1, \quad \sum_{j\in J} |\nabla\chi_{j,h^{1/6}}(z)|^2 \leqslant Ch^{-1/3}, \tag{5.11}$$

[3]We take a partition of unity associated to squares instead of discs.

$$\operatorname{supp} \chi_{j,h^{1/6}} \subset jh^{1/6} + [-h^{1/6}, h^{1/6}]^2. \tag{5.12}$$

We define the following set of indices:

$$J^1_{\tau(h)} := \{j \in \mathbb{Z}^2; \operatorname{supp} \chi_{j,h^{1/6}} \cap \Omega \neq \phi, \operatorname{dist}(\operatorname{supp} \chi_{j,h^{1/6}}, \partial\Omega) \leqslant \tau(h)\},$$

where the number $\tau(h)$ is defined by

$$\tau(h) = h^\delta \quad \text{with } \tfrac{1}{6} \leqslant \delta \leqslant \tfrac{1}{2}, \tag{5.13}$$

and the number δ will be chosen in a suitable manner.

We consider also another scaled partition of unity in $\mathbb{R}$:

$$\psi^2_{0,\tau(h)}(t) + \psi^2_{1,\tau(h)}(t) = 1, \quad |\psi'_{j,\tau(h)}(t)| \leqslant acC\tau(h), \quad j = 0,1, \tag{5.14}$$

$$\operatorname{supp} \psi_{0,\tau(h)} \subset \left[\frac{\tau(h)}{20}, +\infty[, \operatorname{supp}\psi_{1,\tau(h)} \subset]-\infty, \frac{\tau(h)}{10} \right]. \tag{5.15}$$

Note that, for each $j \in J^1_{\tau(h)}$, the function $\psi_{1,\tau(h)}(t)\chi_{j,h^{1/6}}(s,t)$ could be interpreted, by means of boundary coordinates, as a function in $\bar{\Omega}$. Moreover, each $\psi_{1,\tau(h)}(t)\chi_{j,h^{1/6}}(s,t)$ is supported in a rectangle

$$K(j,h) =]-h^{1/6} + s_j, s_j + h^{1/6}[\times [0, h^\delta[$$

near $\partial\Omega$. The role of δ is then to control the size of the width of each rectangle $K(j,h)$. Due to the exponential decay of a ground state away from the boundary (Theorem IV.1), we get the following lemma.

Lemma V.4: Suppose that $\alpha > \frac{1}{2}$. With the above notations, an L^2-normalized ground state $u_{\alpha,\gamma,h}$ of the operator $P^{\alpha,\gamma}_{h,A,\Omega}$ satisfies

$$\left| \sum_{j \in J^1_{\tau(h)}} q^{\alpha,\gamma}_{h,A,\Omega}(\chi_{j,h^{1/6}}\psi_{1,\tau(h)}u_{\gamma,h}) - \mu^{(1)}(\alpha,\gamma,h) \right| \leqslant Ch^{5/3}. \tag{5.16}$$

The proof of (5.16) follows the same lines of that in Ref. 10 (Formulas (10.4), (10.5) and (10.6)).

For each $j \in J^1_{\tau(h)}$, we define a unique point $z_j \in \partial\Omega$ by the relation $s(z_j) = s_j$. We denote then by $\kappa_j = \kappa_r(z_j)$, $a_j(t) = 1 - \kappa_j t$, $A^j(t) = -t(1 - t/2\kappa_j)$, and $\gamma_j = \gamma(z_j)$.

We consider now the k-family of one-dimensional differential operators:

$$H_{h,j,k} = -h^2 a_j^{-1}\partial_t(a_j\partial_t) + (1 + 2\kappa_j t)(hk - A^j)^2, \tag{5.17}$$

where k is a real parameter. We denote by $H^{\alpha,\gamma,D}_{h,j,k}$ the self-adjoint realization on $L^2(]0,h^\delta[; a_j(t)dt)$ of $H_{h,j,k}$ whose domain is given by

$$D(H^{\gamma,D}_{h,j,k}) = \{v \in H^2(]0,h^\delta[); v'(0) = h^\alpha\tilde{\gamma}_j v(0), v(h^\delta) = 0\}. \tag{5.18}$$

The parameter $\tilde{\gamma}_j$ is defined by

$$\tilde{\gamma}_j = \gamma_j + \varepsilon(h),$$

where $\varepsilon(h) = 0$ if the function γ is constant; if γ is not constant, then there are constants $C, h_0 > 0$ such that

$$|\varepsilon(h)| \leqslant Ch^{1/6}, \quad \forall\, h \in]0,h_0].$$

We now introduce

$$\mu_1^j(\alpha,\gamma,h) := \inf_{k\in\mathbb{R}} \inf \mathrm{Sp}(H_{h,j,k}^{\gamma,D}). \tag{5.19}$$

We have now the following lemma:

Lemma V.5: For each $\alpha \in \left[\frac{1}{2}, +\infty\right[$, *we have under the above notations:*

$$\mu^{(1)}(\alpha,\gamma,h) \geqslant \Big(\inf_{j\in J^1_{\tau(h)}} \mu_1^j(\alpha,\gamma,h)\Big) + \mathcal{O}(h^{5/3}). \tag{5.20}$$

Again the proof follows the same lines of Ref. 10 (Sec. 11), but let us explain briefly the main steps. We express each term $q^{\alpha,\gamma}_{h,A,\Omega}(\psi_{1,\tau(h)}\chi_{j,h^{1/6}}u_{\alpha,\gamma,h})$ in boundary coordinates. We work with the local choice of gauge given in Proposition A.2. We expand now all terms by Taylor's formula near $(s_j,0)$. After controlling the remainder terms, thanks to the exponential decay of the ground states away from the boundary, we apply a partial Fourier transformation in the tangential variable s and we get finally the result of the lemma.

We now have to find, uniformly over $k\in\mathbb{R}$, a lower bound for the first eigenvalue $\mu_1^j(k;\alpha,\gamma,h)$ of the operator $H^{\alpha,\gamma,D}_{h,j,k}$. Putting $\beta=\kappa_j$, $\xi=-h^{1/2}k$, and $\eta=\tilde{\gamma}_j$, we get by a scaling argument

$$\mu_1^j(k;\alpha,\gamma,h) = h\mu_1(H^{\alpha,\eta,D}_{h,\beta,\xi}),$$

where $\mu_1(H^{\alpha,\eta,D}_{h,\beta,\xi})$ is the first eigenvalue of the one-dimensional operator:

$$H^{\alpha,\eta,D}_{h,\beta,\xi} = -\partial_t^2 + (t-\xi)^2 + \beta h^{1/2}(1-\beta h^{1/2}t)^{-1}\partial_t + 2\beta h^{1/2}t\left(t-\xi-\beta h^{1/2}\frac{t^2}{2}\right)^2 - \beta h^{1/2}t^2(t-\xi) + \beta^2 h\frac{t^4}{4}, \tag{5.21}$$

whose domain is defined by

$$D(H^{\alpha,\eta,D}_{h,\beta,\xi}) = \{u\in H^2(]0,h^{\delta-1/2}[); u'(0) = h^{\alpha-1/2}\eta u(0), u(h^{\delta-1/2}) = 0\}.$$

We have then to find (when $\eta,\beta\in\,]-M,M[$ and M a given positive constant), uniformly with respect to $\xi\in\mathbb{R}$, a lower bound for the eigenvalue $\mu_1(H^{\alpha,\eta,D}_{h,\beta,\xi})$. The min-max principle gives the following preliminary localization of the spectrum of the operator $H^{\alpha,\eta,D}_{h,\beta,\xi}$:

Lemma V.6: For each $M>0$ *and* $\alpha\in\left[\frac{1}{2},+\infty\right[$, *there exist positive constants* C, h_0 *such that*

$$\forall\ \eta,\beta\in\,]-M,M[, \quad \forall\ \xi\in\mathbb{R}, \quad \forall\ h\in\,]0,h_0],$$

we have

$$|\mu_j(H^{\alpha,\eta,D}_{h,\beta,\xi}) - \mu_j(H^{\alpha,\eta,D}_{0,\xi})| \leqslant Ch^{2\delta-1/2}(1+\mu_j(H^{\alpha,\eta,D}_{0,\xi})), \tag{5.22}$$

where, for an operator T *having a compact resolvent,* $\mu_j(T)$ *denotes the increasing sequence of eigenvalues of* T.

Remark V.7: Note that the min-max principle gives now that

$$\mu_j(H^{\alpha,\eta,D}_{0,\xi}) \geqslant \mu^{(j)}(h^{\alpha-1/2}\eta,\xi),$$

where, for $\tilde{\eta}\in\mathbb{R}$, $\mu^{(j)}(\tilde{\eta},\xi)$ *is the increasing sequence of eigenvalues of the operator* $H[\eta,\xi]$ *introduced in* (2.2).

The following lemma deals with the case when ξ is not localized very close to $\xi(h^{\alpha-1/2}\eta)$.

Lemma V.8: Suppose that $\delta\in\,]1/4,1/2[$. *For each* $\alpha\geqslant\frac{1}{2}$, *there exists* $\rho\in\,]0,\delta-\frac{1}{4}]$, *and for each* $M>0$, *there exist positive constants* $\zeta, h_0>0$ *such that*

$$\forall\ \eta,\beta\in\,]-M,M[, \quad \forall\ \xi \text{ such that } |\xi-\xi(h^{\alpha-1/2}\eta)|\geqslant\zeta h^{\rho}, \quad \forall\ h\in\,]0,h_0],$$

we have

$$\mu_1(H^{\alpha,\eta,D}_{h,\beta,\xi}) \geqslant \Theta(h^{\alpha-1/2}\eta) + h^{2\rho}. \tag{5.23}$$

Proof: It is sufficient to obtain (5.23) for $\mu^{(1)}(h^{\alpha-1/2}\eta,\xi)$, thanks to Lemma V.6 and Remark V.7. We start with the case when $\alpha=\frac{1}{2}$ and $\eta\in\,]-M,M[$. Writing Taylors formula up to the second order for the function $\xi\mapsto\mu^{(1)}(\eta,\xi)$, we get positive constants θ, C_1 such that when $|\xi-\xi(\eta)| \leqslant \theta$, we have

$$\mu^{(1)}(\eta,\xi) \geqslant \Theta(\eta) + C_1|\xi-\xi(\eta)|^2.$$

Then by taking ζ such that $C_1\zeta>\zeta_0$, where $\zeta_0>1$ is a constant to be chosen appropriately, we get when $\zeta h^\rho \leqslant |\xi-\xi(\eta)| \leqslant \theta$,

$$\mu^{(1)}(\eta,\xi) \geqslant \Theta(\eta) + \zeta_0 h^{2\rho},$$

where ρ is also a positive constant to be chosen later. When $|\xi-\xi(\eta)|>\theta$, we get a positive constant ϵ_θ such that

$$\mu^{(1)}(\eta,\xi) \geqslant \Theta(\eta) + \epsilon_\theta.$$

Then by choosing h_0 such that $\zeta_0 h_0^\rho < \epsilon_\theta$, we get for $|\xi-\xi(\eta)| \geqslant \zeta h^\rho$ and $h\in\,]0,h_0]$:

$$\mu^{(1)}(\eta,\xi) \geqslant \Theta(\eta) + \zeta_0 h^{2\rho}. \tag{5.24}$$

We treat now the case when $\alpha>1/2$. Note that the min-max principle gives uniformly for all $\xi \in \mathbb{R}$ and $\eta\in\,]-M,M[$,

$$\mu^{(1)}(h^{\alpha-1/2}\eta,\xi) \geqslant (1 - C\eta_- h^{\alpha-1/2})\mu^{(1)}(0,\xi).$$

Then using (5.24) for $\eta=0$ and $\rho=\inf\left(\delta-\frac{1}{4}, \alpha-\frac{1}{2}\right)$, we can choose ζ_0 large enough so that we have for $|\xi-\xi_0| \geqslant \zeta h^\rho$:

$$\mu^{(1)}(h^{\alpha-1/2}\eta,\xi) \geqslant \Theta(h^{\alpha-1/2}\eta) + \frac{\zeta_0}{2}h^\rho.$$

To finish the proof, we replace ξ_0 by $\xi(h^{\alpha-1/2}\eta)$ getting an error of order $\mathcal{O}(h^{\alpha-1/2})$. □

Now we deal with the case when $|\xi-\xi(h^{\alpha-1/2}\eta)| < \zeta h^\rho$. Let $\tilde{\eta}=h^{\alpha-1/2}\eta$. We look for a formal solution $(\mu, f^{\alpha,\eta}_{h,\beta,\xi})$ of the spectral problem

$$H^{\alpha,\eta}_{h,\beta,\xi} f^{\alpha,\eta}_{h,\beta,\xi} = \mu f^{\alpha,\eta}_{h,\beta,\xi}, \quad (f^{\alpha,\eta}_{h,\beta,\xi})'(0) = h^{\alpha-1/2} f^{\alpha,\eta}_{h,\beta,\xi}(0), \tag{5.25}$$

in the form:

$$\mu = d_0 + d_1(\xi-\xi(\tilde{\eta})) + d_2(\xi-\xi(\tilde{\eta}))^2 + d_3 h^{1/2}, \tag{5.26}$$

$$f^{\alpha,\eta}_{h,\beta,\xi} = u_0 + (\xi-\xi(\tilde{\eta}))u_1 + (\xi-\xi(\tilde{\eta}))^2 u_2 + h^{1/2}u_3, \tag{5.27}$$

where the coefficients d_0,d_1,d_2,d_3 and the functions u_0,u_1,u_2,u_3 are to be determined. We expand the operator $H^{\alpha,\eta,D}_{h,\beta,\xi}$ in powers of $(\xi-\xi(\tilde{\eta}))$ and then we identify the coefficients of the terms of orders $(\xi-\xi(\tilde{\eta}))^j$ $(j=0,1,2)$ and $h^{1/2}$. We then obtain for the coefficients:

$$d_0 = \Theta(\tilde{\eta}), \quad u_0 = \varphi_{\tilde{\eta}},$$

$$d_1 = 0, \quad u_1 = 2\widetilde{R}[\tilde{\eta}]\{(t-\xi(\tilde{\eta}))\varphi_{\tilde{\eta}}\},$$

$$d_2 =: d_2(\alpha,\eta) = 1 - 2\int_{\mathbb{R}_+} (t-\xi(\tilde{\eta}))\varphi_{\tilde{\eta}} u_1 \mathrm{d}t,$$

$$u_2 = \widetilde{R}[\widetilde{\eta}]\{4(t-\xi(\widetilde{\eta}))\widetilde{R}[\widetilde{\eta}][(t-\xi(\widetilde{\eta}))\varphi_{\widetilde{\eta}}] - d_2\},$$

$$d_3 =: d_3(\alpha,\eta) = \beta\int_{\mathbb{R}_+} \varphi_{\widetilde{\eta}}\{\partial_t + (t-\xi(\widetilde{\eta}))^3\}\varphi_{\widetilde{\eta}}\mathrm{d}t,$$

$$u_3 = -\widetilde{R}[\widetilde{\eta}][\beta(\partial_t + (t-\xi(\widetilde{\eta}))^3 - \xi(\widetilde{\eta})^2(t-\xi(\widetilde{\eta}))) - d_3]u_0. \tag{5.28}$$

Using the function $\chi(t/h^{\delta-1/2})f^{\alpha,\eta}_{h,\beta,\xi}$ (where χ is the same as in (3.5)) as a quasimode, we get by the spectral theorem, thanks to the decay results in Propositions II.9 and II.10 and to the localization of the spectrum in Lemma V.6, the following lemma.

Lemma V.9: Suppose that $\delta \in]\frac{1}{4},\frac{1}{2}[$. *For each* $M>0$ *and* $\alpha \in [\frac{1}{2},1]$, *there exist positive constants* $C>0, h_0$ *such that*

$$\forall\ \eta,\beta \in]-M,M[, \quad \forall\ \xi \text{ such that } |\xi-\xi(\widetilde{\eta})| \leqslant \zeta h^{\rho}, \quad \forall\ h \in]0,h_0],$$

we have

$$|\mu_1(H^{\alpha,\eta,D}_{h,\beta,\xi}) - \{\Theta(\widetilde{\eta}) + d_2(\alpha,\eta)(\xi-\xi(\widetilde{\eta}))^2 + d_3(\alpha,\eta)h^{1/2}\}| \leqslant C[h^{1/2}|\xi-\xi(\widetilde{\eta})| + h^{\delta+1/2}], \tag{5.29}$$

where $d_2(\alpha,\eta)$ *and* $d_3(\alpha,\eta)$ *are defined by (5.28)).* Hence we have obtained by this analysis a lower bound for the first eigenvalue $\mu^{(1)}(\alpha,\gamma,h)$. We complete the picture by showing that the term $d_2(\alpha,\eta)$ is positive.

Lemma V.10: For each $\alpha \in [\frac{1}{2},+\infty[$ *and* $M>0$, *there exists a positive constant* h_0 *such that*

$$d_2(\alpha,\eta) > 0, \quad \forall\ h \in]0,h_0], \quad \forall\ \eta \in]-M,M[.$$

Proof: It is actually sufficient to prove the conclusion of the lemma when $\alpha=\frac{1}{2}$. If $\alpha>\frac{1}{2}$, we replace $d_2(\alpha,\eta)$ by its approximation up to the first order, thanks to Proposition II.4, and we obtain that

$$d_2(\alpha,\eta) = d_2\left(\tfrac{1}{2},0\right) + \mathcal{O}(h^{\alpha-1/2}),$$

which gives the lemma. For the particular case $\alpha=\frac{1}{2}$, we show that

$$d_2\left(\tfrac{1}{2},\eta\right) = \tfrac{1}{2}(\partial^2_{\xi}\mu^{(1)}(\eta,\cdot))(\xi(\eta))$$

which is strictly positive. □

We are now able to conclude the asymptotics given in Theorems I.4 and I.5. First we choose $\delta=\frac{5}{12}$. When $\alpha>\frac{1}{2}$ we replace $\Theta(\widetilde{\eta})$ and d_3 by their approximations up to the second and first orders, respectively, thanks to Propositions II.5 and II.4. For $\alpha=\frac{1}{2}$ we get by (2.21) that d_3 is indeed equal to $-2M_3(\frac{1}{2},\gamma)$.

Remark V.11: When $\alpha \in]\frac{1}{2},1[$ *and when the function* γ *is not constant, we get from the above analysis that the upper bound in Remark III.2 is indeed an asymptotic expansion, and we achieve therefore the proof of Theorem I.2.*

We get also that the quadratic form $q^{\alpha,\gamma}_{h,A,\Omega}$ *can be bounded from below by means of a potential* W:

$$q^{\alpha,\gamma}_{h,A,\Omega}(u) \geqslant \int_{\Omega} W(x)|u(x)|^2\mathrm{d}x, \quad \forall\ u \in H^1(\Omega),$$

where W *is defined for some positive constant* C_0 *by*

$$W(x) = \begin{cases} h & \text{if } \operatorname{dist}(x,\partial\Omega) > h^{1/6} \\ h\Theta_0 + 6M_3\gamma(x)h^{\alpha+1/2} - C_0 h^{\inf(3/2,2\alpha)} & \text{if } \operatorname{dist}(x,\partial\Omega) < h^{1/6}. \end{cases}$$

Then, as in Sec. IV, we get by Agmon's technique that a ground state decays exponentially away from the boundary points where γ is minimum and hence we have completed the proof of Theorem I.3.

Remark V.12: Note also that the above analysis permits, under the hypotheses of Theorems I.4 and I.5, to bound the quadratic form $q^{\alpha,\gamma}_{h,A,\Omega}$ from below using a potential W defined either by means of the function $\kappa_r - 3\gamma$ (when $\alpha=1$) or by the scalar curvature κ_r (when γ is constant). Then, by using Agmon's technique, we finish the proofs of Theorems I.4 and I.5.

VI. CONCLUSION

The systematic analysis in the spirit of Ref. 10 has allowed us to understand the role of the boundary condition imposed by De Gennes. We have extended in Theorems I.4 and I.5 the expansion announced by Pan[25] in the particular case when $\alpha=1$ and γ is a positive constant. However, there is a specific difficulty when γ is negative. We have not been able to obtain the localization of the ground state when $\alpha<1/2$ and $\gamma_0>0$. This is strongly related to the question of the localization of the ground state of the Dirichlet realization of the Schrödinger operator with constant magnetic field which is open. Finally, in the spirit of Refs. 12, 26, and 27, we hope to apply this analysis to the onset of superconductivity and to complete the analysis of Ref. 28 (cf. Ref. 18).

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APPENDIX: COORDINATES NEAR THE BOUNDARY

We recall in this appendix well-known coordinates that straighten a portion of the boundary $\partial\Omega$. Let $s \in]-|\partial\Omega|/2, |\partial\Omega|/2] \mapsto M(s) \in \partial\Omega$ be a regular parametrization of $\partial\Omega$. For each $x \in \Omega$ and $\epsilon > 0$ we denote by

$$t(x) = \operatorname{dist}(x,\partial\Omega) \quad \text{and } \Omega_\epsilon = \{x \in \bar{\Omega}; \operatorname{dist}(x,\partial\Omega) < \epsilon\}.$$

Then there exists a positive constant $t_0 > 0$ depending on Ω such that, for each $x \in \Omega_{t_0}$, we can define the coordinates $(s(x), t(x))$ by

$$t(x) = |x - M(s(x))|,$$

and such that the transformation

$$\psi : \Omega_{t_0} \ni x \mapsto (s(x), t(x)) \in \mathbb{S}^1_{|\partial\Omega|/2\pi} \times [0, t_0[$$

is a diffeomorphisim. The Jacobian of this coordinate transformation is given by

$$a(s,t) = \det(D\psi) = 1 - t\kappa_r(s). \tag{A1}$$

To a vector field $A = (A_1, A_2) \in C^\infty(\bar{\Omega}; \mathbb{R}^2)$, we associate the vector field $\tilde{A} = (\tilde{A}_1, \tilde{A}_2) \in C^\infty(\mathbb{S}^1_{|\partial\Omega|/2\pi} \times [0, t_0[)$ by the following relation:

$$\tilde{A}_1 \mathrm{d}s + \tilde{A}_2 \mathrm{d}t = A_1 \mathrm{d}x_1 + A_2 \mathrm{d}x_2. \tag{A2}$$

We get then the following change of variable formulas.

Proposition A.1: Let $u \in H^1(\Omega)$ be supported in Ω_{t_0}. Then we have

$$\int_{\Omega_{t_0}} |(h\nabla - iA)u|^2 \mathrm{d}x = \int_{\mathrm{S}^1_{|\partial\Omega|/2\pi}\times[0,t_0[} [|(h\partial_t - i\tilde{A}_2)v|^2 + a^{-2}|(h\partial_s - i\tilde{A}_1)v|^2] a \mathrm{d}s\mathrm{d}t \tag{A3}$$

and

$$\int_{\Omega_{t_0}} |u(x)|^2 \mathrm{d}x = \int_{\mathrm{S}^1_{|\partial\Omega|/2\pi}\times[0,\epsilon_0[} |v(s,t)|^2 a \mathrm{d}s\mathrm{d}t, \tag{A4}$$

where $v(s,t) = u(\psi^{-1}(s,t))$.

We also have the relation

$$(\partial_{x_1} A_2 - \partial_{x_2} A_1)\mathrm{d}x_1 \wedge \mathrm{d}x_2 = (\partial_s \tilde{A}_2 - \partial_t \tilde{A}_1) a^{-1} \mathrm{d}s \wedge \mathrm{d}t,$$

which gives

$$\mathrm{curl}\,\tilde{A} = (1 - t\kappa_r(s))\mathrm{curl}\,A.$$

We give in the next proposition a standard choice of gauge.

Proposition A.2: Consider a vector field $A = (A_1, A_2) \in C^\infty(\bar{\Omega}; \mathbb{R}^2)$ such that $\mathrm{curl}\,A = 1$. *For each point $x_0 \in \partial\Omega$, there exists a neighborhood $\mathcal{V}_{x_0} \subset \Omega_{t_0}$ of x_0 and a smooth real-valued function ϕ_{x_0} such the vector field $A_{\mathrm{new}} := A - \nabla\phi_{x_0}$ satisfies*

$$\tilde{A}^1_{\mathrm{new}} = -t\left(1 - \frac{t}{2}\kappa_r(s)\right) \quad \textit{and } \tilde{A}^2_{\mathrm{new}} = 0 \quad \textit{in } \mathcal{V}_{x_0}, \tag{A5}$$

with $\tilde{A}_{\mathrm{new}} = (\tilde{A}^1_{\mathrm{new}}, \tilde{A}^2_{\mathrm{new}})$.

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Scalar gauge theory on a cylinder

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In this work, we study the complex bosonic matter coupled to the SU(N_c) gauge fields on a cylinder, which has a circular space part. We extend the ideas used for fermions on a cylinder in [S. G. Rajeev and Guruswamy, Mod. Phys. Lett. A **7**, 3783 (1992)] to this case. Here, the normal ordering rule for bosonic bilinears is found. In the large-N_c limit, we can reformulate the whole problem in terms of a set of basic mesonic operators. The full equations of motion satisfied by these mesonic variables are too complicated. An approximation method, which is a kind of linearization, is suggested for this problem. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Calculation of the bound states from first principles in QCD is a very challenging problem. The perturbative approach is not sufficient to understand this problem. There are various interesting ideas in this direction, but the most promising one seems to be the large-N_c limit, which is first suggested by 't Hooft[1] and elaborated more by Migdal[2,3] and Witten.[4] 't Hooft applied the large-N_c limit to 1+1 dimensional QCD and found his celebrated equation for the mesonic spectrum.[5] Soon after this is generalized by Shei and Tsao to the scalar matter.[6] The same problem is also solved in the Hamiltonian formalism in Ref. 7. The generalized QCD, where the fermionic and bosonic matter fields present together, is solved by Aoki in Ref. 8 following 't Hooft's original approach.

In Ref. 9 Rajeev took a fresh look at the large-N_c limit of 1+1 dimensional QCD and has shown that this is indeed a classical theory which has the restricted Grassmanian as its phase space (see Ref. 10 for a nice review). The linearized equations for the mesonic bilinears are shown to agree with the 't Hooft equation. Being a nonlinear theory it admits also large deviations from the vacuum and they may be taken as the baryons. Krishnaswami gave a detailed study of these solutions in his thesis and showed that the minimum of the baryon mass in this theory goes to zero as the mass of the fermion goes to zero, contrary to what is believed to happen in 3+1 dimensions.[11] An extension of these ideas to bosonic matter is done in Ref. 12 and the linearized equations are shown to agree with what is found by Shei and Tsao. The method proposed in Ref. 9 also can be applied to SO(N_c) gauge theories,[13] the phase space there is an infinite dimensional version of the Siegel disk.

In all these problems the gauge theory sector is not dynamical and only generates a potential between the quarks. When we study the pure Yang-Mills on a cylinder, which has a circular spatial geometry, there is a global degree of freedom left out after the gauge equivalent configurations are removed. Therefore it is natural to try to add only a global degree of freedom to the gauge sector when it is coupled to matter for simplicity, by studying the same problem on a cylinder, which has

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a circle for the space part. This is perhaps the least complicated problem, but as we will see, the resulting theory is much more complex, and we are far from understanding it.

The literature on the pure Yang-Mills theory on such nontrivial spaces is large, we mention just a few of them closely related to our approach taken here, there is an extensive review by Moore *et al.*[14] where further references can be found. The solution of pure Yang-Mills theory on the cylinder is given by Rajeev in Ref. 15, there it is found that this system is equivalent to a particle moving on the group manifold. The Hamiltonian is the quadratic Casimir of the group, the global gauge invariance left out, forces one to restrict the Hilbert space of the theory to the character functions. The key to reduction is accomplished by the Wilson loop operator along the circle. Later, the nonrelativistic matter coupled to the gauge fields is worked out in a geometric setting using the Wilson loop operator to reduce the redundant gauge degrees of freedom in Ref. 16. The large-N_c limit of pure Yang-Mills is understood from different points of views in Refs. 17–20 (see for more the review in Ref. 14). The matter coupled to gauge fields on a cylinder was studied by other authors as well, in Langmann and Semenoff[21] the theory is constructed using the free vacuum and some ideas are suggested to study the spectrum. This problem is studied in Refs. 22 and 23, using again a large-N_c approximation in the path integral perspective. For large values of the radius, the authors give a formula for the eigenvalues of the Hamiltonian. In all these approaches the splitting of the true degrees of freedom of the gauge fields and the matter fields is not so clear. In Ref. 24, Rajeev and Guruswamy reduced the fermionic matter interacting with the gauge fields on the cylinder to matter coupled to quantum mechanics on the tangent bundle of the symmetry group. Again, only global degrees of freedom are left after the removal of gauge equivalent configurations from the gauge fields via the Wilson loop operator (the holonomy along the circle).

Here, we will study non-Abelian gauge theory coupled to scalars in the fundamental representation in $1+1$ dimensions. To decouple the gauge theory sector from the kinetic part of the bosons and reducing the gauge theory sector to its true degrees of freedom, we will use the same method suggested in Ref. 24. There are two essential points, first is the decoupling of the kinetic part of the bosons and gauge fields, since when we have coupling between the leading kinetic parts, the vacuum will change in an uncontrollable way. To start quantizing the fields, we should find the correct vacuum. The second point is the reduction of the gauge fields to their true degrees of freedom *without performing any gauge fixing*. The fermionic problem is more realistic, yet it is interesting to work out the same approach in the bosonic case. In Ref. 24, only the Hamiltonian of the theory is written in this coordinate system and no attempt is made to write down a large-N_c theory. There are some complications coming from the boundary conditions in the case of fermions, it seems to us that they are harder to resolve than the ones in the bosonic theory. In the bosonic theory, as we will see, it is more difficult to find the normal ordering prescription. In a separate section this is developed, which we believe could be useful in other contexts as well.

Following Ref. 24, we will perform our analysis in a coordinate system different from the Cartesian (x,t) coordinates used to solve pure Yang-Mills theory in Ref. 15. We construct a kind of light-cone formalism such that the new coordinates (u,x) are

$$u = t + |x|. \tag{1}$$

Then,

$$\mathrm{d}t = \mathrm{d}u - \mathrm{sgn}(x)\mathrm{d}x. \tag{2}$$

The metric is

$$\mathrm{d}s^2 = \mathrm{d}t \otimes \mathrm{d}t - \mathrm{d}x \otimes \mathrm{d}x = \mathrm{d}u \otimes \mathrm{d}u - \mathrm{sgn}(x)\mathrm{d}u \otimes \mathrm{d}x - \mathrm{sgn}(x)\mathrm{d}x \otimes \mathrm{d}u. \tag{3}$$

Thus the metric tensor becomes

$$\eta_{\mu\nu}=\begin{pmatrix}1 & -\operatorname{sgn}(x)\\ -\operatorname{sgn}(x) & 0\end{pmatrix},\quad \eta^{\mu\nu}=\begin{pmatrix}0 & -\operatorname{sgn}(x)\\ -\operatorname{sgn}(x) & -1\end{pmatrix}. \tag{4}$$

The points (u,x) and $(u,x+2L)$ are the same on the cylinder. These light-cone coordinates avoid the quadratic energy term appearing in the mass shell condition of the Cartesian coordinates,

$$p_0^2-p_1^2=m^2. \tag{5}$$

In Ref. 24, it is noticed that the ordinary light-cone method is not suitable for the elimination of the redundant gauge theory degrees of freedom, but in this coordinate system it can be done in a clever way. For this purpose, *we will use u as our evolution variable*. In this special light-cone coordinate system the mass-shell condition is

$$-2\operatorname{sgn}(x)p_xp_u-p_x^2=m^2 \tag{6}$$

from which we obtain a unique solution for p_u,

$$p_u=-\frac{1}{2}\left(\frac{m^2}{p_x}+p_x\right)\operatorname{sgn}(x). \tag{7}$$

This is important, since it suggests that in second quantization the positive and negative energies will be determined by the sign of $p_x\operatorname{sgn}(x)$. This is essentially correct, the operator that we will find has this as its leading symbol.

II. BOSONS IN THE FUNDAMENTAL REPRESENTATION

The action of the complex bosons in two dimensions interacting with an SU(N_c) gauge field can be written as

$$S=\int \mathrm{d}u\,\mathrm{d}x\sqrt{-\eta}\left[\frac{1}{2}(D_\mu\phi)^\dagger D^\mu\phi-\frac{1}{2}m^2\phi^\dagger\phi+\frac{1}{4g^2}\operatorname{Tr}F^{\mu\nu}F_{\mu\nu}\right], \tag{8}$$

where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu+[A_\mu,A_\nu]$. Here $D_\mu=\partial_\mu+A_\mu$, where A_μ is the gauge potential, D_μ is the covariant derivative. We choose A_μ to be anti-Hermitian with

$$A_\mu=A_\mu^a t^a, \tag{9}$$

$$\operatorname{Tr}(t^at^b)=-\delta^{ab}, \tag{10}$$

where t^a are the generators of the Lie algebra. If we express this in terms of components in the new system of coordinates, we find

$$S=\int \mathrm{d}u\,\mathrm{d}x\left[-\frac{1}{2}\operatorname{sgn}(x)D_u\phi^\dagger D_x\phi-\frac{1}{2}\operatorname{sgn}(x)D_x\phi^\dagger D_u\phi\right]+\int \mathrm{d}u\,\mathrm{d}x\left[-\frac{1}{2}D_x\phi^\dagger D_x\phi-\frac{1}{2}m^2\phi^\dagger\phi\right]$$
$$+\int \mathrm{d}u\,\mathrm{d}x\left[-\frac{1}{g^2}\operatorname{Tr}E(\partial_uA_x-\partial_xA_u+[A_u,A_x])+\frac{1}{2g^2}\operatorname{Tr}E^2\right], \tag{11}$$

where

$$E=\partial_uA_x-\partial_xA_u+[A_u,A_x]. \tag{12}$$

Here we split the E^2 term, namely,

$$\frac{1}{4g^2}\operatorname{Tr}F^{\mu\nu}F_{\mu\nu}=-\frac{1}{2g^2}\operatorname{Tr}E^2=\frac{1}{2g^2}\operatorname{Tr}E^2-\frac{1}{g^2}\operatorname{Tr}E^2, \tag{13}$$

and insert the definition of E in terms of gauge fields in the second part to get

$$-\frac{1}{g^2}\,\mathrm{Tr}\,E(\partial_u A_x-\partial_x A_u+[A_u,A_x]). \tag{14}$$

If we write the action explicitly,

$$\begin{aligned}S=&-\int \mathrm{d}u\,\mathrm{d}x\frac{1}{2}\mathrm{sgn}(x)(\partial_u\phi^\dagger-\phi^\dagger A_u)(\partial_x\phi+A_x\phi)-\int \mathrm{d}u\,\mathrm{d}x\frac{1}{2}\mathrm{sgn}(x)(\partial_x\phi^\dagger-\phi^\dagger A_x)(\partial_u\phi+A_u\phi)\\&-\int \mathrm{d}u\,\mathrm{d}x\left[\frac{1}{2}(\partial_x\phi^\dagger-\phi^\dagger A_x)(\partial_x\phi+A_x\phi)\right]-\int \mathrm{d}u\,\mathrm{d}x\frac{1}{2}m^2\phi^\dagger\phi-\int \mathrm{d}u\,\mathrm{d}x\left[\frac{1}{g^2}\,\mathrm{Tr}\,E(\partial_u A_x-\partial_x A_u\right.\\&\left.+[A_u,A_x])+\frac{1}{2g^2}\,\mathrm{Tr}\,E^2\right].\end{aligned}$$

Now, following Ref. 24, we will define a variable $h(u,x)$ to eliminate the Yang-Mills field *without imposing any gauge condition*:

$$\frac{\partial h}{\partial x}+A_x h=0, \tag{15}$$

$$h(u,-L)=1. \tag{16}$$

The solution is represented as a path ordered exponential

$$h(u,x)=P[e^{\int_{-L}^{x}\mathrm{d}y\,A_x(u,y)}]. \tag{17}$$

The Wilson loop is then given by

$$q=h^{-1}(u,L). \tag{18}$$

We will define new field variables such that

$$\phi=h\tilde{\phi},$$

$$A_u=h\tilde{A}_u h^{-1},$$

$$E=h\tilde{E}h^{-1}. \tag{19}$$

Our aim is to decouple the leading bosonic action from the gauge fields and reduce the gauge field sector to its true dynamical degrees of freedom.

Since we are on a cylinder with $(u,x)\sim(u,x+2L)$, the fields are periodic with period $2L$. Thus

$$\phi(L)=\phi(-L),$$

$$\phi^\dagger(L)=\phi^\dagger(-L),$$

$$E(L)=E(-L). \tag{20}$$

In terms of the new variables, we have

$$\tilde{\phi}(L)=q\tilde{\phi}(-L),$$

$$\tilde{\phi}^\dagger(L)=\tilde{\phi}^\dagger(-L)q^{-1},$$

$$\tilde{E}(L) = q\tilde{E}(-L)q^{-1}. \tag{21}$$

We see that now we are dealing with a complicated boundary condition. We will define $E(-L)=e$. When we insert the new definitions of our variables, we find

$$S = \int \mathrm{d}u\,\mathrm{d}x\left[-\frac{1}{2}\mathrm{sgn}(x)(\partial_u\tilde{\phi}^\dagger\partial_x\tilde{\phi} + \partial_x\tilde{\phi}^\dagger\partial_u\tilde{\phi})\right] - \int \mathrm{d}u\,\mathrm{d}x\frac{1}{2}\mathrm{sgn}(x)[\partial_x\tilde{\phi}^\dagger(\tilde{A}_u + h^{-1}\partial_u h)\tilde{\phi} - \tilde{\phi}^\dagger(\tilde{A}_u + h^{-1}\partial_u h)\partial_x\tilde{\phi}] - \int \mathrm{d}u\,\mathrm{d}x\frac{1}{2}m^2\tilde{\phi}^\dagger\tilde{\phi} - \int \mathrm{d}u\,\mathrm{d}x\frac{1}{g^2}\,\mathrm{Tr}[h\tilde{E}h^{-1}(\partial_u A_x - \{\partial_x A_u + [A_u,A_x]\})] + \int \mathrm{d}u\,\mathrm{d}x\frac{1}{2g^2}\,\mathrm{Tr}[(\tilde{E}^2)]. \tag{22}$$

We used the definition of h to simplify the above expression. Let us now work on the combination below,

$$\partial_x A_u + [A_u,A_x]. \tag{23}$$

We insert identities on both sides in the form of hh^{-1} and use Eq. (15). We see that this term is the expansion of

$$h(\partial_x\tilde{A}_u)h^{-1}. \tag{24}$$

Thus

$$\partial_u A_x - \{\partial_x A_u + [A_u,A_x]\} = hh^{-1}\partial_u A_x hh^{-1} - h(\partial_x\tilde{A}_u)h^{-1}. \tag{25}$$

By using the relation below that can also be derived from (15),

$$h^{-1}(\partial_u A_x)h = -\partial_x(h^{-1}\partial_u h). \tag{26}$$

Equation (25) becomes

$$-h\partial_x(h^{-1}\partial_u h)h^{-1} - h\partial_x(h^{-1}A_u h)h^{-1} = -h\partial_x(h^{-1}\partial_u h + \tilde{A}_u)h^{-1}. \tag{27}$$

As we can see now, it is better to introduce a new variable A via

$$A = \tilde{A}_u + h^{-1}\partial_u h. \tag{28}$$

Let us write down the Yang-Mills part of our action,

$$-\frac{1}{g^2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{Tr}[h\tilde{E}h^{-1}(\partial_u A_x - \{\partial_x A_u + [A_u,A_x]\})] = -\frac{1}{g^2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{Tr}[-\tilde{E}\partial_x(h^{-1}\partial_u h + \tilde{A}_u)], \tag{29}$$

and express this in terms of total derivatives,

$$-\frac{1}{g^2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{Tr}[-\partial_x(\tilde{E}h^{-1}\partial_u h) + (\partial_x\tilde{E})h^{-1}\partial_u h - \partial_x(\tilde{E}\tilde{A}_u) + (\partial_x\tilde{E})\tilde{A}_u] = \frac{1}{g^2}\int \mathrm{d}u\int_{-L}^{L}\mathrm{d}x\,\mathrm{Tr}[\partial_x(\tilde{E}h^{-1}\partial_u h)] - \frac{1}{g^2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{Tr}[(\partial_x\tilde{E})[\tilde{A}_u + h^{-1}\partial_u h]].$$

Here the third term vanished, since the fields cancel out at the boundaries. The total derivative can be expanded as

$$\frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}[\tilde{E}(L)h^{-1}(L)\partial_u h(L) - \tilde{E}(-L)h^{-1}\partial_u h(-L)] - \frac{1}{g^2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{Tr}[(\partial_x \tilde{E})A]. \tag{30}$$

In this expression $\partial_u h(-L)$ gives zero, we insert our boundary conditions; $h^{-1}(L)=q$, or $h(L)=q^{-1}$, obtaining

$$\frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}[q\tilde{E}(-L)q^{-1}q\partial_u q^{-1}] - \frac{1}{g^2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{Tr}[(\partial_x \tilde{E})A]. \tag{31}$$

So the pure gauge theory part of our equation has become

$$-\frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}[q^{-1}\partial_u q e] - \frac{1}{g^2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{Tr}[(\partial_x \tilde{E})A] + \frac{1}{2g^2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{Tr}\,\tilde{E}^2. \tag{32}$$

Having derived the gauge field interaction part in terms of the new variables we can now go back to (22),

$$\begin{aligned} S = &\int \mathrm{d}u\ \mathrm{d}x\left[-\frac{1}{2}\mathrm{sgn}(x)[(\partial_u \tilde{\phi}^\dagger)(\partial_x \tilde{\phi}) + (\partial_x \tilde{\phi}^\dagger)(\partial_u \tilde{\phi})]\right] + \int \mathrm{d}u\ \mathrm{d}x\left[-\frac{1}{2}\mathrm{sgn}(x)[(\partial_x \tilde{\phi}^\dagger)A\tilde{\phi}\right. \\ &\left. - \tilde{\phi}^\dagger A(\partial_x \tilde{\phi})]\right] - \int \mathrm{d}u\ \mathrm{d}x\frac{1}{2}(\partial_x \tilde{\phi}^\dagger)(\partial_x \tilde{\phi}) - \int \mathrm{d}u\ \mathrm{d}x\frac{1}{2}m^2\tilde{\phi}^\dagger\tilde{\phi} - \int \mathrm{d}u\ \mathrm{d}x\left[\frac{1}{g^2}\mathrm{Tr}(\partial_x \tilde{E})A\right. \\ &\left. - \frac{1}{2g^2}\mathrm{Tr}\,\tilde{E}^2\right] - \frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}(q^{-1}\partial_u q e). \end{aligned} \tag{33}$$

We see now that A does not have a time derivative in the action, so it is just a Lagrange multiplier imposing a constraint and can be eliminated. Varying the action with respect to A we obtain a constraint,

$$\frac{1}{g^2}\partial_x \tilde{E}^b \delta A^a\ \mathrm{Tr}[t^b t^a] = -\frac{1}{2}\mathrm{sgn}(x)(\partial_x \tilde{\phi}^\dagger t^a \tilde{\phi} - \tilde{\phi}^\dagger t^a \partial_x \tilde{\phi})\delta A^a. \tag{34}$$

Thus the constraint becomes

$$-\frac{1}{g^2}\partial_x \tilde{E}^a = -\frac{1}{2}\mathrm{sgn}(x)\{(t^a)^\alpha{}_\beta[\tilde{\phi}^\beta(\partial_x \tilde{\phi}^\dagger)_\alpha - (\partial_x \tilde{\phi})^\beta \tilde{\phi}^\dagger_\alpha]\}. \tag{35}$$

In matrix form,

$$\tilde{E} = e - \frac{g^2}{2}\int_{-L}^{x} \mathrm{d}y\ \mathrm{sgn}(y)\{\tilde{\phi}(\partial_y \tilde{\phi}^\dagger) - (\partial_y \tilde{\phi})\tilde{\phi}^\dagger\}. \tag{36}$$

Thus the *classical* action is reduced to

$$\begin{aligned} S = &-\frac{1}{2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{sgn}(x)[(\partial_u \tilde{\phi}^\dagger)(\partial_x \tilde{\phi}) + (\partial_x \tilde{\phi}^\dagger)(\partial_u \tilde{\phi})] - \int \mathrm{d}u\ \mathrm{d}x\frac{1}{2}(\partial_x \tilde{\phi}^\dagger)(\partial_x \tilde{\phi}) - \frac{1}{2}\int \mathrm{d}u\ \mathrm{d}x\ m^2\tilde{\phi}^\dagger\tilde{\phi} \\ &+ \frac{1}{2g^2}\int \mathrm{d}u\ \mathrm{d}x\ \mathrm{Tr}\left[e - \frac{g^2}{2}\int_{-L}^{x}\mathrm{d}y\ \mathrm{sgn}(y)\{\tilde{\phi}(\partial_y \tilde{\phi}^\dagger) - (\partial_y \tilde{\phi})\tilde{\phi}^\dagger\}\right]^2 - \frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}(q^{-1}\partial_u q e). \end{aligned} \tag{37}$$

Here, we see that the action has three parts, the first part consists of (dressed) bosons, the last term represents the true dynamical degrees of freedom for the gauge fields and the rest is the coupling of these two separate systems. There is only a global gauge freedom left, as we will see coming from the constraint equation. We can now start from the beginning and quantize these dynamical systems. The quantized bosonic field will not be related to the original bosonic fields in a simple way, in some sense they are dressed by the gauge fields.

The advantage of the light-cone systems is clear, the action is first order in the time variable u, thus we are already in the Hamiltonian picture. When we write this action in the form

$$S = \int \mathrm{d}u\, \bar{w}^i \omega_{ij} \dot{w}^j - \int \mathrm{d}u\, H \tag{38}$$

we can read off the Hamiltonian as

$$H = \int \mathrm{d}x \frac{1}{2}(\partial_x \tilde{\phi}^\dagger)(\partial_x \tilde{\phi}) + \int \mathrm{d}x \frac{1}{2} m^2 \tilde{\phi}^\dagger \tilde{\phi} - \frac{1}{2g^2} \int \mathrm{d}x\, \mathrm{Tr}\Bigg[e - \frac{g^2}{2} \int_{-L}^{x} \mathrm{d}y\, \mathrm{sgn}(y) \{ \tilde{\phi}(\partial_y \tilde{\phi}^\dagger) - (\partial_y \tilde{\phi}) \tilde{\phi}^\dagger \} \Bigg]^2, \tag{39}$$

the rest belonging to the symplectic part.

In the Hamiltonian formulation, the reduced gauge field theory part becomes the motion on the cotangent bundle of the Lie group SU(N). The geometric meaning of this symplectic form is well described in Ref. 25. This is the same result for the pure Yang-Mills on a cylinder first worked out by Rajeev[15] using the Cartesian coordinates. To help the reader we present a simple derivation of this in the appendix. Here, we state the result,

$$\{q^\alpha{}_\beta, q^\lambda{}_\sigma\} = 0,$$

$$\{\mathrm{Tr}\, \Lambda e, q^\alpha{}_\beta\} = g^2 (q\Lambda)^\alpha{}_\beta,$$

$$\{\mathrm{Tr}\, \Lambda_1 e, \mathrm{Tr}\, \Lambda_2 e\} = g^2 \mathrm{Tr}[\Lambda_1, \Lambda_2] e. \tag{40}$$

We can quantize by Dirac's rule of replacing the Poisson brackets by the commutators, and there is a natural representation of this on the space of square integrable functions on the Lie group SU(N). We set the Hilbert space to be $L^2(\mathrm{SU}(N))$, and

$$(\hat{q}^\alpha{}_\beta f)(q) = q^\alpha{}_\beta f(q), \quad (\mathrm{Tr}\, \Lambda \hat{e} f)(q) = i g^2 \mathcal{L}_\Lambda f(q). \tag{41}$$

One should further assume an ordering rule for the product of operators, one typically takes the Weyl (symmetric) ordering. The solution for the pure gauge theory on a circle can now be given easily, $\mathrm{Tr}\, e^2$ is proportional to the quadratic Casimir on the group. The boundary condition $\tilde{E}(L) = q\tilde{E}(-L)q^{-l}$ becomes

$$[\hat{e} - \hat{q}\hat{e}\hat{q}^{-1}] f(q) = 0, \tag{42}$$

as a result of nondynamical nature of A. Exponentiation of this constraint to the group will give us

$$f(sqs^{-1}) = f(q) \quad \text{for all} \quad s \in \mathrm{SU}(N), \tag{43}$$

and for all wave functions $f(q)$. Indeed the quadratic Casimir leaves this constraint invariant, hence we can reduce the dynamics onto this subspace. The energy eigenvalues are the values of the quadratic Casimir on all the irreducible representations. The eigenfunctions are the characters of the irreducible representations (see Rajeev[15]). It is known from the Peter-Weyl theorem that the characters form an orthonormal complete set in the above subspace.

In the next section we will focus on the quantization of the boson fields, since this will require a rethinking of the usual canonical quantization. What we need is the normal ordering prescription of the bosonic theory, we will give the answer formally, we are not able to compute the resulting integral kernel exactly at the moment.

III. QUANTIZATION AND THE NORMAL ORDERING FOR BOSONS

Looking back to our action in Eq. (37), we take the symplectic form of the field theory part as

$$-\frac{1}{2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{sgn}(x)[(\partial_u\tilde{\phi}^\dagger)(\partial_x\tilde{\phi})+(\partial_x\tilde{\phi}^\dagger)(\partial_u\tilde{\phi})]. \tag{44}$$

Varying with respect to $\tilde{\phi}^\dagger$, we get

$$-\frac{1}{2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{sgn}(x)[(\partial_u\delta\tilde{\phi}^\dagger)(\partial_x\tilde{\phi})+(\partial_x\delta\tilde{\phi}^\dagger)(\partial_u\tilde{\phi})]. \tag{45}$$

Integrating by parts in the first term gives

$$-\frac{1}{2}\int \mathrm{d}u\,\mathrm{d}x\,\mathrm{sgn}(x)[\partial_u(\delta\tilde{\phi}^\dagger\partial_x\tilde{\phi})-\delta\tilde{\phi}^\dagger\partial_u\partial_x\tilde{\phi}+(\partial_x\delta\tilde{\phi}^\dagger)(\partial_u\tilde{\phi})]. \tag{46}$$

The first term drops out since $\delta\tilde{\phi}^\dagger$ is zero at the boundaries $\pm\infty$ of the time coordinate. The same cannot be applied to the x coordinate due to the boundary conditions stated in Eq. (21). Thus we obtain

$$-\frac{1}{2}\int \mathrm{d}u\,\mathrm{d}x[\delta\tilde{\phi}^\dagger(\overleftarrow{\partial}_x\,\mathrm{sgn}(x)-\mathrm{sgn}(x)\overrightarrow{\partial}_x)\partial_u\tilde{\phi}]. \tag{47}$$

The term in parentheses gives the symplectic form. Its inverse can be written formally as

$$(\omega^{-1})^\alpha{}_\beta = 2(\mathrm{sgn}\,\overrightarrow{\partial}_x-\overleftarrow{\partial}_x\,\mathrm{sgn})^{-1}\delta^\alpha{}_\beta, \tag{48}$$

where sgn is defined as

$$\langle x|\mathrm{sgn}|y\rangle = \mathrm{sgn}(x)\,\delta(x-y). \tag{49}$$

We have the previously stated boundary conditions.

To second quantize the theory one must know the annihilation and creation operators. Once we find these operators, we will introduce the normal ordering procedure to make sure that the products of the fields at the same point are well defined.

Apart from the coupling with the gauge field, our problem is like the harmonic oscillator. First we will focus on a finite dimensional problem with constant symplectic and quadratic form.

We are going to make the quantization as in a real vector space. *We can do this since in our case the symplectic and quadratic forms are real operators and the real and imaginary parts of the complex vectors decouple*. We can see this easily by taking our complex fields as

$$\phi = a + ib. \tag{50}$$

Our action has the form

$$\int \mathrm{d}u\frac{1}{2}(\phi^\dagger\omega\dot{\phi}-\phi^\dagger Q\phi) \tag{51}$$

and it can be rewritten by using the antisymmetry of ω and the symmetry of Q,

$$\int \mathrm{d}u\frac{1}{2}[a^\dagger\omega\dot{a}-a^\dagger Qa+b^\dagger\omega\dot{b}-b^\dagger Qb]. \tag{52}$$

Since a and b commute, if we quantize these fields, the normal ordering of ϕ can now be defined in a simple way,

$$:\phi^\dagger\phi: = :(a+ib)^\dagger(a+ib): = :a^\dagger a: + :b^\dagger b: + i[a^\dagger b - b^\dagger a]. \tag{53}$$

At the end, we will subtract twice the commutator of the annihilation and creation operators from the normal ordered product, to get the correct vacuum energy.

For simplicity we work with a finite dimensional (real valued) system, which has coordinates x^i, in our application the indices $(i,j,k,l,\ldots)$ will refer to both a set of continuous indices and a set of discrete indices. To start quantization, the first step is to look at the equations of motion

$$\dot{x}^i = (\omega^{-1})^{ij}Q_{jk}x^k. \tag{54}$$

The next step is to complexify the underlying vector space to get the oscillatory solutions. Indeed the oscillatory solutions are related to a complex structure. (This is not the original complex structure in our complex case.) This quantization method is worked out using the ideas of Rajeev and Bowick in Ref. 26.

The polar decomposition of the operator $\omega^{-1}Q$ will reveal a complex structure J and a positive symmetric operator K. As a result the equations of motion become

$$\dot{x}^i = J^i_k K^k_l x^l, \tag{55}$$

where

$$J^\tau J = 1. \tag{56}$$

Here the transpose is not the usual one but instead it is defined with respect to the metric defined by the quadratic form, Q as

$$J^\tau = Q^{-1}J^T Q. \tag{57}$$

We have,

$$K^\tau = K, \quad K \geq 0. \tag{58}$$

It will be useful to define a new variable as

$$\tilde{\omega} = \omega^{-1}Q. \tag{59}$$

We can see that this operator is antisymmetric in the metric defined by the quadratic form, that is

$$\tilde{\omega}^\tau = -\tilde{\omega}, \tag{60}$$

since,

$$(\omega^{-1}Q)^\tau = Q^{-1}(\omega^{-1}Q)^T Q = Q^{-1}Q^T(\omega^{-1})^T Q = Q^{-1}Q(-\omega^{-1})Q = -\omega^{-1}Q. \tag{61}$$

If we use Eq. (60), we can solve for K and J in terms of $\tilde{\omega}$, giving

$$K = (-\tilde{\omega}^2)^{1/2}, \quad J = (-\tilde{\omega}^2)^{-1/2}\tilde{\omega}. \tag{62}$$

One can check that

$$J^\tau = -(-\tilde{\omega}^2)^{-1/2}\tilde{\omega} = -J, \quad \text{thus,} \quad J^2 = -1. \tag{63}$$

So, *J defines a complex structure*. What follows after the construction of the complex structure is to project the coordinates into $\pm i$ eigenspaces to obtain complex coordinates. But it would be instructive to stop at this point and apply this procedure to the well-known real scalar field in the usual coordinate system. For simplicity we will call this familiar quantization as the Klein-Gordon field. The Hamiltonian of a Klein-Gordon field on $\mathbb{R}^3$ can be written as follows:

$$H = \int d^3x[\pi^2 + (\nabla\phi)^2 + m^2\phi^2]. \tag{64}$$

By partial integration we get the quadratic form

$$H = \int d^3x[\pi^2 + \phi(-\nabla^2 + m^2)\phi] \tag{65}$$

$$= \int d^3x[\Phi^T Q \Phi]. \tag{66}$$

Here we use a two component representation such that

$$\Phi = \begin{pmatrix} \phi \\ \partial_t \phi \end{pmatrix}. \tag{67}$$

We can read off the quadratic form as

$$Q = \begin{pmatrix} (-\nabla^2 + m^2) & 0 \\ 0 & 1 \end{pmatrix}. \tag{68}$$

The symplectic form is

$$\omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{69}$$

Thus

$$\tilde{\omega} = \omega^{-1}Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} (-\nabla^2 + m^2) & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ (-\nabla^2 + m^2) & 0 \end{pmatrix}. \tag{70}$$

One can easily show that the transpose is

$$\tilde{\omega}^\tau = \begin{pmatrix} 0 & 1 \\ (-\nabla^2 + m^2) & 0 \end{pmatrix}. \tag{71}$$

We can now calculate the complex structure J for the Klein-Gordon field easily,

$$J = (\tilde{\omega}^\tau\tilde{\omega})^{-1/2}\tilde{\omega} = \begin{pmatrix} (-\nabla^2 + m^2)^{-1/2} & 0 \\ 0 & (-\nabla^2 + m^2)^{-1/2} \end{pmatrix}\begin{pmatrix} 0 & -1 \\ (-\nabla^2 + m^2) & 0 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & -(-\nabla^2 + m^2)^{-1/2} \\ (-\nabla^2 + m^2)^{1/2} & 0 \end{pmatrix}. \tag{72}$$

At this point we go back to our main line of discussion. We will now project our coordinates into $\pm i$ eigenspaces to obtain complex coordinates. Let us point out that, there is always a basis $\{e_\alpha\}$, and a dual basis $\{e^{*\alpha}\}$ for which

$$J(e^{*\alpha}) = e^{*\alpha+n},$$

$$J(e^{*\alpha+n}) = -e^{*\alpha}, \tag{73}$$

where $\alpha = 1, 2, \ldots, n$, since J is a complex structure[27] (note that these indices have nothing to do with our previous use of color indices, they are just used to denote these special basis elements in the vector space). We may define the coordinates through

$$x^j = e^{*j}(x), \tag{74}$$

where x is a vector in our space. This can easily be verified, by looking at

$$e^{*j}(x) = e^{*j}(x^k e_k), \tag{75}$$

since the dual product gives a delta, $e^{*j}(e_k) = \delta^j_k$. If we do not think about a basis, symbolically we can write the projections as

$$x^j = \tfrac{1}{2}(1 + iJ)^j_s x^s + \tfrac{1}{2}(1 - iJ)^j_s x^s. \tag{76}$$

We can verify that

$$\left[\tfrac{1}{2}(1 \pm iJ)\right]^2 = \tfrac{1}{2}(1 \pm iJ) \tag{77}$$

and

$$(1 + iJ)(1 - iJ) = 0. \tag{78}$$

Here the first part is the projection into the $+i$ eigenspace and the second is into $-i$. Let us make a choice from the linearly independent dual basis elements as

$$\overline{f}^{*\alpha} = \tfrac{1}{2}(1 + iJ)(e^{*\alpha}) \sim \overline{z}^{\alpha},$$

$$f^{*\alpha} = \tfrac{1}{2}(1 - iJ)(e^{*\alpha}) \sim z^{\alpha}, \tag{79}$$

where $\alpha = 1, 2, \ldots, n$.

So we think of dual basis as if they are the coordinates, this simplifies our writing. Now we should compute the Poisson brackets of these projected coordinates. We expect to have nonzero Poisson bracket only for z, $\overline{z}$ term. Let us first check that the others give zero,

$$\left\{\tfrac{1}{2}(\delta^i_k + iJ^i_k)x^k, \tfrac{1}{2}(\delta^j_l + iJ^j_l)x^l\right\} = \tfrac{1}{4}[\{x^i, x^j\} + iJ^i_k\{x^k, x^j\} + iJ^j_l\{x^i, x^l\} - J^i_k J^j_l\{x^k, x^l\}] = \tfrac{1}{4}[(\omega^{-1})^{ij} + iJ^i_k(\omega^{-1})^{kj} + iJ^j_l(\omega^{-1})^{il} - J^i_k J^j_l(\omega^{-1})^{kl}] = \tfrac{1}{4}[(\omega^{-1})^{ij} + iJ^i_k J^k_r K^{rj} - iJ^j_l J^l_r K^{ri} - J^i_k J^j_l J^k_s K^{sl}].$$

Here $K^{ij} = K^i_s (Q^{-1})^{sj}$ and we used the equality of $\omega^{-1}Q$ to JK,

$$\left\{\tfrac{1}{2}(\delta^i_k + iJ^i_k)x^k, \tfrac{1}{2}(\delta^j_l + iJ^j_l)x^l\right\} = \tfrac{1}{4}[(\omega^{-1})^{ij} - i\delta^i_r K^{rj} + i\delta^j_r K^{ri} + J^j_l \delta^i_s K^{sl}] = \tfrac{1}{4}[(\omega^{-1})^{ij} - iK^{ij} + iK^{ji} + J^j_l K^{il}]$$
$$= \tfrac{1}{4}[(\omega^{-1})^{ij} + (\omega^{-1})^{ji}] = 0,$$

where we used the symmetry property of K and antisymmetry of ω.

In the same manner,

$$\left\{\tfrac{1}{2}(\delta^i_k - iJ^i_k)x^k, \tfrac{1}{2}(\delta^j_l - iJ^j_l)x^l\right\} = 0.$$

Now we can compute $\{\overline{z}, z\}$ combinations,

$$\left\{\tfrac{1}{2}(\delta^i_k + iJ^i_k)x^k, \tfrac{1}{2}(\delta^j_l - iJ^j_l)x^l\right\} = \tfrac{1}{4}[\{x^i, x^j\} + iJ^i_k\{x^k, x^j\} - iJ^j_l\{x^i, x^l\} + J^i_k J^j_l\{x^k, x^l\}] = \tfrac{1}{4}[(\omega^{-1})^{ij} + iJ^i_k(\omega^{-1})^{kj} - iJ^j_l(\omega^{-1})^{il} + J^i_k J^j_l(\omega^{-1})^{kl}] = \tfrac{1}{4}[(\omega^{-1})^{ij} + iJ^i_k J^k_r K^{rj} + iJ^j_l J^l_r K^{ri} + J^i_k J^j_l J^k_s K^{sl}]$$
$$= \tfrac{1}{4}[(\omega^{-1})^{ij} - i\delta^i_r K^{rj} - i\delta^j_r K^{ri} - J^j_l \delta^i_s K^{sl}] = \tfrac{1}{4}[2(\omega^{-1})^{ij} - 2iK^{ij}]$$
$$= \tfrac{1}{2}[(\omega^{-1})^{ij} - iK^{ij}] = \tfrac{1}{2}[J^i_s K^{sj} - iK^{ij}] = \tfrac{1}{2}(-i)[\delta^i_s + iJ^i_s]K^{sj}.$$

Alternatively we could switch the indices of the symplectic form in the middle step above, to get

$$\left\{\tfrac{1}{2}(\delta^i_k + iJ^i_k)x^k, \tfrac{1}{2}(\delta^j_l - iJ^j_l)x^l\right\} = \tfrac{1}{2}[-(\omega^{-1})^{ji} - iK^{ij}] = \tfrac{1}{2}(-i)[\delta^i_s - iJ^j_s]K^{si}. \tag{80}$$

Now we note that,

$$\tfrac{1}{2}(-i)[\delta^i_s + iJ^i_s]K^{sj} = \tfrac{1}{2}[-(\omega^{-1})^{ji} - iK^{ij}] = \tfrac{1}{2}(-i)[\delta^j_s - iJ^j_s]K^{si}. \tag{81}$$

We use the fact that the operator acting on K is the projection operator $(1+iJ)$. Now we have

$$(-i)\tfrac{1}{2}[\delta^i_s + iJ^i_s]\tfrac{1}{2}[\delta^s_{s'} + iJ^s_{s'}]K^{s'j} = (-i)\tfrac{1}{2}[\delta^i_s + iJ^i_s]K^{sj}. \tag{82}$$

From the equality of this to the above expressions we write

$$\left\{\tfrac{1}{2}(1+iJ)^i_l x^l, \tfrac{1}{2}(1-iJ)^j_k x^k\right\} = (-i)\tfrac{1}{2}[\delta^i_s + iJ^i_s]\tfrac{1}{2}[\delta^j_{s'} - iJ^j_{s'}]K^{s's}. \tag{83}$$

Indeed the meaning of this equation is clear if we construct a Hermitian product, using our original real inner product as

$$\left[\tfrac{1}{2}(1+iJ)e^{*\alpha}\right](x)\left[\tfrac{1}{2}(1-iJ)e^{*\beta}\right](x)K(e_\alpha, e_\beta)$$

$$= \left[\tfrac{1}{2}(x^\alpha + ix^{\alpha+n})\tfrac{1}{2}(x^\beta - ix^{\beta+n})\right]K(e_\alpha, e_\beta) = H(x,x), \tag{84}$$

or in a dual manner

$$\left[\tfrac{1}{2}(1-iJ)e^{*i}\right](e_s)\left[\tfrac{1}{2}(1+iJ)e^{*j}\right](e_{s'})K(e^{*s}, e^{*s'})$$

$$= e^{*i}\left[\tfrac{1}{2}(1+iJ)e_s\right]e^{*j}\left[\tfrac{1}{2}(1-iJ)e_{s'}\right]K(e^{*s}, e^{*s'}). \tag{85}$$

In a compact form using $x_i e^{*i} = x^*$ this could be expressed as

$$x^*\left[\tfrac{1}{2}(1+iJ)e_s\right]x^*\left[\tfrac{1}{2}(1-iJ)e_{s'}\right]K(e^{*s}, e^{*s'}). \tag{86}$$

If we now use our special basis, $\{e_\alpha\}$, we get

$$= \tfrac{1}{4}x^*(e_\alpha - ie_{\alpha+n})x^*(e_\beta + ie_{\beta+n})K(e^{*\alpha}, e^{*\beta})$$
$$= \tfrac{1}{4}(x_\alpha - ix_{\alpha+n})(x_\beta + ix_{\beta+n})K(e^{*\alpha}, e^{*\beta}) = H(x^*, x^*). \tag{87}$$

So, if we specialize to our choice of coordinates, $(z^\alpha, \bar{z}^\alpha)$, the expression on the right-hand side in Eq. (84) is indeed a Hermitian inner product. We will denote this Hermitian form as $H_{\alpha\underline{\beta}}$ and it has the symmetry

$$\overline{H_{\alpha\underline{\beta}}} = H_{\beta\underline{\alpha}}. \tag{88}$$

We will find the creation and annihilation operators in terms of our special choice of coordinates. By (76),

$$\tfrac{1}{2}(1+iJ)e^{*\alpha} + \tfrac{1}{2}(1-iJ)e^{*\alpha} = e^{*\alpha}. \tag{89}$$

The same is true for the second half, so

$$\tfrac{1}{2}(1+iJ)e^{*\alpha+n} + \tfrac{1}{2}(1-iJ)e^{*\alpha+n} = e^{*\alpha+n}. \tag{90}$$

We can extract the J from the $e^{*\alpha+n}$ term to get $e^{*\alpha}$ and act to the left to obtain

$$\tfrac{1}{2}(J+iJ^2)e^{*\alpha} + \tfrac{1}{2}(J-iJ^2)e^{*\alpha} = e^{*\alpha}. \tag{91}$$

Then we see that,

$$\tfrac{1}{2}(J-i)e^{*\alpha} + \tfrac{1}{2}(J+i)e^{*\alpha} = e^{*\alpha+n}. \tag{92}$$

Hence,

$$(-i)\left[\tfrac{1}{2}(1+iJ)e^{*\alpha}-\tfrac{1}{2}(1-iJ)e^{*\alpha}\right]=e^{*\alpha+n}. \tag{93}$$

Thus, we have the usual relation, such that

$$z^{\alpha}+\bar{z}^{\alpha}=x^{\alpha}, \tag{94}$$

$$(-i)(z^{\alpha}-\bar{z}^{\alpha})=x^{\alpha+n}. \tag{95}$$

Let us assume that we have made this special choice of basis and found

$$\{\bar{z}^{\alpha},z^{\beta}\}=(-i)H^{\underline{\alpha}\beta}. \tag{96}$$

Now we use the Dirac quantization rule and set

$$[a^{\alpha},a^{\dagger\beta}]=H^{\underline{\alpha}\beta}, \tag{97}$$

and we assume there is a vacuum state satisfying,

$$a^{\alpha}|0\rangle=0. \tag{98}$$

It is possible to further diagonalize the Hermitian form $H^{\underline{\alpha}\beta}$, without mixing z and $\bar{z}$ coordinates, they will be the independent excitations, which could be identified as the "particles" of the theory. We will not need this in our work, so not to complicate our notation further we ignore this step. Equation (97) creates a Fock space with positive norm elements as can easily be checked,

$$|\lambda\rangle=\lambda_{\alpha}a^{\dagger\alpha}|0\rangle, \tag{99}$$

$$\langle\lambda|\lambda\rangle=\lambda^{*}_{\underline{\beta}}\lambda_{\alpha}H^{\underline{\beta}\alpha}>0. \tag{100}$$

We will demonstrate in an alternative way that these commutation relations can be realized by operators acting on a Hilbert space and a^{α} and $a^{\dagger\alpha}$ are Hermitian conjugates under the inner product of our Hilbert space. For two functions $f(z^{\alpha})$ and $g(z^{\alpha})$, we define an inner product,

$$\langle f|g\rangle=\int\Pi_{\alpha}\,\mathrm{d}z^{\alpha}\,\mathrm{d}\bar{z}^{\underline{\alpha}}\,e^{-z^{\beta}(H^{-1})_{\beta\underline{\alpha}}\bar{z}^{\underline{\alpha}}}f(z)g(z). \tag{101}$$

The completion of holomorphic functions in this inner product defines our Hilbert space. Then we define,

$$a^{\alpha}=H^{\underline{\alpha}\beta}\frac{\partial}{\partial z^{\beta}},\quad a^{\dagger\beta}=z^{\beta}, \tag{102}$$

which clearly satisfies our commutation relations. A calculation reveals that

$$\langle f|H^{\underline{\gamma\lambda}}\partial_{\lambda}g\rangle=\langle z^{\gamma}f|g\rangle. \tag{103}$$

As a result we have the desired equality

$$\langle f|a^{\dagger\gamma}g\rangle=\langle a^{\gamma}f|g\rangle. \tag{104}$$

We have a well-defined normal ordering rule

$$:a^{\alpha}a^{\dagger\beta}:=a^{\dagger\beta}a^{\alpha}, \tag{105}$$

and no change for all the other combinations.

In general it will not be practical to switch to this special basis, but $\frac{1}{2}(1-iJ)$, $\frac{1}{2}(1+iJ)$ terms are, respectively, projections onto these subspaces and normal ordering brings a negative commutator at the end, so

$$\left[\tfrac{1}{2}(\widehat{(1+iJ)}x)^i, \tfrac{1}{2}(\widehat{(1-iJ)}x)^j\right] = i\tfrac{1}{2}[(\omega^{-1})^{ij} - iK^{ij}] = \tfrac{1}{2}[i(\omega^{-1})^{ij} + K^{ij}]. \tag{106}$$

So we can use this idea to set a normal ordering rule as

$$:\hat{x}^i\hat{x}^j: = \hat{x}^i\hat{x}^j - \tfrac{1}{2}[i(\omega^{-1})^{ij} + K^{ij}]. \tag{107}$$

The discussion on projections imply that there is no reason to look for two different relations, our projections have all the desired properties. (So the net result will be the above commutator relations.)

For complex coordinates as in our case, we can thus postulate the normal ordering with twice the commutator taken out. However, we note a subtle point, what we call as the symplectic structure and the quadratic form are not the same as in the complex case, there is a factor of 2. Thus, when we multiply the above subtracted term by a factor of 2, we should then covert back to the symplectic form and the quadratic form used in the complex case, this means that the factor of 2 disappears again, and we end up with

$$:\hat{\bar{w}}^i\hat{w}^j: = \hat{\bar{w}}^i\hat{w}^j - \tfrac{1}{2}[i(\omega^{-1})^{ij} + K^{ij}]. \tag{108}$$

It should be noted that in this equation the indices are assigned to a discrete set, and *from now on, we will use continuous indices as well as discrete ones; the continuous indices will be shown explicitly in parentheses or as bra-kets and* α, β, γ, *etc, will imply only discrete color degrees of freedom*.

If we go back to our example of Klein-Gordon field we can state our normal ordering as

$$:\Phi(x)\Phi(y): = \Phi(x)\Phi(y) - \tfrac{1}{2}[i(\omega^{-1})(x,y) + KQ^{-1}(x,y)] \tag{109}$$

$$\begin{aligned}=&\begin{pmatrix}\phi(x)\phi(y) & \phi(x)\pi(y)\\ \pi(x)\phi(y) & \phi(x)\phi(y)\end{pmatrix} - \frac{1}{2}\begin{pmatrix}0 & -i\delta(x-y)\\ i\delta(x-y) & 0\end{pmatrix}\\ &-\frac{1}{2}\begin{pmatrix}\langle x|(-\nabla^2+m^2)^{-1/2}|y\rangle & 0\\ 0 & \langle x|(-\nabla^2+m^2)^{\frac{1}{2}}|y\rangle\end{pmatrix}\end{aligned} \tag{110}$$

$$= \begin{pmatrix}\phi(x)\phi(y) & \phi(x)\pi(y)\\ \pi(x)\phi(y) & \phi(x)\phi(y)\end{pmatrix} \tag{111}$$

$$-\frac{1}{2}\begin{pmatrix}\langle x|(-\nabla^2+m^2)^{-1/2}|y\rangle & -i\delta(x-y)\\ i\delta(x-y) & \langle x|(-\nabla^2+m^2)^{\frac{1}{2}}|y\rangle\end{pmatrix}. \tag{112}$$

Let us now write the normal ordering rule in our theory using the formalism developed above,

$$:\phi^\dagger_\alpha(x)\phi^\beta(y): = \phi^\dagger_\alpha(x)\phi^\beta(y) - \tfrac{1}{2}[i(\omega^{-1})^\alpha{}_\beta(x,y) + K^\alpha{}_\beta(x,y)], \tag{113}$$

where

$$(\omega^{-1})^\gamma{}_\beta(x,y) = 2\langle x|(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}|y\rangle\delta^\gamma{}_\beta. \tag{114}$$

Here sgn is

$$\langle x|\mathrm{sgn}|y\rangle = \mathrm{sgn}(x)\,\delta(x-y). \tag{115}$$

The system is diagonal in the color indices, hence we can write it as it is

$$K^\alpha{}_\beta(x,y) = \langle x|([-(\omega^{-1}Q)^2]^{1/2})^\alpha{}_\beta|y\rangle. \tag{116}$$

There is no difference between upper and lower color indices for our purposes here. Thus

$$K^{\alpha}{}_{\beta}(x,y) = \langle x|(-[(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}(-\partial_x^2 + m^2)]^2)^{1/2}|y\rangle \delta^{\alpha}{}_{\beta}. \tag{117}$$

Then, transforming our expression $K^i_j Q^{js}$ to the infinite dimensional case only for the continuous indices, this becomes

$$K^{\alpha}{}_{\beta} = 2(-[(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}(-\partial^2 + m^2)]^2)^{1/2}(-\partial^2 + m^2)^{-1}\delta^{\alpha}{}_{\beta}. \tag{118}$$

We *keep the color index* down in general, since from the group theory point of view the fields have special color indices attached to them. (The operator above has a kernel which should perhaps best be written as $K^{\alpha(x,y)}_{\beta}$, but to keep the notation simple we will keep the usual writing style for the kernels.) It is not so simple to evaluate these expressions. Only as symbols of operators we have some chance. We will not attack this question in the present work. From now on we will denote the colorless part of the subtraction in the normal ordering as the vacuum expectation value $V(x,y)$,

$$V(x,y) \equiv \langle x|(-[(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}(-\partial^2 + m^2)]^2)^{1/2}(-\partial^2 + m^2)^{-1}|y\rangle + i\langle x|(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}|y\rangle.$$

As mentioned, this is defined as a pseudodifferential operator. And of course after quantization we maintain the commutation relations for the bosons,

$$[\tilde{\phi}^{\alpha}(x), \tilde{\phi}^{\dagger}_{\beta}(y)] = i\omega^{-1}(x,y)\delta^{\alpha}{}_{\beta}, \tag{119}$$

where

$$\omega^{-1}(x,y) = \langle x|2(-\overleftarrow{\partial}\,\mathrm{sgn} + \mathrm{sgn}\,\overrightarrow{\partial})^{-1}|y\rangle. \tag{120}$$

IV. GAUGE INVARIANCE CONSTRAINT

When we quantize the theory, we get a normal ordered version of (36), since we have products of the fields at the same point. Thus a reduction at the quantum level should read

$$\hat{E} = \hat{e} - \frac{g^2}{2}\int_{-L}^{x} \mathrm{d}y\ \mathrm{sgn}(y){:}\{\tilde{\phi}(\partial_y\tilde{\phi}^{\dagger}) - (\partial_y\tilde{\phi})\tilde{\phi}^{\dagger}\}{:}\ . \tag{121}$$

With this expression our *quantum* Hamiltonian can be written as

$$\hat{H} = \frac{1}{2}\int \mathrm{d}x{:}(\partial_x\tilde{\phi}^{\dagger})(\partial_x\tilde{\phi}){:} + \frac{1}{2}\int \mathrm{d}x{:}m^2\tilde{\phi}^{\dagger}\tilde{\phi}{:} - \frac{1}{2g^2}\int \mathrm{d}x\ \mathrm{Tr}\left[\hat{e} - \frac{g^2}{2}\int_{-L}^{x}\mathrm{d}y\ \mathrm{sgn}(y){:}\{\tilde{\phi}(\partial_y\tilde{\phi}^{\dagger}) - (\partial_y\tilde{\phi})\tilde{\phi}^{\dagger}\}{:}\right]^2 \tag{122}$$

If we express our previous boundary condition (21), $\tilde{E}(+L) = q\tilde{E}(-L)q^{-1}$ we end up with a constraint,

$$\hat{e} - \frac{g^2}{2}\int_{-L}^{L}\mathrm{d}y\ \mathrm{sgn}(y){:}\{\tilde{\phi}(\partial_y\tilde{\phi}^{\dagger}) - (\partial_y\tilde{\phi})\tilde{\phi}^{\dagger}\} := \hat{q}\hat{e}\hat{q}^{-1}. \tag{123}$$

(For simplicity we are not using any ordering rule for $\hat{q}\hat{e}\hat{q}^{-1}$, we can take it as Weyl ordered, and the result will not change.) This is a too strong condition in the quantum theory. We should impose this constraint on physical states. Its meaning is clear if we define a global color operator as

$$\hat{Q} = \hat{e} - \hat{q}\hat{e}\hat{q}^{-1} - \frac{g^2}{2}\int_{-L}^{L}\mathrm{d}y\ \mathrm{sgn}(y){:}\{\tilde{\phi}(\partial_y\tilde{\phi}^{\dagger}) - (\partial_y\tilde{\phi})\tilde{\phi}^{\dagger}\}{:}\ , \tag{124}$$

which gives zero acting on any color invariant physical state.

Shortly we will demonstrate that $\hat{Q}$ truly generates global gauge transformations. Therefore the constraint tells us to restrict our theory to the color invariant sector. It is not difficult to form the simplest mesonic variable, i.e., a color invariant physical state, in the fundamental representation. We can check that the combination below is a gauge invariant state,

$$\phi^{\dagger}(x)P\{e^{\int_x^y A_x\,\mathrm{d}z}\}\phi(y). \tag{125}$$

Here the fields at these points are brought to the same point by parallel transport operator. When we transform the fields according to Eq. (19) we obtain

$$(\tilde{\phi}^{\dagger}(x)P\{e^{\int_{-L}^{x} A_x\,\mathrm{d}z}\})P\{e^{\int_x^y A_x\,\mathrm{d}z}\}(P\{e^{-\int_{-L}^{y} A_x\,\mathrm{d}z}\}\tilde{\phi}(y)). \tag{126}$$

The path ordered exponentials add up to one due to the boundary conditions of the Wilson loop in (16). We could as well construct a more general state by having several loops such as

$$\phi^{\dagger}(x)P\{e^{\int_x^{y+2KL} A_x\,\mathrm{d}z}\}\phi(y). \tag{127}$$

So the more general expression for the mesonic variable is as follows:

$$\tilde{\phi}_{\alpha}^{\dagger}(x)(q^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y). \tag{128}$$

We should normal order this at the quantum level. The normal ordered versions of these should be the general "mesonic" observables. Nevertheless, we will need even a more general expression for possible observables in our work, as we will see later on.

Now that we have constructed a color invariant physical state we should show that it commutes with our color operator. Typical color invariant state can be constructed through the products of such mesonic states on the vacuum. If we write the quantum constraint as

$$\mathrm{Tr}\,\Lambda\hat{Q}|\text{physical state}\rangle = 0, \tag{129}$$

where Λ is an element of the Lie algebra, after commuting through various mesonic operators eventually $\mathrm{Tr}\,\Lambda\hat{Q}$ acts on the vacuum and that gives zero as desired. So let us take a closer look at the commutator,

$$[\mathrm{Tr}\,\Lambda\hat{Q},{:}\tilde{\phi}_{\alpha}^{\dagger}(z)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(w){:}]. \tag{130}$$

First note that

$$\begin{aligned}
&\frac{g^2}{2}\int_{-L}^{L}\mathrm{d}y\;\Lambda^{\alpha}{}_{\beta}{:}\tilde{\phi}_{\alpha}^{\dagger}(y)(-\overleftarrow{\partial}_y\,\mathrm{sgn}(y)+\mathrm{sgn}(y)\overrightarrow{\partial}_y)\tilde{\phi}^{\beta}(y){:}\\
&\quad=\frac{g^2}{2}\int_{-L}^{L}\int_{-L}^{L}\mathrm{d}y\,\mathrm{d}y'\;\Lambda^{\alpha}{}_{\beta}{:}\tilde{\phi}_{\alpha}^{\dagger}(y')\langle y'|(-\overleftarrow{\partial}\,\mathrm{sgn}+\mathrm{sgn}\,\overrightarrow{\partial})|y\rangle\tilde{\phi}^{\beta}(y){:}\\
&\quad=g^2\int_{-L}^{L}\int_{-L}^{L}\mathrm{d}y\,\mathrm{d}y'\;\Lambda^{\alpha}{}_{\beta}{:}\tilde{\phi}_{\alpha}^{\dagger}(y')\omega(y',y)\tilde{\phi}^{\beta}(y){:}
\end{aligned}$$

Now it is a simple matter to check that,

$$\begin{aligned}
&[\mathrm{Tr}\,\Lambda\hat{e}-\mathrm{Tr}(\Lambda\hat{q}\hat{e}\hat{q}^{-1}),{:}\tilde{\phi}^{\dagger}\hat{q}^K\tilde{\phi}{:}]\\
&\quad=ig^2\sum_R{:}\tilde{\phi}^{\dagger}\hat{q}^R(\hat{q}\Lambda)\hat{q}^{K-R-1}\tilde{\phi}{:}-ig^2\sum_R{:}\tilde{\phi}^{\dagger}\hat{q}^R(\hat{q}\hat{q}^{-1}\Lambda\hat{q})\hat{q}^{K-R-1}\tilde{\phi}{:}\\
&\quad=-ig^2{:}\tilde{\phi}_{\alpha}^{\dagger}(z)[\Lambda,\hat{q}^K]^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(w){:}\;,
\end{aligned}$$

here the last commutator only refers to the color indices. We can now go back and find the action of the bosonic part on mesonic operators,

$$\begin{aligned}
&\left[g^2 \int_{-L}^{L} \int_{-L}^{L} \mathrm{d}y\, \mathrm{d}y'\ \Lambda^{\alpha}{}_{\beta} (: \tilde{\phi}^{\dagger}_{\alpha}(y') \omega(y',y) \tilde{\phi}^{\beta}(y):), : \tilde{\phi}^{\dagger}_{\sigma}(z) (\hat{q}^K)^{\sigma}{}_{\tau} \tilde{\phi}^{\tau}(w): \right] \\
&\quad = i g^2 \int_{-L}^{L} \int_{-L}^{L} \mathrm{d}y\, \mathrm{d}y'\ \Lambda^{\alpha}{}_{\beta} \tilde{\phi}^{\dagger}_{\alpha}(y') \omega(y',y) \omega^{-1}(y,z) \delta^{\beta}{}_{\sigma} (\hat{q}^K)^{\sigma}{}_{\tau} \tilde{\phi}^{\tau}(w) \\
&\qquad + i g^2 \int_{-L}^{L} \int_{-L}^{L} \mathrm{d}y\, \mathrm{d}y'\ \Lambda^{\alpha}{}_{\beta} \omega(y',y) \omega^{-1}(y',\omega) \delta^{\tau}{}_{\alpha} \tilde{\phi}^{\dagger}_{\sigma}(z) (\hat{q}^K)^{\sigma}{}_{\tau} \tilde{\phi}^{\beta}(y) \\
&\quad = i g^2 : \tilde{\phi}^{\dagger}_{\alpha}(z) \Lambda^{\alpha}{}_{\beta} (\hat{q}^K)^{\beta}{}_{\sigma} \tilde{\phi}^{\sigma}(w): - i g^2 : \tilde{\phi}^{\dagger}_{\alpha}(z) (\hat{q}^K)^{\alpha}{}_{\beta} \Lambda^{\beta}{}_{\tau} \tilde{\phi}^{\tau}(w): \\
&\qquad - i V(z,w) \delta^{\sigma}{}_{\alpha} \Lambda^{\alpha}{}_{\beta} (\hat{q}^K)^{\beta}{}_{\sigma} + i V(z,w) \delta^{\tau}{}_{\alpha} \Lambda^{\beta}{}_{\tau} (\hat{q}^K)^{\alpha}{}_{\beta} \\
&\quad = + i g^2 : \tilde{\phi}^{\dagger}_{\alpha}(z) \Lambda^{\alpha}{}_{\beta} (\hat{q}^K)^{\beta}{}_{\sigma} \tilde{\phi}^{\sigma}(w): - i g^2 : \tilde{\phi}^{\dagger}_{\alpha}(z) (\hat{q}^K)^{\alpha}{}_{\beta} \Lambda^{\beta}{}_{\sigma} \tilde{\phi}^{\sigma}(w): \\
&\quad = i g^2 : \tilde{\phi}^{\dagger}_{\alpha}(z) [\Lambda, \hat{q}^K]^{\alpha}{}_{\beta} \tilde{\phi}^{\beta}(w): .
\end{aligned}$$

We may need to deal with even more general operators of the form

$$: \tilde{\phi}^{\dagger}(z) \hat{q}^{K_1} \hat{e}^{S_1} \hat{q}^{K_2} \cdots \tilde{\phi}(w): \tag{131}$$

as we will discuss later on. The operator $\mathrm{Tr}\, \Lambda \hat{Q}$ still generates global color transformations on these operators. To show this it is enough to look at the action of $\mathrm{Tr}\, \Lambda \hat{Q}$ on $\hat{e}^{\alpha}_{\beta}$,

$$\begin{aligned}
[\mathrm{Tr}\, \Lambda \hat{Q}, \hat{e}^{\alpha}_{\beta}] &= [\mathrm{Tr}\, \Lambda \hat{e} - \mathrm{Tr}\, \Lambda \hat{q} \hat{e} \hat{q}^{-1}, \hat{e}^{\alpha}{}_{\beta}] = - i g^2 [\Lambda, \hat{e}]^{\alpha}{}_{\beta} + [(\Lambda \hat{q})^{\lambda}{}_{\sigma}, \hat{e}^{\alpha}{}_{\beta}] (\hat{e} \hat{q})^{\tau}{}_{\lambda} \\
&\quad + (\Lambda \hat{q})^{\lambda}{}_{\sigma} [\hat{e}^{\sigma}{}_{\tau}, \hat{e}^{\alpha}{}_{\beta}] (\hat{q}^{-1})^{\tau}{}_{\lambda} + (\Lambda \hat{q} \hat{e})^{\lambda}{}_{\tau} [(\hat{q}^{-1})^{\tau}{}_{\lambda}, \hat{e}^{\alpha}{}_{\beta}] \\
&= - i g^2 [\Lambda, \hat{e}]^{\alpha}{}_{\beta} - i g^2 \Lambda^{\lambda}{}_{\mu} (\hat{q}^{\mu}{}_{\beta} \delta^{\alpha}{}_{\sigma}) \hat{e}^{\sigma}{}_{\tau} (\hat{q}^{-1})^{\tau}{}_{\lambda} \\
&\quad + i g^2 (\Lambda \hat{q})^{\lambda}{}_{\sigma} (\hat{e}^{\alpha}{}_{\tau} \delta^{\sigma}{}_{\beta} - \hat{e}^{\sigma}{}_{\beta} \delta^{\alpha}{}_{\tau}) (\hat{q}^{-1})^{\alpha}{}_{\lambda} + i g^2 (\Lambda \hat{q} \hat{e})^{\lambda}{}_{\tau} (\hat{q}^{-1})^{\tau}{}_{\mu} \hat{q}^{\mu}{}_{\beta} \delta^{\alpha}{}_{\nu} (\hat{q}^{-1})^{\nu}{}_{\sigma} \\
&= - i g^2 [\Lambda, \hat{e}]^{\alpha}{}_{\beta}.
\end{aligned}$$

(As the reader can verify, the Weyl ordering will not change this result.) This proves that the color operator acts as desired.

V. THE LARGE N_c LIMIT

The basic idea of large N_c limit is to write everything in terms of color invariant observables. In the limit of large N_c, only the color invariant operators survive and the expectation values of color invariant operators split as a product up to order $1/N_c$ corrections, so

$$\langle AB \rangle = \langle A \rangle \langle B \rangle + O\left(\frac{1}{N_c} \right). \tag{132}$$

The equation above implies that the set of color invariant operators becomes classical as N_c goes to infinity. Thus all color invariant operators should be representable as classical observables in the large N_c limit. This is an idea of Migdal,[2] see also Witten.[28] A nice review of how one should think of it as a classical limit is presented in Ref. 29.

We had found the color invariant physical states to be of the form in Eq. (128). A more general expression would be of the form

$$: \tilde{\phi}^{\dagger}_{\alpha}(x) [\hat{q}^{K_1} \hat{e}^{S_1} \hat{q}^{K_2} \hat{e}^{S_2} \cdots \hat{q}^{K_m}]^{\alpha}{}_{\beta} \tilde{\phi}_{\beta}(y): . \tag{133}$$

In the large N_c limit there should be classical observables defined to be

$$N(x,y|K_1,S_1,\cdots,K_m)=\lim_{N_c\to\infty}\frac{1}{N_c}:\tilde{\phi}^{\dagger}_{\alpha}(x)[\hat{q}^{K_1}\hat{e}^{S_1}\hat{q}^{K_2}\hat{e}^{S_2}\cdots\hat{q}^{K_m}]^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y):. \tag{134}$$

We note that its complex conjugate is not an independent variable, but satisfies the relation

$$N^{*}(x,y|K_1,S_1,\cdots,K_m)=\lim_{N_c\to\infty}\frac{1}{N_c}(:\tilde{\phi}^{\dagger}_{\alpha}(x)[\hat{q}^{K_1}\hat{e}^{S_1}\hat{q}^{K_2}\hat{e}^{S_2}\cdots\hat{q}^{K_m}]^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y))^{\dagger}: \tag{135}$$

$$=N(y,x|-K_m,S_{n-1},\ldots,-K_1)(-1)^{S_1+\ldots+S_m}, \tag{136}$$

since, we keep

$$(\hat{e}^{\alpha}{}_{\beta})^{\dagger}=-\hat{e}^{\beta}{}_{\alpha}\quad\text{and}\quad(\hat{q}^{\alpha}{}_{\beta})^{\dagger}=(\hat{q}^{-1})^{\beta}{}_{\alpha} \tag{137}$$

(where † refers to the quantum mechanical Hermitian conjugate). Moreover, we may keep the tracelessness condition of $\hat{e}$ acting on the physical states, $\mathrm{Tr}\,\hat{e}\,|\text{physical}>=0$. When we apply our dynamical boundary conditions, namely

$$\tilde{\phi}(L)=\hat{q}^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(-L), \tag{138}$$

the N observable satisfies the relation

$$:\tilde{\phi}^{\dagger}_{\alpha}(x)[\hat{q}^{K_1}\hat{e}^{S_1}\hat{q}^{K_2}\hat{e}^{S_2}\cdots\hat{q}^{K_m}]^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(L):=:\tilde{\phi}^{\dagger}_{\alpha}(x)[\hat{q}^{K_1}\hat{e}^{S_1}\hat{q}^{K_2}\hat{e}^{S_2}\cdots\hat{q}^{K_m+1}]^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(-L):. \tag{139}$$

In the large N_c limit this condition should be postulated as

$$N(x,L|K_1,S_1,\ldots,K_m)=N(x,-L|K_1,S_1,\ldots,K_m+1). \tag{140}$$

We also define

$$Q(K)=\lim_{N_c\to\infty}\frac{1}{N_c}\,\mathrm{Tr}\,\hat{q}^{K}, \tag{141}$$

and in general more complex variables

$$Q(K_1,S_1,\ldots,K_r,S_r)=\lim_{N_c\to\infty}\frac{1}{N_c}\,\mathrm{Tr}(\hat{q}^{K_1}\hat{e}^{S_1}\cdots\hat{q}^{K_r}\hat{e}^{S_r}). \tag{142}$$

We believe that only the simpler variables will be essential to get the mesonic spectrum of the theory but in principle we have all these observables in our theory. These observables satisfy similar conjugation conditions.

VI. CONSTRAINTS OF THE LARGE-N_c THEORY

Color invariance implies a constraint on the bilinears of the theory, due to our requirement

$$\mathrm{Tr}\,\Lambda\hat{Q}|\text{physical}\rangle=0. \tag{143}$$

We note the following interesting observation about the infinite dimensional trace of the basic variables,

$$g^2\int_{-L}^{L}\int_{-L}^{L}\mathrm{d}x\,\mathrm{d}y\;\omega(y,x):\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^{K})^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y):=(\hat{q}^{K})^{\alpha}{}_{\beta}[\hat{e}^{\beta}{}_{\alpha}-(\hat{q}\hat{e}\hat{q}^{-1})^{\beta}{}_{\alpha}]=[\mathrm{Tr}(\hat{q}^{K}\hat{e})-\mathrm{Tr}(\hat{q}^{K+1}\hat{e}\hat{q}^{-1})]. \tag{144}$$

Let us reorder the last term as

$$\hat{q}^{\lambda}{}_{\sigma}(\hat{q}^K)^{\sigma}{}_{\mu}\hat{e}^{\mu}{}_{\nu}(\hat{q}^{-1})^{\nu}{}_{\lambda} = (\hat{q}^K)^{\sigma}{}_{\mu}(\hat{e}^{\mu}{}_{\nu}\hat{q}^{\lambda}{}_{\sigma}(q^{-1})^{\nu}{}_{\lambda} - [e^{\mu}{}_{\nu}, q^{\lambda}{}_{\sigma}])(q^{-1})^{\nu}{}_{\lambda} = (\hat{q}^K)^{\sigma}{}_{\mu}\hat{e}^{\mu}{}_{\nu}\delta^{\nu}{}_{\sigma} - ig^2\delta^{\mu}{}_{\sigma}\delta^{\lambda}{}_{\lambda}(\hat{q}^K)^{\sigma}{}_{\mu}$$
$$= \mathrm{Tr}(\hat{q}^K\hat{e}) - ig^2N_c\,\mathrm{Tr}\,\hat{q}^K.$$

Hence we get,

$$g^2\int_{-L}^{L}\int_{-L}^{L}\mathrm{d}x\,\mathrm{d}y\;\omega(y,x):\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y) = (\hat{q}^K)^{\alpha}{}_{\beta}[\hat{e}^{\beta}{}_{\alpha} - (\hat{q}\hat{e}\hat{q}^{-1})^{\beta}{}_{\alpha}] = ig^2\,\mathrm{Tr}(\hat{q}^K), \quad (145)$$

or in the large-N_c limit,

$$\lim_{N_c\to\infty}\frac{1}{N_c}\int \mathrm{d}x\,\mathrm{d}y\;\omega(y,x)N(x,y|K) = iQ(K). \quad (146)$$

This is an extra condition on the infinite dimensional trace,

$$\lim_{N_c\to\infty}\frac{1}{N_c}\,\mathrm{tr}(\omega\mathbf{N}(K)) = iQ(K). \quad (147)$$

(Note that this condition tells us what should be the leading divergence of the trace of this operator.)

Let us now look for another relation satisfied by the basic "mesonic" observables, so we compute the following product:

$$\int_{-L}^{L}\mathrm{d}y\,\mathrm{d}y':\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y'):\omega(y',y):\tilde{\phi}^{\dagger}_{\lambda}(y)(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z):. \quad (148)$$

For simplicity of writing we will drop the limits of the integrals. We expand the normal orderings by subtracting the vacuum energies

$$\int \mathrm{d}y\,\mathrm{d}y'[\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y') - V(x,y')\mathrm{Tr}(\hat{q}^K)]\omega(y',y)[\tilde{\phi}^{\dagger}_{\lambda}(y)(\hat{q}^K)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z) - V(y,z)\mathrm{Tr}(\hat{q}^L)]. \quad (149)$$

Collecting the cross terms, and keeping the first term as it is, and normal ordering the other terms again we get, apart from the first term,

$$-\int \mathrm{d}y\,\mathrm{d}y'(\mathrm{Tr}\,\hat{q}^K)V(x,y')\omega(y',y):\tilde{\phi}^{\dagger}_{\lambda}(y)(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z):-\int \mathrm{d}y\,\mathrm{d}y'(\mathrm{Tr}\,\hat{q}^L)V(y,z)\omega(y',y):\tilde{\phi}^{\dagger}_{\alpha}(x)$$
$$\times(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y'):-\int \mathrm{d}y\,\mathrm{d}y'(\mathrm{Tr}\,\hat{q}^L)(\mathrm{Tr}\,\hat{q}^K)V(x,y')\omega(y',y)V(y,z). \quad (150)$$

We will keep this term as it is, what we extract from the first term at the end will be added to this part. Now let us look at the other product coming from (149),

$$\int \mathrm{d}y\,\mathrm{d}y'\,\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y')\omega(y',y)\tilde{\phi}^{\dagger}_{\lambda}(y)(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z). \quad (151)$$

Here we will change the order of $\tilde{\phi}^{\dagger}_{\lambda}(y)$ and $\tilde{\phi}^{\sigma}(z)$ inserting their commutation relations which brings the symplectic form as

$$\int \mathrm{d}y\,\mathrm{d}y'\;\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y')\omega(y',y)[\tilde{\phi}^{\sigma}(z)\tilde{\phi}^{\dagger}_{\lambda}(y) + i\omega^{-1}(y,z)\delta^{\sigma}{}_{\lambda}](\hat{q}^L)^{\lambda}{}_{\sigma}. \quad (152)$$

Hence,

$$\int \mathrm{d}y\ \mathrm{d}y'\ \tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(y')\omega(y',y)\tilde{\phi}^{\sigma}(z)\tilde{\phi}^{\dagger}_{\lambda}(y)(\hat{q}^L)^{\lambda}{}_{\sigma} + i\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z)\mathrm{Tr}(\hat{q}^L). \quad (153)$$

Now the first term in the above expression is

$$\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z)\int \mathrm{d}y\ \mathrm{d}y'\ \tilde{\phi}^{\beta}(y')\omega(y',y)\tilde{\phi}^{\dagger}_{\lambda}(y). \quad (154)$$

The integral part is converted to normal ordering as

$$\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z)\Bigg[\int \mathrm{d}y\ \mathrm{d}y' {:}\tilde{\phi}^{\beta}(y')\omega(y',y)\tilde{\phi}^{\dagger}_{\lambda}(y){:} + \int \mathrm{d}y\ \mathrm{d}y'\,\delta^{\beta}{}_{\lambda}V(y,y')\omega(y',y)$$
$$- i\int \mathrm{d}y\ \mathrm{d}y'\,\omega(y,y')\omega^{-1}(y',y)\delta^{\beta}{}_{\lambda}\Bigg]. \quad (155)$$

The vacuum energy term gives $\mathrm{tr}(V\omega)$, an infinite dimensional trace, and there is another term $\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}(\hat{q}^L)^{\beta}{}_{\sigma}\tilde{\phi}^{\sigma}(z)$. Both of them are of smaller order in $1/N_c$. The last term is also of smaller order in $1/N_c$. Thus we drop these terms as $N_c\to\infty$. The first term in (155) satisfies the following on color invariant states as a result of vanishing color operator on such states;

$$\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}(\hat{q}^L)^{\lambda}{}_{\sigma}\tilde{\phi}^{\sigma}(z)\Bigg[-\frac{1}{g^2}(\hat{q}\hat{e}\hat{q}^{-1})^{\beta}{}_{\lambda}+\frac{1}{g^2}\hat{e}^{\beta}{}_{\lambda}\Bigg]. \quad (156)$$

To set the color indices in the right order we should commute $\hat{e}$ terms with $\hat{q}^L$ terms, which gives us,

$$\frac{1}{\tilde{g}^2}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K\hat{e}\hat{q}^L)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z) - \frac{1}{\tilde{g}^2}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^{K+1}\hat{e}\hat{q}^{L-1})^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z) - \frac{1}{\tilde{g}^2}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\sigma}(z)([\hat{e}^{\beta}_{\lambda},(\hat{q}^L)^{\lambda}{}_{\sigma}]$$
$$-[(\hat{q}\hat{e}\hat{q}^{-1})^{\beta}{}_{\sigma},(\hat{q}^L)^{\lambda}{}_{\sigma}]).$$

Here, $1/g^2$ eats up one of the $1/N_c$ terms via $g^2N_c=\tilde{g}^2$ as $N_c\to\infty$. Now let us normal order these terms again and simplify the commutators by a similar method to finally obtain

$$\frac{1}{\tilde{g}^2}\Bigg({:}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K\hat{e}\hat{q}^L)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z){:} - {:}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^{K+1}\hat{e}\hat{q}^{L-1})^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z){:} - V(x,z)(\mathrm{Tr}(\hat{q}^{K+1}\hat{e}\hat{q}^{L-1}) - \mathrm{Tr}(\hat{q}^K\hat{e}\hat{q}^L))$$
$$- {:}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\sigma}(z){:}\delta^{\beta}{}_{\sigma}(ig^2N_c)\frac{1}{N_c}\,\mathrm{Tr}\,\hat{q}^L + {:}\tilde{\phi}^{\dagger}_{\alpha}(x)(\hat{q}^K)^{\alpha}{}_{\beta}\tilde{\phi}^{\sigma}(z){:}(\hat{q}^L)^{\beta}{}_{\sigma}(ig^2N_c)$$
$$- ig^2V(x,z)(\mathrm{Tr}\,\hat{q}^K\,\mathrm{Tr}\,\hat{q}^L - N_c\,\mathrm{Tr}(\hat{q}^{K+L}))\Bigg).$$

We can use a further simplification,

$$\mathrm{Tr}(\hat{q}^{K+1}\hat{e}\hat{q}^{L-1}) - \mathrm{Tr}(\hat{q}^K\hat{e}\hat{q}^L) = -ig^2\,\mathrm{Tr}\,\hat{q}^K\,\mathrm{Tr}\,\hat{q}^L. \quad (157)$$

We divide the full expression by $1/N_c^2$ and find in terms of the large-N_c variables,

$$-iN(x,z|K)Q(L) + iN(x,z|K+L) + \frac{1}{\tilde{g}^2}[N(x,z|K,1,L) - N(x,z|K+1,1,L-1)] + iV(x,z)Q(K+L). \quad (158)$$

Here, we recall that

$$N(x,z|K,1,L) = \lim_{N_c\to\infty}\frac{1}{N_c}:\tilde{\phi}^{\dagger}_{\alpha}(x)(q^K\hat{e}q^L)^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z):\ ,$$

$$N(x,z|K+1,1,L-1) = \lim_{N_c\to\infty}\frac{1}{N_c}:\tilde{\phi}^{\dagger}_{\alpha}(x)(q^{K+1}\hat{e}q^{L-1})^{\alpha}{}_{\beta}\tilde{\phi}^{\beta}(z):\ .$$

The final result will then be, in terms of the large-N_c variables,

$$\begin{aligned}
&\int \mathrm{d}y'\ \mathrm{d}y\ N(x,y'|K)\omega(y',y)N(y,z|L) + Q(K)\int \mathrm{d}y'\ \mathrm{d}y\ V(x,y')\omega(y',y)N(y,z|L)\\
&\quad + Q(L)\int \mathrm{d}y'\ \mathrm{d}y\ N(x,y'|k)\omega(y',y)V(y,z) + Q(K)Q(L)\int \mathrm{d}y'\ \mathrm{d}y\ V(x,y')\omega(y',y)V(y,z)\\
&= iN(x,z|K+L) + \frac{1}{\tilde{g}^2}[N(x,z|K,1,L) - N(x,z|K+1,1,L-1)] + iV(x,z)Q(K)Q(L)\\
&\quad + iV(x,z)Q(K+L).
\end{aligned}$$

We see that the constraint does not define a familiar algebra (in its present form). There are similar constraints for other variables as well, but they are more complicated to derive although the essential steps are the same. We believe that if we could understand the above sector of this large-N_c theory, a significant part of the mesonic excitations would be understood. This constraint can be put in a more elegant form by assuming that there is an operator $\mathbf{N}$ which satisfies

$$\langle x|\mathbf{N}(K)|y\rangle = N(x,y|K), \tag{159}$$

then, we can write it as a matrix equation,

$$\begin{aligned}
&\mathbf{N}(K)\omega\mathbf{N}(L) + Q(K)V\omega\mathbf{N}(L) + Q(L)\mathbf{N}(K)\omega V + Q(K)Q(L)V\omega V = i\mathbf{N}(K+L)\\
&\quad + \frac{1}{\tilde{g}^2}[\mathbf{N}(K,1,L) - \mathbf{N}(K+1,1,L-1)] + iVQ(K+L) + iVQ(K)Q(L).
\end{aligned} \tag{160}$$

We recall our discussion in the third section, using its original notation (now j,k,l refer only to the continuous indices), that

$$\begin{aligned}
(V\omega)^k{}_l &= \frac{1}{2}[i(\omega^{-1})^{kj} + (KQ^{-1})^{kj}]\omega_{jl} = \frac{1}{2}[i\delta^k{}_l + ([-(\omega^{-1}Q)^2]^{1/2})^k{}_j(Q^{-1}\omega)^j_l]\\
&= \frac{i}{2}\delta^k{}_l + \frac{1}{2}([-(\omega^{-1}Q)^2]^{1/2})^k{}_j[(\omega^{-1}Q)^{-1}]^j{}_l = \frac{1}{2}[i\delta^k{}_l + i[\mathrm{sgn}(i\omega^{-1}Q)]^k{}_l].
\end{aligned} \tag{161}$$

Here the operator $\omega^{-1}Q$ is an antisymmetric matrix, since the usual sign function is defined for Hermitian operators we introduce an extra $i=\sqrt{-1}$ and pull out a factor of i. We also recall that

$$K^{\tau} = Q^{-1}K^TQ = K, \tag{162}$$

which can be written as

$$(KQ^{-1})^T = KQ^{-1}. \tag{163}$$

Now we note the following:

$$\begin{aligned}
\omega_{kj}V^{jl} &= -\tfrac{1}{2}\omega_{jk}[-i\omega^{lj} + (KQ^{-1})^{lj}] = i\tfrac{1}{2}\delta^k{}_l - \tfrac{1}{2}([-(\omega^{-1}Q)^2]^{1/2})^k{}_j[(\omega^{-1}Q)^{-1}]^j{}_l\\
&= i\tfrac{1}{2}\delta^k{}_l - i\tfrac{1}{2}[\mathrm{sgn}(i\omega^{-1}Q)]^k{}_l.
\end{aligned} \tag{164}$$

Hence, by using $\tilde{\omega}=\omega^{-1}Q$, we get

$$\mathbf{N}(K)\omega\,\mathbf{N}(L) + iQ(K)\tfrac{1}{2}[1+\mathrm{sgn}(i\tilde{\omega})]\mathbf{N}(L)$$
$$+ iQ(L)\mathbf{N}(K)\tfrac{1}{2}[1-\mathrm{sgn}(i\tilde{\omega})]$$
$$- Q(K)Q(L)\tfrac{1}{4}[1+\mathrm{sgn}(i\tilde{\omega})]\omega^{-1}[1-\mathrm{sgn}(i\tilde{\omega})] = i\mathbf{N}(K+L) + \frac{1}{\tilde{g}^2}[\mathbf{N}(K,1,L) - \mathbf{N}(K+1,1,L-1)]$$
$$+ iVQ(K+L) + iVQ(K)Q(L). \tag{165}$$

Let us note that the above constraint is invariant under the complex conjugation, or using the matrix form, under the Hermitian conjugation. To check that one should take the Hermitian conjugation and use the constraint equation for the combination $-\mathbf{N}(-K)\omega\mathbf{N}(-L)$, then the two results actually agree.

VII. THE EQUATIONS OF MOTION

The next stage is to write the equations of motion for the simple mesonic variables, to accomplish this we preserve the Heisenberg equations of motion,

$$\frac{\partial N(x,y|K)}{\partial u} = -iN_c\left[N(x,y|K), \frac{H}{N_c}\right], \tag{166}$$

and we take the limit $N_c \to \infty$. Since the Hamiltonian contains various types of observables, we need to know the Poisson brackets among these variables. To calculate the equations of motion it is enough to know these Poisson brackets. The algebraic structure of these Poisson brackets, or the structure of all the Poisson brackets, may actually help us solve the problem. At the moment the calculations are too complex, and a direct attack to the equations of motion as in Refs. 9, 10, and 12 seems to be intractable. It is perhaps much better to look for a variational ansatz as in Ref. 11.

After some computations we can write down the Hamiltonian in a completely well-defined manner. The expression below unfortunately hides the analogies with the usual $\mathbf{R}^{1+1}$ case. As we will see there is a better way to write it which reflects this resemblance,

$$\frac{H}{N_C} = \frac{1}{2}\int \lim_{y\to x} \mathrm{d}x(-\partial_y^2 N(x,y)) + \frac{1}{2}\int \mathrm{d}x\, m^2 N(x,x) - \frac{L}{\tilde{g}^2}\mathrm{Tr}\, e^2$$
$$+ \frac{1}{2}\int \mathrm{d}x \int_{-L}^{x} \mathrm{d}y\ \mathrm{sgn}(y) \lim_{z\to y}[\partial_z N(z,y|0,1,0) - \partial_z N(y,z|0,1,0)]$$
$$- \frac{\tilde{g}^2}{8}\int \mathrm{d}x \int_{-L}^{x} \mathrm{d}y\ \mathrm{sgn}(y) \int_{-L}^{x} \mathrm{d}y'\ \mathrm{sgn}(y') \lim_{z\to y} \lim_{w\to y'} [\partial_w N(w,y)\partial_z N(z,y') - N(y',y)\partial_z\partial_w N(z,w)$$
$$- \partial_z\partial_w N(w,z)N(y,y') + \partial_z N(y',z)\partial_w N(y,w) + \partial_w N(w,y)\partial_z V(z,y') + \partial_z N(z,y')\partial_w V(w,y)$$
$$- N(y',y)\partial_z\partial_w V(z,w) - \partial_z\partial_w N(z,w)V(y',y) - \partial_z\partial_w N(w,z)V(y,y') - N(y,y')\partial_z\partial_w V(w,z)$$
$$+ \partial_z N(y',z)\partial_w V(y,w) + \partial_w N(y,w)\partial_z V(y',z) + i\partial_z N(z,y')\partial_w\omega^{-1}(y,w) - i\partial_z\partial_w N(z,w)\omega^{-1}(y,y')$$
$$- iN(y,y')\partial_z\partial_w\omega^{-1}(z,w) + i\partial_w N(y,w)\partial_z\omega^{-1}(z,y')]. \tag{167}$$

The above form shows that everything in the Hamiltonian is well defined. However, from a conceptual point of view there is a better way to write the Hamiltonian. After some algebra, we can get to the following form:

$$\frac{H}{N_C}=\frac{1}{2}\int_{-L}^{L}\mathrm{d}x'\,\mathrm{d}y'(N\omega)(x',y')\tilde{\omega}(y',x')-\frac{L}{\tilde{g}^2}\mathrm{Tr}\,e^2+\int_{-L}^{L}\mathrm{d}x'\,\mathrm{d}y'(N(0,1,0)\omega)(y',y')\theta(x'-y')$$
$$-\frac{\tilde{g}^2}{2}\int_{-L}^{L}\mathrm{d}x'\,\mathrm{d}y'\,G(x',y')(N\omega)(x',y')(N\omega)(y',x')-\frac{i\tilde{g}^2}{2}\int_{-L}^{L}\mathrm{d}x'\,\mathrm{d}y'G(x',y')$$
$$\times(N\omega)(x',y')\mathrm{sgn}(i\tilde{\omega})(y',x'),\tag{168}$$

where $\theta(x-y)$ denotes the usual step function and we also introduce the Green's function

$$G(y,z)=\frac{L}{2}-\frac{1}{2}(y+z)-\frac{1}{2}|y-z|.\tag{169}$$

For simplicity we write $\mathbf{N}\omega$ in place of $\mathbf{N}(0)\omega$, but the two will be used interchangeably.

To find the equations of motion for the basic large-N_c variables we will first calculate the Poisson brackets among various terms. These Poisson brackets along with the constraints satisfied by these variables, define the underlying classical phase space of the large-N_c theory. Since there is an infinite chain of operators we should compute the most general combinations. However, the Hamiltonian contains only a certain set of these terms and we believe the essentials of the dynamics is contained in the simple mesonic variables $N(x,y|K)$, so we restrict our computations to these variables. In fact, the above form of the Hamiltonian naturally suggests $(\mathbf{N}\omega)=(\mathbf{N}\omega)(x,y)$ as our basic variable, so we will write all the relations in terms of these variables (for simplicity when we use the explicit matrix elements we will not use the boldface notation). Poisson brackets below define an infinite dimensional algebra, a natural question is to ask what kind of algebra this is. Moreover, what should be the underlying symmetry principle, which in some sense will replace the gauge invariance principle in this classical system (see Ref. 30 for a study of these type of algebras)? All these questions are left unanswered here, we hope to return to them in a later work. We first state the commutators between the simple mesonic operators then write down the resulting Poisson brackets,

$$\begin{aligned}[(N(K)\omega)(x,y),(N(K')\omega)(x',y')]=&\frac{i}{N_c}\delta(y'-x)(N(K+K')\omega)(x',y)\\&-\frac{\mathrm{i}}{N_c}\delta(y-x')(N(K+K')\omega)(x,y')\\&-\frac{1}{2N_c}\delta(y'-x)\mathrm{sgn}(i\tilde{\omega})(x',y)Q(K+K')\\&+\frac{1}{2N_c}\delta(y-x')\mathrm{sgn}(i\tilde{\omega})(x,y')Q(K+K').\end{aligned}\tag{170}$$

Multiplying this by $-iN_c$ and taking the limit as $N_c\to\infty$ we postulate the Poisson brackets,

$$\begin{aligned}\{(N(K)\omega)(x,y),(N(K')\omega)(x',y')\}=&[\delta(y'-x)(N(K+K')\omega)(x',y)-\delta(y-x')(N(K+K')\omega)(x,y')]\\&+\frac{i}{2}\delta(y'-x)\mathrm{sgn}(i\tilde{\omega})(x',y)-\delta(y-x')\mathrm{sgn}(i\tilde{\omega})(x,y')Q(K+K').\end{aligned}\tag{171}$$

This is essentially the $U(\infty)$ Lie algebra, graded by $\mathbf{Z}$, and has a central extension determined by the operator $\mathrm{sgn}(i\tilde{\omega})$. If we switch to a basis where the operator is diagonal, we will find that it is the same central extension, apart from the $\mathbf{Z}$ grading, as before in Ref. 9. The next commutator we need is

$$\left[\frac{1}{\tilde{g}^2}\mathrm{Tr}\, e^2,(N(K)\omega)(x,y)\right]=\frac{2i}{N_C}\sum_{k=0}^{K}(N(k,1,K-k)\omega)(x,y)-\frac{2i}{N_C}(N(0,1,K)\omega)(x,y)$$
$$-\frac{K\tilde{g}^2}{N_C}(N(K)\omega)(x,y). \tag{172}$$

As a result we postulate the Poisson bracket, and we define a special variable, $C(2)=(1/\tilde{g}^2)Q(0,2)=(1/\tilde{g}^2)\mathrm{Tr}\,\hat{e}^2$,

$$\{C(2),(N(K)\omega)(x,y)\}=2\sum_{k=0}^{K}(N(k,1,K-k)\omega)(x,y)-2(N(0,1,K)\omega)(x,y)+iK\tilde{g}^2(N(K)\omega)(x,y). \tag{173}$$

The last commutator is the most complicated one, after a long computation we have,

$$\begin{aligned}[(N(K)\omega)(x,y),(N(0,1,0)\omega)(x',y')]=&-\frac{i\tilde{g}^2}{N_C}\sum_{k=0}^{K}[(N(K-k)\omega)(x,y')(N(k)\omega)(x',y)\\
&+(N(k)\omega)(x',y)(V\omega)(x,y')Q(K-k)\\
&+(V\omega)(x',y)Q(k)(N(K-k)\omega)(x,y')\\
&+(V\omega)(x',y)Q(k)(V\omega)(xy')Q(K-k)]\\
&+\frac{i\tilde{g}^2}{N_C}[(N(K)\omega)(x',y)(N\omega)(x,y')\\
&+(N(K)\omega)(x',y)(V\omega)(x,y')\\
&+(V\omega)(x',y)Q(K)(N\omega)(x,y')\\
&+(V\omega)(x',y)Q(K)(V\omega)(x,y')]\\
&-\frac{i}{N_C}[\delta(x'-y)(N(K,1,0)\omega)(x,y')\\
&-\delta(y'-x)(N(0,K,1)\omega)(x',y)]\\
&-\frac{i}{N_C}[\delta(x'-y)(V\omega)(x,y')Q(K,1,0)\\
&-\delta(y'-x)(V\omega)(x',y)Q(0,1,K)]\\
&+\frac{K\tilde{g}^2}{N_C^2}\delta(x'-y')[(N(K)\omega)(x,y)\\
&+(V\omega)(x,y)Q(K)]\\
&+\frac{iK\tilde{g}^2}{N_C^2}[(V\omega)(x',y')(N(K)\omega)(x,y)\\
&+(V\omega)(x,y)(N(K)\omega)(x',y')]\\
&+\frac{iK\tilde{g}^2}{N_C^2}(V\omega)(x',y')(V\omega)(x,y)Q(K).\end{aligned} \tag{174}$$

We take the large-N_c limit and drop terms of smaller order to finally postulate,

$$\{(N(K)\omega)(x,y),(N(0,1,0)\omega)(x',y')\} = -\tilde{g}^2\sum_{k=0}^{K}[(N(K-k)\omega)(x,y')(N(K)\omega)(x',y) + (N(k)\omega)(x',y)$$
$$\times(V\omega)(x,y')Q(K-k) + (V\omega)(x',y)Q(k)(N(K-k)\omega)(x,y')$$
$$+ (V\omega)(x',y)Q(k)(V\omega)(x,y')Q(K-k)] + \tilde{g}^2[(N\omega)(x,y')$$
$$\times(N(K)\omega)(x',y) + (N(K)\omega)(x',y)(V\omega)(x,y')$$
$$+ (V\omega)(x',y)Q(K)(N\omega)(x,y') + (V\omega)(x',y)Q(K)(V\omega)(x,y')]$$
$$+ [\delta(y'-x)(N(0,K,1)\omega)(x',y) - \delta(x'-y)$$
$$\times(N(K,1,0)\omega)(x,y')] + [\delta(y'-x)(V\omega)(x',y)Q(0,1,K)$$
$$- \delta(x'-y)(V\omega)(x,y')Q(K,1,0). \tag{175}$$

In principle we can compute now the equations of motion for the simple mesonic variables, via

$$\frac{\partial N(x,y|K)}{\partial u} = \{N(x,y|K),H_c\}, \tag{176}$$

where H_c denotes the limit of H/N_c as $N_c\to\infty$. However, the answer given in the appendix is not at all easy to work with. In the next section we search for a linear approximation.

VIII. LINEARIZATION

A casual look at the Poisson brackets and the Hamiltonian tells us that the equations are very complicated in the general case, and various terms are coupled. An approximation which keeps the nonperturbative aspects of the theory is needed. One possibility is to again look at a linearized version of these equations. This is a good approximation as we know from the previous work in Ref. 9. It seems natural to assume that the operators with various powers of $\hat{q}$ inserted should be the excited states (see also the nonrelativistic version in Ref. 16). In fact we expect that the operators of the form $N(x,y|K_1,S_1,K_2,S_2..)$ become less and less important when we study states close to the ground state. Of course it is possible that the theory readjusts itself further away from these naive expectations to a more complicated ground state. This can only be answered by a more careful study of the system. It is likely that a variational estimate will be more powerful to settle such questions. From a group theory point of view we cannot neglect products of $Q(K)$'s with themselves, but we will neglect the products of $N(x,y|K)$ with $Q(K)$ variables. This means that our basic variables are of order $\hbar$ fluctuations, or even smaller. Let us first rewrite the constraint for $\mathbf{N}(K)\omega$,

$$\mathbf{N}(K)\omega\mathbf{N}(L)\omega + i\left[\frac{1}{2}Q(K)(\mathbf{N}(L)\omega) + \frac{1}{2}Q(L)(\mathbf{N}(K)\omega) - \mathbf{N}(K+L)\omega\right] + i\frac{1}{2}[Q(K)\mathrm{sgn}(i\tilde{\omega})\mathbf{N}(L)\omega$$
$$+ Q(L)\mathbf{N}(K)\omega\,\mathrm{sgn}(i\tilde{\omega})] - \frac{1}{2}[1+\mathrm{sgn}(i\tilde{\omega})]Q(K+L) = \frac{1}{\tilde{g}^2}[\mathbf{N}(K,1,L)\omega - \mathbf{N}(K+1,1,L-1)\omega]. \tag{177}$$

If we set here $K=L=0$, we get a constraint equation which is

$$\mathbf{N}(0)\omega\mathbf{N}(0)\omega + i\frac{1}{2}[\mathrm{sgn}(i\tilde{\omega})\mathbf{N}(0)\omega + \mathbf{N}(0)\omega\,\mathrm{sgn}(i\tilde{\omega})] - \frac{1}{2}[1+\mathrm{sgn}(i\tilde{\omega})]$$
$$= \frac{1}{\tilde{g}^2}[\mathbf{N}(0,1,0)\omega - \mathbf{N}(1,1,-1)\omega]. \tag{178}$$

This looks very much like the constraints found before in Refs. 10 and 12 apart from terms with $\hat{e}$ in them and also a vacuum correction term. There, the constraint was used to throw away certain

momentum components of the basic variables, here we will use this to eliminate the variable $\mathbf{N}(0,1,0)$ as we will see. The linearized equations of motion will then be

$$\begin{aligned}\frac{\partial}{\partial u}(N\omega)(x,y) = \{(N\omega)(x,y), H_C\} &= -\frac{1}{2}[N\omega,\tilde{\omega}](x,y)\\ &+ \int \mathrm{d}x'\,\mathrm{d}y'\ \theta(x',y')[\delta(y',x)(N(0,1,0)\omega)(y',y) - \delta(y,y')(N(0,1,0)\omega)(x,y')]\\ &+ \frac{i\tilde{g}^2}{2}\int \mathrm{d}x'[G(x,x')\{\mathrm{sgn}(i\tilde{\omega})(x',y),(N\omega)(x,x')\}_+\\ &- G(y,x')\{\mathrm{sgn}(i\tilde{\omega})(x,x'),(N\omega)(x',y)\}_+ - G(x,x')(N\omega)(x',y)\mathrm{sgn}(i\tilde{\omega})(x,x')\\ &+ G(y,x')(N\omega)(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)]\\ &+ \frac{\tilde{g}^2}{4}\int \mathrm{d}x'[G(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)\mathrm{sgn}(i\tilde{\omega})(x,x')\\ &- G(y,x')\mathrm{sgn}(i\tilde{\omega})(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)] \end{aligned} \tag{179}$$

in which $Q(0,1,0)=0$ is imposed (because $\mathrm{Tr}\,\hat{e}=0$ on physical states). We also used $\{.,.\}_+$ to denote symmetrized product. If we now assume that $N(x,y|1,1,-1)$ is of smaller order in comparison to the other terms, we can eliminate $N(x,y|0,1,0)$ in favor of $N(x,y|0)$ in the above constraint and plug it into the equations of motion. This gives us

$$\begin{aligned}\{(N(0)\omega)(x,y), H_c\} &= -\frac{1}{2}[\mathbf{N}(0)\omega,\tilde{\omega}](x,y)\\ &+ \frac{\tilde{g}^2}{2}(y-x)[i[\mathbf{N}(0)\omega,\mathrm{sgn}(i\tilde{\omega})]_+(x,y) - [1+\mathrm{sgn}(i\tilde{\omega})](x,y)]\\ &+ \tilde{g}^2\frac{i}{2}\int \mathrm{d}x'[G(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)(N(0)\omega)(x,x')\\ &- G(y,x')\mathrm{sgn}(i\tilde{\omega})(x,x')(N(0)\omega)(x',y)]\\ &+ \tilde{g}^2\frac{1}{2}\int \mathrm{d}x'[G(x',x) - G(y,x')]\mathrm{sgn}(i\tilde{\omega})(x',y)\mathrm{sgn}(i\tilde{\omega})(x,x'). \end{aligned} \tag{180}$$

It can further be simplified and we reach to,

$$\begin{aligned}\frac{\partial(N(0)\omega)(x,y)}{\partial u} &= \{(N(0)\omega)(x,y), H_c\}\\ &= -\frac{1}{2}[\mathbf{N}(0)\omega,\tilde{\omega}](x,y) + \frac{\tilde{g}^2}{2}(y-x)[i[\mathbf{N}(0)\omega,\mathrm{sgn}(i\tilde{\omega})]_+(x,y) - \mathrm{sgn}(i\tilde{\omega})(x,y)]\\ &+ \tilde{g}^2\frac{i}{2}\int \mathrm{d}x'[G(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)(N(0)\omega)(x,x')\\ &- G(y,x')\mathrm{sgn}(i\tilde{\omega})(x,x')(N(0)\omega)(x',y)]\\ &+ \tilde{g}^2\frac{1}{4}\int \mathrm{d}x'[|x'-x| - |y-x'|]\mathrm{sgn}(i\tilde{\omega})(x',y)\mathrm{sgn}(i\tilde{\omega})(x,x'). \end{aligned} \tag{181}$$

We can reorganize this equation into,

$$\frac{\partial(N(0)\omega)(x,y)}{\partial u} = \{(N(0)\omega)(x,y), H_c\}$$

$$= -\frac{1}{2}[\mathbf{N}(0)\omega, \tilde{\omega}](x,y) + \frac{\tilde{g}^2}{2} i(y-x)[\mathbf{N}(0)\omega, \mathrm{sgn}(i\tilde{\omega})]_+(x,y)$$

$$+ \tilde{g}^2 \frac{i}{2} \int \mathrm{d}x' [G(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)(N(0)\omega)(x,x')$$

$$- G(y,x')\mathrm{sgn}(i\tilde{\omega})(x,x')(N(0)\omega)(x',y)]$$

$$+ \tilde{g}^2 \frac{1}{2} \int_x^y \mathrm{d}x' \left[x' - \frac{1}{2}(x+y) \right] \mathrm{sgn}(i\tilde{\omega})(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y) - \frac{\tilde{g}^2}{2}(y-x)\mathrm{sgn}(i\tilde{\omega})(x,y). \tag{182}$$

Here we face a problem, $\mathbf{N}\omega=0$ is not a solution, so it suggests that the true ground state of the theory is not the naive vacuum but has changed due to the interactions. It is also possible that this is the result of our approximations. This is hard to say at our present level of understanding. The inhomogeneous terms are proportional to the coupling constant, as it becomes weaker and weaker we should approach to the true vacuum. If we set $\tilde{g}=0$, the naive vacuum $N\omega=0$, indeed solves the time independent equations. (There are examples of this type of phenomena, in the Lee model, the coupling of the bosonic fields to a quantum mechanical system leads to a drastic change in the ground state of the system.) It is also possible to think of these inhomogeneous terms as if they were multiplied by some powers of $\hbar$ which allows one to get an idea about in which orders in $\hbar$ these terms make contributions to the naive vacuum of the theory due to the interactions. If one keeps in mind that there are $\hbar$'s both in the commutators of the bosonic sector and in the commutators of the gauge sector, more careful analysis shows that the first term in Eq. (182) is zeroth order in $\hbar$ as expected. Moreover the second, third, and fourth terms are the first order terms in $\hbar$ and the order of the last two terms is two in $\hbar$. The solutions of the equations of motion will not give us the invariant mass, the energy is not a relativistic invariant. We need to find the operator of the field momentum and look for the correct combinations of the simultaneous eigenvalues to determine the mass spectrum. All these can best be done in a variational setting. In Refs. 9 and 12, the ordinary momentum was used to diagonalize all the operators. A natural ansatz for the basic mesonic variables would be of the form $(N\omega)(x,y)=\xi(x-y)e^{iP(x+y)/2}$. The leading symbol of $\mathrm{sgn}(i\tilde{\omega})$ is given by $\mathrm{sgn}\left(\frac{1}{2}(x+y)\right)\mathrm{sgn}(p)$, this is expected and such a symbol expansion may be useful to understand this problem as an alternative. Our elimination method may not be the best approach, it may be better to develop a new kind of symbol calculus by combining the collective field approach of the papers[31,32] with bilinear methods. We hope to return to these issues in a later work.

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APPENDIX A: POISSON BRACKETS OF THE GAUGE SECTOR

In this section, in order to evaluate the Poisson brackets of the gauge sector, the suggestion given in Ref. 28 is followed. The variation of the action for the gauge sector can be given by

$$\delta S = \int \mathrm{d}u\ \delta x^{A\mu}{}_{\nu}\Omega^{AB\nu}{}_{\mu}{}^{\lambda}{}_{\sigma}\dot{x}^{B\sigma}{}_{\lambda} - \int \mathrm{d}u\ \delta H = \int \mathrm{d}u\ \delta x^{A\mu}{}_{\nu}\Omega^{AB\nu}{}_{\mu}{}^{\lambda}{}_{\sigma}\dot{x}^{B\sigma}{}_{\lambda} - \int \mathrm{d}u\ \delta x^{A\mu}{}_{\nu}Q^{AB\nu}{}_{\mu}{}^{\lambda}{}_{\sigma}x^{B\sigma}{}_{\lambda}. \tag{A1}$$

For simplicity δH is given as a quadratic form, its explicit form is not needed here. The indices A,B belong to the coordinates (e,q) and run from (1,2). On top of it, the μ,ν indices refer to matrix form of the Lie algebra. The equations of motion gives

$$\dot{x}^{A\mu}{}_{\nu} = (\Omega^{-1})^{AB\mu}{}_{\nu}{}^{\sigma}{}_{\lambda}Q^{BC\lambda}{}_{\sigma}{}^{\kappa}{}_{\tau}x^{C\tau}{}_{\kappa}. \tag{A2}$$

Since

$$\dot{x}^{A\mu}{}_{\nu} = \{x^{A\mu}{}_{\nu}, x^{B\sigma}{}_{\lambda}\}Q^{BC\lambda}{}_{\sigma}{}^{\kappa}{}_{\tau}x^{C\tau}{}_{\kappa}, \tag{A3}$$

the Poisson brackets can be read off directly from the expression. The variation of the action should be expressed in terms of a set of independent variables ξ, v, e and their variations $\delta\xi, \delta e$ on the group manifold. The variables $\delta\xi$ and v are given by

$$\delta\xi = q^{-1}\delta q,$$

$$v = q^{-1}\dot{q}. \tag{A4}$$

To obtain the Poisson brackets, a variation is made in the action

$$\delta S = -\frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}\ \delta(q^{-1}\dot{q}e). \tag{A5}$$

This variation can be expressed in terms of our proper variables after an integration by parts as

$$\delta S = -\frac{1}{g^2}\int \mathrm{d}u\ \mathrm{Tr}(-\delta\xi v e + \delta\xi e v - \delta\xi\dot{e} + \delta e v) \tag{A6}$$

in which there is no contribution coming from a boundary term since the variation of q at the boundaries gives zero. Equation (A6) can be written in terms of explicit indices

$$\delta S = -\frac{1}{g^2}\int \mathrm{d}u(-\delta\xi^{\mu}{}_{\nu}v^{\nu}{}_{\sigma}e^{\sigma}{}_{\mu} + \delta\xi^{\mu}{}_{\nu}e^{\nu}{}_{\sigma}v^{\sigma}{}_{\mu} - \delta\xi^{\mu}{}_{\nu}e^{\nu}{}_{\mu} + \delta e^{\mu}{}_{\nu}v^{\nu}{}_{\mu}). \tag{A7}$$

After some rearrangements of the indices, Eq. (A7) is given by

$$\delta S = -\frac{1}{g^2}\int \mathrm{d}u[\delta\xi^{\mu}{}_{\nu}(\delta^{\kappa}{}_{\mu}e^{\nu}{}_{\sigma} - \delta^{\nu}{}_{\sigma}e^{\kappa}{}_{\mu})v^{\sigma}{}_{\kappa} - \delta^{\kappa}{}_{\mu}\delta^{\nu}{}_{\sigma}(\delta e^{\mu}{}_{\nu}v^{\sigma}{}_{\kappa} - \delta\xi^{\mu}{}_{\nu}\dot{e}^{\sigma}{}_{\kappa})]. \tag{A8}$$

It is possible to write this variation in a more compact form as

$$\delta S = -\frac{1}{g^2}\int \mathrm{d}u(\delta\xi^{\mu}{}_{\nu} - \delta e^{\mu}{}_{\nu})\begin{pmatrix} A^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} & -\delta^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} \\ \delta^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} & 0 \end{pmatrix}\begin{pmatrix} v^{\sigma}{}_{\kappa} \\ \dot{e}^{\sigma}{}_{\kappa} \end{pmatrix} \tag{A9}$$

in which

$$A^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} = \delta^{\kappa}{}_{\mu}e^{\nu}{}_{\sigma} - \delta^{\nu}{}_{\sigma}e^{\kappa}{}_{\mu},$$

$$\delta^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} = \delta^{\kappa}{}_{\mu}\delta^{\nu}{}_{\sigma}. \tag{A10}$$

The symplectic form can, therefore, be given by a matrix as

$$\Omega^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} = -\frac{1}{g^2}\begin{pmatrix} A^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} & -\delta^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} \\ \delta^{\nu}{}_{\mu}{}^{\kappa}{}_{\sigma} & 0 \end{pmatrix}, \tag{A11}$$

and its inverse is also given by

$$(\Omega^{-1})^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} = -g^2\begin{pmatrix} 0 & \delta^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} \\ -\delta^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} & A^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} \end{pmatrix}. \tag{A12}$$

The equations of motion for ξ and e are expressed in terms of the Poisson brackets by

$$v^{\sigma}{}_{\kappa} = \{\xi^{\sigma}{}_{\kappa}, \xi^{\rho}{}_{\tau}\}\frac{\partial H}{\partial \xi^{\rho}{}_{\tau}} + \{\xi^{\sigma}{}_{\kappa}, e^{\rho}{}_{\tau}\}\frac{\partial H}{\partial e^{\rho}{}_{\tau}},$$

$$\dot{e}^{\sigma}{}_{\kappa} = \{e^{\sigma}{}_{\kappa}, \xi^{\rho}{}_{\tau}\}\frac{\partial H}{\partial \xi^{\rho}{}_{\tau}} + \{e^{\sigma}{}_{\kappa}, e^{\rho}{}_{\tau}\}\frac{\partial H}{\partial e^{\rho}{}_{\tau}}. \tag{A13}$$

Thus the Poisson brackets can be read off with the assistance of Eqs. (A12) and (A13) as follows:

$$\{\xi^{\sigma}{}_{\kappa}, e^{\rho}{}_{\tau}\} = -g^2\delta^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} = -g^2\delta^{\sigma}{}_{\tau}\delta^{\rho}{}_{\kappa}, \tag{A14}$$

$$\{e^{\sigma}{}_{\kappa}, e^{\rho}{}_{\tau}\} = -g^2 A^{\sigma}{}_{\kappa}{}^{\rho}{}_{\tau} = g^2(\delta^{\sigma}{}_{\tau}e^{\rho}{}_{\kappa} - \delta^{\rho}{}_{\kappa}e^{\sigma}{}_{\tau}). \tag{A15}$$

A Poisson bracket between the variables q and e can be introduced by passing q^{-1} in the definition of v to the other side as q in the equation of motion for ξ. This is allowed since the Poisson bracket between the variables ξ themselves is zero. One can therefore end up with

$$\{e^{\mu}{}_{\nu}, q^{\sigma}{}_{\kappa}\} = g^2\delta^{\mu}{}_{\kappa}q^{\sigma}{}_{\nu}. \tag{A16}$$

Contracting e by an element of the Lie algebra, namely Λ, the Poisson brackets can be set in a form as below,

$$\{\mathrm{Tr}\,\Lambda e, q^{\sigma}{}_{\kappa}\} = g^2(g\Lambda)^{\sigma}{}_{\kappa},$$

$$\{\mathrm{Tr}\,\Lambda^1 e, \mathrm{Tr}\,\Lambda^2 e\} = g^2\,\mathrm{Tr}[\Lambda^1, \Lambda^2]e. \tag{A17}$$

There is a natural geometric interpretation for this symplectic structure. It is indeed the canonical form on T^*G; the cotangent bundle on G (see Ref. 25 for a good exposition).

APPENDIX B: THE FULL EQUATIONS OF MOTION

A long and tedious calculation will reveal the full equations of motion for the simple mesonic variables. We give the answer below without any details. One should subtract divergence coming from the renormal ordering of the Hamiltonian, this is not a simple task. We plan to come back to these issues in a later presentation,

$$\begin{aligned}\frac{\partial}{\partial u}(N(K)\omega)(x,y) = \{(N(K)\omega)(x,y), H_C\} = &-\frac{1}{2}[N(K)\omega, \tilde{\omega}](x,y) + i\tilde{g}^2 KL(N(K)\omega)(x,y) \\ &+ 2L\sum_{k=0}^{K} N(k,1,K-k)\omega(x,y) - 2L(N(0,1,K)\omega)(x,y) \\ &- \tilde{g}^2\sum_{k=0}^{K}\int \mathrm{d}x'\,\mathrm{d}y'\,\theta(x',y')[(N(K-k)\omega)(x,y')(N(k)\omega)(y',y) \\ &+ (V\omega)(x,y')Q(K-k)(N(k)\omega)(y',y) + (N(K-k)\omega)(x,y')(V\omega)(y',y)Q(k)\end{aligned}$$

$$
\begin{aligned}
&+ (V\omega)(x,y')(V\omega)(y',y)Q(K-k)Q(k)] \\
&+ \tilde{g}^2 \int \mathrm{d}x'\,\mathrm{d}y'\;\theta(x',y')[(N\omega)(x,y')(N(K)\omega)(y',y) + (V\omega)(x,y') \\
&\times (N(K)\omega)(y',y) + (N\omega)(x,y')(V\omega)(y',y)Q(K) + (V\omega)(x,y')(V\omega)(y',y)Q(K)] \\
&+ \int \mathrm{d}x'\,\mathrm{d}y'\;\theta(x',y')[\delta(y',x)(N(0,1,K)\omega)(y',y) - \delta(y,y')(N(K,1,0)\omega)(x,y')] \\
&+ \int \mathrm{d}x'\,\mathrm{d}y'\;\theta(x',y')[\delta(y',x)(V\omega)(y',y)Q(0,1,K) - \delta(y,y') \\
&\times (V\omega)(x,y')Q(K,1,0)] - \frac{\tilde{g}^2}{2}\int \mathrm{d}x'[G(x,x')\{(N(K)\omega)(x'y),(N\omega)(x,x')\}_+ \\
&- G(y,x')\{(N(K)\omega)(x,x'),(N\omega)(x',y)\}_+] \\
&+ \frac{i\tilde{g}^2}{2}\int \mathrm{d}x'[G(x,x')\{\mathrm{sgn}(i\tilde{\omega})(x',y),(N\omega)(x,x')\}_+Q(K) - G(y,x') \\
&\times \{\mathrm{sgn}(i\tilde{\omega})(x,x'),(N\omega)(x',y)\}_+Q(K) - G(x,x')(N(K)\omega)(x',y)\mathrm{sgn}(i\tilde{\omega})(x,x') \\
&+ G(y,x')(N(K)\omega)(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)] \\
&+ \frac{\tilde{g}^2}{4}\int \mathrm{d}x'[G(x,x')\mathrm{sgn}(i\tilde{\omega})(x',y)Q(K)\mathrm{sgn}(i\tilde{\omega})(x,x') \\
&- G(y,x')\mathrm{sgn}(i\tilde{\omega})(x,x')Q(K)\mathrm{sgn}(i\tilde{\omega})(x',y). \qquad \text{(B1)}
\end{aligned}
$$

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Laurent series expansion of a class of massive scalar one-loop integrals up to $\mathcal{O}(\varepsilon^2)$ in terms of multiple polylogarithms

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In a recent paper we have presented results for a set of massive scalar one-loop master integrals needed in the NNLO parton model description of the hadroproduction of heavy flavors. The one-loop integrals were evaluated in $n=4-2\varepsilon$ dimension and the results were presented in terms of a Laurent series expansion up to $\mathcal{O}(\varepsilon^2)$. We found that some of the ε^2 coefficients contain a new class of functions which we termed the L functions. The L functions are defined in terms of one-dimensional integrals involving products of logarithm and dilogarithm functions. In this paper we derive a complete set of algebraic relations that allow one to convert the L functions of our previous approach to a sum of classical and multiple polylogarithms. Using these results we are now able to present the ε^2 coefficients of the one-loop master integrals in terms of classical and multiple polylogarithms.
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I. INTRODUCTION

Recently, we have calculated the complete set of massive one-loop master integrals[1] needed in the calculation of the next-to-next-to-leading order (NNLO) parton model corrections to the hadroproduction of heavy flavors.[2] We used Feynman parametrization to evaluate the one-loop master integrals in $n=4-2\varepsilon$ dimensions. We obtained the coefficients of the Laurent series expansion of the relevant scalar integrals in terms of the parameter ε up to $\mathcal{O}(\varepsilon^2)$ as needed for the NNLO calculation. We found that the real parts of some of the ε^2 coefficients contain a new class of functions which can be written in terms of one-dimensional integral representations involving products of log and dilog functions. These so-called single and triple index L functions cannot be expressed in terms of classical polylogaritms but can be seen to belong to a generalization of the classical polylogarithms which are called multiple polylogarithms.

Functions analogous to the triple index functions $L_{\sigma_1\sigma_2\sigma_3}$ also arise in the approach of Ref. 3 when one analytically continues their $\mathcal{O}(\varepsilon^2)$ integral representation for a general vertex function. Methods differing from ours have been used for the derivation of master N-point integrals such as the differential equations method[4] or the nested sum method.[5] Depending on the number of scales involved, the results include multiple polylogarithms[6] and/or harmonic[7] or two-dimensional harmonic[8] polylogarithms. The latter functions all are subsets of multiple polylogarithms. Present-

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ing our results in terms of multiple polylogarithms will facilitate a comparison with the results of possible rederivations of the scalar one-loop integrals using other methods. It is very likely that future results of multiloop calculations will be presented in terms of multiple polylogarithms or their subclasses. Alongside with this the necessary tools will be developed to deal with multiple polylogarithms, be it analytically or numerically. In fact, recently a computer code has been written for the numerical evaluation of the multiple polylogarithms.[9] It is therefore timely that we express the results of Ref. 1 also in terms of multiple polylogarithms.

It is a purpose of this paper to show that the single and triple index L functions introduced in Ref. 1 can all be related to multiple polylogarithms. This is done in explicit form. We are thus able to present our results for the scalar massive one-loop master integrals in terms of multiple polylogarithms and classical polylogarithms.[10] In Sec. II we recapitulate material on the definition of the single and triple index L functions as they arise in the approach of Ref. 1. Simple symmetry relations allow one to restrict the discussion to the triple index L functions L_{-++} and L_{+++}, and to the single index L function L_{+}. In Sec. II we also recapitulate the definition of multiple polylogarithms. In the subsequent sections we will write down the formulas needed to transform the L functions to multiple polylogarithms for general arguments. The general formulas are not always applicable when the arguments take special values as they do in the massive one-loop calculation. For these special values one must carefully discuss the limiting behavior of the general formulas. In Sec. III A we derive the general formula which relates the L_{-++} functions to the set of multiple polylogarithms. Section III B considers special cases of the general relation. Similarly, Sec. IV A gives general relations which allow one to express the L_{+++} functions in terms of multiple polylogarithms. In Sec. IV B we discuss special cases for the arguments of the L_{+++} functions. Sections V A and V B repeat the discussion for the single index L_{+} functions. Finally, Sec. VI presents our conclusions.

As remarked on before, the L functions appear only in the real parts of some of the $\mathcal{O}(\varepsilon^2)$ coefficient functions of the masive one-loop integrals. In the notation of Ref. 1 these are the three-point coefficient functions $\mathrm{Re}\, C_1^{(2)}$, $\mathrm{Re}\, C_2^{(2)}$, and $\mathrm{Re}\, C_5^{(2)}$, and the four-point coefficient functions $\mathrm{Re}\, D_1^{(2)}$, $\mathrm{Re}\, D_2^{(2)}$, and $\mathrm{Re}\, D_3^{(2)}$. For the sake of brevity we have decided to present multiple polylogarithm results in this paper only for the four-point coefficient function $\mathrm{Re}\, D_1^{(2)}$. This result is listed in the Appendix. The corresponding results for the other five coefficient functions are readily available in electronic form.[11]

II. BASIC FEATURES

In order to make the paper self-contained, we write down a number of basic definitions for the L functions and the multiple polylogarithms in this section, as well as some symmetry properties and domains of definitions for the single and triple index L functions. These will be of help when presenting the subsequent material.

The definition for the L functions is as follows:[1]

$$L_{\sigma_1\sigma_2\sigma_3}(\alpha_1,\alpha_2,\alpha_3,\alpha_4)=\int_0^1 \mathrm{d}y \frac{\ln(\alpha_1+\sigma_1 y)\ln(\alpha_2+\sigma_2 y)\ln(\alpha_3+\sigma_3 y)}{\alpha_4+y} \tag{1}$$

and

$$L_{\sigma_1}(\alpha_1,\alpha_2,\alpha_3,\alpha_4)=\int_0^1 \mathrm{d}y \frac{\ln(\alpha_1+\sigma_1 y)Li_2(\alpha_2+\alpha_3 y)}{\alpha_4+y}. \tag{2}$$

Here the σ_i $(i=1,2,3)$ take the values ± 1 and the α_j's are either integers $\{1,0,-1\}$ or else kinematical variables. We want to emphasize that the numerical evaluation of the L functions is straightforward.

The L functions possess simple symmetry properties as follows. One notices that a change of the integration variable $y \to 1-y$ results in the identity

$$L_{\sigma_1}(\alpha_1,\alpha_2,\alpha_3,\alpha_4) = -L_{-\sigma_1}(\alpha_1+\sigma_1,\alpha_2+\alpha_3,-\alpha_3,-\alpha_4-1) \tag{3}$$

which implies that L_- can always be related to L_+, and vice versa. We have thus written our results for the three-point and four-point functions in Ref. 1 only in terms of the L_+ functions.

Turning to the triple index L function one notices that $L_{\sigma_1\sigma_2\sigma_3}(\alpha_1,\alpha_2,\alpha_3,\alpha_4)$ is symmetric under permutations of any two pairs of indices and arguments $\{\sigma_i,\alpha_i\}$ and $\{\sigma_j,\alpha_j\}$ for $(i\neq j)$. The same change of variables as above $y\to 1-y$ results in

$$L_{\sigma_1\sigma_2\sigma_3}(\alpha_1,\alpha_2,\alpha_3,\alpha_4) = -L_{-\sigma_1-\sigma_2-\sigma_3}(\alpha_1+\sigma_1,\alpha_2+\sigma_2,\alpha_3+\sigma_3,-\alpha_4-1). \tag{4}$$

Therefore, from the eight functions L_{---}, L_{--+}, L_{-+-}, L_{+--}, L_{-++}, L_{+-+}, L_{++-}, and L_{+++} only two are independent. We have chosen to write our results in terms of L_{-++} and L_{+++}.

The domains of definition of the functions L_{+++}, L_{-++}, and L_+ that follow from the requirement that these functions take real values can be read off from the defining relations Eqs. (1) and (2) considering the arguments of the log and dilog functions in the integrands, as well as from ensuring that the denominator of Eqs. (1) and (2) does not change sign on the integration path. One has

$$L_{+++}(\alpha_1,\alpha_2,\alpha_3,\alpha_4): \quad \alpha_1>0,\alpha_2>0,\alpha_3>0,\alpha_4<-1 \text{ or } \alpha_4>0;$$

$$L_{-++}(\alpha_1,\alpha_2,\alpha_3,\alpha_4): \quad \alpha_1>1,\alpha_2>0,\alpha_3>0,\alpha_4<-1 \text{ or } \alpha_4>0;$$

$$L_{+}(\alpha_1,\alpha_2,\alpha_3,\alpha_4): \quad \alpha_1>0,\alpha_2\leqslant 1,\alpha_2+\alpha_3\leqslant 1,\alpha_3\neq 0,\alpha_4<-1 \text{ or } \alpha_4>0. \tag{5}$$

Looking at the definition of the triple index L function in (1) one concludes that the boundary points $\alpha_1=0$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ can be included in the domain of the definition for L_{+++}. The same holds true for $\alpha_1=1$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ for L_{-++}. Also, from the definition of the single index function L_+ in (2) one concludes that the boundary point $\alpha_1=0$ can be added to its domain of definition.

The points $\alpha_4=\{-1,0\}$ can also be included in the domain if the values taken by the other parameters α_i guarantee the convergence of the integral. We mention that for all of our purposes the conditions (5), with the boundary points included, are satisfied, e.g., our results for the integrals are real. Nevertheless, it is of course always possible to analytically continue the parameters to the complex plane.

There are some further relations for the L functions which result from applying integration-by-parts identities. They are not listed here but can be found in Appendix C of Ref. 1. They have been used to reduce the set of L functions occurring in the master integrals to a subset of L functions having real values in physical phase space.[1]

Multiple polylogarithms are defined as a limit of Z sums,[6] e.g.,

$$Li_{m_k,\ldots,m_1}(x_k,\ldots,x_1) = \lim_{n_1\to\infty} \sum_{n_1>n_2\ldots>n_k>0} \frac{x_1^{n_1}x_2^{n_2}\cdots x_k^{n_k}}{n_1^{m_1}n_2^{m_2}\cdots n_k^{m_k}}. \tag{6}$$

The number $w=m_1+\cdots+m_k$ is called the weight and k is called the depth of the multiple polylogarithm. The power series (6) is convergent for $|x_i|<1$, and can be analytically continued via the iterated integral representation:

$$Li_{m_k,\ldots,m_1}(x_k,\ldots,x_1) = \int_0^{x_1x_2\cdots x_k} \left(\frac{dt}{t}\circ\right)^{m_1-1} \frac{dt}{x_2x_3\cdots x_k-t}\circ \left(\frac{dt}{t}\circ\right)^{m_2-1} \frac{dt}{x_3\cdots x_k-t}\circ\cdots\circ\left(\frac{dt}{t}\circ\right)^{m_k-1}\frac{dt}{1-t}, \tag{7}$$

where the following notation is used for the iterated integrals:

$$\int_0^\lambda \frac{\mathrm{d}t}{a_n - t} \circ \cdots \circ \frac{\mathrm{d}t}{a_1 - t} = \int_0^\lambda \frac{\mathrm{d}t_n}{a_n - t_n} \int_0^{t_n} \frac{\mathrm{d}t_{n-1}}{a_{n-1} - t_{n-1}} \times \cdots \times \int_0^{t_2} \frac{\mathrm{d}t_1}{a_1 - t_1}. \tag{8}$$

III. TRANSFORMATION OF L_{-++} TO MULTIPLE POLYLOGARITHMS

In this section we will show that all our L_{-++} functions can be expressed in terms of multiple polylogarithms.

A. General case for the L_{-++} function

We begin with the L_{-++} function Eq. (1),

$$L_{-++}(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = \int_0^1 \mathrm{d}y \frac{\ln(\alpha_1 - y)\ln(\alpha_2 + y)\ln(\alpha_3 + y)}{\alpha_4 + y}. \tag{9}$$

After changing the integration variable $y = \alpha_1 t$ one gets

$$\begin{aligned}
&\int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(\alpha_1 - \alpha_1 t)\ln(\alpha_2 + \alpha_1 t)\ln(\alpha_3 + \alpha_1 t)}{\frac{\alpha_4}{\alpha_1} + t} \\
&= \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln \alpha_1 \ln(\alpha_2 + \alpha_1 t)\ln(\alpha_3 + \alpha_1 t)}{\frac{\alpha_4}{\alpha_1} + t} \\
&\quad + \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\left[\ln \alpha_1 + \ln\left(\frac{\alpha_2}{\alpha_1} + t\right)\right]\left[\ln \alpha_1 + \ln\left(\frac{\alpha_3}{\alpha_1} + t\right)\right]}{\frac{\alpha_4}{\alpha_1} + t} \\
&= \ln \alpha_1 \int_0^1 \mathrm{d}y \frac{\ln(\alpha_2 + y)\ln(\alpha_3 + y)}{\alpha_4 + y} + \ln^2 \alpha_1 \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_1} + t} \\
&\quad + \ln \alpha_1 \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_2}{\alpha_1} + t\right)}{\frac{\alpha_4}{\alpha_1} + t} + \ln \alpha_1 \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_3}{\alpha_1} + t\right)}{\frac{\alpha_4}{\alpha_1} + t} \\
&\quad + \int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_2}{\alpha_1} + t\right)\ln\left(\frac{\alpha_3}{\alpha_1} + t\right)}{\frac{\alpha_4}{\alpha_1} + t}.
\end{aligned} \tag{10}$$

With the help of (7) the integral in the second term of the last equation of (10) can be written as

$$\int_0^{1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_1} + t} = \int_0^{1/\alpha_1} \frac{\mathrm{d}t_1}{-\frac{\alpha_4}{\alpha_1} - t_1} \int_0^{t_1} \frac{\mathrm{d}t_2}{1 - t_2} = Li_{1,1}\left(-\frac{\alpha_4}{\alpha_1}, -\frac{1}{\alpha_4}\right). \tag{11}$$

The third and fourth terms of the last equation in (10) contain integrals of the form

$$\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\beta_1+t)}{\beta_2+t}. \tag{12}$$

To express such integrals in terms of multiple polylogarithms one proceeds as follows:

$$\begin{aligned}
-Li_{1,1,1}\left(-\beta_2, \frac{\beta_1}{\beta_2}, \frac{-t_m}{\beta_1}\right) &= \int_0^{t_m} \frac{\mathrm{d}t_2}{\beta_1+t_2} \int_0^{t_2} \mathrm{d}t_1 \frac{\ln(1-t_1)}{\beta_2+t_1} = \int_0^{t_m} \mathrm{d}t_1 \frac{\ln(1-t_1)}{\beta_2+t_1} \int_{t_1}^{t_m} \frac{\mathrm{d}t_2}{\beta_1+t_2} \\
&= \ln(\beta_1+t_m) \int_0^{t_m} \mathrm{d}t_1 \frac{\ln(1-t_1)}{\beta_2+t_1} - \int_0^{t_m} \mathrm{d}t_1 \frac{\ln(1-t_1)\ln(\beta_1+t_1)}{\beta_2+t_1} \\
&= \ln(\beta_1+t_m) Li_{1,1}\left(-\beta_2, \frac{-t_m}{\beta_2}\right) - \int_0^{t_m} \mathrm{d}t_1 \frac{\ln(1-t_1)\ln(\beta_1+t_1)}{\beta_2+t_1}.
\end{aligned} \tag{13}$$

In the first line of (13) we have changed the order of integration in the two-dimensional integral. We shall frequently use this trick further on. From Eq. (13) one immediately concludes that

$$\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\beta_1+t)}{\beta_2+t} = Li_{1,1,1}\left(-\beta_2, \frac{\beta_1}{\beta_2}, \frac{-t_m}{\beta_1}\right) + \ln(\beta_1+t_m) Li_{1,1}\left(-\beta_2, \frac{-t_m}{\beta_2}\right). \tag{14}$$

Let us now turn to the more involved integral [first term of Eq. (12)]

$$\begin{aligned}
\int_0^1 \mathrm{d}y \frac{\ln(\alpha_2+y)\ln(\alpha_3+y)}{\alpha_4+y} &\overset{y\to-\alpha_2 t}{=} -\int_0^{-1/\alpha_2} \mathrm{d}t \frac{[\ln\alpha_2+\ln(1-t)]\ln(\alpha_3-\alpha_2 t)}{\frac{\alpha_4}{\alpha_2}-t} \\
&= -\ln\alpha_2 \int_0^{-1/\alpha_2} \mathrm{d}t \frac{\ln(\alpha_3-\alpha_2 t)}{\frac{\alpha_4}{\alpha_2}-t} \\
&\quad - \int_0^{-1/\alpha_2} \mathrm{d}t \frac{\ln(1-t)\left[\ln\alpha_2+\ln\left(\frac{\alpha_3}{\alpha_2}-t\right)\right]}{\frac{\alpha_4}{\alpha_2}-t} \\
&= +\ln\alpha_2 \int_0^1 \mathrm{d}y \frac{\ln(\alpha_3+y)}{\alpha_4+y} - \ln\alpha_2 \int_0^{-1/\alpha_2} \mathrm{d}t \frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_2}-t} \\
&\quad - \int_0^{-1/\alpha_2} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_3}{\alpha_2}-t\right)}{\frac{\alpha_4}{\alpha_2}-t}.
\end{aligned} \tag{15}$$

The integral in the first term can be expressed as

$$\int_0^1 \mathrm{d}y \frac{\ln(\alpha_3+y)}{\alpha_4+y} \overset{y\to-\alpha_3 t}{=} -\int_0^{-1/\alpha_3} \mathrm{d}t \frac{[\ln\alpha_3+\ln(1-t)]}{\frac{\alpha_4}{\alpha_3}-t} = \ln\alpha_3 \ln\left(\frac{\alpha_4+1}{\alpha_4}\right) + Li_{1,1}\left(\frac{\alpha_4}{\alpha_3}, -\frac{1}{\alpha_3}\right). \tag{16}$$

The integral in the second term can be written as

$$\int_0^{-1/\alpha_2} \mathrm{d}t \frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_2}-t} = -Li_{1,1}\left(\frac{\alpha_4}{\alpha_2},-\frac{1}{\alpha_2}\right). \tag{17}$$

The term from the last line of Eq. (15) has a form which is an analog of the integral (12) and can be calculated in a similar way,

$$\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\beta_1-t)}{\beta_2-t} = Li_{1,1,1}\left(\beta_2,\frac{\beta_1}{\beta_2},\frac{t_m}{\beta_1}\right) + \ln(\beta_1-t_m)Li_{1,1}\left(\beta_2,\frac{t_m}{\beta_2}\right). \tag{18}$$

Combining the Eqs. (16)–(18) we arrive at the result for Eq. (15),

$$\begin{aligned}\int_0^1 \mathrm{d}y \frac{\ln(\alpha_2+y)\ln(\alpha_3+y)}{\alpha_4+y} &= Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_2},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right) + \ln\,\alpha_2 Li_{1,1}\left(\frac{\alpha_4}{\alpha_3},-\frac{1}{\alpha_4}\right)\\ &\quad + \ln(1+\alpha_3)Li_{1,1}\left(\frac{\alpha_4}{\alpha_2},-\frac{1}{\alpha_4}\right) + \ln\,\alpha_2\,\ln\,\alpha_3\,\ln\left(\frac{\alpha_4+1}{\alpha_4}\right).\end{aligned} \tag{19}$$

Because the initial integrand is symmetric under the exchange of the parameters α_2 and α_3, the rhs of (19) can be rewritten in a symmetric form if desired.

We are now left with the fifth term in (10). The fifth term is an integral of the type

$$\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1+t)\ln(\gamma_2+t)}{\gamma_3+t}. \tag{20}$$

In order to express such integrals in terms of multiple polylogarithms one can perform the following chain of transformations resulting in a multiple polylogarithm of weight four:

$$\begin{aligned}-Li_{1,1,1,1}\left(-\gamma_3,\frac{\gamma_2}{\gamma_3},\frac{\gamma_1}{\gamma_2},\frac{-t_m}{\gamma_1}\right) &= \int_0^{t_m}\frac{\mathrm{d}t_4}{\gamma_1+t_4}\int_0^{t_4}\frac{\mathrm{d}t_3}{\gamma_2+t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{\gamma_3+t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1}\\ &= -\int_0^{t_m}\frac{\mathrm{d}t_4}{\gamma_1+t_4}\int_0^{t_4}\frac{\mathrm{d}t_3}{\gamma_2+t_3}\int_0^{t_3}\mathrm{d}t_2\frac{\ln(1-t_2)}{\gamma_3+t_2}\\ &= -\int_0^{t_m}\frac{\mathrm{d}t_4}{\gamma_1+t_4}\int_0^{t_4}\mathrm{d}t_2\frac{\ln(1-t_2)}{\gamma_3+t_2}\int_{t_2}^{t_4}\frac{\mathrm{d}t_3}{\gamma_2+t_3}\\ &= -\int_0^{t_m}\mathrm{d}t_4\frac{\ln(\gamma_2+t_4)}{\gamma_1+t_4}\int_0^{t_4}\mathrm{d}t_2\frac{\ln(1-t_2)}{\gamma_3+t_2}\\ &\quad +\int_0^{t_m}\frac{\mathrm{d}t_4}{\gamma_1+t_4}\int_0^{t_4}\mathrm{d}t_2\frac{\ln(1-t_2)\ln(\gamma_2+t_2)}{\gamma_3+t_2}\\ &= -I'(t_m)+\int_0^{t_m}\mathrm{d}t_2\frac{\ln(1-t_2)\ln(\gamma_2+t_2)}{\gamma_3+t_2}\int_{t_2}^{t_m}\frac{\mathrm{d}t_4}{\gamma_1+t_4}\\ &= -I'(t_m)+I''(t_m)-\int_0^{t_m}\mathrm{d}t_2\frac{\ln(\gamma_1+t_2)\ln(\gamma_2+t_2)\ln(1-t_2)}{\gamma_3+t_2},\end{aligned} \tag{21}$$

where we have introduced the notation

$$I'(t_m) = \int_0^{t_m}\mathrm{d}t_4\frac{\ln(\gamma_2+t_4)}{\gamma_1+t_4}\int_0^{t_4}\mathrm{d}t_2\frac{\ln(1-t_2)}{\gamma_3+t_2},$$

$$I''(t_m) = \ln(\gamma_1 + t_m) \int_0^{t_m} \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_2 + t_2)}{\gamma_3 + t_2}. \tag{22}$$

The third term on the last line of (21) is exactly the integral of the required type Eq. (20).

The integral in $I''(t_m)$ has the form of (14). For the integral $I'(t_m)$ we write

$$I'(t_m) = \int_0^{t_m} \mathrm{d}t_4 \frac{\ln(\gamma_2 + t_4)}{\gamma_1 + t_4} \int_0^{t_4} \mathrm{d}t_2 \frac{\ln(1-t_2)}{\gamma_3 + t_2} = \int_0^{t_m} \mathrm{d}t_4 \frac{\ln(\gamma_2 + t_4)}{\gamma_1 + t_4} Li_{1,1}\left(-\gamma_3, \frac{-t_4}{\gamma_3}\right). \tag{23}$$

On the other hand, one has

$$\begin{aligned} Li_{1,1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{\gamma_2}{\gamma_1}, \frac{-t_m}{\gamma_2}\right) &= \int_0^{t_m} \frac{\mathrm{d}t_2}{\gamma_2 + t_2} \int_0^{t_2} \frac{\mathrm{d}t_1}{\gamma_1 + t_1} Li_{1,1}\left(-\gamma_3, \frac{-t_1}{\gamma_3}\right) \\ &= \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma_1 + t_1} Li_{1,1}\left(-\gamma_3, \frac{-t_1}{\gamma_3}\right) \int_{t_1}^{t_m} \frac{\mathrm{d}t_2}{\gamma_2 + t_2} \\ &= \ln(\gamma_2 + t_m) \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma_1 + t_1} Li_{1,1}\left(-\gamma_3, \frac{-t_1}{\gamma_3}\right) \\ &\quad - \int_0^{t_m} \mathrm{d}t_1 \frac{\ln(\gamma_2 + t_1)}{\gamma_1 + t_1} Li_{1,1}\left(-\gamma_3, \frac{-t_1}{\gamma_3}\right) \\ &= -\ln(\gamma_2 + t_m) Li_{1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{-t_m}{\gamma_1}\right) - I'(t_m). \end{aligned} \tag{24}$$

One then concludes that

$$I'(t_m) = -Li_{1,1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{\gamma_2}{\gamma_1}, \frac{-t_m}{\gamma_2}\right) - \ln(\gamma_2 + t_m) Li_{1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{-t_m}{\gamma_1}\right). \tag{25}$$

Finally, substituting $I'(t_m)$ and $I''(t_m)$ into Eq. (21) we write down the result for the integral of the required type Eq. (20),

$$\begin{aligned} &\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1 + t)\ln(\gamma_2 + t)}{\gamma_3 + t} \\ &\quad = \ln(\gamma_1 + t_m)\ln(\gamma_2 + t_m) Li_{1,1}\left(-\gamma_3, \frac{-t_m}{\gamma_3}\right) + \ln(\gamma_2 + t_m) Li_{1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{-t_m}{\gamma_1}\right) \\ &\qquad + \ln(\gamma_1 + t_m) Li_{1,1,1}\left(-\gamma_3, \frac{\gamma_2}{\gamma_3}, \frac{-t_m}{\gamma_2}\right) \\ &\qquad + Li_{1,1,1,1}\left(-\gamma_3, \frac{\gamma_2}{\gamma_3}, \frac{\gamma_1}{\gamma_2}, \frac{-t_m}{\gamma_1}\right) + Li_{1,1,1,1}\left(-\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{\gamma_2}{\gamma_1}, \frac{-t_m}{\gamma_2}\right). \end{aligned} \tag{26}$$

We are now in the position to collect all required contributions to express the L_{-++} function in terms of multiple polylogarithms. Taking into account Eqs. (11), (14), (19), and (26) and we obtain

$$
\begin{aligned}
L_{-++}(\alpha_1,\alpha_2,\alpha_3,\alpha_4) = {} & Li_{1,1,1,1}\left(-\frac{\alpha_4}{\alpha_1},\frac{\alpha_2}{\alpha_4},\frac{\alpha_3}{\alpha_2},-\frac{1}{\alpha_3}\right) + Li_{1,1,1,1}\left(-\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},\frac{\alpha_2}{\alpha_3},-\frac{1}{\alpha_2}\right) \\
& + \ln\,\alpha_1 Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_2},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right) + \ln(1+\alpha_2) Li_{1,1,1}\left(-\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right) \\
& + \ln(1+\alpha_3) Li_{1,1,1}\left(-\frac{\alpha_4}{\alpha_1},\frac{\alpha_2}{\alpha_4},-\frac{1}{\alpha_2}\right) + \ln\,\alpha_1\,\ln\,\alpha_2 Li_{1,1}\left(\frac{\alpha_4}{\alpha_3},-\frac{1}{\alpha_4}\right) \\
& + \ln\,\alpha_1\,\ln(1+\alpha_3) Li_{1,1}\left(\frac{\alpha_4}{\alpha_2},-\frac{1}{\alpha_4}\right) + \ln(1+\alpha_2)\ln(1+\alpha_3) Li_{1,1}\left(-\frac{\alpha_4}{\alpha_1},-\frac{1}{\alpha_4}\right) \\
& + \ln\,\alpha_1\,\ln\,\alpha_2\,\ln\,\alpha_3\,\ln\left(\frac{\alpha_4+1}{\alpha_4}\right). \qquad (27)
\end{aligned}
$$

Some remarks are in order at this place. The final formula (27) contains multiple polylogarithms up to weight four. All multiple polylogarithms up to weight three can be expressed in terms of logarithms and clasical polylogarithms Li_2 and Li_3. This fact is used by us when we reexpress our results for the massive scalar integrals in terms of multiple polylogarithms, i.e., our final results will contain only multiple polylogarithms of weight four. For the variables α_i the conditions (5) are assumed. But in the results for the massive scalar integrals there are also cases when $\alpha_1=1$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ and/or $\alpha_4=\{-1,0\}$. In such cases the general formula (27) is no longer valid and these cases must be studied separately.

B. Special cases for the L_{-++} function

In the Laurent series expansion of the massive scalar one-loop integrals one encounters special values of the arguments α_i for which the general formula Eq. (27) no longer applies. This is quite obvious from the list of special cases discussed in the following.

1. $\alpha_1=1$, $\alpha_4=0$

In such case one can make use of Eq. (26). One should find the limit of the expression on the right-hand side for $t_m=1$, $\gamma_3\to 0$. One obtains

$$
\begin{aligned}
\int_0^1 \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1+t)\ln(\gamma_2+t)}{t} = \lim_{\gamma_3\to 0}\Bigg\{ & \ln(\gamma_1+1)\ln(\gamma_2+1)\int_0^1 \frac{\mathrm{d}t_2}{-\gamma_3-t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1} \\
& + \ln(\gamma_2+1)\int_0^1 \frac{\mathrm{d}t_3}{-\gamma_1-t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{-\gamma_3-t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1} \\
& + \ln(\gamma_1+1)\int_0^1 \frac{\mathrm{d}t_3}{-\gamma_2-t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{-\gamma_3-t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1} \\
& + \int_0^1 \frac{\mathrm{d}t_4}{-\gamma_1-t_3}\int_0^{t_4}\frac{\mathrm{d}t_3}{-\gamma_2-t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{-\gamma_3-t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1} \\
& + \int_0^1 \frac{\mathrm{d}t_4}{-\gamma_2-t_3}\int_0^{t_4}\frac{\mathrm{d}t_3}{-\gamma_1-t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{-\gamma_3-t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1}\Bigg\} \\
= {} & -\ln(\gamma_1+1)\ln(\gamma_2+1)\int_0^1 \frac{\mathrm{d}t_2}{t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1} \\
& - \ln(\gamma_2+1)\int_0^1 \frac{\mathrm{d}t_3}{-\gamma_1-t_3}\int_0^{t_3}\frac{\mathrm{d}t_2}{t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{1-t_1}
\end{aligned}
$$

$$
\begin{aligned}
&- \ln(\gamma_1+1)\int_0^1 \frac{dt_3}{-\gamma_2-t_3}\int_0^{t_3}\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1}\\
&-\int_0^1 \frac{dt_4}{-\gamma_1-t_3}\int_0^{t_4}\frac{dt_3}{-\gamma_2-t_3}\int_0^{t_3}\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1}\\
&-\int_0^1 \frac{dt_4}{-\gamma_2-t_3}\int_0^{t_4}\frac{dt_3}{-\gamma_1-t_3}\int_0^{t_3}\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1}. \qquad (28)
\end{aligned}
$$

In order to get the expression under the sign of the limit in Eq. (28) one applies the definition (7) for the multiple polylogarithms in Eq. (26). Using the same definition for the final multidimensional integrals in (28) and making the change $\gamma_1\to\alpha_2$, $\gamma_2\to\alpha_3$ one finally arrives at the result for the case $\alpha_1=1$ and $\alpha_4=0$,

$$
\begin{aligned}
L_{-++}(1,\alpha_2,\alpha_3,0) &= -Li_{2,1,1}\left(-\alpha_3,\frac{\alpha_2}{\alpha_3},-\frac{1}{\alpha_2}\right)-Li_{2,1,1}\left(-\alpha_2,\frac{\alpha_3}{\alpha_2},-\frac{1}{\alpha_3}\right)-\ln(\alpha_3+1)Li_{2,1}\left(-\alpha_2,-\frac{1}{\alpha_2}\right)\\
&\quad -\ln(\alpha_2+1)Li_{2,1}\left(-\alpha_3,-\frac{1}{\alpha_3}\right)-\ln(\alpha_2+1)\ln(\alpha_3+1)\zeta(2). \qquad (29)
\end{aligned}
$$

2. $\alpha_1=1$, $\alpha_2=\alpha_3=0$

For these values of the parameters α_i one has an integral of the very simple form

$$
L_{-++}(1,0,0,\alpha_4)=\int_0^1 dy\frac{\ln(1-y)\ln^2 y}{\alpha_4+y}.
$$

After a change of variable $y\to 1-t$ one gets

$$
\begin{aligned}
\int_0^1 dt\frac{\ln t\ln^2(1-t)}{\alpha_4+1-t} &= -\int_0^1 dt_1\frac{\ln^2(1-t_1)}{\alpha_4+1-t_1}\int_{t_1}^1\frac{dt_2}{t_2}\\
&= -\int_0^1\frac{dt_2}{t_2}\int_0^{t_2}dt_1\frac{\ln^2(1-t_1)}{\alpha_4+1-t_1}\\
&= -2\int_0^1\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{\alpha_4+1-t_1}\int_0^{t_1}\frac{dt_3}{1-t_3}\int_0^{t_3}\frac{dt_4}{1-t_4}. \qquad (30)
\end{aligned}
$$

Applying the definition (7) one obtains

$$
L_{-++}(1,0,0,\alpha_4)=-2Li_{1,1,2}\left(1,\alpha_4+1,\frac{1}{\alpha_4+1}\right). \qquad (31)
$$

3. $\alpha_1=1$, $\alpha_2=0$ (and $\alpha_4=-1$)

We shall again find the limit of the rhs of (26) for $t_m=1$ and $\gamma_1\to 0$. The first and the third terms are equal to 0 because of the limit $\lim_{\gamma_1\to 0}\ln(\gamma_1+1)=0$. The other terms transform into

$$
\lim_{\gamma_1\to 0} Li_{1,1,1}\left(-\gamma_3,\frac{\gamma_1}{\gamma_3},\frac{-1}{\gamma_1}\right)=-Li_{1,2}\left(-\gamma_3,-\frac{1}{\gamma_3}\right),
$$

$$
\lim_{\gamma_1\to 0} Li_{1,1,1,1}\left(-\gamma_3,\frac{\gamma_2}{\gamma_3},\frac{\gamma_1}{\gamma_2},\frac{-t_m}{\gamma_1}\right)=-Li_{1,1,2}\left(-\gamma_3,\frac{\gamma_2}{\gamma_3},\frac{-1}{\gamma_2}\right),
$$

$$\lim_{\gamma_1\to 0} Li_{1,1,1,1}\left(-\gamma_3,\frac{\gamma_1}{\gamma_3},\frac{\gamma_2}{\gamma_1},\frac{-t_m}{\gamma_2}\right)=-Li_{1,2,1}\left(-\gamma_3,\frac{\gamma_2}{\gamma_3},\frac{-1}{\gamma_2}\right).$$

Finally we write

$$L_{-++}(1,0,\alpha_3,\alpha_4)=-Li_{1,1,2}\left(-\alpha_4,\frac{\alpha_3}{\alpha_4},\frac{-1}{\alpha_3}\right)-Li_{1,2,1}\left(-\alpha_4,\frac{\alpha_3}{\alpha_4},\frac{-1}{\alpha_3}\right)-\ln(\alpha_3+1)Li_{1,2}\left(-\alpha_4,-\frac{1}{\alpha_4}\right). \tag{32}$$

For the special case $\alpha_4=-1$ one gets

$$L_{-++}(1,0,\alpha_3,-1)=-Li_{1,1,2}\left(1,-\alpha_3,\frac{-1}{\alpha_3}\right)-Li_{1,2,1}\left(1,-\alpha_3,\frac{-1}{\alpha_3}\right)-\ln(\alpha_3+1)\zeta(3). \tag{33}$$

4. $\alpha_2=\alpha_3=0$ (and $\alpha_4=-1$)

In this case one proceeds along the following lines:

$$\begin{aligned}
L_{-++}(\alpha_1,0,0,\alpha_4)&=\int_0^1 dy\frac{\ln(\alpha_1-y)\ln^2 y}{\alpha_4+y}\overset{y\to 1-t}{=}\int_0^1 dt\frac{\ln(\alpha_1-1+t)\ln^2(1-t)}{\alpha_4+1-t}\\
&=-\int_0^1 dt_1\frac{\ln^2(1-t_1)}{-\alpha_4-1+t_1}\int_{-\alpha_1+2}^{t_1}\frac{dt_2}{\alpha_1-1+t_2}\\
&=-\int_0^1 dt_1\frac{\ln^2(1-t_1)}{-\alpha_4-1+t_1}\left\{\int_1^{t_1}+\int_{-\alpha_1+2}^1\right\}\frac{dt_2}{\alpha_1-1+t_2}\\
&=\int_0^1\frac{dt_2}{\alpha_1-1+t_2}\int_0^{t_2}dt_1\frac{\ln^2(1-t_1)}{-\alpha_4-1+t_1}-\ln\alpha_1\int_0^1 dt_1\frac{\ln^2(1-t_1)}{-\alpha_4-1+t_1}\\
&=2\int_0^1\frac{dt_2}{\alpha_1-1+t_2}\int_0^{t_2}\frac{dt_1}{-\alpha_4-1+t_1}\int_0^{t_1}\frac{dt_3}{1-t_3}\int_0^{t_3}\frac{dt_4}{1-t_4}-2\ln\alpha_1 Li_3\left(-\frac{1}{\alpha_4}\right).
\end{aligned} \tag{34}$$

Using the definition (7) we arrive at the result

$$L_{-++}(\alpha_1,0,0,\alpha_4)=2Li_{1,1,1,1}\left(1,\alpha_4+1,\frac{1-\alpha_1}{\alpha_4+1},\frac{1}{1-\alpha_1}\right)-2\ln\alpha_1 Li_3\left(-\frac{1}{\alpha_4}\right). \tag{35}$$

For the case $\alpha_4=-1$ one obtains

$$L_{-++}(\alpha_1,0,0,-1)=-2Li_{1,2,1}\left(1,1-\alpha_1,\frac{1}{1-\alpha_1}\right)-2\ln\alpha_1\zeta(3). \tag{36}$$

5. $\alpha_2=0$ (and $\alpha_4=-1$)

For this integral we change the integration variable $y\to 1-t$,

$$\int_0^1 \mathrm{d}y \frac{\ln(\alpha_1 - y)\ln y \ln(\alpha_3 + y)}{\alpha_4 + y} = \int_0^1 \mathrm{d}t \frac{\ln(1-t)\ln(\alpha_1 - 1 + t)\ln(\alpha_3 + 1 - t)}{\alpha_4 + 1 - t}$$
$$= \int_0^1 \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1 + t)\ln(\gamma_2 - t)}{\gamma_3 - t}. \tag{37}$$

One notes that the last integral is an analog of the integral in Eq. (26). The calculation proceeds in a similar way,

$$\begin{aligned}
&- Li_{1,1,1,1}\left(\gamma_3, \frac{\gamma_2}{\gamma_3}, -\frac{\gamma_1}{\gamma_2}, -\frac{1}{\gamma_1}\right) \\
&= \int_0^1 \frac{\mathrm{d}t_4}{\gamma_1 + t_4} \int_0^{t_4} \frac{\mathrm{d}t_3}{\gamma_2 - t_3} \int_0^{t_3} \frac{\mathrm{d}t_2}{\gamma_3 - t_2} \int_0^{t_2} \frac{\mathrm{d}t_1}{1 - t_1} \\
&= -\int_0^{t_m} \frac{\mathrm{d}t_4}{\gamma_1 + t_4} \int_0^{t_4} \frac{\mathrm{d}t_3}{\gamma_2 - t_3} \int_0^{t_3} \mathrm{d}t_2 \frac{\ln(1-t_2)}{\gamma_3 - t_2} = -\int_0^{t_m} \frac{\mathrm{d}t_4}{\gamma_1 + t_4} \int_0^{t_4} \mathrm{d}t_2 \frac{\ln(1-t_2)}{\gamma_3 - t_2} \int_{t_2}^{t_4} \frac{\mathrm{d}t_3}{\gamma_2 - t_3} \\
&= \int_0^1 \mathrm{d}t_4 \frac{\ln(\gamma_2 - t_4)}{\gamma_1 + t_4} \int_0^{t_4} \mathrm{d}t_2 \frac{\ln(1-t_2)}{\gamma_3 - t_2} - \int_0^1 \frac{\mathrm{d}t_4}{\gamma_1 + t_4} \int_0^{t_4} \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2} \\
&= Y'(1) - \int_0^1 \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2} \int_{t_2}^1 \frac{\mathrm{d}t_4}{\gamma_1 + t_4} \\
&= Y'(1) - \ln(\gamma_1 + 1) \int_0^1 \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2} + \int_0^1 \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_1 + t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2} \\
&= Y'(1) - Y''(1) + \int_0^1 \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_1 + t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2},
\end{aligned} \tag{38}$$

where we have introduced the notation

$$Y'(t_m) = \int_0^{t_m} \mathrm{d}t_4 \frac{\ln(\gamma_2 - t_4)}{\gamma_1 + t_4} \int_0^{t_4} \mathrm{d}t_2 \frac{\ln(1-t_2)}{\gamma_3 - t_2},$$

$$Y''(t_m) = \ln(\gamma_1 + t_m) \int_0^{t_m} \mathrm{d}t_2 \frac{\ln(1-t_2)\ln(\gamma_2 - t_2)}{\gamma_3 - t_2}. \tag{39}$$

The last term in (38) is the required integral. The expansion of the integral $Y'(t_m)$ in terms of multiple polylogarithms is similar to the evaluation of $I'(t_m)$ in Eq. (22). The result of the calculation is

$$Y'(t_m) = Li_{1,1,1,1}\left(\gamma_3, -\frac{\gamma_1}{\gamma_3}, -\frac{\gamma_2}{\gamma_1}, \frac{t_m}{\gamma_2}\right) + \ln(\gamma_2 - t_m) Li_{1,1,1}\left(\gamma_3, -\frac{\gamma_1}{\gamma_3}, -\frac{t_m}{\gamma_1}\right). \tag{40}$$

For the calculation of $Y''(t_m)$ one can make use of (18). Finally using Eqs. (38) and (40) one arrives at the result

$$\int_0^1 \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1+t)\ln(\gamma_2-t)}{\gamma_3-t} = -Li_{1,1,1,1}\left(\gamma_3,-\frac{\gamma_1}{\gamma_3},-\frac{\gamma_2}{\gamma_1},\frac{1}{\gamma_2}\right)$$
$$-Li_{1,1,1,1}\left(\gamma_3,\frac{\gamma_2}{\gamma_3},-\frac{\gamma_1}{\gamma_2},-\frac{1}{\gamma_1}\right)-\ln(\gamma_1+1)Li_{1,1,1}\left(\gamma_3,\frac{\gamma_2}{\gamma_3},\frac{1}{\gamma_2}\right)$$
$$-\ln(\gamma_2-1)Li_{1,1,1}\left(\gamma_3,-\frac{\gamma_1}{\gamma_3},-\frac{1}{\gamma_1}\right)$$
$$-\ln(\gamma_1+1)\ln(\gamma_2-1)Li_{1,1}\left(\gamma_3,\frac{1}{\gamma_3}\right). \tag{41}$$

To obtain the formula for the L function with $\alpha_2=0$ we must only change γ_1, γ_2, and γ_3 to α_1-1, α_3+1, and α_4+1 according to Eq. (37):

$$L_{-++}(\alpha_1,0,\alpha_3,\alpha_4)=\int_0^1 \mathrm{d}y \frac{\ln(\alpha_1-y)\ln y\ln(\alpha_3+y)}{\alpha_4+y} = -Li_{1,1,1,1}\left(1+\alpha_4,\frac{1-\alpha_1}{1+\alpha_4},\frac{1+\alpha_3}{1-\alpha_1},\frac{1}{1+\alpha_3}\right)$$
$$-Li_{1,1,1,1}\left(1+\alpha_4,\frac{1+\alpha_3}{1+\alpha_4},\frac{1-\alpha_1}{1+\alpha_3},\frac{1}{1-\alpha_1}\right)-\ln\alpha_1 Li_{1,1,1}\left(1+\alpha_4,\frac{1+\alpha_3}{1+\alpha_4},\frac{1}{1+\alpha_3}\right)$$
$$-\ln\alpha_3 Li_{1,1,1}\left(1+\alpha_4,\frac{1-\alpha_1}{1+\alpha_4},\frac{1}{1-\alpha_1}\right)-\ln\alpha_1\ln\alpha_3 Li_{1,1}\left(1+\alpha_4,\frac{1}{1+\alpha_4}\right). \tag{42}$$

For the case $\alpha_4=-1$ we calculate the limit of the rhs of (42) for $\alpha_4\to-1$ and obtain

$$L_{-++}(\alpha_1,0,\alpha_3,-1)=Li_{2,1,1}\left(1-\alpha_1,\frac{1+\alpha_3}{1-\alpha_1},\frac{1}{1+\alpha_3}\right)$$
$$+Li_{2,1,1}\left(1+\alpha_3,\frac{1-\alpha_1}{1+\alpha_3},\frac{1}{1-\alpha_1}\right)+\ln\alpha_1 Li_{2,1}\left(1+\alpha_3,\frac{1}{1+\alpha_3}\right)$$
$$+\ln\alpha_3 Li_{2,1}\left(1-\alpha_1,\frac{1}{1-\alpha_1}\right)+\ln\alpha_1\ln\alpha_3\zeta(2). \tag{43}$$

IV. TRANSFORMATION OF L_{+++} TO MULTIPLE POLYLOGARITHMS

In this section we will show that all our L_{+++} functions can be expressed in terms of multiple polylogarithms.

A. General case for the L_{+++} function

We now proceed with the transformation of the triple index function L_{+++}

$$L_{+++}(\alpha_1,\alpha_2,\alpha_3,\alpha_4)=\int_0^1 \mathrm{d}y \frac{\ln(\alpha_1+y)\ln(\alpha_2+y)\ln(\alpha_3+y)}{\alpha_4+y}. \tag{44}$$

After changing the integration variable $y=-\alpha_1 t$ we obtain

$$
\begin{aligned}
&-\int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(\alpha_1-\alpha_1 t)\ln(\alpha_2-\alpha_1 t)\ln(\alpha_3-\alpha_1 t)}{\frac{\alpha_4}{\alpha_1}-t} \\
&\quad = -\int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln\alpha_1 \ln(\alpha_2-\alpha_1 t)\ln(\alpha_3+\alpha_1 t)}{\frac{\alpha_4}{\alpha_1}-t} \\
&\qquad -\int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\left[\ln\alpha_1+\ln\left(\frac{\alpha_2}{\alpha_1}-t\right)\right]\left[\ln\alpha_1+\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)\right]}{\frac{\alpha_4}{\alpha_1}-t} \\
&\quad = \ln\alpha_1 \int_0^1 \mathrm{d}y \frac{\ln(\alpha_2+y)\ln(\alpha_3+y)}{\alpha_4+y} - \ln^2\alpha_1 \int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_1}-t} \\
&\qquad -\ln\alpha_1 \int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_2}{\alpha_1}-t\right)}{\frac{\alpha_4}{\alpha_1}-t} - \ln\alpha_1 \int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)}{\frac{\alpha_4}{\alpha_1}-t} \\
&\qquad -\int_0^{-1/\alpha_1} \mathrm{d}t \frac{\ln(1-t)\ln\left(\frac{\alpha_2}{\alpha_1}-t\right)\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)}{\frac{\alpha_4}{\alpha_1}-t}.
\end{aligned} \tag{45}
$$

The first integral on the rhs of (45) has been calculated in Eq. (19). For the second integral one makes use of the formula (17) (the only change is $\alpha_2 \to \alpha_1$). For the evaluation of the third and fourth integrals one uses Eq. (18). We are left with the most complicated fifth integral. Let us consider an integral of the type

$$
\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1-t)\ln(\gamma_2-t)}{\gamma_3-t}. \tag{46}
$$

This integral is an analog of the integral in Eq. (26). The calculation proceeds in a similar way. One obtains the result

$$
\begin{aligned}
\int_0^{t_m} \mathrm{d}t \frac{\ln(1-t)\ln(\gamma_1-t)\ln(\gamma_2-t)}{\gamma_3-t} &= -\ln(\gamma_1-t_m)\ln(\gamma_2-t_m) Li_{1,1}\left(\gamma_3, \frac{t_m}{\gamma_3}\right) \\
&\quad -\ln(\gamma_2-t_m) Li_{1,1,1}\left(\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{t_m}{\gamma_1}\right) \\
&\quad -\ln(\gamma_1-t_m) Li_{1,1,1}\left(\gamma_3, \frac{\gamma_2}{\gamma_3}, \frac{t_m}{\gamma_2}\right) - Li_{1,1,1,1}\left(\gamma_3, \frac{\gamma_2}{\gamma_3}, \frac{\gamma_1}{\gamma_2}, \frac{t_m}{\gamma_1}\right) \\
&\quad - Li_{1,1,1,1}\left(\gamma_3, \frac{\gamma_1}{\gamma_3}, \frac{\gamma_2}{\gamma_1}, \frac{t_m}{\gamma_2}\right).
\end{aligned} \tag{47}
$$

Taking into account everything mentioned above for Eq. (45) we arrive at the final result for the L_{+++} function,

$$
\begin{aligned}
L_{+++}(\alpha_1,\alpha_2,\alpha_3,\alpha_4) &= Li_{1,1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_2}{\alpha_4},\frac{\alpha_3}{\alpha_2},-\frac{1}{\alpha_3}\right)+Li_{1,1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},\frac{\alpha_2}{\alpha_3},-\frac{1}{\alpha_2}\right)\\
&\quad+\ln\alpha_1 Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_2},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right)+\ln(1+\alpha_2)Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right)\\
&\quad+\ln(1+\alpha_3)Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_2}{\alpha_4},-\frac{1}{\alpha_2}\right)+\ln\alpha_1\ln\alpha_2 Li_{1,1}\left(\frac{\alpha_4}{\alpha_3},-\frac{1}{\alpha_4}\right)\\
&\quad+\ln\alpha_1\ln(1+\alpha_3)Li_{1,1}\left(\frac{\alpha_4}{\alpha_2},-\frac{1}{\alpha_4}\right)+\ln(1+\alpha_2)\ln(1+\alpha_3)Li_{1,1}\left(\frac{\alpha_4}{\alpha_1},-\frac{1}{\alpha_4}\right)\\
&\quad+\ln\alpha_1\ln\alpha_2\ln\alpha_3\ln\left(\frac{\alpha_4+1}{\alpha_4}\right). \qquad (48)
\end{aligned}
$$

For this equation the conditions (5) are assumed. We emphasize that the arguments of L_{+++} functions occurring in the actual calculation of the massive scalar one-loop integrals are not of the most general type as assumed in the derivation of (48). We have nevertheless included a discussion of the general case because Eq. (48) may be useful in other applications. In the results for the massive scalar integrals one has only the special cases where $\alpha_1=\alpha_2$ or $\alpha_1=\alpha_3$ as well as the cases $\alpha_1=0$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ and/or $\alpha_4=\{-1,0\}$. If some α's coincide with each other Eq. (48) becomes simpler. In this case one can also make use of symmetry properties to obtain simpler relations between the L_{+++} functions and multiple polylogarithms. For the cases $\alpha_1=0$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ and/or $\alpha_4=\{-1,0\}$ the general formula (48) is no longer valid and these cases must be studied separately.

B. Special cases for the L_{+++} function

In the Laurent series expansion of the massive scalar one-loop integrals the following special cases for the α_i are present.

1. $\alpha_1=\alpha_2$ or $\alpha_1=\alpha_3$

As it was stated in Sec. II the L_{+++} function is symmetric under the permutations $\alpha_i\leftrightarrow\alpha_j$. Therefore, it suffices to consider the case $\alpha_1=\alpha_2$.

We must evaluate the integral

$$
L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4)=\int_0^1 dy\frac{\ln^2(\alpha_1+y)\ln(\alpha_3+y)}{\alpha_4+y}. \qquad (49)
$$

This integral can be expressed in different ways. First of all one can directly use Eq. (48) replacing α_2 by α_1. The second possibility is to use symmetry properties. One takes into account the rhs of Eq. (48) and notes that the part with multiple polylogarithms of weight four is symmetric under the exchange $\alpha_2\leftrightarrow\alpha_3$. It allows one to reduce the number of the multiple polylogarithms from two to one. First we apply Eq. (48) for the case $\alpha_2=\alpha_3$ replacing α_3 by α_2. Second we change $\alpha_1\rightarrow\alpha_3$ and $\alpha_2\rightarrow\alpha_1$. After these transformations one obtains the following result:

$$
\begin{aligned}
L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4) &= \int_0^1 dy\frac{\ln^2(\alpha_1+y)\ln(\alpha_3+y)}{\alpha_4+y}\\
&= +2Li_{1,1,1,1}\left(\frac{\alpha_4}{\alpha_3},\frac{\alpha_1}{\alpha_4},1,-\frac{1}{\alpha_1}\right)+\ln\alpha_3 Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_1}{\alpha_4},-\frac{1}{\alpha_1}\right)\\
&\quad+2\ln(1+\alpha_1)Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_3},\frac{\alpha_1}{\alpha_4},-\frac{1}{\alpha_1}\right)+\ln\alpha_3[\ln(\alpha_1+1)+\ln\alpha_1]Li_{1,1}\left(\frac{\alpha_4}{\alpha_1},-\frac{1}{\alpha_4}\right)
\end{aligned}
$$

$$+\ln^2(1+\alpha_1)Li_{1,1}\left(\frac{\alpha_4}{\alpha_3},-\frac{1}{\alpha_4}\right)+\ln^2\alpha_1\ln\alpha_3\ln\left(\frac{\alpha_4+1}{\alpha_4}\right). \tag{50}$$

There is also the third possibility to express $L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4)$ in terms of multiple polylogarithms:

$$\begin{aligned}
&\int_0^1 \mathrm{d}y\frac{\ln^2(\alpha_1+y)\ln(\alpha_3+y)}{\alpha_4+y}\\
&\overset{y\to-\alpha_1 t}{=} -\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln^2(\alpha_1-\alpha_1 t)\ln(\alpha_3-\alpha_1 t)}{\frac{\alpha_4}{\alpha_1}-t}\\
&=-\int_0^{-1/\alpha_1}\mathrm{d}t\frac{[\ln^2\alpha_1+2\ln\alpha_1\ln(1-t)+\ln^2(1-t)]\left[\ln\alpha_1+\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)\right]}{\frac{\alpha_4}{\alpha_1}-t}\\
&=+\ln^3\alpha_1\int_0^1\frac{\mathrm{d}y}{\alpha_4+y}+\ln^2\alpha_1\int_0^1\mathrm{d}y\frac{\ln(\alpha_3+y)}{\alpha_4+y}-2\ln^2\alpha_1\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln(1-t)}{\frac{\alpha_4}{\alpha_1}-t}\\
&\quad-\ln\alpha_1\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln^2(1-t)}{\frac{\alpha_4}{\alpha_1}-t}-2\ln\alpha_1\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln(1-t)\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)}{\frac{\alpha_4}{\alpha_1}-t}\\
&\quad-\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln^2(1-t)\ln\left(\frac{\alpha_3}{\alpha_1}-t\right)}{\frac{\alpha_4}{\alpha_1}-t}.
\end{aligned} \tag{51}$$

The first term can be integrated immediately. For the second and third term one uses Eq. (16) and Eq. (17), respectively. The integral of the fourth term can be rewritten as

$$\int_0^{-1/\alpha_1}\mathrm{d}t\frac{\ln^2(1-t)}{\frac{\alpha_4}{\alpha_1}-t}=2\int_0^{-1/\alpha_1}\frac{\mathrm{d}t_1}{\frac{\alpha_4}{\alpha_1}-t_1}\int_0^{t_1}\frac{\mathrm{d}t_2}{1-t_2}\int_0^{t_2}\frac{\mathrm{d}t_3}{1-t_3}=2Li_{1,1,1}\left(1,\frac{\alpha_4}{\alpha_1},\frac{-1}{\alpha_4}\right). \tag{52}$$

The fifth term is calculable with Eq. (14). To integrate the last term one first evaluates the following integral:

$$\begin{aligned}
\int_0^{t_m}\mathrm{d}t\frac{\ln^2(1-t)\ln(\beta_1-t)}{\beta_2-t}&=-\int_0^{t_m}\mathrm{d}t_1\frac{\ln^2(1-t_1)}{\beta_2-t_1}\left\{\int_{t_m}^{t_1}+\int_{\beta_1-1}^{t_m}\right\}\frac{\mathrm{d}t_2}{\beta_1-t_2}\\
&=\int_0^{t_m}\frac{\mathrm{d}t_2}{\beta_1-t_2}\int_0^{t_2}\mathrm{d}t_1\frac{\ln^2(1-t_1)}{\beta_2-t_1}+\ln(\beta_1-t_m)\int_0^{t_m}\mathrm{d}t\frac{\ln^2(1-t)}{\beta_2-t}\\
&=2Li_{1,1,1,1}\left(1,\beta_2,\frac{\beta_1}{\beta_2},\frac{t_m}{\beta_1}\right)+2\ln(\beta_1-t_m)Li_{1,1,1}\left(1,\beta_2,\frac{t_m}{\beta_2}\right).
\end{aligned} \tag{53}$$

Then to calculate the last term of Eq. (51) one only has to change β_1, β_2, and t_m by the corresponding combinations of α_i. Finally we arrive at the result for the $L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4)$ function,

$$L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4) = -2Li_{1,1,1,1}\left(1,\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right) - 2\ln(\alpha_3+1)Li_{1,1,1}\left(1,\frac{\alpha_4}{\alpha_1},-\frac{1}{\alpha_4}\right)$$
$$+ 2\ln\alpha_1 Li_{1,1,1}\left(\frac{\alpha_4}{\alpha_1},\frac{\alpha_3}{\alpha_4},-\frac{1}{\alpha_3}\right) + 2\ln\alpha_1\ln(\alpha_3+1)Li_{1,1}\left(\frac{\alpha_4}{\alpha_1},-\frac{1}{\alpha_4}\right)$$
$$+ \ln^2\alpha_1 Li_{1,1}\left(\frac{\alpha_4}{\alpha_3},-\frac{1}{\alpha_4}\right) + \ln^2\alpha_1\ln\alpha_3\ln\left(\frac{\alpha_4+1}{\alpha_4}\right). \tag{54}$$

This is the third possibility to express $L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4)$ function in terms of multiple polylogaritms. Each of the Eqs. (50) and (54) contains only one multiple polylogarithm of weight four and they are both equally acceptable from this point of view. One has a free choice to apply any of these equations for the required L functions. The situation with the $L_{+++}(\alpha_1,\alpha_1,\alpha_3,\alpha_4)$ function is an example of the statement that the expansion of the L functions in terms of multiple polylogarithms is not unique.

2. $\alpha_1=0$ (or $\alpha_2=0$ or $\alpha_3=0$)

For this integral we change the integration variable $y\to 1-t$,

$$L_{+++}(0,\alpha_2,\alpha_3,\alpha_4) = \int_0^1 dy\frac{\ln y\ln(\alpha_2+y)\ln(\alpha_3+y)}{\alpha_4+y} = \int_0^1 dt\frac{\ln(1-t)\ln(\alpha_2+1-t)\ln(\alpha_3+1-t)}{\alpha_4+1-t} \tag{55}$$

and using Eq. (48) we arrive at the result

$$L_{+++}(0,\alpha_2,\alpha_3,\alpha_4) = -Li_{1,1,1,1}\left(1+\alpha_4,\frac{1+\alpha_2}{1+\alpha_4},\frac{1+\alpha_3}{1+\alpha_2},\frac{1}{1+\alpha_3}\right)$$
$$- Li_{1,1,1,1}\left(1+\alpha_4,\frac{1+\alpha_3}{1+\alpha_4},\frac{1+\alpha_2}{1+\alpha_3},\frac{1}{1+\alpha_2}\right)$$
$$- \ln\alpha_2 Li_{1,1,1}\left(1+\alpha_4,\frac{1+\alpha_3}{1+\alpha_4},\frac{1}{1+\alpha_3}\right) - \ln\alpha_3 Li_{1,1,1}\left(1+\alpha_4,\frac{1+\alpha_2}{1+\alpha_4},\frac{1}{1+\alpha_2}\right)$$
$$- \ln\alpha_2\ln\alpha_3 Li_{1,1}\left(1+\alpha_4,\frac{1}{1+\alpha_4}\right). \tag{56}$$

3. $\alpha_1=\alpha_2=0$

To calculate this integral we again change the integration variable $y\to 1-t$,

$$L_{+++}(0,0,\alpha_3,\alpha_4) = \int_0^1 dy\frac{\ln^2 y\ln(\alpha_3+y)}{\alpha_4+y} = \int_0^1 dt\frac{\ln^2(1-t)\ln(\alpha_3+1-t)}{\alpha_4+1-t}. \tag{57}$$

For the last integral we use Eq. (53). An additional simplification can be done if one notes that

$$Li_{1,1,1}\left(1,\alpha_4+1,\frac{1}{\alpha_4+1}\right) = -Li_3\left(-\frac{1}{\alpha_4}\right). \tag{58}$$

Finally one has

$$L_{+++}(0,0,\alpha_3,\alpha_4) = 2Li_{1,1,1,1}\left(1,\alpha_4+1,\frac{\alpha_3+1}{\alpha_4+1},\frac{1}{\alpha_3+1}\right) - 2\ln\alpha_3 Li_3\left(-\frac{1}{\alpha_4}\right). \tag{59}$$

4. $\alpha_1=\alpha_2=0$, $\alpha_4=-1$ (or $\alpha_2=\alpha_3=0$, $\alpha_4=-1$)

In this case one should calculate the limit of the rhs of (59) for $t_m=1$ and $\alpha_4\to-1$. After this procedure one obtains

$$L_{+++}(0,0,\alpha_3,-1)=-2Li_{1,2,1}\left(1,\alpha_3+1,\frac{1}{\alpha_3+1}\right)-2\ln\alpha_3\zeta(3). \tag{60}$$

For the case $\alpha_2=\alpha_3=0$ and $\alpha_4=-1$ one can use the same formula. The only change is $\alpha_3\to\alpha_1$.

5. $\alpha_1=0$, $\alpha_4=-1$

To obtain the solution for these values of the α_i we must find the limit of the rhs of (56) for $\alpha_4\to-1$. After taking the limit one arrives at the result

$$\begin{aligned}L_{+++}(0,\alpha_2,\alpha_3,-1)=&+Li_{2,1,1}\left(1+\alpha_2,\frac{1+\alpha_3}{1+\alpha_2},\frac{1}{1+\alpha_3}\right)+Li_{2,1,1}\left(1+\alpha_3,\frac{1+\alpha_2}{1+\alpha_3},\frac{1}{1+\alpha_2}\right)\\&+\ln\alpha_2 Li_{2,1}\left(1+\alpha_3,\frac{1}{1+\alpha_3}\right)+\ln\alpha_3 Li_{2,1}\left(1+\alpha_2,\frac{1}{1+\alpha_2}\right)+\ln\alpha_2\ln\alpha_3\zeta(2).\end{aligned} \tag{61}$$

V. TRANSFORMATION OF L_+ TO MULTIPLE POLYLOGARITHMS

In this section we will show that all our L_+ functions can be expressed in terms of multiple polylogarithms.

A. General case for the L_+ function

Here we derive the general formula for the single index L_+ function Eq. (2),

$$L_+(\alpha_1,\alpha_2,\alpha_3,\alpha_4)=\int_0^1 dy\frac{\ln(\alpha_1+y)}{\alpha_4+y}Li_2(\alpha_2+\alpha_3 y). \tag{62}$$

After changing the integration variable $y\to(t-\alpha_2)/\alpha_3$ one gets

$$L_+=\int_{\alpha_2}^{\alpha_2+\alpha_3}\frac{dt}{\alpha_3}\frac{\ln\left(\alpha_1+\dfrac{t-\alpha_2}{\alpha_3}\right)}{\alpha_4+\dfrac{t-\alpha_2}{\alpha_3}}Li_2(t)=\int_{\alpha_2}^{\alpha_2+\alpha_3}dt\frac{-\ln\alpha_3+\ln(\alpha_1\alpha_3-\alpha_2+t)}{\alpha_3\alpha_4-\alpha_2+t}Li_2(t). \tag{63}$$

The integration interval can be split into two pieces, $[\alpha_2,0]$ and $[0,\alpha_2+\alpha_3]$. One can then write L_+ as a sum of four terms,

$$L_+=-\ln\alpha_3\left\{\int_0^{\alpha_2+\alpha_3}-\int_0^{\alpha_2}\right\}\frac{dt}{\gamma+t}Li_2(t)+\left\{\int_0^{\alpha_2+\alpha_3}-\int_0^{\alpha_2}\right\}dt\frac{\ln(\alpha+t)}{\gamma+t}Li_2(t), \tag{64}$$

where we have introduced the notation

$$\alpha=\alpha_1\alpha_3-\alpha_2,\quad \gamma=\alpha_3\alpha_4-\alpha_2. \tag{65}$$

Looking at Eq. (64) it is clear that there are only two different types of integrals to be dealt with,

$$\int_0^{t_m} \frac{\mathrm{d}t}{\gamma+t} Li_2(t) \quad \text{and} \quad \int_0^{t_m} \mathrm{d}t \frac{\ln(\alpha+t)}{\gamma+t} Li_2(t). \tag{66}$$

The upper limits are $t_m=\alpha_2+\alpha_3$ or $t_m=\alpha_2$. The first integral can be evaluated analytically in terms of standard logarithms and classical polylogarithms up to Li_3. However, the same integral can also be expressed in terms of multiple polylogarithms via the integral representation (7), e.g.,

$$\int_0^{t_m} \frac{\mathrm{d}t}{\gamma+t} Li_2(t) = \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma+t_1} \int_0^{t_1} \frac{\mathrm{d}t_2}{t_2} \int_0^{t_2} \frac{\mathrm{d}t_3}{1-t_3} = -Li_{2,1}\left(-\gamma, \frac{-t_m}{\gamma}\right). \tag{67}$$

We now deal with the second integral in (66). Consider the following multiple polylogarithm of weight four:

$$\begin{aligned} Li_{2,1,1}\left(-\gamma, \frac{\alpha}{\gamma}, \frac{t_m}{-\alpha}\right) &= \int_0^{t_m} \frac{\mathrm{d}t_2}{-\alpha-t_2} \int_0^{t_2} \frac{\mathrm{d}t_1}{-\gamma-t_1} Li_2(t_1) = \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma+t_1} Li_2(t_1) \int_{t_1}^{t_m} \frac{\mathrm{d}t_2}{\alpha+t_2} \\ &= \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma+t_1} Li_2(t_1) \ln(\alpha+t_m) - \int_0^{t_m} \frac{\mathrm{d}t_1}{\gamma+t_1} Li_2(t_1) \ln(\alpha+t_1). \end{aligned} \tag{68}$$

In the first step we have used the usual trick to change the order of integration. As already noted before [see Eq. (67)] the first term on the second line can be expressed through a multiple polylogarithm of weight three. Thus one has

$$\int_0^{t_m} \mathrm{d}t \frac{\ln(\alpha+t)}{\gamma+t} Li_2(t) = -Li_{2,1,1}\left(-\gamma, \frac{\alpha}{\gamma}, \frac{t_m}{-\alpha}\right) - Li_{2,1}\left(-\gamma, \frac{-t_m}{\gamma}\right) \ln(\alpha+t_m). \tag{69}$$

Finally, substituting Eqs. (67) and (69) into Eq. (64) we arrive at the desired relation

$$\begin{aligned} L_+(\alpha_1,\alpha_2,\alpha_3,\alpha_4) = {} & Li_{2,1,1}\left(\alpha_2-\alpha_3\alpha_4, \frac{\alpha_2-\alpha_1\alpha_3}{\alpha_2-\alpha_3\alpha_4}, \frac{\alpha_2}{\alpha_2-\alpha_1\alpha_3}\right) \\ & - Li_{2,1,1}\left(\alpha_2-\alpha_3\alpha_4, \frac{\alpha_2-\alpha_1\alpha_3}{\alpha_2-\alpha_3\alpha_4}, \frac{\alpha_2+\alpha_3}{\alpha_2-\alpha_1\alpha_3}\right) \\ & + \ln\alpha_1 Li_{2,1}\left(\alpha_2-\alpha_3\alpha_4, \frac{\alpha_2}{\alpha_2-\alpha_3\alpha_4}\right) \\ & - \ln(\alpha_1+1) Li_{2,1}\left(\alpha_2-\alpha_3\alpha_4, \frac{\alpha_2+\alpha_3}{\alpha_2-\alpha_3\alpha_4}\right). \end{aligned} \tag{70}$$

We should note that, similar to Eq. (27), the conditions (5) are assumed for the variables α_i. Also, one cannot directly use Eq. (70) if $\alpha_2-\alpha_3\alpha_4=0$ or $\alpha_2-\alpha_1\alpha_3=0$. However, in the results for the massive scalar integrals precisely these special cases appear, as well as the cases where $\alpha_1=0$ and/or $\alpha_2=0$ and/or $\alpha_3=0$ and/or $\alpha_4=\{-1,0\}$. In such cases the general formula (70) is no longer valid and these cases must be studied separately.

B. Special cases for the L_+ function

In the Laurent series expansion of the massive scalar one-loop integrals the following special cases appear for the arguments of the L_+ functions:

1. $\alpha_2-\alpha_3\alpha_4=0$ (or $\alpha_2-\alpha_1\alpha_3=0$)

In this case one must find the limit of the rhs of Eq. (70) for $\alpha_2 \to \alpha_3\alpha_4$. First we rewrite the rhs of Eq. (70) in terms of multidimensional integrals via the definition (7). Second we replace α_2 by $\alpha_3\alpha_4$. We finally again use the definition (7) to obtain the result

$$L_+(\alpha_1,\alpha_3\alpha_4,\alpha_3,\alpha_4) = -Li_{3,1}\left(\alpha_3(\alpha_4-\alpha_1),\frac{\alpha_4}{\alpha_4-\alpha_1}\right)+Li_{3,1}\left(\alpha_3(\alpha_4-\alpha_1),\frac{\alpha_4+1}{\alpha_4-\alpha_1}\right)$$
$$-\ln\alpha_1 Li_3(\alpha_3\alpha_4)+\ln(\alpha_1+1)Li_3(\alpha_3(\alpha_4+1)). \tag{71}$$

When $\alpha_2-\alpha_1\alpha_3=0$ one must find the limit of the rhs of Eq. (70) for $\alpha_2\to\alpha_1\alpha_3$. We again rewrite the rhs of Eq. (70) in terms of multidimensional integrals. We then replace α_2 by $\alpha_1\alpha_3$ and use the definition (7). We arrive at the result

$$L_+(\alpha_1,\alpha_1\alpha_3,\alpha_3,\alpha_4) = -Li_{2,2}\left(\alpha_3(\alpha_1-\alpha_4),\frac{\alpha_1}{\alpha_1-\alpha_4}\right)+Li_{2,2}\left(\alpha_3(\alpha_1-\alpha_4),\frac{\alpha_1+1}{\alpha_1-\alpha_4}\right)$$
$$+\ln\alpha_1 Li_{2,1}\left(\alpha_3(\alpha_1-\alpha_4),\frac{\alpha_1}{\alpha_1-\alpha_4}\right)-\ln(\alpha_1+1)Li_{2,1}\left(\alpha_3(\alpha_1-\alpha_4),\frac{\alpha_1+1}{\alpha_1-\alpha_4}\right). \tag{72}$$

2. $\alpha_1=0$

Unfortunately in this case one cannot use Eq. (70) for $\alpha_1=0$ because one is immediately faced with the problem of a logarithmic infinity. One must find another algorithm to express the $L_+(0,\alpha_2,\alpha_3,\alpha_4)$ function in terms of multiple polylogarithms. After changing the integration variable $y\to 1-t$ one gets

$$\int_0^1 dy\frac{\ln y}{\alpha_4+y}Li_2(\alpha_2+\alpha_3 y) = \int_0^1 dt\frac{\ln(1-t)}{\alpha_4+1-t}Li_2(\alpha_2+\alpha_3-\alpha_3 t)$$
$$=\int_0^1 dt_1\frac{\ln(1-t_1)}{\alpha_4+1-t_1}\int_{\alpha_2/\alpha_3+1}^{t_1} dt_2\frac{\ln(1-\alpha_2-\alpha_3+\alpha_3 t_2)}{\frac{\alpha_2}{\alpha_3}+1-t_2}$$
$$=\int_0^1 dt_1\frac{\ln(1-t_1)}{\alpha_4+1-t_1}\left\{\int_1^{t_1}+\int_{\alpha_2/\alpha_3+1}^1\right\}dt_2\frac{\ln(1-\alpha_2-\alpha_3+\alpha_3 t_2)}{\frac{\alpha_2}{\alpha_3}+1-t_2}$$
$$=-\int_0^1 dt_2\frac{\ln(1-\alpha_2-\alpha_3+\alpha_3 t_2)}{\frac{\alpha_2}{\alpha_3}+1-t_2}\int_0^{t_2} dt_1\frac{\ln(1-t_1)}{\alpha_4+1-t_1}$$
$$-Li_2(\alpha_2)Li_{1,1}\left(\alpha_4+1,\frac{1}{\alpha_4+1}\right). \tag{73}$$

The last integral is an analog of $I'(t_m)$ in Eq. (22). First one notes that

$$\int_0^{t_2} dt_1\frac{\ln(1-t_1)}{\alpha_4+1-t_1} = -Li_{1,1}\left(\alpha_4+1,\frac{t_1}{\alpha_4+1}\right). \tag{74}$$

Then one considers the following chain of transformations:

$$\int_0^1 \frac{dt_2}{1-\alpha_2-\alpha_3+\alpha_3 t_2}\int_0^{t_2}\frac{dt_1}{\frac{\alpha_2}{\alpha_3}+1-t_1}Li_{1,1}\left(\alpha_4+1,\frac{t_1}{\alpha_4+1}\right)$$
$$=\int_0^1 \frac{dt_1}{\frac{\alpha_2}{\alpha_3}+1-t_1}Li_{1,1}\left(\alpha_4+1,\frac{t_1}{\alpha_4+1}\right)\int_{t_1}^1\frac{dt_2}{1-\alpha_2-\alpha_3+\alpha_3 t_2}$$
$$=\frac{1}{\alpha_3}\ln(1-\alpha_2)\int_0^1\frac{dt_1}{\frac{\alpha_2}{\alpha_3}+1-t_1}Li_{1,1}\left(\alpha_4+1,\frac{t_1}{\alpha_4+1}\right)$$
$$-\frac{1}{\alpha_3}\int_0^1 dt_1\frac{\ln(1-\alpha_2-\alpha_3+\alpha_3 t_1)}{\frac{\alpha_2}{\alpha_3}+1-t_1}Li_{1,1}\left(\alpha_4+1,\frac{t_1}{\alpha_4+1}\right). \tag{75}$$

Using Eq. (74) we see that the last integral is exactly the integral required in Eq. (73). The initial integral of Eq. (75) and the first integral of the rhs of Eq. (75) can be expressed in terms of multiple polylogarithms due to the definition (7). Finally for the $L_+(0,\alpha_2,\alpha_3,\alpha_4)$ function we obtain

$$L_+(0,\alpha_2,\alpha_3,\alpha_4)=Li_{1,1,1,1}\left(\alpha_4+1,\frac{\alpha_2+\alpha_3}{\alpha_3(\alpha_4+1)},\frac{\alpha_2+\alpha_3-1}{\alpha_2+\alpha_3},\frac{\alpha_3}{\alpha_2+\alpha_3-1}\right)$$
$$+\ln(1-\alpha_2)Li_{1,1,1}\left(\alpha_4+1,\frac{\alpha_2+\alpha_3}{\alpha_3(\alpha_4+1)},\frac{\alpha_3}{\alpha_2+\alpha_3}\right)-Li_2(\alpha_2)Li_{1,1}\left(\alpha_4+1,\frac{1}{\alpha_4+1}\right). \tag{76}$$

3. $\alpha_1=0$, $\alpha_4=-1$

For these values of the α_i one uses Eq. (76) to calculate the limit of the rhs for $\alpha_4\to-1$. One arrives at the result

$$L_+(0,\alpha_2,\alpha_3,-1)=-Li_{2,1,1}\left(\frac{\alpha_2+\alpha_3}{\alpha_3},\frac{\alpha_2+\alpha_3-1}{\alpha_2+\alpha_3},\frac{\alpha_3}{\alpha_2+\alpha_3-1}\right)-\ln(1-\alpha_2)Li_{2,1}\left(\frac{\alpha_2+\alpha_3}{\alpha_3},\frac{\alpha_3}{\alpha_2+\alpha_3}\right)$$
$$+Li_2(\alpha_2)\zeta(2). \tag{77}$$

4. $\alpha_1=0$, $\alpha_2+\alpha_3=1$ (and $\alpha_4=-1$)

If one takes a look at Eq. (76) one realizes that there is a problem if $\alpha_2+\alpha_4=1$. To express the L_+ function for this configuration of the α_i the limit of the rhs of (76) for $\alpha_2\to1-\alpha_3$ must be found. The result is

$$L_+(0,1-\alpha_3,\alpha_3,\alpha_4)=-Li_{1,1,2}\left(\alpha_4+1,\frac{1}{\alpha_3(\alpha_4+1)},\alpha_3\right)+\ln\alpha_3 Li_{1,1,1}\left(\alpha_4+1,\frac{1}{\alpha_3(\alpha_4+1)},\alpha_3\right)$$
$$-Li_2(1-\alpha_3)Li_{1,1}\left(\alpha_4+1,\frac{1}{\alpha_4+1}\right). \tag{78}$$

For the case $\alpha_1=0$, $\alpha_2+\alpha_3=1$, and $\alpha_4=-1$ one must find in addition the limit for $\alpha_4\to-1$. One arrives at the result

$$L_+(0,1-\alpha_3,\alpha_3,-1)=Li_{2,2}\left(\frac{1}{\alpha_3},\alpha_3\right)-\ln\alpha_3 Li_{2,1}\left(\frac{1}{\alpha_3},\alpha_3\right)+\zeta(2)Li_2(1-\alpha_3). \tag{79}$$

5. $\alpha_1=0,\ \alpha_2=-\alpha_3$

To obtain the result for this case one must calculate the limit of the rhs of (76) for $\alpha_3\to-\alpha_2$. After taking the limit one has

$$L_+(0,\alpha_2,-\alpha_2,\alpha_4)=-Li_{1,1,2}\left(\frac{\alpha_2}{\alpha_2-1},-\alpha_4,-\frac{1}{\alpha_4}\right)+\ln(1-\alpha_2)Li_{1,2}\left(-\alpha_4,-\frac{1}{\alpha_4}\right)+Li_2(\alpha_2)Li_2\left(-\frac{1}{\alpha_4}\right). \tag{80}$$

6. $\alpha_1=0,\ \alpha_2=0$

For this case one can directly use Eq. (76),

$$L_+(0,0,\alpha_3,\alpha_4)=Li_{1,1,1,1}\left(\alpha_4+1,\frac{1}{\alpha_4+1},\frac{\alpha_3-1}{\alpha_3},\frac{\alpha_3}{\alpha_3-1}\right). \tag{81}$$

But there is also another very simple possibility. We first change the integration variable $y\to t/\alpha_3$,

$$\begin{aligned}\int_0^1 \mathrm{d}y\frac{\ln y}{\alpha_4+y}Li_2(\alpha_3 y)&=\int_0^{\alpha_3}\mathrm{d}t\frac{\ln(t/\alpha_3)}{\alpha_3\alpha_4+t}Li_2(t)\\&=\int_0^{\alpha_3}\frac{\mathrm{d}t_1}{\alpha_3\alpha_4+t_1}Li_2(t_1)\int_{\alpha_3}^{t_1}\frac{\mathrm{d}t_2}{t_2}\\&=-\int_0^{\alpha_3}\frac{\mathrm{d}t_2}{t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{\alpha_3\alpha_4+t_1}Li_2(t_1)\\&=\int_0^{\alpha_3}\frac{\mathrm{d}t_2}{t_2}\int_0^{t_2}\frac{\mathrm{d}t_1}{-\alpha_3\alpha_4+t_1}\int_0^{t_1}\frac{\mathrm{d}t_3}{t_3}\int_0^{t_3}\frac{\mathrm{d}t_4}{1-t_4}.\end{aligned} \tag{82}$$

Now using the definition (7) we obtain the result

$$L_+(0,0,\alpha_3,\alpha_4)=Li_{2,2}\left(-\alpha_3\alpha_4,\frac{-1}{\alpha_4}\right). \tag{83}$$

The reader has a free choice to use either formula (83) or (85). Both equations contain multiple polylogarithms of weight four. The depth of the multiple polylogarithm in Eq. (83) is two against four in Eq. (81). For $\alpha_4=-1$ Eq. (83) can be directly used. However, in the case of Eq. (81) one must first calculate the limit for $\alpha_4\to-1$.

7. $\alpha_1=0,\ \alpha_2=1$

Unfortunately, in this case one cannot use Eq. (76) because of the term $\ln(1-\alpha_2)$. To express this L_+ function in terms of multiple polylogarithms we first make use of a standard relation between dilogs with arguments x and $1-x$ for the function Li_2 under the sign of the integral:

$$\int_0^1 \mathrm{d}y \frac{\ln y}{\alpha_4+y} Li_2(1+\alpha_3 y) = \int_0^1 \mathrm{d}y \frac{\ln y}{\alpha_4+y}[\zeta(2) - \ln(-\alpha_3 y)\ln(1+\alpha_3 y) - Li_2(-\alpha_3 y)]$$
$$= \zeta(2)\int_0^1 \mathrm{d}y \frac{\ln y}{\alpha_4+y} - \int_0^1 \mathrm{d}y \frac{\ln y}{\alpha_4+y} Li_2(-\alpha_3 y)$$
$$- \int_0^1 \mathrm{d}y \frac{\ln y[\ln(-\alpha_3)+\ln y]\ln(1+\alpha_3 y)}{\alpha_4+y}$$
$$= \zeta(2) Li_2\left(-\frac{1}{\alpha_4}\right) - Li_{1,1,1,1}\left(\alpha_4+1, \frac{1}{\alpha_4+1}, \frac{\alpha_3+1}{\alpha_3}, \frac{\alpha_3}{\alpha_3+1}\right)$$
$$- \ln(-\alpha_3)\int_0^1 \mathrm{d}y \frac{\ln y \ln(1+\alpha_3 y)}{\alpha_4+y} - \int_0^1 \mathrm{d}y \frac{\ln^2 y \ln(1+\alpha_3 y)}{\alpha_4+y}, \tag{84}$$

where the $Li_{1,1,1,1}$ function was obtained with the help of Eq. (81). To obtain the last integral in Eq. (84) one proceeds as follows:

$$\int_0^1 \mathrm{d}y \frac{\ln^2 y \ln(1+\alpha_3 y)}{\alpha_4+y} \overset{y\to 1-t}{=} \int_0^1 \mathrm{d}t \frac{\ln^2(1-t)\ln(1+\alpha_3-\alpha_3 t)}{\alpha_4+1-t}$$
$$= \int_0^1 \mathrm{d}t_1 \frac{\ln^2(1-t_1)}{\alpha_4+1-t_1}\int_1^{t_1} \frac{-\alpha_3 \mathrm{d}t_2}{1+\alpha_3-\alpha_3 t_2}$$
$$= \int_0^1 \frac{\mathrm{d}t_2}{\frac{1}{\alpha_3}+1-t_2}\int_0^{t_2} \mathrm{d}t_1 \frac{\ln^2(1-t_1)}{\alpha_4+1-t_1}$$
$$= 2\int_0^1 \frac{\mathrm{d}t_2}{\frac{1}{\alpha_3}+1-t_2}\int_0^{t_2} \frac{\mathrm{d}t_1}{\alpha_4+1-t_1}\int_0^{t_1} \frac{\mathrm{d}t_3}{1-t_3}\int_0^{t_3} \frac{\mathrm{d}t_4}{1-t_4}$$
$$= 2Li_{1,1,1,1}\left(1, \alpha_4+1, \frac{\alpha_3+1}{\alpha_3(\alpha_4+1)}, \frac{\alpha_3}{\alpha_3+1}\right). \tag{85}$$

Similarly one can evaluate the remaining integral

$$\int_0^1 \mathrm{d}y \frac{\ln y \ln(1+\alpha_3 y)}{\alpha_4+y} = -Li_{1,1,1}\left(\alpha_4+1, \frac{\alpha_3+1}{\alpha_3(\alpha_4+1)}, \frac{\alpha_3}{\alpha_3+1}\right). \tag{86}$$

Now combining Eqs. (84)–(86) one arrives at the result

$$L_+(0,1,\alpha_3,\alpha_4) = -2Li_{1,1,1,1}\left(1, \alpha_4+1, \frac{\alpha_3+1}{\alpha_3(\alpha_4+1)}, \frac{\alpha_3}{\alpha_3+1}\right)$$
$$- Li_{1,1,1,1}\left(\alpha_4+1, \frac{1}{\alpha_4+1}, \frac{\alpha_3+1}{\alpha_3}, \frac{\alpha_3}{\alpha_3+1}\right)$$
$$+ \ln(-\alpha_3) Li_{1,1,1}\left(\alpha_4+1, \frac{\alpha_3+1}{\alpha_3(\alpha_4+1)}, \frac{\alpha_3}{\alpha_3+1}\right) + \zeta(2) Li_2\left(-\frac{1}{\alpha_4}\right). \tag{87}$$

8. $\alpha_1=0$, $\alpha_2=-\alpha_3=1$

For these values of the α_i we must find the limit of the rhs of Eq. (87) for $\alpha_3\to-1$. After taking the limit we obtain

$$L_+(0,1,-1,\alpha_4)=Li_{1,1,2}\left(\alpha_4+1,\frac{1}{\alpha_4+1},1\right)+2Li_{1,1,2}\left(1,\alpha_4+1,\frac{1}{\alpha_4+1}\right)+\zeta(2)Li_2\left(-\frac{1}{\alpha_4}\right). \tag{88}$$

VI. CONCLUSIONS

We have presented all the necessary relations to transform the L functions [as defined in Eqs. (1) and (2)] that occur in our $\mathcal{O}(\varepsilon^2)$ results[1] for the Laurent series expansion of massive scalar one-loop integrals to multiple polylogarithms. We have used these relations to transform our results on massive one-loop integrals involving L functions to corresponding results involving multiple polylogarithms. The multiple polylogarithms results are readily available in electronic form.[11]

Despite of the fact that the relations between the L functions and the multiple polylogarithms have been derived having the massive scalar one-loop integrals in mind they can also be used in a more general setting. In fact, any definite integral given by

$$\int_A^B \frac{\ln(a_1+b_1x)\ln(a_2+b_2x)\ln(a_3+b_3x)\mathrm{d}x}{a_4+b_4x} \quad \text{or} \quad \int_A^B \frac{\ln(a_1+b_1x)Li_2(a_2+b_2x)\mathrm{d}x}{a_3+b_3x}$$

can be written in terms of multiple polylogarithms with the help of the relations presented in this paper. It is worthwhile to mention that all the equations presented in the present paper have been also checked numerically.

We have found several examples where the representation of the L functions in terms of multiple polylogarithms is not unique. This reflects the fact that multiple polylogarithms obey quasishuffle and shuffle Hopf algebras and hence satisfy numerous identities as is the case for the classical polylogarithms. More information about identities between multiple polylogarithms can be found, e.g., in Refs. 5 and 9 and references therein.

For future parton model applications of our results numerical efficiency is an important issue. We are presently writing numerical $C++$ codes to compare the numerical efficiency of the two representations in terms of L functions and multiple polylogarithms.

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APPENDIX

In this Appendix we consider as an example the real part of the $\mathcal{O}(\varepsilon^2)$ coefficient $\mathrm{Re}\,D_1^{(2)}$ of the Laurent series expansion of the massive box D_1 with three massive propagators. Using the rules written down in the main text of this paper we have expressed the corresponding results of Ref. 1 involving L functions in terms of multiple polylogarithms. The L function structure of $\mathrm{Re}\,D_1^{(2)}$ in Ref. 1 is sufficiently rich to provide an illustration of the corresponding complexity in terms of multiple polylogarithms when transforming to the latter representation. We mention that all multiple polylogarithms up to weight three have been reexpressed in terms of classical polylogarithms. We then used automatic program codes to simplify the classical polylogarithms as much as possible, as was also done in Ref. 1.

We use the notation and the conventions of Ref. 1. In brief, we use the Mandelstam-type variables

$$s \equiv (p_1+p_2)^2, \quad t \equiv T-m^2 \equiv (p_1-p_3)^2-m^2, \quad u \equiv U-m^2 \equiv (p_2-p_3)^2-m^2 \tag{A1}$$

for the $2\to 2$ partonic process $a(p_1)+b(p_2)\to Q(p_3)+\overline{Q}(p_4)$ with $p_1^2=p_2^2=0$ and $p_3^2=p_4^2=m^2$. We also introduce the abbreviations ($\beta=\sqrt{1-4m^2/s}$)

$$z_3 \equiv (s+2t+s\beta)/2, \quad z_4 \equiv (s+2t-s\beta)/2,$$

$$z_5 \equiv (2m^2+t+t\beta)/2, \quad z_6 \equiv (2m^2+t-t\beta)/2,$$

$$l_s \equiv \ln\frac{s}{m^2}, \quad l_t \equiv \ln\frac{-t}{m^2}, \quad l_T \equiv \ln\frac{-T}{m^2}, \quad l_x \equiv \ln x,$$

$$l_\beta \equiv \ln\beta, \quad l_{z3} \equiv \ln\frac{z_3}{m^2}, \quad l_{z4} \equiv \ln\frac{-z_4}{m^2}. \tag{A2}$$

One finds

$$\begin{aligned}
\mathrm{Re}\, D_1^{(2)} = \frac{1}{st\beta}\Bigg[\frac{1}{192}\{&-109l_s^4+240l_t^4+32l_T^3l_x+264l_T^2l_x^2-200l_Tl_x^3-177l_x^4-96l_T^2l_xl_{z3}+192l_Tl_x^2l_{z3}\\
&+12l_x^3l_{z3}+96l_Tl_xl_{z3}^2-32l_xl_{z3}^3-480l_T^2l_xl_{z4}+24l_Tl_x^2l_{z4}+180l_x^3l_{z4}-144l_x^2l_{z3}l_{z4}\\
&+480l_Tl_xl_{z4}^2-336l_x^2l_{z4}^2-96l_xl_{z3}l_{z4}^2+320l_xl_{z4}^3-168l_{z4}^4+480l_T^2l_xl_\beta-480l_Tl_x^2l_\beta-40l_x^3l_\beta\\
&-192l_Tl_xl_{z3}l_\beta+336l_x^2l_{z3}l_\beta+96l_xl_{z3}^2l_\beta-384l_Tl_xl_{z4}l_\beta+336l_x^2l_{z4}l_\beta+192l_xl_{z3}l_{z4}l_\beta\\
&+96l_xl_{z4}^2l_\beta+192l_{z4}^3l_\beta+96l_Tl_xl_\beta^2+24l_x^2l_\beta^2-96l_xl_{z3}l_\beta^2-96l_{z4}^2l_\beta^2+32l_xl_\beta^3+32l_\beta^4\\
&-32l_t^3(9l_T+20l_x+25l_{z3}+l_{z4}+13l_\beta)-4l_s^3(8l_T-36l_x-9l_{z3}-43l_{z4}+94l_\beta)\\
&-6l_s^2(52l_t^2-28l_T^2+15l_x^2+26l_xl_{z3}+46l_xl_{z4}+24l_{z3}l_{z4}+32l_{z4}^2-4l_T(9l_x+8l_{z3}-15l_{z4}\\
&-4l_\beta)-60l_xl_\beta-24l_{z3}l_\beta-56l_{z4}l_\beta+76l_\beta^2+l_t(-44l_T+60l_x-8l_{z3}-60l_{z4}+8l_\beta))\\
&-24l_t^2(4l_T^2+15l_x^2-8l_T(2l_x+2l_{z3}+4l_{z4}-3l_\beta)+4l_x(3l_{z3}-8l_{z4}+13l_\beta)+2(-4l_{z3}^2\\
&+l_{z4}^2+12l_{z3}l_{z4}-12l_{z3}l_\beta-8l_{z4}l_\beta+10l_\beta^2))+8l_t(8l_T^3-31l_x^3+l_x^2(-6l_{z3}+33l_{z4}+6l_\beta)\\
&+6l_x(3l_{z3}^2-22l_{z4}^2-2l_{z3}(5l_{z4}-9l_\beta)+20l_{z4}l_\beta-10l_\beta^2)+4(-2l_{z3}^3+6l_{z3}^2l_{z4}+16l_{z4}^3\\
&+9l_{z3}(l_{z4}-l_\beta)^2-18l_{z4}^2l_\beta+9l_{z4}l_\beta^2+2l_\beta^3)+6l_T^2(3l_x-4l_{z3}+4l_{z4}-4l_\beta)-3l_T(5l_x^2\\
&-4l_x(5l_{z3}-4l_{z4})-8(l_{z3}^2-2l_{z3}l_{z4}-3l_{z4}^2+4l_{z4}l_\beta+l_\beta^2)))-4l_s(80l_t^3+8l_T^3+18l_x^3\\
&-27l_x^2l_{z3}-8l_{z3}^3-165l_x^2l_{z4}-72l_xl_{z3}l_{z4}+48l_xl_{z4}^2-24l_{z3}l_{z4}^2-64l_{z4}^3+18l_x^2l_\beta+120l_xl_{z3}l_\beta\\
&+24l_{z3}^2l_\beta+72l_xl_{z4}l_\beta+48l_{z3}l_{z4}l_\beta+72l_{z4}^2l_\beta-84l_xl_\beta^2-24l_{z3}l_\beta^2-48l_{z4}l_\beta^2+40l_\beta^3\\
&-12l_T^2(13l_x+2l_{z3}-6l_{z4}+6l_\beta)+12l_t^2(8l_T+5l_x-26l_{z3}-10l_{z4}+12l_\beta)-12l_t(5l_T^2\\
&+6l_x^2-7l_{z3}^2-10l_{z3}l_{z4}-16l_{z4}^2+l_x(14l_{z3}+27l_{z4}-4l_\beta)+10l_{z3}l_\beta+16l_{z4}l_\beta+2l_\beta^2\\
&+l_T(-5l_x-2l_{z3}+4l_{z4}+8l_\beta))+12l_T(11l_x^2+l_x(8l_{z3}+7l_{z4}-4l_\beta)+2l_{z3}^2-6l_{z4}^2-4l_{z3}l_\beta\\
&+8l_{z4}l_\beta+2l_\beta^2))\}
\end{aligned}$$

$$+ (3l_s^2/4 - 7l_t^2/2 + l_T l_x + 3l_x^2/4 + 5l_x l_{z3} + 5l_x l_{z4} + l_{z4}^2/2 + l_t(2l_T - l_x + 10l_{z3} + 2l_{z4} - 15l_\beta) - 8l_x l_\beta$$
$$+ 2l_{z4} l_\beta - 11l_\beta^2 - l_s(7l_t + l_T + 8l_x + 5l_{z3} + l_{z4} + 6l_\beta))\zeta(2) + (-3l_s + 2l_x)\zeta(3) - 35\zeta(4)/4$$
$$- 2Li_2^2\left(\frac{m^2}{z_5}\right) + 2Li_2^2\left(\frac{-t(1-\beta)}{2m^2}\right) + \frac{1}{8}Li_2\left(\frac{m^2}{z_5}\right)(-11l_s^2 - 4l_t^2 + 25l_x^2 + 8l_x l_{z4} - 24l_{z4}^2 + l_s(4l_t$$
$$+ 26l_x + 24l_{z4} - 8l_\beta) + 24l_x l_\beta + 16l_{z4} l_\beta - 8l_\beta^2 - 4l_t(9l_x - 4l_{z4} + 4l_\beta)) + Li_2\left(\frac{m^2 x}{-T}\right)(11l_s^2/8 - l_t^2$$
$$+ 2l_t(l_x + l_{z4} - 2l_\beta) + l_s(-l_t + 7l_x/4 - l_{z4} + 2l_\beta) + l_x(19l_x - 24l_{z4} + 16l_\beta)/8) + \frac{1}{8}Li_2(-x)(-15l_s^2$$
$$+ 4l_t^2 + l_x(-39l_x + 32l_{z4} - 16l_\beta) + 2l_s(10l_t + 5l_x - 8l_\beta) + l_t(-44l_x + 32l_\beta)) + Li_2\left(\frac{z_3}{z_4}\right)$$
$$\times\left(-2Li_2\left(\frac{m^2}{z_5}\right) + \frac{1}{4}(-5l_s^2 + 20l_t^2 - 7l_x^2 - 4l_x l_{z3} + 12l_x l_{z4} - 4l_{z4}^2 + l_s(-2l_t + 4(2l_x + l_{z3} + l_{z4}\right.$$
$$\left. - l_\beta)) - 4l_x l_\beta + l_t(-22l_x - 8l_{z3} + 8l_\beta) - 8\zeta(2))\right) + Li_2(x)\left(2Li_2\left(\frac{m^2}{z_5}\right) + 2Li_2\left(\frac{-t(1-\beta)}{2m^2}\right)\right.$$
$$- 7l_s^2/4 - 3l_t^2/2 - 11l_x^2/4 + l_x l_{z3} + 3l_x l_{z4} + l_{z4}^2 - 2l_x l_\beta + l_t(-4l_x + 2l_{z3} + 4l_\beta) + l_s(4l_t + l_x/2 - l_{z3}$$
$$\left. - l_{z4} - 2l_\beta) - 6\zeta(2)\right) + Li_2\left(\frac{T}{m^2}\right)\left(-4Li_2(x) - 4Li_2\left(\frac{z_3}{z_4}\right) - 4Li_2\left(\frac{m^2}{z_5}\right) + 4Li_2\left(\frac{-t(1-\beta)}{2m^2}\right) + l_s^2/8\right.$$
$$- 3l_t^2/2 + l_x^2/8 + 2l_x l_{z3} - 4l_{z4}^2 + l_t(3l_x/2 + 4l_{z3} + 4l_{z4} - 4l_\beta) - 2l_x l_\beta + 4l_{z4} l_\beta - 2l_\beta^2 - \frac{l_s}{4}(18l_t + 7l_x$$
$$\left. + 8l_{z3} - 16l_{z4} + 8l_\beta) - 4\zeta(2)\right)$$

$$+ Li_2\left(\frac{T}{z_3}\right)\left(-\frac{l_s^2}{8} - 2l_t^2 + l_s\left(\frac{9}{4}l_x - l_{z4}\right) - 2l_t(l_x - l_{z4}) - l_x\left(\frac{17}{8}l_x - l_{z4}\right)\right) + Li_2\left(\frac{-t(1-\beta)}{2m^2}\right)\left(-2Li_2\left(\frac{z_3}{z_4}\right)\right.$$
$$- 7l_t^2 - l_x^2/2 + 2l_x l_{z3} - l_x l_{z4} - l_{z4}^2 + l_s(l_t + 3l_x/2 - 2l_{z3} + l_{z4} - l_\beta) + 3l_x l_\beta + 2l_{z4} l_\beta - l_\beta^2 - l_t(l_x - 4l_{z3} - 2l_{z4}$$
$$\left. + 2l_\beta) + 12\zeta(2)\right) + Li_3\left(\frac{-1+\beta}{2\beta}\right)(4l_s - 7l_t) + 5Li_3\left(\frac{z_5}{t\beta}\right)l_t + Li_3\left(\frac{m^2}{z_5}\right)(5l_s - 6l_t - 11l_x)/2 - Li_3\left(\frac{z_3}{t}\right)$$
$$\times(4l_t + 6l_x) + Li_3\left(\frac{z_6}{m^2}\right)(3l_s/2 - 5l_t - 7l_x/2) + 4Li_3\left(\frac{z_4}{t}\right)(l_s - l_t - 2l_x) + Li_3\left(-\frac{m^2 x z_3}{sT\beta}\right)(l_s - 2l_t - l_x)$$
$$+ Li_3\left(\frac{-x^2}{1-x^2}\right)(l_s - l_t - l_x) + Li_3\left(\frac{z_3}{s\beta}\right)(l_s + 5l_t - l_x) + 2Li_3\left(\frac{m^2}{-t}\right)l_x + Li_3\left(\frac{z_5}{T}\right)\left(-\frac{5}{2}l_s - 3l_t - \frac{5}{2}l_x + 4l_{z4}\right.$$
$$\left. - 4l_\beta\right) + Li_3\left(\frac{-t(1-\beta)}{2z_5}\right)\left(-\frac{5}{2}l_s - l_t - \frac{3}{2}l_x + 4l_{z4} - 4l_\beta\right) + Li_3\left(\frac{-2z_6}{t(1+\beta)}\right)\left(-\frac{3}{2}l_s - 2l_t + 2l_{z4} - \frac{l_x}{2}\right.$$
$$\left. - 2l_\beta\right) + Li_3\left(\frac{z_3}{z_4}\right)\left(\frac{l_s}{2} - l_t - \frac{l_x}{2} + 2l_{z4} - 2l_\beta\right) + 2Li_3(-x)(3l_s + 2l_t + 2l_x - 4l_{z4} + 4l_\beta) + Li_3\left(\frac{z_6}{z_5}\right)\left(\frac{l_s}{2}\right.$$
$$\left. + 4l_t - \frac{l_x}{2} - 2l_{z4} + 2l_\beta\right)$$

$$+ Li_3\left(\frac{2z_6}{m^2(1+\beta)}\right)\left(\frac{3}{2}l_s + 2l_t + \frac{l_x}{2} - 2l_{z4} + 2l_\beta\right) + Li_3\left(\frac{z_4}{T}\right)(3l_s + 3l_t + 3l_x - 4l_{z4} + 4l_\beta)$$
$$+ Li_3\left(\frac{T}{z_3}\right)\left(\frac{l_s}{2} + l_t + \frac{7}{2}l_x - 2l_{z4} + 2l_\beta\right) + Li_3\left(\frac{m^2(1-\beta)}{2z_5}\right)\left(\frac{3}{2}l_s + 3l_t + \frac{5}{2}l_x - 4l_{z4} + 4l_\beta\right)$$
$$+ Li_3(x)\left(\frac{15}{2}l_s - 2l_t + \frac{5}{2}l_x - 6l_{z4} + 6l_\beta\right) + Li_3\left(\frac{T}{z_6}\right)(-2l_s + l_t - 2l_x + 2l_{z4} - 2l_\beta) + 2Li_4(x)$$
$$- 4Li_4\left(\frac{z_3}{t}\right) + 4Li_4\left(\frac{z_4}{t}\right) - Li_4\left(\frac{z_4}{T}\right) - Li_4\left(\frac{Tz_4}{D}\right) + Li_4\left(\frac{z_5}{T}\right) + 2Li_4\left(\frac{s(1-\beta)}{-2t}\right) + 3Li_4\left(\frac{s(1-\beta)}{2z_4}\right)$$
$$+ Li_4\left(\frac{T}{z_6}\right) + 4Li_4\left(\frac{-1+\beta}{2\beta}\right) + 2Li_4\left(\frac{-2t}{s(1+\beta)}\right) + 4Li_4\left(\frac{2\beta}{1+\beta}\right) + 3Li_4\left(\frac{2z_3}{s(1+\beta)}\right)$$
$$+ 2Li_{3,1}\left(-\frac{m^2xz_3}{sT\beta}, \frac{-T}{m^2x}\right) - 2Li_{3,1}\left(-\frac{m^2xz_3}{sT\beta}, \frac{2T}{t(1-\beta)}\right) - 6Li_{1,2,1}\left(1, \frac{s(1-\beta)}{2z_4}, \frac{z_5}{m^2}\right)$$
$$+ 6Li_{1,2,1}\left(1, \frac{s(1+\beta)}{2z_3}, \frac{z_6}{m^2}\right) - 2Li_{2,1,1}\left(1, \frac{z_4}{z_3}, \frac{z_3}{t}\right) - 2Li_{2,1,1}\left(\frac{m^2}{T}, \frac{T}{z_5}, \frac{z_5}{m^2}\right) + 2Li_{2,1,1}\left(\frac{m^2}{T}, \frac{T}{z_6}, \frac{z_6}{m^2}\right)$$
$$- 2Li_{2,1,1}\left(\frac{z_3}{z_4}, \frac{z_4}{z_3}, \frac{z_3}{t}\right) - 2Li_{2,1,1}\left(\frac{m^2}{z_5}, 1, \frac{z_5}{m^2}\right) - 2Li_{2,1,1}\left(\frac{m^2}{z_5}, \frac{z_5}{T}, \frac{T}{m^2}\right) + 2Li_{2,1,1}\left(\frac{s(1-\beta)}{2z_4}, \frac{z_5}{z_6}, \frac{z_6}{m^2}\right)$$
$$+ 2Li_{2,1,1}\left(-\frac{m^2xz_3}{sT\beta}, -\frac{sT\beta}{m^2xz_3}, \frac{z_3}{s\beta}\right) - 2Li_{2,1,1}\left(-\frac{m^2xz_3}{sT\beta}, -\frac{sT\beta}{m^2xz_3}, -\frac{z_6}{t\beta}\right)$$
$$+ 2Li_{2,1,1}\left(\frac{s(1+\beta)}{2z_3}, 1, \frac{z_6}{m^2}\right) + 2Li_{2,1,1}\left(\frac{s(1+\beta)}{2z_3}, \frac{z_6}{T}, \frac{T}{m^2}\right) - 2Li_{2,1,1}\left(\frac{s(1+\beta)}{2z_3}, \frac{z_6}{z_5}, \frac{z_5}{m^2}\right)$$
$$+ Li_{1,1,1,1}\left(1, \frac{T}{z_6}, \frac{z_6}{z_5}, \frac{z_5}{m^2}\right) - Li_{1,1,1,1}\left(1, \frac{s(1-\beta)}{2z_4}, \frac{z_5}{T}, \frac{T}{m^2}\right) + 3Li_{1,1,1,1}\left(1, \frac{s(1-\beta)}{2z_4}, \frac{z_5}{z_6}, \frac{z_6}{m^2}\right)$$
$$+ Li_{1,1,1,1}\left(1, \frac{s(1+\beta)}{2z_3}, \frac{z_6}{T}, \frac{T}{m^2}\right) - 3Li_{1,1,1,1}\left(1, \frac{s(1+\beta)}{2z_3}, \frac{z_6}{z_5}, \frac{z_5}{m^2}\right) - 2Li_{1,1,1,1}\left(\frac{t}{T}, 1, \frac{T}{z_3}, \frac{z_3}{t}\right)$$
$$+ 2Li_{1,1,1,1}\left(\frac{t}{T}, 1, \frac{T}{z_4}, \frac{z_4}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_3}, 1, \frac{z_3}{t}\right)$$

$$- 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_3}, \frac{z_3}{T}, \frac{T}{t}\right) - 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_3}, \frac{z_3}{z_4}, \frac{z_4}{t}\right) - 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_4}, 1, \frac{z_4}{t}\right)$$
$$+ 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_4}, \frac{z_4}{T}, \frac{T}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{T}, \frac{T}{z_4}, \frac{z_4}{z_3}, \frac{z_3}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{z_3}, 1, \frac{z_3}{T}, \frac{T}{t}\right)$$
$$- 2Li_{1,1,1,1}\left(\frac{t}{z_3}, \frac{z_3}{T}, 1, \frac{T}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{z_3}, \frac{z_3}{T}, \frac{T}{z_3}, \frac{z_3}{t}\right) - 2Li_{1,1,1,1}\left(\frac{t}{z_3}, \frac{z_3}{T}, \frac{T}{z_4}, \frac{z_4}{t}\right)$$
$$- 2Li_{1,1,1,1}\left(\frac{t}{z_3}, \frac{z_3}{z_4}, \frac{z_4}{T}, \frac{T}{t}\right) - 2Li_{1,1,1,1}\left(\frac{t}{z_4}, 1, \frac{z_4}{T}, \frac{T}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{z_4}, \frac{z_4}{T}, 1, \frac{T}{t}\right)$$
$$+ 2Li_{1,1,1,1}\left(\frac{t}{z_4}, \frac{z_4}{T}, \frac{T}{z_3}, \frac{z_3}{t}\right) - 2Li_{1,1,1,1}\left(\frac{t}{z_4}, \frac{z_4}{T}, \frac{T}{z_4}, \frac{z_4}{t}\right) + 2Li_{1,1,1,1}\left(\frac{t}{z_4}, \frac{z_4}{z_3}, \frac{z_3}{T}, \frac{T}{t}\right)$$
$$- 2Li_{1,1,1,1}\left(\frac{T}{z_4}, \frac{z_4}{z_3}, 1, \frac{z_3}{t}\right) + Li_{1,1,1,1}\left(\frac{z_4}{T}, \frac{T}{z_3}, 1, \frac{z_3}{t}\right) - Li_{1,1,1,1}\left(\frac{m^2}{z_5}, 1, \frac{z_5}{T}, \frac{T}{m^2}\right)$$

$$
\begin{aligned}
&+ Li_{1,1,1,1}\left(\frac{m^2}{z_5},\frac{z_5}{T},1,\frac{T}{m^2}\right) - Li_{1,1,1,1}\left(\frac{m^2}{z_5},\frac{z_5}{T},\frac{T}{z_5},\frac{z_5}{m^2}\right) - Li_{1,1,1,1}\left(\frac{m^2}{z_6},\frac{z_6}{T},1,\frac{T}{m^2}\right)\\
&- Li_{1,1,1,1}\left(\frac{m^2}{z_6},\frac{z_6}{T},\frac{T}{z_5},\frac{z_5}{m^2}\right) - Li_{1,1,1,1}\left(\frac{m^2}{z_6},\frac{z_6}{z_5},1,\frac{z_5}{m^2}\right) - Li_{1,1,1,1}\left(\frac{m^2}{z_6},\frac{z_6}{z_5},\frac{z_5}{T},\frac{T}{m^2}\right)\\
&- Li_{1,1,1,1}\left(\frac{z_6}{T},\frac{T}{z_5},1,\frac{z_5}{m^2}\right) + Li_{1,1,1,1}\left(\frac{z_6}{z_5},\frac{z_5}{T},1,\frac{T}{m^2}\right) - 3Li_{1,1,1,1}\left(\frac{s(1-\beta)}{2z_4},1,\frac{z_5}{z_6},\frac{z_6}{m^2}\right)\\
&+ Li_{1,1,1,1}\left(\frac{s(1-\beta)}{2z_4},\frac{z_5}{T},\frac{T}{z_6},\frac{z_6}{m^2}\right) - 3Li_{1,1,1,1}\left(\frac{s(1-\beta)}{2z_4},\frac{z_5}{z_6},1,\frac{z_6}{m^2}\right) + Li_{1,1,1,1}\left(\frac{s(1-\beta)}{2z_4},\frac{z_5}{z_6},\frac{z_6}{T},\frac{T}{m^2}\right)\\
&- 3Li_{1,1,1,1}\left(\frac{s(1-\beta)}{2z_4},\frac{z_5}{z_6},\frac{z_6}{z_5},\frac{z_5}{m^2}\right) + Li_{1,1,1,1}\left(\frac{s(1+\beta)}{2z_3},1,\frac{z_6}{T},\frac{T}{m^2}\right) - Li_{1,1,1,1}\left(\frac{s(1+\beta)}{2z_3},1,\frac{z_6}{z_5},\frac{z_5}{m^2}\right)\\
&+ Li_{1,1,1,1}\left(\frac{s(1+\beta)}{2z_3},\frac{z_6}{T},\frac{T}{z_6},\frac{z_6}{m^2}\right) - Li_{1,1,1,1}\left(\frac{s(1+\beta)}{2z_3},\frac{z_6}{z_5},\frac{z_5}{z_6},\frac{z_6}{m^2}\right) - i\pi(l_s-2l_t-l_x)\left(\frac{l_s^2}{2}+l_sl_T\right.\\
&\left.+ l_sl_x + \frac{l_x^2}{2} - l_Tl_{z3} + \frac{l_{z3}^2}{2} - l_sl_{z4} + \frac{l_{z4}^2}{2} + l_sl_\beta + l_Tl_\beta + l_xl_\beta - l_{z4}l_\beta + \frac{l_\beta^2}{2} + 2Li_2(-x) + 2Li_2(x)\right.\\
&\left.- Li_2\left(\frac{m^2x}{-T}\right) + Li_2\left(\frac{T}{z_3}\right) + Li_2\left(\frac{z_3}{z_4}\right) + \zeta(2)\right)\Bigg]. \qquad \text{(A3)}
\end{aligned}
$$

At the very end of the expression one finds an explicit imaginary part. Since the whole expression must be real this clearly indicates that the same imaginary contribution with opposite sign must be contained in multiple polylogarithms, e.g., some of them are sitting on branch cuts. This is in fact true for the multiple polylogarithms

$$
Li_{3,1}\left(-\frac{m^2xz_3}{sT\beta},\frac{-T}{m^2x}\right),\quad Li_{3,1}\left(-\frac{m^2xz_3}{sT\beta},\frac{2T}{t(1-\beta)}\right),
$$

$$
Li_{2,1,1}\left(-\frac{m^2xz_3}{sT\beta},-\frac{sT\beta}{m^2xz_3},\frac{z_3}{s\beta}\right),\quad Li_{2,1,1}\left(-\frac{m^2xz_3}{sT\beta},-\frac{sT\beta}{m^2xz_3},-\frac{z_6}{t\beta}\right).
$$

Indeed, one finds that the imaginary contributions cancel out when one numerically evaluates the result.

As regards the length the representations of $\mathrm{Re}\, D_1^{(2)}$ in terms of L functions in Ref. 1 and in terms of multiple polylogarithms are of similar size. The representation in terms of L functions contains 43 different L function expressions against 59 different multiple polylogarithm expressions.

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A Michelson interferometer in the field of a plane gravitational wave

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We treat the problem of a Michelson interferometer in the field of a plane gravitational wave in the framework of general relativity. The arms of the interferometer are regarded as the world lines of the light beams, whose motion is determined by the Hamilton-Jacobi equation for a massless particle. In the case of a weak monochromatic wave we find that the formula for the delay of a light beam agrees with the result obtained by solving the linearized coupled Einstein-Maxwell equations. We also calculate this delay in the next (quadratic) approximation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2212670]

I. INTRODUCTION

The subject of this work is to investigate the behavior of a Michelson interferometer in the presence of a plane gravitational wave. Sources of gravitational waves include the collapse of massive stars in supernova explosions, and the coalescence of stars in binary systems containing a neutron star and/or a black hole. The large distances from these objects allow us to assume that the gravitational waves detected on the Earth may be regarded as plane waves.

Gravitational waves were predicted by Einstein in his general theory of relativity[1,2] as perturbations of the space-time metric that propagate at the speed of light. Plane gravitational waves were considered first by Rosen,[3] Taub,[4] and McVittie,[5] and their work seemed to indicate that such waves may not physically exist. However, Bondi, Pirani, and Robinson[6–8] proved that this conclusion was wrong, and that these waves not only exist but also carry energy. Exact solutions of the Einstein equations, which describe plane gravitational waves, have also been developed in Refs. 9 and 10. In 1975, Hulse and Taylor[11] found indirect proof for the existence of gravitational waves by observing the pulsar PSR 1913+16. They noticed that the orbital parameters of this pulsar were changing according to a model assuming that such a system radiates gravitational waves.[12,13] This discovery was awarded with the Nobel Prize in physics in 1993.

Research on the possibility of detecting gravitational waves was started in the 1960s by Weber,[14] who constructed the first resonant-mass antenna. His results claiming the discovery of gravitational waves[15] could not be confirmed by other groups who built similar detectors. In the 1970s, another method of detection was suggested using laser interferometry.[16–19] Current and planned ground-based laser interferometric detectors include AIGO (Australia),[20] GEO 600 (Germany/UK),[21] LIGO (USA),[22] TAMA 300 (Japan),[23] and VIRGO (France/Italy).[24] The first search for signals from neutron stars in LIGO and GEO 600 data did not find direct evidence for gravitational waves,[25] but gave upper limits on the strength of periodic gravitational radiation.[26] In 2011, ESA and NASA plan to launch LISA,[27] a space project that will be able to make observations in a low-frequency band that is not achievable by ground-based observatories. A bibliography on gravitational-wave theory and experiment through 1999 is listed in Ref. 28.

Since the search for gravitational waves is mainly based on interferometry, we consider a Michelson interferometer in the presence of a plane gravitational wave. The effect of such a wave

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on a light beam, using the linearized coupled Einstein-Maxwell equations, was studied in Refs. 29 and 30. However, these equations in the quadratic approximation may lead to quite lengthy expressions. Instead, we can treat the light beam as photons whose motion is determined by the geodesic equations for a massless particle.

The equations of motion for a particle in the metric of a strong gravitational wave[13] were derived by Ebner,[31] and all seven integrals of motion can be found in the literature, e.g., Ref. 32. A simple model of a Michelson interferometer in the field of such a wave, based on the above equations of motion, was proposed by Bażański.[33] Here, we generalize this model to the second (quadratic) approximation. For simplicity, we consider a monochromatic plane gravitational wave whose direction is parallel to one arm of the interferometer and perpendicular to the other. Since the energy of gravitational waves contains the factor G/c^5, the amplitude for such waves is very small. Therefore, second-order effects in gravitational-wave detection are irrelevant experimentally, although it might be interesting to explore them.

This paper is organized as follows. In Sec. II we introduce a plane gravitational wave and review the equations of motion for a test particle. In Sec. III we study the behavior of a Michelson interferometer under the action of this wave in the first (linear) approximation. In Sec. IV we proceed to the second approximation. The results are summarized in Sec. V. For the metric tensor and the curvature tensor we use the conventions of Ref. 13.

II. MOTION OF A PARTICLE IN THE FIELD OF A PLANE GRAVITATIONAL WAVE

In this section we derive the motion of a test particle in the presence of a plane gravitational wave[31,33] using the relativistic Hamilton-Jacobi equation. Let us consider the metric tensor whose components are functions of only one variable u, $g_{ab}=g_{ab}(u)$. In this case, it can be shown[13] that the space-time interval in vacuum is of the form

$$ds^2 = dudv + g_{ab}(u)dx^a dx^b, \tag{1}$$

where the letters a,b refer to the coordinates 2,3. For a plane wave propagating in the direction of the x axis we have $u=ct-x$ and $v=ct+x$. If the interval is given by Eq. (1), then all components of the Ricci tensor identically vanish except $R_{uu}=-\frac{1}{2}\dot{\kappa}^a_a-\frac{1}{4}\kappa^a_b\kappa^b_a$, where $\kappa_{ab}=\dot{g}_{ab}$, and the dot denotes differentiation with respect to u. Thus, the Einstein field equations in the case of a plane gravitational wave reduce to one equation, $R_{uu}=0$.

The Hamilton-Jacobi equation for a particle with mass m moving in the gravitational field described by the metric in (1) is given by

$$4\frac{\partial S}{\partial u}\frac{\partial S}{\partial v}+g^{ab}\frac{\partial S}{\partial x^a}\frac{\partial S}{\partial x^b}=m^2c^2, \tag{2}$$

where $S=S(u,v,x^a)$ is a principal function. We seek a solution of (2) in the form $S=\tilde{S}(u)+\frac{1}{2}Bv+p_{0a}x^a$, where $B=p_0+p_x=\text{const}$ and $p_{0a}=\text{const}$. For a timelike geodesic line we have $B>0$. We obtain the principal function given by

$$S=\frac{1}{2B}[(m^2c^2u-G^{ab}(u,0)p_{0a}p_{0b})]+\frac{1}{2}Bv+p_{0a}x^a, \tag{3}$$

where we define

$$G^{ab}(p,q)=\int_q^{q+p} g^{ab}(u)du. \tag{4}$$

The components of four-momentum are given by the derivatives of a principal function, $p_i=\partial S/\partial x^i$. The world line of a particle is determined by Jacobi's theorem, $\partial S/\partial\alpha^k=\beta^k$, where α^k are the constants in the principal function (3), and β^k are new constants. Introducing a finite interval s as a parameter such that $mc(dx^a/ds)=g^{ab}(\partial S/\partial x^b)$ yields $u=(B/mc)(s-s_0)+u_0$. The equations of

motion for a massive particle in the field of a plane gravitational wave in terms of s are (in agreement with Ref. 31)

$$ct(s) = ct(s_0) + \frac{1}{2}\left(\frac{B}{mc} + \frac{mc}{B}\right)(s - s_0) - \frac{1}{2B^2}G^{ab}\left(\frac{B}{mc}(s - s_0), ct(s_0) - x(s_0)\right)p_{0a}p_{0b},$$

$$x(s) = x(s_0) + \frac{1}{2}\left(\frac{mc}{B} - \frac{B}{mc}\right)(s - s_0) - \frac{1}{2B^2}G^{ab}\left(\frac{B}{mc}(s - s_0), ct(s_0) - x(s_0)\right)p_{0a}p_{0b},$$

$$x^a(s) = x^a(s_0) + \frac{1}{B}G^{ab}\left(\frac{B}{mc}(s - s_0), ct(s_0) - x(s_0)\right)p_{0b}. \tag{5}$$

In a similar manner, we can determine the equations of null geodesic lines in the presence of a plane gravitational wave. The Hamilton-Jacobi equation in this case is equivalent to the eikonal equation,

$$4\frac{\partial\Psi}{\partial u}\frac{\partial\Psi}{\partial v} + g^{ab}\frac{\partial\Psi}{\partial x^a}\frac{\partial\Psi}{\partial x^b} = 0, \tag{6}$$

and its solution is of the form $\Psi = \tilde{\Psi}(u) + \frac{1}{2}Cv + k_{0a}x^a$, where $C = k_0 + k_x = \text{const}$ and $k_{0a} = \text{const}$. Consequently we find

$$\Psi = -\frac{1}{C}G^{ab}(u,0)k_{0a}k_{0b} + \frac{1}{2}Cv + k_{0a}x^a, \tag{7}$$

with G^{ab} defined in (4). The components of the four-dimensional wave vector are given by the derivatives of the eikonal, $k_i = \partial\Psi/\partial x^i$. A world line for a massless particle is again determined from Jacobi's theorem.

Let us define the affine parameter π such that $dx^a/d\pi = g^{ab}(\partial\Psi/\partial x^b)$ from which we find $u = C(\pi - \pi_0) + u_0$. As a result, we obtain the null geodesic lines:

$$ct(\pi) = ct(\pi_0) + \frac{1}{2}C(\pi - \pi_0) - \frac{1}{2C^2}G^{ab}(C(\pi - \pi_0), \quad ct(\pi_0) - x(\pi_0))k_{0a}k_{0b},$$

$$x(\pi) = x(\pi_0) - \frac{1}{2}C(\pi - \pi_0) - \frac{1}{2C^2}G^{ab}(C(\pi - \pi_0), \quad ct(\pi_0) - x(\pi_0))k_{0a}k_{0b},$$

$$x^a(\pi) = x^a(\pi_0) + \frac{1}{C}G^{ab}(C(\pi - \pi_0) \quad , ct(\pi_0) - x(\tau_0))k_{0b}, \tag{8}$$

where $G^{ab}(p,q)$ were defined in (4). Formulas (4) are satisfied for all null geodesics, except the curve for which $C = 0$. This condition represents a light beam moving parallel to a gravitational wave. In this case, $k_a = 0$ for an arbitrary π, and the solution is

$$ct = A(\pi - \pi_0) + ct_0, \quad x = A(\pi - \pi_0) + x_0, \quad x^a = x_0^a, \tag{9}$$

where A is a constant.

III. A MICHELSON INTERFEROMETER IN THE PRESENCE OF A PLANE GRAVITATIONAL WAVE

Using the equations of motion for a light beam in the field of a plane gravitational wave, Eqs. (8) and (9), we will show how to build a simple model of a Michelson interferometer.[33] Let us consider three observers at rest:

$$1.\quad ct = s - s_0,\quad x = 0,\quad y = 0,\quad z = 0,$$

$$2.\quad ct = s - s_0,\quad x = l_\parallel,\quad y = 0,\quad z = 0,$$

$$3.\quad ct = s - s_0,\quad x = 0,\quad y = l_\perp,\quad z = 0. \tag{10}$$

Let a light beam leave the world point (0,0,0,0) in the direction of a plane wave, and arrive at the point $(\tilde{s}_1 - s_0, l_\parallel, 0, 0)$. In this case Eqs. (9) lead to

$$\tilde{s}_1 - s_0 = A(\tilde{\pi}_1 - \tilde{\pi}_0),\quad l_\parallel = A(\tilde{\pi}_1 - \tilde{\pi}_0), \tag{11}$$

which gives $\tilde{s}_1 - s_0 = l_\parallel$. Then, let this light beam leave the point $(\tilde{s}_1 - s_0, l_\parallel, 0, 0)$ and arrive at the point $(\tilde{s}_2 - s_0, 0, 0, 0)$ (return to the initial space point). Consequently, the equations of motion (8) are

$$\tilde{s}_2 - \tilde{s}_1 = \frac{1}{2}C(\tilde{\pi}_2 - \tilde{\pi}_1) - \frac{1}{C^2}G^{ab}(C(\tilde{s}_2 - \tilde{s}_1), \tilde{s}_1 - l_\parallel)k_{0a}k_{0b},$$

$$-l_\parallel = -\frac{1}{2}C(\tilde{s}_2 - \tilde{s}_1) - \frac{1}{2C^2}G^{ab}(C(\tilde{s}_2 - \tilde{s}_1), \tilde{s}_1 - l_\parallel)k_{0a}k_{0b},$$

$$0 = \frac{1}{C}G^{ab}(C(\tilde{s}_2 - \tilde{s}_1), \tilde{s}_1 - l_\parallel)k_{0b}. \tag{12}$$

Therefore $\tilde{s}_2 - s_0 = 2l_\parallel$.

Next, let us consider a light beam leaving the point (0,0,0,0) in the direction perpendicular to that of the gravitational wave, and arriving at $(s_1 - s_0, 0, l_\perp, 0)$. In this case Eqs. (8) give

$$s_1 - s_0 = \frac{1}{2}C(\pi_1 - \pi_0) - \frac{1}{2C^2}G^{ab}_{\rightarrow}k_{0a}k_{0b},\quad l_\perp = \frac{1}{C}G^{2b}_{\rightarrow}k_{0b},$$

$$0 = -\frac{1}{2}C(\pi - \pi_0) - \frac{1}{2C^2}G^{ab}_{\rightarrow}k_{0a}k_{0b},\quad 0 = \frac{1}{C}G^{3b}_{\rightarrow}k_{0b}, \tag{13}$$

where $G^{ab}_{\rightarrow} = G^{ab}(C(\pi_1 - \pi_0), s_0) = \int_{s_0}^{s_1} g^{ab}(u)du$. We obtain the equation for s_1:

$$s_1 - s_0 = -\frac{l_\perp^2 G^{33}_{\rightarrow}}{\Delta_{\rightarrow}}, \tag{14}$$

where $\Delta_{\rightarrow} = G^{22}_{\rightarrow}G^{33}_{\rightarrow} - (G^{23}_{\rightarrow})^2$.

Then, let the same light beam go from the point $(s_1, 0, l_\perp, 0)$ to the initial space point $(s_2, 0, 0, 0)$. The equations of motion are (with different constants of motion)

$$s_2 - s_1 = \frac{1}{2}C(\pi_2 - \pi_1) - \frac{1}{2C^2}G^{ab}_{\leftarrow}k_{0a}k_{0b},\quad -l_\perp = -\frac{1}{C}G^{2b}_{\leftarrow}k_{0b},$$

$$0 = -\frac{1}{2}C(\pi_2 - \pi_1) - \frac{1}{2C'^2}G^{ab}_{\leftarrow}k_{0a}k_{0b},\quad 0 = \frac{1}{C}G^{3b}_{\leftarrow}k_{0b}, \tag{15}$$

where $G^{ab}_{\leftarrow} = G^{ab}(C(\pi_2 - \pi_1), s_1) = \int_{s_1}^{s_2} g^{ab}(u)du$. In a similar manner we obtain

$$s_2 - s_1 = -\frac{l_\perp^2 G_{\leftarrow}^{33}}{\Delta_{\leftarrow}}, \tag{16}$$

where $\Delta_{\leftarrow} = G_{\leftarrow}^{22} G_{\leftarrow}^{33} - (G_{\leftarrow}^{23})^2$.

A weak plane gravitational wave in metric (1) can be described by the two-dimensional metric tensor

$$g_{ab} = \begin{bmatrix} -1 + f(u) & h(u) \\ h(u) & -1 - f(u) \end{bmatrix}, \tag{17}$$

where $f(u)$ and $h(u)$ are small quantities. [If we neglect terms quadratic and smaller in f and h, then the metric tensor (17) identically satisfies the field equation $R_{uu}=0$.] The two possible polarizations correspond to setting either quantity to zero. Let us consider a polarization such that $h(u)=0$ and denote it by h_+. From this we find $\Delta_{\rightarrow} = (s_1 - s_0)^2 + O(A^2)$, where A is the amplitude of the gravitational wave. We can linearize Eq. (14), omitting terms quadratic and smaller in A:

$$s_1 - s_0 = -\frac{l_\perp^2}{(s_1 - s_0)^2}\left(-(s_1 - s_0) + \int_{s_0}^{s_1} f(u)du \right). \tag{18}$$

The analogous expression can be derived for Eq. (16).

Let us assume that a plane gravitational wave is monochromatic with wavelength λ, $f(u) = A\cos(2\pi u/\lambda)$. We seek the solution of Eq. (18) in the form $s_1 - s_0 = l_\perp + \Delta s_{\rightarrow}$, where $\Delta s_{\rightarrow}$ is a small quantity on the order of A. Keeping only linear terms in $\Delta s_{\rightarrow}$ we find

$$\Delta s_{\rightarrow} = -\frac{A\lambda}{2\pi} \sin\frac{\pi l_\perp}{\lambda} \cos\frac{2\pi(s_0 + l_\perp/2)}{\lambda}. \tag{19}$$

Similarly, for the returning beam we have $s_2 - s_1 = l_\perp + \Delta s_{\leftarrow}$, where

$$\Delta s_{\leftarrow} = -\frac{A\lambda}{2\pi} \sin\frac{\pi l_\perp}{\lambda} \cos\frac{2\pi(s_0 + 3l_\perp/2)}{\lambda}, \tag{20}$$

where we used $s_1 - s_0 = l_\perp$ since this term is on the order of A. Finally, the total delay of the light beam moving perpendicular to the gravitational wave, relative to the parallel beam, is given by

$$\Delta s = \Delta s_{\rightarrow} + \Delta s_{\leftarrow} = -\frac{A\lambda}{2\pi} \sin\frac{2\pi l_\perp}{\lambda} \cos\frac{2\pi(s_0 + l_\perp)}{\lambda}. \tag{21}$$

The other polarization (denoted by $h_\times$) is described by the metric tensor

$$g_{ab} = \begin{bmatrix} -1 & h(u) \\ h(u) & -1 \end{bmatrix}. \tag{22}$$

In this case, Eq. (14) reduces to $s_1 - s_0 = l_\perp$, whereas for the returning beam we find $s_2 - s_1 = l_\perp$. For this polarization there is no delay.

Equation (21) is what experimentalists use to detect gravitational waves.[28,34] Its relation to incoming gravitational waves with arbitrary propagation directions and polarization states can be found in the literature, e.g., Ref. 29. This equation agrees with the corresponding expression in Ref. 30 if we set the departure moment $s_0=0$ and use the relation $\Delta s = (c/\omega)\Delta\phi$, where ω is the light beam frequency and $\Delta\phi$ denotes the phase shift. Therefore, treating light as massless particles in the field of a weak gravitational wave and solving the linearized coupled Einstein-Maxwell equations lead to the same result.

The delay of a light beam depends on the quantity s_0, which corresponds to the moment when the beam leaves the start point [the time dependence of the gravitational field is fixed by the form of $f(u)$]. If the wavelength of a monochromatic gravitational wave is small compared to the size of the interferometer, we can average this delay over s_0: $\langle \Delta s \rangle = (1/\lambda)\int_0^\lambda \Delta s(s_0) ds_0$. The physical rea-

son for averaging arises from the fact that we do not know when the front of a gravitational wave hits the point of the departure of the beam. However, as for each periodic function, such an expression vanishes and is of no interest.

IV. LIGHT BEAM DELAY IN THE SECOND APPROXIMATION

In this section we will generalize the results of the preceding section and consider quadratic terms. Let the two-dimensional metric tensor g_{ab} of a weak gravitational wave be given by

$$g_{ab}=\begin{bmatrix} -1+f^{(1)} & h^{(1)} \\ h^{(1)} & -1+g^{(1)} \end{bmatrix}, \tag{23}$$

where $f^{(1)}$, $g^{(1)}$, $h^{(1)}$ are small quantities on the same order. In the linear approximation $f^{(1)}+g^{(1)}=O(A^2)$, where A is the amplitude of such a wave on the order of $f^{(1)}$. Therefore, without loss of generality we may assume $f^{(1)}+g^{(1)}=g^{(2)}$. The field equation is obtained from $R_{uu}=0$:

$$\frac{1}{2}(\dot{f}^{(1)2}+2f^{(1)}\ddot{f}^{(1)}+\ddot{g}^{(2)}+\dot{h}^{(1)2}+2h^{(1)}\ddot{h}^{(1)})=0, \tag{24}$$

which gives $g^{(2)}$ as a function of $f^{(1)}$ and $h^{(1)}$.

If we consider a polarization h_+ with $h^{(1)}=0$ and put $s_1-s_0=l_\perp$ in terms on the order of A^2, then Eq. (14) becomes

$$(s_1-s_0)^3-l_\perp^2(s_1-s_0)+l_\perp^2\int_{s_0}^{s_1}(f^{(1)}+f^{(1)2})du-l_\perp\left(\int_{s_0}^{s_1}f^{(1)}du\right)^2=0, \tag{25}$$

Note that this equation does not contain the quantity $g^{(2)}$. Let us apply the above results to the case of a monochromatic plane wave, $f^{(1)}=A\cos(2\pi u/\lambda)$. For such a wave, Eq. (24) leads to $g^{(2)}=(4\pi^2A^2/\lambda^2)[3\cos^2(2\pi u/\lambda)-1]$, and this quantity clearly is not a periodic function of u. [We could assume $f^{(1)}+g^{(1)}=f^{(2)}$, but then Eq. (25) would contain the nonperiodic function $f^{(2)}$. Thus, it would be impossible to average the light beam delay over s_0 (the moment when the beam leaves the start point) independently of the initial conditions.] We seek the solution in the form $s_1-s_0=l_\perp+\Delta s_\rightarrow$, where $\Delta s_\rightarrow$ is again a small quantity on the same order as A. Thus, up to quadratic terms in $\Delta s_\rightarrow$ we obtain

$$\begin{aligned}\Delta s_\rightarrow=&-\frac{A\lambda}{2\pi}\sin\frac{\pi l_\perp}{\lambda}\cos\frac{\pi}{\lambda}(2s_0+l_\perp)-\frac{A^2\lambda}{16\pi}\sin\frac{2\pi l_\perp}{\lambda}\cos\frac{2\pi}{\lambda}(2s_0+l_\perp)-\frac{A^2l_\perp}{4}\\&+\frac{A^2\lambda^2}{8\pi^2l_\perp}\left(\sin\frac{\pi l_\perp}{\lambda}\cos\frac{\pi}{\lambda}(2s_0+l_\perp)\right)^2+\frac{A^2\lambda}{4\pi}\sin\frac{\pi l_\perp}{\lambda}\cos\frac{\pi}{\lambda}(2s_0+l_\perp)\cos\frac{2\pi}{\lambda}(s_0+l_\perp).\end{aligned} \tag{26}$$

The above expression contains the quadratic corrections to Eq. (19). The mean value of this quantity over the moment of the departure of the beam s_0, $\langle\Delta s_\rightarrow\rangle=(1/\lambda)\int_0^\lambda\Delta s_\rightarrow(s_0)ds_0$, is now different from zero:

$$\langle\Delta s_\rightarrow\rangle=\frac{A^2\lambda^2}{16\pi^2l_\perp}\sin^2\frac{\pi l_\perp}{\lambda}-\frac{A^2l_\perp}{4}+\frac{A^2\lambda}{16\pi}\sin\frac{2\pi l_\perp}{\lambda}. \tag{27}$$

We remind that the moment s_0 is relative to the instant when a front of the gravitational wave in question hits the departure point, and we average with respect to s_0 since we do not know the value of this quantity.

For the returning beam we must replace s_1 with s_2 and s_0 with s_1 (since the beam departs from the reflection point right after it arrives there), which gives $s_2-s_1=l_\perp+\Delta s_\leftarrow$, where $\Delta s_\leftarrow$ is described by Eq. (26) in which s_0 is replaced with $s_0+l_\perp+\Delta s_\rightarrow$. The result is

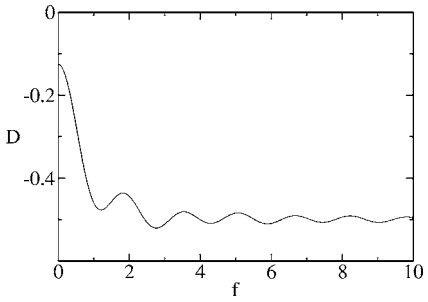

FIG. 1. The normalized average light beam delay D as a function of the normalized wave frequency f for the polarization h_+.

$$\langle \Delta s_{\leftarrow} \rangle = \langle \Delta s_{\rightarrow} \rangle - \frac{A^2 \lambda}{4\pi} \sin^2 \frac{\pi l_\perp}{\lambda} \sin \frac{2\pi l_\perp}{\lambda}. \tag{28}$$

Therefore, the total average delay of the light beam is given by

$$\langle \Delta s \rangle = \frac{A^2 \lambda^2}{8\pi^2 l_\perp} \sin^2 \frac{\pi l_\perp}{\lambda} - \frac{A^2 l_\perp}{2} + \frac{A^2 \lambda}{8\pi} \sin \frac{2\pi l_\perp}{\lambda} - \frac{A^2 \lambda}{4\pi} \sin^2 \frac{\pi l_\perp}{\lambda} \sin \frac{2\pi l_\perp}{\lambda}. \tag{29}$$

We observe that $\langle \Delta s \rangle$ is negative for all values of λ. If $l_\parallel = l_\perp$, then the light beam moving perpendicular to the direction of a gravitational wave lags (on average with respect to the departure moment s_0) behind the one which moves parallel, provided both beams left the light source at the same time. The dependence of the quantity $D = \langle \Delta s \rangle / A^2 l_\perp$ on the variable $f = \pi l_\perp / \lambda$ is shown in Fig. 1.

Now we consider the other polarization $h_\times$ for which $f^{(1)} = 0$. Equation (25) is replaced by

$$(s_1 - s_0)^3 - l_\perp^2 (s_1 - s_0) + l_\perp^2 \int_{s_0}^{s_1} (h^{(1)2}) du - l_\perp \left(\int_{s_0}^{s_1} h^{(1)} du \right)^2 = 0. \tag{30}$$

For a monochromatic plane wave, $h^{(1)} = A \cos(2\pi u / \lambda)$, instead of Eq. (26) we find

$$\Delta s_{\rightarrow} = \frac{A^2 \lambda^2}{2\pi^2 l_\perp} \left(\sin \frac{\pi l_\perp}{\lambda} \cos \frac{\pi}{\lambda} (2s_0 + l_\perp) \right)^2 - \frac{A^2 l_\perp}{4} - \frac{A^2 \lambda}{16\pi} \sin \frac{2\pi l_\perp}{\lambda} \cos \frac{2\pi}{\lambda} (2s_0 + l_\perp). \tag{31}$$

The returning beam again satisfies formula (28). Averaging over the departure moment s_0 gives

$$\langle \Delta s \rangle = \frac{A^2 \lambda^2}{2\pi^2 l_\perp} \sin^2 \frac{\pi l_\perp}{\lambda} - \frac{A^2 l_\perp}{2} - \frac{A^2 \lambda}{4\pi} \sin^2 \frac{\pi l_\perp}{\lambda} \sin \frac{2\pi l_\perp}{\lambda}. \tag{32}$$

We see that $\langle \Delta s \rangle$ is negative for all values of the length of a gravitational wave, and tends asymptotically to zero as $\lambda \to \infty$. In Fig. 2 we show the function $D(f)$. Note that for both polarizations $D \to 1/2$ as $\lambda \to 0$.

From Figs. 1 and 2 we conclude that a one-to-one relation between the average light beam delay and the wavelength exists only for waves longer than $\sim \pi l_\perp$. Moreover, the precision of the measurement of the delay is proportional to the length of the arms of the interferometer. Therefore, if we try to increase the precision by increasing this length, we end up with decrease of the range of waves measurable in this way.

V. SUMMARY

In this work we showed that the time delay of a light beam in a Michelson interferometer, obtained by treating light as massless particles moving on geodesics, agrees with the corresponding solution of the linearized coupled Einstein-Maxwell equations. We also calculated this delay in

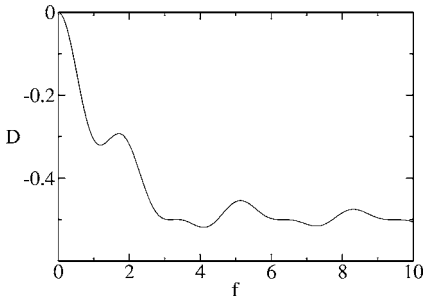

FIG. 2. The normalized average light beam delay D as a function of the normalized wave frequency f for the polarization $h_\times$.

the second (quadratic) approximation. We considered the simple case of a plane wave with the direction parallel to one arm of the interferometer, and treated the two polarizations separately. However, in reality, one should expect a broad spectrum of frequencies and a combination of both polarizations.

Averaging the light beam delay Δs over the moment of the departure of the beam s_0 would make sense if either wavelength λ is much smaller than the arm length $l_\perp$ or we measure $\langle \Delta s \rangle$ many times. Since we excluded the former, this method would not work in the case of supernova explosions that radiate significantly for a few seconds only. Instead, the presented model could be used (in principle) for continuous sources of gravitational waves such as stellar binaries containing a neutron star. As we stated in Sec. I, second-order effects in gravitational-wave detection are extremely small and thus irrelevant experimentally. However, they might be of some academic interest.

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The orbital precession around oblate spheroids

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An exact series will be given for the gravitational potential generated by an oblate gravitating source. To this end the corresponding Epstein-Hubbell type elliptic integral is evaluated. The procedure is based on the Legendre polynomial expansion method and on combinatorial techniques. The result is of interest for gravitational models based on the linearity of the gravitational potential. The series approximation for such potentials is of use for the analysis of orbital motions around a nonspherical source. It can be considered advantageous that the analysis is purely algebraic. Numerical approximations are not required. As an important example, the expression for the orbital precession will be derived for an object orbiting around an oblate homogeneous spheroid. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The basis of the analysis will be the well known expression for the gravitational potential for a point source: $\phi=GM/c^2r$. In this expression M is the mass, G is the gravitational constant, c is the velocity of light, and r is the distance with respect to the point source. One can think of a gravitating body as a collection of point sources. For a linear gravity theory the potential of the complete body simply is the sum over all the point sources: $\phi=\Sigma_i GM_i/c^2r_i$. Wherever possible, it is customary to take the continuum limit and perform the integration. As is known, for a spherical source the result of the integration will also be of the form $\phi=GM/c^2r$, where now M is the mass of the sphere and r is the distance with respect to the center of the sphere. This means that general relativity happens to be linear for the spherical situation. For nonspherical bodies the procedure of adding potentials is valid in the Newtonian limit of general relativity or in a linear gravitation theory. In the latter case the integration will lead to a series expansion for the potential of a nonspherical source.

In Sec. II the series expansion will be derived for the gravitational potential for an oblate spheroid. As a part of the analysis an Epstein-Hubbell type integral has to be solved. The evaluation of the Epstein-Hubbell elliptic type integral originates from 1963.[1] Ever since, various solution methods have been constructed for all kinds of generalizations of the Epstein-Hubbell elliptic integral.[2–4] For the evaluation of the integral under concern, use will be made of the Legendre polynomial expansion method in the same way as it recently has been used for disk galaxies.[5]

In Sec. III a new model for gravitation will be mentioned briefly. The new model describes gravitation in a flat Euclidean spacetime.[6,7] It has the advantage that it is a linear gravitation theory. The new model for gravitation is part of a larger theory.[8–10] According to this theory physics takes place in a Euclidean geometry. The results of the theory are compatible with the results of the theory of relativity. One of the differences with the theory of relativity is that proper time is taken as the fourth dimension. If one wishes, one can regard this fourth dimension as a hidden dimension. Recently, a model for elementary particles in a Eucldean geometry has been proposed on the basis of such a hidden dimension.[11] The results obtained in Sec. II will be applied

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to the new model for gravitation. Although the analysis holds for all kinds of motion, we will focus our attention to the precession of elliptic orbits. A general expression for the orbital precession will be given, with the potential unspecified. The substitution of the potential for a spherical source leads to the correct prediction for the precession of Mercury. In a recent paper the orbital precession has been derived in a pure algebraic manner for the bipole.[12] To significant order the latter equals the prediction as it results from the general theory of relativity and numerical calculations. Because of the novelty of the present theory, the algebraic result will be recalled briefly. It also illustrates that a linear gravitation theory leads to the same result as the general theory of relativity.

In Sec. IV we will consider an oblate spheroid as the source of gravitation. The exact series for the potential will be derived by means of an appropriate integration method. Finally, the exact series for the orbital precession will be given.

In Sec. V the results will be discussed briefly.

II. THE EPSTEIN-HUBBELL INTEGRAL FOR GRAVITATION

We start considering homogeneous disk sources. These disk sources have a cylindrical shape with radius R and thickness S. For convenience, the disk is taken in the $z=0$ or $\theta=0$ plane with the center of the disk in the origin. For such a disk source the potential is given by

$$\phi = \frac{4G\rho}{c^2}\int_0^{S/2}\int_0^{\pi}\int_0^{R} uk\,dk\,d\varphi\,dz, \tag{1}$$

with $u=1/\sqrt{k^2-2kr\cos\varphi+r^2+z^2}$. In this expression ρ is the homogeneous density and k, φ, z are the cylindrical coordinates in the interior of disk.[5] To be specific, φ is the azimuthal angle, z is the height and k is the radial distance in the $z=0$ plane with respect to the center of the disk. The elliptic integral (1) is known as an Epstein-Hubbell type integral. The integral can be evaluated exactly by expanding the function u in terms of Legendre polynomials. First, the function u is written as a Taylor series with respect to k:

$$u = \sum_{n=0}^{\infty} \frac{u^{(n)}(0)k^n}{n!}, \tag{2}$$

where $u^{(n)}(0)$ stands for the nth derivative of u with respect to k and evaluated at $k=0$. In addition, a function v is defined as follows: $v=r\cos\varphi-k$. The functions u and v have the following property: $u^{(1)}=u^3v$ and $v^{(1)}=-1$. By means of this property one finds for the higher order derivatives with respect to k:

$$u^{(n)}(0) = n!\,w^{-(n+1)/2}P_n(w^{-1/2}r\cos\varphi). \tag{3}$$

In the latter equation $w:=r^2+z^2$ and the P_n are the Legendre polynomials: $P_n(x)=(1/2^n)(1/n!)\times(d^n/dx^n)(x^2-1)^n$. Substituting the power series (2) into the equation (1), we obtain for the potential:

$$\phi(r) = \frac{4G\rho}{c^2}\sum_{n=0}^{\infty}\int_0^{R} k^{n+1}\,dk\int_0^{S/2} w^{-(n+1)/2}\int_0^{\pi} P_n(w^{-1/2}r\cos\varphi)d\varphi\,dz. \tag{4}$$

Since the integral vanishes for odd n, the integration over k yields

$$\phi(r) = \frac{4G\rho}{c^2}\sum_{n=0}^{\infty}\frac{1}{2t+2}R^{2t+2}\int_0^{S/2} w^{-(n+1)/2}\int_0^{\pi} P_n(w^{-1/2}r\cos\varphi)d\varphi\,dz. \tag{5}$$

This integral can be evaluated exactly in a systematic way.[5] For the derivative of the gravitational potential with respect to r, the result is

$$d_r\phi = -\frac{GM}{c^2 r^2}\sum_{t=0}^{\infty} A_t B_t(\lambda) C_t(\lambda)\left(\frac{R}{r}\right)^{2t}, \tag{6}$$

where d_r stands for the derivative with respect to r, $M=\pi R^2 S\rho$ is the mass of the disk and where the coefficients A, B, and C are given by

$$A_t = \frac{1}{2^{4t}}\cdot\frac{2t+1}{t+1}\cdot\left(\tfrac{2t}{t}\right)^2, \tag{7}$$

$$B_t(\lambda) = (1+\lambda^2)^{-2t-1/2}, \tag{8}$$

$$C_t(\lambda) = \sum_{i=0}^{t} d_{ti}\lambda^{2i} \tag{9}$$

with

$$d_{ti} = \binom{2t}{t}^{-1}\sum_{j=0}^{i}\frac{(-1)^j(2t+2j)!}{(2j+1)!\,(t+j)!\,(t-i)!\,(i-j)!}. \tag{10}$$

Here λ is defined as $\lambda := S/2r$. In case the distance r with respect to the center of the disk is larger than the size of the disk (either S or R) the derivative of the potential can also be written in an alternative way. That is, expanding the $B_t(\lambda)$, writing λ as $\sigma R/r$ and recollecting equal powers of R/r, we obtain

$$d_r\phi = -\frac{GM}{c^2 r^2}\sum_{t=0}^{\infty} A_t C_{t+1}(\sigma)\left(\frac{R}{r}\right)^{2t}, \tag{11}$$

where $\sigma = S/2R$ is the oblateness of the disk. Explicitly it reads to sixth order as

$$d_r\phi = -\frac{GM}{c^2 r^2}\left[1+\frac{3}{8}\left(1-\frac{4}{3}\sigma^2\right)\left(\frac{R}{r}\right)^2+\frac{15}{64}\left(1-4\sigma^2+\frac{8}{5}\sigma^4\right)\left(\frac{R}{r}\right)^4+\frac{175}{1024}\left(1-8\sigma^2+\frac{48}{5}\sigma^4-\frac{64}{35}\sigma^6\right)\times\left(\frac{R}{r}\right)^6+\ldots\right]. \tag{12}$$

The power series for the derivative of the potential for the disk will serve as the building block for the derivative of the potential for the oblate spheroid. In order to build a general function for an oblate spheroid out of the function for a disk one needs a suitable integration procedure.

First of all, it will be assumed that the cross section of the oblate spheroid through the origin is an ellipse. In analogy with the oblateness of a disk, the oblateness of the ellipse (or the oblateness of the spheroid) is defined as the semiminor axis divided by the semimajor axis: $\sigma = L\sqrt{1-\epsilon^2}/L$ or $\sigma^2 = 1-\epsilon^2$, where ϵ is the eccentricity of the ellipse. In the sequel we will not work with the eccentricity of the elliptic cross section just in order to avoid confusion with the eccentricity of the elliptic orbit. That is, the oblateness of the spheroid will be characterized solely by the oblateness σ. The symbol ϵ will be strictly reserved for the eccentricity of the orbit.

Now we consider a cylinder with radius q inside the spheroid, $q<R$ such that it precisely touches the surface of the spheroid. The cross section then is a rectangle with sizes $2q$ and $2h$, where the h and q are related according to the elliptic shape: $h=\sigma\sqrt{R^2-q^2}$. The value h is with respect to the equatorial plane, thus half the height of the cylinder. We can imagine the spheroid to be build of these cylinders. That is, we start with a cylinder with small radius q_0 and corresponding height $2h_0$ in the middle of the spheroid. Around it one can think a cylindrical tube with inner radius q_0, outer radius q_1, and height $2h_1$. Outside that tube is a next tube with inner radius q_1, outer radius q_2 and height $2h_2$ and so on until the last tube with outer radius equal to R and

height equal to 0. Tube number i with outer radius q_i and height $2h_i$ can be regarded as a cylinder with radius q_i and height $2h_i$ minus a cylinder with radius q_{i-1} and height $2h_i$. The calculation of the influence of a spheroid then is a matter of counting up the influence of all the tubes. For a general function F, this is

$$F = F(q_0,h_0) + F(q_1,h_1) - F(q_0,h_1) + \cdots + F(q_i,h_i) - F(q_{i-1},h_i) + \cdots . \tag{13}$$

Using

$$F(q_i,h_i) - F(q_{i-1},h_i) \approx (q_i - q_{i-1}) \cdot \left(\frac{\partial F}{\partial q}\right), \tag{14}$$

and taking the continuum limit yields the following expression for F:

$$F = \int_0^R \left(\frac{\partial F}{\partial q}\right) dq. \tag{15}$$

Alternatively, we first calculate the partial derivative of F with respect to q and then we substitute the function $h(q)$ for h and perform the integration.

The method will be illustrated by the simple case of the calculation of the mass of a homogeneous spheroid. We start with the mass of a homogeneous cylinder with density ρ, radius q and height $2h$: $2\rho\pi q^2 h$. The partial derivative with respect to q yields $4\rho\pi qh$. Now we substitute $h = \sigma\sqrt{R^2-q^2}$ in the integral for the mass of the spheroid:

$$M = 4\pi\rho\sigma R^3 \int_0^1 x\sqrt{1-x^2}\,dx. \tag{16}$$

An evaluation of the integral yields the correct value for the mass of an oblate spheroid: $M = \frac{4}{3}\pi\rho\sigma R^3$. Now we turn to the calculation of the derivative of the potential for an oblate spheroid. According to Eqs. (6) and (11) the derivative of the potential of a homogeneous cylinder with radius q and thickness $2h$ is given by

$$d_r\phi = -\frac{2\rho\pi q^2 hG}{c^2 r^2} \sum_{t=0}^{\infty} A_t B_t\left(\frac{h}{r}\right) C_t\left(\frac{h}{r}\right)\left(\frac{q}{r}\right)^{2t} \tag{17}$$

and

$$d_r\phi = -\frac{2\rho\pi q^2 hG}{c^2 r^2} \sum_{t=0}^{\infty} A_t C_{t+1}(\sigma)\left(\frac{q}{r}\right)^{2t}, \tag{18}$$

respectively. It does not matter which one we take, since they are identical. As for the mass, we take the partial derivative with respect to q, substitute the expression $\sigma\sqrt{R^2-q^2}$ for h, evaluate the integral Eq. (15), and collect equal powers of $R/2r$. After some elaboration we arrive at the following result:

$$d_r\phi = -\frac{3GM}{c^2 r^2}\left[\frac{1}{3} + \frac{2}{5}(1-\sigma^2)\left(\frac{R}{2r}\right)^2 + \frac{6}{7}(1-\sigma^2)^2\left(\frac{R}{2r}\right)^4 + \frac{20}{9}(1-\sigma^2)^3\left(\frac{R}{2r}\right)^6 + \frac{70}{11}(1-\sigma^2)^4\left(\frac{R}{2r}\right)^8 + \cdots\right], \tag{19}$$

where M is the mass of the spheroid. The latter can also be written as

$$d_r\phi = -\frac{GM}{c^2r^2}\sum_{t=0}^{\infty}\frac{3}{2t+3}\binom{2t}{t}\left(\frac{\alpha}{2}\right)^{2t}, \tag{20}$$

where the quantity α is defined as $\alpha := \sqrt{1-\sigma^2}R/r$. These expressions are identical to the power series of the following function:

$$d_r\phi = \frac{3GM}{2c^2r^2}\left(\frac{\sqrt{1-\alpha^2}}{\alpha^2} - \frac{\arcsin\alpha}{\alpha^3}\right). \tag{21}$$

Note that for a perfect sphere, $\sigma=1$, the latter expressions are reduced to $d_r\phi=-GM/c^2r^2$, exactly as required.

III. GENERAL DIFFERENTIAL EQUATION FOR ORBITAL MOTION

The theory of relativity is based on a Minkowskian geometry and in case of gravitational interactions even on curved spacetime. Recently, there has been proposed an alternative based on a Euclidean geometry.[8–14] Gravitational dynamics does not require an interpretation in terms of a curvature of spacetime.[6–8] According to this new model the proper time of an object is taken as its fourth coordinate: $x_4c := \tau$. As a consequence one obtains a circular spacetime diagram where distances are measured with the flat Euclidean metric: $ds^2=dx^2+dy^2+dz^2+c^2\,d\tau^2$, even in the presence of gravitation. The Schwarzschild counterpart of the Lagrangian for gravitational dynamics in a flat Euclidean spacetime is given by

$$L = m[e^{2\phi}(c\dot{\tau})^2 + e^{4\phi}(\dot{x}^2+\dot{y}^2+\dot{z}^2)], \tag{22}$$

where the overdot represents the derivative with respect to the global time t. In case of a spherical source the latter reads in polar coordinates

$$L = m[e^{2\mu/r}(c\dot{\tau})^2 + e^{4\mu/r}(\dot{r}^2+r^2\omega^2)], \tag{23}$$

where $\mu=GM/c^2$ is half the Schwarzschild radius. It leads to the correct prediction for the deflection of light and the orbital precession of Mercury.[8] Also, the prediction for the orbital precession around the bipole is in excellent agreement with the prediction of general relativity.[12] The new model leads in a straightforward manner to an algebraic expression for the relationship between the precession around the bipole and the distance between the two spheres who constitute the bipole.[12] In contrast, in the general theory of relativity one has to resort to numerical solutions.[15] Both solutions are identical to significant order. The advantage of the new gravitation theory is that it is a linear theory. For two or more spherical bodies, one can add the potentials of all the individual spheres. For bodies with non-spherical shape one can integrate over the volume precisely as we did in the previous section for an oblate spheroid. For the analysis of the orbital motion one has to substitute the resulting potential in the Lagrangian (22). However, one can avoid labor if one first derives the general differential equation for the orbital motion with an unspecified potential and substitutes the expression for the potential afterward. Since we restrict ourselves to motions in the $z=0$ plane, the orbital motion will be derived from the following Lagrangian:

$$L = m[e^{2\phi}(c\dot{\tau})^2 + e^{4\phi}(\dot{r}^2+r^2\omega^2)]. \tag{24}$$

The corresponding Euler-Lagrange equations of motion are

$$me^{4\phi}r^2\omega = A, \tag{25}$$

$$me^{2\phi}c\dot{\tau} = B \tag{26}$$

and

$$m^2c^2 = m^2e^{2\phi}(c\dot{\tau})^2 + m^2e^{4\phi}(\dot{r}^2 + r^2\omega^2). \tag{27}$$

Substituting the Eqs. (25) and (26) into the Eq. (27) and changing coordinates to $u := 1/r$, we obtain

$$m^2c^2 = e^{-2\phi}B^2 + e^{-4\phi}A^2(u'^2 + u^2). \tag{28}$$

The prime denotes the derivative with respect to the orbital angle φ. The derivative with respect to φ followed by the resubstitution of the Eq. (28) gives

$$(d_u\phi)^{-1}e^{-2\phi}A^2(u'' + u) + B^2 - 2e^{2\phi}m^2c^2 = 0, \tag{29}$$

where d_u stands for the derivative with respect to u.

An elliptic orbit without a precession is described as follows:

$$u = \frac{(1 + \epsilon\cos\varphi)}{L(1 - \epsilon^2)}, \tag{30}$$

where ϵ is the eccentricity of the orbit, L is the semimajor axis of the orbit and u is the inverse distance: $u = 1/r$. The equation (30) satisfies the zeroth order equation,

$$u'' + u = \frac{1}{L(1 - \epsilon^2)}. \tag{31}$$

Now we take the derivative of Eq. (29) with respect to φ and substitute the zeroth order equation (31). The result is

$$u''' + u'\left(1 + \frac{2r + r^2\, d_r^2\phi(d_r\phi)^{-1} + 2r^2\, d_r\phi}{L(1 - \epsilon^2)} - \frac{4r^2(d_r\phi)^2m^2c^2}{A^2}\right) = 0. \tag{32}$$

In this expression a factor $e^{4\phi}$ has been set equal to unity in the last term between the brackets, since the difference is of insignificant order. The Eq. (32) is the general differential equation for elliptic orbital motion.

IV. THE ORBITAL PRECESSION FOR OBLATE SPHEROIDS

For elliptic orbits with a precession one cannot neglect the second and last term between the brackets in the differential equation (32). To evaluate these terms we first will substitute the value for A. The constant A is determined by looking for its value at the perihelion.[6] It suffices to substitute the lowest order value for A in the differential equation. In the present analysis the plane of the orbit equals the equatorial plane of the source. For bodies like disks, spheres, and spheroids, the lowest order value for A then reads as

$$A^2 = \mu m^2c^2L(1 - \epsilon^2). \tag{33}$$

With the substitution of this expression for A, the differential equation for u is reduced to

$$u''' + u'\left(1 + \frac{2r + r^2d_r^2\phi(d_r\phi)^{-1} + 2r^2d_r\phi}{L(1 - \epsilon^2)} - \frac{4r^4(d_r\phi)^2}{\mu L(1 - \epsilon^2)}\right) = 0. \tag{34}$$

Now we can substitute the expression (19) for $d_r\phi$. The result is

$$u''' + u'\left(1 - \frac{K}{L(1 - \epsilon^2)}\right), \tag{35}$$

where K stands for the following power series:

$$K = 6\mu + \frac{3r+5\mu}{5}(1-\sigma^2)\left(\frac{R}{r}\right)^2 + \frac{324r+1377\mu}{700}(1-\sigma^2)^2\left(\frac{R}{r}\right)^4 + \frac{8184r+29975\mu}{21\,000}(1-\sigma^2)^3\left(\frac{R}{r}\right)^6 + \frac{7\,390\,528r+23\,695\,625\mu}{21\,560\,000}(1-\sigma^2)^4\left(\frac{R}{r}\right)^8 + \cdots . \tag{36}$$

From a practical point of view we will not consider motions in the vicinity of an extremely dense source. That is, we will restrict ourselves to the situation where $\mu \ll r$. When terms of order μ/r are neglected, the quantity K is reduced to

$$K = 6\mu + \frac{3r}{5}(1-\sigma^2)\left(\frac{R}{r}\right)^2 + \frac{81r}{175}(1-\sigma^2)^2\left(\frac{R}{r}\right)^4 + \frac{341r}{875}(1-\sigma^2)^3\left(\frac{R}{r}\right)^6 + \frac{115\,477r}{336\,875}(1-\sigma^2)^4\left(\frac{R}{r}\right)^8 + \cdots . \tag{37}$$

The latter can be written a little bit more elegantly as follows:

$$K = 6\mu + r\left[3\left(\frac{\alpha^2}{5}\right) + \frac{81}{7}\left(\frac{\alpha^2}{5}\right)^2 + \frac{341}{7}\left(\frac{\alpha^2}{5}\right)^3 + \frac{115\,477}{539}\left(\frac{\alpha^2}{5}\right)^4 + \frac{6\,776\,661}{7007}\left(\frac{\alpha^2}{5}\right)^5 + \frac{59\,419\,831}{13\,377}\left(\frac{\alpha^2}{5}\right)^6 + \frac{7\,380\,857\,431}{357\,357}\left(\frac{\alpha^2}{5}\right)^7 + \cdots\right]. \tag{38}$$

Here and in the sequel, $\alpha = \sqrt{1-\sigma^2}$. As can be inferred from Eq. (21) the latter is a power series of the following function:

$$K = 6\mu - r\left(\frac{\alpha^3 + 3\sqrt{1-\alpha^2}\arcsin\alpha - 3\alpha}{\alpha^3 + \sqrt{1-\alpha^2}\arcsin\alpha - \alpha}\right). \tag{39}$$

According to the averaging method, we approximate K by its average value $\langle K\rangle$:

$$\langle K\rangle \approx = \frac{1}{T}\int_0^T K(t)dt, \tag{40}$$

where T is the period of a revolution. Since $\langle K\rangle$ is independent of $u = 1/r$, an approximate solution for the differential equation (35) can be found. It reads as

$$u(\varphi) = \frac{1+\epsilon\cos[(1-p/2\pi)\varphi]}{L(1-\epsilon^2)}, \tag{41}$$

where the precession per revolution p is given by

$$p = \frac{\pi\langle K\rangle}{L(1-\epsilon^2)}. \tag{42}$$

When the source of gravitation is a perfect sphere, $\sigma = 1$, $\alpha = 0$, $\langle K\rangle = K = 6\mu$, the precession reads as

$$p = \frac{6\pi\mu}{L(1-\epsilon^2)}, \tag{43}$$

precisely in agreement with the prediction from the general theory of relativity. When the source of gravitation is an oblate spheroid, $\sigma < 1$, or a prolate spheroid, $\sigma > 1$, the precession will, in general, differ from the expression (43). For this situation there are two ways to proceed with the analysis of the precession.

One way is to keep the orbit fixed and to vary the radius R of the source. This is appropriate when $R \ll L$. For this situation it suffices to consider terms up to order R^2/r^2:

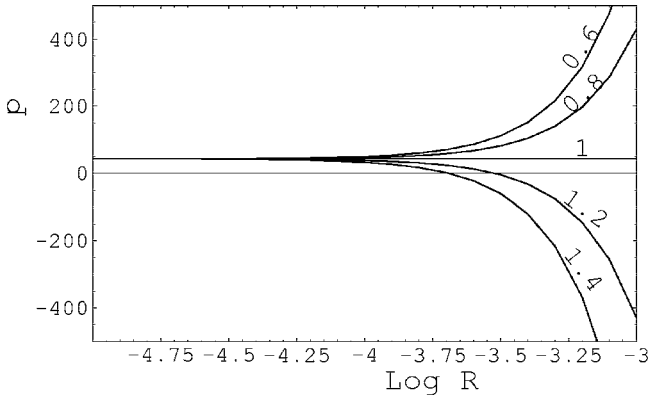

FIG. 1. The orbital precession against the radius of the spheroid for the values 0.6, 0.8, 1.0, 1.2, and 1.4 of the oblateness σ.

$$K \approx 6\mu + \frac{3}{5}\frac{R^2(1-\sigma^2)}{r}. \tag{44}$$

Substitution of the average value $1/L$ for $u=1/r$ gives

$$\langle K \rangle \approx 6\mu + \frac{3}{5}\frac{R^2(1-\sigma^2)}{L}. \tag{45}$$

The expression for the precession (in radians per revolution) then is reduced to

$$p \approx \frac{6\pi\mu}{L(1-\epsilon^2)}\left(1 + \frac{R^2(1-\sigma^2)}{10\mu L}\right). \tag{46}$$

In order to make a comparison, we imagine that Mercury is orbiting around the spheroid. That is, we substitute the values for L and ϵ as they hold for Mercury and the value for μ as it holds for the Sun. The relationship between the radius R (in astronomical units) and the precession p (in arcseconds per century) is then given by

$$p \approx 43'' \cdot \left[1 + (1-\sigma^2) \cdot \left(\frac{R}{2\times 10^{-4}}\right)^2\right]. \tag{47}$$

Figure 1 illustrates the latter relationship between R in astronomical units and the orbital precession p (in arcseconds per century) for various values of σ.

The other way is to keep the radius R of the spheroid fixed and to vary the radius r of the orbit. This seems appropriate when the radius of the orbit does not differ very much from the radius of the spheroid. For this situation we have to use the full equation (38). The averaging method will then give rise to all kinds of powers of $\sqrt{(1-\epsilon^2)}$ in the expression for $\langle K \rangle$. Since we are mainly interested in the consequences of the oblateness of the spheroid, the eccentricity of the orbit will be neglected for convenience. The precession (in radians per revolution) then is given by

$$p = \frac{6\pi\mu}{r} - \pi\left(\frac{\alpha^3 + 3\sqrt{1-\alpha^2}\arcsin\alpha - 3\alpha}{\alpha^3 + \sqrt{1-\alpha^2}\arcsin\alpha - \alpha}\right). \tag{48}$$

In order to make a comparison, we let the spheroid have a mass and radius identical to the Sun. It is obvious to regard the radius of the orbit in units of the Sun radius: $r=xR$. Since we vary the radius of the orbit, also the period of the orbit varies. To obtain the precession per second we have to take the precession per revolution times the number of revolutions per second. The latter, of

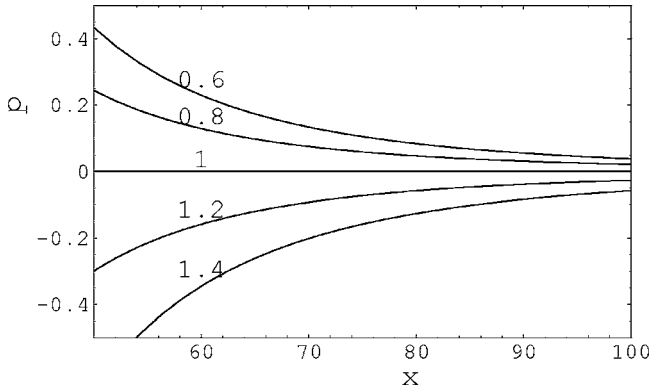

FIG. 2. The orbital precession against the relative radius of the orbit for the values 0.6, 0.8, 1.0, 1.2, and 1.4 of the oblateness σ.

course, is equal to $1/T$ where $T=2\pi\frac{r}{c}\sqrt{r/\mu}$ is the well known expression for the period of the orbit. For the precession in radians per second we then obtain

$$p = 3c\sqrt{\frac{\mu^3}{x^5R^5}} - \frac{c}{2}\sqrt{\frac{\mu}{x^3R^3}}\left(\frac{\alpha^3 + 3\sqrt{1-\alpha^2}\arcsin\alpha - 3\alpha}{\alpha^3 + \sqrt{1-\alpha^2}\arcsin\alpha - \alpha}\right). \tag{49}$$

If we substitute the values for R and μ as they hold for the Sun. The relationship between the relative orbit radius x (in sun radii) and the precession p (in radians per century) is then given by

$$p \approx \frac{13}{\sqrt{x^5}} - \frac{1\times 10^6}{\sqrt{x^3}}\left(\frac{\alpha^3 + 3\sqrt{1-\alpha^2}\arcsin\alpha - 3\alpha}{\alpha^3 + \sqrt{1-\alpha^2}\arcsin\alpha - \alpha}\right). \tag{50}$$

Figure 2 illustrates the relationship between the value x and the orbital precession for various values of σ.

It also is illustrative to consider the situation for a fixed radius of the spheroid at a fixed orbital radius (say the radius of Mercury) and to vary solely the oblateness of the spheroid. Substituting the values for R and μ as they hold for the Sun and of the value for r as it holds for Mercury, we obtain for the precession of the orbit in arcseconds per century:

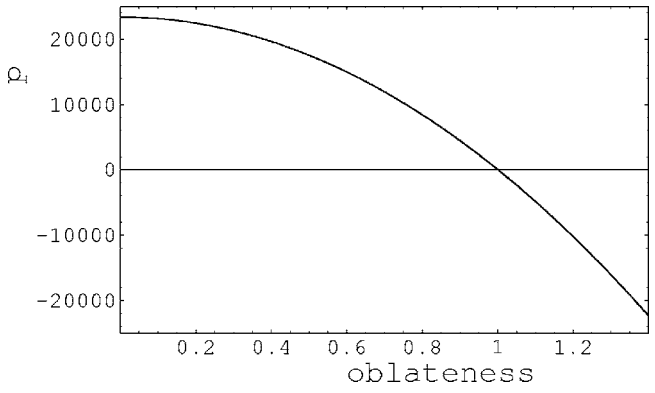

FIG. 3. The orbital precession against the oblateness σ of the gravitational source.

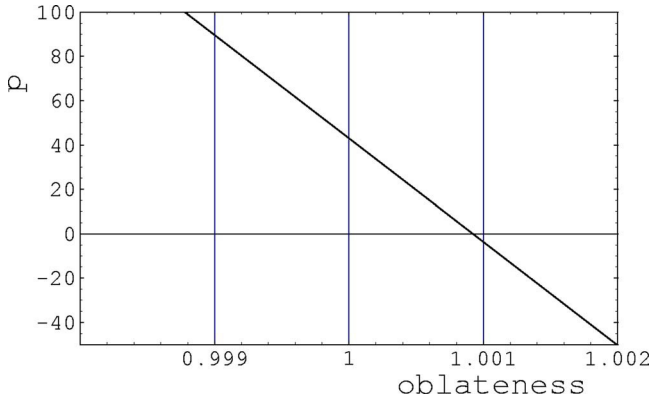

FIG. 4. (Color online) The orbital precession against the oblateness σ for a nearly spherical gravitational source.

$$p \approx 43 - 2.7 \times 10^8 \left(\frac{\lambda^3 + 3\sqrt{1-\lambda^2}\arcsin\lambda - 3\lambda}{\lambda^3 + \sqrt{1-\lambda^2}\arcsin\lambda - \lambda} \right), \tag{51}$$

where $\lambda \approx 0.012\sqrt{1-\sigma^2}$. As can be inferred from Eq. (47) the latter expression is approximately equal to

$$p \approx 43[1 + 550 \cdot (1-\sigma^2)]. \tag{52}$$

In Fig. 3 the precession (in arcseconds per century) is plotted against the oblateness of the spheroid. We see that the precession reaches a maximum value of about 23500 arcseconds per century when $\sigma=0$. That is, if the Sun would be a perfectly flat disk, Mercury would orbit around it with a precession of about 6.5° per century. For the details of the precession around a nearly spherical gravitational source, we have to zoom in at $\sigma \approx 1$. This is done in Fig. 4. We see that for $\sigma=1$ the precession is about 43 arcseconds per century. For the Sun, $\sigma \approx 0.999\,991$. Since the difference with respect to unity is so small, the contribution of the oblateness of the Sun to the precession of Mercury is less than half an arcsecond per century. We also see that the precession decreases for increasing σ. The precession of Mercury would be zero in case of a prolate Sun with $\sigma \approx 1.000\,92$. For larger values the precession rapidly falls off.

V. DISCUSSION OF THE RESULTS

We showed how the Epstein-Hubbell type integral for the gravitational potential for a disk can be evaluated by means of Legendre polynomials. By means of integration by parts one can obtain the expression for the gravitational potential for a spheroid. The method can be applied to gravitational theories based on a linear potential. In the present alternative model the linearity for gravitation is restored. In contrast to general relativity, it is based on a flat and Euclidean spacetime. Nevertheless, it leads to the same prediction for gravitational time dilation, gravitational lensing, and the orbital precession around a point source or a bipole as the general theory of relativity. In this paper we applied the method for the analysis of the orbital precession around an oblate spheroid. Obviously the new model allows for the analysis of gravitational motion in situations that are difficult to solve within the general theory of relativity. The precession of orbits around an oblate spheroid source is derived algebraically. To my knowledge, such a result has never been obtained with the general theory of relativity.

The paper might be of value for mathematicians interested in the mathematical correspondence between two different models for gravitation as well as for mathematicians interested in the applications of Epstein-Hubbell integrals.

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The path topology and the causal completion

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It is shown that the path topology of Hawking, King, and McCarthy can be extended to the causal completion of a globally hyperbolic Lorentzian manifold. The suggested topology $\mathcal{T}$ is defined only in terms of chronological structures and $\mathcal{T}$ is finer than the extended Alexandrov topology. It is also shown that a $\mathcal{T}$-homeomorphism induces a conformal isomorphism and a homeomorphism in the extended Alexandrov topology. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In the sense that the Lorentzian geometry gives mathematical tools and models to Einsten's general relativity, a causality is one of the major areas of the Lorentzian geometry. By a causality, we refer to the general question of which points in a space-time can be joined by causal curves. Relativistically, this is the question of which events can influence a given event. In a particular space-time, a causality may be trivial, but under fairly mild conditions it is closely related to fundamental geometrical properties. For example, it is well known that the Alexandrov topology $\mathcal{A}$ agrees with the given manifold topology $\mathcal{M}$ if and only if the strong causality condition holds.[1]

In connection with this, in 1964, Zeeman[2] has shown that the causal structure of Minkowski space already implies its linear structure. Also, in 1967, he proposed a new topology on Minkowski space that describes timelike and spacelike directions separately. Zeeman's idea on the new topology of Minkowski space was motivated by the fact that Euclidean space is locally isotropic whereas Minkowski space is not; every point has its associated light cone separating spacelike vectors from timelike vectors.

In 1976, Hawking, King, and McCarthy[3] took Zeeman's idea and they proposed a new topology $\mathcal{P}$, called the path topology, on a space-time which is strongly causal. They have shown that $\mathcal{P}$ has several advantages: $\mathcal{P}$ is defined only in terms of timelike curves and a $\mathcal{P}$-continuous curve has a very close relation to timelike curves. One of the advantages of $\mathcal{P}$ is that a $\mathcal{P}$-homeomorphism naturally induces a conformal diffeomorphism and thus $\mathcal{P}$ determines the causal, differential, and conformal structure of the manifold. However, there is a certain disadvantage on $\mathcal{P}$ in the sense that the manifold topology $\mathcal{M}$ is used implicitly in the definition of $\mathcal{P}$.

In 1991, Fullwood[4] proposed a new topology $\tilde{\mathcal{P}}$ defined only in terms of causal structures on the Lorentzian manifold in which the chronological condition is satisfied. He also proved that $\tilde{\mathcal{P}}$ is equivalent to the path topology if and only if the distinguishing condition holds. Thus if the distinguishing condition holds, $\tilde{\mathcal{P}}$ determines the causal, differential, and conformal structure of the manifold. Not only extending the path topology, he has shown that the topology $\tilde{\mathcal{P}}$ can be defined in terms of timelike sequences and its causal limits, which will be used in this paper.

A causal boundary was introduced by the need to control singular points effectively. In 1972, Geroch, Kronheimer, and Penrose[5] constructed the causal boundary of a strongly causal space-

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time. Whereas they constructed the causal boundary only from the properties of a space-time itself, the causal relation cannot be extended to boundary points and the identification rule cannot be given explicitly by the Hausdorff condition of the topology.

In 1974, Budic and Sachs (BS)[6] proposed a new causal boundary construction, ∂M, which states that in a causally continuous space-time, the Hausdorff condition can be naturally satisfied and the causal relation can be extended to the ideal boundary. The topology of the BS-causal completion was defined in terms of the causal relation and is called the extended Alexandrov topology, denoted by $\bar{\mathcal{A}}$. The fact that the BS-causal completion $\bar{M}$ is Hausdorff and is itself an abstract causal set suggests that the Fullwood's method can be applied to the BS-causal completion.

In this paper, it is shown that the path topology can be defined on the BS-causal completion if the manifold is globally hyperbolic. The new topology $\mathcal{T}$ is shown to be finer than the Extended Alexandrov topology $\bar{\mathcal{A}}$ and the inclusion map $i:(M,\tilde{\mathcal{P}})\hookrightarrow(\bar{M},\mathcal{T})$ is shown to be a dense imbedding. Also, it is shown that a $\mathcal{T}$-homeomorphism induces a conformal isomorphism and thus $\mathcal{T}$ determines the causal, differential, and conformal structure of the manifold.

As noted by several authors, in a sense, the structure of a causal boundary determines its inner structure: (1) M is globally hyperbolic if and only if $I^{\pm}(x)=\emptyset$ for $x\in\partial M$; (2) if ∂M is spacelike, then $\bar{M}$ is geodesically connected. Furthermore, Penrose has shown that the strong cosmic censorship is equivalent to $I^{\pm}(x)=\emptyset$ for $x\in\partial M$, which is equivalent to the condition that the space-time be globally hyperbolic. When we consider the fact that the BS-causal completion contains all the singular points of our space-time, the fact that a $\mathcal{T}$-homeomorphism on the BS-causal completion induces a conformal diffeomorphism on M tells us that singularities have deep effects on the structure of our space-time.

II. THE PATH TOPOLOGY

Let M be a time-oriented space-time, that is, M is a connected C^{∞} Hausdorff manifold with a countable basis, a Lorentz metric g of signature $(-,+,+,+)$, and a time orientation

A smooth future-directed curve in M is a smooth curve whose tangent vector is never vanishing, future directed nonspacelike, which means the tangent is always timelike or lightlike. If the tangent is always timelike the curve is said to be a timelike curve. If there is a future-directed timelike curve from x to y, we write $x\ll y$. When there is a future-directed curve from x to y, or when $x=y$, we write $x\leqslant y$. The chronological future $I^{+}(x)$ and the chronological past $I^{-}(x)$ are defined by $I^{+}(x)=\{y\,|\,x\ll y\}$ and $I^{-}(x)=\{y\,|\,y\ll x\}$. When S is a subset of M, one defines $I^{+}(S)=\{y\,|\,s\ll y$ for some $s\in S\}$. The causal future of a point x is defined by $J^{+}(x)=\{y\,|\,x\leqslant y\}$. Furthermore, one may define $J^{-}(x)=\{y\,|\,y\leqslant x\}$, $J^{+}(S)=\{y\,|\,s\leqslant y$ for some $s\in S\}$ and $J^{-}(S)=\{y\,|\,y\leqslant s$ for some $s\in S\}$. $I^{+}(p,N)$ is the set of points that can be reached by a smooth future-directed timelike curve from p in N. $I^{-}(p,N)$ is the dual to the past. $J^{+}(p,N)$ and $J^{-}(p,N)$ allow nonspacelike curves in similar definition to $I^{+}(p,N)$ and $I^{-}(p,N)$.

Throughout this paper, we denote the manifold topology of M by $\mathcal{M}$. It is well known that $I^{+}(p)$ and $I^{-}(p)$ is always $\mathcal{M}$-open and so $I^{+}(p)\cap I^{-}(q)$ is $\mathcal{M}$-open for any pair of points in M. The Alexandrov topology, $\mathcal{A}$, is the topology obtained by taking the set of the form $I^{+}(p)\cap I^{-}(q)$ as a basis. Then the following is a well-known fact.

Theorem 1: *The following are equivalent.*

(1) *The Alexandrov topology $\mathcal{A}$ agrees with the manifold topology $\mathcal{M}$.*
(2) *The strong causality condition holds on M.*
(3) *The Alexandrov topology is Hausdorff.*

Hawking, King, and McCarthy[3] defined that a set $E\subset M$ is $\mathcal{P}$-open if and only if for every timelike curve γ, there is an $O\in\mathcal{M}$ such that $E\cap\gamma=O\cap\gamma$. Then as can easily be shown, $\mathcal{P}$ is finer than $\mathcal{M}$, and we can prove the following.

Proposition 2.1: Let $\gamma:I\to M$ be a curve. If γ is $\mathcal{P}$-continuous, then γ is $\mathcal{M}$-continuous. If γ is timelike, then γ is $\mathcal{P}$-continuous.

Hawking, King, and McCarthy[3] have also shown that the sets of the form $I^+(p,U)\cup I^-(p,U)\cup\{p\}$ form a basis for $\mathcal{P}$ where U is a convex normal neighborhood. Thus we get the following.

Proposition 2: For any $\mathcal{P}$-open neighborhood U of $p\in M$, there is future (past, respectively)-directed timelike curve in U with p its future (past, respectively) end point.

Fullwood[4] defined the $\widetilde{\mathcal{P}}$-topology by taking the sets of the form $[I^+(p)\cap I^-(q)]\cup[I^+(q)\cap I^-(r)]\cup\{q\}$, for $p\ll q\ll r$, as a basis and has shown that $\mathcal{P}=\widetilde{\mathcal{P}}$ if and only if the distinguishing condition holds on M.

Fullwood has shown that the path topology can be obtained in a different manner described as follows. A sequence $\{x_i\}$ of points in M is said to be monotonic timelike if either $x_i\ll x_{i+1}$ or $x_{i+1}\ll x_i$ for each i. A sequence $\{x_i\}$ is said to be causally convergent to $x\in M$ if either $I^-(x)=\cup I^-(x_j)$ for each subsequence of $\{x_i\}$ or $I^+(x)=\cup I^+(x_j)$ for each subsequence of $\{x_i\}$. By the above definition for a sequential convergence, Fullwood defined a set $E\subset M$ to be $\mathcal{P}'$-closed if every monotonic timelike sequence in E that causally converges has a limit in E. Fullwood has proven that, actually, $\mathcal{P}'=\widetilde{\mathcal{P}}$. Since we assume that M is globally hyperbolic throughout in this paper, we do not distinguish $\mathcal{P}$, $\widetilde{\mathcal{P}}$, and $\mathcal{P}'$ and call the equivalent topology as the path topology.

One of the most notable properties of the path topology is that the topology itself determines the causal structure of the space-time. This stems from the fact that the construction of the path topology uses the timelike curve. It thus seems that many calculations involving the causal, differential structure may be made purely topological. We state some of the properties of the $\mathcal{P}$-homeomorphism between Lorentzian manifolds.

Proposition 2.3: A $\mathcal{P}$-homeomorphism is a C^∞ diffeomorphism.

Theorem 2.2: *A $\mathcal{P}$-homeomorphism h is a smooth conformal diffeomorphism and the group of $\mathcal{P}$-homeomorphisms of M coincides with the group of conformal diffeomorphisms of M.*

III. THE BS CAUSAL BOUNDARY

Given an open set $U\subseteq M$, the chronological common past $\downarrow U$ and the common future $\uparrow U$ are defined by $\downarrow U=I^-(\{x|x\ll y \text{ for all } y\in U\})$ and $\uparrow U=I^+(\{x|y\ll x \text{ for all } y\in U\})$, respectively.

A set P is called a past set if $P=I^-(S)$ for some subset S of M. A past set is always open since $I^-(x)$ is open for each $x\in M$. A nonempty past set P is called indecomposable if whenever Q_1 and Q_2 are past sets with $P=Q_1\cup Q_2$, then either $P=Q_1$ or $P=Q_2$. If an indecomposable past set (IP) P is of the form $I^-(x)$ for some $x\in M$, we say that P is a proper indecomposable past set (PIP). If an IP Q cannot be represented by the form $I^-(x)$ for any $x\in M$, we say that Q is a terminal indecomposable past set (TIP). Geroch, Kronheimer, and Penrose[5] have shown that an IP P is a PIP $I^-(x)$ if and only if $P=I^-(\gamma)$ for some timelike curve γ whose end point is x. They have also shown that an IP Q is a TIP if and only if Q can be represented by the form $Q=I^-(\gamma)$ for some inextendible timelike curve γ.[5] Future sets and indecomposable future sets are defined similarly.

Let $\hat{M}$ denote the collection of all indecomposable past sets of M and let $\check{M}$ denote the collection of all indecomposable future sets of M. It is not hard to show that either $\hat{M}\cap\check{M}=\varnothing$ or $\hat{M}\cap\check{M}=\{M\}$.[6] For most space-times, $\hat{M}\cap\check{M}=\varnothing$. Whenever $\hat{M}\cap\check{M}=\{M\}$, we will make a distinction between M considered as an indecomposable past set and M considered as an indecomposable future set.

If $A\in\hat{M}$ and $B\in\check{M}$ are such that $B=\uparrow A$ and $A=\downarrow B$, the pair (A,B) is called a hull pair. An equivalence relation may be defined on the collection $\hat{M}\cup\check{M}$. If $A,B\in\hat{M}\cup\check{M}$ and either (A,B) or (B,A) is a hull pair, we write $A\sim B$. Furthermore, let $A\sim A$ if $A\in\hat{M}$ and $A\sim A$ if $A\in\check{M}$. When M is in both $\hat{M}$ and $\check{M}$, M considered as a past set is not equivalent to M considered as a future set. Budic and Sachs have investigated this equivalence relation. Each equivalence class has at most two elements. The completion $\bar{M}$ is defined to be the set of equivalence classes of $\hat{M}\cup\check{M}$.[6]

In a causally continuous space-time, for each $x\in M$, we have $I^-(x)\in\hat{M}$, $I^+(x)\in\check{M}$ and $(I^-(x),I^+(x))$ is a hull pair. Thus, each point x of M corresponds to exactly one point in $\hat{M}\cup\check{M}/$

$\sim$, and we have an injection $M \hookrightarrow \hat{M} \cup \check{M}/\sim$. The causal completion $\bar{M}$ of the causally continuous space-time M is therefore defined to be $\hat{M} \cup \check{M}/\sim$. Technically, this definition is not the one given by Budic and Sachs, however, they remark that their definition is essentially the same as $\hat{M} \cap \check{M}/\sim$. Our definition is clearly invariant under reversal of time orientation.

Define a map $I: M \to \bar{M}$ by letting $I(x)$ be the equivalence class represented by $I^-(x)$. Since M is distinguishing, this is a one-to-one map into the set $\bar{M}$. The boundary ∂M of M may be defined as $\partial M = \bar{M} - I(M)$. A boundary point of M is represented by an indecomposable subset of M which is not of the form $I^-(x)$ or $I^+(x)$ for any $x \in M$. The map $I: M \to \bar{M}$ will be used to identify M as a subset of $\bar{M}$.

Budic and Sachs defined the causality on $\bar{M}$ by defining relations $\ll$ and $\leqslant$ on $\hat{M} \cup \check{M}$ as in the table to follow. For example, if $(P,Q) \in \hat{M} \times \hat{M}$, $(P,F) \in \hat{M} \times \check{M}$ and $(F,P) \in \check{M} \times \hat{M}$, the table indicates that $P \geqslant Q$ iff $P \supseteq Q$; $P \gg Q$ iff $P \cup (\uparrow Q) \neq \emptyset$; $P \geqslant F$ iff there is a hull pair $(\hat{L}, \check{L})$ such that $P \supseteq \hat{L}$ and $\check{L} \subseteq F$, etc.

	$\cdot \geqslant \cdot$	$\cdot \gg \cdot$
$\hat{M} \times \hat{M}$	$\cdot \supseteq \cdot$	$\cdot \cap (\uparrow \cdot) \neq \emptyset$
$\check{M} \times \check{M}$	$\cdot \subseteq \cdot$	$(\downarrow \cdot) \cap \cdot \neq \emptyset$
$\hat{M} \times \check{M}$	$\cdot \supseteq \hat{L}$ and $\check{L} \subseteq \cdot$	$\cdot \cap \cdot \neq \emptyset$
$\check{M} \times \hat{M}$	$\cdot \subseteq \check{L}$ and $\hat{L} \supseteq \cdot$	$(\downarrow \cdot) \cap (\uparrow \cdot) \neq \emptyset$

The relations $\geqslant$ and $\gg$ may be considered to be defined on $\hat{M} \cup \check{M}/\sim$. If $p, q \in \bar{M}$ and some representative in the equivalence class of p is in the causal future of some representative of q according to the table, then this same relation holds for any representatives of p and any representatives of q. The chronological past of q and causal past of q are defined, respectively, by $\underline{I}^-(q) = \{p \in \bar{M} \,|\, q \gg p\}$ and $\underline{J}^-(q) = \{p \in \bar{M} \,|\, q \geqslant p\}$. The set $\underline{I}^+(q)$ and $\underline{J}^+(q)$ are defined dually.

The extended Alexandrov topology $\bar{A}$ is defined on $\bar{M}$ by taking the smallest topology such that for all $q \in \bar{M}$ each of the following four subsets of $\bar{M}$ is open:

$$\underline{I}^+(q), \quad \underline{I}^-(q), \quad \bar{M} - \underline{J}^-(q), \quad \bar{M} - \underline{J}^+(q).$$

Budic and Sachs[6] have shown that, if the manifold M is causally continuous, the causal completion $\bar{M}$ becomes a causal space which is Hausdorff with respect to the extended Alexandrov topology.

For the following sections, we state some results concerning the extended Alexandrov topology $\bar{\mathcal{A}}$.

Definition: Let $\mathcal{T}$ be a topology on a topological space M and $\gamma: (a,b) \to (M, \mathcal{T})$ be a $\mathcal{T}$-continuous curve. Then $p \in M$ is called a $\mathcal{T}$ end point of γ if for every $\mathcal{T}$-open neighborhood U of p, there exists t_0 such that $\gamma(t) \in U$ for all $t \geqslant t_0$.

A curve is called inextendible, if it does not have an end point in M.

Theorem 3.1: *Let $\gamma: I \to M$ be a timelike curve. Then $I^-(\gamma) \in \partial M$ is the unique $\bar{\mathcal{A}}$ end point in $\bar{M}$.*

Proof: If γ is extendible, see theorem 2.3 in Ref. 5. If γ is inextendible, see Ref. 7. □

IV. THE PATH TOPOLOGY ON THE CAUSAL COMPLETION AND ITS PROPERTIES

Throughout this paper, all the concerned manifolds are always assumed to be globally hyperbolic.

Definition: A sequence $\{x_i\}$ in $\bar{M}$ is timelike if either $x_i \ll x_{i+1}$ or $x_{i+1} \ll x_i$. A timelike sequence $\{x_i\}$ satisfying $x_i \ll x_{i+1}$ ($x_{i+1} \ll x_i$, respectively) is called an increasing (decreasing, respectively)

sequence. A timelike sequence $\{x_i\}$ converges to x if either $\cup I^-(x_i)=I^-(x)$ when $\{x_i\}$ is increasing, or $\cup I^+(x_i)=I^+(x)$ when $\{x_i\}$ is decreasing.

Since we assume that M is globally hyperbolic, we have $I^\pm(x)=\emptyset$ for all $x\in\partial M$.[6] Thus, only the first term in every timelike sequence can be in ∂M.

Proposition 4.1: For increasing timelike sequence $\{x_i\}$, $\cup I^-(x_i)$ *is an indecomposable past set.*

Proof: (This proposition is due to Geroch, Kronheimer, and Penrose[5]) Assume not. Then there exist past sets Q and R such that $\cup I^-(x_i)=Q\cup R$. We must show that $Q\subset R$ or $R\subset Q$. Suppose that there exists $q\in Q-R$ and $r\in R-Q$. Then there exist i_0 and j_0 such that $q\ll x_{i_0}$ and $r\ll x_{j_0}$. Setting $k_0=\max\{i_0,j_0\}$, we have $q\ll x_{k_0}$ and $r\ll x_{k_0}$. If $x_{k_0}\in Q$, then both q and r are in Q since Q is a past set. If $x_{k_0}\in R$, then both q and r are in R since R is a past set. This is a contradiction. Thus, $\cup I^-(x_i)$ is an indecomposable past set. □

From the above proposition, we can easily see that for any increasing timelike sequence $\{x_i\}$, we have a timelike curve γ such that $\cup I^-(x_i)=I^-(\gamma)$. If this timelike curve has an end point x in M with respect to the $\bar{\mathcal{M}}$-topology, then it is also an end point with respect to the $\mathcal{A}$-topology and we have $\cup I^-(x_i)=I^-(x)$. If γ is inextendible, then it is known that $I^-(\gamma)$ is also an end point of γ with respect to the $\bar{\mathcal{A}}$-topology.[7] Thus we can conclude that for any increasing timelike sequence $\{x_i\}$, the corresponding timelike curve has an $\bar{\mathcal{A}}$ end point x in $\bar{M}$ and it is the unique limit of the sequence. Since $I^+(x_i)\cap I^-(\gamma)\neq\emptyset$, we also have $x_i\ll x$ for each i.

Now we define a new topology $\mathcal{T}$ on $\bar{M}$ as follows.

Definition: $U\subset\bar{M}$ is $\mathcal{T}$-closed if every timelike sequence that converges has a limit in U and $V\subset\bar{M}$ is $\mathcal{T}$-open if its complement is $\mathcal{T}$-closed.

Proposition 4.2: The above defines a new topology $\mathcal{T}$ *on* $\bar{M}$.

Proof: (i) Trivially, $\emptyset$ and $\bar{M}$ is closed and so $\emptyset$ and $\bar{M}$ are in $\mathcal{T}$.

(ii) Almost trivially, arbitrary intersection of $\mathcal{T}$-closed sets is also $\mathcal{T}$-closed.

(iii) Now we show that $A\cup B$ is closed when A and B are closed.

Let $\{x_i\}$ be an increasing timelike sequence in $A\cup B$ that converges to x, i.e., $\cup I^-(x_i)=I^-(x)$. If one of A or B contains all but finitely many terms of $\{x_i\}$, then it is trivial since both A and B are closed. Now, we assume that both A and B contain infinitely many terms of $\{x_i\}$. If we break $\{x_i\}$ into $\{y_j\}$ and $\{z_k\}$ such that $y_j\in A$ and $z_k\in B$, then we have $\cup I^-(x_i)=[\cup I^-(y_j)]\cup[\cup I^-(z_k)]$. Since both $\cup I^-(y_j)$ and $\cup I^-(z_k)$ are past sets and $\cup I^-(x_i)$ is an indecomposable past set, without loss of generality, we can have $I^-(x)=\cup I^-(x_i)=\cup I^-(y_j)$, i.e., y_j converges to x. Since $y_j\in B$ and B is closed, we must have $x\in B$, i.e., $x\in A\cup B$. □

In Sec. II, we have seen that the path topology $\mathcal{P}$ is finer than the manifold topology $\mathcal{M}$. We have the same result on the causal completion.

Proposition 4.3: The topology $\mathcal{T}$ *on* $\bar{M}$ *is finer than the extended Alexandrov topology* $\mathcal{A}$ *on* $\bar{M}$.

Proof: Since $I^\pm(y)$ and $\bar{M}-J^\pm(y)$ form a sub-basis of $\bar{\mathcal{A}}$, any $\bar{\mathcal{A}}$-closed subset of $\bar{M}$ can be expressed as an intersection of sets of the form $\bar{M}-I^\pm(y)$ and $J^\pm(y)$. So it is sufficient to show that the above four basic closed subsets are $\mathcal{T}$-closed. In the following four cases, we assume that $\{x_i\}$ is an increasing timelike sequence that $\mathcal{T}$-converges to x (i.e., $\cup I^-(x_i)=I^-(x)$).

(i) Let $\{x_i\}\subset\bar{M}-I^+(y)$.

Assume that $x\notin\bar{M}-I^+(y)$. Then $I^-(x)\cap I^+(y)\neq\emptyset$ and $[\cup I^-(x_i)]\cap I^+(y)\neq\emptyset$. Thus, $I^-(x_i)\cap I^+(y)\neq\emptyset$ for some i. This implies that $x_i\in I^+(y)$ for some i, which contradicts to $x_i\in\bar{M}-I^+(y)$. Thus, $x\in\bar{M}-I^+(y)$ and $\bar{M}-I^+(y)$ is $\mathcal{T}$-closed.

(ii) Let $\{x_i\}\subset\bar{M}-I^-(y)$.

Assume that $x\notin\bar{M}-I^-(y)$. Then $\cup I^-(x_i)=I^-(x)\subset I^-(y)$ and $x_i\ll y$ for some i. This implies that $x_i\in I^-(y)$ which contradicts to $x_i\in\bar{M}-I^-(y)$. Thus, $x\in\bar{M}-I^-(y)$ and $\bar{M}-I^-(y)$ is $\mathcal{T}$-closed.

(iii) Let $\{x_i\}\subset J^+(y)$.

Since $\cup I^-(x_i)=I^-(x)$, we have $x_i\ll x$ for each i by the remark following Proposition 4.1. Thus $y\leqslant x_i\ll x$. In other words, $x\in J^+(y)$ and $J^+(y)$ is $\mathcal{T}$-closed.

(iv) Let $\{x_i\}\subset J^-(y)$.

Since $x_i \leqslant y$, we have $I^-(x_i) \subset I^-(y)$ for each i. Thus, $\cup I^-(x_i) \subset I^-(y)$ and so $I^-(x) \subset I^-(y)$. So we can conclude that $x \in \overline{I^-(x)} \subset \overline{I^-(y)} = J^-(y)$. Thus, $J^-(y)$ is $\mathcal{T}$-closed. □

Since $\mathcal{T}$ is finer than $\bar{\mathcal{A}}$ and $\bar{\mathcal{A}}$ is Hausdorff, we can conclude that $\mathcal{T}$ is a Hausdorff topology on $\bar{M}$.

Proposition 4.4: Let $\gamma:(a,b)\to(\bar{M},\mathcal{T})$ be a curve. Assume that for any sequence $t_i \in (a,b)$ satisfying $t_i \to b$, we have $\gamma(t_i) \to p$ in $\mathcal{T}$-topology. Then $p \in \bar{M}$ is the $\mathcal{T}$ end point of γ.

Proof: Assume there exists a $\mathcal{T}$-open neighborhood U of p such that for any $t_i \in (a,b)$ we can choose $t \geqslant t_i$ such that $\gamma(t) \notin U$. If we let $t_i = b - 1/i$, then $t_i \to b$ and we can choose $s_i \geqslant t_i$ such that $\gamma(s_i) \notin U$. Clearly, $s_i \to b$ but $\gamma(s_i) p$ in $\mathcal{T}$-topology. This is a contradiction. □

We know that any timelike curve $\gamma:(a,b)\to M$ has an end point $I^-(\gamma)$ in $\bar{\mathcal{A}}$-topology. If $t_i \in (a,b)$ is a sequence such that $t_i \to b$, then we have $I^-(\gamma) = \cup I^-(\gamma(t_i))$. Thus, $\gamma(t_i) \to I^-(\gamma)$ in $\mathcal{T}$-topology. By the previous proposition, we have the following.

Corollary: $I^-(\gamma)$ is also an end point of a timelike curve $\gamma:(a,b)\to M$ in $\mathcal{T}$-topology.

Though $\mathcal{T}$ is finer than $\bar{\mathcal{A}}$, we can say that the two topologies $\mathcal{T}$ and $\bar{\mathcal{A}}$ share the same properties in the timelike directions in a sense, by the above corollary.

Let us assume that we have two topologies T_1 and T_2 on M. Then we can consider two sequential convergences with respect to T_1- and T_2-topologies and it is easy to show the following.

Lemma 4.1: Let T_1 and T_2 be two topologies defined on M and x_i be a sequence of points in M. Then ⌜$x_i \to x$ in $T_1 \Rightarrow x_i \to x$ in T_2⌟ if and only if ⌜A is T_2-closed $\Rightarrow A$ is T_1-closed⌟.

Proof: ⇒; Let A be T_2 closed and $\{x_i\} \subset A$ be such that $x_i \to x$ in T_1. Then, $x_i \to x$ in T_2. Since A is T_2-closed, we have $x \in A$ and so A is also T_1-closed.

⇐; Let U be a T_2-neighborhood of x. Then, since U is T_1-open and $x_i \to x$ in T_1, we have $x_i \in U$ for all but finitely many. Thus we have $x_i \to x$ in T_2 □

The construction of $\mathcal{T}$-topology on the causal completion extends the $\tilde{\mathcal{P}}$-topology on M by use of the sequential convergence. By the above lemma, the relation of $\mathcal{T}$ and $\tilde{\mathcal{P}}$ can be given.

Proposition 4.5: The inclusion map $i:(M,\tilde{\mathcal{P}})\hookrightarrow(\bar{M},\mathcal{T})$ is a dense imbedding.

Proof: The imbeddedness follows from the construction of $\mathcal{T}$ and the previous lemma. Let $p \in \partial M$, U be a $\mathcal{T}$-open neighborhood of p and assume that $U \cap M = \emptyset$. Then $\bar{M} - U$ is $\mathcal{T}$-closed and so it must contain all limits of convergent timelike sequence $\{x_i\}$. Since $p \in \partial M$, there exists a timelike sequence $\{x_i\}$ such that $x_i \to p$ with $x_i \in M = M - U$. Since $p \in U$, it is a contradiction. Thus, M with $\tilde{\mathcal{P}}$ topology is dense in $\bar{M}$ with $\mathcal{T}$-topology. □

V. THE PATH TOPOLOGY HOMEOMORPHISM

Definition: A bijection $f:\bar{M}\to\bar{N}$ is a chronological isomorphism if $x \ll y \Leftrightarrow f(x) \ll f(y)$ and antichronological isomorphism if $x \ll y \Leftrightarrow f(y) \ll f(x)$. Likewise, a bijection $f:\bar{M}\to\bar{N}$ is a causal isomorphism if $x \leqslant y \Leftrightarrow f(x) \leqslant f(y)$ and anticausal isomorphism if $x \leqslant y \Leftrightarrow f(y) \leqslant f(x)$. A bijection $f:\bar{M}\to\bar{N}$ is a conformal isomorphism if f is both (anti-) chronological isomorphism and (anti-) causal isomorphism.

In a Lorentzian manifold, it is known that the causal isomorphism and the chronological isomorphism are equivalent.[4]

The topology $\mathcal{T}$ is defined only in terms of chronological relations and so any chronological isomorphism $f:\bar{M}\to\bar{N}$ induces a $\mathcal{T}$-homeomorphism. The chronological isomorphism has the same effects on the $\bar{\mathcal{A}}$-topology.

Proposition 5.1: If M and N are globally hyperbolic and $f:\bar{M}\to\bar{N}$ is either a chronological isomorphism or an antichronological isomorphism, then f is an $\bar{\mathcal{A}}$-homeomorphism.

Proof: We show that the above statement holds in the case of a chronological isomorphism. The case of an antichronological isomorphism can be shown by the similar argument. Let $x \in \partial M$. Without loss of generality, we can assume that $I^+(x) = \emptyset$ since M is globally hyperbolic. Since f is a chronological isomorphism, $I^+(f(x)) = \emptyset$ and $f(x) \in \partial N$. Thus $f(\partial M) \subset \partial N$. Since f^{-1} is

also a chronological isomorphism, we have $f(\partial M)=\partial N$. Thus f induces a chronological isomorphism $f|_M: M \to N$ and $f|_M$ is also a causal isomorphism by Theorem 6.3 of Ref. 4. This implies that $f|_M$ is a conformal isomorphism between M and N. Since the BS-causal boundary and its topology $\bar{\mathcal{A}}$ is constructed only in terms of the causal and chronological relations, we can conclude that f is an $\bar{\mathcal{A}}$-homeomorphism. □

Theorem 5.1: *If $f: \bar{M} \to \bar{N}$ is a $\mathcal{T}$-homeomorphism, then f is either a chronological isomorphism or an antichronological isomorphism.*

Proof: First, we show that $f(\partial M) \subset \partial N$. Let us assume not. Then there are $p \in \partial M$ and $q \in N$ with $f(p)=q$. Since $i: (M, \tilde{\mathcal{P}}) \hookrightarrow (\bar{M}, \mathcal{T})$ is an imbedding, we can choose $\mathcal{T}$-neighborhoods U of p and V of q such that $V \subset N$ and $f: U \to V$ is a $\mathcal{T}$-homeomorphism. Then $f: U - \partial M \to V - f(\partial M)$ is $\tilde{\mathcal{P}}$-homeomorphism since $i: (M, \tilde{\mathcal{P}}) \hookrightarrow (\bar{M}, \mathcal{T})$ is an imbedding. Since M is globally hyperbolic, ∂M is $\mathcal{T}$-closed in $\bar{M}$ and thus $f(\partial M)$ is $\mathcal{T}$-closed in $\bar{N}$. Thus, $V - f(\partial M)$ is $\tilde{\mathcal{P}}$-open in N and so we can choose future-directed timelike curve γ_1 and past-directed timelike curve γ_2 in $V - f(\partial M)$ with q their common end point. Since $f^{-1}: V - f(\partial M) \to U - \partial M$ is a $\tilde{\mathcal{P}}$-homeomorphism, one of $f^{-1} \circ \gamma_1$ and $f^{-1} \circ \gamma_2$ is past-directed with p its end point. Since M is globally hyperbolic, it is a contradiction. Thus we have shown that $f(\partial M) \subset \partial N$. Likewise, since $f^{-1}: \bar{N} \to \bar{M}$ is also a $\mathcal{T}$-homeomorphism, we have $f^{-1}(\partial N) \subset \partial M$ and so we get $f(\partial M)=\partial N$. Therefore, we can conclude that a $\mathcal{T}$-homeomorphism $f: \bar{M} \to \bar{N}$ induces a $\tilde{\mathcal{P}}$-homeomorphism $f|_M: M \to N$. This implies that $f|_M: M \to N$ is either a chronological isomorphism or an antichronological isomorphism by Theorem 2 of Ref. 4. Without loss of generality, we assume that $f|_M: M \to N$ is a chronological isomorphism. It remains to show that $x \ll y$ implies that $f(x) \ll f(y)$ when either x or y is in ∂M. In either case, there exists a future-directed timelike curve from x to y. Since $f|M$ is a conformal diffeomorphism, $f \circ \gamma$ is a future-directed timelike cuve from $f(x)$ to $f(y)$. Thus $f(x) \ll f(y)$. □

As stated above, the causal isomorphism between Lorentzian manifolds is equivalent to the chronological isomorphism. Thus any $\mathcal{T}$-homeomorphism $f: \bar{M} \to \bar{N}$ induces a causal isomorphism $f|_M: M \to N$ and so we have shown the following theorem.

Theorem 5.2: *If $f: \bar{M} \to \bar{N}$ is a $\mathcal{T}$-homeomorphism, then f is a conformal isomorphism.*

Whereas $\mathcal{T}$ is finer than $\bar{\mathcal{A}}$, by combining proposition 5.1 and theorem 5.1, we have the following theorem.

Theorem 5.3: *A $\mathcal{T}$-homeomorphism induces an $\bar{\mathcal{A}}$-homeomorphism.*

We know that if $f: M \to N$ is a $\tilde{\mathcal{P}}$-homeomorphism, then f is a conformal isomorphism. If, in addition, both M and N are strongly causal, the manifold topologies are the same as the Alexandrov topologies since the Alexandrov topology is defined only in terms of a chronological relation. In other words, a $\tilde{\mathcal{P}}$-homeomorphism induces an $\mathcal{M}$-homeomorphism. By the above theorem, this is indeed the case in the path topology of the BS-causal completion. Thus, we know that, in this sense, the extended Alexandrov topology is natural to the causal completion.

VI. DISCUSSION

If two space-times are chronologically isomorphic or causally isomorphic, then, clearly their causal boundaries have the same structures. Conversely, what can be said about the structures of two space-times if their causal boundaries have the same structure? Considering the fact that the causal boundary contains all the past and the future end points of all the inextendible causal curves in our space-time, we can say that, in a sense, the causal boundary contains all the information of the initial and the final states of our space-time. This is similar to the situation of the initial value problems or the boundary value problems of differential equation theories. Therefore, we may expect that the causal boundary determines the inner structure of our space-time to some extent.

In fact, the study of this paper was motivated by the question: To what extent does the structure of the causal boundary determine the inner causal structure of our space-time. If we keep this in mind, it is natural to ask the following: If $f: \partial M \to \partial N$ is a $\mathcal{T}$-homeomorphism, what is the relation, if any, between the structures of M and N?

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Gravitational Aharonov-Bohm effect due to weak fields

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We study the behavior of relativistic quantum particles in the space-times generated by a rotating massive body and a moving mass current, in the weak field approximation. We solve the Dirac equation in these gravitational fields and calculate the currents associated with the particles. It is shown that these solutions and the currents depend on the angular momentum and on the velocity of the sources, in the cases of a massive rotating body and a moving mass current, respectively. These effects may be looked upon as a gravitational analog of the Aharonov-Bohm effect. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218671]

I. INTRODUCTION

The study of relativistic quantum systems under the influence of gravitational fields goes back to the pioneering works by Fock[1] and Schrödinger,[2] when the generalization of quantum mechanics to curved spaces has been discussed, motivated by the idea of constructing a theory combining quantum physics and general relativity. Along this line of research the hydrogen atom, for example, has been studied in particular curved space-times.[3,4] These investigations showed that the energy levels of an atom placed in a gravitational field is shifted as a result of the interaction of the atom with the space-time curvature.[4–6] These shifts of the atomic levels depend on the Riemann curvature tensor at the position of the atom and can be used in principle to measure or put an upper limit on the curvature of space-time at the position of the atom.

In a metric theory of gravitation, a gravitational field is related to a nonvanishing Riemann curvature tensor. However, the presence of localized curvature can produce effects on the geodesic motion and parallel transport in regions where the curvature vanishes. The best known example of this nonlocal (global) effect is provided when a particle is transported along a closed curve which encircles an idealized cosmic string.[7] In this case, the string is noticed at all. This situation corresponds to the gravitational analog[8] of the electromagnetic Aharonov-Bohm effect.[9] These effects are of global origin rather than local. It is worth calling attention to the fact that different from the electromagnetic Aharonov-Bohm effect which is essentially a quantum effect, the gravitational analog appears also at a purely classical context.

We also have an analog of the gravitational Aharonov-Bohm effect when particles are constrained to move in a region where the Riemann curvature does not vanish, but does not depend on certain parameters such as the angular momentum, as in the case of a weak gravitational field arising from a rotating cylindrical shell[10] which we will consider. In this situation, we can have

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gravitational nonlocal effects associated with this parameter. A similar situation occurs when we have a gravitational field generated by a slowly moving mass current.[11] In this case, the Riemann curvature tensor does not depend on the velocity of the source, but we have a nonlocal effect on the quantum system due to this parameter.

The existence of a gravitational analog of the electromagnetic Aharonov-Bohm effect was first pointed out at the end of the 1960s.[12–16] Studies concerning this subject were reported by many authors from that time up to now.[17,18]

The aim of this paper is to investigate the behavior of relativistic particles placed in the gravitational field generated by a slowly rotating cylindrical shell[10] and by a slowly moving mass current.[11] The gravitational effects are taken into account in the weak field approximation in which case the curvature does not depend on the angular momentum or on the velocity of the sources.

This paper is organized follows. In Sec. II, we introduce the gravitational fields to be considered, namely, the gravitational field generated by a rotating cylindrical shell and by a slowly moving massive current. In Sec. III, we obtain the solution of the Dirac equation and determine the associated current. In Sec. IV, we do the same as the previous section, but now in the space-time generated by a moving mass current. Finally, in Sec. IV, we conclude with some remarks.

II. WEAK GRAVITATIONAL FIELDS

In this section, we will present the space-times generated by an infinitely long and thin cylindrical shell of matter which rotates slowly and by a cylindrical distribution of matter with uniform density along the z axis, which moves slowly with velocity v in the z direction.

First, let us consider the space-time generated by an infinitely long, infinitely thin massive cylindrical shell rotating slowly around its axis. In the weak field approximation the metric reads[10]

$$ds^2 = -\left(1 - \frac{a(\rho)}{2}\right)dt^2 + \left(1 + \frac{a(\rho)}{2}\right)(d\rho^2 + \rho^2 d\varphi^2 + dz^2) + 2b dt d\varphi, \tag{1}$$

where

$$a(\rho) = -8\mu\Theta(\rho - \rho_0)\ln\left(\frac{\rho}{\rho_0}\right) \tag{2}$$

and

$$b(\rho) = 4\mu\omega\rho_0\left[\frac{\rho^2}{\rho_0^2}\Theta(\rho_0 - \rho) + \Theta(\rho - \rho_0)\right], \tag{3}$$

with $\Theta(x)$ being the unit step function.

The metric given by Eq. (1) is characterized by two parameters, namely, the linear mass density μ and the linear angular momentum density $j = \mu\omega\rho_0$, with ρ_0 and ω being the radius of the cylinder and the angular velocity of the source, respectively. This approximate solution is justified in a domain in which the Newtonian potential generated by the thin massive cylindrical shell is much less than the unity which means that $|a(\rho)| \ll 1$ and when $b(\rho)^2 \sim 0$. The term with $b(\rho)$, in this metric, being proportional to j is completely due to the rotation of the cylindrical shell.

In the weak field approximation, the Riemann curvature tensor outside the rotating shell is completely determined by the function $a(\rho)$ only, if we neglect terms containing $b(\rho)a(\rho)$, $|a(\rho)|^2$, or $b(\rho)^2$, which is justified by the fact that $|a(\rho)| \ll 1$ and we are considering that the source rotates slowly around the z axis, which means that $b(\rho)^2 \sim 0$, as already stated. Thus, due to these considerations, the angular momentum is not present in the curvature, in this approximation. The contribution of the term with $b(\rho)$ is concentrated on the shell itself. This means that, in the weak field approximation, the local effects of curvature connected with the rotation of the cylindrical shell are absent outside it. In this background space-time a study concerning the gravitational Aharonov-Bohm effect has been done.[10,19]

The other space-time we will consider is generated by a cylindrical distribution of matter with uniform density along the z axis, which moves slowly with velocity v in the z direction. In the weak field approximation, the line element given by[11]

$$ds^2 = -(1-\Phi(\rho))dt^2 + (1+\Phi(\rho))(d\rho^2 + \rho^2 d\varphi^2 + dz^2) - 4v\Phi(\rho)dzdt, \tag{4}$$

where $\Phi(\rho)$ represents the Newtonian potential produced by this source and satisfies the condition $\Phi(\rho)^2 \approx 0$.

For this space-time, the curvature outside the distribution of matter does not depend on its velocity, in the weak field approximation. This means that for the weak gravitational field associated with slowly moving mass currents, the local effects of the curvature associated with the velocity of the source are absent outside it. In this space-time we also have a manifestation of the Aharonov-Bohm effect.[11,20]

III. RELATIVISTIC QUANTUM SYSTEM IN THE SPACE-TIME OF A SLOWLY ROTATING CYLINDRICAL SHELL

In this section we will consider a massive spinor particle in the space-time of a slowly rotating cylindrical shell. This particle obeys the covariant Dirac equation in a curved space-time, for a massive spinor field Ψ, which is given by

$$[i\gamma^\mu(x)\partial_\mu - i\gamma^\mu(x)\Gamma_\mu(x) - m]\Psi(x) = 0, \tag{5}$$

where $\gamma^\mu(x)$ are the generalized Dirac matrices and are given in terms of the standard flat space Dirac matrices $\gamma^{(a)}$ as

$$\gamma^\mu(x) = e^\mu_{(a)}(x)\gamma^{(a)}, \tag{6}$$

where $e^\mu_{(a)}(x)$ are tetrad components defined by

$$e^\mu_{(a)} e^\nu_{(b)} \eta^{(a)(b)} = g^{\mu\nu}. \tag{7}$$

Here and in what follows Greek indices are connected with tensor world indices (coordinate basis system) and Latin indices denote Lorentz indices which are connected with a local Minkowski coordinate system (tetrads).

The product $\gamma^\mu\Gamma_\mu$ that appears in Eq. (5) can be written as[21]

$$\gamma^\mu(x)\Gamma_\mu(x) = \gamma^{(a)}(A_{(a)}(x) + i\gamma^{(5)}B(x)), \tag{8}$$

with $\gamma^{(5)} = i\gamma^{(0)}\gamma^{(1)}\gamma^{(2)}\gamma^{(3)}$ and $A_{(a)}$ and $B_{(a)}$ given by

$$A_{(a)} = \tfrac{1}{2}(\partial_\mu e^\mu_{(a)} + e^\rho_{(a)}\Gamma^\mu_{\rho\mu}) \tag{9}$$

and

$$B_{(a)} = \tfrac{1}{2}\epsilon_{(a)(b)(c)(d)} e^{(b)\mu} e^{(c)\nu} \partial_\mu e^{(d)}_\nu, \tag{10}$$

where $\epsilon_{(a)(b)(c)(d)}$ is the completely antisymmetric fourth-order unit tensor and the Christoffel symbols $\Gamma^\mu_{\rho\mu}$ are given by $\Gamma^\mu_{\rho\mu} = (1/\sqrt{-g})(\partial/\partial x^\rho)(\sqrt{-g})$.

In order to write the Dirac equation in the space-time generated by a rotating cylindrical shell let us choose the following set of tetrads:

$$e^{\mu}_{(a)} = \begin{pmatrix} 1+\frac{a(\rho)}{4} & 0 & \frac{b}{\rho} & 0 \\ 0 & 1-\frac{a(\rho)}{4} & 0 & 0 \\ 0 & 0 & \frac{1-\frac{a(\rho)}{4}}{\rho} & 0 \\ 0 & 0 & 0 & 1-\frac{a(\rho)}{4} \end{pmatrix}. \tag{11}$$

Calculating the expresssions for $A(a)$ and $B(a)$ given by Eqs. (9) and (10), respectively, and substituting these results into Eq. (8), we get the following result:

$$\gamma^{\mu}\Gamma_{\mu} = \frac{1}{2\rho}\left(1+\frac{a(\rho)}{2}\right)\gamma^{(1)}. \tag{12}$$

Using the set of tetrads in (11), we obtain that the generalized matrices $\gamma^{\mu}(x)$, are given by

$$\begin{aligned} \gamma^{0}(x) &= \left(1+\frac{a(\rho)}{4}\right)\gamma^{(0)}, \\ \gamma^{1}(x) &= \left(1-\frac{a(\rho)}{4}\right)\gamma^{(1)}, \\ \gamma^{2}(x) &= \frac{1}{\rho}\left(1-\frac{a(\rho)}{4}\right)\gamma^{(2)}, \\ \gamma^{3}(x) &= \left(1-\frac{a(\rho)}{4}\right)\gamma^{(3)}. \end{aligned} \tag{13}$$

Thus, substituting Eqs. (12) and (13) into the Dirac equation in the curved space-time given by (5), and considering that the particle is restricted to move in a narrow region such that $a(\rho)$ is approximately constant and equal to a_1, we will get

$$\begin{aligned} &\left[i\left(1+\frac{a_1}{4}\right)\partial_t - m\right]\Psi_2 - \frac{b}{\rho}\partial_t\Psi_3 + i\left(1-\frac{a_1}{4}\right)\partial_\rho\Psi_3 - \frac{1}{\rho}\left(1-\frac{a_1}{4}\right)\partial_\varphi\Psi_3 \\ &\quad - i\left(1-\frac{a_1}{4}\right)\partial_z\Psi_3 + i\frac{1}{2\rho}\left(1-\frac{a_1}{4}\right)\Psi_4 = 0, \end{aligned}$$

$$\begin{aligned} &\left[i\left(1+\frac{a_1}{4}\right)\partial_t - m\right]\Psi_1 + \frac{b}{\rho}\partial_t\Psi_4 + i\left(1-\frac{a_1}{4}\right)\partial_\rho\Psi_4 - \frac{1}{\rho}\left(1-\frac{a_1}{4}\right)\partial_\varphi\Psi_4 \\ &\quad - i\left(1-\frac{a_1}{4}\right)\partial_z\Psi_3 + i\frac{1}{2\rho}\left(1-\frac{a_1}{4}\right)\Psi_4 = 0, \end{aligned}$$

$$\left[-i\left(1+\frac{a_1}{4}\right)\partial_t+m\right]\Psi_3-\frac{b}{\rho}\partial_t\Psi_2-i\left(1-\frac{a_1}{4}\right)\partial_\rho\Psi_2-\frac{1}{\rho}\left(1-\frac{a_1}{4}\right)\partial_\varphi\Psi_2$$
$$+i\left(1-\frac{a_1}{4}\right)\partial_z\Psi_1+i\frac{1}{2\rho}\left(1-\frac{a_1}{4}\right)\Psi_2=0,$$

and

$$\left[-i\left(1+\frac{a_1}{4}\right)\partial_t+m\right]\Psi_4+\frac{b}{\rho}\partial_t\Psi_1-i\left(1-\frac{a_1}{4}\right)\partial_\rho\Psi_1-\frac{1}{\rho}\left(1-\frac{a_1}{4}\right)\partial_\varphi\Psi_1$$
$$-i\left(1-\frac{a_1}{4}\right)\partial_z\Psi_1-i\frac{1}{2\rho}\left(1-\frac{a_1}{4}\right)\Psi_1=0, \tag{14}$$

where $\Psi_1,\Psi_2,\Psi_3,\Psi_4$ are the components of the four spinor

$$\Psi=\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\\ \Psi_4\end{pmatrix} \tag{15}$$

and we have used the standard representation of the Dirac matrices $\gamma^{(a)}$.

To solve the set of equations given in (14), let us choose

$$\Psi_1=\sqrt{E+m}e^{-iEt+il\varphi+ikz}u_1(\rho), \tag{16}$$

$$\Psi_2=\sqrt{E-m}e^{-iEt+i(l+1)\varphi+ikz}u_1(\rho), \tag{17}$$

and consider $\Psi_1=\Psi_3$, $\Psi_2=\Psi_4$, reducing this problem to a two-dimensional one. Thus, the set of equations in (14) turns into the following pair of equations for $u_1(\rho)$ and $u_2(\rho)$:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}+\frac{1}{\rho^2}(l+2bE)^2+\left(1-\frac{a_1}{2}\right)(E^2-m^2)\right]u_1(\rho)=0 \tag{18}$$

and

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}+\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}-\frac{1}{\rho^2}(l+2bE+1)^2+\left(1-\frac{a_1}{2}\right)(E^2-m^2)\right]u_2(\rho)=0, \tag{19}$$

whose solutions are given by

$$u_i=C_{i,l}^{(1)}J_{v+i-1}(k\rho)+C_{i,l}^{(2)}N_{v+i-1}(k\rho), \tag{20}$$

where $i=1,2$, $k^2=(1-a_1/2)(E^2-m^2)$, $v=l+2bE$ and $C_{i,l}^{(1)}$, $C_{i,l}^{(2)}$ are constant spinors. The functions $J_{v+i-1}(k\rho)$ and $N_{v+i-1}(k\rho)$ are Bessel functions of first and second kind, respectively.

The results obtained show us that there exist a dependence with the angular momentum of the source, although this quantity does not have any influence on the curvature, in the limit of weak field we are considering.

To calculate the probability current and exhibit explicitly the influence of the spin on the trajactories of the particle, let us write the Dirac probability current in the Gordon decomposition form which is given by

$$j^{\mu}=\frac{1}{2m}\partial_{\mu}(\overline{\Psi}\sigma^{\mu\lambda}\Psi)+\frac{i}{4m}g^{\mu\lambda}[\overline{\Psi}\partial_{\lambda}\Psi-(\partial_{\lambda}\overline{\Psi})\Psi]+\frac{i}{4m}\overline{\Psi}([\partial_{\lambda}\gamma^{\mu},\gamma^{\mu}]+[\gamma^{\mu},\partial_{\lambda}\gamma^{\mu}])\Psi$$
$$+\frac{i}{2m}\overline{\Psi}[\gamma^{\lambda}\Gamma_{\lambda},\gamma^{\mu}]\Psi. \tag{21}$$

In order to calculate the current associated with a particle in this space-time, we need the following relations:

$$\sigma^{01}=i\gamma^{(0)}\gamma^{(1)}+\frac{ib}{\rho}\gamma^{(2)}\gamma^{(1)},$$

$$\sigma^{02}=\frac{i}{\rho}\gamma^{(0)}\gamma^{(2)}+\frac{ib}{\rho^{2}}\gamma^{(2)}\gamma^{(2)},$$

$$\sigma^{03}=i\gamma^{(0)}\gamma^{(3)}+\frac{ib}{\rho}\gamma^{(2)}\gamma^{(3)},$$

$$\sigma^{12}=i\gamma^{(1)}\gamma^{(0)}+\frac{ib}{\rho}\gamma^{(1)}\gamma^{(2)},$$

$$\sigma^{13}=i\gamma^{(1)}\gamma^{(3)},$$

$$\sigma^{23}=i\left(1-\frac{a(\rho)}{2}\right)\gamma^{(1)}\gamma^{(3)},$$

$$[\gamma^{\lambda}\Gamma_{\lambda},\gamma^{0}]=\frac{1}{\rho}\left(1+\frac{a(\rho)}{2}\right)\gamma^{(1)}\gamma^{(0)}+\frac{b}{\rho^{2}}\gamma^{(1)}\gamma^{(2)},$$

$$[\gamma^{\lambda}\Gamma_{\lambda},\gamma^{1}]=0,$$

$$[\gamma^{\lambda}\Gamma_{\lambda},\gamma^{2}]=\frac{2}{\rho^{2}}\gamma^{(1)}\gamma^{(2)},$$

$$[\gamma^{\lambda}\Gamma_{\lambda},\gamma^{3}]=\frac{2}{\rho}\gamma^{(1)}\gamma^{(3)}. \tag{22}$$

Substituting the set of equations (22) into Eq. (21), we obtain the result

$$j_{t}=\vec{\nabla}\cdot\vec{P}-\frac{2b}{\rho}\left[\frac{1}{\rho}M_{z}-(\vec{\nabla}\times\vec{M})_{\varphi}\right]+\rho_{\mathrm{conv}},$$

$$j_{\rho}=-\partial_{t}P_{\rho}+(\vec{\nabla}\times\vec{M})_{\rho}-\frac{2b}{\rho}\partial_{t}M_{z}+j_{\rho,\mathrm{conv}},$$

$$j_{\varphi}=-\partial_{t}P_{\varphi}+(\vec{\nabla}\times\vec{M})_{\varphi}-\frac{1}{\rho}M_{z}+j_{\varphi,\mathrm{conv}}, \tag{23}$$

$$j_z = -\partial_t P_z + (\vec{\nabla} \times \vec{M})_z - \frac{2b}{\rho}\partial_t M_\rho + j_{z,\mathrm{conv}},$$

where the convective part (subscript conv) is derived from $(i/4m)g^{\mu\lambda}[\overline{\Psi}\partial_\lambda\Psi - (\partial_\lambda\overline{\Psi})\Psi]$. The components of the polarization densities are given by

$$P_\rho = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(\rho)}\Psi,$$

$$P_\varphi = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(\varphi)}\Psi, \tag{24}$$

$$P_z = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(z)}\Psi,$$

where $\gamma_\rho = \gamma_1 \cos\varphi + \gamma_2 \sin\varphi$ and $\gamma_\varphi = \gamma_1 \sin\varphi + \gamma_2 \cos\varphi$.

The components of the magnetization current density vector, $\vec{M}$, are

$$M_\rho = \frac{i}{4M}\overline{\Psi}[\gamma_{(\varphi)}, \gamma_{(z)}]\Psi,$$

$$M_\varphi = \frac{i}{4M}\overline{\Psi}[\gamma_{(z)}, \gamma_{(\rho)}]\Psi, \tag{25}$$

$$M_z = \frac{i}{4M}\overline{\Psi}[\gamma_{(\rho)}, \gamma_{(\varphi)}]\Psi.$$

These results show us that the current also depends on the angular moment of the source, as well as on the Newtonian potential, $a(\rho)$, in the region where the particle is living.

It is worth calling attention to the fact that the Riemann curvature tensor, in this case, does not vanish, but does not depend on the angular momentum, and the solution and the current depend on the angular momentum of the source. This is a manifestation of the global features of the space-time generated by a rotating cylindrical shell, in the weak field approximation, and represents a gravitational analog of the Aharonov-Bohm effect.

IV. RELATIVISTIC QUANTUM SYSTEM IN THE SPACE-TIME OF A MOVING MASS CURRENT

In this section, we will consider a massive spinor particle in the weak gravitational field due to a moving mass current which moves slowly with velocity, v, in the z direction.

In order to solve the Dirac equation for a massive particle, given by Eq. (5), in this space-time given by the line element (4), let us choose the following set of tetrads:

$$e^{\mu}_{(a)} = \begin{pmatrix} 1+\frac{\Phi(\rho)}{2} & 0 & 0 & -2v\Phi(\rho) \\ 0 & 1-\frac{\Phi(\rho)}{2} & 0 & 0 \\ 0 & 0 & \frac{1-\frac{\Phi(\rho)}{2}}{\rho} & 0 \\ 0 & 0 & 0 & 1-\frac{\Phi(\rho)}{2} \end{pmatrix}. \tag{26}$$

In this space-time, the product $\gamma^{\mu}\Gamma_{\mu}$ that appears in the Dirac equation is given by

$$\gamma^{\mu}\Gamma_{\mu} = \gamma^{(a)}A_{(a)} = \frac{1}{2\rho}\left(1-\frac{\Phi}{2}\right)\gamma^{(1)}. \tag{27}$$

In this case, the generalized $\gamma^{\mu}(x)$ matrices are expressed in terms of the Dirac matrices as

$$\begin{aligned} \gamma^{0}(x) &= \left(1+\frac{\Phi(\rho)}{2}\right)\gamma^{(0)} - 2v\Phi(\rho)\gamma^{(3)}, \\ \gamma^{1}(x) &= \left(1-\frac{\Phi(\rho)}{2}\right)\gamma^{(1)}, \\ \gamma^{2}(x) &= \frac{1}{\rho}\left(1-\frac{\Phi(\rho)}{2}\right)\gamma^{(2)}, \\ \gamma^{3}(x) &= \left(1-\frac{\Phi(\rho)}{2}\right)\gamma^{(3)}. \end{aligned} \tag{28}$$

Substituting Eqs. (27) and (28) into (5), we obtain the following result for the Dirac equation in this space-time:

$$(AE-m)R_1 - (Bk+i\overline{v}E)aR_1 + \left(iB\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{iBl}{\rho} + \frac{iB}{2\rho}\right)R_2 = 0, \tag{29}$$

$$(AE-m)R_2 - (Bk+i\overline{v}E)R_2 + \left(iB\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{ilB}{\rho} + \frac{iB}{2\rho}\right)R_1 = 0, \tag{30}$$

$$-(AE+m)aR_1 + (Bk+i\overline{v}E)R_1 - \left(iB\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{ilB}{\rho} + \frac{iB}{2\rho}\right)R_2 = 0, \tag{31}$$

$$-(AE+m)bR_2 + (Bk-i\overline{v}E)R_2 + \left(-iB\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{ilB}{\rho} - \frac{iB}{2\rho}\right)R_1 = 0, \tag{32}$$

where $A=1+\Phi_1/2$, $B=1-\Phi_1/2$, and $\overline{v}=2v\Phi_1$, and we have considered that the components of the spinor, Ψ_j, solution of the Dirac equation can be written as

$$\Psi_j = e^{-iEt}e^{i(l\varphi+kz)}R_j(\rho), \quad j=1,2,3,4 \tag{33}$$

with $R_3=R_1$ e $R_4=R_2$.

Combining Eqs. (29)–(32), we obtain the following equations for $R_1(\rho)$ and $R_2(\rho)$,

$$B^2\frac{d^2R_1}{dr^2}+\frac{B^2}{\rho}\left(l+\frac{1}{2}\right)\frac{dR_1}{dr}+\left\{\frac{B^2}{\rho^2}\left[l(l+1)+\frac{1}{4}-\frac{1}{2B}\right]+pq\right\}R_1=0 \tag{34}$$

and

$$B^2\frac{d^2R_2}{dr^2}+\frac{B^2}{\rho}\left(l-\frac{1}{2}\right)\frac{dR_2}{dr}+\left\{\frac{B^2}{\rho^2}\left[l(l+1)-\frac{1}{4}-\frac{1}{2B}\right]-p'q'\right\}R_2=0, \tag{35}$$

where

$$p=AE-m-(Bk+i\overline{v}\overline{E}),$$

$$q=AE-m-(Bk+i\overline{v}\overline{E}),$$

$$p'=\overline{v}\overline{E}+Bk-(AE+m),$$

$$q'=\overline{v}\overline{E}+Bk+(AE+m).$$

The solutions of (34) and (35) are given by

$$R_1(\rho)=C_1\rho^{(1/2-u/2B)}J_\nu\left(\sqrt{\frac{\tau}{B}}\rho\right)+C_2\rho^{(1/2-u/2B)}J_\nu\left(\sqrt{\frac{\tau}{B}}\rho\right) \tag{36}$$

and

$$R_2(\rho)=C_1'\rho^{(1/2-u/2B)}J_{\overline{\nu}}\left(\sqrt{\frac{\overline{\tau}}{B}}\rho\right)+C_2'\rho^{(1/2-u/2B)}N_{\overline{\nu}}\left(\sqrt{\frac{\overline{\tau}}{B}}\rho\right), \tag{37}$$

where

$$\nu=\frac{1}{2}\sqrt{\frac{B^2-2uB+u^2-4\omega^2B}{B^2}},$$

$$\overline{\nu}=\frac{1}{2}\sqrt{\frac{B^2-2\overline{u}B+\overline{u^2}-4\overline{\omega^2}B}{B^2}},$$

$$\omega=B^2\left[l(l-1)+\frac{1}{4}-\frac{1}{2B}\right],$$

$$\tau=pq,$$

$$\overline{u}=-B^2\left(\frac{1}{2}-l\right),$$

$$u=B^2\left(l+\frac{1}{2}\right),$$

$$\overline{\omega}=-B^2\left(l+\frac{1}{4}\right),$$

$$\overline{\tau} = p'q'.$$

Note that these solutions depend on the velocity of the source. In this case the Riemann tensor does not depend on the velocity of the source, and therefore, the obtained result means that the dependence of the solution with the velocity is of purely global origin.

The current can be computed using Eq. (21). To this we will use the following expressions:

$$\sigma^{01} = i[\gamma^{(0)}\gamma^{(1)} - 2v\Phi\gamma^{(3)}\gamma^{(1)}],$$

$$\sigma^{02} = \frac{i}{\rho}[\gamma^{(0)}\gamma^{(2)} - 2v\Phi\gamma^{(3)}\gamma^{(2)}],$$

$$\sigma^{03} = i[\gamma^{(0)}\gamma^{(3)} - 2v\Phi\gamma^{(3)}\gamma^{(3)}],$$

$$\sigma^{12} = \frac{i}{\rho}\gamma^{(1)}\gamma^{(2)}, \tag{38}$$

$$\sigma^{13} = i\gamma^{(1)}\gamma^{(3)},$$

$$\sigma^{32} = \frac{i(1-\Phi)}{\rho}\gamma^{(3)}\gamma^{(2)},$$

$$[\gamma^{\lambda}\Gamma_{\lambda}, \gamma^{0}] = \frac{2}{\rho}\gamma^{(1)}\gamma^{(0)} - \frac{4v\Phi}{\rho}\gamma^{(1)}\gamma^{(3)}, \tag{39}$$

$$[\gamma^{\lambda}\Gamma_{\lambda}, \gamma^{1}] = 0, \tag{40}$$

$$[\gamma^{\lambda}\Gamma_{\lambda}, \gamma^{2}] = \frac{2(1-\Phi)}{\rho}\gamma^{(1)}\gamma^{(3)}. \tag{41}$$

Substituting these results into Eq. (22), we get

$$j_t = \vec{\nabla}\cdot\vec{P} - \frac{2v}{\rho^2}M_{\varphi} + \rho_{\mathrm{conv}},$$

$$j_{\rho} = -\partial_t P_{\rho} + (\vec{\nabla}\times\vec{M})_{\rho} - \frac{2v}{\rho}\partial_t M_{\rho} + j_{\rho,\mathrm{conv}},$$

$$j_{\varphi} = -\partial_t P_{\varphi} + (\vec{\nabla}\times\vec{M})_{\varphi} + j_{\varphi,\mathrm{conv}},$$

$$j_z = -\partial_t P_z + (\vec{\nabla}\times\vec{M})_z - \frac{2v}{\rho}\partial_t M_{\rho} + j_{z,\mathrm{conv}},$$

where the components polarization and magnetization vectors, $\vec{P}$ and $\vec{M}$, respectively, are given by

$$P_{\rho} = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(\rho)}\Psi,$$

$$P_{\varphi} = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(\varphi)}\Psi,$$

$$P_{z} = \frac{i}{2M}\overline{\Psi}\gamma_{(0)}\gamma_{(z)}\Psi,$$

$$M_{\rho} = \frac{i}{4M}\overline{\Psi}[\gamma_{(\theta)}, \gamma_{(z)}]\Psi,$$

$$M_{\varphi} = \frac{i}{4M}\overline{\Psi}[\gamma_{(z)}, \gamma_{(\rho)}]\Psi,$$

$$M_{z} = \frac{i}{4M}\overline{\Psi}[\gamma_{(\rho)}, \gamma_{(\varphi)}]\Psi.$$

From the obtained results, we conclude that the solution of the Dirac equation, as well as the current associated with the particle, depend on the velocity of the source, which does not have any influence on the curvature, in the weak field approximation. This is a manifestation of an analog of the electromagnetic Aharonov-Bohm effect, but in the present case in the context of the gravitational field.

V. CONCLUDING REMARKS

The obtained results show us that the solutions of the Dirac equation and the associated probability currents depend on the angular momentum and on the velocity. The parameters determine the gravitational fields we have considered, namely, the gravitational fields generated by a slowly rotating cylindrical shell and by a slowly moving mass current.

It is worth calling attention to the fact that in the region of motion of the massive spinor-1/2 particle, the Riemann curvature, in the weak field approximation, does not depend on the angular momentum or on the velocity of the source, respectively, for the rotating cylindrical shell and the moving mass current, but the solutions and probability currents for both cases do depend on these quantities. This result means that even in the situation in which the particle is constrained to move in a region where the Riemann curvature does not depend on the angular, or on the velocity of the source, it exhibits a gravitational effect associated with these quantities. This dependence on parameters which do not have any influence on the Riemann curvature tensor, in the weak field approximation, is a manifestation of a global phenomenon associated with these gravitational fields, which is called gravitational Aharonov-Bohm effect.

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Poincaré-Birkhoff periodic orbits for mechanical Hamiltonian systems on $T^*\mathbb{T}^n$

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Here, a version of the Arnol'd conjecture, first studied by Conley and Zehnder, giving a generalization of the Poincaré-Birkhoff last geometrical theorem, is proved inside Viterbo's framework of the generating functions quadratic at infinity. We give brief overviews of some tools that are often utilized in symplectic topology. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2211930]

I. INTRODUCTION

Henri Poincaré has been the main pioneer of the modern dynamical systems theory. Among the large multitude of his contributes, he formulated what is now called "Poincaré's last geometrical theorem" in order to schematize a crucial class of problems related to the search of period solutions in Hamiltonian dynamics:

{P} *Any area preserving diffeomorphism of the annulus* $A=\{(x,y)\in\mathbb{R}^2: a\leqslant x^2+y^2\leqslant b\}$ *into itself, uniformly rotating the two boundary circles of radius a and b in opposite directions, admits at least two geometrically distinct fixed points.*

The first rigorous proof of this statement was given in the 1920s by Birkhoff by means of a technique that seems not easily extendible to greater dimensional systems. In a following paper,[4] he remarked on the power of "maximum-minimum considerations" in the existence of periodic orbits. Nowadays, theseaspects are well ruled in the Lusternik-Schnirelman setting: in this framework, one can select minimax critical values (connected to periodic orbits) of suitable generating functions—quadratic at infinity (see below).

In the 1960s, in a series of papers Arnol'd proposed his celebrated conjecture (see Ref. 1):

{A} *Any Hamiltonian diffeomorphism of a compact symplectic manifold* (M,ω) *possesses at least many fixed points as a function* $f: M\to\mathbb{R}$ *on* M *possesses critical points.*

This new and intriguing topological question has been answered by Conley and Zehnder,[10] in the case where $M=\mathbb{T}^{2n}$; in that same paper they also proved that

{C-Z} *For a Hamiltonian* $H:\mathbb{R}\times T^*\mathbb{T}^n\to\mathbb{R}$, *such that for* $|p|\geqslant C$ *the related vector field* X_H *is p-linear and independent of* $q\in\mathbb{T}^n$ *and* $t\in\mathbb{R}$, *the time-one flow* ϕ_H^1 *of* X_H *admits at least many fixed points as a function* $f:\mathbb{T}^n\to\mathbb{R}$ *on* $\mathbb{T}^n$ *possesses critical points.*

It is interesting to note that this last statement, directly descending from Poincaré's last geometrical theorem, in a sense comes back to the original setting of analytical mechanics in which it arose. E.g., the above Hamiltonians are at once interpreted as describing a physical landscape in which a number of particles does interact among them only under a suitable energy threshold (low energy scattering):

$$H(q,p)=1/2|p|^2+f(q,p),\quad q\in\mathbb{T}^n,\quad f\in O(1).$$

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Incidentally, we can note that this is quite near to a typical Hamiltonian setting of Nekhoroshev perturbation theory: $H(q,p)=1/2|p|^2+\varepsilon f(q,p)$.

Conley and Zehnder introduced a sort of Liapunov-Schmidt reduction technique, now known as *Amann-Conley-Zehnder reduction*, based on a suitable Fourier cutoff on the loop space and giving, at last, a finite dimensional variational problem. Later, Chaperon (see Ref. 5) proposed his new ingenious *broken geodesics reduction*, showing it is not indispensable to start from the infinite dimensional formulation of the problem. In both cases, the estimates on fixed points of ϕ_H^1 are proved using the isolated invariant sets and the Morse index, as presented by Conley.[9]

More recently, Golé[12,13] gave an alternative proof of the statement {C-Z}, extending $\mathbb{T}^n$ to any compact manifold and using a variation of Chaperon's argument. The finite variational problem that in such a way he obtained was solved by utilizing techniques based on the Conley index and further results on it by Floer. Furthermore, the author pointed out that his function, defining the above finite variational problem, was not a generating function quadratic at infinity, an essential property in order to agreeably apply the Lusternik-Schnirelman theory.

Nowadays, a short and nice proof of this theorem can be built up using the fine papers[6,7] by Chaperon.

After the impressive paper,[22] there exists a rather common growing prejudgment that the framework of the generating function quadratics at infinity and the Lusternik-Schnirelman theory should be the right environment to better understand many actual aspects of symplectic topology, as in the Arnol'd conjecture (see Ref. 15, p. 216).

In this paper, by assuming this point of view, we restart from the original statement {C-Z}, for $\mathbb{T}^n$. In genuine framework of the generating function quadratics at infinity, and then using the now classical results of Chaperon, Chekanov, Laudenbach, and Sikorav and Viterbo, we propose a finite variational problem consisting of a generating function quadratic at infinity: a suitable application of the Lusternik-Schnirelman theory in the degenerate case, and the Morse theory in the nondegenerate one, produces the expected result. By making this goal, we give brief overviews on some of the tools used here, and that are often involved in symplectic topology.

II. PRELIMINARIES

A. Generating functions

Let N be a compact manifold and $L\subset T^*N$ a Lagrangian submanifold. If $L=\mathrm{im}(df)=L_f$, where $f:N\to\mathbb{R}$ is a C^2 function, then the set $\mathrm{crit}(f)$ of the critical points of f coincides with the intersection of L_f with the zero section $0_N\subset T^*N$:

$$\mathrm{crit}(f)=L_f\cap 0_N.$$

In the more general case, Lagrangian submanifolds do not have the above graph structure L_f, and a classical argument by Maslov and Hörmander shows that, at least locally, every Lagrangian submanifold is described by some generating function like $S:N\times\mathbb{R}^k\to\mathbb{R}$, $(x,\xi)\mapsto S(x,\xi)$, in the following way:

$$L_S:=\left\{\left(x,\frac{\partial S}{\partial x}(x,\xi)\right):\frac{\partial S}{\partial \xi}(x,\xi)=0\right\},$$

where 0 is a regular value of the map $(x,\xi)\mapsto \partial S/\partial\xi(x,\xi)$.

Some authors (e.g., Benenti, Tulczyjew, and Weinstein) say that in this case the generating function S is a *Morse family*. In order to apply the calculus of variations to generating functions, one needs a condition implying the existence of critical points. In particular, the following class of generating functions has been decisive in many issues:

Definition 2.1: A generating function $S:N\times\mathbb{R}^k\to\mathbb{R}$ is quadratic at infinity (GFQI) if for $|\xi|>C$

$$S(x,\xi)=\xi^T Q\xi, \tag{1}$$

where $\xi^T Q \xi$ is a nondegenerate quadratic form.

In the literature (see, e.g., Refs. 16 and 23) two main operations on the generating functions that leave the corresponding Lagrangian submanifolds invariant are known. Lemmas 2 and 3 below recollect these facts. The globalization was realized by Viterbo (see Ref. 21).

Lemma 2.2: Let $S: N \times \mathbb{R}^k \to \mathbb{R}$ be a GFQI and $N \times \mathbb{R}^k \ni (x, \xi) \mapsto (x, \phi(x, \xi)) \in N \times \mathbb{R}^k$ a map such that, $\forall x \in N$,

$$\mathbb{R}^k \ni \xi \mapsto \phi(x, \xi) \in \mathbb{R}^k$$

is a diffeomorphism. Then $S_1(x, \xi) := S(x, \phi(x, \xi))$ generates the same Lagrangian submanifold: $L_{S_1} = L_S$.

Proof: Since ϕ is a diffeomorphism, $\partial S_1 / \partial \xi = \partial S / \partial \xi \partial \phi / \partial \xi = 0$ if and only if $\partial S / \partial \xi = 0$. Moreover, $\partial S_1 / \partial x = \partial S / \partial x + \partial S / \partial \xi \partial \phi / \partial x$ and it is immediately verified that 0 is a regular value for $\partial S_1 / \partial \xi(x, \xi)$. □

Lemma 2.3: Let $S: N \times \mathbb{R}^k \to \mathbb{R}$ be a GFQI. Then

$$S_1(x, \xi, \eta) := S(x, \xi) + \eta^T B \eta,$$

where $\eta \in \mathbb{R}^l$ and $\eta^T B \eta$ is a nondegenerate quadratic form, generates the same Lagrangian submanifold: $L_{S_1} = L_S$.

Proof. $\partial S_1 / \partial \xi(x, \xi, \eta) = 0$ if and only if $\partial S / \partial \xi(x, \xi) = 0$. Moreover, $\partial S_1 / \partial \eta(x, \xi, \eta) = 0$ if and only if $B\eta = 0$, that is $\eta = 0$. Thus

$$\left. \frac{\partial S_1}{\partial x} \right|_{\partial S_1 / \partial \xi = 0, \partial S_1 / \partial \eta = 0} = \left. \frac{\partial S}{\partial x} \right|_{\partial S / \partial \xi = 0}.$$

□

Finally, as a third—although trivial—invariant operation, we observe that by adding to a generating function S any arbitrary constant $c \in \mathbb{R}$, the described Lagrangian submanifold is invariant: $L_{S+c} = L_S$. Problems 1 and 2 below have been crucial in the global theory of Lagrangian submanifolds and their parameterizations.

1. When does a Lagrangian submanifold $L \subset T^*N$ admit a FGQI?
2. If L admits a GFQI, when can we state the uniqueness of it (up to the operations described above)?

The following theorem (see Ref. 18) partially answers the first question.

Theorem 2.4: *(Chaperon-Chekanov-Laudenbach-Sikorav) Let 0_N be the zero section of T^*N and $(\phi_t)_{t \in [0,1]}$ a Hamiltonian isotopy. Then the Lagrangian submanifold $\phi_1(0_N)$ admits a GFQI.*

The answer to the second problem is due to Viterbo:

Theorem 2.5: *(Viterbo) Let 0_N be the zero section of T^*N and $(\phi_t)_{t \in [0,1]}$ a Hamiltonian isotopy. Then the Lagrangian submanifold $\phi_1(0_N)$ admits a unique (up to the operations described above) GFQI.*

The theorems above (see also Ref. 20) still hold in T^*R^n, provided that $(\phi_t)_{t \in [0,1]}$ is a flow of a compactly supported Hamiltonian vector field.

B. Lusternik-Schnirelman theory

Let $f: N \to \mathbb{R}$ be a C^2 function. We shall assume that either N is compact or f satisfies the Palais-Smale (PS) condition:

(PS) Any sequence $\{x_n\}$ such that $\nabla f(x_n) \to 0$ and $f(x_n)$ is bounded, admits a converging subsequence.

We recall now some results of the Lusternik-Schnirelman theory, which allow us to associate critical values of f to nonvanishing relative cohomology classes and to give a lower bound to the number of critical points of f in terms of the topological complexity of N.

Let us define the sublevel sets

$$N^\nu := \{x \in N : f(x) \leqslant \nu\}. \tag{2}$$

(PS) condition guarantees the well-defined gradient vector field ∇f, whose flow realizes a diffeomorphism between N^μ and N^ν whenever no critical values exist in $[\mu, \nu]$:

Proposition 2.6: Let $\mu < \nu$. If f has no critical points in $N^\nu \backslash N^\mu$, then $H^*(N^\nu, N^\mu) = 0$.

Thus if $H^*(N^\nu, N^\mu) \neq 0$, then in $N^\nu \backslash N^\mu$ there exists at least one critical point of f, with critical value in $[\mu, \nu]$. For $\lambda \in [\mu, \nu]$, let $i_\lambda : N^\lambda N^\nu$ be the inclusion.

Definition 2.7: For every $u \in H^*(N^\nu, N^\mu)$, $u \neq 0$, we define:

$$c(u,f) =: \inf\{\lambda \in [\mu, \nu] : i_\lambda^* u \neq 0\},$$

where

$$i_\lambda^* : H^*(N^\nu, N^\mu) \to H^*(N^\lambda, N^\mu)$$

denotes the pull-back of the inclusion.

This Definition provides a tool to detect critical values, indeed:

Theorem 2.8. *$c(u,f)$ is a critical value of f.*

The main result of this construction consists of the following.

Theorem 2.9. (*Cohomological Lusternik-Schnirelman theory*) *Let $0 \neq u \in H^*(N^\nu, N^\mu)$* and *$v \in H^*(N^\nu) \backslash H^0(N^\nu)$.*

1.

$$c(u \wedge v, f) \geqslant c(u,f). \tag{3}$$

2. *If (3) is an equality ($c(u \wedge v, f) = c(u,f) =: c$), set $K_c = \{x : df(x) = 0, f(x) = c\}$, then, for every neighborhood U of K_c, v is not vanishing in $H^*(U)$, and the common critical level contains infinitely many critical points.*

Corollary 2.10: Let N be a compact manifold. The function $f : N \to \mathbb{R}$ has at least a number of critical points equal to the cup-length of N:

$$\mathrm{cl}(N) := \max\{k : \exists\, v_1, \ldots, v_{k-1} \in H^*(N) \setminus H^0(N) \text{ s . t . } v_1 \wedge \ldots \wedge v_{k-1} \neq 0\}. \tag{4}$$

Proof: Apply Theorem 2.9 with $\mu < \inf f$, $\sup f < \nu$, and $u = 1 \in H^*(N, \emptyset) = H^*(N)$. □

By Corollary 2.11 below, we verify that the preceding estimate on the number of critical points of f still holds in the noncompact case whenever GFQI f are taken into account.

Corollary 2.11: Let N be a compact manifold and $f : N \times \mathbb{R}^n \to \mathbb{R}$ be a GFQI, $f(x, \xi) = Q(\xi)$ out of a compact set in the parameters ξ. Then, for $c > 0$ large enough, there exist $0 \neq u \in H^*(f^c, f^{-c})$ and $v_1, \ldots, v_{k-1}$ as in (4) such that

$$u \wedge p^* v_1 \wedge \ldots \wedge p^* v_{k-1} \neq 0,$$

where $p : N \times \mathbb{R}^n \to N$ is the canonical projection. Consequently, the GFQI $f : N \times \mathbb{R}^n \to \mathbb{R}$ has at least cl(N) *critical points.*

Proof: Let us first observe that for $c > 0$ large enough, the sublevel sets of f are invariant from a homotopical point of view: $f^{\pm c} = N \times Q^{\pm c}$, and $f^{\pm \bar{c}}$ retracts on $f^{\pm c}$ for any $\bar{c} > c$. Let $A := Q^{-(c+\varepsilon)}$, $\varepsilon > 0$ small. Then the isomorphisms below (the first one by excision and the second one by retraction) hold:

$$H^*(Q^c, Q^{-c}) \cong H^*(Q^c \setminus \mathring{A}, Q^{-c} \setminus \mathring{A}) \cong H^*(D^i, \partial D^i),$$

where i is the index of the quadratic form Q and D^i denotes the disk (of radius $\sqrt{c}$) in $\mathbb{R}^i$. Consequently

$$H^h(Q^c,Q^{-c}) \cong H^h(D^i,\partial D^i) = \begin{cases} 0 & \text{if } h \neq i \\ \alpha\mathbb{R} & \text{if } h = i \end{cases}.$$

To conclude in the noncompact case $N\times\mathbb{R}^n$, by the Künneth isomorphism

$$H^*(N) \cong H_c^{*+i}(N\times\mathbb{R}^i)$$

and the homotopy argument

$$H_c^*(N\times\mathbb{R}^i) \cong H^*(N\times D^i, N\times\partial D^i),$$

the following isomorphism,

$$H^*(N) \ni v \mapsto q^*\alpha\wedge p^*v \in H^{*+i}(N\times D^i, N\times\partial D^i),$$

holds, where $p:N\times\mathbb{R}^n\to N$, $q=(q_1,q_2):(N\times D^i,N\times\partial D^i)\to(D^i,\partial D^i)$ are the standard projections. Now we apply Theorem 2.9 with $u=q^*\alpha$; since $q^*\alpha\wedge p^*v_1\wedge\ldots\wedge p^*v_{k-1}=q^*\alpha\wedge p^*(v_1\wedge\ldots\wedge v_{k-1})\neq 0$ whenever $v_1\wedge\ldots v_{k-1}\neq 0$, then the number of critical points of the GFQI $f:N\times\mathbb{R}^n\to\mathbb{R}$ is at least $\mathrm{cl}(N)$. □

III. THE HAMILTONIAN SETTING

Let $T^*\mathbb{R}^n\equiv\mathbb{R}^{2n}=\{(q,p):q\in\mathbb{R}^n,p\in\mathbb{R}^n\}$ be endowed with the standard symplectic form $\omega=dp\wedge dq=\Sigma_{i=1}^n dp_i\wedge dq^i$.

On $(\mathbb{R}^{2n},\omega)$ we consider the-time-dependent globally Hamiltonian vector field X_H given by

$$H(t,q,p) \in C^2(\mathbb{R}\times\mathbb{R}^{2n};\mathbb{R}),$$

periodic in q of period 2π and

$$H(t,q,p) = \frac{1}{2}|p|^2 \text{ if } |p| \geqslant C > 0. \tag{5}$$

Our aim is to draw a new proof of a popular version, due to Arnol'd, of Poincaré's last geometrical theorem (see Refs. 6, 7, 10, and 12) inside Viterbo's framework of symplectic topology.[22]

A. Properties of flows on the cotangent of the torus

In connection with the above Hamiltonian H, let (here, as in other analogous circumstances, we mean $\phi_H^t:=\phi_H^{t,0}$) ϕ_H^t be the flow of the Hamiltonian vector field X_H, $\omega(X_H,\eta)=-dH(\eta)$, so that $X_H=J\nabla H$, where J is the symplectic $2n$-matrix. The n-torus is denoted by $\mathbb{T}^n=\mathbb{R}^n/2\pi\mathbb{Z}^n$. Therefore a Hamiltonian $\bar{H}$ and the related flow $\phi_{\bar{H}}^t$ are well defined on $T^*\mathbb{T}^n$ (see Corollary 3.2 below):

$$\begin{array}{ccc} \mathbb{R}\times T^*\mathbb{R}^n & \xrightarrow{H} & \mathbb{R} \\ {\scriptstyle \mathrm{id}\times\pi}\downarrow & & \downarrow{\scriptstyle id_{\mathbb{R}}} \\ \mathbb{R}\times T^*\mathbb{T}^n & \xrightarrow[\bar{H}]{} & \mathbb{R} \end{array} \qquad \begin{array}{ccc} T^*\mathbb{R}^n & \xrightarrow{\phi_H^t} & T^*\mathbb{R}^n \\ {\scriptstyle \pi}\downarrow & & \downarrow{\scriptstyle \pi} \\ T^*\mathbb{T}^n & \xrightarrow[\phi_{\bar{H}}^t]{} & T^*\mathbb{T}^n \end{array}$$

It is standard matter to see that

Proposition 3.1: The flow ϕ_H^t associated to H satisfies

$$(\phi_H^t)_q(q+2\pi k,p) = (\phi_H^t)_q(q,p) + 2\pi k,$$

$$(\phi_H^t)_p(q+2\pi k,p) = (\phi_H^t)_p(q,p),$$

$\forall k\in\mathbb{R}^n$ *and* $\forall(q,p)\in\mathbb{R}^{2n}$.

We denote by $[q] \in \mathbb{T}^n := \mathbb{R}^n / 2\pi\mathbb{Z}^n$ the class of $q \in \mathbb{R}^n$. From the above deductions it follows that

Corollary 3.2: The flow of $X_{\bar{H}}$ is

$$\phi^t_{X_{\bar{H}}}([q],p) = ([\phi^t_{X_H,q}(q,p)], \phi^t_{X_H,p}(q,p)). \tag{6}$$

B. The splitting $H=H_0+f$

We remind that the Hamiltonian H coincides with $\frac{1}{2}|p|^2$ if $|p| \geqslant C > 0$. Consequently, outside of this compact set (in the p variables) the flow associated to the Hamiltonian H reduces to

$$\mathbb{R}^n \times \{p : |p| \geqslant C\} \to \mathbb{R}^n \times \{p : |p| \geqslant C\},$$

$$(q,p) \mapsto \phi^t_H(q,p) = (q + tp, p).$$

We split H as the sum of the Hamiltonian $H_0 := \frac{1}{2}|p|^2$ and a Hamiltonian f, hence necessarily compactly supported in the p variables,

$$H = H_0 + f : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R},$$

$$(t,q,p) \mapsto H(t,q,p) = H_0(p) + f(t,q,p).$$

Denoting by ϕ^t_0 the flow related to H_0, we define the Hamiltonian K as the pull-back of f with respect to ϕ^t_0:

$$K : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R},$$

$$K := (\phi^t_0)^* f, \quad \text{i.e.,} \quad K(t,q,p) = H(t, q + tp, p) - \frac{|p|^2}{2}.$$

This Hamiltonian K, which is compactly supported in the p variables like f, will be essential in the following sections. We indicate now ϕ^t_K, the flow of K, and write down the following proposition, which is, essentially, a result of Hamilton[14] (see also Ref. 11).

Proposition 3.3: Let ϕ^t_H, ϕ^t_0, and ϕ^t_K be the flows of $H=H_0+(H-H_0)$, H_0, and $K=(\phi^t_0)^*(H-H_0)$, respectively. We have

$$\phi^t_H(q,p) = \phi^t_0 \circ \phi^t_K(q,p),$$

$\forall (q,p) \in \mathbb{R}^n \times \mathbb{R}^n$ *and* $\forall t \in \mathbb{R}$.

We recall some technical premises to the proof of this fact.

Definition 3.4: (Push-forward) Let N be a manifold and ρ a diffeomorphism of N into itself,

$$N \overset{\rho}{\to} N,$$

$$x \mapsto y = \rho(x).$$

The push-forward ρ_* of a vector field X is defined as follows:

$$\rho_* X(y) := d\rho(\rho^{-1}(y)) X(\rho^{-1}(y)).$$

(Below, we will use this definition with $N=T^*R^n$ and $\rho=\phi^t_0$.) The following Lemma is a central result of the canonical transformations theory.

Lemma 3.5: Let M be a manifold and ρ a symplectic diffeomorphism of T^*M into itself, then, for every Hamiltonian function $L : T^*M \to R$,

$$\rho_* X_L = X_{\rho_* L} = X_{L\circ\rho^{-1}}.$$

Proof.

$$\begin{aligned}\frac{d}{dt}(\phi_0^t \circ \phi_K^t)(q,p) &= X_{H_0}(\phi_0^t \circ \phi_K^t(q,p)) + d\phi_0^t(\phi_K^t(q,p))X_K(\phi_K^t(q,p)) = X_{H_0}(\phi_0^t \circ \phi_K^t(q,p)) \\ &\quad + d\phi_0^t(\phi_0^{-t} \circ \phi_0^t \circ \phi_K^t(q,p))X_K(\phi_0^{-t} \circ \phi_0^t \circ \phi_K^t(q,p)) \\ &= X_{H_0}(\phi_0^t \circ \phi_K^t(q,p)) + (\phi_0^t)_* X_K(\phi_0^t \circ \phi_K^t(q,p)) \\ &= [X_{H_0} + X_{(\phi_0^t)_* K}](\phi_0^t \circ \phi_K^t(q,p)) = X_{H_0+f}(\phi_0^t \circ \phi_K^t(q,p)) \\ &= X_H(\phi_0^t \circ \phi_K^t(q,p)).\end{aligned}$$

□

C. The "graph" and the "cotangent" structures of R^{4n}

We introduce now the linear symplectic isomorphism h, from the "graph" structure to the "cotangent" structure:

$$h:(T^*\mathbb{R}^n \times T^*\mathbb{R}^n, \omega_{\mathbb{R}^n} \ominus \omega_{\mathbb{R}^n}) \to (T^*(T^*\mathbb{R}^n), \omega_{\mathbb{R}^{2n}}),$$

$$(q,p,Q,P) \mapsto (q,P,p-P,Q+P-q). \tag{7}$$

The following Lagrangian submanifold F of $(T^*\mathbb{R}^n \times T^*\mathbb{R}^n, \omega_{\mathbb{R}^n} \ominus \omega_{\mathbb{R}^n})$,

$$F := \{(q,p,q-p,p):(q,p) \in T^*\mathbb{R}^n\}, \tag{8}$$

is mapped by h to the zero section $0_{\mathbb{R}^{2n}}$: $h(F) = 0_{\mathbb{R}^{2n}} \subset \mathbb{R}^{4n}$.

Since we are looking for fixed points of ϕ_H^1, we denote by Γ_H and Γ_K the graphs of ϕ_H^1 and ϕ_K^1 in $(T^*\mathbb{R}^n \times T^*\mathbb{R}^n, \omega_{\mathbb{R}^n} \ominus \omega_{\mathbb{R}^n})$, respectively, and by Δ the diagonal of $T^*\mathbb{R}^n \times T^*\mathbb{R}^n = \mathbb{R}^{4n}$. It comes out that

$$(\bar{q},\bar{p}) \in T^*\mathbb{R}^n \text{ is a fixed point of } \phi_H^1,$$

that is, by Proposition 3.3,

$$(\bar{q},\bar{p},(\phi_0^1 \circ \phi_K^1)_q(\bar{q},\bar{p}),(\phi_0^1 \circ \phi_K^1)_p(\bar{q},\bar{p})) \in \Gamma_H \cap \Delta,$$

if and only if, setting

$$\hat{\phi}_0^{-1}(q,p,Q,P) := id_{R^{2n}} \times \phi_0^{-1}(q,p,Q,P) = (q,p,Q-P,P),$$

and using F in (8),

$$(\bar{q},\bar{p},(\phi_K^1)_q(\bar{q},\bar{p}),(\phi_K^1)_p(\bar{q},\bar{p})) \in \hat{\phi}_0^{-1}(\Gamma_H) \cap \hat{\phi}_0^{-1}(\Delta) = \Gamma_K \cap F,$$

if and only if, using h,

$$h(\bar{q},\bar{p},(\phi_K^1)_q(\bar{q},\bar{p}),(\phi_K^1)_p(\bar{q},\bar{p})) \in h(\Gamma_K) \cap h(F) = h(\Gamma_K) \cap 0_{\mathbb{R}^{2n}}.$$

Thus, we claim that the periodic time-one solutions, corresponding to fixed points of ϕ_H^1, are caught by the critical points of a (possible) generating function for $h(\Gamma_K)$. Furthermore, they are contained in the region $\mathbb{T}^n \times \{p:|p|<C\}$. In fact, on $\mathbb{T}^n \times \{p:|p| \geqslant C\}$ the Hamiltonian system is trivially integrable and in such a case the tori $\mathbb{T}^n \times \{p\}$ are invariant under the flow $\phi_H^t:(q,p) \mapsto (q+tp,p)$. Consequently, the nontrivial periodic solutions of ϕ_H^1, corresponding precisely to the fixed points of ϕ_H^1, must lie in $\mathbb{T}^n \times \{p:|p|<C\}$ and are contractible loops on $\mathbb{T}^n$.

IV. EXISTENCE FOR GENERATING FUNCTIONS

Our original problem has been translated into the investigation of $h(\Gamma_K) \cap 0_{\mathbb{R}^{2n}}$. The Lagrangian submanifold $h(\Gamma_K)$,

$$h(\Gamma_K) = \{(q,(\phi_K^1)_p(q,p),p-(\phi_K^1)_p(q,p),(\phi_K^1)_p(q,p)+(\phi_K^1)_q(q,p)-q),$$

$$\forall\,(q,p) \in T^*\mathbb{R}^n\} \subset (T^*\mathbb{R}^{2n},\omega_{\mathbb{R}^{2n}}),$$

in a neighborhood of infinity (in the p variables) results:

$$h(\Gamma_K) = \{(q,p,0,p),\ \forall\, q \in \mathbb{R}^n,\ \forall\, p \in \mathbb{R}^n : |p| \geqslant C\}.$$

In this section we study its structure, proving that it is the image [through a suitable symplectic isomorphism ψ of $(T^*\mathbb{R}^{2n},\omega_{\mathbb{R}^{2n}})$] of another Lagrangian submanifold, denoted by $\bar{h}(\Gamma_K)$, which is isotopic to the zero section of $T^*\mathbb{R}^{2n}$, so that it admits a GFQI (Theorem 2.4). This is crucial in order to gain the existence of a generating function for $h(\Gamma_K)$. In fact, by means of a natural composition of the above generating functions for $\bar{h}(\Gamma_K)$ and for ψ, we will be able to construct a GFQI for $h(\Gamma_K)$.

A. The factorization of the map *h*

We introduce the following linear two maps $\bar{h}$ (introduced by Sikorav in Ref. 19 and used by Viterbo in Ref. 22) and ψ:

$$\bar{h}:(T^*\mathbb{R}^n \times T^*\mathbb{R}^n, \omega_{\mathbb{R}^n} \ominus \omega_{\mathbb{R}^n}) \to (T^*(T^*\mathbb{R}^n),\omega_{\mathbb{R}^{2n}}), \tag{9}$$

$$(q,p,Q,P) \mapsto \left(\frac{q+Q}{2},\frac{p+P}{2},p-P,Q-q\right),$$

$$\psi:(T^*(T^*\mathbb{R}^n) = T^*\mathbb{R}^{2n},\omega_{\mathbb{R}^{2n}}) \to (T^*(T^*\mathbb{R}^n) = T^*\mathbb{R}^{2n},\omega_{\mathbb{R}^{2n}}),$$

$$(q,p,Q,P) =: (x_0,y_0) \mapsto (x_1,y_1) =: \left(\frac{2q-P}{2},\frac{2p-Q}{2},Q,\frac{2P+2p-Q}{2}\right). \tag{10}$$

It results in the following well-defined map on the quotient tori structures:

$$\tilde{\psi}:T^*(T^*\mathbb{T}^n) \to T^*(T^*\mathbb{T}^n),$$

$$([q],p,Q,P) \mapsto \left(\left[\frac{2q-P}{2}\right],\frac{2p-Q}{2},Q,\frac{2P+2p-Q}{2}\right),$$

and the following diagram is commutative:

$$\begin{array}{ccc} T^*(T^*\mathbb{R}^n) & \xrightarrow{\psi} & T^*(T^*\mathbb{R}^n) \\ \pi \downarrow & & \downarrow \pi \\ T^*(T^*\mathbb{T}^n) & \xrightarrow[\tilde{\psi}]{} & T^*(T^*\mathbb{T}^n) \end{array}$$

It is standard matter to see that the maps ψ and $\bar{h}$ are symplectic isomorphisms and it is easy to check that the factorization $h=\psi\circ\bar{h}$ holds:

$$\begin{array}{ccc} T^*\mathbb{R}^n \times T^*\mathbb{R}^n & \xrightarrow{h} & T^*(T^*\mathbb{R}^n) \\ & \searrow^{\bar{h}} & \uparrow \psi \\ & & T^*(T^*\mathbb{R}^n) \end{array}$$

B. The Lagrangian submanifold $\bar{h}(\Gamma_K)$

This section is devoted to the proof of the following

Proposition 4.1: The Lagrangian submanifold $\bar{h}(\Gamma_K)\subset(T^*\mathbb{R}^{2n},\omega_{\mathbb{R}^{2n}})$ *admits a GFQI,* $S_1(q,p;\xi)$, 2π*-periodic in the* q *variables.*

Proof: We observe that like H also the Hamiltonian K is periodic of the 2π-period in the q variables.:

$$K(t,q+2\pi k,p)=H(t,q+2\pi k+tp,p)-\frac{|p|^2}{2}=H(t,q+tp,p)-\frac{|p|^2}{2}=K(t,q,p),$$

$\forall t\in R$, $\forall(q,p)\in R^{2n}$, and $\forall k\in Z^n$. Moreover, the flow $\phi_K^t=\phi_0^{-t}\circ\phi_H^t$ inherits from the flow ϕ_H^t (see Proposition 3.3) the following properties:

$$(\phi_K^t)_q(q+2\pi k,p)=(\phi_K^t)_q(q,p)+2\pi k,$$

$$(\phi_K^t)_p(q+2\pi k,p)=(\phi_K^t)_p(q,p),$$

$\forall(q,p)\in\mathbb{R}^{2n}$, $\forall k\in\mathbb{Z}^n$.

Consequently, for all fixed $t\in\mathbb{R}$ a flow $\tilde{\phi}_K^{t,0}$ in $T^*\mathbb{T}^n$ are well-defined results, in particular, the following definition it is independent of the choice of q in the class $[q]$:

$$\tilde{\phi}_K^{t,0}([q],p)=((\tilde{\phi}_K^{t,0})_q([q],p),(\tilde{\phi}_K^{t,0})_p([q],p)):=([(\phi_K^t)_q(q,p)],(\phi_K^t)_p(q,p)),$$

$$\begin{array}{ccc} T^*\mathbb{R}^n & \xrightarrow{\phi_K^t} & T^*\mathbb{R}^n \\ \pi \downarrow & & \downarrow \pi \\ T^*\mathbb{T}^n & \xrightarrow[\tilde{\phi}_K^{t,0}]{} & T^*\mathbb{T}^n \end{array}$$

Here we mean $\pi:(q,p)\to([q],p)$.

Similarly to Γ_K, we indicate by $\tilde{\Gamma}_K$ the graph of $\tilde{\phi}_K^{1,0}$:

$$\tilde{\Gamma}_K\subset(T^*\mathbb{T}^n\times T^*\mathbb{T}^n,\omega_{\mathbb{T}^n}\ominus\omega_{\mathbb{T}^n}).$$

The Lagrangian submanifold $\bar{h}(\Gamma_K)$,

$$\bar{h}(\Gamma_K) = \left\{ \left(\frac{q + (\phi_K^1)_q(q,p)}{2}, \frac{p + (\phi_K^1)_p(q,p)}{2}, p - (\phi_K^1)_p(q,p), (\phi_K^1)_q(q,p) - q \right), \forall\, (q,p) \in T^*\mathbb{R}^n \right\} \subset (T^*\mathbb{R}^{2n}, \omega_{\mathbb{R}^{2n}}),$$

in a neighborhood of infinity (in the p variables) results:

$$\bar{h}(\Gamma_K) = \{(q,p,0,0),\ \forall\, q \in \mathbb{R}^n,\ \forall\, p \in \mathbb{R}^n : |p| \geqslant C\}.$$

It is easy to verify that if $(q,p,Q,P) \in \bar{h}(\Gamma_K)$, then $\forall k \in \mathbb{Z}^n (q + 2\pi k, p, Q, P) \in \bar{h}(\Gamma_K)$. Therefore the Lagrangian submanifold $\bar{h}(\Gamma_K) \subset (T^*\mathbb{R}^{2n}, \omega_{\mathbb{R}^{2n}})$ has a natural inclusion into $(T^*(T^n \times R^n), \omega_{T^n \times R^n})$. Now, we prove that $\bar{h}(\Gamma_K)$ coincides, up to the symplectic morphism $\tilde{h}$ below from $\tilde{\Gamma}_K$ to $T^*(\mathbb{T}^n \times \mathbb{R}^n)$, with the image of the zero section $\mathbb{T}^n \times \mathbb{R}^n$ through $\tilde{\phi}_K^{1,0}$. In order to see this, we introduce the following well-defined (independent of the choice of q in $[q]$) [We note that, unlike the map $\bar{h}$, it does not exist a natural definition of $\tilde{h}$ from $T^*\mathbb{T}^n \times T^*\mathbb{T}^n$ in $T^*(\mathbb{T}^n \times \mathbb{R}^n)$, since it is essential the property: $(\phi_K^1)_q(q + 2\pi k, p) = (\phi_K^1)_q(q,p) + 2\pi k$.] map

$$\tilde{h} : \tilde{\Gamma}_K \to T^*(\mathbb{T}^n \times \mathbb{R}^n),$$

$$([q], p, [(\phi_K^1)_q(q,p)], (\phi_K^1)_p(q,p)) \mapsto \left(\left[\frac{q + (\phi_K^1)_q(q,p)}{2} \right], \frac{p + (\phi_K^1)_p(q,p)}{2}, p - (\phi_K^1)_p(q,p), (\phi_K^1)_q(q,p) - q \right).$$

Therefore the following commutative diagram results:

$$\begin{array}{ccc} \Gamma_K & \xrightarrow{\bar{h}} & T^*\mathbb{R}^{2n} \\ \pi_1 \downarrow & & \downarrow \pi_2 \\ \tilde{\Gamma}_K & \xrightarrow[\tilde{h}]{} & T^*(\mathbb{T}^n \times \mathbb{R}^n) \end{array}$$

here we mean $\pi_1 : (q,p,Q,P) \to ([q],p,[Q],P)$, $\pi_2 : (q,p,Q,P) \to ([q],p,Q,P)$.

Thus we have proved that $\bar{h}(\Gamma_K)$ results, up to the symplectic diffeomorphism $\tilde{h}$, the image of the zero section $\mathbb{T}^n \times \mathbb{R}^n$ through $\tilde{\phi}_K^{1,0}$. On the other hand, the manifold $\tilde{h}(\tilde{\Gamma}_K)$ is essentially the image of the zero section $\mathbb{T}^n \times \mathbb{R}^n$ through $\tilde{\phi}_K^{1,0}$. In such a hypothesis (see Theorem 2.4) the manifold $\tilde{h}(\tilde{\Gamma}_K)$ admits a GFQI, say, $s([q],p,\xi)$. Then a GFQI for $\bar{h}(\Gamma_K)$, say, $S_1(q,p,\xi)$, can be obtained extending periodically (in the q variables) $s([q],p,\xi)$. □

C. A generating function for $h(\Gamma_K)$

In this section we build (see Lemma 4.2 below) a generating function for the linear symplectomorphism ψ. Combining it with the one above (see Proposition 4.1), we will state the existence of a generating function for $h(\Gamma_K)$ (see Proposition 4.3).

The following composition rule is popular in symplectic geometry and mechanics (see, e.g., Refs. 2 and 3), and it has been handled by Laudenbach and Sikorav in meaningful problems in symplectic topology (see Ref. 18).

Lemma 4.2: The linear symplectomorphism ψ [see (10)] admits the generating function $S_2(x_0, x_1)$:

$$S_2(x_0,x_1)=\frac{1}{2}\left\langle x_0,\begin{pmatrix}0&-2\\-2&0\end{pmatrix}x_0\right\rangle-\left\langle x_0,\begin{pmatrix}0&-2\\-2&0\end{pmatrix}x_1\right\rangle+\frac{1}{2}\left\langle x_1,\begin{pmatrix}0&-2\\-2&1\end{pmatrix}x_1\right\rangle.$$

(See also Ref. 17, p. 280).

Proof: Recalling the map ψ in (10), we proceed to verify by direct computation:

$$-\frac{\partial S_2}{\partial x_0}(x_0,x_1)\Big|_{x_0=(q,p),x_1=(2q-P/2,2p-Q/2)}=-\begin{pmatrix}0&-2\\-2&0\end{pmatrix}\begin{pmatrix}q\\p\end{pmatrix}+\begin{pmatrix}0&-2\\-2&0\end{pmatrix}\begin{pmatrix}\frac{2q-P}{2}\\\frac{2p-Q}{2}\end{pmatrix}$$
$$=(2p,2q)+(Q-2p,P-2q)=(Q,P)=y_0,$$

$$\frac{\partial S_2}{\partial x_1}(x_0,x_1)\Big|_{x_0=(q,p),x_1=(2q-P/2,2p-Q/2)}=-(q,p)\begin{pmatrix}0&-2\\-2&0\end{pmatrix}+\begin{pmatrix}0&-2\\-2&1\end{pmatrix}\begin{pmatrix}\frac{2q-P}{2}\\\frac{2p-Q}{2}\end{pmatrix}$$
$$=(2p,2q)+\left(Q-2p,P-2q+\frac{2p-Q}{2}\right)$$
$$=\left(Q,\frac{2P+2p-Q}{2}\right)=y_1.$$

□

We can now prove the following.

Proposition 4.3: The Lagrangian submanifold $h(\Gamma_K)$ admits the generating function $S(x_1;x_0,\xi)$:

$$S(x_1;x_0,\xi)=S_1(x_0,\xi)+S_2(x_0,x_1).$$

Remark: Note that the variables x_0 now are interpreted as auxiliary parameters, at the same level of ξ.

Proof: The symplectomorphism ψ is generated by $S_2(x_0,x_1)$, that is,

$$\psi(x_0,y_0)=(x_1,y_1)\text{iff}\begin{cases}y_0=-\dfrac{\partial S_2}{\partial x_0}(x_0,x_1)\\ y_1=\dfrac{\partial S_2}{\partial x_1}(x_0,x_1)\end{cases},$$

$$\frac{\partial S}{\partial x_0}(x_1;x_0,\xi)=0\ \text{means}\ \frac{\partial S_1}{\partial x_0}(x_0,\xi)+\frac{\partial S_2}{\partial x_0}(x_0,x_1)=0,\quad \text{that is,}\ y_0=\frac{\partial S_1}{\partial x_0}(x_0,\xi).$$

Furthermore,

$$\frac{\partial S}{\partial \xi}(x_1;x_0,\xi)=0\quad\text{iff}\ \frac{\partial S_1}{\partial \xi}(x_0,\xi)=0.$$

Therefore the Lagrangian submanifold generated by $S(x_1;x_0,\xi)$ results:

$$\left\{(x_1,y_1)=\left(x_1,\frac{\partial S}{\partial x_1}(x_1;x_0,\xi)\right):\frac{\partial S}{\partial x_0}(x_1;x_0,\xi)=0,\frac{\partial S}{\partial \xi}(x_1;x_0,\xi)=0\right\}$$
$$=\left\{(x_1,y_1)=\left(x_1,\frac{\partial S}{\partial x_1}(x_1;x_0,\xi)\right):y_0=\frac{\partial S_1}{\partial x_0}(x_0,\xi),\frac{\partial S_1}{\partial \xi}(x_0,\xi)=0\right\}$$
$$=\left\{(x_1,y_1)=\left(x_1,\frac{\partial S_2}{\partial x_1}(x_0,x_1)\right):y_0=\frac{\partial S_1}{\partial x_0}(x_0,\xi),\frac{\partial S_1}{\partial \xi}(x_0,\xi)=0\right\}$$
$$=\{(x_1,y_1):(x_1,y_1)=\psi(x_0,y_0)\ \text{with}\ (x_0,y_0)\in\bar{h}(\Gamma_K)\}=\psi(\bar{h}(\Gamma_K))=h(\Gamma_K).$$

D. The quadratic at infinity property

We are ready to look for fixed points of ϕ_H^1, that is, to estimate

$$\#(h(\Gamma_K)\cap 0_{\mathbb{R}^{2n}}).$$

These intersection points are exactly the critical points, with respect to all the variables, of the generating function S for $h(\Gamma_K)$. More precisely, by Proposition 4.4 below, we show that they are essentially (that is to say, up to periodicity) the critical points for a GFQI f defined on a domain contracting to the torus $\mathbb{T}^n$: this is crucial in order to gain, in the Lusternik-Schnirelman format, a lower bound estimate of the number of fixed points of ϕ_H^1.

Although in the previous section we managed with a formal expression of S_2, by a straightforward computation we easily find out the simplified structure [here, for opportunity, we write $S_2(q_0,p_0,\dots)$ instead of $S_2(q,p,\dots)$] of it:

$$S_2(x_0,x_1)=S_2(q_0,p_0,q_1,p_1)=2(p_0-p_1)\cdot(q_1-q_0)+\frac{p_1^2}{2}.$$

Proposition 4.4: The fixed points of ϕ_H^1 correspond to the critical points of the GFQI:

$$f:\mathbb{T}^n\times\mathbb{R}^{3n+k}\to\mathbb{R},$$

$$([q_1],p_1,v,p_0,\xi)\overset{f}{\mapsto}S_1([q_1-v],p_0+p_1,\xi)+2p_0\cdot v+\frac{p_1^2}{2}. \tag{11}$$

Proof: Using the notation $x_1=(q_1,p_1)$ and $x_0=(q_0,p_0)$ we can rewrite S as

$$S:\mathbb{R}^{4n+k}\to\mathbb{R},$$

$$(q_1,p_1,q_0,p_0,\xi)\mapsto S_1(q_0,p_0,\xi)+2(p_0-p_1)\cdot(q_1-q_0)+\frac{p_1^2}{2}.$$

There is an evident invariance property:

$$S(q_1+2\pi k,p_1,q_0+2\pi k,p_0,\xi)=S(q_1,p_1;q_0,p_0,\xi),$$

$\forall(q_1,p_1,q_0,p_0,\xi)\in\mathbb{R}^{4n+k}$, and $\forall k\in\mathbb{Z}^n$. This fact is the same as saying that S is constant over the fibers of the surjective map Π below, thus it results in the following well-defined real-valued function $\tilde{S}$:

$$\begin{array}{ccc}\mathbb{R}^{4n+k} & \xrightarrow{\ S\ } & \mathbb{R}\\ \Pi\downarrow & \nearrow_{\tilde{S}} & \\ \mathbb{T}^n\times\mathbb{R}^{3n+k} & & \end{array} \tag{12}$$

$$\begin{array}{ccc} (q_1,p_1,q_0,p_0,\xi) & \xrightarrow{\;S\;} & \mathbb{R} \\ \Pi\downarrow & \nearrow_{\widetilde{S}} & \\ ([q_1],p_1,q_1-q_0,p_0,\xi) & & \end{array} \tag{13}$$

$$\Pi^{-1}([q_1],p_1,v,p_0,\xi)=\{(q_1+2\pi k,p_1,q_1-v+2\pi k,p_1,\xi):k\in\mathbb{Z}^n\}, \tag{14}$$

$$\widetilde{S}:\mathbb{T}^n\times\mathbb{R}^{3n+k}\to\mathbb{R},$$

$$([q_1],p_1,v,p_0,\xi)\mapsto S_1([q_1-v],p_0,\xi)+2(p_0-p_1)\cdot v+\frac{p_1^2}{2}, \tag{15}$$

satisfying the property

$$\widetilde{S}\circ\Pi=S. \tag{16}$$

Furthermore, since $d\widetilde{S}(y)_{|y=\Pi(x)}\circ d\Pi(x)=dS(x)$, we have that ($rk d\Pi=\max$): $\Pi^{-1}(\mathrm{Crit}(\widetilde{S}))=\mathrm{Crit}(S)$. Now $S_1([q_1-v],p_0+p_1,\xi)$ coincides for $|\xi|>C$ with a nondegenerate quadratic form $(A\xi,\xi)$, then for $|p_1|,|v|,|p_0|,|\xi|>C$ and for any fixed $[q_1]\in\mathbb{T}^n$, $f([q_1],p_1,v,p_0,\xi)=Q(p_1,v,p_0,\xi)$ where $Q(p_1,v,p_0,\xi)$ is the nondegenerate quadratic form

$$Q(p_1,v,p_0,\xi):=\begin{pmatrix} \frac{1}{2} & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & A \end{pmatrix}\begin{pmatrix} p_1 \\ v \\ p_0 \\ \xi \end{pmatrix}\begin{pmatrix} p_1 \\ v \\ p_0 \\ \xi \end{pmatrix}.$$

Therefore f is a GFQI. □

E. Fixed points: Degenerate case

We conclude this section with the estimate in the possible degenerate case, first proved by Conley and Zehnder,[10] of which we propose a proof based on the quadratic at infinity property of the generating function f.

Theorem 4.5: *Let ϕ_H^1 be the time-one map of a time-dependent Hamiltonian $H:\mathbb{R}\times\mathbb{R}^{2n}\to\mathbb{R}$ satisfying*

$$H(t,q+2\pi k,p)=H(t,q,p),\quad \forall\,(t,q,p)\in\mathbb{R}\times\mathbb{R}^{2n},\quad \forall\,k\in\mathbb{Z}^n,$$

and

$$H(t,q,p)=\frac{1}{2}|p|^2 \text{ if } |p|\geqslant C>0.$$

Then ϕ_H^1 has at least $n+1$ fixed points and they correspond to homotopically trivial closed orbits of the Hamiltonian flow.

Proof: Fixed points of ϕ_H^1 correspond to critical points of f (see Proposition 4.4). Moreover, via the Lusternik-Schnirelman theory (see Theorem 2.9), critical values of f can be detected involving nonvanishing relative cohomology classes in $H^*(f^c,f^{-c})$. As a consequence, and since $f:\mathbb{T}^n\times\mathbb{R}^{3n+k}\to\mathbb{R}$ is a GFQI, Corollary 2.11 does work, so that we obtain the well-known estimate

$$\#\mathrm{fix}(\phi_H^1) = \#\,\mathrm{crit}(f) \geqslant \mathrm{cl}(\mathbb{T}^n) = n+1.$$

□

V. FIXED POINTS: NONDEGENERATE CASE

Whenever all the fixed points of ϕ_H^1 are *a priori* nondegenerate, so that the corresponding critical points of f are also nondegenerate, it happens that the GFQI f becomes also a so-called Morse function, and in this case we achieve a rather better estimate.

Definition 5.1: Let N be a smooth manifold. A fixed point $x \in N$ of a diffeomorphism $\Phi: N \to N$ is said to be nondegenerate if the graph of Φ intersects the diagonal of $N \times N$ transversally at (x,x), that is,

$$\det(d\Phi(x) - \mathbb{I}) \neq 0.$$

The notion of nondegeneracy for fixed points of diffeomorphisms corresponds to the notion of nondegeneracy for critical points of functions, originally due to Morse.

Definition 5.2: Let N be a smooth manifold and $f: N \to \mathbb{R}$ be a C^2 function. A critical point x for f, $\nabla f(x)=0$, is said to be nondegenerate if the Hessian $\partial^2 f/\partial x^i \partial x^j(x)$ of f at x is nondegenerate.

(Recall that the Hessian of a scalar function f at its critical points is a well-defined tensorial object.) Starting from the study of the sublevel sets N^ν [see (2)], where ν is not a critical value of f, Morse proved the following famous lower bound on the number of critical points of f.

Theorem 5.3: *(Morse inequality) Let N be a compact manifold and $f: N \to \mathbb{R}$ be a Morse function. Then*

$$\mathrm{crit}(f) \geqslant \sum_{k=0}^{\dim N} H^k(N) =: \sum_{k=0}^{\dim N} b_k(N),$$

where the values $b_k(N)$ are called the Betti numbers of N.

As in the degenerate case, the preceding estimate still holds when $f: N \times \mathbb{R}^n \to \mathbb{R}$ is a GFQI (see, for example, Ref. 8):

Theorem 5.4: *Let N be compact manifold and $f: N \times \mathbb{R}^n \to \mathbb{R}$ be A GFQI. If all the critical points of f are nondegenerate, then*

$$\mathrm{crit}(f) \geqslant \sum_{k=0}^{\dim N} b_k(N).$$

The expected estimate on the number of nondegenerate fixed points for the Hamiltonian flow ϕ_H^1 is a straight consequence of Theorem 5.4.

Theorem 5.5: *Same hypothesis of Theorem 4.5. Then ϕ_H^1 has at least 2^n nondegenerate fixed points and they correspond to homotopically trivial closed orbits of the Hamiltonian flow.*

Proof: Nondegenerate fixed points of ϕ_H^1 correspond (via the diffeomorphisms h and ψ) to transversal intersections between $h(\Gamma_K)$ and $0_{R^{2n}}$. We observe now that the Lagrangian submanifold $h(\Gamma_K)$ intersects transversally $0_{R^{2n}}$ in the point $(\bar{q},\bar{p},\bar{u}) := (\bar{x},\bar{u}) \in h(\Gamma_K)$ if

$$\det\left(\frac{\partial^2 S}{\partial x^i \partial x^j}\right)(\bar{x},\bar{u}) \neq 0. \tag{17}$$

Moreover, since the point $(\bar{x},\bar{u}) \in h(\Gamma_K)$, the transversality condition guarantees that

$$\mathrm{rk}\left(\frac{\partial^2 S}{\partial x^i \partial u^j}, \frac{\partial^2 S}{\partial u^i \partial u^j}\right)(\bar{x},\bar{u}) = \max. \tag{18}$$

Then, from conditions (17) and (18), we conclude that the nondegenerate fixed points of ϕ_H^1 correspond exactly to the nondegenerate critical points of S, which are essentially (that is up to

periodicity) the nondegenerate critical points of f. Now $f:\mathbb{T}^n\times\mathbb{R}^{3n+k}\to\mathbb{R}$ is a GFQI, then, as a consequence of Theorem 5.4, we obtain

$$\#\text{non deg} - \text{fix}(\phi_H^1) = \#\text{non deg} - \text{crit}(f) \geqslant 2^n.$$

□

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Quasiperiodic attractors, Borel summability and the Bryuno condition for strongly dissipative systems

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We consider a class of ordinary differential equations describing one-dimensional analytic systems with a quasiperiodic forcing term and in the presence of damping. In the limit of large damping, under some generic nondegeneracy condition on the force, there are quasiperiodic solutions which have the same frequency vector as the forcing term. We prove that such solutions are Borel summable at the origin when the frequency vector is either any one-dimensional number or a two-dimensional vector such that the ratio of its components is an irrational number of constant type. In the first case the proof given simplifies that provided in a previous work of ours. We also show that in any dimension d, for the existence of a quasiperiodic solution with the same frequency vector as the forcing term, the standard Diophantine condition can be weakened into the Bryuno condition. In all cases, under a suitable positivity condition, the quasiperiodic solution is proved to describe a local attractor. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this paper we pursue the study started in Refs. 6 and 2. We consider one-dimensional systems with a quasiperiodic forcing term in the presence of strong damping, described by ordinary differential equations of the form

$$\varepsilon\ddot{x} + \dot{x} + \varepsilon g(x) = \varepsilon f(\boldsymbol{\omega} t), \tag{1.1}$$

where $\boldsymbol{\omega} \in \mathbb{R}^d$ is the frequency vector, $g(x)$ and $f(\boldsymbol{\psi})$ are functions analytic in their arguments, with f quasiperiodic, i.e.,

$$f(\boldsymbol{\psi}) = \sum_{\boldsymbol{\nu} \in \mathbb{Z}^d} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\psi}} f_{\boldsymbol{\nu}}, \tag{1.2}$$

with average $\langle f \rangle = f_0$, and $\varepsilon > 0$ is a real parameter, physically representing the inverse of the damping coefficient. With $\cdot$ we are denoting the scalar product in $\mathbb{R}^d$. A Diophantine condition is assumed on $\boldsymbol{\omega}$ for $d > 1$, that is

$$|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \geqslant C_0 |\boldsymbol{\nu}|^{-\tau} \quad \forall\, \boldsymbol{\nu} \in \mathbb{Z}^d \setminus \{\mathbf{0}\}, \tag{1.3}$$

where $|\boldsymbol{\nu}| = |\boldsymbol{\nu}|_1 \equiv |\nu_1| + \cdots + |\nu_d|$, and C_0 and τ are positive constants. The set of vectors satisfying the condition (1.3) is nonvoid for $\tau \geqslant d-1$ and is of full measure for $\tau > d-1$. For $d=1$ we denote

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the vectors without boldface; in that case ω will be called the frequency number.

In Ref. 6 we show that, under the nondegeneracy condition

$$\exists c_0 \in \mathbb{R} \quad \text{such that } g(c_0) = f_0 \text{ and } g'(c_0) \neq 0, \tag{1.4}$$

the system (1.1) admits a quasiperiodic solution $x(t;\varepsilon)$ with the same frequency vector as the forcing. Such a solution can be obtained by a suitable summation of the formal power series

$$x_0(t;\varepsilon) := \sum_{k=0}^{\infty} \varepsilon^k x^{(k)}(t), \quad x^{(k)}(t) = \sum_{\boldsymbol{\nu} \in \mathbb{Z}^d} e^{i\boldsymbol{\nu}\cdot\boldsymbol{\omega}t} x_{\boldsymbol{\nu}}^{(k)}, \tag{1.5}$$

which solves the equations of motion order by order. For $d=1$ (periodic forcing) the series (1.4) is Borel summable in ε. In Ref. 2 we also show that if $g'(c_0)>0$, for any d such a solution is locally an attractor. In some cases, for instance if $g(x)=x^{2p+1}$, $p \in \mathbb{N}$, and $f_0>0$, the attractor is global.

In this paper we first give a different (simpler) proof of Borel summability in the periodic case (Sec. II), then we prove that the formal series for the solution turns out to be Borel summable also for $d=2$ and $\tau=1$ (Sec. III); this corresponds to frequency vectors with components such that their ratios are irrational numbers of constant type (i.e., numbers with bounded partial quotients in their continued fraction expansion). The proof does not rely on Nevanlinna-type theorems,[7,8] but consists in checking directly that the conditions for the formal series of the solution to be Borel summable are satisfied, and follows the same strategy introduced in Ref. 4 to investigate Borel summability of lower-dimensional tori.

Finally in Sec. IV we show how to relax the Diophantine condition. We show that, in order to have the same results on existence and attractivity of the quasiperiodic solution, one can take $\boldsymbol{\omega}$ to be a Bryuno vector, that is one can assume that, by defining

$$B(\boldsymbol{\omega}) = \sum_{n=0}^{\infty} \frac{1}{2^n} \log \frac{1}{\alpha_n(\boldsymbol{\omega})}, \quad \alpha_n(\boldsymbol{\omega}) = \inf_{|\boldsymbol{\nu}| \leq 2^n} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|, \tag{1.6}$$

then $\boldsymbol{\omega}$ satisfies the Bryuno condition $B(\boldsymbol{\omega})<\infty$. More formal statements will be given in the next sections.

II. BOREL SUMMABILITY FOR $d=1$

First of all let us recall the definition of Borel summability.[8] Let $f(\varepsilon)=\Sigma_{n=1}^{\infty} a_n \varepsilon^n$ be a formal power series (which means that the sequence $\{a_n\}_{n=1}^{\infty}$ is well defined). We say that $f(\varepsilon)$ is *Borel summable* if

(1) $B(p) := \Sigma_{n=1}^{\infty} a_n p^n/n!$ converges in some circle $|p|<\delta$,
(2) $B(p)$ has an analytic continuation to a neighborhood of the positive real axis, and
(3) $g(\varepsilon)=\int_0^{\infty} e^{-p/\varepsilon} B(p) \mathrm{d}p$ converges for some $\varepsilon>0$.

Then the function $B(p)$ is called the *Borel transform* of $f(\varepsilon)$, and $g(\varepsilon)$ is the *Borel sum* of $f(\varepsilon)$. Moreover if the integral defining $g(\varepsilon)$ converges for some $\varepsilon_0>0$ then it converges in the circle $\mathrm{Re}\ \varepsilon^{-1} > \mathrm{Re}\ \varepsilon_0^{-1}$. A function which admits the formal power series expansion $f(\varepsilon)$ is called Borel summable if $f(\varepsilon)$ is Borel summable; in that case the function equals the Borel sum $g(\varepsilon)$.

Theorem 2.1: *Consider the system (1.1) for $d=1$, and assume that the nondegeneracy condition (1.4) is fulfilled. There exists $\varepsilon_0>0$ such that for $|\varepsilon|<\varepsilon_0$ there is a periodic solution $x(t;\varepsilon)$ which has the same frequency number as the forcing term and is Borel summable in ε at the origin. If $g'(c_0)>0$ such a solution describes a local attractor.*

Proof: We consider explicitly the case $g(x)=x^2$ in (1.1), which corresponds to the varactor equation extensively studied in Refs. 6, 1, and 2; the general case can be easily dealt with by reasoning as in Sec. VII of Ref. 6. In Ref. 6 we proved that the formal power series (1.5) is well defined and that to any order k one has

$$|x_\nu^{(k)}| \leqslant A_1 \varepsilon_2^{-k} k!, \quad |x^{(k)}(t)| \leqslant A_1 \varepsilon_2^{-k} k!, \tag{2.1}$$

for suitable constants A_1 and ε_2 [cf. formula (4.5) in Ref. 6]. This means that the first condition, in the definition of Borel summability, is satisfied, with $\delta = \varepsilon_2$.

In Ref. 6 we also proved that the formal power series can be summed, and gives a function

$$x(t;\varepsilon) = \sum_{k=0}^{\infty} \sum_{\nu \in \mathbb{Z}} e^{i\omega\nu t} x_\nu^{[k]}, \tag{2.2}$$

which is real-analytic and periodic in t, and analytic in ε in a suitable domain tangent to the imaginary axis at the origin. The coefficients $x_\nu^{[k]}$ can be written as

$$x_\nu^{[k]} = \sum_{\theta \in \mathcal{T}_{k,\nu}} \mathrm{Val}(\theta), \quad \mathrm{Val}(\theta) = \left(\prod_{\ell \in L(\theta)} g_\ell \right) \left(\prod_{v \in E(\theta) \cup V(\theta)} F_v \right), \tag{2.3}$$

where the symbols are defined as in Sec. V of Ref. 6. We briefly recall the basic definitions and notations, with the purpose of making self-consistent the discussion; reference should be made to Ref. 6 for further details.

A tree θ is a graph, that is a connected set of points and lines, with no cycle, such that all the lines are oriented toward a unique point (root) which has only one incident line (root line). All the points in a tree except the root are denoted nodes. The orientation of the lines in a tree induces a partial ordering relation ($\leqslant$) between the nodes. Given two nodes v and w, we shall write $w \leqslant v$ every time v is along the path (of lines) which connects w to the root. We call $E(\theta)$ the set of endpoints in θ, that is the nodes which have no entering line. The endpoints can be represented either as white bullets or as black bullets; we denote with $E_W(\theta)$ and $E_B(\theta)$ the set of white bullets and the set of black bullets, respectively. With each endpoint v we associate a mode label $\nu_v \in \mathbb{Z}$, such that $\nu_v = 0$ if $v \in E_W(\theta)$ and $\nu_v \neq 0$ if $v \in E_B(\theta)$. We denote with $L(\theta)$ the set of lines in θ. Since ℓ is uniquely identified with the point v which it leaves, we may write $\ell = \ell_v$. With each line ℓ we associate a momentum label $\nu_\ell \in \mathbb{Z}$. The modes of the endpoints and and the momenta of the lines are related as follows: if $\ell = \ell_v$ one has

$$\nu_\ell = \sum_{i=1}^{s_v} \nu_{\ell_i} = \sum_{w \in E_B(\theta): w \leqslant v} \nu_w, \tag{2.4}$$

where s_v denotes the number of lines entering v [one has $s_v = 2$ if $g(x) = x^2$ in (1.1), otherwise $s_v \geqslant 2$], and $\ell_1, \ldots, \ell_{s_v}$ are the lines entering v. We denote by $V(\theta)$ the set of vertices in θ, that is the set of points which have at least one entering line. We set $V_0(\theta) = \{v \in V(\theta) : \nu_{\ell_v} = 0\}$. We call *equivalent* two trees which can be transformed into each other by continuously deforming the lines in such a way that they do not cross each other. Let $\mathcal{T}_{k,\nu}$ be the set of inequivalent trees of order k and total momentum ν, that is the set of inequivalent trees θ such that $|V(\theta)| + |E_B(\theta)| = k$ and the momentum of the root line is ν. We associate with each line ℓ a *propagator*

$$g_\ell = \begin{cases} 1/((i\omega\nu_\ell)(1 + i\varepsilon\omega\nu_\ell)), & \nu_\ell \neq 0, \\ 1, & \nu_\ell = 0, \end{cases} \tag{2.5}$$

with each vertex v a node factor

$$F_v = \begin{cases} -\varepsilon, & v \notin V_0(\theta), \\ -1/2c_0, & v \in V_0(\theta), \end{cases} \tag{2.6}$$

and with each endpoint v a node factor

$$F_v = \begin{cases} c_0, & v \in E_W(\theta), \\ \varepsilon f_{\nu_v}, & v \in E_B(\theta). \end{cases} \tag{2.7}$$

Then (2.3) says that each coefficient $x_\nu^{[k]}$ is given by the sum over all trees of order k and total momentum ν of the corresponding values.

It is more convenient to slightly change the definition of node factors and propagators, by associating the factor ε with the propagator g_ℓ of the line ℓ coming out from v and not with v itself. In this way the propagator of any line with ℓ momentum $\nu_\ell \neq 0$ is

$$g_\ell = g(\omega\nu_\ell;\varepsilon), \quad g(x;\varepsilon) = \frac{\varepsilon}{ix(1+i\varepsilon x)}, \tag{2.8}$$

and the only dependence on ε in $\mathrm{Val}(\theta)$ is through the product of propagators with nonvanishing momentum. [Note that $g(x;\varepsilon)$ in (2.8) has a completely different meaning with respect to the function $g(x)$ appearing in (1.1). The same *caveat* applies to the propagators $g^{[n]}(x;\varepsilon)$ in Sec. III.]

The function (2.8) is Borel summable, and its Borel transform is easily computed to be

$$g_B(x;p) = \frac{e^{-ipx}}{ix} \Rightarrow |g_B(x;p)| \leqslant \frac{e^{|\mathrm{Im}\, p||x|}}{|x|}. \tag{2.9}$$

Moreover $g_B(x;p)$ is an entire function in p, and the integral $\int_0^\infty e^{-p/\varepsilon} g_B(x;p)\mathrm{d}p$ converges (absolutely) for all $\varepsilon > 0$.

For any tree $\theta \in \mathcal{T}_{k,\nu}$ the Borel transform of $\mathrm{Val}(\theta)$ is given by a constant times the Borel transform of the product of the propagators with nonzero momentum. One has

$$(\mathrm{Val}(\theta))_B(p) = \left(\prod_{\ell \in L_0(\theta)} g_\ell\right)\left(\prod_{v \in E(\theta)\cup V(\theta)} F_v\right)\left(\left(\prod_{\ell \in L_2(\theta)} g_\ell\right)_B(p)\right), \tag{2.10}$$

where we have called $L_0(\theta)$ is the set of lines in $L(\theta)$ with zero momentum, and we have set $L_2(\theta) = L(\theta)\setminus L_0(\theta)$ (cf. Sec. IV of Ref. 6). The Borel transform appearing in (2.10) equals the convolution of the Borel transforms of the propagators with nonzero momentum, so that it can be bounded as

$$\left|\left(\prod_{\ell \in L_2(\theta)} g_\ell\right)_B(p)\right| \leqslant \prod_{\ell \in L_2(\theta)}{}^{*} |g_B(\omega\nu_\ell;p)| \leqslant \left(\prod_{\ell \in L_2(\theta)} \frac{1}{|\omega\nu_\ell|}\right) \frac{|p|^{k-1}}{(k-1)!} \exp\left(|\mathrm{Im}\, p| \max_{\ell \in L_2(\theta)} |\omega\nu_\ell|\right), \tag{2.11}$$

where Π^* denotes the convolution product, and $|\omega| < |\omega\nu_\ell| < |\omega| \Sigma_{v \in E_B(\theta)} |\nu_v|$; cf. Remarks (4) to (6) after Definition 1 in Ref. 3 for properties of the Borel transforms we are using here.

Therefore, for p in any strip $\Sigma_\sigma = \{p \in \mathbb{C} : |\mathrm{Im}\, p| < \sigma\}$ of the real axis, we have

$$\left|\prod_{v \in E_B(\theta)} F_v\right| \exp\left(|\mathrm{Im}\, p| \max_{\ell \in L_2(\theta)} |\omega\nu_\ell|\right) \leqslant F^{|E_B(\theta)|} \prod_{v \in E_B(\theta)} e^{-\xi|\nu_v|/2}, \tag{2.12}$$

provided $|\omega|\sigma < \xi/2$, and summability over the Fourier labels in (2.3) is assured. The sum over k in (2.2) produces a quantity bounded proportionally to the exponential $e^{\Gamma|p|}$, for some positive constant Γ. A comparison with Ref. 6 shows that $\Gamma = 1/\varepsilon_0$, where ε_0 is the same as in the statement of the theorem. In particular the Borel transform $x_B(t;p)$ of the series (2.2) turns out to have an analytic continuation to the strip Σ_σ, and admits there the bound $|x_B(t;p)| \leqslant Ce^{\Gamma|p|}$, for a suitable constant C. Hence the integral

$$g(t;\varepsilon) := \int_0^\infty e^{-p/\varepsilon} x_B(t;p)\mathrm{d}p \tag{2.13}$$

absolutely converges provided $0<\varepsilon<\varepsilon_0$. So also the last two conditions for the formal series of $x(t;\varepsilon)$ to be Borel summable are satisfied.

That the solution $x(t;\varepsilon)$ describes a local attractor, under the further condition $g'(c_0)>0$, follows from the analysis performed in Ref. 2. ■

Note that, because of the analyticity properties of $x_B(t;p)$, it follows, as a consequence of Nevanlinna's theorem,[8] that the function defined by the integral (2.13) is analytic in the circle $C_R=\{\varepsilon\in\mathbb{C}:\mathrm{Re}\,\varepsilon^{-1}>R^{-1}\}$, with $R=\varepsilon_0$, and satisfies the bound

$$g(t;\varepsilon)=\sum_{k=0}^{N-1}\varepsilon^k x^{(k)}(t)+\mathfrak{R}_N(\varepsilon),\quad |\mathfrak{R}_N(\varepsilon)|\leqslant AB^N N!|\varepsilon|^N, \tag{2.14}$$

with constants A and B independent of N. This is consistent with Proposition 5.3 of Ref. 6.

III. BOREL SUMMABILITY FOR $d=2$ AND $\tau=1$

In the case of quasiperiodic forcing terms for $d=2$ we obtain the following result.

Theorem 3.1: *Consider the system (1.1) for* $d=2$, *and assume that* $\boldsymbol{\omega}$ *satisfies the Diophantine condition (1.3)* with $\tau=1$ *and that the nondegeneracy condition (1.4) is fulfilled. There exists* $\varepsilon_0>0$ *such that for* $|\varepsilon|<\varepsilon_0$ *there is a quasiperiodic solution* $x(t;\varepsilon)$ *which has the same frequency vector as the forcing term and is Borel summable at the origin. If* $g'(c_0)>0$ *such a solution describes a local attractor.*

Proof: Again we discuss explicitly the case $g(x)=x^2$ in (1.1). Let ψ be a nondecreasing C^∞ function defined in $\mathbb{R}_+$, such that

$$\psi(u)=\begin{cases}1 & \text{for } u\geqslant 1,\\ 0 & \text{for } u\leqslant 1/2,\end{cases} \tag{3.1}$$

and set $\chi(u):=1-\psi(u)$. Define, for all $n\in\mathbb{Z}_+$, $\chi_n(u):=\chi(2^nC_0^{-1}u/4)$ and $\psi_n(u):=\psi(2^nC_0^{-1}u/4)$.

With each line ℓ with zero momentum we associate a scale label $n_\ell=-1$, while with each line with nonzero momentum we associate (arbitrarily) a scale label $n_\ell\in\mathbb{Z}_+=\{0\}\cup\mathbb{N}$. Then we can define cluster and self-energy clusters as in Refs. 4 and 6. A cluster T on scale n is a maximal set of points and lines connecting them such that all the lines have scales $n'\leqslant n$ and there is at least one line with scale n. The lines entering the cluster T and the possible line coming out from it (unique if existing at all) are called the external lines of the cluster T. Given a cluster T on scale n, we shall denote by $n_T=n$ the scale of the cluster; we call $V(T)$, $E(T)$, $E_W(T)$, $E_B(T)$, and $L(T)$ the set of vertices, of endpoints, of white endpoints, of black endpoints, and of lines of T, respectively. We call self-energy cluster any cluster T such that T has only one entering line ℓ_T^2 and one exiting line ℓ_T^1, and one has $\Sigma_{v\in E_B(T)}\boldsymbol{\nu}_v=\mathbf{0}$. With each line ℓ with momentum $\boldsymbol{\nu}_\ell$ and scale n_ℓ we associate a renormalized propagator $g_\ell=g^{[n_\ell]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\varepsilon)$, still to be defined. On the contrary the node factors are defined as in the previous case (with the only trivial difference that now $\boldsymbol{\nu}_v$, replacing ν_v, is a d-dimensional vector).

Define the self-energy value $\mathcal{V}_T(\boldsymbol{\omega}\cdot\boldsymbol{\nu};\varepsilon)$ in terms of the renormalized propagators and node factors as

$$\mathcal{V}_T(\boldsymbol{\omega}\cdot\boldsymbol{\nu};\varepsilon)=\left(\prod_{\ell\in L(T)} g^{[n_\ell]}(\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell;\varepsilon)\right)\left(\prod_{v\in E(T)\cup V(T)} F_v\right), \tag{3.2}$$

where $\boldsymbol{\nu}$ is the momentum of both the external lines of T.

We proceed as in Sec. VI of Ref. 6, with the only two differences that we perform a preliminary summation by including the contribution $-2\varepsilon c_0$ (arising from the self-energy graphs on scale

-1) into the propagator $g^{[0]}(x;\varepsilon)$, and—as in the periodic case of Sec. II—we associate the factors ε to the propagators with nonzero momentum. Therefore we define [see the comment after (2.8) in Sec. II]

$$g^{[0]}(x;\varepsilon)=\frac{\varepsilon\psi_0(|x|)}{ix(1+i\varepsilon x)-2\varepsilon c_0},\quad M^{[0]}(x;\varepsilon)=\varepsilon\sum_{k=1}^{\infty}\sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,0}}\mathcal{V}_T(x;\varepsilon),\tag{3.3}$$

whereas the propagators on scale $n\geqslant 1$ are defined as in Ref. 6, again with a factor ε appearing in the numerator of the propagators with nonzero momentum; this means that one has

$$\begin{aligned}&g^{[n]}(x;\varepsilon)=\frac{\varepsilon\chi_0(|x|)\cdots\chi_{n-1}(|x|)\psi_n(|x|)}{ix(1+i\varepsilon x)-\mathcal{M}^{[n-1]}(x;\varepsilon)},\\&\mathcal{M}^{[n]}(x;\varepsilon)=\sum_{p=1}^{n}\chi_0(|x|)\cdots\chi_{p-1}(|x|)\chi_n(|x|)M^{[p]}(x;\varepsilon),\quad M^{[n]}(x;\varepsilon)=\varepsilon\sum_{k=1}^{\infty}\sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,n}}\mathcal{V}_T(x;\varepsilon),\end{aligned}\tag{3.4}$$

where the set of renormalized self-energy clusters $\mathcal{S}^{\mathcal{R}}_{k,n}$ is defined and the set of self-energy clusters T on scale $n_T=n$ and of order k [that is with $|V(T)|+|E_B(T)|=k$]. With respect to Refs. 6 and 4 a further factor ε appears in $M^{[n]}(x;\varepsilon)$, $n\geqslant 0$, simply because there is one such factor per node (vertex or endpoint) with exiting line carrying a nonzero momentum—cf. Sec. 6 in Ref. 4—and we are associating the factors ε with the lines instead of the nodes.

An easy computation gives, for the Borel transform of $g^{[0]}(x;\varepsilon)$,

$$g^{[0]}_B(x;p)=\frac{\psi_0(|x|)}{ix}\exp\left(-ip\left(x-2\frac{c_0}{x}\right)\right)\Rightarrow|g^{[0]}_B(x;p)|\leqslant\frac{1}{|x|}e^{(|x|+2|c_0|/|x|)|\mathrm{Im}\,p|}.\tag{3.5}$$

If we set, for $n\geqslant 0$,

$$\tilde{g}^{[n]}(x;\varepsilon)=\frac{\varepsilon}{ix(1+i\varepsilon x)-\mathcal{M}^{[n-1]}(x;\varepsilon)}\qquad\forall\,|x|\leqslant 2^{-(n-1)}C_0,\tag{3.6}$$

and define $M^{[n]}(x;\varepsilon)=\mathcal{M}^{[n]}(x;\varepsilon)-\mathcal{M}^{[n-1]}(x;\varepsilon)$, we obtain the recursive equations

$$(\tilde{g}^{[n]}(x;\varepsilon))^{-1}=(\tilde{g}^{[n-1]}(x;\varepsilon))^{-1}-\chi_0(|x|)\cdots\chi_{n-1}(|x|)\varepsilon^{-1}M^{[n-1]}(x;\varepsilon),\quad n\geqslant 1.\tag{3.7}$$

By using these equations we can prove inductively the bound

$$|\tilde{g}^{[n]}_B(x;p)|\leqslant\frac{K_0}{|x|}e^{(c_n+c'_n|x|^{-1/2})|p|+\kappa_0|\mathrm{Im}\,p|(d_n|x|+d'_n|x|^{-1})},\tag{3.8}$$

where K_0 and κ_0 are two constants, and the sequences $\{c_n\}_{n=0}^{\infty}$, $\{c'_n\}_{n=0}^{\infty}$, $\{d_n\}_{n=0}^{\infty}$, $\{d'_n\}_{n=0}^{\infty}$ are to be found.

The proof proceeds as in Appendix A1 of Ref. 3. Set $x_\ell=\boldsymbol{\omega}\cdot\boldsymbol{\nu}_\ell$, and call $L_0(T)$ and $L_2(T)$ the set of lines in $L(T)$ with zero momentum and the set $L_2(T)=L(T)\setminus L_0(T)$, respectively. First we use the inductive bound to obtain

$$\left|\left(\frac{M^{[N]}(x;\varepsilon)}{\varepsilon}\right)_B\right| \leqslant \sum_{k=2}^{\infty} \sum_{T\in\mathcal{S}^{\mathcal{R}}_{k,N-1}} \left(\prod_{\ell\in L_0(T)} |g_\ell|\right)\left(\prod_{v\in E(T)\cup V(T)} |F_v|\right)$$
$$\times \left(\prod_{\ell\in L_2(T)} {}^{*}\frac{K_0}{|x_\ell|} e^{(c_{n_\ell}+c'_{n_\ell}|x_\ell|^{-1/2})|p|+\kappa_0(d_{n_\ell}|x_\ell|+d'_{n_\ell}|x_\ell|^{-1})|\mathrm{Im}\, p|}\right)$$
$$\leqslant \left(\prod_{v\in E_B(\theta)} e^{-\xi|\nu_v|}\right)\sum_{k=2}^{\infty}\Gamma^k\frac{|p|^{k-2}}{(k-2)!}e^{(c_{N-1}+c'_{N-1}2^{N/2})|p|+\kappa_0 d'_{N-1}2^N|\mathrm{Im}\, p|}, \tag{3.9}$$

where $D_0=\Gamma^2$, $r_N=\Gamma+c_{N-1}+\Gamma_0 c'_{N-1}2^{N/2}$, for some N-independent constant Γ_0. The bound in the last line of (3.9) has been obtained by using part of the exponential decay (say one-fourth) of the node factors associated with the endpoints to control the exponent $\kappa_0 d_{N-1}\max_{\ell\in L_2(T)}|x_\ell|$, provided $d_{N-1}<d$ for some N-independent constant d and $|\mathrm{Im}\, p|\leqslant\sigma$, with σ small enough, more precisely $\kappa_0\sigma d|\omega|<\xi/4$.

By explicitly performing the sum over k we obtain from (3.6),

$$\left|\left(\frac{M^{[N]}(x;\varepsilon)}{\varepsilon}\right)_B\right| \leqslant D_0 e^{r_N|p|}e^{-\xi_0 2^N}, \tag{3.10}$$

where we have used the bound $\Sigma_{\nu\in E_B(T)}|\boldsymbol{\nu}_v|\geqslant\Gamma_1 2^N$, for a suitable constant Γ_1—see formula (7.12) of Ref. 4—and again part of the exponential decay (say another one-fourth) of the node factors associated with the endpoints to control the exponent $\kappa_0 d'_{N-1}2^N|\mathrm{Im}\, p|$, provided again $d'_{N-1}<d'$ for some N-independent constant d' and $\kappa_0 d'\sigma<\xi\Gamma_1/4$; in particular one finds $\xi_0=\Gamma_1\xi/4$.

Then, by using (3.10) and, once more, the inductive bound, we obtain from (3.7),

$$|\tilde{g}^{[N]}_B(x,p)| \leqslant \frac{K_0}{|x|}e^{(c_{N-1}+c'_{N-1}|x|^{-1/2})|p|+\kappa_0(d_{N-1}|x|+d'_{N-1}|x|^{-1})|\mathrm{Im}\, p|} * \sum_{k=0}^{\infty}\left((D_0 e^{-r_N|p|}e^{-\xi_0 2^N})\right.$$
$$\left. * \left(\frac{K_0}{|x|}e^{(c_{N-1}+c'_{N-1}|x|^{-1/2})|p|+\kappa_0(d_{N-1}|x|+d'_{N-1}|x|^{-1})|\mathrm{Im}\, p|}\right)\right)^{*k}, \tag{3.11}$$

with $a^{*k}=a*a*\cdots*a$ (k times). This gives

$$|\tilde{g}^{[N]}_B(x,p)| \leqslant \frac{K_0}{|x|}\sum_{k=0}^{\infty}\frac{1}{(2k)!}\left(\frac{K_0|p|^2}{|x|}D_0 e^{-\xi_0 2^N}\right)^K e^{(r_N+c'_{N-1}|x|^{-1/2})|p|+\kappa_0(d_N|x|+d'_N|x|^{-1})|\mathrm{Im}\, p|}, \tag{3.12}$$

which implies the bound (3.5) for $n=N$, with $c_N=r_N=\Gamma+c_{N-1}+\Gamma_0 c'_{N-1}2^{N/2}$, $c'_N=c'_{N-1}+\sqrt{K_0 D_0 e^{-\xi_0 2^N}}$, $d_N=d_{N-1}$ and $d'_N=d'_{N-1}$. In particular one has $d_N=d=1$ and $d_{N'}=d'=2|c_0|$, so that there exists a constant $c>0$ such that $\max\{c_n 2^{-n/2}, c'_n, d_n, d_{n'}\}\leqslant c$ for all $n\geqslant 0$.

The bounds (3.8) for the Borel transforms of the propagators can be used to obtain a bound on the Borel transform $x_B(t;p)$ of $x(t;\varepsilon)$. We omit the details, which can be derived exactly as in Appendix A1 of Ref. 3. Eventually one finds the bound

$$|x_B(t;p)| \leqslant C_1 e^{C_2|p|^2}, \tag{3.13}$$

for suitable constants C_1 and C_2. Again, the bound (3.13) and the analyticity properties of $x_B(t;p)$ implies that $x(t;\varepsilon)$ is Borel summable, and it can be written for $\varepsilon>0$ as

$$x(t;\varepsilon)=\int_0^\infty e^{-p/\varepsilon}x_B(t;p)\mathrm{d}p, \tag{3.14}$$

in terms of its Borel transform.

As in the case $d=1$ the last statement of the theorem has been proved in Ref. 2. ■

In the general case $g(x) \neq x^2$ in (1.1) the quantity $2c_0$ must be replaced with $g'(c_0)$, with $g'(c_0) \neq 0$ by hypothesis. Then the discussion proceeds as in Sec. VII of Ref. 6.

Note also that in the case $d=2$ and $\tau=1$ the Borel transform is still defined in a strip around the real axis, but it does not satisfy any more an exponential bound like in the case $d=1$ (at least the argument given above does not provide an estimate of this kind). Thus, we cannot apply Nevanlinna's theorem to prove Borel summability.[7,8]

IV. BRYUNO FREQUENCY VECTORS

Let $\boldsymbol{\omega} \in \mathbb{R}^d$ be a Bryuno vector. This means that $B(\boldsymbol{\omega}) < \infty$, with $B(\boldsymbol{\omega})$ defined in (1.6).

Theorem 4.1: *Consider the system (1.1) for any $d \geqslant 2$, and assume that $\boldsymbol{\omega}$ satisfies the Bryuno condition $B(\omega) < \infty$ and that the nondegeneracy condition (1.4) is fulfilled. There exists $\varepsilon_0 > 0$ such that for all real $|\varepsilon| < \varepsilon_0$ there is a quasiperiodic solution with frequency vector $\boldsymbol{\omega}$. If $g'(c_0) > 0$ such a solution describes a local attractor.*

For simplicity's sake we discuss the case $g(x)=x^2$ and $\varepsilon \in \mathbb{R}$, but the analysis can be easily generalized to any analytic function g [provided the nondegeneracy condition (1.4) is satisfied]. Furthermore the solution can be showed to extend to a function analytic in ε in the domain $\mathcal{C}_R$ defined in Sec. VI of Ref. 6 (cf. Fig. 16 in Ref. 6).

Let $\psi(x)$ be the nondecreasing C^∞ function defined in (3.1) and set $\chi(x) := 1 - \psi(x)$. Define, for all $n \in \mathbb{Z}_+$, $\chi_n(x) := \chi(\alpha_n^{-1}(\boldsymbol{\omega})x/4)$ and $\psi_n(x) := \psi(\alpha_n^{-1}(\boldsymbol{\omega})x/4)$.

Set $g^{[-1]}(x;\varepsilon)=1$ and $M^{[-1]}(x;\varepsilon)=0$, and define iteratively $g^{[n]}(x;\varepsilon)$ and $M^{[n]}(x;\varepsilon)$ as done in the case of Diophantine vectors. This means that for $n=0$ we can define $g^{[0]}(x;\varepsilon)$ and $M^{[0]}(x;\varepsilon)$ as in (3.3), while for $n \geqslant 1$ we define

$$g^{[n]}(x;\varepsilon) = \frac{\varepsilon \chi_0(|x|) \cdots \chi_{n-1}(|x|)\psi_n(|x|)}{ix(1+i\varepsilon x) - \mathcal{M}^{[n-1]}(x;\varepsilon)},$$
$$\mathcal{M}^{[n]}(x;\varepsilon) = \sum_{p=0}^{n} \chi_0(|x|) \cdots \chi_p(|x|) M^{[p]}(x;\varepsilon), \quad M^{[n]}(x;\varepsilon) = \varepsilon \sum_{k=1}^{\infty} \sum_{T \in \mathcal{S}_{k,n}^{\mathcal{R}}} \mathcal{V}_T(x;\varepsilon), \tag{4.1}$$

where $\mathcal{S}_{k,n}^{\mathcal{R}}$ is the set of renormalized self-energy clusters T on scale n and of order k, and the self-energy value $\mathcal{V}_T(x;\varepsilon)$ is defined as in (3.2). Note that we are using the same definitions of Sec. III, in particular we are associating the factors ε with the propagators rather than with the nodes (contrary to what done in Ref. 6). So far the only difference with respect to the case of the standard Diophantine condition concerns the multiscale decomposition: the factors $2^n C_0^{-1}$ appearing in χ_n and ψ_n are substituted with $\alpha_n^{-1}(\omega)$.

Lemma 4.2: Assume that the renormalized propagators up to scale $n-1$ can be bounded as

$$|g^{[n_\ell]}(\boldsymbol{\omega} \cdot \boldsymbol{\nu}_\ell; \varepsilon)| \leqslant C^{-1} \alpha_{n_\ell}^{-\beta}(\boldsymbol{\omega}) \tag{4.2}$$

for some positive constants β and C. Then for all $p \leqslant n-1$ the number $N_p(\theta)$ of lines on scale p in any renormalized tree θ and the number $N_p(T)$ of lines on scale p in any renormalised self-energy cluster T are bounded both by

$$N_p(\theta) \leqslant K 2^{-p} \sum_{v \in E_B(\theta)} |\boldsymbol{\nu}_v|, \quad N_p(T) \leqslant K 2^{-p} \sum_{v \in E_B(T)} |\boldsymbol{\nu}_v|, \tag{4.3}$$

for some positive constant K. If $|\varepsilon| < \varepsilon_0$, with ε_0 small enough, then for all $p \leqslant n-1$ one has

$$|M^{[p]}(x;\varepsilon)| \leqslant D_1 |\varepsilon|^2 e^{-D_2 2^p}, \quad |\partial_x M^{[p]}(x;\varepsilon)| \leqslant D_1 |\varepsilon|^2 e^{-D_2 2^p}, \tag{4.4}$$

for some positive constants D_1 and D_2. Only the constant D_1 depends on β. The constant ε_0 can be written as $\varepsilon_0 = C_1 \alpha_{n_0}^{\beta}$, with $n_0(\boldsymbol{\omega}, \beta)$ such that

$$K\beta \sum_{n=n_0+1}^{\infty} \frac{1}{2^n} \log \frac{1}{\alpha_n(\boldsymbol{\omega})} \leqslant \frac{\xi}{4}, \tag{4.5}$$

and C_1 *a positive constant dependending on* C *but not on* β.

Proof: The lemma can be proved by reasoning as in Refs. 4 and 5. We simply sketch the proof, and omit the details. First of all note that, if we define $n(\boldsymbol{\nu})=\{n \in \mathbb{Z}_+ : 2^{n-1} < |\boldsymbol{\nu}| \leqslant 2^n\}$ then one has $|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \geqslant \alpha_{n(\boldsymbol{\nu})}(\boldsymbol{\omega})$. Moreover $n' > n$ implies $\alpha_{n'}(\boldsymbol{\omega}) \leqslant \alpha_n(\boldsymbol{\omega})$, and $\alpha_{n'}(\boldsymbol{\omega}) < \alpha_n(\boldsymbol{\omega})$ implies $n' > n$. Set $M(\theta)=\Sigma_{v \in E_B(\theta)}|\boldsymbol{\nu}_v|$ and $M(T)=\Sigma_{v \in E_B(T)}|\boldsymbol{\nu}_v|$. The bound on $N_p(\theta)$ is obtained by proving by induction on the order of the renormalized tree that if $N_p(\theta) \neq 0$ then $N_p(\theta) \leqslant 22^{-p}M(\theta) - 1$ Then, given a renormalized self-energy cluster $T \in \mathcal{S}^{\mathcal{R}}_{k,n}$, one proves first that $M(T) > 2^{n-1}$, hence, again by induction, that if $N_p(T) \neq 0$ then $N_p(T) \leqslant 22^{-p}M(T) - 1$. Therefore (4.3) is proved. An important property is that if a cluster T has two external lines, with momenta $\boldsymbol{\nu}$ and $\boldsymbol{\nu}'$, respectively, with $\boldsymbol{\nu} \neq \boldsymbol{\nu}'$, both on scales greater or equal to n, so that $|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \leqslant \alpha_{n-1}(\boldsymbol{\omega})/4$ and $|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \leqslant \alpha_{n-1}(\boldsymbol{\omega})/4$, then one has $|\boldsymbol{\omega}\cdot(\boldsymbol{\nu}-\boldsymbol{\nu}')| < \alpha_{n-1}(\boldsymbol{\omega})$, hence $n(\boldsymbol{\nu}-\boldsymbol{\nu}') \geqslant n$, so that $M(T) \geqslant |\boldsymbol{\nu} - \boldsymbol{\nu}'| > 2^{n-1}$. For details we refer to Ref. 5.

The bounds (4.4) are obtained by exploiting the just mentioned bound on $M(T)$ and half the exponential decay factors $e^{-\xi|\boldsymbol{\nu}_v|}$ associated with the vertices and endpoints internal to T to derive the factors $e^{-D_2 2^p}$, with D_2 independent of β, and by using the fact that any self-energy cluster T contributing to $M^{[p]}(x;\varepsilon)$ must be of order at least 2 to derive the factors $|\varepsilon|^2$.

Then for any $n_0 \in \mathbb{N}$ and for any tree θ, we can bound each propagator on scale up to n_0 with $C^{-1}\alpha_{n_0}^{-\beta}(\boldsymbol{\omega})$ and the product of propagators on scale greater than n_0 with

$$\prod_{n=n_0+1} (C^{-1}\alpha_n^{-\beta}(\boldsymbol{\omega}))^{N_n(\theta)} = C^{-\Sigma_{n=n_0+1}^{\infty} N_n(\theta)} \exp\left(\beta M(\theta) \sum_{n=n_0+1}^{\infty} \frac{1}{2^n} \log \frac{1}{\alpha_n(\boldsymbol{\omega})} \right), \tag{4.6}$$

so that, by choosing n_0 according to (4.5), the last exponential in (4.6) is controlled by half the exponential decay factor $e^{-\xi M(T)}$ arising from the node factors. Then the sum of the values of all trees of order k is bounded by $(C^{-1}C'\alpha_{n_0}^{-\beta})^k$, for a suitable constant C'—taking into account all the constants other than C and the sums over the trees. Hence also the assertion about the dependence of ε_0 on $\alpha_{n_0}(\boldsymbol{\omega})$ follows, and the proof of the lemma is complete. ■

As in Ref. 6, to prove existence of the quasiperiodic solution we need the following result, which together with Lemma 4.2 provides the proof of Theorem 4.1.

Lemma 4.3: For real ε *small enough the renormalized propagators satisfy the bounds (4.2) with* $\beta=1$. *For* ε *in the domain* $\mathcal{C}_R$ *in Fig.* 16 *of Ref.* 6 *they satisfy the bounds (4.2) with* $\beta=2$.

Proof: The proof can be carried out exactly as in Ref. 6. Indeed it is enough to show that the propagators $g^{[n]}(x;\varepsilon)$ can be bounded proportionally to $|x|^{-\beta}$, for ε small enough in a suitable domain, and this follows from Lemmata 6.2 to 6.5 of Ref. 6, independently on the particular Diophantine condition assumed on $\boldsymbol{\omega}$. ■

The proof of the theorem is completed if we show that the quasiperiodic solution is a local attractor if $g'(c_0) > 0$. But this can be proved as in the case of Diophantine frequency vectors, by reasoning as in Ref. 2: indeed the only property that we need for the argument given in Ref. 2 to work is the existence of the quasiperiodic solution.

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Long-time dynamics of variable coefficient modified Korteweg-de Vries solitary waves[a)]

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We study the long-time behavior of solutions to the Korteweg-de Vries-type equation $\partial_t u=-\partial_x(\partial_x^2 u+f(u)-b(t,x)u)$, with initial conditions close to a stable, $b=0$ solitary wave. The coefficient b is a bounded and slowly varying function, and f is a nonlinearity. For a restricted class of nonlinearities, we prove that for long time intervals, such solutions have the form of the solitary wave, whose center and scale evolve according to a certain dynamical law involving the function $b(t,x)$, plus an $H^1(\mathbb{R})$-small fluctuation. The result is stronger than those previously obtained for general nonlinearities f. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We study the long-time behavior of solutions to a class Korteweg-de Vries-type equations, with an additional term $b(t,x)u$. These equations, hereafter referred to as the bKdV, are of the form

$$\partial_t u = -\partial_x(\partial_x^2 u + f(u) - b(t,x)u), \tag{1}$$

where $b(t,x)$ is a real valued function and f is a nonlinearity. We formulate conditions on the nonlinearity in Sec. II. Our class includes, in particular, $f(u)=u^3$, corresponding to the modified KdV (mKdV). When $b=0$, Eq. (1) reduces to the generalized Korteweg-de Vries equation (GKdV)

$$\partial_t u = -\partial_x(\partial_x^2 u + f(u)). \tag{2}$$

A remarkable property of the GKdV is the existence of spatially localized solitary (or traveling) waves, i.e., solutions of the form $u=Q_c(x-a-ct)$, where $a\in\mathbb{R}$ and c in some interval I. When $f(u)=u^p$ and $p\geq 2$, solitary waves are explicitly computed to be

$$Q_c(x) = c^{1/(p-1)}Q(c^{1/2}x),$$

where

$$Q(x) = \left(\frac{p+1}{2}\right)^{1/(p-1)}\left(\operatorname{sech}\left(\frac{p-1}{2}x\right)\right)^{2/(p-1)}.$$

It is generally believed that an arbitrary, say $H^1(\mathbb{R})$, solution to Eq. (2) eventually breaks up into a collection of solitary waves and radiation. A discussion of this phenomenon for the generalized KdV appears in Bona.[12] For the general, but integrable, case, see Deift and Zhou.[19]

[a)]This paper is part of the first author's Ph.D. thesis.

The GKdV arises in different branches of science and engineering. In particular, the mKdV equation, to which our results apply, is fundamental in many areas of applied mathematics ranging from traffic flow to plasma physics (see Refs. 16, 32, 33, and 35), and arises from an approximation of more complicated systems. The effects of higher order processes can often be collected into a term of the form $b(t,x)u$. Our main result stated at the end of the next section gives, for long time, an explicit, leading order description of a solution to the bKdV initially close to a solitary wave solution of the GKdV.

We assume that the coefficient b and nonlinearity f are such that (1) has global solutions for $H^1(\mathbb{R})$ data and that (1) with $b=0$ possesses solitary wave solutions. Precise conditions will be formulated in the next section. Here we mention that the literature regarding well-posedness of the KdV [$b=0$, $f(u)=u^2$] is extensive and well developed. The Miura transform (see Ref. 34) then gives well-posedness results for the mKdV. Bona and Smith[10] proved global well-posedness of the KdV in $H^2(\mathbb{R})$. See also Ref. 28. Kenig, Ponce, and Vega[30] have proved local well-posedness in $H^s(\mathbb{R})$ for $s\geq -\frac{3}{4}$, and similar results are available for the generalized KdV [$b=0$, monomial nonlinearity $f(u)=u^p$ with $p=2,3,4$].[29] In particular, local well-posedness for the mKdV in $H^s(\mathbb{R})$ with $s\geq \frac{1}{4}$ and global well-posedness for $s\geq 1$ are known. More recently, results extending local well-posedness in negative index Sobolev spaces to global well-posedness have been proven.[17,18] There is little literature on global well-posedness of the bKdV in energy space, however, under a smallness assumption on the coefficient b, Dejak and Sigal[20] proved global well-posedness in $H^1(\mathbb{R})$ of the bKdV with $f(u)=u^p$, $p=2,3,4$. They used results of Ref. 29, and perturbation and energy arguments.

Soliton solutions of the KdV equation are known to be orbitally stable. Although the linearized analysis of Jeffrey and Kakutani[26] suggested orbital stability, the first nonlinear stability result was given by Benjamin.[2] He assumed smooth solutions and used Lyapunov stability and spectral theory to prove his results. Bona[4] later corrected and improved Benjamin's result to solutions in $H^2(\mathbb{R})$. Weinstein[46] used variational methods, avoiding the use of an explicit spectral representation, and extended the orbital stability result to the GKdV. More recently, Grillakis, Satah, and Strauss[24] extended the Lyapunov method to abstract Hamiltonian systems with symmetry. Numerical simulations of soliton dynamics for the KdV were performed by Bona *et al.* See Refs. 6–9.

The long-time dynamics of the bKdV was first studied in Ref. 20. For nonlinear Schrödinger and Hartree equations, long-time dynamics of solitary waves were studied by Bronski and Jerrard,[13] Fröhlich, Tsai, and Yau,[22] Keraani,[31] and Fröhlich and co-workers.[21,27]. For related results and techniques for the nonlinear Schrödinger equations, see also Refs. 14, 15, 23, 39–41, and 43–45.

In this paper we show that for long time intervals [$t\leq \mathrm{O}(|\partial_x b|^{-1})$], the solution of the bKdV initially close to a soliton $Q_{c_0}(x-a_0)$ remains close to a moving soliton $Q_{c(t)}(x-a(t))$ whose center $a(t)$ and shape parameter $c(t)$ satisfy a certain dynamical system. Although the class of nonlinearities consider in this paper is smaller than that of Ref. 20, we obtain more precise dynamical equations for the soliton parameters that are valid for longer time intervals, and hence obtain a better description of solutions to the bKdV. Moreover, our proof is simpler than that of Ref. 20. In our approach, we use the fact that the bKdV is a (nonautonomous if b depends on time) Hamiltonian system. As in Ref. 20, we construct a Hamiltonian reduction of this original, infinite dimensional dynamical system to a two-dimensional dynamical system on a manifold of soliton configurations. The analysis of the bKdV with general nonlinearity immediately runs into the problem that the natural symplectic form ω is not defined on the tangent space of the soliton manifold. However, we show that there is a class of nonlinearities for which the symplectic form is well defined on the tangent space. This is the class of nonlinearities considered in this paper.

II. PRELIMINARIES, ASSUMPTIONS, MAIN RESULTS

The bKdV can be written in Hamiltonian form as

$$\partial_t u = \partial_x H_b'(u), \tag{3}$$

where H_b' is the $L^2(\mathbb{R})$ function corresponding to the Fréchet derivative ∂H_b in the $L^2(\mathbb{R})$ pairing. Here the Hamiltonian H_b is

$$H_b(u) := \int_{-\infty}^{\infty} \frac{1}{2}(\partial_x u)^2 - F(u) + \frac{1}{2}b(t,x)u^2 dx,$$

where the function F is the antiderivative of f with $F(0)=0$. The operator ∂_x is the anti-self-adjoint operator (symplectic operator) generating the Poisson bracket

$$\{G_1, G_2\} := \frac{1}{2}\int_{-\infty}^{\infty} G_1'(u)\partial_x G_2'(u) - G_2'(u)\partial_x G_1'(u)dx,$$

defined for any G_1, G_2 such that $G_1', G_2' \in H^{1/2}(\mathbb{R})$. The corresponding symplectic form is

$$\omega(v_1, v_2) := \frac{1}{2}\int_{-\infty}^{\infty} v_1(x)\partial_x^{-1} v_2(x) - v_2(x)\partial_x^{-1} v_1(x)dx,$$

defined for any $v_1, v_2 \in L^1(\mathbb{R})$. Here the operator ∂_x^{-1} is defined as

$$\partial_x^{-1} v(x) := \int_{-\infty}^{x} v(y)dy.$$

Note that $\partial_x^{-1}\cdot\partial_x = I$ and, on the space $\{u \in L^2(\mathbb{R}) \,|\, \int_{-\infty}^{\infty} u dx = 0\}$, ∂_x^{-1} is formally anti-self-adjoint with inverse ∂_x. Hence, if $\int_{-\infty}^{\infty} v_1(x)dx = 0$, then $\omega(v_1, v_2) = \int_{-\infty}^{\infty} v_1(x)\partial_x^{-1} v_2(x)dx$.

Note that if b depends on time t, then Eq. (3) is nonautonomous. It is, however, in the form of a conservation law, and hence the integral of the solution u is conserved provided u and its derivatives decay to zero at infinity:

$$\frac{d}{dt}\int_{-\infty}^{\infty} u dx = 0.$$

There are also conserved quantities associated to symmetries of (1) when $b=0$. The simplest such corresponds to time translation invariance and is the Hamiltonian itself. This is also true if b is nonzero but time independent. If the potential $b=0$, then (1) is also spatially translation invariant. Noether's theorem then implies that the flow preserves the momentum

$$P(u) := \frac{1}{2}\|u\|_{L^2}^2.$$

In general, when $b \neq 0$, the temporal and spatial translation symmetries are broken, and hence the Hamiltonian and momentum are no longer conserved. Instead, one has the relations

$$\frac{d}{dt}H_b(u) = \frac{1}{2}\int_{-\infty}^{\infty} (\partial_t b)u^2 dx, \tag{4}$$

$$\frac{d}{dt}P(u) = \frac{1}{2}\int_{-\infty}^{\infty} b' u^2 dx, \tag{5}$$

where $b'(t,x) := \partial_x b(t,x)$. For later use, we also state the relation

$$\frac{d}{dt}\frac{1}{2}\int_{-\infty}^{\infty} bu^2 dx = \int_{-\infty}^{\infty} \frac{1}{2}u^2\partial_t b + b'\left(uf(u) - \frac{3}{2}(\partial_x u)^2 - F(u)\right) - b''u\partial_x u dx. \tag{6}$$

Assuming (1) is well-posed in $H^2(\mathbb{R})$, the above equalities are obtained after multiple integration by parts. Then, by density of $H^2(\mathbb{R})$ in $H^1(\mathbb{R})$, the equalities continue to hold for solutions in $H^1(\mathbb{R})$. To avoid these technical details, we assume the Hamiltonian flow on $H^1(\mathbb{R})$ enjoys (4)–(6).

Consider the GKdV, i.e., Eq. (2). Under certain conditions on f, this equation has traveling wave solutions of the form $Q_c(x-ct)$, where Q_c is a positive $H^2(\mathbb{R})$ function. Substituting $u = Q_c(x-ct)$ into the GKdV gives the scalar field equation

$$-\partial_x^2 Q_c + cQ_c - f(Q_c) = 0. \tag{7}$$

The existence of solutions to this equation has been studied by numerous authors. See Refs. 3, 5, and 42. In particular, Berestyki and Lions[3] give sufficient and necessary conditions for a positive and smooth solution Q_c to exist. We assume $g := -cu + f(u)$ satisfies the following conditions:

1. g is locally Lipschitz and $g(0)=0$;
2. $x^* := \inf\{x>0 \,|\, \int_0^x g(y)dy\}$ exists with $x^*>0$ and $g(x^*)>0$; and
3. $\lim_{s\to 0}[g(s)/s] \le -m < 0$.

Then, as shown by Berestycki and Lions, (7) has a unique (modulo translations) solution $Q_c \in C^2$ for c in some interval, which is positive, even (when centered at the origin), and with Q_c, $\partial_x Q_c$, and $\partial_x^2 Q_c$ exponentially decaying to zero at infinity ($\partial_x Q_c < 0$ for $x>0$). Furthermore, if f is C^2, then the implicit function theorem implies that Q_c is C^2 with respect to the parameter c on some interval $I_0 \subset \mathbb{R}_+$. We assume that $x^m \partial_c^n Q_c \in L^1(\mathbb{R})$ for $n=1,2, m=0,1,2$ so that integrals containing $\partial_c^n Q_c$ are continuous and differentiable with respect to c. We also make the assumption that

$$\int_{-\infty}^{\infty} \partial_c Q_c dx = 0 \tag{8}$$

for all $c \in I$. This implies that

$$\int_{-\infty}^{x} \partial_c Q_c(z)dz, \int_{-\infty}^{x} \partial_c^2 Q_c(z)dz \in L^2(\mathbb{R}). \tag{9}$$

To see this, use the isometry property of the Fourier transform and the decay properties of $\partial_c Q_c$. The above requirements of Q_c are implicit assumptions on the nonlinearity f and are true when $f(u)=u^3$. Assumption (8) is a very important and restrictive requirement; it does not hold when $f(x)=x^p$ and $p \neq 3$. For the case where (8) does not hold, see Ref. 20.

The solitary waves Q_c are orbitally stable if $\delta'(c)>0$, where $\delta(c)=P(Q_c)$ [to avoid potential confusion, we remark that the quantity $\delta(c)$ is often written as $d'(c)$ in the literature]. See Weinstein,[46] for the first proof for general nonlinearities. Moreover, in Ref. 24, Grillakis, Shatah, and Strauss proved that $\delta'(c)>0$ is a necessary and sufficient condition for Q_c to be orbitally stable. Bona, Souganidis, and Strauss[11] also gave stability results for KdV-type equations and Albert, Bona, and Henry[1] gave an instability result. The first proof of asymptotic stability for the KdV was given by Pego and Weinstein.[36] In this paper, we assume that Q_c is orbitally stable for all c in some compact interval $I \subset I_0$, or equivalently that $\delta'(c)>0$ on I. For $f(u)=u^p$, we have

$$\delta'(c) = \frac{5-p}{4(p-1)}\|Q_{c=1}\|_{L^2}^2 c^{\{(7-3p)/[2(p-1)]\}},$$

which implies the well-known stability criterion $p<5$ corresponding to subcritical power nonlinearities.

The scalar field equation (7) for the solitary wave can be viewed as a Euler-Lagrange equation for the extremals of the Hamiltonian $H_{b=0}$ subject to constant momentum $P(u)$. Moreover, Q_c is a stable solitary wave if and only if it is a minimizer of $H_{b=0}$ subject to constant momentum P. Thus, if c is the Lagrange multiplier associated to the momentum constraint, then Q_c is an extremal of

$$\Lambda_{ca}(u) := H_{b=0}(u) + cP(u) = \int_{-\infty}^{\infty} \frac{1}{2}(\partial_x u)^2 + \frac{1}{2}cu^2 - F(u)dx, \tag{10}$$

and hence $\Lambda'_{ca}(Q_c)=0$.

The functional Λ_{ca} is translationally invariant. Therefore, $Q_{ca}(x) := Q_c(x-a)$ is also an extremal of Λ_{ca}, and $Q_c(x-ct-a)$ is a solitary wave solution of (1) with $b=0$. All such solutions form the two-dimensional manifold of solitary waves

$$M_s := \{Q_{ca} | c \in I, a \in \mathbb{R}\},$$

with tangent space $T_{Q_{ca}}M_s$ spanned by the vectors

$$\zeta^{tr}_{ca} := \partial_a Q_{ca} = -\partial_x Q_{ca} \quad \text{and} \quad \zeta^{n}_{ca} := \partial_c Q_{ca}, \tag{11}$$

which we call the translation and normalization vectors. Notice that the two tangent vectors are orthogonal in $L^2(\mathbb{R})$.

In addition to the requirement on b that (1) is globally well posed, we assume the potential b is bounded, twice differentiable, and small in the sense that

$$|\partial_t^n \partial_x^m b| \le \epsilon_a \epsilon_t^n \epsilon_x^m, \tag{12}$$

for $n=0,1$, $m=0,1,2$, and $n+m\le 2$. The positive constants ϵ_a, ϵ_x, and ϵ_t are amplitude, length, and time scales of the function b. We assume all are less than or equal to one.

Lastly, we make some explicit assumptions on the local nonlinearity f. We require the nonlinearity to be k times continuously differentiable, $f(0)=f'(0)=0$. These assumptions ensure the Hamiltonian is finite on the space $H^1(\mathbb{R})$ and, since Q_c decays exponentially (see Ref. 3), both $f(Q_c)$ and $f'(Q_c)$ have exponential decay.

We are ready to state our main result. Recall that $I_0 \subset \mathbb{R}_+$ is an interval where Q_c is twice continuously differentiable.

Theorem 2.1: *Let the above assumptions hold and assume $\delta'(c)>0$ for all c in a compact interval $I \subset I_0$. Assume $\epsilon_a \le 1$. Then, if $\epsilon_x \le 1$, ϵ_0 and ϵ_t are small enough ($\ll \inf_I \delta'^2$), there is a positive constant C such that the solution to* (1) *with an initial condition u_0 satisfying $\inf_{Q_{ca}\in M_s} \|u_0 - Q_{ca}\|_{H^1} \le \epsilon_0$ can be written as*

$$u(x,t) = Q_{c(t)}(x - a(t)) + \xi(x,t),$$

where $\|\xi(t)\|_{H^1} = O(\epsilon_0 + (\epsilon_a \epsilon_x \epsilon_0)^{1/2} + \epsilon_x + \epsilon_t)$ for all times $t \le C(\epsilon_a \epsilon_x)^{-1}$. Moreover, during this time interval the parameters $a(t)$ and $c(t)$ satisfy the equations

$$\begin{pmatrix} \dot{a} \\ \dot{c} \end{pmatrix} = \begin{pmatrix} c - b(a) \\ 0 \end{pmatrix} + b'(a)\frac{\delta(c)}{\delta'(c)}\begin{pmatrix} 0 \\ 1 \end{pmatrix} + O((\epsilon_0 + \epsilon_x + \epsilon_t)^2 + (\epsilon_a \epsilon_x \epsilon_0)^{1/2}(\epsilon_x + \epsilon_t + \epsilon_0)),$$

where c is assumed to lie in the compact interval I.

Sketch of Proof and Paper Organization. To realize the Hamiltonian reduction we decompose functions in a neighborhood of the soliton manifold M_s as

$$u = Q_{ca} + \xi,$$

with ξ symplectically orthogonal to $T_{Q_{ca}}M_s$, i.e., $\xi \perp \partial_x^{-1} T_{Q_{ca}} M_s$. We show that there is an $\epsilon_0 = \mathrm{O}(\inf_I \delta'^2) > 0$ such that if the solution u satisfies the estimate $\inf_{Q_{ca}} \|u - Q_{ca}\|_{H^1} < \epsilon_0$, then there are unique C^1 functions $a(u)$ and $c(u)$ such that $u = Q_{c(u)a(u)} + \xi$ with $\xi \perp \partial_x^{-1} T_{Q_{ca}} M_s$.

With the knowledge that the symplectic decomposition exists, we substitute $u = Q_{ca} + \xi$ into the bKdV (1) and split the resulting equation according to the decomposition

$$L^2(\mathbb{R}) = \partial_x^{-1} T_{Q_{ca}} M_s \oplus (\partial_x^{-1} T_{Q_{ca}} M_s)^{\perp}$$

to obtain equations for the parameters c and a, and an equation for the (infinite dimensional) fluctuation ξ. In Sec. IV we isolate the leading order terms in the equations for a and c and estimate the remainder, including all terms containing ξ. In Secs. VI and VII, we establish spectral properties and a lower bound of the Hessian Λ''_{ca} on the space $(\partial_x^{-1} T_{Q_{ca}} M_s)^{\perp}$.

The proof that $\|\xi\|_{H^1}$ is sufficiently small is the final ingredient in the proof of the main theorem. The remaining sections concentrate on proving this crucial result. We employ a Lyapunov method and in Sec. V we construct the Lyapunov function Γ_c and prove an estimate on its time derivative. This estimate is later time maximized over an interval $[0,T]$, and integrated to obtain an upper bound on Γ_c involving the time T and the norms of ξ. We combine this upper bound with the lower bound on Γ_c following from the results of Sec. VII, and obtain an inequality involving $\|\xi\|_{H^1}$. In Sec. VIII we solve the inequality to find an upper bound on $\|\xi\|_{H^1}$ provided $\|\xi(0)\|_{H^1}$ is small enough. We substitute this bound into the bound appearing in the dynamical equation for a and c, and take $\epsilon_a \epsilon_x$and ϵ_0 small enough so that all intermediate results hold to complete the proof. □

III. MODULATION OF SOLUTIONS

As stated in the previous section, we begin the proof by decomposing the solution of (1) into a modulated solitary wave and a fluctuation ξ:

$$u(x,t) = Q_{c(t)a(t)}(x) + \xi(x,t), \tag{13}$$

with a, c, and ξ fixed by the orthogonality condition

$$\xi \perp \partial_x^{-1} T_{Q_{ca}} M_s, \tag{14}$$

where

$$\partial_x^{-1} : g \to \int_{-\infty}^{x} g(z)dz.$$

Note that $\partial_x^{-1} T_{Q_{ca}} M_s$ is a subset of $L^2(\mathbb{R})$ [see (9)].

The existence and uniqueness of parameters a and c such that $\xi = u - Q_{ca}$ satisfies (14) follows from the next lemma concerning a restriction of ∂_x^{-1} and the implicit function theorem. The restriction K of ∂_x^{-1} to the tangent space $T_{Q_{ca}} M_s$ is defined by the equation $KP_T = P_T \partial_x^{-1} P_T$, where P_T is the orthogonal projection onto $T_{Q_{ca}} M_s$. In the natural basis $\{\zeta_{ca}^{tr}, \zeta_{ca}^{n}\}$ of the tangent space $T_{Q_{ca}} M_s$, the matrix representation of K is $N^{-1}\Omega_{ca}$, where

$$N := \begin{pmatrix} \|\zeta_{ca}^{tr}\|_{L^2}^2 & 0 \\ 0 & \|\zeta_{ca}^{n}\|_{L^2}^2 \end{pmatrix}$$

and

$$\Omega_{ca} := \begin{pmatrix} \langle \zeta_{ca}^{tr}, \partial_x^{-1} \zeta_{ca}^{tr} \rangle & \langle \zeta_{ca}^{n}, \partial_x^{-1} \zeta_{ca}^{tr} \rangle \\ \langle \zeta_{ca}^{tr}, \partial_x^{-1} \zeta_{ca}^{n} \rangle & \langle \zeta_{ca}^{n}, \partial_x^{-1} \zeta_{ca}^{n} \rangle \end{pmatrix}. \tag{15}$$

Recall that $\delta(c) = \frac{1}{2}\|Q_c\|_{L^2}^2$.

Lemma 3.1: If $\delta'(c)>0$ on the compact interval $I\subset R_+$, then the matrix Ω_{ca} is invertible for all $c\in I$, and

$$\Omega_{ca}^{-1}=\frac{1}{\delta'(c)}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}. \tag{16}$$

Clearly, $\|\Omega_{ca}^{-1}\|\leq\lfloor\delta'\rfloor^{-1}$, where $\lfloor\delta'\rfloor:=\inf_I\delta'(c)$.

Proof: The lemma follows from the relations $\langle\zeta_{ca}^{tr},\partial_x^{-1}\zeta_{ca}^{tr}\rangle=0$, $\langle\zeta_{ca}^{n},\partial_x^{-1}\zeta_{ca}^{n}\rangle=0$, and $\langle\zeta_{ca}^{tr},\partial_x^{-1}\zeta_{ca}^{n}\rangle=\langle\zeta_{ca}^{n},Q_c\rangle=\delta'(c)$. □

Given $\varepsilon>0$, define the tubular neighborhood

$$U_\varepsilon:=\left\{u\in L^2(\mathbb{R})\,\middle|\,\inf_{(c,a)\in I\times R}\|u-Q_{ca}\|_{L^2}<\varepsilon\right\}$$

of the solitary wave manifold M_s in $L^2(\mathbb{R})$.

Proposition 3.2: Let $I\subset\mathbb{R}_+$ be a compact interval such that $c\mapsto Q_{ca}$ is $C^1(I)$. Then there exists a positive number $\varepsilon_*=\varepsilon_*(I)=\mathrm{O}(\lfloor\delta'\rfloor^2)$ dependent on I and unique C^1 functions $a:U_{\varepsilon_*}\to\mathbb{R}$ and $c:U_{\varepsilon_*}\to I$, such that

$$\langle Q_{c(u)a(u)}-u,\partial_x^{-1}\zeta_{c(u)a(u)}^{tr}\rangle=0\quad\text{and}\quad\langle Q_{c(u)a(u)}-u,\partial_x^{-1}\zeta_{c(u)a(u)}^{n}\rangle=0$$

for all $u\in U_{\varepsilon_*}$. Moreover, there is a positive real number $C=C(I)$ such that

$$\|u-Q_{c(u)a(u)}\|_{H^1}\leq C\inf_{Q_{ca}\in M_s}\|u-Q_{ca}\|_{H^1} \tag{17}$$

for all $u\in U_{\varepsilon_*}\cap H^1(\mathbb{R})$.

Proof: Let $\mu:=(\mu^1,\mu^2)^T\in\mathbb{R}\times I$ and define $G:\mathbb{R}\times I\times H^1(\mathbb{R})\to\mathbb{R}^2$ as

$$G{:}(\mu,u)\to\begin{pmatrix}\langle Q_{ca}-u,\Omega_{ca}\zeta_{ca}^{tr}\rangle\\ \langle Q_{ca}-u,\Omega_{ca}\zeta_{ca}^{n}\rangle\end{pmatrix},$$

where $a=\mu^1$ and $c=\mu^2$. The proposition is equivalent to solving $G(g(u),u)=0$ for a C^1 function g. Let $\mu_0=(ac)^T$. If G is C^1, $G(\mu_0,Q_{ca})=0$, and $\partial_\mu F(\mu_0,Q_{ca})$ is invertible, then the implicit function theorem asserts the existence of an open ball $B_\varepsilon(Q_{ca})$ of radius ε with center Q_{ca}, and a unique function $g_{Q_{ca}}:B_\varepsilon(Q_{ca})\to\mathbb{R}\times I$, such that $G(g_{Q_{ca}}(u),u)=0$ for all $u\in B_\varepsilon(Q_{ca})$.The first two conditions are trivial, and the third follows from Lemma 3.1 since $\partial_\mu G(\mu_0,Q_{ca})=\Omega_{ca}$. The radius ε depends on the parameters c and a, however, since $\lfloor\delta'\rfloor:=\inf_I\delta'(c)>0$, we can choose a smaller ball radius ε_* of order $\lfloor\delta'\rfloor^2$ that works for all $a\in\mathbb{R}$ and $c\in I$. For details, see the proof of the decomposition theorem in Ref. 20. We define $U_{\varepsilon_*}=\cup\{B_{\varepsilon_*}(Q_{ca})\,|\,a\in\mathbb{R},c\in I\}$ and past the C^1 functions $g_{Q_{ca}}$ together into a C^1 function $g_I:U_{\varepsilon_*}\to\mathbb{R}\times I$. This proves existence of the required C^1 functions $a(u)$ and $c(u)$. Uniqueness follows from the uniqueness of the functions $g_{Q_{ca}}$.

Let $u\in U_{\varepsilon_*}$, $c\in I$, and $a\in\mathbb{R}$, and consider the equation

$$u-Q_{c(u)a(u)}=u-Q_{ca}+Q_{ca}-Q_{c(u)a(u)}.$$

Clearly, inequality (17) will follow if $\|Q_{ca}-Q_{c(u)a(u)}\|_{H^1}\leq C\|u-Q_{ca}\|_{H^1}$ for some positive constant C. Since the derivatives ∂_cQ_{ca} and ∂_aQ_{ca} are uniformly bounded in $H^1(\mathbb{R})$ over $\mathbb{R}\times I$, the mean value theorem gives that $\|Q_{ca}-Q_{c(u)a(u)}\|_{H^1}\leq C\|(c,a)^T-(c(u),a(u))^T\|$, where the constant C does not depend on c, a. The relations $g_I(Q_{ca})=(c,a)^T$ and $g_I(u)=(c(u),a(u))^T$ then imply $\|Q_{ca}-Q_{c(u)a(u)}\|_{H^1}\leq C\|g_I(Q_{ca})-g_I(u)\|$. Again, we appeal to the mean value theorem and use the properties of Ω_{ca} and that $\partial_ug_I=\partial_\mu G^{-1}\partial_uG$ is uniformly bounded in the parameters c and a to obtain (17). The last equation is obtained by implicitly differentiating $G(g_I(u),u)=0$ with respect to u.□

IV. EVOLUTION EQUATIONS FOR PARAMETERS ξ, a, AND c

In Sec. III we proved that if u remains close enough to the solitary wave manifold M_s, then we can write a solution u to (1) uniquely as a sum of a modulated solitary wave Q_{ca} and a fluctuation ξ satisfying the orthogonality condition (14). Thus, as u evolves according to the initial value problem (1), the parameters $a(t)$ and $c(t)$ trace out a path in $\mathbb{R}^2$. The goal of this section is to derive the dynamical equations for the parameters a and c, and the fluctuation ξ. We obtain such equations by substituting the decomposition $u=Q_{ca}+\xi$ into (1) and then projecting the resulting equation onto appropriate directions, with the intent of using the orthogonality condition on ξ.

From now on, u is the solution of (1) with initial condition u_0 satisfying $\epsilon_0 := \inf_{Q_{ca}\in M_s}\|u_0 - Q_{ca}\|_{H^1} < \varepsilon_*$, and $T_0=T_0(u_0)$ is the maximal time such that $u(t)\in U_{\varepsilon_*}$ for $0\le t\le T_0$. Then, for $0\le t\le T_0$, u can be decomposed as in (13) and (14).

Proposition 4.1: Assume $\delta'(c)\neq 0$. *Say* $u=Q_{ca}+\xi$ *is a solution to* (1), *where* ξ *satisfies* (14). *Then, if* $\|\xi\|_{H^1}$ *is small enough,* $\epsilon_x\le 1$, *and* $c\in I$,

$$\begin{pmatrix}\dot a\\ \dot c\end{pmatrix} = \begin{pmatrix} c-b(t,a)\\ 0\end{pmatrix} + b'(t,a)\frac{\delta(c)}{\delta'(c)}\begin{pmatrix}0\\1\end{pmatrix} + Z(a,c,\xi), \tag{18}$$

where $Z(a,c,\xi)=\mathrm{O}(\epsilon_a\epsilon_x^2+\epsilon_a\epsilon_x\|\xi\|_{H^1}+\|\xi\|_{H^1}^2)$.

Proof: Recall that the solitary wave Q_{ca} is an extremal of the functional Λ_{ca}. To use this fact we rearrange definition (10) of Λ_{ca} to write the Hamiltonian H_b as

$$H_b(u) = \Lambda_{ca}(u) - cP(u) + \frac{1}{2}\int_{-\infty}^{\infty} bu^2(x)dx,$$

where for notational simplicity we have suppressed the space and time dependency of b. Substituting $Q_{ca}+\xi$ for u in (3) and using the above expression for H_b gives the equation

$$\dot a\zeta_{ca}^{tr} + \dot c\zeta_{ca}^{n} + \dot\xi = \partial_x\Lambda_{ca}'(Q_{ca}+\xi) - c\partial_x[Q_{ca}+\xi] + \partial_x[(Q_{ca}+\xi)b],$$

where the dots indicate time differentiation. Let $\mathcal{L}_Q := \Lambda_{ca}''(Q_{ca})$,

$$\delta b := b(t,x) - b(t,a),$$

and

$$\delta^2 b := b(t,x) - b(t,a) - b'(t,a)(x-a).$$

Taylor expanding $\Lambda_{ca}'(Q_{ca}+\xi)$ to linear order in ξ, using that Q_{ca} is an extremal of Λ_{ca} and the relation $\zeta_{ca}^{tr}=-\partial_x Q_{ca}$ gives that

$$\begin{aligned}\dot\xi = {}& \partial_x[(\mathcal{L}_Q+\delta b + b(a)-c)\xi] + \partial_x N_{ca}'(\xi) - [\dot a - c + b(a)]\zeta_{ca}^{tr} - \dot c\zeta_{ca}^{n} + b'(a)\partial_x[(x-a)Q_{ca}]\\ & + \partial_x[\delta^2 bQ_{ca}].\end{aligned} \tag{19}$$

The nonlinear terms have been collected into $N_{ca}'(\xi)$ given by (A1) in the Appendix.

Define the vectors $\zeta_1 := \zeta_{ca}^{tr}$ and $\zeta_2 := \zeta_{ca}^{n}$. Projecting (19) onto $\partial_x^{-1}\zeta_i$ for $i=1,2$ and using the antisymmetry of ∂_x gives the two equations

$$\begin{aligned}&[\dot a - c + b(a)][\langle\zeta_{ca}^{tr},\partial_x^{-1}\zeta_i\rangle + \langle\xi,\zeta_i\rangle] + \dot c\langle\zeta_{ca}^{n},\partial_x^{-1}\zeta_i\rangle + \langle\dot\xi,\partial_x^{-1}\zeta_i\rangle - \dot a\langle\xi,\zeta_i\rangle\\ &\quad = -b'(t,a)\langle(x-a)Q_{ca},\zeta_i\rangle - \langle\delta^2 bQ_{ca},\zeta_i\rangle - \langle\delta b\xi,\zeta_i\rangle - \langle N_{ca}'(\xi),\zeta_i\rangle - \langle L_Q\xi,\zeta_i\rangle.\end{aligned} \tag{20}$$

We can replace the term containing $\dot\xi$ since the time derivative of the orthogonality condition $\langle\xi,\partial_x^{-1}\zeta_i\rangle=0$ implies $\langle\dot\xi,\partial_x^{-1}\zeta_i\rangle=\dot a\langle\xi,\zeta_i\rangle-\dot c\langle\xi,\partial_c\partial_x^{-1}\zeta_i\rangle$. Note that we have used the relation $\partial_a\zeta_i = -\partial_x\zeta_i$. Thus, in matrix form, (20) becomes

$$(I+B)\Omega_{ca}\begin{pmatrix}\dot{a}-c+b(t,a)\\ \dot{c}\end{pmatrix}=X+Y, \tag{21}$$

where

$$X:=-b'(t,a)\delta(c)\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}\langle\delta^2 bQ_{ca},\zeta_{ca}^{tr}\rangle\\ \langle\delta^2 bQ_{ca},\zeta_{ca}^{n}\rangle\end{pmatrix},$$

$$Y:=-\begin{pmatrix}\langle\delta b\xi,\zeta_{ca}^{tr}\rangle+\langle N'_{ca}(\xi),\zeta_{ca}^{tr}\rangle+\langle L_Q\xi,\zeta_{ca}^{tr}\rangle\\ \langle\delta b\xi,\zeta_{ca}^{n}\rangle+\langle N'_{ca}(\xi),\zeta_{ca}^{n}\rangle+\langle L_Q\xi,\zeta_{ca}^{n}\rangle\end{pmatrix},$$

and

$$B:=\begin{pmatrix}\langle\xi,\zeta_{ca}^{tr}\rangle & \langle\xi,\zeta_{ca}^{n}\rangle\\ \langle\xi,\zeta_{ca}^{n}\rangle & -\langle\xi,\partial_c\partial_x^{-1}\zeta_{ca}^{n}\rangle\end{pmatrix}\Omega_{ca}^{-1}.$$

We have explicitly computed $\langle(x-a)Q_{ca},\zeta_i\rangle$ to obtain the above expression for X.

We now estimate the error terms and solve for $\dot{a}$ and $\dot{c}$. The assumption on the potential implies the bounds

$$|\delta b|\le\epsilon_a\epsilon_x(x-a)\quad\text{and}\quad|\delta^2 b|\le\epsilon_a\epsilon_x^2(x-a)^2. \tag{22}$$

Thus, Hölder's inequality and exponential decay of Q_{ca} imply

$$X=-b'(t,a)\delta(c)\begin{pmatrix}1\\0\end{pmatrix}+\mathrm{O}(\epsilon_a\epsilon_x^2)=\mathrm{O}(\epsilon_a\epsilon_x). \tag{23}$$

Similarly, exponential decay of ζ_{ca}^{tr} and ζ_{ca}^{n} implies $\langle\delta b\xi,\zeta_i\rangle=\mathrm{O}(\epsilon_a\epsilon_x\|\xi\|_{H^1})$. The linear term $\langle\mathcal{L}_Q\xi,\zeta_i\rangle$ is zero since $\mathcal{L}_Q\zeta_{ca}^{tr}=0$, $\mathcal{L}_Q\zeta_{ca}^{n}=-Q_{ca}$, and $\xi\perp\partial_x^{-1}\zeta_{ca}^{tr}=-Q_{ca}$. Lastly, $\langle N'_{ca}(\xi),\zeta_i\rangle\le C\|\xi\|_{H^1}^2$ by the first estimate in Lemma A.A.1. Combining the above estimates gives the bound

$$\|Y\|=\mathrm{O}\Big(\epsilon_a\epsilon_x\|\xi\|_{H^1}+\big\|\xi\big\|_{H^1}^2\Big).$$

By the second inclusion of (9), $\partial_c\partial_x^{-1}\zeta_{ca}^{n}\in L^2(\mathbb{R})$. Hölder's inequality then implies $\|B\|=\mathrm{O}(\|\xi\|_{H^1})$. Thus, if $\|\xi\|_{H^1}$ is sufficiently small, say so that $\|B\|\le 1/2$, then $I+B$ is invertible and $\|(I+B)^{-1}\|\le 2$. Acting on Eq. (21) by $(I+B)^{-1}=I-B(I+B)^{-1}$ and then Ω_{ca}^{-1} gives the equation

$$\begin{pmatrix}\dot{a}-c+V(a)\\ \dot{c}\end{pmatrix}=\Omega_{ca}^{-1}[X+B(I-B)^{-1}X+(I-B)^{-1}Y].$$

Using the above estimates of $\|B\|$, $\|(I-B)^{-1}\|$, $\|X\|$, and $\|Y\|$ implies

$$\begin{pmatrix}\dot{a}-c+V(a)\\ \dot{c}\end{pmatrix}=\Omega_{ca}^{-1}X+\mathrm{O}(\epsilon_a\epsilon_x\|\xi\|_{H^1}+\|\xi\|_{H^1}^2).$$

Replacing X by (23) completes the proof. □

V. THE LYAPUNOV FUNCTIONAL

In the last section we derived dynamical equations for the modulation parameters. These equations contain the $H^1(\mathbb{R})$ norm of the fluctuation. In this section we begin to prove a bound on ξ. Recall that the latter bound is needed to ensure that u remains close to the manifold of solitary waves M_s for a long time.

We employ a Lyapunov argument with a Lyapunov function

$$\Gamma_c(t) := \Lambda_{ca}(Q_{ca}+\xi) - \Lambda_{ca}(Q_{ca}) + b'(a)\langle (x-a)Q_{ca}, \xi\rangle. \tag{24}$$

Remark: If $f(u)=u^3$, the last term in the Lyapunov functional is not needed; however, apart from computational complexity, there is no disadvantage in using the above function for this special case as well.

Lemma 5.1: Say $u=Q_{ca}+\xi$ *is a solution to* (1), *where* ξ *satisfies* (14). *Say* $\epsilon_a \le 1$. *If* $\delta'(c)>0$, *and* ϵ_x *and* $\|\xi\|_{H^1}$ *are less than 1, with* $\|\xi\|_{H^1}$ *small enough, then*

$$\frac{d}{dt}\Gamma_c(t) = \mathrm{O}(\epsilon_a^2\epsilon_x^3 + (\epsilon_a\epsilon_x\epsilon_t + \epsilon_a\epsilon_x^2)\|\xi\|_{H^1}) + \mathrm{O}(\epsilon_a\epsilon_x\|\xi\|_{H^1}^2 + \|\xi\|_{H^1}^4). \tag{25}$$

Proof: Suppressing explicit dependence on x and t, we have by definition

$$\Lambda_{ca}(u) := H_b(u) - \frac{1}{2}\int_{-\infty}^{\infty} u^2 b dx + cP(u).$$

Thus, relations (4)–(6) imply that the time derivative of Λ_{ca} along the solution u is

$$\frac{d}{dt}\Lambda_{ca}(u) = \int_{-\infty}^{\infty} \frac{1}{2}\dot{c}u^2 + b'\left[\frac{1}{2}cu^2 - uf(u) + \frac{3}{2}(\partial_x u)^2 + F(u)\right] + b''u\partial_x u dx.$$

Substituting $Q_{ca}+\xi$ for u, manipulating the result using antisymmetry of ∂_x, and collecting appropriate terms into $b'(a)\langle \mathcal{L}_Q\xi, \partial_x((x-a)Q_{ca})\rangle$, $\langle N'_{ca}(\xi), \partial_x[\delta b(Q_{ca}+\xi)]\rangle$, and $\langle \Lambda'_{ca}(Q_{ca}), \partial_x(\delta b(Q_{ca}+\xi))\rangle$ gives the relation

$$\begin{aligned}\frac{d}{dt}[\Lambda_{ca}(Q_{ca}+\xi) - \Lambda_{ca}(Q_{ca})] &= b'(a)\langle \mathcal{L}_Q\xi, \partial_x((x-a)Q_{ca})\rangle + \dot{c}\langle Q_{ca}, \xi\rangle \\ &+ \dot{c}\frac{1}{2}\|\xi\|_{L^2}^2 + \langle \mathcal{L}_Q\xi, \partial_x(\delta^2 b Q_{ca})\rangle + c\frac{1}{2}\langle b'\xi, \xi\rangle + \frac{3}{2}\langle b'\partial_x\xi, \partial_x\xi\rangle \\ &- \langle f'(Q_{ca})\xi, \partial_x(\delta b\xi)\rangle + \langle N'_{ca}(\xi), \partial_x[\delta b(Q_{ca}+\xi)]\rangle \\ &+ \langle b''\xi, \partial_x\xi\rangle + \langle \Lambda'_{ca}(Q_{ca}), \partial_x[\delta b(Q_{ca}+\xi)]\rangle.\end{aligned}$$

The last term is zero because $\Lambda'_{ca}(Q_{ca})=0$ and since $\xi \perp Q_{ca}$, the quantity $\dot{c}\langle \xi, Q_{ca}\rangle$ is also zero. We use Lemma A.1, assumptions (12) on the potential, estimates (22), and

$$|\partial_x\delta^2 b| \le \epsilon_a\epsilon_x^2(x-a)$$

to estimate the size of the time derivative of $\Lambda_{ca}(Q_{ca}+\xi)-\Lambda_{ca}(Q_{ca})$. We also use that Q_{ca}, $\partial_x Q_{ca}$, $\partial_x^2 Q_{ca}$, and $f'(Q_{ca})$ are exponentially decaying. When $\epsilon_x \le 1$, higher order terms like $\langle b''\xi, \partial_x\xi\rangle$ are bounded above by lower order terms like $\langle b'\xi, \xi\rangle$. Similarly, if $\|\xi\|_{H^1} \le 1$, then $\epsilon_a\epsilon_x\|\xi\|_{H^1}^2 \le \epsilon_a\epsilon_x\|\xi\|_{H^1}$. This procedure gives the estimate

$$\begin{aligned}\frac{d}{dt}[\Lambda_{ca}(Q_{ca}+\xi) - \Lambda_{ca}(Q_{ca})] &= b'(a)\langle \xi, \mathcal{L}_Q\partial_x((x-a)Q_{ca})\rangle \\ &+ \langle N'_{ca}(\xi), \delta b\partial_x\xi\rangle + \mathrm{O}(\|\dot{c}\|\|\xi\|_{H^1}^2 + \epsilon_a\epsilon_x^2\|\xi\|_{H^1} + \epsilon_a\epsilon_x\|\xi\|_{H^1}^2).\end{aligned}$$

Applying the chain rule to the integrand of

$$\int_{-\infty}^{\infty} \partial_x \left[\left(F(Q_{ca}+\xi) - F(Q_{ca}) - f(Q_{ca})\xi - \frac{1}{2} f'(Q_{ca})\xi^2 \right) \delta b \right] dx = 0$$

and using the definition of $N'_{ca}(\xi)$ gives that

$$\langle N'_{ca}(\xi), \delta b \partial_x \xi \rangle = \left\langle N'_{ca}(\xi) + \frac{1}{2} f''(Q_c)\xi^2, \delta b \partial_x Q_c \right\rangle$$

$$- \int_{-\infty}^{\infty} \left((F(Q_{ca})+\xi) - F(Q_{ca}) - f(Q_{ca})\xi - \frac{1}{2} f'(Q_{ca})\xi^2 \right) b' dx.$$

The second estimate and the proof of the third estimate of Lemma A.1 of the Appendix then imply the bound $\langle N'_{ca}(\xi), \delta b \partial_x \xi \rangle = \mathrm{O}(\epsilon_a \epsilon_x \|\xi\|_{H^1}^3)$. Thus, since $\epsilon_a \epsilon_x \|\xi\|_{H^1}^3 \le \epsilon_a \epsilon_x \|\xi\|_{H^1}^2$ when $\|\xi\|_{H^1} \le 1$, we have

$$\frac{d}{dt}[\Lambda_{ca}(Q_{ca}+\xi) - \Lambda_{ca}(Q_{ca})] = b'(a)\langle \xi, \mathcal{L}_Q \partial_x((x-a)Q_{ca})\rangle + \mathrm{O}\left(\|\dot{c}\| \|\xi\|_{H^1}^2 + \epsilon_a \epsilon_x^2 \left\|\xi\right\|_{H^1} + \epsilon_a \epsilon_x \|\xi\|_{H^1}^2 \right). \tag{26}$$

When $f(u)=u^3$, $\langle \xi, L_Q \partial_x((x-a)Q_{ca})\rangle = 0$ since $\zeta^n_{ca} = \partial_x[(x-a)Q_{ca}]$. In this special case the above estimate is sufficient for our purposes, but in general we need to use the corrected Lyapunov functional. When $\xi \in C(\mathbb{R}, H^1(\mathbb{R})) \cap C^1(\mathbb{R}, H^{-2}(\mathbb{R}))$, $b'(a)\langle \xi, (x-a)Q_{ca}\rangle$ is continuously differentiable with respect to time;

$$\frac{d}{dt}[b'(a)\langle \xi, (x-a)Q_{ca}\rangle] = \partial_t b' \langle \xi, (x-a)Q_{ca}\rangle + b'(a)\langle \dot{\xi}, (x-a)Q_{ca}\rangle + \dot{c} b'(a)\langle \xi, (x-a)\zeta^n_{ca}\rangle + \dot{a} b'(a)$$
$$\times \langle \xi, (x-a)\zeta^{tr}_{ca}\rangle + \dot{a} b''(a)\langle \xi, (x-a)Q_{ca}\rangle,$$

where $\langle \xi, Q_{ca}\rangle = 0$ has been used to simplify the derivative. Substituting for $\partial_t \xi$ using (19) gives

$$\begin{aligned}
\frac{d}{dt}[b'(a)\langle \xi, (x-a)Q_{ca}\rangle] = & - b'(a)\langle \xi, \mathcal{L}_Q \partial_x((x-a)Q_{ca})\rangle - [\dot{a} - c + b(a)] b'(a) \frac{1}{2} \|Q_{ca}\|_{L^2}^2 \\
& + \partial_t b' \langle \xi, (x-a)Q_{ca}\rangle + [\dot{a} - c + b(a)] b'(a) \langle \partial_x \xi, (x-a)Q_{ca}\rangle \\
& + [\dot{a} - c + b(a)] b''(a) \langle \xi, (x-a)Q_{ca}\rangle + \dot{c} b'(a) \langle \xi, (x-a)\zeta^n_{ca}\rangle - b'(a) \\
& \times \langle \xi, \delta b \partial_x((x-a)Q_{ca})\rangle \\
& - b'(a)\langle N'_{ca}(\xi), \partial_x((x-a)Q_{ca})\rangle - b'(a)\langle \delta^2 b Q_{ca}, \partial_x((x-a)Q_{ca})\rangle \\
& + [c - b(a)] b''(a) \langle \xi, (x-a)Q_{ca}\rangle.
\end{aligned}$$

We estimate using the same assumptions used to derive (26). If $\|\xi\|_{H^1}$ and ϵ_x are less than 1, then

$$\begin{aligned}
\frac{d}{dt}[b'(a)\langle \xi, (x-a)Q_{ca}\rangle] = & - b'(a)\langle \xi, \mathcal{L}_Q \partial_x((x-a)Q_{ca})\rangle + \mathrm{O}(|\dot{a} - c + b(a)| \epsilon_a \epsilon_x + |\dot{c}| \epsilon_a \epsilon_x \|\xi\|_{H^1}) \\
& + \mathrm{O}(\epsilon_a^2 \epsilon_x^3 + ((1+\epsilon_a)\epsilon_x^2 + \epsilon_x \epsilon_t)\epsilon_a \|\xi\|_{H^1} + \epsilon_a \epsilon_x \|\xi\|_{H^1}^2).
\end{aligned}$$

Adding the above expression to (26) gives an upper bound containing $|\dot{c}|$ and $|\dot{a} - c + b(a)|$. Replacing these quantities using the bounds

$$|\dot{c}| = \mathrm{O}\left(\epsilon_a \epsilon_x + \epsilon_a \epsilon_x \|\xi\|_{H^1} + \|\xi\|_{H^1}^2 \right)$$

and

$$|\dot{a} - c + b(a)| = \mathrm{O}(\epsilon_a \epsilon_x^2 + \epsilon_a \epsilon_x \|\xi\|_{H^1} + \|\xi\|_{H^1}^2)$$

from Proposition 4.1, and bounding higher order terms by lower order terms gives (25). To use the above bounds on $|\dot{c}|$ and $|\dot{a}-c+b(a)|$ we must assume $\|\xi\|_{H^1}$ is small enough so that Proposition 4.1 holds. □

VI. SPECTRAL PROPERTIES OF THE HESSIAN $\mathcal{L}_Q$

The Hessian $\partial^2 \Lambda_{ca}$ at Q_{ca} in the $L^2(\mathbb{R})$ pairing is computed to be the unbounded operator

$$\mathcal{L}_Q := -\partial_x^2 + c - f'(Q_{ca}), \tag{27}$$

defined on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$. We extend this operator to the corresponding complex spaces.

Proposition 6.1: The self-adjoint operator $\mathcal{L}_Q$ has the following properties.

1. $\mathcal{L}_Q \zeta_{ca}^{tr} = 0$ *and* $\mathcal{L}_Q \zeta_{ca}^{n} = -Q_{ca}$.
2. *All eigenvalues of* $\mathcal{L}_Q$ *are simple, and* Null $\mathcal{L}_Q = \mathrm{Span}\{\zeta_{ca}^{tr}\}$.
3. $\mathcal{L}_Q$ *has exactly one negative eigenvalue.*
4. *The essential spectrum is* $[c, \infty) \subset \mathbb{R}_+$.
5. $\mathcal{L}_Q$ *has a finite number of eigenvalues in* $(-\infty, c)$.

Proof: Recall that the vectors $\zeta_{ca}^{tr} := -\partial_x Q_{ca}$ and $\zeta_{ca}^{n} := \partial_c Q_{ca}$ are in the Sobolev space $H^2(\mathbb{R})$. Thus, relations $\mathcal{L}_Q \zeta_{ca}^{tr} = 0$ and $\mathcal{L}_Q \zeta_{ca}^{n} = -Q_{ca}$ make sense, and are obtained by differentiating $\Lambda_{ca}'(Q_{ca}) = 0$ with respect to a and c. The first relation above proves that ζ_{ca}^{tr} is a null vector.

Say ζ, $\eta \in H^2(\mathbb{R})$ are linearly independent eigenvectors of $\mathcal{L}_Q$ with the same eigenvalue. Then, since $\mathcal{L}_Q$ is a second-order linear differential operator without a first-order derivative, the Wronskian

$$W(\eta, \zeta) = \zeta \partial_x \eta - \eta \partial_x \zeta$$

is a nonzero constant. With η and ζ both in $H^2(\mathbb{R})$, however, the limit $\lim_{x \to \infty} W(\eta, \zeta)$ is zero. This contradicts the nonvanishing of the Wronskian, and hence all eigenvalues of $\mathcal{L}_Q$ are simple and, in particular, Null $\mathcal{L}_Q = \mathrm{Span}\{\zeta_{ca}^{tr}\}$.

Next we prove that the operator $\mathcal{L}_Q$ has exactly one negative eigenvalue using the Sturm-Liouville theory on an infinite interval. Recall that the solitary wave $Q_{ca}(x)$ is a differentiable function, symmetric about $x = a$ and monotonically decreasing if $x > a$. This implies that the null vector ζ_{ca}^{tr}, or, equivalently, the derivative of Q_{ca} with respect to x, has exactly one root at $x = a$. Therefore, by the Sturm-Liouville theory, zero is the second eigenvalue and there is exactly one negative eigenvalue.

We use standard methods to compute the essential spectrum. Since the function $f'(Q_{ca}(x))$ is continuous and decays to zero at infinity, the bottom of the essential spectrum begins at $\lim_{x \to \infty}(c - f'(Q_{ca}(x))) = c$ and extends to infinity: $\sigma_{ess}(\mathcal{L}_Q) = [c, \infty)$. Furthermore, the bottom of the essential spectrum is not an accumulation point of the discrete spectrum since $f'(Q_{ca}(x))$ decays faster than x^{-2} at infinity. Hence, there is at most a finite number of eigenvalues in the interval $(-\infty, c)$. For details, see Refs. 25, 37, and 38. □

VII. STRICT POSITIVITY OF THE HESSIAN

In this section we prove strict positivity of the Hessian $\mathcal{L}_Q$ on the orthogonal complement to the two-dimensional space

$$\partial_x^{-1} T_{Q_{ca}} M_s = \mathrm{Span}\{Q_{ca}, \partial_x^{-1} \zeta_{ca}^{n}\}.$$

This result is a crucial ingredient needed to prove the bound on the fluctuation ξ.

Proposition 7.1: Assume $\delta'(c)>0$ *on* $I\subset\mathbb{R}_+$. *If* $\xi\perp\partial_x^{-1}T_{Q_{ca}}M_s$, *then there is a positive constant* ρ *such that* $\langle\mathcal{L}_Q\xi,\xi\rangle\geq\rho\|\xi\|_{H^1}^2$.

Proof: Define $X:=\{\xi\in H^1(\mathbb{R})\,|\,\xi\perp\partial_x^{-1}T_{Q_{ca}}M_s,\|\xi\|_{L^2}=1\}$. By the max-min principle, $\inf_{X\cap H^2(\mathbb{R})}\times\langle\mathcal{L}_Q\xi,\xi\rangle$ is attained or is equal to inf $\sigma_{ess}(\mathcal{L}_Q)=c$. If the latter holds, the proof is complete. In the former case, let η be the minimizer.

We claim the set of vectors $\{\zeta_{ca}^{tr},\zeta_{ca}^{n},\eta\}$ is a linearly independent set. If they were dependent, then, since ζ_{ca}^{tr} and ζ_{ca}^{n} are orthogonal, there are nonzero constants α and β such that $\eta=\alpha\zeta_{ca}^{tr}+\beta\zeta_{ca}^{n}$. Projecting this equation onto $\partial_x^{-1}\zeta_{ca}^{tr}$ and $\partial_x^{-1}\zeta_{ca}^{n}$ gives the equations $\beta\delta'(c)=0$ and $\alpha\delta'(c)=0$. Thus, the assumption $\delta'(c)>0$ implies $\eta=0$, a contradiction since the zero function does not lie in the set X.Note that in deriving $\alpha\delta'(c)=0$ we have used that ∂_x^{-1} is antisymmetric on the span of ζ_{ca}^{n} since $\partial_x^{-1}\zeta_{ca}^{n}\in L^2(\mathbb{R})$.

By the min-max principle, if

$$\lambda_3:=\inf\{\max\{\langle\mathcal{L}_Q\xi,\xi\rangle|\xi\in V,\|\xi\|_{L^2}=1\}|V\subset H^2(\mathbb{R}),\dim V=3\}$$
$$\leq\max\{\langle\mathcal{L}_Q\xi,\xi\rangle|\xi\in\mathrm{Span}\{\zeta_{ca}^{tr},\zeta_{ca}^{n},\eta\}\}$$

is below the essential spectrum, then it is the third eigenvalue counting multiplicity. Let $\xi=\alpha\eta+\beta\zeta_{ca}^{tr}+\gamma\zeta_{ca}^{n}$, where α, β, and γ are arbitrary apart from satisfying $\|\xi\|_{L^2}=1$. Thus, since the third eigenvalue of $\mathcal{L}_Q$ is positive (see Sec. VI),

$$0<\langle\mathcal{L}_Q\xi,\xi\rangle=\alpha^2\langle\mathcal{L}_Q\eta,\eta\rangle-\gamma^2\delta'(c)\leq\alpha^2\langle\mathcal{L}_Q\eta,\eta\rangle,$$

and hence $\langle\mathcal{L}_Q\eta,\eta\rangle>0$. The function $\sigma(c)=\langle\mathcal{L}_Q\eta,\eta\rangle$ is continuous since both $\partial_x^{-1}\zeta_{ca}^{tr}$ and $\partial_x^{-1}\zeta_{ca}^{n}$ are continuous in $L^2(\mathbb{R})$ as functions of c. Set $\varrho=\inf_I\sigma(c)$.

We now improve the result to an $H^1(\mathbb{R})$ norm. If we define the constant $K(I):=\sup_I\|c-f'(Q_{ca})\|_\infty$, then $\langle\mathcal{L}_Q\xi,\xi\rangle\geq\|\partial_x\xi\|_{L^2}^2-K(I)\|\xi\|_{L^2}^2$. Adding to this bound the factor $(K+1)/\varrho$ of the lower bound $\langle\mathcal{L}_Q\xi,\xi\rangle\geq\varrho\|\xi\|_{L^2}^2$ derived above completes the proof. □

VIII. BOUND ON THE FLUCTUATION

We are now ready to prove the bound on the fluctuation.

Proposition 8.1: Say $\epsilon_a\leq1$. *Then, for small enough* $\epsilon_x\leq1$ *and initial fluctuation* $\|\xi\|_{H^1}\leq1$, *there exists a constant* C *such that the bound*

$$\|\xi(t)\|_{H^1}=\mathrm{O}(\epsilon_0+(\epsilon_a\epsilon_x\epsilon_0)^{1/2}+\epsilon_x+\epsilon_t)$$

holds for all times $t\leq T=C(\epsilon_a\epsilon_x)^{-1}$.

Proof: Lemma 5.1 implies

$$\left|\frac{d}{dt}\Gamma_c(t)\right|\leq C(\epsilon_a^2\epsilon_x^3+(\epsilon_a\epsilon_x\epsilon_t+\epsilon_a\epsilon_x^2)\|\xi\|_T+\epsilon_a\epsilon_x\|\xi\|_T^2+\|\xi\|_T^4)$$

for some constant $C>0$ where $\|\xi\|_T:=\sup_{0\leq t\leq T}\|\xi\|_{H^1}$. Integrating over $[0,T]$ gives an upper bound on $\Gamma_c(T)$. A lower bound is obtained by expanding $\Lambda_{ca}(Q_{ca}+\xi)$ to quadratic order, then using Proposition 7.1, the third estimate of Lemma A.1, and $V'(a)\langle\xi,(x-a)Q_{ca}\rangle=\mathrm{O}(\epsilon_a\epsilon_x\|\xi\|_{H^1})$. We obtain, after setting all nonessential constants to one,

$$\|\xi\|_T^2-\|\xi\|_T^3-\epsilon_a\epsilon_x\|\xi\|_T\leq\Gamma_c(T)$$

$$\leq|\Gamma_c(0)|+(\epsilon_a^2\epsilon_x^3+(\epsilon_a\epsilon_x\epsilon_t+\epsilon_a\epsilon_x^2)\|\xi\|_T+\epsilon_a\epsilon_x\|\xi\|_T^2+\|\xi\|_T^4)T$$

for all $T>0$. Take $T=\mathrm{O}((\epsilon_a\epsilon_x)^{-1})$. Then, under the smallness assumption $\|\xi\|_{H^1}\ll(\epsilon_a\epsilon_x)^{1/2}$,

$$\|\xi\|_{H^1} = \mathrm{O}(|\Gamma_c(0)|^{1/2} + \epsilon_x + \epsilon_t).$$

The initial value of the Lyapunov functional $\Gamma_c(0)$ can be bounded by the $H^1(\mathbb{R})$ norm of the initial fluctuation $\|\xi(0)\|_{H^1} \leq C\epsilon_0$ (recall that $\epsilon_0 := \inf_{Q_{ca} \in M_s} \|u_0 - Q_{ca}\|_{H^1}$). Indeed, Taylor expanding $\Lambda_{ca}(Q_{ca}+\xi)$ to second order in ξ and using the third estimate in Lemma A.1 gives $|\Gamma_c(0)| = \mathrm{O}(\epsilon_0^2 + \epsilon_a\epsilon_x\epsilon_0)$ if $\epsilon_0 \ll 1$. To complete the proof we take ϵ_x and ϵ_0 small enough so that $\|\xi(t)\|_{H^1}$ is sufficiently small for Lemma 5.1 to hold. □

We now prove the main theorem.

Proof of Theorem 1: By our choice $\epsilon_0 < \varepsilon_*$, there is a (maximal) time T_0 such that the solution u in (1) is in U_{ε_*} for time $t \leq T_0$. Hence decomposition (13) with (14), and Proposition 8.1 are valid for the solution u over this time and imply the statements of the main theorem. In particular,

$$\|\xi(t)\|_{H^1} = \mathrm{O}(\epsilon_0 + (\epsilon_a\epsilon_x\epsilon_0)^{1/2} + \epsilon_x + \epsilon_t)$$

for times $t \leq \min\{T_0, T\}$. Taking $\epsilon_0 + (\epsilon_a\epsilon_x\epsilon_0)^{1/2} + \epsilon_x + \epsilon_t \ll \varepsilon_*$, we must have $t \leq T$ by maximality of the time T_0. □

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APPENDIX: ESTIMATES OF NONLINEAR REMAINDERS

Define

$$N_{ca}(\xi) := -\int_{-\infty}^{\infty} F(Q_c + \xi) - F(Q_c) - F'(Q_c)\xi - \frac{1}{2}F''(Q_c)\xi^2 dx$$

and

$$N'_{ca}(\xi) := -(f(Q_c + \xi) - f(Q_c) - f'(Q_c)\xi). \tag{A1}$$

Note that $N'_{ca}(\xi) = \partial_\xi N_{ca}(\xi)$ under the $L^2(\mathbb{R})$ pairing.

Lemma A.1: If $\|\xi\|_{H^1} \leq 1$ *and* $f \in C^k(\mathbb{R})$ *for some* $k \geq 3$, *then there are positive constant* C_1, C_2, *and* C_3 *such that*

1. $\|N'_{ca}(\xi)\|_{L^2} \leq C_1\|\xi\|_{H^1}^2$,
2. $\|N'_{ca}(\xi) + \frac{1}{2}f''(Q_{ca})\xi^2\|_{L^2} \leq C_2\|\xi\|_{H^1}^3$,
3. $|N_{ca}(\xi)| \leq C_3\|\xi\|_{H^1}^3$.

Proof: Taylor's remainder theorem implies

$$N'_{ca}(\xi) = -\sum_{n=2}^{k-1} \frac{1}{n!} f^{(n)}(Q_{ca})\xi^n - R(Q_{ca}, \xi),$$

where, since $\|\xi\|_{H^1} \leq 1$, $|R(Q_{ca}, \xi)| \leq C|\xi|^k$. Recall that Q_{ca} is continuous and decays exponentially to zero. Together with the assumption that $f \in C^k(\mathbb{R})$, this implies $f^{(n)}(Q_{ca}) \in L^\infty(\mathbb{R})$ for $2 \leq n \leq k-1$. Thus, after pulling out the largest constant,

$$\|N'_{ca}(\xi)\|_{L^2} \leq C \sum_{n=2}^{k} \|\xi^n\|_{L^2}.$$

To obtain item 1 we use the bound $\|\xi^n\|_{L^2} \leq C\|\xi\|_{H^1}^n$, which is obtained from the inequality $\|\xi\|_{L^\infty} \leq C\|\xi\|_{H^1}$ and the assumption that $\|\xi\|_{H^1} \leq 1$.

Clearly, a slight modification of the above proof gives items 2 and 3. For the latter we use that the assumptions on f imply $F \in C^{k+1}(\mathbb{R})$ with $F^{(k+1)} \in L^\infty(\mathbb{R})$. □

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Eigenvalue problems and their application to the wavelet method of chaotic control

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Controlling chaos via wavelet transform was recently proposed by Wei, Zhan, and Lai [Phys. Rev. Lett. **89**, 284103 (2002)]. It was reported there that by modifying a tiny fraction of the wavelet subspace of a coupling matrix, the transverse stability of the synchronous manifold of a coupled chaotic system could be dramatically enhanced. The stability of chaotic synchronization is actually controlled by the second largest eigenvalue $\lambda_1(\alpha,\beta)$ of the (wavelet) transformed coupling matrix $C(\alpha,\beta)$ for each α and β. Here β is a mixed boundary constant and α is a scalar factor. In particular, $\beta=1$ (respectively, 0) gives the nearest neighbor coupling with periodic (respectively, Neumann) boundary conditions. The first, rigorous work to understand the eigenvalues of $C(\alpha,1)$ was provided by Shieh *et al.* [J. Math. Phys. (to be published)]. The purpose of this paper is twofold. First, we apply a different approach to obtain the explicit formulas for the eigenvalues of $C(\alpha,1)$ and $C(\alpha,0)$. This, in turn, yields some new information concerning $\lambda_1(\alpha,1)$. Second, we shed some light on the question whether the wavelet method works for general coupling schemes. In particular, we show that the wavelet method is also good for the nearest neighbor coupling with Neumann boundary conditions. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218674]

I. INTRODUCTION

Chaotic synchronization (Refs. 1, 8, 12–14, and references cited therein) is a fundamental phenomenon in physical systems with dissipation. It was first observed in Ref. 8 for identical master-slave Lorenz equations. This phenomenon was later observed in many different fields—physics, electrical engineering, biology, laser systems, etc. Experimental observations show that chaotic subsystems in a lattice manifest synchronized chaotic behavior in time provided they are coupled with a dissipative coupling and its coupling strength is greater than some critical value. Specifically, let there be N nodes (oscillators). Assume $\mathbf{u}_i$ is the m-dimensional vector of dynamical variables of the ith node. Let the isolated (uncoupling) dynamics be $\dot{\mathbf{u}}_i=f(\mathbf{u}_i)$ for each node. We assume that $\mathbf{u}_i$ has a chaotic dynamics in the sense that its largest Lyapunov exponent is positive. Let h: $\mathbb{R}^m\to\mathbb{R}^m$ be an arbitrary function describing the coupling within the components of each node. Thus, the dynamics of the ith node are

$$\dot{\mathbf{u}}_i = f(\mathbf{u}_i) + \epsilon\sum_{j=1}^{N} a_{ij}h(\mathbf{u}_j), \quad i=1,2,\ldots,N, \tag{1.1a}$$

where ϵ is a coupling strength. Here sum $\Sigma_{j=1}^{N}a_{ij}=0$. Let $\mathbf{u}=(\mathbf{u}_1,\mathbf{u}_2,\ldots,\mathbf{u}_N)^T$, $F(\mathbf{u})=(f(\mathbf{u}_1),f(\mathbf{u}_2),\ldots,f(\mathbf{u}_N))^T$, $H(\mathbf{u})=(h(\mathbf{u}_1),h(\mathbf{u}_2),\ldots,h(\mathbf{u}_N))^T$, and $A=(a_{ij})$. We may write (1.1a) as

$$\dot{\mathbf{u}} = F(\mathbf{u}) + \epsilon A\times H(\mathbf{u}). \tag{1.1b}$$

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Here $\times$ is the direct product of two matrices B and C defined as follows. Let $B=(b_{ij})_{k_1\times k_2}$ be a $k_1\times k_2$ matrix and $C=(C_{ij})_{k_2\times k_3}$ be a $k_2\times k_3$ block matrix, where each of C_{ij}, $1\leqslant i\leqslant k_2$, $1\leqslant j\leqslant k_3$, is a $k_4\times k_5$ matrix. Then

$$B\times C=\left(\sum_{l=1}^{k_2} b_{il}C_{lj}\right)_{k_1\times k_3}.$$

Many coupling schemes are covered by Eq. (1.1b). For example, if the Lorenz system is used and the coupling is through its three components x, y, and z, then the function h is just the matrix

$$I_3=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}. \tag{1.2}$$

The choice of A will provide the connectivity of nodes. For instance, the nearest neighbor coupling with mixed boundary conditions is given as follows:

$$A=A(\beta)=\begin{pmatrix}-1-\beta&1&0&\cdots&\cdots&\beta\\1&-2&1&\cdots&\cdots&0\\0&1&-2&1&\cdots&0\\\vdots&\ddots&\ddots&\ddots&&\vdots\\\vdots&&\ddots&\ddots&\ddots&\vdots\\\beta&0&\cdots&\cdots&1&-1-\beta\end{pmatrix}_{N\times N}. \tag{1.3}$$

Note that $\beta=1$ corresponds to periodic boundary conditions, while $\beta=0$ is associated with Neumann boundary conditions. The synchronous manifold of the chaotic system (1.1) can be studied by setting $\mathbf{u}_1(t)=\mathbf{u}_2(t)=\cdots=\mathbf{u}_N(t)=\mathbf{s}(t)$. Here the chaotic solution $\mathbf{s}(t)$ satisfies the single oscillator equation $d\mathbf{s}/dt=f[\mathbf{s}(t)]$. The stability property of the synchronous manifold can then be studied in the space of difference variables $\delta\mathbf{u}_i(t)=\mathbf{u}_i(t)-\mathbf{s}(t)$, which are governed by[7,10]

$$\frac{d\delta\mathbf{u}}{dt}=(I_N\times DF+\epsilon A\times DH)\delta\mathbf{u}, \tag{1.4a}$$

where $DH=dH(\mathbf{u})/d\mathbf{u}$, and $\delta\mathbf{u}=(\delta\mathbf{u}_1,\delta\mathbf{u}_2,\ldots,\delta\mathbf{u}_N)^T$. When H is just a matrix E, $DH=E$. The first term in (1.4a) is block diagonal. The second term can be treated by diagonalizing A. The transformation which does this does not affect the first term, since it acts only on the identity matrix I_N. This leaves us with a block diagonalized variational equation with each block having the form[7]

$$\delta\dot{\mathbf{u}}_i=[DF+\epsilon\lambda_i DH]\delta\mathbf{u}_i, \tag{1.4b}$$

where λ_i is an eigenvalue of A, $i=0,1,\cdots,N-1$. The Jacobian functions DF and DH are the same for each block, since they are evaluated on the synchronized state. It then follows from (1.4b) that the largest eigenvalue λ_0 of A being equal to 0 governs the motion on the synchronized manifold, and all of other eigenvalues $\lambda_i(i\neq 0)$ control the transverse stability[9] of the chaotic synchronous state. The stability condition is then given by $L_{\max}+\epsilon\lambda_1\leqslant 0$, where $L_{\max}>0$ is the largest Lyapunov exponent of a single chaotic oscillator. As a consequence, the second largest eigenvalue λ_1 is dominant in controlling the stability of chaotic synchronization, and the critical strength ϵ_c can be determined in term of λ_1,

$$\epsilon_c=\frac{I_{\max}}{-\lambda_1}. \tag{1.4c}$$

Note that the eigenvalues of $A=A(1)$ are given by $\lambda_i=-4\sin^2(\pi i/N)$, $i=0,1,\ldots,N-1$. In general, a larger number of nodes gives a smaller nonzero eigenvalue λ_1 in magnitude, and, hence,

a larger ϵ_c. As a consequence, controlling chaos is apparently of great interest and importance.[4–7,11,12] In Ref. 11, a new efficient strategy for controlling nonlinear dynamics was presented. To be self-contained, we briefly describe such procedures. Let

$$A = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{pmatrix}_{n\times n}, \tag{1.5a}$$

be a matrix with the dimension of each block matrix A_{kl} being $2^i \times 2^i$. By an i-scale wavelet operator W,[2,11] the matrix A is transformed into $W(A)$ of the form

$$W(A) = \begin{pmatrix} \tilde{A}_{11} & \cdots & \tilde{A}_{1n} \\ \vdots & \ddots & \vdots \\ \tilde{A}_{n1} & \cdots & \tilde{A}_{nn} \end{pmatrix}_{n\times n}, \tag{1.5b}$$

where each entry of $\tilde{A}_{kl}$ is the average of entries of A_{kl}, $1 \leqslant k, l \leqslant n$.

For a given matrix, the above wavelet transform allows a perfect reconstruction (inverse wavelet transform), by which there is nothing to gain: $A = W^{-1}(W(A))$. In Ref. 11, a simple operator O_k is introduced to attain a desirable coupling matrix. That is,

$$C = W^{-1}(O_k(W(A))) = A + (k-1)W(A) =: A + \alpha W(A), \tag{1.5c}$$

where O_k is the multiplication of a scalar factor K on each block matrix $\tilde{A}_{kl}$. After such reconstruction, the critical strength ϵ_c is again determined in terms of the second largest eigenvalue of C. A numerical simulation of a coupled system of 512 Lorenz oscillators in Ref. 11 shows that with $h = I_3$ and $A = A(1)$, the critical coupling strength ϵ_c decreases linearly with respect to the increase of α up to a critical value α_c. The smallest ϵ_c is about 6, which is about 10^3 times smaller than the original critical coupling strength, indicating the efficiency of the proposed approach.

To verify this phenomenon mathematically, we first consider the coupling matrix $A = A(\beta)$, as given in (1.3). Let $n = N/2^i \in \mathbb{N}$, where i is a fixed positive integer. We then write A into an $n \times n$ block matrix of the form

$$A = A(\beta) = \begin{pmatrix} A_1(\beta) & A_2(1) & 0 & . & . & 0 & A_2^T(\beta) \\ A_2^T(1) & A_1(1) & A_2(1) & . & . & 0 & 0 \\ 0 & . & . & . & & & . \\ . & & . & . & . & & . \\ . & & & . & . & . & 0 \\ 0 & 0 & . & . & A_2^T(1) & A_1(1) & A_2(1) \\ A_2(\beta) & 0 & . & . & 0 & A_2^T(1) & \bar{A}_1(\beta) \end{pmatrix}_{n\times n}, \tag{1.6a}$$

where

$$A_1(\beta) = \begin{pmatrix} -1-\beta & 1 & & & \\ 1 & -2 & 1 & & \mathbf{0} \\ & . & . & . & \\ & & . & . & . \\ & \mathbf{0} & & . & . & 1 \\ & & & & 1 & -2 \end{pmatrix}_{2^i\times 2^i},$$

$$\bar{A}_1(\beta) = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \mathbf{0} \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \\ & \mathbf{0} & & \ddots & 1 \\ & & & 1 & -1-\beta \end{pmatrix}_{2^i \times 2^i}, \tag{1.6b}$$

and

$$A_2(\beta) = \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & & & & \vdots \\ \vdots & & & & \vdots \\ 0 & & & & 0 \\ \beta & 0 & \cdots & \cdots & 0 \end{pmatrix}_{2^i \times 2^i}. \tag{1.6c}$$

Then the newly transformed coupling matrix $C=C(\alpha,\beta)$ can be written as

$$\begin{aligned} &C(\alpha,\beta) \\ &= \begin{pmatrix} A_1(\beta)+\tilde{A}_1(\beta) & A_2(1)+\tilde{A}_2(1) & 0 & \cdots & 0 & A_2^T(\beta)+\tilde{A}_2^T(\beta) \\ A_2^T(1)+\tilde{A}_2^T(1) & A_1(1)+\tilde{A}_1(1) & A_2(1)+\tilde{A}_2(1) & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & A_2^T(1)+\tilde{A}_2^T(1) & A_1(1)+\tilde{A}_1(1) & A_2(1)+\tilde{A}_2(1) \\ A_2(\beta)+\tilde{A}_2(\beta) & 0 & \cdots & 0 & A_2^T(1)+\tilde{A}_2^T(1) & \tilde{\bar{A}}_1(\beta)+\tilde{\bar{A}}_1(\beta) \end{pmatrix} \\ &=: \begin{pmatrix} C_1(\beta) & C_2(1) & 0 & \cdots & 0 & C_2^T(\beta) \\ C_2^T(1) & C_1(1) & C_2(1) & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & C_2^T(1) & C_1(1) & C_2(1) \\ C_2(\beta) & 0 & \cdots & 0 & C_2^T(1) & \bar{C}_1(\beta) \end{pmatrix}. \end{aligned} \tag{1.7}$$

Here for any matrix B of dimension $2^i \times 2^i$, the kl entry $(\tilde{B})_{kl}$ of $\tilde{B}$ is defined to be

$$(\tilde{B})_{kl} = \frac{\alpha}{2^{2i}} \sum_{l=1}^{2^i} \sum_{k=1}^{2^i} (B)_{kl}.$$

Here α is a scalar factor. The matrix $C(\alpha,\beta)$ carries a new relationship among the coupled oscillators, which might not be as simple as the original matrix A. Nevertheless, the stability of the synchronous states can be determined by matrix $C(\alpha,\beta)$, whose eigenvalues $\lambda_i(\alpha,\beta)$ $(i=0,1,2,\cdots,N-1)$ determine the synchronous stability of the coupled chaotic system. The following theorem of Shieh *et al.*[9] showed, indeed, the dramatic reduction in the critical coupling strength can be achieved with the periodic boundary conditions. We summarize their main results in the following.

Theorem 1.1: *Let $N\times N$, $N=8k$, $k\in N$, be the dimension of the matrix $C(\alpha,1)$. Let the dimension of each block matrix in $C(\alpha,1)$ be $2^i\times 2^i$. Then the following assertions hold.*

(i) $\rho_i := 2\cos(\pi/2^i)-2$ *is an eigenvalue of* $C(\alpha,1)$.

(ii) *The second eigenvalue* $\lambda_1(\alpha,1)$ *of* $C(\alpha,1)$ *is decreasing in* α. *Moreover,* $\lambda_1(\alpha,1)=\rho_i$ *when-*

ever $\alpha \geqslant -2^i \rho_i / 4 \sin^2(2^i \pi / N)$.

Note that $C(\alpha,1)$ is a block circulant matrix (see e.g., Ref. 3). A classical result of a block circulant matrix states that its eigenvalues exactly consist of those of certain linear combinations of its block matrices (see, e.g., Theorem 5.6.4 of Ref. 3). The proof of Theorem 1.1 was then reduced to working on the eigenvalues of those linear combinations of block matrices of $C(\alpha,1)$. Note that $C(\alpha,\beta)$, $\beta \neq 1$ are not block circulant matrix. The objective of the present work is to present another approach to study the eigenvalues of $C(\alpha,\beta)$. Specifically, we use this new method to study two coupling schemes, the nearest neighbor coupling with periodic boundary conditions and the nearest neighbor coupling with Neumann boundary conditions. To simplify our calculation, we consider only the case $i=1$. In both coupling schemes, we are able to obtain, respectively, exact form of eigenvalues $\lambda_m^{\pm}(\alpha,\beta)$ of its corresponding matrix $C(\alpha,\beta)$, see (2.16) and (3.9). Here $\beta=0$ or 1. For each α and β, let $\lambda_1(\alpha,\beta)$ be the second largest eigenvalue of $C(\alpha,\beta)$. We prove that for N being a multiple of 4, then

$$\lambda_1(\alpha,1) = \begin{cases} \lambda_1^+(\alpha,1), & 0 \leqslant \alpha \leqslant \dfrac{1}{\sin^2 \dfrac{z}{n}} \\ \lambda_{n/2}^+(\alpha,1) = -2, & \alpha \geqslant \dfrac{1}{\sin^2 \dfrac{\pi}{n}}. \end{cases}$$

Let $N=2n$ be an even number which is not multiple of 4. We show that $\lambda_1(\alpha,1)=\lambda_{[n/2]}^+(\alpha,1)$ for α sufficiently large, where $[n/2]$=the largest positive integer that is less than or equal to $n/2$. Moreover, we prove that for such N that $\lambda_1(\alpha,1)<-2$, whenever $\alpha>1/\sin^2(\pi/n)$. With those results above, we get considerably more information than those obtained in Ref. 9. Among other, such result suggests that if the number N of oscillators is even but not a multiple of 4, then the wavelet method works even better. Specifically, it is better in the sense that the corresponding second largest eigenvalue $\lambda_1(\alpha,1)$ is further away from 0, and, hence, gives even smaller critical length. Our second main result is concerned with $\lambda_1(\alpha,0)$ of $C(\alpha,0)$, which corresponds to the nearest neighbor coupling with Neumann boundary conditions. We show that for all even number N its second largest eigenvalue $\lambda_1(\alpha,0)$ for each α behaves like its periodic counterpart for which its corresponding N is a multiple of 4.

II. PERIODIC BOUNDARY CONDITIONS

Here, we consider the nearest neighbor coupling with periodic boundary conditions. The resulting coupling matrix $A(1)$ is given as in (1.6). Let the dimension of $A_1(1)$, $A_2(1)$, and $\bar{A}_1(1)$ be 2×2. Then

$$A_1(1) = \begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix} = \bar{A}_1(1), \quad A_2(1) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{2.1a}$$

$$\tilde{A}_1(1) = \alpha \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} = \tilde{\bar{A}}_1(1), \quad \tilde{A}_2(1) = \alpha \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}. \tag{2.1b}$$

Then $C_i(1)=A_i(1)+\tilde{A}_i(1)$, i=1,2, $\bar{C}_1(1)=\bar{A}_1(1)+\tilde{\bar{A}}_1(1)$. Thus,

$$C_1(1)=\begin{pmatrix} -\frac{1}{2}(4+\alpha) & \frac{1}{2}(2-\alpha) \\ \frac{1}{2}(2-\alpha) & -\frac{1}{2}(4+\alpha) \end{pmatrix}=\bar{C}_1(1), \quad C_2(1)=\begin{pmatrix} \frac{\alpha}{4} & \frac{\alpha}{4} \\ \frac{1}{4}(4+\alpha) & \frac{\alpha}{4} \end{pmatrix}. \tag{2.1c}$$

We begin by identifying some trivial eigenvalues of $C(\alpha,1)$.

Proposition 2.1: For each α, 0 *and* -4 *are eigenvalues of* $C(\alpha,1)$. *If, in addition,* $n/2(>1)$ *is a positive integer, then* -2 *is also an eigenvalue of* $C(\alpha,1)$ *for any* α.

Proof: Let $C(\alpha,1)+4I=(\mathbf{c}_1,\mathbf{c}_2,\ldots,\mathbf{c}_N)$, where $\mathbf{c}_i$, $1\leqslant i\leqslant N$, are column vectors. Then $\Sigma_{j=1}^{N}(-1)^{j+1}\mathbf{c}_j=0$. Thus -4 is an eigenvalue of $C(\alpha,1)$ for each $\alpha>0$. Let $C(\alpha,1)+2I=(\mathbf{c}_1,\mathbf{c}_2,\ldots,\mathbf{c}_N)$. If $N=2n(>4)$ is a multiple of four, then $\Sigma_{j=1}^{N}\delta(j)\mathbf{c}_j=0$, where

$$\delta(j)=\begin{cases} 1 & \text{if } j=4k \text{ or } 4k+1 \text{ for some } k \\ -1 & \text{if } j=4k+2 \text{ or } 4k+3 \text{ for some } k. \end{cases}$$

Thus, -2 is an eigenvalue of $C(\alpha,1)$ for each α with such N. □

Writing the corresponding eigenvalue problem $C(\alpha,1)\mathbf{b}=\lambda\mathbf{b}$, where $\mathbf{b}=(\mathbf{b}_1,\mathbf{b}_2,\ldots,\mathbf{b}_n)^T$ and $\mathbf{b}_i\in\mathbb{C}^2$, in block component form, we have

$$C_2^T(1)\mathbf{b}_{i-1}+C_1(1)\mathbf{b}_i+C_2(1)\mathbf{b}_{i+1}=\lambda\mathbf{b}_i, \quad 1\leqslant i\leqslant n. \tag{2.2a}$$

Periodic boundary conditions would yield that

$$C_2^T(1)\mathbf{b}_0+C_1(1)\mathbf{b}_1+C_2(1)\mathbf{b}_2=\lambda\mathbf{b}_1=C_1(1)\mathbf{b}_1+C_2(1)\mathbf{b}_2+C_2^T(1)\mathbf{b}_n$$

and

$$C_2^T(1)\mathbf{b}_{n-1}+C_1(1)\mathbf{b}_n+C_2(1)\mathbf{b}_{n+1}=\lambda\mathbf{b}_n=C_2(1)\mathbf{b}_1+C_2^T(1)\mathbf{b}_{n-1}+\bar{C}_1(1)\mathbf{b}_n,$$

or, equivalently,

$$\mathbf{b}_0=\mathbf{b}_n, \tag{2.2b}$$

$$\mathbf{b}_1=\mathbf{b}_{n+1}. \tag{2.2c}$$

To study the block difference equation (2.2), we first seek to find the solution $\mathbf{b}_i$ of the form

$$\mathbf{b}_i=\delta^i\begin{pmatrix} 1 \\ \nu \end{pmatrix}. \tag{2.3}$$

Substituting (2.3) into (2.2a), we get

$$[C_2^T(1)+\delta(C_1(1)-\lambda I)+\delta^2C_2(1)]\begin{pmatrix} 1 \\ \nu \end{pmatrix}=0. \tag{2.4}$$

To have a nontrivial solution $\binom{1}{\nu}$ to Eq. (2.4), we need to have

$$\det[C_2^T(1)+\delta(C_1(1)-\lambda I)+\delta^2C_2(1)]=0, \tag{2.5a}$$

or, equivalently,

$$\alpha\delta^4+(4\alpha+4+2\alpha\lambda)\delta^3-(8+10\alpha+16\lambda+4\alpha\lambda+4\lambda^2)\delta^2+(4\alpha+4+2\alpha\lambda)\delta+\alpha=0. \tag{2.5b}$$

Equation (2.5b) is to be called the characteristic equation of the block difference equation (2.2a). To study the property of Eq. (2.5b), we need the following proposition.

Proposition 2.2: Let D_1, D_2, and D_3 *be* 2×2 *matrices. Suppose* $D_1=D_3^T$ *and* $D_2=D_2^T$. *Let* x_1,

x_2, x_3, and x_4 be roots of $\det[D_1+xD_2+x^2D_3]=0$, *where* $x\in\mathbb{C}$. *Then we may renumber the subscripts if necessary so that*

$$x_1x_2=1=x_3x_4. \tag{2.6a}$$

If, in addition, diagonal elements of D_1 and D_2, respectively, are both equal, then

$$y_1y_2=1=y_3y_4. \tag{2.6b}$$

Here $\binom{1}{y_i}$, $i=1,2,3,4$, *are vectors satisfying*

$$[D_1+x_iD_2+x_i^2D_3]\begin{pmatrix}1\\ y_i\end{pmatrix}=0. \tag{2.6c}$$

Proof: If D_1, D_2, and D_3 are as assumed, then

$$\det[D_1+xD_2+x^2D_3]=ax^4+bx^3+cx^2+bx+a \tag{2.7}$$

for some constants $a\neq 0$, b, and c. Letting $y=x+1/x$, then (2.7) can be written as $\alpha y^2+\beta y+\gamma$, where α, β, and γ depend on the constants a, b, and c. Thus $\det[D_1+xD_2+x^2D_3]=0$ is equivalent to $x^2-\lambda_{\pm}x+1=0$, where $\lambda_{\pm}$ are the roots $a_1y^2+b_1y+c_1=0$. Consequently, $x_1x_2=1=x_3x_4$.

Letting $D_1=\left(\begin{smallmatrix}a_1 & b_1\\ c_1 & a_1\end{smallmatrix}\right)=D_3^T$ and $D_2=\left(\begin{smallmatrix}a_2 & b_2\\ b_2 & a_2\end{smallmatrix}\right)$, we write (2.6c) in component form,

$$(a_1+y_ib_1)+(a_2+y_ib_2)x_i+(a_1+y_ic_1)x_i^2=0,\quad i=1,2,3,4, \tag{2.8a}$$

$$(c_1+y_ia_1)+(b_2+y_ia_2)x_i+(b_1+y_ia_1)x_i^2=0,\quad i=1,2,3,4, \tag{2.8b}$$

For $i=1$, (2.8a) is equal to

$$(a_1+y_1b_1)+(a_2+y_1b_2)\frac{1}{x_2}+(a_1+y_1c_1)\frac{1}{x_2^2}=0$$

or

$$(a_1+y_1c_1)+(a_2+y_1b_2)x_2+(a_1+y_1b_1)x_2^2=0$$

or

$$\left(c_1+\frac{1}{y_1}a_1\right)+\left(b_2+\frac{1}{y_1}a_2\right)x_2+\left(b_1+\frac{1}{y_1}a_1\right)x_2^2=0. \tag{2.8c}$$

Using Eqs. (2.8c) and (2.8b) with $i=2$, and the uniqueness of y_i, $i=1,2,3,4$, we conclude that $y_1y_2=1$. Similarly, $y_3y_4=1$. We just complete the proof of the proposition. □

We are now in a position to further study Eq. (2.5). We assume, momentarily, that Eq. (2.5) has four distinct roots δ_1, δ_2, δ_3, and δ_4. The general solutions to (2.2a) can then be written as

$$\mathbf{b}_i=c_1\delta_1^i\begin{pmatrix}1\\ \nu_1\end{pmatrix}+c_2\delta_2^i\begin{pmatrix}1\\ \nu_2\end{pmatrix}+c_3\delta_3^i\begin{pmatrix}1\\ \nu_3\end{pmatrix}+c_4\delta_4^i\begin{pmatrix}1\\ \nu_4\end{pmatrix}. \tag{2.9}$$

Here ν_i, $i=1,2,3,4$, are some constants depending on δ_i.

Applying (2.9) to boundary conditions (2.2b) and (2.2c), we get

$$c_1(\delta_1^n-1)\begin{pmatrix}1\\ \nu_1\end{pmatrix}+c_2(\delta_2^n-1)\begin{pmatrix}1\\ \nu_2\end{pmatrix}+c_3(\delta_3^n-1)\begin{pmatrix}1\\ \nu_3\end{pmatrix}+c_4(\delta_4^n-1)\begin{pmatrix}1\\ \nu_4\end{pmatrix}=0 \tag{2.10a}$$

and

$$c_1\delta_1(\delta_1^n-1)\begin{pmatrix}1\\ \nu_1\end{pmatrix}+c_2\delta_2(\delta_2^n-1)\begin{pmatrix}1\\ \nu_2\end{pmatrix}+c_3\delta_3(\delta_3^n-1)\begin{pmatrix}1\\ \nu_3\end{pmatrix}+c_4\delta_4(\delta_4^n-1)\begin{pmatrix}1\\ \nu_4\end{pmatrix}=0. \tag{2.10b}$$

Writing (2.10) in matrix form, we have

$$\begin{pmatrix}1 & 1 & 1 & 1\\ \nu_1 & \nu_2 & \nu_3 & \nu_4\\ \delta_1 & \delta_2 & \delta_3 & \delta_4\\ \nu_1\delta_1 & \nu_2\delta_2 & \nu_3\delta_3 & \nu_4\delta_4\end{pmatrix}\mathrm{diag}(\delta_1^n-1,\delta_2^n-1,\delta_3^n-1,\delta_4^n-1)\begin{pmatrix}c_1\\ c_2\\ c_3\\ c_4\end{pmatrix}=0. \tag{2.11}$$

Now if, $\mathrm{diag}(\delta_1^n-1,\delta_2^n-1,\delta_3^n-1,\delta_4^n-1)$ is singular, then Eq. (2.9) has nontrivial solutions c_i, $i=1,2,3,4$. Note that $\mathrm{diag}(\delta_1^n-1,\delta_2^n-1,\delta_3^n-1,\delta_4^n-1)$ is singular if and only if δ_i, $i=1,2,3,4$, satisfy

$$\delta^n=1 \tag{2.12}$$

and (2.5b). To solve the system of equations (2.12) and (2.5b), we first note that

$$\delta_m=e^{i2m\pi/n},\quad 0\leqslant m\leqslant n-1, \tag{2.13}$$

are roots of Eq. (2.12). Substituting (2.13) and (2.5b), we get that the imaginary part of the resulting equation is

$$\left[-4\sin\frac{4m\pi}{n}\right]\lambda^2+\left[2\alpha\sin\frac{6m\pi}{n}-(4\alpha+16)\sin\frac{4m\pi}{n}+2\alpha\sin\frac{2m\pi}{n}\right]\lambda$$
$$+\left[\alpha\sin\frac{8m\pi}{n}+4(1+\alpha)\sin\frac{6m\pi}{n}-(8+10\alpha)\sin\frac{4m\pi}{n}+4(1+\alpha)\sin\frac{2m\pi}{n}\right]=0. \tag{2.14}$$

Before we proceed to compute the real part of the resulting equation, we need the following lemma.

Lemma 2.1: Let a, b, and c be any complex number, then

$$\cos 2\theta(\sin 4\theta+a\sin 3\theta+b\sin 2\theta+a\sin\theta)=\sin 2\theta(\cos 4\theta+a\cos 3\theta+b\cos 2\theta+a\cos\theta+1). \tag{2.15}$$

Since the proof of the lemma is straightforward, we will skip it.

Using (2.14) and (2.15), we see immediately that the real part of (2.5b) with $\delta=e^{i2m\pi/n}$ is a constant multiple $\sin/\cos(4m\pi/n)/(4m\pi/n)$ of its imaginary part. We next show that (2.14) is indeed the characteristic equation of the matrix $C(\alpha,1)$.

Theorem 2.1: *Let $N\times N$, $N=2k$, $k\in N$, be the dimension of the matrix $C(\alpha,1)$. Let dimension of each block matrix in $C(\alpha,1)$ be 2×2. Then the eigenvalues $\lambda_m^{\pm}(\alpha,1)$ of $C(\alpha,1)$ are of the following form:*

$$\lambda_m^{\pm}(\alpha,1)=\frac{1}{2}\left(\alpha\cos\frac{2m\pi}{n}-\alpha-4\right)\pm\frac{1}{2}\left[\left(\alpha\cos\frac{2m\pi}{n}-\alpha-4\right)^2+4\left(\alpha\cos^2\frac{2m\pi}{n}\right.\right.$$
$$\left.\left.+2(\alpha+1)\cos\frac{2m\pi}{n}-2-3\alpha\right)\right]^{1/2}=:\check{\lambda}_m(\alpha,1)\pm\hat{\lambda}_m(\alpha,1),\quad m=0,1,\ldots,n-1. \tag{2.16}$$

Proof: Solving (2.14), we get (2.16). Using Proposition 2.2, we see that if $\delta=1$ or -1 is a root of Eq. (2.5b), then the multiplicity of $\delta=1$ or -1 is both two. Thus, we have only proved the

following. (i) If $n/2$ is not a positive integer, then for each α, $\lambda_m^{\pm}(\alpha,1)$, $m=1,2,\ldots,n-1$, are eigenvalues of $C(\alpha,1)$. (ii) If $n/2$ is a positive integer, then for each α, $\lambda_m^{\pm}(\alpha,1)$, $m=1,2,\ldots,n/2-1,n/2+1,\ldots,n-1$, are eigenvalues of $C(\alpha,1)$. To complete the proof of the theorem, it remains to show that for each α, $\lambda_0^{\pm}(\alpha,1)(=0,-4)$ are eigenvalues of $C(\alpha,1)$ for each α and that if, additionally, $n/2>1$ is a positive integer, then for each α, $\lambda_{n/2}^{\pm}(\alpha,1)(=-2,-2-2\alpha)$ are also eigenvalues of $C(\alpha,1)$. Using Proposition 2.1, we only need to show that $-2-2\alpha=(\lambda_{n/2}^{-}(\alpha,1))$ is an eigenvalue of $C(\alpha,1)$ for fixed α. To this end, we see that

$$\textit{trace of } C(\alpha,1) = -n(\alpha+4). \tag{2.17}$$

Let $N=2n>4$ be a multiple of four, then

$$\lambda_{n/2}^{+}(\alpha,1)+\left(\sum_{j=1,j\neq n/2}^{n}\lambda_j^{\pm}(\alpha,1)\right)+\lambda_0^{\pm}(\alpha,1) = -2-(n-2)(\alpha+4)-4. \tag{2.18}$$

Using (2.17) and (2.18), we have that the remaining eigenvalue of $C(\alpha,1)$ for each α is $-2-2\alpha$, which is equal to $\lambda_{n/2}^{-}(\alpha,1)$. We thus complete the proof of the theorem. □

Proposition 2.3: For all $\alpha>0$, we have that $\hat{\lambda}_m(\alpha,1)>0$, $\check{\lambda}_m(\alpha,1)<0$ and $\lambda_m^{\pm}(\alpha,1)\leqslant 0$.

Proof: Obviously, $\check{\lambda}_m(\alpha,1)<0$. Now, letting $t=\cos(2m\pi/n)$, we have that

$$4(\hat{\lambda}_m(\alpha,1))^2=(t-1)^2\alpha^2+4(t^2-1)\alpha+8(1+t)=((t-1)\alpha+2(t+1))^2+4(1-t^2)>0$$

for any $\alpha>0$. Thus $\hat{\lambda}_m(\alpha,1)>0$. To prove the last assertion of the proposition, we note, via (2.16), that

$$0>4\left(\alpha\cos^2\frac{2m\pi}{n}+2(\alpha+1)\cos\frac{2m\pi}{n}-2-3\alpha\right)=:l.$$

Thus,

$$2\lambda_m^{\pm}(\alpha,1)=2\check{\lambda}_m(\alpha,1)\pm(4\check{\lambda}_m^2(\alpha,1)+l)^{1/2}\leqslant 0.$$

We just complete the proof of the proposition. □

Proposition 2.4: If $n/2$ is not a positive integer, then the eigencurves $\lambda_m^{\pm}(\alpha,1)$, $m=1,2,\ldots,n-1$, are strictly decreasing in $\alpha\in(0,\infty)$. If $n/2(>1)$ is a positive integer, then $\lambda_m^{\pm}(\alpha,1)$, $m=1,2,\ldots,n/2-1,n/2+1,\ldots,n-1$, and $\lambda_{n/2}^{-}(\alpha,1)$ are strictly decreasing in $\alpha\in(0,\infty)$.

Proof: Letting $t=\cos(2m\pi/n)$, we write (2.16) as

$$\begin{aligned}\lambda_m^{\pm}(\alpha,1)&=\tfrac{1}{2}\{\alpha(t-1)-4\pm[(t-1)^2\alpha^2+4(t^2-1)\alpha+8(1+t)]^{1/2}\}\\&=:\tfrac{1}{2}\{\alpha(t-1)-4\pm(t_\alpha)^{1/2}\}=:\lambda_t^{\pm}(\alpha).\end{aligned} \tag{2.19}$$

Then

$$2\frac{d\lambda_m^{\pm}(\alpha,1)}{d\alpha}=(t-1)\left(1\pm\frac{(t-1)\alpha+2(t+1)}{\sqrt{t_\alpha}}\right).$$

A direct computation would yield that

$$t_\alpha\geqslant((t-1)\alpha+2(t+1))^2.$$

Thus, $d\lambda_m^{\pm}(\alpha,1)/d\alpha\leqslant 0$. The equality holds only if $t=1$ or $t=-1$ for λ_m^{+}. □

Proposition 2.5: (i) In the $\alpha-\lambda$ plane, $\lambda_t^{\lambda}(\alpha,1)$ interest with $\lambda=-2+k$ at $\alpha_{t,k}$, where

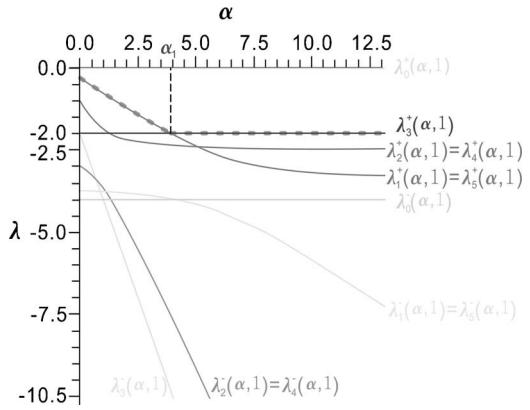

FIG. 1. The curves $\lambda_m^{\pm}(\alpha,1)$ with $N=2n=12$ are provided. As predicted in Theorem 2.2–(i), $\lambda(\alpha,1)$ turns flat after α_1.

$$\alpha_{t,k}=\frac{2(1+t)-k^2}{(1-t)(1+t+k)}. \tag{2.20}$$

(ii) For $-1\leqslant t<1$, $\lim_{\alpha\to\infty}\lambda_t^+(\alpha,1)=-(t+3)$.

Proof: Solving equation $-2+k=\lambda_t^+(\alpha,1)$, we easily get that $\alpha_{t,k}$ are as asserted. Rewriting $\lambda_t^+(\alpha,1)$ as

$$\lambda_t^+(\alpha,1)=\frac{-2\alpha(t-1)(t+3)+4(1-t)}{\alpha(t-1)-4-\sqrt{t_\alpha}},$$

we see that $\lim_{\alpha\to\infty}\lambda_t^+(\alpha,1)=-(t+3)$ for $-1\leqslant t<1$. □

Theorem 2.2: *Let N be any positive even integer. The dimension of each block matrix in* $C(\alpha,1)$ *is* 2×2. *Then (i) suppose N is a multiple of four and* $N>4$. *For each* $\alpha>0$, *let* $\lambda(\alpha,1)$ *be the second largest eigenvalue of* $C(\alpha,1)$. *Then* $\lambda(\alpha,1)=\lambda_1^+(\alpha,1)$, *for* $0\leqslant\alpha\leqslant 1/\sin^2(\pi/n):=\alpha_1$; *and* $\lambda(\alpha,1)=\lambda_{n/2}^+(\alpha,1)=-2$ *for all* $\alpha\in[\alpha_1,\infty)$. *See Fig. 1.*

(ii) Suppose N is not a multiple of four. Then there exists a $\tilde{\alpha}_c$ *such that* $\lambda(\alpha,1)=\lambda_{[n/2]}^+(\alpha)$ *for all* $\alpha\geqslant\tilde{\alpha}_c$. *Here* $[n/2]$=*the largest positive integer that is less than or equal to* $n/2$. *Moreover,* $\lambda(\alpha,1)<-2$ *whenever* $\alpha>\alpha_1$. *See Fig. 2.*

Proof: For $\alpha_{t,k}$ to be positive, we must have

$$2(1+t)>k^2. \tag{2.21}$$

Now,

$$(1-t)^2(1+t+k)^2\frac{\mathrm{d}\alpha_{t,k}}{\mathrm{d}t}=2(t+1)^2-k^3+4k-2tk^2>(1+t)k^2-k^3+4k-2tk^2$$
$$=-k(k^2+(t-1)k-4)=-k(k-t_+)(k-t_-),$$

where $t_\pm=(1-t\pm\sqrt{16+(1-t)^2})/2$. Note that we have used (2.21) to justify the above inequality. Moreover $t_-<0$ and $t_+\geqslant 2$. Thus, $\mathrm{d}\alpha_{t,k}/\mathrm{d}t>0$ whenever $\lambda=-2+k$, $0\leqslant k<2$, and $\lambda=\lambda_t^+(\alpha,1)$ have the intersections intersect at the positive $\alpha_{t,k}$. Upon using Proposition 2.4, we conclude that for $0\leqslant m\leqslant n-1$, the portion of the graphs of $\lambda_m^+(\alpha,1)$ lying above the line $\lambda=-2$ do not intersect each other. Thus, $\lambda(\alpha,1)$ is as asserted.

By Proposition 2.5(ii), we have that

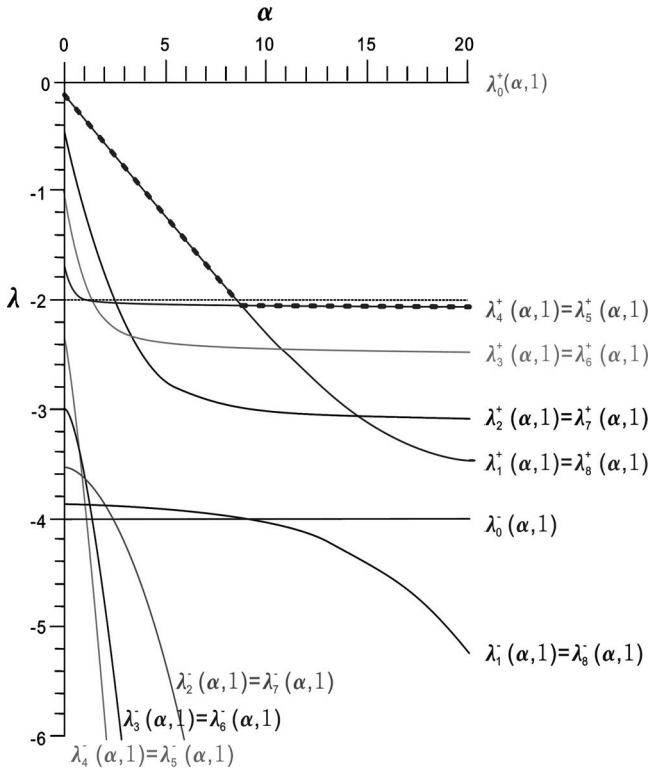

FIG. 2. The curves $\lambda_m^{\pm}(\alpha,1)$ with $N=2n=18$ are provided. As predicted in Theorem 2.2–(ii), $\lambda(\alpha,1)$ lies below -2 eventually.

$$\lim_{\alpha\to\infty}\lambda_m^+(\alpha,1)=-\left(\cos\frac{2m\pi}{n}+3\right)=:\lambda_m^\infty=\lambda_t^\infty.$$

Then $\lambda_m^\infty, 0<m\leqslant n-1$, have a maximum at $m=[n/2]$. Thus, there exists a $\tilde{\alpha}_c$ such that $\lambda(\alpha,1)=\lambda_{[n/2]}^+(\alpha,1)$ for all $\alpha\geqslant\tilde{\alpha}_c$. The last assertion of the theorem follows from Proposition 2.5-(i) and Proposition 2.1. □

Remark 2.1: (i) Since $\lambda_t^+(\alpha,1)$ is increasing in t and λ_t^∞ is decreasing in t, the eigencurves $\lambda_m^+(\alpha,1)$, $0<m\leqslant[n/2]$ must be crossing each other.

(ii) The first column in Table I contains the values of $\lambda_m^{\pm}(1,1)$, $m=0,1,\ldots,5$, while the second column contains the eigenvalues of $C(1,1)$ obtained by using MATHEMATICA. As indicated, the $C(1,1)$ and $C(5,1)$ obtained by both methods are identical. The values $\lambda_m^{\pm}(3,1)$, $m=0,1,\ldots,8$, in the first and third columns of Table II are computed by MAPLE, while those in the second and fourth columns are computed by MATLAB. Some discrepancies between the values in the respective columns occur due to the round-off errors.

(iii) Figure 1 illustrates the graph of $\lambda_m^{\pm}(\alpha,1)$, $m=0,1,\ldots,5$, with $n=6$. The dotted part of the curve is $\lambda(\alpha,1)$. Figure 2 gives the same information with $n=9$.

(iv) We conclude, via the last assertion of Theorem 2.1, that the wavelet approach works even better when N is an even number but not a multiple of four. Indeed, in such case, it synchronizes faster when α is chosen to be the critical value $\tilde{\alpha}_c$.

III. NEUMANN BOUNDARY CONDITIONS

Here, we consider the nearest neighbor coupling with Neumann boundary conditions. The resulting coupling matrix A is then $A(0)$, given as in (1.6a). With $i=1$, we have

TABLE I. The first and third columns contain the values computed by using formulas $\lambda_m^{\pm}(\alpha,1)$ as given in (2.16). The values in the second and fourth columns are eigenvalues of $C(\alpha,1)$ obtained by using MATHEMATICA.

$n=6$			
$\lambda_m^{\pm}(1,1)$	Eigenvalues of $C(1,1)$	$\lambda_m^{\pm}(5,1)$	Eigenvalues of $C(5,1)$
$\lambda_0^+(1,1)=0$	0	$\lambda_0^+(5,1)=0$	0
$\lambda_1^+(1,1)=-\frac{9}{4}+\frac{1}{4}\sqrt{37}$	$-\frac{9}{4}+\frac{1}{4}\sqrt{37}$	$\lambda_1^+(5,1)=-\frac{13}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}+\frac{1}{4}\sqrt{13}$
$\lambda_2^+(1,1)=-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$\lambda_2^+(5,1)=-\frac{23}{4}+\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}+\frac{1}{4}\sqrt{181}$
$\lambda_3^+(1,1)=-2$	-2	$\lambda_3^+(5,1)=-2$	-2
$\lambda_2^+(1,1)=-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$\lambda_4^+(5,1)=-\frac{23}{4}+\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}+\frac{1}{4}\sqrt{181}$
$\lambda_2^+(1,1)=-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}+\frac{1}{4}\sqrt{13}$	$\lambda_5^+(5,1)=-\frac{13}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}+\frac{1}{4}\sqrt{13}$
$\lambda_0^-(1,1)=-4$	-4	$\lambda_0^-(5,1)=-4$	-4
$\lambda_1^-(1,1)=-\frac{9}{4}-\frac{1}{4}\sqrt{37}$	$-\frac{9}{4}-\frac{1}{4}\sqrt{37}$	$\lambda_1^-(5,1)=-\frac{13}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}-\frac{1}{4}\sqrt{13}$
$\lambda_2^-(1,1)=-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$\lambda_2^-(5,1)=-\frac{23}{4}-\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}-\frac{1}{4}\sqrt{181}$
$\lambda_3^-(1,1)=-4$	-4	$\lambda_3^-(5,1)=-12$	-12
$\lambda_4^-(1,1)=-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$\lambda_4^-(5,1)=-\frac{23}{4}-\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}-\frac{1}{4}\sqrt{181}$
$\lambda_5^-(1,1)=-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{11}{4}-\frac{1}{4}\sqrt{13}$	$\lambda_5^-(5,1)=-\frac{13}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}-\frac{1}{4}\sqrt{13}$

TABLE II. The first and third columns contain the values computed by using formulas $\lambda_m^{\pm}(\alpha,1)$ as given in (2.16). The values in the second and fourth columns are eigenvalues of $C(\alpha,1)$ obtained by using MATHEMATICA.

$n=9$			
$\lambda_m^{\pm}(3,1)$	Eigenvalues of $C(3,1)$	$\lambda_m^{\pm}(10,1)$	Eigenvalues of $C(10,1)$
$\lambda_0^+(3,1)=0$	0	$\lambda_0^+(10,1)=0$	0
$\lambda_1^+(3,1)\approx-0.7967$	-0.7967	$\lambda_1^+(10,1)\approx-2.2938$	-2.2930
$\lambda_2^+(3,1)\approx-2.2524$	-2.2525	$\lambda_2^+(10,1)\approx-3.0135$	-3.0140
$\lambda_3^+(3,1)\approx-2.2975$	-2.2974	$\lambda_3^+(10,1)\approx-2.4465$	-2.4466
$\lambda_4^+(3,1)\approx-2.0399$	-2.0399	$\lambda_4^+(10,1)\approx-2.0535$	-2.0542
$\lambda_5^+(3,1)\approx-2.0399$	-2.0399	$\lambda_5^+(10,1)\approx-2.0535$	-2.0542
$\lambda_6^+(3,1)\approx-2.2975$	-2.2974	$\lambda_6^+(10,1)\approx-2.4465$	-2.4466
$\lambda_7^+(3,1)\approx-2.2524$	-2.2525	$\lambda_7^+(10,1)\approx-3.0135$	-3.0140
$\lambda_8^+(3,1)\approx-0.7967$	-0.7967	$\lambda_8^+(10,1)\approx-2.2938$	-2.2930
$\lambda_0^-(3,1)=-4$	-4	$\lambda_0^-(10,1)=-4$	-4
$\lambda_1^-(3,1)\approx-3.9051$	-3.9052	$\lambda_1^-(10,1)\approx-4.0458$	-4.0465
$\lambda_2^-(3,1)\approx-4.2268$	-4.2265	$\lambda_2^-(10,1)\approx-9.2505$	-9.2495
$\lambda_3^-(3,1)\approx-6.2025$	-6.2026	$\lambda_3^-(10,1)\approx-16.5534$	-16.5534
$\lambda_4^-(3,1)\approx-7.7791$	-7.7792	$\lambda_4^-(10,1)\approx-21.3427$	-21.3427
$\lambda_5^-(3,1)\approx-7.7791$	-7.7792	$\lambda_5^-(10,1)\approx-21.3427$	-21.3427
$\lambda_6^-(3,1)\approx-6.2025$	-6.2026	$\lambda_6^-(10,1)\approx-16.5534$	-16.5534
$\lambda_7^-(3,1)\approx-4.2268$	-4.2265	$\lambda_7^-(10,1)\approx-9.2505$	-9.2495
$\lambda_8^-(3,1)\approx-3.9051$	-3.9052	$\lambda_8^-(10,1)\approx-4.0458$	-4.0465

$$A_1(0)=\begin{pmatrix}-1 & 1\\ 1 & -2\end{pmatrix},\quad \bar{A}_1(0)=\begin{pmatrix}-2 & 1\\ 1 & -1\end{pmatrix},\quad A_2(1)=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix},$$

$$A_1(1)=\begin{pmatrix}-2 & 1\\ 1 & -2\end{pmatrix},\quad A_2(0)=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},\quad \tilde{A}_2(0)=\alpha\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},$$

$$\tilde{A}_1(0)=\alpha\begin{pmatrix}-\frac{1}{4} & -\frac{1}{4}\\ -\frac{1}{4} & -\frac{1}{4}\end{pmatrix}=\tilde{\bar{A}}_1(0),\quad \tilde{A}_2(1)=\alpha\begin{pmatrix}\frac{1}{4} & \frac{1}{4}\\ \frac{1}{4} & \frac{1}{4}\end{pmatrix},$$

and

$$\tilde{A}_1(1)=\alpha\begin{pmatrix}-\frac{1}{2} & -\frac{1}{2}\\ -\frac{1}{2} & -\frac{1}{2}\end{pmatrix} \tag{3.1}$$

A direct calculation would yield that

$$C_2(0)=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},$$

$$C_1(0)=\begin{pmatrix}-\frac{1}{4}(4+\alpha) & \frac{1}{4}(4-\alpha)\\ \frac{1}{4}(4-\alpha) & -\frac{1}{4}(8+\alpha)\end{pmatrix},\quad C_2(1)=\begin{pmatrix}\frac{\alpha}{4} & \frac{\alpha}{4}\\ \frac{1}{4}(\alpha+4) & \frac{\alpha}{4}\end{pmatrix},$$

$$C_1(1)=\begin{pmatrix}-\frac{1}{2}(4+\alpha) & \frac{1}{2}(2-\alpha)\\ \frac{1}{2}(2-\alpha) & -\frac{1}{2}(4+\alpha)\end{pmatrix},\quad \bar{C}_1(0)=\begin{pmatrix}-\frac{1}{4}(8+\alpha) & \frac{1}{4}(4-\alpha)\\ \frac{1}{4}(4-\alpha) & -\frac{1}{4}(4+\alpha)\end{pmatrix}. \tag{3.2}$$

As in the case of periodic boundary conditions, the eigenvalue problem $C(\alpha,0)\mathbf{b}=\lambda\mathbf{b}$, where $\mathbf{b}=(\mathbf{b}_1,\mathbf{b}_2,\ldots,\mathbf{b}_n)^T$, $\mathbf{b}_i\in\mathbb{C}^2$, can be formed as block difference equation

$$C_2^T(1)\mathbf{b}_{i-1}+C_1(1)\mathbf{b}_i+C_2(1)\mathbf{b}_{i+1}=\lambda\mathbf{b}_i,\quad 1\leqslant i\leqslant n. \tag{3.3}$$

With Neumann boundary conditions, $\mathbf{b}_0$, and $\mathbf{b}_{n+1}$ must satisfy

$$C_1(0)\mathbf{b}_1+C_2(1)\mathbf{b}_2=\lambda\mathbf{b}_1=C_2^T(1)\mathbf{b}_0+C_1(1)\mathbf{b}_1+C_2(1)\mathbf{b}_2 \tag{3.4a}$$

and

$$C_2^T(1)\mathbf{b}_{n-1}+\bar{C}_1(0)\mathbf{b}_n=\lambda\mathbf{b}_n=C_2^T(1)\mathbf{b}_{n-1}+C_1(1)\mathbf{b}_n+C_2(1)\mathbf{b}_{n+1}. \tag{3.4b}$$

Solving (3.4a) and (3.4b), respectively, we get

$$\mathbf{b}_0=(C_2^T(1))^{-1}(C_1(0)-C_1(1))\mathbf{b}_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\mathbf{b}_1 \tag{3.5a}$$

and

TABLE III. The first and third columns contain the values computed by using formulas $\lambda_m^{\pm}(\alpha,0)$ as given in (3.9). The values in the second and fourth columns are eigenvalues of $C(\alpha,1)$ obtained by using MATHEMATICA.

$n=3$			
$\lambda_m^{\pm}(2,0)$	Eigenvalues of $C(2,0)$	$\lambda_m^{\pm}(5,0)$	Eigenvalues of $C(5,0)$
$\lambda_0^{+}(2,0)=0$	0	$\lambda_0^{+}(5,0)=0$	0
$\lambda_1^{+}(2,0)=-\frac{5}{2}+\frac{1}{2}\sqrt{7}$	$-\frac{5}{2}+\frac{1}{2}\sqrt{7}$	$\lambda_1^{+}(5,0)=-\frac{13}{4}+\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}+\frac{1}{4}\sqrt{13}$
$\lambda_2^{+}(2,0)=-\frac{7}{2}+\frac{1}{2}\sqrt{7}$	$-\frac{7}{2}+\frac{1}{2}\sqrt{7}$	$\lambda_2^{+}(5,0)=-\frac{23}{4}+\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}+\frac{1}{4}\sqrt{181}$
$\lambda_3^{+}(2,0)=-2$	-2	$\lambda_3^{+}(5,0)=-2$	-2
$\lambda_1^{-}(2,0)=-\frac{5}{2}-\frac{1}{2}\sqrt{7}$	$-\frac{5}{2}-\frac{1}{2}\sqrt{7}$	$\lambda_1^{-}(5,0)=-\frac{13}{4}-\frac{1}{4}\sqrt{13}$	$-\frac{13}{4}-\frac{1}{4}\sqrt{13}$
$\lambda_2^{-}(2,0)=-\frac{7}{2}-\frac{1}{2}\sqrt{7}$	$-\frac{7}{2}-\frac{1}{2}\sqrt{7}$	$\lambda_2^{-}(5,0)=-\frac{23}{4}-\frac{1}{4}\sqrt{181}$	$-\frac{23}{4}-\frac{1}{4}\sqrt{181}$

$$\mathbf{b}_{n+1} = C_2(1)^{-1}(\bar{C}_1(0) - C_1(1))\mathbf{b}_n = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\mathbf{b}_n. \tag{3.5b}$$

We then see that the characteristic equation of the block difference equation (3.3) is

$$\det[C_2^T(1) + \delta(C_1(1) - \lambda I) + \delta^2 C_2] = 0. \tag{3.6a}$$

Here δ is such that $\mathbf{b}_i = \delta^i\binom{1}{\nu}$, where ν is a constant depending on δ. Expanding the determinant in (3.6a), we get

$$\alpha\delta^4 + 2(2\alpha + 2 + \lambda\alpha)\delta^3 - 2(4 + 5\alpha + 2(\alpha + 4)\lambda + 2\lambda^2)\delta^2 + 2(2\alpha + 2 + \lambda\alpha)\delta + \alpha = 0. \tag{3.6b}$$

We assume, momentarily, that Eq. (3.6b) has four distinct roots δ_1, δ_2, δ_3, and δ_4. The general solutions to (3.3) can then be written as

$$\mathbf{b}_i = \sum_{j=1}^{4} c_j \delta_j^i \begin{pmatrix} 1 \\ \nu_j \end{pmatrix}. \tag{3.7}$$

Substituting (3.7) into boundary conditions (3.5), we get

$$\begin{pmatrix} \delta_1\nu_1 - 1 & \delta_2\nu_2 - 1 & \delta_3\nu_3 - 1 & \delta_4\nu_4 - 1 \\ \delta_1 - \nu_1 & \delta_2 - \nu_2 & \delta_3 - \nu_3 & \delta_4 - \nu_4 \\ \delta_1^n(\delta_1\nu_1 - 1) & \delta_2^n(\delta_2\nu_2 - 1) & \delta_3^n(\delta_3\nu_3 - 1) & \delta_4^n(\delta_4\nu_4 - 1) \\ \delta_1^n(\delta_1 - \nu_1) & \delta_2^n(\delta_2 - \nu_2) & \delta_3^n(\delta_3 - \nu_3) & \delta_4^n(\delta_4 - \nu_4) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} =: D\mathbf{c} = 0, \tag{3.8}$$

where $\mathbf{c} = (c_1, c_2, c_3, c_4)^T$. We are now in a position to simplify $\det D$,

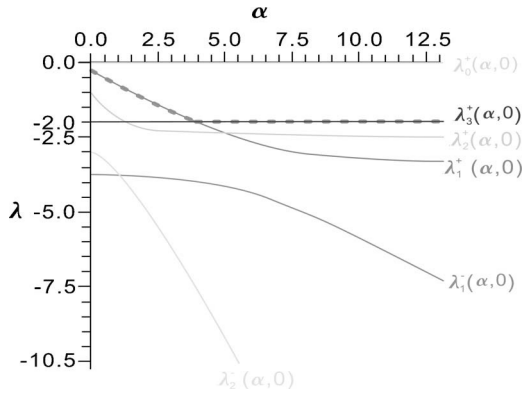

FIG. 3. The curves $\lambda_m^{\pm}(\alpha,0)$ with $N=2n=6$ are provided. As predicted in Theorem 3.2, $\lambda(\alpha,0)$ turns flat after $\bar{\alpha}_1$.

$$\det D=(\delta_2\nu_2)(\delta_4\nu_4)\begin{vmatrix} \delta_1\nu_1-1 & 1-\delta_1\nu_1 & \delta_3\nu_3-1 & 1-\delta_3\nu_3 \\ \delta_1-\nu_1 & \nu_1-\delta_1 & \delta_3-\nu_3 & \nu_3-\delta_3 \\ \delta_1^n(\delta_1\nu_1-1) & \delta_2^n(1-\delta_1\nu_1) & \delta_3^n(\delta_3\nu_3-1) & \delta_4^n(1-\delta_3\nu_3) \\ \delta_1^n(\delta_1-\nu_1) & \delta_2^n(\delta_1-\nu_1) & \delta_3^n(\delta_3-\nu_3) & \delta_4^n(\delta_3-\nu_3) \end{vmatrix}$$

$$=(\delta_2\nu_2)(\delta_4\nu_4)(\delta_1^n-\delta_2^n)(\delta_3^n-\delta_4^n)\begin{vmatrix} 0 & 1-\delta_1\nu_1 & 0 & 1-\delta_3\nu_3 \\ 0 & \nu_1-\delta_1 & 0 & \nu_3-\delta_3 \\ \delta_1\nu_1-1 & \delta_2^n(1-\delta_1\nu_1) & \delta_3\nu_3-1 & \delta_4^n(1-\delta_3\nu_3) \\ \delta_1-\nu_1 & \delta_2^n(\nu_1-\delta_1) & \delta_3-\nu_3 & \delta_4^n(\nu_3-\delta_3) \end{vmatrix}$$

$$=(\delta_2\nu_2)(\delta_4\nu_4)(\delta_1^n-\delta_2^n)(\delta_3^n-\delta_4^n)\Bigg\{[(\delta_1\nu_1-1)(\nu_3-\delta_3)+(\delta_1-\nu_1)(\delta_3\nu_3-1)] \times\begin{vmatrix} 1-\delta_1\nu_1 & 1-\delta_3\nu_3 \\ \nu_1-\delta_1 & \nu_3-\delta_3 \end{vmatrix}\Bigg\}.$$

Therefore, $\det D$ being equal to zero amounts to $\delta_i^{2n}=1$ for $i=1,2,3,4$.

To get the characteristic equation of $C(\alpha,0)$, we need to solve $\delta^{2n}=1$ and Eq. (3.6b). This leads to the following theorem.

Theorem 3.1: *Let N be any positive even integer. The dimension of each block matrix in $C(\alpha,0)$ is 2×2. Let $\lambda_m^{\pm}(\alpha,0)$ be defined as follows:*

$$\lambda_m^{\pm}(\alpha,0)=\frac{1}{2}\left(\alpha\cos\frac{m\pi}{n}-\alpha-4\right)\pm\frac{1}{2}\Bigg[\left(\alpha\cos\frac{m\pi}{n}-\alpha-4\right)^2+4\Bigg(\alpha\cos^2\frac{m\pi}{n}+2(\alpha+1) \times\cos\frac{m\pi}{n}-2-3\alpha\Bigg)\Bigg]^{1/2}. \tag{3.9}$$

Then $\lambda_m^{\pm}(\alpha,0)$, $m=1,2,\ldots,n-1$, $\lambda_0^+(\alpha,0)=0$ and $\lambda_n^+(\alpha,0)=-2$ are eigenvalues of $C(\alpha,0)$ for each $\alpha>0$.

Proof: Substituting $\delta=e^{im\pi/n}$, $0\leqslant m\leqslant n-1$, into (3.6b), we get (3.9). Clearly, if $\delta\neq 1$ or -1, or equivalently, $\cos(m\pi/n)\neq 1$ or -1, then $\lambda_m^{\pm}(\alpha,0)$, $m=1,2,\ldots,n-1$, are eigencurves of $C(\alpha,0)$. Since $0=\lambda_0^+(\alpha,0)$ is an eigenvalue of $C(\alpha,0)$ for all α, we only need to show that $\lambda_n^+(\alpha,0)$ is, indeed, the eigenvalue of $C(\alpha,0)$ for each α. To this end, we see that $\operatorname{trace}(C(\alpha,0))=-(n-2)(\alpha+4)-6-\alpha$. However, $\lambda_0^+(\alpha,0)+\sum_{j=1}^{n-1}\lambda_j^{\pm}(\alpha,0)=-(n-1)(\alpha+4)=:k$. Thus, $\operatorname{trace}(C(\alpha,0))-k=-2=\lambda_n^+(\alpha,0)$. We just complete the proof of the theorem. □

Remark 3.1: (i) Letting $t=\cos(m\pi/n)$, $\lambda_m^{\pm}(\alpha,0)=\lambda_t^{\pm}(\alpha,0)$ and treating t as a real parameter, we see that for fixed $\alpha>0$, the eigenvalues of C with periodic boundary conditions and Neumann

boundary conditions, respectively, lie on the curve $\lambda_t^{\pm}(\alpha,0)$ in $t-\lambda$ plane.

(ii) Note that $\lambda_m^{\pm}(\alpha,0)=\lambda_{2n-m}^{\pm}(\alpha,0)$.

Theorem 3.2: *For each* α, *let* $\lambda(\alpha,0)$ *be the second largest eigenvalue of* $C(\alpha,0)$. *Then* $\lambda(\alpha,0)=\lambda_1^{+}(\alpha,0)$, *for* $0\leqslant\alpha\leqslant 1/\sin^2(\pi/2n)=:\bar{\alpha}_1$; *and* $\lambda(\alpha,0)=\lambda_n^{+}(\alpha,0)=-2$ *for all* $\alpha\in[\bar{\alpha}_1,\infty)$.

We skip the proof of theorem due to its similarity with that of Theorem 2.1 (ii).

Remark 3.2: Table III and Fig. 3 illustrate, again, the accuracy of our theorems.

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Diffraction of light by a planar aperture in a metallic screen

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We present a complete derivation of the formula of Smythe [Phys. Rev. **72**, 1066 (1947)] giving the electromagnetic field diffracted by an aperture created in a perfectly conducting plane surface. The reasoning, valid for any excitating field and any hole shape, makes use only of the free scalar Green function for the Helmoltz equation without any reference to a Green dyadic formalism. We compare our proof with the one previously given by Jackson and connect our reasoning to the general Huygens Fresnel theorem. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Diffraction of electromagnetic waves by an aperture in a perfect metallic plane is not only a mathematical problem of fundamental interest but is connected to many applications in the microwave domain (for example, in waveguides and in cavity resonators[1]) as well as in the optical regime where it is involved in many optical arrangements.[2] The fundamental importance of this phenomenon in near-field optics has been pointed out as early as in 1928 by Synge[3] in his prophetic paper and is currently involved in modern near-field scanning optical microscopy (NSOM).[4]

In the domain of applicability of NSOM where distances and dimensions are smaller than or close to the wavelength of light, we need to know the exact structure of the electromagnetic field, and we cannot in general consider the usual approximations involved in Kirchhoff's theory for a scalar wave.[5–7] In this context, one of the most cited approaches is the one given by Bethe[8] in 1944 and corrected by Bouwkamp.[9,10] It gives the electromagnetic field diffracted by a small circular aperture in a perfect metallic plane in the limit where the optical wavelength is much larger than the aperture. Less known is the more general formula of Smythe[11,12] which expresses in a formal way the Huygens Fresnel principle for any kind of aperture in a metallic screen. Even if this formula is not an explicit solution for the general diffraction problem, it constitutes an integral equation which can be used in a self consistent way in perturbative or numerical calculations of the diffracted field.[13,14] Further efforts have been made by Smythe[11,12] himself in order to justify his formula by means of some arrangements of current sheets fitting the aperture. This method essentially consists of transforming the problem of diffraction by a hole into a physically different one in order to guess the correct integral equation for the original problem. However, if this physical reasoning proves the consistency of the proposed solution with Maxwell equations and boundary conditions for the field, it is not directly connected to the rigorous electromagnetic formulation of the Huygens Fresnel principle obtained by Stratton and Chu.[15] Such a connection is expected naturally because these two formulations of diffraction must be equivalent here.

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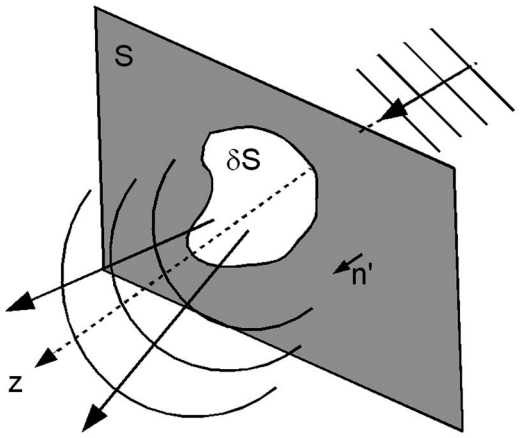

FIG. 1. The problem of diffraction in electromagnetism. The incoming wave comes from the $z<0$ half-space and is diffracted by the aperture δS located in the plane screen S at $z=0$. The unit vector $\vec{n}'=\hat{z}$ used in the text is represented.

Jackson,[16] in the first edition of his textbook on electrodynamics, developed a complete proof of the Smythe formula starting from the Stratton and Chu formula [Eq. (3) of the present paper]. Nevertheless, like in the original paper of Smythe, Jackson transforms the problem into a physically different one in order to guess the correct result. The result is then subjected to the same remarks as above for Smythe's approach. Other justifications of Smythe results are based on the use of the Babinet theorem or of the Green dyadic method. The latter, which uses a tensorial Green function instead of a scalar one like in Kirchhoff's or Stratton and Chu's theories, gives us the most direct justification for Smythe approach in terms of the Huygens Fresnel principle. However, this proof is for the moment not directly connected to the Stratton and Chu approach. It is the aim of this paper to establish such a link.

The paper is organized as follows. We give in Sec. II a description of the general theory of diffraction of electromagnetic waves by an aperture in a screen. In Sec. III, we exploit precedent works by Jackson[16,17] and Levine and Schwinger[18] to justify directly and rigorously the Smythe formula using the Stratton Chu theorem without relying on any ingenious physical "trick." Section IV deals with a vectorial justification of Smythe's approach. The consistency between the various theoretical treatments of diffraction by an aperture in a metallic screen is stressed in Sec. V which also compares our treatment with that obtained within the Green dyadic formalism.[19,20] Our conclusions appear in Sec. VI.

II. THE DIFFRACTION PROBLEM IN ELECTROMAGNETISM

The first coherent theory of diffraction was elaborated by Kirchhoff (1882) on the basis of the Huygens Fresnel principle.[2,21] The method of integral equations allows one to write a solution $\psi(\vec{r})e^{-i\omega t}$ of the Helmholtz propagation equation $[\nabla^2+k^2]\psi(\vec{r})=0$ $(k=\omega/c)$ using the "free" scalar Green function $G(\vec{r},\vec{r}')=e^{ikR}/4\pi R$ which is a solution of the equation $[\nabla^2+k^2]G(\vec{r},\vec{r}')=-\delta^3(\vec{r}-\vec{r}')$.

If, as schematized in Fig. 1, we consider now an aperture δS made in a two-dimensional infinite screen S and illuminated by incident radiation, we can express the field ψ existing at each observation point located behind the screen (i.e., for $z>0$) by the Kirchhoff formula

$$\psi(\vec{r}) = \int_S [\psi(\vec{r}')\vec{n}'\cdot\vec{\nabla}'G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\vec{n}'\cdot\vec{\nabla}'\psi(\vec{r}')]\mathrm{d}S', \tag{1}$$

where the normal unit vector $\vec{n}'$ is oriented into the diffraction half-space.

In a problem of diffraction, we usually impose the additional first Kirchhoff "shadow" approximation $\psi(\vec{r}')=\partial_{n'}\psi(\vec{r}')=0$ which is valid on the unilluminated side of the screen. This per-

mits one to restrict the integral in (1) to the region of the aperture only, which is very useful in some approximations or iterative resolutions. Nevertheless, this intuitive hypothesis has some fundamental inconsistencies because, following a theorem due to Poincaré,[21] a field satisfying the shadow approximation on a finite domain must vanish everywhere.

A classic solution proposed by Rayleigh[22] and Sommerfeld[23] to circumvent this difficulty consists in replacing the free Green function by the Dirichlet G_D or the Neumann G_N Green functions[16] satisfying $\partial_{n'}G_N(\vec{r},\vec{r}')=0$ and $G_D(\vec{r},\vec{r}')=0$ for all points $\vec{r}'$ on S. We can then rigorously reduce the integral to the region of the aperture depending on the nature of the boundary problem. For example, if we impose $\psi=0$ on the screen, we can then write

$$\psi(\vec{r}) = \int_{\text{Aperture}} \psi(\vec{r}')\partial_{n'}G_D(\vec{r},\vec{r}')\mathrm{d}S'. \tag{2}$$

In principle, it could be possible to generalize the preceding methods to the different Cartesian components ψ_α of the electromagnetic field using equations of the form $\psi_\alpha=\int_S[\psi_\alpha\partial_{n'}G - G\partial_{n'}\psi_\alpha]\mathrm{d}S'$. Nevertheless, as pointed out by Stratton, Chu and others,[24–26]the Maxwell equations couple the field components between them and the consistency of these relations must be controlled *a posteriori* if we use an integral equation like Eq. (1) either in an exact or approximative treatment of diffraction. In addition, because the boundary conditions imposed by Maxwell's equations connect the tangential and the normal components of the field on the screen surface, it is not at all trivial to reduce the integral to the region of the aperture directly using Eq. (1).

Due to the uniqueness theorem, such possible reduction of the integral appearing in the Huygens Fresnel principle is expected in the case of a perfectly conducting metallic screen. Indeed, following this uniqueness theorem, the field in the diffracted space must depend only on the tangential electric field on the screen and aperture surface. Because the tangential electric field vanishes on the screen, the integral must depend only on the tangential field at the opening. Numerous authors, especially Stratton and Chu[15] as well as Schelkunoff,[27,28] have discussed a vectorial integral equation satisfying Maxwell's equations automatically. We can effectively write

$$\vec{E}(\vec{x}) = \int_S [ik(\vec{n}'\times\vec{B})G + (\vec{n}'\times\vec{E})\times\vec{\nabla}'G + (\vec{n}'\cdot\vec{E})\vec{\nabla}'G]\mathrm{d}S', \tag{3}$$

hereafter referred to as the Stratton-Chu equation. A similar expression holds for the magnetic field by means of the substitution $\vec{E}\to\vec{B}$ and $\vec{B}\to-\vec{E}$.

It is important to note that Eq. (3) is over-determined although it depends explicitly on the tangential and normal components of the electromagnetic field defined on S. Indeed, due to the equivalence principle of Love and Schelkunoff[24,27,29] and to the uniqueness theorem, we expect that the "most adapted" integral equations depend only on $\vec{n}'\times\vec{E}$ *or* $\vec{n}'\times\vec{B}$ on S. In addition, unlike in the scalar case, we cannot directly reduce the surface integral to the region of the aperture just by choosing an adapted Dirichlet or Neumann Green function. It seems then necessary to apply once again the shadow approximation of Kirchhoff in order to simplify the integration despite the inconsistency of the method. As in the Poincaré theorem, some problems appear here because we need to add a nonphysical contour integral associated with a magnetic line charge in Eq. (3) (or to an electric line charge in the equivalent formula for $\vec{B}$) in order to satisfy Maxwell's equations and to compensate for the arbitrary change imposed to the integration domain.[32] Furthermore, in this Kirchhoff Kottler[26] theory, the introduction of contour integrals induces a logarithmic divergence of the energy at the rim of the aperture, a fact which is forbidden in a diffraction problem.

The particular case of the diffraction by an aperture in a planar screen constitutes an exception in the sense that a rigorous integral equation had been anticipated by Schelkunoff[27] and Bethe[8] for a subwavelength circular aperture and generalized by Smythe[11,12] for any kind of aperture. The integral equation is

$$\vec{E}(\vec{x}) = \frac{1}{2\pi}\vec{\nabla} \times \left(\int_{\text{Aperture}} (\hat{z} \times \vec{E}) \frac{e^{ikR}}{R} \mathrm{d}S' \right). \tag{4}$$

For some applications, it is important to note that in the short wavelength limit ($\lambda \ll$ aperture typical radius) for which the electromagnetic field in the aperture can be identified with the incident plane wave $\vec{B}_i = \hat{z} \times \vec{E}_i$ (first Kirchhoff approximation), the formula of Stratton Chu limited to the aperture domain and the exact solution of Smythe give approximately the same result. Indeed, within the Fraunhofer approximation, Eq. (4) reads

$$\vec{E} \simeq \frac{ike^{ikr}}{r} \hat{r} \times \int_{\text{Aperture}} \left[\frac{\hat{z} \times \vec{E}_i}{2\pi} e^{-ik\hat{\mathbf{r}} \cdot \vec{x}'} \right] \mathrm{d}S', \tag{5}$$

whereas Eq. (3) reduces to

$$\vec{E} \simeq \frac{ike^{ikr}}{r} \frac{\hat{r} + \hat{z}}{2} \times \int_{\text{Aperture}} \left[\frac{\hat{z} \times \vec{E}_i}{2\pi} e^{-ik\hat{\mathbf{r}} \cdot \vec{x}'} \right] \mathrm{d}S'. \tag{6}$$

Both equations are identical in the practical limit of small diffraction angles, i.e., close to the normal axis z going through the aperture. Equation (5) is correct for a subwavelength aperture only because we cannot identify the field in the aperture with the incident one. We can see that the asymptotic diffracted field for $z > 0$ is equivalent to the one produced by an effective magnetic dipole

$$\vec{M}_{\text{eff}} = \int_{\text{Aperture}} \left[\frac{\vec{n}' \times \vec{E}}{2\pi i k} \right] \mathrm{d}S', \tag{7}$$

and by an effective electric dipole

$$\vec{P}_{\text{eff}} = \frac{\hat{z}}{4\pi} \int_{\text{Aperture}} (\vec{x}' \cdot \vec{E}) \mathrm{d}S'. \tag{8}$$

These formula are fundamental in the context of NSOM because they give us the Bethe Bouwkamp[8–10,16] dipoles which, in the particular case of a circular aperture of radius a, are

$$\vec{P}_{\text{eff}} = \frac{a^3}{3\pi} \vec{E}_{\perp}^{(0)}, \quad \vec{M}_{\text{eff}} = -\frac{2a^3}{3\pi} \vec{B}_{\parallel}^{(0)}. \tag{9}$$

$\vec{E}_{\perp}^{(0)}$ and $\vec{B}_{\parallel}^{(0)}$ are, respectively, the locally uniform normal electric field and tangential magnetic field existing in the aperture zone in the absence of the opening (in $z = 0^-$).

III. GREEN DYADIC JUSTIFICATION OF THE SMYTHE FORMULA

The so-called Smythe formula Eq. (4) is generally obtained on the basis of different principles such as the Babinet principle or the equivalence theorem (see Schelkunoff,[27] Bouwkamp,[30] Jackson[17]). In particular, the equivalence theorem shows that the solution of Smythe for $z > 0$ is identical to the one obtained by considering a virtual surface magnetic-current density given by $\vec{J}_s^m = -c\hat{z} \times \vec{E}/(2\pi)$. All these derivations are self consistent if we consider the very fact that the guessed results fulfill Maxwell equations. Then, the uniqueness theorem ensures that the result is the only one possible. Nevertheless, as already noted, the calculation is not direct and not necessarily connected to the Stratton and Chu formalism. A classical calculation due to Schwinger and Levine[19,20] shows, however, that it is possible to rigourously and directly obtain this equation using the tensorial, or dyadic, Green function formalism. Such an electric dyadic Green function[31] $\overleftrightarrow{G}$, which is solution of the equation

$$\vec{\nabla}\times\left(\vec{\nabla}\times\overleftrightarrow{G}_e(\vec{r},\vec{r}')\right)=k^2\overleftrightarrow{G}_e(\vec{r},\vec{r}')+\overleftrightarrow{\delta}\delta^3(\vec{r}-\vec{r}') \tag{10}$$

(with $\overleftrightarrow{\delta}=\Sigma_i\hat{x}_i\hat{x}_i$) satisfying the condition $\vec{\nabla}\cdot\overleftrightarrow{G}_e=-(1/k^2)\vec{\nabla}\delta^3(\vec{r}-\vec{r}')$, can be used to write the integral equation

$$\vec{E}(\vec{r})=\int_S[\left(\vec{n}'\times\vec{E}\right)\cdot\vec{\nabla}'\times\overleftrightarrow{G}-ik\vec{B}\cdot\left(\vec{n}'\times\overleftrightarrow{G}_e\right)]dS' \tag{11}$$

which is defined on the same surface as previously. By imposing the dyadic Dirichlet condition $\vec{n}'\times\overleftrightarrow{G}_e=0$ on S, we can obtain the relation

$$\vec{E}(\vec{r})=\int_{\text{Aperture}}[(\vec{n}'\times\vec{E})\cdot\vec{\nabla}'\times\overleftrightarrow{G}_e]\text{d}S' \tag{12}$$

which depends only on the tangential electric field at the aperture. This is in perfect agreement with the equivalence principle and the uniqueness theorem.

Following Ref. 31, the total Green function $\overleftrightarrow{G}_e$ for the plane can be deduced from the "free" dyadic

$$\overleftrightarrow{G}_e^0(\vec{r},\vec{r}')=\left(\overleftrightarrow{\delta}+\frac{1}{k^2}\vec{\nabla}\vec{\nabla}\right)\frac{e^{ikR}}{4\pi R} \tag{13}$$

[with $R=\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}$] by using the image method. We have

$$\overleftrightarrow{G}_e(\vec{r},\vec{r}')=\left(\overleftrightarrow{\delta}-\frac{1}{k^2}\vec{\nabla}\vec{\nabla}'\right)G_D(\vec{r},\vec{r}')+2\hat{z}\hat{z}\frac{e^{ikR'}}{4\pi R'}, \tag{14}$$

where $G_D=(e^{ikR}/R-e^{ikR'}/R')/4\pi$ is the scalar Dirichlet Green function for the plane screen, and $R'=\sqrt{(x-x')^2+(y-y')^2+(z+z')^2}$. Inserting this Green function into Eq. (12) gives us directly Eq. (4). It is interesting to observe that with the Green dyadic method, we can recover the formula of Smythe by using a magnetic current distribution located in front of a metallic plane or, equivalently, by using a double layer of magnetic currents propagating in the same direction.[13]

In theory, both approaches based either on the scalar Green functions or on the dyadic Green functions are equivalent. In practice however, the difficulties related to the Stratton Chu formula Eq. (3) have imposed the Green dyadic method. An illustration of this statement is that the dyadic formalism has been extensively used in the context of the electromagnetic theory of NSOM.[33–36]

IV. VECTORIAL JUSTIFICATION OF THE SMYTHE FORMULA

We propose now a justification of Eq. (4) based on the Stratton Chu formula Eq. (3). This derivation will directly reveal the equivalence of the scalar and dyadic approaches in the particular case of a planar screen with an aperture. Let the surface S of equation $z=0$ be an infinite, perfectly conducting metallic screen containing an aperture covering the surface δS. By the definition of diffraction, we can always separate the total electric (magnetic) field $\vec{E}$ ($\vec{E}$) into an incident field $\vec{E}^i$ ($\vec{B}^i$) existing independently of the presence of the screen, and into a diffracted field $\vec{E}'$ ($\vec{B}'$) produced by the surface charge and current densities $\rho_s',\vec{J}_s'$ located on the metal.

We have $\vec{B}'=\vec{\nabla}\times\vec{A}'$ and $\vec{E}'=-\vec{\nabla}\Phi'+ik\vec{A}'$ where potentials are expressed in a Lorentz gauge

$$\vec{A}'(\vec{r})=\int_{\text{Screen}}\text{d}S'\left[\frac{\vec{J}_s'}{c}(\vec{r}')\frac{e^{iKR}}{R}\right], \tag{15}$$

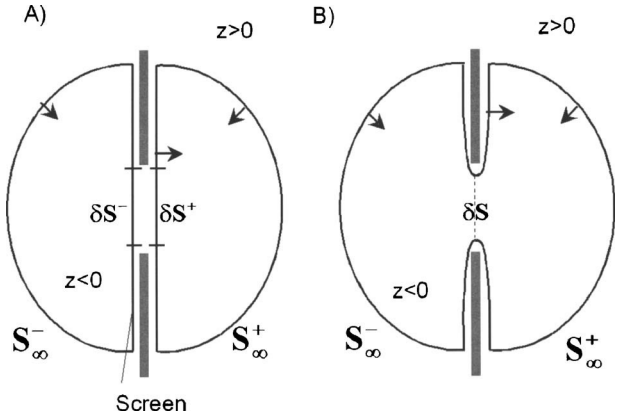

FIG. 2. The two surfaces of integration for the application of the vectorial Kirchhoff theorem.

$$\Phi'(\vec{r}) = \int_{\text{Screen}} dS' \left[\rho_s'(\vec{r}') \frac{e^{iKR}}{R} \right],$$

with $R = \|\vec{r} - \vec{r}'\|$ (we omit here the time dependent factor $e^{-i\omega t}$). Because these potentials are even functions of z we then have the following symmetries:

$$\begin{aligned} &E_x',\ E_y',\ B_z' \text{ are even in } z, \\ &E_z',\ B_x',\ B_y' \text{ are odd in } z. \end{aligned} \tag{16}$$

These symmetries already used by Jackson[16,17] imply in particular $E_z' = B_y' = B_x' = 0$ at the aperture. Therefore, the field is a discontinuous function through the metal.

Let us now consider an observation point **x** located in the half-space $z > 0$. We can apply the vectorial Green theorem on a closed integration surface made up of a half-sphere S_∞^+ "at infinity" and of the S^+ plane ($z = 0^+$) as seen in Fig. 2(A). This surface S^+ can itself be decomposed into an aperture region δS^+ and into a screen region $(S - \delta S)^+$.

We have then

$$\begin{aligned} \vec{E}'(\vec{x}) = &\int_{(S-\delta S)^+} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G] dS' + \int_{\delta S^+} [(\vec{n}' \times \vec{E}') \\ &\times \vec{\nabla}' G] dS' + \int_{S_\infty^+} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G] dS', \end{aligned} \tag{17}$$

where the unit vector $\vec{n}'$ lies on S^+ and is oriented in the positive z direction: $\vec{n}' = \hat{z}$. Similarly we can consider the surface of integration represented in Fig. 2(B). We obtain an integration on the S_∞^+, S_∞^- surfaces and on $(S - \delta S)^+$ and $(S - \delta S)^-$ surfaces. Such integration surfaces have already been used by Schwinger and Levine in the context of diffraction by a scalar wave.[18] Here, due to the symmetries given by Eq. (16), we deduce

$$\begin{aligned} \vec{E}'(\vec{x}) = 2&\int_{(S-\delta S)^+} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G] dS' + \int_{S_\infty^-} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G \\ &+ (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G] dS' + \int_{S_\infty^+} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G] dS' \end{aligned} \tag{18}$$

with $\vec{n}' = \hat{z}$ on the $(S - \delta S)^+$ surface. After identification of Eq. (17) and (18), we obtain

$$\vec{E}'(\vec{x}) = 2\int_{S^+} [(\vec{n}' \times \vec{E}') \times \vec{\nabla}' G]\mathrm{d}S' - \int_{S_\infty^-} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G]\mathrm{d}S'$$

$$+ \int_{S_\infty^+} [ik(\vec{n}' \times \vec{B}')G + (\vec{n}' \times \vec{E}') \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}')\vec{\nabla}' G]\mathrm{d}S'. \tag{19}$$

In order to simplify this formula, it is important to note that the fields $\vec{E}'$, $\vec{B}'$ located on $S_\infty^\pm$ are the reflected fields $\vec{E}^r$, $\vec{B}^r$ which could be produced by the complete metallic screen $z=0$ submitted to the same incident field in the absence of the aperture.

Because this field compensates for the incident field for $z>0$, we have $\vec{E}^r=-\vec{E}^i$, $\vec{B}^r=-\vec{B}^i$ in this half-space. As a consequence, the integral on S_∞^+ in Eq. (19) can be written $-\vec{E}^i(\vec{x})$ $+\int_{S^+}[ik(\vec{n}' \times \vec{B}^i)G + (\vec{n}' \times \vec{E}^i) \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}^i)\vec{\nabla}' G]\mathrm{d}S'$, which is a direct application of the Green theorem for an observation point located on the closed surface composed of S_∞^+ and S^+.

Injecting this last result into Eq. (19) and after subtracting and adding $2\int_{S^+}[(\vec{n}' \times \vec{E}^i)$ $\times \vec{\nabla}' G]\mathrm{d}S'$, we finally obtain $\vec{E}'=\vec{E}^{(1)}+\vec{E}^{(2)}$ where

$$\vec{E}^{(1)}(\vec{x}) = 2\int_{S^+} [(\vec{n}' \times \vec{E}) \times \vec{\nabla}' G]\mathrm{d}S' - \vec{E}^i(\vec{x})\mathrm{d}S' \tag{20}$$

and

$$\vec{E}^{(2)}(\vec{x}) = -\int_{S_\infty^-} [ik(\vec{n}' \times \vec{B}^r)G + (\vec{n}' \times \vec{E}^r) \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}^r)\vec{\nabla}' G]\mathrm{d}S'$$

$$+ \int_{S^+} [ik(\vec{n}' \times \vec{B}^i)G - (\vec{n}' \times \vec{E}^i) \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}^i)\vec{\nabla}' G]\mathrm{d}S'. \tag{21}$$

Because of Eq. (16), we also have

$$E^r_{x,y}(x,y,z) = -E^i_{x,y}(x,y,-z),$$

$$B^r_z(x,y,z) = -B^i_z(x,y,-z),$$

and

$$\begin{aligned} B^r_{x,y}(x,y,z) &= B^i_{x,y}(x,y,-z), \\ E^r_z(x,y,z) &= E^i_z(x,y,-z) \end{aligned} \tag{22}$$

for $z<0$. Using the fact that the integral on S^+ can be written as an integral on S^-: $\int_{S^+}\{\vec{E}^i,\vec{B}^i\}$ $=-\int_{S^-}\{\vec{E}^i,\vec{B}^i\}$, and using Eq. (22), the last two integrals in Eq. (21) can be transformed into $\int_{S^-+S_\infty^-}[ik(\vec{n}' \times \vec{B}^r)G + (\vec{n}' \times \vec{E}^r) \times \vec{\nabla}' G + (\vec{n}' \cdot \vec{E}^r)\vec{\nabla}' G]\mathrm{d}S'$. Because the observation point is outside of the closed surface composed of S_∞^- and of S^-, $\vec{E}^{(2)}(\vec{x})$ is zero. Regrouping all terms, the total electric field in the half-plane $z>0$ is finally given by the Smythe formula

$$\vec{E}(\vec{x}) = 2\int_{\delta S^+} [(\vec{n}' \times \vec{E}) \times \vec{\nabla}' G]\mathrm{d}S' = \frac{1}{2\pi}\vec{\nabla} \times \left(\int_{\text{Aperture}} (\hat{z} \times \vec{E})\frac{e^{ikR}}{R}\mathrm{d}S' \right), \tag{23}$$

where we have applied Maxwell's boundary conditions that annihilate the tangential component of the total electric field on a perfect metal. An equivalent derivation in the $z<0$ half-space gives

$$\vec{E}(\vec{x}) = \vec{E}^0(\vec{x}) + 2\int_{\delta S^-} [(\vec{n}' \times \vec{E}) \times \vec{\nabla}' G] \mathrm{d}S' = \vec{E}^0(\vec{x}) - \frac{1}{2\pi}\vec{\nabla} \times \left(\int_{\text{Aperture}} (\hat{z} \times \vec{\nabla}) \frac{e^{ikR}}{R} \mathrm{d}S' \right), \tag{24}$$

where $\vec{E}^0 = \vec{E}^i + \vec{E}^r$ is now the total electric field existing in the $z<0$ domain for the problem without aperture.

V. CONSISTENCY BETWEEN VARIOUS APPROACHES

As written in the introduction, the proof given by Jackson[16] of the Smythe equation is connected to the theory of vectorial diffraction Eq. (3). In order to solve the problem, Jackson used a volume looking like a flat pancake limited by the two S^+ and S^- surfaces, and he applied Eq. (3) to this boundary. Then, in agreement with Smythe, Jackson imagined a double current sheet such that the surface current on the two S^+ and S^- layers at any point of a given area fitting the aperture are equal and opposite. With such a distribution, it is possible to reduce the integral of Eq. (3) to the one given by the formula of Smythe, Eq. (23). Such a formula is then the correct one to describe the diffraction problem by an aperture in agreement with the uniqueness theorem.

Our justification of the Smythe theorem is more direct because it uses only the Huygens Fresnel theorem without applying the intuitive trick of a virtual surface current distribution associated with a different physical situation (double layer of electric current, or layer of magnetic current confined to the aperture zone). Our result is in fact the direct generalization of a method used by the authors for a scalar wave ψ. Using two different surface integrations, as the ones used in this paper, we are indeed able to prove directly the Rayleigh-Sommerfeld theorem given by Eq. (2). This scalar reasoning, which is similar to the one presented before, is given in the Appendix. It can be observed that the scalar result makes only use of the Green function in vacuum G in order to justify the result obtained with the Dirichlet one G_D. Similarly, our derivation of the Smythe formula uses the scalar Green function in order to justify the result obtained with the "Dirichlet" dyadic Green function. Then, the two reasonings presented in this paper for an electromagnetic and a scalar wave show the primacy of the Huygens-Fresnel theorem given by Eq. (1) for the scalar wave and by Eq. (3) for the electromagnetic field, respectively.

A few further remarks here are relevant: First, the mathematical results described here constitute a justification of the physical "trick" introduced by Smythe and Jackson. However more work must be done in order to see if the method based on scalar Green functions could be extended to other geometries. Second, the Smythe formula allows one to express the electromagnetic field radiated by the aperture (far-field) as a function of the near-field existing in the aperture plane. This method could thus be useful for calculating the field generated by a NSOM aperture if we know the optical near-field (computed, for example, by using numerical methods discussed in Refs. 33–36).

VI. CONCLUSION

In this paper, we have justified the vectorial formula of Smythe expressing the diffracted field produced by an opening created in a perfectly metallic screen. Our justification is based only on the Huygens principle for electromagnetic wave and on the specifical nature of boundary conditions for the Maxwell field. This proof differs from the ones presented in the literature because it does not use the concept of current sheets introduced by Smythe and Jackson. The demonstration uses only the scalar Green function in free space and does not consider Dirichlet or Neumann boundary conditions as involved in the Green dyadic method.

APPENDIX

Let $\Psi(\vec{r})$ be a scalar wave solution of the Helmoltz equation for the problem of diffraction by an opening δS in a plane screen S. In order to define completely the problem, we must impose boundary conditions on the screen surface. Here, we choose $\Psi(\vec{r})|_{S-\delta S}=0$ for any point on the

screen (Dirichlet problem). The Neumann problem can be treated in a similar way. For such a problem, we can in principle always divide the field into an incident one, called $\Psi_{\text{inc}}(\vec{r})$ and existing independently of any screen, and into a scattered field $\Psi'(\vec{r})$, produced by sources in the screen. The problem cannot be solved without postulating some properties of the sources. A way to do this is to introduce a source term $J(\vec{r})$ in the second member of the Helmoltz equation such that this term goes to zero rapidly outside of the pancake volume occupied by the screen. Then, we have $[\nabla^2+k^2]\Psi(\vec{r})=-J(\vec{r})$. Imposing Sommerfeld's radiation condition at infinity gives us the solution

$$\Psi'(\vec{r}) = \int_{\text{pancake}} J(\vec{r}')G(\vec{r},\vec{r}')d^3\vec{r}'. \tag{A1}$$

We deduce the important fact that this potential $\Psi'(\vec{r})$ must be an even function of z. This is consistent with the Kirchhoff formula applied on the surface of Fig. 1(B). Imposing the condition $\Psi'(x,y,z)=\Psi'(x,y,-z)$ implies

$$\Psi(\vec{r}) = -\int_{(S-\delta S)} G(\vec{r},\vec{r}')\hat{z}\cdot\vec{\nabla}'\Psi'(\vec{r}')\mathrm{d}S' \tag{A2}$$

which defines the source term $J_S(x,y)$ (surface density) by $J_S(x,y)=-\lim_{z\to 0^+}\hat{z}\cdot\vec{\nabla}\Psi'(x,y,z)$. It is worth noting that the even character of Ψ' and the field continuity in the aperture impose $\hat{z}\cdot\vec{\nabla}\Psi'(x,y,z=0)$ in the opening. In order to complete the problem, we must define the reflected field $\Psi^r(\vec{r})$ produced by the sources when the plane screen contains no aperture. Since for $z>0$ there is no field, we must choose $\Psi^r(x,y,z)=-\Psi^i(x,y,z)$ in this half-plane. The requirement that the source field is an even function of z imposes $\Psi^r(x,y,z)=-\Psi^i(x,y,-z)$ for $z<0$. In this form, the problem is similar to the one described by Bouwkamp[10] and it can be solved. The rest of the reasoning is similar to the one given for the Smythe formula. Identifying the Kirchhoff integral on the two different surfaces represented in Figs. 2(A) and 2(B), we obtain

$$\Psi'(\vec{r}) = 2\int_{S^+}\Psi'(\vec{r}')\hat{z}\cdot\vec{\nabla}'G(\vec{r},\vec{r}')\mathrm{d}S' + \left(\int_{S_\infty^+} - \int_{S_\infty^-}\right)[\Psi'(\vec{r}')\vec{n}'\cdot\vec{\nabla}'G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\vec{n}'\cdot\vec{\nabla}'\Psi'(\vec{r}')]\mathrm{d}S'. \tag{A3}$$

As for the Smythe formula, we can use the symmetry properties of the field as well as its asymptotic behavior at infinity to transform Eq. (A3) into

$$\Psi(\vec{r}) = 2\int_{\delta S^+}\Psi(\vec{r}')\hat{z}\cdot\vec{\nabla}'G(\vec{r},\vec{r}')\mathrm{d}S' \tag{A4}$$

which is equivalent to the Rayleigh-Sommerfeld result given by Eq. (2).

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Explicit actions for electromagnetism with two gauge fields with only one electric and one magnetic physical field

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We extend the work of Mello *et al.* based on Cabbibo and Ferrari concerning the description of electromagnetism with two gauge fields from a variational principle, i.e., an action. We provide a systematic independent derivation of the allowed actions that have only one magnetic and one electric physical field and are invariant under the discrete symmetries P and T. We conclude that neither the Lagrangian, nor the Hamiltonian, are invariant under the electromagnetic duality rotations. This agrees with the weak-strong coupling mixing characteristic of the duality due to the Dirac quantization condition providing a natural way to differentiate dual theories related by the duality rotations (the energy is not invariant). Also, the standard electromagnetic duality rotations considered in this work violate both P and T by inducing Hopf terms (theta terms) for each sector and a mixed Maxwell term. The canonical structure of the theory is briefly addressed and the magnetic gauge sector is interpreted as a ghost sector. © *2006 American Institute of Physics.*
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I. INTRODUCTION AND DISCUSSION OF RESULTS

The seminal works of Dirac[1] introduced the famous charge quantization relation $eg=n$ that is obtained in the presence of both electric and magnetic poles (charges). The existence of both electric and magnetic charges raised the problem of a variational description of electromagnetism from an action that could actually contain explicitly both types of charges. Also, it is widely accepted that in order to achieve that goal one must consider a description in terms of gauge fields that minimally couple to both currents, so necessarily we need to consider the existence of two distinct gauge fields: A that couples to ordinary electric currents and C that couples to the magnetic current.[2–6] One possible approach first considered by Cabbibo and Ferrari[2] is to consider two physical gauge fields A and C. Although this approach preserves both time-space isotropy and Lorentz invariance has the drawback of the inexistence of experimental observable effects of the second gauge field. Another approach has been to consider mechanisms that, starting from a theory with two gauge fields, give us only one physical gauge field, either by considering solutions (constraints) for the second gauge field[3–6] (this approach has the drawback of not preserving space isotropy or not preserving Lorentz invariance) or by considering a very massive second gauge field.[7] Yet another very simple approach is to consider electromagnetism as an effective theory of an extended theory with two gauge fields such that one gauge field is fixed by the second gauge field obeying the equations of motion.[8] In Mello *et al.*,[9] for the first time an explicit action is built for electromagnetism with two gauge fields based on the work of Cabbibo and Ferrari.[2] In here we build a similar lower order action with two gauge fields A and C of the gauge group $U(1)\times U(1)$. In order to accomplish it, we take an independent approach of the original work[9] by studying in detail and systematically the desired properties of such an action. First, we note that

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due to the different nature of A and C under the discrete symmetries of parity P and time inversion T,[10,11] standard electromagnetic duality[10,12] violates P and T symmetries. So it is desirable that under an electromagnetic duality transformation our action gains terms that explicitly violate these symmetries. This argument is not completely closed once there are ways of implementing duality rotations that preserve P and T symmetries.[13,14] Second, we demand that there is only one electric and one magnetic physical field. Implicitly this assumption means that the group charge flux of each of the $U(1)$'s is of the same nature of the topological flux of the other $U(1)$ group. The action suggested coincides (up to a sign choice) with the one of Ref. 9 and consists of two Maxwell terms with an opposite relative sign, one for each of the gauge fields and a topological cross Hopf term that mixes both gauge sectors allowing for the desired characteristics,

$$S^{\hat{\epsilon}}_{\mathrm{Max}\_} = -\int_M \left[\frac{\sqrt{-g}}{4e^2} F_{\mu\nu}F^{\mu\nu} - \frac{\sqrt{-g}}{4g^2} G_{\mu\nu}G^{\mu\nu} - \frac{\hat{\epsilon}}{4eg}\epsilon^{\mu\nu\rho\delta}F_{\mu\nu}G_{\rho\delta} + \frac{1}{e}(A_\mu - \hat{\epsilon}\tilde{C}_\mu)J^\mu_e - \frac{1}{g}(\hat{\epsilon}C_\mu + \tilde{A}_\mu)J^\mu_g \right],$$

with $\hat{\epsilon} = \pm 1$ corresponding to the two physical fields,

$$E^i = \frac{1}{e}F^{0i} - \frac{\hat{\epsilon}}{2g}\epsilon^{0ijk}G_{jk},$$

$$B^i = \frac{\hat{\epsilon}}{g}G^{0i} + \frac{1}{2e}\epsilon^{0ijk}F_{jk}.$$

However, the Maxwell terms of each of the gauge sectors have an opposite sign; this has no consequences at the classical level, but at the quantum level allows negative energy solutions that clearly violate causality. There are two approaches to overcome this problem. We can consider the C field to be a ghost; this means that upon quantization it has the opposite spin-statistics relations than the one of standard fields and therefore it has anticommutation relations,[15] such kinds of theories both with a matter and a ghost sector were introduced in cosmology by Linde.[16] Alternatively, we can consider some mechanism that allows for a classical treatment of the C field, as examples we have in cosmology the Phantom matter models,[17] and a dynamical symmetry breaking mechanism[8] that allows an effective electric description of the theory. Also compatible with this last mechanism, we can give a vacuum-expectation value to the C field that renders an effective Proca mass to the standard photon, the A field.[18,19]

II. ELECTROMAGNETIC DUALITY

The study of theories with two gauge fields were first considered by Cabbibo and Ferrari.[2] More recently, several studies addressed electromagnetic duality with two gauge fields, namely in Ref. 11 an explicit electromagnetic duality in terms of the gauge fields is presented. Here we review these results.

A. The original duality

The generalized Maxwell equations with both Electric and Magnetic currents[10] read as

$$\boldsymbol{\nabla}\cdot\mathbf{E} = \rho_e,$$

$$\boldsymbol{\nabla}\cdot\mathbf{B} = \rho_g,$$

$$\dot{\mathbf{B}} + \boldsymbol{\nabla}\times\mathbf{E} = -\mathbf{J}_g,$$

$$\dot{\mathbf{E}} - \boldsymbol{\nabla} \times \mathbf{B} = -\mathbf{J}_e. \tag{1}$$

This equation obeys the well known electromagnetic duality that rotates the electric and magnetic fields and currents,[12]

$$\mathbf{E} \to \cos(\theta)\mathbf{E} + \sin(\theta)\mathbf{B},$$

$$\mathbf{B} \to -\sin(\theta)\mathbf{E} + \cos(\theta)\mathbf{B},$$

$$J_e \to \cos(\theta)J_e + \sin(\theta)J_g,$$

$$J_g \to -\sin(\theta)J_e + \cos(\theta)J_g, \tag{2}$$

where $J=(\rho,\mathbf{J})$ stand for the four-vector current densities.

B. Duality with two gauge fields

In order to build an action for electromagnetism with magnetic monopoles it is necessary to consider two $U(1)$ gauge fields that minimally couple to the external electric and magnetic current densities. By introducing gauge fields one is led to the question whether the above duality can be extended to a duality of gauge fields instead of the electric and magnetic fields (i.e., the gauge field connections). By considering that both gauge fields have true physical degrees of freedom it is possible to elevate the duality to a transformation of those gauge fields, as has been shown in Ref. 11. In Ref. 11 the electric and magnetic fields are defined as

$$E^i = \frac{1}{2e}F^{0i} - \frac{1}{4g}\epsilon^{ijk}G_{jk},$$

$$B^i = \frac{1}{2g}G^{0i} + \frac{1}{4e}\epsilon^{ijk}F_{jk}, \tag{3}$$

where $F=dA$ and $G=dC$ are the gauge connections of the gauge fields A and C. In Sec. III B we will properly discuss the physical field definitions; for the time being we use these definitions, which can be found in the literature. The electromagnetic duality reads now as

$$\frac{1}{e}F^{0i} - \frac{1}{2g}\epsilon^{ijk}G_{jk} \to \cos(\theta)\left(\frac{1}{e}F^{0i} - \frac{1}{2g}\epsilon^{ijk}G_{jk}\right) + \sin(\theta)\left(\frac{1}{g}G^{0i} + \frac{1}{2e}\epsilon^{ijk}F_{jk}\right),$$

$$\frac{1}{g}G^{0i} + \frac{1}{2e}\epsilon^{ijk}F_{jk} \to -\sin(\theta)\left(\frac{1}{e}F^{0i} - \frac{1}{2g}\epsilon^{ijk}G_{jk}\right) + \cos(\theta)\left(\frac{1}{g}G^{0i} + \frac{1}{2e}\epsilon^{ijk}F_{jk}\right). \tag{4}$$

There are two ways to implement these transformations, either in terms of each of the $U(1)$ gauge sectors independently or mixing both gauge sectors. If we consider each sector independently, we obtain the standard electromagnetic transformations for each of the connections F and G,

$$F^{0i} \to \cos(\theta)F^{0i} + \sin(\theta)\frac{1}{2}\epsilon^{ijk}F_{jk},$$

$$F_{jk} \to \sin(\theta)\frac{1}{2}\epsilon_{ijk}F^{0i} + \cos(\theta)F_{jk},$$

$$G^{0i} \to \cos(\theta) G^{0i} + \sin(\theta) \frac{1}{2} \epsilon^{ijk} G_{jk},$$

$$G_{jk} \to \sin(\theta) \frac{1}{2} \epsilon^{ijk} G^{0i} + \cos(\theta) G_{jk}. \tag{5}$$

These transformations are not compatible with a transformation of the gauge fields because the $(0i)$ components transform differently from the components (ij).

If we consider mixing between both sectors, we can rewrite the electromagnetic duality in terms of the gauge fields or respective connections,[11]

$$F \to \cos(\theta) F + \sin(\theta) \frac{e}{g} G,$$

$$G \to -\sin(\theta) \frac{g}{e} F + \cos(\theta) G,$$

$$A \to \cos(\theta) A + \sin(\theta) \frac{e}{g} C,$$

$$C \to -\sin(\theta) \frac{g}{e} A + \cos(\theta) C. \tag{6}$$

There is a very simple argument to choose the second kind of duality (6) and exclude the possibility of the transformations (5). Let us consider the Lorentz gauge (or Lorentz condition) for both gauge fields $\partial_\mu A^\mu = \partial_\mu C^\mu = 0$ and assume regular gauge fields (meaning without discontinuities) such that the Bianchi identities are obeyed as $\epsilon^{\mu\nu\rho\delta} \partial_\nu \partial_\rho A_\delta = \epsilon^{\mu\nu\rho\delta} \partial_\nu \partial_\rho C_\delta = 0$. Then the Maxwell equations (1) read simply[11] as

$$\Delta A^\mu = J_e^\mu,$$

$$\Delta C^\mu = J_g^\mu, \tag{7}$$

where the Laplacian is $\Delta = \partial_\mu \partial^\mu$. Taking into account the duality transformations for the current densities expressed in (2), we conclude straight away that only (6) correctly transform the Maxwell equations for these particular *standard* conditions. Here, particular means that the gauge choice is not unique, we could have some other gauge fixing prescription and generally we can have discontinuities on the gauge fields such that the Bianchi identity is not obeyed everywhere. As an example, there are cases of the Dirac string[1] or equivalently the nontrivial fiber bundle of Wu and Yang.[20] However, regular gauge fields describe most of the physical applications and must therefore be a possible choice. There is, however, a serious problem concerning these equations; the two $U(1)$ gauge fields are completely decoupled and we obtain two different interactions corresponding to each of the gauge fields instead of only one, as in standard electromagnetism. Our main aim in the remainder of this work is how to obtain one only interaction described by two physical gauge fields.

So we have reviewed how to elevate electromagnetic duality of the Maxwell equations in terms of the electric and magnetic fields to a electromagnetic duality in terms of the gauge fields. Next, we will briefly describe how the discrete symmetries act on the several fields and how electromagnetic duality breaks parity and time inversion.

C. Discrete symmetries: *P* and *T* violation

We proceed to resume the known results for parity P and time inversion T for the electromagnetic physical quantities. The remaining discrete symmetry is Charge Conjugation C and plays no role in the following discussion.

Parity (P) stands for the inversion of spatial coordinates and time inversion (T) stands for the inversion of the time coordinate. Under these discrete symmetries the fields and current densities transform as[10]

$$
\begin{aligned}
&P: \quad x^i \to -x^i, \quad T: \quad t \to -t,\\
&E^i \to -E^i, \quad E^i \to +E^i,\\
&B^i \to +B^i, \quad B^i \to -B^i,\\
&\rho_e \to +\rho_e, \quad \rho_e \to +\rho_e,\\
&J_e^i \to -J_e^i, \quad J_e^i \to -J_e^i,\\
&\rho_g \to -\rho_g, \quad \rho_g \to -\rho_g,\\
&J_g^i \to +J_g, \quad J_g^i \to +J_g.
\end{aligned} \tag{8}
$$

Electric and magnetic fields transform differently under P and T being, respectively, vectors and pseudovectors. Accordingly, also the electric and magnetic currents have the same properties.[10] Then necessarily the gauge fields A and C also have to transform accordingly as vectors and pseudovectors.[11] The most straightforward way to show this is by considering an action for electromagnetism such that the electric and magnetic current densities are minimally coupled to the gauge fields A and C, respectively (we will return to this discussion later). Demanding invariance of the action under P and T imposes the gauge field C to transform as a pseudovector. We note that the field definitions (3) agree with these results. Then for the two gauge fields and respective gauge connections we have the discrete transformations

$$
\begin{aligned}
&P: \quad A^0 \to +A^0, \quad T: \quad A^0 \to +A^0,\\
&A^i \to -A^i, \quad A^i \to -A^i,\\
&C^0 \to -C^0, \quad C^0 \to -C^0,\\
&C^i \to +C^i, \quad C^i \to +C^i,\\
&F^{0i} \to -F^{0i}, \quad F^{0i} \to +F^{0i},\\
&F^{ij} \to +F^{ij}, \quad F^{ij} \to -F^{ij},\\
&G^{0i} \to +G^{0i}, \quad G^{0i} \to -G^{0i},\\
&G^{ij} \to -G^{ij}, \quad G^{ij} \to +G^{ij}.
\end{aligned} \tag{9}
$$

We want now to show that neither P nor T are maintained by the standard duality rotations (2) or equivalently (6). Here we consider duality as a global transformation independent of space-time

coordinates such that the angle θ is an exterior parameter to the theory used in the redefinition of the fields. Therefore it does not depend on the space-time coordinates and transform as a scalar with respect to the discrete symmetries P and T.

We can see explicitly that the duality transformations mix vector with pseudovectors such that

$$P: \quad \tilde{\mathbf{E}} = \cos(\theta)\mathbf{E} + \sin(\theta)\mathbf{B} \rightarrow -\cos(\theta)\mathbf{E} + \sin(\theta)\mathbf{B}$$

$$\tilde{\mathbf{B}} = -\sin(\theta)\mathbf{E} + \cos(\theta)\mathbf{B} \rightarrow \sin(\theta)\mathbf{E} + \cos(\theta)\mathbf{B}. \tag{10}$$

Clearly $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{B}}$ are not transformed to $-\tilde{\mathbf{E}}$ and $\tilde{\mathbf{B}}$ under parity, as they should. The same argument follows for T:

$$T: \quad \tilde{\mathbf{E}} = \cos(\theta)\mathbf{E} + \sin(\theta)\mathbf{B} \rightarrow \cos(\theta)\mathbf{E} - \sin(\theta)\mathbf{B},$$

$$\tilde{\mathbf{B}} = -\sin(\theta)\mathbf{E} + \cos(\theta)\mathbf{B} \rightarrow -\sin(\theta)\mathbf{E} - \cos(\theta)\mathbf{B}, \tag{11}$$

and the redefined fields do not transform correctly under T. The current duality transformations (2) behave in the same way.

Charge conjugation C is not a space-time symmetry; it exchanges particles with antiparticles. At the classical level this is simply equivalent to change the sign of the current densities and it is preserved by electromagnetic duality.

So, to summarize, at the level of single fields, the electromagnetic duality preserves C, PT, and CPT while it violates P, T, CP, and CT.

The issue of P and T violation by the existence of dyons with both electric and magnetic charge can be found in Ref. 10. As for P and T, the violation by electromagnetic duality is discussed in Ref. 13. The argument is generic and applicable to the original duality transformations (2) independently of considering a gauge field description of electromagnetism. Also, we point out that upon redefinition of the fields one may as well redefine P and T, but in order to do so one would be changing the space-time interpretation of the discrete symmetries and necessarily redefining the action of the Lorentz group. This could be interpreted then as an extended duality of space-time. An alternative interesting construction is to consider θ to be a pseudoscalar;[13] in this way we manage to obtain a duality that preserves the discrete symmetries. Also, it is possible to gauge the duality by considering $\theta = \theta(x)$ to be an additional gauge parameter[14,21] [in this work the duality rotations constitute one further distinct $U(1)$ group].

Here we are considering θ to be a parameter exterior to the theory that transforms as a scalar, then, although the discrete symmetries violations are not explicit in the equations of motion, at the level of the action (a Lagrangian formulation of the theory) they will be explicit. As we will see in detail electromagnetic duality induces P and T violating terms.

In addition, we will demand that there is only one electric and one magnetic physical gauge fields. This requirement is going to reduce the allowed actions.

III. GAUGE SECTOR

In this section we will build a $U(1) \times U(1)$ gauge action such that the physical electric and magnetic fields are identified with the definitions (3). In order to do so, one expects that the group charge flux of each of the $U(1)$'s is coupled to the topological charge flux of the other $U(1)$. It is also desirable that a classical description of electromagnetism preserves both parity P and time inversion T (see, for instance Ref. 10 for a discussion on this topic). So, we are further demanding our action to be invariant under these discrete symmetries. In addition, and from the discussion on the last section, we expect that under an electromagnetic rotation our action explicitly gains terms that violate P and T. This will be the case.

A. Possible actions

Let us consider all the possible lower order terms that are Lorentz and gauge invariant. First, we list the lower order terms containing the gauge connections F and G that are invariant under P and T,

$$\mathcal{L}_{\text{Maxwell}_{FF}} = -\frac{1}{4e^2}F_{\mu\nu}F^{\mu\nu},$$

$$\mathcal{L}_{\text{Maxwell}_{GG}} = -\frac{1}{4g^2}G_{\mu\nu}G^{\mu\nu},$$

$$\mathcal{L}_{\text{Hopf}_{FG}} = -\frac{1}{4eg}\epsilon^{\mu\nu\rho\delta}F_{\mu\nu}G_{\rho\delta}. \tag{12}$$

The last term is a cross Hopf term (or theta term). To show that it is invariant let us rewrite the expression as $\mathcal{L}_{\text{Hopf}}=2\epsilon^{0ijk}(F_{0i}G_{jk}+G_{0i}F_{jk})$; then we see from (9) that F_{0i} and G_{0i} always transform in the same way as G_{jk} and F_{jk} (respectively) such that $\mathcal{L}_{\text{Hopf}_{FG}}$ is invariant under any of the discrete symmetries P and T.

The remaining possible lower order terms that are Lorentz and gauge invariant are not invariant under P and T. They are the cross Maxwell term and the usual Hopf (or theta) terms for each of the gauge sectors,

$$\mathcal{L}_{\text{Maxwell}_{FG}} = -\frac{1}{4eg}F_{\mu\nu}G^{\mu\nu},$$

$$\mathcal{L}_{\text{Hopf}_{FF}} = -\frac{1}{4e^2}\epsilon^{\mu\nu\rho\delta}F_{\mu\nu}F_{\rho\delta},$$

$$\mathcal{L}_{\text{Hopf}_{GG}} = -\frac{1}{4g^2}\epsilon^{\mu\nu\rho\delta}G_{\mu\nu}G_{\rho\delta}. \tag{13}$$

To show that they are not invariant under P and T, we note that, from Eq. (9), (F_{0i},F_{ij}) and (G_{0i},G_{ij}) transform in the opposite way under P and T such that the cross Maxwell term transforms as $\mathcal{L}_{\text{Maxwell}_{FG}}\rightarrow-\mathcal{L}_{\text{Maxwell}_{FG}}$. Concerning the Hopf terms, we note that F_{0i} and G_{0i} transform in the opposite way than F_{ij} and G_{ij} (respectively) under P and T such that $\mathcal{L}_{\text{Hopf}_{FF}}\rightarrow-\mathcal{L}_{\text{Hopf}_{FF}}$ and $\mathcal{L}_{\text{Hopf}_{GG}}\rightarrow-\mathcal{L}_{\text{Hopf}_{GG}}$. This is a known feature of such terms that have been extensively studied to explain the CP violation, both in Abelian and non-Abelian gauge theories (see, for instance Refs. 15 and 22 and references therein).

We have listed all the possible lower order candidate terms to build our action. We also need to study how these several candidate terms behave under electromagnetic duality:

$$\mathcal{L}_{\text{Maxwell}_{FF}} \rightarrow \cos^2(\theta)\mathcal{L}_{\text{Maxwell}_{FF}} + \sin^2(\theta)\mathcal{L}_{\text{Maxwell}_{GG}} + 2\cos(\theta)\sin(\theta)\mathcal{L}_{\text{Maxwell}_{FG}},$$

$$\mathcal{L}_{\text{Maxwell}_{GG}} \rightarrow \sin^2(\theta)\mathcal{L}_{\text{Maxwell}_{FF}} + \cos^2(\theta)\mathcal{L}_{\text{Maxwell}_{GG}} - 2\cos(\theta)\sin(\theta)\mathcal{L}_{\text{Maxwell}_{FG}},$$

$$\mathcal{L}_{\text{Hopf}_{FG}} \rightarrow \sin\theta\cos\theta(\mathcal{L}_{\text{Hopf}_{GG}} - \mathcal{L}_{\text{Hopf}_{FF}}) + (\cos^2\theta - \sin^2\theta)\mathcal{L}_{\text{Hopf}_{FG}},$$

$$\mathcal{L}_{\text{Maxwell}_{FG}} \rightarrow \sin\theta\cos\theta(\mathcal{L}_{\text{Maxwell}_{GG}} - \mathcal{L}_{\text{Maxwell}_{FF}}) + (\cos^2\theta - \sin^2\theta)\mathcal{L}_{\text{Maxwell}_{FG}},$$

$$\mathcal{L}_{\mathrm{Hopf}_{FF}} \to \cos^2(\theta)\mathcal{L}_{\mathrm{Hopf}_{FF}} + \sin^2(\theta)\mathcal{L}_{\mathrm{Hopf}_{GG}} + 2\cos(\theta)\sin(\theta)\mathcal{L}_{\mathrm{Hopf}_{FG}},$$

$$\mathcal{L}_{\mathrm{Hopf}_{GG}} \to \sin^2(\theta)\mathcal{L}_{\mathrm{Hopf}_{FF}} + \cos^2(\theta)\mathcal{L}_{\mathrm{Hopf}_{GG}} - 2\cos(\theta)\sin(\theta)\mathcal{L}_{\mathrm{Hopf}_{FG}}. \tag{14}$$

We are now ready to build an action that describes an electromagnetism with two gauge fields. Demanding the action to be P and T invariant, we are left only with the terms listed in (12). So we conclude that the most standard action that explicitly depends on two gauge fields must be a combination of $\mathcal{L}_{\mathrm{Maxwell}_{FF}}$ and $\mathcal{L}_{\mathrm{Maxwell}_{GG}}$. We will call this action the minimal action,[13,23,24]

$$S_{\mathrm{Min}_+} = -\int_M \sqrt{-g}\left[\frac{1}{4e^2}F_{\mu\nu}F^{\mu\nu} + \frac{1}{4g^2}G_{\mu\nu}G^{\mu\nu}\right], \tag{15}$$

$$S_{\mathrm{Min}_-} = -\int_M \sqrt{-g}\left[\frac{1}{4e^2}F_{\mu\nu}F^{\mu\nu} - \frac{1}{4g^2}G_{\mu\nu}G^{\mu\nu}\right]. \tag{16}$$

We note that from the electric and magnetic fields definition (3) both Maxwell terms must have the same numerical factor (up to the relative sign). The standard would be to consider both with the same sign in order to have the same quantum structure in both sectors, however, for completeness we consider both cases. These actions imply the existence of two electric and two magnetic fields as we will discuss in detail in Sec. III B. Instead, we expect to have only one electric and one magnetic field such that the group charge flux of one $U(1)$ is of the same nature of the flux of the topological charge of the other $U(1)$, as implied by the field definitions (3). As a *weaker* but valid argument, we note that the pure gauge sectors are completely decoupled, *a priori* one would expect that some sort of mixing (meaning coupling) between the two sectors exist that, at least, accomplishes the coupling of topological flux with group charge fluxes. We consider these argument as a drawback of the minimal actions.

From the above arguments we are further considering the remaining allowed term that preserves T and P, the cross Hopf term. We call these actions the maximal actions,

$$S^{\hat{\epsilon}}_{\mathrm{Max}_+} = -\int_M \left[\frac{\sqrt{-g}}{4e^2}F_{\mu\nu}F^{\mu\nu} + \frac{\sqrt{-g}}{4g^2}G_{\mu\nu}G^{\mu\nu} - \frac{\hat{\epsilon}}{4eg}\epsilon^{\mu\nu\rho\delta}F_{\mu\nu}G_{\rho\delta}\right], \tag{17}$$

$$S^{\hat{\epsilon}}_{\mathrm{Max}_-} = -\int_M \left[\frac{\sqrt{-g}}{4e^2}F_{\mu\nu}F^{\mu\nu} - \frac{\sqrt{-g}}{4g^2}G_{\mu\nu}G^{\mu\nu} - \frac{\hat{\epsilon}}{4eg}\epsilon^{\mu\nu\rho\delta}F_{\mu\nu}G_{\rho\delta}\right]. \tag{18}$$

The cross Hopf term couples the flux of the group charges (F^{0i} and G^{0i}) with the flux of the topological charge (G_{ij} and F_{ij}, respectively) of the two different $U(1)$'s. As we are going to show in Sec. III B, the only action that can be defined using only one electric and one magnetic field is $S^{\hat{\epsilon}}_{\mathrm{Max}_-}$, as given by (18). $\hat{\epsilon}=\pm 1$ sets the relative sign of the Hopf term and will be relevant in the definition of the physical fields, as we will show in detail.

We also note that when both Maxwell terms have the same sign the minimal action S_{Min_+}, as given by (15), is invariant under electromagnetic duality, so for an action of this form we have elevated the duality to a symmetry.[14,21] Also, the respective Hamiltonian will be duality invariant. However, this is not necessarily a good feature. As we already pointed out, the standard duality does not preserve either P or T, and this fact is not explicit on the action S_{Min_-}; neither can be on a duality invariant action. This argument is not completely close because one can consider the duality angle parameter θ to be a pseudoscalar.[13] However, another physical argument is that due to the Dirac quantization condition[1] ($eg=n$) we have that the A field obeys a weak coupling regime while the C field obeys a strong coupling regime. Then we expect that the energy (Hamiltonian) not to be conserved under a duality rotation. For these reasons a duality symmetric action does not look like a good choice. The remaining actions, the maximal actions (18) and (17) and

the minimal action (16), are not invariant under duality, but they are P and T invariant. Furthermore, a duality transformation does not preserve P and T invariance, as can explicitly be seen from (14). This is actually a good feature; duality explicitly breaks P and T at the level of the action, as expected from (10) and (11), and the respective Hamiltonians are not invariant under duality.

Finally, as we show in detail in the next subsection, only $S^{\hat{\epsilon}}_{\mathrm{Max\_}}$ is compatible with the existence of only one electric and one magnetic physical field.

B. Physical electric and magnetic fields

Due to the fact that a second gauge field C has been introduced, we now have twice the degrees of freedom than the usual electromagnetism. Accordingly, we expect to have as well a new interaction such that generally we have two *electric fields* and two *magnetic fields*. From a theoretical point of view this is standard; each of the gauge fields carry a different kind of interaction. Nevertheless, we are led to the question of whether both definitions are physical fields or not. Here we will show that for both the minimal actions (15) and (16) and the maximal action (17) we have indeed four physical fields (two electric and two magnetic), while for the maximal action (18) we have only two physical fields (one electric and one magnetic).

Let us consider the generic definitions of electric and magnetic fields corresponding to the gauge fields A and C,

$$E^i_A = \frac{1}{e}F^{0i}, \quad E^i_C = -\frac{1}{2g}\epsilon^{ijk}G_{jk},$$

$$B^i_A = \frac{1}{2e}\epsilon^{ijk}F_{jk}, \quad B^i_C = \frac{1}{g}G^{0i}. \tag{19}$$

We note that the definitions of electric and magnetic fields for C are reversed to the ones of the A field and for reasons that will become clear in the remainder of this section we consider a minus sign in the definition of $\mathbf{E_C}$. Both in order to define the electric and magnetic fields accordingly to (3) and to preserve the properties of the fields in relation to the discrete symmetries, i.e., the electric field is a vector and the magnetic field is a pseudovector. Then we take the following linear combinations of the above definitions (19):

$$E^i_+ = \frac{1}{2}(E^i_A + E^i_C) = +\frac{1}{2e}F^{0i} - \frac{1}{4g}\epsilon^{ijk}G_{jk},$$

$$B^i_+ = \frac{1}{2}(B^i_A + B^i_C) = +\frac{1}{2g}G^{0i} + \frac{1}{4e}\epsilon^{ijk}F_{jk},$$

$$E^i_- = \frac{1}{2}(E^i_A - E^i_C) = +\frac{1}{2e}F^{0i} + \frac{1}{4g}\epsilon^{ijk}G_{jk},$$

$$B^i_- = \frac{1}{2}(B^i_A - B^i_C) = -\frac{1}{2g}G^{0i} + \frac{1}{4e}\epsilon^{ijk}F_{jk}. \tag{20}$$

To consider these combinations is the approach of several authors that consider only $\mathbf{E}_+$ and $\mathbf{B}_+$ as physical fields.[11,23] As already explained in the Introduction, the main motivation is to achieve a generalized description of electromagnetism with both electric and magnetic particles.[2] Also, these combinations are used to implement an explicit electromagnetic duality between the two sectors in terms of two distinct gauge fields, as we explained in Sec. II.

For what follows we will need the identities

$$\frac{1}{2e^2}F^{0i}F_{0i}=\frac{1}{2}(E_+^i+E_-^i)(E_+^i+E_-^i)=\frac{1}{2}(+E_+^iE_+^i+E_-^iE_-^i+2E_+^iE_-^i),$$

$$\frac{1}{4e^2}F^{ij}F_{ij}=-\frac{1}{2}(B_+^i+B_-^i)(B_+^i+B_-^i)=\frac{1}{2}(-B_+^iB_+^i-B_-^iB_-^i-2B_+^iB_-^i),$$

$$\frac{1}{2g^2}G^{0i}G_{0i}=\frac{1}{2}(B_+^i-B_-^i)(B_+^i-B_-^i)=\frac{1}{2}(+B_+^iB_+^i+B_-^iB_-^i-2B_+^iB_-^i),$$

$$\frac{1}{4g^2}G^{ij}G_{ij}=-\frac{1}{2}(-E_+^i+E_-^i)(-E_+^i+E_-^i)=\frac{1}{2}(-E_+^iE_+^i-E_-^iE_-^i+2E_+^iE_-^i),$$

$$\frac{1}{2eg}\epsilon^{0ijk}F_{0i}G_{jk}=(E_+^i+E_-^i)(-E_+^i+E_-^i)=-E_+^iE_+^i+E_-^iE_-^i,$$

$$\frac{1}{2eg}\epsilon^{0ijk}G_{0i}F_{jk}=(B_+^i+B_-^i)(B_+^i-B_-^i)=+B_+^iB_+^i-B_-^iB_-^i, \tag{21}$$

where the minus sign and the factor of 2 in the second and fourth lines are due to the contraction of the indices of the antisymmetric tensor, i.e., $\epsilon^{0jki}\epsilon_{0jk}^{\ \ \ i'}=-2\delta^{ii'}$.

Let us consider both the minimal actions (15) and (16) and the maximal actions (17) and (18) and rewrite the respective Lagrangians in terms of the above combinations (20) using the identities (21). We obtain that

$$\mathcal{L}_{\mathrm{Min}_+}=-2(E_+^iE_-^i-B_+^iB_-^i),$$

$$\mathcal{L}_{\mathrm{Min}_-}=-(E_+^iE_+^i+E_-^iE_-^i-B_+^iB_+^i-B_-^iB_-^i),$$

$$\mathcal{L}^{\hat{\epsilon}}_{\mathrm{Max}_+}=-2(E_+^iE_-^i-B_+^iB_-^i)-\hat{\epsilon}(E_+^iE_+^i-E_-^iE_-^i-B_+^iB_+^i+B_-^iB_-^i),$$

$$\mathcal{L}^{\hat{\epsilon}}_{\mathrm{Max}_-}=-2(E_{\hat{\epsilon}}^iE_{\hat{\epsilon}}^i-B_{\hat{\epsilon}}^iB_{\hat{\epsilon}}^i). \tag{22}$$

Here we use the usual convention in classical electrodynamics;[10] we sum over repeated indices i that are considered always upstairs such that the metric is no longer explicit; because $E^i=-E_i$ we have that $\mathbf{E}^2=-E^iE_i=E^iE^i\geqslant 0$. The indices of the electric and magnetic fields correspond to $\pm$ depending, respectively, on what choice of $\hat{\epsilon}=\pm 1$ is taken.

We readily conclude that the only action that can be written in terms of only two fields ($\mathbf{E}_+$ and $\mathbf{B}_+$ for $\hat{\epsilon}=+1$ or $\mathbf{E}_-$ and $\mathbf{B}_-$ for $\hat{\epsilon}=-1$) is the maximal action (18). This is only possible if the cross Hopf term is present and the two Maxwell terms have opposite signs. We also note that the choice of $\hat{\epsilon}$ is relevant to the physical field definitions.

As a worm up for what follows, we can argue that, after our field redefinition (20), the form of the maximal Lagrangian $\mathcal{L}^{\hat{\epsilon}}_{\mathrm{Max}_-}$, as given in the last line of (22), is essentially the same as the one of standard electromagnetism, therefore we have a very strong indication that, for this Lagrangian, the physical fields are

$$E^i = \frac{1}{e}F^{0i} - \frac{\hat{\epsilon}}{2g}\epsilon^{0ijk}G_{jk},$$

$$B^i = \frac{\hat{\epsilon}}{g}G^{0i} + \frac{1}{2e}\epsilon^{0ijk}F_{jk}. \tag{23}$$

This is only possible for the maximal Lagrangian $\mathcal{L}^{\hat{\epsilon}}_{\mathrm{Max\_}}$.

To show that this is indeed the case, we will formalize this argument and analyze the four possible actions. Let us compute the equations of motion for the actions and check which fields appear in them. We will properly discuss how to couple each type of current density to both the gauge fields in the next section; for the moment being let us assume the standard minimal coupling,

$$S_{\mathrm{Sources,Min}_{\pm}} = -\frac{1}{e}\int A_\mu J_e^\mu \pm \frac{1}{g}\int C_\mu J_g^\mu, \tag{24}$$

where the $\pm$ correspond to the relative sign between the Maxwell terms.

For the minimal actions we have that the equations of motion are

$$\begin{cases} \frac{1}{e}\partial_\mu F^{\mu\nu} = J_e^\mu \\ \frac{1}{g}\partial_\mu G^{\mu\nu} = J_g^\mu \end{cases} \Leftrightarrow \begin{cases} \boldsymbol{\nabla}\cdot\mathbf{E}_A = \rho_e, \\ \boldsymbol{\nabla}\cdot\mathbf{B}_C = \rho_g, \\ \dot{\mathbf{B}}_C + \boldsymbol{\nabla}\times\mathbf{E}_C = -\mathbf{J}_g, \\ \dot{\mathbf{E}}_A - \boldsymbol{\nabla}\times\mathbf{B}_A = -\mathbf{J}_e. \end{cases} \tag{25}$$

The electric and magnetic equations are completely decoupled, and we have two electric and two magnetic fields. Also, in addition to this equation, we have the Bianchi identities for each gauge field. There is a way to couple both sectors by using nonhomogeneous Bianchi identities; for that consider nonregular gauge fields such that we have the respective Bianchi identities $dF = *\tilde{J}_g$ and $dG = *\tilde{J}_e$. Then by an appropriate combination of the equations of motion with the Bianchi identities we obtain $d(*F - G) = *J_e - *\tilde{J}_e$ and $d(F + *G) = *J_g + *\tilde{J}_g$ that correspond to the generalized Maxwell equations (1) with the current densities changed from $J_e \to J_e - \tilde{J}_e$ and $J_g \to J_g + \tilde{J}_g$. Here $*$ denotes the usual Hodge duality operation and we used form notation for compactness. There are two drawbacks for this approach: first the current densities are no longer the ones that minimally couple to the gauge fields at the level of the action and, second, the identification of the topological charge fluxes with the group charge fluxes of different gauge groups is imposed (by hand) not emerging naturally from the action. These problems are solved by using the maximal action with opposite signs for the Maxwell terms as given by (18).

In order to analyze the maximal action (18), we note that the above procedure of the redefinition of fields (20) and rewriting the Lagrangians in terms of the redefined fields (22) is equivalent to rewriting the Lagrangian in terms of the new 2-form *gauge connections*[13]

$$(\mathcal{F}^{\hat{\epsilon}}_{+})^{\mu\nu} = \frac{1}{2}(F + \hat{\epsilon} * G)^{(\mu\nu)} = \frac{1}{2e}F^{\mu\nu} + \frac{\hat{\epsilon}}{4g}\epsilon^{\mu\nu\rho\delta}G_{\rho\delta},$$

$$(\mathcal{F}^{\hat{\epsilon}}_{-})^{\mu\nu} = \frac{1}{2}(F - \hat{\epsilon} * G)^{(\mu\nu)} = \frac{1}{2e}F^{\mu\nu} - \frac{\hat{\epsilon}}{4g}\epsilon^{\mu\nu\rho\delta}G_{\rho\delta}, \tag{26}$$

or their Hodge duals

$$(\mathcal{G}_{+}^{\hat{\epsilon}})^{\mu\nu} = - * (\mathcal{F}_{-}^{\hat{\epsilon}})^{(\mu\nu)} = \frac{\hat{\epsilon}}{2g} G^{\mu\nu} + \frac{1}{4g} \epsilon^{\mu\nu\rho\delta} F_{\rho\delta},$$

$$(\mathcal{G}_{-}^{\hat{\epsilon}})^{\mu\nu} = - * (\mathcal{F}_{+}^{\hat{\epsilon}})^{(\mu\nu)} = \frac{\hat{\epsilon}}{2e} G^{\mu\nu} - \frac{1}{4g} \epsilon^{\mu\nu\rho\delta} F_{\rho\delta}. \tag{27}$$

Then the maximal Lagrangian (18) is rewritten in both equivalent expressions as

$$\mathcal{L}_{\mathrm{Max}_{-}}^{\hat{\epsilon}} = - (\mathcal{F}_{+}^{\hat{\epsilon}})^{\mu\nu} (\mathcal{F}_{+}^{\hat{\epsilon}})_{\mu\nu} = + (\mathcal{G}_{-}^{\hat{\epsilon}})^{\mu\nu} (\mathcal{G}_{-}^{\hat{\epsilon}})_{\mu\nu}, \tag{28}$$

where we used the Hodge duality property $**G=-G$ for 2-forms G in Lorentzian four dimensional (4D) manifolds. This is basically the reason why in (19) we defined $E_C^i = -\epsilon^{ijk} G^{jk}$ with a minus sign.[11,23] We note that these two ways of rewriting are algebraically equivalent. However, physically they have an important meaning, we can have both an electric and a magnetic description of the theory. This is seen in the equations of motion. Upon variation of the maximal action with respect to A and C, we obtain

$$\partial_\mu (\mathcal{F}_{+}^{\hat{\epsilon}})^{\mu\nu} = J_e^\nu,$$

$$\partial_\mu (\mathcal{G}_{-}^{\hat{\epsilon}})^{\mu\nu} = \hat{\epsilon} J_g^\nu, \tag{29}$$

which indeed correspond to the generalized Maxwell equations (1) and are expressed only in terms of the fields **E** and **B**, as given by (23). So these must be the physical fields! This is only possible for the maximal action. As for $\mathcal{L}_{\mathrm{Max}_{+}}^{\hat{\epsilon}}$ corresponding to the action (17), this construction is not possible; we obtain that

$$\mathcal{L}_{\mathrm{Max}_{+}}^{\hat{\epsilon}} = - \frac{1}{2} (\mathcal{F}_{+}^{\hat{\epsilon}})^{\mu\nu} (\mathcal{F}_{+}^{\hat{\epsilon}})_{\mu\nu} + \frac{1}{2} (\mathcal{F}_{-}^{\hat{\epsilon}})^{\mu\nu} (\mathcal{F}_{-}^{\hat{\epsilon}})_{\mu\nu} - (\mathcal{F}_{+}^{\hat{\epsilon}})^{\mu\nu} (\mathcal{F}_{-}^{\hat{\epsilon}})_{\mu\nu} \tag{30}$$

such that we need two distinct *gauge connections* in order to define it, hence, as expected, four physical fields.

One must be careful with the way we couple the source to both gauge fields depending on the choice of $\hat{\epsilon}$ due to the definitions of the physical fields and the current sign in the second line of (29). We will discuss this issue in detail in Sec. IV.

There is a subtlety here. The reader may by now be recalling the Bianchi identities (or homogeneity conditions for Abelian gauge fields) on the gauge connection and claiming that as usual for topological terms, the variation

$$\delta \mathcal{L}_{\mathrm{Hopf}_{FG}} = \frac{1}{2eg} \epsilon^{\mu\nu\delta\rho} (\partial_\nu G_{\delta\rho}\, \delta A_\mu + \partial_\nu F_{\delta\rho}\, \delta C_\mu) \tag{31}$$

should be always null and does not contribute to the equations of motion. This is true for regular fields, however, as already mentioned in the first section and in the analysis of the minimal actions, if nonregular gauge fields are allowed, then this contribution to the equations of motion is not null everywhere and must be taken into account, and (29) are actually the correct ones. By discontinuities we mean that $\partial_\mu \partial_\nu C \neq \partial_\nu \partial_\mu C$. Allowing for corrections to the Bianchi identities allows for the inclusion of magnetic charge in standard electromagnetism [with only one $U(1)$ gauge field] and is in the basis of the original construction that originates the Dirac string[1] or the equivalent nontrivial fiberbundle of Wu and Yang.[20] We present this argument only to show that algebraically (29) are correct, we do not need to *necessarily* have these discontinuities to describe both electric and magnetic charge as long as we work with two distinct gauge fields. However, we show in Ref. 8 that in order to have effective theories obtained from the maximal action only with one gauge field, we still have discontinuities, but the discontinuities will be present on the extra field (instead of the physical field of the effective theory as in Refs. 1 and 20).

An important result here is that for the maximal action the topological fluxes of one $U(1)$ are identified with the charge fluxes of the other $U(1)$ as desired for the existence of only one electric and one magnetic physical field. We must stress that this does not imply that we are constraining the fundamental fields A and C; we are maintaining the same degrees of freedom. We have four physical degrees of freedom (two for each of the gauge fields A and C) that are still maintained in the electric and magnetic fields (again two for each of the fields E and B). In standard electromagnetism with only one gauge field there is only two degrees of freedom. The interpretation in terms of the fields is quite interesting. For each of the $U(1)$ fields the two physical degrees of freedom correspond to the transverse modes while the longitudinal modes are not physical and do not constitute physical degrees of freedom. When combining the gauge connections as in (26) the degrees of freedom of the second gauge field C are combined with the degrees of freedom of the original gauge field A in such a way that they play the role of two Longitudinal modes of the gauge field A; simply, we have now two longitudinal modes instead of a single one, as is usual in theories with massive photons. These degrees of freedom constitute here physical degrees of freedom and are due to the inclusion of a second $U(1)$ gauge group.

Our discussion would not be complete without discussing the canonical variables. We do so next and also discuss briefly the expression for the Hamiltonians corresponding to the minimal and maximal actions.

C. Canonical variables and Hamiltonian formulation

The canonical momenta for the minimal actions (15) and (16) are

$$\pi^i_{A,\mathrm{Min}} = \frac{1}{e^2}F^{0i} = \frac{1}{e}E^i_A,$$

$$\pi^i_{C,\mathrm{Min}_\pm} = \pm\frac{1}{g^2}G^{0i} = \pm\frac{1}{g}B^i_C, \tag{32}$$

where the $\pm$ refers respectively to $\mathcal{L}_{\mathrm{Min}_+}$ (the $+$ sign) and $\mathcal{L}_{\mathrm{Min}_-}$ (the $-$ sign). This means that the canonical momenta are each of the $U(1)$ group charge fluxes. The Hamiltonian depends on both gauge sectors, but each of them are completely decoupled,

$$\mathcal{H}_{\mathrm{Min}_\pm} = \frac{1}{2}\left(e^2\pi^i_{A,\mathrm{Min}}\pi^i_{A,\mathrm{Min}} + \frac{1}{2e^2}F_{ij}F_{ij}\right) \pm \frac{1}{2}\left(g^2\pi^i_{C,\mathrm{Min}_\pm}\pi^i_{C,\mathrm{Min}_\pm} + \frac{1}{2g^2}G_{ij}G_{ij}\right), \tag{33}$$

such that the Hilbert space factorizes into states carrying charge fluxes of both gauge sectors. The topological charge fluxes are present only trough the potential $F_{ij}F_{ij}$ and $G_{ij}G_{ij}$, as in standard electromagnetism. So basically we have two distinct copies of standard electromagnetism and no interaction terms between the two sectors.

The canonical momenta for the maximal action (17) and (18) are

$$(\pi^{\hat{\epsilon}}_{A,\mathrm{Max}_\pm})^i = \frac{1}{e^2}F^{0i} \pm \frac{\epsilon}{2eg}\epsilon^{ijk}G_{jk} = +\frac{2}{e}E^i_{(\pm\hat{\epsilon})},$$

$$(\pi^{\hat{\epsilon}}_{C,\mathrm{Max}_\pm})^i = \pm\frac{1}{g^2}G^{0i} - \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}F_{jk} = -\frac{2\hat{\epsilon}}{g}B^i_\pm, \tag{34}$$

where the $\pm$ refers, respectively, to $\mathcal{L}_{\mathrm{Max}_+}$ (the $+$ sign) and $\mathcal{L}_{\mathrm{Max}_-}$ (the $-$ sign). In the electric field the subscript $(\pm\hat{\epsilon})$ means the product of ± 1 by $\hat{\epsilon}$. The canonical momenta coincide up to constants with the physical electric and magnetic fields, this is a good indication that, indeed, also at the quantum level, we can have the correct identifications between group charge and topological charge fluxes from the opposite $U(1)$'s.

After a straightforward computation, we obtain the following Hamiltonians:

$$\mathcal{H}^{\hat{\epsilon}}_{\mathrm{Max}_+} = +\frac{e^2}{2}\left(\pi^i_{A,\mathrm{Max}_+} + \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}G_{jk}\right)\left(\pi^i_{A,\mathrm{Max}_+} - \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}G_{jk}\right)$$
$$+\frac{g^2}{2}\left(\pi^i_{C,\mathrm{Max}_+} + \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}F_{jk}\right)\left(\pi^i_{C,\mathrm{Max}_+} - \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}F_{jk}\right)$$
$$+\frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}(\pi^i_{A,\mathrm{Max}_+}G_{jk} + \pi^i_{C,\mathrm{Max}_+}F_{jk}) - \frac{3}{4e^2}F_{ij}F_{ij} + \frac{5}{4g^2}G_{ij}G_{ij} \tag{35}$$

and

$$\mathcal{H}^{\hat{\epsilon}}_{\mathrm{Max}_-} = +\frac{e^2}{2}\left(\pi^i_{A,\mathrm{Max}_-} + \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}G_{jk}\right)\left(\pi^i_{A,\mathrm{Max}_-} - \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}G_{jk}\right)$$
$$-\frac{g^2}{2}\left(\pi^i_{C,\mathrm{Max}_-} + \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}F_{jk}\right)\left(\pi^i_{C,\mathrm{Max}_-} - \frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}F_{jk}\right)$$
$$+\frac{\hat{\epsilon}}{2eg}\epsilon^{ijk}(\pi^i_{A,\mathrm{Max}_-}G_{jk} - \pi^i_{C,\mathrm{Max}_-}F_{jk}) + \frac{5}{4e^2}F_{ij}F_{ij} - \frac{5}{4g^2}G_{ij}G_{ij}. \tag{36}$$

The first lines of both these equations are interpreted as usual with $a^i_+a^i_-$, where $a_\pm$ are creation and annihilation operators of electric excitations and the second lines correspond to $b^i_+b^i_-$, where $b_\pm$ are creation and annihilation operators of magnetic excitations. The third lines contain a generalized *angular momenta* term between the two gauge sectors and the potentials $F_{ij}F_{ij}$ and $G_{ij}G_{ij}$. We note that the potential terms have nonstandard factors and opposite signs in both Hamiltonians. In particular, the factors for the potentials in $\mathcal{H}^{\hat{\epsilon}}_{\mathrm{Max}_+}$, as given in (35), have different weights (i.e., besides, the opposite sign has different numerical factors independent of the coupling constants) while they have the same numerical weight for $\mathcal{H}^{\hat{\epsilon}}_{\mathrm{Max}_-}$, as given in (36). This is also a good indication that the Maximal action (18) is the correct one since there is no reason for the potentials $F_{ij}F_{ij}$ and $G_{ij}G_{ij}$ having different numerical weights (beside the coupling constants).

The Hilbert space is not generally factorizable, the states should only be factorizable for states that have null eigenvalues of the generalized angular momenta.

The main problem in quantizing this theory is that the $b^i_+b^i_-$ has the opposite sign (than the standard fields) and, using the usual commutation relations for the C field, makes the existence of negative energy states possible. In order to solve this issue the standard way out is to consider anticommutation relations for the C gauge sector.[15] In this case we are in the presence of a ghost field,[16] not a standard boson. An alternative approach is to consider some mechanism that allows us to quantize only the electric sector, as done in.[26] As such examples we have Phantom matter in cosmology,[17] where such fields are considered at classical level (i.e., we may consider them to be a collective field, meaning a statistical effective field) in inflationary models. Also, we can consider a dynamical symmetry breaking mechanism;[8] a possible application is considered in Refs. 18 and 19 as a way to generate a Proca mass for the usual photon.

We are not discussing any further the quantization procedure here.

IV. INCLUSION OF CURRENT DENSITIES

Here, we analyze in detail the current densities coupling to both the gauge fields for the Maximal action (18) and accordingly derive the Lorentz force with both gauge fields.

A. Current coupling terms

Concerning the inclusion of currents, let us consider the standard action,

$$S^{\hat{\epsilon}}_{\text{Sources,Max\_}} = -\int_M \left[\frac{1}{e}A_\mu J^\mu_e - \frac{\hat{\epsilon}}{g}C_\mu J^\mu_g\right], \tag{37}$$

where $\hat{\epsilon}$ correctly sets the current sign in the generalized Maxwell equations (29). This action is both P and T invariant but it is not invariant under electromagnetic duality rotation. Under a duality rotation we effectively couple each current density with both gauge fields obtaining violating terms.

From the discussion of the last section we concluded that the physical electric and magnetic fields are given by (23). So each of the currents need to couple in some way to both $U(1)$ gauge fields. The question is how to do it maintaining P and T symmetries and having the variation of the action with respect to space-time coordinates holding the Lorentz force defined in terms of the fields (3). We note that (37) is not enough since it holds that we would have two Lorentz forces, one for each $U(1)$ in terms of the decoupled fields as given in (19).

The way out is to consider the dual fields $\tilde{A}$ and $\tilde{C}$ defined in terms of the original gauge fields by the differential equations

$$\begin{cases} \tilde{F} = *F \\ \tilde{G} = *G \end{cases} \Leftrightarrow \begin{cases} d\tilde{A} = *dA \\ d\tilde{C} = *dC \end{cases}, \tag{38}$$

where again $*$ denotes the Hodge duality operation. We note that the dual fields have only longitudinal modes, so by dual we mean that we are exchanging transverse modes in A and C by longitudinal modes in $\tilde{A}$ and $\tilde{C}$. So the extra action for the current densities read as

$$S_{\text{Dual Sources,Max\_}} = +\int_M \left[\frac{\hat{\epsilon}}{g}\tilde{C}_\mu J^\mu_e + \frac{1}{e}\tilde{A}_\mu J^\mu_g\right]. \tag{39}$$

Both terms are P and T invariant because $\tilde{A}$ and $\tilde{C}$ are, respectively, a pseudovector and a vector due to (38). Again, the sign choice is not arbitrary, we already fixed it in order to obtain the correct Lorentz forces. Electromagnetic duality couples both current densities with both gauge fields $\tilde{A}$ and $\tilde{C}$ such that it induces P and T violating terms. For this action we indeed have that the group charges of each $U(1)$ (given by the J's) are coupled to the topological charges of the other $U(1)$ (in terms of $\tilde{A}$ and $\tilde{C}$). This is what is expressed in the definition of the dual fields as given by (38). Also, there are a couple of very important points we must address. These terms do not contribute to the equations of motion of the gauge fields. The reason is that due to (38) we exchange transverse with longitudinal modes in the definitions of $\tilde{A}$ and $\tilde{C}$ and that the current densities only carry transverse modes. Let us be more precise: the variation of a term $\tilde{A}_\mu X^\mu$ reads as

$$\frac{\delta\tilde{A}_\mu}{\delta A_\nu}X^\mu = \left(\frac{\delta\tilde{F}_{\alpha\beta}}{\delta\tilde{A}_\mu}\right)^{-1}\frac{\delta\tilde{F}_{\alpha\beta}}{\delta F_{\delta\rho}}\frac{\delta F_{\delta\rho}}{\delta A_\nu}X^\mu = 8\epsilon_\mu{}^\nu{}_\alpha{}^\beta(\partial_\alpha)^{-1}\,\partial_\beta X^\mu. \tag{40}$$

Now, considering the gauge invariance condition (continuity condition) for current densities $d*J=\partial_\mu J^\mu=0$, we obtain that the currents are given in terms of a regular antisymmetric 2-tensor ϕ (a 2-form) as

$$J^\mu = \epsilon^{\mu\delta\rho\lambda}\,\partial_\delta\phi_{\rho\lambda} + c^\mu, \tag{41}$$

where c_μ is a constant. This same result is already expressed in Refs. 25 and 26. We note that the above expression is obtained from the Hodge decomposition of the current densities $J=d\varphi + *\,d\phi+c$. Then, replacing this expression for $X=J$ in the above action variation (40), we have the

derivatives in μ and δ contracted with the antisymmetric tensor. Therefore we obtain a null variation. We note that although we may generally consider nonregular fields, we cannot consider nonregular current densities; the continuity equation for currents $\partial_\mu J^\mu=0$ is demanded everywhere for gauge invariance, while for the gauge fields F and G are gauge invariant independently of A and C being regular or not (as long as the gauge transformation parameter is regular and well understood). The second point to stress is that for regular gauge fields this term is a total derivative, however, for nonregular gauge fields it is not. So by admitting the existence of nonregular gauge fields, the term is present in the action and cannot be integrated to the boundary.

To clarify we give an explicit example. Let us rewrite the first term of the above expression (39) in terms of ϕ as given in (41) as

$$S_\phi=-\frac{\hat{\epsilon}}{g}\int_M G_{\mu\nu}\phi^{\mu\nu}, \tag{42}$$

being, as usual, $G_{\mu\nu}=\partial_\mu C_\nu-\partial_\nu C_\mu$. One can notice that for regular fields we would integrate by parts, obtaining $S_\phi=-\hat{\epsilon}/g\int_M C_\mu\,\partial_\nu\phi^{\mu\nu}=0$ because $\partial_\nu\phi^{\mu\nu}=0$. However, take as an example of a nonregular gauge field $C_1=H[x_2]$, and all the remaining components null, $C_0=C_2=C_3=0$. Here $H(x)$ is the Heaviside function (also known as a unit step function). Then the above action reads as

$$S_\phi=-\frac{\hat{\epsilon}}{g}\int_M \delta(x_2)\phi^{21}=-\frac{\hat{\epsilon}}{g}\int dt\,dx^1\,dx^3\,dx^4\,\phi^{21}\neq 0. \tag{43}$$

Clearly we are not allowed to integrate by parts for nonregular gauge fields. However, when computing the equations of motion for S_ϕ we obtain upon a functional derivation on C_μ the null contribution for the equations of motion $\partial_\nu\phi^{\mu\nu}=0$, as desired.

As a last remark, we note that adding a current carrying both electric and magnetic charges (corresponding to a dyon) we obtain an explicit P and T violation,

$$S_{\text{Mix Sources}}=-\int_M\left(\frac{1}{e}A_\mu-\frac{1}{g}C_\mu\right)J^\mu_{eg}. \tag{44}$$

This violation is independent of electromagnetic duality by the simple fact that J_{eg} must be a combination both of a vector and a pseudovector. So we are assuming that we have no dyons, meaning particles with both electric and magnetic charge. If they do exist then P and T are not valid symmetries.[10]

In the next subsection we derive the Lorentz force, checking that we actually have the usual expression but with the electric and magnetic fields defined as in (3).

B. Lorentz force and the physical fields

In order to derive the Lorentz force, consider the Lagrangian for a relativistic classical electron with charge $-e$ described by the current density $J^\mu_e=-e(1,\dot{\mathbf{x}})$,

$$\mathcal{L}_{\text{Lorentz-e}}=-m\gamma^{-1}-\left(\frac{1}{e}A_\mu-\frac{\hat{\epsilon}}{g}\tilde{C}_\mu\right)J^\mu_e, \tag{45}$$

where the first term accounts for the rest mass and, as usual, $\gamma^{-1}=\sqrt{1-\dot{x}^2}$. We have set $c=1$. Varying this action with respect to the coordinates x_i is equivalent to the Euler-Lagrange equations, and we obtain after a straightforward computation that

$$\frac{dp^i}{dt}=+e\left[\left(\frac{1}{e}F^{0i}-\frac{\hat{\epsilon}}{g}\tilde{G}^{0i}\right)+\dot{x}_j\left(\frac{1}{e}F^{ij}-\frac{\hat{\epsilon}}{g}\tilde{G}^{ij}\right)\right]=+e[E^i+\epsilon^{ijk}\dot{x}_jB_k], \tag{46}$$

where we used the definition of the dual fields $\tilde{G}$ as given in (38), and E^i and B_i are given by (23).

If instead we consider the Lagrangian for a relativistic classical magnetic monopole with charge $+g$ and current given by $J_g^\mu = +g(1, \dot{\mathbf{x}})$, we obtain

$$\mathcal{L}_{\text{Lorentz-g}} = -m\gamma^{-1} + \left(\frac{\hat{\epsilon}}{g}C_\mu + \frac{1}{e}\tilde{A}_\mu\right)J_g^\mu. \tag{47}$$

Then we obtain

$$\frac{dp^i}{dt} = +g\left[\left(\frac{\hat{\epsilon}}{g}G^{0i} + \frac{\hat{\epsilon}}{g}\tilde{F}^{0i}\right) + \dot{x}_j\left(\frac{\hat{\epsilon}}{g}G^{ij} + \frac{1}{e}\tilde{F}^{ij}\right)\right] = +g[B^i - \epsilon^{ijk}\dot{x}_j E_k], \tag{48}$$

where again we used the definition of the dual fields $\tilde{F}$ as given in (38), and E^i and B_i are given by (23). We note that here we considered a positive magnetic charge with rest energy positive; for that reason we obtain a plus sign in the definition of the Lorentz force.

We note that both Lorentz forces are duality invariant.[13]

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Generalized Ornstein-Uhlenbeck processes

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We solve a physically significant extension of a classic problem in the theory of diffusion, namely the Ornstein-Uhlenbeck process [Ornstein and Uhlenbeck, Phys. Rev. **36**, 823 (1930)]. Our generalized Ornstein-Uhlenbeck systems include a force which depends upon the position of the particle, as well as upon time. They exhibit anomalous diffusion at short times, and non-Maxwellian velocity distributions in equilibrium. Two approaches are used. Some statistics are obtained from a closed-form expression for the propagator of the Fokker-Planck equation for the case where the particle is initially at rest. In the general case we use spectral decomposition of a Fokker-Planck equation, employing nonlinear creation and annihilation operators to generate the spectrum which consists of two staggered ladders. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2206878]

I. INTRODUCTION

This paper introduces a physically important extension of a classic problem in the theory of diffusion, namely the Ornstein-Uhlenbeck process.[1] Our results are obtained by spectral decomposition of a linear operator. The spectrum of this operator consists of two ladders of eigenvalues with, respectively, odd and even parity. The ladders of eigenvalues are staggered, that is the odd-even step is different from the even-odd step (see Fig. 1). The corresponding eigenfunctions are generated by a raising operator. A concise account of our work on these staggered ladder spectra appeared earlier.[2] In the following we show how the results summarized in Ref. 2 were obtained. We also derive new results, not included in our earlier report: a closed-form solution for example, and the generalization of our previous results to a continuous family of diffusion processes.

A. The Ornstein-Uhlenbeck process

Before we discuss our extension of the Ornstein-Uhlenbeck process, we describe its usual form.[1] This considers a particle of momentum p subjected to a rapidly fluctuating random force $f(t)$ and subject to a drag force $-\gamma p$, so that the equation of motion is

$$\dot{p} = -\gamma p + f(t). \tag{1}$$

The random force has statistics $\langle f(t)\rangle = 0$, $\langle f(t)f(t')\rangle = C(t-t')$ (angular brackets denote ensemble averages throughout). If the correlation time τ of $f(t)$ is sufficiently short ($\gamma\tau \ll 1$), the equation of motion may be approximated by a Langevin equation:

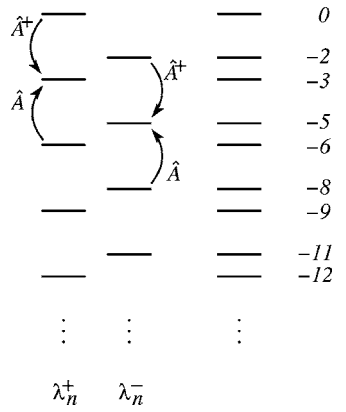

FIG. 1. The spectrum of $\hat{H}$ consists of two equally spaced (ladder) spectra λ_n^- and λ_n^+ which are "staggered" (that is, they are interleaved with uneven spacings). $\hat{A}$ and $\hat{A}^+$ do not change the parity of the eigenfunctions.

$$\mathrm{d}p = -\gamma p \mathrm{d}t + \mathrm{d}w, \tag{2}$$

where the Brownian increment $\mathrm{d}w$ has statistics $\langle \mathrm{d}w \rangle = 0$ and $\langle \mathrm{d}w^2 \rangle = 2D_0 \mathrm{d}t$. The diffusion constant is

$$D_0 = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t \, \langle f(t) f(0) \rangle. \tag{3}$$

This problem is discussed in many textbooks (for example, Ref. 3).

B. Generalized Ornstein-Uhlenbeck processes

Our extension arises when the force depends upon position as well as time. We consider the case where the fluctuations of the force on the particle are mainly a consequence of the spatial, rather the temporal, fluctuations of the force $f(x,t)$. A consequence of this difference is that the impulse δw supplied to the particle in a short time δt depends upon the momentum of the particle. If the particle is at position x_0 at time t_0, this impulse is

$$\delta w = \int_{t_0}^{t_0+\delta t} \mathrm{d}t \, f(x_0 + p(t-t_0)/m, t) + O(\delta t^2). \tag{4}$$

In particular, the impulse approaches zero as the speed $|p|/m$ of the particle increases, because the motion of the particle effects an average over the spatial fluctuations of the force. This can be seen clearly by considering the second moment of δw. We assume that the force $f(x,t)$ has the following statistics:

$$\langle f(x,t) \rangle = 0, \quad \langle f(x,t) f(x',t') \rangle = C(x-x', t-t'). \tag{5}$$

The spatial and temporal correlation scales of the random force $f(x,t)$ are ξ and τ, respectively. We consider the case where (for most of the time) the momentum of the particle is large compared to $p_0 = m\xi/\tau$, then the force experienced by the particle decorrelates much more rapidly than the force experienced by a stationary particle. If δt is large compared to τ but small compared to $1/\gamma$, we can estimate the variance of the impulse $\langle \delta w^2 \rangle = 2D(p)\delta t$ as follows (due to translational invariance, we consider without loss of generality a particle which starts from position $x = 0$ at time $t = 0$):

$$\langle \delta w^2 \rangle = \int_0^{\delta t} \mathrm{d}t_1 \int_0^{\delta t} \mathrm{d}t_2 \, \langle f(pt_1/m,t_1) f(pt_2/m,t_2) \rangle = \delta t \int_{-\infty}^{\infty} \mathrm{d}t \; C(pt/m,t) + O(\tau^2). \tag{6}$$

We define the momentum diffusion constant by writing $\langle \delta w^2 \rangle = 2D(p)\,\delta t + O(\delta t^2)$, and find

$$D(p) = \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}t \; C(pt/m,t). \tag{7}$$

When $p \ll p_0$ we recover $D(p) = D_0$. When $p \gg p_0$, we can approximate (7) to obtain

$$D(p) = \frac{D_1 p_0}{|p|} + O(p^{-2}), \quad D_1 = \frac{m}{2p_0} \int_{-\infty}^{\infty} \mathrm{d}X \; C(X,0). \tag{8}$$

When the force is the gradient of a potential $V(x,t)$ with a correlation function having continuous derivatives, we find that D_1 is zero. This case is discussed in Sec. VIII, where it is shown that $D(p) \sim |p|^{-3}$ provided the correlation function of $V(x,t)$ is sufficiently differentiable. Another variation, also discussed in Sec. VIII, arises when the correlation function of the force exhibits a discontinuity at $t=0$ [as when the potential $V(x,t)$ is itself generated by an Ornstein-Uhlenbeck process]. In this case $D(p) \sim |p|^{-2}$, and other exponents are also possible. We therefore consider a general situation where $D(p) \sim |p|^{-\zeta}$ and give exact results for the case

$$D(p) = D_\zeta (p_0/|p|)^\zeta \tag{9}$$

with $\zeta \geqslant 0$. We analyze the dynamics by solving a Fokker-Planck equation which determines the probability density for the Langevin process in which the momentum has diffusion constant given by (9). We discuss the form of this Fokker-Planck equation in Sec. II; the remainder of this introduction will set our work in context with earlier research on related topics.

C. Earlier work

The motion of a damped particle subjected to a force fluctuating in both space and time was first studied by Deutsch,[4] who addressed an entirely different aspect of the problem. Deutsch considered the case where the momentum of the particle remains small compared to p_0, and posed the question of whether particles aggregate. He discovered that there is a phase transition between coalescing and noncoalescing trajectories. (Two of the authors of the present paper subsequently solved Deutsch's one-dimensional model exactly,[5] and results for two and three spatial dimensions are discussed in Refs. 6 and 7). All of these papers only considered cases where $p \ll p_0$.

Sturrock[8] analyzed the motion of a particle subjected to a spatially varying force field without damping. He introduced the concept of a momentum diffusion constant which varies as a function of the momentum: that is, he considered the same problem as is addressed in the present paper, but in the limit of damping constant $\gamma = 0$. Subsequently Golubovic, Feng, and Zeng[9] identified the importance of the relation $D(p) \sim |p|^{-3}$ (in the case of a potential force), and discussed the nature of the Fokker-Planck equation and its solution in the case where $\gamma = 0$. It was argued that the particle exhibits anomalous diffusion and solution for the propagator of the Fokker-Planck equation with initial value $p = 0$ was proposed. Later Rosenbluth[10] pointed to an error in the evaluation of this propagator. The results of Refs. 8–10 were applied to the stochastic acceleration[11] of particles in plasmas, and subsequent contributions have concentrated on refining models for the calculation of $D(p)$ (see, for example, Refs. 12 and 13).

In the following we analyze the problem with the damping term, proportional to γ, included. Surprisingly, we find that this more general problem is more tractable: we are able, for example, to obtain precise results concerning the problems considered in Refs. 9 and 10 by taking, in our solutions, the limit $\gamma \to 0$.

There is a large literature devoted to the motion of particles advected in random velocity fields (corresponding to the large-γ limit of the model we study). In the case where the velocity field is independent of time, subdiffusive motion is typically found.[14,15] The advection of tracers in a

turbulent fluid is described by models with rapidly fluctuating velocity fields.[16] In our problem the inertia of the particles plays an important role. Particles suspended in a turbulent fluid can show surprising clustering properties when inertia effects are significant. These were first proposed by Maxey;[17] the current state of knowledge is summarized in Ref. 7. In cases where the random force results from motion of the surrounding fluid, it is not possible for the condition $p \gg p_0$ to be realized.[7]

Although our generalized Ornstein-Uhlenbeck process exhibits anomalous diffusion (at short times), this is not a result of power-law distributions that are built into the model. This distinguishes it from the anomalous diffusion of Levy flights or walks, reviewed in Ref. 18, which are a consequence of power-law distributions of the step lengths or waiting times for random jumps. Our model is thus distinct from the 'fractional Ornstein-Uhlenbeck process' described in Ref. 18.

Finally, we remark that a brief summary of many of the results of this paper has already been published.[2] The closed-form solution of Sec. III, the Wentzel-Kramers-Brillouin (WKB) analysis, and most of the results for general values of ζ were not discussed in Ref 2.

D. Description of our results and outline of this paper

In order to simplify the presentation, we describe in detail only our results for the case $\zeta=1$, corresponding to a generic random force. Corresponding expressions for general values of ζ are obtained using the same method, and we quote the most important results for general values of ζ in Sec. VIII at the end of the paper.

In Sec. II, the Fokker-Planck equation for the generalized Ornstein-Uhlenbeck processes is described. In Sec. III we briefly discuss a particular closed-form solution, which enables us to determine the steady state momentum distribution (which is non-Maxwellian) and some statistics, such as the time evolution of the variance of the momentum. The results of Sec. III are not sufficient to enable all statistics to be calculated, and in the general case we obtain statistics via a spectral decomposition of the Fokker-Planck equation. Section IV discusses this spectral decomposition. We transform the Fokker-Planck operator into a Hermitean operator and determine the eigenvalues and eigenvectors of this "Hamiltonian" operator by generating them using a new type of raising and lowering operators, which are nonlinear second-order differential operators. We show that the resulting spectrum is a ladder spectrum, consisting of separate ladders for the odd and even parity states. These are staggered: the odd-even separation differs from even-odd. Section V contains calculations of the matrix elements needed for computing correlation functions and expectation values. In Sec. VI we summarize our results on diffusion and anomalous diffusion for generic random forcing.

Section VII discusses a technical issue concerning our evaluation of the spectrum. When the index of the eigenvalue is large, it is possible to apply standard WKB approximation methods everywhere except in the vicinity of a singularity of the Hamiltonian. We show that the singularity introduces phase shifts which explain the staggered-ladder structure of the spectrum.

Finally, in Sec. VIII we explain in more detail how other values of ζ can arise and summarize our results for general ζ.

II. FOKKER-PLANCK EQUATIONS

We consider a particle with equations of motion

$$\dot{x} = p/m, \quad \dot{p} = -\gamma p + f(x,t) \tag{10}$$

where the force $f(x,t)$ is random, with statistics given by Eq. (5). In the limit as the correlation time τ of the force approaches zero, the equation of motion of the momentum may be approximated by a Langevin equation, (2), where the random increment $\mathrm{d}w$ has second moment $\langle \mathrm{d}w^2 \rangle = 2D(p)\mathrm{d}t$ with $D(p)$ given by (7). This Langevin equation for the stochastic evolution of $p(t)$ corresponds to a Fokker-Planck equation (generalized diffusion equation) for the probability density of the momentum, $P(p,t)$. Using standard results,[3] the Fokker-Planck equation is

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial p}(v(p)P) + \frac{\partial^2}{\partial^2 p}(D(p)P), \tag{11}$$

where

$$v(p) = \frac{\langle \mathrm{d}p \rangle}{\mathrm{d}t}, \quad D(p) = \frac{\langle \mathrm{d}p^2 \rangle}{2\mathrm{d}t}. \tag{12}$$

Note that we can replace dp by dw in the expression for $D(p)$, because the neglected terms are of higher order in dt, and that $D(p)$ has already been obtained in Eq. (7). In order to determine the correct form of the Fokker-Planck equation it remains to determine $\langle \mathrm{d}p \rangle = -\gamma p\, \mathrm{d}t + \langle \mathrm{d}w \rangle$.

Expanding the impulse (4) about a reference trajectory $x(t) = pt/m$, and using the fact that $\langle f(x,t) \rangle = 0$, we obtain

$$\langle \delta w \rangle = \frac{1}{m} \int_0^{\delta t} \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \exp[-\gamma(t_2 - t_3)] \left\langle \frac{\partial f}{\partial x}(pt_1/m, t_1) f(pt_3/m, t_3) \right\rangle. \tag{13}$$

Note that throughout the three-dimensional region of integration, we have $0 \leqslant t_3 \leqslant t_2 \leqslant t_1 \leqslant \delta t$, and the short correlation time implies that the integrand is negligible unless $|t_1 - t_3| < \tau$. The integrand is therefore significant along a line rather than a surface, because t_2 must lie between t_1 and t_3. The integral is therefore $O(\delta t)$, rather than $O(\delta t^2)$ which would obtain if the integrand were significant on a surface. We replace the factor $\exp[-\gamma(t_2 - t_3)]$ by unity because $\gamma\tau \ll 1$, and the other factor is negligible when $|t_2 - t_3| > \tau$. The integral over t_2 then gives simply $t_1 - t_3$. Writing $t = t_1 - t_3$, in the limit $\gamma\tau \ll 1$, the result is therefore

$$\langle \delta w \rangle = \frac{\delta t}{2m} \int_{-\infty}^{\infty} \mathrm{d}t\, t \left\langle \frac{\partial f}{\partial x}(0,0) f(pt/m, t) \right\rangle = \delta t\, \frac{\mathrm{d}}{\mathrm{d}p} D(p). \tag{14}$$

This implies

$$v(p) = -\gamma p + \frac{\mathrm{d}}{\mathrm{d}p} D(p). \tag{15}$$

Rosenbluth[10] has pointed out that this relation can also be obtained as a consequence of applying the principle of detailed balance.

With (7) and (15), the following Fokker-Planck equation obtains:

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p + D(p) \frac{\partial}{\partial p} \right) P. \tag{16}$$

Sturrock[8] introduced a related Fokker-Planck equation (without the damping term) and also gave an expression for $D(p)$ analogous to Eq. (7).

In the following we discuss our solution of (16) with $D(p)$ given by Eq. (9), for the particular case of generic random forcing (corresponding to $\zeta = 1$). Results for other values of ζ are obtained in an analogous fashion. The general case is briefly described in Sec. VIII.

III. A PARTICULAR CLOSED-FORM SOLUTION

In this section we introduce a particular solution of the Fokker-Planck equation (16) with $D(p)$ given by (9). We restrict ourselves to the case of generic random forcing (corresponding to $\zeta = 1$):

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p + D_1 \frac{p_0}{|p|} \frac{\partial}{\partial p} \right) P. \tag{17}$$

Consider the distribution $P(p,t)$ of momentum p for particles initially at rest. It satisfies the initial condition $P(p,0)=\delta(p)$ where $\delta(p)$ is the Dirac δ-function. For this particular initial condition, we have found the following closed-form solution of (17):

$$P(p,t)=\frac{1}{2\Gamma(4/3)}\frac{\gamma^{1/3}}{[3p_0D_1(1-e^{-3\gamma t})]^{1/3}}\exp\left[-\frac{\gamma|p|^3}{3p_0D_1(1-e^{-3\gamma t})}\right]. \tag{18}$$

Equation (18) determines how the moments of momentum grow for a particle initially at rest:

$$\langle p^{2l}(t)\rangle=\left(\frac{3D_1p_0}{\gamma}\right)^{2/3}\frac{\Gamma((2l+1)/3)}{\Gamma(1/3)}(1-e^{-3\gamma t})^{2l/3} \tag{19}$$

for positive integers l. This result is consistent with the result obtained in Ref. 2 [Eq. (8) in that paper]. In the limit of small times (19) gives rise to anomalous diffusion

$$\langle p^{2l}(t)\rangle\sim t^{2l/3}. \tag{20}$$

At large times ($\gamma t\gg 1$), by contrast, we obtain a stationary non-Maxwellian momentum distribution

$$P_0(p)=\frac{1}{2\Gamma(4/3)}\frac{\gamma^{1/3}}{(3p_0D_1)^{1/3}}\exp[-\gamma|p|^3/(3p_0D_1)]. \tag{21}$$

The particular solution (18) generalizes in a natural way to other values of ζ.

However, in order to determine the momentum correlation function and the spatial diffusion properties, the particular solution (18) is not sufficient, the general solution for arbitrary initial condition is required. We have not been able to obtain the general solution to (16) in closed form. Therefore, we determine it using spectral decomposition: we construct the eigenvalues λ_n and eigenfunctions ψ_n of a Hermitian operator $\hat{H}$ corresponding to the Fokker-Planck equation (17). We identify raising and lowering operators $\hat{A}^+$ and $\hat{A}$ which map one eigenfunction to another with, respectively, two more or two fewer nodes. We use these to obtain the spectrum and eigenfunctions of $\hat{H}$ which in turn allow us to construct the propagator, expectation values, and correlation functions. This approach is described in Secs. IV and V.

IV. SPECTRAL DECOMPOSITION

Introducing dimensionless variables ($t'=\gamma t$ and $p=zp_0[D_1/(\gamma p_0^2)]^{1/3}$) we write (17) as

$$\frac{\partial P}{\partial t'}=\frac{\partial}{\partial z}\left(z+\frac{1}{|z|}\frac{\partial}{\partial z}\right)P\equiv\hat{F}P. \tag{22}$$

It is convenient to transform the Fokker-Planck operator $\hat{F}$ to a Hermitian form which we shall refer to as the Hamiltonian operator:

$$\hat{H}=P_0^{-1/2}\hat{F}P_0^{1/2}=\frac{1}{2}-\frac{|z|^3}{4}+\frac{\partial}{\partial z}\frac{1}{|z|}\frac{\partial}{\partial z}. \tag{23}$$

Here $P_0(z)\propto\exp(-|z|^3/3)$ is the stationary solution (21) satisfying $\hat{F}P_0=0$. We solve the diffusion problem by constructing the eigenfunctions of the Hamiltonian operator. In the following we make use of Dirac notation[19] of quantum mechanics to write the equations in a compact form and to emphasize their structure.

The eigenfunctions of the Fokker-Planck equation (16) are alternately even and odd functions, defined on the interval $(-\infty,\infty)$. The operator $\hat{H}$, describing the limiting case of this Fokker-Planck operator, is singular at $z=0$. We identify two eigenfunctions of $\hat{H}$ by inspection, $\psi_0^+(z)=\mathcal{C}_0^+\exp(-|z|^3/6)$ which has eigenvalue $\lambda_0^+=0$ and $\psi_0^-(z)=\mathcal{C}_0^-z|z|\exp(-|z|^3/6)$ with eigenvalue λ_0^-

$=-2$. These eigenfunctions are of even and odd parity, respectively (zero and one node, respectively). Our approach to determining the full spectrum is to define a raising operator $\hat{A}^+$ which maps any eigenfunction $\psi_n^{\pm}(z)$ to its successor with the same parity, $\psi_{n+1}^{\pm}(z)$, having two additional nodes.

A. Algebra of raising and lowering operators

We write

$$\hat{H} = \hat{a}^- |z|^{-1} \hat{a}^+. \tag{24}$$

Here $a^{\pm} = (\partial_z \pm z|z|/2)$. We introduce the operators

$$\hat{A} = \hat{a}^+ |z|^{-1} \hat{a}^+ \quad \text{and} \quad \hat{A}^+ = \hat{a}^- |z|^{-1} \hat{a}^- \tag{25}$$

as well as

$$\hat{G} = \hat{a}^+ |z|^{-1} \hat{a}^-. \tag{26}$$

Note that $\hat{A}^+$ is the Hermitian conjugate of $\hat{A}$. The commutator of $\hat{A}$ and $\hat{A}^+$ is

$$[\hat{A}, \hat{A}^+] = -3(\hat{H} + \hat{G}). \tag{27}$$

Note also that $\hat{H} - \hat{G} = \hat{I}$ (where $\hat{I}$ is the identity operator).

1. Eigenvalues

It can be verified that

$$[\hat{H}, \hat{A}] = 3\hat{A} \quad \text{and} \quad [\hat{H}, \hat{A}^+] = -3\hat{A}^+. \tag{28}$$

These expressions show that the action of $\hat{A}$ and $\hat{A}^+$ on any eigenfunction is to produce another eigenfunction with eigenvalue increased or decreased by three, or else to produce a function which is identically zero. The operator $\hat{A}^+$ adds two nodes, and repeated action of $\hat{A}^+$ on $\psi_0^+(z)$ and $\psi_0^-(z)$ therefore exhausts the set of eigenfunctions. Together with $\lambda_0^+ = 0$ and $\lambda_0^- = -2$ this establishes that the spectrum of $\hat{H}$ is (see Fig. 1)

$$\lambda_n^+ = -3n \quad \text{and} \quad \lambda_n^- = -3n - 2 \quad n = 0, \ldots, \infty. \tag{29}$$

2. Eigenfunctions

We represent the eigenfunctions by of $\hat{H}$ by kets $|\psi_n^-\rangle$ and $|\psi_n^+\rangle$. The actions of $\hat{A}$ and $\hat{A}^+$ are

$$\hat{A}^+ |\psi_n^{\pm}\rangle = C_{n+1}^{\pm} |\psi_{n+1}^{\pm}\rangle \quad \text{and} \quad \hat{A} |\psi_n^{\pm}\rangle = C_n^{\pm} |\psi_{n-1}^{\pm}\rangle. \tag{30}$$

The normalization factor C_{n+1}^- is determined as follows:

$$1 = \langle \psi_{n+1}^- | \psi_{n+1}^- \rangle = (C_{n+1}^-)^{-2} \langle \psi_n^- | \hat{A} \hat{A}^+ | \psi_n^- \rangle = (C_{n+1}^-)^{-2} \langle \psi_n^- | [\hat{A}, \hat{A}^+] + \hat{A}^+ \hat{A} | \psi_n^- \rangle. \tag{31}$$

It follows

$$(C_{n+1}^-)^2 = (3(-2\lambda_n^- + 1) + (C_n^-)^2). \tag{32}$$

By recursion we obtain

$$C_n^- = [3n(3n+2)]^{1/2}. \tag{33}$$

This determines the normalization of the states $(\hat{A}^+)^n|\psi_0^-\rangle$,

$$|\psi_n^-\rangle = N_n^-(\hat{A}^+)^n|\psi_0^-\rangle \tag{34}$$

with

$$N_n^- = \left(\prod_{k=1}^{n} 3k(3k+2)\right)^{-1/2} N_0^-. \tag{35}$$

For the positive-parity states we proceed in a similar fashion and obtain

$$C_n^+ = [3n(3n-2)]^{1/2}. \tag{36}$$

This implies

$$|\psi_n^+\rangle = N_n^+(\hat{A}^+)^n|\psi_0^+\rangle \tag{37}$$

with

$$N_n^+ = \left(\prod_{k=1}^{n} 3k(3k-2)\right)^{-1/2} N_0^+. \tag{38}$$

The operators $\hat{A}^+$ and $\hat{A}$ differ from the usual examples of raising and lowering operators in that they are of second order in $\mathrm{d}/\mathrm{d}z$, whereas other examples of raising and lowering operators are of first order in the derivative. The difference is associated with the fact that the spectrum is a staggered ladder: only states of the same parity have equal spacing, so that the raising and lowering operators must preserve the odd-even parity. This suggests replacing a first-order operator which increases the quantum number (total number of nodes) by one with a second-order operator which increases the quantum number by two, preserving parity.

There is an alternative approach to generating the eigenfunctions of $\hat{H}$. This equation falls into one of the classes considered in Ref. 20, and we have written down first-order operators which map one eigenfunction into another. However, these operators are themselves functions of the quantum number n, making the algebra cumbersome. The approach is briefly described in the next section.

B. Schrödinger factorization

Consider the eigenvalue problem

$$\hat{H}|\psi\rangle = \lambda|\psi\rangle \tag{39}$$

with Hamiltonian (23). For $z>0$ it can be transformed by the variable change $x=z^3$:

$$\left[(3x)^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 3x\frac{\mathrm{d}}{\mathrm{d}x} - x\left(\frac{1}{4}x + \lambda - \frac{1}{2}\right)\right]\psi(x) = 0. \tag{40}$$

Equation (40) is a Fuchsian linear differential equation with regular singular points of rank less than or equal to two. Equation (40) can therefore be factorized using a generalized Schrödinger factorization scheme (see Ref. 20 for a review of this method).

Applying this scheme we have obtained raising and lowering operators generating the spectrum (29). The raising operator acting on $\psi_n^\pm$ is given by

$$T_{\pm,n+1} = -3x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{x}{2} - 3(n+\delta_\pm) \tag{41}$$

with $\delta_+ = 1/3$ and $\delta_- = 1$. The lowering operator acting on $\psi_n^\pm$ is

$$\tilde{T}_{\pm,n} = -3x\frac{\mathrm{d}}{\mathrm{d}x} - \frac{1}{2}x + 3(n+\eta_\pm) \tag{42}$$

with $\eta_+ = 0$ and $\eta_- = 2/3$. Note that the Hermitian conjugates of $T_{\pm,n+1}$ and $\tilde{T}_{\pm,n}$ are

$$(T_{\pm,n+1})^+ = -\tilde{T}_{\pm,n+1} + 3, \tag{43}$$

$$(\tilde{T}_{\pm,n})^+ = -T_{\pm,n} + 3. \tag{44}$$

The raising and lowering operators satisfy

$$T_{\pm,n+1}|\psi_n^\pm\rangle = C_{n+1}^\pm|\psi_{n+1}^\pm\rangle \quad \text{and} \quad \tilde{T}_{\pm,n}|\psi_n^\pm\rangle = C_n^\pm|\psi_{n-1}^\pm\rangle \tag{45}$$

with $C_n^\pm$ given by (33) and (36), generating the spectrum (29). The operators differ from $\hat{A}$ and $\hat{A}^+$ introduced in Sec. IV in that they are of first order in $\mathrm{d}/\mathrm{d}x$, and in that they depend on the state they are applied to.

V. CORRELATION FUNCTIONS AND MATRIX ELEMENTS

A. Correlation functions

The required solutions of the Fokker-Planck equation may be expressed in terms of the propagator $K(y,z,t)$ which is the probability density for the scaled momentum to reach z after time t, starting from y. It satisfies the Fokker-Planck equation $\partial_{t'}K = \hat{F}K$ and can be expressed in terms of the eigenvalues λ_n^σ and eigenfunctions $\phi_n^\sigma(z) = P_0^{-1/2}(z)\psi_n^\sigma(z)$ of $\hat{F}$:

$$K(y,z;t') = \sum_{n\sigma} a_n^\sigma(y)\phi_n^\sigma(z)\exp(\lambda_n^\sigma t') \tag{46}$$

for $t' > 0$. The expansion coefficients $a_n^\sigma(y)$ are determined by the initial condition $K(y,z;0) = \delta(z-y)$, namely $a_n^\sigma(y) = P_0^{-1/2}\psi_n^\sigma(y)$. In terms of the eigenfunctions of $\hat{H}$ we have (for $t' > 0$)

$$K(y,z;t') = \sum_{n\sigma} P_0^{-1/2}(y)\psi_n^\sigma(y)P_0^{1/2}(z)\psi_n^\sigma(z)\exp(\lambda_n^\sigma t'). \tag{47}$$

Equilibrium correlation functions of an observable $O(z)$ are given by

$$\langle O(z_0)O(z_{t'})\rangle_{\mathrm{eq.}} = \int_{-\infty}^{\infty}\mathrm{d}z\int_{-\infty}^{\infty}\mathrm{d}y\, O(z)O(y)K(y,z;t')P_0(y). \tag{48}$$

Since $P_0^{1/2}(y) = \psi_0^+(y)$ this corresponds to

$$\langle O(z_0)O(z_{t'})\rangle_{\mathrm{eq.}} = \sum_{n\sigma}|\langle\psi_0^+|\hat{O}|\psi_n^\sigma\rangle|^2\exp(\lambda_n^\sigma t') \tag{49}$$

for $t' > 0$. The momentum correlation function in equilibrium, for instance, is

$$\langle p_{t'}p_0\rangle_{\mathrm{eq.}} = p_0^2\left(\frac{D_1}{\gamma p_0^2}\right)^{2/3}\sum_n\langle\psi_0^+|\hat{z}|\psi_n^-\rangle^2\exp(\lambda_n^- t') \tag{50}$$

for $t' > 0$, which requires the evaluation of matrix elements $\langle\psi_0^+|\hat{z}|\psi_n^-\rangle$.

Consider on the other hand the time-dependence of $\langle x^2(t)\rangle$, with particles initially at rest at the origin. We need to evaluate

$$\langle x^2(t)\rangle = \frac{1}{m^2}\int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \,\langle p_{t_1} p_{t_2}\rangle. \tag{51}$$

In dimensionless variables this corresponds to

$$\langle x^2(t)\rangle = \frac{1}{\gamma^2}\left(\frac{p_0 D_1}{\gamma}\right)^{2/3} \frac{1}{m^2}\int_0^{t'} \mathrm{d}t_1' \int_0^{t'} \mathrm{d}t_2' \,\langle z_{t_1'} z_{t_2'}\rangle. \tag{52}$$

The required correlation function is (assuming $t_2' > t_1' > 0$)

$$\begin{aligned}\langle z_{t_2'} z_{t_1'}\rangle &= \int_{-\infty}^{\infty} \mathrm{d}z_1 \int_{-\infty}^{\infty} \mathrm{d}z_2 \, z_1 z_2 K(z_1, z_2; t_2' - t_1') K(0, z_1; t_1') \\ &= \sum_{n,m} \frac{\psi_m^+(0)}{\psi_0^+(0)} \langle \psi_0^+ | \hat{z} | \psi_n^- \rangle \langle \psi_n^- | \hat{z} | \psi_m^+ \rangle \exp[\lambda_n^-(t_2' - t_1') + \lambda_m^+ t_1'].\end{aligned} \tag{53}$$

In order to evaluate (53), the ratios of wave-function amplitudes $\psi_m^+(0)/\psi_0^+(0)$ are required in addition to matrix elements of $\hat{z}$. The matrix elements $\langle \psi_n^- | \hat{z} | \psi_m^+ \rangle$ are determined in Sec. V B, while the ratios of eigenfunctions are calculated in Sec. V C.

B. Matrix elements $\langle \psi_m^+ | \hat{z} | \psi_n^- \rangle$

To evaluate the matrix elements $Z_{mn} = \langle \psi_m^+ | \hat{z} | \psi_n^- \rangle$ we proceed in three steps: we first evaluate Z_{0n}, in a second step the matrix elements Z_{mn} are related to $Z_{0,n-m}$ for $m \leqslant n$. Third, Z_{mn} is evaluated for $m > n$.

1. Matrix elements $\langle \psi_0^+ | \hat{z} | \psi_n^- \rangle$

Consider first $Z_{0n} = \langle \psi_0^+ | \hat{z} | \psi_n^- \rangle$. These matrix elements are obtained by recursion. To evaluate

$$Z_{0,n+1} = \langle \psi_0^+ | \hat{z} \hat{A}^+ | \psi_n^- \rangle / C_{n+1}^- \tag{54}$$

we write $\hat{z}\hat{A}^+ = \hat{z}\hat{G} + \hat{z}(\hat{A}^+ - \hat{G}) = \hat{z}(\hat{H} - \hat{I}) + \hat{z}(\hat{A}^+ - \hat{G})$. It follows

$$\langle \psi_0^+ | \hat{z} \hat{A}^+ | \psi_n^- \rangle = (\lambda_n^- - 1) Z_{0n} + \langle \psi_0^+ | \hat{z}(\hat{A}^+ - \hat{G}) | \psi_n^- \rangle. \tag{55}$$

Using $(\hat{A}^+ - \hat{G}) = -\hat{z}\hat{a}^-$ and $[\hat{z}^2, \hat{a}^-] = -2\hat{z}$ we obtain

$$\langle \psi_0^+ | \hat{z} \hat{A}^+ | \psi_n^- \rangle = (\lambda_n^- + 1) Z_{0n}. \tag{56}$$

This corresponds to the recursion

$$Z_{0n} = (-1)^n \frac{\prod_{k=0}^{n-1} (3k+1)}{\sqrt{\prod_{k=0}^{n-1} 3(k+1)(3k+5)}} Z_{00}. \tag{57}$$

With $Z_{00} = 3^{-5/12}\sqrt{\pi}/\Gamma(2/3)$ (found by direct evaluation of an integral) we obtain

$$Z_{0n} = (-1)^n \frac{3^{-5/12}}{\sqrt{2\pi}} \sqrt{\Gamma(2/3)} \frac{\Gamma(n + 1/3)}{\sqrt{\Gamma(n+1)\Gamma(n+5/3)}}. \tag{58}$$

2. Matrix elements $\langle\psi_m^+|\hat{z}|\psi_n^-\rangle$ for $m\leqslant n$

Consider now the case $m\leqslant n$. Let

$$J_{mn}=\langle\psi_0^+|\hat{A}^m\hat{z}(\hat{A}^+)^n|\psi_0^-\rangle=\langle\psi_0^+|\hat{A}^m[\hat{z},\hat{A}^+](\hat{A}^+)^{n-1}|\psi_0^-\rangle+\langle\psi_0^+|\hat{A}^m\hat{A}^+\hat{z}(\hat{A}^+)^{n-1}|\psi_0^-\rangle.$$

We use $[\hat{z},\hat{A}^+]=-(|\hat{z}|^{-1}\hat{a}^-+\hat{a}^-|\hat{z}|^{-1})$ to write

$$\begin{aligned}J_{mn}&=-\langle\psi_0^+|\hat{A}^m|\hat{z}|^{-1}\hat{a}^-(\hat{A}^+)^{n-1}|\psi_0^-\rangle-\langle\psi_0^+|\hat{A}^m\hat{a}^-|\hat{z}|^{-1}(\hat{A}^+)^{n-1}|\psi_0^-\rangle+\langle\psi_0^+|\hat{A}^m\hat{A}^+\hat{z}(\hat{A}^+)^{n-1}|\psi_0^-\rangle\\&=J_{mn}^{(1)}+J_{mn}^{(2)}+J_{mn}^{(3)}\end{aligned}\tag{59}$$

and evaluate the three terms separately. The third one gives

$$J_{mn}^{(3)}=\langle\psi_0^+|\hat{A}^m\hat{A}^+\hat{z}(\hat{A}^+)^{n-1}|\psi_0^-\rangle=(C_m^+)^2\langle\psi_0^+|\hat{A}^{m-1}\hat{z}(\hat{A}^+)^{n-1}|\psi_0^-\rangle=(C_m^+)^2J_{m-1n-1}.\tag{60}$$

Consider next the first term: $\hat{A}^m|\hat{z}|^{-1}\hat{a}^-(\hat{A}^+)^{n-1}=\hat{A}^{m-1}\hat{a}^+|\hat{z}|^{-1}\hat{a}^+|\hat{z}|^{-1}\hat{a}^-(\hat{A}^+)^{n-1}=\hat{A}^{m-1}\hat{a}^+|\hat{z}|^{-1}\hat{G}(\hat{A}^+)^{n-1}$, and thus

$$\langle\psi_0^+|\hat{A}^m|\hat{z}|^{-1}\hat{a}^-(\hat{A}^+)^{n-1}|\psi_0^-\rangle=(\lambda_{n-1}^--1)\langle\psi_0^+|\hat{A}^{m-1}\hat{a}^+|\hat{z}|^{-1}(\hat{A}^+)^{n-1}|\psi_0^-\rangle.\tag{61}$$

Using $\hat{A}^{m-1}\hat{a}^+|\hat{z}|^{-1}(\hat{A}^+)^{n-1}=\hat{A}^{m-1}\hat{a}^+|\hat{z}|^{-1}\hat{a}^-|\hat{z}|^{-1}\hat{a}^-(\hat{A}^+)^{n-2}=\hat{A}^{m-1}\hat{G}|\hat{z}|^{-1}\hat{a}^-\hat{A}^{+n-2}$ we obtain the recursion

$$J_{mn}^{(1)}=(\lambda_{n-1}^--1)(\lambda_{m-1}^+-1)J_{m-1n-1}^{(1)}=3n(3m-2)J_{m-1n-1}^{(1)}.\tag{62}$$

Now consider $J_{mn}^{(2)}$. Using $\hat{a}^-|\hat{z}|^{-1}(\hat{A}^+)^{n-1}=\hat{A}^+|\hat{z}|^{-1}\hat{a}^-\hat{A}^{+n-2}$ it follows

$$J_{mn}^{(2)}=(C_m^+)^2J_{m-1n-1}^{(1)}.\tag{63}$$

This implies

$$J_{mn}^{(2)}=\frac{(C_m^+)^2}{(\lambda_{n-1}^--1)(\lambda_{m-1}^+-1)}J_{mn}^{(1)}=\frac{m}{n}J_{mn}^{(1)}.\tag{64}$$

Note also that $J_{0n}^{(3)}=0$, as well as $J_{0n}^{(2)}=0$. This gives $J_{0n}^{(1)}=J_{0n}$ [consistent with (64)]. We obtain

$$J_{mn}^{(1)}=\prod_{k=1}^{m}3(n-m+k)(3k-2)J_{0n-m},\tag{65}$$

which results in

$$J_{mn}^{(1)}=(-1)^{m+n}\frac{\Gamma(2/3)3^{m+n+5/6}}{6\pi}\frac{\Gamma(n+1)\Gamma(m+1/3)\Gamma(n-m+1/3)}{\Gamma(n-m+1)}.\tag{66}$$

Equation (66) allows us to write down an inhomogeneous recursion for J_{mn}:

$$J_{mn}=3m(3m-2)J_{m-1n-1}+(1+m/n)J_{mn}^{(1)},\tag{67}$$

where the inhomogeneous term is given by (66). Iterating this recursion we obtain

$$J_{mn}=\sum_{l=0}^{m}\left(\prod_{k=l+1}^{m}3k(3k-2)\right)\left(1+\frac{l}{n-m+l}\right)J_{ln-m+l}^{(1)},\tag{68}$$

which results in

$$J_{mn} = (-1)^{m-n} \frac{3^{m+n+1}\Gamma(2/3)^2}{4\pi^2}(m+n+1)\frac{\Gamma(n+1)\Gamma(m+1/3)\Gamma(n-m+1/3)}{\Gamma(n-m+2)}J_{00}. \tag{69}$$

This determines J_{mn} for $n \geqslant m$.

3. Matrix elements $\langle \psi_m^+ | \hat{z} | \psi_n^- \rangle$ for $m > n$

For $m > n$ we use instead

$$J_{mn} = \langle \psi_0^+ | \hat{A}^m \hat{z} \hat{A}^{+n} | \psi_0^- \rangle = \langle \psi_0^+ | \hat{A}^{m-1} [\hat{A}, \hat{z}] \hat{A}^{+n} | \psi_0^- \rangle + \langle \psi_0^+ | \hat{A}^{m-1} \hat{z} \hat{A} (\hat{A}^+)^n | \psi_0^- \rangle \tag{70}$$

and proceed as before. We find that $J_{mn}=0$ for $m > n+1$. For $m=n+1$ we obtain

$$\begin{aligned} J_{n+1n} &= \langle \psi_0^+ | \hat{A}^n |\hat{z}|^{-1} \hat{a}^+ (\hat{A}^+)^n | \psi_0^- \rangle + \langle \psi_0^+ | \hat{A}^n \hat{a}^+ |\hat{z}|^{-1} (\hat{A}^+)^n | \psi_0^- \rangle + \langle \psi_0^+ | \hat{A}^n |\hat{z}| \hat{A} (\hat{A}^+)^n | \psi_0^- \rangle \\ &= \tilde{J}^{(1)}_{n+1n} + \tilde{J}^{(2)}_{n+1n} + \tilde{J}^{(3)}_{n+1n}. \end{aligned} \tag{71}$$

Consider first $\tilde{J}^{(3)}_{n+1n}$:

$$\tilde{J}^{(3)}_{n+1n} = (C_n^-)^2 \tilde{J}^{(3)}_{nn-1} = 3n(3n+2)\tilde{J}^{(3)}_{nn-1}. \tag{72}$$

Second, using $\hat{A}^n |\hat{z}|^{-1} \hat{a}^+ (\hat{A}^+)^n = \hat{A}^{n-1} \hat{a}^+ |\hat{z}|^{-1} \hat{A} (\hat{A}^+)^n$ we determine $\tilde{J}^{(1)}_{n+1n}$:

$$\tilde{J}^{(1)}_{n+1n} = (C_n^-)^2 \tilde{J}^{(2)}_{nn-1} = 3n(3n+2)\tilde{J}^{(2)}_{nn-1}. \tag{73}$$

Third,

$$\tilde{J}^{(2)}_{n+1n} = (\lambda_n^+ - 1)(\lambda_{n-1}^- - 1)\tilde{J}^{(2)}_{nn-1} = (3n+1)3nJ^{(2)}_{nn-1}. \tag{74}$$

We deduce that

$$\tilde{J}^{(1)}_{n+1n} = \frac{3n+2}{3n+1}\tilde{J}^{(2)}_{n+1n} \tag{75}$$

and obtain the recursion

$$J_{n+1n} = \tilde{J}^{(1)}_{n+1n} + \tilde{J}^{(2)}_{n+1n} + \tilde{J}^{(3)}_{n+1n} = 3n(3n+2)J_{nn-1} + \left(1 + \frac{3n+2}{3n+1}\right)\tilde{J}^{(2)}_{n+1n}. \tag{76}$$

Iterating (74) we obtain

$$\tilde{J}^{(2)}_{n+1n} = \left(\prod_{k=1}^{n} 3k(3k+1)\right)\tilde{J}^{(2)}_{10} = \frac{3\sqrt{3}}{2\pi} 9^n \Gamma(2/3)\Gamma(n+1)\Gamma(n+4/3)J_{00} \tag{77}$$

and thus from (76)

$$J_{n+1n} = \frac{\sqrt{3}}{2\pi} 9^n \Gamma(2/3)\Gamma(2+n)\Gamma(n+4/3)J_{00}. \tag{78}$$

Comparing this result to (69) we find that (69) gives the correct result for $m=n+1$, although it was derived assuming $m \leqslant n$. Normalizing to obtain Z_{mn} our final result is

$$Z_{mn} = (-1)^{m-n}\frac{3^{5/6}}{6\pi}(m+n+1)\Gamma(2/3)\frac{\sqrt{\Gamma(n+1)\Gamma(m+1/3)}}{\sqrt{\Gamma(m+1)\Gamma(n+5/3)}}\frac{\Gamma(n-m+1/3)}{\Gamma(n-m+2)} \tag{79}$$

for $n \geqslant m-1$ and zero otherwise.

C. Ratios of eigenfunctions

In this section we show how to evaluate $\psi_n^+(0)/\psi_0^+(0)$. For $z>0$, the eigenfunctions $\psi_n^+(z)$ are of the form $N_n^+ g_n(z)\exp(-z^3/6)$, where $g_n(z)$ is polynomial in z^3, of the form

$$g_n(z) = g_n^{(0)} + g_n^{(1)} z^3 + \cdots . \tag{80}$$

We determine how $\hat{A}^+$ and $\hat{H}$ act on these polynomials. To this end we define

$$\hat{A}'^+ = e^{z^3/6}\hat{A}^+ e^{-z^3/6} = (\partial_z - z^2)z^{-1}(\partial_z - z^2), \tag{81}$$

$$\hat{H}' = e^{z^3/6}\hat{H}e^{-z^3/6} = (\partial_z - z^2)z^{-1}\partial_z. \tag{82}$$

This implies

$$\hat{A}'^+ - \hat{H}' = -(\partial_z - z^2)z = z^3 - z\partial_z - 1 \tag{83}$$

and thus

$$(\hat{A}'^+ - \hat{H}')g_n = -g_n^{(0)} + O(z^3). \tag{84}$$

Using $\lambda_n^+ = -3n$ we obtain

$$\hat{H}' g_n = -3n g_n^{(0)} + O(z^3) \tag{85}$$

from the eigenvalue equation. Taking (84) and (85) together we have

$$\hat{A}'^+ g_n = -(3n+1) g_n^{(0)} + O(z^3). \tag{86}$$

Equation (86) implies

$$g_{n+1}^{(0)} = -(3n+1) g_n^{(0)}. \tag{87}$$

With (30) it follows

$$\psi_{n+1}^+(0) = N_{n+1}^+ g_{n+1}^{(0)} = -(3n+1)N_{n+1}^+/N_n^+ \psi_n^+(0) = -\sqrt{\frac{3n+1}{3(n+1)}}\psi_n^+(0). \tag{88}$$

Our final result for the ratio of wave-function amplitudes is therefore

$$\psi_n^+(0)/\psi_0^+(0) = (-1)^n \sqrt{\frac{\sqrt{3}\Gamma(2/3)}{2\pi}\frac{\Gamma(n+1/3)}{\Gamma(n+1)}}. \tag{89}$$

VI. EQUILIBRIUM CORRELATIONS, DIFFUSION, AND ANOMALOUS DIFFUSION

In the following the momentum correlation function in equilibrium and the time dependence of $\langle x^2(t)\rangle$ are determined.

A. Momentum correlation function in equilibrium

The correlation function of momentum in equilibrium is obtained from (49). We have

$$\langle p_{t'} p_0 \rangle_{\text{eq.}} = p_0^2 \left(\frac{D_1}{\gamma p_0^2}\right)^{2/3} \sum_n Z_{0n}^2 \exp(\lambda_n^- t'). \tag{90}$$

Using (79) we obtain

$$\langle p_t p_0 \rangle_{\text{eq.}} = \frac{\Gamma(4/3)}{3^{1/3}\Gamma(5/3)} \left(\frac{p_0 D_1}{\gamma} \right)^{2/3} e^{-2\gamma t} F_{21}\left(\frac{1}{3}, \frac{1}{3}; \frac{5}{3}; e^{-3\gamma t} \right) \tag{91}$$

for $t>0$. Here F_{21} is a hypergeometric function.[21] It follows that $\langle p_t p_0 \rangle_{\text{eq.}}$ decays as $\exp(-2\gamma t)$ at large times as opposed to $\exp(-\gamma t)$ in the Ornstein-Uhlenbeck process.

B. Diffusion at long times

We now turn to $\langle x^2(t) \rangle$. This expectation value is calculated using Eqs. (52), (53), (79), and (89). We have

$$\langle x^2(t) \rangle = \left(\frac{p_0 D_1}{\gamma} \right)^{2/3} \frac{1}{m^2 \gamma^2} \sum_{k=0}^{\infty} \sum_{l=k-1}^{\infty} \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} T_{kl} \tag{92}$$

with

$$T_{kl}(t') = \int_0^{t'} \mathrm{d}t_1' \int_{t_1'}^{t'} \mathrm{d}t_2' \, e^{\lambda_l^-(t_2'-t_1')+\lambda_k^+ t_1'} + \int_0^{t'} \mathrm{d}t_1' \int_0^{t_1'} \mathrm{d}t_2' \, e^{\lambda_l^-(t_1'-t_2')+\lambda_k^+ t_2'} = 2\frac{\lambda_k^+(1-e^{\lambda_l^- t'}) - \lambda_l^-(1-e^{\lambda_k^+ t'})}{\lambda_l^- \lambda_k^+ (\lambda_k^+ - \lambda_l^-)}. \tag{93}$$

We define

$$A_{kl} \equiv \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} = \frac{3^{2/3}\Gamma(2/3)^2}{12\pi^2} \frac{(k+l+1)\Gamma(k+1/3)\Gamma(l+1/3)\Gamma(l-k+1/3)}{\Gamma(k+1)\Gamma(l+5/3)\Gamma(l-k+2)} \tag{94}$$

for $k \geqslant l-1$ and zero otherwise. In order to determine $\langle x^2(t) \rangle$, the sum

$$S(t') = \sum_{kl} A_{kl} T_{kl}(t') \tag{95}$$

is required. Note that $A_{kl}=0$ for $k<l-1$. Consider the behavior of (95) at large values of t'. We write the $k=0$ term separately

$$T_{0l} = -\frac{2t'}{\lambda_l^-} + \frac{2}{\lambda_l^{-2}}(e^{\lambda_l^- t'} - 1). \tag{96}$$

This gives

$$\langle x^2(t) \rangle = 2\mathcal{D}_x t + \left(\frac{p_0 D_1}{\gamma} \right)^{2/3} \frac{1}{m^2\gamma^2} \sum_{l=0}^{\infty} Z_{0l}^2 \frac{2}{\lambda_l^{-2}} (e^{\lambda_l^- t'} - 1) + \left(\frac{p_0 D_1}{\gamma} \right)^{2/3} \frac{1}{m^2\gamma^2} \sum_{k=1}^{\infty} \sum_{l=k-1}^{\infty} \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} T_{kl}(t'). \tag{97}$$

At large t' the secular term dominates and diffusion is thus recovered. The diffusion constant is obtained as[2]

$$\mathcal{D}_x = \frac{(p_0 D_1)^{2/3}}{m^2 \gamma^{5/3}} \frac{\pi 3^{-5/6}}{2\Gamma(2/3)^2} F_{32}\left(\frac{1}{3}, \frac{1}{3}, \frac{2}{3}; \frac{5}{3}, \frac{5}{3}; 1 \right). \tag{98}$$

C. Anomalous diffusion at short times

Next we consider short times. In order to evaluate (95) at small values of t', we replace the sums in (95) by integrals:

$$S(t') = \int_0^\infty \mathrm{d}l \int_0^l \mathrm{d}k\, T(k,l,t)A(k,l). \tag{99}$$

In order to evaluate (99) we use the asymptotic form of the coefficients A_{kl}:

$$A(k,l) \sim \frac{3^{2/3}\Gamma(2/3)^2}{12\pi^2}\frac{k+l}{k^{2/3}l^{4/3}(l-k)^{5/3}}. \tag{100}$$

The coefficients $A(k,l)$ exhibit nonintegrable divergence $k \to l$. In view of this divergence we make use of a sum rule of the A_{kl}:

$$\sum_{k=0}^{l+1} A_{kl} = 0. \tag{101}$$

It can be derived by considering

$$\sum_{k=0}^{l+1} \psi_k^+(z)\langle\psi_k^+|\hat{z}|\psi_l^-\rangle = \sum_{k=0}^{\infty} \psi_k^+(z)\langle\psi_k^+|\hat{z}|\psi_l^-\rangle = \sum_{k=0}^{\infty} \langle z|\psi_k^+\rangle\langle\psi_k^+|\hat{z}|\psi_l^-\rangle = \langle z|\hat{z}|\psi_l^-\rangle, \tag{102}$$

which vanishes for $z=0$. Replacing sums by integrals the sum rule amounts to

$$\int_0^l \mathrm{d}k\, A(k,l) = 0. \tag{103}$$

Equation (103) allows us to write

$$S(t') = \int_0^\infty \mathrm{d}l \int_0^l \mathrm{d}k\, [T(k,l;t') - \lim_{k\to l} T(k,l;t')]A(k,l). \tag{104}$$

We find that the divergence of $A(k,l)$ is reduced to an integrable divergence by the fact that $T(k,l;t) - \lim_{k\to l} T(k,l;t) = O(k-l)$. Approximately, $T(k,l;t)$ is given by

$$T(k,l;t) = -2\frac{3k[1-\exp(-3lt)] - 3l[1-\exp(-3kt)]}{27lk(l-k)}. \tag{105}$$

Changing the integration variables in (104) to $x=3lt$ and $xy=3kt$, we have $k=xy/(3t)$ and $l=x/(3t)$, and

$$A(x,y,t) = \frac{3^{10/3}\Gamma(2/3)^2}{12\pi^2}t^{8/3}x^{-8/3}\frac{1+y}{y^{2/3}(1-y)^{5/3}}. \tag{106}$$

The Jacobian of the transformation is $J=x/(9t^2)$. In the new variables,

$$T(x,y;t) = -2\frac{t^2}{x}\left[\frac{a(x)-a(xy)}{1-y}\right] \tag{107}$$

where

$$a(x) = [1-\exp(-x)]/x. \tag{108}$$

Using

$$\lim_{y\to 1} T(x,y;t) = -2\frac{t^2}{x}\left[\frac{\partial}{\partial y}a(xy)\right]\Bigg|_{y=1} = -2\frac{t^2}{x}xa'(x) \tag{109}$$

we finally obtain

$$T(k,l;t) - \lim_{k\to l} T(k,l;t) = -2\frac{t^2}{x}\left[\frac{a(x)-a(xy)}{1-y} - xa'(x)\right]. \tag{110}$$

This gives

$$S(t) = -C\,t^{8/3}\int_0^\infty \mathrm{d}x\, x^{-8/3}\int_0^1 \mathrm{d}y\left[\frac{a(x)-a(xy)}{1-y} - xa'(x)\right]\frac{1+y}{y^{2/3}(1-y)^{5/3}} \tag{111}$$

with $C=3^{1/3}\Gamma(2/3)^2/(2\pi^2)$. Equation (111) implies anomalous spatial diffusion at short times:

$$\langle x^2(t)\rangle = \mathcal{C}_x(p_0D_1)^{2/3}m^{-2}t^{8/3} \tag{112}$$

with

$$\mathcal{C}_x = -C\int_0^\infty \mathrm{d}x\, x^{-8/3}\int_0^1 \mathrm{d}y\left[\frac{a(x)-a(xy)}{1-y} - xa'(x)\right]\frac{1+y}{y^{2/3}(1-y)^{5/3}}. \tag{113}$$

This anomalous diffusion is analogous to that described by Golubovic, Feng, and Zeng[9] in the case where there is no damping (they considered the case where $\zeta=3$ in their paper). Our results give the prefactor as well as the scaling behavior. It is noteworthy that we are able to solve the problem discussed in Ref. 9 by solving a more complex set of equations exactly, and taking a limit.

In Ref. 2, Fig. 2b shows plots of Eqs. (97) and (112) in comparison with numerical simulations of the equations of motion (10), exhibiting anomalous spatial diffusion at short times, and a crossover to diffusion at long times.

VII. WKB ANALYSIS

The staggered ladder spectrum discussed in Sec. IV is surprising, especially in view of the fact that for large quantum number n we expect that the eigenfunctions of the Hamiltonian (23) might be obtained by WKB theory. In this section we show how to determine the spectrum (29) of $\hat{H}$ using asymptotic WKB analysis. We show how phase shifts associated with the singularity at $z=0$ of the Hamiltonian (23) are the source of the staggered spectrum. It turns out that the WKB procedure gives rise to the exact eigenvalues.

In dimensionless coordinates, the classical Hamilton function corresponding to (23) is

$$H_{\mathrm{cl}} = \frac{1}{2} - \frac{z^3}{4} - p^2/z. \tag{114}$$

Solving $H_{\mathrm{cl}}=\lambda$ for p we obtain $p(z,\lambda)=\pm\frac{1}{2}\sqrt{(2-4\lambda)z-z^4}$, while the velocity is

$$\dot{z} = \partial H_{\mathrm{cl}}/\partial p = -2p/z. \tag{115}$$

The classical trajectories are figure-of-eight orbits, illustrated in Fig. 2.

The WKB wave function is of the form

$$f(z) = [z/p(z,\lambda)]^{1/2}\exp\left(\pm\mathrm{i}\int^z \mathrm{d}z p(z,\lambda)\right). \tag{116}$$

The phase of the wave function can be determined as follows. We discuss separately the behaviors of the wave function at the origin $z_0=0$ and in the vicinity of the regular turning point $z_{\mathrm{t.p.}}=(2-4\lambda)^{1/3}$. In the latter case, the wave function at $z<z_{\mathrm{t.p.}}$ connected with the turning point is

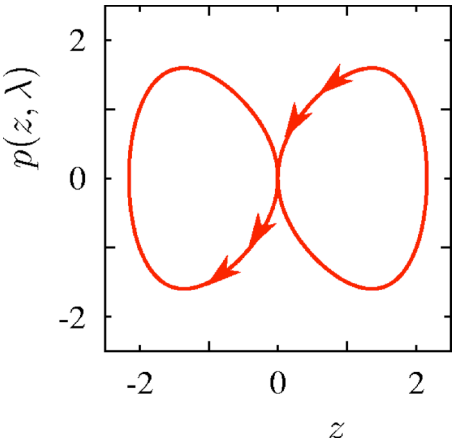

FIG. 2. (Color online) The trajectories of the classical Hamiltonian (114) are figure-of-eight orbits.

$$f_{\text{t.p.}}(z) = C_{\text{t.p.}}[z/p(z,\lambda)]^{1/2} \sin\left(\int_z^{z_{\text{t.p.}}} \mathrm{d}z\, p(z,\lambda) + \frac{\pi}{4} \right). \tag{117}$$

Consider now the behavior of the wave function near the origin. The Hamiltonian has a singularity at $z=0$. We find an exact solution of the equation when $\gamma=0$. This equation has a continuous spectrum, but we identify solutions $f_+(z)$ and $f_-(z)$ which correspond, respectively, to even and odd solutions of the full equation for $\gamma>0$ (with discrete spectrum). Close to $z=0$, the damping term in the Hamiltonian is negligible, and for $z>0$ the eigenfunctions resemble solutions of the equation

$$\partial_z z^{-1} \partial_z f(z) = -\Lambda f(z) \tag{118}$$

where $\Lambda(=-\lambda)$ is a positive constant. Write $f=F'$, and find that

$$\frac{\partial}{\partial z}\left(\frac{F'' + \Lambda z F}{z} \right) = 0 \tag{119}$$

so that $F''+\Lambda zF=Cz$ for some constant C. Thus we find $G(z)=F(z)-C/\Lambda$ satisfies $G''+z\Lambda G=0$, which has solution $G(z)=\mathrm{Ai}(-\Lambda^{1/3}z)$, and a similar solution constructed from $\mathrm{Bi}(x)$ [here $\mathrm{Ai}(y)$ and $\mathrm{Bi}(y)$ are Airy Ai and Bi functions[21]]. The general solution is

$$f(z) = A_1 \mathrm{Ai}'(-\Lambda^{1/3}z) + A_2 \mathrm{Bi}'(-\Lambda^{1/3}z). \tag{120}$$

We must find solutions of this form which resemble the behavior of the eigenfunctions of the equation with $\gamma>0$ which obey the boundary conditions

$$\frac{\mathrm{d}^2 f_+(0)}{\mathrm{d}z^2} = 0 \text{ and } f_-(0) = 0. \tag{121}$$

The functions Ai' and Bi' have the following forms in the neighborhood of $z=0$

$$\mathrm{Ai}'(y) = c_1\left(\frac{y^2}{2} + \mathcal{O}(y^5) \right) - c_2\left(1 + \frac{y^3}{3} + \mathcal{O}(y^6) \right), \tag{122}$$

$$\mathrm{Bi}'(y) = \sqrt{3}c_1\left(\frac{y^2}{2} + \mathcal{O}(y^5)\right) + \sqrt{3}c_2\left(1 + \frac{y^3}{3} + \mathcal{O}(y^6)\right) \tag{123}$$

with $y=-\Lambda^{1/3}z$, $c_1=3^{-2/3}/\Gamma(2/3)$, and $c_2=3^{-1/3}/\Gamma(1/3)$. So the positive-parity solution corresponds to the choice

$$A_1^+ = -\sqrt{3} \text{ and } A_2^+ = 1 \tag{124}$$

while

$$A_1^- = \sqrt{3} \text{ and } A_2^- = 1. \tag{125}$$

At large values of y the corresponding wave functions are of the form

$$f_\pm(y) \sim (-y)^{1/4} \sin\left(\frac{2}{3}(-y)^{3/2} + \frac{\pi}{4} \pm \frac{\pi}{3}\right). \tag{126}$$

Noting that, near $z=0$, $\int_0^z \mathrm{d}z p(z,\lambda)=(2/3)(-y)^{3/2}$ and $(z/p(z,\lambda))^{1/2} \propto (-y)^{1/4}$, the solution coming from the origin is

$$f_{O,\pm}(z) = C_{O,\pm}[z/p(z,\lambda)]^{1/2} \sin\left(\int_0^z \mathrm{d}z'\, p(z',\lambda) + \frac{\pi}{4} \pm \frac{\pi}{3}\right). \tag{127}$$

The forms (117) and (127) should be smoothly connected for $0<z<z_{\mathrm{t.p.}}$. This requires

$$\int_0^{z_{\mathrm{t.p.}}} \mathrm{d}z\, p(z,\lambda) + \frac{\pi}{2} \pm \frac{\pi}{3} = (n+1)\pi, \tag{128}$$

for $n=0,1,\ldots$ together with $C_{\mathrm{t.p.}}=(-1)^n C_{O,\pm}$. Writing

$$S(\lambda) = \int_0^{z_{\mathrm{t.p.}}} \mathrm{d}z\, p(z,\lambda) = \frac{\pi}{12}(-4\lambda + 2), \tag{129}$$

we find the quantization condition

$$S(\lambda_\pm) = \left(n + \tfrac{1}{2} \mp \tfrac{1}{3}\right)\pi. \tag{130}$$

Using (129) the quantization condition takes the form

$$\lambda = \begin{cases} -3n & \text{even parity} \\ -3n-2 & \text{odd parity}, \end{cases} \tag{131}$$

which corresponds exactly to the spectrum (29) obtained by algebraically diagonalizing $\hat{H}$.

VIII. RESULTS FOR OTHER VALUES OF ζ

Up to now we have only considered the case of generic random forcing [where the constant D_1 in Eq. (8) is not zero], corresponding to the case $\zeta=1$ in Eq. (9). In this section we explain two cases where other values of ζ arise and briefly describe results for arbitrary positive values of ζ, analogous to the results obtained in Sec. VI.

First consider the case where the force is the gradient of a potential, $f(x,t)=\partial V(x,t)/\partial x$. We assume that the potential has mean value zero and correlation function $\mathcal{C}(X,T)=\langle V(x+X,t+T)V(x,t)\rangle$. Assuming that $\mathcal{C}(X,T)$ is sufficiently differentiable at $T=0$, the diffusion constant is

$$D(p) = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t \left\langle \frac{\partial V}{\partial x}(pt/m,t)\frac{\partial V}{\partial x}(0,0) \right\rangle = \frac{-m}{2|p|}\int_{-\infty}^{\infty} \mathrm{d}X \frac{\partial^2 \mathcal{C}}{\partial X^2}(X,mX/p)$$
$$= \frac{-m}{2|p|}\int_{-\infty}^{\infty} \mathrm{d}X \left[\frac{\partial^2 \mathcal{C}}{\partial x^2}(X,0) + \frac{mX}{p}\frac{\partial^3 \mathcal{C}}{\partial^2 X \partial T}(X,0) + \frac{m^2X^2}{2p^2}\frac{\partial^4 \mathcal{C}}{\partial^2 X \partial^2 T}(X,0) + O(X^3) \right]. \quad (132)$$

Integration by parts shows that the integral over the first term of the expansion is zero, and the integral over the second term is zero by symmetry. The leading-order contribution in $|p|^{-1}$ comes from the third term. Integrating this term by parts twice gives

$$D(p) \sim \frac{-m^3}{2|p|^3}\int_{-\infty}^{\infty} \mathrm{d}X \frac{\partial^2 \mathcal{C}}{\partial T^2}(X,0). \quad (133)$$

Thus in the case of a potential force with a sufficiently smooth correlation function we have $\zeta = 3$.

An exceptional case which is worthy of comment is when the potential $V(x,t)$ is itself generated from a set of Ornstein-Uhlenbeck processes $A_j(t)$ by writing $V(x,t)=\Sigma_j A_j(t)\Phi_j(x)$, where the $\Phi_j(x)$ are elements of some suitable set of basis functions. In this case the correlation function of $V(x,t)$ is of the form $c(x)\exp(-\gamma|t|)$ [for some function $c(x)$]. Then the second term in the expansion on the final line of Eq. (132) does not vanish by symmetry and we find $D(p) \propto |p|^{-2}$, that is $\zeta=2$.

For general positive values of ζ the Hamiltonian (22) is replaced by

$$\hat{H} = \frac{1}{2} - \frac{1}{4}|z|^{2+\zeta} + \frac{\partial}{\partial z}\frac{1}{|z|^{\zeta}}\frac{\partial}{\partial z}. \quad (134)$$

Its ground state

$$\lambda_0^+ = 0 \text{ and } \psi_0^+(z) = \mathcal{C}_0^+ e^{-|z|^{\zeta+2}/(4+2\zeta)} \quad (135)$$

and first excited state

$$\lambda_0^- = -1-\zeta \text{ and } \psi_0^-(z) = \mathcal{C}_0^- z|z|^{\zeta} e^{-|z|^{\zeta+2}/(4+2\zeta)} \quad (136)$$

are found by inspection. Raising and lowering operators can be introduced in a manner analogous to Eqs. (24)–(26). We write

$$\hat{H} = \hat{a}^-|z|^{-\zeta}\hat{a}^+ \quad (137)$$

with $\hat{a}^{\pm}=\partial_z \pm z|z|^{\zeta}/2$. The operators

$$\hat{A} = \hat{a}^+|z|^{-\zeta}\hat{a}^+ \text{ and } \hat{A}^+ = \hat{a}^-|z|^{-\zeta}\hat{a}^- \quad (138)$$

satisfy

$$[\hat{H},\hat{A}] = (2+\zeta)\hat{A} \text{ and } [\hat{H},\hat{A}^+] = -(2+\zeta)\hat{A}^+ \quad (139)$$

and act as lowering and raising operators. For the spectrum of $\hat{H}$ we obtain

$$\lambda_n^+ = -(2+\zeta)n \text{ and } \lambda_n^- = -(2+\zeta)n - 1 - \zeta. \quad (140)$$

These expressions replace (29). Note also that the commutator of $\hat{A}$ and $\hat{A}^+$ is

$$[\hat{A},\hat{A}^+] = -(2+\zeta)(\hat{H}+\hat{G}) \quad (141)$$

where $\hat{G}=\hat{a}^+|z|^{-\zeta}\hat{a}^-$ and $\hat{H}-\hat{G}=\hat{I}$. The normalization of the eigenstates

$$\hat{A}^+|\psi_n^-\rangle = C_{n+1}^-|\psi_{n+1}^-\rangle, \tag{142}$$

$$\hat{A}|\psi_n^-\rangle = C_n^-|\psi_{n-1}^-\rangle \tag{143}$$

is determined as in Sec. IV A 2. We obtain

$$(C_{n+1}^-)^2 = (2+\zeta)(n+1)[(2+\zeta)n+3+2\zeta] \tag{144}$$

and

$$(C_{n+1}^+)^2 = (2+\zeta)(n+1)[(2+\zeta)n+1]. \tag{145}$$

The results of Sec. V for the matrix elements $Z_{mn}=\langle\psi_m^-|\hat{z}|\psi_n\rangle$ and for $\psi_n^+(0)/\psi_0^+(0)$ generalize as follows:

$$Z_{mn} = (-1)^{n-m}\frac{(2+\zeta)^{-(1+\zeta)/(2+\zeta)}}{\Gamma\left(\frac{\zeta}{2+\zeta}\right)}(m+n+1)\frac{\Gamma\left(\frac{\zeta}{2+\zeta}-m+n\right)\sqrt{\Gamma(n+1)\Gamma\left(\frac{1}{2+\zeta}+m\right)}}{\Gamma(2-m+n)\sqrt{\Gamma\left(\frac{3+2\zeta}{2+\zeta}+n\right)\Gamma(m+1)}}, \tag{146}$$

$$\psi_n^+(0)/\psi_0^+(0) = (-1)^n\sqrt{\frac{\Gamma[((2+\zeta)n+1)/(2+\zeta)]}{\Gamma(n+1)\Gamma(1/(2+\zeta))}}. \tag{147}$$

This allows us to obtain, for example, the diffusion constant

$$\mathcal{D}_x = \frac{1}{m^2}\left(\frac{p_0^{2\zeta}D_\zeta^2}{\gamma^{4+\zeta}}\right)^{1/(2+\zeta)}\frac{(2+\zeta)^{-(4+3\zeta)/(2+\zeta)}\pi F_{32}\left(\frac{\zeta}{2+\zeta},\frac{\zeta}{2+\zeta},\frac{1+\zeta}{2+\zeta};\frac{3+2\zeta}{2+\zeta},\frac{3+2\zeta}{2+\zeta};1\right)}{\sin\left(\frac{\pi}{2+\zeta}\right)\Gamma\left(\frac{3+2\zeta}{2+\zeta}\right)^2} \tag{148}$$

describing the dynamics at large times. Upon substituting $\zeta=0$, Eq. (148) reproduces the standard Ornstein-Uhlenbeck result, and it gives (98) for $\zeta=1$.

For the short-time anomalous diffusion we obtain

$$\langle x^2(t)\rangle = \mathcal{C}_x((p_0^\zeta D_\zeta)^{2/(2+\zeta)}m^{-2})t^{(6+2\zeta)/(2+\zeta)} \tag{149}$$

with

$$\mathcal{C}_x = -C\int_0^\infty \mathrm{d}x\, x^{-(6+2\zeta)/(2+\zeta)}\int_0^1 \mathrm{d}y\left[\frac{a(x)-a(xy)}{1-y}-xa'(x)\right]\frac{1+y}{y^{(1+\zeta)/(2+\zeta)}(1-y)^{(4+\zeta)/(2+\zeta)}}, \tag{150}$$

where $a(x)$ is the same as in (113), and

$$C = \frac{2(2+\zeta)^{-2\zeta/(2+\zeta)}}{\Gamma\left(\frac{\zeta}{2+\zeta}\right)^2}. \tag{151}$$

This reproduces (112) for $\zeta=1$ and concludes our summary of results for other than generic random forcing.

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Heat equilibrium distribution in a turbulent flow

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We consider a shear flow of a scale invariant Gaussian random velocity field that does not depend on the coordinates in the direction of the flow. We investigate a heat advection coming from a Gaussian random homogeneous source. We discuss a relaxation at large time of a temperature distribution determined by the forced advection-diffusion equation. We represent the temperature correlation functions by means of the Feynman-Kac formula. Jensen inequalities are applied for lower and upper bounds on the correlation functions. We show that at finite time there is no velocity dependence of long range temperature correlations (low momentum asymptotics) in the direction of the flow but the equilibrium heat distribution has large distance correlations (low momentum behavior) with an index depending on the scaling index of the random flow and of the index of the random forcing. If the velocity has correlations growing with the distance (a turbulent flow), then the large distance correlations depend in a crucial way on the scaling index of the turbulent flow. In such a case the correlations increase in the direction of the flow and decrease in the direction perpendicular to the flow, making the stream of heat more coherent. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217808]

I. INTRODUCTION

We investigate a heat advection in a random flow that is supposed to be "turbulent." The turbulence is a complex phenomenon that is difficult to define in precise mathematical terms. The complexity of turbulence can be related to its dependence on the length scale relevant for undergoing experiments. In this paper we apply only some aspects of the turbulent flow: randomness of the velocity field, its self-similarity, and long range correlations. The appearance of the turbulence should have an impact on transport phenomena described by an advection-diffusion equation of a passive scalar.[1] Such an equation can describe transport of heat, a mass, or some impurities. We are interested in the equilibrium distribution of solutions of the random advection-diffusion equation. The equilibrium is possible only under an external forcing (a heat source). We are interested in the equilibrium distribution at all scales. Such an equilibrium will depend on the forcing. The universality is possible only in the inertial range[2–4] where the external forcing should not be relevant (see Ref. 5 for some recent shear flow experiments). Although the precise equilibrium distribution depends on the form of the forcing. the asymptotic behavior of correlation functions depends solely on the asymptotic behavior of the random forcing. We investigate the way the long range correlations of the fluid velocity influence the long range correlations of the temperature.

We assume that there is a distinguished direction of the fluid velocity $\mathbf{V}$. We make a decomposition $X=(\mathbf{x},\mathbf{z})\in R^D$ with $\mathbf{x}\in R^d$ and $\mathbf{z}\in R^{D-d}$; $\mathbf{V}(\tau,\mathbf{x})$ depends only on $\mathbf{x}\in R^d$ and has nonvanishing components only in R^{D-d} (in such a case it automatically satisfies $\nabla\mathbf{V}=0$; for physical applications $D=3$ and $d=2$ or $d=1$). As a typical example we could consider a fluid flow $V_z(x,y)$ in the direction of the z axis, which does not depend on z. We can impose such an anisotropy of

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the flow by an external force $\mathbf{R}$, which depends only on $\mathbf{x}$ and has nonzero components solely in the $\mathbf{z}$ direction. So, we consider the Navier-Stokes equation with such a random force $\mathbf{R}$:

$$\partial_t \mathbf{V} + \mathbf{V} \nabla \mathbf{V} - \nu \Delta \mathbf{V} = \mathbf{R}.$$

The $(0, \mathbf{V}(\mathbf{x}))$ solution of the Navier-Stokes equation is the solution of the linear equation (for the $\mathbf{z}$ component)

$$\partial_t \mathbf{V} - \nu \Delta_{\mathbf{x}} \mathbf{V} = \mathbf{R}$$

(together with a zero solution for the $\mathbf{x}$ component). By properly choosing the external force $\mathbf{R}$ we can simulate a large class of $\mathbf{x}$-dependent flows.

In Secs. II and III we discuss the advection-diffusion equation, the random velocity, and a random forcing. The advection-diffusion equation can be solved by means of the Feynman-Kac formula. The Feynman-Kac solution has already been discussed by other authors.[6,7] These authors have been interested in the asymptotic behavior of the advection-diffusion equation without forcing. Our main interest (Secs. IV and V) is in the asymptotic behavior for large time and distances of correlation functions of the temperature field resulting from the advection-diffusion equation with forcing describing the heat injection. First, in Sec. III we simulate forcing by a constant gradient term in the temperature. We obtain a simple soluble model of advection illustrating some general features. In general, we can obtain some lower and upper bounds on the correlation functions by means of the Jensen inequalities (Sec. V). For the sake of simplicity we concentrate on the two-point correlations. In Sec. VI we show how our methods can be extended to multipoint correlations. We obtain asymptotic behavior of the Fourier transform of the correlation functions for small and large momenta. We compare our methods and results (in Secs. IV–VI and in Appendix B) with an exactly soluble model of Kraichnan[4,8,9] (defined by a velocity field, which is a white noise in time). The random advection is closely connected with diffusion. In fact, under some natural assumptions random advection enforces diffusion[10–12] and vice versa the diffusion can be expressed as a white noise advection.[13] However, when we choose no diffusion (zero molecular diffusivity) in the initial equation of advection describing the temperature evolution, then we obtain a model of advection (discussed in Appendix A) as a limit of the solution of the random advection-diffusion equation. The limit of zero molecular diffusivity has been discussed earlier in Refs. 14 and 15.

In the text some positive constants arise (denoted usually as K, c_1, etc.) that are not described at each case and are not related one to another.

II. THE ADVECTION-DIFFUSION EQUATION

We consider the advection in a random velocity field $\mathbf{V}$ (described in Sec. I) forced by a random source f:

$$\partial_\tau \theta_\tau + \mathbf{V} \nabla \theta_\tau - \frac{\mu^2}{2} \Delta \theta_\tau = f, \tag{1}$$

where μ^2 is the molecular diffusivity. If the random velocity $\mathbf{V}$ has singular correlation functions at small time, then Eq. (1) needs a careful interpretation. If the singularity of the velocity's covariance is of the form $\delta(t-t')D(\mathbf{x}-\mathbf{x}')$, then there are two standard interpretations, either Ito or Stratonovitch.[16,17] The difference between them in Eq. (1) is $1/2 D(\mathbf{0}) \nabla^2_{\mathbf{z}} \theta$. Hence, choosing one of them will change only the diffusion constant. We choose the Stratonovitch interpretation throughout the paper and also in Appendix B.

First, let us consider $\mathbf{V}=0$ and $f=0$. Let N be a (deterministic) solution of the heat equation

$$\partial_\tau N_\tau - \frac{\mu^2}{2} \Delta N_\tau = 0. \tag{2}$$

We expand θ around the solution N of the diffusion equation

$$\theta = T + N$$

(if the mean value of $\mathbf{V}$ is zero, then T describes fluctuations of the temperature). From Eq. (1)

$$\partial_\tau T_\tau + \mathbf{V}\nabla T_\tau - \frac{\mu^2}{2}\Delta T_\tau = F, \tag{3}$$

where

$$F = f - \mathbf{V}\nabla N_\tau.$$

As the simplest example of a physical relevance we consider the mean gradient[18,19]

$$N = -\mathbf{gX}, \tag{4}$$

where $\mathbf{g}$ is a constant vector. The mean gradient is a stationary solution of the heat equation between two planes kept at fixed temperatures. For such a static solution

$$F = f + \mathbf{Vg}. \tag{5}$$

We can see that even if $f=0$ then F is nontrivial. This is a frequent realization of an advection in experiments.[20,21] In such a case the source F has the same distribution as the velocity. A constant mean gradient distinguishes a direction in space. It breaks the rotational symmetry. As a model we could consider $\mathbf{g}=(0,0,g_z)$ and $\mathbf{V}=(0,0,V_z)$.

We define the spectral measure ρ of the temperature T, which is directly measurable in experiments[22]

$$\langle T_\tau(\mathbf{x},\mathbf{z})T_\tau(\mathbf{x}',\mathbf{z}')\rangle - \langle T_\tau(\mathbf{x},\mathbf{z})\rangle\langle T_\tau(\mathbf{x}',\mathbf{z}')\rangle = \int d\mathbf{k}d\mathbf{p}\,\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}') + i\mathbf{p}(\mathbf{z}-\mathbf{z}'))\rho_\tau(\mathbf{k},\mathbf{p}). \tag{6}$$

We have

$$\int d\mathbf{x}(\langle \tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p})\tilde{\mathrm{T}}_\tau(\mathbf{x}',\mathbf{p}')\rangle - \langle \tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p})\rangle\langle \tilde{\mathrm{T}}_\tau(\mathbf{x}',\mathbf{p}')\rangle) = \delta(\mathbf{p}+\mathbf{p}')\rho_\tau(0,\mathbf{p}) \tag{7}$$

and

$$\langle \tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p})\tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p}')\rangle - \langle \tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p})\rangle\langle \tilde{\mathrm{T}}_\tau(\mathbf{x},\mathbf{p})\rangle = \delta(\mathbf{p}+\mathbf{p}')\int d\mathbf{k}\rho_\tau(\mathbf{k},\mathbf{p}),$$

$$\langle T_\tau(\mathbf{x},\mathbf{z})T_\tau(\mathbf{x},\mathbf{z})\rangle - \langle T_\tau(\mathbf{x},\mathbf{z})\rangle\langle T_\tau(\mathbf{x},\mathbf{z})\rangle = \int d\mathbf{p}\int d\mathbf{k}\rho_\tau(\mathbf{k},\mathbf{p}).$$

When the spectral function has singularities at low momenta, then the Fourier transform in Eq. (6) may need a careful definition in the sense of generalized functions. Instead of the correlation functions of $T_\tau(\mathbf{x},\mathbf{y})$, we could consider the structure functions

$$\mathcal{G}_\tau^{(2n)}(\mathbf{x},\mathbf{z}) = \langle (T_\tau(0,0) - \langle T_\tau(0,0)\rangle - T_\tau(\mathbf{x},\mathbf{z}) + \langle T_\tau(\mathbf{x},\mathbf{z})\rangle)^{2n}\rangle.$$

For $n=1$ we have

$$\mathcal{G}_\tau^{(2)}(\mathbf{x},\mathbf{z}) = 2\int d\mathbf{k}d\mathbf{p}\rho_\tau(\mathbf{k},\mathbf{p})(1-\exp(i\mathbf{kx}+i\mathbf{p}z)).$$

$\mathcal{G}_\tau^{(2)}$ scales in the same way as $\langle TT\rangle$ but has better infrared behavior. The structure functions $\mathcal{G}^{(2n)}$ are expressed by the correlation functions of the Fourier transforms of T_τ.

It can be seen that the spectral measure ρ of the temperature T depends on the spectral measure of the source f and the scaling properties of the random velocity field.

III. GAUSSIAN MODEL OF THE SHEAR FLOW

We decompose the fluid velocity

$$\mathbf{V} = \mathbf{U} + \mathbf{v}$$

into the mean value $\mathbf{U}$ and random fluctuations $\mathbf{v}$. We assume that the velocity $\mathbf{v}$ is a Gaussian Euclidean R^d invariant random field with the mean zero and the covariance

$$\langle v_j(s,\mathbf{x})v_k(s',\mathbf{x}')\rangle = G_{jk}(s-s',\mathbf{x},\mathbf{x}'), \tag{8}$$

where $j,k=d+1,\ldots,D$. For the sake of simplicity of the arguments we shall sometimes separate the time dependence, choosing G of the product form ΓD. If G is a decaying function of the distance $|\mathbf{x}-\mathbf{x}'|$ then a model of the vector field $\mathbf{v}$ can be determined by a translation invariant G, e.g.,

$$G_{jk}(s-s',\mathbf{x},\mathbf{x}') \equiv \delta_{jk}\Gamma(s-s')D(\mathbf{x}-\mathbf{x}') = \delta_{jk}\Gamma(s-s')\int d\mathbf{p}\,\exp(i\mathbf{p}(\mathbf{x}-\mathbf{x}'))\tilde{D}(\mathbf{p}), \tag{9}$$

where $\tilde{D}$ is a locally integrable function.

In a description of the turbulence we consider growing long range correlations. In such a case G cannot be translation invariant. We consider a model with Euclidean R^d invariant correlation functions of $\mathbf{v}(\mathbf{x})-\mathbf{v}(\mathbf{x}')$. Then

$$G_{jk}(s-s',\mathbf{x},\mathbf{x}') = \delta_{jk}\Gamma(s-s')(|\mathbf{x}|^{2\beta}+|\mathbf{x}'|^{2\beta}-|\mathbf{x}-\mathbf{x}'|^{2\beta}). \tag{10}$$

This G is positive definite if Γ is positive definite and $0<\beta<1$ [the covariance (10) determines Levy's model[23] of the Brownian motion depending on d parameters]. When $2\beta<2$ then the vector field $\mathbf{v}(\mathbf{x})$ does not satisfy the Lipschitz condition. In such a case we could expect difficulties with the uniqueness of the flow and the uniqueness of the solution of Eq. (1) at $\mu=0$. Fortunately, a definition of the unique solution of Eq. (1) in a weak probabilistic sense is possible[24,25] even without the Lipschitz condition.

The source f is an independent Gaussian field with the covariance

$$\langle f(s,\mathbf{x},\mathbf{z})f(s',\mathbf{x}',\mathbf{z}')\rangle = M(s-s',\mathbf{x}-\mathbf{x}',\mathbf{z}-\mathbf{z}'). \tag{11}$$

We take the Fourier transform of Eq. (3) in the $\mathbf{z}$ variable. Then, this equation reads

$$\partial_\tau \tilde{T}_\tau(\mathbf{x},\mathbf{p}) + \left(i\mathbf{p}\mathbf{V}(\tau,\mathbf{x}) + \frac{\mu^2\mathbf{p}^2}{2} - \frac{\mu^2}{2}\Delta_{\mathbf{x}}\right)\tilde{T}_\tau(\mathbf{x},\mathbf{p}) = \tilde{F}(\tau,\mathbf{x},\mathbf{p}). \tag{12}$$

We apply the Feynman-Kac formula[17] in order to express the solution of Eq. (12) with the initial condition $T_0 \in L^2(dX)$ in the form (the uniqueness of the solution is discussed in Refs. 24 and 25)

$$\tilde{T}_\tau(\mathbf{x},\mathbf{p}) = \exp\left(-\frac{\mu^2\mathbf{p}^2\tau}{2}\right)E\left[\exp(-i\mathbf{p}\int_0^\tau \mathbf{V}(\tau-s,\mathbf{x}+\mu\mathbf{b}(s))ds)\tilde{T}_0(\mathbf{x}+\mu\mathbf{b}(\tau),\mathbf{p})\right] + \int_0^\tau dt\exp\left(-\frac{\mu^2\mathbf{p}^2(\tau-t)}{2}\right)E\left[\exp\left(-i\mathbf{p}\int_0^{\tau-t}\mathbf{V}(\tau-s,\mathbf{x}+\mu\mathbf{b}(s))ds\right)\times\tilde{F}(t,\mathbf{x}+\mu\mathbf{b}(\tau-t),\mathbf{p})\right]. \quad (13)$$

In Eq. (13) b_j $(j=1,2,\ldots,d)$ is the Brownian motion defined as the Gaussian process with the covariance[17]

$$E[b_j(s)b_k(t)] = \delta_{jk}\min(s,t).$$

We are interested in the equilibrium distribution of T_τ, i.e., in the limit $\tau\to\infty$. When $\tau\to\infty$ and $T_0 \in L^2(dX)$, then the first term in Eq. (13) is vanishing. For this reason we may set $T_0=0$ from the beginning. The stationary solutions N being harmonic functions are not square integrable in R^D. Admitting such functions as initial conditions, we could regain the solution N from Eq. (13) (with $F=0$). In particular, the mean gradient (4) comes from a generalized function $\tilde{T}_0$ with its support concentrated at $\mathbf{p}=0$.

Before discussing more general correlations let us consider the constant mean gradient [Eqs. (4) and (5)] with $f=0$ and $F=\mathbf{g}V$. Then, from Eq. (13) (with $T_0=0$),

$$\tilde{T}_t(\mathbf{x},\mathbf{p}) = \delta(\mathbf{p})E\left[\int_0^\tau dt\mathbf{g}\mathbf{V}(t,\mathbf{x}+\mu\mathbf{b}(\tau-t))\right]. \quad (14)$$

We shall see that some properties of the general advection (3) appear already at the level of the simple model (14). It follows from Eq. (14) that

$$\langle T_\tau(\mathbf{X})\rangle = \delta(\mathbf{p})E\left[\int_0^\tau dt\mathbf{g}\mathbf{U}(t,\mathbf{x}+\mu\mathbf{b}(\tau-t))\right]$$

and

$$\langle\tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle - \langle\tilde{T}_\tau(\mathbf{x},\mathbf{p})\rangle\langle\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle = \delta(\mathbf{p})\delta(\mathbf{p}')\int_0^\tau dt\int_0^\tau dt' E[\mathbf{g}G(t-t',\mathbf{x}-\mathbf{x}'+\mu\mathbf{b}(\tau-t) - \mu\mathbf{b}'(\tau-t'))\mathbf{g}].$$

We calculate the integral over time. First, if the covariance G is time independent (a steady flow), then

$$\langle T_\tau(\mathbf{x},\mathbf{z})T_\tau(\mathbf{x}',\mathbf{z}')\rangle - \langle T_\tau(\mathbf{X})\rangle\langle T_\tau(\mathbf{X}')\rangle = 4\mu^{-4}\int d\mathbf{k}\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}'))\mathbf{g}\tilde{G}(\mathbf{k})\mathbf{g}|\mathbf{k}|^{-4}\left(1-\exp\left(-\frac{\mu^2}{2}\mathbf{k}^2\tau\right)\right)^2. \quad (15)$$

Next, let us consider

$$G(t-t',\mathbf{x}-\mathbf{x}') = \delta(t-t')D(\mathbf{x}-\mathbf{x}'). \quad (16)$$

The covariance (16) does not have any physical foundations but the virtue of the assumption (16) is the solubility of the model (3) (Ref. 8) (the Kraichnan model) in the sense that one can obtain a closed set of partial differential equations for the correlation functions (see Appendix B). In our simplified version (14)

$$\langle T_\tau(\mathbf{x},\mathbf{z})T_\tau(\mathbf{x}',\mathbf{z}')\rangle - \langle T_\tau(\mathbf{X})\rangle\langle T_\tau(\mathbf{X}')\rangle = \mu^{-2}\int d\mathbf{k}\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}'))\mathbf{g}\tilde{D}(\mathbf{k})\mathbf{g}|\mathbf{k}|^{-2}(1-\exp(-\mu^2\mathbf{k}^2\tau)). \tag{17}$$

If the **v** correlations are growing as in Eq. (10), then expression (17) can be infrared divergent (especially at $\tau=\infty$). In such a case we should rather consider

$$\langle (T_\tau(\mathbf{0},\mathbf{0}) - \langle T_\tau(\mathbf{0},\mathbf{0})\rangle - T_\tau(\mathbf{x},\mathbf{z}) + \langle T_\tau(\mathbf{x},\mathbf{z})\rangle)^2\rangle$$
$$= 8\mu^{-4}\int d\mathbf{k}(1-\exp(i\mathbf{k}\mathbf{x}))\tilde{G}(\mathbf{k})|\mathbf{k}|^{-4}\left(1-\exp\left(-\frac{\mu^2}{2}\mathbf{k}^2\tau\right)\right)^2. \tag{18}$$

In general, let

$$G(t-t',\mathbf{x}-\mathbf{x}) = \int d\omega d\mathbf{k}\tilde{G}(\omega,\mathbf{k})\exp(i\omega(t-t') + i\mathbf{k}(\mathbf{x}-\mathbf{x}')), \tag{19}$$

then

$$\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle - \langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\rangle\langle \tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle$$
$$= \delta(\mathbf{p})\delta(\mathbf{p}')\int_0^\tau dt\int_0^\tau dt'\int d\mathbf{k}\mathbf{g}\tilde{G}(t-t',\mathbf{k})\mathbf{g}\exp\left(i\mathbf{k}(\mathbf{x}-\mathbf{x}') - \frac{1}{2}\mu^2\mathbf{k}^2(2\tau-t-t')\right).$$

After the time integration

$$\langle T_\tau(\mathbf{x},\mathbf{z})T_\tau(\mathbf{x}',\mathbf{z}')\rangle - \langle T_\tau(X)\rangle\langle T_\tau(X')\rangle$$
$$= \int d\mathbf{k}d\omega\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}'))\mathbf{g}\tilde{G}(\omega,\mathbf{k})\mathbf{g}\left(\frac{1}{4}\mu^4|\mathbf{k}|^4+\omega^2\right)^{-1}\left|1-\exp\left(-\frac{1}{2}\mu^2\mathbf{k}^2\tau - i\omega\tau\right)\right|^2. \tag{20}$$

We assume that G is scale invariant:

$$G(ct,\lambda\mathbf{x}) = c^{-\alpha}\lambda^{-2\gamma}G(t,\mathbf{x}) \tag{21}$$

[$\alpha+\gamma<1$ if the time integral in Eq. (14) is to be finite]. This assumption has simple consequences for heat transport. It may not be exact in mathematical models. As an example, for the shear flow solution of the Navier-Stokes equation discussed in Sec. I, if $C_{jl}(\omega,\mathbf{k})$ is the spectral function of the force distribution **R**, then the spectral function of the stationary velocity distribution (obtained as a solution of the Navier-Stokes equation with the initial condition at t_0 and then letting $t_0\to -\infty$) is

$$\tilde{G}_{jl}(\omega,\mathbf{k}) = C_{jl}(\omega,\mathbf{k})\left(\left(\frac{\nu}{2}\mathbf{k}^2\right)+\omega^2\right)^{-1}. \tag{22}$$

We must choose a specific C in order to obtain a scale invariant $\tilde{G}$.

We can see from Eqs. (15)–(20) that at finite τ the large distance behavior of the temperature correlations is the same as that of the velocity correlations because the behavior of ρ_τ for small momenta does not change. However, if $\langle \mathbf{v}(\mathbf{x})\mathbf{v}(0)\rangle \simeq |\mathbf{x}|^{2\beta}$, then at $\tau=\infty$ for a steady flow we obtain in Eq. (18)

$$\langle (T_\infty(\mathbf{x},\mathbf{z}) - \langle T_\infty(\mathbf{x},\mathbf{z})\rangle - T_\infty(\mathbf{0},\mathbf{0}) + \langle T_\infty(\mathbf{0},\mathbf{0})\rangle)^2\rangle \simeq |\mathbf{x}|^{2\beta+4},$$

and for the Kraichnan model[8]

$$\langle (T_\infty(\mathbf{x},\mathbf{z}) - \langle T_\infty(\mathbf{x},\mathbf{z})\rangle - T_\infty(\mathbf{0},\mathbf{0}) + \langle T_\infty(\mathbf{0},\mathbf{0})\rangle)^2\rangle \simeq |\mathbf{x}|^{2\beta+2}$$

in Eq. (17). For a general time-dependent $G(t,\mathbf{x})$ of the form (19), we shall have the $|\mathbf{x}|^{2\beta-2\alpha+4}$ behavior of the structure functions $S_\infty^{(2)}$ in Eq. (20) if G scales as in Eq. (21) ($\gamma=-\beta$). We can establish the behavior for large $\mathbf{x}-\mathbf{x}'$ by means of a change of variables in the integrals (15)–(20), $\mathbf{k}=\tilde{\mathbf{k}}|\mathbf{x}-\mathbf{x}'|^{-1}$ and $\omega=\tilde{\omega}|\mathbf{x}-\mathbf{x}'|^{-2}$ and an estimate of the remainder. Note that the long range correlations of the velocity field ($\gamma<0$) lead to an increase of the temperature correlations.

IV. GAUSSIAN WHITE NOISE SOURCE

In this section we consider $F=f$ as a Gaussian random field independent of $\mathbf{v}$. Estimates on the equilibrium distribution are simplified if the sources at different times are independent:

$$M(t-t',\mathbf{x}-\mathbf{x}',\mathbf{z}-\mathbf{z}') = \delta(t-t')m(\mathbf{x}-\mathbf{x}',\mathbf{z}-\mathbf{z}'). \tag{23}$$

We assume the form (23) of M as a technical simplification. This is a mathematical idealization still justified by an application of physical sources of heat (as heat injections are independent at each time).

For a lower bound we need an assumption that the dependence on $\mathbf{x}-\mathbf{x}'$ is of the form of the Laplace transform (such an assumption includes the scale invariant distributions m, which do not increase at large distances) either in the form

$$\begin{aligned} m(\mathbf{x}-\mathbf{x}',\mathbf{z}-\mathbf{z}') &\equiv m_1(\mathbf{x}-\mathbf{x}')m_0(\mathbf{z}-\mathbf{z}') = \int d\mathbf{k}d\mathbf{p}\,\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}')+i\mathbf{p}(\mathbf{z}-\mathbf{z}'))\tilde{m}_1(\mathbf{k})\tilde{m}_0(\mathbf{p}) \\ &= \int_0^\infty da\,\nu_1(a)\exp(-a|\mathbf{x}-\mathbf{x}'|^2)m_0(\mathbf{z}-\mathbf{z}') \end{aligned} \tag{24}$$

or in the Euclidean invariant way

$$\begin{aligned} m(\mathbf{x}-\mathbf{x}',\mathbf{z}-\mathbf{z}') &= \int_0^\infty da\,\nu(a)\exp(-a(|\mathbf{x}-\mathbf{x}'|^2+|\mathbf{z}-\mathbf{z}'|^2)) \\ &\equiv \int_0^\infty da \int d\mathbf{p}\,\exp(i\mathbf{p}(\mathbf{z}-\mathbf{z}'))\exp(-a|\mathbf{x}-\mathbf{x}'|^2)\nu(a,\mathbf{p}). \end{aligned} \tag{25}$$

In Eqs. (24) and (25) ν_1 and ν are non-negative functions.

$\mathbf{v}$ in Eq. (13) enters T_τ in the form

$$\exp(i\mathbf{v}(\mathbf{J})),$$

where

$$\mathbf{v}(\mathbf{J}) = \int d\mathbf{u}\int_0^\tau ds\mathbf{v}(s,\mathbf{u})\mathbf{J}(s,\mathbf{u})$$

with

$$\mathbf{J}(s,\mathbf{u}) = -\theta(s)\mathbf{p}\,\delta(\mathbf{u}-\mathbf{x}-\mu\mathbf{b}(\tau-s)).$$

It follows that the expected values of n products of T_τ are expressed by

$$\langle \exp(i\mathbf{v}(\mathbf{J}_n))\rangle = S(\mathbf{J}_n),$$

where $S(\mathbf{J})$ is the characteristic function of the random field $\mathbf{v}$. For a Gaussian random field,

$$S(\mathbf{J}) = \exp\left(-\frac{1}{2}\mathbf{J}G\mathbf{J}\right). \tag{26}$$

Let us note that because of the translation invariance in the $\mathbf{z}$ variable of the source f, we have a conservation of momenta

$$\langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_n,\mathbf{p}_n)\rangle = \delta(\mathbf{p}_1+\cdots+\mathbf{p}_n)\mathcal{H} \tag{27}$$

The correlation functions (27) are expressed by the characteristic function (26) with $\mathbf{J}_n$ satisfying the condition (for $n>1$)

$$\int \mathbf{J}_n(s,\mathbf{u})d\mathbf{u} = 0. \tag{28}$$

It follows that in the Gaussian case with the covariance (10) the part of G that is not translation invariant does not contribute to the correlation functions.

We calculate the equal time expectation values of T_τ [Eq. (13) with the zero initial condition] under the assumption that the random fields f and $\mathbf{v}$ are independent:

$$\begin{aligned}&\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle \\ &\quad = \delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dt\,\exp(-\mu^2\mathbf{p}^2(\tau-t)) \\ &\qquad \times E\left[\exp\left(-i\mathbf{p}\int_0^{\tau-t}\mathbf{U}(\tau-s,\mathbf{x}+\mu\mathbf{b}(s))ds\right)\tilde{m}(\mathbf{x}-\mathbf{x}'+\mu\mathbf{b}(\tau-t)-\mu\mathbf{b}'(\tau-t),\mathbf{p})S(\mathbf{J}_2)\right],\end{aligned} \tag{29}$$

where

$$\mathbf{J}_2(\mathbf{u}) = \mathbf{p}\,\theta(s)\,\delta(\mathbf{u}-\mathbf{x}-\mathbf{b}(\tau-s)) - \mathbf{p}\,\theta(s)\,\delta(\mathbf{u}-\mathbf{x}'-\mathbf{b}'(\tau-s)).$$

For the Gaussian field (26)

$$\begin{aligned}S(\mathbf{J}_2) = \exp\Bigg(&-\frac{1}{2}\int_0^{\tau-t}\int_0^{\tau-t} dsds'\mathbf{p}G_0(s-s',\mu\mathbf{b}(s)-\mu\mathbf{b}(s'))\mathbf{p} \\ &-\frac{1}{2}\int_0^{\tau-t}\int_0^{\tau-t} dsds'\mathbf{p}G_0(s-s',\mu\mathbf{b}'(s)-\mu\mathbf{b}'(s'))\mathbf{p} \\ &+\int_0^{\tau-t}\int_0^{\tau-t} dsds'\mathbf{p}G_0(s-s',\mathbf{x}-\mathbf{x}'+\mu\mathbf{b}(s)-\mu\mathbf{b}'(s'))\mathbf{p}\Bigg),\end{aligned} \tag{30}$$

where G_0 is the translation invariant part of G. If

$$|\tilde{m}(\mathbf{x},\mathbf{p})| \leq K|\tilde{m}_0|(\mathbf{p}), \tag{31}$$

then from $|S(\mathbf{J})|\leq 1$ there follows the bound

$$|\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle| \leq K\delta(\mathbf{p}+\mathbf{p}')|\tilde{m}_0|(\mathbf{p})\mu^{-2}\mathbf{p}^{-2}(1-\exp(-\mu^2\mathbf{p}^2\tau)). \tag{32}$$

For a small $\mathbf{p}$ and a finite τ the correlations (32) are bounded by $\tau|\tilde{m}_0|(\mathbf{p})$ whereas at $\tau=\infty$ by $|\tilde{m}_0|(\mathbf{p})\mathbf{p}^{-2}$.

Next, we apply the scale invariance of the Brownian motion

$$\mathbf{b}(at) = \sqrt{a}\mathbf{b}(t) \tag{33}$$

in Eq. (29). We write $s=(\tau-t)\sigma$. Then, using the scaling properties (21) and (33) and denoting by G_0 the translation invariant part of G we can rewrite Eqs. (29) and (30) in the form

$$\begin{aligned}\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle = \delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dt\,\exp(-\mu^2\mathbf{p}^2(\tau-t))\\ \times E\Bigg[\exp\Bigg(-i\mathbf{p}\int_0^{\tau-t}\mathbf{U}(\tau-s,\mathbf{x}+\mu\mathbf{b}(s))ds\Bigg)\tilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{\tau-t}\mathbf{b}(1)\\ -\mu\sqrt{\tau-t}\mathbf{b}'(1),\mathbf{p})\\ \times\exp\Bigg(-\frac{1}{2}(\tau-t)^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}(\sigma)-\mu\mathbf{b}(\sigma'))\mathbf{p}\\ -\frac{1}{2}(\tau-t)^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}'(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}\\ +(\tau-t)^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',(\tau-t)^{-1/2}(\mathbf{x}-\mathbf{x}')\\ +\mu\mathbf{b}(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}\Bigg)\Bigg].\end{aligned} \tag{34}$$

For the Kraichnan model[8] $\Gamma(s-s\prime)=\delta(s-s\prime)$ in Eqs. (9) and (10), then $\alpha=1$ in Eq. (22) and formula (34) reads

$$\begin{aligned}\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle = \delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dt\,\exp(-\mu^2\mathbf{p}^2(\tau-t))\\ \times E\Bigg[\exp\Bigg(-i\mathbf{p}\int_0^{\tau-t}\mathbf{U}(\tau-s,\mathbf{x}+\mu\mathbf{b}(s))ds\Bigg)\tilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{\tau-t}\mathbf{b}(1)\\ -\mu\sqrt{\tau-t}\mathbf{b}'(1),\mathbf{p})\\ \times\exp\Bigg(-(\tau-t)^{1-\gamma}\mathbf{p}D(0)\mathbf{p}+(\tau-t)^{1-\gamma}\int_0^1 d\sigma\mathbf{p}D((\tau-t)^{-1/2}(\mathbf{x}-\mathbf{x}')\\ +\mu\mathbf{b}(\sigma)-\mu\mathbf{b}'(\sigma))\mathbf{p}\Bigg)\Bigg].\end{aligned} \tag{35}$$

V. JENSEN INEQUALITIES FOR THE TEMPERATURE CORRELATIONS

We are going to estimate the spectral measure (6) and (7) by an application of the Jensen inequality. We can obtain an upper bound on the correlation functions by applying the Jensen inequality $[\int d\nu \exp f \geqslant \exp(\int d\nu f)$ if $\int d\nu=1]$ (Ref. 26) to the time integral in Eqs. (29) and (30):

$$|\langle\widetilde{T}_\tau(\mathbf{x},\mathbf{p})\widetilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle| \leqslant 2\delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dr\int_0^1 d\sigma\int_0^\sigma d\sigma'\,\exp(-\mu^2\mathbf{p}^2 r)E\Big[|\widetilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{b}(1)$$
$$-\mu\sqrt{r}\mathbf{b}'(1),\mathbf{p})|\times\exp\Big(-\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}(\sigma)-\mu\mathbf{b}(\sigma'))\mathbf{p}$$
$$-\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}'(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}$$
$$+r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',r^{-1/2}(\mathbf{x}-\mathbf{x}')+\mu\mathbf{b}(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}\Big)\Big]. \tag{36}$$

Let $p(s,\mathbf{u};t,\mathbf{w})$ be the transition function for the Brownian motion to pass from $\mathbf{u}$ at time s to $\mathbf{w}$ at time t. Then, the expectation value (36) reads

$$|\langle\widetilde{T}_\tau(\mathbf{x},\mathbf{p})\widetilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle|$$
$$\leqslant 2\delta(\mathbf{p}+\mathbf{p}')\int d\mathbf{u}d\mathbf{u}'d\mathbf{w}d\mathbf{w}'\int_0^\tau dr\int_0^1 d\sigma\int_0^\sigma d\sigma'\,\exp(-\mu^2\mathbf{p}^2 r)$$
$$\times p(0,\mathbf{0};\sigma',\mathbf{u})p(\sigma',\mathbf{u};\sigma,\mathbf{w})p(\sigma,\mathbf{w};1,\mathbf{z})p(0,\mathbf{0};\sigma',\mathbf{u}')p(\sigma',\mathbf{u}';\sigma,\mathbf{w}')p(\sigma,\mathbf{w}';1,\mathbf{z}')$$
$$\times|\widetilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{z}-\mu\sqrt{r}\mathbf{z}',\mathbf{p})|\times\exp\Big(-\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{w}-\mu\mathbf{u})\mathbf{p}$$
$$-\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{w}'-\mu\mathbf{u}')\mathbf{p}+\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',r^{-1/2}(\mathbf{x}-\mathbf{x}')+\mu\mathbf{w}-\mu\mathbf{u}')\mathbf{p}$$
$$+\frac{1}{2}r^{2-\alpha-\gamma}\mathbf{p}G_0(\sigma-\sigma',r^{-1/2}(\mathbf{x}-\mathbf{x}')+\mu\mathbf{w}'-\mu\mathbf{u})\mathbf{p}\Big). \tag{37}$$

Till now we have kept the mean velocity $\mathbf{U}$ as an arbitrary nonzero function. We can obtain a lower bound only if

$$\mathbf{U}=0.$$

As claimed by some authors (see, e.g., the standard textbook[27]) the mean velocity does not play any essential role in turbulence. So, setting it equal to zero we do not lose much. Moreover, for the lower bound we must assume m of the form (24) [or (25)] with $\widetilde{m}_0(\mathbf{p})\geqslant 0$. Then, we can apply the Jensen inequality to the expectation value over the Brownian motion

$$\langle\widetilde{T}_\tau(\mathbf{x},\mathbf{p})\widetilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dr\,\exp(-\mu^2\mathbf{p}^2 r)\int_0^\infty da\,\nu_1(a)$$
$$\times\widetilde{m}_0(\mathbf{p})\exp E\Big[-\frac{1}{2}r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}(\sigma)-\mu\mathbf{b}(\sigma'))\mathbf{p}$$
$$-\frac{1}{2}r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}'(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}$$
$$+r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',r^{-1/2}(\mathbf{x}-\mathbf{x}')+\mu\mathbf{b}(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}$$
$$-a|\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{b}(1)-\mu\sqrt{r}\mathbf{b}'(1)|^2\Big]. \tag{38}$$

For m of the form (25) the inequality (38) reads

$$\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dr\,\exp(-\mu^2\mathbf{p}^2 r)\int_0^\infty da\,\nu(a,\mathbf{p})$$
$$\times \exp E\Bigg[-\frac{1}{2}r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma' \mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}(\sigma)-\mu\mathbf{b}(\sigma'))\mathbf{p}$$
$$-\frac{1}{2}r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma' \mathbf{p}G_0(\sigma-\sigma',\mu\mathbf{b}'(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}$$
$$+r^{2-\alpha-\gamma}\int_0^1\int_0^1 d\sigma d\sigma' \mathbf{p}G_0(\sigma-\sigma',r^{-1/2}(\mathbf{x}-\mathbf{x}')+\mu\mathbf{b}(\sigma)-\mu\mathbf{b}'(\sigma'))\mathbf{p}$$
$$-a|\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{b}(1)-\mu\sqrt{r}\mathbf{b}'(1)|^2\Bigg]. \tag{39}$$

The correlation functions (36)–(39) in general will essentially depend on the source distribution m. We consider m such that (i) m_1 is bounded from above by a constant [Eq. (31)] and, in addition, (ii) $m_1(\mathbf{x})$ is decreasing like a power 2Ω of $|\mathbf{x}|$. From Eq. (32) it follows that under the assumption (31) the limit $\tau\to\infty$ exists. We wish to estimate the correlation functions at $\tau=\infty$ under various conditions on $m_1(\mathbf{x})$. Using the inequality (for $A\geqslant 0$)

$$2\exp(-\mu^2\mathbf{p}^2 r - A(\mathbf{x}-\mathbf{x}',\mathbf{b})r^{2-\alpha-\gamma}\mathbf{p}^2) \leqslant \exp(-\mu^2\mathbf{p}^2 r)+\exp(-A(\mathbf{x}-\mathbf{x}',\mathbf{b})r^{2-\alpha-\gamma}\mathbf{p}^2),$$

and a change of variables in the r integral in Eqs. (36) and (37), $r=t|\mathbf{p}|^{-(2/2-\alpha-\gamma)}$, we obtain [when m_1 is a bounded function (31)]

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x},\mathbf{p}')\rangle \leqslant \delta(\mathbf{p}+\mathbf{p}')|\tilde{m}_0|(\mathbf{p})\left(c_1\theta\left(|\mathbf{p}|-\frac{1}{\mu}\right)|\mathbf{p}|^{-2}+c_2\theta\left(\frac{1}{\mu}-|\mathbf{p}|\right)|\mathbf{p}|^{-(2/2-\alpha-\gamma)}\right), \tag{40}$$

where on the right-hand side (rhs) of Eq. (36), after an integral over r (which can be performed by a change of variables), we obtain a function $|A(\mathbf{x}-\mathbf{x}',\mathbf{b})|^{-(1/2-\alpha-\gamma)}$ (where $\mathbf{b}$ depends on σ and $\sigma\prime$) whose expectation value is expressed by the rhs of Eq. (37). This is an integrable function of $\mathbf{u},\mathbf{w},\mathbf{z},\mathbf{u}',\mathbf{w}'$, and $\mathbf{z}'$. Hence, the integral can be bounded by a constant c_2. Under a stronger assumption that

$$\int d\mathbf{x} m_1(\mathbf{x}) < \infty \tag{41}$$

from Eq. (37) we obtain in a similar way the bound

$$\int d\mathbf{x}\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle \leqslant \delta(\mathbf{p}+\mathbf{p}')|\tilde{m}_0|(\mathbf{p})\left(c_3\theta\left(|\mathbf{p}|-\frac{1}{\mu}\right)|\mathbf{p}|^{-2}+c_4\theta\left(\frac{1}{\mu}-|\mathbf{p}|\right)|\mathbf{p}|^{-(2/2-\alpha-\gamma)}\right). \tag{42}$$

This is a bound on the spectral measure on the rhs of Eq. (7).

We wish to estimate the dependence of the correlation functions (34) on $\mathbf{x}-\mathbf{x}'$ in a more explicit form. Note that if the velocity correlations are defined by Eq. (9), where $\tilde{D}(\mathbf{k})$ is an integrable function, then on the basis of the Lebesgue lemma G is vanishing at large $|\mathbf{x}-\mathbf{x}'|$. In such a case the term depending on $\mathbf{x}-\mathbf{x}'$ in the exponential on the rhs of Eq. (34) can be neglected. If m is in addition a slowly varying function of $\mathbf{x}-\mathbf{x}'$ then

$$\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle \simeq \langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x},\mathbf{p}')\rangle. \tag{43}$$

A discussion of the turbulent flow (10) remains. We are unable to prove precise upper bounds for large $|\mathbf{x}-\mathbf{x}'|$ and general β. However, if $0<2\beta<1$ and $d=1$ then $g(\mathbf{x})=-|\mathbf{x}|^{2\beta}$ is a convex function[26]

$$g\left(\frac{1}{2}(\mathbf{x}+\mathbf{y})\right) \leqslant \frac{1}{2}g(\mathbf{x}) + \frac{1}{2}g(\mathbf{y}).$$

As a consequence,

$$\exp(-r^{2-\alpha+\beta}\mathbf{p}^2\Gamma(\sigma-\sigma')|r^{-1/2}(\mathbf{x}-\mathbf{x}') + \mu\mathbf{b}(\sigma) - \mu\mathbf{b}'(\sigma')|^{2\beta})$$
$$\leqslant \exp\left(-\frac{1}{2}r^{2-\alpha+\beta}\mathbf{p}^2\Gamma(\sigma-\sigma')(|2r^{-1/2}(\mathbf{x}-\mathbf{x}')|^{2\beta} + |2\mu\mathbf{b}(\sigma) - 2\mu\mathbf{b}'(\sigma')|^{2\beta})\right).$$

Hence, under the assumption (31) (after the r integration) the inequalities (36) and (37) at $\tau=\infty$ for $0<2\beta<1$ read

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle \leqslant K|\mathbf{p}|^{-(2/2-\alpha)}|\tilde{m}_0|(\mathbf{p})|\mathbf{x}-\mathbf{x}'|^{-(2\beta/2-\alpha)}. \tag{44}$$

We expect the inequality (44) to hold true in general [under the assumption (31)] for large $|\mathbf{x}-\mathbf{x}'|$ because we obtain such a behavior of the two-point function if in a formal way we take the limit $|\mathbf{x}-\mathbf{x}'|\to\infty$ in Eq. (34), neglecting terms of order $|\mathbf{x}-\mathbf{x}'|^{-1}$.

We discuss now the Jensen inequality (38) for the lower bound. It is sufficient to calculate the expectation value in the exponential (38). First, in the Kraichnan model (35) for the term $-W$ in the exponential appearing in Eq. (38), we obtain

$$\exp(-W(\mathbf{x}-\mathbf{x}')) = \exp\left(-r^{1-\gamma}\int d\mathbf{k}\mathbf{p}\tilde{D}(\mathbf{k})\mathbf{p}\right.$$
$$\left.\times(1-\mu^{-2}\mathbf{k}^{-2}\exp(i\mathbf{k}r^{-1/2}(\mathbf{x}-\mathbf{x}'))(1-\exp(-\mu^2\mathbf{k}^2)))\right). \tag{45}$$

It is easy to see that

$$\exp(-W(0)) = \exp\left(-r^{1-\gamma}\int d\mathbf{k}\mathbf{p}\tilde{D}(\mathbf{k})\mathbf{p}\times(1-\mu^{-2}\mathbf{k}^{-2}(1-\exp(-\mu^2\mathbf{k}^2)))\right) \geqslant \exp(-cr^{1-\gamma}\mathbf{p}^2) \tag{46}$$

under the assumptions that $\mathbf{p}\tilde{D}\mathbf{p} \geqslant |\tilde{D}|\mathbf{p}^2$, $\int d\mathbf{k}|\tilde{D}|(\mathbf{k})\theta(|\mathbf{k}|-(1/\mu))<\infty$, and

$$\int d\mathbf{k}|\tilde{D}|(\mathbf{k})\mathbf{k}^2\theta\left(\frac{1}{\mu}-|\mathbf{k}|\right) < \infty.$$

In such a case we can take the limit $\tau\to\infty$. In this limit

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x},\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})\int_0^\infty dr\int da\,\nu_1(a)\exp(-\mu^2\mathbf{p}^2r - c\mathbf{p}^2r^{1-\gamma} - 2a\mu^2r)$$
$$= \tilde{m}_0(\mathbf{p})\,\delta(\mathbf{p}+\mathbf{p}')\int_0^\infty dr m_1(\mu\sqrt{2r})\exp(-\mu^2\mathbf{p}^2r - c\mathbf{p}^2r^{1-\gamma}). \tag{47}$$

The behavior of the integral (47) depends on the behavior of the source correlations m_1 as a function of $|\mathbf{x}-\mathbf{x}'|$. If

$$m_1(\mu\sqrt{2r}) \geqslant K, \tag{48}$$

then

$$(\tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x},\mathbf{p}')) \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})\left(c_5\theta\left(|\mathbf{p}|-\frac{1}{\mu}\right)|\mathbf{p}|^{-2}+c_6\theta\left(\frac{1}{\mu}-|\mathbf{p}|\right)|\mathbf{p}|^{-(2/1-\gamma)}\right). \tag{49}$$

This lower bound coincides with the upper bound (40) (where $\alpha=1$). If m_1 satisfies a stronger condition ($\Omega<1$)

$$m_1(|\mathbf{x}|) \geqslant K|\mathbf{x}|^{-2\Omega} \tag{50}$$

[$\Omega\geqslant 0$ if it is to be of the form (24), i.e., $\nu_1(a)\geqslant Ka^{\Omega-1}$], then

$$\langle\tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x},\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})\left(c_7\theta\left(|\mathbf{p}|-\frac{1}{\mu}\right)|\mathbf{p}|^{-2+2\Omega}+c_8\theta\left(\frac{1}{\mu}-|\mathbf{p}|\right)|\mathbf{p}|^{-[(2-2\Omega)/(1-\gamma)]}\right). \tag{51}$$

The inequality (51) results from the following estimate (for $\alpha+\gamma<1$):

$$\begin{aligned}\int_0^\infty drr^{-\Omega}\exp(-\mu^2\mathbf{p}^2r-c\mathbf{p}^2r^{2-\alpha-\gamma}) &= \int_0^1 drr^{-\Omega}\exp(-\mu^2\mathbf{p}^2r-c\mathbf{p}^2r^{2-\alpha-\gamma})\\ &\quad+\int_1^\infty drr^{-\Omega}\exp(-\mu^2\mathbf{p}^2r-c\mathbf{p}^2r^{2-\alpha-\gamma})\\ &\geqslant \int_0^1 drr^{-\Omega}\exp(-(\mu^2\mathbf{p}^2+c\mathbf{p}^2)r)\\ &\quad+\int_1^\infty drr^{-\Omega}\exp(-(\mu^2\mathbf{p}^2+c\mathbf{p}^2)r^{2-\alpha-\gamma})\\ &= |\mathbf{p}|^{-2+2\Omega}\int_0^{\mathbf{p}^2} t^{-\Omega}\exp(-(\mu^2+c)t)dt\\ &\quad+|\mathbf{p}|^{-[(2-2\Omega)/(2-\alpha-\gamma)]}\int_{a(\mathbf{p})}^\infty t^{-\Omega}\exp(-(\mu^2+c)t^{2-\alpha-\gamma})dt,\end{aligned} \tag{52}$$

where $a(\mathbf{p})=|\mathbf{p}|^{2/(2-\alpha-\gamma)}$ and $\alpha=1$ in application to Eq. (47).

Next, we wish to estimate the behavior of the temperature correlations at large $\mathbf{x}-\mathbf{x}'$ in the turbulent case (10) when $\gamma=-\beta<0$ [if $\gamma>0$ and m_1 is a bounded function then the temperature correlations are bounded from below and from above as functions of $\mathbf{x}-\mathbf{x}'$, Eq. (43)]. First, we consider the Kraichnan model (35) [$\Gamma(s-s')=\delta(s-s')$ in Eq. (10)] with the mean velocity $\mathbf{U}=0$ and

$$\tilde{D}(\mathbf{k}) \simeq |\mathbf{k}|^{-d+2\gamma}. \tag{53}$$

The integral in Eq. (45) is convergent for large $\mathbf{k}$ if $\gamma<0$ and for small $\mathbf{k}$ if $-\gamma<1$. We consider the model (10) with $0<\beta=-\gamma<1$. Let us change the integration variable in Eq. (45):

$$\mathbf{k} = |\mathbf{x}-\mathbf{x}'|^{-1}\sqrt{r}\mathbf{q}. \tag{54}$$

Then, after an estimate of the remainder,

$$\exp(-W(\mathbf{x}-\mathbf{x}')) \geqslant \exp(-cr\mathbf{p}^2|\mathbf{x}-\mathbf{x}'|^{2\beta}). \tag{55}$$

As a consequence,

$$\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})(\mu^2\mathbf{p}^2+c\mathbf{p}^2|\mathbf{x}-\mathbf{x}'|^{2\beta})^{-1}(1-\exp(-\tau(\mu^2\mathbf{p}^2+c\mathbf{p}^2|\mathbf{x}-\mathbf{x}'|^{2\beta}))).$$

Hence, for large $|\mathbf{x}-\mathbf{x}\prime|$ we obtain

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})c^{-1}\mathbf{p}^{-2}|\mathbf{x}-\mathbf{x}'|^{-2\beta}. \tag{56}$$

This lower bound for the Kraichnan model is the same as the upper bound (44) (here $\alpha=1$). Let us calculate the expectation value in the exponential of Eq. (38) (denoted by $-W$) for the general G of Eq. (19):

$$\begin{aligned} W(\mathbf{x}-\mathbf{x}') = r^{2-\alpha-\gamma}\int d\omega d\mathbf{k}\mathbf{p}\tilde{G}(\omega,\mathbf{k})\mathbf{p} \\ \times\left(2\left(\frac{1}{2}\mu^2\mathbf{k}^2-i\omega\right)^{-1}\left(1-\left(\frac{1}{2}\mu^2\mathbf{k}^2-i\omega\right)^{-1}\left(1-\exp\left(-\frac{1}{2}\mu^2\mathbf{k}^2+i\omega\right)\right)\right)\right) \\ -\left(\frac{1}{4}\mu^4|\mathbf{k}|^4+\omega^2\right)^{-1}\exp(i\mathbf{k}r^{-1/2}(\mathbf{x}-\mathbf{x}'))\left|1-\exp\left(-\frac{1}{2}\mu^2\mathbf{k}^2+i\omega\right)\right|^2\Bigg). \end{aligned} \tag{57}$$

We estimate this integral at $\mathbf{x}=\mathbf{x}\prime$ first. Similarly, as in Eq. (46), the scale invariance (21) leads to

$$W(\mathbf{0}) \geqslant cr^{2-\alpha-\gamma}\mathbf{p}^2 \tag{58}$$

if

$$\int d\mathbf{k}d\omega\tilde{G}(\omega,\mathbf{k})\left(\frac{1}{2}\mu^2\mathbf{k}^2-i\omega\right)^{-1}\theta\left(|\mathbf{k}|-\frac{1}{\mu}\right)<\infty$$

and

$$\int\int d\mathbf{k}d\omega\tilde{G}(\omega,\mathbf{k})\left(\frac{1}{4}\mu^4|\mathbf{k}|^4+\omega^2\right)^{1/2}\theta\left(\frac{1}{\mu}-|\mathbf{k}|\right)<\infty.$$

Hence, under the assumption (50), on the basis of the inequalities (52) and (58), we have the lower bound [generalizing that of Eq. (51) to $\alpha\neq 1$]

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x},\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})\left(c\,\theta\left(|\mathbf{p}|-\frac{1}{\mu}\right)|\mathbf{p}|^{-2+2\Omega}+c'\,\theta\left(\frac{1}{\mu}-|\mathbf{p}|\right)|\mathbf{p}|^{-[(2-2\Omega)/(2-\alpha-\gamma)]}\right) \tag{59}$$

[at $\Omega=0$ this lower bound coincides with the upper bound (40)]. Next, if $|\mathbf{x}-\mathbf{x}'|$ is large, then for $0<-\gamma=\beta<1$ we obtain from Eqs. (21) and (57) the lower bound

$$\exp(-W(\mathbf{x}-\mathbf{x}')) \geqslant \exp(-c\mathbf{p}^2r^{2-\alpha}|\mathbf{x}-\mathbf{x}'|^{2\beta}),$$

where the form of the rhs comes from a change of variables $\mathbf{k}=\mathbf{k}\prime|\mathbf{x}-\mathbf{x}'|^{-1}$ and $\omega=\omega'|\mathbf{x}-\mathbf{x}\prime|^{-2}$ and an estimate of the remainder in Eq. (57).

If we restrict ourselves to G of the form (10) and $2\beta\geqslant 1$, then we can derive a more precise lower bound for $\exp(-W)$ with an application of the Hölder inequality

$$|\mathbf{x}+\mathbf{y}|^{2\beta} \leqslant 2^{2\beta-1}(|\mathbf{x}|^{2\beta}+|\mathbf{y}|^{2\beta}).$$

From Eq. (38) and the Hölder inequality we obtain, after an elementary calculation of the expectation value over the Brownian paths,

$$\exp(-W(\mathbf{x}-\mathbf{x}')) \geqslant \exp(-Cr^{2-\alpha-\gamma}\mathbf{p}^2 - cr^{2-\alpha}|\mathbf{x}-\mathbf{x}'|^{2\beta}\mathbf{p}^2). \tag{60}$$

Hence, after a calculation of the expectation value in the exponential in Eq. (38), the remaining r and the a integrals [from the representation (24)] in the correlation function (38) read

$$\int_0^\infty dr \int da\,\nu_1(a)\exp(-W-a|\mathbf{x}-\mathbf{x}'|^2-2\mu^2 ra) \geqslant \frac{1}{2}\int_0^\infty dr \int da\,\nu_1(a)\exp(-W-a|\mathbf{x}-\mathbf{x}'|^2) + \frac{1}{2}\int_0^\infty dr \int da\,\nu_1(a)\exp(-W-2\mu^2 ra),$$

where $\exp(-W)$ is lower bounded by Eq. (60). An easy estimate of this integral leads to the following inequality for large $\mathbf{x}-\mathbf{x}'$:

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle \geqslant \delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})(K_1|\mathbf{p}|^{-[(2-2\Omega)/(2-\alpha)]}|\mathbf{x}-\mathbf{x}'|^{-2\sigma} + K_2|\mathbf{p}|^{-2/(2-\alpha)}|\mathbf{x}-\mathbf{x}'|^{-[2\beta/(2-\alpha)]-2\Omega}), \tag{61}$$

where

$$\sigma = \frac{\beta(1-\Omega)}{2-\alpha}. \tag{62}$$

For $0<2\beta<1$ this lower bound coincides with the upper bound (44) (derived for $\Omega=0$). We expect that Eq. (61) gives the asymptotic behavior of the two-point correlation function for any $0<2\beta<2$ because such a behavior is a consequence of a formal exchange of the limit $|\mathbf{x}-\mathbf{x}'| \to \infty$ with the integral over t and the expectation value over the Brownian motion in Eq. (34).

The lower bound (59) for small $\mathbf{p}$ is obtained by neglecting the $|\mathbf{x}-\mathbf{x}'|$-dependent term on the rhs of Eq. (60). We can see from Eq. (59) that if $\tilde{m}_0(\mathbf{p}) \simeq |\mathbf{p}|^{-\nu}$ and $m_1(\mathbf{k}) \simeq |\mathbf{k}|^{-d+2\Omega}$ then the $\langle \tilde{T}\tilde{T}\rangle$ correlations behave as $|\mathbf{p}|^{-2-\nu+2\Omega}$ for large momenta (short distances in the $\mathbf{z}$ direction), whereas the low momentum behavior (large distance) is $|\mathbf{p}|^{-\nu-[(2-2\Omega)/(2-\alpha-\gamma)]}$. These estimates show the effect of the random flow on the temperature correlations in the $\mathbf{z}$ direction. The effect on the temperature correlations in the $\mathbf{x}$ direction is described by the lower bound (61) and the upper bound (44). Again the decay of temperature correlations is determined by scaling indices of the velocity and source correlations.

VI. HIGHER ORDER CORRELATION FUNCTIONS

Let us consider the multipoint correlation functions

$$\langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_{2n},\mathbf{p}_{2n})\rangle = \sum_{\text{pairs}} \int_0^\tau dt_1\cdots dt_{2n} \prod_{(j,k)} \delta(\mathbf{p}_j+\mathbf{p}_k)\delta(t_j-t_k)\exp\left(-\frac{1}{2}\mu^2\sum_j \mathbf{p}_j^2(\tau-t_j)\right) \times E\left[\prod_{(j,k)} \tilde{m}(\mathbf{x}_j-\mathbf{x}_k+\mu\mathbf{b}_j(\tau-t_j)-\mu\mathbf{b}_k(\tau-t_k),\mathbf{p}_j) \times \exp\left(-\frac{1}{2}\sum_{il}\int_0^{\tau-t_i}\int_0^{\tau-t_l} ds\,ds'\,\mathbf{p}_i G_0(s-s',\mathbf{x}_i-\mathbf{x}_l+\mu\mathbf{b}_i(s) - \mu\mathbf{b}_l(s'))\mathbf{p}_l\right)\right], \tag{63}$$

where the sum is over all pairings in accordance with the Gaussian combinatorics. From (63) we have

$$|\langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_{2n},\mathbf{p}_{2n})\rangle| \leqslant \sum_{\text{pairs}} \int_0^t dt_1\cdots dt_{2n} \times \prod_{(j,k)} \delta(\mathbf{p}_j+\mathbf{p}_k)\delta(t_j-t_k)\exp\left(-\frac{1}{2}\mu^2\sum_j \mathbf{p}_j^2(\tau-t_j)\right)$$
$$\times E\left[\prod_{(j,k)} |\tilde{m}(\mathbf{x}_j-\mathbf{x}_k+\mu\mathbf{b}_j(\tau-t_j)-\mu\mathbf{b}_k(\tau-t_k),\mathbf{p}_j)|\right] < \infty.$$

Hence, the equilibrium limit $\tau\to\infty$ exists.

If m is either of the form (24) or (25) then we can apply the Jensen inequality to the expectation value in the form $E[\exp f]\geqslant \exp E[f]$. We obtain an analogue of the lower bound (38). For the upper bound we apply the Jensen inequality to the time integral

$$\exp\left(-\frac{1}{2}\int_0^\tau\int_0^\tau dsds' \int\int J_k(s)J_l(s')\langle v_k(s)v_l(s')\rangle\right)$$
$$\leqslant \tau^{-2}\int_0^\tau\int_0^\tau dsds' \exp\left(-\frac{\tau^2}{2}\int\int J_k(s)J_l(s')\langle v_k(s)v_l(s')\rangle\right), \tag{64}$$

where

$$\mathbf{J}(s,\mathbf{u}) = -\theta(s)\sum_{k=1}^{2n}\mathbf{p}_k\delta(\mathbf{u}-\mathbf{x}_k-\mu\mathbf{b}_k(\tau-s))$$

and the additional integral in Eq. (64) is over the spatial variable $\mathbf{u}$.

We can repeat the basic estimates concerning the behavior for low $\mathbf{z}$ momenta and large $\mathbf{x}$ distances by means of the methods applied for the two-point correlations. First, by means of the Jensen inequalities, we reduce the estimates of the expectation values to finite dimensional integrals. From the Jensen inequalities we can see that the correlation functions are bounded in τ when $\tau\to\infty$. Next, the results concerning the scaling behavior for $2n$-point functions can be obtained by an introduction of spherical coordinates in the $dt_1\cdots dt_n$ integral in Eq. (63). Then, the correlation functions scale in a simple way with respect to the temporal radius r. Let us explain such estimates in more detail for $n=2$. Then,

$$\langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_4,\mathbf{p}_4)\rangle = \delta(\mathbf{p}_1+\mathbf{p}_3)\delta(\mathbf{p}_2+\mathbf{p}_4)\times\int_0^\tau dt_1\int_0^\tau dt_2\exp(-\mu^2\mathbf{p}_1^2(\tau-t_1)-\mu^2\mathbf{p}_2^2(\tau-t_2))$$
$$\times E\Bigg[\tilde{m}(\mathbf{x}_1-\mathbf{x}_3+\mu\mathbf{b}_1(\tau-t_1)-\mu\mathbf{b}_3(\tau-t_1),\mathbf{p}_1)\times\tilde{m}(\mathbf{x}_2-\mathbf{x}_4+\mu\mathbf{b}_2(\tau$$
$$-t_2)-\mu\mathbf{b}_4(\tau-t_2),\mathbf{p}_2)\times\exp\Bigg(-\sum_{j=1,2}\int_0^{\tau-t_j}\int_0^{\tau-t_j}dtdt'\mathbf{p}_jG_0(t-t',\mu\mathbf{b}_j(t)$$
$$-\mu\mathbf{b}_j(t'))\mathbf{p}_j+\sum_{j<k}\int_0^{\tau-t_j}\int_0^{\tau-t_k}dtdt'\mathbf{p}_jG_0(t-t',\mathbf{x}_j-\mathbf{x}_k+\mu\mathbf{b}_j(t)$$
$$-\mu\mathbf{b}_k(t'))\mathbf{p}_k\Bigg)\Bigg]+\text{permut.}, \tag{65}$$

where the sum is over permutations of the numbers from 1 to 4 in accordance with the Gaussian combinatorics; in the sum in the exponential we set $t_1=t_3$ and $t_2=t_4$. Let $\tau-t_1=r\cos\theta$, $\tau-t_2=r\sin\theta$, $t=r\sigma\cos\theta$, and $t'=r\sigma'\sin\theta$. In such a case r scales in the exponential in the same way as in Eqs. (37) and (38). The integral $dt_1dt_2=drrd\theta$ adds an additional power of r. Under the assumption (31) the small $\mathbf{p}$ behavior of the correlation functions (65) at $\tau=\infty$ is determined by the integral

$$|\langle \tilde{T}_\infty(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\infty(\mathbf{x}_4,\mathbf{p}_4)\rangle| \simeq |\tilde{m}_0|(\mathbf{p}_1)|\tilde{m}_0|(\mathbf{p}_2)\int_0^\infty drrE\left[\exp\left(-r^{2-\alpha-\gamma}\sum_{jk}\mathbf{p}_jG_0\mathbf{p}_k\right)\right] + \text{permut.}$$
$$\simeq |\tilde{m}_0|(\mathbf{p}_1)|\tilde{m}_0|(\mathbf{p}_2)E\left[\left|\sum_{jk}\mathbf{p}_jG_0\mathbf{p}_k\right|^{-[2/(2-\alpha-\gamma)]}\right] + \text{permut.} \quad (66)$$

For large distances, $\gamma=-\beta<0$ and G of Eq. (10), we can expand the dependence on the Brownian motion in Eq. (66) in powers of $\mu|\mathbf{x}_j-\mathbf{x}_k|^{-1}$. The leading order reads

$$|\langle \tilde{T}_\infty(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\infty(\mathbf{x}_4,\mathbf{p}_4)\rangle| \simeq |\tilde{m}_0|(\mathbf{p}_1)|\tilde{m}_0|(\mathbf{p}_2)\left|\sum_{jk}\mathbf{p}_j\mathbf{p}_k|\mathbf{x}_j-\mathbf{x}_k|^{2\beta}\right|^{-[2/(2-\alpha)]} + \text{permut.} \quad (67)$$

Note that the power describing the low $\mathbf{p}$ behavior in Eq. (66) and large $\mathbf{x}$ behavior in Eq. (67) is twice as big as that for the two-point function (34) and (40) indicating the asymptotic scale invariance of the temperature $\tilde{T}_\infty(\mathbf{x},\mathbf{p})$ at low momenta or large distances. This property can be extended to the $2n$ correlation functions where the scaling index is proportional to n as a consequence of the drr^{n-1} time integral in the spherical time coordinates. Such a behavior of the integrals suggests that if the velocities and the sources are scale invariant then the temperatures scale at large distances with the scale dimension determined by the two-point function.

VII. DISCUSSION

The power-law behavior of turbulent velocity correlation functions and passive scalar correlation functions in a homogeneous isotropic turbulent flow has been widely discussed in the literature since the basic papers of Kolmogorov[2] followed by Obukhov,[28] Corrsin,[29] and Batchelor[30] (concerning the scalar advection). The universal Kolmogorov 5/3 law for spectral velocity distribution as well as passive scalar distribution is derived by means of dimensional arguments (independent of any dynamical model). A statistical homogeneity and isotropy of the turbulence at a microscale in a sufficiently large space interval (called the "inertial range") is at the basis of the Kolmogorov theory. Under these assumptions the velocity (or passive scalar) correlation functions are universal, i.e., independent of the source distribution m. An experimental verification is not simple. Turbulent flows are usually nonhomogeneous and nonisotropic at a macro scale. However, if a flow satisfying Kolmogorov assumptions is created, then the spectral Kolmogorov law is satisfied in the inertial range.[31] Nevertheless, it is common for flows in nature that Kolmogorov assumptions are not satisfied (for some studies of such turbulent flows, see Refs. 32 and 33). Even if the velocity is satisfying the Kolmogorov law, the analogous Obukhov law for ρ may fail.[32–34] As the authors in Ref. 32 point out, some problems with the verification of Kolmogorov's theory concern a construction of a flow that would be homogeneous and isotropic in a sufficiently large inertial range (usually boundary conditions or sources violate a global symmetry). They suggest a study of nonisotropic flows.

An investigation of a general class of dynamical models of randomly forced Navier-Stokes and passive scalar equations is still beyond the reach of analytical as well as numerical methods. Substantial progress has been achieved in the white noise randomly forced passive scalar (Kraichnan model).[4,8,9] However, the white noise distribution of velocities is quite unrealistic. Our main motivation in these studies was a derivation of the scaling behavior for velocities that are not of the white noise type. A passive scalar in a shear flow independent of the coordinates in the direction of the flow was studied before in Refs. 6 and 7. However, these authors were interested in the anomalous free decay of solutions of the advection-diffusion equation.

Our results predict a power law of the passive scalar correlations in nonisotropic flows. The results depend on the source distribution m because the source f is present at any scale. We do not specify any inertial range in our model. In general, the correlations must depend on the source (for a discussion of random forcing, see Ref. 35). This can be seen from the detailed calculations in Refs. 36 and 37 performed in the isotropic Kraichnan model (white noise in time).[4,8,9] The two-

point passive scalar correlations depend explicitly on the source and on the molecular diffusivity μ^2. Only in a proper limit of the source covariance m and $\mu\to 0$ does the universal scaling law come out.

Before we summarize our results let us begin with simple models. First, consider a pure diffusion corresponding to $\mathbf{V}=0$. Then

$$\langle \tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle = 2\delta(\mathbf{p}+\mathbf{p}')\int_0^\tau dr\,\exp(-\mu^2\mathbf{p}^2 r)\times E[\tilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{b}(1)-\mu\sqrt{r}\mathbf{b}'(1),\mathbf{p})]$$

$$= 2\delta(\mathbf{p}+\mathbf{p}')(2\pi)^{-D+d}\int_0^\tau dr\,\exp(-\mu^2\mathbf{p}^2 r)$$

$$\times\int d\mathbf{u}d\mathbf{w}\,\exp\left(-\frac{\mathbf{u}^2}{2}-\frac{\mathbf{w}^2}{2}\right)[\tilde{m}(\mathbf{x}-\mathbf{x}'+\mu\sqrt{r}\mathbf{u}-\mu\sqrt{r}\mathbf{w},\mathbf{p})]$$

$$= \mu^{-2}\delta(\mathbf{p}+\mathbf{p}')\int d\mathbf{k}\,\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}'))\tilde{m}_1(\mathbf{k})\tilde{m}_0(\mathbf{p})(\mathbf{p}^2+\mathbf{k}^2)^{-1}$$

$$\times(1-\exp(-\mu^2(\mathbf{p}^2+\mathbf{k}^2)\tau)).$$

In the limit $\tau\to\infty$

$$\langle T_\infty(\mathbf{x},\mathbf{z})T_\infty(\mathbf{x}',\mathbf{z}')\rangle = \mu^{-2}\int d\mathbf{k}d\mathbf{p}\,\exp(i\mathbf{k}(\mathbf{x}-\mathbf{x}'))\exp(i\mathbf{p}(\mathbf{z}-\mathbf{z}'))\tilde{m}(\mathbf{k},\mathbf{p})(\mathbf{p}^2+\mathbf{k}^2)^{-1}. \quad (68)$$

Hence

$$\rho_\infty(\mathbf{k},\mathbf{p}) = \mu^{-2}(\mathbf{p}^2+\mathbf{k}^2)^{-1}\tilde{m}_1(\mathbf{k})\tilde{m}_0(\mathbf{p}). \quad (69)$$

Let us note that the behavior of the temperature correlations changes abruptly for large $|\mathbf{z}-\mathbf{z}'|$ at $\tau=\infty$ in this simple model. At finite τ it is the same as that of the source (say $|\mathbf{z}-\mathbf{z}'|^{-d+\nu}$) whereas at $\tau=\infty$ it becomes $|\mathbf{z}-\mathbf{z}'|^{-d+\nu+2}$. However, it can be seen from Eq. (68) that after the limit $\tau\to\infty$, the limit $\mu\to 0$ does not exist in the model without the advection. If we first take $\mu\to 0$ then the subsequent limit $\tau\to\infty$ is linearly divergent in τ. The strong μ dependence of the asymptotic behavior means that this parameter sets a scale on time and space that determines different scaling behavior. In Appendix A we show that the limits $\mu\to 0$ and $\tau\to\infty$ can be interchanged in the model with a random advection. The correlation functions $\mathcal{S}^{(2n)}$ in a nonisotropic Kraichnan model are discussed in Appendix B. The correlation functions $\mathcal{S}^{(2n)}(\mathbf{x}_1,\mathbf{p}_1,\ldots,\mathbf{x}_{2n},\mathbf{p}_{2n})$ can be calculated exactly in the limit $\mu\to 0$ [Eq. (86)]. They show no anomalous scaling (encountered in the isotropic model[4,8]) as long as the points $\mathbf{x}_j$ are different. The scaling behavior can change after a transformation to the configuration space (the Fourier transform does not exist in the usual sense).

Let us compare the two-point temperature correlation function (68) with the one in a random flow, which is bounded in space and time, i.e., $G=\langle\mathbf{vv}\rangle\simeq$ const. Under the assumption (31) we obtain

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle \simeq K\delta(\mathbf{p}+\mathbf{p}')\tilde{m}_0(\mathbf{p})\int_0^\infty dr\,\exp(-\mu^2\mathbf{p}^2 r - c\mathbf{p}^2 r^2). \quad (70)$$

The integral (70) behaves as $\tilde{m}_0(\mathbf{p})\mathbf{p}^{-2}$ for large $\mathbf{p}$ and as $\tilde{m}_0(\mathbf{p})|\mathbf{p}|^{-1}$ for a small $\mathbf{p}$ in agreement with Eq. (59) for $\Omega=\alpha=\gamma=0$. Our results of Secs. IV and V give an extension of the simple observations on the temperature correlation functions derived in this section for a pure diffusion and for an advection by a uniformly bounded random flow.

In our model (defined by the assumption that the velocity does not depend on coordinates in the direction of the flow) the spectral distribution in the corresponding momentum is proportional to the source distribution $\tilde{m}$, as can be seen from Eq. (34). We could consider a source f with the covariance $m(\mathbf{x},\mathbf{z})$, which (approximately in a certain range as in Refs. 36 and 37) is independent

of $\mathbf{x}$. In such a case the spectral equilibrium distribution (6) for a pure diffusion $\rho_\infty(\mathbf{k},\mathbf{p})$ (67) is $\delta(\mathbf{k})\tilde{m}_0(\mathbf{p})\mathbf{p}^{-2}$, where the $\mathbf{p}^{-2}$ behavior comes from the molecular diffusivity. The temperature correlations remain independent of $\mathbf{x}$ and the limit $\mu\to 0$ does not exist. A random advection is changing the behavior of temperature correlations in $\mathbf{x}$ as well as in $\mathbf{p}$. This change involves a nonperturbative mechanism that could not be seen in an expansion in $\mathbf{V}$. It comes from an exponential of G in Eq. (34). In particular, a steady flow bounded in $\mathbf{x}$ gives $\rho_\infty(\mathbf{k},\mathbf{p})=\delta(\mathbf{k})|\mathbf{p}|^{-1}$ for $|\mathbf{p}|\ll 1/\mu$, whereas for the random velocity growing in space with the index β [Eq. (10)] we have for a small $\mathbf{k}$ the behavior $\rho_\infty(\mathbf{k},\mathbf{p})\simeq|\mathbf{k}|^{-d+[2\beta/(2-\alpha)]}$, as follows from Eq. (61).

In experiments ($D=3$) we could create an anisotropic flow with the Kolmogorov index (10) $\beta=1/3$ in $d=2$ or $d=1$. In such a case we obtain definite predictions concerning the temperature distribution. This will be $|\mathbf{x}-\mathbf{x}'|^{-2/3}|\mathbf{z}-\mathbf{z}'|^{\nu}$ where

$$\nu=\frac{2}{2-\alpha}-(D-d),$$

and $D-d$ is either 1 or 2, and there is a restriction $\alpha-\beta<1$ coming from the requirement of the integrability of the expression in the exponential of (34).

In general, we can see from Eqs. (40), (42), (44), (59), and (61) that the turbulent behavior $\gamma=-\beta<0$ of the velocity field will (in comparison to pure diffusion) decrease the temperature correlations in the direction orthogonal to the flow and increase the correlations (at the fixed α)in the direction of the flow. These effects contribute to the more coherent heat distribution in a turbulent stream.

APPENDIX A: THE LIMIT $\mu\to 0$

If there is no diffusion ($\mu=0$), then our formulas in Secs. IV–VI at finite τ remain valid but need some interpretation. There is no expectation value over the Brownian motion. In such a case, in some formulas [as in Eqs. (34) and (35)] $\gamma=0$. Let us consider as an example the formula (34) at $\mu=0$:

$$\begin{aligned}\langle\tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle=\delta(\mathbf{p}+\mathbf{p}')\tilde{m}(\mathbf{x}-\mathbf{x}',\mathbf{p})\int_0^\tau dt\exp\left(-i\mathbf{p}\int_0^{\tau-t}ds\mathbf{U}(\tau-s,\mathbf{x})\right)\\ \times\exp\left(-(\tau-t)^{2-\alpha}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',0)\mathbf{p}\right.\\ \left.+(\tau-t)^{2-\alpha}\int_0^1\int_0^1 d\sigma d\sigma'\mathbf{p}G_0(\sigma-\sigma',\mathbf{x}-\mathbf{x}')\mathbf{p}\right).\end{aligned}\tag{71}$$

For the Kraichnan model[8] (35) the formula (71) reads (with the Stratonovitch interpretation of the gradient term; see the discussion at the beginning of Sec. II)

$$\begin{aligned}\langle\tilde{T}_\tau(\mathbf{x},\mathbf{p})\tilde{T}_\tau(\mathbf{x}',\mathbf{p}')\rangle=\delta(\mathbf{p}+\mathbf{p}')\tilde{m}(\mathbf{x}-\mathbf{x}',\mathbf{p})\int_0^\tau dt\exp\left(-i\mathbf{p}\int_0^{\tau-t}\mathbf{U}(\tau-s,\mathbf{x})ds\right)\\ \times\exp(-(\tau-t)\mathbf{p}D_0(0)\mathbf{p}+(\tau-t)\mathbf{p}D_0(\mathbf{x}-\mathbf{x}')\mathbf{p}).\end{aligned}\tag{72}$$

In the limit $\tau\to\infty$ and for $\mathbf{U}=0$ we can calculate the integral over time in Eq. (71) with the result

$$\langle \tilde{T}_\infty(\mathbf{x},\mathbf{p})\tilde{T}_\infty(\mathbf{x}',\mathbf{p}')\rangle = C\delta(\mathbf{p}+\mathbf{p}')\tilde{m}(\mathbf{x}-\mathbf{x}',\mathbf{p})\Bigg(\int_0^1\int_0^1 d\sigma d\sigma' \mathbf{p}G_0(\sigma-\sigma',0)\mathbf{p} - \int_0^1\int_0^1 d\sigma d\sigma' \mathbf{p}G_0(\sigma-\sigma',\mathbf{x}-\mathbf{x}')\mathbf{p}\Bigg)^{-[1/(2-\alpha)]}, \tag{73}$$

in agreement with the bounds (56) and (61). We can also calculate the higher order correlation functions. As an example, the four-point function (65) reads

$$\langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_4,\mathbf{p}_4)\rangle = \delta(\mathbf{p}_2+\mathbf{p}_4)\delta(\mathbf{p}_1+\mathbf{p}_3)\tilde{m}(\mathbf{x}_1-\mathbf{x}_3,\mathbf{p}_1)\tilde{m}(\mathbf{x}_2-\mathbf{x}_4,\mathbf{p}_2) \times \int_0^\tau dt_1\int_0^\tau dt_2 \exp\Bigg(-\sum_{j=1,2}\int_0^{\tau-t_j}\int_0^{\tau-t_j} dtdt'\mathbf{p}_j G_0(t-t',0)\mathbf{p}_j + \sum_{j<k}\int_0^{\tau-t_j}\int_0^{\tau-t_k} dtdt'\mathbf{p}_j G_0(t-t',\mathbf{x}_j-\mathbf{x}_k)\mathbf{p}_k\Bigg) + \text{permut.}$$

We can obtain detailed estimates of the time integrals for any α. In some special cases the integrals can be explicitly calculated. In Appendix B we give the formula [Eq. (88)] for the Kraichnan model ($\alpha=1$). For a steady flow [$\Gamma(s)=1$ in Eq. (10), $\alpha=0$] at $\tau=\infty$ the integration over t_j gives

$$\langle \tilde{T}_\infty(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\infty(\mathbf{x}_4,\mathbf{p}_4)\rangle = \delta(\mathbf{p}_2+\mathbf{p}_4)\delta(\mathbf{p}_1+\mathbf{p}_3)\tilde{m}(\mathbf{x}_1-\mathbf{x}_3,\mathbf{p}_1)\tilde{m}(\mathbf{x}_2-\mathbf{x}_4,\mathbf{p}_2) \times (4\mathbf{p}_1^2\mathbf{p}_2^2 D_0(\mathbf{x}_1-\mathbf{x}_3)D_0(\mathbf{x}_2-\mathbf{x}_4) - (\mathbf{p}_1\mathbf{p}_2)^2(D_0(\mathbf{x}_1-\mathbf{x}_4)+D_0(\mathbf{x}_2-\mathbf{x}_3) + D_0(\mathbf{x}_1-\mathbf{x}_2)+D_0(\mathbf{x}_3-\mathbf{x}_4))^2)^{-1/2} + \text{permut.}, \tag{74}$$

where $D_0(\mathbf{x}_j-\mathbf{x}_k)=-|\mathbf{x}_j-\mathbf{x}_k|^{2\beta}$ in the model (10).

APPENDIX B: THE KRAICHNAN MODEL

If $\Gamma(t-t')=\delta(t-t')$, then we obtain a closed set of equations for the correlation functions

$$\mathcal{S}_\tau^{(n)}(\mathbf{x}_1,\ldots,\mathbf{x}_n;\mathbf{p}_1,\ldots,\mathbf{p}_n) = \langle \tilde{T}_\tau(\mathbf{x}_1,\mathbf{p}_1)\cdots\tilde{T}_\tau(\mathbf{x}_n,\mathbf{p}_n)\rangle. \tag{75}$$

These equations have been derived by Kraichnan[8] for velocities depending on all coordinates. In our simplified model (9) and (10) they read (the odd order correlation functions are zero)

$$\partial_\tau \mathcal{S}_\tau^{(2n)} = \frac{1}{2}\mu^2\sum_{j=1}^{j=2n}\Delta_j\mathcal{S}_\tau^{(2n)} - \frac{1}{2}(\mu^2+D_0(\mathbf{0}))\sum_{j=1}^{j=2n}\mathbf{p}_j^2\mathcal{S}_\tau^{(2n)} + \sum_{\langle j,k\rangle}\mathbf{p}_j D_0(\mathbf{x}_j-\mathbf{x}_k)\mathbf{p}_k\mathcal{S}_\tau^{(2n)} + \sum_{\langle j,k\rangle}\delta(\mathbf{p}_j+\mathbf{p}_k)\tilde{m}(\mathbf{x}_j-\mathbf{x}_k,\mathbf{p}_j)\mathcal{S}_\tau^{(2n-2)}(jk) \equiv \mathcal{M}\mathcal{S}_\tau^{(2n)} + \mathcal{R}\mathcal{S}_\tau^{(2n-2)}, \tag{76}$$

where D_0 is the translation invariant part of D and $\mathcal{S}(jk)$ means that the coordinates $\mathbf{x}_j$ and $\mathbf{x}_k$ are lacking in $\mathcal{S}$. The term $D(\mathbf{0})$ (adding to μ^2) comes from the Stratonovitch interpretation of Eq. (1). The solution of Eq. (76) reads

$$\mathcal{S}_\tau^{(2n)} = \exp(\tau\mathcal{M})S_0^{(2n)} + \int_0^\tau dt\,\exp((\tau-t)\mathcal{M})\mathcal{R}\mathcal{S}_t^{(2n-2)}. \tag{77}$$

If the operator $\mathcal{M}$ is strictly negative in the space $L^2(R^{2dn})$, then the limit $\tau\to\infty$ exists and does not depend on the initial condition $\mathcal{S}_0^{(2n)}$.

We can express the solution of Eq. (76) by means of the Feynman-Kac formula for the heat kernel

$$(\exp(r\mathcal{M})g)(\mathbf{x}_1, \ldots, \mathbf{x}_{2n}) = E\left[\exp\left(\int_0^r ds W(\mathbf{b}(s))\right) g(\mathbf{x}_1 + \mu\mathbf{b}_1(r), \ldots, \mathbf{x}_{2n} + \mu\mathbf{b}_{2n}(r))\right], \tag{78}$$

where

$$W(s) = -\frac{1}{2}(\mu^2 + D_0(0)) \sum_{j=1}^{j=2n} \mathbf{p}_j^2 + \sum_{\langle j,k\rangle} \mathbf{p}_j D_0(\mathbf{x}_j + \mu\mathbf{b}_j(s) - \mathbf{x}_k - \mu\mathbf{b}_k(s))\mathbf{p}_k. \tag{79}$$

We obtain an upper bound on the correlation functions (78) from the Jensen inequality as applied to the time integral

$$((\exp r\mathcal{M})g)(\mathbf{x}_1, \ldots, \mathbf{x}_{2n}) \leqslant \frac{1}{r}\int_0^r ds E[\exp(rW(\mathbf{b}(s)))|g|(\mathbf{x}_1 + \mu\mathbf{b}_1(r), \ldots, \mathbf{x}_{2n} + \mu\mathbf{b}_{2n}(r))]. \tag{80}$$

If $g = \exp h$ [or a superposition with positive coefficients of such functions as in Eq. (25)], then we have the lower bound from the Jensen inequality as applied to the expectation value

$$(\exp(r\mathcal{M})\exp h)(\mathbf{x}_1, \ldots, \mathbf{x}_{2n}) \geqslant \exp E\left[\int_0^r ds W(\mathbf{b}(s)) + h(\mathbf{x}_1 + \mu\mathbf{b}_1(r), \ldots, \mathbf{x}_{2n} + \mu\mathbf{b}_{2n}(r))\right]. \tag{81}$$

As an example, the formula for the two-point function (in the limit $\tau \to \infty$) with the velocity correlations defined by Eq. (10) reads

$$\mathcal{S}_\infty^{(2)}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2) = \delta(\mathbf{p}_1 + \mathbf{p}_2)\int_0^\infty dr \exp(-r\mu^2\mathbf{p}_1^2) \times E\left[\exp\left(-\mathbf{p}_1^2\int_0^r ds|\mathbf{x}_1 - \mathbf{x}_2 + \mu\mathbf{b}_1(s) - \mu\mathbf{b}_2(s)|^{2\beta}\right)\tilde{m}(\mathbf{x}_1 + \mu\mathbf{b}_1(r) - \mathbf{x}_2 - \mu\mathbf{b}_2(r), \mathbf{p}_1)\right]. \tag{82}$$

Then, the resulting correlation functions are controlled from below and from above by the Jensen inequalities. For the lower bound (81) we obtain an explicit formula [using the representation (24) for m_1]

$$\mathcal{S}_\infty^{(2)}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2) \geqslant \delta(\mathbf{p}_1 + \mathbf{p}_2)\tilde{m}_0(\mathbf{p}) \int d\nu_1(a) \int_0^\infty dr \exp(-r\mu^2\mathbf{p}_1^2) \times \exp(-\mathbf{p}^2 r^{\beta+1} h(r^{-1/2}|\mathbf{x}_1 - \mathbf{x}_2|) - a|\mathbf{x}_1 - \mathbf{x}_2|^2 - 2\mu^2 ra), \tag{83}$$

where

$$h(\rho) = K\rho^{2(1+\beta)}\int_0^{\rho^{-2}} d\lambda \int_0^\infty db b^{-1-\beta}\left(1 - (1 + 2\mu^2\lambda b)^{-d/2}\exp\left(-\frac{b}{2(1 + 2\mu^2 b\lambda)}\right)\right); \tag{84}$$

here K is a positive constant. From Eq. (84) it can easily be seen that for large $\mathbf{x} - \mathbf{x}'$ [small ρ in Eq. (84)] the r integrand in Eq. (83) behaves as

$$\exp(-Kr\mathbf{p}^2|\mathbf{x}_1 - \mathbf{x}_2|^{2\beta} - a|\mathbf{x}_1 - \mathbf{x}_2|^2 - 2\mu^2 ra)$$

[as shown in another way in Eq. (60); here $\alpha = 1$], leading as a consequence to the estimate (61) for the correlation functions. We can continue the Jensen inequalities for higher correlation functions because it follows from Eqs. (77) and (78) that the correlation functions are again in the form of superpositions of exponentials.

For lower order correlations a direct study of the differential equation (76) can be equally efficient. As an example, if $D=3$ and $d=2$, then Eq. (76) at $\tau=\infty$ [with the velocity covariance (10)] reads (here $\rho=|\mathbf{x}_1-\mathbf{x}_2|$)

$$\left(\mu^2\frac{1}{\rho}\partial_\rho\rho\partial_\rho-\mu^2p^2-p^2\rho^{2\beta}\right)T_\infty^{(2)}(\rho,p;\mu)=\tilde{m}(\rho,p), \tag{85}$$

where we defined

$$\mathcal{S}^{(2)}(\rho,p_1,p_2;\mu)=\delta(p_1+p_2)\mathcal{T}^{(2)}(\rho,p_1;\mu).$$

In contradistinction to the spherically symmetric case,[8] Eq. (85) is not explicitly soluble but its asymptotic solution (61) is easy to obtain. This asymptotic behavior is the same as the limit $\mu=0$ of the solution (85):

$$\mathcal{T}_\infty^{(2)}(\rho,p;0)=-p^{-2}\rho^{-2\beta}\tilde{m}(\rho,p). \tag{86}$$

In general, from Eq. (76), the limit $\mu=0$ can be obtained inductively:

$$\mathcal{S}_\infty^{(2n)}(\mathbf{x}_1,\ldots,\mathbf{x}_{2n};\mathbf{p}_1,\ldots,\mathbf{p}_{2n};0)=\left(\frac{1}{2}D_0(\mathbf{0})\sum_{j=1}^{j=2n}\mathbf{p}_j^2-\sum_{\langle j,k\rangle}\mathbf{p}_jD_0(\mathbf{x}_j-\mathbf{x}_k)\mathbf{p}_k\right)^{-1}$$
$$\times\sum_{\langle i,l\rangle}\delta(\mathbf{p}_i+\mathbf{p}_l)\tilde{m}(\mathbf{x}_i-\mathbf{x}_l,\mathbf{p}_i)\mathcal{S}_\infty^{(2n-2)}(il;0). \tag{87}$$

The formulas for the asymptotic behavior (61) ($\alpha=1$) and (66) ($\alpha=1$, $\gamma=0$) agree with the exact solution (87). For $n=1$ the solution (82) takes the form (86), whereas for $n=2$ we have

$$\mathcal{S}_\infty^{(4)}(\mathbf{x}_1,\ldots,\mathbf{x}_4;\mathbf{p}_1,\ldots,\mathbf{p}_4;0)=\left(\frac{1}{2}D_0(\mathbf{0})\sum_{j=1}^{j=4}\mathbf{p}_j^2-\sum_{\langle j,k\rangle}\mathbf{p}_jD_0(\mathbf{x}_j-\mathbf{x}_k)\mathbf{p}_k\right)^{-1}$$
$$\times(\delta(\mathbf{p}_1+\mathbf{p}_2)\delta(\mathbf{p}_3+\mathbf{p}_4)(\mathbf{p}_1D_0(\mathbf{0})\mathbf{p}_1-\mathbf{p}_1D_0(\mathbf{x}_1-\mathbf{x}_2)\mathbf{p}_1)^{-1}$$
$$\times\tilde{m}(\mathbf{x}_1-\mathbf{x}_2,\mathbf{p}_1)\tilde{m}(\mathbf{x}_3-\mathbf{x}_4,\mathbf{p}_3)+\text{permut.}). \tag{88}$$

For the scale invariant random velocity field (10), $D_0(\mathbf{0})=0$ and $D_0(\mathbf{x}_j-\mathbf{x}_k)=-|\mathbf{x}_j-\mathbf{x}_k|^{2\beta}$. It follows from Eqs. (87) and (88) that the temperature correlation functions are scale invariant under scale transformations of the coordinates $\mathbf{x}_j$ as well as $\mathbf{p}_j$. When $\mu=0$, then the correlation functions $\mathcal{S}_\infty^{(2n)}$ are singular at coinciding points (the limit $\mu\to0$ has been studied earlier by other methods in Refs. 14 and 15). The bound (40) is valid for $\mu>0$.

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Quantum macrostates, equivalence of ensembles, and an *H*-theorem

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Before the thermodynamic limit, macroscopic averages need not commute for a quantum system. As a consequence, aspects of macroscopic fluctuations or of constrained equilibrium require a careful analysis, when dealing with several observables. We propose an implementation of ideas that go back to John von Neumann's writing about the macroscopic measurement. We apply our scheme to the relation between macroscopic autonomy and an *H*-theorem, and to the problem of equivalence of ensembles. In particular, we show how the latter is related to the asymptotic equipartition theorem. The main point of departure is an expression of a law of large numbers for a sequence of states that start to concentrate, as the size of the system gets larger, on the macroscopic values for the different macroscopic observables. Deviations from that law are governed by the entropy. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217810]

I. INTRODUCTION

"It is a fundamental fact with macroscopic measurements that everything which is measurable at all, is also simultaneously measurable, i.e. that all questions which can be answered separately can also be answered simultaneously." That statement by von Neumann enters his introduction to the macroscopic measurement.[16] He then continues to discuss in more detail how that view could possibly be reconciled with the non-simultaneous-measurability of quantum mechanical quantities. The main qualitative suggestion by von Neumann is to consider, for a set of noncommuting operators $A,B,\ldots$ a corresponding set of *mutually commuting* operators $A',B',\ldots$ which are each, in a sense, good approximations, $A'\approx A, B'\approx B,\ldots$. The whole question is: *in exactly what sense?* Especially in statistical mechanics, one is interested in fluctuations of macroscopic quantities or in the restriction of certain ensembles by further macroscopic constraints which only make sense for finite systems. In these cases, general constructions of a common subspace of observables become very relevant. Interestingly, at the end of his discussion on the macroscopic measurement,[16] von Neumann turns to the quantum *H*-theorem and to the relation between entropy and macroscopic measurement. He refers to the then recent work of Pauli,[13,15] who by using "disorder assumptions" or what we could call today, a classical Markov approximation, obtained a general argument for the *H*-theorem.

In the present paper, we are dealing exactly with the problems above and as discussed in Chapter V.4 of Ref. 16. While it is indeed true that averages of the form $A=(a_1+\cdots+a_N)/N, B=(b_1+\cdots+b_N)/N$, for which all commutators $[a_i,b_j]=0$ for $i\neq j$, have their commutator $[A,B]=O(1/N)$ going to zero (in the appropriate norm, corresponding to $[a_i,b_i]=O(1)$) as $N\uparrow+\infty$, it is not true in general that

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$$\lim_{N\to+\infty}\frac{1}{N}\log \mathrm{Tr}[e^{NA}e^{NB}]\stackrel{?}{=}\lim_{N\to+\infty}\frac{1}{N}\log \mathrm{Tr}[e^{NA+NB}].$$

These generating functions are obviously important in fluctuation theory, such as in the problem of large deviations for quantum systems.[12] It is still very much an open question to discuss the joint large deviations of quantum observables, or even to extend the Laplace-Varadhan formula to applications in quantum spin systems. The situation is better for questions about normal fluctuations and the central limit theorem, for which the so-called fluctuation algebra provides a nice framework, see, e.g., Ref. 8. There the pioneering work of André Verbeure will continue to inspire coming generations who are challenged by the features of noncommutativity in quantum mechanics.

These issues are also important for the question of convergence to equilibrium. For example, one would like to specify or to condition on various macroscopic values when starting off the system. Under these constrained equilibria not only the initial energy but also, e.g., the initial magnetization or particle density, etc., are known, and simultaneously installed. As with the large deviation question above, we enter here again in the question of equivalence of ensembles but we are touching also a variety of problems that deal with nonequilibrium aspects. The very definition of configurational entropy as related to the size of the macroscopic subspace has to be rethought when the macroscopic variables get their representation as noncommuting operators. One could again argue that all these problems vanish in the macroscopic limit, but the question (indeed) arises before the limit, for very large but finite N where one can still speak about finite dimensional subspaces or use arguments like the Liouville-von Neumann theorem.

In the following, there are three sections. In Sec. II we write about quantum macrostates and about how to define the macroscopic entropy associated to values of several noncommuting observables. As in the classical case, there is the Gibbs equilibrium entropy. The statistical interpretation, going back to Boltzmann for classical physics, is however not immediately clear in a quantum context. We will define various quantum H-functions. Second, in Sec. III, we turn to the equivalence of ensembles. The main result there is to give a counting interpretation to the thermodynamic equilibrium entropy. In that light we discuss quantum aspects of large deviation theory. Finally, in Sec. IV, we study the relation between macroscopic autonomy and the second law, as done before in Ref. 5 for classical dynamical systems. We prove that if the macroscopic observables give rise to a first-order autonomous equation, then the H-function, defined on the macroscopic values, is monotone. That is further illustrated using a quantum version of the Kac ring model.

II. QUANTUM MACROSTATES AND ENTROPY

Having in mind a macroscopically large closed quantum dynamical system, we consider a sequence $\mathcal{H}=(\mathcal{H}^N)_{N\uparrow+\infty}$ of finite-dimensional Hilbert spaces with the index N labeling different finitely extended approximations, and playing the role of the volume or the particle number, for instance. On each space $\mathcal{H}^N$ we have the standard trace Tr^N. Macrostates are usually identified with subspaces of the Hilbert spaces or, equivalently, with the projections on these subspaces. For any collection $(X_k^N)_{k=1}^n$ of mutually commuting self-adjoint operators there is a projection-valued measure (Q^N) on $\mathbb{R}^n$ such that for any function $F\in C(\mathbb{R}^n)$,

$$F(X_1^N,\ldots,X_n^N)=\int_{\mathbb{R}^n}Q^N(\mathrm{d}z)F(z).$$

A macrostate corresponding to the respective values $x=(x_1,x_2,\ldots,x_n)$ is then represented by the projection

$$Q^{N,\delta}(x) = \int_{\times_k(x_k-\delta,x_k+\delta)} Q^N(\mathrm{d}z)$$

for small enough $\delta>0$. Furthermore, the Boltzmann H-function, in the classical case counting the cardinality of macrostates, is there defined as

$$H^{N,\delta}(x) = \frac{1}{N}\log \mathrm{Tr}^N[Q^{N,\delta}(x)]$$

with possible further limits $N\uparrow+\infty$, $\delta\downarrow 0$. However, a less trivial problem that we want to address here, emerges if the observables (X_k^N) chosen to describe the system on a macroscopic scale do not mutually commute.

Consider a family of sequences of self-adjoint observables $(X_k^N)_{N\uparrow+\infty,k\in K}$ where K is some index set, and let each sequence be uniformly bounded, $\sup_N\|X_k^N\|<+\infty$, $k\in K$. We call these observables macroscopic, having in mind mainly averages of local observables but that will not always be used explicitly in what follows; it will however serve to make the assumptions plausible.

In what follows, we define concentrating states as sequences of states for which the observables X_k^N assume sharp values. Those concentrating states will be labeled by possible "outcomes" of the observables X_k^N; for these values we write $x=(x_k)_{k\in K}$ where each $x_k\in\mathbb{R}$.

A. Microcanonical setup

1. Concentrating sequences

A sequence $(P^N)_{N\uparrow+\infty}$ of projections is called concentrating at x whenever

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N(F(X_k^N)|P^N) = F(x_k) \tag{2.1}$$

for all $F\in C(\mathbb{R})$ and $k\in K$; we have used the notation

$$\mathrm{tr}^N(\cdot|P^N) = \frac{\mathrm{Tr}^N(P^N\cdot P^N)}{\mathrm{Tr}^N(P^N)} = \frac{\mathrm{Tr}^N(P^N\cdot)}{\mathrm{Tr}^N(P^N)} \tag{2.2}$$

for the normalized trace state on $P^N\mathcal{H}^N$. To indicate that a sequence of projections is concentrating at x we use the shorthand $P^N\overset{\mathrm{mc}}{\longrightarrow}x$.

2. Noncommutative functions

The previous lines, in formula (2.1), consider functions of a single observable. By properly defining the joint functions of two or more operators that do not mutually commute, the concentration property extends as follows.

Let $\mathcal{I}_K$ denote the set of all finite sequences from K, and consider all maps $G:\mathcal{I}_K\to\mathbb{C}$ such that

$$\sum_{m\geqslant 0}\sum_{(k_1,\ldots,k_m)\in\mathcal{I}_K} |G(k_1,\ldots,k_m)|\prod_{i=1}^{m} r_{k_i} < \infty \tag{2.3}$$

for some fixed $r_k>\sup_N\|X_k^N\|, k\in K$. Slightly abusing the notation, we also write

$$G(X^N) = \sum_{m\geqslant 0}\sum_{(k_1,\ldots,k_m)\in\mathcal{I}_K} G(k_1,\ldots,k_m)X_{k_1}^N\cdots X_{k_m}^N \tag{2.4}$$

defined as norm-convergent series. We write $\mathcal{F}$ to denote the algebra of all these maps G, defining noncommutative "analytic" functions on the multidisc with radii $(r_k), k\in K$.

Proposition 2.1: Assume that $P^N\overset{\mathrm{mc}}{\longrightarrow}x$. *Then, for all* $G\in\mathcal{F}$,

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N[G(X^N)|P^N] = G(x). \tag{2.5}$$

Remark 2.2: In particular, the limit expectations on the left-hand side of (2.5) coincide for all classically equivalent noncommutative functions. As example, for any complex parameters $\lambda_k, k \in R$ with R a finite subset of K and for $P^N \overset{\mathrm{mc}}{\to} x$,

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N(e^{\sum_{k\in R}\lambda_k(X_k^N - x_k)}|P^N) = \lim_{N\uparrow+\infty} \mathrm{tr}^N\left(\prod_{k\in R} e^{\lambda_k(X_k^N - x_k)}|P^N\right) = 1$$

no matter in what order the last product is actually performed.

Proof of Proposition 2.1: For any monomial $G(X^N) = X_{k_1}^N \cdots X_{k_m}^N$, $m \geqslant 1$, we prove the statement of the proposition by induction, as follows. Using the shorthands $Y^N = X_{k_1}^N \cdots X_{k_{m-1}}^N$ and $y = x_{k_1} \cdots x_{k_{m-1}}$, the induction hypothesis reads $\lim_{N\uparrow+\infty} \mathrm{tr}^N(Y^N|P^N) = y$ and we get

$$|\mathrm{tr}^N(Y^N X_{k_m}^N - y x_{k_m}|P^N)|$$

$$= |\mathrm{tr}^N(Y^N(X_{k_m}^N - x_{k_m})|P^N) + x_{k_m}\mathrm{tr}^N(Y^N - y|P^N)|$$

$$\leqslant \|Y^N\|\{\mathrm{tr}^N((X_{k_m}^N - x_{k_m})^2|P^N)\}^{\frac{1}{2}} + |x_{k_m}||\mathrm{tr}^N(Y^N - y|P^N)| \to 0$$

since $P^N \overset{\mathrm{mc}}{\to} x$ and (Y^N) are uniformly bounded. That readily extends to all noncommutative polynomials by linearity, and finally to all uniform limits of the polynomials by a standard continuity argument. □

3. H-function

Only the concentrating sequences of projections on the subspaces of the largest dimension become candidates for noncommutative variants of macrostates associated with $x = (x_k)_{k\in K}$, and that maximal dimension yields the (generalization of) Boltzmann's H-function. More precisely, to any macroscopic value $x = (x_k)_{k\in K}$ we assign

$$H^{\mathrm{mc}}(x) = \limsup_{P^N \overset{\mathrm{mc}}{\to} x} \frac{1}{N} \log \mathrm{Tr}^N[P^N], \tag{2.6}$$

where $\limsup_{P^N \overset{\mathrm{mc}}{\to} x} = \sup_{P^N \overset{\mathrm{mc}}{\to} x} \limsup_{N\uparrow+\infty}$ is the maximal limit point over all sequences of projections concentrating at x. By construction, $H^{\mathrm{mc}}(x) \in \{-\infty\} \cup [0, +\infty]$ and we write Ω to denote the set of all $x \in \mathbb{R}^K$ for which $H^{\mathrm{mc}}(x) \geqslant 0$; these are all admissible macroscopic configurations. Slightly abusing the notation, any sequence $P^N \overset{\mathrm{mc}}{\to} x$, $x \in \Omega$ such that $\limsup_N (1/N)\log \mathrm{Tr}^N[P^N] = H^{\mathrm{mc}}(x)$, will be called a microcanonical macrostate at x.

4. Example

Take a spin system of N spin-1/2 particles for which the magnetization in the α-direction, $\alpha = 1, 2, 3$, is given by

$$X_\alpha^N = \frac{1}{N}\sum_{i=1}^N \sigma_i^\alpha \tag{2.7}$$

in terms of (copies of) the Pauli matrices σ^α.

Let δ_N be a sequence of positive real numbers such that $\delta_N \downarrow 0$ as $N \uparrow +\infty$. For $\vec{m} = (m_1, m_2, m_3) \in [-1,1]^3$, let $\vec{e} \| \vec{m}$ be a unit vector for which $\vec{m} = m\vec{e}$ with $m \geqslant 0$. Consider $Y^N(\vec{m}) = \Sigma_{\alpha=1}^3 m_\alpha X_\alpha^N$ and its spectral projection $Q^N(\vec{m})$ on $[m-\delta_N, m+\delta_N]$. One easily checks that if $N^{1/2}\delta_N \uparrow +\infty$, then $(Q^N(\vec{m}))_N$ is a microcanonical macrostate at $\vec{m}$, and

$$H^{\mathrm{mc}}(\vec{m}) = \begin{cases} -\dfrac{1-m}{2}\log\dfrac{1-m}{2} - \dfrac{1+m}{2}\log\dfrac{1+m}{2} & \text{for } m \leqslant 1 \\ -\infty & \text{otherwise.} \end{cases}$$

B. Canonical setup

The concept of macrostates as above and associated with projections on certain subspaces on which the selected macroscopic observables take sharp values is physically natural and restores the interpretation of "counting microstates." Yet, sometimes it is not very suitable for computations. Instead, at least when modeling thermal equilibrium, one usually prefers canonical or grand-canonical ensembles, and one relies on certain equivalence of all these ensembles.

1. Concentrating states

For building the ensembles of quantum statistical mechanics, one does not immediately encounter the problem of noncommutativity. One requires a certain value for a number of macroscopic observables and one constructs the density matrix that maximizes the von Neumann entropy.

We write $\omega^N \overset{1}{\longrightarrow} x$ for a sequence of states (ω^N) on $\mathcal{H}^N$ whenever $\lim_{N\uparrow+\infty} \omega^N(X_k^N) = x_k$ (convergence in mean).

That construction and that of the concentrating sequences of projections of Sec. II A 1 still has other variants. We say that a sequence of states (ω^N) is concentrating at x and we write $\omega^N \to x$, when

$$\lim_{N\uparrow+\infty} \omega^N(G(X^N)) = G(x) \tag{2.8}$$

for all $G \in \mathcal{F}$. The considerations of Proposition 2.1 apply also here and one can equivalently replace the set of all noncommutative analytic functions with functions of a single variable.

2. Gibbs-von Neumann entropy

The counting entropy of Boltzmann extends to general states such as the von Neumann entropy which is the quantum variant of the Gibbs formula, both being related to the relative entropy defined with respect to a trace reference state. Analogous to (2.6), we define

$$H^{\mathrm{can}}(x) = \limsup_{\omega^N \to x} \frac{1}{N}\mathcal{H}(\omega^N), \tag{2.9}$$

where $\mathcal{H}(\omega^N) \geqslant 0$ is, upon identifying the density matrix σ^N for which $\omega^N(\cdot) = \mathrm{Tr}^N(\sigma^N \cdot)$,

$$\mathcal{H}(\omega^N) = -\mathrm{Tr}[\sigma^N \log \sigma^N]. \tag{2.10}$$

Second, we consider

$$H_1^{\mathrm{can}}(x) = \limsup_{\omega^N \overset{1}{\to} x} \frac{1}{N} \mathcal{H}(\omega^N). \tag{2.11}$$

Obviously, H_1^{can} is the analog of the canonical entropy in thermostatics and the easiest to compute, see also under Sec. II B 3. To emphasize that, we call any sequence of states (ω^N), $\omega^N \overset{1}{\to} x$ such that $\limsup_N (1/N)\mathcal{H}(\omega^N) = H_1^{\mathrm{can}}(x)$ a canonical macrostate at x.

Another generalization of the H-function is obtained when replacing the trace state (corresponding to the counting) with a more general reference state $\rho = (\rho^N)_N$. In that case we consider the H-function as derived from the relative entropy, and differing from the above-used convention by the sign and an additive constant:

$$H_1^{\mathrm{can}}(x|\rho) = \liminf_{\omega^N \overset{1}{\to} x} \frac{1}{N} \mathcal{H}(\omega^N|\rho^N). \tag{2.12}$$

Here, defining σ^N and σ_0^N as the density matrices such that $\omega^N(\cdot) = \mathrm{Tr}[\sigma^N \cdot]$ and $\rho^N(\cdot) = \mathrm{Tr}[\sigma_0^N \cdot]$,

$$\mathcal{H}(\omega^N|\rho^N) = \mathrm{Tr}[\sigma^N(\log \sigma^N - \log \sigma_0^N)]. \tag{2.13}$$

Remark that this last generalization enables one to cross the border between closed and open thermodynamic systems. Here, the state (ρ^N) can be chosen as a nontrivial stationary state for an open system, and the above-defined H-function $H_1^{\mathrm{can}}(x|\rho)$ may lose natural counting and thermodynamic interpretations. Nevertheless, its monotonicity properties under dynamics satisfying suitable conditions justify this generalization, see Sec. IV.

3. Canonical macrostates

The advantage of the canonical formulation of the variational problem for the H-function as in (2.11) is that it can often be solved in a very explicit way. A class of general and well-known examples of canonical macrostates have the following Gibbsian form.[3]

If $\lambda = (\lambda_1, \ldots, \lambda_n)$ are such that the sequence of states (ω_λ^N), $\omega_\lambda^N(\cdot) = \mathrm{Tr}^N(\sigma_\lambda^N \cdot)$ defined by

$$\sigma_\lambda^N = \frac{1}{\mathcal{Z}_\lambda^N} e^{N\Sigma_k \lambda_k X_k^N}, \quad \mathcal{Z}_\lambda^N = \mathrm{Tr}^N\left(e^{N\Sigma_k \lambda_k X_k^N}\right) \tag{2.14}$$

satisfies $\lim_{N\uparrow+\infty} \omega_\lambda^N(X_k^N) = x_k$, $k = 1, \ldots, n$, then (ω_λ^N) is a canonical macrostate at x, and

$$H_1^{\mathrm{can}}(x) = \limsup_N \frac{1}{N} \log \mathcal{Z}_\lambda^N - \sum_k \lambda_k x_k. \tag{2.15}$$

III. EQUIVALENCE OF ENSEMBLES

A basic intuition of statistical mechanics is that adding those many new concentrating states in the variational problem, as done in Sec. II B, does not actually change the value of the H-function. In the same manner of speaking, one would like to understand the definitions (2.9) and (2.11) in counting-terms. In what sense do these entropies represent a dimension (the size) of a (microscopic) subspace?

Trivially, $H^{\mathrm{mc}} \leqslant H^{\mathrm{can}} \leqslant H_1^{\mathrm{can}}$, and $H^{\mathrm{can}}(x) = H_1^{\mathrm{can}}(x)$ iff some canonical macrostate $\omega^N \overset{1}{\to} x$ is actually concentrating at x, $\omega^N \to x$. We give general conditions under which the full equality can be proven. We have again a sequence of observables X_k^N with spectral measure given by the projections $Q_k^N(\mathrm{d}z), k \in K$.

Theorem 3.1: *Assume that for a sequence of density matrices* $\sigma^N > 0$, *the corresponding* $(\omega^N)_N$ *is a canonical macrostate at x and that the following two conditions are verified*:

(i) (Exponential concentration property.)

For every $\delta>0$ *and* $k\in K$ *there are* $C_k(\delta)>0$ *and* $N_k(\delta)$ *so that*

$$\int_{x_k-\delta}^{x_k+\delta}\omega^N(Q_k^N(\mathrm{d}z))\geqslant 1-e^{-C_k(\delta)N} \tag{3.1}$$

for all $N>N_k(\delta)$.

(ii) (Asymptotic equipartition property.)

For all $\delta>0$,

$$\lim_{N\uparrow+\infty}\frac{1}{N}\log\int_{-\delta}^{\delta}\omega^N(\tilde{Q}^N(\mathrm{d}z))=0, \tag{3.2}$$

where $\tilde{Q}^N$ *denotes the projection operator-valued measure of the operator* $(1/N)(\log\sigma^N-\omega^N(\log\sigma^N))$.

Then, $H^{\mathrm{mc}}(x)=H^{\mathrm{can}}(x)=H_1^{\mathrm{can}}(x)\geqslant 0$.

Theorem 3.1 evidently expresses that the microcanonical and the canonical ensembles are equivalent. Results of that kind are well-known in the literature, see e.g., Ref. 14 or 7. An example of a similar type of reasoning for the quantum case is given in Ref. 11. Theorem 3.1 is, however, slightly different from these results in the following aspects,

(1) When considering the quantum microcanonical ensemble, one usually starts out with spectral projections P^N associated with one macroscopic observable. That at least is the approach in Ref. 11 and it is also sketched at the very beginning of Sec. II. Our approach is, however, not limited to one macroscopic observable. Indeed, remember that the $(X_k^N)_k$ need not commute (Sec. II A).

(2) Results on equivalence of ensembles, including those contained in, e.g., Refs. 14, 7, and 11 are mostly dealing solely with translation-invariant lattice spin systems. We do not have that limitation here; instead we have the assumptions (3.2) and (3.1).

(3) Even within the context of translation-invariant lattice spin systems, the results in Refs. 14, 7, and 11 do not yield Theorem 3.1. In these references the microcanonical state is defined as the average of projections P^N, translated over all lattice vectors. That lattice average is translation-invariant by construction (and hence technically easier to handle), but of course it is itself not longer a projection and hence it is not a microcanonical state in the sense of the present paper.

Remarks on the conditions of Theorem 3.1: Whether one can prove the assumptions of Theorem 3.1, depends heavily on the particular model.

The exponential concentration property (3.1) is not trivial even for quantum lattice spin systems, and not even in their one-phase region. Let us mention one criterion under which (3.1) can be checked, which indicates its deep relation to the problem of quantum large deviations. Consider the generating functions

$$\psi_k(t)=\lim_{N\uparrow+\infty}\frac{1}{N}\log\omega^N(e^{tNX_k^N}),\quad k\in K. \tag{3.3}$$

Their existence together with their differentiability at $t=0$ imply by an exponential Chebyshev inequality that ω^N exponentially concentrates at $x=(\psi_k'(0);k\in K)$. However, to our knowledge, the differentiability of $\psi_k(t)$ has only been proven so far for lattice averages over local observables for quantum spin lattice systems in a "high-temperature regime," see Ref. 12, Theorem 2.15 and Remark 7.13, where a cluster expansion technique has been used. The existence of the generating functions (3.3) has also been studied in Ref. 10.

The asymptotic equipartition property (3.2) is easier. The terminology, originally in information theory, comes from its immediate consequence (3.7) below, where P^N projects on a "high

probability" region: as in the classical case, the Gibbs-von Neumann entropy measures in some sense the size of the space of "sufficiently probable" microstates. For (3.2) it is enough to prove that the state ω^N is concentrating for the observable

$$A^N = \frac{1}{N} \log \sigma^N. \tag{3.4}$$

Explicitly, it is enough to show that for all $F \in C(\mathbb{R})$,

$$\lim_{N\uparrow+\infty} [\omega^N(F(A^N)) - F(\omega^N(A^N))] = 0. \tag{3.5}$$

In particular, if (ω^N), $\omega^N = \omega_\lambda^N$ is given by formula (2.14), a sufficient condition for the asymptotic equipartition property to be satisfied is that the pressure $p(\lambda)$ defined as

$$p(\lambda) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathcal{Z}_\lambda^N \tag{3.6}$$

exists and is continuously differentiable at $\lambda = \lambda(x)$.

Remark that for ergodic states of spin lattice systems, the asymptotic equipartition as expressed by (3.2) and (3.7) follows from the quantum Shannon-McMillan theorem, see Ref. 2, and the references therein. An interesting variant of that result, which touches the problem of quantum large deviations, is the quantum Sanov theorem, proven for i.i.d. processes in Ref. 1. In contrast, our result focuses on the intimate relation of the asymptotic equipartition property to the problem of equivalence of ensembles in the noncommutative context, and Theorem 3.1 formulates sufficient conditions under which such an equivalence follows. An advantage of this approach is that it is not restricted to the framework of spin lattice models with its underlying quasilocal structure.

As $H^{\mathrm{mc}} \leqslant H^{\mathrm{can}} \leqslant H_1^{\mathrm{can}}$, we only need to establish that there is a concentrating sequence of projections for which its H-function equals the Gibbs-von Neumann entropy. Hence, the proof of Theorem 3.1 follows from the following lemma:

Lemma 3.2: If a sequence of states (ω^N) *satisfies conditions* (*i*) *and* (*ii*) *of Theorem 3.1*, *then there exists a sequence of projections* (P^N) *exponentially concentrating at x and satisfying*

$$\lim_{N\uparrow+\infty} \frac{1}{N} (\log \mathrm{Tr}^N(P^N) - \mathcal{H}(\omega^N)) = 0. \tag{3.7}$$

Proof: There exists a sequence $\delta_N \downarrow 0$ such that when substituted for δ, (3.2) is still satisfied. Take such a sequence and define $P^N = \int_{-\delta_N}^{\delta_N} \mathrm{d}\tilde{Q}^N(z)$. By construction,

$$e^{N(h_N - \delta_N)} P^N \leqslant (\sigma^N)^{-1} P^N \leqslant e^{N(h_N + \delta_N)} P^N \tag{3.8}$$

for any $N = 1, 2, \ldots$, with the shorthand $h_N = (1/N)\mathcal{H}(\omega^N)$. That yields the inequalities

$$\mathrm{Tr}^N(P^N) = \omega^N((\sigma^N)^{-1} P^N) \leqslant e^{N(h_N + \delta_N)} \omega^N(P^N) \tag{3.9}$$

and

$$\mathrm{Tr}^N(P^N) \geqslant e^{N(h_N - \delta_N)} \omega^N(P^N). \tag{3.10}$$

Using that $\lim_{N\uparrow+\infty} (1/N) \log \omega^N(P^N) = 0$ proves (3.7).

To see that (P^N) is exponentially concentrating at x, observe that for all $Y^N \geqslant 0$,

$$\begin{aligned} \omega^N(Y^N) &= \mathrm{Tr}^N((\sigma^N)^{1/2} Y^N (\sigma^N)^{1/2}) \geqslant \mathrm{Tr}^N(P^N (\sigma^N)^{1/2} Y^N (\sigma^N)^{1/2} P^N) \\ &= \mathrm{Tr}^N((Y^N)^{1/2} P^N \sigma^N (Y^N)^{1/2}) \\ &\geqslant e^{N(h_N - \delta_N)} \mathrm{Tr}^N(P^N) \mathrm{tr}^N(Y^N | P^N) \geqslant e^{-2N\delta_N} \omega^N(P^N) \mathrm{tr}^N(Y^N | P^N), \end{aligned} \tag{3.11}$$

where we used inequalities (3.8)–(3.10). By the exponential concentration property of (ω^N), inequality (3.1), for all $k \in K$, $\epsilon > 0$, and $N > N_k(\epsilon)$,

$$\int_{\mathbb{R}\setminus(x_k-\epsilon,x_k+\epsilon)} \mathrm{tr}^N(\mathrm{d}Q_k^N(z)|P^N) \leqslant e^{-(C_k(\epsilon)-2\delta_N)N}(\omega^N(P^N))^{-1}. \tag{3.12}$$

Choose $N_k'(\epsilon)$ such that $\delta_N \leqslant C_k(\epsilon)/8$ and $(1/N)\log \omega^N(P^N) \geqslant -C_k(\epsilon)/4$ for all $N > N_k'(\epsilon)$. Then (3.12) $\leqslant \exp[-C_k(\epsilon)N/2]$ for all $N > \max\{N_k(\epsilon), N_k'(\epsilon)\}$. □

IV. *H*-THEOREM FROM MACROSCOPIC AUTONOMY

When speaking about an *H*-theorem or about the monotonicity of entropy one often refers, and even more so for a quantum setup, to the fact that the relative entropy verifies the contraction inequality

$$\mathcal{H}(\omega^N\tau^N|\rho^N\tau^N) \leqslant \mathcal{H}(\omega^N|\rho^N) \tag{4.1}$$

for all states ω^N, ρ^N on $\mathcal{H}^N$ and for all completely positive maps τ^N on $\mathcal{B}(\mathcal{H}^N)$. That is true classically, quantum mechanically and for all small or large N. When the reference state ρ^N is invariant under τ^N, (4.1) yields the contractivity of the relative entropy with respect to ρ^N. However tempting, such inequalities should not be confused with second law or with *H*-theorems; note in particular that $\mathcal{H}(\omega^N)$ defined in (2.10) is constant whenever τ^N is an automorphism: $\mathcal{H}(\omega^N\tau^N) = \mathcal{H}(\omega^N)$.

In contrast, an *H*-theorem refers to the (usually strict) monotonicity of a quantity on the macroscopic trajectories as obtained from a microscopically defined dynamics. Such a quantity is often directly related to the fluctuations in a large system and its extremal value corresponds to the equilibrium or, more generally, to a stationary state.

In the previous section we have obtained how to represent a macroscopic state and constructed a candidate *H*-function. Imagine now a time-evolution for the macroscopic values, always referring to the same set of (possibly noncommuting macroscopic) observables X_k^N. To prove an *H*-theorem, we need basically two assumptions: macroscopic autonomy and the semigroup property, or that there is a first-order autonomous equation for the macroscopic values. A classical version of this study and more details can be found in Ref. 5.

A. Microcanonical setup

Assume a family of automorphisms $\tau_{t,s}^N$ is given as acting on the observables from $\mathcal{B}(\mathcal{H}^N)$ and satisfying

$$\tau_{t,s}^N = \tau_{t,u}^N \tau_{u,s}^N, \quad t \geqslant u \geqslant s. \tag{4.2}$$

It follows that the trace Tr^N is invariant for $\tau_{t,s}^N$.

Recall that $\Omega \subset \mathbb{R}^K$ is the set of all admissible macroscopic configurations, $H^{\mathrm{mc}}(x) \geqslant 0$. On this space we want to study the emergent macroscopic dynamics.

Autonomy condition. There are maps $(\phi_{t,s})_{t \geqslant s \geqslant 0}$ on Ω and there is a microcanonical macrostate (P^N), $P^N = P^N(x)$ for each $x \in \Omega$, such that for all $G \in \mathcal{F}$ and $t \geqslant s \geqslant 0$,

$$\lim_{N\uparrow+\infty} \mathrm{tr}^N(\tau_{t,s}^N G(X^N)|P^N) = G(\phi_{t,s}x). \tag{4.3}$$

Semigroup property. The maps are required to satisfy the semigroup condition,

$$\phi_{t,u}\phi_{u,s} = \phi_{t,s} \tag{4.4}$$

for all $t \geqslant u \geqslant s \geqslant 0$.

Theorem 4.1: *Assume that the autonomy condition* (4.3) *and the semigroup condition* (4.4) *are both satisfied. Then, for every* $x \in \Omega$, $H^{\mathrm{mc}}(x_t)$ *is nondecreasing in* $t \geqslant 0$ with $x_t = \phi_{t,0}x$.

Proof: Given $x \in \Omega$, fix a microcanonical macrostate $P^N \overset{\text{mc}}{\to} x$ and $t \geq s \geq 0$. Using that $(\tau^N_{t,s})^{-1}$ is an automorphism and $\mathrm{Tr}^N((\tau^N_{t,s})^{-1}\cdot) = \mathrm{Tr}^N(\cdot)$, the identity

$$\mathrm{tr}^N(\tau^N_{t,s} G(X^N)|P^N) = \frac{\mathrm{Tr}^N(G(X^N)(\tau^N_{t,s})^{-1}P^N)}{\mathrm{Tr}^N((\tau^N_{t,s})^{-1}P^N)} = \mathrm{tr}^N(G(X^N)|(\tau^N_{t,s})^{-1}P^N)$$

yields $(\tau^N_{t,s})^{-1}P^N \overset{\text{mc}}{\to} \phi_{t,s}x$ due to autonomy condition (4.3). Hence,

$$H^{\text{mc}}(\phi_{t,s}x) \geq \limsup_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}^N((\tau^N_{t,s})^{-1}P^N) = H^{\text{mc}}(x).$$

In particular, one has that $x_s = \phi_{s,0}x \in \Omega$. The statement then follows by the semigroup property (4.3):

$$H^{\text{mc}}(x_t) = H^{\text{mc}}(\phi_{t,0}x) = H^{\text{mc}}(\phi_{t,s}x_s) \geq H^{\text{mc}}(x_s).$$

□

It is important to realize that a macroscopic dynamics, even autonomous in the sense of (4.3), need not satisfy the semigroup property (4.1). In that case one actually does not expect the H-function to be monotone; see Ref. 4 and below for an example. As obvious from the proof, without that semigroup property of $(\phi_{t,s})$, (4.3) only implies $H(x_t) \geq H(x)$, $t \geq 0$. Or, in a bit more generality, it implies that for all $s \geq 0$ and $x \in \Omega$ the macrotrajectory $(x_t)_{t\geq s}$, $x_t = \phi_{t,s}(x)$ satisfies $H(x_t) \geq H(x_s)$ for all $t \geq s$.

Remark that while the set of projections is invariant under the automorphisms $(\tau^N_{t,s})$, this is not true any longer for more general microscopic dynamics defined as completely positive maps, and describing possibly an open dynamical system interacting with its environment. In the latter case the proof of Theorem 4.1 does not go through and one has to allow for macrostates described via more general states, as in Sec. II B. The revision of the argument for the H-theorem within the canonical setup is done in the next section.

B. Canonical setup

We have completely positive maps $(\tau^N_{t,s})_{t\geq s\geq 0}$ on $\mathcal{B}(\mathcal{H}^N)$ satisfying

$$\tau^N_{t,s} = \tau^N_{t,u}\tau^N_{u,s}, \quad t \geq u \geq s \geq 0 \tag{4.5}$$

and leaving invariant the state ρ^N; they represent the microscopic dynamics. The macroscopic dynamics is again given by maps $\phi_{t,s}$.

As a variant of autonomy condition (4.3), we assume that the maps $\phi_{t,s}$ are reproduced along the time-evolution in the mean. Namely, see definition (2.12), for every $x \in \Omega_1(\rho) = \{x; H_1^{\text{can}}(x|\rho) < \infty\}$ we ask that a canonical macrostate $\omega^N \overset{1}{\to} x$ exists such that, for all $t \geq s \geq 0$,

$$\phi_{t,s}x = \lim_{N\uparrow+\infty} \omega^N(\tau^N_{t,s}X^N). \tag{4.6}$$

At the same time, we still assume the semigroup condition (4.4).

Theorem 4.2: *Under conditions* (4.6) and (4.4), *the function* $H_1^{\text{can}}(\phi_{t,0}x|\rho)$ *is nonincreasing in* $t \geq 0$ *for all* $x \in \Omega_1(\rho)$.

Proof: If $\omega^N \overset{1}{\to} x$ is a canonical macrostate at x then, by the monotonicity of the relative entropy,

$$H_1^{\text{can}}(x|\rho) = \liminf_{N\uparrow+\infty} \frac{1}{N}\mathcal{H}(\omega^N|\rho^N) \geq \liminf_{N\uparrow+\infty} \frac{1}{N}\mathcal{H}(\omega^N\tau^N_{t,s}|\rho^N).$$

On the other hand, by (4.6), the sequence $(\omega^N\tau^N_{t,s})$ is concentrating in the mean at $\phi_{t,s}(x)$, yielding

$$H_1^{\mathrm{can}}(x|\rho) \geqslant H_1^{\mathrm{can}}(\phi_{t,s}x|\rho).$$

Using (4.4), the proof is now finished as in Theorem 4.1. □

C. Example: The quantum Kac model

A popular toy model to illustrate and to discuss essential features of relaxation to equilibrium has been introduced by Mark Kac.[9] Here we review an extension that can be called a quantum Kac model, we described it extensively in Ref. 4, to learn only later that essentially the same model was considered by Max Dresden and Frank Feiock in Ref. 6. However, there is an interesting difference in interpretation to which we return at the end of the section.

At each site of a ring with N sites there is a quantum bit $\psi_i \in \mathbb{C}^2$ and a classical binary variable $\xi_i = \pm 1$ (which we also consider to be embedded in $\mathbb{C}^2$). The microstates are thus represented as vectors $(\psi;\xi)=(\psi_1,\ldots,\psi_N;\xi_1,\ldots,\xi_N)$, being elements of the Hilbert space $\mathcal{H}^N=\mathbb{C}^{2N}\otimes\mathbb{C}^{2N}$. The time is discrete and at each step two operations are performed: a right shift, denoted below by S^N and a local scattering or update V^N. The unitary dynamics is given as

$$U^N = S^N V^N, \quad U_t^N = (U^N)^t \quad \text{for } t \in \mathbb{N} \tag{4.7}$$

with the shift

$$S^N(\psi;\xi) = (\psi_N, \psi_1, \ldots, \psi_{N-1};\xi) \tag{4.8}$$

and the scattering

$$V^N(\psi;\xi) = \left(\frac{1-\xi_1}{2}V_1\psi_1 + \frac{1+\xi_1}{2}\psi_1, \ldots, \frac{1-\xi_N}{2}V_N\psi_N + \frac{1+\xi_N}{2}\psi_N;\xi\right) \tag{4.9}$$

extended to an operator on $\mathcal{H}^N$ by linearity. Here, V is a unitary 2×2 matrix and V_i its copy at site $i=1,\ldots,N$.

We consider the family of macroscopic observables

$$X_0^N = \frac{1}{N}\sum_{i=1}^N \xi_i, \quad X_\alpha^N = \frac{1}{N}\sum_{i=1}^N \sigma_i^\alpha, \quad \alpha = 1,2,3,$$

where $\sigma_i^1, \sigma_i^2, \sigma_i^3$ are the Pauli matrices acting at site i and embedded to operators on $\mathcal{H}^N$. We fix macroscopic values $x=(\mu,m_1,m_2,m_3)\in[-1,+1]^4$ and we construct a microcanonical macrostate (P^N) in x in the following way.

Let δ_N be a positive sequence in $\mathbb{R}$ such that $\delta_N \downarrow 0$ and $N^{1/2}\delta_N \uparrow +\infty$ as $N\uparrow+\infty$. For $\mu\in[-1,1]$, let $Q_0^N(\mu)$ be the spectral projection associated to X_0^N, on the interval $[\mu-\delta_N,\mu+\delta_N]$. For $\vec{m}=(m_1,m_2,m_3)\in[-1,1]^3$, we already constructed a microcanonical macrostate $Q^N(\vec{m})$ in Sec. II A 4. Obviously, $Q_0^N(\mu)$ and $Q^N(\vec{m})$ commute and the product $P^N=Q_0^N(\mu)Q^N(\vec{m})$ is a projection. It is easy to check that P^N is a microcanonical macrostate at $x=(\mu,\vec{m})$.

The construction of the canonical macrostate is standard along the lines of Sec. II B 3. The corresponding H-functions are manifestly equal:

$$H^{\mathrm{mc}}(x) = H_1^{\mathrm{can}}(x) = \eta\left(\frac{1+m}{2}\right) + \eta\left(\frac{1-m}{2}\right) + \eta\left(\frac{1+\mu}{2}\right) + \eta\left(\frac{1-\mu}{2}\right) \tag{4.10}$$

with $\eta(x)=-x\log x$ for $x\in(0,1]$ and $\eta(0)=0$, otherwise $\eta(x)=-\infty$.

We now come to the conditions of Theorem 4.1. The construction of the macroscopic dynamics and the proof of its autonomy was essentially done in Ref. 4. The macroscopic equation $\xi_t=\xi$ is obvious and the equation for $\vec{m}_t$ can be written, associating $\vec{m}_t$ with the reduced 2×2 density matrix $\nu_t=(1+\vec{m}_t\cdot\vec{\sigma})/2$, in the form $\nu_t=\Lambda_\mu^t\nu$, $t=0,1,\ldots$, where $\Lambda_\mu^t=(\Lambda_\mu)^t$ and

$$\Lambda_\mu(\nu) = \frac{1-\mu}{2} V\nu V^* + \frac{1+\mu}{2}\nu. \tag{4.11}$$

The semigroup condition (4.4) is then also automatically checked.

In order to understand better the necessity of the semigroup property for an H-theorem to be true, compare the above with another choice of macroscopic variables. Assume we had started out with

$$X_0^N = \frac{1}{N}\sum_{i=1}^N \xi_i, \quad X_1^N = \frac{1}{N}\sum_{i=1}^N \sigma_i^1$$

as the only macroscopic variables, as was done in Ref. 6. A microcanonical macrostate can again be easily constructed by setting $Q_0^N(\mu)$ the spectral projection associated to X_0^N on the interval $[\mu-\delta_N, \mu+\delta_N]$ and $Q_1^N(\vec{m})$ the spectral projection for X_1^N on $[\mu-\delta_N, \mu+\delta_N]$, and finally $P^N = Q_0^N(\mu)Q_1^N(\vec{m})$ as before. The sequence (P^N) defines a microcanonical macrostate at $(\mu, \vec{m})$ and the autonomy condition (4.3) is satisfied. However, the macroscopic evolution does not satisfy the semigroup property (4.4) and, in agreement with that, the corresponding H-functions are not monotonous in time (see Ref. 4).

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Uniqueness of solutions to the helically reduced wave equation with Sommerfeld boundary conditions

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We consider the helical reduction of the wave equation with an arbitrary source on $(n+1)$-dimensional Minkowski space, $n \geqslant 2$. The reduced equation is of mixed elliptic-hyperbolic type on $\mathbf{R}^n$. We obtain a uniqueness theorem for solutions on a domain consisting of an n-dimensional ball B centered on the reduction of the axis of helical symmetry and satisfying ingoing or outgoing Sommerfeld conditions on $\partial B \approx S^{n-1}$. Nonlinear generalizations of such boundary value problems (with $n=3$) arise in the intermediate phase of binary inspiral in general relativity. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2212667]

I. INTRODUCTION

Recent approaches to the quasistationary approximation of the intermediate phase of binary inspiral in general relativity have led to the consideration of reductions of the Einstein equations by a helical Killing vector field (see Refs. 1–3 and references therein). To date, model problems have been analyzed consisting of helical reductions of linear and nonlinear wave equations in $(3+1)$-dimensional Minkowski space–time with various sources using Sommerfeld conditions on a spherical boundary.[1] These helically reduced equations have the challenging feature of being of mixed elliptic-hyperbolic type on their three-dimensional domain. More precisely, they are elliptic in an inner cylindrical region surrounding the sources and hyperbolic outside this cylindrical region. There appear to be no general theorems to handle existence and uniqueness of solutions to partial differential equations of mixed type. Results tend to be specific to individual equations or limited classes of equations, and even then the equations which have been most studied are defined in two dimensions.[4] From the investigations of Ref. 1 it appears that the boundary value problem arising from helical reduction of (linear and nonlinear) wave equations using Sommerfeld conditions on an exterior boundary is well-posed. Solutions have been constructed and appear to be unique. This is somewhat remarkable since the boundary intersects both the hyperbolic and elliptic domains. In particular, one might not expect a single (Sommerfeld) condition on a closed boundary to enforce uniqueness of solutions.[1]

Some light was shed on this issue by the work of Ref. 5, where the helical reduction of the $(2+1)$-dimensional wave equation was shown to define a symmetric-positive system on an annular region in $\mathbf{R}^2$ such that the Sommerfeld boundary value problem was well-posed—solutions exist and, in particular, are unique. Unfortunately, it is not known how to generalize these results (i.e., symmetric positivity of the reduced equation) to higher dimensions. Moreover, the helical reduction of the $(2+1)$-dimensional wave equation leads to a boundary value problem on a two-dimensional region with an outer circular boundary which need never intersect the circle of degeneracy of the symbol of the reduced partial differential equation. In higher dimensions, the spherical outer boundary necessarily intersects the "light cylinder" where the symbol is degenerate so the boundary conditions *must* be imposed both in the elliptic and in the hyperbolic regions. (Unless, of course, the boundary is completely contained in the elliptic region, which is not of physical interest and which, in any case, leads to a standard elliptic boundary value problem). This

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makes the problem qualitatively different in the physical $(3+1)$ space–time dimensions (and in higher dimensions).

Thus, it is of interest both from mathematical physics and gravitational physics viewpoints to better understand the nature of boundary value problems arising from helical reduction of wave equations. Here we shall provide a uniqueness theorem for the helical reduction of the $(n+1)$-dimensional wave equation with arbitrary sources and with Sommerfeld boundary conditions. The proof is remarkably elementary and employs an approach used by Protter to study a generalization of the Tricomi problem.[6]

II. THE HELICALLY REDUCED WAVE EQUATION

We will be considering the helical reduction of the wave equation with an arbitrary source on $(n+1)$-dimensional Minkowski space, with $n \geqslant 2$. The space-time manifold is $N=\mathbf{R}^{n+1}$ with metric

$$\eta = -dt \otimes dt + dx \otimes dx + dy \otimes dy + \delta_{ij} dz^i \otimes dz^j, \tag{2.1}$$

where Latin indices $i,j=1,2,\ldots,n-2$. The wave equation for $\Psi: N \to \mathbf{R}$ with a prescribed source $F: N \to \mathbf{R}$ is

$$-\Psi_{tt} + \Psi_{xx} + \Psi_{yy} + \delta^{ij}\Psi_{ij} = F. \tag{2.2}$$

Note we use the notation where subscripts on a function indicate partial derivatives. The helical reduction is accomplished by assuming the source and solutions are invariant with respect to the isometry group (G) generated by

$$K = \partial_t + \Omega(x\partial_y - y\partial_x), \quad \Omega = \text{const.}, \tag{2.3}$$

which is equivalent to

$$\mathcal{L}_K F = \mathcal{L}_K \Psi = 0. \tag{2.4}$$

In cylindrical coordinates (t,ρ,ϕ,z^i), the metric and Killing vector field are

$$\eta = -dt \otimes dt + d\rho \otimes d\rho + \rho^2 d\phi \otimes d\phi + \delta_{ij} dz^i \otimes dz^j, \tag{2.5}$$

$$K = \partial_t + \Omega \partial_\phi, \tag{2.6}$$

the wave equation is

$$-\Psi_{tt} + \frac{1}{\rho}\partial_\rho(\rho\Psi_\rho) + \frac{1}{\rho^2}\Psi_{\phi\phi} + \delta^{ij}\Psi_{ij} = F, \tag{2.7}$$

and the invariance condition (2.4) is

$$\Psi_t = -\Omega\Psi_\phi, \quad F_t = -\Omega F_\phi. \tag{2.8}$$

Introducing $\varphi = \phi - \Omega t$, (2.8) means there exists functions u and f such that

$$\Psi(t,\rho,\phi,z^i) = u(\rho,\varphi,z^i), \quad F(t,\rho,\phi,z^i) = f(\rho,\varphi,z^i). \tag{2.9}$$

We then get the reduced equation defining helically invariant solutions to (2.2)

$$\frac{1}{\rho}\partial_\rho(\rho u_\rho) + \frac{\chi(\rho)}{\rho^2}u_{\varphi\varphi} + \delta^{ij}u_{ij} = f, \tag{2.10}$$

where

$$\chi(\rho) = 1 - \Omega^2\rho^2. \tag{2.11}$$

The locus of points where $\chi(\rho)=0$ is the "light cylinder". Inside the light cylinder ($\rho<1/\Omega$) Eq. (2.10) is elliptic and outside the light cylinder ($\rho>1/\Omega$) Eq. (2.10) is hyperbolic.

A useful geometric interpretation of this reduction is as follows. The set of orbits of the group generated by K defines a manifold $M=N/G\approx\mathbf{R}^n$. The functions (ρ,φ,z^i) are G-invariant and define cylindrical coordinates on M. In these coordinates the projection $\pi:N\to M$ is simply

$$\pi(t,x,y,z^i)=(\rho,\varphi,z^i), \tag{2.12}$$

and satisfies $\pi_* K=0$. The G-invariant functions F and Ψ on N correspond to functions f and u on M, respectively, via

$$F=\pi^* f, \quad \Psi=\pi^* u. \tag{2.13}$$

The inverse metric on N is given by

$$\eta^\sharp=-\partial_t\otimes\partial_t+\partial_\rho\otimes\partial_\rho+\frac{1}{\rho^2}\partial_\phi\otimes\partial_\phi+\delta^{ij}\partial_i\otimes\partial_j. \tag{2.14}$$

Being G-invariant, $\eta^\sharp$ projects to a tensor field q on M. Using (2.12),

$$q=\pi_*\eta^\sharp=\partial_\rho\otimes\partial_\rho+\frac{\chi(\rho)}{\rho^2}\partial_\varphi\otimes\partial_\varphi+\delta^{ij}\partial_i\otimes\partial_j. \tag{2.15}$$

This tensor field is well-defined everywhere on M, but it does not determine a metric on M because q has no inverse on the light cylinder. While the metric on N does not induce a metric on M, the metric volume form ϵ on N does define a volume form ν on M as follows. Define

$$\omega=K\rightharpoonup\epsilon, \tag{2.16}$$

which satisfies

$$L_K\omega=0, \quad K\rightharpoonup\omega=0. \tag{2.17}$$

Consequently, ω is the pull-back by π of a volume form ν on M. It is easy to check that

$$\nu=\rho d\rho\wedge d\varphi\wedge dz^1\wedge\cdots\wedge dz^{n-2}. \tag{2.18}$$

The volume form ν defines a scalar density of weight 1, $\sigma=\rho$, on M.

We will use Greek indices to label tensor fields on M. Introduce a torsion-free derivative operator ∇_α. The reduced equation (2.10) is equivalent to

$$\frac{1}{\sigma}\nabla_\alpha(\sigma q^{\alpha\beta}\nabla_\beta u)=f. \tag{2.19}$$

To see this, we first note that because of the density weights (2.19) is in fact independent of the choice of torsion-free derivative ∇_α. Using the cylindrical coordinate derivative operator, $\nabla_\alpha=\partial_\alpha$, in (2.19) we obtain (2.10). For what follows we rewrite (2.19) as

$$\nabla_\alpha(h^{\alpha\beta}\nabla_\beta u)=\partial_\alpha(h^{\alpha\beta}u_\beta)=\tilde{f}, \tag{2.20}$$

where $\tilde{f}=\sigma f$ is a scalar density of weight 1 and $h^{\alpha\beta}=\sigma q^{\alpha\beta}$ is a tensor density of weight 1 given by

$$h^{\rho\rho}=\rho, \quad h^{ij}=\rho\delta^{ij}, \quad h^{\varphi\varphi}=\frac{1}{\rho}\chi=\frac{1}{\rho}-\Omega^2\rho. \tag{2.21}$$

III. ENERGY INTEGRAL

The key ingredient in our uniqueness theorem is the following generalized energy integral. Fix a domain $B \subset M$ and define

$$E[u] = \int_B [(au + b^\gamma u_\gamma)\partial_\alpha(h^{\alpha\beta}u_\beta)], \tag{3.1}$$

where a and $b^\alpha\partial_\alpha$ are a function and vector field to be specified later. The integrand involving a can be written as

$$au\partial_\alpha(h^{\alpha\beta}u_\beta) = \frac{1}{2}\partial_\alpha(h^{\alpha\beta}a_\beta)u^2 - ah^{\alpha\beta}u_\alpha u_\beta + \partial_\alpha\left[auh^{\alpha\beta}u_\beta - \frac{1}{2}h^{\alpha\beta}a_\beta u^2\right]. \tag{3.2}$$

The integrand involving b^γ can be written as

$$b^\gamma u_\gamma\partial_\alpha(h^{\alpha\beta}u_\beta) = \frac{1}{2}\partial_\gamma(h^{\alpha\beta}b^\gamma)u_\alpha u_\beta - b^\gamma_{,\alpha}h^{\alpha\beta}u_\gamma u_\beta + \partial_\alpha\left[b^\gamma u_\gamma h^{\alpha\beta}u_\beta - \frac{1}{2}b^\alpha h^{\beta\gamma}u_\gamma u_\beta\right]. \tag{3.3}$$

Again, while these expressions use the coordinate derivative, they are in fact independent of the choice of torsion-free derivative operator. The divergences integrate to the boundary and we have

$$\begin{aligned} E[u] = &\int_B \left\{\frac{1}{2}\partial_\alpha(h^{\alpha\beta}a_\beta)u^2 - ah^{\alpha\beta}u_\alpha u_\beta + \frac{1}{2}\partial_\gamma(h^{\alpha\beta}b^\gamma)u_\alpha u_\beta - b^\gamma_{,\alpha}h^{\alpha\beta}u_\gamma u_\beta\right\} \\ &+ \int_{\partial B} n_\alpha\left\{(au + b^\gamma u_\gamma)h^{\alpha\beta}u_\beta - \frac{1}{2}h^{\alpha\beta}a_\beta u^2 - \frac{1}{2}b^\alpha h^{\beta\gamma}u_\gamma u_\beta\right\}. \end{aligned} \tag{3.4}$$

If there were a metric on B, n_α could be defined in terms of the unit normal to the boundary and the metric-induced volume element of the boundary. Without a metric n_α is still defined, of course, but its definition is necessarily more involved. We give the definition in the Appendix.

IV. UNIQUENESS THEOREM

We are now ready to formulate the boundary value problem of interest. We consider solutions to Eq. (2.20) on a ball of radius R,

$$B = \{(\rho, \varphi, z^i) | 0 \leqslant \rho^2 + \delta_{ij}z^i z^j \leqslant R^2\}. \tag{4.1}$$

The boundary ∂B is the sphere S^{n-1} of radius R. Using (A7), we have in spherical coordinates $(r, \theta_1, \ldots, \theta_{n-1})$,

$$n_\alpha dx^\alpha = dr. \tag{4.2}$$

We impose Sommerfeld-type conditions on ∂B of the type used in Ref. 1. These take the form (in cylindrical coordinates)

$$\frac{1}{R}(\rho u_\rho + z^i u_i) \pm \Omega\partial_\varphi u = \tau, \quad \text{on } \partial B, \tag{4.3}$$

where we have included a function $\tau: \mathbf{S}^n \to \mathbf{R}$ to allow for nonradiative (e.g., monopole) contributions to u (see Remark (ii) below). These boundary conditions can be understood as follows. Sommerfeld conditions for Ψ are, strictly speaking, decay conditions on $\Psi_r \mp \Psi_t$ at spatial infinity in N, where r denotes the spatial radius at fixed t in N (see, e.g., Ref. 7 for a discussion of Sommerfeld conditions). These conditions select ingoing/outgoing radiation. At a finite radius—necessary for numerical computations—one imposes conditions of the form

$$\Psi_r \mp \Psi_t = \tau, \quad \text{on } \partial B. \tag{4.4}$$

Applying the helical symmetry reduction the conditions (4.4) reduce to (4.3).

Remark: (i) If $R > 1/\Omega$ the boundary passes through both the elliptic and hyperbolic domains. (ii) The functions τ and $\tilde{f}$ cannot be specified independently. Using (4.3) the integral of (2.20) over B implies

$$\int_B \tilde{f} = \int_{\partial B} \sigma\tau. \tag{4.5}$$

Since (2.20) and the boundary conditions (4.3) only involve derivatives of u, solutions to these equations can only be unique up to an additive constant. In fact, this is the only freedom in the solution. Our main result is the following.

Theorem: *Given* Ω, $\tilde{f}: B \to \mathbf{R}$, *and* $\tau: \partial B \to \mathbf{R}$, *any two solutions to* (2.20) *on B with boundary conditions* (4.3) *differ at most by a constant.*

Proof: Consider the difference of two solutions, $u = u_1 - u_2$; u satisfies (2.20) and (4.3) with $\tilde{f} = 0$ and $\tau = 0$, respectively. Consequently, $E[u] = 0$ for any choices of the function a and vector field $b = b^\alpha \partial_\alpha$. We choose these as

$$a = -1, \quad b = \frac{2}{1-n}[\rho\partial_\rho + z^i\partial_i \pm R\Omega\partial_\varphi]. \tag{4.6}$$

Note that

$$b^\alpha u_\alpha = 0, \quad \text{on } \partial B. \tag{4.7}$$

A straightforward computation, using (4.3) with $\tau = 0$ in the boundary integral, then gives

$$0 = \int_B \left\{ \left(\frac{1}{n-1}\right)\sigma\left[(u_\rho^2 + \delta^{ij}u_i u_j) + \left(\frac{1}{\rho^2} + \Omega^2\right)u_\varphi^2 \right] \right\} + \int_{\partial B} \left(\frac{1}{n-1}\right)\sigma\frac{R}{\rho^2}\{(z^i z^j + \rho^2\delta^{ij})u_i u_j + (1 + \Omega^2\delta_{ij}z^i z^j)u_\varphi^2 \pm 2R\Omega z^i u_i u_\varphi\}. \tag{4.8}$$

The volume integrand (in the first integral) is manifestly non-negative for $n \geqslant 2$. We now show that the boundary integrand (in the second integral) is also non-negative.

We first note that the boundary integrand is invariant under orthogonal transformations of the z^i. Thus, given any point (ρ, φ, z^i), we can rotate the z^i axes such that $z^i = (z, 0, 0, \ldots, 0)$, where $z^2 = \delta_{ij}z^i z^j$. The boundary integrand at the given point is then

$$\begin{aligned}
&\left(\frac{1}{n-1}\right)\sigma\frac{R}{\rho^2}\{(z^i z^j + \rho^2\delta^{ij})u_i u_j + (1 + \Omega^2\delta_{ij}z^i z^j)u_\varphi^2 \pm 2R\Omega z^i u_i u_\varphi\} \\
&= \left(\frac{1}{n-1}\right)\sigma\frac{R}{\rho^2}\{z^2 u_1^2 + \rho^2\delta^{ij}u_i u_j + (1 + \Omega^2 z^2)u_\varphi^2 \pm 2R\Omega z u_1 u_\varphi\} \\
&\geqslant \left(\frac{1}{n-1}\right)\sigma\frac{R}{\rho^2}\{u_\varphi^2 + (Ru_1 \pm \Omega z u_\varphi)^2\} \geqslant 0.
\end{aligned} \tag{4.9}$$

Because both integrands in (4.8) are non-negative they must each vanish. From the volume integrand it follows immediately that

$$u_\alpha = 0. \tag{4.10}$$

□

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APPENDIX: THE DIVERGENCE THEOREM WITHOUT A METRIC

Consider an n-dimensional orientable manifold M, a torsion-free derivative operator ∇_α on M, and a vector density of weight 1, V^α. Given $B \subset M$, Stokes theorem implies an identity of the form

$$\int_B \nabla_\alpha V^\alpha = \int_{\partial B} n_\alpha V^\alpha. \tag{A1}$$

Normally this divergence theorem is proved using a metric on M. However, this is not necessary. Here, we shall give a version of the divergence theorem and, in particular, give a formula for n_α without using a metric.

The manifold M, being orientable, comes equipped with a nowhere vanishing n-form density of weight minus 1, denoted by $\eta_{\alpha_1,\ldots,\alpha_n}$, and a totally antisymmetric contravariant tensor density of weight 1, $\tilde{\eta}^{\alpha_1,\ldots,\alpha_n}$, such that

$$\tilde{\eta}^{\alpha_1,\ldots,\alpha_n}\eta_{\beta_1,\ldots,\beta_n} = n!\,\delta^{[\alpha_1}_{\beta_1}\cdots\delta^{\alpha_n]}_{\beta_n}. \tag{A2}$$

Both $\eta_{\alpha_1,\ldots,\alpha_n}$ and $\tilde{\eta}^{\alpha_1,\ldots,\alpha_n}$ are constant for any choice of ∇_u.

The boundary ∂B is an oriented submanifold in M embedded by $i: S \to M$, i.e., $\partial B = i(S)$. S is equipped with an $(n-1)$-form density of weight minus 1, $\xi_{a_1,\ldots,a_{n-1}}$, and a skew, contravariant rank $(n-1)$ tensor density of weight 1, $\tilde{\xi}^{a_1,\ldots,a_{n-1}}$, satisfying

$$\tilde{\xi}^{a_1,\ldots,a_{n-1}}\xi_{b_1,\ldots,b_{n-1}} = (n-1)!\,\delta^{[a_1}_{b_1}\cdots\delta^{a_{n-1}]}_{b_{n-1}}. \tag{A3}$$

(In this appendix only we use Latin indices to denote tensors on S.)

To apply Stokes theorem we define an $(n-1)$-form

$$\omega_{\alpha_1,\ldots,\alpha_{n-1}} = V^\beta \eta_{\beta\alpha_1,\ldots,\alpha_{n-1}}. \tag{A4}$$

We then have (using differential form notation)

$$\int_B \nabla_\alpha V^\alpha = \int_B d\omega = \int_{\partial B} \omega = \int_S \frac{1}{(n-1)!}\xi^{a_1,\ldots,a_{n-1}}(i^*\omega)_{a_1,\ldots,a_{n-1}}. \tag{A5}$$

Now, at points of ∂B we can write

$$\xi^{a_1,\ldots,a_{n-1}}(i^*\omega)_{a_1,\ldots,a_{n-1}} = (i_*\xi)^{\alpha_1,\ldots,\alpha_{n-1}}\omega_{\alpha_1,\ldots,\alpha_{n-1}} = (i_*\xi)^{\alpha_1,\ldots,\alpha_{n-1}}\eta_{\beta\alpha_1,\ldots,\alpha_{n-1}}V^\beta. \tag{A6}$$

Thus we have

$$n_\beta = \frac{1}{(n-1)!}(i_*\xi)^{\alpha_1,\ldots,\alpha_{n-1}}\eta_{\beta\alpha_1,\ldots,\alpha_{n-1}}. \tag{A7}$$

An alternative approach to the integral over B in (A1) is to note that it is independent of the choice of ∇_α. If we fix a Riemannian metric $g_{\alpha\beta}$ on M, and use the metric-compatible derivative operator, we have available the more traditional form of the divergence theorem,

$$\int_B \nabla_\alpha V^\alpha = \int_{\partial B} \sqrt{\gamma}\hat{n}_\alpha W^\alpha, \tag{A8}$$

where

$$W^{\alpha} = \frac{1}{\sqrt{g}} V^{\alpha}, \tag{A9}$$

$\hat{n}_{\alpha}$ is the outwardly oriented unit normal to ∂B, and $\sqrt{\gamma}$ is the induced volume element on ∂B. The result (A8) is, of course, equivalent to the manifestly metric independent result (A5) above, as can be verified by using the identity

$$\hat{n}_{\beta} = \frac{1}{(n-1)!} \frac{\sqrt{g}}{\sqrt{\gamma}} (i_{*}\xi)^{\alpha_1,\ldots,\alpha_{n-1}} \eta_{\beta\alpha_1,\ldots,\alpha_{n-1}}. \tag{A10}$$

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Feynman path integral of Riemann type

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In this paper, we shall define a kind of operator-valued integration and define the Feynman path integrals of Riemann integral type. It seems that it is one of the best possible conditions of the existence of the path integrals of Riemann integral type for the Schrödinger equation with singular potentials. Our class of potentials is wide enough: the real measurable potential U should be continuous except for a closed set of measure zero. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Heuristic Feynman path integrals have played a remarkable role in various aspects of quantum physics. But rigorous mathematical treatment of this integral is not enough. It is well known that Feynman path integrals for Schrödinger equations are not represented by scalar-valued measure (see Ref. 9).

In this paper, we discuss a kind of operator-valued integration and define the path integral of Riemann type, analogously to Riemann integration of scalar functions. So our integration is different from the one of Nelson's (see Ichinose,[5] Nelson,[9] and Takeo[11]).

We shall show that the solution to the Schrödinger equation in $\mathbb{R}^N (N \geqslant 2)$,

$$\frac{\partial}{\partial t}u(t,x) = i\Delta u(t,x) - iU(t,x)u(t,x), \quad u(0,x) = \varphi(x), \quad \varphi \in L^2(\mathbb{R}^N;\mathbb{C}) \tag{1}$$

is written as the path integral

$$u(t,x) = \int_{\Omega_{[0,t]}} e^{-i\int_0^t U(\tau,\gamma(\tau))\mathrm{d}\tau}\varphi(\gamma(0))\mathrm{d}\mu(\gamma), \quad \varphi \in L^2(\mathbb{R}^N;\mathbb{C}) \tag{2}$$

of Riemann type. Here we denote by γ a path on $\mathbb{R}^N$, that is, $\gamma \in \Omega_{[0,t]} \equiv \Pi_{\alpha\in[0,t]}\mathbb{R}^N_\alpha$ ($\mathbb{R}^N_\alpha$=a copy of $\mathbb{R}^N$): $\gamma=(x_\alpha \in \mathbb{R}^N)_{\alpha\in[0,t]}$ (or $\gamma(\alpha)=x_\alpha$).

We study the conditions to define the path integrals of Riemann integral type for Schrödinger equation with singular potentials. Our class of potentials is wide enough: the real valued measurable potential U should be locally essentially bounded except a closed set of measure zero.

The paper of Nelson[9] is concerned with the Schrödinger operator $i[(1/2m)\Delta - V(x)]$, except for a set $\mathcal{N}$ of m with measure 0 and he assumes that V is continuous on the complement of a closed set F of capacity 0. In this paper Nelson mentions that "*The restriction to almost every real value of the mass parameter is an unsatisfactory feature of the theory*" (Ref. 9, p. 335). As Johnson and Lapidus point out that it is a serious weakness (Ref. 6, p. 295). Notice that we have no restriction of this type.

This paper is organized as follows: In Sec. II we state some fact about abstract evolution equations that will be used later. The main purpose of Sec. III is to provide basic notions of path integral of Riemann type. The concepts of path integral of Riemann type are introduced in Sec.

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III A. In Sec. III B we discuss the relationship between the iteration integral and the multiple integral. Section III C deals with sufficient conditions for μ^Q-integrability on $\mathbb{R}^N$. In Sec. IV we investigate the integrability for potentials with singularity. Integration on bounded domain treated in Sec. IV A. The goal of Sec. IV B is to provide strong integrability for non-negative potentials with singularity. Section IV C deals with the integrability for more general real potentials with singularity (see Refs. 7 and 8).

II. ABSTRACT EVOLUTION EQUATION

We begin by introducing the following class of functions.

Definition 1: The space of functions f in $L^\infty(\mathbb{R}^N;\mathbb{C})$ *such that f is uniformly continuous on* $\mathbb{R}^N$ *will be denoted* $C_\infty(\mathbb{R}^N;\mathbb{C})$ *where* $L^\infty(\mathbb{R}^N;\mathbb{C})$ *consisting of all essentially bounded functions on* $\mathbb{R}^N$.

Equation (1) is written as an evolution equation

$$\frac{d}{\mathrm{d}t}u(t) - (A + V(t))u(t), \quad u(0) = \varphi, \tag{3}$$

where $A=i\Delta$ and $V(t)=-iU(t,\cdot)$ is a $C_\infty(\mathbb{R}^N;\mathbb{C})$-valued function.

The associate semigroup with $V\equiv 0$ is written as $\{S_t\}$. More precisely, $\{S_t|-\infty<t<\infty\}\subset L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))$ is a group of unitary operators, where $L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))$ is the space of all bounded linear operators from $L^2(\mathbb{R}^N;\mathbb{C})$ to $L^2(\mathbb{R}^N;\mathbb{C})$.

Let m be a natural number and $\theta=t/m$, $s_0=0$, $s_{j+1}=s_j+\theta$, for $j=0,\ldots,m-1$, $s_m=t$. The subject of this section is that the solution $u(t)$ to the equation (3) is approximated as

$$u(t,x) \sim \left(\prod_{j=1}^{m} S_\theta e^{V(\tau_j,x)\theta}\right)\varphi(x), \quad s_{j-1} \leqslant \tau_j < s_j, \quad j = 1,\ldots,m. \tag{4}$$

We wish to provide some background in abstract evolution equation theory. Let $H=(H,\|\cdot\|)$ be a Hilbert space. Here $\|\cdot\|$ is a norm of H.

We consider the following abstract evolution equation in H:

$$\frac{d}{\mathrm{d}t}u(t) = (A + B(t))u(t), \quad u(0) = \varphi \in H, \tag{5}$$

where A is the generator of a semigroup of unitary operators and $B(t)$ is a bounded linear operator for any $t>0$.

Definition 2: A function u which is differentiable almost everywhere on $[0,T]$ *such that* $\mathrm{d}u/\mathrm{d}t \in L^1(0,T;H)$ *is called a strong solution of the initial value problem* (5) *if* $u(0)=\varphi$ *and* $(d/\mathrm{d}t)u(t)=(A+B(t))u(t)$ *a.e. on* $[0,T]$.

Lemma 1: The strong solution to

$$\frac{d}{\mathrm{d}t}u(t) = (A + B(t))u(t), \quad u(0) = \varphi \in D(A), \tag{6}$$

is given by

$$u(t) = e^{tA}u(0) + \int_0^t e^{(t-s)A}B(s)u(s)\mathrm{d}s, \tag{7}$$

if $B(t)$ *is an* $L(D(A),D(A))$*-valued continuous function. Here* $D(A)$ *is the domain of A equipped with the graph norm* $\|f\|_{D(A)}=(\|f\|^2+\|Af\|^2)^{1/2}$.

Definition 3: The solution to the integral equation (7) *is called the mild solution to the evolution equation* (6), *if it uniquely exists.*

Lemma 2: The mild solution to (6) *uniquely exists if* $B(t)$ *is an* $L(H,H)$*-valued continuous function.*

From Eq. (7) we have

$$u(t+\theta) = e^{\theta A}u(t) + \int_0^\theta e^{(\theta-s)A}B(t+s)u(t+s)\mathrm{d}s. \tag{8}$$

In general $e^{A+B} \neq e^A e^B$. This is because A and B need not commute. Therefore we shall approximate $u(t+\theta)$ by $e^{\theta A}e^{\theta B(t)}u(t)$.

Lemma 3: Let $T>0$ and $B(t)$ be a $L(H,H)$-valued continuous function. Then we have for each $\varepsilon>0$, there exists $\theta_0>0$ such that

$$\|\varepsilon^{\theta A}e^{\theta B(t)}u(t) - u(t+\theta)\| < \theta\varepsilon \quad \textit{for } 0<\theta\leqslant\theta_0 \textit{ and } 0\leqslant t\leqslant T. \tag{9}$$

Proof: Note that the set $\mathcal{C}=\{u(t)\,|\,0\leqslant t\leqslant T\}$ is compact. Since $B(t)$, $u(t)$, and e^{tA} are continuous in t, we may assume for each $\varepsilon_1>0$, there exists $\theta_1>0$ such that

$$\|(B(t)-B(t+s))u(t)\| < \varepsilon_1, \quad \|B(t+s)(u(t)-u(t+s))\| < \varepsilon_1, \quad \|(e^{\theta A}-e^{sA})B(t)u(t)\| < \varepsilon_1$$

$$\textit{for } 0\leqslant s,\theta\leqslant\theta_1, \textit{ and } 0\leqslant t\leqslant T.$$

Since $B(t)$ is linear bounded operator, there exists $M>0$ such that

$$e^{sB(t)}u(t) = (1+sB(t))u(t) + s^2\eta \textit{ for } \|\eta\| < M.$$

Hence by (8), for any $\varepsilon>0$ it follows that

$$\begin{aligned}
\|e^{\theta A}e^{\theta B(t)}u(t) - u(t+\theta)\| &= \left\| e^{\theta A}e^{\theta B(t)}u(t) - e^{\theta A}u(t) - \int_0^\theta e^{(\theta-s)A}B(t+s)u(t+s)\mathrm{d}s \right\| \\
&= \left\| \theta e^{\theta A}B(t)u(t) + \theta^2 e^{\theta A}\eta - \int_0^\theta e^{(\theta-s)A}B(t+s)u(t+s)\mathrm{d}s \right\| \\
&= \left\| \theta^2 e^{\theta A}\eta + \int_0^\theta (e^{\theta A}-e^{(\theta-s)A})B(t)u(t)\mathrm{d}s \right. \\
&\quad + \int_0^\theta e^{(\theta-s)A}(B(t)-B(t+s))u(t)\mathrm{d}s \\
&\quad \left. + \int_0^\theta e^{(\theta-s)A}B(t+s)(u(t)-u(t+s))\mathrm{d}s \right\| \\
&\leqslant \|\theta^2\eta\| + \left\| \int_0^\theta (e^{\theta A}-e^{(\theta-s)A})B(t)u(t)\mathrm{d}s \right\| \\
&\quad + \left\| \int_0^\theta e^{(\theta-s)A}(B(t)-B(t+s))u(t)\mathrm{d}s \right\| \\
&\quad + \left\| \int_0^\theta e^{(\theta-s)A}B(t+s)(u(t)-u(t+s))\mathrm{d}s \right\| \\
&< \theta^2 M + \theta\varepsilon_1 + \theta\varepsilon_1 + \theta\varepsilon_1 < 4\theta\varepsilon_1 = \theta\varepsilon \quad \textit{for } 0\leqslant\theta\leqslant\min\{\theta_1,\varepsilon_1/M\} \\
&= \theta_0, \quad \textit{and } \varepsilon_1 = \varepsilon/4.
\end{aligned}$$

We turn now to the solution $u(t)$ to Eq. (3). □

Lemma 4: Let $u(t)$ be the solution to the equation (3). *If $V(t)$ is an $L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))$-valued continuous function, then it holds that*

$$u(t,x)=\lim_{\theta\to 0}\left(\prod_{j=1}^{m}S_\theta e^{\theta V(\tau_j)}\right)\varphi(x)\quad \text{for } s_{j-1}\leqslant\tau_j<s_j,\quad \text{and } \theta=t/m. \tag{10}$$

Proof: Set $u_k=(\Pi_{j=1}^{k}S_\theta e^{\theta V(s_j-1)})\varphi$ and $B=\sup_{0\leqslant s\leqslant t}\|V(s)\|_{L^\infty}$.

Given $\varepsilon>0$ it follows from (3) that

$$\begin{aligned}\|u_{k+1}-u(s_{k+1})\|&=\|e^{\theta A}e^{\theta V(s_k)}u_k-u(s_k+\theta)\|\leqslant e^{\theta\|V(s_k)\|_{L^\infty}}\|u_k-u(s_k)\|+\|e^{\theta A}e^{\theta V(s_k)}u(s_k)-u(s_k+\theta)\|\\&\leqslant e^{\theta\|V(s_k)\|_{L^\infty}}\|u_k-u(s_k)\|+\theta\varepsilon\leqslant e^{\theta\|V(s_k)\|_{L^\infty}}\{e^{\theta\|V(s_{k-1})\|_{L^\infty}}\|u_{k-1}-u(s_{k-1})\|+\theta\varepsilon\}+\theta\varepsilon\\&\leqslant\cdots\leqslant e^{k\theta B}k\theta\varepsilon\leqslant e^{tB}t\varepsilon\quad \text{for } k=1,\ldots,m-1.\end{aligned}$$

Since $\varepsilon>0$ is arbitrary the proof is complete. □

III. PATH INTEGRAL OF RIEMANN TYPE

A. Operator-valued integral of Riemann type

In this section we express the operator $S_te^V:\varphi\mapsto S_t(e^V\varphi)$ as the integral of $e^V\varphi$ by $\mathrm{d}S_t$. We denote by $\mathbb{Z}$ the set of integers. We consider a division of $\mathbb{R}^N$,

$$\bigcup_{k\in\mathbb{Z}^N}I_k^h=\mathbb{R}^N,\quad I_k^h=[hk_1,hk_1+h)\times\cdots\times[hk_N,hk_N+h),\quad k=(k_1,\ldots,k_N),\quad k_j\in\mathbb{Z}.$$

A function e^V in $L^\infty(\mathbb{R}^N;\mathbb{C})$ is considered as an operator in $L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))$:

$$e^V:L^2(\mathbb{R}^N;\mathbb{C})\ni\varphi\mapsto e^V\varphi\in L^2(\mathbb{R}^N;\mathbb{C}).$$

For simplicity we denote $L^\infty=L^\infty(\mathbb{R}^N;\mathbb{C})$. This implies the following estimates:

$$\begin{aligned}&\|e^{V(x)}\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))}\leqslant\|e^{V(x)}\|_{L^\infty},\\&\|S_te^{V(x)}\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))}\leqslant\|e^{V(x)}\|_{L^\infty}\leqslant e^{\|V(x)\|_{L^\infty}},\\&\|S_te^{\theta V(x)}\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))}\leqslant(1+\theta\|V(x)\|_{L^\infty})e^{\theta\|V(x)\|_{L^\infty}},\\&\|S_t(e^{\theta V(x)}-1)\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))}\leqslant\theta\|V(x)\|_{L^\infty}e^{\theta\|V(x)\|_{L^\infty}}.\end{aligned}\tag{11}$$

The characteristic function $\chi(I_k^h)$ of I_k^h is at the same time an operator in

$$L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C})):(\chi(I_k^h)\cdot\varphi)(x)\equiv\chi(I_k^h)(x)\cdot\varphi(x)=\begin{cases}\varphi(x) & \text{for } x\in I_k^h,\\ 0 & \text{for } x\notin I_k^h.\end{cases}$$

Note that $\varphi(x)=\Sigma_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)\varphi(x)$. We denote

$$\Delta_k^hS_t=S_t\chi(I_k^h)\in L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C})):\varphi\to S_t(\chi(I_k^h)\varphi). \tag{12}$$

Lemma 5: If e^V in $C_\infty(\mathbb{R}^N;\mathbb{C})$ then the sum $S_te^V=\Sigma_{k\in\mathbb{Z}^N}\Delta_k^hS_te^V$ is unconditionally strongly convergent. That is, for any φ in $L^2(\mathbb{R}^N;\mathbb{C})$, $\Sigma_{k\in\mathbb{Z}^N}\Delta_k^hS_te^V\varphi$ strongly converges independent of the order of the sum.

Proof: The lemma follows from the unconditional strong convergence of $\varphi=\Sigma_{k\in\mathbb{Z}^N}\chi(I_k^h)\varphi$ or $e^V\varphi=\Sigma_{k\in\mathbb{Z}^N}\chi(I_k^h)(e^V\varphi)$. In fact we get

$$\text{if } \chi(I_k^h)\varphi \perp \chi(I_{k'}^h)\varphi \text{ for } k \neq k' \text{ then } S_t\chi(I_k^h)\varphi \perp S_t\chi(I_{k'}^h 0)\varphi \text{ for } k \neq k',$$

since S_t is unitary. Therefore

$$\text{if } \mathbb{Z}_1 \subset \mathbb{Z}_2 \subset \mathbb{Z}^N \text{ then } \left\| S_t e^V - \sum_{k\in\mathbb{Z}_1} \Delta_k^h S_t e^V \right\| \geqslant \left\| S_t e^V - \sum_{k\in\mathbb{Z}_2} \Delta_k^h S_t e^V \right\|.$$

□

Definition 4: For $h>0$ and $k \in \mathbb{Z}^N$, let an element $x_h^k \in I_k^h$ be fixed. $\Sigma_k \Delta_k^h S_t e^{V(x_h^k)}$ is called the Riemann sum. $\lim_{h\to 0}\Sigma_k \Delta_k^h S_t e^{V(x_h^k)}$ is called the Riemann integral of $e^{V(x)}$ by $\mathrm{d}S_t(x)$ and denoted by

$$R-\int_{\mathbb{R}^N} \mathrm{d}S_t(x)e^{V(x)} = \int_{\mathbb{R}^N} S_t(\mathrm{d}x)e^{V(x)} = \lim_{h\to 0} \sum_{k\in\mathbb{Z}^N} \Delta_k^h S_t e^{V(x_h^k)} \in L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C})). \quad (13)$$

$\mathrm{d}S_t$ is finitely additive and may be called an operator-valued "Riemann measure."

B. Iterated integral and multiple integral

From the definition of Riemann integral, we obtain that

$$\prod_{j=1}^m S_\theta e^{\theta V(\tau_j,x)}\varphi = R-\int_{\mathbb{R}^N} dS_\theta(x)e^{\theta V(\tau_m,x)}\cdots R-\int_{\mathbb{R}^N} dS_\theta(x)e^{\theta V(\tau_1,x)}\varphi,$$

with $\theta=t/m$. This is the iterated integral. We shall express this by the multiple integral.

We denote by $C([0,t],C_\infty(\mathbb{R}^N;\mathbb{C}))$ the space of continuous functions on $[0,t]$ with values in $C_\infty(\mathbb{R}^N;\mathbb{C})$. Note that for all $V \in C([0,t],C_\infty(\mathbb{R}^N;\mathbb{C}))$ and for each $\varepsilon>0$, there exists $\delta>0$ such that

$$\begin{gathered} |V(s,x)-V(s',x')|<\varepsilon, \quad |e^{\theta V(s,x)}-e^{\theta V(s',x')}|<\varepsilon\theta, \\ \text{for } |s-s'|\leqslant\delta, \quad |x-x'|<\delta, \quad \text{and } 0\leqslant\theta\leqslant 1. \end{gathered} \quad (14)$$

Lemma 6: Let $\mathcal{C}$ be a compact subset of $L^2(\mathbb{R}^N;\mathbb{C})$. Let A^j and A_n^j be operators in $L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))$ for $1\leqslant j\leqslant m$.

Then for each $\varepsilon>0$, there exists $n_0>1$ such that for all $n\geqslant n_0$, (a) if

$$\|A_n^j - A^j\|_{L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))} < \varepsilon$$

then

$$\left\| \prod_{j=1}^m A_n^j - \prod_{j=1}^m A^j \right\|_{L^2(\mathbb{R}^N;\mathbb{C})} < \varepsilon m M^{m-1}, \quad (15)$$

(b) if

$$\sup_{\varphi\in\mathcal{C}_j} \|(A_n^j - A^j)\varphi\|_{L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))} < \varepsilon, \quad \textit{for all } \mathcal{C}_j\textit{:compact}$$

then

$$\sup_{\varphi\in\mathcal{C}} \left\| \left(\prod_{j=1}^m A_n^j - \prod_{j=1}^m A^j \right)\varphi \right\|_{L^2(\mathbb{R}^N;\mathbb{C})} < \varepsilon m M^{m-1}. \quad (16)$$

Here we write $\Pi_{j=1}^m A^j = A^m\cdots A^1$ and

$$M = \max\{1, \sup(\|A_n^j\|_{L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))}, \|A^j\|_{L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))}; n\in\mathbb{N}, j=1,\ldots,m)\}.$$

Proof: In this proof for simplicity we denote $\|\cdot\|=\|\cdot\|_{L(L^2(\mathbb{R}^N;\mathbb{C}),L^2(\mathbb{R}^N;\mathbb{C}))}$. Note that for each $\varepsilon>0$, there exists n_0 such that $\|A_n^j-A^j\|<\varepsilon$ for all $n\geqslant n_0$, and $j=1,\ldots,m$. We have

$$\prod_{j=1}^{m}A_n^j-\prod_{j=1}^{m}A^j=\left(\prod_{j=2}^{m}A_n^j\right)(A_n^1-A^1)+\sum_{k=2}^{m-1}\left(\left(\prod_{j=k+1}^{m}A_n^j\right)(A_n^k-A^k)\prod_{j=1}^{k-1}A^j\right)+(A_n^m-A^m)\prod_{j=1}^{m-1}A^j.$$

Then from (3.2), we obtain

$$\begin{aligned}\left\|\prod_{j=1}^{m}A_n^j-\prod_{j=1}^{m}A^j\right\|&\leqslant\left\|\left(\prod_{j=2}^{m}A_n^j\right)(A_n^1-A^1)+\sum_{k=2}^{m-1}\left(\left(\prod_{j=k+1}^{m}A_n^j\right)(A_n^k-A^k)\prod_{j=1}^{k-1}A^j\right)+(A_n^m-A^m)\prod_{j=1}^{m-1}A^j\right\|\\&\leqslant\left(\prod_{j=2}^{m}\|A_n^j\|\right)\|A_n^1-A^1\|+\sum_{k=2}^{m-1}\left(\left(\prod_{j=k+1}^{m}\|A_n^j\|\right)\|A_n^k-A^k\|\prod_{j=1}^{k-1}\|A^j\|\right)\\&\quad+\|A_n^m-A^m\|\prod_{j=1}^{m-1}\|A^j\|<\varepsilon mM^{m-1}\ \textit{for any}\ n\geqslant n_0.\end{aligned}$$

Set $\mathcal{C}_1=\mathcal{C}$ and $\mathcal{C}_k=(\Pi_{j=1}^{k-1}A^j)\mathcal{C}$ for $k>1$. Each $\mathcal{C}_k$ is compact, since it is the continuous image of the compact set $\mathcal{C}$. From the right-hand side of (16) we have for each $\varepsilon>0$ that there exists n_0 such that $\sup_{\phi\in\mathcal{C}_k}\|(A_n^k-A^k)\phi\|<\varepsilon$ for all $n\geqslant n_0$ and $j=1,\ldots,m$.

Hence

$$\begin{aligned}&\sup_{\varphi\in\mathcal{C}}\left\|\left(\prod_{j=1}^{m}A_n^j-\prod_{j=1}^{m}A^j\right)\varphi\right\|\\&\quad=\sup_{\varphi\in\mathcal{C}}\left\|\left(\left(\prod_{j=2}^{m}A_n^j\right)(A_n^1-A^1)+\sum_{k=2}^{m-1}\left(\left(\prod_{j=k+1}^{m}A_n^j\right)(A_n^k-A^k)\prod_{j=1}^{k-1}A^j\right)+(A_n^m-A^m)\prod_{j=1}^{m-1}A^j\right)\varphi\right\|\\&\quad\leqslant\sup_{\varphi\in\mathcal{C}_m}\left\|\left(\prod_{j=2}^{m}A_n^j\right)(A_n^1-A^1)\varphi\right\|+\sum_{k=2}^{m-1}\sup_{\varphi\in\mathcal{C}_k}\left\|\left(\prod_{j=k+1}^{m}A_n^j\right)(A_n^k-A^k)\prod_{j=1}^{k-1}A^j\varphi\right\|\\&\quad\quad+\sup_{\varphi\in\mathcal{C}}\left\|(A_n^m-A^m)\prod_{j=1}^{m-1}A^j\varphi\right\|\leqslant\left(\prod_{j=2}^{m}\|A_n^j\|\right)\sup_{\varphi\in\mathcal{C}_1}\|(A_n^1-A^1)\varphi\|\\&\quad\quad+\sum_{k=2}^{m-1}\left(\left(\prod_{j=k+1}^{m}\|A_n^j\|\right)\sup_{\phi\in\mathcal{C}_k}\|(A_n^k-A^k)\phi\|\right)\\&\quad\quad+\sup_{\phi\in\mathcal{C}_m}\|(A_n^m-A^m)\phi\|<\varepsilon mM^{m-1}.\end{aligned}$$

□

Lemma 7: Let V in $C([0,t],C_\infty(\mathbb{R}^N;\mathbb{C}))$. *Then we have*

$$\prod_{j=1}^{m}S_\theta e^{\theta V(\tau_j,\cdot)}\varphi=\lim_{h\to0}\prod_{j=1}^{m}S_\theta\sum_k\chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)}\varphi\quad\textit{for}\ x_h^k\in I_k^h\quad\textit{with}\ \theta=t/m.\tag{17}$$

Proof: From (14) we recall for each $\varepsilon>0$, there exists $h>0$ such that $|e^{V(\tau_j,x)\theta}-e^{V(\tau_j,x_h^k)\theta}|<\varepsilon\theta$ for all x in I_k^h and for all k in $\mathbb{Z}^N$. Then we have

$$\left\| e^{\theta V(\tau_j,\cdot)}\varphi - \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)}\varphi \right\| \leqslant \left\| \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)(e^{\theta V(\tau_j,\cdot)} - e^{\theta V(\tau_j,x_h^k)}) \right\|_{L^\infty} \|\varphi\| < \varepsilon\theta\|\varphi\|$$

$$\text{for all } \varphi \in L^2(\mathbb{R}^N;\mathbb{C}).$$

This means

$$\left\| e^{\theta V(\tau_j,\cdot)}\varphi - \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)} \right\|_{L^\infty} < \varepsilon\theta.$$

From (11) we have

$$\|S_\theta e^{\theta V(\tau_j,\cdot)}\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} \leqslant e_{L^\infty}^{\theta\|V(\tau_j,\cdot)\|},$$

$$\left\| S_\theta \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)} \right\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} \leqslant e_{L^\infty}^{\theta\|V(\tau_j,\cdot)\|} + \varepsilon h,$$

$$\left\| S_\theta e^{\theta V(\tau_j,\cdot)} - S_\theta \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)} \right\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} < \varepsilon\theta. \tag{18}$$

Hence from Lemma 6 we obtain that

$$\begin{aligned} &\left\| \prod_{j=1}^m S_\theta e^{\theta V(\tau_j,\cdot)} - \prod_{j=1}^m S_\theta \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)} \right\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} < \varepsilon\theta m e^{t\|V\|_{L^\infty}} = \varepsilon t e^{t\|V\|_{L^\infty}}, \\ &\left\| \prod_{j=1}^m S_\theta e^{\theta V(\tau_j,\cdot)}\varphi - \prod_{j=1}^m S_\theta \sum_{k\in\mathbb{Z}^N} \chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)}\varphi \right\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} < \varepsilon t e^{t\|V\|_{L^\infty}}\|\varphi\|. \end{aligned} \tag{19}$$

This means (17). □

Denote $\kappa=(k(1),\ldots,k(m)) \in \mathbb{Z}^{N\times m}$ where $k(j)=(k_1(j),\ldots,k_N(j)) \in \mathbb{Z}^N$.

Note that $\Delta_{k(j)}^h S_\theta$ and $e^{\theta V(\tau_j,x_h^{k(j)})}$ commute since each $e^{\theta V(\tau_j,x_h^{k(j)})}$ is a constant function. Thus we have

$$\begin{aligned} \prod_{j=1}^m S_\theta \sum_{k\in\mathbb{Z}^N} \chi(I_{k(j)}^h)e^{\theta V(\tau_j,x_h^k)} &= \sum_{\kappa\in\mathbb{Z}^{N\times m}} \prod_{j=1}^m (S_\theta \chi(I_{k(j)}^h)e^{\theta V(\tau_j,x_h^{k(j)})}) = \sum_{\kappa\in\mathbb{Z}^{N\times m}} \prod_{j=1}^m (\Delta_{k(j)}^h S_\theta e^{\theta V(\tau_i,x_h^{k(j)})}) \\ &= \sum_{\kappa\in\mathbb{Z}^{N\times m}} \prod_{j=1}^m (\Delta_{k(j)}^h S_\theta) e^{\sum_{l=1}^m \theta V(\tau_l,x_h^{k(l)})}, \end{aligned} \tag{20}$$

since the sum $\Sigma_{k\in\mathbb{Z}^N}\chi(I_k^h)e^{\theta V(\tau_j,x_h^k)}$ is unconditionally convergent. The multiple integral is defined as follows.

Definition 5: The multiple integral of $\exp(\Sigma_{l=1}^m \theta V(\tau,\gamma(\tau_l)))$ *is defined by*

$$\begin{aligned} R - \int \cdots \int \mathrm{d}S_\theta(\gamma(\tau_1)) \cdots \mathrm{d}S_\theta(\gamma(\tau_m)) e^{\Sigma_{l=1}^m \theta V(\tau,\gamma(\tau_l))} \\ = \lim_{h\to 0} \sum_{\kappa\in\mathbb{Z}^{Nm}} \prod_{j=1}^m (\Delta_{k(j)}^h S_\theta) e^{\Sigma_{l=1}^m \theta V(\tau_l,x_h^{k(l)})} \quad \text{with } \theta = t/m. \end{aligned} \tag{21}$$

Let $h\to 0$ in (20) and we get the following lemma by (19), (13), and (17).

Lemma 8: Let $V \in C([0,\mathfrak{t}],C_\infty(\mathbb{R}^N;\mathbb{C}))$. *Then we have*

$$\prod_{j=1}^{m} S_\theta e^{\theta V(\tau_j,x)} = R - \int \cdots \int \mathrm{d}S_\theta(\gamma(\tau_1)) \cdots \mathrm{d}S_\theta(\gamma(\tau_m)) e^{\sum_{j=1}^{m} \theta V(\tau,\gamma(\tau_j))},$$

where $\gamma(\tau_j)$ *runs over* $\mathbb{R}^N$ *for each* j *and*

$$\int \mathrm{d}S_\theta(\gamma(\tau_j)) e^{\theta V(\tau,\gamma(\tau_j))} \quad \textit{means} \int_{\mathbb{R}^N} \mathrm{d}S_\theta(x) e^{\theta V(\tau_j,x)}.$$

Roughly speaking,

$$\prod_{j=1}^{m} \Delta^h_{k(j)} S_\theta \sim \prod_{j=1}^{m} \mathrm{d}S_\theta(\gamma(\tau_j)) \quad \text{for } \gamma \in \Omega_{[0,t]}, \quad \gamma(\tau_j) \in I^h_{k(j)} \text{ as } h \to 0.$$

C. Path integral of Riemann type

Now we define the path integral of the Riemann type.

Definition 6: The Riemann type path integral of $F(V;t,\gamma) = e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau}$ *is defined by*

$$R - \int_{\Omega_{[0,t]}} e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau} \varphi \, \mathrm{d}\mu^Q(\gamma) = \lim_{m\to\infty} \lim_{h\to 0} \sum_{\kappa \in \mathbb{Z}^{N_m}} \prod_{j=1}^{m} \Delta^h_{k(j)} S_\theta e^{\sum \theta V(\tau_j, x_h^{k(j)})} \varphi,$$

$$= \lim_{m\to\infty} \lim_{h\to 0} \sum_{\kappa \in \mathbb{Z}^{N_m}} \Delta^h_k S_\theta e^{\sum \theta V(\tau_j, x_h^{k(j)})} \varphi, \tag{22}$$

where $\Delta^h_\kappa S_\theta = \Pi_{j=1}^m \Delta^h_{k(j)} S_\theta$ *with* $\theta = t/m$.

Thus from Definition 5, Lemma 8, and Definition 6 we obtain that

$$R - \int_{\Omega_{[0,t]}} e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau} \varphi d\mu^Q(\gamma) = \lim_{m\to\infty} R - \int \cdots \int \mathrm{d}S_\theta(\gamma(\tau_1)) \cdots \mathrm{d}S_\theta(\gamma(\tau_m)) e^{\sum_{j=1}^{m} \theta V(\tau_j,\gamma(\tau_j))} \varphi$$

$$= \lim_{m\to\infty} \left(\prod_{j=1}^{m} S_\theta e^{\theta V(\tau_j,x)} \varphi \right).$$

Remark: In general we have not defined the function $F(V;t,\gamma) = e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau}$, nor the (generalized) measure μ^Q. Since $F(V;t,\gamma)$ might not exist for a path γ. Nevertheless the path integral (22) is defined for some V.

A sufficient (but not necessary) condition for a function $F(V;t,\gamma)$ to be μ^Q-integrable is given in our next theorem.

Theorem 1: *Let* $V \in C([0,\mathfrak{t}], C_\infty(\mathbb{R}^N;\mathbb{C}))$. *Then the function* $F(V;t,\gamma) = e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau}$ *is* μ^Q*-integrable.*

That is,

$$R - \int_{\Omega_{[0,t]}} e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau} \varphi(\gamma(0)) \mathrm{d}\mu^Q(\gamma) = \lim_{m\to\infty} \left(\prod_{j=1}^{m} S_\theta e^{\theta V(\tau_j,x)} \right) \varphi(x) \quad \textit{with } \theta = t/m \tag{23}$$

exists.

Proof: From (22) of Definition 6 it suffices to show $\lim_{m\to\infty} \Pi_{j=1}^m S_\theta e^{\theta V(\tau_j,x)}$ exists.

For each $\varepsilon > 0$, there exists $m \in \mathbb{N}$ such that $\| e^{\theta' V(\tau,x)} - e^{\theta' V(\sigma,x)} \|_{L^\infty} \leqslant \varepsilon \theta'$ for $|\tau - \sigma| \leqslant \theta = t/m$ and $0 < \theta' \leqslant \theta$. Hence

$$\|S_{\theta'}e^{\theta' V(\tau,x)} - S_{\theta'}e^{\theta' V(\sigma,x)}\|_{L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))} \leqslant \varepsilon\theta' e^{\theta'\|V\|_{L^\infty}}. \tag{24}$$

We divide each time interval $[s_j, s_{j+1}]$. Let m' be a natural number and $\theta' = \theta/m'$, $\sigma_{j0} = s_j$, $\sigma_{jj'} = s_j + \theta'$, $\sigma_{jm'} = s_{j+1}$ for $j' = 0, \ldots, m'-1$.

By Lemma 6 and (24) we have

$$\left\| S_\theta e^{\theta V(\tau_j,x)} - \prod_{j'=1}^{m'} S_{\theta'}e^{\theta' V(\sigma_{jj'},x)} \right\| = \left\| \prod_{j'=1}^{m'} S_{\theta'}e^{\theta' V(\tau_j,x)} - \prod_{j'=1}^{m'} S_{\theta'}e^{\theta' V(\sigma_{jj'},x)} \right\|$$
$$\leqslant \varepsilon m'\theta'(e^{\theta'\|V\|_{L^\infty}})^{m-1} \leqslant \varepsilon\theta e^{\theta\|V\|_{L^\infty}}.$$

In the same way as above we have

$$\left\| \prod_{j=1}^{m} S_\theta e^{\theta V(\tau_j,x)} - \prod_{j=1}^{m}\prod_{j'=1}^{m'} S_{\theta'}e^{\theta' V(\sigma_{jj'},x)} \right\| \leqslant \varepsilon\theta e^{\theta\|V\|_{L^\infty}} m(e^{\theta\|V\|_{L^\infty}})^{m-1} \leqslant \varepsilon t e^{t\|V\|_{L^\infty}}, \tag{25}$$

and the proof is complete. □

A direct consequence of Theorem 1 is the following theorem.

Theorem 2: *Let a real function U in $C([0,t], C_\infty(\mathbb{R}^N;\mathbb{C}))$. Then the mild solution to the Schrödinger equation (1) is expressed as the Riemann type integral*

$$u(t,x) = R - \int_{\Omega_{[0,t]}} e^{-i\int_0^t U(\tau,\gamma(\tau))\mathrm{d}\tau}\varphi(\gamma(0))\mathrm{d}\mu^Q(\gamma). \tag{26}$$

IV. INTEGRABLE FUNCTIONS

In this section we study the Schrödinger equations with singular potentials.

A. Integration on a bounded domain

Let subset D of $\mathbb{R}^N$ be a bounded open domain with smooth boundary and V be a continuous function on $\bar{D}$. Denote

$$\Omega_{[0,t]}(D) = \prod_{\alpha\in[0,t]} D_\alpha,$$

where D_α=a copy of $D=\{\gamma|\,\gamma(s)\in\bar{D}, \forall s\in[0,t]\}$.

We consider the integration on $\Omega_{[0,t]}(D)$.

The family of solutions to the Schrödinger equation in D with Dirichlet boundary condition

$$\frac{\partial}{\partial t}u(t,x) = i\Delta u(t,x), \quad u(t,x)\big|_{x\in\partial D} = 0, \quad u(0,x) = \varphi(x)\big|_{x\in D} \tag{27}$$

is written as $u(t)=S_t\varphi$ by a group $\{S_t|-\infty<t<\infty\}$ of unitary operators.

Let

$$\bigcup_{k\in\mathbb{Z}^N} I_k^h(D) = D, \quad I_k^h(D) = D\cap([hk_1, hk_1+h)\times\cdots\times[hk_N, hk_N+h)), \quad k=(k_1,\ldots,k_N), \quad k_j\in\mathbb{Z}.$$

Definition 7: If the Riemann sum $\Sigma_{k\in\mathbb{Z}^N}\mu(I_k^h(D))(\cdot)e^{V(x_h^k)}$ converges as $h\to 0$ independently of the choice of $\{I_k^h(D)\}$ and $\{x_h^k\}$, the function $e^{V(x)}$ is said to be Riemann integrable, where $\mu(I_k^h(D))$ is the volume of $I_k^h(D)$.

If the function $G(x)=e^{-iU(x)}$, $U(x)\in\mathbb{R}$, is a scalar valued Riemann integrable in a bounded domain D, the operator-valued integral $R-\int_D \mathrm{d}S_t(x)e^{V(x)}=\lim_{h\to 0}\Sigma_{k\in\mathbb{Z}^N}\Delta_k^h S_t e^{V(x_h^k)}$ also exists. Moreover the multiple integral exists.

As is well known, a bounded function on a bounded domain is Riemann integrable if and only if the set of discontinuous points is of measure zero. In our case, we have the following.

Lemma 9: A function $G(x)=e^{-iU(x)}$, $U(x)\in\mathbb{R}$ for a bounded function U, is Riemann integrable in a bounded domain D if and only if the set of discontinuous points of U is of measure zero.

Let $\mathcal{N}_{V(t)}(D)=\{x\in\bar{D}\,|\,V(t)$ is not continuous at$\}$ and $\mathcal{N}_V(D)=\cup_{t\in[0,T]}\mathcal{N}_{V(t)}(D)$.

Our next theorem is analogous to Theorem 1.

Theorem 3: *If a function V in $C([0,T];L^\infty(\mathbb{R}^n;\mathbb{C}))$ and for any t in $[0,T]V(t)$ is Riemann integrable on $\bar{D}$ and $\mathcal{N}_V(D)$ is a closed set of measure zero, then the function $e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau}$ is μ^Q-integrable on $\Omega_{[0,t]}(D)$. That is,*

$$R-\int_{\Omega_{[0,t]}(D)} e^{\int_0^t V(\tau,\gamma(\tau))\mathrm{d}\tau}\varphi(\gamma(0))\mathrm{d}\mu^Q(\gamma)=\lim_{m\to\infty}\prod_{j=1}^{m} S_\theta e^{\theta V(\tau_j,x)}\varphi(x),\quad x\in\text{a.e. } D \text{ with } \theta=t/m \tag{28}$$

exists.

Proof: Note that $\mathcal{N}_{V(t)}(D)$ is of measure zero since $V(t)$ is Riemann integrable on $\bar{D}$. Therefore we have for each $\varepsilon>0$ there exist open sets $J_j(D)\subset D(j=1,\ldots,n)$ such that $\cup_{j=1}^n J_j(D)\supset\mathcal{N}_V(D)$ and $\Sigma_{j=1}^n\mu(J_j(D))<\varepsilon^2$. Set $J(\varepsilon)=^{\mathrm{def}}\cup_{j=1}^n J_j(D)$. Since $\bar{D}\backslash J(\varepsilon\theta)$ is compact,V is uniformly continuous on $[0,T]\times\{\bar{D}\backslash J(\varepsilon\theta)\}$.

For each V and for each $\varepsilon>0$, there exists $\delta>0$, such that

$$|V(s,x)-V(s',x')|<\varepsilon,\quad |e^{\theta V(s,x)}-e^{\theta V(s',x')}|<\varepsilon\theta$$

for

$$|s-s'|<\delta,\quad s,s'\in[0,T],\quad |x-x'|<\delta,\quad x,x'\in\bar{D}\setminus J(\varepsilon\theta),\quad 0\leqslant\theta\leqslant 1. \tag{29}$$

If necessary we take finer division, we assume that $J(\varepsilon\theta)\cap[I_k^h(D)]^o=\emptyset$ for all $k\in\mathbb{Z}_1$, $J(\varepsilon\theta)\supset I_k^h(D)$ for all $k\in\mathbb{Z}_2$, $\mathbb{Z}^N=\mathbb{Z}_1\cup\mathbb{Z}_2$ and $\mathbb{Z}_1\cap\mathbb{Z}_2=\emptyset$. Here A^o is the interior of A. Thus we have

$$\begin{aligned}
&\left\|e^{\theta V(\tau_j,\cdot)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)}\right\|_{L(L^2(D;\mathbb{C});L^2(D;\mathbb{C}))}\\
&\quad=\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left\|\left(e^{\theta V(\tau_j,\cdot)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(\cdot)e^{\theta V(\tau_j,x_h^k)}\right)\varphi\right\|_{L^2(D;\mathbb{C})}\\
&\quad=\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_D\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.\\
&\qquad\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}\\
&\quad=\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\left(\int_{D\backslash J(\varepsilon\theta)}+\int_{J(\varepsilon\theta)}\right)\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.\\
&\qquad\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}
\end{aligned}$$

$$\leqslant \sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_{D\setminus J(\varepsilon\theta)}\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.$$
$$\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}$$
$$+\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_{J(\varepsilon\theta)}\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.$$
$$\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}$$
$$=\mathrm{I}+\mathrm{II}$$

since $\sqrt{A+B}\leqslant\sqrt{A}+\sqrt{B}$ for $A\geqslant 0$, $B\geqslant 0$.

From (29) it follows that

$$\mathrm{I}=\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_{D\setminus J(\varepsilon\theta)}\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.$$
$$\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}\leqslant\varepsilon\theta\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_D\varphi(x)\overline{\varphi(x)}\mathrm{d}x\right)^{1/2}=\varepsilon\theta.$$

By the definition of $J(\varepsilon\theta)$, we have

$$\mathrm{II}=\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_{J(\varepsilon\theta)}\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)\right.$$
$$\left.\times\overline{\left(e^{\theta V(\tau_j,x)}-\sum_{k\in\mathbb{Z}^N}\chi(I_k^h)(x)e^{\theta V(\tau_j,x_h^k)}\right)\varphi(x)}\mathrm{d}x\right)^{1/2}\leqslant 2e^{\|V\|_\infty}\sup_{\|\varphi\|_{L^2(D;\mathbb{C})}=1}\left(\int_{J(\varepsilon\theta)}\varphi(x)\overline{\varphi(x)}\mathrm{d}x\right)^{1/2}$$
$$\leqslant 2e^{\|V\|_\infty}\|\varphi\|_{L^2(D;\mathbb{C})}\mu(J(\varepsilon\theta))^{1/2}<2\varepsilon\theta e^{\|V\|_\infty}.$$

So the rest of the proof is obtained in a way similar to that of Theorem 1. □

B. Strong integrability for non-negative potentials with singularity

For simplicity we shall discuss the time-independent case. We use the following notations:

$$\mathcal{N}=\text{a fixed closed subset of } \mathbb{R}^N \text{ of measure } 0, \tag{30}$$

$$C(\mathbb{R}^N\setminus\mathcal{N},\mathbb{R}^+)=\{U\in C(\mathbb{R}^N\setminus\mathcal{N},\mathbb{R})\,|\,U(x)\geqslant 0,\ \text{for all } x\in\mathbb{R}^N\}. \tag{31}$$

In this section we consider the integrability of the function $e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ for a function $U\in C(\mathbb{R}^N\setminus\mathcal{N},\mathbb{R}^+)$. Let $D_n=\{x\in\mathbb{R}^N\,|\,n>U(x)\}$ for $n\in\mathbb{N}$. $\{D_n\}_{n=1}^\infty$ is an increasing sequence such that $\bar{D}_n\subset D_{n+1}$ and $\cup_{n=1}^\infty D_n=\mathbb{R}^N\setminus\mathcal{N}$. Here D_n is a finite sum of E_k^n for $k\in\mathbb{N}$ and each E_k^n is a bounded open connected set with smooth boundary.

For $U\in C(\mathbb{R}^N\setminus\mathcal{N},\mathbb{R}^+)$ we define a sequence of functions U_n such that

$$U_n(x)=\min\{n,U(x)\}\quad\text{for } n\in\mathbb{N}.$$

Lemma 10: Let U in $C(\mathbb{R}^N\setminus\mathcal{N},\mathbb{R}^+)$. Then $e^{-i\int_0^t U_n(\gamma(s))\mathrm{d}s}$ is Riemann integrable.

Proof: From Theorem 3 we obtain this lemma. □

We denote that

$$T_n(t)\phi = \int_{\Omega_{[0,t]}(D_n)} e^{-i\int_0^t U_n(\gamma(s))\mathrm{d}s}\phi \,\mathrm{d}\mu^Q \quad \text{for } \phi \in L^2(\mathbb{R}^N;\mathbb{C}).$$

When a function U is not bounded the Riemann integral of $e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ does not exist for U in $C(\mathbb{R}^N\backslash\mathcal{N},\mathbb{R}^+)$. Therefore we introduce the definition of improper Riemann integration with respect to μ^Q.

Definition 8: For a function $U \in C(\mathbb{R}^N\backslash\mathcal{N},\mathbb{R}^+)$, the function $e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is said to be improper Riemann integrable by μ^Q if

$$\lim_{n\to\infty} R - \int_{\Omega_{[0,t]}(D_n)} e^{-i\int_0^t U_n(\gamma(s))\mathrm{d}s}\phi \,\mathrm{d}\mu^Q$$

exists for any $\phi \in L^2(\mathbb{R}^N;\mathbb{C})$ independently of the choice of $\{D_n\}$.

The main result of this section is the following theorem.

Theorem 4: *Let a function U in $C(\mathbb{R}^N\backslash\mathcal{N},\mathbb{R}^+)$. Then the function $F(-iU;t,\gamma) = e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is improper Riemann integrable by μ^Q.*

For the proof of this theorem we shall use the subdifferential of convex functionals.

Denote $H_R^1 = H^1(\mathbb{R}^N;\mathbb{R})$ and $H_R^2 = H^2(\mathbb{R}^N;\mathbb{R})$, where $H^1(\mathbb{R}^N;\mathbb{R})$ is the first Sovolev space on $\mathbb{R}^N$ and $H_R^2 = H^2(\mathbb{R}^N;\mathbb{R})$ is the second Sovolev space on $\mathbb{R}^N$. The subdifferential of a lower semicontinuous convex functional $\Psi: L^2(\mathbb{R}^N;\mathbb{R}) \to (-\infty,\infty]$ is defined as

$$\partial\Psi: \psi \mapsto \{\phi \in L^2(\mathbb{R}^N;\mathbb{R}) \,|\, \Psi(\varphi) \geqslant \Psi(\psi) + \langle \phi, \varphi - \psi\rangle \text{ for all } \varphi \in L^2(\mathbb{R}^N;\mathbb{R})\}. \tag{32}$$

For the basic property of lower semicontinuous convex functionals and their subdifferentials, we refer to the book[1] by Brézis.

For $U \in C(\mathbb{R}^N\backslash\mathcal{N},\mathbb{R}^+)$, the functional $\|\sqrt{U}\phi\|^2$ is lower semicontinuous and convex.

$H_1^0(\Omega)$ denote the first Sobolev space defined as the closure of the space of test functions on the open set $\Omega \subset \mathbb{R}^N$ with respect to the Hilbert norm $(\|\cdot\|_2^2 + \|\nabla\cdot\|_2^2)^{1/2}$.

Lemma 11: Let φ_1 and φ_2 be properly lower semicontinuous and convex such that $D(\varphi_1) \cap D(\varphi_2) \neq \emptyset$ where $D(\varphi_1)$ and $D(\varphi_2)$ are effective domain. Then $\varphi_1 + \varphi_2$ is properly lower semicontinuous and convex and $\partial\varphi_1 + \partial\varphi_2 \subset \partial(\varphi_1 + \varphi_2)$. Moreover $\partial\varphi_1 + \partial\varphi_2$ is maximal monotone if and only if $\partial\varphi_1 + \partial\varphi_2 = \partial(\varphi_1 + \varphi_2)$.

Lemma 12: Each functional $\Psi_n(\phi) \equiv \frac{1}{2}(\|(-\Delta)^{1/2}\phi\|^2 + \|\sqrt{U_n}\phi\|^2)$ or $\Psi(\phi) \equiv \frac{1}{2}(\|(-\Delta)^{1/2}\phi\|^2 + \|\sqrt{U}\phi\|^2)$, is lower semicontinuous and convex. Its effective domain is

$$D(\Psi_n)(\equiv\{f \in L^2(\mathbb{R}^N;\mathbb{R}) \,|\, \Psi_n(f) < \infty\}) = H_R^1 \text{ or } D(\Psi) = D((-\Delta)^{1/2}) \cap D(\sqrt{U}).$$

Roughly speaking, $\Psi(\phi)$ is a closed extension of $\langle -\Delta\phi + U\phi, \phi\rangle$.

Lemma 13: The resolvent $\phi_n = (I + \partial\Psi_n)^{-1}\varphi_0$ of the subdifferential $\partial\Psi_n$ is given by the projection of φ_0 to B_n where $B_n = \{\phi \in L^2(\mathbb{R}^N;\mathbb{R}) \,|\, \Psi_n(\phi) \leqslant \Psi_n(\phi_n)\}$:

$$\mathrm{proj}_{B_n}\varphi_0 = (I + \partial\Psi_n)^{-1}\varphi_0. \tag{33}$$

Proof: Since B_n is closed convex, the projection $\mathrm{proj}_{B_n}\varphi_0$, $\|\varphi_0 - \mathrm{proj}_{B_n}\varphi_0\| = \inf\{\|\varphi_0 - \phi\| \,|\, \phi \in B_n\}$, uniquely exists. Using $\partial\Psi_n(\phi_n) = \varphi_0 - \phi_n$ and (32) we have

$$\Psi_n(\phi) \geqslant \Psi_n(\phi_n) + \langle \partial\Psi_n(\phi_n), \phi - \phi_n\rangle = \Psi_n(\phi_n) + \langle \varphi_0 - \phi_n, \phi - \phi_n\rangle, \quad \text{for all } \phi \in L^2(\mathbb{R}^N;\mathbb{R}).$$

This implies $\langle \varphi_0 - \phi_n, \phi - \phi_n\rangle \leqslant 0$, for all $\phi \in B_n$, since $\Psi_n(\phi) \leqslant \Psi_n(\phi_n)$ if $\phi \in B_n$. Thus we have

$$\begin{aligned}\|\varphi_0 - \phi\|^2 &= \|(\varphi_0 - \phi_n) - (\phi - \phi_n)\|^2 = \|\varphi_0 - \phi_n\|^2 - 2\langle \varphi_0 - \phi_n, \phi - \phi_n\rangle + \|\phi - \phi_n\|^2 \geqslant \|\varphi_0 - \phi_n\|^2 \\ &\quad + \|\phi - \phi_n\|^2 \\ &\geqslant \|\varphi_0 - \phi_n\|^2 \quad \text{for all } \phi \in B_n. \end{aligned} \tag{34}$$

The relation $\|\varphi_0-\phi\|^2 \geqslant \|\varphi_0-\phi_n\|^2$, for all $\phi \in B_n$, $\phi_n \in B_n$ means $\phi_n = \mathrm{proj}_{B_n}\varphi_0$. □

Lemma 14: The resolvent $(I+\partial\Psi_n)^{-1}$ *strongly converges to the resolvent* $(I+\partial\Psi)^{-1}$,

$$(I+\partial\Psi)^{-1}\varphi_0 = \lim_{n\to\infty}(I+\partial\Psi_n)^{-1}\varphi_0 \quad \textit{for any } \varphi_0 \in L^2(\mathbb{R}^N;\mathbb{R}). \tag{35}$$

Proof: Denote $B \equiv \{\phi \in L^2 \,|\, \Psi(\phi) \leqslant \Psi((I+\partial\Psi)^{-1}\varphi_0)\}$, $\phi_n = (I+\partial\Psi_n)^{-1}\varphi_0$ and $\phi_m = (I+\partial\Psi_m)^{-1}\varphi_0$. By virtue of Lemma 13 $\phi_n = \mathrm{proj}_{B_n}\varphi_0$ and $\phi_m = \mathrm{proj}_{B_m}\varphi_0$. Since effective domain $D(\Psi_n) \subset D(\Psi)$ implies $\Psi_n \downarrow \Psi$, we have $B_m \uparrow \cup_{n=1}^{\infty} B_n$ and $B = \cup B_n$. For $n > m$ we have $B_n \supset B_m$ and

$$\|\varphi_0-\phi_n\| = \|\varphi_0-\mathrm{proj}_{B_n}\varphi_0\| \leqslant \|\varphi_0-\mathrm{proj}_{B_m}\varphi_0\| = \|\varphi_0-\phi_m\|,$$

since $\phi_m \in (B_m \subset) B_n$. $\{\|\varphi_0-\phi_m\|\}_{m\in\mathbb{N}}$ is a non-negative decreasing sequence. Hence $\|\varphi_0-\phi_m\| - \|\varphi_0-\phi_n\|$ converges to 0 as $n \geqslant m$ tends to infinity. From (34) it follows that

$$\|\varphi_0-\phi_m\|^2 \geqslant \|\varphi_0-\phi_n\|^2 + \|\phi_m-\phi_n\|^2 \quad \text{for all } \phi_m \in B_m.$$

We have

$$\|\mathrm{proj}_{B_m}\varphi_0 - \mathrm{proj}_{B_n}\varphi_0\| = \|\phi_m-\phi_n\| \leqslant \|\varphi_0-\phi_m\|^2 - \|\varphi_0-\phi_n\|^2 \downarrow 0 \quad \text{as } n,m \to \infty.$$

Therefore we obtain (35). □

Proposition 1: $-\partial\Psi$ *generates a* C_0*-semigroup, hence it is a linear operator and* $R(I+\partial\Psi) = L^2(\mathbb{R}^N;\mathbb{R})$. *Here* $R(A)$ *is a range of the operator* A.

Proof: Since $R((I+\partial\Psi)^{-1})$ is dense in $L^2(\mathbb{R}^N;\mathbb{R})$, $-\partial\Psi$ generates a C_0-semigroup. Because of the maximal monotonicity of $\partial\Psi$, we have $R(I+\partial\Psi) = L^2(\mathbb{R}^N;\mathbb{R})$. □

Proposition 2: Let $S(t)$ *and* $S_n(t)$ *be the semigroups generated by infinitesimal generator* $-\partial\Psi$ *and* $-\partial\Psi_n$, *respectively. Then we obtain the following equation:*

$$\lim_{n\to\infty} S_n(t)\varphi = S(t)\varphi \quad \textit{for all } \varphi \in L^2(\mathbb{R}^N;\mathbb{R}). \tag{36}$$

Proof: We obtain (36) by using (35) and Trotter-Kato theorem (see Ref. 12). □

Let $\partial\widetilde{\Psi}$ and $\partial\widetilde{\Psi}_n : L^2(\mathbb{R}^N;\mathbb{C}) \to L^2(\mathbb{R}^N;\mathbb{C})$ be the complex extension of $\partial\Psi$ and $\partial\Psi_n : L^2(\mathbb{R}^N;\mathbb{R}) \to L^2(\mathbb{R}^N;\mathbb{R})$, respectively. From Proposition 1, $R(I+\partial\Psi) = L^2(\mathbb{R}^N;\mathbb{R})$. Hence we obtain $R(I+\partial\widetilde{\Psi}) = L^2(\mathbb{R}^N;\mathbb{C})$.

Lemma 15: The operator $\partial\widetilde{\Psi}$ *is a self-adjoint positive operator.*

Proof: If a symmetric operator T satisfies $R(I+T) = L^2(\mathbb{R}^N;\mathbb{C})$, then it is self-adjoint. The positivity of $\partial\widetilde{\Psi}$ is evident, since $\langle\partial\Psi(\phi),\phi\rangle \geqslant 0$ for all $\phi \in L^2(\mathbb{R}^N;\mathbb{R})$. □

Theorem 5 (Stone): *A is the infinitesimal generator of a* C_0 *group of unitary operator on a Hilbert space H if and only if iA is self-adjoint.*

Theorem 6: *If a function U in* $C(\mathbb{R}^N \backslash \mathcal{N}, \mathbb{R}^+)$ *then the Schrödinger equation*

$$\frac{d}{dt}u(t) = -i\partial\widetilde{\Psi}(u(t)) \quad (\equiv i(\Delta - U)u(t))$$

has a unique solution. Moreover the semigroup $\{T(t)\}$ *of solution family is unitary..*

Proof: Since $\partial\widetilde{\Psi} \equiv -(\Delta - U)$ is self-adjoint, $-i\partial\widetilde{\Psi} \equiv i(\Delta - U)$ generates a semigroup of unitary operators by virtue of Stone's theorem. □

Definition 9: Let A be the linear operator in complex Hilbert space $H = (H, \|\cdot\|)$.

(a) *The operator A is called monotone if and only if*

$$\mathrm{Re}(x,Ax) \geqslant 0 \quad \textit{for all } x \in D(A).$$

(b) *The operator A is called maximal monotone if and only if any monotone extension of A coincides with A.*

Lemma 16: Let $-A$ be a maximal monotone operator. Then

$$\|A(I-A)^{-1}\| \leqslant 1.$$

Proof: The monotonicity of $-A$ implies

$$\|Ay\|^2 \leqslant \|y\|^2 + 2\,\mathrm{Re}(-Ay,y) + \|Ay\|^2 = \|(I-A)y\|^2.$$

Let $y=(I-A)x$. Then we have

$$\|A(I-A)^{-1}x\| \leqslant \|(I-A)(I-A)^{-1}x\| = \|x\|.$$

□

Lemma 17: Let $-A$ and $-A_n$ be maximal monotone operators. Then $(I-(1+\alpha)A)^{-1}$ and $(I-(1+\alpha)A_n)^{-1}$ are bounded operators for $|\alpha|<1$.

Moreover if

$$\lim_{n\to\infty}(I-A_n)^{-1}\varphi = (I-A)^{-1}\varphi \quad \textit{for all } \varphi \in H,$$

then we have

$$\lim_{n\to\infty}(I-(1+\alpha)A_n)^{-1}\varphi = (I-(1+\alpha)A)^{-1}\varphi \quad \textit{for all } \varphi \in H.$$

Proof: From Lemma 16 we have $\|A_n(I-A_n)^{-1}\| \leqslant 1$.

Therefore,

$$I-(1+\alpha)A_n = (I-A_n)(I-\alpha A_n(I-A_n)^{-1}) \text{ and } |\alpha|<1$$

implies

$$(I-(1+\alpha)A_n)^{-1} = (I-\alpha A_n(I-A_n)^{-1})^{-1}(I-A_n)^{-1} = \left(\sum_{k=0}^{\infty}\alpha^k(A_n(I-A_n)^{-1})^k\right)(I-A_n)^{-1}$$
$$= \left(\sum_{k=0}^{K}\alpha^k(A_n(I-A_n)^{-1})^k\right)(I-A_n)^{-1} + \left(\sum_{k=K+1}^{\infty}\alpha^k(A_n(I-A_n)^{-1})^k\right)(I-A_n)^{-1}.$$

Since for any fixed K, we obtain that

$$\lim_{n\to\infty}\left(\sum_{k=0}^{K}\alpha^k(A_n(I-A_n)^{-1})^k\right)(I-A_n)^{-1} = \left(\sum_{k=0}^{K}\alpha^k(A(I-A)^{-1})^k\right)(I-A)^{-1}$$

and the monotonicity of A_n and Lemma 16 we have

$$\left\|\left(\sum_{k=K+1}^{\infty}\alpha^k(A_n(I-A_n)^{-1})^k\right)(I-A_n)^{-1}\right\| \leqslant \left(\sum_{k=K+1}^{\infty}|\alpha^k|\|(A_n(I-A_n)^{-1})\|^k\right)\|(I-A_n)^{-1}\|$$
$$\leqslant \sum_{k=K+1}^{\infty}|\alpha|^k = \frac{|\alpha|^{K+2}}{1-|\alpha|}.$$

For any $\varepsilon>0$ there exists $K\in\mathbb{N}$ such that $|\alpha|^{K+2}/(1-|\alpha|)<\varepsilon$. Then the proof is complete. □

Lemma 18: Let $-A$ and $-A_n$ be self-adjoint positive operators.

If $(I-e^{i\theta}A)^{-1}$ and $(I-e^{i\theta}A_n)^{-1}$ are bounded operators for $0\leqslant\theta\leqslant\pi/2$ and

$$\lim_{n\to\infty}(I-A_n)^{-1}\varphi = (I-A)^{-1}\varphi \quad \textit{for all } \varphi \in H,$$

then

$$\lim_{n\to\infty}(I-iA_n)^{-1}\varphi=(I-iA)^{-1}\varphi \quad \textit{for all } \varphi\in H.$$

Proof: By using Lemma 17 we get

$$\lim_{n\to\infty}\left(I-\frac{1+i}{\sqrt{2}}A_n\right)^{-1}\varphi=\left(I-\frac{1+i}{\sqrt{2}}A\right)^{-1}\varphi \quad \textit{for all } \varphi\in H, \tag{37}$$

since $|\alpha|<1$ for $\alpha=[(1+i)/\sqrt{2}]-1$. Note that $-[(1+i)/\sqrt{2}]A_n$ and $-[(1+i)/\sqrt{2}]A$ are maximal monotone. By virtue of Lemma 17 and

$$(1+\alpha)\frac{1+i}{\sqrt{2}}=\left(\frac{1+i}{\sqrt{2}}\right)^2=i$$

we have

$$\lim_{n\to\infty}(I-iA_n)^{-1}\varphi=(I-iA)^{-1}\varphi \quad \textit{for all } \varphi\in H.$$

□

Remark: $(-i+c)A$ and $(-i+c)iA_n$ are not maximal monotone operators for any $c>0$.

Proposition 3: Let $T(t)$ and $T_n(t)$ be the semigroups generated by infinitesimal generator $-i\partial\Psi$ and $-i\partial\tilde{\Psi}_n$, respectively. Then it follows that

$$\lim_{n\to\infty}T_n(t)\phi=T(t)\phi \quad \textit{for all } \phi\in L^2(\mathbb{R}^N;\mathbb{C}).$$

Proof: Denote $A=-i\partial\tilde{\Psi}$ and $A_n=-i\partial\tilde{\Psi}_n$. Fix $\phi\in L^2(\mathbb{R}^N;\mathbb{C})$ and an interval $0\leqslant t\leqslant T$. We consider

$$\begin{aligned}\|(T_n(t)-T(t))(I-A)^{-1}\phi\| &\leqslant \|T_n(t)((I-A)^{-1}-(I-A_n)^{-1})\phi\|+\|(I-A_n)^{-1}(T_n(t)-T(t))\phi\| \\ &\quad +\|((I-A)^{-1}-(I-A_n)^{-1})T(t)\phi\|=I_1+I_2+I_3.\end{aligned} \tag{38}$$

Since $\|T_n(t)\|$ is bounded for $0\leqslant t\leqslant \mathfrak{t}$ it follows from Lemma 18 that $I_1\to 0$ as $n\to\infty$ uniformly on $[0,\mathfrak{t}]$. The rest of the proof is obtained in a way similar to that of Pazy (Ref. 9, Chap. 3, Theorem 4.2). □.

Proof of the Theorem 4: From Proposition 3, it follows that $\lim_{n\to\infty}R-\int_{\Omega_{[0,t]}}e^{-i\int_0^t U_n(\gamma(s))\mathrm{d}s}\phi\,\mathrm{d}\mu^Q=\lim_{n\to\infty}T_n(t)\phi$ uniquely exists.

Therefore from Definition 7 we obtain that $e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is Riemann integrable by μ^Q. □

Corollary 1: Let a function $U\in C(\mathbb{R}^N\backslash\mathcal{N},\mathbb{R})$ and there exist $m\in\mathbb{R}$ such that $U(x)\geqslant m$ for any $x\in\mathbb{R}^N\backslash\mathcal{N}$. Then the function $F(-iU;t,\gamma)=e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is improper Riemann integrable by μ^Q.

For a time dependent case we give the following theorem.

Theorem 7: *Let $U(t,\cdot)$ be a $C(\mathbb{R}^N;\mathbb{R})\cap L^\infty(\mathbb{R}^N;\mathbb{R})$-valued function and be continuous in t on every compact set $\subset\mathbb{R}$. Then the function $F(-iU;t,\gamma)=e^{-i\int_0^t U(s,\gamma(s))\mathrm{d}s}$ is Riemann integrable by μ^Q.*

Proof: For a fixed t, the integrability follows from the integrability of $U+\|U\|_\infty$. We recall $U+\|U\|_\infty$ is non-negative. Since $V(t)=-iU(t,x)$ is a $L(L^2(\mathbb{R}^N;\mathbb{C});L^2(\mathbb{R}^N;\mathbb{C}))$-valued strongly continuous function, we get the result by virtue of Lemma 4. □

C. Weak integrability for real potentials with singularity

In this section we study about more general potentials. We consider the following equation:

$$\frac{\partial}{\partial t}u(t,x)=i\Delta u(t,x)-iU(x)u(t,x), \quad u(0,x)=\varphi(x), \quad \varphi\in H^2(\mathbb{R}^N;\mathbb{C}). \tag{39}$$

Recall that we set

$$\mathcal{N} = \text{a fixed closed subset of } \mathbb{R}^N \text{ of measure } 0. \tag{40}$$

Let $\mathcal{D}=\{D\}$ be the maximum family such that each element $D \subset \bar{D} \subset \mathbb{R}^N \backslash \mathcal{N}$ is a finite union of connected bounded open sets. The family $\mathcal{D}=\{D\}$ satisfies $\cup_{D\in\mathcal{D}} D = \mathbb{R}^N \backslash \mathcal{N}$.

We denote the restriction of f to D by $f|_D$, or simply, by f_D. We use the following notation:

$$L^\infty_{\mathrm{loc}}(\mathbb{R}^N \backslash \mathcal{N}, \mathbb{R}) = \{f | f(x) \in \mathbb{R},\ f|_D \in\ L^\infty(D;\mathbb{R})),\ \forall\, D \in \mathcal{D}\}. \tag{41}$$

Let U in $L^\infty_{\mathrm{loc}}(\mathbb{R}^N \backslash \mathcal{N}, \mathbb{R})$. We assume for any neighborhood of any point of $\mathcal{N}, U$ is not essentially bounded.

First we cite a result of Kōmura.[7] Let

$$B(n) = \{x \in \mathbb{R}^N | n > U(x) > -n\}, \quad n = 1,2,3, \ldots\ . \tag{42}$$

We have $B(m) \supset B(n)$ for $m > n$ and from the assumption that

$$\text{for any } D \text{ in } \mathcal{D}, \text{ there exists } B(n) \text{ such that } D \subset \bar{D} \subset B(n). \tag{43}$$

[Strictly speaking, $\bar{D} \backslash B(n)$ is a null set.]

We denote

$$U_n(x) = \min\{n, \max\{-n, U(x)\}\}, \quad n \in \mathbb{N}.$$

Thus U_n in $L^\infty(\mathbb{R}^N;\mathbb{R})$.

For U in $L^\infty_{\mathrm{loc}}(\mathbb{R}^N \backslash \mathcal{N}, \mathbb{R})$ we consider the approximate equation

$$\frac{d}{dt} u_n(t) = A_n u_n(t), \quad \text{where } A_n = i(\Delta - U_n). \tag{44}$$

In this case the operator $-iA_n$ is essentially self-adjoint and hence the semigroup $\{T_n(t)\}$ of the family of solutions to (44) is a group of unitary operators: $\|T_n(t)\varphi\| = \|\varphi\|, -\infty < t < \infty$ for all $\varphi \in L^2(\mathbb{R}^N;\mathbb{C})$.

Theorem 8 (Kōmura): *For any U in $L^\infty_{\mathrm{loc}}(\mathbb{R}^N \backslash \mathcal{N};\mathbb{R})$, there exists a closed extension of $(i\Delta - iU)|_{C_0^\infty(\mathbb{R}^N \backslash \mathcal{N})}$ in $L^2(\mathbb{R}^N;\mathbb{C}) \to L^2(\mathbb{R}^N;\mathbb{C})$ which generates a contraction C_0-semigroup $\{T(t) | t \geqslant 0\}$ such that*

$$T(t)\varphi = w - \lim_{n\to\infty} T_n(t)\varphi, \quad \forall\ \varphi \in L^2(\mathbb{R}^N;\mathbb{C}), \tag{45}$$

where $T_n(t)\varphi$ is the solution to

$$\frac{d}{dt} u_n(t) = A_n u_n(t), \quad \textit{where } A_n = i(\Delta - U_n) \tag{46}$$

and $w-\lim$ means the weak convergence.

Definition 10: For a function U in $C(\mathbb{R}^n \backslash \mathcal{N};\mathbb{R})$, the function $e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is said to be weakly Riemann integrable by μ^Q if

$$w - \lim_{m,n\to\infty} R - \int_{\Omega_{[0,t]}(D_{m,n})} e^{-i\int_0^t U_{m,n}(\gamma(s))\mathrm{d}s} \phi \, \mathrm{d}\mu^Q$$

exists for any ϕ in $L^2(\mathbb{R}^N;\mathbb{C})$ independently of the choice of $\{D_{m,n}\}$.

Now we return to (39). Let U in $C(\mathbb{R}^N \backslash \mathcal{N}, \mathbb{R})$. In order to use the previous theorem we define a sequence of functions $U_{m,n}$ and $D_{m,n}$ such that

$$U_{m,n}(x) = \min\{m, \max\{-n, U(x)\}\}, \quad m,n = 1,2,3, \ldots\ ,$$

$$D_{m,n} = \{x \in \mathbb{R}^N | m > U(x) > -n\}, \quad m,n = 1,2,3, \ldots .$$

By virtue of Corollary 1 the solution $u_{m,n}$ to the Schrödinger equation in $\mathbb{R}^N$,

$$\frac{\partial}{\partial t}u_{m,n}(t,x) = i\Delta u_{m,n}(t,x) - iU_{m,n}(x)u_{m,n}(t,x),$$
$$u_{m,n}(0,x) = \varphi(x), \quad \varphi \in L^2(\mathbb{R}^N;\mathbb{C}), \tag{47}$$

exists.

Theorem 9: *For any U in $L^\infty_{\mathrm{loc}}(\mathbb{R}^N\backslash\mathcal{N};\mathbb{R})$, there exists a closed extension of $i(\Delta - U)|_{C_0^\infty(\mathbb{R}^N\backslash\mathcal{N})}$ in $L^2(\mathbb{R}^N;\mathbb{C}) \to L^2(\mathbb{R}^N;\mathbb{C})$ which generates a contraction C_0-semigroup $\{T(t)|t \geqslant 0\}$ such that*

$$T(t)\varphi = w - \lim_{n\to\infty} T_{m,n}(t)\varphi, \quad \forall\, \varphi \in L^2(\mathbb{R}^N;\mathbb{C}), \tag{48}$$

where $T_{m,n}(t)\varphi$ is the solution to

$$\frac{d}{\mathrm{d}t}u_{m,n}(t) = A_{m,n}u_{m,n}(t), \quad \text{where } A_{m,n} = i(\Delta - U_{m,n}) \tag{49}$$

and $w-\lim$ means the weak convergence.

Proof: Let $U^+_{m,n}(x) = \max\{0, U_{m,n}(x)\}$ and $U^-_{m,n}(x) = \max\{0, -U_{m,n}(x)\}$. Then $U_{m,n}(x) = U^+_{m,n}(x) - U^-_{m,n}(x)$. Note the following:

(a) In the case that there exists $M \geqslant 0$ such that $U^+_{m,n}(x) \leqslant M$ for $x \in D_{m,n}$ and $m,n \in \mathbb{N}$, there exists $n_0 \in \mathbb{N}$ such that $D_{m,n} \subset B(n)$ for any $n \geqslant n_0 \geqslant M$.
(b) In the case that there exists $M \geqslant 0$ such that $U^-_{m,n}(x) \leqslant M$ for $x \in D_{m,n}$ and $m,n \in \mathbb{N}$, there exists $m_0 \in \mathbb{N}$ such that $D_{m,n} \subset B(m)$ for any $m \geqslant m_0 \geqslant M$.
(c) In another case we obtain that

$$\max\{B(n),B(m)\} \supset D_{m,n} \supset \min\{B(n),B(m)\}, \quad m,n \in \mathbb{N}.$$

Note that

$$D = \bigcup_{n,m=1}^{\infty} D_{m,n}.$$

Therefore from the result of Theorem 8 we obtain the consequence. □

Note that $\{T_t\}$ is independent of the choice of $\{D_{m,n}\}$.

We conclude this section with a condition for $F(-iU;t,\gamma)$ to be weakly Riemann integrable. (See Refs. 2–4 and 10).

Theorem 10: *Let the associated scalar function $G(x) = e^{-iU(x)}$ be the Riemann integrable on any bounded domain in $\mathbb{R}^N$. Then the function $F(-iU;t,\gamma) = e^{-i\int U(\gamma(s))\mathrm{d}s}$ is weakly Riemann integrable.*

Proof: Let $D \subset \mathbb{R}^N$ be a bounded domain. As is well known, $\int_D G(x)\mathrm{d}x$ is Riemann integrable if and only if $G(x)$ is continuous except a closed set $\mathcal{N}_G(D)$ of measure zero, since $G(x)$ is bounded. Hence $U(x) = i\log G(x)$ is continuous except a closed set $\mathcal{N}_G = \cup_D \mathcal{N}_G(D)$. In this case $F(-iU;t,\gamma)$ is weakly Riemann integrable. □

Corollary 2: Let U be continuous and real valued function on the complement of $\mathcal{N}$. Then the function $F(-iU;t,\gamma) = e^{-i\int_0^t U(\gamma(s))\mathrm{d}s}$ is weakly Riemann integrable.

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Dimensional reduction of Dirac operator

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We construct an explicit example of dimensional reduction of the free massless Dirac operator with an internal SU(3) symmetry, defined on a 12-dimensional manifold that is the total space of a principal SU(3)-bundle over a four-dimensional (nonflat) pseudo-Riemannian manifold. Upon dimensional reduction the free 12-dimensional Dirac equation is transformed into a rather nontrivial four-dimensional one: a pair of massive Lorentz spinor SU(3)-octets interacting with an SU(3)-gauge field with a source term depending on the curvature tensor of the gauge field. The SU(3) group is complicated enough to illustrate features of the general case. It should not be confused with the color SU(3) of quantum chromodynamics where the fundamental spinors, the quark fields, are SU(3) triplets rather than octets. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217811]

I. INTRODUCTION

It is well known that when we look for a solution with some symmetry, we can reduce the number of variables and thus simplify the problem of solving differential equations. The Schwarzschild solution of the nonlinear Hilbert-Einstein equation is a typical example. A point of view, different from this calculational aspect of symmetry, is essential for the so-called "Kaluza-Klein approach." It is observed in the pioneer work of Kaluza (1921, English translation in Ref. 1) that there is one-to-one correspondence between the U(1)-invariant metrics on a five-dimensional manifold and the triples [metric on four-dimensional manifold, linear connection with structure group U(1) (electromagnetic potential), scalar field]. The scalar curvature of five-dimensional U(1)-invariant metric is equivalent to the Einstein-Maxwell action for the mentioned fields. This action describes the really observed interaction between gravity and electromagnetic field. This demonstrates the general idea: We consider a "simple" field and "simple" equations but in a "multidimensional" universe. Imposing some symmetry conditions, after dimensional reduction we obtain a set of fields with different nature involved in complicated differential equations. Our hope is that the fields and differential equations, obtained in this way, may describe a real process, and that this investigation may be a step to the unification of different interactions in nature. The natural generalizations of the Kaluza-Klein ansatz are considered in the literature: the group of symmetry G is arbitrary, the group G acts on a manifold as on a total space of a principal bundle, and the group G acts on a manifold with one type orbits. See, for example, Ref. 2.

In this paper the starting point is the free Dirac operator with an SU(3) symmetry defined on a twelve-dimensional Minkowski space that is interpreted as an SU(3) principal bundle over four-dimensional Minkowski space. Should we interpret the outcome in physical terms we should relate the structure group with the "flavor SU(3)" of the quark model, identifying the resulting

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SU(3)-octets Dirac particles with observed baryons. Such an interpretation would again be a nonstandard one however since, unlike the flavor SU(3) of the standard model, our structure group appears as a local gauge group in four-space-time. We prefer, in fact, to view the present paper as a mathematical model illustrating some surprising features of dimensional reduction.

Our purpose is to consider the simplest possible case because then the arising structures after dimensional reduction are imperative. The initial manifold, denoted by E in the text, is the 12-dimensional total space of a principal SU(3) bundle, which admits a real spinor bundle with standard fiber $\mathbb{R}^{64}$. In the real case, the spinor connection is uniquely defined if it is compatible with the Levi-Civita connection of the metric on E. For physical reasons we consider a complex spinor bundle, a complexification of the real-valued one. The spinor connection is also considered as a complexification of the real one. Thus we avoid the necessity to fix a connection with structure group U(1). Further, when we fix the SU(3)-action on spinor fields we choose the trivial lifting. And thus we avoid some additional terms in the reduced Dirac operator. Also the scalar field in the Kaluza-Klein ansatz is taken to be constant—the Killing metric in the Lie algebra of SU(3). In this way, in the reduced Dirac operator there are only structures whose presence is necessary. We also point out the steps in which, imposing the symmetry, the new structures arise (the gauge field with structure group $G=\mathrm{SU}(3)$, its curvature tensor, the Clifford algebra for a four-dimensional manifold, the four-dimensional Dirac operator, the spinor octets, the mass term etc.).

We choose the group of symmetry to be SU(3) acting freely on the 12D manifold because of its connection to the standard model and because we wanted the arising after the reduction gauge field to have structure group SU(3). In the same way one can obtain the dimensional reduction of Dirac operator when the symmetry group is an arbitrary connected Lie group acting freely on the multidimensional manifold.

The article is organized as follows.

In Sec. II the necessary constructions from differential geometry and the algebraic origin of the Kaluza-Klein ansatz are presented. We give the coordinate expression of the Levi-Civita connection for the metric in nonholonomic basis. These formulas are applied to the canonical basis of the SU(3)-invariant metric on E. This basis determines a horizontal subbundle $T^h(E)\hookrightarrow T(E)$. The subbundle $T^h(E)$ is invariant under the action of SU(3) and defines a linear connection [gauge field with structure group SU(3)]. The components of the Levi-Civita connection for the SU(3)-invariant metric are calculated and they contain components of the gauge field and its stress tensor [Eq. (16)].

In Sec. III the Dirac operator for the SU(3)-invariant metric (the Kaluza-Klein ansatz) is considered. The crucial moment here is that the sum $T(E)=T^h(E)\oplus T^v(E)$ is orthogonal with respect to the SU(3)-invariant metric. According to the classifying theorem for Clifford algebras, the Clifford algebra $\mathrm{Cl}(T_z(E),g(x))\approx M_{64}(\mathbb{R})$ is realized as a tensor product of the Clifford algebras of $T^h_z(E)$ and $T^v_z(E)$. So the standard fiber $\mathbb{C}^{64}$ of the spinor bundle on E takes the structure of tensor product $\mathbb{C}^4\otimes\mathbb{C}^{16}$.

In Sec. IV we give the dimensional reduction of the Dirac operator for the SU(3)-invariant metric. We introduce an action of SU(3) on the spinor bundle, compatible with the action of SU(3) on $T(E)$. This condition of compatibility does not fix uniquely the action of SU(3) on the spinors. So we choose, as we mentioned above, the simplest case in which the lifting of the SU(3) action on E to the total space of the spinor bundle is trivial in the canonical basis.

In Sec. V we list the steps in the procedure of dimensional reduction where the new structures presented in the reduced Dirac operator arise.

II. BASIC CONSTRUCTIONS AND NOTATIONS

Let E be a smooth manifold, g a metric on E (with arbitrary signature), and ∇ the corresponding Levi-Civita connection. Let $\{\mathbf{h}_\mu\}$ be a (local) nonholonomic basis of $T(E)$ and $\{\mathbf{h}^\mu\}$ the corresponding dual basis on $T^*(E)$. In this basis we have the following notation:

$$\nabla(\mathbf{h}_\beta) = \Gamma^\rho_{\alpha\beta}\mathbf{h}^\alpha \otimes \mathbf{h}_\rho, \quad \nabla_{\mathbf{h}_\alpha}(\mathbf{h}_\beta) = \nabla_\alpha(\mathbf{h}_\beta) = \Gamma^\rho_{\alpha\beta}\mathbf{h}_\rho,$$

$$[\mathbf{h}_\alpha, \mathbf{h}_\beta] = C^\rho_{\alpha\beta}\mathbf{h}_\rho, \quad g(\mathbf{h}_\alpha, \mathbf{h}_\beta) = g_{\alpha\beta},$$

$$g(\nabla_\alpha(\mathbf{h}_\beta), \mathbf{h}_\gamma) = \Gamma^\rho_{\alpha\beta}g_{\rho\gamma} = \Gamma_{\alpha\beta\gamma}, \quad g([\mathbf{h}_\alpha, \mathbf{h}_\beta], \mathbf{h}_\gamma) = C^\rho_{\alpha\beta}g_{\rho\gamma} = C_{\alpha\beta\gamma}.$$

The condition $\nabla(g)=0$ and the requirement for the vanishing of the torsion reads:

$$\begin{aligned} &\mathbf{h}_\rho(g_{\mu\nu}) = g(\nabla_\rho(\mathbf{h}_\mu), \mathbf{h}_\nu) + g(\mathbf{h}_\mu, \nabla_\rho(\mathbf{h}_\nu)) \Rightarrow \Gamma_{\rho\mu\nu} + \Gamma_{\rho\nu\mu} = \mathbf{h}_\rho(g_{\mu\nu}), \\ &\nabla_\mu(\mathbf{h}_\nu) - \nabla_\nu(\mathbf{h}_\mu) = [\mathbf{h}_\mu, \mathbf{h}_\nu] \Rightarrow \Gamma_{\mu\nu\rho} - \Gamma_{\nu\mu\rho} = C_{\mu\nu\rho}, \end{aligned} \tag{1}$$

and from here it follows that

$$2\Gamma_{\alpha\beta\gamma} = C_{\alpha\beta\gamma} + C_{\gamma\beta\alpha} + C_{\alpha\gamma\beta} + \mathbf{h}_\alpha(g_{\beta\gamma}) + \mathbf{h}_\beta(g_{\alpha\gamma}) - \mathbf{h}_\gamma(g_{\alpha\beta}). \tag{2}$$

We follow the classical construction of the generalized Kaluza-Klein ansatz. The point structure of the ansatz is the description of the metric on the vector space L, which is the middle term in the short exact sequence:

$$0 \to L_0 \overset{i}{\to} L \overset{j}{\to} L_1 \to 0. \tag{3}$$

We realize this in coordinates by choosing a basis $\{\mathbf{h}\}=\{\mathbf{f},\mathbf{e}\}$ in L; $\mathbf{h}_\mu=\mathbf{f}_\mu$, $\mu=1,2,\ldots,m=\dim(L_1)$, $\mathbf{h}_k=\mathbf{e}_k$, $k=m+1,\ldots,m+n, n=\dim(L_0)$. The vector space $L_0=\mathrm{span}(\mathbf{e}_1,\ldots,\mathbf{e}_n)$, and the vector space L_1 is identified with $\mathrm{span}(\mathbf{f}_1,\ldots,\mathbf{f}_m)$ and $i(\mathbf{e}_k)=\mathbf{e}_k$; $j(\mathbf{e}_k)=\mathbf{0}$, $j(\mathbf{f}_\mu)=\mathbf{f}_\mu$. Every splitting of the exact sequence (3) is given by a linear map $S: L_1 \to L$ with the property $j\circ S=\mathbf{1}$, i.e., is given by defining the vectors:

$$\hat{\mathbf{f}}_\mu = S(\mathbf{f}_\mu) = \mathbf{f}_\mu - A^k_\mu \mathbf{e}_k. \tag{4}$$

In these formulas we have summation over repeated indices. Here the matrix A^k_μ is arbitrary. Every metric g_L on L, for which the restriction on $i(L_0)$ is nondegenerate is uniquely determinate by the conditions:

$$\begin{aligned} &g_L(\hat{\mathbf{f}}_\mu, \hat{\mathbf{f}}_\nu) = g_{\mu\nu}, \\ &g_L(\hat{\mathbf{f}}_\mu, \mathbf{e}_k) = 0, \\ &g_L(\mathbf{e}_k, \mathbf{e}_l) = g_{0kl}, \end{aligned} \tag{5}$$

where g_{0kl} and $g_{\mu\nu}$ are metrics on L_0 and L_1. In this manner we have one-to-one correspondence between the metrics on L, non degenerated on L_0 and the triples {metric on L_1, metric on L_0, splitting of (3)}.

In the basis $\{\mathbf{f}_\mu, \mathbf{e}_k\}$ the metric, defined by Eq. (5) has components:

$$\{g_L\} = \begin{pmatrix} g_{\mu\nu} + A_\mu{}^i A_\nu{}^j g_{0ij} & A_\mu{}^i g_{0il} \\ g_{0ki}A^i_\nu & g_{0kl} \end{pmatrix}. \tag{6}$$

The above construction is the algebraic origin of the Kaluza-Klein ansatz. In the case of the general Kaluza-Klein ansatz this construction arises in the tangent space of each point of the manifold where the group of symmetry acts. More precisely, let (E,p,M) be a principal bundle with structure group $G=\mathrm{SU}(3)$. We assume for simplicity that the principal bundle is trivial and the manifold M is isomorphic to $\mathbb{R}^4$ as a topological manifold. We take a global trivialization $E=M\times\mathrm{SU}(3)$ and the right group action is $R_{\mathbf{g}}(\mathbf{x},\mathbf{z})=(\mathbf{x},\mathbf{zg})$ where $(\mathbf{x},\mathbf{z})\in M\times\mathrm{SU}(3)$ and $\mathbf{g}$

$\in \mathrm{SU}(3)$. We also fix coordinates on the total space E, $(x^\mu, z^k)=(x,z)$, $\mu=1,2,3,4$, $k=5,\ldots,12$, $p(x^\mu,z^k)=(x^\mu)$. Because of the assumed triviality of M the coordinates x^μ are global. Let $T^v(E)\hookrightarrow T(E)$ be the vertical subbundle, $\mathbf{f}_\mu$ the nonholonomic basis of $T(M)$, $\mathbf{e}_k$ the fundamental fields on E corresponding to a basis $\hat{\mathbf{e}}_5,\ldots,\hat{\mathbf{e}}_{12}$ of the Lie algebra $su(3)$. The fields $\mathbf{f}_\mu,\mathbf{e}_k$ form a nonholonomic basis on $TE=T(M\times \mathrm{SU}(3))$, and have the form

$$\mathbf{f}_\mu = f_\mu^\nu(x)\frac{\partial}{\partial x^\nu}, \quad \mathbf{e}_k = e_k^l(z)\frac{\partial}{\partial z^l}. \tag{7}$$

The natural exact sequence

$$0 \to T^v(E) \to T(E) \to p^*(T(M)) \to 0 \tag{8}$$

realizes the exact sequence (3) at the tangent space of each point of the manifold E. Here $p^*(T(M))$ is the pull back of the tangent bundle of M (see Ref. 3). Each metric g_E on E can be written in the form:

$$\{g_E(x,z)\} = \begin{pmatrix} g_{\mu\nu}(x,z) + A_\mu{}^i(x,z)A_\nu{}^j(x,z)g_{0ij}(x,z) & A_\mu{}^i(x,z)g_{0il}(x,z) \\ g_{0ki}(x,z)A_\nu^i(x,z) & g_{0kl}(x,z) \end{pmatrix}, \tag{9}$$

where $g_{\mu\nu}(x,z)=g_E(x,z)(\mathbf{f}_\mu(x),\mathbf{f}_\nu(x))$, $g_{0kl}(x,z)=g_E(x,z)(\mathbf{e}_k(z),\mathbf{e}_l(z))$. The vector fields $\hat{\mathbf{f}}_\mu(x,z) = \mathbf{f}_\mu(x)-A_\mu^k(x,z)\mathbf{e}_k(z)$ span a horizontal subbundle $T^h(E)\hookrightarrow T(E)$ orthogonal to $T^v(E)$ with respect to the metric (9). The ansatz (9) is convenient to describe the metrics on E invariant under the action of the group $G=\mathrm{SU}(3)$. The invariant metrics g on E have the form

$$\{g_E(x,z)\} = \begin{pmatrix} g_{\mu\nu}(x) + A_\mu{}^i(x)A_\nu{}^j(x)g_{0ij}(x) & A_\mu{}^i(x)g_{0il}(x) \\ g_{0ki}(x)A_\nu^i(x) & g_{0kl}(x) \end{pmatrix}. \tag{10}$$

This is the Kaluza-Klein ansatz in our case. In this formula $g_{\mu\nu}(x)=g(\mathbf{f}_\mu,\mathbf{f}_\nu)(x)$ is an arbitrary metric on M. Because $\mathbf{f}_\mu$ is a nonholonomic basis on M, without loss of generality we can think that $g_{\mu\nu}$ is in canonical form, i.e. $\mathbf{f}_\mu$ are tetrada. This will be used in our calculation later. $g_{0kl}(x)$ at each point $x\in M$ is invariant metric on the Lie algebra $su(3)$, i.e., g_0 is a field defined on M taking values in the set of invariant metrics on the Lie algebra $su(3)$. The vector fields $\hat{\mathbf{f}}_\mu(x,z) = \mathbf{f}_\mu(x)-A_\mu^k(x)\mathbf{e}_k(z)$ span orthogonal horizontal subbundle $T^h(E)$ which is invariant under the action of the structure group of the principal bundle $G=\mathrm{SU}(3)$. So $A_\mu^k(x)$ define a linear connection in the principal bundle with a structure group $G=\mathrm{SU}(3)$. A classical result is that there is one-to-one correspondence between the G-invariant metrics on E and the triples {metric on M, linear connection with values in the Lie algebra of G, "scalar field"}. In the basis $\{\hat{\mathbf{f}}_\mu,\mathbf{e}_k\}$ for the metric (10) we have

$$\begin{gathered} g_E(\hat{\mathbf{f}}_\mu(x),\hat{\mathbf{f}}_\nu(x)) = g(\mathbf{f}_\mu(x),\mathbf{f}_\nu(x)) = g_{\mu\nu}(x), \\ g_E(\hat{\mathbf{f}}_\mu(x),\mathbf{e}_k(x)) = 0, \\ g_E(\mathbf{e}_k(z),\mathbf{e}_l(z)) = g_{0kl}(x). \end{gathered} \tag{11}$$

The next step is to construct the Dirac operator on E corresponding to the metric (10). To calculate the Levi-Civita connection (2) of the metric (10) we have to introduce the commutator coefficients for the basis $\{\mathbf{f}_\mu,\mathbf{e}_k\}$:

$$[\mathbf{f}_\mu,\mathbf{f}_\nu](x) = C_{\mu\nu}^\rho(x)\mathbf{f}_\rho(x),$$

$$[\mathbf{f}_\mu,\mathbf{e}_k] = \left[f_\mu^\nu(x)\frac{\partial}{\partial x^\nu}, e_k^l(z)\frac{\partial}{\partial z^l}\right] = 0,$$

$$[\mathbf{e}_k,\mathbf{e}_l](z)=t_{kl}^m\mathbf{e}_m(z). \tag{12}$$

Here $C_{\mu\nu}^\rho(x)$ are determined by the choice of the nonholonomic basis $\mathbf{f}_\mu$ in $T(M)$, t_{kl}^m are the structure constants of the Lie algebra $su(3)$ for the basis $\hat{\mathbf{e}}_5,\ldots,\hat{\mathbf{e}}_{12}$. The non-holonomic basis $\{\hat{\mathbf{f}}_\mu,\mathbf{e}_k\}$, because of (11), is convenient for the construction of the Dirac operator. By means of (12) and (4) we calculate

$$\begin{gathered}[\hat{\mathbf{f}}_\mu,\hat{\mathbf{f}}_\nu](x,z)=C_{\mu\nu}^\rho(x)\hat{\mathbf{f}}_\rho(x)-F_{\mu\nu}^k(x)\mathbf{e}_k(z),\\ [\hat{\mathbf{f}}_\mu,\mathbf{e}_k](x,z)=-A_\mu^l(x)t_{lk}^m\mathbf{e}_m(z),\\ [\mathbf{e}_k,\mathbf{e}_l](z)=t_{kl}^m\mathbf{e}_m.\end{gathered} \tag{13}$$

Here

$$F_{\mu\nu}^m=\mathbf{f}_\mu(A_\nu^m)-\mathbf{f}_\nu(A_\mu^m)+t_{\mu\nu}^\rho A_\rho^m-C_{\mu\nu}^\rho A_\rho^m \tag{14}$$

is the curvature tensor of the linear connection, determined by the one-form $A_\mu=A_\mu^m a_m$. Then the coefficients $C_{\alpha\beta\gamma}$ in (2) for the basis $\{\hat{\mathbf{f}}_\mu,\mathbf{e}_k\}$ are

$$\begin{gathered}C_{\mu\nu\rho}=g([\mathbf{f}_\mu,\mathbf{f}_\nu],\mathbf{f}_\rho)=C_{\mu\nu}^\sigma g_{\sigma\rho},\quad C_{\mu\nu k}=-g_{0kl}F_{\mu\nu}^l=-F_{\mu\nu k},\\ C_{\mu k\nu}=-C_{k\mu\nu}=0,\quad C_{\mu kl}=-A_\mu^k t_{mkl}=-C_{k\mu l},\\ C_{kl\mu}=0,\quad C_{klm}=t_{klm},\end{gathered} \tag{15}$$

where $t_{mkl}=g_{0li}t_{mk}^i$. From (2) we obtain the components of Levi-Civita connection in the basis $\{\hat{\mathbf{f}}_\mu,\mathbf{e}_k\}$:

$$\begin{gathered}\Gamma_{\mu\nu\rho}^E=\Gamma_{\mu\nu\rho},\quad \Gamma_{\mu\nu k}^E=-\tfrac{1}{2}F_{\mu\nu k},\\ \Gamma_{\mu k\nu}^E=\tfrac{1}{2}F_{\mu\nu k},\quad \Gamma_{\mu kl}^E=\tfrac{1}{2}A_\mu^m(t_{mlk}-t_{mkl})+\tfrac{1}{2}\mathbf{f}_\mu(g_{0kl}),\\ \Gamma_{k\mu\nu}^E=\tfrac{1}{2}F_{\mu\nu k},\quad \Gamma_{k\mu l}^E=\tfrac{1}{2}A_\mu^m(t_{mkl}+t_{mlk})+\tfrac{1}{2}\mathbf{f}_\mu(g_{0kl}),\\ \Gamma_{kl\mu}^E=-\tfrac{1}{2}A_\mu^m(t_{mkl}+t_{mlk})+\tfrac{1}{2}\mathbf{f}_\mu(g_{0kl}),\quad \Gamma_{klm}^E=\tfrac{1}{2}(t_{klm}+t_{mlk}+t_{mkl}).\end{gathered} \tag{16}$$

In these formulas $\Gamma_{\mu\nu}^\rho$ are the components of the Levi-Civita connection in the basis $\{\mathbf{f}_\mu\}$ for the metric g on M.

III. DIRAC OPERATOR FOR THE KALUZA-KLEIN METRIC

To describe the Dirac operator for the Kaluza-Klein metric (10) we need some preliminary constructions. Let L be a real vector space and η a metric on L of type (p,q); $\eta=\mathrm{diag}(-1,\ldots,-1,1,\ldots,1)$, $\{\text{number of }(1)\}=p$, $\{\text{number of }(1)\}=q$, $p+q=\dim(L)$. We denote by ϑ the canonical embedding

$$\vartheta:L\to \mathrm{Cl}(\eta) \tag{17}$$

of the vector space L into the corresponding Clifford algebra.[4,5] $\vartheta(\mathbf{x})^2=\eta(\mathbf{x},\mathbf{x})\mathbf{1},\mathbf{x}\in L$, where $\mathbf{1}$ is the unit of the algebra $\mathrm{Cl}(\eta)\equiv\mathrm{Cl}^{p,q}$. If $\mathbf{a}_1,\ldots,\mathbf{a}_n$ is an arbitrary basis of L, $\vartheta(\mathbf{a}_i)=\gamma_i$, $\gamma_i\gamma_j-\gamma_j\gamma_i=2\eta_{ij}\mathbf{1}$, $\eta_{ij}=\eta(\mathbf{a}_i,\mathbf{a}_j)$. If $\mathbf{a}_1,\ldots,\mathbf{a}_n$ is oriented orthonormal basis, the volume element $\omega=\gamma_1\ldots\gamma_n$ is uniquely determined and $\omega^2=\pm\mathbf{1}$. We will assume that L has fixed orientation. The symmetry of

the metric on L gives rise to some structures on the spinor bundle on L. In order to describe them we need some facts for the classificationof the Clifford algebras.

The first step in the classification and realizations of the Clifford algebras for arbitrary metric is the following statement:[4,5] If $(L_1 \oplus L_2, \eta_1 \oplus \eta_2)$ is an orthogonal direct sum of metric vector spaces (L_1, η_1) and (L_2, η_2) then $\mathrm{Cl}(\eta_1 \oplus \eta_2) = \mathrm{Cl}(\eta_1) \widehat{\otimes} \mathrm{Cl}(\eta_2)$, where $\widehat{\otimes}$ is the $\mathbb{Z}_2$-graded tensor product of the naturally $\mathbb{Z}_2$-graded Clifford algebras. In some exceptional cases the $\mathbb{Z}_2$-graded tensor product may be replaced with the usual tensor product. In our example is realized one of these exceptional cases.

Let $\dim(L) = p+q = 2k$ be even. We say that $\mathrm{Cl}(\eta) > 0$ or $\mathrm{Cl}(\eta) < 0$ if $\omega^2 = +1$ or $\omega^2 = -1$. Let (L_1, η_1) and (L_2, η_2) be vector spaces with metrics η_1 and η_2, and $(L_1 \oplus L_2, \eta_1 \oplus \eta_2)$ be an orthogonal direct sum. Then (see Ref. 4 and 5)

$$\begin{aligned} \mathrm{Cl}(\eta_1) > 0 \Rightarrow \mathrm{Cl}(\eta_1 \oplus \eta_2) = \mathrm{Cl}(\eta_1) \otimes \mathrm{Cl}(\eta_2), \\ \mathrm{Cl}(\eta_1) < 0 \Rightarrow \mathrm{Cl}(\eta_1 \oplus \eta_2) = \mathrm{Cl}(\eta_1) \otimes \mathrm{Cl}(-\eta_2). \end{aligned} \tag{18}$$

Let $\{\mathbf{a}_{1i}\}$, $\{\mathbf{a}_{2j}\}$ be bases in L_1 and L_2. The isomorphisms in (18) are given by

$$\begin{aligned} \gamma_{1i} \otimes \mathbf{1}_2 \mapsto \gamma_i = \vartheta(\mathbf{a}_{1i}, \mathbf{0}), \quad i = 1,2,\ldots,n_1 = \dim(L_1), \\ \omega_1 \otimes \gamma_{2j}, \mapsto \gamma_{n_1+j} = \vartheta(\mathbf{0}, \mathbf{a}_{2j}), \quad j = 1,2,\ldots,n_2 = \dim(L_2). \end{aligned} \tag{19}$$

These isomorphisms give the classification of the Clifford algebras.

For physical reasons we will consider complex spinor fields and we will need a complexification of the Clifford algebra:

$$\mathrm{Cl}^{p,q} \otimes \mathbb{C} = \mathrm{Cl}(L \otimes \mathbb{C}, \eta) = \mathrm{Cl}^n, \quad n = p+q. \tag{20}$$

It is known[4,5] that $\mathrm{Cl}^{2k} \approx M_{2^k}(\mathbb{C})$, $\mathrm{Cl}^{2k+1} \approx M_{2^k}(\mathbb{C}) \oplus M_{2^k}(\mathbb{C})$. In our case the Clifford algebra Cl^{12} is even and thus $\mathrm{Cl}^{12} \approx M_{64}(\mathbb{C})$ has only one simple module. We have the following isomorphisms:

$$\begin{aligned} \mathrm{Cl}^{1,3} \approx M_4(\mathbb{R}), \quad \mathrm{Cl}^{1,3} < 0 \\ \mathrm{Cl}^{0,8} = \mathrm{Cl}^{8,0} \approx M_{16}(\mathbb{R}), \quad \mathrm{Cl}^{0,8} > 0, \quad \mathrm{Cl}^{8,0} > 0. \end{aligned} \tag{21}$$

So we have

$$\mathrm{Cl}^{1,11} = \mathrm{Cl}^{1,3} \otimes \mathrm{Cl}^{8,0} \approx M_4(\mathbb{R}) \otimes M_{16}(\mathbb{R}). \tag{22}$$

Let (E,g) be an oriented even dimensional manifold with metric g, $\mathrm{sign}(g) = (p,q)$. This means that the tangent bundle over E has a cocycle $\psi_{\alpha\beta}(x) \in \mathrm{Aut}(\mathbb{R}^{2k}, \eta) = O(p,q)$. An element $A \in \mathrm{Aut}(\mathbb{R}^{2k}, \eta)$ uniquely determines an element $\widetilde{A} \in \mathrm{Aut}(\mathrm{Cl}^{p,q})$. So $\widetilde{\psi}(x) \in \mathrm{Aut}(\mathrm{Cl}^{p,q})$ is a cocycle which defines the Clifford bundle $\mathrm{Cl}(TE)$ over E. In this bundle the fiber $\mathrm{Cl}(TE)_x$ is the Clifford algebra for the vector space $(T_x(E), g(x))$. The standard fiber of the complex Clifford bundle $\mathrm{Cl}^{\mathbb{C}}(TE)$ is $\mathrm{Cl}^{2k} = M_{2^k}(\mathbb{C})$. A spin$^{\mathbb{C}}$ structure on E is equivalent to a bundle ζ of simple complex modules over the Clifford bundle $\mathrm{Cl}^{\mathbb{C}}(TE)$. We will point out some details in the construction of the complexified bundle ζ because they are important in our later study on the structures arising in ζ. Let $\widehat{L} = \vartheta(L) \hookrightarrow \mathrm{Cl}(\eta)$ be the image of the linear space L in the Clifford algebra. $\vartheta: L \to \widehat{L}$ is an isomorphism and we will identify L and $\widehat{L}$ by means of ϑ. The Clifford group $\mathcal{F}$ is defined by

$$\mathcal{F}^{p,q} = \{c \in \mathrm{Cl}^*(p,q) | c\widehat{L}c^{-1} \subset L\}, \tag{23}$$

where Cl^* is the set of invertible elements. In the complexified case we have similarly

$$\mathcal{F}^{2k} = \{c \in \mathrm{Cl}^{*2k} | c\hat{L}c^{-1} \subset L\}. \tag{24}$$

The linear map $j(c):\hat{L}\to\hat{L}$; $\mathbf{u}\to j(c)(\mathbf{u})=c\mathbf{u}c^{-1}$ is orthogonal and $j:\mathcal{F}\to O(p,q)$ is surjective and gives the exact sequence

$$1 \to \mathbb{C}^* \to \mathcal{F}^{2k} \overset{j^{\mathbb{C}}}{\to} O(p,q) \to \mathbf{1}. \tag{25}$$

And in the real case we have

$$1 \to \mathbb{R}^* \to \mathcal{F}^{p,q} \overset{j}{\to} O(p,q) \to \mathbf{1}. \tag{26}$$

A spin$^{\mathbb{C}}$ bundle ζ is a complex vector bundle on E and each fiber $\zeta_{(\mathbf{x},\mathbf{z})}, (\mathbf{x},\mathbf{z}) \in E = M \otimes G$, is a simple complex module over the algebra $\mathrm{Cl}(T_{(x,z)}E)$. Let $\psi_{\alpha\beta}(x) \in \mathrm{Aut}(\mathbb{R}^{2k}, \eta)$ be a cocycle of $T(E)$ and $\widetilde{\psi}_{\alpha\beta}(x) \in \mathrm{Aut}(\mathrm{Cl}^{2k})$ be the cocycle of $\mathrm{Cl}^{\mathbb{C}}(TE)$. Because the standard fiber of $\mathrm{Cl}(TE)$ is $\mathrm{Cl}^{2k} \approx M_{2^k}(\mathbb{C}) \approx \mathrm{Hom}(\mathbb{C}^{2^k}, \mathbb{C}^{2^k})$, and $\mathbb{C}^{2^k}$ (the standard fiber of the spinor bundle ζ)is the simple module of $M_{2^k}(\mathbb{C})$, the spin$^{\mathbb{C}}$ bundle has a cocycle $\varphi_{\alpha\beta}(x) \in \mathrm{Aut}(\mathbb{C}^{2^k}) \subset M_{2^k}(\mathbb{C}) \approx \mathrm{Cl}^{2k}$ of invertible elements $\varphi_{\alpha\beta} \in \mathcal{F}^{2k}$ and

$$j(\varphi_{\alpha\beta}(x)) = \psi_{\alpha\beta}(x). \tag{27}$$

In general, not every manifold admits a spin$^{\mathbb{C}}$ structure, and even if it admits there may exist different spin$^{\mathbb{C}}$ structures. In our example the base manifold has only one (up to isomorphism) spin$^{\mathbb{C}}$-structure.

The Dirac operator

$$D: C^{\infty}(\zeta) \to C^{\infty}(\zeta) \tag{28}$$

is determined by a linear connection on the spinor bundle and the requirement that its symbol $\sigma(D):T^*(E)\to\zeta^*\otimes\zeta$ be the unique irreducible representation of the Clifford algebra Cl^{2k} at each fiber (see Ref. 6).

In our example we choose E to be a total space of a principal SU(3) bundle over M and M to be isomorphic to $\mathbb{R}^4$ as a topological manifold. We also choose the metric on M to be $g_{\mu\nu} = \mathrm{diag}(-1,1,1,1)$, the basis $\{\mathbf{f}_{\mu}(\mathbf{x})\}$ to be a nonholonomic basis in $T(M)$, and the metric $g_{0kl}(x) = g_{0kl} = \mathrm{diag}(-1,\ldots,-1)$ to be the Killing metric on the Lie algebra $su(3)$. We consider the simplest case in which the "scalar fields" in Kaluza-Klein ansatz are constants.

Because of (11) the direct sum $T(E)=T^h(E)\oplus T^v(E)$ is orthogonal. And from (17)

$$\mathrm{Cl}(TE) = \mathrm{Cl}(T^hE) \otimes \mathrm{Cl}(T^vE), \tag{29}$$

i.e., the standard fiber of $\mathrm{Cl}(TE)$ is $\mathrm{Cl}^{1,3}\otimes\mathrm{Cl}^{0,8}$ in the real (Majorana) case and $\mathbb{C}^4\otimes\mathbb{C}^8$ in the complexified case. So the standard fiber of the spinor bundle ζ is isomorphic to $\mathbb{R}^4\otimes\mathbb{R}^{16}$ in the Majorana case and $\mathbb{C}^4\otimes\mathbb{C}^{16}$ in the complexified case. In the nonholonomic basis (7) of TE according to (19) we have

$$\begin{aligned} &\mathbf{f}_{\mu}(x) \mapsto \gamma_{\mu}\otimes\mathbf{1} \in \mathrm{Cl}(T^h_{(x,z)}E \oplus T^v_{(x,z)}E) = \mathrm{Cl}(T^h_{(x,z)}E, g) \otimes \mathrm{Cl}(T^h_{(x,z)}E, -g_0), \\ &\mathbf{e}_k(x) \mapsto \omega \otimes \gamma_k \in \mathrm{Cl}(T^h_{(x,z)}E \oplus T^v_{(x,z)}E) = \mathrm{Cl}(T^h_{(x,z)}E, g) \otimes \mathrm{Cl}(T^h_{(x,z)}E, -g_0). \end{aligned} \tag{30}$$

In the real case the Levi-Civita connection determines a unique connection on the Majorana spinor bundle. Let ∇ be the Levi-Civita connection for the metric g_E on E and $\mathbf{h}_{\alpha}$ be an orthonormal with respect of g_E nonholonomic basis of TE. If

$$\nabla_{\mathbf{h}_{\alpha}}(\mathbf{h}_{\beta}) \equiv \nabla_{\alpha}(\mathbf{h}_{\beta}) = \Gamma^{E\rho}_{\alpha\beta}\mathbf{h}_{\rho}, \tag{31}$$

then in the real case there is a unique corresponding connection on ζ,

$$\nabla_{\mathbf{h}_\alpha} = \mathbf{h}_\alpha + S_\alpha,$$

$$S_\alpha = -\tfrac{1}{4}\Gamma_\alpha^{E\rho\sigma}\gamma_\rho\gamma_\sigma = -\tfrac{1}{4}\Gamma_{\alpha\rho\sigma}\gamma^\rho\gamma^\sigma, \tag{32}$$

$$\Gamma_{\alpha\beta\sigma} = g^E_{\sigma\rho}\Gamma^\rho_{\alpha\beta}, \quad g^E_{\alpha\beta} = g^E(\mathbf{h}_\alpha, \mathbf{h}_\beta) = \text{const}.$$

If in the complexified case we want to have a soldering between the parallel transport in TE and ζ there remains freedom for the choice of the $U(1)$-connection. In our example we fix the complexification of (32). Then the Dirac operator reads:

$$D = \hat{\mathbf{h}}^\mu\nabla_\mu = g^{E\mu\beta}\hat{\mathbf{h}}_\beta\nabla_\mu = \gamma^{E\mu}(\mathbf{h}_\mu + S_\mu), \quad \hat{\mathbf{h}}^\mu = \vartheta(\mathbf{h}^\mu),$$
$$(D\psi)^a = \gamma^{E\mu}(\mathbf{h}_\mu(\psi^a) + S^a_{\mu b}\psi^b), \quad \psi \in C^\infty(\zeta^{\mathbb{C}}). \tag{33}$$

For the Kaluza-Klein metric we specify $g_{\mu\nu} = g(\mathbf{f}_\mu, \mathbf{f}_\nu) = \text{const} = \text{diag}(-1,1,1,1)$, $g_{0kl} = \text{const} = \text{diag}(-1,\ldots,-1)$. Because $\{\mathbf{f}_\mu\}$ is nonholonomic basis on $T(M)$, "tetrada," g can be an arbitrary metric on M. For simplicity we take the "scalar fields" g_{0kl} to be constant: the Killing form in the Lie algebra $su(3)$. In the global basis $\{\hat{\mathbf{f}}_\mu, \mathbf{e}_k\}$ the metric (10) has the form:

$$\{g^E\} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & . & . & 0 \\ 0 & 1 & 0 & 0 & 0 & . & . & 0 \\ 0 & 0 & 1 & 0 & 0 & . & . & 0 \\ 0 & 0 & 0 & 1 & 0 & . & . & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ . & . & . & . & 0 & . & . & 0 \\ . & . & . & . & 0 & . & . & 0 \\ 0 & 0 & 0 & 0 & 0 & . & . & -1 \end{pmatrix}. \tag{34}$$

The coefficients of the Levi-Civita connection of the metric (34)

$$\begin{aligned}
\nabla_{\hat{\mathbf{f}}_\mu}(\hat{\mathbf{f}}_\nu) &= \Gamma^{E\rho}_{\mu\nu}\hat{\mathbf{f}}_\rho + \Gamma^{Ek}_{\mu\nu}\mathbf{e}_k; & \Gamma^E_{\mu\nu\rho} &= g_{\rho\sigma}\Gamma^{E\sigma}_{\mu\nu}, & \Gamma^E_{\mu\nu k} &= -g_{0ki}\Gamma^{Ei}_{\mu\nu},\\
\nabla_{\hat{\mathbf{f}}_\mu}(\mathbf{e}_k) &= \Gamma^{E\nu}_{\mu k}\hat{\mathbf{f}}_\nu + \Gamma^{El}_{\mu k}\mathbf{e}_l; & \Gamma^E_{\mu k\nu} &= g_{\nu\sigma}\Gamma^{E\sigma}_{\mu k}, & \Gamma^E_{\mu kl} &= -g_{0li}\Gamma^{Ei}_{\mu k},\\
\nabla_{\mathbf{e}_k}(\hat{\mathbf{f}}_\mu) &= \Gamma^{E\nu}_{k\mu}\hat{\mathbf{f}}_\nu + \Gamma^{El}_{k\mu}\mathbf{e}_l; & \Gamma^E_{k\mu\nu} &= g_{\nu\sigma}\Gamma^{E\sigma}_{k\mu}, & \Gamma^E_{k\mu l} &= -g_{0li}\Gamma^{Ei}_{k\mu},\\
\nabla_{\mathbf{e}_k}(\mathbf{e}_l) &= \Gamma^{E\mu}_{kl}\hat{\mathbf{f}}_\mu + \Gamma^{Em}_{kl}\mathbf{e}_m; & \Gamma^E_{kl\mu} &= g_{\mu\sigma}\Gamma^{E\sigma}_{kl}, & \Gamma^E_{klm} &= -g_{0mi}\Gamma^{Ei}_{kl}
\end{aligned} \tag{35}$$

are defined in the general case in (16). Because of the form of the metric in (34) the Clifford bundle $\text{Cl}(TE)$ has global generators:

$$\gamma^E_\mu = \gamma_\mu \otimes \mathbf{1}, \quad \mu = 1,2,3,4,$$
$$\gamma^E_k = \omega \otimes \gamma_k, \quad k = 5,\ldots,12, \tag{36}$$

where γ_μ are generators of $\text{Cl}^{1,3}$, γ_k are generators of $Cl^{0,8}$ (30), $\omega = \gamma_1\gamma_2\gamma_3\gamma_4$, $\omega^2 = -1$. After these specifications the Dirac operator (32) and (36) for the Kaluza-Klein metric (10) reads:

$$\begin{aligned}
D &= \gamma^{E\mu}\nabla_{\hat{\mathbf{f}}_\mu} + \gamma^{Ek}\nabla_{\mathbf{e}_k} = (\gamma^\mu \otimes \mathbf{1})(\hat{\mathbf{f}}_\mu + S_\mu) + (\omega \otimes \gamma^k)(\mathbf{e}_k + S_k)\\
&= (\gamma^\mu \otimes \mathbf{1})(\mathbf{f}_\mu - A^k_\mu\mathbf{e}_k) + (\omega \otimes \gamma^k)\mathbf{e}_k\\
&\quad + (\gamma^\mu \otimes \mathbf{1})\left(-\frac{1}{4}\right)(\Gamma^E_{\mu\nu\rho}\gamma^\nu\gamma^\rho \otimes \mathbf{1} + \Gamma^E_{\mu\nu k}(\gamma^\nu \otimes \mathbf{1})(\omega \otimes \gamma^k)
\end{aligned}$$

$$+\Gamma^E_{\mu k\nu}(\omega\otimes\gamma^k)(\gamma^\nu\otimes\mathbf{1})+\Gamma^E_{\mu kl}(\omega\otimes\gamma^k)(\omega\otimes\gamma^l))$$
$$+(\omega\otimes\gamma^k)\left(-\frac{1}{4}\right)(\Gamma^E_{k\mu\nu}\gamma^\mu\gamma^\nu\otimes\mathbf{1}+\Gamma^E_{k\mu l}(\gamma^\mu\otimes\mathbf{1})(\omega\otimes\gamma^l)$$
$$+\Gamma^E_{kl\mu}(\omega\otimes\gamma^l)(\gamma^\mu\otimes\mathbf{1})+\Gamma^E_{klm}(\omega\otimes\gamma^l)(\omega\otimes\gamma^m)). \tag{37}$$

Here $\gamma^\mu=g^{\mu\sigma}\gamma_\sigma$ and $\gamma^k=-g_0^{ki}\gamma_i$. Using (16) we obtain

$$D=(\gamma^\mu\otimes\mathbf{1})(\mathbf{f}_\mu-A^k_\mu\mathbf{e}_k)+(\omega\otimes\gamma^k)\mathbf{e}_k-\frac{1}{4}(\gamma^\mu\otimes\mathbf{1})\left(\Gamma_{\mu\nu\rho}\gamma^\nu\gamma^\rho\otimes\mathbf{1}+F_{\mu\nu k}\omega\gamma^\nu\right.$$
$$\left.\otimes\gamma^k-\frac{1}{2}A^m_\mu(t_{mlk}-t_{mkl})\mathbf{1}\otimes\gamma^k\gamma^l\right)-\frac{1}{4}(\omega\otimes\gamma^k)\left(\frac{1}{2}F_{\mu\nu k}\gamma^\mu\gamma^\nu\otimes\mathbf{1}-A^m_\mu(t_{mlk}+t_{mkl})\omega\gamma^\mu\right.$$
$$\left.\otimes\gamma^l-\frac{1}{2}(t_{klm}+t_{mlk}+t_{mkl})\mathbf{1}\otimes\gamma^l\gamma^m\right). \tag{38}$$

The Dirac operator (38) for the Kaluza-Klein metric (10) acts on spinor fields which have 64 components. Due to (30) the standard fiber of the complex spinor bundle is $\mathbb{C}^4\otimes\mathbb{C}^{16}$.

IV. DIMENSIONAL REDUCTION OF THE DIRAC OPERATOR

We need to specify the action of the symmetry group $G=\mathrm{SU}(3)$ on the spinor bundle. The action $R_g(x,z)=(x,zg)$ on the base $E=M\times\mathrm{SU}(3)$ of the spinor bundle ζ must be lifted to a bundle morphism action on the spinor bundle ζ. This lifting must be in agreement with the action of SU(3) on $T(E)$. More precisely, let $R_\mathbf{g}:(\mathbf{x},\mathbf{z})\to(\mathbf{x},\mathbf{zg})$ be the action of $\mathbf{g}\in G=\mathrm{SU}(3)$ on E. For the Kaluza-Klein metric (10) the tangent lifting $R^T_\mathbf{g}:T_{(\mathbf{x},\mathbf{z})}(E)\to T_{(\mathbf{x},\mathbf{zg})}(E)$ is an isometry. In our trivialization, in the basis $\{\hat{\mathbf{f}}_\mu,\mathbf{e}_k\}$ the tangent lifting $R^T_\mathbf{g}:\mathbb{R}^{12}\to\mathbb{R}^{12}$ is the identity. Let $\mathcal{F}:\mathbb{C}^4\otimes\mathbb{C}^{16}\to\mathbb{C}^4\otimes\mathbb{C}^{16}$be the lifting of the action $L_\mathbf{g}$ to the complexified spinor bundle $\zeta^\mathbb{C}$. $\mathcal{F}_\mathbf{g}$ must satisfy (in the same trivialization)

$$j^\mathbb{C}(\mathcal{F}_\mathbf{g})=R^T_\mathbf{g}=\mathbf{1} \tag{39}$$

with $j^\mathbb{C}$ given from (25). Our purpose is to construct explicitly the simplest example of the Dirac operator with SU(3) symmetry and its reduction to the Dirac operator acting on spinors over four-dimensional manifold. So we fix $\mathcal{F}_\mathbf{g}=\mathbf{1}$ and then the action of $G=\mathrm{SU}(3)$ on spinor fields, i.e., the sections on ζ, is

$$R_\mathbf{g}(\psi)^{\mu a}(\mathbf{x},\mathbf{z})=\psi^{\mu a}(\mathbf{x},\mathbf{zg}). \tag{40}$$

The Dirac operator (38) for the Kaluza-Klein metric (10) is SU(3)-invariant, when the action of SU(3) on spinor fields is specified as in (40). For the invariant spinor fields, from (40) we have

$$R_\mathbf{g}(\psi)^{\mu a}=\psi^{\mu a}\Rightarrow\psi^{\mu a}(\mathbf{x},\mathbf{zg})=\psi^{\mu a}(\mathbf{x},\mathbf{e})\equiv\psi^{\mu a}(\mathbf{x}). \tag{41}$$

The set of all invariant spinor fields $C^\infty(\zeta)_G$ is identified, due to (41), with $C^\infty(\zeta|_{M\times\{e\}})\equiv C^\infty(\zeta|_M)$. The dimensional reduction of the Dirac operator (38) is a restriction of (38) on the set of SU(3)-invariant spinor fields and we obtain the reduced Dirac operator D_r:

$$D_r:C^\infty(\zeta|_M)\to C^\infty(\zeta|_M). \tag{42}$$

To calculate D_r we have to put in (38) a SU(3) invariant spinor field. For invariant spinor fields $\psi^{\mu a}(\mathbf{x})$ we have from (41), $\mathbf{e}_k(\psi^{\mu a})=0$. For the reduced Dirac operator D_r we obtain

$$D_r = (\gamma^\mu \otimes \mathbf{1})\left(\mathbf{f}_\mu - \frac{1}{4}\Gamma_{\mu\nu\rho}(x)\gamma^\nu\gamma^\rho\right) - \frac{1}{8}F_{\mu\nu k}(x)\omega\gamma^\mu\gamma^\nu \otimes \gamma^k + \frac{1}{4}A^m_\mu(x)t_{mlk}\gamma^\mu \otimes \gamma^k\gamma^l + \frac{1}{4}t_{mlk}\omega \otimes \gamma^k\gamma^l\gamma^m, \tag{43}$$

where the coefficients t_{mlk} are totally antisymmetric in all indices. The reduced Dirac operator (43) acts on the sections $\psi \in C^\infty(\zeta|_M)$. The standard fiber is $\mathbb{C}^4 \otimes \mathbb{C}^{16}$. The bundle $\zeta|_M$ is canonically isomorphic to $\zeta^M \otimes \zeta^{\mathrm{SU}(3)}$:

$$\zeta|_M \approx \zeta^M \otimes \zeta^{\mathrm{SU}(3)}, \tag{44}$$

where ζ^M is the (complex) spinor bundle on M and $\zeta^{\mathrm{SU}(3)}$ is a vector bundle on M with standard fiber $\mathbb{C}^{16}$ considered as a simple module of the Clifford algebra $Cl^{0,8}$ corresponding to the Lie algebra $su(3)$ with the Killing metric g. $\{\mathbf{f}_\mu\}$ is a nonholonomic global basis of $T(M)$ and tetrada for the metric g. $\Gamma_{\mu\nu\rho}(x)$ are the components of the Levi-Civita connection of g in the basis $\{\mathbf{f}_\mu\}$ and $-\frac{1}{4}\Gamma_{\mu\nu\rho}(x)\gamma^\nu\gamma^\rho$ are the components of the spinor connection in ζ^M, so

$$D^M = (\gamma^\mu \otimes \mathbf{1})\left(\mathbf{f}_\mu - \frac{1}{4}\Gamma_{\mu\nu\rho}(x)\gamma^\nu\gamma^\rho\right) \tag{45}$$

is the Dirac operator for the metric g acting on spinor fields with isotopic indices. $A^m_\mu(x)$ is a gauge field with values in the Lie algebra $su(3)$ and $F_{\mu\nu k}(x)$ is its curvature tensor. We can write (45) in the form

$$D_r = (\gamma^\mu \otimes \mathbf{1})\left(\mathbf{f}_\mu - \frac{1}{4}\Gamma_{\mu\nu\rho}\gamma^\nu\gamma^\rho + \frac{1}{4}A^m_\mu t_{mkl}\mathbf{1} \otimes \gamma^k\gamma^l\right) - \frac{1}{8}F_{\mu\nu k}\omega\gamma^\mu\gamma^\nu \otimes \gamma^k + \omega \otimes \boldsymbol{\epsilon}, \tag{46}$$

where $\boldsymbol{\epsilon} = \frac{1}{4}t_{klm}\gamma^k\gamma^l\gamma^m$.

The interpretation of (46) is that the reduced free massless Dirac operator for the Kaluza-Klein metric acting on spinor fields with an "isotopic" index on M is equivalent to the usual Dirac operator in the presence of a gravitation field (the metric) and external gauge field with gauge group SU(3), source term depending on the curvature $F^k_{\mu\nu}$ and a mass term $\omega \otimes \boldsymbol{\epsilon}$.

The "isotopic" bundle $\zeta^{\mathrm{SU}(3)}$ in (44) has a standard fiber $\mathbb{C}^{16}$. $\mathbb{C}^{16}$ is the unique simple module of the Clifford algebra $\mathrm{Cl}(su(3), -g_0) = \mathrm{Cl}^{0,8} = M_{16}(\mathbb{R})$. The algebra $su(3)$, as a real vector space, is isomorphic to $\mathbb{R}^8$ and g_0 is the negative defined Killing metric. In the chosen basis $\{\hat{\mathbf{e}}_k\}$ of $su(3)$, $g_0 = \mathrm{diag}(-1, \ldots, -1)$. The group of symmetry of the Killing metric g_0 on $su(3)$ (considered as a vector space, isomorphic to $\mathbb{R}^8$) is $O(8)$. According to the standard procedure,[4,5] the Lie algebra $o(8)$has a complex spinor representation in $\mathbb{C}^{16}$, which is a direct sum of two irreducible representations and $\mathbb{C}^{16} = \mathbb{C}^8 \oplus \mathbb{C}^8$. These representations are realized on the eigenspaces of the operator $\omega_0 = \Pi_{k=4}^{12}\gamma^k$. Let $\rho: O(8) \to \mathrm{End}(\mathbb{C}^{16})$ be the spinor representation, $s \in o(8)$ and $s(\hat{\mathbf{e}}_i) = s^j_i\hat{\mathbf{e}}_j$. Then

$$\rho(s) = -\frac{1}{4}s_{ij}\gamma^j\gamma^j. \tag{47}$$

But the Lie algebra $su(3)$ has a natural adjoint representation: $b \in su(3), ad(b) \in End(su(3) \approx \mathbb{R}^6)$,

$$\mathrm{ad}(\hat{\mathbf{e}}_k)(\hat{\mathbf{e}}_i) = [\hat{\mathbf{e}}_k, \hat{\mathbf{e}}_i] = t^j_{ki}\hat{\mathbf{e}}_j. \tag{48}$$

The adjoint representation "ad" takes values in the Lie algebra $so(8)$, i.e. $\{t_k\} \in so(8)$. So we can take the composition of the two natural representations:

$$\rho \circ \mathrm{ad}: su(3) \to \mathrm{End}(\mathbb{C}^{16}) \tag{49}$$

$$(\rho \circ \mathrm{ad})(\hat{\mathbf{e}}_k) = -\frac{1}{4} t_{kij} \gamma^i \gamma^j.$$

This is a representation of $su(3)$ in $\mathbb{C}^{16}$ which is a direct sum of two eight-dimensional representations of $su(3)$. So the bundle $\zeta^{su(3)}$ on M is a Whitney sum of two eight-dimensional bundles. Due to this fact, the SU(3) invariant spinors, i.e., the sections $C^\infty(\zeta|_M) = C^\infty(\zeta^M \otimes \zeta^{\mathrm{SU}(3)})$ have the natural interpretation as two $su(3)$ spinor octets.

The main result of this paper is that the free massless SU(3)-invariant Dirac operator on the manifold E (the total space of principal SU(3)-bundle on four-dimensional manifold M) after dimensional reduction is equivalent to the Dirac operator on 4-dimensional manifold M, acting on two SU(3) spinor octets, in the presence of gravitational field, external SU(3) gauge field with a source depending on the curvature tensor of the SU(3) gauge field and mass term as it is in (46).

V. COMMENTS

One of the ideas of the "Kaluza-Klein approach" is that a collection of fields with different nature involved in complicated differential equations may be considered as "simple" differential equations for one-type field in a multidimensional case, but having some symmetry, and considered only on the invariant fields. In the spirit of this idea we comment here on the steps in the reduction procedure, where the structures of new type arise. In this example E is 12-dimensional manifold with trivial tangent bundle. For arbitrary metric g_E on E there is just one spinor structure and the spinor fields have 64-components. The group of symmetry $G = \mathrm{SU}(3)$ acts on E as on a total space of a principal bundle. This separate the vertical subbundle $T^v(E) \hookrightarrow T(E)$. The metric under consideration g_E determines a horizontal subbundle $T^h(E) \hookrightarrow T(E)$ as an orthogonal complement of $T^v(E)$. The metric g_E is G-invariant, so the horizontal subbundle $T^h(E)$ is G-invariant and is a linear connection with structure group $G = \mathrm{SU}(3)$. Further, the linear connection in the spinor bundle, coming from the Levi-Civita connection for g_E and needed for the Dirac operator, is expressed interms of this SU(3)-connection. This leads to the appearance of the SU(3) gauge field and its stress tensor. These are classical results for the Kaluza-Klein ansatz. The orthogonal splitting $T(E) = T^h(E) \oplus T^v(E)$ according to the classifying theorem for Clifford algebras leads to the representation (29) and to appearance of spinors on Four-dimensional base manifold after the reduction. The metric in the vertical subspace is the Killing metric. There is a natural adjoint representation of Lie algebra $su(3)$ on itself, orthogonal to the Killing metric and a natural representation of the orthogonal group of the Killing metric on corresponding 16-dimensional spinors. Due to the representations (29), this leads to the appearance of two SU(3) spinor octets after the reduction. Finally, the G-invariance of the spinor fields in the simple case that we consider leads to vanishing of the vertical derivatives and we obtain the reduced operator acting on the fields defined on the Four-dimensional base manifold.

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Second and fourth Painlevé hierarchies and Jimbo-Miwa linear problems

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The relations between the different linear problems for Painlevé equations is an intriguing open problem. Here we consider our previously given second and fourth Painlevé hierarchies [Publ. Res. Inst. Math. Sci. (Kyoto) **37**, 327-347 (2001)], and show that they could alternatively have been derived using the linear problems of Jimbo and Miwa. That is, we give a gauge transformation of our linear problems for these two hierarchies which maps those of the second and fourth Painlevé equations themselves onto those of Jimbo and Miwa. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217647]

I. INTRODUCTION

The discovery of the inverse monodromy transform[1–4] saw the inclusion of the six Painlevé equations amongst the panoply of integrable equations, i.e., of equations solvable using underlying linear problems. Recently, the question of obtaining linear problems for hierarchies of higher order analogues of the Painlevé equations has absorbed the attention of many authors. In particular, in a series of recent papers,[5–8] nonisospectral scattering problems have been used as a means of deriving new completely integrable hierarchies of partial differential equations (PDEs) in $2+1$ and $1+1$ dimensions, and, by reduction, new hierarchies of ordinary differential equations (ODEs), all together with corresponding underlying linear problems.

In Ref. 8 we presented a generalized nonisospectral dispersive water wave hierarchy in $2+1$ dimensions; amongst the reductions to ODEs of this hierarchy we obtained a generalized $P_{\mathrm{IV}}-P_{\mathrm{II}}$ hierarchy which includes as special cases both a hierarchy of ODEs having the fourth Painlevé equation (P_{IV}) as first member, and a hierarchy having the second Painlevé equation (P_{II}) as first member. We believe that the P_{II} hierarchy of Ref. 8 is not equivalent to the standard P_{II} hierarchy given in Refs. 9 and 1. We note in particular that for the first members of these two hierarchies, that is for P_{II} itself, there is no known gauge transformation between their respective linear problems (see the Appendix). We thus believe that both the P_{II} and P_{IV} hierarchies of Ref. 8 were previously unknown.

The aim of the present paper is to explore the relationship between the linear problems for the P_{II} and P_{IV} hierarchies presented in Ref. 8, and other linear problems for these hierarchies. We

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give the important result that there exist gauge transformations which map the linear problems for these P_{II} and P_{IV} hierarchies onto two new sequences of linear problems, whose first members are the linear problems of P_{II} and P_{IV} given by Jimbo and Miwa.[3]

II. A SECOND PAINLEVÉ HIERARCHY

One of the hierarchies of ODEs obtained in Ref. 8, as a reduction of a (2+1)-dimensional nonisospectral hierarchy, can be expressed as

$$\mathcal{R}^n \mathbf{u}_x + \sum_{i=0}^{n-2} c_i \mathcal{R}^i \mathbf{u}_x + g_{n+1} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad n \geqslant 1, \tag{1}$$

where $g_{n+1}(\neq 0)$ and each of the c_i are constants. Here $\mathbf{u}=(u(x),v(x))^T$ and $\mathcal{R}$ is the recursion operator of the dispersive water wave hierarchy as given in Ref. 10,

$$\mathcal{R} = \frac{1}{2} \begin{pmatrix} \partial_x u \partial_x^{-1} - \partial_x & 2 \\ 2v + v_x \partial_x^{-1} & u + \partial_x \end{pmatrix}. \tag{2}$$

In Ref. 8, we also gave the following matrix linear problem for the hierarchy (1):

$$\boldsymbol{\Psi}_x = F \boldsymbol{\Psi}, \tag{3}$$

$$\left(\frac{1}{2} g_{n+1} \right) \boldsymbol{\Psi}_\lambda = H_n \boldsymbol{\Psi} = \left[\left(\lambda^n + \sum_{i=0}^{n-2} c_i \lambda^i \right) F + G_n + \sum_{i=1}^{n-2} c_i G_i \right] \boldsymbol{\Psi}, \tag{4}$$

where $\boldsymbol{\Psi}=(\psi_1,\psi_2)^T$ and the matrices F and G_i are given by

$$F = \begin{pmatrix} -\frac{1}{2}(2\lambda - u) & 1 \\ -v & \frac{1}{2}(2\lambda - u) \end{pmatrix}, \tag{5}$$

$$G_n = \begin{pmatrix} -\frac{1}{4}((2\lambda - u)P_n + P_{n,x}) & \frac{1}{2}P_n \\ \frac{1}{2}g_{n+1} + \frac{1}{2}\lambda^n u_x - \frac{1}{2}M_n & \frac{1}{4}((2\lambda - u)P_n + P_{n,x}) \\ -\frac{1}{4}((2\lambda - u)P_n + P_{n,x})_x - \frac{1}{2}vP_n & \end{pmatrix}, \tag{6}$$

and, for $i<n$,

$$G_i = \begin{pmatrix} -\frac{1}{4}((2\lambda - u)P_i + P_{i,x}) & \frac{1}{2}P_i \\ \frac{1}{2}\lambda^i u_x - \frac{1}{2}M_i & \frac{1}{4}((2\lambda - u)P_i + P_{i,x}) \\ -\frac{1}{4}((2\lambda - u)P_i + P_{i,x})_x - \frac{1}{2}vP_i & \end{pmatrix}. \tag{7}$$

In the above, M_i and P_i are given, respectively, by

$$\begin{pmatrix} M_n \\ N_n \end{pmatrix} = \mathcal{R}^n \mathbf{u}_x + g_{n+1} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{8}$$

$$\begin{pmatrix} M_i \\ N_i \end{pmatrix} = \mathcal{R}^i \mathbf{u}_x, \quad \text{for } i < n, \tag{9}$$

and

$$P_i = \partial_x^{-1} \sum_{j=0}^{i-1} \lambda^{i-1-j} M_j. \tag{10}$$

The compatibility condition of the matrix linear problem (3), (4) is Eq. (1).

Since each member of the dispersive water wave hierarchy is in conservation form, each component of our hierarchy (1) integrates immediately to give

$$\begin{pmatrix} \tilde{M}_n \\ \tilde{N}_n \end{pmatrix} \equiv \begin{pmatrix} \partial_x^{-1} & 0 \\ 0 & \partial_x^{-1} \end{pmatrix} \left[\mathcal{R}^n \mathbf{u}_x + \sum_{i=0}^{n-2} c_i \mathcal{R}^i \mathbf{u}_x \right] + \begin{pmatrix} g_{n+1} x \\ -\delta_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{11}$$

where δ_n is one of the constants of integration; our assumption that $g_{n+1} \neq 0$ allows us to set the second constant of integration to zero without loss of generality. It is this hierarchy that is our P_{II} hierarchy; as we shall see, in the case $n=1$, this system of equations yields P_{II} itself. We note, however, that higher order members of this hierarchy are different from those of the P_{II} hierarchy presented in Refs. 9 and 1.

It is a simple matter to write down a linear problem whose compatibility condition gives the hierarchy (11) directly; this is given by the pair of equations

$$\boldsymbol{\Psi}_x = F \boldsymbol{\Psi}, \tag{12}$$

$$\boldsymbol{\Psi}_\lambda = K_n \boldsymbol{\Psi}, \tag{13}$$

where

$$K_n = \frac{1}{g_{n+1}} \left[2H_n + \begin{pmatrix} -\tilde{M}_n & 0 \\ 2\tilde{N}_n & \tilde{M}_n \end{pmatrix} \right] = \begin{pmatrix} (K_n)_{11} & (K_n)_{12} \\ (K_n)_{21} & (K_n)_{22} \end{pmatrix}. \tag{14}$$

Here we have added to H_n in the linear equation (4) a matrix whose entries (being the integrated equations themselves) are identically zero. This matrix is obtained by taking into account the dependence of H_n on the higher order derivatives u_{nx} and v_{nx}, as well as that of $\tilde{M}_n$ and $\tilde{N}_n$ on these derivatives: $\tilde{M}_n \sim (-\frac{1}{2})^n u_{nx}$, $\tilde{N}_n \sim (\frac{1}{2})^n v_{nx}$. The addition of this matrix to H_n in (4) is equivalent to substituting higher order derivatives in H_n in order to obtain as compatibility condition the integrated hierarchy (11) rather than the original hierarchy (1). The compatibility condition of the linear problem (12), (13) is

$$F_\lambda - K_{n,x} + [F, K_n] = R_1 \lambda + R_0 = 0, \tag{15}$$

where

$$(R_1)_{21} = \frac{4}{g_{n+1}} \tilde{N}_n, \quad (R_0)_{12} = \frac{2}{g_{n+1}} \tilde{M}_n, \tag{16}$$

all other $(R_1)_{ij}=0$, and all other $(R_0)_{ij}=0$ modulo $\tilde{M}_n=0$, $\tilde{N}_n=0$.

A. The relationship with the Jimbo-Miwa linear problem for the second Painlevé equation

Let us consider the linear problem for the hierarchy (11) given by the system of equations (12) and (13), where F and K_n are as above. We now consider the gauge transformation

$$\mathbf{\Psi} = M\mathbf{\Phi}, \tag{17}$$

where the matrix M is given by

$$M = \begin{pmatrix} e^{(1/2)s(x)} & 0 \\ 0 & e^{-(1/2)s(x)} \end{pmatrix}, \tag{18}$$

and where $s_x = u$. This maps the linear system (12) and (13) onto

$$\mathbf{\Phi}_x = A\mathbf{\Phi}, \tag{19}$$

$$\mathbf{\Phi}_\lambda = B_n\mathbf{\Phi}, \tag{20}$$

where (noting that $M_\lambda = 0$)

$$A = M^{-1}FM - M^{-1}M_x = \begin{pmatrix} -\lambda & \frac{w}{2} \\ -2\frac{v}{w} & \lambda \end{pmatrix}, \tag{21}$$

$$B_n = M^{-1}K_nM = \begin{pmatrix} (K_n)_{11} & \frac{w}{2}(K_n)_{12} \\ \frac{2}{w}(K_n)_{21} & (K_n)_{22} \end{pmatrix}, \tag{22}$$

and where we have introduced the auxiliary function $w = w(x)$ defined by $w = 2e^{-s}$, and which therefore satisfies the relation $w_x/w = -u$.

Thus we obtain a different sequence of linear problems (19), (20) for the P_{II} hierarchy (11): the first of these is, up to a trivial change of variables (see the next section), the linear problem for P_{II} given by Jimbo and Miwa.[3] We thus obtain the result that the P_{II} hierarchy obtained in Ref. 8 could also have been obtained by expanding in powers of λ (or $\mu = -2\lambda$; again, see the next section) in the Jimbo-Miwa linear problem for P_{II}, i.e., by using an Ablowitz-Kaup-Newell-Segur (AKNS) type approach[11] therein. We now illustrate this remark with some examples.

B. Examples

1. Example n=1

For the case $n = 1$ of the hierarchy (11) we have the system of equations

$$v + \tfrac{1}{2}(u^2 - u_x) + g_2 x = 0, \tag{23}$$

$$uv + \tfrac{1}{2}v_x - \delta_1 = 0. \tag{24}$$

This system is equivalent to the second order ODE,

$$u_{xx} = 2u^3 + 4g_2xu + 2(g_2 + 2\delta_1), \tag{25}$$

which for $g_2 \neq 0$ is just the second Painlevé equation P_{II}. We have the corresponding linear problem given by Eqs. (12) and (13), where

$$F = \begin{pmatrix} -\lambda + \frac{1}{2}u & 1 \\ -v & \lambda - \frac{1}{2}u \end{pmatrix}, \tag{26}$$

$$K_1 = \frac{1}{g_2}\sum_{j=0}^{2} K_{1,j}\lambda^j, \tag{27}$$

and where the matrices $K_{1,j}$ are given by

$$K_{1,2} = 2\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad K_{1,1} = 2\begin{pmatrix} 0 & 1 \\ -v & 0 \end{pmatrix}, \quad K_{1,0} = \begin{pmatrix} -v - g_2 x & u \\ uv - 2\delta_1 & v + g_2 x \end{pmatrix}. \tag{28}$$

After the gauge transformation (17) we obtain the linear problem (19), (20) with

$$A = \begin{pmatrix} -\lambda & \frac{w}{2} \\ -2\frac{v}{w} & \lambda \end{pmatrix}, \tag{29}$$

$$B_1 = \frac{1}{g_2}\sum_{j=0}^{2} B_{1,j}\lambda^j, \tag{30}$$

where each $B_{1,j} = M^{-1}K_{1,j}M$, and where w satisfies $w_x/w = -u$. This transformation leads to the introduction of factors $(w/2)$ and $(2/w)$ in the off-diagonal elements of the matrix B_1, as in (22).

If in the linear system (19), (20), with A and B_1 given as above, we set $\lambda = -(\mu/2)$, $v = z/2$, $g_2 = 1/4$, $u = y$ and $4\delta_1 = \alpha - \frac{1}{2}$, then we obtain the linear system for P_{II} as given by Jimbo and Miwa,[3] i.e.,

$$\mathbf{\Phi}_x = \tilde{A}\mathbf{\Phi}, \tag{31}$$

$$\mathbf{\Phi}_\mu = \tilde{B}_1\mathbf{\Phi} \tag{32}$$

with

$$\tilde{A} = \frac{1}{2}\begin{pmatrix} \mu & w \\ -2\frac{z}{w} & -\mu \end{pmatrix}, \tag{33}$$

$$\tilde{B}_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\mu^2 + \begin{pmatrix} 0 & w \\ -2\frac{z}{w} & 0 \end{pmatrix}\mu + \begin{pmatrix} z + \frac{1}{2}x & -wy \\ \frac{2\alpha - 1 - 2zy}{w} & -z - \frac{1}{2}x \end{pmatrix}. \tag{34}$$

The compatibility condition of the latter gives $w_x = -yw$ and, after elimination of w, the system of equations

$$z_x = -2yz + \alpha - \tfrac{1}{2}, \tag{35}$$

$$y_x = y^2 + z + \frac{x}{2}. \tag{36}$$

These two equations imply that y satisfies P_{II}:

$$y_{xx} = 2y^3 + xy + \alpha. \tag{37}$$

2. Example n=2

In the case $n=2$ of the hierarchy (11) we have the system of equations

$$\frac{1}{4}(u_{xx} - 3uu_x + u^3 + 6uv) + c_0 u + g_3 x = 0, \tag{38}$$

$$\frac{1}{4}(v_{xx} + 3v^2 + 3uv_x + 3u^2 v) + c_0 v - \delta_2 = 0. \tag{39}$$

This system arises as the compatibility condition of the linear problem (12), (13) where F is given by (26) and K_2 by

$$K_2 = \frac{1}{g_3}\sum_{j=0}^{3} K_{2,j}\lambda^j, \tag{40}$$

where the matrices $K_{2,j}$ are as follows:

$$K_{2,3} = 2\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{41}$$

$$K_{2,2} = 2\begin{pmatrix} 0 & 1 \\ -v & 0 \end{pmatrix}, \tag{42}$$

$$K_{2,1} = \begin{pmatrix} -v - 2c_0 & u \\ -v_x - uv & v + 2c_0 \end{pmatrix}, \tag{43}$$

$$K_{2,0} = \begin{pmatrix} -\frac{1}{2}v_x - uv - g_3 x & \frac{1}{2}(u^2 - u_x) + v + 2c_0 \\ \frac{1}{2}(v^2 + uv_x - u_x v) + u^2 v - 2\delta_2 & \frac{1}{2}v_x + uv + g_3 x \end{pmatrix}. \tag{44}$$

After the gauge transformation (17) we obtain the linear problem (19), (20) with

$$A = \begin{pmatrix} -\lambda & \frac{w}{2} \\ -2\frac{v}{w} & \lambda \end{pmatrix}, \tag{45}$$

$$B_2 = \frac{1}{g_3}\sum_{j=0}^{3} B_{2,j}\lambda^j, \tag{46}$$

where as before each $B_{2,j} = M^{-1}K_{2,j}M$. We note that this particular member of our P_{II} hierarchy was also obtained by Kitaev[12] (see the Appendix).

3. Example n=3

In the case $n=3$ the system of equations (11) is

$$\frac{1}{8}(-u_{xxx}+6v^2+2v_{xx}+4uu_{xx}-6vu_x-6u^2u_x+3u_x^2+12u^2v+u^4)+c_1\left(v+\frac{1}{2}u^2-\frac{1}{2}u_x\right)+c_0u+g_4x=0, \tag{47}$$

$$\frac{1}{8}(v_{xxx}+6vv_x+2vu_{xx}+2u_xv_x+12v^2u+4u^3v+6u^2v_x+4uv_{xx})+c_1\left(uv+\frac{1}{2}v_x\right)+c_0v-\delta_3=0. \tag{48}$$

This system arises as the compatibility condition of the linear problem (12), (13), where F is given by (26) and K_3 by

$$K_3=\frac{1}{g_4}\sum_{j=0}^{4}K_{3,j}\lambda^j, \tag{49}$$

and where the matrices $K_{3,j}$ are

$$K_{3,4}=2\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}, \tag{50}$$

$$K_{3,3}=2\begin{pmatrix}0 & 1\\ -v & 0\end{pmatrix}, \tag{51}$$

$$K_{3,2}=\begin{pmatrix}-v-2c_1 & u\\ -v_x-uv & v+2c_1\end{pmatrix}, \tag{52}$$

$$K_{3,1}=\begin{pmatrix}-\frac{1}{2}v_x-uv-2c_0 & \frac{1}{2}(u^2-u_x)+v+2c_1\\ -\frac{1}{2}(v_{xx}+2v^2+u^2v+2uv_x+u_xv) & \frac{1}{2}v_x+uv+2c_0\\ -2c_1v & \end{pmatrix}, \tag{53}$$

$$K_{3,0}=\begin{pmatrix}-\frac{1}{4}(v_{xx}+3v^2+3u^2v+3uv_x) & \frac{1}{4}(u_{xx}-3uu_x+6uv+u^3)\\ -c_1v-g_4x & +c_1u+2c_0\\ \frac{1}{4}(vu_{xx}+uv_{xx}+3u^2v_x-3uvu_x & \frac{1}{4}(v_{xx}+3v^2+3u^2v+3uv_x)\\ -u_xv_x+3u^3v+6uv^2) & +c_1v+g_4x\\ +c_1uv-2\delta_3 & \end{pmatrix}. \tag{54}$$

Again, after the gauge transformation (17) we obtain the linear problem (19), (20) with

$$A=\begin{pmatrix}-\lambda & \frac{w}{2}\\ -2\frac{v}{w} & \lambda\end{pmatrix}, \tag{55}$$

$$B_3 = \frac{1}{g_4}\sum_{j=0}^{4} B_{2,j}\lambda^j, \tag{56}$$

and where as before $B_{3,j}=M^{-1}K_{3,j}M$.

III. A FOURTH PAINLEVÉ HIERARCHY

We now consider the P_{IV} hierarchy which, together with its linear problem, we introduced in Ref. 8. Without any loss of generality we assume that our P_{IV} hierarchy is of the form

$$\mathcal{R}^n \mathbf{u}_x + \sum_{i=1}^{n-1} c_i \mathcal{R}^i \mathbf{u}_x + g_n \mathcal{R}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}, \quad n \geqslant 1, \tag{57}$$

where again $g_n(\neq 0)$ and c_i are constants, and where $\mathcal{R}$ is the recursion operator of the dispersive water wave hierarchy (2). Bäcklund transformations for this hierarchy have been given in Ref. 13. We also note that a detailed singularity analysis of the case $n=2$, which presented certain difficulties, was undertaken in Ref. 14. Here we concentrate on the linear problem for (57), whose matrix form is[8]

$$\mathbf{\Psi}_x = F\mathbf{\Psi}, \tag{58}$$

$$\left(\frac{1}{2}\lambda g_n\right)\mathbf{\Psi}_\lambda = H_n\mathbf{\Psi} = \left[\left(\lambda^n + \sum_{i=1}^{n-1} c_i\lambda^i\right)F + G_n + \sum_{i=1}^{n-1} c_i G_i\right]\mathbf{\Psi}, \tag{59}$$

where $\mathbf{\Psi}=(\psi_1,\psi_2)^T$ and the matrices F, G_n, and G_i for $i<n$, are given by

$$F = \begin{pmatrix} -\frac{1}{2}(2\lambda - u) & 1 \\ -v & \frac{1}{2}(2\lambda - u) \end{pmatrix}, \tag{60}$$

$$G_n = \begin{pmatrix} -\frac{1}{4}((2\lambda-u)P_n + P_{n,x}) & \frac{1}{2}P_n \\ \frac{1}{2}\lambda g_n + \frac{1}{2}\lambda^n u_x - \frac{1}{2}M_n & \frac{1}{4}((2\lambda-u)P_n + P_{n,x}) \\ -\frac{1}{4}((2\lambda-u)P_n + P_{n,x})_x - \frac{1}{2}vP_n & \end{pmatrix}, \tag{61}$$

where

$$\begin{pmatrix}M_n\\N_n\end{pmatrix} = \mathcal{R}^n\mathbf{u}_x + g_n\mathcal{R}\begin{pmatrix}1\\0\end{pmatrix}, \tag{62}$$

$$\begin{pmatrix}M_{n-1}\\N_{n-1}\end{pmatrix} = \mathcal{R}^{n-1}\mathbf{u}_x + g_n\begin{pmatrix}1\\0\end{pmatrix}, \tag{63}$$

$$\begin{pmatrix}M_j\\N_j\end{pmatrix} = \mathcal{R}^j\mathbf{u}_x, \quad \text{for } j < n-1, \tag{64}$$

and

$$P_n = \partial_x^{-1} \sum_{j=0}^{n-1} \lambda^{n-1-j} M_j; \tag{65}$$

and (for $i < n$)

$$G_i = \begin{pmatrix} -\frac{1}{4}((2\lambda - u)P_i + P_{i,x}) & \frac{1}{2}P_i \\ \frac{1}{2}\lambda^i u_x - \frac{1}{2}\widehat{M}_i & \frac{1}{4}((2\lambda - u)P_i + P_{i,x}) \\ -\frac{1}{4}((2\lambda - u)P_i + P_{i,x})_x - \frac{1}{2}vP_i & \end{pmatrix}, \tag{66}$$

where

$$\begin{pmatrix} \widehat{M}_i \\ \widehat{N}_i \end{pmatrix} = \mathcal{R}^i \mathbf{u}_x \tag{67}$$

and now

$$P_i = \partial_x^{-1} \sum_{j=0}^{i-1} \lambda^{i-1-j} \widehat{M}_j. \tag{68}$$

The compatibility condition of the matrix linear problem (58), (59) is Eq. (57).

Again, as in the case of the P_{II} hierarchy discussed in Sec. II, this hierarchy (57) can be integrated. The integrated version of this hierarchy was presented in Ref. 8 and its derivation was given in Ref. 15. A general statement of this integration process can be found in Ref. 16. The integrated form of (57), or equivalently of

$$B_2 \mathbf{K}_n[\mathbf{u}] = 0, \quad B_2 = \frac{1}{2}\begin{pmatrix} 2\partial_x & \partial_x u - \partial_x^2 \\ u\partial_x + \partial_x^2 & v\partial_x + \partial_x v \end{pmatrix}, \tag{69}$$

where

$$\mathbf{K}_n[\mathbf{u}] = \begin{pmatrix} K_n \\ L_n \end{pmatrix} = \mathbf{L}_n[\mathbf{u}] + \sum_{i=1}^{n-1} c_i \mathbf{L}_i[\mathbf{u}] + g_n \begin{pmatrix} 0 \\ x \end{pmatrix}, \tag{70}$$

is

$$\widetilde{M}_n \equiv L_{n,x} - 2K_n - uL_n - (g_n - 2\alpha_n) = 0, \tag{71}$$

$$\widetilde{N}_n \equiv K_{n,x} - \frac{\left(K_n + \frac{1}{2}g_n - \alpha_n\right)^2 - \frac{1}{4}\beta_n^2}{L_n} + vL_n = 0, \tag{72}$$

α_n and β_n^2 being the two arbitrary constants of integration.

A matrix linear problem whose compatibility condition is precisely the integrated hierarchy (71), (72) can easily be given. This can be done, in the same way as for the P_{II} hierarchy, by adding to H_n in the linear equation (59) a matrix whose entries (being the integrated equations themselves) are identically zero. This matrix is obtained by taking into account the dependence of H_n on the higher order derivatives u_{nx} and v_{nx}, as well as that of $\widetilde{M}_n$ and $\widetilde{N}_n$ on these derivatives: $\widetilde{M}_n \sim \left(-\frac{1}{2}\right)^{n-1} u_{nx}$, $\widetilde{N}_n \sim \left(\frac{1}{2}\right)^{n-1} v_{nx}$. We thus obtain the linear problem

$$\mathbf{\Psi}_x = F\mathbf{\Psi}, \tag{73}$$

$$\mathbf{\Psi}_\lambda = K_n\mathbf{\Psi}, \tag{74}$$

where the matrix K_n is given by

$$K_n = \frac{1}{\lambda g_n}\left[2H_n + \begin{pmatrix} \frac{1}{2}\tilde{M}_n & 0 \\ \tilde{N}_n & -\frac{1}{2}\tilde{M}_n \end{pmatrix}\right] = \begin{pmatrix} (K_n)_{11} & (K_n)_{12} \\ (K_n)_{21} & (K_n)_{22} \end{pmatrix}. \tag{75}$$

The compatibility condition of the linear problem (73), (74) is the integrated hierarchy (71), (72):

$$F_\lambda - K_{n,x} + [F,K_n] = S_0 + \frac{1}{\lambda}S_{-1} = 0, \tag{76}$$

where

$$(S_0)_{21} = \frac{2}{g_n}\tilde{N}_n, \quad (S_{-1})_{12} = -\frac{1}{g_n}\tilde{M}_n, \tag{77}$$

all other $(S_0)_{ij}=0$, and all other $(S_{-1})_{ij}=0$ modulo $\tilde{M}_n=0$, $\tilde{N}_n=0$.

A. The relationship with the Jimbo-Miwa linear problem for the fourth Painlevé equation

As for the P_{II} hierarchy discussed in Sec. II, we now consider a gauge transformation of the linear problem (73), (74): we set

$$\mathbf{\Psi} = M\mathbf{\Phi}, \tag{78}$$

where as before

$$M = \begin{pmatrix} e^{(1/2)s(x)} & 0 \\ 0 & e^{-(1/2)s(x)} \end{pmatrix} \tag{79}$$

and $s_x=u$. The linear system (73), (74) is then mapped to

$$\mathbf{\Phi}_x = A\mathbf{\Phi}, \tag{80}$$

$$\mathbf{\Phi}_\lambda = B_n\mathbf{\Phi}, \tag{81}$$

where A and B_n are now

$$A = M^{-1}FM - M^{-1}M_x = \begin{pmatrix} -\lambda & w \\ -\frac{v}{w} & \lambda \end{pmatrix}, \tag{82}$$

$$B_n = M^{-1}K_nM = \begin{pmatrix} (K_n)_{11} & w(K_n)_{12} \\ \frac{1}{w}(K_n)_{21} & (K_n)_{22} \end{pmatrix}, \tag{83}$$

and where we have introduced the auxiliary function $w=w(x)$ defined—differently from in Sec. II—by $w=e^{-s}$, and which therefore satisfies the relation $w_x/w=-u$.

We now consider some examples. In particular we will see how, using the above gauge transformation, the linear problem for the first nontrivial flow of our hierarchy is mapped onto the

linear problem for P_{IV} given by Jimbo and Miwa.[3] This then means that our P_{IV} hierarchy (71), (72) could alternatively have been obtained using an AKNS type approach in the Jimbo-Miwa linear problem for P_{IV}.

B. Examples

1. Example n=1

The first nontrivial flow of the hierarchy (71), (72) consists of the pair of equations

$$u_x = 2v + u^2 + g_1 x u - 2\alpha_1, \tag{84}$$

$$v_x = \frac{\left[v - \alpha_1 + \frac{1}{2}g_1\right]^2 - \frac{1}{4}\beta_1^2}{(u + g_1 x)} - v(u + g_1 x), \tag{85}$$

where α_1 and β_1 are two independent constants of integration. Eliminating v between these equations and performing the change of variables

$$u = y - g_1 x, \tag{86}$$

we obtain

$$y_{xx} = \frac{1}{2}\frac{y_x^2}{y} + \frac{3}{2}y^3 - 2g_1 x y^2 + 2[(g_1^2 x^2/4) - \alpha_1]y - \frac{1}{2}\frac{\beta_1^2}{y}. \tag{87}$$

Setting $g_1 = -2$, which can be done without loss of generality for $g_1 \neq 0$, gives

$$y_{xx} = \frac{1}{2}\frac{y_x^2}{y} + \frac{3}{2}y^3 + 4xy^2 + 2(x^2 - \alpha_1)y - \frac{1}{2}\frac{\beta_1^2}{y}, \tag{88}$$

i.e., P_{IV}. Corresponding to the system (84), (85) we have the linear problem given by Eqs. (73), (74) where

$$F = \begin{pmatrix} -\lambda + \frac{1}{2}u & 1 \\ -v & \lambda - \frac{1}{2}u \end{pmatrix}, \tag{89}$$

$$K_1 = \frac{1}{g_1}\sum_{j=-1}^{1} K_{1,j}\lambda^j, \tag{90}$$

with $K_{1,j}$ given by

$$K_{1,1} = 2\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{91}$$

$$K_{1,0} = \begin{pmatrix} -g_1 x & 2 \\ -2v & g_1 x \end{pmatrix}, \tag{92}$$

$$K_{1,-1}=\begin{pmatrix} -v-\frac{1}{2}g_1+\alpha_1 & u+g_1x \\ -\dfrac{\left[v-\alpha_1+\frac{1}{2}g_1\right]^2-\frac{1}{4}\beta_1^2}{(u+g_1x)} & v+\frac{1}{2}g_1-\alpha_1 \end{pmatrix}. \tag{93}$$

Our gauge transformation then yields the alternative linear problem (80), (81) with

$$A=\begin{pmatrix} -\lambda & w \\ -\dfrac{v}{w} & \lambda \end{pmatrix}, \tag{94}$$

$$B_1=\frac{1}{g_1}\sum_{j=-1}^{1} B_{1,j}\lambda^j, \tag{95}$$

where w satisfies $\frac{w_x}{w}=-u$ and each $B_{1,j}=M^{-1}K_{1,j}M$. This transformation leads to the introduction of factors w and $(1/w)$ in the off-diagonal elements of the matrix B_1, as in (83).

If in the linear system (80), (81), with A and B_1 given as above, we set $\lambda=-\mu$ and choose $g_1=-2$, make the transformation

$$u=y+2x, \tag{96}$$

$$v=-2z+2(\theta_0+\theta_\infty), \tag{97}$$

and redefine the parameters α_1 and β_1 as

$$\alpha_1=2\theta_\infty-1, \tag{98}$$

$$\beta_1^2=16\theta_0^2, \tag{99}$$

we obtain the linear problem

$$\mathbf{\Phi}_x=\widetilde{A}\mathbf{\Phi}, \tag{100}$$

$$\mathbf{\Phi}_\mu=\widetilde{B}_1\mathbf{\Phi}, \tag{101}$$

where

$$\widetilde{A}=\begin{pmatrix} \mu & w \\ \dfrac{2(z-\theta_0-\theta_\infty)}{w} & -\mu \end{pmatrix}, \tag{102}$$

$$\widetilde{B}_1=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\mu+\begin{pmatrix} x & w \\ \dfrac{2(z-\theta_0-\theta_\infty)}{w} & -x \end{pmatrix}+\begin{pmatrix} -z+\theta_0 & -\frac{1}{2}wy \\ \dfrac{2z(z-2\theta_0)}{wy} & z-\theta_0 \end{pmatrix}\frac{1}{\mu}, \tag{103}$$

and where we now have the relation $w_x/w=-y-2x$. The compatibility condition of this linear problem gives this last relation and, after elimination of w, the system of equations

$$z_x = -\frac{2}{y}z^2 - yz + \frac{4\theta_0}{y}z + (\theta_0 + \theta_\infty)y, \tag{104}$$

$$y_x = -4z + y^2 + 2xy + 4\theta_0, \tag{105}$$

which is of course equivalent to P_{IV}. The above linear problem is the linear problem for P_{IV} given by Jimbo and Miwa in Ref. 3.

2. Example n=2

As a further example we give here the results for the second member of our P_{IV} hierarchy (71), (72),

$$u_{xx} = 3uu_x - u^3 - 6uv - 2g_2xu + 2c_1(u_x - 2v - u^2) + 4\alpha_2, \tag{106}$$

$$v_{xx} = 2\left(\frac{\left[uv + \frac{1}{2}v_x + c_1v - \alpha_2 + \frac{1}{2}g_2\right]^2 - \frac{1}{4}\beta_2^2}{v + \frac{1}{2}u^2 - \frac{1}{2}u_x + g_2x + c_1u}\right) - 2(uv)_x - 2v\left(v + \frac{1}{2}u^2 - \frac{1}{2}u_x + g_2x\right) - 2c_1(v_x + uv), \tag{107}$$

where α_2 and β_2 are two independent constants of integration.

Corresponding to the system (106), (107) we have the linear problem given by Eqs. (73), (74) where

$$F = \begin{pmatrix} -\lambda + \frac{1}{2}u & 1 \\ -v & \lambda - \frac{1}{2}u \end{pmatrix}, \tag{108}$$

$$K_2 = \frac{1}{g_2}\sum_{j=-1}^{2} K_{2,j}\lambda^j, \tag{109}$$

with $K_{2,j}$ given by

$$K_{2,2} = 2\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{110}$$

$$K_{2,1} = \begin{pmatrix} -2c_1 & 2 \\ -2v & 2c_1 \end{pmatrix}, \tag{111}$$

$$K_{2,0} = \begin{pmatrix} -v - g_2x & u + 2c_1 \\ -v_x - uv - 2c_1v & v + g_2x \end{pmatrix}, \tag{112}$$

$$K_{2,-1}=\begin{pmatrix} -\frac{1}{2}(2uv+v_x) & \frac{1}{2}(2v+u^2-u_x) \\ -c_1v-\frac{1}{2}g_2+\alpha_2 & +c_1u+g_2x \\ -\dfrac{\left[uv+\frac{1}{2}v_x+c_1v-\alpha_2+\frac{1}{2}g_2\right]^2-\frac{1}{4}\beta_2^2}{v+\frac{1}{2}u^2-\frac{1}{2}u_x+g_2x+c_1u} & \frac{1}{2}(2uv+v_x) \\ & +c_1v+\frac{1}{2}g_2-\alpha_2 \end{pmatrix}. \tag{113}$$

Our gauge transformation then yields the alternative linear problem (80), (81), with

$$A=\begin{pmatrix} -\lambda & w \\ -\dfrac{v}{w} & \lambda \end{pmatrix}, \tag{114}$$

$$B_2=\frac{1}{g_2}\sum_{j=-1}^{2}B_{2,j}\lambda^j, \tag{115}$$

where w satisfies $w_x/w=-u$ and where each $B_{2,j}=M^{-1}K_{2,j}M$.

IV. CONCLUSIONS

We have studied in detail the P_{II} and P_{IV} hierarchies derived in Ref. 8. We have shown that the corresponding linear problems can be mapped on to alternative linear problems such that those for the first members of our hierarchies (i.e., for P_{II} and P_{IV} themselves) are precisely the linear problems given by Jimbo and Miwa.[3] This then means that our hierarchies could alternatively have been obtained by using an AKNS type approach, i.e., expanding in powers of λ, in the Jimbo-Miwa linear problems for P_{II} and P_{IV}. Our work here then raises the interesting problem of whether other Jimbo-Miwa linear problems can be used to obtain hierarchies based on Painlevé equations. This is a topic that we will pursue in subsequent studies.

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APPENDIX

In this Appendix we briefly consider the linear problems for P_{II} given in Refs. 1 and 3,

$$\mathbf{\Phi}_t=\mathcal{U}\mathbf{\Phi}, \quad \mathbf{\Phi}_\xi=\mathcal{V}\mathbf{\Phi}, \tag{A1}$$

which we take here in the forms presented in Ref. 17, i.e., respectively in the form of Ref. 1 with

$$\mathcal{U}=\begin{pmatrix} -i\xi & ip \\ -ip & i\xi \end{pmatrix}, \tag{A2}$$

$$\mathcal{V}=\begin{pmatrix} -i(4\xi^2+t+2p^2) & i(4p\xi-\beta/\xi)-2p_t \\ -i(4p\xi-\beta/\xi)-2p_t & i(4\xi^2+t+2p^2) \end{pmatrix}, \tag{A3}$$

or, corresponding to Ref. 3, with

$$\mathcal{U}=\begin{pmatrix} -i\xi & iq \\ -ir & i\xi \end{pmatrix}, \tag{A4}$$

$$\mathcal{V}=\begin{pmatrix} -i(4\xi^2+t+2qr) & 4iq\xi-2q_t \\ -4ir\xi-2r_t & i(4\xi^2+t+2qr) \end{pmatrix}. \tag{A5}$$

The compatibility condition of each of these linear problems yields P_{II} (in the case of (A4), (A5) after integrating twice). The linear problem (A1) with (A4), (A5) is put into standard Jimbo-Miwa form (31)–(34) by making the change of variables

$$q=-\frac{1}{2}i\gamma w, \quad r=-i\gamma\frac{z}{w}, \quad t=\frac{x}{\gamma}, \quad \xi=\frac{1}{2}i\gamma\mu, \tag{A6}$$

and using the relations

$$q_t=\frac{1}{2}i\gamma^2 wy, \quad r_t=-i\gamma^2\left(\frac{\alpha-(1/2)-zy}{w}\right), \tag{A7}$$

where $\gamma^3=-2$. This identification means that our P_{II} hierarchy described in Sec. II could also have been derived beginning with an AKNS type linear problem, which then explains why Kitaev obtained the second member of our hierarchy when seeking to isolate examples of higher order ODEs related to such a linear problem.[12]

It is argued in Ref. 17 that there is no elementary relation between the linear problems given by (A1) with (A2), (A3), and (A1) with (A4), (A5); for example, there is no gauge transformation mapping one into the other. However, while there is no known gauge transformation, we give a general linear problem which encapsulates both Lax pairs. Consider the linear problem (A1) with

$$\mathcal{U}=\begin{pmatrix} -i\xi & iq \\ -ir & i\xi \end{pmatrix}, \tag{A8}$$

$$\mathcal{V}=\begin{pmatrix} -i(4\xi^2+t+2qr) & i(4q\xi-\beta/\xi)-2q_t \\ -i(4r\xi-\beta/\xi)-2r_t & i(4\xi^2+t+2qr) \end{pmatrix}. \tag{A9}$$

The compatibility condition of this linear problem yields the three equations

$$q_{tt}=2q^2r+tq+\beta, \tag{A10}$$

$$r_{tt}=2qr^2+tr+\beta, \tag{A11}$$

$$\beta(q-r)=0, \tag{A12}$$

the third of which tells us that we must either have $q=r$ or $\beta=0$, corresponding to the choices (A2), (A3) and (A4), (A5), respectively. That is, the linear problems with (A2), (A3) and (A4), (A5) are in fact both special cases of (A8), (A9).

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Whitham systems and deformations

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We consider the deformations of Whitham systems including the "dispersion terms" and having the form of Dubrovin-Zhang deformations of Frobenius manifolds. The procedure is connected with the B. A. Dubrovin problem of deformations of Frobenius manifolds corresponding to the Whitham systems of integrable hierarchies. Under some nondegeneracy requirements we suggest a general scheme of the deformation of the hyperbolic Whitham systems using the initial nonlinear system. The general form of the deformed Whitham system coincides with the form of the "low-dispersion" asymptotic expansions used by B. A. Dubrovin and Y. Zhang in the theory of deformations of Frobenius manifolds. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217648]

I. INTRODUCTION

The classical Whitham method[1–4] is connected with the slow modulations of the exact periodic or quasiperiodic solutions of nonlinear PDE's,

$$F^i(\boldsymbol{\varphi},\boldsymbol{\varphi}_t,\boldsymbol{\varphi}_x,\boldsymbol{\varphi}_{tt},\boldsymbol{\varphi}_{xt},\boldsymbol{\varphi}_{xx},\dots)=0,\quad i=1,\dots,n, \tag{1.1}$$

where $\boldsymbol{\varphi}=(\varphi^1,\dots,\varphi^n)$.

It is assumed that the system (1.1) admits the finite-parametric family of exact solutions

$$\varphi^i(x,t)=\boldsymbol{\Phi}^i(\mathbf{k}(\mathbf{U})x+\boldsymbol{\omega}(\mathbf{U})t+\boldsymbol{\theta}_0,\mathbf{U}), \tag{1.2}$$

where $\boldsymbol{\theta}=(\theta^1,\dots,\theta^n)$, $\Phi^i(\boldsymbol{\theta},\mathbf{U})$ are smooth functions 2π-periodic with respect to each θ^α, $\mathbf{k}(\mathbf{U})=(k^1(\mathbf{U}),\dots,k^m(\mathbf{U}))$, $\boldsymbol{\omega}(\mathbf{U})=(\omega^1(\mathbf{U}),\dots,\omega^m(\mathbf{U}))$ are "wave numbers" and "frequencies" of the solution, $\mathbf{U}=(U^1,\dots,U^N)$ are parameters of the solution, and $\boldsymbol{\theta}_0=(\theta_0^1,\dots,\theta_0^m)$ are arbitrary initial phases.

The functions $\boldsymbol{\Phi}(\boldsymbol{\theta},\mathbf{U})$ satisfy the nonlinear system

$$F^i(\boldsymbol{\Phi},\omega^\alpha(\mathbf{U})\boldsymbol{\Phi}_{\theta^\alpha},k^\beta(\mathbf{U})\boldsymbol{\Phi}_{\theta^\beta},\omega^\gamma(\mathbf{U})\omega^\delta(\mathbf{U})\boldsymbol{\Phi}_{\theta^\gamma\theta^\delta},\dots)=0. \tag{1.3}$$

We can introduce the families $\Lambda_{\mathbf{k},\boldsymbol{\omega}}$ and the full family $\Lambda=\cup\Lambda_{\mathbf{k},\boldsymbol{\omega}}$ of the functions $\boldsymbol{\Phi}(\boldsymbol{\theta},\mathbf{U})$ satisfying the system (1.3) in the space of 2π-periodic with respect to each θ^α function. Let us choose (in a smooth way) at every $(U^1,\dots,U^N)$ some function $\boldsymbol{\Phi}(\boldsymbol{\theta},\mathbf{U})$ as having "zero initial phase shifts" and represent the full family of m-phase solutions of system (1.1) in the form (1.2).

In Whitham method we make a rescaling $X=\epsilon x$, $T=\epsilon t$ $(\epsilon\to 0)$ of both variables x and t and try to find a function

$$\mathbf{S}(X,T)=(S^1(X,T),\dots,S^m(X,T)) \tag{1.4}$$

and 2π-periodic functions

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$$\Psi^i(\boldsymbol{\theta},X,T,\epsilon)=\sum_{k\geqslant 0}\Psi^i_{(k)}(\boldsymbol{\theta},X,T)\epsilon^k \tag{1.5}$$

such that the functions

$$\phi^i(\boldsymbol{\theta},X,T,\epsilon)=\Psi^i\left(\frac{\mathbf{S}(X,T)}{\epsilon}+\boldsymbol{\theta},X,T,\epsilon\right) \tag{1.6}$$

satisfy the system

$$F^i(\phi,\epsilon\phi_T,\epsilon\phi_X,\epsilon^2\phi_{TT},\dots)=0 \tag{1.7}$$

at every X, T, and $\boldsymbol{\theta}$.

It is easy to see that the function $\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ satisfies the system (1.3) at every X and T with

$$k^\alpha=S^\alpha_X,\quad \omega^\alpha=S^\alpha_T$$

and so belongs at every (X,T) to the family Λ. We can write then

$$\Psi^i_{(0)}(\boldsymbol{\theta},X,T)=\Phi^i(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T),\mathbf{U}(X,T))$$

and introduce the functions $U^\nu(X,T)$, $\theta^\alpha_0(X,T)$ as the parameters characterizing the main term in (1.5) which should satisfy the condition

$$[k^\alpha(\mathbf{U})]_T=[\omega^\alpha(\mathbf{U})]_X. \tag{1.8}$$

The functions $\Psi^i_{(1)}(\boldsymbol{\theta},X,T)$ are defined from the linear system

$$\hat{L}^i_j\Psi^j_{(1)}(\boldsymbol{\theta},X,T)=f^i_{(1)}(\boldsymbol{\theta},X,T) \tag{1.9}$$

where

$$\begin{aligned}\hat{L}^i_j=\hat{L}^i_{(X,T)j}=&\frac{\partial F^i}{\partial\varphi^j}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)+\frac{\partial F^i}{\partial\varphi^j_t}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)\omega^\alpha(X,T)\frac{\partial}{\partial\theta^\alpha}\\&+\frac{\partial F^i}{\partial\varphi^j_x}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)k^\beta(X,T)\frac{\partial}{\partial\theta^\beta}+\cdots\end{aligned} \tag{1.10}$$

is the linearization of system (1.3) and $\mathbf{f}_{(1)}(\boldsymbol{\theta},X,T)$ is discrepancy given by

$$\begin{aligned}f^i_{(1)}(\boldsymbol{\theta},X,T)=&-\frac{\partial F^i}{\partial\varphi^j_t}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)\Psi^j_{(0)T}(\boldsymbol{\theta},X,T)-\frac{\partial F^i}{\partial\varphi^j_x}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)\Psi^j_{(0)X}(\boldsymbol{\theta},X,T)\\&-\frac{\partial F^i}{\partial\varphi^j_{tt}}(\boldsymbol{\Psi}_{(0)}(\boldsymbol{\theta},X,T),\dots)(2\omega^\alpha(X,T)\Psi^j_{(0)\theta^\alpha T}+\omega^\beta_T(X,T)\Psi^j_{(0)\theta^\beta})-\dots.\end{aligned} \tag{1.11}$$

We have here

$$\frac{\partial}{\partial T}=U^\nu_T\frac{\partial}{\partial U^\nu}+\theta^\alpha_{(0)T}\frac{\partial}{\partial\theta^\alpha},\quad \frac{\partial}{\partial X}=U^\nu_X\frac{\partial}{\partial U^\nu}+\theta^\alpha_{(0)X}\frac{\partial}{\partial\theta^\alpha}$$

for the functions

$$\Psi^i_{(0)}(\boldsymbol{\theta},X,T)=\Phi^i(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T),\mathbf{U}(X,T)).$$

We will assume that k^α and ω^α can be considered (locally) as the independent parameters on the family Λ and the total family of solutions of (1.3) depends (for generic k^α, ω^α) on $N=2m+s$, $(s\geqslant 0)$ parameters U^ν and m initial phases θ^α_0.

It is easy to see that the functions $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T),\mathbf{U}(X,T))$ and $\nabla_{\boldsymbol{\xi}}\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T),\mathbf{U}(X,T))$ where $\boldsymbol{\xi}$ is any vector in the space of parameters U^ν tangential to the surface $\mathbf{k}=\text{const}$, $\boldsymbol{\omega}=\text{const}$ belong to the kernel of the operator $\hat{L}^i_{(X,T)j}$.

Let us put now some "regularity" conditions on the family (1.2) of quasiperiodic solutions of (1.1)

Definition 1.1: We call the family (1.2) the full regular family of m-phase solutions of (1.1) if:

(1) The functions $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{U})$, $\mathbf{\Phi}_{U^\nu}(\boldsymbol{\theta},\mathbf{U})$ *are linearly independent (almost everywhere) on the set* Λ;

(2) The $m+s$ *linearly independent functions* $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{U})$, $\nabla_{\boldsymbol{\xi}}\mathbf{\Phi}(\boldsymbol{\theta},\mathbf{U})$ $(\nabla_{\boldsymbol{\xi}}\mathbf{k}=0,\nabla_{\boldsymbol{\xi}}\boldsymbol{\omega}=0)$ *give the full kernel of the operator* $\hat{L}^i_{[\mathbf{U}]j}$ *(here* $\boldsymbol{\theta}_0=0$*) for generic* $\mathbf{k}$ *and* $\boldsymbol{\omega}$.

(3) There are exactly $m+s$ *linearly independent "left eigen-vectors"* $\boldsymbol{\kappa}^{(q)}_{[\mathbf{U}]}(\boldsymbol{\theta})$, $q=1,\dots,m+s$ *of the operator* $\hat{L}^i_{[\mathbf{U}]j}$ *(for generic* $\mathbf{k}$ *and* $\boldsymbol{\omega}$*) corresponding to zero eigenvalues, i.e.,*

$$\int_0^{2\pi}\dots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{U}]i}(\boldsymbol{\theta})\hat{L}^i_{[\mathbf{U}]j}\psi^j(\boldsymbol{\theta})\frac{d^m\theta}{(2\pi)^m}\equiv 0$$

for any periodic $\psi^j(\boldsymbol{\theta})$.

It is not difficult to see that the Definition 1.1 is connected with the regularity properties of the submanifold Λ given by the set of functions $\mathbf{\Phi}(\boldsymbol{\theta},\mathbf{U})$ in the space of 2π-periodic functions. In fact, for our purposes we can use also the weaker definition of the full regular family of m-phase solutions of (1.1). Namely, let us represent the space of parameters $\mathbf{U}$ in the form $\mathbf{U}=(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ where $\mathbf{k}$ are the wave numbers, $\boldsymbol{\omega}$ are the frequencies of m-phase solutions, and $\mathbf{n}=(n^1,\dots,n^s)$ are some additional parameters (if they exist). Let us give now the "weak" definition of the full regular family of m-phase solutions in the form:

Definition 1.1′: We call the family Λ *the full regular family of m-phase solutions of (1.1) if*

(1) The functions $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$, $\mathbf{\Phi}_{n^l}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ *are linearly independent and give (for generic* $\mathbf{k}$ *and* $\boldsymbol{\omega}$*) the full basis in the kernel of the operator* $\hat{L}^i_{j[\boldsymbol{\theta}_0,\mathbf{k},\boldsymbol{\omega},\mathbf{n}]}$;

(2) The operator $\hat{L}^i_{j[\boldsymbol{\theta}_0,\mathbf{k},\boldsymbol{\omega},\mathbf{n}]}$ *has (for generic* $\mathbf{k}$ *and* $\boldsymbol{\omega}$*) exactly* $m+s$ *linearly independent "left eigenvectors"*

$$\boldsymbol{\kappa}^{(q)}_{[\mathbf{U}]}(\boldsymbol{\theta}+\boldsymbol{\theta}_0)=\boldsymbol{\kappa}^{(q)}_{[\mathbf{k},\boldsymbol{\omega},\mathbf{n}]}(\boldsymbol{\theta}+\boldsymbol{\theta}_0)$$

depending on the parameters $\mathbf{U}$ *in a smooth way and corresponding to zero eigenvalues.*

We will assume now that the system (1.1) has a full regular family of quasiperiodic m-phase solutions in strong or weak sense in all our considerations.

To find the function $\mathbf{\Psi}_{(1)}(\boldsymbol{\theta},X,T)$ we have to put now the $m+s$ conditions of orthogonality of the discrepancy $\mathbf{f}_{(1)}(\boldsymbol{\theta},X,T)$ to the functions $\boldsymbol{\kappa}^{(q)}_{[\mathbf{U}(X,T)]}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T))$

$$\int_0^{2\pi}\dots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{U}(X,T)]i}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T))f^i_{(1)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}=0. \tag{1.12}$$

The system (1.12) together with (1.8) gives $m+(m+s)=2m+s=N$ conditions at each X and T on the parameters of zero approximation $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ necessary for the construction of the first $\boldsymbol{\epsilon}$-term in the solution (1.5).

Let us prove now the following Lemma about the orthogonality conditions (1.12):

Lemma 1.1: Under all the assumptions of regularity formulated above the orthogonality conditions (1.12) do not contain the functions $\theta^\alpha_0(X,T)$ *and give just the restrictions on the functions* $U^\nu(X,T)$ *having the form*

$$C^{(q)}_\nu(\mathbf{U})U^\nu_T-D^{(q)}_\nu(\mathbf{U})U^\nu_X=0 \tag{1.13}$$

(with some functions $C^{(q)}_\nu(\mathbf{U})$, $D^{(q)}_\nu(\mathbf{U})$*).*

Proof: Let us write down the part $\mathbf{f}'_{(1)}$ of the function $\mathbf{f}_{(1)}$ which contains the derivatives $\theta^\beta_{0T}(X,T)$ and $\theta^\beta_{0X}(X,T)$. We have from (1.11)

$$f'^{\,i}_{(1)}(\boldsymbol{\theta},X,T) = -\frac{\partial F^i}{\partial \varphi^j_t}(\boldsymbol{\Psi}_{(0)},\dots)\Psi^j_{(0)\theta^\beta}\theta^\beta_{0T} - \frac{\partial F^i}{\partial \varphi^j_x}(\boldsymbol{\Psi}_{(0)},\dots)\Psi^j_{(0)\theta^\beta}\theta^\beta_{0X}$$
$$-\frac{\partial F^i}{\partial \varphi^j_{tt}}(\boldsymbol{\Psi}_{(0)},\dots)2\omega^\alpha(X,T)\Psi^j_{(0)\theta^\alpha\theta^\beta}\theta^\beta_{0T} - \frac{\partial F^i}{\partial \varphi^j_{xx}}(\boldsymbol{\Psi}_{(0)},\dots)2k^\alpha(X,T)\Psi^j_{(0)\theta^\alpha\theta^\beta}\theta^\beta_{0X} - \dots .$$

Let us choose again the set of parameters $\mathbf{U}$ in the form

$$\mathbf{U} = (k^1,\dots,k^m,\omega^1,\dots,\omega^m,n^1,\dots,n^s),$$

where k^α are the wave numbers, ω^α are the frequencies of m-phase solutions, and $(n^1,\dots,n^s)$ are additional parameters (except the initial phases).

We can write then

$$f'^{\,i}_{(1)}(\boldsymbol{\theta},X,T) = \left[-\frac{\partial}{\partial\boldsymbol{\omega}^\beta}F^i(\boldsymbol{\Phi}(\boldsymbol{\theta}+\boldsymbol{\theta}_0,\mathbf{U}),\dots) + \hat{L}^i_j\frac{\partial}{\partial\boldsymbol{\omega}^\beta}\Phi^j(\boldsymbol{\theta}+\boldsymbol{\theta}_0,\mathbf{U})\right]\theta^\beta_{0T}$$
$$+\left[-\frac{\partial}{\partial k^\beta}F^i(\boldsymbol{\Phi}(\boldsymbol{\theta}+\boldsymbol{\theta}_0,\mathbf{U}),\dots) + \hat{L}^i_j\frac{\partial}{\partial k^\beta}\Phi^j(\boldsymbol{\theta}+\boldsymbol{\theta}_0,\mathbf{U})\right]\theta^\beta_{0X}.$$

The derivatives $\partial F^i/\partial\omega^\beta$ and $\partial F^i/\partial k^\beta$ are identically zero on Λ according to (1.3). We have then

$$\int_0^{2\pi}\dots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{U}(X,T)]i}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T))f'^{\,i}_{(1)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}\equiv 0$$

since all $\boldsymbol{\kappa}^{(q)}(\boldsymbol{\theta},X,T)$ are the left eigenvectors of $\hat{L}$ with zero eigenvalues.

It is easy to see also that all $\boldsymbol{\theta}_0(X,T)$ in the arguments of $\boldsymbol{\Phi}$ and $\boldsymbol{\kappa}^{(q)}$ will disappear after the integration with respect to $\boldsymbol{\theta}$ so we get the statement of the Lemma.

Lemma 1.1 is proved.

The system

$$\frac{\partial k^\alpha}{\partial U^\nu}U^\nu_T = \frac{\partial\omega^\alpha}{\partial U^\nu}U^\nu_X,\quad \alpha=1,\dots,m,$$
$$C^{(q)}_\nu(\mathbf{U})U^\nu_T = D^{(q)}_\nu(\mathbf{U})U^\nu_X,\quad q=1,\dots,m+s \tag{1.14}$$

is called the Whitham system for the m-phase solutions of system (1.1).

Let us note that we have rank $\|\partial k^\alpha/\partial U^\nu\| = m$ according to our assumption above. In the generic case the derivatives U^ν_T can be expressed through U^μ_X and the Whitham system (1.14) can be written in the form

$$U^\nu_T = V^\nu_\mu(\mathbf{U})U^\mu_X,\quad \nu,\mu=1,\dots,N, \tag{1.15}$$

where $V^\nu_\mu(U)$ is some $N\times N$ matrix depending on the variables $U^1,\dots,U^N$.

Let us say that quite often the system (1.1) can be written in the evolution form

$$\varphi^i_t = Q^i(\boldsymbol{\varphi},\boldsymbol{\varphi}_x,\boldsymbol{\varphi}_{xx},\dots). \tag{1.16}$$

For systems (1.16) the form (1.15) of the corresponding Whitham system has then a natural motivation.

We will assume here that if the conditions (1.14) are satisfied then the system (1.9) is resolvable on the space of 2π-periodic with respect to each θ^α function. The solution $\boldsymbol{\Psi}_{(1)}(\boldsymbol{\theta},X,T)$ is

defined then modulo a linear combination of the "right eigenfunctions" of $\hat{L}^i_{(X,T)j}$ $(\boldsymbol{\Psi}_{(0)\theta^\alpha}, \boldsymbol{\Psi}_{(0)n^l})$ introduced above. According to common approach[4,12] we can try to use the corresponding coefficients to make the systems analogous to (1.9) resolvable in the next orders and try to find recursively all the terms of series (1.5).

Different aspects and numerous applications of the Whitham method were studied in many different works[1–51] (we apologize for the impossibility to give here the full list of numerous works on the Whitham method) and the Whitham method is considered now as one of the classical methods of investigation of nonlinear systems.

It was pointed out by G. Whitham[1–3] that the Whitham system (1.14) has a local Lagrangian structure in case when the initial system has a local Lagrangian structure

$$\delta \int \int \mathcal{L}(\boldsymbol{\varphi}, \boldsymbol{\varphi}_t, \boldsymbol{\varphi}_x, \ldots)\mathrm{d}x\, \mathrm{d}t = 0$$

on the space $\{\boldsymbol{\varphi}(x,t)\}$.

The procedure of construction of Lagrangian formalism for the Whitham system (1.14) is given by the averaging of the Lagrangian function $\mathcal{L}$ on the family of m-phase solutions of system (1.1).[1–3] Let us note also that in the case of the presence of additional parameters n^l the additional method of Whitham pseudophases should be used.

The important procedure of averaging of local field-theoretical Hamiltonian structures was suggested by B. A. Dubrovin and S. P. Novikov.[14,18,28,32] The Dubrovin-Novikov procedure gives the local field-theoretical Hamiltonian formalism for the Whitham system (1.15) in the case when the initial system (1.16) has a local Hamiltonian formalism of general type. The Dubrovin-Novikov bracket for the Whitham system has a general form

$$\{U^\nu(X), U^\mu(Y)\} = g^{\nu\mu}(\mathbf{U})\delta'(X-Y) + b^{\nu\mu}_\lambda(\mathbf{U})U^\lambda_X\delta(X-Y) \tag{1.17}$$

and was called the local Poisson bracket of hydrodynamic type. The theory of the brackets (1.17) is closely related with differential geometry[14,28,32] and is connected with different coordinate systems in the (pseudo) Euclidean spaces. Let us say also that during the last years the important weakly nonlocal generalizations of Dubrovin-Novikov brackets (Mokhov-Ferapontov bracket and Ferapontov brackets) were introduced and studied.[53–59]

The Hamiltonian structure (1.17) for the systems (1.15) has a direct relation to the integrability of the systems of this class. Thus it was conjectured by S. P. Novikov that any diagonalizable system (1.15) Hamiltonian with respect to the bracket of hydrodynamic type is integrable. The conjecture of S. P. Novikov was proved by S. P. Tsarev,[52] who suggested the "generalized Hodograph method" for solving the diagonal Hamiltonian systems (1.15). Let us say that the Tsarev method has become especially important for the Whitham systems corresponding to integrable hierarchies and provided a lot of very important solutions for such systems in different cases. We note here that the Whitham systems of integrable hierarchies can usually be written in diagonal form[3,11,25] and admit the (multi-) Hamiltonian structures given by the averaging of the Lagrangian or the field-theoretical Hamiltonian structures of the initial system.

During the last years the theory of compatible Poisson brackets (1.17) and their deformations in connection with Quantum Field Theory was intensively developed.[60–72] Namely, the theory of compatible Poisson brackets (1.17) plays the main role in the theory of "Frobenius manifolds" constructed by B. A. Dubrovin and connected with the classification of the topological quantum field theories (based on the Witten-Dijkgraaf-Verlinde-Verlinde equation). Every "Frobenius manifold" is connected also with the integrable hierarchy of hydrodynamic type

$$U^\nu_{t_s} = V^\nu_{(s)\mu}(\mathbf{U})U^\mu_X \tag{1.18}$$

having the bi-Hamiltonian structure in Dubrovin-Novikov sense with a pair of Poisson brackets (1.17). [The hierarchy (1.18) and the corresponding pair of Poisson brackets also possess some additional properties (the existence of "unit vector field," Euler field, τ-symmetry, etc.)]

The "ϵ-deformations" of the integrable hierarchies and the Poisson brackets (1.17) are connected with the "higher" corrections in the quantum field theories and are being intensively investigated now.[64–72] According to B. A. Dubrovin and Y. Zhang the ϵ-deformation of Frobenius manifold is given by the infinite series polynomial with respect to derivatives $\mathbf{U}_X, \mathbf{U}_{XX}, \mathbf{U}_{XXX}, \ldots$ and representing the "small dispersion" deformation of the hierarchy (1.18) and the corresponding bi-Hamiltonian structure of hydrodynamic type. The deformed hierarchy and bi-Hamiltonian structure should possess also the additional properties of Frobenius manifolds ("unit vector field," Euler field, τ-symmetry etc.,…) and give then the "deformation" of the corresponding Frobenius manifold.[64,66,68] The general problem of classification of deformations of bi-Hamiltonian hierarchies (1.18) is being also intensively studied by now and very important results were obtained recently in this area.[67–72]

The dispersive corrections to the Whitham systems were first considered by M. Y. Ablowitz and D. J. Benney (see Ref. 5, also Refs. 6 and 7) where the first consideration of multiphase Whitham method was also made. As was shown in Ref. 5 the dispersive corrections to Whitham systems can naturally arise and, besides that, can be generalized to the multiphase situation.

In this paper we will consider the deformations of the Whitham systems (1.15) having Dubrovin-Zhang form, i.e., the dispersive corrections to (1.15) containing the higher X-derivatives of the parameters $\mathbf{U}$. The problem in this form is connected with the problem set by B. A. Dubrovin, which is formulated as the problem of deformations of Frobenius manifolds corresponding to the Whitham systems of integrable hierarchies. B. A. Dubrovin problem contains both the problem of deformation of Whitham systems (1.15) and the corresponding bi-Hamiltonian structures of hydrodynamic type giving the dispersive corrections to these structures.

We will consider here the first part of the B. A. Dubrovin problem and suggest a general scheme of recursive construction of terms of the deformation of the Whitham system (1.15) using the initial system (1.1) or (1.16). The second part of the B. A. Dubrovin problem will then be considered in the next paper. We will not require, however, the "integrability" of the system (1.15) and all the considerations below can be applicable for both integrable and nonintegrable systems (1.1) and (1.16). Thus, we do not require also the bi-Hamiltonian property of the Whitham system (1.15).

In the next section we will make more detailed investigation of the asymptotic series (1.5) and describe the construction of the deformation procedure for general Whitham systems.

II. THE DEFORMATION OF THE WHITHAM SYSTEMS

Let us start again with the description of the construction of asymptotic series (1.5) connected with the Whitham method. We will assume that we have the initial system having the general form (1.1) which has an N-parametric (modulo the initial phases θ_0^α) family of m-phase solutions

$$\varphi^i(x,t) = \Phi^i(\mathbf{k}(\mathbf{U})x + \boldsymbol{\omega}(\mathbf{U})t + \boldsymbol{\theta}_0, \mathbf{U}) \tag{2.1}$$

with the functions $\boldsymbol{\Phi}(\boldsymbol{\theta}, \mathbf{U})$ satisfying the system

$$F^i(\boldsymbol{\Phi}, \omega^\alpha(\mathbf{U})\boldsymbol{\Phi}_{\theta^\alpha}, k^\beta(\mathbf{U})\boldsymbol{\Phi}_{\theta\beta}, \omega^\gamma(\mathbf{U})\omega^\delta(\mathbf{U})\boldsymbol{\Phi}_{\theta\gamma\theta\delta}, \ldots) = 0 \tag{2.2}$$

(and 2π-periodic with respect to all θ^α).

The choice of the functions $\Phi^i(\boldsymbol{\theta}, \mathbf{U})$ at each $\mathbf{U}$ is defined modulo the initial phase $\boldsymbol{\theta}_0$ and the full family of solutions of (2.2) is given by all the functions $\boldsymbol{\Phi}(\boldsymbol{\theta}+\boldsymbol{\theta}_0, \mathbf{U})$ with arbitrary $\boldsymbol{\theta}_0 = (\theta_0^1, \ldots, \theta_0^m)$. We will just assume here that the choice of $\Phi^i(\boldsymbol{\theta}, \mathbf{U})$ is smooth on the family of m-phase solutions Λ.

We will assume also that the parameters $(\mathbf{k}, \boldsymbol{\omega})$ are independent on the family Λ such that $N \geqslant 2m$. It will be convenient to use the parameters $(k^1, \ldots, k^m, \omega^1, \ldots, \omega^m, n^1, \ldots, n^s)$ on the family Λ where k^α are the "wave numbers," ω^α are frequencies, and $(n^1, \ldots, n^s)$ are additional parameters (if they present). The linearly independent solutions of the linearized system (2.2) will then be given by $m+s$ functions $\boldsymbol{\Phi}_{\theta^\alpha}(\boldsymbol{\theta}, \mathbf{U})$, $\boldsymbol{\Phi}_{n^l}(\boldsymbol{\theta}, \mathbf{U})$.

As we already said above we assume that the family Λ represents the "full regular family" of m-phase solutions of (2.3) such that the requirements formulated in Definition 1.1 or Definition 1.1′ are satisfied. We thus have exactly $m+s$ functions $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{U})$, $\mathbf{\Phi}_{n^l}(\boldsymbol{\theta},\mathbf{U})$ giving the basis in the kernel of linearized system (2.2) and exactly $m+s$ linearly independent functions $\boldsymbol{\kappa}^{(q)}_{[\mathbf{U}]}(\boldsymbol{\theta}+\boldsymbol{\theta}_0)$ giving the basis in the kernel of the adjoint operator (for generic $\mathbf{k}$, $\boldsymbol{\omega}$) and depending in a smooth way on the parameters $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$.

As we mentioned already we make a rescaling of coordinates $X=\epsilon x$, $T=\epsilon t$ and try to find the solutions of system

$$F^i(\boldsymbol{\varphi},\epsilon\boldsymbol{\varphi}_T,\epsilon\boldsymbol{\varphi}_X,\epsilon^2\boldsymbol{\varphi}_{TT},\epsilon^2\boldsymbol{\varphi}_{XT},\epsilon^2\boldsymbol{\varphi}_{XX},\dots)=0,\quad i=1,\dots,n \tag{2.3}$$

having the form

$$\phi^i(\boldsymbol{\theta},X,T,\epsilon)=\Psi^i\left(\frac{\mathbf{S}(X,T)}{\epsilon}+\boldsymbol{\theta},X,T,\epsilon\right), \tag{2.4}$$

$$\Psi^i(\boldsymbol{\theta},X,T,\epsilon)=\sum_{k\geqslant 0}\Psi^i_{(k)}(\boldsymbol{\theta},X,T)\epsilon^k. \tag{2.5}$$

The function $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ belongs to the family Λ at every fixed X and T,

$$\Psi^i_{(0)}(\boldsymbol{\theta},X,T)=\Phi^i(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T),\mathbf{k}(X,T),\boldsymbol{\omega}(X,T),\mathbf{n}(X,T)), \tag{2.6}$$

and the compatibility conditions (1.12) for the system

$$\hat{L}^i_j\Psi^j_{(1)}(\boldsymbol{\theta},X,T)=f^i_{(1)}(\boldsymbol{\theta},X,T) \tag{2.7}$$

give the Whitham system (1.13) on the parameters $\mathbf{U}(X,T)$ of the zero approximation. The function $\mathbf{\Psi}_{(1)}(\boldsymbol{\theta},X,T)$ is defined from the system (2.7) modulo the linear combination of functions $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{U})$, $\mathbf{\Phi}_{n^l}(\boldsymbol{\theta},\mathbf{U})$ at every X and T.

All the other approximations $\mathbf{\Psi}_{(k)}(\boldsymbol{\theta},X,T)$ satisfy the linear systems

$$\hat{L}^i_j\Psi^j_{(k)}(\boldsymbol{\theta},X,T)=f^i_{(k)}(\boldsymbol{\theta},X,T), \tag{2.8}$$

where the functions $\mathbf{f}_{(k)}(\boldsymbol{\theta},X,T)$ represent the higher order discrepancies given by system (2.3).

The compatibility conditions of the systems (2.8) ($k\geqslant 2$) give the restrictions on the "initial phases" θ^α_0 of the zero approximation and on the previous corrections $\mathbf{\Psi}_{(k')}(\boldsymbol{\theta},X,T)$.

Let us make now one more general assumption about the systems (2.7) and (2.8). Namely we omit here the special investigation of the solvability of systems (2.7) and (2.8) on the space of 2π-periodic functions and assume that the orthogonality conditions

$$\int_0^{2\pi}\dots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{U}(X,T)]_i}(\boldsymbol{\theta}+\boldsymbol{\theta}_0(X,T))f^i_{(k)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}=0 \tag{2.9}$$

give the necessary and sufficient conditions of solvability of these systems. So, we will assume that under the conditions (2.9) we can always find a smooth 2π-periodic solution of (2.7) and (2.8) defined modulo the linear combination

$$\sum_{\alpha=1}^{m}c^\alpha_{(k)}(X,T)\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},X,T)+\sum_{l=1}^{s}d^l_{(k)}(X,T)\mathbf{\Phi}_{n^l}(\boldsymbol{\theta},X,T). \tag{2.10}$$

Let us consider now the construction of the asymptotic series (2.5). We note first that the solution $\mathbf{\Psi}_{(k)}(\boldsymbol{\theta},X,T)$ is defined from the system (2.8) modulo the linear combination (2.10) which is equivalent in the main order to the addition of the values $\epsilon^{k+1}c^\alpha_{(k)}(X,T)$ to the phases $S^\alpha(X,T)$ of

the zero approximation $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ and to the addition of the values $\epsilon^k d^l_{(k)}(X,T)$ to the parameters $n^l(X,T)$ of $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ according to the formulas (2.4) and (2.5). It is easy to see also that we can add the values $\epsilon^{k+1}c^\alpha_{(k)X}(X,T)$ and $\epsilon^{k+1}c^\alpha_{(k)T}(X,T)$ to the parameters k^α and ω^α in the **U**-dependence of $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ which does not affect the kth order of ϵ in the series (2.5).

Let us change now the procedure of construction of series (2.5) in the following way:

(1) At every step k we choose the solution $\mathbf{\Psi}_{(k)}(\boldsymbol{\theta},X,T)$ in arbitrary way;

(2) We allow the regular ϵ-dependence

$$S^\alpha(X,T,\epsilon)=\sum_{k\geqslant 0} S^\alpha_{(k)}(X,T)\epsilon^k,$$

$$n^l(X,T,\epsilon)=\sum_{k\geqslant 0} n^l_{(k)}(X,T)\epsilon^k$$

of the phases S^α and the parameters $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ of the zero approximation $\mathbf{\Psi}_{(0)}(\boldsymbol{\theta},X,T)$ such that

$$k^\alpha(X,T,\epsilon)=S^\alpha_X(X,T,\epsilon),\quad \omega^\alpha(X,T,\epsilon)=S^\alpha_T(X,T,\epsilon)$$

(3) We use the higher orders $S^\alpha_{(k)}$, $n^l_{(k)}$ of the functions $S^\alpha(X,T,\epsilon)$, $n^l(X,T,\epsilon)$ to provide the orthogonality conditions (2.9) for the systems (2.8).

We can now write the asymptotic solution of (2.3) in the form

$$\phi^i(\boldsymbol{\theta},X,T,\epsilon)=\Phi^i\left(\frac{\mathbf{S}(X,T,\epsilon)}{\epsilon}+\boldsymbol{\theta},\mathbf{S}_X(X,T,\epsilon),\mathbf{S}_T(X,T,\epsilon),\mathbf{n}(X,T,\epsilon)\right)+\sum_{k\geqslant 1}\tilde{\Psi}^i_{(k)}\left(\frac{\mathbf{S}(X,T,\epsilon)}{\epsilon}+\boldsymbol{\theta},X,T\right)\epsilon^k. \tag{2.11}$$

Let us note that the phase shift $\boldsymbol{\theta}_0(X,T)$ of the initial approximation now becomes the ϵ-term in ϵ-expansion of the function $\mathbf{S}(X,T,\epsilon)$.

It is not difficult to see that the series (2.11) can be always represented in the form (2.4) and (2.5) and give the same set of the asymptotic solutions of system (2.3). However, the series (2.11) contains a big "renormalization freedom" since we can change in arbitrary way the higher orders corrections $\mathbf{S}_{(2)}(X,T)$, $\mathbf{S}_{(3)}(X,T),\ldots$, $\mathbf{n}_{(1)}(X,T)$, $\mathbf{n}_{(2)}(X,T),\ldots$ and then adjust the functions $\tilde{\mathbf{\Psi}}_{(k)}$ in the appropriate way.

Let us now "fix the normalization" of the solution (2.11) in the following way.

We require that the first term

$$\Phi^i\left(\frac{\mathbf{S}(X,T,\epsilon)}{\epsilon}+\boldsymbol{\theta},\mathbf{S}_X(X,T,\epsilon),\mathbf{S}_T(X,T,\epsilon),\mathbf{n}(X,T,\epsilon)\right)$$

of (2.11) gives "the best approximation" of the asymptotic solution (2.11) by the modulated m-phase solution of (1.1). To be more precise, we require that the rest of the series (2.11) is orthogonal (at every X and T) to the vectors $\mathbf{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},X,T)$, $\mathbf{\Phi}_{n^l}(\boldsymbol{\theta},X,T)$ "tangent" to Λ at the "point" $[\mathbf{S}(X,T,\epsilon),\mathbf{n}(X,T,\epsilon)]$.

Thus we will now put the conditions

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\sum_{i=1}^n \Phi^i_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\left[\sum_{k=1}^\infty \tilde{\Psi}^i_{(k)}(\boldsymbol{\theta},X,T)\epsilon^k\right]\frac{d^m\theta}{(2\pi)^m}=0, \tag{2.12}$$

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\sum_{i=1}^n \Phi^i_{n^l}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\left[\sum_{k=1}^\infty \tilde{\Psi}^i_{(k)}(\boldsymbol{\theta},X,T)\epsilon^k\right]\frac{d^m\theta}{(2\pi)^m}=0 \tag{2.13}$$

(for all ϵ).

The representation (2.6) defines in fact the first correction $\mathbf{S}_{(1)}=\boldsymbol{\theta}_{(0)}(X,T)$. As we saw above, the functions $\tilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$ are defined modulo the linear combinations of the functions $\boldsymbol{\Phi}_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})$, $\boldsymbol{\Phi}_{n^l}(\boldsymbol{\theta},\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})$ which are linearly independent for the full regular family of m-phase solutions of (1.1). Using this fact it is not difficult to prove that the conditions (2.12) and (2.13) fix uniquely all the terms $\mathbf{S}_{(k+1)}$, $\mathbf{n}_{(k)}$, and $\tilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$ $(k\geqslant 1)$ for a given solution (2.4) and (2.5) which gives then the representation (2.11).

Let us say now that the choice of the normalization (2.12) and (2.13) is not unique. In particular, it depends on the choice of the variables $\varphi^i(x,t)$ for the "vector" $(i>1)$ systems (1.1). We will speak about the normalization (2.12) and (2.13) as about one possible way to fix the functions $\tilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$.

The solution $\phi(\boldsymbol{\theta},X,T)$ can now be defined as the asymptotic solution of the system (2.3) having the form (2.11) which satisfies the conditions

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\sum_{i=1}^{n}\Phi^i_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\phi^i\left(\boldsymbol{\theta}-\frac{\mathbf{S}}{\epsilon},X,T,\epsilon\right)\frac{d^m\theta}{(2\pi)^m}=0,$$

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\sum_{i=1}^{n}\Phi^i_{n^l}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\left[\phi^i\left(\boldsymbol{\theta}-\frac{\mathbf{S}}{\epsilon},X,T,\epsilon\right)-\Phi^i(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\right]\frac{d^m\theta}{(2\pi)^m}=0$$

(for all ϵ).

To find a solution in the form (2.11) we substitute the series (2.11) in the system (2.3) and try to find the functions $\tilde{\Psi}^i_{(k)}(\boldsymbol{\theta},X,T)$ from the linear systems

$$\hat{L}^i_{j[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}\tilde{\Psi}^j_{(k)}(\boldsymbol{\theta},X,T)=\tilde{f}^i_{(k)}(\theta,X,T) \tag{2.14}$$

analogous to (2.8).

The functions $\tilde{f}^i_{(k)}(\boldsymbol{\theta},X,T)$ are different from the functions $f^i_{(k)}(\boldsymbol{\theta},X,T)$ since we included "a part of ϵ-dependence" in the first term of (2.11). The functions $\tilde{\mathbf{f}}_{(k)}(\boldsymbol{\theta},X,T)$ should be orthogonal to the functions $\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}(\boldsymbol{\theta},X,T)$, $q=1,\ldots,m+s$ and we use the conditions (2.12) and (2.13) for the recurrent determination of $\tilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$. The functions $S^\alpha_{(k)}(X,T)$, $n^l_{(k)}(X,T)$ are used now to provide the resolvability of the systems (2.14) in all orders of ϵ.

Let us investigate now the systems arising on the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{S}_{(1)}(X,T),\ldots$, $\mathbf{n}_{(0)}(X,T)$, $\mathbf{n}_{(1)}(X,T),\ldots$. Let us note that we have in our notations $\mathbf{S}(X,T)=\mathbf{S}_{(0)}(X,T)$, $\boldsymbol{\theta}_0(X,T)=\mathbf{S}_{(1)}(X,T)$. We saw in Lemma 1.1 that the function $\boldsymbol{\theta}_0(X,T)$ does not appear in the solvability conditions of the system (1.9). For the asymptotic solution written in the form (2.11) with the normalization conditions (2.12) and (2.13) we can prove here even stronger statement.

Lemma 2.1: The functions $S^\alpha_{(k)}(X,T)$, $n^l_{(k)}(X,T)$ do not appear in the expression for the discrepancy $\tilde{\mathbf{f}}_{(k)}(\boldsymbol{\theta},X,T)$ and do not affect the solution $\tilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$.

Proof: The way we get the discrepancy $\tilde{\mathbf{f}}_{(k)}(\boldsymbol{\theta},X,T)$ can be described as follows:

(1) We substitute the solution (2.11) in the system (2.3);

(2) After "making all differentiations" we can omit the argument shift $\mathbf{S}(X,T,\epsilon)/\epsilon$ in all functions depending on $\boldsymbol{\theta}$;

(3) Then collecting together all the terms of order ϵ^k we get the system (2.14).

It is not difficult to see that in this approach the kth order of ϵ containing the functions $\mathbf{S}_{(k)}(X,T)$ or $\mathbf{n}_{(k)}(X,T)$ have the form

$$\frac{\mathrm{d}F^i}{\mathrm{d}k^\alpha}S^\alpha_{(k)X},\quad \frac{\mathrm{d}F^i}{\mathrm{d}\omega^\alpha}S^\alpha_{(k)T}\quad \frac{\mathrm{d}F^i}{\mathrm{d}n^l}n^l_{(k)},$$

where F^i are the constraints (2.2) defining the m-phase solutions of (1.1). The derivatives $\mathrm{d}/\mathrm{d}k^\alpha$, $\mathrm{d}/\mathrm{d}\omega^\alpha$, $\mathrm{d}/\mathrm{d}n^l$ here are the total derivatives including the dependence of the functions $\Phi^i(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ on the corresponding parameters view the form of (2.11). However, all these derivatives are identically equal to zero on the family Λ, so we get the first part of the Lemma. To finish the proof we have to note also that the values $\mathbf{S}_{(k)}(X,T)$, $\mathbf{n}_{(k)}(X,T)$ do not appear in the kth order of $\boldsymbol{\epsilon}$ of the normalization conditions (2.12) and (2.13) either.

Lemma 2.1 is proved.

We can now formulate the procedure in the following form:

We try to solve the systems (2.14) recursively in all orders and find the functions $\widetilde{\boldsymbol{\Psi}}_{(k)}(\boldsymbol{\theta},X,T)$ satisfying the conditions (2.12) and (2.13). At each kth step of our procedure we get a system on the functions $\mathbf{S}_{(k-1)}(X,T)$, $\mathbf{n}_{(k-1)}(X,T)$ from the solvability conditions of (2.14). The full set of Whitham solutions will then be parametrized by the set of all functions $\{\mathbf{S}_{(k)}(X,T),\mathbf{n}_{(k)}(X,T)\}$, $k\geqslant 0$ satisfying the conditions of solvability of systems (2.14).

Now let us investigate the systems arising on the functions $\mathbf{S}_{(k-1)}(X,T)$, $\mathbf{n}_{(k-1)}(X,T)$ from the solvability conditions of (2.14)

$$\int_0^{2\pi}\cdots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T)\widetilde{f}^i_{(k)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}\equiv 0,\quad q=1,\ldots,m+s \tag{2.15}$$

in the kth order of $\boldsymbol{\epsilon}$. We note first that the solvability conditions of (2.14) for $k=1$ give a nonlinear system on the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$. It is not difficult to prove the following Lemma:

Lemma 2.2: The system arising for $k=1$ coincides with the Whitham system for the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$.

Proof: Indeed, using Lemma 2.1 it is not difficult to see that the discrepancy $\mathbf{f}_{(1)}(\boldsymbol{\theta},X,T)$ differs from $\widetilde{\mathbf{f}}_{(1)}(\boldsymbol{\theta},X,T)$ just by the terms containing derivatives $\boldsymbol{\theta}_{0X}$ and $\boldsymbol{\theta}_{0T}$. However, according to Lemma 1.1 these terms do not affect the orthogonality conditions (1.12) which then coincide with orthogonality conditions for $\widetilde{\mathbf{f}}_{(1)}(\boldsymbol{\theta},X,T)$.

Lemma 2.2 is proved.

The Whitham system (orthogonality conditions) for the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ can be written in the following general form:

$$\begin{aligned}
W^{(q)}[\mathbf{S}_{(0)},\mathbf{n}_{(0)}](X,T) &\equiv \langle\boldsymbol{\kappa}^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}\cdot\widetilde{\mathbf{f}}_{(1)}[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]\rangle(X,T)\\
&=\int_0^{2\pi}\cdots\int_0^{2\pi}\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T)\widetilde{f}^i_{(1)}[\mathbf{S}_{(0)},\mathbf{n}_{(0)}](\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}\\
&=A^{(q)}_\alpha(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\alpha_{(0)TT}\\
&\quad+B^{(q)}_\alpha(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\alpha_{(0)XT}+C^{(q)}_\alpha(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\alpha_{(0)XX}\\
&\quad+G^{(q)}_l(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})n^l_{(0)T}+H^{(q)}_l(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})n^l_{(0)X}=0
\end{aligned}\tag{2.16}$$

with some functions $A^{(q)}_\alpha$, $B^{(q)}_\alpha$, $C^{(q)}_\alpha$, $G^{(q)}_l$, $H^{(q)}_l$, $q=1,\ldots,m+s$, $\alpha=1,\ldots,m$, $l=1,\ldots,s$.

Let us prove now the following Lemma about the systems on $\mathbf{S}_{(k)}$, $\mathbf{n}_{(k)}$, $k\geqslant 1$.

Lemma 2.3: The orthogonality conditions of $\widetilde{\mathbf{f}}_{(k+1)}(\boldsymbol{\theta},X,T)$ to the functions $\boldsymbol{\kappa}^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}$ give the following linear systems for the functions $\mathbf{S}_{(k)}(X,T)$, $\mathbf{n}_{(k)}(X,T)$, $k\geqslant 1$:

$$\int\int \frac{\delta W^{(q)}(X,T)}{\delta S^{\alpha}_{(0)}(X',T')} S^{\alpha}_{(k)}(X',T')dX'dT' + \int\int \frac{\delta W^{(q)}(X,T)}{\delta n^{l}_{(0)}(X',T')} n^{l}_{(k)}(X',T')\mathrm{d}X'\mathrm{d}T'$$
$$= V^{(q)}_{(k)}[\mathbf{S}_{(0)},\ldots,\mathbf{S}_{(k-1)},\mathbf{n}_{(0)},\ldots,\mathbf{n}_{(k-1)}](X,T),$$

where

$$\frac{\delta W^{(q)}(X,T)}{\delta S^{\alpha}_{(0)}(X',T')} = \frac{\partial W^{(q)}}{\partial S^{\alpha}_{(0)T}}\delta'(T-T')\delta(X-X') + \frac{\partial W^{(q)}}{\partial S^{\alpha}_{(0)X}}\delta(T-T')\delta'(X-X')$$
$$+ \frac{\partial W^{(q)}}{\partial S^{\alpha}_{(0)TT}}\delta''(T-T')\delta(X-X') + \frac{\partial W^{(q)}}{\partial S^{\alpha}_{(0)XT}}\delta'(T-T')\delta'(X-X') + \frac{\partial W^{(q)}}{\partial S^{\alpha}_{(0)XX}}\delta(T-T')\delta''(X-X'),$$

$$\frac{\delta W^{(q)}(X,T)}{\delta n^{l}_{(0)}(X',T')} = \frac{\partial W^{(q)}}{\partial n^{l}_{(0)}}\delta(T-T')\delta(X-X') + \frac{\partial W^{(q)}}{\partial n^{l}_{(0)T}}\delta'(T-T')\delta(X-X') + \frac{\partial W^{(q)}}{\partial n^{l}_{(0)X}}\delta(T-T')\delta'(X-X').$$

In other words, the functions $\mathbf{S}_{(k)}(X,T)$, $\mathbf{n}_{(k)}(X,T)$ satisfy the linearized Whitham system on the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ with additional right-hand part depending on the functions $\mathbf{S}_{(0)},\ldots,\mathbf{S}_{(k-1)}$, $\mathbf{n}_{(0)},\ldots,\mathbf{n}_{(k-1)}$.

Proof: Let us look at the terms in $\widetilde{\mathbf{f}}_{(k+1)}(\boldsymbol{\theta},X,T)$ which contain the functions $\mathbf{S}_{(k)}(X,T)$, $\mathbf{n}_{(k)}(X,T)$:

(1) As we proved in Lemma 2.1 the functions $\widetilde{f}^{i}_{(1)}(\boldsymbol{\theta},X,T)$ contain only the terms depending on $\mathbf{S}_{(0)}$, $\mathbf{n}_{(0)}$. It is easy to see that the functions $\widetilde{f}^{i}_{(k+1)}(\boldsymbol{\theta},X,T)$ will then contain the terms

$$\int\int \frac{\delta\widetilde{f}^{i}_{(1)}(\boldsymbol{\theta},X,T)}{\delta S^{\alpha}_{(0)}(X',T')} S^{\alpha}_{(k)}(X',T')\mathrm{d}X'\,\mathrm{d}T' + \int\int \frac{\delta\widetilde{f}^{i}_{(1)}(\boldsymbol{\theta},X,T)}{\delta n^{l}_{(0)}(X',T')} n^{l}_{(k)}(X',T')\mathrm{d}X'\,\mathrm{d}T'$$

according to the form of the first term in (2.11).

(2) There are terms containing the functions $\mathbf{S}_{(k)}$, $\mathbf{n}_{(k)}$ and the function $\widetilde{\boldsymbol{\Psi}}_{(1)}(\boldsymbol{\theta},X,T)$. All such terms can be written in the form:

$$-\int\int\left[S^{\alpha}_{(k)}(X',T')\frac{\delta\hat{L}^{i}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(X,T)}{\delta S^{\alpha}_{(0)}(X',T')} + n^{l}_{(k)}(X',T')\frac{\delta\hat{L}^{i}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(X,T)}{\delta n^{l}_{(0)}(X',T')}\right]\widetilde{\Psi}^{j}_{(1)}(\boldsymbol{\theta},X,T)\mathrm{d}X'\,\mathrm{d}T',$$

where $\hat{L}^{i}_{j[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}$ is the linear operator (1.10) given by the linearization of the system (2.2) on the family of m-phase solutions.

(3) There are terms of the form

$$-\int\ldots\int\frac{\delta^{2}F^{i}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}(\boldsymbol{\theta},X,T)}{\delta S^{\alpha}_{(0)}(X',T')\,\delta S^{\beta}_{(0)}(X'',T'')} S^{\alpha}_{(k)}(X',T')S^{\beta}_{(1)}(X'',T'')\mathrm{d}X'\,\mathrm{d}T'\,\mathrm{d}X''\,\mathrm{d}T'' - \cdots,$$

where $F^{i}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]}(\boldsymbol{\theta},X,T)$ is the left-hand part of the system (2.2).

However, the sum of all such terms is equal to zero since they all correspond to the expansion of the "shift of parameters" $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ on the family Λ where we have $F^{i}(\boldsymbol{\theta},X,T)\equiv 0$ identically.

Let us look now at the terms in the orthogonality conditions

$$\int_{0}^{2\pi}\ldots\int_{0}^{2\pi}\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T)\widetilde{f}^{i}_{(k+1)}(\boldsymbol{\theta},X,T)\frac{d^{m}\theta}{(2\pi)^{m}} = 0 \tag{2.17}$$

containing the terms (1) and (2).

We have identically

$$\int_0^{2\pi} \cdots \int_0^{2\pi} \kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T) L^i_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(\boldsymbol{\theta},\boldsymbol{\theta}',X,T)\frac{d^m\theta}{(2\pi)^m} \equiv 0 \tag{2.18}$$

on Λ (where $L^i_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(\boldsymbol{\theta},\boldsymbol{\theta}',X,T)$ is the "core" of the operator $\hat{L}^i_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(X,T)$).

It is easy to see then that the inner product of $\boldsymbol{\kappa}^{(q)}$ with the terms (2) is equal to

$$\int_0^{2\pi} \cdots \int_0^{2\pi} \int\int \left[S^\alpha_{(k)}(X',T')\frac{\delta\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T)}{\delta S^\alpha_{(0)}(X',T')} + n^l_{(k)}(X',T')\frac{\delta\kappa^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]i}(\boldsymbol{\theta},X,T)}{\delta n^l_{(0)}(X',T')}\right] \mathrm{d}X'\,\mathrm{d}T'$$

$$\times \hat{L}^i_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]j}(X,T)\tilde{\Psi}^j_{(1)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m}.$$

It is not difficult to see now that the terms of orthogonality conditions containing the terms (1) and (2) can be written together in the form

$$\int\int S^\alpha_{(k)}(X',T')\frac{\delta}{\delta S^\alpha_{(0)}(X',T')}\langle \boldsymbol{\kappa}^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]} \cdot \tilde{\mathbf{f}}_{(1)}[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]\rangle(X,T)\mathrm{d}X'\,\mathrm{d}T'$$

$$+ \int\int n^l_{(k)}(X',T')\frac{\delta}{\delta n^l_{(0)}(X',T')}\langle \boldsymbol{\kappa}^{(q)}_{[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]} \cdot \tilde{\mathbf{f}}_{(1)}[\mathbf{S}_{(0)},\mathbf{n}_{(0)}]\rangle(X,T)\mathrm{d}X'\,\mathrm{d}T'$$

(where $\langle\cdots\cdots\rangle$ is the inner product of $\boldsymbol{\kappa}^{(q)}$ and $\tilde{\mathbf{f}}_{(1)}$).

All the other terms in the orthogonality conditions (2.17) are the smooth functionals of $\mathbf{S}_{(0)},\ldots,\mathbf{S}_{(k-1)}$, $\mathbf{n}_{(0)},\ldots,\mathbf{n}_{(k-1)}$, so we get the statement of the Lemma.

Lemma 2.3 is proved.

Let us consider now the systems (1.1) satisfying the special nondegeneracy conditions. Namely, we will assume that the corresponding Whitham system (2.16) can be resolved with respect to the highest T derivatives of the functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ and written in the "evolution" form:

$$S^\alpha_{(0)TT} = M^\alpha_{(0)\beta}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\beta_{(0)XX} + N^\alpha_{(0)\beta}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\beta_{(0)TX} + P^\alpha_{(0)p}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})n^p_{(0)X},$$

$$\alpha = 1,\ldots,m, \tag{2.19}$$

$$n^l_{(0)T} = T^l_{(0)\beta}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\beta_{(0)XX} + L^l_{(0)\beta}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})S^\beta_{(0)TX} + R^l_{(0)p}(\mathbf{S}_{(0)X},\mathbf{S}_{(0)T},\mathbf{n}_{(0)})n^p_{(0)X},$$

$$l = 1,\ldots,s. \tag{2.20}$$

After the introduction of the variables $k^\alpha_{(0)} = S^\alpha_{(0)X}$, $\omega^\alpha_{(0)} = S^\alpha_{(0)T}$ we can write the system (2.19) and (2.20) in the form

$$k^\alpha_{(0)T} = \omega^\alpha_{(0)X},$$

$$\omega^\alpha_{(0)T} = M^\alpha_{(0)\beta}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})k^\beta_{(0)X} + N^\alpha_{(0)\beta}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})\omega^\beta_{(0)X} + P^\alpha_{(0)p}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})n^p_{(0)X},$$

$$n^l_{(0)T} = T^l_{(0)\beta}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})k^\beta_{(0)X} + L^l_{(0)\beta}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})\omega^\beta_{(0)X} + R^l_{(0)p}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})n^p_{(0)X}, \tag{2.21}$$

i.e., in the form (1.15).

We will consider now the hyperbolic systems (2.21), i.e., such that the matrix

$$V_{\mu}^{\nu}(\mathbf{k}_{(0)},\boldsymbol{\omega}_{(0)},\mathbf{n}_{(0)})=\begin{pmatrix}0 & I_m & 0\\ M_{(0)} & N_{(0)} & P_{(0)}\\ T_{(0)} & L_{(0)} & R_{(0)}\end{pmatrix}$$

has exactly $N=2m+s$ real eigenvalues with N linearly independent real eigenvectors. For hyperbolic systems (2.21) it is natural to consider the Cauchy problem with the smooth initial data $\mathbf{k}_{(0)}(X,0)$, $\boldsymbol{\omega}_{(0)}(X,0)$, $\mathbf{n}_{(0)}(X,0)$ (or $\mathbf{S}_{(0)}(X,0)$, $\mathbf{S}_{(0)T}(X,0)$, $\mathbf{n}_{(0)}(X,0)$). The smooth solution of (2.21) exists in general up to some finite time T_0 until the breakdown occurs. So we can write the zero (global in X) approximation for the solution (2.11) just in the time interval where we have a smooth solution of the Whitham system. Using Lemma 2.3 it is not difficult to prove then the following Lemma:

Lemma 2.4: For nondegenerate hyperbolic Whitham system (2.21) and the global solution $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ *defined on the interval* $[0,T_0]$ *the higher orders approximations in (2.11) are all defined for all* X *and* $T\in[0,T_0)$ *and are parametrized by the initial values* $\mathbf{S}_{(k)}(X,0)$, $\mathbf{S}_{(k)T}(X,0)$, $\mathbf{n}_{(k)}(X,0)$. [Let us recall that we assume that all systems (2.14) are solvable if the corresponding orthogonality conditions are satisfied.]

Proof: Indeed, as follows from Lemma 2.3 the functions $\mathbf{S}_{(k)}(X,T)$, $\mathbf{n}_{(k)}(X,T)$ are defined by the initial values $\mathbf{S}_{(k)}(X,0)$, $\mathbf{S}_{(k)T}(X,0)$, $\mathbf{n}_{(k)}(X,0)$ and can be found from the linear system using the characteristic directions of (2.21) (defined by $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$) provided that all the smooth solutions $\mathbf{S}_{(0)}(X,T),\dots,\mathbf{S}_{(k-1)}(X,T)$, $\mathbf{n}_{(0)}(X,T)\dots,\mathbf{n}_{(k-1)}(X,T)$ and $\tilde{\boldsymbol{\Psi}}_{(1)}(\boldsymbol{\theta},X,T),\dots,\tilde{\boldsymbol{\Psi}}_{(k-2)}(\boldsymbol{\theta},X,T)$ exist on the interval $[0,T_0)$. According to Lemma 2.1 and Lemma 2.3 we can find then the functions $\tilde{\Psi}^{i}_{(k-1)}(\boldsymbol{\theta},X,T)$ which are the local expressions (in X and T) of $\mathbf{S}_{(0)}(X,T),\dots,\mathbf{S}_{(k-1)}(X,T)$, $\mathbf{n}_{(0)}(X,T)\dots,\mathbf{n}_{(k-1)}(X,T)$ and their derivatives. Using the induction we then finish the proof of the Lemma.

Lemma 2.4 is proved.

According to Lemma 2.4 we can formulate now the following statement:

For the initial system (1.1) having the nondegenerate hyperbolic Whitham system (2.21) the corresponding Whitham solutions (2.11) (or (2.4) and (2.5)) are defined by the initial values $\mathbf{S}(X,0,\epsilon)$, $\mathbf{S}_T(X,0,\epsilon)$, $\mathbf{n}(X,0,\epsilon)$ and exist in the time interval $[0,T_0)$ defined by the Whitham system (2.21) and the initial data $\mathbf{S}_{(0)}(X,0)=\mathbf{S}(X,0,0)$, $\mathbf{S}_{(0)T}(X,0)=\mathbf{S}_T(X,0,0)$, and $\mathbf{n}_{(0)}(X,0)=\mathbf{n}(X,0,0)$.

The deformation procedure: Let us note now that the series (2.11) (or (2.4) and (2.5)) give in fact the one-parametric formal solutions of (1.1) with a parameter ϵ. Let us rewrite now the solutions (2.11) in the form which gives the concrete (formal) solution of (1.1) and is not connected with the additional one-parametric ϵ-family including this given solution. We omit now the ϵ-dependence of functions $\mathbf{S}(X,T,\epsilon)$, $\mathbf{n}(X,T,\epsilon)$ (or put formally $\epsilon=1$) and say that the Whitham solution is defined now by functions $\mathbf{S}(X,T)$, $\mathbf{n}(X,T)$ determined by the initial values $\mathbf{S}(X,0)$, $\mathbf{S}_T(X,0)$, and $\mathbf{n}(X,0)$. (Let us keep here the notations X and T for the spatial and time coordinates just to emphasize that we consider the "slow" functions $\mathbf{S}_X(X,T)$, $\mathbf{S}_T(X,T)$, $\mathbf{n}(X,T)$.)

Thus, we define now the Whitham solution as the solution of the system

$$F^{i}(\boldsymbol{\varphi},\boldsymbol{\varphi}_T,\boldsymbol{\varphi}_X,\boldsymbol{\varphi}_{TT},\boldsymbol{\varphi}_{XT},\boldsymbol{\varphi}_{XX},\dots)=0,\quad i=1,\dots,n \tag{2.22}$$

having the form

$$\phi^{i}(\boldsymbol{\theta},X,T)=\Phi^{i}(\mathbf{S}(X,T)+\boldsymbol{\theta},\mathbf{S}_X(X,T),\mathbf{S}_T(X,T),\mathbf{n}(X,T))+\sum_{k\geqslant 1}\Phi^{i}_{(k)}(\mathbf{S}(X,T)+\boldsymbol{\theta},X,T) \tag{2.23}$$

where the functions $\Phi^{i}_{(k)}$:

(1) Are 2π-periodic with respect to each θ^{α};

(2) Have degree k (introduced below);

(3) Satisfy the normalization conditions (2.12) and (2.13) which will be written now in the form:

$$\int_0^{2\pi} \dots \int_0^{2\pi} \sum_{i=1}^{n} \Phi^i_{\theta^\alpha}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\Phi^i_{(k)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m} = 0, \tag{2.24}$$

$$\int_0^{2\pi} \dots \int_0^{2\pi} \sum_{i=1}^{n} \Phi^i_{n^l}(\boldsymbol{\theta},\mathbf{S}_X,\mathbf{S}_T,\mathbf{n})\Phi^i_{(k)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m} = 0 \tag{2.25}$$

$k \geqslant 1$, $(\alpha = 1, \dots, m,\ l = 1, \dots, s)$.

Let us introduce now the gradation used for the formal expansion (2.23). Namely, for the systems (1.1) having the nondegenerate hyperbolic Whitham system (2.21) we put the following gradation on the functions $\mathbf{S}_X(X,T)$, $\mathbf{S}_T(X,T)$, $\mathbf{n}(X,T)$ and their derivatives:

(1) The functions $k^\alpha(X,T) = S^\alpha_X(X,T)$, $\omega^\alpha(X,T) = S^\alpha_T(X,T)$, and $n^l(X,T)$ have degree 0;

(2) Every differentiation with respect to X adds 1 to the degree of the function;

(3) The degree of the product of two functions having certain degrees is equal to the sum of their degrees.

In other words, for the parameters $\mathbf{U} = (\mathbf{k}, \boldsymbol{\omega}, \mathbf{n})$ we have the gradation rule of Dubrovin-Zhang type, i.e.,

All the functions $f(\mathbf{U})$ have degree 0;

The derivatives U^ν_{kX} have degree k;

The degree of the product of functions having certain degrees is equal to the sum of their degrees.

We put now the evolution conditions to the functions $\mathbf{S}(X,T)$, $\mathbf{n}(X,T)$ having the form:

$$S^\alpha_{TT} = \sum_{k\geqslant 1} \sigma^\alpha_{(k)}(\mathbf{k},\boldsymbol{\omega},\mathbf{n},\mathbf{k}_X,\boldsymbol{\omega}_X,\mathbf{n}_X,\dots), \tag{2.26}$$

$$n^l_T = \sum_{k\geqslant 1} \eta^l_{(k)}(\mathbf{k},\boldsymbol{\omega},\mathbf{n},\mathbf{k}_X,\boldsymbol{\omega}_X,\mathbf{n}_X,\dots), \tag{2.27}$$

where $\sigma^\alpha_{(k)}$, $\eta^l_{(k)}$ are general polynomials in derivatives $\mathbf{k}_X, \boldsymbol{\omega}_X, \mathbf{n}_X, \mathbf{k}_{XX}, \boldsymbol{\omega}_{XX}, \mathbf{n}_{XX}, \dots$ (with coefficients depending on $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$) having degree k.

We now substitute the expansion (2.23) in the system (2.22) and use the relations (2.26) and (2.27) to remove all the time derivatives of parameters $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$. After that we can divide the system (2.22) into the terms of certain degrees and try to find recursively all the terms $\boldsymbol{\Phi}_{(k)}(\boldsymbol{\theta},X,T)$ for $k = 1,2,\dots$.

It is easy to see again that for any $\boldsymbol{\Phi}_{(k)}(\boldsymbol{\theta},X,T)$ we will have the linear system analogous to (2.8) and (2.14), i.e.,

$$\hat{L}^i_{[\mathbf{S}(X,T),\mathbf{n}(X,T)]j}\Phi^i_{(k)}(\boldsymbol{\theta},X,T) = \hat{f}^i_{(k)}(\boldsymbol{\theta},X,T), \tag{2.28}$$

where $\hat{\mathbf{f}}_{(k)}(\boldsymbol{\theta},X,T)$ is the discrepancy having degree k according to the definition above.

We have to put again the orthogonality conditions

$$\int_0^{2\pi} \dots \int_0^{2\pi} \kappa^{(q)}_{[\mathbf{S},\mathbf{n}]i}(\boldsymbol{\theta},X,T)\hat{f}^i_{(k)}(\boldsymbol{\theta},X,T)\frac{d^m\theta}{(2\pi)^m} \equiv 0 \tag{2.29}$$

on the functions $\hat{f}^i_{(k)}(\boldsymbol{\theta},X,T)$ and then find the unique $\boldsymbol{\Phi}_{(k)}(\boldsymbol{\theta},X,T)$ satisfying the normalization conditions (2.24) and (2.25).

It is not difficult to prove the following Lemma:

Lemma 2.5: (1) For any system (1.1) having the nondegenerate hyperbolic Whitham system

(2.21) the functions $\sigma^{\alpha}_{(k)}$, $\eta^{l}_{(k)}$ *are uniquely determined by the orthogonality conditions (2.29) in the order k.*

(2) The functions $\sigma^{\alpha}_{(1)}$, $\eta^{l}_{(1)}$ *give the Whitham system (2.19) and (2.20) for the functions* $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$. [In fact, the functions $\mathbf{S}(X,T,\epsilon)$, $\mathbf{n}(X,T,\epsilon)$ introduced previously satisfy the full system (2.26) and (2.27).]

Proof: Indeed, using Lemma 2.1 it is easy to see that the functions $\hat{f}^{i}_{(1)}(\boldsymbol{\theta},X,T)$ coincide with the functions $\tilde{f}^{i}_{(1)}(\boldsymbol{\theta},X,T)$ introduced in (2.14) after the replacement of functions $\mathbf{S}_{(0)}(X,T)$, $\mathbf{n}_{(0)}(X,T)$ by $\mathbf{S}(X,T)$, $\mathbf{n}(X,T)$. Comparing then the orthogonality conditions (2.29) with (2.15) we get the second part of the Lemma.

To prove the first part we just note that all $\sigma^{\alpha}_{(k)}$, $\eta^{l}_{(k)}$ arise in the kth order of system (2.22) "in the same way." We can conclude then that the orthogonality conditions (2.29) in the kth order always contain the functions $\sigma^{\alpha}_{(k)}$, $\eta^{l}_{(k)}$ in one particular way which coincides with the appearance of $\sigma^{\alpha}_{(1)}$, $\eta^{l}_{(1)}$ in the Whitham system arising for $k=1$. From the definition of the nondegenerate Whitham system we now obtain the first part of the Lemma.

Lemma 2.5 is proved.

Definition 2.1: We call the system (2.26) and (2.27) or the equivalent system

$$k^{\alpha}_{T}=\omega^{\alpha}_{X},$$

$$\omega^{\alpha}_{T}=\sum_{k\geqslant 1}\sigma^{\alpha}_{(k)}(\mathbf{k},\boldsymbol{\omega},\mathbf{n},\mathbf{k}_{X},\boldsymbol{\omega}_{X},\mathbf{n}_{X},\dots),$$

$$n^{l}_{T}=\sum_{k\geqslant 1}\eta^{l}_{(k)}(\mathbf{k},\boldsymbol{\omega},\mathbf{n},\mathbf{k}_{X},\boldsymbol{\omega}_{X},\mathbf{n}_{X},\dots) \tag{2.30}$$

the deformation of the Whitham system (2.19) and (2.20) (or (2.21)).

The functions $k^{\alpha}(X,T)$, $\omega^{\alpha}(X,T)$, $n^{l}(X,T)$ are the "slow" functions of the variables x and t and the system (2.30) gives the analog of the "low-dispersion" expansion in our case. The asymptotic solutions (2.23) of the initial system (2.22) are parametrized by the asymptotic solutions $k^{\alpha}(X,T)$, $\omega^{\alpha}(X,T)$, $n^{l}(X,T)$ of the system (2.30) and arbitrary (constant) initial phases θ^{α}_{0}. As follows from our considerations above the solutions (2.23) give all the "particular solutions" (2.4) and (2.5), however, they do not contain the additional information about the one-parametric ϵ-family given by (2.4) and (2.5)

Remark 1: Let us note that the full set of parameters of m-phase solutions of (1.1) is given by $\mathbf{k}$, $\boldsymbol{\omega}$, $\mathbf{n}$, and $\boldsymbol{\theta}_{0}$. However the functions $\boldsymbol{\theta}_{0}(X,T)$ do not present as the parameters of solutions (2.23) in this approach. This shows in fact that the introduction of the functions $\theta^{\alpha}_{0}(X,T)$ does not give "new" formal solutions of (1.1) and is responsible for the additional ϵ-dependence of one-parametric families (2.4) and (2.5). Here they are "absorbed" by the total phase $\mathbf{S}(X,T)$ connected with the "particular" formal solution of (1.1).

Remark 2: In our consideration we fixed some functions $\Phi^{i}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ on the family Λ (for each $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$) as having zero initial phases. However, the choice of the functions $\Phi^{i}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ is not unique. In particular, the natural change of the functions $\boldsymbol{\Phi}^{i}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ on Λ can be written in the form

$$\boldsymbol{\Phi}'(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})=\boldsymbol{\Phi}(\boldsymbol{\theta}+\boldsymbol{\theta}_{0}(\mathbf{k},\boldsymbol{\omega},\mathbf{n}),\mathbf{k},\boldsymbol{\omega},\mathbf{n}), \tag{2.31}$$

where $\theta^{\alpha}_{0}(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ are arbitrary smooth functions.

It is not difficult to see also that the system (2.30) depends on the choice of the functions $\Phi^{i}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ in the high $(k\geqslant 2)$ orders.

Let us give here the definition given by B. A. Dubrovin and Y. Zhang[64,66] and connected with the "equivalence" of different infinite (or finite) systems.

Definition 2.2 (B. A. Dubrovin, Y. Zhang): *Consider the system of the form*

$$U_T^\nu = \sum_{k\geqslant 1} V_{(k)}^\nu(\mathbf{U}, \mathbf{U}_X, \mathbf{U}_{XX}, \dots), \quad \nu = 1, \dots, N \tag{2.32}$$

for arbitrary parameters U^ν where all $V_{(k)}^\nu$ are smooth functions polynomial in $\mathbf{U}_X, \mathbf{U}_{XX}, \dots$ and having degree k. We say that two systems (2.32) are connected by the triviality transformation (or equivalent) if they are connected by the formal substitution

$$\widetilde{U}^\nu = \sum_{k\geqslant 0} \widetilde{U}_{(k)}^\nu(\mathbf{U}, \mathbf{U}_X, \mathbf{U}_{XX}, \dots),$$

where all $\widetilde{U}_{(k)}^\nu$ are smooth functions polynomial in $\mathbf{U}_X, \mathbf{U}_{XX}, \dots$ and having degree k.

Let us say actually that the definition of B. A. Dubrovin and Y. Zhang is applied usually to the whole integrable hierarchies and plays the important role in the classification of integrable hierarchies having the form (2.32). We will prove here the following Lemma:

Lemma 2.6: The deformations of the Whitham system (2.30) written for the initial functions $\mathbf{\Phi}(\boldsymbol{\theta}, \mathbf{k}, \boldsymbol{\omega}, \mathbf{n})$ and $\mathbf{\Phi}'(\boldsymbol{\theta}, \mathbf{k}, \boldsymbol{\omega}, \mathbf{n})$ connected by the transformation (2.31) are equivalent in Dubrovin-Zhang sense.

Proof: Let us prove first the following statement:

For any transformation (2.31) there exists a unique change of functions $S^\alpha(X)$, $n^l(X)$:

$$S'^\alpha = S^\alpha - \theta_0^\alpha(\mathbf{k}, \boldsymbol{\omega}, \mathbf{n}) + \sum_{k\geqslant 1} S_{(k)}^\alpha(\mathbf{k}, \boldsymbol{\omega}, \mathbf{n}, \mathbf{k}_X, \dots),$$

$$n'^l = n^l + \sum_{k\geqslant 1} n_{(k)}^l(\mathbf{k}, \boldsymbol{\omega}, \mathbf{n}, \mathbf{k}_X, \dots) \tag{2.33}$$

such that:

(1) All $\mathbf{S}_{(k)}$, $\mathbf{n}_{(k)}$ are polynomial in derivatives of $(\mathbf{k}, \boldsymbol{\omega}, \mathbf{n})$ and have degree k;

(2) For any solution (2.23) $(\phi_{[\mathbf{S},\mathbf{n}]}(\boldsymbol{\theta}, X, T))$ of (2.22) the functions $\Phi'^i(\mathbf{S}'(X,T) + \boldsymbol{\theta}, \mathbf{S}'_X, \mathbf{S}'_T, \mathbf{n}')$ satisfy the normalization conditions

$$\int_0^{2\pi} \dots \int_0^{2\pi} \sum_{i=1}^n \Phi'^i_{\theta^\alpha}(\mathbf{S}' + \boldsymbol{\theta}, \mathbf{S}'_X, \mathbf{S}'_T, \mathbf{n}') \phi^i_{[\mathbf{S},\mathbf{n}]}(\boldsymbol{\theta}, X, T) \frac{d^m\theta}{(2\pi)^m} \equiv 0, \tag{2.34}$$

$$\int_0^{2\pi} \dots \int_0^{2\pi} \sum_{i=1}^n \Phi'^i_{n'^l}(\mathbf{S}' + \boldsymbol{\theta}, \mathbf{S}'_X, \mathbf{S}'_T, \mathbf{n}')[\phi^i_{[\mathbf{S},\mathbf{n}]}(\boldsymbol{\theta}, X, T) - \Phi'^i(\mathbf{S}' + \boldsymbol{\theta}, \mathbf{S}'_X, \mathbf{S}'_T, \mathbf{n}')] \frac{d^m\theta}{(2\pi)^m} \equiv 0. \tag{2.35}$$

For the proof of this statement let us note first that we can always express all the time derivatives of $\mathbf{k}$, $\boldsymbol{\omega}$, and $\mathbf{n}$ using the system (2.30) in terms of X-derivatives of these functions. Using this procedure we try to find the transformation (2.33) recursively in all degrees by substitution of (2.33) in (2.34) and (2.35). It is not difficult to check then that the functions $S_{(k)}^\alpha$, $n_{(k)}^l$ are defined in the kth order of (2.34) and (2.35) from a linear system. The matrix of this linear system coincides with the Gram matrix of functions Φ_{θ^α}, Φ_{n^l} at every X and T. Thus, for the full nondegenerate family of m-phase solutions of (1.1) this system has a unique solution at every degree k. The transformation (2.33) is evidently invertible in sense of the infinite series (polynomial with respect to derivatives of $(\mathbf{k}, \boldsymbol{\omega}, \mathbf{n})$) so we can also express the functions $(\mathbf{S}, \mathbf{n})$ in terms of $(\mathbf{S}', \mathbf{n}')$.

We can now try to use the functions $\Phi'^i(\mathbf{S}' + \boldsymbol{\theta}, \mathbf{S}'_X, \mathbf{S}'_T, \mathbf{n}')$ as the zero approximation in the $(\mathbf{S}', \mathbf{n}')$-expansion of the corresponding solution (2.23). It is not difficult to see that the difference

$$\Phi'^{i}(\mathbf{S}'+\theta,\mathbf{S}'_X,\mathbf{S}'_T,\mathbf{n}')-\phi^i_{[\mathbf{S},\mathbf{n}]}(\boldsymbol{\theta},X,T)$$

can be represented as the infinite series polynomial with respect to derivatives of $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ and starting with the terms of degree 1. After the expression of the functions $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ in terms of $(\mathbf{k}',\boldsymbol{\omega}',\mathbf{n}')$ in this difference we get finally the $(\mathbf{S}',\mathbf{n}')$-expansion of the solution $\phi^i_{[\mathbf{S},\mathbf{n}]}(\boldsymbol{\theta},X,T)$.

The functions $(\mathbf{S}',\mathbf{n}')$ now satisfy the new deformed Whitham system (2.26) and (2.27) corresponding to the choice of the functions $\boldsymbol{\Phi}'(\boldsymbol{\theta},\mathbf{k}',\boldsymbol{\omega}',\mathbf{n}')$ as the functions of zero approximation.

It is easy to see also that the transformation (2.33) remains polynomial in X-derivatives of $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ after the expression of time derivatives of $(\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ using the system (2.30).

We obtain then that the transformation (2.33) gives a "triviality" connection between the systems (2.30) written for the initial functions $\boldsymbol{\Phi}(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$ and $\boldsymbol{\Phi}'(\boldsymbol{\theta},\mathbf{k},\boldsymbol{\omega},\mathbf{n})$.

Lemma 2.6 is proved.

At the end let us note again that Lemma 2.6 is important in fact for the integrable hierarchies rather than for the one particular system (1.1) according to Dubrovin-Zhang approach to classification of integrable systems.

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Geometrical classification of Killing tensors on bidimensional flat manifolds

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Valence two Killing tensors in the Euclidean and Minkowski planes are classified under the action of the group which preserves the type of the corresponding Killing web. The classification is based on an analysis of the system of determining partial differential equations for the group invariants and is entirely algebraic. The approach allows one to classify both characteristic and noncharacteristic Killing tensors. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2217649]

I. INTRODUCTION AND BASIC PROPERTIES

A. Killing tensors and separable webs

A Killing tensor (KT) on a pseudo-Riemannian space $(M,\mathbf{g})$ is a tensor $\mathbf{K}$ of type $(0,k)$ which satisfies

$$\nabla_{(j} K_{i_1\ldots i_k)} = 0, \tag{1}$$

where ∇ denotes the covariant derivative defined by the Levi-Civita connection of the pseudo-Riemannian metric $\mathbf{g}$ and where the parentheses signify symmetrization of the enclosed indices. It was shown by Eisenhart[5] that such tensors arise naturally from first integrals of the geodesic flow on $(M,\mathbf{g})$ in the form

$$I = K_{i_1\ldots i_k}\frac{\mathrm{d}q^{i_1}}{\mathrm{d}s}\cdots\frac{\mathrm{d}q^{i_k}}{\mathrm{d}s}.$$

The function I, defined on the tangent bundle TM, is a first integral of the geodesic equations (i.e., it is constant along each geodesic) if and only if the Killing tensor equation (1) holds. Killing tensors may also be characterized in contravariant form by means of the following function defined on the cotangent bundle T^*M:

$$I^* = K^{i_1\ldots i_k}p_{i_1}\ldots p_{i_k},$$

where (q^i,p_i) denote canonical coordinates on T^*M. Condition (1) is then equivalent to

$$\{I^*,H\} = 0,$$

where $\{\cdot,\cdot\}$ denotes the Poisson bracket and

$$H = \tfrac{1}{2}g^{ij}p_ip_j,$$

the geodesic Hamiltonian.

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The set of all Killing tensors of valence k, on an n-dimensional manifold M, is a real vector space which we denote by $\mathcal{K}^k(M)$. Its dimension d satisfies the Delong-Takeuchi-Thompson inequality[4,15,16]

$$d \leqslant \frac{1}{n}\binom{n+k}{k+1}\binom{n+k-1}{k}.$$

Equality is achieved for manifolds of constant curvature. Moreover, in this case the Killing tensors of valence k are sums of symmetrized products of the Killing vectors of the manifold. In manifolds with isometry groups of less than the maximal dimension there may exist Killing tensors which are not expressible in this way. For example, such a situation occurs in the Kerr space-time.[3]

Killing tensors of type (0, 2) which we call Killing 2-tensors, are particularly important. Indeed, if the eigenvalues of a Killing 2-tensor are real and simple and the eigenvectors are normal (orthogonally integrable), then the Killing tensor defines an orthogonally separable web on M, that is n foliations of mutually orthogonal $(n-1)$-dimensional hypersurfaces. To the separable web are associated systems of coordinates with respect to which the Hamilton-Jacobi equation for the geodesic flow is solvable by separation of variables (see Benenti[1]). Killing 2-tensors with the above properties are called characteristic Killing tensors (CKTs).

It is well known that in the Euclidean plane there exist four types of orthogonally separable webs (see, for example, Miller[11]). Nevertheless, it is not a trivial task to determine which type of web is defined by a given characteristic Killing tensor. The converse problem of characterizing the Killing tensors which define the same separable web is also challenging. This problem becomes even more difficult in dimension greater than two where the preliminary problem of identifying the characteristic Killing tensors is itself a daunting task. It is thus clear that finding an effective method of classifying Killing tensors would be very useful indeed.

The classification of separable coordinates in two- and three-dimensional Euclidean space by Killing tensors dates back to the work of Eisenhart.[5] A similar classification for two- and three-dimensional Minkowski space was undertaken by Kalnins,[8] who classified the symmetric second-order differential operators that commute with the wave operator and solved the Eisenhart integrability conditions[5] to obtain the metric in the two-dimensional case. A classification of KTs in the Euclidean and Minkowski planes based on an analysis of their singular sets (i.e., the points where the eigenvalues of the Killing tensors are not real and simple) is given by Benenti and Rastelli[2] and Rastelli.[13] Recently remarkable progress in the classification problem was achieved by McLenaghan, Smirnov, Horwood, The, and Yue by means of the invariant theory of Killing tensors on spaces of constant curvature.[7,9,10,14] In this theory Killing tensors are classified modulo the group which consists of the transformations on $\mathcal{K}^2(M)$ induced by the isometries of the underlying pseudo-Riemannian manifold $(M,\mathbf{g})$ and the transformation which maps any Killing tensor $\mathbf{K}$ into $\mathbf{K}+b\mathbf{g}$, where b is any real number. More specifically to any isometry ϕ on M is associated the transformation on $\mathbf{K}\mapsto\hat{\mathbf{K}}$ on $\mathcal{K}^2(M)$ defined with respect to a system of local coordinates (q^i) by

$$\hat{K}^{ij}(q) = J^i_k(\Phi^{-1}(q))J^j_l(\Phi^{-1}(q))K^{kl}(\Phi^{-1}(q)), \tag{2}$$

where $J^i_j(q)=\partial\Phi^i/\partial q^j$ is the Jacobian of the transformation Φ. Two Killing tensors are considered equivalent if one can be obtained from the other in this way. Clearly all CKTs in the same equivalence class define the same orthogonal web. The classification is based on set of algebraic invariants of $\mathcal{K}^2(M)$ under the action of the group, from which a classification scheme for the type of the separable web can be constructed in the cases considered, namely, $\mathbb{E}_2$, $\mathbb{M}_2$, and $\mathbb{E}_3$.

The approach presented in this paper is related but somewhat different than that developed by McLenaghan *et al.* It is based on two observations: (i) the transformations on $\mathcal{K}^2(M)$ induced by the isometries are not the only ones which preserve the type of web defined by a given CKT. Indeed, any transformation of the form $\mathbf{K}\mapsto a\mathbf{K}+b\mathbf{g}$ also preserves the web (in Refs. 9 and 10, $a=1$ was assumed); (ii) two webs of the same type are not necessarily isometric. For example two elliptic-hyperbolic in the Euclidean plane webs with different interfocal distances are of the same

type but are not isometric but are rather related by a dilatation transformation. In the following we do not focus on the transformations of the manifold M, but directly on the transformations of $\mathcal{K}^2(M)$ that preserve the type of separable web defined by a given characteristic Killing tensor. In the Euclidean and Minkowski planes these transformations are well known and generate a Lie group with dimension equal to that of $\mathcal{K}^2(M)$. This further fact allows the determination of the equivalence classes in a purely algebraic way which is described in the sequel.

There are both advantages and disadvantages to the extension of the group of transformation used in our classification scheme. On the positive side is the very natural way in which the classes of KTs which define the distinct types of separable webs are obtained. Restriction of the transformations of KTs to those that preserve the web has the result that the CKTs which define the same type of web are scattered through many classes. The method also leaves open the possibility of classifying noncharacteristic KTs. On the negative side, while the isometry group of pseudo-Riemannian manifold is known in many cases, it is not easy to identify the additional transformations of $\mathcal{K}^2(M)$ that preserve the type of a Killing web. This makes it very difficult to extend the method to higher dimensions and to spaces with nonvanishing curvature.

The plan of the paper is as follows: in Sec. I B we outline the necessary theory of Lie transformation groups to be applied later in the paper. In Sec. II we perform the classification in the Euclidean plane. The classification in the Minkowski plane is undertaken in Sec. III. Section IV contains the conclusion.

B. Orbit of Lie group actions

Let $\Psi: G\times\mathcal{K}\to\mathcal{K}$ be a linear action of a finite-dimensional Lie group G on the vector space $\mathcal{K}$. According to the notation of Ref. 12, the infinitesimal generators of the action form a finitely generated and involutive distribution Δ of nonconstant rank (isomorphic to the Lie algebra of G).

Proposition 1:[6,12] *A distribution on a manifold is integrable if and only if it is involutive and rank-invariant. Finitely generated involutive distributions are always rank-invariant and so integrable.*

By this generalized Frobenius theorem the distribution Δ is integrable, and for the rank-invariance property it is tangent to any of the sets

$$r_j = \{x \in \mathcal{K}: \operatorname{rank}(\Delta)|_x = j\},$$

which are unions of maximal connected integral submanifolds S_x of Δ, but in general not (immersed) submanifolds.

All the connected components of the Lie group G are diffeomorphic to the normal subgroup G_0 which is the connected component containing the identity. Then $G=\cup_{g\in Z} gG_0$ where Z is a set of cosets representatives.

The orbit $\mathcal{O}_x$ of the action Ψ can be obtained as union of maximal integral manifolds of Δ mapped one into the other by the diffeomorphisms Ψ_g with $g\in Z$,

$$\mathcal{O}_x = \bigcup_{g\in Z} \Psi_g(S_x) = \bigcup_{g\in Z} S_{g\cdot x}.$$

Lemma 2: If r_j is a submanifold of dimension j then for any $x\in r_j$ S_x is the connected component of r_j containing x and the orbit $\mathcal{O}_x$ is the union of the connected components of r_j which are images of S_x through the action of the elements of Z.

If $\dim G=\dim \mathcal{K}=n$ then we are able to determine the orbits where the distribution Δ has maximal rank by looking for the connected components of r_n and gluing the ones mapped into the others by the elements of Z. Moreover the other orbits are contained in the sets where the rank of Δ change and, if the condition $\dim r_j=j$ still holds, they can all be determined in an algebraic way.

Some tools useful to detect the components connected by arcs (equal to topological connected components in our case) of a subset of $\mathbb{R}^n$ are now introduced. Let us consider a set $A\subset\mathbb{R}^n$ and let $\{A_i\}_{i\in I}$ be its partition in connected components. We consider the natural decomposition $\mathbb{R}^n\to\mathbb{R}^m\times\mathbb{R}^{n-m}$, so that any point of $P\in\mathbb{R}^n$ can be labeled as $P=(v,p)$ with $v\in\mathbb{R}^m$ and

$p \in R^{n-m}$. In this way we get a partition $\{V^v\}_{v \in \mathbb{R}^m}$ of $\mathbb{R}^n$ in parallel hyperplanes of dimension $n-m$, where $V^v = \{P \in \mathbb{R}^n : P = (v,p), p \in \mathbb{R}^{n-m}\}$. We call $A^v = A \cap V^v$ the section of A determined by the hyperplane V^v and construct its partition in connected components

$$A^v = \bigcup_{\alpha \in I^v} A^v_\alpha.$$

On the family $\{A^v_\alpha\}_{\alpha \in I^v, v \in \mathbb{R}^m}$ of the connected components of the sections of A we define the relation

$$A^v_\alpha \sim A^w_\beta \Leftrightarrow \exists\, !i \in I : A^v_\alpha \subseteq A_i \text{ and } A^w_\beta \subseteq A_i$$

It's easy to check that the following Lemma holds:

Lemma 3: The relation $\sim$ is an equivalence relation. There is a one-to-one correspondence between the equivalence classes $[A^v_\alpha]$ and the (arc)-connected components A_i of A. If there exists a continuous arc $f : [0,1] \to \mathbb{R}^m \times \mathbb{R}^{n-m}$ such that $f([0,1]) \subseteq A$, $f(0) = (v,p)$, $f(1) = (w,q)$ with $p \in A^v_\alpha$, $q \in A^w_\beta$ then $A^v_\alpha \sim A^w_\beta$.

Hence, the study of the connected components of A can be reduced to the study of connected components of all sections A^v (of lower dimension) under the equivalence relation.

II. KILLING TENSORS IN THE EUCLIDEAN PLANE

In the Euclidean plane $\mathbb{E}_2$, with Cartesian coordinates (x,y) and the standard metric $\mathbf{g}$, the general Killing 2-tensor $\mathbf{K}$ has the following contravariant form:

$$\|K^{ij}\| = \begin{pmatrix} A + 2\alpha y + \gamma y^2 & C - \alpha x - \beta y - \gamma xy \\ C - \alpha x - \beta y - \gamma xy & B + 2\beta x + \gamma x^2 \end{pmatrix}.$$

We denote by $\mathcal{K}(\mathbb{E}_2)$ the vector space of KTs on the Euclidean plane. On this space there exist six kinds of transformation preserving the type of the web associated to each KT: three of them correspond to isometries, a fourth corresponds to the dilatation of $\mathbb{E}_2$. The last two are not associated with any coordinate transformation in the plane but act directly on the tensor $\mathbf{K}$ and correspond to the addition of a multiple of the metric tensor ($\mathbf{K} \mapsto \mathbf{K} + \tau\mathbf{g}$) and to the multiplication of the tensor for a nonvanishing constant ($\mathbf{K} \mapsto \lambda\mathbf{K}$). The infinitesimal generators of these transformations are easily calculated (see Ref. 9 for the generators corresponding to isometries and addition of a multiple of the metric). With respect to the basis of the vector fields on $\mathcal{K}(\mathbb{E}_2)$ given by $(\partial_A, \partial_B, \partial_C, \partial_\alpha, \partial_\beta, \partial_\gamma)$ the infinitesimal generators are spanned by:

Translations

$$V_1 = (0, -2\beta, \alpha, 0, -\gamma, 0),$$

$$V_2 = (-2\alpha, 0, \beta, -\gamma, 0, 0).$$

Rotation

$$V_3 = (-2C, 2C, A - B, \beta, -\alpha, 0).$$

Dilatation of $\mathbb{E}_2$,

$$V_4 = (2A, 2B, 2C, \alpha, \beta, 0).$$

Addition of the metric

$$V_5 = (1, 1, 0, 0, 0, 0).$$

Scalar multiplication

$$V_6 = (A, B, C, \alpha, \beta, \gamma).$$

These vector fields form a Lie algebra and therefore generate an integrable distribution, denoted by Δ_E. In order to study the rank of Δ_E we gather the components of the V_i in the matrix

$$M = \begin{pmatrix} 0 & -2\beta & \alpha & 0 & -\gamma & 0 \\ -2\alpha & 0 & \beta & -\gamma & 0 & 0 \\ -2C & 2C & A-B & \beta & -\alpha & 0 \\ 2A & 2B & 2C & \alpha & \beta & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ A & B & C & \alpha & \beta & \gamma \end{pmatrix} \tag{3}$$

with determinant $\det M = -2\gamma[(\alpha^2-\beta^2-\gamma(A-B))^2+4(\alpha\beta+\gamma C)^2]$. We are led naturally to consider the two surfaces where $\det M = 0$,

$$S_1: \quad \gamma = 0 \quad \dim S_1 = 5, \tag{4}$$

$$S_2: \quad \begin{cases} \alpha^2 - \beta^2 = \gamma(A-B) \\ \alpha\beta = -\gamma C \end{cases} \qquad \dim S_2 = 4, \tag{5}$$

whose intersection is the vector subspace $\alpha=\beta=\gamma=0$. The sections of S_1, obtained using as parameters A, B, and C, are always planes; on the other hand the sections of S_2 are curves described by the following lemma:

Lemma 4: If the parameters A, B, and C have the values $C=0$ and $A=B$ then the section of S_2 is given by the axis γ, for other values of the parameters the section is given by two parabolas contained in two orthogonal planes, with vertex in the origin and foci on the γ axis symmetric with respect to the origin.

Proof: When $C \neq 0$ Eq. (5) become

$$(\alpha^2 - \beta^2)C + \alpha\beta(A-B) = 0,$$

$$\alpha\beta = -\gamma C.$$

The first equation can be factorized as $C(\alpha - k_+\beta)(\alpha - k_-\beta)$ where

$$k_\pm = \frac{B - A \pm \sqrt{(A-B)^2 + 4C^2}}{2C}.$$

Thus the section of S_2 is the union of the two parabolas

$$\begin{cases} \alpha = k_+\beta \\ \gamma = -\dfrac{k_+}{C}\beta^2 \end{cases} \cup \begin{cases} \alpha = k_-\beta \\ \gamma = -\dfrac{k_-}{C}\beta^2 \end{cases}.$$

We observe that $k_+k_- = -1$ thus the two parabolas are contained in two orthogonal planes. Their foci lie on the γ axis with

$$\gamma = \pm\tfrac{1}{4}\sqrt{(A-B)^2 + 4C^2};$$

being $k_+/C > 0$ the first parabola is always downward, while the second one is always upward. For $C=0$ the second equation in (5) becomes $\alpha\beta = 0$. Then when $A \neq B$ we have the two parabolas

$$\begin{cases} \alpha = 0 \\ \gamma = -\dfrac{\beta^2}{B-A} \end{cases} \cup \begin{cases} \beta = 0 \\ \gamma = \dfrac{\alpha^2}{A-B} \end{cases}$$

for which the previous considerations on foci hold. Finally when $A=B$ we have $\alpha=\beta=0$ and then the two parabolas degenerate in the γ axis.

We remark that the functions $\delta=(\alpha^2-\beta^2-\gamma(A-B))^2+4(\alpha\beta+\gamma C)^2$ and γ, defining the surfaces S_1 and S_2, are the fundamental invariant of $\mathcal{K}_2(\mathbb{R}^2)$ determined by McLenaghan *et al.*[9] under the action of the group induced by the isometries and the addition of a multiple of the metric.

Proposition 5: Outside of the union of the surfaces S_1 and S_2, the distribution Δ_E has rank 6 and the space $\mathcal{K}(\mathbb{E}_2)-(S_1\cup S_2)$ is an orbit of the action.

Proof: The distribution has maximal rank outside of $S_1\cup S_2$ because the determinant of the matrix (3) vanishes only on that set. Since $\mathcal{K}(\mathbb{E}_2)-(S_1\cup S_{2\,1})$ has the same dimension of the distribution, each connected component is an orbit of the action generated by the vector fields V_i. The connected components are two: one for $\gamma>0$ and the other for $\gamma<0$. However, the two components are linked together by the finite transformation that change the sign of the KT and so they form a unique orbit with respect to the disconnected group generated by the vector fields and this transformation.

Proposition 6: On S_1-S_2 the rank of Δ_E is 5 and this space is an orbit of the action.

Proof: In order to determine the rank of Δ_E on S_1 we set $\gamma=0$ in the matrix M: all the nonvanishing 5×5 minors contain the factor $\alpha^2+\beta^2$, and one of them is $2(\alpha^2+\beta^2)^2$. Thus the rank of M is lesser than 5 if and only if $\alpha=\beta=0$, that is on $S_1\cap S_2$. Because S_1-S_2 is connected and has dimension five it is an orbit of the action.

Proposition 7: On S_2-S_1 the rank of Δ_E is 4 and this space is an orbit of the action.

Proof: Assume $\gamma\neq0$, from Eq. (5) we obtain the relation

$$B = A - \frac{\alpha^2-\beta^2}{\gamma}, \quad C = -\frac{\alpha\beta}{\gamma},$$

which substituted in adj(M) make it identically zero. Then on S_2-S_1 the rank of the distribution is at most 4, but one 4×4 minor is $\gamma^3\neq0$. Thus outside of $S_1\cap S_2$ the rank is exactly 4. From Lemma 4 it follows that for any fixed values of $A-B$ and C (not both vanishing) the section of S_2-S_1 is formed by four disjoint parabola's arcs. But it is always possible to find a continuous deformation of the parameter A,B,C gluing together the two upward and downward arcs, respectively. Indeed with the change in the space of parameters $A-B=\rho\cos\theta$, $2C=\rho\sin\theta$ we have that the directions of the two planes containing the parabolas depends only on θ, while the amplitude of the two parabolas is inversely proportional to ρ, thus letting ρ go to zero with a fixed value of θ has the effect to glue together the arcs of the two parabolas along the γ axis. Hence, S_2-S_1 has two connected components only, which can be connected using the change of sign of the KT.

Finally we study the intersection $S_1\cap S_2$ which is the three-dimensional vector space with coordinates A, B, and C. On $S_1\cap S_2$ the only independent vector fields among the V_i are V_3, V_5, and V_6, whose components, with respect to $(\partial_A,\partial_B,\partial_C)$, form the matrix

$$\tilde{M} = \begin{pmatrix} -2C & 2C & A-B \\ A & B & C \\ 1 & 1 & 0 \end{pmatrix}. \tag{6}$$

Introducing the one-dimensional line

$$S_3: \begin{cases} \alpha=\beta=\gamma=0 \\ C=0 \\ A=B \end{cases} \qquad \dim S_3 = 1 \tag{7}$$

we are able to individuate the last two orbits.

Proposition 8: The rank of Δ_E *on* $(S_1 \cap S_2) - S_3$ *is* 3 *and then this space is an orbit of the action.*

Proof: The determinant of the matrix (6) is $\det \tilde{M} = 4C^2 + (A-B)^2$, then it vanishes only on S_3. Because $(S_1 \cap S_2) - S_3$ is connected it is an orbit. □

Proposition 9: The rank of Δ_E *on* S_3 *is* 1 *and then this space is an orbit of the action, containing the (noncharacteristic) tensors of the form* $\tau \mathbf{g}$.

Proof: The only independent vector field on S_3 is the constant vector V_5, generated by the addition of a multiple of the metric. □

We remark that the discrete transformation $(A \leftrightarrow B, \alpha \leftrightarrow \beta)$ induced by the discrete isometry of the Euclidean plane $(\{\overline{x}=y, \overline{y}=x\})$ does not allow one to glue together the above found orbits.

In conclusion five orbits of the action of the web preserving group are found.

E1) The set $\mathcal{K}(\mathbb{E}_2) - (S_1 \cup S_2)$, the tensors on this orbit generate elliptic-hyperbolic coordinates. A tensor of this type is

$$\begin{pmatrix} y^2 & 1-xy \\ 1-xy & x^2 \end{pmatrix}.$$

E2) The set $S_1 - S_2$, the tensors on this orbit generate parabolic coordinates. Two tensors of this type are

$$\begin{pmatrix} 2y & -x \\ -x & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -y \\ -y & 2x \end{pmatrix}.$$

E3) The set $S_2 - S_1$, the tensors on this orbit generate polar coordinates. A tensor of this type is

$$\begin{pmatrix} y^2 & -xy \\ -xy & x^2 \end{pmatrix}.$$

E4) The set $(S_1 \cap S_2) - S_3$, the tensors on this orbit generate Cartesian coordinates. Three tensors of this type are

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

E5) The line S_3, the tensors on this orbit are multiples of the metric.

This classification coincides with that given by McLenaghan *et al.*[9] where the four types of separable webs in $\mathbb{E}_2$ are characterized by the vanishing or not of the fundamental invariants γ and δ. The orbits are strictly related to the set of singular points discussed by Benenti and Rastelli.[2] Indeed, the discriminant of the characteristic polynomial of $\mathbf{K}$ vanishes on points satisfying

$$\gamma xy + \alpha x + \beta y - C = 0,$$

$$\gamma(y^2 - x^2) + 2(\alpha y - \beta x) + A - B = 0. \tag{8}$$

If $\gamma \neq 0$ (i.e., outside S_1), Eq. (8) describes two hyperbolas both centered in $(-\beta/\gamma, -\alpha/\gamma)$. For tensors belonging to $S_2 - S_1$ both conics degenerate into two couples of lines through the center (polar web). Otherwise, they have two points in common (elliptic-hyperbolic web). For tensor belonging to S_1 $(\gamma = 0)$ the system (8) is linear: if $\mathbf{K} \in S_1 - S_2$, it represents the intersection of two orthogonal lines (parabolic web); if $\mathbf{K} \in (S_1 \cap S_2) - S_3$ the system has no solution (Cartesian web), while for $\mathbf{K} \in S_3$ all points are singular.

III. KILLING TENSORS IN THE MINKOWSKI PLANE

On the Minkowski plane $\mathbb{M}_2$ with pseudo-Cartesian coordinates (t,x) and metric $\mathbf{g}$ with contravariant components

$$\|g^{ij}\| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

the general Killing tensor $\mathbf{K}$ has contravariant components:

$$\|K^{ij}\| = \begin{pmatrix} A + 2\alpha x + \gamma x^2 & C + \alpha t + \beta x + \gamma t x \\ C + \alpha t + \beta x + \gamma t x & B + 2\beta t + \gamma t^2 \end{pmatrix}.$$

We denote by $\mathcal{K}(\mathbb{M}_2)$ the vector space of all the KTs on $\mathbb{M}_2$. On this space six kinds of transformation are defined, which preserve the type of the web associated to the KT: three are induced by the isometries of the Minkowski plane and a fourth by its dilatation; the last two do not depend on any transformation of $\mathbb{M}_2$ and are defined directly on $\mathcal{K}(\mathbb{M}_2)$: adding a multiple of the metric tensor ($\mathbf{K} \mapsto \mathbf{K} + \tau\mathbf{g}$) and multiplying the tensor for a nonvanishing constant ($\mathbf{K} \mapsto \lambda\mathbf{K}$). With respect to the basis of the vector fields on $\mathcal{K}(\mathbb{M}_2)$ given by $(\partial_A, \partial_B, \partial_C, \partial_\alpha, \partial_\beta, \partial_\gamma)$ the infinitesimal generators are spanned by:

Translation:

$$V_1 = (0, -2\beta, -\alpha, 0, -\gamma, 0),$$

$$V_2 = (-2\alpha, 0, -\beta, -\gamma, 0, 0).$$

Boost (hyperbolic rotation):

$$V_3 = (2C, 2C, A + B, \beta, \alpha, 0).$$

Dilatation of $\mathbb{M}_2$:

$$V_4 = (2A, 2B, 2C, \alpha, \beta, 0).$$

Addition of the metric:

$$V_5 = (1, -1, 0, 0, 0, 0).$$

Scalar multiplication:

$$V_6 = (A, B, C, \alpha, \beta, \gamma)$$

(see Ref. 10 for the computation of V_1, V_2, V_3, and V_5).

Moreover, similar to the Euclidean case, there are the following discrete transformations which are analyzed in detail in Sec. III B: the first is the change in sign of the Killing tensor

$$R_0 : K \to -K.$$

The others are induced from the discrete isometries of $\mathbb{M}_2\{\bar{t} = t, \bar{x} = -x\}$ and $\{\bar{t} = -t, \bar{x} = x\}$, they are

$$R_1 : C \to -C, \alpha \to -\alpha,$$

$$R_2 : C \to -C, \beta \to -\beta,$$

In Refs. 8 and 10 the transformations used are R_1 together with

$$\hat{R}_2: A \leftrightarrow B, \alpha \leftrightarrow \beta,$$

which arises from a change of signature of the metric. We prefer transformation R_2 instead of $\hat{R}_2$ because it preserves the interior (and exterior) of the null cone in $\mathbb{M}_2$.

A. Study of the distribution rank

The vector fields V_i form a Lie algebra and therefore generate an integrable distribution, denoted by Δ_M. In to order to study the rank of Δ_M we gather the components of the V_i in the matrix

$$M = \begin{pmatrix} 0 & -2\beta & -\alpha & 0 & -\gamma & 0 \\ -2\alpha & 0 & -\beta & -\gamma & 0 & 0 \\ 2C & 2C & A+B & \beta & \alpha & 0 \\ 2A & 2B & 2C & \alpha & \beta & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ A & B & C & \alpha & \beta & \gamma \end{pmatrix} \tag{9}$$

with determinant:

$$\det M = 2\gamma[\gamma(A+B-2C)-(\alpha-\beta)^2][\gamma(A+B+2C)-(\alpha+\beta)^2].$$

Thus we consider the two surfaces

$$S_1: \gamma = 0, \quad \dim S_1 = 5, \tag{10}$$

$$S_2: [\gamma(A+B-2C)-(\alpha-\beta)^2][\gamma(A+B+2C)-(\alpha+\beta)^2] = 0, \quad \dim S_2 = 5. \tag{11}$$

We remark that the functions

$$f_1 = \gamma, \quad f_2 = [\gamma(A+B-2C)-(\alpha-\beta)^2][\gamma(A+B+2C)-(\alpha+\beta)^2],$$

coincide with the two fundamental algebraic invariants of $\mathcal{K}(\mathbb{M}_2)$ under the action of the isometry group augmented by addition of a multiple of the metric given in Ref. 10.

The surface S_2 is formed by two branches B_1 and B_2 given, respectively, by the equations $\gamma(A+B-2C)=(\alpha-\beta)^2$ and $\gamma(A+B+2C)=(\alpha+\beta)^2$. Nevertheless these two branches are mapped one in the other by the transformation R_1 and thus it is appropriate to consider them as a unique object. The intersection of B_1 and B_2 is the surface

$$B_1 \cap B_2 = S_3: \begin{cases} \gamma(A+B) = \alpha^2 + \beta^2 \\ \gamma C = \alpha\beta \end{cases} \qquad \dim S_3 = 4 \tag{12}$$

The intersection of S_1 and S_2 is described by the equations $\gamma=0$ and $\alpha^2=\beta^2$, while $S_1 \cap S_3$ has equations $\alpha=\beta=\gamma=0$.

The surfaces in Fig. 1 represent all the possible (generic) sections of S_2 in the space α, β, γ. These sections can be grouped in four kinds, corresponding to the following open sets in the space of parameters $A+B$ and C:

$$\text{region I}: \{A+B-2C>0, A+B+2C>0\},$$

$$\text{region II}: \{A+B-2C<0, A+B+2C>0\},$$

$$\text{region III}: \{A+B-2C<0, A+B+2C<0\},$$

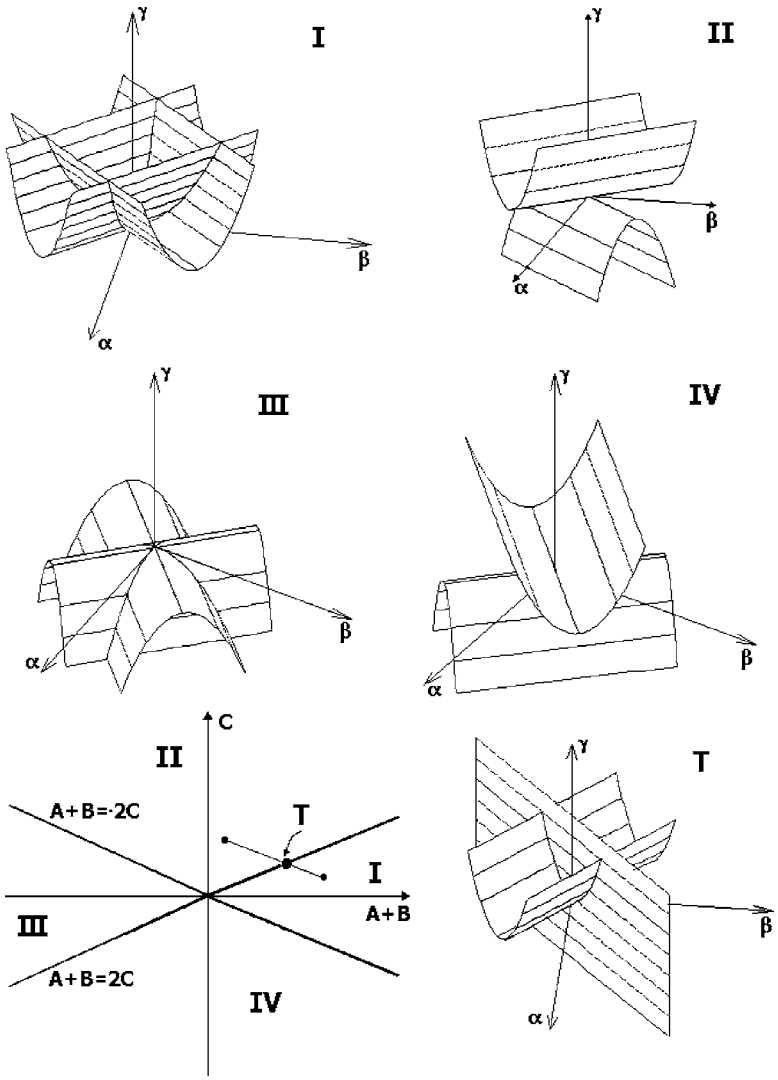


FIG. 1. The sections of surface S_2.

$$\text{region IV:}\{A+B-2C>0, A+B+2C<0\}.$$

Moreover, there are some nongeneric sections corresponding to the boundaries of the above regions, where at least one of the functions $A+B\pm 2C$ vanishes; in these cases the corresponding paraboloid becomes a plane (an example is given by the section T). Figure 2 describes the relation between the surfaces S_1, S_2, and S_3 for parameters belonging to region I.

Proposition 10: The rank of Δ_M *is* 6 *on* $\mathcal{K}(\mathbb{M}_2)-(S_1\cup S_2)$.

Proof: Since the determinant of the matrix (9) vanishes only on $S_1\cup S_2$, outside of this set the rank of Δ_M is maximal.

Proposition 11: The rank of Δ_M *on* S_1-S_2 *is* 5.

Proof: In order to study the rank of Δ_M on S_1 we set $\gamma=0$ in the matrix M: all the nonvanishing 5×5 minors contain the factor $\alpha^2-\beta^2$, and one of them is $2(\alpha^2-\beta^2)^2$. Thus the rank is lesser than 5 only when $\alpha^2=\beta^2$ that is on $S_1\cap S_2$. □

Proposition 12: The rank of Δ_M *on* $S_2-(S_1\cup S_3)$ *is* 5.

Proof: Let us study now the rank of the distribution on S_2 without its intersection with S_1: using the condition $\gamma\neq 0$ Eq. (11) of the two branches of S_2 becomes

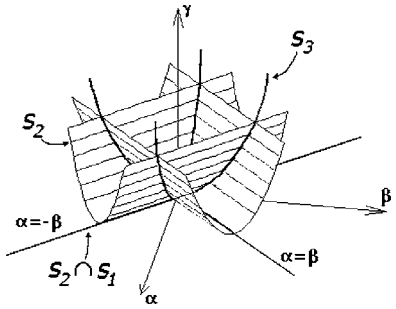


FIG. 2. The section of S_1, S_2, S_3 in region I.

$$B = \frac{(\alpha-\beta)^2}{\gamma} - A + 2C \quad \text{on the branch } B_1,$$

$$B = \frac{(\alpha+\beta)^2}{\gamma} - A - 2C \quad \text{on the branch } B_2.$$

Substituting them in the matrix M (9) and calculating the adjoint we obtain that in both cases all the nonvanishing 5×5 minors contain the factor $\alpha\beta-\gamma C$ and one of them is $\gamma^2(\alpha\beta-\gamma C)$. Then the rank is 5 except when $\gamma C=\alpha\beta$, that is outside of $S_3=B_1\cap B_2$. □

The surface $S_2-(S_1\cup S_3)$ is formed by several connected components: in Sec. III B we will study which of these components are mapped one in the other by the discrete transformations and then generate the same type of coordinates system.

Proposition 13: The rank of Δ_M on S_3-S_1 is 4.

Proof: From the previous proposition the rank of Δ_M on S_3-S_1 is at most 4 and it is lesser if all the 4×4 minors of M vanish. Outside of the intersection with S_1 (i.e., for $\gamma\neq0$) Eq. (12) of S_3 is

$$B = \frac{\alpha^2+\beta^2}{\gamma}, \quad C = \frac{\alpha\beta}{\gamma}$$

and substituting them in M one of the 4×4 minors is $\gamma^3\neq0$. Hence, the rank of Δ_M on S_3-S_1 is always 4. □

Let us now analyze the intersection between S_1 and S_2: $S_1\cap S_2$ is formed by two branches isomorphic to $\mathbb{R}^4$ intersecting in the three-dimensional vector space $\alpha=\beta=\gamma=0$. The first branch is described by the equations $\gamma=0$ and $\alpha=\beta$, while the second by the equations $\gamma=0$ and $\alpha=-\beta$. Inside $S_1\cap S_2$ we point out the surface (union of two branches, named, respectively, C_1 and C_2)

$$S_4:\begin{cases}\gamma=0\\ \alpha=\beta\\ A+B=2C\end{cases}\cup\begin{cases}\gamma=0\\ \alpha=-\beta\\ A+B=-2C\end{cases}\qquad \dim S_4=3. \tag{13}$$

We observe that the branches C_1 and C_2 are both isomorphic to $\mathbb{R}^4$ and their intersection (belonging entirely to $S_1\cap S_3$) is the line

$$C_1\cap C_2=S_5:\begin{cases}\alpha=\beta=\gamma=0\\ B=-A\\ C=0\end{cases}\qquad \dim S_5=1. \tag{14}$$

Proposition 14: The rank of Δ_M on $(S_1\cap S_2)-(S_3\cup S_4)$ is 4.

Proof: We study the rank of Δ_M on the two branches of $S_1\cap S_2$ separately. Moreover we work

outside of the intersection with S_3 (α and β both different from zero). On the first branch, where $\gamma=0$ and $\alpha=\beta$, we get that all the nonvanishing 4×4 minors contain the factor $\alpha^2(2C-B-A)$; on the other branch, where $\gamma=0$ and $\alpha=-\beta$, all the nonvanishing minors contain the factor $\alpha^2(B+A+2C)$. Then the rank is 4 outside S_4. □

Proposition 15: The rank of Δ_M on S_4-S_3 is 3.

Proof: We study the rank of the distribution on the two branches C_1 and C_2 of S_4. On C_1, where $\beta=\alpha$ and $2C=A+B$ it is straightforward that

$$V_2 = V_1 - 2\alpha V_5,$$

$$V_4 = V_3 + (A-B)V_5,$$

$$2V_6 = V_3 + V_4 + \frac{A+B}{2\alpha}(V_1+V_2)$$

and so outside of $S_4\cap S_3$, where $\alpha=0$. In a similar way, on $C_2\beta=-\alpha$ and $2C=-A-B$ hold, hence

$$V_2 = -V_1 - 2\alpha V_5,$$

$$V_4 = -V_3 + (A-B)V_5,$$

$$2V_6 = -V_3 + V_4 + \frac{A+B}{2\alpha}(V_2-V_1).$$

In both cases, the independent vector fields are V_1, V_3, and V_5 only. All the nonvanishing 3×3 minors of the two matrices constructed with these three vectors (restricted on C_1 and C_2, respectively) are real multiples of α^2, thus outside of $S_4\cap S_3$ the rank is 3. □

The rank of the distribution on $S_1\cap S_3$ remains to be evaluated. The space $S_1\cap S_3$ (see Fig. 4) is a three-dimensional vector space described by the equations $\alpha=\beta=\gamma=0$, with coordinates A, B, and C. We recall that $S_3\cap S_4\subset S_3\cap S_1$. On $S_3\cap S_1$ the only independent V_i are V_3, V_5, and V_6 and their components, with respect to $(\partial_A,\partial_B,\partial_C)$ can be collected in the matrix

$$\tilde{M} = \begin{pmatrix} 2C & 2C & A+B \\ 1 & -1 & 0 \\ A & B & C \end{pmatrix}. \tag{15}$$

Proposition 16: The rank of Δ_M on $(S_3\cap S_1)-S_4$ is 3.

Proof: The determinant of the matrix (15) is $\det\tilde{M}=(A+B+2C)(2C-A-B)$ and it vanishes only on the intersection with S_4. □

Proposition 17: The rank of Δ_M on $(S_3\cap S_4)-S_5$ is 2.

Proof: Evaluating the matrix $\tilde{M}$ on the two branches of $S_3\cap S_4$ we get in both cases that all the nonvanishing 2×2 minors contain the factor $A+B$, and one of them is exactly $-(A+B)$, then the rank is lesser than 2 only on the intersection of the branches given by $B=-A$, that is on the line S_5. □

Proposition 18: The rank of Δ_M on S_5 is 1.

Proof: On S_5 the only independent vector field is the constant vector V_5. □

B. Discrete transformations

As we already mentioned besides the continuous transformations associated with the vector fields V_i we have to consider also some discrete transformation leaving unchanged the web associated with a given Killing tensor: the first one is the change of the sign of the tensor

$$R_0{:}K \to -K$$

and the others are induced from the discrete isometries of the Minkowski plane $\{\overline{t}=t,\overline{x}=-x\}$ and $\{\overline{t}=-t,\overline{x}=x\}$, they are

$$R_1{:}C \to -C, \alpha \to -\alpha,$$

$$R_2{:}C \to -C, \beta \to -\beta.$$

Now we have to study the connected components of the sets determined in the Sec. III A and which of them are linked through one of the above discrete transformations. Since some of these sets have a quite high dimension we use the sectioning technique presented in Sec. I B.

In order to study the open set $\mathcal{K}(\mathbb{M}_2)-S_1-S_2$ we observe that it is the set where the three functions

$$\gamma,$$

$$Z_+ = \gamma(A+B-2C) - (\alpha-\beta)^2,$$

$$Z_- = \gamma(A+B+2C) - (\alpha+\beta)^2$$

are all different from zero, where the notation of Ref. 10 has been used. Then, the continuous function $\mathcal{K}(\mathbb{M}_2) \to \mathbb{R}^3$ given by $\Phi=(\gamma,Z_+,Z_-)$ maps $\mathcal{K}(\mathbb{M}_2)-S_1-S_2$ in the eight connected components of $\mathbb{R}^3$ without the coordinate planes. We introduce the eight (not empty) sets $\Gamma_1,\ldots,\Gamma_8$ such that

$$\Phi(\Gamma_1)=(+,+,+), \quad \Phi(\Gamma_5)=(-,+,+),$$

$$\Phi(\Gamma_2)=(+,+,-), \quad \Phi(\Gamma_6)=(-,+,-),$$

$$\Phi(\Gamma_3)=(+,-,+), \quad \Phi(\Gamma_7)=(-,-,+),$$

$$\Phi(\Gamma_4)=(+,-,-), \quad \Phi(\Gamma_8)=(-,-,-).$$

The sets $\Gamma_1,\ldots,\Gamma_8$ form a partition of $\mathcal{K}(\mathbb{M}_2)-S_1-S_2$.

Proposition 19: All the sets $\Gamma_1,\ldots,\Gamma_8$ *are connected and then the set* $\mathcal{K}(\mathbb{M}_2)-(S_1\cup S_2)$ *has* 8 *connected components. We have three orbits of the action:* $\Gamma_1\cup\Gamma_5$, $\Gamma_4\cup\Gamma_8$ (*both linked by the transformation* R_0) *and* $\Gamma_2\cup\Gamma_3\cup\Gamma_6\cup\Gamma_7$ (*linked by* R_0 *and* R_1).

Proof: We prove that all the sets $\Gamma_1,\ldots,\Gamma_8$ are connected by showing that all the connected components of their sections are equivalent in the sense of Lemma 3. First of all we remark that for any two sections with parameter belonging to same region of Fig. 1, the corresponding connected components (of any Γ_i) are trivially equivalent. Hence the sets Γ_1 and Γ_5 are connected because their sections are nonempty only for parameters in regions I and III, respectively. For any of the other Γ_i there exists a region of the parameter space in which the corresponding section has a unique connected component. On the other hand it is possible to construct a continuous path connecting a point of any connected components of the section of a given Γ_i to a point in the one with a unique connected component. For instance moving the parameters along the path shown in Fig. 1 (with $A+B+2C=$const) and leaving α, β, and γ fixed we link any point in one of the two connected components of Γ_3 obtained for parameter in region I, to a point in the unique connected component of the section of Γ_3, obtained for parameters in region II. We conclude, by applying Lemma 3, that the sets Γ_i are all connected. From the definition of transformation R_0 and R_1 we get that Γ_1 is in the same orbit of Γ_5, Γ_4 is in the same orbit of Γ_8, and all the other Γ_i are in the same orbit. Moreover, because all the transformations R_i maps any of the sets $\Gamma_1\cup\Gamma_5$, $\Gamma_4\cup\Gamma_8$, $\Gamma_2\cup\Gamma_3\cup\Gamma_6\cup\Gamma_7$ into themselves, they form distinct orbits. □

In order to study the set $S_2-(S_1\cup S_3)$ we introduce the eight (not empty) sets $\Theta_1,\dots,\Theta_8$ such that

$$\Phi(\Theta_1)=(+,0,+),\quad \Phi(\Theta_5)=(-,0,+),$$

$$\Phi(\Theta_2)=(+,0,-),\quad \Phi(\Theta_6)=(-,0,-),$$

$$\Phi(\Theta_3)=(+,+,0),\quad \Phi(\Theta_7)=(-,+,0),$$

$$\Phi(\Theta_4)=(+,-,0),\quad \Phi(\Theta_8)=(-,-,0).$$

The sets $\Theta_1,\dots,\Theta_8$ form a partition of $S_2-(S_1\cup S_3)$.

Proposition 20: All the sets $\Theta_1,\dots,\Theta_8$ are connected and then the set $S_2-(S_1\cup S_3)$ has 8 connected components. We have two orbits of the action: $\Theta_1\cup\Theta_3\cup\Theta_5\cup\Theta_7$ and $\Theta_2\cup\Theta_4\cup\Theta_6\cup\Theta_8$ (both linked by the transformations R_0 and R_1).

Proof: As in the previous proposition we prove that all the sets $\Theta_1,\dots,\Theta_8$ are connected by showing that all the connected components of their sections are equivalent in the sense of Lemma 3. Also in this case for any two sections with parameter belonging to same region of Fig. 1, the corresponding connected components (of any Θ_i) are trivially equivalent. We observe that because the plane $\gamma=0$ is removed all the paraboloids that form the sections of the sets Θ_i consist of at least two disconnected parts. For any Θ_i a section with a unique connected component exists. For instance in the section labeled T, in Fig. 1, the sets Θ_1 and Θ_5 have a connected section. Moreover it is possible to construct a continuous path connecting a point of any connected components of the section of a given Θ_i to a point in the one with a unique connected component. We conclude, by applying Lemma 3, that the sets Θ_i are all connected. From the definition of transformation R_0 and R_1 we get that Θ_1, Θ_3, Θ_5, and Θ_7 are mapped one into the other and then are in the same orbit, as well Θ_2, Θ_4, Θ_6, and Θ_8. Moreover, because all the transformations R_i maps the two sets $\Theta_1\cup\Theta_3\cup\Theta_5\cup\Theta_7$ and $\Theta_2\cup\Theta_4\cup\Theta_6\cup\Theta_8$ into themselves, they form distinct orbits. □

Proposition 21: The set S_3-S_1 has two connected components mapped one in the other by R_0, and so it forms a unique orbit of the action.

Proof: A section of the set S_3-S_1 is not empty only if its parameters (A,B,C) belong to the closure of regions I and III, referring to the notation of Fig. 1. All sections with parameters belonging to the interior of I (respectively, III) have four connected components which are equivalent to the positive part of the axis γ (respectively, the negative part) in the sections with parameters $A+B=C=0$. The sections with parameters on the boundary of I (respectively, III) and $C\neq 0$ have two connected components, also equivalent to the positive part of the axis γ (respectively, the negative part) in the sections with parameters $A+B=C=0$. Hence just two different equivalence classes of sections exist, corresponding to two connected components of S_3-S_1: one corresponds to positive values of γ, while the other to negative ones. Since the transformation R_0 maps the positive part of the γ axis in the negative one, these two connected components form a unique orbit. □

Proposition 22: The set S_1-S_2 is formed by 4 connected components. Each pair of components symmetric with respect to the origin are linked by R_0, thus two orbit of the action are present.

Proof: S_1 is homeomorphic to $\mathbb{R}^5$, then it is divided in four connected parts by the two four-dimensional hyperplanes that form $S_1\cap S_2$. The transformation R_0 represents a central symmetry and links together components symmetric with respect to the origin. The two transformations R_1 and R_2 on S_1-S_2 are symmetries with respect to the α and β axes, hence they map the two orbits into themselves. □

Proposition 23: The set $(S_1\cap S_2)-(S_3\cup S_4)$ contains eight connected components. They can be linked together using the three discrete transformation R_0, R_1, and R_2 and so they form a unique orbit of the action.

Proof: Each of the two branches of $S_1\cap S_2$ is homeomorphic to $\mathbb{R}^4$. Cutting out from the first

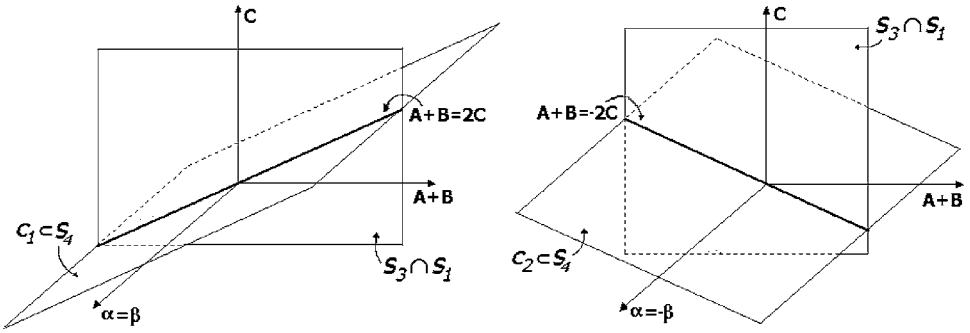


FIG. 3. The two branches of S_4 in $S_1 \cap S_2$.

one the two three-dimensional hyperplanes $S_3 \cap S_1$ and C_1, and from the second one $S_3 \cap S_1$ and C_2, respectively, we obtain four connected components in each case. In order to prove that all the components form a unique orbit, we can consider just the branch defined by $\alpha=\beta$, because R_1 (or equivalently R_2) maps each branch into the other. The transformation R_0 maps one in the other the components symmetric with respect to the origin (see Fig. 3), while the transformation $R_1 \circ R_2$ (corresponding in this branch to the inversion of the $\alpha=\beta$ axis) maps one in the other the components symmetric with respect to the hyperplane $S_3 \cap S_1$. Therefore all the eight connected components form a unique orbit. □

Proposition 24: The set $S_4 - S_3$ contains four connected components. They can be linked together using R_0 and one between R_1 and R_2 and so they form a unique orbit of the action.

Proof: Each of the two branches C_1 and C_2 of S_4 is homeomorphic to $\mathbb{R}^3$. Cutting out from the first one the two two-dimensional hyperplane $S_3 \cap S_4$, we obtain two connected components in each case. Each of the transformations R_1 or R_2 maps C_1 in C_2 and R_0 links the two connected components of C_2. Thus we have a unique orbit. □

Proposition 25: The space $(S_3 \cap S_1) - S_4$ has four connected components. The two pairs of components symmetric with respect to the origin (linked by R_0) form two different orbits of the action.

Proof: As shown in Fig. 4, in the space of coordinates A, B, and C, the set $(S_3 \cap S_1) - S_4$ is composed by the four dihedra determined by the two planes $A+B=2C$ and $A+B=-2C$. Hence it has four connected components. The transformation R_0 links together the two dihedra containing the plane $C=0$ as well as the other pair of dihedra. Unfortunately neither R_1 nor R_2 is able to connect together these two pairs of dihedra. Hence in $(S_3 \cap S_1) - S_4$ we have two different orbits: indeed, the KTs belonging to the pair that contains the plane $C=0$ define pseudo-Cartesian coordinates, while the ones belonging to the other pair are not characteristic tensors, with everywhere imaginary eigenvalues. □

Proposition 26: The space $(S_3 \cap S_4) - S_5$ has four connected components. They are mapped one into the other by the two discrete transformations R_0 and R_1, hence they form a unique orbit of the action.

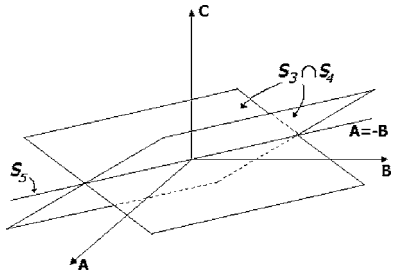


FIG. 4. The space $S_3 \cap S_1$.

Proof: As shown in Fig. 4, in the space of coordinates A, B, and C, the set $(S_3 \cap S_4) - S_5$ is formed by two planes intersecting on the line $A+B=0$, $C=0$ (S_5) without their intersection. Hence it has four connected components. The transformation R_0 maps an half of each plane in the other; moreover, the transformation R_1 maps each plane into the other. □

Proposition 27: The line S_5 formed by the (noncharacteristic) tensors of the kind $\tau \mathbf{g}$ is a connected orbit of the action.

The following list contains all orbits of the action of the group generated by the vector fields V_i, extended with the three finite transformations. For each orbit a representative tensor is given. Orbits of characteristic Killing tensors are labeled according both to Refs. 10 and 8 and the associated *complete* web is plotted. In each picture the set of singular points and the two distinct foliations of the web are emphasized completing the partial representation given in Refs. 10 and 8: the leaves belonging to the two foliations are plotted dashed and continuous, respectively, the grey lines represent the boundaries of the singular set of the web.

M1) The set $\Gamma_1 \cup \Gamma_5$, contained in $\mathcal{K}(\mathbb{M}_2) - (S_1 \cup S_2)$, where $Z_+ > 0$ and $Z_- > 0$: SC9, elliptic coordinates of type I. A tensor of this type is

$$\begin{pmatrix} x^2 & xt \\ xt & t^2+1 \end{pmatrix}.$$

M2) The set $\Gamma_2 \cup \Gamma_3 \cup \Gamma_6 \cup \Gamma_7$, contained in $\mathcal{K}(\mathbb{M}_2) - (S_1 \cup S_2)$, where Z_+ and Z_- have different sign: SC8, hyperbolic coordinates of type I. A tensor of this type is

$$\begin{pmatrix} x^2 & 1+xt \\ 1+xt & t^2 \end{pmatrix}.$$

M3) The set $\Gamma_4 \cup \Gamma_8$, contained in $\mathcal{K}(\mathbb{M}_2) - (S_1 \cup S_2)$, where $Z_+ < 0$ and $Z_- < 0$: SC5 and SC10, elliptic coordinates of type II. A tensor of this type is

$$\begin{pmatrix} x^2 & xt \\ xt & t^2-1 \end{pmatrix}.$$

M4) The set $\Theta_1 \cup \Theta_3 \cup \Theta_5 \cup \Theta_7$ contained in $S_2 - (S_1 \cup S_3)$, where the nonvanishing one of the two functions $Z_\pm$ is positive: SC6, hyperbolic coordinates of type II. Two tensors of this type are

$$\begin{pmatrix} x^2+1 & xt+1 \\ xt+1 & t^2+1 \end{pmatrix}, \quad \begin{pmatrix} x^2+1 & xt-1 \\ xt-1 & t^2+1 \end{pmatrix}.$$

M5) The set $\Theta_2 \cup \Theta_4 \cup \Theta_6 \cup \Theta_8$ contained in $S_2 - (S_1 \cup S_3)$, where the nonvanishing one of the two functions $Z_\pm$ is negative: SC7, hyperbolic coordinates of type III. Two tensors of this type are

$$\begin{pmatrix} x^2-1 & xt-1 \\ xt-1 & t^2-1 \end{pmatrix}, \quad \begin{pmatrix} x^2-1 & xt+1 \\ xt+1 & t^2-1 \end{pmatrix}.$$

M6) The set $S_3 - S_1$: SC2, polar coordinates. A tensor of this type is

$$\begin{pmatrix} x^2 & xt \\ xt & t^2 \end{pmatrix}.$$

M7) The subset of $S_1 - S_2$ containing the α axis: first web for SC4, parabolic coordinate of type I. A tensor of this type is

$$\begin{pmatrix} 2x & t \\ t & 0 \end{pmatrix}.$$

M8) The subset of S_1-S_2 containing the β axis: second web for SC4, parabolic coordinate of type I. A tensor of this type is

$$\begin{pmatrix} 0 & x \\ x & 2t \end{pmatrix}.$$

M9) The set $(S_1 \cap S_2)-(S_3 \cup S_4)$: SC3, parabolic coordinate of type II. Two tensors of this type are

$$\begin{pmatrix} 1+2x & x+t \\ x+t & 1+2t \end{pmatrix}, \quad \begin{pmatrix} 2x+1 & x+t-1 \\ x+t-1 & 2t+1 \end{pmatrix}.$$

M10) The set S_4-S_3: no characteristic tensors. A tensor of this type is

$$\begin{pmatrix} 2x & x+t \\ x+t & 2t \end{pmatrix}.$$

M11) The subset of $(S_1 \cap S_3)-S_4$ containing the plane $C=0$, that is where $\alpha=\beta=\gamma=0$ and $|A+B|>2|C|$: SC1, Cartesian coordinates. A tensor of this type is

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

M12) The subset of $(S_1 \cap S_3)-S_4$ not containing the plane $C=0$, that is where $\alpha=\beta=\gamma=0$ and $|A+B|<2|C|$: no characteristic tensors. A tensor of this type is

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

M13) The set $(S_3 \cap S_4)-S_5$, that is where $\alpha=\beta=\gamma=0$ and $|A+B|=2|C|$: no characteristic tensors. A tensor of this type is

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

M14) The line S_5, containing tensors multiple of the metric.

As in the Euclidean case, our classification is closely related to the one of Rastelli[13] based on the analysis of the singular set of the tensors. The discriminant of the characteristic polynomial of the general KT of the Minkowski plane is

$$\Delta = (\gamma(x+t)^2 + 2(\alpha+\beta)(x+t) + A + B + 2C)(\gamma(x-t)^2 + 2(\alpha-\beta)(x-t) + A + B - 2C).$$

For $\gamma \neq 0$ (i.e., outside of S_1), we rewrite Δ as

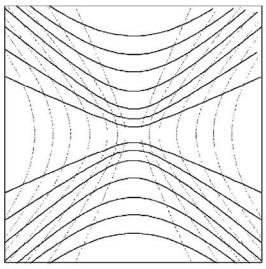
$$\gamma^2\left(\left(x+t+\frac{\alpha+\beta}{\gamma}\right)^2 + \frac{1}{\gamma^2}Z_+\right)\left(\left(x-t+\frac{\alpha-\beta}{\gamma}\right)^2 + \frac{1}{\gamma^2}Z_-\right).$$

In this case the set $\Delta=0$ is made of two couples of lines parallel to $x=t$ and $x=-t$, respectively. It is immediate to see that the lines of the first (second) pair are real and distinct, real and coinciding, imaginary according to the fact that Z_+ (Z_-) is negative, zero, or positive. So the singular set is empty when both $Z_\pm$ are positive (SC9); a strip when $Z_+Z_-<0$ (SC8); two intersecting strips without their intersection when $Z_\pm$ are negative (SC5,SC10); a line when one of $Z_\pm$ vanishes and the other is positive (SC6); a strip and a line orthogonal to it when one of $Z_\pm$ vanishes and the other is positive (SC7); two orthogonal lines if both $Z_\pm$ vanish.

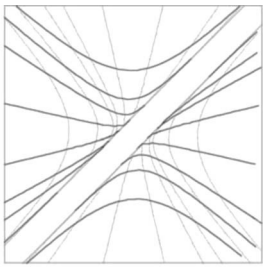
On S_1 we have $\gamma=0$ and the discriminant reduces to

$$(2(\alpha+\beta)(x+t)+A+B+2C)(2(\alpha-\beta)(x-t)+A+B-2C).$$

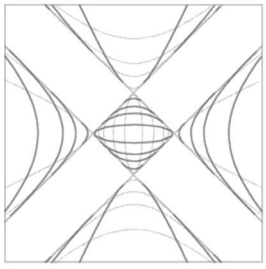
On S_4 the discriminant identically vanishes, so the singular set is all the plane and the corresponding tensors are not characteristic tensors. Outside of S_4, if the discriminant is not constant (i.e., outside of $S_1\cap S_3$), then $\Delta=0$ is a pair of orthogonal lines or a single line and the singular set is made of two opposite quadrants (the two webs corresponding to SC4) or of a half-plane (SC3). If Δ is a positive constant, the singular set is empty (SC1), while if it is negative all points are singular and the tensor is not characteristic ($(S_1\cap S_3)-S_4$ not containing the plane $C=0$). The classification given here can also be compared with that given in Table III of Ref. 10, where the type of any separable web in $\mathbb{M}_2$ is characterized in terms gamma and $I_\pm=\mathrm{sgn}(Z_\pm)$. Note that in Ref. 10 (as in Ref. 8) the discrete transformation $\hat{R}_2$ is used, with the consequence that the number of distinct types of separable webs is reduced from the ten described in the present paper to nine. See the following diagrams:



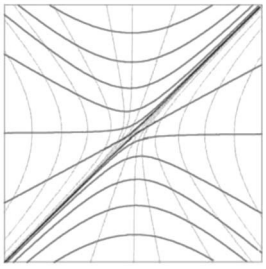
Web for SC9



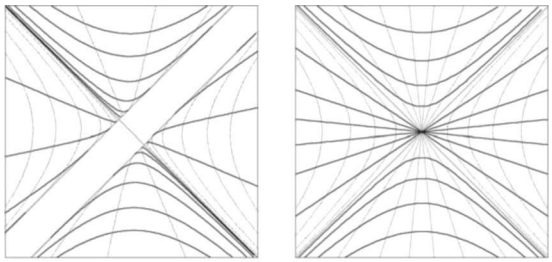
Web for SC8



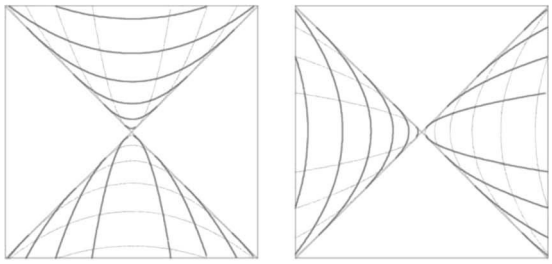
Web for SC5 and SC10



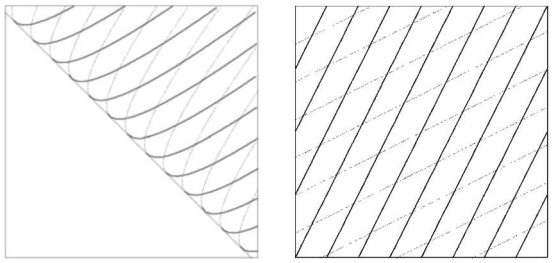
Web for SC6



Web for SC7 Web for SC2



First web for SC4 Second web for SC4



Web for SC3 Web for SC1

IV. CONCLUSION

We have classified Killing tensors of valence two in the Euclidean and Minkowski planes under the action of a group that preserves the type of the Killing web. The method is based on a detailed analysis of the rank of the determining system of partial differential equations for the group invariants and depends crucially on the fact the generic rank of the system is six, which equals the dimension of the space of Killing two-tensors. This result is dimensionally dependent. It is thus unclear whether the method or a modification thereof can be extended to flat spaces of higher dimension or to spaces of nonzero constant curvature. Nonetheless for the cases where the method is applicable it provides a very elegant algebraic classification for the type of the Killing web defined by a characteristic Killing tensor. This classification is equivalent to the classification of quadratic symmetric operators in the generators of the isometries of $\mathbb{M}_2$, given in Ref. 8 and to the classification given in Ref. 10 in terms of Killing tensor invariants, up to the exchange between space and time: since we do not allow a change in signature of the metric, the coordinates of type SC4 (parabolic of type I in Ref. 8) splits into the classes M7 and M8. Our classification, not being restricted to characteristic Killing tensors, extends the classification given in Ref. 10 through the invariant theory of Killing tensors.

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Stochastic quantization of topological field theory: Generalized Langevin equation with memory kernel

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We use the method of stochastic quantization in a topological field theory defined in an Euclidean space, assuming a Langevin equation with a memory kernel. We show that our procedure for the Abelian Chern-Simons theory converges regardless of the nature of the Chern-Simons coefficient. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2219158]

I. INTRODUCTION

In the Euclidean version of field theory, we are interested in computing the Schwinger functions of a theory. In order to obtain these functions, Parisi and Wu introduced the stochastic quantization.[1] This formalism was introduced as an alternative quantization scheme, different from the usual canonical and the path integral field quantization, based in the Hamiltonian and the Lagrangian, respectively. The method starts from a classical equation of motion, but not from Hamiltonian or Lagrangian, and consequently can be used to quantize dynamical systems without canonical formalism and therefore it is useful in situations where the other methods lead to difficult problems.

The main idea of the stochastic quantization is that a d-dimensional quantum system is equivalent to a $(d+1)$-dimensional classical system that undergoes random fluctuations. Some of the most important papers in the subject can be found in Ref. 2. A brief introduction to the stochastic quantization can be found in Ref. 3 and Ref. 4. See also Ref. 5.

In a previous paper,[6] we studied the stochastic quantization of a self-interacting scalar field theory, assuming a non-Markovian process, modifying the Langevin equation by introducing a memory kernel.[7–9] We have shown that although a system with a stationary, Gaussian, non-Markovian Langevin equation with a memory kernel and a colored noise converges in the asymptotic limit of the Markov parameter τ to the equilibrium, we obtain a nonregularized theory.

In this paper we would like to continue to investigate the virtues of this non-Markovian stochastic quantization method, now employed in the case of a topological field theory. One of the peculiar features within this kind of theory is the appearance of a factor of i in front of the topological action in Euclidean space. Since the topological theory does not depend on the metric of space-time, the path integral measure weighing remains to be e^{iS}, even after the Wick rotation. Another feature of a topological action is that it is the integral of a density that is not bounded from below in Euclidean space. So, if one attempts to use a Markovian Langevin equation with a white noise to quantize this theory, one will find serious problems if the factor of i is ignored. This Langevin equation will not tend to any equilibrium in the large τ limit. So, in this sense, the use of a Langevin equation with a complex action[10] becomes essential for stochastically quantizing a topological action.[11–13]

There is, in the literature, an approach to solve the above mentioned convergence problem. Studying the purely topological Chern-Simons theory, Ferrari *et al.* introduced a nontrivial kernel

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in the Langevin equation.[14] On the other way, Wu *et al.*[15] showed that the Langevin equation for a Maxwell-Chern-Simons theory converges to the usual equilibrium result without the need to introduce such a kernel. Their method, however, only works in the case where the Chern-Simons coefficient is real.

We show in this paper that, if one uses a non-Markovian Langevin equation with a colored random noise, this convergence problem may be solved in a different way. We will apply this approach to three-dimensional Abelian Chern-Simons theory and prove that we obtain convergence toward equilibrium, even with an imaginary Chern-Simons coefficient. To simplify the calculations we assume the units to be such that $\hbar=c=1$.

II. STOCHASTIC QUANTIZATION OF ABELIAN CHERN-SIMONS THEORY

Let us consider the following action for the three-dimensional Maxwell-Chern-Simons theory, in Euclidean space:

$$S=\int d^3x\left(\frac{1}{4\epsilon^2}A_\mu(x)(-\Delta\delta_{\mu\nu}+\partial_\mu\partial_\nu)A_\nu(x)-i\frac{\kappa}{8\pi}\epsilon_{\mu\nu\rho}A_\mu(x)\partial_\nu A_\rho(x)\right), \tag{1}$$

where Δ is the three-dimensional Laplace operator. At the end of our calculations we set $\epsilon\to\infty$ to obtain the results for the purely topological theory, as discussed in Ref. 15. Notice the factor of i in front of the topological term, as mentioned before. In order to obtain the Schwinger functions of the theory, let us use the stochastic quantization method. Let us introduce a non-Markovian Langevin equation given by

$$\frac{\partial}{\partial\tau}A_\mu(\tau,x)=-\int_0^\tau ds\, M_\Lambda(\tau-s)\frac{\delta S}{\delta A_\mu(x)}\Big|_{A_\mu(x)=A_\mu(s,x)}+\eta_\mu(\tau,x), \tag{2}$$

where $M_\Lambda(\tau-s)$ is a memory kernel and Λ is a arbitrary parameter. We will have, from Eqs. (1) and (2), in momentum space:

$$\frac{\partial}{\partial\tau}A_\mu(\tau,k)=-\frac{k^2}{\epsilon^2}\left(\delta_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)\int_0^\tau ds\, M_\Lambda(\tau-s)A_\nu(s,k)-\frac{\kappa}{4\pi}\epsilon_{\mu\nu\rho}k_\rho\int_0^\tau ds\, M_\Lambda(\tau-s)A_\nu(s,k)$$
$$+\eta_\mu(\tau,k), \tag{3}$$

where the stochastic field $\eta_\mu(\tau,k)$ satisfies the modified Einstein relations:

$$\langle\eta_\mu(\tau,k)\rangle_\eta=0, \tag{4}$$

and also

$$\langle\eta_\mu(\tau,k)\,\eta_\nu(\tau',k')\rangle_\eta=2\,\delta_{\mu\nu}M_\Lambda(|\tau-\tau'|)\,\delta^d(k+k'). \tag{5}$$

For the initial condition $A_\mu(\tau,k)|_{\tau=0}=0$, it is easy to see that the solution of Eq. (3) is given by

$$A_\mu(\tau,k)=\int_0^\infty d\tau'\, G_{\mu\nu}(k;\tau-\tau')\,\eta_\nu(\tau',k), \tag{6}$$

where we introduced the retarded Green's function $G_{\mu\nu}(k,r)$, which satisfies

$$\frac{\partial}{\partial\tau}G_{\mu\nu}(k,\tau)=-\frac{k^2}{\epsilon^2}\left(\delta_{\mu\rho}-\frac{k_\mu k_\rho}{k^2}\right)\int_0^\tau ds\, M_\Lambda(\tau-s)G_{\rho\nu}(k,s)-\frac{\kappa}{4\pi}\epsilon_{\mu\rho\sigma}k_\sigma\int_0^\tau ds\, M_\Lambda(\tau-s)G_{\rho\nu}(k,s)$$
$$+\delta_{\mu\nu}\delta(\tau), \tag{7}$$

for $\tau>0$ and $G_{\mu\nu}(k,\tau)=0$ for $\tau<0$.

To proceed the calculations, let us introduce the Laplace transform of Eq. (7):

$$zG_{\mu\nu}(k,z) = -\frac{k^2}{\epsilon^2}\left(\delta_{\mu\rho} - \frac{k_\mu k_\rho}{k^2}\right)M_\Lambda(z)G_{\rho\nu}(k,z) - \frac{\kappa}{4\pi}\epsilon_{\mu\rho\sigma}k_\sigma M_\Lambda(z)G_{\rho\nu}(k,z) + \delta_{\mu\nu}, \tag{8}$$

where

$$M_\Lambda(z) = \int_0^\infty d\tau\, M_\Lambda(\tau)e^{-z\tau}. \tag{9}$$

For the result without memory [or, formally, when $M_\Lambda(\tau) \to \delta(\tau)$], we have, from Eq. (7),

$$\frac{\partial}{\partial\tau}G_{\mu\nu}(k,\tau) = -\frac{k^2}{\epsilon^2}\left(\delta_{\mu\rho} - \frac{k_\mu k_\rho}{k^2}\right)G_{\rho\nu}(k,\tau) - \frac{\kappa}{4\pi}\epsilon_{\mu\rho\sigma}k_\sigma G_{\rho\nu}(k,\tau) + \delta_{\mu\nu}\delta(\tau), \tag{10}$$

whose Laplace transform reads as

$$zG_{\mu\nu}(k,z) = -\frac{k^2}{\epsilon^2}\left(\delta_{\mu\rho} - \frac{k_\mu k_\rho}{k^2}\right)G_{\rho\nu}(k,z) - \frac{\kappa}{4\pi}\epsilon_{\mu\rho\sigma}k_\sigma G_{\rho\nu}(k,z) + \delta_{\mu\nu}. \tag{11}$$

Note the similarity between Eqs. (8) and (11). The solution to Eq. (10) is given by[15]

$$G_{\mu\nu}(k,\tau) = \frac{k_\mu k_\nu}{k^2} + \left(\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)\cos\left(\frac{\kappa}{4\pi}k\tau\right) \quad - \epsilon_{\mu\nu\sigma}\frac{k_\sigma}{k}\sin\left(\frac{\kappa}{4\pi}k\tau\right)\right)\exp\left(\frac{-k^2}{\epsilon^2}\tau\right), \tag{12}$$

whose Laplace transform is

$$G_{\mu\nu}(k,z) = \frac{k_\mu k_\nu}{k^2}\frac{1}{z} + \frac{\left(\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)z - \epsilon_{\mu\nu\sigma}k_\sigma\left(\frac{\kappa}{4\pi}\right)\right)}{\left(z + \frac{k^2}{\epsilon^2}\right)^2 + \left(\frac{\kappa}{4\pi}\right)^2 k^2}. \tag{13}$$

Comparing Eqs. (8) and (11), it is trivial to obtain the analog of Eq. (13) with memory:

$$G_{\mu\nu}(k,z) = \frac{k_\mu k_\nu}{k^2}\frac{1}{z} + \frac{\left(\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)z - \epsilon_{\mu\nu\sigma}k_\sigma\left(\frac{\kappa'}{4\pi}\right)\right)}{\left(z + \frac{k^2}{\epsilon'^2}\right)^2 + \left(\frac{\kappa'}{4\pi}\right)^2 k^2}, \tag{14}$$

where

$$\frac{1}{\epsilon'^2} \equiv \frac{M_\Lambda(z)}{\epsilon^2} \tag{15}$$

and

$$\kappa' \equiv \kappa M_\Lambda(z). \tag{16}$$

In the Appendix , we derive in detail the inverse Laplace transform of Eq. (14). It is given by

$$G_{\mu\nu}(k,\tau) = \left(\frac{k_\mu k_\nu}{k^2} + g_{\mu\nu}G_1(k,\tau) + \tilde{g}_{\mu\nu}G_2(k,\tau)\right)\theta(\tau), \tag{17}$$

where the quantities $G_i(k,\tau)$, $i=1,2$, $g_{\mu\nu}$ and $\tilde{g}_{\mu\nu}$ are defined in the Appendix . We see that our $G_{\mu\nu}(k,\tau)$ does not approach zero as $\tau\to\infty$. The reason for such behavior is the presence of the longitudinal term $k_\mu k_\nu/k^2$, which is common in the stochastic quantization of all gauge theories without gauge fixing and can be eliminated by a suitable stochastic gauge fixing. In spite of this, the presence of this term will not give any contribution to gauge invariant quantities.

After this discussion, we are able to present the two-point correlation function. We have that $D_{\mu\nu}(k;\tau,\tau')$ is given by

$$\begin{aligned} D_{\mu\nu}(k,\tau,\tau') &\equiv \langle A_\mu(\tau,k)A_\nu(\tau' k')\rangle_\eta \\ &= \delta^d(k+k')\int_0^\infty ds\int_0^\infty ds'\, G_{\mu\kappa}(k,\tau-s)G_{\lambda\nu}(k,\tau'-s')\langle \eta_k(s,k)\,\eta_\lambda(s',k')\rangle_\eta \\ &= 2\delta^d(k+k')\int_0^\infty ds\int_0^\infty ds'\, G_{\mu\lambda}(k,\tau-s)G_{\lambda\nu}(k,\tau'-s')M_\Lambda(|s-s'|). \end{aligned} \tag{18}$$

So, inserting Eq. (17) in the above equation and splitting the result in five different contributions yields

$$D_{\mu\nu}(k;\tau,\tau') = 2\delta^d(k+k')(J_1+J_2+J_3+J_4+J_5) \tag{19}$$

where:

$$J_1 \equiv \int_0^\tau ds\int_0^{\tau'} ds'\frac{k_\mu k_\nu}{k^2}M_\Lambda(|s-s'|), \tag{20}$$

$$J_2 \equiv \int_0^\tau ds\int_0^{\tau'} ds'\, g_{\mu\lambda}g_{\lambda\nu}G_1(k;\tau-s)G_1(k;\tau'-s')M_\Lambda(|s-s'|), \tag{21}$$

$$J_3 \equiv \int_0^\tau ds\int_0^{\tau'} ds'\, \tilde{g}_{\mu\lambda}\tilde{g}_{\lambda\nu}G_2(k;\tau-s)G_2(k;\tau'-s')M_\Lambda(|s-s'|), \tag{22}$$

$$J_4 \equiv \int_0^\tau ds\int_0^{\tau'} ds'\, g_{\mu\lambda}\tilde{g}_{\lambda\nu}G_1(k;\tau-s)G_2(k;\tau'-s')M_\Lambda(|s-s'|), \tag{23}$$

and, finally,

$$J_5 \equiv \int_0^\tau ds\int_0^{\tau'} ds'\, \tilde{g}_{\mu\lambda}g_{\lambda\nu}G_2(k;\tau-s)G_1(k;\tau'-s')M_\Lambda(|s-s'|). \tag{24}$$

We can solve these equations by ordering the fictitious times s and s', $s>s'$ for instance, and solving the integrals in s (s') in the interval $[0,t]$ ($[0,s]$). We obtain for J_1, in the limit $\tau\to\infty$,

$$J_1 = \frac{1}{2}\frac{k_\mu k_\nu}{k^2}\left(\tau-\frac{1}{\Lambda^2}\right). \tag{25}$$

The integrals J_2 and J_3 can be solved by analogy with the scalar case.[6] Making the following replacements:

$$(k^2+m^2)_1 \to \frac{\alpha}{\Lambda^2}(1-\Lambda^4)+\Lambda^2 y_1+\frac{(\alpha^2-y_1^2)}{\Lambda^2}, \tag{26}$$

$$(k^2+m^2)_2 \to \frac{\alpha}{\Lambda^2}(1+\Lambda^4)-\Lambda^2 y_1-\frac{(\alpha^2-y_1^2)}{\Lambda^2}, \tag{27}$$

where the subscript 1 (2) stands for the G_1 (G_2) case (see the Appendix), we will have, in the asymptotic limit $\tau\to\infty$, that

$$J_2 = \left(\frac{\alpha}{\Lambda^2}(1-\Lambda^4) + \Lambda^2 y_1 + \frac{(\alpha^2 - y_1^2)}{\Lambda^2}\right)^{-1}\left[\frac{\Lambda^2}{(\sigma\gamma)^2}\left(\frac{\Lambda^4}{4} + \frac{(\sigma+\gamma)^2}{4}\right)\left(\frac{\kappa}{4\pi}\right)\epsilon_{\mu\nu\rho}k_\rho\right.$$
$$\left. + (\sigma\gamma)^{-2}\left(\left(\frac{\Lambda^4}{4} + \frac{(\sigma+\gamma)^2}{4}\right)^2 - \frac{\Lambda^4}{4}k^2\left(\frac{\kappa}{4\pi}\right)^2\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)\right], \tag{28}$$

and

$$J_3 = \left(\frac{\alpha}{\Lambda^2}(1+\Lambda^4) - \Lambda^2 y_1 - \frac{(\alpha^2 - y_1^2)}{\Lambda^2}\right)^{-1}\left[-\frac{\Lambda^2}{(\sigma\gamma)^2}\left(\frac{\Lambda^4}{4} + \frac{(\sigma-\gamma)^2}{4}\right)\left(\frac{\kappa}{4\pi}\right)\epsilon_{\mu\nu\rho}k_\rho\right.$$
$$\left. + (\sigma\gamma)^{-2}\left(\left(\frac{\Lambda^4}{4} + \frac{(\sigma-\gamma)^2}{4}\right)^2 - \frac{\Lambda^4}{4}k^2\left(\frac{\kappa}{4\pi}\right)^2\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)\right]. \tag{29}$$

The remaining integrals J_4 and J_5 can be solved without any further complications.[16] Again, in the asymptotic limit $\tau\to\infty$, we obtain

$$J_4 + J_5 = \frac{f(\Lambda,\sigma,\gamma)}{g(\Lambda,\sigma,\gamma)}\left[-\frac{\Lambda^2}{(2\sigma\gamma)}\left(\frac{\kappa}{4\pi}\right)\epsilon_{\mu\nu\rho}k_\rho \quad + (\sigma\gamma)^{-2}\left(\left(\frac{\Lambda^4}{4} + \frac{(\sigma+\gamma)^2}{4}\right)\left(\frac{\Lambda^4}{4} + \frac{(\sigma-\gamma)^2}{4}\right)\right.\right.$$
$$\left.\left. + \frac{\Lambda^4}{4}k^2\left(\frac{\kappa}{4\pi}\right)^2\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)\right], \tag{30}$$

where

$$f(\Lambda,\sigma,\gamma) \equiv 153\Lambda^{14} + \Lambda^{10}[18(\sigma+\gamma)^2 + 17(\sigma-\gamma)^2 + 9\sigma\gamma] + \Lambda^6\left[(\sigma+\gamma)^4 + (\sigma-\gamma)^4\right.$$
$$\left. + \frac{\sigma\gamma}{2}((\sigma+\gamma)^2 + (\sigma-\gamma)^2) - \frac{9}{2}\sigma\gamma((\sigma+\gamma)^2 - \sigma\gamma(1-2\sigma\gamma))\right]$$
$$+ \Lambda^2\sigma\gamma\left[\frac{(\sigma+\gamma)^2}{2} - \sigma\gamma(\sigma+\gamma)^2 - \frac{1}{2}(\sigma+\gamma)^2(\sigma-\gamma)^2\right], \tag{31}$$

and

$$g(\Lambda,\sigma,\gamma) \equiv (9\Lambda^4 + (\sigma-\gamma)^2)(9\Lambda^4 + (\sigma+\gamma)^2)(\Lambda^4 + \sigma^2)(\Lambda^4 + \gamma^2). \tag{32}$$

As mentioned before, the linearly divergent longitudinal term, found in Eq. (25), can be eliminated by stochastic gauge fixing. Now, taking the limit $\epsilon\to\infty$, it is easy to see that the contribution $J_2 + J_3$ vanishes identically. Then, finally, we obtain, for the purely topological two-point correlation function:

$$D_{\mu\nu}(k;\tau,\tau') = 2\delta^{ij}(k+k')\left[\frac{1}{2}\frac{k_\mu k_\nu}{k^2}\left(\tau - \frac{1}{\Lambda^2}\right) + \frac{f'(\Lambda,\sigma,\gamma)}{g'(\Lambda,\sigma,\gamma)}\left(-\frac{\Lambda^2}{2Q(y_1')}\left(\frac{\kappa}{4\pi}\right)\epsilon_{\mu\nu\rho}k_\rho\right.\right.$$
$$\left.\left. + \left(\frac{\beta'}{Q^2(y_1')} - 1\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right)\right)\right], \tag{33}$$

where $\beta' = \beta|_{\epsilon\to\infty} = (\Lambda^4/4)k^2(\kappa/4\pi)$, $y_1' = y_1|_{\varepsilon\to\infty}$, and

$$f'(\Lambda,\sigma,\gamma) = f\Big|_{\varepsilon\to\infty} = 120\Lambda^{14} + \frac{19}{2}\Lambda^{10}Q(y_1') + 9\Lambda^6Q^2(y_1') - \frac{\Lambda^6}{2}Q(y_1') + \frac{9}{2}\Lambda^4Q(y_1') + \Lambda^2Q^2(y_1')$$
$$- 18Q^2(y_1') + \frac{9}{2}Q(y_1'), \tag{34}$$

$$g'(\Lambda,\sigma,\gamma) = g|_{\epsilon\to\infty} = 64\Lambda^8 Q^2(y_1') + 32\Lambda^4 Q^3(y_1') + 4Q^4(y_1'), \tag{35}$$

$$Q(y_1') \equiv (\Lambda^4 y_1' - (y_1')^2)^{1/2}. \tag{36}$$

We see that in our last expression for the propagator remained a term proportional to the Maxwell transversal propagator. This is a anomalous situation, since the Maxwell contribution is absent in the usual purely topological Chern-Simons theory. The origin of this anomalous situation is the use of a non-Markovian Langevin equation. To circumvent this problem and recover the usual result, we have to make the following choice:

$$\beta' = Q^2(y_1'), \tag{37}$$

which leads us to

$$y_1' = \frac{\Lambda}{2} \pm \frac{(\Lambda^8 - 4\beta')^{1/2}}{2}. \tag{38}$$

So, if we choose

$$y_1 = \frac{\Lambda}{2} \pm \frac{(\Lambda^8 - 4\beta')^{1/2}}{2} + \frac{C}{\varepsilon^n}, \tag{39}$$

where C is a real constant and n is an arbitrarily large integer number. Inserting this latter equation in Eq. (A23), we will get a cubic equation in C. From the usual Galois theory of radical solutions for polynomials,[16–18] we can always choose a real root from the three possible ones. So, in other words, we can always choose a real constant such that the two-point correlation function converges to a "purely topological" term, with some minor differences from the usual one. We notice as well that our approach still works when κ is purely imaginary [which is mathematically analogous to writing $A_\mu = A'_\mu + iA'_\mu$, where A'_μ is real, and taking the real part of the Langevin Eq. (3) in coordinate space].

III. CONCLUSIONS

In this paper we discussed the stochastic quantization for Maxwell Chern-Simons theory using a non-Markovian Langevin equation and examined the field theory that appears in the asymptotic limit of this non-Markovian process.

This paper is the second one of a program where the possibility that the Parisi-Wu quantization method can be extended is investigated, assuming a Langevin equation with a memory kernel with the modified Einstein relations. To make sure that this modification can be used, one must first check that the system evolves to the equilibrium in the asymptotic limit. Second, we have to show that it converges to the correct equilibrium distribution. We proved that although the system evolves to equilibrium, in the propagator remained a term proportional to the Maxwell transversal propagator. This is an anomalous situation, since the Maxwell contribution is absent in the usual purely topological Chern-Simons theory. To circumvent this problem and recover the usual result, we have imposed a constraint in the parameters of our theory.

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APPENDIX: DERIVATION OF THE RETARDED GREEN'S FUNCTION FOR THE DIFFUSION PROBLEM

In this Appendix, we derive the retarded Green's function for the diffusion problem $G_{\mu\nu}(k,\tau)$. Expanding the denominator in Eq. (A1), given by

$$G_{\mu\nu}(k,z)=\frac{k_\mu k_\nu}{k^2}\frac{1}{z}+\frac{\left(\left(\delta_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)z-\epsilon_{\mu\nu\sigma}k_\sigma\left(\frac{\kappa'}{4\pi}\right)\right)}{\left(z+\frac{k^2}{\epsilon'^2}\right)^2+\left(\frac{\kappa'}{4\pi}\right)^2k^2}, \tag{A1}$$

we have

$$G_{\mu\nu}(k,z)=\frac{k_\mu k_\nu}{k^2}\frac{1}{z}+\left(\delta_{\mu\nu}-\frac{k_\mu k_\nu}{k^2}\right)I_1(z)-\epsilon_{\mu\nu\sigma}k_\sigma\left(\frac{\kappa}{4\pi}\right)I_2(z), \tag{A2}$$

where

$$I_1(z)\equiv\frac{z}{P(z)}, \tag{A3}$$

$$I_2(z)\equiv\frac{M_\Lambda(z)}{P(z)}, \tag{A4}$$

and

$$P(z)\equiv z^2+2\frac{k^2}{\varepsilon^2}M_\Lambda(z)z+\frac{k^4}{\varepsilon^4}M_\Lambda^2(z)+\left(\frac{\kappa}{4\pi}\right)^2k^2M_\Lambda^2(z). \tag{A5}$$

Using the following exponential representation for the memory kernel $M_\Lambda(\tau)$:

$$M_\Lambda^n(\tau)=\frac{1}{2n!}\Lambda^2(\Lambda^2|\tau|)^n\exp(-\Lambda^2|\tau|), \tag{A6}$$

where Λ is a parameter, we will have, for the case $n=0$,

$$I_1(z)=\frac{z^3+2\Lambda^2z^2+\Lambda^4z}{\Omega(z)}, \tag{A7}$$

$$I_2(z)=\frac{\frac{\Lambda^2}{2}z+\frac{\Lambda^4}{2}}{\Omega(z)}, \tag{A8}$$

and

$$\Omega(z)\equiv z^4+2\Lambda^2z^3+(\Lambda^4+\alpha)z^2+\alpha\Lambda^2z+\beta, \tag{A9}$$

where

$$\alpha\equiv\frac{k^2\Lambda^2}{\varepsilon^2}, \tag{A10}$$

and

$$\beta\equiv\left(\frac{k^4}{\varepsilon^4}+\left(\frac{\kappa}{4\pi}\right)^2k^2\right)\frac{\Lambda^4}{4}. \tag{A11}$$

In order to get the inverse Laplace transform of Eq. (A2), we must seek for the solutions of the quartic equation $\Omega(z)=0$. As it is well known, a general quartic equation is a fourth-order polynomial equation of the form:

$$z^4 + a_3 z^3 + a_2 z^2 + a_1 z + a_0 = 0. \tag{A12}$$

Using the familiar algebraic technique developed by Ferrari and Cardano,[19] it is easy to show that the roots of Eq. (A12) are given by

$$z_1 = -\frac{1}{4}a_3 + \frac{1}{2}R + \frac{1}{2}D, \tag{A13}$$

$$z_2 = -\frac{1}{4}a_3 + \frac{1}{2}R - \frac{1}{2}D, \tag{A14}$$

$$z_3 = -\frac{1}{4}a_3 - \frac{1}{2}R + \frac{1}{2}E, \tag{A15}$$

$$z_4 = -\frac{1}{4}a_3 - \frac{1}{2}R - \frac{1}{2}E, \tag{A16}$$

where

$$R \equiv \left(\frac{1}{4}a_3^2 - a_2 + y_1\right)^{1/2}, \tag{A17}$$

$$D \equiv \begin{cases} (F(R)+G)^{1/2}, & \text{for } R \neq 0, \\ (F(0)+H)^{1/2}, & \text{for } R = 0, \end{cases} \tag{A18}$$

$$E \equiv \begin{cases} (F(R)-G)^{1/2}, & \text{for } R \neq 0, \\ (F(0)-H)^{1/2}, & \text{for } R = 0, \end{cases} \tag{A19}$$

$$F(R) \equiv \frac{3}{4}a_3^2 - R^2 - 2a_2, \tag{A20}$$

$$H \equiv 2(y_1^2 - 4a_0)^{1/2}, \tag{A21}$$

$$G \equiv \frac{1}{4}(4a_3a_2 - 8a_1 - a_3^3)R^{-1}, \tag{A22}$$

and y_1 is a real root of the following cubic equation:

$$y^3 - a_2 y^2 + (a_1 a_3 - 4a_0)y + (4a_2 a_0 - a_1^2 - a_3^2 a_0) = 0. \tag{A23}$$

Therefore, the inverse Laplace transform of $I_1(z)$ and $I_2(z)$ reads

$$I_1(\tau) = \frac{z_1^3 + 2\Lambda^2 z_1^2 + \Lambda^4 z_1}{(z_1 - z_2)(z_1 - z_3)(z_1 - z_4)} e^{z_1\tau} + \frac{z_2^3 + 2\Lambda^2 z_2^2 + \Lambda^4 z_2}{(z_2 - z_1)(z_2 - z_3)(z_2 - z_4)} e^{z_2\tau} + \frac{z_3^3 + 2\Lambda^2 z_3^2 + \Lambda^4 z_3}{(z_3 - z_1)(z_3 - z_2)(z_3 - z_4)} e^{z_3\tau} + \frac{z_4^3 + 2\Lambda^2 z_4^2 + \Lambda^4 z_4}{(z_4 - z_1)(z_4 - z_2)(z_4 - z_3)} e^{z_4\tau}, \tag{A24}$$

and

$$I_2(\tau) = \frac{\frac{\Lambda^2}{2} z_1 + \frac{\Lambda^4}{2}}{(z_1 - z_2)(z_1 - z_3)(z_1 - z_4)} e^{z_1\tau} + \frac{\frac{\Lambda^2}{2} z_2 + \frac{\Lambda^4}{2}}{(z_2 - z_1)(z_2 - z_3)(z_2 - z_4)} e^{z_2\tau} + \frac{\frac{\Lambda^2}{2} z_3 + \frac{\Lambda^4}{2}}{(z_3 - z_1)(z_3 - z_2)(z_3 - z_4)} e^{z_3\tau} + \frac{\frac{\Lambda^2}{2} z_4 + \frac{\Lambda^4}{2}}{(z_4 - z_1)(z_4 - z_2)(z_4 - z_3)} e^{z_4\tau}. \tag{A25}$$

Now, let us study a simple convergence criterion in order that $G_{\mu\nu}(k,\tau) \to 0$ as the Markov parameter goes to infinity, i.e., $\tau \to \infty$. In this situation, the system converges to an equilibrium. Comparing the polynomial $\Omega(z)$ with expression Eq. (A12), it is trivial to make the following identifications: $a_0 = \beta$, $a_1 = \alpha\Lambda^2$, $a_2 = \alpha + \Lambda^4$ and, finally, $a_3 = 2\Lambda^2$.

For convenience, let us assume that R, defined by Eq. (A17), does not vanish. To proceed with the calculations, let us introduce the following real quantities σ and γ defined, respectively, by

$$\sigma \equiv \left(a_2 - \frac{1}{4} a_3^2 - y_1 \right)^{1/2} = (\alpha - y_1)^{1/2} \tag{A26}$$

and

$$\gamma \equiv \left(a_2 + y_1 - \frac{1}{2} a_3^2 \right)^{1/2} = (\alpha + y_1 - \Lambda^4)^{1/2}, \tag{A27}$$

where we used the identifications $a_2 = \alpha + \Lambda^4$ and $a_3 = 2\Lambda^2$. Then, we shall have

$$R = i\sigma \tag{A28}$$

and

$$E = i\gamma. \tag{A29}$$

So, with the above identifications, it is easy to see to prove that G, defined by Eq. (A22), vanishes identically. Therefore, we will have, from Eq. (A18) and Eq. (A19), that $D = E$. We also see that

$$\sigma^2 + \gamma^2 = 2\alpha - \Lambda^4 > 0, \tag{A30}$$

which implies

$$k^2 > \frac{\varepsilon^2 \Lambda^2}{2}, \tag{A31}$$

where we used Eq. (A10), which is a convergence criterion similar to the massless scalar field case.[6]

Thus, from Eqs. (A13)–(A16), Eq. (A28), and Eq. (A29), we obtain the following solutions to $\Omega(z) = 0$:

$$z_1 = -\frac{\Lambda^2}{2} + \frac{1}{2} i\sigma + \frac{1}{2} i\gamma, \tag{A32}$$

$$z_2 = -\frac{\Lambda^2}{2} + \frac{1}{2}i\sigma - \frac{1}{2}i\gamma, \tag{A33}$$

$$z_3 = -\frac{\Lambda^2}{2} - \frac{1}{2}i\sigma + \frac{1}{2}i\gamma, \tag{A34}$$

$$z_4 = -\frac{\Lambda^2}{2} - \frac{1}{2}i\sigma - \frac{1}{2}i\gamma. \tag{A35}$$

So, from these last results, we will have, finally, for $G_{\mu\nu}(k,\tau)$,

$$G_{\mu\nu}(k,\tau) = \left(\frac{k_\mu k_\nu}{k^2} + g_{\mu\nu}G_1(k,\tau) + \tilde{g}_{\mu\nu}G_2(k,\tau)\right)\theta(\tau), \tag{A36}$$

where:

$$G_1(k,\tau) \equiv \left(\frac{\Lambda^2}{(\sigma+\gamma)}\sin\left(\frac{(\sigma+\gamma)}{2}\tau\right) + \cos\left(\frac{(\sigma+\gamma)}{2}\tau\right)\right)e^{-(\Lambda^2/2)\tau}, \tag{A37}$$

$$G_2(k,\tau) \equiv \left(\frac{\Lambda^2}{(\sigma-\gamma)}\sin\left(\frac{(\sigma-\gamma)}{2}\tau\right) + \cos\left(\frac{(\sigma-\gamma)}{2}\tau\right)\right)e^{-(\Lambda^2/2)\tau}, \tag{A38}$$

and $g_{\mu\nu}$ and $\tilde{g}_{\mu\nu}$ appearing in Eq. (A36) are defined by

$$g_{\mu\nu} \equiv \Pi_{\mu\nu} - h_{\mu\nu}, \tag{A39}$$

$$\tilde{g}_{\mu\nu} \equiv h_{\mu\nu} - \tilde{\Pi}_{\mu\nu}, \tag{A40}$$

with

$$h_{\mu\nu} \equiv -\frac{\Lambda^2}{2\gamma\sigma}\epsilon_{\mu\nu\rho}k_\rho\left(\frac{\kappa}{4\pi}\right), \tag{A41}$$

$$\Pi_{\mu\nu} \equiv \frac{1}{\gamma\sigma}\left(\frac{\Lambda^4}{4} + \frac{(\sigma+\gamma)^2}{4}\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right), \tag{A42}$$

and

$$\tilde{\Pi}_{\mu\nu} \equiv -\frac{1}{\gamma\sigma}\left(\frac{\Lambda^4}{4} + \frac{(\sigma-\gamma)^2}{4}\right)\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\right). \tag{A43}$$

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Symmetry of quantum torus with crossed product algebra

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In this paper, we study the symmetry of quantum torus with the concept of crossed product algebra. As a classical counterpart, we consider the orbifold of classical torus with complex structure and investigate the transformation property of classical theta function. An invariant function under the group action is constructed as a variant of the classical theta function. Then our main issue, the crossed product algebra representation of a quantum torus with complex structure under the symplectic group, is analyzed as a quantum version of orbifolding. We perform this analysis with Manin's so-called model II quantum theta function approach. The symplectic group $Sp(2n,\mathbb{Z})$ satisfies the consistency condition of a crossed product algebra representation of quantum torus times the algebra of functions on the Siegel space. However, only a subgroup of $Sp(2n,\mathbb{Z})$ satisfies the consistency condition for orbifolding of the quantum torus. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Classical theta functions[1] can be regarded as state functions on classical tori, and have played an important role in the string loop calculation.[2,3] Recently, Manin[4–6] introduced the concept of quantum theta function as a quantum counterpart of classical theta function. In our previous work,[7] we clarified the relationship between Manin's quantum theta function and the theta vector[8–10] that Schwarz introduced earlier. In Ref. 7 we showed the connection between the classical theta function and the so-called *kq* representation that appeared in the physics literature.[11,12] Then we showed that the Manin's quantum theta function corresponds to the quantum version of the *kq* representation. In the physics literature, quantum theta functions are related with noncommutative solitons[13] whose solutions are given in terms of projection operators.[13–15] Under the lattice translation, quantum theta function maintains the transformation property of a classical theta function. Manin's construction of quantum theta function[5,6] is based on the algebra valued inner product of the theta vector, and this construction is a generalization of Boca's construction of projection operators on the $\mathbb{Z}_4$ orbifold of a noncommutative two torus.[16]

In the algebra valued inner product one can make the inner product of the dual algebra, the representation of the perpendicular lattice space, be invertible or proportional to the identity operator. This makes the algebra valued inner product be a projection operator.[17] In Boca's work,[16] the projection operators on the $\mathbb{Z}_4$ orbifold of the noncommutative two torus were constructed based on the algebra valued inner product that Rieffel[17] used in his classic work on projective modules over noncommutative tori.

One can consider a symmetry group defining an orbifold from the view point of the crossed product algebra of the original algebra with the given symmetry group.[13,18,19] Therefore in order to

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find a representation of an orbifold algebra, one has to find a representation of the group compatible to that of the original algebra. In Boca's work, the action of the $\mathbb{Z}_4$ quotient was represented as the Fourier transformation, and the algebra valued inner product was evaluated with the eigenstates of Fourier transformation.[16]

When the consistency conditions for the representation of crossed product algebra are fulfilled, the group of the crossed product algebra behaves as a symmetry group of the original algebra. The consistency conditions for crossed product algebra are basically having compatible actions of the group acting on the original algebra and on the module.

For quantum tori, there are two types of symmetries. One is a symmetry under a group action, and the other is a symmetry under deformation of the algebra, the so-called Morita equivalence.[20] Here, we restrict our discussion to the symmetry under a group action that is not related to the Morita equivalence.

In this paper, we first consider classical functions under orbifolding of torus and try to find an invariant function under the symplectic group $Sp(2n,\mathbb{Z})$. We then look into the representation of crossed product algebra as a way of orbifolding in the quantum (noncommutative) case.

The organization of the paper is as follows. In Sec. II, we review orbifolding of the classical torus and construct an invariant function under the action of $Sp(2n,\mathbb{Z})$. In Sec. III, we first review the crossed product algebra and its consistency conditions. Then, we check the consistency conditions of our crossed product algebra with the group $Sp(2n,\mathbb{Z})$ via the approach of Manin's model II quantum theta function. In Sec. IV, we conclude with a discussion.

II. ORBIFOLDING AND CLASSICAL THETA FUNCTION

In this section, we first consider orbifolding under a group action. A classical function f on an orbifold $X=M/G$ should satisfy

$$f(g\cdot x)=f(x), \quad {}^{\forall}g\in G, \quad x\in M. \tag{1}$$

Now, we consider the case in which M is a complex torus. Let $M=\mathbb{C}^n/\Lambda$ ($\Lambda\cong\mathbb{Z}^{2n}$) be a complex torus. If M can be embedded in a projective space $\mathbb{C}P^N$ for some N, then it is called an Abelian variety. For M to be an Abelian variety, there must exist a polarization, a positive line bundle on M. A positive line bundle L on M should satisfy that $\int_C c_1(L)>0$, for any curve C in M, where $c_1(L)$ is the first Chern class of L as an element of $H^2(M,\mathbb{Z})\cap H^{1,1}(M,\mathbb{R})$. Explicitly, $c_1(L)=\Sigma\delta_\alpha dx_\alpha\wedge dy_\alpha=\Sigma q_\beta dz_\beta\wedge d\overline{z_\beta}$, $\delta_\alpha\in\mathbb{Z}$, and q_β is pure imaginary. In particular, if $\delta_\alpha=1$, for all α, then the Abelian variety is called *principally polarized*.[21] The moduli space $\mathfrak{M}$ of principally Polarized abelian varieties is the collection of the pair $\{(M,L)\,|\,M=\mathbb{C}^n/\Lambda;\ L$ is a principally polarized line bundle$\}$. Let $\mathbb{H}_n=\{T\,|\,T\in M_n(\mathbb{C}), T^t=T, \mathrm{Im}\,T>0\}$ on which $Sp(2n,\mathbb{Z})$ acts as follows:

$$g\cdot T=(AT+B)(CT+D)^{-1}, \quad \text{for } g=\begin{pmatrix} A & B \\ C & D\end{pmatrix}\in Sp(2n,\mathbb{Z}).$$

Then, $\mathfrak{M}=Sp(2n,\mathbb{Z})\backslash\mathbb{H}_n$.

Now, we consider an action of a group G on M. In other words, a map from $G\times M$ to M, such that for every $g\in G$, g is an automorphism of M preserving complex structure T and the group structure. Then, g induces a linear map from $\mathbb{C}^n$ to $\mathbb{C}^n$, sending Λ to Λ. It means that g belongs to $GL(n,\mathbb{C})$ and also $GL(2n,\mathbb{Z})$, which is given in terms of the basis of $\Lambda(\cong\mathbb{Z}^{2n})$, whose determinant is ±1. Additionally, if we impose that g preserves L, then g preserves $c_1(L)$, so that

$$c_1(L)=\sum dx_\alpha\wedge dy_\alpha=g^*(c_1(L))=\sum d(g^*x_\alpha)\wedge d(g^*y_\alpha).$$

It implies that $g\in Sp(2n,\mathbb{Z})$. Then we can define an orbifold M/G with the preserved polarization L.

If $g\in GL(n,\mathbb{C})$ and $g\in Sp(2n,\mathbb{Z})$, then $T'=g\cdot T=T$, as we see later. Hence, only a subgroup of $Sp(2n,\mathbb{Z})$, namely $GL(n,\mathbb{C})\cap Sp(2n,\mathbb{Z})$, acts as a symmetry group for orbifolding.

For $g\in Sp(2n,\mathbb{Z})$, it acts on the basis as follows:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} T \\ I \end{pmatrix} = \begin{pmatrix} AT+B \\ CT+D \end{pmatrix} \sim \begin{pmatrix} (AT+B)(CT+D)^{-1} \\ I \end{pmatrix} = \begin{pmatrix} T' \\ I \end{pmatrix}.$$

On the other hand, for $g \in GL(n,\mathbb{C})$ it acts as follows:

$$\begin{pmatrix} T \\ I \end{pmatrix} \cdot g^t = \begin{pmatrix} T \cdot g^t \\ I \cdot g^t \end{pmatrix} \sim \begin{pmatrix} T \cdot g^t \cdot g^{-t} \\ I \end{pmatrix} = \begin{pmatrix} T \\ I \end{pmatrix}.$$

Since the two actions should yield the same result, we get to the result that $T' = g \cdot T = T$.

We now consider whether the classical theta function θ is well defined on the above mentioned orbifold. The classical theta function θ is a complex valued function on $\mathbb{C}^n$ satisfying the following relation.

$$\theta(z+\lambda') = \theta(z), \quad \text{for } z \in \mathbb{C}^n, \quad \lambda' \in \Lambda', \tag{2}$$

$$\theta(z+\lambda) = c(\lambda)e^{q(\lambda,z)}\theta(z), \quad \text{for } \lambda \in \Lambda, \tag{3}$$

where $\Lambda' \oplus \Lambda \subset \mathbb{C}^n$ is a discrete sublattice of rank $2n$ split into the sum of two sublattices of rank n, isomorphic to $\mathbb{Z}^n$, and $c:\Lambda \to \mathbb{C}$ is a map and $q:\Lambda \times \mathbb{C} \to \mathbb{C}$ is a biadditive pairing linear in z.

The above property reflects the fact that the classical theta function lives on $\mathbb{C}^n$, not on $\mathbb{T}^{2n}$. The function $\theta(z,T)$ satisfying (2) and (3) can be defined as

$$\theta(z,T) = \sum_{k \in \mathbb{Z}^n} e^{\pi i(k^t T k + 2k^t z)}, \tag{4}$$

where $T \in \mathbb{H}_n$. With the above definition, $c(\lambda)$ and $q(\lambda,z)$ in (3) are given explicitly by $c(\lambda) = e^{-\pi i m^t T m}$ and $q(\lambda,z) = -2\pi i m^t z$ when $\lambda = Tm$, $m \in \mathbb{Z}^n$. Also, $z \in \mathbb{C}^n$ transforms as

$$g \cdot z = z' = (CT+D)^{-t}z, \quad \text{for } g = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp(2n,\mathbb{Z}), \tag{5}$$

where "$-t$" denotes the transposed inverse. Under this modular transformation, the classical theta function transforms as follows:

$$g \cdot \theta(z,T) = \theta(z',T') = \xi_g \det(CT+D)^{1/2} e^{\pi i\{z^t(CT+D)^{-1}Cz\}}\theta(z,T), \quad {}^\forall g \in Sp(2n,\mathbb{Z}), \tag{6}$$

where ξ_g is an eighth root of unity depending on the group element g.[1]

Now, we like to find a compatible function on the orbifold in which the complex structure is preserved, $g \cdot T = T$. For this, we first try to construct a new function that has the symmetry properties of the classical theta function, (2) and (3). We define a new function as a linear combination of the classical theta functions under the group action

$$\Theta_1(z,T) = \sum_{g \in G} g \cdot \theta(z,T). \tag{7}$$

Clearly the above function is invariant under the group action,

$$h \cdot \Theta_1(z,T) = \sum_{g \in G} h \cdot g \cdot \theta(z,T) = \sum_{g' \in G} g' \cdot \theta(z,T) = \Theta_1(z,T), \quad {}^\forall h \in G. \tag{8}$$

However, this function does not possess the symmetry properties of the classical theta function (2) and (3). This is because the condition (2) is not satisfied by $\Theta_1(z,T)$, since

$$g \cdot \theta(z+\lambda',T) = \theta(g \cdot (z+\lambda'), g \cdot T) = \theta(g \cdot z + g \cdot \lambda', T) \neq \theta(g \cdot z, T), \tag{9}$$

where $g \cdot \lambda' \in \Lambda + \Lambda'$ for some $\lambda' \in \Lambda'$ due to the modular transformation $g \cdot \lambda' = (CT+D)^{-t}\lambda'$. For the condition (3), each $g \cdot \theta$ in $\Theta_1(z,T)$ in (7) gets a different factor for a lattice shift in Λ:

$$g \cdot \theta(z+\lambda,T) = \theta(g\cdot(z+\lambda), g\cdot T) = \theta(g\cdot z + g\cdot\lambda, T) \neq \theta(g\cdot z+\lambda,T), \quad \text{for } \lambda \in \Lambda, \tag{10}$$

since again $g\cdot\lambda=(CT+D)^{-t}\lambda \neq \lambda$ and belongs to $\Lambda+\Lambda'$ in general. Thus the function $\Theta_1(z,T)$ fails to preserve the transformation properties of the classical theta function, (2) and (3), though it is a well defined function on the orbifold.

In (4), the above result was due to the product $k^t z$ in the exponent. So we need to find a new combination of this type of product under the modular transformation that preserves the complex structure. Since a symplectic product preserves the complex structures, we modify the classical theta function as follows:

$$\tilde{\Theta}(z,T) = \sum_{\underline{k}} \exp(-\pi H_T(\underline{k},\underline{k}) + 2\pi i \,\mathrm{Im}[H_T(\underline{k},z)]), \tag{11}$$

where

$$H_T(s,z) \equiv s^t(\mathrm{Im}\, T)^{-1} z^*, \quad \text{for } s,z \in \mathbb{C}^n. \tag{12}$$

Here, T is the complex structure given before, and $\underline{k}$ denotes the lattice point given by $\underline{k}=Tk_1+k_2$ with $k_1,k_2\in\mathbb{Z}^n$, and $z\in\mathbb{C}^n$ is given as usual with $z=Tx_1+x_2$ with $x_1,x_2\in\mathbb{R}^n$. Here, we notice that $\mathrm{Im}[H_T(\underline{k},z)]=\mathrm{Im}[\underline{k}^t(\mathrm{Im}\,T)^{-1}z^*]=k_1^t x_2 - k_2^t x_1$. If we denote $\underline{x}$ as $z=Tx_1+x_2\equiv\underline{x}$ and the same for $\underline{y}=Ty_1+y_2$ with $y_1,y_2\in\mathbb{R}^n$, then $H_T(\underline{x},\underline{y})=\underline{x}^t(\mathrm{Im}\,T)^{-1}\underline{y}^*$ is an invariant combination under the modular transformation, $T'=(AT+B)(CT+D)^{-1}$, $\underline{x}'=(CT+D)^{-t}\underline{x}$ and the same for $\underline{y}$, for any

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp(2n,\mathbb{Z}).$$

One can check that the above transformation of the complex coordinate $\underline{x}$ is compatible with the following coordinate transformation in the real basis:

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-t} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{13}$$

The first term in the exponent in (11) is invariant under the modular transformation as we shall see in the next section, and the second term is also invariant since it is a symplectic product that preserves the complex structure. Thus, our modified theta function $\tilde{\Theta}$ is invariant under the modular transformation, and it is a well defined function on the above orbifold.

In fact, we can view this as follows. The classical theta function θ in (4) is summed over only one of the two $\mathbb{Z}^n$ lattices Λ,Λ' in the $2n$-torus. Our modified theta function $\tilde{\Theta}$ is summed over both lattices, and its property under lattice translation is changed from that of the classical theta function. The new function $\tilde{\Theta}$ is invariant under the lattice translation in both directions, Λ and Λ'. And this property is preserved under the group action.

In general, for a manifold M on which a group G is acting, one can define invariant functions on M under the action of the group G as the functions on the orbifold M/G. In the next section, we will do a quantum counterpart of the above analysis with crossed product algebra.

III. QUANTUM TORUS WITH CROSSED PRODUCT ALGEBRA

In order to consider an orbifolding of a quantum torus, we have to express the group action in terms of the representation of the crossed product algebra. So, in this section we first review briefly about the crossed product algebra and its representation, then we will investigate the representation of crossed product algebra for orbifolding.

A. Crossed product algebra

We now consider the crossed product algebra and its representation.[13,18]

Let G, a group, act on an algebra $\mathcal{A}$. More explicitly, there is a group homomorphism,

$$\varepsilon: G \to \mathrm{Aut}(\mathcal{A}).$$

Then we define the crossed product algebra $\mathcal{B}=\mathcal{A}\rtimes_{\varepsilon}G$, which is $\mathcal{A}[G]=\{b|\, b: G\to\mathcal{A}\}$ as a set. And we formally express $b\in\mathcal{B}$ as $\Sigma_{g\in G}b_g g$, where $b_g=b(g)\in\mathcal{A}$. Here, the addition and scalar product are defined naturally. To define multiplication we require the following relation:

$$g\cdot b_{g'}g^{-1}=\varepsilon(g)(b_{g'}),\quad g,g'\in G,\quad b_{g'}\in\mathcal{A}. \tag{14}$$

For $b,c,d\in\mathcal{B}$ with $b=\Sigma_{g\in G}b_g g$, $c=\Sigma_{g'\in G}c_{g'}g'$, $d=\Sigma_{h\in G}d_h h$, we can express the multiplication $b*_{\varepsilon}c=d$ as

$$b*_{\varepsilon}c=\sum_g b_g g\cdot\sum_{g'}c_{g'}g'=\sum_{g,g'}b_g g\cdot c_{g'}g'=\sum_{g,h}b_g\varepsilon(g)(c_{g^{-1}h})h=\sum_h d_h h=d, \tag{15}$$

where we set $g'=g^{-1}h$, $d_h=b_g\varepsilon(g)(c_{g^{-1}h})$, and used the relation (14).

If there are representations π, u that are a representation of $\mathcal{A}$ and a representation of the group G, respectively, on a module $\mathcal{H}$,

$$\pi:\mathcal{A}\to\mathrm{End}(\mathcal{H}),\quad u: G\to\mathrm{Aut}(\mathcal{H}),$$

then (14) leads to the following condition for any representation of the crossed product algebra that should satisfy

$$u(g)\pi(a)u(g^{-1})=\pi(\varepsilon(g)(a)),\quad {}^{\forall}a\in\mathcal{A},\quad {}^{\forall}g\in G. \tag{16}$$

With the above condition, we can define a representation π_u of $\mathcal{B}$ on $\mathcal{H}$ as follows:

$$\pi_u\left(\sum_g b_g g\right)=\sum_g \pi(b_g)u(g),\quad \text{for } b_g\in\mathcal{A},\quad {}^{\forall}g\in G. \tag{17}$$

When the condition (16) is satisfied, G is called a symmetry group for the algebra representation π. Furthermore, if there exists an $\mathcal{A}$ valued inner product ${}_{\mathcal{A}}\langle\langle,\rangle\rangle$ on $\mathcal{H}$, then the following should be also satisfied for consistency:[18]

$$\varepsilon(g)({}_{\mathcal{A}}\langle\langle\xi,\eta\rangle\rangle)={}_{\mathcal{A}}\langle\langle u(g)\xi,u(g)\eta\rangle\rangle,\quad \text{for } g\in G,\quad \xi,\eta\in\mathcal{H}. \tag{18}$$

Here, ${}_{\mathcal{A}}\langle\langle\xi,\eta\rangle\rangle$ denotes the $\mathcal{A}$-algebra valued inner product to be defined below, which belongs to $\mathcal{A}$. We changed the notation for the algebra valued inner product from the single bracket in our previous work[7] to the double bracket to distinguish it from the usual scalar product that we will denote with the single bracket below.

B. Symmetry transformation

In Ref. 6, Manin constructed the quantum theta function in two ways that he called model I and model II. The model I basically follows the Rieffel's way of constructing projective modules over noncommutative tori. Thus, in model I, one deals with Schwartz functions on $\mathbb{R}^n$ a for complex n-torus. And the scalar product is defined as

$$\langle\xi,\eta\rangle=\int\xi(x_1)\overline{\eta(x_1)}d\mu(x_1),\quad x_1\in\mathbb{R}^n \tag{19}$$

where $\overline{\eta(x_1)}$ denotes the complex conjugation of $\eta(x_1)$, and $d\mu(x_1)$ denotes the Haar measure in which $\mathbb{Z}^n$ has covolume 1.

In model II, one deals with holomorphic functions on $\mathbb{C}^n$, and the scalar product is defined as

$$\langle \xi, \eta \rangle_T = \int_{\mathbb{C}^n} \xi(\underline{x}) \overline{\eta(\underline{x})} e^{-\pi H_T(\underline{x},\underline{x})} \, d\nu \tag{20}$$

where $d\nu$ is the translation invariant measure making $\mathbb{Z}^{2n}$ a lattice of covolume 1 in $\mathbb{R}^{2n}$. Here, $\underline{x}=Tx_1+x_2$ with $x_1,x_2 \in \mathbb{R}^n$. The complex structure T is given by an $n \times n$ complex valued matrix, and $H_T(\underline{x},\underline{x})=\underline{x}^t(\mathrm{Im}\, T)^{-1}\underline{x}^*$ as in (12).

Now, we do the analysis with model II quantum theta function. For consistency of the representation of a crossed product algebra $\mathcal{B}=\mathcal{A} \rtimes G$, we need to define the following as explained in Sec. III A:

(I) $\pi: \mathcal{A} \to \mathrm{End}(\mathcal{H})$
(II) $u: G \to \mathrm{Aut}(\mathcal{H})$
(III) $\varepsilon: G \to \mathrm{Aut}(\mathcal{A})$, such that $u(g)\pi(a)u(g^{-1})=\pi(\varepsilon(g)(a))$
(IV) $\langle\langle , \rangle\rangle$: $\mathcal{H} \times \mathcal{H} \to \mathcal{A}$, such that $\varepsilon(g)\langle\langle f,h\rangle\rangle=\langle\langle u(g)f, u(g)h\rangle\rangle$.

Let M be any locally compact Abelian group and $\hat{M}$ be its dual group and define $\mathcal{G} \equiv M \times \hat{M}$. And, let π be a representation of $\mathcal{G}$ on $L^2(M)$ such that

$$\pi_x \pi_y = \alpha(x,y)\pi_{x+y} = \alpha(x,y)\overline{\alpha}(y,x)\pi_y \pi_x, \quad \text{for } x,y \in \mathcal{G}, \tag{21}$$

where α is a map $\alpha: \mathcal{G} \times \mathcal{G} \to \mathbb{C}^*$ satisfying

$$\alpha(x,y) = \alpha(y,x)^{-1}, \quad \alpha(x_1+x_2,y) = \alpha(x_1,y)\alpha(x_2,y).$$

We also define $S(D)$ as the space of Schwartz functions on D that we take as a discrete subgroup of $\mathcal{G}$. For $\Phi \in S(D)$, it can be expressed as $\Phi=\Sigma_{w \in D}\Phi(w)e_{D,\alpha}(w)$, where $e_{D,\alpha}(w)$ is a delta function with support at w and obeys the following relation:

$$e_{D,\alpha}(w_1)e_{D,\alpha}(w_2) = \alpha(w_1,w_2)e_{D,\alpha}(w_1+w_2). \tag{22}$$

From now on, we take M as $\mathbb{R}^n$. Let $\mathcal{A}$ be $S(D)$ valued functions on the Siegel space, $\mathbb{H}_n$. More explicitly,

$$\mathcal{A} = S(D) \otimes \mathcal{F}(\mathbb{H}_n) = \{a | a: \mathbb{H}_n \to S(D)\}, \tag{23}$$

where $\mathcal{F}(\mathbb{H}_n)$ is an algebra of smooth complex functions on $\mathbb{H}_n$. Then $a(T)=\Sigma_{w \in D}a_{T,w}e(w)$, where $a_{T,w} \in \mathbb{C}$. Let $\mathcal{H}$ be given as follows:

$$\mathcal{H} = \left\{ f | f: \mathbb{R}^n \times \hat{\mathbb{R}}^n \times \mathbb{H}_n \to \mathbb{C}, \ \langle f(x,T), f(x,T)\rangle_T = \int |f(x,T)|^2 e^{-\pi H_T(x,x)} \, dx < \infty, {}^{\forall}T \right\}, \tag{24}$$

where $x \in \mathbb{R}^n \times \hat{\mathbb{R}}^n$, $T \in \mathbb{H}_n$ and from here on $H_T(x,y)$ that we used above denotes $H_T(\underline{x},\underline{y})$ defined in the Sec. II for notational convenience. In other words, $\mathcal{H}$ are global sections of $\bar{\mathbb{H}}$, a vector bundle over $\mathbb{H}_n$, where the fiber over T is

$$\mathbb{H}_T = \{\xi | \xi: \mathbb{R}^n \times \hat{\mathbb{R}}^n \to \mathbb{C}, \ \langle \xi, \xi \rangle_T < \infty\}. \tag{25}$$

Let the group G be $Sp(2n,\mathbb{Z})$ and we now carry out steps (I)–(IV) that we listed previously.
(I) Before we define π, we need to define a map π_0 from $S(D)$ to $\mathrm{End}(\mathcal{H})$:

$$\pi_0: e(w) \to \pi_w, \quad \text{for } w \in D$$

where

$$(\pi_w f)(x,T) = e^{-\pi H_T(x,w)-(\pi/2)H_T(w,w)} f(x+w,T). \tag{26}$$

Let $a \in \mathcal{A}$, where $a(T)=\Sigma_w a_{T,w}e(w)$. Now, we define π as follows:

$$(\pi(a)f)(x,T) = [\pi_0(a(T))f](x,T). \tag{27}$$

(II) We define u as follows:

$$(u(g)f)(x,T) = f(g\cdot x, g\cdot T), \tag{28}$$

where

$$g = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp(2n,\mathbb{Z}), \quad g\cdot x = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-t} x,$$

and $g\cdot T=(AT+B)(CT+D)^{-1}$.

For the remaining steps we need to use the following two lemmas.

Lemma 1:

$$H_T(x,y) = H_{g\cdot T}(g\cdot x, g\cdot y). \tag{29}$$

Lemma 2:

$$\langle f,h\rangle_{g\cdot T} = \langle u(g)f, u(g)h\rangle_T. \tag{30}$$

Proof of Lemma 1: We first want to show that

$$\mathrm{Im}(g\cdot T) = \mathrm{Im}((AT+B)(CT+D)^{-1}) = (C\overline{T}+D)^{-t}\,\mathrm{Im}(T)(CT+D)^{-1}. \tag{31}$$

Then the proof of Lemma 1 is given by the following steps:

$$\begin{aligned} H_{g\cdot T}(g\cdot x, g\cdot y) &= ((CT+D)^{-t}\underline{x})^t(\mathrm{Im}(g\cdot T))^{-1}((CT+D)^{-t}\underline{y})^* \\ &= \underline{x}^t(CT+D)^{-1}(CT+D)(\mathrm{Im}(T))^{-1}(C\overline{T}+D)^t(C\overline{T}+D)^{-t}\underline{y}^* \\ &= \underline{x}^t(\mathrm{Im}(T))^{-1}\underline{y}^* = H_T(x,y). \end{aligned}$$

Thus, we only have to show (31). We can prove it with the three generators of $Sp(2n,\mathbb{Z})$:[1]

$$(i)\ g = \begin{pmatrix} A & 0 \\ 0 & A^{-t} \end{pmatrix}, \quad A \in GL(n,\mathbb{Z}) \tag{32}$$

$$(ii)\ g = \begin{pmatrix} I & B \\ 0 & I \end{pmatrix}, \quad B^t = B, \quad B \in gl(n, \quad \mathbb{Z}) \tag{33}$$

$$(iii)\ g = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \tag{34}$$

For the first two cases, (31) can be shown trivially. For case (iii), we need to show the following:

$$\mathrm{Im}\ T' = \overline{T}^{-t}(\mathrm{Im}\ T)T^{-1} = \overline{T}^{-1}(\mathrm{Im}\ T)T^{-1}, \tag{35}$$

where $T'=g\cdot T=-T^{-1}$.

Now, we prove (35).

Let $T=T_1+iT_2$ and $T'=T_1'+iT_2'$. Then from $T'T=-I$, we get $T_1'T_1-T_2'T_2=-I$ and $T_2'T_1+T_1'T_2=0$. Then the statement we want to prove becomes $T_2'=\overline{T}^{-1}T_2T^{-1}$, or equivalently,

$$\overline{T}T_2'T = T_2. \tag{36}$$

The left hand side of (36) is

$$\text{lhs} = (T_1 - iT_2)T_2'(T_1 + iT_2) = (T_1T_2'T_1 + T_2T_2'T_2) + i(-T_2T_2'T_1 + T_1T_2'T_2).$$

Using $T_1'T_1 - T_2'T_2 = -I$ and $T_2'T_1 + T_1'T_2 = 0$ together with the property that T_i, T_i' are symmetric, then we can easily show that

$$\text{lhs} = T_2 = \text{rhs}.$$

Proof of Lemma 2: The left hand side of (30) is

$$\text{lhs} = \langle f,h\rangle_{g\cdot T} = \int f(x,g\cdot T)\overline{h(x,g\cdot T)}e^{-\pi H_{g\cdot T}(x,x)}\,dx,$$

and the right hand side of (30) is

$$\text{rhs} = \langle u(g)f,u(g)h\rangle_T = \int f(g\cdot x,g\cdot T)\overline{h(g\cdot x,g\cdot T)}e^{-\pi H_T(x,x)}\,dx$$

$$= \int f(x,g\cdot T)\overline{h(x,g\cdot T)}e^{-\pi H_{g\cdot T}(x,x)}\,dx,$$

where we used Lemma 1 in the final step.

(III) We define $\varepsilon: G \to \text{Aut}(\mathcal{A})$ such that $u(g)\pi(a)u(g^{-1}) = \pi(\varepsilon(g)(a))$.

Let $a(T)$ be $\Sigma a_{T,w}e(w)$. The left hand side can be evaluated as follows:

$$(u(g)\pi(a)u(g^{-1})f)(x,T) = (\pi(a)u(g^{-1})f)(g\cdot x,g\cdot T)$$

$$= \sum_w a_{g\cdot T,w}e^{-\pi H_{g\cdot T}(g\cdot x,w)-(\pi/2)H_{g\cdot T}(w,w)}f(x+g^{-1}\cdot w,T).$$

If we define $\varepsilon(g)(a)(T) = \Sigma_w a_{g\cdot T,w}e(g^{-1}\cdot w)$, then the right hand side is given by

$$\pi(\varepsilon(g)(a)f)(x,T) = \sum_w a_{g\cdot T,w}\pi(g^{-1}\cdot w)f(x,T) = \sum_w a_{g\cdot T,w}e^{-\pi H_{g\cdot T}(g\cdot x,w)-(\pi/2)H_{g\cdot T}(w,w)}f(x+g^{-1}\cdot w,T).$$

In the last equality we used Lemma 1. So those two sides are equal. Using Lemma 1, one can also show the following:

$$u(g)\pi_w u(g^{-1}) = \varepsilon(g)\pi_w = \pi_{g^{-1}\cdot w}. \tag{37}$$

(IV) We define an $\mathcal{A}$-valued inner product on $\mathcal{H}$ as follows:

$$\langle\langle f,h\rangle\rangle(T) = \sum_w \langle f,\pi_w h\rangle_T e(w), \tag{38}$$

where $\langle f,\pi_w(h)\rangle_T = \langle f(x,T),\pi_w h(x,T)\rangle_T$.

In other words, if $a = \langle\langle f,h\rangle\rangle$ then $a_{T,w} = \langle f,\pi_w h\rangle_T$.

Now, we want to check that $\varepsilon(g)\langle\langle f,h\rangle\rangle = \langle\langle u(g)f,u(g)h\rangle\rangle$ holds.

Recall that

$$\varepsilon(g)(a)(T) = \sum_w a_{g\cdot T,w}e(g^{-1}\cdot w).$$

The left hand side is given by

$$(\varepsilon(g)(\langle\langle f,h\rangle\rangle))(T) = \sum_w \langle f,\pi_w h\rangle_{g\cdot T}e(g^{-1}\cdot w) = \sum_w \langle f,\pi_{g\cdot w}h\rangle_{g\cdot T}e(w).$$

The right hand side is given by

$$\langle\langle u(g)f,u(g)h\rangle\rangle_T=\sum_w \langle u(g)f,\pi_w u(g)h\rangle_T e(w)=\sum_w \langle f,u(g)^{-1}\pi_w u(g)h\rangle_{g\cdot T}e(w)=\sum_w \langle f,\pi_{g\cdot w}h\rangle_{g\cdot T}e(w),$$

where we used Lemma 2 and (37).

C. Orbifolding quantum torus

We consider an orbifolding of quantum torus with a polarized complex structure T. The symmetry group preserving the polarized complex structure is the subgroup $G_T=\{g \in Sp(2n,\mathbb{Z})|g\cdot T=T\}$ of $Sp(2n,\mathbb{Z})$. Orbifolding the quantum torus with a complex structure T corresponds to the crossed product algebra discussed in the previous section with fixed T.

Let $A_T=S(D)$ and $\mathbb{H}_T=\{f_T|f_T:\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{C},\|f_T\|^2=\int|f_T(x)|^2e^{-\pi H_T(x,x)}dx<\infty\}$. Now, we can define the crossed product algebra, $A_T\rtimes G_T$, naturally from the construction in Sec. III B:

(1) $\pi_T:A_T\to \mathrm{End}(\mathbb{H}_T)$
(2) $u_T:G_T\to \mathrm{Aut}(\mathbb{H}_T)$
(3) $\varepsilon_T:G_T\to \mathrm{Aut}(A_T)$, such that $u_T(g)\pi_T(a)u_T(g^{-1})=\pi_T(\varepsilon_T(g)(a))$
(4) $\langle\langle,\rangle\rangle_T:\mathbb{H}_T\times\mathbb{H}_T\to A_T$ such that $\varepsilon_T(g)\langle\langle f_T,h_T\rangle\rangle_T=\langle\langle u_T(g)f_T,u_T(g)h_T\rangle\rangle_T$.

Here, π_T, u_T, ε_T, $\langle\langle,\rangle\rangle_T$, f_T satisfy the following relations:

$$(\pi_T(a(T))f_T)(x)=(\pi(a)f)(x,T),$$

$$(u_T(g)f_T)(x)=(u(g)f)(x,T),$$

$$(\varepsilon(g)(a))(T)=\varepsilon_T(g)(a(T)),$$

$$\langle\langle f_T,h_T\rangle\rangle_T=\langle\langle f,h\rangle\rangle(T),$$

where $f_T(x)=f(x,T)$, $a\in S(D)\otimes\mathcal{F}(\mathbb{H}_n)$, and $g\in G_T$. If we choose $f(x,T)=1$, then $\varepsilon(g)\langle\langle 1,1\rangle\rangle=\langle\langle u(g)1,u(g)1\rangle\rangle=\langle\langle 1,1\rangle\rangle$, and thus $\langle\langle 1,1\rangle\rangle$, which belongs to the algebra $\mathcal{A}$ is $Sp(2n,\mathbb{Z})$ invariant. Since $\langle\langle 1,1\rangle\rangle(T)=\Sigma_{w\in D}e^{-(\pi/2)H_T(w,w)}e(w)$ is Manin's model II quantum theta function; this also tells us that the model II quantum theta function is well defined on the orbifolds of a quantum complex torus. We further notice that Boca's projection operator[16] on the $\mathbb{Z}/4\mathbb{Z}$ orbifold of a quantum 2-torus with $T=i$ corresponds to a special case of this construction.

IV. CONCLUSION

In this paper, we investigate the symmetry of quantum torus with the group $Sp(2n,\mathbb{Z})$.

First, we investigate the orbifolding of the classical complex torus. It turns out that the orbifold group for a complex n torus leaving the complex structure and its polarization intact is a subgroup of $Sp(2n,\mathbb{Z})$. Also, the classical theta function is not invariant under the $Sp(2n,\mathbb{Z})$ transformation, and we construct a variant of the classical theta function as an invariant function under the transformation of $Sp(2n,\mathbb{Z})$. Then, as a quantum counterpart, we investigate the representation of crossed product algebra of quatum torus with $Sp(2n,\mathbb{Z})$ via Manin's model II quantum theta function approach.

In Manin's model I approach, the dimension of the Hilbert space variable x_1, which is n for quantum $\mathbb{T}^{2n}$, does not match the dimension of the fundamental representation of $Sp(2n,\mathbb{Z})$, which is $2n$. On the other hand, in the model II case the dimension of the Hilbert space variable $x=(x_1,x_2)$ exactly matches that of the group. Therefore in the model I case the group action cannot act directly on the variables of the Hilbert space. Thus, one has to devise a transformation such as Fourier transformation as in the Boca's work,[16] where $\mathbb{Z}_4$ acts directly on the functions as a Fourier transformation, not on the variables of the functions. This type of difficulty comes from the fact that in the model I case the number of variables of the functions is half that of the phase space, as

is typical in the conventional quantization. In the model II approach, the above mentioned difficulty does not arise. The group action can be defined nicely on the module as it acts on the variables.

In conclusion, in the model II case $Sp(2n,\mathbb{Z})$ turns out to be the symmetry group for the quantum torus times $\mathbb{H}_n$. The orbifolding of quantum torus with a complex structure corresponds to the crossed product algebra, $S(D)\rtimes G_T$, where G_T is the subgroup of $Sp(2n,\mathbb{Z})$ fixing the complex structure, $g\cdot T=T$ for $g\in Sp(2n,\mathbb{Z})$. And Manin's model II quantum theta function turns out to be a well defined function over the above orbifold of the quantum torus.

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The Gell-Mann-Okubo and Coleman-Glashow relations for octet and decuplet baryons in the $SU_q(3)$ quantum algebra

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The q-deformed Clebsch-Gordan coefficients corresponding to the $\{3\}\times\{21\}$ reduction of the $SU_q(3)$ quantum algebra are computed. From these results and using the quantum Clebsch-Gordan coefficients for the $\{21\}\times\{21\}$ reduction found by Z. Q. Ma, the q-deformed Gell-Mann-Okubo mass relations for octet and decuplet baryons are determined by generalizing the procedure used for the SU(3) algebra. We also determine the Coleman-Glashow relations for octet and decuplet baryons in the $SU_q(3)$ algebra. Finally, by using the experimental particle masses of the octet and decuplet baryons, two values of the q-parameter are found and adjusted for the predicted expressions of the masses (one for the Gell-Mann-Okubo mass relations and the other for the Coleman-Glashow relations) and a possible physical interpretation is given. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The q-deformed algebras extend the domain of classical group theory and constitute a new and growing field of mathematics with a vast potential for applications in physics.[1–6] The quantum algebra $SU_q(3)$, as a generalization of the SU(3) algebra, has been studied by several authors[7–11] with several applications in particle physics, conformal field theory, statistical mechanics, quantum optics, condensed matter, molecular, atomic and nuclear spectroscopy.[1,3,7,12] In these applications either an existing model is identified with a quantum algebraic structure or a standard model is deformed to show a underlying quantum algebraic structure which reveals new features.[3]

Applications of quantum algebras in particle physics have been explored in several works.[12] In hadronic phenomenology q-deformed mass relations between particle families in the octet and decuplet baryons have been determined from the computation of the mass operator's expectation value. In these works, the mass operator has been defined in terms of generators of $SU_q(4)$ and $SU_q(5)$ and its expectation value has been computed from the determination of their matrix elements.

Our aim in this article is to determine the q-deformed Gell-Mann-Okubo and Coleman-Glashow relations for octet and decuplet baryons in the $SU_q(3)$ quantum algebra. First, we develop the $SU_q(3)$ quantum algebra and use it to compute the q-deformed Clebsch-Gordan coefficients corresponding to the $\{3\}\times\{21\}$ reduction. Second, to derive the q-deformed Gell-Mann-Okubo mass relations for octet and decuplet baryons in the $SU_q(3)$ quantum algebra we generalize the traditional procedure for the SU(3) algebra[13] and use the previous results together with the quantum Clebsch-Gordan coefficients corresponding to the $\{21\}\times\{21\}$ reduction.[8] After that, we obtain the q-deformed Coleman-Glashow relations for octet and decuplet baryons by following the same procedure used for the SU(3) algebra.[14] Finally, by using the experimental particle masses of the

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octet and decuplet baryons, two values of the q-parameter are found and adjusted for the Gell-Mann-Okubo and Coleman-Glashow mass relations and a possible physical interpretation is given.

II. THE $SU_q(3)$ QUANTUM ALGEBRA

The quantum algebra $SU_q(3)$ is generated by the operators $\hat{I}$, $\hat{h}_1$, $\hat{h}_2$, $\hat{X}_1^{\pm}$, $\hat{X}_2^{\pm}$, which satisfy the following commutation relations[10]:

$$[\hat{h}_i,\hat{h}_j]=0, \quad [\hat{h}_i,\hat{X}_j^{\pm}]=\pm a_{ij}\hat{X}_j^{\pm}, \tag{1}$$

$$[\hat{X}_i^{+},\hat{X}_j^{-}]=\delta_{ij}[\hat{h}_i]_q=\delta_{ij}\frac{q^{\hat{h}_i}-q^{-\hat{h}_i}}{q-q^{-1}}, \quad i,j=1,2 \tag{2}$$

together with

$$(\hat{X}_i^{\pm})^2\hat{X}_j^{\pm}+\hat{X}_j^{\pm}(\hat{X}_i^{\pm})^2-[2]_q\hat{X}_i^{\pm}\hat{X}_j^{\pm}\hat{X}_i^{\pm}=0, \quad i\neq j, \tag{3}$$

where a_{ij} is the Cartan matrix given by

$$a_{ij}=\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}. \tag{4}$$

Additional generators $\hat{X}_3^{\pm}$ are introduced by[9]:

$$\hat{X}_3^{+}=q^{1/2}[\hat{X}_1^{+},\hat{X}_2^{+}]_{q^{-1}}, \quad \hat{X}_3^{-}=-q^{-1/2}[\hat{X}_2^{-},\hat{X}_1^{-}]_q, \tag{5}$$

where

$$\hat{X}_1^{\pm}=\hat{T}_{\pm}, \quad \hat{X}_2^{\pm}=\hat{U}_{\pm}, \quad \hat{h}_1=2\hat{T}_3, \tag{6}$$

$$\hat{h}_2=-\hat{T}_3+\tfrac{3}{2}\hat{Y}, \quad [\hat{A},\hat{B}]_q=\hat{A}\hat{B}-q\hat{B}\hat{A}. \tag{7}$$

From the previous expressions, we obtain

$$[\hat{X}_3^{+},\hat{X}_3^{-}]=-\frac{q^{\widehat{h_3}}-q^{-\widehat{h_3}}}{q-q^{-1}}=-[\hat{h}_3]_q, \tag{8}$$

$$[\hat{h}_i,\hat{X}_3^{\pm}]=\pm\hat{X}_3^{\pm} \quad \text{with} \quad \hat{h}_3=\hat{h}_1+\hat{h}_2=\hat{T}_3+\tfrac{3}{2}\hat{Y}. \tag{9}$$

According to the standard coproduct definition at $SU_q(3)$, the following expressions are obtained[7]:

$$\Delta\hat{T}_{\pm}=\hat{T}_{\pm}\otimes q^{\hat{T}_3}+q^{-\hat{T}_3}\otimes\hat{T}_{\pm}, \tag{10}$$

$$\Delta\hat{U}_{\pm}=\hat{U}_{\pm}\otimes q^{(3\hat{Y}-2\hat{T}_3)/4}+q^{-(3\hat{Y}-2\hat{T}_3)/4}\otimes\hat{U}_{\pm}. \tag{11}$$

Hence, the coproduct of two $SU_q(3)$ irreps is defined as[7]:

$$\hat{T}_{\pm}(\psi_{\eta}^{\{\lambda_1,\lambda_2\}}\psi_{\beta}^{\{\mu_1,\mu_2\}})=(q^{-\hat{T}_3}\psi_{\eta}^{\{\lambda_1,\lambda_2\}})(\hat{T}_{\pm}\psi_{\beta}^{\{\mu_1,\mu_2\}})+(\hat{T}_{\pm}\psi_{\eta}^{\{\lambda_1,\lambda_2\}})(q^{\hat{T}_3}\psi_{\beta}^{\{\mu_1,\mu_2\}}),$$

$$\hat{U}_{\pm}(\psi_{\eta}^{\{\lambda_1,\lambda_2\}}\psi_{\beta}^{\{\mu_1,\mu_2\}}) = (\hat{U}_{\pm}\psi_{\eta}^{\{\lambda_1,\lambda_2\}})(q^{(3\hat{Y}-2\hat{T}_3)/4}\psi_{\beta}^{\{\mu_1,\mu_2\}}) + (q^{-(3\hat{Y}-2\hat{T}_3)/4}\psi_{\eta}^{\{\lambda_1,\lambda_2\}})(\hat{U}_{\pm}\psi_{\beta}^{\{\mu_1,\mu_2\}}),$$

where $\psi_{\alpha}^{\{\nu\}}$, with $\alpha=1,2,\ldots,\dim(\{\nu\})$, is the state with eigenvalues t_{α}, $t_{3\alpha}$, and y_{α}, which belongs to the $SU_q(3)$ representation $\{\nu\}=\{\nu_1,\nu_2\}$. (In this article, we consider $q\in R$ following the Quesne's prescription.)

III. THE *q*-DEFORMED GELL-MANN-OKUBO MASS RELATIONS FOR OCTET AND DECUPLET BARYONS

In order to get expressions of the masses corresponding to the octet and decuplet baryons, we introduce the following mass operator:

$$\hat{M} = \hat{M}_S + \hat{M}_T, \tag{12}$$

where $\hat{M}_S$ is a $SU_q(3)$ invariant and $\hat{M}_T$ is an isospin escalar.

By computing the expectation value of the mass operator in a $|\psi_{\alpha}^{\{\lambda\}}\rangle$ state belonging to a $\{\lambda\}$ representation, we obtain that the mass of the particle corresponding to this state is given by

$$m(\{\lambda\},\{\mu\}) = \langle\psi_{\alpha}^{\{\lambda\}}|\hat{M}_S|\psi_{\alpha}^{\{\lambda\}}\rangle + \langle\psi_{\alpha}^{\{\lambda\}}|\hat{M}_T|\psi_{\alpha}^{\{\lambda\}}\rangle \tag{13}$$

with

$$|\psi_{\alpha}^{\{\lambda\}}\rangle = |\{\lambda\},\{\mu\}\rangle = |\{\lambda\},y,t,t_z\rangle, \quad \{\mu\}=\{y,t,t_z\}, \tag{14}$$

where in order to simplify the notation we have taken $y=y_{\alpha}$, $t=t_{\alpha}$, and $t_z=t_{3\alpha}$ with y, t, and t_z being the hypercharge, the isospin, and the z isospin component, respectively.

As $\hat{M}_S$ is a $SU_q(3)$ scalar, its expectation value is the same for all members of the multiplet corresponding to a $\{\lambda\}$ representation. Therefore, according to the previous, we obtain

$$\langle\psi_{\alpha}^{\{\lambda\}}|\hat{M}_S|\psi_{\alpha}^{\{\lambda\}}\rangle = m_S(\{\lambda\}). \tag{15}$$

We also note that the $\hat{M}_T$ operator can be written as an expansion of irreducible tensor operators of $SU_q(3)$, according to

$$\hat{M}_T = \sum_{\mu\nu} \hat{T}_{\mu}^{\{\nu\}}. \tag{16}$$

Then, by taking into account that $[\hat{M}_T,\hat{Y}]=[\hat{M}_T,\hat{T}]=0$, from the previous expression we obtain that the irreducible tensor operators $\hat{T}_{\mu}^{\{\lambda\}}$ should satisfy the following conditions:

$$[\hat{T}_{\mu}^{\{\nu\}},\hat{Y}] = 0, \quad [\hat{T}_{\mu}^{\{\nu\}},\hat{T}] = 0. \tag{17}$$

On the other hand, according to the Wigner-Eckart theorem for the quantum group $SU_q(3)$, we have that the matrix element of the irreducible tensor operator $\hat{T}_{\mu_2}^{\{\lambda_2\}}$ is given by[15]

$$\langle\{\lambda_3\},y_3,t_3,t_{3z}|\hat{T}_{\mu_2}^{\{\lambda_2\}}|\{\lambda_1\},y_1,t_1,t_{1z}\rangle = \sum_{\gamma} \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda_{3\gamma} \\ \mu_1 & \mu_2 & \mu_3 \end{pmatrix}_q \langle\{\lambda_3\}||\hat{T}^{\{\lambda_2\}}||\{\lambda_1\}\rangle_{\gamma}, \tag{18}$$

where the reduced matrix element $\langle\{\lambda_3\}||\hat{T}^{\{\lambda_2\}}||\{\lambda_1\}\rangle_{\gamma}$ only depends on the representations involved and the sum is performed over γ, being γ the index which labels the copies of the $\{\lambda_3\}$ representation in the $\{\lambda_1\}\otimes\{\lambda_2\}$ reduction. We also have that the coupling factor in the expression (18) corresponds to the q-deformed Clebsch-Gordan Coefficient of $SU_q(3)$.[15]

Moreover, in the $|\psi_{\alpha}^{\{\lambda\}}\rangle=|\{\lambda\},y,t,t_z\rangle$ basis, we have

$$\langle\{\lambda\}y't't_z'|\hat{T}_{\mu}^{\{\nu\}}|\{\lambda\}ytt_z\rangle = \delta_y^{y'}\delta_t^{t'}\delta_{t_z}^{t_z'}\langle\{\lambda\}||\hat{T}_{\mu}^{\{\nu\}}||\{\lambda\}\rangle. \tag{19}$$

Therefore, by comparing the previous result with the corresponding one to the q-deformed Wigner-Eckart theorem, we obtain that μ should be $(ytt_z)=(000)$.

Then, according to the previous we have that the $\hat{M}_T$ operator is given by

$$\hat{M}_T=\sum_{\nu}\hat{T}^{\{\nu\}}_{000}, \tag{20}$$

where the sum is performed over all physically allowed $SU_q(3)$ representations. Hence, we have $\{\nu\}=\{0\},\{21\},\{42\},\ldots$.

Therefore, the particle mass corresponding to a $|\psi^{\{\lambda\}}_{\alpha}\rangle=|\{\lambda\},y,t,t_z\rangle$ state of a multiplet belonging to a $\{\lambda\}$ representation of $SU_q(3)$ is given by

$$m(\{\lambda\},y,t,t_z)=m_S(\{\lambda\})+\sum_{\nu}\langle\{\lambda\},y,t,t_z|\hat{T}^{\{\nu\}}_{000}|\{\lambda\},y,t,t_z\rangle. \tag{21}$$

It is important to point out that the $\langle\psi^{\{\lambda\}}_{\alpha}|\hat{T}^{\{0\}}_{000}|\psi^{\{\lambda\}}_{\alpha}\rangle$ term remains absorbed in the $m_S(\{\lambda\})$ term, which is a $SU_q(3)$ scalar. We also have that the dominant contribution comes from the $\hat{T}^{\{21\}}_{000}$ component of the octet tensor operator. Hence, according to the previous we obtain[7]

$$m(\{\lambda\},y,t,t_z)=m_S(\{\lambda\})+\langle\{\lambda\},y,t,t_z|\hat{T}^{\{21\}}_{000}|\{\lambda\},y,t,t_z\rangle. \tag{22}$$

On the other hand, it is well known that the product of the $SU_q(3)$ representations $\{21\}$ and $\{21\}$ is given by

$$\{21\}\times\{21\}=\{42\}+\{3\}+\{3^2\}+\{21\}_S+\{21\}_A+\{0\}, \tag{23}$$

where $\{42\}$, $\{3\}$, $\{3^2\}$, $\{21\}$, and $\{0\}$ are representations with dimensions equal to 27, 10, 10, 8, and 1, respectively. Moreover, $\{21\}_S$ and $\{21\}_A$ are symmetric and antisymmetric representations with the same transformation properties under the quantum group $SU_q(3)$.

We also have that the $\{21\}$ representation corresponding to the octet baryon exhibits the following descomposition under the subgroup $U(1)_Y\times SU_q(2)_T$:

$$\{21\}\downarrow\{3\}\times\{1\}+\{0\}\times\{2\}+\{0\}\times\{0\}+\{\overline{3}\}\times\{1\}, \tag{24}$$

where the products $\{3\}\times\{1\}$, $\{0\}\times\{2\}$, $\{0\}\times\{0\}$, and $\{\overline{3}\}\times\{1\}$ represent 2, 3, 1, and 2 states corresponding to the N, Σ, Λ, and Ξ particles of the octet baryon.[16]

Then, by applying the q-deformed Wigner-Eckart theorem to the second term of expression (22) taking into account that in the $\{21\}\times\{21\}$ reduction, the $\{3\}\times\{1\}$, $\{0\}\times\{2\}$, $\{0\}\times\{0\}$, and $\{\overline{3}\}\times\{1\}$ states of the first $\{21\}$ representation are coupled to the $\{0\}\times\{0\}$ state of the second one $\{21\}$, where the coupling coefficients are the q-deformed isoscalar factors, we obtain the following expressions corresponding to the masses of the particle families in the octet baryon[7]:

$$\begin{aligned}m_N=m_S(\{21\})&+\begin{pmatrix}\{21\} & \{21\} & \| & \{21\}_S\\ \frac{1}{2}1 & 00 & \| & \frac{1}{2}1\end{pmatrix}_q\langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_S\\&+\begin{pmatrix}\{21\} & \{21\} & \| & \{21\}_A\\ \frac{1}{2}1 & 00 & \| & \frac{1}{2}1\end{pmatrix}_q\langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_A,\end{aligned} \tag{25}$$

$$\begin{aligned}m_\Sigma=m_S(\{21\})&+\begin{pmatrix}\{21\} & \{21\} & \| & \{21\}_S\\ 10 & 00 & \| & 10\end{pmatrix}_q\langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_S\\&+\begin{pmatrix}\{21\} & \{21\} & \| & \{21\}_A\\ 10 & 00 & \| & 10\end{pmatrix}_q\langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_A,\end{aligned} \tag{26}$$

$$m_{\Lambda} = m_S(\{21\}) + \begin{pmatrix} \{21\} & \{21\} & \| & \{21\}_S \\ 00 & 00 & \| & 00 \end{pmatrix}_q \langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_S + \begin{pmatrix} \{21\} & \{21\} & \| & \{21\}_A \\ 00 & 00 & \| & 00 \end{pmatrix}_q \langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_A, \tag{27}$$

$$m_{\Xi} = m_S(\{21\}) + \begin{pmatrix} \{21\} & \{21\} & \| & \{21\}_S \\ \frac{1}{2}-1 & 00 & \| & \frac{1}{2}-1 \end{pmatrix}_q \langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_S + \begin{pmatrix} \{21\} & \{21\} & \| & \{21\}_A \\ \frac{1}{2}-1 & 00 & \| & \frac{1}{2}-1 \end{pmatrix}_q \langle\{21\}||\hat{T}^{\{21\}}||\{21\}\rangle_A. \tag{28}$$

We also have that according to Racah's factorization lemma, the q-deformed isoscalar factors for the $SU_q(3)$ quantum algebra are given by[11]

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \| & \lambda_{3\gamma} \\ t_1 y_1 & t_2 y_2 & \| & ty \end{pmatrix}_q = \frac{\begin{pmatrix} \lambda_1 & \lambda_2 & | & \lambda_{3\gamma} \\ \mu_1 & \mu_2 & | & \mu_3 \end{pmatrix}_q}{{}_qC^{t_1 t_2 t}_{t_{1z} t_{2z} t_z}} = \frac{{}_qC^{\{\lambda_1\}\times\{\lambda_2\}}_{(\alpha_1\alpha_2)\{\lambda_3\}(\alpha_3)}}{{}_qC^{t_1 t_2 t}_{t_{1z} t_{2z} t_z}}, \tag{29}$$

where ${}_qC^{t_1 t_2 t}_{t_{1z} t_{2z} t_z}$ is the q-deformed Clebsch-Gordan coefficient for $SU_q(2)$. For this case, we have[1,7]

$${}_qC^{1/2\ 0\ 1/2}_{1/2\ 0\ 1/2} = {}_qC^{101}_{101} = {}_qC^{000}_{000} = 1. \tag{30}$$

Then, for the octet baryon we get

$$\begin{pmatrix} \{21\} & \{21\} & \| & \{21\}_{S,A} \\ ty & 00 & \| & ty \end{pmatrix}_q = {}_qC^{\{21\}\times\{21\}}_{(\alpha 5)\{21\}_{S,A}(\alpha)}. \tag{31}$$

Therefore, by combining expressions (25)–(28) and using the quantum Clebsch-Gordan coefficients corresponding to the $\{21\}\times\{21\}$ reduction obtained in Ref. 8, the following q-deformed mass relation for octet baryons is obtained[7]:

$$[3]_q \sqrt{\frac{[3]_q+[2]_q}{[4]_q+1}} m_{\Lambda} + m_{\Sigma}(C(q)-E(q)-D(q)) = m_N \left\{ q^{-2}E(q) + \frac{q^2}{2}\left(A(q) + \frac{\left(\left[\frac{3}{2}\right]_q\right)^2 \sqrt{[5]_q}}{[3]_q \left[\frac{1}{2}\right]_q \left[\frac{5}{2}\right]_q} B(q) \right) \right\} + m_{\Xi} \left\{ q^2 E(q) + \frac{q^3}{2}\left(A(q) - \frac{\left(\left[\frac{3}{2}\right]_q\right)^2 \sqrt{[5]_q}}{[3]_q \left[\frac{1}{2}\right]_q \left[\frac{5}{2}\right]_q} B(q) \right) \right\}, \tag{32}$$

where $A(q)$, $B(q)$, $C(q)$, and $D(q)$ are functions of the q-real parameter given by

$$A(q) = 1 - q^{-1} + q^{-2} + q^{-3} - q^{-4} + q^{-5}, \quad B(q) = 1 + q^{-1} + q^{-2} - q^{-3} - q^{-4} - q^{-5},$$

$$E(q) = \sqrt{\frac{[3]_q+[2]_q}{[4]_q+1}},$$

$$C(q) = \frac{q^{5/2}([2]_q+1)(q^{3/2}+q^{-3/2})}{2[3]_q} A(q), \quad D(q) = \frac{q^{5/2}([2]_q-1)(q^{3/2}-q^{-3/2})\left(\left[\frac{3}{2}\right]_q\right)^2 \sqrt{[5]_q}}{2([3]_q)^2 \left[\frac{1}{2}\right]_q \left[\frac{5}{2}\right]_q} B(q). \tag{33}$$

By replacing the average multiplet masses[17] in the expression (32) and performing a program in C that finds the roots of this expression, we obtain (In this article we choose between the roots of the mass relations which satisfy $0 \leqslant q \leqslant 1$.)

$$q_1 = 0.9870 \pm 0.0002. \tag{34}$$

Throughout this article, the errors of the q-parameters were obtained by applying the formula:

$$\Delta q = \sqrt{\sum_{i=1}^{N} \left(\frac{\partial q}{\partial m_i} \right)^2 (\Delta m_i)^2}, \tag{35}$$

where N is the number of particles under consideration, Δm_i is the error of their masses and $\partial q/\partial m_\Lambda$, $\partial q/\partial m_\Sigma$, $\partial q/\partial m_N$, $\partial q/\partial m_\Xi$, obtained by performing an implicit differentiation of expression (32) are respectively given by

$$\frac{\partial q}{\partial m_\Lambda} = \frac{-F(q)}{m_\Lambda \frac{dF(q)}{dq} + m_\Sigma \frac{dG(q)}{dq} - m_N \frac{dH(q)}{dq} - m_\Xi \frac{dI(q)}{dq}},$$

$$\frac{\partial q}{\partial m_\Sigma} = \frac{-G(q)}{m_\Lambda \frac{dF(q)}{dq} + m_\Sigma \frac{dG(q)}{dq} - m_N \frac{dH(q)}{dq} - m_\Xi \frac{dI(q)}{dq}}$$

$$\frac{\partial q}{\partial m_N} = \frac{H(q)}{m_\Lambda \frac{dF(q)}{dq} + m_\Sigma \frac{dG(q)}{dq} - m_N \frac{dH(q)}{dq} - m_\Xi \frac{dI(q)}{dq}},$$

$$\frac{\partial q}{\partial m_\Xi} = \frac{I(q)}{m_\Lambda \frac{dF(q)}{dq} + m_\Sigma \frac{dG(q)}{dq} - m_N \frac{dH(q)}{dq} - m_\Xi \frac{dI(q)}{dq}}.$$

With the functions $F(q)$, $G(q)$, $H(q)$, and $I(q)$ given by

$$F(q) = [3]_q \sqrt{\frac{[3]_q + [2]_q}{[4]_q + 1}},$$

$$G(q) = C(q) - E(q) - D(q),$$

$$H(q) = q^{-2}E(q) + \frac{q^2}{2}\left(A(q) + \frac{\left(\left[\frac{3}{2} \right]_q \right)^2 \sqrt{[5]_q}}{[3]_q \left[\frac{1}{2} \right]_q \left[\frac{5}{2} \right]_q} B(q) \right),$$

$$I(q) = q^2 E(q) + \frac{q^3}{2}\left(A(q) - \frac{\left(\left[\frac{3}{2} \right]_q \right)^2 \sqrt{[5]_q}}{[3]_q \left[\frac{1}{2} \right]_q \left[\frac{5}{2} \right]_q} B(q) \right).$$

To determine the q-deformed mass relations for the decuplet baryon, we follow the same procedure used for the octet baryon, taking into account that when the q-deformed Wigner-Eckart theorem is applied to the second term of expression (22), the $\{3\} \times \{3\}$, $\{0\} \times \{2\}$, $\{\bar{3}\} \times \{1\}$, and

$\{\overline{6}\}\times\{0\}$ states of the $\{3\}$ representation (which represent 4, 3, 2, and 1 states respectively, corresponding to the Δ, Σ, Ξ, and Ω particles of the decuplet baryon) are coupled to the $\{0\}\times\{0\}$ state of the $\{21\}$ representation, where the coupling coefficients are the q-deformed isoscalar factors. Hence, according to the previous, we obtain the following expressions corresponding to the masses of the particle families in the decuplet baryon[7]:

$$m_{\Delta} = m_S(\{3\}) + \begin{pmatrix} \{3\} & \{21\} & \| & \{3\} \\ \frac{3}{2}1 & 00 & \| & \frac{3}{2}1 \end{pmatrix}_q \langle\{3\}||\hat{T}^{\{21\}}||\{3\}\rangle, \tag{36}$$

$$m_{\Sigma} = m_S(\{3\}) + \begin{pmatrix} \{3\} & \{21\} & \| & \{3\} \\ 10 & 00 & \| & 10 \end{pmatrix}_q \langle\{3\}||\hat{T}^{\{21\}}||\{3\}\rangle, \tag{37}$$

$$m_{\Xi} = m_S(\{3\}) + \begin{pmatrix} \{3\} & \{21\} & \| & \{3\} \\ \frac{1}{2}-1 & 00 & \| & \frac{1}{2}-1 \end{pmatrix}_q \langle\{3\}||\hat{T}^{\{21\}}||\{3\}\rangle, \tag{38}$$

$$m_{\Omega} = m_S(\{3\}) + \begin{pmatrix} \{3\} & \{21\} & \| & \{3\} \\ 0-2 & 00 & \| & 0-2 \end{pmatrix}_q \langle\{3\}||\hat{T}^{\{21\}}||\{3\}\rangle. \tag{39}$$

Where for this case, we have[1,7]

$${}_qC^{3/2\ 0\ 3/2}_{3/2\ 0\ 3/2} = {}_qC^{101}_{101} = {}_qC^{1/2\ 0\ 1/2}_{1/2\ 0\ 1/2} = 1. \tag{40}$$

Then, for the decuplet baryon we have

$$\begin{pmatrix} \{3\} & \{21\} & \| & \{3\} \\ ty & 00 & \| & ty \end{pmatrix}_q = {}_qC^{\{3\}\times\{21\}}_{(\alpha 5)\{3\}(\alpha)} \tag{41}$$

Therefore, by combining expressions (36)–(39) and using the q-deformed Clebsch-Gordan coefficients corresponding to the $\{3\}\times\{21\}$ reduction given in the Appendix, the following q-deformed mass relations for decuplet baryons is obtained[7]:

$$m_{\Sigma^*} - m_{\Omega} = \frac{1+q}{[2]_q}(m_{\Delta} - m_{\Xi^*}), \tag{42}$$

$$m_{\Xi^*} - m_{\Omega} = \frac{q^3}{1+q}(m_{\Sigma^*} - m_{\Omega}), \tag{43}$$

$$m_{\Omega} - m_{\Xi^*} = \frac{q^3}{1+q-q^3}(m_{\Xi^*} - m_{\Sigma^*}), \tag{44}$$

where the q-deformation parameter, according to expression (42) is given by

$$q = \frac{m_{\Delta} - m_{\Xi^*} \pm \sqrt{(m_{\Delta} - m_{\Xi^*})^2 - 4(m_{\Sigma^*} - m_{\Omega})(m_{\Sigma^*} + m_{\Xi^*} - m_{\Omega} - m_{\Delta})}}{2(m_{\Sigma^*} + m_{\Xi^*} - m_{\Omega} - m_{\Delta})}. \tag{45}$$

As in the case of the octet baryons, we replace the average multiplet masses obtaining the following values for the q-parameter:

$$q_2 = 0.917 \pm 0.012, \quad q_3 = 0.986 \pm 0.003, \quad q_4 = 0.985 \pm 0.002. \tag{46}$$

With the aim to determine a unique q-parameter for the q-deformed Gell-Mann-Okubo mass relations for octet and decuplet baryons, we perform a χ^2 adjustment given by the fitted function:

TABLE I. Error percentages of the Gell-Mann-Okubo mass relations for the $SU_q(3)$ and SU(3) algebras.

Mass relation	q	$\frac{\lvert\text{rhs}-\text{lhs}\rvert}{\text{rhs}}\%$
(32)	0.970	0.33
(32)	1.000	0.58
(42)	0.970	2.99
(42)	1.000	4.49
(43)	0.970	4.26
(43)	1.000	3.40
(44)	0.970	7.95
(44)	1.000	8.23

$$\chi^2 = \sum_{i=1}^{4} \frac{(q_i - q)^2}{q^2}. \tag{47}$$

By minimizing the χ^2 function, we obtain the fitted q-parameter given by

$$q = 0.970 \pm 0.003. \tag{48}$$

Besides that, by comparing the generalization of the Gell-Mann-Okubo mass formula for pseudoscalar meson with its q-deformed version, the following relation is obtained:[12]

$$\frac{f_K^2}{f_\pi^2} = \frac{[2]_q}{2([2]_q - [3]_q)}, \tag{49}$$

where f_K and f_π are the decay constants for the K and π mesons, respectively.

Moreover, the ratio f_K/f_π can be expressed in terms of the Cabbibo angle as follows[12]:

$$\tan^2\theta_C = \frac{\frac{m_\pi^2}{m_K^2}}{\frac{f_K}{f_\pi} - \frac{m_\pi^2}{m_K^2}}. \tag{50}$$

From expressions (49) and (50), a connection between the q-deformation parameter and the Cabbibo angle is observed.[12]

On the other hand, as we have chosen before that $0 \leqslant q \leqslant 1$, we can introduce a new τ parameter according to:

$$q = \cos\tau. \tag{51}$$

Then, from expressions (48) and (51) we get:

$$\tau = (0.246 \pm 0.012)\text{rad}. \tag{52}$$

As the Cabbibo angle is equal to $\theta_C = (0.226 \pm 0.002)\text{rad}$,[17] expression (52) implies:

$$\tau = (1.085 \pm 0.063)\,\theta_C. \tag{53}$$

Hence, according to the previous result, it is possible to interpret the q-deformation parameter with the cosine of the Cabbibo angle.

By replacing the q-deformation parameter obtained by the χ^2 fitting in the Gell-Mann-Okubo mass relations and comparing with the $q=1$ case, we obtain Table I. In Table I we can see that for the q-deformed Gell-Mann-Okubo mass relations for the octet and decuplet baryons, a better

agreement with the experimental masses than the predicted by the SU(3) algebra is obtained, except for expression (43) corresponding to the decuplet baryon, where the difference between the error percentages is only 0.86%.

IV. THE *q*-DEFORMED COLEMAN-GLASHOW RELATIONS FOR OCTET AND DECUPLET BARYONS

The center of the octet baryon is degenerate and so the U eigenfunctions differ from isoespin eigenfunctions. The $U=1$ and $U=0$ eigenfuntions are

$$|\Sigma_U^0\rangle = \frac{\sqrt{[3]_q}}{[2]_q}|\Lambda^0\rangle - \frac{1}{[2]_q}|\Sigma^0\rangle, \tag{54}$$

$$|\Lambda_U^0\rangle = \frac{\sqrt{[3]_q}}{[2]_q}|\Lambda^0\rangle + \frac{1}{[2]_q}|\Sigma^0\rangle. \tag{55}$$

For this case, we consider the following expression for the mass operator:

$$\hat{M} = \hat{M}_S + \hat{M}_T + \hat{M}_U, \tag{56}$$

where the operators $\hat{M}_S$, $\hat{M}_T$, and $\hat{M}_U$ are $\mathrm{SU}_q(3)$ scalar, isospin scalar and U spin scalar, respectively.

The mass operators $\hat{M}_T$ and $\hat{M}_U$ have matrix elements related by

$$m_T(n) = m_T(p), \quad m_T(\Sigma^+) = m_T(\Sigma^0), \quad m_U(n) = m_U(\Sigma_U^0), \quad m_U(p) = m_U(\Sigma_U^+),$$

$$m_T(\Sigma^-) = m_T(\Sigma^0), \quad m_T(\Xi^-) = m_T(\Xi^0), \quad m_U(\Sigma^-) = m_U(\Xi^-), \quad m_U(\Xi^0) = m_U(\Sigma_U^0). \tag{57}$$

Moreover, by taking into account that

$$m_U(\Sigma_U^0) = \langle\Sigma_U^0|\hat{M}_U|\Sigma_U^0\rangle \quad \langle\Sigma_U^0|\hat{M}_U|\Lambda_U^0\rangle = 0,$$

$$m(\Sigma^0\Lambda^0) = \langle\Sigma^0|\hat{M}|\Lambda^0\rangle = \langle\Sigma^0|\hat{M}_U|\Lambda^0\rangle = m_U(\Sigma^0\Lambda^0)$$

and using the expressions corresponding to the $|\Sigma_U^0\rangle$, $|\Lambda_U^0\rangle$ states, we get:

$$m_U(\Sigma_U^0) = \frac{[3]_q m_U(\Lambda^0) + m_U(\Sigma^0) - 2\sqrt{[3]_q}m_U(\Sigma^0\Lambda^0)}{([2]_q)^2}, \tag{58}$$

$$m_U(\Lambda^0) - m_U(\Sigma^0) = -\frac{[4]_q}{[2]_q\sqrt{[3]_q}}m(\Sigma^0\Lambda^0). \tag{59}$$

Then, from expressions (56)–(58), we find

$$m(n) - m(p) + m(\Sigma^+) - m(\Sigma^0) = \frac{[3]_q}{([2]_q)^2}(m_U(\Lambda^0) - m_U(\Sigma^0)) - \frac{2\sqrt{[3]_q}}{([2]_q)^2}m_U(\Sigma^0\Lambda^0), \tag{60}$$

$$m(\Xi^-) - m(\Xi^0) + m(\Sigma^0) - m(\Sigma^-) = \frac{2\sqrt{[3]_q}}{([2]_q)^2}m_U(\Sigma^0\Lambda^0) + \frac{[3]_q}{([2]_q)^2}(m_U(\Sigma^0) - m_U(\Lambda^0)). \tag{61}$$

Therefore, by replacing (59) in expressions (60) and (61), the following relations are obtained:

$$m_n - m_p + m_{\Sigma^+} - m_{\Sigma^0} = -\sqrt{[3]_q} m_{\Sigma^0\Lambda^0}, \tag{62}$$

$$m_{\Xi^-} - m_{\Xi^0} + m_{\Sigma^0} - m_{\Sigma^-} = \sqrt{[3]_q} m_{\Sigma^0\Lambda^0}. \tag{63}$$

From the linear combinations of the previous relations we find

$$m_{\Xi^-} - m_{\Xi^0} = m_{\Sigma^-} - m_{\Sigma^+} + m_p - m_n. \tag{64}$$

Hence, the Colemann-Glashow relation for the octet baryon is independent of q.

On the other hand, it is known that when the electromagnetic interactions are neglected, we have that the mass operator for hadron multiplets is given by

$$\hat{M} = \hat{M}_S + \hat{M}_T, \tag{65}$$

where $\hat{M}_S$ is a $\mathrm{SU}_q(3)$ invariant whereas $\hat{M}_T$ is an operator corresponding to the $\mathrm{SU}_q(3)$ symmetry breaking.

We also have that under $\mathrm{SU}_q(2)_U \times \mathrm{U}(1)_Q$ the $\hat{M}_T$ operator in expression (65) transforms as the sum of a U vector spin and a U scalar.[14] Applying the $\mathrm{SU}_q(2)$ Wigner-Eckart theorem to this subgroup, we have

$$M(U,U_3) = A + C(U,q) q^{-U_3} U_3, \tag{66}$$

where $C(U,q)$ is given by[11]

$$C(U,q) = \frac{q^{U+1/2}}{[2U+1]_q} \langle \alpha U || \hat{M}_U || \alpha U \rangle. \tag{67}$$

From expressions (66) and (67) we get

$$m(U,U_3) - m(U,U_3-1) = C(U,q) q^{-U_3+1} + C(U,q) q^{-U_3} (1-q) U_3. \tag{68}$$

By applying the previous formula to the octet baryon, we find that

$$m(n) - m(\Sigma_U^0) = C(1,q) q^{-1},$$

$$m(\Sigma_U^0) - m(\Xi^0) = C(1,q) q.$$

Then, the following relation holds:

TABLE II. Error percentages of the Coleman-Glashow relations for the $\mathrm{SU}_q(3)$ and SU(3) algebras.

Mass relation	q	$\frac{\lvert \mathrm{rhs}-\mathrm{lhs} \rvert}{\mathrm{rhs}}\%$
(70)	0.973	0.14
(70)	1.000	0.60
(74)	0.973	1.29
(74)	1.000	1.42
(74)	0.973	1.27
(74)	1.000	7.03
(74)	0.973	1.03
(74)	1.000	9.72
(75)	0.973	2.97
(75)	1.000	2.51

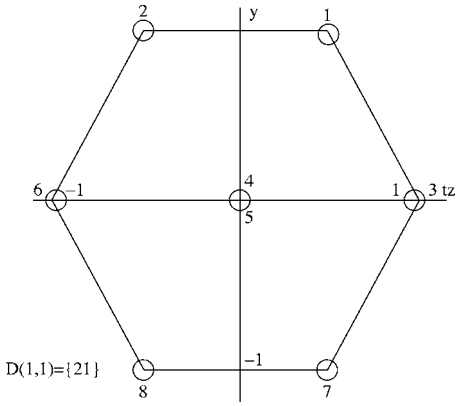

FIG. 1. Representation {21} of $SU_q(3)$ (Ref. 7).

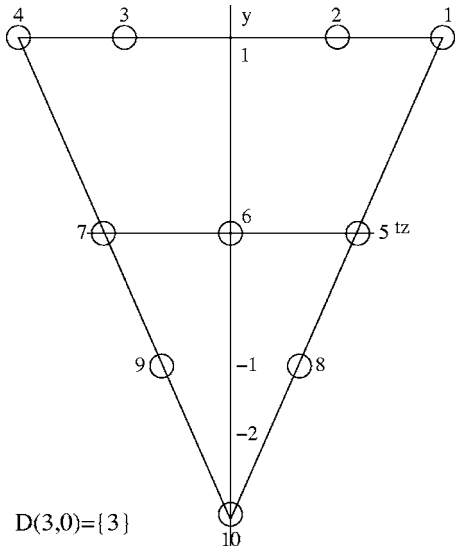

FIG. 2. Representation {3} of $SU_q(3)$ (Ref. 7).

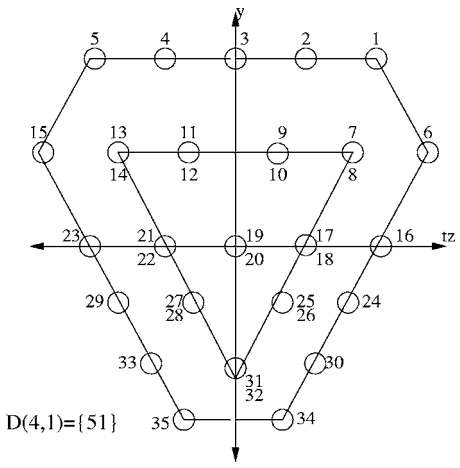

FIG. 3. Representation {51} of $SU_q(3)$ (Ref. 7).

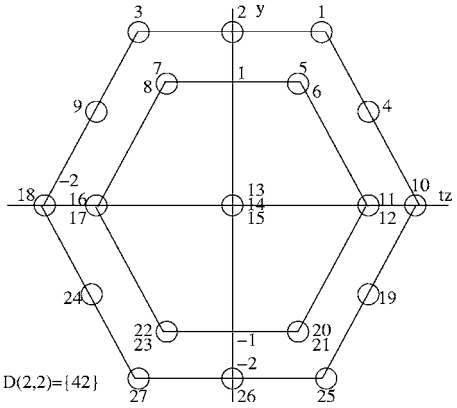

FIG. 4. Representation {42} of $SU_q(3)$ (Ref. 7).

$$q(m_n - m_{\Sigma_U^0}) = q^{-1}(m_{\Sigma_U^0} - m_{\Xi^0}). \tag{69}$$

Hence, by using (58), (59), and (69) we obtain a q deformed mass relation for the particles in the octet baryon:

$$q^2 m_n + m_p + q^{-2} m_{\Xi^0} + m_{\Xi^-} = [3]_q m_{\Lambda^0} + m_{\Sigma^+} + m_{\Sigma^-} - m_{\Sigma^0} \tag{70}$$

with the q deformation parameter given by

$$q = \pm \sqrt{\frac{s \pm \sqrt{s^2 - 4(m_n - m_{\Lambda^0})(m_{\Xi^0} - m_{\Lambda^0})}}{2(m_n - m_{\Lambda^0})}} \tag{71}$$

where the s parameter has been introduced according to

$$s = m_{\Sigma^+} + m_{\Sigma^-} + m_{\Lambda^0} - m_p - m_{\Xi^-} - m_{\Sigma^0}. \tag{72}$$

By replacing the experimental octet particle masses in expression (71), we obtain

$$q_1 = 0.965 \pm 0.001. \tag{73}$$

On the other hand, when formula (68) is applied to the decuplet baryon, we get the following expressions:

$$m_{\Delta^-} - m_{\Sigma^{*-}} = \tfrac{1}{2} C\left(\tfrac{3}{2}, q\right) q^{-3/2}(3 - q),$$

$$m_{\Sigma^{*-}} - m_{\Xi^{*-}} = \tfrac{1}{2} C\left(\tfrac{3}{2}, q\right) q^{-1/2}(1 + q),$$

$$m_{\Xi^{*-}} - m_{\Omega^-} = \tfrac{1}{2} C\left(\tfrac{3}{2}, q\right) q^{1/2}(3q - 1),$$

$$m_{\Delta^0} - m_{\Sigma^{*0}} = C(1, q) q^{-1},$$

$$m_{\Sigma^{*0}} - m_{\Xi^{*0}} = C(1, q) q.$$

Hence, for the decuplet baryons we obtain:

$$\frac{q^{3/2}(m_{\Delta^-} - m_{\Sigma^{*-}})}{3 - q^{-1}} = \frac{q^{1/2}(m_{\Sigma^{*-}} - m_{\Xi^{*-}})}{1 + q} = \frac{q^{-1/2}(m_{\Xi^{*-}} - m_{\Omega^-})}{3q - 1}, \tag{74}$$

$$q(m_{\Delta^0} - m_{\Sigma^{*0}}) = q^{-1}(m_{\Sigma^{*0}} - m_{\Xi^{*0}}). \tag{75}$$

Then, from expressions (74) and (75) and using the experimental decuplet particle masses we obtain:

$$q_2 = 0.976 \pm 0.007, \quad q_3 = 0.965 \pm 0.004, \tag{76}$$

$$q_4 = 0.970 \pm 0.003, \quad q_5 = 0.988 \pm 0.008. \tag{77}$$

Up to this point we have obtained five different values for the q-deformation parameter from the q-deformed Coleman-Glashow relations for octet and decuplet baryons. In order to obtain a unique q-parameter we perform a χ^2 adjustment obtaining

$$q = 0.973 \pm 0.002. \tag{78}$$

For this case, we have obtained the τ parameter given by

$$\tau = (0.233 \pm 0.010)\text{rad} = (1.030 \pm 0.053)\,\theta_C, \tag{79}$$

which implies that the q-deformation parameter can be interpreted with the cosine of the Cabbibo angle.

By replacing the q-deformation parameter obtained by the χ^2 adjustment in the Coleman-Glashow relations and comparing with the predicted by the SU(3) algebra, we obtain the Table II. From Table II, a better agreement of the q-deformed Coleman-Glashow relations with the experiment than the predicted by the SU(3) algebra is obtained in all cases except in the last [relation (75)], where the difference between the error percentages is only 0.46%.

V. CONCLUSIONS

The quantum group $SU_q(3)$ provides a good tool to solve problems in particle physics, especially when one needs to describe the mass splitting for particles from isomultiplets within octet and decuplet baryons.

The q-deformed Clebsch-Gordan coefficients corresponding to the $\{3\}\times\{21\}$ reduction of the $SU_q(3)$ algebra were computed. The q-deformed mass relations for octet and decuplet baryons have been explicity obtained from the quantum Clebsch-Gordan coefficients corresponding to the $\{21\}\times\{21\}$ and $\{3\}\times\{21\}$ reductions. The Coleman-Glashow relations for octet and decuplet baryons have been found in the $SU_q(3)$ quantum algebra. From the Coleman-Glashow relation for the octet baryon, a q-deformed mass relation between its particles has been obtained.

By performing an adjustment of the q-deformation parameter in the q-deformed Gell-Mann-Okubo and Coleman-Glashow relations for octet and decuplet baryons, we obtain that the corresponding values for this parameter are $q=0.970\pm0.003$ and $q=0.973\pm0.002$, respectively. These values are directly connected with the cosine of the Cabbibo angle. That is, a unique relation between the q-deformation parameter and the Cabbibo angle has been found, which differs with the results given in Ref. 12 in the fact that in this reference two different relations, $q=e^{2i\theta_C}$ and $q=e^{i\theta_C}$, between these parameters have been obtained for the octet and decuplet baryons, respectively, exhibiting error percentages of approximately 0.07% and 0.53% when these relations are replaced in the q deformed masses expressions.

In spite of the fact that the error percentages of the q-deformed mass relations obtained in Ref. 12 are lower than those obtained in this article, it is important to point out that we have shown that when two approximately equivalent values of the q-deformation parameter are used, the q-deformed Gell-Mann-Okubo and Coleman-Glashow relations for octet and decuplet baryons exhibit a very good agreement with the experimental results, in most cases better than the predicted by the SU(3) algebra. The error percentages of the q-deformed Gell-Mann-Okubo and Coleman-Glashow relations are lower than 7.95% and 2.97%, respectively.

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APPENDIX: QUANTUM CLEBSCH-GORDAN COEFFICIENTS FOR THE {3}×{21} REDUCTION

The product of the $SU_q(3)$ representations {3} and {21} is given by

$$\{3\} \times \{21\} = \{51\} + \{42\} + \{3\} + \{21\}, \tag{A1}$$

where {51}, {42}, {3}, and {21} are representations with dimensions equal to 35, 27, 10, and 8, respectively. These representations are shown in Figs. 1–4.

Through a straightforward calculation in which the angular momentum addition rules are taken into account together with the requirements of orthogonality, the q-deformed Clebsch-Gordan coefficients corresponding to the {3}×{21} reduction are determined and shown in the Table III. In this case, we have that χ_i, $i=1,2,\ldots,8$ and ξ_j, $j=1,2,\ldots,10$ are the wave functions which describe the octet and decuplet baryons states corresponding to the {21} and {3} representations.

TABLE III. The q-deformed Clebsch-Gordan coefficients for the {3}×{21} reduction.

		(a) $\psi_1^{\{51\}}$	(b) $\psi_5^{\{51\}}$	(c) $\psi_6^{\{51\}}$	(d) $\psi_{15}^{\{51\}}$	(e) $\psi_{34}^{\{51\}}$	(f) $\psi_{35}^{\{51\}}$
(a) $\xi_1\chi_1$	(d) $\xi_4\chi_6$						
(b) $\xi_4\chi_2$	(e) $\xi_{10}\chi_7$			1			
(c) $\xi_1\chi_3$	(f) $\xi_{10}\chi_8$						
		(a) $\psi_2^{\{51\}}$	$-\psi_1^{\{42\}}$	(b) $\psi_4^{\{51\}}$	$\psi_3^{\{42\}}$	(c) $\psi_3^{\{51\}}$	$-\psi_2^{\{42\}}$
		(d) $\psi_{16}^{\{51\}}$	$\psi_{30}^{\{51\}}$	(e) $\psi_{10}^{\{42\}}$	$\psi_{25}^{\{42\}}$	(f) $\psi_{24}^{\{51\}}$	$\psi_{19}^{\{42\}}$
		(g) $\psi_{23}^{\{51\}}$	$\psi_{33}^{\{51\}}$	(h) $\psi_{18}^{\{42\}}$	$\psi_{27}^{\{42\}}$	(i) $\psi_{29}^{\{51\}}$	$\psi_{24}^{\{42\}}$
(a) $\xi_2\chi_1$	(b) $\xi_3\chi_2$						
(d) $\xi_5\chi_3$	(e) $\xi_8\chi_7$	$\sqrt{\frac{q[3]_q}{[4]_q}}$	$\sqrt{\frac{1}{q^3[4]_q}}$	$\sqrt{\frac{[3]_q}{q[4]_q}}$	$-\sqrt{\frac{q^3}{[4]_q}}$	0	0
(g) $\xi_7\chi_6$	(h) $\xi_9\chi_8$						
(c) $\xi_2\chi_2$	(c) $\xi_3\chi_1$					$q^{-1}\sqrt{\frac{[2]_q}{[4]_q}}$	$-q\sqrt{\frac{[2]_q}{[4]_q}}$
(f) $\xi_5\chi_7$	(f) $\xi_8\chi_3$	0	0	0	0		
(c) $\xi_7\chi_8$	(c) $\xi_9\chi_6$					$q\sqrt{\frac{[2]_q}{[4]_q}}$	$q^{-1}\sqrt{\frac{[2]_q}{[4]_q}}$
(a) $\xi_1\chi_2$	(b) $\xi_4\chi_1$						
(d) $\xi_1\chi_7$	(e) $\xi_{10}\chi_3$	$\sqrt{\frac{1}{q^3[4]_q}}$	$-\sqrt{\frac{q[3]_q}{[4]_q}}$	$\sqrt{\frac{q^3}{[4]_q}}$	$\sqrt{\frac{[3]_q}{q[4]_q}}$	0	0
(g) $\xi_4\chi_8$	(h) $\xi_{10}\chi_6$						

		(a) $\psi_{31}^{\{51\}}$	$\psi_{32}^{\{51\}}$	$\psi_{26}^{\{42\}}$	$\psi_{10}^{\{3\}}$	(b) $\psi_{19}^{\{51\}}$	$\psi_{20}^{\{51\}}$
(a)$\xi_{10}\chi_4$	(b)$\xi_5\chi_6$	$\sqrt{\frac{q^3}{[4]_q}}$	0	$\sqrt{\frac{[3]_q}{q[4]_q}}$	0	$\frac{\sqrt{q^{-3}[2]_q}}{[4]_q}$	$\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^3[6]_q}}$
(a)$\xi_{10}\chi_5$	(b)$\xi_7\chi_3$	0	$\sqrt{\frac{q^3[3]_q}{[6]_q}}$	0	$\sqrt{\frac{[3]_q}{q^3[6]_q}}$	$\frac{\sqrt{q^5[2]_q}}{[4]_q}$	$-\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^3[6]_q}}$
(a)$\xi_8\chi_8$	(b)$\xi_3\chi_7$	$\sqrt{\frac{q^{-2}[3]_q}{[2]_q[4]_q}}$	$\sqrt{\frac{q^{-2}[3]_q}{[2]_q[6]_q}}$	$-\frac{q}{\sqrt{[2]_q[4]_q}}$	$-\sqrt{\frac{q^4[3]_q}{[2]_q[6]_q}}$	$\frac{\sqrt{q^{-1}[2]_q}}{[4]_q}$	$-\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^9[6]_q}}$

TABLE III. (*Continued.*)

		(a) $\psi_{31}^{\{51\}}$	$\psi_{32}^{\{51\}}$	$\psi_{26}^{\{42\}}$	$\psi_{10}^{\{3\}}$	(b) $\psi_{19}^{\{51\}}$	$\psi_{20}^{\{51\}}$
(a)$\xi_9\chi_7$	(b)$\xi_2\chi_8$	$\sqrt{\frac{[3]_q}{[2]_q[4]_q}}$	$-\sqrt{\frac{q^{-4}[3]_q}{[2]_q[6]_q}}$	$-\frac{q^2}{\sqrt{[2]_q[4]_q}}$	$\sqrt{\frac{q^2[3]_q}{[2]_q[6]_q}}$	$\frac{\sqrt{q^{-5}[2]_q}}{[4]_q}$	$\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^5[6]_q}}$
(a)$\xi_8\chi_7$	(b)$\xi_6\chi_4$	0	0	0	0	$\frac{[2]_q\sqrt{q[2]_q}}{[4]_q}$	$\frac{(1-q^{-2})[2]_q}{[4]_q\sqrt{q[6]_q}}$
(a)$\xi_9\chi_8$	(b)$\xi_8\chi_2$	0	0	0	0	0	$\sqrt{\frac{1}{q^5[6]_q}}$
(a)$\xi_9\chi_5$	(b)$\xi_9\chi_1$	0	0	0	0	0	$\sqrt{\frac{1}{q^3[6]_q}}$
(a)$\xi_9\chi_4$	(b)$\xi_6\chi_5$	0	0	0	0	0	$\sqrt{\frac{[3]_q}{[6]_q}}$

		(a) $\psi_{26}^{\{51\}}$	$\psi_{20}^{\{42\}}$	$\psi_{21}^{\{42\}}$	$\psi_{8}^{\{3\}}$	$\psi_{7}^{\{21\}}$	(b) $\psi_{5}^{\{21\}}$
(a) $\xi_{10}\chi_1$	(b) $\xi_9\chi_1$	$q^3\sqrt{\frac{[3]_q}{[4]_q[6]_q}}$	0	$\frac{q[3]_q}{\sqrt{[2]_q[4]_q[5]_q}}$	$\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{q^3[5]_q}}$	$-\sqrt{\frac{1}{[5]_q}}$
(a) $\xi_9\chi_3$	(b) $\xi_7\chi_3$	$-\frac{q^{-1}}{\sqrt{[4]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{[3]_q[4]_q}}$	$-\frac{q^{-1}([5]_q+q^{-1}[2]_q)}{\sqrt{[2]_q[3]_q[4]_q[5]_q}}$	$\frac{q^2}{\sqrt{[2]_q[6]_q}}$	$\sqrt{\frac{q[2]_q}{[3]_q[5]_q}}$	$-\frac{q^{-2}}{\sqrt{[5]_q}}$
(a) $\xi_5\chi_8$	(b) $\xi_5\chi_6$	$\frac{q^{-2}[2]_q}{\sqrt{[4]_q[6]_q}}$	$-\sqrt{\frac{[2]_q}{[3]_q[4]_q}}$	$-\sqrt{\frac{[2]_q}{[3]_q[4]_q[5]_q}}$	$-q\sqrt{\frac{[2]_q}{[6]_q}}$	$\sqrt{\frac{q^5[2]_q}{[3]_q[5]_q}}$	$\frac{-q^2}{\sqrt{[5]_q}}$
(a) $\xi_6\chi_7$	(b) $\xi_8\chi_2$	$-\sqrt{\frac{[2]_q}{q^7[4]_q[6]_q}}$	$-\frac{q^{3/2}[2]_q}{\sqrt{[3]_q[4]_q}}$	$\sqrt{\frac{1}{q^3[3]_q[4]_q[5]_q}}$	$\sqrt{\frac{1}{q[6]_q}}$	$-\frac{q}{\sqrt{[3]_q[5]_q}}$	$\frac{q^{-1}}{\sqrt{[5]_q}}$
(a) $\xi_8\chi_5$	(b) $\xi_6\chi_4$	$\frac{[3]_q\sqrt{q[3]_q}}{\sqrt{[2]_q[4]_q[6]_q}}$	0	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q^5}{[4]_q[5]_q}}$	$\frac{([2]_q-q^3)\sqrt{[3]_q}}{[2]_q\sqrt{q^3[6]_q}}$	$-\sqrt{\frac{1}{[5]_q}}$	$\frac{q}{\sqrt{[5]_q}}$
(a) $\xi_8\chi_4$	(b) $\xi_2\chi_8$	$\sqrt{\frac{q}{[2]_q[4]_q[6]_q}}$	$\frac{[2]_q}{\sqrt{q^3[3]_q[4]_q}}$	$\frac{[2]_q+q[5]_q}{[2]_q\sqrt{q[3]_q[4]_q[5]_q}}$	$\frac{-1}{[2]_q}\sqrt{\frac{q^7}{[6]_q}}$	$-\frac{q^2}{\sqrt{[3]_q[5]_q}}$	0

		(a) $\psi_{14}^{\{42\}}$	$\psi_{6}^{\{3\}}$	$\psi_{4}^{\{21\}}$	(b) $\psi_{14}^{\{42\}}$	$\psi_{6}^{\{3\}}$	$\psi_{4}^{\{21\}}$
(a) $\xi_8\chi_2$	(b) $\xi_9\chi_1$	$\sqrt{\frac{1}{q[2]_q[5]_q}}$	$\sqrt{\frac{1}{q^3[6]_q}}$	$\frac{q^{-3}}{\sqrt{[3]_q[5]_q}}$	$\sqrt{\frac{q}{[2]_q[5]_q}}$	$\sqrt{\frac{1}{q[6]_q}}$	$\frac{q^{-2}}{\sqrt{[3]_q[5]_q}}$
(a) $\xi_2\chi_8$	(b) $\xi_6\chi_5$	$-\frac{1}{[4]_q}\sqrt{\frac{[2]_q}{q[5]_q}}$	$-\sqrt{\frac{q}{[6]_q}}$	$\frac{q^2[2]_q}{\sqrt{[3]_q[5]_q}}$	$-\sqrt{\frac{q^3[3]_q}{[2]_q[5]_q}}$	$\frac{q^{-5/2}-q^{-3/2}}{[2]_q\sqrt{[6]_q([3]_q)^{-1}}}$	$\frac{-q^{-1}}{\sqrt{[5]_q}}$
(a) $\xi_6\chi_4$	(b) $\xi_3\chi_7$	$\frac{(1+q^4-q^{-4}-q^2)\sqrt{[2]_q}}{[4]_q\sqrt{q[5]_q}}$	$\frac{q^{1/2}-q^{5/2}}{\sqrt{[6]_q}}$	$\frac{q^{-1}-q}{\sqrt{[3]_q[5]_q}}$	$\frac{\sqrt{q^{-5}[2]_q}}{[4]_q\sqrt{[5]_q}}$	$\frac{[3]_q+[2]_q-q^5}{([2]_q)^2\sqrt{q^5[6]_q}}$	$\frac{-[2]_q}{\sqrt{[3]_q[5]_q}}$
(a) $\xi_5\chi_6$	(b) $\xi_7\chi_3$	$\frac{([2]_q+q^5)\sqrt{[2]_q}}{[4]_q\sqrt{q^5[5]_q}}$	$-\sqrt{\frac{q^3}{[6]_q}}$	$\frac{-1}{\sqrt{[3]_q[5]_q}}$	$\frac{-(q^{-4}+q^{-2}+q^2)}{[4]_q\sqrt{[5]_q(q[2]_q)^{-1}}}$	$\sqrt{\frac{q^3}{[6]_q}}$	$\sqrt{\frac{1}{[3]_q[5]_q}}$

		$\psi_{28}^{\{51\}}$	$\psi_{22}^{\{42\}}$	$\psi_{23}^{\{42\}}$	$\psi_{9}^{\{3\}}$	$\psi_{8}^{\{21\}}$
	$\xi_{10}\chi_2$	$q^3\sqrt{\frac{[3]_q}{[4]_q[6]_q}}$	0	$\frac{q[3]_q}{\sqrt{[2]_q[4]_q[5]_q}}$	$\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{q^3[5]_q}}$
	$\xi_8\chi_6$	$\frac{1}{\sqrt{[4]_q[6]_q}}$	$q^{-2}\sqrt{\frac{[2]_q}{[3]_q[4]_q}}$	$-\frac{q^{-5/2}([5]_q+q[2]_q)}{\sqrt{[2]_q[3]_q[4]_q[5]_q}}$	$-\frac{q^3}{\sqrt{[2]_q[6]_q}}$	$-\sqrt{\frac{q^3[2]_q}{[3]_q[5]_q}}$
	$\xi_7\chi_7$	$-\frac{q^{-3}[2]_q}{\sqrt{[4]_q[6]_q}}$	$-q^2\sqrt{\frac{[2]_q}{[3]_q[4]_q}}$	$-q^{-1}\sqrt{\frac{[2]_q}{[3]_q[4]_q[5]_q}}$	$\sqrt{\frac{[2]_q}{[6]_q}}$	$-\sqrt{\frac{q^3[2]_q}{[3]_q[5]_q}}$
	$\xi_6\chi_8$	$\sqrt{\frac{[2]_q}{q^3[4]_q[6]_q}}$	$-\frac{q^{1/2}[2]_q}{\sqrt{[3]_q[4]_q}}$	$\sqrt{\frac{q}{[3]_q[4]_q[5]_q}}$	$-\sqrt{\frac{q^3}{[6]_q}}$	$\frac{q^3}{\sqrt{[3]_q[5]_q}}$

TABLE III. (*Continued.*)

		$\psi_{28}^{\{51\}}$	$\psi_{22}^{\{42\}}$	$\psi_{23}^{\{42\}}$	$\psi_{9}^{\{3\}}$	$\psi_{8}^{\{21\}}$
	$\xi_9\chi_5$	$\frac{[3]_q\sqrt{q[3]_q}}{\sqrt{[2]_q[4]_q[6]_q}}$	0	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q^5}{[4]_q[5]_q}}$	$\frac{([2]_q-q^3)\sqrt{[3]_q}}{[2]_q\sqrt{q^3[6]_q}}$	$\sqrt{\frac{1}{[5]_q}}$
	$\xi_9\chi_4$	$-\sqrt{\frac{1}{q^3[2]_q[4]_q[6]_q}}$	$\frac{[2]_q}{\sqrt{q[3]_q[4]_q}}$	$-\frac{[2]_q+q[5]_q}{[2]_q\sqrt{q^5[3]_q[4]_q[5]_q}}$	$\frac{1}{[2]_q}\sqrt{\frac{q^3}{[6]_q}}$	$\frac{1}{\sqrt{[3]_q[5]_q}}$
		(a) $\psi_{8}^{\{51\}}$	$\psi_{7}^{\{51\}}$	$\psi_{4}^{\{42\}}$	$\psi_{1}^{\{3\}}$	(b) $\psi_{13}^{\{42\}}$
(a) $\xi_1\chi_4$	(b) $\xi_8\chi_2$	$\frac{[3]_q}{\sqrt{q^3[2]_q[4]_q[5]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{q^3[5]_q}}$	$\frac{1}{[2]_q}\sqrt{\frac{q[3]_q}{[4]_q}}$	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q^3}{[6]_q}}$	$-\frac{[3]_q}{[4]_q}\sqrt{\frac{q^3[2]_q}{[3]_q}}$
(a) $\xi_1\chi_5$	(b) $\xi_5\chi_6$	$\sqrt{\frac{[3]_q[5]_q}{q^3[2]_q[4]_q[6]_q}}$	0	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q}{[4]_q}}$	$-\frac{1}{[2]_q}\sqrt{\frac{q^3[3]_q}{[6]_q}}$	$\frac{1}{[4]_q}\sqrt{\frac{[2]_q}{q^7[3]_q}}$
(a) $\xi_2\chi_3$	(b) $\xi_7\chi_3$	$-q^{-4}\sqrt{\frac{[3]_q}{[4]_q[5]_q[6]_q}}$	$q\sqrt{\frac{[3]_q}{[5]_q}}$	$-q^{-2}\sqrt{\frac{1}{[2]_q[4]_q}}$	$q^{-1}\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$\frac{1}{[4]_q}\sqrt{\frac{q[2]_q}{[3]_q}}$
(a) $\xi_5\chi_1$	(b) $\xi_2\chi_8$	$q\sqrt{\frac{[3]_q[5]_q}{[4]_q[6]_q}}$	0	$q^{-1}\sqrt{\frac{1}{[2]_q[4]_q}}$	$q^{-2}\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$-\frac{[3]_q}{[4]_q}\sqrt{\frac{[2]_q}{q[3]_q}}$
(a) $\xi_1\chi_3$	(b) $\xi_6\chi_4$	0	0	0	0	$\frac{[2]_q}{[4]_q}\sqrt{\frac{[2]_q}{q^3[3]_q}}$
		(a) $\psi_{14}^{\{51\}}$	$\psi_{13}^{\{51\}}$	$\psi_{9}^{\{42\}}$	$\psi_{4}^{\{3\}}$	(b) $\psi_{15}^{\{42\}}$
(a) $\xi_4\chi_4$	(b) $\xi_8\chi_2$	$\frac{[3]_q}{\sqrt{q^7[2]_q[4]_q[5]_q[6]_q}}$	$\sqrt{\frac{q^3[2]_q}{[5]_q}}$	$-\frac{1}{[2]_q}\sqrt{\frac{[3]_q}{q^3[4]_q}}$	$\frac{[3]_q}{[2]_q}\sqrt{\frac{1}{q[6]_q}}$	$\sqrt{\frac{q^3[3]_q}{[2]_q[5]_q}}$
(a) $\xi_4\chi_5$	(b) $\xi_5\chi_6$	$\sqrt{\frac{[3]_q[5]_q}{q^3[2]_q[4]_q[6]_q}}$	0	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q}{[4]_q}}$	$-\frac{1}{[2]_q}\sqrt{\frac{q^3[3]_q}{[6]_q}}$	$\sqrt{\frac{[2]_q}{q[3]_q[5]_q}}$
(a) $\xi_3\chi_6$	(b) $\xi_7\chi_3$	$q^{-1}\sqrt{\frac{[3]_q}{[4]_q[5]_q[6]_q}}$	$q^{-1}\sqrt{\frac{[3]_q}{[5]_q}}$	$q\sqrt{\frac{1}{[2]_q[4]_q}}$	$-q^2\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{q^5[3]_q[5]_q}}$
(a) $\xi_7\chi_2$	(b) $\xi_9\chi_1$	$q\sqrt{\frac{[3]_q[5]_q}{[4]_q[6]_q}}$	0	$q^{-1}\sqrt{\frac{1}{[2]_q[4]_q}}$	$q^{-2}\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$-\sqrt{\frac{q[3]_q}{[2]_q[5]_q}}$
(a) $\xi_1\chi_3$	(b) $\xi_6\chi_4$	0	0	0	0	$-\sqrt{\frac{[2]_q}{q^3[3]_q[5]_q}}$
		$\psi_{18}^{\{51\}}$	$\psi_{17}^{\{51\}}$	$\psi_{11}^{\{42\}}$	$\psi_{12}^{\{42\}}$	$\psi_{5}^{\{3\}}$	$\psi_{3}^{\{21\}}$
$\xi_5\chi_5$		$\sqrt{\frac{[3]_q}{q[6]_q}}$	0	0	$-\sqrt{\frac{q^3[3]_q}{[2]_q[5]_q}}$	$\frac{q^{-5/2}-q^{-3/2}}{[2]_q}\sqrt{\frac{[3]_q}{[6]_q}}$	$-\frac{q^{-1}}{\sqrt{[5]_q}}$
$\xi_1\chi_8$		$\frac{q^{-3}}{[4]_q}\sqrt{\frac{[2]_q[3]_q}{[6]_q}}$	$\frac{q^{-3}}{[4]_q}$	$-\frac{q^{-1}\sqrt{[3]_q}}{[4]_q}$	$-\frac{q^{-1}}{[4]_q}\sqrt{\frac{[3]_q}{[5]_q}}$	$-\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$\sqrt{\frac{q^3[2]_q}{[5]_q}}$
$\xi_8\chi_1$		$q^{-2}\sqrt{\frac{[2]_q}{[6]_q}}$	0	0	$\sqrt{\frac{1}{[5]_q}}$	$q^{-1}\sqrt{\frac{[2]_q}{[6]_q}}$	$\sqrt{\frac{[2]_q}{q^5[3]_q[5]_q}}$
$\xi_2\chi_7$		$-\frac{q^{-5}}{[4]_q}\sqrt{\frac{[2]_q}{[6]_q}}$	$\frac{\sqrt{[3]_q}}{q[4]_q}$	$-\frac{q[3]_q}{[4]_q}$	$\frac{q^{-3}}{[4]_q}\sqrt{\frac{1}{[5]_q}}$	$\frac{[3]_q+(1-q^{3/2})[2]_q-q^5}{[2]_q\sqrt{q^3[2]_q[6]_q}}$	$-\sqrt{\frac{[2]_q}{q[3]_q[5]_q}}$
$\xi_5\chi_4$		$\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^5[6]_q}}$	$\frac{\sqrt{[2]_q[3]_q}}{q^{1/2}[4]_q}$	$\frac{q^{-5/2}\sqrt{[2]_q}}{[4]_q}$	$\frac{[2]_q+q^5}{[4]_q}\sqrt{\frac{[2]_q}{q^3[5]_q}}$	$-\sqrt{\frac{q^5}{[6]_q}}$	$-\frac{q}{\sqrt{[3]_q[5]_q}}$

TABLE III. (*Continued.*)

	$\psi_{18}^{\{51\}}$	$\psi_{17}^{\{51\}}$	$\psi_{11}^{\{42\}}$	$\psi_{12}^{\{42\}}$	$\psi_{5}^{\{3\}}$	$\psi_{3}^{\{21\}}$
$\xi_6\chi_3$	$-\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q[6]_q}}$	$\frac{\sqrt{q^3[2]_q[3]_q}}{[4]_q}$	$\frac{q^{-1/2}\sqrt{[2]_q}}{[4]_q}$	$-\frac{q^{-4}+q^{-2}+q^2}{[4]_q}\sqrt{\frac{[2]_q}{q[5]_q}}$	$\sqrt{\frac{q}{[6]_q}}$	$\frac{q^{-1}}{\sqrt{[3]_q[5]_q}}$
	$\psi_{9}^{\{51\}}$	$\psi_{10}^{\{51\}}$	$\psi_{5}^{\{42\}}$	$\psi_{6}^{\{42\}}$	$\psi_{2}^{\{3\}}$	$\psi_{1}^{\{21\}}$
$\xi_3\chi_3$	$q^2\sqrt{\frac{[2]_q[3]_q}{[4]_q[5]_q}}$	$-\frac{q^{-3}[2]_q}{\sqrt{[4]_q[5]_q[6]_q}}$	$-\frac{q^{-1}\sqrt{[2]_q}}{\sqrt{[3]_q[4]_q}}$	$\frac{q^{-4}\sqrt{[2]_q}}{\sqrt{[3]_q[4]_q[5]_q}}$	$\sqrt{\frac{[2]_q}{[6]_q}}$	$-\sqrt{\frac{[2]_q}{q^3[3]_q[5]_q}}$
$\xi_6\chi_1$	0	$\sqrt{\frac{q^3[2]_q[5]_q}{[4]_q[6]_q}}$	$\sqrt{\frac{1}{q[3]_q[4]_q}}$	$-\frac{[4]_q+q^{-1}-1}{\sqrt{[3]_q[4]_q[5]_q}}$	$\sqrt{\frac{1}{q^3[6]_q}}$	$-\frac{q^{-3}}{\sqrt{[3]_q[5]_q}}$
$\xi_2\chi_4$	$\frac{[2]_q\sqrt{[3]_q}}{\sqrt{q[4]_q[5]_q}}$	$\frac{q^{-1/2}([2]_q-q^{-5})}{\sqrt{[2]_q[4]_q[5]_q[6]_q}}$	$\frac{q^{3/2}([2]_q-q^{-4})}{[2]_q\sqrt{[3]_q[4]_q}}$	$-\frac{[2]_q}{\sqrt{q^5[3]_q[4]_q[5]_q}}$	$\frac{q^{5/2}(q^{-5}-[2]_q)}{[2]_q\sqrt{[6]_q}}$	$\frac{[2]_q}{\sqrt{[3]_q[5]_q}}$
$\xi_5\chi_2$	0	$\sqrt{\frac{[5]_q}{[4]_q[6]_q}}$	$\frac{q^{-2}}{\sqrt{[2]_q[3]_q[4]_q}}$	$\frac{q^3(1+q^3[3]_q)\sqrt{[2]_q}}{\sqrt{[3]_q[4]_q[5]_q}}$	$\frac{q^{-3}}{\sqrt{[2]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{q^3[3]_q[5]_q}}$
$\xi_1\chi_6$	$\frac{q^{-3}\sqrt{[2]_q}}{\sqrt{[4]_q[5]_q}}$	$\frac{q^{-3}\sqrt{[3]_q}}{\sqrt{[4]_q[5]_q[6]_q}}$	$\frac{q^{-1}}{\sqrt{[2]_q[4]_q}}$	$\frac{q^{-1}\sqrt{[2]_q}}{\sqrt{[4]_q[5]_q}}$	$-\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$-\sqrt{\frac{q^3[2]_q}{[5]_q}}$
$\xi_2\chi_5$	0	$\sqrt{\frac{[3]_q[5]_q}{q^3[2]_q[4]_q[6]_q}}$	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q}{[4]_q}}$	0	$-\frac{1}{[2]_q}\sqrt{\frac{q^3[3]_q}{[6]_q}}$	0
	$\psi_{22}^{\{51\}}$	$\psi_{21}^{\{51\}}$	$\psi_{16}^{\{42\}}$	$\psi_{17}^{\{42\}}$	$\psi_{7}^{\{3\}}$	$\psi_{6}^{\{21\}}$
$\xi_7\chi_5$	$\sqrt{\frac{[3]_q}{q[6]_q}}$	0	0	$-\sqrt{\frac{q^3[3]_q}{[2]_q[5]_q}}$	$\frac{q^{-5/2}-q^{-3/2}}{[2]_q}\sqrt{\frac{[3]_q}{[6]_q}}$	$-\frac{q^{-1}}{\sqrt{[5]_q}}$
$\xi_4\chi_7$	$\frac{-q^{-4}}{[4]_q}\sqrt{\frac{[2]_q[3]_q}{[6]_q}}$	$\frac{1}{[4]_q}$	$-\frac{q^2\sqrt{[3]_q}}{[4]_q}$	$\frac{q^{-2}}{[4]_q}\sqrt{\frac{[3]_q}{[5]_q}}$	$\frac{1+q^{-1}}{q^2[2]_q}\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$-\sqrt{\frac{q[2]_q}{[5]_q}}$
$\xi_9\chi_2$	$q^{-2}\sqrt{\frac{[2]_q}{[6]_q}}$	0	0	$\sqrt{\frac{1}{[5]_q}}$	$q^{-1}\sqrt{\frac{[2]_q}{[6]_q}}$	$\sqrt{\frac{[2]_q}{q^5[3]_q[5]_q}}$
$\xi_3\chi_8$	$\frac{q^{-2}}{[4]_q}\sqrt{\frac{[2]_q}{[6]_q}}$	$\frac{\sqrt{[3]_q}}{q^2[4]_q}$	$-\frac{[3]_q}{[4]_q}$	$-\frac{1}{[4]_q}\sqrt{\frac{1}{[5]_q}}$	$-q\sqrt{\frac{1}{[2]_q[6]_q}}$	$\sqrt{\frac{q^3[2]_q}{[3]_q[5]_q}}$
$\xi_6\chi_6$	$\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q[6]_q}}$	$\frac{\sqrt{[2]_q[3]_q}}{q^{5/2}[4]_q}$	$\frac{q^{-5/2}\sqrt{[2]_q}}{[4]_q}$	$\frac{[5]_q+q^{-2}}{[2]_q[4]_q}\sqrt{\frac{q[2]_q}{[5]_q}}$	$-\sqrt{\frac{q^5}{[6]_q}}$	$-\frac{q}{\sqrt{[3]_q[5]_q}}$
$\xi_7\chi_4$	$-\frac{[2]_q}{[4]_q}\sqrt{\frac{1}{q^5[6]_q}}$	$\frac{\sqrt{q^3[2]_q[3]_q}}{[4]_q}$	$\frac{q^{-1/2}\sqrt{[2]_q}}{[4]_q}$	$-\frac{q^{-4}+q^{-2}+q^2}{[4]_q}\sqrt{\frac{[2]_q}{q[5]_q}}$	$\sqrt{\frac{q}{[6]_q}}$	$\frac{q^{-1}}{\sqrt{[3]_q[5]_q}}$
	$\psi_{11}^{\{51\}}$	$\psi_{12}^{\{51\}}$	$\psi_{7}^{\{42\}}$	$\psi_{8}^{\{42\}}$	$\psi_{3}^{\{3\}}$	$\psi_{2}^{\{21\}}$
$\xi_2\chi_6$	$q^{-2}\sqrt{\frac{[2]_q[3]_q}{[4]_q[5]_q}}$	$\frac{q^{-2}[2]_q}{\sqrt{[4]_q[5]_q[6]_q}}$	$\sqrt{\frac{[2]_q}{[3]_q[4]_q}}$	$\sqrt{\frac{[2]_q}{[3]_q[4]_q[5]_q}}$	$-q\sqrt{\frac{[2]_q}{[6]_q}}$	$-\sqrt{\frac{q^5[2]_q}{[3]_q[5]_q}}$
$\xi_6\chi_2$	0	$\sqrt{\frac{q[2]_q[5]_q}{[4]_q[6]_q}}$	$\sqrt{\frac{1}{q[3]_q[4]_q}}$	$\frac{q^{-1/2}(1+q^3[3]_q)}{\sqrt{[3]_q[4]_q[5]_q}}$	$\sqrt{\frac{1}{q^5[6]_q}}$	$\frac{q^{-1}}{\sqrt{[3]_q[5]_q}}$
$\xi_3\chi_4$	$\frac{[2]_q\sqrt{q[3]_q}}{\sqrt{[4]_q[5]_q}}$	$\frac{q^{1/2}(1-q^{-5}[2]_q)}{\sqrt{[2]_q[4]_q[5]_q[6]_q}}$	$\frac{q^{-5/2}(q^5-[2]_q)}{[2]_q\sqrt{[3]_q[4]_q}}$	$-\frac{[2]_q}{\sqrt{q^3[3]_q[4]_q[5]_q}}$	$\frac{q^{-3/2}([2]_q-q^5)}{[2]_q\sqrt{[6]_q}}$	$\frac{q[2]_q}{\sqrt{[3]_q[5]_q}}$
$\xi_7\chi_1$	0	$q^2\sqrt{\frac{[5]_q}{[4]_q[6]_q}}$	$\frac{1}{\sqrt{[2]_q[3]_q[4]_q}}$	$-\sqrt{\frac{[2]_q[4]_q}{[3]_q[5]_q}}$	$\frac{q^{-1}}{\sqrt{[2]_q[6]_q}}$	$-\sqrt{\frac{[2]_q}{q^5[3]_q[5]_q}}$

TABLE III. (*Continued.*)

	$\psi_{11}^{\{51\}}$	$\psi_{12}^{\{51\}}$	$\psi_{7}^{\{42\}}$	$\psi_{8}^{\{42\}}$	$\psi_{3}^{\{3\}}$	$\psi_{2}^{\{21\}}$
$\xi_4\chi_3$	$\frac{q^3\sqrt{[2]_q}}{\sqrt{[4]_q[5]_q}}$	$\frac{-q^{-2}\sqrt{[3]_q}}{\sqrt{[4]_q[5]_q[6]_q}}$	$-\frac{1}{\sqrt{[2]_q[4]_q}}$	$\frac{q^{-3}\sqrt{[2]_q}}{\sqrt{[4]_q[5]_q}}$	$q\sqrt{\frac{[3]_q}{[2]_q[6]_q}}$	$-\sqrt{\frac{[2]_q}{q[5]_q}}$
$\xi_3\chi_5$	0	$\sqrt{\frac{[3]_q[5]_q}{q^3[2]_q[4]_q[6]_q}}$	$-\frac{[3]_q}{[2]_q}\sqrt{\frac{q}{[4]_q}}$	0	$-\frac{1}{[2]_q}\sqrt{\frac{q^3[3]_q}{[6]_q}}$	0

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Study of the validity of the phase-integral connection formula for potential barriers of arbitrary thickness

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The validity of the phase-integral connection matrix for potential barriers is discussed in a concrete way for a particular parabolic barrier, for the symmetric Eckart-Epstein barrier, and for the inverted Morse potential, when the first-order phase-integral approximation is used. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The first *correct* phase-integral connection formula for a real, single-hump potential barrier was published by Fröman and Fröman in 1965 for the first-order approximation,[1] and in 1970 for an arbitrary-order approximation, but a particular choice of the base function.[2] The formula is valid also for underdense barriers, if the energy does not lie too high above the top of the barrier. The corresponding connection formula for a possibly complex potential barrier, when the phase-integral appoximation of arbitrary order generated from an unspecified base function (which is described in Sec. 1.3.1 of Ref. 3 and in Sec. 2.2 of Ref. 4) is used, was derived by Fröman *et al.* in Chap. 5 of Ref. 3 by means of comparison equation technique and by Fröman and Fröman[4] by initially using the fact that the wave function is single valued and then, only finally, comparison equation technique; see Sec. 3.44 in Ref. 4. The previously mentioned connection formula for a real, single-hump potential barrier was derived and presented in an alternative way in Ref. 4; see their Secs. 2.5 and 3.45. It is valid for a barrier of arbitrary thickness with approximately parabolic top, when an arbitrary order of the phase-integral approximation is used. The purpose of the present article is to verify the correctness of this connection formula for a particular parabolic barrier, for the symmetric Eckart-Epstein barrier, and for the inverted Morse potential, when the first order of the phase-integral approximation is used. For the background we refer to Sec. 1.3.1 in Ref. 3 or to Sec. 2.2 in Ref. 4.

II. FIRST-ORDER PHASE-INTEGRAL CONNECTION FORMULA FOR A REAL, SINGLE-HUMP BARRIER

For a real, single-hump potential barrier of arbitrary thickness with the turning points t' and t'' (where $t'<t''$ if the barrier is superdense), we write in the first order of the phase-integral approximation generated from an unspecified base function $Q(z)$ the wave function on the real axis as

$$\Psi(x')=\tilde{A}'(x')|Q^{-1/2}(x')|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x'}Q(z)dz\right|\right]+\tilde{B}'(x')|Q^{-1/2}(x')|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x'}Q(z)dz\right|\right], \tag{2.1}$$

with x' lying to the left of the barrier, and

$$\Psi(x'') = \tilde{A}''(x'')|Q^{-1/2}(x'')|\exp\left[i \left| \mathrm{Re} \int_{t''}^{x''} Q(z)dz \right| \right] + \tilde{B}''(x'')|Q^{-1/2}(x'')|\exp\left[-i \left| \mathrm{Re} \int_{t''}^{x''} Q(z)dz \right| \right], \tag{2.2}$$

with x'' lying to the right of the barrier.

The coefficients $\tilde{A}'(x')$, $\tilde{B}'(x')$, and $\tilde{A}''(x'')$, $\tilde{B}''(x'')$ in (2.1) and (2.2) are related to each other according to Eq. (3.45.8) in Ref. 4, i.e.,

$$\begin{pmatrix} \tilde{A}''(x'') \\ \tilde{B}''(x'') \end{pmatrix} = \tilde{\mathbf{M}} \begin{pmatrix} \tilde{A}'(x') \\ \tilde{B}'(x') \end{pmatrix}, \tag{2.3}$$

with the connection matrix $\tilde{\mathbf{M}}$ given by approximate formula (3.45.9a) in Ref. 4, i.e., in the first-order approximation

$$\tilde{\mathbf{M}} = \begin{pmatrix} -i\exp(K_0) & [\exp(2K_0)+1]^{1/2}\exp(i\tilde{\varnothing}) \\ [\exp(2K_0)+1]^{1/2}\exp(-i\tilde{\varnothing}) & i\exp(K_0) \end{pmatrix}, \tag{2.4}$$

where K_0 is the first-order phase integral with t' and t'' as limits of integration, i.e.,

$$K_0 = -\mathrm{i}\int_{t'}^{t''} Q(z)dz, \tag{2.5}$$

with the phase of $Q(z)$ chosen such that K_0 is positive when the barrier is superdense but negative when the barrier is underdense, and $\tilde{\varnothing}$ is the parabolic phase correction given by Eqs. (2.5.11) and (2.5.13a-c) in Ref. 4, i.e., in the first order of the phase-integral approximation,

$$\tilde{\varnothing} = \arg\Gamma(1/2 + i\overline{K_0}) - \overline{K_0}\ln|\overline{K_0}| + \overline{K_0}, \quad \overline{K_0} = K_0/\pi. \tag{2.6}$$

The matrix (2.4) has the property that

$$\tilde{\mathbf{M}}^{-1} = \tilde{\mathbf{M}}, \tag{2.7}$$

and therefore it follows from (2.3) that

$$\begin{pmatrix} \tilde{A}'(x') \\ \tilde{B}'(x') \end{pmatrix} = \tilde{\mathbf{M}} \begin{pmatrix} \tilde{A}''(x'') \\ \tilde{B}''(x'') \end{pmatrix}. \tag{2.8}$$

Formulas (2.3) and (2.8) along with (2.4) and (2.6) are valid under the assumptions that the coefficient function in the Schrödinger equation is in some sense large and that the top of the barrier is approximately parabolic. One can express the first assumption more precisely by saying that the quantity ϵ_0, defined by Eq. (2.2.1) in Ref. 4, be small compared to unity in the relevant region of the complex x plane. The second assumption means that the distance from the two transition points of the barrier to the transition points that are not associated with the barrier is much larger than the distance between the transition points of the barrier.

III. CONNECTION FORMULA FOR A REAL PARABOLIC BARRIER, OBTAINED FROM EXACT SOLUTIONS

The time-independent Schrödinger equation for a particular parabolic barrier can be written as

$$\frac{d^2\Psi}{dx^2} + R(x)\Psi = 0, \tag{3.1}$$

with

$$R(x) = \tfrac{1}{4}x^2 - a, \tag{3.2}$$

where a is a real constant.

According to Secs. 19.21.1 and 19.17.10 in Ref. 5, differential equation (3.1) along with (3.2) has a solution $E(a,x)$ such that

$$E(a,x) \sim \left(\frac{2}{x}\right)^{1/2} \exp\left\{ i\left[\frac{1}{4}x^2 - a\ln x + \frac{1}{2}\arg\Gamma(1/2+ia) + \frac{\pi}{4}\right]\right\}, \quad x \to +\infty. \tag{3.3}$$

Using Secs. 19.17.9, 19.21.1, 19.17.10, 19.21.4, 19.21.5, 19.21.6, and 19.18.3 in Ref. 5, and noting that $\arg\Gamma(1/2+ia)$ is a real quantity, one finds that the behavior of $E(a,x)$ as $x \to -\infty$ is

$$\begin{aligned} E(a,x) \sim{}& \left(\frac{2}{|x|}\right)^{1/2} \exp\left\{ \pi a + i\left[\frac{1}{4}x^2 - a\ln|x| + \frac{1}{2}\arg\Gamma(1/2+ia) - \frac{\pi}{4}\right]\right\} \\ &+ [\exp(2\pi a)+1]^{1/2}\left(\frac{2}{|x|}\right)^{1/2} \exp\left\{ -i\left[\frac{1}{4}x^2 - a\ln|x| + \frac{1}{2}\arg\Gamma(1/2+ia) - \frac{\pi}{4}\right]\right\}, \\ & x \to -\infty. \end{aligned} \tag{3.4}$$

By expressing the right-hand sides of (3.3) and (3.4) in terms of phase-integral quantities we shall derive the connection formula described in Sec II.

Choosing

$$Q(x) = R^{1/2}(x) \tag{3.5}$$

with the phase of $R^{1/2}(x)$ in agreement with what is said following (2.5), and denoting the zeros of $Q^2(x)$ by t' and t'', where $t' < t''$ if the barrier is superdense, we obtain from (2.5), with the use of (3.2),

$$K_0 = -\,\mathrm{i}\int_{t'}^{t''} Q(x)dx = \int_{t'}^{t''} \left(a - \frac{1}{4}x^2\right)^{1/2} dx = \pi a = \pi\overline{K}_0, \tag{3.6}$$

where

$$\overline{K}_0 = K_0/\pi = a. \tag{3.7}$$

With the use of (3.2) and (3.5) we obtain

$$\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right| = \mathrm{Re}\int_{2\sqrt{a}}^{x}\left(\frac{1}{4}z^2 - a\right)^{1/2} dz = \frac{1}{4}x(x^2-4a)^{1/2} - a\ln[(x^2-4a)^{1/2}+x] + a\ln(2\sqrt{|a|}), \tag{3.8}$$

with x lying to the right of the barrier, and hence, by neglecting terms of the order $O(x^{-2})$,

$$\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right| \sim \frac{1}{4}x^2 - a\ln x + \frac{1}{2}a(\ln|a| - 1), \quad x \to +\infty. \tag{3.9}$$

Because of the symmetry of $Q^2(x)$ we obtain from (3.8)

$$\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right| = \left|\mathrm{Re}\int_{t''}^{|x|} Q(z)dz\right| = \frac{1}{4}|x|(x^2-4a)^{1/2} - a\ln[(x^2-4a)^{1/2}+|x|] + a\ln(2\sqrt{|a|}), \tag{3.10}$$

with x lying to the left of the barrier, and hence, by neglecting terms of the order $O(x^{-2})$,

$$\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right| \sim \frac{1}{4}x^2 - a\ln|x| + \frac{1}{2}a(\ln|a| - 1), \quad x \to -\infty. \tag{3.11}$$

Recalling (3.2), (3.5), (3.7), (3.9), and (3.11), one can write (3.3) and (3.4) as

$$E(a,x) \sim |Q^{-1/2}(x)|\exp\left\{ i\left[\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right| + \frac{\tilde{\varnothing}}{2} + \frac{\pi}{4}\right]\right\}, \quad x \to +\infty, \tag{3.12}$$

$$\begin{aligned} E(a,x) \sim{}& |Q^{-1/2}(x)|\exp\left\{ K_0 + i\left[\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right| + \frac{\tilde{\varnothing}}{2} - \frac{\pi}{4}\right]\right\} \\ &+ [\exp(2K_0) + 1]^{1/2}|Q^{-1/2}(x)|\exp\left\{ - i\left[\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right| + \frac{\tilde{\varnothing}}{2} - \frac{\pi}{4}\right]\right\}, \\ & x \to -\infty, \end{aligned} \tag{3.13}$$

with

$$\tilde{\varnothing} = \arg\Gamma(1/2 + i\overline{K_0}) - \overline{K_0}\ln|\overline{K_0}| + \overline{K_0}. \tag{3.14}$$

From (3.12) and (3.13) one finds that the function

$$\Psi_1(x) = \exp\left[- i\left(\frac{\tilde{\varnothing}}{2} + \frac{\pi}{4}\right)\right]E(a,x) \tag{3.15}$$

for sufficiently large positive and negative values of x is given by

$$\Psi_1(x) \sim |Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right|\right], \quad x \to +\infty, \tag{3.16}$$

$$\Psi_1(x) \sim b_1|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right] + b_2|Q^{-1/2}(x)|\exp\left[- i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right], \quad x \to -\infty, \tag{3.17}$$

where

$$b_1 = -i\exp(K_0), \tag{3.18}$$

$$b_2 = [\exp(2K_0) + 1]^{1/2}\exp(-i\tilde{\varnothing}). \tag{3.19}$$

The function

$$\Psi_2(x) = \Psi_1^*(x) \tag{3.20}$$

is another approximate solution of (3.1) along with (3.2). It behaves for large positive and negative values of x as

$$\Psi_2(x) \sim |Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right|\right], \quad x \to +\infty, \tag{3.21}$$

$$\Psi_2(x) \sim b_2^*|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right] + b_1^*|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right], \quad x \to -\infty. \tag{3.22}$$

As $x \to +\infty$ the general solution is according to (3.16) and (3.21)

$$\Psi(x) \sim \tilde{A}''|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right|\right] + \tilde{B}''|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t''}^{x} Q(z)dz\right|\right], \quad x \to +\infty, \tag{3.23}$$

where $\tilde{A}''$ and $\tilde{B}''$ are arbitrary constants. When $x \to -\infty$ this solution behaves according to (3.17) and (3.22) as

$$\begin{aligned}\Psi(x) \sim{}& \tilde{A}''\left\{b_1|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right] + b_2|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right]\right\} \\ &+ \tilde{B}''\left\{b_2^*|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right] + b_1^*|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right]\right\} \\ ={}& \tilde{A}'|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right] + \tilde{B}'|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x} Q(z)dz\right|\right], \quad x \to -\infty,\end{aligned} \tag{3.24}$$

where

$$\tilde{A}' = b_1\tilde{A}'' + b_2^*\tilde{B}'', \tag{3.25}$$

$$\tilde{B}' = b_2\tilde{A}'' + b_1^*\tilde{B}'', \tag{3.26}$$

i.e.,

$$\begin{pmatrix}\tilde{A}' \\ \tilde{B}'\end{pmatrix} = \tilde{\mathbf{M}}\begin{pmatrix}\tilde{A}'' \\ \tilde{B}''\end{pmatrix}, \tag{3.27}$$

with

$$\tilde{\mathbf{M}} = \begin{pmatrix}b_1 & b_2^* \\ b_2 & b_1^*\end{pmatrix}. \tag{3.28}$$

Inserting (3.18) and (3.19) into (3.28) one obtains

$$\tilde{\mathbf{M}} = \begin{pmatrix}-i\exp(K_0) & [\exp(2K_0)+1]^{1/2}\exp(i\tilde{\varnothing}) \\ [\exp(2K_0)+1]^{1/2}\exp(-i\tilde{\varnothing}) & i\exp(K_0)\end{pmatrix}. \tag{3.29}$$

It is seen that (3.27) along with (3.29) and (3.14) agrees with the first-order phase-integral result given by (2.8) along with (2.4) and (2.6). This is true for any real value of the constant a in (3.2). According to (3.6) $K_0 = \pi a$, so the barrier can therefore be of arbitrary thickness (overdense or underdense).

Of the conditions stated following (2.8) for the validity of the general connection formula for a real barrier described in Sec. II the second condition is automatically fulfilled for the particular barrier now considered. Further, in the present section we did not use the first condition, i.e., the requirement that the absolute value of ϵ_0 be much smaller than unity in the relevant region of the complex plane. The reason for this is that the Schrödinger equation with a parabolic barrier was used as comparison equation in the derivation of the general connection formula presented in Sec. III, and therefore the condition in question is not needed here.

IV. CONNECTION FORMULA FOR THE REAL, SYMMETRIC ECKART-EPSTEIN BARRIER, OBTAINED FROM EXACT SOLUTIONS

Consider the real, symmetric Eckart-Epstein potential barrier

$$V(x) = \frac{4V_0 \exp(x/x_0)}{[\exp(x/x_0) + 1]^2}, \tag{4.1}$$

where x_0 is a positive constant with the dimension of length, and V_0 is a positive constant, which has the dimension of energy and is equal to the height of the barrier. With obvious notations the time-independent Schrödinger equation for a quantal particle in the potential (4.1) is

$$\frac{d^2\Psi}{dx^2} + R(x)\Psi = 0, \tag{4.2}$$

where

$$R(x) = \frac{2m}{\hbar^2}\left\{E - \frac{4V_0 \exp(x/x_0)}{[\exp(x/x_0) + 1]^2}\right\}. \tag{4.3}$$

From Eckart's[6] paper one finds that there is a solution $\Psi(x)$ of (4.2) along with (4.3) that for large positive and negative values of x behaves as

$$\Psi(x) \sim \left(\frac{\alpha}{x_0}\right)^{-1/2} \exp(i\alpha x/x_0), \quad x \to +\infty, \tag{4.4}$$

$$\begin{aligned}\Psi(x) \sim{}& \frac{\Gamma(-2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2 + i(\beta - 2\alpha))\Gamma(1/2 - i(\beta + 2\alpha))}\left(\frac{\alpha}{x_0}\right)^{-1/2} \exp(i\alpha x/x_0) \\ &+ \frac{\Gamma(2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2 + i\beta)\Gamma(1/2 - i\beta)}\left(\frac{\alpha}{x_0}\right)^{-1/2} \exp(-i\alpha x/x_0), \quad x \to -\infty,\end{aligned} \tag{4.5}$$

where

$$\alpha = \left(\frac{2mEx_0^2}{\hbar^2}\right)^{1/2} \tag{4.6}$$

is a dimensionless, positive parameter. By expressing the right-hand sides of (4.4) and (4.5) in terms of phase-integral quantities we shall in the following derive the phase-integral connection formula for a real barrier described in Sec. II.

When x lies sufficiently close to an arbitrary pole x_p of $R(x)$ one has the formula

$$\frac{\exp(x/x_0)}{4x_0^2[\exp(x/x_0) + 1]^2} \approx -\frac{1}{4(x - x_p)^2}. \tag{4.7}$$

Referring to Sec. 2.2 in Ref. 4, we therefore choose

$$Q^2(x) = R(x) + \frac{\exp(x/x_0)}{4x_0^2[\exp(x/x_0)+1]^2} \tag{4.8}$$

and hence, with the use of (4.3),

$$Q^2(x) = \frac{\alpha^2[\exp(x/x_0)+1]^2 - \beta^2\exp(x/x_0)}{x_0^2[\exp(x/x_0)+1]^2} \tag{4.9}$$

$$= \frac{\alpha^2[\exp(2x/x_0) - (\gamma^2-2)\exp(x/x_0)+1]}{x_0^2[\exp(x/x_0)+1]^2} \tag{4.10}$$

where α (dimensionless and positive) is defined by (4.6), and

$$\beta = \left(\frac{8mV_0x_0^2}{\hbar^2} - \frac{1}{4}\right)^{1/2}, \tag{4.11}$$

$$\gamma = \frac{\beta}{\alpha}, \tag{4.12}$$

are other dimensionless parameters, which are also assumed to be positive.

One finds from (4.10) that the turning points t' and t'' (where $t' < t''$ when the barrier is superdense), i.e., the zeros of $Q^2(x)$ on the real axis, are obtained from

$$-t' = t'' = x_0 \ln\frac{\gamma^2 - 2 + \gamma(\gamma^2-4)^{1/2}}{2} = x_0 \ln\frac{[\gamma+(\gamma^2-4)^{1/2}]^2}{4} = x_0 \ln\frac{\gamma+(\gamma^2-4)^{1/2}}{\gamma-(\gamma^2-4)^{1/2}}$$
$$= x_0 \ln\frac{1+(1-4/\gamma^2)^{1/2}}{1-(1-4/\gamma^2)^{1/2}},$$

i.e.,

$$-t' = t'' = x_0 \ln\frac{1+(1-4/\gamma^2)^{1/2}}{1-(1-4/\gamma^2)^{1/2}}. \tag{4.13}$$

According to (2.5) one has

$$K_0 = -\mathrm{i}\int_{t'}^{t''} Q(z)dz = \int_{t'}^{t''} [-Q^2(z)]^{1/2}dz, \tag{4.14}$$

where the phase of the integrand is to be chosen appropriately. In Appendices A and B it is shown that by inserting the expression for $Q(z)$ obtained from (4.9) into (4.14) and evaluating the integral one obtains

$$K_0 = \pi(\beta - 2\alpha), \tag{4.15}$$

where α and β are given by (4.6) and (4.11), respectively.

One finds with the use of (4.10) that

$$\lim_{x\to-\infty}|Q^{-1/2}(x)| = \lim_{x\to+\infty}|Q^{-1/2}(x)| = \left(\frac{\alpha}{x_0}\right)^{-1/2}, \tag{4.16}$$

and according to (C3) and (C4) in Appendix C one has

$$\lim_{x\to+\infty}\left[\left|\mathrm{Re}\int_{t''}^{x}Q(z)dz\right|-\frac{\alpha}{x_0}x\right]=\lim_{x\to-\infty}\left[\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|+\frac{\alpha}{x_0}x\right]=2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)$$
$$+\frac{\beta-2\alpha}{2}\ln|\beta-2\alpha|. \tag{4.17}$$

With the use of (4.4), (4.5), (4.16), and (4.17) one finds that the function

$$\Psi_1(x)=\exp\left\{i\left[2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)+\frac{\beta-2\alpha}{2}\ln|\beta-2\alpha|\right]\right\}\Psi(x) \tag{4.18}$$

has the following behavior for large positive and negative values of x

$$\Psi_1(x)\sim|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t''}^{x}Q(z)dz\right|\right],\quad x\to+\infty, \tag{4.19}$$

$$\Psi_1(x)\sim b_1|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]+b_2|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right],\quad x\to-\infty, \tag{4.20}$$

where

$$b_1=\frac{\Gamma(2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2+i\beta)\Gamma(1/2-i\beta)}, \tag{4.21}$$

$$b_2=\exp\left\{2i\left[2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)+\frac{\beta-2\alpha}{2}\ln|\beta-2\alpha|\right]\right\}$$
$$\times\frac{\Gamma(-2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2+i(\beta-2\alpha))\Gamma(1/2-i(\beta+2\alpha))}. \tag{4.22}$$

Using the formulas in Secs. 6.1.17 and 6.1.30 of Ref. 5 and (4.15), one can write (4.21) as

$$b_1=\frac{\cosh(\pi\beta)}{\sin(2i\pi\alpha)}=-i\frac{\exp(\pi\beta)+\exp(-\pi\beta)}{\exp(2\pi\alpha)-\exp(-2\pi\alpha)}=-i\exp[\pi(\beta-2\alpha)]\frac{1+\exp(-2\pi\beta)}{1-\exp(-4\pi\alpha)}$$
$$=-i\exp(K_0)\frac{1+\exp(-2\pi\beta)}{1-\exp(-4\pi\alpha)}, \tag{4.23}$$

and with the use of the formulas in Secs. 6.1.15, 6.1.29, and 6.1.30 of Ref. 5 one obtains from (4.22)

$$|b_2|=\left|\frac{\Gamma(-2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2+i(\beta-2\alpha))\Gamma(1/2-i(\beta+2\alpha))}\right|=\left|\frac{-2i\alpha[\Gamma(-2i\alpha)]^2}{\Gamma(1/2+i(\beta-2\alpha))\Gamma(1/2-i(\beta+2\alpha))}\right|$$
$$=\frac{2\alpha|\Gamma(-2i\alpha)|^2}{[|\Gamma(1/2+i(\beta-2\alpha))|^2|\Gamma(1/2-i(\beta+2\alpha))|^2]^{1/2}}=\frac{\cosh^{1/2}[\pi(\beta-2\alpha)]\cosh^{1/2}[\pi(\beta+2\alpha)]}{\sinh(2\pi\alpha)}$$
$$=\frac{\{1+\exp[-2\pi(\beta+2\alpha)]\}^{1/2}\{\exp[2\pi(\beta-2\alpha)]+1\}^{1/2}}{1-\exp(-2\pi\alpha)}. \tag{4.24}$$

The conditions under which the phase-integral connection formula given by (2.3) or (2.8) together with (2.4) and (2.6) is valid are stated following (2.8). They require that ϵ_0, defined by Eq. (2.2.1) in Ref. 4, be small compared to unity in the relevant region of the complex plane, and

that the distance from the two transition points of the barrier to the transition points not associated with the barrier be much larger than the distance between the transition points of the barrier.

The requirement that the distance between the transition points of the barrier, obtained from (4.13), be small compared to their distance from the other transition points yields

$$2x_0 \ln\left|\frac{1+(1-4/\gamma^2)^{1/2}}{1-(1-4/\gamma^2)^{1/2}}\right| \ll \pi x_0, \tag{4.25}$$

and this requirement is fulfilled when $|(1-4/\gamma^2)^{1/2}| \ll \pi/4$, i.e., when $|\gamma-2|^{1/2} \ll \pi/4$, which is the case when

$$|\gamma-2|^{1/2} \ll 1. \tag{4.26}$$

In order for the phase-integral approximation to be valid, one requires the absolute value of ϵ_0 to be small compared to unity in the relevant region of the complex plane. According to (4.8), (4.10), and (4.26) and definition (2.2.1) in Ref. 4 of ϵ_0 this is the case when α is sufficiently large. For the moment we do not know how large α must be, and therefore we now impose only the condition

$$\alpha \gg 1 \tag{4.27}$$

without specifiying for the moment how large α must be. From (4.12), (4.26), and (4.27) it follows that

$$\beta \approx 2\alpha \gg 1, \tag{4.28}$$

and hence (4.23) gives

$$b_1 \approx -i\exp(K_0)[1+\exp(-4\pi\alpha)+\exp(-2\pi\beta)]. \tag{4.29}$$

Having already obtained formula (4.24) for $|b_2|$, one needs a formula for $\arg b_2$ in order to obtain b_2. To derive it one recalls (4.22), (4.27), and (4.28), and starts by making, with the use of asymptotic expansion (5) in Luke (Ref. 7, p. 32), i.e.,

$$\ln\Gamma(1/2+z) \sim z\ln z - z + \ln(2\pi)^{1/2} - \frac{1}{24z}, \quad z\to\infty, \quad |\arg z| < \pi-\epsilon, \quad \epsilon>0, \tag{4.30}$$

the following calculation:

$$\begin{aligned}
\ln\frac{\Gamma(-2i\alpha)\Gamma(1-2i\alpha)}{\Gamma(1/2-i(\beta+2\alpha))} &= \ln\frac{-2i\alpha[\Gamma(-2i\alpha)]^2}{\Gamma(1/2-i(\beta+2\alpha))} = \ln(-2i\alpha)+2\ln\Gamma(-2i\alpha)-\ln\Gamma(1/2-i(\beta+2\alpha)) \\
&= \ln(-2i\alpha)+2\ln\Gamma(1/2-(1/2+2i\alpha))-\ln\Gamma(1/2-i(\beta+2\alpha)) \\
&\sim \ln(2\alpha)-i\frac{\pi}{2}+2\left\{\ln(2\pi)^{1/2}+(-1/2-2i\alpha)[\ln(-1/2-2i\alpha)-1]\right. \\
&\quad \left.-\frac{1}{24(-1/2-2i\alpha)}\right\}-\left\{\ln(2\pi)^{1/2}-i(\beta+2\alpha)\{\ln[-i(\beta+2\alpha)]-1\}\right. \\
&\quad \left.-\frac{1}{24[-i(\beta+2\alpha)]}\right\} \approx \ln(2\alpha)-i\frac{\pi}{2}+2\left\{\ln(2\pi)^{1/2}-(1/2+2i\alpha)\right. \\
&\quad \left.\times\left[\ln(4\alpha^2+1/4)^{1/2}-i\left(\frac{\pi}{2}+\frac{1}{4\alpha}\right)-1\right]-\frac{i}{48\alpha}\right\}-\left\{\ln(2\pi)^{1/2}-i(\beta+2\alpha)\right. \\
&\quad \left.\times\left[\ln(\beta+2\alpha)-i\frac{\pi}{2}-1\right]-\frac{i}{24(\beta+2\alpha)}\right\} \approx \ln(2\pi)^{1/2}+(\beta-2\alpha)\frac{\pi}{2}
\end{aligned}$$

$$-\frac{1}{32\alpha^2}+i\Bigg[(\beta+2\alpha)\ln(\beta+2\alpha)-4\alpha\ln(2\alpha)-(\beta-2\alpha)+\frac{1}{12\alpha}+\frac{1}{24(\beta+2\alpha)}\Bigg]. \tag{4.31}$$

From (4.22) and (4.31) one obtains

$$\ln b_2 \approx \ln(2\pi)^{1/2}+(\beta-2\alpha)\frac{\pi}{2}-\frac{1}{32\alpha^2}-\ln\Gamma(1/2+i(\beta-2\alpha))+i\Bigg[(\beta-2\alpha)\ln|\beta-2\alpha|-(\beta-2\alpha)+\frac{1}{12\alpha}+\frac{1}{24(\beta+2\alpha)}\Bigg]. \tag{4.32}$$

With the use of the formula in Sec. 6.1.30 of Ref. 5 together with (4.27) and (4.28) one can confirm that (4.32) is in approximate agreement with the exact formula (4.24). From (4.32) one obtains

$$\arg b_2 = \operatorname{Im}\ln b_2 \approx (\beta-2\alpha)\ln|\beta-2\alpha|-(\beta-2\alpha)+\frac{1}{12\alpha}+\frac{1}{24(\alpha+2\beta)}-\arg\Gamma(1/2+i(\beta-2\alpha)). \tag{4.33}$$

With the use of (4.15) and (4.28) one obtains from (4.24) and (4.33)

$$b_2 \approx [\exp(2K_0)+1]^{1/2}\Bigg\{1+\exp(-2\pi\alpha)+\frac{1}{2}\exp[-2\pi(\beta+2\alpha)]\Bigg\}\times\exp\Bigg\{-i\Bigg[\tilde{\varnothing}-\frac{1}{12\alpha}-\frac{1}{24(\alpha+2\beta)}\Bigg]\Bigg\}, \tag{4.34}$$

where

$$\tilde{\varnothing} = \arg\Gamma(1/2+i\overline{K_0})-\overline{K_0}\ln|\overline{K_0}|+\overline{K_0} \tag{4.35}$$

with

$$\overline{K_0} = K_0/\pi. \tag{4.36}$$

We have thus found that the solution $\Psi_1(x)$ behaves for large positive and negative values of x according to (4.19) and (4.20), where b_1 and b_2 are given by (4.29) and (4.34).

Putting

$$\Psi_2(x) = \Psi_1^*(x), \tag{4.37}$$

one obtains with the use of (4.19) and (4.20)

$$\Psi_2(x) \sim |Q^{-1/2}(x)|\exp\Bigg[-i\Bigg|\operatorname{Re}\int_{t''}^{x}Q(z)dz\Bigg|\Bigg], \quad x\to+\infty, \tag{4.38}$$

$$\Psi_2(x) \sim b_2^*|Q^{-1/2}(x)|\exp\Bigg[i\Bigg|\operatorname{Re}\int_{t'}^{x}Q(z)dz\Bigg|\Bigg]+b_1^*|Q^{-1/2}(x)|\exp\Bigg[-i\Bigg|\operatorname{Re}\int_{t'}^{x}Q(z)dz\Bigg|\Bigg], \quad x\to-\infty. \tag{4.39}$$

When $x\to+\infty$ the general solution $\tilde{A}''\Psi_1(x)+\tilde{B}''\Psi_2(x)$, where $\tilde{A}''$ and $\tilde{B}''$ are arbitrary constants, behaves according to (4.19) and (4.38) as

$$\tilde{A}''\Psi_1(x)+\tilde{B}''\Psi_2(x)\sim\tilde{A}''|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t''}^{x}Q(z)dz\right|\right]$$
$$+\tilde{B}''|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t''}^{x}Q(z)dz\right|\right],\quad x\to+\infty. \tag{4.40}$$

When $x\to-\infty$ this solution behaves according to (4.20) and (4.39) as

$$\begin{aligned}\tilde{A}''\Psi_1(x)+\tilde{B}''\Psi_2(x)\sim{}&\tilde{A}''\Bigg\{b_1|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]+b_2|Q^{-1/2}(x)|\\&\times\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]\Bigg\}+\tilde{B}''\Bigg\{b_2^{*}|Q^{-1/2}(x)|\\&\times\exp\left[i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]+b_1^{*}|Q^{-1/2}(x)|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]\Bigg\}\\={}&\tilde{A}'|Q^{-1/2}(x)|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right]+\tilde{B}'|Q^{-1/2}(x)|\\&\times\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x}Q(z)dz\right|\right],\quad x\to-\infty,\end{aligned} \tag{4.41}$$

where

$$\tilde{A}'=b_1\tilde{A}''+b_2^{*}\tilde{B}'', \tag{4.42}$$

$$\tilde{B}'=b_2\tilde{A}''+b_1^{*}\tilde{B}'', \tag{4.43}$$

i.e.,

$$\begin{pmatrix}\tilde{A}'\\ \tilde{B}'\end{pmatrix}=\tilde{\mathbf{M}}\begin{pmatrix}\tilde{A}''\\ \tilde{B}''\end{pmatrix}, \tag{4.44}$$

with

$$\tilde{\mathbf{M}}=\begin{pmatrix}b_1 & b_2^{*}\\ b_2 & b_1^{*}\end{pmatrix}. \tag{4.45}$$

Inserting (4.29) and (4.34) into (4.45) and recalling (4.28), one obtains, when 12α is much larger than unity,

$$\tilde{\mathbf{M}}\approx\begin{pmatrix}-i\exp(K_0) & [\exp(2K_0)+1]^{1/2}\exp(i\tilde{\varnothing})\\ [\exp(2K_0)+1]^{1/2}\exp(-i\tilde{\varnothing}) & i\exp(K_0)\end{pmatrix}. \tag{4.46}$$

It is seen that (4.44) along with (4.46) and (4.35) agrees with the first-order phase-integral connection formula given by (2.8) along with (2.4) and (2.6). This result is obtained under the conditions (4.26), which with the use of (4.12), (4.15), and (4.36) can be written as $|\overline{K_0}/\alpha|^{1/2}\ll 1$, and (4.27), or more precisely $12\alpha\gg 1$ according to what is said immediately prior to (4.46). For any value of K_0 (positive or negative) it is possible to find values of α such that these conditions are fulfilled. The barrier may thus be of arbitrary thickness.

V. CONNECTION FORMULA FOR THE INVERTED, REAL MORSE POTENTIAL BARRIER, OBTAINED FROM EXACT SOLUTIONS

The present section concerns the inverted Morse potential

$$V(x) = V_0[2\exp(-x/b) - \exp(-2x/b)], \quad V_0 > 0, \quad b > 0. \tag{5.1}$$

When the energy E is positive, the Schrödinger equation associated with this potential describes a quantal particle subject to the influence of a single-hump potential barrier with the top at $x=0$ and $V(0)=V_0$, where V_0 is the height of the barrier. Lundborg[8] has treated the connection problem for a barrier given by (5.1) with the use of exact solutions of the Schrödinger equation. According to Eqs. (4) and (3a–c) in Ref. 8 the time-independent Schrödinger equation in question can be written as

$$\frac{d^2\Psi}{dz^2} + R(z)\Psi = 0 \tag{5.2}$$

with

$$R(z) = G^2[p^2 - 2\exp(-z) + \exp(-2z)] \tag{5.3}$$

where, with obvious notations,

$$z = x/b, \tag{5.4}$$

$$G = b\left(\frac{2mV_0}{\hbar^2}\right)^{1/2} > 0, \tag{5.5}$$

$$p = \left(\frac{E}{V_0}\right)^{1/2} > 0. \tag{5.6}$$

Lundborg[8] relates the exact solution to the phase-integral approximation generated from an unspecified base function and chooses the square of the base function to be

$$Q^2(z) = R(z). \tag{5.7}$$

The barrier is superdense for $0<p<1$ but underdense for $p>1$. The transition zeros, i.e., the zeros of $Q^2(z)$, obtained from (5.7) and (5.3), are $t'+2\pi ki$ and $t''+2\pi ki$, $k=0,\pm1,\pm2,\ldots$, with

$$t' = \ln\frac{1-(1-p^2)^{1/2}}{p^2}, \tag{5.8}$$

$$t'' = \ln\frac{1+(1-p^2)^{1/2}}{p^2}, \tag{5.9}$$

t' and t'' being the zeros of $Q^2(z)$ associated with the barrier. From (5.8) and (5.9) one obtains

$$t''-t' = \ln\frac{1+(1-p^2)^{1/2}}{1-(1-p^2)^{1/2}}. \tag{5.10}$$

According to what is said following (2.8), the phase-integral expression (2.4) for the connection matrix $\tilde{\mathbf{M}}$ is valid when the quantity ϵ_0, defined in Eq. (2.2.1) in Ref. 4, is much smaller than unity in the relevant region of the complex plane, and the distances from t' and t'' to the transition points not associated with the barrier are much larger than $|t''-t'|$. Recalling (5.3) and (5.7) one sees that the first of these conditions is fulfilled when G is sufficiently large. With the use of (5.10) the second condition can be written as

$$\ln\left|\frac{1+(1-p^2)^{1/2}}{1-(1-p^2)^{1/2}}\right| \ll 2\pi, \tag{5.11}$$

and this condition is undoubtedly fulfilled when

$$|1-p|^{1/2} \ll 1. \tag{5.12}$$

According to Ref. 8 (p. 466) the functions f_1 and f_2 are the same in Lundborg[8] as in Fröman and Fröman.[2] According to Eqs. (16a,b), (17a,b), and (9a,b) in the latter paper one therefore has in the first order of the phase-integral approximation and with the notation of the present paper

$$f_1(x') = |Q^{-1/2}(x')|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x'} Q(z)dz\right|\right], \tag{5.13}$$

with x' lying to the left of the barrier,

$$f_2(x') = |Q^{-1/2}(x')|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x'} Q(z)dz\right|\right], \tag{5.14}$$

with x' lying to the left of the barrier, and

$$f_1(x'') = |Q^{-1/2}(x'')|\exp\left[+K_0 - i\left|\mathrm{Re}\int_{t''}^{x''} Q(z)dz\right| + i\pi/2\right], \tag{5.15}$$

with x'' lying to the right of the barrier,

$$f_2(x'') = |Q^{-1/2}(x'')|\exp\left[-K_0 + i\left|\mathrm{Re}\int_{t''}^{x''} Q(z)dz\right| - i\pi/2\right], \tag{5.16}$$

with x'' lying to the right of the barrier, where x' and x'' are points in the classically allowed regions to the left and to the right, respectively, of the barrier. According to Eq. (24a) in Lundborg[8] the first-order quantity K_0 in (5.15) and (5.16) is given by

$$K_0 = \pi\overline{K_0} = \pi G(1-p). \tag{5.17}$$

With the use of Eq. (18) in Ref. 2, i.e.,

$$\Psi(z) = a_1(z)f_1(z) + a_2(z)f_2(z), \tag{5.18}$$

together with (5.13)–(5.16) in the present paper one obtains

$$\Psi(x') = \tilde{A}'|Q^{-1/2}(x')|\exp\left[i\left|\mathrm{Re}\int_{t'}^{x'} Q(z)dz\right|\right] + \tilde{B}'|Q^{-1/2}(x')|\exp\left[-i\left|\mathrm{Re}\int_{t'}^{x'} Q(z)dz\right|\right], \tag{5.19}$$

where

$$\tilde{A}' = a_2(x'), \tag{5.20}$$

$$\tilde{B}' = a_1(x'), \tag{5.21}$$

and

$$\Psi(x'') = \tilde{A}''|Q^{-1/2}(x'')|\exp\left[i \left| \mathrm{Re} \int_{t''}^{x''} Q(z)dz \right| \right] + \tilde{B}''|Q^{-1/2}(x'')|\exp\left[-i \left| \mathrm{Re} \int_{t''}^{x''} Q(z)dz \right| \right], \tag{5.22}$$

where

$$\tilde{A}'' = i \exp(-K_0) a_2(x''), \tag{5.23}$$

$$\tilde{B}'' = i \exp(K_0) a_1(x''). \tag{5.24}$$

With the use of the formula (30) for $\mathbf{F}(-\infty, +\infty)$ in Lundborg,[8] and (5.20), (5.21), (5.23), and (5.24) in the present paper one can write Eq. (19) in Ref. 2, i.e.,

$$\begin{pmatrix} a_1(x') \\ a_2(x') \end{pmatrix} = \mathbf{F}(x', x'') \begin{pmatrix} a_1(x'') \\ a_2(x'') \end{pmatrix} \tag{5.25}$$

in the first order of the phase-integral approximation and in the limit when $x' \to -\infty$ and $x'' \to +\infty$ as

$$\begin{pmatrix} \tilde{A}' \\ \tilde{B}' \end{pmatrix} = \tilde{\mathbf{M}} \begin{pmatrix} \tilde{A}'' \\ \tilde{B}'' \end{pmatrix} \tag{5.26}$$

where

$$\tilde{M}_{11} = \tilde{M}_{22}^* = -i|F_{22}|\exp(K_0 + i \arg F_{22}) \tag{5.27}$$

$$\tilde{M}_{12} = \tilde{M}_{21}^* = |F_{12}|\exp(K_0 - 2i\sigma), \tag{5.28}$$

Lundborg's notation σ being related to our notation $\tilde{\varphi}$ according to the formula

$$\tilde{\varphi} = -2\sigma. \tag{5.29}$$

Using (5.29) and Lundborg's[8] formulas (32a,b) for $|F_{12}|$ and $|F_{22}|$ in the first-order approximation, one can write (5.27) and (5.28) as

$$\tilde{M}_{11} = \tilde{M}_{22}^* = -i\left[\frac{1 + \exp[-2\pi G(1+p)]}{1 - \exp(-4\pi G p)} \right]^{1/2} \exp(K_0 + i \arg F_{22}), \tag{5.30}$$

$$\tilde{M}_{12} = \tilde{M}_{21}^* = \left[\frac{\exp(2K_0) + 1}{1 - \exp(-4\pi G p)} \right]^{1/2} \exp(i\tilde{\varphi}). \tag{5.31}$$

For the first-order phase-integral approximation one obtains from (5.29) and Lundborg's[8] Eq. (33a)

$$\tilde{\varphi} = \arg \Gamma(1/2 + i\overline{K_0}) - \overline{K_0} \ln|\overline{K_0}| + \overline{K_0} + \mathrm{Im} \ln \Gamma(2iGp) - 2Gp[\ln(2Gp) - 1] + \pi/4, \tag{5.32}$$

and from Lundborg's[8] Eq. (34a), after correction by addition of a term $-\pi/4$ on the right-hand side,

$$\arg F_{22} = \operatorname{Im} \ln \Gamma(1/2 + iG(1+p)) - G(1+p)\{\ln[G(1+p)] - 1\} - \operatorname{Im} \ln \Gamma(2iGp) + 2Gp[\ln(2Gp) - 1] - \pi/4. \tag{5.33}$$

The logarithms of the gamma functions $\Gamma(2iGp)$ and $\Gamma(1/2+iG(1+p))$ in (5.32) and (5.33) are expanded for large arguments by the use of the asymptotic expansion (4.30), yielding

$$\operatorname{Im} \ln \Gamma(2iGp) \sim 2Gp[\ln(2Gp) - 1] - \frac{\pi}{4} - \frac{1}{24Gp}, \tag{5.34}$$

$$\operatorname{Im} \ln \Gamma(1/2 + iG(1+p)) \sim G(1+p)\{\ln(G(1+p)) - 1\} + \frac{1}{24G(1+p)}, \tag{5.35}$$

Inserting (5.34) and (5.35) into (5.32) and (5.33) we obtain

$$\tilde{\varnothing} \sim \arg \Gamma(1/2 + i\overline{K_0}) - \overline{K_0} \ln|\overline{K_0}| + \overline{K_0} - \frac{1}{24Gp}, \tag{5.36}$$

$$\arg F_{22} \sim \frac{1}{24G(1+p)} + \frac{1}{24Gp}. \tag{5.37}$$

Recalling condition (5.12) and assuming that $24G \gg 1$, one can in (5.36) and (5.37) neglect the terms containing G. Inserting the resulting formulas for $\tilde{\varnothing}$ and $\arg F_{22}$ into (5.30) and (5.31), where the terms containing G can also be neglected, one obtains (2.4) along with (2.6). With the use of (5.17) condition (5.12) can be written as $|\overline{K_0}/G|^{1/2} \ll 1$. For any value of $\overline{K_0}$ (positive or negative) it is possible to find values of G such that the condition $24G \gg 1$ and $|\overline{K_0}/G|^{1/2} \ll 1$ are fulfilled. The barrier may thus be of arbitrary thickness.

APPENDIX A: PREPARATION FOR THE DERIVATIONS OF (4.15) and (4.17)

With the use of (4.9) and (4.12) one obtains

$$\begin{aligned}[\pm Q^2(x)]^{1/2} &= \frac{\alpha\{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{1/2}}{x_0[\exp(x/x_0)+1]} \\ &= \frac{\alpha\{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}}{x_0[\exp(x/x_0)+1]\{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{1/2}} \\ &= \frac{\alpha\{\pm[\exp(x/x_0)+1] \mp \gamma^2 \exp(x/x_0)/[\exp(x/x_0)+1]\}}{x_0\{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{1/2}}.\end{aligned} \tag{A1}$$

Using (A1) one gets

$$\begin{aligned}\int [\pm Q^2(x)]^{1/2} dx = &\pm \frac{\alpha}{x_0} \int \{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{-1/2} \exp(x/x_0) dx \\ &\pm \frac{\alpha}{x_0} \int \{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{-1/2} dx \\ &\mp \frac{\alpha\gamma^2}{x_0} \int \{\pm[\exp(x/x_0)+1]^2 \mp \gamma^2 \exp(x/x_0)\}^{-1/2} \frac{\exp(x/x_0)}{[\exp(x/x_0)+1]} dx.\end{aligned} \tag{A2}$$

Here one introduces instead of the integration variable x in the first integral

$$y_1 = y_1(x) = \frac{2\exp(x/x_0) + 2 - \gamma^2}{\gamma(\gamma^2 - 4)^{1/2}}, \tag{A3}$$

in the second integral

$$y_2 = y_2(x) = \frac{\gamma^2 - 2 - 2\exp(-x/x_0)}{\gamma(\gamma^2 - 4)^{1/2}}, \tag{A4}$$

and in the third integral

$$y_3 = y_3(x) = \frac{2\gamma}{(\gamma^2 - 4)^{1/2}}\left[\frac{1}{2} - \frac{1}{\exp(x/x_0) + 1}\right], \tag{A5}$$

the functions $y_1(x)$, $y_2(x)$, and $y_3(x)$ being equal to -1 and $+1$ at the turning points t' and t'', respectively. With the aid of (A2)–(A5) one obtains

$$\int [\pm Q^2(x)]^{1/2} dx = \pm\alpha \int \frac{dy_1}{[\pm(y_1^2 - 1)]^{1/2}} \pm \alpha \int \frac{dy_2}{[\pm(y_2^2 - 1)]^{1/2}} \mp \alpha\gamma \int \frac{dy_3}{[\pm(y_3^2 - 1)]^{1/2}}. \tag{A6}$$

APPENDIX B: DERIVATION OF (4.15)

Inserting (A6) with the lower signs into (4.14), one obtains

$$K_0 = -\alpha \int_{-1}^{1} \frac{dy_1}{(1 - y_1^2)^{1/2}} - \alpha \int_{-1}^{1} \frac{dy_2}{(1 - y_2^2)^{1/2}} + \alpha\gamma \int_{-1}^{1} \frac{dy_3}{(1 - y_3^2)^{1/2}} = (\alpha\gamma - 2\alpha) \int_{-1}^{1} \frac{dy}{(1 - y^2)^{1/2}}$$
$$= \pi(\alpha\gamma - 2\alpha) = \pi(\beta - 2\alpha), \tag{B1}$$

where the last equality has been obtained with the use of (4.12).

APPENDIX C: DERIVATION OF (4.17)

Using (A6) with the upper signs, and recalling that $y_1(t'') = y_2(t'') = y_3(t'') = +1$, one obtains when x is real and lies to the right of the barrier

$$\left| \mathrm{Re} \int_{t''}^{x} Q(z)dz \right| = \mathrm{Re} \int_{t''}^{x} [Q^2(z)]^{1/2} dz = \alpha\, \mathrm{Re} \int_{+1}^{y_1(x)} \frac{dy_1}{(y_1^2 - 1)^{1/2}} + \alpha\, \mathrm{Re} \int_{+1}^{y_2(x)} \frac{dy_2}{(y_2^2 - 1)^{1/2}}$$
$$- \alpha\gamma\, \mathrm{Re} \int_{+1}^{y_3(x)} \frac{dy_3}{(y_3^2 - 1)^{1/2}}, \tag{C1}$$

and after evaluation of the integrals

$$\left| \mathrm{Re} \int_{t''}^{x} Q(z)dz \right| = \alpha\, \mathrm{Re}\ln\{y_1(x) + [y_1^2(x) - 1]^{1/2}\} + \alpha\, \mathrm{Re}\ln\{y_2(x) + [y_2^2(x) - 1]^{1/2}\}$$
$$- \alpha\gamma\, \mathrm{Re}\ln\{y_3(x) + [y_3^2(x) - 1]^{1/2}\}. \tag{C2}$$

From this formula one obtains with the aid of (A3)–(A5) and (4.12)

$$\lim_{x\to+\infty}\left[\left|\operatorname{Re}\int_{t''}^{x}Q(z)dz\right|-\frac{\alpha}{x_0}x\right]=\alpha\operatorname{Re}\ln\frac{4}{\gamma(\gamma^2-4)^{1/2}}+\alpha\operatorname{Re}\ln\frac{\gamma}{(\gamma^2-4)^{1/2}}-\alpha\gamma\operatorname{Re}\ln\frac{\gamma+2}{(\gamma^2-4)^{1/2}}$$

$$=\alpha\operatorname{Re}\left[\ln\frac{4}{\gamma^2-4}-\frac{\gamma}{2}\ln\frac{\gamma+2}{\gamma-2}\right]=2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)$$

$$+\frac{\beta-2\alpha}{2}\operatorname{Re}\ln(\beta-2\alpha)=2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)$$

$$+\frac{\beta-2\alpha}{2}\ln|\beta-2\alpha|. \tag{C3}$$

As the barrier is symmetric, one obtains with the use of (C3)

$$\lim_{x\to-\infty}\left[\left|\operatorname{Re}\int_{t'}^{x}Q(z)dz\right|+\frac{\alpha}{x_0}x\right]=\lim_{x\to+\infty}\left[\left|\operatorname{Re}\int_{t''}^{x}Q(z)dz\right|-\frac{\alpha}{x_0}x\right]=2\alpha\ln(2\alpha)-\frac{\beta+2\alpha}{2}\ln(\beta+2\alpha)$$

$$+\frac{\beta-2\alpha}{2}\ln|\beta-2\alpha|. \tag{C4}$$

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Coherent states expectation values as semiclassical trajectories

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We study the time evolution of the expectation value of the anharmonic oscillator coordinate in a coherent state as a toy model for understanding the semiclassical solutions in quantum field theory. By using the deformation quantization techniques, we show that the coherent state expectation value can be expanded in powers of $\hbar$ such that the zeroth-order term is a classical solution while the first-order correction is given as a phase-space Laplacian acting on the classical solution. This is then compared to the effective action solution for the one-dimensional ϕ^4 perturbative quantum field theory. We find an agreement up to the order $\lambda\hbar$, where λ is the coupling constant, while at the order $\lambda^2\hbar$ there is a disagreement. Hence the coherent state expectation values define an alternative semiclassical dynamics to that of the effective action. The coherent state semiclassical trajectories are exactly computable and they can coincide with the effective action trajectories in the case of two-dimensional integrable field theories. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227259]

I. INTRODUCTION

The notion of a semiclassical trajectory as a quantum corrected classical trajectory is a very useful idea in various areas of physics. In the case of field theories, the classical trajectory represents a classical field configuration, and the semiclassical field configurations are usually calculated from the effective action,[2,3] i.e., by solving the corresponding equations of motion. However, the semiclassical dynamics depends on the initial quantum state, so that one can have in principle many different semiclassical dynamics (for a review see Ref. 1).

In the effective action approach the initial state is the in-vacuum state. (This state can be described as a vacuum state of the Hamiltonian coupled to a source with appropriate boundary conditions.[4]) Since the effective action approach was tailor-made for the problems of scattering of the elementary particles, one is not calculating the expectation value of an appropriate operator, but a matrix element between the "in" and the "out" vacuum. This means that the obtained values can be complex and this is a problem in the context of quantum gravity and quantum cosmology applications because the field operator is a metric, and the effective metric has to be real. This problem can be resolved by using the effective action formalism where the field variable is a true expectation value.[5,6] However, in order to obtain a semiclassical trajectory, one needs to solve the corresponding effective equation of motion, which is often a difficult task.

These types of problems were encountered in the context of two-dimensional dilaton gravity models of quantum black holes, where the effective metric gives the information about the back-reaction of the black hole evaporation (for a review and references see Ref. 7). These models are exactly integrable two-dimensional field theories, and in the case of the CGHS model,[8] it was

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demonstrated in Ref. 9 that a relevant one-loop ($O(\hbar)$) solution could be obtained as an expectation value of the metric operator in the coherent state corresponding to the initial matter distribution. Furthermore, a two-loop ($O(\hbar^2)$) solution was found by using this approach,[10] which was otherwise impossible to do by solving the corresponding two-loop effective action equations.

These results suggest an approach to constructing semiclassical trajectories for field theories via expectation values of the appropriate operators in the coherent states. A coherent state (and a related squeezed state) is the best possible description of a classical phase-space point, since they saturate the Heisenberg uncertainty relations. In quantum mechanics one can prove that for a general quadratic Hamiltonian, a coherent state wave packet follows the classical trajectory, while in the case of interactions, the wave packet is well approximated by the coherent state during the Ehrenfest time.[11–14] In the case of field theories one then expects that the coherent state trajectories should be the same as the effective action trajectories in the case of free-field theories, while in the case of interactions one expects that the coherent state trajectories should be a good approximation for the effective action ones.

The effective action quantum dynamics can be studied via the anharmonic oscillator (AHO) toy model.[15,16] One can then study the time evolution of the coherent states for the AHO and compare it to the effective action trajectories. However, the effective action trajectories were obtained only in the effective potential approximation. It is possible to improve this approximation by including more relevant terms in the effective action,[15] but there is no simple expression for the complete one-loop contribution, i.e., the $\hbar$ correction. On the other hand, it has been known from the deformation quantization applications to quantum optics how to evaluate the coherent states expectation values.[17] Hence one can apply these techniques to the case of the AHO and calculate the complete $\hbar$ contribution for the coherent states. The result can then be expanded perturbatively in the coupling constant and compared to the corresponding effective action expansion.

Given that it is easier to obtain semiclassical trajectories from the coherent states expectation values than from solving the equations of motion of the effective action, a natural question is to what extent one can approximate the effective action trajectories by the coherent states trajectories. In this paper we explore this and related issues by studying the example of the anharmonic oscilator. We calculate the coherent states trajectories by using the deformation quantization techniques, while for the effective action trajectories we use the Feynman diagram techniques and the results are compared order by order in the perturbative expansion. In Sec. II we introduce the basic concepts of deformation quantization (DQ) and derive a new formula for the expectation value (EV) of a generic dynamical variable in an arbitrary state. We then use this result in Sec. III to derive the $O(\hbar)$ contribution to the coherent state EV of a generic dynamical variable. We then derive the corresponding quantum equation of motion for the coordinate EV and in Sec. IV we specialize to the case of an AHO. In Sec. V we derive the perturbative quantum equations of motion for an AHO coming from the effective action formalism and compare the results of the two approaches. In Sec. VI we present our conclusions and in the Appendix we describe how to solve the perturbative equations of motion.

II. EXPECTATION VALUES

Let us consider an N-dimensional system with coordinates $q=(q_1,\ldots,q_N)$ and canonical momenta $p=(p_1,\ldots,p_N)$. We shall assume a flat phase space $T^*M\simeq\mathbb{R}^{2N}$ with symplectic form $\sigma(z,z')=q\cdot p'-p\cdot q'$, where $z=(p,q)$, $z'=(p',q')$.

In the context of deformation quantization[17–34]one computes the expectation value of a generic operator $\hat{A}(\hat{z},t)$ from the algebra of observables at time t in a state $\psi\in L^2(\mathbb{R}^N,dq)$ as

$$A(t)\equiv\langle\psi|\hat{A}(\hat{z},t)|\psi\rangle=\int \mathrm{d}z\, F_W(z)A_W(z,t), \tag{1}$$

where $F_W(z)$ is the Wigner function[19] associated with ψ,

$$F_W(p,q) = \frac{1}{(\pi\hbar)^N} \int \mathrm{d}y\, e^{-2ip\cdot y/\hbar} \psi^*(q-y)\psi(q+y). \tag{2}$$

$A_W(z,t)$ is the Weyl symbol[18] associated with $\hat{A}(\hat{z},t)$ given by

$$A_W(z,t) = \left(\frac{\hbar}{2\pi}\right)^N \int \mathrm{d}\xi\, \mathrm{Tr}\{\hat{A}(\hat{z},t)e^{i\xi\cdot\hat{z}}\}e^{-i\xi\cdot z}. \tag{3}$$

The Weyl symbol defines a noncommutative twisted product,[20]

$$(\hat{A}\cdot\hat{B})_W \equiv \; A_W \star_W B_W = \exp\left[\frac{i\hbar}{2}\sigma\left(\frac{\partial}{\partial z_1},\frac{\partial}{\partial z}\right)\right] A_W(z_1)B_W(z)\Big|_{z_1=z} = A_W(z)B_W(z) + \mathcal{O}(\hbar), \tag{4}$$

where $\partial/\partial z = (\partial/\partial p, \partial/\partial q)$. Likewise, one may define a bracket—the Moyal bracket—according to[21]

$$[A_W,B_W]_W \equiv \left(\frac{1}{i\hbar}[\hat{A},\hat{B}]\right)_W = \frac{1}{i\hbar}(A_W\star_W B_W - B_W\star_W A_W) = \; \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\sigma\left(\frac{\partial}{\partial z_1},\frac{\partial}{\partial z}\right)\right] A_W(z_1)B_W(z)\Big|_{z_1=z}$$
$$= \{A_W(z),B_W(z)\} + O(\hbar^2). \tag{5}$$

These algebraic operations are formal deformations of the usual product and of the Poisson bracket with deformation parameter $\hbar$.

The dynamics is governed by the Moyal equation

$$\dot{A}_W(z,t) = [H_W(z),A_W(z,t)]_W = \{H_W(z),A_W(z,t)\} + O(\hbar^2), \tag{6}$$

where H_W is the Weyl symbol of the quantum Hamiltonian.

The following remark is important for the sequel. If the Hamiltonian is of the form

$$H = \frac{p^2}{2m} + U(q), \tag{7}$$

then there are no ordering ambiguities and we conclude that Eq. (6) only yields corrections of even order in $\hbar$ to the classical solution $A_{\mathrm{cl}}(z,t)$ so that

$$A_W(z,t) = A_{\mathrm{cl}}(z,t) + O(\hbar^2). \tag{8}$$

The Wigner function being a square integrable function admits a Fourier transform:

$$\widetilde{F}_W(a) = \int dz F_W(z)e^{ia\cdot z} = \int \mathrm{d}x\, e^{iv\cdot x}\psi^*\left(x - \frac{\hbar u}{2}\right)\psi\left(x + \frac{\hbar u}{2}\right), \tag{9}$$

with the inverse

$$F_W(z) = \frac{1}{(2\pi)^{2N}} \int \mathrm{d}a\, \widetilde{F}_W(a)e^{-ia\cdot z}. \tag{10}$$

Here $a=(u,v)$ lives in the dual of the phase space. The function $\widetilde{F}(\tilde{a})$, with $\tilde{a}=(u,-v)$, is known as the symplectic Fourier transform or chord function and finds many applications in the context of deformation quantization and decoherence.[32–34]

If we substitute (10) into (1), we obtain

$$A(t) = \widetilde{F}_W\left(\frac{1}{i}\frac{\partial}{\partial z}\right)A_W(z,t)\Big|_{z=0}. \tag{11}$$

Equation (11) has a nice interpretation in the context of deformation quantization. In Eq. (1) the objects appearing on the right-hand side are defined up to an isomorphism, in the following sense. The Weyl symbol stems from a correspondence rule according to which operators are first written in a fully symmetric form—the Weyl order—before they are "dequantized." Alternatively, one may choose other ordering prescriptions for the operators (e.g., normal ordering). The price to pay is that one also needs to change the corresponding quasidistribution, in order to leave the expectation value (1) unchanged. This ambiguity has been systematized by Cohen.[31] Each correspondence rule is associated with an analytic so-called Cohen function $f(\xi)$, such that $f(0)=1$, which allows us to define a new f-symbol[17]

$$A_f(z,t) = f\left(\frac{1}{i}\frac{\partial}{\partial z}\right)A_W(z,t), \tag{12}$$

and the corresponding quasidistribution

$$F_f(z) = f^{-1}\left(i\frac{\partial}{\partial z}\right)F_W(z). \tag{13}$$

Likewise one naturally defines a $\star_f$-product and an f-bracket

$$A_f\star_f B_f = f\left(\frac{1}{i}\frac{\partial}{\partial z}\right)A_W\star_W B_W, \quad [A_f,B_f]_f = f\left(\frac{1}{i}\frac{\partial}{\partial z}\right)[A_W,B_W]_W. \tag{14}$$

The dynamics is then dictated by

$$\dot{A}_f(z,t) = [H_f(z),A_f(z,t)]_f. \tag{15}$$

Equation (11) can thus be interpreted in the following terms. If we regard $\widetilde{F}_W$ as one of Cohen's functions, then $A_{\tilde{F}}(z,t)\equiv\widetilde{F}_W((1/i)(\partial/\partial z))A_W(z,t)$ is just the $\widetilde{F}_W$ symbol associated with the operator $\hat{A}$. The only difference is that one eventually sets $z=0$. The symbol $A_{\tilde{F}}(t)$ is a solution of Eq. (15).

Note that Eq. (11) remains valid even if F_W is the Wigner function of a mixed state given by a density matrix ρ. However, in this paper we will be concerned with the pure states only.

III. COHERENT STATES

Equation (11) derived in Sec. II simplifies drastically if we choose the state ψ to be the coherent state

$$\psi_{\alpha_0}(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{N/4}\exp\left[-\frac{m\omega}{2\hbar}(q-q_0)^2 + \frac{ip_0}{\hbar}\cdot\left(q-\frac{q_0}{2}\right)\right], \tag{16}$$

where in the standard notation

$$\alpha_0 \equiv \sqrt{\frac{m\omega}{2\hbar}}q_0 + \frac{ip_0}{\sqrt{2m\omega\hbar}}. \tag{17}$$

From (9) we have

$$\widetilde{F}_W(u,v) = \exp\left[-\frac{m\omega\hbar u^2}{4} - \frac{\hbar v^2}{4m\omega} + iu\cdot p_0 + iv\cdot q_0\right]. \tag{18}$$

Substituting into (11), we obtain

$$A_{\alpha_0}(t) = \exp\left[\frac{\hbar}{4m\omega}\frac{\partial^2}{\partial q^2} + \frac{\hbar m\omega}{4}\frac{\partial^2}{\partial p^2}\right] A_W(p+p_0, q+q_0, t)\Big|_{q=p=0}$$
$$= \exp\left[\frac{\hbar}{4m\omega}\frac{\partial^2}{\partial q_0^2} + \frac{\hbar m\omega}{4}\frac{\partial^2}{\partial p_0^2}\right] A_W(p_0, q_0, t). \tag{19}$$

The last expression is well known to be the phase space symbol stemming from normal ordering.[17] Now, this equation is particularly well suited for semiclassical expansions in powers of $\hbar$. Following the remark after Eq. (6), we conclude that if the Hamiltonian is of the form (7), then we get at the order $\hbar$ (cf. (8), (19)),

$$A_{\alpha_0}(t) = A_{\mathrm{cl}}(p_0, q_0, t) + \left[\frac{\hbar}{4m\omega}\frac{\partial^2}{\partial q_0^2} + \frac{\hbar m\omega}{4}\frac{\partial^2}{\partial p_0^2}\right] A_{\mathrm{cl}}(p_0, q_0, t) + O(\hbar^2). \tag{20}$$

Expression (20) is valid for any trace-class operator $\hat{A}$ and any Hamiltonian of the form (7) provided the wave function is the coherent state (16).

In fact these semiclassical expansions can be performed for other states, by using (11), as long as the chord function admits a regular expansion in powers of $\hbar$,

$$\tilde{F}_W(a) = \sum_{n=0}^{\infty} \rho_n(a)\hbar^n. \tag{21}$$

In most applications one is interested in the case $\hat{A} = \hat{q}$. For simplicity, we shall henceforth consider a one-dimensional system. Let us define $Q(p_0, q_0, t) \equiv \langle \psi_{\alpha_0} | \hat{q} | \psi_{\alpha_0} \rangle$ and $q_{\mathrm{cl}}(p_0, q_0, t) \equiv q(p_0, q_0, t)$. In order to compare to the effective action approach, let us derive the equations of motion to order $\hbar$ for $Q(p_0, q_0, t)$. From (20) we have

$$m\ddot{Q} = m\ddot{q} + \frac{\hbar}{4\omega}\frac{\partial^2}{\partial q_0^2}\ddot{q} + \frac{\hbar m^2\omega}{4}\frac{\partial^2}{\partial p_0^2}\ddot{q} + O(\hbar^2) = -U'(q) - \frac{\hbar}{4m\omega}\frac{\partial^2}{\partial q_0^2}U'(q) - \frac{\hbar m\omega}{4}\frac{\partial^2}{\partial p_0^2}U'(q) + O(\hbar^2). \tag{22}$$

Notice that $U(q)$ depends on p_0, q_0 only through $q(p_0, q_0, t)$. Consequently

$$m\ddot{Q} = -U'(q) - \frac{\hbar}{4m\omega}\left[U'''(q)\left(\frac{\partial q}{\partial q_0}\right)^2 + U''(q)\frac{\partial^2 q}{\partial q_0^2}\right] - \frac{\hbar m\omega}{4}\left[U'''(q)\left(\frac{\partial q}{\partial p_0}\right)^2 + U''(q)\frac{\partial^2 q}{\partial p_0^2}\right] + O(\hbar^2). \tag{23}$$

We then obtain

$$U'(q) = U'(Q) - U''(q)\left[\frac{\hbar}{4m\omega}\frac{\partial^2 q}{\partial q_0^2} + \frac{\hbar m\omega}{4}\frac{\partial^2 q}{\partial p_0^2}\right] + O(\hbar^2). \tag{24}$$

By substituting (24) into (23), we finally obtain

$$m\ddot{Q} = -U'(Q) - \frac{\hbar}{4}U'''(Q)\left[\frac{1}{m\omega}\left(\frac{\partial Q}{\partial q_0}\right)^2 + m\omega\left(\frac{\partial Q}{\partial p_0}\right)^2\right] + O(\hbar^2). \tag{25}$$

This is a partial differential equation for $Q(p_0, q_0, t)$ where (p_0, q_0) play a double role. They are variables, but also the initial conditions

$$Q(p_0, q_0, t)|_{t=0} = q_0, \qquad \dot{Q}(p_0, q_0, t)|_{t=0} = \frac{p_0}{m}. \tag{26}$$

One may instead derive an ordinary differential equation for Q and its time derivatives which is more suited for comparison with the effective action formalism. In order to do this let us consider the solution for q of the classical equations of motion given by

$$t = \pm \int_{q_0}^{q} \mathrm{d}x \left[\frac{2}{m}(E - U(x)) \right]^{-1/2}, \tag{27}$$

where

$$E = \frac{p_0^2}{2m} + U(q_0) = \frac{1}{2}m\dot{q}^2 + U(q) \tag{28}$$

is the total energy of the classical system. Taking into account that E and q depend on p_0 and q_0, and applying the implicit function theorem we obtain

$$\frac{\partial q}{\partial q_0} = \frac{m}{p_0}\dot{q} + \frac{\dot{q}U'(q_0)}{2}\sqrt{\frac{m}{2}}f(q,p_0,q_0), \quad \frac{\partial q}{\partial p_0} = \frac{p_0\dot{q}}{2\sqrt{2m}}f(q,p_0,q_0), \tag{29}$$

where

$$f(q,p_0,q_0) \equiv \int_{q_0}^{q} \mathrm{d}x[E - U(x)]^{-3/2}. \tag{30}$$

In Eq. (25) it is immaterial whether we write q or Q in the terms proportional to $\hbar$. From (29) we then obtain

$$m\ddot{Q} = -U'(Q) - \frac{\hbar}{4}\dot{Q}^2U'''(Q)\left\{ \frac{m}{\omega p_0^2} + \frac{U'(q_0)}{\omega p_0}\sqrt{\frac{m}{2}}f(Q,p_0,q_0) + \left[\frac{(U'(q_0))^2}{8\omega} + \frac{\omega p_0^2}{8} \right] f^2(Q,p_0,q_0) \right\} + O(\hbar^2). \tag{31}$$

If we neglect the $O(\hbar^2)$ terms in (31) we obtain a second-order nonlinear ordinary differential equation for $Q(t)$ with the initial conditions (26).

IV. THE ANHARMONIC OSCILLATOR

As an application we consider the quartic anharmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2q^2 + \frac{\lambda}{4!}q^4, \tag{32}$$

where λ is a positive coupling constant. Let us define $\Lambda = \lambda/4!$ and

$$\alpha^2 \equiv \frac{\sqrt{m^2\omega^4 + 16E\Lambda} - m\omega^2}{4\Lambda}, \quad \beta^2 \equiv \frac{\sqrt{m^2\omega^4 + 16E\Lambda} + m\omega^2}{4\Lambda}. \tag{33}$$

By substituting

$$x = \frac{\alpha\beta \sin\varphi}{\sqrt{\beta^2 + \alpha^2\cos^2\varphi}} \tag{34}$$

into (30) we obtain

$$f(q,p_0,q_0)=\frac{1}{[\Lambda(\alpha^2+\beta^2)]^{3/2}}\left\{\frac{1}{\beta^2}E(\varphi(q)|n)+\frac{1}{\alpha^2}[\tan\varphi(q)\sqrt{1-n\sin^2\varphi(q)}+F(\varphi(q)|n)\right.$$
$$\left.-E(\varphi(q)|n)]-(q\leftrightarrow q_0)\right\}, \tag{35}$$

where $\{h(q)-(q\leftrightarrow q_0)\}=\{h(q)-h(q_0)\}$,

$$\varphi(q)\equiv\arcsin\sqrt{\frac{q^2}{n(q^2+\alpha^2)}},\quad n\equiv\frac{\alpha^2}{\alpha^2+\beta^2},\quad 0\leqslant n\leqslant 1, \tag{36}$$

and

$$F(\phi|m)\equiv\int_0^\phi \mathrm{d}\theta\frac{1}{\sqrt{1-m\sin^2\theta}},\quad E(\phi|m)\equiv\int_0^\phi \mathrm{d}\theta\sqrt{1-m\sin^2\theta} \tag{37}$$

are the incomplete elliptic integrals of the first and second kind, respectively.[35]

In order to compare this with the equations of motion stemming from the effective action, let us expand the right-hand side of (31) in powers of λ,

$$\ddot{Q}=-\omega^2Q-\frac{\lambda}{6m}Q^3-\hbar\lambda\frac{k_t^2x_t}{4m^2}\left\{\frac{1}{\omega p_0^2}+\frac{m\omega q_0}{p_0\sqrt{2m}}f_0(x_t,p_0,q_0)+\frac{\omega E_0}{4}f_0^2(x_t,p_0,q_0)\right\}+O(\hbar\lambda^2), \tag{38}$$

where x_t and k_t are the classical harmonic oscillator (HO) solutions for the coordinate and the momentum

$$x_t=q_0\cos(\omega t)+\frac{p_0}{m\omega}\sin(\omega t),\quad k_t=p_0\cos(\omega t)-m\omega q_0\sin(\omega t), \tag{39}$$

with the energy

$$E_0=\frac{p_0^2}{2m}+\frac{1}{2}m\omega^2q_0^2. \tag{40}$$

Moreover

$$f_0(x_t,p_0,q_0)=\int_{q_0}^{x_t}\mathrm{d}x\left(E_0-\frac{1}{2}m\omega^2x^2\right)^{-3/2}=\frac{\sqrt{2m}}{E_0}\left(\frac{x_t}{k_t}-\frac{q_0}{p_0}\right). \tag{41}$$

The terms proportional to $\hbar\lambda$ in (38) yield $-\hbar\lambda x_t/4m^2\omega$ and up to order $\hbar\lambda$ we may replace x_t by Q in the terms proportional to $\hbar\lambda$. By neglecting the $O(\hbar\lambda^2)$ terms we obtain

$$\ddot{Q}+\left(\omega^2+\frac{\hbar\lambda}{4m^2\omega}\right)Q+\frac{\lambda}{6m}Q^3=0, \tag{42}$$

as a semiclassical equation of motion.

V. THE EFFECTIVE ACTION RESULTS

Let us consider a D-dimensional scalar field theory given by the action

$$S[\phi]=\int\mathrm{d}^Dx\left[\frac{1}{2}(\partial_\mu\phi)^2-\frac{1}{2}M^2\phi^2-V(\phi)\right], \tag{43}$$

where $V(\phi)$ is polynomial in ϕ. The corresponding effective action can be written as[36]

$$\Gamma[\phi] = \sum_{n=2}^{\infty} \int \mathrm{d}^D x_1 \cdots \int \mathrm{d}^D x_1 \frac{1}{n!} \Gamma^{(n)}(x_1, \ldots, x_n) \phi(x_1) \cdots \phi(x_n), \tag{44}$$

where

$$\Gamma^{(n)}(x_1, \ldots, x_n) = \int \mathrm{d}^D p_1 \cdots \int \mathrm{d}^D p_n e^{i(p_1 x_1 + \cdots + p_n x_n)} (\Gamma^{(n)}(p_1, \ldots, p_n))^{\epsilon_n}. \tag{45}$$

The $\Gamma^{(n)}(p)$ are the momentum space n-particle irreducible Greens functions whose external legs are amputated for $n>2$ and $\epsilon_n=-1$ for $n=2$ and $\epsilon_n=1$ for $n>2$. These objects can be calculated perturbatively via the Feynman diagrams and for $V=\lambda\phi^4/4!$ the perturbative expansion can be organized in powers of λ (number of the vertices) and in powers of $\hbar$ (number of the loops), so that

$$\Gamma^{(n)}(p) = \sum_{v,l} \lambda^v \hbar^l \Gamma^{(n)}_{v,l}(p). \tag{46}$$

Up to the order of $\lambda\hbar$ only the tadpole diagram contributes,[36] so that in the case of $D=1$ field theory, i.e., quantum mechanics (QM), one obtains

$$\Gamma^{(2)}_E(p) = \frac{1}{p^2+M^2} - \frac{\lambda\hbar/2}{(p^2+M^2)^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{q^2+M^2} + O(\lambda^2\hbar) = \frac{1}{p^2+M^2} - \frac{\lambda\hbar}{2(p^2+M^2)^2} \frac{1}{2M} + O(\lambda^2\hbar), \tag{47}$$

where Γ_E is the Euclidean propagator. The physical (Minkowski) propagator is given by $\Gamma^{(2)}(p) = -\Gamma^{(2)}_E(ip)$, and the position space vertex function is given by

$$\Gamma^{(2)}(x_1,x_2) = 2\pi \int \frac{\mathrm{d}p_1}{2\pi} \int \frac{\mathrm{d}p_2}{2\pi} \delta(p_1+p_2)(\Gamma^{(2)}(p_1))^{-1} e^{i(p_1x_1+p_2x_2)}. \tag{48}$$

This gives

$$\Gamma[\phi] = S[\phi] + \frac{\lambda\hbar}{8M} \int_{x_1}^{x_2} \mathrm{d}x\, \phi^2(x) + O(\lambda^2\hbar). \tag{49}$$

Passing to the anharmonic oscillator parameters $(M\to\omega, \lambda\to\lambda/m^2)$ gives

$$\Gamma[q] = S[q] + \frac{\lambda\hbar}{8m^2\omega} \int_{t_1}^{t_2} \mathrm{d}t\, q^2(t) + O(\lambda^2\hbar). \tag{50}$$

Up to order $O(\hbar\lambda)$ this action gives the same equation of motion as (42).

When going to higher orders in perturbation theory, one obtains the nonlocal terms in the effective action. For example, at the order $\lambda^2\hbar$ one has to include four $\Gamma^{(4)}$ diagrams (one three-diagram plus three one-loop diagrams[36]) so that

$$\Gamma^{(4)}_E(p) = -\lambda + \lambda^2\hbar \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{q^2+M^2} \frac{1}{(p_1+p_2-q)^2+M^2} + \lambda^2\hbar \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{q^2+M^2} \frac{1}{(p_1-p_3+q)^2+M^2} + \lambda^2\hbar \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{q^2+M^2} \frac{1}{(p_1-p_4+q)^2+M^2}. \tag{51}$$

This gives

$$\Gamma^{(4)}_E(p) = -\lambda + \frac{\lambda^2\hbar}{M} \left[-\frac{1}{(p_1+p_2)^2+4M^2} + \frac{1}{(p_1-p_3)^2+4M^2} + \frac{1}{(p_1-p_4)^2+4M^2} \right]. \tag{52}$$

The physical vertex function is given by $\Gamma^{(4)}(p)=\Gamma_E^{(4)}(ip)$, and the position space vertex function is given by

$$\Gamma^{(4)}(x_1,\ldots,x_4)=2\pi\int\frac{dp_1}{2\pi}\cdots\int\frac{dp_4}{2\pi}\delta(p_1+\cdots+p_4)\Gamma^{(4)}(p_1,\ldots,p_4)e^{i(p_1x_1+\cdots+p_4x_4)}. \tag{53}$$

One then obtains the effective action contribution

$$\int dx\left[-\frac{\lambda}{4!}\phi^4-\frac{\lambda^2\hbar}{4!\,M}\int dy\,G_{2M}(x-y)\phi^2(x)\phi^2(y)\right], \tag{54}$$

where

$$G_\mu(x)=Re\int\frac{dp}{2\pi}\frac{e^{ipx}}{p^2-\mu^2+i\epsilon}=\frac{1}{2\mu}\sin(\mu x)[\theta(-x)-\theta(x)] \tag{55}$$

is the real part of the $D=1$ Feynman propagator and $\theta(x)=1$ for $x>0$ and $\theta(x)=0$ for $x\leqslant 0$.

By going to the QM parameters via $\lambda\to\lambda/m^2$, $M\to\omega$, and $\phi\to\sqrt{m}q$, one obtains the following effective equations of motion:

$$0=\ddot{q}+\omega^2q+\frac{\lambda}{6m}q^3+\frac{\lambda\hbar}{4m^2\omega}q+\frac{\lambda^2\hbar}{6m^3\omega}q\int_{-\infty}^{\infty}d\tau\,G_{2\omega}(t-\tau)q^2(\tau)+O(\lambda^3\hbar). \tag{56}$$

This effective equation of motion can be solved perturbatively as

$$q(t)=q_{0,0}(t)+\sum_{m\geqslant 1,n\geqslant 0}\lambda^m\hbar^nq_{n,m}(t), \tag{57}$$

where $q_{0,0}(t)$ is the classical HO solution. The first and the second quantum correction will satisfy

$$\ddot{q}_{1,1}+\omega^2q_{1,1}=-\frac{1}{4m^2\omega}q_{0,0}, \tag{58}$$

$$\ddot{q}_{1,2}+\omega^2q_{1,2}=-\frac{1}{2m}q_{0,0}^2q_{1,1}-\frac{1}{4m^2\omega}q_{0,1}-\frac{1}{6m^3\omega}q_{0,0}\int_{-\infty}^{\infty}d\tau\,G_{2\omega}(t-\tau)q_{0,0}^2(\tau). \tag{59}$$

The solution (57) has a classical part given by

$$q_c=q_{0,0}+\lambda q_{0,1}+\lambda^2q_{0,2}+\cdots. \tag{60}$$

Up to the order of λ^2 the classical solution is given by

$$q_{0,0}=a\cos\omega t+b\sin\omega t, \tag{61}$$

$$q_{0,1}=a_1\cos 3\omega t+b_1\sin 3\omega t+(c_1t+e_1)\cos\omega t+(d_1t+f_1)\sin\omega t, \tag{62}$$

$$\begin{aligned}q_{0,2}=&\,a_2\cos 5\omega t+b_2\sin 5\omega t+(c_2t+c_2')\cos 3\omega t+(d_2t+d_2')\sin 3\omega t+(e_2t^2+e_2't+g_2)\cos\omega t\\&+(f_2t^2+f_2't+h_2)\sin\omega t,\end{aligned} \tag{63}$$

where $a=q_0$, $b=p_0/m\omega$ and the coefficients $a_k,b_k,\ldots$ are the homogeneous polynomials of a and b of the order $2k+1$, see Eqs. (A4) and (A5).

From (61) and (58) it follows that

$$q_{1,1} = \frac{t}{8m^2\omega^2}(b\cos\omega t - a\sin\omega t) - \frac{b}{8m^2\omega^3}\sin\omega t, \tag{64}$$

which coincides with the coherent state result

$$Q_{1,1} = \frac{1}{4m\omega}\left(\frac{\partial^2}{\partial a^2} + \frac{\partial^2}{\partial b^2}\right)q_{0,1}. \tag{65}$$

This is an expected result since the equations of motion coincide up to this order.

In order to solve the equation for $q_{1,2}$ we need to evaluate

$$\begin{aligned} I(t) &= \int_{-\infty}^{\infty} \mathrm{d}\tau G_{2\omega}(t-\tau)[a\cos(\omega\tau) + b\sin(\omega\tau)]^2 \\ &= \frac{\xi}{32\omega^2}[(b^2-a^2)\cos(2\omega t) - 2ab\sin(2\omega t) - 4(a^2+b^2)], \end{aligned} \tag{66}$$

where $\xi = \int_0^\infty \mathrm{d}x \sin x$. The divergent integral can be regularized by the formula

$$\int_0^\infty \mathrm{d}x\, e^{-\epsilon x + ix} = (\epsilon - i)^{-1}, \quad \epsilon > 0, \tag{67}$$

which in the $\epsilon \to 0$ limit gives $\xi = 1$. The solution will then have the form

$$q_{1,2} = (\gamma_2 t + \gamma_2')\cos 3\omega t + (\delta_2 t + \delta_2')\sin 3\omega t + (\epsilon_2 t^2 + \epsilon_2' t + \kappa_2)\cos\omega t + (\phi_2 t^2 + \phi_2' t + \chi_2)\sin\omega t, \tag{68}$$

see Eq. (A7).

The coherent state expectation value will give the correction of the form

$$\begin{aligned} Q_{1,2} = \frac{1}{4m\omega}\left(\frac{\partial^2}{\partial a^2} + \frac{\partial^2}{\partial b^2}\right)q_{0,2} &= (\tilde{c}_2 t + \tilde{c}_2')\cos 3\omega t + (\tilde{d}_2 t + \tilde{d}_2')\sin 3\omega t + (\tilde{e}_2 t^2 + \tilde{e}_2' t + \tilde{g}_2)\cos\omega t \\ &+ (\tilde{f}_2 t^2 + \tilde{f}_2' t + \tilde{h}_2)\sin\omega t, \end{aligned} \tag{69}$$

see Eq. (A6), which could in principle coincide with (68) if the corresponding coefficients were identical. However, by comparing (A6) to (A7) one can see that $q_{1,2} \neq Q_{1,2}$, and therefore there is a discrepancy at the order $\lambda^2\hbar$.

One can also try to obtain a nonperturbative in λ effective action equations of motion, which amounts to summing all the diagrams with different powers of λ at a fixed order in $\hbar$. This can be achieved by using the saddle point approximation in the path-integral formalism, see Ref. 36. This then boils down to evaluating the traces of D-dimensional differential operators. The drawback of this approach is that one can only obtain certain terms at a fixed order of $\hbar$, i.e., not the complete correction. The standard approximation is

$$\Gamma[\phi] \approx \int \mathrm{d}^D x\left[\frac{1}{2}(1+Z(\phi))(\partial_\mu\phi)^2 - \frac{1}{2}M^2\phi^2 - V_{\mathrm{eff}}(\phi)\right], \tag{70}$$

where V_{eff} is the effective potential. In the $D=1$ case one obtains at $O(\hbar)$,[15]

$$V_{\mathrm{eff}}(q) = V(q) + \frac{\hbar\omega}{2}\left(\sqrt{1 + \frac{V''(q)}{m\omega^2}} - 1\right), \quad Z(q) = \frac{\hbar}{32m^3}\frac{(V'''(q))^2}{\left(\omega^2 + \frac{V''(q)}{m}\right)^{5/2}}, \tag{71}$$

so that

$$\Gamma[q] \approx \int_{t_1}^{t_2} \mathrm{d}t \left[\frac{1}{2} m(1+Z(q))(\dot{q})^2 - \frac{1}{2} m\omega^2 q^2 - V_{\mathrm{eff}}(q) \right]. \tag{72}$$

The equations of motion coming from (72) are given by

$$0 = (1+Z)\ddot{q} + \frac{1}{2} Z'(q)(\dot{q})^2 + \omega^2 q + V'_{\mathrm{eff}}(q). \tag{73}$$

By using

$$V_{\mathrm{eff}}(q) = \lambda \frac{q^4}{4!} + \hbar\, \lambda \frac{q^2}{8m\omega} - \hbar\, \lambda^2 \frac{q^4}{64 m^2 \omega^3} + O(\lambda^3 \hbar), \tag{74}$$

$$Z(q) = \hbar\, \lambda^2 \frac{q^2}{32 m^3 \omega^5} + O(\lambda^3 \hbar), \tag{75}$$

(73) can be expanded in powers of λ and one can see that (73) agrees with (56) up to $O(\lambda\hbar)$. At $O(\lambda^2\hbar)$ there is a disagreement, reflecting the fact that there are other terms contributing at $O(\hbar)$ which we have not included in the approximation (72) (for example, $\int \mathrm{d}t\, A(q)(\dot{q})^4$ or nonlocal terms).

One can also compare the perturbative solutions, and it can be shown by using the techniques from the Appendix that the $O(\hbar\lambda^2)$ perturbative solution of (73) has a form

$$\tilde{q}_{1,2} = \tilde{\gamma}'_2 \cos 3\omega t + \tilde{\delta}'_2 \sin 3\omega t + (\tilde{\epsilon}_2 t^2 + \tilde{\epsilon}'_2 t + \tilde{\kappa}_2)\cos \omega t + (\tilde{\phi}_2 t^2 + \tilde{\phi}'_2 t + \tilde{\chi}_2)\sin \omega t, \tag{76}$$

which differs from the coherent state and the perturbative effective action results by the absence of the $t \cos 3\omega t$ and $t \sin 3\omega t$ terms.

VI. CONCLUSIONS

Comparing the effective action equations of motion (56) and (73) to the coherent state expectation value equation of motion (38) gives an agreement up to $O(\lambda\hbar)$. For the higher orders it is simpler to compare the solutions and we find that at $O(\lambda^2\hbar)$ there are discrepancies between all three approaches. Although all three solutions (68), (69), and (76) are linear combinations of $t^n \cos(2k+1)\omega t$ and $t^n \sin(2k+1)\omega t$ functions, the corresponding coefficients differ.

Note that the effective action perturbative solution (68) depends on a regularization dependent parameter ξ. However, the ξ-independent coefficients are different from the corresponding expectation value solution coefficients, see the Appendix. Hence the discrepancy cannot be explained as a regularization scheme artifact. Therefore the state whose EV gives the effective action trajectory is not the coherent state in the AHO case. This agrees with the assumption made in Ref. 16, where the effective action state was taken to be the ground state of the AHO with a source. The arguments for this state were first presented in Ref. 4.

The discrepancy between the perturbative effective action solution (68) and the perturbative effective potential solution (76) is simply due to the fact that the effective potential method is an approximation which did not take into account all possible terms which could contribute at a given order.

Although the formula (20) is valid for the coherent states, it can be used as an approximation for the field expectation value coming from the effective action. We expect that the expansion (20) can give the same result as the effective action in the case of two-dimensional integrable field theories. This happens in the case of the CGHS dilaton gravity model and the rationale is that the two-dimensional integrable field theories are closely related to the free-field theories, and for these the effective action and the coherent state expectation values give the same dynamics. In order to use formula (20) in the field theory case, one would have to extend the DQ formalism to the field theory case, see Ref. 37.

Our results imply that the coherent state expectation values define in general an alternative semiclassical dynamics to that coming from the effective action. The reason is that the effective action initial state is different from the coherent state in the case when the interactions are present. The coherent states expectation values could then be used as an approximation for the effective action trajectories, or one can obtain the exact trajectories in the situations where the system is prepared to be in the initial coherent state. The advantage of studying the semiclassical dynamics of coherent states is that one can obtain directly a semiclassical trajectory through computable $\hbar^n$ corrections to the classical one. In contrast, in the effective action case one has to obtain first the $\hbar^n$ corrections to the classical equations of motion, which can be only done approximately. Furthermore, the corresponding effective action equations of motion are nonlocal and difficult to solve nonperturbatively in the coupling constant.

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APPENDIX

The classical AHO equation of motion can be solved perturbatively via the expansion (60). One then obtains

$$Lq_{0,1} = -\frac{q_{0,0}^3}{6m}, \quad Lq_{0,2} = -\frac{q_{0,0}^2 q_{0,1}}{2m}, \ldots, \tag{A1}$$

where $L = \mathrm{d}^2/\mathrm{d}t^2 + \omega^2$. These equations can be solved by the method of undetermined coefficients for the forced HO equation of motion $Lq = f(t)$.

In order to solve the first two equations in (A1) we will need a particular solution for

$$f(t) = (At + A')\cos \Omega t + (Bt + B')\sin \Omega t.$$

It is given by

$$q(t) = \left(\frac{At + A'}{\omega^2 - \Omega^2} - \frac{2B\Omega}{(\omega^2 - \Omega^2)^2}\right)\cos \Omega t + \left(\frac{Bt + B'}{\omega^2 - \Omega^2} + \frac{2A\Omega}{(\omega^2 - \Omega^2)^2}\right)\sin \Omega t, \tag{A2}$$

for $\Omega \neq \omega$ and by

$$q(t) = \frac{1}{4\omega}\left(-Bt - 2B' + \frac{A}{\omega}\right)t \cos \omega t + \frac{1}{4\omega}\left(At + 2A' + \frac{B}{\omega}\right)t \sin \omega t, \tag{A3}$$

for $\Omega = \omega$.

By using formulas (A2) and (A3) we obtain (62) and (63). The initial conditions

$$q(0) = a, \quad \dot{q}(0) = \omega b$$

are imposed by requiring

$$q_{n,m}(0) = 0, \quad \dot{q}_{n,m}(0) = 0,$$

for $(n,m) \neq (0,0)$. These conditions determine the coefficients of the HO terms as

$$e_1 = -a_1, \quad f_1 = -\frac{c_1}{\omega}, \quad g_2 = -a_2 - c_2', \quad h_2 = -5b_2 - \frac{c_2 + e_2'}{\omega},$$

etc.

One then obtains

$$q_{0,1} = \frac{1}{192m\omega^2}\{a(a^2-3b^2)\cos 3\omega t - b(b^2-3a^2)\sin 3\omega t + [-a^3+3ab^2+12b(a^2+b^2)\omega t]\cos \omega t + [21a^2b+9b^3+4a(a^2+b^2)\omega t]\sin \omega t\}, \tag{A4}$$

and

$$q_{0,2} = \frac{1}{36\,864m^2\omega^4}\{(a^5-10a^3b^2+5ab^4)\cos 5\omega t - 12[2a^5-15a^3b^2-(9a^4b+6a^2b^3-3b^5)\omega t]\cos 3\omega t + [23a^5-170a^3b^2-113ab^4-48b(7a^4+19a^2b^2+8b^4)\omega t - 72a(a^2+b^2)^2\omega^2t^2]\cos \omega t + (b^5-10a^2b^3+5a^4b)\sin 5\omega t + [132a^4b+12a^2b^3+48b^5-(36a^5-72a^3b^2-108ab^4)\omega t]\sin 3\omega t + [599a^4b+854a^2b^3+271b^5+(96a^5+528a^3b^2+240ab^4)\omega t + (72a^4b-144a^2b^3-72b^5)\omega^2t^2]\sin \omega t\}. \tag{A5}$$

The coherent state expectation value is then obtained from (20). This gives (64) and

$$Q_{1,2} = \frac{1}{6144m^3\omega^5}\{[24(3a^2b-b^3)\omega t+99ab^2-5a^3]\cos 3\omega t - [63a^2b-41b^3+24(a^3-3ab^2)\omega t]\sin 3\omega t + [5a^3-99ab^2-396b(a^2+b^2)\omega t - 72a(a^2+b^2)\omega^2t^2]\cos \omega t + [27b(19a^2+11b^2)+4a(31a^2+63b^2)\omega t - 72b(a^2+b^2)\omega^2t^2]\sin \omega t\}. \tag{A6}$$

The $O(\hbar\lambda^2)$ correction from the effective action equation of motion (56) can be obtained by solving

$$Lq_{1,2} = -\frac{1}{2m}q_{0,0}^2q_{1,1} - \frac{1}{4m\omega^2}q_{0,1} + \frac{\xi}{96m^3\omega^2}\left(2a^2+2b^2+\frac{a^2-b^2}{2}\cos 2\omega t + ab\sin \omega t\right)q_{0,0},$$

where ξ is a regularization dependent constant. The Cauchy problem solution will have the form (68), and the ξ independent coefficients are γ_2, δ_2, ϵ_2, and ϕ_2. For $\xi=1$ one obtains

$$q_{1,2} = \frac{1}{3072m^3\omega^5}\{[27ab^2-5a^3+6(3a^2b-b^3)\omega t]\cos 3\omega t + [11b^3-21a^2b+6(3ab^2-a^3)]\sin 3\omega t + [5a^3-27ab^2-6b(21a^2+25b^2)\omega t - 24a(a^2+b^2)\omega^2t^2]\cos \omega t + [3b(57a^2+41b^2)+2a(31a^2+51b^2)\omega t - 24b(a^2+b^2)\omega^2t^2]\sin \omega t\}. \tag{A7}$$

We have checked the results (A4)–(A7) by using the MATHEMATICA program.[38]

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Minimally disturbing Heisenberg–Weyl symmetric measurements using hard-core collisions of Schrödinger particles

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In a previous paper we have presented a general scheme for the implementation of symmetric generalized measurements (POVMs) on a quantum computer. This scheme is based on representation theory of groups and methods to decompose matrices that intertwine two representations. We extend this scheme in such a way that the measurement is minimally disturbing, i.e., it changes the state vector $|\Psi\rangle$ of the system to $\sqrt{\Pi}|\Psi\rangle$ where Π is the positive operator corresponding to the measured result. Using this method, we construct quantum circuits for measurements with Heisenberg–Weyl symmetry. A continuous generalization leads to a scheme for optimal simultaneous measurements of position and momentum of a Schrödinger particle moving in one dimension such that the outcomes satisfy $\Delta x \Delta p \geqslant \hbar$. The particle to be measured collides with two probe particles, one for the position and the other for the momentum measurement. The position and momentum resolution can be tuned by the entangled joint state of the probe particles which is also generated by a collision with hard-core potential. The parameters of the POVM can then be controlled by the initial widths of the wave functions of the probe particles. We point out some formal similarities and differences to simultaneous measurements of quadrature amplitudes in quantum optics. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2222080]

I. INTRODUCTION

The question of how to implement quantum measurements is an important issue of quantum information theory. Even though the standard model of quantum computers uses only 1 qubit measurements in the computational basis at the end or during the computation,[1] other measurements are also relevant for quantum information for several reasons.

In quantum computing, models have been proposed where collective measurements on more than 1 qubit are necessary.[2] In Ref. 3 a quantum algorithm is described which uses even more general measurements than the usual von Neumann measurements, i.e., they are not described by a family of mutually orthogonal projections but by a so-called positive operator-valued measure (POVM).

In noncomputing applications of quantum information theory, like future nanoscience, it may, for instance, be useful to implement approximative simultaneous measurements of observables which are actually incompatible when measured accurately. An important example would be the position and the momentum of a Schrödinger particle.

The implementation of generalized measurements is not trivial since this is also true for the smaller class of von Neumann measurements.[4] Even though it is known that it is in principle possible to reduce every POVM measurement to a von Neumann measurement on an extended

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quantum system it is little known so far about how to realize the required transformation by physical processes, particularly when the implementation should disturb the quantum state in a minimal way. In Refs. 5 and 6 the class of POVMs is described which can be measured using linear optics. Some special POVM measurements on low-dimensional spaces are described in Refs. 7–12.

In Ref. 13 we have described a general design principle to implement symmetric POVMs on a quantum register where universal quantum computation capabilities are available. However, these implementations are not minimally disturbing.

Here we describe an extension of the theory of Ref. 13 such that the symmetric measurements disturb the state in a minimal way and apply it to the Heisenberg–Weyl group in finite dimensions. Since the latter actually defines a *family* of groups it is desirable to have an implementation which is efficient in the sense that its running time scales polynomially in the logarithm of the dimension, i.e., with the number of qubits. We show that this can indeed be achieved for Heisenberg–Weyl groups with a power of 2 as dimension.

We then adapt the implementation scheme to the continuous situation. The corresponding POVM provides a good example for a measurement where the feature of minimal disturbance makes sense: Given the motivation to measure position and momentum of a particle in order to monitor its motion one would clearly try to avoid disturbance as far as possible.

The general idea of the paper is to show that the finite dimensional circuits provide a paradigm for the continuous variable implementation. By replacing the finite dimensional gates with appropriate analogs, we also obtain a possible measurement scheme even though it is not *a priori* clear how the required "gates" could be implemented physically. However, we show that a modification of the gate sequence could in principle be realized by three hard-core scattering processes. This kind of idealized scattering is not unphysical since hard-core potential can be a useful approximation in many real collision processes.

We proceed as follows. In Sec. II we recapitulate the definition of POVMs and recall a general scheme for the implementation of general measurements by orthogonal measurements. In Sec. III we define the symmetry of POVMs and present a method for designing measurement algorithms for symmetric POVMs. In Sec. IV we consider the implementation for two special classes of POVMs to illustrate the latter. Explicitly, we consider POVMs on qubits with cyclic symmetry groups and POVMs on d-dimensional quantum systems with Heisenberg–Weyl symmetry. In Sec. V we convert the implementation to quantum systems with Hilbert spaces of infinite dimension and describe a potential realization by scattering processes on an abstract level. In Sec. VI we compare this scheme to a quantum optical implementation of simultaneous measurements for the quadrature amplitudes.

II. MINIMALLY DISTURBING IMPLEMENTATION BY VON NEUMANN MEASUREMENTS

In this section we briefly outline a general scheme[1] for the minimally disturbing implementation of a POVM. Consider a quantum system with Hilbert space $\mathbb{C}^d$. A POVM consists of n operators $\Pi_j \in \mathbb{C}^{d\times d}$ with $\Pi_j \geqslant 0$ and $\Sigma_j \Pi_j = I_d$, where I_d denotes the identity matrix of size $d\times d$. A definition for POVMs on infinite dimensional quantum systems and an infinite number of results can be found in Ref. 14. In Sec. V we use this more general definition but here we start with finite POVMs since we consider implementation schemes on *quantum computers* at first. Following Refs. 15 and 16 we define:

Definition 1 (Minimally disturbing measurement): Let (Π_j) *be a POVM. Then a measurement is called minimally disturbing if it changes the state vector according to*

$$|\Psi\rangle \mapsto \frac{\sqrt{\Pi_j}|\Psi\rangle}{\|\sqrt{\Pi_j}|\Psi\rangle\|},$$

given that the measurement result is j.

The motivation for this definition is given by a theorem in Ref. 15 stating that the above type of measurements maximizes the average fidelity between the input and the output state if the input is drawn from a uniformly distributed ensemble of pure states.

The following lemma[1] reduces the implementation of this kind of measurements to von Neumann measurements (with Lüder's projection postulate) in the standard basis.

Lemma 2 (Reduction of a POVM to a von Neumann measurement): Let P be a POVM with the n operators $\Pi_j \in \mathbb{C}^{d\times d}$. *Furthermore, let* $\mathbb{C}^n$ *be the Hilbert space of an ancilla that is initialized with* $|0\rangle$. *Then, a minimally disturbing measurement of P can be achieved by a measurement in the standard basis of the ancilla after the implementation of a unitary* $U \in \mathbb{C}^{dn\times dn}$ *satisfying the equation*

$$U(|0\rangle \otimes |\Psi\rangle) = \sum_{j=0}^{n-1} |j\rangle \otimes \sqrt{\Pi_j}|\Psi\rangle. \tag{1}$$

Equation (1) states that U is a unitary extension of the matrix

$$M := \sum_j |j\rangle \otimes \sqrt{\Pi_j} = (\sqrt{\Pi_1}, \sqrt{\Pi_2}, \ldots, \sqrt{\Pi_n})^T \in \mathbb{C}^{dn\times d}, \tag{2}$$

which is defined by P. In the following section we consider this extension for symmetric POVMs. In some cases, the following observations help to show that a unitary U implements a POVM in a minimally disturbing way:

Lemma 3 (Linear assignment of Kraus operators): Let $U \in \mathbb{C}^{dn\times dn}$ *be a unitary operating on a bipartite system which is initialized with* $|\Phi\rangle \otimes |\Psi\rangle$ *where* $|\Phi\rangle \in \mathbb{C}^n$ *and* $|\Psi\rangle \in \mathbb{C}^d$. *Let the first component be measured in the standard basis after the joint system has been subjected to the unitary U*. *Then the conditional postmeasurement state is pure*.

Let $A_{U,\Phi,j}$ *be the Kraus operator describing the corresponding state change*

$$|\Psi\rangle \mapsto \frac{A_{U,\Phi,j}|\Psi\rangle}{\|A_{U,\Phi,j}|\Psi\rangle\|},$$

where j is the measurement result. For each U and *j*, *the mapping* $|\Phi\rangle \mapsto A_{U,\Phi,j}$ *is linear*.

The proof is straightforward since the projected state of the composed system is a product state and the map given by the partial trace is linear. We find:

Corollary 4 (Minimally disturbing Kraus operators): *Let P be a POVM with operators* Π_j. *Furthermore, let U*, $|\Phi\rangle$, *and* $A_{U,\Phi,j}$ *be as defined in Lemma 3. If the equation*

$$A_{U,\Phi,j} = \sqrt{\Pi_j}$$

holds for all j then U gives rise to a minimally disturbing measurement of P. *In other words*, *whenever* $A_{U,\Phi,j}$ *is positive for each j*, *it defines a minimally disturbing measurement for the POVM given by*

$$\Pi_j := A_{U,\Phi,j}^2.$$

III. IMPLEMENTATION OF SYMMETRIC POVMS

In this section we analyze how the symmetry of a POVM can be used for the implementation scheme of Lemma 2. Here, we follow the approach of Ref. 13 where we have obtained a general implementation scheme for POVMs without consideration of the disturbance of the measurement process. This implementation scheme also relies on the unitary extension of a matrix that is defined by the POVM operators. It turned out that the symmetry of the POVM leads to a symmetry of the matrix which can be exploited for the extension. In this section we show that a similar construction is possible for the minimally disturbing implementation of POVMs.

To begin with, we define the symmetry of POVMs:

Definition 5 (Symmetric POVMs): Let $\sigma: G \to \mathbb{C}^{d\times d}$ *be a unitary representation of a finite group* G. *A POVM with operators* $\Pi_0, \ldots, \Pi_{n-1}$ *is called* (σ, π) *symmetric if there is a permutation representation* $\pi: G \to S_n$ *of the indices such that*

$$\sigma(g)\Pi_j\sigma(g)^\dagger = \Pi_{\pi(g)j}.$$

Here, S_n *denotes the symmetric group consisting of all permutations of n objects.*

As mentioned above, the symmetry of a matrix is a useful tool for the implementation of POVMs. Here we define the symmetry of a matrix as in Refs. 17–19.

Definition 6 (Matrices with symmetry and intertwining spaces): Let G *be a finite group and* $\sigma: G \to \mathbb{C}^{m\times m}$ *as well as* $\tau: G \to \mathbb{C}^{n\times n}$ *be unitary representations. A matrix* $A \in \mathbb{C}^{m\times n}$ *is* (σ, τ) *symmetric if it satisfies*

$$\sigma(g)A = A\tau(g)$$

for all $g \in G$. *We also write* $\sigma M = M\tau$ *for the* (σ, τ) *symmetry. We call the set*

$$\mathrm{Int}(\sigma, \tau) = \{A \in \mathbb{C}^{m\times n} : \sigma A = A\tau\}$$

of all such matrices the intertwining space of σ *and* τ.

The structure of the intertwining space of two representations can be easily specified if both representations are decomposed into a direct sum of irreducible representations of the group as the following lemma[19] shows:

Lemma 7 (Structure of intertwining space): Let σ *and* τ *be decomposed into the direct sums*

$$\sigma = \bigoplus_j (I_{m_j} \otimes \kappa_j) \text{ and } \tau = \bigoplus_j (I_{n_j} \otimes \kappa_j)$$

of different irreducible representations κ_j *of the group* G. *Then*

$$\mathrm{Int}(\sigma, \tau) = \bigoplus_j (\mathbb{C}^{m_j\times n_j} \otimes I_{\deg(\kappa_j)})$$

where $\deg(\kappa_j)$ *denotes the degree of* κ_j. *For* $m_j = 0$ *and* $n_j = 0$ *we insert* $n_j \deg(\kappa_j)$ *zero columns or* $m_j \deg(\kappa_j)$ *zero rows, respectively.*

The key observation used for the extension of the matrix M from Eq. (2) to a unitary is that the symmetry of a POVM leads to a matrix M with symmetry. This is summarized in the following lemma which can be proved by direct calculation:

Lemma 8 (Symmetry of a POVM and its matrix): If the POVM with operators $\Pi_1, \ldots, \Pi_n$ *is* (σ, π) *symmetric then the corresponding matrix* M *is* $(\sigma_\pi \otimes \sigma, \sigma)$ *symmetric with the permutation matrix representation* $\sigma_\pi(g) = \Sigma_j |\pi(g)j\rangle\langle j|$.

The following theorem explicitly shows how the $(\sigma_\pi \otimes \sigma, \sigma)$ symmetry of M can be extended to a $(\sigma_\pi \otimes \sigma, \sigma \oplus \widetilde{B}^\dagger \sigma' \widetilde{B})$ symmetry of U where σ' is an appropriate representation and $\widetilde{B}$ a unitary.

Theorem 9 (Implementation of symmetric POVMs): Let M *be the matrix of Eq. (2) for a* (σ, π) *symmetric POVM with symmetry group* G. *Let* A *and* B *be transformations that decompose* $\sigma_\pi \otimes \sigma$ *and* σ *into irreducible representations, respectively. Then there is a representation* σ' *of* G *such that* $B\sigma B^\dagger \oplus \sigma'$ *is equal to* $A(\sigma_\pi \otimes \sigma)A^\dagger$ *up to a permutation of the irreducible components. Furthermore, there is a transformation* $W \in \mathrm{Int}[A(\sigma_\pi \otimes \sigma)A^\dagger, B\sigma B^\dagger \oplus \sigma']$ *which is a unitary extension of* $AMB^\dagger$. *Then*

$$U := A^\dagger W(B \oplus \widetilde{B})$$

implements the POVM for every unitary $\widetilde{B}$. *The unitary* U *is* $(\sigma_\pi \otimes \sigma, \sigma \oplus \widetilde{B}\sigma'\widetilde{B}^\dagger)$ *symmetric.*

Proof: We decompose $\sigma_\pi \otimes \sigma$ and σ with the unitaries $A \in \mathbb{C}^{dn\times dn}$ and $B \in \mathbb{C}^{d\times d}$, i.e., we obtain the equations

$$A(\sigma_\pi \otimes \sigma)A^\dagger = \bigoplus_j (I_{m_j} \otimes \kappa_j) \quad \text{and} \quad B\sigma B^\dagger = \bigoplus_j (I_{n_j} \otimes \kappa_j).$$

Therefore, the equation

$$\left[\bigoplus_j (I_{m_j} \otimes \kappa_j)\right] AMB^\dagger = AMB^\dagger \left[\bigoplus_j (I_{n_j} \otimes \kappa_j)\right]$$

holds. Following Lemma 7 the matrix $N := AMB^\dagger$ has the decomposition

$$N = \bigoplus_j (A_j \otimes I_{d_j})$$

with $A_j \in \mathbb{C}^{m_j \times n_j}$ and $d_j := \deg(\kappa_j)$. From Theorem 5 of Ref. 13 it follows that $B\sigma B^\dagger$ can be extended to $A(\sigma_\pi \otimes \sigma)A^\dagger$, i.e., the representations $A(\sigma_\pi \otimes \sigma)A^\dagger$ and $B\sigma B^\dagger \oplus \sigma'$ with

$$\sigma' = \bigoplus_j (I_{m_j - n_j} \otimes \kappa_j)$$

are equal up to a permutation of the irreducible components. We choose a unitary extension $W \in \mathrm{Int}[A(\sigma_\pi \otimes \sigma)A^\dagger, B\sigma\widetilde{B} \oplus \sigma']$ of N. This extension can be achieved by appending appropriate columns to the right side of N since the matrix N has orthogonal columns. We can write $W = (N|\widetilde{N})$ for this extension if we denote the new columns by $\widetilde{N}$. With this matrix we obtain for an arbitrary unitary $\widetilde{B} \in \mathbb{C}^{n(d-1)\times n(d-1)}$ the unitary extension

$$A^\dagger(N|\widetilde{N})(B \oplus \widetilde{B}) = (M|A^\dagger \widetilde{N}\widetilde{B})$$

of M. □

As shown in the following section, the unitary W of Theorem 9 can be chosen to be sparse for some POVMs. Within the standard model of quantum computing, this can be used for obtaining efficient decompositions into elementary gates for the cases discussed in the next section. Furthermore, there are methods known to decompose the transformations A and $B \oplus \widetilde{B}$ into products of simpler matrices.[17–19]

IV. EXAMPLES

In this section we explicitly construct quantum circuits and implementation schemes for the minimally disturbing implementation of two families of symmetric POVMs. First, we introduce the following notations: For $m \in \mathbb{N}$ define $\omega_m := \exp(-2\pi i/m)$ and let

$$X_m := \sum_{j=0}^{m-1} |(j+1) \bmod m\rangle\langle j| \in \mathbb{C}^{m\times m}$$

be the cyclic shift of the basis vectors of an m-dimensional space. Furthermore, define the diagonal phase matrix

$$Z_m := \sum_{j=0}^{m-1} \omega_m^j |j\rangle\langle j| \in \mathbb{C}^{m\times m}$$

and the Fourier transform

$$F_m := \sqrt{\frac{1}{m}} \sum_{j,k=0}^{m-1} \omega_m^{jk} |j\rangle\langle k| \in \mathbb{C}^{m\times m}.$$

We obtain the equalities $F_m X_m F_m^\dagger = Z_m$ and $Z_m X_m = \omega_m X_m Z_m$ which we will use in the following without proof.

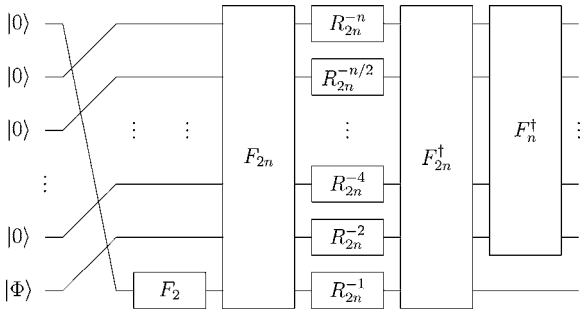

FIG. 1. Circuit for the implementation of POVMs with cyclic symmetry group C_{2^m} on a qubit. The circuit operates on $m+1$ qubits. On the right side the upper m qubits are measured in the standard basis.

A. Cyclic groups

Simple examples for our implementation scheme are POVMs operating on a qubit with a cyclic symmetry. Measurements with cyclic symmetry can, for instance, provide an estimation of time when applied to a dynamical quantum system. The reason for this is that the time evolution of a quantum system with energy eigenvalues being rational multiples of each other is periodic and the dynamics is therefore a unitary representation of SO(2). This leads naturally to the finite cyclic groups after discretization.

Fix $n \geqslant 2$. We consider the cyclic group $C_n = \langle r : r^n = 1 \rangle$ with n elements, the unitary matrix representation $\sigma : C_n \to \mathbb{C}^{2\times 2}$ with $\sigma(j) = R_n^j$ for

$$R_n := \begin{pmatrix} 1 & 0 \\ 0 & \omega_n \end{pmatrix} \in \mathbb{C}^{2\times 2}, \tag{3}$$

and the orbit of the vector $\sqrt{1/n}(1,1)^T \in \mathbb{C}^2$ with respect to this representation of C_n. We have the POVM operators

$$\Pi_j := \frac{1}{n}\begin{pmatrix} 1 & 0 \\ 0 & \omega_n^j \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & \omega_n^{-j} \end{pmatrix} = \frac{1}{n}\begin{pmatrix} 1 & \omega_n^{-j} \\ \omega_n^j & 1 \end{pmatrix} \tag{4}$$

for $j \in \{0, \ldots, n-1\}$.

Applying the methods discussed in Sec. III we obtain the following unitary for the minimally disturbing implementation of the POVM with cyclic symmetry:

Theorem 10 (Implementation of POVMs with cyclic symmetry): *The POVM with the operators of Eq. (4) can be implemented by the unitary*

$$U := (F_n^{\dagger} \otimes I_2) X_{2n}^{\dagger} (I_n \otimes F_2) K^{\dagger} \in \mathbb{C}^{2n\times 2n}$$

where K denotes the permutation matrix which is defined by

$$K|2j\rangle = |j\rangle \quad \text{and} \quad K|2j+1\rangle = |n+j\rangle.$$

The rather technical proof can be found in the Appendix. The idea is as follows: The transformation A must diagonalize the cyclic shift $X_n \otimes I_2$. This can be achieved by $F_n^{\dagger} \otimes I_2$. Furthermore, we need the cyclic shift $X_{2n}^{\dagger}$ to obtain the correct order of the irreducible representations. The transformation B is trivial since σ is already diagonal. The remaining transformation $(I_n \otimes F_2)K^{\dagger}$ is the sparse matrix in the intertwining space.

If n is a power of 2 the ancilla system can be a qubit register and the unitary of Theorem 10 can be implemented efficiently as the following corollary states.

Corollary 11 (Circuits for cyclic POVM): For $n = 2^m$, $m \geqslant 1$, the unitary U of Theorem 10 can be implemented efficiently with the circuit of Fig. 1.

Proof: Since Fourier transforms can be implemented with a polynomial number[1,20] of elemen-

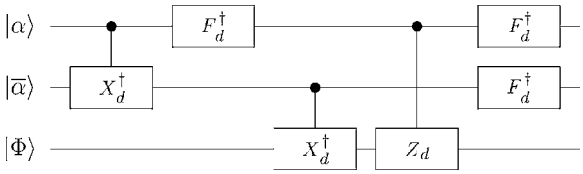

FIG. 2. Schematic circuit for the POVM with Heisenberg–Weyl symmetry. The basis state $|j\rangle$ of the control wire causes the implementation of the jth power of the controlled operation. On the right side of the circuit the two upper systems are measured in the standard basis.

tary gates, i.e., 1 and 2 qubit gates, $F_n^\dagger \otimes I_2$ can be implemented efficiently. Furthermore, the cyclic shift $X_{2n}^\dagger$ can be written as $X_{2n}^\dagger = F_{2n}^\dagger Z_{2n}^\dagger F_{2n}$ with

$$Z_{2n}^\dagger = R_{2n}^{-n} \otimes R_{2n}^{-n/2} \otimes \ \ldots \ \otimes R_{2n}^{-1}.$$

The unitary K is only a cyclic shift of qubits. □

B. Heisenberg–Weyl groups

The operators X_d and Z_d are discrete analogs of translations in position and momentum space. If $\mathbb{C}^d$ denotes the d possible positions of a particle on a cyclic chain, the eigenvectors of Z_d can be interpreted as positions eigenstates and the eigenvectors of X_d as eigenvectors of crystal momentum.[21] As for continuous quantum systems these observables are incompatible and it can be desirable to have approximative simultaneous measurements such that the result can be interpreted as a point in $2d$-dimensional "phase space." In Sec. V we discuss the continuous analog.

The basis of simultaneous measurements of position and momentum are POVMs with Heisenberg–Weyl symmetry. For all $d \geqslant 2$, the Heisenberg–Weyl group is given by $G = \langle X_d, Z_d \rangle$ and has order d^3. For a positive operator μ with $\mathrm{tr}(\mu) = 1/d$ we consider the POVM with the d^2 operators

$$Z_d^k X_d^j \mu X_d^{-j} Z_d^{-k} \quad \text{for } k,j = 0, \ldots, d-1. \tag{5}$$

The following theorem shows how to implement this type of POVMs:

Theorem 12 (POVMs with Heisenberg–Weyl symmetry): *Given the Heisenberg–Weyl POVM P with the d^2 operators from Eq. (5) with $\mu := |\alpha\rangle\langle\alpha|/d$ for some state vector $|\alpha\rangle$. Then P can be implemented by the circuit in Fig. 2 where the inputs of the ancillas are given by $|\alpha\rangle \otimes |\overline{\alpha}\rangle$ with the complex conjugated wave function $\overline{\alpha}$. For general μ the ancilla input has to be replaced with the state vector*

$$|\gamma\rangle := \sqrt{d} \sum_{j,k=0}^{d-1} \sqrt{\mu}_{jk} |j\rangle \otimes |k\rangle \in \mathbb{C}^{d^2},$$

where $\sqrt{\mu}_{jk}$ denotes the entry of $\sqrt{\mu}$ in the jth row and kth column.

The proof of the theorem can be found in the Appendix. In the following we briefly sketch the main points of the proof. For the decomposition of $\sigma_\pi \otimes \sigma$ we observe that the permutation π given by the action of the Heisenberg–Weyl group on the operators is a translation in the finite plane $(\mathbb{Z}/d\mathbb{Z})^2$. This translation is diagonalized by the inverse Fourier transform $F_d^\dagger \otimes F_d^\dagger \otimes I_d$ at the end of the circuit in Fig. 2. This transformation already block diagonalizes $\sigma_\pi \otimes \sigma$. However, the irreducible components are only equivalent, but not equal, to σ. We apply the controlled Z and controlled $X^\dagger$ operations to obtain equality. Hence, these operations correspond to the matrix A. The matrix B is trivial since σ is an irreducible representation. The unitary extension W used in Theorem 12 is decomposed into two components. One component is given by the first two gates of the circuit in Fig. 2, the other is absorbed into the preparation procedure for the initial state.

As already stated, we can efficiently implement F_d by elementary gates on a qubit register. We also obtain efficient implementations of controlled X and Z gates by concatenations of controlled

R_d gates as defined in Eq. (3). Hence, we can implement the POVM with initial operator $\mu = |\alpha\rangle\langle\alpha|/d$ efficiently if the same is true for the preparation of the states $|\alpha\rangle$ and $|\bar{\alpha}\rangle$.

V. CONTINUOUS MEASUREMENTS

Here we want to address how to implement Heisenberg–Weyl symmetric POVMs for continuous quantum systems such that we have also minimal disturbance. For a detailed mathematical description of such POVMs we refer also to Refs. 22 and 23.

The continuous degree of freedom can either be a Schrödinger wave of a quantum particle moving on a line (where the Heisenberg–Weyl group formalizes translations in position and momentum space) or a quantum optical light mode (where the translations shift the quadrature amplitudes). The most natural representation of the Hilbert space of a particle in one dimension is $\mathcal{H} := L^2(\mathbb{R})$, the space of square integrable functions over the real line. For a light mode, it is often more appropriate to choose the isomorphic Hilbert space $l^2(\mathbb{N}_0)$ of square-summable sequences. In this section, we will focus on Schrödinger particles since simultaneous measurements of quadrature amplitudes in quantum optics have already been implemented.[24] We will compare our implementation to the latter in the next section.

We first describe the continuous analogs of the "gates" in Fig. 2 and show that their concatenation leads indeed to a correct implementation. Later we will discuss a modification of the scheme which can be implemented by hard-core scattering processes. The description below refers to the Schrödinger representation where the position operator X, defined on a dense subspace of $\mathcal{H}$, is the multiplication operator

$$X\psi(x) := x\psi(x).$$

The momentum operator is

$$P\psi(x) := -i\frac{d}{dx}\psi(x),$$

where we have chosen the units such that $\hbar = 1$. Following Sec. 3.4 of Ref. 14 (with a slight modification of the sign) we introduce a family $(U_{s,t})$ of unitaries

$$(U_{s,t}\psi)(x) := e^{-ixs}\psi(x-t),$$

which formalize shifts in momentum and position space. These unitaries define a measurement by the positive operators

$$\Pi_{s,t} := \frac{1}{2\pi}U_{s,t}|\alpha\rangle\langle\alpha|U_{s,t}^{\dagger},$$

where $|\alpha\rangle \in \mathcal{H}$ is a wave function which is sufficiently localized in momentum and position space. The probability density for the result (s,t) is $\mathrm{tr}(\rho\Pi_{s,t})$ if the system state is described by the density operator ρ. The outcome (s,t) is interpreted as momentum s and position t of the particle in a "coarse grained phase space." We can clearly generalize the POVM above by replacing $|\alpha\rangle\langle\alpha|/(2\pi)$ with any operator μ having trace $1/(2\pi)$.

In agreement with the discussions of finite POVMs in the preceding sections we want to implement the POVM in such a way that the state changes according to

$$\rho \mapsto \frac{\sqrt{\Pi_{s,t}}\rho\sqrt{\Pi_{s,t}}}{\mathrm{tr}(\Pi_{s,t}\rho)},$$

given that the measurement outcome is (s,t).

Now we describe how to find a continuous analog of the circuit in Fig. 2. The system Hilbert space $(\mathbb{C}^d)^{\otimes 3}$ is replaced by $\mathcal{H}^{\otimes 3}$, i.e., in additional to the particle to be measured one uses two

particles in one dimension as an ancilla system. The final von Neumann measurement is a position measurement on both ancillas. (One could also use the remaining two dimensions of a particle in three dimensions as an ancilla system.)

The continuous analogs of the required gates are as follows. The discrete Fourier transform (whose inverse is occurring three times in Fig. 2) is replaced with the continuous unitary Fourier transform

$$(F\psi)(x) = \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} e^{-ixy}\psi(y)\mathrm{d}y. \tag{6}$$

The controlled cyclic shift is replaced by a unitary Y describing controlled translations on the real line. It acts on the wave function ψ of two particles according to

$$(Y\psi)(x,y) = \psi(x,y-x), \tag{7}$$

since this transformation would correspond to the transformation

$$|x\rangle \otimes |y\rangle \mapsto |x\rangle \otimes |x+y\rangle,$$

if such position eigenstates $|x\rangle$ and $|y\rangle$ existed. Conjugating Y with the Fourier transform on the second tensor component makes it more apparent that it is indeed a unitary map since we obtain then the multiplication operator

$$V := [(I\otimes F)Y(I\otimes F^{\dagger})\psi](x,y) = e^{-ixy}\psi(x,y). \tag{8}$$

Here I denotes the identity operator on $\mathcal{H}$. The unitary in Eq. (8) is the straightforward generalization of the controlled phase-shift operation that is the fourth gate in Fig. 2. The following theorem shows that the above described replacements provide in fact the desired measurement procedure:

Theorem 13: *Replace the gates in Fig. 2 with their continuous analogs as follows:*

(1) *Set the inverse of the continuous unitary Fourier transform given by Eq. (6) instead of* $F_d^{\dagger}$;
(2) *Set the inverse of Y given in Eq. (7) instead of the controlled* $X_d^{\dagger}$ *gate*; and
(3) *Set V as given by Eq. (8) instead of the controlled* Z_d *gate*.

Let μ *be an arbitrary positive operator with* $\mathrm{tr}(\mu)=1/(2\pi)$ *and the two ancilla systems be in the state* γ *with*

$$|\gamma\rangle := \sum_{j=0}^{\infty} \sqrt{\lambda_j}|\alpha_j\rangle \otimes |\bar{\alpha}_j\rangle, \tag{9}$$

where $|\alpha_j\rangle$ *is an eigenvector basis of* μ *such that*

$$2\pi\mu = \sum_j \lambda_j |\alpha_j\rangle\langle\alpha_j|.$$

Then the resulting transformation on $\mathcal{H}^{\otimes 3}$ *implements a minimally disturbing measurement for the POVM*

$$\Pi_{s,t} := U_{s,t}\mu U_{s,t}^{\dagger},$$

when followed by position measurements on both ancillas at the end and interpreting the position of the first particle in Fig. 2 as t and the position of the second as s.

Proof: Due to Lemma 3 and its corollary it is sufficient to restrict the attention to rank-one operators $\mu := |\alpha\rangle\langle\alpha|/(2\pi)$ and show that the unnormalized output state coincides with the desired state. The linearity argument holds also if μ is an infinite series since one can check that the map

$$\Phi \mapsto A_{U,\Phi,j}$$

is continuous with respect to the topologies induced by the Hilbert space norm and the operator norm, respectively. This is seen from

$$\|\Phi\|^2 = \mathrm{tr}(A^\dagger_{U,\Phi,j} A_{U,\Phi,j}) \leqslant \|A^\dagger_{U,\phi,j} A_{U,\Phi,j}\| = \|A_{U,\Phi,j}\|^2.$$

The whole "circuit" creates some wave function $\tilde{\Psi} \in \mathcal{H}^{\otimes 3}$. After measuring t and s we obtain an unnormalized conditional state vector given by the wave function

$$z \mapsto \tilde{\Psi}(t,s,z) := \tilde{\Psi}_{t,s}(z).$$

We want to show that it satisfies

$$|\tilde{\Psi}_{t,s}\rangle = \sqrt{\Pi_{s,t}}|\Psi\rangle = \sqrt{\frac{1}{2\pi}} U_{s,t}|\alpha\rangle\langle\alpha|U^\dagger_{s,t}\Psi\rangle.$$

This means explicitly that

$$\tilde{\Psi}_{t,s}(z) = \sqrt{\frac{1}{2\pi}} e^{-izs}\alpha(z-t)\int_{-\infty}^{\infty} \bar{\alpha}(u-t)e^{ius}\Psi(u)\mathrm{d}u. \tag{10}$$

Now we calculate the effect of the circuit starting with the joint state

$$\alpha(x)\bar{\alpha}(y)\Psi(z),$$

where Ψ is the wave function of the measured particle. First, we apply the controlled inverse translation and obtain

$$\alpha(x)\bar{\alpha}(y+x)\Psi(z).$$

The inverse Fourier transform changes this state to

$$\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} e^{iux}\alpha(u)\bar{\alpha}(y+u)\Psi(z)\mathrm{d}u.$$

The second controlled inverse shift followed by the controlled phase yields

$$\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} e^{iux}\alpha(u)\bar{\alpha}(y+u)e^{-ixz}\Psi(z+y)\mathrm{d}u.$$

After applying the inverse Fourier transform to both ancilla registers we obtain

$$\sqrt{\frac{1}{8\pi^3}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{iyw}e^{ixv}e^{iuv}\alpha(u)\bar{\alpha}(w+u)e^{-ivz}\Psi(z+w)\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w.$$

We simplify this term into

$$\sqrt{\frac{1}{8\pi^3}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{iyw}e^{i(x-z+u)v}\alpha(u)\bar{\alpha}(w+u)\Psi(z+w)\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w.$$

The integral over v is only nonvanishing for $x-z+u=0$. Hence, we obtain

$$\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} e^{iyw}\alpha(z-x)\bar{\alpha}(z+w-x)\Psi(z+w)\mathrm{d}w.$$

With the substitution $u := z+w$ we get

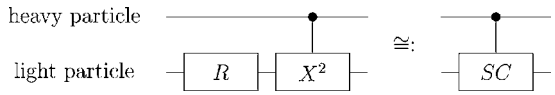

FIG. 3. Correspondence between gates and a scattering of two particles with extreme mass ratio. The scattering is called controlled SC gate.

$$\sqrt{\frac{1}{2\pi}}e^{-iyz}\alpha(z-x)\int_{-\infty}^{\infty}e^{iyu}\bar{\alpha}(u-x)\Psi(u)\mathrm{d}u.$$

The conditional state given that we obtain the result $x=t$ and $y=s$ coincides with Eq. (10). □

In order to realize the transformation in Theorem 13 by a physical process we first observe that scattering processes realize quantum gates which are close to the controlled phase shift in Eq. (7): Consider two particles interacting with hard-core potential, i.e., the interaction energy is zero whenever their distance is larger than some $a>0$ and infinite if the distance is smaller than a. In Ref. 25 we have discussed the state change caused by such a scattering provided that the considered time scale is small compared to the time scale on which the width of wave packets grows by dispersion. We will first explain the scattering process in momentum space since the change of momenta of classical particles provide a good intuition about the quantum case. The momentum p_2 of the light particle obtains a sign change since it is reflected. Due to the conservation of total momentum, the heavy particle acquires an additional momentum $2p_2$. The vector of momenta of both particles is therefore changed according to a linear transformation N given by

$$N\begin{pmatrix}p_1\\p_2\end{pmatrix}=\begin{pmatrix}p_1+2p_2\\-p_2\end{pmatrix}.$$

Neglecting irrelevant translations in position space, the corresponding linear transformation M in position space is already given by the requirement that the 4×4 matrix transformation $M\oplus N$ acting on the two positions and the two momenta has to be symplectic. We have therefore $M=(N^T)^{-1}$ and obtain in agreement with Ref. 25

$$M=\begin{pmatrix}1&0\\2&-1\end{pmatrix}.$$

The scattering process S acts therefore on the wave function in position space by multiplying the coordinate vector with M, i.e.,

$$(S\psi)(\mathbf{x}):=\psi(M\mathbf{x}),\quad \mathbf{x}\in\mathbb{R}^2.$$

We obtain

$$(S\psi)(x,y)=\psi(x,-y+2x).$$

In order to understand the relation to the gates in Theorem 13, we may represent this operation by the circuit in Fig. 3. The "reflection" gate R corresponds to a change of the wave function according to

$$(R\psi)(x):=\psi(-x).$$

Elementary calculations show that Fig. 2 is equivalent to the circuit in Fig. 4 where we have absorbed the Fourier transform on the wire in the middle by replacing an X measurement with a P measurement.

After we have converted the desired circuit into the equivalent one that avoids controlled phase gates in Fig. 4 we still have the problem that it requires controlled X gates and its inverse instead of a controlled X^2 gate which implements the shift twice. However, we observe that we may convert these gates into each other by conjugating them with the unitary squeezing operator

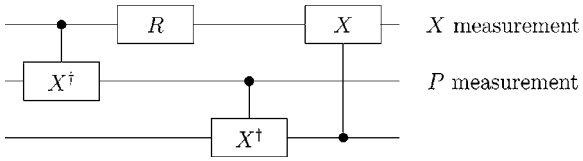

FIG. 4. Circuit equivalent to the circuit in Fig. 2.

$$S_2|x\rangle := |2x\rangle$$

combined with reflections when needed. (Note that the described reduction of controlled SC to controlled X is also possible in finite dimensions d. The definition $R|x\rangle := |-x\rangle$ is always possible and $|x\rangle \mapsto |2x \bmod d\rangle$ is bijective if d is odd. Then the ring $\mathbb{Z}/d\mathbb{Z}$ allows division by 2.) We will see later that we do not have to worry about the physical realization of S_2 since we need this gate and its inverse only at the end or at the beginning of the first or the second wire. Hence, they can either be absorbed into the preparation procedure or into the measurement by reinterpreting the result.

We will furthermore modify the entangling operation on ancilla 1 and 2, i.e., the first gate of the circuit in Fig. 4 for the following reason. An important feature of the circuits in Figs. 2 and 4 is that the POVM consists of rank-one operators if the input ancilla state is the product state $|\alpha\rangle \otimes |\bar{\alpha}\rangle$ and entangled inputs lead to POVM operators of higher rank. The preparation of these entangled states was not considered in Subsection IV B. Here we also want to describe *how to entangle* ancilla 1 and 2 when POVMs of higher rank are desired. The goal is therefore to change the operation on ancilla 1 and 2 preceding the interaction with the system to be measured such that a family of *product* input states allows the implementation of POVMs of higher rank. In other words, we want to tune the achieved information and the caused disturbance of the measurements by plugging different product states into the circuit.

After subsequently replacing the gates in Fig. 4 with scattering processes combined with squeezing operations and reflections and modifying the entangling operation between the ancillas, we found that an interesting class of POVMs can indeed be implemented by three scattering processes as depicted in Fig. 5 when the initial ancilla states are Gaussian wave packets.

To understand the effect of the "circuit" in Fig. 5 we shall compute a 3×3 matrix that describes the effect of the whole circuit on the three position coordinates. For doing so, we recall (see Fig. 5) that the masses of the particles satisfy

$$m_1 \ll m_3 \ll m_2.$$

First, we implement a collision between particles 1 and 2. Here, the position of particle 2 controls the position of particle 1. In analogy to the remarks above we describe the scattering and reflection by matrices that act on the vector of position coordinates of the three particles. The scattering processes with the pairs (2,1), (2,3), and (3,1) correspond to the matrices

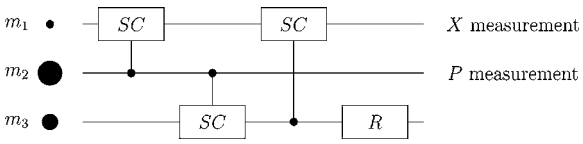

FIG. 5. Implementation of minimally disturbing simultaneous measurement of position and momentum by three scattering processes and one reflection. The masses m_1 and m_2 of the two ancilla particles are extremely small or extremely large compared to the mass m_3 of the particle to be measured.

$$S_{21} := \begin{pmatrix} -1 & 2 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad S_{23} := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & -1 \end{pmatrix}, \quad S_{31} := \begin{pmatrix} -1 & 0 & 2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The scatterings are followed by a reflection of the z coordinate (the R gate). Taking into account that we have to concatenate the effect on the coordinates from the left to the right, the complete transformations in position coordinate space is given by

$$A := S_{31}S_{23}S_{21}R_3 = \begin{pmatrix} 1 & 2 & 2 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix}.$$

Let the initial state of the three particles be given by the wave function

$$\alpha(x)\beta(y)\psi(z).$$

After subjecting the arguments to A we obtain

$$\alpha(x+2y+2z)\beta(y)\psi(2y+z). \tag{11}$$

In order to reduce a momentum measurement on the second wire to a position measurement we apply a Fourier transform to the state (11) and obtain

$$\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} \alpha(x+2\tilde{w}+2z)\beta(\tilde{w})\psi(2\tilde{w}+z)e^{-i\tilde{w}y}\,\mathrm{d}\tilde{w}.$$

With $w := 2\tilde{w}+z$ we get

$$\sqrt{\frac{1}{8\pi}}\int_{-\infty}^{\infty} \alpha(x+w+z)\beta[(w-z)/2]\psi(w)e^{i(-y/2)(w-z)}\,\mathrm{d}w.$$

We define the integral kernel

$$k_{x,y}(z,w) := \sqrt{\frac{1}{8\pi}}\alpha(x+w+z)\beta[(w-z)/2]e^{i(-y/2)(w-z)}.$$

It defines for fixed x,y an operator $K_{x,y}$ on $\mathcal{H}$ by

$$(K_{x,y}\psi)(z) := \int_{-\infty}^{\infty} k_{x,y}(z,w)\psi(w)\mathrm{d}w.$$

Note that the Kraus operators $K_{x,y}$ describe the unnormalized output state $K_{x,y}|\psi\rangle$ of particle 3 given that we have measured x and y on the first and second particle, respectively (in straightforward analogy to the Kraus operators in Lemma 3 for the discrete setting).

Now we show that $K_{x,y}$ can be obtained by subjecting $K_{0,0}$ to the Heisenberg–Weyl group elements by

$$K_{x,y} = U_{-x/2,-y}K_{0,0}U^{\dagger}_{-x/2,-y}.$$

To see this, we observe that the translation by $-x/2$ in position space changes the integral kernel $k_{0,0}(z,w)$ into $k_{0,0}(z+x/2,w+x/2)$ and the additional translation in momentum space by $-y/2$ changes it into

$$k_{0,0}(z+x,w+x)e^{i(-y/2)(w-z)} = k_{x,y}(z,w).$$

This shows that the process in Fig. 5 implements a measurement for the POVM

$$\Pi_{s,t} := U_{s,t} K_{0,0}^{\dagger} K_{0,0} U_{s,t},$$

when reinterpreting the measurement outcomes x,y on particles 1 and 2 as $t=-x/2$ and $s=-y$, respectively. In order to obtain a minimally disturbing implementation, we have to ensure that $K_{0,0}$ is positive (in straightforward generalization of Corollary 4 to the continuous setting) because it can then be interpreted as $\sqrt{\mu}$. If α and β are real and β is an even function, i.e., $\beta(-y)=\beta(y)$, $K_{0,0}$ is self-adjoint due to

$$k_{0,0}(z,w) = \overline{k_{0,0}(w,z)}.$$

The integral kernel of $K_{0,0}$ is explicitly given by

$$k_{0,0}(z,w) = \frac{1}{\sqrt{2\pi}} \alpha(w+z)\beta[(w-z)/2].$$

Now we assume that α and β are both real Gaussian wave functions with widths σ_1 and σ_2, respectively, i.e.,

$$\alpha(x) := \frac{1}{\sqrt{\sigma_1}\pi^{1/4}} \exp\left(-\frac{x^2}{2\sigma_1^2}\right) \quad \text{and } \beta(y) := \frac{1}{\sqrt{\sigma_1}\pi^{1/4}} \exp\left(-\frac{y^2}{2\sigma_2^2}\right).$$

Under these conditions, $k_{0,0}$ defines a positive operator whenever $\sigma_1 \geqslant 2\sigma_2$. This follows from the following lemma after replacing a and b with $1/(2\sigma_1^2)$ and $1/(8\sigma_2^2)$, respectively.

Lemma 14: The operator given by the integral kernel

$$k(x,y) := de^{-a(x+y)^2 - b(x-y)^2}$$

with $d>0$ is for all $b>a\geqslant 0$ positive.

Proof: Rewrite the kernel as

$$k(x,y) = \mathrm{d}e^{-2ax^2} e^{-(b-a)(x-y)^2} e^{-2ay^2}. \tag{12}$$

It is known that the integral kernel

$$\tilde{k}(x,y) := \mathrm{d}e^{-c(x-y)^2}$$

defines for all positive c,d a positive operator[26] which we shall denote by $\tilde{K}$. Then the operator K given by the kernel (12) can be written as $K=D\tilde{K}D$ where D is the multiplication operator

$$(D\psi)(x) := e^{-2ax^2}\psi(x).$$

Hence, K is also positive. □

Since we have now described sufficient conditions for which $K_{0,0}$ is positive, we would like to better understand the POVM operator $\mu=K_{0,0}^2$. As simple computations show, it is (up to the normalization factor 2π) given by the reduced state of one particle in a two-particle system, if the latter is described by the wave function

$$\phi(x,y) := \sqrt{2\pi}k_{0,0} = \alpha(x+y)\beta[(x-y)/2]. \tag{13}$$

It can be obtained from the state $|\alpha\rangle\otimes|\beta\rangle$ by a linear mapping of the wave function arguments according to

$$\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} 1 & 1 \\ 1/2 & -1/2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} =: G \begin{pmatrix} x \\ y \end{pmatrix}.$$

Such a linear operation transforms the initial Gaussian state into an entangled Gaussian state. Since Gaussian states are completely determined by their covariance matrix,[27] we will compute the latter for the state in Eq. (13).

For doing so, we must describe the linear transformation corresponding to G that acts on the arguments of the wave function in momentum space. According to the remarks at the beginning of this section, it is given by the transposed inverse:

$$\begin{pmatrix} p_x \\ p_y \end{pmatrix} \mapsto (G^T)^{-1} \begin{pmatrix} p_x \\ p_y \end{pmatrix}.$$

The covariance matrix of a two-particle state ρ consists of the entries

$$\mathrm{tr}(\rho X_i X_j) - \mathrm{tr}(\rho X_i)\mathrm{tr}(\rho X_j) \quad \text{with } i,j = 1, \ldots, 4$$

where X_1, X_2 denote the position operators and X_3, X_4 the momentum operators of particles 1 and 2, respectively. For the state $|\alpha\rangle \otimes |\beta\rangle$ it is given by (see Ref. 27)

$$\sigma = \begin{pmatrix} \sigma_1^2/2 & 0 & 0 & 0 \\ 0 & \sigma_2^2/2 & 0 & 0 \\ 0 & 0 & 1/(2\sigma_1^2) & 0 \\ 0 & 0 & 0 & 1/(2\sigma_2^2) \end{pmatrix}.$$

If the coordinate vector in the position wave function is subjected to some area-preserving linear map G and the coordinates of the momentum wave function to $(G^T)^{-1}$, the covariance matrix transforms in the following way:

$$\sigma' := \begin{pmatrix} G^{-1} & 0 \\ 0 & G^T \end{pmatrix} \sigma \begin{pmatrix} (G^T)^{-1} & 0 \\ 0 & G \end{pmatrix} = \frac{1}{8} \begin{pmatrix} \sigma_1^2 + 4\sigma_2^2 & \sigma_1^2 - 4\sigma_2^2 & 0 & 0 \\ \sigma_1^2 - 4\sigma_2^2 & \sigma_1^2 + 4\sigma_2^2 & 0 & 0 \\ 0 & 0 & \dfrac{4}{\sigma_1^2} + \dfrac{1}{\sigma_2^2} & \dfrac{4}{\sigma_1^2} - \dfrac{1}{\sigma_2^2} \\ 0 & 0 & \dfrac{4}{\sigma_1^2} - \dfrac{1}{\sigma_2^2} & \dfrac{4}{\sigma_1^2} + \dfrac{1}{\sigma_2^2} \end{pmatrix},$$

as simple computations show. The covariance matrix of the reduced state of each particle is given by the 2×2 submatrices that refer to its position and momentum. Due to the symmetry of our state, it is for both particles given by

$$\frac{1}{8} \begin{pmatrix} \sigma_1^2 + 4\sigma_2^2 & 0 \\ 0 & \dfrac{4}{\sigma_1^2} + \dfrac{1}{\sigma_2^2} \end{pmatrix}. \tag{14}$$

It is known[27] that such a state is pure if and only if the determinant is $\frac{1}{4}$. This is given for $\sigma_1 = 2\sigma_2$. One can rewrite a Gaussian state of a single mode having diagonal covariance matrix as a thermal state of a harmonic oscillator with frequency ω, mass m, and average phonon number N. (In quantum optics, one would also need squeezing transformations to obtain a general diagonal Gaussian state. But here the product of frequency and mass of the oscillator provides an additional free parameter.) It is explicitly given by

$$\rho_{N,\nu} = (1 - e^{-1/N}) \sum_{n=0}^{\infty} e^{-n/N} |n\rangle\langle n|,$$

where $|n\rangle$ with $n \in \mathbb{N}_0$ denotes the nth energy eigenstate of the oscillator. We will first use dimensionless position and momentum variables

$$X' := \frac{1}{\sqrt{2}}(a + a^\dagger) = \sqrt{m\omega} X \tag{15}$$

and

$$P' := \frac{1}{i\sqrt{2}}(a - a^\dagger) = \frac{1}{\sqrt{m\omega}} P, \tag{16}$$

with creation operator $a^\dagger$ and annihilation operator a. In these coordinates, the covariance matrix of the thermal state with average phonon number N is the identity matrix times $(N+1)/2$. This follows, e.g., from Eqs. (2.16) in Ref. 27. In natural units, we therefore have the covariance matrix

$$\frac{N+1}{2} \begin{pmatrix} \frac{1}{m\omega} & 0 \\ 0 & m\omega \end{pmatrix}. \tag{17}$$

Comparing Eq. (14) to Eq. (17) we obtain

$$(m\omega)^2 = \frac{4/\sigma_1^2 + 1/\sigma_2^2}{\sigma_1^2 + 4\sigma_2^2}$$

and

$$(N+1)^2 = \frac{1}{4}(\sigma_1^2 + 4\sigma_2^2)\left(\frac{1}{\sigma_1^2} + \frac{1}{4\sigma_2^2}\right).$$

Hence

$$N = \frac{1}{2}\sqrt{2 + \frac{4\sigma_2^2}{\sigma_1^2} + \frac{\sigma_1^2}{4\sigma_2^2}} - 1.$$

For $\sigma_1 = 2\sigma_2$ one obtains $N=0$, i.e., the ground state of the oscillator that corresponds to a rank-one operator μ. We rephrase the findings implied by the above discussion as a theorem:

Theorem 15: *Given three particles such that their masses satisfy*

$$m_1 \ll m_3 \ll m_2.$$

Let the first and the second particle be in Gaussian states with real wave functions such that their widths satisfy $\sigma_1 \geq 2\sigma_2$. *Then the sequence of scattering processes depicted in Fig. 5 implements the Heisenberg–Weyl POVM* $(U_{s,t}\mu U_{s,t}^\dagger)_{s,t}$ *in a minimally disturbing way when the position of particle 1 and the momentum of particle 2 is measured and the result* (x,y) *is interpreted as* $t=-x/2$ *and* $s=-y$. *The initial operator* μ *of the POVM is given by*

$$\mu = \frac{1}{2\pi}\rho_{N,m\omega},$$

where $\rho_{N,m\omega}$ *is the thermal equilibrium state of a harmonic oscillator with mass m and frequency* ω *when the temperature is chosen such that the average phonon number is N. The parameters N and* $m\omega$ *are determined by the widths* σ_1 and σ_2 *according to*

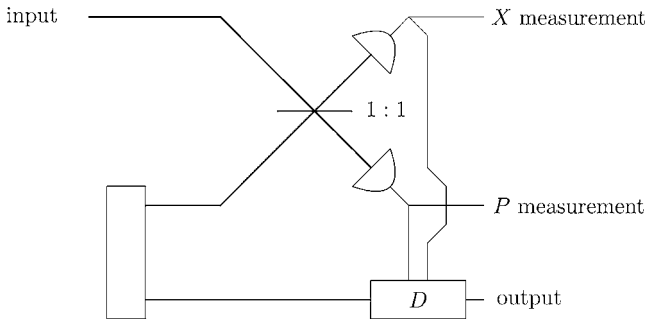

FIG. 6. Measurement scheme of Ref. 24. The box at the beginning of mode 2 and 3 indicate the entangled input on these two modes. The entanglement tunes the POVM. In the limit of infinite entanglement the output coincides with the input state and no information is gained. If mode 2 and 3 start in a product state, a rank-one POVM is implemented. The input interferes with mode 2 in a balanced beam splitter where one output mode is subjected to a position measurement and the other to a momentum measurement. The results determine the displacements in position and momentum the output is subjected to.

$$(m\omega)^2 = \frac{4/\sigma_1^2 + 1/\sigma_2^2}{\sigma_1^2 + 4\sigma_2^2},$$

and

$$N = \frac{1}{2}\sqrt{2 + \frac{4\sigma_2^2}{\sigma_1^2} + \frac{\sigma_1^2}{4\sigma_2^2}} - 1.$$

We want to briefly explain qualitatively how the measured POVM is tuned by the parameters σ_1 and σ_2. The ratio of both determine the purity of μ, for $\sigma_1 = 2\sigma_2$ we obtain a rank-one measurement. By increasing or decreasing both we can achieve a better resolution in momentum space or in position space: Small values σ_1, σ_2 lead to good position measurements for the cost of having large errors in the momentum measurement. If $\sigma_1 \gg 2\sigma_2$ both position and momentum measurements are bad and we obtain a measurement with small disturbance.

For detailed discussions on the disturbance and accuracy of the measurements we also refer to Refs. 22 and 23. It is shown that the outcomes for position and momentum in POVMs of the above type satisfy the inequality $\Delta x \Delta p \geqslant \hbar$ in contrast to the Heisenberg uncertainty relation $\Delta x \Delta p \geqslant \hbar/2$.

VI. Comparison to quantum optics implementations

Meanwhile there are several methods known to measure the quadrature amplitudes of a light mode simultaneously (see Ref. 24). We will consider the scheme shown in Fig. 6 which has some nice similarities to the continuous analog of our circuit in Fig. 2. In the following, we will use the dimensionless formal position and momentum operators as given in Eqs. (15) and (16) which generate the momentum and position translations in the Heisenberg–Weyl group and furthermore define implicitly a Schrödinger representation of a single mode state as wave function $\psi \in L^2(\mathbb{R})$ in position state.

The method in Fig. 6 also uses two ancilla modes. As in our proposal, the entanglement of the two modes tunes the POVM operator. One part of an entangled two-mode state (wires 2 and 3 in Fig. 6) interferes with the input state (wire 1) in a beam splitter. One of its output modes is subjected to a position measurement, the other to a momentum measurement. The results of the measurement determine furthermore displacements performed on the second component of the entangled input. The idea behind the scheme is to perform a teleportation using a nonmaximally entangled bipartite state (a maximally entangled state does not exist anyway in continuous variables) as a resource. Then the transfer of quantum information is not perfect but the measurements

performed during the "bad" teleportation provide some information on the input state. Similar to our scheme, the more entangled the joint state, the less information provides the measurement and the less disturbance on the output state will be observed.

One technical difference to our scheme is that the input and output are not on the same wire. The main difference is, however, that the interaction between input and entangled ancilla is given by a beam splitter, whereas we use scattering processes. This is geometrically the difference between a rotation or a shear in coordinate space (for details see Ref. 25). Note, however, that the effect of the controlled displacements of Fig. 6 could be mimicked by a controlled-X gate from wire 1 to 3 and a controlled-Z gate from wire 2 to 3 if the latter gate is conjugated by a Fourier transform on wire 2. The reason is that it does not make a difference whether the controlled operation is performed before the measurement or afterward. The scheme therefore contains elements quite similar to ours.

In Ref. 24 we did not find an explicit remark stating that their implementation scheme is minimally disturbing in the sense considered here since the authors use the term "minimally disturbing" in a different sense. Furthermore, the attention was restricted to Gaussian states for both the input as well as for the ancilla states. We have observed that the implementation is also applicable for non-Gaussian states and non-Gaussian POVM operators:

Theorem 16: *The scheme of Ref. 6 can in principle be used for a minimally disturbing implementation of any Heisenberg–Weyl symmetric POVM*

$$U_{s,t}\mu U_{s,t}^{\dagger}$$

by preparing the ancilla state

$$\sum_j \sqrt{\lambda_j}|\alpha_j\rangle \otimes |\overline{\alpha_j}\rangle,$$

where the $|\alpha_j\rangle$ *denote the eigenvector basis for* μ *and* $\lambda_j/(2\pi)$ *the corresponding eigenvalues.*

Proof: Due to the linearity argument in Lemma 3 we may prove our statement for the case where the two ancillas are in a product state. The initial three mode wave function is then given by

$$\phi(x,y,z) = \psi(x)\alpha(y)\beta(z),$$

where ψ is the wave function of the mode to be measured. The beam splitter transfers it to the wave function

$$\psi[(x+y)/\sqrt{2}]\alpha[(x-y)/\sqrt{2}]\beta(z).$$

We simulate the momentum measurement by an inverse Fourier transform followed by a position measurement. Conditioned on the measurement result (x,y) we therefore obtain a one-mode wave function (having z as argument) which is given by

$$\sqrt{\frac{1}{2\pi}}\left\{\int_{-\infty}^{\infty}\psi[(x+w)/\sqrt{2}]\alpha[(-x+w)/\sqrt{2}]e^{iwy}dw\right\}\beta(z).$$

After obtaining the measurement results x and y on wires 1 and 2, respectively, the conditioned displacement of position and momentum by $\sqrt{2}x$ and $\sqrt{2}y$, respectively, leads to

$$\sqrt{\frac{1}{2\pi}}\left\{\int_{-\infty}^{\infty}\psi[(x+w)/\sqrt{2}]\alpha[(-x+w)/\sqrt{2}]e^{iwy}dw\right\}\beta(z-\sqrt{2}x)e^{-iz\sqrt{2}y}$$
$$=\sqrt{\frac{1}{2\pi}}\left[\int\psi(w)\alpha(-\sqrt{2}x+w)e^{iw\sqrt{2}y}dw\right]\beta(z-\sqrt{2}x)e^{-iz\sqrt{2}y}.$$

This shows that the unnormalized state vector of the third particle, given that x,y was measured, reads

$$U_{\sqrt{2}y,\sqrt{2}x}|\beta\rangle\langle\bar{\alpha}|U^{\dagger}_{\sqrt{2}y,\sqrt{2}x}|\psi\rangle.$$

After taking into account that the quantum optics convention for position and momentum differs from the canonical definition of Eqs. (15) and (16) by the factor $\sqrt{2}$ (see Ref. 27), this is exactly the desired output state.

By choosing the input $|\bar{\alpha}\rangle\otimes\langle\alpha|$ we therefore have $\mu=|\alpha\rangle\langle\alpha|=\sqrt{\mu}$. Similarly we can obtain operators μ with higher rank by choosing entangled input states. □

Note that the calculations which show that the scheme does indeed implement a minimally disturbing POVM is very similar to the calculations in Sec. V which show the close formal analogy of both methods.

VII. CONCLUSIONS

We have presented a general scheme to implement minimally disturbing symmetric measurements by quantum circuits. By applying it to the Heisenberg–Weyl group, we obtain circuits for simultaneous measurements of position and momentum of a particle moving on a discrete cyclic chain. We show that an infinite dimensional generalization of this circuit leads to a well-defined measurement process on a Schrödinger particle moving on the real line using two probe particles. The "circuit" for this continuous variable quantum system can, in principle, be obtained by particle collisions with hard-core potential. The whole measurement process on the three particles shows some analogies but also differences to simultaneous measurements of the quadrature amplitudes in quantum optics using two ancilla modes.

ACKNOWLEDGMENT

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APPENDIX

1. Proof of Theorem 10

The $(2n\times 2)$ matrix M of Eq. (2) has the $(\sigma_\pi\otimes\sigma,\sigma)$ symmetry that is defined by

$$(X_n\otimes R_n)M=MR_n,$$

as straightforward computation shows, i.e., we have $(\sigma_\pi\otimes\sigma)(j)=X_n^j\otimes R_n^j$ and $\sigma(j)=R_n^j$. To find the diagonalizing operations A and B of Theorem 9 we observe that σ is already decomposed into irreducible representations and B is therefore trivial. To decompose $\sigma_\pi\otimes\sigma$ we diagonalize σ_π by the Fourier transform F_n. The eigenvalues of $(F_nX_nF^\dagger)\otimes R_n$ are in the order $1,\omega_n,\omega_n,\omega_n^2,\omega_n^2,\ldots,\omega_n^{n-1},\omega_n^{n-1},1$. We apply the cyclic shift X_{2n} to group them into a sequence of pairs (ω_n^j,ω_n^j) as in Lemma 7. Therefore, we have $A=X_{2n}(F_n\otimes I_2)$. Following Theorem 9 we only have to find $W\in\mathrm{Int}[A(\sigma_\pi\otimes\sigma)A^\dagger,B\sigma B^\dagger\oplus\sigma']$ which is a unitary extension of $N:=A^\dagger MB$. Hence, we can choose

$$W := \sqrt{\frac{1}{2}} \begin{pmatrix} 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 & -1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & -1 \end{pmatrix},$$

since the first two columns of this matrix coincide with N. This is verified by straightforward computations, too. One can also easily check that W can be written as $W=(I_n \otimes F_2)K^\dagger$ where K is defined in Theorem 10.

2. Proof of Theorem 12

To define M as in Eq. (2) we have to define a correspondence between ancilla basis states and POVM operators. Since our ancilla system is a tensor product of two d-dimensional systems, this correspondence is canonical and we obtain

$$M = \sum_{j,k=0}^{d-1} |j\rangle \otimes |k\rangle \otimes Z_d^k X_d^j \sqrt{\mu} X_d^{-j} Z_d^{-k} \in \mathbb{C}^{d^3 \times d}. \tag{A1}$$

The symmetry $(\sigma_\pi \otimes \sigma)M = M\sigma$ of M is defined by

$$(I_d \otimes X_d \otimes Z_d)M = MZ_d \quad \text{and} \quad (X_d \otimes I_d \otimes X_d)M = MX_d,$$

as straightforward computations show. Following Theorem 9 we decompose the representation on the left side into a direct sum of irreducible representations. First of all, we diagonalize the shifts X_d in the first and second tensor components by the Fourier transform. We obtain

$$(I_d \otimes Z_d \otimes Z_d)(F_d \otimes F_d \otimes I_d)M = (F_d \otimes F_d \otimes I_d)MZ_d$$

and

$$(Z_d \otimes I_d \otimes X_d)(F_d \otimes F_d \otimes I_d)M = (F_d \otimes F_d \otimes I_d)MX_d.$$

The matrices on the left side can be written as

$$(I_d \otimes Z_d \otimes Z_d) = \bigoplus_{j=0}^{d^2-1} \omega_d^{j \bmod d} Z_d \quad \text{and} \quad (Z_d \otimes I_d \otimes X_d) = \bigoplus_{j=0}^{d^2-1} \omega_d^{j \operatorname{div} d} X_d.$$

Therefore, the representation is decomposed into a direct sum of representations that are equal to σ up to phase factors. We now eliminate these factors. To simplify notation we define the block diagonal matrices

$$X_{\mathrm{mod}} := \bigoplus_{j=0}^{d^2-1} X_d^{j \bmod d} \quad \text{and} \quad Z_{\mathrm{div}} := \bigoplus_{j=0}^{d^2-1} Z_d^{j \operatorname{div} d}.$$

Using $Z_d^\dagger X_d Z_d = \omega_d^{-1} X_d$ and $X_d Z_d X_d^\dagger = \omega_d^{-1} Z_d$ we obtain

$$X_{\mathrm{mod}} \left(\bigoplus_{j=0}^{d^2-1} \omega_d^{j \bmod d} Z_d \right) X_{\mathrm{mod}}^\dagger = \bigoplus_{j=0}^{d^2-1} Z_d$$

and

$$Z_{\mathrm{div}}^{\dagger}\left(\bigoplus_{j=0}^{d^2-1}\omega_d^{j\ \mathrm{div}\ d}X_d\right)Z_{\mathrm{div}}=\bigoplus_{j=0}^{d^2-1}X_d.$$

Using both equations we can write

$$X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(I_d\otimes Z_d\otimes Z_d)Z_{\mathrm{div}}X_{\mathrm{mod}}^{\dagger}=(I_d\otimes I_d\otimes Z_d)$$

and

$$X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(Z_d\otimes I_d\otimes X_d)Z_{\mathrm{div}}X_{\mathrm{mod}}^{\dagger}=(I_d\otimes I_d\otimes X_d),$$

where we have no phase factors. Consequently, we obtain

$$(I_d\otimes I_d\otimes Z_d)X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)M=X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)MZ_d$$

and

$$(I_d\otimes I_d\otimes X_d)X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)M=X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)MX_d.$$

We can rewrite this as

$$(I_d\otimes I_d\otimes\sigma)N=N\sigma \tag{A2}$$

with $N=X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)M$. Hence, using the notation of Theorem 9 we have

$$A:=X_{\mathrm{mod}}Z_{\mathrm{div}}^{\dagger}(F_d\otimes F_d\otimes I_d)\quad\text{and}\quad B=I_d$$

since σ is an irreducible representation. The matrix N is an element of the intertwining space $\mathrm{Int}(\oplus_{j=0}^{d^2-1}\sigma,\sigma)$. Following Lemma 7 it has the decomposition

$$N=|\Phi_1\rangle\otimes I_d\in\mathbb{C}^{d^3\times d}$$

with $|\Phi_1\rangle\in\mathbb{C}^{d^2}$. Elementary but cumbersome computations (write $\sqrt{\mu}=\Sigma_{j=0}^{d-1}X_d^j\Delta_j$ with appropriate diagonal matrices Δ_j and powers of the shift X_d) show

$$|\Phi_1\rangle=(F_d^{\dagger}\otimes I_d)\left(\sum_{q=0}^{d-1}|q\rangle\langle q|\otimes X_d^{-q}\right)\left(\sqrt{d}\sum_{j,k=0}^{d-1}\sqrt{\mu}_{jk}|j\rangle\otimes|k\rangle\right). \tag{A3}$$

We extend the representation σ on the right side of Eq. (A2) to the direct sum of d^2 copies of σ. The matrix W of the resulting intertwining space has the decomposition $C\otimes I_d$ with $C\in\mathbb{C}^{d^2\times d^2}$. Therefore, we extend $\{|\Phi_1\rangle\}$ to an orthonormal basis $\{|\Phi_1\rangle,|\Phi_2\rangle,\ldots,|\Phi_{d^2}\rangle\}$ of $\mathbb{C}^{d^2}$. We can define the unitary

$$U:=A^{\dagger}W(B\oplus\tilde{B})=A^{\dagger}[(|\Phi_1\rangle|\Phi_2\rangle\ldots|\Phi_{d^2}\rangle)\otimes I_d]$$

that extends M with $\tilde{B}:=I_{(n-1)d}$. Now we show how to simplify the implementation by preparing an appropriate ancilla state. We have

$$U(|0\rangle\otimes|\Psi\rangle)=A^{\dagger}[(|\Phi_1\rangle|\Phi_2\rangle\ldots|\Phi_{d^2}\rangle)\otimes I_d](|0\rangle\otimes|\Psi\rangle)=A^{\dagger}(|\Phi_1\rangle\otimes|\Psi\rangle).$$

Hence, we can omit the implementation of W if we initialize the ancilla with $|\Phi_1\rangle$ of Eq. (A3). In summary, we have to implement the unitary

$$(F_d^{\dagger}\otimes F_d^{\dagger}\otimes I_d)Z_{\mathrm{div}}X_{\mathrm{mod}}^{\dagger}(F_d^{\dagger}\otimes I_d\otimes I_d)\left(\sum_{q=0}^{d-1}|q\rangle\langle q|\otimes X_d^{-q}\otimes I_d\right)$$

after we have initialized the ancillas with the state vector

$$|\gamma\rangle := \sqrt{d}\sum_{j,k=0}^{d-1}\sqrt{\mu}_{jk}|j\rangle\otimes|k\rangle \in \mathbb{C}^{d^2}. \tag{A4}$$

As a special case consider the initial operator $\mu=|\alpha\rangle\langle\alpha|/d$ with $|\alpha\rangle\in\mathbb{C}^d$ and $\langle\alpha|\alpha\rangle=1$. In this case we have $\sqrt{\mu}=|\alpha\rangle\langle\alpha|/\sqrt{d}$. Furthermore, we have

$$|\gamma\rangle = |\alpha\rangle\otimes|\bar{\alpha}\rangle.$$

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Zero energy resonance and the logarithmically slow decay of unstable multilevel systems

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The long time behavior of the reduced time evolution operator for unstable multilevel systems is studied based on the *N*-level Friedrichs model in the presence of a zero energy resonance. The latter means the divergence of the resolvent at zero energy. Resorting to the technique developed by Jensen and Kato [Duke Math. J. **46**, 583 (1979)], the zero energy resonance of this model is characterized by the zero energy eigenstate that does not belong to the Hilbert space. It is then shown that for some kinds of the rational form factors the logarithmically slow decay proportional to $(\log t)^{-1}$ of the reduced time evolution operator can be realized. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227260]

I. INTRODUCTION

The exponential decay of unstable systems has been a well-known law since the early days of quantum theory. The quantum description of those systems, however, allows deviation from exponential decay both at shorter and longer times[1] than those times over which the exponential decay law dominates.[2,3] The short time deviation was actually found in a quantum tunneling experiment,[4] while the long time deviation seems still not to have been detected in any quantum system.[5] The main cause that hinders the detection is considered as the smallness of the deviation at such long times.[6]

In a recent study, a method enhancing the long time deviation was proposed.[7] The decay of the unstable systems is theoretically modeled in the time evolution of the survival probability of unstable initial state. The survival probability is just the probability of finding the initial state in the state at a later time t. Since it is rewritten in a Fourier integral of the spectral function, its behavior at long times is determined by that of the spectral function near the threshold of the energy continuum.[2,3] The essential aspect of the method is then distorting the spectral function from the Breit-Wigner form and dislocating its peak toward the threshold energy. Mathematically, this causes a divergence of the spectral function, i.e., the resolvent at the threshold. Then, it is expected that the exponential decay period disappears and the survival probability at long times is increased. A similar idea was also considered in a related context.[5,8] In addition, in the analysis of the Friedrichs model[9,10] that is often used for the study on the decays of the unstable systems, the survival probability at long times sometimes exhibits a power decay law slower than that in cases of no divergence.[11–13]

These facts remind the author of the zero energy resonance proposed by Jensen and Kato.[14] According to them, such zero energy singularities are classified by the zero energy eigenstates of the total Hamiltonian that either belong to or do not belong to the Hilbert space. The cases where such eigenstates exist are called the exceptional cases; otherwise they are referred to as the regular case. The result in Ref. 14 is concerned with the three-dimensional system of the one particle in short-range potentials, and they proved that the time evolution operator asymptotically decreases as $O(t^{-1/2})$ for the exceptional cases, which is slower than $O(t^{-3/2})$ for the regular case. However,

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to the author's knowledge, the zero energy resonance for the Friedrichs model seems not to have been examined in the previous studies including Refs. 7 and 11–13, in spite of the wide applicability of the model to the various physical systems.[8,11,13,15,16]

In the present paper, we examine the zero energy singularities of the resolvent at the threshold energy for the Friedrichs model from the viewpoint of the zero energy resonance,[14] and clarify how the asymptotic behavior of the survival probability at long times is affected. The Friedrichs model[9,10] describes the system of the finite discrete levels coupled with the continuous spectrum, in which the former can be interpreted as the unstable excited levels of atoms and the latter as the environmental electromagnetic fields.[11,15,16] We emphasize that the model is not restricted to the single level case[7–13,15,16] but, rather, the N-level case.[10,17–21] In addition, we assume that the square modulus of the form factors vanishes at zero energy with an integer power,[15,16,22] however it is treated without restriction to a specific form to some extent. Furthermore, since we only consider the initial state spanned by the discrete states, it is sufficient for us to see the reduced resolvent $\widetilde{R}(z)$ that is just the restriction of the resolvent to the subspace spanned by the discrete states. Then, the Fourier integral of $\widetilde{R}(z)$ that we call the reduced time evolution operator $\widetilde{U}(t)$ enables us to calculate the survival probability. In fact it is expressed by the square modulus of the expectation value of$\widetilde{U}(t)$ in a given initial state. We first study the zero energy eigenstates of the model which either belong to or do not belong to the Hilbert space. It is then possible to estimate correctly the asymptotic behavior of $\widetilde{R}(z)$ at small energies both in the regular case and the exceptional cases. The latter cases are examined in detail only for the first kind, where only the zero energy eigenstate not belonging to the Hilbert space exists. On the basis of this analysis, we can derive the long-time asymptotic formula for $\widetilde{U}(t)$ in those cases. In particular, the logarithmic decay proportional to $(\log t)^{-1}$ of $\widetilde{U}(t)$ is shown to occur in the exceptional case of the first kind for our form factors, which is extremely slower than the power decays in the regular case and in the exceptional case for another type of form factor.[11–13] These results are shown in Theorems VII.1 and VII.2.

The organization of the paper is as follows. We first explain in Sec. II the N-level Friedrichs model with an appropriate Hilbert space, and then in Sec. III we introduce the reduced resolvent $\widetilde{R}(z)$. Section IV is devoted to the identification of zero energy eigenstates in this model. It is then possible to obtain the asymptotic expansion of $\widetilde{R}(z)$ at small energies in Sec. V, where we examine the regular and the exceptional case of the first kind. By making sure of the relation between $\widetilde{R}(z)$ and $\widetilde{U}(t)$ in Sec. VI, the asymptotic formula for $\widetilde{U}(t)$ in the regular and the exceptional case of the first kind are derived in Sec. VII. Concluding remarks are given in Sec. VIII.

II. HILBERT SPACE AND THE *N*-LEVEL FRIEDRICHS MODEL

We shall use bracket notation; however it can be understood in a standard treatment based on functional analysis as in Refs. 10 and 17. The Hilbert space describing the unstable multilevel systems is here defined by

$$\mathcal{H} := \mathbb{C}^N \oplus L^2((0,\infty)). \tag{1}$$

A vector $|c\rangle \in \mathbb{C}^N$ is expressed by $|c\rangle = \Sigma_{n=1}^N c_n |n\rangle$, where $|n\rangle$'s are the orthonormal basis of $\mathbb{C}^N$, so that $\langle n|n'\rangle = \delta_{nn'}$, where $\delta_{nn'}$ is Kronecker's delta. $L^2((0,\infty))$ is the Hilbert space of the square-integrable complex function $|f\rangle$ of the variable ω defined on $(0,\infty)$, i.e.,

$$|f\rangle \in L^2((0,\infty)) \Leftrightarrow \int_0^\infty |f(\omega)|^2 \mathrm{d}\omega < \infty\,. \tag{2}$$

In a standard notation using the (generalized) eigenstate $|\omega\rangle$ of the multiplication operator by ω, $|f\rangle$ is nothing more than

$$|f\rangle = \int_0^\infty f(\omega)|\omega\rangle \mathrm{d}\omega, \tag{3}$$

where $\langle\omega|\omega'\rangle = \delta(\omega-\omega')$ and $\delta(\omega-\omega')$ is Dirac's delta. Then, an arbitrary vector $|\Psi\rangle \in \mathcal{H}$ composed of $|c\rangle \in \mathbb{C}^N$ and $|f\rangle \in L^2((0,\infty))$ is denoted by

$$|\Psi\rangle := |c\rangle + |f\rangle, \tag{4}$$

and the inner product between any two vectors $|\Psi\rangle$ and $|\Phi\rangle \in \mathcal{H}$ is defined by[23]

$$\langle\Phi|\Psi\rangle := \langle \mathrm{d}|c\rangle + \langle g|f\rangle = \sum_{n=1}^{N} \mathrm{d}_n^* c_n + \int_0^\infty g^*(\omega) f(\omega) \mathrm{d}\omega, \tag{5}$$

where $(^*)$ denotes the complex conjugate and $|\Phi\rangle = |\mathrm{d}\rangle + |g\rangle$ with $|\mathrm{d}\rangle \in \mathbb{C}^N$ and $|g\rangle \in L^2((0,\infty))$. In particular, the associated norm of $|\Psi\rangle$ is $\|\Psi\| := \sqrt{\langle\Psi|\Psi\rangle}$, which is ensured to be finite for all $|\Psi\rangle \in \mathcal{H}$.

Let us now introduce the N-level Friedrichs model for a description of the decay of the unstable multilevel systems. The Hamiltonian H of this model is defined by

$$H := H_0 + \lambda V, \tag{6}$$

where H_0 is the free part and V the interaction part of H, respectively, and $\lambda \in \mathbb{R}$ is the coupling constant. H_0 is defined by

$$H_0 := \sum_{n=1}^{N} \omega_n |n\rangle\langle n| + \int_0^\infty \omega|\omega\rangle\langle\omega| \mathrm{d}\omega, \tag{7}$$

where $\omega_n \in \mathbb{R}$ with $\omega_1 \leqslant \omega_2 \leqslant \cdots \leqslant \omega_N$, and its action is prescribed by $H_0|\Psi\rangle = \Sigma_{n=1}^N \omega_n c_n |n\rangle + \omega|f\rangle$ for any $|\Psi\rangle = |c\rangle + |f\rangle \in D(H_0)$. $D(H_0)$ is the domain of H_0 defined by $D(H_0) := \{|\Psi\rangle \in \mathcal{H} \,|\, \int_0^\infty |\omega f(\omega)|^2 \mathrm{d}\omega < \infty\}$, and then the self-adjointness of H_0 is guaranteed. The interaction part V is defined by

$$V := \sum_{n=1}^{N} \int_0^\infty [v_n^*(\omega)|n\rangle\langle\omega| + v_n(\omega)|\omega\rangle\langle n|] \mathrm{d}\omega, \tag{8}$$

where we assumed that $|v_n\rangle \in L^2((0,\infty))$.[24] We call the L^2-functions $v_n(\omega)$ the form factors of the system under consideration. The action of V is then given by $V|\Psi\rangle = \Sigma_{n=1}^N \langle v_n|f\rangle |n\rangle + \Sigma_{n=1}^N c_n |v_n\rangle$ for any $|\Psi\rangle \in \mathcal{H}$. Note that since $D(V) = \mathcal{H}$ and V is a bounded self-adjoint operator, H is self-adjoint with the domain $D(H) = D(H_0) \cap D(V) = D(H_0)$.

In the whole of the paper, we will restrict ourselves to the special kind of the form factor: Suppose that the product $v_m^*(\omega)v_n(\omega)$ between an arbitrary pair of $v_m^*(\omega)$ and $v_n(\omega)$ is written in a rational function, i.e., it is expressed by

$$v_m^*(\omega)v_n(\omega) = \frac{\pi_{mn}(\omega)}{\rho_{mn}(\omega)}, \tag{9}$$

where $\pi_{mn}(\omega)$ and $\rho_{mn}(\omega)$ are the polynomials of the degree M_{mn} and N_{nm}, respectively, and we assume that $\rho_{mn}(\omega)$ has no zeros in $[0,\infty)$. It is also assumed that $M_{mn}+2 \leqslant N_{mn}$ and $\pi_{mn}(0) = 0$. The former condition ensures that $v_m^*(\omega)v_n(\omega)$ is integrable in $[0,\infty)$ and $\lim_{\omega\to\infty} v_m^*(\omega)v_n(\omega) = 0$, while the latter condition implies that the rational function $v_m^*(\omega)v_n(\omega) = O(\omega)$ as $\omega \to +0$. The form factors with such properties are often found in actual systems involving the process of the spontaneous emission of photons from the hydrogen atom,[15,22] and quantum dots.[16] We do not treat the algebraic form factor that behaves as $O(\omega^{1/2})$ as $\omega \to +0$ instead, associated with the photodetachment of electrons from the negative ion[8,12,13,25] and the spontaneous emission from the

atoms in the photonic crystals;[11] however, the discussion developed in the following could be easily extended to such a case.

III. REDUCED RESOLVENT FOR THE *N*-LEVEL FRIEDRICHS MODEL

In the following, we introduce the reduced resolvent that is simply the restriction of the resolvent of H to the N dimensional subspace $\mathbb{C}^N \oplus \{0\}$. Since we only consider the initial state belonging to this subspace, this restriction is sufficient for our study. In a technical sense, this treatment corresponds to the appropriate choice of a weighted Sobolev space.[14,30] In the later sections, we do not distinguish the vector in $\mathbb{C}^N$ from that in $\mathbb{C}^N \oplus \{0\}$. After introducing the reduced resolvent, we see the existence of the boundary values of the reduced resolvent on the positive real line. The large-energy behavior of the reduced resolvent is also examined, which is necessary for a rigorous estimation of the long time behavior of the reduced time evolution operator.

A. Reduced resolvent

The resolvent of H_0 and that of H are defined by $R_0(z)=(H_0-z)^{-1}$ and $R(z)=(H-z)^{-1}$, respectively, where we assume that $z \in \mathbb{C}\backslash(\sigma(H_0) \cup \sigma(H))$. $\sigma(H_0)$ (or $\sigma(H)$) is the spectrum of H_0 (or H), i.e., the set of the singular points of $R_0(z)$ (or R(z)). Then, we have

$$R(z) - R_0(z) = -R_0(z)VR(z) \tag{10}$$

$$= -R_0(z)VR_0(z) + R_0(z)VR_0(z)VR(z). \tag{11}$$

From Eq. (10), one obtains the equation $R(z)=(1+R_0(z)V)^{-1}R_0(z)$, which is the starting point of the asymptotic expansion of $R(z)$ for the short-range potential systems.[14] On the other hand, we instead start from Eq. (11) to obtain

$$[H_0 - z - VR_0(z)V]R(z) = 1 - VR_0(z). \tag{12}$$

This equation can be solved for our model if we confine ourselves to the state subspace $\mathbb{C}^N \oplus \{0\}$.[10] In fact, from the fact that $\langle n|VR_0(z)|n'\rangle = 0$ for any $|n\rangle$ and $|n'\rangle \in \mathbb{C}^N \oplus \{0\}$, Eq. (12) reads

$$\sum_{m=1}^{N} [(\omega_n - z)\delta_{nm} - \lambda^2 S_{nm}(z)]\tilde{R}_{mn'}(z) = \delta_{nn'}, \tag{13}$$

where $S(z)$ and $\tilde{R}(z)$ are the $N \times N$ matrix defined with the matrix components

$$S_{mn}(z) := \langle m|VR_0(z)V|n\rangle = \int_0^\infty \frac{v_m^*(\omega)v_n(\omega)}{\omega - z} d\omega, \quad \tilde{R}_{mn}(z) := \langle m|R(z)|n\rangle. \tag{14}$$

We call $S(z)$ and $\tilde{R}(z)$ the *self energy* and the *reduced resolvent*, respectively. Note that $S(z)$ can be analytically defined for all $z \in \mathbb{C}\backslash[0,\infty)$. For a later convenience, we also introduce the matrix K_0 and $K(z)$ by

$$K_{0mn} := \langle m|H_0|n\rangle = \omega_n \delta_{mn}, \quad K_{mn}(z) := [K_0 - \lambda^2 S(z)]_{mn}, \tag{15}$$

respectively. Then, Eq. (13) is equivalent to

$$[K(z) - z]\tilde{R}(z) = 1, \quad \forall z \in \mathbb{C}\backslash(\sigma(H_0) \cup \sigma(H)), \tag{16}$$

which implies that $\det[K(z)-z]\det[\tilde{R}(z)]=1$, so that $\det[K(z)-z] \neq 0$ and $\det[\tilde{R}(z)] \neq 0$ for all $z \in \mathbb{C}\backslash(\sigma(H_0) \cup \sigma(H))$. Thus, the inverse of $K(z)-z$ exists, and we have

$$\tilde{R}(z) = [K(z) - z]^{-1}, \quad \forall z \in \mathbb{C}\backslash(\sigma(H_0) \cup \sigma(H)). \tag{17}$$

B. The boundary values of $\tilde{R}(z)$ and its large energy behavior

From the assumption on the form factors, every $v_m^*(\omega)v_n(\omega)$ is continued to the whole complex plane as a meromorphic function which we merely denote as $v_m^*(z)v_n(z)$. It may have a finite number of poles. Then, it follows from Lemma A.1 that $S(z)$ can be reduced to the form

$$S(z) = S(0) + A(z) - (\log(-z))\Gamma(z), \tag{18}$$

where we choose $\arg(-z)=\arg(z)-\pi$ and $0<\arg(z)<2\pi$. The matrix $\Gamma(z)$ is defined with the components

$$\Gamma_{mn}(z) := v_m^*(z)v_n(z), \tag{19}$$

and satisfies $\Gamma(z)\to 0$ as $z\to 0$ in $\mathbb{C}$. $S(0)$ is the limit of $S(z)$ as $z\to 0$ in $\mathbb{C}\backslash[0,\infty)$, which turns out to be unique. Indeed, as we see from the Appendix in Ref. 21, $S_{mn}(0)=\int_0^\infty v_m^*(\omega)v_n(\omega)/\omega \mathrm{d}\omega$. $A(z)$ is then defined through Eq. (18) and becomes a Hermitian matrix for real ω, whose components are the rational functions of z without any singularity on $[0,\infty)$. By definition, $A(z)$ satisfies $A(z)\to 0$ as $z\to 0$. One sees that the boundary values of $S(z)$ at the half line $(0,\infty)$ exist and satisfy[10]

$$\lim_{\epsilon\to+0} S(\omega \pm i\epsilon) = D(\omega) \pm \pi i\Gamma(\omega), \tag{20}$$

where

$$D(\omega) := S(0) + A(\omega) - (\log \omega)\Gamma(\omega). \tag{21}$$

The matrix $D(\omega)$ is just of the components

$$D_{mn}(\omega) := P\int_0^\infty \frac{v_m^*(\omega')v_n(\omega')}{\omega'-\omega}\mathrm{d}\omega', \tag{22}$$

where P denotes the principal value of the integral. Note that both $D(\omega)$ and $\Gamma(\omega)$ are Hermitian matrices and $\Gamma(\omega)\geqslant 0$.

In all the discussion developed in the following, we assume that

$$\det[K^\pm(\omega)-\omega]\neq 0, \quad \forall\ \omega>0, \tag{23}$$

where we introduced

$$K^\pm(\omega) := \lim_{\epsilon\to+0} K(\omega\pm i\epsilon) = K_0 - \lambda^2 D(\omega) \mp \lambda^2\pi i\Gamma(\omega), \quad \forall\ \omega>0. \tag{24}$$

It is worth noting that condition (23) is equivalent to the requirement of no positive eigenvalues of H_0, whose eigenstates are normalizable. Indeed, if $\det[K^\pm(\omega)-\omega]=0$ for some $\omega>0$, there is a nonzero vector $|\eta\rangle=\Sigma_{n=1}^N \eta_n|n\rangle\in\mathbb{C}^N$ such that $[K^\pm(\omega)-\omega]|\eta\rangle=0$. Since both $D(\omega)$ and $\Gamma(\omega)$ are Hermitian matrices, the latter equation implies that

$$\langle\eta|[K_0-\omega-\lambda^2 D(\omega)]|\eta\rangle = 0, \quad \langle\eta|\Gamma(\omega)|\eta\rangle = \left|\sum_{n=1}^N v_n(\omega)\eta_n\right|^2 = 0. \tag{25}$$

Note that the latter relation means that $\Gamma(\omega)|\eta\rangle=0$ because $\Gamma(\omega)\geqslant 0$. Thus, Eq. (25) implies that $\Gamma(\omega)|\eta\rangle=0$ and $[K_0-\lambda^2 D(\omega)]|\eta\rangle=\omega|\eta\rangle$, i.e.,

$$\sum_{n=1}^N v_n(\omega)\eta_n = 0, \quad \sum_{n=1}^N [\omega_m\delta_{mn}-\lambda^2 D_{mn}(\omega)]\eta_n = \omega\eta_m, \tag{26}$$

for all $m=1,\ldots,N$. This is merely the condition for the existence of a positive eigenvalue ω of H.[21]

Lemma III.1: *Under the assumption* (23), *it holds that* $\tilde{R}^{\pm}(\omega) := \lim_{\epsilon \to +0} \tilde{R}(\omega \pm i\epsilon)$ *exists for all* $\omega > 0$ *and* $\tilde{R}^{\pm}(\omega) = [K^{\pm}(\omega) - \omega]^{-1}$.

Proof: Under the assumption (23), $[K^{\pm}(\omega) - \omega]^{-1}$ exists. Then

$$\begin{aligned} &\| [K^{\pm}(\omega) - \omega]^{-1} - \tilde{R}(\omega \pm i\epsilon) \| \\ &\quad \leqslant \| [K^{\pm}(\omega) - \omega]^{-1} \| \, \| \pm i\epsilon + \lambda^2 S(\omega \pm i\epsilon) - \lambda^2 D(\omega) \mp \lambda^2 \pi i \Gamma(\omega) \| \, \| \tilde{R}(\omega \pm i\epsilon) \|. \end{aligned} \tag{27}$$

Note that for any nonzero $|y\rangle \in \mathbb{C}^N$ $(\neq 0)$ there is a nonzero $|x\rangle \in \mathbb{C}^N$ such that $|y\rangle = [K(\omega \pm i\epsilon) - \omega \mp i\epsilon]|x\rangle$. We then obtain

$$\begin{aligned} \frac{\| \tilde{R}(\omega \pm i\epsilon)|y\rangle \|}{\|y\|} &\leqslant \frac{\|x\|}{\| \| [K^{\pm}(\omega) - \omega]|x\rangle \| - \| [\pm i\epsilon + \lambda^2 S(\omega \pm i\epsilon) - \lambda^2 D(\omega) \mp \lambda^2 \pi i \Gamma(\omega)]|x\rangle \|} \\ &\leqslant \left[\inf_{|x\rangle \neq 0, |x\rangle \in \mathbb{C}^N} \frac{\| [K^{\pm}(\omega) - \omega] \|}{\|x\|} - \| \pm i\epsilon + \lambda^2 S(\omega \pm i\epsilon) - \lambda^2 D(\omega) \mp \lambda^2 \pi i \Gamma(\omega) \| \right]^{-1}, \end{aligned} \tag{28}$$

which implies that

$$\overline{\lim_{\epsilon \to +0}} \| \tilde{R}(\omega \pm i\epsilon) \| \leqslant \left[\inf_{|x\rangle \neq 0, |x\rangle \in \mathbb{C}^N} \frac{\| K^{\pm}(\omega) - \omega \|}{\|x\|} \right]^{-1} < \infty, \tag{29}$$

where the norm of an $N \times N$ matrix A is defined by $\|A\| = \sup_{|x\rangle \neq 0, |x\rangle \in \mathbb{C}^N} \|A|x\rangle\| / \|x\|$. In Eq. (28), we used the fact that there is some $\epsilon_0 > 0$ such that for any positive $\epsilon < \epsilon_0$ and for any nonzero $|x\rangle \in \mathbb{C}^N$,

$$\begin{aligned} \frac{\| [K^{\pm}(\omega) - \omega]|x\rangle \|}{\|x\|} &\geqslant \inf_{|x\rangle \neq 0, |x\rangle \in \mathbb{C}^N} \frac{\| [K^{\pm}(\omega) - \omega]|x\rangle \|}{\|x\|} > \| \pm i\epsilon + \lambda^2 S(\omega \pm i\epsilon) - \lambda^2 D(\omega) \mp \lambda^2 \pi i \Gamma(\omega) \| \\ &\geqslant \frac{\| [\pm i\epsilon + \lambda^2 S(\omega \pm i\epsilon) - \lambda^2 D(\omega) \mp \lambda^2 \pi i \Gamma(\omega)]|x\rangle \|}{\|x\|}, \end{aligned} \tag{30}$$

where the assumption (23) is taken into account. Thus, by using Eq. (29), Eq. (27) leads us to

$$\lim_{\epsilon \to +0} \| [K^{\pm}(\omega) - \omega]^{-1} - \tilde{R}(\omega \pm i\epsilon) \| = 0, \tag{31}$$

which completes the proof of the lemma. □

Lemma III.2: *Under the assumption* (23), $\tilde{R}^{\pm}(\omega)$ *is r-times differentiable in* $\omega \in (0, \infty)$, *and it behaves as*

$$\frac{\mathrm{d}^r \tilde{R}^{\pm}(\omega)}{\mathrm{d}\omega^r} = O(\omega^{-r-1}) \text{ as } \omega \to \infty. \tag{32}$$

Proof: We first show the statement for $r = 0$. From the assumption on the form factors and Lemma A.1, one sees that

$$\lim_{\omega \to \infty} D(\omega) = 0, \quad \lim_{\omega \to \infty} \Gamma(\omega) = 0. \tag{33}$$

Since from the assumption (23) $K^{\pm}(\omega) - \omega$ is invertible for all $\omega > 0$, it holds that there is some positive $\bar{\omega} > \omega_N$ such that for any $\omega > \bar{\omega}$,

$$\frac{\| \tilde{R}^{\pm}(\omega)|y\rangle \|}{\|y\|} \leqslant \frac{\|x\|}{\| (K_0 - \omega)|x\rangle \| - \lambda^2 \| [D(\omega) \pm \pi i \Gamma(\omega)]|x\rangle \|} \tag{34}$$

$$\leqslant \frac{1}{\omega - \omega_N - \lambda^2 \|D(\omega) \pm \pi i \Gamma(\omega)\|} = O(\omega^{-1}), \tag{35}$$

where the last inequality is obtained as follows: we can choose some positive $\bar{\omega} > \omega_N$ such that for any $\omega > \bar{\omega}$,

$$\frac{\|[K_0 - \omega]|x\rangle\|}{\|x\|} \geqslant \min_n\{\omega - \omega_n\} = \omega - \omega_N > \lambda^2 \|D(\omega) \pm \pi i \Gamma(\omega)\| \geqslant \lambda^2 \frac{\|[D(\omega) \pm \lambda^2 \pi i \Gamma(\omega)]|x\rangle\|}{\|x\|}, \tag{36}$$

where Eq. (33) was used. Thus Eq. (35) reads just as Eq. (32) does for $r=0$. In the case of $r \geqslant 1$, we first note that from our assumptions on the form factors and Lemma A.1 again, $A(\omega)$ and $\Gamma(\omega)$, which are connected through $D(\omega)=S_0+A(\omega)-\log \omega\Gamma(\omega)$, also satisfy

$$\frac{\mathrm{d}^r A(\omega)}{\mathrm{d}\omega^r} = O(\omega^{-1-r}), \quad \frac{\mathrm{d}^r \log \omega\Gamma(\omega)}{\mathrm{d}\omega^r} = O(\omega^{-1-r}\log \omega), \tag{37}$$

as $\omega \to \infty$, where we used the estimation that $\mathrm{d}^r\Gamma(\omega)/\mathrm{d}\omega^r = O(\omega^{-1-r})$. Thus, for $r=1$, we have

$$\frac{\mathrm{d}\tilde{R}^{\pm}(\omega)}{\mathrm{d}\omega} = \tilde{R}^{\pm}(\omega)\frac{\mathrm{d}}{\mathrm{d}\omega}[\omega + \lambda^2 D(\omega) \pm \lambda^2 \pi i \Gamma(\omega)]\tilde{R}^{\pm}(\omega) = O(\omega^{-2}), \tag{38}$$

as $\omega \to \infty$, where Eq. (32) for $r=0$ was used. For $r \geqslant 1$, we obtain

$$\frac{\mathrm{d}^r \tilde{R}^{\pm}(\omega)}{\mathrm{d}\omega^r} = \sum_{j=1}^{r} {\sum_{\{s_i\}_{i=1}^j}}' a^{(r)}(\{s_i\}_{i=1}^j) \left\{ \prod_{i=1}^{j} \tilde{R}^{\pm}(\omega) \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2 \pi i \Gamma(\omega)] \right\} \tilde{R}^{\pm}(\omega), \tag{39}$$

where $a^{(r)}(\{s_i\}_{i=1}^j)$ is an appropriate positive integer. Note that the symbol $(')$ means that the summation over $\{s_i\}_{i=1}^j$ is taken under the condition that $s_i \geqslant 1$ for all i and $\Sigma_{i=1}^j s_i = r$. If $r=1$, Eq. (39) reproduces Eq. (38) with $a^{(1)}(\{s_i\}_{i=1}^1)=1$. In the general case, if Eq. (39) holds for $r=k$, then its derivative is made up of a linear combination of

$$\left\{ \prod_{i=1}^{j+1} \tilde{R}^{\pm}(\omega) \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2 \pi i \Gamma(\omega)] \right\} \tilde{R}^{\pm}(\omega), \tag{40}$$

where $\Sigma_{i=1}^{j+1} s_i = k+1$ for $1 \leqslant j \leqslant k$, and

$$\left\{ \prod_{i=1}^{j+1} \tilde{R}^{\pm}(\omega) \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2 \pi i \Gamma(\omega)] \right\} \tilde{R}^{\pm}(\omega), \tag{41}$$

where $\Sigma_{i=1}^{j} s_i = k+1$ for $1 \leqslant j \leqslant k$. On the other hand, they are actually included in the right-hand side (rhs) of Eq. (39) for $r=k+1$. Thus Eq. (39) is valid for all integer $r \geqslant 1$. Let us now evaluate the asymptotic behavior of $\mathrm{d}^r\tilde{R}^{\pm}(\omega)/\mathrm{d}\omega^r$ for large ω. One can see that the summand for $j=r$ in Eq. (39), where all $s_i=1$, contributes $O(\omega^{-r-1})$ to $\mathrm{d}^r\tilde{R}^{\pm}(\omega)/\mathrm{d}\omega^r$, while the other summands for $j<r$ specified by $\{s_i\}_{i=1}^j$ contribute $O(\omega^{-r-1-2s_0}(\log \omega)^{s_0}))$ at most, where s_0 is a number of s_i satisfying $s_i \geqslant 2$ and never vanishes for $j<r$. Therefore, the summand dominating for large ω is that for $j=r$. Since we recursively show $a^{(r)}(\{s_1\}_{i=1}^r)=r!$, which never vanishes, the statement is proved. □

IV. CLASSIFICATION OF THE ZERO-ENERGY SINGULARITY OF $\tilde{R}^{\pm}(\omega)$

In order to prescribe the zero energy resonance in the N-level Friedrichs model, we should identify the zero energy eigenstates in this model which either belong to or do not belong to $\mathcal{H}$. In

the case of the short-range potential systems,[14] this task needs some elaborate examination with an appropriately extended Hilbert space. On the other hand, in our case, it is rather easily performed, as is seen in the following.

Let us first see whether the eigenvector $|\psi\rangle \in \mathbb{C}^N$ of $K_0 - \lambda^2 S(0)$, belonging to the zero eigenvalue, can be actually extended to the eigenvector of H belonging to the zero eigenvalue of H. If $|\Psi\rangle = |\psi\rangle + |f\rangle \in D(H) \subset \mathcal{H}$ is a zero eigenvector of H, it should satisfy $H|\Psi\rangle = 0$, or equivalently[21]

$$\omega_n \psi_n + \lambda \langle v_n | f \rangle = 0 \text{ for } n = 1, \ldots, N, \quad \omega f(\omega) + \lambda \sum_{n=1}^{N} \psi_n v_n(\omega) = 0. \tag{42}$$

The latter equation of Eq. (42) is immediately solved as

$$f(\omega) = -\lambda \frac{\sum_{n=1}^{N} \psi_n v_n(\omega)}{\omega}, \tag{43}$$

which should be square integrable because we intend to find $|\Psi\rangle$ in $\mathcal{H}$. If this is the case, $\omega f(\omega) \in L^2((0,\infty))$, i.e., $|\Psi\rangle \in D(H)$ is ensured, and the substitution of Eq. (43) into $\langle v_n | f \rangle$ is safely done. Then, we find that the former equation of Eq. (42) is nothing more than

$$(K_0 - \lambda^2 S(0))|\psi\rangle = K(0)|\psi\rangle = 0, \tag{44}$$

where $K(0) := K^{\pm}(0) = K_0 - \lambda^2 S(0)$. However, it is noted that such an $f(\omega)$ associated with $|\psi\rangle$ is not necessarily square integrable. Hence, we shall decompose the zero eigenspace of $K(0)$, denoted by $M = \{|\psi\rangle \in \mathbb{C}^N | K(0)|\psi\rangle = 0\}$, into two kinds of subspaces: $M_1 = (M_0 \oplus M_2)^{\perp}$ and $M_2 = \{|\psi\rangle \in M | f(\omega) \in L^2((0,\infty))\}$. Here $M_0 = M^{\perp}$, and $D^{\perp}$ denotes the orthogonal complement of the subspace D. In short we have $\mathbb{C}^N = M_0 \oplus M_1 \oplus M_2$. Then, as is expected from the definition, we have

$$M_1 \subset \{|\psi\rangle \in M | f(\omega) \notin L^2((0,\infty))\}. \tag{45}$$

Note that in general the subset on the rhs of the above is not a subspace. We call 0 the *zero energy resonance* (or merely *zero resonance*) of H if M_1 is not empty. We also introduce the projection operators Q_0, Q_1, and Q_2, associated with M_0, M_1, and M_2, respectively. What we next do is to introduce the terminology following the study of Jensen and Kato.[14]

Definition IV.1: We call the system a *regular* case if it holds that $0 \notin \sigma(K(0))$, i.e.,

$$\det[K(0)] \neq 0. \tag{46}$$

In this case, 0 is said to be a *regular* point for H.

Definition IV.2: We call the system the *exceptional* case if, instead of Eq. (46), it holds that $0 \in \sigma(K(0))$, i.e.,

$$\det[K(0)] = 0. \tag{47}$$

In particular, if 0 is a resonance but not an eigenvalue ($Q_1 \neq 0$, $Q_2 = 0$), 0 is said to be an *exceptional* point for H of the *first kind*. If 0 is not a resonance, but an eigenvalue ($Q_1 = 0$, $Q_2 \neq 0$), 0 is said to be an exceptional point of the *second kind*. If 0 is both a resonance and an eigenvalue ($Q_1 \neq 0$, $Q_2 \neq 0$), 0 is said to be an exceptional point of the *third kind*.

We here remark that in general a nontrivial solution of Eq. (44) does not exist, however we can find a special case where such a solution surely exists. Suppose that N_+ eigenvalues ω_n of H_0 are positive, and all form factors $v_n(\omega)$ satisfying the assumption (9) are linearly independent. Then increasing λ gradually from 0 to ∞, we can find some critical values of λ for which $K(0)$ has the zero eigenvalue. Let us denote the nth eigenvalue of $K(0)$ by $\kappa_n(0)$ where $\kappa_1(0) \leqslant \kappa_2(0) \leqslant \cdots \leqslant \kappa_N(0)$. Then, $\kappa_n(0)$ turns out to satisfy the inequality

$$\omega_n - \lambda^2\sigma_N(0) \leqslant \kappa_n(0) \leqslant \omega_n - \lambda^2\sigma_1(0), \tag{48}$$

where both of $\sigma_1(0)$ and $\sigma_N(0)$ are positive constants and ensured not to vanish.[21] Thus, for a sufficiently small $|\lambda|$ $\kappa_n(0)$ for each $n \geqslant N-N_+ +1$ should be positive, while for a sufficiently large $|\lambda|$ they should be negative. Furthermore, one easily sees that all $\kappa_n(0)$ are continuous functions of λ^2. Therefore, we conclude from the intermediate value theorem that there is at least one critical value of λ to make $\kappa_n(0)=0$ for each $n \geqslant N-N_+ +1$. We can actually find such special values of λ in Fig. 1 depicted in Ref. 21. The example mentioned here could be treated in a more general way with resort to the analytic Fredholm theorem,[26,27] which tells us at most a finite number of the critical values exists.

It is also worth remarking that the existence of the zero energy eigenstates that either belong to or not to the Hilbert space necessarily prescribes the small energy behavior of the form factors in the following way. Remember that under the assumption on the form factors, $\Gamma(\omega)$ defined by Eq. (19) has an asymptotic form like

$$\Gamma(\omega) = \sum_{n=1}^{N} \omega^n \Gamma_n + O(\omega^{N+1}), \tag{49}$$

as $\omega \to +0$. Then, if $|\psi\rangle \in M_1$ exists, it should satisfy

$$\langle\psi|\Gamma_1|\psi\rangle \neq 0. \tag{50}$$

In fact, if $\langle\psi|\Gamma_1|\psi\rangle=0$, we see that $f(\omega)$ in Eq. (43) has to satisfy $|f(\omega)|^2=\lambda^2\langle\psi|\Gamma(\omega)|\psi\rangle/\omega^2 = O(1)$ as $\omega \to +0$, however which concludes that $f(\omega)$ is square integrable. This contradicts the assumption that $|\psi\rangle \in M_1$. In order to make the condition (50) be satisfied, at least Γ_1 should not vanish identically. We can find such form factors in the physical systems for the spontaneous emission process of photons from the hydrogen atom[15,22] and the quantum dot.[16] On the other hand, the discussion mentioned here immediately implies the fact that if $|\psi\rangle \in M_2$ exists, this time it should satisfy

$$\langle\psi|\Gamma_1|\psi\rangle = 0, \tag{51}$$

which just ensures the requirement that $f(\omega) \in L^2((0,\infty))$. However, note that Eq. (51) does not imply $\Gamma_1=0$ identically and only requires $\Gamma_1=0$ on the subspace M_2.

A. The small-energy behavior of $\tilde{R}^{\pm}(\omega)$ in the regular case

In this case, the same as in Eq. (31), we can show that $\tilde{R}^{\pm}(0)=(K(0))^{-1}$. Furthermore, we can choose some positive $\omega_0>0$ such that

$$\|(K(0))^{-1}\|\,\|[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega) - \lambda^2 S(0)]\| < 1, \tag{52}$$

for all positive $\omega<\omega_0$. Then, $\tilde{R}^{\pm}(\omega)$ is expanded as a Neumann series,

$$\tilde{R}^{\pm}(\omega) = \{K(0)[1-(K(0))^{-1}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega) - \lambda^2 S(0)]]\}^{-1} = \lim_{N\to\infty} S_N(\omega), \tag{53}$$

where

$$S_N(\omega) = \sum_{j=0}^{N} \{(K(0))^{-1}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega) - \lambda^2 S(0)]\}^j (K(0))^{-1}, \tag{54}$$

for all positive $\omega<\omega_0$ with $\{(K(0))^{-1}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)-\lambda^2 S(0)]\}^0=1$. Under our assumptions on the form factors, $A(\omega)$ defined in Eq. (21) is asymptotically expanded as

$$A(\omega) = \sum_{n=1}^{N} \omega^n A_n + O(\omega^{N+1}), \tag{55}$$

as $\omega \to 0$. By using Eqs. (49) and (55), it also follows that

$$D(\omega) = S(0) - \omega \log \omega \Gamma_1 + \omega A_1 + O(\omega^2 \log \omega), \tag{56}$$

as $\omega \to +0$. Then, Eq. (53) tells us the dominant asymptotic behavior of $\tilde{R}^{\pm}(\omega)$ becomes

$$\tilde{R}^{\pm}(\omega) = (K(0))^{-1} + O(\omega \log \omega), \tag{57}$$

as $\omega \to +0$, where $(K(0))^{-1}$ never vanishes in the regular case.

B. The small-energy behavior of $\tilde{R}(z)$ in the exceptional case of the first kind

In the exceptional case of the first kind, from the definition, $Q_1 \neq 0$ while $Q_2 = 0$, so that $Q_0 + Q_1 = 1$. Then, $\tilde{R}(z)$ is divided into the following four terms,

$$\tilde{R}(z) = Q_0 \tilde{R}(z) Q_1 + Q_0 \tilde{R}(z) Q_0 + Q_1 \tilde{R}(z) Q_0 + Q_1 \tilde{R}(z) Q_1. \tag{58}$$

We now introduce the four matrices:

$$E_{kl}(z) = Q_k [K(z) - z] Q_l = Q_k [K_0 - z - \lambda^2 [S(0) + A(z) - (\log z)\Gamma(z) + i\pi\Gamma(z)]] Q_l, \tag{59}$$

where $k, l = 0, 1$, and $\log(-z) - \log z = -i\pi$ is used. From the relation that $[K(z) - z]\tilde{R}(z) = 1$, they satisfy

$$E_{k0} Q_0 \tilde{R} Q_l + E_{k1} Q_1 \tilde{R} Q_l = Q_k \delta_{kl}, \tag{60}$$

for $k, l = 0, 1$. To solve the above equations we need to check whether E_{11} and E_{00} are invertible in the subspaces M_1 and M_0, respectively. By using Eq. (49), $E_{11}(z)$ is rewritten as

$$E_{11}(z) = \lambda^2 z (\log z) Q_1 \Gamma_1 Q_1 - z Q_1 - \lambda^2 Q_1 \{A(z) - (\log z)[\Gamma(z)] - z\Gamma_1] + i\pi\Gamma(z)\} Q_1, \tag{61}$$

where $Q_1 K(0) Q_1 = 0$ is used. Note that $A(z) = O(z)$ and $\Gamma(z) - z\Gamma_1 = O(z^2)$ for our form factors, so that all terms excepting the first one of the rhs of Eq. (61) are of the order of $O(z)$. Furthermore, the exceptional case of the first kind imposes the fact that $Q_1 \Gamma_1 Q_1 \neq 0$ [see Eq. (50)], and $Q_1 \Gamma_1 Q_1$ is positive definite in M_1 and thus invertible in M_1. Hence, $E_{11}(\omega)$ is invertible for sufficiently small $|z| > 0$, and the inverse can be expanded by the Neumann series as

$$E_{11}^{-1}(z) = \sum_{j=0}^{\infty} (\tilde{E}_{11}(z))^j \frac{1}{\lambda^2 z \log z} (Q_1 \Gamma_1 Q_1)^{-1} \tag{62}$$

$$= \frac{1}{\lambda^2 z \log z} (Q_1 \Gamma_1 Q_1)^{-1} + O(z^{-1} (\log z)^{-2}) = O(z^{-1} (\log z)^{-1}), \tag{63}$$

for small $|z|$, where we define

$$\tilde{E}_{11}(z) := \frac{1}{\lambda^2 z \log z} (Q_1 \Gamma_1 Q_1)^{-1} \{z Q_1 + \lambda^2 Q_1 \{A(z) - (\log z)[\Gamma(z) - z\Gamma_1] + \pi i \Gamma(z)\} Q_1\}, \tag{64}$$

which behaves as $1/\log z$ as $z \to 0$. For E_{00} we have

$$E_{00}(z) = Q_0K(0)Q_0 - Q_0[z + \lambda^2[A(z) - (\log z)\Gamma(z) + i\pi\Gamma(z)]]Q_0, \tag{65}$$

where the first term of the above is invertible in M_0, and the last term vanishes as $z \to 0$. Hence, $E_{00}(z)$ is invertible in M_0 for sufficiently small $|z| > 0$ and is expanded as

$$E_{00}^{-1}(z) = -\sum_{j=0}^{\infty} \{[Q_0K(0)Q_0]^{-1}[z + \lambda^2[A(z) - (\log z)\Gamma(z) + i\pi\Gamma(z)]]Q_0\}^j[Q_0K(0)Q_0]^{-1} = O(1), \tag{66}$$

for small $|z|$. Furthermore, we obtain

$$E_{kl}(z) = -\lambda^2 Q_k[A(z) - (\log z)\Gamma(z) + \pi i\Gamma(z)]Q_l = O(z \log z), \tag{67}$$

for $k \neq l$ as $z \to 0$, because $Q_0K(0)Q_1 = Q_1K(0)Q_0 = 0$. Solving Eq. (60), we obtain[28]

$$Q_0\tilde{R}Q_0 = (E_{00} - E_{01}E_{11}^{-1}E_{10})^{-1} = O(1), \tag{68}$$

$$Q_0\tilde{R}Q_1 = -E_{00}^{-1}E_{01}Q_1\tilde{R}Q_1 = -E_{00}^{-1}E_{01}(E_{11} - E_{10}E_{00}^{-1}E_{01})^{-1} = O(1), \tag{69}$$

$$Q_1\tilde{R}Q_0 = -Q_1\tilde{R}Q_1E_{10}E_{00}^{-1} = -(E_{11} - E_{10}E_{00}^{-1}E_{01})^{-1}E_{10}E_{00}^{-1} = O(1), \tag{70}$$

$$Q_1\tilde{R}Q_1 = (E_{11} - E_{10}E_{00}^{-1}E_{01})^{-1} = O(z^{-1}(\log z)^{-1}). \tag{71}$$

It is worth noting that since the relation $[K(z) - z]\tilde{R}(z) = 1$ is analytically continued to the second Riemann sheet through the cut $[0, \infty)$, the above-mentioned results are also valid for such a continued region and the estimations obtained here can be applied without any corrections.

When we consider the small energy behavior of $\tilde{R}^-(\omega)$, it is convenient to expand E_{11}, differently from Eq. (61), as

$$E_{11}(z) = \lambda^2 z(\log z - 2\pi i)Q_1\Gamma_1Q_1 - zQ_1 - \lambda^2 Q_1\{A(z) - (\log z - 2\pi i)[\Gamma(z) - z\Gamma_1] - i\pi\Gamma(z)\}Q_1. \tag{72}$$

All the above-obtained results are only changed by replacing the term $\log z$ with $\log z - 2\pi i$. Then, we can obtain from Eq. (61)

$$E_{11}^+(\omega) = \lim_{\epsilon \to +0} E_{11}(\omega + i\epsilon) = \lambda^2(\log \omega)Q_1\Gamma(\omega)Q_1 - \omega Q_1 - \lambda^2 Q_1[A(\omega) - i\pi\Gamma(\omega)]Q_1, \tag{73}$$

while from Eq. (72)

$$E_{11}^-(\omega) = \lim_{\epsilon \to +0} E_{11}(\omega - i\epsilon) = \lambda^2(\log \omega)Q_1\Gamma(\omega)Q_1 - \omega Q_1 - \lambda^2 Q_1[A(\omega) + i\pi\Gamma(\omega)]Q_1. \tag{74}$$

C. The small-energy behavior of $\tilde{R}(z)$ in the exceptional case of the second kind

In the exceptional case of the second kind, it follows that $Q_1 = 0$, $Q_2 \neq 0$, and $Q_0 + Q_2 = 1$. Let us consider the asymptotic behavior of the reduced resolvent at small energies, which is written in the following form, $\tilde{R}(z) = \Sigma_{k,l=0,2}Q_k\tilde{R}(z)Q_l$. We now introduce the four matrices again,

$$E_{kl}(z) = Q_k[K(z) - z]Q_l, \tag{75}$$

where $k, l = 0, 2$. From the relation that $[K(z) - z]\tilde{R}(z) = 1$, they satisfy that

$$E_{k0}Q_0\tilde{R}Q_l + E_{k2}Q_2\tilde{R}Q_l = Q_k\delta_{kl}, \tag{76}$$

for $k,l=0,2$. This time, E_{22} and E_{00} are invertible in M_2 and M_0, respectively. In fact, from Eqs. (49) and (55) we have

$$E_{22}(z) = -zQ_2(1+\lambda^2 A_1)Q_2 - \lambda^2 Q_2[A(z) - zA_1 - (\log z)\Gamma(z) + i\pi\Gamma(z)]Q_2, \tag{77}$$

where $Q_2K(0)Q_2=0$ was used. Note that since $A(z)-zA_1=O(z^2)$ and $Q_2\Gamma_1Q_2=0$ [see Eq. (51)], the second term of the rhs of Eq. (77) is of the order of $O(z^2\log z)$. Furthermore, since $Q_2A_1Q_2\geqslant 0$ from $Q_2\Gamma_1Q_2=0$ and Lemma A.2, $Q_2(1+\lambda^2A_1)Q_2>0$ and invertible in M_2. These facts bring us the fact that $E_{22}(z)$ is invertible in M_2 for sufficiently small $z>0$, that is

$$E_{22}^{-1}(z) = -\sum_{j=0}^{\infty}(-\tilde{E}_{22}(z))^j\frac{1}{z}[Q_2(1+\lambda^2A_1)Q_2]^{-1} \tag{78}$$

$$= \frac{1}{z}[Q_2(1+\lambda^2A_1)]Q_2{}^{-1} + O(\log z) = O(z^{-1}), \tag{79}$$

where

$$\tilde{E}_{22}(z) := \frac{1}{z}[Q_2(1+\lambda^2A_1)Q_2]^{-1}\lambda^2Q_2[A(z) - zA_1 - (\log z)\Gamma(z) + i\pi\Gamma(z)]Q_2. \tag{80}$$

For E_{00}, we next have

$$E_{00}(z) = Q_0K(0)Q_0 - Q_0[z + \lambda^2[A(z) - (\log z)\Gamma(z) + i\pi\Gamma(z)]]Q_0, \tag{81}$$

where the first term of the above is invertible in M_0, and the last term vanishes as $|z|\to 0$. Hence, $E_{00}(z)$ is invertible in M_0 for sufficiently small $|z|>0$, and the inverse is obtained as a Neumann series. On the other hand, E_{20} and E_{02} behave as

$$E_{kl}(z) = Q_k[-z(1+\lambda^2A_1) - \lambda^2[A(z) - zA_1 - (\log z)\Gamma(z) + \pi i\Gamma(z)]]Q_l = O(z), \tag{82}$$

for small $|z|$ where $k\neq l$. Solving Eq. (76) as in Eqs. (68)–(71), one sees that $Q_0\tilde{R}Q_0=O(1)$, for $k,l=0,2$, except

$$Q_2\tilde{R}Q_2 = (E_{22} - E_{20}E_{00}^{-1}E_{02})^{-1} = O(z^{-1}), \tag{83}$$

as $z\to 0$. In particular, the last equation is expanded as

$$Q_2\tilde{R}(z)Q_2 = \sum_{j=0}^{\infty}[E_{22}^{-1}E_{20}E_{00}^{-1}E_{02}]^jE_{22}^{-1} = -\frac{1}{z}[Q_2(1+\lambda^2A_1)Q_2]^{-1} + O(\log z), \tag{84}$$

for small $|z|$, where we used Eq. (79).

We now remark that the zero energy eigenspace of H denoted by $\mathcal{N}_0$ is completely characterized by M_2. That is, there is a bijection from $M_2\oplus\{0\}$ to $\mathcal{N}_0$. From the discussion concerning Eqs. (42)–(44), for any $|\Psi\rangle\in\mathcal{M}_0$, there is a vector $|\psi\rangle\in M_2\oplus\{0\}$ such that

$$|\Psi\rangle = |\psi\rangle - \lambda\int_0^{\infty}\frac{\sum_{n=1}^{N}v_n(\omega)\psi_n}{\omega}|\omega\rangle d\omega = [1-\lambda R_0(0)V]|\psi\rangle, \tag{85}$$

where V is restricted to $\mathbb{C}^N\oplus\{0\}$ and $R_0(0)$ is the (unbounded) multiplication operator of $1/\omega$ in $L^2((0,\infty))$. Then we see $V|\psi\rangle\in D(R_0(0))$ because $|\psi\rangle\in M_2\oplus\{0\}$. Thus $1-\lambda R_0(0)V$ is well defined as an operator from $M_2\oplus\{0\}$ to $\mathcal{H}$. Now, Eq. (85) tells us that $1-\lambda R_0(0)V$ is a surjection from $M_2\oplus\{0\}$ to $\mathcal{N}_0$. On the other hand, for any $|\Psi\rangle\in\mathcal{N}_0$,if $|\Psi\rangle=0$, i.e., $0=\langle\Psi|\Psi\rangle$, Eq. (85) implies

that $0=\langle\Psi|\Psi\rangle \geqslant \langle\psi|\psi\rangle$. Therefore, $1-\lambda R_0(0)V$ is also an injection from $M_2 \oplus \{0\}$ to $\mathcal{N}_0$, and the proof is completed.

D. The small-energy behavior of $\tilde{R}^{\pm}(\omega)$ in the exceptional case of the third kind

In the exceptional case of the third kind, from the definition, $Q_1 \neq 0$, $Q_2 \neq 0$, and $Q_0+Q_1+Q_2=1$. The reduced resolvent is written in the form, $\tilde{R}^{\pm}(\omega)=\Sigma_{k,l=0}^{2} Q_k \tilde{R}^{\pm}(\omega) Q_l$. This time, we need nine matrices,

$$E_{kl}^{\pm}(\omega) = Q_k[K^{\pm}(\omega) - \omega]Q_l, \tag{86}$$

for $k,l=0,1,2$. From the relation that $[K^{\pm}(\omega)-\omega]\tilde{R}^{\pm}(\omega)=1$, they satisfy that

$$E_{k0}^{\pm} Q_0 \tilde{R}^{\pm} Q_l + E_{k1}^{\pm} Q_1 \tilde{R}^{\pm} Q_l + E_{k2}^{\pm} Q_2 \tilde{R}^{\pm} Q_l = Q_k \delta_{kl}, \tag{87}$$

for $k,l=0,1,2$. The asymptotic behaviors of $E_{kl}^{\pm}(\omega)$ are essentially examined in the preceding subsections, except for $E_{12}^{\pm}(\omega)$ and $E_{21}^{\pm}(\omega)$. Then, $E_{12}^{\pm}(\omega)$ becomes

$$E_{12}^{\pm}(\omega) = -\omega\lambda^2 Q_1 A_1 Q_2 - \lambda^2 Q_1[A(\omega) - \omega A_1 - (\log\omega)[\Gamma(\omega) - \omega\Gamma_1] \pm \pi i[\Gamma(\omega) - \omega\Gamma_1]]Q_2 \tag{88}$$

$$= -\omega\lambda^2 Q_1 A_1 Q_2 + O(\omega^2 \log\omega), \tag{89}$$

where $Q_1 K(0) Q_2=0$, $Q_1 Q_2=0$, and $\Gamma_1 Q_2=0$ are used. The last relation follows from the fact that $Q_2\Gamma_1 Q_2=0$ and $\Gamma_1 \geqslant 0$. In addition, since $Q_1\Gamma(\omega)Q_2=O(\omega^2)$, we see that $Q_1 A_1 Q_2 = \int_0^\infty Q_1\Gamma(\omega)Q_2\omega^{-2}\mathrm{d}\omega$. By the same way, we also see that

$$E_{21}^{\pm}(\omega) = -\omega\lambda^2 Q_1 A_1 Q_2 + O(\omega^2 \log\omega). \tag{90}$$

To solve Eq. (87), let us now put the $N\times N$ matrix $\mathbf{E}$ as

$$\mathbf{E} = \begin{bmatrix} E_{00} & E_{01} & E_{02} \\ E_{10} & E_{11} & E_{12} \\ E_{20} & E_{21} & E_{22} \end{bmatrix}, \tag{91}$$

and partition it into $\mathbf{A}=\begin{bmatrix} E_{00} & E_{01} \\ E_{10} & E_{11} \end{bmatrix}$, $\mathbf{B}=\begin{bmatrix} E_{02} \\ E_{12} \end{bmatrix}$, $\mathbf{C}=[E_{20} \;\; E_{21}]$, $\mathbf{D}=[E_{22}]$. Then, from the inverse matrix formula again, $\mathbf{E}^{-1}$ $(=\tilde{R})$ is expressed as[28]

$$\mathbf{E}^{-1} = \begin{bmatrix} [\mathbf{A}-\mathbf{B}\mathbf{D}^{-1}\mathbf{C}]^{-1} & -\mathbf{A}^{-1}\mathbf{B}[\mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}]^{-1} \\ -[\mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}]^{-1}\mathbf{C}\mathbf{A}^{-1} & [\mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}]^{-1} \end{bmatrix}. \tag{92}$$

The validities of $\mathbf{A}^{-1}$ and $\mathbf{D}^{-1}$ are already ensured in the exceptional cases of the first and second kinds, respectively. Then, one sees that since $\mathbf{A}^{-1}=O(\omega^{-1}(\log\omega)^{-1})$, $\mathbf{B}=O(\omega)$, $\mathbf{C}=O(\omega)$, and $\mathbf{D}^{-1}=O(\omega^{-1})$, it holds that $\mathbf{A}^{-1}\mathbf{B}\mathbf{D}^{-1}\mathbf{C}=O((\log\omega)^{-1})$. Thus, $[\mathbf{A}-\mathbf{B}\mathbf{D}^{-1}\mathbf{C}]^{-1}$ exists for small ω and $[\mathbf{A}-\mathbf{B}\mathbf{D}^{-1}\mathbf{C}]^{-1}=O(\omega^{-1}(\log\omega)^{-1})$. We also show that $[\mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}]^{-1}$ exists for small ω and $[\mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}]^{-1}=O(\omega^{-1})$. To obtain the asymptotic forms of the matrix components of $\mathbf{E}^{-1}$ explicitly, some redundant calculation is required; however, it could be achieved by a manner as similar to that used in the preceding subsections.

V. ASYMPTOTIC EXPANSION OF THE REDUCED RESOLVENT AT SMALL *z*

We examine the small-energy behavior of the reduced resolvent only for the regular case and the exceptional case of the first kind. This analysis is crucial for determining the asymptotic behavior of the reduced time evolution operator at long times.

A. The regular case

Here, we introduce $\tilde{A}(\omega) := \omega/\lambda^2 + A(\omega)$ and suppose that $\tilde{A}(\omega)$ and $\Gamma(\omega)$ behave as

$$\tilde{A}(\omega) := \frac{1}{\lambda^2}\omega + A(\omega) = \sum_{n=n_a}^{n_a+N} \omega^n \tilde{A}_n + O(\omega^{n_a+N+1}), \quad \Gamma(\omega) = \sum_{n=n_b}^{n_b+N} \omega^n \Gamma_n + O(\omega^{n_b+N+1}), \tag{93}$$

as $\omega \to 0$, respectively, that is, $\tilde{A}_n = 0$ for all $n < n_a$ and $\Gamma_{n_b} = 0$ for all $n < n_b$, while $\tilde{A}_{n_a} \neq 0$ and $\Gamma_{n_b} \neq 0$. Then, we obtain

$$\frac{1}{\lambda^2}\omega + D(\omega) = S(0) + \tilde{A}(\omega) - (\log \omega)\Gamma(\omega) = S(0) - \omega^{n_b} \log \omega \Gamma_{n_b} + \omega^{n_a}\tilde{A}_{n_a} + O(\omega h(\omega)), \tag{94}$$

as $\omega \to +0$, where

$$h(\omega) = \begin{cases} \omega^{n_b} \log \omega & (n_b \leqslant n_a) \\ \omega^{n_a} & (n_b > n_a) \end{cases} \tag{95}$$

It is important to note that the values of two parameters n_a and n_b are not determined independently. We shall here consider n_b as a controllable one. We first note that if $n_b \geqslant 2$ then $n_a = 1$ should be concluded, because from Lemma A.2 we have $A_1 > 0$, so that $\tilde{A}_1 = 1/\lambda^2 + A_1 > 0$ holds. Therefore, the conditions $n_b \leqslant n_a$ and $n_b > n_a$ can be realized only in the situations

$$n_b = 1 \text{ and } n_a \geqslant 1, \quad n_b \geqslant 2 \text{ and } n_a = 1, \tag{96}$$

respectively.

Lemma V.1: *Assume that* 0 *is a regular point for H. Then the rth derivative of* $\tilde{R}^{\pm}(\omega)$ *asymptotically behaves as*

$$\frac{d^r \tilde{R}^{\pm}(\omega)}{d\omega^r} = \begin{cases} O(1) & (r=0) \\ O(\omega^{1-r}(\log \omega)^{\theta(1-r)}) & (r \geqslant 1) \end{cases}, \quad or \quad \begin{cases} O(1) & (r=0) \\ O(\omega^{[1-r]^+}) & (1 \leqslant r < n_b) \\ O(\omega^{n_b-r}(\log \omega)^{\theta(n_b-r)}) & (n_b \leqslant r \leqslant 2n_b), \end{cases} \tag{97}$$

for $n_b = 1$, *or* $n_b \geqslant 2$, *respectively, as* $\omega \to 0$, *where* $[x]^+ = \max\{x, 0\}$ *and* $\theta(x) = 1$ *for* $x \geqslant 0$ *or* 0 *for* $x < 0$. *In addition, the rth derivative of* $\tilde{R}^{\pm}(\omega)$ *is approximated by that of a finite series*

$$(K(0))^{-1} + (K(0))^{-1}[-\omega^{n_b}(\log \omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\tilde{A}_{n_a} \pm \lambda^2 \pi i \omega^{n_b}\Gamma_{n_b}](K(0))^{-1}, \tag{98}$$

that is, it is shown that

$$\left\| \frac{d^r}{d\omega^r}\{\tilde{R}^{\pm}(\omega) - (K(0))^{-1} - (K(0))^{-1}[-\omega^{n_b}(\log \omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\tilde{A}_{n_a} \pm \lambda^2 \pi i \omega^{n_b}\Gamma_{n_b}](K(0))^{-1}\} \right\|$$

$$= O(\omega^{2-r}(\log \omega)^{1+\theta(2-r)}) \ (r \geqslant 0)$$

$$or \begin{cases} O(\omega^{[2-r]^+}) & (0 \leqslant r \leqslant n_b) \\ O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}) & (n_b + 1 \leqslant r \leqslant 2n_b) \end{cases}, \tag{99}$$

for $n_b = 1$, *or* $n_b \geqslant 2$, *respectively, as* $\omega \to 0$. *Here,* n_a *is restricted to the condition* (96).

Proof: The left-hand side (lhs) of Eq. (99) is written as follows:

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\widetilde{R}^{\pm}(\omega) - (K(0))^{-1} - (K(0))^{-1}[-\omega^{n_b}(\log\omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\widetilde{A}_{n_a} \pm \lambda^2\pi i\omega^{n_b}\Gamma_{n_b}](K(0))^{-1}\} \right\|$$

$$\leqslant \left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\widetilde{R}^{\pm}(\omega) - S_1(\omega)\} \right\| + \left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{S_1(\omega) - (K(0))^{-1} - (K(0))^{-1}[-\omega^{n_b}(\log\omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\widetilde{A}_{n_a} \pm \lambda^2\pi i\omega^{n_b}\Gamma_{n_b}](K(0))^{-1}\} \right\| \tag{100}$$

where $S_N(\omega)$ is defined by Eq. (54). When $r=0$, the first term on the rhs of Eq. (100) is estimated from the special case of Eq. (101) for $N=1$,

$$\|\widetilde{R}^{\pm}(\omega) - S_N(\omega)\| \leqslant \frac{\|\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega) - \lambda^2 S(0)\|^{N+1}\|(K(0))^{-1}\|^{N+2}}{1 - \|(K(0))^{-1}\|\,\|[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega) - \lambda^2 S(0)]\|} = O(h(\omega)^{N+1}), \tag{101}$$

as $\omega \to 0$. When $r \geqslant 1$, instead we have

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\widetilde{R}^{\pm}(\omega) - S_1(\omega)\} \right\|$$

$$\leqslant \left\| \sum_{j=2}^{r} {\sum_{\{s_i\}_{i=1}^{j}}}' a^{(r)}(\{s_i\}_{i=1}^{j}) \left\{ \prod_{i=1}^{j} \widetilde{R}^{\pm}(\omega) \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega)] \right\} \widetilde{R}^{\pm}(\omega) \right\|$$

$$+ \left\| \widetilde{R}^{\pm}(\omega) \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega)]\widetilde{R}^{\pm}(\omega) - \frac{\mathrm{d}^r}{\mathrm{d}\omega^r} S_1(\omega) \right\|, \tag{102}$$

where Eq. (39) is used, and here $s_i \geqslant 1$ and $\Sigma_{i=1}^{j} s_i = r$ should be satisfied. Note that the first term on the rhs of Eq. (102) in the following appears only for $r \geqslant 2$, which is estimated in the following. In the following estimations, we temporarily forget the restriction (96) and consider the two general cases: $n_b \leqslant n_a$ and $n_b > n_a$. In the case of $n_b \leqslant n_a$, we can obtain for $r \geqslant 2$,

$$\left\| \sum_{j=2}^{r} {\sum_{\{s_i\}_{i=1}^{j}}}' a^{(r)}(\{s_i\}_{i=1}^{j}) \left\{ \prod_{i=1}^{j} \widetilde{R}^{\pm}(\omega) \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega)] \right\} \widetilde{R}^{\pm}(\omega) \right\|$$

$$\leqslant \sum_{j=2}^{r} {\sum_{\{s_i\}_{i=1}^{j}}}' a^{(r)}(\{s_i\}_{i=1}^{j}) \|\widetilde{R}^{\pm}(\omega)\|^{j+1} O(\omega^{jn_b - r}) \prod_{i=1}^{j} O((\log\omega)^{\theta(n_b - s_i)})$$

$$= O(\omega^{2n_b - r}(\log\omega)^{\theta(n_b + 1 - r) + \theta(2n_b + 1 - r)}), \tag{103}$$

as $\omega \to 0$. For $n_a < n_b$,

$$\left\| \sum_{j=2}^{r} {\sum_{\{s_i\}_{i=1}^{j}}}' a^{(r)}(\{s_i\}_{i=1}^{j}) \widetilde{R}^{\pm}(\omega) \prod_{i=1}^{j} \left\{ \frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega + \lambda^2 D(\omega) \pm \lambda^2\pi i\Gamma(\omega)]\widetilde{R}^{\pm}(\omega) \right\} \right\|$$

$$= \begin{cases} O(\omega^{[2n_a - r]^+}) & (2 \leqslant r \leqslant n_a + n_b - 1) \\ O(\omega^{n_a + n_b - r}(\log\omega)^{\theta(n_a + n_b - r)}) & (n_a + n_b \leqslant r \leqslant 2n_b), \end{cases} \tag{104}$$

as $\omega \to 0$. We here used that

$$\frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)-\lambda^2 S(0)]$$

$$=O(\omega^{n_b-r}(\log\omega)^{\theta(n_b-r)}),\quad \text{or}\quad \begin{cases} O(\omega^{[n_a-r]^+}) & (0\leqslant r<n_b)\\ O(\omega^{n_b-r}(\log\omega)^{\theta(n_b-r)}) & (r\geqslant n_b)\end{cases}, \tag{105}$$

for $n_b\leqslant n_a$, or $n_a<n_b$, respectively, as $\omega\to 0$. Equation (105) follows from

$$\frac{\mathrm{d}^r\widetilde{A}(\omega)}{\mathrm{d}\omega^r}=O(\omega^{[n_a-r]^+}),\frac{\mathrm{d}^r\Gamma(\omega)}{\mathrm{d}\omega^r}=O(\omega^{[n_b-r]^+}),\quad \frac{\mathrm{d}^r(\log\omega)\Gamma(\omega)}{\mathrm{d}\omega^r}=O(\omega^{n_b-r}(\log\omega)^{\theta(n_b-r)}), \tag{106}$$

as $\omega\to 0$. Incorporating Eqs. (103)–(105), with

$$\left\|\frac{\mathrm{d}^r\widetilde{R}^{\pm}(\omega)}{\mathrm{d}\omega^r}\right\|\leqslant\left\|\sum_{j=2}^{r}{\sum_{\{s_i\}_{i=1}^{j}}}'a^{(r)}(\{s_i\}_{i=1}^{j})\left\{\widetilde{R}^{\pm}(\omega)\prod_{i=1}^{j}\frac{\mathrm{d}^{s_i}}{\mathrm{d}\omega^{s_i}}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)]\right\}\widetilde{R}^{\pm}(\omega)\right\|$$
$$+\left\|\widetilde{R}^{\pm}(\omega)\frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)]\widetilde{R}^{\pm}(\omega)\right\|, \tag{107}$$

we have

$$\left\|\frac{\mathrm{d}^r\widetilde{R}^{\pm}(\omega)}{\mathrm{d}\omega^r}\right\|$$

$$=\begin{cases} O(1) & (r=0)\\ O(\omega^{n_b-r}(\log\omega)^{\theta(n_b-r)}) & (r\geqslant 1)\end{cases}\quad or\quad \begin{cases} O(1) & (r=0)\\ O(\omega^{[n_a-r]^+}) & (1\leqslant r<n_b)\\ O(\omega^{n_b-r}(\log\omega)^{\theta(n_b-r)}) & (n_b\leqslant r\leqslant 2n_b)\end{cases}, \tag{108}$$

for $n_b\leqslant n_a$, or $n_a<n_b$, respectively, as $\omega\to 0$. Then, the first part of the statement can be shown under the restriction (96). Let us next examine the second term on the rhs of Eq. (102), which reads for $r\geqslant 1$,

$$\left\|\widetilde{R}^{\pm}(\omega)\frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)]\widetilde{R}^{\pm}(\omega)-\frac{\mathrm{d}^r}{\mathrm{d}\omega^r}S_1(\omega)\right\|$$

$$\leqslant 2\|\widetilde{R}^{\pm}(\omega)-(K(0))^{-1}\|\left\|\frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[\omega+\lambda^2 D(\omega)\pm\lambda^2\pi i\Gamma(\omega)]\right\|\|\widetilde{R}^{\pm}(\omega)\|$$

$$=O(\omega^{2n_b-r}(\log\omega)^{1+\theta(n_b-r)}),\quad or\quad \begin{cases} O(\omega^{n_a+[n_a-r]^+}) & (r<n_b)\\ O(\omega^{n_a+n_b-r}(\log\omega)^{\theta(n_b-r)}) & (r\geqslant n_b),\end{cases} \tag{109}$$

for $n_b\leqslant n_a$ or $n_b>n_a$, respectively, as $\omega\to 0$. We here used Eq. (101) with $N=0$. Therefore, substituting Eqs. (103), (104), and (109) into Eq. (102), one has for $r\geqslant 1$,

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\widetilde{R}^{\pm}(\omega) - S_1(\omega)\} \right\|$$

$$= O(\omega^{2n_b - r}(\log \omega)^{1+\theta(n_b+1-r)}), \quad \text{or} \quad \begin{cases} O(\omega^{[2n_a - r]^+}) & (r \leqslant n_a + n_b - 1) \\ O(\omega^{n_a+n_b-r}(\log \omega)^{\theta(n_a+n_b-r)}) & (n_a + n_b \leqslant r \leqslant 2n_b) \end{cases} \tag{110}$$

for $n_b \leqslant n_a$ or $n_b > n_a$, respectively, as $\omega \to 0$. Note that this estimation is also valid for $r=0$ because it reproduces Eq. (101) for $N=1$.

Let us now evaluate the last term in Eq. (100). For $r \geqslant 0$, we have

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\left\{S_1(\omega) - (K(0))^{-1} - (K(0))^{-1}[-\omega^{n_b}(\log \omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\widetilde{A}_{n_a} \pm \lambda^2\pi i\omega^{n_b}\Gamma_{n_b}](K(0))^{-1}\right\} \right\|$$

$$\leqslant \|(K(0))^{-1}\|^2 \left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}[-(\log \omega)\lambda^2(\Gamma(\omega) - \omega^{n_b}\Gamma_{n_b}) + \lambda^2(\widetilde{A}(\omega) - \omega^{n_a}\widetilde{A}_{n_a})) \pm \lambda^2\pi i(\Gamma(\omega) - \omega^{n_b}\Gamma_{n_b})] \right\|$$

$$= O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}), \quad \text{or} \quad \begin{cases} O(\omega^{[n_a+1-r]^+}) & (0 \leqslant r \leqslant n_b) \\ O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}) & (r \geqslant n_b + 1) \end{cases}, \tag{111}$$

for $n_b \leqslant n_a$ or $n_b > n_a$, respectively, as $\omega \to 0$ for any $r \geqslant 0$. We here used that for $r \geqslant 0$,

$$\frac{\mathrm{d}^r(\Gamma(\omega) - \omega^{n_b}\Gamma_{n_b})}{\mathrm{d}\omega^r} = O(\omega^{[n_b+1-r]^+}), \quad \frac{\mathrm{d}^r(\log \omega)(\Gamma(\omega) - \omega^{n_b}\Gamma_{n_b})}{\mathrm{d}\omega^r} = O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}) \tag{112}$$

as $\omega \to 0$, and so forth. Thus, setting Eqs. (110) and (111) into Eq. (100), we conclude that

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\widetilde{R}^{\pm}(\omega) - (K(0))^{-1} - (K(0))^{-1}[-\omega^{n_b}(\log \omega)\lambda^2\Gamma_{n_b} + \omega^{n_a}\lambda^2\widetilde{A}_{n_a} \pm \lambda^2\pi i\omega^{n_b}\Gamma_{n_b}](K(0))^{-1}\} \right\|$$

$$= \begin{cases} O(\omega^{2n_b-r}(\log \omega)^{1+\theta(n_b+1-r)}) & (r \geqslant 0, n_b = 1) \\ O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}) & (r \geqslant 0, n_b \geqslant 2), \end{cases}$$

$$\text{or} \begin{cases} O(\omega^{[n_a+1-r]^+}) & (0 \leqslant r \leqslant n_b) \\ O(\omega^{n_b+1-r}(\log \omega)^{\theta(n_b+1-r)}) & (n_b + 1 \leqslant r \leqslant 2n_b), \end{cases} \tag{113}$$

for $n_b \leqslant n_a$ or $n_b > n_a$, respectively, as $\omega \to 0$. By taking into account the restriction (96), we can show the last part of the lemma. □

To estimate the long time behavior of the reduced time evolution operator, the above-mentioned lemma seems not precisely appropriate because the reduced time evolution operator is obtained from the Fourier transform of the imaginary part of $\widetilde{R}^+(\omega)$, not from $\widetilde{R}^+(\omega)$ itself, which is explained in the next section. Hence, the following lemma is more appropriate for our purpose.

Lemma V.2: *Assume that* 0 *is a regular point for H. Then the rth derivative of* $\mathrm{Im}\,\widetilde{R}^+(\omega) := (\widetilde{R}^+(\omega) - \widetilde{R}^-(\omega))/2i$ *is approximated by that of*

$$(K(0))^{-1}\lambda^2\pi\omega^{n_b}(\Gamma_{n_b} + \omega\Gamma_{n_b+1} + \omega^2\Gamma_{n_b+2})(K(0))^{-1}, \tag{114}$$

in the sense that for $0 \leqslant r \leqslant n_b + 1$ *the remainder is estimated as*

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\mathrm{Im}\,\tilde{R}^+(\omega) - (K(0))^{-1}\lambda^2\pi\omega^{n_b}(\Gamma_{n_b} + \omega\Gamma_{n_b+1} + \omega^2\Gamma_{n_b+2})(K(0))^{-1}\} \right\|$$

$$= O(\omega^{2-r}\log\omega) \quad \text{or} \quad O(\omega^{1+n_b-r}), \tag{115}$$

for $n_b=1$, *or* $n_b\geqslant 2$, *respectively*, *as* $\omega\to 0$. *For* $r=n_b+2$, *the estimation is replaced by* $O(\omega^{-1})$ *for* $n_b=1$, $O(\log\omega)$ *for* $n_b=2$, *or* $O(1)$ *for* $n_b\geqslant 3$, *respectively*, *as* $\omega\to 0$.

Proof: Since $\mathrm{Im}\,\tilde{R}^+(\omega)=\lambda^2\pi\tilde{R}^+(\omega)\Gamma(\omega)\tilde{R}^-(\omega)$, one has

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}\omega^r}\{\mathrm{Im}\,\tilde{R}^+(\omega) - (K(0))^{-1}\lambda^2\pi\omega^{n_b}(\Gamma_{n_b} + \omega\Gamma_{n_b+1} + \omega^2\Gamma_{n_b+2})(K(0))^{-1}\} \right\| \tag{116}$$

$$\leqslant \lambda^2\pi \sum_{\substack{s\geqslant 0,t\geqslant 0,u\geqslant 0,\\ (s+t+u=r)}}^{r} [F_1(s,t,u) + F_2(s,t,u) + F_3(s,t,u)], \tag{117}$$

with

$$F_1(s,t,u) = C_{stu}\left\| \frac{\mathrm{d}^s\tilde{R}^+(\omega)}{\mathrm{d}\omega^s} \right\| \left\| \frac{\mathrm{d}^t\Gamma(\omega)}{\mathrm{d}\omega^t} \right\| \left\| \frac{\mathrm{d}^u}{\mathrm{d}\omega^u}\{\tilde{R}^-(\omega) - (K(0))^{-1}\} \right\|, \tag{118}$$

$$F_2(s,t,u) = C_{stu}\left\| \frac{\mathrm{d}^s\tilde{R}^+(\omega)}{\mathrm{d}\omega^s} \right\| \left\| \frac{\mathrm{d}^t}{\mathrm{d}\omega^t}\{\Gamma(\omega) - \omega^{n_b}(\Gamma_{n_b} + \omega\Gamma_{n_b+1} + \omega^2\Gamma_{n_b+2})\} \right\| \left\| \frac{\mathrm{d}^u(K(0))^{-1}}{\mathrm{d}\omega^u} \right\|, \tag{119}$$

$$F_3(s,t,u) = C_{stu}\left\| \frac{\mathrm{d}^s}{\mathrm{d}\omega^s}\{\tilde{R}^+(\omega) - (K(0))^{-1}\} \right\| \left\| \frac{\mathrm{d}^t}{\mathrm{d}\omega^t}\omega^{n_b}(\Gamma_{n_b} + \omega\Gamma_{n_b+1} + \omega^2\Gamma_{n_b+2}) \right\| \left\| \frac{\mathrm{d}^u(K(0))^{-1}}{\mathrm{d}\omega^u} \right\|, \tag{120}$$

where C_{stu}'s are appropriate constants. For $1\leqslant r\leqslant n_b+1$, the summation of the first summand in Eq. (117) can be estimated as

$$\sum_{\substack{s\geqslant 0,t\geqslant 0,u\geqslant 0,\\ (s+t+u=r)}}^{r} F_1(s,t,u) = F_1(0,r,0) + \sum_{t\geqslant 0,u\geqslant 1}^{r} F_1(0,t,u) + \sum_{s\geqslant 1,t\geqslant 0}^{r} F_1(s,t,0) + \sum_{\min\{s,u\}\geqslant 1}^{r} F_1(s,t,u)$$

$$= O(F_1(0,r-1,1)) = O(\omega^{2n_b-r}\log\omega) \qquad \text{or} \quad O(\omega^{n_a+n_b-r}), \tag{121}$$

for $n_b\leqslant n_a$ or $n_b>n_a$, respectively, as $\omega\to 0$. Note that from Eq. (101) for $N=0$ this estimation is valid for $r=0$ too. For $r=n_b+2$, it is estimated as

$$\begin{cases} O(\omega^{n_b-1}\log\omega) & (n_b\geqslant 2) \\ O((\log\omega)^2) & (n_b=1) \end{cases} \quad \text{or } O(\omega^{n_a-1}), \tag{122}$$

for $n_b\leqslant n_a$ or $n_b>n_a$, respectively, as $\omega\to 0$. The summation of the second summand in Eq. (117) for $0\leqslant r\leqslant n_b+3$ is also estimated as

$$\lambda^2\pi \sum_{\substack{s\geqslant 0,t\geqslant 0,u\geqslant 0,\\ (s+t+u=r)}}^{r} F_2(s,t,u) = \sum_{(s+t=r)}^{r} F_2(s,t,0) = O(F_2(0,r,0)) = O(\omega^{n_b+3-r}), \tag{123}$$

both for $n_b \leqslant n_a$ and for $n_b > n_a$, as $\omega \to 0$. The summation of the last summand in Eq. (117) for $0 \leqslant r \leqslant n_b+1$ is estimated as

$$\lambda^2\pi \sum_{\substack{s\geqslant 0,t\geqslant 0,u\geqslant 0,\\ (s+t+u=r)}}^{r} F_3(s,t,0) = \sum_{(s+t=r)}^{r} F_3(s,t,0) = O(F_3(1,r-1,0))$$

$$= O(\omega^{2n_b-r}\log\omega), \quad \text{or} \quad O(\omega^{n_a+n_b-r}), \tag{124}$$

for $n_b \leqslant n_a$ or $n_a < n_b$, respectively, as $\omega \to 0$. For $r = n_b+2$, the estimation is replaced by

$$O(\omega^{n_b-2}(\log\omega)^{\theta(n_b-2)}), \quad \text{or} \quad \begin{cases} O(\omega^{[n_a-2]^+}) & (n_b \geqslant 3) \\ O(\log\omega) & (n_b = 2), \end{cases} \tag{125}$$

for $n_b \leqslant n_a$ or $n_a < n_b$, respectively, as $\omega \to 0$. Then, by summarizing the above-noted estimations from Eqs. (121) and (125), and by taking into account the restriction (96) again, the proof of the lemma is completed. □

B. The exceptional case of the first kind

In this case, we first remember that from the discussion around Eq. (50) it necessarily holds that $\Gamma_1 \neq 0$, i.e., $n_b = 1$ in Eq. (93).

Lemma V.3: *Assume that* 0 *is an exceptional point of the first kind for H. the* 0*th and the first derivative of* $\tilde{R}(z)$ *are approximated by those of a finite series*

$$\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} + \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1)(Q_1\Gamma_1Q_1)^{-1}, \tag{126}$$

that is, it is shown that

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}z^r}\left[\tilde{R}(z) - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \right.\right.$$
$$\left.\left. \times(Q_1\Gamma_1Q_1)^{-1} \right] \right\| = O(z^{-1}(\log z)^{-3}) \quad \textit{for} \quad r=0, \quad \textit{or } O(z^{-2}(\log z)^{-3}) \quad \textit{for} \quad r=1, \tag{127}$$

as $z \to 0$.

Proof: Let us first consider the quantity that

$$\left\| \frac{\mathrm{d}^r}{\mathrm{d}z^r}\left[\tilde{R}(z) - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \right.\right.$$
$$\left.\left. \times(Q_1\Gamma_1Q_1)^{-1} \right] \right\| \leqslant \left\| \frac{\mathrm{d}^r}{\mathrm{d}z^r}[\tilde{R}(z) - Q_1\tilde{R}(z)Q_1] \right\| + \left\| \frac{\mathrm{d}^r}{\mathrm{d}z^r}\left[Q_1\tilde{R}(z)Q_1 - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} \right.\right.$$
$$\left.\left. - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1)(Q_1\Gamma_1Q_1)^{-1} \right] \right\|. \tag{128}$$

For $r=0$, the first term on the rhs of Eq. (128) is estimated as follows:

$$\|\tilde{R}(z) - Q_1\tilde{R}(z)Q_1\| \leqslant \|Q_0\tilde{R}(z)Q_0\| + \|Q_0\tilde{R}(z)Q_1\| + \|Q_1\tilde{R}(z)Q_0\| = O(1), \tag{129}$$

as $z \to 0$, where Eqs. (68)–(70) are used. For $r=1$, one obtains

$$\left\| \frac{\mathrm{d}\tilde{R}(z)}{\mathrm{d}z} - \frac{\mathrm{d}Q_1\tilde{R}(z)Q_1}{\mathrm{d}z} \right\| \leqslant \left\| \frac{\mathrm{d}Q_0\tilde{R}(z)Q_0}{\mathrm{d}z} \right\| + \left\| \frac{\mathrm{d}Q_0\tilde{R}(z)Q_1}{\mathrm{d}z} \right\| + \left\| \frac{\mathrm{d}Q_1\tilde{R}(z)Q_0}{\mathrm{d}z} \right\| = O(z^{-1}). \tag{130}$$

In fact, by using expression (68) the first term on the rhs of Eq. (130) is estimated as follows:

$$\frac{\mathrm{d}Q_0\tilde{R}(z)Q_0}{\mathrm{d}z} = -Q_0\tilde{R}(z)Q_0\left(\frac{\mathrm{d}E_{00}}{\mathrm{d}z} - \frac{\mathrm{d}E_{01}}{\mathrm{d}z}E_{11}^{-1}E_{10} - E_{01}\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z}E_{10} - E_{01}E_{11}^{-1}\frac{\mathrm{d}E_{10}}{\mathrm{d}z} \right) Q_0\tilde{R}(z)Q_0 \tag{131}$$

$$= O(\log z). \tag{132}$$

Four derivatives in Eq. (131) have the same order, which can be shown from the use of Eqs. (61), (63), (65), and (67): We here note that

$$\frac{\mathrm{d}E_{00}}{\mathrm{d}z} = O(\log z), \quad \frac{\mathrm{d}E_{01}}{\mathrm{d}z} = O(\log z), \quad \frac{\mathrm{d}E_{10}}{\mathrm{d}z} = O(\log z), \tag{133}$$

and from Eqs. (61) and (63)

$$\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z} = E_{11}^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}Q_1\{z + \lambda^2[A(z) - \log z\Gamma(z) + \pi i\Gamma(z)]\}Q_1 \right\}E_{11}^{-1} \tag{134}$$

$$= E_{11}^{-1}Q_1\left\{ 1 + \lambda^2\left[\frac{\mathrm{d}A(z)}{\mathrm{d}z} - \Gamma(z)/z - \log z\frac{\mathrm{d}\Gamma(z)}{\mathrm{d}z} + \pi i\frac{\mathrm{d}\Gamma(z)}{\mathrm{d}z} \right] \right\}Q_1E_{11}^{-1} \tag{135}$$

$$= O(z^{-2}(\log z)^{-1}). \tag{136}$$

In the same way, the second term in the rhs of Eq. (130) is also estimated as follows:

$$\frac{\mathrm{d}Q_0\tilde{R}(z)Q_1}{\mathrm{d}z} = -\left(\frac{\mathrm{d}E_{00}^{-1}}{\mathrm{d}z}E_{01} + E_{00}^{-1}\frac{\mathrm{d}E_{01}}{\mathrm{d}z} \right)Q_1\tilde{R}Q_1 + E_{00}^{-1}E_{01}Q_1\tilde{R}Q_1\left(\frac{\mathrm{d}E_{11}}{\mathrm{d}z} - \frac{\mathrm{d}E_{10}}{\mathrm{d}z}E_{00}^{-1}E_{01} - E_{10}\frac{\mathrm{d}E_{00}^{-1}}{\mathrm{d}z}E_{01} - E_{10}E_{00}^{-1}\frac{\mathrm{d}E_{01}}{\mathrm{d}z} \right)Q_1\tilde{R}Q_1 \tag{137}$$

$$= O(z^{-1}), \tag{138}$$

where we used Eq. (69) and the fact that

$$\frac{\mathrm{d}E_{00}^{-1}}{\mathrm{d}z} = O(\log z), \quad \frac{\mathrm{d}E_{11}}{\mathrm{d}z} = O(\log z). \tag{139}$$

In a similar manner, we can also show

$$\frac{\mathrm{d}Q_1\tilde{R}(z)Q_0}{\mathrm{d}z} = O(z^{-1}). \tag{140}$$

Let us next consider the last term in Eq. (128). For $r=0$, it reads

$$\left\| Q_1\tilde{R}(z)Q_1 - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \times(Q_1\Gamma_1Q_1)^{-1}\right\| \tag{141}$$

$$\leqslant \left\| E_{11}^{-1} - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \times(Q_1\Gamma_1Q_1)^{-1}\right\| + \left\|(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}E_{11}^{-1}-E_{11}^{-1}\right\| \tag{142}$$

$$\leqslant \left\| \tilde{E}_{11}(z)\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \times(Q_1\Gamma_1Q_1)^{-1}\right\| + \left\|\sum_{j=2}^{\infty}(\tilde{E}_{11}(z))^j\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1}\right\| + O(1) \tag{143}$$

$$= O(z^{-1}(\log z)^{-3}), \tag{144}$$

where in the second inequality we used Eq. (62) and that

$$\left\|(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}E_{11}^{-1}-E_{11}^{-1}\right\| \leqslant \frac{\left\|E_{11}^{-1}E_{10}E_{00}^{-1}E_{01}\right\|\left\|E_{11}^{-1}\right\|}{1-\left\|E_{11}^{-1}E_{10}E_{00}^{-1}E_{01}\right\|} = O(1), \tag{145}$$

as $z\to 0$. Substituting Eqs. (129) and (144) into Eq. (128), we can obtain the estimation (127) for $r=0$.

For $r=1$, we can obtain

$$\left\| \frac{\mathrm{d}}{\mathrm{d}z}\left[Q_1\tilde{R}(z)Q_1 - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1Q_1) \times(Q_1\Gamma_1Q_1)^{-1}\right]\right\| \tag{146}$$

$$\leqslant \left\| \frac{\mathrm{d}}{\mathrm{d}z}\left[E_{11}^{-1} - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z)^2}(Q_1\Gamma_1Q_1)^{-1}(Q_1+\lambda^2Q_1A_1Q_1 + \lambda^2\pi i Q_1\Gamma_1Q_1)(Q_1\Gamma_1Q_1)^{-1}\right]\right\| + \left\| \frac{\mathrm{d}}{\mathrm{d}z}\left\{(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}E_{11}^{-1}-E_{11}^{-1}\right\}\right\| \tag{147}$$

$$\leqslant \left\| E_{11}^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z} Q_1\{z+\lambda^2[A(z)+\pi i\Gamma(z)]\}Q_1 \right\} E_{11}^{-1} - \frac{1}{\lambda^4 z^2 (\log z)^2}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 \right.$$
$$\left. + \lambda^2 Q_1 A_1 Q_1 + \lambda^2 \pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1} \right\| + \left\| - E_{11}^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z) Q_1\Gamma(z)Q_1 \right\} E_{11}^{-1} \right.$$
$$- \frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} - z\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^4 z^2(\log z)^2} \right\}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 + \lambda^2 Q_1 A_1 Q_1$$
$$\left. + \lambda^2 \pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1} \right\| + \left\| \{(Q_{11} - E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1} - Q_{11}\}\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z} \right\|$$
$$+ \left\| \left\{ \frac{\mathrm{d}}{\mathrm{d}z}(Q_{11} - E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1} \right\} E_{11}^{-1} \right\| \tag{148}$$

$$= O(z^{-2}(\log z)^{-3}), \tag{149}$$

where we used the expression for $\mathrm{d}E_{11}^{-1}/\mathrm{d}z$ in Eq. (134). Actually, the first term in Eq. (148) is estimated as

$$\left\| E_{11}^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z} Q_1\{z+\lambda^2[A(z)+\pi i\Gamma(z)]\}Q_1 \right\} E_{11}^{-1} - \frac{1}{\lambda^4 z^2(\log z)^2}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 + \lambda^2 Q_1 A_1 Q_1 \right.$$
$$\left. + \lambda^2 \pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1} \right\| \leqslant \left\| E_{11}^{-1} - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} \right\| \left\| \frac{\mathrm{d}}{\mathrm{d}z} Q_1\{z+\lambda^2[A(z) \right.$$
$$\left. + \pi i\Gamma(z)]\}Q_1 \right\| \|E_{11}^{-1}\| + \frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|}{\lambda^2|z\log z|} \left\| \frac{\mathrm{d}}{\mathrm{d}z} Q_1\{z+\lambda^2[A(z)+\pi i\Gamma(z)]\}Q_1 \right\| \left\| E_{11}^{-1} \right\|$$
$$\left. - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} \right\| + \frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|^2}{\lambda^4 z^2(\log z)^2} \left\| \frac{\mathrm{d}}{\mathrm{d}z} Q_1\{z+\lambda^2[A(z)+\pi i\Gamma(z)]\}Q_1 - Q_1(1+\lambda^2 A_1 \right.$$
$$\left. + \lambda^2 \pi i\Gamma_1)Q_1 \right\| \tag{150}$$

$$= O(z^{-2}(\log z)^{-3}), \tag{151}$$

as $z \to 0$. On the other hand, the second term in Eq. (148) is slightly complicated to evaluate:

$$\left\| - E_{11}^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z) Q_1\Gamma(z)Q_1 \right\} E_{11}^{-1} - \frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} \right.$$
$$\left. - z\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^4 z^2(\log z)^2} \right\}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 + \lambda^2 Q_1 A_1 Q_1 + \lambda^2 \pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1} \right\| \tag{152}$$

$$\leqslant \left\| - \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z) Q_1\Gamma(z)Q_1 \right\} \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} - \frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} \right.$$
$$- \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z) Q_1\Gamma(z)Q_1 \right\} \widetilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}$$
$$\left. - \widetilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{ \frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z) Q_1\Gamma(z)Q_1 \right\} \frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1} \right.$$

$$+ z\frac{2}{(\lambda^2 z\log z)^3}\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)(Q_1\Gamma_1 Q_1)^{-1}(Q_1+\lambda^2 Q_1 A_1 Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1}\Big\|$$

$$+\left\|\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}\sum_{j=2}^{\infty}\tilde{E}_{11}^{j}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right\| \tag{153}$$

$$+\left\|\tilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}\sum_{j=1}^{\infty}\tilde{E}_{11}^{j}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right\|$$

$$+\left\|\sum_{j=2}^{\infty}\tilde{E}_{11}^{j}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}E_{11}^{-1}\right\|$$

$$\begin{aligned}\leqslant&\left\|-\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2\log z Q_1\Gamma(z)Q_1\right\}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right.\\&\left.-\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right\|\\&+\left\|-\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}\tilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right.\\&\left.+z\frac{1}{(\lambda^2 z\log z)^3}\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)(Q_1\Gamma_1 Q_1)^{-1}z(Q_1+\lambda^2 Q_1 A_1 Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1}\right\|\\&+\left\|-\tilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right.\\&\left.+z\frac{1}{(\lambda^2 z\log z)^3}\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)(Q_1\Gamma_1 Q_1)^{-1}(Q_1+\lambda^2 Q_1 A_1 Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1}\right\|\\&+O(z^{-2}(\log z)^{-3})\end{aligned} \tag{154}$$

$$=O(z^{-2}(\log z)^{-3}). \tag{155}$$

In fact, the first term in Eq. (154) reads

$$\begin{aligned}&\left\|-\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2\log z Q_1\Gamma(z)Q_1\right\}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}-\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right\|\\&\quad\leqslant\left\|-(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}+\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z(\log z)Q_1\right\|\frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|}{(\lambda^2 z\log z)^2}\end{aligned} \tag{156}$$

$$\begin{aligned}\leqslant&\lambda^2\left\{\left\|-(Q_1\Gamma_1 Q_1)^{-1}Q_1\frac{\Gamma(z)}{z}Q_1+Q_1\right\|+\left\|-(Q_1\Gamma_1 Q_1)^{-1}Q_1\frac{\mathrm{d}\Gamma(z)}{\mathrm{d}z}Q_1+Q_1\right\|(\log z)\right\}\\&\times\|(Q_1\Gamma_1 Q_1)^{-1}\|\frac{1}{\lambda^2 z\log z}\end{aligned} \tag{157}$$

$$=O((z\log z)^{-1}). \tag{158}$$

The second term in Eq. (154) also reads

$$\left\| -\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}\tilde{E}_{11}\frac{1}{\lambda^2 z\log z}(Q_1\Gamma_1 Q_1)^{-1}\right.$$
$$\left. +z\frac{1}{(\lambda^2 z\log z)^3}\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)(Q_1\Gamma_1 Q_1)^{-1}(Q_1+\lambda^2 Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1}\right\|$$
$$\leqslant \|(Q_1\Gamma_1 Q_1)^{-1}\|\left\|-\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}(Q_1\Gamma_1 Q_1)^{-1}\{zQ_1+\lambda^2 Q_1\{A(z)-\log z[\Gamma(z)-z\Gamma_1]\right.\right.$$
$$\left.\left. +\pi i\Gamma(z)\}Q_1\}+z\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)(Q_1+\lambda^2 Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)\right\|\frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|}{(\lambda^2 z\log z)^3} \tag{159}$$

$$\leqslant \|(Q_1\Gamma_1 Q_1)^{-1}\|\left\|\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}(Q_1\Gamma_1 Q_1)^{-1}\right\|\left\|-\{zQ_1+\lambda^2 Q_1\{A(z)-\log z[\Gamma(z)-z\Gamma_1]\right.\right.$$
$$\left.\left. +\pi i\Gamma(z)\}Q_1\}+z(Q_1+\lambda^2 Q_1A_1Q_1+\lambda^2\pi i Q_1\Gamma_1 Q_1)\right\|\frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|}{(\lambda^2 z\log z)^3}+\|(Q_1\Gamma_1 Q_1)^{-1}\|$$
$$\times\left\|-\left\{\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2(\log z)Q_1\Gamma(z)Q_1\right\}(Q_1\Gamma_1 Q_1)^{-1}+\left(\frac{\mathrm{d}}{\mathrm{d}z}\lambda^2 z\log z\right)Q_1\right\|\left\|z(Q_1+\lambda^2 Q_1A_1Q_1\right.$$
$$\left.+\lambda^2\pi i Q_1\Gamma_1 Q_1)\right\|\frac{\|(Q_1\Gamma_1 Q_1)^{-1}\|}{(\lambda^2 z\log z)^3} \tag{160}$$

$$=O((z\log z)^{-1}), \tag{161}$$

as $z\to 0$. The third term gives the same contribution to the order as the second one does. Furthermore, the last term in Eq. (154) comes from the estimations of the second, third, and last terms in Eq. (153), where each contributes the same order as $O(z^{-2}(\log z)^{-3})$. Therefore, Eq. (155) is proved.

On the other hand, the third term in Eq. (148) reads

$$\left\|\{(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}-Q_{11}\}\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z}\right\|\leqslant\frac{\left\|E_{11}^{-1}E_{10}E_{00}^{-1}E_{01}\right\|}{1-\left\|E_{11}^{-1}E_{10}E_{00}^{-1}E_{01}\right\|}\left\|\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z}\right\|=O(z^{-1}), \tag{162}$$

as $z\to 0$, where Eqs. (63), (65), (67), and (136) are used. In the same way, the last term in Eq. (148) reads

$$\left\|E_{11}^{-1}\frac{\mathrm{d}}{\mathrm{d}z}(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}\right\|\leqslant\|E_{11}^{-1}\|\|(Q_{11}-E_{11}^{-1}E_{10}E_{00}^{-1}E_{01})^{-1}\|^2\left[\left\|\frac{\mathrm{d}E_{11}^{-1}}{\mathrm{d}z}E_{10}E_{00}^{-1}E_{01}\right\|\right.$$
$$\left.+\left\|E_{11}^{-1}\frac{\mathrm{d}E_{10}}{\mathrm{d}z}E_{00}^{-1}E_{01}\right\|+\left\|E_{11}^{-1}E_{10}E_{00}^{-1}\frac{\mathrm{d}E_{01}}{\mathrm{d}z}\right\|+\left\|E_{11}^{-1}E_{10}\frac{\mathrm{d}E_{00}^{-1}}{\mathrm{d}z}E_{01}\right\|\right] \tag{163}$$

$$=O(z^{-1}\log z), \tag{164}$$

as $z\to 0$. By substituting Eqs. (151), (155), (162), and (164) into Eq. (148), one finally obtains Eq. (149). We can now show Eq. (127) for $r=1$ by setting Eqs. (130) and (149) into Eq. (128). □

If we start with expression (72), we obtain the following lemma instead of Lemma V.3.

Lemma V.4: *Assume that* 0 *is an exceptional point of the first kind for* H. *Then the* 0*th and the first derivative* of $\tilde{R}(z)$ *are approximated by those of a finite series*

$$\frac{1}{\lambda^2 z(\log z - 2\pi i)}(Q_1\Gamma_1 Q_1)^{-1} + \frac{1}{\lambda^4 z(\log z - 2\pi i)^2}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 + \lambda^2 Q_1 A_1 Q_1 - \lambda^2 \pi i Q_1\Gamma_1 Q_1) \times (Q_1\Gamma_1 Q_1)^{-1}, \tag{165}$$

that is, it is shown that

$$\left\| \frac{d^r}{dz^r}\left[\tilde{R}(z) - \frac{1}{\lambda^2 z(\log z - 2\pi i)}(Q_1\Gamma_1 Q_1)^{-1} - \frac{1}{\lambda^4 z(\log z - 2\pi i)^2}(Q_1\Gamma_1 Q_1)^{-1}(Q_1 + \lambda^2 Q_1 A_1 Q_1 - \lambda^2 \pi i Q_1\Gamma_1 Q_1)(Q_1\Gamma_1 Q_1)^{-1} \right] \right\| = O(z^{-1}(\log z - 2\pi i)^{-3}) \quad for \quad r = 0, \ or \ O(z^{-2}(\log z - 2\pi i)^{-3}) \quad for \ r = 1, \tag{166}$$

as $z \to 0$.

VI. THE REDUCED TIME EVOLUTION OPERATOR

In this section, we show that the reduced time evolution operator is expressed by the Fourier transform of the imaginary part of the reduced resolvent both in the regular case and the exceptional case of the first kind. We here define the reduced time evolution operator by the $N \times N$ matrix $\tilde{U}(t)$ of the components $\tilde{U}_{mn}(t) := \langle m | Pe^{-itH}P | n \rangle$, where $P = E((0,\infty))$ and $\{E(B) | B \in \mathbb{B}\}$ is the spectral measure of H, which is a family of the projection operator. $\mathbb{B}$ is the Borel field of $\mathbb{R}$.

Lemma VI.1: *We assume that Eq.* (23) *holds so that there is no positive eigenvalue. Then, for the system with the rational form-factor* (9), *it holds that*

$$\tilde{U}(t) = \frac{1}{\pi}\int_{(0,\infty)} e^{-it\omega} \mathrm{Im}\, \tilde{R}^+(\omega) d\omega = \lim_{r \to +0} \frac{1}{\pi}\int_r^\infty e^{-it\omega} \mathrm{Im}\, \tilde{R}^+(\omega) d\omega, \tag{167}$$

both in the regular case and the exceptional case of the first kind, where

$$\mathrm{Im}\, \tilde{R}^+(\omega) := \frac{1}{2i}[\tilde{R}^+(\omega) - \tilde{R}^-(\omega)], \tag{168}$$

which is sometimes called the spectral density.

Proof: Let us remember that the matrix $\tilde{U}(t)$ is expressed by the spectral measure as

$$\tilde{U}_{mn}(t) = \int_{(0,\infty)} e^{-it\lambda} d\langle m | E(\lambda) | n \rangle = \int_{(0,\infty)} e^{-it\lambda} d\tilde{E}_{mn}(\lambda), \tag{169}$$

where $\tilde{E}(B)$ is the matrix of the components $\langle m | E(B) | n \rangle$. Therefore, what we first should do is to clarify the relation between $\mathrm{Im}\, \tilde{R}^+(\omega)$ and $\tilde{E}(\lambda)$. Resorting to Stone's formula between $E(B)$ and $R(z)$, we clearly see

$$\frac{1}{2}[\tilde{E}([a,b]) + \tilde{E}((a,b))] = \lim_{\epsilon \to +0} \frac{1}{2\pi i}\int_a^b [\tilde{R}(\omega + i\epsilon) - \tilde{R}(\omega - i\epsilon)] d\omega, \tag{170}$$

for $a, b \in \mathbb{R}$ with $a < b$. Under the assumption (23), Lebesgue's dominated convergence theorem and the proof of Lemma III.1 tell us that the exchange between the limit and the integration in Eq. (170) is allowed for $[a,b] \subset (0,\infty)$. If $[a,b] \subset (-\infty, 0) \setminus \sigma(H)$, then $\tilde{R}^\pm(\omega) = \tilde{R}(\omega)$, and thus $\tilde{E}([a,b]) = \tilde{E}((a,b)) = 0$. In addition, by the continuity of $\tilde{R}^\pm(\omega)$, Eq. (170) tells us that $\tilde{E}(\{a\}) = 0$ for all $a > 0$, which leads to

$$\widetilde{E}((a,b)) = \widetilde{E}([a,b]) = \frac{1}{\pi}\int_a^b \mathrm{Im}\,\widetilde{R}^+(\omega)\mathrm{d}\omega, \tag{171}$$

for all a,b with $b>a>0$.

Let us now consider the regular case and in particular the validity of the expression (171) for the interval including the origin. In this case, $\widetilde{R}^{\pm}(0) \coloneqq \lim_{\omega\to+0}\widetilde{R}^{\pm}(\omega)$ exists to be finite. Furthermore, $\lim_{\omega\to\infty}\widetilde{R}^{\pm}(\omega)=0$ from Lemma III.2. Thus, $\widetilde{R}^{\pm}(\omega)$ is uniformly continuous on $(0,\infty)$. Therefore, we can take the limit of Eq. (171) as $a\to+0$ to obtain $\lim_{a\to+0}E([a,b])=E((0,b])$. We next see that all components of $\mathrm{Im}\,\widetilde{R}^+(\omega)$ are integrable, i.e., belong to $L^1((0,\infty))$. Suppose that $|\psi\rangle \in \mathbb{C}^N$,then $\langle\psi|\widetilde{E}((0,\lambda))|\psi\rangle$ is positive and a monotonically increasing function of λ, and it is also differentiable in this case. Thus Eq. (171) tells us that $\langle\psi|\mathrm{Im}\,\widetilde{R}^+(\omega)|\psi\rangle \geqslant 0$. In addition,

$$\|\psi\|^2 \geqslant \lim_{\lambda\to\infty}\langle\psi|\widetilde{E}((0,\lambda))|\psi\rangle = \lim_{\lambda\to\infty}\frac{1}{\pi}\int_0^\lambda \langle\psi|\mathrm{Im}\,\widetilde{R}^+(\omega)|\psi\rangle\mathrm{d}\omega = \frac{1}{\pi}\int_0^\infty \langle\psi|\mathrm{Im}\,\widetilde{R}^+(\omega)|\psi\rangle\mathrm{d}\omega. \tag{172}$$

Hence, from the monotonic convergence theorem, we see that $\langle\psi|\mathrm{Im}\,\widetilde{R}^+(\omega)|\psi\rangle \in L^1((0,\infty))$. From this fact and the use of the polarization identity, we can prove that all components of the matrix $\mathrm{Im}\,\widetilde{R}^+(\omega)$ are integrable. Thus, extending the rhs of Eq. (171) to arbitrary $B\in\{B \in \mathbb{B}|B\subset(0,\infty)\}$, $\int_B \mathrm{Im}\,\widetilde{R}^+(\omega)\mathrm{d}\omega$ defines a measure. We can now see from Eq. (171) and from E. Hopf's extension theorem that

$$\widetilde{E}(B) = \frac{1}{\pi}\int_B \mathrm{Im}\,\widetilde{R}^+(\omega)\mathrm{d}\omega \tag{173}$$

holds for all $B\in\{B\in\mathbb{B}|B\subset(0,\infty)\}$. Note that this expression means that the restriction of $\widetilde{E}_{mn}(B)$ to $\{B\in\mathbb{B}|B\subset(0,\infty)\}$ is absolutely continuous. Therefore, rewriting of $\widetilde{U}(t)$ in Eq. (169) into (167) is straightforward.

In the exceptional case of the first kind, from the assumption (23), $\widetilde{R}^{\pm}(\omega)$ is continuous on $(0,\infty)$, while $\widetilde{R}^{\pm}(\omega)=O((\omega\log\omega)^{-1})$ as $\omega\to+0$, so that it is not integrable around 0. See, Eq. (71). However, $\mathrm{Im}\,\widetilde{R}^+(\omega)$ is of the order $O(\omega^{-1}(\log\omega)^{-2})$ from Lemmas V.3 and V.4, and thus it is integrable around 0. Hence, Eq. (173) holds again, and Eq. (167) is valid for this exceptional case. □

We remark that in the case of no negative eigenvalues (point spectrum) of H,[21] the restriction of $\widetilde{U}(t)$ to the continuous energy spectrum is removed because in such a case $P=I$ the identity. Furthermore, the connection between $\widetilde{U}(t)$ and the observables is easily found, e.g., $|\langle\psi|\widetilde{U}(t)|\psi\rangle|^2/\|P|\psi\rangle\|^4$ for $|\psi\rangle\in\mathbb{C}^N$ (or $\mathbb{C}^N\oplus\{0\}$) is the survival probability of $P|\psi\rangle$ which is the probability of finding the system in the state $P|\psi\rangle$ at the later time t, where $P|\psi\rangle$ is just the decaying component of the initial state$|\psi\rangle$.

VII. THE ASYMPTOTIC EXPANSION OF THE REDUCED TIME EVOLUTION OPERATOR

We can finally show the asymptotic formula for $\widetilde{U}(t)$ at long times for the rational form factors satisfying our assumptions. In the following, we assume that Eq. (23) holds, i.e., there is no positive eigenvalue. However, this is not explicitly mentioned in the statements of the theorems. Let us first consider the regular case. For this purpose, according to Lemma V.2, we introduce the remainder $F(\omega)$ in the following way:

$$\frac{1}{\pi}\mathrm{Im}\,\widetilde{R}^{+}(\omega)=\lambda^{2}(K(0))^{-1}\omega^{n_b}(\Gamma_{n_b}+\omega\Gamma_{n_b+1}+\omega^{2}\Gamma_{n_b+2})(K(0))^{-1}+F(\omega), \tag{174}$$

for $\omega>0$.

Theorem VII.1: *Assume that* 0 *is a regular point for H. For a system with the rational form factor* (9) *characterized by the positive integers* n_a *and* n_b *that satisfy that* $n_b\geqslant 2$ *and* $n_a=1$, *the reduced time evolution operator* $\widetilde{U}(t)$ *behaves asymptotically as*

$$\widetilde{U}(t)=\lambda^{2}\frac{\Gamma(1+n_b)}{(it)^{n_b+1}}(K(0))^{-1}\Gamma_{n_b}(K(0))^{-1}+O(t^{-n_b-2}), \tag{175}$$

as $t\to\infty$. *When* $n_b=1$ *and* $n_a\geqslant 1$, *the error term is replaced by* $O(t^{-3}\log t)$.

Proof: We first summarize the several properties of $\mathrm{Im}\,\widetilde{R}^{+}(\omega)$. By Lemma V.2, we see that the remainder $F(\omega)$ in Eq. (174) is arbitrary-times differentiable. Particularly it holds that $\lim_{\omega\to 0}\mathrm{d}^{r}F(\omega)/\mathrm{d}\omega^{r}=0$ for all $r\leqslant n_b$, and

$$\left\|\frac{\mathrm{d}^{n_b+1}F(\omega)}{\mathrm{d}\omega^{n_b+1}}\right\|=O(\log\omega),\quad \text{or } O(1), \tag{176}$$

for $n_b=1$ and $n_a\geqslant 1$, or $n_b\geqslant 2$ and $n_a=1$, respectively, and

$$\left\|\frac{\mathrm{d}^{n_b+2}F(\omega)}{\mathrm{d}\omega^{n_b+2}}\right\|=O(\omega^{-1}),\quad \text{or}\begin{cases} O(1) & (n_b\geqslant 3)\\ O(\log\omega) & (n_b=2)\end{cases}, \tag{177}$$

for $n_b=1$ and $n_a\geqslant 1$, or $n_b\geqslant 2$ and $n_a=1$, respectively, as $\omega\to 0$. On the other hand, we see from Lemma III.2 that $(\mathrm{d}/\mathrm{d}\omega)^{r}\mathrm{Im}\,\widetilde{R}^{+}(\omega)=O(\omega^{-r-1})$ as $\omega\to\infty$. In particular, if $m\geqslant 1$, $(\mathrm{d}/\mathrm{d}\omega)^{m}\mathrm{Im}\,\widetilde{R}^{+}(\omega)$ is integrable on $[\delta,\infty)$ for an arbitrary $\delta>0$.

Let us now split the integral in Eq. (167) into two parts by writing

$$\mathrm{Im}\,\widetilde{R}^{+}(\omega)=\phi(\omega)\mathrm{Im}\,\widetilde{R}^{+}(\omega)+(1-\phi(\omega))\mathrm{Im}\,\widetilde{R}^{+}(\omega), \tag{178}$$

where $\phi\in C_0^{\infty}([0,\infty))$ and satisfies $\phi(\omega)=1$ in a neighborhood of $\omega=0$. Such a function is realized by $f(\omega)=1-\int_0^{\omega}g(x)\mathrm{d}x$, where $g(x)=h(x)/\int_{\mathbf{R}}h(x)\mathrm{d}x$ and $h(x)=\exp(-1/[a^2-(x-\mathrm{d})^2])$ $(|x-\mathrm{d}|<a)$ or 0 $(|x-\mathrm{d}|\geqslant a)$ with $\mathrm{d}>a>0$.

From Lemma 10.1 in Ref. 14 and the above-mentioned discussion, we see that $(1-\phi(\omega))\mathrm{Im}\,\widetilde{R}^{+}(\omega)$ has a contribution of $O(t^{-m})$ to $\widetilde{U}(t)$ for an arbitrary $m\geqslant 1$, i.e., this term decays faster than any negative power of t.

On the other hand, the contribution of $\phi(\omega)\mathrm{Im}\,\widetilde{R}^{+}(\omega)$ to $\widetilde{U}(t)$ gives the main part of the asymptotic expansion. Then, the coefficient of Γ_{n_b}, Γ_{n_b+1}, and Γ_{n_b+2} is given by the form[29]

$$\int_0^{\infty}\phi(\omega)\omega^{q}e^{-it\omega}\mathrm{d}\omega=\sum_{k=0}^{N-1}\frac{1}{(it)^{k+1}}\left.\frac{\mathrm{d}^{k}\omega^{q}\phi(\omega)}{\mathrm{d}\omega^{k}}\right|_{\omega=0}+R_N(t)=\frac{\Gamma(1+q)}{(it)^{1+q}}+R_N(t), \tag{179}$$

for all $N\geqslant 1+q$, where q takes the value n_b, n_b+1, or n_b+2. We here used that

$$\left.\frac{\mathrm{d}^{k}\omega^{q}\phi(\omega)}{\mathrm{d}\omega^{k}}\right|_{\omega=0}=\sum_{j=0}^{\min\{k,q\}}\binom{k}{j}\left.\frac{\mathrm{d}^{j}\omega^{q}}{\mathrm{d}\omega^{j}}\right|_{\omega=0}\left.\frac{\mathrm{d}^{k-j}\phi(\omega)}{\mathrm{d}\omega^{k-j}}\right|_{\omega=0}=\Gamma(1+q)\delta_{kq}, \tag{180}$$

where $\Gamma(1+n)=\int_0^{\infty}x^{n}e^{-x}\mathrm{d}x$ is the gamma function. In addition, the remainder $R_N(t)$ is bounded above by

$$|R_N(t)| \leqslant \frac{1}{t^N}\left|\int_0^\infty \frac{\mathrm{d}^N\omega^q\phi(\omega)}{\mathrm{d}\omega^N}e^{-i\omega t}\mathrm{d}\omega\right| = o(t^{-N}). \tag{181}$$

Note that since all derivatives of $\phi(\omega)$ vanish in the neighborhood of $\omega=0$, Eq. (179) is valid for all $N\geqslant q+1$ and thus $R_N(t)$ decays faster than any negative power of t. Furthermore, we understand, by applying Eq. (B1) in Lemma B.1 directly to $\phi(\omega)F(\omega)$ with the discussion in the first part of this section, that the contribution of the Fourier transform of the remainder $\phi(\omega)F(\omega)$ to $\widetilde{U}(t)$ is

$$O(t^{-3}\log t) \quad \text{or } (t^{-n_b-2}), \tag{182}$$

for $n_b=1$ and $n_a\geqslant 1$, or $n_b\geqslant 2$ and $n_a=1$, respectively, as $\omega\to 0$, where we used the formula of the indefinite integral that $\int(\log\omega)^2\mathrm{d}\omega=\omega[(\log\omega)^2-2\log\omega+2]$. Summarizing the above-noted results, we finally obtain that

$$\left\|\widetilde{U}(t)-\lambda^2(K(0))^{-1}\left[\frac{\Gamma(1+n_b)}{(it)^{n_b+1}}\Gamma_{n_b}+\frac{\Gamma(2+n_b)}{(it)^{n_b+2}}\Gamma_{n_b+1}+\frac{\Gamma(3+n_b)}{(it)^{n_b+3}}\Gamma_{n_b+2}\right](K(0))^{-1}\right\| \leqslant \left\|\frac{1}{\pi}\int_0^\infty(1-\phi(\omega))\mathrm{Im}\,\widetilde{R}^+(\omega)e^{-it\omega}\mathrm{d}\omega\right\| + \left\|\frac{1}{\pi}\int_0^\infty\phi(\omega)F(\omega)e^{-it\omega}\mathrm{d}\omega\right\| + O(t^{-N}) = O(t^{-3}\log t) \text{ or } O(t^{-n_b-2}), \tag{183}$$

for $n_b=1$ and $n_a\geqslant 1$, or $n_b\geqslant 2$ and $n_a=1$, respectively, as $t\to\infty$, where $O(t^{-N})$ is due to the contribution from $R_N(t)$. This is just the asymptotic expansion of $\widetilde{U}(t)$ in the statement. □

It is worth noting that if we resort to Lemma V.1, instead of Eqs. (176) and (177), we have

$$\frac{\mathrm{d}^rF(\omega)}{\mathrm{d}\omega^r} = O(\omega^{2-r}(\log\omega)^{1+\theta(2-r)}), \quad \text{or} \begin{cases} O(\omega^{[2-r]^+}) & (0\leqslant r\leqslant n_b) \\ O(\omega^{n_b+1-r}(\log\omega)^{\theta(n_b+1-r)}) & (r\geqslant n_b+1), \end{cases} \tag{184}$$

for $n_b=1$ and $n_a\geqslant 1$, or $n_b\geqslant 2$ and $n_a=1$, respectively. However, in the latter case, we see that the Fourier transform of $\phi(\omega)F(\omega)$ gives the contribution of the order $O(t^{-n_b-1})$, which is just the same order as that coming from the dominant one. Hence, we can only obtain a useless estimation.

We next show the asymptotic formula for $\widetilde{U}(t)$ at long times for a system with an exceptional point of the first kind. To this end, we write $\mathrm{Im}\,\widetilde{R}^+(\omega)$ with the remainder $F(\omega)$ again as follows:

$$\frac{1}{\pi}\mathrm{Im}\,\widetilde{R}^+(\omega) = \frac{1}{\lambda^2\omega(\log\omega)^2}(Q_1\Gamma_1Q_1)^{-1}+F(\omega). \tag{185}$$

Theorem VII.2: *Assume that* 0 *is an exceptional point of the first kind for H, which necessarily imposes that* $n_b=1$. *Then, the reduced time evolution operator* $\widetilde{U}(t)$ *for the rational form factor* (9) *behaves asymptotically as*

$$\widetilde{U}(t) = \frac{1}{\lambda^2\log t}(Q_1\Gamma_1Q_1)^{-1}+O((\log t)^{-2}), \tag{186}$$

as $t\to\infty$.

Proof: Let us first look over some properties of $\mathrm{Im}\,\widetilde{R}^+(\omega)$ again. By Lemmas V.3 and V.4, we see that the remainder $F(\omega)$ in Eq. (185) is arbitrary-times differentiable, satisfies that $F(\omega)=O(\omega^{-1}(\log\omega)^{-3})$, and $\mathrm{d}F(\omega)/\mathrm{d}\omega=O(\omega^{-2}(\log\omega)^{-3})$, as $\omega\to+0$. On the other hand, we see from Lemma III.2 that $(\mathrm{d}/\mathrm{d}\omega)^r\mathrm{Im}\,\widetilde{R}^+(\omega)=O(\omega^{-r-1})$ as $\omega\to\infty$. In particular, if $m\geqslant 1$, $(\mathrm{d}/\mathrm{d}\omega)^m\mathrm{Im}\,\widetilde{R}^+(\omega)$ is integrable on $[\delta,\infty)$ for an arbitrary $\delta>0$.

We now split the integral in Eq. (167) into two parts as in Eq. (178) again using the C_0^∞-function $\phi(\omega)$. From Lemma 10.1 in Ref. 14 and the above-mentioned discussion, $(1-\phi(\omega))\mathrm{Im}\,\widetilde{R}^+(\omega)$ has a contribution of $O(t^{-m})$ to $\widetilde{U}(t)$ for an arbitrary $m \geqslant 1$. On the other hand, the contribution of $\phi(\omega)\mathrm{Im}\,\widetilde{R}^+(\omega)$ to $\widetilde{U}(t)$ gives the dominant part of the asymptotic expansion. Then, the dominant time dependence of the asymptote of $\widetilde{U}(t)$ follows from Lemma B.2, that is,

$$\int_0^\infty \phi(\omega)(\omega(\log\omega)^2)^{-1}e^{-it\omega}\mathrm{d}\omega = (\log t)^{-1} + O((\log t)^{-2}). \tag{187}$$

Furthermore, the contribution of the Fourier transform of the remainder $\phi(\omega)F(\omega)$ to $\widetilde{U}(t)$ can be estimated by a similar manner to Lemma B.2, rather than Lemma B.1. By setting $\sigma(\omega) = F(\omega)e^{-it\omega}$ instead in the proof of Lemma B.1 of inverse-lagarithmic-fourier-integral, we can apply it to this case, and we have

$$\int_0^\infty F(\omega)\phi(\omega)e^{-it\omega}\mathrm{d}\omega = -\lim_{\omega\to+0}(\hat{I}\sigma)(\omega) + (-1)^N\int_0^\infty (\hat{I}^N\sigma)(\omega)\frac{\mathrm{d}^N\phi(\omega)}{\mathrm{d}\omega^N}\mathrm{d}\omega. \tag{188}$$

Then, corresponding to Eq. (B10), we have

$$\|(\hat{I}\sigma)(\omega)\| \leqslant \left\| ie^{-it\omega}\int_0^\infty F(\omega - i\eta)e^{-t\eta}\mathrm{d}\eta \right\| + E(t) \leqslant C\int_0^\infty |(\omega - i\eta)^{-1}[\log(\omega - i\eta)]^{-3}|e^{-t\eta}\mathrm{d}\eta + E(t), \tag{189}$$

with an appropriate constant C. Note that in this procedure, $\widetilde{R}^+(\omega)$ is analytically continued to the lower plane of the second Riemann sheet, while $\widetilde{R}^-(\omega)$ still remains in the lower plane of the first Riemann sheet. Then, both are ensured to contribute the remainders of the same order to $F(\omega - i\eta)$ in the above integral from Lemmas V.3 and V.4. The remainder term $E(t)$ in Eq. (189) that gives the order of $O(e^{-\gamma t})$ for some $\gamma > 0$ is responsible for the possible poles of $\widetilde{R}^+(\omega)$ continued to the second Riemann sheet, the number of which are guaranteed to be finite from the analytic Fredholm theorem[26] and Lemma III.2 for the continued $\widetilde{R}^+(\omega)$. Thus, it follows from Lemma B.2 that $\lim_{\omega\to+0}\|(\hat{I}\sigma)(\omega)\| = O((\log t)^{-2})$. By the same argument as in Lemma B.2, one also sees that the remainder term in Eq. (188) is of the order of $O(t^{-N+1})$. Summarizing these arguments, we can finish the proof of the theorem. □

VIII. CONCLUDING REMARKS

We have rigorously derived the asymptotic formula of the reduced time evolution operator for the N-level Friedrichs model in the context of the zero energy resonance[14] both for the regular case and the exceptional case of the first kind. Then, in the latter case, the logarithmically slow decay proportional to $(\log t)^{-1}$ has been found, and the expansion coefficient has been explicitly presented by the projection operator associated with the zero energy eigenstates of the total Hamiltonian, which is an extended state not belonging to the Hilbert space. We note that the decay involving the logarithmic function expressed by $t^{-j}(\log t)^k$ ($j=1,2,\ldots$ and $k=0,\pm1,\ldots$) can occur in the short range potential systems in the even dimensional space.[30] It should be noted that a realization of the exceptional cases requires the parameters, e.g., the coupling constant λ, to take such special values that the matrix $K(0)$ in Eq. (44) has a zero eigenvalue. In addition, some of the form factors $v_n(\omega)$ have to behave as $|v_n(\omega)|^2 \sim c_n\omega$ around $\omega=0$. In other words, if all of them behave as $|v_n(\omega)|^2 \sim c_n\omega^{q_n}$ with $q_n \geqslant 2$, the exceptional case of the first kind never occurs though that of the second kind could happen. These circumstances explain how the exceptional cases are surely exceptional. The presented results also enable us to calculate the asymptotic formula for the survival probability of an arbitrary initial state $|\psi\rangle$ localized over the N discrete levels. If we choose the special initial state to satisfy $\Gamma_{n_b}(K(0))^{-1}|\psi\rangle = 0$ in Eq. (175) or $(Q_1\Gamma_1Q_1)^{-1}|\psi\rangle = 0$ in

Eq. (186)), our estimations are useless and other decay laws could appear.[20] The long time behavior of the reduced time evolution operator for the exceptional case of the second and the third kind are not examined. As is expected, in the former case, the nondecaying component associated with the localized zero energy eigenstate will appear due to the divergent behavior of $Q_2\tilde{R}(z)Q_2 = O(z^{-1})$ in Eq. (83). The latter case can occur in the N-level cases of the model only for $N \geqslant 3$, which yields a more complicated situation. In the whole of the paper, we assumed that there is no bound eigenstate with a positive eigenenergy. This situation is actually realized in the weak coupling cases.[17,21]However, its compatibility with the existence of the extended zero energy eigenstate is still not clear in the multilevel cases (except the single level case). The emergence of the logarithmic decay $(\log t)^{-1}$ is just due to the logarithmic energy dependence of the self energy $S(\omega)$ and it comes from the assumption (9) where $|v_n(\omega)|^2 \sim c_n\omega^{q_n}$ with a positive integer q_n is required. Therefore, if we choose another type of form factor, it is not necessary for such a slow decay to occur even in the exceptional case.[11–13] However, we stress that our assumption is often satisfied by actual systems.[15,16] The experimental realization of the exceptional case requires the setup of parameters like $\omega_1 \simeq \lambda^2\Lambda$, where Λ is a typical cutoff constant. This seems to be naturally satisfied in a strong coupling region,[7,31] and hence it could be suggested to invoke the artificial quantum structures for a realization.

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APPENDIX A: CHARACTERISTICS OF SELF ENERGY FOR THE RATIONAL FORM FACTOR

Lemma A.1: *Suppose that* $\eta(\omega)$ *is a rational function*, *i.e.*, *it is expressed by* $\eta(\omega) = \pi(\omega)/\rho(\omega)$, *where* $\pi(\omega)$ *and* $\rho(\omega)$ *are the polynomials of the degree m and n*, *respectively*. *Furthermore*, *we assume that* $n \geqslant m+1$ *and* $\rho(z)$ *has no zeros in* $[0,\infty)$. *Then*

$$\int_0^\infty \frac{\eta(\omega)}{\omega-\zeta}\mathrm{d}\omega = \frac{P_{n-1}(\zeta) - \pi(\zeta)\log(-\zeta)}{\rho(\zeta)}, \tag{A1}$$

for all $\zeta \in \mathbb{C}\backslash([0,\infty)\cup\{a_k\}_{k=1}^N)$, *where* a_k *is a pole of* m_k*-th order of* $\eta(z)$, N *is the number of such poles*, *and* $P_n(\zeta)$ *is a polynomial of* ζ *of the degree not greater than n. For* $\zeta = |\zeta|e^{i\theta}$ *with* $0 \leqslant \theta \leqslant 2\pi$, *we define* $-\zeta = |\zeta|e^{i\phi}$ *with* $-\pi \leqslant \phi \leqslant \pi$.

Proof: From the fundamental theorems for the complex functions, it holds that

$$\int_0^\infty \frac{\eta(\omega)}{\omega-\zeta}\mathrm{d}\omega = -\sum_{k=1}^{N+1}\mathrm{Res}\left(\frac{\eta(z)}{z-\zeta}\log(-z), z=a_k\right), \tag{A2}$$

where $a_{N+1} = \zeta$. Then the residue at $z = a_k$ for $k \leqslant N$ is deduced to explicitly

$$\frac{1}{(m_k-1)!}\sum_{j=0}^{m_k-1}\binom{m_k-1}{j}\left[\left(\frac{\mathrm{d}^{m_k-1-j}}{\mathrm{d}z^{m_k-1-j}}(z-a_k)^{m_k}\frac{\eta(z)}{z-\zeta}\right)\left(\frac{\mathrm{d}^j}{\mathrm{d}z^j}\log(-z)\right)\right]_{z=a_k}$$
$$=-\sum_{j=1}^{m_k-1}\frac{P_{m_k-1-j}(\zeta)}{(a_k-\zeta)^{m_k-j}}-\frac{P_{m_k-1}(\zeta)}{(a_k-\zeta)^{m_k}}\log(-a_k). \tag{A3}$$

For $z=\zeta$, which is a simple pole, the residue becomes

$$\mathrm{Res}\left(\frac{\eta(z)}{z-\zeta}\log(-z),z=\zeta\right)=\eta(\zeta)\log(-\zeta). \tag{A4}$$

Therefore, by setting Eqs. (A3) and (A4) into Eq. (A2), one obtains Eq. (A1), and the proof is completed. □

Lemma A.2: *Suppose that the function* $\eta(\omega)$ *belonging to* $L^1([0,\infty))$ *is of the form*

$$\eta(\omega):=\omega^p r(\omega), \tag{A5}$$

where $p>1$ *and* $r(\omega)$ *is a* C^1*-function defined in* $[0,\infty)$. *Then it holds that both* $\eta(\omega)/\omega$ *and* $\eta(\omega)/\omega^2\in L^1([0,\infty))$, *and*

$$\lim_{E\to+0}\frac{1}{E}\left[P\int_0^\infty\frac{\eta(\omega)}{\omega-E}\mathrm{d}\omega-\int_0^\infty\frac{\eta(\omega)}{\omega}\mathrm{d}\omega\right]=\int_0^\infty\frac{\eta(\omega)}{\omega^2}\mathrm{d}\omega. \tag{A6}$$

Proof: From the proof of Proposition 3.2.2 in Ref. 10, the principal value of the integral on the rhs is written by the absolutely integrable function as follows:

$$P\int_0^\infty\frac{\eta(\omega)}{\omega-E}\mathrm{d}\omega=\int_0^\infty\frac{\eta(\omega)-\eta(E)\varphi_\delta(\omega-E)}{\omega-E}\mathrm{d}\omega, \tag{A7}$$

for all $E>0$, where $\varphi_\delta(\omega)$ is a C_0^∞-function with support $[-\delta,\delta]$ $(0<\delta<E)$, even with respect to the origin, and such that $\varphi_\delta(0)=1$. In the following, we choose such that $\varphi_\delta(\omega)=\exp[1-1/(1-(\omega/\delta)^2)]$ for $\omega\in(-\delta,\delta)$ or 0 otherwise, and $\delta=E/2$. Then, the proof of Eq. (A6) is equivalent to that of

$$\lim_{E\to+0}\int_0^\infty\left\{\frac{1}{E}\left[\frac{\eta(\omega)}{\omega}-\frac{\eta(\omega)-\eta(E)\varphi_\delta(\omega-E)}{\omega-E}\right]+\frac{\eta(\omega)}{\omega^2}\right\}\mathrm{d}\omega=0, \tag{A8}$$

which will be shown in the following. We note that the above-mentioned integrand can be rewritten as

$$-E\frac{\eta(\omega)}{\omega^2(\omega-E)}+\frac{\eta(E)\varphi_\delta(\omega-E)}{E(\omega-E)} \tag{A9}$$

$$=\frac{\eta(E)\varphi_\delta(\omega-E)}{E\omega}-\frac{E\eta(\omega)-\omega\eta(E)\varphi_\delta(\omega-E)}{\omega^2(\omega-E)}. \tag{A10}$$

We also put $I_1=(0,E/2]$, $I_2=(E/2,3E/2)$, and $I_3=[3E/2,\infty)$.

Let us first consider the case that $\omega\in I_1\cup I_3$. Then, since $\varphi_\delta(\omega-E)=0$, we can use Eq. (A9) to estimate the integrand in Eq. (A8), which reads

$$\left|E\frac{\eta(\omega)}{\omega^2(\omega-E)}\right|\leqslant 2\left|\frac{\eta(\omega)}{\omega^2}\right|, \tag{A11}$$

where the rhs is absolutely integrable and independent of E. Furthermore, it follows that $\lim_{E\to+0}E\chi_{I_1\cup I_3}(\omega)\eta(\omega)/[\omega(\omega-E)]=0$ for every $\omega\in(0,\infty)$, where $\chi_{I_1\cup I_3}(\omega)=1$ $(\omega\in I_1\cup I_3)$ or 0

($\omega \in I_2$), being the characteristic function. Thus, by the dominated convergence theorem, we can see that

$$\lim_{E\to+0}\int_{I_1\cup I_3} E\frac{\eta(\omega)}{\omega^2(\omega-E)}\mathrm{d}\omega = \lim_{E\to+0}\int_0^\infty E\chi_{I_1\cup I_3}(\omega)\frac{\eta(\omega)}{\omega^2(\omega-E)}\mathrm{d}\omega = 0. \tag{A12}$$

Next, for $\omega \in I_2$, we can use Eq. (A10). The integration of the first term of Eq. (A10) is estimated by

$$\left|\int_{I_2}\frac{\eta(E)\varphi_\delta(\omega-E)}{E\omega}\mathrm{d}\omega\right| \leqslant \frac{\eta(E)}{E^2/2}\int_{I_2}\varphi_\delta(\omega-E)\mathrm{d}\omega = \frac{\eta(E)}{E}\int_{-1}^{1}\varphi_1(x)\mathrm{d}x \to 0, \tag{A13}$$

as $E\to+0$, because $\eta(\omega)=O(\omega^p)$ where $p>1$. The second term of Eq. (A10) is also estimated with the decomposition

$$|E\eta(\omega)-\omega\eta(E)\varphi_\delta(\omega-E)| \leqslant |(E-\omega)\eta(\omega)| + |\omega(\eta(\omega)-\eta(E))| + |\omega\eta(E)||1-\varphi_\delta(\omega-E)|. \tag{A14}$$

The integral corresponding to the first term on the rhs of Eq. (A14) is evaluated as

$$\int_{I_2}\frac{|(E-\omega)\eta(\omega)|}{\omega^2|\omega-E|}\mathrm{d}\omega \to 0, \tag{A15}$$

as $E\to+0$, because of the fact $\eta(\omega)/\omega^2 \in L^1([0,\infty))$. The integral corresponding to the second term is also evaluated as

$$\int_{I_2}\frac{\omega|\eta(\omega)-\eta(E)|}{\omega^2|\omega-E|}\mathrm{d}\omega \leqslant (\ln 3)\sup_{\omega\in I_2}|\eta'(\omega)| \to 0, \tag{A16}$$

as $E\to+0$, because of the assumption on $\eta(\omega)$, where $\eta'(\omega)$ is the derivative of $\eta(\omega)$. The integral corresponding the last term on the rhs of Eq. (A14) is also estimated as

$$\int_{I_2}\frac{\omega|\eta(E)||1-\varphi_\delta(\omega-E)|}{\omega^2|\omega-E|}\mathrm{d}\omega \leqslant (\ln 3)\frac{|\eta(E)|}{\delta}\sup_{|x|\leqslant 1}|\varphi_1'(x)| \to 0, \tag{A17}$$

as $E\to+0$. Thus, we see from Eqs. (A15)–(A17),

$$\lim_{E\to+0}\int_{I_2}\frac{E\eta(\omega)-\omega\eta(E)\varphi_\delta(\omega-E)}{\omega^2(\omega-E)}\mathrm{d}\omega = 0. \tag{A18}$$

Equations (A12), (A13), and (A18) mean the completion of the proof of Eq. (A8). □

APPENDIX B: ASYMPTOTIC EXPANSION OF THE FOURIER INTEGRALS

We have to estimate the integrals of the form $U(t)=\int_0^\infty e^{-it\lambda}F(\lambda)\mathrm{d}\lambda$ in which $F(\lambda)=0$ identically either for small $\lambda>0$ or for large λ where F is supposed to take values in an arbitrary Banach space **B**. The following lemma is essentially the same as Lemma 10.2 in Ref. 14.

Lemma B.1: *Suppose that* $F(\lambda)=0$ *for* $\lambda>a>0$, $(F\in C^{k+1}(\delta,\infty;\mathbf{B}))$, $F^{(k+1)}\in L^1(\delta,\infty;\mathbf{B})$ *for any* $\delta>0$ *and for an integer* $k\geqslant 0$, *and that* $F^{(j)}(0)=0$ *for* $j\leqslant k-1$. *Then*

$$\|U(t)\| \leqslant \frac{1}{t^k}\left(\int_0^{2\pi/t}\|F^{(k)}(\lambda)\|\mathrm{d}\lambda + \frac{\pi}{2t}\int_{\pi/t}^{a}\sup_{\mu\in[\lambda,\lambda+\pi/t]}\|F^{(k+1)}(\mu)\|\mathrm{d}\lambda\right), \tag{B1}$$

for all $t>\pi/a$. *Here* $F^{(k)}(\lambda)$ *denotes the kth derivative of* $F(\lambda)$ *and so forth*.

Proof: By extending F by $F(\lambda)=0$ to $\lambda<0$, we obtain a function F on $(-\infty,\infty)$ with $F^{(k)}\in L^1(-\infty,\infty;\mathbf{B})$. Then we have that

$$\int_{-\infty}^{\infty} \|F^{(k)}(\lambda+h)-F^{(k)}(\lambda)\|\mathrm{d}\lambda = \left(\int_{-\infty}^{h} + \int_{h}^{a}\right)\|F^{(k)}(\lambda+h)-F^{(k)}(\lambda)\|\mathrm{d}\lambda \tag{B2}$$

$$\leqslant 2\int_{0}^{2h} \|F^{(k)}(\lambda)\|\mathrm{d}\lambda + \int_{h}^{a}\mathrm{d}\lambda\int_{\lambda}^{\lambda+h}\|F^{(k+1)}(\mu)\|\mathrm{d}\mu \tag{B3}$$

$$\leqslant 2\int_{0}^{2h} \|F^{(k)}(\lambda)\|\mathrm{d}\lambda + h\int_{h}^{a}\sup_{\mu\in[\lambda,\lambda+h]}\|F^{(k+1)}(\mu)\|\mathrm{d}\lambda. \tag{B4}$$

By noting that $e^{-it\lambda}=-e^{-it(\lambda-\pi/t)}$, one sees that the lhs of Eq. (B2) is just an upper bound of the Fourier transform of $2F^{(k)}$. Remember that the Fourier transform of $F^{(k)}$ is equal to $(it)^k U(t)$ under the assumption of the lemma, i.e., $F^{(j)}(0)=0$ for $j\leqslant k-1$, then the desired result follows. □

Lemma B.2: *Suppose that* $\phi\in C_0^{\infty}([0,\infty))$ *and satisfies* $\phi(\omega)=1$ *in a neighborhood of* $\omega=0$. *It then holds that for any positive integer* $q\geqslant 2$ *and* $N\geqslant 1$,

$$\int_{0}^{\infty}\omega^{-1}(\log\omega)^{-q}\phi(\omega)e^{-it\omega}\mathrm{d}\omega = \frac{(-1)^q}{q-1}\sum_{j=0}^{N-1}\binom{q+j-2}{j}(\log t)^{1-q-j}\left(\frac{\mathrm{d}}{\mathrm{d}\nu}-\frac{\pi}{2}i\right)^{j}\Gamma(\nu)\big|_{\nu=1} + O((\log t)^{1-q-N}) \tag{B5}$$

as $t\to\infty$.

Proof: We first put $\sigma(\omega)=\omega^{-1}(\log\omega)^{-q}e^{-it\omega}$ and introduce the indefinite integral operator $\hat{I}$ as[29]

$$(\hat{I}\sigma)(\omega) = \int_{c}^{\omega} s^{-1}(\log s)^{-q}e^{-its}\mathrm{d}s, \tag{B6}$$

where c is an arbitrary complex number. We can also recursively show

$$(\hat{I}^k\sigma)(\omega) = \frac{1}{(k-1)!}\int_{c}^{\omega}(\omega-s)^{k-1}s^{-1}(\log s)^{-q}e^{-its}\mathrm{d}s. \tag{B7}$$

Then, repeating the partial integration, we obtain

$$\int_{0}^{\infty}\omega^{-1}(\log\omega)^{-q}\phi(\omega)e^{-it\omega}\mathrm{d}\omega = -(\hat{I}\sigma)(\omega)\phi(\omega)\big|_{\omega=0} + R_N(t), \tag{B8}$$

for all $N\geqslant 1$ with

$$R_N(t) = (-1)^N\int_{0}^{\infty}(\hat{I}^N\sigma)(\omega)\mathrm{d}^N\phi(\omega)/\mathrm{d}\omega^N\mathrm{d}\omega, \tag{B9}$$

where we used the fact that $\mathrm{d}^k\phi(\omega)/\mathrm{d}\omega^k=\delta_{k0}$ at $\omega=0$ for any $k\geqslant 0$, and $\mathrm{d}^k\phi(\omega)/\mathrm{d}\omega^k=0$ at $\omega=\infty$ for any $k\geqslant 0$. We now choose $c=\omega-i\infty$ and change the variable as $s:=\omega-i\eta$, which leads to

$$(\hat{I}\sigma)(\omega) = ie^{-it\omega}\int_{0}^{\infty}(\omega-i\eta)^{-1}[\log(\omega-i\eta)]^{-q}e^{-t\eta}\mathrm{d}\eta. \tag{B10}$$

Then, we can use the dominated convergence theorem to obtain

$$\lim_{\omega\to+0}(\hat{I}\sigma)(\omega)=i\int_0^\infty(-i\eta)^{-1}[\log(-i\eta)]^{-q}e^{-t\eta}\mathrm{d}\eta. \tag{B11}$$

Here we used the fact that there is a positive number $\omega_0<1/(e^q\sqrt{2})$ such that

$$\begin{aligned}|(\omega-i\eta)^{-1}[\log(\omega-i\eta)]^{-q}e^{-t\eta}| &\leqslant \begin{cases}\eta^{-1}|\log\eta|^{-q}e^{-t\eta} & (0<\eta<\omega_0)\\ Ce^{-t\eta} & (\omega_0\leqslant\eta)\end{cases}\\ &\leqslant[\chi_{\eta\leqslant\omega_0}(\eta)\eta^{-1}|\log\eta|^{-q}+C]e^{-t\eta},\end{aligned} \tag{B12}$$

for all $0<\omega\leqslant\omega_0$ and all $0<\eta<\infty$, where $\chi_{\eta\leqslant\omega_0}(\eta)=1$ for $\eta\leqslant\omega_0$ or 0 otherwise, and C is an appropriate constant. The existence of such a C is ensured by the fact that $\log(\omega-i\eta)$ has no zeros in the rectangular region $\{\omega-i\eta|0<\omega\leqslant\omega_0,\omega_0\leqslant\eta<\infty\}$, and its modulus diverges as $\eta\to\infty$. The function on the rhs of Eq. (B12) is integrable, so that the use of the dominated convergence theorem is valid. To evaluate the asymptotic behavior of Eq. (B11), putting $\epsilon=(\log t)^{-1}$ and $t\eta=\xi$, one obtains

$$\lim_{\omega\to+0}(\hat{I}\sigma)(\omega)=i(-\epsilon)^q\int_0^\infty\frac{-i\epsilon^{-1}}{1-q}\left(\frac{\mathrm{d}}{\mathrm{d}\xi}[1-\epsilon\log(-i\xi)]^{1-q}\right)e^{-\xi}\mathrm{d}\xi \tag{B13}$$

$$=-\frac{(-\epsilon)^{q-1}}{1-q}\int_0^\infty[1-\epsilon\log(-i\xi)]^{1-q}e^{-\xi}\mathrm{d}\xi \tag{B14}$$

$$\begin{aligned}=&-\frac{(-\epsilon)^{q-1}}{1-q}\left\{\sum_{j=0}^{N-1}\binom{q+j-2}{j}\epsilon^j\left(\frac{\mathrm{d}}{\mathrm{d}\nu}-\frac{\pi}{2}i\right)^j\Gamma(\nu)\big|_{\nu=1}\right.\\ &\left.+\epsilon^N N\binom{q+N-2}{N}\int_0^\infty\left[\int_0^1\frac{(1-u)^{N-1}}{[1-\epsilon u\log(-i\xi)]^{q+N}}\mathrm{d}u\right][\log(-i\xi)]^N e^{-\xi}\mathrm{d}\xi\right\},\end{aligned} \tag{B15}$$

where we used the formulas that $f(\epsilon)=\sum_{j=0}^{N-1}\epsilon^j f^{(j)}(0)/j!+[\epsilon^N/(N-1)!]\int_0^1(1-u)^{N-1}f^{(N)}(\epsilon u)\mathrm{d}u$ with $f(\epsilon)=[1-\epsilon\log(-i\xi)]^{1-q}$, and $\int_0^\infty x^{\nu-1}e^{-\mu x}(\log x)^j\mathrm{d}x=\partial^j[\mu^{-\nu}\Gamma(\nu)]/\partial\nu^j$. The last integral in Eq. (B15) turns out to be finite because we have

$$\left|\int_0^\infty\left[\int_0^1\frac{(1-u)^{N-1}}{[1-\epsilon u\log(-i\xi)]^{q+N}}\mathrm{d}u\right][\log(-i\xi)]^N e^{-\xi}\mathrm{d}\xi\right|\leqslant\int_0^\infty\frac{[(\pi/2)^2+(\log\xi)^2]^{q/2+N}}{(\pi/2)^{q+N}}e^{-\xi}\mathrm{d}\xi, \tag{B16}$$

where we used that

$$|1-\epsilon u\log(-i\xi)|^2=(1-\epsilon u\log\xi)^2+(\epsilon u\pi/2)^2\geqslant\frac{(\pi/2)^2}{(\pi/2)^2+(\log\xi)^2}. \tag{B17}$$

Let us now evaluate the upperbound of $|(\hat{I}^N\sigma)(\omega)|$. Using the estimation (B12), we have

$$|(\hat{I}^N\sigma)(\omega)|=\frac{1}{(N-1)!}\left|\int_0^\infty(i\eta)^{N-1}(\omega-i\eta)^{-1}[\log(\omega-i\eta)]^{-q}e^{-t\eta}\mathrm{d}\eta\right| \tag{B18}$$

$$\leqslant\frac{1}{(N-1)!}\int_0^\infty[\eta^{N-2}|\log\omega_0|^{-q}+C\eta^{N-1}]e^{-t\eta}\mathrm{d}\eta=O(t^{-N+1}). \tag{B19}$$

Substituting this result into the error term $R_N(t)$ in Eq. (B9), we see that $R_N(t)=O(t^{-N+1})$ for any integer $N\geqslant2$. This proves the statement of the lemma. □

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[23] As is usual, the inner product between $|c\rangle$ and $|\mathrm{d}\rangle \in \mathbb{C}^N$ is defined by $\langle \mathrm{d}|c\rangle := \Sigma_{n=1}^{N} \mathrm{d}_n^* c_n$, and then the norm of $|c\rangle$ is defined by $\||c\rangle\| = \sqrt{\langle c|c\rangle}$. Furthermore, the inner product between $|f\rangle$ and $|g\rangle \in L^2((0,\infty))$ is also given by $\langle g|f\rangle := \int_0^\infty g^*(\omega) f(\omega) \mathrm{d}\omega$ and the norm of $|f\rangle$ is $\||f\rangle\| = \sqrt{\langle f|f\rangle}$.
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Some physical applications of fractional Schrödinger equation

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The fractional Schrödinger equation is solved for a free particle and for an infinite square potential well. The fundamental solution of the Cauchy problem for a free particle, the energy levels and the normalized wave functions of a particle in a potential well are obtained. In the barrier penetration problem, the reflection coefficient and transmission coefficient of a particle from a rectangular potential wall is determined. In the quantum scattering problem, according to the fractional Schrödinger equation, the Green's function of the Lippmann-Schwinger integral equation is given. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Schrödinger equation is the fundamental equation of physics for describing nonrelativistic quantum mechanical behavior. It is also often called the Schrödinger wave equation, and is a partial differential equation that describes how the wave function of a physical system evolves over time. The time-dependent one-dimensional Schrödinger equation is given by

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x,t)\psi(x,t), \tag{1}$$

where i is the imaginary unit, $\psi(x,t)$ is the time-dependent wave function, $\hbar$ is Planck's constant (strictly speaking, is Plank's constant divided by 2π; this is Dirac's notation), $V(x,t)$ is the potential.

It is well known that Feynman and Hibbs[1] used path integrals over Brownian paths to derive the standard (nonfractional) Schrödinger equation. In quantum physics, the Feynman path integral approach to quantum mechanics was the first successful attempt applying the fractality concept that was first introduced by Mandelbrot.[2] Recently, Laskin[3–6] extended the fractality concept and formulated fractional quantum mechanics as a path integral over the Lévy flights paths. Through introducing the quantum Riesz fractional derivative

$$(-\hbar^2\Delta)^{\alpha/2}\psi(x,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}e^{ipx/\hbar}|p|^{\alpha}\varphi(p,t)\mathrm{d}p, \tag{2}$$

$1<\alpha\leqslant 2$, they constructed the space fractional Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=D_{\alpha}(-\hbar^2\Delta)^{\alpha/2}\psi+V(x,t)\psi \tag{3}$$

(here $\Delta=\partial^2/\partial x^2$ is the Laplacian). Laskin showed the Hermiticity of the fractional Hamilton operator and established the parity conservation law. Energy spectra of a hydrogenlike atom and of

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a fractional oscillator were also computed. Afterwards, Naber[7] considered the Schrödinger equation with the first-order time derivative changed to a Caputo fractional detivative, the time fractional Schrödinger equation, and discussed the solutions of this kind of equation for a free particle and for a potential well.

In this paper, some other physical applications of the space fractional Schrödinger equation are considered, which are organized as follows. In Sec. II we solve the time-dependent fractional Schrödinger equation for a free particle and give the fundamental solution of the Cauchy problem, using the properties of Fox's H function. In Sec. III the energy levels and the normalized wave functions of a particle in an infinite square potential well are discussed. In Sec. IV according to the time-independent fractional Schrödinger equation we calculate the reflection coefficient and transmission coefficient of a particle from a rectangular potential wall. The quantum scattering problem is the basis of the quantum mechanics. Lippmann-Schwinger equation as the fundamental equation of quantum scattering theory obtains the widespread application in the three-dimensional quantum scattering.[8,9] In Sec. V the Lippmann-Schwinger equation equivalent to the fractional time-independent Schrödinger equation is considered, and the Green's function of it is determined in terms of Fox's H function. Finally, the paper is concluded with a discussion and summary.

II. FREE PARTICLE SOLUTION

The fractional Schrödinger equation for a free particle is given by

$$i\hbar\frac{\partial\psi}{\partial t}=D_\alpha(-\hbar^2\Delta)^{\alpha/2}\psi. \tag{4}$$

Taking into account the definitions of the Fourier transforms on the spatial coordinate

$$\varphi(p,t)=\int_{-\infty}^{+\infty}e^{-ipx/\hbar}\psi(x,t)\mathrm{d}x \tag{5}$$

and the quantum Riesz fractional derivative (2), we have

$$i\hbar\frac{\partial\varphi(p,t)}{\partial t}=D_\alpha|p|^\alpha\varphi(p,t), \tag{6}$$

and

$$\varphi(p,t)=C\exp\{-iD_\alpha|p|^\alpha t/\hbar\}, \tag{7}$$

where C is a constant. Inverse Fourier transforming gives the final solution

$$\psi(x,t)=\frac{C}{2\pi\hbar}\int_{-\infty}^{+\infty}e^{ipx/\hbar}\exp\{-iD_\alpha|p|^\alpha t/\hbar\}\mathrm{d}p, \tag{8}$$

which also can be expressed in terms of Fox's H functions

$$\psi(x,t)=\frac{C}{\alpha|x|}H_{2,2}^{1,1}\left[\frac{1}{\hbar}\left(\frac{\hbar}{iD_\alpha t}\right)^{1/\alpha}|x|\,\middle|\begin{matrix}(1,1/\alpha),(1,1/2)\\(1,1),(1,1/2)\end{matrix}\right], \tag{9}$$

by using the identical formula and the formula of the Fourier cosine transform of Fox's H function.[10,11] When $C=1$, Eq. (9) is the fundamental solution of the Cauchy problem, i.e., the solution to Eq. (4) with the initial condition $\psi(x,0)=\delta(x)$.

III. POTENTIAL WELL SOLUTION

Now consider a particle in a potential well

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ \infty & \text{for } |x| > a. \end{cases} \tag{10}$$

We need to solve Eq. (4) for $|x|<a$, with the condition $\psi(x,t)=0$, *for* $|x|\geqslant a$.

By separation of variables $\psi=f(t)\phi(x)$, we get

$$f(t) = e^{-(iE/\hbar)t} \tag{11}$$

(let $f(t=0)=1$),

$$D_\alpha(-\hbar^2\Delta)^{\alpha/2}\phi = E\phi, \tag{12}$$

in which E is the energy of the particle.

Let

$$k^\alpha = \frac{E}{D_\alpha \hbar^\alpha}. \tag{13}$$

Then considering

$$(-\hbar^2\Delta)^{\alpha/2} \exp\left\{ i\frac{px}{\hbar} \right\} = |p|^\alpha \exp\left\{ i\frac{px}{\hbar} \right\}, \tag{14}$$

and $E=D_\alpha|p|^\alpha$, the solution of Eq. (12) is

$$\phi(x) = e^{\pm ikx}, \tag{15}$$

or

$$\phi(x) = A\sin(kx) + B\cos(kx). \tag{16}$$

The boundary conditions $\phi(-a)=\phi(a)=0$ give

$$\begin{aligned} A\sin(ka) &= 0, \\ B\cos(ka) &= 0. \end{aligned} \tag{17}$$

So the solutions fall into two classes: those with $A=0$ and those with $B=0$.

The odd solutions have $B=0$, so $ka=n\pi/2$, for $n=2,4,6,\ldots$,

$$E_n^{(o)} = D_\alpha\left(\frac{\hbar n\pi}{2a} \right)^\alpha, \tag{18}$$

$$\phi_n^{(o)}(x) = \begin{cases} A\sin\left(\dfrac{n\pi}{2a}x \right) & \text{for } |x| < a \\ 0 & \text{for } |x| \geqslant a. \end{cases} \tag{19}$$

The even solutions have $A=0$, so $ka=n\pi/2$, for $n=1,3,5,\ldots$,

$$E_n^{(e)} = D_\alpha\left(\frac{\hbar n\pi}{2a} \right)^\alpha, \tag{20}$$

$$\phi_n^{(e)}(x) = \begin{cases} B\cos\left(\dfrac{n\pi}{2a}x\right) & \text{for } |x| < a \\ 0 & \text{for } |x| \geqslant a. \end{cases} \tag{21}$$

Combining even and odd solutions gives the energy levels

$$E_n = D_\alpha\left(\frac{\hbar n\pi}{2a}\right)^\alpha, \tag{22}$$

$$\phi_n(x) = \begin{cases} C_0 \sin\dfrac{n\pi}{2a}(x+a) & \text{for } |x| < a \\ 0 & \text{for } |x| \geqslant a, \end{cases} \tag{23}$$

for $n=1,2,3,\ldots$. Normalizing gives $\int_{-\infty}^{+\infty}|\phi(x)|^2 \mathrm{d}x=1$, so $C_0=1/\sqrt{a}$.

Thus the time-dependent wave functions of a particle in a one-dimensional infinite square potential well are

$$\psi_n(x,t) = e^{-(i/\hbar)E_n t}\phi_n(x) = C_0 e^{-(i/\hbar)E_n t}\sin\frac{n\pi}{2a}(x+a), \tag{24}$$

for $n=1,2,3,\ldots$ and $|x|<a$, which also can be expressed in terms of exponential function

$$\psi_n(x,t) = C_1 e^{i/\hbar(n\pi\hbar x/2a - E_n t)} + C_2 e^{i/\hbar(n\pi\hbar x/2a + E_n t)}, \tag{25}$$

where C_1 and C_2 are constants.

It should be noted that the results [Eqs. (22) and (23)] are equivalent to those given by Laskin.[6]

IV. BARRIER PENETRATION

Let us consider the motion of particles in a rectangular potential barrier

$$V(x) = \begin{cases} V_0, & 0 < x < a \\ 0, & x < 0, x > a. \end{cases} \tag{26}$$

According to classical physics, a particle of energy E less than the height V_0 of a barrier could not penetrate the region inside the barrier. But the wave function associated with a free particle must be continuous at the barrier and will show an exponential decay inside the barrier. The wave function must also be continuous on the far side of the barrier, so there is a finite probability that the particle will tunnel through the barrier.

First we suppose that the energy of the particle satisfies $E>V_0$ and the incident particle is moving from the left of the potential wall to the right. Then for $x<0$ or $x>a$, the time-independent fractional Schrodinger equation is Eq. (12). Its solution is (15), with (13). For $0<x<a$, the time-independent fractional Schrödinger equation is

$$D_\alpha(-\hbar^2\Delta)^{\alpha/2}\phi(x) + V_0\phi(x) = E\phi(x). \tag{27}$$

Solving this equation yields

$$\phi(x) = e^{\pm i\kappa x}, \tag{28}$$

in which

$$\kappa = \left(\frac{E - V_0}{D_\alpha \hbar^\alpha} \right)^{1/\alpha}. \tag{29}$$

Then we have for the time-independent wave function ϕ in the different regions expressions of the form

$$\text{for } x < 0, \quad \phi = e^{ikx} + Re^{-ikx}, \tag{30}$$

$$\text{for } 0 < x < a, \quad \phi = Ae^{i\kappa x} + Be^{-i\kappa x}, \tag{31}$$

$$\text{for } x > a, \quad \phi = Se^{ikx}. \tag{32}$$

In (30), the first term corresponds to a particle incident on the barrier (we suppose ϕ normalized so that the coefficient of this term is unity); the second term represents a particle reflected from the barrier. In (32), the wave function describes a particle, which has passed "above the wall" and is moving in the positive direction of x. The fractional probability current density in the incident wave is (see Ref. 5)

$$j_i(x) = \frac{D_\alpha \hbar}{i} \left[\phi^*(x)(-\hbar^2\Delta)^{\alpha/2-1} \frac{\partial}{\partial x} \phi(x) - \phi(x)(-\hbar^2\Delta)^{\alpha/2-1} \frac{\partial}{\partial x} \phi^*(x) \right]. \tag{33}$$

Then we have

$$j_i(x) = \frac{D_\alpha \hbar}{i} \left[e^{-ikx}(-\hbar^2\Delta)^{\alpha/2-1} \frac{\partial}{\partial x} e^{ikx} - e^{ikx}(-\hbar^2\Delta)^{\alpha/2-1} \frac{\partial}{\partial x}\ e^{-ikx}] \right] = 2D_\alpha (k\hbar)^{\alpha-1}. \tag{34}$$

Similarly, the fractional probability current density in the reflected wave is $2D_\alpha(k\hbar)^{\alpha-1}|R|^2$, in the transmitted wave $2D_\alpha(k\hbar)^{\alpha-1}|S|^2$. Then the transmission coefficient T of the particle as the ratio of the probability current density in the transmitted wave to that in the incident wave is $|S|^2$, and the reflection coefficient of the particle as the ratio of the probability current density in the reflected wave to that in the incident wave is $|R|^2$. The constants R and S are determined from the conditions that ϕ and $(-\hbar^2\Delta)^{\alpha/2-1}\phi$ are continuous at $x=0$:

$$1 + R = A + B, \tag{35}$$

$$(ik)^{\alpha-1} + (-ik)^{\alpha-1} R = (i\kappa)^{\alpha-1} A + (-i\kappa)^{\alpha-1} B, \tag{36}$$

at $x=a$:

$$Ae^{i\kappa a} + Be^{-i\kappa a} = Se^{ika}, \tag{37}$$

$$(i\kappa)^{\alpha-1} Ae^{i\kappa a} + (-i\kappa)^{\alpha-1} Be^{-i\kappa a} = (ik)^{\alpha-1} Se^{ika}. \tag{38}$$

Combining (35) and (36) gives

$$A = \frac{1}{1 + (-1)^\alpha} \left\{ \left[1 - \left(\frac{k}{-\kappa} \right)^{\alpha-1} \right] + R \left[1 - \left(\frac{k}{\kappa} \right)^{\alpha-1} \right] \right\},$$

$$B = \frac{1}{1 + (-1)^\alpha} \left\{ \left[1 - \left(\frac{k}{\kappa} \right)^{\alpha-1} \right] + R \left[1 - \left(\frac{k}{-\kappa} \right)^{\alpha-1} \right] \right\}.$$

Combining (37) and (38) gives

$$A = \frac{S}{1 + (-1)^\alpha} \left[1 - \left(\frac{k}{-\kappa} \right)^{\alpha-1} \right] e^{i(ka+\kappa a)},$$

$$B = \frac{S}{1+(-1)^{\alpha}}\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]e^{i(ka-\kappa a)}.$$

Then we have

$$\frac{1}{1+(-1)^{\alpha}}\left\{\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]+R\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]\right\} = \frac{S}{1+(-1)^{\alpha}}\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]e^{i(ka+\kappa a)},$$

$$\frac{1}{1+(-1)^{\alpha}}\left\{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]+R\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]\right\} = \frac{S}{1+(-1)^{\alpha}}\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]e^{i(ka-\kappa a)}.$$

Hence

$$Se^{ika} = \frac{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2}{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2 e^{i\kappa a}-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2 e^{-i\kappa a}}, \tag{39}$$

$$R = \frac{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right](e^{-i\kappa a}-e^{i\kappa a})}{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2 e^{i\kappa a}-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2 e^{-i\kappa a}}. \tag{40}$$

Finally the transmission coefficient T is given by

$$T = |S|^2 = \frac{\left\{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\right\}^2}{\left\{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\right\}^2+4\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\sin^2\kappa a},$$

$$T = \left\{1+\frac{4\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\sin^2\kappa a}{\left\{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\right\}^2}\right\}^{-1}, \tag{41}$$

and the reflection coefficient is

$$|R|^2 = \frac{4\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\sin^2\kappa a}{\left\{\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2-\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\right\}^2+4\left[1-\left(\frac{k}{\kappa}\right)^{\alpha-1}\right]^2\left[1-\left(\frac{k}{-\kappa}\right)^{\alpha-1}\right]^2\sin^2\kappa a}. \tag{42}$$

Obviously $|R|^2+|S|^2=1$.

For $E<V_0$, the corresponding expressions for T and $|R|^2$ are also obtained by replacing κ by k', where $k'=(-1)^{1/\alpha}((V_0-E)/D_{\alpha}\hbar^{\alpha})^{1/\alpha}$.

When the particle is passing over a rectangular potential well instead of a potential barrier, i.e.,

$$V(x)=\begin{cases}-V_0, & 0<x<a\\ 0, & x<0, x>a\end{cases}$$

($V_0>0$), the above theory still holds, in which $\kappa=((E+V_0)/D_\alpha\hbar^\alpha)^{1/\alpha}\geqslant k=(E/D_\alpha\hbar^\alpha)^{1/\alpha}$. In that case, it is interesting to note that $T=1$ ($|R|^2=0$), if $\sin^2\kappa a=0$, i.e., $a\kappa=n\pi$, thus $E=E_n=-V_0+D_\alpha(n\pi\hbar/a)^\alpha$, for $n=1,2,3,\ldots$. This phenomenon is called resonance transmission, and E_n is resonance energy levels.

V. THE GREEN'S FUNCTION IN QUAUTUM SCATTERING

Consider the incident particles with $E=D_\alpha|p|^\alpha$ are scattered by potential field $V(x)$. This problem sums up for solving the one-dimensional fractional Schrödinger equation

$$[-D_\alpha(-\hbar^2\Delta)^{\alpha/2}+E]\phi(x)=V(x)\phi(x). \tag{43}$$

According to the theory of Green's function of a fractional differential equation,[12] the solution of Eq. (43) can be expressed by

$$\phi(x)=\phi^0(x)+\int_{-\infty}^{+\infty}G(x,x')V(x')\phi(x')\mathrm{d}x', \tag{44}$$

in which $G(x,x')$ is the Green's function, satisfying

$$[-D_\alpha(-\hbar^2\Delta)^{\alpha/2}+E]G(x,x')=\delta(x-x'), \tag{45}$$

and $\phi^0(x)$ is an arbitrary solution of the homogeneous equation

$$[-D_\alpha(-\hbar^2\Delta)^{\alpha/2}+E]\phi(x)=0. \tag{46}$$

Supposing the incident wave $\phi_i(x)=e^{ikx}$, with $k^\alpha=E/D_\alpha\hbar^\alpha$, then the quantum scattering problem sums up for solving the generalized Lippmann-Schwinger integral equation equivalent to Eq. (43) as follows:

$$\phi(x)=e^{ikx}+\int_{-\infty}^{+\infty}G(x,x')V(x')\phi(x')\mathrm{d}x'. \tag{47}$$

In the following we calculate the Green's function. From Eq. (45), using Fourier transform we have

$$G(x,x')=G(x-x')=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{E-D_\alpha\hbar^\alpha|q|^\alpha}e^{iq(x-x')}\mathrm{d}q=\frac{1}{\pi}\int_0^\infty\frac{1}{E-D_\alpha\hbar^\alpha q^\alpha}\cos q(x-x')\mathrm{d}q$$
$$=\frac{1}{\pi E}\int_0^\infty\frac{1}{1-\dfrac{D_\alpha\hbar^\alpha}{E}q^\alpha}\cos q(x-x')\mathrm{d}q.$$

Considering the identical formula

$$\frac{z^\beta}{1+az^\alpha}=a^{-\beta/\alpha}H_{1,1}^{1,1}\left[az^\alpha\middle|\begin{matrix}(\beta/\alpha,1)\\(\beta/\alpha,1)\end{matrix}\right],$$

the properties of Fox's H function and the formula of the Fourier cosine transform of Fox's H functions,[11] we get

$$G(x-x') = \frac{1}{\pi E}\int_0^\infty H_{1,1}^{1,1}\left[\left(-\frac{D_\alpha \hbar^\alpha}{E}\right)q^\alpha \middle| \begin{matrix}(0,1)\\(0,1)\end{matrix}\right] \cos q(x-x')\mathrm{d}q$$

$$= \frac{1}{\alpha E|x-x'|}H_{2,3}^{2,1}\left[\frac{|x-x'|}{\left(-\frac{D_\alpha \hbar^\alpha}{E}\right)^{1/\alpha}} \middle| \begin{matrix}(1,1/\alpha) & (1,1/2)\\(1,1) & (1,1/\alpha)(1,1/2)\end{matrix}\right]$$

$$= \frac{-1}{\alpha D_\alpha \hbar^\alpha}\left(-\frac{D_\alpha \hbar^\alpha}{E}\right)^{1-1/\alpha} H_{2,3}^{2,1}\left[\frac{|x-x'|}{\left(-\frac{D_\alpha \hbar^\alpha}{E}\right)^{1/\alpha}} \middle| \begin{matrix}(1-1/\alpha,1/\alpha) & (1/2,1/2)\\(0,1) & (1-1/\alpha,1/\alpha)\quad (1/2,1/2)\end{matrix}\right]. \tag{48}$$

VI. CONCLUSION

Some physical applications of the fractional Schrödinger equation have been studied. The time-dependent free particle fractional Schrödinger equation was solved, using method of integral transform. The fundamental solution of the Cauchy problem was obtained in term of Fox's H function, which can be used for calculating boundary value problem in quantum mechanics. The motion of a particle in an infinite square potential well was discussed. We outlined the energy levels and wave functions. Also the reflection and transmission coefficient of a particle from a potential barrier or a potential well was derived. Last we gave the Green's function of the generalized Lippmann-Schwinger equation equivalent to time-independent fractional Schrödinger equation in quantum scattering processes. Equations (9), (22), (25), (41), (42), and (48) include the well-known equations as their special cases at $\alpha=2$.

On the other hand, we also can show that Eq. (48) is consistent with more general three-dimensional Green's function Eq. (47) obtained by Laskin.[13] According to his ideas, the one-dimensional fixed-energy kernel, i.e., the one-dimensional Green's function can be given by (using the expressions in Ref. 13)

$$k_L^{(0)}(x_2x_1;E) = \int_{t_1}^\infty \mathrm{d}t_2 e^{(i/\hbar)E(t_2-t_1)}K_L^{(0)}(x_2t_2|x_1t_1),$$

where

$$K_L^{(0)}(x_2t_2|x_1t_1) = \frac{1}{\alpha|x_2-x_1|}H_{2,2}^{1,1}\left[\frac{1}{\hbar}\left(\frac{\hbar}{iD_\alpha(t_2-t_1)}\right)^{1/\alpha}|x_2-x_1| \middle| \begin{matrix}(1,1/\alpha),(1,1/2)\\(1,1),(1,1/2)\end{matrix}\right].$$

Then we get the one-dimensional Green's function

$$k_L^{(0)}(x_2x_1;E) = \frac{i\hbar}{\alpha E|x_2-x_1|}H_{2,3}^{2,1}\left[\frac{|x_2-x_1|}{\left(-\frac{D_\alpha \hbar^\alpha}{E}\right)^{1/\alpha}} \middle| \begin{matrix}(1,1/\alpha)(1,1/2)\\(1,1)(1,1/\alpha)(1,1/2)\end{matrix}\right].$$

So we can see that Eq. (48) in this paper is a particular case of the more general Laskin's Eq. (47) in Ref. 13.

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Thin layer quantization in higher dimensions and codimensions

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We consider the thin layer quantization with use of only the most elementary notions of differential geometry. We consider this method in higher dimensions and get an explicit formula for quantum potential. For codimension 1 surfaces the quantum potential is presented in terms of principal curvatures, and equivalence with Prokhorov quantization method is proved. It is shown that, in contrast with original da Costa method, Prokhorov quantization can be generalized directly to higher codimensions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We consider free particle motion on a curved surface. Probably, the first quantum theory of it was proposed by Podolsky in Ref. 1; he postulated that the Hamiltonian operator is $\hat{H}=-(\hbar^2/2)\Delta_{\mathrm{LB}}$ with Δ_{LB} being the Laplace-Beltrami operator on the surface. One may try to get the Podolsky theory by some quantization procedure. Different methods of quantization yield various results which usually have the following general form:

$$\hat{H}=-\frac{\hbar^2}{2}\Delta_{\mathrm{LB}}+V_q(x), \tag{1}$$

the function $V_q(x)$ is commonly called "quantum potential." The Dirac canonical quantization[2] and the Abelian conversion method[3,4] were discussed in our previous work[5] for surfaces of codimension 1 in $\mathbb{R}^n$. (The codimension is the difference between the bulk space dimension and the dimension of the submanifold. In particular, codimension 1 surfaces can be defined by one equation and have one-dimensional normal space at each point. For these surfaces all notions of classical differential geometry are valid after obvious generalizations in the number of coordinates. For example, in the next section we would use the principal curvatures[6] of codimension 1 surfaces. At the same time, higher-codimensional surfaces present certain difficulties, and we encounter some of them in Sec. VI). This paper is devoted to another theory: the thin layer quantization. In this approach the particle moves between two equidistant infinite potential walls[7] or it is subject to some potential force which in a proper limit makes it moving strictly along the surface.[8]

The thin layer method seems to be natural for description of low dimensional motions in nanoelectronics. Recent progress in nanotechnology caused a great activity in the field. Free particle energy spectrum was investigated for thin layers around cylinders,[9] tori,[10] and arbitrary surfaces of revolution.[11] In this paper we clarify the general properties of the thin layer method and establish its equivalence with Prokhorov quantization procedure[12,13] for codimension 1 surfaces. For a vast majority of higher codimensional cases the thin layer method fails to yield meaningful results,[14] at least of the general form (1), while the Prokhorov quantization can be generalized directly as we show in Sec. VI.

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In Sec. II we describe the thin layer quantization method in a geometrically clear manner which allows us to deal with any codimension 1 surface in $\mathbb{R}^n$ without any complications in comparison with two-dimensional surfaces in $\mathbb{R}^3$. In contrast with Ref. 8 we use only the most elementary notions of differential geometry. In Sec. III we establish the equivalence of the thin layer approach with Prokhorov quantization method[12,13]. In Sec. IV a method of quantization with Hermitian momenta recently proposed by Encinosa[15] is analyzed. In Secs. V and VI we consider surfaces of codimension greater than 1.

II. QUANTIZATION FOR CODIMENSION 1 SURFACES

We consider $(n-1)$-dimensional smooth surface in $\mathbb{R}^n$ and two infinite potential walls at the distance $\delta\to 0$ from the surface. Free quantum particle moves in the thin layer of width 2δ between these potential walls. We introduce a curvilinear coordinate system in which $|x_n|$ equals the distance from the surface to the given point, and the coordinate lines of $x_1,\ldots,x_{n-1}$ are orthogonal to coordinate lines of x_n. We have the boundary condition $\Psi|_{x_n=\delta}=\Psi|_{x_n=-\delta}=0$ and Hamiltonian $\widetilde{H}=-(\hbar^2/2)\widetilde{\Delta}$ with $\widetilde{\Delta}$ being the Laplace operator in $\mathbb{R}^n$,

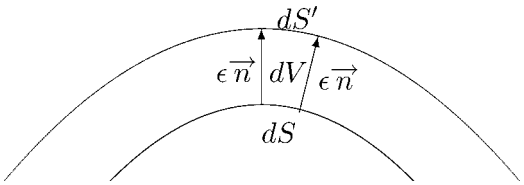
$$\widetilde{\Delta}=\sum_{i=1}^{n}\sum_{k=1}^{n}\tilde{g}^{-1/2}\partial_i\tilde{g}^{1/2}\tilde{g}^{ik}\partial_k=\partial_n^2+(\tilde{g}^{-1/2}\partial_n\tilde{g}^{1/2})\partial_n+\Delta_{\mathrm{LB}},$$

$$\tilde{g}_{ik}=\begin{pmatrix} g_{ab} & 0\\ 0 & 1\end{pmatrix},$$

where Δ_{LB} is the Laplace-Beltrami operator on the surface $x_n=\mathrm{const}$. One can prove[5] that $\tilde{g}^{-1/2}\partial_n\tilde{g}^{1/2}=\mathrm{div}\,\vec{n}$ with $\vec{n}$ being a unit normal vector to the surface, hence

$$\widetilde{\Delta}=\partial_n^2+\mathrm{div}(\vec{n})\cdot\partial_n+\Delta_{\mathrm{LB}}. \tag{2}$$

Indeed, let us consider two surfaces, $x_n=0$ and $x_n=\epsilon$. Suppose we have an infinitesimal area $\mathrm{d}S$ at the surface $x_n=0$. We denote the corresponding area element on $x_n=\epsilon$ surface by $\mathrm{d}S'$:



We have $\mathrm{div}(\vec{n})=[(\mathrm{d}S'-\mathrm{d}S)/\mathrm{d}V]+\mathcal{O}(\epsilon)=[(\mathrm{d}S'-\mathrm{d}S)/\epsilon\mathrm{d}S]+\mathcal{O}(\epsilon)$, so $\tilde{g}^{-1/2}\partial_n\tilde{g}^{1/2}=\mathrm{div}(\vec{n})$.

Now, let us take some point at the surface and consider another coordinate system $y_1,\ldots,y_n$. We choose it to be Cartesian and such that at the given point the tangent paraboloid of the surface is presented in its canonical form: $y_n=\frac{1}{2}\Sigma_{a=1}^{n-1}k_a y_a^2$. So, in the vicinity of the chosen point ($\vec{y}=0$) the equation of surface is $y_n=\frac{1}{2}\Sigma_{a=1}^{n-1}k_a y_a^2+\mathcal{O}(y_a^3)$, k_a's are the principal curvatures. The unit normal is

$$n_a=\frac{k_a y_a}{\sqrt{1+\sum_{a=1}^{n-1}k_a^2 y_a^2}}+\mathcal{O}(y_a^2)=k_a y_a+\mathcal{O}(y_a^2),\quad n_n=-1+\mathcal{O}(y_a^2)$$

and

$$\mathrm{div}\,\vec{n}=\sum_{a=1}^{n-1}k_a+\mathcal{O}(y_a). \tag{3}$$

The surface $x_n=\epsilon$ can be obtained by $\vec{y}\to\vec{y}'=\vec{y}+\epsilon\vec{n}$, and $\mathrm{d}y_a'=\mathrm{d}y_a(1+\epsilon k_a+\mathcal{O}(y_a))$. It yields

$$\frac{dS'}{dS} = \frac{\prod_{a=1}^{n-1}(1+\mathcal{O}(y_a'2))dy_a'}{\prod_{a=1}^{n-1}(1+\mathcal{O}(y_a^2))dy_a} = \prod_{a=1}^{n-1}(1+\epsilon k_a) + \mathcal{O}(y_a)$$

near the point $\vec{y}=0$. At the line $y_a=0\ \forall a=1,\ldots,n-1$ one has

$$\frac{dS'}{dS} = 1 + \epsilon\sum_{a=1}^{n-1} k_a + \frac{1}{2}\epsilon^2\left(\left(\sum_{a=1}^{n-1} k_a\right)^2 - \sum_{a=1}^{n-1} k_a^2\right) + \mathcal{O}(\epsilon^3). \tag{4}$$

The relation (4) is valid at every point of the surface provided that one takes the principal curvatures at the same point.

Following Refs. 7 and 8 we introduce a wave function

$$\chi(x) = \Psi(x)\sqrt{\frac{dS'}{dS}}.$$

It is natural because

$$\int_{|x_n|\le\delta} dV|\Psi(x)|^2 = \int_{-\delta}^{\delta} dx_n \int dS|\chi(x)|^2,$$

so that the normal and tangential coordinates are completely separated. For the lowest energy solutions the normal motion is restricted only to the factor of $\cos(\pi x_n/2\delta)$, and the integration over x_n yields just the constant number. It means that the conservation of norm for $\chi(x)$ is satisfied. From (2)–(4) one gets

$$\tilde{\Delta}\Psi(x) = \tilde{\Delta}\frac{\chi(x)}{\sqrt{\frac{dS'}{dS}}} = \Delta_{\mathrm{LB}}\frac{\chi(x)}{\sqrt{\frac{dS'}{dS}}} + \frac{\partial_n^2\chi(x)}{\sqrt{\frac{dS'}{dS}}} + \chi(x)\partial_n^2\frac{1}{\sqrt{\frac{dS'}{dS}}} + 2\partial_n\chi(x)\partial_n\frac{1}{\sqrt{\frac{dS'}{dS}}} + \mathrm{div}\,\vec{n}\cdot\frac{\partial_n\chi(x)}{\sqrt{\frac{dS'}{dS}}}$$

$$+ \mathrm{div}\,\vec{n}\cdot\chi(x)\partial_n\frac{1}{\sqrt{\frac{dS'}{dS}}} = \Delta_{\mathrm{LB}}\chi(x) + \partial_n^2\chi(x) + \left(\frac{1}{2}\sum_{a=1}^{n-1} k_a^2 - \frac{1}{4}\left(\sum_{a=1}^{n-1} k_a\right)^2\right)\chi(x) + \mathcal{O}(x_n).$$

For the lowest energy levels we have

$$\chi(x_1,\ldots,x_n) = f(x_1,\ldots,x_{n-1})\cos\frac{\pi x_n}{2\delta} \tag{5}$$

and, after taking $\delta\to 0$ limit and subtracting an infinite (proportional to $1/\delta^2$) energy, the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\Delta_{\mathrm{LB}} + \frac{\hbar^2}{8}\left(\left(\sum_{a=1}^{n-1} k_a\right)^2 - 2\sum_{a=1}^{n-1} k_a^2\right) \tag{6}$$

is obtained. In simple cases the factorization (5) works very good even for not so small values of δ.[11]

What was presented before (infinite potential walls) is rather the approach of Ref. 7 than of Ref. 8. But the difference is not very important. One could use an appropriate confining potential instead of infinite walls. It would lead to the lowest energy level function of the potential $V_{\mathrm{conf}}(x_n/\delta)$ instead of $\cos(\pi x_n/2\delta)$ and to another infinite energy.

Hamiltonian (6) contains quantum potential

$$V_q = \frac{\hbar^2}{8}\left(\left(\sum_{a=1}^{n-1} k_a\right)^2 - 2\sum_{a=1}^{n-1} k_a^2\right).$$

For two-dimensional surfaces in $\mathbb{R}^3$ we get the result of da Costa:[8] $V_q=-(\hbar^2/8)(k_1-k_2)^2$. For a sphere $k_a=1/R$ and the potential is $V_q=\hbar^2(n-1)(n-3)/8R^2$.

Physically this quantization can describe lower dimensional motions in nanoelectronics provided that the restricting potential makes a layer of uniform effective width. Of course, it would be still a severe problem to check this potential experimentally due to the great energy proportional to the width of layer powered by −2. (Actually, it is not so great in comparison with the kinetic energy of chaotic motion at ordinary temperatures. It means that the method would not work well due to excitation of higher energy levels of the transverse motion. So, a cryogenic experiment is needed.) This energy is constant on the physical surface if the potential depends only on a distance from the surface. For more complex potentials the results may differ. One can get different infinite energies in different parts of the surface. It would mean infinite tangential forces, of course. But if variation of width becomes smaller and smaller while $\delta\to 0$ it is obviously possible to obtain some finite additional potential.

III. EQUIVALENCE WITH PROKHOROV QUANTIZATION

We should mention that there is one more method of quantization proposed by Prokhorov.[12] The motion of a particle is considered as a system with two second class constraints but the only one condition is imposed on the physical sector: $\hat{P}_n\Psi_{\text{phys}}(x)=0$ with $\hat{P}_n=-i\hbar\,(1/\tilde{g}^{1/4})(\partial/\partial x_n)\tilde{g}^{1/4}$. It means that

$$\partial_n\left(\sqrt{\frac{dS'}{dS}}\Psi_{\text{phys}}(x)\right)=0. \tag{7}$$

Having solved some task by this method, one should set $x_n=0$ in the results *after* all the differentiations over x_n are performed. Due to (7) the probability to find a particle at the distance $|x_n|$ from the surface *does not depend* on the value of x_n, and we choose one value we need. For Prokhorov's view see Refs. 12 and 13.

From (7) and (4) we conclude that

$$\partial_n\Psi_{\text{phys}}(x) = -\frac{\Psi_{\text{phys}}(x)}{\sqrt{\frac{dS'}{dS}}}\partial_n\sqrt{\frac{dS'}{dS}} = -\Psi_{\text{phys}}(x)\left(\frac{1}{2}\sum_{a=1}^{n-1} k_a - \frac{1}{2}x_n\sum_{a=1}^{n-1} k_a^2 + \mathcal{O}(x_n^2)\right),$$

$$\partial_n^2\Psi_{\text{phys}}(x) = \Psi_{\text{phys}}(x)\left(\frac{1}{4}\left(\sum_{a=1}^{n-1} k_a\right)^2 + \frac{1}{2}\sum_{a=1}^{n-1} k_a^2 + \mathcal{O}(x_n)\right).$$

Now (2) and (3) yield

$$-\frac{\hbar^2}{2}\tilde{\Delta}\Psi_{\text{phys}}(x) = -\frac{\hbar^2}{2}\Delta_{\text{LB}}\Psi_{\text{phys}}(x) + \frac{\hbar^2}{8}\left(\left(\sum_{a=1}^{n-1} k_a\right)^2 - 2\sum_{a=1}^{n-1} k_a^2\right)\Psi_{\text{phys}}(x).$$

So, the quantum potential coincides with the one obtained by the thin layer method. The reason is clear. The lowest energy level wave functions (in the model with two infinite potential walls) have nodes at $x_n=\pm\delta$ and the bunch at $x_n=0$: $\partial_n\chi=0$ or, equivalently, $\hat{P}_n\Psi=0$. The methods of da Costa and Prokhorov are equivalent (disregarding the infinite energy of the thin layer quantization).

Actually, one could use the calculation of $\tilde{\Delta}\Psi(x)$ from Sec. II and set $\partial_n\chi\equiv 0$ (but note that in Prokhorov method one uses Ψ as a wave function, not χ).

IV. ON HERMITIAN MOMENTA OF ENCINOSA

Recently Encinosa[15] proposed one more quantization method for a constrained free motion. The starting point is the Hamiltonian in curvilinear coordinates x_i,

$$H=\frac{1}{2}\left(\sum_{i-1}^{n-1}\frac{p_i^2}{h_i(x)}+p_n^2\right),$$

and the recipe is simple, $p_i\to\hat{p}_i=-i\hbar\tilde{g}^{-1/4}\partial_i\tilde{g}^{1/4}$ followed by the thin layer method. According to these rules we have in our notations

$$\hat{H}\frac{f(x_1,\ldots,x_{n-1})\cos\dfrac{\pi x_n}{2\delta}}{\sqrt{\dfrac{\mathrm{d}S'}{\mathrm{d}S}}}=\frac{1}{2}\sum_{i-1}^{n-1}\frac{\hat{p}_i^2}{h_i(x)}\frac{f(x_1,\ldots,x_{n-1})\cos\dfrac{\pi x_n}{2\delta}}{\sqrt{\dfrac{\mathrm{d}S'}{\mathrm{d}S}}}-\frac{1}{2}\frac{\hbar^2 f(x_1,\ldots,x_{n-1})}{\sqrt{\dfrac{\mathrm{d}S'}{\mathrm{d}S}}}\partial_n^2\cos\frac{\pi x_n}{2\delta}.$$

Effectively this result may be considered as zero quantum potential (geometric potential in the terminology of Ref. 15). We should make two important comments on this point.

(a) Quantization in curvilinear coordinates is dangerous, because the results usually depend on the choice of coordinate system. Nevertheless, the meaning of the method considered could be clear if momenta operators were self-adjoint, but it is not the case even for spherical coordinates on the sphere.

(b) Strictly speaking, the recipe is not defined correctly, because the operator ordering problem in $\hat{p}_i^2/h_i(x)$ terms is not solved. It is not difficult to deduce the correct ordering for the zero potential theory from the relation

$$-\hbar^2\tilde{\Delta}=-\hbar^2\sum_{i=1}^{n}\sum_{k=1}^{n}\tilde{g}^{-1/2}\partial_i\tilde{g}^{1/2}\tilde{g}^{ik}\partial_k=\sum_{i=1}^{n}\tilde{g}^{-1/4}\hat{p}_i\tilde{g}^{1/4}\tilde{g}^{ii}\hat{p}_i$$

in any orthogonal coordinate system. But this particular ordering is not natural *a priori*. Let us turn to the case of $\mathcal{S}^2$ with stereographic coordinates $x_1=2(R+x_3)\cot(\vartheta/2)\cos\varphi$ and $x_2=2(R+x_3)\cot(\vartheta/2)\sin\varphi$. In Ref. 16 it was shown that in these coordinates the Laplace-Beltrami operator on the sphere of radius $R+x_3$ equals

$$-\frac{\hbar^2}{2}\Delta_{\mathrm{LB}}=\left(1+\frac{x_1^2+x_2^2}{4(R+x_3)^2}\right)\frac{(\hat{p}_1^2+\hat{p}_2^2)}{2}\left(1+\frac{x_1^2+x_2^2}{4(R+x_3)^2}\right).$$

Even less natural it would seem for $\mathcal{S}^n$ in $\mathbb{R}^{n+1}$,

$$-\frac{\hbar^2}{2}\Delta_{\mathrm{LB}}=\frac{1}{2}\left(1+\frac{x_1^2+\cdots+x_n^2}{4(R+x_{n+1})^2}\right)^{n/2}\times\sum_{i=1}^{n}\left(\hat{p}_i\left(1+\frac{x_1^2+\cdots+x_n^2}{4(R+x_{n+1})^2}\right)^{2-n}\hat{p}_i\right)\left(1+\frac{x_1^2+\cdots+x_n^2}{4(R+x_{n+1})^2}\right)^{n/2}.$$

And, of course, for coordinates of Sec. 5 in Ref. 16 the situation would not be better.

V. ELEMENTARY CASES OF CODIMENSION >1

In general let us consider m-dimensional smooth surface in $\mathbb{R}^n$ represented by its tangent paraboloid at some point,

$$y_\alpha=\frac{1}{2}\sum_{a=1}^{m}\sum_{b=1}^{m}k_{ab}^{(\alpha)}y_a y_b+\mathcal{O}(y_a^3),\tag{8}$$

$\alpha=m+1,\ldots,n$, $k_{ab}^{(\alpha)}=k_{ba}^{(\alpha)}$. In general $n-m$ curvature forms $k^{(\alpha)}$ cannot be diagonalized simultaneously and the notion of principal curvatures does not exist, but in this section we treat the simplest cases for which the diagonalization can be performed.

First of all, for one-dimensional manifolds (curves) curvature forms $k^{(\alpha)}$ are just real numbers. In this case by a rotation in the space of y_α one can get $y_2=\frac{1}{2}ky_1^2+\mathcal{O}(y_1^3)$, $y_3,\ldots,y_n=\mathcal{O}(y_1^3)$. The unit normal vectors are $n_1^{(2)}=ky_1+\mathcal{O}(y_1^2)$, $n_2^{(2)}=-1+\mathcal{O}(y_1^2)$, $n_3^{(2)}=\cdots=n_n^{(2)}=\mathcal{O}(y_1^2)$; $n_i^{(\alpha)}=-\delta_{i\alpha}+\mathcal{O}(y_1^2)$ for $\alpha\geq 3$. We have $\vec{n}^{(\alpha)}\vec{n}^{(\beta)}=\delta_{\alpha\beta}+\mathcal{O}(y_1^2)$ and after the transformation $\vec{y}\to\vec{y}'=\vec{y}+\Sigma_{\alpha=2}^n\epsilon_\alpha\vec{n}^{(\alpha)}$ one gets $dy_1'=(1+\epsilon_2 k+\mathcal{O}(y_1))dy_1$, $dy_\alpha'=(1+\mathcal{O}(y_1))dy_\alpha$.

Now we consider a smooth family of such coordinate systems and normals along the curve. We introduce a curvilinear coordinate system in which x_1 is just the length along the curve while $x_\alpha=\vec{n}^{(\alpha)}\cdot\vec{r}$ where $\vec{r}$ is the minimal norm radius vector from the curve to a given point and $\vec{n}^{(\alpha)}$ is taken at the same point on the curve as $\vec{r}$. In this coordinate system we have

$$\tilde{g}_{ik}=\begin{pmatrix}(1+x_2k)^2 & 0\\ 0 & I\end{pmatrix}$$

and

$$\tilde{\Delta}=\Delta_c+\Delta_n+\left(\frac{1}{1+x_2k}\partial_2(1+x_2k)\right)\partial_2=\Delta_c+\Delta_n+\frac{k}{1+x_2k}\partial_2,$$

where Δ_c is Laplace-Beltrami operator on a curve $x_\alpha=\text{const}$ and $\Delta_n=\Sigma_{\alpha=2}^n\partial_\alpha^2$ is the Laplace operator in a hyperplane $x_1=\text{const}$.

To proceed with the thin layer quantization we introduce a thin layer $\Sigma_{\alpha=2}^n x_\alpha^2=\delta^2$ around the curve and a wave function $\chi(x)=\sqrt{1+x_2k}\,\Psi(x)$ such that $\int dx_1\int dS_{\text{normal}}|\chi(x)|^2=\int dV|\Psi(x)|^2$:

$$\tilde{\Delta}\Psi(x)=\tilde{\Delta}\frac{\chi(x)}{\sqrt{1+x_2k}}=\Delta_c\chi(x)+\Delta_n\chi(x)+\frac{k^2}{4}\chi(x)+\mathcal{O}(x_\alpha).$$

After subtracting an infinite energy due to $\Delta_n\chi(x)$ it yields the quantum potential $V_q=-(\hbar^2/8)k^2$ as in Ref. 8.

We should mention that it is very important for this result that the thin layer is spherical at every point of the curve. Indeed, suppose we have a straight line in $\mathbb{R}^3$. We can first embed a cylinder of any radius R into $\mathbb{R}^3$ and after that, with much more thin layer, we embed a line into the cylinder. The first embedding results in $V_q=-\hbar^2/8R^2$ and the second one changes nothing because the line is geodesic in the cylinder. Note that it is possible to generalize our considerations to the case of embedding into non-Euclidean spaces in a sense that, if one has a free particle Hamiltonian (probably, with some quantum potential) in a Riemannian manifold, he may consider a thin layer of constant width around any codimension 1 submanifold. For a cylinder it would literally reproduce the demonstrations of Sec. II because in intrinsic geometry the cylinder is flat.

As another simple example we consider two-dimensional flat torus isometrically embedded in $\mathbb{R}^4$,

$$x_1^2+x_2^2=R_1^2,$$

$$x_3^2+x_4^2=R_2^2.$$

We use the following coordinate system:

$$\phi_1=\arctan\frac{x_2}{x_1},$$

$$\phi_2=\arctan\frac{x_4}{x_3},$$

$$r_1 = \sqrt{x_1^2 + x_2^2} - R_1,$$

$$r_2 = \sqrt{x_3^2 + x_4^2} - R_2$$

with

$$\tilde{g}_{ik} = \begin{pmatrix} (r_1+R_1)^2 & 0 & 0 & 0 \\ 0 & (r_1+R_1)^2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and $\tilde{\Delta} = \Delta_t + \Delta_n + [1/(r_1+R_1)]\partial_{r_1} + [1/(r_2+R_2)]\partial_{r_2}$ where Δ_t is the Laplace-Beltrami operator on the torus $r_1 = \text{const}$, $r_2 = \text{const}$. We have the volume element $dV = (r_1+R_1)(r_2+R_2)dr_1\, dr_2\, d\phi_1\, d\phi_2$, the wave function $\chi = \sqrt{[1+(r_1/R_1)][1+(r_2/R_2)]}\Psi$ and the quantum potential $V_q = -(\hbar^2/8)(k_1^2+k_2^2)$ with $k_a = 1/R_a$.

VI. GENERAL THEORY

In general the geometric construction is very similar to that of the one-dimensional case. The unit normals to the surface (8) at $\vec{y}=0$ are $n_\beta^{(\alpha)} = \delta_{\alpha\beta}(-1+\mathcal{O}(y_a^2))$, $n_a^{(\alpha)} = \sum_{b=1}^m k_{ab}^{(\alpha)} y_b + \mathcal{O}(y_a^2)$, $\alpha, \beta = m+1, \ldots, n$, $a, b = 1, \ldots, m$, and after the replacement $\vec{y} \to \vec{y}' = \vec{y} + \sum_{\alpha=m+1}^n \epsilon_\alpha \vec{n}^{(\alpha)}$ one gets

$$dy_a' = \sum_{b=1}^m \left(\delta_{ab} + \sum_{\alpha=m+1}^n \epsilon_\alpha k_{ab}^{(\alpha)} + \mathcal{O}(y_c) \right) dy_b,$$

$dy_\alpha' = (1+\mathcal{O}(y_c))dy_\alpha$. It means that in curvilinear coordinate system

$$g_{ab}(x_1, \ldots, x_n) = \sum_{c=1}^m \left(\delta_{ca} + \sum_{\alpha=m+1}^n x_\alpha k_{ca}^{(\alpha)} \right) \times \left(\delta_{cb} + \sum_{\beta=m+1}^n x_\beta k_{cb}^{(\beta)} \right) f_{ab}(x_1, \ldots, x_m)$$

with $x_\alpha = \vec{n}^{(\alpha)} \cdot \vec{r}$ as in the preceding section and $f_{ab}(x_1, \ldots, x_m) = g_{ab}(x_1, \ldots, x_m, 0, \ldots, 0)$. In this system if some point has coordinates $(x_1, \ldots, x_n)$ then its position can be found by adding the vector $\sum_{\alpha=m+1}^n x_\alpha \vec{n}^{(\alpha)}$ to the radius vector of the initial surface point with coordinates $(x_1, \ldots, x_m)$. If we choose $x_a = y_a$ at the surface $x_\alpha = 0$, then at the $x_a = 0$ hyperplane $f_{ab} = \delta_{ab}$, $x_\alpha = \epsilon_\alpha$, and $g_{ab} = \delta_{ab} + 2\sum_\alpha \epsilon_\alpha k_{ab}^{(\alpha)} + \sum_{\alpha,\beta,c} \epsilon_\alpha \epsilon_\beta k_{ac}^{(\alpha)} k_{bc}^{(\beta)}$. An easy computation yields

$$g = 1 + 2\sum_{\alpha,a} \epsilon_\alpha k_{aa}^{(\alpha)} + 2 \sum_{\alpha,\beta,a,b} \epsilon_\alpha \epsilon_\beta k_{aa}^{(\alpha)} k_{bb}^{(\beta)} - 2 \sum_{\alpha,\beta,a} \epsilon_\alpha \epsilon_\beta k_{aa}^{(\alpha)} k_{aa}^{(\beta)} + 3\sum_{a,b} \left(\sum_\alpha \epsilon_\alpha k_{ab}^{(\alpha)} \right)^2 - 2\sum_a \left(\sum_\alpha \epsilon_\alpha k_{aa}^{(\alpha)} \right)^2 + \mathcal{O}(\epsilon^3).$$

The problem is that the coordinates x_i are not orthogonal. Parallel translations of the surface along one of the normals breaks its orthogonality to other normals. Indeed, we have $\partial n_b^{(\alpha)} / \partial y_a = k_{ab}^{(\alpha)} + \mathcal{O}(y_c)$ and $\partial n_\beta^{(\alpha)} / \partial y_a = \mathcal{O}(y_c)$. We suppose that all normals have unit length, hence

$$0 = \frac{\partial \vec{n}^{(\alpha)}}{\partial y_a} \cdot \vec{n}^{(\alpha)} = \sum_{b,c} k_{bc}^{(\alpha)} y_c k_{ab}^{(\alpha)} - \frac{\partial n_\alpha^{(\alpha)}}{\partial y_a} + \mathcal{O}(y_c^2)$$

and

$$\frac{\partial n_\alpha^{(\alpha)}}{\partial y_a} = \sum_{b,c} k_{ab}^{(\alpha)} k_{bc}^{(\alpha)} y_c + \mathcal{O}(y_c^2).$$

Now we see that parallel translations lead to violation of orthogonality condition because

$$\frac{\partial \vec{n}^{(\beta)}}{\partial y_a} \cdot \vec{n}^{(\alpha)} = \sum_{b,c} (k_{ab}^{(\beta)} - k_{ab}^{(\alpha)}) k_{bc}^{(\alpha)} y_c + \mathcal{O}(y_c^2) \neq 0.$$

We introduce a notation $f_{\alpha a}^{(\beta)} = f_{a\alpha}^{(\beta)} = \Sigma_{b,c}(k_{ab}^{(\beta)} - k_{ab}^{(\alpha)}) k_{bc}^{(\alpha)} y_c$ and find the metric tensor

$$\tilde{g}_{ik} = \begin{pmatrix} g_{ab} & \sum_\gamma f_{a\beta}^{(\gamma)} \epsilon_\gamma + \mathcal{O}(\epsilon^2) \\ \sum_\gamma f_{\beta a}^{(\gamma)} \epsilon_\gamma + \mathcal{O}(\epsilon^2) & \delta_{\alpha\beta} \end{pmatrix},$$

its determinant $\tilde{g} = g + \mathcal{O}(\epsilon^2)$ and the reciprocal tensor

$$\tilde{g}^{ik} = \begin{pmatrix} g^{ab} & -\sum_{c,\gamma} g^{ac} f_{c\beta}^{(\gamma)} \epsilon_\gamma + \mathcal{O}(\epsilon^2) \\ -\sum_{c,\gamma} f_{\alpha c}^{(\gamma)} g^{cb} \epsilon_\gamma + \mathcal{O}(\epsilon^2) & \delta_{\alpha\beta} \end{pmatrix}.$$

Da Costa concluded[14] that the thin layer quantization would not work well in this situation because $\tilde{\Delta}$ contains terms with both derivatives ∂_a and ∂_α.

The situation is quite different for the method proposed in Ref. 12. All new terms in $\tilde{\Delta}$ have coefficients of order $\mathcal{O}(\epsilon)$; the only suspicious term,

$$\sum_{a,\alpha} (\partial_\alpha g^{a\alpha}) \partial_a = \left(- \sum_{a,c,\alpha,\beta} g^{ac} f_{c\alpha}^{(\beta)} \delta_{\alpha\beta} + \mathcal{O}(\epsilon) \right) \partial_a = \mathcal{O}(\epsilon) \partial_a,$$

is not dangerous because $f_{c\alpha}^{(\alpha)} = 0$. In Prokhorov quantization method the condition $\partial_\alpha (g^{1/4} \Psi_{\text{phys}}) = 0$, $\forall \alpha = m+1, \ldots, n$ is imposed. For a function $\chi(x) = (g/f)^{1/4} \Psi(x)$ it means $\partial_\alpha \chi = 0$, and we get

$$\tilde{\Delta} \frac{\chi(x)}{\left(\frac{g}{f}\right)^{1/4}} = \Delta_{\text{LB}} \frac{\chi(x)}{\left(\frac{g}{f}\right)^{1/4}} + \chi(x) \Delta_n \frac{1}{\left(\frac{g}{f}\right)^{1/4}} + \chi(x) \sum_{\alpha=m+1}^{n} \left(\frac{1}{\sqrt{g}} \partial_\alpha \sqrt{g} \right) \partial_\alpha \frac{1}{\left(\frac{g}{f}\right)^{1/4}} + \mathcal{O}(x_\alpha),$$

$\Delta_n \equiv \Sigma_{\alpha=m+1}^n \partial_\alpha^2$. It is easy to see that $(1/\sqrt{g}) \partial_\alpha \sqrt{g} = -2 g^{1/4} \partial_\alpha g^{-1/4}$, and the Hamiltonian is $\hat{H} = -(\hbar^2/2) \Delta_{\text{LB}} + V_q(x)$,

$$V_q = -\frac{\hbar^2}{2} \left(g^{1/4} \Delta_n g^{-1/4} - 2 \sum_{\alpha=m+1}^{n} (g^{1/4} \partial_\alpha g^{-1/4})^2 \right) \Bigg|_{x_\alpha = 0}.$$

One more (not too difficult) calculation yields

$$V_q = \frac{\hbar^2}{8} \sum_{\alpha=m+1}^{n} \left(\left(\sum_{a=1}^{m} k_{aa}^{(\alpha)} \right)^2 + 6 \sum_{a=1}^{m} \sum_{b=1}^{m} (k_{ab}^{(\alpha)})^2 - 8 \sum_{a=1}^{m} (k_{aa}^{(\alpha)})^2 \right). \tag{9}$$

The thin layer method would not give this answer because in this method we have $\partial_\alpha \chi = 0$ only at the original surface and generally $\partial_\alpha \chi \sim 1/\delta$, so that terms with $\partial_\alpha \chi$ are not negligible and factorization similar to (5) is not a good approximation of the exact thin layer solution. It is not surprising. Let us take a small element of the surface and its δ-neighborhood, $\delta \to 0$. The well-known theorem states that $\int \mathrm{d}V \, \Delta\Psi = \int \mathrm{d}\vec{S} \cdot \vec{\nabla} \Psi$. We have $\Delta\Psi \approx \int \mathrm{d}\vec{S} \cdot \vec{\nabla} \Psi / V$ and in the codimension 1 case the normal projection of $\vec{\nabla} \Psi$ leads to $1/\delta^2$ term in $\Delta\Psi$ (because $\partial_n \Psi \sim 1/\delta$ and $V \sim \delta$). Tangential components of $\vec{\nabla} \Psi$ result in finite values of $\Delta\Psi$ due to $\mathrm{d}S_\perp \sim \delta$. In the general case $V \sim \delta^{n-m}$ and $\mathrm{d}S \sim \delta^{n-m}$, hence the tangential components of $\vec{\nabla} \Psi$ yield finite terms in $\Delta\Psi$ again; but normal projections gain some components orthogonal to transverse hyperplanes (x_a

=const). The corresponding angles are of order δ but $\partial_\alpha \Psi \sim 1/\delta$. It results in finite terms in $\Delta\Psi$. So, normal components of $\vec{\nabla}\Psi$ influence the tangential dynamics. Hence, the thin layer method of Refs. 7, 8, and 14 *does not* yield the result of the general form (1). It means that the Prokhorov method in such cases *does not* correspond to the motion in the uniform thin layer but it turns out to be more powerful as an abstract quantization method for second class constrained systems. One could find, of course, some orthogonal coordinate system in the whole vicinity of the surface with normals depending on x_α and, maybe, one would be able to determine a geometry of the thin layer for which some factorization similar to (5) would be a good approximation. Quantum potential in this approach is likely to coincide with (9) at least with a certain realization of it, but generally the layer would not have constant width and the setup of the quantization would not be as easy and clear as the original one.

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Analytic plane wave solutions for the quaternionic potential step

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By using the recent mathematical tools developed in quaternionic differential operator theory, we solve the Schrödinger equation in the presence of a quaternionic step potential. The analytic solution for the stationary states allows one to explicitly show the qualitative and quantitative differences between this quaternionic quantum dynamical system and its complex counterpart. A brief discussion on reflected and transmitted times, performed by using the stationary phase method, and its implication on the experimental evidence for deviations of standard quantum mechanics is also presented. The analytic solution given in this paper represents a fundamental mathematical tool to find an analytic approximation to the quaternionic barrier problem (up to now solved by numerical method). © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227635]

I. INTRODUCTION

Since a quaternionic equation can be equivalently written as a two-component complex equation, it is natural to ask whether the quaternionic Schrödinger equation is simply another way of rewriting complex quantum mechanics. The answer to this question is given in the famous book[1] by Adler. Probabilities in quaternionic dynamical system are different from those of standard complex theory. In the first papers on the quaternionic Schrödinger equation, deviations from complex quantum mechanics were studied by considering quaternionic perturbation potentials.[2,3] Recent progress on the solution of quaternionic differential equations[4–6] has improved the physical discussion on quaternionic tunneling phenomena[7] and bound states.[8]

In this paper, an interesting simple quaternionic quantum mechanical system is *analytically* solved. This allows one to discuss both qualitative and quantitative differences between quaternionic and complex quantum mechanics. The explicit stationary wave solution for the quaternionic potential step shows some important results which could be very useful in looking for deviations from the standard quantum theory. For example, the quaternionic step diffusion is characterized by reflected and transmitted waves which are *not* instantaneous. The analytic solution is also very useful to understand the effect that quaternionic potentials play on the phase of stationary waves. The advantage to analytically solve a quaternionic problem is surely represented by the possibility to deeply study the quaternionic solution and understand where and if deviations from complex quantum theory could be seen.

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II. FQUATERNIONIC SCHRÖDINGER EQUATION

In the quaternionic formulation of nonrelativistic quantum mechanics, the dynamics of a particle without spin subject to the influence of the anti-Hermitian scalar potential,

$$iV_1(\boldsymbol{r},t)+jV_2(\boldsymbol{r},t)+kV_3(\boldsymbol{r},t),$$

is described by

$$\hbar\,\partial_t\Psi(\boldsymbol{r},t)=\left[i\frac{\hbar^2}{2m}\nabla^2-iV_1(\boldsymbol{r},t)-jV_2(\boldsymbol{r},t)-kV_3(\boldsymbol{r},t)\right]\Psi(\boldsymbol{r},t), \tag{1}$$

with

$$V_{1,2,3}:\quad (\mathbb{R}^3,\mathbb{R})\to\mathbb{R}\quad\text{and}\quad \Psi:(\mathbb{R}^3,\mathbb{R})\to\mathbb{H}.$$

Equation (1) is known as the Schrödinger equation for quaternionic quantum mechanics.[1] It is natural to try to relate the new results coming from this quaternionic formulation with the well-known phenomena discussed in the standard textbooks of (complex) quantum mechanics.[9–11] In this spirit, the complex limit, i.e., $V_{2,3}\to 0$, surely represents a useful mathematical tool to test quaternionic calculations and to understand, by explicitly showing the difference between the quaternionic and complex formulation, if and where quaternionic deviations from standard quantum mechanics could be seen and investigated.

The linearity in ∂_t of the evolution time operator in Eq. (1) guarantees to obtain a positive probability density

$$\rho(\boldsymbol{r},t)=\overline{\Psi}(\boldsymbol{r},t)\Psi(\boldsymbol{r},t), \tag{2}$$

together with a continuity equation

$$\partial_t\rho(\boldsymbol{r},t)+\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{r},t)=0. \tag{3}$$

To find the explicit form of the current density $\boldsymbol{J}(\boldsymbol{r},t)$, let us first derive the Schrödinger equation for $\overline{\Psi}(\boldsymbol{r},t)$ [the quaternionic conjugate of $\Psi(\boldsymbol{r},t)$, i.e., $(i,j,k)\to-(i,j,k)$],

$$\hbar\,\partial_t\overline{\Psi}(\boldsymbol{r},t)=-\frac{\hbar^2}{2m}\nabla^2\overline{\Psi}(\boldsymbol{r},t)i+\overline{\Psi}(\boldsymbol{r},t)[iV_1(\boldsymbol{r},t)+jV_2(\boldsymbol{r},t)+kV_3(\boldsymbol{r},t)]. \tag{4}$$

Combining Eq. (1) [multiplied from the left by $\overline{\Psi}(\boldsymbol{r},t)$] and Eq. (4) [multiplied from the right by $\Psi(\boldsymbol{r},t)$], we obtain

$$\partial_t[\overline{\Psi}(\boldsymbol{r},t)\Psi(\boldsymbol{r},t)]+\frac{\hbar}{2m}\{[\nabla^2\overline{\Psi}(\boldsymbol{r},t)]i\Psi(\boldsymbol{r},t)-\overline{\Psi}(\boldsymbol{r},t)i\nabla^2\Psi(\boldsymbol{r},t)\}=0.$$

Consequently, the density current in quaternionic quantum mechanics is formally equal to that one of the usual complex theory, i.e.,

$$\boldsymbol{J}(\boldsymbol{r},t)=\frac{\hbar}{2m}\{[\nabla\overline{\Psi}(\boldsymbol{r},t)]i\Psi(\boldsymbol{r},t)-\overline{\Psi}(\boldsymbol{r},t)i\,\nabla\,\Psi(\boldsymbol{r},t)\}. \tag{5}$$

It is worth pointing out that, due to the noncommutativity nature of quaternions, the position of the imaginary unit i is not a choice but it is imposed by the anti-Hermiticity of evolution time operator in Eq. (1).

A. Time independent potentials

In this paper, we are going to be concerned with a particle in a time independent potential. In complex quantum mechanics, the rapid spatial variations of a square potential introduce purely

quantum effects in the motion of the particle. The same is valid for perturbative quaternionic potentials. Before beginning our investigation, we shall discuss some important mathematical properties of the quaternionic Schrödinger equation in the presence of time independent potentials,

$$\hbar\,\partial_t\Psi(\boldsymbol{r},t)=\left[i\frac{\hbar^2}{2m}\nabla^2-iV_1(\boldsymbol{r})-jV_2(\boldsymbol{r})-kV_3(\boldsymbol{r})\right]\Psi(\boldsymbol{r},t). \tag{6}$$

Taking into account that $\Psi(\boldsymbol{r},t)$ is a quaternionic function, we apply the method of separation of variables with the time dependent function appearing on the right-hand side,[4]

$$\Psi(\boldsymbol{r},t)=\Phi(\boldsymbol{r})\exp\left[-\frac{i}{\hbar}Et\right], \tag{7}$$

with

$$\Phi:\quad \mathbb{R}^3\rightarrow\mathbb{H}.$$

This stationary solution of the Schrödinger equation leads to a time-independent probability density $\rho(\boldsymbol{r})$. Consequently, the current density satisfies

$$\boldsymbol{\nabla}\cdot\{[\nabla\overline{\Phi}(\boldsymbol{r})]i\Phi(\boldsymbol{r})-\overline{\Phi}(\boldsymbol{r})i\,\nabla\,\Phi(\boldsymbol{r})\}=0. \tag{8}$$

By using the separation of variable (7), Eq. (6) reduces to the following quaternionic (right) eigenvalue problem:[12,13]

$$\left[i\frac{\hbar^2}{2m}\nabla^2-iV_1(\boldsymbol{r})-jV_2(\boldsymbol{r})-kV_3(\boldsymbol{r})\right]\Phi(\boldsymbol{r})+\Phi(\boldsymbol{r})iE=0. \tag{9}$$

B. Time reversal invariance

From Eq. (6), we can immediately obtain the time-reversed Schrödinger equation

$$\hbar\,\partial_t\Psi_T(\boldsymbol{r},-t)=-\left[i\frac{\hbar^2}{2m}\nabla^2-iV_1(\boldsymbol{r})-jV_2(\boldsymbol{r})-kV_3(\boldsymbol{r})\right]\Psi_T(\boldsymbol{r},-t). \tag{10}$$

In complex quantum mechanics the *-conjugation yields a time-reversed version of the original Schrödinger equation. In quaternionic quantum mechanics there does *not* exist a universal time reversal operator.[1] Only a *restricted* class of time-independent quaternionic potentials $[V_2(\boldsymbol{r})\propto V_3(\boldsymbol{r})]$, i.e.,

$$W(\boldsymbol{r})=V_2(\boldsymbol{r})-iV_3(\boldsymbol{r})=|W(\boldsymbol{r})|\exp[i\theta]\quad(\theta=\text{const}),$$

is time reversal invariant. For these potentials,

$$\Psi_T(\boldsymbol{r},-t)=u\Psi(\boldsymbol{r},t)\overline{u},\quad u=k\exp[i\theta]. \tag{11}$$

In the standard quantum mechanics limit, due to the complex nature of the wave function $\Psi_{\mathbb{C}}(\boldsymbol{r},t)$, we recover the well-known result

$$\Psi_{\mathbb{C},T}(\boldsymbol{r},-t)=\Psi^*_{\mathbb{C}}(\boldsymbol{r},t).$$

C. One-dimensional square potentials

Let us consider one-dimensional potentials. In the case of square shapes, the potential is a quaternionic constant in certain regions of space. In such regions, the stationary wave function $\Phi(x)$ is obtained by solving the following second-order differential equation with (left) constant quaternionic coefficients,

$$\left[i\frac{\hbar^2}{2m}\Phi''(x) - iV_1 - jV_2 - kV_3 \right]\Phi(x) = -\Phi(x)iE. \tag{12}$$

It is not our purpose here to discuss the theory of quaternionic differential equations and we refer the interested reader to the papers cited in Refs. 4–6 where a detailed exposition of the subject is found. The solution of Eq. (12) is

$$\Phi(x) = (1+jw)\{\exp[\nu_- x]c_1 + \exp[-\nu_- x]c_2\} + (z+j)\{\exp[\nu_+ x]c_3 + \exp[-\nu_+ x]c_4\}, \tag{13}$$

where $c_{1,\ldots,4}$ are complex coefficients to be determined by the boundary conditions and

$$\nu_\pm = \sqrt{2m(V_1 \pm \sqrt{E^2 - V_2^2 - V_3^2})}/\hbar\ ,$$

$$z = i(V_2 + iV_3)/(E + \sqrt{E^2 - V_2^2 - V_3^2}),$$

$$w = -i(V_2 - iV_3)/(E + \sqrt{E^2 - V_2^2 - V_3^2}) \in \mathbb{C}(1,i).$$

In the free potential region ($V_{1,2,3}=0$) the previous solution reduces to

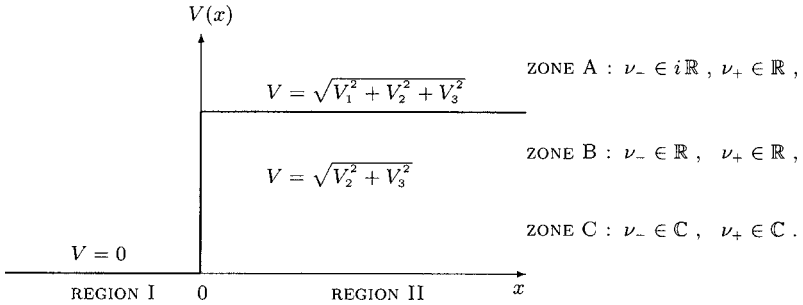
$$\Phi(x) = \exp[i\epsilon x]c_1 + \exp[-i\epsilon x]c_2 + j\{\exp[\epsilon x]c_3 + \exp[-\epsilon x]c_4\}, \tag{14}$$

where

$$\epsilon = \sqrt{2mE}/\hbar\ \in \mathbb{R}.$$

III. BOUNDED SOLUTIONS AND CURRENT DENSITY

Let us now calculate the stationary states in the case of a quaternionic step potential. The procedure follows the standard one. We use Eq. (13) in the region where the potential is a constant and Eq. (14) in the free region. We then impose that such solutions remain bounded and, finally, we match these functions by requiring the continuity of $\Phi(x)$ and its derivative in $x=0$. Before proceeding with our calculations, the only point deserving further discussion concerns the classification of the energy zones in the potential region (in order to distinguish between partial and total reflection). To do this, we have to analyze the complex exponential factors $\nu_\pm$. The possible cases are sketched in the following figure



To avoid any confusion between real and imaginary coefficients and to facilitate the reading of this paper, in the sequel, we shall adopt the following notation:

zone A:	$\nu_- = i\rho_-$,	ν_+,
zone B:	ν_-,	ν_+,
zone C:	$\nu_- = \sigma_+ - i\sigma_-$,	$\nu_+ = \sigma_+ + i\sigma_-$,

where

$$\rho_- = \sqrt{\frac{2m}{\hbar^2}(\sqrt{E^2 - V_2^2 - V_3^2} - V_1)}, \quad \sigma_\pm = \sqrt{\frac{m}{\hbar^2}(\sqrt{V_1^2 + V_2^2 + V_3^2 - E^2} \pm V_1)} \in \mathbb{R}.$$

A. Region I

For the solution to remain bounded when $x \to -\infty$, it is necessary to have $c_4=0$ in Eq. (14). So, the solution in region I becomes

$$\Phi_{\mathrm{I}}(x) = e^{i\epsilon x} + re^{-i\epsilon x} + j\tilde{r}e^{\epsilon x}, \tag{15}$$

where $c_2=r$ and $c_3=\tilde{r}$ represent the reflection coefficients to be determined by the matching conditions. From Eq. (8), we immediately find the constant value of the current density in this region, i.e.,

$$J_{\mathrm{I}} = (1 - |r|^2)\,\hbar\,\epsilon/m. \tag{16}$$

B. Region II - zone A: Partial reflection

The condition on the boundedness of the solution implies that $c_3=0$ in Eq. (13). Since the incident particle is coming from $x=-\infty$, we also have to impose $c_2=0$. The stationary wave function, in zone A, is then given by

$$\Phi_{\mathrm{II,A}}(x) = (1 + jw)te^{i\rho_- x} + (z + j)\tilde{t}e^{-\rho_+ x}, \tag{17}$$

where $c_1=t$ and $c_4=\tilde{t}$ represent the transmission coefficients to be determined by the matching conditions. In this region the current density is

$$J_{\mathrm{II,A}} = (1 - |w|^2)|t|^2\,\hbar\,\rho_-/m. \tag{18}$$

This means a non-null transmission probability and consequently partial reflection in region I.

C. Region II - zone B: Total reflection

For the solution to remain bounded when $x \to +\infty$, it is necessary that $c_2=c_4=0$ in Eq. (13). Thus, the solution in zone B is

$$\Phi_{\mathrm{II,B}}(x) = (1 + jw)te^{-\nu_- x} + (z + j)\tilde{t}e^{-\nu_+ x}. \tag{19}$$

In this zone, the current density is null

$$J_{\mathrm{II,B}} = 0. \tag{20}$$

This characterizes a total reflection in region I.

D. Region II - zone C: Total reflection

The boundedness condition of the solution implies that $c_1=c_3=0$ in Eq. (13). Thus, we have

$$\Phi_{\mathrm{II,C}}(x) = [(1 + jw)te^{i\sigma_- x} + (z + j)\tilde{t}e^{-i\sigma_- x}]e^{-\sigma_+ x}, \tag{21}$$

with

$$w = -i\frac{V_2 - iV_3}{\sqrt{V_2^2 + V_3^2}}e^{-i\varphi}, \quad z = i\frac{V_2 + iV_3}{\sqrt{V_2^2 + V_3^2}}e^{-i\varphi}, \quad \varphi = \arctan\left[\frac{\sqrt{V_2^2 + V_3^2 - E^2}}{E}\right].$$

As in the previous zone, the current density is null

$$J_{\mathrm{II,C}} = 0. \tag{22}$$

This implies total reflection in region I.

E. Relation between reflection and transmission coefficients

The stationary wave solution of the Schrödinger equation in the presence of a quaternionic step potential can then be expressed in terms of complex reflection $(r,\tilde{r})$ and transmission $(t,\tilde{t})$ coefficients:

$$\Phi_{\mathrm{I}}(x) = e^{i\epsilon x} + re^{-i\epsilon x} + j\tilde{r}e^{\epsilon x}, \tag{23}$$

$$\Phi_{\mathrm{II}}(x) = \begin{cases} (1+jw)te^{i\rho_- x} + (z+j)\tilde{t}e^{-\nu_+ x} & \text{zone A} \\ (1+jw)te^{-\nu_- x} + (z+j)\tilde{t}e^{-\nu_+ x} & \text{zone B} \\ [(1+jw)te^{i\sigma_- x} + (z+j)\tilde{t}e^{-i\sigma_- x}]e^{-\sigma_+ x} & \text{zone C}. \end{cases} \tag{24}$$

As we saw, the current density assumes a constant value. This value has been calculated in the free potential region and in each of the three different zones of region II. The continuity of $\Phi(x)$ and its derivative in $x=0$ implies the continuity of the current density, i.e., $J_{\mathrm{I}}=J_{\mathrm{II}}$. This gives an immediate relation between reflection and transmission coefficients,

$$R + T = 1, \tag{25}$$

with

$$R = |r|^2 \quad \text{and} \quad T = \frac{\rho_-}{\epsilon}(1-|w|^2)|t|^2 \quad \text{for } E > \sqrt{V_1^2+V_2^2+V_3^2},$$

$$R = |r|^2 \quad \text{and} \quad T = 0 \quad \text{for } E < \sqrt{V_1^2+V_2^2+V_3^2}.$$

Observe that both in complex and quaternionic quantum mechanics, to find the relation between R and T we do not have the necessity to find the explicit value of plane wave coefficients r and t.

IV. EXPLICIT PLANE WAVE SOLUTIONS

The usual method for determining the stationary states in a square potential requires the continuity of $\Phi(x)$ and its derivative at the point where the potential is discontinuous (in this case $x=0$). Then, we impose that

$$\begin{aligned} \Phi_{\mathrm{I}}(0) &= \Phi_{\mathrm{II}}(0), \\ \Phi_{\mathrm{I}}'(0) &= \Phi_{\mathrm{II}}'(0). \end{aligned} \tag{26}$$

A. Region II - zone A: Continuity

Matching the conditions at $x=0$, we get

$$1 + r + j\tilde{r} = (1+jw)t + (z+j)\tilde{t},$$

$$i\epsilon(1-r) + j\epsilon\tilde{r} = (1+jw)i\rho_- t - (z+j)\nu_+\tilde{t}.$$

After separating the complex from the pure quaternionic part, we find

$$1 + r = t + z\tilde{t},$$

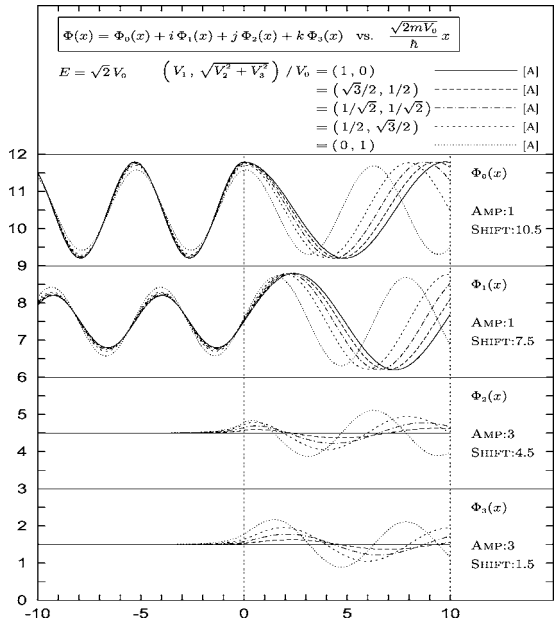


FIG. 1. Space is divided into region I ($x<0$) and region II ($x>0$). There is a constant quaternionic potential ($iV_1+jV_2+kV_3$) in region II whereas in region I there is no potential. The space dependence of the quaternionic stationary wave function $\Phi(x)$ is plotted for the energy zone A ($E>V_0=\sqrt{V_1^2+V_2^2+V_3^2}$) and for different complex/pure quaternionic potential ratios. The plots for the complex part of $\Phi(x)$ exhibit an oscillatory behavior both for region I and region II. The pure quaternionic part is practically absent in the free potential region.

$$\tilde{r} = wt + \tilde{t},$$

$$1 - r = \frac{\rho_-}{\epsilon}t + i\frac{\nu_+}{\epsilon}\tilde{zt},$$

$$\tilde{r} = i\frac{\rho_-}{\epsilon}wt - \frac{\nu_+}{\epsilon}\tilde{t},$$

which gives

$$\begin{aligned}
t &= \frac{2\epsilon}{\epsilon+\rho_-}\left[1 - zw\frac{\epsilon+i\nu_+}{\epsilon+\nu_+}\frac{\epsilon-i\rho_-}{\epsilon+\rho_-}\right]^{-1},\\
r &= \frac{\epsilon-\rho_-}{2\epsilon}\left[1 - zw\frac{\epsilon-i\nu_+}{\epsilon+\nu_+}\frac{\epsilon-i\rho_-}{\epsilon-\rho_-}\right]t,\\
\tilde{t} &= -\frac{\epsilon-i\rho_-}{\epsilon+\nu_+}wt,\\
\tilde{r} &= \frac{\nu_+ + i\rho_-}{\epsilon+\nu_+}wt.
\end{aligned} \tag{27}$$

We have determined the stationary states of a particle in the presence of a quaternionic step potential for plane waves of energy $E>V_0=\sqrt{V_1^2+V_2^2+V_3^2}$. In Fig. 1, we plot, for different ratios of the complex and pure quaternionic potential $(V_1/\sqrt{V_2^2+V_3^2}\,)$, the four real component of $\Phi(x)$

versus the adimensional space variable $\sqrt{2mV_0}x/\hbar$. In region I, only the complex part of $\Phi(x)$ presents an oscillatory behavior. The pure quaternionic part decreases exponentially due to the presence of the evanescent wave $e^{\epsilon x}$. In region II, we have a new oscillatory pure quaternionic wave. It is also important to note here that increasing the value of pure quaternionic potential, we smooth the phase changes expected in the potential region by standard quantum mechanics. Thus, we can conclude that this change in the phase is caused by the complex part of the quaternionic potential.

These plane waves do not represent a physical state for a localized incoming particle. They have to be linearly superposed to form wave packets. It is not our purpose to introduce the wave packet treatment for quaternionic wave functions in this paper. This topic deserves a deeper analysis and is, currently, under investigation. Nevertheless, a simple discussion can done at this stage. By using the stationary phase method,[9] we can follow the maximum of the reflected and transmitted wave packets. The use of a real modulation function $g(\epsilon)$ implies that the incident wave packets reach the point $x=0$ at $t=0$. Any phase in the reflected and/or transmitted waves will introduce a shift in time. To clarify this point, it can be useful to rewrite the reflection and transmission coefficients in terms of their modulus and phases. By simple algebraic manipulations, we find

$$\begin{aligned} r &= \frac{(\epsilon-\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2-\rho_-\nu_+)+izw\epsilon(\rho_-+\nu_+)}{(\epsilon+\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2+\rho_-\nu_+)+izw\epsilon(\rho_--\nu_+)} \\ &= \sqrt{\frac{[(\epsilon-\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2-\rho_-\nu_+)]^2+z^2w^2\epsilon^2(\rho_-+\nu_+)^2}{[(\epsilon+\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2+\rho_-\nu_+)]^2+z^2w^2\epsilon^2(\rho_--\nu_+)^2}}\exp[i(\theta_n-\theta_d)] \end{aligned} \tag{28}$$

and

$$\begin{aligned} t &= \frac{2\epsilon}{\epsilon+\rho_-}\left[\frac{(\epsilon+\rho_-)(\epsilon+\nu_+)}{(\epsilon+\rho_-)(\epsilon+\nu_+)-zw(\epsilon-i\rho_-)(\epsilon+i\nu_+)}\right] \\ &= \frac{2\epsilon(\epsilon+\nu_+)}{\sqrt{[(\epsilon+\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2-\rho_-\nu_+)]^2+z^2w^2\epsilon^2(\rho_-+\nu_+)^2}}\exp[-i\theta_d], \end{aligned} \tag{29}$$

where

$$\theta_n = \arctan\left[\frac{zw\epsilon(\rho_-+\nu_+)}{(\epsilon-\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2-\rho_-\nu_+)}\right], \tag{30}$$

$$\theta_d = \arctan\left[\frac{zw\epsilon(\rho_--\nu_+)}{(\epsilon+\rho_-)(\epsilon+\nu_+)-zw(\epsilon^2+\rho_-\nu_+)}\right]. \tag{31}$$

The phases of the reflected and transmitted waves are then given by

$$\begin{aligned} \theta_r(\epsilon;x,t) &= \theta_n(\epsilon)-\theta_d(\epsilon)-\epsilon x-\frac{\hbar\epsilon^2}{2m}t, \\ \theta_t(\epsilon;x,t) &= -\theta_d(\epsilon)+\rho_-(\epsilon)x-\frac{\hbar\epsilon^2}{2m}t. \end{aligned} \tag{32}$$

The stationary phase method suggests that the maximum of the reflected and transmitted waves is found at the point $x=0$ for the following time values:

$$\tau_r = \frac{m}{\hbar}\frac{\theta_n'(\epsilon_0)-\theta_d'(\epsilon_0)}{\epsilon_0},$$

$$\tau_t = -\frac{m}{\hbar}\frac{\theta_d'(\epsilon_0)}{\epsilon_0}, \tag{33}$$

where ϵ_0 is the maximum of the modulation function $g(\epsilon)$. In this energy zone ($E > V_0$), an immediate *qualitative* difference between complex and quaternionic quantum mechanics is found. For quaternionic potential the reflection and transmission are *not* instantaneous. We shall come back to this point later.

B. Region II - zone A: Complex limit

Performing the complex limit, $V_{2,3} \to 0$, we obtain

$$\nu_+ \to \sqrt{2m(E+V_1)}/\hbar\ ,$$

$$\rho_- \to \sqrt{2m(E-V_1)}/\hbar\ ,$$

$$z, w \to 0.$$

From Eq. (27), we find the reflection and transmission coefficient of standard (complex) quantum mechanics

$$t_{\mathrm{C}} = 2\sqrt{E}/(\sqrt{E}+\sqrt{E-V_1}),$$

$$r_{\mathrm{C}} = (\sqrt{E}-\sqrt{E-V_1})/(\sqrt{E}+\sqrt{E-V_1}),$$

$$\tilde{r}_{\mathrm{C}}, \tilde{t}_{\mathrm{C}} = 0.$$

Due to the real nature of r_{C} and t_{C}, we find instantaneous reflection and transmission. This means that at time zero, the maximum of the incident, reflected and transmitted waves are at $x=0$.

C. Region II - zone B: Continuity

Matching the continuity conditions at $x=0$, we obtain

$$t = \frac{2\epsilon}{\epsilon + i\nu_-}\left[1 - zw\frac{\epsilon+\nu_-}{\epsilon+i\nu_-}\frac{\epsilon+i\nu_+}{\epsilon+\nu_+}\right]^{-1},$$

$$r = \frac{\epsilon - i\nu_-}{2\epsilon}\left[1 - zw\frac{\epsilon+\nu_-}{\epsilon-i\nu_-}\frac{\epsilon-i\nu_+}{\epsilon+\nu_+}\right]t, \tag{34}$$

$$\tilde{t} = -\frac{\epsilon+\nu_-}{\epsilon+\nu_+}wt,$$

$$\tilde{r} = \frac{\nu_+ - \nu_-}{\epsilon+\nu_+}wt.$$

In Fig. 2, we plot the four real component of $\Phi(x)$ versus the adimensional space variable $\sqrt{2mV_0}x/\hbar$. Zone B is characterized by $\sqrt{V_2^2+V_3^2} < E < V_0$. In Fig. 2, we have considered the case $E = V_0/\sqrt{2}$. Consequently, the behavior of the stationary waves in this zone is given by the plots corresponding to $\sqrt{V_2^2+V_3^2}/V_0 < 1/\sqrt{2}$. In this zone, due to the presence of evanescent exponentials in the transmitted waves, we find a nonzero probability to find the particle in the region of space where x is positive only for short times. The stationary phase method can be applied to the reflected wave. The coefficient r can be rewritten as follows

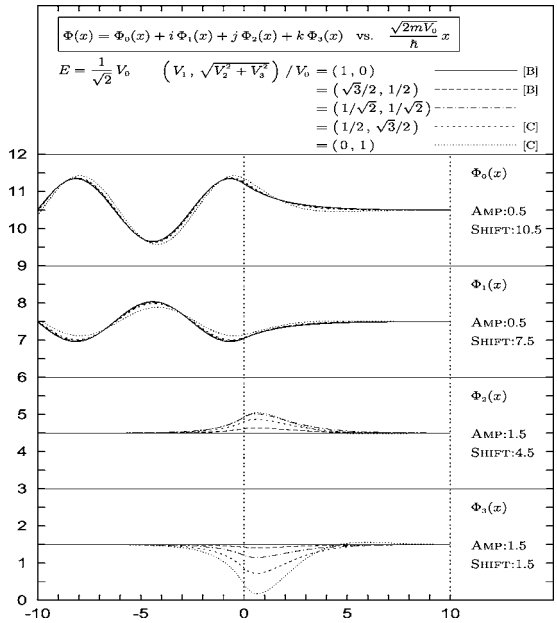


FIG. 2. The space dependence of the quaternionic stationary wave function $\Phi(x)$ is plotted for the energy zone B ($\sqrt{V_2^2+V_3^2}<E<V_0$) and C ($E<\sqrt{V_2^2+V_3^2}$), and for different complex/pure quaternionic potential ratios. The plots for the complex part of $\Phi(x)$ exhibit an evanescent behavior in region II. The pure quaternionic part is practically zero far from the discontinuity point. An interesting oscillatory behavior smoothed by the evanescent waves is also present in region II for energy values in zone C. This remembers the Klein zone in the Dirac equation.

$$r = \frac{\epsilon[(\epsilon+\nu_+) - zw(\epsilon+\nu_-)] + i[zw\nu_+(\epsilon+\nu_-) - \nu_-(\epsilon+\nu_+)]}{\epsilon[(\epsilon+\nu_+) - zw(\epsilon+\nu_-)] - i[zw\nu_+(\epsilon+\nu_-) - \nu_-(\epsilon+\nu_+)]} = \exp[2i\theta], \tag{35}$$

where

$$\theta = \arctan\left[\frac{zw\nu_+(\epsilon+\nu_-) - \nu_-(\epsilon+\nu_+)}{\epsilon(\epsilon+\nu_+) - zw\epsilon(\epsilon+\nu_-)}\right].$$

The phase of the reflected wave is then given by

$$\theta_r(\epsilon;x,t) = 2\theta(\epsilon) - \epsilon x - \frac{\hbar\epsilon^2}{2m}t. \tag{36}$$

It is important to observe that here we have a *quantitative* difference between complex and quaternionic quantum mechanics. Indeed, also for the standard quantum theory the reflection is not instantaneous. The reflect wave reaches $x=0$ at time

$$\tau_r = 2\frac{m}{\hbar}\frac{\theta'(\epsilon_0)}{\epsilon_0}. \tag{37}$$

D. Region II - zone B: Complex limit

Performing the complex limit, $V_{2,3}\to 0$, we obtain

$$t \to t_C = 2\sqrt{E}/(\sqrt{E} + i\sqrt{V_1 - E}),$$

$$r \to r_C = (\sqrt{E} - i\sqrt{V_1 - E})/(\sqrt{E} + i\sqrt{V_1 - E}),$$

$$\tilde{r},\tilde{t}\to 0.$$

The presence of the phase

$$\theta_{\mathrm{C}}=\arctan\left(-\sqrt{\frac{V_1-E}{E}}\right)$$

in r_{C} shows that the reflection is not instantaneous. The delay time[9] is

$$\tau_{r,\mathrm{C}}=2\frac{m}{\hbar}\frac{\theta_{\mathrm{C}}'(\epsilon_0)}{\epsilon_0}=\frac{\hbar}{E_0}\sqrt{\frac{E_0}{V_1-E_0}}. \tag{38}$$

E. Region II - zone C: Continuity

The last zone is characterized by $E<\sqrt{V_2^2+V_3^2}$. Continuity conditions give

$$\begin{aligned}
t&=\frac{2\epsilon}{\epsilon+\sigma_-+i\sigma_+}\left[1-zw\frac{\epsilon+\sigma_+-i\sigma_-}{\epsilon+\sigma_-+i\sigma_+}\frac{\epsilon-\sigma_-+i\sigma_+}{\epsilon+\sigma_++i\sigma_-}\right]^{-1},\\
r&=\frac{\epsilon-\sigma_--i\sigma_+}{2\epsilon}\left[1-zw\frac{\epsilon+\sigma_+-i\sigma_-}{\epsilon-\sigma_--i\sigma_+}\frac{\epsilon+\sigma_--i\sigma_+}{\epsilon+\sigma_++i\sigma_-}\right]t,\\
\tilde{t}&=-\frac{\epsilon+\sigma_+-i\sigma_-}{\epsilon+\sigma_++i\sigma_-}wt,\\
\tilde{r}&=\frac{2i\sigma_-}{\epsilon+\sigma_++i\sigma_-}wt.
\end{aligned} \tag{39}$$

The stationary waves corresponding to this case are also shown in Fig. 2, see the plots with $\sqrt{V_2^2+V_3^2}/V_0>1/\sqrt{2}$. To discuss the time reflection, we rewrite r in terms of its modulus and phase,

$$r=\frac{(\epsilon-\sigma_--i\sigma_+)(\epsilon+\sigma_++i\sigma_-)e^{i\varphi}-(\epsilon+\sigma_+-i\sigma_-)(\epsilon+\sigma_--i\sigma_+)e^{-i\varphi}}{(\epsilon+\sigma_++i\sigma_-)(\epsilon+\sigma_-+i\sigma_+)e^{i\varphi}-(\epsilon+\sigma_+-i\sigma_-)(\epsilon-\sigma_-+i\sigma_+)e^{-i\varphi}}=\exp[2i\theta] \tag{40}$$

where

$$\theta=\arctan\left[\frac{\epsilon(\epsilon+\sigma_+)\tan\varphi+\epsilon\sigma_-}{\epsilon\sigma_--(\epsilon\sigma_++\sigma_-^2+\sigma_+^2)\tan\varphi}\right].$$

In this zone, we do not have a complex limit case. It is important to observe that a *new* phenomenon appears. The oscillatory behavior of the particle in region II is damped due to the presence of the evanescent wave $e^{-\sigma_+x}$. Thus, a nonzero probability to find the particle in the potential region only exists for short times.

V. RELATIONSHIPS BETWEEN COMPLEX AND QUATERNIONIC QUANTUM MECHANICS

In the last several years, the Schrödinger equation in the presence of quaternionic (constant) potentials has been a matter of study and discussion in the literature. This is justified in view of a possible understanding of the role that a quaternionic quantum theory could play in the real physical world. As remarked by Adler[1] all known physical phenomena appear to be very well described by complex quantum mechanics. Nevertheless, to see if quaternionic quantum mechanics represents a possible way to describe the nature or if it is only an interesting mathematical exercise, we have to use and test this formalism in simple quantum mechanical systems. With

respect to previous works regarding potential barrier diffusion[2,3,7] and potential well bound states,[8] in this paper, we have preferred to go back in our analysis of nonrelativistic quaternionic quantum mechanics by studying the potential step.

The study presented in this paper can be seen as an attempt to understand, by starting from an *analytic* solution of a simple quantum mechanical system, where and if differences between standard quantum mechanics and theoretical solutions obtained by solving the Schrödinger equation in the presence of a quaternionic step perturbation can be observed. The main difficulty in obtaining quaternionic solutions of a physical problem is due to the fact that, in general, the standard mathematical methods of resolution break down. Nevertheless, the recent progress in quaternionic differential theory[4–6] and linear algebra[12,13] gives the possibility to use "new" quaternionic mathematical tools. As a direct consequence of this, we have been able to find an analytic solution for the stationary states in the presence of a quaternionic potential step. This means that we have now (for the first time) the possibility of describing in detail *qualitative* differences between complex and quaternionic quantum mechanics.

A. Experimental proposals in quaternionic quantum mechanics

The earliest experimental proposals to test quaternionic deviations from complex quantum mechanics[14] suggested that the noncommutativity of quaternionic phases could be observed in Bragg scattering by crystal made of three different atoms, in neutron interferometry and in meson regeneration. In 1984, the neutron interferometric experiment was realized by Kaiser, George, and Werner.[15] The neutron wave function traversing slabs of two dissimilar materials (titanium and aluminum) should experience the noncommutativity of the phase shifts when the order in which the barriers are traversed is reversed. The experimental result showed that the phase shifts commute to better than one part in 3×10^4. To explain this null result, Klein postulated[16] that quaternionic potentials act only for some of the fundamental forces and proposed an experiment for testing possible violations of the Schrödinger equation by permuting the order in which nuclear, magnetic, and gravitational potentials act on neutrons in an interferometer.

The first theoretical analysis of two quaternionic potential barriers was developed by Davies and McKellar.[3] In their paper, by translating the quaternionic Schrödinger equation into a pair of coupled complex equations and solving the corresponding complex system by numerical methods, Davies and McKellar showed that, notwithstanding the presence of complex *instead* of quaternionic phases, the predictions of quaternionic quantum mechanics differ from those of the usual theory. In particular, they pointed out that different from the complex quantum mechanics prediction, where the left and right transmission amplitudes, t_L and t_R, are equal in magnitude and in phase, in the quaternionic quantum mechanics only the magnitudes $|t_L|$ and $|t_R|$ are equal. So, the measurement of a phase shift should be an indicator of quaternionic effects *and* of space dependent phase potentials. However, this conclusion leads to the embarrassing question of why there was no phase change in the experiment proposed by Peres[14] and realized by Kaiser, George, and Werner.[15] To reconcile the theoretical predictions with the experimental observations, Davies and McKellar reiterated the Klein conclusion and suggested to subject the neutron beam to different interactions in permuted order.

In the final chapter of the Adler book,[1] we find an intriguing question. Do the Kayser and colleagues'[1] experiment, and the elaborations on it proposed by Klein actually test for residual quaternionic effects? According to the nonrelativistic quaternionic scattering theory developed by Adler[1] the answer is clearly *no*. Experiments to detect a phase shift are equivalent to detect *time reversal violation*, which so far has not been detectable in neutron-optical experiments.

B. Quaternionic potential step, CP violation, and kaons system

Based on the previous considerations, experimental proposals to test quaternionic deviations from standard quantum mechanics should involve CP violation dynamical systems. A natural candidate to such an investigation could be the system of K-mesons.[17,18] The quaternionic time reversal violation potential (see Sec. II)

$$W(\mathbf{r}) = |W(\mathbf{r})|\exp[i\theta(\mathbf{r})]$$

should be directly responsible for CP violation effects. The experimental results on $K_{S,L}$ (a K_L meson decays more often to $\pi^- e^+ \overline{\nu_e}$ than to $\pi^+ e^- \nu_e$ Ref. 19) could be useful to estimate the modulus and phase of the pure quaternionic part of this "effective" potential.

Once determined the magnitude of the quaternionic perturbation, by using the analytic solution obtained in this paper, could be possible (through a stationary phase analysis) to explicitly calculate the reflection and transmission times of a K-meson particle scattered by a complex potential step in the presence of a quaternionic (CP violating) perturbation. In the case of an above-potential incident particle the diffusion from a pure complex potential (standard quantum mechanics) happens instantaneously, i.e.,

$$\tau_{r,\mathbb{C}} = \tau_{t,\mathbb{C}} = 0.$$

The possibility to *analytically* solve the corresponding quaternionic problem gives us the chance to see an immediate *qualitative* difference between complex and quaternionic quantum mechanics. The presence of a quaternionic potential surprisingly modifies the reflection and transmission times which are now nonzero,

$$\tau_r = \frac{m}{\hbar}\frac{\theta_n'(\epsilon_0) - \theta_d'(\epsilon_0)}{\epsilon_0}, \quad \tau_t = -\frac{m}{\hbar}\frac{\theta_d'(\epsilon_0)}{\epsilon_0},$$

where ϵ_0 is the maximum of the wave packet modulation function.

With this paper, we would have liked to close the debate on the role that quaternionic potentials could play in quantum mechanics, but more realistically, we simply contribute to the general discussion. Physical interpretations of quaternionic solutions still represent a *delicate* question and before proposing a detailed experimental test, we think that more mathematical questions should be addressed and deeply investigated.

C. Complex and quaternionic geometries

To give a satisfactory probability interpretation, amplitudes of probability must be defined in *associative division algebras*.[1] Amplitudes of probabilities defined in nondivision algebras fail to satisfy the requirement that in the absence of quantum interference effects, probability amplitude superposition should reduce to probability superposition. The associative law of multiplication (which fails for the octonions) is needed to satisfy the completeness formula and to guarantee that the Schrödinger anti-self-adjoint operator leaves invariant the inner product.

At first glance it appears that we cannot formulate quantum theories by using wave functions defined in nondivision or nonassociative algebras. This is an erroneous conclusion because the constraint concerns the inner product and *not* the kind of Hilbert space in which we define our wave functions. Amplitudes of probability have to be given in $\mathbb{C}$ or $\mathbb{H}$ (complex or quaternionic geometry) but vectors in the Hilbert space have no limitation. We can formulate a consistent complexified quaternionic[20–24] or octonionic[25,26] quantum mechanics by adopting complex inner products. The use of complex inner product represents a fundamental tool in applying a Clifford algebraic formalism to physics and plays a fundamental role in looking for geometric interpretation of the algebraic structures in relativistic equations and gauge theories.[27–31] The choice of quaternionic inner product seems to be best adapted to investigate deviations from the standard complex theory in quantum mechanics[32,33] and field theory.[34,35]

D. Conclusions and outlooks

We conclude this paper by listing the most interesting features of our analysis and future investigations suggested by our results.

(1) An *analytic* solution for a simple quantum mechanical system (quaternionic potential step) has been given (previous studies on the quaternionic Schrödinger equation have been performed by numerical calculations).

(2) Our plane wave analysis immediately show *qualitative* differences between complex and quaternionic quantum mechanics (see, for example, the reflection and transmission times for above-potential diffusion and the oscillatory behavior in the new region below the potential).

(3) A plane wave analysis for a quaternionic barrier can be now developed by using an analytic *two step approach*.

(4) The plane wave results (valid in the physical situation of complete interference) should be revised by introducing a quaternionic *wave packet* formalism (particle viewpoint). This should confirm and explain the reflection and transmission times obtained by the stationary phase method.

(5) In the quaternionic barrier analysis, we expect *qualitative* differences between complex and quaternionic quantum dynamical system.

(5.1) For above-potential diffusion, the quaternionic wave packets will be characterized by *new* reflection and transmission times with respect to the standard (complex) case.[36,37]

(5.2) In the tunneling zone, the quaternionic *Hartman* effect has to be investigated and confronted with the standard one which predicts (for a long barrier) instantaneous transmission.[38–40]

(5.3) In the *new* below-potential region, a *Klein-like* phenomenon[41,42] appears and it should be interpreted within a nonrelativistic context.

(6) The natural candidate to quaternionic experimental proposals seems to be the system of *K*-mesons. The above-suggested investigations should give a more clear idea about the possibility to *really* perform an experiment involving nonrelativistic oscillating particles and CP violating potential barriers. This probably should close the debate on the use of a quaternionic mathematical formalism in quantum theories.

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Toeplitz algebras and spectral results for the one-dimensional Heisenberg model

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We determine the structure of the spectrum and obtain nonpropagation estimates for a class of Toeplitz operators acting on a subset of the lattice $\mathbb{Z}^N$. This class contains the Hamiltonian of the one-dimensional Heisenberg model. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2222083]

I. INTRODUCTION

Spectral theory of Toeplitz operators and its connection with C^*-algebras is a vast topic. We only indicate Ref. 6 as a textbook systematization of part of the early theory. Since the appearance of Douglas' book, the theory has evolved by extension and abstraction in many directions. The works closest to the present paper are the ones relating Toeplitz operators and Toeplitz algebras to ordered groups.[11,13,20,21]

Our interest in the topic has been aroused by the remark[15,16,14] that the one-dimensional Heisenberg Hamiltonian H of ferromagnetism can be written as a direct sum $H=\oplus_{N\in\mathbb{N}}H_N$, where H_N can be interpreted as the Laplace operator on the subgraph

$$\mathbb{Z}^N_< := \{(x_1, \ldots, x_N) \in \mathbb{Z}^N : x_1 < x_2 < \cdots < x_N\}$$

of the standard (Cayley) graph $\mathbb{Z}^N$. In Sec. II we show that H_N (when suitably restricted to $\mathbb{Z}^N_<$) is equal to the sum of a Toeplitz operator and a multiplicative potential, both belonging to the Toeplitz-like C^*-algebra $\mathcal{T}^<(\mathbb{Z}^N)$ generated by the unilateral shifts on $\mathbb{Z}^N_<$.

Although $\mathcal{T}^<(\mathbb{Z}^N)$ is of none of the types thoroughly studied in the literature, its structure is simple enough to suggest spectral results for the operators it contains (see Sec. III). Since the elements of $\mathcal{T}^<(\mathbb{Z}^N)$ can be written as direct integrals over a torus, we are mainly concerned with spectral properties of the fibers (this presents a particular interest in the case of the one-dimensional Heisenberg model (see Refs. 14 and 22)). In Sec. IV we express the essential spectrum of the fibers as a union of spectra of a family of subhamiltonians, improving part of the statements of Zholondek,[23] which concerns a larger class of operators but imposes an unnecessary exponential decay condition. We consider that our formalism and proofs are much more simple and natural than those of Zholondek.[23] In Sec. V we show the following type of result concerning the whole Hamiltonian H_N. If κ is a continuous real function with suitable support, then there exists a natural family of multiplication operators $\{\chi_n\}_{n\in\mathbb{N}}$ for which $\|\chi_n\kappa(H_N)\|$ is arbitrarily small if n is large enough. This can be reformulated in terms of the evolution group $\{e^{-itH_N}\}_{t\in\mathbb{R}}$: at

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energies belonging to $\mathrm{supp}(\kappa)$, the system governed by H_N stays "out of $\mathrm{supp}(\chi_n)$" uniformly in time. Practically, $\mathrm{supp}(\kappa)$ must not intersect the spectrum of a certain subhamiltonian associated to some ideal of $\mathcal{T}^<(\mathbb{Z}^N)$. For the Heisenberg model we put into evidence a nice interpretation involving cluster properties of N-magnon states. The related issue of determining a Plancherel formula for the one-dimensional Heisenberg model has been discussed in Refs. 17 and 4 in the isotropic case and in Ref. 3 for the *XXZ* model.

We think that the structure of $\mathcal{T}^<(\mathbb{Z}^N)$ may also be crucial for proving finer spectral and scattering properties. The attainment of a Mourre estimate, which is a first step in this direction, is a problem under review.

Actually the setting generalizes from $\mathbb{Z}^N$ to $(\mathbb{Z}^m_{\mathrm{lex}})^N$, where $\mathbb{Z}^m_{\mathrm{lex}}$ is the group $\mathbb{Z}^m$ ordered lexicographically. This relies on rather deep results of Murphy[13] on Toeplitz algebras associated to certain ordered groups. The statements of the present paper can be pushed to this more general case; they just require more involved notations. Unfortunately, this is *not* the right framework to study the m-dimensional Heisenberg model (another type of Toeplitz algebra is needed), so we refrained from giving explicit detailed results in this situation; see however Remark 4.3.

Let us finally mention that our treatment has few direct connections with previous work on the spectral theory of Toeplitz operators. We were actually guided by the C^*-algebra approach to spectral analysis for Schrödinger operators, as in Refs. 1, 5, 8, 9, and 2.

II. THE ONE-DIMENSIONAL HEISENBERG MODEL

In order to justify the class of operators we study, we present here briefly and rather formally the one-dimensional Heisenberg model. Further details may be found in Refs. 14–17.

We consider the one-dimensional lattice $\mathbb{Z}$ with a spin-$\frac{1}{2}$ attached at each vertex. Let

$$\mathbb{F}(\mathbb{Z}) := \{\alpha : \mathbb{Z} \to \{0,1\} : \mathrm{supp}(\alpha) \text{ is finite}\},$$

and write $\{e^0, e^1\} := \{(0,1),(1,0)\}$ for the canonical basis of the spin-$\frac{1}{2}$ Hilbert space $\mathbb{C}^2$. For any $\alpha \in \mathbb{F}(\mathbb{Z})$ we denote by e^α the element $\{e^{\alpha(x)}\}_{x\in\mathbb{Z}}$ of the direct product $\Pi_{x\in\mathbb{Z}}\mathbb{C}^2_x$. We distinguish the vector e^{α_0}; where $\alpha_0(x) := 0$ for all $x \in \mathbb{Z}$. Each element e^α is interpreted as a pure state of the system of spins, and e^{α_0} as its ground state with all spins pointing down. The Hilbert space $\mathcal{L}$ of the system (which is spanned by the states with all but finitely many spins pointing down) is the incomplete tensor product Ref. 15, Sec. II, and Ref. 16, Sec. II)

$$\mathcal{L} := \bigotimes_{x\in\mathbb{Z}}^{\alpha_0} \mathbb{C}^2_x \equiv \text{closed span}\{e^\alpha : \alpha \in \mathbb{F}(\mathbb{Z})\}.$$

The dynamics of the spins is given by the nearest-neighbor Heisenberg Hamiltonian

$$L := -\frac{1}{2}\sum_{|x-y|=1}[a(\sigma_1^{(x)}\sigma_1^{(y)} + \sigma_2^{(x)}\sigma_2^{(y)}) + b(\sigma_3^{(x)}\sigma_3^{(y)} - 1)].$$

The operator $\sigma_j^{(x)}$ acts in $\mathcal{L}$ as the identity operator on each factor $\mathbb{C}^2_y$, except on the component $\mathbb{C}^2_x$ where it acts as the Pauli matrix σ_j. The scalars $a, b \in \mathbb{R}$ prescribe the anisotropy of the system. The case $a \neq b$ corresponds to the *XXZ* model, whereas the standard Heisenberg model is obtained for $a = b$.

Let $\mathcal{H} := \ell^2[\mathbb{F}(\mathbb{Z})]$. Then the Hilbert spaces $\mathcal{L}$ and $\mathcal{H}$ are isomorphic due to the unitarity of the mapping $\mathfrak{s} : \mathcal{L} \to \mathcal{H}$ sending e^α onto $\chi_{\{\alpha\}}$ for all α ($\chi_{\{\alpha\}}$ stands for the characteristic function of the singleton α). In particular, the set $\mathbb{F}(\mathbb{Z})$ may be considered as the configuration space for the system of spins. The Hamiltonian L is unitarily equivalent to a difference operator in $\mathcal{H}$. Given $\alpha \in \mathbb{F}(\mathbb{Z})$ and $x \in \mathrm{supp}(\alpha), y \notin \mathrm{supp}(\alpha)$, we write α_x^y for the function of $\mathbb{F}(\mathbb{Z})$ such that $\mathrm{supp}(\alpha_x^y) = \mathrm{supp}(\alpha) \sqcup \{y\} \setminus \{x\}$.

Lemma 2.1: For any $f \in \mathcal{H}$, $\alpha \in \mathbb{F}(\mathbb{Z})$, one has the equality

$$(\varsigma L\varsigma^{-1}f)(\alpha) = -2\sum_{|x-y|=1}\alpha(x)[1-\alpha(y)][af(\alpha_x^y)-bf(\alpha)].$$

Proof: The claim follows from a direct calculation using the properties of the Pauli matrices.□

For $N\in\mathbb{N}$, let $\mathbb{F}_N(\mathbb{Z}):=\{\alpha\in\mathbb{F}(\mathbb{Z}):\mathrm{supp}(\alpha)$ has N elements$\}$ and set $\mathcal{H}_N:=\ell^2[\mathbb{F}_N(\mathbb{Z})]$. Lemma 2.1 shows that the subspace $\mathcal{H}_N$ of $\mathcal{H}$ is left invariant by $\varsigma L\varsigma^{-1}$. This is due to the fact that the Hamiltonian L commutes with the (magnon) number operator $\frac{1}{2}\Sigma_{x\in X}(\sigma_3^{(x)}+1)$. Moreover it is straightforward to show that the restriction $H_N:=(\varsigma L\varsigma^{-1})\restriction\mathcal{H}_N$ is bounded and symmetric.

The operator H_N has a more convenient form in another representation, which deserves the introduction of some notations. Elements of $\mathbb{Z}^N$ are denoted generically by $\xi\equiv(x_1,\ldots,x_N)$, $\eta\equiv(y_1,\ldots,y_N)$, or $\zeta\equiv(z_1,\ldots,z_N)$, and $P^<$ stands for the multiplication operator in $\ell^2(\mathbb{Z}^N)$ by the characteristic function $\chi_{\mathbb{Z}^N_<}$. We shall often interpret this projection as an operator from $\ell^2(\mathbb{Z}^N)$ to $\ell^2(\mathbb{Z}^N_<)$. For each $\eta\in\mathbb{Z}^N$ we define the unitary "bilateral shift" u_η in $\ell^2(\mathbb{Z}^N)$by

$$(u_\eta f)(\xi):=f(\xi-\eta),\quad f\in\ell^2(\mathbb{Z}^N),\quad \xi\in\mathbb{Z}^N.$$

We also define the "unilateral shift" $v_\eta^<:=P^<u_\eta\restriction\ell^2(\mathbb{Z}^N_<)$, which is a partial isometry in $\ell^2(\mathbb{Z}^N_<)$. Thus, for any $\varphi\in\ell^1(\mathbb{Z}^N)$, one can consider the convolution operator

$$C_\varphi:=\sum_{\eta\in\mathbb{Z}^N}\varphi(\eta)u_\eta$$

in $\ell^2(\mathbb{Z}^N)$, and the Toeplitz operator

$$T_\varphi^<:=\sum_{\eta\in\mathbb{Z}^N}\varphi(\eta)v_\eta^<$$

in $\ell^2(\mathbb{Z}^N_<)$. These operators are related by the formula $T_\varphi^<=P^<C_\varphi\restriction\ell^2(\mathbb{Z}^N_<)$. Let us also consider the projections $q_\eta^<:=v_\eta^<(v_\eta^<)^*$ on the range of the partial isometries $v_\eta^<$. One sees easily that $q_\eta^<$ is the multiplication operator by the characteristic function of the set $\mathbb{Z}^N_<\cap(\mathbb{Z}^N_<+\eta)$. Finally, among the multiplication operators in $\ell^2(\mathbb{Z}^N_<)$, we distinguish those of the form

$$V_\varphi^<:=\sum_{\eta\in\mathbb{Z}^N}\varphi(\eta)q_\eta^<,\quad \varphi\in\ell^1(\mathbb{Z}^N).$$

We identify now the Heisenberg Hamiltonian as an operator of the form above. The set S stands for the collection of vectors $\{s_i^\pm\}_{i=1}^N\subset\mathbb{Z}^N$ with components $(s_i^\pm)_j:=\pm\delta_{ij}$. Notice that S is a symmetric family of generators for the group $\mathbb{Z}^N$.

Proposition 2.2: The Hamiltonian H_N is unitarily equivalent to the operator $T_\varphi^<+V_\psi^<$, where $\varphi:=-2a\chi_S$ and $\psi:=2b\chi_S$.

Proof: Let $\phi:\mathbb{Z}^N_<\to\mathbb{F}_N(\mathbb{Z})$ be the one-to-one map $\xi\mapsto\chi_{\{x_1,\ldots,x_N\}}$. Let $\Phi:\mathcal{H}_N\to\ell^2(\mathbb{Z}^N_<)$ be the unitary operator given by $\Phi(f):=f\circ\phi$ for any $f\in\mathcal{H}_N$. Then one has for $g\in\ell^2(\mathbb{Z}^N_<)$, $\xi\in\mathbb{Z}^N_<$

$$(\Phi H\Phi^{-1}g)(\xi)=-2\sum_{j=1}^N\sum_{\substack{y=x_j\pm1\\ y\notin\{x_1,\ldots,x_N\}}}\{ag[\phi^{-1}(\chi_{\{x_1,\ldots,x_{j-1},y,x_{j+1},\ldots,x_N\}})]-bg(\xi)\}.$$

On the other hand

$$\phi^{-1}(\alpha)=[\min\alpha,\ \min(\alpha\setminus\{\min\alpha\}),\ \ldots]$$

for any $\alpha\in\mathbb{F}_N(\mathbb{Z})$. Thus

$$\Phi^{-1}(\chi_{\{x_1,\ldots,x_{j-1},y,x_{j+1},\ldots,x_N\}})=(x_1,\ldots,x_{j-1},y,x_{j+1},\ldots,x_N)$$

if $y=x_j\pm1$, $y\notin\{x_1,\ldots,x_N\}$ and $x_1<\cdots<x_N$. This implies that

$$(\Phi H \Phi^{-1} g)(\xi) = -2 \sum_{s \in S} \chi_{\mathbb{Z}^N_<}(\xi - s)[ag(\xi - s) - bg(\xi)]$$

$$= -2 \sum_{s \in S} [(av_s^< - bq_s^<)g](\xi) = [(T_\varphi^< + V_\psi^<)g](\xi).$$

□

Proposition 2.2 is one of the motivations to study operators of the form $T_\varphi^< + V_\psi^<$ for general functions $\varphi, \psi \in \ell^1(\mathbb{Z}^N)$. Actually, we can even indicate a larger class of operators $T_\varphi^< + V_\psi^<$ which have an interpretation on their own, outside the Toeplitz theory. If $M \subset \mathbb{Z}^N$ is a finite subset such that $\eta \in M$ implies $-\eta \in M$, then one can associate to it a Cayley graph having $\mathbb{Z}^N$ as a set of vertices by declaring that η and ζ are connected iff $\eta - \zeta \in M$. The Laplace operator Δ^M of this Cayley graph is a convolution operator in $\ell^2(\mathbb{Z}^N)$, easy to understand when applying a Fourier transformation. On the other hand Laplacians Δ_E^M on subgraphs E of this Cayley graph could be complicated objects. However it easy to show the identity $\Delta^M_{\mathbb{Z}^N_<} = T^<_{\chi_M} + V^<_{-\chi_M}$, which essentially applies to the Heisenberg model in the case $M = S$. Thus the Laplacians $\Delta^M_{\mathbb{Z}^N_<}$ are subject of the spectral results that follow below.

III. TOEPLITZ ALGEBRAS

In this section we collect some results on the Toeplitz-like algebra $\mathcal{T}^<(\mathbb{Z}^N)$. We first introduce the appropriate abstract setting.

Let X be a (discrete) Abelian group and E be a nonvoid subset of X. The projection $P^E: \ell^2(X) \to \ell^2(E)$ is defined in $\ell^2(X)$ as the multiplication operator by the characteristic function χ_E. As before we introduce the unitary translation operators $\{u_\eta\}_{\eta \in X}$ in $\ell^2(X)$ and the partial isometries $\{v_\eta^E := P^E u_\eta \restriction \ell^2(E)\}_{\eta \in X}$ in $\ell^2(E)$. Once again, for $\varphi \in \ell^1(X)$, the "Toeplitz operator"

$$T_\varphi^E := \sum_{\eta \in X} \varphi(\eta) v_\eta^E$$

and the "potential"

$$V_\varphi^E := \sum_{\eta \in X} \varphi(\eta) q_\eta^E \equiv \sum_{\eta \in X} \varphi(\eta) v_\eta^E (v_\eta^E)^*$$

are available as operators in $\ell^2(E)$.

Definition 3.1: The C^*-algebra $\mathcal{T}^E(X) \subset \mathcal{B}[\ell^2(E)]$ generated by the family $\{v_\eta^E\}_{\eta \in X}$ is called the Toeplitz algebra of the group X with respect to the subset E.

Obviously $\mathcal{T}^E(X)$ contains all the operators of the form $T_\varphi^E + V_\psi^E$, $\varphi, \psi \in \ell^1(\mathbb{Z}^N)$ (and many others). In fact $\mathcal{T}^E(X)$ is also generated by the family $\{T_\varphi^E : \varphi \in \ell^1(X)\}$ as in the case of usual Toeplitz algebras. If $E = X$, $\mathcal{T}^E(X)$ is equal to $C_r^*(X)$, the reduced group C^*-algebra of X. Since X is Abelian, we may identify it with $C^*(X)$, the enveloping C^*-algebra of the convolution Banach $*$-algebra $\ell^1(X)$. The identification puts into correspondence u_η with $\delta_\eta := \chi_{\{\eta\}}$. Due to the Fourier transform, $C^*(X)$ is isomorphic to the C^*-algebra $C(\hat{X})$ of continuous complex functions on $\hat{X}$, where $\hat{X}$ is the (compact, Abelian) dual group of X. The conventions "in dimension zero" are clear: The group is $X = \{0\}$, with subset $E = \{0\}$, all functions are scalars, and for $\varphi \in \mathbb{C}$ one sets $T_\varphi = V_\varphi := \varphi 1$ in $\ell^2(X) \equiv \mathbb{C}$.

The algebras $\mathcal{T}^E(X)$ were mainly studied for X an ordered group and E its positive cone.[11,13,20,21] The standard case is the "classical" Toeplitz algebra $\mathcal{T}^{\mathbb{N}}(\mathbb{Z}) \equiv \mathcal{T}$ (Ref. 6) associated with the unilateral shift on $\ell^2(\mathbb{N})$ (often presented in a Fourier transformed realization). In our proofs the isomorphic algebra $\mathcal{T}^* := \mathcal{T}^{\mathbb{N}^*}(\mathbb{Z})$, $\mathbb{N}^* := \{1, 2, \ldots\}$, will appear more naturally. The case $X = \mathbb{Z}^2$, $E = \mathbb{N}^2$ is studied in Ref. 7. The most relevant Toeplitz algebra for us is $\mathcal{T}^<(\mathbb{Z}^N) := \mathcal{T}^{\mathbb{Z}^N_<}(\mathbb{Z}^N)$, which is *not* of ordered type. We shall point out its structure, which will be the main tool in analyzing the operators $T_\varphi^< + V_\psi^<$.

The key facts are as follows:

(A) If $\theta: X \to X'$ is a group isomorphism sending E onto E', then $\mathcal{T}^E(X)$ and $\mathcal{T}^{E'}(X')$ are naturally isomorphic, the element v_η^E of $\mathcal{T}^E(X)$ being sent onto $v_{\theta(\eta)}^{E'} \in \mathcal{T}^{E'}(X')$.

(B) If E_j is a subset of a group X_j, $j=1,\ldots,m$, then $\mathcal{T}^{E_1\times\cdots\times E_m}(X_1\times\cdots\times X_m)$ can be identified with the spatial tensor product C^*-algebra $\otimes_{j=1}^m \mathcal{T}^{E_j}(X_j)$, $v^E_{(\eta_1,\ldots,\eta_m)}$ being identified with $\otimes_{j=1}^m v^{E_j}_{\eta_j}$.

Both isomorphisms are unitarily implemented, but this will not be used explicitly in the sequel.

Let $\theta: \mathbb{Z}^N \to \mathbb{Z}^N$ be the group automorphism defined by

$$\theta(y_1,\ldots,y_N) := (y_1, y_2 - y_1, \ldots, y_N - y_{N-1}),$$

with inverse

$$\theta^{-1}(z_1,\ldots,z_N) = (z_1, z_1+z_2, \ldots, z_1+\cdots+z_N).$$

Obviously, $\mathcal{E} := \theta(\mathbb{Z}^N_<) = \mathbb{Z}\times(\mathbb{N}^*)^{N-1}$. Thus, by (A), $\mathcal{T}^<(\mathbb{Z}^N)$ and $\mathcal{T}^{\mathcal{E}}(\mathbb{Z}^N)$ are isomorphic, $v_\eta^<$ being sent onto $v^{\mathcal{E}}_{\theta(\eta)}$ for any $\eta\in\mathbb{Z}^N$. Consequently, this isomorphism sends $T_\varphi^<$ onto $T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}$ and $V_\psi^<$ onto $V^{\mathcal{E}}_{\psi\circ\theta^{-1}}$. In the next few lines we only consider the case of $T_\varphi^<$.

By applying (B), one gets an isomorphism between $\mathcal{T}^{\mathcal{E}}(\mathbb{Z}^N)$ and $\mathcal{T}^{\mathbb{Z}}(\mathbb{Z})\otimes[\mathcal{T}^{\mathbb{N}^*}(\mathbb{Z})]^{\otimes(N-1)} \equiv C^*(\mathbb{Z})\otimes(\mathcal{T}^*)^{\otimes(N-1)}$, under which $T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}$ is transformed into

$$\sum_{(z_1,\ldots,z_N)\in\mathbb{Z}^N} (\varphi\circ\theta^{-1})(z_1,\ldots,z_N)\,\delta_{z_1}\otimes v_{z_2}^{\mathbb{N}^*}\otimes\cdots\otimes v_{z_N}^{\mathbb{N}^*}. \tag{3.1}$$

Now we apply the partial Fourier transform on the first variable. It maps $\delta_{z_1}\in C^*(\mathbb{Z})$ onto $\mathrm{e}_{z_1}\in C(\mathbb{T})$, where $\mathbb{T}$ is equal to the interval $[0,1]$ (with 0 identified to 1) and $\mathrm{e}_z(\tau) := \mathrm{e}^{-2\pi i z\tau}$ for all $z\in\mathbb{Z}$, $\tau\in\mathbb{T}$. Namely we use $\mathcal{F}_1 := \mathcal{F}\otimes 1$, where $(\mathcal{F}f)(\tau) := \Sigma_{z\in\mathbb{Z}}\mathrm{e}_z(\tau)f(z)$ for all $\tau\in\mathbb{T}$, $f\in\ell^1(\mathbb{Z})$. When performing the sum over z_1, the operator (3.1) becomes

$$\sum_{(z_2,\ldots,z_N)\in\mathbb{Z}^{N-1}} [\mathcal{F}_1(\varphi\circ\theta^{-1})](\cdot,z_2,\ldots,z_N)\,v_{z_2}^{\mathbb{N}^*}\otimes\cdots\otimes v_{z_N}^{\mathbb{N}^*},$$

which will be regarded as an element of $C(\mathbb{T})\otimes\mathcal{T}^{\otimes(N-1)} \equiv C[\mathbb{T};\mathcal{T}^{\otimes(N-1)}]$. Similar arguments can be carried on for $V_\psi^<$. When summing up we get the following lemma. For any $\rho\in\ell^1(\mathbb{Z}^N)$ and $\tau\in\mathbb{T}$ we define $\mu(\tau)\rho\in\ell^1(\mathbb{Z}^{N-1})$ by

$$[\mu(\tau)\rho](z_2,\ldots,z_N) := [\mathcal{F}_1(\rho\circ\theta^{-1})](\tau,z_2,\ldots,z_N).$$

Lemma 3.2: The C^*-algebras $\mathcal{T}^<(\mathbb{Z}^N)$ and $C(\mathbb{T})\otimes\mathcal{T}^{\otimes(N-1)}$ are naturally isomorphic. The isomorphism sends $T_\varphi^<+V_\psi^<$ onto the direct integral

$$\int_{\mathbb{T}}^{\oplus} \mathrm{d}\tau\,(T^{N-1}_{\mu(\tau)\varphi} + V^{N-1}_{\mu(0)\psi}),$$

where the exponent of the Toeplitz operators refers to the subset $(\mathbb{N}^*)^{N-1}$ of the group $\mathbb{Z}^{N-1}$.

The presence of a direct integral is connected to the invariance of our operators under a natural action of $\mathbb{Z}$ on $\mathbb{Z}^N_<$ by translations. For the Heisenberg model, this can be traced back to any of the earlier representations of the Hamiltonian.

As a rule, the spectral results will be stated only for operators of the form $T_\varphi^<+V_\psi^<$. By introducing suitable notations, they could be extended to all the elements of $\mathcal{T}^<(\mathbb{Z}^N)$.

Corollary 3.3: For any real functions $\varphi,\psi\in\ell^1(\mathbb{Z}^N)$, one has

$$\sigma_{\mathrm{ess}}(T_\varphi^<+V_\psi^<) = \sigma(T_\varphi^<+V_\psi^<) = \bigcup_{\tau\in\mathbb{T}} \sigma(T^{N-1}_{\mu(\tau)\varphi} + V^{N-1}_{\mu(0)\psi}). \tag{3.2}$$

Proof: The essential spectrum of an element A of a C^*-algebra $\mathcal{C}$ composed of bounded

operators in a Hilbert space $\mathcal{G}$ coincides with the spectrum of its image in the quotient $\mathcal{C}/[\mathcal{C}\cap\mathcal{K}(\mathcal{G})]$, where $\mathcal{K}(\mathcal{G})$ denotes the compact operators in $\mathcal{G}$. Thus the first equality follows from the obvious fact that there is no nontrivial compact operator in $C(\mathbb{T})\otimes\mathcal{T}^{\otimes(N-1)}$. For the second equality, we apply Lemma 3.2 and the discussion in Ref. 1, Sec. 8.2.4 on the spectrum of observables defined by a continuous family of selfadjoint operators. Note that the union on the right-hand side (r.h.s.) is automatically closed. □

If $N=1$, then $T_{\varphi}^{<}$ is the convolution operator C_{φ} and $V_{\psi}^{<}$ is the multiplication operator by $\Sigma_{z\in\mathbb{Z}}\psi(z)=(\mathcal{F}\psi)(0)\in\mathbb{R}$. Thus the spectrum (3.2) reduces to

$$\sigma(T_{\varphi}^{<}+V_{\psi}^{<})=(\mathcal{F}\varphi)(\mathbb{T})+(\mathcal{F}\psi)(0)=[\min(\mathcal{F}\varphi),\max(\mathcal{F}\varphi)]+(\mathcal{F}\psi)(0)$$

as it should be.

IV. THE ESSENTIAL SPECTRUM OF THE FIBER HAMILTONIANS

The fiber Hamiltonians $H(\tau):=T_{\mu(\tau)\varphi}^{N-1}+V_{\mu(0)\psi}^{N-1}$ can be interpreted physically as "energy operators at fixed quasi-momentum τ." We now study their essential spectrum. We again use the well known fact that, given a Hilbert space $\mathcal{G}$, the essential spectrum of an operator $A\in\mathcal{B}(\mathcal{G})$ coincides with the spectrum of its image in the Calkin algebra $\mathcal{B}(\mathcal{G})/\mathcal{K}(\mathcal{G})$, where $\mathcal{K}(\mathcal{G})$ is the ideal of compact operators.

The fibers $H(\tau)$ act in $\ell^2[(\mathbb{N}^*)^{N-1}]\simeq\ell^2(\mathbb{N}^*)^{\otimes(N-1)}$ and belong to the C^*-algebra $(\mathcal{T}^*)^{\otimes(N-1)}$. So we are faced with the problem of understanding the quotient of $(\mathcal{T}^*)^{\otimes(N-1)}$ by $\mathcal{K}[\ell^2(\mathbb{N}^*)^{\otimes(N-1)}]$, the latter being identified as $(\mathcal{K}^*)^{\otimes(N-1)}$, where $\mathcal{K}^*:=\mathcal{K}[\ell^2(\mathbb{N}^*)]$. The discussion in Ref. 7 is relevant here, especially in the case $N=2$. We start by proving a result in a more abstract setting (see Ref. 8, Theorem 2.3 for an alternate proof).

Lemma 4.1: Let $\mathcal{I}_j$ be an ideal of a nuclear C^*-algebra $\mathcal{C}_j$, $j=1,2$. Let $\pi_j:\mathcal{C}_j\to\mathcal{C}_j/\mathcal{I}_j$ be the canonical $*$-morphism. Then the mapping

$$\bar{\pi}:\mathcal{C}_1\otimes\mathcal{C}_2\to[(\mathcal{C}_1/\mathcal{I}_1)\otimes\mathcal{C}_2]\oplus[\mathcal{C}_1\otimes(\mathcal{C}_2/\mathcal{I}_2)]$$

$$A\mapsto\{(\pi_1\otimes 1)(A),(1\otimes\pi_2)(A)\}$$

is a $*$-morphism, and $\ker(\bar{\pi})=\mathcal{I}_1\otimes\mathcal{I}_2$.

Proof: Since $\mathcal{C}_1$ and $\mathcal{C}_2$ are nuclear, the mappings $\pi_1\otimes 1$ and $1\otimes\pi_2$ are (surjective) $*$-morphisms with $\ker(\pi_1\otimes 1)=\mathcal{I}_1\otimes\mathcal{C}_2$ and $\ker(1\otimes\pi_2)=\mathcal{C}_1\otimes\mathcal{I}_2$ (Ref. 12, Theorem 6.5.2). From this it follows that $\bar{\pi}$ is a $*$-morphism with $\ker(\bar{\pi})=(\mathcal{I}_1\otimes\mathcal{C}_2)\cap(\mathcal{C}_1\otimes\mathcal{I}_2)$. Since ideals in nuclear C^*-algebras are nuclear, the triple $(\mathcal{I}_1,\mathcal{C}_2,\mathcal{I}_2)$ verifies the (right) slice map conjecture (Ref. 19, Proposition 10). Thus one gets the equality $\ker(\bar{\pi})=\mathcal{I}_1\otimes\mathcal{I}_2$ by an easy adaptation of the proof of (Ref. 18, Corollary 5). □

We need two more notations. For any $j\in\{2,\ldots,N\}$, $\varrho\in\ell^1(\mathbb{Z}^{N-1})$ and $\tau\in\mathbb{T}$, we define $\nu_j(\tau)\varrho\in\ell^1(\mathbb{Z}^{N-2})$ by

$$[\nu_j(\tau)\varrho](z_2,\ldots,z_{j-1},z_{j+1},\ldots,z_N):=(\mathcal{F}_j\varrho)(z_2,\ldots,z_{j-1},\tau,z_{j+1},\ldots,z_N),$$

$\mathcal{F}_j$ being the Fourier transformation in the jth variable. Furthermore we denote by $\Sigma_j(\tau,\tau')$ the spectrum of the Toeplitz operator (relative to the pair $\{\mathbb{Z}^{N-2},(\mathbb{N}^*)^{N-2}\}$)

$$T_{\nu_j(\tau')\mu(\tau)\varphi}^{N-2}+V_{\nu_j(0)\mu(0)\psi}^{N-2}$$

acting in $\ell^2[(\mathbb{N}^*)^{N-2}]$.

Theorem 4.2: *Let $\varphi,\psi\in\ell^1(\mathbb{Z}^N)$ be real functions and $\tau\in\mathbb{T}$. Then one has*

$$\sigma_{\mathrm{ess}}(T_{\mu(\tau)\varphi}^{N-1}+V_{\mu(0)\psi}^{N-1})=\bigcup_{j=2}^{N}\bigcup_{\tau'\in\mathbb{T}}\Sigma_j(\tau,\tau').$$

Proof: By analogy to (the Fourier transformed version of) the isomorphism $\mathcal{T}/\mathcal{K}[\ell^2(\mathbb{N})] \simeq C(\mathbb{T})$ (Ref. 6, Theorem 7.23) one has a canonical isomorphism $\mathcal{T}^*/\mathcal{K}^* \simeq C(\mathbb{T})$, uniquely defined by the fact that for any $z \in \mathbb{Z}$ the operator $v_z^{\mathbb{N}^*} \in \mathcal{T}^*$ is sent onto the function $\mathrm{e}_z \in C(\mathbb{T})$. Therefore the class of operators $T_f^{\mathbb{N}^*} \in \mathcal{T}^*$, $f \in \ell^1(\mathbb{Z})$, must be sent onto the class of functions $\mathcal{F}f \in C(\mathbb{T})$.

The Toeplitz algebra $\mathcal{T}^*$ is nuclear, since it is the extension of the Abelian quotient $\mathcal{T}^*/\mathcal{K}^* \simeq C(\mathbb{T})$ by the nuclear ideal $\mathcal{K}^*$. So we may use the analog of Lemma 4.1 for the $N-1$ factors $\mathcal{C}_2=\cdots=\mathcal{C}_N=\mathcal{T}^*$ and $\mathcal{I}_2=\cdots=\mathcal{I}_N=\mathcal{K}^*$. We get an injective $*$-morphism

$$(\mathcal{T}^*)^{\otimes(N-1)}/(\mathcal{K}^*)^{\otimes(N-1)} \hookrightarrow \oplus_{j=2}^N(\mathcal{T}_*^{\otimes(j-2)} \otimes C(\mathbb{T}) \otimes \mathcal{T}_*^{\otimes(N-j)})$$

$$\simeq \oplus_{j=2}^N(C(\mathbb{T}) \otimes \mathcal{T}_*^{\otimes(N-2)}),$$

sending $T_{\mu(\tau)\varphi}+V_{\mu(0)\psi}$ onto the collection

$$\left\{\int_{\mathbb{T}}^{\oplus} \mathrm{d}\tau'(T^{N-2}_{\nu_j(\tau')\mu(\tau)\varphi} + V^{N-2}_{\nu_j(0)\mu(0)\psi})\right\}_{j=2,\ldots,N}.$$

One concludes by using Ref. 1, Sec. 8.2.4. □

As an example, if $N=2$, one has

$$\sigma_{\mathrm{ess}}(T^1_{\mu(\tau)\varphi} + V^1_{\mu(0)\psi}) = \{(\mathcal{F}_1\mathcal{F}_2\varphi)(\tau-\tau',\tau') + (\mathcal{F}_1\mathcal{F}_2\psi)(0,0): \tau' \in \mathbb{T}\}.$$

In the case of the Heisenberg model (see Proposition 2.2), one has to take $\varphi=-2a\chi_S$ and $\psi=2b\chi_S$. Since $(\mathcal{F}_1\mathcal{F}_2\chi_S)(\tau-\tau',\tau')=2\cos(2\pi\tau')+2\cos[2\pi(\tau-\tau')]$, the essential spectrum of the fiber operator coincides with the interval $\{8b-4a\cos(2\pi\tau')-4a\cos[2\pi(\tau-\tau')]: \tau' \in [0,1]\}$.

Remark 4.3: Results of this section (*and also of the next one*) *can easily be generalized to Toeplitz-like operators* $T^<_\varphi+V^<_\psi$ *acting on the subset*

$$E = (\mathbb{Z}^m_{\mathrm{lex}})^N_< := \{(x_1,\ldots,x_N) \in (\mathbb{Z}^m_{\mathrm{lex}})^N : x_1 < x_2 < \cdots < x_N\}$$

of $X=(\mathbb{Z}^m_{\mathrm{lex}})^N$, *where* $\mathbb{Z}^m_{\mathrm{lex}}$ *is the group* $\mathbb{Z}^m$ *ordered lexicographically. In analyzing the structure of* $\mathcal{T}^E(X)$ *for this case, the Toeplitz algebra* $\mathcal{T}$ *should be replaced by* $\mathcal{T}_m := \mathcal{T}^{(\mathbb{Z}^m_{\mathrm{lex}})_+}(\mathbb{Z}^m_{\mathrm{lex}})$, *where* $(\mathbb{Z}^m_{\mathrm{lex}})_+ := \{x \in \mathbb{Z}^m_{\mathrm{lex}} : 0 \le x\}$. *The only important change concerns the calculation of the quotients* $\mathcal{T}_m/\mathcal{K}_m$, *where* $\mathcal{K}_m := \mathcal{K}\{\ell^2[(\mathbb{Z}^m_{\mathrm{lex}})_+]\}$. *Namely one has to call for the rather deep result* (Ref. 13, Theorem 2.3), *which implies that* $\mathcal{T}_m/\mathcal{K}_m$ *and* $\mathcal{T}_{m-1} \otimes C(\mathbb{T})$ *are* $*$*-isomorphic*.

V. LOCALIZATION

In the sequel we determine localization properties of the operators $T^<_\varphi+V^<_\psi$ by adapting them to the Toeplitz algebra $\mathcal{T}^<(\mathbb{Z}^N)$, a technique developed in Ref. 2 (see also Ref. 10) for crossed product C^*-algebras, with applications to Schrödinger operators in $\mathbb{R}^n$.

Let H be a self-adjoint operator in $\ell^2(\mathbb{Z}^N_<)$ (or in some other L^2 space) and χ a nontrivial multiplication operator (for example the characteristic function of a set having a strictly positive measure). If κ is a continuous function with support intersecting the spectrum of H, the operator $\chi\kappa(H)$ has no reason to be small in general. The unique *a priori* bound would be

$$\|\chi\kappa(H)\| \le \|\chi\|_\infty \sup_{\lambda \in \sigma(H)} |\kappa(\lambda)|. \tag{5.1}$$

We are going to correlate χ to κ in such a way to make the norm small without asking any of the two factors on the r.h.s. of (5.1) to be small.

Theorem 5.1: *Fix* $j \in \{2,\ldots,N\}$ *and let* φ,ψ *be real elements of* $\ell^1(\mathbb{Z}^N)$. *For any* $n \in \mathbb{N}$ *set*

$$\Omega_j(n) := \{(y_1,\ldots,y_N) \in \mathbb{Z}^N_< : y_j - y_{j-1} \ge n\}.$$

Let $\kappa: \mathbb{R} \to \mathbb{R}$ *be a continuous function with*

$$\operatorname{supp}\kappa \cap [\cup_{\tau,\tau'\in\mathbb{T}}\Sigma_j(\tau,\tau')] = \emptyset\ .$$

Then for each $\varepsilon>0$ *there exists* $n_\varepsilon\in\mathbb{N}$ *such that*

$$\|\chi_{\Omega_j(n)}\kappa(T^<_\varphi + V^<_\psi)\| \le \varepsilon \tag{5.2}$$

for each $n\ge n_\varepsilon$.

Proof: Denote by $T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}}$ the image of $T^<_\varphi+V^<_\psi$ through the isomorphism $\mathcal{T}^<(\mathbb{Z}^N)\simeq C(\mathbb{T})\otimes(\mathcal{T}^*)^{\otimes(N-1)}$, defined by the change of variables θ. One verifies easily that the estimate (5.2) is equivalent to

$$\|\chi_{\widetilde{\Omega_j(n)}}\kappa(T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}})\|\le\varepsilon,$$

where $\widetilde{\Omega_j(n)}:=\theta[\Omega_j(n)]=\{(z_1,\ldots,z_N)\in\mathbb{Z}\times(\mathbb{N}^*)^{(N-1)}: z_j\ge n\}$. Moreover the operator $\kappa(T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}})$ belongs to the ideal

$$\mathcal{I}_j := C(\mathbb{T})\otimes(\mathcal{T}^*)^{\otimes(j-2)}\otimes\mathcal{K}^*\otimes(\mathcal{T}^*)^{\otimes(N-j)}$$

of $\mathcal{C}:=C(\mathbb{T})\otimes(\mathcal{T}^*)^{\otimes(N-1)}$. Indeed the image of $T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}}$ in the quotient

$$\mathcal{C}/\mathcal{I}_j\simeq C(\mathbb{T})\otimes(\mathcal{T}^*)^{\otimes(j-2)}\otimes C(\mathbb{T})\otimes(\mathcal{T}^*)^{\otimes(N-j)}\simeq C(\mathbb{T})^{\otimes 2}\otimes(\mathcal{T}^*)^{\otimes(N-2)}$$

is

$$\int^{\oplus}_{\mathbb{T}^2}\mathrm{d}\tau\,\mathrm{d}\tau'\,(T^{N-2}_{\nu_j(\tau')\mu(\tau)\varphi}+V^{N-2}_{\nu_j(0)\mu(0)\psi}),$$

with spectrum $\cup_{\tau,\tau'\in\mathbb{T}}\Sigma_j(\tau,\tau')\equiv\sigma_{\mathcal{I}_j}(T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}})$. Thus, since $\operatorname{supp}(\kappa)\cap[\cup_{\tau,\tau'\in\mathbb{T}}\Sigma_j(\tau,\tau')]=\emptyset$, it follows by Ref. 2, Lemma 1 that $\kappa(T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}})\in\mathcal{I}_j$. Now

$$\chi_{\widetilde{\Omega_j(n)}}=1_{j-1}\otimes\chi_{\{z_j\ge n\}}\otimes 1_{N-j},$$

where $\chi_{\{z_j\ge n\}}$ converges strongly to 0 in $\mathcal{B}[\ell^2(\mathbb{N}^*)]$ as $n\to\infty$. Thus, by examining the structure of $\mathcal{J}_j$, one gets

$$\|\chi_{\widetilde{\Omega_j(n)}}\kappa(T^{\mathcal{E}}_{\varphi\circ\theta^{-1}}+V^{\mathcal{E}}_{\psi\circ\theta^{-1}})\|\to 0$$

as $n\to\infty$. □

Let H be a self-adjoint operator in a Hilbert space $\mathcal{G}$ with spectral measure E^H, and let $f\in\mathcal{G}$ be an arbitrary vector. We call *spectral support of* f *with respect to* H, and write $\operatorname{supp}(f;H)$, for the smallest closed subset F of $\mathbb{R}$ such that $E^H(F)f=f$. Alternatively one can characterize $\operatorname{supp}(f;H)$ as follows:

$$\lambda\notin\operatorname{supp}(f;H)\quad\text{iff }\exists\,\varepsilon>0\text{ such that }E^H(\lambda-\varepsilon,\lambda+\varepsilon)f=0.$$

Obviously one has $\operatorname{supp}(f;H)\subset\sigma(H)$. If H is the Hamilton operator describing some quantum system in $\mathcal{G}$, we say that f is *a state with energy in* $\operatorname{supp}(f;H)$.

Corollary 5.2: Let φ,ψ *and* j *be as in Theorem 5.1. Then, for any* $\varepsilon>0$, *there exists* $n_\varepsilon\in\mathbb{N}$ *such that*

$$\|\chi_{\Omega_j(n)}e^{-it(T^<_\varphi+V^<_\psi)}f\|\le\varepsilon\|f\|$$

for all $n\ge n_\varepsilon$, $t\in\mathbb{R}$ *and all* $f\in\ell^2(\mathbb{Z}^N_<)$ *satisfying*

$$\operatorname{supp}(f;T^<_\varphi+V^<_\psi)\cap[\cup_{\tau,\tau'\in\mathbb{T}}\Sigma_j(\tau,\tau')]=\emptyset\ .$$

Corollary 5.2 follows trivially from Theorem 5.1. We put it into evidence for its physical interpretation in the case of the one-dimensional Heisenberg model: Intuitively, if f is a normalized initial state with energy outside $\cup_{\tau,\tau' \in \mathbb{T}} \Sigma_j(\tau,\tau')$, the decomposition of the system into two clusters of spins pointing up, one "at the left" composed of $j-1$ elements, and the other one "at the right" composed of $N-j+1$ elements, is highly unprobable *uniformly in time* if the distance n between the clusters is large enough.

It is obvious that several variants are available. One can consider ideals smaller than $\mathcal{I}_j$, by collapsing more than one factor to the ideal of compact operators in $\ell^2(\mathbb{N}^*)$. In this way, one gets more detailed clustering information for the one-dimensional Heisenberg model, but for *a priori* smaller sets of energy values. The fiber Hamiltonians $T^{N-1}_{\mu(\tau)\varphi}+V^{N-1}_{\mu(0)\psi}$ can be studied identically by using ideals in the C^*-algebra $(\mathcal{T}^*)^{\otimes(N-1)}$.

From Corollary 3.3 and Theorem 4.2 we know that

$$\bigcup_{j=2}^{N} \bigcup_{\tau,\tau' \in \mathbb{T}} \Sigma_j(\tau,\tau') = \bigcup_{\tau \in \mathbb{T}} \sigma_{\mathrm{ess}}(T^{N-1}_{\mu(\tau)\varphi} + V^{N-1}_{\mu(0)\psi}) \subset \sigma(T^{<}_{\varphi} + V^{<}_{\psi}).$$

It does not seem easy to determine under which conditions there is room in the spectrum of $T^{<}_{\varphi} + V^{<}_{\psi}$ outside $\cup_{\tau,\tau' \in \mathbb{T}} \Sigma_j(\tau,\tau')$ for a given j. However one may expect it is often the case.

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Group-theoretical approach to reflectionless potentials

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We examine the general form of potentials with zero reflection coefficient in one-dimensional Hamiltonians connected with Casimir invariants of non-compact groups. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2259579]

I. INTRODUCTION

There are a number of potentials for the Schrödinger equation in one dimension for which the reflection amplitude vanishes identically while the transmission amplitude is a complex number of modulus 1 for all energy values.[1,2] Such potentials are called the reflectionless or transparent potentials. The best known of these is a modified Pöschl-Teller potential hole.[3] (For scattering of the Gaussian wave packet by the modified Pöschl-Teller potential hole see Ref. 4.) A number of authors have already discussed reflectionless potentials within the frameworks of inverse scattering theory,[5–12] supersymmetric quantum mechanics,[13–17] and a Darbox transformation approach.[18] The relation between the reflectionless potentials and the soliton solutions of nonlinear (such as Korteweg-de Vries, sine-Gordon, and nonlinear Schrödinger) equations has been investigated in Refs. 7 and 19–21 In the present work, we provide a group-theoretical approach to the problem.

In a previous paper,[22] G. A. K. discussed one-dimensional scattering problems related to the principal series of SO(2,2), in the sense that the Hamiltonian, H, of the system is related to the Casimir operator, C, of SO(2,2) as follows:

$$Q(H-E) = (C^{\mathrm{SO}(2,2)} - \sigma(\sigma+2))|_{\mathcal{H}},$$

where $\mathcal{H}$ are the subspaces occurring in the subgroup reductions, $\sigma(\sigma+2)$ is an eigenvalue of C, and Q is some nontrivial operator. In Ref. 22 it was shown that the scattering problem can be completely solved within the framework of group theory, without explicit knowledge of the interaction potentials. Namely, the S-matrices for systems under consideration are determined by diagonal elements of the intertwining operator, A, between Weyl-equivalent representations of SO(2,2).[23] At this stage we note that the operator A is said to be intertwining if relation

$$AU^{\chi}(g) = U^{\tilde{\chi}}(g)A \quad \text{for all } g \in G \tag{1}$$

or relation

$$AdU^{\chi}(b) = \mathrm{d}U^{\tilde{\chi}}(b)A \quad \text{for all } b \in \mathfrak{g} \tag{2}$$

holds, where U^{χ} and $U^{\tilde{\chi}}$ are Weyl-equivalent unitary irreducible representation's (UIRs) of principal series of the group G, while $\mathrm{d}U^{\chi}$ and $\mathrm{d}U^{\tilde{\chi}}$ are the corresponding representations of the algebra $\mathfrak{g}$ of G. It is worthwhile to point out that representations U^{χ} and $U^{\tilde{\chi}}$ have the same Casimir eigenvalues. Such representations are called Weyl equivalent. Equations (1) and (2) have much

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restriction power, determining the intertwining operator up to a constant. Therefore, one can evaluate the *S*-matrix without writing a Schrödinger equation, or computing the wave functions.[24]

Reference 22 explained a method of extracting the corresponding (Natanzon) potentials from the Casimir operator and applied it in detail to the reductions $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(2),\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes E(1)$, and $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$. The same article explained the occurrence of reflection and transmission amplitudes in the *S*-matrix for potentials related to $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\otimes\mathrm{SO}(1,1)$ reduction: this happens because within a principal series of SO(2,2) each UIR of SO(1,1) appears twice. We notice that, in one-dimensional scattering problems, the *S*-matrix can be written as a 2×2 matrix[1]

$$S=\begin{pmatrix} R_l & T_r \\ T_l & R_r \end{pmatrix}, \tag{3}$$

where R_l and T_l are the reflection and transmission amplitudes for a wave incident from the left while R_r and T_r are the reflection and transmission amplitudes for a wave incident from the right. (For other definitions of *S*-matrix see, e. g., Ref. 25, and references therein.) If potential $V(x)$ is real and symmetric (i.e., $V(-x)=V(x)$) then $T_l=T_r$ and $R_l=R_r$.

If one chooses the chain $\mathrm{SO}(2,2)\supset\mathrm{SO}(2,1)\supset\mathrm{SO}(2)$ then both principal and discrete series representations of SO(2,1) appear in the reduction. Moreover, the principal series representation of SO(2,1) is double degenerate therein, while the discrete series representation of SO(2,1) appears at most once. One can calculate the matrix form of the intertwining operator in the basis corresponding to the reduction with respect to SO(2,1). Everything here follows exactly as in Appendix A of Ref. 23. As a result, we come to following conclusion: the *S*-matrices of one-dimensional scattering systems related to the $\mathrm{SO}(2,2)\supset\mathrm{SO}(2,1)\supset\mathrm{SO}(2)$ reduction have the form (3) with $R_l=R_r=R$ and $T_l=T_r=T$ where

$$R=c\frac{1}{\pi}\sin(\pi j)\Gamma(\sigma+j+2)\Gamma(\sigma-j+1),$$

$$T=c\frac{1}{\pi}\sin(\pi\sigma)\Gamma(\sigma+j+2)\Gamma(\sigma-j+1).$$

Here, c is a complex number of unit modulus, $j=-1/2-i\tau$, for principal series representations of SO(2,1), while $j=0,1,2,\ldots$, for discrete series representations of SO(2,1) and $\sigma=-1-i\rho$ labels the principal series of the most degenerate representations of SO(2,2) (see Sec. II).

The square modulus of the transmission amplitude is

$$|T|^2=\frac{\sinh^2\pi\rho}{\cosh^2\pi\tau+\sinh^2\pi\rho} \tag{4}$$

if j belongs to the continuous series, while

$$|T|^2=1, \tag{5}$$

if j belongs to the discrete series. Hence, the corresponding class of Natanzon potentials contains symmetric reflectionless potentials.

Moreover, it is not difficult to see that all the potentials related to the Poincaré group in 2+1 dimensions, ISO(2,1), are reflectionless, too. Indeed, the connection between anti de-Sitter group in 2+1 dimensions SO(2,2) and Poincaré group in 2+1 dimensions ISO(2,1) naturally indicates a connection between intertwining operators of these groups. We notice that the group SO(2,2) contracts with respect to SO(2,1) to the group ISO(2,1) in the sense of Inönü and Wigner (see, e.g., Refs. 26 and 27, and references therein). Thus, the intertwining operator of the group ISO(2,1) must arise through a limiting process $\rho\to\infty$ from the intertwining operators of the group SO(2,2). As a result, we obtain $|T|^2=1$ for all potentials related to ISO(2,1). Moreover, due to $|T|^2=1$ for both the discrete spectrum ($j=0,1,2,\ldots$) and the continuous spectrum $\left(j=-\frac{1}{2}-i\tau\right)$ of

$C^{\mathrm{SO}(2,1)}$, we can restrict ourselves to the Poincaré group in $1+1$ dimensions in our study. In fact, one can show that the one-dimensional potentials connected with Poincaré group in $n+1$ dimensions have the same shape. (The intertwining operators of ISO(1,1) are discussed in Sec. 4.2.3 of Ref. 28.) The general form of Hamiltonians for reflectionless potentials connected with Casimir invariants of noncompact groups SO(2,2) and ISO(1,1) will be constructed in the following in a systematic way. We show that the reflectionless potentials under considerations are given by solutions of nonlinear equations (33) and (95).

II. REFLECTIONLESS POTENTIALS RELATED TO SO(2,2)

By SO(2,2) we denote the connected component of the group of linear transformations of $R^{2,2}$ preserving the bilinear form

$$\xi\cdot\eta\equiv\xi_1\eta_1+\xi_2\eta_2-\xi_3\eta_3-\xi_4\eta_4,$$

with $\xi,\eta\in R^{2,2}$. We consider SO(2,2) matrices acting on $R^{2,2}$ on the right. In accordance with this, we write four-vectors ξ in row form: $\xi=(\xi_1\xi_2\xi_3\xi_4)$.

Let us denote $\{g_{ij}(t)\}, i<j, i,j=1,2,3,4$ the six one-parameter subgroups of SO(2,2) consisting of rotations or pseudorotations in the $\xi_i-\xi_j$ planes, that is, transformations of the form

$$\xi_k'=\xi_k,\quad k\neq i,j,\quad \xi_i'=\xi_i\cos t+\xi_j\sin t,\quad \xi_j'=-\xi_i\sin t+\xi_j\cos t,$$

or

$$\xi_k'=\xi_k,\quad k\neq i,j,\quad \xi_i'=\xi_i\cosh t+\xi_j\sinh t,\quad \xi_j'=\xi_i\sinh t+\xi_j\cosh t.$$

The matrices

$$a_{ij}=\frac{\mathrm{d}}{\mathrm{d}t}g_{ij}(t)|_{t=0},\quad i<j \tag{6}$$

form a basis of the Lie algebra, SO(2,2), of the group, with commutation relations

$$[a_{12},a_{13}]=a_{23},\quad [a_{12},a_{14}]=a_{24},$$

$$[a_{12},a_{23}]=-a_{13},\quad [a_{12},a_{24}]=-a_{14},$$

$$[a_{13},a_{23}]=-a_{12},\quad [a_{14},a_{24}]=-a_{12},$$

$$[a_{23},a_{24}]=-a_{34},\quad [a_{13},a_{14}]=-a_{34},$$

$$[a_{23},a_{34}]=-a_{24},\quad [a_{13},a_{34}]=-a_{14},$$

$$[a_{24},a_{34}]=a_{23},\quad [a_{14},a_{34}]=a_{13}.$$

The unitary irreducible representations (UIRs) of SO(2,2) are known to form three series:[26,28] principal, supplementary, and discrete. It is also known that only the principal series of SO(2,2) describe scattering states. Consequently, the relevant UIRs are those in the principal series. Moreover, the discussion will be limited to the most degenerate representations.

The principal series of the most degenerate representations of SO(2,2) is characterized by the pair of quantum numbers $\chi=(\rho,\varepsilon)$, where $\varepsilon=0$, or 1 and $0\leqslant\rho<+\infty$. The representations specified by labels $\chi=(\rho,\varepsilon)$ and $\tilde{\chi}=(-\rho,\varepsilon)$ are Weyl-equivalent. For the sake of simplicity, we consider here the representations with $\varepsilon=0$.

We want to construct the Hamiltonians for which the relation

$$Q(H-E) = [C^{\mathrm{SO}(2,2)} - \sigma(\sigma+2)]|_{\mathcal{H}}, \tag{7}$$

holds, where $\sigma=-1-i\rho$ specifies the most degenerate principal series of SO(2,2) and $\mathcal{H}$ is a subspace occurring in $\mathrm{SO}(2,2)\supset\mathrm{SO}(2,1)\supset\mathrm{SO}(2)$ subgroup reduction. The key to the construction of it lies in the observation that the Schrödinger energy eigenvalue equation for such systems is nothing but the condition imposed on the carrier space of SO(2,2) to be irreducible. Thus, in order to find the Hamiltonians for the systems under consideration, we should look for a reducible representation of SO(2,2) containing the principal series.

Let us consider a quasiregular representation $T(g)$ of SO(2,2) realized in the Hilbert space of square-integrable functions $f(\xi)$ on the hyperboloid $\Xi\sim\mathrm{SO}(2,2)/\mathrm{SO}(2,1)$ defined by

$$\xi_1^2+\xi_2^2-\xi_3^2-\xi_4^2=1. \tag{8}$$

In general, one can use for construction of the quasiregular representation the carrier space $L^2(\Xi,\mathrm{d}\mu)$ with any quasi-invariant measure $\mathrm{d}\mu(\xi)$ on Ξ.[26] Representations with different measures are unitarily equivalent, and are given by

$$T(g)f(\xi)=\left(\frac{\mathrm{d}\mu(\xi g)}{\mathrm{d}\mu(\xi)}\right)^{1/2} f(\xi g), \tag{9}$$

where $\mathrm{d}\mu(\xi g)/\mathrm{d}\mu(\xi)$ is the Radon-Nikodym derivative.

Without loss of generality, we can put

$$\mathrm{d}\mu(\xi)=h(\xi)\mathrm{d}\xi, \tag{10}$$

where $\mathrm{d}\xi=\mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3/|\xi_4|$ is an invariant measure on Ξ. The requirement that the measure is quasi-invariant implies the condition

$$h(\xi)\geqslant 0. \tag{11}$$

Then, it is not difficult to see that the Hermitian infinitesimal operators

$$A_{jk}=-i\frac{\mathrm{d}}{\mathrm{d}t}T(g_{jk}(t))|_{t=0} \tag{12}$$

of the representation $T(g)$ corresponding to the one-parameter subgroup are given by

$$iA_{12}=h^{-1/2}\circ\left(\xi_2\frac{\partial}{\partial\xi_1}-\xi_1\frac{\partial}{\partial\xi_2}\right)\circ h^{1/2},$$

$$iA_{13}=h^{-1/2}\circ\left(\xi_3\frac{\partial}{\partial\xi_1}+\xi_1\frac{\partial}{\partial\xi_3}\right)\circ h^{1/2},$$

$$iA_{23}=h^{-1/2}\circ\left(\xi_3\frac{\partial}{\partial\xi_2}+\xi_2\frac{\partial}{\partial\xi_3}\right)\circ h^{1/2},$$

$$iA_{14}=h^{-1/2}\circ\left(\xi_4\frac{\partial}{\partial\xi_1}\right)\circ h^{1/2},$$

$$iA_{24}=h^{-1/2}\circ\left(\xi_4\frac{\partial}{\partial\xi_2}\right)\circ h^{1/2},$$

$$iA_{34} = h^{-1/2} \circ \left(\xi_4 \frac{\partial}{\partial \xi_3} \right) \circ h^{1/2}. \tag{13}$$

where $\circ$ denotes composition of operators. Here, we have assumed ξ_1, ξ_2, and ξ_3 as the independent variables on Ξ.

The representation $T(g)$ is decomposed into principal and discrete series of most degenerate UIRs of SO(2,2).[27] The irreducible components are obtained if all functions f are eigenfunctions of the Casimir operator $C^{\mathrm{SO}(2,2)}$,

$$C^{\mathrm{SO}(2,2)} f = \sigma(\sigma+2) f, \tag{14}$$

where $\sigma = -1 - i\rho, 0 \leqslant \rho < +\infty$ for the principal series representations, while $\sigma = l, l = 0,1,2,\ldots$, for discrete series representations and

$$C^{\mathrm{SO}(2,2)} = A_{12}^2 + A_{34}^2 - A_{13}^2 - A_{14}^2 - A_{23}^2 - A_{24}^2 = h^{-1/2} \circ \left[-\frac{\partial^2}{\partial \xi_1^2} - \frac{\partial^2}{\partial \xi_2^2} + \frac{\partial^2}{\partial \xi_3^2} + L(L+2) \right] \circ h^{1/2}, \tag{15}$$

with

$$L = \xi_1 \frac{\partial}{\partial \xi_1} + \xi_2 \frac{\partial}{\partial \xi_2} + \xi_3 \frac{\partial}{\partial \xi_3}. \tag{16}$$

Since we are interested only in the continuum, we put $\sigma = -1 - i\rho$. Next, imposing the reduction condition, we can extract the corresponding one-dimensional potentials from the Casimir operator.

We want to consider the $\mathrm{SO}(2,2) \supset \mathrm{SO}(2,1) \supset \mathrm{SO}(2)$ reduction chain; but there are four subgroups which are isomorphic to SO(2,1). Namely, the subgroups G_1, G_2, G_3, and G_4 generated by $\{a_{12}, a_{13}, a_{23}\}, \{a_{12}, a_{14}, a_{24}\}, \{a_{23}, a_{24}, a_{34}\}$, and $\{a_{13}, a_{14}, a_{34}\}$, respectively. Although these subgroups are mathematically equivalent, they may be related to different physical problems. For this reason we shall consider various SO(2,1) subgroup reductions

(i) The $\mathrm{SO}(2,2) \supset G_1$ reduction. Then, the reduction conditions are

$$A_{12} f_{jm} = m f_{jm}, \quad C^{G_1} f_{jm} = j(j+1) f_{jm}$$

where

$$C^{G_1} = A_{12}^2 - A_{13}^2 - A_{23}^2 = h^{-1/2} \circ \left[(1+\xi_4^2) \left(-\frac{\partial^2}{\partial \xi_1^2} - \frac{\partial^2}{\partial \xi_2^2} + \frac{\partial^2}{\partial \xi_3^2} \right) + L(L+1) \right] \circ h^{1/2}. \tag{17}$$

It is known that[26,27] the spectrum of C^{G_1} consists of a discrete part

$$j = l, \quad l = 0,1,2,\ldots \quad (|m| = l+1+n, n = 0,1,2,\ldots)$$

and a continuous part

$$j = -\tfrac{1}{2} - i\tau, \quad 0 \leqslant \tau < \infty \quad (m = 0, \pm 1, \pm 2, \ldots).$$

According to this, we impose $\mathrm{d}\mu$ to be invariant under G_1,

$$h(\xi g) = h(\xi), \tag{18}$$

where $g \in G_1$. Hence we can, without loss of generality, put $h = h(u)$, $u = \xi_1^2 + \xi_2^2 - \xi_3^2$.

The parametrization that we seek for manifold (8) must be such as to make A_{12} and C^{G_1} particularly simple. The corresponding coordinate system on (8) is obtained by sections of the manifold (8) by the planes $\xi_4 = c$. These sections are one-sheeted hyperboloids

$$\xi_1^2 + \xi_2^2 - \xi_3^2 = 1 + c^2$$

being invariant under G_1. Hence we introduce in place of ξ_1, ξ_2, and ξ_3 the new variables x, α, and φ by

$$\xi_1 = \frac{1}{\sqrt{1 - z^2(x)}} \cosh \alpha \cos \varphi,$$

$$\xi_2 = \frac{1}{\sqrt{1 - z^2(x)}} \cosh \alpha \sin \varphi,$$

$$\xi_3 = \frac{1}{\sqrt{1 - z^2(x)}} \sinh \alpha,$$

$$\xi_4 = \frac{z(x)}{\sqrt{1 - z^2(x)}}, \tag{19}$$

where $-\infty < x, \alpha < \infty, 0 \leqslant \varphi < 2\pi$ and $z(x)$ is a differentiable function on R with values in $[-1, +1]$. Then

$$A_{12} = i\frac{\partial}{\partial \varphi}, \quad C^{G_1} = \frac{\partial^2}{\partial \alpha^2} + \tanh \alpha \frac{\partial}{\partial \alpha} - \frac{1}{\cosh^2 \alpha} \frac{\partial^2}{\partial \varphi^2} \tag{20}$$

while

$$C^{\mathrm{SO}(2,2)} = \left(\frac{1 - z^2}{\dot{z}}\right)^2 \left[\frac{\partial^2}{\partial x^2} + \left(\frac{\dot{h}}{h} - \frac{\ddot{z}}{\dot{z}}\right) \frac{\partial}{\partial x} + \frac{1}{2}\frac{\ddot{h}}{h} - \frac{1}{4}\left(\frac{\dot{h}}{h}\right)^2 - \frac{\ddot{z}}{\dot{z}}\frac{\dot{h}}{2h} \right.$$
$$\left. + \frac{(\dot{z})^2}{1 - z^2}\left(\frac{\partial^2}{\partial \alpha^2} + \tanh \alpha \frac{\partial}{\partial \alpha} - \frac{1}{\cosh^2 \alpha} \frac{\partial^2}{\partial \varphi^2} \right) \right], \tag{21}$$

where dots represent derivatives with respect to x, i.e., $\dot{z} = \mathrm{d}z/\mathrm{d}x$, $\ddot{z} = \mathrm{d}^2 z/\mathrm{d}x^2$, and so on.

In order to eliminate the term that is linear in $\partial/\partial x$, we impose

$$\frac{\dot{h}}{h} - \frac{\ddot{z}}{\dot{z}} = 0. \tag{22}$$

Equation (22) is obviously satisfied by

$$h = \varkappa \dot{z}, \tag{23}$$

where $\varkappa$ is a constant. Substituting Eq. (23) into formula (21), we readily obtain

$$C^{\mathrm{SO}(2,2)} = \left(\frac{1 - z^2}{\dot{z}}\right)^2 \left[\frac{\partial^2}{\partial x^2} + \frac{1}{2}\frac{\dddot{z}}{\dot{z}} - \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2 + \frac{(\dot{z})^2}{1 - z^2}\left(\frac{\partial^2}{\partial \alpha^2} + \tanh \alpha \frac{\partial}{\partial \alpha} - \frac{1}{\cosh^2 \alpha} \frac{\partial^2}{\partial \varphi^2} \right) \right]. \tag{24}$$

Let us denote by $C_{jm}^{\mathrm{SO}(2,2)}$ a restriction of $C^{\mathrm{SO}(2,2)}$ on the subspace $\mathcal{H}_{jm}$ spanned by functions f_{jm} with fixed j and m. It turns out that

$$C_{jm}^{\mathrm{SO}(2,2)} = \left(\frac{1 - z^2}{\dot{z}}\right)^2 \left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\frac{\dddot{z}}{\dot{z}} - \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2 + j(j+1)\frac{(\dot{z})^2}{1 - z^2} \right], \tag{25}$$

where we have replaced the Casimir operator of G_1 on the right-hand side of formula (24) with its eigenvalue.

We allow now the eigenvalues of $C^{\mathrm{SO}(2,2)}$ and of C^{G_1} to be linear functions of the energy, i.e.,

$$j(j+1) = \gamma_1 E + \delta_1 \tag{26}$$

and

$$1 + \rho^2 = \gamma_2 E + \delta_2. \tag{27}$$

On the above-given conditions, we have

$$C_{jm}^{\mathrm{SO}(2,2)} - \sigma(\sigma+2) = -\left(\frac{1-z^2}{\dot{z}}\right)^2\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{2}\frac{\dddot{z}}{\dot{z}} + \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2 + \dot{z}^2\frac{ER(z) + \delta_1(1-z^2) + \delta_2}{(1-z^2)^2}\right], \tag{28}$$

where

$$R(z) = \gamma_1(1-z^2) + \gamma_2. \tag{29}$$

This equation is easily reduced to the form (7) with

$$Q = -\left(\frac{1-z^2}{\dot{z}}\right)^2, \tag{30}$$

and

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(z) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{2}\frac{\dddot{z}}{\dot{z}} + \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2 - \frac{\delta_1(1-z^2) + \delta_2}{R} \tag{31}$$

provided that

$$(\dot{z})^2 = \frac{(1-z^2)^2}{R(z)}. \tag{32}$$

(We are using units with $2M = \hbar = 1$.)

Taking into account Eq. (32), the potential, V, in Eq. (31) can be rewritten in the form

$$V(z) = -\frac{(4\delta_1+1)(1-z^2) + 4\delta_2 - 5}{4R(z)} - \frac{1}{2}\left[2\gamma_2 + \gamma_1 + \frac{\gamma_2}{2(1-z^2)} + \frac{5\Delta}{8R(z)}\right]\frac{1-z^2}{R(z)^2}, \tag{33}$$

where $\Delta = -4(\gamma_1+\gamma_2)\gamma_2$.

To make the potential V vanish as $|x| \to \infty$ (i.e., as $|z| \to 1$) we set $\delta_2 = 1$. Hence the relation (27) reduces to

$$\rho^2 = \gamma_2 E. \tag{34}$$

According to this we shall assume that $\gamma_2 > 0$.

The expression (33) simplifies for some convenient choice of γ_1 and γ_2. Let us start with the simplest case when $\gamma_1 = 0$, but γ_2 and δ_1 are still arbitrary. Then Eq. (32) reduces to

$$(\dot{z})^2 = \frac{1}{\gamma_2}(1-z^2)^2. \tag{35}$$

The solution to this equation is given by

$$z = \tanh\frac{x}{\sqrt{\gamma_2}}. \tag{36}$$

With this z, the Hamiltonian in (31) simplifies to the modified Pöschl-Teller Hamiltonian,[3]

$$H_{\mathrm{PT}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{j(j+1)}{\gamma_2 \cosh^2(x/\sqrt{\gamma_2})}. \tag{37}$$

It is also worth noting that potentials (33) include important families of Ginocchio potentials.[29] Indeed, putting

$$\gamma_1 = \frac{1}{\lambda^2} - \frac{1}{\lambda^4}, \quad \gamma_2 = \frac{1}{\lambda^4}, \quad \delta_1 = \nu(\nu+1), \quad \delta_2 = 1 \tag{38}$$

with $0 < \lambda < \infty$ and introducing a new variable y, $-1 \leqslant y \leqslant 1$,

$$y = \frac{z}{\sqrt{z^2 + \lambda^2(1-z^2)}}, \tag{39}$$

Eqs. (33) and (32) reduce to

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \lambda^2\nu(\nu+1)(1-y^2) + \frac{(1-\lambda^2)}{4}[5(1-\lambda^2)y^4 - (7-\lambda^2)y^2 + 2](1-y^2) \tag{40}$$

and

$$\frac{\mathrm{d}y}{\mathrm{d}x} = (1-y^2)[1-(1-\lambda^2)y^2], \tag{41}$$

respectively. Moreover, it follows from (41) that

$$x = \frac{1-\lambda^2}{\lambda^2}\int \frac{\mathrm{d}y}{(1-\lambda^2)y^2 - 1} - \frac{1}{\lambda^2}\int \frac{\mathrm{d}y}{y^2-1}$$

or[30]

$$x = \begin{cases} \dfrac{1}{\lambda^2}[\operatorname{arctanh}(y) - \sqrt{1-\lambda^2}\,\operatorname{arctanh}(\sqrt{1-\lambda^2}y)] & \text{if } 0 < \lambda < 1 \\ \dfrac{1}{\lambda^2}[\operatorname{arctanh}(y) + \sqrt{\lambda^2-1}\,\arctan(\sqrt{\lambda^2-1}y)] & \text{if } 1 \leqslant \lambda < \infty, \end{cases} \tag{42}$$

which is just relation (2.8) of Ref. 29.

The family of potentials given in (40) is a two parameter generalization of the modified Pöschl-Teller potential hole. (Observe that (40) reduces to the modified Pöschl-Teller Hamiltonian when $\lambda = 1$.) They are symmetric about the origin as we expected. The parameter λ is related to the shape of the potential while the parameter ν is related to the depth of the potential and determines the nature of the scattering. If the depth parameter ν is an integer then $|T|^2 = 1$, $|R| = 0$ (see Eqs. (5.9) and (5.10) of Ref. 29).

By making use of traditional techniques, i.e., by considering the asymptotic behavior of the scattering wavefunctions, one can check that the potentials in (33) are reflectionless when j is an integer. In order to apply such a technique we require first a solution for the Schrödinger equation

$$H\Psi = E\Psi$$

with Hamiltonian (31). If we substitute $\Psi = (\dot{z})^{-1/2}\check{\Psi}$ the equation for $\check{\Psi}$ becomes

$$\left\{-(\dot{z})^2\frac{\mathrm{d}^2}{\mathrm{d}z^2} - \frac{\dot{z}^2}{(1-z^2)^2}[\delta_1(1-z^2) + \delta_2]\right\}\check{\Psi} = E\check{\Psi}. \tag{43}$$

Taking into account Eqs. (32), (26), and (27), we arrive at

$$\left[-(1-z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2} - j(j+1)(1-z^2) + \sigma(\sigma+2)\right]\check{\Psi} = 0. \tag{44}$$

If we set $w=z^2$ and substitute $\check{\Psi}=(1-w)^{(\sigma+2)/2}u$, this differential equation becomes

$$w(1-w)\frac{\mathrm{d}^2u}{\mathrm{d}w^2} + \left[\frac{1}{2} - \left(\sigma+\frac{5}{2}\right)w\right]\frac{\mathrm{d}u}{\mathrm{d}w} - \frac{1}{4}[(\sigma+2)(\sigma+1) - j(j+1)]u = 0. \tag{45}$$

This is equivalent to the hypergeometric equation[30]

$$w(1-w)\frac{\mathrm{d}^2u}{\mathrm{d}w^2} + [c-(a+b+1)w]\frac{\mathrm{d}u}{\mathrm{d}w} - abu = 0, \tag{46}$$

which has two linear independent solutions

$$u_1 = {}_2F_1(a,b;c;w),$$

$$u_2 = w^{1-c}{}_2F_1(a-c+1,b-c+1;2-c;w).$$

Before proceeding further, we note that with $\gamma_2>0$ the function z carries the points $x=\pm\infty$ to $z=\pm1$, respectively. It follows from (32) that

$$z \to \pm\left[1-2e^{-2(|x|-x_0)/\sqrt{\gamma_2}}\right] \quad \text{for } x \to \pm\infty, \tag{47}$$

where x_0 is a constant depending on γ_1 and γ_2. Hence, two linear independent scattering solutions Ψ_l and Ψ_r satisfying the boundary conditions

$$\Psi_l = \begin{cases} e^{ikx} + R_l e^{-ikx} & \text{for } x \to -\infty \\ T_l e^{ikx} & \text{for } x \to +\infty, \end{cases} \tag{48}$$

and

$$\Psi_r = \begin{cases} T_r e^{-ikx} & \text{for } x \to -\infty \\ e^{-ikx} + R_r e^{ikx} & \text{for } x \to +\infty \end{cases} \tag{49}$$

with $E=k^2$, are given by

$$\Psi_l = N\sqrt[4]{\gamma_1(1-z^2)+\gamma_2}(1-z^2)^{(\sigma+1)/2}\left[\Gamma\left(\frac{\sigma+j+2}{2}\right)\Gamma\left(\frac{\sigma-j+1}{2}\right)u_1 - \Gamma\left(\frac{\sigma+j+3}{2}\right)\Gamma\left(\frac{\sigma-j+2}{2}\right)u_2\right]$$

and

$$\Psi_r = N\sqrt[4]{\gamma_1(1-z^2)+\gamma_2}(1-z^2)^{(\sigma+1)/2}\left[\Gamma\left(\frac{\sigma+j+2}{2}\right)\Gamma\left(\frac{\sigma-j+1}{2}\right)u_1 + \Gamma\left(\frac{\sigma+j+3}{2}\right)\Gamma\left(\frac{\sigma-j+2}{2}\right)u_2\right],$$

where

$$N = \frac{\exp\left[\left(\frac{x_0}{\sqrt{\gamma_2}} + \ln\sqrt{2}\right)(\sigma+1)\right]}{2\sqrt{\pi}(\gamma_2)^{1/4}\Gamma(\sigma+1)}, \tag{50}$$

$$u_1 = {}_2F_1\left(\frac{\sigma+j+2}{2}, \frac{\sigma-j+1}{2}; \frac{1}{2}; z^2\right), \tag{51}$$

$$u_2 = z\,{}_2F_1\left(\frac{\sigma+j+3}{2}, \frac{\sigma-j+2}{2}; \frac{3}{2}; z^2\right). \tag{52}$$

Using (47) together with the transformation[30]

$$\begin{aligned} {}_2F_1(a,b;c;w) &= A_1\,{}_2F_1(a,b;a+b-c+1;1-w) \\ &\quad + A_2(1-w)^{c-a-b}\,{}_2F_1(c-a,c-b;c-a-b+1;1-w), \end{aligned}$$

where

$$A_1 = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, \quad A_2 = \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)},$$

one can check that the reflection and transmission amplitudes are

$$R_l = R_r = c\frac{1}{\pi}\sin(\pi j)\Gamma(\sigma+j+2)\Gamma(\sigma-j+1) \tag{53}$$

and

$$T_l = T_r = c\frac{1}{\pi}\sin(\pi\sigma)\Gamma(\sigma+j+2)\Gamma(\sigma-j+1), \tag{54}$$

where c is a complex number of unit modulus

$$c = \frac{\Gamma(-1-\sigma)}{\Gamma(1+\sigma)}\exp\left[\left(\frac{2x_0}{\sqrt{\gamma_2}} - \ln 2\right)(\sigma+1)\right]. \tag{55}$$

Thus, when j is an integer the family of potentials given in (33) is reflectionless as we expected.

Finally, by arguments very similar to those used to obtain (33) we can show that the potentials gained for $\mathrm{SO}(2,2) \supset G_2$ reduction have just the same shape as (33).

(ii) The $\mathrm{SO}(2,2) \supset G_3$ reduction. Then, the reduction conditions are

$$A_{34} f_{jm} = m f_{jm}, \quad C^{G_3} f_{jm} = j(j+1) f_{jm}, \tag{56}$$

where

$$C^{G_3} = A_{34}^2 - A_{23}^2 - A_{24}^2 = h^{-1/2} \circ \left[(\xi_1^2 - 1)\left(\frac{\partial^2}{\partial \xi_2^2} - \frac{\partial^2}{\partial \xi_3^2}\right) + M(M+1)\right] \circ h^{1/2} \tag{57}$$

with

$$M = \xi_2 \frac{\partial}{\partial \xi_2} + \xi_3 \frac{\partial}{\partial \xi_3}.$$

According to this, we impose $\mathrm{d}\mu$ to be invariant under G_3,

$$h(\xi g) = h(\xi), \tag{58}$$

where $g \in G_3$. Hence we can, without loss of generality, put $h = h(v)$, $v = \xi_2^2 - \xi_3^2 - \xi_4^2$.

Since A_{34} and $A_{34}^2 - A_{23}^2 - A_{24}^2$ are sought to be diagonal, the appropriate parametrization for (8) in these circumstances is obtained by sections of the manifold (8) by the planes $\xi_1 = c$. It is not difficult to see that the sections are one-sheeted hyperboloids

$$-\xi_2^2+\xi_3^2+\xi_4^2=c^2-1$$

if $|c|>1$ and two-sheeted hyperboloids

$$\xi_2^2-\xi_3^2-\xi_4^2=1-c^2$$

if $|c|<1$. The whole of Ξ can be expressed as the union of two regions, Ξ_1 in which $|\xi_1|>1$ and Ξ_2 in which $|\xi_1|<1$. Since the discrete series of SO(2,1) is related to the one-sheeted hyperboloid we shall restrict ourselves to Ξ_1.

We proceed with the determination of the new coordinates in Ξ_1:

$$\xi_1=\frac{z(x)}{\sqrt{z^2(x)-1}},$$

$$\xi_2=\frac{1}{\sqrt{z^2(x)-1}}\sinh\alpha,$$

$$\xi_3=\frac{1}{\sqrt{z^2(x)-1}}\cosh\alpha\sin\varphi,$$

$$\xi_4=\frac{1}{\sqrt{z^2(x)-1}}\cosh\alpha\cos\varphi, \tag{59}$$

where $-\infty<x,\ \alpha<\infty,\ 0\leqslant\varphi<2\pi$ and $z(x)$ is a differentiable function on R with values in $(-\infty,1)\cup(1,\infty)$. Then

$$A_{34}=-i\frac{\partial}{\partial\varphi},\quad C^{G_3}=\frac{\partial^2}{\partial\alpha^2}+\tanh\alpha\frac{\partial}{\partial\alpha}-\frac{1}{\cosh^2\alpha}\frac{\partial^2}{\partial\varphi^2} \tag{60}$$

while

$$C^{\mathrm{SO}(2,2)}=\left(\frac{1-z^2}{\dot z}\right)^2\left[\frac{\partial^2}{\partial x^2}+\left(\frac{\dot h}{h}-\frac{\ddot z}{\dot z}\right)\frac{\partial}{\partial x}+\frac{1}{2}\frac{\ddot h}{h}-\frac{1}{4}\left(\frac{\dot h}{h}\right)^2-\frac{\ddot z}{\dot z}\frac{\dot h}{2h}\right.$$
$$\left.+\frac{(\dot z)^2}{1-z^2}\left(\frac{\partial^2}{\partial\alpha^2}+\tanh\alpha\frac{\partial}{\partial\alpha}-\frac{1}{\cosh^2\alpha}\frac{\partial^2}{\partial\varphi^2}\right)\right]. \tag{61}$$

Although the operators (21) and (61) have the same form (in terms of z, α,φ), the functions z are not the same.

It is immediately evident from the above-noted sets of equations that the potentials gained for $\mathrm{SO}(2,2)\supset G_3$ reduction are also given by (33), but the values of z are in $(-\infty,1)\cup(1,\infty)$. Hence we have a new family of reflectionless potentials. For example, if $\gamma_1=0$ then z satisfies Eq. (35) whose (nonsingular) solution now becomes

$$z=\begin{cases}\coth\dfrac{x-a}{\sqrt{\gamma_2}} & \text{for } x<0\\[2ex] \coth\dfrac{x+a}{\sqrt{\gamma_2}} & \text{for } x>0,\end{cases} \tag{62}$$

where a, $0<a$, is a constant of integration. So that

$$V=\begin{cases}\dfrac{j(j+1)}{\gamma_2\sinh^2\left(\dfrac{x-a}{\sqrt{\gamma_2}}\right)} & \text{for } x<0\\ \dfrac{j(j+1)}{\gamma_2\sinh^2\left(\dfrac{x+a}{\sqrt{\gamma_2}}\right)} & \text{for } x>0.\end{cases} \tag{63}$$

(Observe that the potential (63) is symmetric about the origin.) This reflectionless potential has been discussed in detail in the context of supersymmetric quantum mechanics.[17]

Finally, we note that we have the same results for the $\mathrm{SO}(2,2)\supset G_4$ reduction.

III. REFLECTIONLESS POTENTIALS RELATED TO ISO(1,1)

We denote by M a two-dimensional Minkowski space with bilinear form

$$\xi\cdot\eta\equiv\xi_1\eta_1-\xi_2\eta_2. \tag{64}$$

Poincaré transformations in M are translations and hyperbolic rotations of the type[28]

$$\xi_1'=\xi_1\cosh\theta+\xi_2\sinh\theta+b_1,$$

$$\xi_2'=\xi_1\sinh\theta+\xi_2\cosh\theta+b_2,$$

where the three parameters b_1, b_2, and θ range from $-\infty$ to $+\infty$. The above-noted transformations can be conveniently written in matrix form

$$\xi'=\xi g, \tag{65}$$

with

$$g=\begin{pmatrix}\cosh\theta & \sinh\theta & 0\\ \sinh\theta & \cosh\theta & 0\\ b_1 & b_2 & 1\end{pmatrix},\quad \xi=(\xi_1,\xi_2,1). \tag{66}$$

The UIRs of the Poincaré group in $1+1$ dimensions are labeled with a quantum number, ρ, ranging from 0 to $+\infty$. Representations labeled with ρ and $-\rho$ are Weyl-equivalent.

The matrices corresponding to translations along the ξ_1 axis and the ξ_2 axis, as well as to hyperbolic rotations are, respectively,

$$g_1(t)=\begin{pmatrix}1&0&0\\0&1&0\\t&0&1\end{pmatrix},\quad g_2(t)=\begin{pmatrix}1&0&0\\0&1&0\\0&t&1\end{pmatrix},\quad g_3(t)=\begin{pmatrix}\cosh t&\sinh t&0\\\sinh t&\cosh t&0\\0&0&1\end{pmatrix}. \tag{67}$$

The generators of the corresponding Lie algebra, $\mathrm{ISO}(1,1)$, denoted by $a_k(k=1,2,3)$, are, by definition

$$a_k=\left.\frac{\mathrm{d}g_k}{\mathrm{d}t}\right|_{t=0}. \tag{68}$$

They satisfy the following commutation relations:

$$[a_1,a_2]=0,\quad [a_3,a_1]=-a_2,\quad [a_3,a_2]=-a_1. \tag{69}$$

Now, we want to construct the Hamiltonian H for which

$$Q(H-E) = (C-\rho^2)|_{\mathcal{H}_\tau}, \tag{70}$$

where $\mathcal{H}_\tau$ is a one-dimensional subspace occurring in the $\mathrm{ISO}(1,1)\supset\mathrm{SO}(1,1)$ reduction.

Let us consider a quasiregular representation of ISO(1,1) induced by a one-dimensional identity representation of SO(1,1). It is known that[28] this representation is decomposed into the direct integral of UIRs of ISO(1,1) labeled with $\rho(0<\rho<\infty)$ and each UIR appears in the decomposition four times.

The quasiregular representation can be realized in the Hilbert space $L^2(M,\mathrm{d}\mu)$ of square-integrable functions defined on $M\sim\mathrm{ISO}(1,1)/\mathrm{SO}(1,1)$. In general, for construction of the quasi-regular representation, one can use the carrier space, $L^2(M,\mathrm{d}\mu)$, with any quasi-invariant measure $\mathrm{d}\mu(\xi)$ on M. The representations with different measure are unitarily equivalent, and given by

$$T(g)f(\xi) = \left[\frac{\mathrm{d}\mu(\xi g)}{\mathrm{d}\mu(\xi)}\right]^{1/2} f(\xi g), \tag{71}$$

with inner product

$$(f,f') = \int \overline{f(\xi)} f'(\xi)\mathrm{d}\mu(\xi), \tag{72}$$

where $\overline{f(\xi)}$ is the complex conjugate of $f(\xi)$ and $\mathrm{d}\mu(\xi g)/\mathrm{d}\mu(\xi)$ is the Radon-Nikodym derivative.

Without loss of generality, we can put

$$\mathrm{d}\mu(\xi) = h(\xi)\mathrm{d}\xi, \tag{73}$$

where $\mathrm{d}\xi=\mathrm{d}\xi_1\mathrm{d}\xi_2$ is an invariant measure on M.

It is not difficult to show that the infinitesimal operators $A_k = -i(\mathrm{d}/\mathrm{d}t)T(g_k(t))|_{t=0}$ of the representation (71) corresponding to the three one-parameter subgroups of ISO(1,1) are given by

$$iA_1 = \frac{\partial}{\partial\xi_1} + \frac{1}{2h}\frac{\partial h}{\partial\xi_1}, \tag{74}$$

$$iA_2 = \frac{\partial}{\partial\xi_2} + \frac{1}{2h}\frac{\partial h}{\partial\xi_2}, \tag{75}$$

$$iA_3 = \xi_2\frac{\partial}{\partial\xi_1} + \xi_1\frac{\partial}{\partial\xi_2} + \frac{1}{2h}\left(\xi_2\frac{\partial h}{\partial\xi_1} + \xi_1\frac{\partial h}{\partial\xi_2}\right). \tag{76}$$

If we compute the Casimir operator $C=A_1^2-A_2^2$, it becomes

$$C = -\frac{\partial^2}{\partial\xi_1^2} + \frac{\partial^2}{\partial\xi_2^2} - \frac{1}{2h}\left(\frac{\partial h}{\partial\xi_1}\frac{\partial}{\partial\xi_1} - \frac{\partial h}{\partial\xi_2}\frac{\partial}{\partial\xi_2}\right) - \frac{1}{2h}\left(\frac{\partial^2 h}{\partial\xi_1^2} - \frac{\partial^2 h}{\partial\xi_2^2}\right) + \frac{1}{4h^2}\left(\left(\frac{\partial h}{\partial\xi_1}\right)^2 - \left(\frac{\partial h}{\partial\xi_2}\right)^2\right). \tag{77}$$

Hence, we can construct the irreducible representations of ISO(1,1) as subrepresentations of the quasi-regular representation (71). To do this, we require the representation space to be irreducible. Such a restriction is obtained if all functions f are eigenfunctions of the Casimir operator C of (71),

$$Cf = \rho^2 f. \tag{78}$$

Next, imposing the reduction condition, we can choose a different basis in the carrier space. In order to diagonalize the SO(1,1) subgroup, we exploit the reduction condition

$$A_3 f_\tau = \tau f_\tau. \tag{79}$$

According to this, we want $d\mu$ to be invariant under SO(1,1), i.e.,

$$h(g_3\xi) = h(\xi), \quad g_3 \in \mathrm{SO}(1,1). \tag{80}$$

As a consequence, we find

$$\left(\xi_2 \frac{\partial}{\partial \xi_1} + \xi_1 \frac{\partial}{\partial \xi_2}\right) h = 0. \tag{81}$$

The parametrization of M we are searching for must be such as to make A_3 particularly simple. For this purpose, we must introduce hyperbolic variables; this requires dividing the Minkowski space into two regions. The new variables x and α, both ranging from $-\infty$ to $+\infty$, are introduced in each region in this way:

$$\xi_1^2 > \xi_2^2: \quad \xi_1 = z(x)\cosh\alpha, \quad \xi_2 = z(x)\sinh\alpha, \tag{82}$$

$$\xi_1^2 < \xi_2^2: \quad \xi_1 = z(x)\sinh\alpha, \quad \xi_2 = z(x)\cosh\alpha, \tag{83}$$

where $z(x)$, $-\infty < z < \infty$, is a differentiable function on R.

Without loss of generality, we replace ξ_1 and ξ_2 with the new variables x and α via Eq. (82). Then, Eq. (81) reduces to

$$\frac{\partial h}{\partial \alpha} = 0. \tag{84}$$

Then operator A_3 (76) is simply

$$A_3 = i\frac{\partial}{\partial \alpha}, \tag{85}$$

as expected, and the Casimir operator becomes, in the new parametrization,

$$C = -\frac{1}{(\dot{z})^2}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{1}{h}\frac{\mathrm{d}h}{\mathrm{d}x} + \frac{\dot{z}}{z} - \frac{\ddot{z}}{\dot{z}}\right)\frac{\partial}{\partial x} - \left(\frac{\dot{z}}{z}\right)^2 \frac{\partial^2}{\partial \alpha^2} - \frac{1}{4h^2}\left(\frac{\mathrm{d}h}{\mathrm{d}x}\right)^2 + \frac{1}{2h}\left(\frac{\mathrm{d}^2 h}{\mathrm{d}x^2} - \frac{\ddot{z}}{\dot{z}}\frac{\mathrm{d}h}{\mathrm{d}x} + \frac{\dot{z}}{z}\frac{\mathrm{d}h}{\mathrm{d}x}\right)\right], \tag{86}$$

where $\dot{z} \equiv \mathrm{d}z/\mathrm{d}x$, $\ddot{z} \equiv \mathrm{d}^2 z/\mathrm{d}x^2$, and so on. In order to eliminate the term containing $\partial/\partial x$, we require

$$\frac{1}{h}\frac{\mathrm{d}h}{\mathrm{d}x} + \frac{\dot{z}}{z} - \frac{\ddot{z}}{\dot{z}} = 0. \tag{87}$$

The solution to this equation is given by

$$h = \chi\frac{\dot{z}}{z}, \tag{88}$$

where χ is a constant. Substituting Eq. (88) into formula (86), we get

$$C = -\frac{1}{(\dot{z})^2}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{\dot{z}}{z}\right)^2\left(\frac{1}{4} - \frac{\partial^2}{\partial \alpha^2}\right) + \frac{1}{2}\frac{\dddot{z}}{\dot{z}} - \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right]. \tag{89}$$

Let $\mathcal{H}_\tau$ be a one-dimensional subspace spanned by functions f_τ with fixed τ: the Casimir operator restricted to $\mathcal{H}_\tau$ becomes a differential operator in x alone; it turns out that

$$C_\nu = -\frac{1}{(\dot{z})^2}\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (1+\nu^2)\left(\frac{\dot{z}}{z}\right)^2 + \frac{1}{2}\frac{\dddot{z}}{\dot{z}} - \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right], \tag{90}$$

where C_τ denotes the restriction of C to $\mathcal{H}_\tau$.

Let the quantum numbers τ^2 and ρ^2 be linear functions of energy, E. Without loss of generality, we can assume

$$\tau^2 + \tfrac{1}{4} = \alpha_1 E + \beta_1, \tag{91}$$

and

$$\rho^2 = \alpha_2 E + \beta_2. \tag{92}$$

Then, formula (90) becomes

$$C_\nu - \rho^2 = \frac{1}{(\dot{z})^2}\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - (ER(z) + \beta_2 z^2 + \beta_1)\left(\frac{\dot{z}}{z}\right)^2 - \frac{1}{2}\frac{\dddot{z}}{\dot{z}} + \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2\right], \tag{93}$$

where now

$$R(z) = \alpha_2 z^2 + \alpha_1. \tag{94}$$

In order that relation (70) be satisfied, with $Q = 1/(\dot{z})^2$, we now impose

$$(\dot{z})^2 = \frac{z^2}{R(z)}. \tag{95}$$

If the above-presented condition holds, the operator within square brackets on the right-hand side of Eq. (93) can be written as $H - E$, where

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(z) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{2}\frac{\dddot{z}}{\dot{z}} + \frac{3}{4}\left(\frac{\ddot{z}}{\dot{z}}\right)^2 - \frac{\beta_2 z^2 + \beta_1}{R}.$$

Hence, the ISO(1,1) related potentials V are given by

$$V = -\frac{\beta_2 z^2 + \beta_1}{R} + \frac{3\alpha_1}{2R^2} - \frac{5\alpha_1^2}{4R^3}. \tag{96}$$

In order to make the potential V vanish as $|x| \to \infty$ (i.e., as $|z| \to \infty$) we set $\beta_2 = 0$. Hence relation (92) reduces to

$$\rho^2 = \alpha_2 E. \tag{97}$$

A simple case comes about by choosing $\alpha_1 = 0$. In this case Eq. (95) reduces to

$$(\dot{z})^2 = 1/\alpha_2, \tag{98}$$

whose solution is given by

$$z = \begin{cases} (x-a)/\sqrt{\alpha_2}, & \text{for } x < 0 \\ (x+a)/\sqrt{\alpha_2}, & \text{for } x > 0, \end{cases} \tag{99}$$

where a, $0 < a$, is a constant of integration. According to (96) and (99) we obtain

$$V(x)=\begin{cases} -\dfrac{\frac{1}{4}+\tau^2}{(x-a)^2}, & \text{for } x<0 \\ -\dfrac{\frac{1}{4}+\tau^2}{(x+a)^2}, & \text{for } x>0. \end{cases} \tag{100}$$

Furthermore one can check that the potential (63) with $j=-1/2-i\tau$ goes over in the limit $\gamma_2 \to \infty$ into (100). Hence (see Eq. (34)) we can obtain the S-matrix for (100) by the limiting process $\rho \to \infty$ from (53) and (54) as mentioned in Sec. I.

It is worthwhile to point out that potential (100) was obtained in the supersymmetric approach[17] as a partner of the null potential. (In Ref. 31 a singular potential $V \sim 1/x^2$ has been studied on the line.) Finally, we note that the potentials related to $\mathrm{ISO}(2,1) \supset \mathrm{SO}(2,1)$ are also given by (96), but the left-hand side of (91) must be replaced by $-j(j+1)$, where $j=-1/2-i\tau$, for principal series representations of SO(2,1), while $j=0,1,2,\ldots$, for discrete series representations of SO(2,1).

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Decompositions of unitary evolutions and entanglement dynamics of bipartite quantum systems

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We describe a decomposition of the Lie group of unitary evolutions for a bipartite quantum system of arbitrary dimensions. The decomposition is based on a recursive procedure that systematically uses the Cartan classification of the symmetric spaces of the Lie group $SO(n)$. The resulting factorization of unitary evolutions clearly displays the local and entangling character of each factor. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2245205]

I. INTRODUCTION

Decompositions of a Lie group G are methods to factorize every element $X \in G$ as

$$X = X_1 X_2 \dots X_m, \tag{1.1}$$

where the factors $X_1, \dots, X_m$ belong to one dimensional subgroups. Decompositions of unitary evolutions in simpler terms are of interest in quantum control and information theory for at least three reasons. They allow us to simplify the task of controlling the evolution of a quantum system to a target into a sequence of simpler subtasks, consisting of control problems to more easily reachable targets (see, e.g., Refs. 1–3). They allow the analysis of several features of quantum dynamics such as entanglement generation, time optimality, and parameter identification (see, e.g., Refs. 4–7). They give methods to produce unitary evolutions in a laboratory by combining a sequence of readily reproducible evolutions. In particular, in quantum information theory, a decomposition can be seen as a method to generate a quantum logic operation from a sequence of elementary operations.[6,8]

In many cases, decompositions of the unitary group $U(n)$ correspond to vector space decompositions of the corresponding Lie algebra $\mathfrak{u}(n)$, and each element $H \in i\mathfrak{u}(n)$ represents the Hamiltonian of a possible evolution. In the analysis of multipartite quantum systems, it is useful to distinguish Hamiltonians acting on single subsystems, called *local Hamiltonians*, and Hamiltonians describing the coupling between two or more systems, called *interaction (or entangling) Hamiltonians*. In the unitary group, these Hamiltonians generate local and entangling evolutions, respectively. In particular, if one considers a multipartite system composed of N subsystems of dimensions $n_1, \dots, n_N$, the space of all possible Hamiltonians is given by $i\mathfrak{u}(n_1 n_2 \cdots n_N)$. Once we have an orthogonal basis in $i\mathfrak{u}(n_j)$, $j=1, \dots, N$, given by $H_{l_j}^j$, $l_j=1, \dots, n_j^2$, then a basis of $\mathfrak{u}(n_1 n_2 \cdots n_N)$ is given by

$$iH_{l_1}^1 \otimes H_{l_2}^2 \otimes \cdots \otimes H_{l_N}^N. \tag{1.2}$$

The subalgebra of local Hamiltonians is spanned by elements where all the factors in the tensor product are equal to the identity except one. They produce unitary evolutions of the factorized form $X_1 \otimes X_2 \otimes \cdots \otimes X_N$, which correspond to transformations on the single subsystems. In this spirit, the decomposition given in Ref. 6 recursively factorizes a unitary transformation on n qubits

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in local and entangling transformations, the latter one acting on two subsystems at a time only. In a recent paper,[9] a method was given to generate decompositions in the tensor product space for general multipartite quantum systems of arbitrary dimensions, starting from decompositions of evolutions on the single subsystems.

In the spirit of the last two works cited, we present in this paper a recursive procedure to decompose the unitary evolution of a bipartite system *of arbitrary dimensions* so that every evolution is factorized into simple terms, and it is clear what the entangling and local contributions of a single transformation are. The procedure we present applies recursively the Cartan decomposition of the Lie algebra $\mathfrak{so}(n)$ by keeping the tensor product basis representation of the Lie algebra $\mathfrak{u}(n)$. In this basis, at the end of the procedure, it is easy to analyze the local and entangling character of each factor.

The paper is organized as follows: in the next section we review some basic concepts and results on the Cartan classification of symmetric spaces and Cartan decompositions. We shall mention only the facts needed in the sequel of the paper. A detailed treatment can be found in Ref. 10. The decomposition procedure we describe consists of an initial step that reduces the problem to a decomposition of the orthogonal group and a recursive procedure, which allows us to decompose further the elements of the orthogonal group. These steps are described in Secs. III and IV, respectively. We give several remarks highlighting the local and entangling factors needed in the factorization. Section V is devoted to a discussion and a numerical example.

Notation: In the following we will use several times the definition of the elementary matrices E_{mn},

$$(E_{mn})_{rs} = \delta_{mr}\delta_{ns}, \tag{1.3}$$

and of their antisymmetric and symmetric superposition, respectively as

$$\Delta_{mn} := E_{mn} - E_{nm}, \quad \Omega_{mn} := E_{mn} + E_{nm}. \tag{1.4}$$

We denote by A^T the transposed of the matrix A. An $n \times m$ rectangular matrix is denoted by $A_{n\times m}$; the $n \times n$ identity matrix by $\mathbf{1}_n$. Finally, we call a *sign* matrix a matrix of the form $\mathrm{diag}(\pm 1, \pm 1, \ldots, \pm 1)$ with all the possible combinations of + and −.

II. BACKGROUND MATERIAL

In the following, we shall use (in a recursive manner) *Cartan decompositions* of the Lie algebras $\mathfrak{su}(n)$ and $\mathfrak{so}(n)$ as well as Cartan decompositions of direct products of (isomorphic copies of) these Lie algebras. A Cartan decomposition of a semisimple Lie algebra $\mathfrak{L}$ is a vector space decomposition

$$\mathfrak{L} = \mathfrak{k} \oplus \mathfrak{p}, \tag{2.1}$$

where $\mathfrak{k}$ is a subalgebra, namely

$$[\mathfrak{k},\mathfrak{k}] \subseteq \mathfrak{k}, \tag{2.2}$$

and the complement subspace $\mathfrak{p} = \mathfrak{k}^{\perp}$ is such that

$$[\mathfrak{p},\mathfrak{p}] \subseteq \mathfrak{k}, \quad [\mathfrak{p},\mathfrak{k}] \subseteq \mathfrak{p}. \tag{2.3}$$

Here the orthogonal complement $\perp$ is with respect to the *Killing form*. The Killing form on a Lie algebra $\mathfrak{L}$ is an inner product defined in terms of the adjoint representation of $\mathfrak{L}$. In particular, every $l \in \mathfrak{L}$ acts on the vector space $\mathfrak{L}$ according to the linear map ad_l, defined as

$$\mathrm{ad}_l(x) := [l,x]. \tag{2.4}$$

The Killing form *Kill* is a bilinear form defined as

$$\mathrm{Kill}(x,y) := \mathrm{Tr}(\mathrm{ad}_x \mathrm{ad}_y). \tag{2.5}$$

For the Lie algebras $su(n)$ and $so(n)$, which are the main Lie algebras considered in this work, the Killing form is proportional to the matrix inner product $\langle x,y\rangle := \mathrm{Tr}(xy^*)$.[10] Therefore, we shall refer to this inner product in the following any time we mention orthogonality relations.

To a Cartan decomposition of $\mathfrak{L}$ there corresponds a factorization of $e^{\mathfrak{L}}$, the connected Lie group associated to $\mathfrak{L}$, such that every element $X \in e^{\mathfrak{L}}$ can be written as

$$X = KP, \tag{2.6}$$

where K belongs to $e^{\mathfrak{k}}$, the connected Lie group corresponding to $\mathfrak{k}$, and P is the exponential of an element in $\mathfrak{p}$. The coset space $e^{\mathfrak{L}}/e^{\mathfrak{k}}$ is called a *symmetric space* of $e^{\mathfrak{L}}$. A maximal Abelian subalgebra of $\mathfrak{L}$ in $\mathfrak{p}$ is called a *Cartan subalgebra* associated to the decomposition, and it is denoted by $\mathfrak{a}$. One can show, under appropriate assumptions, that

$$\bigcup_{K \in e^{\mathfrak{k}}} K\mathfrak{a}K^{-1} = \mathfrak{p}, \tag{2.7}$$

so that the factorization (2.6) refines to

$$X = K_1 A K_2, \tag{2.8}$$

with $K_1, K_2 \in e^{\mathfrak{k}}$, and $A \in e^{\mathfrak{a}}$. The dimension of the Cartan subalgebra $\mathfrak{a}$ is called the *rank* of the decomposition (or of the associated symmetric space).

Cartan has classified all the symmetric spaces of the classical Lie groups, i.e., the Lie groups $SU(n)$, $Sp(n)$, and $SO(n)$, and has shown that, up to conjugacy, the corresponding decompositions fall in one of few classes that he has described. [A conjugacy on $\mathfrak{L}$ is a map $m:\mathfrak{L}\to\mathfrak{L}$ such that $m(L)=MLM^{-1}$ for some $M \in e^{\mathfrak{L}}$.] In particular, for $\mathfrak{L}=\mathfrak{su}(n)$, there are three types of decompositions labeled by AI, AII, AIII. In the following, we shall use only decompositions of the type AI, given by

$$\mathfrak{k} = \mathfrak{so}(n), \quad \mathfrak{p} = \mathfrak{so}(n)^{\perp}, \tag{2.9}$$

with $\mathfrak{so}(n)^{\perp}$ the subspace of $\mathfrak{su}(n)$ spanned by purely imaginary matrices. The rank of this decomposition is $n-1$. Decompositions of the type AII and AIII will not be considered here.

We consider now the Lie algebra $\mathfrak{L}=\mathfrak{so}(n)$. If $n=1$, this algebra contains only the null matrix $\mathbf{0}$. For $n>2$, when n is odd there is only one type of Cartan decomposition, denoted by BDI. Fixing two positive integers r and q such that $r \geqslant q \geqslant 1$ and $r+q=n$, the matrices $k \in \mathfrak{k}$ have the form

$$k = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}, \tag{2.10}$$

with $A \in \mathfrak{so}(r)$ and $B \in \mathfrak{so}(q)$. Matrices $p \in \mathfrak{p}$ have the form

$$p = \begin{pmatrix} 0 & C \\ -C^T & 0 \end{pmatrix}, \tag{2.11}$$

for a general $r \times q$ matrix C. The rank of this decomposition is q. In this paper, we will not consider other decompositions.

III. DECOMPOSITION OF UNITARY EVOLUTIONS IN $U(d_1d_2)$; INITIAL STEP

Consider two interacting quantum systems $\mathcal{S}_1$ and $\mathcal{S}_2$ whose associated Hilbert spaces have dimensions d_1 and d_2, respectively. According to the procedure described in Ref. 9, it is possible to obtain a decomposition for $\mathfrak{su}(d_1d_2)$ from decompositions of type AI of the Lie algebras associated to each subsystem, i.e., $\mathfrak{su}(d_1)$ and $\mathfrak{su}(d_2)$. In the following instead of decompositions of $su(n)$ we shall refer to decompositions of $u(n)$. To a decomposition of $su(n)$,

$$su(n) = \mathfrak{k} \oplus \mathfrak{p}, \tag{3.1}$$

with $\mathfrak{k}$ and $\mathfrak{p}$ satisfying the conditions (2.2) and (2.3), there corresponds a decomposition of $u(n)$,

$$u(n) = \mathfrak{k} \oplus \mathfrak{p}', \tag{3.2}$$

where $\mathfrak{p}'$ is defined by $\mathfrak{p}' := \mathfrak{p} \oplus \text{span}\{i\mathbf{1}\}$. $\mathfrak{k}$ and $\mathfrak{p}'$ still satisfy the relations (2.2) and (2.3), with $\mathfrak{p}$ replaced by $\mathfrak{p}'$. What we have said in the previous section, in particular for the decomposition of the associated Lie group, can be repeated by including $\text{span}\{i\mathbf{1}\}$ in the maximal Abelian subalgebra. With some abuse of terminology, we shall refer to this decomposition also as a *Cartan decomposition of* $u(n)$. We write

$$\mathfrak{u}(d_1) = \mathfrak{so}(d_1) \oplus \mathfrak{so}(d_1)^{\perp}, \quad \mathfrak{u}(d_2) = \mathfrak{so}(d_2) \oplus \mathfrak{so}(d_2)^{\perp}. \tag{3.3}$$

Let σ^j, $j=1,2$, be a generic element of an orthogonal basis of $i\mathfrak{so}(d_j)$, and S^j, $j=1,2$, a generic element of an orthogonal basis of $i\mathfrak{so}(d_j)^{\perp}$. Then the subalgebra of $\mathfrak{u}(d_1 d_2)$, defined by

$$\mathfrak{k} := \text{span}\{i\sigma^1 \otimes S^2, iS^1 \otimes \sigma^2\}, \tag{3.4}$$

along with its orthogonal complement in $\mathfrak{u}(d_1 d_2)$,

$$\mathfrak{p} := \text{span}\{i\sigma^1 \otimes \sigma^2, iS^1 \otimes S^2\}, \tag{3.5}$$

define a Cartan decomposition of $\mathfrak{u}(d_1 d_2)$ as

$$\mathfrak{u}(d_1 d_2) = \mathfrak{k} \oplus \mathfrak{p}. \tag{3.6}$$

This decomposition is of type AI[9] as $\mathfrak{k}$ is conjugate to $\mathfrak{so}(d_1 d_2)$ and $\mathfrak{p}$ to $\mathfrak{so}(d_1 d_2)^{\perp}$. The rank of this decomposition is $d_1 d_2$. A basis of the maximal Abelian subalgebra $\mathfrak{a} \subseteq \mathfrak{p}$ is given by tensor products of elements of the orthogonal basis of the maximal Abelian subalgebras associated to the single subsystems, which are of dimensions d_1 and d_2, respectively. Denoting by D^1 the diagonal elements of the type S^1, and by D^2 those of the type S^2, $\mathfrak{a}$ is given by

$$\mathfrak{a} := \text{span}\{iD^1 \otimes D^2\}. \tag{3.7}$$

The associated Cartan factorization of $X \in U(d_1 d_2)$ is

$$X = K_1 A K_2, \tag{3.8}$$

according to the notation of the previous section.

Remark III.1: Only in the simplest case of the decomposition of $\mathfrak{su}(4)$ (i.e., $d_1=2$ and $d_2=2$), studied, for example, in Ref. 7, the decomposition (3.8) is a decomposition in local and nonlocal transformations. The local transformations are products of exponentials of matrices of the form $iH \otimes \mathbf{1}$ or $\mathbf{1} \otimes iH$, where $\mathbf{1}$ is the identity matrix of appropriate dimensions and H is a generic matrix in $i\mathfrak{u}(d_1)$ or $i\mathfrak{u}(d_2)$. Both local and nonlocal transformations are possibly present in the K_1 and K_2 factors as well as in the A factor. However, obtaining a decomposition in terms of tensor product matrices will allow us to identify exactly where the local and nonlocal transformations are present in the final transformation.

Remark III.2: We notice that, in general, only one nonlocal transformation, along with the set of the local transformations, is sufficient to obtain all the possible values for A in (3.8). To see this, notice that the factor A is the finite product of exponentials of elements of the form $i\alpha_{jk} E_{jj} \otimes E_{kk}$, with $j=1,\ldots,d_1$, $k=1,\ldots,d_2$, and α_{jk} real numbers. Since, for every l, E_{ll} is unitarily equivalent to E_{11}, the Hamiltonian $H=E_{11} \otimes E_{11}$, along with local transformations, is sufficient to generate any element of the form A. Notice that an alternative (universal) *nonlocal Hamiltonian* is given by an Ising interaction between two spins, which in our notation reads as $(E_{11}-E_{d_1 d_1}) \otimes (E_{11}-E_{d_2 d_2})$.

We now turn our attention to decomposing the elements K_1 and K_2 in (3.8). This will be obtained through a recursive procedure via iterate decompositions of $\mathfrak{so}(n)$.

IV. DECOMPOSITION OF UNITARY EVOLUTIONS IN $U(d_1d_2)$; RECURSIVE PROCEDURE

The Lie algebra $\mathfrak{k}$ defined in (3.4) is conjugate to $\mathfrak{so}(d_1d_2)$. We rewrite its definition below:

$$\mathfrak{k} := \mathrm{span}\{i\sigma^1 \otimes S^2, iS^1 \otimes \sigma^2\},$$

with σ^j, $j=1,2$, belonging to an orthogonal basis of $i\mathfrak{so}(d_j)$ and S^j, $j=1,2$, belonging to an orthogonal basis of $i\mathfrak{so}(d_j)^{\perp}$.

A special case arises when $d_1=d_2=1$, and only the matrix $\mathbf{0}$ belongs to the corresponding Lie algebra. This case is not of physical interest, as it would imply a one-dimensional quantum system. However, it may arise as the final step of the recursive procedure we are going to present. A special, nonphysical case is also $d_1=2$ and $d_2=1$, or vice versa. In this case, the Lie algebra $\mathfrak{k}$ contains only one element. Another special case is given by $d_1=d_2=2$. In this case, consider the Pauli matrices,

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.1}$$

and the 2×2 identity matrix $\mathbf{1}$. Then $\mathfrak{k}=\mathfrak{so}(4)$ is the direct sum of two commuting subalgebras, $\mathfrak{s}_1$ and $\mathfrak{s}_2$, each isomorphic to $\mathfrak{so}(3)$, and given by

$$\begin{aligned} \mathfrak{s}_1 &:= \mathrm{span}\{i\sigma_y \otimes \mathbf{1}, i\sigma_x \otimes \sigma_y, i\sigma_z \otimes \sigma_y\}, \\ \mathfrak{s}_2 &:= \mathrm{span}\{i\mathbf{1} \otimes \sigma_y, i\sigma_y \otimes \sigma_x, i\sigma_y \otimes \sigma_z\}. \end{aligned} \tag{4.2}$$

Therefore K_1 (and analogously K_2) in (3.8) can be written as the product

$$K_1 = F_1F_2 = F_2F_1, \tag{4.3}$$

with F_1 and F_2 in the Lie group corresponding to $\mathfrak{s}_1$ and $\mathfrak{s}_2$, respectively. A Cartan decomposition can be performed on $\mathfrak{s}_1$ (and analogously on $\mathfrak{s}_2$), which is an Euler decomposition as $\mathfrak{s}_1$ is isomorphic to $\mathfrak{so}(3)$, and allows us to express F_1 as

$$F_1 = L_1NL_2, \tag{4.4}$$

with $L_j=e^{\alpha_j i\sigma_y\otimes\mathbf{1}}$, $j=1,2$, for real parameters α_j, and $N=e^{\beta i\sigma_x\otimes\sigma_y}$ for a real parameter β. Notice that L_1 and L_2 are local transformations while N is nonlocal. The same can be done for F_2, moreover, the nonlocal transformation for F_2 can be obtained using a local similarity transformation from the one for F_1, or vice versa, so that for F_1 and F_2 we need only one nonlocal Hamiltonian.

Consider now the case where at least one between d_1 and d_2 is greater than 2. As it was done for the initial step in the previous section, we look for decompositions concerning the single subsystems to induce a decomposition on the total bipartite system. The elements of the type $i\sigma^1$ and $i\sigma^2$ are real, skew-symmetric, square matrices of dimensions d_1 and d_2, respectively. Let $d_1>2$ without loss of generality. On the Lie algebra of $d_1\times d_1$, skew-symmetric matrices (that is, matrices of the type σ^1), we perform a decomposition of the type BDI (see the previous section) by selecting two positive integers $r_1\geqslant q_1\geqslant 1$ so that $r_1+q_1=d_1$. In the resulting Cartan decomposition, $\mathfrak{so}(d_1)=\mathfrak{k}\oplus\mathfrak{p}$, the Lie algebra $\mathfrak{k}$ is spanned by block diagonal skew-symmetric matrices with the upper block of dimension r_1 and the lower block of dimension q_1. We denote this type of matrices by $i\sigma^{1,D}$ (where D stands for "diagonal"). The skew-symmetric matrices in the complement $\mathfrak{p}$ will be denoted by $i\sigma^{1,A}$ (where A stands for "antidiagonal"). We as well separate matrices of the type S^1 into block diagonal and block antidiagonal and denote them by $iS^{1,D}$ and $iS^{1,A}$, respectively. Analogously, we define a decomposition of type BDI on $\mathfrak{so}(d_2)$ introducing two positive integers $r_2\geqslant q_2\geqslant 1$, with $r_2+q_2=d_2$ and matrices of the type $i\sigma^{2,D}$, $i\sigma^{2,A}$, $iS^{2,D}$ and $iS^{2,A}$. In the special case where $d_2=2$, we can only choose $r_2=q_2=1$ and we do not, in fact, obtain a decomposition of $\mathfrak{so}(d_2)$ of the type BDI. However, we still formally decompose matrices of the

form σ^2 and S^2 in (block) diagonal and (block) antidiagonal components and notice that, in this case, the only matrix of the type $i\sigma^{2,D}$ and $iS^{2,A}$ is the 2×2 zero matrix.

These decompositions on the two subsystems induce a decomposition on the overall bipartite system. More precisely we decompose $\mathfrak{k}$ in (3.4) as follows:

$$\mathfrak{k} := \mathfrak{k}' \oplus \mathfrak{p}', \tag{4.5}$$

with

$$\begin{aligned}\mathfrak{k}' &= \mathrm{span}\{i\sigma^{1,D}\otimes S^{2,D}, iS^{1,D}\otimes\sigma^{2,D}, i\sigma^{1,A}\otimes S^{2,A}, iS^{1,A}\otimes\sigma^{2,A}\},\\ \mathfrak{p}' &= \mathrm{span}\{i\sigma^{1,A}\otimes S^{2,D}, i\sigma^{1,D}\otimes S^{2,A}, iS^{1,D}\otimes\sigma^{2,A}, iS^{1,A}\otimes\sigma^{2,D}\}.\end{aligned} \tag{4.6}$$

The following Theorem summarizes the features of this decomposition. It also gives, in its proof, a coordinate transformation to write the elements of the subalgebra $\mathfrak{k}'$ and its complement $\mathfrak{p}'$ in the standard form.

Theorem 1: *The decomposition of* $\mathfrak{k}$ *defined in* (4.5), (4.6) *is a Cartan decomposition*, *i.e.*,

$$[\mathfrak{k}',\mathfrak{k}']\subseteq\mathfrak{k}', \quad [\mathfrak{k}',\mathfrak{p}']\subseteq\mathfrak{p}', \quad [\mathfrak{p}',\mathfrak{p}']\subseteq\mathfrak{k}'.$$

As a decomposition of $\mathfrak{so}(d_1d_2)$, *it is a Cartan decomposition of type BDI with indices r and q satisfying* $r\geqslant q\geqslant 1$, $r+q=d_1d_2$, *and with*

$$r = r_1r_2 + q_1q_2, \quad q = r_1q_2 + q_1r_2. \tag{4.7}$$

Accordingly, *the dimension of the associated Cartan subalgebra* $\mathfrak{a}'\subseteq\mathfrak{p}'$ *is* $q=r_1q_2+q_1r_2$.

Proof: We explicitly exhibit a conjugacy that transforms elements of $\mathfrak{k}'$ into the form (2.10) and elements of $\mathfrak{p}'$ into the form (2.11). In particular, notice that the matrices $i\sigma^{1,D}\otimes S^{2,D}$, $iS^{1,D}\otimes\sigma^{2,D}$ have the form

$$k_1 := \begin{pmatrix} A_{r_1\times r_1}\otimes C_{r_2\times r_2} & 0 & 0 & 0\\ 0 & A_{r_1\times r_1}\otimes D_{q_2\times q_2} & 0 & 0\\ 0 & 0 & B_{q_1\times q_1}\otimes C_{r_2\times r_2} & 0\\ 0 & 0 & 0 & B_{q_1\times q_1}\otimes D_{q_2\times q_2}\end{pmatrix}, \tag{4.8}$$

while the matrices $i\sigma^{1,A}\otimes S^{2,A}$ and $iS^{1,A}\otimes\sigma^{2,A}$ are of the form

$$k_2 := \begin{pmatrix} 0 & 0 & 0 & F_{r_1\times q_1}\otimes G_{r_2\times q_2}\\ 0 & 0 & \pm F_{r_1\times q_1}\otimes G^T_{q_2\times r_2} & 0\\ 0 & \mp F^T_{r_1\times q_1}\otimes G_{r_2\times q_2} & 0 & 0\\ -F^T_{q_1\times r_1}\otimes G^T_{q_2\times r_2} & 0 & 0 & 0\end{pmatrix}. \tag{4.9}$$

A straightforward calculation shows that, defining

$$R := \begin{pmatrix} \mathbf{1}_{r_1r_2} & 0 & 0 & 0\\ 0 & 0 & 0 & \mathbf{1}_{q_1q_2}\\ 0 & \mathbf{1}_{r_1q_2} & 0 & 0\\ 0 & 0 & \mathbf{1}_{r_2q_1} & 0\end{pmatrix}, \tag{4.10}$$

the matrices

$$\tilde{k}_1 := Rk_1R^T, \quad \tilde{k}_2 := Rk_2R^T, \tag{4.11}$$

have the form given in (2.10), where the upper block has dimension $r=r_1r_2+q_1q_2$ and the lower block has dimension $q=r_1q_2+q_1r_2$. Analogously one shows that the conjugacy defined in (4.10) transforms elements in $\mathfrak{p}'$ into elements of the form p in (2.11). □

In view of the decomposition (4.5), any element K_1 (and analogously for K_2) in (3.8) can be written as

$$K_1 = K_1' A' K_2', \tag{4.12}$$

where K_1' and K_2' belong to the Lie group associated with the Lie algebra $\mathfrak{k}'$, conjugate to $\mathfrak{so}(r) \oplus \mathfrak{so}(q)$, and are to be further factorized. The matrix A' belongs to the Abelian Lie subgroup associated to the maximal Abelian subalgebra $\mathfrak{a}' \in \mathfrak{p}'$. In the following proposition we find an orthogonal basis for such a Cartan subalgebra expressing it in terms of tensor products. [An alternative procedure is to transform the Lie algebra $\mathfrak{k}'$ according to the change of coordinates (4.10) and to find the Cartan subalgebra in the standard basis.]

Proposition IV.1: The $(r_1+q_1)q_2$ matrices

$$N_{jk} := E_{jj} \otimes \Delta_{k,r_2+k}, \quad j = 1, \ldots, r_1 + q_1, \quad k = 1, \ldots, q_2, \tag{4.13}$$

along with the $(r_2-q_2)q_1$ matrices

$$M_{fl} := \Delta_{f,r_1+f} \otimes E_{ll}, \quad l = q_2 + 1, \ldots, r_2, \quad f = 1, \ldots, q_1, \tag{4.14}$$

span a Cartan subalgebra $\mathfrak{a}' \in \mathfrak{p}'$.

Proof: The dimension of the vector space spanned by the matrices in (4.13) and (4.14) is, in fact, $(r_1+q_1)q_2+(r_2-q_2)q_1=r_1q_2+q_1r_2$. Therefore, we only have to verify that matrices of the type (4.13) and (4.14) commute with each other. The commutator between two matrices of the type (4.13) always vanishes. Analogously, matrices of the type (4.14) commute with each other. The Lie bracket of matrices of the type (4.13) and (4.14) vanishes too, since the products of matrices Δ_{k,r_2+k} and E_{ll} in the second factors are always zero.

Remark IV.2: It follows from Proposition IV.1 that the element A' in (4.12) is the exponential of a linear combination of matrices (4.13) and (4.14) or (equivalently) the product of exponentials of matrices proportional to these. The resulting unitary transformations may be entangling or local. However, since all the matrices of the form E_{jj} are unitarily equivalent to each other and the matrices of the type Δ_{kl} are also unitarily equivalent to each other, only one (entangling) Hamiltonian of the type (4.13), one of the type (4.14) along with local operations are sufficient (and necessary) to generate all the possible factors A' in (4.12).

Remark IV.3: A further reduction of the nonlocal Hamiltonians to be used is obtained by noticing that all the transformations in Remark III.2 and in Proposition IV.1 can be obtained with only one Ising Hamiltonian and local transformations. Therefore only one nonlocal Hamiltonian is needed to implement all of these transformations.

We now further factorize the elements K_1' and K_2' in (4.12) using, once again, a Cartan decomposition of the Lie algebra $\mathfrak{k}'$ isomorphic to $\mathfrak{so}(r) \oplus \mathfrak{so}(q)$, with r and q defined in (4.7). In particular, we decompose $\mathfrak{k}'$ as follows:

$$\mathfrak{k}' = \mathfrak{k}'' \oplus \mathfrak{p}'', \tag{4.15}$$

with

$$\begin{aligned} \mathfrak{k}'' &= \mathrm{span}\{i\sigma^{1,D} \oplus S^{2,D}, S^{1,D} \oplus i\sigma^{2,D}\}, \\ \mathfrak{p}'' &= \mathrm{span}\{i\sigma^{1,A} \otimes S^{2,A}, S^{1,A} \otimes i\sigma^{2,A}\}. \end{aligned} \tag{4.16}$$

The matrices in $\mathfrak{k}''$ are block diagonal matrices and $\mathfrak{k}''$ is

$$\mathfrak{k}'' = \mathfrak{so}(r_1 r_2) \oplus \mathfrak{so}(r_1 q_2) \oplus \mathfrak{so}(q_1 r_2) \oplus \mathfrak{so}(q_1 q_2), \tag{4.17}$$

where each term refers to a block on the diagonal. For example, the first block corresponding to $\mathfrak{so}(r_1 r_2)$ contains matrices obtained as tensor products $i\sigma^{1,D} \otimes S^{2,D}$ or $S^{1,D} \otimes \sigma^{2,D}$, where all matrices involved have the second block equal to zero. This corresponds to two decompositions of the type BDI: one on $\mathfrak{so}(r)$ and the other on $\mathfrak{so}(q)$. The Cartan subalgebra in $\mathfrak{p}''$ is the direct sum of the two Cartan subalgebras of the two decompositions. It has dimension $q_1 q_2 + \min\{r_1 q_2, q_1 r_2\}$. The following proposition explains how to find a basis of this Cartan subalgebra as tensor product matrices. [Alternatively, one can construct a basis for this Cartan subalgebra working in the standard representation using the conjugacy given in (4.10).]

Proposition IV.4: A Cartan subalgebra of the decomposition (4.15), (4.16) is spanned by the $q_1 q_2$ matrices,

$$N_{jm,ln} := \begin{pmatrix} 0 & E_{jl} \\ -E_{jl}^T & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & E_{mn} \\ E_{mn}^T & 0 \end{pmatrix} + \begin{pmatrix} 0 & E_{jl} \\ E_{jl}^T & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & E_{mn} \\ -E_{mn}^T & 0, \end{pmatrix} \tag{4.18}$$

with $1 \leqslant j \leqslant r_1$, $1 \leqslant l \leqslant q_1$ and $1 \leqslant m \leqslant r_2$, $1 \leqslant n \leqslant q_2$ satisfying

$$(j-1) r_2 + m = s, \quad (l-1) q_2 + n = s, \tag{4.19}$$

with $s = 1, \ldots, q_1 q_2$, along with matrices

$$M_{jm,ln} := \begin{pmatrix} 0 & E_{jl} \\ -E_{jl}^T & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & E_{mn} \\ E_{mn}^T & 0 \end{pmatrix} - \begin{pmatrix} 0 & E_{jl} \\ E_{jl}^T & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & E_{mn} \\ -E_{mn}^T & 0 \end{pmatrix}, \tag{4.20}$$

with $1 \leqslant j \leqslant r_1$, $1 \leqslant l \leqslant q_1$ and $1 \leqslant m \leqslant r_2$, $1 \leqslant n \leqslant q_2$ satisfying

$$(j-1) q_2 + n = s, \quad (l-1) r_2 + m = s, \tag{4.21}$$

with $s = 1, \ldots, \min\{r_1 q_2, q_1 r_2\}$.

Remark IV.5: For all s, there is a unique pair (l,n) so that the second relation in (4.19) is verified. There is some freedom in choosing the pairs (j,m) satisfying the first relation in (4.19). However, for every value of s, and therefore of l and n, one is allowed to choose a *unique* pair (j,m). The notation in (4.20) and (4.21) has an analogous meaning.

Proof: Matrices of the form (4.18) commute with matrices of the form (4.20), since these matrices form Cartan subalgebras associated to decompositions of $\mathfrak{so}(r)$ and $\mathfrak{so}(q)$, respectively. To show that matrices of type (4.18) commute, one verifies that the commutators of two matrices corresponding to indices $(j_1 m_1, l_1 n_1)$ and $(j_2 m_2, l_2 n_2)$ vanish. In fact, all the blocks of such matrices are zero except for the $1,1$ and $2,2$ blocks, which, from a direct calculation, turn out to be equal to

$$4(E_{j_2 j_1} \delta_{l_1 l_2} \otimes E_{m_2 m_1} \delta_{n_1 n_2} - E_{j_1 j_2} \delta_{l_1 l_2} \otimes E_{m_1 m_2} \delta_{n_1 n_2}), \tag{4.22}$$

and

$$4(E_{l_2 l_1} \delta_{j_1 j_2} \otimes E_{n_2 n_1} \delta_{m_1 m_2} - E_{l_1 l_2} \delta_{j_1 j_2} \otimes E_{n_1 n_2} \delta_{m_1 m_2}), \tag{4.23}$$

respectively. However these are also zero if $n_1 \neq n_2$ and/or $l_1 \neq l_2$ as well as in the case $l_1 = l_2$, $n_1 = n_2$ (and therefore $j_1 = j_2$, $m_1 = m_2$; see Remark IV.5). A perfectly analogous argument holds in the case of commutators of matrices of the form (4.20). □

Remark IV.6: Notice that all the Hamiltonians (4.18) are locally unitarily equivalent to each other. The same is true for the Hamiltonians (4.20). Therefore only two more entangling Hamiltonians are needed.

At this point we are left with the Lie algebra $\mathfrak{so}(p_1 p_1) \oplus \mathfrak{so}(q_1 q_2) \oplus \mathfrak{so}(p_1 q_2) \oplus \mathfrak{so}(p_2 q_1)$. The construction proceeds recursively by decomposing each one of the four component Lie algebras

and so on, until one finds one of the Lie algebras $\mathfrak{so}(1)$ (which we define as the element zero), $\mathfrak{so}(2)$ (which consists of a single element), $\mathfrak{so}(3)$, or $\mathfrak{so}(4)$ (which are treated as it was explained at the beginning of the procedure).

V. DISCUSSION AND AN EXAMPLE

In order to illustrate the Lie group decomposition described in the previous sections, we consider the *generalized SWAP* operator X_{sw} acting on three qubits and rotating their states in a cyclic fashion. Its action is defined in the tensor product basis as

$$X_{\mathrm{sw}}:|i\rangle_1 \otimes |j\rangle_2 \otimes |k\rangle_3 \rightarrow |k\rangle_1 \otimes |i\rangle_2 \otimes |j\rangle_3, \tag{5.1}$$

where $i,j,k=0,1$ and $\{|0\rangle,|1\rangle\}_{1,2,3}$ are orthonormal bases for the Hilbert spaces of the three systems.

This operator is relevant in quantum information and computation since it enables us to switch the quantum states of different systems. For example, assume that one is interested in the state of the third system, but only the first system is accessible and can be controlled; then the application of the generalized SWAP operator will enable to transfer the state of the third system to the first system. As local operations alone clearly cannot implement the generalized SWAP, this has to involve some degree of entanglement among the various subsystems. We consider an hypothetical situation where it is possible to create an interaction between the first qubit and the other two as a whole although it is difficult to create interactions with the single qubits 2 and 3. This justifies to consider the total Hilbert space as the tensor product of a two-dimensional subspace with a four-dimensional one (that is, $d_1=2$ and $d_2=4$). Therefore $X_{\mathrm{sw}} \in U(8)$ will be decomposed accordingly. (We believe that extensions of the procedure presented here to multipartite systems are possible at the price of an increased notational complexity.)

In the specified basis, with standard ordering, the matrix representation of this operator is given by

$$X_{\mathrm{sw}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.2}$$

This transformation belongs to $SO(8)$, therefore the first step of the decomposition of $U(8)$ is trivial: $K_1=X_{sw}$ and $A=K_2=\mathbf{1}$.

For the first step of the recursive part of the procedure, we choose $r_1=q_1=1$ and $r_2=q_2=2$. We find it convenient to work in the basis of the Hilbert space such that $\mathfrak{k}'=\mathfrak{so}(2)\oplus\mathfrak{so}(4)$, obtained by performing the change of basis $R|ijk\rangle \rightarrow |ijk\rangle'$, with R given in (4.10), which, in this particular case ($r_1=q_1=1$, $r_2=q_2=2$), takes the form

$$R = \begin{pmatrix} \mathbf{1}_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1}_2 \\ 0 & \mathbf{1}_2 & 0 & 0 \\ 0 & 0 & \mathbf{1}_2 & 0 \end{pmatrix}. \tag{5.3}$$

In these coordinates, the SWAP operator is written as $\tilde{X}_{\mathrm{sw}}=RX_{\mathrm{sw}}R^T$, that is

$$\widetilde{X}_{\mathrm{sw}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}. \tag{5.4}$$

The elements of the Cartan subalgebra $\mathfrak{a}'$ (defined in Proposition IV.1), which in this case are only of the form (4.13), are transformed by R into elements of the form

$$\widetilde{a}' = \begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix}.$$

The computational problem is to find two 4×4 diagonal matrices, D_1 and D_2, with

$$\widetilde{A}' = e^{\widetilde{a}'} = \begin{pmatrix} D_1 & D_2 \\ -D_2 & D_1 \end{pmatrix},$$

$\widetilde{A}' \in SO(8)$, and matrices $K_{ij} \in SO(4)$, $i,j=1,2$, such that

$$\widetilde{K}_1' = \begin{pmatrix} K_{11} & 0 \\ 0 & K_{12} \end{pmatrix}, \quad \widetilde{K}_2' = \begin{pmatrix} K_{21} & 0 \\ 0 & K_{22} \end{pmatrix} \tag{5.5}$$

and $\widetilde{X}_{\mathrm{sw}} = \widetilde{K}_1' \widetilde{A}' \widetilde{K}_2'$. To perform this task we propose an algorithm that uses ideas similar to the ones for other Cartan decompositions (cf., e.g., Ref. 5 and references therein). We illustrate this algorithm for the dimensions of our problem but generalizations to other dimensions are obvious. Let us write $\widetilde{X}_{\mathrm{sw}}$ with 4×4 blocks $\widetilde{X}_{ij}$, $i,j=1,2$, as

$$\widetilde{X}_{\mathrm{sw}} = \begin{pmatrix} \widetilde{X}_{11} & \widetilde{X}_{12} \\ \widetilde{X}_{21} & \widetilde{X}_{22} \end{pmatrix}. \tag{5.6}$$

Equation (5.5) is equivalent to the four matrix equations:

$$\widetilde{X}_{11} = K_{11} D_1 K_{21}, \tag{5.7}$$

$$\widetilde{X}_{12} = K_{11} D_2 K_{22}, \tag{5.8}$$

$$\widetilde{X}_{21} = -K_{12} D_2 K_{21}, \tag{5.9}$$

$$\widetilde{X}_{22} = K_{12} D_1 K_{22}. \tag{5.10}$$

From the first one, we obtain

$$\widetilde{X}_{11} \widetilde{X}_{11}^T K_{11} = K_{11} D_1^2, \tag{5.11}$$

which is an eigenvalue equation as D_1^2 is diagonal. In the generic case, when all the eigenvalues of $\widetilde{X}_{11}\widetilde{X}_{11}^T$ are different, Eq. (5.11) determines K_{11} and D_1 up to the right product by a sign matrix [and the fact that $\det(K_{11})=1$]. Moreover, D_1 gives D_2 up to a sign matrix from the requirement that $D_1^2 + D_2^2 = \mathbf{1}_4$. Using K_{11} and D_2 in (5.8), we obtain K_{22} up to a sign matrix. Plugging K_{22} in (5.10),

we get K_{12} up to a sign matrix and from (5.9) we find K_{21}. Finally, we adjust the sign matrices to make (5.7)–(5.10) consistently verified. In the case where $\tilde{X}_{11}\tilde{X}_{11}^T$ has multiple eigenvalues, there is more freedom in the choice of K_{11} at the initial step, but then one proceeds in the same way and determines the other matrices up to some degree of freedom. At the end of the procedure, these degrees of freedom are exploited to make (5.7)–(5.10) jointly satisfied.

Using this procedure, we have found, for our example,

$$K_{11}=\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&-1\end{pmatrix},\quad K_{12}=-\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},$$

$$K_{21}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad K_{22}=\begin{pmatrix}0&-1&0&0\\0&0&0&1\\1&0&0&0\\0&0&1&0\end{pmatrix},\tag{5.12}$$

$$D_1=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-1\end{pmatrix},\quad D_2=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix}.$$

We can repeat the same procedure as above to further factorize K_{11}, K_{12}, K_{21}, K_{22}, and to obtain $\tilde{K}_1'=\tilde{K}_1''\tilde{A}_1''\tilde{K}_2''$ and $\tilde{K}_2'=\tilde{K}_3''\tilde{A}_2''\tilde{K}_4''$. We finally get the decomposition of $\tilde{X}_{\mathrm{sw}}$,

$$\tilde{X}_{\mathrm{sw}}=\tilde{K}_1''\tilde{A}_1''\tilde{K}_2''\tilde{A}'\tilde{K}_3''\tilde{A}_2''\tilde{K}_4'',\tag{5.13}$$

where

$$\tilde{A}_1''=\mathrm{diag}\left\{\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&-1&0&0\end{pmatrix},\begin{pmatrix}0&0&-1&0\\0&0&0&1\\1&0&0&0\\0&-1&0&0\end{pmatrix}\right\},$$

$$\tilde{A}_2''=\mathrm{diag}\left\{\mathbf{1}_4,\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&-1&0&0\end{pmatrix}\right\},$$

$$\begin{aligned}\tilde{K}_1''&=\mathrm{diag}\left\{\mathbf{1}_2,\begin{pmatrix}0&-1\\1&0\end{pmatrix},\begin{pmatrix}0&-1\\1&0\end{pmatrix},\begin{pmatrix}0&1\\-1&0\end{pmatrix}\right\},\\ \tilde{K}_2''&=\mathrm{diag}\left\{\mathbf{1}_2,\begin{pmatrix}0&-1\\1&0\end{pmatrix},\mathbf{1}_2,\mathbf{1}_2\right\},\\ \tilde{K}_3''&=\mathrm{diag}\left\{\mathbf{1}_2,\mathbf{1}_2,\mathbf{1}_2,\begin{pmatrix}0&-1\\1&0\end{pmatrix}\right\},\end{aligned}\tag{5.14}$$

$$\tilde{K}_4'' = \mathrm{diag}\left\{\mathbf{1}_2, \mathbf{1}_2, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \mathbf{1}_2\right\}.$$

We now use the transformation R in (5.3) to write X_{sw} in the original coordinates as

$$X_{\mathrm{sw}} = K_1'' A_1'' K_2'' A' K_3'' A_2'' K_4'', \tag{5.15}$$

with $A' = R^T \tilde{A}' R$, $A'' = R^T \tilde{A}'' R$, and $K_j'' = R^T \tilde{K}_j'' R$, $j = 1, 2$. We can write all the factors in (5.15) as exponentials of appropriate matrices in the tensor product basis:

$$\begin{gathered} A' = e^{a'}, \quad A_k'' = e^{a_k''}, \quad k = 1,2, \\ K_j'' = e^{k_j''}, \quad j = 1, \ldots, 4 \end{gathered} \tag{5.16}$$

where

$$a' = \frac{\pi}{2}(E_{11} \otimes \Delta_{24}) + \frac{3\pi}{2}(E_{22} \otimes \Delta_{13}) + \pi(E_{22} \otimes \Delta_{24}),$$

$$a_1'' = \frac{\pi}{4}(\Delta_{12} \otimes \Omega_{24} + \Omega_{12} \otimes \Delta_{24}) + \frac{\pi}{4}(\Delta_{12} \otimes \Omega_{24} - \Omega_{12} \otimes \Delta_{24}) + \frac{3\pi}{4}(\Delta_{12} \otimes \Omega_{13} - \Omega_{12} \otimes \Delta_{13}),$$

$$a_2'' = \frac{\pi}{4}(\Delta_{12} \otimes \Omega_{24} - \Omega_{12} \otimes \Delta_{24}),$$

$$k_1'' = \frac{3\pi}{2}(E_{22} \otimes \Delta_{34}) + \frac{\pi}{2}(E_{22} \otimes \Delta_{12}) + \frac{3\pi}{2}(E_{11} \otimes \Delta_{34}), \tag{5.17}$$

$$k_2'' = \frac{3\pi}{2}(E_{22} \otimes \Delta_{34}),$$

$$k_3'' = \frac{3\pi}{2}(E_{22} \otimes \Delta_{12}),$$

$$k_4'' = \frac{3\pi}{2}(E_{11} \otimes \Delta_{34}).$$

It is interesting to observe what number of nonlocal transformations are needed to perform the given task if we are able to perform any local transformation on the two subsystems. Notice that we are considering the system as a bipartite system of a two level system with a four level system. In essence, we assume that we have to decide appropriate interactions between the two subsystems (two and four dimensional), which along with local transformations will allow us to perform the given task. By grouping the matrices that are equivalent through local similarity transformations it is clear that the Hamiltonians

$$H_1 := E_{11} \otimes \Delta_{34},$$

$$H_2 := \Delta_{12} \otimes \Omega_{24} + \Omega_{12} \otimes \Delta_{24}, \tag{5.18}$$

$$H_3 := \Delta_{12} \otimes \Omega_{24} - \Omega_{12} \otimes \Delta_{24},$$

are sufficient. [In view of (5.17), one can replace H_2 with $\tilde{H}_2 := \Delta_{12} \otimes \Omega_{24}$.]

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Finitely many Dirac-delta interactions on Riemannian manifolds

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This work is intended as an attempt to study the nonperturbative renormalization of bound state problem of finitely many Dirac-delta interactions on Riemannian manifolds, $\mathbb{S}^2$, $\mathbb{H}^2$, and $\mathbb{H}^3$. We formulate the problem in terms of a finite dimensional matrix, called the characteristic matrix Φ. The bound state energies can be found from the characteristic equation $\Phi(-\nu^2)A=0$. The characteristic matrix can be found after a regularization and renormalization by using a sharp cut-off in the eigenvalue spectrum of the Laplacian, as it is done in the flat space, or using the heat kernel method. These two approaches are equivalent in the case of compact manifolds. The heat kernel method has a general advantage to find lower bounds on the spectrum even for compact manifolds as shown in the case of $\mathbb{S}^2$. The heat kernels for $\mathbb{H}^2$ and $\mathbb{H}^3$ are known explicitly, thus we can calculate the characteristic matrix Φ. Using the result, we give lower bound estimates of the discrete spectrum. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2259581]

I. INTRODUCTION

It is well known that the exactly solvable Dirac-delta interactions on the plane and three-dimensional Euclidean space in quantum mechanics give rise to some unphysical results for physical observables, i.e., bound state energy and scattering cross section are infinite and the problem is said to be ultraviolet divergent. Nevertheless, there is a systematic way to dispense with these infinities by means of a so-called regularization and renormalization, which is first introduced in quantum field theory for the same reason. This problem constitutes an analytical example of regularization and renormalization in quantum mechanics so that it helps us to understand and deal with it in a more elementary context rather than field theory and it has been studied in the literature from several point of views.[1–13] Moreover, a single point interaction in two-dimensional flat space is an instructive example of dimensional transmutation in nonrelativistic quantum mechanics.[3,14–16] That is, the original Hamiltonian does not contain any intrinsic energy scale due to the dimensionless coupling constant in natural units. Nevertheless, a new parameter μ^2, which specifies the bound state energy, must be introduced after the renormalization procedure which then fixes the energy scale of the system. (A detailed discussion of dimensional transmutation in nonrelativistic quantum mechanics is given in a relatively recent article.[16])

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In this study, we consider a bound state problem in which a nonrelativistic particle living in a Riemannian manifold (in particular $\mathbb{S}^2$, $\mathbb{H}^2$, and $\mathbb{H}^3$) interacts with finitely many Dirac-delta interactions. Similar to the corresponding bound state problem on $\mathbb{R}^2$ and $\mathbb{R}^3$, we encounter divergences in this case as well. The main purpose of this paper is to show how to nonperturbatively regularize and renormalize the problem by means of heat kernel (even in the case where we do not have an explicit expression for it). After the renormalization, we estimate a lower bound for the ground state energy for each particular Riemannian manifold. This problem on two-dimensional Riemannian manifolds, such as $\mathbb{S}^2$ and $\mathbb{H}^2$, also displays a kind of dimensional transmutation,[16] where new energy scales different from the intrinsic energy scales of the system appear after the renormalization. We will briefly discuss it in Secs. III and IV B.

Many body version of this problem on $\mathbb{R}^2$ and $\mathbb{R}^3$ is known as the formal nonrelativistic limit of the $\lambda\phi^4$ scalar field theory in $(2+1)$ and $(3+1)$ dimensions. All these are extensively discussed first by Hoppe[31] and later from a new perspective in Ref. 17. Our primary motivation here is coming from the question of how the renormalization method for the singular interactions in quantum mechanics would be performed on Riemannian manifolds, hoping that this may help us to understand the problem in the realm of quantum field theory. However, we shall postpone the discussion of the many body extension of it for future work and study first the one-particle Schrödinger problem.

The paper is organized as follows. In Sec. II, we first define the bound state problem on compact and connected Riemannian manifolds and reformulate the problem in terms of a finite dimensional matrix Φ, which we will call the characteristic matrix.[17] Then, we emphasize the relation of the characteristic matrix with the corresponding spectral functions, resolvent and heat kernel. This allows us to reformulate the renormalization in terms of heat kernel. After that we continue to the discussion in the following sections by working out concrete examples. In Sec. III, we consider the delta interaction problem on $\mathbb{S}^2$ as an example for compact and connected manifolds. Considering the properties of the operator Φ and using some properties and upper bound estimates of the heat kernel, Geršgorin theorem allows us to estimate a lower bound for the ground state energy of the system. In Sec. IV, we apply a similar methodology, developed in the section of heat kernel method for $\mathbb{S}^2$, to the noncompact manifolds, such as $\mathbb{H}^2$ and $\mathbb{H}^3$, and show that the methods developed for compact manifolds work for some particular noncompact manifolds as well. Therefore, we renormalize the problem on hyperbolic spaces and give estimates on the ground state energy of each system.

II. RENORMALIZATION OF FINITELY MANY DIRAC-DELTA INTERACTIONS ON COMPACT AND CONNECTED RIEMANNIAN MANIFOLDS (M,g)

The canonical quantization on nontrivial manifolds is known to have some ambiguities in quantum mechanics. For the path integral approach to the quantum system, the ambiguity in the canonical formalism is replaced by the undetermined parameter λ and it can take various possible values.[18] We remove this term for simplicity in all our examples, in which the curvature term is constant and it corresponds to an overall shift in energy levels so that we can safely set λ to be zero.

Now, we consider a nonrelativistic point particle living on a Riemannian manifold M interacting with a finite number of delta interactions located on the manifold and study bound states of the problem. We first investigate the delta interactions on a compact and connected Riemannian manifold (M,g) without boundary, of dimension $D=2,3$ with the Riemannian metric g. The kinetic energy operator on Riemannian manifold (M,g) is just the Laplace-Beltrami operator or simply Laplacian, which is defined, in local coordinates $x\equiv(x^1,\ldots,x^D)$ for a neighborhood in the manifold, as follows:

$$\Delta_g = -\frac{1}{\sqrt{\det g}} \sum_{\alpha,\beta=1}^{D} \frac{\partial}{\partial x^\alpha}\left(g^{\alpha\beta}\sqrt{\det g}\frac{\partial}{\partial x^\beta}\right), \tag{1}$$

where $g_{\alpha\beta}$ is the metric tensor and $g=(g_{\alpha\beta})$. We shall usually denote the Laplacian as Δ_g to specify which metric structure on Riemannian manifold it is associated with.

The spectral theorem[19,20] states that the eigenvalue problem $\Delta_g\phi_l=\lambda_l\phi_l$ on a compact and connected Riemannian manifold (M,g) has a complete orthonormal system of C^∞ eigenfunctions $\phi_0,\phi_1,\ldots$ in $L^2(M)$ and the spectrum $\mathrm{Spec}\,(\Delta_g)\equiv\mathrm{Spec}(M,g)=\{\lambda_l\}=\{0=\lambda_0<\lambda_1\leqslant\lambda_2\leqslant\ldots\}$, with λ_l tending to infinity as $l\to\infty$. As a corollary of this theorem, the Laplacian on (M,g) provides us with all the tools of Fourier analysis, so that we can expand any "sufficiently good" function $\psi(x)$ on M in terms of the complete orthonormal eigenfunctions $\phi_l(x)$,

$$\psi(x) = \sum_{l\geqslant 0} C_l\phi_l(x), \tag{2}$$

with the normalization

$$\int_M \phi_l(x)\phi_{l'}^*(x)\sqrt{\det g}\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^D = \delta_{ll'},$$

where C_l's are expansion coefficients. Note that extra labels in the eigenfunction expansion must be taken into account if the problem admits degeneracy. Delta functions on M can also assumed to be represented by these eigenfunctions

$$\delta^D(x-a_i) = \sum_{l\geqslant 0}\phi_l(x)\phi_l^*(a_i), \tag{3}$$

with $a_i\in M$ and $\delta^D(x-a_i)$ being the D-dimensional normalized delta function at point a_i,

$$\int_M \delta^D(x-a_i)\sqrt{\det g}\,\mathrm{d}x^1\wedge\cdots\wedge\mathrm{d}x^D = 1.$$

A typical Hamiltonian operator in quantum theory consists of a kinetic term, the Laplacian Δ_g with the factor $\hbar^2/2m$, and a potential function of position, attractive delta interactions in our problem. The time-independent Schrödinger equation on M for the bound states of a particle under the influence of N attractive delta interactions reads

$$\left[\frac{\hbar^2}{2m}\Delta_g - \sum_{i=1}^{N} g_i\delta^D(x-a_i)\right]\psi(x) = -\nu^2\psi(x), \tag{4}$$

where $g_i\in\mathbb{R}^+$ is the strength of the delta interaction at a_i and $-\nu^2$ is the bound state energy of the system. If we substitute (2) and (3) into the Schrödinger equation, it yields

$$\sum_{l\geqslant 0}\left[\frac{\hbar^2}{2m}\lambda_l C_l - \sum_{i=1}^{N} A_i g_i\phi_l^*(a_i) + \nu^2 C_l\right]\phi_l(x) = 0,$$

where $A_i\equiv\psi(a_i)$ for simplicity of notation. The fact that ϕ_l's form a complete orthonormal system allows us to write C_l in terms of them:

$$C_l = \frac{1}{\dfrac{\hbar^2}{2m}\lambda_l+\nu^2}\sum_{i=1}^{N} A_i g_i\phi_l^*(a_i). \tag{5}$$

Substituting (5) into the definition of A_i,

$$A_i = \sum_{j=1}^{N} A_j g_j \sum_{l \geqslant 0} \frac{\phi_l(a_i)\phi_l^*(a_j)}{\frac{\hbar^2}{2m}\lambda_l + \nu^2},$$

and grouping the A_i terms we find

$$\left[g_i^{-1} - \sum_{l \geqslant 0} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \nu^2} \right] A_i - \sum_{\substack{j=1 \\ j \neq i}}^{N} \left[\frac{g_j}{g_i} \sum_{l \geqslant 0} \frac{\phi_l(a_i)\phi_l^*(a_j)}{\frac{\hbar^2}{2m}\lambda_l + \nu^2} \right] A_j = 0.$$

The observation that the preceding equation is linear in A_i permits us to write it naturally as a matrix equation

$$\Phi(-\nu^2)A = 0, \tag{6}$$

where $\Phi(-\nu^2)$ is called the characteristic matrix and defined as

$$\Phi_{ij}(-\nu^2) = \begin{cases} g_i^{-1} - \sum_{l \geqslant 0} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \nu^2} & \text{if } i = j \\ -\frac{g_j}{g_i} \sum_{l \geqslant 0} \frac{\phi_l(a_i)\phi_l^*(a_j)}{\frac{\hbar^2}{2m}\lambda_l + \nu^2} & \text{if } i \neq j. \end{cases} \tag{7}$$

As we shall see in the following the resolvent is intimately related to it and this allows us to state that the equation $\det \Phi(-\nu^2)=0$ gives the bound state energies of our problem. In other words, this equation is considered to be the determining equation of the ground state energy. Unfortunately, this nontrivial eigenvalue problem cannot be solved analytically, that is, we cannot obtain an exact expression for the bound state energy for arbitrary N since the characteristic matrix depends *nonlinearly* on the bound state energy. Indeed, the problem is even worse than that, because we do not have finite expressions in the matrix elements of $\Phi_{ij}(-\nu^2)$. Fortunately, there exists a way to redefine the problem so that the physical observables yield finite values with the help of regularization and renormalization. Before introducing this procedure for our problem, it would be good to review first the problem in flat spaces. The infinite sums in the characteristic matrix on $\mathbb{R}^2$ or $\mathbb{R}^3$ are then replaced by integrals. The idea in that case is to take Fourier transform of the wave function

$$\psi(x) = \int \tilde{\psi}(k) e^{ik.x} \frac{\mathrm{d}^D k}{(2\pi)^D},$$

and substitute into the Schrödinger equation. Then we find that the diagonal part of the characteristic matrix is

$$\frac{1}{g_i} - \frac{1}{(2\pi)^D} \int \frac{\mathrm{d}^D k}{k^2 + \nu^2},$$

where $D=2,3$. This integral does not converge as it stands. The well-known method to remove the divergence is to put a cut-off Λ to the integral's upper limit and consider the equation as a determining equation of bound state energy for a given coupling constant g. If this regularization is performed, we realize that as the cut-off goes to infinity, ground state energy becomes divergent. In order to get a physically acceptable result, one assumes that the coupling constant depends on this cut-off and performs the limit $\Lambda \to \infty$ in such a way that bound state energy remains finite. These infinities should be removed properly since all the physical observables are measured experimentally as finite quantities. The cut-off dependence of the coupling constant is chosen as

$$\frac{1}{g_i(\Lambda)} = \frac{1}{(2\pi)^D}\int_{|k|<\Lambda} \frac{\mathrm{d}^D k}{k^2+\mu_i^2}. \tag{8}$$

The determination of this coupling constant is called renormalization. Now, we follow the same idea to remove the divergence from our problem. By using Weyl's asymptotic formula,[21] one expects that the diagonal term

$$\sum_{l\geqslant 0} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \nu^2}$$

in the above-noted matrix does not converge and this will be explicitly seen for a particular manifold $\mathbb{S}^2$. For a general compact manifold, we introduce cut-off to the upper bound of the infinite sum and choose the coupling constant as

$$g_i^{-1}(\Lambda) = \sum_{l=0}^{\Lambda} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \mu_i^2}, \tag{9}$$

where $-\mu_i^2$ is the measured binding energy to a single delta interaction. Then, we take the limit $\Lambda\to\infty$,

$$\lim_{\Lambda\to\infty}\left[\sum_{l=0}^{\Lambda} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \mu_i^2} - \sum_{l=0}^{\Lambda} \frac{|\phi_l(a_i)|^2}{\frac{\hbar^2}{2m}\lambda_l + \nu^2}\right], \tag{10}$$

and this should give us a finite result in two and three dimensions. Hence, the divergence has been removed and bound state energy becomes finite. A rigorous proof of this is not trivial, so we will stay at a heuristic level and study special cases only.

As we will show in Sec. II, the heat kernel is intimately related to the characteristic matrix Φ and this relation helps us to see easily which part of the matrix is divergent or convergent and then how to renormalize the problem nonperturbatively. Furthermore, heat kernel is especially very helpful to remove the divergences for our problem on noncompact manifolds, as we shall discuss in Sec. IV. We will see that the above-noted method can easily be extended to find the renormalized resolvent of the singular Hamiltonian.

A. The relation of matrix Φ with heat kernel and resolvent

The resolvent (or Green's function) and heat kernel play a very essential role in establishing the connection between spectral properties of the operator and corresponding geometrical notions. Up to now, we have been dealing with a matrix Φ, and do not refer to resolvent and heat kernel. In order to see the relation between the matrix Φ and heat kernel we consider the separable Hamiltonians $H=H_0-\Sigma_{i=1}^N g_i|f_i\rangle\langle f_i|$, where $|f_i\rangle$ is a particular Dirac ket. We work out the resolvent formula of H in terms of H_0 and assume that the two Dirac kets $|\psi\rangle$ and $|\chi\rangle$ are related in such a way that the equality $(H-z)|\psi\rangle=|\chi\rangle$ is satisfied. Then, we have

$$\left[H_0 - z - \sum_{j=1}^{N} g_j|f_j\rangle\langle f_j|\right]|\psi\rangle = |\chi\rangle, \tag{11}$$

assuming complex number $z\notin \mathrm{Spec}(H_0)$. Acting the operator $(H_0-z)^{-1}$ on both sides and projecting it onto $\langle f_i|$, we obtain

$$\sum_{j=1}^{N} \Phi_{ij}(z)\langle f_j|\psi\rangle = g_i^{-1}\langle f_i|(H_0-z)^{-1}|\chi\rangle,$$

where we define a matrix $\Phi_{ij}(z)$ as[1]

$$\Phi_{ij}(z) = \begin{cases} g_i^{-1} - \langle f_i|(H_0-z)^{-1}|f_i\rangle & \text{if } i=j \\ -\dfrac{g_j}{g_i}\langle f_i|(H_0-z)^{-1}|f_j\rangle & \text{if } i\neq j. \end{cases} \tag{12}$$

After a little algebra, it is evident that

$$(H-z)^{-1} = (H_0-z)^{-1} + (H_0-z)^{-1}\left[\sum_{i,j=1}^{N} |f_i\rangle\Phi_{ij}(z)^{-1}\langle f_j|\right](H_0-z)^{-1}, \tag{13}$$

as long as $\Phi_{ij}(z)^{-1}$ exists. Such formulas were extensively discussed in problems associated with self-adjoint extensions of operators, notably by Krein and his school, and also for such singular interactions in flat spaces.[12,22] Therefore, our problem can also be considered as a kind of self-adjoint extension of the free Hamiltonian. It is defined through regulating (or controlling) the behavior of the wave function in the vicinity of these interaction points.

If we take the matrix element of (13) by projecting on to the Dirac kets $\langle x|$ and $|y\rangle$, we have found the resolvent kernel $R(x,y|z)\equiv\langle x|(H-z)^{-1}|y\rangle$ corresponding to (11)

$$\begin{aligned} R(x,y|z) &= R_0(x,y|z) + \int \mathrm{d}x'\mathrm{d}y' R_0(x,x'|z)\left[\sum_{i,j=1}^{N} f_i(x')\Phi_{ij}(z)^{-1}f_j(y')\right]R_0(y',y|z) \\ &= R_0(x,y|z) + \sum_{i,j=1}^{N}\left[\int \mathrm{d}x' R_0(x,x'|z)f_i(x')\right]\Phi_{ij}(z)^{-1}\left[\int \mathrm{d}y' R_0(y',y|z)f_j(y')\right]. \end{aligned}$$

By choosing the functions $f_i(x)$'s as bump functions centered at $x=a_i$ such that the sequences of the functions admit the limit $f_i(x)\to\delta^D(x-a_i)$ (in the appropriate topology), it turns out that

$$R(x,y|z) = R_0(x,y|z) + \sum_{i,j=1}^{N} R_0(x,a_i|z)\Phi_{ij}(z)^{-1}R_0(a_j,y|z). \tag{14}$$

The important point to note here is the relation between the resolvent operator, defined on an infinite dimensional space and the characteristic matrix, defined on a finite dimensional space. This allows us to find the bound state spectrum of the separable Hamiltonian operator H with the help of a finite dimensional matrix $\Phi(z)^{-1}$. Since discrete spectrum is the set of complex numbers such that the resolvent does not exist, this proves that the equation $\det\Phi=0$ gives the bound state spectrum of our system. The fact that the free Hamiltonian is bounded from below allows us to write the free resolvent operator as an integral for $\Re(z)<0$,

$$(H_0-z)^{-1} = \frac{1}{\hbar}\int_0^{\infty} e^{-(t/\hbar)((\hbar^2/2m)\Delta_g - z)}\mathrm{d}t, \tag{15}$$

the result of which should be continued analytically to its largest set in the entire complex plane. As a consequence of this, the free resolvent kernel is

[1]There is no confusion in notation because we will see that this matrix Φ is exactly the same matrix considered in the previous sections.

$$\langle f_i|(H_0-z)^{-1}|f_j\rangle=\frac{1}{\hbar}\int_0^\infty e^{zt/\hbar}\langle f_i|e^{-\left[\frac{t}{\hbar}\right](\hbar^2/2m)\Delta_g}|f_j\rangle \mathrm{d}t.$$

Taking the limit $f_i(x)\to\delta^D(x-a_i)$, it results in

$$R_0(a_i,a_j|z)=\langle a_i|(H_0-z)^{-1}|a_j\rangle=\frac{1}{\hbar}\int_0^\infty e^{zt/\hbar}K_t(a_i,a_j)\mathrm{d}t, \tag{16}$$

where $K_t(a_i,a_j)$ is the so-called heat kernel, and the operator $e^{-[t/\hbar](\hbar^2/2m)\Delta_g)}$ is the formal solution to the heat equation.[19,20] Hence, the matrix Φ is written in terms of the heat kernel in the following way:

$$\Phi_{ij}(z)=\begin{cases} g_i^{-1}-\dfrac{1}{\hbar}\displaystyle\int_0^\infty e^{zt/\hbar}K_t(a_i,a_i)\mathrm{d}t & \text{if } i=j \\ -\dfrac{g_j}{g_i}\dfrac{1}{\hbar}\displaystyle\int_0^\infty e^{zt/\hbar}K_t(a_i,a_j)\mathrm{d}t & \text{if } i\neq j. \end{cases} \tag{17}$$

The matrix Φ_{ij} is exactly the same matrix mentioned in the previous sections. This can be shown easily from the spectral theorem[19] for compact manifolds

$$K_t(a_i,a_j)=\sum_{l\geqslant 0}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\phi_l(a_i)\phi_l^*(a_j), \tag{18}$$

which converges uniformly on $M\times M$ for each $t>0$:

$$\begin{aligned}\langle f_i|(H_0-z)^{-1}|f_j\rangle\to\int_0^\infty e^{zt/\hbar}K_t(a_i,a_j)\frac{\mathrm{d}t}{\hbar}&=\sum_{l\geqslant 0}\phi_l(a_i)\phi_l^*(a_j)\int_0^\infty e^{-((\hbar^2/2m)\lambda_l-z)[t/\hbar]}\mathrm{d}t/\hbar \\ &=\sum_{l\geqslant 0}\frac{\phi_l(a_i)\phi_l^*(a_j)}{\frac{\hbar^2}{2m}\lambda_l-z},\end{aligned}$$

where summation and integral are interchanged since summation converges uniformly. This is the same result for $z=-\nu^2$ that we already obtained for the nondiagonal part of the characteristic matrix in Sec. II. One can understand how the nondiagonal part of it in (7) is convergent by using the smooth behavior of the heat kernel and the integral $\int_0^\infty(\mathrm{d}t/\hbar)e^{zt/\hbar}K_t(a_i,a_j)$ is convergent for $a_i\neq a_j$. However, the asymptotic behavior of the heat kernel as $t\to 0^+$ for every point x on a compact manifold M[19] is given by

$$K_t(x,x)\sim\left(4\pi\frac{\hbar t}{2m}\right)^{-D/2}\sum_{k=0}^\infty u_k(x,x)\left(\frac{\hbar t}{2m}\right)^k, \tag{19}$$

where D is the dimension of the manifold and the $u_k(x,x)$ are functions given in terms of the curvature tensor of M and its covariant derivatives at the point x. This result shows that the diagonal part of the heat kernel as $t\to 0^+$ for $D=2,3$ leads to a divergence since $u_0(x,x)=1$ (there are no infinities for $D=1$ as it can be easily realized). In other words, the sum in the diagonal term in Φ is divergent while the sum in the nondiagonal term is convergent. However, we have already shown that bound state energies are related to the characteristic matrix, i.e., $\det\Phi(z)=0$ contains information about bound states. If some of the elements of the characteristic matrix have infinities, it is impossible to get sensible bound state energies for our problem. Before establishing the renormalization of our problem with the help of heat kernel, we must indicate why this problem occurs. Although the delta interactions may approximately describe a system in which a particle interacting with a point-like centers when its de Broglie wavelength is large compared to the typical range of a potential, we have not encountered in nature this type of contact interaction.

This means that substituting the Dirac-Delta interactions into the Hamiltonian for $D=2,3$ directly is not a proper way. Therefore, we must modify our problem such that it has a finite range and then consider the zero range limit. In our renormalization method with heat kernel, short range is replaced with the short time as we will see.

We introduce a small constant ϵ, in the lower limit of the integral. We then take the limit as the cut-off ϵ goes to zero in such a way that the experimentally measured ground state energy remains finite. This requires that some quantities in the problem, e.g., coupling constant, should have a cut-off dependence in a definite way. For our problem, we naturally choose

$$g_i^{-1}(\epsilon,\mu_i)=\frac{1}{\hbar}\int_{\epsilon}^{\infty}e^{-\mu_i^2 t/\hbar}K_t(a_i,a_i)\mathrm{d}t. \tag{20}$$

After performing the limit $\epsilon\to 0$, we have the renormalized characteristic matrix

$$\Phi_{ij}(z)=\begin{cases}\dfrac{1}{\hbar}\displaystyle\int_0^{\infty}K_t(a_i,a_i)\left[e^{-\mu_i^2 t/\hbar}-e^{zt/\hbar}\right]\mathrm{d}t & \text{if } i=j\\ -\dfrac{1}{\hbar}\displaystyle\int_0^{\infty}e^{zt/\hbar}K_t(a_i,a_j)\mathrm{d}t & \text{if } i\neq j,\end{cases} \tag{21}$$

where $\Re(z)<0$ and $\Phi_{ij}(z)$ can be analytically continued to its largest set in the entire complex plane. One can naturally ask whether the renormalization performed with heat kernel is compatible with the one introduced in Sec. II. The answer is affirmative and one can easily show that the cut-off Λ for the infinite sum introduced in Sec. II corresponds to the cut-off ϵ for the lower bound of integral in the heat kernel method. This can be realized easily by using the spectral theorem in the diagonal part of Eq. (21) and taking $z=-\nu^2$:

$$\begin{aligned}&g_i^{-1}(\epsilon,\mu_i)-\frac{1}{\hbar}\int_{\epsilon}^{\infty}e^{-\nu^2 t/\hbar}\sum_{l\geq 0}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\phi_l(a_i)\phi_l^*(a_i)\mathrm{d}t\\ &\quad=g_i^{-1}(\epsilon,\mu_i)-\frac{1}{\hbar}\sum_{l\geq 0}\phi_l(a_i)\phi_l^*(a_i)\int_{\epsilon}^{\infty}e^{-\nu^2 t/\hbar}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\mathrm{d}t,\end{aligned} \tag{22}$$

where we have used the uniform convergence of the sum. Now, in order to remove the divergence, we can naturally choose the coupling constant as

$$g_i^{-1}(\epsilon,\mu_i)=\frac{1}{\hbar}\sum_{l\geq 0}\phi_l(a_i)\phi_l^*(a_i)\int_{\epsilon}^{\infty}e^{-\mu_i^2 t/\hbar}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\mathrm{d}t. \tag{23}$$

Then, we have

$$\begin{aligned}&\lim_{\epsilon\to 0}\left\{\frac{1}{\hbar}\sum_{l\geq 0}\phi_l(a_i)\phi_l^*(a_i)\left[\int_{\epsilon}^{\infty}e^{-\mu_i^2 t/\hbar}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\mathrm{d}t-\int_{\epsilon}^{\infty}e^{-\nu^2 t/\hbar}e^{-(\hbar^2/2m)\lambda_l[t/\hbar]}\mathrm{d}t\right]\right\}\\ &\quad=\frac{1}{\hbar}\sum_{l\geq 0}\frac{[\nu^2-\mu_i^2]\phi_l(a_i)\phi_l^*(a_i)}{\left[\dfrac{\hbar^2}{2m}\lambda_l+\mu_i^2\right]\left[\dfrac{\hbar^2}{2m}\lambda_l+\nu^2\right]},\end{aligned} \tag{24}$$

which is the same result we would have obtained by the eigenfunction expansion by introducing a cut-off Λ (Eq. (10)). After finding the renormalized characteristic matrix, the resolvent can be written explicitly

$$R(x,y|z) = R_0(x,y|z) + \sum_{i,j=1}^{N} R_0(x,a_i|z)\Phi_{ij}(z)^{-1}R_0(a_j,y|z), \tag{25}$$

where

$$R_0(x,y|z) = \frac{1}{\hbar}\int_0^\infty e^{zt/\hbar}K_t(x,y)\mathrm{d}t. \tag{26}$$

Once we have given the resolvent of an operator, all the information about the operator is contained in it. Nevertheless, it is instructive to check that the wave functions can also be obtained and they are normalizable. We write the normalized wave function with a cut-off Λ and then take the limit $\Lambda\to\infty$, this way we will not get a vanishing wave function. So the normalization constant can be found easily

$$\begin{aligned}|C(\Lambda)|^{-2} &= \sum_{i,j=1}^{N} g_i(\Lambda)g_j(\Lambda)A_i^*(\Lambda)A_j(\Lambda)\int \mathrm{d}^D x\sqrt{g}\sum_{l,l'=0}^{\Lambda}\frac{\phi_l(a_i)\phi_l^*(x)}{\left(\frac{\hbar^2}{2m}\lambda_l+\nu^2\right)}\frac{\phi_{l'}^*(a_j)\phi_{l'}(x)}{\left(\frac{\hbar^2}{2m}\lambda_{l'}+\nu^2\right)}\\ &= \sum_{i,j=1}^{N} g_i(\Lambda)g_j(\Lambda)A_i^*(\Lambda)A_j(\Lambda)\sum_{l=0}^{\Lambda}\frac{\phi_l(a_i)\phi_l^*(a_j)}{\left(\frac{\hbar^2}{2m}\lambda_l+\nu^2\right)^2}.\end{aligned} \tag{27}$$

One expects from the Weyl asymptotic formula that the wave function is not normalizable if we are on a space of dimension bigger than three. Moreover, we can see that the summation over the eigenmodes is exactly the derivative of $\Phi(-\nu^2)$ with respect to ν, hence we get

$$|C(\Lambda)|^{-2} = \frac{1}{2\nu}\sum_{i,j=1}^{N} g_j(\Lambda)^2A_i^*(\Lambda)\frac{\partial\Phi_{ij}(\Lambda,-\nu^2)}{\partial\nu}A_j(\Lambda). \tag{28}$$

Performing the limit $\Lambda\to\infty$, the properly normalized wave function of nth state becomes

$$\psi_n(x) = \sqrt{2\nu_n}\left[\sum_{r,s=1}^{N}A_r^*(\nu_n)\left.\frac{\partial\Phi_{rs}(-\nu^2)}{\partial\nu}\right|_{\nu=\nu_n}A_s(\nu_n)\right]^{-1/2}\sum_{l\geqslant 0}\sum_{i=1}^{N}A_i(\nu_n)\frac{\phi_l^*(a_i)\phi_l(x)}{\left(\frac{\hbar^2}{2m}\lambda_l+\nu_n^2\right)},$$

where ν_n is the nth root of the energy equation $\det\Phi(-\nu^2)=0$. This can further be simplified to an expression in terms of the heat kernel

$$\begin{aligned}\psi_n(x) &= \sqrt{2\nu_n}\left[\sum_{r,s=1}^{N}A_r^*(\nu_n)\left.\frac{\partial\Phi_{rs}(-\nu^2)}{\partial\nu}\right|_{\nu=\nu_n}A_s(\nu_n)\right]^{-1/2}\\ &\quad\times\sum_{l\geqslant 0}\sum_{i=1}^{N}A_i(\nu_n)\phi_l^*(a_i)\phi_l(x)\int_0^\infty e^{-(t/\hbar)((\hbar^2/2m)\lambda_l+\nu_n^2)}\frac{\mathrm{d}t}{\hbar}\\ &= \sqrt{2\nu_n}\left[\sum_{r,s=1}^{N}A_r^*(\nu_n)\left.\frac{\partial\Phi_{rs}(-\nu^2)}{\partial\nu}\right|_{\nu=\nu_n}A_s(\nu_n)\right]^{-1/2}\int_0^\infty e^{-t\nu_n^2/\hbar}\sum_{i=1}^{N}A_i(\nu_n)K_t(a_i,x)\frac{\mathrm{d}t}{\hbar},\end{aligned} \tag{29}$$

in which one can easily see that $\psi_n(x)$ is finite.

III. FINITELY MANY DIRAC-DELTA INTERACTIONS ON $\mathbb{S}^2$

Since the simplest and one of the most familiar compact manifolds is the sphere $\mathbb{S}^2$, we shall work out the problem of point interactions on a sphere as a concrete example. Suppose that point interactions are located at the points given by the local coordinates $(\theta_i, \phi_i)_{i=1}^N$ on a sphere of radius R. Then, the Schrödinger equation for the bound states of a particle living on the sphere under the influence of N attractive delta interactions becomes

$$\left[\frac{\hbar^2}{2m}\Delta_{\mathbb{S}^2} - \sum_{i=1}^{N} g_i \delta^2(\theta-\theta_i, \phi-\phi_i)\right]\psi = -\nu^2\psi, \tag{30}$$

where $\Delta_{\mathbb{S}^2}$ is Laplacian on the sphere in spherical coordinates

$$\Delta_{\mathbb{S}^2} = -\frac{1}{R^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{R^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}, \tag{31}$$

and $\delta^2(\theta-\theta_i, \phi-\phi_i) = \delta(\theta-\theta_i)\delta(\phi-\phi_i)/R^2\sin^2\theta$ is the two-dimensional delta function on the sphere centered at (θ_i, ϕ_i). It is well known that spherical harmonics Y_l^m are eigenfunctions of the Laplacian $\Delta_{\mathbb{S}^2}$ with the eigenvalues $l(l+1)/R^2$ and form a complete orthonormal basis on $\mathbb{S}^2$. In order to be consistent with the standard normalization of spherical harmonics, we choose $\phi_{lm} = Y_l^m/R$. From the following identity

$$\sum_{m=-l}^{l} Y_l^m(\theta_i, \phi_i) Y_l^{m*}(\theta_j, \phi_j) = \frac{2l+1}{4\pi} P_l(\cos\theta_i\cos\theta_j + \cos(\phi_i-\phi_j)\sin\theta_i\sin\theta_j) = \frac{2l+1}{4\pi}P_l\left(1-\frac{\mathrm{d}_{ij}^2}{2}\right),$$

where $\mathrm{d}_{ij} = d_{ij}/R = |\hat{r}_i - \hat{r}_j| \in [0,2]$ being rescaled distance between point centers with radius of the sphere R, the matrix $\Phi_{ij}(-\nu^2)$ in (7) becomes

$$\Phi_{ij}(-\nu^2) = \begin{cases} g_i^{-1} - \dfrac{1}{4\pi R^2}\displaystyle\sum_{l\geqslant 0}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\nu^2} & i=j \\ -\dfrac{g_j}{g_i}\dfrac{1}{4\pi R^2}\displaystyle\sum_{l\geqslant 0}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\nu^2}P_l\left(1-\dfrac{\mathrm{d}_{ij}^2}{2}\right) & i\neq j. \end{cases} \tag{32}$$

It follows easily from the Cauchy-MacLaurin integral test that the infinite sum

$$\frac{1}{4\pi R^2}\sum_{l\geqslant 0}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\nu^2}$$

is divergent. To get a sensible result for our problem, we must modify our original problem as outlined in Sec. II. Therefore, considering our problem in light of this method, we first define the coupling constant g_i as a function of the parameter Λ (cut-off). Then, by choosing $g_i^{-1}(\Lambda)$'s naturally

$$g_i^{-1}(\Lambda) = \frac{1}{4\pi R^2}\sum_{l=0}^{\Lambda}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\mu_i^2},$$

where μ_i is the experimentally measured value of bound state energy for the single delta interaction and taking the limit $\Lambda\to\infty$ of the difference, we have obtained

$$\lim_{\Lambda\to\infty}\left[\frac{1}{4\pi R^2}\sum_{l=0}^{\Lambda}\frac{2l+1}{\frac{\hbar^2}{2mR^2}l(l+1)+\mu_i^2}-\frac{1}{4\pi R^2}\sum_{l=0}^{\Lambda}\frac{2l+1}{\frac{\hbar^2}{2mR^2}l(l+1)+\nu^2}\right]$$
$$\to\frac{1}{4\pi R^2\mu_R^2}\left[\phi\left(\frac{\mu_i}{\mu_R}\right)-\phi\left(\frac{\nu}{\mu_R}\right)\right],$$

where $\mu_R^2\equiv\hbar^2/2mR^2$. The function ϕ here is defined as

$$\phi(x)\equiv\frac{1}{x^2}-H_{1/2-\sqrt{1/4-x^2}}-H_{1/2+\sqrt{1/4-x^2}},\quad x\in\mathbb{R}^+,$$

where H's are the harmonic numbers, commonly defined on integers as $H_n=\Sigma_{k=1}^n 1/k$ and can be extended by analytical continuation to its largest domain in the entire complex plane as $H_z=\psi(z+1)+\gamma$, where $\psi(z)=\Gamma'(z)/\Gamma(z)$ being the digamma function and γ being the Euler-Mascheroni constant. The digamma function has several useful integral representations,[23] some of which are

$$\psi(z)=\int_0^\infty\left(\frac{e^{-t}}{t}-\frac{e^{-zt}}{1-e^{-t}}\right)dt, \tag{33}$$

$$\psi(z)=\log z+\int_0^\infty\left(\frac{1}{1-e^{-t}}+\frac{1}{t}-1\right)e^{-zt}dt, \tag{34}$$

where $\Re(z)>0$ and these can be useful for the estimates of its upper and lower bounds. Due to the Schwarz reflection principle of harmonic numbers ($\overline{H_z}=H_{\bar{z}}$), the function $\phi(x)$ is real valued ($\phi\in\mathbb{R}$) for all $x\in\mathbb{R}^+$. It is also easy to check $\lim_{\Lambda\to\infty}g_j(\Lambda)/g_j(\Lambda)\to 1$ in the nondiagonal part of (32), simply because of their same form of the divergence. Then, the renormalized matrix $\Phi(-\nu^2)$ for bound states can be eventually written as

$$\Phi_{ij}(-\nu^2)=\frac{1}{4\pi R^2\mu_R^2}\begin{cases}\phi\left(\frac{\mu_i}{\mu_R}\right)-\phi\left(\frac{\nu}{\mu_R}\right) & i=j\\ -\sum_{l\geqslant 0}\frac{2l+1}{l(l+1)+\frac{\nu^2}{\mu_R^2}}P_l\left(1-\frac{d_{ij}^2}{2}\right) & i\neq j.\end{cases} \tag{35}$$

By the analytical continuation of the characteristic matrix to its largest domain in the entire complex plane, we have

$$\Phi_{ij}(z)=\frac{1}{4\pi R^2\mu_R^2}\begin{cases}\phi\left(\frac{\mu_i}{\mu_R}\right)-\phi\left(\frac{\sqrt{-z}}{\mu_R}\right) & i=j\\ -\sum_{l\geqslant 0}\frac{2l+1}{l(l+1)-\frac{z}{\mu_R^2}}P_l\left(1-\frac{d_{ij}^2}{2}\right) & i\neq j,\end{cases} \tag{36}$$

from which we can write the resolvent equation (14). Hence, we have obtained a well-defined formulation of our problem, that is, the infinities have been removed. Moreover, we see that the problem realizes a generalized dimensional transmutation. In this case, the coupling constants g_i have the same dimension as $\hbar^2/2m$ by dimensional analysis. In contrast to the flat case, we have one more parameter R coming from the geometry of the space. Thus, we expect that the system must have an intrinsic energy scale $\hbar^2/2mR^2$ as well as $\hbar^2/md_{ij}^2$ terms. However, after the renormalization, we obtain a set of new dimensional parameters μ_i^2. Hence, the first set of scales we expect by naive dimensional analysis at the beginning is not sufficient. Instead, a specific combi-

nation of all these parameters together determine the scale of our problem. This means that delta potentials on a sphere are an example of a kind of dimensional transmutation. However, there is a slight difference, especially in the case of single delta attractor: in the flat case there is no combination of dimensional parameters to come up with an energy scale, whereas in the case of a sphere we have a geometric length scale R which already defines an energy scale $\hbar^2/2mR^2$. The dimensional transmutation is most striking in such cases where there is no intrinsic energy scale.

In order to estimate the nondiagonal part of the matrix Φ for sphere $\mathbb{S}^2$, we follow a different strategy, using the heat kernel.

A. Lower bound of E_{gr} by heat kernel method for $\mathbb{S}^2$

Heat kernel $K_t(x,y)$ is the unique fundamental solution to the heat equation $(\hbar^2/2m)\Delta_g\phi = -\hbar\,\phi_t$. It has the symmetry $(K_t(x,y)=K_t(y,x))$ and semigroup property.[19,20] As well as being a useful computational tool in establishing the existence and some of the properties of the spectrum of the Laplacian of the eigenfunctions on Riemannian manifolds, it is very helpful to understand the nature of the divergences for our purposes, as we have shown in the previous section.

By means of relation (21) and explicit form of the heat kernel, one can calculate the matrix Φ_{ij}. However, there are some situations in which one cannot calculate the heat kernel explicitly, e.g., we do not have an explicit expression of the heat kernel for two-dimensional sphere. In this case, one can still find some bound estimates on matrix Φ_{ij} without having an explicit form of the heat kernel, but instead some properties of it. In order to analyze this for $\mathbb{S}^2$, we will use some estimates on the heat kernel, based on a work by Li and Yau.[24] Let us recall the corollary of the theorem (3.1) in Ref. 24.

Let M be a complete manifold without boundary. If the Ricci curvature of M is bounded from below by $-K$, for some constant $K \geqslant 0$, then for $1<\alpha<2$ and $0<\varepsilon<1$, the heat kernel satisfies

$$K_t(x,y) \leqslant \frac{C(\varepsilon)^\alpha}{\sqrt{V(x,\sqrt{t})V(y,\sqrt{t})}} e^{C_7\varepsilon(\alpha-1)^{-1}Kt - d(x,y)^2/(4+\varepsilon)t},$$

where $V(x,r)=\mu(B(x,r))$, $B(x,r)$ is the geodesic ball of radius r centered at $x \in M$ and $d(x,y)$ is the geodesic distance between two points x and y on the manifold. The constant C_7 depends only on the dimension of the manifold D, while $C(\varepsilon)$ depends on ε with $C(\varepsilon)\to\infty$ as $\varepsilon\to 0$. When $K=0$, the above-noted estimate, after letting $\alpha\to 1$, can be written as

$$K_t(x,y) \leqslant \frac{C(\varepsilon)}{\sqrt{V(x,\sqrt{t})V(y,\sqrt{t})}} e^{-d(x,y)^2/(4+\varepsilon)t}. \tag{37}$$

Since $\mathbb{S}^2$ satisfies the above-noted conditions as a particular case, this corollary can be applied to it as well. On the other hand, we have a different purpose from the original corollary of the theorem for the estimates on the upper bound of the heat kernel, in which the sharp estimate for the heat kernel is found. Instead, we are trying to find a best lower bound of the ground state energy of the system. Therefore, we shall modify the original corollary in Ref. 24. Using this theorem with relaxed condition $0<\varepsilon<1$, we have found the upper bound estimate for heat kernel of sphere $\mathbb{S}^2$ in our problem:

$$K_t(a_i,a_j) \leqslant \frac{C'(\delta)}{\sqrt{V\left(x,\sqrt{\frac{\hbar t}{2m}}\right)V\left(y,\sqrt{\frac{\hbar t}{2m}}\right)}} e^{-2md_{ij}^2/D(\delta)\hbar t}, \tag{38}$$

where

$$C'(\delta) \equiv (1+\delta)^2 \exp\left[\frac{1}{4\delta(1+\delta)(1+2\delta)} + \frac{1}{2\delta(2+\delta)} + \frac{1}{4\delta}\right], \tag{39}$$

and

$$D(\delta) \equiv 4(1+2\delta)(1+\delta)^2, \tag{40}$$

δ is merely required to be positive. When we want to find a lower bound for the energy, the numerical values of the coefficients $C'(\delta)$ and $D(\delta)$ will be determined explicitly. It is easy to see that $V(x,\sqrt{\hbar t/2m})=V(y,\sqrt{\hbar t/2m})=2\pi R^2(1-\cos\sqrt{\hbar t/2mR^2})$ as long as $0\leqslant t\leqslant 2m\pi^2R^2/\hbar$. For $t \geqslant 2m\pi^2R^2/\hbar$, we have $V(x,\sqrt{\hbar t/2m})=V(y,\sqrt{\hbar t/2m})=4\pi R^2$. According to our corollary and positive definiteness of heat kernel, the following integral has an upper bound:

$$\frac{1}{\hbar}\int_0^\infty e^{-\nu^2 t/\hbar}K_t(a_i,a_j)\mathrm{d}t$$

$$\leqslant \frac{C'(\delta)}{\hbar}\int_0^{2m\pi^2R^2/\hbar}\frac{e^{-2md_{ij}^2/D(\delta)\hbar t-\nu^2 t/\hbar}}{2\pi R^2\left(1-\cos\sqrt{\dfrac{\hbar t}{2mR^2}}\right)}\mathrm{d}t+\frac{C'(\delta)}{4\pi R^2\hbar}\int_{2m\pi^2R^2/\hbar}^\infty e^{-2md_{ij}^2/D(\delta)\hbar t-\nu^2 t/\hbar}\mathrm{d}t,$$

where we have taken z as $-\nu^2$. With the help of the identity $1-\cos\sqrt{\hbar t/2mR^2}=2\sin^2\sqrt{\hbar t/8mR^2}$ and the inequality $1/\sin\theta\leqslant\pi/2\theta$ for $0\leqslant\theta\leqslant\pi/2$, we obtain

$$\frac{1}{\hbar}\int_0^\infty e^{-\nu^2 t/\hbar}K_t(a_i,a_j)\mathrm{d}t\leqslant\frac{m\pi C'(\delta)}{2\hbar^2}\int_0^\infty\frac{e^{-2md_{ij}^2/D(\delta)\hbar t-\nu^2 t/\hbar}}{t}\mathrm{d}t+\frac{C'(\delta)}{4\pi R^2\hbar}\int_0^\infty e^{-2md_{ij}^2/D(\delta)\hbar t-\nu^2 t/\hbar}\mathrm{d}t.$$

Evaluating these integrals, we find

$$|-\Phi_{i\neq j}(-\nu^2)|\equiv|\mathcal{K}_{ij}|=\frac{1}{\hbar}\int_0^\infty e^{-\nu^2 t/\hbar}K_t(a_i,a_j)\mathrm{d}t\leqslant C'(\delta)\left[\frac{m\pi}{\hbar^2}K_0(\alpha_{ij}\nu)+\frac{\alpha_{ij}}{4\pi}\frac{K_1(\alpha_{ij}\nu)}{\nu R^2}\right],$$

where

$$\alpha_{ij}\equiv\sqrt{\frac{8md_{ij}^2}{D(\delta)\hbar^2}}, \tag{41}$$

and $K_0(x)$, $K_1(x)$ are modified Bessel functions. This shows us that the infinite series in the nondiagonal part of the characteristic matrix is finite and bounded from above according to (41). In order to find a lower bound for the diagonal part, denoted by $\mathcal{D}$, of the matrix Φ for sphere $\mathbb{S}^2$, we first recall how the diagonal part of the matrix Φ appears in (36):

$$\mathcal{D}_i=\frac{1}{4\pi R^2}\lim_{\Lambda\to\infty}\left[\sum_{l=0}^{\Lambda}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\mu_i^2}-\sum_{l=0}^{\Lambda}\frac{2l+1}{\dfrac{\hbar^2}{2mR^2}l(l+1)+\nu^2}\right]\geqslant 0.$$

Instead of calculating explicitly this limit as we have done in Sec. III, we estimate a lower bound of it by means of integrals replaced by the sums as follows:

$$\mathcal{D}_i\geqslant\frac{1}{4\pi R^2}\lim_{\Lambda\to\infty}\left[\int_0^{\Lambda+1}\frac{2t+1}{\dfrac{\hbar^2}{2mR^2}t(t+1)+\mu_i^2}\mathrm{d}t-\int_0^{\Lambda}\frac{2t+1}{\dfrac{\hbar^2}{2mR^2}t(t+1)+\nu^2}\mathrm{d}t-\frac{1}{\nu^2}\right].$$

After taking the limit we find

$$\mathcal{D}_i\geqslant\left[\frac{m}{\pi\hbar^2}\log(\nu/\mu_i)-\frac{1}{4\pi R^2\nu^2}\right], \tag{42}$$

and using the estimate for logarithmic functions in Ref. 25

$$\log x > \frac{x-1}{x} \quad \text{for } x > 0,\ x \neq 1, \tag{43}$$

we obtain

$$\mathcal{D}_i \geqslant \left[\frac{m}{\pi\hbar^2} \log(\nu/\mu_i) - \frac{1}{4\pi R^2 \nu^2} \right] > \left[\frac{m}{\pi\hbar^2} - \frac{m\mu_i}{\pi\hbar^2 \nu} - \frac{1}{4\pi R^2 \nu^2} \right] > 0. \tag{44}$$

For positive definiteness, we have assumed ν is sufficiently large, which is not a particularly restrictive condition. In fact, one can try to find sharper estimates by means of the integral representations of digamma functions (33) and (34) without this assumption. However, the estimated functions in this case are too complicated to suggest a bound for ground state energy.

A well-known theorem in matrix analysis, called Geršgorin Theorem,[26] states that all the eigenvalues λ_i of the renormalized matrix Φ are located in the union of N discs

$$\bigcup_{i=1}^{N} \{|\lambda_i - \Phi_{ii}| \leqslant R_i'(\Phi)\} \equiv G(\Phi), \tag{45}$$

where $R_i'(\Phi) \equiv \Sigma_{i\neq j=1}^{N} |\Phi_{ij}|$ and $1 \leqslant i \leqslant N$. If we want $\lambda = 0$ not to be an eigenvalue, then none of the discs should contain $\lambda = 0$. Then, we should impose

$$|-\mathcal{D}_i(\nu)| > \sum_{i\neq j}^{N} |\mathcal{K}_{ij}(\nu)|, \tag{46}$$

for all i. This is possible for a critical value $\nu > \nu^*$ since the left-hand side is an increasing function of ν and the right-hand side is a decreasing function of it for a given d and N. In fact, this inequality obviously provides a lower bound for the bound state energy by just plotting the functions on both sides in spite of how complicated the form of functions are. However, we shall try to find an explicit expression for the lower bound of the ground state energy depending on the number of delta interactions. In order to achieve this, we choose ν such that

$$|-\mathcal{D}_i(\nu)| > \left[\frac{m}{\pi\hbar^2} - \frac{m\mu_i}{\pi\hbar^2 \nu} - \frac{1}{4\pi R^2 \nu^2} \right],$$

$$(N-1)C'(\delta) \left[\frac{m\pi}{\hbar^2} K_0(\alpha\nu) + \frac{\alpha}{4\pi} \frac{K_1(\alpha\nu)}{\nu R^2} \right] > \sum_{i\neq j}^{N} |\mathcal{K}_{ij}(\nu)|, \tag{47}$$

where we have used the monotonic behavior of the functions in $\mathcal{D}_{ij}$ and $\mathcal{K}_{ij}$ and defined $\mu \equiv \max_i \mu_i$ and $\alpha \equiv \min_{i\neq j} \alpha_{ij}$ or $d \equiv \min_{i\neq j} d_{ij}$. From the integral representations of the Bessel functions for $z \in \mathbb{R}^+$,[27]

$$K_0(z) = \int_0^\infty e^{-z \cosh t} dt,$$

$$K_1(z) = z \int_0^\infty e^{-z \cosh t} \sinh^2 t dt,$$

and using the inequalities $e^t/2 < \cosh t$, $\sinh^2 t < e^{2t}/4$ for all $t \in \mathbb{R}^+$, we can find the upper bounds for the functions K_0 and K_1,

$$K_0(\alpha\nu) < \frac{2e^{-\alpha\nu/2}}{\alpha\nu},$$

$$K_1(\alpha\nu) < e^{-\alpha\nu/2}\left(\frac{1}{\alpha\nu}+\frac{1}{2}\right), \tag{48}$$

where $\alpha\nu \in \mathbb{R}^+$. Considering the estimated bounds for Bessel functions, it is easy to see that

$$\frac{m}{\pi\hbar^2}(N-1)C'(\delta)\left[\frac{2\pi^2 e^{-\alpha\nu/2}}{\alpha\nu}+\frac{e^{-\alpha\nu/2}\mu_R^2}{2\nu^2}+\frac{e^{-\alpha\nu/2}\mu_R^2\alpha}{4\nu}\right]$$
$$> (N-1)C'(\delta)\left[\frac{m\pi}{\hbar^2}K_0(\alpha\nu)+\frac{\alpha}{4\pi}\frac{K_1(\alpha\nu)}{\nu R^2}\right].$$

Using the argument $\nu > \sqrt{2}\mu_R$ in Eq. (44) and the last inequality, we impose the following inequality with the help of the Geršgorin Theorem:

$$\nu > \mu + \frac{\mu_R}{2\sqrt{2}} + (N-1)C'(\delta)e^{-\alpha\nu/2}\left[\frac{2\pi^2}{\alpha}+\frac{\mu_R}{2\sqrt{2}}+\frac{\mu_R^2\alpha}{4}\right]. \tag{49}$$

Let us make the following reasonable assumptions and take these for granted for the present (we will later show that they indeed satisfy these conditions by finding the extremum of ground state energy with respect to the parameter δ)

$$\frac{\mu_R^2\alpha}{4} < \frac{2\pi^2}{\alpha}, \tag{50}$$

$$\frac{\mu_R}{2\sqrt{2}} < \frac{2\pi^2}{\alpha}, \tag{51}$$

$$\frac{1}{\sqrt{D(\delta)}} > \frac{1}{5}, \tag{52}$$

so that the inequality becomes

$$\nu > \mu + \frac{\mu_R}{2\sqrt{2}} + 3\pi^2\mu_d(N-1)C'(\delta)\sqrt{D(\delta)}e^{-\nu/5\mu_d}, \tag{53}$$

from which we conclude that there exists a critical value $\nu > \nu^*$ for a given N such that $\lambda \neq 0$ and then the ground state energy cannot be less than $-\nu^{*2}$:

$$E_{\mathrm{gr}} \geqslant -\nu^{*2} = -\left\{\mu + \frac{\mu_R}{2\sqrt{2}} + 5\mu_d W\left[\frac{3\pi^2}{5}C'(\delta)\sqrt{D(\delta)}(N-1)e^{-(\mu+\mu_R/2\sqrt{2})/5\mu_d}\right]\right\}^2, \tag{54}$$

where W is the Lambert W function, also called the Omega function or product-log function.[28] Now, we choose δ in such a way that the energy bound takes its minimum value. This is accomplished if δ is chosen approximately 0.508, which is independent of the parameters in the problem. This independence can be easily realized from the form of inequality (53). By substituting the values of $C'(\delta)$ and $D(\delta)$, we estimate a lower bound for the ground state energy:

$$E_{\mathrm{gr}} \geqslant -\nu^{*2} = -\left\{\mu + \frac{\mu_R}{2\sqrt{2}} + 5\mu_d W\left[28\pi^2(N-1)e^{-(\mu+\mu_R/2\sqrt{2})/5\mu_d}\right]\right\}^2. \tag{55}$$

By using this value of δ and the fact that $d < 2\pi R$, the consistency of the assumption we made can be shown easily. Finally, we shall consider the large N behavior of the ground state energy. The asymptotic expansion of product-log function W[28] for large z is given as

$$W(z) \sim \log z - \log\log z. \tag{56}$$

Hence, this leads to

$$E_{\mathrm{gr}} \sim -\mu_d^2[\log(N) - \log\log(N)]^2. \tag{57}$$

The method we have introduced for the two-dimensional sphere $\mathbb{S}^2$ can also be applied to a general compact manifold. The main idea is based on finding an upper and lower bound for the characteristic matrix or heat kernel (based on the work by Li and Yau). Then, Geršgorin theorem allows us to estimate a lower bound for the ground state energy.

IV. FINITELY MANY DIRAC-DELTA INTERACTIONS ON HYPERBOLIC SPACES

The hyperbolic space $\mathbb{H}^n$ is defined as maximally symmetric and simply connected complete n-dimensional Riemannian manifold with a constant negative sectional curvature $-1/R$, which is also in some sense considered to be the negative curvature analog of the sphere $\mathbb{S}^n$. We shall deal with the delta interactions on the hyperbolic spaces $\mathbb{H}^3$ and $\mathbb{H}^2$ in the following sections. The method developed in the previous sections for $\mathbb{S}^2$ will be useful as well for the hyperbolic spaces. The heat kernel on hyperbolic spaces,[29] written in terms of dimensionless quantities:

$$K_t(x,y) = \frac{1}{(4\pi t)^{3/2}} \frac{d}{\sinh d} e^{-t-d^2/4t} \quad \text{on } \mathbb{H}^3,$$

$$K_t(x,y) = \frac{\sqrt{2}}{(4\pi t)^{3/2}} e^{-t/4} \int_d^\infty \frac{s e^{-s^2/4t}}{(\cosh s - \cosh d)^{1/2}} \mathrm{d}s \quad \text{on } \mathbb{H}^2, \tag{58}$$

where $d \equiv \mathrm{dist}(x,y)$, geodesic distance between two points x and y on $\mathbb{H}^n$.

Although spectral theorem and asymptotic expansion of heat kernel discussed in the previous sections may not be valid for general noncompact manifolds, we shall demonstrate that for the specific examples in noncompact manifolds, such as $\mathbb{H}^2$ and $\mathbb{H}^3$, our viewpoint still works. It would be desirable to show the equivalence between the eigenfunction expansion and the heat kernel method for the regularization in noncompact manifolds rigourously. Nevertheless, we have not been able to do this. The main idea is similar in spirit to the renormalization procedure introduced for the compact manifolds.

A. Finitely many Dirac-delta interactions on hyperbolic space $\mathbb{H}^3$

In the hyperbolic space $\mathbb{H}^3 = \{x \in \mathbb{R}^3 \,|\, x_3 > 0\}$, the geodesic distance d is defined as

$$\cosh \frac{d(x,y)}{R} = 1 + \frac{|x-y|^2}{2x_3 y_3},$$

where R is the scaling parameter. The Schrödinger equation for the bound states of a particle living on $\mathbb{H}^3$ under the influence of N attractive delta interactions is

$$\left[\frac{\hbar^2}{2m} \Delta_{\mathbb{H}^3} - \sum_{i=1}^{N} g_i \delta^3(\chi - \chi_i, \theta - \theta_i, \phi - \phi_i) \right] \psi = -\nu^2 \psi, \tag{59}$$

where Laplacian $\Delta_{\mathbb{H}^3}$ in polar coordinates (χ, θ, ϕ),

$$\Delta_{\mathbb{H}^3} = -\frac{1}{R^3} \frac{\partial^2}{\partial \psi^2} - \frac{2\coth\psi}{R^3} \frac{\partial}{\partial \psi} + \frac{1}{R \sinh^2 \psi} \Delta_{\mathbb{S}^2}. \tag{60}$$

We have an explicit formula[29] for the heat kernel of the three-dimensional hyperbolic plane $\mathbb{H}^3$ written by using physical constants

$$K_t(x,y) = \frac{1}{R^3} \frac{\frac{d(x,y)}{R}}{\left(4\pi\left[\frac{\hbar}{2mR^2}\right]t\right)^{3/2} \sinh\frac{d(x,y)}{R}} \exp\left(-\frac{\hbar t}{2mR^2} - \frac{md(x,y)^2}{2\hbar t}\right) \tag{61}$$

such that as $R\to\infty$, we can obtain the heat kernel on $\mathbb{R}^3$. Hence we have the free resolvent kernel as

$$\begin{aligned}\langle a_i|(H_0-z)^{-1}|a_j\rangle &= \frac{1}{\hbar R^3}\int_0^\infty \frac{\frac{d_{ij}}{R}\exp\left(\frac{zt}{\hbar}-\frac{\hbar t}{2mR^2}-\frac{md_{ij}^2}{2\hbar t}\right)}{\left(4\pi\left[\frac{\hbar}{2mR^2}\right]t\right)^{3/2}\sinh\frac{d_{ij}}{R}}\mathrm{d}t \\ &= \left[\frac{1}{4\pi R^3}\frac{\frac{d_{ij}}{R}}{\sinh\frac{d_{ij}}{R}}\exp\left(-\frac{\mu_R}{\mu_{d_{ij}}}\sqrt{1-\frac{z}{\mu_R^2}}\right)\right]\frac{\mu_{d_{ij}}}{\mu_R^3},\end{aligned} \tag{62}$$

where $d_{ij}\equiv d(a_i,a_j)$, $\mu_R^2\equiv\hbar^2/2mR^2$, $\mu_{d_{ij}}^2\equiv\hbar^2/2md_{ij}^2$. It follows easily that this term gives infinity when $i=j$, that is, the diagonal term in the characteristic matrix is divergent. Then, we can now proceed to the regularization and renormalization schemes analogously for the hyperbolic spaces. However, the divergence in hyperbolic space $\mathbb{H}^3$ is due to fact that the lower bound t of integral (62) is zero. Hence we regularize the divergent term by introducing a lower cut-off ϵ, as we have shown in Sec. II and we expect this should in some way be related to the ultraviolet regularization. We next define the coupling constant as a function of this cut-off:

$$\Phi_{ii}(z) = \lim_{\epsilon\to 0^+}\left[g_i^{-1}(\epsilon) - \frac{1}{(4\pi)^{3/2}\mu_R^2R^3}\int_\epsilon^\infty u^{-3/2}e^{-[1-z/\mu_R^2]u}\mathrm{d}u\right],$$

where the integration variable $u\equiv(\hbar^2/2mR^2)t$ is introduced for simplicity. The natural choice for $g_i^{-1}(\epsilon)$ is simply

$$g_i^{-1}(\epsilon) = \frac{1}{(4\pi)^{3/2}\mu_R^2R^3}\int_\epsilon^\infty u^{-3/2}e^{-[1+\mu_i^2/\mu_R^2]u}\mathrm{d}u,$$

where μ_i is an experimentally measured bound state energy for the single delta interaction and it helps us to keep track of the strength of point interactions. In $\epsilon\to 0^+$ limit, we have found the explicit renormalized characteristic matrix for $\mathbb{H}^3$,

$$\Phi_{ij}(z) = \frac{1}{4\pi}\frac{1}{\mu_R^2R^3}\begin{cases}\sqrt{1-\frac{z}{\mu_R^2}}-\sqrt{1+\frac{\mu_i^2}{\mu_R^2}} & \text{if } i=j \\ -\frac{\mu_{d_{ij}}}{\mu_R}\frac{\frac{d_{ij}}{R}}{\sinh\frac{d_{ij}}{R}}\exp\left(-\frac{\mu_R}{\mu_{d_{ij}}}\sqrt{1-\frac{z}{\mu_R^2}}\right) & \text{if } i\neq j.\end{cases} \tag{63}$$

Then, we have the resolvent equation (14) with the free resolvent kernel $R_0(x,y|z)$ for $\mathbb{H}^3$ given by

$$R_0(x,y|z)=\frac{1}{4\pi}\frac{1}{\mu_R^2R^3}\frac{\mu_{d(x,y)}}{\mu_R}\frac{\dfrac{d(x,y)}{R}}{\sinh\dfrac{d(x,y)}{R}}\exp\left(-\frac{\mu_R}{\mu_{d(x,y)}}\sqrt{1-\frac{z}{\mu_R^2}}\right), \tag{64}$$

from which we can get all information about the system. Using the Geršgorin Theorem (45) for this matrix, and following the same ideas introduced for $\mathbb{S}^2$ we obtain

$$\left[\sqrt{1+\frac{\nu^2}{\mu_R^2}}-\sqrt{1+\frac{\mu^2}{\mu_R^2}}\right]>(N-1)\frac{\mu_d}{\mu_R}\frac{d}{R\sinh\dfrac{d}{R}}\exp\left(-\frac{\mu_R}{\mu_d}\sqrt{1+\frac{\nu^2}{\mu_R^2}}\right),$$

where we have taken $z=-\nu^2$ and chosen $d\equiv\min_{i\neq j}d_{ij}$, and $\mu\equiv\max_i\mu_i$. It turns out that this inequality indicates that there exists a critical $\nu>\nu^*$ for a given d and N for which this inequality is satisfied and zero is not an eigenvalue. Therefore, the ground state energy cannot be less than $-\nu^{*2}$:

$$\begin{aligned}E_{\mathrm{gr}}\geqslant-\nu^{*2}=&-\mu^2-2\mu_d\sqrt{\mu_R^2+\mu^2}W\left[\frac{e^{-(\mu_R/\mu_d)\sqrt{1+\mu^2/\mu_R^2}d(N-1)}}{R\sinh\dfrac{d}{R}}\right]\\&-\mu_d^2W\left[\frac{e^{-(\mu_R/\mu_d)\sqrt{1+\mu^2/\mu_R^2}d(N-1)}}{R\sinh\dfrac{d}{R}}\right]^2.\end{aligned} \tag{65}$$

For the large N behavior of the ground state energy, the estimate becomes

$$E_{\mathrm{gr}}\sim-2\mu_d\sqrt{\mu_R^2+\mu^2}[\log N-\log\log N]-\mu_d^2[\log N-\log\log N]^2.$$

Now let us consider the two center case on the hyperbolic plane $\mathbb{H}^3$ and assume again that their strengths (or bound state energies of each center) are the same. In this way, determining equation ($\det\Phi=0$) becomes

$$\sqrt{1+\frac{\nu^2}{\mu_R^2}}-\sqrt{1+\frac{\mu^2}{\mu_R^2}}=\pm\frac{\mu_d}{\mu_R}\frac{\dfrac{d}{R}}{\sinh\dfrac{d}{R}}\exp\left(-\frac{\mu_R}{\mu_d}\sqrt{1+\frac{\nu^2}{\mu_R^2}}\right).$$

If we expand it for small d we have

$$\sqrt{1+\frac{\nu^2}{\mu_R^2}}-\sqrt{1+\frac{\mu^2}{\mu_R^2}}=\pm\frac{\mu_d}{\mu_R}\left[1-\sqrt{\frac{\mu_R^2}{\mu_d^2}+\frac{\nu^2}{\mu_d^2}}\right],$$

from which we can conclude

$$E_{\mathrm{gr}}=-\nu^2\simeq\frac{3}{4}\mu_R^2-\frac{\mu^2}{4}-\frac{\mu_d^2}{4}-\frac{\mu_d\mu_R}{2}\sqrt{1+\frac{\mu^2}{\mu_R^2}}.$$

Similarly, for large values of d, the right-hand side of the energy equation for two dirac delta interactions vanishes, so that we obtain the ground state energy $E_{\mathrm{gr}}=-\nu^2=-\mu^2$.

B. Finitely many Dirac-delta interactions on hyperbolic plane $\mathbb{H}^2$

The geodesic distance on the hyperbolic plane $\mathbb{H}^2$ is defined by

$$\cosh\frac{d(x,y)}{R}=1+\frac{|x-y|^2}{2x_2y_2},$$

where R is a scale distance. Then, the Schrödinger equation for the bound states of a particle living on $\mathbb{H}^2$ in the presence of N attractive delta interactions is

$$\left[\frac{\hbar^2}{2m}\Delta_{\mathbb{H}^2}-\sum_{i=1}^{N}g_i\delta^2(\theta-\theta_i,\phi-\phi_i)\right]\psi=-\nu^2\psi, \tag{66}$$

where the Laplacian $\Delta_{\mathbb{H}^2}$ in polar coordinates (θ,ϕ) is given by

$$\Delta_{\mathbb{H}^2}=-\frac{1}{R^2}\frac{\partial^2}{\partial\theta^2}-\frac{2\coth\theta}{R^2}\frac{\partial}{\partial\theta}-\frac{1}{R^2\sinh^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{67}$$

The heat kernel for $\mathbb{H}^2$ (Ref. 29) with the proper physical parameters is

$$K_t(x,y)=\frac{\sqrt{2}}{\left(4\pi\left[\frac{\hbar}{2mR^2}\right]t\right)^{3/2}}\frac{e^{-(\hbar/2mR^2)t/4}}{R^2}\int_{\frac{d(x,y)}{R}}^{\infty}\frac{re^{-(r^2/4)(2mR^2/\hbar)1/t}}{\sqrt{\cosh r-\cosh\frac{d(x,y)}{R}}}\mathrm{d}r. \tag{68}$$

One can check that this goes to the heat kernel on $\mathbb{R}^2$ as $R\to\infty$. Then, the free resolvent kernel is immediately obtained

$$\begin{aligned}\langle a_i|(H_0-z)^{-1}|a_j\rangle&=\frac{1}{\hbar R^2}\int_0^{\infty}e^{zt/\hbar}\frac{\sqrt{2}}{\left(4\pi\left[\frac{\hbar}{2mR^2}\right]t\right)^{3/2}}e^{-(\hbar/2mR^2)t/4}\left[\int_{d_{ij}/R}^{\infty}\frac{re^{-(r^2/4)(2mR^2/\hbar)1/t}}{\sqrt{\cosh r-\cosh\frac{d_{ij}}{R}}}\mathrm{d}r\right]\mathrm{d}t\\&=\frac{1}{4\pi\mu_R^2R^2}\int_{d_{ij}/R}^{\infty}\frac{e^{-(1/2)r\sqrt{1-4z/\mu_R^2}}}{\sqrt{\cosh r-\cosh\frac{d_{ij}}{R}}}\mathrm{d}r.\end{aligned}$$

We see that the diagonal term, which corresponds to $d_{ij}=0$, is divergent, as expected. Therefore we again repeat the similar regularization and renormalization procedure as we have done for $\mathbb{H}^3$. After introducing a cut-off to the lower limit of the integral

$$\begin{aligned}\Phi_{ii}(z)&=\lim_{\epsilon\to0^+}\left[g_i^{-1}(\epsilon)-\frac{1}{4\pi\mu_R^2R^2}\int_{\epsilon}^{\infty}\frac{e^{-(1/2)r\sqrt{1-4z/\mu_R^2}}}{\sqrt{\cosh r-1}}\mathrm{d}r\right]\\&=\lim_{\epsilon\to0^+}\left[g_i^{-1}(\epsilon)-\frac{\sqrt{2}}{4\pi\mu_R^2R^2}\int_{\epsilon/2}^{\infty}\frac{e^{-u\sqrt{1-4z/\mu_R^2}}}{\sinh u}\mathrm{d}u\right].\end{aligned}$$

and by the natural choice for $g_i^{-1}(\epsilon)$,

$$g_i^{-1}(\epsilon)=\frac{\sqrt{2}}{4\pi\mu_R^2R^2}\int_{\epsilon/2}^{\infty}\frac{e^{-u\sqrt{1+4\mu_i^2/\mu_R^2}}}{\sinh u}\mathrm{d}u,$$

we have obtained the renormalized characteristic matrix for $\mathbb{H}^2$ in the $\epsilon\to0$ limit,

$$\Phi_{ij}(z)=\frac{1}{4\pi R^2}\frac{1}{\mu_R^2}\begin{cases}\sqrt{2}\left[\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{z}{\mu_R^2}}\right)-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu_i^2}{\mu_R^2}}\right)\right] & \text{if } i=j\\ -\int_{\frac{d_{ij}}{R}}^{\infty}\frac{e^{-(1/2)r\sqrt{1-4z/\mu_R^2}}}{\sqrt{\cosh r-\cosh\frac{d_{ij}}{R}}}\mathrm{d}r & \text{if } i\neq j,\end{cases} \tag{69}$$

where ψ is the digamma function. Then, we have the resolvent equation (14) in which the free resolvent kernel $R_0(x,y|z)$ for $\mathbb{H}^2$ is given by

$$R_0(x,y|z)=\frac{1}{4\pi R^2}\frac{1}{\mu_R^2}\int_{d(x,y)/R}^{\infty}\frac{e^{-(1/2)r\sqrt{1-4z/\mu_R^2}}}{\sqrt{\cosh r-\cosh\frac{d(x,y)}{R}}}\mathrm{d}r. \tag{70}$$

The integral on the right-hand side is in fact one of the integral representations of the Legendre polynomials of second type[27]

$$\sqrt{2}Q_\lambda\left(\cosh\frac{d(x,y)}{R}\right)=\int_{d(x,y)/R}^{\infty}\frac{e^{-(\lambda+1/2)r}}{\sqrt{\cosh r-\cosh\frac{d(x,y)}{R}}}\mathrm{d}r, \tag{71}$$

which are defined for $\Re(\lambda)>-1$ and in our case $\Re(\lambda)=\Re\left(\frac{1}{2}\sqrt{1-4z/\mu_{R^2}}-1/2\right)>-1$. Therefore, the free resolvent in terms of Q_λ,

$$R_0(x,y|z)=\frac{1}{4\pi R^2}\frac{1}{\mu_R^2}\sqrt{2}Q_{1/2\sqrt{1-4z/\mu_{R^2}}-1/2}\left(\cosh\frac{d(x,y)}{R}\right). \tag{72}$$

Geršgorin theorem allows us to estimate the lower bound for the bound state energy as done for $\mathbb{S}^2$ and $\mathbb{H}^3$. In order not to have zero as an eigenvalue, we must have

$$\sqrt{2}\left[\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\nu^2}{\mu_R^2}}\right)-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu_i^2}{\mu_R^2}}\right)\right]>\sum_{i\neq j}\int_{d_{ij}/R}^{\infty}\frac{e^{-(1/2)r\sqrt{1+4\nu^2/\mu_R^2}}}{\sqrt{\cosh r-\cosh d_{ij}/R}}\mathrm{d}r, \tag{73}$$

for all i and we have taken $z=-\nu^2$ and $\nu>\max_i\mu_i$. It is easy to see this inequality is satisfied for some values of ν because the left-hand side is an increasing function, whereas the right-hand side is a decreasing function of ν. However, it is not so easy to give an explicit estimate for ν by this inequality so we will estimate the functions on both sides. The inequality for the digamma functions[30]

$$\psi(x)>\log x-\frac{1}{x},\quad x>0, \tag{74}$$

which can be obtained from the integral representation (34), and $1/2+\sqrt{1/4+x^2}\geqslant x$ for all $x>0$ helps us that we can find the following inequality by assuming ν is sufficiently large,

$$\left[\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\nu^2}{\mu_R^2}}\right)-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu_i^2}{\mu_R^2}}\right)\right]>\left[\log\frac{\nu}{\mu_R}-\frac{\mu_R}{\nu}-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu_i^2}{\mu_R^2}}\right)\right]. \tag{75}$$

Since the right-hand side of Eq. (73) is $(N-1)\sqrt{2}Q_\lambda(\cosh d_{ij}/R)$ we can find an upper bound for this function, using another integral representation of the second type Legendre polynomials:[27]

$$Q_\lambda\left(\cosh\frac{d_{ij}}{R}\right)=\frac{1}{\Gamma(\lambda+1)}\int_0^\infty e^{-t\cosh d_{ij}/R}K_0\left(t\sinh\frac{d_{ij}}{R}\right)t^\lambda \mathrm{d}t, \tag{76}$$

where $\Im(d_{ij}/R)=0$ and $\lambda=\frac{1}{2}\sqrt{1+4\nu^2/\mu_R^2}-1/2$. Using the estimate for the function K_0 given in Eq. (48), we obtain

$$\sqrt{2}Q_\lambda\left(\cosh\frac{d_{ij}}{R}\right)<\frac{2\sqrt{2}}{\Gamma(\lambda+1)\sinh\dfrac{d_{ij}}{R}}\int_0^\infty e^{-t(\cosh d_{ij}/R+(1/2)\sinh d_{ij}/R)}t^{\lambda-1}\mathrm{d}t$$

and the right-hand side is just the gamma function, then the estimate becomes

$$\sqrt{2}Q_\lambda\left(\cosh\frac{d_{ij}}{R}\right)<\frac{2\sqrt{2}\Gamma(\lambda)}{\Gamma(\lambda+1)\left(\cosh\dfrac{d_{ij}}{R}+\dfrac{1}{2}\sinh\dfrac{d_{ij}}{R}\right)^\lambda\sinh\dfrac{d_{ij}}{R}}.$$

Using identity $\Gamma(\lambda+1)=\lambda\Gamma(\lambda)$ and the assumption $\nu/\mu_R>1$ and $\sqrt{1+4\nu^2/\mu_R^2}>2\nu/\mu_R$, we get

$$\begin{aligned}\sqrt{2}Q_\lambda\left(\cosh\frac{d_{ij}}{R}\right)&<\frac{4\sqrt{2}}{\left(\dfrac{2\nu}{\mu_R}-1\right)}\frac{1}{\left(\cosh\dfrac{d_{ij}}{R}+\dfrac{1}{2}\sinh\dfrac{d_{ij}}{R}\right)^\lambda\sinh\dfrac{d_{ij}}{R}}\\&<\frac{4\sqrt{2}}{\dfrac{\nu}{\mu_R}}\frac{e^{-(\nu/\mu_R-1/2)\log(\cosh d_{ij}/R+(1/2)\sinh d_{ij}/R)}}{\sinh\dfrac{d_{ij}}{R}}.\end{aligned} \tag{77}$$

Also, by choosing $d\equiv\min_{i\neq j}d_{ij}$ and $\mu\equiv\max_i\mu_i$, we easily find

$$\left[\log\frac{\nu}{\mu_R}-\frac{\mu_R}{\nu}-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu_i^2}{\mu_R^2}}\right)\right]>\left[\log\frac{\nu}{\mu_R}-\frac{\mu_R}{\nu}-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu^2}{\mu_R^2}}\right)\right], \tag{78}$$

and

$$\frac{e^{-(\nu/\mu_R-1/2)\log(\cosh d_{ij}/R+(1/2)\sinh d_{ij}/R)}}{\sinh\dfrac{d_{ij}}{R}}<\frac{e^{-(\nu/\mu_R-1/2)\log(\cosh d/R+(1/2)\sinh d/R)}}{\sinh\dfrac{d}{R}}. \tag{79}$$

Therefore, we impose

$$\left[\log\frac{\nu}{\mu_R}-\frac{\mu_R}{\nu}-\psi\left(\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\mu^2}{\mu_R^2}}\right)\right]>\frac{4(N-1)}{\dfrac{\nu}{\mu_R}}\frac{e^{-(\nu/\mu_R-1/2)\log(\cosh d/R+(1/2)\sinh d/R)}}{\sinh\dfrac{d}{R}}. \tag{80}$$

It is immediately seen that there exists a critical value $\nu>\nu^*$ for a given d and N for which this inequality is satisfied and zero is not an eigenvalue. The last inequality can be written as

$$e^{(\nu/\mu_R-1/2)\log(\cosh d/R+(1/2)\sinh d/R)}\left(\frac{\nu}{\mu_R}\log\left(\frac{\nu}{\mu_R e^{\psi(1/2+\sqrt{1/4+\mu^2/\mu_R^2})}}\right)-1\right)>\frac{4(N-1)}{\sinh\dfrac{d}{R}}.$$

If $\nu/\mu_R>e^{\psi(1/2+\sqrt{1/4+\mu^2/\mu_R^2})+1}$ (independent of N), then we have the lower bound of the ground state energy

$$E_{\mathrm{gr}} \geqslant -\nu^{*2} = -\mu_R^2 \left[\frac{A + W\left(\dfrac{4(N-1)Ae^{-A/2}}{\sinh \dfrac{d}{R}} \right)}{A} \right]^2, \tag{81}$$

where we define $A \equiv \log(\cosh d/R + (1/2)\sinh d/R)$ for simplicity of notation. For large values of N as long as the ratio μ/μ_R and d/R is finite, the behavior of the bound state energy is given by

$$E_{\mathrm{gr}} \sim -\mu_R^2 \left[\frac{\log N - \log\log N}{\log\left(\cosh \dfrac{d}{R} + \dfrac{1}{2} \sinh \dfrac{d}{R} \right)} \right]^2. \tag{82}$$

This problem again is an example of a certain kind of dimensional transmutation in nonrelativistic quantum mechanics. By dimensional analysis, the Hamiltonian of the system contains intrinsic energy scales $\hbar^2/md_{ij}^2$ and $\hbar^2/2mR^2$. However, after the renormalization, we obtain new parameters μ_i^2 with energy dimensions. Hence, the number of parameters we expect for the energy at the beginning has changed after the renormalization. As it happens in the $\mathbb{S}^2$ case, the delta potentials on $\mathbb{H}^2$ are an example of a generalized dimensional transmutation.

V. CONCLUSION

In this work, we studied a particle moving under the influence of N attractive Dirac delta interactions on some special Riemannian manifolds. We renormalized the problem and find a finite dimensional matrix Φ, called the characteristic matrix, by means of which a well-defined expression for the resolvent can be written. All the information about the bound states can be obtained from the characteristic matrix. The renormalization can be done by means of the heat kernel and this is equivalent to the sharp cut-off method for the eigenvalues of the Laplacian, in the case of compact manifolds. We have studied the problem on particular compact and noncompact manifolds, $\mathbb{S}^2$, $\mathbb{H}^2$, and $\mathbb{H}^3$ and we give explicit lower bound estimates on the bound state energies for each problem. Although we are concerned with particular manifolds, the basic idea for the renormalization can be applied also to general manifolds.

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Anomaly-free sets of fermions

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We present new techniques for finding anomaly-free sets of fermions. Although the anomaly cancellation conditions typically include cubic equations with integer variables that cannot be solved in general, we prove by construction that any chiral set of fermions can be embedded in a larger set of fermions which is chiral and anomaly-free. Applying these techniques to extensions of the standard model, we find anomaly-free models that have arbitrary quark and lepton charges under an additional U(1) gauge group. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Gauge symmetries successfully describe the electromagnetic, weak, and strong interactions of particle physics. Nevertheless, unitarity and renormalizability of the standard model do not necessarily follow from a classical invariance of the Lagrangian under $SU(3)_C \times SU(2)_W \times U(1)_Y$ gauge transformations: one-loop SU(N) and U(1) gauge anomalies must also be absent.[1–3]

In order to avoid these local gauge anomalies, the sum over triangle diagrams with gauge bosons as external lines and charged fermions running in the loops must vanish. As a consequence, the sums over loops with more external lines and over higher-order diagrams automatically vanish.[4,2] Similarly, the sum over triangle diagrams involving two gravitons and one U(1) gauge boson in the external lines must vanish, or else this mixed gravitational U(1) anomaly will also lead to an explicit breaking of the gauge symmetry by gravitational interactions (for a review see Ref. 5). Finally, the SU(2) gauge symmetry may suffer from a global gauge anomaly unless the number of Weyl fermion doublets is even.[6]

A remarkable property of all elementary fermions discovered so far is that they form a chiral set—none of them can have a gauge invariant mass term. The cancellation of anomalies within a chiral set of fermions is highly nontrivial. Given the observed $SU(3)_C \times SU(2)_W$ representations found in the standard model, the anomaly cancellation conditions are restrictive enough to uniquely determine the $U(1)_Y$ charges, assuming that not all of them are zero. More strikingly, the *minimal* anomaly-free chiral set of fermions charged under $SU(3)_C \times SU(2)_W \times U(1)_Y$ is exactly given by a standard model generation.[7] Therefore, anomaly cancellation provides an explanation for the fermion structure of the standard model which is an alternative to the explanation provided by grand unified theories where, for example, an entire standard model generation and right-handed neutrino can be embedded in a single, anomaly-free SO(10) representation—although it must be noted that many low energy hypercharge assignments are consistent with this embedding.[8]

Anomaly cancellation will constrain the charges of the standard model fermions under any newly discovered gauge groups, whether these groups follow from grand unification or not. Many models of physics beyond the standard model incorporate new gauge groups, and the couplings of

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the standard model fermions to the gauge bosons associated with these groups are completely determined by the spectrum of charges. It is therefore useful to have methods that allow finding, in general, sets of fermions which are anomaly free under arbitrary gauge groups. Since vector-like pairs of fermions do not contribute to these anomalies, a complete description of anomaly-free sets hinges only on the identification of all *chiral* anomaly-free sets.

Furthermore, if the chiral set of standard model fermions is charged under a new gauge group, anomaly cancellation usually dictates the presence of additional fermions. The complete set of fermions under the full gauge group would most likely be chiral. Imagine instead that the full theory was completely vector-like—after the breaking of the extended gauge symmetry to $SU(3)_C \times SU(2)_W \times U(1)_Y$, one would be left with both the observed standard model fields and a set of conjugate partners. To avoid mixing with the standard model fields, these conjugate partners should have large masses that proceed through electroweak symmetry breaking, which would induce too large corrections to electroweak observables.

In the case of SU(N) gauge groups, comprehensive lists of anomaly-free sets have been identified using numerical methods.[9] By contrast, anomaly-free sets of chiral fermions charged under a U(1) gauge group, or under direct products of gauge groups including at least one U(1) group, have been less thoroughly catalogued, despite the common appearance of extra U(1) groups in connection to flavor symmetry (see, e.g., Refs. 10 and 11), supersymmetry breaking (see, e.g., Ref. 12), neutrino masses,[13–17] and many other model building issues (see, e.g., Ref. 18). Many of these constructions depend on the existence of a chiral set of fermions.

If the quarks and leptons have arbitrary charges under a new U(1), then there are a number of gauge anomalies that need to be cancelled. Usually, this is achieved by the inclusion of additional fermions with carefully chosen charges. An alternative is available in the context of string theory, when the U(1) symmetry is spontaneously broken at a scale close to the string scale: the four-dimensional gauge anomalies associated with the U(1) can be cancelled by the Green–Schwartz mechanism.[19] The question of when can anomalies be cancelled by additional fermions has not been given a general answer. It is often stated, though, that there are cases where the anomalies can be cancelled *only* by the Green–Schwartz mechanism[20,10] (in these cases it is usually said that there is an "anomalous U(1)," albeit this is a misleading phrase).

In this paper we prove that any set of fermions with arbitrary charges under a gauge symmetry involving any number of non-Abelian and U(1) groups can be embedded in an anomaly-free chiral set that contains additional fermions—even when any ratio of charges is a rational number. This conclusion is far from obvious: it involves cubic Diophantine equations (i.e., cubic equations with integer solutions), which include for the case of three fermions the (in)famous Fermat's last theorem.

We focus on rational charges since such charges seem more natural, but more importantly, they solve a real problem: any U(1) gauge theory eventually hits a Landau pole unless it is embedded in a non-Abelian group, which is possible only if these fermions have commensurate charges. (i.e., rational up to a normalization of the gauge coupling).[21] Even in string theory the gauge charges appear to be commensurate, although we are not aware of a general proof of this statement.

In particular, we find that any "anomalous U(1)" that can be made nonanomalous by the Green–Schwartz mechanism can also be made nonanomalous by new fermions. More importantly, our theorem shows that it is possible to add new fermions such that the anomalies cancel for any charges of the standard model fermions under a new U(1). This is relevant for the experimental searches for Z' bosons,[22,23] because the Z' couplings to quarks and lentons are fixed, up to an overall normalization, by the U(1) charges.

In Sec. II we discuss U(1) gauge anomalies, and derive our main results. These results are then generalized to any gauge group in Secs. III and IV. In Sec. V we apply our results to the phenomenologically interesting case of a U(1) extension of the standard model gauge group. Our conclusions are presented in Sec. VI.

II. U(1) GAUGE ANOMALIES

Consider a set of n left-handed Weyl fermions with charges $z_i, i=1,\ldots,n$ under a U(1) gauge theory. The $[\mathrm{U}(1)]^3$ and mixed U(1)-gravitational anomaly cancellation conditions are given by

$$\sum_{i=1}^{n} z_i^3 = 0,$$

$$\sum_{i=1}^{n} z_i = 0. \tag{2.1}$$

We are interested in chiral sets, so the charges of the fermions must satisfy

$$z_i + z_j \neq 0 \tag{2.2}$$

for any i, j, and in particular $z_i \neq 0$. For $n \leqslant 4$, the first Eq. (2.1) can be easily solved once the constraint given by the second Eq. (2.1) is imposed, and the result is that all the fermions are vector-like, i.e., do not satisfy Eq. (2.2). Hence, at least five chiral fermions are needed to satisfy Eqs. (2.1).[14,16]

When the charges are arbitrary real numbers, it is evident that there are solutions to Eqs. (2.1) for any $n \geqslant 5$. In realistic physics theories, however, it is generally expected that the charges are rational numbers up to an overall normalization of the gauge coupling. The reason for that is that the U(1) gauge coupling increases with the energy, and the gauge theory appears to need a cutoff above which some new physics would have to soften the running of the gauge coupling. Typically, that new physics involves the embedding of the U(1) group in a non-Abelian gauge group, which guarantees that the ratio of U(1) charges are rational numbers. We will therefore concentrate on the case where the ratio of any two z_i charges is rational. Furthermore, the overall normalization of the U(1) charges is arbitrary, so we can take all z_i to be integers without loss of generality. For integer charges z_i, Eqs. (2.1) are equivalent to identifying the integer points in the intersection of a cubic hypersurface and a hyperplane in $\mathbb{R}^n$. The first Eq. (2.1) is a cubic Diophantine equation, and there are no known methods of solving it in general for a fixed but arbitrary value of n.

A. Construction of anomaly-free chiral sets

There is often a more straightforward problem that arises in model building: given a chiral set of fermions, which is anomalous, is it possible to include more fermions such that the larger set is chiral and anomaly free? To address this issue, we make the important observation that any fermion with integer charge z is part of the following anomaly-free set:

$$\left\{1 \times (z), \quad \frac{z}{6}(z^2-1) \times (-2), \quad \frac{z}{3}(z^2-4) \times (1)\right\}. \tag{2.3}$$

where the notation $p \times (x)$ means that there are $|p|$ left-handed fermions with charge $\pm x$, the + and − signs corresponding to $p>0$ and $p<0$, respectively. It is not surprising that the two anomaly conditions can be satisfied by two numbers, the numbers of fields of charge 1 and −2. What is nontrivial is that the coefficients p are always integers for any integer z, as a physical number of fields must be. Since fermions with charge ±1, ±2 are central to this construction, we call them basic charges for U(1). If z is one of the basic charges, then the set is vector-like. Otherwise, the set is chiral.

Given a chiral set of charges $S=\{z_i, i=1,\ldots,n\}$ that may not be anomaly free, we construct a chiral anomaly free set that consists only of charges in S and, for each one, the appropriate number of fermions with the basic charges, ±1 and ±2, as in Eq. (2.3). If some of the charges in S are themselves basic charges, then we must initially rescale all charges so this is no longer the case. In many cases the resulting anomaly-free set will still contain some vector-like pairs of ±1 and ±2,

TABLE I. Anomaly-free chiral sets with $n=5,\ldots,9$ integer charges.

Number of fermions	Charges
5	{1,5,−7,−8,9}
	{2,4,−7,−9,10}
6	{1,1,1,−4,−4,5}
	{−1,2,3,−5,−5,6}
7	{1,2,2,−3,−3,−3,4}
	{−1,−1,3,4,−6,−6,7}
	{1,3,−4,5,−6,−6,7}
	{2,3,3,−4,−5,−6,7}
8	{1,1,2,3,−4,−4,−5,6}
	{2,2,2,2,−5,−5,−5,7}
9	{2,2,2,−3,−3,4,−5,−5,6}
	{1,1,1,2,−4,5,−7,−9,10}
	{1,−3,4,5,5,−6,−7,−9,10}

so the final step is to remove all such pairs. This completes our proof by construction that *for any chiral set of charges S there is a larger set which includes S and is chiral and anomaly free.*

B. Anomaly-free chiral sets with a small number of fermions

The above successful construction of chiral, anomaly-free sets often requires a disturbingly large number of basic charges. We now discuss methods for obtaining smaller sets of fermions which have the advantage of pushing the Landau pole to higher energies.

First, to show that smaller sets are even possible, let us first observe that *for any number* $n \geqslant 5$ *of chiral fermions there is a chiral set of* $U(1)$ *charges that is anomaly free.* To prove this statement it is sufficient to show that there is a chiral set for each $n=5,\ldots,9$. An anomaly-free chiral set with arbitrary $n \geqslant 10$ can always be constructed using linear combinations of chiral sets with $n=5,\ldots,9$. In Table I we show anomaly-free chiral sets with $n=5,\ldots,9$ integer charges that have the maximum charge, chosen to be positive, as small as possible (we include all sets with the two smallest values of the maximum charge).

To reduce the numbers of fermions in a set S we again rely on the construction of Eq. (2.3). Just as the anomaly contribution from a single charge z can be cancelled by the prescribed number of fields with charges $+1$ and -2, the reverse is also true: the anomaly contribution from a number of fields of charges $+1$ and -2 can be cancelled off by a single charge z'. In this way, large numbers of basic charges are exchanged for a single fermion with a large charge.

The numerical techniques that can address the problem of finding small anomaly-free sets are defined on lattices. For our purposes, a lattice is any set of vectors in $\mathbb{R}^n$, that is closed under addition and subtraction (i.e., for any two vectors x, y in a lattice, both $x+y$ and $x-y$ are also in the lattice). Each axis of $\mathbb{R}^n$ represents a possible value of fermion charge, and the coordinates on an axis indicate the *number* of fermions with that charge. Negative coordinates correspond to positive numbers of fermions with the conjugate charge.

The set of chiral, anomaly-free sets forms a lattice, denoted L. For any chiral set X, let $V(X)$ denote the vectorization of X, which is the image of X in the space $\mathbb{R}^n$. For example, if X is the set $\{1,5,-7,-8,9\}$, we would define $V(X)$ to be the vector $[1,0,0,0,1,0,-1,-1,1,0,0,\ldots]$ corresponding to the fact that there is one fermion of charge 1, zero of charge 2, one of charge -7, etc. Let L denote the set of all such vectorizations $L=\{V(X)\,|\,X \text{ is chiral and anomaly free}\}$. We can add elements of L: for any two chiral, anomaly-free sets X and Y, the sum $V(X)+V(Y)$ corresponds to the anomaly-free chiral set that contains all the fermions in both X and Y, followed by the removal of all vector-like pairs. We can similarly subtract any two elements of L to find another element of L; therefore L is a lattice.

For a given z, the vectorization of the construction given in Eq. (2.3) is an element of L, which we call $C(z)$. $C(z)$ contains one fermion with charge z, and the needed number of basic charges to

satisfy the anomaly equations. The set $\{C(z_i)|z_i \in \pm 3,4,5,\ldots\}$ actually spans L: any element of L can be written, by construction, as a unique linear combination of the $C(z_i)$.

It follows that finding the smallest sets of anomaly-free chiral fermions is similar to finding the shortest vectors in L. This latter problem is called the "short vector problem" and has been studied extensively by mathematicians and computer scientists (for a review, see Ref. 24). An important distinction is that short vectors are here defined in terms of the ℓ^2 norm, which can differ from the ℓ^1 norm actually used to determine the number of fermions. Nevertheless, shortness in the ℓ^2 norm is a good approximation to shortness in the ℓ^1 norm, and sufficient for our purposes of finding small sets.

Even finding a vector which is at most $\sqrt{2}$ times as long as the shortest vector remains an nondeterministic polynomial (NP)-hard problem, i.e., at least as hard as any NP time problem.[25] This means that for very large numbers of fermions, it is impossible to have both accuracy and speed in an algorithm.

To set up the problem concretely, consider searching for an anomaly-free, chiral set with at most N fermions, whose maximum charge is m. A simple iterative approach over all possible numbers of fermions has a time complexity of the order of

$$2^{m-1}\frac{(N+m)!}{N!\,m!}. \tag{2.4}$$

Given a computing power of 10^{10} operations per second, it would take ~ 100 years to find the shortest solution for $N=30$, $m=20$. A better algorithm would be to search over all linear combinations of the basis vectors, $C(z_i)$. This has a time complexity of the order of

$$2^{m-3}\frac{(N+m-2)!}{N!\,(m-2)}, \tag{2.5}$$

and would take ~ 1 year for $N=30$, $m=20$.

Consider instead the Lenstra–Lenstra–Lovasz (LLL) algorithm,[26] readily available in mathematical packages, for attacking the shortest vector problem. The LLL algorithm requires as input the basis vectors $C(z_i)$ for $|z_i| < m$, and outputs a shorter, closer to orthogonal set of basis vectors that span the same lattice. The LLL algorithm has a time complexity of $\mathcal{O}(m^4 \log m)$, and takes $\sim 10^{-5}$ s for $m=20$. Note that this is polynomial in m instead of exponential, and does not involve the number of fermions N (this is possible because the solutions found using the LLL algorithm are by no means guaranteed to be minimal). In fact, they can be up to $2^{(m-1)/2}$ times larger than the minimal solutions. In practice, however, the solutions found are almost always reasonably short, and the significant decrease in time and ease of implementation make this approach worthwhile.

Since the LLL algorithm actually returns a new basis of short vectors which spans L, the algorithm can easily be adapted to solving another common problem in polynomial time: finding the shortest vector that contains a specific spectrum of fermion charges. Consider a specific set of charges $\{x_i\}$. To make the LLL algorithm handle this problem, we exchange the basis vectors $C(x_i)$ for the single basis vector $\Sigma_i C(x_i)$. The output basis set is guaranteed to include at least one short vector that includes the specified charges $\{x_i\}$.

Since we are interested in numbers of fermions that are not particularly large, it may eventually prove useful to adapt even exponential-time solutions to the shortest vector problem in order to identify anomaly-free sets. Although these solutions are exponential in m, a recent algorithm has a time complexity of order $\mathcal{O}(2^{m \log m})$, which take ~ 1 s for $m=20$.[24]

III. $U(1)_1 \times \cdots \times U(1)_m$

Now consider a set of fermions, $\psi_i, i=1,\ldots,n$, which are charged under $U(1)_1 \times \cdots \times U(1)_m$ gauge group. Let us denote the charges of ψ_i under $U(1)_a$, $a=1,\ldots,m$, by $z_{a,i}$. The

construction of anomaly-free sets will proceed as in the case of a single U(1): we will identify the number and structure of basic charges that are needed to cancel off the anomalies for any single fermion.

A. $m=2$

In the case of $U(1)_1 \times U(1)_2$ gauge group there are six types of anomalies: $[U(1)_1]^3$, mixed $U(1)_1$ gravitational, $[U(1)_2]^3$, mixed $U(1)_2$ gravitational, $[U(1)_1]^2 U(1)_2$, and $U(1)_1[U(1)_2]^2$. These anomalies cancel if and only if

$$\sum_{i=1}^{n} z_{1,i}^3 = \sum_{i=1}^{n} z_{1,i} = \sum_{i=1}^{n} z_{2,i}^3 = \sum_{i=1}^{n} z_{2,i} = \sum_{i=1}^{n} z_{1,i}^2 z_{2,i} = \sum_{i=1}^{n} z_{1,i} z_{2,i}^2 = 0. \tag{3.1}$$

A set of fermions is chiral with respect to $U(1)_1 \times U(1)_2$ if

$$z_{1,i} + z_{1,j} \neq 0 \quad \text{or} \quad z_{2,i} + z_{2,j} \neq 0, \tag{3.2}$$

for any i and j. Note that a chiral set with respect to $U(1)_1 \times U(1)_2$ may be chiral, partially vector-like, or entirely vector-like with respect to each of the individual U(1)s.

We now show that any set of fermions which is chiral with respect to $U(1)_1 \times U(1)_2$ can be embedded into an anomaly-free set of chiral fermions, as we showed in the previous section for a U(1) gauge theory. This follows from the fact that any fermion with integer charges (z_1, z_2), is part of the following anomaly-free set

$$\left\{ (z_1,z_2), \quad -\frac{z_1 z_2}{2}(z_1+z_2)\times(1,1), \quad -\frac{z_1 z_2}{2}(z_1-z_2)\times(-1,1), \quad -\frac{z_1}{6}(z_1^2-1)\times(2,0), \right.$$
$$\left. \frac{z_1}{3}(z_1^2+3z_2^2-4)\times(1,0), \quad -\frac{z_2}{6}(z_2^2-1)\times(0,2), \quad \frac{z_2}{3}(3z_1^2+z_2^2-4)\times(0,1) \right\} \tag{3.3}$$

where the notation $p\times(x_1,x_2)$ means that there are $|p|$ left-handed fermions with $U(1)_1 \times U(1)_2$ charges (x_1,x_2) for $p>0$, or $(-x_1,-x_2)$ for $p<0$. We now have 12 basic pairs of charges $\pm\{(1,1),(1,-1),(2,0),(1,0),(0,2),(0,1)\}$ that are needed to ensure anomaly cancellation. Note that the number of fermions with basic charges prescribed by Eq. (3.3) is automatically an integer. The proof for constructing an anomaly-free chiral set from any chiral set S proceeds exactly as in Sec. II A.

Finding small anomaly-free sets from this construction proceeds through a lattice construction similar to that of Sec. II B. With the larger gauge group $U(1)\times U(1)$, the only change we make is to make each axis of $\mathbb{R}^n$ correspond to a specific (z_1,z_2) charge, instead of a single U(1) charge z. This adaptation works for finding small anomaly-free sets for all of the other gauge groups considered in the remainder of this paper.

B. $m\geqslant 3$

In the case where the number of U(1) gauge groups is $m\geqslant 3$, there are $m(m^2+3m+8)/6$ equations that must be satisfied to ensure that the theory is anomaly free:

$$\sum_{i=1}^{n} z_{a,i} = \sum_{i=1}^{n} z_{a,i} z_{b,i} z_{c,i} = 0, \tag{3.4}$$

for any a, b, $c=1,\ldots,m$.

We construct anomaly-free chiral sets by showing that the anomalies of any fermion ψ_i can be cancelled by the anomalies of a set of additional chiral fermions, which is a generalization of the basic charges $\{(1,1),(1,-1),(2,0),(1,0),(0,2),(0,1)\}$ from Eq. (3.3).

Consider a fermion ψ with charges $(z_1,\ldots,z_m)$. Its $U(1)_a U(1)_b U(1)_c$ anomalies can be cancelled for any unequal a, b, $c=1,\ldots,m$ by a number $(-z_a z_b z_c)$ of fermions, labeled by χ_{abc}, a

TABLE II. Anomaly-free chiral set of charges under three U(1) groups.

Number of fermions	$U(1)_1$	$U(1)_2$	$U(1)_3$
1	z_1	z_2	z_3
$-z_1z_2z_3$	+1	+1	+1
$-z_1z_2(z_1+z_2-2z_3)/2$	+1	+1	0
$-z_1z_2(z_1-z_2)/2$	−1	+1	0
$-z_2z_3(z_2+z_3-2z_1)/2$	0	+1	+1
$-z_2z_3(z_2-z_3)/2$	0	−1	+1
$-z_3z_1(z_3+z_1-2z_2)/2$	+1	0	+1
$-z_3z_1(z_3-z_1)/2$	+1	0	−1
$-z_1(z_1^2-1)/6$	+2	0	0
$z_1(z_1^2-4)/3+z_1(z_2^2+z_3^2-z_2z_3)$	+1	0	0
$-z_2(z_2^2-1)/6$	0	+2	0
$z_2(z_2^2-4)/3+z_2(z_3^2+z_1^2-z_3z_1)$	0	+1	0
$-z_3(z_3^2-1)/6$	0	0	+2
$z_3(z_3^2-4)/3+z_3(z_1^2+z_2^2-z_1z_2)$	0	0	+1

$<b<c$, with charges $(+1,+1,+1)$ under $U(1)_a\times U(1)_b\times U(1)_c$ and charge 0 under all other groups. Then the $[U(1)_a]^2U(1)_b$ anomalies of ψ and χ_{abc} can be cancelled for any unequal $a,b=1,\ldots,m$ by a set of fermions composed of N_{ab}^{ω} fermions, labeled by $\omega_{ab}, a<b$, with charges $(+1,+1)$ under $U(1)_a\times U(1)_b$ and charge 0 under all other groups, $N_{ab}^{\omega\prime}$ fermions, labeled by $\omega'_{ab}, a<b$, with charges $(-1,+1)$ under $U(1)_a\times U(1)_b$ and charge 0 under all other groups, where

$$N_{ab}^{\omega}=z_az_b\left[\sum_{c=1}^{m}z_c-\frac{3}{2}(z_a+z_b)\right],$$

$$N_{ab}^{\omega\prime}=-\frac{1}{2}z_az_b(z_a-z_b). \tag{3.5}$$

The remaining $[U(1)_a]^3$ and mixed $U(1)_a$ gravitational anomalies can be cancelled for any $a=1,\ldots,m$ by a set of fermions composed of N_a^{ξ} fermions, labeled by ξ_a, with charges +2 under $U(1)_a$ and charge 0 under all other groups, and $N_a^{\xi\prime}$ fermions, labeled by ξ'_a, with charges +1 under $U(1)_a$ and charge 0 under all other groups, where

$$N_a^{\xi}=-\frac{1}{6}z_a(z_a^2-1),$$

$$N_a^{\xi\prime}=\frac{1}{3}z_a(z_a^2-4)+z_a\sum_{b\neq a}\left(z_b^2-z_b\sum_{c\neq a,c>b}z_c\right). \tag{3.6}$$

Therefore, we have constructed an anomaly-free chiral set that includes a fermion ψ of arbitrary charges $(z_1,\ldots,z_m)$

$$\left\{\psi,\quad -z_az_bz_c\times(\chi_{abc}),\quad N_{ab}^{\omega}\times(\omega_{ab}),\quad N_{ab}^{\omega\prime}\times(\omega'_{ab}),\quad N_a^{\xi}\times(\xi_a),\quad N_a^{\xi\prime}\times(\xi'_a)\right\} \tag{3.7}$$

In Table II we show the charges in the particular case $m=3$. Here, the basic charges are the fields χ,ω,ξ.

The proof for constructing an anomaly-free chiral set S' from any set chiral set S proceeds exactly as in Sec. II A.

IV. GENERALIZATION TO ANY GAUGE GROUP

We now extend our results to $G\times U(1)$ gauge groups, where G is any non-Abelian group. Consider a set of chiral fermions ψ_i, $i=1,\ldots,n$, whose charges are (R_i,z_i) under $G\times U(1)$. R_i are some irreducible representations of G. In addition to the $U(1)$ and $U(1)^3$ anomalies, the G^3 and $G^2U(1)$ anomalies also must cancel (all other mixed anomalies are zero). The G^3 anomaly is given by

$$A_{GGG}=\sum_i A(R_i), \tag{4.1}$$

where the anomaly of R_i, $A(R_i)$, is defined by

$$\mathrm{Tr}\big(\{T^a(R_i),T^b(R_i)\}T^c(R_i)\big)=\tfrac{1}{2}A(R_i)d^{abc}. \tag{4.2}$$

The totally symmetric tensor d^{abc} is determined by the anticommutation relation among the group generators $T^a(R_i)$. The $G^2U(1)$ anomaly is given by

$$A_{GG1}=\sum_i C(R_i)z_i, \tag{4.3}$$

where the Casimir of R_i, $C(R_i)$, is defined by

$$\mathrm{Tr}\big(T^a(R_i)T^b(R_i)\big)=\delta_{ab}C(R_i). \tag{4.4}$$

Finally, the $U(1)$ and $U(1)^3$ anomalies take the following form up to an overall normalization:

$$A_{1GG}=\sum_i d(R_i)z_i,$$

$$A_{111}=\sum_i d(R_i)z_i^3, \tag{4.5}$$

where $d(R_i)$ is the dimension of R_i. The set of fermions ψ_i is anomaly free if

$$A_{GGG}=A_{GG1}=A_{1gg}=A_{111}=0. \tag{4.6}$$

If any of these conditions is not satisfied, then we prove by construction that one can add more fermions such that the larger set is both chiral and anomaly free.

For each fermion with charges (R,z) with $z\neq 0$, we can construct an anomaly-free set

$$\left\{(R,z),\quad \frac{z}{6}(z^2-1)\times(R,-2),\quad \frac{z}{3}(z^2-4)\times(\overline{R},1),\quad \frac{1}{6}(z+1)(z+2)(z-3)\times(R,0)\right\}, \tag{4.7}$$

where $\overline{R}$ is the conjugate of R: $A(\overline{R})=-A(R)$, $C(\overline{R})=C(R)$, $d(\overline{R})=d(R)$. The notation $p\times(R,x)$ means that if $p\geqslant 0$ then there are p left-handed fermions with charge (R,x), while if $p<0$ then there are $-p$ left-handed fermions with charge $(\overline{R},-x)$. The additional fermions with charge $(R,0)$ are included to make the entire set vector-like under the G group. We have chosen a basis that is easy to write down explicitly, but in many cases is larger than necessary—one could instead make some of the $(R,1)$ fermions into $(\overline{R},1)$ fermions and remove the appropriate number of $(R,0)$ fermions leaving at most one fermion with charge 0 under $U(1)$.

To render the entire set $\{\psi_i,i=1,\ldots,n\}$ anomaly free and chiral, we first rescale the z_i charges to be different than $+1$ and -2, add the fermions for each field ψ according to Eq. (4.7), then discard any remaining vector-like pairs. Note that if any of the z_i charges is zero, then one could

add other fermions which are neutral with respect to U(1) that belong to nontrivial representations of G such that the entire set is anomaly free and chiral [as done in Ref. 9 for the case where $G=\mathrm{SU}(N)$].

Typically, the total number of additional fermions can be further reduced if instead of fermions transforming nontrivially under G we add some fermions which are singlets (belong to the 1 representation of G). For example, consider the case where the set $\{\psi_i, i=1,\ldots,n\}$ is anomaly free with respect to the non-Abelian group $G(A_{GGG}=0)$. In order to cancel the $G^2\mathrm{U}(1)$ anomaly we could add two more fermions with charges (R,z) and $(\overline{R},z')$ such that

$$z+z'=-\frac{1}{C(R)}\sum_i C(R_i)z_i. \tag{4.8}$$

One may ensure that all the U(1) charges are integers by an appropriate rescaling. The U(1) and $\mathrm{U}(1)^3$ anomalies can be finally cancelled by including a number N_1 of fermions with charges $(1,+1)$, and a number N_2 of fermions with charges $(1,-2)$, as prescribed in Sec. II A

$$N_1=\frac{1}{3}\left\{\sum_i d(R_i)z_i(z_i^2-4)+d(R)[z(z^2-4)+z'(z'^2-4)]\right\},$$

$$N_2=\frac{1}{6}\left\{\sum_i d(R_i)z_i(z_i^2-1)+d(R)[z(z^2-1)+z'(z'^2-1)]\right\}. \tag{4.9}$$

The remarkable feature that enables this construction is that N_1 and N_2 are integers for any integer charges z, z', z_i.

This procedure can immediately be extended to groups of the form $G_1\times\ldots\times G_m\times\mathrm{U}(1)$, where G_i are non-Abelian gauge groups. For example, a single fermion ψ with charge $(R_i,\ldots,R_m,z)$ is part of the anomaly free set

$$\left\{(R_1,\ldots,R_m,z),\quad \frac{z}{6}(z^2-1)\times(R_1,\ldots,R_m,-2),\quad \frac{z}{3}(z^2-4)\times(\overline{R}_1,\ldots,\overline{R}_m,1),\right.$$
$$\left.\frac{1}{6}(z+1)(z+2)(z+3)\times(R_1,\ldots,R_m,0)\right\}. \tag{4.10}$$

To extend these results to arbitrary $G_1\times\ldots\times G_m\times\mathrm{U}(1)_1\times\ldots\times\mathrm{U}(1)_{m'}$ groups, one may simply use the coefficients and the set of fermions χ, ω, ω', ξ, ξ' described in Sec. III B in place of the single z charges written above.

V. U(1) EXTENSION OF THE STANDARD MODEL GAUGE GROUP

The results presented in the previous sections have various applications to physics beyond the standard model. In this section we study a particularly important application. The elementary fermions discovered in experiments so far, with charges under the $\mathrm{SU}(3)_C\times\mathrm{SU}(2)_W\times\mathrm{U}(1)_Y$ gauge group listed in Table III, may be charged under a new Abelian gauge group, $\mathrm{U}(1)_z$, provided this is spontaneously broken. The $\mathrm{U}(1)_z$ charges of these standard model fermions determine the relative couplings of the Z' boson [the heavy gauge boson associated with $\mathrm{U}(1)_z$], and therefore its experimental signatures.

The discovery of a Z' boson with couplings to the known fermions which are not proportional to hypercharge would imply the existence of certain additional fermions[27] or antisymmetric tensor fields in extra dimensions.[19] Here, as an application of our results, we show that *any* couplings of a Z' boson to the standard model fermions are allowed by anomaly cancellation if additional fermions are present. For simplicity, we concentrate on generation-independent couplings. The same method can be easily applied to generation-dependent couplings (in that case, though, there are stronger phenomenological constraints from flavor-changing neutral currents).[28,23]

TABLE III. Gauge charges of the Standard Model fermions in the presence of a new U(1) group. An index labeling the three generations is implicit.

	$SU(3)_C$	$SU(2)_W$	$U(1)_Y$	$U(1)_z$
q_L	3	2	$+1/3$	z_q
u_R	3	1	$-4/3$	z_u
d_R	3	1	$-2/3$	z_d
l_L	1	2	-1	z_l
e_R	1	1	-2	z_e

The $U(1)_z$ charges of the standard model fermions lead in general to six different gauge anomalies: $SU(3)_C^2U(1)_z$, $SU(2)_W^2U(1)_z$, $U(1)_Y^2U(1)_z$, $U(1)_YU(1)_z^2$, $U(1)_z^3$, and $U(1)_z$. It is imperative to ask whether these anomalies can all be cancelled simultaneously by including additional fermions. According to the prescription outlined in Sec. IV one can construct anomaly-free sets for any rational values of the $U(1)_z$ charges.

However, realistic extensions of the standard model need additional constraints to be satisfied. One constraint is that there are no new stable particles with fractional electric charges (for a review of experimental limits, see Ref. 29). To avoid fractional electric charges, we choose to introduce only fermions that transform under the standard model gauge group in the same representations (or the conjugated ones) as the observed fermions, or are not charged under the standard model gauge group. One could relax this restriction, for example, by including fermions with larger integer electric charges, but we will not need this freedom here.

Electroweak measurements restrict severely the number of new chiral fermions charged under $SU(2)_W$. In order to satisfy this constraint, we require the new fermions to be vector-like with respect to the $SU(3)_C \times SU(2)_W \times U(1)_Y$, but chiral with respect to $U(1)_z$. Another constraint is that both the standard model fermions and the new ones must have masses, so that some Yukawa-type couplings to Higgs fields need to be gauge invariant. For any specified Higgs sector, this leads to constraints on the $U(1)_z$ charges. However, one can keep the $U(1)_z$ charges of the fermions arbitrary and still give masses to all fermions by including a sufficient number of scalars with $U(1)_z$-breaking Vacuum Expectation Value (VEV)s that have higher-dimensional interactions with the fermions.

To allow for completely arbitrary charge for the standard model fields under the new $U(1)_z$, the spectrum of fields listed in Table IV suffice, although other choices are possible as long as

TABLE IV. New fermions which, together with the three standard model generations (see Table III), form an anomaly-free set. The charges under the new $U(1)_z$ gauge group are restricted by Eqs. (5.1) and (5.3), while N_1 and N_2 are given in Eq. (5.4)

	$SU(3)_C$	$SU(2)_W$	$U(1)_Y$	$U(1)_z$
ψ_L^l ψ_R^l	1	2	-1	z_L^l z_R^l
ψ_L^e ψ_R^e	1	1	-2	z_L^e z_R^e
ψ_L^d ψ_R^d	3	1	$\frac{2}{3}$	z_L^d z_R^d
$\nu_R^j, j=1,\ldots,N_1$	1	1	0	-1
$\nu_R'^k, k=1,\ldots,N_2$	1	1	0	$+2$

there is at least one fermion charged under SU(3), another one charged under $SU(2)_W$, and yet another one charged under $U(1)_Y$. We will eventually show that the anomaly cancellation conditions can be solved for arbitrary rational values of z_q, z_u, z_d, z_e, and z_l, as well as rational values of all other charges. Given the freedom in choosing the normalization of the gauge coupling, we can take z_q, z_u, z_d, z_e, and z_l to be integers. Our method of approach is to first impose that all of the anomalies cancel except for the $U(1)_z$ gravitational and $U(1)_z^3$ ones. Finding the $U(1)_z$ charges of the ψ fields requires solving three linear equations, corresponding to the $SU(3)_C^2U(1)_z$, $SU(2)_W^2U(1)_z$, and $U(1)_Y^2U(1)_z$ anomalies, and one quadratic equation, corresponding to the $U(1)_YU(1)_z^2$ anomaly. Note that if we can guarantee that the $U(1)_z$ values of all fields are still rational after having imposed these relations, then the $U(1)_z$ and $U(1)_z^3$ anomaly equations can be cancelled as described in Sec. II by adding the needed number of fields ν_R and ν_R'. The remaining anomaly conditions are not affected by the ν_R and ν_R' fields, so the most difficult part of satisfying the anomaly conditions, the cubic $U(1)_z^3$ equation, is removed from the process.

Notice that we have chosen some of the fermions in Tables III and IV to be right handed. Their contributions to the anomalies are the same as those of a left-handed fermion in the complex conjugated representation. The three linear equations due to the $SU(3)^2U(1)_z$, $SU(2)^2U(1)_z$, and $U(1)_Y^2U(1)_z$ anomalies constrain linear combinations of the charges of the new fields to be

$$z_L^d - z_R^d = -3(2z_q - z_u - z_d),$$

$$z_L^l - z_R^l = -3(3z_q + z_l),$$

$$z_L^e - z_R^e = 3(2z_q + z_u + z_e). \tag{5.1}$$

To proceed with the $U(1)_YU(1)_z^2$ anomaly cancellation condition, given by

$$(z_L^d)^2 - (z_R^d)^2 + (z_L^l)^2 - (z_R^l)^2 + (z_L^e)^2 - (z_R^e)^2 = 3(z_q^2 - 2z_u^2 + z_d^2 - z_l^2 + z_e^2), \tag{5.2}$$

we consider the particular case where the three remaining linear combinations of ψ charges can also be written as linear combinations of z_q, z_u, z_l, z_d, and z_e. This reduces the $U(1)_YU(1)_z^2$ anomaly equation to a linear equation in the unknown coefficients which has a three parameter solution for general values of z_q, z_u, z_l, z_d, and z_e. We find that the charges of the new fields are given by

$$z_L^d = \left(-2 - \frac{3}{2}a_2 + a_1\right)z_q + \left(1 + \frac{a_1}{2}\right)z_u + 2z_d - \frac{a_2}{2}z_l + \frac{a_1}{2}z_e,$$

$$z_L^l = (-6 + a_2 - a_3)z_q - \frac{1}{2}(a_2 + a_3)z_u - \frac{a_2}{2}z_d - z_l - \frac{a_3}{2}z_e,$$

$$z_L^e = \left(2 + a_1 - \frac{3}{2}a_3\right)z_q + \left(1 - \frac{a_1}{2}\right)z_u - \frac{a_1}{2}z_d - \frac{a_3}{2}z_l + 2z_e, \tag{5.3}$$

where a_1, a_2, and a_3 are arbitrary even integers.

To complete the proof, we add the necessary number of ν_R and ν_R' fields as described in Sec. II to cancel the $U(1)_z$ gravitational and $U(1)_z^3$ anomalies

$$N_1 = \frac{1}{3}\sum_f d_f z_f(z_f^2 - 4) = (z_L^d)^3 - (z_R^d)^3 + \frac{2}{3}[(z_L^l)^3 - (z_R^l)^3] + \frac{1}{3}[(z_L^e)^3 - (z_R^e)^3] + 6z_q^3 - 3z_u^3 - 3z_d^3 + 2z_l^3 - z_e^3 + 16z_q - 4z_u,$$

$$N_2 = \frac{1}{6}\sum_f d_f z_f(z_f^2 - 1) = \frac{1}{2}(N_1 - 12z_q + 3z_u), \tag{5.4}$$

where f runs over all fermions, z_f is the $U(1)_z$ charge of the fermion, and d_f is the dimensionality of the $SU(3)_C \times SU(2)_W$ representation times ± 1 for left-handed and right-handed fermions, respectively. We emphasize that Eqs. (5.4) yield integer values for N_1 and N_2 for any integers z_q, z_u, z_d, z_e, and z_l and the values of N_1 and N_2 can be reduced using the numerical methods of Sec. II B. Our construction shows that all couplings of a Z' boson to the standard model fermions are allowed by anomaly cancellation, as long as additional fermions are present.

For illustration, let us pick some simple $U(1)_z$ charges for the standard model fermions, $z_d = z_l = z_e = 0$ and $z_q = z_u = 1$, and compute the number of right-handed neutrinos in Table IV that need to be included in an anomaly-free set. We could use the freedom to choose a_1, a_2, and a_3 in order to minimize N_1 and N_2, but for this simple case we just take $a_1 = a_2 = a_3 = 0$. Therefore, the charges of the ψ fermions follow from Eqs. (5.3) and (5.2): $z_L^d = -1$, $z_R^d = 2$, $z_L^l = z_R^e = -6$, and $z_R^l = z_L^e = 3$. Equation (5.4) then gives $N_1 = -75$ and $N_2 = -42$, which means that there are 75 right-handed neutrinos of $U(1)_z$ charge $+1$ and 42 right-handed neutrinos of $U(1)_z$ charge -2. This large number of right-handed neutrinos can be substantially reduced using Eq. (2.3). For example, the set $\{42 \times (-2), 75 \times (+1)\}$ can be replaced by one of the following sets of five right-handed neutrinos: $\{2 \times (-5), 1 \times (-3), 2 \times (+2)\}$ or $\{1 \times (-6), 2 \times (-3), 1 \times (+2), 1 \times (+1)\}$.

VI. CONCLUSIONS

The need to embed new U(1) gauge groups in non-Abelian groups forces a focus on integer-valued charges, up to a possible rescaling of the gauge coupling constant. Our results show that anomaly cancellation in a gauge theory, while highly constraining, can occur for *any* set of integer fermion charges through the addition of new integer-charged fields. This is akin to gauging $U(1)_{B-L}$ in the standard model: one is forced to add a right-handed neutrino to prevent gauge anomalies from appearing. That such anomaly-free sets exist is obvious when one constructs vector-like sets, but highly nontrivial for chiral integer-valued sets.

The main result is presented in Sec. II A for fermions charged under a U(1) gauge group, and subsequently extended to any other gauge groups. The key observation is that there always exists a certain *integer* number of basic charges that can cancel off the anomaly from a single fermion. When the sets are large, the numerical techniques discussed in Sec. II B allow a quick reduction of the set size.

Our solution is a complete description of chiral anomaly-free sets for $U(1)^m$ gauge theories. For gauge groups that have additional non-Abelian factors $G_1 \times \ldots \times G_m \times U(1)^{m'}$ we have concentrated on chiral anomaly-free sets that include vector-like fermions with respect to some of the non-Abelian groups. This is sufficient to prove that any fermion can be included in a larger chiral set of fermions that is anomaly free. Nevertheless, it would be interesting to extend our results and find a complete description of anomaly-free sets under gauge groups of the form $G_1 \times \ldots \times G_m \times U(1)^{m'}$ which are chiral with respect to each of the G_i groups.

If a gauge extension of the standard model is discovered, then we have argued that the full spectrum of the new theory will still be chiral: a completely vector-like theory would leave behind both the observed standard model fermions *and* a set of conjugate partners after the extended gauge symmetry breaks to $SU(3)_C \times SU(2)_W \times U(1)_Y$, which is not phenomenologically acceptable. Therefore, our results should have applications to a variety of extensions of the standard model. In Sec. V we have presented a particular application: if the standard model gauge group is extended to include a new U(1) group, then the standard model fermions may have arbitrary rational charges under the new U(1) and still the anomalies would cancel in the presence of certain additional fermions with rational charges.

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Exact analytical solution to the relativistic Klein-Gordon equation with noncentral equal scalar and vector potentials

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We present an alternative and simple method for the exact solution of the Klein-Gordon equation in the presence of the noncentral equal scalar and vector potentials by using Nikiforov-Uvarov method. The exact bound state energy eigenvalues and corresponding eigenfunctions are obtained for a particle bound in a potential of $V(r,\theta)=\alpha/r+\beta/(r^2\sin^2\theta)+\gamma\cos\theta/(r^2\sin^2\theta)$ type. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227258]

I. INTRODUCTION

In nuclear and high energy physics, one of the interesting problems is to obtain exact solutions of the Klein-Gordon, Duffin-Kemmer-Petiau, and Dirac equations for mixed vector and scalar potentials. The Klein-Gordon, Dirac, and Duffin-Kemmer-Petiau wave equations are frequently used to describe the particle dynamics in relativistic quantum mechanics. In recent years, a great deal of effort has been spent to solve these relativistic wave equations for various potentials by using different methods. These relativistic equations contain two objects: the four-vector linear momentum operator and the scalar rest mass. They allow us to introduce two types of potential coupling, which are the four vector potential (V) and the space-time scalar potential (S).

The Klein-Gordon equation with the vector and scalar potentials can be written as follows:

$$\left[-\left(i\frac{\partial}{\partial t}-V(\vec{r})\right)^2-\vec{\nabla}^2+(S(\vec{r})+M)^2\right]\psi(\vec{r})=0. \tag{1}$$

For the case $S(\vec{r})=\pm V(\vec{r})$, the solution of the Klein-Gordon equation has been studied recently.[1,2] The exact solutions of these equations are possible only for certain potentials such as Coulomb, Morse, Pöschl-Teller, Hulthen, and harmonic oscillator, etc., by using different methods.[3] The other exactly solvable ones are the ring-shaped potentials introduced by Hartmann[4] and Quesne.[5] These potentials involve an attractive Coulomb potential with a repulsive inverse square potential one. In particular, the Coulombic ring-shaped potential[6] revived in quantum chemistry by Hartmann and co-workers[7] and the oscillatory ring-shaped potential, systematically studied by Quesne,[5] have been investigated from a quantum mechanical viewpoint by using various approaches. The special case of the potential in spherical coordinates is

$$V(r,\theta)=\frac{\alpha}{r}+\frac{\beta}{r^2\sin^2\theta}+\gamma\frac{\cos\theta}{r^2\sin^2\theta} \tag{2}$$

introduced by Makarov *et al.*[8] This potential can be used in quantum chemistry and nuclear physics to describe the ring-shaped molecules like benzene and the interactions between the deformed pairs of the nuclei.

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In this paper, we introduce an alternative and simple method for the exact solution of the Klein-Gordon equation for the case where $S(\vec{r})=\pm V(\vec{r})$, considering a general angle dependent (noncentral) potential by using Nikiforov-Uvarov (NU) method.[9] This method is based on solving the second-order linear differential equations by reducing to a generalized equation of hypergeometric type.

The NU method is used to solve Schrödinger, Dirac, Klein-Gordon, and Duffin-Kemmer-Petiau wave equations in the presence of the exponential type potentials such as Woods-Saxon, Pöschl-Teller,[10] and Hulthen[11,12] and noncentral potential.[13] The aim of this study is to show that the NU method can be used to obtain exact solutions of noncentral potentials for Klein-Gordon equation. Thus, radial and angular parts of the Klein-Gordon equation with noncentral potential are solved by the NU method and it is seen that this method is applicable to noncentral type potential for relativistic wave equations.

In Sec. II, the Klein-Gordon equation with equal scalar and vector potentials is examined. In Sec. III, the Klein-Gordon equation in spherical coordinates for a particle in the presence of noncentral potential is separated into radial and angular parts. Section IV is devoted to a brief description of the NU method. Solutions of the radial and angular parts of the Klein-Gordon equation by using the NU method are presented in Sec. V. Finally, concluding remarks are given in Sec. VI.

II. KLEIN-GORDON EQUATION WITH EQUAL SCALAR AND VECTOR POTENTIALS

For the time-independent potentials we can write the total wave function as $\psi(\vec{r},t)=e^{-i\varepsilon t}\psi(\vec{r})$, where ε is the relativistic energy. The three-dimensional Klein-Gordon equation with the mixed vector and scalar potentials can be written as follows:

$$[\vec{\nabla}^2+(V(\vec{r})-\varepsilon)^2-(S(\vec{r})+M)^2]\psi(\vec{r})=0, \tag{3}$$

where M is the mass, ε is the energy, and $S(\vec{r})$ and $V(\vec{r})$ are the scalar and vectorial potentials, respectively. Now, if we take $S(\vec{r})=\pm V(\vec{r})$, the Klein-Gordon equation becomes

$$[\vec{\nabla}^2-2(\varepsilon\pm M)V(\vec{r})+\varepsilon^2-M^2]\psi(\vec{r})=0. \tag{4}$$

This equation describes a scalar particle, i.e., spin-0 particle. It is the Schrödinger equation for the potential $2V$ in the nonrelativistic limit. Thus, Alhaidari *et al.* conclude that only the choice $S=+V$ produces a nontrivial nonrelativistic limit with a potential function $2V$, and not V. Accordingly, it would be natural to scale the potential terms in Eq. (3) so that in the relativistic limit the interaction potential becomes V, not $2V$. Therefore, they modify Eq. (3) to read as follows:[1]

$$\left[\vec{\nabla}^2+\left(\tfrac{1}{2}V(\vec{r})-\varepsilon\right)^2-\left(\tfrac{1}{2}S(\vec{r})+M\right)^2\right]\psi(\vec{r})=0. \tag{5}$$

Thus, Eq. (4) is acquired as

$$[\vec{\nabla}^2-(\varepsilon\pm M)V(\vec{r})+\varepsilon^2-M^2]\psi(\vec{r})=0. \tag{6}$$

In Sec. III, for $S(\vec{r})=+V(\vec{r})$, if we take $V(\vec{r})$ as a general noncentral potential, the three-dimensional Klein-Gordon equation is separated into variables and the equation can be solved using the NU method.

III. SEPARATING VARIABLES OF THE KLEIN-GORDON EQUATION WITH NONCENTRAL POTENTIAL

In the spherical coordinates, the Klein-Gordon equation for a particle in the presence of a general noncentral potential $V(r,\theta)$ becomes

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}-(\varepsilon+M)V(r,\theta)+\varepsilon^2-M^2\right]\psi(r,\theta,\varphi)=0, \tag{7}$$

where $V(r,\theta)$ is a general noncentral potential as given by Eq. (2). If one assigns the corresponding spherical total wave function as $\psi(r,\theta,\varphi)=(1/r)R(r)Y(\theta,\varphi)$, then by selecting $Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$, the wave equation (7) for a general noncentral potential is separated into variables and the following equations are obtained:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{\lambda}{r^2}-(\varepsilon+M)\frac{\alpha}{r}+\varepsilon^2-M^2\right]R(r)=0, \tag{8}$$

$$\frac{\mathrm{d}^2\Theta(\theta)}{\mathrm{d}\theta^2}+\cot\theta\frac{\mathrm{d}\Theta(\theta)}{\mathrm{d}\theta}+\left[\lambda-\frac{m^2}{\sin^2\theta}-(\varepsilon+M)\left(\frac{\beta+\gamma\cos\theta}{\sin^2\theta}\right)\right]\Theta(\theta)=0, \tag{9}$$

$$\frac{\mathrm{d}^2\Phi(\varphi)}{\mathrm{d}\varphi^2}+m^2\Phi(\varphi)=0, \tag{10}$$

where m^2 and λ are the separation constants. The solution of Eq. (10) is well known and it is the azimuthal angle solution,

$$\Phi_m=Ae^{im\varphi}\quad(m=0,\pm1,\pm2,\ldots). \tag{11}$$

Equations (8) and (9) are radial and polar-angle equations and they will be solved by using the NU method,[9] given briefly in the following Sec. IV.

IV. NIKIFOROV-UVAROV METHOD

The nonrelativistic Schrödinger equation or similar time-independent second-order differential equations can be solved by using the NU method which is based on solutions of a general second-order linear differential equation with special orthogonal functions. In this method, for a given real or complex potential, the Schrödinger equation is transformed into a generalized equation of hypergeometric type with an appropriate $s=s(r)$ coordinate transformation and it can be written in the following form:

$$\psi(s)''+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s)=0, \tag{12}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Hence, from Eq. (12), the Schrödinger equation or the Schrödinger-type equations can be solved by means of this method for potentials we consider. In order to find a particular solution of Eq. (12), we use the separation of variables with the transformation

$$\psi(s)=\phi(s)y(s), \tag{13}$$

it reduces Eq. (12) to an equation of hypergeometric type,

$$\sigma(s)y''+\tau(s)y'+\lambda y=0 \tag{14}$$

and $\phi(s)$ is defined as a logarithmic derivative in the following form and its solutions can be obtained from

$$\phi'(s)/\phi(s)=\pi(s)/\sigma(s). \tag{15}$$

The other part $y(s)$ is the hypergeometric type function whose polynomial solutions are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{\mathrm{d}^n}{\mathrm{d}s^n}[\sigma^n(s)\rho(s)], \tag{16}$$

where B_n is a normalizing constant and the weight function $\rho(s)$ must satisfy the condition

$$(\sigma\rho)' = \tau\rho. \tag{17}$$

The function π and the parameter λ required for this method are defined as follows:

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \tag{18}$$

$$\lambda = k + \pi'. \tag{19}$$

On the other hand, in order to find the value of k, the expression under the square root must be square of a polynomial. Thus, a new eigenvalue equation for the Schrödinger equation becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \tag{20}$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \tag{21}$$

and its derivative is negative. By comparison of Eqs. (19) and (20), we obtain the energy eigenvalues.

V. SOLUTIONS OF THE RADIAL AND ANGLE-DEPENDENT EQUATIONS

A. Solutions of the radial equation and energy eigenvalues

The radial part of the Klein-Gordon equation is given as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\lambda}{r^2} - (\varepsilon + M)\frac{\alpha}{r} + \varepsilon^2 - M^2\right]R(r) = 0. \tag{22}$$

This equation can be further arranged as

$$R''(r) + (-\eta^2 r^2 - \xi^2 r - \lambda)\frac{1}{r^2}R(r) = 0 \tag{23}$$

with

$$\varepsilon^2 - M^2 = -\eta^2, \quad (\varepsilon + M) = \xi^2, \quad \lambda = \ell(\ell+1), \quad \alpha = -Ze^2, \tag{24}$$

which is now amenable to a NU solution. In order to find the solution of this equation, it is necessary to compare Eq. (23) with Eq. (12). By comparison, we obtain the following polynomials:

$$\tilde{\tau} = 0, \quad \sigma = r, \quad \tilde{\sigma} = -\eta^2 r^2 - \xi^2 r - \lambda. \tag{25}$$

Substituting these polynomials in Eq. (18), we obtain π function as

$$\pi = \tfrac{1}{2} \pm \tfrac{1}{2}\sqrt{4\eta^2 r^2 + 4r(k + \xi^2) + 4\lambda + 1}. \tag{26}$$

The expression in the square root must be the square of polynomial in respect to the NU method.

Therefore, we can determine the constant k by using the condition that the discriminant of the square root is zero, that is

$$k = -\xi^2 \pm 2\sqrt{\eta^2}\left(\ell + \tfrac{1}{2}\right). \tag{27}$$

In view of that, one can find new possible functions for each k as

$$\pi = \begin{cases} \dfrac{1}{2} \pm \left[\sqrt{\eta^2} r + \left(\ell + \dfrac{1}{2}\right)\right], & \text{for } k = -\xi^2 + 2\sqrt{\eta^2}\left(\ell + \dfrac{1}{2}\right) \\ \dfrac{1}{2} \pm \left[\sqrt{\eta^2} r - \left(\ell + \dfrac{1}{2}\right)\right], & \text{for } k = -\xi^2 - 2\sqrt{\eta^2}\left(\ell + \dfrac{1}{2}\right). \end{cases} \tag{28}$$

For the polynomial of $\tau = \tilde{\tau} + 2\pi$ which has a negative derivative, we get

$$k = -\xi^2 - 2\sqrt{\eta^2}\left(\ell + \tfrac{1}{2}\right), \quad \pi = \tfrac{1}{2} - \left[\sqrt{\eta^2} r - \left(\ell + \tfrac{1}{2}\right)\right]. \tag{29}$$

Using $\chi = k + \pi'$ together with the values k and π, τ and χ can be respectively obtained as

$$\tau = 2(\ell + 1 - \sqrt{\eta^2} r), \tag{30}$$

$$\chi = -\xi^2 - \sqrt{\eta^2}(2\ell + 2). \tag{31}$$

Another definition of χ_N is given at Eq. (20),

$$\chi_N = 2N\sqrt{\eta^2}. \tag{32}$$

Comparing this with Eq. (31) and inserting the values of η and ξ, the exact energy eigenvalues of the radial part of the Klein-Gordon equation with the noncentral potential are derived as

$$\varepsilon_{N\ell} = M \frac{\left((N + \ell + 1)^2 - \dfrac{\alpha^2}{4}\right)}{\left((N + \ell + 1)^2 + \dfrac{\alpha^2}{4}\right)}, \tag{33}$$

where N denotes the radial quantum number. This is not equal to the well-known positive energy spectrum of the relativistic Klein-Gordon-Coulomb problem but gives the correct nonrelativistic limit in the case of weak coupling.

Using σ and π in Eqs. (14)–(16), we can find the wave functions $y(r) = y_{N\ell}(r)$ and $\phi(r)$:

$$R_{N\ell}(z) = C_{N\ell} z^{\ell+1} \exp\left(-\frac{z}{2}\right) L_N^{2\ell+1}(z), \tag{34}$$

where $L_N^{2\ell+1}(z)$ stands for the associated Laguerre functions whose argument is equal to $z = [(\varepsilon + M)Ze^2/(N + \ell + 1)]r$ and $C_{N\ell}$ is normalization constant determined by $\int_0^\infty R_{N\ell}^2(r)dr = 1$,[14] the corresponding normalized wave functions are finally obtained as

$$R_{n'\ell}(r) = \left(\frac{2(\varepsilon + M)Ze^2}{n'}\right)^{1/2} \left(\frac{(n' - \ell - 1)!}{n'\Gamma(n' + \ell + 1)}\right)^{1/2} \left(\frac{2(\varepsilon + M)Ze^2}{n'}\right)^{\ell+1} \times r^{\ell+1} \exp\left(-\frac{(\varepsilon + M)Ze^2}{n'} r\right) L_{n'-\ell-1}^{2\ell+1}\left(\frac{(\varepsilon + M)Ze^2}{n'} r\right), \tag{35}$$

where $n' = N + \ell + 1$. This equation is also stands for solution of the radial Klein-Gordon equation with Coulomb potential, since the radial Klein-Gordon equation with noncentral potential contains only Coulombic potential terms.

B. Eigenvalues and eigenfunctions of the angle-dependent equation

As for the solutions of the angle-dependent part of the Klein-Gordon equation, we may also derive eigenvalues and eigenfunctions of the polar angle part of the Klein-Gordon equation similar to the method as given in Sec. IV.

Equation (9) can be written in the following form by introducing a new variable, $x=\cos\theta$,

$$\frac{d^2\Theta(x)}{dx^2}-\frac{2x}{1-x^2}\frac{d\Theta(x)}{dx}+\left(\frac{\lambda(1-x^2)-m^2-(\varepsilon+M)(\beta+\gamma x)}{(1-x^2)^2}\right)\Theta(x)=0. \tag{36}$$

To apply the NU method, we compare Eq. (36) with Eq. (12). By comparison, we obtain the following polynomials:

$$\tilde{\tau}=-2x,\quad \sigma=1-x^2,\quad \tilde{\sigma}=-\lambda x^2-\gamma x+(\lambda-m^2-\beta). \tag{37}$$

The function π is obtained by putting the above-noted expression in Eq. (18),

$$\pi=\pm\sqrt{x^2(\lambda-k)+\gamma x-(\lambda-m^2-\beta-k)}. \tag{38}$$

The expression in the square root must be square of a polynomial. Then, one can find new possible functions for each k as

$$\pi=\pm\begin{cases} x\sqrt{\dfrac{m^2+\beta+u}{2}}+\sqrt{\dfrac{m^2+\beta-u}{2}}, & \text{for } k=\dfrac{2\lambda-m^2-\beta}{2}-\dfrac{1}{2}u \\ x\sqrt{\dfrac{m^2+\beta-u}{2}}+\sqrt{\dfrac{m^2+\beta+u}{2}}, & \text{for } k=\dfrac{2\lambda-m^2-\beta}{2}+\dfrac{1}{2}u, \end{cases} \tag{39}$$

where $u=\sqrt{(m^2+\beta)^2-\gamma^2}$. For the polynomial of $\tau=\tilde{\tau}+2\pi$ which has a negative derivative,

$$\tau=-2\sqrt{\frac{m^2+\beta-u}{2}}-2x\left(1+\sqrt{\frac{m^2+\beta+u}{2}}\right). \tag{40}$$

Using $\chi=k+\pi'$ and its other definition $\chi_n=-n\tau'-[n(n-1)/2]\sigma''$ given by Eqs. (19) and (20), following expressions for χ are obtained, respectively,

$$\chi=\frac{2\lambda-(m^2+\beta)}{2}-\frac{1}{2}u-\sqrt{\frac{m^2+\beta+u}{2}}, \tag{41}$$

$$\chi_n=2n\left(1+\sqrt{\frac{m^2+\beta+u}{2}}\right)+n(n-1). \tag{42}$$

Equating Eqs. (41) and (42) and using the definition of $\lambda=\ell(\ell+1)$, we obtain the ℓ values as

$$\ell=\sqrt{\frac{m^2+\beta+\sqrt{(m^2+\beta)^2-\gamma^2}}{2}}+n. \tag{43}$$

If we insert ℓ values obtained by Eq. (43) into eigenvalues of the radial part of the Klein-Gordon equation with the noncentral potential given by Eq. (33), we finally find the energy eigenvalues for a bound electron in the presence of a noncentral potential by Eq. (2)

$$E_{Nnm} = M\frac{\left[\left(N+\sqrt{\frac{m^2+\beta+\sqrt{(m^2+\beta)^2-\gamma^2}}{2}}n+1\right)^2-\frac{\alpha^2}{4}\right]}{\left[\left(N+\sqrt{\frac{m^2+\beta+\sqrt{(m^2+\beta)^2-\gamma^2}}{2}}+n+1\right)^2+\frac{\alpha^2}{4}\right]}, \tag{44}$$

where $\beta=(\varepsilon+M)\beta$ and $\gamma=(\varepsilon+M)\gamma$. The nonrelativistic limit ($\alpha\ll 1$) of the energy spectrum for the Hartmann problem where $\beta\neq 0$ and $\gamma=0$ is

$$E_{Nnm} = -\frac{M\alpha^2}{2}(N+n+1+\sqrt{m^2+\beta(\varepsilon+M)}). \tag{45}$$

Then, the wave functions of the polar-angle part of the Klein-Gordon equation, using σ and π in Eqs. (14)–(16), are obtained:

$$\phi = (1-x)^{B+C/2}(1+x)^{B-C/2}, \tag{46}$$

$$\rho = (1-x^2)^B\left(\frac{1+x}{1-x}\right)^{-C}, \tag{47}$$

$$y_n = B_n(1-x)^{-(B+C)}(1+x)^{-(B-C)}\frac{d^n}{dx^n}[(1+x)^{n+B-C}(1-x)^{n+B+C}], \tag{48}$$

where $B=\sqrt{[(m^2+\beta+u)/2]}$ and $C=\sqrt{[(m^2+\beta-u)/2]}$. The polynomial solution of y_n is expressed in terms of Jacobi polynomials which are one of the orthogonal polynomials, giving $\approx P_n^{(B+C,B-C)}(x)$. Substituting Eqs. (46)–(48) into Eq. (13), the corresponding wave functions are found to be

$$\Theta_n(x) = N_n(1-x)^{(B+C)/2}(1+x)^{(B-C)/2}P_n^{(B+C,B-C)}(x), \tag{49}$$

where N_n is normalization constant determined by $\int_{-1}^{+1}[\Theta_n(x)]^2 dx=1$ and using the orthogonality relation of Jacobi polynomials,[14,15] the normalization constant becomes

$$N_n = \sqrt{\frac{(2n+2B+1)\Gamma(n+1)\Gamma(n+2B+1)}{2^{2B+1}\Gamma(n+B+C+1)\Gamma(n+B-C+1)}}. \tag{50}$$

VI. CONCLUSIONS

This paper presented a different approach, the NU method, to the calculation of the nonzero angular momentum solutions of the relativistic Klein-Gordon equation. Exact eigenvalues and eigenfunctions for the Klein-Gordon equation in the presence of the noncentral equal scalar and vector potentials are derived easily. In the nonrelativistic limit, the energy eigenvalue spectrum is shown to be equivalent to the Hartmann one and the radial and polar angle wave functions are found in terms of Laguerre and Jacobi polynomials, respectively. The method presented in this study is general and worth extending to the solution of other interaction problems.

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Quantum energy inequalities and local covariance. I. Globally hyperbolic spacetimes

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We begin a systematic study of quantum energy inequalities (QEIs) in relation to local covariance. We define notions of locally covariant QEIs of both "absolute" and "difference" types and show that existing QEIs satisfy these conditions. Local covariance permits us to place constraints on the renormalized stress-energy tensor in one spacetime using QEIs derived in another, in subregions where the two spacetimes are isometric. This is of particular utility where one of the two spacetimes exhibits a high degree of symmetry and the QEIs are available in simple closed form. Various general applications are presented, including *a priori* constraints (depending only on geometric quantities) on the ground-state energy density in a static spacetime containing locally Minkowskian regions. In addition, we present a number of concrete calculations in both two and four dimensions that demonstrate the consistency of our bounds with various known ground- and thermal-state energy densities. Examples considered include the Rindler and Misner spacetimes, and spacetimes with toroidal spatial sections. In this paper we confine the discussion to globally hyperbolic spacetimes; subsequent papers will also discuss spacetimes with boundary and other related issues. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2212669]

I. INTRODUCTION

Over the past 30 years, much effort has been devoted to calculations of the renormalized stress-energy tensor in ground states of quantum fields on stationary background spacetimes. Many analogous calculations have been made in flat spacetime equipped with reflecting boundaries, in connection with the Casimir effect. However, it would be fair to say that only limited qualitative insight has been gained. For example, the energy density is sometimes positive and sometimes negative, and there is no known way of predicting the sign in any general situations without performing the full calculations.[1] At least analytically, these calculations are restricted to cases exhibiting a high degree of symmetry. The aim of this paper, and a companion paper,[2] is to point out that there are situations in which one may gain some qualitative insight into the possible magnitude of the stress-energy tensor based on simple geometric considerations.

The situation we study in this paper arises when a spacetime contains a subspacetime that is isometric to (a subspacetime of) another spacetime, which will usually have nontrivial symmetries. By using quantum energy inequalities (QEIs) together with the locality properties of quantum field theory, we are then able to use information about the second (symmetric) spacetime to yield information about the stress-energy tensor of states on the first spacetime (which need have no global symmetries) in the region where the isometry holds. We will work on globally hyperbolic

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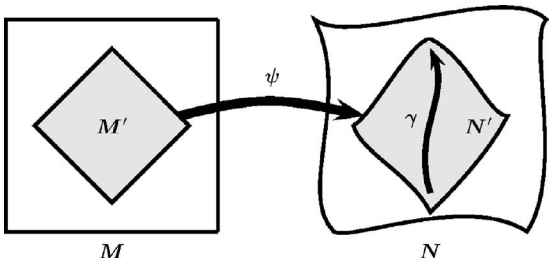

FIG. 1. Illustration for Example 1: The curve γ in $\boldsymbol{N}$ is enclosed in a causally embedded globally hyperbolic subspacetime $\boldsymbol{N}'$, which is causally isometric to a causally embedded globally hyperbolic subspacetime $\boldsymbol{M}'$ of four-dimensional Minkowski space $\boldsymbol{M}$ under $\psi:\boldsymbol{M}'\to\boldsymbol{N}'$.

spacetimes in this paper, deferring the issue of spacetimes with boundary to a companion paper.[2] As well as setting out the theory behind the method, we will demonstrate it in several locally Minkowskian spacetimes. Marecki[3] has also illustrated our approach by considering the case of spacetimes locally isometric to portions of exterior Schwarzschild. Also begun here for the free massless scalar field is a similar discussion for conformally related regions of two-dimensional spacetimes. In a separate paper we will extend this to the generalized Maxwell field in higher dimensional manifolds related by conformal diffeomorphisms.

To be more specific, consider a globally hyperbolic spacetime $\boldsymbol{N}$, consisting of a manifold of dimension $d\geqslant 2$, a Lorentzian metric with signature $+-\cdots-$, and choices of orientation and time-orientation (which, together, are required to fulfill the demands of global hyperbolicity.[4] Suppose an open subset of $\boldsymbol{N}$, when equipped with the metric and (time) orientation inherited from $\boldsymbol{N}$, is a globally hyperbolic spacetime $\boldsymbol{N}'$ in its own right. If, moreover, any causal curve in $\boldsymbol{N}$ whose endpoints lie in $\boldsymbol{N}'$ is contained completely in $\boldsymbol{N}'$, then we will call $\boldsymbol{N}'$ a *causally embedded globally hyperbolic subspacetime* (c.e.g.h.s.) of $\boldsymbol{N}$. Our main interest will be in the situation where a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$ is isometric to a c.e.g.h.s. $\boldsymbol{M}'$ of a second globally hyperbolic spacetime $\boldsymbol{M}$, with the isometry also respecting the (time) orientation. (We speak of a *causal isometry* in this case.) By the principle of locality, we expect that any experiment conducted within $\boldsymbol{N}'$ should have the same results as the same experiment (i.e., its isometric image) conducted in $\boldsymbol{M}'$. No observer in $\boldsymbol{N}'$ should be able to discern, by such local experiments that she does not, in fact, inhabit $\boldsymbol{M}'$; in particular, energy densities in $\boldsymbol{N}'$ should be subject to the same QEIs as those in $\boldsymbol{M}'$. We will demonstrate explicitly that these expectations are met by the QEIs we employ.

Among our results are the following, which we state for the case of a Klein-Gordon field of mass $m\geqslant 0$ in four dimensions:

Example 1: Suppose a timelike *geodesic* segment γ of proper duration τ_0 in a globally hyperbolic spacetime $\boldsymbol{N}$ can be enclosed in a c.e.g.h.s. $\boldsymbol{N}'$ that is causally isometric to a c.e.g.h.s. of four-dimensional Minkowski space as shown in Fig. 1. Then any state ω of the Klein-Gordon field (of mass $m\geqslant 0$) on $\boldsymbol{N}$ obeys

$$\sup_{\gamma}\langle T_{ab}u^a u^b\rangle_\omega \geqslant -\frac{C_4}{\tau_0^4}, \tag{1}$$

where the constant $C_4=3.169858\ldots$ (if $m>0$, one may obtain even more rapid decay).

Example 2: Suppose a globally hyperbolic spacetime $\boldsymbol{N}$ is stationary with respect to a timelike Killing field t^a and admits the smooth foliation into constant time surfaces $\boldsymbol{N}\cong\mathbb{R}\times\Sigma$. Suppose the metric takes the Minkowski form (with respect to some coordinates) on $\mathbb{R}\times\Sigma_0$ for some subset Σ_0 of Σ with nonempty interior. (We may suppose that Σ_0 has been taken to be maximal.) For any x in the interior of Σ_0, let $r(x)$ be the radius of the largest Euclidean 3-ball that can be isometrically embedded in Σ_0, centered on x, as in Fig. 2. Then any stationary Hadamard state[5] ω_N on $\boldsymbol{N}$ obeys the bound

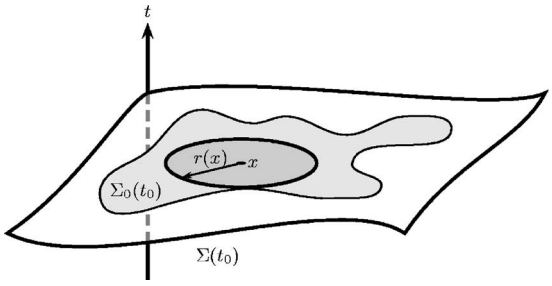

FIG. 2. Diagram showing open ball about the point x in Example 2.

$$\langle T_{ab}n^a n^b\rangle_{\omega_N}(t,x) \geqslant -\frac{C_4}{(2r(x))^4} \tag{2}$$

for any $x \in \Sigma_0$, where n^a is the unit vector along t^a.

Example 3: Suppose $\gamma: \mathbb{R} \to \boldsymbol{N}$ is a uniformly accelerated trajectory (parametrized by proper time) with proper acceleration α, and suppose γ can be enclosed within a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$ that is causally isometric to a c.e.g.h.s. of four-dimensional Minkowski space. Then, for any Hadamard state ω on $\boldsymbol{N}$, and any smooth compactly supported real-valued g, with $\int_{-\infty}^{\infty} g(\tau)^2 \mathrm{d}\tau = 1$,

$$\liminf_{\tau_0 \to \infty} \frac{1}{\tau_0} \int_\gamma \langle T_{ab}u^a u^b\rangle_\omega \, g(\tau/\tau_0)^2 \mathrm{d}\tau \geqslant -\frac{11\alpha^4}{480\pi^2}. \tag{3}$$

Note the remarkable fact that the right-hand side is precisely the expected energy density in the Rindler vacuum state along the trajectory with constant proper accleration α. In particular, if the energy density in some state ω is constant along γ, it must exceed or equal that of the Rindler vacuum. We emphasize that our derivation does not involve the Rindler vacuum, but only the Minkowski vacuum state two-point function and the QEIs.

Variants of these results hold in other dimensions, and also for other linear field equations such as the Maxwell and Proca fields (which we will treat elsewhere).

To prepare for our main discussion, it will be useful to make a few general remarks about QEIs, also often called simply quantum inequalities (QIs). QEIs have been quite intensively developed over the past decade, following Ford's much earlier insight[6] that quantum field theory might act to limit the magnitude and duration of negative energy densities and/or fluxes, thereby preventing macroscopic violations of the second law of thermodynamics (see Ref. 7 for rigorous links between QEIs and thermodynamical stability). Detailed reviews of QEIs may be found in Refs. 8–10.

QEIs take various forms, but we will distinguish two basic types: absolute QEIs and difference QEIs. An absolute QEI bound consists of a set $\mathcal{F}$ of *sampling tensors*, i.e., second rank contravariant tensor fields against which the renormalized stress-energy tensor will be averaged, a class $\mathcal{S}$ of states of the theory (which may be chosen to have nice properties) and a map $\mathcal{Q}: \mathcal{F} \to \mathbb{R}$ such that

$$\int \langle T_{ab}\rangle_\omega \, f^{ab} \mathrm{dvol} \geqslant -\mathcal{Q}(\mathsf{f}) > -\infty \tag{4}$$

for all states $\omega \in \mathcal{S}$. [It would also be natural to demand that $\mathcal{F}$ be convex (i.e., if f_1 and f_2 are in $\mathcal{F}$ then so is $\lambda\mathsf{f}_1 + (1-\lambda)\mathsf{f}_2$ for all $\lambda \in [0,1]$, and for $\mathcal{Q}$ to obey $\mathcal{Q}(\lambda\mathsf{f}_1 + (1-\lambda)\mathsf{f}_2) \leqslant \lambda\mathcal{Q}(\mathsf{f}_1) + (1-\lambda)\mathcal{Q}(\mathsf{f}_2)$, but we shall not make these requirements.] Here T_{ab} is the renormalized stress-energy tensor defined in a manner compatible with Wald's axioms,[11] and we have adopted the convention that the same tensor may be written f (without indices) or f^{ab} (with). We will permit $\mathcal{F}$ to include tensors singularly supported on timelike curves or other submanifolds of spacetime, so, for example, we can treat worldline averages such as

$$\int_\gamma \langle T_{ab}\rangle_\omega f^{ab} \mathrm{d}\tau = \int_I \langle T_{ab}(\gamma(\tau))\rangle_\omega \, u^a u^b g(\tau)^2 \mathrm{d}\tau, \tag{5}$$

where γ is a smooth timelike curve parametrized by an open interval I of proper time τ, with velocity u^a, and for $g \in C_0^\infty(I)$. (To be precise, $\mathcal{F}$ is required to be a set of compactly supported distributions on smooth rank two covariant test tensor fields.)

Absolute QEIs are known (with explicit formulae for $\mathcal{Q}$, and specific $\mathcal{F}$ and $\mathcal{S}$) for (a) the scalar field of mass $m \geqslant 0$ in d-dimensional Minkowski space[12–14] (see also Ref. 15 for $d \geqslant 2$), (b) the massless scalar and Fermi fields in arbitrary two-dimensional globally hyperbolic spacetimes,[16–19] (c) general (interacting) conformal field theories in two-dimensional Minkowski space,[20] and (d) a variety of higher spin linear fields in two- and four-dimensional Minkowski space.[13,21–26] For the most part only worldline bounds involving averages of the form Eq. (5) have been studied; it has been found that replacing g by a scaled version $\tau_0^{-1/2} g(\tau/\tau_0)$ has the effect of sending the QEI bound to zero as τ_0^{-d} (or faster, for massive fields) as $\tau_0 \to \infty$, where d is the spacetime dimension.

Difference QEI bounds also involve the specification of $\mathcal{F}$ and $\mathcal{S}$ as before, but now the bound sought takes the form

$$\int [\langle T_{ab}\rangle_\omega - \langle T_{ab}\rangle_{\omega_0}] f^{ab} \mathrm{dvol} \geqslant -\mathcal{Q}(\mathsf{f}, \omega_0) > -\infty, \tag{6}$$

where ω_0 is called the reference state. If the theory were represented in a Fock space built on ω_0 (when this is possible), the left-hand side would be an average of the normal ordered stress-energy tensor. However, it is not always necessary to assume that ω and ω_0 are represented in this way. Difference QEIs have proved to be the easiest to establish in curved spacetimes, or where boundaries are present. First developed in the case of (ultra)static spacetimes with the (ultra)static ground state chosen as the reference state ω_0,[21,27–29] they are now known for scalar, spin-1/2, and spin-1 fields in arbitrary globally hyperbolic spacetimes.[22,30,31] In these general results, $\mathcal{S}$ is the class of Hadamard states and the bounds are sufficiently general that ω_0 may be any element of $\mathcal{S}$, so $\mathcal{Q}$ becomes a function $\mathcal{Q}: \mathcal{F} \times \mathcal{S} \to \mathbb{R}$. The general results do not make use of a Hilbert space representation.

Clearly, difference and absolute QEIs are quite closely related. In particular, Wald's fourth axiom requires $\langle T_{ab}\rangle_{\omega_0}$ to vanish identically if ω_0 is the Minkowski vacuum, so difference QEIs become absolute in this case. (The extension of this observation to locally Minkowskian spaces is a key idea in this paper.) More generally, we may convert a difference QEI to an absolute QEI by moving all the terms in ω_0 onto the right-hand side. In cases where the renormalized stress-energy tensor is known explicitly for the reference state, this is perfectly satisfactory. However, there are two (related) drawbacks: (i) there is no canonical choice of reference state ω_0 in a general spacetime (which might have no timelike Killing fields, for example); (ii) one does not normally have available a closed form expression for $\langle T_{ab}\rangle_{\omega_0}$ for *any* state on a general spacetime, so the QEI bound becomes somewhat inexplicit. This weakens the power of QEIs to constrain exotic spacetime configurations such as macroscopic traversable wormholes or "warp drive." (On sufficiently small scales, one expects that the absolute QEI bounds should strongly resemble those of Minkowski space—as first argued in Ref. 32, and proven in various situations in Refs. 28 and 19—however one still needs to know the magnitude of $\langle T_{ab}\rangle_{\omega_0}$ to know on what scales this approximation holds.)

The present paper and its companion represent first steps towards absolute QEIs in more general spacetimes, starting with spacetimes containing regions isometric to others where reference states are known. Work is under way on generally applicable absolute QEIs and will be reported elsewhere; however, we expect the results and methods presented here to be of continuing interest, as they reduce to very simple geometrical conditions.

The paper is structured as follows. In Sec. II we give a brief introduction to some of the relevant notions of locally covariant quantum field theory before defining locally covariant QEIs

and developing their simple properties in Sec. II C. The following two subsections show how existing QEIs in the literature may be expressed in the locally covariant framework, and address some technical points along the way. In Sec. III we show how local covariance permits *a priori* bounds to be placed on energy densities in spacetimes with Minkowskian subspacetimes using geometric data. The main technique here, in addition to local covariance, is the conversion of QEIs to eigenvalue problems, first introduced in Ref. 33. These are applied in Sec. IV to specific spacetime models where the energy densities of ground states and thermal states are known, permitting comparison with our *a priori* bounds. In some cases these bounds are saturated by the exact values. After a summary, the appendices collect various results needed in the main text.

II. QUANTUM ENERGY INEQUALITIES AND LOCAL COVARIANCE

A. Geometrical preliminaries

Suppose two globally hyperbolic spacetimes of the same dimension, $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$, are given (we denote the corresponding manifolds and metrics by M_i, $\boldsymbol{g}_i$ for $i=1,2$). An *isometric embedding* of $\boldsymbol{M}_1$ in $\boldsymbol{M}_2$ is a smooth map $\psi: M_1 \to M_2$ which is a diffeomorphism of M_1 onto its range $\psi(M_1)$ in M_2 and so that the pull-back $\psi^* \boldsymbol{g}_2$ is everywhere equal to $\boldsymbol{g}_1$ on M_1. In local coordinates,

$$g_{1ab}(x) = \frac{\partial y^{a'}}{\partial x^a} \frac{\partial y^{b'}}{\partial x^b} g_{2a'b'}(y) \tag{7}$$

should hold for all $x \in M_1$, where $y = \psi(x)$. We *do* require that all of M_1 is mapped into M_2, but we do *not* require that the image of M_1 under ψ consists of the whole of M_2. There are two possible choices of orientation and time orientation on $\psi(M_1)$: that induced by ψ from the (time) orientation of $\boldsymbol{M}_1$, and that inherited from $\boldsymbol{M}_2$. If these coincide and we have the further property that every causal curve in $\boldsymbol{M}_2$ with endpoints in $\psi(M_1)$ lies entirely in $\psi(M_1)$, then we say that ψ is a *causal isometric embedding*. An important class of examples arises where $\boldsymbol{M}_1$ is a causally embedded globally hyperbolic subspacetime (c.e.g.h.s.) of $\boldsymbol{M}_2$ as defined in Sec. I, in which case ψ is simply the identity map. It is also worth mentioning an example of a noncausal embedding, namely, the "helical strip" described by Kay.[34] In this example a long thin diamond region of two-dimensional Minkowski space is isometrically embedded in a "timelike cylinder" that is the quotient of Minkowski space by a spacelike translation. The wrapping is arranged so that points that are spacelike separated in the original diamond are timelike separated in the geometry of the timelike cylinder. The definition of a causal embedding is designed precisely to ensure that the induced and inherited causal structures cannot differ in this way.

B. Local covariance

The relevance of local covariance to quantum field theory on manifolds has long been understood[35,36] but has recently been put in a new setting by Brunetti, Fredenhagen, and Verch[37] (see also Refs. 38 and 39) and related work of Hollands and Wald (see, e.g., Refs. 40 and 41). This provides a very elegant and general framework for local covariance in the language of category theory. The recent interest in local covariance has already had a significant impact in completing the renormalization program in curved spacetimes,[40,41] in providing a rigorous spin-statistics connection in curved spacetimes,[38] and in the theory of superselection sectors.[42] For our current purposes, we will only need a few of the main ideas of this analysis and will not describe the whole structure, referring the reader to the references just mentioned for further details. A discussion of QEIs in the categorical description of local covariance will appear elsewhere.[43]

In this section we will restrict ourselves to the Klein-Gordon field of mass $m \geqslant 0$, although similar comments can be made for the Dirac, Maxwell, and Proca fields. There is a well-defined quantization of the theory on any globally hyperbolic spacetime $\boldsymbol{M}$, in terms of an algebra of observables $\mathfrak{A}_{\boldsymbol{M}}$ and a space of Hadamard states $\mathcal{S}_{\boldsymbol{M}}$ which determine expectation values for observables in $\mathfrak{A}_{\boldsymbol{M}}$. For the purposes of this section, it suffices to know that $\mathfrak{A}_{\boldsymbol{M}}$ is generated by smeared field objects $\Phi_{\boldsymbol{M}}(f)$ labeled by smooth, compactly supported test functions $f \in C_0^\infty(\boldsymbol{M})$,

subject to relations expressing the field equation and commutation relations, and the hermiticity of the field. (The structure is given in detail in Appendix A.) The Hadamard states of the theory are those states on $\mathfrak{A}_{\boldsymbol{M}}$ whose two-point functions have singularities of the Hadamard form, which at leading order are just those of the Minkowski vacuum two-point function. More precisely,[44] on any causal normal neighborhood $\mathcal{O}$ in $\boldsymbol{M}$ there is a sequence of bidistributions H_n so that (for any n) the two-point function of any Hadamard state differs from H_n on $\mathcal{O}$ by a state-dependent function of class C^n. It is of key importance that $H_n(x,x')$ is fixed entirely by the local metric and causal structure, through the Hadamard recursion relations. Given a Hadamard state ω, we may construct the expected renormalized stress-energy tensor $\langle T_{ab}\rangle_\omega$ by the point-splitting technique (see, e.g., Ref. 11): first subtract H_n from the two-point function (for $n \geqslant 2$), then apply appropriate derivatives before taking the points together again. Next, one subtracts a term of the form Qg_{ab}, where Q is locally determined (and state independent), in order to ensure that the resulting tensor is conserved and vanishes in the Minkowski vacuum state. The tensor defined in this way obeys Wald's axioms mentioned above; however, these axioms would also be satisfied if one were to add a conserved local curvature term. Such terms are sometimes described as undetermined or arbitrary; we take the view, however, that they are part of the specification of the theory, just as the mass and conformal coupling are, even though they do not appear explicitly in the Lagrangian (a similar attitude is expressed in Ref. 45). For simplicity, and because our main applications will concern locally Minkowskian spacetimes, we will assume that these terms are absent—that is, we restrict to those scalar particle species for which this is the case.

The above structure is locally covariant in the following sense. Suppose a globally hyperbolic spacetime $\boldsymbol{M}$ is embedded in a globally hyperbolic spacetimes $\boldsymbol{N}$ by a causal isometry ψ, and let ψ_* denote the push-forward map on test functions. That is, $\psi_*: C_0^\infty(\boldsymbol{M}) \to C_0^\infty(\boldsymbol{N})$ is defined by

$$(\psi_* f)(y) = \begin{cases} f(\psi^{-1}(y)) & \text{if } y = \psi(x) \text{ for some } x \in \boldsymbol{M} \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

Then there is a natural mapping of the field on $\boldsymbol{M}$ to the field on $\boldsymbol{N}$ given by $\Phi_{\boldsymbol{M}}(f) \mapsto \Phi_{\boldsymbol{N}}(\psi_* f)$; we also write this as $\psi_*(\Phi_{\boldsymbol{M}}(f)) = \Phi_{\boldsymbol{N}}(\psi_* f)$. Moreover, ψ_* can be extended to any element of $\mathfrak{A}_{\boldsymbol{M}}$, respecting the algebraic relations and mapping the identity in $\mathfrak{A}_{\boldsymbol{M}}$ to the identity in $\mathfrak{A}_{\boldsymbol{N}}$; technically, it is a unit-preserving injective $*$-homomorphism of $\mathfrak{A}_{\boldsymbol{M}}$ into $\mathfrak{A}_{\boldsymbol{N}}$.

On account of the correspondence $\Phi_{\boldsymbol{M}}(f) \mapsto \Phi_{\boldsymbol{N}}(\psi_* f)$, we say that the field is covariant (the transformation goes "in the same direction" as ψ; see the remarks below on the underlying category theory at the end of Appendix A). By contrast, the state spaces transform in a contravariant way (in the "opposite direction" to ψ): for any state ω on $\mathfrak{A}_{\boldsymbol{N}}$ there is a pulled-back state, which we denote $\psi^*\omega$, on $\mathfrak{A}_{\boldsymbol{M}}$, so that the expectation values of $A \in \mathfrak{A}_{\boldsymbol{M}}$ and $\psi_* A \in \mathfrak{A}_{\boldsymbol{N}}$ are related by

$$\langle A \rangle_{\psi^*\omega} = \langle \psi_* A \rangle_\omega. \tag{9}$$

The correspondences just described are summarized graphically in Fig. 3. The use of pull-back notation may be justified by the observation that Eq. (9) entails that the n-point functions of the two states are related by

$$\langle \Phi_{\boldsymbol{M}}(x_1) \cdots \Phi_{\boldsymbol{M}}(x_n) \rangle_{\psi^*\omega} = \langle \Phi_{\boldsymbol{N}}(\psi(x_1)) \cdots \Phi_{\boldsymbol{N}}(\psi(x_n)) \rangle_\omega \tag{10}$$

(adopting an "unsmeared" notation). That is, the n-point function of $\psi^*\omega$ is simply the pull-back of the n-point function of ω by ψ (or more precisely, by the duplication of ψ across n copies of $\boldsymbol{M}$). This has an important consequence when the state ω is Hadamard, i.e., $\omega \in \mathcal{S}_{\boldsymbol{N}}$: because the Hadamard condition is based on the local metric and causal structure, both of which are preserved by ψ, it is clear that $\psi^*\omega$ is also Hadamard. (A more elegant proof of this[37] is to use Radzikowski's characterization of the Hadamard condition in terms of the wave-front set of the two-point function,[46] and the transformation properties of the wave-front set under pull-backs.) This may be expressed by the inclusion $\psi^* \mathcal{S}_{\boldsymbol{N}} \subset \mathcal{S}_{\boldsymbol{M}}$.

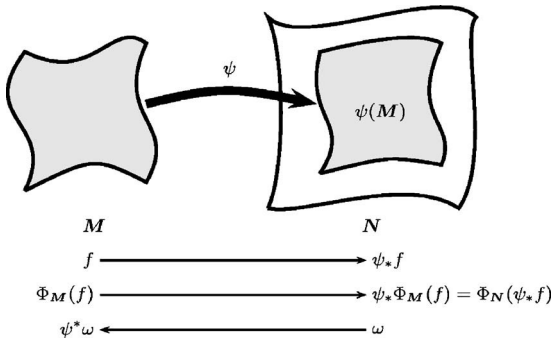

FIG. 3. If $\boldsymbol{M}$ is embedded in $\boldsymbol{N}$ by a causal isometry ψ, then test functions and smeared fields may be pushed forwards from $\boldsymbol{M}$ to $\boldsymbol{N}$, while states (and expectation values) are pulled back from $\boldsymbol{N}$ to $\boldsymbol{M}$.

As noted above, the expectation values of the stress-energy tensor are also constructed in a purely local fashion from the two-point function of the state. It therefore follows that

$$\langle T_{\boldsymbol{M}ab}(x)\rangle_{\psi^*\omega} = \frac{\partial y^{a'}}{\partial x^a}\frac{\partial y^{b'}}{\partial x^b}\langle T_{\boldsymbol{N}a'b'}(y)\rangle_{\omega}, \tag{11}$$

where we have written $y=\psi(x)$: like the n-point functions, the expected stress-energy tensor in state $\psi^*\omega$ is simply the pull-back of that in state ω. In coordinate-free notation we may write

$$\langle \mathbf{T}_{\boldsymbol{M}}\rangle_{\psi^*\omega} = \psi^*\langle \mathbf{T}_{\boldsymbol{N}}\rangle_{\omega}. \tag{12}$$

In the above equations we have written the stress-energy tensor as if it is an element of the algebra $\mathfrak{A}_{\boldsymbol{M}}$, which it is not. One may proceed in two ways: either interpreting Eq. (12) as the extension of Eq. (9) to an algebra of Wick polynomials that contains $\mathfrak{A}_{\boldsymbol{M}}$ as a subalgebra, and in which $\mathbf{T}_{\boldsymbol{M}}$ may be defined as a locally covariant field.[40,47] For our purposes, however, it will be simpler to define the smeared stress-energy tensor only through its expectation values; more technically, we think of it as a linear functional on the space of Hadamard states, with the notation $\langle \mathbf{T}_{\boldsymbol{M}}(\mathsf{f})\rangle_{\omega}$ expressing the value of this functional applied to the state ω. This has the advantage that one may deal with all Hadamard states, rather than those which extend to the Wick algebra.[47]

We emphasize the fact that states are pulled back in this setting; although one could push forward a state $\omega\in\mathcal{S}_{\boldsymbol{M}}$ to obtain a state on $\mathfrak{A}_{\psi(\boldsymbol{M})}$, there is no guarantee that this can be extended to a Hadamard state on $\mathfrak{A}_{\boldsymbol{N}}$, and indeed, such extensions do not always exist. For example, the Rindler vacuum state on the Rindler wedge is Hadamard in the interior of the wedge,[48] but cannot be extended to a Hadamard state on the whole of Minkowski because its stress-energy tensor diverges at the boundary of the wedge. See Ref. 49 for further discussion of these issues.

C. QEIs in a locally covariant setting

We now introduce two types of locally covariant QEIs. A more abstract (and general) definition can be given in the language of categories—this will be pursued elsewhere. Recall that a set of sampling tensors on a globally hyperbolic spacetime is a set of compactly supported distributions on smooth second rank covariant tensor fields.

Definition II.1: A locally covariant absolute QEI *assigns to each globally hyperbolic spacetime* $\boldsymbol{M}$ *a set of sampling tensors* $\mathcal{F}_{\boldsymbol{M}}$ *on* $\boldsymbol{M}$ *and a map* $\mathcal{Q}_{\boldsymbol{M}}:\mathcal{F}_{\boldsymbol{M}}\to\mathbb{R}$ *such that (i) we have*

$$\langle \mathbf{T}_{\boldsymbol{M}}(\mathsf{f})\rangle_{\omega} \geqslant -\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}) \tag{13}$$

for all $\mathsf{f}\in\mathcal{F}_{\boldsymbol{M}}$ *and* $\omega\in\mathcal{S}_{\boldsymbol{M}}$, *and (ii) if* $\psi:\boldsymbol{M}\to\boldsymbol{N}$ *is a causal isometric embedding then* $\psi_*\mathcal{F}_{\boldsymbol{M}}\subset\mathcal{F}_{\boldsymbol{N}}$ *and*

$$\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{N}}(\psi_*\mathsf{f}) \tag{14}$$

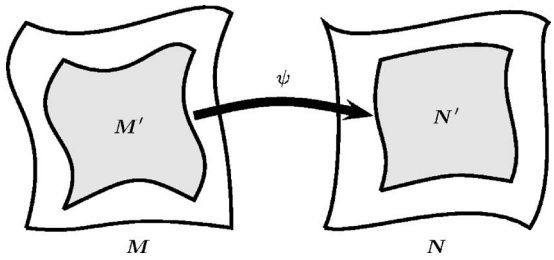

FIG. 4. (Color online) Diagram showing the various spacetimes and embeddings in Sec. II C.

for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}}$. (*We might also express this in the form* $\mathcal{Q}_{\boldsymbol{M}} = \psi^* \mathcal{Q}_{\boldsymbol{N}}$.)

A locally covariant difference QEI *assigns to each globally hyperbolic* $\boldsymbol{M}$ *a set of sampling tensors* $\mathcal{F}_{\boldsymbol{M}}$ *as before, and a map* $\mathcal{Q}_{\boldsymbol{M}}: \mathcal{F}_{\boldsymbol{M}} \times \mathcal{S}_{\boldsymbol{M}} \to \mathbb{R}$ *such that (i)*

$$\langle \mathsf{T}_{\boldsymbol{M}}(\mathsf{f}) \rangle_{\omega} - \langle \mathsf{T}_{\boldsymbol{M}}(\mathsf{f}) \rangle_{\omega_0} \geqslant - \mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}, \omega_0) \tag{15}$$

for each $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}}$ *and all* $\omega, \omega_0 \in \mathcal{S}_{\boldsymbol{M}}$; (*ii*)

$$\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}, \psi^* \omega_0) = \mathcal{Q}_{\boldsymbol{N}}(\psi_* \mathsf{f}, \omega_0) \tag{16}$$

holds for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}}$ *and* $\omega_0 \in \mathcal{S}_{\boldsymbol{N}}$.

We will shortly give examples of each type: Flanagan's two-dimensional QEIs for massless fields[18] will be exhibited as a locally covariant absolute QEI, while (generalizations of) the QEI obtained in Ref. 30 provide examples of locally covariant difference QEIs. Before that, let us examine some simple consequences of these definitions.

First, suppose that $\boldsymbol{M}'$ is a c.e.g.h.s. of $\boldsymbol{M}$, so the identity map $\iota: \boldsymbol{M}' \to \boldsymbol{M}$ is a causal isometric embedding, and we must have $\iota_* \mathcal{F}_{\boldsymbol{M}'} \subset \mathcal{F}_{\boldsymbol{M}}$ and $\mathcal{Q}_{\boldsymbol{M}'}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{M}}(\iota_* \mathsf{f})$. It is sensible to drop the identity mappings, and write the above in the form

$$\mathcal{F}_{\boldsymbol{M}'} \subset \mathcal{F}_{\boldsymbol{M}}, \quad \text{and } \mathcal{Q}_{\boldsymbol{M}'}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}) \text{ for all } \mathsf{f} \in \mathcal{F}_{\boldsymbol{M}'}. \tag{17}$$

If $\psi: \boldsymbol{M}' \to \boldsymbol{N}$ is a causal isometric embedding, as shown in Fig. 4, we then obtain

$$\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{M}'}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{N}}(\psi_* \mathsf{f}) \tag{18}$$

for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}'}$. As one would expect, this shows that locally covariant absolute QEIs are indifferent to the larger spacetime; one obtains the same bound whether one is in $\boldsymbol{M}'$ or its image $\boldsymbol{N}'$ in $\boldsymbol{N}$. Although this barely extends the original definition, it is worth isolating it as a separate result.

Proposition II.2: Suppose a c.e.g.h.s. $\boldsymbol{M}'$ *of* $\boldsymbol{M}$ *is causally isometric to a c.e.g.h.s.* $\boldsymbol{N}'$ *of* $\boldsymbol{N}$ *under the map* ψ. *Then a locally covariant absolute QEI obeys*

$$\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}) = \mathcal{Q}_{\boldsymbol{N}}(\psi_* \mathsf{f}) \tag{19}$$

for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}'} \subset \mathcal{F}_{\boldsymbol{M}}$.

Let us now examine locally covariant difference QEIs in this situation. Given arbitrary Hadamard states $\omega_{\boldsymbol{M}} \in \mathcal{S}_{\boldsymbol{M}}$ and $\omega_{\boldsymbol{N}} \in \mathcal{S}_{\boldsymbol{N}}$ on the parent spacetimes $\boldsymbol{M}$ and $\boldsymbol{N}$, there are states $\iota^* \omega_{\boldsymbol{M}}$ and $\psi^* \omega_{\boldsymbol{N}}$ in $\mathcal{S}_{\boldsymbol{M}'}$, i.e., Hadamard states on $\mathfrak{A}_{\boldsymbol{M}'}$. Applying the difference QEI to $\psi^* \omega_{\boldsymbol{N}}$ with $\iota^* \omega_{\boldsymbol{M}}$ as reference state, we find

$$\langle \mathsf{T}_{\boldsymbol{M}'}(\mathsf{f}) \rangle_{\psi^* \omega_{\boldsymbol{N}}} - \langle \mathsf{T}_{\boldsymbol{M}'}(\mathsf{f}) \rangle_{\iota^* \omega_{\boldsymbol{M}}} \geqslant - \mathcal{Q}_{\boldsymbol{M}'}(\mathsf{f}, \iota^* \omega_{\boldsymbol{M}}) = - \mathcal{Q}_{\boldsymbol{M}}(\iota_* \mathsf{f}, \omega_{\boldsymbol{M}}), \tag{20}$$

where we have used the transformation property Eq. (16). On the other hand, we could equally well apply the difference QEI to $\iota^* \omega_{\boldsymbol{M}}$, with $\psi^* \omega_{\boldsymbol{N}}$ as reference state, to obtain

$$\langle \mathbf{T}_{\boldsymbol{M}'}(\mathsf{f})\rangle_{\iota^*\omega_{\boldsymbol{M}}} - \langle \mathbf{T}_{\boldsymbol{M}'}(\mathsf{f})\rangle_{\psi^*\omega_{\boldsymbol{N}}} \geqslant -\mathcal{Q}_{\boldsymbol{M}'}(\mathsf{f}, \psi^*\omega_{\boldsymbol{N}}) = -\mathcal{Q}_{\boldsymbol{N}}(\psi_*\mathsf{f}, \omega_{\boldsymbol{N}}). \tag{21}$$

Combining these inequalities yields

$$\mathcal{Q}_{\boldsymbol{N}}(\psi_*\mathsf{f}, \omega_{\boldsymbol{N}}) \geqslant \langle \mathbf{T}_{\boldsymbol{M}'}(\mathsf{f})\rangle_{\psi^*\omega_{\boldsymbol{N}}} - \langle \mathbf{T}_{\boldsymbol{M}'}(\mathsf{f})\rangle_{\iota^*\omega_{\boldsymbol{M}}} \geqslant -\mathcal{Q}_{\boldsymbol{M}}(\iota_*\mathsf{f}, \omega_{\boldsymbol{M}}); \tag{22}$$

we may also use the covariance of $\mathbf{T}$ to reexpress the central member of this inequality in terms of expectation values on $\boldsymbol{N}$ and $\boldsymbol{M}$, rather than $\boldsymbol{M}'$. The result, on dropping identity mappings from the notation, is the following.

Proposition II.3: Suppose a c.e.g.h.s. $\boldsymbol{M}'$ of $\boldsymbol{M}$ is causally isometric to a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$ under the map ψ. *Then a locally covariant difference QEI obeys*

$$\mathcal{Q}_{\boldsymbol{N}}(\psi_*\mathsf{f}, \omega_{\boldsymbol{N}}) \geqslant \langle \mathbf{T}_{\boldsymbol{N}}(\psi_*\mathsf{f})\rangle_{\omega_{\boldsymbol{N}}} - \langle \mathbf{T}_{\boldsymbol{M}}(\mathsf{f})\rangle_{\omega_{\boldsymbol{M}}} \geqslant -\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}, \omega_{\boldsymbol{M}}), \tag{23}$$

for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}'} \subset \mathcal{F}_{\boldsymbol{M}}$ *and any* $\omega_{\boldsymbol{M}} \in \mathcal{S}_{\boldsymbol{M}}$, $\omega_{\boldsymbol{N}} \in \mathcal{S}_{\boldsymbol{N}}$.

Note that the QEIs used are those associated with the full spacetimes $\boldsymbol{M}$ and $\boldsymbol{N}$; similarly, the states $\omega_{\boldsymbol{M}}$, $\omega_{\boldsymbol{N}}$ are states of the field on the full spacetimes. However, the isometry ψ connects only portions of the spacetime together and the restriction on the support of f is therefore crucial: in general, the above result will not hold when sampling extends outside the isometric region. It is also worth noting that we have both lower and upper bounds.

In this paper we will study the simplest possible setting for this result, in which $\boldsymbol{M}$ is Minkowski spacetime and $\omega_{\boldsymbol{M}}$ is the Minkowski vacuum state. However, other situations are possible. For example, Marecki[3] has employed our framework in the case where $\boldsymbol{M}$ is the exterior Schwarzschild spacetime and $\omega_{\boldsymbol{M}}$ is the Boulware vacuum. In the Minkowski case, the result simplifies because the renormalized stress-energy tensor vanishes in the state $\omega_{\boldsymbol{M}}$, and we have the following statement.

Corollary II.4: Suppose a c.e.g.h.s. $\boldsymbol{M}'$ of Minkowski space $\boldsymbol{M}$ is causally isometric to a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$ under the map ψ. Then a locally covariant difference QEI obeys

$$\mathcal{Q}_{\boldsymbol{N}}(\psi_*\mathsf{f}, \omega_{\boldsymbol{N}}) \geqslant \langle \mathbf{T}_{\boldsymbol{N}}(\psi_*\mathsf{f})\rangle_{\omega_{\boldsymbol{N}}} \geqslant -\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}, \omega_{\boldsymbol{M}}) \tag{24}$$

for all $\mathsf{f} \in \mathcal{F}_{\boldsymbol{M}'} \subset \mathcal{F}_{\boldsymbol{M}}$ *and any* $\omega_{\boldsymbol{N}} \in \mathcal{S}_{\boldsymbol{N}}$, *where* $\omega_{\boldsymbol{M}}$ *is the Minkowski vacuum state.*

D. A locally covariant absolute QEI for massless fields in two dimensions

The QEI we now describe was originally developed by Flanagan[16] for the massless scalar field in two-dimensional Minkowski space, in work which was subsequently generalized to curved spacetimes[17–19] and also to arbitrary unitary positive energy conformal field theories in two-dimensional Minkowski space.[20] The results of Ref. 18 were obtained for two-dimensional spacetimes globally conformal to the whole of Minkowski space; as noted in Ref. 19, however, any point of a globally hyperbolic two-dimensional spacetime has a (causally embedded) neighborhood that is conformal to the whole of Minkowski space, and to which Flanagan's result applies.

We first state the result of Ref. 18, and then show that it meets our definition of a locally covariant absolute QEI. Let $\boldsymbol{M}$ be a globally hyperbolic two-dimensional spacetime, and suppose that γ is a smooth, future-directed timelike curve, parametrized by proper time $\tau \in I$, which is completely contained within a c.e.g.h.s. $\boldsymbol{M}'$ of $\boldsymbol{M}$, such that $\boldsymbol{M}'$ is globally conformal to the whole of two-dimensional Minkowski space. Then all Hadamard states ω on $\boldsymbol{M}$ obey the QEI

$$\int_I \langle T_{\boldsymbol{M}ab} u^a u^b \rangle_\omega(\gamma(\tau)) g(\tau)^2 \mathrm{d}\tau \geqslant -\frac{1}{6\pi}\int_I [g'(\tau)^2 + g(\tau)^2\{R_{\boldsymbol{M}}(\gamma(\tau)) - a^c(\tau)a_c(\tau)\}]\mathrm{d}\tau \tag{25}$$

for any smooth, real-valued g compactly supported in I,[50] where u^a is the two-velocity of γ, a^c is its acceleration and $R_{\boldsymbol{M}}$ is the scalar curvature on $\boldsymbol{M}$. (Note that Ref. 18 uses conventions in which $u^a u_a < 0$ for timelike u^a; the bound is therefore modified slightly.)

As we now describe, Flanagan's bound is a locally covariant absolute QEI. Given I, γ, and g as above, we may define a compactly supported distribution $\mathsf{f}_{I,\gamma,g}$ acting on smooth second rank covariant tensor fields t, by

$$\mathsf{f}_{I,\gamma,g}(\mathsf{t}) = \int_I g(\tau)^2 u^a u^b t_{ab}|_{\gamma(\tau)} \mathrm{d}\tau. \tag{26}$$

Our set of sampling tensors $\mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}}$ ("conf" abbreviating "conformal") will be the set of all distributions formed in this way. [A distribution of the form $\mathsf{f}_{I,\gamma,g}$ is singularly supported on the curve γ; we could also write it in the form

$$f^{ab}_{I,\gamma,g}|_p = \int_I u^a u^b g(\tau)^2 \delta_{\gamma(\tau)}(p) \mathrm{d}\tau, \tag{27}$$

where $\delta_q(p)$ is the δ function at q, obeying $\int_{\boldsymbol{M}} \delta_q(p) F(p) \mathrm{dvol} = F(q)$.]

The QEI bound $\mathcal{Q}^{\mathrm{conf}}_M$ is then defined by

$$\mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{M}}(\mathsf{f}) = \frac{1}{6\pi} \int_I [g'(\tau)^2 + g(\tau)^2 \{R_{\boldsymbol{M}}(\gamma(\tau)) - a^c(\tau) a_c(\tau)\}] \mathrm{d}\tau \tag{28}$$

for any I, γ, g for which $\mathsf{f} = \mathsf{f}_{I,\gamma,g}$. For this to make sense, we must ensure that the right-hand side is unchanged if we replace I, γ, and g by $\widetilde{I}$, $\widetilde{\gamma}$ and $\widetilde{g}$ such that $\mathsf{f}_{I,\gamma,g} = \mathsf{f}_{\widetilde{I},\widetilde{\gamma},\widetilde{g}}$. Since γ and γ' are both assumed to be parametrized by proper time, our two sampling tensors must be related in a simple way: supp $\widetilde{g}$ is the translation of supp g by some τ_0, so that $\widetilde{\gamma}(\tau) = \gamma(\tau + \tau_0)$, $\widetilde{g}(\tau)^2 = g(\tau + \tau_0)^2$ for all $\tau \in$ supp $\widetilde{g}$. The only possible ambiguity stems from the fact that $\widetilde{g}(\tau)$ and $g(\tau + \tau_0)$ might differ by a relative sign that can change at zeros of $\widetilde{g}$ of infinite order. However, it is simple to show that, nevertheless, $\widetilde{g}(\tau)^2 = g'(\tau + \tau_0)^2$,[51] ensuring that the right-hand side of Eq. (28) is unchanged under the reparametrization of f.

The bound Eq. (25) now takes the form of Eq. (13), so it remains only to verify that $\mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}}$ and $\mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{M}}$ have the required transformation properties. Suppose $\psi : \boldsymbol{M} \to \boldsymbol{N}$ is a causal isometric embedding. The push-forward ψ_* acts on $\mathsf{f}_{I,\gamma,g} \in \mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}}$ so that, for any smooth tensor field t_{ab} on $\boldsymbol{N}$, we have

$$(\psi_* \mathsf{f}_{I,\gamma,g})(\mathsf{t}) = \mathsf{f}_{I,\gamma,g}(\psi^* \mathsf{t}) = \int_I g(\tau)^2 u^a u^b (\psi^* \mathsf{t})_{ab}|_{\gamma(\tau)} \mathrm{d}\tau = \int_I g(\tau)^2 (\psi^* \mathsf{u})^a (\psi^* \mathsf{u})^b t_{ab}|_{\gamma(\tau)} \mathrm{d}\tau = \mathsf{f}_{I,\psi\circ\gamma,g}(\mathsf{t}). \tag{29}$$

Now the image curve $\psi \circ \gamma$ can certainly be enclosed in a c.e.g.h.s. of $\boldsymbol{N}$ which is conformal to the whole of Minkowski space: namely the image under ψ of that which enclosed γ. Moreover, the image curve has velocity $\psi^* \mathsf{u}$. It is therefore clear that $\psi_* \mathsf{f}_{I,\gamma,g} = \mathsf{f}_{I,\psi\circ\gamma,g}$ is a legitimate sampling tensor in $\mathcal{F}^{\mathrm{conf}}_{\boldsymbol{N}}$, so we have shown that $\psi_* \mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}} \subset \mathcal{F}^{\mathrm{conf}}_{\boldsymbol{N}}$. It is obvious that $\mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{M}}(\mathsf{f}) = \mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{N}}(\psi_* \mathsf{f})$ because all quantities involved in the bound are invariant under the isometry.

We have thus shown that two-dimensional massless fields obey a locally covariant absolute QEI. One need not restrict to worldline averages such as those described above: see Refs. 16 and 18 for averages along spacelike or null curves, and Ref. 20 for worldvolume averages (in Minkowski space). We summarize as follows:

Theorem II.5: *Let $\boldsymbol{M}$ be a two-dimensional globally hyperbolic spacetime and let $\mathcal{S}_{\boldsymbol{M}}$ be the class of Hadamard states of the massless Klein-Gordon field on $\boldsymbol{M}$. Let $\mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}}$ consist of all sampling tensors of the form Eq. (26) where (i) $\gamma : I \to \boldsymbol{M}$ is a smooth future-directed timelike curve parametrized by proper time, with velocity $\mathsf{u} = \dot{\gamma}$; (ii) γ may be enclosed in a c.e.g.h.s. of $\boldsymbol{M}$ globally conformal to the whole of Minkowski space; (iii) $g \in C^\infty_0(I; \mathbb{R})$. Then, defining $\mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{M}}(\mathsf{f})$ by Eq. (28) for any I, γ, g for which $\mathsf{f} = \mathsf{f}_{I,\gamma,g}$, the absolute QWEI*

$$\int_\gamma \langle T_{\boldsymbol{M}ab}\rangle_\omega \, u^a u^b g(\tau)^2 \mathrm{d}\tau \geqslant -\mathcal{Q}^{\mathrm{conf}}_{\boldsymbol{M}}(\mathsf{f}_{I,\gamma,g}) \tag{30}$$

holds for all $\omega \in \mathcal{S}_{\boldsymbol{M}}$ *and* $\mathsf{f}_{I,\gamma,g} \in \mathcal{F}^{\mathrm{conf}}_{\boldsymbol{M}}$, *and is locally covariant.*

E. Examples of locally covariant difference QEIs

We now give two related examples of locally covariant difference QEIs, based on methods first introduced in Ref. 30. The first is a quantum null energy inequality (QNEI), constraining averages of the null-contracted stress-energy tensor along timelike curves,[52] while the second is a quantum weak energy inequality (QWEI), constraining averages of the energy density along timelike curves.[30]

Suppose that $\boldsymbol{M}$ is any globally hyperbolic spacetime of dimension $d \geqslant 2$, and $\gamma: I \to M$ is any smooth, future-directed timelike curve. Suppose further that k^a is a smooth nonzero null vector field defined near γ. Then for any smooth, real-valued g, compactly supported in I, there is a difference QNEI,[52]

$$\int_\gamma [\langle T_{\boldsymbol{M}ab}\rangle_\omega - \langle T_{\boldsymbol{M}ab}\rangle_{\omega_0}] k^a k^b g(\tau)^2 \mathrm{d}\tau \geqslant -\int_0^\infty \frac{d\alpha}{\pi} \hat{F}_{\gamma,g,\mathsf{k},\omega_0}(-\alpha,\alpha) \tag{31}$$

for all $\omega, \omega_0 \in \mathcal{S}_{\boldsymbol{M}}$, where the hat denotes Fourier transform and

$$F_{\gamma,g,\mathsf{k},\omega_0}(\tau,\tau') = g(\tau)g(\tau')\langle \nabla_{\mathsf{k}}\Phi_{\boldsymbol{M}}(\gamma(\tau))\nabla_{\mathsf{k}}\Phi_{\boldsymbol{M}}(\gamma(\tau'))\rangle_{\omega_0}. \tag{32}$$

in which we have written ∇_{k} for $k^a\nabla_a$. (More precisely, the last factor is a distributional pull-back of the differentiated two-point function. We also adopt the nonstandard convention

$$\hat{f}(\lambda) = \int \mathrm{d}t \; e^{i\lambda t} f(t) \tag{33}$$

for Fourier transforms; for purposes of comparison, we note that the same convention was used in Ref. 30, but not in Ref. 52.) The integral on the right-hand side of Eq. (31) is finite as a consequence of ω_0 being Hadamard. We emphasize that there is no necessity for ω and ω_0 to be represented as vectors or density matrices in a common Hilbert space representation in order to prove the QEIs described in this section, because the proof may be phrased entirely in the algebraic formulation of QFT.

The above result was derived in Ref. 52 based on an earlier result in Ref. 30, described below. However, it is slightly easier to show that it is locally covariant, which is why we have presented it first. To accomplish our task, we define $\mathcal{F}^{\mathrm{null}}_{\boldsymbol{M}}$ to consist of all compactly supported distributions $\mathsf{f}_{I,\gamma,\mathsf{k},g}$ on smooth second rank covariant tensor fields t on $\boldsymbol{M}$, such that

$$\mathsf{f}_{I,\gamma,\mathsf{k},g}(\mathsf{t}) = \int_I g(\tau)^2 k^a k^b t_{ab} \mathrm{d}\tau \tag{34}$$

for γ, k^a, g, obeying the conditions already mentioned in this subsection *and* with g having connected support with no zeros of infinite order in its interior, for reasons to be explained shortly. We write $\widetilde{C}^\infty_0(I;\mathbb{R})$ for the set of functions g of this type. As in the two-dimensional case it is clear that the assignment $\boldsymbol{M} \to \mathcal{F}^{\mathrm{null}}_{\boldsymbol{M}}$ is covariant in the required sense.

The QEI bound is then defined by setting $\mathcal{Q}^{\mathrm{null}}_{\boldsymbol{M}}(\mathsf{f},\omega_0)$ equal to minus the right-hand side of Eq. (31), for any I, γ, k, and g such that $\mathsf{f}=\mathsf{f}_{I,\gamma,\mathsf{k},g}$. The particular parametrization is not important, for reasons similar to those explained in the previous subsection. However, here it is important that $g \in \widetilde{C}^\infty_0(I;\mathbb{R})$: otherwise we could change g to $h(\tau)=\sigma(\tau)g(\tau)$ with σ changing sign from $+1$ to -1 at a zero of g of infinite order, say at τ_0; although $\mathsf{f}_{I,\gamma,k,h}=\mathsf{f}_{I,\gamma,\mathsf{k},g}$, the two functions $F_{\gamma,h,\mathsf{k},\omega_0}$ and

$F_{\gamma,g,\mathsf{k},\omega_0}$ differ when, for example, $\tau<\tau_0<\tau'$. [The restriction to $\widetilde{C}_0^\infty(I;\mathbb{R})$ is not, however, very significant because it is dense in $C_0^\infty(I;\mathbb{R})$, as is shown in Appendix C.] Finally, the covariance property Eq. (16) follows because Eq. (10) (for the case $n=2$) implies

$$F_{\gamma,g,\mathsf{k},\psi^*\omega_0}(\tau,\tau')=F_{\psi\circ\gamma,g,\psi_*\mathsf{k},\omega_0}(\tau,\tau'). \tag{35}$$

We summarize what has been proved.

Theorem II.6: *Let $\boldsymbol{M}$ be a globally hyperbolic spacetime of dimension $d\geqslant 2$ and let $\mathcal{S}_{\boldsymbol{M}}$ be the class of Hadamard states of the Klein-Gordon field of mass $m\geqslant 0$ on $\boldsymbol{M}$. Let $\mathcal{F}_{\boldsymbol{M}}^{\mathrm{null}}$ consist of all sampling tensors of the form Eq. (34) where $\gamma:I\to\boldsymbol{M}$ is a smooth future-directed timelike curve parametrized by proper time, k is a smooth nonzero null field defined near the track of γ and $g\in\widetilde{C}_0^\infty(I;\mathbb{R})$. For each $\mathsf{f}\in\mathcal{F}_{\boldsymbol{M}}^{\mathrm{null}}$ and reference state $\omega_0\in\mathcal{S}_{\boldsymbol{M}}$ define*

$$\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{null}}(\mathsf{f},\omega_0)=\int_0^\infty\frac{\mathrm{d}\alpha}{\pi}\hat{F}_{\gamma,g,\mathsf{k},\omega_0}(-\alpha,\alpha) \tag{36}$$

for any I,γ,k,g with $\mathsf{f}=\mathsf{f}_{I,\gamma,k,g}$. Then the difference QNEI

$$\int_\gamma[\langle T_{\boldsymbol{M}ab}\rangle_\omega-\langle T_{\boldsymbol{M}ab}\rangle_{\omega_0}]k^ak^bg(\tau)^2\mathrm{d}\tau\geqslant-\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{null}}(\mathsf{f},\omega_0) \tag{37}$$

holds for all $\omega,\omega_0\in\mathcal{S}_{\boldsymbol{M}}$, and $\mathsf{f}_{I,\gamma,\mathsf{k},g}\in\mathcal{F}_{\boldsymbol{M}}^{\mathrm{null}}$, and is locally covariant.

Our second example of a locally covariant difference QEI constrains the energy density. We keep γ and g as before, but replace k^a by the velocity u^a of the trajectory. Then the following difference QWEI holds for all $\omega,\omega_0\in\mathcal{S}_{\boldsymbol{M}}$ (Ref. 30):

$$\int_\gamma[\langle T_{\boldsymbol{M}ab}\rangle_\omega-\langle T_{\boldsymbol{M}ab}\rangle_{\omega_0}]u^au^bg(\tau)^2\mathrm{d}\tau\geqslant-\int_0^\infty\frac{d\alpha}{\pi}\hat{G}_{\gamma,g,e,\omega_0}(-\alpha,\alpha), \tag{38}$$

where

$$G_{\gamma,g,\boldsymbol{e},\omega_0}(\tau,\tau')=\frac{1}{2}g(\tau)g(\tau')[\delta^{\mu\mu'}\langle\nabla_{\mathrm{e}_\mu}\Phi_{\boldsymbol{M}}(\gamma(\tau))\nabla_{\mathrm{e}_{\mu'}}\Phi_{\boldsymbol{M}}(\gamma(\tau'))\rangle_{\omega_0}+m^2\langle\Phi_{\boldsymbol{M}}(\gamma(\tau))\Phi_{\boldsymbol{M}}(\gamma(\tau'))\rangle_{\omega_0}] \tag{39}$$

and $\boldsymbol{e}=(e_\mu^a)_{\mu=0\ldots,d-1}$ is a smooth d-bein defined in a neighborhood of γ with $e_0^a=u^a$ on γ.

The frame $\boldsymbol{e}$ adds a new ingredient to the discussion of covariance, which was not explored in Ref. 30. Subject to the condition $e_0^a|_\gamma=u^a$, any choice of $\boldsymbol{e}$ will give a QEI bound, which may have differing numerical values. When considering a causal isometry $\psi:\boldsymbol{M}\to\boldsymbol{N}$, we must therefore find a way of choosing frames in the two spacetimes so as to give equal values to the QWEI bound, in accordance with covariance. One solution would be to incorporate the frame as part of the data in the QWEI, [i.e., writing $\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{weak}}(\mathsf{f},\boldsymbol{e},\omega_0)$ and using the push-forward $\psi_*\boldsymbol{e}$ on $\psi(\boldsymbol{M})$] but this seems rather inelegant. Fortunately, a better solution is at hand: it turns out that we can covariantly specify a subclass of frames guaranteed to yield the same numerical bound. This is accomplished by requiring, in addition to $e_0^a|_\gamma=u^a$, that the d-bein $\boldsymbol{e}$ be invariant under Fermi-Walker transport along γ, i.e.,

$$\frac{D_{\mathrm{FW}}e_\mu^a}{\mathrm{d}\tau}\equiv u^b\nabla_be_\mu^a+a_be_\mu^bu^a-u_be_\mu^ba^a=0 \tag{40}$$

for each $\mu=0,\ldots,d-1$, where a^a is the acceleration of γ. If $\boldsymbol{e}'$ is another d-bein also invariant under Fermi-Walker transport and with $e'^a_0=e_0^a=u^a$, then it must be that $\boldsymbol{e}'$ is related to $\boldsymbol{e}$ by a rigid rotation along γ, i.e., $e'^a_i|_{\gamma(\tau)}=S_i^je_j^a|_{\gamma(\tau)}$ for some fixed $S\in\mathrm{SO}(d-1)$, because Fermi-Walker transport preserves inner products. It is now easy to see that $G_{\gamma,g,\boldsymbol{e},\omega_0}=G_{\gamma,g,\boldsymbol{e}',\omega_0}$, because the form of $\boldsymbol{e}$

off the curve γ is irrelevant, provided it is smooth. Accordingly this QEI depends only on the smearing tensor f [defined by analogy with Eq. (34)] and the reference state.

We emphasize that this is only one method of constructing a locally covariant bound in this setting, and others may be convenient in other contexts. For example, it would be possible to simply take the infimum of the bound over all d-beins with $\mathsf{e}_0=\mathsf{u}$; this is certainly locally covariant, but impractical for calculational purposes.

With this detail addressed, it is now straightforward to show that this QEI is locally covariant by exactly the same arguments as used in the null-contracted case, and the additional observation that $\psi_*\boldsymbol{e}$ is Fermi-Walker transported along $\psi\circ\gamma$ if $\boldsymbol{e}$ is along γ. Again, we summarize what has been established.

Theorem II.7: *Let $\boldsymbol{M}$ be a globally hyperbolic spacetime of dimension $d\geqslant 2$ and let $\mathcal{S}_{\boldsymbol{M}}$ be the class of Hadamard states of the Klein-Gordon field of mass $m\geqslant 0$ on $\boldsymbol{M}$. Let $\mathcal{F}^{\mathrm{weak}}_{\boldsymbol{M}}$ consist of all sampling tensors of the form Eq. (26) where $\gamma: I\to\boldsymbol{M}$ is a smooth future-directed timelike curve parametrized by proper time and with velocity $\mathsf{u}=\dot{\gamma}$, and $g\in\tilde{C}^\infty_0(I;\mathbb{R})$. For each $\mathsf{f}\in\mathcal{F}^{\mathrm{weak}}_{\boldsymbol{M}}$ and reference state $\omega_0\in\mathcal{S}_{\boldsymbol{M}}$ define*

$$\mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}}(\mathsf{f},\omega_0)=\int_0^\infty\frac{\mathrm{d}\alpha}{\pi}\hat{G}_{\gamma,g,\boldsymbol{e},\omega_0}(-\alpha,\alpha) \tag{41}$$

for any I, γ, g with $\mathsf{f}=\mathsf{f}_{I,\gamma,g}$, and any smooth tetrad $\boldsymbol{e}$ defined near the track of γ with $\boldsymbol{e}_0|_\gamma=\mathsf{u}$ and which is invariant under Fermi-Walker transport along γ. Then the difference QWEI

$$\int_\gamma[\langle T_{\boldsymbol{M}ab}\rangle_\omega-\langle T_{\boldsymbol{M}ab}\rangle_{\omega_0}]u^au^bg(\tau)^2\mathrm{d}\tau\geqslant-\mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}}(\mathsf{f},\omega_0) \tag{42}$$

hold for all $\omega,\omega_0\in\mathcal{S}_{\boldsymbol{M}}$ and $\mathsf{f}_{I,\gamma,g}\in\mathcal{F}^{\mathrm{weak}}_{\boldsymbol{M}}$, and is locally covariant.

Most cases considered in the sequel will actually involve averages in static spacetimes along timelike curves that are static trajectories (i.e., orbits of a hypersurface orthogonal timelike Killing field ξ) and with ω_0 chosen to be a static Hadamard state (with respect to the same Killing field). In these cases the bounds derived above simplify considerably, because the two-point function of ω_0 obeys

$$w_2(\psi_tx,\psi_tx')=w_2(x,x') \tag{43}$$

for any t, x,x', where ψ_t is the one-parameter group of isometries obtained from ξ. We fix a particular orbit $\gamma(\tau)=\psi_\tau(x_0)$, which may be assumed to be a proper-time parametrization (as $\xi_a\xi^a$ is constant along γ and may be set equal to unity). Then the two-point function, restricted to γ, can be expressed as

$$w_2(\gamma(\tau),\gamma(\tau'))=w_2(\psi_\tau(x_0),\psi_{\tau'}(x_0))=w(\tau-\tau'), \tag{44}$$

where $w(\tau)=w_2(\psi_\tau(x_0),x_0)$. The same time-translational invariance is obtained for derivatives $(\nabla_{\mathsf{v}}\otimes\nabla_{\mathsf{v}})w_2(\gamma(\tau),\gamma(\tau'))$, provided that v is invariant under the Killing flow, or equivalently, has vanishing Lie derivative with respect to ξ on γ, i.e., $\pounds_\xi\mathsf{v}|_\gamma=0$.

This simplifies the QWEI bound (38) as follows. If $\boldsymbol{e}$ is Lie-transported along γ then

$$G_{\gamma,g,\boldsymbol{e},\omega_0}(\tau,\tau')=g(\tau)g(\tau')T_{\gamma,\omega_0}(\tau-\tau') \tag{45}$$

holds for some "single variable" distribution T_{γ,ω_0}; moreover, $\boldsymbol{e}$ is also invariant under Fermi-Walker transport along γ (owing to hypersurface orthogonality of ξ).[53] Then, as shown in Refs. 7 and 30 the QEI Eq. (38) becomes

$$\int_\gamma [\langle T_{\mathbf{M}ab}\rangle_\omega - \langle T_{\mathbf{M}ab}\rangle_{\omega_0}]u^a u^b g(\tau)^2 \mathrm{d}\tau \geqslant -\int_{-\infty}^{\infty} du |\hat{g}(u)|^2 Q_{\gamma,\omega_0}(u), \tag{46}$$

where $Q_{\gamma,\omega_0}(u)$ is a positive polynomially bounded function defined by

$$Q_{\gamma,\omega_0}(u) = \frac{1}{2\pi^2}\int_{(-\infty,u)} \mathrm{d}v \hat{T}_{\gamma,\omega_0}(v). \tag{47}$$

Additionally, if ω_0 is a ground state (as was the case in Ref. 30) one may show that $\hat{T}_{\gamma,\omega_0}(\sigma)=0$ for $\sigma<0$, and so the function Q_{γ,ω_0} is supported on the positive half-line only. More generally, it is always the case that $\hat{T}_{\gamma,\omega_0}(\sigma)$ decays rapidly as $\sigma\to-\infty$, so Q_{γ,ω_0} is always well defined.[7] Technically, $\hat{T}_{\gamma,\omega_0}(\sigma)$ is a measure, and may have δ-function spikes that would exhibit themselves as discontinuities in $Q_{\gamma,\omega_0}(u)$. Since we define $Q_{\gamma,\omega_0}(u)$ as an integral over the open interval $(-\infty,u)$, it is continuous from the left.

A similar analysis holds for the QNEI Eq. (31), provided that the null vector field k has vanishing Lie derivative along γ, $\pounds_\xi \mathsf{k}=0$, because we have

$$F_{\gamma,g,\mathsf{k},\omega_0}(\tau,\tau') = g(\tau)g(\tau')S_{\gamma,\mathsf{k},\omega_0}(\tau-\tau') \tag{48}$$

for some distribution $S_{\gamma,\mathsf{k},\omega_0}$.

To conclude this section, we mention that more general QEI bounds may be constructed along similar lines, based on other decompositions of the contracted stress-energy tensor as a sum of squares. This includes bounds averaged over spacetime volumes (see, e.g., Ref. 9). However, we will not need this generality here, and observe only that one would need to ensure that such decompositions are made in a canonical fashion to obtain a locally covariant bound.

III. APPLICATIONS: GENERAL EXAMPLES

In this section we develop some simple consequences of the QEIs described in Secs. II D and II E specialized to Minkowski space. These will then be utilized in more general spacetimes using the local covariance properties of these bounds. Our results are obtained by converting QEI bounds into eigenvalue problems that can then be solved.

For the most part, we will consider the scalar field of mass $m\geqslant 0$ on d-dimensional globally hyperbolic spacetimes for $d\geqslant 2$; special features of massless fields in two dimensions will be treated in Sec. III C. Accordingly, let $\boldsymbol{N}$ be a d-dimensional globally hyperbolic spacetime, and let $\boldsymbol{M}_d$ denote d-dimensional Minkowski space. As illustrated in Fig. 1, let $\gamma: I\to\boldsymbol{N}$ be a smooth, future-directed timelike curve, parametrized by proper time $\tau\in I$, and assume γ may be enclosed in a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$ so that $\boldsymbol{N}'$ is the image of a c.e.g.h.s. $\boldsymbol{M}'$ of $\boldsymbol{M}_d$ under a causal isometric embedding $\psi:\boldsymbol{M}'\to\boldsymbol{N}$. Thus the curve γ is the image of a curve $\tilde{\gamma}(\tau)=\psi^{-1}(\gamma(\tau))$ in $\boldsymbol{M}_d$; because ψ is an isometry, $\tau\mapsto\tilde{\gamma}(\tau)$ is also a proper time parametrization, and $\tilde{\gamma}$ has the same proper acceleration as γ for each $\tau\in I$.

Given any $g\in\tilde{C}_0^\infty(I;\mathbb{R})$, define a sampling tensor on Minkowski space $\mathsf{f}\in\mathcal{F}_{M_d}^{\mathrm{weak}}$ by

$$\mathsf{f}(\mathsf{t}) = \int_I t_{ab}|_{\tilde{\gamma}(\tau)}\tilde{u}^a\tilde{u}^b g(\tau)^2 \mathrm{d}\tau \tag{49}$$

on smooth covariant rank-two tensor fields t on $\boldsymbol{M}_d$, where $\tilde{\mathsf{u}}$ is the velocity of $\tilde{\gamma}$. [Recall that $g\in\tilde{C}_0^\infty(I;\mathbb{R})$ means that g is a real-valued smooth function whose support is compact, connected and contained in I, and that g has no zeros of infinite order in the interior of its support.] Under the isometry, f is mapped to $\psi_*\mathsf{f}$, with action

$$\psi_* \mathsf{f}(\mathsf{t}) = \int_I t_{ab}|_{\gamma(\tau)} u^a u^b g(\tau)^2 \mathrm{d}\tau, \tag{50}$$

where t is now any smooth covariant rank-2 tensor field on $\boldsymbol{N}$. Applied to the stress-energy tensor, $\psi_* \mathsf{f}$ therefore provides a weighted average of the energy density along γ. Our aim is to place constraints on these averages using the locally covariant difference QWEI given in Theorem II.7. By local covariance, Corollary II.4 guarantees that

$$\int_I \langle T_{\boldsymbol{N}ab} \rangle_\omega (\gamma(\tau)) u^a u^b g(\tau)^2 \mathrm{d}\tau = \langle \mathbf{T}_{\boldsymbol{N}}(\psi_* \mathsf{f}) \rangle_\omega \geqslant - \mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}_d}(\mathsf{f}, \omega_{\boldsymbol{M}_d}), \tag{51}$$

where $\omega_{\boldsymbol{M}_d}$ is the Minkowski vacuum state.

We will be particularly interested in the least upper bound of the energy density along γ,

$$\mathcal{E} := \sup_\gamma \langle T_{\boldsymbol{N}ab} u^a u^b \rangle_\omega. \tag{52}$$

Since the energy density is smooth, this value must be the maximum value taken by the field on the closure of the track of γ. Using the trivial estimate $\mathcal{E} \geqslant \langle T_{\boldsymbol{N}ab} u^a u^b \rangle_\omega (\gamma(\tau))$ for each $\tau \in I$, we have

$$\mathcal{E} \int_I g(\tau)^2 \mathrm{d}\tau \geqslant \int_I \langle T_{\boldsymbol{N}ab} \rangle_\omega (\gamma(\tau)) u^a u^b g(\tau)^2 \mathrm{d}\tau \tag{53}$$

and, putting this together with Eq. (51), we obtain the inequality

$$\mathcal{E} \int_I g(\tau)^2 \mathrm{d}\tau \geqslant - \mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}_d}(\mathsf{f}, \omega_{\boldsymbol{M}_d}), \tag{54}$$

which holds, in the first place, for all $g \in \widetilde{C}^\infty_0(I; \mathbb{R})$. In the next two subsections we will analyze this in two special cases: namely, inertial motion and uniform acceleration.

A. Inertial curves

When γ is inertial the QWEI of Theorem II.7 takes the simpler form described in Eqs. (46) and (47) above:[14]

$$\mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}_d}(\mathsf{f}, \omega_{\boldsymbol{M}_d}) = K_d \int_m^\infty \frac{\mathrm{d}u}{\pi} u^d |\hat{g}(u)|^2 Q_d(u/m), \tag{55}$$

where

$$Q_d(x) = \frac{d}{x^d} \int_1^x \mathrm{d}y \; y^2 (y^2 - 1)^{(d-3)/2}, \tag{56}$$

and the constant K_d is $K_d = A_{d-2}/(2d(2\pi)^{d-1})$, where A_k is the area of the unit k-sphere. (Notation varies slightly from that used in Ref. 14.)

For all $d \geqslant 3$, it is clear that $Q_d(x) \leqslant 1$ for all $x \geqslant 1$, while one may show that $Q_2(x) < 1.2$ on the same domain.[54] Using these results, we may estimate Eq. (55) rather crudely by

$$\mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{M}_d}(\mathsf{f}, \omega_{\boldsymbol{M}_d}) \leqslant K'_d \int_0^\infty \frac{\mathrm{d}u}{\pi} u^d |\hat{g}(u)|^2, \tag{57}$$

with $K'_d = K_d$ for $d \geqslant 3$ and $K'_2 = 1.2 K_2$. Note that we have made two changes here: (a) $Q_d(u/m)$ has been replaced by unity; (b) the lower integration limit m has been replaced by zero.

We now specialize to even dimensions $d=2k$, $k\geqslant 1$. Because g is real-valued, $|\hat{g}(u)|$ is even and we may write

$$\int_0^\infty \frac{\mathrm{d}u}{\pi} u^d |\hat{g}(u)|^2 = \int_{-\infty}^\infty \frac{\mathrm{d}u}{\pi} u^{2k} |\hat{g}(u)|^2 = \int_I \mathrm{d}\tau\, |(D^k g)(\tau)|^2, \tag{58}$$

where D is the differential operator $D=-i\mathrm{d}/\mathrm{d}\tau$ and we have used Parseval's theorem, and the fact that g vanishes outside I.

Inserting the above in Eq. (54), we have shown that $\mathcal{E}$ obeys the inequality

$$\mathcal{E}\int_I |g(\tau)|^2 d\tau \geqslant -K'_d \int_I d\tau\, |(D^k g)(\tau)|^2 \tag{59}$$

for all $g\in\widetilde{C}_0^\infty(I;\mathbb{R})$. The class $\widetilde{C}_0^\infty(I;\mathbb{R})$ is inconvenient to work with directly; fortunately, the same inequality holds for general $g\in C_0^\infty(I)$, as we now show. First, any $g\in\widetilde{C}_0^\infty(I;\mathbb{R})$ is the limit of a sequence of $g_n\in\widetilde{C}_0^\infty(I;\mathbb{R})$ for which $g_n\to g$ and $D^k g_n\to D^k g$ in $L^2(I)$ (see Appendix C). Applying the above inequality to each g_n, we may take the limit $n\to\infty$ to conclude that it holds for g as well. Having established the result for arbitrary real-valued $g\in C_0^\infty(I)$, we extend to general complex-valued g by applying it to real and imaginary parts separately, and then adding. Accordingly the inequality Eq. (59) holds for all $g\in C_0^\infty(I)$.

Integrating by parts k times, and noting that no boundary terms arise because g vanishes near the boundary ∂I of I, Eq. (59) may be rearranged to give

$$-\frac{\mathcal{E}}{K'_d} \leqslant \frac{\langle g|Lg\rangle}{\langle g|g\rangle}, \tag{60}$$

where $\langle\cdot|\cdot\rangle$ denotes the usual L^2-inner product on I, and the operator $L=(-1)^k\mathrm{d}^{2k}/\mathrm{d}\tau^{2k}$ on $C_0^\infty(I)$. Our aim is now to minimize the right-hand side over the class of g at our disposal (excluding the identically zero function). Now the operator L is symmetric[55] and positive, i.e., $\langle g|Lg\rangle\geqslant 0$ for all $g\in C_0^\infty(I)$. By Theorem X.23 in Ref. 56, the solution to our minimization problem is the lowest element λ_0 of the spectrum of $\hat{L}$, the so-called *Friedrichs extension* of L. This is a self-adjoint operator with the same action as L on $C_0^\infty(I)$, but which is defined on a larger domain in $L^2(I)$. In particular, every function in the domain of $\hat{L}$ obeys the boundary condition $g=g'=\cdots=g^{(k-1)}=0$ at ∂I. (See Ref. 33, where the technique of reformulating quantum energy inequalities as eigenvalue problems was first introduced, and which contains a self-contained exposition of the necessary operator theory.) One may think of this as a precise version of the Rayleigh-Ritz principle. Once we have determined λ_0, we then have the bound

$$\mathcal{E}\geqslant -\lambda_0 K'_d, \tag{61}$$

so the problem of determining the lower bound is reduced to the analysis of a Schrödinger-like equation, subject to the boundary conditions mentioned above.

The two examples of greatest interest to us are $k=1$ and $k=2$, representing two- and four-dimensional spacetimes. Starting with $k=1$, let us suppose that I is the interval $(-\tau_0/2,\tau_0/2)$ for some $\tau_0>0$. We therefore solve $-g''=\lambda g$ subject to Dirichlet boundary conditions at $\pm\tau_0/2$; as is well known, the lowest eigenvalue is $\lambda_0=\pi^2/\tau_0^2$ and corresponds to the eigenfunction $g(\tau)=\cos(\pi\tau/\tau_0)$. [A possible point of confusion is that, if g is extended so as to vanish outside I, it will not be smooth. However, there is no contradiction here: the point is that the infimum is not attained on $C_0^\infty(I)$.] Thus we have

$$\mathcal{E} \geqslant -\frac{3\pi}{10\tau_0^2}, \tag{62}$$

because $K_2' = 1.2K_2 = 1.2/(4\pi) = 3/(10\pi)$ (by convention, the zero sphere has area $A_0 = 2$). We may infer, without further calculation, that the bound must be zero if $I = \mathbb{R}$, because [returning to the Ritz quotient Eq. (60)], the infimum over all functions in $C_0^\infty(\mathbb{R})$ must be less than or equal to the infimum over all functions in $C_0^\infty(I)$ for any bounded I (a similar argument applies to the semi-infinite case). Thus λ_0 can be no greater than zero; on the other hand, the minimum cannot be negative either, because the original functional is nonnegative. Accordingly Eq. (62) holds in all cases, with τ_0 equal to the length of the interval I.

In the four-dimensional case $k=2$, we proceed in a similar way, solving $g'''' = \lambda g$ subject to $g = g' = 0$ at ∂I. In the case where I is bounded, $I = (-\tau_0/2, \tau_0/2)$ (without loss of generality), the spectrum consists only of positive eigenvalues. It is easy to see that the solutions to the eigenvalue equation $g'''' = \beta^4 g$ are linear combinations of trigonometric and hyperbolic functions. The lowest eigenfunction solution that obeys the boundary conditions is

$$g(\tau) = \cosh(\beta\tau/\tau_0) - \frac{\cosh(\beta/2)}{\cos(\beta/2)} \cos(\beta\tau/\tau_0), \tag{63}$$

where $\beta \approx 4.730\,040\,745$ is the minimum positive solution to

$$\tan(\beta/2) = -\tanh(\beta/2). \tag{64}$$

Since $K_4' = 1/(16\pi^2)$, we obtain

$$\mathcal{E} \geqslant -\frac{500.5639}{16\pi^2\tau_0^4} = -\frac{3.169\,858}{\tau_0^4}. \tag{65}$$

If I is semi-infinite or infinite, we may argue exactly as in the two-dimensional case that the bound vanishes, in agreement with the formal limit $\tau_0 \to \infty$.

Clearly this approach will give similar results in any even dimension, with a consequent increase in complexity in solving the eigenvalue problem. Nonetheless, it is clear that the resulting bound will always scale as τ_0^{-d}. In fact, this is even true in odd spacetime dimensions, where the eigenvalue problem would involve a nonlocal operator and is not easily tractable.

We summarize what has been proved so far in the following way.

Proposition III.1: Let $\mathbf{N}$ *be a globally hyperbolic spacetime of dimension* $d \geqslant 2$ *and suppose that a timelike geodesic segment* γ *of proper duration* τ_0 *may be enclosed in a c.e.g.h.s. of* $\mathbf{N}$, *which is causally isometric to a c.e.g.h.s. of Minkowski space* $\mathbf{M}_d$, *then*

$$\sup_\gamma \langle T_{\mathbf{N}ab} u^a u^b \rangle_\omega \geqslant -\frac{C_d}{\tau_0^d} \tag{66}$$

for all Hadamard states ω *of the Klein-Gordon field of mass* $m \geqslant 0$ *on* $\mathbf{N}$. *The constants* C_d *depend only on* d. *In particular*, $C_2 = 3\pi/10 = 0.942\,478\ldots$, *while* $C_4 = 3.169\,858\ldots$.

Remark: When the field has nonzero mass, we can expect rather more rapid decay than given by this estimate. To see why, return to the argument leading to Eq. (57). If we reinstate m as the lower integration limit, we have

$$\mathcal{Q}^{\text{weak}}_{\mathbf{M}_d}(\mathrm{f}, \omega_{\mathbf{M}_d}) \leqslant K_d' \int_m^\infty \frac{\mathrm{d}u}{\pi} u^d |\hat{g}(u)|^2. \tag{67}$$

Suppose for simplicity that $I = (-\tau_0/2, \tau_0/2)$. If we write $g_{\tau_0}(\tau) = \tau_0^{-1/2} g_0(\tau/\tau_0)$, for $g_0 \in C_0^\infty(-1/2, 1/2)$, a change of variables yields

$$\mathcal{Q}_{\boldsymbol{M}_d}(\mathsf{f}, \omega_{\boldsymbol{M}_2}) \leqslant \frac{K'_d G_d(m\tau_0)}{\tau_0^d}, \tag{68}$$

where the nonnegative quantity

$$G_d(x) = \int_x^\infty \frac{\mathrm{d}y}{\pi} y^d |\hat{g}_0(y)|^2 \tag{69}$$

decays rapidly as $x \to \infty$, owing to the rapid decay of $\hat{g}$. Thus the estimate Eq. (66) is quite crude when $m\tau_0 \gg 1$; it is hoped to return to this elsewhere.

Equipped with Proposition III.1, we may now address the first two examples presented in Sec. I. First, the proposition asserts that no Hadamard state can maintain an energy density lower than $-C_d/\tau_0^d$ for proper time τ_0 along an inertial curve in a Minkowskian c.e.g.h.s. of $\boldsymbol{N}$. In particular, this justifies the claim made in Example 1 in Sec. I.

Our bounds clearly depend only on τ_0, which in turn is controlled by the size of the Minkowskian region $\boldsymbol{N}'$. By choosing the curve γ and $\boldsymbol{N}'$ in an appropriate way, fairly simple geometrical considerations can thus provide good *a priori* bounds on the magnitude and duration of negative energy density. A good illustration is the following (which includes Example 2 in Sec. I).

Suppose that a d-dimensional globally hyperbolic spacetime $\boldsymbol{N}$ with metric $\boldsymbol{g}$ is stationary with respect to timelike Killing vector t^a and admits the smooth foliation into constant time surfaces $N \cong \mathbb{R} \times \Sigma$. Suppose there is a (maximal) subset Σ_0 of Σ, with nonempty interior, for which $\boldsymbol{g}$ takes the Minkowski form on $\mathbb{R} \times \Sigma_0$. Choose any point (t,x) in N, with $x \in \Sigma_0$, and suppose that we may isometrically embed a Euclidean $(d-1)$ ball of radius r in Σ_0, centered at x (see Fig. 2). Then the interior of the double cone $J^+(\{(t-r,x)\}) \cap J^-(\{(t+r,x)\})$ is a c.e.g.h.s. of $\boldsymbol{N}$, which is isometric to a c.e.g.h.s. of Minkowski space, and contains an inertial curve segment $\gamma(\tau) = (\tau, x)$ parametrized by the interval $(t-r, t+r)$ of proper time. Any Hadamard state ω on $\boldsymbol{N}$ therefore obeys

$$\sup_\gamma \langle T_{\boldsymbol{N}ab} u^a u^b \rangle_\omega \geqslant -\frac{C_d}{(2r)^d} \tag{70}$$

along γ. Writing $r(x)$ for the minimum distance from x to the boundary of Σ_0, it is clear that this inequality holds for all $r < r(x)$ and hence, by continuity, for $r = r(x)$. Moreover, if the state is stationary (for example, if it is the ground state), then the energy density takes a constant value along γ and we obtain

$$\langle T_{ab} n^a n^b \rangle_\omega (t,x) \geqslant -\frac{C_d}{(2r(x))^d} \tag{71}$$

for any $x \in \Sigma_0$, where n^a is the unit vector along t^a. In this way we obtain a universal bound on the fall-off of negative energy densities in such spacetimes, which could be used to provide a quantitative check on exact calculations, if these are possible, or to provide some precise information in situations where they are not. The bound is of course very weak close to the boundary of Σ_0: this does not imply that the energy density diverges as this boundary is approached, of course, but merely indicates that it would not be incompatible with the quantum inequalities for there to exist geometries on $\mathbb{R} \times (\Sigma \backslash \Sigma_0)$ for which the stationary energy density just outside might be very negative.

To conclude this subsection, let us briefly discuss the null-contracted QEI Eq. (31) in the present context. For simplicity, we restrict ourselves to four dimensions. Suppose $\tilde{k}^a$ is a nonzero null vector field that is covariantly constant along $\tilde{\gamma}$, so, in particular, $\tilde{u}^a \tilde{k}_a$ is also constant on $\tilde{\gamma}$. Our sampling tensor is now defined to be $\mathsf{f} \in \mathcal{F}^{\mathrm{null}}_{\boldsymbol{M}_4}$ with action

$$\mathsf{f}(t) = \int_I t_{ab}|_{\tilde{\gamma}(\tau)} \tilde{k}^a \tilde{k}^b g(\tau)^2 \mathrm{d}\tau \tag{72}$$

on smooth covariant rank-2 tensor fields t on $\boldsymbol{M}_4$. In exactly the same way as for the QWEI discussed above, we may apply local covariance to the QNEI of Theorem II.6, so yielding

$$\int \langle T_{\boldsymbol{N}ab} \rangle_\omega \, k^a k^b g(\tau)^2 \mathrm{d}\tau \geqslant - \mathcal{Q}^{\mathrm{null}}_{\boldsymbol{M}_4}(\mathsf{f}, \omega_{\boldsymbol{M}_4}), \tag{73}$$

where, as shown in Ref. 52,

$$\mathcal{Q}^{\mathrm{null}}_{\boldsymbol{M}_4}(\mathsf{f}, \omega_{\boldsymbol{M}_4}) = - \frac{(u^a k_a)^2}{12\pi^2} \int_{-\infty}^{\infty} g''(\tau)^2 \mathrm{d}\tau \tag{74}$$

for the massless scalar field (and in fact this bound also constrains the massive field too). This differs from the corresponding QWEI by a factor of $4(u^a k_a)^2/3$ [recall that $K_4' = 1/(16\pi^2)$], so we may immediately deduce the following result.

Proposition III.2: Let $\boldsymbol{N}$ *be a four-dimensional globally hyperbolic spacetime and suppose that a timelike geodesic segment* γ *of proper duration* τ_0 *may be enclosed in a c.e.g.h.s. of* $\boldsymbol{N}$*, which is causally isometric to a c.e.g.h.s. of Minkowski space. If* k^a *is a covariantly constant null vector field on* γ *then we have*

$$\sup_\gamma \langle T_{\boldsymbol{N}ab} \rangle_\omega k^a k^b \geqslant - \frac{C_4' (u^a k_a)^2}{\tau_0^4} \tag{75}$$

for any Hadamard state ω *of the Klein-Gordon field, where* $C_4' = 4C_4/3 = 4.226\,477\ldots$.

This result justifies the claim made above Eq. (38) of Ref. 57, where an application is presented.

B. Uniformly accelerated trajectories in four dimensions

We now turn to the case where γ has uniform constant proper acceleration α. For simplicity we consider only massless fields in four dimensions, but expect similar results in more general cases. We need to estimate $\mathcal{Q}^{\mathrm{weak}}_{M_4}(\mathsf{f}, \omega_{\boldsymbol{M}_4})$ where f is supported on the uniformly accelerated worldline $\tilde{\gamma}$ in $\boldsymbol{M}_4$. It will be convenient to drop the tilde from $\tilde{\gamma}$ and the subscript from $\boldsymbol{M}_4$. Without loss of generality, we may assume $\gamma: I \to \boldsymbol{M}$ is parametrized so that

$$\gamma(\tau) = \begin{pmatrix} \xi_o \sinh(\tau/\xi_o) \\ \xi_o \cosh(\tau/\xi_o) \\ y_o \\ z_o \end{pmatrix} \quad \text{with} \quad u^a(\tau) = \frac{\mathrm{d}\gamma(\tau)^a}{\mathrm{d}\tau} = \begin{pmatrix} \cosh(\tau/\xi_o) \\ \sinh(\tau/\xi_o) \\ 0 \\ 0 \end{pmatrix}, \tag{76}$$

where $\xi_o = \alpha^{-1}$.

The first step in our calculation is to set up an orthonormal tetrad field surrounding the worldline,

$$e_0^a = \frac{1}{\sqrt{x^2 - t^2}} \begin{pmatrix} x \\ t \\ 0 \\ 0 \end{pmatrix}, \quad e_1^a = \frac{1}{\sqrt{x^2 - t^2}} \begin{pmatrix} t \\ x \\ 0 \\ 0 \end{pmatrix}, \quad e_2^a = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_3^a = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \tag{77}$$

which satisfies the two properties required: namely, that e_0^a agrees with the velocity u^a on γ, and that the frame is invariant under Fermi-Walker transport along γ. The required bound is then given by

$$\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{weak}}(\mathsf{f},\omega_{\boldsymbol{M}}) = \int_0^\infty \frac{\mathrm{d}\alpha}{2\pi}\hat{G}_{\gamma,g,\boldsymbol{e},\omega_{\boldsymbol{M}}}(-\alpha,\alpha), \tag{78}$$

where

$$G_{\gamma,g,\boldsymbol{e},\omega_{\boldsymbol{M}}}(\tau,\tau') = \frac{1}{2}g(\tau)g(\tau')\delta^{\mu\mu'}\langle\nabla_{\mathrm{e}_\mu}\Phi_{\boldsymbol{M}}(\gamma(\tau))\nabla_{\mathrm{e}_{\mu'}}\Phi_{\boldsymbol{M}}(\gamma(\tau'))\rangle_{\omega_{\boldsymbol{M}}}. \tag{79}$$

We evaluate this quantity in stages, beginning by noting that

$$\begin{aligned}&\delta^{\mu\mu'}\langle\nabla_{\mathrm{e}_\mu}\Phi_{\boldsymbol{M}}(x)\nabla_{e_{\mu'}}\Phi_{\boldsymbol{M}}(x')\rangle_{\omega_{\boldsymbol{M}}}\\ &\quad= \left[\frac{(xx'+tt')(\partial_t\partial_{t'}+\partial_x\partial_{x'})+(xt'+tx')(\partial_t\partial_{x'}+\partial_x\partial_{t'})}{\sqrt{x^2-t^2}\sqrt{x'^2-t'^2}}+\partial_y\partial_{y'}+\partial_z\partial_{z'}\right]W_{\boldsymbol{M}}^{(2)}(x,x'),\end{aligned} \tag{80}$$

where

$$W_{\boldsymbol{M}}^{(2)}(x,x') = -\lim_{\epsilon\to 0^+}\frac{1}{4\pi^2}[(t-t'-i\epsilon)^2-|\boldsymbol{x}-\boldsymbol{x}'|^2]^{-1} \tag{81}$$

is the Wightman function of the vacuum state. Performing the necessary derivatives and pulling back to the worldline, we obtain, after some calculation,

$$G_{\gamma,g,\boldsymbol{e},\omega_0}(\tau,\tau') = g(\tau)g(\tau')T(\tau-\tau'), \tag{82}$$

where T is the limit (in the distributional sense) as $\epsilon\to 0^+$ of

$$T_\epsilon(\sigma) = \frac{3}{32\pi^2\xi_o^4}\operatorname{cosech}^4\left(\frac{\sigma}{2\xi_o}-i\frac{\epsilon}{\xi_o}\right). \tag{83}$$

Thus we are in the situation of Eq. (45), and the bound becomes

$$\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{weak}}(\mathsf{f},\omega_{\boldsymbol{M}}) = \int_{-\infty}^\infty \mathrm{d}u|\hat{g}(u)|^2 Q(u), \tag{84}$$

where

$$Q(u) = \frac{1}{2\pi^2}\int_{(-\infty,u)}\mathrm{d}v\hat{T}(v). \tag{85}$$

To obtain the required Fourier transform, we first use contour integration[58] to find

$$\hat{T}_\epsilon(u) = \frac{e^{-2u\epsilon}}{2\pi\xi_o^4}\left(\frac{\xi_o^4u^3+\xi_o^2u}{1-e^{-2\pi\xi_o u}}\right), \tag{86}$$

which decays exponentially as $u\to-\infty$, provided $\epsilon<\pi\xi_o$. Taking the limit $\epsilon\to 0^+$ it is easy to check that

$$\hat{T}(u) = \frac{1}{2\pi\xi_o^4}\left(\frac{\xi_o^4u^3+\xi_o^2u}{1-e^{-2\pi\xi_o u}}\right). \tag{87}$$

Note that this Fourier transform has support on the whole real line, not just the positive half-line. Thus

$$Q(u) = \frac{1}{4\pi^3 \xi_o^4} \int_{-\infty}^{u} \frac{\xi_o^4 v^3 + \xi_o^2 v}{1 - e^{-2\pi\xi_o v}} dv. \tag{88}$$

Our aim is now to estimate $Q(u)$ in order to obtain a bound that may be analyzed by eigenvalue techniques as in the previous subsection. Beginning in the half-line $u<0$, we may estimate

$$Q(u) < Q(0) = \frac{11}{960\pi^3 \xi_o^4} \tag{89}$$

since $Q(u)$ is everywhere increasing. On the other hand, for $u \geqslant 0$, we may split the integral into $Q(0)$ and the contribution from $[0,u]$ to give

$$Q(u) = \frac{11}{960\pi^3 \xi_o^4} + \frac{1}{4\pi^3 \xi_o^4} \left[\int_0^u (\xi_o^4 v^3 + \xi_0^2 v) \mathrm{d}v + \int_0^u \frac{\xi_o^4 v^3 + \xi_o^2 v}{e^{2\pi\xi_o v} - 1} \mathrm{d}v \right] \tag{90}$$

after rearranging. Now the last integral is increasing in u, so we may bound it by its limit as $u \to +\infty$ to yield

$$Q(u) \leqslant \frac{1}{16\pi^3 \xi_o^4} \left(\xi_o^4 u^4 + 2\xi_o^2 u^2 + \frac{11}{30} \right) \tag{91}$$

for $u>0$. Using the estimates Eqs. (89) and (91), and the fact that $|\hat{g}(u)|^2$ is even,

$$\begin{aligned} \mathcal{Q}_{\boldsymbol{M}}^{\mathrm{weak}}(\mathsf{f}, \omega_{\boldsymbol{M}}) &\leqslant \frac{11}{960\pi^3 \xi_o^4} \int_{-\infty}^{0} \mathrm{d}u |\hat{g}(u)|^2 + \frac{1}{16\pi^3 \xi_o^4} \int_0^{\infty} \mathrm{d}u |\hat{g}(u)|^2 \left(\xi_o^4 u^4 + 2\xi_o^2 u^2 + \frac{11}{30} \right) \\ &= \frac{1}{16\pi^2 \xi_o^4} \int_{-\infty}^{\infty} \frac{\mathrm{d}u}{2\pi} |\hat{g}(u)|^2 \left(\xi_o^4 u^4 + 2\xi_o^2 u^2 + \frac{11}{20} \right). \end{aligned} \tag{92}$$

Applying Parseval's theorem, we arrive at

$$\mathcal{Q}_{\boldsymbol{M}}^{\mathrm{weak}}(\mathsf{f}, \omega_{\boldsymbol{M}}) \leqslant \frac{1}{16\pi^2} \int_{-\infty}^{\infty} \mathrm{d}\tau \left(|g''(\tau)|^2 + \frac{2}{\xi_o^2} |g'(\tau)|^2 + \frac{11}{20\xi_o^4} |g(\tau)|^2 \right), \tag{93}$$

and, together with Eq. (54), we now have

$$\mathcal{E} \int_I |g(\tau)|^2 \mathrm{d}\tau \geqslant \frac{1}{16\pi^2} \int_{-\infty}^{\infty} \mathrm{d}\tau \left(|g''(\tau)|^2 + \frac{2}{\xi_o^2} |g'(\tau)|^2 + \frac{11}{20\xi_o^4} |g(\tau)|^2 \right), \tag{94}$$

for any $g \in \widetilde{C}_0^{\infty}(I;\mathbb{R})$. As in the previous subsection, we may extend this inequality to arbitrary $g \in C_0^{\infty}(I)$, and then optimize over this class. This leads to the conclusion that

$$\mathcal{E} \geqslant -\frac{\mu_0}{16\pi^2}, \tag{95}$$

where μ_0 is the lowest (positive) eigenvalue for the equation

$$g'''' - \frac{2}{\xi_o^2} g'' + \frac{11}{20\xi_o^4} g = \mu g \tag{96}$$

on I, subject to boundary conditions $g=g'=0$ at ∂I.

Let us suppose that I is bounded, writing $I=(-\tau_0/2, \tau_0/2)$ without loss of generality. It is convenient to write

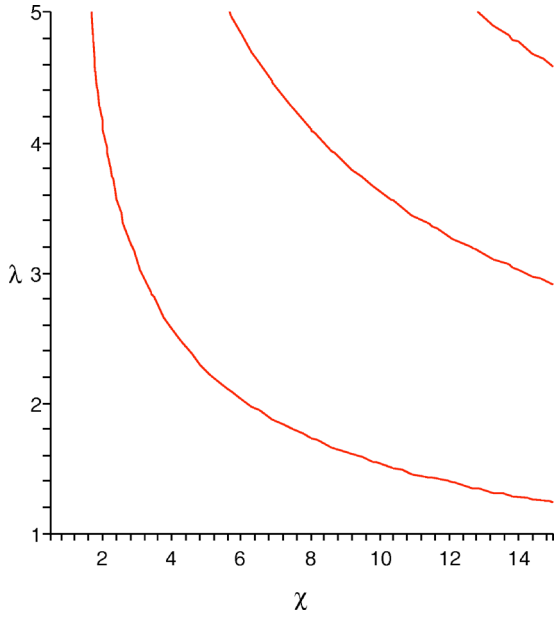

FIG. 5. (Color online) The first three solutions λ to Eq. (100), showing the dependence on $\chi=\tau_0/\xi_0$.

$$\mu = \frac{20\lambda^2 - 9}{20\xi_o^4} \tag{97}$$

for then the eigensolutions must be scalar multiples of

$$g(\tau) = \cosh \frac{\sqrt{\lambda+1}\,\tau}{\xi_o} + A \cos \frac{\sqrt{\lambda-1}\,\tau}{\xi_o}, \tag{98}$$

where

$$A = \frac{\sqrt{\lambda+1}\,\sinh(\sqrt{\lambda+1}\,\tau_0/(2\xi_o))}{\sqrt{\lambda-1}\,\sin(\sqrt{\lambda-1}\,\tau_0/(2\xi_o))} \tag{99}$$

and $\lambda > 1$ solves

$$\sqrt{\lambda+1}\,\tanh \frac{\sqrt{\lambda+1}\,\tau_0}{2\xi_o} = -\sqrt{\lambda-1}\,\tan \frac{\sqrt{\lambda-1}\,\tau_0}{2\xi_o}. \tag{100}$$

We shall denote the minimum solution to this equation in $(1,\infty)$ by λ_0 (see Fig. 5); clearly λ_0 depends only on the ratio of the sampling time τ_0 to the acceleration scale ξ_o. Two limits are of interest. First, when $\tau_0/\xi_0 \ll 1$, one may show that $\lambda_0^2 \sim \beta^4 \xi_o^4/\tau_0^4$ where β is as in Eq. (64). Thus we regain the usual short-timescale constraint Eq. (66). This supports the "usual assumption" (see Ref. 19 for references) that sampling at scales shorter than those determined by the acceleration or curvature is governed by the bound obtained for inertial curves in Minkowski space. On the other hand, if we take $\tau_0 \gg \xi_o$, we see that $\lambda_0 \to 1$, so

$$\mathcal{E} \gtrsim -\frac{11}{320\pi^2\xi_o^4} \tag{101}$$

in this limit.

In fact, more can be said for the inextendible case $\tau_0=\infty$, because the approximations made to gain Eq. (91) are rather wasteful in this limit. Choose any $g\in C_0^\infty((-1/2,1/2))$ with $g(0)\neq 0$ and define $g_{\tau_0}(\tau)=\tau_0^{-1/2}g(\tau/\tau_0)$, denoting the corresponding sampling tensor f_{τ_0}. Then a simple change of variables argument applied to Eq. (84) shows that

$$\mathcal{Q}_{\boldsymbol{M}}^{\text{weak}}(\mathsf{f}_{\tau_0},\omega_{\boldsymbol{M}})=\int_{-\infty}^{\infty}\mathrm{d}v|\hat{g}(v)|^2Q(v/\tau_0), \tag{102}$$

and the limit $\tau_0\to\infty$ may be taken under the integral sign to yield

$$\lim_{\tau_0\to\infty}\mathcal{Q}_{\boldsymbol{M}}(\mathsf{f}_{\tau_0},\omega_{\boldsymbol{M}})=2\pi Q(0)\int_{-\infty}^{\infty}\mathrm{d}\tau|g_{\tau_0}(\tau)|^2. \tag{103}$$

In particular, if g has unit L^2-norm, we have

$$\liminf_{\tau_0\to\infty}\frac{1}{\tau_0}\int_\gamma\langle T_{ab}u^au^b\rangle_\omega g(\tau/\tau_0)^2\mathrm{d}\tau\geqslant-\frac{11\alpha^4}{480\pi^2}, \tag{104}$$

where $\alpha=\xi_o^{-1}$ is the proper acceleration of the curve, as asserted in Example 3 in Sec. I. Thus long term averages of the energy density measured along the curve are bounded from below, and no energy density can be less than this bound over the entire worldline. This is an improvement by a factor of 3/2 over the bound given in Eq. (101). Using a more refined analysis one could presumably extract it as the limit of a result for general τ_0, but we will not pursue this here. To summarize, we have reached the following conclusions.

Proposition III.3: Let $\boldsymbol{N}$ *be a four-dimensional globally hyperbolic spacetime containing a timelike curve* γ *of proper duration* τ_0 *and constant proper acceleration* α. *If* γ *may be enclosed in a c.e.g.h.s. of* $\boldsymbol{N}$, *which is causally isometric to a c.e.g.h.s. of Minkowski space, then we have*

$$\sup_\gamma\langle T_{\boldsymbol{N}ab}u^au^b\rangle_\omega\geqslant-\frac{(20\lambda_0^2-9)\alpha^4}{320\pi^2} \tag{105}$$

for any Hadamard state ω *of the massless Klein-Gordon field, where* λ_0 *is the smallest solution to Eq.* (100) *in* $[1,\infty)$ *and depends on* $\alpha\tau_0$. *If* γ *has infinite proper duration, we also have the more stringent constraint Eq.* (104).

C. Massless fields in two dimensions

So far, we have only utilized the locally covariant difference QEIs of Sec. II E. For massless fields in two dimensions, however, we also have the absolute QEI developed by Flanagan and others, described in Sec. II D, which are also known to be optimal bounds. In this subsection we briefly discuss how the results of the previous subsections may be sharpened and generalized in this context. In fact the formula for the QEI bound is sufficiently simple that we may work directly in curved spacetime, rather than in Minkowskian subregions.

Let $\gamma:I\to\boldsymbol{N}$ be a smooth future-directed timelike curve, with velocity u^a and accleration a^c in a two-dimensional globally hyperbolic spacetime $\boldsymbol{N}$. As before, I is an open interval of proper time. In order to apply Flanagan's bound, we make the additional assumption that γ may be enclosed within a c.e.g.h.s. $\boldsymbol{N}'$ of $\boldsymbol{N}$, which is globally conformal to the whole of Minkowski space. Then Flanagan's QEI asserts that

$$\int_I\langle T_{\boldsymbol{N}ab}u^au^b\rangle_\omega(\gamma(\tau))g(\tau)^2\mathrm{d}\tau\geqslant-\frac{1}{6\pi}\int_I[g'(\tau)^2+g(\tau)^2\{R_{\boldsymbol{N}}(\gamma(\tau))-a^c(\tau)a_c(\tau)\}]\mathrm{d}\tau \tag{106}$$

for all Hadamard states ω and any smooth, real-valued g compactly supported in I, i.e., $g\in C_0^\infty(I;\mathbb{R})$.

We proceed as above, obtaining the estimate

$$\mathcal{E}\int_I g(\tau)^2 \mathrm{d}\tau \geqslant -\frac{1}{6\pi}\int_I [g'(\tau)^2 + g(\tau)^2\{R_{\boldsymbol{N}}(\gamma(\tau)) - a^c(\tau)a_c(\tau)\}]\mathrm{d}\tau, \tag{107}$$

for all $g \in C_0^\infty(I;\mathbb{R})$, where $\mathcal{E}=\sup_\gamma \langle T_{\mathbf{M}ab}u^a u^b\rangle_\omega$ as usual. Converting to an eigenvalue problem, we deduce that

$$\mathcal{E} \geqslant -\frac{\lambda_0}{6\pi}, \tag{108}$$

where λ_0 is the lowest element in the spectrum of the Friedrichs extension of the operator

$$(Lg)(\tau) = -g''(\tau) + (R_{\boldsymbol{N}}(\gamma(\tau)) - a^c(\tau)a_c(\tau))g(\tau), \tag{109}$$

on $C_0^\infty(I)$. Provided $R_{\boldsymbol{N}}$ and $a^c a_c$ are bounded along γ, the correct boundary conditions are Dirichlet conditions $g=0$ on ∂I (see, e.g., Ref. 33). We now give two illustrative examples.

Proposition III.4: Suppose $\boldsymbol{N}$ *is a globally hyperbolic two-dimensional spacetime with a c.e.g.h.s.* $\boldsymbol{N}'$*, which is globally conformal to the whole of Minkowski space. Then the following hold for all Hadamard states* ω *on* $\boldsymbol{N}$:

(*a*) *If* γ *is a curve of proper duration* τ_0 *contained in* $\boldsymbol{N}'$*, with* $R_{\boldsymbol{N}} - a^c a_c \equiv S$ *constant along* γ*, then*

$$\sup_{\tau\in I}\langle T_{\boldsymbol{N}ab}u^a u^b\rangle_\omega(\gamma(\tau)) \geqslant \frac{S}{6\pi} - \frac{\pi}{6\tau_0^2}. \tag{110}$$

(*b*) *If* $\gamma:\mathbb{R}\to\boldsymbol{N}$ *has (signed) proper acceleration growing linearly with proper time,* $\mathrm{d}\alpha/\mathrm{d}\tau = p$, and $R_{\boldsymbol{N}}\equiv 0$ on γ, then

$$\sup_{\tau\in I}\langle T_{\boldsymbol{N}ab}u^a u^b\rangle_\omega(\gamma(\tau)) \geqslant -\frac{|p|}{6\pi}. \tag{111}$$

The proof is straightforward: for (a), the eigenvalue problem is $-g''(\tau)=(\lambda+6\pi S)g(\tau)$ on an interval of length τ_0 subject to Dirichlet boundary conditions, which easily yields the stated result. For (b), we may choose the origin of proper time so that $a^c a_c = -p^2\tau^2$ for some constant p. The eigenvalue problem is then

$$-g''(\tau) + p^2\tau^2 g(\tau) = \lambda g(\tau), \tag{112}$$

which is the harmonic oscillator equation (and the Friedrichs extension is also the standard harmonic oscillator Hamiltonian). The minimum value of λ is therefore the "zero-point" value $\lambda_0 = |p|$. (The comparison with the usual quantum mechanical harmonic oscillator would correspond to units in which the mass and Planck's constant are both set to 2.) Thus we obtain the required result.

IV. CALCULATIONS IN SPECIFIC SPACETIMES

In this section we illustrate our general method by some concrete calculations in a variety of locally Minkowskian spacetimes in both two and four dimensions. For the most part, we focus on the lower bounds, but upper bound calculations are included where they are enlightening. For each spacetime we consider, exact values of the renormalized stress-energy tensor are known (or easily obtained from existing results) for one or more states. This permits comparison with the results of our method.

A. Two-dimensional timelike cylinder

Consider the massless scalar field on the two-dimensional timelike cylinder, $\boldsymbol{C}$, i.e., Minkowski space $\boldsymbol{M}_2$ quotiented by the group of translations $(t,x)\mapsto(t,x+nL)$ $(n\in\mathbb{Z})$. The Casimir vacuum $\omega_{\boldsymbol{C}}$ is the ground state of the scalar field on $\boldsymbol{C}$ (more precisely, it is a state on the

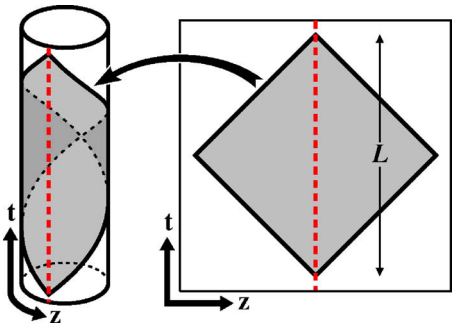

FIG. 6. (Color online) Diagram showing the "largest" causal diamond in two-dimensional Minkowski space that can be isometrically embedded into the two-dimensional cylinder spacetime with periodicity L in the z direction. To an observer inside the diamond in the cylinder spacetime, the quantum field theory and states would be indistinguishable from that in Minkowski space. The dashed vertical line is the worldline of a stationary observer.

algebra of first derivatives of the field—we will ignore this subtlety, which does not modify any of our conclusions below). The renormalized expectation value of the vacuum stress-tensor has the form

$$\langle T_{\boldsymbol{C}ab}\rangle_{\omega_{\boldsymbol{C}}}(x) = \rho_{\boldsymbol{C}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{113}$$

where $\rho_{\boldsymbol{C}}$ is a constant. Our aim is to use quantum inequalities to provide upper and lower bounds on $\rho_{\boldsymbol{C}}$. The value of $\rho_{\boldsymbol{C}}$ is, of course, well known, and will satisfy the bounds we now derive; our aim is to demonstrate how it may be bounded without direct calculation.

In order to apply our method, we must identify suitable globally hyperbolic subspacetimes of $\boldsymbol{C}$. For any $0<\tau_0\leqslant L$, we may define a timelike geodesic $\gamma:(0,\tau_0)\to\boldsymbol{C}$ by $\gamma(\tau)=(\tau,0)$. Then the double cone $\mathrm{int}(J^+(\gamma(0))\cap J^-(\gamma(\tau_0)))$ is a causally embedded globally hyperbolic subspacetime of $\boldsymbol{C}$, containing γ. As this subspacetime is globally conformal to the whole of Minkowski space and the energy density is constant along γ, we have the lower bound

$$\rho_{\boldsymbol{C}} \geqslant -\frac{\pi}{6\tau_0^2}, \tag{114}$$

from Proposition III.4(a) (in the case $S=0$). This bound clearly becomes more stringent as τ_0 is increased, so we obtain the best bound possible (within this method) by taking $\tau_0=L$. As shown in Fig. 6, the corresponding diamond is one for which the corners of the diamond just barely fail to touch on the back of the cylinder. This gives the final result

$$\rho_{\boldsymbol{C}} \geqslant -\frac{\pi}{6L^2}. \tag{115}$$

We now demonstrate how to find an upper bound on $\rho_{\boldsymbol{C}}$ for which we must employ our locally covariant difference QWEI. Let $\tilde{\gamma}$ be the curve $\tilde{\gamma}(\tau)=(\tau,0)$ in $\boldsymbol{M}_2$ and let $\boldsymbol{M}'=\mathrm{int}\, J^+(\tilde{\gamma}(0))\cap J^-(\tilde{\gamma}(\tau_0))$, for some $0<\tau_0<L$, which is a c.e.g.h.s. of $\boldsymbol{M}_2$. Then the quotient map $q:\boldsymbol{M}_2\to\boldsymbol{C}$ defines a causal isometric embedding of $\boldsymbol{M}'$ in $\boldsymbol{C}$, with $q(\boldsymbol{M}')$ equal to the double cone constructed earlier in this subsection. By Corollary II.4 we have

$$\langle T_{\boldsymbol{C}}(q_*\mathsf{f})\rangle_{\omega_{\boldsymbol{C}}} \leqslant \mathcal{Q}^{\mathrm{weak}}_{\boldsymbol{C}}(\mathsf{f},\omega_{\boldsymbol{C}}) \tag{116}$$

for any sampling tensor $\mathsf{f}\in\mathcal{F}^{\mathrm{weak}}_{M'}$. We define f by Eq. (49) for $g\in\tilde{C}^\infty_0((0,\tau_0);\mathbb{R})$ and then use the constancy of the energy density along γ to find

$$\rho_C \int_0^{\tau_0} g(\tau)^2 \mathrm{d}\tau \leqslant \mathcal{Q}_C^{\mathrm{weak}}(\mathsf{f}, \omega_C) \leqslant \frac{1}{2\pi} \int (g'(\tau))^2 \mathrm{d}\tau, \tag{117}$$

where the last inequality is derived in Appendix B. As usual, this may be converted into an eigenvalue problem: here, $\rho_C \leqslant \lambda_0/(2\pi)$ where $\lambda_0 = (\pi/\tau_0)^2$ is the minimum eigenvalue of $-\mathrm{d}^2/\mathrm{d}\tau^2$ on $(0, \tau_0)$ subject to Dirichlet boundary conditions. Combining with our earlier lower bound, we thus have

$$-\frac{\pi}{6L^2} \leqslant \rho_C \leqslant \frac{\pi}{2L^2}. \tag{118}$$

The known value of ρ_C is exactly $-\pi/(6L^2)$ (see Ref. 59), which, remarkably, saturates the lower bound. Thus we have shown that, in the cylinder spacetime, the Casimir vacuum energy density is the lowest possible static energy density compatible with the quantum energy inequalities. This, however, is not always the case, as we will see in later examples.

Because the energy density is in fact negative, the upper bound was not particularly enlightening in this example. However, the situation is different for thermal equilibrium states. Let $\omega_{C,\beta}$ be the thermal equilibrium (KMS) state at inverse temperature β, relative to the static time translations. The stress-energy tensor is again diagonal

$$\langle T_{Cab} \rangle_{\omega_{C,\beta}}(x) = \rho_{C,\beta} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{119}$$

where

$$\rho_{C,\beta} = -\frac{\pi}{6L^2} + \frac{\pi}{L^2} \sum_{n=1}^{\infty} \operatorname{cosech}^2 \frac{n\pi\beta}{L}, \tag{120}$$

see, e.g., Sec. 4.2 of Ref. 59. By our general theory, these states should be constrained by the same lower bound as before, and this is evidently true, because the series contribution to $\rho_{C,\beta}$ is clearly positive. The upper bound depends on the temperature according to the formula

$$\rho_{C,\beta} \leqslant \frac{\mathcal{Q}_C^{\mathrm{weak}}(\mathsf{f}, \omega_{C,\beta})}{\displaystyle\int_0^{\tau_0} g(\tau)^2 \mathrm{d}\tau} \tag{121}$$

for any $g \in \widetilde{C}_0^\infty((0, \tau_0); \mathbb{R})$. In Appendix B we obtain the estimate

$$\mathcal{Q}_C^{\mathrm{weak}}(\mathsf{f}, \omega_{C,\beta}) \leqslant \frac{\mathcal{Q}_C^{\mathrm{weak}}(\mathsf{f}, \omega_C)}{1 - e^{-2\pi\beta/L}} + \frac{\pi e^{\pi\beta/L}}{2L^2 \sinh^3 \pi\beta/L} \int_{-\infty}^{\infty} |g(\tau)|^2 \mathrm{d}\tau \tag{122}$$

and we may now immediately optimize over g using our result for the ground state to obtain

$$-\frac{\pi}{6L^2} \leqslant \rho_{C,\beta} \leqslant \frac{\pi}{2L^2(1 - e^{-2\pi\beta/L})} + \frac{\pi e^{\pi\beta/L}}{2L^2 \sinh^3 \pi\beta/L}. \tag{123}$$

As shown in Fig. 7 this is consistent with the known value of $\rho_{C,\beta}$.

B. Spatial topology $\mathbb{R}^{3-j} \times \mathbb{T}^j$, $j = 1, 2, 3$

Let us now consider various quotients of four-dimensional Minkowksi space by subgroups of the group of spatial translations. To begin, consider the quotient of four-dimensional Minkowski space, with inertial coordinates (t, x, y, z) by the spatial translation subgroup $(t, x, y, z) \mapsto (t, x, y, z + nL_1)$ $(n \in \mathbb{Z})$ for some fixed periodicity length $L_1 > 0$. We will denote the resulting spacetime by $\boldsymbol{N}_1$, and consider the ground state $\omega_{\boldsymbol{N}_1}$, which has a nonzero Casimir

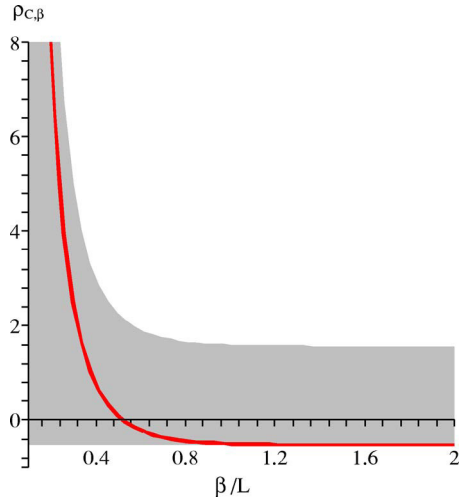

FIG. 7. (Color online) A graph showing the energy density $\rho_{C,\beta}$ in units of L^{-2} of the thermal equilibrium state at temperature β^{-1} on a cylinder of circumference L. The shaded region indicates the range permitted by the upper and lower bounds obtained from QEIs, illustrating Eq. (123).

vacuum stress-energy tensor. A calculation using the method of images and the Minkowski space vacuum two-point function yields the renormalized vacuum stress-tensor for the massless scalar field in this spacetime, (see, e.g., Ref. 60)

$$\langle T_{\boldsymbol{N}_1 ab}\rangle_{\omega_{\boldsymbol{N}_1}} = -\frac{\pi^2}{90L_1^4}\,\mathrm{diag}[1,-1,-1,3]. \tag{124}$$

We will now show that this is consistent with the lower bound arising from the QEIs. To this end, let $\gamma(\tau)=(\tau,x_0)$ for some fixed $x_0\in\mathbb{R}^2\times\mathbb{T}$. Then the double cone $\mathrm{int}(J^+(\gamma(0))\cap J^-(\gamma(L_1)))$ is a c.e.g.h.s. of $\boldsymbol{N}_1$, which is causally isometric to a double cone in Minkowski space. Thus the portion of γ parametrized by $(0,L_1)$ meets the hypotheses of Proposition III.1 and we have

$$\sup_{\gamma}\langle T_{\boldsymbol{N}_1 00}\rangle_\omega \geqslant -\frac{C_4}{L_1^4} \tag{125}$$

for any Hadamard state ω of the Klein-Gordon field. In particular, the state $\omega_{\boldsymbol{N}_1}$ obeys this bound, as $\pi^2/90\approx 0.109\,662 < C_4$. In fact, the energy density is about 30 times smaller than the QEI bound in this case.

Thus the QEI bounds can be rather weak. But this is necessary, as can be seen from the next examples, in which the same lower bound must constrain a more negative energy density. Consider the spacetime $\boldsymbol{N}_2\cong\mathbb{R}\times\mathbb{R}\times\mathbb{T}^2$, which may be obtained by quotienting $\boldsymbol{N}_1$ by the translation group $(t,x,y,z)\mapsto(t,x,y+nL_2,z)$ $(n\in\mathbb{Z})$ for some nonnegative L_2, which, without loss of generality, we take to be no less than L_1. Because $L_2\geqslant L_1$ we may apply Proposition III.1 to a double cone of the same size as before, so the lower bound is unchanged. However the stress tensor is now[60]

$$\langle T_{\boldsymbol{N}_2 ab}\rangle_{\omega_{\boldsymbol{N}_2}} = -\frac{1}{2\pi^2 L_1^4}\sum_{(m,n)\in\mathbb{Z}^2\setminus\{0\}}\frac{1}{(m^2+n^2)^2}\,\mathrm{diag}[1,-1,1,1] \tag{126}$$

in the special case $L_2=L_1$. The sum can no longer be given in closed form, but numerically the overall prefactor [equal to the energy density on the worldline $\tau\mapsto(\tau,x_0)$] is given in Ref. 60 as $-0.305/L_1^4$. This is still consistent with Eq. (125), with energy density now only around ten times smaller than the bound.

In exactly the same way we may quotient $\boldsymbol{N}_2$ by the translation subgroup $(t,x,y,z)\mapsto(t,x+nL_3,y,z)$ $(n\in\mathbb{Z})$, thereby forming $\boldsymbol{N}_3\cong\mathbb{R}\times\mathbb{T}^3$. If we again suppose that $L_1\leqslant L_2\leqslant L_3$, then the bound Eq. (125) still applies to the ground state on this spacetime. (Since this spacetime supports normalizable zero modes for the massless scalar field, one must regard this as a state on the algebra of derivatives of the field, much as for massless fields in two dimensions.) On the other hand, the stress-energy tensor in the natural ground state is

$$\langle T_{\boldsymbol{N}_3 ab}\rangle_{\omega_{\boldsymbol{N}_3}} = -\frac{1}{2\pi^2 L_1^4}\sum_{(l,m,n)\in\mathbb{Z}^3\setminus\{0\}}\frac{1}{(l^2+m^2+n^2)^2}\,\mathrm{diag}\left[1,\frac{1}{3},\frac{1}{3},\frac{1}{3}\right] \tag{127}$$

in the special case $L_1=L_2=L_3$. The energy density along $\tau\mapsto(\tau,x_0)$ in this case is numerically computed to be $0.838/L_1^4$, which is again consistent with the QEI constraint Eq. (125), which is now weaker by a factor of less than 4.

Let us note that the massless QEI bound also provides a lower bound on the ground state energy densities of *massive* scalar fields in these spacetimes. Consistency here is seen from the fact that the mass diminishes the magnitude of the energy density[61] (note the misprints in Ref. 61 noted in Ref. 62 that do not, however, affect the final result).

C. Misner universe

Our third example concerns (the globally hyperbolic portion of) the Misner universe $\boldsymbol{U}$; namely, the quotient of $(0,\infty)\times\mathbb{R}^3$ with metric

$$\mathrm{d}s^2 = \mathrm{d}t^2 - t^2(\mathrm{d}x^1)^2 - (\mathrm{d}x^2)^2 - (\mathrm{d}x^3)^2, \tag{128}$$

by the translation group $(t,x^1,x^2,x^3)\mapsto(t,x^1+na,x^2,x^3)$ $(n\in\mathbb{Z})$ for some constant $a>0$. That is, the x^1 coordinate has been compactified onto a circle. We restrict to $t>0$ to avoid the closed null geodesics that would appear at $t=0$ and the closed timelike curves appearing for $t<0$. Under the coordinate transformation

$$y^0 = t\cosh(x^1),\quad y^1 = t\sinh(x^1),\quad y^2 = x^2,\quad y^3 = x^3, \tag{129}$$

we may, equivalently, regard Misner space as the wedge $y^0>|y^1|$ of Minkowski spacetime with the points (y^0,y^1,y^2,y^3) and $(y^0\cosh(na)+y^1\sinh(na),y^1\cosh(na)+y^0\sinh(na),y^2,y^3)$ identified for each $n\in\mathbb{Z}$.

Define a curve $\gamma(\tau)=(\tau,\boldsymbol{x}_o)$ in the original coordinates, for some constant $x_0\in\mathbb{T}\times\mathbb{R}^2$. This is a timelike geodesic, with velocity $u^a=(1,0)$. In the Minkowski space cover, this worldline is given by

$$\gamma(\tau) = \begin{pmatrix}\tau\cosh(x_o^1)\\ \tau\sinh(x_o^1)\\ x_o^2\\ x_o^3\end{pmatrix}\quad\text{with}\quad u^a(\tau) = \begin{pmatrix}\cosh(x_o^1)\\ \sinh(x_o^1)\\ 0\\ 0\end{pmatrix}, \tag{130}$$

which is a constant velocity geodesic, as shown by the bold dashed line in Fig. 8. Let us consider a portion of this curve, running between $P=\gamma(\tau_P)$ and $F=\gamma(\tau_F)$, which is such that $\mathrm{int}(J^+(P)\cap J^-(F))$ is a c.e.g.h.s. of Misner space isometric to a double cone in Minkowski space. Assuming that this region is maximal, it must be that the geodesic joining the $n=+1$ image P_{+1} of P to F is null. Setting $\tau_O=(\tau_F+\tau_P)/2$ and $L=(\tau_F-\tau_P)/2$, this yields the condition

$$\left[\left(\tau_O+\frac{L}{2}\right)\cosh(x_o^1)-\left(\tau_O-\frac{L}{2}\right)\cosh(x_o^1+a)\right]^2-\left[\left(\tau_O+\frac{L}{2}\right)\sinh(x_o^1)-\left(\tau_O-\frac{L}{2}\right)\sinh(x_o^1+a)\right]^2=0, \tag{131}$$

which entails

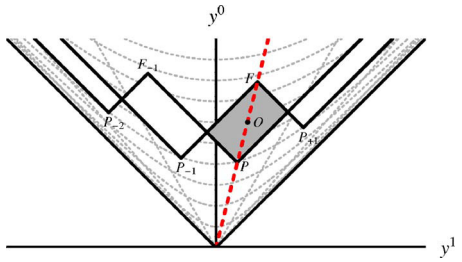

FIG. 8. (Color online) The covering space of the Misner universe is the wedge $y^0>|y^1|$ of Minkowski spacetime, shown here in cross section in the y^0-y^1 coordinates. Points in the covering space are identified, as described in the text, along the background hyperbolæ. Also shown is a stationary geodesic in the Misner universe, which in the covering space is a constant velocity observer (dashed line). For such an observer, the largest causal diamond for a given center point that is isomorphic to a subset of Minkowski space is shown in gray. Identified images of this diamond are also shown in white.

$$L = 2\tau_O \tanh\left(\frac{a}{2}\right). \tag{132}$$

This is the largest double cone of this type, centered on O, in which an observer cannot detect the compactified nature of the x^1 direction. We may therefore apply Proposition III.1 to the portion γ_{PF} of γ lying between P and F. This gives

$$\sup_{\gamma_{PF}} \langle T_{Uab} u^a u^b \rangle_\omega \geqslant -\frac{C_4}{L^4} = -\frac{C_4}{(2\tau_O \tanh(a/2))^4} \tag{133}$$

for any Hadamard state ω on Misner space. In particular, an energy density $\rho(\tau) = \langle T_{Uab} u^a u^b \rangle_\omega(\gamma(\tau))$ of the form $\rho(\tau) = -C/\tau^4$, for which $\sup_\gamma \rho = -C/\tau_F^4$, would be subject to the constraint

$$C \leqslant \frac{C_4}{16}(2 + \coth(a/2))^4. \tag{134}$$

By adapting the eigenvalue method, we may obtain a better bound. Let us suppose that ρ obeys

$$\rho(\tau) \leqslant \frac{K}{16\pi^2\tau^4} \tag{135}$$

on $I = (\tau_O - L/2, \tau_0 + L/2)$. Then by exactly the same arguments as in Sec. III A, we may deduce

$$K \geqslant -\inf_g \frac{\int |g''(\tau)|^2 \mathrm{d}\tau}{\int \tau^{-4}|g(\tau)|^2 \mathrm{d}\tau}, \tag{136}$$

where the τ^{-4} in the denominator comes from the form of ρ, and the infimum is taken over all $g \in C_0^\infty(I)$. The denominator can be reinterpreted as the norm of g in $L^2(I, \tau^{-4}d\tau)$. Integrating by parts twice, we may rewrite the numerator as $-\langle g | Lg \rangle$, where the inner product is that of $L^2(I, \tau^{-4}d\tau)$ and L is defined on $C_0^\infty(I)$ by

$$(Lg)(\tau) = \tau^4 g''''(\tau) \tag{137}$$

and is symmetric, i.e., $\langle h | Lg \rangle = \langle Lh | g \rangle$ for all $g, h \in C_0^\infty(I)$. The minimization problem is then solved by finding the lowest spectral point of the Friedrichs extension of L. It may be shown that the Friedrichs extension again amounts to the imposition of Dirichlet boundary conditions $g = g' = 0$ on ∂I,[63] and the problem now reduces to the study of the ODE

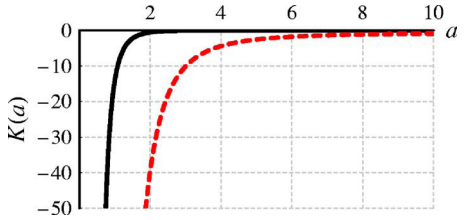

FIG. 9. (Color online) The numerical factor $K(a)$ for the vacuum stress tensor in the Misner universe (solid line) plotted for a range of the closure scale a. Also shown is the lower bounds from $-\lambda(a)$ (dashed line). The lower bound from Eq. (134) is so weak (it asymptotically approaches ~ -2500 from below for large a) that it is not included to preserve detail in the figure above.

$$g''''(\tau) - \frac{\lambda}{\tau^4} g(\tau) = 0. \tag{138}$$

Again we wish to determine the minimum eigenvalue λ for eigensolutions that satisfy the boundary conditions. The substitution $g(\tau) = h\left(\frac{1}{2}\ln(\tau)\right)$ converts the equation to a constant coefficient linear equation, and one may determine the general solution (e.g., using *Mathematica*) as

$$h(l) = c_1 e^{3l} \cos(l\sqrt{4\sqrt{\lambda+1}-5}) + c_2 e^{3l} \sin(l\sqrt{4\sqrt{\lambda+1}-5}) + c_3 e^{(3+\sqrt{4\sqrt{\lambda+1}+5})l} + c_4 e^{(3-\sqrt{4\sqrt{\lambda+1}+5})l}, \tag{139}$$

where (c_1, c_2, c_3, c_4) are constants. Imposing three of the boundary conditions fixes three of the constants in terms of the fourth, which serves as an overall magnitude for the test function. The fourth boundary condition can then be used to determine the eigenvalues. A somewhat involved calculation leads to the transcendental equation to determine λ implicitly in terms of a:

$$\frac{\sqrt{16\lambda-9}}{5} = \frac{\sin\left(\frac{a}{2}\sqrt{4\sqrt{\lambda+1}-5}\right)\sinh\left(\frac{a}{2}\sqrt{4\sqrt{\lambda+1}+5}\right)}{\cos\left(\frac{a}{2}\sqrt{4\sqrt{\lambda+1}-5}\right)\cosh\left(\frac{a}{2}\sqrt{4\sqrt{\lambda+1}+5}\right)-1}. \tag{140}$$

We denote λ, so determined, as $\lambda(a)$; this constrains our original value K by

$$K \geqslant -\lambda(a). \tag{141}$$

Our interest in energy densities proportional to τ^{-4} stems from the state constructed by Hiscock and Konkowski.[64] This quasifree state, which we denote ω_U, is obtained by applying the method of images to the Minkowski space two-point function in the wedge $y^0 > |y^1|$, and then carrying it back to the original Misner coordinates to find the renormalized vacuum expectation value of the stress tensor. Hiscock and Konkowski considered the conformally coupled scalar field, but their calculations can be easily reproduced in the minimally coupled case to yield

$$\langle T_{Uab}\rangle_{\omega_U}(t) = \frac{K(a)}{16\pi^2 t^4}\,\mathrm{diag}[1, 3t^2, -1, -1], \tag{142}$$

where

$$K(a) = -\sum_{n=1}^{\infty} \mathrm{cosech}^4\left(\frac{na}{2}\right) \tag{143}$$

is a negative constant depending on the x^1-period a.[65] Both the coefficient $K(a)$ and the numerical evaluation of the lower bound $-\lambda(a)$ are plotted in Fig. 9. It is obvious that $K(a)$, and thus the energy density obey the QEI constraint for all values of a. The bound Eq. (134) is still weaker.

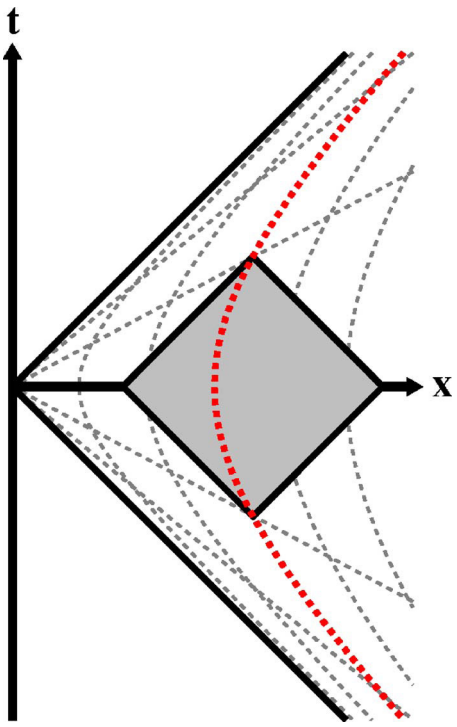

FIG. 10. Diagram showing Rindler spacetime (with the two perpendicular space dimensions suppressed) embedded into Minkowski spacetime. The dashed hyperbolic line, the worldline of a constantly accelerating observer, is the image of a constant ξ observer's worldline in Rindler coordinates. The gray diamond is a causal region that can be isometrically identified between the two "different" coordinate systems.

D. Rindler spacetime

The Rindler spacetime $\boldsymbol{R}$ is the "right wedge" of Minkowski space, i.e., the region $\{(t,x,y,z)\in\mathbb{R}^4: x>|t|\}$ in inertial coordinates (t,x,y,z). We may also make the coordinate transformation

$$t=\xi\sinh(\eta),\quad y=y,$$

$$x=\xi\cosh(\eta),\quad z=z, \tag{144}$$

to obtain the metric in the form

$$\mathrm{d}s^2=\xi^2\mathrm{d}\eta^2-\mathrm{d}\xi^2-\mathrm{d}y^2-\mathrm{d}z^2, \tag{145}$$

with coordinate ranges $\eta,y,z\in\mathbb{R}$, $\xi\in(0,\infty)$. Lines of constant ξ, when mapped into Minkowski space, are worldlines for observers undergoing constant proper acceleration $\alpha=\xi^{-1}$. Rindler spacetime is static with respect to η (corresponding to Lorentz invariance in the xt plane) and is invariant under Euclidean transformations of the yz plane. (See Fig. 10.)

Clearly any line of constant ξ meets the conditions of Proposition III.3 and we may immediately read off that any static Hadamard state ω on $\boldsymbol{R}$ must obey

$$\langle T_{\boldsymbol{R}ab}u^a u^b\rangle_\omega(\eta,\xi,y,z)\geqslant-\frac{11}{480\pi^2\xi^4}, \tag{146}$$

where u^a is the unit vector parallel to $\partial/\partial\eta$. In particular, this provides a constraint on the energy density $\rho_{\boldsymbol{R}}=\langle T_{\boldsymbol{R}ab}u^a u^b\rangle_{\omega_{\boldsymbol{R}}}$ in the ground state $\omega_{\boldsymbol{R}}$ (which is Hadamard). This may also be computed exactly: it was first computed for the conformally coupled scalar field by Candelas and Deutsch[66]

and one can easily generalize their results to the minimally coupled scalar field to obtain[67]

$$\rho_{\boldsymbol{R}} = -\frac{11}{480\pi^2\xi_o^4}, \tag{147}$$

which is exactly the lower bound given above. Thus, remarkably, the Rindler ground state saturates the QEI constraints, which were obtained using local covariance and the Minkowski vacuum, and nowhere involved $\omega_{\boldsymbol{R}}$.

Let us also examine how an upper bound might be obtained. Let $\gamma(\tau)=(\tau/\xi_o,\xi_o,0,0)$ in (η,ξ,y,z) coordinates and set $\mathsf{u}=\dot{\gamma}$ as usual. We consider sampling along γ, with sampling tensors of form

$$\mathsf{f}(\mathsf{t}) = \int t_{ab}|_{\gamma(\tau)} u^a u^b g(\tau)^2 \mathrm{d}\tau \tag{148}$$

for $g \in \widetilde{C}_0^\infty(\mathbb{R};\mathbb{R})$. Since the energy density is constant along γ, the upper bound of Corollary II.4 gives

$$\rho_{\boldsymbol{R}} \int g(\tau)^2 \mathrm{d}\tau = \langle \mathsf{T}_{\boldsymbol{R}}(\mathsf{f})\rangle_{\omega_{\boldsymbol{R}}} \leqslant \mathcal{Q}_{\boldsymbol{R}}^{\mathrm{weak}}(\mathsf{f},\omega_{\boldsymbol{R}}). \tag{149}$$

The right-hand side can be read off from the difference QEI derived by Pfenning[21] for the electromagnetic field, because the corresponding bound for the scalar field is exactly half of the electromagnetic expression[68]

$$\mathcal{Q}_{\boldsymbol{R}}^{\mathrm{weak}}(\mathsf{f},\omega_{\boldsymbol{R}}) = \frac{1}{16\pi^3}\int_0^\infty |\hat{g}(u)|^2(u^4+2\xi_o^{-2}u^2)\mathrm{d}u = \frac{1}{16\pi^2}\int_{-\infty}^\infty (|g''(\tau)|^2+2\xi_o^{-2}|g'(\tau)|^2)\mathrm{d}\tau. \tag{150}$$

Next consider scaling the test function, replacing g by $g_\alpha(\tau)=\alpha^{-1/2}g(\tau/\alpha)$. We find, considering the scaling behavior of the above expression,

$$\rho_{\boldsymbol{R}} \leqslant \frac{1}{16\pi^2}\frac{\displaystyle\int (|g''(\tau)|^2+2\alpha^2\xi_o^{-2}|g'(\tau)|^2)\mathrm{d}\tau}{\displaystyle\alpha^4\int g(\tau)^2\mathrm{d}\tau} \tag{151}$$

for which the right-hand side vanishes in the limit of $\alpha\to\infty$. Thus we find consistency with the known fact that the expectation value of the Rindler ground state is bounded above by zero, i.e., $\rho_{\boldsymbol{R}}\leqslant 0$.

V. SUMMARY

In this paper we have initiated the study of interrelations between quantum energy inequalities and local covariance. We have formulated definitions of locally covariant QEIs, and shown that existing QEIs obey them, modulo small additional restrictions (Sec. II). The main thrust of our work has been directed at providing *a priori* constraints on renormalized energy densities in locally Minkowskian regions, accomplished in Sec. III. The simple geometric nature of these bounds makes them easy to apply in practice, and a number of future applications are envisaged. In particular, we will discuss applications to the Casimir effect in a companion paper;[2] at the theoretical level, it is possible to place the present discussion in the categorical language of Ref. 37, and this will be done elsewhere. Equally important are the specific calculations reported in Sec. IV. Here we saw that, in some situations, the QEI bounds give best-possible constraints on the energy density, and that typical ground-state energy densities are not overestimated by the QEI bound by more than a factor of about 30 at worst (in the examples studied so far).

Finally, although we confined our attention largely to locally Minkowskian spacetimes in Secs. III and IV, we emphasize again that other interesting cases may be studied using our general formalism, as, for example, in the work of Marecki[3] on spacetimes with locally Schwarzschild subregions.

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APPENDIX A: THE LOCALLY COVARIANT QUANTUM FIELD THEORY OF A SCALAR FIELD

In this Appendix we describe the construction of the quantized Klein-Gordon field within the algebraic approach to quantum field theory, and explain the construction of pulled back states used in Sec. II B.

The free scalar field of mass $m \geqslant 0$ may be quantized on any globally hyperbolic spacetime $\boldsymbol{M}$ in the sense that one may construct a complex unital $*$-algebra $\mathfrak{A}(\boldsymbol{M})$ whose elements may be interpreted as "polynomials in smeared fields." A typical element of the algebra is a complex linear combination of the identity $\mathbf{1}$ and a finite number of terms, each of which is a finite product of a number of objects $\Phi_{\boldsymbol{M}}(f)$, where f is a test function (i.e., smooth and compactly supported) on M. The algebra also satisfies a number of relations:

1. $\Phi_{\boldsymbol{M}}(\lambda f+\mu g)=\lambda\Phi_{\boldsymbol{M}}(f)+\mu\Phi_{\boldsymbol{M}}(g)$
2. $\Phi_{\boldsymbol{M}}(f)^*=\Phi_{\boldsymbol{M}}(\bar{f})$
3. $\Phi_{\boldsymbol{M}}((\Box+m^2)f)=0$
4. $[\Phi_{\boldsymbol{M}}(f),\Phi_{\boldsymbol{M}}(g)]=iE_{\boldsymbol{M}}(f,g)\mathbf{1}$

for all test functions f,g on M and complex scalars λ,μ, where $E_{\boldsymbol{M}}$ is the advanced-minus-retarded fundamental solution to $\Box+m^2$ on $\boldsymbol{M}$. The first two axioms are necessary for compatibility with the idea of $\Phi_{\boldsymbol{M}}(f)$ as a smeared hermitian field; the third expresses the field equation in "weak" form; the fourth expresses the commutation relations.

Now let ψ be a causal isometric embedding of $\boldsymbol{M}_1$ into $\boldsymbol{M}_2$. Any test function f on M_1 now corresponds to a test function $\psi_* f$ on M_2, defined by $(\psi_* f)(x)=f(\psi^{-1}(x))$ for $x\in\psi(M_1)$ and $(\psi_* f)(x)=0$ otherwise. We may use this to define a map α_ψ between $\mathfrak{A}(\boldsymbol{M}_1)$ and $\mathfrak{A}(\boldsymbol{M}_2)$ such that

1. $\alpha_\psi\mathbf{1}_{\mathfrak{A}(\boldsymbol{M}_1)}=\mathbf{1}_{\mathfrak{A}(\boldsymbol{M}_2)}$
2. $\alpha_\psi(\Phi_{\boldsymbol{M}_1}(f))=\Phi_{\boldsymbol{M}_2}(\psi_* f)$ for all test functions f on M_1
3. α_ψ extends to general elements of $\mathfrak{A}(\boldsymbol{M}_1)$ as a $*$-homomorphism, i.e., α_ψ is linear and obeys $\alpha_\psi(AB)=\alpha_\psi(A)\alpha_\psi(B)$ and $\alpha_\psi(A^*)=\alpha_\psi(A)^*$ for all $A,B\in\mathfrak{A}(\boldsymbol{M}_1)$.

In the body of the text we have used the notation ψ_* for α_ψ, relying on the context for the appropriate meaning; here, it is convenient to distinguish the two maps. One must check that the last statement is compatible with the axioms stated above—the only nontrivial one is the commutation relation, where the causal nature of ψ plays a key role and guarantees that α_ψ is well-defined. What needs to be proved boils down to checking that

$$E_{\boldsymbol{M}_1}(f,g) = E_{\boldsymbol{M}_2}(\psi_* f, \psi_* g) \tag{A1}$$

for all test functions f,g on M_1. This equivalence is proved as follows. Writing $E^{\pm}_{\boldsymbol{M}}$ for the advanced $(-)$ and retarded $(+)$ Green functions on $\boldsymbol{M}$, $E^{\pm}_{\boldsymbol{M}_2}\psi_* f$ solves the inhomogeneous Klein-Gordon equation on $\boldsymbol{M}_2$ with source $\psi_* f$ and support in $J^{\pm}_{\boldsymbol{M}_2}(\mathrm{supp} f)$. Because ψ is a causal isometry, the pull-back $\psi^* E^{\pm}_{\boldsymbol{M}_2}\psi_* f$ solves the inhomogeneous Klein-Gordon equation on $\boldsymbol{M}_1$ with source f and support in $J^{\pm}_{\boldsymbol{M}_1}(\mathrm{supp} f)$; by uniqueness of solution, we have $E^{\pm}_{\boldsymbol{M}_1} f = \psi^* E^{\pm}_{\boldsymbol{M}_2}\psi_* f$. Accordingly $\psi_* E_{\boldsymbol{M}_1} = E_{\boldsymbol{M}_2}\psi_*$ and the required result follows.

In the algebraic approach we have been pursuing, a state of the quantum field on $\boldsymbol{M}$ is a linear map ω from $\mathfrak{A}(\boldsymbol{M})$ to the complex numbers, obeying $\omega(\mathbf{1})=1$ and $\omega(A^*A)\geqslant 0$ for any $A\in\mathfrak{A}(\boldsymbol{M})$. One interprets $\omega(A)$ as the expectation value of observable A in state ω. In particular, each state yields a hierarchy of n-point functions, i.e., maps of the form

$$(f_1,\ldots,f_n)\mapsto \omega(\Phi_{\boldsymbol{M}}(f_1)\cdots\Phi_{\boldsymbol{M}}(f_n)); \tag{A2}$$

we will restrict attention to those states whose corresponding n-point functions are distributions. A state ω is Hadamard if its two-point function has a particular singular structure, which is determined by the local metric and causal properties of the spacetime. Note that none of the structures introduced so far invoke any particular Hilbert space representation of the theory.

Now suppose again that ψ is a causal isometric embedding of $\boldsymbol{M}_1$ into $\boldsymbol{M}_2$ and let ω_2 be a state on $\mathfrak{A}(\boldsymbol{M}_2)$. We obtain a state ω_1 on $\mathfrak{A}(\boldsymbol{M}_2)$ by

$$\omega_1(A) = \omega_2(\alpha_\psi(A)) \tag{A3}$$

for any $A\in\mathfrak{A}(\boldsymbol{M}_1)$; that is, $\omega_1=\alpha^*_\psi\omega_2$, where α^*_ψ is the dual map to α_ψ (in the body of the text, we have written ψ^* for α^*_ψ). The n-point functions are therefore related by

$$\omega_1(\Phi_{\boldsymbol{M}_1}(f_1)\cdots\Phi_{\boldsymbol{M}_1}(f_n)) = \omega_2(\alpha_\psi(\Phi_{\boldsymbol{M}_1}(f_1)\cdots\Phi_{\boldsymbol{M}_1}(f_n))) = \omega_2(\Phi_{\boldsymbol{M}_2}(\psi_* f_1)\cdots\Phi_{\boldsymbol{M}_2}(\psi_* f_n)). \tag{A4}$$

It is useful to write this in "unsmeared" notation. Let $w^{(n)}_j$ be the n-point functions of ω_j. Then the last equation becomes

$$\begin{aligned}
&\int_{\boldsymbol{M}_1}\mathrm{dvol}_{g_1}(x_1)\cdots\int_{\boldsymbol{M}_1}\mathrm{dvol}_{g_1}(x_n)w^{(n)}_1(x_1,\ldots,x_n)f_1(x_1)\cdots f_n(x_n)\\
&\quad=\int_{\boldsymbol{M}_2}\mathrm{dvol}_{g_2}(y_1)\cdots\int_{\boldsymbol{M}_2}\mathrm{dvol}_{g_2}(y_n)w^{(n)}_2(y_1,\ldots,y_n)\psi_* f_1(y_1)\cdots\psi_* f_n(y_n)\\
&\quad=\int_{\boldsymbol{M}_1^{\times n}}\mathrm{dvol}_{g_1}(x_1)\cdots\mathrm{dvol}_{g_1}(x_n)w^{(n)}_1(\psi(x_1),\ldots,\psi(x_n))f_1(x_1)\cdots f_n(x_n),
\end{aligned} \tag{A5}$$

where the change of variables employed in the last step is justified by the fact that ψ is an isometry. As this holds for all choices of f_k, we may deduce that

$$w^{(n)}_1(x_1,\ldots,x_n) = w^{(n)}_2(\psi(x_1),\ldots,\psi(x_n)); \tag{A6}$$

that is, the n-point functions of ω_1 are the pull-backs by ψ of those of ω_2. It follows that if ω_2 is Hadamard then so too is ω_1, because the two-point function is simply pulled back under ψ and the Hadamard series is constructed from the local causal and metric structure, which is preserved under ψ. Since the stress-energy tensor is renormalized by subtracting the first few terms of the Hadamard series from the two-point function, and then taking suitable derivatives before taking the coincidence limit (making a further locally constructed correction to ensure conservation of the stress tensor), we have the following important consequence, which we isolate as a theorem.

Theorem A.1: *Suppose ψ is a causal isometric embedding of globally hyperbolic spacetime*

$\boldsymbol{M}_1$ in a globally hyperbolic spacetime $\boldsymbol{M}_2$. Any Hadamard state of the massive Klein-Gordon quantum field on $\boldsymbol{M}_2$ induces a Hadamard state of the same theory on $\boldsymbol{M}_1$, whose n-point functions and renormalized expected stress-energy tensor are the pull-backs by ψ of the corresponding quantities on $\boldsymbol{M}_2$.

This fits in with the principle that one should not be able to tell, by local experiments, whether one is in $\boldsymbol{M}_1$ or its image within the larger spacetime $\boldsymbol{M}_2$. It also justifies us in the abuse of notation perpetrated in Sec. II B, where we wrote ψ^* in place of α^*_ψ, and (dually) ψ_* in place of α_ψ.

Let us conclude by briefly describing more of the structure set out by Ref. 37. The key is the observation that the globally hyperbolic spacetimes of given dimension form the objects of a category in which the morphisms are causal isometric embeddings. One may also consider a category of unital $*$-algebras with injective unit-preserving $*$-homomorphisms as morphisms. The association of a globally hyperbolic spacetime $\boldsymbol{M}$ with the corresponding algebra $\mathfrak{A}(\boldsymbol{M})$ is then shown to be a covariant functor between these categories and gives a precise meaning to the notion of "the same field theory on different spacetimes" (and the same would be true even for theories not necessarily described in terms of a Lagrangian). A similar functorial description may be given to the association of the state space of the theory, and quantum fields are reinterpreted as natural transformations between functors. We refer the reader to Ref. 37 for full details.

APPENDIX B: DERIVATION OF A SCALAR FIELD QUANTUM WEAK ENERGY INEQUALITY IN THE CYLINDER SPACETIME

In this Appendix we calculate quantum weak energy inequalities for the massless, minimally coupled real scalar field in the two-dimensional cylinder spacetime relative to the ground and thermal equilibrium states. We use the notation of Sec. IV A. The KMS state $\omega_{\boldsymbol{C},\beta}$ at inverse temperature β has two-point function [see, e.g., Eq. (2.43) of Ref. 69]

$$w_{2,\beta}(x,x') = \frac{1}{2L}\sum_{n\in\mathbb{Z}\setminus\{0\}} \frac{e^{ik_n(z-z')}}{\omega_n(1-e^{-\beta\omega_n})}(e^{-i\omega(t-t')} + e^{-\beta\omega_n}e^{i\omega(t-t')}), \tag{B1}$$

where $k_n = 2\pi n/L$ and $\omega_n = |k_n|$, and the sum converges in the distributional sense (i.e., after smearing each term with test functions, the resulting series converges and its sum depends continuously on the test functions). We exclude the zero mode $n=0$ as usual, regarding $\omega_{\boldsymbol{C},\beta}$ as a state on the derivative fields. The two-point function of the ground state $\omega_{\boldsymbol{C}}$ is obtained as the zero temperature ($\beta\to\infty$) limit of this expression. We will be interested in the static curve $\gamma(\tau) = (\tau, 0)$, and employ the tetrad $e_0 = \partial/\partial t$, $e_1 = \partial/\partial z$, which is invariant under Fermi-Walker transport along γ. Following the procedure of Sec. II E, we find

$$Q_{\gamma,\omega_{\boldsymbol{C},\beta}}(u) = \frac{1}{2\pi^2}\int_{(-\infty,u)} \mathrm{d}v\, \hat{T}_{\gamma,\omega_{\boldsymbol{C},\beta}}(v) \tag{B2}$$

and

$$T_{\gamma,\omega_{\boldsymbol{C},\beta}}(\sigma) = \frac{1}{L}\sum_{n=1}^{\infty} \frac{\omega_n}{1-e^{-\beta\omega_n}}(e^{-i\omega_n\sigma} + e^{-\beta\omega_n}e^{i\omega_n\sigma}). \tag{B3}$$

Taking the Fourier transform, we have

$$\hat{T}_{\gamma,\omega_{\boldsymbol{C},\beta}}(v) = \frac{2\pi}{L}\sum_{n=1}^{\infty} \frac{\omega_n}{1-e^{-\beta\omega_n}}(\delta(v-\omega_n) + e^{-\beta\omega_n}\delta(v+\omega_n)) \tag{B4}$$

and therefore obtain

$$Q_{\gamma,\omega_{C,\beta}}(u) = \frac{1}{\pi L}\left\{ \sum_{\substack{n\in\mathbb{N} \\ \text{s.t.}\omega_n<u}} \frac{\omega_n}{1-e^{-\beta\omega_n}} + \sum_{\substack{n\in\mathbb{N} \\ \text{s.t.}-\omega_n<u}} \frac{\omega_n e^{-\beta\omega_n}}{1-e^{-\beta\omega_n}} \right\}. \tag{B5}$$

Note that $Q_{\gamma,\omega_{C,\beta}}$ is supported on $\mathbb{R}^+$ in the $\beta=\infty$ case, but otherwise on the whole of $\mathbb{R}$, albeit exponentially suppressed on the negative half-line.

To arrive at convenient QEI bounds we estimate $Q_{\gamma,\omega_{C,\beta}}$ by

$$Q_{\gamma,\omega_{C,\beta}}(u) \leqslant Q_{\gamma,\omega_{C,\beta}}(0) + \frac{\vartheta(u)}{\pi L(1-e^{-2\pi\beta/L})} \sum_{\substack{n\in\mathbb{N} \\ \text{s.t.}\omega_n<u}} \omega_n, \tag{B6}$$

where ϑ is the Heaviside step function. To see that this estimate is valid, we note that $Q_{\gamma,\omega_{C,\beta}}(u)$ is clearly increasing on the negative half-line, so it is valid to bound it by $Q_{\gamma,\omega_{C,\beta}}(0)$ on $u\leqslant 0$; the second term in the estimate arises by noting that $(1-e^{-\beta\omega_n})^{-1}\leqslant(1-e^{-2\pi\beta/L})^{-1}$ for all n. Using this estimate again, we also have

$$Q_{\gamma,\omega_{C,\beta}}(0) = \sum_{n\in\mathbb{N}} \frac{\omega_n e^{-\beta\omega_n}}{1-e^{-\beta\omega_n}} \leqslant \frac{1}{\pi L(1-e^{-2\pi\beta/L})} \sum_{n=1}^{\infty} \frac{2\pi n}{L} e^{-2\pi\beta n/L} = \frac{e^{\pi\beta/L}}{4L^2\sinh^3\pi\beta/L}, \tag{B7}$$

while for $u>0$

$$\frac{1}{\pi L} \sum_{\substack{n\in\mathbb{N} \\ \text{s.t.}\omega_n<u}} \omega_n = \frac{1}{L^2}\tilde{n}(\tilde{n}+1) \leqslant \frac{2}{L^2}\tilde{n}^2 \leqslant \frac{u^2}{2\pi^2}, \tag{B8}$$

where $\tilde{n}$ is the greatest integer *strictly* less than $uL/(2\pi)$. Thus we have the estimate

$$Q_{\gamma,\omega_{C,\beta}}(u) \leqslant \frac{e^{\pi\beta/L}}{4L^2\sinh^3\pi\beta/L} + \frac{\vartheta(u)u^2}{2\pi^2(1-e^{-2\pi\beta/L})}. \tag{B9}$$

It then follows that, in the notation of Sec. IV A

$$\begin{aligned} \mathcal{Q}_C^{\text{weak}}(\mathsf{f},\omega_{C,\beta}) &= \int_{-\infty}^{\infty} \mathrm{d}u |\hat{g}(u)|^2 Q_{\gamma,\omega_{C,\beta}}(u) \\ &\leqslant \frac{e^{\pi\beta/L}}{4L^2\sinh^3\pi\beta/L} \int_{-\infty}^{0} |\hat{g}(u)|^2 \mathrm{d}u + \frac{1}{2\pi^2(1-e^{-2\pi\beta/L})} \int_0^{\infty} u^2 |\hat{g}(u)|^2 \mathrm{d}u \qquad \text{(B10)} \\ &\leqslant \frac{\pi e^{\pi\beta/L}}{2L^2\sinh^3\pi\beta/L} \int_{-\infty}^{\infty} |g(\tau)|^2 \mathrm{d}\tau + \frac{1}{2\pi(1-e^{-2\pi\beta/L})} \int_{-\infty}^{\infty} |g'(\tau)|^2 \mathrm{d}\tau, \qquad \text{(B11)} \end{aligned}$$

where we have used Parseval's theorem and the fact that $|\hat{g}(u)|$ is even for real-valued g to convert the integral over $\mathbb{R}^+$ into one over $\mathbb{R}$. For the ground state, of course, this yields

$$\mathcal{Q}_C^{\text{weak}}(\mathsf{f},\omega_C) \leqslant \frac{1}{2\pi}\int_{-\infty}^{\infty} |g'(\tau)|^2 \mathrm{d}\tau \tag{B12}$$

and Eq. (122) follows immediately. Although our estimates are not very sharp, they have led to a very simple quantum inequality. In fact, for the ground state, this inequality is only three times less restrictive than the optimal quantum inequality bound found in two-dimensional Minkowski spacetime.

APPENDIX C: A LEMMA CONCERNING SMOOTH FUNCTIONS

Recall from Sec. II E that we define $\tilde{C}_0^\infty(I;\mathbb{R})$ to be the set of smooth compactly supported real-valued functions g on I whose support is connected and which have no zeros of infinite order in the interior of that support (equivalently, g has no zeros in $(\inf \operatorname{supp} g, \sup \operatorname{supp} g)$ of infinite order). Our aim is to prove the following result.

Lemma 1: Let $g \in C_0^\infty(I;\mathbb{R})$ *and choose any* $\chi \in \tilde{C}_0^\infty(I;\mathbb{R})$ *with* $\chi=1$ *on* $\operatorname{supp} g$. *Then there is a sequence* $\epsilon_n \to 0$ *for which each* $g_n = g + \epsilon_n \chi$ *is an element of* $\tilde{C}_0^\infty(I;R)$.

Proof: If g is identically zero the result is trivial, so we assume henceforth that it is not, so $M = \sup|g''|$ is strictly positive. Suppose the stated result is false, so there exists an $\epsilon_0 > 0$ such that $g + \epsilon\chi \notin \tilde{C}_0^\infty(I;\mathbb{R})$ for all $|\epsilon| \leqslant \epsilon_0$. Choose $N \in \mathbb{N}$ sufficiently large that $(N-1)\sqrt{2\epsilon_0/(MN)}$ exceeds the diameter of the support of g. By hypothesis, for each $|\epsilon| < \epsilon_0$ the function $g + \varepsilon_n \chi$ has a zero of infinite order within its support; since $\chi \in \tilde{C}_0^\infty(I;\mathbb{R})$ this zero must lie in the support of g and is therefore a point at which g' vanishes, while g takes the value $-\epsilon_n$. We may therefore choose $z_1 < z_2 < \ldots < z_N$ such that $g'(z_k) = 0$ for each k and $g(z_k)$ runs through the values $\{-k\epsilon_0/N : k = 1, \ldots, N\}$ (not necessarily in order). Using Taylor's theorem with remainder at each z_k,

$$\frac{\epsilon_0}{N} \leqslant |g(z_{k+1}) - g(z_k)| \leqslant \frac{M}{2}(z_{k+1} - z_k)^2 \tag{C1}$$

so

$$z_N - z_1 = \sum_{k=1}^{N-1} (z_{k+1} - z_k) \geqslant (N-1)\sqrt{\frac{2\epsilon_0}{MN}} \geqslant \operatorname{diam} \operatorname{supp} g \tag{C2}$$

which is a contradiction, since z_1 and z_N must belong to the support of g. ■

Since $g_n - g = \epsilon_n \chi$, it is clear that $g_n \to g$ and $g_n^{(k)} \to g^{(k)}$ in $L^2(I)$ as $n \to \infty$. This is the property required in Sec. III A.

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[51] We have $\tilde{g}(\tau)^2=g(\tau+\tau_0)^2$, and want to show that $\tilde{g}(\tau)^2=g'(\tau+\tau_0)^2$ for all τ. Differentiating and squaring yields $4\tilde{g}(\tau)^2\tilde{g}(\tau)^2=4g(\tau+\tau_0)^2g'(\tau+\tau_0)^2$ from which it follows that $\tilde{g}(\tau)^2=g'(\tau+\tau_0)^2$ except perhaps at zeros of $\tilde{g}(\tau)$. If $\tilde{g}$ vanishes in a neighborhood of τ then so must $\tilde{g}$ and the result holds trivially. For the remaining case, choose a sequence $\tau_n\to\tau$ with $\tilde{g}(\tau_n)\neq 0$; since $\tilde{g}(\tau_n)^2=g'(\tau_n+\tau_0)^2$, we conclude the required result by continuity as $n\to\infty$.
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Liouville theory and uniformization of four-punctured sphere

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A few years ago Zamolodchikov and Zamolodchikov proposed an expression for the four-point classical Liouville action in terms of the three-point actions and the classical conformal block [Nucl. Phys. B **477**, 577 (1996)]. In this paper we develop a method of calculating the uniformizing map and the uniformizing group from the classical Liouville action on n-punctured sphere and discuss the consequences of Zamolodchikovs conjecture for an explicit construction of the uniformizing map and the uniformizing group for the sphere with four punctures. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2234272]

I. INTRODUCTION

The uniformization problem for n-punctured ($n \geqslant 3$) spheres can be formulated as follows:[2]

Given $X=\mathbb{C}\backslash\{z_1,\ldots,z_{n-1}\}$, *find the (unique to within conjugacy) Fuchsian group* $G\subset \mathrm{PSU}(1,1)$ *which makes* X *conformally equivalent to the quotient* Δ/G *of the unit disc* $\Delta=\{z\in\mathbb{C}:|z|<1\}$ *by* G.

The existence of solution to this problem, called the *uniformization theorem*, was first proved by Poincaré and Koebe in 1907. The universal covering map $\lambda:\Delta\to\Delta/G$ is however explicitly known only for the thrice-punctured sphere[3] and in a few very special, symmetric cases with a higher number of punctures.[2] In particular an explicit construction of this map for the four-punctured sphere is a long-standing and still open problem.

One possible approach, going back to Poincaré, is based on the relation of the uniformization problem to a certain Fuchs equation on X. If $\lambda:\Delta\to\Delta/G\cong X$ is the universal covering map, the inverse $\rho=\lambda^{-1}:X\to\Delta$ is a multivalued function with branching points z_j and with branches related by elements of the covering group $G\subset\mathrm{PSU}(1,1)$. One can show that the Schwarzian derivative of ρ is a holomorphic function on X of the form[2]

$$\{\rho,z\}=\frac{1}{2}\sum_{k=1}^{n-1}\frac{1}{(z-z_k)^2}+\sum_{k=1}^{n-1}\frac{2c_k}{z-z_k}, \tag{1.1}$$

$$\{\rho,z\}\overset{z\to\infty}{=}\frac{1}{2z^2}+\mathcal{O}(z^{-3}), \tag{1.2}$$

where the *accessory parameters* c_j satisfy the relations

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$$\sum_{k=1}^{n-1} c_k = 0, \quad \sum_{k=1}^{n-1} (4c_k z_k + 1) = 1. \tag{1.3}$$

It is a well-known property of the Schwarzian derivative[2,4] that the map ρ is, to within a Möbius transformation, a quotient of two linearly independent solutions of the Fuchs equation

$$\partial_z^2 \Psi + \frac{1}{2}\{\rho, z\}\Psi = 0. \tag{1.4}$$

This, in particular, means that there exists a unique to within SU(1,1) transformation fundamental system $\{\Psi_1, \Psi_2\}$ of normalized (i.e., with the Wronskian equal to 1) solutions for which

$$\rho = \frac{\Psi_1}{\Psi_2}. \tag{1.5}$$

Note that any such system has to have an SU(1,1) monodromy with respect to all punctures.

Whether the Fuchs equation can be used to calculate the map ρ depends on our ability to calculate the accessory parameters and to choose an appropriate fundamental system of normalized solutions. The first problem can be easily solved for three punctures where the accessory parameters are completely determined by relations (1.3). It is, however, difficult and still unsolved for $n > 3$.

One can get some more insight by relating this problems to the Liouville equation on X. Since PSU(1,1) is the isometry group of the Poincaré hyperbolic metric $g_\Delta = 4d\rho d\bar{\rho}/(1-|\rho|^2)^2$ on Δ the pull back

$$\rho^* g_\Delta = \frac{4}{(1-|\rho|^2)^2} \left| \frac{\partial \rho}{\partial z} \right|^2 \mathrm{d}z\, \mathrm{d}\bar{z} = e^{\varphi(z,\bar{z})} \mathrm{d}z\, \mathrm{d}\bar{z} \tag{1.6}$$

is a regular hyperbolic metric on X, conformal to the standard flat metric $\mathrm{d}z\, \mathrm{d}\bar{z}$ on $X \subset \mathbb{C}$. Its conformal factor φ satisfies the Liouville equation

$$\partial_z \partial_{\bar{z}} \varphi(z,\bar{z}) = \tfrac{1}{2} e^{\varphi(z,\bar{z})} \tag{1.7}$$

and has the following asymptotic behavior at punctures

$$\varphi(z,\bar{z}) = \begin{cases} -2\log|z-z_j| - 2\log|\log|z-z_j|| + O(1) & \text{as } z \to z_j \\ -2\log|z| - 2\log|\log|z|| + O(1) & \text{as } z \to \infty. \end{cases} \tag{1.8}$$

It is known that there exists a unique solution to (1.7) and (1.8).[5] One can show that the *energy-momentum tensor* $T(z)$ of this solution is equal to one half of the Schwarzian derivative (1.1):

$$T(z) \equiv -\tfrac{1}{4}(\partial\varphi)^2 + \tfrac{1}{2}\partial^2\varphi = \tfrac{1}{2}\{\rho, z\}. \tag{1.9}$$

This allows one to calculate all accessory parameters once the classical solution φ is known.

The problem of selecting an appropriate fundamental system is slightly less demanding. As we shall see it is sufficient to know the next to the first two leading terms of the asymptotic of the classical solution φ at one arbitrary puncture.

Unfortunately, the problem to find solutions to the Liouville equation seems to be at least as hard as the problem of calculating the map ρ itself, and the reformulation does not help much on this stage. In this framework however one can consider a more general problem of spheres with n elliptic singularities characterized by real parameters $0 < \xi_j < 1$. Instead of asymptotic conditions (1.8) we impose

$$\varphi(z,\bar{z}) = \begin{cases} -2(1-\xi_j)\log|z-z_j| + O(1) & \text{as } z \to z_j \\ -2(1+\xi_n)\log|z-z_j| + O(1) & \text{as } z \to \infty. \end{cases} \tag{1.10}$$

The existence and uniqueness of φ was in this case proved by Picard[6,7] (see also Ref. 8). The solution can be interpreted as a conformal factor of the complete, hyperbolic metric with the Gaussian curvature $R=-1$ on $X=\mathbb{C}\backslash\{z_1,\ldots,z_{n-1}\}$ and conical singularities of the opening angles $0<2\pi\xi_j<2\pi$ at the points z_j. The n-punctured sphere discussed so far corresponds to the limiting case $\xi_j \to 0$ for all $j=1,\ldots,n$.

The notion of accessory parameters can be introduced in terms of the energy momentum tensor of the solution φ. In the present case it takes the form:[4]

$$T(z) = \sum_{j=1}^{n-1} \left[\frac{\delta_j}{(z-z_j)^2} + \frac{c_j}{z-z_j} \right],$$
$$T(z) \overset{z\to\infty}{=} \frac{\delta_n}{z^2} + \mathcal{O}(z^{-3}), \tag{1.11}$$

where $\delta_j=(1-\xi_j^2)/4$, $j=1,\ldots,n$ are *classical conformal weights*. The multivalued function $\rho: X \to \Delta$ is still of interest although it is no longer an inverse to the universal covering of X. It can be used as before in formula (1.6) to construct solutions to the Liouville equation with asymptotic behavior (1.10).

The above-described ideas are classic and most of them were already pursued by Poincaré. For almost a century the problem of accessory parameters had remainded unsolved. An essentially new insight was brought in by the so-called Polyakov conjecture in 1982.[9] It states that the (properly defined and normalized) Liouville action functional evaluated on the classical solution $\varphi_{\mathrm{cl}}(z,\bar{z})$ is a generating function for the accessory parameters:

$$c_j = -\frac{\partial S^{(\mathrm{cl})}(\delta_i;z_i)}{\partial z_j}. \tag{1.12}$$

This formula was derived within path integral approach to the quantum Liouville theory as the quasiclassical limit of the conformal Ward identity.[10] In the case of the parabolic singularities on n-punctured Riemann sphere a rigorous proof based on the theory of quasiconformal mappings was given by Zograf and Takhtajan.[11] Other proofs, valid both in the case of parabolic and general elliptic singularities, were proposed in Refs. 12 and 14.

The next significant step was done by Zamolodchikov and Zamolodchikov.[1] Analyzing the classical limit of the four-point function of the quantum Liouville theory they argued that the classical Liouville action for four elliptic (parabolic) singularities can be expressed in terms of the classical Liouville action for three singularities and some special function called the *classical conformal block*. Recently this conjecture has been successfully tested by symbolic and numerical calculations in Ref. 13. It should be stressed however that it is still far from being rigorously proved. The basic problem is the classical block itself which is so far accessible only via term by term calculation of the classical limit of the quantum conformal block.

The aim of the present paper is to analyze to what extent the Zamolodchikovs conjecture can provide an explicit construction of the uniformization of four-punctured sphere. Our motivation is to get a better insight into a geometric content of this conjecture and to develop a theoretical framework for its new numerical tests. The results indicate that the classical conformal block plays a central role in the problem and certainly deserves further investigation.

The content of the paper is as follows. In Sec. II we analyze the problem of selecting an appropriate pair of solutions to the Fuchs equation in the case of elliptic weights. It is shown that all the information required is encoded in the derivatives of the classical Liouville action with respect to the parameters ξ_j. The case of parabolic singularities is obtained by taking an appro-

priate limit. The main result is that in order to calculate the map ρ from the Fuchs equation it is sufficient to know the classical Liouville action as a function of z_j's and ξ_j's.

In Sec. III we analyze the problem of calculating monodromies of the Fuchs equation once the accessory parameters are known. Only the case of four punctures is considered. For the standard locations $0,x,1,\infty$ we develop systematic expansions of monodromy matrices at $0,x,1$ in terms of power expansions in x and $1-x$. The results of Secs. II and III are general and are independent of the form in which the classical Liouville action is available.

In Sec. IV the Zamolodchikovs conjecture is formulated and some schemes of calculation of the classical Liouville action and accessory parameters are developed. They lead to very efficient methods of numerical calculations. It should be stressed, however, that many steps in their derivation still require sound mathematical proofs. Concluding this section we discuss some open problems and possible extensions of our work.

II. MAP $\rho: X \to \Delta$

In the case of the sphere with n elliptic singularities with weights $\delta_j=(1-\xi_j^2)/4$ we define the functional

$$S_L[\delta_i;\phi]=\frac{1}{4\pi}\lim_{\epsilon\to 0} S_L^{\epsilon}[\delta_i;\phi],$$

$$S_L^{\epsilon}[\delta_i;\phi]=\int_{X_\epsilon} \mathrm{d}^2z[|\partial\phi|^2+e^{\phi}]+\sum_{j=1}^{n-1}(1-\xi_j)\int_{|z-z_j|=\epsilon}|\mathrm{d}z|\kappa_z\phi+(1+\xi_n)\int_{|z|=1/\epsilon}|\mathrm{d}z|\kappa_z\phi$$
$$-2\pi\sum_{j=1}^{n-1}(1-\xi_j)^2\log\epsilon-2\pi(1+\xi_n)^2\log\epsilon,$$

where $X_\epsilon=\mathbb{C}\setminus(\cup_{j=1}^{n}\{|z-z_j|<\epsilon\}\cup\{|z|>1/\epsilon\})$.

The classical Liouville action $\mathcal{S}^{(\mathrm{cl})}(\delta_i;z_i)$ is then defined as[4,12]

$$S^{(\mathrm{cl})}(\delta_i,z_i)=S_L[\delta_i;\varphi_{\mathrm{cl}}],$$

where $\varphi_{\mathrm{cl}}(z,\bar{z})$ is the unique solution to (1.7) and (1.10).

Once the classical action is known one can use the Polyakov conjecture (1.12) to calculate the accessory parameters and write down the corresponding Fuchs equation

$$\partial_z^2\Psi+T\Psi=0, \tag{2.1}$$

with the energy momentum tensor T given by (1.11). Our aim in this section is to select a fundamental system of solutions to this equation such that their quotient yields a multivalued function $\rho: X\to\Delta$ with SU(1,1) monodromy at each z_j and regular for all $z\in X$.

To this end let us first observe that (1.7) and (1.9) imply that $e^{-\varphi(z,\bar{z})/2}$ is a real solution to the Fuchs equations (2.1) and its complex conjugate. It can therefore be expressed as a bilinear combination of any fundamental system and its complex conjugate. In order to fix the freedom related to the SU(1,1) transformations let us choose a normalized system with diagonal monodromy at an arbitrarily chosen singular point z_j:

$$\Psi_{\xi,\pm}^{(j)}(z)=\frac{A_j^{\pm 1}}{\sqrt{\xi_j}}(z-z_j)^{(1\pm\xi_j)/2}(1+\mathcal{O}(z-z_j)),\quad A_j\in\mathbb{R}. \tag{2.2}$$

It follows from reality, positivity, and single valuedness of $e^{-\varphi(z,\bar{z})/2}$ on X that the parameter A_j can be adjusted such that

$$e^{-\varphi(z,\bar{z})/2} = \frac{D_j}{2}[|\Psi^{(j)}_{\xi,-}(z)|^2 - |\Psi^{(j)}_{\xi,+}(z)|^2],$$

where D_j is a positive constant. Although the above-presented formula is derived by considering a small neighborhood of z_j, it holds for all $z \in X$. Using it one easily derives all the required properties of the map

$$\rho_j(z) = \frac{\Psi^{(j)}_{\xi,+}(z)}{\Psi^{(j)}_{\xi,-}(z)}.$$

One can in particular apply the formula (1.6) to construct the hyperbolic metric with Gaussian curvature -1 on X. As this metric coincides with $e^{\varphi(z,\bar{z})}\mathrm{d}z\,\mathrm{d}\bar{z}$, the constant D_j has to be equal to 1 and

$$e^{-\varphi(z,\bar{z})/2} = \tfrac{1}{2}[|\Psi^{(j)}_{\xi,-}(z)|^2 - |\Psi^{(j)}_{\xi,+}(z)|^2]. \tag{2.3}$$

Analyzing the limit $z \to z_j$ one finds that $A_j^2 = (1/2\xi_j)e^{(1/2)f_j}$, where f_j is the next to the leading term in the $\varphi_{\mathrm{cl}}(z,\bar{z})$ asymptotic at $z \to z_j$. On the other hand,

$$\frac{\partial S^{(\mathrm{cl})}(\delta_i;z_i)}{\partial \xi_j} = \lim_{\epsilon\to 0}\left[(1-\xi_j)\log\epsilon - \frac{1}{4\pi}\int_{|z-z_j|=\epsilon} |\mathrm{d}z|\,\kappa_z\phi\right] = \frac{1}{2}f_j, \tag{2.4}$$

and consequently

$$A_j^2 = \frac{1}{2\xi_j}\exp\left\{\frac{\partial}{\partial\xi_j}S^{(\mathrm{cl})}(\delta_i;z_i)\right\}. \tag{2.5}$$

This equation, along with the Polyakov conjecture, shows that the classical Liouville action contains all the information needed to calculate the map $\rho: X \to \Delta$ from the Fuchs equation.

To study the parabolic limit $\xi_j \to 0$ we shall first define the pair $\widetilde{\Psi}^{(j)}_{\xi,\pm}(z)$, related to $\Psi^{(j)}_{\xi,\pm}(z)$ through the SU(1,1) transformation,

$$\begin{pmatrix} \widetilde{\Psi}^{(j)}_{\xi,+}(z) \\ \widetilde{\Psi}^{(j)}_{\xi,-}(z) \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \xi_j^{1/2} + \xi_j^{-1/2} & \xi_j^{1/2} - \xi_j^{-1/2} \\ \xi_j^{1/2} - \xi_j^{-1/2} & \xi_j^{1/2} + \xi_j^{-1/2} \end{pmatrix}\begin{pmatrix} \Psi^{(j)}_{\xi,+}(z) \\ \Psi^{(j)}_{\xi,-}(z) \end{pmatrix}.$$

From (2.5) it can be shown in the general case (and will be illustrated by the explicit calculation in the next section) that

$$A_j = 1 + \xi_j a_j + \mathcal{O}(\xi_j^2) = e^{\xi_j a_j} + \mathcal{O}(\xi_j^2), \tag{2.6}$$

with a_j independent of ξ_j. From this fact and (2.2) it follows that the limit

$$\begin{pmatrix} \Psi^{(j)}_{+}(z) \\ \Psi^{(j)}_{-}(z) \end{pmatrix} = \lim_{\xi_j\to 0}\begin{pmatrix} \widetilde{\Psi}^{(j)}_{\xi,+}(z) \\ \widetilde{\Psi}^{(j)}_{\xi,-}(z) \end{pmatrix} \tag{2.7}$$

exists.

The inverse of the map

$$\rho^{(j)}(z) = \frac{\Psi^{(j)}_{-}(z)}{\Psi^{(j)}_{+}(z)} \tag{2.8}$$

is the universal covering map of the punctured sphere X by the Poincaré disc Δ. In particular, as

$$\left| \lim_{z \to z_j} \frac{\Psi_-^{(j)}(z)}{\Psi_+^{(j)}(z)} \right| = 1,$$

the puncture is mapped onto the point on the boundary of the Poincaré disc.

III. MONODROMY MATRICES

In this section we shall consider the Riemann sphere with four punctures at the standard locations $z=0,x,1$ and ∞. In this case

$$T(z) = \frac{1}{4z^2} + \frac{1}{4(z-x)^2} + \frac{1}{4(z-1)^2} + \frac{c_1(x)}{z} + \frac{c_2(x)}{z-x} + \frac{c_3(x)}{z-1},$$

and the relations (1.3) can be written in the form

$$c_1(x) = \tfrac{1}{2} - (1-x)c_2(x), \quad c_3(x) = -\tfrac{1}{2} - xc_2(x). \tag{3.1}$$

Our aim is to calculate in this case the monodromies of the fundamental systems of solutions to the Fuchs equation (1.4) constructed in the previous section.

To this end we shall split $T(z)$ onto the "free" term $T_0(z)$ and the "interaction" $-V(z)$,

$$T(z) = T_0(z) - V(z).$$

$T_0(z)$ contains by construction all terms in $T(z)$ singular at $z=0$, term with a second-order pole at $z=x$ plus a "correction" enforcing the behavior $\sim z^{-2}$ at the infinity,

$$T_0(z) = \frac{1}{4z^2} + \frac{1}{4(z-x)^2} + \frac{c_1(x)}{z} - \frac{c_1(x)}{z-x} = \frac{1}{4z^2} + \frac{1}{4(z-x)^2} - \frac{xc_1(x)}{z(z-x)} \equiv \frac{1}{4z^2} + \frac{1}{4(z-x)^2} - \frac{1+\nu^2(x)}{4z(z-x)}$$

with

$$\nu^2(x) = 4xc_1(x) - 1 = -4x(1-x)c_2(x) + x - (1-x), \tag{3.2}$$

and

$$V(z) = -\frac{(1-x)c_3(x)}{(z-x)(z-1)} - \frac{1}{4(z-1)^2}.$$

Solutions to the "free" equation

$$\partial_z^2 f(z) + T_0(z) f(z) = 0$$

are then expressible through the hypergeometric functions with the well-known monodromies around $z=0,x$, while the solutions (and monodromies) of the "full" equation

$$\partial_z^2 \Psi(z) + T_0(z)\Psi(z) = V(z)\Psi(z) \tag{3.3}$$

can be obtained by perturbation theory with an nth order correction proportional to x^n.

One then repeats the above-presented calculation with $x \to 1-x$. Since this problem is related through the global conformal transformation $z \to w = 1-z$ to our original problem with the points 0 and 1 exchanged (and opposite orientation of the z and w planes) it is clear that the monodromy matrix around $w=0$ yields the monodromy matrix around $z=1$. Note however that this time the parameter in the perturbative expansion is $1-x$. Our method thus yields all three monodromy matrices (the monodromy matrix around the puncture $z=\infty$ is equal to the inverse of the product of the remaining three matrices) only for those x for which both x and $1-x$ are small enough.

Let

$$T_0^{(\xi,\epsilon)}(z) = \frac{1-\epsilon^2}{4z^2} + \frac{1-\xi^2}{4(z-x)^2} + \frac{\xi^2+\epsilon^2-\nu^2-1}{4z(z-x)}. \tag{3.4}$$

We can choose the normalized basis in the space of solutions to

$$\partial^2 f(z) + T_0^{(\xi,\epsilon)}(z) f(z) = 0$$

in the form of the pair of functions with the diagonal monodromy matrix around $z=0$,

$$\phi_\pm^{(\xi,\epsilon)}(z) = \sqrt{\frac{x}{\epsilon}}\left(\frac{z}{x}\right)^{(1\pm\epsilon)/2}\left(1-\frac{z}{x}\right)^{(1+\xi)/2} {}_2F_1\left(\frac{1+\xi+\nu\pm\epsilon}{2}, \frac{1+\xi-\nu\pm\epsilon}{2}, 1\pm\epsilon, \frac{z}{x}\right),$$

or in the form of the pair of functions with the diagonal monodromy matrix around $z=x$,

$$\psi_\pm^{(\xi,\epsilon)}(z) = e^{\pm\xi a}\sqrt{\frac{x}{\xi}}\left(\frac{z}{x}\right)^{(1+\epsilon)/2}\left(1-\frac{z}{x}\right)^{(1\pm\xi)/2} {}_2F_1\left(\frac{1\pm\xi+\nu+\epsilon}{2}, \frac{1\pm\xi-\nu+\epsilon}{2}, 1\pm\xi, 1-\frac{z}{x}\right).$$

These two pairs of functions are obviously expressible through each other,

$$\begin{pmatrix} \psi_+^{(\xi,\epsilon)}(z) \\ \psi_-^{(\xi,\epsilon)}(z) \end{pmatrix} = \mathcal{C}^{(\xi,\epsilon)} \cdot \begin{pmatrix} \phi_+^{(\xi,\epsilon)}(z) \\ \phi_-^{(\xi,\epsilon)}(z) \end{pmatrix}$$

with[14]

$$\mathcal{C}^{(\xi,\epsilon)} = \sqrt{\frac{\epsilon}{\xi}}\begin{pmatrix} \dfrac{e^{\xi a}\Gamma(-\epsilon)\Gamma(1+\xi)}{\Gamma\left(\frac{1+\xi+\nu-\epsilon}{2}\right)\Gamma\left(\frac{1+\xi-\nu-\epsilon}{2}\right)} & \dfrac{\Gamma(\epsilon)\Gamma(1+\xi)}{\Gamma\left(\frac{1+\xi+\nu+\epsilon}{2}\right)\Gamma\left(\frac{1+\xi-\nu+\epsilon}{2}\right)} \\ \dfrac{\Gamma(-\epsilon)\Gamma(1-\xi)}{\Gamma\left(\frac{1-\xi+\nu-\epsilon}{2}\right)\Gamma\left(\frac{1-\xi-\nu-\epsilon}{2}\right)} & \dfrac{e^{-\xi a}\Gamma(\epsilon)\Gamma(1-\xi)}{\Gamma\left(\frac{1-\xi+\nu+\epsilon}{2}\right)\Gamma\left(\frac{1-\xi-\nu+\epsilon}{2}\right)} \end{pmatrix}.$$

To take the limit $\epsilon\to 0$ we define, similar to (2.7),

$$\begin{pmatrix} \phi_+^{(\xi)}(z) \\ \phi_-^{(\xi)}(z) \end{pmatrix} = \lim_{\epsilon\to 0} B_\epsilon \begin{pmatrix} \phi_+^{(\xi,\epsilon)}(z) \\ \phi_-^{(\xi,\epsilon)}(z) \end{pmatrix} \tag{3.5}$$

and

$$\mathcal{C}^{(\xi)} = \lim_{\epsilon\to 0} \mathcal{C}^{(\xi,\epsilon)} \cdot B_\epsilon^{-1}$$

with

$$B_\epsilon = \frac{1}{2}\begin{pmatrix} \sqrt{\epsilon}+\dfrac{1}{\sqrt{\epsilon}} & \sqrt{\epsilon}-\dfrac{1}{\sqrt{\epsilon}} \\ \sqrt{\epsilon}-\dfrac{1}{\sqrt{\epsilon}} & \sqrt{\epsilon}+\dfrac{1}{\sqrt{\epsilon}} \end{pmatrix}.$$

For $z\to x$,

$$\phi_\pm^{(\xi)}(z) = \sqrt{z}\left(1 \pm \frac{1}{2}\log\frac{z}{x}\right) + o(z),$$

and the monodromy matrix of this pair around $z=0$ (for $z\to e^{2\pi i}z$) is

$$M_{\phi^{(\xi)}}^{(z=0)} = -\begin{pmatrix} 1+\frac{i\pi}{2} & \frac{i\pi}{2} \\ -\frac{i\pi}{2} & 1-\frac{i\pi}{2} \end{pmatrix}.$$

One thus gets a monodromy matrix of the pair $\psi_{\pm}^{(\xi)}=\lim_{\epsilon\to 0}\psi_{\pm}^{(\xi,\epsilon)}$ around $z=0$ in the form

$$M_{\psi^{(\xi)}}^{(z=0)} = \mathcal{C}^{(\xi)} \cdot M_{\phi^{(\xi)}}^{(z=0)} \cdot (\mathcal{C}^{(\xi)})^{-1}.$$

The limit $\xi\to 0$ can be taken as in (2.7),

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \lim_{\xi\to 0} B_\xi \cdot \begin{pmatrix} \psi_+^{(\xi)} \\ \psi_-^{(\xi)} \end{pmatrix} \tag{3.6}$$

with

$$B_\xi = \frac{1}{2}\begin{pmatrix} \sqrt{\xi}+\frac{1}{\sqrt{\xi}} & \sqrt{\xi}-\frac{1}{\sqrt{\xi}} \\ \sqrt{\xi}-\frac{1}{\sqrt{\xi}} & \sqrt{\xi}+\frac{1}{\sqrt{\xi}} \end{pmatrix}.$$

We have

$$\psi_+(z) = \sqrt{x-z}(1+a) + \frac{1}{2}\sqrt{x-z}\log\left(1-\frac{z}{x}\right) + o(z-x),$$

$$\psi_-(z) = \sqrt{x-z}(1-a) - \frac{1}{2}\sqrt{x-z}\log\left(1-\frac{z}{x}\right) + o(z-x).$$

The monodromy matrix of this pair around $z=x$ (in the counterclockwise direction, $(z-x)\to e^{2\pi i}(z-x)$) thus reads

$$M_{\psi}^{(z=x)} = -\begin{pmatrix} 1-\frac{i\pi}{2} & -\frac{i\pi}{2} \\ \frac{i\pi}{2} & 1+\frac{i\pi}{2} \end{pmatrix},$$

and the monodromy matrix of the $\psi_\pm$ pair around $z=0$ (in the counterclockwise direction, $z\to e^{2\pi i}z$) can be calculated as

$$M_{\psi}^{(z=0)} = \lim_{\xi\to 0} B_\xi \cdot M_{\psi^{(\xi)}}^{(z=0)} \cdot B_\xi^{-1} = \frac{i}{2\pi}\begin{pmatrix} 2i\pi + (\beta^2(x)-4)\cos^2\frac{\pi\nu(x)}{2} & (\beta(x)-2)^2\cos^2\frac{\pi\nu(x)}{2} \\ -(\beta(x)+2)^2\cos^2\frac{\pi\nu(x)}{2} & 2i\pi - (\beta^2(x)-4)\cos^2\frac{\pi\nu(x)}{2} \end{pmatrix}. \tag{3.7}$$

Here

$$\beta(x) \equiv \psi_0\left(\frac{1-\nu(x)}{2}\right) + \psi_0\left(\frac{1+\nu(x)}{2}\right) + 2\gamma_E - 2a(x),$$

$\psi_0(z)=(\mathrm{d}/\mathrm{d}z)\log\Gamma(z)$ is the digamma function and γ_E denotes the Euler-Mascheroni constant.

Monodromy matrix around $z=1$ can now be obtained (paying attention to the opposite orientation of the planes z and $w=1-z$) by repeating the above-presented calculation with x substituted by $1-x$. As these calculations are fairly straightforward we refrain from writing them down explicitly.

We shall now turn to the power-like corrections. Define

$$(\hat{\mathcal{G}}f)(z)=\int_x^z \mathrm{d}z'(\psi_+(z)\psi_-(z')-\psi_-(z)\psi_+(z'))f(z')$$

with $\psi_\pm$ given by (3.6). Since

$$(\partial^2+T_0)\hat{\mathcal{G}}=1,$$

we can rewrite (3.3) in the form of an integral equation

$$\Psi_\pm=\psi_\pm+\hat{\mathcal{G}}V\Psi_\pm$$

with a (formal) solution

$$\Psi_\pm=(1-\hat{\mathcal{G}}V)^{-1}\psi_\pm. \tag{3.8}$$

From (3.8) one can read off the nth order correction to the functions $\psi_\pm(z)$,

$$\delta^{(n)}\psi_\pm(z)=\int_x^z \mathrm{d}z_n\mathcal{G}(z,z_n)V(z_n)\int_x^{z_n}\mathrm{d}z_{n-1}\mathcal{G}(z_n,z_{n-1})V(z_{n-1})\cdots\int_x^{z_2}\mathrm{d}z_1\mathcal{G}(z_2,z_1)V(z_1)\psi_\pm(z_1). \tag{3.9}$$

Let us discuss in some detail the case $n=1$,

$$\delta^{(1)}\psi_\pm(z)=\psi_+(z)\int_x^z \mathrm{d}z'\ \psi_-(z')V(z')\psi_\pm(z')-\psi_-(z)\int_x^z \mathrm{d}z'\ \psi_+(z')V(z')\psi_\pm(z').$$

The functions $\psi_\pm(z')V(z')\psi_\pm(z')$ have integrable (logarithmic) singularities for $z\to x$ and $z\to 0$. Consequently,

$$\delta^{(1)}\psi_\pm(z)=o(z-x)\quad \text{for } z\to x,$$

which means that the monodromy matrix of the $\psi_\pm$ pair remains unchanged. For $z\to 0$ the leading correction takes the form

$$\delta^{(1)}\psi_\pm(z)=\alpha^{(1)}_{\pm,+}\cdot\psi_+(z)+\alpha^{(1)}_{\pm,-}\cdot\psi_-(z)+o(z),$$

with

$$\alpha^{(1)}_{\pm,\pm}=\int_x^0 \mathrm{d}z'\ \psi_\pm(z')V(z')\psi_\pm(z').$$

The monodromy matrix of the $\psi_\pm+\delta^{(1)}\psi_\pm$ pair is therefore given by

$$M^{(0)}_{\psi+\delta^{(1)}\psi}=(1+\alpha^{(1)})M^{(0)}_{\psi}(1+\alpha^{(1)})^{-1}.$$

Notice further that $(1/\sqrt{x})\psi_\pm(x\zeta)$ does not depend on x and $V(xz)=\mathcal{O}(x^{-1})$, so that (with $z'=x\zeta$)

$$\alpha^{(1)}_{\pm,\pm}=x\int_1^0 \mathrm{d}\zeta\left(\frac{1}{\sqrt{x}}\psi_\pm(x\zeta)\right)xV(x\zeta)\left(\frac{1}{\sqrt{x}}\psi_\pm(x\zeta)\right)=\mathcal{O}(x).$$

Similarly one gets

$$\delta^{(n)}\psi_{\pm}(z) = o(z-x) \quad \text{for } z \to x,$$

and

$$\delta^{(n)}\psi_{\pm}(z) = \alpha^{(n)}_{\pm,+}\cdot\psi_{+}(z) + \alpha^{(n)}_{\pm,-}\cdot\psi_{-}(z) + o(z) \quad \text{for } z \to 0,$$

with

$$\alpha^{(n)}_{\pm,\pm} = \mathcal{O}(x^n).$$

Up to this order the monodromy of the pair $\Psi_{\pm}$ around $z=0$ is therefore given by

$$M^{(0)}_{\Psi} = \left(1 + \sum_{k=1}^{n}\alpha^{(k)}\right) M^{(0)}_{\psi} \left(1 + \sum_{k=1}^{n}\alpha^{(k)}\right)^{-1}.$$

Let us remark that although the matrices $\alpha^{(k)}$ are difficult to evaluate analytically, their numerical calculation is rather straightforward.

IV. ZAMOLODCHIKOVS CONJECTURE

The four-point function of the DOZZ theory with the operator insertions at $z_1=0$, $z_3=1$, $z_4=\infty$, and $z_2=x$, can be expressed as an integral of s-channel conformal blocks and DOZZ couplings over the continuous spectrum of the theory. In the semiclassical limit the integrand can be written in terms of three-point classical Liouville actions and the classical block,[1]

$$\langle V_4(\infty,\infty)V_3(1,1)V_2(x,\bar{x})V_1(0,0)\rangle \sim \int_0^{\infty} \mathrm{d}p\; e^{-Q^2 S(\delta_i;x;\delta)}, \tag{4.1}$$

where $\delta=\frac{1}{4}+p^2$ and

$$S(\delta_i;x;\delta) = S^{(\mathrm{cl})}(\delta_4,\delta_3,\delta) + S^{(\mathrm{cl})}(\delta,\delta_2,\delta_1) - f_{\delta}\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(x) - \bar{f}_{\delta}\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(\bar{x}). \tag{4.2}$$

The three-point classical Liouville action with a parabolic $\delta_1=\frac{1}{4}$, an elliptic $\delta_2=\frac{1}{4}(1-\xi^2)$, and a hyperbolic weight $\delta=\frac{1}{4}+p^2$, reads[1,15]

$$S^{(\mathrm{cl})}(\delta,\delta_2,\delta_1) = -(1-\xi)\log 2 + 2F\left(\frac{1-\xi}{2}+ip\right) + 2F\left(\frac{1-\xi}{2}-ip\right) - F(\xi) + H(2ip) + \pi|p| + \text{const}, \tag{4.3}$$

where

$$F(x) = \int_{1/2}^{x} \mathrm{d}y \log\frac{\Gamma(y)}{\Gamma(1-y)}, \quad H(x) = \int_0^x \mathrm{d}y \log\frac{\Gamma(-y)}{\Gamma(y)}.$$

$f_{\delta}\left[\begin{smallmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{smallmatrix}\right](x)$ is the classical conformal block[1] (or the "classical action" of Refs. 16 and 17), defined as the semiclassical asymptotic

$$\mathcal{F}_{1+6Q^2,\Delta}\begin{bmatrix}\Delta_3 & \Delta_2\\ \Delta_4 & \Delta_1\end{bmatrix}(x) \sim \exp\left(Q^2 f_{\delta}\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(x)\right) \tag{4.4}$$

of the BPZ conformal block.[18]

In the classical limit $Q^2\to\infty$ the integral on the right-hand side of relation (4.1) is dominated by its saddle point value. One thus gets

$$S^{(\mathrm{cl})}(\delta_i;x)=S(\delta_i;x;\delta_s)=S^{(\mathrm{cl})}(\delta_4,\delta_3,\delta_s)+S^{(\mathrm{cl})}(\delta_s,\delta_2,\delta_1)-f_{\delta_s}\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(x)-\bar{f}_{\delta_s}\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(\bar{x}), \tag{4.5}$$

where $\delta_s=\frac{1}{4}+p_s^2(x)$ and the *saddle point momentum* $p_s(x)$ is determined by

$$\frac{\partial}{\partial p}S\left(\delta_i;x;\frac{1}{4}+p^2\right)_{|p=p_s}=0. \tag{4.6}$$

Since the semiclassical limit should be independent of the choice of the channel in the factorization of the DOZZ four-point function the Zamolodchikovs' conjecture (4.5) yields three different expressions for the four-point classical Liouville action. The corresponding consistency equations (*classical bootstrap equations*) have been numerically verified for punctures[13] and for punctures and one and two elliptic singularities.[19]

Taking into account the classical geometry corresponding to hyperbolic weights[20] one may expect that the saddle point momentum $p_s(x)$ in the s-channel is related to the length $\ell_s(x)$ of the closed geodesic separating the "initial" $z=0,x$ from the "final" $z=1,\infty$ singularities:

$$\ell_s(x)=4\pi p_s(x). \tag{4.7}$$

In the case of punctures this conjecture has strong numerical support.[13]

The classical limit of the quantum conformal block is up to now the only method of calculating the classical conformal block. Let us note that it is by no means obvious that the quantum conformal block for "heavy" weights does have the asymptotic of the form assumed in (4.4). This is however very well supported by symbolic calculations for the first few terms in a number of cases. An efficient recursive method of calculating coefficients of the expansion of the quantum block in powers of x was developed by Zamolodchikov.[16] Using this method and taking the limit $Q\to\infty$ one can calculate term by term the coefficients of the power expansion

$$f_\delta\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(x)=(\delta-\delta_1-\delta_2)\log x+\sum_{n=1}^{\infty}x^n f_\delta^n\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}. \tag{4.8}$$

In the case of three punctures and one elliptic singularity the first few terms of this expansion read

$$f_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1-\xi^2}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(x)=\left(p^2-\frac{1-\xi^2}{4}\right)\log x+\left(\frac{1-\xi^2}{8}+\frac{p^2}{2}\right)x$$
$$+\left(\frac{9(1-\xi^2)}{128}+\frac{13p^2}{64}+\frac{(1-\xi^2)^2}{1024(1+p^2)}\right)x^2+\mathcal{O}(x^3). \tag{4.9}$$

The limitation of formulas (4.8) and (4.9) is that the power series involved are supposed to converge only for $|x|<1$. A more convenient representation of the conformal block was developed by Zamolodchikov in Ref. 17, where he proposed to regard the block as a function of the variable

$$q(x)=e^{-\pi[K(1-x)/K(x)]},\quad K(x)=\int_0^1\frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-xt^2)}}.$$

In terms of q the classical conformal block reads:

$$f_\delta\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(x)=\left(\frac{1}{4}-\delta_1-\delta_2\right)\log x+\left(\frac{1}{4}-\delta_2-\delta_3\right)\log(1-x)$$
$$+\left(\frac{3}{2}-2(\delta_1+\delta_2+\delta_3+\delta_4)\right)\log\left(\frac{2}{\pi}K(x)\right)$$
$$+\left(\delta-\frac{1}{4}\right)\log 16-\left(\delta-\frac{1}{4}\right)\pi\frac{K(1-x)}{K(x)}+h_\delta\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(q), \tag{4.10}$$

where

$$h_\delta\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix}(q)=\sum_{n=1}^{\infty}(16q)^n h_\delta^n\begin{bmatrix}\delta_3 & \delta_2\\ \delta_4 & \delta_1\end{bmatrix} \tag{4.11}$$

is supposed to converge uniformly on each subset $\{q:|q|<e^{-\epsilon}<1\}$.

The coefficients of power series (4.11) can be determined term by term using Zamolodchikovs recursive method to calculate coefficients in the q-expansion of the quantum block[17] and then taking the limit $Q\to\infty$. This for instance yields:

$$h_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1-\xi^2}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(q)=\frac{(1-\xi^2)^2}{4(1+p^2)}q^2+\left[\frac{(1-\xi^2)^2(15+18\xi^2-\xi^4)}{128(1+p^2)}+\frac{(1-\xi^2)^2(9-\xi^2)^2}{128(4+p^2)}\right.$$
$$\left.+\frac{3(1-\xi^2)^4}{128(1+p^2)^2}-\frac{(1-\xi^2)^4}{32(1+p^2)^3}\right]q^4+\mathcal{O}(q^6). \tag{4.12}$$

In the case of four punctures the saddle point equation determining $p_s(x)$ reads

$$0=\frac{\partial}{\partial p}S\left(\frac{1}{4};x;\frac{1}{4}+p^2\right)=2\pi+4i\log\frac{\Gamma^2\left(\frac{1}{2}+ip\right)\Gamma(-2ip)}{\Gamma^2\left(\frac{1}{2}-ip\right)\Gamma(2ip)}-2\Re\frac{\partial}{\partial p}f_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(x), \tag{4.13}$$

and the classical Liouville action is given by

$$\mathcal{S}^{(\mathrm{cl})}\left(\frac{1}{4};x\right)=S\left(\frac{1}{4};x;\frac{1}{4}+p_s^2(x)\right). \tag{4.14}$$

Using (4.2), (4.3), and (4.9) one gets

$$c_2(x)=-\frac{\partial\mathcal{S}^{(\mathrm{cl})}\left(\frac{1}{4};x\right)}{\partial x}=-\left.\frac{\partial S\left(\frac{1}{4};x;\frac{1}{4}+p^2\right)}{\partial p}\right|_{p=p_s(x)}\cdot\frac{\partial p_s(x)}{\partial x}-\left.\frac{\partial S\left(\frac{1}{4};x;\frac{1}{4}+p^2\right)}{\partial x}\right|_{p=p_s(x)}$$
$$=-\left.\frac{\partial S\left(\frac{1}{4};x;\frac{1}{4}+p^2\right)}{\partial x}\right|_{p=p_s(x)}=\left.\frac{\partial}{\partial x}f_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(x)\right|_{p=p_s(x)}$$
$$=\frac{4p_s^2(x)-1}{4x}+\frac{1}{8}(4p_s^2(x)+1)+\left[\frac{9}{2}+13p_s^2(x)+\frac{1}{8}\frac{1}{1+p_s^2(x)}\right]\frac{x}{32}+\mathcal{O}(x^2) \tag{4.15}$$

or, employing the q expansion of the classical block,

$$c_2(x) = -\frac{1}{4x(1-x)}\left(\frac{E(x)}{K(x)} - x\right) - \frac{\pi^2}{4x(1-x)K^2(x)}\left[p_s^2(x) + \frac{1}{1+p_s^2(x)}\frac{q^2}{2} + \left(\frac{15}{1+p_s^2(x)} + \frac{81}{4+p_s^2(x)} + \frac{3}{(1+p_s^2(x))^2} - \frac{4}{(1+p_s^2(x))^3}\right)\frac{q^4}{32} + \mathcal{O}(q^6)\right], \tag{4.16}$$

where $E(x)$ denotes the complete elliptic integral of the second kind. Equations (4.15) and (4.16) are simple consequences of the Zamolodchikovs conjecture. They provide a new relation between the accessory parameters, the classical conformal block, and the geodesic length function $\ell_s(x)$ which is certainly worth further investigations.

In order to calculate $a_2 \equiv a$ for four punctures one can replace one puncture by an elliptic singularity and then take the limit

$$2a = \lim_{\xi\to 0}\frac{1}{\xi}\log A^2.$$

Using (2.5), (4.2), (4.3), and (4.9) one obtains

$$\begin{aligned} 2a(x) &= \lim_{\xi\to 0}\left\{\frac{1}{\xi}\log\frac{\Gamma\left(\frac{1+\xi}{2} - ip_s(x)\right)\Gamma\left(\frac{1+\xi}{2} + ip_s(x)\right)}{\Gamma\left(\frac{1-\xi}{2} - ip_s(x)\right)\Gamma\left(\frac{1-\xi}{2} + ip_s(x)\right)} - \frac{2}{\xi}\Re\frac{\partial}{\partial\xi}\ f_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1-\xi^2}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(x)\Bigg|_{p=p_s(x)}\right\} \\ &= \psi_0\left(\frac{1}{2} + ip_s(x)\right) + \psi_0\left(\frac{1}{2} - ip_s(x)\right) - \frac{2}{\xi}\Re\frac{\partial}{\partial\xi}\ f_{(1/4)+p^2}\begin{bmatrix}\frac{1}{4} & \frac{1-\xi^2}{4}\\ \frac{1}{4} & \frac{1}{4}\end{bmatrix}(x)\Bigg|_{p=p_s(x),\xi=0} \\ &= \psi_0\left(\frac{1}{2} + ip_s(x)\right) + \psi_0\left(\frac{1}{2} - ip_s(x)\right) - \frac{1}{2}\log x\bar{x} + \frac{\Re x}{2} + \left[36 + \frac{1}{1+p_s^2(x)}\right]\frac{\Re x^2}{2^7} + \mathcal{O}(x^3), \end{aligned} \tag{4.17}$$

or, using (4.10) and (4.12):

$$\begin{aligned} 2a(x) = \psi_0\left(\frac{1}{2} + ip_s(x)\right) + \psi_0\left(\frac{1}{2} - ip_s(x)\right) - \frac{1}{2}\log x\bar{x} - \frac{1}{2}\log|1-x|^2 - \log\left|\frac{2}{\pi}K(x)\right|^2 \\ + \frac{2}{1+p_s^2(x)}\Re q^2 + \left[\frac{45}{4+p_s^2(x)} + \frac{3}{1+p_s^2(x)} + \frac{3}{(1+p_s^2(x))^2} - \frac{4}{(1+p_s^2(x))^3}\right]\frac{\Re q^4}{8} + \mathcal{O}(q^6). \end{aligned} \tag{4.18}$$

Note that in the above-mentioned formulas one only needs the saddle point momentum $p_s(x)$ for four punctures (ξ=0).

Let us finally turn to the problem of determining the saddle point momentum $p_s(x)$. As was discussed in Ref. 13 $p_s(x)$ can be determined numerically, using the q expansion of the classical block, with an essentially arbitrary high precision everywhere but at small vicinities of the singular points $x=1$ and $x=\infty$. On the other hand, the problem of analytic determination of the saddle point momentum still remains to be solved and only partial results are available.

Both geometrical arguments and the form of (4.9) indicate that for $x\to 0$ the solution of (4.13) should also tend to zero. For $p\to 0$,

$$4i\log\frac{\Gamma^2\left(\frac{1}{2}+ip\right)\Gamma(-2ip)}{\Gamma^2\left(\frac{1}{2}-ip\right)\Gamma(2ip)}=-4\pi+32p\log 2+16\sum_{k=1}^{\infty}\frac{(-1)^k\zeta(2k+1)}{2k+1}(2^{2k}-1)p^{2k+1} \tag{4.19}$$

so that, up to the leading terms, the saddle point equation (4.13) takes the form

$$-\pi+16p\log 2-p\log x\bar{x}=0 \tag{4.20}$$

and, to this order,

$$p_s(x)\sim\varepsilon(x)\equiv\frac{\pi}{-\log x\bar{x}+16\log 2}. \tag{4.21}$$

We can now solve (4.13) by iteration, in the form of a double series expansion in $\Re x$ and $\varepsilon(x)$ (since $x=\exp(-1/[1/(-\log x)])$, the powers of x can be viewed as "nonperturbative" corrections to the $\varepsilon(x)$ series). For instance, keeping in (4.13) terms up to p^3 and x^2 we get

$$\begin{aligned}
p_s&=\frac{\pi}{-\log x\bar{x}+16\log 2-\Re x-\frac{207}{512}\Re x^2}\\
&\quad+\frac{8\zeta(3)+\frac{1}{256}\Re x^2}{-\log x\bar{x}+16\log 2-\Re x-\frac{207}{512}\Re x^2}p_s^3+\mathcal{O}(\varepsilon(x)^6,x^3\varepsilon(x))\\
&=\frac{\pi}{-\log x\bar{x}+16\log 2-\Re x-\frac{207}{512}\Re x^2}\\
&\quad+\frac{8\pi^3\zeta(3)+\frac{\pi^3}{256}\Re x^2}{\left(-\log x\bar{x}+16\log 2-\Re x-\frac{207}{512}\Re x^2\right)^4}+\mathcal{O}(\varepsilon(x)^6,x^3\varepsilon(x))\\
&=\varepsilon(x)+\frac{8\zeta(3)}{\pi}\varepsilon^4(x)+\left(\frac{1}{\pi}\varepsilon^2(x)+\frac{32\zeta(3)}{\pi^2}\varepsilon^5(x)\right)\Re x+\frac{\varepsilon^2(x)}{\pi^2}(\Re x)^2\\
&\quad+\left(\frac{207}{512\pi}\varepsilon^2(x)+\frac{1}{256\pi}\varepsilon^4(x)+\frac{207\zeta(3)}{16\pi^2}\varepsilon^5(x)\right)\Re x^2+\mathcal{O}(\varepsilon(x)^6,x^3\varepsilon(x)).
\end{aligned} \tag{4.22}$$

As in the case of the accessory parameters, one can also work out the formula for the saddle point momentum involving the q expansion of the classical conformal block.

For a sufficiently small x the right-hand side of (4.22) agrees with the numerically calculated saddle point momentum and is well within the know analytic bounds on $\ell_s(x)/4\pi$.[2,13] However, to determine the radius of convergence of the series in (4.22) or to give an estimate on the omitted terms one would need to know the classical conformal block exactly.

As discussed in the previous section in order to determine the monodromy matrix at $x=1$ one needs a power expansion of $p_s(x)$ at this point. In other words, an analytic continuation of the classical block from the vicinity of $x=0$ to $x=1$ is required. One possible approach to this problem is to consider the classical limit of the braiding relation for the quantum BPZ block (for conformal blocks corresponding to degenerated fields this calculation is quite straightforward).

We believe that a better understanding of the classical conformal block and the geodesic length function may provide an essentially new insight into the problem of finding an analytic expressions for the map ρ and the uniformizing group. Further studies of these structures are definitely worth pursuing.

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Gauge theories of Dirac type

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A specific class of gauge theories is geometrically described in terms of fermions. In particular, it is shown how the geometrical frame presented naturally includes spontaneous symmetry breaking of Yang-Mills gauge theories without making use of a Higgs potential. In more physical terms, it is shown that the Yukawa coupling of fermions, together with gravity, necessarily yields a symmetry reduction provided the fermionic mass is considered as a globally well-defined concept. The structure of this symmetry breaking is shown to be compatible with the symmetry breaking that is induced by the Higgs potential of the minimal Standard Model. As a consequence, it is shown that the fermionic mass has a simple geometrical interpretation in terms of curvature and that the (semiclassical) "fermionic vacuum" determines the intrinsic geometry of space-time. We also discuss the issue of "fermion doubling" in some detail and introduce a specific projection onto the "physical subspace" that is motivated by the Standard Model. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218673]

I. INTRODUCTION

The aim of this article is to put emphasis on the role of fermions in a geometrically unified description of different kinds of gauge theories as, for instance, Yang-Mills and Einstein's theory. Especially, we discuss in some detail the role of the "Yukawa coupling" of fermions with respect to the mechanism of spontaneous symmetry breaking. This may provide us with a better geometrical understanding of the relation between inertia and gravity.

Let us start out with some general remarks on the notion of "gauge symmetry." The notion of gauge symmetry, in general terms, expresses certain redundancies in the mathematical description of the interactions considered. In mathematics, by gauge theory one usually refers to gauge theories of the Yang-Mills type with the underlying geometry given by a principal G-bundle over a smooth orientable (compact) manifold endowed, in addition, with a (semi-)Riemannian structure (see, for instance, in Refs. 5, 34, 35, 38, and 49). This notion of gauge theory, however, is clearly far too restrictive when considered from a physical point of view. For instance, gravity is also usually regarded as a kind of gauge theory though it is certainly not of the Yang-Mills type. The underlying geometrical structure of gravity, regarded as a gauge theory, is that of a fiber bundle naturally associated with the frame bundle of the base manifold $\mathcal{M}$ with typical fiber given by $\mathrm{GL}(n)/\mathrm{SO}(p,q)$. Here, respectively, $\dim(\mathcal{M}) \equiv n = p+q$ equals the dimension of the oriented base manifold and $s = p-q$ is the signature. The bundle structure of the two gauge theories is obviously very different. In contrast to Yang-Mills theory, the bundle structure of gravity is fully determined (modulo diffeomorphisms) by fixing the (topology of the) base manifold and the signature s. In this sense, the bundle structure in Einstein's theory of gravity is more natural than in the Yang-Mills theory. Moreover, the mathematical notion of a local trivialization has a physical meaning in

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the case of gravity, however, not in Yang-Mills gauge theories (there is no "exponential map" defined in Yang-Mills theories for, in contrast to gravity, Yang-Mills connections only determine second order vector fields but no spray fields).

The respective Lagrangian densities of gravity and Yang-Mills gauge theory differ in that the former is known to be linear in the curvature of the base manifold whereas the latter is quadratic in the curvature of the bundle space. This difference is known to yield far-reaching consequences, for example, when quantization is taken into account. But also on the purely "classical" level (i.e., gravity and electromagnetism) there are fundamental differences in these two kinds of gauge theories. For example, electromagnetism (more general, Yang-Mills gauge theories over even-dimensional base manifolds) is known to be scale invariant but not invariant with respect to the action of the diffeomorphism group (except isometries). In contrast, gravity is covariant with respect to diffeomorphisms but not scale invariant. Of course, despite these profound mathematical and physical differences there are, nonetheless, formal similarities between these two types of gauge theories. Especially, the dynamics that is defined by both theories can be expressed with respect to top-forms on the base manifold with the property of being invariant with respect to the action of their respective symmetry groups. A natural question then is whether these two fundamental kinds of gauge theories have a common geometrical root (for a discussion about the "naturality" of these two top-forms see Refs. 50 and 33).

Of course, over the last few decades there have been various attempts to geometrically unify gravity with the Yang-Mills gauge theory. This holds true for string theory and, in particular, for various aspects of noncommutative geometry, see, e.g., Refs. 8, 9, 14, and 40, and references there. The fruitful idea to consider the Higgs boson of the Standard Model as an integral part of the Yang-Mills theory goes back to fundamental works, e.g., Refs. 15–17 and 10. It is well known that this idea actually has had a tremendous impact on a vast variety of articles of the same theme (see, for instance, Refs. 18, 27, 36, and 37 in the context of noncommutative geometry, or Refs. 25 and 39 in the case of "superalgebras"). Basically, all of these geometrical descriptions of gauge theory use the purely algebraic content of gauge theories of the Yang-Mills type (e.g., the exterior differential is a nilpotent derivation and a connection is the sum of the latter and a one-form) as their starting point. However, gravity seems not to fit in this basic algebraic vision. Also, spontaneous symmetry breaking is described only in terms of (the algebraic aspects of) Yang-Mills gauge theories without using gravity. The notion of fermions only arises because in the algebraic context the exterior differential is defined in terms of specific generalizations of the notion of a Dirac operator. These purely algebraic generalizations of the latter, however, seem to have no geometrical counterpart (see, for instance, the "internal Dirac operator" in the geometrical description of the Standard Model in terms of "almost commutative models)."[26]

In the following we shall discuss a specific class of gauge theories including Einstein's theory of gravity and (spontaneously broken) Yang-Mills theory from the point of view of fermions. The latter will be geometrically treated as certain Hermitian vector bundles over arbitrary smooth orientable manifolds of even dimension. These "fermion bundles" correspond to a global specification of a certain class of first order differential operators, called "Dirac type operators." We introduce a canonical mapping which associates with every Dirac type operator a specific top-form on the base manifold. This canonical mapping is then referred to as the "Dirac-Lagrangian" on the setup to be discussed. The Dirac-Lagrangian turns out to be equivariant with respect to bundle equivalence. In particular, it is invariant with respect to the action of the Yang-Mills and the Einstein-Hilbert gauge groups. The diffeomorphism group of the base manifold is naturally included by the pull-back action. We also consider a distinguished class of Dirac type operators within this setup. The corresponding top-form associated with these Dirac type operators is shown to define a spontaneously broken gauge theory without referring to a Higgs potential. In more physical terms, it is shown that the Yukawa coupling together with gravity yields a symmetry reduction which is compatible with the symmetry breaking induced by a Higgs potential of the form used in the (minimal) Standard Model of Particle Physics. In fact, the latter is shown to be

naturally generated by a "fluctuation of the fermionic vacuum." We will also reformulate the notion of "unitary gauge" in terms of Dirac type operators and give necessary and sufficient conditions for its global existence.

The geometrical description of gauge theories discussed in the present article is a considerable refinement of the geometrical frame that has been introduced in Ref. 45 in the case of elliptic Dirac type operators on a smooth even-dimensional closed Riemannian spin manifold. In contrast to the latter we will consider in this article the more physically appropriate case of arbitrary signature and noncompact manifolds. Also, we do not assume that "space-time" has a spin structure (please see the following discussion). For this, however, we will focus on (globally defined) densities instead of action functionals. Accordingly, we have to demand that the densities themselves are covariant with respect to the underlying symmetry action and thus well defined on the appropriate moduli spaces. This is achieved mainly since the densities in question are derived from evaluating a natural object (within the frame considered) with respect to specific first order differential operators. As a consequence, one ends up with densities which are linear in the curvature of the base manifold and quadratic in the curvature of the bundle space. For instance, it is shown that the total curvature of the "fermionic vacuum" decomposes into the sum of the curvature of the base manifold together with the (square of the) fermionic mass operator. Also a basic difference relative to the frame considered here (and subsequent articles thereof) is that all bundles, including the Higgs and the Yang-Mills bundles, are considered as specific subbundles of the fermion bundle (respectively, of the bundle of endomorphisms of the latter). The fermion density will be considered as a specific mapping on the affine set of all Dirac type operators on a fermion bundle. Here, we also discuss the issue of the doubling of the fermionic degrees of freedom that is necessary to apply the general Bochner-Lichnerowicz-Weizenböck formula.

Finally, we want to comment on the notion of "fermions" without assuming the existence of spin structures. At least in the so-called "semi-classical approximation" of a full quantum field theory it is common to geometrically treat the "states of a fermion" as sections of a (twisted) spinor bundle over space-time. For this, of course, the topology of space-time must guarantee the existence of a spin structure (i.e., the vanishing of the second Stiefel-Whitney classes). Moreover, it is known that a noncompact Lorentzian four manifold possesses a spin structure if and only if its frame bundle is trivial ("Geroch's Theorem," c.f. Refs. 19 and 20). Therefore, the existence of a spin structure provides severe restrictions to the topology of space-time. However, the experiments performed to demonstrate that the double cover of the (proper orthochroneous) Lorentz group is more fundamental are purely local in nature. Also, in order to obtain a topologically nontrivial statement about the existence of spin structures, space-time has to be covered by at least three (trivializing) local charts. This, of course, raises the question of the physical sense of "locality" in this context to give the mathematical construction a physical meaning. Hence, from our point of view, the assumption of the existence of a spin structure is a purely mathematical one without a physically meaningful counterpart. In fact, in this respect the notion of locality, as it is used in mathematics, seems physically as spurious as in the case of the Yang-Mills gauge theories which do not provide any scale. Basically, this is the reason to consider in this work the more general notion of "Clifford module bundles" instead of "twisted spinor bundles" as an appropriate geometrical background. In contrast to the latter, the existence of Clifford module bundles yields no more topological restrictions on space-time than the existence of a metric itself. For instance, the bundle of Grassmann algebras serves as a natural Clifford module bundle for every space-time manifold. However, the topology of the Clifford module bundles cannot be arbitrary. The physical interpretation of the sections of Clifford module bundles in terms of the states of fermions yields restrictions to the topology of the considered Clifford module bundles (please, see the following text).

This article is organized as follows. In the next section we introduce the concept of fermion bundles as a specific class of Clifford module bundles and define Dirac type gauge theories. In the third section we consider a distinguished class of such gauge theories and discuss spontaneous symmetry breaking in this context. In the Sec. IV we introduce the fermionic density within the presented geometrical setup and discuss the issue of fermionic doubling. In the fifth section we

want to specify what we mean by a fluctuation of the fermionic vacuum. This is done in terms of yet another class of Dirac type operators. Finally, in Sec. VI we close with an outlook. In the Appendix we present a detailed proof of the explicit form of "simple type Dirac operators" of arbitrary signature, for these operators turn out to be fundamental, e.g., in our discussion of spontaneous symmetry breaking.

II. FERMION BUNDLES AND DIRAC TYPE GAUGE THEORIES

In this section we introduce a specific class of Clifford module bundles which will serve as our geometrical background for gauge theories. With respect to this background there exists a canonical mapping which permits to associate with the local data of a fermion bundle a specific top form on the base manifold. This top form turns out to be equivariant with respect to the automorphism group of the underlying geometrical structure.

A. Fermion bundles, Dirac type operators and connections

In this subsection we define our notion of *fermion bundles* as a specific class of Clifford module bundles. For this let $\xi := (\mathcal{E}, \pi_\varepsilon, \mathcal{M})$ be a smooth complex vector bundle with total space $\mathcal{E}$, base manifold $\mathcal{M}$ and projection map $\pi_\varepsilon : \mathcal{E} \to \mathcal{M}$. The rank, $\mathrm{rk}(\xi) \in \mathbb{N}$, of the bundle is $\mathrm{N} \geqslant 1$. In what follows the base manifold is assumed to be orientable and of even dimension $n \equiv 2k$. As a topological space $\mathcal{M}$ is a paracompact and (simply) connected Hausdorff-space. On this geometrical background we consider the following local data:

$$(\mathrm{G}, \rho_\mathrm{F}, D). \tag{1}$$

Here, G is a semisimple, compact and real Lie group and $\rho_\mathrm{F} : \mathrm{G} \to \mathrm{SU}(\mathrm{N}_\mathrm{F})$ is a unitary and faithful representation thereof. Moreover, $D : \Gamma(\xi) \to \Gamma(\xi)$ is a first order differential operator, acting on sections of the bundle ξ such that the bilinear extension g_M of the mapping $(df, dh) \mapsto \mathrm{tr}([D,f] \times [D,h])/\mathrm{rk}(\xi)$ is nondegenerated for all smooth functions $f, g \in \mathcal{C}^\infty(\mathcal{M})$. The operator D is said to have the signature $s \in \mathbb{Z}$, provided that the quadratic form associated with the (semi-) Riemannian metric g_M has signature s. The mapping g_M corresponds to a section of the "Einstein-Hilbert bundle" $\xi_\mathrm{EH} := (FM \times_{\mathrm{GL(n)}} \mathrm{GL}(n)/\mathrm{O}(p,q), \pi_\mathrm{EH}, \mathcal{M})$, with, respectively, FM the total space of the frame bundle $\mathcal{FM}$ of the base manifold $\mathcal{M}$ and $n \equiv p+q, s \equiv p-q$.

Let $\tau_\mathrm{Cl} \equiv \tau_\mathrm{Cl}^{(\pm)}$ be the algebra bundle of Clifford algebras which are point-wise generated by $(\tau_\mathrm{M}^*, g_\mathrm{M})$, with τ_M^* being the cotangent bundle of $\mathcal{M}$ (with total space T^*M). The corresponding Clifford relations are defined by $\alpha^2 := \pm g_\mathrm{M}(\alpha, \alpha)$ for all $\alpha \in T^*M \subset Cl(M)$ (the total space of τ_Cl). In the following, it is assumed that the principal symbol of the operator D induces a Clifford (left) action $\gamma : \tau_\mathrm{Cl} \to \mathrm{End}(\xi)$ via the mapping

$$\begin{aligned} \tau_\mathrm{Cl} \times \xi &\to \xi, \\ (df, \mathfrak{z}) &\mapsto [D,f]\mathfrak{z}, \end{aligned} \tag{2}$$

for all smooth functions $f \in \mathcal{C}^\infty(\mathcal{M})$. In other words, besides the assumption that $[D,f]^2$ induces an isomorphism $\tau_\mathrm{M} \simeq \tau_\mathrm{M}^*$, it is also supposed to be in the commutant of $\mathrm{End}(\xi)$. As a consequence, the algebra bundle of endomorphisms on ξ globally decomposes as

$$\mathrm{End}(\xi) \simeq \tau_\mathrm{Cl}^\mathbb{C} \otimes_\mathcal{M} \mathrm{End}_\mathrm{Cl}(\xi). \tag{3}$$

Here, $\mathrm{End}_\mathrm{Cl}(\xi) \subset \mathrm{End}(\xi)$ denotes the subbundle of endomorphisms which supercommute with the Clifford action γ (c.f., for instance, in Refs. 2 and 3).

Definition 2.1: *The vector bundle* $\xi \equiv \xi_\mathrm{F}$ *is called a "fermion bundle" with respect to the* (*local*) *data* (1) *if the structure group of* ξ *can be reduced to* $\mathrm{Spin}(p,q) \times \rho_\mathrm{F}(\mathrm{G})$. *A fermion bundle is called "chiral" provided* $\xi_\mathrm{F} = \xi_\mathrm{F}^+ \oplus \xi_\mathrm{F}^-$ *is* $\mathbb{Z}_2$*-graded with respect to some involution* $\Gamma \equiv \gamma_\mathrm{M} \otimes \chi \in \Gamma(\mathrm{End}(\xi_\mathrm{F}))$. *Here, the canonical involution* $\gamma_\mathrm{M} \in \Gamma(\tau_\mathrm{Cl}^\mathbb{C})$ *is defined in terms of the* (*semi-*) *Riemannian volume form* $\mu_\mathrm{M} \in \Omega^n(\mathcal{M})$ *that is induced by* g_M. *Moreover,* ξ_F *is called "real" if all of*

its odd Chern classes vanish. With respect to Γ *the operator* D *is supposed to be odd and the representation* ρ_{F} *is assumed to be even. In this case*, D *is called a "Dirac type operator" and* (1) *a "Dirac triple."*

A fermion bundle encodes the global data of a Dirac type gauge theory. With respect to these data we consider the set $\mathcal{D}(\xi_{\mathrm{F}})$ of all Dirac type operators $D' \in \mathcal{D}(\xi_{\mathrm{F}})$ to satisfy the condition $[D'-D,f] \equiv 0$ for all $f \in \mathcal{C}^{\infty}(\mathcal{M})$. The set $\mathcal{D}(\xi_{\mathrm{F}})$ naturally becomes an affine space with vector space $\Gamma(\mathrm{End}^{-}(\xi_{\mathrm{F}}))$. In what follows we summarize the basic features of this affine space.

The affine space $\mathcal{A}(\xi_{\mathrm{F}})$ of linear connections on ξ_{F} has a distinguished affine sub-space $\mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}}) \subset \mathcal{A}(\xi_{\mathrm{F}})$ that is defined by all linear connections which are compatible with the Clifford action γ. That is, $A \in \mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ defines a covariant derivative ∂_A satisfying $[\partial_A, \gamma(a)] = \gamma(\nabla^{\mathrm{Cl}} a)$ for all sections $a \in \Gamma(\tau_{\mathrm{Cl}}^{\mathbb{C}})$ with ∇^{Cl} being the covariant derivative with respect to the lifted Levi-Civita connection of g_{M}. Accordingly, such a connection is referred to as a "Clifford connection." Hence, every $D' \in \mathcal{D}(\xi_{\mathrm{F}})$ may be written as $D' = \partial\!\!\!/_A + \Phi$ where, respectively, $\partial\!\!\!/_A \equiv \gamma \circ \partial_A$ is the analogue of a twisted spin Dirac operator in the case where $\mathcal{M}$ denotes a spin manifold and $\Phi \equiv D - \partial\!\!\!/_A \in \Gamma(\mathrm{End}(\xi_{\mathrm{F}}))$. Notice, however, that in general the zero order operator Φ also depends on the Clifford connection A. Moreover, the relation between the two affine spaces $\mathcal{D}(\xi_{\mathrm{F}})$ and $\mathcal{A}(\xi_{\mathrm{F}})$ on a fermion bundle is given by the (signature independent) bijection (c.f. Ref. 45)

$$\mathcal{D}(\xi_{\mathrm{F}}) \simeq \mathcal{A}(\xi_{\mathrm{F}})/\ker(\delta_{\gamma}), \tag{4}$$

where

$$\delta_{\gamma}\colon \Omega^1(\mathcal{M},\mathrm{End}(\mathcal{E})) \to \Omega^0(\mathcal{M},\mathrm{End}(\mathcal{E}))\ \alpha \mapsto \gamma(\alpha). \tag{5}$$

Therefore, to each Dirac type operator on ξ_{F} there corresponds an equivalence class of connections. However, each connection class has a natural representative that is constructed as follows: First, on every chiral fermion bundle there is a canonical odd one-form $\Theta \in \Omega^1(\mathcal{M},\mathrm{End}^{-}(\mathcal{E}))$ that is given by the (normalized) lifted soldering form of $\mathcal{FM}$. More precisely, let $\vartheta \in \Omega^1_{\mathrm{eq,hor}}(FM,\mathbb{R}^n)$ be the soldering form on the (total space of the) frame bundle of $\mathcal{M}$. Here, the canonical identification $\Omega^*_{\mathrm{eq,hor}}(FM,\mathbb{R}^n) \simeq \Omega^*(\mathcal{M},T\mathcal{M})$ and the injection (here, $\Omega^*_{\mathrm{eq,hor}}(FM,\mathbb{R}^n)$ denotes the "right-equivariant" and "horizontal" forms on the total space of the frame bundle of $\mathcal{M}$)

$$\Gamma(\tau_{\mathrm{M}}^* \otimes_{\mathcal{M}} \tau_{\mathrm{M}}) \overset{\mathrm{id}\otimes\ \flat}{\to} \Gamma(\tau_M^* \otimes_{\mathcal{M}} \tau_M^*) \hookrightarrow \Gamma(\tau_M^* \otimes_{\mathcal{M}} \tau_{\mathrm{Cl}}) \overset{\mathrm{id}\otimes\gamma}{\to} \Gamma(\tau_M^* \otimes_M \mathrm{End}(\xi_{\mathrm{F}})) \tag{6}$$

yields $\Theta := \pm\widetilde{\vartheta}/n$ with $\widetilde{\vartheta} \equiv \gamma \circ \vartheta^{\flat} \in \Omega^1(\mathcal{M},\mathrm{End}(\mathcal{E}))$. If $(X_1,\ldots,X_n)$ denotes a local frame on $\mathcal{M}$ and $(X^1,\ldots,X^n)$ its dual, then (throughout this article Einstein's summation convention is used in local formulas except where this may lead to confusions) $\widetilde{\vartheta} \overset{loc.}{=} X^k \otimes \gamma(X_k^{\flat}) \otimes \mathrm{id}$, with the usual "musical" isomorphism $u^{\flat}(v) := g_{\mathrm{M}}(u,v)$ for all $u,v \in T\mathcal{M}$. The normalized soldering form Θ has the two basic properties: It is covariantly constant with respect to every Clifford connection and it induces a canonical right inverse of the Clifford action, i.e., $\delta_{\gamma} \circ \mathrm{ext}_{\Theta} = \mathrm{id}$. Here, $\mathrm{ext}_{\Theta} \in \mathrm{End}(\tau^*_{\Lambda\mathrm{M}} \otimes_{\mathcal{M}} \mathrm{End}(\xi))$ denotes the operator of (point-wise) left-multiplication by Θ, and $\tau^*_{\Lambda\mathrm{M}}$ is the bundle of Grassmann algebras that is, again, generated by τ^*_{M}. Note that the linear equivalence $\tau_{\mathrm{Cl}} \simeq \tau^*_{\Lambda\mathrm{M}}$ is used but not explicitly indicated. Second, to each Dirac type operator $D' \in \mathcal{D}(\xi_{\mathrm{F}})$ there exists a correspondingly unique connection $\hat{A}'_{\mathrm{D}} \in \mathcal{A}(\xi_{\mathrm{F}})$ such that $D'^2 - \triangle'_{\mathrm{D}} \in \Gamma(\mathrm{End}(\xi_{\mathrm{F}}))$. The second order operator $\triangle'_{\mathrm{D}} := -\mathrm{tr}(\hat{\nabla}^{T^*\mathcal{M}\otimes\mathcal{E}} \circ \hat{\nabla}^{\mathcal{E}})$ is called the "Bochner-Laplacian" of D' (c.f., e.g., Refs. 3 and 6, or 21). Here, $\hat{\nabla}^{\mathcal{E}}$ denotes the covariant derivative that corresponds to the connection $\hat{A}'_{\mathrm{D}}$. As a consequence, the covariant derivative that is defined by

$$\partial_{D'} := \hat{\nabla}^{\mathcal{E}} + \Theta \wedge (D' - \gamma \circ \hat{\nabla}^{\mathcal{E}}) \tag{7}$$

yields a connection $A'_{\mathrm{D}} \in \mathcal{A}(\xi_{\mathrm{F}})$ which clearly represents the Dirac type operator D', i.e., $D' = \gamma \circ \partial_{D'}$. We call, respectively, A'_{D} the Dirac connection associated with D' and the one-form

$$\varpi'_{\mathrm{D}} := \Theta \wedge (D' - \gamma \circ \hat{\nabla}^{\mathcal{E}}) \in \Omega^1(\mathcal{M}, \mathrm{End}(\mathcal{E})) \tag{8}$$

the "Dirac form" associated with $D' \in \mathcal{D}(\xi_{\mathrm{F}})$. Of course, if the connections $\hat{A}'_{\mathrm{D}}$ and A'_{D} are identified with the respective connection forms $\hat{\omega}, \omega'_{\mathrm{D}} \in \Omega^1(\mathcal{E}, T\mathcal{E})$, then

$$\pi^*_{\mathcal{E}} \varpi'_{\mathrm{D}} = \omega'_{\mathrm{D}} - \hat{\omega}. \tag{9}$$

Remark: *As a first order differential operator each Dirac type operator D is known to be of the* (*local*) *form*: $D = \gamma^\mu(\partial_\mu + \omega_\mu)$ *with the appropriate* "γ-matrices" $\gamma^\mu \in \mathrm{End}(\mathbb{C}^{2^k})$ *satisfying either of the Clifford relations* $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu \equiv \pm 2g^{\mu\nu}\mathbf{1}$, *and*

$$\omega_\mu \equiv \omega^{\mathrm{Cl}}_\mu \otimes \mathbf{1} + \mathbf{1} \otimes A_\mu \pm \tfrac{1}{n} g_{\mu\nu} \sum_{0 \leqslant k \leqslant n} \sum_{1 \leqslant i_1 < i_2 \cdots < i_k \leqslant n} \gamma^\nu \gamma^{j_1} \gamma^{j_2} \cdots \gamma^{j_k} \otimes \theta_{i_1 i_2 \cdots i_k}. \tag{10}$$

Here, *respectively*, ω^{Cl}_μ *is the component of the lifted Levi-Civita form with respect to the appropriate metric coefficients* $g_{\mu\nu}$, *and* $A_\mu, \theta_{i_1 i_2 \cdots i_k}$ *are the components of locally defined differential forms of various degrees which take their values in* $\rho'_{\mathrm{F}}(\mathrm{Lie}(\mathrm{G})) \subset \mathrm{End}(\mathbb{C}^{N_{\mathrm{F}}})$. *Obviously*, *these forms determine each specific Dirac type operator* $D \in \mathcal{D}(\xi_{\mathrm{F}})$ *locally. More precisely*, *let* $\{(U_\alpha, \chi_\alpha) \,|\, \alpha \in \Lambda\}$ *be a family of local trivializations of the underlying vector bundle* ξ, *i.e.*, $\chi_\alpha : \pi^{-1}_{\mathcal{E}}(U_\alpha) \xrightarrow{\simeq} U_\alpha \times \mathbb{C}^{\mathrm{N}}$. *Accordingly*, *let* $\chi_{\alpha\beta} : U_\alpha \cap U_\beta \to \mathrm{GL}(\mathrm{N}, \mathbb{C})$ *be the appropriate transition functions. Then*, *a family of first order differential operators* D_α *of the form* $D_\alpha = \gamma_\alpha \circ \nabla_\alpha$, *with* $\nabla_\alpha \equiv d + \omega_\alpha$ and ω_α *defined by* (10), *gives rise to a Dirac type operator D on* ξ *provided the principal symbols* γ_α *define a family of Clifford mappings* $\mathbb{R}^{p,q} \to \mathrm{End}(\mathbb{C}^{2^k}) \simeq \mathbb{C} \otimes \mathrm{Cl}_{p,q}$ *and the transition functions take their values in the subgroup* $\mathrm{Spin}(p,q) \times \rho_{\mathrm{F}}(\mathrm{G})$ *such that the family* $\{(U_\alpha, D_\alpha) \,|\, \alpha \in \Lambda\}$ *fulfills the compatibility condition* $D_\alpha = \chi_{\alpha\beta} \circ D_\beta \circ \chi^{-1}_{\alpha\beta}$ *for all* $x \in U_\alpha \cap U_\beta \subset \mathcal{M}$. *Hence*, *the notion of a Dirac triple on* ξ (i.e., ξ_{F}) *globalizes what is encoded in the local data specifying D. In other words*, *the notion of a fermion bundle simply permits globalization of the local data* $(U_\alpha, D_\alpha)_{\alpha \in \Lambda}$ *usually encountered in physics*.

B. Gauge theories of Dirac type and their gauge groups

In this subsection we show that the geometrical setup of fermion bundles permits to naturally introduce a specific class of gauge theories which we call *gauge theories of Dirac type* (GTDT). The corresponding gauge group is the automorphism group of the underlying geometrical structure. It is shown that this group decomposes into certain subgroups which can be identified with the usual Yang-Mills gauge group, the Einstein-Hilbert gauge group, and the diffeomorphism group of the base manifold.

Definition 2.2: *Two fermion bundles* ξ_{F} *and* ξ'_{F} *are considered to be equivalent if* $\mathrm{G} \simeq \mathrm{G}'$ *and* ρ_{F} *is similar to* ρ'_{F}. *Moreover*, *there is a bundle isomorphism* $(\alpha, \beta) : \xi \to \xi'$ (*i.e., diffeomorphisms* $\alpha : \mathcal{M} \to \mathcal{M}'$ *and* $\beta : \mathcal{E} \to \mathcal{E}'$, *with* β *being fiber-wise linear and* $\alpha \circ \pi_{\mathcal{E}} = \pi_{\mathcal{E}'} \circ \beta$) *such that* $D' = \beta \circ D \circ \beta^{-1}$.

Notice that the condition $D' = \beta \circ D \circ \beta^{-1}$ actually is equivalent to $g_{\mathrm{M}'} = \alpha^{-1*} g_{\mathrm{M}}$.

The presented geometrical setup permits the formulation of a class of gauge theories which are based on a "universal Lagrangian" that is covariant with respect to the action of the automorphism group

$$\mathcal{G}_{\mathrm{F}} \equiv \mathrm{Aut}(\xi_{\mathrm{F}}) := \{(\alpha, \beta) \in \mathrm{Diff}(\mathcal{M}) \times \mathrm{Aut}(\mathcal{E}) \,|\, \pi_{\mathcal{E}} \circ \beta = \alpha \circ \pi_{\mathcal{E}}\} \tag{11}$$

of the fermion bundle in question. This group may be identified with the group of right-equivariant automorphisms of the frame bundle associated with ξ_{F}. That is,

$$\mathcal{G}_{\mathrm{F}} \simeq \mathrm{Aut}_{\mathrm{eq}}(\mathcal{FE}) := \{f \in \mathrm{Aut}(F\mathcal{E}) | R_g \circ f = f \circ R_g, g \in \mathrm{G_F}\}, \tag{12}$$

where, respectively, $\mathcal{FE} \equiv (F\mathcal{E}, \mathcal{M}, \pi, \mathrm{G_F})$ is the associated frame bundle of the fermion bundle considered, $\mathrm{G_F} \equiv \mathrm{Spin}(p,q) \times \rho_{\mathrm{F}}(\mathrm{G})$ its structure group and R the right action of the latter on the total space $F\mathcal{E}$ of the frame bundle.

Therefore, the automorphism group (11) has several important subgroups. In particular, it contains the "inner gauge group" of the fermion bundle ξ_{F}:

$$\mathcal{G}_{\mathrm{in}} := \{(\alpha, \beta) \in \mathcal{G}_{\mathrm{F}} | \alpha := \mathrm{id}_{\mathcal{M}}\}, \tag{13}$$

which may be identified with the gauge group of $\mathcal{FE}$. The latter contains two mutually commuting normal subgroups $\mathcal{G}_{\mathrm{EH}}$ and $\mathcal{G}_{\mathrm{YM}}$, such that $\mathcal{G}_{\mathrm{EH}} \cap \mathcal{G}_{\mathrm{YM}} = \{e\}$. Therefore,

$$\mathcal{G}_{\mathrm{in}} \simeq \mathcal{G}_{\mathrm{EH}} \times_{\mathcal{M}} \mathcal{G}_{\mathrm{YM}}. \tag{14}$$

Here, the "Yang-Mills gauge group" $\mathcal{G}_{\mathrm{YM}}$ can be identified with the subgroup $\{(\alpha, \beta) \in \mathrm{Aut}(\xi_{\mathrm{F}}) | \alpha = \mathrm{id}_{\mathcal{M}}, \beta \in \mathrm{Aut}_{\mathrm{Cl}}(\mathcal{E})\}$ of the inner gauge group (14). Note that the Yang-Mills gauge group is in fact an invariant subgroup of the inner gauge group. Hence, with respect to the above-mentioned identification, the "Einstein-Hilbert gauge group" $\mathcal{G}_{\mathrm{EH}}$ may be identified with the quotient group $\mathcal{G}_{\mathrm{in}}/\mathcal{G}_{\mathrm{YM}}$ according to the decomposition (3).

Moreover, the diffeomorphism group of the base manifold $\mathcal{M}$ has a natural nontrivial embedding into $\mathrm{Aut}(\xi_{\mathrm{F}})$. Indeed, if ξ_{F} is merely considered as a vector bundle, one gets the (trivial) embedding

$$\begin{gathered} \mathrm{Diff}(\mathcal{M}) \hookrightarrow \mathrm{Aut}(\xi_{\mathrm{F}}), \\ \alpha \mapsto (\alpha, \beta := \pi_{\mathcal{E}}^{*} \alpha \times \mathrm{id}_{\mathcal{E}}). \end{gathered} \tag{15}$$

This embedding may actually be identified with the inclusion according to the definition (11) of the automorphism group and the identification

$$\alpha^{-1*}\mathcal{E} \equiv \{(y, \mathfrak{z}) \in \mathcal{M} \times \mathcal{E} | \pi_{\mathcal{E}}(\mathfrak{z}) = \alpha^{-1}(y)\} = \{(\pi^{*}\alpha(\mathfrak{z}), \mathfrak{z}) | \mathfrak{z} \in \mathcal{E}\} \simeq \mathcal{E}. \tag{16}$$

Hence, one has $\alpha^{-1*}\xi_{\mathrm{F}} = (\alpha^{-1*}\mathcal{E}, \mathcal{M}, \mathrm{pr}_1) = (\mathcal{E}, \mathcal{M}, \pi^{*}\alpha)$, which permits to replace $\beta = \pi^{*}\alpha \times \mathrm{id}_{\mathcal{E}}$ (with inverse given by pr_2) simply by $\beta := \mathrm{id}_{\mathcal{E}}$. However, as ξ_{F} is a Clifford module bundle over $(\mathcal{M}, g_{\mathrm{M}})$, the embedding of $\mathrm{Diff}(\mathcal{M})$ into $\mathrm{Aut}(\xi_{\mathrm{F}})$ becomes non-trivial. In other words, there is an inner automorphism on $\mathrm{End}(\mathcal{E})$, induced by α, such that $\gamma' = \widetilde{\alpha} \circ \gamma \circ \widetilde{\alpha}^{-1}$. Here, $\gamma'|_{TM} \equiv \gamma|_{TM} \circ T\alpha^{-1}$ is the Clifford action on $\alpha^{-1*}\xi_{\mathrm{F}}$ that is defined with respect to $\alpha^{-1*}g_{\mathrm{M}}$ and $\widetilde{\alpha} \in \mathrm{End}(\mathcal{E})$ an appropriate lift of α.

As a consequence, one obtains

$$\begin{gathered} \mathrm{Diff}(\mathcal{M}) \hookrightarrow \mathrm{Aut}(\xi_{\mathrm{F}}), \\ \alpha \mapsto (\alpha, \beta := \widetilde{\alpha}). \end{gathered} \tag{17}$$

We call the image of this embedding the "outer gauge group" of the fermion bundle ξ_{F}. It is denoted by $\mathcal{G}_{\mathrm{ex}}$.

Finally, since $\mathcal{G}_{\mathrm{in}} \subset \mathcal{G}_{\mathrm{F}}$ is normal and $\mathcal{G}_{\mathrm{in}} \cap \mathcal{G}_{\mathrm{ex}} = \{e\}$, one ends up with the semidirect decomposition of the automorphism group into the gauge and diffeomorphism group, i.e.,

$$\mathcal{G}_{\mathrm{F}} = \mathcal{G}_{\mathrm{in}} \rtimes \mathcal{G}_{\mathrm{ex}}. \tag{18}$$

In fact, each $g \in \mathcal{G}_{\mathrm{F}}$ may be written as $g = g_{\mathrm{in}} g_{\mathrm{ex}} \in \mathcal{G}_{\mathrm{in}} \rtimes \mathcal{G}_{\mathrm{ex}}$ such that

$$\mathcal{G}_{\mathrm{F}} \ni gg' = (g_{\mathrm{in}} g_{\mathrm{ex}})(g'_{\mathrm{in}} g'_{\mathrm{ex}}) \equiv (g_{\mathrm{in}} g_{\mathrm{ex}} g'_{\mathrm{in}} g_{\mathrm{ex}}^{-1})(g_{\mathrm{ex}} g'_{\mathrm{ex}}) \in \mathcal{G}_{\mathrm{in}} \rtimes \mathcal{G}_{\mathrm{ex}}. \tag{19}$$

We call the automorphism group $\mathcal{G}_{\mathrm{F}} \equiv \mathrm{Aut}(\xi_{\mathrm{F}})$ the "(fermionic) gauge group" of the fermion bundle ξ_{F}.

In order to define a $\mathcal{G}_{\mathrm{F}}$–covariant theory (by which we mean that symbolically $\mathcal{L} \circ (\alpha, \beta) = \alpha^{-1^*}\mathcal{L}$, where $\mathcal{L}$ is an appropriate "Lagrangian density" defining the theory) we first consider, for a given fermion bundle ξ_{F}, the canonical mapping

$$V_{\mathrm{D}} : \mathcal{D}(\xi_{\mathrm{F}}) \to \mathcal{C}^{\infty}(\mathcal{M})$$

$$D' \mapsto \mathrm{tr}(D'^2 - \triangle'_{\mathrm{D}}), \tag{20}$$

which is called the "Dirac potential" on ξ_{F}. Here again, the second order differential operator $\triangle'_{\mathrm{D}}$ denotes the Bochner-Laplacian that is uniquely defined with respect to D' such that $\triangle'_{\mathrm{D}} + (D'^2 - \triangle'_{\mathrm{D}})$ is the (general) Lichnerowicz decomposition of D'^2 (c.f. in Refs. 3 and 21).

The universal top form

$$\mathcal{L}_{\mathrm{D}} : \mathcal{D}(\xi_{\mathrm{F}}) \to \Omega^n(\mathcal{M}),$$

$$D' \to * V_{\mathrm{D}}(D') \tag{21}$$

is called the "Dirac-Lagrangian" on the fermion bundle ξ_{F}. This canonical mapping is universal in the sense that it is indeed covariant with respect to the action of $\mathcal{G}_{\mathrm{F}}$. In particular, it is invariant with respect to the action of the inner gauge group $\mathcal{G}_{\mathrm{in}} \subset \mathcal{G}_{\mathrm{F}}$.

Definition 2.3: *Let ξ_{F} be the fermion bundle with respect to the data $(\mathrm{G}, \rho_{\mathrm{F}}, D)$. We call* (*the* "*bosonic part*" *of*) *the theory defined by the corresponding Lagrangian density $\mathcal{L}_{\mathrm{D}}(D) \in \Omega^n(\mathcal{M})$ a* "*gauge theory of Dirac type*".

Let again $\mathcal{A}(\xi_{\mathrm{F}})$ be the set of all linear connections on ξ_{F} and $\mathcal{A}_{\mathrm{D}}(\xi_{\mathrm{F}}) \subset \mathcal{A}(\xi_{\mathrm{F}})$ be the subset of all connections which yield D (i.e., $\gamma \circ \nabla^{\mathcal{E}} = D$, with $\nabla^{\mathcal{E}}$ a corresponding covariant derivative). Then, the top form $\mathcal{L}_{\mathrm{D}}(D) \in \Omega^n(\mathcal{M})$ is indeed well-defined on the moduli-space $\mathfrak{M}_{\mathrm{D}}(\xi_{\mathrm{F}}) \equiv \mathcal{A}_{\mathrm{D}}(\xi_{\mathrm{F}})/\mathcal{G}_{\mathrm{in}}$. Moreover, it transforms covariantly with respect to the (left) action of the fermionic gauge group $\mathcal{G}_{\mathrm{F}}$, i.e.,

$$\mathcal{L}'_{\mathrm{D}}(\beta \circ D \circ \beta^{-1}) = (\alpha^{-1^*}\mathcal{L}_{\mathrm{D}})(D). \tag{22}$$

To obtain an explicit formula for the top form $\mathcal{L}_{\mathrm{D}}(D)$ associated with a Dirac type operator D, one could use the generalized Bochner-Lichnerowicz-Weizenböck formula of $D^2 - \triangle_{\mathrm{D}} \in \Gamma(\mathrm{End}(\xi_{\mathrm{F}}))$. As a consequence, the Dirac potential reads

$$V_{\mathrm{D}}(D) = \mathrm{tr}(\gamma(\mathcal{F}_D) + \mathrm{ev}_{g_{\mathrm{M}}}(\partial_D^{T^*\mathcal{M} \otimes \mathrm{End}(\mathcal{E})} \Xi + \Xi^2)). \tag{23}$$

Here, respectively, $\mathcal{F}_D \in \Omega^2(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ is the total curvature with respect to the Dirac connection $A_{\mathrm{D}} \in \mathcal{A}(\xi_{\mathrm{F}})$ and the one-form $\Xi \in \Omega^1(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ measures the deviation of A_{D} from being a Clifford connection. With respect to a local co-frame $(X^1, \ldots, X^n)$ on $\mathcal{M}$ this one-form reads

$$\Xi \overset{loc.}{=} -\tfrac{1}{2} g_{li} X^l \otimes \gamma(X^j)([\partial_{D,X_j}, \gamma(X^i)] + \omega^i_{jk} \gamma(X^k)), \tag{24}$$

where $(X_1, \ldots, X_n)$ is the dual frame of $(X^1, \ldots, X^n)$ and $\omega^i_{jk} := X^i(\nabla^{TM}_{X_j} X_k)$ are the corresponding Levi-Civita connection coefficients with respect to g_{M} and the chosen frame. Again, $g_{ij} \in \mathcal{C}^{\infty}(U_\alpha)$ is the matrix element of $(g_{\mathrm{M}}(X^i, X^j))^{-1}$. Also, $\mathrm{ev}_{g_{\mathrm{M}}}$ denotes the evaluation map (contraction) with respect to the isomorphism $\tau^*_{\mathrm{M}} \simeq \tau_{\mathrm{M}}$ of the tangent and the cotangent bundle of $\mathcal{M}$ that is provided by g_{M} (c.f. Refs. 1 and 45).

Remark: Let again, $\{(U_\alpha, \chi_\alpha) \,|\, \alpha \in \Lambda\}$ be a family of local trivializations of a given fermion bundle ξ_{F}. According to (10), *$D_\alpha := \chi_\alpha \circ D \circ \chi_\alpha^{-1}$ is fully determined by $(\gamma_\alpha, A_\alpha, \theta_\alpha)$. Hence, $\mathcal{A}_{\mathrm{D}}(\xi_{\mathrm{F}}) \subset \mathcal{A}(\xi_{\mathrm{F}})$ may locally be identified with the set of differential forms ω_α*

$\in \Omega^*(U_\alpha, \mathrm{End}(\mathbb{C}^N))$ *which, together with* $g^{ik} \in \mathcal{C}^\infty(U_\alpha)$, *determine* D_α. *Accordingly, the Euler-Lagrange equations*

$$\mathcal{EL}_D(D) = 0 \tag{25}$$

are obtained by the first variation of the (*locally defined*) *functional* ($\Omega \subset U_\alpha$, *compact*)

$$\mathcal{S}[\gamma_\alpha, A_\alpha, \theta_\alpha] := \int_\Omega \mathcal{L}(\gamma_\alpha, A_\alpha, \theta_\alpha), \tag{26}$$

with $\mathcal{L}(\gamma_\alpha, A_\alpha, \theta_\alpha) \equiv (\chi_\alpha^{-1*}\mathcal{L}_D)(D) \in \Omega^n(U_\alpha)$. *Notice, however, it can easily be inferred from the local version of the Dirac potential* (20) that $\mathcal{S} = \mathcal{S}[\gamma_\alpha, \theta_\alpha]$. *Indeed, the local version of* (23) *reads*

$$V(\gamma_\alpha, A_\alpha, \theta_\alpha) \equiv (\chi_\alpha^{-1*}V_D)(D) = \tfrac{N}{2} r_M + \tfrac{1}{2}\,\mathrm{tr}([\gamma_\alpha^j, \gamma_\alpha^j][\theta_{\alpha,i}, \theta_{\alpha,j}]) + \tfrac{1}{8} g_{ij}\mathrm{tr}(\gamma_\alpha^k[\theta_{\alpha,k}, \gamma_\alpha^j]\gamma_\alpha^j[\theta_{\alpha,l}, \gamma_\alpha^j]). \tag{27}$$

The notation used is as follows: $\theta_\alpha \equiv X^i \otimes \theta_{\alpha,i} := \pm(1/n) g_{\mu\nu} \Sigma_{0 \leqslant k \leqslant n} \Sigma_{1 \leqslant i_1 < i_2 \cdots < i_k \leqslant n} X^\mu \otimes \gamma_\alpha^\nu \gamma_\alpha^{j_1} \gamma_\alpha^{j_2} \cdots \gamma_\alpha^{j_k} \otimes \theta_{i_1 i_2 \cdots i_k}$, *with the abbreviation* $\gamma_\alpha^j := \gamma_\alpha(X^i) \equiv \chi_\alpha \circ \gamma(X^i) \circ \chi_\alpha^{-1}$. *Moreover,* $r_M \in \mathcal{C}^\infty(\mathcal{M})$ *denotes the scalar curvature of* $\mathcal{M}$ *with regard to* g_M.

It follows that Einstein's field equation of gravity is an integral part of the Euler-Lagrange equations of Dirac type gauge theories. In particular, the "energy-momentum tensor" is specified by the Dirac type operator in question (i.e., locally fixed by the one-form $\theta \in \Omega^1(U, \mathrm{End}(\mathcal{E}))$).

In the next section we discuss a specific class of Dirac type operators which is distinguished by its Lichnerowicz decomposition (c.f. Ref. 30). Moreover, it is shown that, as a solution of the Euler-Lagrange equations, these Dirac type operators spontaneously break the gauge symmetry.

III. SIMPLE TYPE DIRAC OPERATORS AND SPONTANEOUS SYMMETRY BREAKING

In what follows we discuss a specific class of Dirac type gauge theories. The main feature of this class consists of permitting us to naturally include the notion of "spontaneous symmetry breaking" in the realm of Dirac type gauge theories. Eventually, we will show that the Yukawa coupling of the fermions, together with gravity, induces spontaneous symmetry breaking without use of a "Higgs potential." The inner geometry of $\mathcal{M}$ (i.e., of space-time in the case of $(n,s) = (4, \mp 2)$) in the "ground state" of the gauge theory is fully determined (up to boundary conditions) by the "fermionic masses." Here, the latter are shown to correspond to the spectrum of a certain Hermitian section of the bundle $\mathrm{End}(\xi_F)$. Because this spectrum turns out to be constant over $\mathcal{M}$ one may thus decompose the fermion bundle ξ_F into the Whitney sum of the appropriate eigenbundles of the "fermionic mass operator" that is induced by spontaneous symmetry breaking. If the spectrum is non-degenerated (like in the case of the Standard Model) the eigenbundles are Hermitian line bundles which one may consider to geometrically model "asymptotically free fermions."

Let ξ_F be a chiral fermion bundle with respect to some Dirac triple (G, ρ_F, D).

Definition 3.1: A Dirac type operator $D' \in \mathcal{D}(\xi_F)$ *is called of "simple type" if the Bochner-Laplacian of* D' *is defined by a Clifford connection, i.e.,* $\hat{A}'_D \in \mathcal{A}_{Cl}(\xi_F) \subset \mathcal{A}(\xi_F)$.

We denote the corresponding covariant derivative again by ∂_A. As a result, the covariant derivative of the Dirac connection $A'_D \in \mathcal{A}(\xi_F)$ reads

$$\partial_{D'} = \partial_A + \varpi'_D \tag{28}$$

with a unique one-form $\varpi'_D \in \Omega^1(\mathcal{M}, \mathrm{End}(\mathcal{E}))$. The next Proposition permits us to characterize the Dirac forms of simple type Dirac operators of arbitrary signature.

Proposition 3.1: A Dirac type operator $D' \in \mathcal{D}(\xi_F)$ *is of simple type if and only if it reads*

$$D' = \not{\partial}_A + \gamma_M \otimes \phi, \tag{29}$$

with $\phi \in \Gamma(\mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$.

Proof: The proof of the statement is lengthy and somewhat technical though elementary. It is similar to the proof already presented in Ref. 1 for the special case $s=n$. A detailed proof for arbitrary signature s can be found in the Appendix. □

Note that a simple type Dirac operator is fully determined by a Clifford connection in the case where ξ_{F} is not chiral and thus has a vanishing Dirac form. In general, however, the Dirac connection of a simple type Dirac operator is given by a unique Clifford connection $A \in \mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ together with the specific Dirac form

$$\varpi'_{\mathrm{D}} = \Theta \wedge (\gamma_{\mathrm{M}} \otimes \phi). \tag{30}$$

With respect to a local trivialization (U_α, χ_α) of ξ_{F} the Dirac form is determined by

$$\theta_\alpha = \pm \tfrac{1}{n} g_{ij} X^i \otimes \gamma^j_\alpha \gamma_{\mathrm{M}} \otimes \phi_\alpha, \tag{31}$$

with $1 \otimes \phi_\alpha := \chi_\alpha \circ (1 \otimes \phi) \circ \chi_\alpha^{-1} \in \mathcal{C}^\infty(U_\alpha, \mathrm{End}^-(\mathbb{C}^{\mathrm{N_F}}))$ and $\theta_\alpha \equiv \chi_\alpha^{-1*} \varpi'_{\mathrm{D}}$.

Dirac operators of simple type define the largest class of Dirac type operators with the corresponding Bochner-Laplace operators defined by Clifford connections. Of course, the most important subclass of Dirac type operators is given by $D' = \not{\partial}_A$. They correspond to "twisted spin Dirac operators" in the case where $\mathcal{M}$ denotes a spin manifold. Notice that in the elliptic case, Dirac operators of simple type turn out to be of importance in the discussion of the family index theorem (c.f. Refs. 4 and 41). They are also known to play a fundamental role in the description of the minimal Standard Model within the realm of noncommutative geometry (please see, e.g., the corresponding references already cited in Sec. I). This kind of first order differential operator is thus well known in physics (please, see the following), as well as in mathematics. However, in this article we discuss them from a purely geometrical perspective of gauge theories.

We turn now to the discussion of spontaneous symmetry breaking within the realm of the presented geometrical frame. For this let again ξ_{F} be a chiral fermion bundle with respect to $(\mathrm{G}, \rho_{\mathrm{F}}, D)$ where D is of simple type.

Proposition 3.2: Let D be a global solution of the Euler-Lagrange equation

$$\mathcal{EL}_{\mathrm{D}}(D) = 0 \tag{32}$$

such that $\mathcal{G}_{\mathrm{YM}}$ *acts transitively on the image of* $D - \not{\partial}_A$. *Consequently*, *there exists a constant* (*skew-Hermitian*) *section* $\mathcal{D} \in \Gamma(\mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$ *such that* $(\mathcal{M}, g_{\mathrm{M}})$ *is an Einstein manifold with the scalar curvature given by*

$$r_{\mathrm{M}} = \lambda \|\mathrm{M_F}\|^2. \tag{33}$$

Here, $\|\mathrm{M_F}\|^2 \equiv \mathrm{tr}(\mathrm{M_F^\dagger M_F})$ *with* $i\mathrm{M_F} := \gamma_{\mathrm{M}} \otimes \mathcal{D}$ *representing the* "*total fermionic mass operator*"; $\lambda \in \mathbb{R}$ *is an appropriate nonzero constant which may also depend on a suitable normalization of* $\mathcal{L}_{\mathrm{D}}(D)$.

Proof: The Dirac-Lagrangian of a simple type Dirac operator reads

$$\mathcal{L}_{\mathrm{D}}(D) = 2^k (\mathrm{N_F} r_{\mathrm{M}} + \mathrm{tr}\,\phi^2) \mu_{\mathrm{M}}. \tag{34}$$

We remark that this Lagrangian depends on the connection that is defined only with respect to (g_{M}, ϕ). Moreover, the Euler-Lagrange equation concerning $\phi \in \Gamma(\mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$ is trivial. Whence, one may conclude that a global solution of (32) yields: $D = \not{\partial}_A$ with $A \in \mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ arbitrary and $(\mathcal{M}, g_{\mathrm{M}})$ Ricci flat. However, there is actually a bigger class of solutions of (32). As the latter does not provide any dynamical condition on the sections ϕ one may treat the latter as "background fields", similar to the metric in the case of pure Yang-Mills gauge theory. The Euler-Lagrange equations with respect to the corresponding Dirac-Lagrangian then reduces to the Einstein equation

$$\mathrm{Ric}(g_{\mathrm{M}}) = \lambda_{\mathrm{gr}} \mathrm{tr}\phi^2 \mathrm{id}_{\mathrm{TM}} \tag{35}$$

with $\lambda_{\mathrm{gr}} \in \mathbb{R}$ being some nonzero constant which also depends on the chosen normalization of $\mathcal{L}_{\mathrm{D}}(D)$. It also takes into account the appropriate physical (length) dimension, where ϕ is accordingly rescaled. The section $\mathrm{Ric} \in \Gamma(\mathrm{End}(\tau_{\mathrm{M}}))$ denotes the Ricci tensor with respect to g_{M}. From the Einstein equation it follows that $\mathrm{d}(\mathrm{tr}\,\phi^2)=0$. Hence, the Dirac-Lagrangian (34) of a simple type Dirac operator reduces, in general, to the Einstein-Hilbert Lagrangian with a "cosmological constant" included. This constant is generated by a section $\phi \in \Gamma(\mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$ subject to the condition that $\|\phi\|^2 := <\phi,\phi> \equiv \mathrm{tr}(\phi^\dagger\phi)$ must be constant. Note that $\phi^\dagger = \pm\phi$, depending on whether D is supposed to be Hermitian or skew-Hermitian. The basic idea here is to make a polar decomposition $\phi \overset{loc.}{=} \rho_{\mathrm{F}}(g)\circ\mathcal{D}\circ\rho_{\mathrm{F}}(g)^{-1}$ with $\mathcal{D}$ being a fixed vector of the same length as ϕ. To make this more precise let $\mathcal{W} := \mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ be the Hermitian vector bundle of (complex) rank $\mathrm{N}_{\mathrm{F}}^2$ with total space $W := \mathrm{End}^-_{\mathrm{Cl}}(\mathcal{E})$. Accordingly, let $\mathfrak{P} := (P,\mathcal{M},\pi_{\mathrm{P}})$ be the frame bundle associated with $\mathcal{W}$. Also, let $\mathfrak{E} := (E,\mathcal{M},\pi_{\mathrm{E}})$ be the associated Hermitian vector bundle with total space defined by $E := P\times_{\mathrm{G}}\mathrm{End}(\mathbb{C}^{\mathrm{N_F}})$. By construction $\mathfrak{E} \simeq \mathcal{W}$, and we do not distinguish between these two vector bundles. In particular, we may write $W \ni \mathfrak{Z} = [(p,\mathfrak{z})]$. Equivalently, if $\phi \neq 0$ we may consider the normalized section $\varphi := \phi/\|\phi\| \in \Gamma(\mathcal{S})$ with $\mathcal{S} \subset \mathcal{W}$ being the sphere sub-bundle. According to the identification $\mathfrak{E} \simeq \mathcal{W}$ any section φ corresponds to a G-equivariant mapping $\tilde{\varphi}: P \to \mathrm{S}^{\mathrm{N}'-1}$ ($\mathrm{N}' = 2\mathrm{N}_{\mathrm{F}}^2$), such that $\varphi(x) = [(p,\tilde{\varphi}(p)]\big|_{p\in\pi_{\mathrm{P}}^{-1}(x)}$. By assumption, G acts transitively on $\mathrm{im}(\tilde{\varphi}) \subset \mathrm{S}^{\mathrm{N}'-1}$. Hence, for arbitrarily chosen $\mathfrak{z}_0 \in \mathrm{im}(\tilde{\varphi})$ we may identify the orbit of $\mathfrak{z}_0$, $\mathrm{orbit}(\mathfrak{z}_0)$, with $\mathrm{im}(\tilde{\varphi})$. Let $\mathrm{I}(\mathfrak{z}_0) \subset \rho_{\mathrm{F}}(\mathrm{G})$ be the isotropy group of $\mathfrak{z}_0$. The mapping

$$\nu_\phi : P \to \mathrm{orbit}(\mathfrak{z}_0).$$

$$p \mapsto \rho_{\mathrm{F}}(g)\mathfrak{z}_0\rho_{\mathrm{F}}(g^{-1}), \tag{36}$$

defines an "H-reduction" $(\mathcal{Q}_\phi, \iota_\phi)$ of $\mathfrak{P}$ with $g \in \mathrm{G}$ being determined (modulo $\mathrm{I}(\mathfrak{z}_0)$) by the relation $\tilde{\varphi}(pg) = \mathfrak{z}_0$. Indeed, the corresponding section

$$\mathcal{V}_\phi : \mathcal{M} \to P\times_{\mathrm{G}}\mathrm{G/H}$$

$$x \mapsto \left[(p,\nu_\phi(p))\right]\Big|_{p\in\pi_{\mathrm{P}}^{-1}(x)} \tag{37}$$

is known to be equivalent to a specific principal H-bundle $\mathcal{Q}_\phi \equiv (Q,\mathcal{M},\pi_{\mathrm{Q}},\mathrm{H})$ together with an equivariant embedding $\iota_\phi : \mathcal{Q}_\phi \hookrightarrow \mathcal{P}$ of principal bundles (c.f., e.g., Ref. 29). For "bundle reduction" in the context of Yang-Mills-Higgs gauge theories see also, e.g., Refs. 11, 43, and 49. Here, $\mathrm{H} \subset \mathrm{G}$ is the unique sub-group equivalent to $\mathrm{I}(\mathfrak{z}_0)$, and thus $\mathrm{orbit}(\mathfrak{z}_0) \simeq \mathrm{G/H}$. Finally, we may define $\mathcal{D} \in \Gamma(\mathrm{End}^-_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$ by the section

$$\mathcal{D} : \mathcal{M} \to E$$

$$x \mapsto [(\iota_\phi(q),\mathfrak{z}_0)]\big|_{q\in\pi_{\mathrm{Q}}^{-1}(x)}. \tag{38}$$

Of course, the section $\mathcal{D}$ also gives rise to an (equivalent) H-reduction $(\mathcal{Q},\iota)$ of $\mathfrak{P}$ which may be identified with $(\mathcal{Q}_\phi,\iota_\phi)$ by $\mathrm{H} \simeq \mathrm{I}(\tilde{g}\mathfrak{z}_0\tilde{g}^{-1})$. Here, $\tilde{g} \in \mathrm{G}$ is determined (up to $\mathrm{I}(\mathfrak{z}_0)$) by a choice of $q_0 \in \mathcal{Q}_\phi$ and the corresponding relation $\varphi(\iota_\phi(q_0)) \equiv \tilde{\mathfrak{z}}_0 =: \tilde{g}\mathfrak{z}_0\tilde{g}^{-1}$. The rest of the statement is a direct consequence of the Einstein equation. □

A simple type Dirac operator D is said to be in the unitary gauge provided it reads

$$D = \not{\partial}_A + \gamma_{\mathrm{M}} \otimes \mathcal{D}. \tag{39}$$

A necessary condition for the existence of the unitary gauge is that $D-\not{b}_A \neq 0$. If $\mathcal{G}_{\mathrm{YM}}$ acts transitively on the image of the latter operator, this condition is also sufficient. A simple type Dirac operator in the unitary gauge spontaneously breaks the Yang-Mills gauge symmetry since in general

$$\mathcal{H}_{\mathrm{YM}} := \{g \in \mathcal{G}_{\mathrm{YM}} | [\mathcal{D}, g] = 0\} \tag{40}$$

is a proper sub-group of the Yang-Mills gauge group $\mathcal{G}_{\mathrm{YM}} \subset \mathcal{G}_{\mathrm{F}}$. In this case, the Lagrangian $\mathcal{L}_{\mathrm{D}}(D)$ is said to define a "spontaneously broken fermionic gauge theory." Note that in the case where $\mathcal{G}_{\mathrm{YM}}$ acts transitively on the sphere subbundle $\mathcal{S} \subset \mathrm{End}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ any global solution of (32) satisfying $D-\not{b}_A \neq 0$ defines a spontaneously broken fermionic gauge theory.

Remark: The notion of unitary gauge and its existence is similar to that presented in (Ref. 46) (Proposition 3.2) *in the case of rotationally symmetric Higgs potentials. However, the* "*mass term*" $\|\phi\|^2$ *in the Lagrangian of a simple type Dirac operator itself does not break the symmetry, of course. The symmetry breaking is caused by assuming that the fermionic mass generates a non-trivial geometry. Indeed, the geometry is fully determined by the spectrum of the* (*square of the*) *fermionic mass operator* $\mathrm{M}_{\mathrm{F}}^2 \in \Gamma(\mathrm{End}(\xi_{\mathrm{F}}))$. *Also, since the spectrum* $\mathrm{spec}(\mathrm{M}_{\mathrm{F}}^2)$ *is constant throughout* $\mathcal{M}$, *one may decompose the fermion bundle into the Whitney sum of the corresponding eigenbundles of* $\mathrm{M}_{\mathrm{F}}^2$, *i.e.* (c.f. Ref. 47),

$$\xi_{\mathrm{F}} = \bigoplus_{\mathrm{m}^2 \in \mathrm{spec}(\mathrm{M}_{\mathrm{F}}^2)} \xi_{\mathrm{F},\mathrm{m}^2} = \ker(\mathrm{M}_{\mathrm{F}}^2) \oplus \left[\bigoplus_{\mathrm{m}^2 \in \mathrm{spec}(\mathrm{M}_{\mathrm{F}}^2)\setminus\{0\}} \xi_{\mathrm{F},\mathrm{m}^2} \right]. \tag{41}$$

The total curvature on ξ_{F} *with respect to a simple type Dirac operator satisfying* (32) *is given by*

$$\mathcal{F}_D = \not{R} + F_A + \mathrm{M}_{\mathrm{F}}^2 \Theta \wedge \Theta - \partial_A^{\mathrm{End}(\mathcal{E})} \mathrm{M}_{\mathrm{F}} \wedge \Theta. \tag{42}$$

Here, respectively, $\not{R} \in \Omega^2(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ *is the lifted* (*semi-*)*Riemannian curvature with respect to* g_{M}, *and* $F_A \equiv \mathcal{F}_{\not{b}_A} - \not{R} \in \Omega^2(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ *is the* "*twisting curvature*" *with respect to the Clifford connection* $A \in \mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$ *that is determined by D. In contrast to* $\not{R}$, *which is determined by the spectrum of* $\mathrm{M}_{\mathrm{F}}^2$, *the twisting curvature* F_A *is completely arbitrary. For this reason it is natural to assume that A is purely topological, i.e., flat. In this case, the curvature of* ξ_{F} *is fully determined by the spectrum of the fermionic mass operator. As a consequence, for* $n=4$ *the chiral fermion bundle must indeed be real. If in addition* $\mathcal{M}$ *is a spin manifold, then* $\xi_{\mathrm{F},\mathrm{m}^2} \simeq \tau_{\mathrm{spin}} \otimes_{\mathcal{M}} \zeta_{\mathrm{F},\mathrm{m}^2}$, *where the latter is a Hermitian line bundle if and only if* $\mathrm{spec}(\mathrm{M}_{\mathrm{F}}^2)\setminus\{0\}$ *is non-degenerated. Consequently, when restricted to the residual group H, the fermionic representation* ρ_{F} *decomposes into the sum of the trivial representation and irreducible* $U(1)$*-representations.* (*To date, electromagnetism is the only Abelian gauge theory that is physically well-established. Moreover, as a matter of fact, massless but electrically charged particles are unknown in nature*). *The latter are either trivial, and hence* $\xi_{\mathrm{F},\mathrm{m}^2}$ *corresponds to an electrically uncharged but massive fermion or, for non-trivial representations,* $\xi_{\mathrm{F},\mathrm{m}^2}$ *corresponds to a massive electrically charged particle. Apparently, together with spin, the assumption that the Clifford connection A is flat imposes crucial restrictions on the fermion bundle. In fact, in this case* (*up to algebraic torsion*) $\xi_{\mathrm{F}} \simeq \oplus_{k=1}^{\mathrm{N_F}} \tau_{\mathrm{spin}}$. *Note that, if* $n=4$ *and* $\mathrm{spec}(\mathrm{M}_{\mathrm{F}}^2)$ *is nondegenerate, the existence of a flat Clifford connection on* ξ_{F} (*again, up to torsion*) *becomes equivalent to the reality of the latter.*

Definition 3.2: A fermion bundle ξ_{F} *is said to be in the unitary gauge provided it is defined with respect to a Dirac triple* $(\mathrm{G}, \rho_{\mathrm{F}}, D)$ *such that D is in the unitary gauge. More generally, a fermion bundle is called* "*massive*" *if it is gauge equivalent to a fermion bundle in the unitary gauge. The corresponding element of* $\mathcal{G}_{\mathrm{YM}} \subset \mathcal{G}_{\mathrm{F}}$ *is referred to as a* "*unitary gauge transformation.*"

On a massive fermion bundle there exists a distinguished class of connections.

Definition 3.3: A connection $A \in \mathcal{A}(\xi_{\mathrm{F}})$ *on a massive fermion bundle* ξ_{F} *is called compatible with D provided the corresponding covariant derivative* $\nabla^{\mathcal{E}}$ *commutes with the appropriate total fermionic mass operator. That is,*

$$\nabla_X^{\mathrm{End}(\mathcal{E})} \mathrm{M}_{\mathrm{F}} = 0 \tag{43}$$

for all smooth tangent vector fields $X \in \Gamma(\tau_M)$.

This definition expresses the H-reducibility of a connection on ξ_F in terms of Dirac type operators which spontaneously break the gauge symmetry. The Definition (3.3) is in fact analogous to the Definition 2.1 in Ref. 46 for a spontaneously broken Yang-Mills-Higgs gauge theory. Note that (43) is equivalent to the condition

$$D' \circ M_F = - M_F \circ D', \tag{44}$$

with $D' \in \mathcal{D}(\xi_F)$ being identified with $\gamma \circ \nabla^{\mathcal{E}}$. In particular, one may assume that the Clifford connection which defines the Bochner-Laplacian of $D = \not{\partial}_A + iM_F$ is compatible with the latter. This holds true if and only if

$$D^2 = \not{\partial}_A^2 - M_F^2. \tag{45}$$

Hence, the Clifford connection of the Bochner-Laplacian $\triangle_D$ is compatible with spontaneous symmetry breaking if and only if "the square of the sum equals the sum of the squares." We note that, from a geometrical point of view, it is the condition $\nabla^{\mathrm{End}(\mathcal{E})} M_F \neq 0$ that yields "massive vector bosons" (please see the following). In other words, the existence of a nontrivial "Yang-Mills mass operator" can be expressed by the violation of compatibility condition (45).

Definition 3.4: We consider a Dirac operator D of simple type to define a "(*semi-classical*) *fermionic vacuum*" *if D is gauge equivalent to* $\not{\partial}_A + iM_F$ *where the corresponding Clifford connection* $A \in \mathcal{A}(\xi_F)$ *is purely topological. In this case*, *D in the unitary gauge is denoted by*

$$\not{\partial}_{\mathcal{D}} \equiv \not{\partial} + iM_F. \tag{46}$$

Clearly, when restricted to the appropriate eigenbundles this operator corresponds to Dirac's well-known first order differential operator $i\not{\partial} - m$ and thus provides us with the appropriate physical interpretation of $\mathrm{spec}(M_F^2)$ (and hence also with $\mathcal{D}$). For example, in the case of $(n,s) = (4, \mp 2)$ there is always a local frame such that the total symbol $\sigma(i\not{\partial}_{\mathcal{D}})$ coincides with the principal symbol of (46). Every time-like $\xi \in T^*\mathcal{M} \subset \mathrm{End}(\mathcal{E})$ and eigenvector $\mathfrak{z} \in \mathcal{E}$ of M_F^2 (with eigenvalue m^2) yields $\sigma(i\not{\partial})(\xi)\mathfrak{z} \overset{loc}{=} \gamma(\xi)\mathfrak{z} = \pm m\mathfrak{z}$. Hence, one obtains the usual relation between momentum and mass: $g_M(\xi,\xi) = \pm m^2$ of a point-like particle.

From a geometrical point of view a fermionic vacuum may be regarded as a fermion bundle $\xi_{F,\mathrm{red}} := (\mathcal{E}_{\mathrm{red}}, \mathcal{M}, \pi_{\mathcal{E},\mathrm{red}})$ with respect to the Dirac triple $(H, \rho_{F,\mathrm{red}}, \not{\partial}_{\mathcal{D}})$. Here, respectively, $\mathcal{E}_{\mathrm{red}} := Q \times_H \mathbb{C}^{2^k} \otimes \mathbb{C}^{N_F}$ and $\rho_{F,\mathrm{red}} := \rho_F|_H$. Notice that $\xi_F \simeq \xi_{F,\mathrm{red}}$ via the bundle mapping $[(q,z)] \mapsto [(\iota(q),z)]$. Accordingly, we shall not distinguish between these two bundles and proceed to say that a fermion bundle ξ_F can be generated from a fermionic vacuum if it is determined by a Dirac triple of the form $(H, \rho_{F,\mathrm{red}}, \not{\partial}_{\mathcal{D}})$. In other words, ξ_F is generated from a fermionic vacuum provided the corresponding frame bundle $\mathcal{P}$ can be considered as a prolongation of the frame bundle $\mathcal{Q}$ that corresponds to some fermion bundle $\xi_{F,\mathrm{red}}$. Finally, the Dirac potential of a fermionic vacuum has the particular simple form (c.f. Ref. 47)

$$V_D(\not{\partial}_{\mathcal{D}}) = \frac{\lambda}{2} < M_F^2 >, \tag{47}$$

where $< M_F^2 > := (1/N_F) \Sigma_{a=1}^{N_F} m_a^2$ and $\lambda \in \mathbb{R}$ is a suitable nonzero constant.

The idea of a fermionic vacuum is mainly motivated by a geometrical description of perturbation theory used in quantum field theory. As already mentioned the fermion bundle ξ_F is considered as a "perturbation" of a fermionic vacuum $\xi_{F,\mathrm{red}}$. Such a perturbation cannot change the topology of ξ_F but its geometry. The notion of a fermionic vacuum itself puts severe topological restrictions on a fermion bundle. (One might speculate that "quantum fluctuations" will lead to a change of the topology of the fermionic vacuum for it basically adds "quantum corrections" to the fermionic mass spectrum). Before we explain this in more detail, however, we shall discuss in the next section a more specific class of simple type Dirac operators which takes into account that, within the Standard Model of Particle Physics, the Higgs boson is described by a subrepresenta-

tion of ρ_F instead of the fundamental representation. Moreover, we shall discuss the need for "fermionic doubling" and the fermionic Lagrangian within the presented setup.

IV. DIRAC-YUKAWA OPERATORS AND THE FERMIONIC LAGRANGIAN

In the previous section we discussed a distinguished class of Dirac type operators on a fermion bundle. Their basic feature is to give rise to a reduction of the underlying gauge symmetry. Moreover, these Dirac type operators also determine a distinguished class of connections on the fermion bundle. In the next two sections we specialize the presented frame in order to geometrically describe the action of the Standard Model of Particle Physics in terms of a specific Dirac-Lagrangian. For this, we first discuss a certain "refinement" of simple type Dirac operators which we call "Dirac-Yukawa operators." In what follows, we also discuss an important consequence of the occurrence of the grading involution γ_M in the definition of simple type Dirac operators. This turns out to parallel the occurrence of this grading involution in A. Connes' noncommutative geometry (c.f., e.g., Refs. 12, 22, 23, 28, 31, 32, and 42).

A. Yukawa bundles and Dirac operators of Yukawa type

To start with, let again ξ_F be a chiral fermion bundle with respect to (G,ρ_F,D), where D is of simple type. Also let $\xi_H \subset \xi_F$ be a sub-vector bundle of rank $N_H < N_F$ on which τ_{Cl} acts trivially. We denote its dual by ξ_H^*. The structure group of ξ_H is a specific subgroup of $\rho_F(G)$. It will be denoted by $\rho_H(G)$. The gauge group of ξ_H is accordingly denoted by $\mathcal{G}_H \subset \mathcal{G}_{YM} \subset \mathrm{Aut}(\xi_H) \subset \mathrm{Aut}(\xi_F)$ (the bundle automorphisms of ξ_H over the identity on $\mathcal{M}$.)

Definition 4.1: *Let $E_H \subset \mathcal{E}$ be the total space of ξ_H, and let π_H be the appropriate projection mapping onto the base manifold $\mathcal{M}$. Also, let again $W := \mathrm{End}_{Cl}^-(\mathcal{E})$. We call the subvector bundle $\xi_Y \subset \xi_H^* \otimes_{\mathcal{M}} \xi_W$ the "Yukawa bundle" (with respect to the previous data) if its structure group acts as follows: For each $h \in \mathrm{Aut}(E_H)$ there is a unique $g \in \mathrm{Aut}_{Cl}^+(\mathcal{E})$ such that $\mathcal{Y}(h^{-1}\mathfrak{z}) = \mathrm{Ad}_{g^{-1}}(\mathcal{Y}(\mathfrak{z}))$ for all $\mathfrak{z} \in E_H$ and $\mathcal{Y} \in E_H^* \otimes W$. In this case we call ξ_H the "Higgs bundle" (again, with respect to the previous data). A section $\mathcal{Y} \in \Gamma(\xi_Y)$ of the Yukawa bundle is called a "Yukawa mapping" provided that it fulfills the following conditions: Considered as a bundle mapping the Yukawa mapping $\mathcal{Y}$ is injective and anti-Hermitian, i.e., $\mathcal{Y}(\mathfrak{z})^\dagger = -\mathcal{Y}(\mathfrak{z})$ for all $\mathfrak{z} \in E_H$. Moreover, we assume that it satisfies the requirement $\mathcal{Y}(\partial_{A,X}\varphi) = [\partial_{A,X}, \mathcal{Y}(\varphi)]$ for all Clifford connections on ξ_F (and thus for all induced connections on ξ_H), sections $\varphi \in \Gamma(\xi_H)$ and tangent vector fields $X \in \Gamma(\tau_M)$.*

Note that for each connection on ξ_F with covariant derivative $\nabla^{\mathcal{E}}$, the operator

$$[\nabla_X^{\mathcal{E}}, \mathcal{Y}(\varphi)] - \mathcal{Y}(\nabla_X^{E_H}\varphi) \tag{48}$$

on the fermion bundle ξ_F defines a connection on $\xi_H^* \otimes \xi_W$ with the covariant derivative $\nabla^{E_H^* \otimes W} \equiv \nabla^{E_H^*} \otimes 1 + 1 \otimes \nabla^W$. Hence, a Yukawa mapping is assumed to be covariantly constant with respect to any Clifford connection. By the definition of the Yukawa bundle it then follows that a Yukawa mapping (4.1) has to be a constant section. For instance, in the case of the Standard Model the Yukawa mapping (4.1) is parameterized by the "Yukawa coupling constants." The representations ρ_H and ρ_F are known to be related by the "hypercharges" of the fermions and the Higgs boson.

Definition 4.2: *We call a Dirac type operator D on a fermion bundle ξ_F a "Dirac-Yukawa operator" if there is a section of the Higgs bundle, $\varphi \in \Gamma(\xi_H)$, such that*

$$D = \not{\partial}_A + \gamma_M \otimes \mathcal{Y}(\varphi). \tag{49}$$

According to its physical interpretation we call the section $\mathcal{Y}(\varphi) \in \Gamma(\mathrm{End}_{Cl}^-(\xi_F))$ the "Yukawa coupling term" with respect to $(\mathcal{Y},\varphi) \in \Gamma(\xi_Y \times_{\mathcal{M}} \xi_H)$.

A Yukawa mapping defines an additional data on a fermion bundle which in some sense is not natural within the frame of Dirac type gauge theories. For this reason we shall refer to the data (G,ρ_F,D), with D being a Dirac-Yukawa operator, as a "Dirac-Yukawa model." A necessary condition for a Dirac-Yukawa operator to spontaneously break the underlying gauge symmetry is that $\varphi \in \Gamma(\xi_H)$ does not vanish. Again, this condition is also sufficient provided G acts transitively

on the image of the section $\mathcal{Y}(\varphi)$. Assuming this is the case it follows from the definition of the Higgs bundle and the Yukawa mapping that there must exist a constant section $\mathcal{V} \in \Gamma(\xi_H) \backslash \{\mathcal{O}\}$ (with $\mathcal{O}$ being the zero-section) such that in the unitary gauge

$$D = \partial\!\!\!/_A + \gamma_M \otimes \mathcal{Y}(\mathcal{V}). \tag{50}$$

Analogously to our previous definition we consider a Dirac-Yukawa operator to define a (semiclassical) fermionic vacuum if it is gauge equivalent to $\partial\!\!\!/_{\mathcal{V}} \equiv \partial\!\!\!/ + iM_F$ with the total fermionic mass operator $iM_F := \gamma_M \otimes \mathcal{Y}(\mathcal{V})$. Notice that the spectrum of the total fermionic mass operator is independent of the choice of $\mathfrak{Z}_0 \in \mathrm{End}(\mathbb{C}^{N_F})$. This reduces to $\mathfrak{Z}_0 = G_Y(\mathbf{z}_0)$ in the case where the gauge symmetry is spontaneously broken by a Dirac-Yukawa operator. Here, $G_Y \in \mathrm{Hom}(\mathbb{C}^{N_H}, \mathrm{End}(\mathbb{C}^{N_F}))$ is the matrix of the Yukawa coupling constants and $\mathbf{z}_0 \in \mathbb{C}^{N_H}$. In particular, we obtain $\mathrm{orbit}(\mathfrak{Z}_0) = G_Y(\mathrm{orbit}(\mathbf{z}_0))$. Hence, from the properties of the Yukawa mapping it can be inferred that the "little group" $H \subset G$ crucially depends on $\rho_H \subset \rho_F$.

B. The fermionic Lagrangian

Next, we discuss the fermionic Lagrangian within the presented frame. By definition, the grading involution of a chiral fermion bundle $\xi_F = \xi_F^+ \oplus \xi_F^-$ reads $\Gamma = \gamma_M \otimes \chi$. Consequently, the total space $\mathcal{E}$ of the fermion bundle decomposes as

$$\mathcal{E} = \mathcal{E}^+ \oplus \mathcal{E}^- = (\mathcal{E}_{LL} \oplus \mathcal{E}_{RR}) \oplus (\mathcal{E}_{RL} \oplus \mathcal{E}_{LR}), \tag{51}$$

where, respectively,

$$\begin{aligned}
\mathcal{E}_{LL} &:= \{\mathfrak{z} \in \mathcal{E} | (\gamma_M \otimes 1)\mathfrak{z} = -\mathfrak{z}, (1 \otimes \chi)\mathfrak{z} = -\mathfrak{z}\},\\
\mathcal{E}_{RR} &:= \{\mathfrak{z} \in \mathcal{E} | (\gamma_M \otimes 1)\mathfrak{z} = \mathfrak{z}, (1 \otimes \chi)\mathfrak{z} = \mathfrak{z}\},\\
\mathcal{E}_{RL} &:= \{\mathfrak{z} \in \mathcal{E} | (\gamma_M \otimes 1)\mathfrak{z} = \mathfrak{z}, (1 \otimes \chi)\mathfrak{z} = -\mathfrak{z}\},\\
\mathcal{E}_{LR} &:= \{\mathfrak{z} \in \mathcal{E} | (\gamma_M \otimes 1)\mathfrak{z} = -\mathfrak{z}, (1 \otimes \chi)\mathfrak{z} = \mathfrak{z}\}.
\end{aligned} \tag{52}$$

Let $\pi_{R/L} := \frac{1}{2}(1 \pm (\gamma_M \otimes 1))$ and $\rho_{R/L} := \frac{1}{2}(1 \pm (1 \otimes \chi))$. The appropriate projection mappings of the respective subspaces (52) of $\mathcal{E}$ are denoted by $\pi_{LL} \equiv \pi_L \circ \rho_L = \rho_L \circ \pi_L$, $\pi_{RR} \equiv \pi_R \circ \rho_R = \rho_R \circ \pi_R$, $\pi_{RL} \equiv \pi_R \circ \rho_L = \rho_L \circ \pi_R$ and $\pi_{LR} \equiv \pi_L \circ \rho_R = \rho_R \circ \pi_L$. Consequently, $\pi_+ = \pi_{RR} + \pi_{LL}$ and $\pi_- = \pi_{RL} + \pi_{LR}$. For $\phi \in \Gamma(\mathrm{End}_{Cl}(\xi_F))$ we also define $1 \otimes \phi_{LL} := \rho_L \circ (1 \otimes \phi) \circ \rho_L \in \Gamma(\mathrm{End}_{Cl}(\xi_{F,LL} \oplus \xi_{F,RL})) \simeq \Gamma(\mathrm{End}_{Cl}(\xi_{F,LL})) \oplus \Gamma(\mathrm{End}_{Cl}(\xi_{F,RL}))$, $1 \otimes \phi_{RL} := \rho_R \circ (1 \otimes \phi) \circ \rho_L \in \Gamma(\mathrm{Hom}_{Cl}(\xi_{F,LL} \oplus \xi_{F,RL}, \xi_{F,LR} \oplus \xi_{F,RR})) \simeq \Gamma(\mathrm{Hom}_{Cl}(\xi_{F,LL}, \xi_{F,LR})) \oplus \Gamma(\mathrm{Hom}_{Cl}(\xi_{F,RL}, \xi_{F,RR}))$, etc.

If $\mathcal{M}$ denotes a spin manifold, then $\mathcal{E} \simeq S \otimes E_F$, where S is the total space of the spinor bundle τ_{spin} (with respect to some chosen spin structure) and E_F is the total space of some Hermitian vector bundle ζ_F. In this case, the fermion bundle $\xi_F \simeq \tau_{spin} \otimes \zeta_F$ is chiral if and only if ζ_F is $\mathbb{Z}_2$−graded, i.e., $E_F = E_{F,R} \oplus E_{F,L}$. Here, $E_{F,R/L}$ are considered as the eigenspaces of χ with respect to the eigenvalues ± 1. Then, for instance, $\mathcal{E}_{LL} \simeq S_L \otimes E_{F,L}$, etc. Consequently, like in noncommutative geometry, the fermionic degrees of freedoms are doubled in the geometrical description presented here (c.f. again the corresponding discussion in Refs. 31 and 32). Indeed, as far as the Standard Model is concerned only

$$\mathcal{E}_{phy} \equiv \mathcal{E}^+ = (\mathcal{E}_{LL} \oplus \mathcal{E}_{RR}) \tag{53}$$

represents the "true" physical degrees of freedom.

With this in mind the "fermionic Lagrangian" of D may be defined as the following specific quadratic form on $\Gamma(\xi_F)$ (taking its value in the top forms of $\mathcal{M}$):

$$\mathcal{L}_F : \mathcal{D}(\xi_F) \to \Gamma(\xi_F \otimes_{\mathcal{M}} \Lambda^n \tau_M^*)$$

$$D \mapsto \begin{cases} \Gamma(\xi_{\mathrm{F}}) & \to & \Omega^{\mathrm{n}}(\mathcal{M}) \\ \psi & \mapsto & <\psi, D_+\psi>_{\mathcal{E}}\mu_{\mathrm{M}}. \end{cases} \tag{54}$$

Here, $<\cdot,\cdot>_{\mathcal{E}}$ is the Hermitian product on $\mathcal{E}$ and $D_\pm \equiv \pi_{\mp}\circ D\circ \pi_\pm : \Gamma(\xi_{\mathrm{F}}^{\pm}) \to \Gamma(\xi_{\mathrm{F}}^{\mp})$ such that $D \in \mathcal{D}(\xi_{\mathrm{F}})$ reads

$$D = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix} : \begin{matrix} \Gamma(\xi_{\mathrm{F}}^{+}) \\ \oplus \\ \Gamma(\xi_{\mathrm{F}}^{-}) \end{matrix} \to \begin{matrix} \Gamma(\xi_{\mathrm{F}}^{+}) \\ \oplus \\ \Gamma(\xi_{\mathrm{F}}^{-}) \end{matrix}. \tag{55}$$

It is common use to also refer to the operators $D_\pm$ themselves as Dirac type operators although the square of these operators is usually not defined. (Equivalently, if, for instance, the operator $D_+ : \Gamma(\xi_{\mathrm{F}}^{+}) \to \Gamma(\xi_{\mathrm{F}}^{-})$ is identified by the operator $\begin{pmatrix} 0 & 0 \\ D_+ & 0 \end{pmatrix} : \Gamma(\xi_{\mathrm{F}}) \to \Gamma(\xi_{\mathrm{F}})$ it follows that $D_+^2 \equiv 0$. Hence, it is not a Dirac type operator in the sense presented here. However, every (anti-) symmetric Dirac type operator D is fully determined by D_+.) The Hermitian product on $\mathcal{E}$ depends on the signature of D. For instance, in the respective cases of Lorentzian and Euclidean signature the following is obtained for all $\mathfrak{z}, \mathfrak{z}' \in \mathcal{E}$:

$$<\mathfrak{z}, \mathfrak{z}'>_{\mathcal{E}} := \begin{cases} \overline{\mathfrak{z}}_-\mathfrak{z}'_+ + \overline{\mathfrak{z}}_+\mathfrak{z}'_- & \text{(Lorentzian sign.)} \\ \overline{\mathfrak{z}}_+\mathfrak{z}'_+ + \overline{\mathfrak{z}}_-\mathfrak{z}'_- & \text{(Euclidean sign.)}, \end{cases}$$

where $\overline{\mathfrak{z}}$ means either the Dirac or Hermitian conjugate of the "spinor degrees" of freedom of $\mathfrak{z}$. More precisely, let $\pi : \mathrm{F}\mathcal{E} \to \mathcal{M}$ be the frame bundle of ξ_{F}, such that $\mathcal{E} \ni \mathfrak{z} \simeq [(p, \mathbf{z} = \Sigma_{i=1}^{2^{\mathrm{k}}} \mathbf{s}_i \otimes \mathbf{z}_i)] \in \mathrm{F}\mathcal{E} \times_{\mathrm{spin(n)} \times \rho_{\mathrm{F}}(\mathrm{G})} \mathbb{C}^{2^{\mathrm{k}}} \otimes \mathbb{C}^{\mathrm{N_F}}$. Then, the notation $\overline{\mathfrak{z}_1}\mathfrak{z}_2$ means: $\overline{\mathfrak{z}_1}\mathfrak{z}_2 \equiv \overline{\mathbf{z}_1}\mathbf{z}_2 := \Sigma_{i=1}^{2^{\mathrm{k}}} (\overline{\mathbf{s}_{1,i}}\, \mathbf{s}_{2,i})(\mathbf{z}_{1,i}^{\dagger}\, \mathbf{z}_{2,i})$. By the definition of the fermion bundle, this value is clearly independent of the choice of $p \in \mathrm{F}\mathcal{E}$ and thus independent of the representative $\mathbf{z}$ of $\mathfrak{z}$. Hence, in the cases considered, the fermionic Lagrangian (54) reads

$$\mathcal{L}_{\mathrm{F}}(D)(\psi) := \begin{cases} (\overline{\psi_+} D_+ \psi_+)\mu_{\mathrm{M}} & \text{(Lorentzian sign.)} \\ (\overline{\psi_-} D_+ \psi_+)\mu_{\mathrm{M}} & \text{(Euclidean sign.)}. \end{cases}$$

The D_+ part of simple type Dirac operators has the form

$$D_+ = \begin{pmatrix} \partial\!\!\!/_A & \Phi_{\mathrm{LR}} \\ -\Phi_{\mathrm{RL}} & \partial\!\!\!/_A \end{pmatrix} \equiv \partial\!\!\!/_A + \gamma_{\mathrm{M}} \otimes \phi_+ \tag{56}$$

where, respectively, $\Phi_{\mathrm{LR}} := \gamma_{\mathrm{M}} \otimes \widetilde{\phi}_{\mathrm{LR}} \in \Gamma(\mathrm{Hom}(\xi_{\mathrm{F,RR}}, \xi_{\mathrm{F,RL}}))$ and $\Phi_{\mathrm{RL}} := -\gamma_{\mathrm{M}} \otimes \widetilde{\phi}_{\mathrm{RL}} \in \Gamma(\mathrm{Hom}(\xi_{\mathrm{F,LL}}, \xi_{\mathrm{F,LR}}))$. The mapping $\widetilde{\phi}_{\mathrm{LR}}$ equals ϕ_{LR} restricted to $\Gamma(\mathrm{Hom}_{\mathrm{Cl}}(\xi_{\mathrm{F,LL}}, \xi_{\mathrm{F,LR}}))$ and $\widetilde{\phi}_{\mathrm{RL}}$ equals $-\phi_{\mathrm{RL}}$, restricted to the sub-space $\Gamma(\mathrm{Hom}_{\mathrm{Cl}}(\xi_{\mathrm{F,RR}}, \xi_{\mathrm{F,RL}}))$. As (56) formally looks like a simple type Dirac operator, we also refer to it as a Dirac operator of simple type. For Lorentzian or Euclidean signature the corresponding fermionic Lagrangian reads:

$$\mathcal{L}_{\mathrm{F}}(\partial\!\!\!/_A + \gamma_{\mathrm{M}} \otimes \phi)(\psi) = \begin{cases} (\overline{\psi_+}(\partial\!\!\!/_A + \gamma_{\mathrm{M}} \otimes \phi_+)\psi_+)\mu_{\mathrm{M}} & \text{(Lorentzian sign.)} \\ (\overline{\psi_-}(\partial\!\!\!/_A + \gamma_{\mathrm{M}} \otimes \phi_+)\psi_+)\mu_{\mathrm{M}} & \text{(Euclideansign.)} \end{cases}$$

$$= \begin{cases} (\overline{\psi_{\mathrm{LL}}}\partial\!\!\!/_A\psi_{\mathrm{LL}} + \overline{\psi_{\mathrm{RR}}}\partial\!\!\!/_A\psi_{\mathrm{RR}})\mu_{\mathrm{M}} + \\ (\overline{\psi_{\mathrm{LL}}}(1 \otimes \widetilde{\phi}_{\mathrm{LR}})\psi_{\mathrm{RR}} + \overline{\psi_{\mathrm{RR}}}(1 \otimes \widetilde{\phi}_{\mathrm{RL}})\psi_{\mathrm{LL}})\mu_{\mathrm{M}}, \\ (\overline{\psi_{\mathrm{RL}}}\partial\!\!\!/_A\psi_{\mathrm{LL}} + \overline{\psi_{\mathrm{LR}}}\partial\!\!\!/_A\psi_{\mathrm{RR}})\mu_{\mathrm{M}} + \\ (\overline{\psi_{\mathrm{RL}}}(1 \otimes \widetilde{\phi}_{\mathrm{LR}})\psi_{\mathrm{RR}} + \overline{\psi_{\mathrm{LR}}}(1 \otimes \widetilde{\phi}_{\mathrm{RL}})\psi_{\mathrm{LL}})\mu_{\mathrm{M}}. \end{cases}$$

Note that D is formally self-adjoint if and only if $D_-=D_+^\dagger$. Also note that $\phi^\dagger=-\phi$ if and only if $\phi_+^\dagger=-\phi_+$, which in turn is equivalent to $(1\otimes\tilde{\phi}_{\mathrm{RL}})=(1\otimes\tilde{\phi}_{\mathrm{LR}})^\dagger$. Here, all mappings are considered to be defined on the total space $\Gamma(\xi_{\mathrm{F}})$. In case of D being (anti-) Hermitian we may set, respectively, $(1\otimes\tilde{\phi}):=(1\otimes\tilde{\phi}_{\mathrm{LR}})$ and $\tilde{\Phi}\equiv\gamma_{\mathrm{M}}\otimes\tilde{\phi}$.

Finally, for a Dirac-Yukawa operator one obtains

$$D_+=\begin{pmatrix} \partial\!\!\!/_A & \mathcal{G}_{\mathrm{Y}}(\varphi) \\ -\mathcal{G}_{\mathrm{Y}}(\varphi)^\dagger & \partial\!\!\!/_A \end{pmatrix} \equiv \partial\!\!\!/_A+\gamma_{\mathrm{M}}\otimes\tilde{\mathcal{Y}}(\varphi), \tag{57}$$

with a smooth mapping

$$\mathcal{G}_{\mathrm{Y}}:\Gamma(\xi_{\mathrm{H}})\to\Gamma(\mathrm{Hom}(\xi_{\mathrm{F,RR}},\xi_{\mathrm{F,RL}}))$$

$$\varphi\mapsto\gamma_{\mathrm{M}}\otimes\tilde{\phi}:=\mathcal{G}_{\mathrm{Y}}(\varphi) \tag{58}$$

that is induced by an appropriate Yukawa mapping (4.1) and where $\varphi\in\Gamma(\xi_{\mathrm{H}})$ is a section of the Higgs bundle. We may therefore formally refer to the operator (57) also as a Dirac-Yukawa operator.

As an example, we consider the fermionic Lagrangian of a Dirac-Yukawa type operator of Lorentzian signature which spontaneously breaks the gauge symmetry. In the case of $\mathrm{N}_{\mathrm{F,L}}:=2,\mathrm{N}_{\mathrm{F,R}}:=1$ the fermionic Lagrangian (54) reads

$$\mathcal{L}_{\mathrm{F}}(iD)(\psi)=<\nu_{\mathrm{L}},i\partial\!\!\!/\nu_{\mathrm{L}}>_{\mathcal{E}_\nu}\mu_{\mathrm{M}}+<e,(i\partial\!\!\!/-m)e>_{\mathcal{E}_e}\mu_{\mathrm{M}}, \tag{59}$$

with the physical notation $\psi_{\mathrm{LL}}\equiv(\nu_{\mathrm{L}},e_{\mathrm{L}})$ and $\psi_{\mathrm{RR}}\equiv e_{\mathrm{R}}$ for the "state" of the left-handed and right-handed leptons, respectively. Here, $\nu_{\mathrm{L}}\equiv\nu_{\mathrm{LL}}\oplus\nu_{\mathrm{RL}}$ and $e\equiv e_{\mathrm{L}}\oplus e_{\mathrm{R}}$ are considered as eigensections of the total fermionic mass matrix which correspond to the eigenvalues zero and $m\in\mathbb{R}_+^\times$. Physically, one may interpret the corresponding (isomorphism class of) eigenbundles ξ_{F}^ν and ξ_{F}^e (with $\xi_{\mathrm{F}}\simeq\xi_{\mathrm{F}}^\nu\oplus\xi_{\mathrm{F}}^e$) as "asymptotically free particles."

Remark: *To "lowest order" (c.f. our discussion in the next section) the energy-momentum current* $\mathcal{L}_{\mathrm{tot}}^*\vartheta_{\mathrm{M}}\in\Gamma(\mathrm{End}(\tau_{\mathrm{M}}))$ *of the "total Lagrangian"*

$$\mathcal{L}_{\mathrm{tot}}(i\partial\!\!\!/-\mathrm{M}_{\mathrm{F}})(\psi)\equiv\mathcal{L}_{\mathrm{F}}(i\partial\!\!\!/-\mathrm{M}_{\mathrm{F}})(\psi)+\mathcal{L}_{\mathrm{D}}(i\partial\!\!\!/-\mathrm{M}_{\mathrm{F}}) \tag{60}$$

reads

$$\mathcal{L}_{\mathrm{tot}}^*\vartheta_{\mathrm{M}}\sim_{\epsilon\to0}\lambda_{\mathrm{gr}}\mathrm{tr}\,\mathrm{M}_{\mathrm{F}}^2\mathrm{id}_{\mathrm{TM}}+\mathcal{O}(\epsilon). \tag{61}$$

This holds true for every gauge theory that is based on a Dirac-Yukawa type operator.

In this section we introduced the Higgs bundle as a specific Hermitian subvector bundle of a chiral fermion bundle and discussed a specific subclass of simple type Dirac operators, called Dirac-Yukawa operators. We also introduced the fermionic Lagrangian within our geometrical setup. In particular, in the case of the Lorentzian signature the definition of the fermionic Lagrangian simply looks like the restriction to the physical subbundle ξ_{phy} of the fermion bundle. However, this is not the case. In order to obtain the "correct" fermionic couplings one also needs $\xi_{\mathrm{F}}^-\subset\xi_{\mathrm{F}}$. Indeed this doubling of the fermionic degrees of freedom is necessary in order to consider a Dirac type operator as an endomorphism on the vector space of sections of a fermion bundle. It is only in this case that one can make use of the general Lichnerowicz decomposition of (the square of) a Dirac type operator which in turn permits to consider the universal Lagrangian (21) as a canonical mapping between the affine set of all Dirac type operators on a fermion bundle and the top forms of the underlying base manifold $\mathcal{M}$.

In the next section we will consider a natural generalization of Dirac-Yukawa type operators which encodes the dynamics of the sections of the Higgs bundle ξ_{H} and the "Yang-Mills bundle"

ξ_{YM}. It also yields the appropriate mass matrices in such a way that spontaneous symmetry breaking induced by a minimum of the Higgs potential is in accordance with spontaneous symmetry breaking induced by the Yukawa coupling and gravity.

V. THE LAGRANGIAN OF THE STANDARD MODEL AS THE "SQUARE" OF PAULI-DIRAC-YUKAWA TYPE OPERATORS

From our discussion of the preceding section it follows that the total Lagrangian of a simple type Dirac operator to lowest order only yields the "free field" equations of the eigensections of the fermionic mass matrix. (This is because the energy momentum current is at least homogeneous of degree two with respect to the appropriate sections.) Moreover, space-time should be an Einstein manifold that is physically determined by the (sum of the) fermionic masses. As a consequence, one has to appropriately generalize simple type Dirac operators in order to obtain nontrivial Euler-Lagrange equations also for the Yang-Mills gauge fields and the sections of the Higgs bundle. Of course, such a generalization of a simple type Dirac operator on a fermion bundle must be done in such a way that it is consistent with spontaneous symmetry breaking induced by the Yukawa coupling and gravity. For this we first introduce a new class of Dirac type operators which we call "Dirac operators of Pauli type" (PD). These operators act on sections of a specific subbundle of the doubled fermion bundle, where the latter is defined by the data of a simple type Dirac operator that underlies the corresponding PD. Doubling the fermion bundle has the physical meaning of simultaneously dealing with "particles and antiparticles." The above mentioned subbundle turns out to be equivalent to the fermion bundle one starts with, and the corresponding fermionic Lagrangian reduces to the one which is defined only by the underlying Dirac operator of simple type. To make this precise, we have to consider real fermion bundles.

A. Real fermion bundles and operators of Pauli type

Let $\zeta_{2\mathrm{F}}$ be a real vector bundle of rank 2N and total space $\mathcal{W}_{2\mathrm{F}}$. Also let $\mathcal{I}_{2\mathrm{F}} \in \mathrm{End}_{\mathbb{R}}(\zeta_{2\mathrm{F}})$ be a complex structure. We denote by ξ_{F} the complex vector bundle of rank N which is defined by the $\mathbb{C}$–action: $z\mathfrak{z} := x\mathfrak{z} + y\mathcal{I}_{2\mathrm{F}}(\mathfrak{z})$, for all $z \equiv x + iy \in \mathbb{C}$ and $\mathfrak{z} \in \mathcal{W}_{2\mathrm{F}}$. The corresponding total space is denoted again by $\mathcal{E}$. Also, let $\xi_{2\mathrm{F}} := \mathbb{C} \otimes \zeta_{2\mathrm{F}}$ with total space $\mathcal{E}_{2\mathrm{F}} := \mathbb{C} \otimes \mathcal{W}_{2\mathrm{F}}$. The complex vector bundle $\xi_{2\mathrm{F}}$ of rank 2N is naturally $\mathbb{Z}_2$–graded as

$$\xi_{2\mathrm{F}} \simeq \xi_{\mathrm{F}} \oplus \overline{\xi_{\mathrm{F}}}. \tag{62}$$

Here, $\overline{\xi_{\mathrm{F}}}$ is the conjugate complex vector bundle of ξ_{F}. The elements of its total space $\overline{\mathcal{E}}$ are denoted by $\overline{\mathfrak{z}}$. They may be identified either with elements $\mathfrak{z} \in \mathcal{W}_{2\mathrm{F}}$, such that $z\mathfrak{z} := x\mathfrak{z} - y\mathcal{I}_{2\mathrm{F}}(\mathfrak{z})$, or considered as antilinear functionals on $\mathcal{E}^*$ (dual of $\mathcal{E}$). Of course, the subspaces of decomposition (62) are but the eigenspaces of $\mathcal{I}_{2\mathrm{F}}$ (considered as a complex linear mapping) with respect to the eigenvalues $\pm i$.

The canonical real structure on $\xi_{2\mathrm{F}}$ is denoted by $\mathcal{J}_{2\mathrm{F}}$. It is given by $\mathcal{J}_{2\mathrm{F}}(\mathfrak{z}_1, \overline{\mathfrak{z}_2}) := (\mathfrak{z}_2, \overline{\mathfrak{z}_1})$. The corresponding real sub-space

$$\{(\mathfrak{z}, \overline{\mathfrak{z}}) \in \mathcal{E}_{2\mathrm{F}} | \mathfrak{z} \in \mathcal{E}\} \simeq \mathcal{W}_{2\mathrm{F}} \tag{63}$$

can be identified with $\mathcal{E}$ via the canonical complex structure: $i(\mathfrak{z}, \overline{\mathfrak{z}}) := (i\mathfrak{z}, -i\overline{\mathfrak{z}})$. Note that, likewise, $\mathcal{E}_{2\mathrm{F}}$ may be viewed as the complex space $\mathcal{W}_{4\mathrm{F}} \equiv \mathcal{W}_{2\mathrm{F}} \oplus \mathcal{W}_{2\mathrm{F}}$ with the complex structure given by the action $\mathcal{I}_{4\mathrm{F}}(\mathfrak{w}_1, \mathfrak{w}_2) := (-\mathfrak{w}_2, \mathfrak{w}_1)$. Clearly, this complex structure in turn can be identified with $\mathcal{I}_{2\mathrm{F}}$ under the identification of $\mathcal{W}_{2\mathrm{F}}$ with $\mathcal{E}$.

In what follows, it is assumed that the complex vector bundle ξ_{F} is a fermion bundle with respect to $(\mathrm{G}, \rho_{\mathrm{F}}, D)$. Both the signature $s \in \mathbb{Z}$ of D and the dimension $n = 2k \in \mathbb{N}$ of the orientable base manifold $\mathcal{M}$ are again arbitrary, although we are mainly interested in the physically distinguished case of $(n, s) = (4, \mp 2)$. Likewise, the complex vector bundle $\overline{\xi_{\mathrm{F}}}$ is treated as the conjugate complex ("charge conjugate") fermion bundle with respect to $(\mathrm{G}, \overline{\rho}_{\mathrm{F}}, \overline{D})$. Here, $\overline{\rho}_{\mathrm{F}}$ is the conjugate representation of G, and the (charge conjugate) Dirac type operator $\overline{D}$ is defined by $\overline{D}\overline{\psi} := \overline{D\psi}$ for

all $\overline{\psi} \in \Gamma(\overline{\xi_F})$. If $<\cdot,\cdot>_{\mathcal{E}}$ denotes again the Hermitian product (the Hermitian product on $\mathcal{E}$ is assumed to be antilinear in the first, and linear in the second argument; also, the "bar" notation, as for instance $\bar{\mathfrak{z}}$, should not be confounded with the Dirac conjugation in the case of the Lorentz signature) on $\mathcal{E}$, one has $<\bar{\mathfrak{z}}_1,\bar{\mathfrak{z}}_2>_{\bar{\mathcal{E}}} := <\mathfrak{z}_2,\mathfrak{z}_1>_{\mathcal{E}}$. Hence, the sum $<\psi,D\psi>_{\mathcal{E}} + <\overline{\psi},\bar{D}\overline{\psi}>_{\bar{\mathcal{E}}}$ vanishes if D is anti-symmetric.

Although they are anti-isomorphic to each other, there is no natural way to identify the fermion bundle ξ_F with its charge conjugate $\overline{\xi_F}$. In order to do so we still have to give additional input. For this let $\mathcal{J}$ be a real structure on ξ_F such that

$$\mathcal{C}:\mathcal{E} \to \bar{\mathcal{E}}$$

$$\mathfrak{z} \mapsto \bar{\mathcal{J}}(\mathfrak{z}) \tag{64}$$

defines a linear bundle isomorphism over the identity on $\mathcal{M}$, usually referred to as "charge conjugation" (see, for instance, in Ref. 7 in the context of Clifford algebras and in Ref. 13 in the context of noncommutative geometry). Notice that $\mathcal{C}^{-1}(\bar{\mathfrak{z}}) = \mathcal{J}(\mathfrak{z})$. As a result, the charge conjugate Dirac operator may be written as

$$\bar{D} = \mathcal{C}_J \circ D \circ \mathcal{C}_J^{-1}, \tag{65}$$

where $\mathcal{C}_J(\mathfrak{z}) := \mathcal{C}(\mathcal{J}(\mathfrak{z})) = \bar{\mathfrak{z}}$.

The existence of $\mathcal{J}$ depends on the topology of ξ_F. Indeed, it can be shown that a complex vector bundle possesses a real structure if and only if all of its odd Chern classes vanish (see, for instance, Ref. 24).

Definition 5.1 *Let ξ_F be a real fermion bundle over $\mathcal{M}$ with respect to the Dirac triple (G,ρ_F,D). Also, let $F_D \in \Omega^2(\mathcal{M},\mathrm{End}^+_{Cl}(\mathcal{E}))$ be the twisting curvature of ∂_D. We call the associated first order differential operator*

$$D_P := \begin{pmatrix} D + i\gamma(F_D) & 0 \\ 0 & \mathcal{C}_J^{-1} \circ (\overline{D - i\gamma(F_D)}) \circ \mathcal{C}_J \end{pmatrix} : \begin{matrix} \Gamma(\xi_F) & \Gamma(\xi_F) \\ \oplus & \to \quad \oplus \\ \Gamma(\xi_F) & \Gamma(\xi_F) \end{matrix} \tag{66}$$

a Dirac operator of "*Pauli type*" (*or* "*Pauli-Dirac operator*") *with respect to the grading involution Γ_{2F} that is defined by the action $\Gamma_{2F}(\mathfrak{z}_1,\mathfrak{z}_2) := (\Gamma(\mathfrak{z}_2),\Gamma(\mathfrak{z}_1))$ and the real structure $\mathcal{J}$.*

Equivalently, one may also express a Pauli-Dirac operator with respect to the diagonal representation of the grading involution Γ_{2F} (i.e., where $\Gamma_{2F} = \mathrm{diag}(\Gamma,-\Gamma)$), in which case

$$D_P = \begin{pmatrix} D & -\gamma(F_D) \\ \gamma(F_D) & D \end{pmatrix} \equiv D + \mathcal{I} \otimes \gamma(F_D). \tag{67}$$

The bundle mapping $\mathcal{I} \in \mathrm{End}_C(\mathcal{E} \oplus \mathcal{E})$, which is defined by $\mathcal{I}(\mathfrak{z}_1,\mathfrak{z}_2) := (-\mathfrak{z}_2,\mathfrak{z}_1)$, corresponds to the complex structure $\mathcal{I}_{4F}$ with help of the identification of $\mathcal{W}_{2F} \subset \mathcal{E} \oplus \bar{\mathcal{E}}$ with $\mathcal{E}$.

If $D \equiv \not{\partial}_A$, then the zero order term $D_P - \not{\partial}_A$ formally looks like the well-known "Pauli-term" $i\gamma(F_A)$ which has been introduced by physicists in order to correctly describe the anomalous magnetic moment of the proton. However, the first order operator $\not{\partial}_A + i\gamma(F_A)$ is not a Dirac type operator in our sense for the Pauli term is an even operator. To remedy this flaw we again have to "double the fermionic degrees of freedom," in this case, however, by adding the corresponding "antifermions." As a consequence, for diagonal sections, which one may physically interpret as representing the state of a "particle-antiparticle" (with the help of the identification $\overline{\xi_F} \simeq \xi_F$), $\Psi \equiv (\psi,\psi) \in \Gamma(\xi_F) \oplus \Gamma(\xi_F) = \Gamma(\xi_F \oplus \xi_F) \simeq \Gamma(\xi_{2F})$, we obtain the identity

$$<\Psi, D_{\mathrm{P}}\Psi>_{\mathcal{E}_{2\mathrm{F}}} = 2<\psi, D\psi>_{\mathcal{E}}. \tag{68}$$

Hence, the Pauli term does not contribute to the fermionic Lagrangian as far as "particle-anti-particle states" are simultaneously taken into account. This is certainly desirable, for it is well-known that the coupling of the fermions to the curvature actually spoils the theory of their renormalizability. Hence, to lift the first order differential operator $\not{\partial}_A + i\gamma(F_{\mathrm{A}})$ to a true Dirac type operator restores a basic feature of (perturbative) quantum field theory. Again, by formal similarity we also refer to the operator $\not{\partial}_A + i\gamma(F_{\mathrm{A}})$ itself as a Dirac operator of Pauli type, analogous to operator (57) is formally referred to as Dirac operator of Yukawa type.

Let ξ_{F} be the real chiral fermion bundle with respect to $(\mathrm{G}, \rho_{\mathrm{F}}, D)$, with D being of simply type.

Proposition 5.1: The top form of D_{P} decomposes into the sum

$$\mathcal{L}_{\mathrm{D}}(D_{\mathrm{P}}) = \mathcal{L}_{EH} \pm \mathcal{L}_{YM} \pm \mathcal{L}_{H} \tag{69}$$

where, respectively, $\mathcal{L}_{EH}$ is the Einstein-Hilbert Lagrangian, $\mathcal{L}_{YM}$ the Yang-Mills Lagrangian and $\mathcal{L}_{H}$ the "Higgs" Lagrangian of the Standard Model of Particle Physics.

Proof: The proof is basically a copy of the proof of the corresponding statement that has been presented already in Ref. 45 in the case of $s=n$ (c.f. Theorem 1). We note that the top form $\mathcal{L}_{\mathrm{D}}(D') \in \Omega^{\mathrm{n}}(\mathcal{M})$ is independent of the connection representing $D' \in \mathcal{D}(\xi_{\mathrm{F}})$. Hence, one may choose any representative of the connection class that corresponds to D_{P} to define the Pauli term $i\gamma(F_A)$. The relative signs of (69) depend on the signature of D and of the definition of the Clifford multiplication. In particular, the relative sign in front of the kinetic term $\langle \partial_A^W \phi, \partial_A^W \phi \rangle$ of the Higgs Lagrangian depends on whether (the complexified) $\tau_{\mathrm{Cl}}^{(+)}$ or $\tau_{\mathrm{Cl}}^{(-)}$ is considered to act on ξ_{F}. Finally, we stress that decomposition (69) is actually independent of the existence of a real structure on ξ_{F}. In particular, it does not depend on the choice of $\mathcal{J}$. □

The top form (69) clearly reduces to the combined Einstein-Hilbert-Yang-Mills Lagrangian in the case where ξ_{F} is not chiral. However, if D denotes a Dirac-Yukawa type operator, then the total Lagrangian

$$\mathcal{L}_{\mathrm{tot}}(D_{\mathrm{P}})(\Psi) \equiv \mathcal{L}_{\mathrm{F}}(D_{\mathrm{P}})(\Psi) + \mathcal{L}_{\mathrm{D}}(D_{\mathrm{P}}) = \mathcal{L}_{\mathrm{F}}(D)(\psi) + \mathcal{L}_{\mathrm{D}}(D_{\mathrm{P}}) \tag{70}$$

equals the total Lagrangian of the Standard Model, including Einstein's theory of gravity. Here, we used the homogeneity property of the fermionic density: $\mathcal{L}_{\mathrm{F}}(D_{\mathrm{P}})(\lambda\Psi) = \lambda^2 \mathcal{L}_{\mathrm{F}}(D_{\mathrm{P}})(\Psi)$ and put $\Psi \equiv (\psi, \psi)/\sqrt{2}$. Note that the corresponding Euler-Lagrange equations form a dynamically closed system. For this reason, we refer to D_{P} also as a Dirac operator of "Pauli-Yukawa" type (or "Pauli-Dirac-Yukawa" operator, PDY) if operator (66) is defined in terms of a Dirac-Yukawa type operator (49). Therefore,

$$(\xi_{\mathrm{F}}, D_{\mathrm{P}}) \tag{71}$$

may be regarded as a "square root" of (the Lagrangian of) the Standard Model. (Of course, the data $(\xi_{\mathrm{F}}, D_{\mathrm{P}})$ covers the geometrical properties of the Standard Model only up to the semiclassical approximation of the latter. It also seems worth noting that because decomposition (69) is independent of the existence of the reality of the fermion bundle, it is possible to also take into account magnetic monopoles within the Standard Model as topologically nontrivial ground states of the Higgs boson. Moreover, it is well-known that the weak interaction actually spoils the symmetry under charge conjugation).

B. "Fluctuation" of a fermionic vacuum and the YM-mass matrix

Before we proceed let us come back to the notion of a "(semiclassical) fermionic vacuum" and how this is related to the reality of a fermion bundle. Essentially, a chiral fermion bundle $\xi_{\mathrm{F}} = \xi_{\mathrm{F}}^{+} \oplus \xi_{\mathrm{F}}^{-}$ is related to a Dirac triple $(\mathrm{G}, \rho_{\mathrm{F}}, D)$, with D being of simple type. The existence of a fermionic vacuum crucially depends on the existence of a non-vanishing section $\phi \in \Gamma(\mathrm{End}_{\mathrm{Cl}}^{-}(\xi_{\mathrm{F}}))$ and a purely topological Clifford connection $A \in \mathcal{A}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$. This in fact reduces the

previous Dirac triple to $(\mathrm{H},\rho_{\mathrm{F,red}},\not{\partial})$ and ξ_{F} may be regarded, accordingly, as a perturbation of the corresponding $\xi_{\mathrm{F,red}}$. Clearly, such a reduction causes severe topological restrictions on a fermion bundle. Of course, this holds true also for the existence of a Dirac-Yukawa type operator. For example, in the case of the electroweak interaction, a fermionic vacuum exists if and only if the corresponding Yang-Mills gauge bundle of the electroweak interaction is trivial. This in turn holds true if and only if the (charged) electroweak vector bosons are charge conjugate to each other (c.f. Ref. 48). In the (algebraic) torsion free case this is equivalent to the existence of a flat Yang-Mills connection. This example may motivate the following

Definition 5.2: A fermion bundle ξ_{F} is called "perturbative" provided there is a Dirac type operator $D\in\mathcal{D}(\xi_{\mathrm{F}})$ such that $\mathcal{F}_D=\not{R}$.

A fermionic vacuum is thus geometrically described by a perturbative massive fermion bundle. Next, we introduce a specific subvector bundle of $\xi_{\mathrm{F}}^{*}\otimes_{\mathcal{M}}\xi_{\mathrm{F}}$ and discuss the "bosonic mass matrix" within the presented fermionic frame.

Definition 5.3: Let again ξ_{F} be a massive fermion bundle with respect to a Dirac-Yukawa model $(\mathrm{G},\rho_{\mathrm{F}},D)$. The real sub-bundle

$$\xi_{\mathrm{YM}}:=\tau_{\mathrm{M}}^{*}\otimes_{\mathcal{M}}\mathrm{End}_{\mathrm{Cl}}^{+}(\xi_{\mathrm{F}})\subset\mathrm{End}(\xi_{\mathrm{F}}) \tag{72}$$

is called the Yang-Mills bundle with respect to the appropriate fermionic vacuum $\xi_{\mathrm{F,red}}$.

With respect to a fermionic vacuum the (real form of the) Higgs bundle decomposes into the Whitney sum of two real vector bundles

$$\xi_{\mathrm{H}}\simeq\xi_{\mathrm{G}}\oplus\xi_{\mathrm{H,phys}} \tag{73}$$

with $\xi_{\mathrm{G}}\subset\xi_{\mathrm{H}}\subset\xi_{\mathrm{F}}$ being the "Goldstone bundle" and $\xi_{\mathrm{H,phys}}\subset\xi_{\mathrm{F}}$ being the "physical Higgs bundle" (c.f. Lemma 3.1 in Ref. 46 for Yang-Mills-Higgs gauge theories). Therefore, any Dirac-Yukawa type operator on a massive fermion bundle ξ_{F} is parametrized by $(A,\varphi_{\mathrm{H}})\in\Gamma(\xi_{\mathrm{YM}}\times_{\mathcal{M}}\xi_{\mathrm{H,phys}})$. In particular, for $t\in[0,1]$ one may consider the one-parameter family $(A_t,\varphi_t)\in\mathcal{A}(\xi_{\mathrm{H}})\times\Gamma(\xi_{\mathrm{H}})$ which is defined by $\partial_{A,t}:=\partial+tA$, $\varphi_t:=\mathcal{V}+t\varphi_{\mathrm{H}}$. Hence, the "Yang-Mills-Higgs pair" $(A,\varphi_{\mathrm{H}})\in\Gamma(\xi_{\mathrm{YM}}\times_{\mathcal{M}}\xi_{\mathrm{H,phys}})$ may be physically regarded as a "fluctuation" of the corresponding fermionic vacuum $\xi_{\mathrm{F,red}}$.

Like in the Yang-Mills-Higgs gauge theories, a fluctuation (A,φ_{H}) of a fermionic vacuum yields a self-adjoint section $\mathrm{M}_{\mathrm{H}}\in\Gamma(\mathrm{End}(\xi_{\mathrm{H}}))\subset\Gamma(\mathrm{End}_{\mathrm{Cl}}(\xi_{\mathrm{F}}))$ such that the rank of the Goldstone bundle equals the dimension of the kernel of the "Higgs mass operator" M_{H}. Moreover, $\xi_{\mathrm{H,phys}}$ decompose into the Whitney sum of eigenbundles of the Higgs mass matrix. Likewise, since in general $A\in\Gamma(\xi_{\mathrm{YM}})$ gives rise to a connection on ξ_{F} that is not compatible with the fermionic vacuum (i.e., the corresponding covariant derivative does not commute with the total fermionic mass operator), a fluctuation of the fermionic vacuum also yields a nontrivial Yang-Mills mass operator $\mathrm{M}_{\mathrm{YM}}\in\Gamma(\mathrm{End}(\xi_{\mathrm{YM}}))$ (see Ref. 46). As a consequence, the Yang-Mills bundle decomposes into the eigenbundles of M_{YM} for again $\mathrm{spec}(\mathrm{M}_{\mathrm{YM}})$ is constant throughout $\mathcal{M}$. In particular, one obtains the decomposition (see, again, Ref. 46)

$$\xi_{\mathrm{YM}}\simeq\tau_{\mathrm{M}}^{*}\otimes_{\mathcal{M}}(\mathfrak{ad}(\mathcal{Q})\oplus\xi_{\mathrm{G}}) \tag{74}$$

with $\mathfrak{ad}(\mathcal{Q})\equiv\mathrm{Lie}(\mathcal{H}_{\mathrm{YM}})$ being the "adjoint bundle" of the reduced frame bundle $\mathcal{Q}\overset{\iota}{\hookrightarrow}\mathcal{P}$ associated with the fermionic vacuum $\xi_{\mathrm{F,red}}$. As $\mathrm{rk}(\mathrm{M}_{\mathrm{YM}})=\mathrm{rk}(\xi_{\mathrm{G}})$ the equivalence (74) is a geometrical variant of the famous "Higgs-Dinner." It follows that $A\in\Gamma(\xi_{\mathrm{YM}})$ decomposes into $A=A_{\mathrm{YM}}+A_{\mathrm{G}}$. Hence, the deviation from A being compatible with the fermionic vacuum can be expressed by

$$\partial_A^{\mathrm{End}(\mathcal{E})}\mathrm{M}_{\mathrm{F}}=\mathrm{ad}(A_{\mathrm{G}})\mathrm{M}_{\mathrm{F}}. \tag{75}$$

As already mentioned, the nonvanishing of the right-hand side (i.e., of $A_{\mathrm{G}}\in\tau_{\mathrm{M}}^{*}\otimes_{\mathcal{M}}\xi_{\mathrm{G}}$) yields a nontrivial Yang-Mills mass operator M_{YM}. In fact, one has

$$\mathrm{M}_{\mathrm{YM}}(A) = \mathrm{ad}(\mathrm{M}_{\mathrm{F}})(A) \tag{76}$$

with $\|\mathrm{M}_{\mathrm{YM}}(A)\|^2 = \mathrm{M}^2_{\mathrm{YM}}(A,A)$ and the symmetric bilinear form

$$\mathrm{M}^2_{\mathrm{YM}}: \Gamma(\xi_{\mathrm{YM}} \times_{\mathcal{M}} \xi_{\mathrm{YM}}) \to \mathcal{C}^\infty(\mathcal{M})$$

$$(A, A') \mapsto \tfrac{1}{2}\mathrm{M}^2_{\mathrm{YM}}(T_a, T_b) g_{\mathrm{M}}(A^a, A'^b). \tag{77}$$

Here, respectively, $\overset{\mathrm{loc}}{A} = A^a \otimes T_a, \overset{\mathrm{loc}}{A'} = A'^a \otimes T_a$ and

$$\mathrm{M}^2_{\mathrm{YM}}(T_a, T_b)|_x := 2\|\mathcal{G}_{\mathrm{Y}}\|^2 < \mathcal{V}(x), [T_a, T_b]_+ \mathcal{V}(x) >_{\mathcal{E}} \tag{78}$$

is the (squared) "Yang-Mills mass matrix," with $[\cdot,\cdot]_+$ being the anticommutator. Note that we used $\xi_{\mathrm{H}} \subset \xi_{\mathrm{F}}$, such that a vacuum section $\mathcal{V}$ can also be regarded as a section of the fermion bundle. We also extensively used the properties of the Yukawa mapping (4.1). In particular, we made use of the fact that $\mathrm{ad}(\mathcal{D})A = \mathcal{Y}(A\mathcal{V})$ where, by abuse of notation, A refers to two different representations. Also note that the eigenvalues of (78) are actually independent of $x \in \mathcal{M}$. Of course, the rank of (78) equals the rank of the Goldstone bundle $\xi_{\mathrm{G}} \subset \xi_{\mathrm{F}}$. Accordingly, one may rewrite (75) as

$$\|\partial_A^{\mathrm{End}(\mathcal{E})} \mathrm{M}_{\mathrm{F}}\|^2 = 2^n \mathrm{M}^2_{\mathrm{YM}}(A, A). \tag{79}$$

That is, the fermionic mass matrix is covariantly constant with respect to a Clifford connection on a massive fermion bundle iff this Clifford connection is in the kernel of the Yang-Mills mass matrix. The latter, of course, is in one-to-one correspondence with the residual gauge fields.

Let $D \in \mathcal{D}(\xi_{\mathrm{F}})$ be a Dirac operator of simple type such that $D - \not{b}_A \neq 0$ and $\mathcal{G}_{\mathrm{YM}}$ acts transitively on the image of $D - \not{b}_A$. Then, there is a nonvanishing smooth function $\chi \in \mathcal{C}^\infty(\mathcal{M})$ such that $D = \not{b}_A + i\chi \mathrm{M}_{\mathrm{F}}$. Let $\xi_{\mathrm{F,red}} \simeq \xi_{\mathrm{F}}$ be a fermionic vacuum with respect to $(\mathrm{H}, \rho_{\mathrm{F,red}}, \not{b}_{\mathcal{D}})$. Then, D defines a fluctuation of $\xi_{\mathrm{F,red}}$ iff

$$D = \not{b}_A + \chi(\not{b}_{\mathcal{D}} - \not{b}). \tag{80}$$

Note that this condition is in full accordance with the usual definition of the Higgs boson as being in the unitary gauge. Here, however, this condition is expressed purely in terms of fermions.

Proposition 5.2: Let $\xi_{\mathrm{F,red}} \simeq \xi_{\mathrm{F}}$ be a fermionic vacuum with respect to a Dirac-Yukawa model $(\mathrm{H}, \rho_{\mathrm{F,red}}, \not{b}_{\mathcal{V}})$. Also, let $(A, \varphi_{\mathrm{H}}) \in \Gamma(\xi_{\mathrm{YM}} \times_{\mathcal{M}} \xi_{\mathrm{H,phys}})$ be a fluctuation of the fermionic vacuum. Then, the total curvature on ξ_{F} of the connection determined by the Dirac-Yukawa operator

$$D = \not{b}_A + \gamma_{\mathrm{M}} \otimes \not{\phi} = \not{b} + \gamma_{\mathrm{M}} \otimes \mathcal{Y}(\mathcal{V}) + \gamma(A) + \gamma_{\mathrm{M}} \otimes \mathcal{Y}(\varphi_{\mathrm{H}}) \equiv \not{b}_{\mathcal{D}} + \gamma(A_{\mathrm{fl}}) \tag{81}$$

reads

$$\mathcal{F}_D = \mathbb{R} + F_A + F_{\mathrm{H}} + F_{\mathrm{mass}} = \mathbb{R} + F_{\mathrm{YM}} + F_{\mathrm{G}} + F_{\mathrm{H}} + F_{\mathrm{mass}}. \tag{82}$$

Here, respectively,

$$F_{\mathrm{YM}} := \partial A_{\mathrm{YM}} + A_{\mathrm{YM}} \wedge A_{\mathrm{YM}},$$

$$F_{\mathrm{G}} := \partial A_{\mathrm{G}} + A_{\mathrm{G}} \wedge A_{\mathrm{G}},$$

$$F_{\mathrm{H}} := \partial A_{\mathrm{H}} + A_{\mathrm{H}} \wedge A_{\mathrm{H}} \tag{83}$$

are the Yang-Mills curvature with respect to the reduced Yang-Mills gauge group $\mathcal{H}_{\mathrm{YM}} \subset \mathcal{G}_{\mathrm{YM}} \subset \mathcal{G}_{\mathrm{F}}$, the curvature on ξ_{F} of the (massive) vector boson that corresponds to the Goldstone boson and the curvature induced by the (physical part of the) Higgs boson according to the decomposition

$$A_{\mathrm{fl}} = A + A_{\mathrm{H}} = A_{\mathrm{YM}} + A_{\mathrm{G}} + A_{\mathrm{H}}, \tag{84}$$

with $A_{\mathrm{H}} := \mathrm{ext}_{\Theta}(\gamma_{\mathrm{M}} \otimes \mathcal{Y}(\varphi_{\mathrm{H}}))$.

Finally, the "mass-curvature" $F_{\mathrm{mass}} \in \Omega^2(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ *is given by*

$$F_{\mathrm{mass}} := (1 - 2\|\varphi_{\mathrm{H}}\|)\mathrm{M}_{\mathrm{F}}^2\Theta \wedge \Theta + (1 + \|\varphi_{\mathrm{H}}\|)\mathrm{M}_{\mathrm{YM}}(A_{\mathrm{G}}) \wedge \Theta = \mathrm{ext}_{\Theta}[(1 - 2\|\varphi_{\mathrm{H}}\|)\mu_{\mathrm{F}} + (1 + \|\varphi_{\mathrm{H}}\|)\mu_{\mathrm{YM}}]. \tag{85}$$

We call, respectively, $\mu_{\mathrm{F}} := \mathrm{ext}_{\Theta}(\mathrm{M}_{\mathrm{F}}^2) \in \Omega^1(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ *and* $\mu_{\mathrm{YM}} := \mathrm{M}_{\mathrm{YM}}(A_{\mathrm{G}}) \equiv \gamma_{\mathrm{M}} \otimes \mathrm{M}_{\mathrm{YM}}(A) \in \Omega^1(\mathcal{M}, \mathrm{End}(\mathcal{E}))$ *the "fermionic mass form" and the "Yang-Mills mass form."*

Proof: First, note that the Yang-Mills mass form μ_{YM} contributes to the total curvature even if $F_{\mathrm{A}} = \varphi_{\mathrm{H}} = 0$ is supposed to hold true. Hence, it also gives rise to a fluctuation of g_{M}. In contrast to what one may infer from F_{mass}, however, the contribution of the bosonic mass is of "higher order" in comparison to the curvature that is induced by the fermionic mass. In other words, $F_{\mathrm{mass}} = \mathrm{ext}_{\Theta}(\mu_{\mathrm{F}}) + \mathcal{O}(t)$ in accordance with (42). We stress that (82) indeed reduces to (42) if $\varphi_{\mathrm{H}} = 0$. Hence, it gives a physical interpretation, in particular, of the last term of the decomposition (42) of the curvature of a simple type Dirac operator which spontaneously breaks the gauge symmetry. One may express this also in more physical terms by saying that it is the interaction of the gauge field with the fermionic vacuum that yields massive vector bosons.

To prove decomposition (82) one uses decomposition (73) and the Higgs-Dinner (74), as well as $[\mathrm{M}_{\mathrm{F}}^2, \Theta] = [\mathrm{M}_{\mathrm{YM}}, \Theta] = 0$. Moreover, due to our previous remark concerning fluctuations one may take into account that $\varphi_{\mathrm{H}} = \|\varphi_{\mathrm{H}}\| \mathcal{V}$ (where $\|\mathcal{V}\| = 1$ is assumed without loss of generality). Note also that both the (lifted) soldering form Θ and the Yukawa-mapping $\mathcal{Y}$ are covariantly constant with respect to any Clifford connection. Finally, taking also into account that ∂ acts on A_{fl} like the usual exterior derivative, the proof actually becomes a straightforward calculation. □

We emphasize that spontaneous symmetry breaking induced by a fermionic vacuum is compatible with spontaneous symmetry breaking induced by the Higgs potential arising from a fluctuation of the fermionic vacuum (i.e., $\not{\partial}_{\mathcal{D}} \mapsto D_{\mathrm{P}}$). Clearly, G acts transitively on $\mathrm{im}(\phi) \subset \mathrm{Orbit}(\mathfrak{Z}_0) \simeq \mathrm{P} \times_{\mathrm{G}} \mathrm{G}/\mathrm{H}$ for any chosen minimum $\mathfrak{Z}_0 \in \mathrm{End}(\mathbb{C}^{\mathrm{N_H}})$ of the Higgs potential induced by D_{P}. Therefore, the condition $\phi \in \Gamma(\mathrm{End}(\xi_{\mathrm{H}})) \backslash \{\mathcal{O}\}$ is necessary and sufficient for the unitary gauge to exist. In particular, if ξ_{F} is defined with respect to a Dirac-Yukawa model, then for each $\varphi \in \Gamma(\xi_{\mathrm{H}}) \backslash \{\mathcal{O}\}$ there exists a "vacuum section" $\mathcal{V}_{\varphi} \in \Gamma(\mathcal{O}rbit(\mathbf{z}_0)) \subset \Gamma(\xi_{\mathrm{H}})$ such that $\varphi \in \Gamma(\xi_{\mathrm{H,phys}})$. This holds true for any rotationally symmetric Higgs potential (like the Higgs potential generated by a Pauli-Dirac type operator). By the very definition of the Yukawa mapping the structure group G then acts transitively also on $\mathrm{im}(\mathcal{Y}(\varphi)/\|\mathcal{Y}(\varphi)\|) \subset \mathcal{S} \subset \mathrm{End}_{\mathrm{Cl}}(\xi_{\mathrm{F}})$.

VI. OUTLOOK

We discussed a certain class of gauge theories with the basic property of having a square root in the sense of the data of Dirac type operators. These Dirac type gauge theories have in common that they are derived by a universal Lagrangian which is shown to be equivariant with respect to bundle automorphisms. Moreover, these gauge theories naturally include Einstein's theory of gravity, and the fermionic gauge group of the universal (Dirac-) Lagrangian contains both Yang-Mills and Einstein-Hilbert type symmetry groups. In particular, the action of the diffeomorphism group of the base manifold is naturally represented by pull-back. We also considered a distinguished class of Dirac type operators whose associated top form gives rise to spontaneous symmetry breaking without using Higgs-like potentials. Indeed, the latter naturally arises when a fluctuation of the fermionic vacuum is taken into account. The geometrical meaning of the induced bosonic mass operators can be shown to consist of defining the extrinsic curvature of the "physical space-time" $\mathcal{M}_{\mathrm{phys}}$. The intrinsic curvature of the latter, however, was shown to be defined by the fermionic vacuum. In the case where the fermionic vacuum is defined with respect to a Dirac-Yukawa model, the appropriate Higgs and Yang-Mills bundle can be naturally regarded as specific sub-vector bundles of ξ_{F}, respectively, of $\xi_{\mathrm{F}}^* \otimes_{\mathcal{M}} \xi_{\mathrm{F}}$. For this we discussed the Yukawa couplings from a geometrical point of view in terms of specific sections of the Yukawa bundle, which is

shown to yield the connection between the fermion and the Higgs bundle. To consider the Yukawa bundle ξ_Y as a specific sub-vector bundle of $\xi_H^* \otimes_{\mathcal{M}} \xi_F^* \otimes_{\mathcal{M}} \xi_F$ permits a geometrical understanding of the well-known "hypercharge relations" between the physical Higgs boson $\xi_{H,phy}$ and the asymptotically free fermions $\xi_{F,m^2} \subset \xi_F$ in the case of the minimal Standard Model. In this sense, the presented frame makes it possible to treat the geometrical properties of spontaneously broken Yang-Mills-Higgs gauge theories in terms of fermions, as discussed in Ref. 46. In particular, it is shown that this kind of gauge theories can be expressed in the geometrical setup needed to describe fermions without use of spin structures. Note that the latter actually has no obvious physical meaning. Indeed, all experiments carried out to date demonstrating the physical significance of the twofold cover of SO(3) are local. The assumption of orientability, however, is necessary to derive the Einstein equation from a globally defined density which seems to also have some significance in our understanding of mass.

The "fermion doubling" within the presented geometrical setup is shown to be tied to the Lichnerowicz decomposition of a Dirac type operator. As the latter gives rise to the universal Lagrangian and, moreover, to a specific class of Dirac type operators which yield spontaneous symmetry breaking, the projection onto the physical sub-space $\xi_{phy} \subset \xi_F$ clearly indicates a nontrivial relation between the fermionic Lagrangian $\mathcal{L}_F$ and the Dirac Lagrangian $\mathcal{L}_D$.

As the Dirac Lagrangian is a canonical element within the presented geometrical frame, it will be useful to discuss it also in terms of the geometry of variational bicomplexes. This may offer a more profound mathematical understanding of operators of Pauli-Dirac type as has been introduced here as a "fluctuation of a fermionic vacuum." These kinds of Dirac type operators obviously play a fundamental role in the Standard Model of Particle Physics. In a forthcoming article we shall thus discuss the Dirac triple of the Standard Model in more detail. In particular, we shall show how this triple permits specification of $\mathrm{spec}(M_H)$. In the case of the "minimal" Standard Model $\mathrm{rk}(\xi_{H,phys})=1$ which allows a prediction of the mass of the Higgs boson. For this, however, one still has to carefully take into account possible "coupling constants" within the frame of Dirac type gauge theories. In general, one may modify the total Lagrangian $\mathcal{L}_{tot}$ as

$$\mathcal{L}_{tot}(D)(\psi) \rightsquigarrow \mathcal{L}_{phys}(D)(\psi) := \mathcal{L}_F(D)(\psi) + \lambda \mathcal{L}_D(D), \tag{86}$$

with the Dirac-Lagrangian being refined by

$$\mathcal{L}_D(D) := * \,\mathrm{tr}(\zeta[D^2 - \triangle_D]). \tag{87}$$

Here, respectively, $\lambda \in \mathbb{R}$ is a "relative weight" between the fermionic and bosonic Lagrangian and ζ is the most general element of the commutant with respect to the fermionic representation ρ_F of the structure group G. More precisely, $\zeta \in \Gamma(\mathrm{End}^+_{Cl}(\xi_F))$ is a positive Hermitian operator satisfying: $[D,\zeta]=0=[\zeta,g]$, for all $g \in \mathcal{G}_{YM}$. It therefore may be considered as generalizing the Yang-Mills coupling constant of a "pure" Yang-Mills gauge theory. Actually, the constant λ may be fixed by an appropriate normalization of the Einstein-Hilbert Lagrangian.

Due to formula (78) the Yang-Mills mass matrix is proportional to the (squared) norm of the Yukawa-coupling constants $\mathcal{G}_Y$. However, the "physical" Yang-Mills mass matrix is known to be proportional to the Yang-Mills coupling constants $g_{YM}>0$ which parameterize the most general Killing form on Lie(G). Hence, we have to re-scale A_G by a positive constant g_G for each simple factor of G, i.e., $A^a_G \rightsquigarrow A^a_G / g^{(a)}_G$ (no summation involved), such that

$$g^{(a)}_{YM} = g^{(a)}_G g_Y \tag{88}$$

with the abbreviation $g_Y \equiv \|\mathcal{G}_Y\|$.

Finally, one also has to take into account that in general $\|\mathcal{V}\| \neq 1$, and that the various differential forms defining the Dirac type operator in question have different dimensions. Besides the "Planck scale" (which comes in because of the generic Einstein-Hilbert part of the total Lagrangian) this will bring in an additional length scale within Dirac type gauge theories. However, in the case of the Lagrangian of a PDY this additional length scale turns out to be proportional to the (inverse of the) Higgs mass. Hence, in the case of the Standard Model the two length scales

decouple within GTDT, and gravity effects can be neglected as it is commonly expected. For this to be consistent, however, we stress again the necessity of the compatibility of the two different symmetry reductions obtained by the fermionic vacua (i.e., simple type Dirac operators) and the ground states of the Higgs boson (i.e., Pauli type Dirac operators).

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APPENDIX

Because of its relevance within Dirac type gauge theories we present here in some detail the proof of Proposition 3.1. In particular, it is shown that it holds true for arbitrary signature of D. In Ref. 1 a similar proof was presented for the special case of elliptic Dirac type operators.

1. Tensor decomposition

In this subsection we collect some useful formulas which will be needed to prove the explicit form of the Dirac forms $\varpi_{\rm D} \in \Omega^1(\mathcal{M}, {\rm End}(\mathcal{E}))$ of simple type Dirac operators. Though interesting in its own we will not prove these formulae here (since the proof would be technical but straightforward).

To get started let $\omega \in \Gamma(\tau^*_{\rm M} \otimes_{\mathcal{M}} \Lambda^{\rm n-1} \tau^*_{\rm M} \otimes_{\mathcal{M}} {\rm End}(\xi_{\rm F}))$. Throughout this Appendix, let $(X_1, \ldots, X_n)$ be a locally defined orthonormal frame on $\mathcal{M}$ and $(X^1, \ldots, X^n)$ its dual frame. Then, locally one has

$$\begin{aligned} \omega(X_{i_1}, \ldots, X_{i_n}) &=: \omega_{i_1 \cdots i_n} \equiv \omega_{i_1[i_2 \cdots i_n]}, \\ \gamma(\omega) &=: \not{\omega} \equiv \gamma^{j_1} \ldots \gamma^{j_n} \circ \omega_{i_1 \cdots i_n}. \end{aligned} \tag{A1}$$

Here, the square brackets $[\cdots]$ indicate skew-symmetrization with the convention: $n!\,\omega_{[i_1 \cdots i_n]} = \Sigma_{\sigma \in S_n} \mathrm{sgn}\,\sigma \omega_{\sigma(\mathrm{i}_1) \cdots \sigma(\mathrm{i}_n)}$ and, again, $\gamma^k \equiv \gamma(X^k)$. In what follows, we restrict ourselves to the Clifford relation $\alpha\beta + \beta\alpha = +2g_{\rm M}(\alpha, \beta)$ for all $\alpha, \beta \in T^*M \hookrightarrow Cl(M)$ (the total space of $\tau^{(+)}_{\rm Cl}$).

First, we have the following decomposition (the "$\underset{j}{\uparrow}$" means that i_1 is at the jth position)

$$\omega_{i_1 \cdots i_n} = \omega_{[i_1 \cdots i_n]} + \frac{1}{n} \sum_{j=2}^{n} \left(\omega_{i_1 \cdots i_n} + \omega_{\substack{ij \;\; i_2 \;\; \cdots \;\; i_1 \;\; \cdots \;\; i_n \\ \uparrow \\ j}} \right). \tag{A2}$$

As a consequence, it follows that $\gamma(\omega)$ may locally be written as

$$\begin{aligned} \gamma^{j_1} \gamma^{j_3} \cdots \gamma^{j_n} \circ \omega_{i_1 \mu i_3 \cdots i_n} = &- \frac{n}{n-1} \gamma^{j_1} \gamma^{j_3} \cdots \gamma^{j_n} \circ \omega_{[\mu i_1 i_3 \cdots i_n]} + \frac{1}{n-1} \gamma^{j_1} \gamma^{j_3} \cdots \gamma^{j_n} \circ \omega_{\mu i_1 i_3 \cdots i_n} \\ &- (n-2) g^{\alpha\beta} \gamma^{j_4} \cdots \gamma^{j_n} \circ \omega_{\alpha\beta\mu i_4 \cdots i_n} \end{aligned} \tag{A3}$$

where, again, $g^{ij} \equiv g_{\rm M}(X^i, X^j)$.

Using these two formulas one finally proves the following local decomposition which turns out to be particularly useful in what follows:

$$\gamma(\omega) \overset{loc.}{=} \gamma^{j_1} \cdots \gamma^{j_n} \circ \omega_{[i_1 \cdots i_n]} + (n-1) g^{\alpha\beta} \gamma^{j_3} \cdots \gamma^{j_n} \circ \omega_{\alpha\beta i_3 \cdots i_n}. \tag{A4}$$

2. Proof of Proposition 3.1

Let $\xi=(\mathcal{E},\mathcal{M},\pi_\epsilon)$ be an arbitrary $\mathbb{Z}_2$−graded Clifford module bundle over any smooth (semi-) Riemannian manifold $(\mathcal{M},g_{\mathrm{M}})$ with $\dim\mathcal{M}=n$ and n even. Every Dirac type operator D may be globally decomposed as $D=\not{\partial}_A+\not{\omega}$, with A being a Clifford connection and $\omega\in\Omega^1(\mathcal{M},\mathrm{End}^+(\mathcal{E}))$ being given by $\omega:=\Theta\wedge(D-\not{\partial}_A)$. Notice again that ω may also depend on the choice of A unless D is of simple type. Locally, ω reads

$$\overset{loc.}{\omega}=X^i\otimes\omega_i^a\otimes\mathfrak{e}_a\equiv X^i\otimes\left(\sum_{k=0}^{n}\gamma^{j_1}\cdots\gamma^{j_k}\omega^a_{ij_1\cdots j_k}\right)\otimes\mathfrak{e}_a, \tag{A5}$$

with $\omega^a_{ij_1\cdots j_k}=\omega^a_{i[j_1\cdots j_k]}$ and $(\mathfrak{e}_1,\ldots,\mathfrak{e}_N)$ being a local frame in $\mathrm{End}_{\mathrm{Cl}}(\xi)$ such that ω is odd with respect to the total grading.

By definition, D is of simple type if the Clifford connection A also defines the Bochner-Laplacian of D. Using the general Bochner-Lichnerowicz-Weizenböck decomposition of D^2 it can be shown that, independently of the signature of g_{M}, this holds true if and only if (in the case $s=n$ this has been proved in Ref. 1; the more general case of arbitrary signature has been proved in Ref. 44)

$$2g^{ij}\omega^a_j+\gamma^i[\omega^a_j,\gamma^j]=0. \tag{A6}$$

As this relation is linear with respect to the frame $(\mathfrak{e}_1,\ldots,\mathfrak{e}_N)$ we may suppress the index a in what follows.

Lemma 7.1: Let $\omega\in\Gamma(\overset{*}{\tau}_{\mathrm{M}}\otimes_{\mathcal{M}}\tau^{(+)}_{\mathrm{Cl}})$ *be a Clifford algebra valued one-form where the coefficients* ω_ν *fulfill the relation* (A6). *Then, the most general form of* ω_ν *reads*

$$\omega_\nu=\sum_{k=0}^{n}\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{\nu[j_1\cdots j_k]} \tag{A7}$$

where the coefficients satisfy the relations:

$$\omega^{(n)}_{[\nu i_1\cdots i_n]}=0,$$

$$\omega^{(n-1)}_{[\nu i_1\cdots i_{n-1}]}=\varepsilon_{\nu i_1\cdots i_{n-1}}f,$$

$$kg^{\alpha\beta}\omega^{(k)}_{\alpha\beta i_1\cdots i_{k-1}}+\omega^{(k-2)}_{[i_1\cdots i_{k-1}]}=0,\quad k=n-1,\ldots,2,$$

$$g^{\alpha\beta}\omega^{(1)}_{\alpha\beta}=0. \tag{A8}$$

Here, respectively, $\omega^{(k)}_{\nu i_1\cdots i_k}\equiv\omega^{(k)}_{\nu[i_1\cdots i_k]}:=\omega^{(k)}_\nu(X_{i_1},\ldots,X_{i_k})$ *are the local coefficients of appropriate k-forms* $\omega^{(k)}_\nu\in\Omega^1(U)$ $(U\subset\mathcal{M}$ *open,* $\nu=1,\ldots,n)$, $f\in\mathcal{C}^\infty(U)$ *and* $\epsilon_{i_1\ldots i_n}\equiv\mu_{\mathrm{M}}(X_{i_1},\ldots,X_{i_n})$ *the Levi-Civita symbol.*

Proof: To get started we rewrite condition (A6) as $\gamma^\mu\gamma^\nu\omega_\nu+\gamma^\nu\omega_\nu\gamma^\mu=0$ and then appropriately rearrange both terms on the left-hand side.

$$\gamma^\nu\omega_\nu\gamma^\mu=\sum_{k=0}^{n}(-1)^k(\gamma^\nu\gamma^\nu\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{\nu i_1\cdots i_k}-2kg^{\mu i_1}\gamma^\nu\gamma^{j_2}\cdots\gamma^{j_k}\omega^{(k)}_{\nu i_1 i_2\cdots i_k}). \tag{A9}$$

Using this re-arrangement and formula (A3) one obtains

$$0=\sum_{k=0}^{n}((1-(-1)^k)(\gamma^\mu\gamma^\nu\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\nu i_1\cdots i_k]}+k\gamma^\mu\gamma^{j_2}\cdots\gamma^{j_k}g^{\alpha\beta}\omega^{(k)}_{\alpha\beta i_2\cdots i_k})+(-1)^k2(k+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\nu i_1\cdots i_k]}+(-1)^k2k(k-1)g^{\mu\nu}\gamma^{j_3}\cdots\gamma^{j_k}g^{\alpha\beta}\omega^{(k)}_{\alpha\beta\nu i_3\cdots i_k}). \tag{A10}$$

This sum may be further split into two sums of an even and odd number of Clifford elements. Since these terms are linearly independent one may evaluate each sum separately. For example, the sum of an odd number of Clifford elements gives rise to the condition:

$$0=\sum_{\substack{k=1\\(\text{k odd})}}^{n}(\gamma^\mu\gamma^\nu\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\nu i_1\cdots i_k]}+k\gamma^\mu\gamma^{j_2}\cdots\gamma^{j_k}g^{\alpha\beta}\omega^{(k)}_{\alpha\beta i_2\cdots i_k}-(k+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\nu i_2\cdots i_k]}-k(k-1)g^{\mu\nu}\gamma^{j_3}\cdots\gamma^{j_k}g^{\alpha\beta}\omega^{(k)}_{\alpha\beta\nu i_3\cdots i_k}). \tag{A11}$$

As (the caret denotes the omission of the "hated" object)

$$\gamma^\mu\gamma^\nu\gamma^{j_1}\cdots\gamma^{j_{n-1}}\omega^{(n-1)}_{[\nu i_1\cdots i_{n-1}]}=ng^{\mu\nu}\gamma^{j_1}\cdots\hat{\gamma^{j_\mu}}\cdots\gamma^{j_n}\omega^{(n-1)}_{[\nu i_1\cdots\hat{i_\mu}\cdots i_n]}, \tag{A12}$$

condition (A11) becomes equivalent to

$$0=\gamma^\mu\gamma^{j_2}\cdots\gamma^{j_{n-1}}((n-1)g^{\alpha\beta}\omega^{(n-1)}_{\alpha\beta i_2\cdots i_{n-1}}+\omega^{(n-3)}_{[i_2\cdots i_{n-1}]})+\sum_{\substack{k=3\\(\text{k odd})}}^{n-3}(-(k+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_k}((k+2)g^{\alpha\beta}\omega^{(k+2)}_{\alpha\beta\nu i_1\cdots i_k}+\omega^{(k)}_{[\nu i_1\cdots i_k]})+\gamma^\mu\gamma^{j_2}\cdots\gamma^{j_k}(kg^{\alpha\beta}\omega^{(k)}_{\alpha\beta i_2\cdots i_k}+\omega^{(k-2)}_{[i_2\cdots i_k]}))+\gamma^\mu g^{\alpha\beta}\omega^{(1)}_{\alpha\beta}. \tag{A13}$$

The term with the highest degree in the γ^{j_j} vanishes. By an induction argument one ends up with the recursion relation:

$$kg^{\alpha\beta}\omega^{(k)}_{\alpha\beta i_2\cdots i_k}+\omega^{(k-2)}_{[i_2\cdots i_k]}=0,\quad k=3,\ldots,n-1. \tag{A14}$$

As a consequence, it follows that $g^{\alpha\beta}\omega^{(1)}_{\alpha\beta}=0$. Moreover, the term $\omega^{(n-1)}_{[\nu i_1\ldots i_{n-1}]}$ drops out and thus is undetermined. Its most general form is given by

$$\omega^{(n-1)}_{[\nu i_1\ldots i_{n-1}]}=\varepsilon_{\nu i_1\ldots i_{n-1}}f, \tag{A15}$$

with f being an arbitrary locally defined smooth function on $\mathcal{M}$.

Next, we consider the sum of an even number of Clifford elements. This yields the relation

$$\sum_{\substack{k=0\\(\text{k even})}}^{n}((k+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\nu i_1\cdots i_k]}+k(k-1)g^{\mu\nu}\gamma^{j_3}\cdots\gamma^{j_k}g^{\alpha\beta}\omega^{(k)}_{\alpha\beta\nu i_3\cdots i_k})=0, \tag{A16}$$

which in turn gives rise to the following constraint equations:

$$0=(n+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_n}\omega^{(n-1)}_{[\nu i_1\cdots i_n]},$$

$$0=(n-1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_{n-2}}(ng^{\alpha\beta}\omega^{(n)}_{\alpha\beta\nu i_1\cdots i_{n-2}}+\omega^{(n-2)}_{[\nu i_1\cdots i_{n-2}]}),$$

$$\vdots$$

$$0=(k+1)g^{\mu\nu}\gamma^{j_1}\cdots\gamma^{j_k}((k+2)g^{\alpha\beta}\omega^{(k+2)}_{\alpha\beta\nu i_1\cdots i_k}+\omega^{(k)}_{[\nu i_1\cdots i_k]}),$$

$$\vdots$$

$$0 = g^{\mu\nu}\gamma^j\gamma^j(2g^{\alpha\beta}\omega^{(2)}_{\alpha\beta\nu} + \omega^{(0)}_{\nu}). \tag{A17}$$

These are satisfied provided that

$$0 = \omega^{(n)}_{[\nu i_1\cdots i_n]}$$

$$0 = (k+2)g^{\alpha\beta}\omega^{(k+2)}_{\alpha\beta\nu i_1\cdots i_k} + \omega^{(k)}_{[\nu i_1\cdots i_k]}, \quad k = 0, \ldots, n \tag{A18}$$

which, when combined with our previous result with respect to the sum of an odd number of Clifford elements, finally proves the statement. □

Corollary 7.1: Let ξ_F *be the chiral fermion bundle with respect to the Dirac triple* (G, ρ_F, D), *with D being of simple type and of arbitrary signature. The Dirac form of D reads* $\varpi_D = \Theta \wedge (\gamma_M \otimes \phi)$, *with* $\phi \in \Gamma(\mathrm{End}^-_{Cl}(\xi_F))$ *uniquely determined by D.*

Proof: Again, in the sequel we shall suppose that the induced Clifford relations, defining τ_{Cl}, are given by $\alpha\beta + \beta\alpha = +2g_M(\alpha, \beta)$. Locally, we may write $\varpi_D(X_\mu) = \omega^a_\mu \otimes \mathfrak{e}_a$ and, again, decompose the coefficients into the sum of odd and even terms with respect to the canonical involution $\alpha \mapsto -\alpha$ for all $\alpha \in T^*M \hookrightarrow Cl(M)$:

$$\omega^a_\mu = \sum_{k=1}^{n} \gamma^{j_1}\cdots\gamma^{j_k}\omega^a_{\mu[i_1\cdots i_k]} = \sum_{\substack{k=1 \\ (\text{k odd})}}^{n-1} \gamma^{j_1}\cdots\gamma^{j_k}\omega^a_{\mu[i_1\cdots i_k]} + \sum_{\substack{k=0 \\ (\text{k even})}}^{n} \gamma^{j_1}\cdots\gamma^{j_k}\omega^a_{\mu[i_1\cdots i_k]} \equiv \alpha^a_\mu + \beta^a_\mu. \tag{A19}$$

We then compute $\gamma^\mu\omega^a_\mu \equiv \gamma^\mu\alpha^a_\mu + \gamma^\mu\beta^a_\mu$ to show that $\gamma^\mu\omega^a_\mu \otimes \mathfrak{e}_a = \gamma_M \otimes \phi$.

With the help of formula (A4) one obtains (for notational convenience the index a is again suppressed)

$$\gamma^\mu\alpha_\mu = \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_{n-1}}\omega^{(n-1)}_{[\mu i_1\cdots i_{n-1}]} + 2g^{ij}\omega^{(1)}_{ij} + \sum_{\substack{k=1 \\ (\text{k odd})}}^{n-3} ((k+2)\gamma^{j_2}\cdots\gamma^{j_{k+2}}g^{ij}\omega^{(k+2)}_{ij[i_2\cdots i_{k+2}]}$$
$$+ \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\mu i_1\cdots i_k]}). \tag{A20}$$

Hence, using Lemma 7.1, one concludes that

$$\gamma^\mu\alpha_\mu = \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_{n-1}}\omega^{(n-1)}_{[\mu i_1\cdots i_{n-1}]}. \tag{A21}$$

Next, we consider $\gamma^\mu\beta_\mu$ and find, using similar arguments like those given earlier, that

$$\gamma^\mu\beta_\mu = \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_n}\omega^{(n)}_{[\mu i_1\cdots i_n]} + \sum_{\substack{k=0 \\ (\text{k even})}}^{n-2} ((k+2)\gamma^{j_2}\cdots\gamma^{j_{k+2}}g^{ij}\omega^{(k+2)}_{ij[i_2\cdots i_{k+2}]} + \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_k}\omega^{(k)}_{[\mu i_1\cdots i_k]}) = 0. \tag{A22}$$

Finally, using Lemma 7.1 again, we end up with

$$\gamma^\mu\omega_\mu = \gamma^\mu\gamma^{j_1}\cdots\gamma^{j_{n-1}}\omega^{(n-1)}_{[\mu i_1\cdots i_{n-1}]} = f\gamma^1\cdots\gamma^n = \tilde{f}\gamma_M. \tag{A23}$$

If we set $\phi \equiv \tilde{f}^\alpha\mathfrak{e}_a$, where $(\mathfrak{e}_1, \ldots, \mathfrak{e}_{N^-})$ is a local frame in $\mathrm{End}^-_{Cl}(\xi_F)$, we obtain the desired result and thus have also proved Proposition 3.1 in the case of τ_M. Of course, for $\tau^{(-)}_{Cl}$ the proof is similar. □

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q stars in scalar-tensor gravitational theories in extra dimensions

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We present Jordan-Brans-Dicke and general scalar-tensor gravitational theory in extra dimensions in an asymptotically flat or anti de Sitter spacetime. We consider a special gravitating, boson field configuration, a *q* star, in three, four, five, and six dimensions, within the framework of the above gravitational theory, and find that the parameters of the stable stars are a few percent different from the case of General Relativity. © *2006 American Institute of Physics.*
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I. INTRODUCTION — JORDAN-BRANS-DICKE THEORY IN ANY DIMENSION

Boson stars are stable configurations of a massive, complex scalar field coupled to gravity.[1,2] Self-interactions,[3,4] the coupling of the matter scalar field to a gauge field,[5] or the rotation of the solitonic object,[6] were taken into account. When the nonrelativistic theory admits nontopological soliton solutions, the corresponding relativistic generalizations, which are very large field configurations, are the soliton stars.[7–9] *Q* balls is a special class of nontopological solitons, appearing in Lagrangians with a global $U(1)$ symmetry,[10] a local $U(1)$,[11] or a non-Abelian $SU(3)$ or $SO(3)$ symmetry.[12] Q-stars have been investigated in various models, with one and two scalar fields,[13] non-Abelian symmetries,[14] with a scalar and a fermion field,[15] and with a local $U(1)$ symmetry[16] in asymptotically anti de Sitter spacetime,[17] and in four or more dimensions.[18]

Scalar-tensor gravitational theories appeared in the original papers of Brans and Dicke and Jordan.[19,20] The Newtonian constant G is replaced by the inverse mean value of a scalar field, ϕ_{BD}, and the total action contains kinetic terms for the new field times an ω_{BD} quantity, which is regarded as a constant in the original theory. The theory can be generalized by replacing the constant ω_{BD} by a function usually of the Brans-Dicke (BD) scalar field.[21,22] The theory of a scalar field with quartic self-interactions coupled to the metric and the BD scalar formulated in Ref. 23. Various properties of such configurations have been studied in a series of papers,[24,25] where especially the matter of gravitational memory of boson stars in scalar tensor gravity has been analyzed.[26,27] Their results generalized in scalar-tensor gravitational theories with ω_{BD} no more a constant, but a function of the BD scalar.[30–32]

The purpose of the present work is two-fold: We write the BD gravitational theory in D dimensions and apply our results in a realistic case of a scalar field, admitting *q*-ball type solutions in the absence of gravity. We compare our results with the corresponding ones obtained in General Relativity and we investigate the influence of the space-time dimensionality in the parameters of the star.

All the field configurations under consideration are spherically symmetric and static, so we use a static, spherically symmetric metric in D dimensions:

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$$ds^2 = -e^{\nu}\,dt^2 + e^{\lambda}\,d\rho^2 + \rho^2\,d\Omega_{D-2}^2, \tag{1}$$

with $g_{tt}=-e^{\nu}$ and $d\Omega_{D-2}^2$ the line element on a $(D-2)$-dimensional unit sphere. The action is

$$S = \frac{1}{16\pi}\int d^D x\sqrt{-g_D}\left[\phi_{\mathrm{BD}}(R-2\Lambda) - \frac{\omega_{\mathrm{BD}} g^{\mu\nu}\,\partial^{\lambda}\phi_{\mathrm{BD}}\,\partial_{\lambda}\phi_{\mathrm{BD}}}{\phi_{\mathrm{BD}}^2}\right] + S_{\mathrm{matter}}, \tag{2}$$

with S_{matter} the contribution to the total action of the matter fields. Λ stands for the negative, or zero, cosmological constant. The Einstein equations take the form

$$G_{\mu\nu} = \frac{8\pi}{\phi_{\mathrm{BD}}}T_{\mu\nu} + \frac{\omega_{\mathrm{BD}}}{\phi_{\mathrm{BD}}^2}\left(\partial_{\mu}\phi_{\mathrm{BD}}\,\partial_{\nu}\phi_{\mathrm{BD}} - \frac{1}{2}g_{\mu\nu}\,\partial^{\lambda}\phi_{\mathrm{BD}}\,\partial_{\lambda}\phi_{\mathrm{BD}}\right) + \frac{1}{\phi_{\mathrm{BD}}}\left(\phi_{\mathrm{BD},\mu;\nu} - g_{\mu\nu}\phi_{\mathrm{BD}}{}_{;\lambda}^{;\lambda}\right) - \Lambda g_{\mu\nu}, \tag{3}$$

where $T_{\mu}^{\nu}=\mathrm{diag}(-\varepsilon,p,\ldots,p)$ is the energy momentum tensor with trace $T=\varepsilon+Dp$. The equation of motion for the BD field is

$$\frac{2\omega_{\mathrm{BD}}}{\phi_{\mathrm{BD}}}\phi_{\mathrm{BD}}{}_{;\lambda}^{;\lambda} - \frac{\omega_{\mathrm{BD}}\,\partial^{\lambda}\phi_{\mathrm{BD}}\,\partial_{\lambda}\phi_{\mathrm{BD}}}{\phi_{\mathrm{BD}}^2} + R - 2\Lambda = 0. \tag{4}$$

Contracting Eq. (3), and substituting the trace in Eq. (4), we find the final form for the equation of motion of the BD field

$$\phi_{\mathrm{BD}}{}_{;\lambda}^{;\lambda} = \frac{8\pi T - 2\Lambda\phi_{\mathrm{BD}}}{(D-2)\omega_{\mathrm{BD}} + D - 1}. \tag{5}$$

Equation (5) reveals the dimensional sensitivity of the BD theory. Both T and the ω_{BD}-dependent factor depend on the space-time dimensionality.

We will now find the asymptotic relation for the BD field. For $p \ll \varepsilon$ and $\Lambda=0$, the tt component of the Einstein equations gives

$$G_t^t = -\frac{8\pi\varepsilon}{\phi_{\mathrm{BD}}}\frac{(D-2)\omega_{\mathrm{BD}} + D}{(D-2)\omega_{\mathrm{BD}} + D - 1}. \tag{6}$$

The corresponding result of the Einstein gravity is

$$G_t^t = -8\pi G_D\varepsilon. \tag{7}$$

We know that for $\varepsilon \ll$, the limit of the BD theory is the Einstein gravity. So, for localized matter configurations, the right boundary value at infinity for the BD field is

$$\phi_{\mathrm{BD}} = \frac{1}{G_D}\frac{(D-2)\omega_{\mathrm{BD}} + D}{(D-2)\omega_{\mathrm{BD}} + D - 1}. \tag{8}$$

One can verify that Eqs. (6) and (8) give the right result for the well-known four-dimensional case. We will now apply our results to a certain case of gravitating scalar matter, namely q stars. See (Figs. 1–4).

II. *q* STARS IN BD GRAVITATIONAL THEORY

The Lagrangian resulting from the presence of a matter scalar field is:

$$\mathcal{L}_{\mathrm{matter}} = -(\partial_{\mu}\phi)^{*}(\partial^{\nu}\phi) - U, \tag{9}$$

where ϕ is the matter scalar and U a suitable potential, admitting q-ball type solutions in the absence of gravity. We will now insert the q-soliton ansatz:

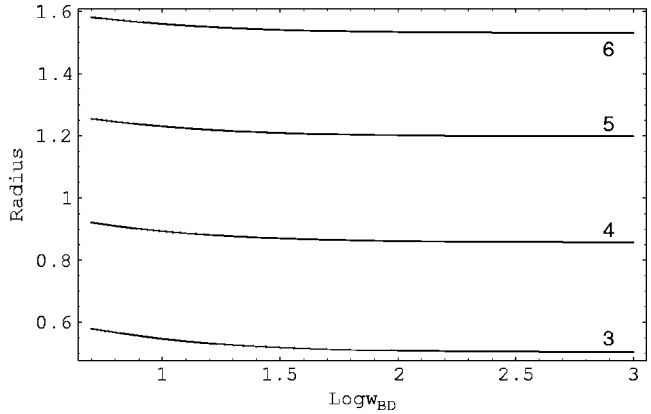

FIG. 1. The radius of a q star as a function of ω_{BD}. The numbers within the figures denote the space-time dimensionality. For $\omega_{BD} \simeq 1000$, the results of General Relativity are approximately reproduced. In Figs. 1–4 and 6–14 (later) we use $\omega=0.45$; equivalently $A_{sur}=0.81$. When decreasing ω_{BD}, the star parameters are a few percent larger.

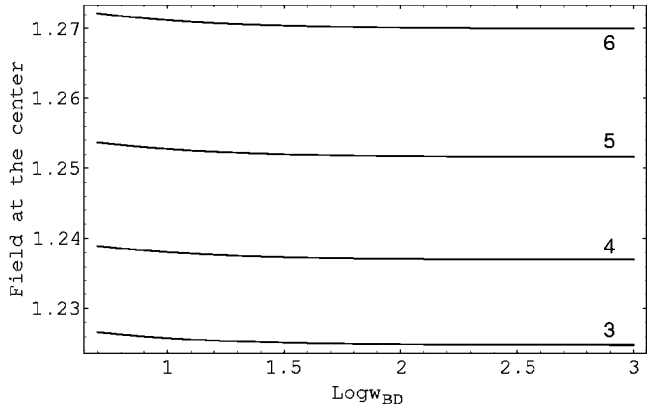

FIG. 2. The value of the matter scalar field at the center of the q star as a function of ω_{BD}.

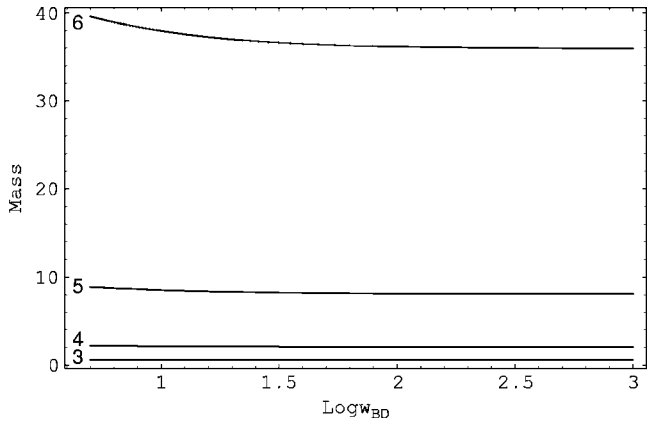

FIG. 3. The total energy of a q star as a function of ω_{BD}.

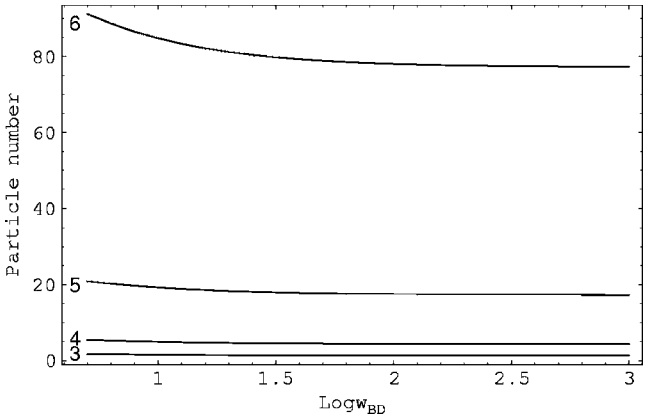

FIG. 4. The particle number of a q star as a function of ω_{BD}.

$$\phi(\vec{\rho},t)=\sigma(\rho)e^{-\iota\omega t}. \tag{10}$$

The equation of motion for the scalar field,

$$\phi_{;\lambda}{}^{;\lambda}-\frac{dU}{d|\phi|^2}\phi=0, \tag{11}$$

now takes the form

$$\sigma''+\left[\frac{D-2}{\rho}+\frac{1}{2}(\nu'-\lambda')\right]\sigma'+e^{\lambda}\omega^2e^{-\nu}\sigma-e^{\lambda}\frac{dU}{d\sigma^2}\sigma=0, \tag{12}$$

where the prime denotes the derivative with respect to ρ. We define

$$A=e^{-\lambda},\quad B=e^{-\nu}, \tag{13}$$

$$W\equiv e^{-\nu}\left(\frac{\partial\phi}{\partial t}\right)^{*}\left(\frac{\partial\phi}{\partial t}\right)=e^{-\nu}\omega^2\sigma^2,$$

$$V\equiv e^{-\lambda}\left(\frac{\partial\phi}{\partial\rho}\right)^{*}\left(\frac{\partial\phi}{\partial\rho}\right)=e^{-\lambda}\sigma'^2, \tag{14}$$

and rescale:

$$\tilde{\rho}=\rho m,\quad \tilde{\omega}=\omega/m,\quad \tilde{\phi}=\phi/m^{D-2/2},$$

$$\widetilde{U}=U/m^D,\quad \widetilde{W}=W/m^D,\quad \widetilde{V}=V/m^D. \tag{15}$$

We also rescale for convenience the BD scalar field:

$$\Phi_{\mathrm{BD}}=\phi_{\mathrm{BD}}G_D\frac{(D-2)\omega_{\mathrm{BD}}+D-1}{(D-2)\omega_{\mathrm{BD}}+D}. \tag{16}$$

Comparing Eqs. (8) and (16) we find that $\Phi_{\mathrm{BD}}\to 1$ for $\rho\to\infty$ and for localized field configurations.

Gravity becomes important when $R^{D-3}\sim G_DM(R)$, where $M(R)$ is a parameter, dependent on the mass trapped within a sphere of radius R. We define

$$\epsilon \equiv \sqrt{8\pi G_D m^{D-2}}, \tag{17}$$

which is a very small quantity for m of the order of magnitude of some (hundreds) GeV. We find for the interior of a q star that $U \sim W \sim m^D$, $V \sim \epsilon^2 m^D$, so the energy resulting from the spatial variation of matter field can be neglected within the star. We also define

$$\tilde{r} = \epsilon \tilde{\rho}. \tag{18}$$

We use a rescaled potential:

$$\tilde{U} = |\tilde{\phi}|^2 \left(1 - |\tilde{\phi}|^2 + \frac{1}{3}|\tilde{\phi}|^4\right) = \tilde{\sigma}^2 \left(1 - \tilde{\sigma}^2 + \frac{1}{3}\tilde{\sigma}^4\right). \tag{19}$$

This potential admits q-ball type solutions in the absence of gravity with $1 > \omega \geqslant (\sqrt{U/|\phi|^2}_{\min}) = 1/2$. Dropping from now on the overtildes and the $O(\epsilon)$ quantities, we find an analytical solution for the scalar field:

$$\sigma = (1 + \omega B^{1/2})^{1/2}, \quad W = B\omega^2(1 + \omega B^{1/2}), \quad U = \frac{1}{3}(1 + \omega^3 B^{3/2}). \tag{20}$$

The eigenvalue equation for the frequency ω of the scalar field can be found from the equation of motion of the matter field within the surface. As we know from Refs. 13–15 q-type solitons are characterized by a large interior where the scalar field is approximately constant and a thin surface of width of order of m^{-1}, where the scalar field varies rapidly from the σ value at the inner edge of the surface, to the zero value at the outer edge. The soliton exterior is clearly distinguished from the soliton interior and the surface, because the scalar field vanishes at the exterior. The situation is different in the case of *nonsolitonic* boson stars, where the star radius is of order of m^{-1}, the scalar field varies from $\sim M_{\mathrm{PI}}$ at the center of the soliton to the zero value outside, and there is no clear distinction between the star interior and the star surface. In the case of solitonic stars, the soliton radius is uniquely definned by the outer edge of the surface. Dropping the $O(\epsilon)$ quantities from the Lagrange equation within the surface, we find

$$V + W - U = 0. \tag{21}$$

The above equation holds true only within the surface. At the inner edge of the surface σ' and, consequently, V are zero, in order to match the interior with the surface solution, so $W = U$. Using also Eq. (20), we find

$$\omega = \frac{A_{\mathrm{sur}}^{1/2}}{2} = \frac{B_{\mathrm{sur}}^{-1/2}}{2}, \tag{22}$$

where $A_{\mathrm{sur}}, B_{\mathrm{sur}}$ denote the value of the metrics at the surface of the star. In the absence of gravity, $A(r) = B(r) = 1$, so $\omega = 1/2$.

We will now turn to the Einstein equations. In D dimensions,

$$G_t^{\ t} = \frac{A-1}{2r^2}(D-3)(D-2) + \frac{A'}{2r}(D-2),$$

$$G_r^{\ r} = \frac{A-1}{2r^2}(D-3)(D-2) - \frac{AB'}{2Br}(D-2). \tag{23}$$

The energy-momentum tensor for the matter scalar field is

$$T_{\mu\nu} = (\partial_\mu \phi)^*(\partial_\nu \phi) + (\partial_\mu \phi)(\partial_\nu \phi)^* - g_{\mu\nu}[g^{\alpha\beta}(\partial_\alpha \phi)^*(\partial_\beta \phi)] - g_{\mu\nu}U. \tag{24}$$

Using Eqs. (10), (13)–(15), and (20), and dropping the $O(\epsilon)$ quantities, we can write the Einstein equations:

$$G_t^{\ t} = \frac{(D-2)\omega_{\rm BD}+D-1}{[(D-2)\omega_{\rm BD}+D]\Phi_{\rm BD}} \times \left[-W-U-\frac{(D-2)W-DU-2\Lambda\Phi_{\rm BD}\dfrac{(D-2)\omega_{\rm BD}+D}{(D-2)\omega_{\rm BD}+D-1}}{(D-2)\omega_{\rm BD}+D-1} \right] - \frac{\omega_{\rm BD}A\Phi'^{\,2}_{\rm BD}}{2\Phi^2_{\rm BD}} - \frac{AB'\Phi'_{\rm BD}}{2\Phi_{\rm BD}B}, \tag{25}$$

$$G_r^{\ r} = \frac{(D-2)\omega_{\rm BD}+D-1}{[(D-2)\omega_{\rm BD}+D]\Phi_{\rm BD}} \times \left[W-U-\frac{(D-2)W-DU-2\Lambda\Phi_{\rm BD}\dfrac{(D-2)\omega_{\rm BD}+D}{(D-2)\omega_{\rm BD}+D-1}}{(D-2)\omega_{\rm BD}+D-1} \right] - \frac{\omega_{\rm BD}A\Phi'^{\,2}_{\rm BD}}{2\Phi^2_{\rm BD}} + \frac{A\Phi''_{\rm BD}}{\Phi_{\rm BD}} + \frac{A'\Phi'_{\rm BD}}{2\Phi_{\rm BD}}, \tag{26}$$

and the equation of motion for the BD field,

$$A\left[\Phi''_{\rm BD}+\left(\frac{D-2}{r}+\frac{A'}{2A}-\frac{B'}{2B}\right)\Phi'_{\rm BD}\right] = \frac{(D-2)W-DU-2\Lambda\Phi_{\rm BD}\dfrac{(D-2)\omega_{\rm BD}+D}{(D-2)\omega_{\rm BD}+D-1}}{(D-2)\omega_{\rm BD}+D}. \tag{27}$$

We numerically solve the coupled system of equations (25)–(27).

We can find the total mass of the field configuration by the relation

$$A(\rho) = 1 - \frac{2G_D m_\rho}{\rho^{D-3}} - \frac{2\Lambda\rho^2}{(D-2)(D-1)}, \tag{28}$$

where m_ρ is straightforward connected to the total mass, M_ρ, trapped within a sphere of radius ρ:

$$M_\rho = \frac{D-2}{8\pi}\frac{2\pi^{(D-2)/2}}{\Gamma\left(\dfrac{D-1}{2}\right)} m_\rho, \tag{29}$$

which, with our rescalings, gives for the total mass, M:

$$M = (D-2)\frac{\pi^{(D-1)/2}}{\Gamma\left(\dfrac{D-1}{2}\right)} r^{D-3}\left[1-A(r)-\frac{2\Lambda r^2}{(D-2)(D-1)}\right], \quad r\to\infty. \tag{30}$$

In the case of a rotating star, one should embed General Relativity in a more general framework, Metric-affine Gravity, where the correct renormalized mass is (in four dimensions):

$$\frac{M}{1+\dfrac{\Lambda}{3}\dfrac{J^2}{M^2}},$$

with J the total angular momentum of the star.[28,29] In our case the anti de Sitter mass is identical with the above renormalized mass, because $J=0$. The mass of Eqs. (28)–(30) is the Schwarzschild mass, which corresponds to the ADM mass in the Jordan frame. In the literature,[25,26] apart from the above mentioned mass, one also defines the ADM mass in the Einstein frame, or tensor mass M_T, and the Keplerian mass, $M_{\rm K}$. In the framework of a scalar tensor gravitational theory, these masses are obtained from the relations

$$M_{\mathrm{K}} = M + \Phi_1 \quad M_T = M + \frac{\Phi_1}{2}, \tag{31}$$

with

$$\Phi_1 = \lim_{r\to\infty}(r^2 \Phi'_{\mathrm{BD}}). \tag{32}$$

In our case we used the ADM mass in the Jordan frame for three reasons: It comes naturally from the Schwarzschild mass, we can deduce the Keplerian and tensor mass from Eqs. (31) and (32), and in our case is always larger from M_{K} and M_T. For the $\omega_{\mathrm{BD}}=-1$ case, and according to the literature,[25,26] $\Phi'_{\mathrm{BD}}>0$ holds at infinity. For our case ($\omega_{\mathrm{BD}}>5$), we found numerically that $\Phi'_{\mathrm{BD}}<0$, not only at infinity, but also for the whole region outside the soliton star. Because, in our case, $M>M_{\mathrm{K}}, M_T$, and because the energy of the same number of free particles is larger than M, we find that the energy of the free particles is always larger than M_{K} and M_T, confirming the stability of the soliton with respect to fission into free particles.

The Noether current that leads to the conserved particle number is

$$j^{\mu} = i\sqrt{-g_D}\, g^{\mu\nu}(\phi\, \partial_\nu \phi^* - \phi^*\, \partial_\nu \phi), \tag{33}$$

which gives a conserved Noether charge:

$$N = \int_0^{\infty} d^{D-1}x\, j^t = \frac{4\pi^{(D-2)/2}}{\Gamma\left(\frac{D-1}{2}\right)} \int_0^R dr\, \omega\sigma^2 r^{D-2} \sqrt{\frac{B}{A}}. \tag{34}$$

III. GENERAL SCALAR-TENSOR THEORY

In the original BD gravitational theory ω_{BD} is a constant. In a more general theory it may be regarded as a function, usually of the BD scalar. We use one of the simple functions investigated in a cosmological framework,[33,34] namely,

$$(D-2)\omega_{\mathrm{BD}} + D - 1 = \omega_0 \phi_{\mathrm{BD}}^n, \tag{35}$$

with ω_0 and n constants. The equation of motion for the BD field is

$$\phi_{\mathrm{BD}_{;\lambda}}{}^{;\lambda} = \frac{1}{(D-2)\omega_{\mathrm{BD}} + D - 1}\left(8\pi T - \frac{d\omega_{\mathrm{BD}}}{d\phi_{\mathrm{BD}}} \phi_{\mathrm{BD}}{}^{,\rho} \phi_{\mathrm{BD};\rho}\right). \tag{36}$$

We set for simplicity $\Lambda=0$. We rescale

$$\tilde{\omega}_0 = \frac{(D-2)\omega_{\mathrm{BD}} + D - 1}{(D-2)\omega_{\mathrm{BD}} + D} G_D^n \omega_0, \tag{37}$$

and the other quantities as in Eqs. (15)–(18). We will use for our calculations $n=1$. For $n=2,3,4$ the behavior of the star parameters is similar. Dropping the overtildes and the $O(\epsilon)$ quantities we find for the Einstein equations:

$$G_t{}^t = \frac{\omega_0}{\omega_0\Phi_{\mathrm{BD}} + 1}\left[-W - U - \frac{1}{\omega_0 \Phi_{\mathrm{BD}}} \quad \times \left((D-2)W - DU - \frac{A\Phi'^2_{\mathrm{BD}}}{D-2}\frac{\omega_0\Phi_{\mathrm{BD}} + 1}{\Phi_{\mathrm{BD}}}\right)\right]$$

$$- \frac{\omega_0\Phi_{\mathrm{BD}} - D + 1}{D-2}\frac{A\Phi'^2_{\mathrm{BD}}}{2\Phi^2_{\mathrm{BD}}} - \frac{AB'\Phi'_{\mathrm{BD}}}{2\phi_{\mathrm{BD}} B}, \tag{38}$$

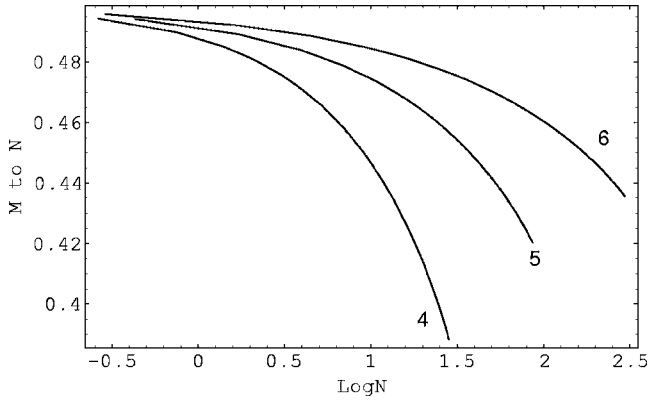

FIG. 5. The ratio of the star mass to its particle number as a function of the particle number for $\omega_{\mathrm{BD}}=500$. Small values of the particle number correspond to small stars, whose limiting value is the nongravitating q ball.

$$G_r{}^r = \frac{\omega_0}{\omega_0\Phi_{\mathrm{BD}}+1}\left[W-U-\frac{1}{\omega_0\Phi_{\mathrm{BD}}} \quad \times\left((D-2)W-DU-\frac{A\Phi'^{\,2}_{\mathrm{BD}}}{D-2}\frac{\omega_0\Phi_{\mathrm{BD}}+1}{\Phi_{\mathrm{BD}}}\right)\right]$$

$$-\frac{\omega_0\Phi_{\mathrm{BD}}-D+1}{D-2}\frac{A\Phi'^{\,2}_{\mathrm{BD}}}{2\Phi^2_{\mathrm{BD}}}+\frac{A\Phi''_{\mathrm{BD}}}{\phi_{\mathrm{BD}}}+\frac{A'\Phi'_{\mathrm{BD}}}{2\Phi_{\mathrm{BD}}}. \tag{39}$$

The equation of motion for the BD field is

$$A\left[\Phi''_{\mathrm{BD}}+\left(\frac{D-2}{r}+\frac{A'}{2A}-\frac{B'}{2B}\right)\Phi'_{\mathrm{BD}}\right]$$

$$=\frac{1}{\omega_0\Phi_{\mathrm{BD}}+1}\left[(D-2)W-DU-\frac{A\Phi'^{\,2}_{\mathrm{BD}}}{D-2}\frac{\omega_0\Phi_{\mathrm{BD}}+1}{\Phi_{\mathrm{BD}}}\right]. \tag{40}$$

We solve numerically the coupled system of equations (38)–(40). The mass and particle number of the star are given by Eqs. (30) and (34), respectively. We start from $\omega_0=5$ up to $\omega_0=1000$, where the results of general relativity are approximately reproduced.

IV. CONCLUSIONS

In the present work we write the Brans-Dicke and a simple scalar-tensor gravitational theory in D dimensions and apply it in a special case of stable, gravitating, scalar field configuration, namely that of a q star. The results of general relativity are reproduced for $\omega_{\mathrm{BD}},\omega_0\to\infty$. A generally accepted, lower experimental limit is $\omega_{\mathrm{BD}}\simeq 500$. Even for this value, the results almost coincide with General Relativity, and one can regard that the results of General Relativity are practically obtained from our figures when $\omega_{\mathrm{BD}},\omega_0=1000$. We investigate the phase space from $\omega_{\mathrm{BD}},\omega_0=5$ up to 1000 so as to gain a detailed picture of the behavior of the star parameters, radius, value of the matter scalar field at the center of the star, total mass, and particle number. For $\omega_{\mathrm{BD}},\omega_0<500$ the star parameters are a few percent larger than in the case of General Relativity. These differences are D dependent. For example, for $\omega_{\mathrm{BD}}=5$ the particle number is 33%, 24%, 21%, and 18% larger from the corresponding results in General Relativity, for $D=3,4,5$, and 6 dimensions, respectively; the radius is 15%, 7%, 4%, and 3% larger, respectively; and the total mass is $\gtrsim$0%, 7%, 9%, and 10% larger. One can find similar differences for the scalar-tensor theory.

The results of Figs. 1–5 and 11–14 refer to a zero cosmological constant. Figure 5 shows the ratio M/N of the star as a function of its particle number (M is the ADM star mass and N is the

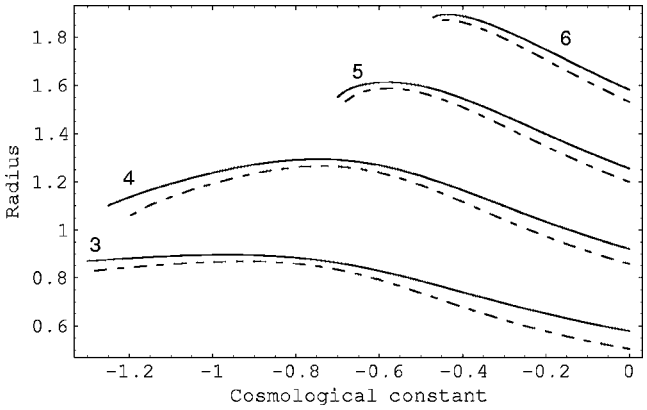

FIG. 6. The radius of a q star as a function of the cosmological constant. In Figs. 6–10, the dashed lines correspond to $\omega_{\mathrm{BD}}=500$ and the solid lines to $\omega_{\mathrm{BD}}=5$.

particle number). As one can see, every field configuration is stable with respect to fission into free particles. This feature is characteristic for solitonic gravitating objects, which are stable even in the absence of gravity. For example, a q star with very small particle number and mass corresponds to a (nongravitating) q ball (in the thin-wall approximation). For small q stars, one can see from Fig. 5 that $M/(mN)\rightarrow 0.5$, with m the mass of the free particles (here equal to unity with our rescalings). This is the correct limiting value in the absence of gravity, for the potential of 19, for which $\omega_{\mathrm{min}}\equiv(\sqrt{U/\sigma^2})_{\mathrm{min}}=0.5$. The picture is absolutely different for nonsolitonic boson stars,[35] where gravity and not the scalar potential is the main stabilizing factor. This means that for some region of the phase space, gravity is not strong enough to make the binding energy negative [equivalently, to make $M/(mN)<1$]. In Figs. 6–9 and for four, five, and six dimensions we start from a zero value of the cosmological constant, gradually decrease its value, and stop our calculations when $B(0)\rightarrow\infty$, or $\sigma(0)\rightarrow\infty$, showing in this way the formation of an anomaly at the center of the star. For $D=3$, when decreasing the value of Λ, we find that both mass and particle number increase up to their maximum value at approximately $\lambda\simeq -3$, and below this value, the energy is approximately constant, when the particle number decreases slowly. Below $\Lambda\simeq -10$, the energy of the free particles (identified with the particle number for $m=1$) is less than the soliton energy, which means that the decay into free particles is energetically favorable. All the other field configurations depicted in our figures are stable with respect to decay into free particles. (See Figs. 10–14).

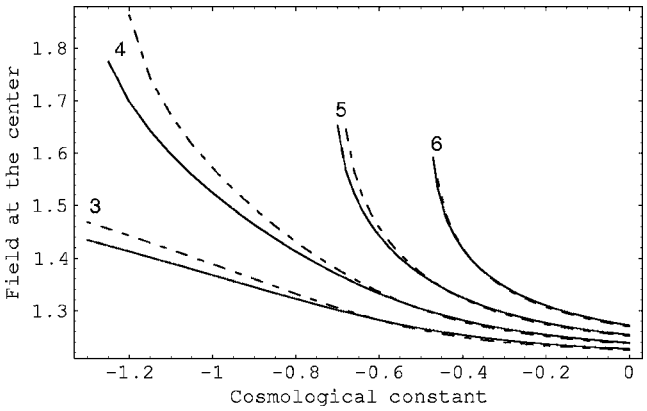

FIG. 7. The value of the matter scalar field at the center of a q star as a function of the cosmological constant.

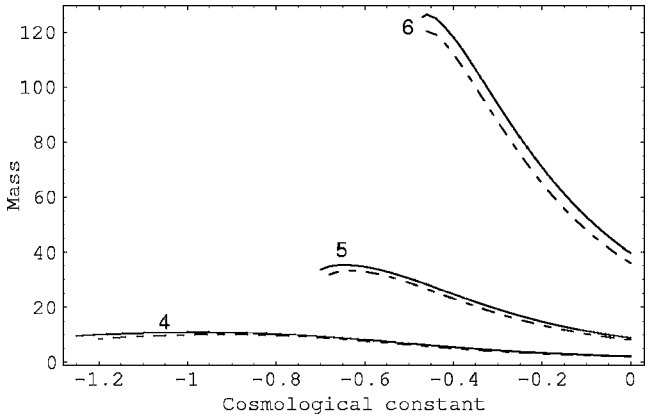

FIG. 8. The mass of a q star as a function of the cosmological constant.

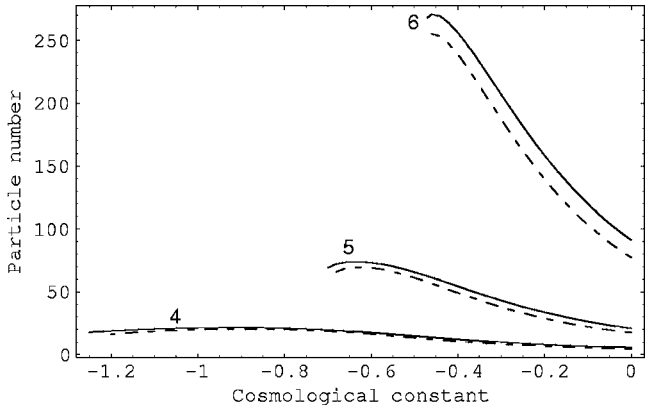

FIG. 9. The particle number of a q star as a function of the cosmological constant.

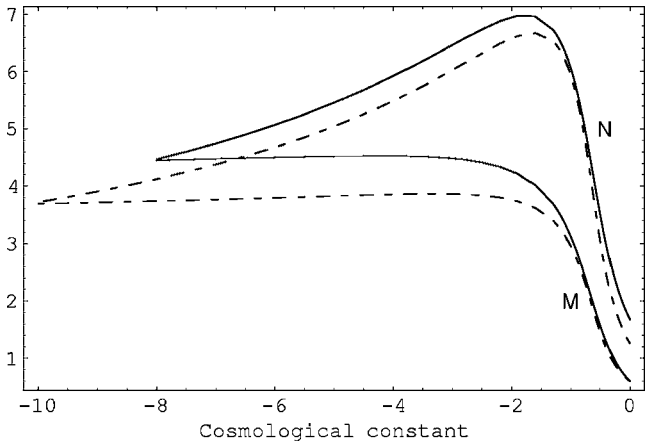

FIG. 10. The mass, M, and the particle number, N, of a q star in 2+1 dimensions as a function of the cosmological constant.

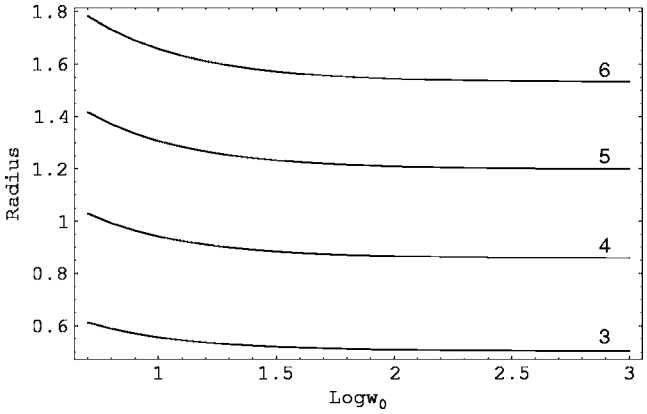

FIG. 11. The radius of a q star as a function of ω_0.

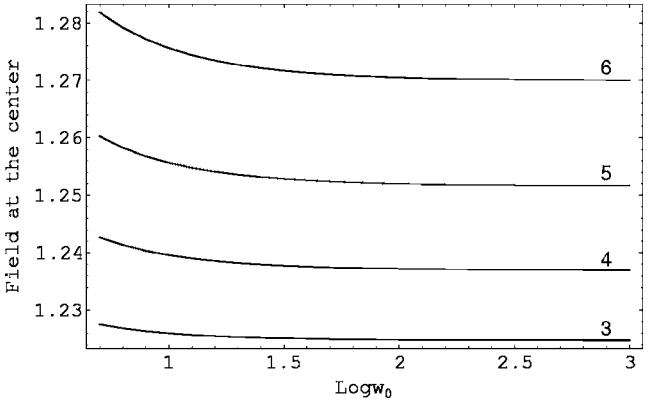

FIG. 12. The value of the matter scalar field at the center of the q star as a function of ω_0.

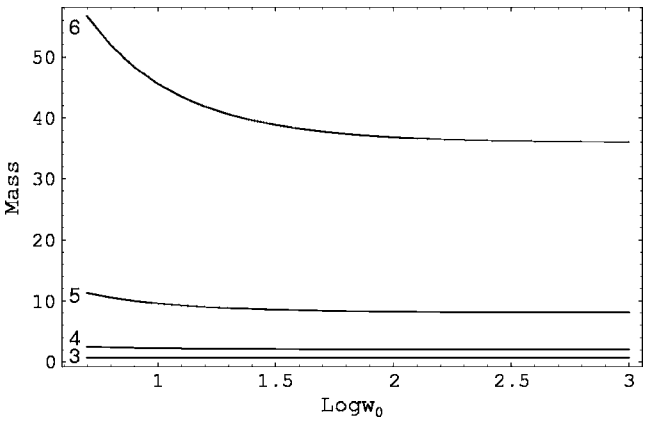

FIG. 13. The total energy of a q star as a function of ω_0.

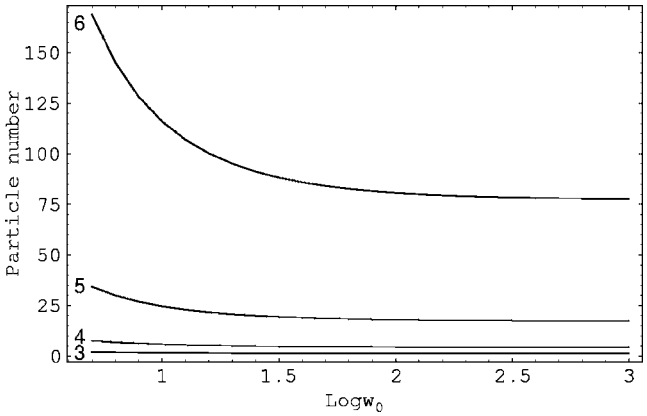

FIG. 14. The particle number of a q star as a function of ω_0.

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Mathematical analysis of the wavelet method of chaos control

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In this paper, we provide mathematical analysis for the controllability of chaos in wavelet subspaces. We prove that depending on the scale of the wavelet operation and the number of the coupled oscillators, the critical coupling strength for the occurrence of chaos synchronization becomes many times smaller if the original coupling matrix is appropriately treated with the wavelet transform. Moreover, we obtain rigorous relations connecting the critical values and the wavelet subspace operations. Our mathematical results are completely consistent with early numerical simulations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2203229]

I. INTRODUCTION

Chaos is ubiquitous in nature. Controlling chaos is of both theoretical and of practical importance.[1–5] Recently, a new paradigm of chaos control via wavelet transform has been introduced by Wei, Zhan, and Lai in Ref. 6 (also see Ref. 7). It is found that the transverse stability of the synchronous manifold of a chaotic system could be dramatically enhanced by the means of modifying a tiny fraction of the wavelet subspaces of a coupling matrix. Nevertheless, rigorous mathematical analysis of the aforementioned control has not been reported in the literature. Our objective in the present work is to present detailed mathematical analyses of the wavelet approach.[6]

To be more precise, let $du/dt=f(u)$ be a given chaotic oscillator. Consider a coupled nonlinear dynamical system of N chaotic oscillators,

$$\frac{d\mathbf{u}}{dt}=\mathbf{F}(\mathbf{u})+\epsilon\mathbf{A}\mathbf{u},\quad \mathbf{u}=(u_1,u_2,\ldots,u_N)^{\mathsf{T}}, \tag{1.1}$$

where $(\mathbf{F}(\mathbf{u}))_i=f(u_i)$ is a nonlinear function of the ith oscillator, which has a state function $u_i \in [0,\infty)\times\mathbb{R}^n$, ϵ is a coupling strength, and $\mathbf{A}$ is a coupling matrix having the periodic structure at the boundaries.

The synchronous manifold of the chaotic system, as a subspace of the original coupled system, Eq. (1.1), can be studied by setting $u_1(t)=u_2(t)=\cdots=u_N(t)=s(t)$, where the chaotic solution $s(t)$ satisfies the single oscillator equation $ds/dt=f(s(t))$. The stability property of the synchronous manifold can be studied in the space of difference variables $\delta u_i(t)=u_i(t)-s(t)$, which are governed by

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$$\frac{d\delta\mathbf{u}}{dt} = (D\mathbf{F}(\mathbf{S}(t)) + \epsilon\mathbf{A})\delta\mathbf{u}, \quad \delta\mathbf{u} = (\delta u_1, \delta u_2, \cdots, \delta u_N)^{\mathsf{T}}, \tag{1.2}$$

where $D\mathbf{F}(\mathbf{u}) = \mathrm{diag}(f'(u_1), f'(u_2), \cdots, f'(u_N))$ and $\mathbf{S}(t)^T = (s(t), s(t), \ldots, s(t))_{1\times N}$. The second largest eigenvalue λ_2 of the matrix $\mathbf{A}$ plays a dominant role in controlling the stability of chaotic synchronization.[8–10] A critical coupling strength ϵ_c can be determined in terms of λ_2,

$$\epsilon_c = \frac{L_{\max}}{-\lambda_2}, \tag{1.3}$$

where $L_{\max} > 0$ is the largest Lyapunov exponent of a single chaotic oscillator.

For the nearest neighbor coupling case, the eigenvalue spectrum of an appropriately normalized $\mathbf{A}$ is given by

$$-4\sin^2\frac{\pi(i-1)}{N}, \quad i = 1,2,\ldots,N. \tag{1.4}$$

In general, a wider coupling width gives a smaller λ_2, while a larger number of oscillators requires a larger ϵ_c. In controlling a given system, it is desirable to reduce the critical coupling strength ϵ_c.

Denote the two dimensional wavelet decomposition and its inverse with periodic boundary condition by $\mathbf{W}$ and $\mathbf{W}^{-1}$, respectively. For a given matrix $\mathbf{A}$, the wavelet decomposition allows a perfect reconstruction, by which there is nothing to gain: $\mathbf{A} = \mathbf{W}^{-1}(\mathbf{W}(\mathbf{A}))$. In Ref. 6, a simple operation is used to attain a desirable coupling matrix:

$$\tilde{\mathbf{A}} = \mathbf{W}^{-1}(\mathbf{O}_K(\mathbf{W}(\mathbf{A}))), \tag{1.5}$$

where $\mathbf{O}_K$ is limited to be the multiplication of a scalar factor K on the elements of subspaces $\mathbf{LL}_1$, which corresponds to the lowest resolution subspace in both the horizontal and vertical directions in a two-dimensional multiscale wavelet decomposition. A numerical simulation of a coupled system of 512 Lorenz oscillators in Ref. 6 shows that for the nearest neighbor coupling case, the critical coupling strength ϵ_c decreases linearly with respect to the increase of K up to a critical value K_c. The smallest ϵ_c is about 6, which is about 10^3 times smaller than the original critical coupling strength, indicating the efficiency of the proposed approach.

In this paper we will provide a rigid mathematical analysis of the above wavelet scheme. For simplicity and without loss of generality, we only consider the wavelet transformation and the reverse transformation based on the Daubechies wavelet, $db1$.[11]

By an i-scale wavelet operation $\mathbf{W} = \mathbf{W}(i)$ based on the $db1$ wavelet, a $2^k \times 2^k$ matrix $\mathbf{A}$ is transformed into another $2^k \times 2^k$ matrix $\mathbf{W}(\mathbf{A})$. Moreover, the subspaces $\mathbf{LL}_1$ or equally the $2^{k-i} \times 2^{k-i}$ up-left block of $\mathbf{W}(\mathbf{A})$ equals $\mathbf{\Omega A \Omega}^{\mathsf{T}}$, where

$$\mathbf{\Omega} = \frac{1}{2^{2i}}\begin{bmatrix} \mathbf{e} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{e} & \cdots & \mathbf{0} & \mathbf{0} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{e} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{e} \end{bmatrix}_{2^{k-i}\times 2^k},$$

with $\mathbf{e} = (1,1,\ldots,1)_{1\times 2^i}$ and $\mathbf{0} = (0,0,\ldots,0)_{1\times 2^i}$. In other words, every entry of $\mathbf{\Omega A \Omega}^{\mathsf{T}}$ is the average value of all items of some $2^i \times 2^i$ block of $\mathbf{A}$. With the transformation $\mathbf{O}_K$, $\mathbf{\Omega A \Omega}^{\mathsf{T}}$ is transformed into $K\mathbf{\Omega A \Omega}^{\mathsf{T}}$. Since $\mathbf{A} = \mathbf{W}^{-1}(\mathbf{W}(\mathbf{A}))$, we have that

$$\tilde{\mathbf{A}} = \mathbf{W}^{-1}(\mathbf{O}_K(\mathbf{W}(\mathbf{A}))) = \mathbf{A} + (K-1)\mathbf{\Omega A \Omega}^{\mathsf{T}}. \tag{1.6}$$

Before stating the main theorem, we introduce some notations. Define series $\{\rho_i\}_{i=1}^{\infty}$ by

$$\rho_i = 2\cos\frac{\pi}{2^i} - 2, \quad i = 1,2,3,\ldots . \tag{1.7}$$

Moreover, we denote

$$K_c(i,N) = \frac{-2^i\rho_i}{4\sin^2\dfrac{2^i\pi}{N}} + 1, \quad i = 1,2,3,\ldots . \tag{1.8}$$

Theorem 1: *For any $i \in \mathcal{N}$, assume ρ_i is defined as in* (1.7) *and the nature numbers N satisfy $N/2^{i+2} \in \mathcal{N}$. Let* $\mathbf{A}$ *be the nearest neighbor-coupling matrix of order $N \times N$ defined as in Eq.* (1.1). *Suppose by i-scale wavelet operation* (1.5) *with the scalar factor $K \geq 1$ that the coupling matrix is transformed from* $\mathbf{A}$ *to* $\tilde{\mathbf{A}}$. *Then for any such K, all the eigenvalues of* $\tilde{\mathbf{A}}$ *are nonpositive; Moreover, it holds that ρ_i is an eigenvalue of the matrix* $\tilde{\mathbf{A}}$.

Theorem 2: *Let i, ρ_i, N,* $\mathbf{A}$, $\tilde{\mathbf{A}}$, *K be defined as in Theorem 1. Assume $K_c(i,N)$ are defined by* (1.8). *Then the second largest eigenvalue of* $\tilde{\mathbf{A}}$ *is a decreasing function of K. Moreover, the second largest eigenvalue of* $\tilde{\mathbf{A}}$ *is equal to ρ_i for any $K \geq K_c(i,N)$ and is strictly larger than ρ_i (thus its absolute value is strictly less than $-\rho_i$) for any $1 \leq K < K_c(i,N)$.*

Since the critical coupling strength is determined in terms of the second largest eigenvalue of the coupling matrix, by Theorem 2 and (1.4) we have the following result.

Corollary 1.1: *The i-scale wavelet control method with $K_c(i,N)$ as the scalar factor can enhance the stability of a synchronous manifold of an N coupled system by reducing the critical coupling strength as much as $\rho_i/4\sin^2(\pi/N)$ time.*

In the following, we denote a "block circulant matrix" with blocks $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_n$ by

$$b\mathrm{circ}(\mathbf{A}_1,\mathbf{A}_2,\ldots,\mathbf{A}_n) = \begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 & \mathbf{A}_3 & \cdots & \cdots & \mathbf{A}_n \\ \mathbf{A}_n & \mathbf{A}_1 & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \mathbf{A}_4 & \ddots & \ddots & \ddots & \mathbf{A}_2 & \mathbf{A}_3 \\ \mathbf{A}_3 & \mathbf{A}_4 & \ddots & \ddots & \mathbf{A}_1 & \mathbf{A}_2 \\ \mathbf{A}_2 & \mathbf{A}_3 & \mathbf{A}_4 & \cdots & \mathbf{A}_n & \mathbf{A}_1 \end{bmatrix}.$$

Moreover, we denote average values of all elements of a matrix $\mathbf{A} = (a_{ij})_{n\times n}$ by $\mathrm{aver}(\mathbf{A})$, that is, $\mathrm{aver}(\mathbf{A}) = (1/n^2)\sum_{i,j=1}^{n} a_{ij}$.

II. PROOF OF THE MAIN THEOREMS

In this section, we will prove Theorem 1 and Theorem 2. First, we introduce some useful lemmas.

A. Preliminaries

Lemma 2.1: Assume matrix $\mathbf{A}$ *is of order $N \times N$ and* $\tilde{\mathbf{A}}$ *is defined by i-scale wavelet operation* (1.5) *with the scalar factor $K \geq 1$. Then it holds that*

$$\tilde{\mathbf{A}} - \mathbf{A} = \frac{K-1}{2^{2i}}\mathbf{A}_{N_i} \otimes \mathbf{B}_i, \tag{2.1}$$

with

$$\mathbf{A}_{N_i}=\begin{bmatrix} -2 & 1 & & & 1 \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & 1 & -2 \end{bmatrix}_{N_i\times N_i}$$

and

$$\mathbf{B}_i=\mathbf{e}^{\mathsf{T}}\mathbf{e},$$

where $N_i=N/2^i$, $\mathbf{e}$ *is defined as in the introduction, and* $\otimes$ *represents tensor product of matrices.*

Proof: First note that the nearest neighbor matrix $\mathbf{A}$ can be written in the form

$$b\text{circ}(\mathbf{A}_1,\mathbf{A}_2,\ldots,\mathbf{A}_{N_i}),\quad N_i=\frac{N}{2^i},$$

where matrix $\mathbf{A}_j$ of order $2^i\times 2^i$ $(j=1,2,\ldots,N_i)$ satisfies

$$\mathbf{A}_1=\begin{bmatrix} -2 & 1 & & \cdots & 0 \\ 1 & -2 & \ddots & & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & \ddots & 1 \\ 0 & \cdots & & 1 & -2 \end{bmatrix},\quad \mathbf{A}_2=\mathbf{A}_{N_i}^{\mathsf{T}}=\begin{bmatrix} 0 & \ldots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \ldots & 0 & 0 \\ 1 & \ldots & 0 & 0 \end{bmatrix},\tag{2.2}$$

$$\mathbf{A}_l=\mathbf{0},\quad 3\le l\le\frac{N}{2^i}-1.\tag{2.3}$$

It is obvious to see that $\text{aver}(\mathbf{A}_1)=-1/2^{2i-1}$ and $\text{aver}(\mathbf{A}_2)=\text{aver}(\mathbf{A}_{N_i})=1/2^{2i}$.

From (1.6), we obtain that $\tilde{\mathbf{A}}$ is of the form

$$\tilde{\mathbf{A}}=b\text{circ}(\tilde{\mathbf{A}}_1,\tilde{\mathbf{A}}_2,\ldots,\tilde{\mathbf{A}}_{N_i}),\tag{2.4}$$

with

$$\tilde{\mathbf{A}}_1=-\frac{K-1}{2^{2i-1}}\mathbf{B}_i+\mathbf{A}_1,\quad \tilde{\mathbf{A}}_2=\frac{K-1}{2^{2i}}\mathbf{B}_i+\mathbf{A}_2,\quad \tilde{\mathbf{A}}_{N_i}=\frac{K-1}{2^{2i}}\mathbf{B}_i+\mathbf{A}_{N_i},$$

$$\tilde{\mathbf{A}}_j=\mathbf{0},\quad 3\le j\le N_i-1.\tag{2.5}$$

Thus the lemma can be obtained easily. □

Proposition 2.1: Let $\mathbf{A}=b\text{circ}(\mathbf{A}_1,\mathbf{A}_2,\ldots,\mathbf{A}_n)$ *be a real symmetric block circulant matrix. Denote* $\mathbf{C}_k=\Sigma_{j=1}^{n}e^{\iota[k(j-1)/n]2\pi}\mathbf{A}_j$, $k=0,1,\ldots,n-1$, $\iota=\sqrt{-1}$. *Then eigenvalues of* $\mathbf{A}$ *consist of eigenvalues of* $\mathbf{C}_k$, $k=0,1,\ldots,n-1$.

Proof: See p. 211 in Ref. 12. □

B. Proof of Theorem 1

Proof of nonpositivity: First, we prove that for any $K\ge 1$, all the eigenvalues of $\tilde{\mathbf{A}}$ are nonpositive. From Lemma 2.1, we have that

$$\tilde{\mathbf{A}} = \mathbf{A} + \frac{K-1}{2^{2i}} \mathbf{A}_{N_i} \otimes \mathbf{B}_i. \tag{2.6}$$

We will prove that $[(K-1)/2^{2i}]\mathbf{A}_{N_i} \otimes \mathbf{B}_i$ is seminegative definite. Then by the seminegative definiteness of $\mathbf{A}$ and the fact that the sum of two seminegative definite matrices is seminegative definite, we obtain that $\tilde{\mathbf{A}}$ is also seminegative definite. Thus all its eigenvalues are nonpositive. Since $[(K-1)/2^{2i}]\mathbf{A}_{N_i} \otimes \mathbf{B}_i$ is a real symmetric block circulant, by Proposition 2.1, it is sufficient to prove the nonpositivity of eigenvalues of matrices,

$$-2\mathbf{B}_i + e^{\mathrm{i}(k2^i/N)2\pi}\mathbf{B}_i + e^{\mathrm{i}[k(N-2^i)/N]2\pi}\mathbf{B}_i, \quad k = 0,1,\ldots,\frac{N}{2^i} - 1, \tag{2.7}$$

or equally,

$$\left(-2 + 2\cos\frac{k2^i}{N}2\pi\right)\mathbf{B}_i, \quad k = 0,1,\ldots,\frac{N}{2^i} - 1. \tag{2.8}$$

Obviously, $\mathbf{B}_i$ has 0 and 1 as its eigenvalues and the term in the parentheses is less than or equal to 0. Thus, each eigenvalue of the matrices defined in (2.7) and (2.8) is nonpositive. Then from the symmetry, we obtain that $(K-1)/2^{2j}\mathbf{A}_{N_i} \otimes \mathbf{B}_i$ is seminegative definite. Thus, the proof is completed. □

Remark 2.1: From the fact that $\mathbf{A}$ *has only one zero eigenvalue, we conclude that* $\tilde{\mathbf{A}}$ *has at most one zero eigenvalue. On the other hand, since the sum of elements in every column of* $\tilde{\mathbf{A}}$ *is zero, we obtain that* $\tilde{\mathbf{A}}$ *has at least one zero eigenvalue. In a word, it has and only has one zero eigenvalue.*

Now we prove the second part of Theorem 1, that is, for any $K \geq 1$, ρ_i is an eigenvalue of the matrix $\tilde{\mathbf{A}}$.

Combining (2.4), (2.5) and Proposition 2.1, we have that the set of eigenvalues of $\tilde{\mathbf{A}}$ is equal to the collection of the eigenvalue of the $2^i \times 2^i$ matrix,

$$\mathbf{D}_1(l) + d_l\mathbf{D}_2(l) := \begin{bmatrix} -2 & 1 & & & e^{-i(2\pi l/n)} \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ e^{i(2\pi l/n)} & & & 1 & -2 \end{bmatrix} + d_l \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} [1 \ldots 1],$$

$$l = 0,1,\ldots,n-1,$$

with $n = N/2^i$, $d_l = (c/2^{2i})[2\cos(2\pi l/n) - 2]$, $c = K-1$.

The following two propositions are useful for the proof of Theorem 1 and Theorem 2.

Proposition 2.2 (rank one update for Hermitian matrices): *Let* $\mathbf{A}$ *be an* $N \times N$ *Hermitian matrix and* $\mathbf{u} \in \mathcal{C}^{\mathbf{N}}$. *Suppose* $(\lambda_k, \mathbf{u}_k)$ *and* $(\tilde{\lambda}_k(\alpha), \tilde{\mathbf{u}}_k(\alpha))$, $k = 1,\ldots,N$, *be, respectively, the eigenpairs for* $\mathbf{A}$ *and* $\mathbf{A} + \alpha\mathbf{u}\mathbf{u}^H$ *with the order* $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ *and* $\tilde{\lambda}_1 \leq \tilde{\lambda}_2 \leq \cdots \leq \tilde{\lambda}_N$.

(i) Assume $\alpha > 0$. *If* $\mathbf{u}^H\mathbf{u}_k \neq 0$ *and* $\mathbf{u}^H\mathbf{u}_{k'} \neq 0$ *for some* $k' > k$; *then* $\lambda_k \leq \tilde{\lambda}_k(\alpha) \leq \lambda_{k'}$.

(ii) If $\mathbf{u}^H\mathbf{u}_{k''} = 0$ *for some* k''; *then* $\tilde{\lambda}_{k''}(\alpha) = \lambda_{k''}$ *for all* α.

Proof: See Ref. 13. □

Proposition 2.3: Denote $(\lambda_k, \mathbf{u}_k)$, $k=0,\ldots,m-1$, *the eigenpair of the matrix*

$$\mathbf{G} = \begin{bmatrix} -2 & 1 & & & e^{-\imath\alpha} \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ e^{\imath\alpha} & & & 1 & -2 \end{bmatrix}_{m\times m}$$

with α *any real number. Then*

$$\lambda_k = 2\cos\theta_k - 2$$

and

$$\mathbf{u}_k = (u_{k,j})_{j=1}^{m},$$

where

$$\theta_k = \frac{2k\pi}{m} + \frac{\alpha}{m}, \quad k = 0, \ldots, m-1,$$

and

$$u_{k,j} = \begin{cases} 1, & \text{if } k^2+\alpha^2 = 0, \\ c_1(\sin j\theta_k + e^{-\imath\alpha}\sin(m+j)\theta_k) + c_2(\sin(m+1+j)\theta_k + e^{\imath\alpha}\sin(j+1)\theta_k), & \text{otherwise.} \end{cases}$$

Here c_1 *and* c_2 *are arbitrary complex numbers.*

Proof: By directly solving the eigenvalue problem for $\mathbf{G}$, $\mathbf{Gu}=\lambda\mathbf{u}$, we obtain the difference equation

$$u_{j+1} - (2+\lambda)u_j + u_{j-1} = 0, \quad j = 2, \ldots, m-1, \tag{2.9}$$

with

$$u_0 = e^{-\imath\alpha}u_m,$$

$$u_{m+1} = e^{\imath\alpha}u_1. \tag{2.10}$$

Equation (2.9) has characteristic equation $r^2-(2+\lambda)r+1=0$, which yields

$$r_{1,2} = \frac{(2+\lambda) \pm \sqrt{(2+\lambda)^2-4}}{2} =: e^{\pm\imath\theta}. \tag{2.11}$$

The second equality holds since eigenvalues of $\mathbf{G}$ are nonpositive. Now set

$$u_j = Ar_1^j + Br_2^j = Ae^{\imath j\theta} + Be^{-\imath j\theta}, \tag{2.12}$$

where A and B are constant coefficient to be determined. Substituting (2.12) into (2.10), we obtain

$$A + B = e^{-\imath\alpha}(Ae^{\imath m\theta} + Be^{-\imath m\theta}),$$

$$Ae^{\imath(m+1)\theta} + Be^{-\imath(m+1)\theta} = e^{\imath\alpha}(Ae^{\imath\theta} + Be^{-\imath\theta}). \tag{2.13}$$

Since (A,B) is a nonzero solution of Eq. (2.13), it turns out that

$$\begin{vmatrix} 1-e^{\imath(m\theta-\alpha)} & 1-e^{-(\imath m\theta+\alpha)} \\ e^{\imath(m+1)\theta}-e^{\imath(\theta+\alpha)} & e^{-\imath(m+1)\theta}-e^{-\imath(\theta-\alpha)} \end{vmatrix} = 0,$$

or, equivalently,

$$\cos m\theta = \cos \alpha.$$

Thus, $\theta_k = 2k\pi/m + \alpha/m$, $k=0,\ldots,m-1$, and, hence, by using (2.11), we have $\lambda_k = 2\cos\theta_k - 2$. This gives the proof of the first assertion.

To see the eigenvector of $\mathbf{G}$ corresponding to eigenvalue λ_k, we first consider that for $\alpha=0$ and $k=0$, i.e., $\lambda_0=0$. It is easy to see that the vector $(1,\ldots,1)^{\mathsf{T}}$ is the eigenvector of $\mathbf{G}$ corresponding to 0. Now, assume $\alpha\neq 0$ and $k\neq 0$. For convenience, we write $\theta=\theta_k$ and $u_j=u_{k\cdot j}$. Choose $A_1=1-e^{\imath(m\theta-\alpha)}$, $B_1=-1+e^{-\imath(m\theta+\alpha)}$, $A_2=e^{\imath(m+1)\theta}-e^{\imath(\theta+\alpha)}$, and $B_2=-e^{-\imath(m+1)\theta}+e^{-\imath(\theta-\alpha)}$ with $\theta=\theta_k$ for some k. Note that (A_1,B_1) and (A_2,B_2) are solutions of (2.13). Set $u_j=\frac{1}{2}(c_1A_1+c_2A_2)e^{\imath j\theta}+\frac{1}{2}(c_1B_1+c_2B_2)e^{-\imath j\theta}=c_1(\sin j\theta_k+e^{-\imath\alpha}\sin(m+j)\theta_k)+c_2(\sin(m+1+j)\theta_k+e^{\imath\alpha}\sin(j+1)\theta_k)$ and the second assertion follows. □

Proof of the second part of Theorem 1: Let $\alpha=\pi$ and $m=2^i$. From Proposition 2.3, it follows that ρ_i is an eigenvalue of $\mathbf{D}_1(n/2)$. To see that ρ_i is also an eigenvalue of $\mathbf{D}_1(n/2)+d_{n/2}\mathbf{D}_2(n/2)$, we choose $c_1=1$ and $c_2=0$. From Proposition 2.3 again, $\mathbf{D}_1(n/2)$ has an eigenvector $\mathbf{u}=[\sin(j\pi/m)]_{j=1}^m$ corresponding to the eigenvalue ρ_i. Since $\mathbf{D}_2=\mathbf{e}\mathbf{e}^{\mathsf{T}}$ and $\mathbf{e}^{\mathsf{T}}\mathbf{u}=\Sigma_{j=1}^m\sin(j\pi/m)=0$, applying (ii) of Proposition 2.2, we see that ρ_i is an eigenvalue of $\mathbf{D}_1(n/2)+d_{n/2}\mathbf{D}_2(n/2)$. □

C. Proof of Theorem 2

Proof of the first part of Theorem 2: Let $n=N/2^i$ and $\mathbf{D}_1(l),\mathbf{D}_2(l),d_l,l=0,1,\cdots,n-1$ be defined as in the last subsection. Since $d_l\leq 0$, applying Proposition 2.2 to $-\mathbf{D}_1(l)-d_l\mathbf{D}_2(l)$, we have that the eigenvalues of $\mathbf{D}_1(l)+d_l\mathbf{D}_2(l)$ are increasing functions of d_l, which, by Proposition 2.1, implies the first part of Theorem 2, that is, the second largest eigenvalue of $\tilde{\mathbf{A}}$ is a decreasing function of K. □

Now we are in a position to prove the second part of Theorem 2.

Denote $\alpha=2\pi l/n$. We have

$$\mathbf{D}_1(l)=\begin{bmatrix} -2 & 1 & & & e^{-\imath\alpha} \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ e^{\imath\alpha} & & & 1 & -2 \end{bmatrix}. \tag{2.14}$$

From Proposition 2.3, we have that any eigenvalue of $\mathbf{D}_1(l)$ can be written in the form

$$\lambda = 2\cos\theta(k,l) - 2,$$

with $\theta(k,l)=2k\pi/2^i+\alpha/2^i$, $k=0,1,\ldots,2^i-1$, $l=0,1,\ldots,n-1$. Obviously, for every such l and k_1,k_2 with $k_1\neq k_2$, it holds that $|\theta(k_1,l)-\theta(k_2,l)|\geq 2\cdot\pi/2^i$, which implies that there is at most one $k\in\{0,1,\ldots,2^i-1\}$ such that $|\theta(k,l)|\leq\pi/2^i$. Then we have that for every matrix $\mathbf{D}_1(l)+d_l\mathbf{D}_2(l)$ $(l=0,1,\ldots,n-1)$, there is at most one nonzero eigenvalue that is larger than or equal to $\rho_i=2\cos(\pi/2^i)-2$. It implies that if for some $d_l=d_l^*$, $\mathbf{D}_1(l)+d_l\mathbf{D}_2(l)$ has eigenvalue ρ_i, then all its other eigenvalues are less than ρ_i.

Remark 2.2: If such d_l^* exists for $\mathbf{D}_1(l)+d_l\mathbf{D}_2(l)$, then by the first part of Theorem 2, we have that all its eigenvalues will be less than or equal to ρ_i for all $d_l<d_l^*$. Then for the proof of the second part of Theorem 2, it is sufficient to prove that the existence of such d_l^* for every l.

The following proposition will help us to complete the proof of Theorem 2.

Proposition 2.4: Let $d=[2\cos(\pi/m)-2]/m$. *Then the matrix*

$$\mathbf{G}=\begin{bmatrix} -2 & 1 & & & e^{-\imath\alpha} \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ e^{\imath\alpha} & & & 1 & -2 \end{bmatrix}+d\begin{bmatrix} 1 \\ \vdots \\ \vdots \\ 1 \end{bmatrix}[1,\ldots,1]\in\mathbb{R}^{m\times m},$$

has eigenvalue $2\cos(\pi/m)-2$ *for and* $\alpha\neq 0,\pm\pi$.

Proof: Consider the eigenproblem of the matrix **G**, which is equivalent to

$$u_{k-1}-(\lambda+2)u_k+u_{k+1}+d\sum_{j=1}^{m}u_j=0,\quad k=2,\ldots,m-1, \tag{2.15}$$

$$u_2-2u_1+e^{-\imath\alpha}u_m+d\sum_{j=1}^{m}u_j=0, \tag{2.16}$$

$$u_{m-1}-2u_m+e^{\imath\alpha}u_1+d\sum_{j=1}^{m}u_j=0. \tag{2.17}$$

Denote $\tilde{u}_k=u_k/\Sigma_{j=1}^{m}u_j$. Then we have

$$\tilde{u}_{k-1}-(\lambda+2)\tilde{u}_k+\tilde{u}_{k+1}+d=0,$$

$$\tilde{u}_2-2\tilde{u}_1+e^{-\imath\alpha}\tilde{u}_m+d=0,$$

$$\tilde{u}_{m-1}-2\tilde{u}_m+e^{\imath\alpha}\tilde{u}_1+d=0. \tag{2.18}$$

In the following, for the sake of notation without leading confusion, we use the notation u_k with the restriction $\Sigma_{j=1}^{m}u_j=1$ to replace the notation $\tilde{u}_k$.

Obviously, (2.18) has a special solution of the form $u_k=d/\lambda$, $k=1,\ldots,m$. Thus the general solution of (2.18) is of the form

$$u_k=C_1e^{\imath k\theta}+C_2e^{-\imath k\theta}+\frac{d}{\lambda}, \tag{2.19}$$

with the boundary condition

$$u_0=e^{-\imath\alpha}u_m,\quad u_{m+1}=e^{\imath\alpha}u_1, \tag{2.20}$$

where $\cos\theta=(\lambda+2)/2$.

Now we determine C_1 and C_2 with the boundary condition

$$C_1+C_2+\frac{d}{\lambda}=C_1e^{\imath(-\alpha+m\theta)}+C_2e^{-\imath(\alpha+m\theta)}+e^{-\imath\alpha}\frac{d}{\lambda} \tag{2.21}$$

and

$$C_1e^{\imath(m+1)\theta}+C_2e^{-\imath(m+1)\theta}+\frac{d}{\lambda}=C_1e^{\imath(\theta+\alpha)}+C_2e^{\imath(-\theta+\alpha)}+e^{i\alpha}\frac{d}{\lambda}. \tag{2.22}$$

Thus we have

$$\begin{bmatrix} 1 & 1 \\ -e^{\imath(\theta+\alpha)} & -e^{\imath(-\theta+\alpha)} \end{bmatrix} \begin{bmatrix} 1-e^{\imath(-\alpha+m\theta)} & 0 \\ 0 & 1-e^{-\imath(\alpha+m\theta)} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \frac{d}{\lambda} \begin{bmatrix} e^{-\imath\alpha}-1 \\ e^{\imath\alpha}-1 \end{bmatrix}.$$

Then we have

$$C_1 = \frac{-(e^{-\imath\alpha}-1)e^{-\imath(\theta-\alpha)} - (e^{\imath\alpha}-1)}{(1-e^{\imath(-\alpha+m\theta)})(e^{\imath(\theta+\alpha)} - e^{\imath(-\theta+\alpha)})} \frac{d}{\lambda} \tag{2.23}$$

and

$$C_2 = \frac{e^{\imath\alpha} - 1 + (e^{-\imath\alpha}-1)e^{\imath(\theta+\alpha)}}{(1-e^{-\imath(\alpha+m\theta)})(e^{\imath(\theta+\alpha)} - e^{\imath(-\theta+\alpha)})} \frac{d}{\lambda}. \tag{2.24}$$

From $\Sigma_{j=1}^{m} u_j = 1$, we obtain that

$$C_1 \frac{e^{\imath\theta}(1-e^{\imath m\theta})}{1-e^{\imath\theta}} + C_2 \frac{e^{-\imath\theta}(1-e^{-\imath m\theta})}{1-e^{-\imath\theta}} + m\frac{d}{\lambda} = 1. \tag{2.25}$$

Combining (2.23)–(2.25), we have

$$\frac{e^{\imath\alpha}-1}{e^{\imath\theta}-e^{-\imath\theta}} \left(\frac{1-e^{\imath m\theta}}{e^{\imath\alpha}-e^{\imath m\theta}} - \frac{1-e^{-\imath m\theta}}{e^{\imath\alpha}-e^{-\imath m\theta}} \right) + m = \frac{\lambda}{d}. \tag{2.26}$$

We note that $\theta = \arccos[(\lambda+2)/2] = \pi/m$. Substituting $d = [2\cos(\pi/m) - 2]/m$ into (2.26) and by direct computation, we obtain that $2\cos(\pi/m) - 2$ is a root of (2.26) thus an eigenvalue of $\mathbf{G}$. □

Proof of the second part of Theorem 2: Denote $\lambda_1^{(l)}(K)$ and $\lambda_2^{(l)}(K)$, respectively, the largest and second largest eigenvalue of $\mathbf{D}_1(l) + d_l \mathbf{D}_2(l)$. From Proposition 2.3, it follows that

$$\lambda_1^{(l)}(1) = \begin{cases} 2\cos\left(\dfrac{2\pi l}{mn}\right) - 2, & 0 < l < \dfrac{n}{2}, \\ 2\cos\dfrac{\pi}{m} - 2 = \rho_i, & l = \dfrac{n}{2}, \\ 2\cos\left(\dfrac{2(m-1)\pi}{m} + \dfrac{2\pi l}{mn}\right) - 2, & \dfrac{n}{2} + 1 < l < n-1, \end{cases}$$

and

$$\lambda_2^{(l)}(1) = \begin{cases} 2\cos\left(\dfrac{2(m-1)\pi}{m} + \dfrac{2\pi l}{mn}\right) - 2, & 0 < l < \dfrac{n}{2}, \\ 2\cos\dfrac{\pi}{m} - 2 = \rho_i, & l = \dfrac{n}{2}, \\ 2\cos\left(\dfrac{2\pi l}{mn}\right) - 2, & \dfrac{n}{2} + 1 < l < n-1, \end{cases}$$

where $m = 2^i$ and $n = N/m$. Here we note that $\lambda_1^{(l)}(1) > \rho_i > \lambda_2^{(l)}(1)$ for $l = 0, \ldots, n/2-1, n/2+1, \ldots, n-1$. Since the largest eigenvalue of $\tilde{\mathbf{A}}$ equals $0 = \lambda^{(0)}(K) \equiv \bar{\lambda}_1(K)$, we see that the second largest eigenvalue of $\tilde{\mathbf{A}}$ at $K=1$ equals $\max\{\lambda_1^{(l)}(1) \,|\, l = 0, \ldots, n/2-1, n/2+1, \ldots, n-1\}$. On the other hand, applying Proposition 2.4 with $m = 2^i$, we have that for $l \neq 0, n/2$ and $d_l = \rho_i/m$, i.e.,

$$K = \frac{m\rho_i}{2\cos\dfrac{2\pi l}{n} - 2} + 1 \equiv K_c^{(l)},$$

$\mathbf{D}_1(l) + d_l \mathbf{D}_2(l)$ has eigenvalue ρ_i. By using Proposition 2.2, $\lambda_1^{(l)}(K)$ is decreasing in K. Hence

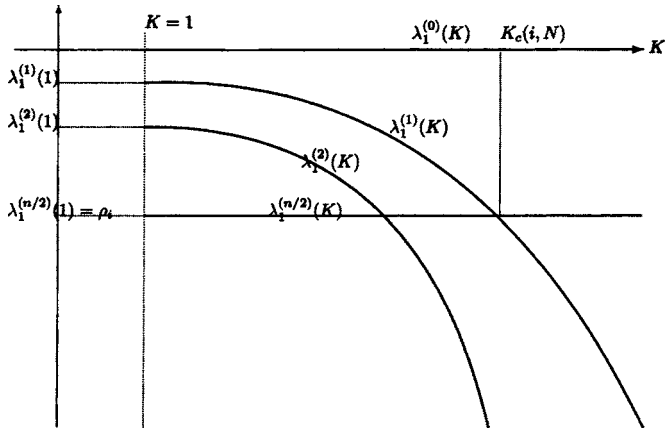

FIG. 1. An illustration of the eigenvalues curves of $\tilde{\mathbf{A}}$.

$$\lambda_1^{(l)}(K) < \rho_i,$$

for $K > K_c^{(l)}$ and $l \neq 0, n/2$. Thus, for $K > \max_{l\neq 0,n/2}\{K_c^{(l)}\} = K_c^{(1)} = K_c(i,N)$, we have $\bar{\lambda}_2(K) = \rho_i$. Also, for $1 < K < K_c(i,N)$, $\bar{\lambda}_2 = \max_{l\neq 0,n/2} \lambda_1^{(l)}(K)$ (see Fig. 1 for an illustration). This completes the proof. □

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Goldfishing by gauge theory

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A new *solvable* many-body problem of goldfish type is identified and used to revisit the connection between two different approaches to *solvable* dynamical systems. An *isochronous* variant of this model is identified and investigated. Alternative versions of these models are presented. The behavior of the alternative *isochronous* model near its equilibrium configurations is investigated, and a remarkable *Diophantine* result, as well as related *Diophantine* conjectures, are thereby obtained. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2235035]

I. INTRODUCTION

Recently a method has been introduced and exploited to identify new *exactly solvable* (namely solvable by purely algebraic operations, such as diagonalizing a matrix) many-body problems characterized by equations of motion of Newtonian type ("the acceleration of each particle is determined by the positions and velocities of all particles"), including in particular models of goldfish type (see, for instance, Ref. 4, and the following). The main idea of this approach—hereafter referred to as the *direct* method—is to start from an *explicitly solvable* matrix evolution equation (possibly even quite a trivial one), and to then focus on the time evolution of the *eigenvalues* of this matrix. For an overview of this method (including an explanation of the terminology used herein) of the main results yielded by it so far, and the quotation of relevant references, we refer to the very recent paper Ref. 2.

Another method has been introduced some years ago to treat certain well-know *solvable* dynamical systems and to illuminate their connection with developments in theoretical particle physics. The main idea of this approach—hereafter referred to as the *gauge theory* method—is to start from a *gauge invariant* matrix evolution equation and to exploit the possibility that in one gauge this evolution be trivially simple hence *solvable* while in another gauge it can be related to interesting evolutions, in particular to the equations of motion of Newtonian type of certain many-body problems. For an overview of this approach and the quotation of relevant references, we refer to the relatively recent paper (Ref. 1). An analysis of the *gauge theory* approach entailing a clarification of the relation of this method to the *direct* approach is already provided in the more recent paper published by one of us.[11]

In the present paper, in the context of revisiting this connection, we identify a new *solvable* many-body problem of goldfish type. This finding hinges on a result obtained many years ago by Inozemtsev.[10] We also present the *isochronous* variant of this many-body problem, as well as alternative formulations of these two models, and by investigating the behavior of the alternative *isochronous* model in the neighborhood of its equilibrium configurations we identify certain remarkable *Diophantine* relations.

The main *new* results obtained in this paper are reported in Sec. II. The hasty browser eager

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to see immediately the equations of motion of the new *solvable* many-body problems of goldfish type should jump to (1) and for the *isochronous* variant to (6), and for the alternative versions of these models to (14) and (21); a *Diophantine* finding and related conjectures are reported at the end of Sec. II. In Sec. III the *solvable* character of the new many-body problems of goldfish type is demonstrated, first via the *direct* method and then via the *gauge theory* method; the connection among these two approaches is thereby illuminated. In Sec. IV *solvable* dynamical systems are derived, which constitute nontrivial alternative reformulations of the many-body problems of goldfish type treated in Sec. III. In Sec. V the behavior of the alternative *isochronous* model in the neighborhood of its equilibrium configurations is investigated and remarkable *Diophantine* relations are thereby obtained. In Sec. VI possible future developments are mentioned. The Appendix contains some findings the insertion of which where they are first mentioned (see *Remark 2.9* in Sec. II) would have been too distracting.

II. MAIN RESULTS

In this section we report the main *new* findings obtained in subsequent sections.

The *solvable N*-body problem of goldfish type identified in this paper is characterized by the following equations of motion of Newtonian type:

$$\ddot{z}_n = 2z_n(z_n^2 - a^2) + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n + z_n^2 - a^2)(\dot{z}_m + z_m^2 - a^2)}{z_n - z_m}. \tag{1}$$

Notation: $z_n \equiv z_n(t)$ are the dependent variables, t is the independent variable ("time"), superimposed dots denote time-differentiations, a^2 is an *arbitrary* constant (we use a^2 rather than a merely for notational convenience, see the following), N is a positive integer (generally we assume $N>1$), and indices such as n,m generally take all the values $1,2,\ldots,N$ unless otherwise mentioned.

Remark 2.1: Trivially related models involving additional arbitrary constants could of course be obtained by rescaling the (dependent and independent) variables and by shifting by a constant amount the dependent variables; note incidentally that the first factor 2 on the right-hand side of (1) could be changed by rescaling (we put it there for notational convenience, see the following), while the second factor 2 (that multiplying the sum) cannot of course be changed.

Remark 2.2: Although for *real* a^2 and for *real* initial data $z_n(0)$, $\dot{z}_n(0)$ the time evolution (for *real* time) of this many-body model entails that the dependent variables $z_n(t)$ are as well *real*, we generally assume the time evolution to take place in the *complex* z-plane (and generally allow the constant a to be as well *complex*); indeed such an evolution is much more interesting due to the possibility of the "particles" characterized by the *complex* coordinates $z_n(t)$ to go round each other and the related fact that initial data $z_n(0)$, $\dot{z}_n(0)$ leading to particle collisions are then *exceptional* (they generally have vanishing dimensionality relative to *generic* initial data). (If attention is instead restricted to *real* motions, then the trivial change of dependent variables $z_n \to iy_n$ with y_n *real* might be expedient in order to deal with *confined* motions.) It is possible to reformulate these *complex* equations of motions as *real* (and even *covariant*, even *rotation-invariant*) equations of motion describing the motion of *real* point particles in the *real* (say, *horizontal*) plane, but we will not take space here to reformulate them in this manner, since the technique to do so is well known (see for instance Ref. 5).

The *solvable* character of these equations of motion is evidenced by the well-known fact[10,5] that the $N\times N$ matrix evolution equation

$$\ddot{U} = 2U(U^2 - a^2) \tag{2}$$

is itself *solvable* (in terms of appropriate sigma functions[10]), together with the following.

Proposition 2.3: *The solution of the initial-value problem for the equations of motion (1) is provided by the following prescription: the coordinates* $z_n(t)$ *are the N eigenvalues of the* $N\times N$ *matrix* $U(t)$ *solution of (2) and determined by the following initial data:*

$$U_{nm}(0) = \delta_{nm} z_n(0), \tag{3a}$$

$$\dot{U}_{nm}(0) = -\delta_{nm}[z_n^2(0) - a^2] + [\dot{z}_n(0) + z_n^2(0) - a^2]^{1/2}[\dot{z}_m(0) + z_m^2(0) - a^2]^{1/2}. \tag{3b}$$

Note that the matrix $U(0)$ is *diagonal*, while the matrix $\dot{U}(0)$ is the sum of a *diagonal* matrix and a *dyadic* matrix.

Notation: here and hereafter $\delta_{nm} \equiv \delta_{n,m}$ is the Kronecker delta symbol, $\delta_{nm}=1$ if $n=m$, $\delta_{nm}=0$, if $n \neq m$.

To obtain the *isochronous* variant of this many-body problem one starts from the equations of motion

$$\zeta_n'' = 2\zeta_n^3 + 2 \sum_{m=1, m\neq n}^{N} \frac{(\zeta_n' + \zeta_n^2)(\zeta_m' + \zeta_m^2)}{\zeta_n - \zeta_m}, \tag{4}$$

which correspond to (1) with $a=0$ and with the merely notational replacement of the dependent variables $z_n(t)$ with the dependent variables $\zeta_n(\tau)$ (and of course now the appended primes denote differentiations with respect to τ). One can then apply the procedure usually referred to as "the trick" (see for instance Refs. 4 and 5), i.e. (in this case) the following change of dependent and independent variables:

$$\tilde{z}_n(t) = \exp(it)\zeta_n(\tau), \tag{5a}$$

$$\tau = i[1 - \exp(it)]. \tag{5b}$$

This yields the equations of motion

$$\ddot{\tilde{z}}_n = 3i\dot{\tilde{z}}_n + 2\tilde{z}_n(1 + \tilde{z}_n^2) + 2 \sum_{m=1, m\neq n}^{N} \frac{(\dot{\tilde{z}}_n - i\tilde{z}_n + \tilde{z}_n^2)(\dot{\tilde{z}}_m - i\tilde{z}_m + \tilde{z}_m^2)}{\tilde{z}_n - \tilde{z}_m}. \tag{6}$$

The solution of the initial-value problem is then obviously given by the solution (via Proposition 2.3) of the problem (4) and by the "trick" relations (5), which clearly also imply

$$\zeta_n(0) = \tilde{z}_n(0), \quad \zeta'(0) = \dot{\tilde{z}}_n(0) - i\tilde{z}_n(0). \tag{7}$$

Equivalently, the solution of this model (6) is clearly given by the following.

Proposition 2.4: *The dependent variables $\tilde{z}_n(t)$ that solve the initial-value problem for the Newtonian N-body problem (6) are the N eigenvalues of the $N \times N$ matrix $\tilde{U}(t)$ evolving according to the solvable matrix evolution equation*

$$\ddot{\tilde{U}} - 3i\dot{\tilde{U}} - 2\tilde{U} = 2\tilde{U}^3 \tag{8}$$

and being moreover characterized by the following initial data:

$$\tilde{U}_{nm}(0) = \delta_{nm}\tilde{z}_n(0), \tag{9a}$$

$$\dot{\tilde{U}}_{nm}(0) = -\delta_{nm}[\tilde{z}_n^2(0)] + [\dot{\tilde{z}}_n(0) - i\tilde{z}_n(0) + \tilde{z}_n^2(0)]^{1/2}[\dot{\tilde{z}}_m(0) - i\tilde{z}_m(0) + \tilde{z}_m^2(0)]^{1/2}. \tag{9b}$$

Note that the matrix $\tilde{U}(0)$ is *diagonal*, while the matrix $\dot{\tilde{U}}(0)$ is the sum of a *diagonal* matrix and a *dyadic* matrix.

The *solvable* character of the matrix evolution equation (8) is implied by the "trick" formula

$$\widetilde{U}(t) = \exp(it)U(\tau), \quad \tau = i[1 - \exp(it)] \tag{10}$$

relating the $N \times N$ matrix $\widetilde{U}(t)$ evolving according to (8) to the $N \times N$ matrix $U(t)$ evolving according to (2) with $a=0$.

Remark 2.5: The *solvable* character[10] of the matrix evolution equation (2) entails that *all* its solutions $U(t)$ are *meromorphic* functions of the independent variable t. Hence (see (10)) *all* the *nonsingular* solutions $\widetilde{U}(t)$ of the matrix evolution equation (8) are *periodic* with period 2π,

$$\widetilde{U}(t + 2\pi) = \widetilde{U}(t). \tag{11}$$

The *singular* solutions of (8) are *exceptional*, corresponding to a set of initial data having *vanishing* measure with respect to the set of *generic* initial data.

As an immediate consequence of Proposition 2.4 and of this *Remark 2.5* there holds the following.

Proposition 2.6: *All the solutions of the many-body problem (6) (except those* exceptional *ones that run into a collision of two or more particles, which correspond to* nongeneric *initial data) are* completely periodic *with a period which is a* positive integer multiple p *of* 2π:

$$\widetilde{z}_n(t + 2p\pi) = \widetilde{z}_n(t), \quad p = 1 \text{ or } 2 \text{or} \ldots \text{or } N. \tag{12}$$

The positive integer p *accounts for the possibility that the eigenvalues get exchanged among each other through the motion: it depends on the initial data, but it does not change for sufficiently small, if finite, changes of these data and it clearly is* not larger *than* N.

This proposition displays the *isochronous* character of the N-body problem (6), indeed it justifies considering it as one more instance of *nonlinear harmonic oscillators*.[7]

There exists a, by now rather standard, technique to reformulate these types of N-body problems, by identifying the N "particle coordinates" $z_n(t)$ as the N zeros of a (*monic*) polynomial in z of degree N, and by then focusing on the corresponding time evolution of the N coefficients $c_m(t)$ of this polynomial (see for instance Refs. 6 and 5):

$$\psi(z,t) = \prod_{n=1}^{N} [z - z_n(t)] = \sum_{m=0}^{N} c_m(t) z^{N-m}, \quad c_0 = 1. \tag{13}$$

In Sec. IV we show how such a procedure is applicable in our case, and we thereby obtain the following alternative formulation of the N-body problem (1):

$$\ddot{c}_m + 2(m-1)\dot{c}_{m+1} - 2c_1\dot{c}_m + 2(N+1-m)a^2\dot{c}_{m-1} + (m+2)(m-3)c_{m+2} - 2(m-1)c_1c_{m+1} + 2[m(N + 2 - m)a^2 + \dot{c}_1 - c_1^2 + 3c_2]c_m - 2(N+1-m)a^2c_1c_{m-1} + (N+2-m)(N+1-m)a^4c_{m-2} = 0,$$
$$m = 1, \ldots, N, \quad c_0 = 1, \quad c_{-1} = c_{N+1} = c_{N+2} = 0. \tag{14}$$

Remark 2.7: The ODE of this system with $m=0$ is identically satisfied; the ODE with $m=N+1$ is also satisfied provided one sets $c_{N+3}=0$, and even the ODE with $m=N+2$ is identically satisfied if one moreover sets $c_{N+4}=0$.

Remark 2.8: A superficial look at this system of ODEs might suggest that it is a *linear* system of evolution equations for the quantities $c_m(t)$; but this is of course *not* the case, due to the presence of the quantities $c_1(t)$ and $c_2(t)$. Indeed the highly nonlinear character of this system is already evident by looking at the $N=2$ case, in which case it yields the following (*solvable*!) fourth-order ODE for $f(t) \equiv c_1(t)$:

$$f'''' f^2 - 2f''' f' f^2 - 2f''' f^3 - 2(f'')^2 f + 2f''(f')^2 + 4f'' f' f^2 - 2f'' f^4 - 4(f')^2 f^3 + 4f' f^5 + 4a^2(f'' f^2 - 2f' f^3) = 0 \tag{15}$$

(here for typographical convenience differentiations are denoted by appended primes rather than superimposed dots).

Remark 2.9: Two equilibrium (namely, time-independent) solutions of this system (14) are provided by the formula

$$c_m = (\pm a)^m \binom{N}{m}. \tag{16}$$

They are not, however, the only equilibrium configurations of this system. A technique to obtain *all* these configurations (including this one!) is described in the Appendix.

As indicated earlier, see (13), the quantities $c_m(t)$ that evolve according to the system of ODEs (14) are just the *coefficients* of the *monic* polynomial $\psi(z,t)$ of degree N in z, the N zeros $z_n(t)$ of which evolve according to the equations of motion (1). Hence (see Proposition 2.3) the solution of the system of ODEs (14) is given by the following.

Proposition 2.10: *The dependent variables $c_m(t)$ that solve the initial-value problem for the system of nonlinear ODEs (14) are the N coefficients of the polynomial $\psi(z,t)$, see (13), which is itself given by the formula*

$$\psi(z,t) = \det[z - U(t)], \tag{17}$$

where the $N \times N$ matrix $U(t)$ evolves according to the solvable *matrix evolution equation (2) and is moreover characterized by the initial data (3), with the initial values $z_n(0)$, $\dot{z}_n(0)$ related to the initial values $c_m(0)$, $\dot{c}_m(0)$ by the formulas implied by (13),*

$$\prod_{n=1}^{N} [z - z_n(0)] = \sum_{m=0}^{N} c_m(0) z^{N-m}, \quad c_0 = 1, \tag{18a}$$

$$-\sum_{n=1}^{N} \dot{z}_n(0) \prod_{m=1, m\neq n}^{N} [z - z_n(0)] = \sum_{m=1}^{N} \dot{c}_m(0) z^{N-m}. \tag{18b}$$

To obtain an alternative version of the *isochronous N*-body problem (6) we use the following version of the "trick:"

$$\tilde{c}_m(t) = (-i)^m \exp(mit)\, \gamma_m(\tau), \tag{19a}$$

$$\tau = i[1 - \exp(it)]. \tag{19b}$$

Here the quantities $\gamma_m(\tau)$ are the dependent variables of the previous model, (14), with $a=0$, up to the (purely notational) change consisting in calling the independent variable τ (instead of t) and the dependent variables γ_m (instead of c_m), so that these variables satisfy the following system of ODEs:

$$\gamma_m'' + 2(m-1)\gamma_{m+1}' - 2\gamma_1\gamma_m' + (m+2)(m-3)\gamma_{m+2} - 2(m-1)\gamma_1\gamma_{m+1} + 2(\gamma_1' - \gamma_1^2 + 3\gamma_2)\gamma_m = 0,$$

$$m = 1, \ldots, N, \quad \gamma_0 = 1, \quad \gamma_{-1} = \gamma_{N+1} = \gamma_{N+2} = 0, \tag{20}$$

where of course appended primes denote differentiations with respect to the independent variable τ (which we allow to be complex, see (19b)).

Then clearly by applying the "trick" (19) to the system (20) the following new system of nonlinear ODEs is obtained:

$$\ddot{\tilde{c}}_m + 2(m-1)i\dot{\tilde{c}}_{m+1} - (2m+1+2\tilde{c}_1)i\dot{\tilde{c}}_m - (m+2)(m-3)\tilde{c}_{m+2} + 2(m-1)(m+1+\tilde{c}_1)\tilde{c}_{m+1}$$
$$+ [-m(m+1) + 2i\dot{\tilde{c}}_1 - 2(m-1)\tilde{c}_1 + 2\tilde{c}_1^2 - 6\tilde{c}_2]\tilde{c}_m = 0,$$

$$m = 1, \ldots, N, \quad \tilde{c}_0 = 1, \quad \tilde{c}_{-1} = \tilde{c}_{N+1} = \tilde{c}_{N+2} = 0. \tag{21}$$

Remark 2.11: The prefactor $(-i)^m$ in (19a) is of course unessential, it has been introduced merely to give a marginally nicer look to this system (21) and to some other formulas, see the following. With this version, (19), of the "trick" the relation among the particle coordinates satisfying the equations of motion of the *isochronous N*-body problem (6) and the quantities $\tilde{c}_m(t)$ satisfying this system of ODEs (21) reads now

$$\tilde{\psi}(z,t) = \prod [z - \tilde{z}_n(t)] = \sum_{m=0}^{N} (i)^m \tilde{c}_m(t) z^{N-m}, \quad \tilde{c}_0 = 1, \tag{22}$$

see (5), (19), and (13). Note that we introduced here the (new) *monic* polynomial $\tilde{\psi}(z,t)$ having as its N zeros the N dependent variables $\tilde{z}_n(t)$ satisfying (6) and as its N coefficients the N dependent variables $\tilde{c}_m(t)$ satisfying (21).

This model, (21), is obviously just as *solvable* as the previous one, (14), indeed the solution of its initial-value problem can be obtained from the solution of the corresponding problem for (14) via the formulas (19) that clearly imply the following relations among the initial data of the two models:

$$\tilde{c}_m(0) = (-i)^m \gamma_m(0), \tag{23a}$$

$$\dot{\tilde{c}}_m(0) - mi\tilde{c}_m(0) = (-i)^m \gamma_m(0). \tag{23b}$$

Equivalently, the solution of this model (21) is clearly given by the following.

Proposition 2.12: *The dependent variables $\tilde{c}_m(t)$ that solve the initial-value problem for the system of nonlinear ODEs (21) are the N coefficients of the polynomial $\tilde{\psi}(z,t)$, see (22), which is itself given by the formula*

$$\tilde{\psi}(z,t) = \det[z - \tilde{U}(t)], \tag{24}$$

where the $N \times N$ matrix $\tilde{U}(t)$ evolves according to the solvable *matrix evolution equation* (8) *and is moreover characterized by the initial data (9) with the initial values $\tilde{z}_n(0)$, $\dot{\tilde{z}}_n(0)$ related to the initial values $\tilde{c}_m(0)$, $\dot{\tilde{c}}_m(0)$ by the following formulas implied by (22),*

$$\prod_{n=1}^{N} [z - \tilde{z}_n(0)] = \sum_{m=0}^{N} (i)^m \tilde{c}_m(0) z^{N-m}, \quad \tilde{c}_0 = 1, \tag{25a}$$

$$-\sum_{n=1}^{N} [\dot{\tilde{z}}_n(0) - i\tilde{z}_n(0)] \prod_{m=1, m\neq n}^{N} [z - \tilde{z}_n(0)] = \sum_{m=1}^{N} (i)^m \dot{\tilde{c}}_m(0) z^{N-m}. \tag{25b}$$

As an immediate consequence of this Proposition 2.12 and of *Remark 2.5* there holds the following.

Proposition 2.13: *All the* nonsingular *solutions of the system of ODEs (21) are* completely periodic *with period* 2π,

$$\tilde{c}_m(t + 2\pi) = \tilde{c}_m(t), \tag{26}$$

while the singular *solutions are* exceptional, *corresponding to a set of initial data having* vanishing *measure with respect to the set of* generic *initial data.*

This proposition displays the *isochronous* character of the *N*-body problem (21), indeed it justifies considering it as one more instance of *nonlinear harmonic oscillators*.[7]

Finally, in Sec. V we obtain *all* the *equilibrium configurations* of the *isochronous* systems (6) and (21) and we study the behavior of the system of *nonlinear harmonic oscillators* (21) in the neighborhood of its equilibrium configurations. The interested reader will find these results in that

section, but we advertise here the *Diophantine* findings arrived at via this study.

Proposition 2.14: *Let the two $N\times N$ matrices A and B be defined componentwise as follows:*

$$A_{nm} = 2(n-1)\,\delta_{n+1,m} - (2n+1+2\bar{c}_1)\,\delta_{n,m} + 2\bar{c}_n\delta_{1,m}, \tag{27a}$$

$$B_{nm} = (n+2)(n-3)\,\delta_{n+2,m} - 2(n-1)(n+1+\bar{c}_1)\,\delta_{n+1,m} + [n(n+1) + 2(n-1)\bar{c}_1 - 2\bar{c}_1^2 + 6\bar{c}_2]\,\delta_{n,m} + 2[-(n-1)\bar{c}_{n+1} + (n-1-2\bar{c}_1)\bar{c}_n]\,\delta_{1,m} + 6\bar{c}_n\delta_{2,m}, \tag{27b}$$

with the numbers $\bar{c}_m$ defined as follows:

$$\text{for } \nu=0, \quad \bar{c}_m = (-)^m\binom{\mu}{m}, \tag{28a}$$

$$\text{for } \nu=1, \quad \bar{c}_m = \delta_{0m} + \delta_{1m} \text{ if } \mu=1, \quad \bar{c}_m = (-)^m\left[\binom{\mu-2}{m} - \binom{\mu-2}{m-2}\right] \text{ if } \mu>1, \tag{28b}$$

$$\text{for } \nu=3, \ \bar{c}_m = (-)^m\left[\binom{\mu-3}{m} + 6\binom{\mu-3}{m-1} + 14\binom{\mu-3}{m-2} + 14\binom{\mu-3}{m-3}\right], \tag{28c}$$

$$\text{for } \nu=4, \quad \bar{c}_m = (-)^m\sum_{k=0}^{4}\binom{\mu-4}{m-k}\binom{5}{k}, \tag{28d}$$

$$\text{for } \nu=5, \quad \bar{c}_m = (-)^m\left[c\binom{\mu-5}{m-5} + \sum_{k=0}^{5}\binom{\mu-5}{m-k}\binom{5}{k}\right], \quad c \text{ arbitrary}. \tag{28e}$$

As indicated earlier the parameter ν (the role of which here is mainly to distinguish five different cases) can take any one of the 5 *values* 0, 1, 3, 4, 5, *while the parameter μ can take any* positive integer *value in the range $\nu\leqslant\mu\leqslant N$. Let the* $2N$ *numbers $p_n^{(\pm)}$ be the eigenvalues of the generalized eigenvalue problem*

$$(p^2 + Ap + B)\underline{r} = 0, \tag{29a}$$

(where $\underline{r}\equiv(r_1,\ldots,r_N)$ denotes the corresponding eigenvector) implying

$$\det(p^2 + Ap + B) = \prod_{n=1}^{N}[(p - p_n^{(+)})(p - p_n^{(-)})]. \tag{29b}$$

Then the $2N$ *numbers $p_n^{(\pm)}$ are* all integers.

Notation: here and throughout the symbol $\binom{x}{y}$ is the standard binomial coefficient,

$$\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}. \tag{30}$$

We have verified with the help of symbolic programing languages (we used MAPLE and MATHEMATICA) and for an ample sample of values of N and of the other parameters the validity of this proposition (proven in Sec. V), and from these computer-aided checks we are led to formulate the following *Diophantine* conjectures.

Conjecture 2.15: *For ν=*0, 1, 3, 4, 5 *and μ integer in the range $\nu\leqslant\mu\leqslant N$ the eigenvalues of the generalized eigenvalue problem (29a) (with (27) and (28)) are given by the following formulas:*

$$\text{for } \nu=0, \quad \det(p^2+Ap+B)=\left\{\prod_{n=1}^{N-\mu}[(p-n)(p-n-1)]\right\}\left\{\prod_{n=1}^{\mu}[(p+n)(p+n-5)]\right\}, \tag{31a}$$

$$\text{for } \nu=1, \quad \det(p^2+Ap+B)=(p+1)(p-4)\left\{\prod_{n=1}^{N-\mu}[(p-n)(p-n-5)]\right\} \times\left\{\prod_{n=1}^{\mu-1}[(p+n)(p+n-7)]\right\}, \tag{31b}$$

$$\text{for } \nu=3, \quad \det(p^2+Ap+B)=(p+1)(p-4)\left\{\prod_{n=1}^{N-\mu}[(p-n)(p-n+5)]\right\} \times\left\{\prod_{n=1}^{\mu-1}[(p+n)(p-n+\mu-7)]\right\}, \tag{31c}$$

$$\text{for } \nu=4, \quad \det(p^2+Ap+B)=(p+1)\left[\prod_{n=1}^{3}(p-n-1)\right]\left\{\prod_{n=1}^{N-\mu}[(p-n)(p-n+1)]\right\}\left[\prod_{n=1}^{\mu-4}(p+n)\right] \times\left[\prod_{n=1}^{\mu}(p+n+1)\right], \tag{31d}$$

$$\text{for } \nu=5, \quad \det(p^2+Ap+B)=\left\{\prod_{n=1}^{N-\mu}[(p-n)(p-n-1)]\right\}\left\{\prod_{n=1}^{\mu}[(p+n)(p-n+\mu-4)]\right\}. \tag{31e}$$

Here we use the standard convention according to which a product equals unity *if the lower limit of the running index exceeds the upper limit.*

Remark 2.16: For $\mu=\nu=0$ the validity of this conjecture is certainly true, indeed trivially so (see below the *Remark 5.4*).

The Conjecture 2.15 only refers to *integer* values of the parameter μ in the range $\nu\leqslant\mu\leqslant N$. But our computer-aided exploration also indicates the validity, for *arbitrary* values of the parameter μ, of the following conjecture (which is only formulated in the following for sufficiently large values of N, to avoid less interesting complications).

Conjecture 2.17: *The generalized eigenvalue problem* (29a) (*with* (27) and (28a)) *features, for* arbitrary μ, *the* $N-1$ *eigenvalues*

$$2,3,4,5-\mu,6-\mu,\ldots,N-\mu, \quad \textit{if } \nu=0 \textit{ or } \nu=5 \textit{ and } N\geqslant 5, \tag{32a}$$

$$2,3,4,4-\mu,5-\mu,\ldots,N-1-\mu, \quad \textit{if } \nu=4 \textit{ and } N\geqslant 5, \tag{32b}$$

and the $N-4$ *eigenvalues*

$$-1,4,6,8-\mu,9-\mu,\ldots,N-\mu, \quad \textit{if } \nu=1 \textit{ and } N\geqslant 8, \tag{32c}$$

$$-1,4,6,3-\mu,4-\mu,\ldots,N-5-\mu, \quad \textit{if } \nu=3 \textit{ and } N\geqslant 8. \tag{32d}$$

Remark 2.18: The Conjecture 2.17—in contrast to the Conjecture 2.15—does *not* provide the *entire* spectrum of the eigenvalue problem (29a), which of course features $2N$ eigenvalues.

Some aspects of these conjectures are easy to prove. For instance Conjecture 2.15 can be proven by induction for all $N>\mu$ if one assumes its validity for $N=\mu$. But complete proofs of them do not seem quite trivial (see Sec. VI).

III. TWO PROOFS OF PROPOSITION 2.3

In this section (part of) the results reported in the Sec. II are proven, first by the *direct* method, then by the *gauge theory* method.

A. Direct method

The starting point of the *direct* method is the *solvable* $N\times N$ matrix evolution equation (2). We then introduce the eigenvalues of the matrix $U(t)$ and the corresponding diagonalizing matrix $R(t)$ via the formulas

$$U(t)=R(t)Z(t)[R(t)]^{-1}, \tag{33a}$$

$$Z(t)=\mathrm{diag}[z_n(t)], \tag{33b}$$

with moreover

$$R(0)=\mathbf{1}. \tag{33c}$$

Here and in the following $\mathbf{1}$ is the $N\times N$ identity matrix. Note that the first two of these equations, (33a) and (33b), identify (consistent with Proposition 2.3) the N coordinates $z_n(t)$ as the N eigenvalues of the $N\times N$ matrix $U(t)$, while the third, (33c), is consistent via the first two with the assignment (3a).

It is then easy to see (for the derivation of these formulas see, if need be, for instance Ref. 2) that, after introducing the $N\times N$ matrix $M(t)$ via the assignment

$$M(t)=[R(t)]^{-1}\dot{R}(t), \tag{34}$$

one gets

$$\dot{U}(t)=R(t)\{\dot{Z}(t)+[M(t),Z(t)]\}[R(t)]^{-1}, \tag{35a}$$

entailing (see (33c))

$$\dot{U}(0)=\dot{Z}(0)+[M(0),Z(0)], \tag{35b}$$

as well as the following system of evolution ODEs for the coordinates $z_n(t)$ and for the matrix elements $M_{nm}(t)$ of the matrix $M(t)$:

$$\ddot{z}_n=2z_n(z_n^2-a^2)+2\sum_{m=1,m\neq n}^{N}(z_n-z_m)M_{nm}M_{mn}, \tag{36a}$$

$$\frac{\dot{M}_{nm}}{M_{nm}}=-2\frac{\dot{z}_n-\dot{z}_m}{z_n-z_m}-M_{nn}+M_{mm}+\sum_{\ell=1;\ell\neq n,m}^{N}\frac{(z_n+z_m-2z_\ell)}{z_n-z_m}\frac{M_{n\ell}M_{\ell m}}{M_{nm}},\quad n\neq m. \tag{36b}$$

Note that the time evolutions of the *diagonal* elements $M_{nn}(t)$ of the matrix $M(t)$ remain unrestricted: it is indeed clear from (33) (implying that $R(t)$ is defined only up to multiplication from the right by an *arbitrary* diagonal matrix $D(t)$) and from (34) that these N functions of time can be chosen arbitrarily without affecting the eigenvalues of $U(t)$, namely the coordinates $z_n(t)$. Indeed it is clear that the $N\times N$ matrix evolution equation (2), characterizing the time evolution of the N^2 matrix elements $M_{nm}(t)$, has now been turned into the system (36), characterizing the time evo-

lution of the N coordinates $z_n(t)$ and the $N(N-1)$ *off-diagonal* elements $M_{nm}(t)$ (with $n \neq m$) of the $N \times N$ matrix $M(t)$.

Clearly this system (36) is *no less solvable* than the original matrix evolution (2), because its solution can be retrieved from the solution of (2) by purely algebraic operations (essentially, by diagonalizing an $N \times N$ matrix).

But we are interested in obtaining an N-body problem involving *only* the N "particle coordinates" $z_n(t)$, hence our next task is to eliminate the $N(N-1)$ "auxiliary quantities" $M_{nm}(t)$ (with $n \neq m$). To do this one must find (assuming it exists) an appropriate *ansatz* expressing the $N(N-1)$ auxiliary quantities $M_{nm}(t)$ (with $n \neq m$) in terms of the N particle coordinates $z_n(t)$, taking advantage if need be of the freedom to assign the N quantities $M_{nn}(t)$ at our convenience.

An *ansatz* that works (in the sense of turning the $N(N-1)$ evolution equations (36b) into identities) is

$$M_{nn}(t) = -\sum_{\ell=1}^{N} \frac{g}{[z_n(t) - z_\ell(t)]^2}, \tag{37a}$$

$$M_{nm}(t) = \frac{g}{[z_n(t) - z_m(t)]^2}, \quad n \neq m, \tag{37b}$$

with g an *arbitrary constant*. This leads however to an N-body model the *solvable* character of which is already well known,[9,13,3,12] hence we do not pursue this development here (we elaborate on this point a little further in the following version of the proof).

Remark 3.1: Clearly insertion of this *ansatz* (37) in the more general matrix evolution equation

$$\ddot{U} = \Phi(U), \tag{38a}$$

with $\Phi(z)$ an *arbitrary* scalar function would also work (since this does not depend on the equations of motion satisfied by the coordinates z_n, see the following), and it would lead to the N-body problem characterized by the Newtonian equations of motion

$$\ddot{z}_n = \Phi(z_n) - 2\sum_{n=1, m\neq n}^{N} \frac{g^2}{(z_n - z_m)^3}. \tag{38b}$$

This was already noted, many years ago, by Veselov.[12] But it appears that, so far, the most general (up to trivial transformations) *solvable* $N \times N$ matrix evolution of type (38a) is just (2).

Another *ansatz* that also does (as it were *miraculously*) work (namely, transform the evolution equations (36b) into identities) reads as follows:

$$M_{nm}(t) = -\frac{\{[\dot{z}_n + z_n^2 - a^2][\dot{z}_m + z_m^2 - a^2]\}^{1/2}}{z_n - z_m}, \quad n \neq m. \tag{39}$$

Note that this *ansatz,* in contrast to the previous one, contains no arbitrary ("coupling") constant g. In this case the appropriate assignment for the diagonal elements $M_{nn}(t)$ is quite trivial: $M_{nn}(t) = 0$, or equivalently (see (36b)) $M_{nn}(t) = \mu(t)$, $\mu(t)$ being an arbitrary function of time (but independent of the index n). The truth of this assertion can be verified by a trivial if tedious calculation: note that the evolution equations (36a) must also be used in the process.

And it is now clear that the insertion of this *ansatz* in (36a) yields (1), while its insertion in (35b) yields the assignment (3b). The proof of Proposition 2.3 is thus completed.

B. Gauge theory approach

Let us now prove again Proposition 2.3, but via the *gauge theory* method. Although this entails some repetitions we believe it is useful to go through this exercise in some detail, especially because we will now use a somewhat different language—and one purpose of this paper is precisely to clarify the relations among these two different approaches. Moreover this presentation provides some indication of the extent to which these kinds of fishing expeditions are likely to yield new goldfishes, namely new interesting *solvable* models.

Let us start by reviewing (but in a notation more conducive to a direct comparison with the preceding treatment) the gauge theory approach to a more standard model referred to in the literature as rCM[1,11] characterized by the Newtonian equations of motion

$$\ddot{z}_n = -z_n - 2\sum_{m=1,m\neq n}^{N} \frac{g^2}{(z_n - z_m)^3}. \tag{40}$$

We then present a variant of this approach which leads us to the new *solvable N*-body model of goldfish type presented earlier.

We start with the following system of dynamical equations for the $N\times N$ matrices $U\equiv U(t)$, $M\equiv M(t)$, and $W\equiv W(t)$:

$$\dot{U} + [M,U] = W, \tag{41a}$$

$$\dot{W} + [M,W] = \Phi(U), \tag{41b}$$

with the square brackets indicating matrix commutators. As discussed in the following, to get the rCM model one should assign the function $\Phi(U)$ as follows:

$$\Phi(U) = -U. \tag{42}$$

It is however convenient to leave this function Φ unspecified for the moment; but we require that it contain no other matrix besides U, so that $R^{-1}\Phi(U)R=\Phi(R^{-1}UR)$ for any (invertible) matrix R.

Equation (41) has a natural interpretation as gauge theory in $0+1$ dimensions: they are indeed of the form $[D_t,U]=P$, $[D_t,P]=\Phi(U)$, with $D_t=\partial_t+M$ being the so-called *covariant time derivative* with M regarded as *gauge field*. In particular, they are invariant under the following *gauge transformations*,

$$U \to \tilde{U} = R^{-1}UR, \quad W \to \tilde{W} = R^{-1}WR, \tag{43a}$$

$$M \to \tilde{M} = R^{-1}MR + R^{-1}\dot{R}, \tag{43b}$$

where the matrix $R\equiv R(t)$ characterizing the gauge transformation is an arbitrarily time-dependent invertible matrix (the transformation rule for M follows from $R^{-1}D_tR=\partial_t+R^{-1}\dot{R}+R^{-1}MR$). One can exploit this invariance to impose additional conditions. In particular for any solution $U(t)$, $M(t)$, and $W(t)$ of (41), one can find a gauge transformation $R(t)$ such that the gauge-transformed matrix $\tilde{M}(t)$, see (43b), vanishes, $\tilde{M}(t)=0$. Indeed, this is implied by the fact that the linear first-order matrix ODE

$$\dot{R} + MR = 0, \quad R(0) = \mathbf{1} \tag{44a}$$

always has a (unique) solution, which can be written as

$$R(t) = \mathcal{T}\exp\left[-\int_0^t \mathrm{d}s\, M(s)\right] \tag{44b}$$

where the symbol $\mathcal{T}$ denotes time-ordering. This shows that we can impose the condition

$$M(t) = 0 \tag{45}$$

for all times t, without loss of generality. Note that this also implies that, if we impose (45), we will not lose any solution: indeed any solution to our gauge theory equations can be obtained by solving these equations with the condition (45) imposed, and performing a gauge transformation afterwards. In particle physics this latter condition is often called *Weyl gauge*. We will also use another gauge condition, namely

$$U_{nm}(t) = \delta_{nm} z_n(t) \tag{46}$$

for all times t, which we call *diagonal Coulomb gauge*. Note that we can impose this latter condition if the matrix $U(t)$ is such that there exists an invertible matrix $R(t)$ such that $R^{-1}(t)U(t)R(t)$ is a *diagonal* matrix, and this is obviously true in the generic case when the matrix $U(t)$ is nondegenerate. The cases when the matrix $U(t)$ is degenerate correspond to particles in our N-body system colliding, and then our solution breaks down (as it should): but this can only happen for exceptional—i.e., *nongeneric*—initial data, if we allow the particle coordinates $z_n(t)$ to move in the complex plane, as we generally do (see *Remark 2.2*).

The idea now is that, by imposing the gauge condition (45), we get the matrix equation $\ddot{U} = \Phi(U)$ which might be (chosen to be) exactly solvable, whereas by imposing the condition (46), we get a (hopefully) interesting dynamical system for the variables $z_n(t)$. The latter dynamical system can then be solved explicitly as follows: one first determines the solution $U(t)$ of the matrix equation obtained from (41) in the Weyl gauge and with the initial conditions

$$U_{nm}(0) = \delta_{nm} z_n(0), \quad \dot{U}_{nn}(0) = \dot{z}_n(0). \tag{47}$$

Then the eigenvalues of $U(t)$ give the solution of the dynamical system. Note that we can only assign the *diagonal* elements of $\dot{U}(0)$ since, as we will see, the *off-diagonal* elements of $\dot{U}(0)$ are determined by another condition which we have to add.

Indeed, to get an interesting dynamical system, we need to add one more gauge invariant equation to (41). In particular, to get the rCM model (40), one has to add

$$[W, U] = J, \tag{48}$$

which is often called *Gauss law* or *momentum map*. This latter equation is gauge invariant if the matrix $J=J(t)$ introduced here transforms under gauge transformations as $J \to \widetilde{J} = R^{-1}JR$. It turns out indeed[1,11] that if one makes the assignment

$$J_{nm}(0) = g(1 - \delta_{nm}) \tag{49}$$

and chooses $\Phi(U)$ as in (42), then the coordinates $z_n(t)$ obey the equations of motion of the rCM model (40).

To obtain goldfish type dynamical systems one must instead replace the Gauss' law condition (48) by

$$B_{nm}B_{n'm'} = B_{nm'}B_{n'm} \tag{50a}$$

with

$$B = W + f(U), \tag{50b}$$

where $f(x)$ is another function to be assigned later. To see that this condition is gauge invariant we note that it can be written as $B \otimes B = \mathcal{P}B \otimes B$ where $\otimes$ is the tensor product (so that $(B \otimes B)(u$

$\otimes v)=(Bu)\otimes(Bv)$ where u and v are N-vectors) and $\mathcal{P}$ is the permutation matrix defined as follows, $\mathcal{P}u\otimes v=v\otimes u$: the gauge invariance of (50a) follows from the obvious fact that $\mathcal{P}$ commutes with $R\otimes R$.

A new finding (proved at the end of this section) is then given by the following.

Proposition 3.2: *The gauge theory equations (41) and (50) are consistent if*

$$f(x)=\alpha+\beta x+\gamma x^2, \tag{51a}$$

$$\Phi(x)=(\alpha+\beta x+\gamma x^2)(\beta+2\gamma x)=f(x)f'(x), \tag{51b}$$

for arbitrary constants α,β,γ. *Imposing the diagonal Coulomb gauge (46) these equations imply*

$$\ddot{z}_n=\Phi(z_n)+\sum_{m=1,m\neq n}^{N}\frac{[\dot{z}_n+f(z_n)][\dot{z}_m+f(z_m)]}{z_n-z_m}, \tag{52}$$

and thus the solution of the initial-value problem for this dynamical system can be obtained by solving the corresponding gauge theory equations in the Weyl gauge, see (45). More specifically: the solution of the initial-value problem for this dynamical system, (52), is given by the eigenvalues of the matrix equation

$$\ddot{U}=\Phi(U) \tag{53}$$

with the initial conditions

$$U_{nm}(0)=\delta_{mn}z_n(0) \tag{54}$$

and

$$\dot{U}_{nn}(0)=\dot{z}_n, \tag{55a}$$

$$\dot{U}_{nm}(0)=\{[\dot{z}_n(0)+f[z_n(0)]\}^{1/2}\{[\dot{z}_m(0)+f[z_m(0)]\}^{1/2},\quad n\neq m. \tag{55b}$$

Remark 3.3: In the special case $\gamma=0$ a model is obtained whose solvability was already known.[8] Our new model reported in Sec. II (and already derived by our other method in Sec. III A) is obtained for $\beta=0$, $\gamma=1$, and $\alpha=-a^2$. But the greater generality of the result as formulated in Proposition 3.2 is only apparent: if $\gamma\neq 0$, one can always reduce this more general case to the special case with $\beta=0$ by the (rather trivial) transformations $U\to\breve{U}=U-(\beta/2\gamma)\mathbf{1}$, $t\to\breve{t}=\gamma t$. And note that, for $f(z)=z^2-a^2$, the right-hand sides of (55) and (3b) coincide: the apparent differences are merely notational.

Let us end this section by outlining the proof of this result, whose analogy with that proven in the first part of this section is we trust evident enough not to require further elaboration. We first write out (41) and (50) by imposing condition (45). Then (41a) becomes

$$\delta_{nm}\dot{z}_n+M_{nm}(z_m-z_n)=W_{nm}, \tag{56}$$

which for the *diagonal* elements (i.e., $n=m$) implies

$$W_{nn}=\dot{z}_n. \tag{57}$$

For the *off-diagonal* elements we obtain the assignment

$$M_{nm}=-\frac{1}{z_n-z_m}W_{nm},\quad n\neq m, \tag{58}$$

whereas the diagonal elements M_{nn} remain unassigned. Then (41b) reads

$$\dot{W}_{nm} + \sum_{\ell=1}^{N} (M_{n\ell} W_{\ell m} - W_{n\ell} M_{\ell m}) = \delta_{nm} \Phi(z_n). \tag{59}$$

The *diagonal* elements of this equation give (via (58) and (57))

$$\ddot{z}_n - 2 \sum_{\ell=1, \ell \neq n}^{N} \frac{W_{n\ell} W_{\ell n}}{z_n - z_\ell} = \Phi(z_n), \tag{60}$$

while the *off-diagonal* elements imply the following important consistency conditions,

$$W_{nm} + (M_n - M_m)\dot{W}_{nm} + \frac{\dot{z}_n - \dot{z}_m}{z_n - z_m} W_{nm} - \sum_{\ell=1, \ell \neq n,m}^{N} W_{n\ell} W_{\ell m} \left(\frac{1}{z_n - z_\ell} - \frac{1}{z_\ell - z_m} \right) = 0, \quad n \neq m. \tag{61}$$

In particular (50a) implies $B_{nm}B_{mn} = B_{nn}B_{mm}$. Inserting in this equation the assignment $B_{nm} = W_{nm} + \delta_{nm} f(z_n)$ (see (50b)) and in particular $B_{nn} = \dot{z}_n + f(z_n)$ (see (57)), we get

$$W_{nm} W_{mn} + \delta_{nm} [2\dot{z}_n + f(z_n)] f(z_n) = [\dot{z}_n + f(z_n)][\dot{z}_m + f(z_m)]. \tag{62}$$

Thus the solution of (50) for $n' = m$ and $m' = n$ is

$$W_{nm} = \exp(\varphi_n - \varphi_m) \{ - \delta_{nm} [2\dot{z}_n + f(z_n)] f(z_n) + [\dot{z}_n + f(z_n)][\dot{z}_m + f(z_m)] \}^{1/2}, \tag{63}$$

where the functions $\varphi_n(t)$ are *arbitrary*, and it is easy to check that this is a solution of (50) also for all the other values of n', m'. Inserting this in (60) we obtain

$$\ddot{z}_n = \Phi(z_n) + 2 \sum_{\ell=1, \ell \neq n}^{N} \frac{[\dot{z}_n + f(z_n)][\dot{z}_\ell + f(z_\ell)]}{z_n - z_\ell}. \tag{64}$$

It remains to check the consistency relations (61). We note that, for $\ell \neq n, m$ and $n \neq m$, (63) entails $W_{n\ell} W_{\ell m} = W_{nm} [\dot{z}_\ell + f(z_\ell)]$, hence (61) is implied by

$$\frac{\dot{W}_{nm}}{W_{nm}} = - (M_n - M_m) - \frac{\dot{z}_n - \dot{z}_m}{z_n - z_m} + \sum_{\ell=1, \ell \neq n,m}^{N} [\dot{z}_\ell + f(z_\ell)] \left(\frac{1}{z_n - z_\ell} - \frac{1}{z_\ell - z_m} \right), \quad n \neq m. \tag{65}$$

Inserting the logarithmic derivative of (63) for $n \neq m$ and using (64) we find by straightforward computations that the condition (61) is identically satisfied provided

$$\dot{\varphi}_n = - M_n \tag{66}$$

and the functions f and Φ satisfy the following functional equations,

$$f'(x) + f'(y) = 2 \frac{f(x) - f(y)}{x - y}, \quad \Phi(x) = f(x) f'(x), \tag{67}$$

for all $x \neq y$. The general solution of these functional equations is given by (51), and this concludes our proof. Note that at the end we can make the simplifying assignment $\varphi_n = M_n = 0$.

IV. ALTERNATIVE FORMULATIONS

The strategy to obtain alternative formulations of "goldfish-type" N-body problems is by now standard (and quite old;[6] for a convenient up-to-date presentation see Ref. 2). One introduces a *monic* polynomial $\psi(z,t)$ of degree N in z, the N zeros $z_n(t)$ of which evolve according to the equations of motion of the N-body problem under consideration, and then investigates the corresponding evolution of the N coefficients $c_m(t)$ of this polynomial. The route we follow to obtain the equations of motions satisfied by the coefficients $c_m(t)$—equations that are of course no less

solvable than the equations of motion satisfied by the zeros $z_n(t)$, since the relationship among these quantities, the N zeros z_n and the N coefficients c_m of a polynomial of degree N, is purely *algebraic*—is via the evolution equation satisfied by the polynomial $\psi(z,t)$: note that this entails that this evolution equation is itself *solvable*. Since this technique is by now standard, and appropriate formulas to implement it are available (see in particular the Appendix in Ref. 2), we present without further ado the relevant results.

The evolution equation satisfied by the polynomial $\psi(z,t)$ (see (13)) the zeros of which evolve according to the equations of motion (1) reads

$$\psi_{tt} - 2(z^2-a^2)\psi_{tz} + 2[(N-2)z - c_1]\psi_t + (z^2-a^2)^2\psi_{zz} - 2[(N-3)z - c_1](z^2-a^2)\psi_z + \{N(N-5)z^2 - 2(N-2)c_1 z + 2[2Na^2 + \dot{c}_1 - c_1^2 + 3c_2]\}\psi = 0. \tag{68}$$

Notation: Here and hereafter subscripted variables denote partial differentiations with respect to them.

Remark 4.1: This evolution equation, (68), contains also certain coefficients $c_m \equiv c_m(t)$, which are obviously (linearly) related to the function $\psi(z,t)$, indeed clearly (see (13))

$$c_m(t) = [(N-m)!]^{-1} \left.\frac{\partial^{N-m}\psi(z,t)}{\partial z^{N-m}}\right|_{z=0}. \tag{69}$$

Hence (68) is in fact a nonlinear functional equation satisfied by the polynomial $\psi(z,t)$, and the fact that it is indeed satisfied by a polynomial of degree N in z, while not evident, is implied by the way it has been obtained.

From this evolution equation one obtains (using if need be the results in Ref. 2) the corresponding system of ODEs satisfied by the coefficients $c_m(t)$, see (14); and this of course justifies the relevant results about the solvability of this system reported in Sec. II.

Exactly the same procedure yields (21) from (6), although a more direct route is via the "trick" formula (5), as indicated in Sec. II. Anyway we also display here, for completeness, the equation for the polynomial $\tilde{\psi}(z,t)$ (see (22)) that provides the bridge connecting these two systems of ODEs (deriving this equation is particularly easy using the formulas given in the Appendix in Ref. 2; but beware of the slight notational change in the definition of the coefficients c_m due to the $(i)^m$ factor on the right-hand side of (22)):

$$\tilde{\psi}_{tt} - 2z(z-i)\tilde{\psi}_{tz} + [2(N-2)z - (2N+1)i - 2i\tilde{c}_1]\tilde{\psi}_t + z^2(z-i)^2\tilde{\psi}_{zz} - 2z(z-i)[N(z-i) - 3z - i\tilde{c}_1]\tilde{\psi}_z + [N(N-5)z^2 - 2N^2 iz - N(N+1) - 2(N-2)i\tilde{c}_1 z - 2(N-1)\tilde{c}_1 + 2(i\cdot\tilde{c}_1 + \tilde{c}_1^2 - 3\tilde{c}_2)]\tilde{\psi} = 0. \tag{70}$$

V. EQUILIBRIUM CONFIGURATIONS, BEHAVIOR IN THEIR VICINITY, *DIOPHANTINE* RELATIONS

In this section we discuss the equilibrium configurations (namely, the time-independent solutions) of the *isochronous* models (6) and (21) and the behavior of these models in the vicinity of their equilibria. A motivation for focusing on the *isochronous* models is that they lead to the remarkable *Diophantine* relations reported at the end of Sec. II, as indicated below.

Clearly the equilibrium configuration $\tilde{c}_m(t) = \bar{c}_m$, $\dot{c}_m(t) = 0$ of the system of ODEs (21) is characterized by the following system of N algebraic equations:

$$-(m+2)(m-3)\bar{c}_{m+2} + 2(m-1)(m+1+\bar{c}_1)\bar{c}_{m+1} + [-m(m+1) - 2(m-1)\bar{c}_1 + 2\bar{c}_1^2 - 6\bar{c}_2]\bar{c}_m = 0,$$

$$m = 1, \ldots, N, \quad \bar{c}_0 = 1, \quad \bar{c}_{-1} = \bar{c}_{N+1} = \bar{c}_{N+2} = 0. \tag{71}$$

Likewise the equilibrium configuration $\tilde{z}_n(t) = \bar{z}_n$, $\dot{\tilde{z}}_n = 0$, of the N-body problem (6) is characterized by the following N algebraic equations:

$$\bar{z}_n(\bar{z}_n - i)\left[\bar{z}_n + i + \sum_{m=1, m\neq n}^{N} \frac{\bar{z}_m(\bar{z}_m - i)}{\bar{z}_n - \bar{z}_m}\right] = 0. \tag{72}$$

These two configurations are related to each other by the polynomial formula (see (22))

$$\bar{\psi}(z) = \prod_{n=1}^{N} (z - \bar{z}_n) = \sum_{n=0}^{N} (i)^m \bar{c}_m z^{N-m}, \quad \bar{c}_0 = 1, \tag{73}$$

where $\bar{\psi}(z)$ is the "equilibrium" (namely, time-independent) polynomial solution of (70).

The general solution of the algebraic problem (72) can clearly be broken down as follows:

$$\bar{z}_n + i + \sum_{m=1, m\neq n}^{\nu} \frac{\bar{z}_m(\bar{z}_m - i)}{\bar{z}_n - \bar{z}_m} = 0 \quad \text{for } n = 1, \ldots, \nu, \tag{74a}$$

$$\bar{z}_n = i \quad \text{for } n = \nu + 1, \ldots, \mu, \tag{74b}$$

$$\bar{z}_n = 0 \quad \text{for } n = \mu + 1, \ldots, N, \tag{74c}$$

with ν and μ *non-negative integers*, $0 \leqslant \nu \leqslant \mu \leqslant N$. Of course each of these three sectors will be empty if the corresponding range of values of n is empty (recall that $n = 1, \ldots, N$).

Remark 5.1: In any equilibrium configuration the labeling of the particles can be freely permuted. To write the breakdown (74) we identified, without loss of generality, a (somewhat) definite assignment of particle labels.

Remark 5.2: Genuine equilibrium configurations of the N-body problem (6) are characterized by the requirement that $\bar{z}_n \neq \bar{z}_m$ if $n \neq m$: indeed, whenever this condition is violated, the equilibrium condition (72) becomes *ambiguous* due to the vanishing of some denominator in the sum, compensated by a vanishing of the corresponding numerator or by some other cancellation. Hence a *necessary* condition in order that the configuration associated with the breakdown indicated in (74) correspond to a *genuine* equilibrium configuration of the N-body problem (6) is that $\mu \geqslant N - 1$ and $\nu \geqslant \mu - 1$, so that at most one of the $\bar{z}_n$'s vanishes (in which case we assign to it the highest label, $\bar{z}_N = 0$) and at most one takes the value i (in which case we assign to it the highest or next-to-highest label, $\bar{z}_N = i$, or $\bar{z}_{N-1} = i$ if $\bar{z}_N = 0$). But in the following it is convenient to consider *all* possible equilibrium configurations, including *nongenuine* ones, because, as we will see, such configurations, while problematic to deal with in the context of the N-body problem (6), correspond to equilibrium configurations $\bar{c}_m$ of the system of ODEs (21) which are instead perfectly legitimate in the context of this *nonlinear harmonic oscillators* model. Indeed their consideration in such a context yields interesting findings (see the following).

To get more information on the roots $\bar{z}_n$ of (74a) we now introduce a *monic* polynomial $\varphi(z)$ of degree ν having the ν numbers $\bar{z}_n$ with $n = 1, \ldots, \nu$ as its zeros:

$$\varphi(z) = \prod_{n=1}^{\nu} (z - \bar{z}_n) = \sum_{m=0}^{\nu} (i)^m \varphi_m z^{\nu-m}, \quad \varphi_0 = 1. \tag{75}$$

Note that via this formula we also introduced the ν coefficients φ_m of this polynomial.

It is now straightforward (and particularly easy using the formulas given in the Appendix in Ref. 2; but beware of the slight notational change in the definition of the coefficients $\bar{c}_m$ due to the $(i)^m$ factor on the right-hand side of (75)) to conclude that this polynomial must then satisfy the following equation, implied by (74a):

$$z^2\varphi'' - 2(\nu - 3)z\varphi' + \nu(\nu - 5)\varphi = i[z\varphi'' - 2(\nu + \varphi_1)\varphi']. \tag{76}$$

It is now easily seen that, via (75), this ODE (76) yields for the coefficients φ_m the recurrence relation

$$m(m-5)\varphi_m = (m-\nu-1)(m+\nu+2\varphi_1)\varphi_{m-1}, \tag{77a}$$

which must be complemented by the two extremal conditions (see (75))

$$\varphi_{-1} = \varphi_{\nu+1} = 0 \tag{77b}$$

and by the normalization condition (see (75))

$$\varphi_0 = 1. \tag{77c}$$

Clearly the two extremal conditions (77b) are identically satisfied (for $m=0$, respectively, $m=\nu+1$), while the condition (77c) yields (for $m=1$)

$$\varphi_1 = \frac{\nu(\nu+1)}{2(2-\nu)}, \tag{78}$$

entailing the requirement (hereafter assumed to hold)

$$\nu \neq 2. \tag{79}$$

Insertion of (78) in (77a) yields finally the recursion

$$m(m-5)\varphi_m = (m-\nu-1)\left(m+\frac{3\nu}{2-\nu}\right)\varphi_{m-1}, \tag{80}$$

the solution of which is easily seen to exist only if $\nu \leqslant 5$. For the remaining cases,

$$\nu = 0 \text{ or } 1 \text{ or } 3 \text{ or } 4 \text{ or } 5, \tag{81}$$

see (79), we get the following solutions (recall (77c)):

$$\text{for } \nu = 0, \quad \varphi(z) = \varphi_0 = 1, \tag{82a}$$

$$\text{for } \nu = 1, \quad \varphi_0 = \varphi_1 = 1, \quad \varphi(z) = z + i, \tag{82b}$$

$$\text{for } \nu = 3, \quad \varphi_0 = 1, \quad \varphi_1 = -6, \quad \varphi_2 = 14, \quad \varphi_3 = -14, \tag{82c}$$

$$\text{for } \nu = 4, \quad \varphi_m = (-)^m \binom{5}{m}, \quad m = 0,1,\ldots,4, \tag{82d}$$

$$\text{for } \nu = 5, \quad \varphi_m = (-)^m \binom{5}{m}, \quad m = 0,1,\ldots,4, \quad \varphi_5 \text{ arbitrary}. \tag{82e}$$

Via (74) and (75) it is clear that the *monic* polynomial $\bar{\psi}(z)$ of degree N in z, see (73)—which identifies as its N zeros $\bar{z}_n$, respectively, its N coefficients $\bar{c}_m$ the equilibrium configurations of the models (6), respectively, (21)—is given by the formula

$$\bar{\psi}(z) = \varphi(z)(z-i)^{\mu-\nu} z^{N-\mu}. \tag{83}$$

It is thereby seen, via (82), that the coefficients $\bar{c}_m$ are given by the formulas (28) (with the *arbitrary* constant $c=\varphi_5-1$ in (28e), see (28e)).

Remark 5.3: Clearly the coefficients $\bar{c}_m$ vanish for $m>\mu$, hence they *all* vanish (except of course $\bar{c}_0=1$) if $\mu=0$ (this assignment provides indeed a solution of (71)).

Next, let us discuss the behavior of the system (21) in the neighborhood of its equilibrium configurations. To this end we set

$$\tilde{c}_n(t) = \bar{c}_n + \varepsilon\rho_n(t) + O(\varepsilon^2), \tag{84}$$

with $\bar{c}_m$ the coefficients c_m at equilibrium (as determined in the following) and ε a small parameter. We thereby obtain in the standard manner the *linearized* equations of motion

$$\ddot{\rho}_m + 2(m-1)i\dot{\rho}_{m+1} - (2m+1+2\bar{c}_1)i\dot{\rho}_m - (m+2)(m-3)\rho_{m+2} + 2(m-1)(m+1+\bar{c}_1)\rho_{m+1} + [-m(m+1) - 2(m-1)\bar{c}_1 + 2\bar{c}_1^2 - 6\bar{c}_2]\rho_m + 2i\bar{c}_m\dot{\rho}_1 + 2[(m-1)\bar{c}_{m+1} - (m-1-2\bar{c}_1)\bar{c}_m]\rho_1 - 6\bar{c}_m\rho_2 = 0,$$

$$m = 1, \ldots, N, \quad \rho_0 = 0, \quad \rho_{N+1} = \rho_{N+2} = 0. \tag{85}$$

The general solution of this linear system of ODEs, (85), reads

$$\rho_m(t) = \sum_{n=1}^{N} [a_n^{(+)} r_m^{(+)(n)} \exp(ip_n^{(+)}t) + a_n^{(-)} r_m^{(-)(n)} \exp(ip_n^{(-)}t)], \tag{86}$$

where the $2N$ numbers $a_n^{(\pm)}$ are *arbitrary* (to be fixed by the initial data) while the $2N$ numbers $p_n^{(\pm)}$, respectively, the $2N$ corresponding (t-independent) N-vectors $\underline{r}^{(\pm)(n)} \equiv (r_1^{(\pm)(n)}, \ldots, r_N^{(\pm)(n)})$, are the eigenvalues, respectively, the eigenvectors, of the (N-vector) generalized eigenvalue equation (29a). This implies (29b) with the two $N \times N$ matrices A and B defined (componentwise) by the formulas (27). But we know (see Proposition 2.13) that *all* the *nonsingular* solutions of the system of *nonlinear harmonic oscillators* (21) are *completely periodic* with period 2π, hence the (certainly *nonsingular*) solutions describing the behavior of this system around equilibrium must have the same periodicity property, implying that *all* the eigenvalues $p_n^{(\pm)}$ yielded by the generalized eigenvalue problem (29a) must be *integers.* And this entails the validity of Proposition 2.14.

Remark 5.4: In the special case of the equilibrium configuration $\bar{c}_m = 0$ (for $m = 1, \ldots, N$, while of course $\bar{c}_0 = 1$; see the *Remark 5.3*), the matrices A and B become *triangular* and the computation of the eigenvalues $p_n^{(\pm)}$ is then a trivial task, yielding

$$p_n^{(+)} = n + 1, \quad p_n^{(-)} = n. \tag{87}$$

VI. OUTLOOK

It is remarkable that a research project started with the main purpose to clarify a methodological issue—namely, the relationship among two different approaches to the same question: that of identifying *solvable* many-body problems—resulted in the identification of a *novel* solvable many-body problem. To the readers who might imagine—in view of the recent discovery of several such new models, as reviewed in Ref. 2—that this is a relatively trivial task, we suggest to try and find themselves some new model. Our educated guess is that such a task is quite challenging. We are nevertheless ourselves hopeful that new many-body models exist, and that they might be discovered/manufactured by the techniques described in this paper. In any case this possibility remains as a tantalizing prospect, until a way is found to ascertain conclusively that these approaches have exhausted their capability to yield many-body models of the kind investigated herein which are both new and interesting (although the second of these two qualities involves of course a value judgment).

Another research direction (perhaps suitable as a PhD project) is toward proving the *Diophantine* conjectures proffered in this paper (see the end of Sec. II) and in previous ones (see Ref. 2) and other papers referred to there), as well as obtaining additional findings of this kind (for instance by applying techniques analogous to those of Sec. V to the model (14), taking advantage of the results reported in the Appendix).

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APPENDIX: EQUILIBRIUM CONFIGURATIONS OF MODELS (14) AND (1)

In *Remark 2.9* it was mentioned that there exist additional equilibrium (i.e., time-independent) solutions of the model (14) besides (16). In this appendix we first list *all* these equilibrium configurations (as obtained via MAPLE) for $N=2$, 3, 4, and 5. We then outline a technique allowing one to obtain *all* the equilibrium configurations for *arbitrary N* (we of course did check that these findings reproduce, for $N=2,3,4,5$, those obtained via MAPLE).

These equilibrium configurations are clearly solutions of the following set of N algebraic equations (see (14)):

$$(m+2)(m-3)c_{m+2}-2(m-1)c_1c_{m+1}+2[m(N+2-m)a^2-c_1^2+3c_2]c_m-2(N+1-m)a^2c_1c_{m-1}$$
$$+(N+2-m)(N+1-m)a^4c_{m-2}=0,$$

$$m=1,\ldots,N,\quad c_0=1,\quad c_{-1}=c_{N+1}=c_{N+2}=0. \tag{A1}$$

The following solutions of this algebraic system have been obtained via MAPLE.

For $N=2$

$$c_1=0,\quad c_2=-a^2, \tag{A2a}$$

or

$$c_2=\frac{c_1^2}{3}-\frac{a^2}{3},\quad c_1 \text{ arbitrary} \tag{A2b}$$

(the equilibrium configurations (16) correspond to the latter one, (A2b), with $c_1=\pm 2a$).

For $N=3$,

$$c_2=\frac{c_1^2}{3}\pm\frac{ac_1}{3}-a^2,\quad c_3=\pm\frac{ac_1^2}{3}-\frac{2a^2c_1}{3},\quad c_1 \text{ arbitrary} \tag{A3}$$

(the equilibrium configurations (16) obtain for $c_1=\pm 3a$).

For $N=4$,

$$c_2=\frac{c_1^2}{3}-\frac{4a^2}{3},\quad c_3=-a^2c_1,\quad c_4=-\frac{a^2c_1^2}{3}+\frac{a^4}{3},\quad c_1 \text{ arbitrary}, \tag{A4a}$$

or

$$c_2 = \frac{c_1^2}{3} \pm \frac{2ac_1}{3} - 2a^2, \quad c_3 = \pm \frac{2ac_1^2}{3} - \frac{5a^2c_1}{3},$$

$$c_4 = \frac{a^2c_1^2}{3} \mp \frac{4a^3c_1}{3} + a^4, \quad c_1 \text{ arbitrary} \tag{A4b}$$

(the equilibrium configurations (16) obtain from (A4b) for $c_1 = \pm 4a$.

For $N=5$,

$$c_2 = \frac{c_1^2}{3} \pm \frac{ac_1}{3} - 2a^2, \quad c_3 = \pm \frac{ac_1^2}{3} - \frac{5a^2c_1}{3}, \quad c_4 = -\frac{a^2c_1^2}{3} \mp \frac{a^3c_1}{3} + a^4,$$

$$c_5 = \mp \frac{a^3c_1^2}{3} + \frac{2a^4c_1}{3}, \quad c_1 \text{ arbitrary}, \tag{A5a}$$

or

$$c_2 = \frac{c_1^2}{3} \pm ac_1 - \frac{10a^2}{3}, \quad c_3 = \pm ac_1^2 - 3a^2c_1, \quad c_4 = a^2c_1^2 p 5a^3c_1 + 5a^4,$$

$$c_5 = \pm \frac{a^3c_1^2}{3} - 2a^4c_1 \pm \frac{8a^5}{3}, \quad c_1 \text{ arbitrary} \tag{A5b}$$

(the equilibrium configurations (16) obtain from (A5b) for $c_1 = \pm 5a$).

The route we follow to obtain *all* the solutions of the system (A1) is analogous to that followed in Sec. V. The starting point is to introduce a *monic* polynomial $\bar{\psi}(z)$ of degree N that has the N numbers c_m solutions of (A1) as its N coefficients:

$$\bar{\psi}(z) = \prod_{n=1}^{N} (z - \bar{z}_n) = \sum_{m=0}^{N} c_m z^{N-m}, \quad c_0 = 1. \tag{A6}$$

Note the analogy of these formulas with (13), and the fact that we also introduced the N zeros $\bar{z}_n$ of this polynomial $\bar{\psi}(z)$, which clearly provide the equilibrium configuration of the N-body problem (1) (although not necessarily a *genuine* equilibrium configuration), hence satisfy the following system of N algebraic ODEs:

$$(\bar{z}_n^2 - a^2)\left[\bar{z}_n + \sum_{m=1, m\neq n}^{N} \frac{\bar{z}_m^2 - a^2}{\bar{z}_n - \bar{z}_m}\right] = 0. \tag{A7}$$

Our strategy to find all the solutions of the system (A1) is to find first all the solutions of this system, (A7), and then use (A6).

Clearly the solutions of (A7) can be broken down as follows:

$$\bar{z}_n + \sum_{m=1, m\neq n}^{\nu} \frac{\bar{z}_m^2 - a^2}{\bar{z}_n - \bar{z}_m} = 0 \quad \text{for } n = 1, \ldots, \nu, \tag{A8a}$$

$$\bar{z}_n = a \quad \text{for } n = \nu + 1, \ldots, \nu + \mu, \tag{A8b}$$

$$\bar{z}_n = -a \quad \text{for } n = \nu + \mu + 1, \ldots, N, \tag{A8c}$$

with the two *non-negative integers* ν and μ *arbitrary* except for the constraint

$$\nu + \mu \leqslant N \tag{A8d}$$

(implying of course that neither one of these two non-negative integers can exceed N).

This assignment, (A8), clearly entails that

$$\bar{\psi}(z) = (z-a)^{\mu}(z+a)^{N-\mu-\nu}\phi_{\nu}(z), \tag{A9a}$$

with $\phi_{\nu}(z)$ the *monic* polynomial of degree ν,

$$\phi_{\nu}(z) = \prod_{n=1}^{\nu}(z-\bar{z}_n) = \sum_{m=0}^{\nu} f_m z^{\nu-m}, \quad f_0 = 1, \tag{A9b}$$

the zeros of which satisfy the algebraic relations (A8a). Hence this polynomial $\phi_{\nu}(z)$ satisfies

$$(z^2-a^2)\phi_{\nu}'' - 2[(\nu-3)z - f_1]\phi_{\nu}' + \nu(\nu-5)\phi_{\nu} = 0, \tag{A10}$$

as implied by the (by now standard) technique to transform algebraic equations such as (A8a) into differential equations (see for instance the Appendix in Ref. 2). Here and in the following primes denote of course differentiations with respect to the argument of the function they are appended to.

Before proceeding to discuss the solution of this equation let us consider the special case with $\nu=0$ entailing $\phi_0(z)=1$ (which solves (A10) trivially). In this case (A9a) and (A8d) yield

$$\bar{\psi}(z) = (z-a)^{\mu}(z+a)^{N-\mu}, \quad \mu = 0,1,\ldots,N. \tag{A11a}$$

It is then easily seen from (A6) that this entails

$$c_m = a^m \sum_{\ell=\max(0,m+\mu-N)}^{\min(\mu,m)} (-)^{\ell}\binom{\mu}{\ell}\binom{N-\mu}{m-\ell}. \tag{A11b}$$

This formula provides a set of equilibrium configurations, characterized by the integer μ in the range $0 \leqslant \mu \leqslant N$; in particular the two solutions corresponding to $\mu=0$ and to $\mu=N$ are easily seen to yield the two solutions (16).

Let us now return to (A10), assuming hereafter that the integer ν is *positive*, $\nu>0$ (to avoid unnecessary notational complications). To solve this equation, (A10), we set

$$\phi_{\nu}(z) = a^{\nu}\chi(x), \quad z = a(x-1). \tag{A12}$$

This formula implies that $\chi(x)$ is again a *monic* polynomial of degree ν (although for notational simplicity we do not signal this via a subscript ν). We also set (in analogy to (A9b))

$$\chi(x) = \prod_{n=1}^{\nu}(x-x_n) = \sum_{m=0}^{\nu}\chi_m x^{\nu-m}, \quad \chi_0 = 1, \tag{A13}$$

and we then note that this formula, together with (A9b), entails

$$f_m = a^m \sum_{\ell=0}^{m}\binom{\nu-\ell}{m-\ell}\chi_{\ell}, \tag{A14a}$$

hence in particular

$$f_1 = a(\nu + \chi_1). \tag{A14b}$$

Via this formula and (A12) the differential equation (A10) now reads

$$x(x-2)\chi'' - 2[(\nu-3)x - 2\nu + 3 - \chi_1]\chi' + \nu(\nu-5)\chi = 0, \tag{A15a}$$

entailing, via (A13), the two-term recurrence

$$m(m-5)\chi_m = 2(\nu+1-m)(3-\nu-\chi_1-m)\chi_{m-1}, \tag{A15b}$$

implying (for $m=0$ and $m=\nu+1$) the extremal conditions $\chi_{-1}=\chi_{\nu+1}=0$ (consistent with (A13)).

For $m=1$ the recurrence formula (A15b) (together with $\chi_0=1$, see (A13)) yields the relation

$$(\nu-2)\chi_1 = -\nu(\nu-2), \tag{A16}$$

requiring that the two cases with $\nu=2$ and $\nu\neq 2$ be treated separately.

For $\nu=2$ one easily obtains the solution

$$\chi_0 = 1, \quad \chi_1 \text{ arbitrary}, \quad \chi_2 = \frac{\chi_1(\chi_1+1)}{3}. \tag{A17a}$$

Remark A.1: Let us note as a curiosity that the recursion (A15b) with $\nu=2$ allows this solution (A17a) to be extended as follows:

$$\chi_3 = \chi_4 = 0, \quad \chi_5 \text{ also arbitrary},$$

$$\chi_m = \frac{2^{m-3}15}{m(m-1)(m-2)}\binom{m-1+\chi_1}{m-5}\chi_5, \quad m=5,6,\ldots . \tag{A17b}$$

But we are only interested in the solution (A17a) with $\chi_m=0$ for $m>2$, entailing that $\chi(x)$ is a polynomial of degree $\nu=2$.

So in this $\nu=2$ case we get

$$\chi(x) = x^2 + \chi_1 x + \frac{\chi_1(\chi_1+1)}{3} \tag{A18}$$

hence, via (A12),

$$\phi_2(z) = z^2 + f_1 z + \frac{f_1^2 - a^2}{3}, \quad f_1 \text{ arbitrary}, \tag{A19}$$

where we set, consistent with (A9b), $f_1=(2+\chi_1)a$.

For $\nu\neq 2$ the recursion (A15b) with (A16) yields

$$\chi_0 = 1, \quad \chi_1 = -\nu, \quad \chi_2 = \frac{\nu(\nu-1)}{3}, \quad \chi_3 = \chi_4 = 0, \quad \chi_5 \text{ arbitrary},$$

$$\chi_m = \frac{(-)^{m-1}2^{m-3}15}{m(m-1)(m-2)}\binom{\nu-5}{m-5}\chi_5, \quad m=6,\ldots,\nu. \tag{A20}$$

Of course the second line of this equation is only relevant if $\nu>5$, which can only happen if $N>5$.

From these results, via (A9a) with (A8d) and (A12), we arrive finally, after a bit of trivial algebra, at the following two determinations of the polynomial $\bar{\psi}(z)$ (see (A6)):

$$\bar{\psi}(z) = \left(z^2 + cz + \frac{c^2-a^2}{3}\right)(z-a)^{\mu}(z+a)^{N-2-\mu}, \quad \mu=0,1,\ldots,N-2, \tag{A21a}$$

$$\bar{\psi}(z) = (z-a)^{\mu}(z+a)^{N-\mu}\left[1 - \frac{\nu a}{z+a} + \frac{\nu(\nu-1)a^2}{3(z+a)^2} + c\sum_{\ell=0}^{\nu-5}\frac{(-2)^{\ell}}{(\ell+5)(\ell+4)(\ell+3)}\binom{\nu-5}{\ell}\left(\frac{a}{z+a}\right)^{\ell+5}\right],$$

$$\nu = 5,6,\ldots,N, \quad \mu = 0,1,\ldots,N-\nu. \tag{A21b}$$

The first, (A21a), of these two formulas is applicable for $N \geqslant 2$, having been obtained from the previous results corresponding to $\nu=2$, with $c=f_1$ an *arbitrary* number. It includes the results obtainable from the cases with $\nu=1$ and $\nu=3$; likewise, the result corresponding to $\nu=4$ has not be reported, as it is encompassed by the result (A11a). The second, (A21b), of these two formulas is of course only applicable provided $N \geqslant 5$, having being obtained from (A20) for $\nu \geqslant 5$, with $c = \chi_5/60$ an *arbitrary* number. Together with (A11a) these two formulas determine *all* the equilibrium configurations c_m of the system (14) (and as well *all* the equilibrium configurations–not necessarily *genuine*—of the N-body problem (1))—up to a final (trivial but tedious) step, to be performed using (A6) (as done earlier to obtain (A11b) from (A11a)), which we leave as a task for the diligent reader.

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Optimization problems for an elastic plate

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This paper concerns optimization problems related to bi-harmonic equations subject to either Navier or Dirichlet homogeneous boundary conditions. Physically, in dimension two, our equation models the deformation of an elastic plate which is either hinged or clamped along the boundary, under load. We discuss existence, uniqueness, and properties of the optimizers. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Let Ω be a bounded domain in $\mathbb{R}^N$. This paper is concerned with optimization problems related to either the following boundary value problem (with Navier boundary conditions)

$$\Delta^2 u = f \text{ in } \Omega, \quad u = \Delta u = 0, \quad \text{on } \partial\Omega, \tag{1}$$

or to the problem (with Dirichlet boundary conditions)

$$\Delta^2 v = f \text{ in } \Omega, \quad v = |\nabla v| = 0, \quad \text{on } \partial\Omega. \tag{2}$$

As usual, $\Delta^2 = \Delta(\Delta)$. Let $f_0 \in L^2(\Omega)$, $f_0 \not\equiv 0$, and let $\mathcal{F} = \mathcal{F}(f_0)$ be the class of rearrangements of f_0. Similarly, let $g_0 \in L^2(\Omega)$, $g_0 \not\equiv 0$, and let $\mathcal{G} = \mathcal{G}(g_0)$ be the class of rearrangements of g_0. We say that $f(x) \not\equiv 0$ if the set $\{x \in \Omega : f(x) \neq 0\}$ has a positive measure. We are interested in the following problems:

$$\sup_{f\in\mathcal{F}, g\in\mathcal{G}} \int_\Omega g u_f \, dx, \quad \inf_{f\in\mathcal{F}, g\in\mathcal{G}} \int_\Omega g u_f \, dx, \tag{3}$$

$$\sup_{f\in\mathcal{F}, g\in\mathcal{G}} \int_\Omega g v_f \, dx, \quad \inf_{f\in\mathcal{F}, g\in\mathcal{G}} \int_\Omega g v_f \, dx, \tag{4}$$

where u_f is the (unique) solution of (1), and v_f is the (unique) solution of (2).

In dimension two, problem (1) models the deformation of an elastic plate which is hinged along the boundary (under load f), whereas problem (2) models the deformation of an elastic plate which is clamped along the boundary. The solution u_f stands for the deformation of the hinged plate from the rest position. Therefore, the functional $\int_\Omega g u_f \, dx$ measures the average deformation (with respect to the measure $g \, dx$) of the plate and similarly for v_f. Thus, any solution to (3) or (4) determines an *extremal* configuration.

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Our interest in the above-mentioned optimization problems spans questions such as existence, uniqueness (in case Ω is a ball), and qualitative properties of maximizers or minimizers. The case of the equation $-\Delta u=f$ is well understood, see Refs. 3–6 and 13. As far as we know, the optimization problems for bi-harmonic equations have not been investigated yet. We show that the corresponding results of existence continue to hold. In the case of hinged plates we also find a result of representation of the optimizers and, for the maximizer, a result of uniqueness in the ball. An example of interest is the following.

Example 1: Suppose $g_0=1$ and $f_0=\chi_{F_0}$, where χ_{F_0} is the characteristic functions of the measurable sets $F_0\subset\Omega$ with $|F_0|<|\Omega|$. Denoting by f_M a maximizer of (3) in this special situation, and denoting by w the solution to problem (1) with $f=1$, we show that (see Theorem 5) $f_M=\chi_{F_M}$ for the measurable set $F_M=\{w(x)>t_M\}$ with t_M such that $|F_M|=|F_0|$. Moreover, denoting by f_m a minimizer of (3) we prove that $f_m=\chi_{F_m}$ for the measurable set $F_m=\{w(x)<t_m\}$ with t_m such that $|F_m|=|F_0|$. So, physically speaking, in order to maximize the average deformation of the linear hinged plate under uniform loads (given by the appropriate rearrangement class) it is best to place the load away from the boundary (independent of the geometry of the plate); in order to minimize the average deformation it is best to place the load in a tubular neighborhood of the boundary. The above-mentioned results give some information on the location of extremal domains.

For clamped plates the representation result seems to be more difficult due to the lack of appropriate maximum principles for the corresponding equation; however, if the domain is a ball we prove a particular result of symmetry for the optimizers. A special example is the following.

Example 2: Let Ω be a disc. Suppose $g=\chi_G$, where $G\subset\Omega$ is a disc concentric with Ω. Let $f_0=\chi_{F_0}$, with $F_0\subset\Omega$. Denoting a maximizer of

$$\sup_{f\in\mathcal{F}}\int_\Omega gv_f\,dx$$

by $\bar{f}$ we show that (see Theorem 7) $\bar{f}=\chi_{F_M}$, where F_M is the disc concentric with Ω with $|F_M|=|F_0|$. Similarly, denoting a minimizer of

$$\inf_{f\in\mathcal{F}}\int_\Omega gv_f\,dx$$

by $\underline{f}$ we have $\underline{f}=\chi_{F_m}$, where F_m is the annulus concentric with Ω with $|F_m|=|F_0|$ and such that its exterior boundary coincides with $\partial\Omega$. So, physically speaking, in order to maximize the average deformation over the set G of the linear circular clamped plate under uniform loads (given by the appropriate rearrangement class) it is best to place the load centered with Ω. To minimize the analogous deformation it is best to place the load close to the boundary of Ω. Of course, these results agree with the physical intuition.

Some theorems of the present paper are based on results by Burton summarized by Lemmas 1–3 in the following. Burton and McLeod have used these results to investigate the problems

$$\sup_{f\in\mathcal{F}}\int_\Omega fu_f\,dx,\quad \inf_{f\in\mathcal{F}}\int_\Omega fu_f\,dx,$$

where u_f is the solution of the homogeneous Dirichlet problem $-\Delta u=f$.

We study the problems (3) and (4), where $\mathcal{F}$ and $\mathcal{G}$ are two (possibly different) classes of rearrangements. A remarkable fact is that (Theorem 3) when $\mathcal{F}=\mathcal{G}$ then

$$\sup_{f,g\in\mathcal{F}}\int_\Omega gu_f\,dx=\sup_{f\in\mathcal{F}}\int_\Omega fu_f\,dx.$$

II. PRELIMINARIES

In this section we collect some well-known results.

Recall that a function $u \equiv u_f \in W_0^{1,2}(\Omega)$ with $\Delta u_f \in W_0^{1,2}(\Omega)$ is a weak solution of (1) provided

$$\int_\Omega \Delta u \Delta \phi \, dx = \int_\Omega f\phi \, dx, \quad \forall\, \phi \in W_0^{1,2}(\Omega) \quad \text{with } \Delta\phi \in W_0^{1,2}(\Omega).$$

This problem can be described by a system of second-order elliptic equations with Dirichlet boundary conditions. It is well known that it has a unique solution. Alternatively, in smooth domains, one could work in $H^2(\Omega) \cap H_0^1(\Omega)$ with the test functions in the same space. The difference between these two approaches in nonsmooth domains is investigated in Ref. 12. See also, Refs. 8, 9, and 16. Using standard results on regularity (see Refs. 1 and 10) we find that u is a classical solution in the sense that $u \in W^4(\Omega) \cap C^3(\Omega)$. Moreover, using the continuity (with respect to weak convergence) of the inverse of the Laplacian, one proves the following result: If $\{f_i\}$ is a sequence of functions in $L^2(\Omega)$ which converges weakly (in $L^2(\Omega)$) to a function ξ then the corresponding solutions u_{f_i} to problem (1) converge strongly in $L^2(\Omega)$ to the solution u_ξ.

A function $v \equiv v_f \in W_0^{2,2}(\Omega)$ is a weak solution of (2) provided

$$\int_\Omega \Delta v \Delta \psi \, dx = \int_\Omega f\psi \, dx, \quad \forall\, \psi \in W_0^{2,2}(\Omega).$$

For results of the existence and regularity of this problem we refer to Refs. 1 and 11. It has a unique solution. Moreover, if $\{f_i\}$ is a sequence of functions in $L^2(\Omega)$ which converges weakly (in $L^2(\Omega)$) to a function ξ then the corresponding solutions v_{f_i} to problem (2) converges weakly in $W_0^{2,2}(\Omega)$ to the solution v_ξ. As a consequence, v_{f_i} converges strongly in $L^2(\Omega)$ to the solution v_ξ.

If u_g is the solution of (1) with f replaced by g then we have

$$\int_\Omega g u_f \, dx = \int_\Omega (\Delta u_g)(\Delta u_f) dx = \int_\Omega f u_g \, dx. \tag{5}$$

Similarly, if v_g is the solution of (2) with f replaced by g then we have

$$\int_\Omega g v_f \, dx = \int_\Omega (\Delta v_g)(\Delta v_f) dx = \int_\Omega f v_g \, dx. \tag{6}$$

Definition: Suppose $f, f_0 : \Omega \to \mathbb{R}$ are (Lebesgue) measurable functions. We say that f and f_0 are rearrangements of each other if and only if

$$|\{f(x) \geqslant \alpha\}| = |\{f_0(x) \geqslant \alpha\}|, \quad \forall\, \alpha \in \mathbb{R}.$$

Here and in what follows we write $\{f(x) \geqslant \alpha\}$ instead of $\{x \in \Omega : f(x) \geqslant \alpha\}$, and denote with $|E|$ the Lebesgue measure of the (measurable) set E. For any $f : \Omega \to \mathbb{R}$, f^* denotes the decreasing Schwarz rearrangement of f; that is, f^* is radially symmetric, decreases as $|x|$ increases, and it is a rearrangement of f. Recall that f^* is defined on B, the ball centered at the origin with volume equal to $|\Omega|$.

Lemma 1: *Let $f, u \in L^2(\Omega)$. Suppose that every level set of u (that is, sets of the form $u^{-1}(\{\alpha\})$) has measure zero. Then there exists an increasing function ϕ such that $\phi \circ u$ is a rearrangement of f.*

Lemma 2: *Let $\mathcal{F}$ be the set of rearrangements of a fixed function $f_0 \in L^2(\Omega)$, $f_0 \not\equiv 0$, and let $u \in L^2(\Omega)$, $u \not\equiv 0$. If there is an increasing function ϕ such that $\phi(u) \in \mathcal{F}$ then*: (*a*)

$$\int_\Omega f u \, dx \leqslant \int_\Omega \phi(u) u \, dx, \quad \forall\, f \in \bar{\mathcal{F}};$$

(*b*) *the function* $\phi(u)$ *is the unique maximizer relative to* $\bar{\mathcal{F}}$.

Lemma 3: *Let* $\mathcal{F}$ *be the set of rearrangements of a fixed function* $f_0 \in L^2(\Omega)$, $f_0 \not\equiv 0$, *and let* $u \in L^2(\Omega)$, $u \not\equiv 0$. *There exists* $\hat{f} \in \mathcal{F}$ *such that*

$$\int_\Omega fu \, dx \leqslant \int_\Omega \hat{f}u \, dx, \quad \forall f \in \bar{\mathcal{F}}.$$

In the above-mentioned lemmas and in what follows, we denote with $\bar{\mathcal{F}}$, the weak closure of $\mathcal{F}$ in $L^2(\Omega)$. For the proof of Lemma 1, see Ref. 4 (Lemma 2.9), and for Lemmas 2 and 3, see Ref. 4 (Lemma 2.4).

Next we recall a well-known rearrangement inequality. If $u \in W_0^{1,2}(\Omega)$ is non-negative and if u^* denotes the Schwarz rearrangement of u, then $u^* \in W_0^{1,2}(\Omega)$ and the inequality

$$\int_B |\nabla u^*|^2 \, dx \leqslant \int_\Omega |\nabla u|^2 \, dx \tag{7}$$

holds. The case of equality in (7) has been considered in Ref. 2. The following result can be deduced from Lemma 3.2, Theorem 1.1, and Lemma 2.3(v), in Ref. 2.

Theorem 1: *Let* $u \in W_0^{1,2}(\Omega)$ *be non-negative*, *and suppose equality holds in* (7). *Then* $u^{-1}(\alpha, \infty)$ *is a translate of* $u^{*-1}(\alpha, \infty)$, *for every* $\alpha \in [0, M]$, *where* M *is the essential superior of* u *over* Ω, *modulo sets of measure zero*. *Moreover*, *if*

$$|\{x \in \Omega : \nabla u(x) = 0, 0 < u(x) < M\}| = 0, \tag{8}$$

then u *is a translation of* u^*.

III. EXISTENCE RESULTS

To state the next theorem we use the notion of weak continuity in the following sense: A linear operator $K : L^2(\Omega) \to L^2(\Omega)$ is weakly continuous if for every sequence f_i which converges weakly in $L^2(\Omega)$ to f, the sequence Kf_i converges strongly to Kf.

The existence of solutions to problems (3) and (4) follows from the following.

Theorem 2: *Let* $K : L^2(\Omega) \to L^2(\Omega)$ *be a linear operator weakly continuous and such that*

$$\int_\Omega gKf \, dx = \int_\Omega fKg \, dx, \quad \forall g, f \in L^2(\Omega).$$

Then there exist $f_M \in \mathcal{F}$ *and* $g_M \in \mathcal{G}$ *such that*

$$\int_\Omega g_M K f_M \, dx = \sup_{g \in \mathcal{G}, f \in \mathcal{F}} \int_\Omega gKf \, dx;$$

furthermore, *there exist* $f_m \in \mathcal{F}$ *and* $g_m \in \mathcal{G}$ *such that*

$$\int_\Omega g_m K f_m \, dx = \inf_{g \in \mathcal{G}, f \in \mathcal{F}} \int_\Omega gKf \, dx.$$

Proof: Let

$$I = \sup_{g \in \mathcal{G}, f \in \mathcal{F}} \int_\Omega gKf \, dx.$$

We first show that I is finite. Since K is continuous we must have

$$\|Kf\|_2 \leqslant C\|f\|_2, \quad \forall f \in L^2(\Omega).$$

Moreover, since

$$\|g\|_2\|Kf\|_2 \leqslant C\|g_0\|_2\|f_0\|_2,$$

I is finite. Let $\{g_i,f_i\}$ be a maximizing sequence and let $u_i=Kf_i$. Since $\{f_i\}$ is bounded in $L^2(\Omega)$, it must contain a subsequence (still denoted $\{f_i\}$) converging weakly to $\xi \in L^2(\Omega)$. Note that $\xi \in \bar{\mathcal{F}}$, the weak closure of $\mathcal{F}$ in $L^2(\Omega)$. Since K is assumed to be weakly continuous, Kf_i converges (strongly) in $L^2(\Omega)$ to $K\xi$. Moreover, $\{g_i\}$ must contain a subsequence (still denoted $\{g_i\}$) converging weakly to $\eta \in L^2(\Omega)$, with $\eta \in \bar{\mathcal{G}}$. Thus,

$$I = \lim_{i\to\infty}\int_\Omega g_i Kf_i \,\mathrm{d}x = \int_\Omega \eta K\xi \,\mathrm{d}x. \tag{9}$$

By Lemma 3 we infer existence of $g_M \in \mathcal{G}$ that maximizes the linear functional $\int_\Omega hK\xi \,\mathrm{d}x$, relative to $h \in \bar{\mathcal{G}}$. As a consequence we obtain

$$\int_\Omega \eta K\xi \,\mathrm{d}x \leqslant \int_\Omega g_M K\xi \,\mathrm{d}x. \tag{10}$$

By assumption we also have

$$\int_\Omega g_M K\xi \,\mathrm{d}x = \int_\Omega \xi K g_M \,\mathrm{d}x.$$

Applying again Lemma 3, we find $f_M \in \mathcal{F}$ such that

$$\int_\Omega g_M K\xi \,\mathrm{d}x = \int_\Omega \xi K g_M \,\mathrm{d}x \leqslant \int_\Omega f_M K g_M \,\mathrm{d}x = \int_\Omega g_M K f_M \,\mathrm{d}x \leqslant I.$$

From (9) and (10) and the last inequality it follows that

$$I = \int_\Omega g_M K f_M \,\mathrm{d}x.$$

Thus (g_M,f_M) is a maximizer, as desired.

Now define $-\mathcal{G}=\{h \in L^2(\Omega): -h \in \mathcal{G}\}$. The class $-\mathcal{G}$ coincides with the class of all rearrangements of $-g_0$. Since

$$\inf_{g\in\mathcal{G},f\in\mathcal{F}}\int_\Omega gKf \,\mathrm{d}x = -\sup_{g\in\mathcal{G},f\in\mathcal{F}}\int_\Omega (-g)Kf \,\mathrm{d}x = -\sup_{h\in-\mathcal{G},f\in\mathcal{F}}\int_\Omega hKf \,\mathrm{d}x,$$

the existence of a minimizer follows by the proof for the maximizer. □

Theorem 3: *Let* $K: L^2(\Omega)\to L^2(\Omega)$ *satisfy the assumptions of Theorem 2 and, in addition,*

$$\int_\Omega fKf \,\mathrm{d}x \geqslant 0, \quad \forall f \in L^2(\Omega), \quad \int_\Omega fKf \,\mathrm{d}x = 0 \Leftrightarrow f = 0.$$

Then,

$$\sup_{f,g\in\mathcal{F}}\int_\Omega gKf \,\mathrm{d}x = \sup_{f\in\mathcal{F}}\int_\Omega fKf \,\mathrm{d}x.$$

Proof: Let (g_M,f_M) be a maximizing pair. From

$$0 \leqslant \int_\Omega (g_M - f_M)K(g_M - f_M)\mathrm{d}x = \int_\Omega g_M K g_M \,\mathrm{d}x + \int_\Omega f_M K f_M \,\mathrm{d}x - 2\int_\Omega g_M K f_M \,\mathrm{d}x,$$

it follows that

$$2\int_\Omega g_M K f_M \leqslant \int_\Omega f_M K f_M \,\mathrm{d}x + \int_\Omega g_M K g_M \,\mathrm{d}x$$

with equality if and only if $g_M = f_M$. We can rewrite the latter inequality as

$$\int_\Omega g_M K f_M \leqslant \int_\Omega \frac{f_M + g_M}{2}\frac{Kf_M + Kg_M}{2}. \tag{11}$$

Since $\bar{\mathcal{F}}$ is convex (Ref. 3, Theorem 6), we have $(f_M+g_M)/2 \in \bar{\mathcal{F}}$. Moreover, since K is linear we have $(Kf_M+Kg_M)/2=K((f_M+g_M)/2)$. Hence, using (11) we find

$$I = \int_\Omega g_M K f_M \leqslant \int_\Omega \frac{f_M + g_M}{2} K\left(\frac{f_M + g_M}{2}\right) \leqslant I.$$

It follows that equality must hold in (11). Hence, $g_M = f_M$. The theorem follows. □

Remark: Note that all conditions in Theorems 2 and 3 hold when $Kf = u_f$, the solution to problem (1), and when $Kf = v_f$, the solution to problem (2). In particular, by theorems 2 and 3 we have existence for the problems

$$\sup_{f\in\mathcal{F}}\int_\Omega f u_f \,\mathrm{d}x, \quad \sup_{f\in\mathcal{F}}\int_\Omega f v_f \,\mathrm{d}x.$$

We cannot have, in general, a corresponding result for the inferior.

IV. NAVIER BOUNDARY CONDITIONS

In this section we consider optimizers of problems (3). We will use a strong maximum principle for Eq. (1). That is, if $f(x) \geqslant 0$, $f \not\equiv 0$, we must have $-\Delta u_f(x) > 0$ in Ω. This fact follows easily from the strong maximum principle of the Laplacian and from the special boundary conditions of problem (1). A further application of the strong maximum principle for the Laplacian yields $u_f(x) > 0$ in Ω.

Theorem 4: *Let* $g_0(x) \not\equiv 0$ *with either* $g_0(x) \geqslant 0$ *or* $g_0(x) \leqslant 0$, *and let* $\mathcal{G} = \mathcal{G}(g_0)$. *Let* $f_0(x) \not\equiv 0$ *with either* $f_0(x) \geqslant 0$ *or* $f_0(x) \leqslant 0$, *and let* $\mathcal{F} = \mathcal{F}(f_0)$.

(i) If (g_M, f_M) *is a maximizing pair of* (3) *then there exist increasing functions* ϕ *and* ψ *such that*

$$f_M = \phi(u_{g_M}), \quad g_M = \psi(u_{f_M}), \tag{12}$$

almost everywhere in Ω.

(ii) If (g_m, f_m) *is a minimizing pair of* (3) *then there exist decreasing functions* $\underline{\phi}$ *and* $\underline{\psi}$ *such that*

$$f_m = \underline{\phi}(u_{g_m}), \quad g_m = \underline{\psi}(u_{f_m}), \tag{13}$$

almost everywhere in Ω.

Proof: (i) Let (g_M, f_M) be a maximizing pair and let u_{g_M} (u_{f_M}) be the corresponding solutions to (1) with g_M (f_M) in place of f. If $g_0(x) \geqslant 0$, the set $\{x \in \Omega : g_M(x) > 0\}$ has a positive measure, and by (1) (with g_M in place of f) we get $-\Delta u_{g_M}(x) > 0$ in Ω. If $g_0(x) \leqslant 0$, the set $\{x \in \Omega : g_M(x) < 0\}$ has a positive measure, and by (1) we get $-\Delta u_{g_M}(x) < 0$ in Ω. In both cases, all level sets $A_\alpha = \{x \in \Omega : u_{g_M}(x) = \alpha\}$ have measure zero (this follows from Ref. 10, Lemma 7.7). By Lemma 1

we infer the existence of ϕ increasing such that $\phi(u_{g_M})$ is a rearrangement of f_M. Since f_M is a maximizer of $\int_\Omega f u_{g_M}\,dx$ for $f\in\mathcal{F}$, by Lemma 2 we must have $f_M=\phi(u_{g_M})$. We have proved the first equation of (12). To prove the second equation of (12), we can proceed as before interchanging the roles of f_M and g_M. We find a function ψ increasing such that $g_M=\psi(u_{f_M})$.

(ii) Let (g_m,f_m) be a minimizing pair. As already observed in the proof of Theorem 2, we have

$$\int_\Omega g_m u_{f_m}\,dx=-\sup_{h\in-\mathcal{G},f\in\mathcal{F}}\int_\Omega hu_f\,dx,$$

where $-\mathcal{G}=\mathcal{G}$ $(-g_0)$. We can write the previous equation as

$$\int_\Omega(-g_m)u_{f_m}\,dx=\sup_{h\in-\mathcal{G},f\in\mathcal{F}}\int_\Omega hu_f\,dx.$$

By our previous result there exist $\tilde{\phi}$ and $\tilde{\psi}$ increasing such that

$$f_m=\tilde{\phi}(u_{-g_m}),\quad -g_m=\tilde{\psi}(u_{f_m}).$$

We can rewrite the previous equations as

$$f_m=\tilde{\phi}(-u_{g_m})=\underline{\phi}(u_{g_m}),\quad g_m=-\tilde{\psi}(u_{f_m})=\underline{\psi}(u_{f_m}),$$

with $\underline{\phi}(s)=\tilde{\phi}(-s)$, and $\underline{\psi}(s)=-\tilde{\psi}(s)$. Of course, $\underline{\phi}(s)$ and $\underline{\psi}(s)$ are decreasing. The theorem is proved. □

Theorem 5: *Let $g_0(x)\geqslant 0$, $g_0(x)\not\equiv 0$, $f_0(x)\geqslant 0$, $f_0(x)\not\equiv 0$. Let (g_M,f_M) be a maximizing pair of* (3). *If $G_M=\{g_M(x)>0\}$ then (up to sets of zero measure) we have*

$$G_M=\{u_{f_M}(x)>t_M\},\quad t_M=\inf_{x\in G_M}u_{f_M}(x);\tag{14}$$

if $F_M=\{f_M(x)>0\}$ then (up to sets of zero measure) we have

$$F_M=\{u_{g_M}(x)>\tau_M\},\quad \tau_M=\inf_{x\in F_M}u_{g_M}(x).\tag{15}$$

Moreover, let (g_m,f_m) be a minimizing pair of (3). *If $G_m=\{g_m(x)>0\}$ then (up to sets of zero measure) we have*

$$G_m=\{u_{f_m}(x)<t_m\},\quad t_m=\sup_{x\in G_m}u_{f_m}(x);\tag{16}$$

if $F_m=\{f_m(x)>0\}$ then (up to sets of zero measure) we have

$$F_m=\{u_{g_m}(x)<\tau_m\},\quad \tau_m=\sup_{x\in F_m}u_{g_m}(x).\tag{17}$$

Proof: Let us prove that

$$\{u_{f_M}(x)>t_M\}\subset G_M\subset\{u_{f_M}(x)\geqslant t_M\}.\tag{18}$$

The inclusion on the right follows from the definition of t_M. If we define

$$\delta=\sup_{x\in\Omega\setminus G_M}u_{f_M}(x),$$

the inclusion on the left is clear if we prove that $t_M\geqslant\delta$. To derive a contradiction assume $t_M<\delta$. Let us fix $t_M<\xi_1<\xi_2<\delta$. Since $\xi_1>t_M$, there exists a set $A\subset G_M$, with positive measure, such that $u_{f_M}(x)\leqslant\xi_1$ on A. Similarly, $\xi_2<\delta$ implies that there exists a set $B\subset\Omega\setminus G_M$, with positive measure, such that $u_{f_M}(x)\geqslant\xi_2$ on B. Without loss of generality we may assume that $|A|=|B|$. Next,

consider a measure preserving map $T:A\to B$, see Ref. 14. Using T we define a particular rearrangement of $g_M(x)$, denoted $\bar{g}$,

$$\bar{g}(x)=\begin{cases} g_M(Tx), & x\in A \\ g_M(T^{-1}x), & x\in B \\ g_M(x) & \Omega\setminus(A\cup B). \end{cases}$$

Thus

$$\int_\Omega \bar{g}u_{f_M}\,dx-\int_\Omega g_M u_{f_M}\,dx=\int_{A\cup B}\bar{g}u_{f_M}\,dx-\int_{A\cup B}g_M u_{f_M}\,dx=\int_B \bar{g}u_{f_M}\,dx-\int_A g_M u_{f_M}\,dx$$
$$\geqslant \xi_2\int_B \bar{g}\,dx-\xi_1\int_A g_M\,dx=(\xi_2-\xi_1)\int_A g_M\,dx>0.$$

Therefore

$$\int_\Omega \bar{g}u_{f_M}\,dx>\int_\Omega g_M u_{f_M}\,dx,$$

which contradicts the maximality of g_M. Hence, $t_M\geqslant\delta$, and (18) follows. By the proof of Theorem 4 we know that the level sets of $u_{f_M}(x)$ have zero measure, hence, (14) follows from (18). The proof of (15) is the same (interchanging the roles of g_M and f_M). To prove (16), we observe that

$$\int_\Omega g_m u_{(-f_m)}=\sup_{g\in\mathcal{G},f\in\mathcal{F}}\int_\Omega g u_{(-f)}.$$

If $G_m=\{g_m(x)>0\}$, by our previous result we have

$$G_m=\{u_{(-f_m)}(x)>\bar{t}_M\},\quad \bar{t}_M=\inf_{x\in G_m}u_{(-f_m)}(x).$$

Equivalently, since $u_{(-f_m)}=-u_{f_m}$, we have

$$G_m=\{u_{f_m}(x)<t_m\},\quad t_m=\sup_{x\in G_m}u_{f_m}(x),$$

with $t_m=-\bar{t}_M$. Similarly, one proves (17) interchanging the roles of g_m and f_m. The proof of the theorem is complete. □

Remark: Note that $|\{g_M(x)>0\}|=|\{g_m(x)>0\}|=|\{g_0(x)>0\}|$. Therefore, if $|\{g_0(x)>0\}|<|\Omega|$, by Theorem 5 it follows that t_M and t_m are strictly positive. If we assume $f_0\in L^\infty(\Omega)$ then we have the continuity of the solutions u_{f_M} and u_{f_m} (see Ref. 10). In this situation, by Theorem 5 we have

$$\partial G_M\subset\{u_{f_M}=t_M\},\quad \partial(\Omega\setminus G_m)\subset\{u_{f_m}=t_m\}.$$

This result establishes a link between g_M and f_M or g_m and f_m. We remark that we may have different solutions of the optimization problems, and the above link holds for any solution.

We now address the question of uniqueness in a ball.

Theorem 6: *Suppose* Ω *is a ball centered at the origin. Suppose* $f_0(x)\geqslant 0$, $f_0(x)\not\equiv 0$ *and* $g_0(x)\geqslant 0$, $g_0(x)\not\equiv 0$. *Then the maximization problem in* (3) *has a unique solution, namely*, (g_0^*,f_0^*).

Proof: Let (g,f) be a maximizing pair. If u_f and u_g are the solutions of problem (1) with f and g, respectively, put

$$-\Delta u_f=z_f,\quad -\Delta u_g=z_g.$$

We have

$$-\Delta z_f = f \text{ in } \Omega, \quad z_f = 0 \text{ on } \partial\Omega, \tag{19}$$

and

$$-\Delta z_g = g \text{ in } \Omega, \quad z_g = 0 \text{ on } \partial\Omega. \tag{20}$$

Then

$$\int_\Omega g u_f \, dx = \int_\Omega (\Delta u_g)(\Delta u_f) \, dx = \int_\Omega z_g z_f \, dx. \tag{21}$$

By a well-known result of Talenti (Ref. 15) we have

$$z_f^*(x) \leqslant z_{f^*}(x), \quad z_g^*(x) \leqslant z_{g^*}(x) \text{ in } \Omega, \tag{22}$$

where $z_{f^*}(x)$ is the solution to problem (19) with f^* in place of f and $z_{g^*}(x)$ is the solution to problem (20) with g^* in place of g. Using (21), the Hardy-Littlewood inequality and (22) we find

$$\int_\Omega g u_f \, dx = \int_\Omega z_g z_f \, dx \leqslant \int_\Omega z_g^* z_f^* \, dx \leqslant \int_\Omega z_{g^*} z_{f^*} \, dx = \int_\Omega g^* u_{f^*} \, dx \leqslant \int_\Omega g u_f \, dx,$$

where u_{f^*} denotes the solution to (1) with f^* in place of f. Therefore

$$\int_\Omega z_g^* z_f^* \, dx = \int_\Omega z_{g^*} z_{f^*} \, dx.$$

The latter equation and (22) yield

$$z_f^*(x) = z_{f^*}(x), \quad z_g^*(x) = z_{g^*}(x) \text{ in } \Omega. \tag{23}$$

By using (23), the variational characterization of the solution of (19) and standard inequalities about rearrangements we find

$$\int_\Omega |\nabla z_f|^2 \, dx = \int_\Omega (2 f z_f - |\nabla z_f|^2) dx \leqslant \int_\Omega (2 f^* z_f^* - |\nabla z_f^*|^2) dx = \int_\Omega (2 f^* z_{f^*} - |\nabla z_{f^*}|^2) dx$$

$$= \int_\Omega |\nabla z_{f^*}|^2 \, dx = \int_\Omega |\nabla z_f^*|^2 \, dx.$$

The last inequality and (7) yield

$$\int_\Omega |\nabla z_f^*|^2 \, dx = \int_\Omega |\nabla z_f|^2 \, dx.$$

We find easily that

$$|\{x \in \Omega : \nabla z_f^*(x) = 0\}| = |\{x \in \Omega : \nabla z_{f^*}(x) = 0\}| = 0.$$

Therefore, using Theorem 1 and (23) we find $z_f(x) = z_f^*(x) = z_{f^*}(x)$. As a consequence, by (19) we get $f(x) = f^*(x) = f_0^*(x)$. Similarly, one finds that $g(x) = g^*(x) = g_0^*(x)$. The theorem is proved. □

V. DIRICHLET BOUNDARY CONDITIONS

This problem seems to be more complicated than that with Navier boundary conditions. We prove the following (partial) result.

Theorem 7: *Let Ω be an N-ball centered at the origin. Let $0 \leqslant g(x) \leqslant M$, $g(x) \not\equiv 0$, $g(x) = g^*(x)$ in Ω, and let $0 \leqslant f_0(x) \leqslant M$, $f_0(x) \not\equiv 0$. Let $\mathcal{F}$ be the family of rearrangements of f_0 in Ω. For $f \in \mathcal{F}$, let v_f be the solution to problem* (2). *Then*

$$\sup_{f\in\mathcal{F}}\int_\Omega gv_f\,\mathrm{d}x \tag{24}$$

has a unique solution $\bar{f}$; *namely* $\bar{f}=f_0^*$. *Moreover*,

$$\inf_{f\in\mathcal{F}}\int_\Omega gv_f\,\mathrm{d}x \tag{25}$$

has a unique solution $\underline{f}$; *namely* $\underline{f}=-(-f_0)^*$.

The following lemma, which is an extension of Ref. 3, Theorem 2.4 to weak solutions, will be used in the proof of Theorem 7.

Lemma 4: Suppose $0\leqslant g(x)\leqslant M$ *is a radial function defined in the N-ball* Ω, *and suppose* $v=v_g$ *is the corresponding solution to problem* (2). *Then* $v(x)=v^*(x)$, *almost everywhere in* Ω.

Proof: We begin by showing that $v(x)$ is radial. To do this we fix a rotation map R. Let G denote the Green function given by (see Ref. 7)

$$G(x,y)=C_N|x-y|^{4-N}\int_0^{(1-|x|^2)(1-|y|^2)/|x-y|^2} t(1+t)^{-\frac{N}{2}}\,\mathrm{d}t,$$

where C_N is a positive constant. Then

$$v(x)=\int_\Omega G(x,y)g(y)\mathrm{d}y.$$

Simple calculations confirm that $G(Rx,Ry)=G(x,y)$, hence

$$v(Rx)=\int_\Omega G(Rx,y)g(y)\mathrm{d}y=\int_\Omega G(Rx,Ry)g(Ry)\mathrm{d}y=\int_\Omega G(x,y)g(y)\mathrm{d}y=v(x),$$

so v is radial. Next, note that $v(x)$ is non-negative since $g(x)$ is non-negative. Consider a radial test function $\psi\in C_0^\infty(\mathbb{R}^N)$, say

$$\psi(x)=\begin{cases} c_N e^{-1/(1-\|x\|^2)}, & \|x\|<1\\ 0, & \|x\|\geqslant 1,\end{cases}$$

where c_N is a suitable normalizing constant. Let us set $\psi_\epsilon(x)=\epsilon^{-n}\psi(x/\epsilon)$, the standard mollifier. By extending g to all of $\mathbb{R}^N$, defining it to be zero outside Ω, we have $g_\epsilon:=\phi_\epsilon * g\to g$, in $L^2(\Omega)$, as $\epsilon\to 0$. Next we consider

$$\Delta^2 v_\epsilon=g_\epsilon \text{ in } \Omega,\quad v_\epsilon=|\nabla v_\epsilon|=0 \text{ on } \partial\Omega. \tag{26}$$

Since $g_\epsilon\in C_0^\infty(\bar{\Omega})$, v_ϵ belongs (at least) to $C^4(\bar{\Omega})$. Also g_ϵ is radial, indeed for R, a rotation map, we have

$$g_\epsilon(Rx)=\int_{\mathbb{R}^N} g(y)\psi_\epsilon(Rx-y)\mathrm{d}y=\int_{\mathbb{R}^N} g(Ry)\psi_\epsilon(Rx-Ry)\mathrm{d}y=\int_{\mathbb{R}^N} g(y)\psi_\epsilon(x-y)\mathrm{d}y=g_\epsilon(x).$$

Now applying Ref. 3, Theorem 2.4 we derive $v_\epsilon=v_\epsilon^*$. By the weak formulation of the solutions of (26) we have

$$\int_\Omega \Delta v_\epsilon\Delta w\,\mathrm{d}x=\int_\omega g_\epsilon w\,\mathrm{d}x,\quad \forall\, w\in H_0^2(\Omega).$$

So $\|v_\epsilon\|^2_{H_0^2(\Omega)}=\int_\Omega g_\epsilon v_\epsilon\,\mathrm{d}x\leqslant\|g_\epsilon\|_{L^2(\Omega)}\|v_\epsilon\|_{L^2(\Omega)}$. An application of the Sobolev embedding theorem then yields $\|v_\epsilon\|_{H_0^2(\Omega)}\leqslant C$, for some constant C. Thus $\{v_\epsilon\}$ is bounded (uniformly with respect to ϵ)

in $H_0^2(\Omega)$. Therefore it has a subsequence, denoted $\{v_i\}$, that converges to some $\bar{v} \in H_0^2(\Omega)$, weakly in $H_0^2(\Omega)$ and strongly in $L^2(\Omega)$. As a consequence we find

$$\int_\Omega \Delta \bar{v} \Delta w \, dx = \int_\Omega g w \, dx, \quad \forall \, w \in H_0^2(\Omega),$$

since $g_i \to g$ in $L^2(\Omega)$. Therefore $\bar{v}$ is the solution of the following boundary value problem:

$$\Delta^2 \bar{v} = g \text{ in } \Omega, \quad \bar{v} = |\nabla \bar{v}| = 0, \text{ on } \partial\Omega,$$

and $\bar{v}=v$. On the other hand, from a standard property of rearrangements, we have

$$\|v_i^* - v^*\|_{L^2(\Omega)} \leqslant \|v_i - v\|_{L^2(\Omega)},$$

so $v_i^* \to v^*$, in $L^2(\Omega)$, since $v_i \to v$, in $L^2(\Omega)$. Since $v_i^* = v_i$, it readily follows that $v=v^*$, almost everywhere in Ω, as desired. □

We are now ready to prove Theorem 7.

Proof of Theorem 7: Let v_g denote the solution of

$$\Delta^2 v_g = g \text{ in } \Omega, \quad v_g = |\nabla v_g| = 0 \text{ on } \partial\Omega.$$

Since $0 \leqslant g(x) \leqslant M$, $g(x) \not\equiv 0$, an inspection of the representation formula via Green's function shows that $v_g(x)$ is strictly positive in Ω and continuous on $\bar{\Omega}$.

It is easy to show that

$$\int_\Omega g v_f \, dx = \int_\Omega f v_g \, dx,$$

for every $f \in \mathcal{F}$, where v_f is the solution of (2). Therefore, we are interested in the following maximization problem:

$$\sup_{f \in \mathcal{F}} \int f v_g \, dx.$$

By Lemma 3 we know that there is a maximizer $\bar{f}$. Now let us prove that all level sets $A_\alpha = \{x \in \Omega : v_g(x) = \alpha\}$ have measure zero. If B is the ball $\{x \in \Omega : g(x) > 0\}$, the set $A_\alpha \cap B$ has measure zero because $\Delta^2 v_g = g > 0$ there. The boundary of B has (N-dimensional) measure zero. On $\Omega \backslash \bar{B}$ we have $\Delta^2 v_g = 0$. If the set $A_\alpha \cap (\Omega \backslash \bar{B})$ has a positive measure then $v_g(x) = \alpha$ on $\Omega \backslash \bar{B}$. Since $v_g(x) = 0$ on $\partial\Omega$, if $\alpha > 0$ we find a contradiction. If $\alpha = 0$ we have $v_g(x) = 0$ on a set of positive measures, but we know that $v_g(x) > 0$ in Ω. Therefore, all sets A_α have measure zero. Then, by Lemma 1, there is an increasing function ϕ such that $\phi(v_g(x))$ is a rearrangement of $\bar{f}$. Finally, by Lemma 2 we get $\bar{f} = \phi(v_g(x))$. As a consequence, since (by Lemma 4) $v_g(x) = v_g^*(x)$ and ϕ is increasing, we must have $\bar{f}(x) = \bar{f}^*(x) = f_0^*(x)$. The first assertion of the theorem is proved. The proof of the second assertion is very similar. We have

$$-\inf_{f \in \mathcal{F}} \int_\Omega g v_f \, dx = \sup_{f \in \mathcal{F}} \int_\Omega (-g) v_f \, dx = \sup_{f \in \mathcal{F}} \int_\Omega f v_{-g} \, dx,$$

where v_{-g} denotes the solution to (2) with $-g$ in place of f. By Lemma 3 we find a maximizer (of the last functional) $\underline{f}$. The level sets $A_\alpha = \{x \in \Omega : v_{-g}(x) = \alpha\}$ have measure zero (note that $v_{-g} = -v_g$, with v_g as in the previous case). Therefore, by Lemma 1, there is an increasing function $\tilde{\psi}$

such that $\tilde{\psi}(v_{-g}(x))$ is a rearrangement of $\underline{f}$. Finally, by Lemma 2 we get $\underline{f}=\tilde{\psi}(v_{-g}(x))$. Equivalently, since $v_{-g}(x)=-v_g(x)$, we have $-\underline{f}=\psi(v_g(x))$, with ψ increasing. As a consequence, since $v_g(x)=v_g^*(x)$ and ψ is increasing, we must have $-\underline{f}(x)=(-\underline{f})^*(x)=(-f_0)^*(x)$. Therefore, $f(x)=-(-f0)^*(x)$ as claimed. The theorem is proved. □

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Application of a variational iteration method to linear and nonlinear viscoelastic models with fractional derivatives

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Two nonlinear anelastic models with fractional derivatives, describing the properties of a series of materials as polymers, and polycrystalline materials are presented in this paper. These models are studied analytically, using a variational iteration method. The paper clarifies the different ways in which the fractional differentiation operator can be defined. A Volterra series method of model parameters identification from the experimental data is also presented. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2234273]

I. INTRODUCTION

In order to describe accurately the anelastic properties of polymers, anelastic rheologic equations were used, in which terms containing fractional derivatives[1–3] appear. The validity of these models is extensively discussed.

Linear five-parameter fractional anelastic models[4] are currently used to explain the anelastic properties of plastics or rubber.

It was found that the difference between the order of strain and stress time derivatives is related to the high frequency limit value of the loss factor.[5]

The investigation of the constitutive equations, which describes these models, is based on Fourier[6,7] and Laplace transform,[8] averaging methods,[9] finite element method,[4] and numerical methods.[10,11]

Unfortunately, only a restricted number of differential equations involving fractional derivatives have exact, or closed form solutions.

The aim of this paper is to build a nonlinear anelastic model with fractional damping, and to express the efficiency of the variational iteration method of He,[12–15] based on the Lagrange multiplier. The advantages of this method were widely presented in Ref. 16 as being useful for all kinds of differential equations, including strongly nonlinear equations. The method is strongly convergent, and was applied to a series of problems as waves,[17] fractional differential equations,[18] and differential equations with convolution product nonlinearity.[19] It is important to underline that the variational iteration method of He is not yet sufficiently investigated, which in the case of linear differential equations yields the solution after one iteration.

While the method has been applied to various nonlinear problems by many authors, a complete review is available in the He's monograph.[20]

This paper also tries to clarify the different ways in which the fractional differentiation operator can be defined.

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II. FRACTIONAL DIFFERENTIATION

The fractional derivative represents a generalization of the standard derivative and was introduced 300 years ago by Leibniz, and investigated by mathematicians such as Liouville, Riemann, Fourier, and Laplace.

The fractional derivative $D_{t,a}^{\mu}$, operator represents a linear operator, which can be written with the aid of the Riemann-Liouville definition as[21]

$$D_{t,a}^{\mu}x(t) = \begin{cases} \dfrac{1}{\Gamma(n-\mu)}\dfrac{\mathrm{d}^n}{\mathrm{d}t^n}\displaystyle\int_a^t (t-y)^{n-\mu-1}f(y)\mathrm{d}y, & n-1<\mu<n \\ \dfrac{\mathrm{d}^n}{\mathrm{d}x^n}f(t), & \mu=n, \end{cases} \tag{1}$$

where μ is a noninteger number which verifies $n-1<\mu<n$, $n=0,1,\ldots$. This definition of the fractional derivative is useful since for negative values of μ, the operator D^{μ} represents the fractional integration operator.

The fractional differentiation operator also verifies the following rules:

Composition or semigroup rule:

$$D_{t,a}^{\alpha}D_{t,a}^{\beta} = D_{t,a}^{\alpha+\beta}.$$

Zero rule:

$$D_{t,a}^{0}x(t) = x(t).$$

Fractional differentiation of a product of two functions $f(t)g(t)$ (Leibniz rule):

$$D_{t,a}^{\mu}f(t)g(t) = \sum_{k=0}^{\infty}\binom{k}{\mu}D_{t,a}^{k}f(t)D_{t,a}^{\mu-k}g(t). \tag{2}$$

For different values of a, different particular derivatives result, for which different differentiation rules result. This apparent contradiction was discussed and pointed out in the paper of Lavoie, Osler, and Tremblay.[22]

The value $a=-\infty$ gives the $D_{t,-\infty}^{\mu}$ operator, to which the following differentiation rule corresponds:

$$D_{t,-\infty}^{\mu}\exp(ut) = u^{\mu}\exp(ut), \tag{3}$$

where u is a complex valued quantity, $u \in C$.

The following differentiation rules result:

$$D_{t,-\infty}^{\mu}\exp(iat) = a^{\mu}\exp\left(i\left(at+\frac{\pi}{2}\mu\right)\right),$$

$$D_{t,-\infty}^{\mu}\sin(\omega t) = \omega^{\mu}\sin\left(\omega t+\frac{\pi}{2}\mu\right), \tag{4}$$

$$D_{t,-\infty}^{\mu}\cos(\omega t) = \omega^{\mu}\cos\left(\omega t+\frac{\pi}{2}\mu\right).$$

For $a=0$ the differentiation operator,

$$D_t^\mu = D_{t,0}^\mu, \tag{5}$$

results, which will be used in our calculation since the process investigated by us corresponds to positive values of time. For this kind of fractional derivative it results:[21,22,28]

$$D_t^\mu t^k = \frac{n!}{\Gamma(k-\mu+1)} t^{k-\mu}, \tag{6}$$

where $k \in N$.

The differentiation rule for the constant function $f(t)=1$[21,22] is

$$D_t^\mu 1 = \frac{n!}{\Gamma(1-\mu)} t^{-\mu}, \tag{7}$$

and it is valid for $\mu \geqslant 0$ and $t>0$, where Γ represents the Euler function.[27]

An interesting category of functions are the Mittag-Leffler functions, $E_\alpha(t)$ and $E_{\alpha,\beta}(t)$:[21]

$$E_\mu(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k+1)}, \quad E_{\mu,\alpha}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k+\alpha)}, \tag{8}$$

valid for $\mu \geqslant 0$, $\alpha \in C$ and $z \in C$.

It is important to note that the eigenfunctions $\psi_\mu(t)$ of the $D_{t,0}^\mu$ operator can be expressed in terms of $E_{\mu,\alpha}$ and the initial conditions $x(0)=x_0$, $\dot{x}(0)=x_1$, $\ddot{x}(0)=x_2,\ldots$, in the form[23]

$$\psi_\mu(t) = \sum_{j=0}^{[\mu]-1} x_j E_{\mu,j+1}(\lambda t^\mu), \tag{9}$$

which obeys the eigenvalue equation:

$$D_{t,0}^\mu \psi_\mu(t) = \lambda \psi_\mu(t). \tag{10}$$

The identity:

$$D_{t,0}^\mu E_\mu(-(at)^\mu) = -a^\mu E_\mu(-(at)^\mu), \tag{11}$$

can also be proved.

III. THE FRACTIONAL ANELASTIC MODELS

So far, a series of linear fractional anelastic models have been introduced in the literature for the investigation of a number of materials, as presented in Sec. II. We introduce the stress σ and the strain ε. A general linear anelastic model of this type can be written in the following form:[6]

$$\sigma + \sum_{i=1}^{n} \tau_\varepsilon^{\alpha_i} D_{t,a}^{\alpha_i} \sigma = E_0 \left(\varepsilon + \sum_{j=1}^{m} \tau_\sigma^{\beta_j} D_{t,a}^{\beta_j} \varepsilon \right), \tag{12}$$

where $n, m \in N$ are positive integers, $\tau_\sigma, \tau_\varepsilon$ are time constants, α_i, β_j are fractional and/or integer parameters (where $\alpha_i>0$, $0<\beta_j<1$), and E_0 the relaxed elastic modulus. $D_{t,a}^{\alpha_i,\beta_j}$ are the Riemann-Liouville differentiation operators.

There are known nonlinear anelastic models with fractional damping,[24] used for the study of rubbers and plastic materials.

Also, there are nonlinear anelastic models, based on the structural properties of polycrystalline solids, in which the rate of the relaxation process is a linear function of the stress applied on the grain boundaries:[25]

$$v \sim \frac{1}{\tau} = \frac{\alpha\sigma + \beta}{\tau_0}, \tag{13}$$

where τ is the nonlinear relaxation time, α and β are constants of the material, and τ_0 is the time constant in the linear model approximation.

The relaxed and the unrelaxed Young moduli, will be denoted by E_r and by $E_u = E_r + \delta E$, respectively. If the nonlinear processes are weak, α is a small parameter, and $\beta \approx 1$. For this kind of material, the nonlinear constitutive equation was established:[25]

$$(\dot{\sigma} - E_r\dot{\varepsilon}) + \frac{1}{\tau_0}[\alpha(\sigma - E_r\varepsilon) + \beta](\sigma - E_r\varepsilon) = \delta E\dot{\varepsilon}. \tag{14}$$

We consider the case of harmonic excitation

$$\varepsilon = A \sin \omega t,$$

where A is the amplitude of the excitation strain and ω is the angular frequency of the excitation.

Equation (14) can be written in a more general form, considering the dependency on fractional derivatives:

$$D^1_{t,a}x + \gamma D^\mu_{t,a}x + \beta x + \alpha x^2 = \mathcal{A}_0 \cos \omega t, \tag{15}$$

where $x = \sigma - E_r\varepsilon$, $\mathcal{A}_0 = \delta E \omega A$, μ has noninteger values, and γ and β are positive material constants.

Assuming that the initial condition at $t=0$ is

$$\sigma_0 = (E_r + \delta E)\varepsilon_0, \tag{16}$$

it corresponds to instantaneous response to the constant strain ε_0.

If $\beta = 1$ and $\alpha = 0$ the standard case of linear anelastic model results. Considering that α is a small parameter $0 < \alpha < 1$) the anelastic solid with small nonlinearities is obtained.

By optimal selection of the parameters of this model solutions with a strong linear behavior of the response to vibrations and with a nonlinear manifestation for the exponential response can be obtained.

IV. VARIATIONAL ITERATION METHOD

In order to find an analytical solution of Eq. (15) we will use a powerful variational iteration method established by He,[12,13] a new type of Lagrange multiplier method.

This universal method gives the possibility to solve all kinds of nonlinear equations. The application of the powerful method is limited to the case of a nonlinear system of type:

$$Lx(t) + Nx(t) = g(t), \tag{17}$$

where L is a linear operator, N is a nonlinear operator, and $g(t)$ is a known excitation function.

The variational iteration method gives the possibility to write the solution of Eq. (17) with the aid of the correction functional:

$$x_{n+1}(t) = x_n(t) + \int_0^t \lambda(\tau)(Lx(\tau) + N\tilde{x}(\tau) - g(\tau))\mathrm{d}\tau, \tag{18}$$

where x_n is an initial approximation with possible unknowns, λ is a Lagrange multiplier, and $\tilde{y}$ represents a term with a restricted variation, i.e., $\delta\tilde{y} = 0$. The λ multiplier can be found from the stationary condition of the correction functional $\delta x_{n+1} = 0$.

The variational iteration method was proposed in 1998, and it is used to solve fractional differential equations arising in seepage flow.[14]

We will use this method to obtain the solution of the constitutive equation (15). In our case we take

$$L = \frac{\mathrm{d}x}{\mathrm{d}t} + \beta x,$$

$$g = \mathcal{A}_0 \cos \omega t,$$

$$N = \gamma D^{\mu}_{t,a} x + \alpha x^2.$$

Imposing the stationary condition ($\delta x_{n+1}=0$) on the correction functional it results

$$\dot{\lambda}(\tau) - \beta\lambda(\tau) = 0, \tag{19}$$

$$[1 + \lambda(\tau)]\big|_{\tau=t} = 0, \tag{20}$$

from which the Lagrange multiplier can be identified as

$$\lambda(\tau) = -\exp(\beta(\tau - t)). \tag{21}$$

We will consider an initial approximation of the solution of

$$x_0(t) = c\exp(-\beta t) + \frac{\mathcal{A}_0\omega}{\omega^2+\beta^2}\sin\omega t + \frac{\mathcal{A}_0\beta}{\omega^2+\beta^2}\cos\omega t \tag{22}$$

containing the integration constant c.

We will investigate the solution of Eq. (15) for two particular forms of the fractional derivative, i.e., for $D^{\mu}_{t,0}$ and $D^{\mu}_{t,-\infty}$.

A. Case of $D^{\mu}_{t,0}$

A fractional oscillator was studied on the basis of He's method in a previous paper.[26]

In this case, for the linear model $\alpha=0$ replacing (19), (21), and (22) in (18) based on differentiation rules (6) and (7), it results:

$$\begin{aligned} x_{\mathrm{lin}}(t) = c\Bigg\{ & \exp(-\beta t) - \frac{\gamma}{\beta t^{\mu}\Gamma(1-\mu)}\Bigg[-e^{-\beta t}\sum_{n=0}^{\infty}\frac{(-\beta t)^n {}_1F_1(n-\mu;n+1-\mu;\beta t)}{(1-\mu)_n} \\ & + {}_1F_1(1;1-\mu;-\beta t)\Bigg]\Bigg\} + \frac{\mathcal{A}_0\omega}{\omega^2+\beta^2}\sin\omega t + \frac{\mathcal{A}_0\beta}{\omega^2+\beta^2}\cos\omega t - \gamma\mathcal{A}_0\frac{1}{(\omega^2+\beta^2)\beta t^{\mu}\Gamma(1-\mu)} \\ & \times\Bigg\{(\beta - i\omega)\Bigg[-e^{-\beta t}\sum_{n=0}^{\infty}\frac{(i\omega t)^n {}_1F_1(n-\mu;n+1-\mu;\beta t)}{(1-\mu)_n} + {}_1F_1(1;1-\mu;i\omega t)\Bigg] \\ & + (\beta + i\omega)\Bigg[-e^{-\beta t}\sum_{n=0}^{\infty}\frac{(-i\omega t)^n {}_1F_1(n-\mu;n+1-\mu;\beta t)}{(1-\mu)_n} + {}_1F_1(1;1-\mu;-i\omega t)\Bigg]\Bigg\}, \end{aligned} \tag{23}$$

where ${}_1F_1(a;b;z)$ represents the confluent hypergeometric function:[27,28]

$${}_1F_1(a;b;z) = \sum_{n=0}^{\infty}\frac{(a)_n z^n}{(b)_n n1}.$$

The quantity $(a)_n$ represents[27]

$$(a)_n = a(a+1)(a+2)\ldots(a+n-1),$$

where $(a)_0=1$. The quantity $(a)_n$ is connected to the Γ function by

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}.$$

For the nonlinear case ($\alpha \neq 0$) we obtain

$$x_1(t) = x_{\text{lin}}(t) + x_n(t), \tag{24}$$

where $x_n(t)$ is

$$\begin{aligned} x_n(t) = -\frac{\alpha}{\beta}e^{-\beta t}\Bigg\{ & c^2(1-e^{-\beta t}) + \frac{1}{2}\frac{\mathcal{A}_0^2}{(\omega^2+\beta^2)}(e^{\beta t}-1) + \frac{1}{2}\frac{\mathcal{A}_0^2(\beta^2-\omega^2)\beta}{(\omega^2+\beta^2)^2(4\omega^2+\beta^2)} \\ & \times[-\beta+\beta e^{\beta t}\cos 2\omega t + 2\omega e^{\beta t}\sin 2\omega t] + \frac{\mathcal{A}_0^2(\beta^2\omega)}{(\omega^2+\beta^2)^2(4\omega^2+\beta^2)} \\ & \times[2\omega - 2\omega e^{\beta t}\cos 2\omega t + \beta e^{\beta t}\sin 2\omega t] + 2\frac{\mathcal{A}_0 c}{(\omega^2+\beta^2)}\left[-2\beta(\cos\omega t - 1) + \frac{\beta^2}{\omega}\sin\omega t\right]\Bigg\}, \end{aligned} \tag{25}$$

It is important to underline that for the linear case, the first iteration of solution (23) must be in principle the exact solution.

It can be noted that, using the properties of the hypergeometric functions, the series which appear in (23) can be written in a more compact form:

$$\sum_{n=0}^{\infty}\frac{(at)^n F(n-\mu;n+1-\mu;\beta t)}{(1-\mu)_n} = \sum_{n=0}^{\infty}\frac{(at)^n}{(-\mu)_n}\left(\frac{\mathrm{d}}{\mathrm{d}(\beta t)}\right)^n F(-\mu;1-\mu;\beta t) = HF(-\mu;1-\mu;\beta t),$$

where H is a linear operator.

An alternate way to find the solution consists of taking the linear operator L from (17) as $L = D^{\mu}_{t,a}x + (\beta/\gamma)x$ and expressing the solution for $Lx_0=0$ in terms of Mittag-Leffler E_{μ} or $E_{\mu,j}$ functions due to properties (10) and (11).

The stress response resulting after the use of the initial condition (16), for the both cases, is

$$\sigma(t) = x + E_r A\sin\omega t,$$

where $x=x_{\text{lin}}$ or $x=x_1$.

B. Case of $D^{\mu}_{t,-\infty}$

In this case, for the linear model $\alpha=0$ replacing (19), (21), and (22) in (18), based on differentiation rules (3) and (4) it results:

$$\begin{aligned} x_{\text{lnr}}(t) = {} & c(1-\gamma(-\beta)^{\mu}t)\exp(-\beta t) + \frac{\mathcal{A}_0\omega}{\omega^2+\beta^2}\sin\omega t + \frac{\mathcal{A}_0\beta}{\omega^2+\beta^2}\cos\omega t - \frac{\gamma\mathcal{A}_0}{\omega^2+\beta^2}e^{-\beta t} \\ & \times\Bigg[-\frac{\omega\left(-\omega\cos\left(\frac{\pi\mu}{2}\right)+\beta\sin\left(\frac{\pi\mu}{2}\right)+\omega e^{\beta t}\cos\left(\omega t+\frac{\pi\mu}{2}\right)-\beta e^{\beta t}\sin\left(\omega t+\frac{\pi\mu}{2}\right)\right)}{\beta^2+\omega^2} \\ & -\frac{\beta\left(\beta\cos\left(\frac{\pi\mu}{2}\right)+\omega\sin\left(\frac{\pi\mu}{2}\right)-\beta e^{\beta t}\cos\left(\omega t+\frac{\pi\mu}{2}\right)-\omega e^{\beta t}\sin\left(\omega t+\frac{\pi\mu}{2}\right)\right)}{\beta^2+\omega^2}\Bigg]. \end{aligned} \tag{26}$$

For the nonlinear case ($\alpha \neq 0$) the solution will be of the form:

$$x_1(t) = x_{\text{lnr}}(t) + x_n(t), \tag{27}$$

where x_n is given by (25).

It is important to underline that also for this linear case, the first iteration of solution (26) must be in principle the exact solution.

The use of $D^{\mu}_{t,-\infty}$ differentiation operator gives different results with respect to $D^{\mu}_{t,0}$. It must be noted that this situation is more restrictive, and can be considered similar to the use of the Fourier transform for solving nonhomogeneous differential linear equations: this case gives only the part of solution connected to the permanent response.

Also, the results become incorrect when $(-\beta)^{\mu}$ are complex valued. Consequently, in order to obtain valid solutions, the terms containing complex valued quantities must be eliminated from the solution.

The stress response that results after the use of the initial condition (16), for the both cases, is

$$\sigma(t) = x + E_r A \sin \omega t,$$

where $x = x_{\text{lnr}}$ or $x = x_1$.

V. VOLTERRA SERIES METHOD

There are methods for the identification of nonlinear systems from experimental data. For a nonlinear system described by equations of type (15) the response can be expressed in terms of Volterra series:[29,30]

$$\begin{aligned} x(t) = &\int_0^{\infty} h_1(\tau_1) u(t-\tau_1) \mathrm{d}\tau_1 + \int_0^{\infty}\int_0^{\infty} h_2(\tau_1,\tau_2) u(t-\tau_1) u(t-\tau_2) \mathrm{d}\tau_1 \mathrm{d}\tau_2 \\ &+ \int_0^{\infty}\int_0^{\infty}\int_0^{\infty} h_3(\tau_1,\tau_2,\tau_3) u(t-\tau_1) u(t-\tau_2) u(t-\tau_3) \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 + \cdots , \end{aligned} \tag{28}$$

where $h_i(\tau_1, \tau_2, \ldots)$ (with $i = 1, 2, 3, \ldots.$) is the ith order transfer function, and u represents the input function. In our case $u(t) = \dot{\varepsilon}(t)$.

If we consider that the excitation is $\varepsilon(t) = Ae^{i\omega t}$, by replacing (28) in (15) we can calculate different orders of the transfer function for harmonic excitation. In this case the response will have the form:[29,30]

$$x(t) = \sum_{i=1}^{+\infty} (i\tau_0 \omega \delta E)^n H_i(\omega, \omega, \ldots.) \exp[in\omega t] = \sum \xi_n e^{in\omega t}, \tag{29}$$

representing a superposition of harmonics.

The amplitudes ξ_n can be found from the constitutive equation (15). The problem can be correctly formulated only for systems described by constitutive equations with fractional differentiation operators connected to the Fourier transforms, i.e., for $D^{\mu}_{t,-\infty}$. We take (15), for the case of $D^{\mu}_{t,-\infty}$, and use the notation:

$$F(p) = ip + \gamma e^{i(\pi\mu/2)} \omega^{\mu} \beta.$$

Thus, the following results are obtained:

$$\xi_1 = \frac{1}{F(\omega)},$$

$$\xi_2 = -2 \frac{\alpha}{\tau_0} \frac{\xi_1^2}{F(2\omega)}, \tag{30}$$

$$\xi_3 = -6\frac{\alpha}{\tau_0}\frac{\xi_1\xi_2}{F(3\omega)}.$$

The different amplitudes ξ_1 and finally the parameters of the rheologic model may be obtained from experimental data.

VI. CONCLUSIONS

In order to find an analytical solution of Eq. (15) we used a powerful variational iteration method established by He,[12,13] a new type of Lagrange multiplier method. The strength of this method consists in its convergence. We limited our investigations to the first iteration.

We used these methods to establish the solution for a class of linear and nonlinear anelastic models, (15), in which the dependency of fractional damping process (fractional differentiation) appears.

We introduced an anelastic model using a more general definition of fractional differentiation of order μ, using Riemann-Liouville $D_{t,a}^{\mu}$ operator.

Two cases were investigated. For $a=0$ we established the solution for linear and nonlinear cases. It is important to underline that for the linear case, the first iteration of the solution (23) must be in principle the exact solution.

The case $a=-\infty$ was also investigated, establishing the solution for linear and nonlinear situations. The obtained solution was simpler. It was underlined that this situation was more restrictive, and could be considered similar to the use of the Fourier transform for solving nonhomogeneous differential linear equations: this case gives only the part of solution connected to the permanent response. The results cannot be valid when $(-\beta)^{\mu}$ are complex valued.

The variational iteration method of He can be used for finding general solutions for the partial differential equations, starting with a particular solution, as suggested in Ref. 31.

As a generalization of the Fourier transform rheology we introduced the Volterra-Fourier series in order to study the response of nonlinear systems to harmonic excitation.

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On the simultaneous presence of unilateral and kinetic constraints in time-dependent impulsive mechanics

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The simultaneous presence of unilateral and kinetic constraints acting on a mechanical system with a finite number of degrees of freedom is framed in the geometric context of left and right jet-bundles of the classical space–time bundle of the system. The survey gives three main cases and several subcases, some of which are mathematically correct but physically meaningless. The existence of at least one frame of reference for which the whole set of constraints can be at rest is the criterion selecting the physically relevant systems. For these systems, the conservation of kinetic energy, possibly together with a standard Gauss's requirement on the impulsive reaction, is shown to give a well posed criterion of ideality of the constraints. The application of the criterion to several examples is presented and the corresponding results are critically analyzed. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Differential geometric techniques have been recently discovered again as useful tools for the study of classical impulsive mechanics of systems with a finite number of degrees of freedom, in both cases of free or constrained systems. Besides the usual instruments of differential geometry (for whose applications to impulsive mechanics see, e.g. Refs. 1–5), several results in time-dependent impulsive mechanics were obtained by the author by introducing the framework of left and right jet-bundles of the classical configuration space–time of the mechanical system. In particular, this setup allows deeper insights into the study of the behavior of free systems subject to active impulses,[6] of constrained systems subject to ideal bilateral positional or kinetic constraints,[7,8] and in the study of the concept of ideality for unilateral positional constraints.[9]

In this paper, going in the same direction as the previous cited papers of the author, we present a geometric framework for the study of impulsive systems simultaneously subject to unilateral and kinetic constraints. In particular, we distinguish three different cases: when the system is subject to a kinetic constraint only when it impacts with a unilateral positional constraint (the kinetic constraint "lives" on the positional unilateral constraint); when the system is permanently subject to a kinetic constraint and impacts with unilateral positional constraints; when both situations simultaneously occur, i.e., the system is subject to a permanent kinetic constraint and impacts with a unilateral positional constraint where an ulterior kinetic constraint acts on the system.

For all three cases, following the same line of thought presented in Ref. 9, we propose an ideality criterion of the constraints based on the conservation of the kinetic energy of the system together with, when this requirement turns out to be insufficient to restore the principle of determinism, a Gauss's "extremality" requirement for the impulsive reaction. As usually happens in impulsive problems involving kinetic constraints, Gauss's condition is automatically well posed if

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the kinetic constraint has a linear-affine nature, but, if the constraint has a nonlinear nature, the existence of the extremum, in general, is not ensured (see Ref. 7). Nevertheless, linear-affine constraints can provide several meaningful examples.

The paper is divided into four sections. Section II presents, in order to fix notation, a brief survey on the general geometric setup for the study of systems subject to bilateral constraints, positional or kinetic, and systems subject to unilateral positional ones. Almost all its material is not new and can be found in literature (see, for example, Refs. 10, 11, 6, 7, and 9). Nevertheless, the reorganization of this material in a form suitable to approach the subsequent problems is new stuff. Section III presents the geometric framing of the three possible cases of coexistence of kinetic and positional unilateral constraints in the general context illustrated in Sec. II, together with a detailed discussion on the conditions determined by the geometry itself on the impulsive reaction. Moreover it presents, for all three possibilities, the ideality criterion based on the conservation of kinetic energy and Gauss's principle. Section IV is devoted to examples of the three possibilities, and it presents a detailed discussion of the behavior of four simple mechanical systems: a cogwheel moving in the plane and impacting with a linear rack; a cogwheel rolling on a horizontal rack and impacting in a smooth vertical wall; a ball rolling on a horizontal plane and impacting in a smooth vertical wall; a ball rolling on a horizontal plane and impacting in a rough vertical wall. Section V briefly presents a critical analysis of the results obtained in Sec. IV, together with conclusions.

II. PRELIMINARIES

A. Geometric aspects of bilateral constraints

The configuration space–time of a mechanical system with a finite number n of degrees of freedom is a bundle $\pi:\mathcal{V}\to\mathbb{E}_1$, where $\mathbb{E}_1$ is the affine line. The set $\mathcal{V}$ is an $(n+1)$-dimensional differentiable manifold (noncanonically) diffeomorphic to the Cartesian product $\mathbb{R}\times\mathcal{Q}$, where the manifold $\mathcal{Q}$ is the usual configuration space of the system. The composition of π with the Cartesian coordinate of $\mathbb{E}_1$ determines the absolute time function $t:\mathcal{V}\to\mathbb{R}$. The bundle $\mathcal{V}$ will be referred to admissible coordinates $(t,x^1,\ldots,x^n)$.

The first jet-extension $\pi:J_1(\mathcal{V})\to\mathcal{V}$ of the configuration space–time represents the absolute velocity space of the system. It can be viewed as a subbundle of the tangent bundle $T(\mathcal{V})$ of $\mathcal{V}$ given by those vectors having the form $\mathbf{p}=\partial/(\partial t)+\dot{x}^i\partial/(\partial x^i)$ or, that is the same, determined by the condition $\{\mathbf{X}\in T(\mathcal{V})\,|<dt,\mathbf{X}>=1\}$. This condition also shows that $J_1(\mathcal{V})$ is an affine bundle, modeled on the so-called vertical vector bundle $\pi:V(\mathcal{V})\to\mathcal{V}$ of the tangent vectors $\mathbf{X}\in T(\mathcal{V})$ satisfying the condition $\{\mathbf{X}\in T(\mathcal{V})\,|<dt,\mathbf{X}>=0\}$, or that is the same, having the form $\mathbf{V}=X^i\partial/(\partial x^i)$. The bundles $J_1(\mathcal{V})$ and$V(\mathcal{V})$ will be both referred to admissible jet-coordinates $(t,x^i,\dot{x}^i)$.

The fibers of $V(\mathcal{V})$ are endowed with a positive definite scalar product $\Phi:V(\mathcal{V})\times_{\mathcal{V}}V(\mathcal{V})\to\mathbb{R}$, where $\times_{\mathcal{V}}$ denotes the usual fiber product of bundles on $\mathcal{V}$. The map Φ is called the vertical scalar product of $\mathcal{V}$ and can be locally described by the functions $g_{ij}(p)=\Phi((\partial/(\partial x^i))_p,(\partial/(\partial x^j))_p)$. We recall that Φ takes intrinsically into account the mass properties of the system (for a detailed discussion of these arguments, see, e.g., Ref. 11, and the references therein).

A frame of reference for the system (without any assumption of rigidity) is a global section $\mathbf{h}:\mathcal{V}\to J_1(\mathcal{V})$. It can be represented by a globally defined vector field $\mathbf{h}=\partial/(\partial t)+H^i(t,x^j)\partial/(\partial x^i)$ and it determines a "vectorialization" of $J_1(\mathcal{V})$, i.e., a diffeomorphism $\Delta_{\mathbf{h}}$ defined by

$$\Delta_{\mathbf{h}}:J_1(\mathcal{V})\to V(\mathcal{V})\quad\text{such that}\quad\Delta_{\mathbf{h}}(\mathbf{p})=\mathbf{p}-\mathbf{h}(\pi(\mathbf{p})).$$

Given a frame $\mathbf{h}$, the vertical vector

$$\Delta_{\mathbf{h}}(\mathbf{p})=\mathbf{p}-\mathbf{h}=(\dot{x}^i-H^i(t,x^j))\frac{\partial}{\partial x^i}$$

represents the *relative velocity* of $\mathbf{p}\in J_1(\mathcal{V})$ with respect to $\mathbf{h}$. Moreover, the function

$$ {}^{\mathbf{h}}\mathcal{K}: J_1(\mathcal{V}) \to \mathbb{R} \quad \text{such that} \quad {}^{\mathbf{h}}\mathcal{K}(\mathbf{p}) = \tfrac{1}{2}\Phi(\mathbf{p}-\mathbf{h}, \mathbf{p}-\mathbf{h}) \tag{1} $$

is the *kinetic energy* of the system with respect to **h**.

Additional positional constraints acting on the system are given by a globally time-fibered subbundle $i: \mathcal{S} \to \mathcal{V}$, where the manifold $\mathcal{S}$ has dimension $(r+1), r<n$. Of course, the bundle $t: \mathcal{S} \to \mathbb{R}$ is the space–time bundle of the system that takes into account the constraint $\mathcal{S}$ as a bilateral constraint. The bundle $\mathcal{S}$ will be referred to admissible coordinates $(t, q^1, \ldots, q^r)$, and the immersion i can be briefly described by the relations $x^i = x^i(t, q^1, \ldots, q^r)$. The bundle $\mathcal{S}$ determines its own first jet-extension $\pi: J_1(\mathcal{S}) \to \mathcal{S}$ with its vertical bundle $\pi: V(\mathcal{S}) \to \mathcal{S}$. They both are described by admissible jet-coordinates $(t, q^\eta, \dot{q}^\eta)$, and their elements have the vector representations $\mathbf{q} = \partial/(\partial t) + \dot{q}^\eta \partial/(\partial q^\eta)$ and $\mathbf{V} = V^\eta \partial/(\partial q^\eta)$, respectively.

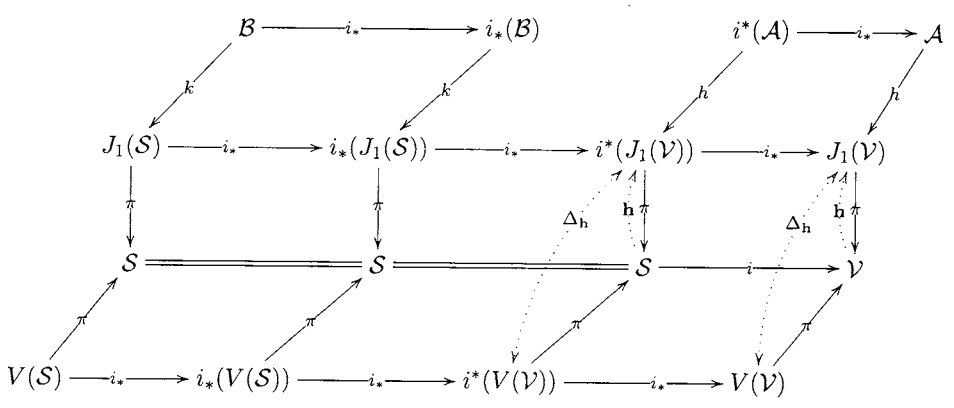
The tangent map $i_*: T(\mathcal{S}) \to T(\mathcal{V})$ determines by restriction the fibered immersions $i_*: J_1(\mathcal{S}) \to J_1(\mathcal{V})$ and $i_*: V(\mathcal{S}) \to V(\mathcal{V})$. As a consequence, the vertical scalar product Φ of $\mathcal{V}$ can be pulled back to $V(\mathcal{S})$, defining the vertical scalar product φ of $\mathcal{S}$.

The standard pull-back techniques allow the construction of the pull-back bundles $\pi: i^*(J_1(\mathcal{V})) \to \mathcal{S}$ and $\pi: i^*(V(\mathcal{V})) \to \mathcal{S}$ (see Ref. 9), both referred to fibered admissible coordinates $(t, q^\eta, \dot{x}^i)$. A frame of reference **h** and the corresponding vectorialization $\Delta_{\mathbf{h}}$ and kinetic energy ${}^{\mathbf{h}}\mathcal{K}$ can be naturally restricted to maps $\mathbf{h}: \mathcal{S} \to i^*(J_1(\mathcal{V})), \Delta_{\mathbf{h}}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ and ${}^{\mathbf{h}}\mathcal{K}: i^*(J_1(\mathcal{V})) \to \mathbb{R}$.

The framing of kinetic constraints in this global geometric context needs some clarifications. The presence of kinetic constraints permanently acting on the system (without considering the possible presence of additional positional constraint) is modeled, as it is well known (see, e.g., Ref. 10), by a subbundle $h: \mathcal{A} \to J_1(\mathcal{V})$. The manifold $\mathcal{A}$ is globally fibered over $\mathcal{V}$ (and then over the real line), and $\mathcal{A}$ has dimension $(n+s+1), s<n$. The bundle $\mathcal{A}$ will be called a *permanent* kinetic constraint and will be referred to admissible coordinates $(t, x^i, \dot{\xi}^A)$. The standard pull-back procedure determines the subbundle $\pi: i^*(\mathcal{A}) \to \mathcal{S}$ of the bundle $\pi: i^*(J_1(\mathcal{V})) \to \mathcal{S}$ described by admissible coordinates $(t, q^\alpha, \dot{\xi}^A)$.

However, in the presence of an additional positional constraint $\mathcal{S}$, a kinetic constraint can be defined only on $\mathcal{S}$. Then a subbundle $k: \mathcal{B} \to J_1(\mathcal{S})$ can be introduced for the bundle $J_1(\mathcal{S})$, with the manifold $\mathcal{B}$ globally fibered over $\mathcal{S}$, and $\mathcal{B}$ of dimension $(r+m+1)$, $m<r$. The bundle $\mathcal{B}$ will be referred to admissible coordinates $(t, q^\eta, \dot{\theta}^Y)$. This kinetic constraint can act on the system only when the system is in a configuration of $\mathcal{S}$: for this reason, slightly improperly, $\mathcal{B}$ will be called an *instantaneous* kinetic constraint.

Of course, both kinds of kinetic constraints can be simultaneously present on the system. The whole situation is summarized with the following diagram:



B. Geometric aspects of impulsive constraints

In order to approach the study of impulsive aspects of the system, it is useful to introduce the bundles $\pi: L_1(\mathcal{V}) \to \mathcal{V}$ of the left velocities of the system and $\pi: R_1(\mathcal{V}) \to \mathcal{V}$ of the right velocities

of the system (see Ref. 6). They are both affine bundles canonically diffeomorphic to $J_1(\mathcal{V})$ in the geometric sense, with diffeomorphism $Id_L: J_1(\mathcal{V}) \to L_1(\mathcal{V})$ and $Id_R: J_1(\mathcal{V}) \to R_1(\mathcal{V})$, but their physical interpretation is slightly different from that of $J_1(\mathcal{V})$. The action of the diffeomorphisms Id_L and Id_R will frequently be implicitly understood. We will use jet-coordinates $(t, x^i, \dot{x}^i_L)$ to describe $L_1(\mathcal{V})$ and $(t, x^i, \dot{x}^i_R)_i$ to describe $R_1(\mathcal{V})$. The elements $\mathbf{p}_L$ of $L_1(\mathcal{V})$ can be represented in the vector form $\mathbf{p}_L = \partial/(\partial t) + \dot{x}^i_L \partial/(\partial x^i)$, and, analogously, $\mathbf{p}_R \in R_1(\mathcal{V})$ can be written as $\mathbf{p}_R = \partial/(\partial t) + \dot{x}^i_R \partial/(\partial x^i)$.

Due to the affine structure of $L_1(\mathcal{V})$ and $R_1(\mathcal{V})$ and to the diffeomorphisms Id_L and Id_R, we can define two fibered maps

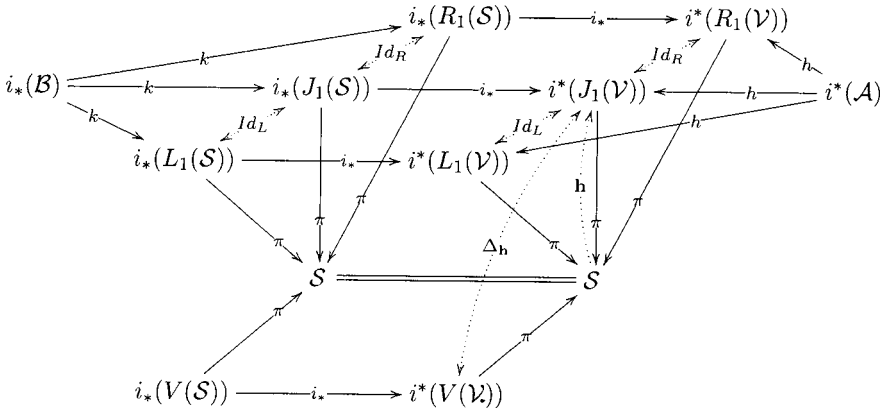
$$\begin{aligned} &\Xi\colon L_1(\mathcal{V}) \times_{\mathcal{V}} V(\mathcal{V}) \to R_1(\mathcal{V}) \text{such that} \quad \Xi(\mathbf{p}_L, \mathbf{V}) = \mathbf{p}_L + \mathbf{V}, \\ &\Delta\colon L_1(\mathcal{V}) \times_{\mathcal{V}} R_1(\mathcal{V}) \to V(\mathcal{V}) \quad \text{such that} \quad \Delta(\mathbf{p}_L, \mathbf{p}_R) = \mathbf{p}_R - \mathbf{p}_L. \end{aligned} \tag{2}$$

In the presence of additional positional constraints, identical constructions can be repeated for the bundle $t: \mathcal{S} \to \mathbb{R}$, obtaining the bundles $L_1(\mathcal{S})$ and $R_1(\mathcal{S})$ canonically diffeomorphic to $J_1(\mathcal{S})$ with diffeomorphisms $Id_L: J_1(\mathcal{S}) \to L_1(\mathcal{S})$ and $Id_R: J_1(\mathcal{S}) \to R_1(\mathcal{S})$. They are described by jet-coordinates $(t, q^\eta, \dot{q}^\eta_L)$ and $(t, q^\eta, \dot{q}^\eta_R)$ respectively, and their elements admit the vector representation $\mathbf{q}_L = \partial/(\partial t) + \dot{q}^\eta_L \partial/(\partial q^\eta)$ and $\mathbf{q}_R = \partial/(\partial t) + \dot{q}^\eta_R \partial/\partial q^\eta$.

The immersion $i_*: J_1(\mathcal{S}) \to J_1(\mathcal{V})$ determines, thanks to the diffeomorphisms Id_L, Id_R, the immersions $i_*: L_1(\mathcal{S}) \to L_1(\mathcal{V})$ and $i_*: R_1(\mathcal{S}) \to R_1(\mathcal{V})$. Therefore, applying once again the pull-back procedure, we can construct the bundles $\pi: i^*(L_1(\mathcal{V})) \to \mathcal{S}$ and $\pi: i^*(R_1(\mathcal{V})) \to \mathcal{S}$, locally described by coordinates $(t, q^\eta, \dot{x}^i_L)$ and $(t, q^\eta, \dot{x}^i_R)$, respectively. Of course, as it happens for the immersion $i_*: J_1(\mathcal{S}) \to i^*(J_1(\mathcal{V}))$, the images $i_*(L_1(\mathcal{S}))$ and $i_*(R_1(\mathcal{S}))$ are affine subbundles of $i^*(L_1(\mathcal{V}))$ and $i^*(R_1(\mathcal{V}))$, respectively.

The pull-back bundle $h: i^*(\mathcal{A}) \to i^*(J_1(\mathcal{V}))$ of the permanent kinetic constraint $\mathcal{A}$ determines, using the diffeomorphisms Id_L and Id_R, the subbundles $h: i^*(\mathcal{A}) \to i^*(L_1(\mathcal{V}))$ and $h: i^*(\mathcal{A}) \to i^*(R_1(\mathcal{V}))$. Similarly, the instantaneous constraint $\mathcal{B}$ gives rise to subbundles $k: i_*(\mathcal{B}) \to i_*(L_1(\mathcal{S}))$ and $k: i_*(\mathcal{B}) \to i_*(R_1(\mathcal{S}))$. Later on, when no confusion can arise, the action of the immersion h and k will be often omitted and implicitly understood.

Focusing our attention only on the part of the construction that will be intensively used in the paper, the geometric setup is synthesized by the following diagram:



(3)

An impulse acting on the system can be equivalently described by a map $\mathcal{I}: L_1(\mathcal{V}) \to R_1(\mathcal{V})$ assigning to each left velocity $\mathbf{p}_L$ of the system a corresponding right velocity $\mathbf{p}_R$, or, preferably in order to preserve some similarities with the usual definition of forces (see, e.g., Refs. 10 and 11), by a map $\mathbf{I}: J_1(\mathcal{V}) \to V(\mathcal{V})$ assigning to each velocity $\mathbf{p}$ of the system the corresponding jump of velocity $\mathbf{V} = \mathbf{I}(\mathbf{p})$ (see, e.g., Ref. 6). The equivalence of the two definitions is synthesized by the relation $\mathbf{p}_R = \mathbf{p}_L + \mathbf{I}(\mathbf{p}_L)$ and it is easily proved taking into account the maps (2).

C. Geometric aspects of unilateral constraints

The bundle $i^*(J_1(\mathcal{V}))$ is, by its very nature, the set of all possible absolute velocities of the system when the system itself is in a configuration of $\mathcal{S}$, but without thinking of $\mathcal{S}$ as a constraint. Therefore, $i^*(J_1(\mathcal{V}))$ is the most suitable geometric environment to approach the analysis of $\mathcal{S}$ as a unilateral constraint acting on the system.

Every map $\mathbf{I}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ defined on the bundle $i^*(J_1(\mathcal{V}))$ can be thought of as an assignment of the impulsive reaction of $\mathcal{S}$ considered as a unilateral constraint acting on the system: given an "entrance" velocity of the system in a configuration of $\mathcal{S}$, the map $\mathbf{I}$ determines, through the map Ξ defined in (2), a corresponding "exit" velocity of the system from the same configuration of $\mathcal{S}$. Therefore, once $\mathcal{S}$ is assigned, every criterion fit to determine a unique impulse $\mathbf{I}: i^*(J_1(\mathcal{V})) \to i^*(V(\mathcal{V}))$ is a so-called (impulsive) *constitutive characterization* of the unilateral constraint $\mathcal{S}$ (see Ref. 9).

The immersions $i_*: J_1(\mathcal{S}) \to i^*(J_1(\mathcal{V}))$ and $i_*: V(\mathcal{S}) \to i^*(V(\mathcal{V}))$ play a crucial role in the geometric model of $\mathcal{S}$ as unilateral constraint. Since their images $i_*(J_1(\mathcal{S}))$ and $i_*(V(\mathcal{S}))$ are an affine subbundle of $i^*(J_1(\mathcal{V}))$ and a vector subbundle of $i^*(V(\mathcal{V}))$, respectively, then the vertical metric Φ defined on $i^*(V(\mathcal{V}))$ determines, with obvious meaning of the notation, the splits

$$i^*(V(\mathcal{V})) = i_*(V(\mathcal{S})) \oplus (i_*(V(\mathcal{S})))^\perp,$$

$$\Phi = \varphi \otimes \psi, \tag{4}$$

and the projection operators

$$\mathcal{P}^{\|}: i^*(V(\mathcal{V})) \to i_*(V(\mathcal{S})), \quad \mathcal{P}^{\perp}: i^*(V(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp.$$

It is a straightforward matter[9] to show that an analogous split

$$i^*(J_1(\mathcal{V})) = i_*(J_1(\mathcal{S})) \oplus (i_*(V(\mathcal{S})))^\perp \tag{5}$$

and analogous projection operators

$$\mathcal{P}^{\|}_{\mathcal{S}}: i^*(J_1(\mathcal{V})) \to i_*(J_1(S)), \quad \mathcal{P}^{\perp}_{\mathcal{S}}: i^*(J_1(\mathcal{V})) \to (i_*(V(\mathcal{S})))^\perp$$

can be introduced for the affine bundle $i^*(J_1(\mathcal{V}))$. Note moreover that (see, for example, Refs. 10 and 3), from the computational point of view, the operators $\mathcal{P}^{\|}_{\mathcal{S}}$ and $P^{\perp}_{\mathcal{S}}$ can be determined through a minimum principle, since, for every point $\mathbf{p} \in i^*(J_1(\mathcal{V}))$, the projection $\mathcal{P}^{\|}_{\mathcal{S}}(\mathbf{p})$ realizes the minimum of the scalar function

$$f_{\mathbf{p}}: i_*(J_1(\mathcal{S})) \to \mathbb{R} \quad \text{such that} \quad f_{\mathbf{p}}(\mathbf{y}) = \Phi(\mathbf{p}-\mathbf{y}, \mathbf{p}-\mathbf{y}).$$

The presence of the constraint $\mathcal{S}$ allows the selection of the class $\mathcal{H}$ of the frames of reference that are tangent to $\mathcal{S}$. The set $\mathcal{H}$ is formed by all the frames of reference whose one-parameter group of transformations maps the constraint $\mathcal{S}$ into itself. The kinematical meaning of this property is that $\mathcal{H}$ is formed by those frames for which $\mathcal{S}$ can be "at rest" (see Ref. 9).

For every absolute velocity $\mathbf{p} \in i^*(J_1(\mathcal{V}))$, the component $\mathcal{P}^{\perp}(\mathbf{p}-\mathbf{h}) \in (i_*(V(\mathcal{S})))^\perp$ of the relative velocity $\mathbf{p}-\mathbf{h}$ orthogonal to the constraint $\mathcal{S}$ is invariant with respect to the choice of the frame $\mathbf{h}$ in $\mathcal{H}$. Equivalently, given an absolute velocity $\mathbf{p} \in i^*(J_1(\mathcal{V}))$, the condition $\mathcal{P}^{\perp}(\mathbf{p}-\mathbf{h}) = \mathcal{P}^{\perp}_{\mathcal{S}}(\mathbf{p})$ holds if and only if $\mathbf{h} \in \mathcal{H}$ (see Ref. 9). Restricting our attention to the frames in $\mathcal{H}$, the vertical vector $\mathcal{P}^{\perp}_{\mathcal{S}}(\mathbf{p}) \in (i_*(V(\mathcal{S})))^\perp$ assumes the absolute (in the sense of independent of the frame) meaning of *orthogonal* (to $\mathcal{S}$) absolute velocity of $\mathbf{p}$. The component $\mathcal{P}^{\|}_{\mathcal{S}}(\mathbf{p}) \in i_*(J_1(\mathcal{S}))$ can be called the *tangent* (component of the) absolute velocity.

Suitable splits and projection operators defined on vector or affine bundles and special classes of frames of reference will turn out to be very useful in the analysis of possible constitutive characterizations also when both kinetic and unilateral constraints act on the system. For the analysis of these cases we need the following two lemmas:

Lemma 1.1: Let $\mathbf{K}$ *be an affine space modeled on a* (*finite dimensional*) *vector space* $\mathbf{W}$ *endowed with a scalar product* Φ, *and let* $\mathbf{A}$ *be an affine subspace of* $\mathbf{K}$ *modeled on the vector subspace* $\mathbf{U}$ *of* $\mathbf{W}$. *Then*

(1) $\mathbf{K}=\mathbf{A}\oplus\mathbf{U}^{\perp}$ (*where, of course,* $\mathbf{W}=\mathbf{U}\oplus\mathbf{U}^{\perp}$) *or, that is the same,* $\forall k\in\mathbf{K}$ *there exists a unique pair* $a\in\mathbf{A},\mathbf{u}\in\mathbf{U}^{\perp}$ *such that* $k-a=\underline{\mathbf{u}}$;
(2) *introduced the natural projection operators* $\mathcal{P}_{\mathbf{W},\mathbf{U}^{\perp}}:\mathbf{W}\to\mathbf{U}^{\perp}$ *and* $\mathcal{P}_{\mathbf{K},\mathbf{U}^{\perp}}:\mathbf{K}\to\mathbf{U}^{\perp}$, *determined by the splits* $\mathbf{W}=\mathbf{U}+\mathbf{U}^{\perp}$ *and* $\mathbf{K}=\mathbf{A}\oplus\mathbf{U}^{\perp}$, *then* $\mathcal{P}_{\mathbf{W},\mathbf{U}^{\perp}}(k-a)=\mathcal{P}_{\mathbf{K},\mathbf{U}^{\perp}}(k)$ *if and only if* $a\in\mathbf{A}$.

To prove the first part of the lemma, it is sufficient to consider the pair $a\in\mathbf{A},\mathbf{u}\in\mathbf{U}^{\perp}$ that realizes the minimum of the function

$$f_k{:}A\to\mathbb{R}\quad\text{such that}\quad f_k(x)=\Phi(k-x,k-x).$$

This is the unique pair giving the split.

To prove the second part, it is sufficient to show that, due to the linearity of the operators involved, for every pair $k_1,k_2\in\mathbf{K}$, the identity

$$\mathcal{P}_{\mathbf{W},\mathbf{U}^{\perp}}(k_1-k_2)=\mathcal{P}_{\mathbf{K},\mathbf{U}^{\perp}}(k_1)-\mathcal{P}_{\mathbf{K},\mathbf{U}^{\perp}}(k_2)$$

holds. The details of both these proofs are straightforward and left to the reader.

Lemma 1.2: Let $\mathbf{K}$ *be an affine space modeled on the vector space* $\mathbf{W}$, *and let* $\mathbf{A}$, $\mathbf{B}$ *be two affine subspaces of* $\mathbf{K}$ *respectively modeled on the vector subspaces* $\mathbf{U}$, $\mathbf{V}$ of $\mathbf{W}$. *Let* $\mathbf{A}$, $\mathbf{B}$ *be such that* $\mathbf{A}\cap\mathbf{B}\neq\emptyset$. *Then* $\mathbf{A}\cap\mathbf{B}$ *is an affine subspace of* $\mathbf{K}$ (*possibly given by a single point of* $\mathbf{K}$) *modeled on the vector space* $\mathbf{U}\cap\mathbf{V}$.

Once again the proof is straightforward and it is left to the reader.

III. CLASSIFICATION OF CONSTRAINTS AND IDEALITY CRITERION

Taking into account diagram (3), we can note that three distinct impulsive situations can occur to the system when it impacts with a unilateral positional constraint $\mathcal{S}$:

Case I: No permanent kinetic constraints $\mathcal{A}$ act on the system, and an impulsive kinetic constraint $\mathcal{B}$ must be satisfied when the system impacts with $\mathcal{S}$. The geometric setup is illustrated in diagram (3) without the part on the right involving the bundle $\mathcal{A}$. A simple mechanical system described by this situation is a cogwheel moving in a plane and impacting with a linear rack.

Case II: The motion of the system obeys a permanent kinetic condition $\mathcal{A}$ before and after the impact with $\mathcal{S}$, but no impulsive kinetic constraint $\mathcal{B}$ is present on $\mathcal{S}$. The geometric setup is illustrated by (3) but this time without the part on the left involving the bundle $\mathcal{B}$. Examples of this situation are a cogwheel rolling on a horizontal rack and impacting with a smooth vertical wall or, more significantly, a sphere rolling on a horizontal plane and impacting with a smooth vertical wall.

Case III: Both a permanent kinetic constraint $\mathcal{A}$ and an impulsive kinetic constraint $\mathcal{B}$ must be satisfied by the motion of the system, the first before and after the impact with $\mathcal{S}$, and the second during the impact. This case requires the whole diagram (3) to be illustrated. A simple example of this situation is a sphere rolling on a horizontal plane and impacting with a rough vertical wall where an ulterior condition of rolling must be satisfied.

The next part of the section presents a separate analysis of the three cases, in the following hypotheses:

H1: The positional constraint $\mathcal{S}$ has codimension 1 as subbundle of $\mathcal{V}$, or, that is the same, $r=n-1$.

H2: The kinetic constraints $\mathcal{A}$ and $\mathcal{B}$ are affine subbundles of $J_1(\mathcal{V})$ and $J_1(\mathcal{S})$, respectively.

The first hypothesis is required mainly with the intention of avoiding some pathological (and physically almost meaningless) systems, such as a point mass moving in a three-dimensional space and impacting with a one-dimensional thread. This intention will permeate through the whole section, since it will be shown that, depending on the nature of the constraints $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{S}$ (in

Cases II and III), several physically meaningless situations can occur. Note moreover that hypothesis *H1* implies that the vector bundle $(i_*(V(\mathcal{S})))^\perp$ is a (line) bundle whose fibers have dimension 1. Therefore we can introduce a vector field $\mathbf{V}_{\mathcal{S}}^{\perp}$ such that $(i_*(V(\mathcal{S})))^\perp = \mathcal{L}\{\mathbf{V}_{\mathcal{S}}^{\perp}\}$.

The second hypothesis, as we already pointed out, is required mainly in order to avoid technicalities regarding the existence of the extremum in the Gauss's requirement about the reaction. Using admissible coordinates, this means that the immersion $h:\mathcal{A}\to J_1(\mathcal{V})$ can be synthesized by the relations $\dot{x}^i = E_A^i \dot{\xi}^A + F^i$, and the immersion $k:\mathcal{B}\to J_1(\mathcal{S})$ can be synthesized by the relations $\dot{q}^\alpha = M_\Upsilon^\alpha \dot{\theta}^\Upsilon + N^\alpha$, with the coefficients $E_A^i, F^i, M_\Upsilon^\alpha, N^\alpha$ independent of dotted coordinates. In particular, when *H2* holds, the affine structure of the constraints $\mathcal{A}$ and $\mathcal{B}$ implies that the sets

$$V(\mathcal{A}) = \{\mathbf{A} = \mathbf{a}_1 - \mathbf{a}_2 | \mathbf{a}_1, \mathbf{a}_2 \in i^*(\mathcal{A})\},$$

$$V(\mathcal{B}) = \{\mathbf{B} = \mathbf{b}_1 - \mathbf{b}_2 | \mathbf{b}_1, \mathbf{b}_2 \in i_*(\mathcal{B})\}, \tag{6}$$

have the structure of vector subbundles of $i^*(V(\mathcal{V}))$ and $i_*(V(\mathcal{S}))$, respectively.

We underline however that, even imposing conditions *H1* and *H2*, the situation remains general enough to describe a wide variety of mechanical systems, such as the four examples described earlier.

The determination of a constitutive characterization of the constraints follows the same line of thought for all three cases. This line of thought is analogous to the one presented in Ref. 9, when a single unilateral positional constraint acts on the system, and it is synthetically described by the following step-by-step procedure:

Step 1: A geometric analysis of the case is performed in order to determine the set of the admissible left and right velocities $\mathbf{p}_L, \mathbf{p}_R$ of the system, the corresponding admissible impulsive reactions $\mathbf{I}(\mathbf{p}_L)$, the set $\mathcal{H}$ of the frames of reference for which all the constraints can be at rest (if it exists), and a particular component $\mathbf{V}^\perp(\mathbf{p}_L)$ of the left velocity that, in the simplest cases, coincides with the component orthogonal to the whole set of constraints.

Step 2: Conservation of kinetic energy before and after the impact is required, if possible, for all the frames in $\mathcal{H}$.

Step 3: If the impulsive reaction is not uniquely determined, a Gauss's criterion is imposed.

We will show that the procedure can already fail at the first step since the set $\mathcal{H}$ of rest frames can be empty. However, the corresponding systems do not have a clear physical meaning. In fact, the integral lines of the elements of $\mathcal{H}$ represent the possible motions of the system respecting the whole set of constraints, and the condition $\mathcal{H}=\emptyset$ implies that no such motions exist. This is mathematically admissible, but physically meaningless. In a Poisson-type approach, with the impulsive reaction divided in a first part determined by the entrance of the system in the unilateral constraint and a second part determined by the exit of the system out of the constraint (see Ref. 9), if $\mathcal{H}=\emptyset$ the first part of the impulse is undeterminable. Two simple examples should clarify these situations:

Example 1: A point mass moving in the xy-plane is subject to the permanent kinetic constraint $\dot{y}=c_1\neq 0$ and impacts with a horizontal guide $y=0$.

Example 2: A point mass moving in the xy-plane is subject to the permanent kinetic constraint $\dot{x}=c_1$ and impacts with a horizontal guide $y=0$ where an instantaneous kinetic constraint $\dot{x}=c_2$, $c_2\neq c_1$ is defined.

When the first step can be performed with meaningful results, taking into account (1), the second step consists in the requirement

$${}^{\mathbf{h}}\mathcal{K}(\mathbf{p}_L) = {}^{\mathbf{h}}\mathcal{K}(\mathbf{p}_R), \quad \forall\, \mathbf{h} \in \mathcal{H}.$$

A straightforward calculation shows that this condition is equivalent to

$$\Phi(2(\mathbf{p}_L - \mathbf{h}), \mathbf{I}(\mathbf{p}_L)) + \Phi(\mathbf{I}(\mathbf{p}_L), \mathbf{I}(\mathbf{p}_L)) = 0, \quad \forall\, \mathbf{h} \in \mathcal{H} \tag{7}$$

or, that is the same,

$$\Phi(2(\mathbf{p}_L - \mathbf{h}) + \mathbf{I}(\mathbf{p}_L), \mathbf{I}(\mathbf{p}_L)) = 0, \quad \forall\, \mathbf{h} \in \mathcal{H}. \tag{8}$$

Of course, the trivial solution $\mathbf{I}(\mathbf{p}_L)=0$ is not admissible, since it implies that the constraints do not act on the system.

However, depending on the nature of the constraints, conditions (7) or (8) could not determine a unique nontrivial impulsive reaction $\mathbf{I}(\mathbf{p}_L)$. In this case, in order to restore the principle of determinism, we should perform the third step of the procedure.

We advance that, in all the meaningful situations, the result of the above-described procedure is $\mathbf{I}(\mathbf{p}_L)=-2\mathbf{V}^{\perp}(\mathbf{p}_L)$, once again analogous to the impulsive reaction in the case of single unilateral positional constraint acting on the system. However, this conclusion is the result of a detailed analysis of two subcases of Case I, four subcases (with only two of them physically meaningful) of Case II and the other five (once again with only three of them physically meaningful) subcases of Case III. Before delving, in the following, into this analysis, we list the vector expressions in admissible coordinates of the elements of the involved affine and vector spaces, recalling that the vectors must be thought of as having base point in $\mathcal{S}$:

$$\begin{aligned}
i^*(J_1(\mathcal{V})) &= \left\{ \mathbf{p} = \frac{\partial}{\partial t} + \dot{x}^i \frac{\partial}{\partial x^i} \right\}, \\
i^*(V(\mathcal{V})) &= \left\{ \mathbf{V} = X^i \frac{\partial}{\partial x^i} \right\} = \mathcal{L}\left\{ \frac{\partial}{\partial x^i} \right\}, \\
i^*(J_1(\mathcal{S})) &= \left\{ \mathbf{q} = \frac{\partial}{\partial t} + \left(\frac{\partial x^i}{\partial t} + \dot{q}^\alpha \frac{\partial x^i}{\partial q^\alpha} \right) \frac{\partial}{\partial x^i} \right\}, \\
i_*(V(\mathcal{S})) &= \left\{ \mathbf{U} = Q^\alpha \frac{\partial x^i}{\partial q^\alpha} \frac{\partial}{\partial x^i} \right\} = \mathcal{L}\left\{ \frac{\partial x^i}{\partial q^\alpha} \frac{\partial}{\partial x^i} \right\}, \\
i^*(\mathcal{A}) &= \left\{ \mathbf{a} = \frac{\partial}{\partial t} + \left(E^i_A \dot{\xi}^A + F^i \right) \frac{\partial}{\partial x^i} \right\}, \\
V(\mathcal{A}) &= \left\{ \boldsymbol{\Xi} = \Xi^A E^i_A \frac{\partial}{\partial x^i} \right\} = \mathcal{L}\left\{ E^i_A \frac{\partial}{\partial x^i} \right\}, \\
i_*(\mathcal{B}) &= \left\{ \mathbf{b} = \frac{\partial}{\partial t} + \left(\frac{\partial x^i}{\partial t} + \left(M^\alpha_\Upsilon \dot{\theta}^\Upsilon + N^\alpha \right) \frac{\partial x^i}{\partial q^\alpha} \right) \frac{\partial}{\partial x^i} \right\}, \\
V(\mathcal{B}) &= \left\{ \Theta = \Theta^\Upsilon M^\alpha_\Upsilon \frac{\partial x^i}{\partial q^\alpha} \frac{\partial}{\partial x^i} \right\} = \mathcal{L}\left\{ M^\alpha_\Upsilon \frac{\partial x^i}{\partial q^\alpha} \frac{\partial}{\partial x^i} \right\}.
\end{aligned} \tag{9}$$

A. Case I

By the nature of the constraints acting on the system, the admissible left velocities $\mathbf{p}_L$ of the system are elements of $i^*(L_1(\mathcal{V}))$, and the admissible right velocities $\mathbf{p}_R$ of the system are elements of $i^*(R_1(\mathcal{V}))$. Then, the reactive impulse $\mathbf{I}(\mathbf{p}_L)=\mathbf{p}_R-\mathbf{p}_L$ given by the constraints must be in general an element of $i^*(V(\mathcal{V}))$.

Since $i_*(\mathcal{B})$ is an affine subbundle of $i_*(J_1(\mathcal{S}))$, applying Lemma 1.1 to $i_*(J_1(\mathcal{S}))$, modeled on the vector bundle $i_*(V(\mathcal{S}))$ endowed with the scalar product φ induced by Φ, we obtain the splits

$$i_*(V(\mathcal{S})) = V(\mathcal{B}) \oplus (V(\mathcal{B}))^\perp,$$

$$i_*(J_1(\mathcal{S})) = i_*(\mathcal{B}) \oplus (V(\mathcal{B}))^\perp. \tag{10}$$

Replacing them in (4) and (5), we have

$$i_*(V(\mathcal{V})) = V(\mathcal{B}) \oplus (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp,$$

$$i^*(J_1(\mathcal{V})) = i_*(\mathcal{B}) \oplus (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp. \tag{11}$$

The space $\mathcal{H}$ of the frames of rest of the whole set of constraints coincides with $i_*(\mathcal{B})$. In fact, since $i^*(\mathcal{B}) \subset i_*(J_1(\mathcal{S}))$, every $\mathbf{h} \in i^*(\mathcal{B})$ is automatically tangent to $\mathcal{S}$. This implies that $\mathcal{H}$ is not empty (even if it can be given by a single point).

Given a left velocity $\mathbf{p}_L \in i^*(L_1(\mathcal{V})) \simeq i^*(J_1(\mathcal{V}))$, we can therefore determine, by introducing the natural projection operators $\mathcal{P}^{\parallel}{}_{\mathcal{B}}: i^*(J_1(\mathcal{V})) \to i_*(\mathcal{B})$ and $\mathcal{P}^{\perp}{}_{\mathcal{B}}: i^*(J_1(\mathcal{V})) \to (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp$ induced by the second split of (11), the component $\mathbf{V}^\perp(\mathbf{p}_L) = \mathcal{P}^{\perp}{}_{\mathcal{B}}(\mathbf{p}_L)$ of the velocity orthogonal to the whole set of constraints. Lemma 1.1 ensures that, introducing the natural projection operators $\mathcal{P}^{\parallel}: i^*(V(\mathcal{V})) \to V(\mathcal{B})$ and $\mathcal{P}^{\perp}: i^*(V_1(\mathcal{V})) \to (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp$ induced by the first split of (11), for every $\mathbf{h} \in i_*(\mathcal{B})$ the vector $\mathbf{V}^\perp(\mathbf{p}_L)$ coincides with the component $\mathcal{P}^\perp(\mathbf{p}_L - \mathbf{h})$ of the relative velocity $\mathbf{p}_L - \mathbf{h}$. This concludes Step 1 of the procedure.

In order to determine possible constitutive characterizations $\mathbf{I}(\mathbf{p}_L)$ of the constraints, we impose the conservation of kinetic energy in the impact with respect to all the frames in $\mathcal{H}$. Taking into account the natural decompositions $\mathbf{p}_L - \mathbf{h} = \mathcal{P}^{\parallel}(\mathbf{p}_L - \mathbf{h}) + \mathcal{P}^{\perp}(\mathbf{p}_L - \mathbf{h})$ and $\mathbf{I}(\mathbf{p}_L) = \mathcal{P}^{\parallel}(\mathbf{I}(\mathbf{p}_L)) + \mathcal{P}^{\perp}((\mathbf{p}_L))$, condition (7) gives

$$\begin{aligned}\Phi(2(\mathcal{P}^{\parallel}(\mathbf{p}_L - \mathbf{h}), \mathcal{P}^{\parallel}(\mathbf{I}(\mathbf{p}_L))) + \Phi(2\mathbf{V}^\perp(\mathbf{p}_L), \mathcal{P}^\perp(\mathbf{I}(\mathbf{p}_L))) + \Phi(\mathcal{P}^{\parallel}(\mathbf{I}(\mathbf{p}_L)), \mathcal{P}^{\parallel}(\mathbf{I}(\mathbf{p}_L)))\\ + \Phi(\mathcal{P}^\perp(\mathbf{I}(\mathbf{p}_L)), \mathcal{P}^\perp(\mathbf{I}(\mathbf{p}_L))) = 0.\end{aligned} \tag{12}$$

The first addendum is the only one depending on the frame $\mathbf{h} \in \mathcal{H}$. So (omitting for brevity the dependence on $\mathbf{p}_L$) we have that:

Case Ia: If $\mathcal{H}$ is not formed by a single frame, a straightforward computation using admissible coordinates (see Ref. 9) shows that $\mathcal{P}^{\parallel}(\mathbf{I}) = 0$ and then $\mathbf{I} = \mathcal{P}^\perp(\mathbf{I})$. The conservation of kinetic energy can be expressed by the condition

$$\Phi(2\mathbf{V}^\perp + \mathcal{P}^\perp(\mathbf{I}), \mathcal{P}^\perp(\mathbf{I})) = 0, \tag{13}$$

completely analogous to the one presented in Ref. 9. This concludes Step 2 of the procedure.

However, in this situation, both $\mathbf{V}^\perp$ and $\mathcal{P}^\perp(\mathbf{I})$ belong to $(V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp$, that is a vector bundle whose fibers have dimension greater than 1, and therefore condition (13) alone does not determine $\mathcal{P}^\perp(\mathbf{I}) = -2\mathbf{V}^\perp$ as unique nontrivial solution. In complete analogy with Ref. 9, this result can be recovered only with an additional Gauss's "maximality" requirement on the impulsive admissible reaction $\mathbf{I}$. This concludes Step 3 and the whole procedure.

To conclude the analysis of this case, note moreover that, with obvious notation, the impulsive reaction $\mathbf{I}(\mathbf{p}_L) \in (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp$ can be decomposed a part $\mathbf{I}^\perp{}_{\mathcal{B}}$ tangent to the unilateral constraint $\mathcal{S}$ but orthogonal to the instantaneous kinetic constraint $\mathcal{B}$, and a part $\mathbf{I}^\perp{}_{\mathcal{S}}$ orthogonal to the unilateral constraint $\mathcal{S}$.

Case Ib: if $\mathcal{H} = \{\overline{\mathbf{h}}\}$, then $V(\mathcal{B}) = \{\underline{\mathbf{0}}\}$, and the splits (4) and (5) become

$$i^*(V(\mathcal{V})) = \{\underline{\mathbf{0}}\} \oplus (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp, \quad i^*(J_1(\mathcal{V})) = \{\overline{\mathbf{h}}\} \oplus (V(\mathcal{B}))^\perp \oplus (i_*(V(\mathcal{S})))^\perp.$$

Then, for every admissible impulsive reaction $\mathbf{I} \in i^*(V(\mathcal{V}))$, we have $\mathcal{P}^{\parallel}(\mathbf{I}) = 0$ and for every admissible left velocity $\mathbf{p}_L \in i^*(J_1(\mathcal{V}))$ we have $\mathbf{p}_L = \overline{\mathbf{h}} + \mathbf{V}^\perp$. Condition (8) directly assumes the form (13) and, using the same arguments of Case Ia about the Gauss's "maximality" requirement, we obtain the impulsive reaction $\mathbf{I}(\mathbf{p}_L) = -2\mathbf{V}^\perp(\mathbf{p}_L)$.

B. Case II

By the nature of the constraints acting on the system, both the admissible left velocities $\mathbf{p}_L$ and the admissible right velocities $\mathbf{p}_R$ of the system are elements of $i^*(\mathcal{A})$. Then, the reactive impulse $\mathbf{I}(\mathbf{p}_L)=\mathbf{p}_R-\mathbf{p}_L$ given by the constraints must be an element of $V(\mathcal{A})$. Moreover, the set $\mathcal{H}$ is obviously given by the intersection $\mathcal{H}=i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))$. Taking into account Lemma 1.2 and recalling that the fibers of the vector bundles $V(\mathcal{A})$ and $i_*(V(\mathcal{S}))$ have dimensions $s<n$ and $n-1$, respectively (so that, in particular, the fibers of $i_*(V(\mathcal{S}))$ have codimension 1), we have three possible situations:

- $V(\mathcal{A})\subset i_*(V(\mathcal{S}))$ and $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))=\emptyset$. Then $\mathcal{H}=\emptyset$ and the system does not have physical meaning (this is the situation of Example 1 described earlier).
- $V(\mathcal{A})\subset i_*(V(\mathcal{S}))$ and $i^*(\mathcal{A})\subset i_*(J_1(\mathcal{S}))$. Then the system cannot impact with the positional constraint $\mathcal{S}$, since every admissible left velocity $\mathbf{p}_L\in i^*(\mathcal{A})$ is already tangent to the positional constraint $\mathcal{S}$. In this case $\mathbf{V}^\perp(\mathbf{p}_L)=0$ and the corresponding impulsive reaction is $\mathbf{I}(\mathbf{p}_L)=0$.
- $V(\mathcal{A})\neq\subset i_*(V(\mathcal{S}))$. This situation can be divided into two cases: $V(\mathcal{A})\cap i_*(V(\mathcal{S}))\neq\{\underline{\mathbf{0}}\}$, which we will study as Case IIa, and $V(\mathcal{A})\cap i_*(V(\mathcal{S}))=\{\underline{\mathbf{0}}\}$, which we will study as Case IIb.

The only nontrivial situation is the last one. To start the geometric analysis when $V(\mathcal{A})\not\subset i_*(V(\mathcal{S}))$, we need the following:

Lemma 2.1: $V(\mathcal{A})\not\subset i_*(V(\mathcal{S}))$ if and only if $i^*(\mathcal{A})\not\subset i_*(J_1(\mathcal{S}))$ and $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))\neq\emptyset$.

Proof: "$\Leftarrow$" Let $\bar{a}\in i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))$ and let a be such that $a\in i^*(\mathcal{A})$ and $a\notin i_*(J_1(\mathcal{S}))$. Then $a-\bar{a}\in V(\mathcal{A})$ and $a-\bar{a}\notin i_*(V(\mathcal{S}))$.

"$\Rightarrow$" Of course $i^*(\mathcal{A})\not\subset i_*(J_1(\mathcal{S}))$, since otherwise, for the definition (6) of $V(\mathcal{A})$, it would follow the inclusion $V(\mathcal{A})\subset i_*(V(\mathcal{S}))$. Moreover, since $V(\mathcal{A})\not\subset i_*(V(\mathcal{S}))$ and $i_*(V(\mathcal{S}))$ has dimension $n-1$, the (nondirect) sum $V(\mathcal{A})+i_*(V(\mathcal{S}))$ generates the whole $i^*(V(\mathcal{V}))$. Introducing two bases of the vector bundles $V(\mathcal{A})$ and $i_*(V(\mathcal{S}))$, or equivalently taking into account the vector forms (9), the existence of an element in $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))$can be proved by solving a nonhomogeneous underdetermined linear system with maximum rank. □

Case IIa: If $V(\mathcal{A})\cap i_*(V(\mathcal{S}))\neq\{\underline{\mathbf{0}}\}$, then, applying Lemma 2.1, we have $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))\neq\emptyset$. Now taking into account Lemma 1.2, we have that $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))$ is an affine subspace of $i^*(\mathcal{A})$ modeled on the vector space $V(\mathcal{A})\cap i_*(V(\mathcal{S}))$. Therefore we have the splits

$$V(\mathcal{A})=(V(\mathcal{A})\cap i_*(V(\mathcal{S})))\otimes(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp,$$

$$i^*(\mathcal{A})=(i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S})))\otimes(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp. \tag{14}$$

This case is then structurally similar to Case Ia, with the vector bundle $V(\mathcal{A})$ of the admissible impulsive reaction split into a vector bundle $V(\mathcal{A})\cap i_*(V(\mathcal{S}))$ modeling the affine bundle of the frames of rest of the constraints and the vector bundle $(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp$ of the admissible orthogonal velocities. The requirement (12) of conservation of kinetic energy for all the frames in $\mathcal{H}$ implies once again $\mathcal{P}^{\|}(\mathbf{I})=0$ and then $\mathbf{I}=\mathcal{P}^\perp(\mathbf{I})$. Furthermore, the conservation of kinetic energy can be once again expressed by condition (13). However, in this case, the result $\mathbf{I}=-2\mathbf{V}^\perp$ can be obtained without imposing additional Gauss's "maximality" requirement as in Case Ia, but as a straightforward consequence of the following:

Proposition 2.1: The vector bundle $(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp$ is a line bundle. In particular, if $\mathbf{U}_{\mathcal{A}}^\perp$ is the projection on $V(\mathcal{A})$ of the velocity $\mathbf{V}_{\mathcal{S}}^\perp$, then $(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp=\mathcal{L}\{\mathbf{U}_{\mathcal{A}}^\perp\}$.

Proof: The first statement easily follows by dimensionality arguments: since the fibers of $i_*(V(\mathcal{S}))$ are of dimension $n-1$, then those of $V(\mathcal{A})\cap i_*(V(\mathcal{S}))$ have dimension $s-1$ (that is greater than 0, for the condition $V(\mathcal{A})\cap i_*(V(\mathcal{S}))\neq\{\underline{\mathbf{0}}\}$). Then $(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp$ is a line bundle.

The second statement can be proved in two steps: the first shows that $\mathbf{U}_{\mathcal{A}}^\perp\neq 0$, the second shows that $\mathbf{U}_{\mathcal{A}}^\perp\in(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^\perp$.

If $\mathbf{U}_{\mathcal{A}}^{\perp}=0$, then, since $\mathbf{U}_{\mathcal{A}}^{\perp}$ is the projection on $V(\mathcal{A})$ of $\mathbf{V}_{S}^{\perp}$, we should have $\Phi(\mathbf{V}_{S}^{\perp},\boldsymbol{\Xi})=0\ \forall \boldsymbol{\Xi}(\mathcal{A})$, and therefore $V(\mathcal{A})\subset i_*(V(\mathcal{S}))$, that is not possible in this case.

Moreover, a straightforward computation using admissible coordinates and the vector representations (9) shows that for every $\boldsymbol{\Xi}\in V(\mathcal{A})$ we have that $\Phi(\boldsymbol{\Xi},\mathbf{U}_{\mathcal{A}}^{\perp})=0$ if and only if $\Phi(\boldsymbol{\Xi},\mathbf{V}_{S}^{\perp})=0$, that is if and only if $\boldsymbol{\Xi}\in i_*(V(\mathcal{S}))$. Then $\mathbf{U}_{\mathcal{A}}^{\perp}$ is orthogonal to $V(\mathcal{A})\cap i_*(V(\mathcal{S}))$, or, that is the same, $\mathbf{U}_{\mathcal{A}}^{\perp}\in(V(\mathcal{A})\cap i_*(V(\mathcal{S})))^{\perp}$.

Case IIb: If $V(\mathcal{A})\cap i_*(V(\mathcal{S}))=\{\underline{\mathbf{0}}\}$ with the condition $V(\mathcal{A})\not\subset i_*(V(\mathcal{S}))$, then the fibers of $V(\mathcal{A})$ must have dimension 1. However, applying Lemma 2.1, we have once again $i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))\neq\emptyset$ and then $\mathcal{H}=\{\overline{\mathbf{h}}\}$.

The splits (14) assume the trivial aspect

$$V(\mathcal{A})=\{\underline{\mathbf{0}}\}\oplus V(\mathcal{A}),$$

$$i^*(\mathcal{A})=\{\overline{\mathbf{h}}\}\oplus V(\mathcal{A}).$$

Similar to Case Ib, for every admissible impulsive reaction $\mathbf{I}\in V(\mathcal{A})$, we have $\mathcal{P}^{\|}(\mathbf{I})=0$ and for every admissible left velocity $\mathbf{p}_L\in i^*(\mathcal{A})$ we have $\mathbf{p}_L=\overline{\mathbf{h}}+\mathbf{V}^{\perp}$. Condition (8) directly assumes the form (13) and, if we take into account that $V(\mathcal{A})$ is a line bundle, once again without Gauss's requirement, it follows that $\mathbf{I}=-2\mathbf{V}^{\perp}$.

C. Case III

Clearly, since both kinds of kinetic constraints $\mathcal{A}$ and $\mathcal{B}$ and the unilateral constraint $\mathcal{S}$ simultaneously act on the system, both splits (10) and (14) hold.

Once again, both the admissible left and right velocities $\mathbf{p}_L$ and $\mathbf{p}_R$ are elements of $i^*(\mathcal{A})$. Then, the reactive impulse $\mathbf{I}(\mathbf{p}_L)=\mathbf{p}_R-\mathbf{p}_L$ given by the constraints must be an element of $V(\mathcal{A})$. Moreover, the set $\mathcal{H}$ is obviously given by the intersection $\mathcal{H}=i_*(\mathcal{B})\cap i^*(\mathcal{A})$. Since $i_*(\mathcal{B})\subset i_*(J_1(\mathcal{S}))$ and $V(\mathcal{B})\subset i_*(V(\mathcal{S}))$, the splits (14) do not have relevance in this case.

Taking into account Lemma 1.2 and recalling that the fibers of the vector bundles $V(\mathcal{B})$ and $V(\mathcal{A})$ have dimensions $m<n-1$ and $s<n$, respectively (so that this time, in the general case, we do not have bundles with fibers of codimension 1), we have five possibilities about the nature of $\mathcal{H}$:

- The intersection $i_*(\mathcal{B})\cap i^*(\mathcal{A})$ is not trivial. Then we have two possible situations:

(1) $V(\mathcal{B})\cap V(\mathcal{A})\neq\{\underline{\mathbf{0}}\}$, which we will study as Case IIIa;
(2) $V(\mathcal{B})\cap V(\mathcal{A})=\{\underline{\mathbf{0}}\}$, which we will study as Case IIIb.

- The intersection $i_*(\mathcal{B})\cap i^*(\mathcal{A})$ is trivial. Then we have three possible situations:

(1) $i_*(\mathcal{B})\cap i^*(\mathcal{A})=\emptyset$. Then $\mathcal{H}=\emptyset$ and the system does not have physical meaning (this is the situation of Example 2 described earlier).
(2) $i^*(\mathcal{A})\subset i_*(\mathcal{B})$. Then the system cannot impact with the positional constraint $\mathcal{S}$, since every admissible left velocity $\mathbf{p}_L\in i^*(\mathcal{A})$ is already tangent to the positional constraint $\mathcal{S}$ and $\mathbf{p}_L$ also obeys the instantaneous kinetic constraint $\mathcal{B}$. In this case $\mathbf{V}^{\perp}(\mathbf{p}_L)=0$ and the corresponding impulsive reaction is $\mathbf{I}(\mathbf{p}_L)=0$.
(3) $i_*(\mathcal{B})\subset i^*(\mathcal{A})$, which can be considered as a particular case of Case IIIa if the fibers of $i_*(\mathcal{B})$ are not given by a single point, or a particular case of Case IIIb otherwise.

Case IIIa: If $i_*(\mathcal{B})\cap i^*(\mathcal{A})\neq\emptyset$ and $V(\mathcal{B})\cap V(\mathcal{A})\neq\{\underline{\mathbf{0}}\}$, taking into account Lemma 1.2, with obvious notation we have the splits

$$V(\mathcal{A})=(V(\mathcal{B})\cap V(\mathcal{A}))\oplus(V(\mathcal{B})\cap V(\mathcal{A}))^{\perp},$$

$$i^*(\mathcal{A}) = (i_*(\mathcal{B}) \cap i^*(\mathcal{A})) \oplus (V(\mathcal{B}) \cap V(\mathcal{A}))^\perp.$$

The procedure is then completely similar to Cases Ia and IIa. The conservation of kinetic energy (12) for all the frames in $\mathcal{H}$ implies once again $\mathcal{P}^{\|}(\mathbf{I})=0$, so that $\mathbf{I}=\mathcal{P}^{\perp}(\mathbf{I})$. The conservation of kinetic energy can therefore be rewritten as (13) and, if the vector bundle $(V(\mathcal{B})\cap V(\mathcal{A}))^\perp$ is a line bundle, this suffices to conclude that $\mathbf{I}=-2\mathbf{V}^\perp$. If the bundle $(V(\mathcal{B})\cap V(\mathcal{A}))^\perp$ has fibers of dimension greater than 1, we need Gauss's requirement to reach the same conclusion.

Case IIIb: If $i_*(\mathcal{B})\cap\ i^*(\mathcal{A})\neq\emptyset$ and $V(\mathcal{B})\cap V(\mathcal{A})=\{\underline{\mathbf{0}}\}$, then $\mathcal{H}=i_*(\mathcal{B})\cap i^*(\mathcal{A})=\{\overline{\mathbf{h}}\}$. With obvious notation we have the splits

$$V(\mathcal{A}) = \{\underline{\mathbf{0}}\} \oplus V(\mathcal{A}),$$

$$i^*(\mathcal{A}) = \{\overline{\mathbf{h}}\} \oplus V(\mathcal{A}).$$

Similar to Cases Ib and IIb, for every admissible impulsive reaction $\mathbf{I}\in V(\mathcal{A})$, we have $\mathcal{P}^{\|}(\mathbf{I})=0$ and for every admissible left velocity $\mathbf{p}_L\in i^*(\mathcal{A})$ we have $\mathbf{p}_L=\overline{\mathbf{h}}+\mathbf{V}^\perp$. Condition (8) directly assumes the form (13). Similar to Case IIIa, dimension of the bundle $V(\mathcal{A})$ of the admissible impulsive reactions determines whether or not we need Gauss's requirement to obtain the result $\mathbf{I}=-2\mathbf{V}^\perp$.

IV. EXAMPLES

It is clear that a list of examples exhausting all the possibilities described in the previous section would be very tedious and, in some cases, even of minimum interest, since the corresponding mechanical systems would be rather artful. Therefore, although several significant examples could be listed and analyzed, in this section we present only the four examples described at the beginning of Sec. II.

In the following we extensively use the representations in admissible coordinates listed in (9) of the elements of the various bundles involved in the description.

A. Example of Case I

A cogwheel of mass m and radius R is moving in a plane and impacts with a straight rack. The space–time bundle $\mathcal{V}$ is a four-dimensional manifold, locally described by admissible coordinates (t,x,y,ϑ) where x,y are the Cartesian coordinates of the center of the cogwheel in the plane of the motion and ϑ is the orientation of the cogwheel. The vertical scalar product Φ on $\mathcal{V}$ is described by the matrix $g_{ij}=\mathrm{diag}(m,m,A)$ with $A=\frac{1}{2}mR^2$. The unilateral constraint $\mathcal{S}$ can be described by the condition $y=R$ or, choosing admissible coordinates (t,x,ϑ) in $\mathcal{S}$, by the injection

$$i:S\to\mathcal{V} \quad \text{such that} \quad (t,x,\vartheta)\rightsquigarrow(t,x,R,\vartheta).$$

The instantaneous kinetic constraint $\mathcal{B}$ is given by the condition $\dot{x}+R\dot{\vartheta}=0$, or by the injection

$$k:\mathcal{B}\to J_1(\mathcal{S}) \quad \text{such that} \quad (t,x,\vartheta,\dot{\vartheta})\rightsquigarrow(t,x,\vartheta,-R\dot{\vartheta},\dot{\vartheta}).$$

The velocity and vertical spaces are

$$i^*(J_1(\mathcal{V})) = \left\{\mathbf{p}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{y}\frac{\partial}{\partial y}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i^*(V(\mathcal{V})) = \mathcal{L}\left\{\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial\vartheta}\right\},$$

$$i^*(J_1(\mathcal{S})) = \left\{ \mathbf{q} = \frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$i_*(V(\mathcal{S})) = \mathcal{L}\left\{ \frac{\partial}{\partial x}, \frac{\partial}{\partial \vartheta} \right\},$$

$$(i_*(V(\mathcal{S})))^\perp = \mathcal{L}\left\{ \frac{\partial}{\partial y} \right\},$$

$$i_*(\mathcal{B}) = \left\{ \mathbf{b} = \frac{\partial}{\partial t} - R\dot{\vartheta}\frac{\partial}{\partial x} + \dot{\vartheta}\frac{\partial}{\partial \vartheta} \right\},$$

$$V(\mathcal{B}) = \mathcal{L}\left\{ -R\frac{\partial}{\partial x} + \frac{\partial}{\partial \vartheta} \right\},$$

$$(V(\mathcal{B}))^\perp = \mathcal{L}\left\{ -\frac{A}{mR}\frac{\partial}{\partial x} + \frac{\partial}{\partial \vartheta} \right\}.$$

Since $\mathcal{H} = i_*(\mathcal{B})$ is not given by a single frame, the situation is the one described in Case Ia.

Given a left velocity $\mathbf{p}_L = \partial/(\partial t) + \dot{x}_L \partial/(\partial x) + \dot{y}_L \partial/(\partial y) + \dot{\vartheta}_L \partial/(\partial \vartheta)$, we have

$$\mathbf{V}^\perp(\mathbf{p}_L) = \frac{A}{mR^2 + A}(\dot{x}_L + R\dot{\vartheta}_L)\frac{\partial}{\partial x} + \dot{y}_L\frac{\partial}{\partial y} + \frac{mR}{mR^2 + A}(\dot{x}_L + R\dot{\vartheta}_L)\frac{\partial}{\partial \vartheta}.$$

The corresponding ideal reactive impulse $\mathbf{I}(\mathbf{p}_L) = -2\mathbf{V}^\perp(\mathbf{p}_L)$ gives then the right velocity

$$\mathbf{p}_R = \mathbf{p}_L + \mathbf{I}(\mathbf{p}_L) = \frac{\partial}{\partial t} + \left(\frac{mR^2 - A}{mR^2 + A}\dot{x}_L - \frac{2A}{mR^2 + A}R\dot{\vartheta}_L \right)\frac{\partial}{\partial x} - \dot{y}_L\frac{\partial}{\partial y} + \left(-\frac{2mR}{mR^2 + A}\dot{x}_L + \frac{A - mR^2}{mR^2 + A}\dot{\vartheta}_L \right)\frac{\partial}{\partial \vartheta}.$$

Clearly the result does not have an immediate physical interpretation. However it is worth noticing that, such as in the case of smooth unilateral constraint (i.e., in the absence of the instantaneous constraint $\mathcal{B}$—see Ref. 9), the velocity of the cogwheel along the y-axis simply reverses.

Simple tests of reasonableness of the result follow from the analysis of particular impact configurations. A first possibility is the impact of the cogwheel without initial spin, that is in the case $\mathbf{p}_L = \partial/(\partial t) + \dot{x}_L \partial/(\partial x) + \dot{y}_L \partial/(\partial y)$. The corresponding right velocity is

$$\mathbf{p}_R = \frac{\partial}{\partial t} + \frac{mR^2 - A}{mR^2 + A}\dot{x}_L\frac{\partial}{\partial x} - \dot{y}_L\frac{\partial}{\partial y} - \frac{2mR}{mR^2 + A}\dot{x}_L\frac{\partial}{\partial \vartheta}.$$

This result shows that, unlike the smooth situation, the rule "incidence angle equal to reflection angle" is not fulfilled, since the rack clasps the cogwheel, giving it a (correctly directed) spin but bringing the exit direction nearer to the direction orthogonal to the rack.

A second possibility of particular impact is when the cogwheel has an initial "pure rolling" spin, that is in the case $\mathbf{p}_L = \partial/(\partial t) - R\dot{\vartheta}_L \partial/(\partial x) + \dot{y}_L \partial/(\partial y) + \dot{\vartheta}_L \partial/(\partial \vartheta)$. The corresponding right velocity is $\mathbf{p}_R = \partial/(\partial t) - R\dot{\vartheta}_L \partial/(\partial x) - \dot{y}_L \partial/(\partial y) + \dot{\vartheta}_L \partial/(\partial \vartheta)$, which shows that, this time, the rack does not clasp the cogwheel and the rule "incidence angle equal to reflection angle" is fulfilled.

B. Examples of Case II

Example 1: A cogwheel of mass m and radius R is moving in a plane rolling on a horizontal rack and impacts with a vertical smooth wall. Due to the integrability of the pure rolling kinetic constraint given by the rack on the cogwheel, the system can be studied as a "one degree of

freedom" system subject to an ideal unilateral constraint given by the wall, without the introduction of kinetic constraints. The results presented in Ref. 9 immediately give the (obvious) behavior of the cogwheel.

Nevertheless, the system can also be viewed as a "two degrees of freedom" system subject to a kinetic constraint. The space–time bundle $\mathcal{V}$ can be chosen as a three-dimensional manifold, locally described by admissible coordinates (t,x,ϑ) where x is the Cartesian abscissa of the center of the cogwheel in the plane of the motion and ϑ is the orientation of the cogwheel. The vertical scalar product Φ on $\mathcal{V}$ is described by the matrix $g_{ij}=\mathrm{diag}(m,A)$ with $A=\frac{1}{2}mR^2$. The unilateral constraint $\mathcal{S}$ is given by the condition $x=K=$constant or, choosing admissible coordinates (t,ϑ) in $\mathcal{S}$, by the injection

$$i:\mathcal{S}\to\mathcal{V} \quad \text{such that} \quad (t,\vartheta)\rightsquigarrow(t,K,\vartheta).$$

The kinetic constraint $\mathcal{A}$ is given by the condition $\dot{x}+R\dot{\vartheta}=0$, or by the injection

$$h:\mathcal{A}\to J_1(\mathcal{V}) \quad \text{such that} \quad (t,x,\vartheta,\dot{\vartheta})\rightsquigarrow(t,x,\vartheta,-R\dot{\vartheta},\dot{\vartheta}).$$

The velocity and vertical spaces are

$$i^*(J_1(\mathcal{V}))=\left\{\mathbf{p}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i^*(V(\mathcal{V}))=\mathcal{L}\left\{\frac{\partial}{\partial t},\frac{\partial}{\partial\vartheta}\right\},$$

$$i_*(J_1(\mathcal{S}))=\left\{\mathbf{q}=\frac{\partial}{\partial t}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$i_*(V(\mathcal{S}))=\mathcal{L}\left\{\frac{\partial}{\partial\vartheta}\right\},$$

$$(i_*(V(\mathcal{S})))^\perp=\mathcal{L}\left\{\frac{\partial}{\partial x}\right\},$$

$$i^*(\mathcal{A})=\left\{\mathbf{a}=\frac{\partial}{\partial t}-R\dot{\vartheta}\frac{\partial}{\partial x}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}\right\},$$

$$V(\mathcal{A})=\mathcal{L}\left\{-R\frac{\partial}{\partial x}+\frac{\partial}{\partial\vartheta}\right\}.$$

Since $V(\mathcal{A})\cap i_*(V(\mathcal{S}))=\{\underline{\mathbf{0}}\}$, the situation is the one described in Case IIb. In fact we have $\mathcal{H}=i^*(\mathcal{A})\cap i_*(J_1(\mathcal{S}))=\{\partial/\partial t\}$.

Given a left velocity $\mathbf{p}_L=\partial/(\partial t)-R\dot{\vartheta}_L\partial/(\partial x)+\dot{\vartheta}_L\partial/(\partial\vartheta)$, we have

$$\mathbf{V}^\perp(\mathbf{p}_L)=-R\dot{\vartheta}_L\frac{\partial}{\partial x}+\dot{\vartheta}_L\frac{\partial}{\partial\vartheta}.$$

The corresponding ideal reactive impulse $\mathbf{I}(\mathbf{p}_L)=-2\mathbf{V}^\perp(\mathbf{p}_L)$ gives then a right velocity $\mathbf{p}_R=\partial/(\partial t)+R\dot{\vartheta}_L\partial/(\partial x)-\dot{\vartheta}_L\partial/(\partial\vartheta)$, as it can be easily foreseen.

Passing over the obviousness of the result, this approach shows that the impulsive reaction $\mathbf{I}(\mathbf{p}_L)=2R\dot{\vartheta}_L\partial/(\partial x)-2\dot{\vartheta}_L\partial/(\partial\vartheta)$ cannot be due only to the smooth unilateral constraint $\mathcal{S}$, that can give only impulsive reactions in $(i_*(V(\mathcal{S})))^\perp$, but also to the kinetic constraint $\mathcal{A}$.

Example 2: A homogeneous billiard ball of mass m and radius R is rolling on a horizontal plane and impacts with a smooth vertical wall. The space–time bundle $\mathcal{V}$ is a six-dimensional manifold, locally described by admissible coordinates $(t,x,y,\psi,\vartheta,\varphi)$ where x,y are the Cartesian coordinates of the center of the ball and ψ,ϑ,φ are the usual Euler angles describing the orientation of the ball. The vertical scalar product Φ on $\mathcal{V}$ is given by the matrix

$$g_{ij}=\begin{pmatrix} m & 0 & 0 & 0 & 0 \\ 0 & m & 0 & 0 & 0 \\ 0 & 0 & A & 0 & A\cos\vartheta \\ 0 & 0 & 0 & A & 0 \\ 0 & 0 & A\cos\vartheta & 0 & A \end{pmatrix}$$

with $A=\frac{2}{5}mR^2$ (and it is nonsingular when $\sin\vartheta\neq 0$). The unilateral constraint $\mathcal{S}$ is given by the condition $y=R$ or, choosing admissible coordinates $(t,x,\psi,\vartheta,\varphi)$ in $\mathcal{S}$, by the injection

$$i:\mathcal{S}\to\mathcal{V} \quad \text{such that} \quad (t,x,\psi,\vartheta,\varphi)\rightsquigarrow(t,x,R,\psi,\vartheta,\varphi).$$

The permanent kinetic constraint $\mathcal{A}$ is given by the conditions

$$\dot{x}-R\dot{\vartheta}\sin\psi+R\dot{\varphi}\sin\vartheta\cos\psi=0,$$

$$\dot{y}+R\dot{\vartheta}\cos\psi+R\dot{\varphi}\sin\vartheta\sin\psi=0,$$

or by the injection

$$h:\mathcal{A}\to J_1(\mathcal{V}) \quad \text{such that}$$

$$(t,\psi,\vartheta,\varphi,\dot{\psi},\dot{\vartheta},\dot{\varphi})\rightsquigarrow(t,\psi,\vartheta,\varphi,R\dot{\vartheta}\sin\psi-R\dot{\varphi}\sin\vartheta\cos\psi,-R\vartheta\cos\psi-R\dot{\varphi}\sin\vartheta\sin\psi,\dot{\psi},\dot{\vartheta},\dot{\varphi}).$$

The velocity and vertical spaces are

$$i^*(J_1(\mathcal{V}))=\left\{\mathbf{p}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{y}\frac{\partial}{\partial y}+\dot{\psi}\frac{\partial}{\partial y}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}+\dot{\varphi}\frac{\partial}{\partial\varphi}\right\},$$

$$i^*(V(\mathcal{V}))=\mathcal{L}\left\{\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial\psi},\frac{\partial}{\partial\vartheta},\frac{\partial}{\partial\varphi}\right\},$$

$$i_*(J_1(\mathcal{S}))=\left\{\mathbf{q}=\frac{\partial}{\partial t}+\dot{x}\frac{\partial}{\partial x}+\dot{\psi}\frac{\partial}{\partial\psi}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}+\dot{\varphi}\frac{\partial}{\partial\varphi}\right\},$$

$$i_*(V(\mathcal{S}))=\mathcal{L}\left\{\frac{\partial}{\partial x},\frac{\partial}{\partial\psi},\frac{\partial}{\partial\vartheta},\frac{\partial}{\partial\varphi}\right\},$$

$$(i_*(V(\mathcal{S})))^\perp=\mathcal{L}\left\{\frac{\partial}{\partial y}\right\},$$

$$
\begin{aligned}
i^*(\mathcal{A}) = \Bigg\{ & \mathbf{a} = \frac{\partial}{\partial t} + (R\dot{\vartheta}\sin\psi - R\dot{\varphi}\sin\vartheta\cos\psi)\frac{\partial}{\partial x} \\
& + (-R\dot{\vartheta}\cos\psi - R\dot{\varphi}\sin\vartheta\sin\psi)\frac{\partial}{\partial y} + \dot{\psi}\frac{\partial}{\partial\psi} + \dot{\vartheta}\frac{\partial}{\partial\vartheta} + \dot{\varphi}\frac{\partial}{\partial\varphi}\Bigg\}, \\
V(\mathcal{A}) = \Bigg\{ & \mathbf{V} = (RV^4\sin\psi - RV^5\sin\vartheta\cos\psi)\frac{\partial}{\partial x} \\
& + (-RV^4\cos\psi - RV^5\sin\vartheta\sin\psi)\frac{\partial}{\partial y} + V^3\frac{\partial}{\partial\psi} + V^4\frac{\partial}{\partial\vartheta} + V^5\frac{\partial}{\partial\varphi}\Bigg\}.
\end{aligned} \tag{15}
$$

Since $V(\mathcal{A}) \cap i_*(V(\mathcal{S})) \neq \{\underline{\mathbf{0}}\}$, the situation is the one described in Case IIa. Given a left velocity

$$
\begin{aligned}
\mathbf{p}_L = & \frac{\partial}{\partial t} + (R\dot{\vartheta}_L\sin\psi - R\dot{\varphi}_L\sin\vartheta\cos\psi)\frac{\partial}{\partial x} + (-R\dot{\vartheta}_L\cos\psi - R\dot{\varphi}_L\sin\vartheta\sin\psi)\frac{\partial}{\partial y} \\
& + \dot{\psi}_L\frac{\partial}{\partial\psi} + \dot{\vartheta}_L\frac{\partial}{\partial\vartheta} + \dot{\varphi}_L\frac{\partial}{\partial\varphi},
\end{aligned} \tag{16}
$$

we have

$$
\begin{aligned}
\mathbf{V}^{\perp}(\mathbf{p}_L) = & (-R\dot{\vartheta}_L\cos\psi - R\dot{\varphi}_L\sin\vartheta\sin\psi)\frac{\partial}{\partial y} + \left(-\dot{\vartheta}_L\frac{\cos\vartheta\sin\psi\cos\psi}{\sin\vartheta} - \dot{\varphi}_L\cos\vartheta\sin^2\psi\right)\frac{\partial}{\partial\psi} \\
& + \left(\dot{\vartheta}_L\cos^2\psi + \dot{\varphi}_L\sin\vartheta\sin\psi\cos\psi\right)\frac{\partial}{\partial\vartheta} + \left(\dot{\vartheta}_L\frac{\sin\psi\cos\psi}{\sin\vartheta} + \dot{\varphi}_L\sin^2\psi\right)\frac{\partial}{\partial\varphi}.
\end{aligned}
$$

The corresponding ideal reactive impulse $\mathbf{I}(\mathbf{p}_L) = -2\mathbf{V}^{\perp}(\mathbf{p}_L)$ gives then a right velocity

$$
\begin{aligned}
\mathbf{p}_R = & \frac{\partial}{\partial t} + (R\dot{\vartheta}\sin\psi - R\dot{\varphi}\sin\vartheta\cos\psi)\frac{\partial}{\partial x} \\
& + (R\dot{\vartheta}_L\cos\psi + R\dot{\varphi}_L\sin\vartheta\sin\psi)\frac{\partial}{\partial y} \\
& + \left(\dot{\psi}_L + 2\dot{\vartheta}_L\frac{\cos\vartheta\sin\psi\cos\psi}{\sin\vartheta} + 2\dot{\varphi}_L\cos\vartheta\sin^2\psi\right)\frac{\partial}{\partial\psi} \\
& + \left(\dot{\vartheta}_L(1-\cos^2\psi) - 2\dot{\varphi}_L\sin\vartheta\sin\psi\cos\psi\right)\frac{\partial}{\partial\vartheta} \\
& + \left(-2\dot{\vartheta}_L\frac{\sin\psi\cos\psi}{\sin\vartheta} + \dot{\varphi}_L(1-\sin^2\psi)\right)\frac{\partial}{\partial\varphi}.
\end{aligned}
$$

Although the result seems quite complicated, some tests can be performed in order to prove the reasonableness of the result. The results $\dot{x}_R = \dot{x}_L, \dot{y}_R = -\dot{y}_L$ show that the impact obeys the rule "incidence angle equal to reflection angle." Moreover, if we assume a very classical point of view, and we denote with $\underline{\omega} = \omega^1\underline{\mathbf{e}}_1 + \omega^2\underline{\mathbf{e}}_2 + \omega^3\underline{\mathbf{e}}_3$ the usual angular velocity of the ball, where $\underline{\mathbf{e}}_1$ is a unit vector in the direction x, $\underline{\mathbf{e}}_2$ is a unit vector in the direction y, and $\underline{\mathbf{e}}_3$ is a unit vector in the direction orthogonal to the horizontal plane where the ball rolls, a tedious but straightforward calculation shows that, independent of the angles $(\psi, \vartheta, \varphi)$ for which the impact happens, we have $\omega_R^1 = -\omega_L^1, \omega_R^2 = \omega_L^2$ (that once again proves the rule "incidence angle equal to reflection angle") and $\omega_R^3 = \omega_L^3$, which proves that the smooth vertical wall (obviously) does not clasp the ball during the impact.

Note also that, such as in the previous example, the impulsive reaction cannot be due only to the smooth unilateral constraint $\mathcal{S}$, which can give only impulsive reactions in $(i_*(V(\mathcal{S})))^\perp$, but also to the kinetic constraint $\mathcal{A}$.

C. Example of Case III

The same billiard ball of the previous example is rolling on the horizontal plane but this time impacts with a rough vertical wall where a kinetic condition of rolling must be fulfilled. The space–time bundle $\mathcal{V}$, the admissible coordinates $(t,x,y,\psi,\vartheta,\varphi)$, and the vertical scalar product Φ on $\mathcal{V}$ are the same as in the previous example, such as the unilateral constraint $\mathcal{S}$ and the permanent kinetic constraint $\mathcal{A}$, with their Cartesian or parametric representations. The instantaneous kinetic constraint $\mathcal{B}$ is given by the conditions

$$\begin{aligned}&\dot{x}+R\dot{\psi}+R\dot{\varphi}\cos\vartheta=0,\\&\dot{y}=0,\\&\dot{\vartheta}\cos\psi+\dot{\varphi}\sin\vartheta\sin\psi=0\end{aligned}$$

(with the second condition that simply expresses the fact that $\mathcal{B}$ "lives" on $i_*(J_1(\mathcal{S}))$ or by the injection

$$k:\mathcal{B}\to J_1(\mathcal{S}) \quad \text{such that}$$

$$(t,x,\psi,\vartheta,\varphi,\dot{\psi},\dot{\varphi})\rightsquigarrow\left(t,x,\psi,\vartheta,\varphi,-R\dot{\psi}-R\dot{\varphi}\cos\vartheta,\dot{\psi},-\dot{\varphi}\frac{\sin\vartheta\sin\psi}{\cos\psi},\dot{\vartheta}\right).$$

Then, together with the spaces given by (15), we have also the bundles

$$i_*(\mathcal{B})=\left\{\mathbf{b}=\frac{\partial}{\partial t}+(-R\dot{\psi}-R\dot{\varphi}\cos\vartheta)\frac{\partial}{\partial x}+\dot{\psi}\frac{\partial}{\partial\psi}-\dot{\varphi}\frac{\sin\vartheta\sin\psi}{\cos\psi}\frac{\partial}{\partial\vartheta}+\dot{\varphi}\frac{\partial}{\partial\varphi}\right\},$$

$$V(\mathcal{B})=\left\{\mathbf{W}=(-RV^3-RV^5\cos\vartheta)\frac{\partial}{\partial x}+V^3\frac{\partial}{\partial\psi}-\frac{\sin\vartheta\sin\psi}{\cos\psi}V^5\frac{\partial}{\partial\vartheta}+V^5\frac{\partial}{\partial\varphi}\right\}.$$

We have $V(\mathcal{B})\cap V(\mathcal{A})\neq\{\underline{\mathbf{0}}\}$ and the space $\mathcal{H}$ is given by

$$\mathcal{H}=\left\{\frac{\partial}{\partial t}-R\dot{\varphi}\frac{\sin\vartheta}{\cos\psi}\frac{\partial}{\partial x}+\dot{\varphi}\left(\frac{\sin\vartheta}{\cos\psi}-\cos\vartheta\right)\frac{\partial}{\partial\psi}-\dot{\varphi}\frac{\sin\vartheta\sin\psi}{\cos\psi}\frac{\partial}{\partial\vartheta}+\dot{\varphi}\frac{\partial}{\partial\varphi}\right\}.$$

Then the situation is the one described in Case IIIa. Given a left velocity $\mathbf{p}_L$ as in (16), we obtain

$$\begin{aligned}\mathbf{V}^\perp(\mathbf{p}_L)=&[R(\dot{\vartheta}_L\sin\psi-\dot{\varphi}_L\sin\vartheta\cos\psi-\Gamma_L)]\frac{\partial}{\partial x}+[R(-\dot{\vartheta}_L\cos\psi-\dot{\varphi}_L\sin\vartheta\sin\psi)]\frac{\partial}{\partial y}\\&+\left[\dot{\psi}_L-\left(1-\frac{\cos\vartheta\cos\psi}{\sin\vartheta}\right)\Gamma_L\right]\frac{\partial}{\partial\psi}+\left[\dot{\vartheta}_L+(\sin\psi)\Gamma_L\right]\frac{\partial}{\partial\vartheta}+\left[\dot{\varphi}_L-\left(\frac{\cos\psi}{\sin\vartheta}\right)\Gamma_L\right]\frac{\partial}{\partial\varphi}\end{aligned}$$

with

$$\Gamma_L=\frac{A}{mR^2+2A}\dot{\psi}_L-\left(\frac{mR^2+A}{mR^2+2A}\sin\psi\right)\dot{\vartheta}_L+\left(\frac{mR^2+A}{mR^2+2A}\sin\vartheta\cos\psi+\frac{A}{mR^2+2A}\cos\vartheta\right)\dot{\varphi}_L.$$

The corresponding ideal reactive impulse $\mathbf{I}(\mathbf{p}_L)=-2\mathbf{V}^\perp(\mathbf{p}_L)$ gives the right velocity

$$\mathbf{p}_R = \frac{\partial}{\partial t} + [-R(\dot{\vartheta}_L \sin\psi - \dot{\varphi}_L \sin\vartheta\cos\psi + 2\Gamma_L)]\frac{\partial}{\partial x} + [R(\dot{\vartheta}_L \cos\psi + \dot{\varphi}_L \sin\vartheta \sin\psi)]\frac{\partial}{\partial y}$$
$$+ \left[-\dot{\psi}_L + 2\left(1 - \frac{\cos\vartheta\cos\psi}{\sin\vartheta}\right)\Gamma_L\right]\frac{\partial}{\partial\psi} + [-\dot{\vartheta}_L - 2(\sin\psi)\Gamma_L]\frac{\partial}{\partial\vartheta}$$
$$+ \left[-\dot{\varphi}_L + 2\left(\frac{\cos\psi}{\sin\vartheta}\right)\Gamma_L\right]\frac{\partial}{\partial\varphi}.$$

Once again, the result does not have an immediate reading. If we assume the classical point of view, denoting with $\underline{\omega} = \omega^1\underline{\mathbf{e}}_1 + \omega^2\underline{\mathbf{e}}_2 + \omega^3\underline{\mathbf{e}}_3$ the angular velocity of the ball and with $\underline{\mathbf{u}} = \dot{x}\underline{\mathbf{e}}_1 + \dot{y}\underline{\mathbf{e}}_2$ the linear velocity of the center of mass of the ball, a straightforward calculation shows that, independent of the angles $(\psi, \vartheta, \varphi)$ for which the impact happens, we have the relations

$$\dot{x}_L = R\omega_L^2, \quad \dot{x}_R = R\left(\frac{mR^2}{mR^2 + 2A}\omega_L^2 - \frac{2A}{mR^2 + 2A}\omega_L^3\right),$$

$$\dot{y}_L = -R\omega_L^1, \quad \dot{y}_R = R\omega_L^1.$$

This shows that, in general, the rule "incidence angle equal to reflection angle" is not fulfilled, and that the vertical wall clasps the ball. Moreover, this also shows that the exit direction is influenced by the initial spin in the direction $\underline{\mathbf{e}}_3$ orthogonal to the horizontal plane. The same result can be deduced by the relations

$$\omega_R^1 = -\omega_L^1,$$

$$\omega_R^2 = \frac{mR^2}{mR^2 + 2A}\omega_L^2 - \frac{2A}{mR^2 + 2A}\omega_L^3,$$

$$\omega_R^3 = -2\frac{mR^2 + A}{mR^2 + 2A}\omega_L^2 - \frac{mR^2}{mR^2 + 2A}\omega_L^3,$$

which prove that the impact with the vertical wall changes the spin in the direction $\underline{\mathbf{e}}_3$ orthogonal to the horizontal plane.

V. FINAL REMARKS AND CONCLUSIONS

Let us delve more deeply into the analysis of the results of the examples described in Sec. III.

It is intuitively clear that the behavior of the billiard ball of Example 2 of Case II is the most natural and foreseeable. Unfortunately, we cannot say the same for the examples of Cases I and III.

We focus our attention on the example of Case III in the particular situation when the motion of the ball before the impact is a *pure* rolling, so that $\omega_L^3 = 0$: if we denote with μ_L the "incident" angle formed by the direction of the entrance velocity $\underline{\mathbf{u}}_L = \dot{x}_L\underline{\mathbf{e}}_1 + \dot{y}_L\underline{\mathbf{e}}_2$ of the center of mass of the ball and the orthogonal to the vertical wall and with μ_R the "reflection" angle formed by the direction of the exit velocity $\underline{\mathbf{u}}_R = \dot{x}_R\underline{\mathbf{e}}_1 + \dot{y}_R\underline{\mathbf{e}}_2$ and the orthogonal to the vertical wall, we have the relation

$$\tan\mu_R = \frac{mR^2}{mR^2 + 2A}\tan\mu_L = \frac{5}{9}\tan\mu_L. \tag{17}$$

If, on the one side, this relation has some correct behaviors (such as $\mu_R = 0$ if and only if $\mu_L = 0$ or $\lim_{\mu_L \to \pi/2}\mu_R = \pi/2$), on the other side Eq. (17) shows that the vertical wall clasps the ball very hard (too much with respect to the behavior of the true billiard game, like every billiard player

knows). Moreover, the wall gives to the ball a (correctly oriented but) very great spin $\omega_R^3 = -\frac{14}{9}\omega_L^2$ in the vertical direction. Furthermore, the "clasp" effect shows itself both for almost orthogonal ($\dot{x}_L \simeq 0$) and almost tangent ($\dot{x}_L \gg \dot{y}_L$) impacts with the vertical wall.

Completely analogous considerations can be done for the results of Example 1. Let us denote with $\underline{\mathbf{u}} = \dot{x}\underline{\mathbf{e}}_1 + \dot{y}\underline{\mathbf{e}}_2$ the linear velocity of the center of mass of the cogwheel, where $\underline{\mathbf{e}}_1$ is a unit vector in the direction x of the rack, $\underline{\mathbf{e}}_2$ is a unit vector in the direction y orthogonal to the rack, and once again let us denote with μ_L and μ_R the "incident" and the "reflection" angles formed by the direction of the entrance and exit velocities with the direction orthogonal to the rack. Then, in the case of initial motion of the cogwheel without spin, we obtain the relation

$$\tan \mu_R = \frac{mR^2 - A}{mR^2 + A} \tan \mu_L = \frac{1}{3} \tan \mu_L.$$

Moreover, the cogwheel assumes (with obvious notation) an angular velocity $\underline{\omega} = -\frac{4}{3}(\dot{x}_L/R)\underline{\mathbf{e}}_3$. If it is intuitively clear that a rack clasps very hard a cogwheel, it is also intuitively clear that a similar situation is very difficult to realize in practice.

Then we must conclude by pointing out that the theoretical approach described in the paper gives results that are correct from the qualitative point of view but, when compared with the real (in the sense of "in the real world") behaviors of some simple and well-known systems, the results are improvable from the quantitative point of view. This improvability is obviously due to the sternness of the ideality requirement on the constraints: the analysis of nonideal unilateral constraints, starting from a coherent definition of the coefficient of restitution, should improve the results in this direction and will be the argument of a forthcoming paper.

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Nonlinear stability of boundary layers of the Boltzmann equation for cutoff hard potentials

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Many physical models have boundaries. For the Boltzmann equation, the study on the boundary layer in the region of the width in the order of the Kundsen number along the boundary is important both in mathematics and physics. In this paper, we consider the nonlinear stability of boundary layer solutions to the Boltzmann equation for hard potentials with angular cut-off. The boundary condition is imposed on incoming particles of the Dirichlet type and the solution tends to a global Maxwellian in the far field. For the existence of the boundary layer solutions, it is proved by Chen *et al.* [Anal. Appl. **2**, 337–363 (2004)] by introducing a weight function which is a function of both position and velocity to overcome the difficulty from the sublinear growth in the collision frequency. Unlike the hard sphere model, even for stability in the case when the Mach number of the far field is less than -1, exponential decay in time cannot be expected for the cutoff hard potentials. Instead, an algebraic decay in time to the boundary layer solution is proved in this paper by using some recursive weighted energy estimates and the bootstrap argument. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2229421]

I. INTRODUCTION

Consider the Boltzmann equation for the rarefied gas

$$F_t + \xi \cdot \nabla_x F = \frac{1}{\kappa} Q(F,F),$$

where $F(t,x,\xi)$ is the number density distribution function of particles at space-time $(t,x) = (t,x_1,x_2,x_3)$ with velocity ξ. When the problem involves a boundary, there is usually a layer of width of order κ along the boundary which is called the boundary layer. The equation for the boundary layer is a stationary equation which can be obtained by the standard scaling in the neighborhood of the boundary. In this paper, we consider the case when the boundary is an infinite plane, such as the (x_2,x_3) plane, and the layer depends only on (t,x_1,ξ). In this case, the dimension of the space variable becomes one, while the velocity variable is still three dimensional. In what follows, we still use x to denote x_1 for simplicity of notations. For general knowledge of the Boltzmann equation, please refer to Refs. 3–5, 10, and 11 and references therein.

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Since it is expected that the gas tends to an equilibrium away from the layer, the distribution function is assumed to be a global Maxwellian. Moreover, for the problem to be well-posed, the Dirichlet boundary condition is imposed by giving the incoming particle distribution. Under these assumptions, the problem in its linearized version and some other settings has been extensively studied, cf. Refs. 2, 12, 13, and 7–9. In addition, there are some elaborate numerical studies on this problem, cf. Ref. 1, and references therein. For the nonlinear problem, the existence for both hard sphere model and hard potentials with angular cut-off were obtained in Refs. 15 and 6, respectively. Furthermore, the stability of the boundary layer for the hard sphere model was proved when the Mach number of the far field is less than -1 in Ref. 16. In this stability analysis, the linear growth in the collision frequency is crucially used where exponential decay in time to the boundary layer can be proved by combining the energy method and a bootstrap argument. However, for the cut-off hard potentials, the sublinear growth in the collision frequency prevents the exponential decay both in space and time. Therefore, the analysis on the stability which is the topic in this paper is more subtle. By using some new recursive energy estimates, an algebraic decay rate will be proved for the convergence of the time evolutional solution to the boundary layer when Mach number of the far field is also less than -1.

From now on, F is assumed to be a function of time $t \in \mathbf{R}_+$, position $x \in \mathbf{R}$ and particle velocity $\xi=(\xi_1,\xi_2,\xi_3) \in \mathbf{R}^3$. Here, ξ_1 stands for the velocity component along the x axis. The boundary layer $F(x,\xi)$ is governed by the stationary Boltzmann equation

$$\xi_1 F_x = Q(F,F), \quad x>0,\ \xi \in \mathbf{R}^3,$$

$$F|_{x=0} = F_b(\xi), \quad \xi_1 > 0,\ (\xi_2,\xi_3) \in \mathbf{R}^2, \tag{1.1}$$

$$F \to M_\infty(\xi)(x \to \infty), \quad \xi \in \mathbf{R}^3,$$

where

$$M_\infty = M_{(\rho_\infty,u_\infty,T_\infty)}(\xi) = \frac{\rho_\infty}{(2\pi T_\infty)^{3/2}} \exp\left(-\frac{|\xi-u_\infty|^2}{2T_\infty}\right). \tag{1.2}$$

Here $\rho_\infty>0, u_\infty=(u_{\infty,1},u_{\infty,2},u_{\infty,3}) \in \mathbf{R}^3$ and $T_\infty>0$ represent the macroscopic density, velocity, and temperature, respectively, and the gas constant R is normalized to one. Up to a linear transformation in the ξ variable, $u_{\infty,2}$ and $u_{\infty,3}$ can be assumed to be zero. In this case, the sound speed and Mach number of the far field equilibrium state are given, respectively, by

$$c_\infty = \sqrt{\frac{5}{3}T_\infty}, \quad \mathcal{M}^\infty = \frac{u_{\infty,1}}{c_\infty}.$$

As usual, the collision operator Q which is a bilinear integral operator takes the form

$$Q(F,F) = \int \int_{\mathbf{R}^3\times\mathbf{S}^2} (F(\xi')F(\xi'_*) - F(\xi)F(\xi_*))q(V,\theta)\mathrm{d}\xi_*\mathrm{d}\omega,$$

where

$$\xi' = \xi - [(\xi-\xi_*)\cdot\omega]\omega, \quad \xi'_* = \xi_* + [(\xi-\xi_*)\cdot\omega]\omega$$

are the relations between velocities before and after an elastic collision by using the conservation of momentum and energy. Here the relative velocity $V=\xi-\xi_*$ and collision angle $\theta=\cos^{-1}(\langle V,\omega\rangle/|V|)$ with $\omega \in S^2$.

Set

$$F = M_\infty + M_\infty^{1/2} f.$$

Then the problem (1.1) is reduced to

$$\xi_1 f_x - Lf = h, \quad x > 0,\ \xi \in \mathbf{R}^3,$$

$$f|_{x=0} = b_0(\xi) = M_\infty^{-1/2}(F_b(\xi) - M_\infty), \quad \xi_1 > 0,\ (\xi_2, \xi_3) \in \mathbf{R}^2, \tag{1.3}$$

$$f \to 0\ (x \to \infty), \quad \xi \in \mathbf{R}^3,$$

where

$$h \equiv \Gamma(f,f) = M_\infty^{-1/2} Q(M_\infty^{1/2} f, M_\infty^{1/2} f), \quad Lf = M_\infty^{-1/2}\{Q(M_\infty, M_\infty^{1/2} f) + Q(M_\infty^{1/2} f, M_\infty)\}$$

are the nonlinear and linear parts in the collision operator.

It is known that the operator L can be written as, cf. Ref. 6,

$$L = -\nu(|\xi|) - K_1 + K_2,$$

where K_1 and K_2 are compact operators with kernels $k_1(\xi, \xi_*)$ and $k_2(\xi, \xi_*)$, respectively. For cut-off hard potentials, there exists $0 \leqslant \delta_1 < 1$ such that

$$k_1(\xi, \xi_*) \leqslant C(|\xi - \xi_*| + |\xi - \xi_*|^{-\delta_1}) \exp\left(-\frac{|\xi - u_\infty|^2}{4T_\infty} - \frac{|\xi_* - u_\infty|^2}{4T_\infty}\right),$$

$$k_2(\xi, \xi_*) \leqslant C|\xi - \xi_*|^{-1} \exp\left(-\frac{(|\xi - u_\infty|^2 - |\xi_* - u_\infty|^2)^2}{8T_\infty |\xi - \xi_*|^2} - \frac{|\xi - \xi_*|^2}{8T_\infty}\right).$$

Sometimes, we use the notation $K = -K_1 + K_2$.

In the following discussion, the same assumption on the collision kernel as in Ref. 6 for the existence of the boundary layer is imposed. That is, assume, cf. Ref. 14:

Assumption 1: There is $0 \leqslant \delta_1 < 1$ such that

$$0 \leqslant q(V, \theta) \leqslant c(|V| + |V|^{-\delta_1})|\cos\theta|.$$

Assumption 2: There exists a positive constant $c > 0$ such that

$$\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} e^{-|\xi_*|^2/2} q(\xi - \xi_*, \theta) \mathrm{d}\xi_* \mathrm{d}\omega \left(\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} e^{-|\xi_*|^2} q(\xi - \xi_*, \theta) \mathrm{d}\xi_* \mathrm{d}\omega\right)^{-1} \leqslant c.$$

Assumption 3: There are constants $0 < \beta_1 \leqslant \beta_2 \leqslant 1$ such that

$$c_1(1 + |\xi|)^{\beta_1} \leqslant \nu(\xi) \leqslant c_2(1 + |\xi|)^{\beta_2}.$$

For both hard sphere model and cut-off hard potentials, the results in Refs. 15 and 6 show that the existence of boundary layer solution depends on the Mach number $\mathcal{M}^\infty$ at $x = \infty$. When $\mathcal{M}^\infty \neq 0, \pm 1$, a solvability condition can be obtained implicitly with given co-dimensions of the manifold for the admissible boundary data $F_b(\xi)$. In particular, when $\mathcal{M}^\infty < -1$, the boundary layer solution exists as long as the boundary data $F_b(\xi)$ is close to the Maxwellian at $x = \infty$ because all the information at infinity in some sense goes into the layer.

To prove the existence of the boundary layers for the cut-off hard potentials, the following weight function $\sigma(x, \xi)$ is introduced in Ref. 6. Let $\eta: [0, \infty) \to \mathbf{R}$ be a smooth nonincreasing function satisfying $\eta(s) = 1$, for $s \leqslant 1$, $\eta(s) = 0$ for $s \geqslant 2$, and $0 \leqslant \eta \leqslant 1$. The weight function to cope with the sublinear growth in the collision frequency is

$$\sigma(x,\xi) = 5(\delta x + l)^{2/(3-\beta_1)}\left(1 - \eta\left(\frac{\delta x + l}{(1+|\xi - u_\infty|)^{3-\beta_1}}\right)\right)$$
$$+\left(\frac{\delta x + l}{(1+|\xi - u_\infty|)^{1-\beta_1}} + 3|\xi - u_\infty|^2\right)\eta\left(\frac{\delta x + l}{(1+|\xi - u_\infty|)^{3-\beta_1}}\right),$$

for some large positive constant l and a small positive constant δ. For later use, set

$$\mathbf{W}_\beta(\xi) = (1+|\xi|)^{-\beta}(M_{[1,u_\infty,T_\infty]})^{1/2}. \tag{1.4}$$

In the study on the nonlinear stability of the boundary layer for the hard sphere model when $\mathcal{M}^\infty < -1$ given in Ref. 16, the perturbation decays exponentially in time because the collision frequency has linear growth in the velocity. However, for the hard potentials with angular cutoff, the convergence rate will be shown to be algebraic depending on the spatial decay of the initial data.

In what follows, we will use the following norm for the perturbation of the layer in the time evolution equation,

$$[[f]]_\beta = \sup_{x,\xi} \sigma_x^{1/2}(1+|\xi|)^\beta |f(x,\xi)|.$$

Consider the initial boundary value problem,

$$\begin{gathered} F_t + \xi_1 F_x = Q(F,F), \quad t>0, x>0,\ \xi \in \mathbf{R}^3, \\ F|_{t=0} = F_0(x,\xi), \quad x>0,\ \xi \in \mathbf{R}^3, \\ F|_{x=0} = F_b(\xi), \quad t>0, \xi_1>0,\ (\xi_2,\xi_3) \in \mathbf{R}^2, \\ F \to M_\infty(\xi),\ (x \to \infty), \quad t>0,\ \xi \in \mathbf{R}^3. \end{gathered} \tag{1.5}$$

The main result in this paper can be stated as follows.

Theorem 1.1: *When the Mach number $\mathcal{M}^\infty < -1$, if the boundary data satisfy*

$$|F_b(\xi) - M_\infty(\xi)| \leqslant \epsilon_0 \sigma_x^{-1/2}(0,\xi) e^{-\epsilon\sigma(0,\xi)} \mathbf{W}_\beta(\xi), \quad \xi \in \mathbf{R}^3_+, \quad \beta > \tfrac{5}{2},$$

where the weight function $\mathbf{W}_\beta$ and $\sigma(x,\xi)$ are defined above and ϵ_0 is a sufficiently small positive constant, then there exists a boundary layer solution $\bar{F}(x,\xi)$ to (1.1) *obtained in Ref.* 6. *For the initial boundary value problem* (1.5), *if the initial data satisfy*

$$\|\sigma_x^{-1} e^{\epsilon\sigma(x,\xi)} M_\infty^{-1/2}(F_0 - \bar{F})\|_{L^2_{x,\xi}} + [[e^{\epsilon\sigma(x,\xi)} M_\infty^{-1/2}(F_0 - \bar{F})]]_\beta < \epsilon_1, \quad \beta > 3 - \frac{\beta_1}{2}, \tag{1.6}$$

where $\epsilon_1 > 0$ is a sufficiently small constant, and l satisfies $l \geqslant \epsilon^{-3+\beta_1}$, then there exists a unique solution $F(t,x,\xi)$ such that

$$[[e^{\epsilon\sigma(x,\xi)} M_\infty^{-1/2}(F - \bar{F})]]_\beta \leqslant C\epsilon_1 (1+t)^{-3/2}.$$

This implies that the perturbation of the boundary layer converges to zero in time with an algebraic rate $(1+t)^{-3/2}$, that is, the boundary layer solution is nonlinearly stable.

Remark 1.2: If we impose faster spatial decay on the initial data, then faster time decay on the perturbation can be obtained. More precisely, for $m \geqslant 2$, if we replace (1.6) by

$$\|\sigma_x^{-m/2} e^{\epsilon\sigma(x,\xi)} M_\infty^{-1/2}(F_0 - \bar{F})\|_{L^2_{x,\xi}} + [[e^{\epsilon\sigma(x,\xi)} M_\infty^{-1/2}(F_0 - \bar{F})]]_\beta < \epsilon_1, \quad \text{for } \beta > \frac{m+4}{2} - \frac{m-1}{2}\beta_1,$$

then similar analysis gives that the decay rate as $(1+t)^{-(m+1)/2}$.

The rest of the paper is organized as follows. In Sec. II, we will recall some lemmas from Ref. 6 and present some basic lemmas for the later stability analysis. In Sec. III, we will consider the linearized equation and derive some recursive energy estimates using various weight functions. Based on this, the time decay estimate of perturbation is proved by a bootstrap argument in the last section.

II. PRELIMINARIES

For later use, we introduce some notations $\Theta=(1-\beta_1)/(3-\beta_1)$ and $\tilde{\xi}=\xi-u_\infty$. c and C are generic positive numbers. For the weight function $\sigma(x,\xi)$ defined in the previous section, we have the following estimates on its derivative by straightforward calculation.

Lemma 2.1: There exists a constant $c>0$ such that

$$\sigma_x(x,\xi)=\begin{cases}\delta(1+|\tilde{\xi}|)^{-1+\beta_1} & (x,\xi)\in\Omega_1\\ c\,\delta((\delta x+l)^{-\Theta}+|\tilde{\xi}|^{-1+\beta_1}) & (x,\xi)\in\Omega_2\\ \dfrac{10\delta}{3-\beta_1}(\delta x+l)^{-\Theta} & (x,\xi)\in\Omega_3,\end{cases}$$

where

$$\Omega_1=\{(x,\xi)|\,\delta x+l<(1+|\tilde{\xi}|)^{3-\beta_1}\},\quad \Omega_3=\{(x,\xi)|\,\delta x+l\geqslant 2(1+|\tilde{\xi}|)^{3-\beta_1}\},$$

$$\Omega_2=\{(x,\xi)|(1+|\tilde{\xi}|)^{3-\beta_1}\leqslant\delta x+l<2(1+|\tilde{\xi}|)^{3-\beta_1}\}.$$

Furthermore,

$$|\sigma_{xx}(x,\xi)|\leqslant\begin{cases}0 & (x,\xi)\in\Omega_1\\ c(\delta x+l)^{-\Theta-1} & (x,\xi)\in\Omega_2\cup\Omega_3.\end{cases}$$

It is well known that the collision operator Q has five collision invariants

$$\varrho_0=1,\quad \varrho_i=\xi(i=1,2,3),\quad \varrho_4=|\xi|^2,$$

satisfying

$$\langle\varrho_\alpha,Q(F,F)\rangle=0,\quad \alpha=0,1,\ldots,4,$$

for any distribution function F. Here $\langle .,.\rangle$ is the inner product in L^2_ξ. The null space of the linearized collision operator L in the space L^2_ξ is

$$\mathbf{N}=\mathrm{span}\{M_\infty^{1/2}\varrho_\alpha,\alpha=0,1,2,3,4\}=\mathrm{span}\{\psi_\alpha,\alpha=0,1,2,3,4\}.$$

In what follows, $\mathbf{N}^\perp$ denotes the orthogonal complement of $\mathbf{N}$ in L^2_ξ. With these notations, the dissipation of the modified linearized collision operator on $\mathbf{N}^\perp$ is given as follows.

Lemma 2.2: There is constant $\epsilon_2>0$ such that for $0<\epsilon<\epsilon_2$ and $g\in\mathbf{N}^\perp$,

$$\langle g,\sigma_x^{-m/2}e^{\epsilon\sigma}Le^{-\epsilon\sigma}\sigma_x^{m/2}g\rangle\leqslant-\nu_1\langle\nu(|\xi|)g,g\rangle,\quad m=-1,0,1,2,$$

for some positive constant $\nu_1=\nu_1(\epsilon_2)$.

Proof: Similar to Lemma 2.2 in Ref. 6, we only need to estimate the term related to the operator K_2 as follows. It is because $L=-\nu(|\xi|)-K_1+K_2$ and $\nu(|\xi|)$ commutes with the multiple operator and the estimation on the terms related to K_1 is simpler. Set

$$s(\epsilon,\xi,\xi_*)=\sigma_x^{-m/2}(x,\xi)\exp\left(-\frac{1}{8T_\infty}\frac{(|\tilde{\xi}|^2+|\tilde{\xi}_*|^2)^2}{|\xi-\xi_*|^2}-\frac{1}{8T_\infty}|\xi-\xi_*|^2\right)$$
$$\times(\exp[\epsilon(\sigma(x,\xi)-\sigma(x,\xi_*))]-1)\sigma_x^{m/2}(x,\xi_*).$$

It suffices to show that

$$\sup_{\xi,\xi_*} s(\epsilon,\xi,\xi_*)\to 0 \quad as\ \epsilon\to 0, \tag{2.1}$$

because of the classical dissipative effect of L on the functions in $\mathbf{N}^\perp$. (2.1) can be proved by considering the cases when (x,ξ) in different $\Omega_i, i=1,2,3$. For illustration, we only consider two cases for $m=-1$ because the other cases can be discussed similarly.

Case 1: When (x,ξ) *and* $(x,\xi_*)\in\Omega_3$, $\sigma_x(x,\xi)=\sigma_x(x,\xi_*)=[10\delta/(3-\beta_1)](\delta x+l)^{-\Theta}$. In this case, we have

$$|\sigma(x,\xi)-\sigma(x,\xi_*)|\leqslant c\|\tilde{\xi}|^2-|\tilde{\xi}_*|^2|,$$

which implies (2.1).

Case 2: When $(x,\xi)\in\Omega_1$ *and* $(x,\xi_*)\in\Omega_3, \sigma_x(x,\xi)^{-1}\leqslant c(1+|\tilde{\xi}|)^{1-\beta_1}+(1+|\xi-\xi_*|)^{1-\beta_1})$ and $|\sigma(x,\xi)-\sigma(x,\xi_*)|\leqslant c\|\tilde{\xi}|^2-|\tilde{\xi}_*|^2|$. In this case, we have

$$s(\epsilon,\xi,\xi_*)\leqslant\exp\left(-\frac{1}{16T_\infty}\frac{(|\tilde{\xi}|^2-|\tilde{\xi}_*|^2)^2}{|\xi-\xi|^2}-\frac{1}{16T_\infty}|\xi-\xi_*|^2\right)(\exp[\epsilon\|\tilde{\xi}|^2-|\tilde{\xi}_*|^2|]-1),$$

which also implies (2.1).

This completes the proof of the lemma.

To apply the energy method, define the following orthogonal projections on the macroscopic and microscopic subspaces:

$$\mathbf{P}_0:L^2_\xi\to\mathbf{N},\quad \mathbf{P}_1:L^2_\xi\to\mathbf{N}^\perp.$$

Notice that the macroscopic convection $A=\mathbf{P}_0\xi_1\mathbf{P}_0$ is a linear bounded self-adjoint operator on $\mathbf{N}$. It is straightforward to show that A has five eigenvalues

$$\lambda_1=u_{\infty,1}-c_\infty,\quad \lambda_i=u_{\infty,1}(i=2,3,4),\quad \lambda_5=u_{\infty,1}+c_\infty.$$

Thus, A is negative definite on $\mathbf{N}$ when $\mathcal{M}^\infty<-1$. For later use, denote

$$\phi_0=\mathbf{P}_0\phi=\sum_{j=0}^{4}b_j\psi_j=\sum_{j=0}^{4}\langle\phi,\psi_j\rangle\psi_j,\quad \phi_1=\mathbf{P}_1\phi=\phi-\mathbf{P}_0\phi.$$

The following lemma is from Ref. 6 and we include it here for the self-containess of the paper.

Lemma 2.3: Assume $\mathcal{M}^\infty<-1$, *and the constant* l *in* $\sigma(x,\xi)$ *is sufficiently large. Then there is* $\nu_2>0$ *such that for any* $\phi\in L^2_\xi$,

$$\int_{|\tilde{\xi}|^{3-\beta_1}\leqslant l/2}\phi\mathbf{P}_0\xi_1\mathbf{P}_0\phi\mathrm{d}\xi\leqslant-\nu_2\int_{\mathbf{R}^3}^{s}\phi_0^2\mathrm{d}\xi.$$

Denote $L_\epsilon=e^{\epsilon\sigma}Le^{-\epsilon\sigma}$. Lemmas 2.2 and 2.3 imply the following lemma.

Lemma 2.4: Assume that $\mathcal{M}^\infty<-1$, ϵ *is sufficiently small, and* $l\geqslant\epsilon^{-1}$. *Then there exist* $c,C>0$ *such that*

$$-\langle\sigma_x\xi_1\phi,\phi\rangle\geqslant\frac{C\nu_2}{4}\langle(\delta x+l)^{-\Theta/2}\phi_0,(\delta x+l)^{-\Theta/2}\phi_0\rangle-c\langle\nu(\xi)\phi_1,\phi_1\rangle,$$

$$-\langle L_\epsilon \phi, \phi\rangle \geqslant -c\epsilon^2\langle(\delta x+l)^{-\Theta/2}\phi_0,(\delta x+l)^{-\Theta/2}\phi_0\rangle + C\nu_2\langle\nu(\xi)\phi_1,\phi_1\rangle.$$

Furthermore,

$$-\varepsilon\langle\sigma_x\xi_1\phi,\phi\rangle - \langle L_\epsilon\phi,\phi\rangle \geqslant \frac{C\nu_2\epsilon}{8}\langle(\delta x+l)^{-\Theta/2}\phi,(\delta+l)^{-\Theta/2}\phi\rangle.$$

The following lemma is also needed in the convergence rates analysis.

Lemma 2.5: When $\mathcal{M}^\infty<-1$, ϵ *is sufficiently small, and* $l\geqslant\epsilon^{-3+\beta_1}$, *there exists a constant* $c>0$ *such that for any* ϕ,

$$\left|\int_{\mathbf{R}^3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi^2\mathrm{d}\xi\right| \leqslant c\epsilon^2(\delta x+l)^{-\Theta}\langle\phi_0,\phi_0\rangle + c\epsilon^{4/3}\langle\nu(|\xi|)\phi_1,\phi_1\rangle.$$

Proof: The integral on the left-hand side of the above-presented estimate can be discussed as follows. First, notice that by Lemma 2.1,

$$\left|\frac{\sigma_{xx}}{\sigma_x}\right| \leqslant \begin{cases} 0 & (x,\xi)\in\Omega_1 \\ c(\delta x+l)^{-1}\leqslant c(\delta x+l)^{-1+\Theta}\sigma_x & (x,\xi)\in\Omega_2\cup\Omega_3. \end{cases}$$

Then, for $l\geqslant\epsilon^{3-\beta_1}$, we have

$$\begin{aligned}\left|\int_{\mathbf{R}^3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi_0^2\mathrm{d}\xi\right| &= \left|\int_{\Omega_2\cup\Omega_3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi_0^2\mathrm{d}\xi\right| \leqslant c(\delta x+l)^{-1}\langle|\xi|\phi_0,\phi_0\rangle \\ &\leqslant c\epsilon^2(\delta x+l)^{-\Theta}\langle\phi_0,\phi_0\rangle. \end{aligned} \tag{2.2}$$

Thus,

$$\begin{aligned}\int_{\mathbf{R}^3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi_0^2\mathrm{d}\xi &\leqslant 2\int_{\mathbf{R}^3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi_0^2\mathrm{d}\xi + \ +2\int_{\mathbf{R}^3}\frac{\sigma_{xx}}{\sigma_x}\xi_1\phi_0^2\mathrm{d}\xi \\ &\leqslant c\epsilon^2(\delta x+l)^{-\Theta}\langle\phi_0,\phi_0\rangle + c(\delta x+l)^{-1+\Theta}\langle\nu(|\xi|)\phi_1,\phi_1\rangle \\ &\leqslant c\epsilon^2(\delta x+l)^{-\Theta}\langle\phi_0,\phi_0\rangle + c\epsilon^{4/3}\langle\nu(|\xi|)\phi_1,\phi_1\rangle.\end{aligned}$$

Here we have used $|\sigma_x\xi_1|\leqslant c\nu(|\xi|)$, $-1\leqslant-1+\Theta<-\frac{2}{3}$ for $0<\beta_1\leqslant1$, $(\delta x+l)^{-1+\Theta}\leqslant\epsilon^{2(3-\beta_1)/3}\leqslant\epsilon^{4/3}$ when $l\geqslant\epsilon^{3-\beta_1}$. And this completes the proof of the lemma.

Denote $\widetilde{K}=e^{\epsilon\sigma}Ke^{-\epsilon\sigma}$. The following properties of the operator $\widetilde{K}$ are also proved in Ref. 6.

Lemma 2.6: When ϵ *is sufficiently small, then* $\widetilde{K}$ *satisfies*:

1. $\sigma_x^{1/2}\widetilde{K}\sigma_x^{-1/2}$ *is a bounded operator from* L^2_ξ *to itself.*
2. $\sigma_x^{1/2}\widetilde{K}\sigma_x^{-1/2}$ *is a bounded operator from* L^2_ξ *to* L^∞_ξ.
3. $[[\widetilde{K}h]]_\beta\leqslant c[[h]]_{\beta-1}$, *for* $\beta\in\mathbf{R}$.

We now recall some property on the nonlinear term $\Gamma(g,h)$ from Lemma 4.5 in Ref. 6.

Lemma 2.7: The projection of $\Gamma(g,h)$ *on the null space of L vanishes and there exists a positive constant c such that, for all* $(x,\xi)\in\mathbf{R}\times\mathbf{R}^3$,

$$|\sigma_x^{1/2}\nu^{-1}(e^{\epsilon\sigma}g,e^{-\epsilon\sigma}h)(x,\xi)| \leqslant C(1+|\xi|)^{-\beta}\exp(-\epsilon^2(\delta x+l)^{2/(3-\beta_1)})[[g]]_\beta[[h]]_\beta$$

for any $\beta>(1-\beta_1)/2$ *and sufficiently small constant* $\epsilon>0$.

The last lemma in this section is about how to transfer the decay in space to the decay in time through some recursive relations in terms of energy inequalities. This lemma is used to obtain the time convergence rate for the solution to the initial boundary value problem (1.5).

Lemma 2.8: Suppose that y *and* $\Xi(t,x,\xi)\geqslant1$ *are functions of* (t,x,ξ). *Define*

$$\mathbf{I}_m(t) = \int_{\mathbf{R}\times\mathbf{R}^3} \Xi(t,x,\xi)^m y(t,x,\xi)^2 \mathrm{d}x\,\mathrm{d}\xi \quad \textit{for all } m \geqslant -1.$$

If there exists a positive constant ϵ *such that*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_{-1} \leqslant 0, \cdots, \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_{m-1} + \epsilon\mathbf{I}_{m-2} \leqslant 0, \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_m + \epsilon\mathbf{I}_{m-1} \leqslant 0, \tag{2.3}$$

then there exists constant $c_{m,\epsilon}$, *for* $-1 \leqslant n \leqslant m$, *we have*

$$(1+t)^{m-n}\mathbf{I}_n(t) \leqslant c_{m,\epsilon}\mathbf{I}_m(0). \tag{2.4}$$

Proof: By definition, notice that $\mathbf{I}_{-1}(t) \leqslant \mathbf{I}_0(t) \leqslant \cdots \leqslant \mathbf{I}_m(t)$ *for all* $t \geqslant 0$ because $\Xi \geqslant 1$. Define

$$F(t) = \frac{m!\,\epsilon}{(m+1)!}(1+t)^{m+1}\mathbf{I}_{-1} + \frac{m!}{m!}(1+t)^m\mathbf{I}_0 + \cdots + \frac{m!}{1!}\epsilon^{-m+1}(1+t)\mathbf{I}_{m-1} + \frac{m!}{0!}\epsilon^{-m}\mathbf{I}_m.$$

From (2.3), it is straightforward to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = \frac{(1+t)^{m+1}\epsilon}{m+1}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_{-1} + (1+t)^m\left[\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_0 + \epsilon\mathbf{I}_{-1}\right] + \cdots + m!\,\epsilon^{-m}\left[\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_m + \epsilon\mathbf{I}_{m-1}\right] \leqslant 0.$$

Thus, $F(t) \leqslant F(0)$ which implies that there exists a constant $c_{m,\epsilon}$ such that

$$(1+t)^{m-n}\mathbf{I}_n(t) \leqslant c_{m,\epsilon}\mathbf{I}_m(0) \quad \textit{for } -1 \leqslant n \leqslant m.$$

The proof of the lemma is then completed.

III. LINEARIZED PROBLEM

The purpose of this section is to obtain some time decay estimate on the solutions to the linearized problem. Recall $F = M_\infty + M_\infty^{1/2} f$, and let $f = e^{-\epsilon\sigma} g$. Then the problem (1.5)

$$\begin{aligned}
&g_t + \xi_1 g_x - \epsilon\sigma_x\xi_1 g - L_\epsilon g = e^{\epsilon\sigma}\Gamma(e^{-\epsilon\sigma}g, e^{-\epsilon\sigma}g), \quad t>0,\ x>0,\ \xi\in\mathbf{R}^3,\\
&g|_{t=0} = g_0(x,\xi) = e^{\epsilon\sigma}M_\infty^{-1/2}(F_0 - M_\infty), \quad x>0,\ \xi\in\mathbf{R}^3,\\
&g|_{x=0} = b_0(\xi) = e^{\epsilon\sigma}M_\infty^{-1/2}(F_b - M_\infty), \quad t>0,\ \xi_1>0,\ (\xi_2,\xi_3)\in\mathbf{R}^2,\\
&g \to 0 (x\to\infty), \quad t>0,\ \xi\in\mathbf{R}^3.
\end{aligned} \tag{3.1}$$

Denote the corresponding stationary boundary layer solution to (3.1) by $\bar{g}$ and let the initial g_0 be a small perturbation of $\bar{g}$. Then the problem on the perturbation $\tilde{g}$ is

$$\begin{aligned}
&\tilde{g}_t + \xi_1\tilde{g}_x - \epsilon\sigma_x\xi_1\tilde{g} - L_\epsilon\tilde{g} = e^{\epsilon\sigma}\{\bar{L}_\epsilon\tilde{g} + \Gamma(e^{-\epsilon\sigma}\tilde{g}, e^{-\epsilon\sigma}\tilde{g})\}, \quad t>0,\ x>0,\ \xi\in\mathbf{R}^3,\\
&\tilde{g}|_{t=0} = \tilde{g}_0 = e^{\epsilon\sigma}M_\infty^{-\frac{1}{2}}(F_0 - \bar{F}), \quad x>0,\ \xi\in\mathbf{R}^3,\\
&\tilde{g}|_{x=0} = 0(\xi_1>0), \quad t>0,\ (\xi_2,\xi_3)\in\mathbf{R}^2,\\
&\tilde{g} \to 0 (x\to\infty), \quad t>0,\ \xi\in\mathbf{R}^3.
\end{aligned} \tag{3.2}$$

here $\tilde{g} = g - \bar{g}$, $\tilde{g}_0 = g_0 - \bar{g}$ and $\bar{L}_\epsilon = 2\Gamma(e^{-\epsilon\sigma}\bar{g}, e^{-\epsilon\sigma}\tilde{g})$.

We are going to derive some energy estimates on the solution to the corresponding linearized equation using several weight functions. Let $S(t)$ be the solution operator of the linear problem:

$$h_t + \xi_1 h_x - \varepsilon\sigma_x\xi_1 h - L_\epsilon h = 0, \quad t > 0,\ x > 0,\ \xi \in \mathbf{R}^3,$$

$$h\big|_{x=0} = 0(\xi_1 > 0), h \to 0(x \to \infty), \quad t > 0,\ \xi \in \mathbf{R}^3, \tag{3.3}$$

$$h\big|_{t=0} = h_0(x,\xi), \quad x > 0,\ \xi \in \mathbf{R}^3.$$

That is, $h(t)=S(t)h_0(x,\xi)$.

For the hard sphere model, the solution operator $S(t)$ has exponential decay property when the Mach number $\mathcal{M}^\infty$ is less than -1. For the cut-off hard potentials, we will use the spatial-temporal estimates in Lemma 2.8 to derive an algebraic decay.

In what follows, $(\cdot,\cdot)$ denotes the inner product of $L^2_{x,\xi}$ with norm $\|\cdot\|=\|\cdot\|_{L^2_{x,\xi}}$. The inner product corresponding to the boundary value is $<\cdot,\cdot>_-=(\cdot,\cdot)_{L^2_{x,\xi}(\xi_1>0)}$.

Set

$$\rho^{-1} = \sigma_x^{1/2}h, \quad \rho^0 = h, \quad \rho^1 = \sigma_x^{-1/2}h, \quad \rho^2 = \sigma_x^{-1}h.$$

It is straightforward to derive the following equations for $\rho^i, i=-1,\dots,2$:

$$\begin{aligned}
&\rho_t^{-1} + \xi_1\rho_x^{-1} - \frac{\sigma_{xx}}{2\sigma_x}\xi_1\rho^{-1} - \epsilon\sigma_x\xi_1\rho^{-1} - \sigma_x^{1/2}L_\epsilon\sigma_x^{-1/2}\rho^{-1} = 0,\\
&\rho_t^0 + \xi_1\rho_x^0 - \epsilon\sigma_x\xi_1\rho^0 - L_\epsilon\rho^0 = 0,\\
&\rho_t^1 + \xi_1\rho_x^1 + \frac{\sigma_{xx}}{2\sigma_x}\xi_1\rho^1 - \epsilon\sigma_x\xi_1\rho^1 - \sigma_x^{-1/2}L_\epsilon\sigma_x^{1/2}\rho^1 = 0,\\
&\rho_t^2 + \xi_1 j_x^2 + \frac{\sigma_{xx}}{\sigma_x}\xi_1\rho^2 - \epsilon\sigma_x\xi_1\rho^2 - \sigma_x^{-1}L_\epsilon\sigma_x\rho^2 = 0.
\end{aligned} \tag{3.4}$$

By multiplying $(3.4)_1$ by ρ^{-1} and integrating it over $\mathbf{R}^+\times\mathbf{R}^3$, when ϵ is sufficiently small, Lemmas 2.4 and 2.5 give

$$(\rho^{-1},\rho^{-1})_t + \langle|\xi_1|\rho^{-1},\rho^{-1}\rangle_- + c\epsilon((\delta x+l)^{-\Theta/2}\rho^{-1}, \quad (\delta x+l)^{-\frac{\Theta}{2}}\rho^{-1}) \leqslant 0. \tag{3.5}$$

Similarly, for sufficiently small ϵ, we have

$$\begin{aligned}
&(\rho^0,\rho^0)_t + \langle|\xi_1|\rho^0,\rho^0\rangle_- + c\epsilon((\delta x+l)^{-\Theta/2}\rho^0, \quad (\delta x+l)^{-\Theta/2}\rho^0) \leqslant 0,\\
&(\rho^1,\rho^1)_t + \langle|\xi_1|\rho^1,\rho^1\rangle_- + c\epsilon((\delta x+l)^{-\Theta/2}\rho^1, \quad (\delta x+l)^{-\Theta/2}\rho^1) \leqslant 0,\\
&(\rho^2,\rho^2)_t + \langle|\xi_1|\rho^2,\rho^2\rangle_- + c\epsilon((\delta x+l)^{-\Theta/2}\rho^2, \quad (\delta x+l)^{-\Theta/2}\rho^2) \leqslant 0.
\end{aligned}$$

Since $\sigma_x(x,\xi)\leqslant(\delta x+l)^{-\Theta}$ and $\langle|\xi_1|\rho^i,\rho^i\rangle_-\geqslant 0$ *for* $i=-1,\dots,2$, by the definition of ρ^i, $i=-1,0,1,2$, we have

$$\begin{aligned}
&(\rho^{-1},\rho^{-1})_t \leqslant 0, \quad (\rho^0,\rho^0)_t + c\epsilon(\rho^{-1}, \quad \rho^{-1}) \leqslant 0,\\
&(\rho^1,\rho^1)_t + c\epsilon(\rho^0,\rho^0) \leqslant 0, \quad (\rho^2,\rho^2)_t + c\epsilon(\rho^1,\rho^1) \leqslant 0.
\end{aligned}$$

Corresponding to Lemma 2.8, if we choose $y=\rho^{-1}, \Xi=\sigma_x^{-1/2}, m=2$ and $n=-1$, then

$$(\rho^{-1},\rho^{-1})(t) \leqslant c_\epsilon(1+t)^{-3}(\rho^2,\rho^2)(0),$$

that is,

$$\|\sigma_x^{1/2}S(t)h_0\|_{L^2_{x,\xi}} \leqslant c_\epsilon(1+t)^{-\frac{3}{2}}\|\sigma_x^{-1}h_0\|_{L^2_{x,\xi}}. \tag{3.6}$$

Based on this energy estimate, the following decay estimate on the solution operator $S(t)$ in $[[\cdot]]_\beta$ norm is essential to obtain the global existence and convergence rate for the nonlinear problem through the fixed point theorem in Sec. IV. That is, we want to show that for some $\beta > 0$,

$$[[S(t)h_0]]_\beta \leqslant c(1+t)^{-3/2}\{[[h_0]]_\beta + \|\sigma_x^{-1}h_0\|_{L^2_{x,\xi}}\}, \tag{3.7}$$

where $[[\cdot]]_\beta$ is defined in Sec. I. To prove (3.7), we consider a simpler linear solution operator. Let $S_0(t)$ be the solution operator of

$$\begin{gathered} h_t + \xi_1 h_x - \epsilon\sigma_x\xi_1 h + \nu(\xi)h = 0, \quad t>0,\ x>0,\ \xi\in\mathbf{R}^3, \\ h|_{t=0} = h_0(x,\xi), \quad x>0,\ \xi\in\mathbf{R}^3, \\ h|_{x=0} = 0, \quad t>0,\ \xi_1>0,\ (\xi_2,\xi_3)\in\mathbf{R}^2, \\ h\to 0 (x\to\infty), \quad t>0,\ \xi\in\mathbf{R}^3. \end{gathered} \tag{3.8}$$

It is straightforward to check that the solution to the above-presented linear initial boundary value problem has the following explicit expression:

$$h(x,t) = S_0(t)h_0 = h_0(x-\xi_1 t,\xi)\chi(x-\xi_1 t)\exp\left(-\int_0^t [\nu(\xi) - \epsilon\sigma_x(x-\xi_1(t-s),\xi)\xi_1]\mathrm{d}s\right),$$

where $\chi(y)$ is the characteristic function for $y>0$. By using this expression and the positive lower bound of the collision frequency $\nu(|\xi|)$, the following lemma gives the exponential decay estimate on the operator $S_0(t)$.

Lemma 3.1: For $S_0(t)$ defined earlier, there exist positive constants C and κ such that

$$\|S_0(t)h_0\|_X \leqslant Ce^{-\kappa t}\|h_0\|_X, \tag{3.9}$$

where the norm in X can be $[[\cdot]]_\beta$ and $\|\cdot\|_{L^2_{x,\xi}}$.

Proof: We only prove (3.9) for the norm $[[\cdot]]_\beta$, and the case for the norm $\|\cdot\|_{L^2_{x,\xi}}$ can be proved similarly.

For δ being sufficiently small, $|\sigma_x\xi_1| \leqslant \nu(|\xi|)$ and $\nu(|\xi|)\geqslant \nu_0$. Thus, there exists a positive constant κ such that

$$|(1+|\xi|)^\beta\sigma_x^{1/2}(x,\xi)h(t,x,\xi)| \leqslant H(t,x,\xi)e^{-\kappa t}[[h_0]]_\beta,$$

where $H(x,t,\xi)=\sigma_x^{1/2}(x,\xi)\sigma_x^{-1/2}(x,-\xi_1 t,\xi)e^{-\nu(|\xi|)t/4}$. We now show that there exists a constant c such that $H(t,x,\xi)\leqslant c$ by considering the following two cases.

Case 1: When $(x,\xi)\in\Omega_1\cup\Omega_2$, if $(x-\xi_1 t,\xi)\in\Omega_1\cup\Omega_2$, we have both $\sigma_x(x,\xi)\sim(1+|\widetilde{\xi}|)^{-1+\beta_1}$ and $\sigma_x^{-1}(x-\xi_1 t,\xi)\sim(1+|\widetilde{\xi}|)^{1-\beta_1}$. Thus, it is obvious that there exists a constant c such that $H(t,x,\xi)\leqslant c$. On the other hand, if $(x-\xi_1 t,\xi)\in\Omega_3$, we have $\sigma_x(x,\xi)\leqslant c(\delta x+l)^{-\Theta}$ and $\sigma_x(x-\xi_1 t,\xi)=10\delta/(3-\beta_1)(\delta x+l)^{-\Theta}$ which also immediately implies $H(t,x,\xi)\leqslant c$ for some c.

Case 2: For $(x,\xi)\in\Omega_3$. If $(x-\xi_1 t,\xi)\in\Omega_1$, then $|\xi_1|t=|(\delta x+l)-(\delta x+l-\xi_1 t)|\geqslant(1+|\widetilde{\xi}|)^{3-\beta_1}\geqslant c(1+|\xi|)^{3-\beta_1}$. Thus, for $\xi_1\neq 0$,

$$\nu(|\xi|)t \geqslant c(1+|\xi|)^{\beta_1}t \geqslant c(1+|\xi|)^{\beta_1}\frac{(1+|\xi|)^{3-\beta_1}}{|\xi_1|} \geqslant c(1+|\xi|)^2.$$

This implies that

$$H(t,x,\xi) \leqslant c(1+|\xi|)^{(1-\beta_1)/2} e^{-c(1+|\xi|)^2} \leqslant c.$$

If $(x-\xi_1 t,\xi) \in \Omega_2 \cup \Omega_3$, then $\sigma_x^{-1}(x-\xi_1 t,\xi) \leqslant c(\delta(x-\xi_1 t)+l)^{\Theta}$. Since $\sigma_x(x,\xi) = 10\delta/(3-\beta_1)(\delta x + l)^{-\Theta}$. Hence, it is straightforward to see that there exists constant c such that $H(t,x,\xi) \leqslant c$ by using the decay property of $e^{-\nu(|\xi|)^t/4}$ and $\beta_1 > 0$. This completes the proof of the lemma.

As in Ref. 16, from (3.3) and (3.8), we can rewrite $S(t)$ in terms of $S_0(t)$ and $\tilde{K} = e^{\epsilon\sigma} K e^{-\epsilon\sigma}$:

$$\begin{aligned} S(t)h_0 &= S_0(t)h_0 + \int_0^t S_0(t-s)\tilde{K}S(s)h_0 \mathrm{d}s \\ &= \sum_{j=0}^{m-1} I_j(t) + J_m(t), \end{aligned}$$

$$I_0(t) = S_0(t)h_0,$$

$$I_j(t) = \int_0^t S_0(t-s)\tilde{K}I_{j-1}(s)ds = S_0\tilde{K} * I_{j-1},$$

$$J_m(t) = \underbrace{(S_0\tilde{K}) * (S_0\tilde{K}) * \cdots * (S_0\tilde{K})}_{m} * h,$$

with $h = S(t)h_0$. Here, the notation $*$ stands for the convolution in t. By using the estimate (3.9) and the regularizing property of the compact operator $\tilde{K}$ given in Lemma 2.6, we have for $\beta \geqslant j \geqslant 0$, cf. Ref. 16,

$$[[I_j(t)]]_\beta \leqslant C_j e^{-\kappa t}[[h_0]]_\beta.$$

The estimate on J_m given in the following is more complicated and can be obtained by a bootstrap argument as in Ref. 16 for the hard sphere model.

Lemma 3.2: For $\beta \geqslant 0$, there exists a constant C such that

$$[[J_{\beta+3}(t)]]_\beta \leqslant C(1+t)^{-3/2}\|\sigma_x^{-1}h_0\|_{L_x^\infty(L_\xi^2)}.$$

Proof: The following proof mainly follows from the proof of Lemma 2.2 in Ref. 16 with K replaced by $\sigma_x^{1/2}\tilde{K}\sigma_x^{-1/2}$ and the norm $\|\cdot\|_\beta$ replaced by $[[\cdot]]_\beta$. Moreover, the exponential decay for the hard sphere model in Ref. 16 becomes the algebraic decay.

By using the property of $\sigma_x^{1/2}\tilde{K}\sigma_x^{-1/2}$ in Lemma 2.6 and (3.9), it is straightforward to have

$$[[J_{\beta+3}(t)]]_\beta \leqslant \frac{C}{\beta!}\int_0^t (t-\tau)^\beta e^{-\kappa\tau}\|J_2\|_{L_{x,\xi}^2}(\tau)\mathrm{d}\tau, \tag{3.10}$$

where

$$J_2(t) = \sigma_x^{1/2}(S_0\tilde{K}) * (S_0\tilde{K}) * h = S_0 * \bar{J}, \tag{3.11}$$

with

$$\bar{J} = \sigma_x^{1/2}\tilde{K}S_0\tilde{K} * h = \int_0^t \bar{J}_0(t-s,s)\mathrm{d}s.$$

$\bar{J}_0(t,s)$ can be estimated as follows by using the properties of the operator $\sigma_x^{1/2}\tilde{K}\sigma_x^{-1/2}$. In fact, since

$$\bar{J}_0(t,s) = \sigma_x^{1/2}\widetilde{K}S_0(t)\widetilde{K}h(s) = \int_{\mathbf{R}^3\times\mathbf{R}^3} \sigma_x^{1/2}\widetilde{K}(\xi,\xi')\widetilde{K}(\xi',\xi'')$$
$$\times\exp\left(-\int_0^t [\nu(\xi') - \epsilon\xi_1'\sigma_y(x-\xi_1's,\xi')]\mathrm{d}s\right)\chi(y)h(t,y,\xi'')\mathrm{d}\xi'\,\mathrm{d}\xi'',$$

where $y=x-\xi_1't$, we have

$$|\bar{J}_0(t,s)| \leqslant e^{-\kappa t}\int_{\mathbf{R}\times\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\chi(y)\sigma_x^{1/2}h(t,y,\xi'')\mathrm{d}\xi'\,\mathrm{d}\xi'',$$

where

$$\widetilde{K}_0(\xi,\xi_1',\xi'') = \int_{\mathbf{R}^2} \sigma_x^{1/2}|\widetilde{K}(\xi,\xi')|\sigma_x^{-1/2}\sigma_x^{1/2}|\widetilde{K}(\xi',\xi'')|\sigma_x^{-1/2}\mathrm{d}\xi_2'\mathrm{d}\xi_3', \quad \xi' = (\xi_1',\xi_2',\xi_3').$$

Similar to the properties of the kernel $K(\xi,\xi')$ stated in Ref. 16, it is straightforward to check that the following estimates hold:

$$\int_{\mathbf{R}^3} \sigma_x^{1/2}|\widetilde{K}(\xi,\xi')|\sigma_x^{-1/2}\mathrm{d}\xi' = \int_{\mathbf{R}^3} \sigma_x^{1/2}|\widetilde{K}(\xi',\xi)|\sigma_x^{-1/2}\mathrm{d}\xi' \leqslant C_0,$$

$$\int_{\mathbf{R}^3} \sigma_x^{1/2}|\widetilde{K}(\xi,\xi')|\sigma_x^{-1/2}\mathrm{d}\xi_2'\,\mathrm{d}\xi_3' \leqslant C_1,$$

where C_0 and C_1 are some positive constants depending only on the parameters ρ_∞, u_∞, T_∞. Thus,

$$\int_{\mathbf{R}\times\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\mathrm{d}\xi_1'\,\mathrm{d}\xi'' \leqslant C_0^2, \quad \int_{\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\mathrm{d}\xi \leqslant C_0C_1,$$

which implies that

$$|\bar{J}_0(t,s)|^2 \leqslant e^{-2\kappa t}\left[\int_{\mathbf{R}\times\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\mathrm{d}\xi_1'\,\mathrm{d}\xi''\right]\left[\int_{\mathbf{R}\times\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\chi(y)|\sigma_x^{1/2}h(s,y,\xi'')|^2\mathrm{d}\xi_1'\,\mathrm{d}\xi''\right]$$
$$\leqslant C_0^2e^{-2\kappa t}\int_{\mathbf{R}\times\mathbf{R}^3} \widetilde{K}_0(\xi,\xi_1',\xi'')\chi(y)|\sigma_x^{1/2}h(s,y,\xi'')|^2\mathrm{d}\xi_1'\,\mathrm{d}\xi''.$$

Hence, we have

$$\|\bar{J}_0(t,s)\|^2_{L_x^\infty(L_\xi^2)} = \sup_{x>0}\int_{\mathbf{R}^3} |\bar{J}_0(t,s)|^2\mathrm{d}\xi \leqslant C_0^2C_0C_1e^{-2\kappa t}\int_{\mathbf{R}\times\mathbf{R}^3} \chi(y)|\sigma_x^{1/2}h(s,y,\xi'')|^2\mathrm{d}\xi_1'\,\mathrm{d}\xi''$$
$$= \frac{ce^{-2\kappa t}}{t}\int_0^\infty\int_{\mathbf{R}^3} |\sigma_x^{1/2}h(s,y,\xi'')|^2\mathrm{d}\xi''\,\mathrm{d}y \leqslant \frac{ce^{-2\kappa t}}{t}(1+s)^{-3}\|\sigma_x^{-1}h_0\|^2_{L^2_{x,\xi}}.$$

Here, we have used the $L^2_{x,\xi}$ decay estimate (3.6). Hence, the definition of $\bar{J}$ and the above-presented estimate give

$$\|\bar{J}(t)\|_{L_x^\infty(L_\xi^2)} \leqslant \int_0^t \|\bar{J}_0(t-s,s)\|_{L_x^\infty(L_\xi^2)}\mathrm{d}s \leqslant c\int_0^t \frac{e^{-\kappa t-s}}{\sqrt{t-s}}(1+s)^{-3/2}\|\sigma_x^{-1}h_0\|_{L^2_{x,\xi}}\mathrm{d}s \leqslant c(1+t)^{-3/2}\|\sigma_x^{-1}h_0\|_{L^2_{x,\xi}}.$$

Thus, (3.9) and (3.11) yield

$$\|J_2(t)\|_{L_x^\infty(L_\xi^2)} = c\|S_0 * \bar{J}\|_{L_x^\infty(L_\xi^2)} \int_0^t e^{-\kappa(t-s)} \|\bar{J}\|_{L_x^\infty(L_\xi^2)}(s)\mathrm{d}s$$

$$\leqslant c\int_0^t e^{-\kappa(t-s)}(1+s)^{-3/2}\mathrm{d}s\|\sigma_x^{-1}h_0\|_{L_x^\infty(L_\xi^2)} \leqslant c(1+t)^{-3/2}\|\sigma_x^{-1}h_0\|_{L_x^\infty(L_\xi^2)},$$

which together with (3.10) give

$$[[J(t)]]_{\beta+3} \leqslant \frac{C}{\beta!}\int_0^t (t-\tau)^\beta e^{-\kappa(t-\tau)}\|\sigma_x^{1/2}h\|_{L_x^\infty(L_\xi^2)}(\tau)\mathrm{d}\tau \leqslant C(1+t)^{-3/2}\|\sigma_x^{-1}h_0\|_{L_x^\infty(L_\xi^2)}.$$

This completes the proof of the lemma.

As a consequence of Lemmas 3.1 and 3.2,. the main estimate in this section stated in (3.7) about the time decay for the solutions to the linearized Boltzmann equation holds.

IV. NONLINEAR STABILITY

In this section, we will prove the main result on the stability of the boundary layer. In order to estimate the nonlinear term and the coupling term with the boundary layer defined in (3.2), we need the following lemma.

Lemma 4.1: When $\beta>0$, *for the two semigroups* S_0 *and* S *defined in* Sec. III, *we have*

$$[[S_0 * \nu h]]_\beta(t) \leqslant C(1+t)^{-3/2}\sup_{0\leqslant\tau\leqslant t}\{(1+\tau)^{3/2}[[h]]_\beta(\tau)\},$$

$$[[S * \nu h]]_\beta(t) \leqslant C(1+t)^{-3/2}\sup_{0\leqslant\tau\leqslant t}\{(1+\tau)^{3/2}[[h]]_\beta(\tau) + (1+\tau)^{3/2}\|\sigma_x^{-1}\nu h\|_{L^2_{x,\xi}}(\tau)\},$$

for any function $h(t,x,\xi)$ *with the corresponding norm bounded.*

Proof: The explicit expression for S_0 gives

$$[[S_0(t) * \nu h]]_\beta \leqslant \sup_{x,\xi}\int_0^t \sigma_x^{1/2}(1+|\xi|)^\beta e^{-\nu(\xi)/2(t-s)}\chi(x-\xi_1 s)\nu h(s,x-\xi_1 s,\xi)\mathrm{d}s$$

$$\leqslant c\sup_{0\leqslant\tau\leqslant t}\{(1+\tau)^{3/2}[[h]]_\beta(\tau)\}\sup_\xi\left\{\int_0^t e^{-(\nu/2)(t-s)}(1+s)^{-3/2}\nu(\xi)\mathrm{d}s\right\}$$

$$\leqslant c(1+t)^{-3/2}\sup_{0\leqslant\tau\leqslant t}\{(1+\tau)^{3/2}[[h]]_\beta(\tau)\}.$$

The estimate on $S(t)$ can be obtained by using the relation between $S(t)$ and $S_0(t)$:

$$S(t) = S_0(t) + S_0(t) * \tilde{K}S(t).$$

Since (3.7) implies that

$$[[S(t)h_0]]_\beta \leqslant C(1+t)^{-3/2}\{\{h_0\}\}_\beta \tag{4.1}$$

with

$$\{\{h\}\}_\beta \equiv [[h]]_\beta + \|\sigma_x^{-1}h\|_{L^2_{x,\xi}}, \quad \beta>0.$$

For $\beta\geqslant 1$, by the regularizing property of the operator $\tilde{K}$, we have

$$
\begin{aligned}
[[S_0 * \tilde{K}S * \nu h]]_\beta &\leqslant \int_0^t e^{-\kappa(t-s)}[[\tilde{k}S * \nu h]]_\beta(s)\mathrm{d}s \leqslant \int_0^t e^{-\kappa(t-s)}[[S * \nu h]]_{\beta-1}(s)\mathrm{d}s \\
&\leqslant \int_0^t e^{-\kappa(t-s)} \int_0^s (1+s-\tau)^{-3/2}\{\{\nu h\}\}_{\beta-1}(\tau)\mathrm{d}\tau\,\mathrm{d}s \\
&\leqslant c \sup_{0\leqslant\tau\leqslant t}\left[(1+\tau)^{3/2}\{\{\nu h\}\}_{\beta-1}(\tau)\right]\int_0^t e^{-\kappa(t-s)}(1+s)^{-3/2}\mathrm{d}s \\
&\leqslant c(1+t)^{-3/2} \sup_{0\leqslant\tau\leqslant t}[(1+\tau)^{3/2}\{\{\nu h\}\}_{\beta-1}(\tau)].
\end{aligned}
$$

Combining this with the estimate for S_0 yields

$$
[[S * \nu h]]_\beta \leqslant C(1+t)^{-3/2} \sup_{0\leqslant\tau\leqslant t}[(1+\tau)^{3/2}[[h]]_\beta(\tau) + (1+\tau)^{3/2}\{\{\nu h\}\}_{\beta-1}(\tau)].
$$

With this estimate, the sublinear growth of $\nu(\xi)$ and the definition $\{\{\cdot\}\}$ give the estimate in the lemma.

With the above-presented estimates, the global solution to the nonlinear problem (3.2) can be proved as follows. Note that, we formally have

$$
\tilde{g} = S(t)\tilde{g}_0 + S * \{e^{\epsilon\sigma}(\bar{L}_\epsilon\tilde{g} + \Gamma(e^{-\epsilon\sigma}\tilde{g}, e^{-\epsilon\sigma}\tilde{g}))\}.
$$

By denoting the right-hand side of the above equation by $T[\tilde{g}]$, we have

$$
\begin{aligned}
[[T[\tilde{g}]]]_\beta &\leqslant [[S(t)\tilde{g}_0]]_\beta + [[S * \nu\nu^{-1}e^{\epsilon\sigma}(L_\epsilon\tilde{g} + \Gamma(\epsilon^{-\epsilon\sigma}\tilde{g}, e^{-\epsilon\sigma}\tilde{g}))]]_\beta \\
&\leqslant C(1+t)^{-3/2}\Bigg\{\{\{\sigma_x^{-1}\tilde{g}_0\}\}_\beta + \sup_{0\leqslant\tau\leqslant t}((1+\tau)^{3/2}[[\nu^{-1}e^{\epsilon\sigma}(\bar{L}_\epsilon\tilde{g} + \Gamma(e^{-\epsilon\sigma}\tilde{g}, e^{-\epsilon\sigma}\tilde{g}))]]_\beta) \\
&\quad + \sup_{0\leqslant\tau\leqslant t}((1+\tau)^{3/2}\|\sigma_x^{-1}\nu\nu^{-1}e^{\epsilon\sigma}(\bar{L}_\epsilon\tilde{g} + \Gamma(e^{-\epsilon\sigma}\tilde{g}, e^{-\epsilon\sigma}\tilde{g}))\|_{L^2_{x,\xi}})\Bigg\} \\
&\leqslant c(1+t)^{\frac{3}{2}}\{\{\{\tilde{g}_0\}\}_\beta + [[\bar{g}]]|||\tilde{g}||| + |||\tilde{g}|||^2\},
\end{aligned}
$$

where

$$
|||h||| = \sup_{t\geqslant 0}\{(1+t)^{\frac{3}{2}}[[h]]_\beta(t)\}.
$$

Here, we have used Lemma 2.7 in estimating

$$
\begin{aligned}
\|\sigma_x^{-1}e^{\epsilon\sigma}\Gamma(e^{-\epsilon\sigma}g, e^{-\epsilon\sigma}h)\|^2_{L^2_{x,\xi}} &= \int_0^\infty \mathrm{d}x \int_{\mathbf{R}^3} |\sigma_x^{-3}\nu(|\xi|)^2||\nu(|\xi|)^{-1}\sigma_x^{1/2}e^{\epsilon\sigma}\Gamma(e^{-\epsilon\sigma}g, e^{-\epsilon\sigma}h)|^2\mathrm{d}\xi \\
&\leqslant c\int_0^\infty \mathrm{d}x \int_{\mathbf{R}^3} |\sigma_x^{-3}\nu(|\xi|)^2|e^{-c\epsilon^2}(\delta x + l)^{2/(3-\beta_1)}(1+|\xi|)^{-2\beta}\mathrm{d}\xi[[g]]_\beta[[h]]_\beta \\
&\leqslant c\int_0^\infty \mathrm{d}x \int_{\mathbf{R}^3} ((\delta x + l)^{3\Theta} + (1+|\tilde{\xi}|)^{3(1-\beta_1)})e^{-c\epsilon^2(\delta x + l)2/(3-\beta_1)} \\
&\quad \times (1+|\xi|)^{-2(\beta-\beta_1)}\mathrm{d}\xi[[g]]_\beta[[h]]_\beta \leqslant c[[g]]_\beta[[h]]_\beta \quad \text{for } \beta > 3 - \frac{\beta_1}{2}.
\end{aligned}
$$

Consequently,

$$
|||T[\tilde{g}]||| \leqslant c(\{\{\tilde{g}_0\}\}_\beta + [[\bar{g}]]_\beta|||\tilde{g}||| + |||\tilde{g}|||^2).
$$

Similar argument gives

$$|||T[\tilde{g}] - T[\tilde{h}]||| \leqslant c([[\bar{g}_0]]_\beta |||\tilde{g} - \tilde{h}||| + |||\tilde{g} + \tilde{h}|||||\tilde{g} - \tilde{h}|||),$$

for the some constant c.

Finally, the smallness assumptions on $\{\{\tilde{g}_0\}\}_\beta$ and $[[\tilde{g}]]_\beta$ coming from the smallness assumption on the initial data $\tilde{g}_0$ and the boundary data b_0 in (3.1) assure that the nonlinear map T is contractive in a small neighborhood of the origin in the Banach space with the norm $[[\cdot]]_\beta$. Therefore, there is a unique fixed point which implies that (3.2) has a unique global in time solution converging to 0 with an algebraic rate as $c(1+t)^{-3/2}$. This gives the proof of Theorem 1.1.

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Statistical quantum probabilities in coherent bosonic and fermionic states

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A derivation of the statistical nature of quantum probabilities is presented by considering a system of bosonic particles in a coherent state. A comparison between the current approach and a former derivation is also discussed. The current approach, which is an evaluation of the field operator matrix in the coherent Glauber state, proved to be a concise method which can be applied to relativistic particles as well. An extension of the coherent state method to the fermionic type of particles is also presented and thus the generality of the coherent state method is established.
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I. INTRODUCTION

In an attempt to relate the quantum probabilities to the statistical probabilities the Wigner transform[1] was applied[2] to the field operator $\hat{\psi}^{\dagger}(\vec{x})$, the operator which creates a particle at point $\vec{x}$, and the resulting function was related to the quantum mechanical state function, the square of which should yield the probability density. Wigner transforms[3] are transformation procedures which assign a classical function to every quantum operator. When applying the Wigner transformation to the density operator one gets the Wigner function which has been widely used to investigate quantum mechanics in phase space.[4] However, usage of the Wigner transformation to deduce the statistical nature of the quantum probabilities turned out to be a difficult, if not impossible, method. For example, one of the steps that was needed to connect the quantum probability to the statistical probability was to impose the ansatz $\phi_i(\vec{x}\pm\vec{z}/2)=\phi_i(\vec{x})\phi_i(\pm\vec{z}/2)$. This condition is not satisfied if the set $\{\phi_i\}$ consists of single particle solutions of the Schrödinger equation with a nonzero potential operator. Another difficult condition to satisfy was the neglect of fluctuations. The relative fluctuations[5] are defined as $f=\langle n_k\rangle^{-1}-a$ where $\langle n_k\rangle$ is the average occupation number per mode and a is a constant which depends on particle type. For classical Maxwell-Boltzmann particles $a=0$, for bosons $a=-1$, and for fermions $a=+1$. Therefore, one may neglect relative fluctuations for classical particles only, and in the limit when $\langle n_k\rangle \gg 1$. Yet another disadvantage of the previous method[2] is the fact that the result for N particles needed to be inductive in the sense that the general result for N particles relied on the result for two and three particles and that one may not do the calculations for N particles in an exact way.

A far more legitimate and elegant way of relating the quantum probabilities to statistical probabilities is by calculating the field operator $\hat{\psi}^{\dagger}(\vec{x},t)$ in the coherent state which is a clever quantum state invented by Glauber.[6] One will not need the above-mentioned disadvantageous approximations, and the calculations are quite simple and exact. A possible shortcoming in using the coherent state is the fact that the method is limited to bosons only as one may not speak of a single particle state being occupied by more than one fermion. However, the application of the coherent states method to fermionic particles is simple as one will just need to reinterpret the results of the coherent state for bosons. A more serious problem to think about in the current approach is the fact that there needs to be a physical justification for the presence of the N bosons,

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or the N fermionic orbitals, by means of which one may attribute a statistical nature to the wave function $\psi(\vec{x},t)$ for the single bosonic or the single fermionic particle at $\vec{x}$ and t. For bosons one can contemplate an analogy between this situation and that of the zero point field (ZPF) bosons. Haisch *et al.*[7] argue that while the quantization of the radiation field predicts the existence of an electromagnetic ZPF, there is, on theoretical grounds, a possibility of assuming a ZPF *a priori*. In fact, they explain, that several quantum effects can be derived by assuming a ZPF and using the theoretical method of stochastic electrodynamics. while it is tempting to think of the ZPF bosons as the N bosons needed for the present situation, the fact is the N bosons in the present paper are massive and the ZPF bosons are massless. Thus, one is compelled to assume the existence of massive bosons with an uncertainty in their number which promotes the statistical nature of the bosonic particle field. As for fermions one needs to assume the existence of an infinite number of orbitals which by themselves are bosons, nevertheless they are occupied by fermions and their numerical uncertainty will promote an uncertainty in the number of fermions and this will lead to a formalism appropriate for fermions yet quite similar to that of the bosons.

II. DERIVATION OF THE BOSONIC STATISTICAL QUANTUM PROBABILITY

The best theoretical way to describe a physical state with an uncertainty in particle number is by means of the coherent state.[8,9] The general coherent state is given by $|\ \rangle=\Pi_{j=1}^{\infty}|\alpha_j\rangle=|\alpha_1\alpha_2\cdots\alpha_k\cdots\rangle$, where for the jth mode, or the jth quantum number, the coherent state is given by

$$|\alpha_j\rangle=\sum_{n_j=0}^{\infty}\frac{\alpha_j^{n_j}}{\sqrt{n_j!}}e^{-1/2|\alpha_j|^2}|n_j\rangle \tag{1}$$

and where $\{|n_j\rangle\}_{n_j=0}^{\infty}$ is a complete orthonormal set of basis in the Fock space. The norm $|\alpha_j|^2=\alpha_j^*\alpha_j$ is equal to the average occupation number for the jth mode, and that can be seen by calculating the number operator $\hat{n}=\hat{a}_j^{\dagger}\hat{a}_j$ in the coherent state representation

$$\begin{aligned}\langle\alpha_j|\hat{n}_j|\alpha_j\rangle&=\sum_{m_j=0}^{\infty}\sum_{n_j=0}^{\infty}\frac{\alpha_j^{*m_j}\alpha_j^{n_j}}{\sqrt{m_j!}\sqrt{n_j!}}e^{-|\alpha_j|^2}n_j\langle m_j|n_j\rangle=\sum_{n_j=0}^{\infty}\frac{\alpha_j^{*n_j}\alpha_j^{n_j}}{n_j!}n_je^{-|\alpha_j|^2}\\&=e^{-|\alpha_j|^2}\alpha_j^*\alpha_j\sum_{n_j=1}^{\infty}\frac{\alpha_j^{*n_j-1}\alpha_j^{n_j-1}}{(n_j-1)!}=e^{-|\alpha_j|^2}\alpha_j^*\alpha_je^{|\alpha_j|^2}=\alpha_j^*\alpha_j=|\alpha_j|^2\end{aligned} \tag{2}$$

or by observing the fact that the norm square of the coefficients in the coherent state expansion is just the Poisson distribution $P(n_j)=(|\alpha_j|^{2n_j}e^{-|\alpha_j|^2})/n_j!$,[9]

$$\langle n_j\rangle=\sum_{n_j=0}^{\infty}n_jP(n_j)=\sum_{n_j=0}^{\infty}\frac{n_j|\alpha_j|^{2n_j}}{n_j!}e^{-|\alpha_j|^2}=\left(\frac{1}{2}|\alpha_j|\frac{\mathrm{d}e^{|\alpha_j|^2}}{\mathrm{d}\alpha_j}\right)e^{-|\alpha_j|^2}=|\alpha_j|^2. \tag{3}$$

Equation (2) relates a diagonal element to an expectation value which is the quantum mechanical method of calculating average values, however, Eq. (3) does not follow that recipe and for that reason it is better to refer to Eq. (3) in this derivation. Given the complete orthonormal set $\{\phi_j(\vec{x})\}_{j=1}^{\infty}$, where each function $\phi_j(\vec{x})$ is the solution to the Schrödinger equation for a particle with mass m, the evaluation of the field operator $\hat{\psi}^{\dagger}(\vec{x})=\Sigma_{j=1}^{\infty}\hat{a}_j^{\dagger}\phi_j^*(\vec{x})$, which creates a particle at point $\vec{x}$, in the coherent states representation will make the relation of quantum probabilties to statistical probabilities evident. Therefore one should evaluate the matrix element given by

$$\langle\,|\hat{\psi}^{\dagger}(\vec{x})|\,\rangle=\sum_{j=1}^{\infty}\langle\alpha_1\alpha_2\cdots\alpha_k\cdots|\hat{a}_j^{\dagger}\phi_j^{*}(\vec{x})|\alpha_1\alpha_2\cdots\alpha_k\cdots\rangle=\langle\alpha_1|\hat{a}_1^{\dagger}|\alpha_1\rangle\phi_1^{*}(\vec{x})\prod_{j=2}^{\infty}\langle\alpha_j|\alpha_j\rangle$$

$$+\langle\alpha_2|\hat{a}_2^{\dagger}|\alpha_2\rangle\phi_2^{*}(\vec{x})\prod_{\substack{j=1\\ j\neq 2}}^{\infty}\langle\alpha_j|\alpha_j\rangle+\cdots+\langle\alpha_k|\hat{a}_k^{\dagger}|\alpha_k\rangle\phi_k^{*}(\vec{x})\prod_{\substack{j=1\\ j\neq k}}^{\infty}\langle\alpha_j|\alpha_j\rangle+\cdots$$

$$=\sum_{j=1}^{\infty}\langle\alpha_j|\hat{a}_j^{\dagger}|\alpha_j\rangle\phi_j^{*}(\vec{x})=\sum_{m_j=0}^{\infty}\sum_{n_j=0}^{\infty}\sum_{j=1}^{\infty}\frac{\alpha_j^{*m_j}\alpha_j^{n_j}}{\sqrt{m_j!}\sqrt{n_j!}}e^{-|\alpha_j|^2}\langle m_j|\hat{a}_j^{\dagger}|n_j\rangle\phi_j^{*}(\vec{x}),\tag{4}$$

where $\langle\alpha_j|\alpha_j\rangle=1$, and where $|\alpha_j\rangle$ is given by Eq. (1). The equation $\hat{a}_j^{\dagger}|n_j\rangle=\sqrt{n_j+1}|n_j+1\rangle$, and the orthonormal property of the Fock space basis $\{|n_j\rangle\}_{n_j=0}^{\infty}$ can be used in Eq. (4),

$$\langle\,|\hat{\psi}^{\dagger}(\vec{x})|\,\rangle=\sum_{j=1}^{\infty}\sum_{n_j=0}^{\infty}\frac{\alpha_j^{*(n_j+1)}\alpha_j^{n_j}}{\sqrt{(n_j+1)!}\sqrt{n_j!}}e^{-|\alpha_j|^2}\sqrt{n_j+1}\,\phi_j^{*}(\vec{x})=\sum_{j=1}^{\infty}\sum_{n_j=0}^{\infty}\frac{\alpha_j^{*n_j}\alpha_j^{*}\alpha_j^{n_j}}{\sqrt{n_j!}\sqrt{n_j!}}e^{-|\alpha_j|^2}\phi_j^{*}(\vec{x}).\tag{5}$$

A simple rearrangement of Eq. (5) will give the final result

$$\langle\,|\hat{\psi}^{\dagger}(\vec{x})|\,\rangle=\sum_{j=1}^{\infty}\alpha_j^{*}\left(\sum_{n_j=0}^{\infty}\frac{|\alpha_j|^{2n_j}}{n_j!}\right)e^{-|\alpha_j|^2}\phi_j^{*}(\vec{x})=\sum_{j=1}^{\infty}\alpha_j^{*}e^{|\alpha_j|^2}e^{-|\alpha_j|^2}\phi_j^{*}(\vec{x})=\sum_{j=1}^{\infty}\alpha_j^{*}\phi_j^{*}(\vec{x}).\tag{6}$$

The coefficients in the final form of Eq. (6) are complex, and one may write them as $\alpha_j=|\alpha_j|e^{i\delta_{\alpha_j}}$. Also, Eq. (3) indicates that $|\alpha_j|=\sqrt{\langle n_j\rangle}$ which means that $\alpha_j^{*}=|\alpha_j|e^{-i\delta_{\alpha_j}}$ or

$$\alpha_j^{*}=\sqrt{\langle n_j\rangle}e^{-i\delta_{\alpha_j}}.\tag{7}$$

Now define the function

$$\psi^{*}(\vec{x})=\frac{\langle\,|\hat{\psi}^{\dagger}(\vec{x})|\,\rangle}{\sqrt{N}},\tag{8}$$

which along with Eqs. (6) and (7) will give

$$\psi^{*}(\vec{x})=\sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{-i\delta_{\alpha_j}}\phi_j^{*}(\vec{x}).\tag{9}$$

By employing the grand canonical equation[5] $N=\Sigma_{j=1}^{\infty}\langle n_j\rangle$, and the orthonormal property of the set $\{\phi_j(\vec{x})\}_{j=1}^{\infty}$ one can show that the integral of the product $\psi^{*}(\vec{x})\psi(\vec{x})\mathrm{d}^3x$ is unity

$$\int\psi^{*}(\vec{x})\psi(\vec{x})\mathrm{d}^3x=\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}\left(\frac{\langle n_k\rangle}{N}\right)^{1/2}e^{-i\delta_{\alpha_j}}e^{i\delta_{\alpha_k}}\int\phi_j^{*}(\vec{x})\phi_k(\vec{x})\mathrm{d}^3x=\sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)=1.\tag{10}$$

Furthermore the function $\psi(\vec{x})$, defined as the Hermitian conjugate of Eq. (9), obeys the Schrödinger equation for a particle at point $\vec{x}$ as one can see by applying the Hamiltonian, $\hat{H}=-(\hbar^2/2m)\nabla^2+V(\vec{x})$, to the function $\psi(\vec{x},t)$,

$$\hat{H}\psi(\vec{x},t)=\sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{i\delta_{\alpha_j}}\hat{H}\phi_j(\vec{x},t)=\sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{i\delta_{\alpha_j}}i\hbar\frac{\partial\phi_j(\vec{x},t)}{\partial t}$$

$$=i\hbar\frac{\partial}{\partial t}\sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2}e^{i\delta_{\alpha_j}}\phi_j(\vec{x},t)=i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t},\tag{11}$$

where

$$\hat{H}\phi_j(\vec{x},t)=i\hbar\frac{\partial\phi_j(\vec{x},t)}{\partial t}$$

and where $\phi_j(\vec{x},t)=\phi_j(\vec{x})e^{-i\epsilon_j t/\hbar}$, which is the time dependence that one gets when solving the Heisenberg equation for the annihilation operator.[2] Alternatively, one can evaluate the bosonic field equation

$$-\frac{\hbar^2}{2m}\nabla^2\hat{\psi}(\vec{x},t)+V(\vec{x})\hat{\psi}(\vec{x},t)=i\hbar\frac{\partial\hat{\psi}(\vec{x},t)}{\partial t}\tag{12}$$

in the coherent state representation and that, together with the Hermitian conjugate of Eq. (8), will prove that the function $\psi(\vec{x},t)$ obeys the Schrödinger equation. In fact, using the alternative method one can show that the relativistic $\psi(\vec{x},t)$ function can be retrieved from the field operator $\hat{\psi}(\vec{x},t)$ which obeys[10]

$$\nabla^2\hat{\psi}(\vec{x},t)-\frac{1}{c^2}\frac{\partial^2\hat{\psi}(\vec{x},t)}{\partial t^2}=\frac{m^2c^2}{\hbar^2}\hat{\psi}(\vec{x},t),\tag{13}$$

where the relation between $\psi(\vec{x},t)$ and $\hat{\psi}(\vec{x},t)$ is again given by the Hermitian conjugate of Eq. (8). The field operator in Eq. (13) satisfies the equal-time commutation relations, and consequently will satisfy the Bose-Einstein statistics.[10] For a charged Klein-Gordon field[10] one may write the box normalized non-Hermitian field as

$$\hat{\psi}(\vec{x},t)=\hat{\psi}^{(+)}(\vec{x},t)+\hat{\psi}^{(-)}(\vec{x},t)=\sum_{\ell}\hat{a}_{p_\ell}\phi_{p_\ell}(\vec{x},t)+\hat{b}^{\dagger}_{p_\ell}\phi^{*}_{p_\ell}(\vec{x},t),\tag{14}$$

where the positive sign indicates particle, and the negative sign indicates antiparticle. The set $\{\phi_{p_\ell}(\vec{x},t)\}$ is a complete orthonormal set of solutions to the Klein-Gordon equation, and for a box volume $V=L^3$ the momentum is $\vec{p}_\ell=(2\pi/L)\vec{\ell}$ with $\vec{\ell}=(\ell_1,\ell_2,\ell_3)$, and $\ell_i=0,\pm1,\pm2,\ldots$, where $i=1,2,3$. The Glauber state which should be used in Eq. (8) is

$$|\ \rangle=\prod_{\ell=1}^{\infty}|\alpha_\ell\rangle\prod_{\ell=1}^{\infty}|\overline{\alpha_\ell}\rangle\tag{15}$$

and the total number of particles is given by $N=\Sigma_\ell(\langle n_\ell\rangle+\langle\overline{n_\ell}\rangle)$, where $\langle\overline{n_\ell}\rangle$ is the average number of antiparticles that occupies the ℓth mode. The elements of the set $\{|\alpha_\ell\rangle\}$ are coherent states which correspond to particles and are defined in Eq. (1). Those of the set $\{|\overline{\alpha_\ell}\rangle\}$ correspond to antiparticles and one may define them as

$$|\overline{\alpha_\ell}\rangle=\sum_{\overline{n_\ell}=0}^{\infty}\frac{\overline{\alpha_\ell}^{\overline{n_\ell}}}{\sqrt{\overline{n_\ell}!}}e^{-1/2|\overline{\alpha_\ell}|^2}|\overline{n_\ell}\rangle.$$

One may define the relativistic wave function by means of the Hermitian conjugate of Eqs. (8), (14), and (15). Therefore, using plane wave solutions to the Klein-Gordon equation one can write the relativistic $\psi(\vec{x},t)$ as

$$\psi(\vec{x},t) = \frac{1}{\sqrt{N}}\langle\,|\hat{\psi}(\vec{x},t)|\,\rangle = \frac{1}{\sqrt{N}}(\langle\,|\hat{\psi}^{(+)}(\vec{x},t)|\,\rangle + \langle\,|\hat{\psi}^{(-)}(\vec{x},t)|\,\rangle)$$

$$= \frac{1}{\sqrt{N}}\sum_{\ell}\langle\alpha_\ell|\hat{a}_\ell|\alpha_\ell\rangle N_\ell e^{(i/\hbar)(\vec{p}_\ell\cdot\vec{x}-|E_\ell|t)} + \frac{1}{\sqrt{N}}\sum_{\ell}\langle\overline{\alpha_\ell}|\hat{b}_\ell^{\dagger}|\overline{\alpha_\ell}\rangle N_\ell^{*} e^{-(i/\hbar)(\vec{p}_\ell\cdot\vec{x}-|E_\ell|t)}, \tag{16}$$

where $N_\ell=(mc^2/L^3|E_\ell|)^{1/2}$ is the normalization constant,[11] $|E_\ell|=\sqrt{p^2c^2+m^2c^4}$, and the summation index is simplified. The particle part in Eq. (16) should be evaluated using the coherent state defined in Eq. (1),

$$\sum_{\ell}\langle\alpha_\ell|\hat{a}_\ell|\alpha_\ell\rangle\phi_\ell(\vec{x},t) = \sum_{\ell}\sum_{n_\ell=0}^{\infty}\frac{\alpha_\ell^{*(n_\ell-1)}\alpha_\ell^{n_\ell}}{\sqrt{(n_\ell-1)!}\sqrt{n_\ell!}}\sqrt{n_\ell}e^{-|\alpha_\ell|^2}\phi_\ell(\vec{x},t) = \sum_{\ell}\sum_{n_\ell=0}^{\infty}\frac{\alpha_\ell^{*n_\ell}\alpha_\ell^{n_\ell}}{\sqrt{n_\ell!}\sqrt{n_\ell!}}\frac{n_\ell}{\alpha_\ell^{*}}e^{-|\alpha_\ell|^2}\phi_\ell(\vec{x},t)$$

$$= \sum_{\ell}\sum_{n_\ell=0}^{\infty}\frac{|\alpha_\ell|^{2n_\ell}}{n_\ell!}\frac{n_\ell}{\alpha_\ell^{*}}e^{-|\alpha_\ell|^2}\phi_\ell(\vec{x},t) = \sum_{\ell}\left(\frac{1}{2}|\alpha_\ell|\frac{de^{|\alpha_\ell|^2}}{d\alpha_\ell}\right)\frac{1}{\alpha_\ell^{*}}e^{-|\alpha_\ell|^2}\phi_\ell(\vec{x},t)$$

$$= \sum_{\ell}\frac{|\alpha_\ell||\alpha_\ell|}{|\alpha_\ell|e^{-i\delta_{\alpha_\ell}}}\phi_\ell(\vec{x},t) = \sum_{\ell}|\alpha_\ell|e^{i\delta_{\alpha_\ell}}\phi_\ell(\vec{x},t) = \sum_{\ell}\sqrt{\langle n_\ell\rangle}e^{i\delta_{\alpha_\ell}}\phi_\ell(\vec{x},t), \tag{17}$$

where in getting Eq. (17) one needs to refer to Eq. (7). The antiparticle part in Eq. (16) is similar to the result in Eq. (9) except that the average occupation number will be for antiparticles. With Eqs. (9) and (17) one may write Eq. (16) in terms of average occupation numbers of particles and antiparticles

$$\psi(\vec{x},t) = \sum_{\ell}\left(\frac{\langle n_\ell\rangle}{N}\right)^{1/2}e^{i\delta_{\alpha_\ell}}N_\ell e^{(i/\hbar)(\vec{p}_\ell\cdot\vec{x}-|E_\ell|t)} + \sum_{\ell}\left(\frac{\langle\overline{n_\ell}\rangle}{N}\right)^{1/2}e^{-i\delta_{\overline{\alpha}_\ell}}N_\ell^{*}e^{-(i/\hbar)(\vec{p}_\ell\cdot\vec{x}-|E_\ell|t)}. \tag{18}$$

Equation (18) can now be substituted into the equation which is supposed to be the probability density for relativistic particles[11]

$$\rho(\vec{x}) = \frac{i\hbar}{2mc^2}\left(\psi^{*}(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t} - \psi(\vec{x},t)\frac{\partial\psi^{*}(\vec{x},t)}{\partial t}\right). \tag{19}$$

Integration of Eq. (19) along with the orthonormal property of the basis set[12] will give

$$\int d^3x\rho(\vec{x}) = \sum_{\ell}\frac{\langle n_\ell\rangle - \langle\overline{n_\ell}\rangle}{N}. \tag{20}$$

Equation (20) can be utilized to investigate a possible physical condition which will cause the failure of Eq. (19) to represent the probability density. It states that if particles and antiparticles are equal in number then there is no chance of finding any massive entity which may be interpreted as a total annihilation. This can be seen be setting $\langle n_\ell\rangle=\langle\overline{n_\ell}\rangle$ which will lead to

$$\int d^3x\rho(\vec{x}) = 0. \tag{21}$$

On the other hand, if there are no antiparticles present then the system consists of particles only and $N=\Sigma_\ell\langle n_\ell\rangle$ which will lead to

$$\int d^3x\rho(\vec{x}) = \sum_{\ell}\frac{\langle n_\ell\rangle}{N} = 1, \tag{22}$$

which is similar to the result Eq. (10). The third possibility is when there are no particles and the system consists of antiparticles only in which case Eq. (20) will be

$$\int \mathrm{d}^3x\rho(\vec{x}) = -\sum_{\ell} \frac{\langle \overline{n_\ell} \rangle}{N} = -1. \tag{23}$$

However, a negative sign for a function which is supposed to represent a probability density is a direct indication that Eq. (19) fails to be a probability density for the third possibility being discussed here. The reasons for the negative sign have been traced to Eq. (19) which one derives from the Klein-Gordon equation.[11] It is said that since $\psi(\vec{x},t)$ and its time derivative may have arbitrary value the function in Eq. (19) can be negative. Nevertheless, one may think in terms of Eq. (20) in which the function that is supposed to represent the probability density will acquire a negative sign only under one physical circumstance, and that is whenever the total number of antiparticles exceed the total number of particles. On physical grounds this line of reasoning provides a better arguement for the failure of that function to represent the probability density.

The application of the coherent states method to fermions is an important task which will generalize the statistical nature of quantum wave functions and will render it nonaxiomatic. However, to apply it to fermions one needs to make up a state that does not include uncertainties in particle number and that suggests a different kind of Glauber state, one which does not consist of a superposition of states with many particles in each state. Although that might seem to be a formidable task at first, the fact is one can easly extend the bosonic formalism to include the fermionic particles as well.

III. DERIVATION OF THE FERMIONIC STATISTICAL QUANTUM PROBABILITY

Here one needs to think in terms of quantum orbitals and fermions which can occupy the orbitals in accordance with the Pauli principle. The orbitals may be occupied by either one fermion or no fermion. If the total number of orbitals in the jth quantum state is k_j then n_j will be the number of orbitals which are filled with a single fermion. This situation is similar to the Bernoulli trials[13] in which there are two possible outcomes for each trial. The probabilities of the two outcomes are denoted by p as the probability of a success S, and q as the probability of a failure F. In this approach the trials are independent, and the probability of any specific sequence, say $(SSFSF\cdots FFS)$, is given by

$$P\{(SSFSF\cdots FFS)\} = ppqpq\cdots qqp. \tag{24}$$

Thus if one defines a filled orbital as a success and an empty one as a failure then the above sequence can be written for the jth quantum state

$$P\{(11010\cdots001)\} = p_jp_jq_jp_jq_j\cdots q_jq_jp_j, \tag{25}$$

where there are k_j elements in the set $(11010\cdots001)$, n_j of them are ones and k_j-n_j of them are zeros, and where $p_j+q_j=1$; $\forall j$. For example, if $n_j=1$ then there are k_j ways of placing the one fermion in the orbitals with the jth quantum state. One can define the mutually exclusive sets $A_1=(10000\cdots000)_j, A_2=(01000\cdots000)_j, A_3=(00100\cdots000)_j, \cdots, A_{k_j}=(00000\cdots001)_j$, and that will give $\cap_{i=1}^{k_j} A_i=\varnothing$, which along with the definition $P\{\varnothing\}=0$ will give the probability of the union of all the events as[13]

$$P\left\{\bigcup_{i=1}^{k_j} A_i\right\} = \sum_{i=1}^{k_j} P\{A_i\} = p_jq_jq_j\cdots q_j + q_jp_jq_j\cdots q_j + q_jq_jp_j\cdots q_j + \cdots + q_jq_jq_j\cdots p_j$$

$$= k_jp_jq_jq_j\cdots q_j = \frac{k_j!}{1!(k_j-1)!}p_j^1q_j^{(k_j-1)}. \tag{26}$$

In general, the probability that k_j orbitals (Bernoulli trials), with probabilities p_j for finding a fermion in one of the k_j orbitals and $q_j=1-p_j$ for failure to find one, results in n_j successes (filled orbitals) and k_j-n_j failures (empty orbitals) is

$$P(n_j) = \frac{k_j!}{n_j!(k_j - n_j)!} p_j^{n_j} q_j^{(k_j - n_j)}, \tag{27}$$

which is the binomial distribution. Note that the multiplicative factor in Eq. (27) is precisely the one which corresponds to the Fermi-Dirac statistics of distributing n_j fermions among k_j energy levels. This probability satistfies the axiom of a probability function as one can see by summing over all possible values of n_j,

$$\sum_{n_j=0}^{k_j} P(n_j) = \sum_{n_j=0}^{k_j} \frac{k_j!}{n_j!(k_j - n_j)!} p_j^{n_j} q_j^{(k_j - n_j)} = (p_j + q_j)^{k_j} = 1. \tag{28}$$

When considering the limit $k_j \gg 1$ such that the product $k_j p_j$ is moderate then the binomial distribution may be approximated by the Poisson distribution.[13] Therefore, the probability that n_j orbitals among a total of k_j orbitals are filled is

$$P(n_j) = \frac{\lambda_j^{n_j}}{n_j!} e^{-\lambda_j}, \tag{29}$$

where $\lambda_j = k_j p_j$, and $k_j \gg 1$. Accordingly

$$\langle n_j \rangle = \sum_{n_j=0}^{\infty} n_j P(n_j) = \sum_{n_j=0}^{\infty} n_j \frac{\lambda_j^{n_j}}{n_j!} e^{-\lambda_j} = \sum_{n_j=1}^{\infty} \frac{\lambda_j^{n_j}}{(n_j - 1)!} e^{-\lambda_j} = \lambda_j e^{-\lambda_j} \sum_{n_j=1}^{\infty} \frac{\lambda_j^{n_j - 1}}{(n_j - 1)!} = \lambda_j e^{-\lambda_j} e^{+\lambda_j} = \lambda_j \tag{30}$$

and therefore

$$P(n_j) = \frac{\langle n_j \rangle^{n_j}}{n_j!} e^{-\langle n_j \rangle}. \tag{31}$$

Now one can construct a state for fermions which may be expanded in terms of the Fock space basis given by the form $|\beta_j\rangle = \Sigma_{n_j=0}^{\infty} C_{n_j} |n_j\rangle$, where $|C_{n_j}|^2$ should be the probability that n_j of the k_j orbitals are filled with fermions. To ensure the normalization of the set $\{|\beta_j\rangle\}$ it must be true that $\Sigma_{n_j}^{\infty} |C_{n_j}|^2 = 1$ which along with Eq. (31) suggests that

$$C_{n_j} = \frac{(\langle n_j \rangle e^{i\delta_j})^{n_j/2}}{\sqrt{n_j!}} e^{-\langle n_j \rangle/2}. \tag{32}$$

Now define the annihilation operator $\hat{a}_j$, which annihilates an orbital of the filled type when it operates on the state $|n_j\rangle$. One needs to be aware of the fact that the state $|\beta_j\rangle$ describes fermionic particles by using a formalism which is similar to the bosonic particles. There are no bosonic particles here, however, for the jth quantum state there can be an infinite number of orbitals and any number of these may be occupied by fermions such that each fermion occupy only one orbital. It is easy to show the equality

$$\hat{a}_j |\beta_j\rangle = \sqrt{\langle n_j \rangle} e^{i\delta_j/2} |\beta_j\rangle \tag{33}$$

from which it follows that

$$\langle \beta_j | \hat{a}_j^{\dagger} = \langle \beta_j | \sqrt{\langle n_j \rangle} e^{-i\delta_j/2}. \tag{34}$$

The operator $\hat{\psi}(\vec{x}) = \Sigma_j \hat{a}_j \phi_j(\vec{x})$ annihilates a filled orbital at position $\vec{x}$, and hence annihilates one fermion at that position. The quantum state of the totality of all the fermions can be defined by the direct product

$$|\ \rangle = \prod_{j=1}^{\infty} |\beta_j\rangle. \tag{35}$$

This state accommodates an infinite number of orbitals for each quantum state j with each orbital either being filled with one fermion or with no fermion. The function

$$\psi(\vec{x}) = \frac{1}{\sqrt{N}}\langle\ |\hat{\psi}(\vec{x})|\ \rangle \tag{36}$$

will now be the state function for a fermionic particle, and $N=\Sigma_j\langle n_j\rangle$ is the total number of filled orbitals, or the total number of fermions. With Eq. (35) a direct evaluation of Eq. (36) will give

$$\psi(\vec{x}) = \frac{1}{\sqrt{N}}\sum_{j=1}^{\infty}\langle\beta_1\beta_2\cdots\beta_k\cdots|\hat{a}_j|\beta_1\beta_2\cdots\beta_k\cdots\rangle\phi_j(\vec{x}) = \frac{1}{\sqrt{N}}\sum_{j=1}^{\infty}\langle\beta_j|\hat{a}_j|\beta_j\rangle\phi_j(\vec{x}). \tag{37}$$

With the help of Eq. (33) one can achieve the final form of the fermionic state function which embeds the statistical information

$$\psi(\vec{x}) = \sum_{j=1}^{\infty}\left(\frac{\langle n_j\rangle}{N}\right)^{1/2} e^{i\delta_j/2}\phi_j(\vec{x}). \tag{38}$$

The orthonormality of the set $\{\phi_j(\vec{x})\}$ will directly lead to the result

$$\int \mathrm{d}^3x\psi^*(\vec{x})\psi(\vec{x}) = 1, \tag{39}$$

which makes clear the statistical interpretation of the fermionic state function $\psi(\vec{x})$.

In conclusion, using coherent states is a far superior way to derive the statistical nature of quantum probabilities as the Wigner transformation method necessitated some unfavorable approximations. The coherent state method can be applied to relativistic as well as nonrelativistic particles. It can also be applied to both bosons and fermions which makes the coherent state method as general as the previous method but at the same time more reliable and much more precise.

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Cartan calculi on the quantum superplane

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Cartan calculi on the extended quantum superplane are given. To this end, the noncommutative differential calculus on the extended quantum superplane is extended by introducing inner derivations and Lie derivatives. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227638]

I. INTRODUCTION

Noncommutative geometry[1] has started to play an important role in different fields of mathematical physics over the past decade. The basic structure giving a direction to the noncommutative geometry is a differential calculus on an associative algebra. The noncommutative differential geometry of quantum groups was introduced by Woronowicz.[2,3] In this approach the differential calculus on the group is deduced from the properties of the group and it involves functions on the group, differentials, differential forms, and derivatives. The other approach, initiated by Wess and Zumino,[4] followed Manin's emphasis[5] on the quantum spaces as the primary objects. Differential forms are defined in terms of noncommuting coordinates, and the differential and algebraic properties of quantum groups acting on these spaces are obtained from the properties of the spaces. The natural extension of their scheme to superspace[6] was introduced by Soni in Ref. 7 and Chung in Ref. 8. The noncommutative geometry of the quantum superplane was given in Ref. 9.

The differential calculus on the quantum superplane similarly involves functions on the superplane, differentials, differential forms, and derivatives. The exterior derivative is a linear operator d acting on k-forms and producing $(k+1)$-forms, such that for scalar functions (0-forms) f and g we have

$$\begin{aligned} \mathsf{d}(1) &= 0, \\ \mathsf{d}(fg) &= (\mathsf{d}f)g + (-1)^{\deg(f)} f(\mathsf{d}g), \end{aligned} \tag{1}$$

where $\deg(f)=0$ for even variables and $\deg(f)=1$ for odd variables, and for a k-form ω_1 and any form ω_2,

$$\mathsf{d}(\omega_1 \wedge \omega_2) = (\mathsf{d}\omega_1) \wedge \omega_2 + (-1)^k \omega_1 \wedge (\mathsf{d}\omega_2). \tag{2}$$

A fundamental property of the exterior derivative d is

$$\mathsf{dd} =: \mathsf{d}^2 = 0. \tag{3}$$

There is a relationship between the exterior derivative and the Lie derivative. To describe the relation between exterior derivative and the Lie derivative, we introduce a new operator: the inner derivation. Hence the differential calculus on the quantum superplane can be extended into a large calculus. We call this new calculus the Cartan calculus. The connection of the inner derivation denoted by $\mathbf{i}_a$ and the Lie derivative denoted by $\mathcal{L}_a$ is given by the Cartan formula:

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$$\mathcal{L}_a = \mathrm{d} \circ \mathbf{i}_a + \mathbf{i}_a \circ \mathrm{d}. \tag{4}$$

This and other formulas are explained in Refs. 10–12. Here we do not give any details. In the related section we shall give a brief overview without much discussion.

The extended calculus on the quantum plane was introduced in Ref. 13 using the approach of Ref. 10. In this work we explicitly set up the Cartan calculi on the quantum superplane. In Secs. II and III we give some information on the Hopf algebra structures of the quantum superplane and its differential calculus which we shall use in order to establish our notions. The differential structures of Types II and III which appeared in Sec. III A exist in Ref. 8, but here they are repeated because we need them. In Sec. IV we present the commutation rules of the inner derivations and the Lie derivatives with functions on the quantum superplane, differentials, and partial differentials.

II. REVIEW OF HOPF ALGEBRA $\mathcal{A}$

Elementary properties of the quantum superplane are described in Ref. 9. We state briefly the properties we are going to need in this work.

A. The algebra of functions on the quantum superplane

Let us begin with the definition of the coordinate ring of the quantum superplane $\mathcal{R}_q^{1|1}$. It is well known that the quantum superplane[6] is defined as an associative algebra generated by two noncommuting coordinates x and θ with the relations

$$\begin{aligned} x\theta &= q\theta x, \\ \theta^2 &= 0, \end{aligned} \tag{5}$$

where q is a nonzero complex deformation parameter. The algebra of q polynomials will be called the algebra of functions on the quantum superplane and will be denoted by $\mathcal{A}_0 =: A(\mathcal{R}_q^{1|1})$. In the limit $q \to 1$, this algebra is commutative and can be considered as the algebra of polynomials $\mathcal{R}^{1|1}$ over the usual superplane, where x and θ are the two coordinate functions.

Let $\mathcal{A}_0 = A(\mathcal{R}_q^{1|1})$ be a free unital associative algebra generated by even coordinate x and odd coordinate θ obeying relations (5). We extend the algebra $\mathcal{A}_0$ by including the inverse of x which satisfies

$$xx^{-1} = 1 = x^{-1}x$$

and we denote it by $\mathcal{A}$. We know that the algebra $\mathcal{A}$ is a graded Hopf algebra with the following costructures.[9]

B. Hopf algebra structure on $\mathcal{A}$

The definitions of a coproduct, a counit, and a coinverse on the algebra $\mathcal{A}$ are as follows:

(1) the coproduct $\Delta_{\mathcal{A}}: \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}$ is an algebra homomorphism and is defined by

$$\begin{aligned} \Delta_{\mathcal{A}}(x) &= x \otimes x, \\ \Delta_{\mathcal{A}}(\theta) &= \theta \otimes x + x \otimes \theta. \end{aligned} \tag{6}$$

(2) The counit $\epsilon_{\mathcal{A}}$ is an algebra homomorphism from $\mathcal{A}$ to the complex numbers $\mathcal{C}$ and is given by

$$\begin{aligned} \epsilon_{\mathcal{A}}(x) &= 1, \\ \epsilon_{\mathcal{A}}(\theta) &= 0. \end{aligned} \tag{7}$$

(3) The antipode $S_{\mathcal{A}}:\mathcal{A}\to\mathcal{A}$ is an algebra antihomomorphism and is given by

$$S_{\mathcal{A}}(x)=x^{-1},$$
$$S_{\mathcal{A}}(\theta)=-x^{-1}\theta x^{-1}. \tag{8}$$

These comaps satisfy the Hopf algebra axioms:

$$(\Delta_{\mathcal{A}}\otimes \mathrm{id})\circ\Delta_{\mathcal{A}}=(\mathrm{id}\otimes\Delta_{\mathcal{A}})\circ\Delta_{\mathcal{A}},$$
$$m_{\mathcal{A}}\circ(\epsilon_{\mathcal{A}}\otimes \mathrm{id})\circ\Delta_{\mathcal{A}}=m_{\mathcal{A}}\circ(\mathrm{id}\otimes\epsilon_{\mathcal{A}})\circ\Delta_{\mathcal{A}}, \tag{9}$$
$$m_{\mathcal{A}}\circ(S_{\mathcal{A}}\otimes \mathrm{id})\circ\Delta_{\mathcal{A}}=\epsilon_{\mathcal{A}}=m_{\mathcal{A}}\circ(\mathrm{id}\otimes S_{A})\circ\Delta_{\mathcal{A}},$$

where id denotes the identity map on $\mathcal{A}$ and $m_{\mathcal{A}}$ stands for the algebra product $\mathcal{A}\otimes\mathcal{A}\to\mathcal{A}$. The multiplication in $\mathcal{A}\otimes\mathcal{A}$ is defined with the rule

$$(A\otimes B)(C\otimes D)=(-1)^{\deg(B)\deg(C)}(AC\otimes BD). \tag{10}$$

III. DIFFERENTIAL CALCULI ON THE QUANTUM SUPERPLANE

Here, we shall build up the noncommutative differential calculi on the quantum superplane with help of the covariance point of view, using the Hopf algebra structure of the quantum superplane.[14]

A. Differential algebra

It is well known that in classical differential calculus, functions commute with differentials. From algebraic point of view, the space of one-forms is a free bimodule over the algebra of smooth functions generated by the first-order differentials and the commutativity shows how its left and right structures are related to each other.

In order to establish a noncommutative differential calculus on the quantum superplane, we assume that the commutation relations between the coordinates and their differentials are of the following form:

$$x\mathrm{d}x=Q\mathrm{d}xx,$$
$$x\mathrm{d}\theta=Q_{11}\mathrm{d}\theta x+Q_{12}\mathrm{d}x\theta,$$
$$\theta\mathrm{d}x=Q_{21}\mathrm{d}x\theta+Q_{22}\mathrm{d}\theta x, \tag{11}$$
$$\theta\mathrm{d}\theta=\mathrm{d}\theta\theta.$$

The coefficients Q and Q_{ij} $(1\leqslant i,j\leqslant 2)$ will be determined using the covariance of the noncommutative differential calculus. We also have assumed that

$$\mathrm{d}x\wedge\mathrm{d}\theta=Q'\mathrm{d}\theta\wedge\mathrm{d}x,\quad \mathrm{d}x\wedge\mathrm{d}x=0, \tag{12}$$

where Q' is a parameter that will be described later.

We shall denote the algebra generated with relations (11) by Ω^1 and the algebra generated with relations (12) by Ω^2.

B. Covariance

We first note that consistency of a differential calculus with commutation relations (5) means that the differential algebra is a graded associative algebra generated by the elements of the set

$\{x,\theta,\mathrm{d}x,\mathrm{d}\theta\}$. Let Ω be a free left module over the algebra $\mathcal{A}$ generated by the elements of this set. So the Ω has to be generated by $\Omega^0\cup\Omega^1\cup\Omega^2$, where Ω^0 is isomorphic to $\mathcal{A}$. One says that (Ω,d) is a *first-order differential calculus* over the Hopf algebra $(\mathcal{A},\Delta_{\mathcal{A}},\epsilon_{\mathcal{A}},S_{\mathcal{A}})$. We begin with the definitions of a left- and right-covariant bimodule.

(1) Let Ω be a bimodule over $\mathcal{A}$ and $\Delta^R:\Omega\to\Omega\otimes\mathcal{A}$ be a linear homomorphism. We say that (Ω,Δ^R) is a right-covariant bimodule if

$$\Delta^R(a\rho+\rho' a')=\Delta_{\mathcal{A}}(a)\Delta^R(\rho)+\Delta^R(\rho')\Delta_{\mathcal{A}}(a') \tag{13}$$

for all $a,a'\in\mathcal{A}$ and $\rho,\rho'\in\Omega$, and

$$\begin{gathered}(\Delta^R\otimes\mathrm{id})\circ\Delta^R=(\mathrm{id}\otimes\Delta_{\mathcal{A}})\circ\Delta^R,\\ (\mathrm{id}\otimes\epsilon)\circ\Delta^R=\mathrm{id}.\end{gathered} \tag{14}$$

The action of Δ^R on the first-order differentials is

$$\begin{gathered}\Delta^R(\mathrm{d}x)=\mathrm{d}x\otimes x,\\ \Delta^R(\mathrm{d}\theta)=\mathrm{d}\theta\otimes x+\mathrm{d}x\otimes\theta\end{gathered} \tag{15}$$

since

$$\Delta^R(\mathrm{d}a)=(\mathrm{d}\otimes\mathrm{id})\Delta_{\mathcal{A}}(a);\quad \forall\, a\in\mathcal{A}. \tag{16}$$

We now apply the linear map Δ^R to relations (11):

$$\begin{gathered}\Delta^R(x\mathrm{d}x)=\Delta_{\mathcal{A}}(x)\Delta^R(\mathrm{d}x)=Q\Delta^R(\mathrm{d}xx),\\ \Delta^R(x\mathrm{d}\theta)=\Delta^R(Q_{11}\mathrm{d}\theta x+Q_{12}\mathrm{d}x\theta)+(qQ-Q_{11}-qQ_{12})\mathrm{d}xx\otimes\theta x,\\ \Delta^R(\theta\mathrm{d}x)=\Delta^R(Q_{21}\mathrm{d}x\theta+Q_{22}\mathrm{d}\theta x)-(q^{-1}Q+Q_{21}+q^{-1}Q_{22})\mathrm{d}xx\otimes x\theta,\\ \Delta^R(\theta\mathrm{d}\theta)=\Delta^R(\mathrm{d}\theta\theta)+(q^{-1}Q_{11}+Q_{22}-1)\mathrm{d}\theta x\otimes x\theta+(Q_{12}+qC_{21}+1)\mathrm{d}x\theta\otimes\theta x.\end{gathered} \tag{17}$$

So we must have

$$\begin{gathered}Q_{11}+qQ_{12}=qQ,\quad Q_{11}+qQ_{22}=q,\\ Q_{12}+qQ_{21}=-1,\quad qQ_{21}+C_{22}=-Q.\end{gathered} \tag{18}$$

(2) Let Ω be a bimodule over $\mathcal{A}$ and $\Delta^L:\Omega\to\mathcal{A}\otimes\Omega$ be a linear homomorphism. We say that (Ω,Δ^L) is a left-covariant bimodule if

$$\Delta^L(a\rho+\rho' a')=\Delta_{\mathcal{A}}(a)\Delta^L(\rho)+\Delta^L(\rho')\Delta_{\mathcal{A}}(a') \tag{19}$$

for all $a,a'\in\mathcal{A}$ and $\rho,\rho'\in\Omega$, and

$$\begin{gathered}(\Delta_{\mathcal{A}}\otimes\mathrm{id})\circ\Delta^L=(\mathrm{id}\otimes\Delta^L)\circ\Delta^L,\\ (\epsilon\otimes\mathrm{id})\circ\Delta^L=\mathrm{id}.\end{gathered} \tag{20}$$

Since

$$\Delta^L(\mathrm{d}a)=(\tau\otimes\mathrm{d})\Delta_{\mathcal{A}}(a),\quad \forall\, a\in\mathcal{A} \tag{21}$$

the action of Δ^L on the first-order differentials gives rise to the relations

$$\Delta^L(\mathrm{d}x) = x \otimes \mathrm{d}x,$$
$$\Delta^L(\mathrm{d}\theta) = x \otimes \mathrm{d}\theta - \theta \otimes \mathrm{d}x. \tag{22}$$

Here $\tau: \Omega \to \Omega$ is the linear map of degree zero which gives $\tau(a) = (-1)^{\deg(a)}a$. If we apply Δ^L to relations (11), we do not have any new relations between Q's. Consequently, we may have three distinct solutions:

Type I: includes one deformation parameter

$$Q_{12} = 0, \quad Q_{22} = 0 \Rightarrow \begin{cases} Q = 1 \\ Q_{11} = q \\ Q_{21} = -q^{-1} \\ Q' = q. \end{cases} \tag{23}$$

Type II: includes two parameters

$$Q_{22} = 0, \quad Q = r \Rightarrow \begin{cases} Q_{11} = q \\ Q_{12} = r - 1 \\ Q_{21} = -q^{-1}r \\ Q' = qr^{-1}. \end{cases} \tag{24}$$

Type III: includes two parameters

$$Q_{12} = 0, \quad Q = p \Rightarrow \begin{cases} Q_{11} = pq \\ Q_{21} = -q^{-1} \\ Q_{22} = 1 - p \\ Q' = pq. \end{cases} \tag{25}$$

Hence we see that solution of the form Type I is a special case of solution of the form Type II for $r=1$ or Type III for $p=1$. Therefore it may be omitted. However the Type I solution, as we will see in Sec. IV, gives rise to interesting and important results. Therefore it is convenient as a special type.

Note that it can be checked that the identities (14) and (20) and also the following identities are satisfied:

$$(\mathrm{id} \otimes \mathrm{d})\Delta_{\mathcal{A}}(a) = \Delta^L(\mathrm{d}a),$$
$$(\mathrm{d} \otimes \mathrm{id})\Delta_{\mathcal{A}}(a) = \Delta^R(\mathrm{d}a), \tag{26}$$
$$(\Delta^L \otimes \mathrm{id}) \circ \Delta^R = (\mathrm{id} \otimes \Delta^R) \circ \Delta^L.$$

Note that the Type I has a special importance. We will see in Sec. IV, that in this case the extended calculus on the quantum superplane has linear commutation relations, for example, the commutation rules of the Lie derivatives with functions do not contain the inner derivations.

We call the $\mathcal{A}_0 = A(\mathcal{R}_q^{1|1})$-bimodule generated by $\mathrm{d}x$, $\mathrm{d}\theta$ with relations (11) a *cotangent bimodule* and denote it by $\Omega(T^*\mathcal{R}_q^{1|1})$. Further work on this and on the tangent bimodule is in progress.

C. Cartan-Maurer one-forms on $\mathcal{A}$

In analogy with the left-invariant one-forms on a Lie group in classical differential geometry, one can construct two one-forms using the generators of $\mathcal{A}$ as follows:[9]

$$\omega_x = \mathrm{d}x x^{-1},$$
$$\omega_\theta = \mathrm{d}\theta x^{-1} - \mathrm{d}x x^{-1}\theta x^{-1}. \tag{27}$$

The commutation relations between the generators of $\mathcal{A}$ and one-forms are

$$x\omega_x = Q\omega_x x,$$
$$x\omega_\theta = Q_{11}\omega_\theta x,$$
$$\theta\omega_x = -Q\omega_x\theta + Q_{22}\omega_\theta x, \tag{28}$$
$$\theta\omega_\theta = Q_{11}\omega_\theta\theta.$$

The commutation rules of the one-forms ω_x and ω_θ are

$$\omega_x \wedge \omega_\theta = \omega_\theta \wedge \omega_x,$$
$$\omega_x \wedge \omega_x = 0. \tag{29}$$

We denote the algebra of the forms generated by the two elements ω_x and ω_θ by $\mathcal{W}$. We make the algebra $\mathcal{W}$ into a graded Hopf algebra with the following co-structures:[9] the coproduct $\Delta_\mathcal{W}: \mathcal{W} \to \mathcal{W} \otimes \mathcal{W}$ is defined by

$$\Delta_\mathcal{W}(\omega_x) = \omega_x \otimes 1 + 1 \otimes \omega_x,$$
$$\Delta_\mathcal{W}(\omega_\theta) = \omega_\theta \otimes 1 + 1 \otimes \omega_\theta. \tag{30}$$

The counit $\epsilon_\mathcal{W}: \mathcal{W} \to \mathcal{C}$ is given by

$$\epsilon_\mathcal{W}(\omega_x) = 0,$$
$$\epsilon_\mathcal{W}(\omega_\theta) = 0 \tag{31}$$

and the coinverse $S_\mathcal{W}: \mathcal{W} \to \mathcal{W}$ is defined by

$$S_\mathcal{W}(\omega_x) = -\omega_x,$$
$$S_\mathcal{W}(\omega_\theta) = -\omega_\theta. \tag{32}$$

D. The algebra of partial derivatives

Here, we introduce commutation relations between the coordinates of the quantum superplane and their partial derivatives. Later, we illustrate the connection between the relations in Sec. III E.

To proceed, let us obtain the relations of the coordinates with their partial derivatives. We know that the exterior differential d can be expressed in the form

$$\mathrm{d}f = (\mathrm{d}x\partial_x + \mathrm{d}\theta\partial_\theta)f. \tag{33}$$

Then, for example,

$$\mathrm{d}(xf) = \mathrm{d}x f + x\mathrm{d}f = [\mathrm{d}x(1 + Qx\partial_x + Q_{12}\theta\partial_\theta) + Q_{11}\mathrm{d}\theta\partial_\theta]f = (\mathrm{d}x\partial_x x + \mathrm{d}\theta\partial_\theta x)f$$

so that, after some calculations

$$\partial_x x = 1 + Qx\partial_x + Q_{12}\theta\partial_\theta,$$

$$\partial_x \theta = -Q_{21}\theta\partial_x,$$

$$\partial_\theta x = Q_{11}x\partial_\theta, \tag{34}$$

$$\partial_\theta \theta = 1 - \theta\partial_\theta - Q_{22}x\partial_x.$$

We shall denote the $\mathcal{A}$-module generated by the partial derivatives ∂_x and ∂_θ with relations (34) by $\mathcal{D}^1$. This space $\mathcal{D}^1$ is the bimodule of first-order partial differential operators.

The commutation relations between derivatives are

$$\partial_x\partial_\theta = Q'\partial_\theta\partial_x,$$

$$\partial_\theta^2 = 0. \tag{35}$$

The relations between partial derivatives and differentials are found as

$$\partial_x \mathsf{d}x = Q^{-1}\mathsf{d}x\partial_x - (1 + Q'^{-1}Q_{21}^{-1})\mathsf{d}\theta\partial_\theta,$$

$$\partial_x \mathsf{d}\theta = Q_{11}^{-1}\mathsf{d}\theta\partial_x,$$

$$\partial_\theta \mathsf{d}x = Q_{21}^{-1}\mathsf{d}x\partial_\theta, \tag{36}$$

$$\partial_\theta \mathsf{d}\theta = \mathsf{d}\theta\partial_\theta + (1 - Q'Q_{11}^{-1})\mathsf{d}x\partial_x.$$

The relations between partial derivatives and the exterior derivative, which guarantee the consistence with the basic requirement for the nilpotency of d, are

$$\partial_x \mathsf{d} = Q^{-1}\mathsf{d}\partial_x,$$

$$\partial_\theta \mathsf{d} = -Q^{-1}\mathsf{d}\partial_\theta. \tag{37}$$

E. Quantum Lie superalgebra

The commutation relations of Cartan-Maurer forms allow us to construct the algebra of the generators. In order to obtain the quantum Lie superalgebra of the algebra generators we first write the Cartan-Maurer forms as

$$\mathsf{d}x = \omega_x x,$$

$$\mathsf{d}\theta = \omega_x\theta + \omega_\theta x. \tag{38}$$

The differential d can then be expressed in the form

$$\mathsf{d} = \omega_x H + \omega_\theta \nabla\,. \tag{39}$$

Here H and ∇ are the quantum Lie superalgebra generators (vector fields). We now shall obtain the commutation relations of these generators. Considering an arbitrary function f of the coordinates of the quantum superplane and using that $\mathsf{d}^2 = 0$ and

$$\mathsf{d}\omega_x = 0,$$

$$\mathsf{d}\omega_\theta = 0, \tag{40}$$

one has the following commutation relations for the quantum Lie superalgebra:

$$H\nabla = \nabla H,$$
$$\nabla^2 = 0. \tag{41}$$

The commutation relation (41) of the algebra generators should be consistent with monomials of the coordinates of the quantum superplane. To do this, we evaluate the commutation relations between the generators of algebra and the coordinates. The commutation relations of the generators with the coordinates can be extracted from the graded Leibniz rule:

$$\mathrm{d}(xf) = (\mathrm{d}x)f + x(\mathrm{d}f) = \omega_x(x + QxH)f + \omega_\theta(x\nabla)f = (\omega_x H + \omega_\theta \nabla)xf$$

and

$$\mathrm{d}(\theta f) = (\mathrm{d}\theta)f + \theta(\mathrm{d}f) = \omega_x(\theta + Q\theta H)f + \omega_\theta(x - Q_{11}\theta\nabla - Q_{22}xH)f = (\omega_x H + \omega_\theta \nabla)\theta f.$$

This yields

$$Hx = x + QxH,$$
$$H\theta = \theta + Q\theta H,$$
$$\nabla x = Q_{11}x\nabla, \tag{42}$$
$$\nabla\theta = x - Q_{11}\theta\nabla - Q_{22}xH.$$

We know, from Sec. III D, that the exterior differential d can be expressed in the form (33), which we repeat here,

$$\mathrm{d}f = (\mathrm{d}x\partial_x + \mathrm{d}\theta\partial_\theta)f.$$

Considering (39) together with (33) and using (27) one has

$$H \equiv x\partial_x + \theta\partial_\theta,$$
$$\nabla \equiv x\partial_\theta. \tag{43}$$

Note that, using relations (34) and (35) one can check that the relation of the generators in (43) coincide with (41). It can also be verified that the action of the generators in (43) on the coordinates coincide with (42). Of course, these relations can also be found using the dual pairing. This case will be considered at the end of this section.

The commutation relations of the vector fields H and ∇ with the differentials are the following:

$$H\mathrm{d}x = \mathrm{d}xH,$$
$$H\mathrm{d}\theta = \mathrm{d}\theta H,$$
$$\nabla\mathrm{d}x = QQ_{21}^{-1}\mathrm{d}x\nabla, \tag{44}$$
$$\nabla\mathrm{d}\theta = Q_{11}\mathrm{d}\theta\nabla + Q_{12}\mathrm{d}xH.$$

Here we used that

$$Q_{22} - Q_{11}Q_{21} - Q_{11}Q'^{-1} = 0, \quad Q_{12} + Q_{21}(Q_{11} - Q') = 0,$$
$$Q(Q_{11} - Q') - Q_{11}Q_{12} = 0, \tag{45}$$

$$Q_{12}(1+Q'Q_{21})=0, \quad Q_{22}(Q_{11}-Q')=0.$$

Using relations (44) together with (42) we obtain the commutation rules of the vector fields with one-forms as follows:

$$\begin{aligned} H\omega_x &= -Q^{-1}\omega_x + Q^{-1}\omega_x H, \\ H\omega_\theta &= -Q^{-1}\omega_\theta + Q^{-1}\omega_\theta H, \\ \nabla\omega_x &= -\omega_x \nabla, \\ \nabla\omega_\theta &= Q^{-1}\omega_x + \omega_\theta \nabla + (Q-1)\omega_x H \end{aligned} \tag{46}$$

or taking

$$T = \mathbf{1} + (Q-1)H \tag{47}$$

one has

$$\begin{aligned} T\omega_x &= Q^{-1}\omega_x T, \\ T\omega_\theta &= Q^{-1}\omega_\theta T, \\ \nabla\omega_x &= -\omega_x \nabla, \\ \nabla\omega_\theta &= \omega_\theta \nabla + Q^{-1}\omega_x T. \end{aligned} \tag{48}$$

Here we used that

$$Q_{12} - Q_{22} = Q - 1. \tag{49}$$

Similarly, we can find the commutation relations between the vector fields and the partial derivatives as

$$\begin{aligned} \partial_x H &= \partial_x + QH\partial_x, \\ \partial_\theta H &= \partial_\theta + QH\partial_\theta, \\ \partial_x \nabla &= \partial_\theta + QQ' \nabla \partial_x, \\ \partial_\theta \nabla &= -\nabla\partial_\theta. \end{aligned} \tag{50}$$

We here again used that

$$Q_{12} - Q'Q_{21} = 1, \quad Q_{11} - Q'(Q + Q_{22}) = 0. \tag{51}$$

We know that the differential operator d satisfies the graded Leibniz rule. Therefore, the generators H and ∇ are endowed with a natural coproduct. To find them, we need the following commutation relation:

$$Hx^m = \frac{1-Q^m}{1-Q}x^m + Q^m x^m H, \tag{52}$$

where use was made of the first relation of (42). Relation (52) is understood as an operator equation. This implies that when H acts on arbitrary monomials $x^m\theta$,

$$H(x^m\theta) = \frac{1-Q^{m+1}}{1-Q}(x^m\theta) + Q^{m+1}(x^m\theta)H \tag{53}$$

from which we obtain

$$H = \frac{\mathbf{1}-Q^N}{1-Q}, \tag{54}$$

where N is a number operator acting on a monomial as

$$N(x^m\theta) = (m+1)x^m\theta. \tag{55}$$

We also have

$$\nabla(x^m\theta) = Q_{11}^m x^{m+1} - Q_{11}^{m+1}(x^m\theta)\,\nabla - Q_{11}Q_{22}x^{m+1}H. \tag{56}$$

So, applying the graded Leibniz rule to the product of functions f and g, we write

$$\mathsf{d}(fg) = [(\omega_x H + \omega_\theta \nabla)f]g + f(\omega_x H + \omega_\theta \nabla)g \tag{57}$$

with help of (39). From the commutation relations of the Cartan-Maurer forms with the coordinates of the quantum superplane, we can compute the corresponding relations of ω_x and ω_θ with functions of the coordinates. From (28) we have

$$\begin{aligned}(x^m\theta)\omega_x &= -Q^{m+1}\omega_x(x^m\theta) + Q^m Q_{22}\omega_\theta x^{m+1},\\ (x^m\theta)\omega_\theta &= Q_{11}^{m+1}\omega_\theta(x^m\theta).\end{aligned} \tag{58}$$

Inserting (58) in (57) and equating coefficients of the Cartan-Maurer forms, we get, for example,

$$H(fg) = (Hf)g + (\mathbf{1} + (Q-1)H)f(Hg). \tag{59}$$

Consequently, we have the coproducts for Type II

$$\begin{aligned}\Delta(H) &= H\otimes\mathbf{1} + (\mathbf{1} + (r-1)H)\otimes H,\\ \Delta(\nabla) &= \nabla\otimes\mathbf{1} + (\mathbf{1} + (r-1)H)^{h_2/h_1}\otimes\nabla,\end{aligned} \tag{60}$$

where

$$h_1 = \ln r, \quad h_2 = \ln q, \tag{61}$$

or with (54)

$$\begin{aligned}\Delta(N) &= N\otimes\mathbf{1} + \mathbf{1}\otimes N,\\ \Delta(\nabla) &= \nabla\otimes\mathbf{1} + q^N\otimes\nabla.\end{aligned} \tag{62}$$

The counit and coinverse may be calculated by using the axioms of Hopf algebra:

$$\begin{aligned}m(\epsilon\otimes\mathrm{id})\Delta(u) &= u = m(\mathrm{id}\otimes\epsilon)\Delta(u),\\ m(\mathrm{id}\otimes S)\Delta(u) &= \epsilon(u) = m(S\otimes\mathrm{id})\Delta(u).\end{aligned} \tag{63}$$

So we have

$$\epsilon(N) = 0,$$

$$\epsilon(\nabla) = 0,$$
$$S(N) = -N, \tag{64}$$
$$S(\nabla) = -q^N \nabla .$$

The dual of $\mathcal{A}$, denoted by $\mathcal{U}$ is generated by the elements H and ∇ obeying relations (41). Multiplication and comultiplication in $\mathcal{U}$ can be obtained from the corresponding ones in its dual $\mathcal{A}$, but in the above we get the relevant formulas [Eqs. (41), (62), and (64)] without using its duality with $\mathcal{A}$. We now call $\langle U,a\rangle$ the evaluation of U on a where $U \in \mathcal{U}$ and $a \in \mathcal{A}$. Using

$$\langle U_1 U_2, a\rangle = \langle U_1 \otimes U_2, \Delta_{\mathcal{A}}(a)\rangle,$$
$$\langle U, a_1 a_2\rangle = \langle \Delta_{\mathcal{U}}(U), a_1 \otimes a_2\rangle \tag{65}$$

and

$$\langle U, \mathbf{1}_{\mathcal{A}}\rangle = \epsilon_{\mathcal{U}}(U), \quad \langle \mathbf{1}_{\mathcal{U}}, a\rangle = \epsilon_{\mathcal{A}}(a) \tag{66}$$

we then can compute all possible pairings from those between the generators H, ∇, and x, θ. They are given by for Type II

$$\left\langle T, \begin{pmatrix} x \\ \theta \end{pmatrix} \right\rangle = \begin{pmatrix} r \\ 0 \end{pmatrix}, \quad \left\langle \nabla, \begin{pmatrix} x \\ \theta \end{pmatrix} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{67}$$

To obtain the (left) action of the elements of $\mathcal{U}$ on the elements of $\mathcal{A}$, we now may use the following properties:[15]

$$U[a] = a_{(1)}\langle U, a_{(2)}\rangle,$$
$$U[af] = m \circ \Delta_{\mathcal{U}}(U)[a \otimes f], \tag{68}$$

where $\Delta_{\mathcal{A}}(a) = \Sigma a_{(1)} \otimes a_{(2)}$ is the coproduct of a. For example, one has

$$T[xf] = m \circ \Delta_{\mathcal{U}}(T)[x \otimes f] = m(T \otimes T)[x \otimes f] = T[x]T[f] = rxT[f], \tag{69}$$

so that

$$Tx = rxT. \tag{70}$$

Similarly, we find

$$T\theta = r\theta T,$$
$$\nabla x = qx\nabla , \tag{71}$$
$$\nabla\theta = x - q\theta\nabla .$$

IV. EXTENDED CALCULUS ON THE QUANTUM SUPERPLANE

A Lie derivative is a derivation on the algebra of tensor fields over a manifold. The Lie derivative should be defined in three ways: on scalar functions, vector fields, and tensors.

The Lie derivative can also be defined on differential forms. In this case, it is closely related to the exterior derivative. The exterior derivative and the Lie derivative are set to cover the idea of a derivative in different ways. These differences can be hasped together by introducing the idea of an antiderivation which is called an inner derivation.

A. Inner derivations

Let us begin with some information about the inner derivations. Generally, for a smooth vector field X on a manifold the inner derivation, denoted by $\mathbf{i}_X$, is a linear operator which maps k-forms to $(k-1)$-forms. If we define the inner derivation $\mathbf{i}_X$ on the set of all differential forms on a manifold, we know that $\mathbf{i}_X$ is an antiderivation of degree -1:

$$\mathbf{i}_X(\alpha \wedge \beta) = (\mathbf{i}_X\alpha) \wedge \beta + (-1)^k \alpha \wedge (\mathbf{i}_X\beta), \tag{72}$$

where α and β are both differential forms. The inner derivation $\mathbf{i}_X$ acts on zero- and one-forms as follows:

$$\begin{aligned} \mathbf{i}_X(f) &= 0, \\ \mathbf{i}_X(\mathrm{d}f) &= X(f). \end{aligned} \tag{73}$$

We now wish to find the commutation relations between the coordinates x, θ, and the inner derivations associated with them. In order to obtain the commutation rules of the coordinates with inner derivations, we shall assume that they are of the following form:

$$\begin{aligned} \mathbf{i}_x x &= A_1 x \mathbf{i}_x + A_2 \theta \mathbf{i}_\theta, \\ \mathbf{i}_x \theta &= A_3 \theta \mathbf{i}_x + A_4 x \mathbf{i}_\theta, \\ \mathbf{i}_\theta x &= A_5 x \mathbf{i}_\theta + A_6 \theta \mathbf{i}_x, \\ \mathbf{i}_\theta \theta &= A_7 \theta \mathbf{i}_\theta + A_8 x \mathbf{i}_x. \end{aligned} \tag{74}$$

The coefficients A_k $(1 \leqslant k \leqslant 8)$ will be determined in terms of the deformation parameters in relations (11). But the use of the relations (5) does not give rise to any solution in terms of the parameters Q and Q_{ij} $(1 \leqslant i, j \leqslant 2)$ in (11). Howover, we have, at least, the system

$$\begin{aligned} &A_4(A_1 - qA_5) = 0, \quad A_4(A_3 + qA_7) = 0, \quad A_2A_8 = 0, \\ &A_8(A_5 - qA_1) = 0, \quad A_8(qA_1 + A_7) = 0, \quad A_4A_8 = 0. \end{aligned} \tag{75}$$

To find the coefficients, we need the commutation relations of the inner derivations with the differentials of x and θ. Since

$$\mathbf{i}_{X_i}(\mathrm{d}X_j) = \delta_{ij} \tag{76}$$

we can assume that the relations between the differentials and the inner derivations are of the following form

$$\begin{aligned} \mathbf{i}_x \mathrm{d}x &= 1 + a_1 \mathrm{d}x \mathbf{i}_x + a_2 \mathrm{d}\theta \mathbf{i}_\theta, \\ \mathbf{i}_x \mathrm{d}\theta &= a_3 \mathrm{d}\theta \mathbf{i}_x + a_4 \mathrm{d}x \mathbf{i}_\theta, \\ \mathbf{i}_\theta \mathrm{d}x &= a_5 \mathrm{d}x \mathbf{i}_\theta + a_6 \mathrm{d}\theta \mathbf{i}_x, \\ \mathbf{i}_\theta \mathrm{d}\theta &= 1 + a_7 \mathrm{d}\theta \mathbf{i}_\theta + a_8 \mathrm{d}x \mathbf{i}_x. \end{aligned} \tag{77}$$

Using relations (12) we get the system

$$a_2(a_5 - Q') = 0, \quad a_5 = Q'(1 + a_8), \quad a_1 = -1,$$
$$a_2(a_7 - Q'a_3) = 0, \quad a_2 = Q'a_3 - 1, \quad a_2 a_6 = 0. \tag{78}$$

Now the use of the relations (11) will give

$$A_1 = Q, \quad A_2 = Q_{12}, \quad A_3 = Q_{21}, \quad A_4 = 0,$$
$$A_5 = Q_{11}, \quad A_6 = 0, \quad A_7 = 1, \quad A_8 = Q_{22} \tag{79}$$

and some additional relations consisting A_k, a_k and

$$a_6 = 0.$$

To find the remaining parameters a_k, this time we assume that the commutation relations of the inner derivations with the partial derivatives ∂_x and ∂_θ are in the following form:

$$\mathbf{i}_x \partial_x = B_1 \partial_x \mathbf{i}_x + B_2 \partial_\theta \mathbf{i}_\theta,$$
$$\mathbf{i}_x \partial_\theta = B_3 \partial_\theta \mathbf{i}_x + B_4 \partial_x \mathbf{i}_\theta,$$
$$\mathbf{i}_\theta \partial_x = B_5 \partial_x \mathbf{i}_\theta + B_6 \partial_\theta \mathbf{i}_x, \tag{80}$$
$$\mathbf{i}_\theta \partial_\theta = B_7 \partial_\theta \mathbf{i}_\theta + B_8 \partial_x \mathbf{i}_x.$$

Then using the relations (34) we obtain

$$B_1 = Q^{-1}, \quad B_2 = 0,$$
$$B_3 = Q_{21}^{-1}, \quad B_4 = -Q_1^{-1} Q_{21}^{-1} Q_{12},$$
$$B_5 = Q_{11}^{-1}, \quad B_6 = -Q_{11}^{-1} Q_{21}^{-1} Q_{22}, \tag{81}$$
$$B_7 = 1, \quad B_8 = 0.$$

If we demand that the commutation rules of the inner derivations with d in the form

$$\mathbf{i}_x \circ \mathsf{d} - F \mathsf{d} \circ \mathbf{i}_x = \partial_x,$$
$$\mathbf{i}_\theta \circ \mathsf{d} - F' \mathsf{d} \circ \mathbf{i}_\theta = \partial_\theta, \tag{82}$$

one has

$$F = -Q^{-1}, \quad F' = -F,$$
$$a_2 = -Q^{-1} Q_{12}, \quad a_4 = 0, \quad a_7 = Q^{-1}, \tag{83}$$
$$a_3 = -Q^{-1} Q_{21}, \quad a_5 = Q^{-1} Q_{11}, \quad a_8 = Q'^{-1} Q^{-1} Q_{22}.$$

Consequently, we have the following commutation relations:

- the commutation relations of the inner derivations with x and θ

$$\mathbf{i}_x x = Q x \mathbf{i}_x + Q_{12} \theta \mathbf{i}_\theta,$$

$$\begin{aligned}
\mathbf{i}_x\theta &= Q_{21}\theta\mathbf{i}_x,\\
\mathbf{i}_\theta x &= Q_{11}x\mathbf{i}_\theta,\\
\mathbf{i}_\theta\theta &= \theta\mathbf{i}_\theta + Q_{22}x\mathbf{i}_x,
\end{aligned} \tag{84}$$

- the commutation relations between the differentials and the inner derivations

$$\begin{aligned}
\mathbf{i}_x\mathrm{d}x &= 1 - \mathrm{d}x\mathbf{i}_x - Q^{-1}Q_{12}\mathrm{d}\theta\mathbf{i}_\theta,\\
\mathbf{i}_x\mathrm{d}\theta &= -Q^{-1}Q_{21}\mathrm{d}\theta\mathbf{i}_x,\\
\mathbf{i}_\theta\mathrm{d}x &= Q^{-1}Q_{11}\mathrm{d}x\mathbf{i}_\theta,\\
\mathbf{i}_\theta\mathrm{d}\theta &= 1 + Q^{-1}\mathrm{d}\theta\mathbf{i}_\theta + (QQ')^{-1}Q_{22}\mathrm{d}x\mathbf{i}_x,
\end{aligned} \tag{85}$$

- the relations of the inner derivations with the partial derivatives ∂_x and ∂_θ,

$$\begin{aligned}
\mathbf{i}_x\partial_x &= Q^{-1}\partial_x\mathbf{i}_x,\\
\mathbf{i}_x\partial_\theta &= Q_{21}^{-1}\partial_\theta\mathbf{i}_x - (Q_{11}Q_{21})^{-1}Q_{12}\partial_x\mathbf{i}_\theta,\\
\mathbf{i}_\theta\partial_x &= Q_{11}^{-1}\partial_x\mathbf{i}_\theta - (Q_{11}Q_{21})^{-1}Q_{22}\partial_\theta\mathbf{i}_x,\\
\mathbf{i}_\theta\partial_\theta &= \partial_\theta\mathbf{i}_\theta.
\end{aligned} \tag{86}$$

B. Lie derivatives

We know, from the classical differential geometry, that the Lie derivative $\mathcal{L}$ can be defined as a linear map from the exterior algebra into itself which takes k-forms to k-forms. For a zero-form, that is, an ordinary function f, the Lie derivative is just the contraction of the exterior derivative with the vector field X:

$$\mathcal{L}_X f = \mathbf{i}_X\mathrm{d}f. \tag{87}$$

For a general differential form, the Lie derivative is likewise a contraction, taking into account the variation in X:

$$\mathcal{L}_X\alpha = \mathbf{i}_X\mathrm{d}\alpha + \mathrm{d}(\mathbf{i}_X\alpha). \tag{88}$$

The Lie derivative has the following properties. If $\mathcal{F}(M)$ is the algebra of functions defined on the manifold M then

$$\mathcal{L}_X{:}\mathcal{F}(M) \to \mathcal{F}(M) \tag{89}$$

is a derivation on the algebra $\mathcal{F}(M)$:

$$\begin{aligned}
\mathcal{L}_X(af + bg) &= a(\mathcal{L}_X f) + b(\mathcal{L}_X g),\\
\mathcal{L}_X(fg) &= (\mathcal{L}_X f)g + f(\mathcal{L}_X g),
\end{aligned} \tag{90}$$

where a and b real numbers.

The Lie derivative is a derivation on $\mathcal{F}(M)\times\mathcal{V}(M)$ where $\mathcal{V}(M)$ is the set of vector fields on M:

$$\mathcal{L}_{X_1}(fX_2) = (\mathcal{L}_{X_1}f)X_2 + f(\mathcal{L}_{X_1}X_2). \tag{91}$$

The Lie derivative also has an important property when acting on differential forms. If α and β are two differential forms on M then

$$\mathcal{L}_X(\alpha \wedge \beta) = (\mathcal{L}_X\alpha) \wedge \beta + (-1)^k \alpha \wedge (\mathcal{L}_X\beta), \tag{92}$$

where α is a k-form.

In this section we now wish to find the commutation rules of the Lie derivatives with functions, i.e., the elements of the algebra $\mathcal{A}$, their differentials, etc. For example, the relation of $\mathcal{L}_x$ with x can be obtained, using relations (74) and (77), as follows:

$$\begin{aligned}
\mathcal{L}_x x &= (\mathbf{i}_x \circ \mathsf{d} + \mathsf{d} \circ \mathbf{i}_x)x \\
&= \mathbf{i}_x \mathsf{d}x + \mathsf{d}(\mathbf{i}_x x) \\
&= 1 + a_1 \mathsf{d}x \mathbf{i}_x + a_2 \mathsf{d}\theta \mathbf{i}_\theta + \mathsf{d}(A_1 x \mathbf{i}_x + A_2 \theta \mathbf{i}_\theta) \\
&= 1 + A_1 x \mathcal{L}_x + A_2 \theta \mathcal{L}_\theta + (A_1 + a_1)\mathsf{d}x \mathbf{i}_x + (A_2 + a_2)\mathsf{d}\theta \mathbf{i}_\theta = 1 + Qx\mathcal{L}_x + Q_{12}\theta\mathcal{L}_\theta + (Q-1)(\mathsf{d}x\mathbf{i}_x \\
&\quad + Q^{-1}Q_{12}\mathsf{d}\theta\mathbf{i}_\theta).
\end{aligned} \tag{93}$$

Similarly, one has

$$\mathcal{L}_x\theta = -Q_{21}\theta\mathcal{L}_x + Q_{21}(1-Q^{-1})\mathsf{d}\theta\mathbf{i}_x,$$

$$\mathcal{L}_\theta x = (\mathbf{i}_\theta \circ \mathsf{d} - \mathsf{d} \circ \mathbf{i}_\theta)x = Q_{11}x\mathcal{L}_\theta + Q_{11}(Q^{-1}-1)\mathsf{d}x\mathbf{i}_\theta, \tag{94}$$

$$\mathcal{L}_\theta\theta = 1 - \theta\mathcal{L}_\theta - Q_{22}x\mathcal{L}_x - Q_{22}((QQ')^{-1}-1)\mathsf{d}x\mathbf{i}_x + (Q^{-1}-1)\mathsf{d}\theta\mathbf{i}_\theta.$$

The following relations can be obtained from (85):

$$\begin{aligned}
\mathcal{L}_x\mathsf{d}x &= \mathsf{d}x\mathcal{L}_x + Q^{-1}Q_{12}\mathsf{d}\theta\mathcal{L}_\theta, \\
\mathcal{L}_x\mathsf{d}\theta &= -Q^{-1}Q_{21}\mathsf{d}\theta\mathcal{L}_x, \\
\mathcal{L}_\theta\mathsf{d}x &= -Q^{-1}Q_{11}\mathsf{d}x\mathcal{L}_\theta, \\
\mathcal{L}_\theta\mathsf{d}\theta &= Q^{-1}\mathsf{d}\theta\mathcal{L}_\theta + (QQ')^{-1}Q_{22}\mathsf{d}x\mathcal{L}_x.
\end{aligned} \tag{95}$$

Other commutation relations can be similarly obtained. To complete the description of the above-presented scheme, we get in the following the remaining commutation relations as follows:

- the Lie derivatives and partial derivatives

$$\begin{aligned}
\mathcal{L}_x\partial_x &= \partial_x\mathcal{L}_x, \\
\mathcal{L}_x\partial_\theta &= -QQ_{21}^{-1}\partial_\theta\mathcal{L}_x + Q(Q_{11}Q_{21})^{-1}Q_{12}\partial_x\mathcal{L}_\theta, \\
\mathcal{L}_\theta\partial_x &= QQ_{11}^{-1}\partial_x\mathcal{L}_\theta - Q(Q_{11}Q_{21})^{-1}Q_{22}\partial_\theta\mathcal{L}_x, \\
\mathcal{L}_\theta\partial_\theta &= -Q\partial_\theta\mathcal{L}_\theta,
\end{aligned} \tag{96}$$

- the inner derivations

$$\mathbf{i}_x\mathbf{i}_\theta = -Q_{11}(Q_{12}-Q)^{-1}\mathbf{i}_\theta\mathbf{i}_x,$$
$$\mathbf{i}_x\mathbf{i}_x = 0. \tag{97}$$

- the Lie derivatives and the inner derivations

$$\mathcal{L}_x\mathbf{i}_x = \mathbf{i}_x\mathcal{L}_x,$$

$$\mathcal{L}_x\mathbf{i}_\theta = -QQ_{21}^{-1}\mathbf{i}_\theta\mathcal{L}_x + Q_{12}(Q-Q_{12})^{-1}\mathbf{i}_x\mathcal{L}_\theta,$$
$$\mathcal{L}_\theta\mathbf{i}_x = -QQ_{11}^{-1}\mathbf{i}_x\mathcal{L}_\theta - (Q'Q_{21})^{-1}QQ_{22}\mathbf{i}_\theta\mathcal{L}_x, \tag{98}$$

$$\mathcal{L}_\theta\mathbf{i}_\theta = Q^{-1}\mathbf{i}_\theta\mathcal{L}_\theta,$$

- the Lie derivatives

$$\mathcal{L}_x\mathcal{L}_\theta = Q_{21}^{-1}(Q_{12}-Q)\mathcal{L}_\theta\mathcal{L}_x,$$
$$\mathcal{L}_\theta^2 = 0. \tag{99}$$

Note that the Lie derivatives can be written as follows:

$$\mathcal{L}_x = \partial_x + (1-Q^{-1})\mathsf{d}\circ\mathbf{i}_x,$$
$$\mathcal{L}_\theta = \partial_\theta - (1-Q^{-1})\mathsf{d}\circ\mathbf{i}_\theta, \tag{100}$$

or in terms of vector fields and coordinates

$$\mathcal{L}_x = x^{-1}H - x^{-1}\theta x^{-1}\nabla + (1-Q^{-1})\mathsf{d}\circ\mathbf{i}_x,$$
$$\mathcal{L}_\theta = x^{-1}\nabla - (1-Q^{-1})\mathsf{d}\circ\mathbf{i}_\theta. \tag{101}$$

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Yang-Baxter maps and symmetries of integrable equations on quad-graphs

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A connection between the Yang-Baxter relation for maps and the multidimensional consistency property of integrable equations on quad-graphs is investigated. The approach is based on the symmetry analysis of the corresponding equations. It is shown that the Yang-Baxter variables can be chosen as invariants of the multiparameter symmetry groups of the equations. We use the classification results by Adler, Bobenko, and Suris to demonstrate this method. Some new examples of Yang-Baxter maps are derived in this way from multifield integrable equations. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2227641]

I. INTRODUCTION

The quantum Yang-Baxter (YB) equation has its origins in the theory of solvable models in statistical mechanics[1,2] and the quantum inverse scattering method.[3] The fact that this equation has also found many applications in representation theory, the construction of invariants in knot theory and that it lies at the foundation of quantum groups, gives to the quantum YB equation a prominent position among the basic equations in mathematical physics, see, e.g., Refs. 4 and 5, and references therein.

In its original form, the quantum YB equation is a relation for a linear operator $R: V \otimes V \to V \otimes V$, where V is a vector space. The relation has the form

$$R^{23}R^{13}R^{12} = R^{12}R^{13}R^{23}, \tag{1}$$

in End $(V \otimes V \otimes V)$, where R^{13} is meant as the identity in the second factor of the tensor product $V \otimes V \otimes V$ and as R in the first and third factors, and analogously for R^{12}, R^{23}. Supposing that X is any set, the maps R from the Cartesian product $X \times X$ into itself, which satisfy the relation (1) of composite maps are called set theoretic solutions of the quantum YB relation. The study of set theoretic solutions of the quantum YB equation was originally suggested by Drinfeld[6] (see also earlier work by Sklyanin[7] where the first interesting example of such solutions was found) and since then they have attracted the interest of many researchers.

More recently, a general theory on the set theoretic solutions to the YB relation was developed in Ref. 8 and the notion of transfer maps, which can be considered as the dynamical analogues of the monodromy and transfer matrices in the theory of solvable models in statistical mechanics, was introduced in Ref. 9. In many interesting examples of YB maps,[10] such as maps arising from

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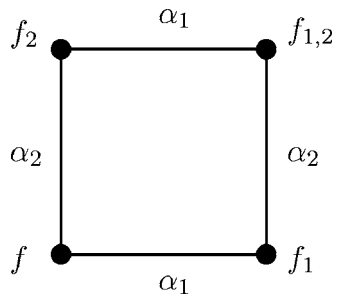

FIG. 1. An elementary quadrilateral.

geometric crystals,[11] the set X has the structure of an algebraic variety and R is a birational isomorphism. The case of $\mathbb{CP}^1 \times \mathbb{CP}^1$ has been recently discussed in Ref. 12 in relation to the classification of the so-called *quadrirational maps*.

In this paper we investigate the relation between the YB property for maps and the *multidimensional consistency* condition for equations on quad-graphs, which is now commonly accepted as a definition of integrability for such equations (see Refs. 13–15). Although the link between these two notions was known before (see, e.g., concluding remarks in Ref. 15) it was never explored systematically.

Our approach is based on the symmetry analysis of integrable equations on quad-graphs. The main idea is that the YB variables are suitable invariants of their symmetry groups. A good example is the *discrete potential Korteweg–de Vries* equation (dpKdV)[16–18]

$$(f_{1,2}-f)(f_1-f_2)-\alpha_1+\alpha_2=0 \tag{2}$$

(see notation in Fig. 1). It is clearly invariant under the translation $f \to f+\text{const}$. The invariants

$$x=f_1-f, \quad y=f_{1,2}-f_1, \quad u=f_{1,2}-f_2, \quad v=f_2-f, \tag{3}$$

satisfy the relation

$$x+y=u+v. \tag{4}$$

and Eq. (2) is written in terms of them as

$$(x+y)(x-v)=\alpha_1-\alpha_2. \tag{5}$$

This allows one to express u,v as functions of x,y, which leads to the following YB map:

$$u=y+\frac{\alpha_1-\alpha_2}{x+y}, \quad v=x-\frac{\alpha_1-\alpha_2}{x+y}, \tag{6}$$

known as the Adler map.[19] Note that the YB variables x, y, u, v, are attached to the edges of the lattice. The fact that the corresponding map satisfies the YB property follows directly from the three dimensional (3D) consistency property of dpKdV (see Fig. 5). This construction works for integrable equations on quad-graphs with one-parameter symmetry group.

One of the main findings of our paper is that this idea works for multiparameter symmetry groups if one considers the extension of the equation on a multidimensional lattice. In that case the edges are replaced by higher dimensional faces. We show that in such a way one can derive from the same discrete potential KdV the following YB map:

$$u=yQ, \quad v=xQ^{-1}, \quad Q=\frac{(1-\gamma_2)+(\gamma_2-\gamma_1)x+\gamma_2(\gamma_1-1)xy}{(1-\gamma_1)+(\gamma_1-\gamma_2)y+\gamma_1(\gamma_2-1)xy}. \tag{7}$$

We will call it *Harrison* map since it is closely related to the superposition formula of the

Bäcklund transformation for the Ernst equation in general relativity introduced by Harrison.[20] After the change of variables $x \mapsto 1/x, v \mapsto 1/v, y \mapsto y/\gamma_2, u \mapsto u/\gamma_1$ it coincides with the F_I quadrirational map in Ref. 12, which corresponds to the most general case of two conics. Note that the most degenerate case F_V in the classification of Ref. 12 is simply related to the Adler map.

The plan of the paper is the following. We start in Sec. II with the discussion of the 3D consistency property for equations on quad-graphs. As examples we choose three equations from the classification list in Ref. 15. By considering the invariants of their one-parameter symmetry groups we derive all five types of the quadrirational maps from Ref. 12. Next, in Sec. III, we show how this symmetry method can be generalized in the case where the lattice equation admits a multiparameter symmetry group. This is demonstrated on the example of the lattice KdV equation by extending it to a three-dimensional cube and using the invariants of a two-parameter symmetry group as YB variables. Finally, we show how the Harrison map can be retrieved from the lattice KdV equation by exploiting its full three-parameter symmetry group and the consistency property on a four-dimensional cube.

In Sec. IV we show that the same idea works equally well for multifield integrable lattice equations and we derive certain examples of multidimensional YB maps from lattice equations in the Boussinesq family, vector Calapso equation and its specialization to an integrable discrete version of the $O(n+2)$ nonlinear σ model, introduced recently by Schief.[21] The paper concludes with perspectives where we address some questions for future study.

II. MULTIDIMENSIONAL CONSISTENCY AND YB MAPS

A. Equations on quad-graphs and the 3D consistency property

Central to our considerations are integrable discrete equations on quad-graphs, which are specific equations associated to planar graphs with elementary quadrilaterals faces. In the simplest case one has complex fields $f: \mathbb{Z}^2 \to \mathbb{C}$ assigned on the vertices at sites (n_1, n_2) and two complex lattice parameters α_1, α_2 assigned on the edges of an elementary square being equal on opposite edges (see Fig. 1). The basic building block of such equations consists of a relation of the form

$$\mathcal{E}(f, f_1, f_2, f_{1,2}; \alpha_1, \alpha_2) = 0, \tag{8}$$

between the values of four fields residing on the vertices of each elementary quadrilateral for which we use the shorthand notation:

$$f := f(n_1, n_2), \quad f_1 := f(n_1+1, n_2), \quad f_2 := f(n_1, n_2+1), \quad f_{1,2} := f(n_1+1, n_2+1). \tag{9}$$

Integrable discrete equations of the above mentioned type (8) are listed in a recent classification[15] where the 3D consistency property (see the following) and some additional conditions were imposed. From that list we consider the following:

$$\mathcal{E}_1: \quad (f_{1,2} - f)(f_1 - f_2) - \alpha_1 + \alpha_2 = 0, \tag{10}$$

$$\mathcal{E}_2: \quad \alpha_1(f f_1 + f_2 f_{1,2}) - \alpha_2(f f_2 + f_1 f_{1,2}) + \delta(\alpha_1^2 - \alpha_2^2) = 0, \tag{11}$$

$$\mathcal{E}_3: \quad (1-\alpha_2^2)(f_1 - \alpha_1 f)(f_2 - \alpha_1 f_{1,2}) - (1-\alpha_1^2)(f_2 - \alpha_2 f)(f_1 - \alpha_2 f_{1,2}) = 0. \tag{12}$$

Equation $\mathcal{E}_1$ is already mentioned as the dpKdV equation. Equation $\mathcal{E}_2$ with $\delta=0$ is the modified discrete KdV or *Hirota equation*.[16] If $\delta \neq 0$, we may always assume that $\delta=1$ using an appropriate gauge. Equation $\mathcal{E}_3$ corresponds to the equation labeled as $Q3_{\delta=0}$ in the classification of Ref. 15. It is contained in the four-parameter family of the equations derived earlier in Ref. 22, which contains also discrete versions of potential KdV, modified KdV, and Schwarzian KdV (see Ref. 23 for a more recent discussion).

The integrability of such equations can be defined using the *three-dimensional consistency* property. This means that the overdetermined system consisting of the difference equations

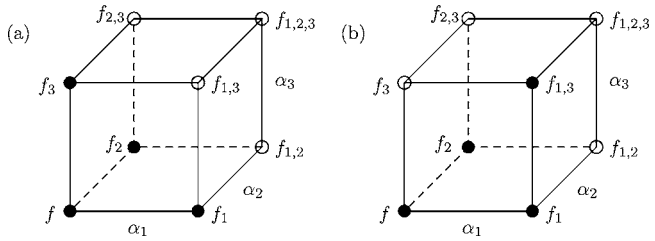

FIG. 2. Elementary initial value problems on the cube.

$$\mathcal{E}(f,f_i,f_j,f_{i,j};\alpha_i,\alpha_j)=0, \quad 1\leqslant i<j\leqslant 3, \tag{13}$$

and their shifted versions, is consistent on the three-dimensional lattice $\mathbb{Z}^3$. In practice, this property is verified as follows.[13–15] Consider an elementary initial value problem on the three-dimensional cube with initial data assigned on four vertices, exactly three of them lying on the same face. One such initial configuration is depicted in Fig. 2(a) with initial values $f,f_i,1\leqslant i\leqslant 3$. Using Eq. (13) on the three faces adjacent to the vertex with value f, we determine uniquely the values $f_{i,j},1\leqslant i<j\leqslant 3$, in terms of the initial data. Then using shifted versions of (13) on each of the remaining three faces, we evaluate $f_{1,2,3}$ in three different ways. Consistency means that one obtains the same value for $f_{1,2,3}$ in terms of the initial data $f,f_i,1\leqslant i\leqslant 3$ (independent of the way we choose to evaluate it). For the dpKdV equation (2) this value is

$$f_{1,2,3}=\frac{(\alpha_1-\alpha_2)f_1f_2+(\alpha_3-\alpha_1)f_1f_3+(\alpha_2-\alpha_3)f_2f_3}{(\alpha_2-\alpha_1)f_3+(\alpha_1-\alpha_3)f_2+(\alpha_3-\alpha_2)f_1}. \tag{14}$$

Note that the right-hand side of Eq. (14) is invariant under any permutation of the indices (1,2,3) which label the field variables and the associated lattice parameters.

Another initial data configuration, which is best adapted to the YB property that we consider, is depicted in Fig. 2(b). A third possible initial configuration is to give the values $f,f_1,f_2,f_{1,2,3}$. The latter two configurations are equivalent to the first one by using the equation on one of the faces. For example, by using the front face equation we can exchange the value $f_{1,3}$ to f_3 in the set of initial data.

Using the fact that dpKdV equation possesses the 3D consistency property, one can show in a similar manner that it can be consistently imposed on each two-dimensional face of a four-cube. Since we are going to use this property later on we describe explicitly its derivation.

For given initial values $f,f_i\ i=1,2,3,4$, we determine the shifted values of the fields involving any two different directions, using

$$(f_{i,j}-f)(f_i-f_j)=\alpha_i-\alpha_j, \tag{15}$$

$1\leqslant i<j\leqslant 4$ (see Fig. 3). Successively, since dpKdV is three-dimensional consistent, we determine the values $f_{ijk},1\leqslant i<j<k\leqslant 4$. Then the value $f_{1,2,3,4}$ can be found in six different ways, using the dpKdV equations on the six two-dimensional facets containing the vertex where the value $f_{1,2,3,4}$ is assigned. This vertex is contained also in four cubes, each one of them containing three of the six facets, and the incidence relations are such that taking into account the three-dimensional consistency on each of the four cubes one proves that the value $f_{1,2,3,4}$ is uniquely determined in terms of initial data. By direct calculations also we find that this value is independent of the way that we used to calculate it, and equals

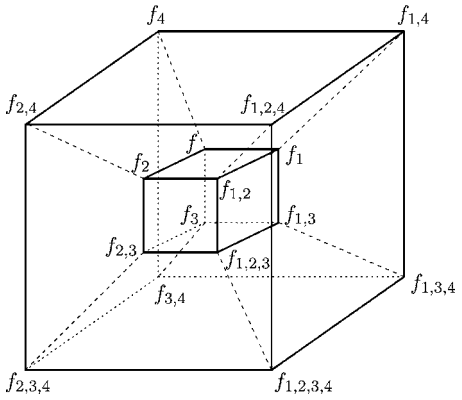

FIG. 3. Discrete potential KdV in $\mathbb{Z}^4$.

$$f_{1,i,j,k} = \frac{\boldsymbol{\sigma}_{ijk}(\alpha_1\alpha_i f_{i,j} + \alpha_j\alpha_k f_{j,k})(f_1 - f_i)(f_j - f_k)}{\boldsymbol{\sigma}_{ijk}(\alpha_1\alpha_i + \alpha_j\alpha_k)(f_1 - f_i)(f_j - f_k)}, \tag{16}$$

where $\boldsymbol{\sigma}_{ijk}$ denotes the cyclic sum over the subscripts $(i,j,k)=(2,3,4),(4,2,3),(3,4,2)$. It can be easily checked that $f_{1,2,3,4}$ given by (16) remains invariant under any permutation of the indices (1,2,3,4), thus dpKdV is four-dimensional consistent.

B. YB relation and 3D consistency property

Let $\mathbb{X}$ be any set and R a map of $\mathbb{X}\times\mathbb{X}$ into itself. Let R^{ij}: $\mathbb{X}^n \to \mathbb{X}^n$, where $\mathbb{X}^n = \mathbb{X}\times\mathbb{X}\times\cdots\times\mathbb{X}$, denotes the map which acts as R on the i and j factors and as the identity on the others. More explicitly, let us write $R(x,y), x,y \in \mathbb{X}$, as

$$R(x,y) = (f(x,y), g(x,y)). \tag{17}$$

Then, for $n \geqslant 2$ and $1 \leqslant i,j \leqslant n, i \neq j$ we define

$$R^{ij}(x^1,x^2,\ldots,x^n) = \begin{cases} (x^1,\ldots,x^{i-1},f(x^i,x^j),x^{i+1},\ldots,x^{j-1},g(x^i,x^j),x^{j+1},\ldots,x^n), & i<j \\ (x^1,\ldots,x^{j-1},g(x^i,x^j),x^{j+1},\ldots,x^{i-1},f(x^i,x^j),x^{i+1},\ldots,x^n), & i>j \end{cases}. \tag{18}$$

In particular, for $n=2$ we find that $R^{12}=R$ and $R^{21}(x,y)=(g(y,x),f(y,x))$. The latter map can be written as a composition of maps as follows:

$$R^{21} = PRP, \tag{19}$$

where P is the permutation map, i.e., $P(x,y)=(y,x)$.

A map R is called a *YB map* if it satisfies the YB relation (1), regarded as an equality of maps from $\mathbb{X}\times\mathbb{X}\times\mathbb{X}$ into itself. If in addition the relation $R^{21}R=\mathrm{Id}$ holds, then R is called reversible YB map.

In a more general setting we may consider a whole family of YB maps parametrized by continuous parameters α_i rather than a single map. The YB relation then takes the parameter-dependent form

$$R^{23}(\alpha_2,\alpha_3)R^{13}(\alpha_1,\alpha_3)R^{12}(\alpha_1,\alpha_2) = R^{12}(\alpha_1,\alpha_2)R^{13}(\alpha_1,\alpha_3)R^{23}(\alpha_2,\alpha_3), \tag{20}$$

and the reversibility condition becomes

$$R^{21}(\alpha_2,\alpha_1)R(\alpha_1,\alpha_2) = \mathrm{Id}. \tag{21}$$

The relation between YB maps and integrable equations on quad-graphs can be demonstrated in the example of the discrete potential KdV equation $\mathcal{E}_1$. As we have already shown in Sec. I, by considering the differences of the values of the fields assigned on two adjacent vertices (3), we arrive at the Adler map (6). There is a different combination for the variables assigned on the edges of the square, namely

$$x = ff_1, \quad y = f_1 f_{1,2}, \quad u = f_2 f_{1,2}, \quad v = ff_2. \tag{22}$$

From the above-noted relations (22) we deduce that

$$xu = yv. \tag{23}$$

Moreover, dpKdV can also be written in terms of the variables (22) as follows:

$$y + v - x - u = \alpha_1 - \alpha_2. \tag{24}$$

Solving Eqs. (23) and (24) for (u,v) we get the following map:

$$u = y\left(1 + \frac{\alpha_1 - \alpha_2}{x - y}\right), \quad v = x\left(1 + \frac{\alpha_1 - \alpha_2}{x - y}\right). \tag{25}$$

The maps (6) and (25) *automatically* satisfy the parameter dependent YB relation (20). Indeed, it is easily shown that the consistency property for a configuration of initial data on the vertices of a cube, as depicted in Fig. 2, is equivalent to that with initial values $f, f_1, f_{1,2}, f_{1,2,3}$. These initial data correspond to the values (x,y,z) on the edges (Fig. 5). The 3D consistency property guarantees that the composite maps

$$(a): \quad (x,y,z) \overset{R^{12}}{\to} (x_2,y_{-1},z) \overset{R^{13}}{\to} (x_{2,3},y_{-1},z_{-2}) \overset{R^{23}}{\to} (x_{2,3},y_{-1,3},z_{-1,-2}), \tag{26}$$

$$(b): \quad (x,y,z) \overset{R^{23}}{\to} (x,y_3,z_{-2}) \overset{R^{13}}{\to} (x_3,y_3,z_{-1,-2}) \overset{R^{12}}{\to} (x_{2,3},y_{-1,3},z_{-1,-2}) \tag{27}$$

appearing in Eq. (20), applied on (x,y,z) give identical values for $(x_{2,3}, y_{-1,3}, z_{1,-2})$.

Analyzing these two examples one notices that the variables x,y,u,v, which we call YB variables, are *invariants* of certain *symmetry groups* of the relevant lattice equation. Now we are going to show that this symmetry method can be applied in more general situations as well.

C. Lattice invariants of symmetry groups and YB variables

Let us first recall the basic notions of Lie symmetry methods applied to lattice equations of the form (8). With minor modifications these are in accordance with the symmetry methods applied to algebraic or differential equations (see, e.g., Ref. 24 for an extensive study on the subject).

Consider a lattice equation of the form (8) involving one field $f: \mathbb{Z}^2 \to \mathbb{C}$(or $\mathbb{CP}^1$). Let G be a one-parameter group of transformations acting on the domain of the dependent variables,

$$G: f \mapsto \Phi(n_1,n_2,f;\varepsilon), \quad \varepsilon \in \mathbb{C}. \tag{28}$$

The prolongation of the group action on the lattice jet space J with coordinates $(f,f_1,f_2,f_{1,2})$ is specified by

$$G: (f,f_1,f_2,f_{1,2}) \mapsto (\Phi(n_1,n_2,f;\varepsilon), \Phi(n_1+1,n_2,f_1;\varepsilon), \Phi(n_1,n_2+1,f_2;\varepsilon), \Phi(n_1+1,n_2+1,f_{1,2};\varepsilon)). \tag{29}$$

The infinitesimal generator of the group action of G on f is the vector field

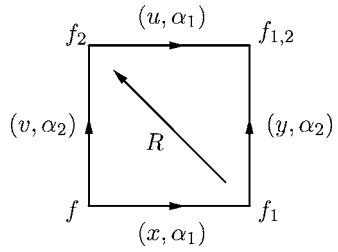

FIG. 4. An oriented quadrilateral for the map $R(x,y)=(u,v)$.

$$\mathbf{v} = Q(n_1,n_2,f)\partial_f, \quad \text{where } Q(n_1,n_2,f) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Phi(n_1,n_2,f;\varepsilon)_{\varepsilon=0}. \tag{30}$$

There is a one-to-one correspondence between connected groups of transformations and their associated infinitesimal generators since the group action is reconstructed by the flow of the vector field $\mathbf{v}$ by exponentiation

$$\Phi(n_1,n_2,f;\varepsilon) = \exp(\varepsilon\mathbf{v})f. \tag{31}$$

The prolongation of the infinitesimal action of G given by (29) is generated by the prolonged vector field

$$\hat{\mathbf{v}} = Q\partial_f + Q_1\partial_{f_1} + Q_2\partial_{f_2} + Q_{1,2}\partial_{f_{1,2}}, \tag{32}$$

where subscripts denote $Q_1=Q(n_1+1,n_2,f_1), Q_{1,2}=Q(n_1+1,n_2+1,f_{1,2})$, and so on.

The transformation G is a symmetry of the lattice equation (8), if it transforms any solution of (8) to another solution of the same equation. Equivalently, G is a symmetry of Eq. (8), if the equation is not affected by the transformation (29). The infinitesimal criterion for G to be a symmetry of Eq. (8) is

$$\hat{\mathbf{v}}(\mathcal{E}(f,f_1,f_2,f_{1,2};\alpha_1,\alpha_2)) = 0, \tag{33}$$

whenever Eq. (8) holds.

A function $I:J\to\mathbb{C}$ is a *lattice invariant* of the transformation group G, if I is not affected under the action of G. The infinitesimal invariance condition for the lattice invariants is

$$\hat{\mathbf{v}}(I) = 0. \tag{34}$$

Once we have determined a symmetry generator $\mathbf{v}$ of the lattice equation (8), the corresponding lattice invariants can be found from the solution of the first-order partial differential equation (34), by using the method of characteristics. From the corresponding system of ordinary differential equations we may easily obtain the general solution, since it consists of equations with separated variables. We assign now to the edges of an elementary quadrilateral the following YB variables (Fig. 4):

$$x = I(f,f_1), \quad y = I(f_1,f_{1,2}), \quad u = I(f_2,f_{1,2}), \quad v = I(f,f_2), \tag{35}$$

where I is an invariant depending on two neighboring values of f. Since G is a symmetry of the lattice equation, the latter can be written in terms of these variables:

$$\mathcal{D}(x,y,u,v;\alpha_1,\alpha_2) = 0. \tag{36}$$

This can be done in different ways since the variables (35) are not independent; there exists a relation among them

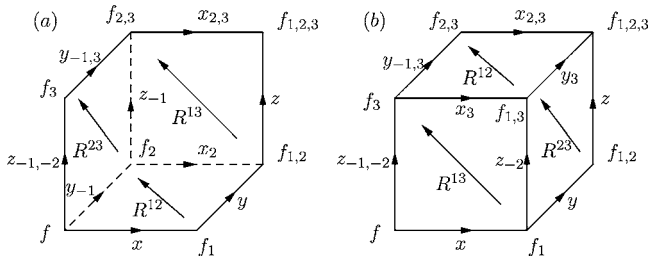

FIG. 5. Three-dimensional representation of the YB relation.

$$\mathcal{F}(x,y,u,v;\alpha_1,\alpha_2)=0, \tag{37}$$

following from the fact that the space of G-orbits is three-dimensional.

Solving the system of equations (36) and (37) for u,v in terms of x,y and assuming that the solution is unique, we obtain a map $R(x,y)=(u,v)$.

Proposition II.1: *If the discrete equation $\mathcal{E}$ satisfies the 3D consistency property, then the map $R(x,y)=(u,v)$, which relates the lattice invariants* (35)*, satisfies the YB relation.*

The proof follows from Fig. 5. Similar considerations hold for multifield lattice equations, which give rise to multicomponent YB maps (see Sec. IV).

Example II.2: Consider the dpKdV equation (2). Two infinitesimal symmetry generators of the latter equation are

$$\mathbf{v}_1=\partial_f, \quad \mathbf{v}_2=(-1)^{n_1+n_2}f\partial_f \tag{38}$$

(see Ref. 25). They generate the symmetry transformations

$$G^1{:}f\mapsto f+\varepsilon_1, \quad G^2{:}f\mapsto f\exp(\varepsilon_2(-1)^{n_1+n_2}), \quad \varepsilon_1,\varepsilon_2\in\mathbb{C}, \tag{39}$$

respectively. The lattice invariants assigned on the edges of a square for each one of the above-noted symmetry transformations are the variables (3) and (22), respectively.

The consideration of the remaining two equations from the list (10)–(12), with the corresponding symmetry generators

$$\mathbf{v}_{\mathcal{E}_2}=(-1)^{n_1+n_2}f\partial_f, \quad \mathbf{v}_{\mathcal{E}_3}=f\partial_f, \tag{40}$$

leads to the results summarized in the Table I.

These maps are simply related to quadrirational maps $F_{\mathrm{I}}-F_{\mathrm{III}}$ from the Adler-Bobenko-Suris (ABS) list of Ref. 12. Namely, setting $\delta=0$ in the YB map constructed from $\mathcal{E}_2$, we retrieve the map labeled as F_{III} map in Ref. 12. The case $\delta=-1$ corresponds to the F_{II} map. Finally, the YB map constructed from $\mathcal{E}_3$ under the transformation $x\mapsto 1/x$, $v\mapsto 1/v$, $y\mapsto y/\gamma_2$, $u\mapsto u/\gamma_1$ turns into

$$u=\gamma_1 y\widetilde{Q}, \quad v=\gamma_2 x\widetilde{Q}, \quad \widetilde{Q}=\frac{(1-\gamma_2)x+\gamma_2-\gamma_1+(\gamma_1-1)y}{\gamma_2(1-\gamma_1)x+(\gamma_1-\gamma_2)xy+\gamma_1(\gamma_2-1)y}, \tag{41}$$

which corresponds to the F_{I} map in the classification in Ref. 12. As we have already mentioned it is closely related to the superposition formula of the Bäcklund transformation for the Ernst equation in general relativity introduced by Harrison,[20] cf. Ref. 26.

The remaining maps F_{IV} and F_{V} from Ref. 12 are related in a simple way to the maps (6) and (25) derived from dpKdV already in Sec. II B.

Thus all five types of quadrirational maps from the ABS classification are equivalent to the YB maps coming from the integrable equations on quad-graphs.

Remark II.3: We should mention that the equivalence of the quadrirational maps considered in Ref. 12 allows independent change of variables x,y,u,v and therefore does not respect the YB property, which is preserved in general only under the diagonal action of the Möbius group. In

TABLE I. YB maps arising from equations $\mathcal{E}_2$ and $\mathcal{E}_3$.

	YB variables	Functional relation and lattice equation	YB Map
$\mathcal{E}_2$	$x=ff_1/\alpha_1$ $y=f_1f_{1,2}/\alpha_2$ $u=f_2f_{1,2}/\alpha_1$ $v=ff_2/\alpha_2$	$\gamma_1xu=\gamma_2yv$ $\gamma_1(x+u+\delta)=\gamma_2(y+v+\delta)$ where $\gamma_i=\alpha_i^2$	$u=\frac{y}{\gamma_1}\frac{\gamma_1(x+\delta)-\gamma_2(y+\delta)}{x-y}$ $v=\frac{x}{\gamma_2}\frac{\gamma_1(x+\delta)-\gamma_2(y+\delta)}{x-y}$
$\mathcal{E}_3$	$x=f_1/(\alpha_1f)$ $y=f_{1,2}/(\alpha_2f_1)$ $u=f_{1,2}/(\alpha_1f_2)$ $v=f_2/(\alpha_2f)$	$xy=uv$ $\frac{1-x^{-1}}{1-v^{-1}}=\frac{1-\gamma_1}{1-\gamma_2}\frac{1-\gamma_2y}{1-\gamma_1u}$ where $\gamma_i=\alpha_i^2$	$u=yQ,\quad v=xQ^{-1}$ $Q=\frac{(1-\gamma_2)+(\gamma_2-\gamma_1)x+\gamma_2(\gamma_1-1)xy}{(1-\gamma_1)+(\gamma_1-\gamma_2)y+\gamma_1(\gamma_2-1)xy}$

particular, quadrirational maps in general do not satisfy the YB relation (contrary to what one might conclude from Ref. 12). However sometimes two YB maps are related by nondiagonal action (see the example of Harrison map and F_V noted earlier). The question how many such pairs exist needs further investigation (see the discussion of this in Ref. 27).

III. MULTIPARAMETER SYMMETRY GROUPS AND MULTIDIMENSIONAL CONSISTENCY

The purpose of this section is to show that the symmetry method described in the preceding section works equally well for multiparameter symmetry groups. The idea is to consider the extension of the equation into many dimensions using the 3D-consistency property and then prescribe the YB variables not to the edges but, for example, to higher dimensional faces.

We demonstrate how the method works in the example of dpKdV equation, which is invariant under the three-parameter symmetry group G with infinitesimal generators

$$\mathbf{v}_1=\partial_f,\quad \mathbf{v}_2=(-1)^{n_1+n_2}f\partial_f,\quad \mathbf{v}_3=(-1)^{n_1+n_2}\partial_f. \tag{42}$$

Their commutators are

$$[\mathbf{v}_1,\mathbf{v}_2]=\mathbf{v}_3,\quad [\mathbf{v}_2,\mathbf{v}_3]=-\mathbf{v}_1,\quad [\mathbf{v}_1,\mathbf{v}_3]=0, \tag{43}$$

from which it is immediately seen that $\{\mathbf{v}_1,\mathbf{v}_2,\mathbf{v}_3\}$ span a solvable Lie algebra. This algebra is actually isomorphic to the Lie algebra of the group Iso $(\mathbb{R}^{1,1})$ of isometries of the Minkowski plane, so G can be considered as the connected component of identity of this group.

A. Consistency of dpKdV around a three-cube and the F_{III} map

Consider the dpKdV equation imposed on each face of an elementary cube (see Fig. 2) and the Abelian subgroup H of the full symmetry group G generated by $\{\mathbf{v}_1,\mathbf{v}_3\}$ (translations of the Minkowski plane). These two symmetries can be extended to the corresponding system on $\mathbb{Z}^3$, e.g., $\mathbf{v}_3=(-1)^{n_1+n_2+n_3}\partial_f$.

We consider now the following invariants of the subgroup H:

$$x=f_1-f_3,\quad y=f_{1,2}-f_{1,3},\quad u=f_{1,2}-f_{2,3},\quad v=f_2-f_3, \tag{44}$$

assigned on four faces of the three-cube. Using the dpKdV equations

$$f_{1,2}-f=\frac{\alpha_1-\alpha_2}{f_1-f_2},\quad f_{1,3}-f=\frac{\alpha_1-\alpha_3}{f_1-f_3},\quad f_{2,3}-f=\frac{\alpha_2-\alpha_3}{f_2-f_3}, \tag{45}$$

we easily find that the invariants (44) are related by

$$uv=xy,\quad u-\frac{\beta_1}{x}=y-\frac{\beta_2}{v}, \tag{46}$$

where $\beta_1=\alpha_1-\alpha_3,\beta_2=\alpha_2-\alpha_3$. Solving the system (46) for (u,v) in terms of (x,y) we obtain the map

$$u=yP,\quad v=xP^{-1},\quad P=\frac{\beta_1+xy}{\beta_2+xy}, \tag{47}$$

which satisfies the YB relation as it can be checked by direct calculations. This fact is also related to the higher dimensional consistency of dpKdV on $\mathbb{Z}^4$ as it is explained in the following.

Considering the five initial values $f_3,f_{1,3},f_1,f_{1,2},f_{1,2,4}$ on the vertices of the four-cube (see Fig. 3) one can find the values on all other vertices in a unique way using the dpKdV equation on each two-dimensional face because of its four-dimensional consistency. From these five initial values we form the differences

$$x=f_1-f_3,\quad y=f_{1,2}-f_{1,3}\quad z=f_{1,2,4}-f_{1,2,3}, \tag{48}$$

which are assigned on (the diagonals of) the two-dimensional faces of the four-cube (Fig. 3). We note that the value $f_{1,2,3}$ can be expressed already in terms of $f_3,f_{1,3},f_1,f_{1,2}$ through the three-dimensional consistency of dpKdV on the "inner" cube. Next we apply successively the map $R:(x,y)\mapsto(u,v)$ given by (47) on the (a) "inner," "front," "left" and (b) "right," "back," "outer" three-dimensional cubes to obtain the following composite maps:

$$(a):\quad (x,y,z)\overset{R^{12}}{\to}(x_2,y_{-1},z)\overset{R^{13}}{\to}(x_{2,4},y_{-1},z_{-1})\overset{R^{23}}{\to}(x_{2,4},y_{-1,4},z_{-1,-2}), \tag{49}$$

$$(b):\quad (x,y,z)\overset{R^{23}}{\to}(x,y_4,z_{-2})\overset{R^{13}}{\to}(x_4,y_4,z_{-1,-2})\overset{R^{12}}{\to}(x_{2,4},y_{-1,4},z_{-1,-2}). \tag{50}$$

The fact that the two ways of obtaining the values for $(x_{2,4},y_{-1,4},z_{-1,-2})$ lead to identical results, and thus to the YB property of the map (47), is guaranteed by the four-dimensional consistency. One can notice that the evolution of the Yang-Baxter variables takes place on two parallel layers of the $\mathbb{Z}^3$ lattice, i.e., $\{(n_1,n_2,0),(n_1,n_2,1),n_1,n_2\in\mathbb{Z}\}$. This is reflected to the fact that there are six out of the eight three-dimensional faces (cubes) of the four-cube involved in the compatibility.

A final comment about the map (47) is that under the transformation $x\mapsto -x^{-1}$, $v\mapsto v^{-1}$, $u\mapsto\beta_1 u$, $y\mapsto\beta_2 y$ it becomes the first YB map in Table I for $\delta=0$. Thus the F_{III} map in the classification of Ref. 12 is also retrieved from dpKdV in $\mathbb{Z}^3$, by using the invariants of the symmetry subgroup H.

B. Consistency of dpKdV around a four-cube and the Harrison map

We are going to show that the Harrison map (7) appears in a similar manner as previously using now the invariants of the *full* symmetry group G of dpKdV and extending both the equation and its symmetry group in $\mathbb{Z}^4$.

The symmetry group G can be naturally extended to the corresponding system in $\mathbb{Z}^4$. Now let us consider the following invariants of this group:

$$x=\frac{f_1-f_3}{f_2-f_3},\quad v=\frac{f_1-f_4}{f_2-f_4},\quad y=\left(\frac{f_1-f_4}{f_2-f_4}\right)_3,\quad u=\left(\frac{f_1-f_3}{f_2-f_3}\right)_4, \tag{51}$$

where the subscript i means the shift in the ith direction. The natural place for them to live in are the corresponding two-dimensional faces. Next we derive the relations between these variables.

First of all Eq. (15) and its forward shifts with respect to the lattice directions 3 and 4 imply that the following relations:

$$(f_1-f_3)(f_1-f_4)_3=(f_1-f_4)(f_1-f_3)_4, \tag{52a}$$

$$(f_2-f_3)(f_2-f_4)_3=(f_2-f_4)(f_2-f_3)_4, \tag{52b}$$

$$(f_{1,3}-f)(f_{1,4}-f)_3=(f_{1,4}-f)(f_{1,3}-f)_4, \tag{52c}$$

$$(f_{2,3}-f)(f_{2,4}-f)_3=(f_{2,4}-f)(f_{2,3}-f)_4, \tag{52d}$$

hold on the "back" and "left" three-cubes of the four-cube depicted in Fig. 3. Dividing memberwise Eqs. (52a), (52b) and rearranging terms we get

$$\frac{f_1-f_3}{f_2-f_3}\left(\frac{f_1-f_4}{f_2-f_4}\right)_3=\frac{f_1-f_4}{f_2-f_4}\left(\frac{f_1-f_3}{f_2-f_3}\right)_4. \tag{53}$$

In terms of the variables (51) Eq. (53) reads

$$xy=uv. \tag{54}$$

On the other hand, we can rewrite Eq. (52c) in the equivalent form

$$(f_{1,3}-f)\left(1-\frac{(f_{2,3}-f)_4}{(f_{1,3}-f)_4}\right)=(f_{1,4}-f)\left(1-\frac{(f_{2,4}-f)_3}{(f_{1,4}-f)_3}\right), \tag{55}$$

which by using Eq. (15) reads

$$\frac{\alpha_1-\alpha_3}{f_1-f_3}\left(1-\frac{\alpha_2-\alpha_3}{\alpha_1-\alpha_3}\left(\frac{f_1-f_3}{f_2-f_3}\right)_4\right)=\frac{\alpha_1-\alpha_4}{f_1-f_4}\left(1-\frac{\alpha_2-\alpha_4}{\alpha_1-\alpha_4}\left(\frac{f_1-f_4}{f_2-f_4}\right)_3\right). \tag{56}$$

Multiplying both terms of Eq. (56) with $(\alpha_1-\alpha_2)(f_1-f_2)$ and rearranging terms, the latter takes the form

$$\left(1-\frac{\alpha_2-\alpha_4}{\alpha_1-\alpha_4}\right)\left(1-\frac{f_2-f_3}{f_1-f_3}\right)\left(1-\frac{\alpha_2-\alpha_3}{\alpha_1-\alpha_3}\left(\frac{f_1-f_3}{f_2-f_3}\right)_4\right)=\left(1-\frac{\alpha_2-\alpha_3}{\alpha_1-\alpha_3}\right)\left(1-\frac{f_2-f_4}{f_1-f_4}\right)\left(1-\frac{\alpha_2-\alpha_4}{\alpha_1-\alpha_4}\left(\frac{f_1-f_4}{f_2-f_4}\right)_3\right). \tag{57}$$

Finally, recalling the defining relations of the variables x,y,u,v, Eq. (57) becomes

$$(1-\gamma_2)(1-x^{-1})(1-\gamma_1 u)=(1-\gamma_1)(1-v^{-1})(1-\gamma_2 y), \tag{58}$$

where

$$\gamma_1=\frac{\alpha_2-\alpha_3}{\alpha_1-\alpha_3},\quad \gamma_2=\frac{\alpha_2-\alpha_4}{\alpha_1-\alpha_4}. \tag{59}$$

A similar calculation starting with (52d) and using (54), delivers the same relation (58).

Proposition III.1: *The invariants* (51) *of the symmetry group G of the dpKdV equation extended to* $\mathbb{Z}^4$ *are related by the YB map*, *which coincides with the Harrison map* (7).

Indeed, comparing (54) and (58) with the relations from which we obtain the last map in Table I, we deduce that x,y and u,v are related by the Harrison map. The fact that this map satisfies the YB relation can also be derived from the consistency property and geometry of the five-dimensional lattice.

IV. MULTICOMPONENT YB MAPS

In this section we show that YB maps can be constructed equally well from 3D consistent multifield discrete equations, for which no classification scheme exploiting the multidimensional consistency property has been obtained yet.

A. YB map from the discrete modified Boussinesq system

The discrete modified Boussinesq (dmBSQ) equations[28] involve two fields $f,g:\mathbb{Z}^2\to\mathbb{CP}^1$ and are given by the system

$$f_{1,2}=g\frac{\alpha_1 f_2-\alpha_2 f_1}{\alpha_1 g_1-\alpha_2 g_2},\quad g_{1,2}=\frac{g}{f}\frac{\alpha_1 f_1 g_2-\alpha_2 f_2 g_1}{\alpha_1 g_1-\alpha_2 g_2}. \tag{60}$$

Its 3D consistency is provided by a lengthy but straightforward calculation that delivers the symmetric values

$$f_{1,2,3}=f\frac{\underset{ijk}{\boldsymbol{\sigma}}\alpha_i\alpha_j f_k(\alpha_i g_i-\alpha_j g_j)}{\underset{ij}{\boldsymbol{\sigma}}\alpha_i\alpha_j(\alpha_i f_i g_j-\alpha_j f_j g_i)},\quad g_{1,2,3}=g\frac{\underset{ijk}{\boldsymbol{\sigma}}\alpha_i\alpha_j g_k(\alpha_i f_j-\alpha_j f_i)}{\underset{ij}{\boldsymbol{\sigma}}\alpha_i\alpha_j(\alpha_i f_i g_j-\alpha_j f_j g_i)}, \tag{61}$$

with respect to any permutation of the indices (1,2,3). Here the cyclic sum $\boldsymbol{\sigma}$ is over the subscripts $(i,j,k)=(1,2,3)$, (3,1,2), (2,3,1), and similarly the cyclic sum $\underset{ij}{\boldsymbol{\sigma}}$ is over $(i,j)=(1,2)$, (2,3), (3,1). The explicit dependence of $f_{1,2,3},g_{1,2,3}$ on the values f,g implies that dmBSQ does not satisfy the so-called *tetrahedron* property, which is an additional assumption in the classification scheme in Ref. 15 for one-field discrete equations.

Using the symmetry generators

$$\mathbf{v}_1=f\partial_f,\quad \mathbf{v}_2=g\partial_g, \tag{62}$$

of the dmBSQ equations, we define as YB variables the following joint lattice invariants:

$$x^1=\frac{f_1}{f},\quad y^1=\frac{f_{1,2}}{f_1},\quad u^1=\frac{f_{1,2}}{f_2},\quad v^1=\frac{f_2}{f}, \tag{63}$$

$$x^2=\frac{g_1}{g},\quad y^2=\frac{g_{1,2}}{g_1},\quad u^2=\frac{g_{1,2}}{g_2},\quad v^2=\frac{g_2}{g}. \tag{64}$$

It is immediately seen that the above-mentioned equations imply that

$$x^1y^1=u^1v^1,\quad x^2y^2=u^2v^2. \tag{65}$$

Moreover, the lattice equation (60) can be expressed in terms of the above-noted invariants as follows:

$$u^1v^1=\frac{\alpha_1 v^1-\alpha_2 x^1}{\alpha_1 x^2-\alpha_2 v^2},\quad u^2v^2=\frac{\alpha_1 x^1v^2-\alpha_2 v^1x^2}{\alpha_1 x^2-\alpha_2 v^2}. \tag{66}$$

Finally, solving Eqs. (65), (66) for (u^i,v^i) we obtain the reversible YB map

$$u^1 = y^1 A, \quad v^1 = x^1 A^{-1}, \quad A = \frac{\alpha_1^2 x^1 + \alpha_2^2 x^1 x^2 y^1 + \alpha_1 \alpha_2 x^2 y^2}{\alpha_1 \alpha_2 x^1 + \alpha_1^2 x^1 x^2 y^1 + \alpha_2^2 x^2 y^2}, \tag{67a}$$

$$u^2 = y^2 B, \quad v^2 = x^2 B^{-1}, \quad B = \frac{\alpha_1^2 x^1 + \alpha_2^2 x^1 x^2 y^1 + \alpha_1 \alpha_2 x^2 y^2}{\alpha_2^2 x^1 + \alpha_1 \alpha_2 x^1 x^2 y^1 + \alpha_1^2 x^2 y^2}. \tag{67b}$$

B. YB map from the discrete potential Boussinesq system

Discrete potential Boussinesq (dpBSQ) equations is the second member in the so-called lattice Gel'fand-Dikii hierarchy.[29] The dpBSQ equations, in the form they were studied recently in Ref. 30, involve three fields $f, g, h: \mathbb{Z}^2 \to \mathbb{CP}^1$, and they are given by the following system:

$$h_1 = f f_1 - g, \tag{68a}$$

$$h_2 = f f_2 - g, \tag{68b}$$

$$h = f f_{1,2} - g_{1,2} - \frac{\alpha_1 - \alpha_2}{f_1 - f_2}. \tag{68c}$$

For the purposes of the present discussion, Eq. (68) exhibits the interesting feature that the joint invariants of two symmetry generators are enough to construct a YB map. In connection with this issue we note that for an elementary Cauchy problem on a staircase, we should impose initial values (f, g, h), (f_1, g_1), (f_2, g_2), only. From these data the values (h_1, h_2) and $(f_{1,2}, g_{1,2}, h_{1,2})$ are determined uniquely. In particular, Eqs. (68a), (68b) imply that

$$f_{1,2} = \frac{g_1 - g_2}{f_1 - f_2}, \tag{69}$$

and subsequently the values $h_{1,2}$ and $g_{1,2}$ are determined from Eq. (68a) [or equivalently (68b) and (68c)], respectively.

Using the infinitesimal invariance criterion (33) to determine the symmetries of Eq. (68), we find that two particular symmetry generators are given by the following vector fields:

$$\mathbf{v}_1 = \partial_f + f\partial_g + f\partial_h, \quad \mathbf{v}_2 = \partial_g - \partial_h. \tag{70}$$

They generate the symmetry transformations

$$G^1: (f, g, h) \mapsto \left(f + \varepsilon_1, g + \varepsilon_1 f + \frac{\varepsilon_1^2}{2}, h + \varepsilon_1 f + \frac{\varepsilon_1^2}{2} \right), \tag{71}$$

$$G^2: (f, g, h) \mapsto (f, g + \varepsilon_2, h - \varepsilon_2), \tag{72}$$

respectively. We now define as YB variables the following invariants:

$$\begin{aligned}
&x^1 = f_1 - f, && y^1 = f_{1,2} - f_1, \\
&x^2 = g_1 - g - f(f_1 - f), && y^2 = g_{1,2} - g_1 - f_1(f_{1,2} - f_1), \\
&x^3 = h_1 - h - f(f_1 - f), && y^3 = h_{1,2} - g_1 - f_1(f_{1,2} - f_1), \\
&u^1 = f_{1,2} - f_2, && v^1 = f_2 - f, \\
&u^2 = g_{1,2} - g_2 - f_2(f_{1,2} - f_2), && v^2 = g_2 - g - f(f_2 - f), \\
&u^3 = h_{1,2} - h_2 - f_2(f_{1,2} - f_2), && v^3 = h_2 - h - f(f_2 - f).
\end{aligned} \tag{73}$$

They are functionally related by

$$u^1 + v^1 = x^1 + y^1, \tag{74a}$$

$$u^2 + v^2 = x^2 + y^2 + x^1y^1 - u^1v^1, \tag{74b}$$

$$u^3 + v^3 = x^3 + y^3 + x^1y^1 - u^1v^1 \tag{74c}$$

Moreover, the system of equations formed by (68a)–(68c), (68b), (68c), and (69) can be written in terms of the above-mentioned invariants as follows:

$$x^1 = -y^1 + \frac{x^2}{x^1 - v^1} - \frac{v^2}{x^1 - v^1}, \tag{75a}$$

$$x^3 = x^2 + y^2 + x^1y^1 + \frac{\alpha_1 - \alpha_2}{x^1 - v^1}, \tag{75b}$$

$$v^3 = u^2 + v^2 + u^1v^1 + \frac{\alpha_1 - \alpha_2}{x^1 - v^1}. \tag{75c}$$

Solving the system of Eqs. (74), (75) for (u^i, v^i) we obtain the following YB map:

$$\begin{aligned}
&u^1 = y^1 - (\alpha_1 - \alpha_2)\Gamma^{-1}, && v^1 = x^1 + (\alpha_1 - \alpha_2)\Gamma^{-1},\\
&u^2 = y^2 + (\alpha_1 - \alpha_2)(\alpha_1 - \alpha_2 - 2y^1\Gamma)\Gamma^{-2}, && v^2 = x^2 + (\alpha_1 - \alpha_2)(x^1 + y^1)\Gamma^{-1},\\
&u^3 = y^3 + (\alpha_1 - \alpha_2)(\alpha_1 - \alpha_2 + (x^1 - y^1)\Gamma)\Gamma^{-2}, && v^3 = x^3,
\end{aligned} \tag{76}$$

where $\Gamma = x^2 - x^3 + x^1y^1 + y^2$.

C. YB map from discrete Calapso equation and nonlinear σ-model

In a recent study on discrete isothermic surfaces, Schief[21] introduced the following vector generalization of the dpKdV:

$$(\boldsymbol{f}_{1,2} - \boldsymbol{f}) = \frac{\alpha_1 - \alpha_2}{|\boldsymbol{f}_1 - \boldsymbol{f}_2|^2}(\boldsymbol{f}_1 - \boldsymbol{f}_2), \tag{77}$$

$\boldsymbol{f}: \mathbb{Z}^2 \mapsto \mathbb{C}^n$, under the name *discrete Calapso equation*. Equation (77) is three-dimensional consistent since for an initial value configuration $\boldsymbol{f}, \boldsymbol{f}_i$ as in Fig. 2(a), one finds that the value $\boldsymbol{f}_{1,2,3}$ is given by

$$\boldsymbol{f}_{1,2,3} = \frac{\lambda|\boldsymbol{f}_2 - \boldsymbol{f}_3|^2\boldsymbol{f}_1 - \mu|\boldsymbol{f}_1 - \boldsymbol{f}_3|^2\boldsymbol{f}_2 + \nu|\boldsymbol{f}_1 - \boldsymbol{f}_2|^2\boldsymbol{f}_3}{\lambda|\boldsymbol{f}_2 - \boldsymbol{f}_3|^2 - \mu|\boldsymbol{f}_1 - \boldsymbol{f}_3|^2 + \nu|\boldsymbol{f}_1 - \boldsymbol{f}_2|^2}, \tag{78}$$

where

$$\lambda = (\alpha_1 - \alpha_2)(\alpha_1 - \alpha_3), \quad \mu = (\alpha_1 - \alpha_2)(\alpha_2 - \alpha_3), \quad \nu = (\alpha_1 - \alpha_3)(\alpha_2 - \alpha_3). \tag{79}$$

The consistency property is readily checked since $\boldsymbol{f}_{1,2,3}$ is invariant under any permutation of the indices (1, 2, 3) labeling the field variables and the corresponding lattice parameters.

The aim now is to construct a YB map from Eq. (77). Using the translational invariance of Eq. (77), we define the following YB variables:

$$\boldsymbol{x} = \boldsymbol{f}_1 - \boldsymbol{f}, \quad \boldsymbol{y} = \boldsymbol{f}_{1,2} - \boldsymbol{f}_1, \quad \boldsymbol{u} = \boldsymbol{f}_{1,2} - \boldsymbol{f}_2, \quad \boldsymbol{v} = \boldsymbol{f}_2 - \boldsymbol{f}, \tag{80}$$

on the edges of a square, which are related by

$$\boldsymbol{x}+\boldsymbol{y}=\boldsymbol{u}+\boldsymbol{v}. \tag{81}$$

On the other hand, Eq. (10) can be written in terms of the variables (80) in the form

$$(\boldsymbol{u}-\boldsymbol{y})=\frac{\alpha_1-\alpha_2}{|\boldsymbol{x}+\boldsymbol{y}|^2}(\boldsymbol{x}+\boldsymbol{y}). \tag{82}$$

Hence, Eqs. (81) and (82) deliver the following reversible YB map:

$$\boldsymbol{u}=\boldsymbol{y}+\frac{\alpha_1-\alpha_2}{|\boldsymbol{x}+\boldsymbol{y}|^2}(\boldsymbol{x}+\boldsymbol{y}),\quad \boldsymbol{v}=\boldsymbol{x}-\frac{\alpha_1-\alpha_2}{|\boldsymbol{x}+\boldsymbol{y}|^2}(\boldsymbol{x}+\boldsymbol{y}). \tag{83}$$

Moreover, in Ref. 21 it was shown that discrete Calapso equation (77) can be specialized to an integrable discrete version of the $O(n+2)$ nonlinear σ-model. This reduction is accomplished by imposing the constraint

$$|\boldsymbol{f}|^2=1, \tag{84}$$

on the discrete Calapso equation (77). Since the shifted values of $\boldsymbol{f}$ with respect to any lattice directions should also satisfy constraint (84), Eq. (77) is compatible with this constraint whenever

$$2\boldsymbol{f}\cdot\boldsymbol{f}_2-2\boldsymbol{f}\cdot\boldsymbol{f}_1=\alpha_1-\alpha_2. \tag{85}$$

This requirement can be satisfied by taking

$$-2\boldsymbol{f}\cdot\boldsymbol{f}_1=\alpha_1,\quad -2\boldsymbol{f}\cdot\boldsymbol{f}_2=\alpha_2. \tag{86}$$

In terms of the variables (80), the above-mentioned constraints translate to

$$|\boldsymbol{x}|^2=2+\alpha_1,\quad |\boldsymbol{y}|^2=2+\alpha_2. \tag{87}$$

In view of the previous relations the map (83) obtains the form

$$\boldsymbol{u}=\boldsymbol{y}+\frac{|\boldsymbol{x}|^2-|\boldsymbol{y}|^2}{|\boldsymbol{x}+\boldsymbol{y}|^2}(\boldsymbol{x}+\boldsymbol{y}),\quad \boldsymbol{v}=\boldsymbol{x}-\frac{|\boldsymbol{x}|^2-|\boldsymbol{y}|^2}{|\boldsymbol{x}+\boldsymbol{y}|^2}(\boldsymbol{x}+\boldsymbol{y}). \tag{88}$$

By straightforward calculations one finds that

$$|\boldsymbol{u}|^2=|\boldsymbol{x}|^2,\quad |\boldsymbol{v}|^2=|\boldsymbol{y}|^2. \tag{89}$$

Using the above-mentioned identity it is easily established that the map $R:(\boldsymbol{x},\boldsymbol{y})\mapsto(\boldsymbol{u},\boldsymbol{v})$ given by (88) is a reversible YB map. Up to a permutation this map was first considered by Adler[31] in the geometric problem about recuttings of polygons.

V. PERSPECTIVES

We have shown how the symmetry analysis of integrable equations on quad-graphs can be used in order to construct YB maps. In particular, we derived the Harrison map from the consistently extended discrete potential Korteweg–de Vries equation to the four-dimensional lattice. The main question now is how far this example can be generalized. In particular, for a given multiparametric symmetry group, is there a general relation between the structure of the invariants and the geometry of the objects which the YB variables are assigned to? What is the dimension of the lattice in which the discrete equation should be extended to? The analysis of other equations from Ref. 15 may clarify these issues.

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A new multisymplectic scheme for generalized Kadomtsev-Petviashvili equation

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From the multisymplectic Euler box scheme, we derive a new multisymplectic 16-point scheme for the generalized Kadomtsev-Petviashvili equation by eliminating the auxiliary variables. The new scheme is an explicit scheme in sense that it does not need iteration. The results of backward error analysis for the Euler box scheme show that the modified equation associated with the new scheme is not multisymplectic but of a high order approximation to a multisymplectic partial differential equations with a modified structure. Numerical results on one soliton and lump-type solitary waves are reported to illustrate the efficiency of the multisymplectic scheme. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Many years ago, Korteweg and de Vries[1] (KdV) derived an equation equivalent to

$$u_t + (3u^2)_x + u_{xxx} = 0 \ (t > 0, -\infty < x < +\infty), \tag{1.1}$$

to describe approximately the slow evolution of long water waves of moderate amplitude as they propagate under the influence of gravity in one direction in shallow of uniform depth.

The two-dimensional KdV, or the generalized Kadomtsev-Petviashvili (GKP) equation

$$(u_t + \partial_x f(u) + u_{xxx})_x + \sigma u_{yy} = 0 \ (t > 0, -\infty < x, y < +\infty), \tag{1.2}$$

was first introduced by Kadomtsev and Petviashvili[2] in order to study the stability of one-dimensional solitons against transverse perturbations, where σ is a constant and $f(u)$ is a smooth function. In the case of $f(u)=3u^2$ and $\sigma=-3$, Eq. (1.2) is usually called the KPI equation, whereas the KPII equation with $f(u)=3u^2$ and $\sigma=3$. In this paper, we mainly discuss the KPI equation. The KPII equation can be discussed similarly.

As far as we know, several numerical schemes have been proposed for the KP equation. These include the following: the explicit finite difference method proposed by Katsis;[3] the pseudospectral method developed by Fornberg and Whitham;[4,5] a linearized implicit method proposed by Feng,[6] and so on.

Recently, Marsden, Patrik, and Shkoller[7] and Bridges and Reich[8] proposed the concept of multisymplectic partial differential equations (PDEs) and multisymplectic schemes that can be viewed as the generalization of symplectic schemes. The KPI equation can be described in the language of multisymplectic geometry and reformulated to the multisymplectic form, which was first proposed by Bridges in Ref. 9. Liu and Qin,[10] from the Preissman scheme for multisymplectic equations, derived a multisymplectic numerical scheme for the KPI equation that can be simplified to an implicit 45-point scheme. They also claimed the robusticity of the 45-point scheme by several numerical experiments. In this paper, the multisymplectic Euler box scheme for the KPI equation is investigated and an explicit scheme is derived. So, the first question we must address is, why another study of numerics for the KPI equation? We start with several reasons: First, the 45-point scheme, as well as many other schemes for the GKP equation, is fully implicit and thus

cumbersome and expensive to work with for the high dimensional equations like the GKP equation. An efficient explicit scheme is of value in this case. Second, there is growing interest in the multisymplectic PDEs and multisymplectic schemes. As we know, there are two basic multisymplectic schemes: the Preissman scheme and the Euler box scheme. For details, we refer to Refs. 8, 19, and 22 for a recent survey. The Preissman scheme has been a hot topic in the past years,[10–15] however, little work has been done with the Euler box scheme. We know that the Preissman scheme is compact while the Euler box scheme is not. So, we want to know whether the noncompact Euler box scheme has as good a numerical performance as has the Preissman scheme. Third, many of numerical experiments have been reported to illustrate the good numerical performance of the multisymplectic schemes. However, all of them are implicit. We may ask the following question, as to whether only implicit multisymplectic schemes have a good numerical performance.

In this paper, we derive a new multisymplectic numerical scheme for the GKP equation that can be simplified to the 16-point scheme. This is an explicit scheme in sense that it does not need iteration in each time integration because the nonlinear term $(f(u))_{xx}$ is treated explicitly. Numerical results show that it is a good-performance scheme. Furthermore, the new scheme can be easily carried out, so it may be a useful tool for engineering applications to study the GKP equation.

The backward error analysis (BEA) for ODEs is a useful technique for studying the qualitative behavior of a discretization. This helps us to understand why the symplectic schemes for Hamiltonian systems can give accurate and efficient results for long time integration.[16,17] BEA for multisymplectic schemes was developed by Moore and Reich[18,19] and later by Islas and Schober in Ref. 20. Though their results show that the multisymplectic structure of the modified system has changed, they still help us to get further insight into the multisymplectic discretizations. In this paper, following their methods, we take BEA for the Euler box scheme for the KPI equation. We obtain the associated modified equations and the modified multisymplectic structure. However, the auxiliary variables in the modified equations cannot be eliminated completely to generate the corresponding modified equation associated with the 16-point scheme. Actually, a high order approximation is generated.

The paper is organized as follows: In Sec. II we take a brief view of multisymplectic structure of the KPI equation. We derive a new scheme and verify that it satisfies the multisymplectic conservation law. In Sec. III we implement BEA for PDE discretizations of the Euler box scheme for the KPI equation. In Sec. IV, some numerical results on one soliton and lump-type solitary waves over long time intervals are given. Section V gives concluding remarks.

II. DERIVATION OF A NEW EXPLICIT SCHEME FOR THE KPI EQUATION

The KPI equation can be written as

$$(u_t + 6uu_x + u_{xxx})_x + \sigma u_{yy} = 0 \ (t > 0, -\infty < x, y < +\infty), \tag{2.1}$$

where $\sigma = -3$. To put the KPI equation in the variational framework, we let $\varphi_{xx} = u$, then φ satisfies the following equation:

$$\varphi_{xxxt} + 6\varphi_{xx}\varphi_{xxxx} + 6\varphi_{xxx}^2 + \varphi_{xxxxxx} + \sigma\varphi_{xxyy} = 0. \tag{2.2}$$

Now, we introduce some variables: $v = \varphi_x$, $u = \varphi_{xx}$, $w = \varphi_{xy}$, $p = \frac{1}{2}\varphi_{xt}$, $p^x = -\varphi_{xxt} - 6\varphi_{xx}\varphi_{xxx} - \sigma\varphi_{xyy} - \varphi_{xxxxx}$, $p^{xx} = \frac{1}{2}\varphi_{xt} + 3\varphi_{xx}^2 + \varphi_{xxxx}$, $p^{xt} = \varphi_{xx}$, $p^{xy} = \sigma\varphi_{xy}$, and $p^{xxx} = -\varphi_{xxx}$.

According to the covariant De Donder-Weyl Hamilton function theories and the multisymplectic concept introduced by Bridges,[21] the KPI equation can be reformulated as a system of ten first-order partial differential equations, which can be written in the form

$$Mz_t + Kz_x + Lz_y = \nabla_z S(z), \quad z = (\varphi, v, u, w, p, p^x, p^{xx}, p^{xy}, p^{xt}, p^{xxx})^T \in R^{10}, \tag{2.3}$$

where

$$\mathbf{M} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{K} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{L} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where $S(z)=up+\frac{1}{2}(p^{xxx})^2+\sigma/2w^2+u^3-p^xv-p^{xx}u-p^{xt}p-p^{xy}w$. For details, we refer to Ref. 10. $\nabla_z S(z)$ is the gradient of $S(z)$ with respect to the standard inner product on R^{10}. The system (2.3) is a Hamiltonian formulation of the KPI equation on a multisymplectic structure, where $M,K,L \in R^{n\times n}$ are skew-symmetric matrices and $S(z):R^n\to R$ is a smooth function of the $z(x,y,t)$.

For Eq. (2.3), one of the most important characteristic is that it satisfies the multisymplectic conservation law

$$\frac{\partial w}{\partial t}+\frac{\partial k}{\partial x}+\frac{\partial q}{\partial y}=0, \tag{2.4}$$

where

$$w = \frac{1}{2}(dz \wedge Mdz), \quad k = \frac{1}{2}(dz \wedge Kdz), \quad q = \frac{1}{2}(dz \wedge Ldz), \tag{2.5}$$

are differential two-forms. So, when a numerical scheme is developed, we expect that the multisymplectic conservation law (2.4) should be preserved. Bridges and Reich defined a numerical scheme as a multisymplectic scheme if the scheme preserves a discrete multisymplectic conservation law.[8] Specifically, if we discretize Hamiltonian PDEs (2.3) as follows,

$$M\partial_t^{i,j,n} z_{i,j}^n + K\partial_x^{i,j,n} z_{i,j}^n + L\partial_y^{i,j,n} z_{i,j}^n = (\nabla_z S(z))_{i,j}^n, \tag{2.6}$$

where $z_{i,j}^n = z(x_i, y_j, t_n)$, $\partial_t^{i,j,n}$, $\partial_x^{i,j,n}$, and $\partial_y^{i,j,n}$ are the discretizations of the derivatives ∂_t, ∂_x, and ∂_y, respectively, then the scheme is multisymplectic provided that it can preserve the following discrete conservation law:

$$\partial_t^{i,j,n} w_{i,j}^n + \partial_x^{i,j,n} k_{i,j}^n + \partial_y^{i,j,n} q_{i,j}^n = 0, \tag{2.7}$$

where

$$w_{i,j}^n = \frac{1}{2}(dz_{i,j}^n \wedge Mdz_{i,j}^n), \quad k_{i,j}^n = \frac{1}{2}(dz_{i,j}^n \wedge Kdz_{i,j}^n), \quad q_{i,j}^n = \frac{1}{2}(dz_{i,j}^n \wedge Ldz_{i,j}^n). \tag{2.8}$$

Set t_n, $n=1,2,\ldots,N_1$; x_i, $i=1,2,\ldots,N_2$; y_j, $j=1,2,\ldots,N_3$ is the regular grids of the integral domain, $z_{i,j}^n$ is an approximation to $z(x_i, y_j, t_n)$, Δt is the time step, Δx is the x direction step, Δy is the y direction step, and

$$D_t^{\pm} z_{i,j}^n = \pm \frac{z_{i,j}^{n\pm1} - z_{i,j}^n}{\Delta t}, \quad D_x^{\pm} z_{i,j}^n = \pm \frac{z_{i\pm1,j}^n - z_{i,j}^n}{\Delta x}, \quad D_y^{\pm} z_{i,j}^n = \pm \frac{z_{i,j\pm1}^n - z_{i,j}^n}{\Delta y}.$$

The Euler box scheme for (2.3) is

$$M_+ D_t^+ z_{i,j}^n + M_- D_t^- z_{i,j}^n + K_+ D_x^+ z_{i,j}^n + K_- D_x^- z_{i,j}^n + L_+ D_y^+ z_{i,j}^n + L_- D_y^+ z_{i,j}^n = (\nabla_z S(z))_{i,j}^n, \tag{2.9}$$

where M_+, M_-, K_+, K_-, L_+, and L_- are matrix splitting for the symplectic structure matrices M, K, and L, respectively, s.t.,

$$M = M_+ + M_-, \quad M_+^T = -M_-,$$

$$K = K_+ + K_-, \quad K_+^T = -K_-,$$

$$L = L_+ + L_-, \quad L_+^T = -L_-. \tag{2.10}$$

Scheme (2.9) satisfies the discrete multisymplectic conservation law.

Theorem 1. (Ref. 19) Euler box scheme (2.9) is multisymplectic with the following discrete multisymplectic conservation law:

$$D_t^+ w_{i,j}^n + D_x^+ k_{i,j}^n + D_y^+ q_{i,j}^n = 0, \tag{2.11}$$

where

$$w_{i,j}^n = \frac{1}{2}(dz_{i,j}^{n-1} \wedge M_+ dz_{i,j}^n), \quad k_{i,j}^n = \frac{1}{2}(dz_{i-1,j}^n \wedge K_+ dz_{i,j}^n), \quad q_{i,j}^n = \frac{1}{2}(dz_{i,j-1}^n \wedge L_+ dz_{i,j}^n).$$

Proof: The variational equation associated with (2.9) is

$$M_+ D_t^+ dz_{i,j}^n + M_- D_t^- dz_{i,j}^n + K_+ D_x^+ dz_{i,j}^n + K_- D_x^- dz_{i,j}^n + L_+ D_y^+ dz_{i,j}^n + L_- D_y^- dz_{i,j}^n = S_{zz} dz_{i,j}^n. \tag{2.12}$$

For $dz_{i,j}^n \wedge S_{zz} dz_{i,j}^n = 0$, then we have

$$dz_{i,j}^n \wedge (M_+ D_t^+ dz_{i,j}^n + M_- D_t^- dz_{i,j}^n + K_+ D_x^+ dz_{i,j}^n + K_- D_x^- dz_{i,j}^n + L_+ D_y^+ dz_{i,j}^n + L_- D_y^- dz_{i,j}^n) = 0. \tag{2.13}$$

Note that

$$dz_{i,j}^n \wedge M_+ D_t^+ dz_{i,j}^n + dz_{i,j}^n \wedge M_- D_t^- dz_{i,j}^n = dz_{i,j}^n \wedge M_+ D_t^+ dz_{i,j}^n + D_t^- dz_{i,j}^n \wedge M_+ dz_{i,j}^n = - D_t^+ dz_{i,j}^n \wedge M_+ dz_{i,j}^n - dz_{i,j}^n \wedge D_t^- M_+ dz_{i,j}^n = - D_t^+ (dz_{i,j}^{n-1} \wedge M_+ dz_{i,j}^n); \tag{2.14}$$

similarly, we have

$$dz_{i,j}^n \wedge K_+ D_x^+ dz_{i,j}^n + dz_{i,j}^n \wedge K_- D_x^- dz_{i,j}^n = - D_x^+ (dz_{i-1,j}^n \wedge K_+ dz_{i,j}^n), \tag{2.15}$$

$$dz_{i,j}^n \wedge L_+ D_y^+ dz_{i,j}^n + dz_{i,j}^n \wedge L_- D_y^- dz_{i,j}^n = - D_y^+ (dz_{i,j-1}^n \wedge L_+ dz_{i,j}^n). \tag{2.16}$$

Combining (2.14)–(2.16), we have

$$D_t^+ (dz_{i,j}^{n-1} \wedge M_+ dz_{i,j}^n) + D_x^+ (dz_{i-1,j}^n \wedge K_+ dz_{i,j}^n) + D_y^+ (dz_{i,j-1}^n \wedge L_+ dz_{i,j}^n) = 0. \tag{2.17}$$

The proof is completed. □

We start from the Euler box scheme (2.9). Note that the matrix splitting (2.10) is not unique. We can obtain different schemes with different splitting methods. Now we take M_+, K_+, and L_+ as upper triangle matrices. They are

$$\mathbf{M}_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{K}_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{L}_+ = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0 \end{pmatrix}.$$

Substituting the above splitting into Euler box scheme (2.10), we get the discrete forms of the multisymplectic PDEs (2.3):

$$D_x^+ p^x = 0, \tag{2.18}$$

$$\frac{1}{2} D_t^+ p^{xt} + D_x^+ p^{xx} + D_y^+ p^{xy} = -p^x, \tag{2.19}$$

$$D_x^+ p^{xxx} = p + 3u^2 - p^{xx}, \tag{2.20}$$

$$p^{xy} = \sigma w, \tag{2.21}$$

$$p^{xt} = u, \tag{2.22}$$

$$D_x^- \varphi = v, \tag{2.23}$$

$$D_x^- v = u, \tag{2.24}$$

$$D_y^- v = w, \tag{2.25}$$

$$\frac{1}{2} D_t^- v = p, \tag{2.26}$$

$$D_x^- u = -p^{xxx}. \tag{2.27}$$

Substituting (2.26) and (2.27) into (2.20), we have

$$-D_x^+ D_x^- u = \frac{1}{2} D_t^- v + 3u^2 - p^{xx}. \tag{2.28}$$

Combining (2.21), (2.22), (2.25), and (2.19), then

$$\frac{1}{2} D_t^+ u + D_x^+ p^{xx} + \sigma D_y^+ D_y^- v = -p^x. \tag{2.29}$$

Applying D_x^- to Eq. (2.28), $D_x^+ D_x^-$ to (2.29), noting that the finite difference operators mutually commute, and combining (2.18), we have

$$-D_x^+D_x^-D_x^-u=\frac{1}{2}D_t^-D_x^-v+3D_x^-(u^2)-D_x^-p^{xx}, \tag{2.30}$$

$$\frac{1}{2}D_x^+D_x^-D_t^+u+D_x^+D_x^+D_x^-p^{xx}+\sigma D_x^+D_y^+D_y^-D_x^-v=-D_x^+p^x=0. \tag{2.31}$$

Note that $D_x^-v=u$, (2.30) and (2.31) can be reformulated as follows:

$$D_x^-p^{xx}=\frac{1}{2}D_t^-u+3D_x^-(u^2)+D_x^+D_x^-D_x^-u, \tag{2.32}$$

$$\frac{1}{2}D_x^+D_x^-D_t^+u+D_x^+D_x^+D_x^-p^{xx}+\sigma D_x^+D_y^+D_y^-u=0. \tag{2.33}$$

Substituting (2.32) into (2.33), we obtain the following multisymplectic 16-point scheme:

$$\frac{1}{2}D_t^+D_x^-D_x^+u_{i,j}^n+D_x^+D_x^+\left(\frac{1}{2}D_t^-u_{i,j}^n+3D_x^-f_{i,j}^n+D_x^+D_x^-D_x^-u_{i,j}^n\right)+\sigma D_x^+D_y^+D_y^-u_{i,j}^n=0, \tag{2.34}$$

where $f=u^2$. In finite difference format the 16-point scheme is given as follows:

$$\begin{aligned}\frac{1}{2\Delta t(\Delta x)^2}(u_{i+1,j}^{n+1}-2u_{i,j}^{n+1}+u_{i-1,j}^{n+1})=&\frac{1}{2\Delta t(\Delta x)^2}(u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n})\\&-\frac{1}{2\Delta t(\Delta x)^2}(u_{i+2,j}^{n}-2u_{i+1,j}^{n}+u_{i,j}^{n}-u_{i+2,j}^{n-1}+2u_{i+1,j}^{n-1}-u_{i,j}^{n-1})\\&-\frac{3}{(\Delta x)^3}((u^2)_{i+2,j}^{n}-3(u^2)_{i+1,j}^{n}+3(u^2)_{i,j}^{n}-(u^2)_{i-1,j}^{n})\\&-\frac{1}{(\Delta x)^5}(u_{i+3,j}^{n}-5u_{i+2,j}^{n}+10u_{i+1,j}^{n}-10u_{i,j}^{n}+5u_{i-1,j}^{n}-u_{i-2,j}^{n})\\&-\frac{\sigma}{\Delta x(\Delta y)^2}(u_{i+1,j+1}^{n}-u_{i,j+1}^{n}-2u_{i+1,j}^{n}+2u_{i,j}^{n}+u_{i+1,j-1}^{n}-u_{i,j-1}^{n}).\end{aligned} \tag{2.35}$$

It couples three time levels (see Figs. 1 and 2). It is an explicit scheme in the sense that the scheme does not need iteration because the third time level ($t=n+1$) does not include nonlinear terms.

III. BACKWARD ERROR ANALYSIS FOR THE SCHEME

We now assume z is a sufficiently smooth function that, when evaluated at the lattice points, satisfies (2.10). Using the Taylor series expansions in t about $z(x_i,y_j,t_n)$,

$$z_{i,j}^{n\pm1}=z_{i,j}^n\pm\Delta t(z_{i,j}^n)_t+\frac{1}{2}(\Delta t)^2(z_{i,j}^n)_{tt}\pm\ \dots, \tag{3.1}$$

and equivalent expansions in x and y, then we have the following first order equation:

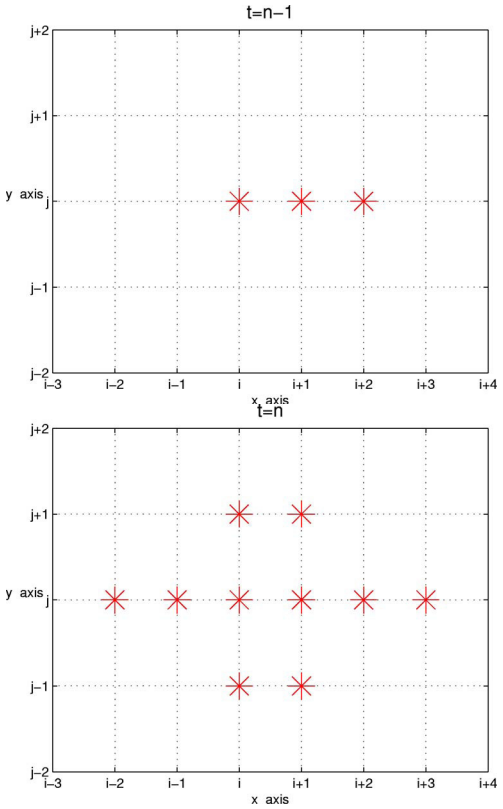

FIG. 1. (Color online) Left: points used by the first time level. Right: points used by the second time level.

$$Mz_t = (M_+ + M_-)z_t = \left[\left(M_+ z_t + \frac{1}{2}\Delta t M_+ z_{tt}\right) + \left(M_- z_t - \frac{1}{2}\Delta t M_- z_{tt}\right)\right] + o(\Delta t)$$

$$= Mz_t + \frac{1}{2}\Delta t(M_+ - M_-)z_{tt} + o(\Delta t). \tag{3.2}$$

Similarly, the space terms are approximated by

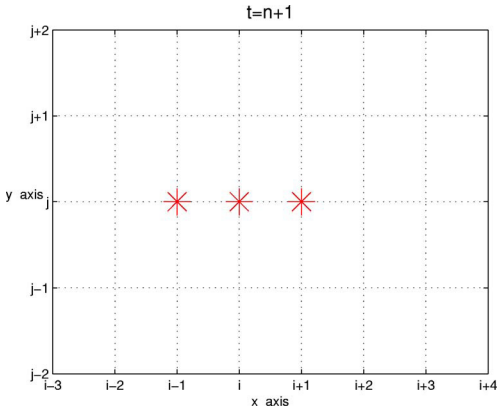

FIG. 2. (Color online) Points used by the third time level.

$$Kz_x = Kz_x + \frac{1}{2}\Delta x(K_+ - K_-)z_{xx} + o(\Delta x), \tag{3.3}$$

$$Lz_y = Lz_y + \frac{1}{2}\Delta y(L_+ - L_-)z_{yy} + o(\Delta y). \tag{3.4}$$

Substituting these expansions into (2.3), we obtain to first order the following modified equation:

$$Mz_t + \frac{1}{2}\Delta t(M_+ - M_-)z_{tt} + Kz_x + \frac{1}{2}\Delta x(K_+ - K_-)z_{xx} + Lz_y + \frac{1}{2}\Delta y(L_+ - L_-)z_{yy} = \nabla_z S(z). \tag{3.5}$$

Equation (3.5) can be written in the multisymplectic form:

$$\widetilde{M}\widetilde{z}_t + \widetilde{K}\widetilde{z}_x + \widetilde{L}\widetilde{z}_y = (\nabla_{\widetilde{z}}\widetilde{S}(\widetilde{z})), \tag{3.6}$$

where $\widetilde{z}=(z,z_t,z_x,z_y)^T$ and

$$\widetilde{\mathbf{M}} = \begin{pmatrix} M & \Delta tP & 0 & 0 \\ -\Delta tP & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \widetilde{\mathbf{K}} = \begin{pmatrix} K & 0 & \Delta xQ & 0 \\ 0 & 0 & 0 & 0 \\ -\Delta xQ & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\widetilde{\mathbf{L}} = \begin{pmatrix} L & 0 & 0 & \Delta yR \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\Delta yR & 0 & 0 & 0 \end{pmatrix},$$

$\widetilde{S}(\widetilde{z})=S-\frac{1}{2}\Delta t z_t^T P z_t - \frac{1}{2}\Delta x z_x^T Q z_x - \frac{1}{2}\Delta y z_y^T R z_y$, P, Q, and R are new matrices

$$P = \frac{1}{2}(M_+ - M_-), \quad Q = \frac{1}{2}(K_+ - K_-), \quad R = \frac{1}{2}(L_+ - L_-). \tag{3.7}$$

Applying Eq. (3.5) to the example, we can obtain

$$(p^x)_x + \frac{1}{2}\Delta x(p^x)_{xx} = 0,$$

$$\frac{1}{2}(p^{xt})_t + (p^{xx})_x + (p^{xy})_y + \frac{1}{4}\Delta t(p^{xt})_{tt} + \frac{1}{2}\Delta x(p^{xx})_{xx} + \frac{1}{2}\Delta y(p^{xy})_{yy} = -p^x,$$

$$(p^{xxx})_x + \frac{1}{2}\Delta x(p^{xxx})_{xx} = p + 3u^2 - p^{xx},$$

$$p^{xy} = \sigma w,$$

$$p^{xt} = u,$$

$$(\varphi)_x - \frac{1}{2}\Delta x(\varphi)_{xx} = v,$$

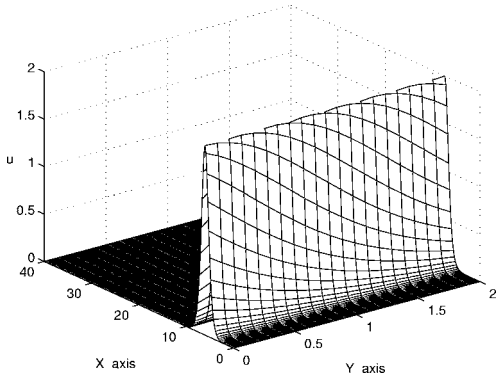

FIG. 3. The wave form of one soliton at $t=0$.

$$(v)_x - \frac{1}{2}\Delta x(v)_{xx} = u,$$

$$(v)_y - \frac{1}{2}\Delta y(v)_{yy} = w,$$

$$\frac{1}{2}(v)_t - \frac{1}{4}\Delta t(v)_{tt} = p,$$

$$(u)_x - \frac{1}{2}\Delta x(u)_{xx} = -p^{xxx}. \tag{3.8}$$

We tried to eliminate the auxiliary variables in Eqs. (3.8) to get the expected modified equation associated with the 16-point scheme. Unfortunately, we failed. We just obtain the following approximate equation, by ignoring the high order items,

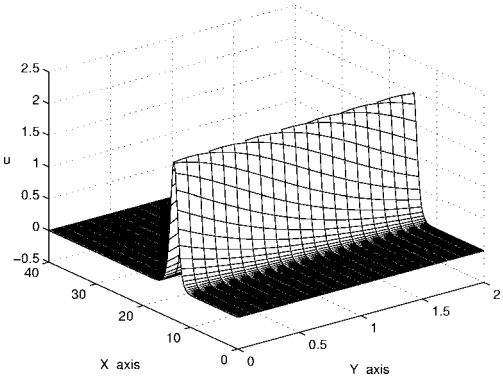

FIG. 4. Numerical solution of one soliton at $t=3$ with $\Delta x=0.1$, $\Delta y=0.1$, and $\Delta t=0.00005$.

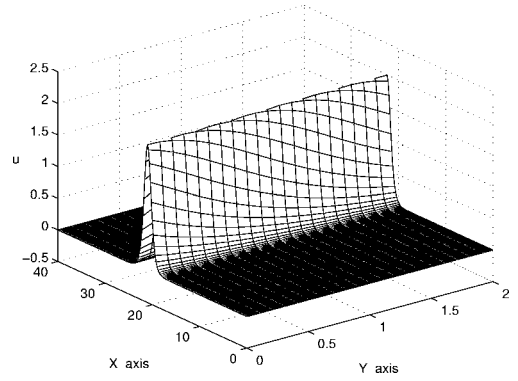

FIG. 5. Numerical solution of one soliton at $t=6$ with $\Delta x=0.1$, $\Delta y=0.1$, and $\Delta t=0.00005$.

$$(u_t + 6uu_x + u_{xxx})_x + \sigma u_{yy} = -\Delta x[u_{xxt} + (3u^2)_{xxx} + u_{xxxxx} + \sigma u_{xyy}] + \frac{1}{4}\Delta x\Delta t(u_{xxtt}) + \frac{1}{4}\Delta y^2(u_{yyyy}) + \frac{1}{4}\Delta x\Delta y^2(u_{xyyyy}) + O(\Delta t^2 + \Delta x^2 + \Delta y^3), \tag{3.9}$$

which is an $O(\Delta t+\Delta x+\Delta y^2)$ perturbation of the KPI.

IV. SOME NUMERICAL RESULTS

For our numerical experiments, we test the 16-point scheme on one soliton and lump-type solitary over long time intervals. We consider the KPI equation with an exact boundary condition. First we consider the one soliton with initial conditions

$$u(x,y,0) = 2\,\mathrm{sech}^2\left(x - \frac{\sqrt{2}}{2}y - 6\right). \tag{4.1}$$

The KPI equation has the theoretic solution

$$u(x,y,t) = 2\,\mathrm{sech}^2\left(x - \frac{\sqrt{2}}{2}y - \frac{5}{2}t - 6\right), \tag{4.2}$$

which represents one soliton propagating with the velocity $\frac{5}{2}$ in the direction with the angle of $\tan^{-1}(\sqrt{2})$ to the positive x axis. We carry out our numerical computation on the domain

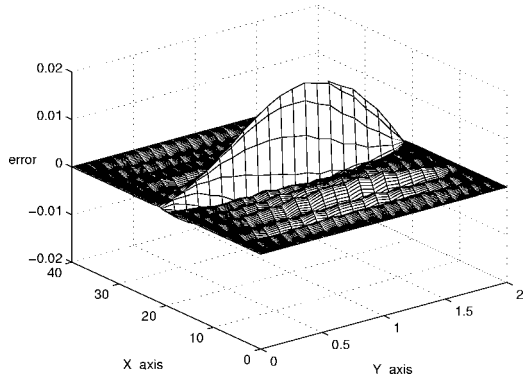

FIG. 6. The error between the numerical solution and the exact solution of one soliton at $t=6$ with $\Delta x=0.1$, $\Delta y=0.1$, and $\Delta t=0.00005$.

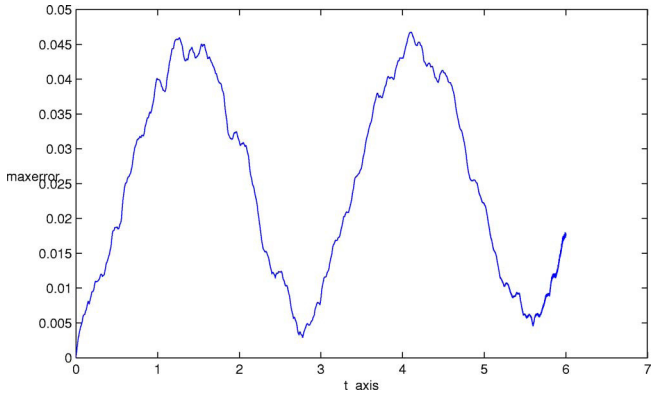

FIG. 7. (Color online) The trend of the maxerror(n) of one soliton as time evolves with $\Delta x=0.1$, $\Delta y=0.1$, and $\Delta t=0.00005$.

$[0,40]\times[0,2]$ and choose $\Delta x=0.1$, $\Delta y=0.1$, $\Delta t=0.00005$. Figure 3 shows the wave form of one soliton at $t=0$. Figures 4 and 5 show the numerical solution at $t=3$ and $t=6$, respectively. We can see the moving of one soliton from the graph. Figure 6 shows the error between the numerical solution and the exact solution at $t=6$. For fixed n, we give the definition of maxerror(n):

$$\text{maxerror}(n) = \max_{ij} |u_{i,j}^n - u(x_i, y_j, t_n)|, \tag{4.3}$$

where $u_{i,j}^n$ is the numerical solution while $u(x_i, y_j, t_n)$ is the exact solution. Figure 7 shows the trend of the maxerror(n) as time evolves. From that, we can see that the scheme has the good numerical performance over long time intervals.

Next, we try the lump-type solitary waves of the KPI equation with the following initial condition:

$$u(x,y,0) = 4\frac{\left(-(x-x_0)^2 + \mu^2(y-y_0)^2 + \frac{1}{\mu^2}\right)}{\left((x-x_0)^2 + \mu^2(y-y_0)^2 + \frac{1}{\mu^2}\right)^2}. \tag{4.4}$$

We compute in a rectangle $[0,20]\times[0,20]$ with the parameters $\mu^2=1.0$, $x_0=10.0$, $y_0=10.0$, and choose $\Delta x=0.1$, $\Delta y=0.2$, $\Delta t=0.00005$. The lump solution of the KPI equation can be expressed as

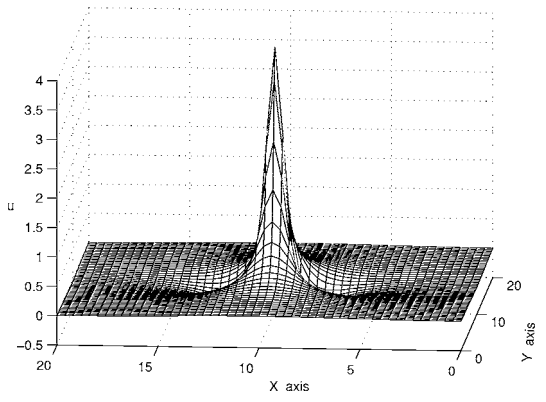

FIG. 8. The lump-type solitary wave at $t=0$.

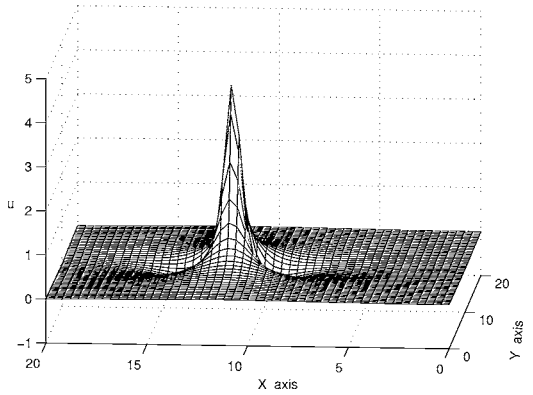

FIG. 9. Numerical solution of lump-type solitary wave at $t=0.5$ with $\Delta x=0.1$, $\Delta y=0.2$, and $\Delta t=0.00005$.

$$u(x,y,t)=4\frac{\left(-(x-x_0-3\mu^2t)^2+\mu^2(y-y_0)^2+\frac{1}{\mu^2}\right)}{\left((x-x_0-3\mu^2t)^2+\mu^2(y-y_0)^2+\frac{1}{\mu^2}\right)^2}. \tag{4.5}$$

Figure 8 shows the lump-type solitary wave at $t=0$. Figures 9 and 10 show the numerical solution at $t=0.5$ and $t=1$, respectively. Figure 11 shows the error between the numerical solution and the exact solution at $t=1$.

According to (4.5), this lump-type solitary wave will move to the positive x direction with velocity $3\mu^2$. Figures 9 and 10 shows the moving of the lump-type solitary wave.

V. CONCLUDING REMARKS

We investigate the noncompact Euler box for the GKP equation. A new equivalent scheme 16-point for KPI equation is derived. It is an explicit scheme, therefore it could be faster, less storage consuming, and more easy to carry out than the multisymplectic 45-point scheme when it is applied into computers. The good numerical performance of the derived scheme in several numerical experiments illustrates that the multisymplectic Euler box scheme is as good the as multisymplectic Preissman scheme. Thus we may draw the conclusion that not only compact implicit multisymplectic schemes but also noncompact explicit multisymplectic can be high quality schemes for the long time integration of nonlinear PDEs.

Remark. In Ref. 23, Frank, Moore, and Reich have shown that the explicit noncompact

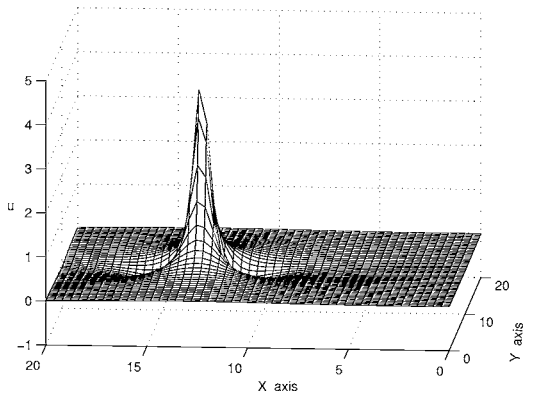

FIG. 10. Numerical solution of lump-type solitary wave at $t=1$ with $\Delta x=0.1$, $\Delta y=0.2$, and $\Delta t=0.00005$.

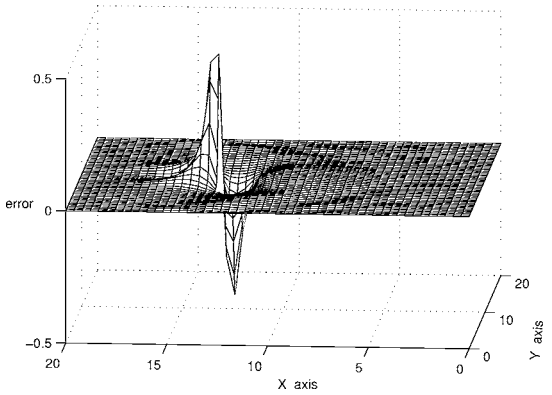

FIG. 11. The error between the numerical solution and the exact solution of lump-type solitary wave at $t=1$ with $\Delta x=0.1$, $\Delta y=0.2$, and $\Delta t=0.00005$.

midpoint multisymplectic scheme may exhibit spurious roots in the numerical dispersion relation for any value of $\Delta t/\Delta x$. This may lead to numerical instabilities. Our 16-point scheme is also an explicit multisymplectic and the numerical experiments do not exhibit instabilities. In future work, we will take the dispersion relation analysis for the new scheme and the von Neumann stability analysis to get a linear stability condition. Further, we will test numerically the scheme on a more challenging problem, which was reported by Bridges in Ref. 24.

ACKNOWLEDGMENTS

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Yang–Mills fields on CR manifolds

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We study *pseudo Yang–Mills fields* on a compact strictly pseudoconvex CR manifold M, i.e., the critical points of the functional $\mathcal{PYM}(D)=\frac{1}{2}\int_M \|\pi_H R^D\|^2\theta\wedge(d\theta)^n$, where D is a connection in a Hermitian CR holomorphic vector bundle $(E,h)\to M$. Let $\Omega=\{\varphi<0\}\subset\mathbb{C}^n$ be a smoothly bounded strictly pseudodoconvex domain and g the Bergman metric on Ω. We show that boundary values D_b of Yang–Mills fields D on (Ω,g) are pseudo Yang–Mills fields on $\partial\Omega$, provided that $i_T R^{D_b}=0$ and $i_N R^D=0$ on $H(\partial\Omega)$. If $S^1\to C(M)\xrightarrow{\pi} M$ is the canonical circle bundle and π^*D is a Yang–Mills field with respect to the Fefferman metric F_θ of (M,θ) then D is a pseudo Yang–Mills field on M. The Yang–Mills equations $\delta^{\pi^*D}R^{\pi^*D}=0$ project on the Euler–Lagrange equations $\delta_b^D R^D=0$ of the variational principle $\delta\mathcal{PYM}(D)=0$, provided that $i_T R^D=0$. When M has vanishing pseudohermitian Ricci curvature the pullback π^*D of the (CR invariant) Tanaka connection D of (E,h) is a Yang–Mills field on $C(M)$. We derive the second variation formula $\{d^2\mathcal{PYM}(D^t)/dt^2\}_{t=0}=\int_M\langle\mathcal{S}_b^D(\varphi),\varphi\rangle\theta\wedge(d\theta)^n$, $D^t=D+A^t$ [provided that D is a pseudo Yang–Mills field and $\varphi\equiv\{dA^t/dt\}_{t=0}\in\mathrm{Ker}(\delta^D)$], and show that $\mathcal{S}_b^D(\varphi)\equiv\Delta_b^D\varphi+\mathcal{R}_b^D(\varphi)$, $\varphi\in\Omega^{0,1}[\mathrm{Ad}(E)]$, is a subelliptic operator. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2222082]

I. INTRODUCTION

A series of papers published in the last decade[21,24,25] are devoted to exploring the relationship among CR structures on three-dimensional manifolds and null solutions to Einstein equations, Maxwell equations, and Yang–Mills equations (see also Ref. 28). Specifically, if $[M,T_{1,0}(M)]$ is a nondegenerate three-dimensional CR manifold endowed with the contact form θ and with the (locally defined) complex 1-form θ^1 such that $\theta^1(T_1)=1$, $\theta^1(T_{\bar{1}})=0$ [where T_1 is a local generator of the CR structure $T_{1,0}(M)$] let us consider the semi-Riemannian metric

$$F=2p^2[(\pi^*\theta^1)\odot(\pi^*\theta^{\bar{1}})-(\pi^*\theta)\odot\sigma], \tag{1}$$

on $M\times\mathbb{R}$, where p is a real valued function on $M\times\mathbb{R}$ and σ is a real 1-form on $M\times\mathbb{R}$ such that

$$\pi^*(\theta\wedge\theta^1\wedge\theta^{\bar{1}})\wedge\sigma\neq 0.$$

Here $\pi: M\times\mathbb{R}\to M$ is the projection. Nurowski[24] has determined local solutions to the Yang–Mills equations on $(M\times\mathbb{R},F)$, under the additional assumption that the shear-free congruence of

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null geodesics tangent to $\partial/\partial\gamma$ (γ is the natural coordinate function on $\mathbb{R}$) possesses three linearly independent symmetries $\{X_i: 1\leqslant i\leqslant 3\}$. Let D be a SU(3) connection in a vector bundle $\hat{E}\to M\times\mathbb{R}$ locally described by a matrix of 1-forms $A=b\pi^*\theta^1+\bar{b}\pi^*\theta^{\bar{1}}+c\pi^*\theta+e\sigma$, where a, b, c, and e are $\mathcal{G}\otimes\mathbb{C}$-valued functions $[\mathcal{G}=\mathbf{su}(3)]$ on $M\times\mathbb{R}$. When the Lie group G_3 (whose Lie algebra is generated by the X_is) consists of symmetries of D (i.e., each element of G_3 induces a gauge transformation of A) then (by a result of Harnad *et al.*[12]) up to some gauge transformation A is strictly invariant under G_3. Then $\mathcal{L}_{X_i}A=0$, conditions which may be exploited to show that locally D may be looked for in the form $A=B\pi^*\Omega^1+\bar{B}\pi^*\Omega^{\bar{1}}+C\pi^*\Omega$, with $B,C\in\mathcal{G}\otimes\mathbb{C}$. Here Ω and Ω^1 are a new contact form and a new local coframe such that

$$\mathcal{L}_{\tilde{X}_i}\Omega=0,\quad \mathcal{L}_{\tilde{X}_i}\Omega^1=0,\quad d\Omega=2\sqrt{-1}\Omega^1\wedge\Omega^{\bar{1}}, \tag{2}$$

while $\tilde{X}_i$ are the projections on M of the (nontrivial) symmetries X_i. Finally the Yang–Mills equations [for SU(3) fields] on $M\times\mathbb{R}$ may be solved [together with the condition that D is null, i.e., $dA+A\wedge A=(\pi^*\Omega)\wedge(\Phi\pi^*\Omega^1+\bar{\Phi}\pi^*\Omega^{\bar{1}})$, for some $\mathcal{G}\otimes\mathbb{C}$-valued function Φ]. For instance [see Eq. (5.10) in Ref. 24, p. 805]

$$A=\rho\mathbf{n}\cdot f\pi^*(e^{i\phi}\Omega^1+e^{-i\phi}\Omega^{\bar{1}}) \tag{3}$$

is a solution, where $\mathbf{n}\in\mathbb{R}^3$ is a unit vector, $\rho\in\mathbb{R}$, $\phi\in[0,2\pi]$, and $f=(e_1,e_2,e_3)$ is a basis in $\mathcal{G}$. It is noteworthy that $\tilde{X}_i$ turn out to be symmetries of the CR structure $T_{1,0}(M)$ (in a sense that will be explained in Sec. III) and that the CR structures admitting the three-dimensional symmetry group G_3 are fully classified in Ref. 21, according to the Bianchi type of G_3. For instance, if $M=\{(x,y,z)\in\mathbb{R}^3: y\neq 0\}$ carries the CR structure $T_{1,0}(M)=\mathbb{C}T_1$ with

$$T_1=\frac{y}{1+y^2}\frac{\partial}{\partial x}-\frac{iy}{2}\frac{\partial}{\partial y}+\frac{1}{y(1+y^2)}\frac{\partial}{\partial z} \tag{4}$$

and the contact form $\theta=(1/y)dx-ydz$ (such M possesses a symmetry group of Bianchi type VI_0) then a local solution A (to the Yang–Mills equations) of the form (3) may be produced. The example (4) of a CR structure on $\mathbb{R}^3\setminus\{y=0\}$ will be encountered again in Sec. III. Now let M be a compact strictly pseudoconvex CR manifold, of arbitrary CR dimension n. Let $S^1\to C(M)\xrightarrow{\pi}M$ be the canonical circle bundle (cf. Sec. III for definitions). Note that $C(M)$ and $M\times\mathbb{R}$ are locally diffeomorphic. If θ is a contact form on M then $C(M)$ carries a natural Lorentz metric F_θ (the Fefferman metric) and a moment's thought [compare to Eq. (70) in Sec. V] shows that when M is three-dimensional the Fefferman metric F_θ is of the form (1). Then, under the symmetry assumptions above, (3) is a (local) solution to the Yang–Mills equations

$$\delta^{\mathrm{D}}R^{\mathrm{D}}=0 \tag{5}$$

on $[C(M),F_\theta]$ (with $n=1$), and in general it is conceivable that when the CR structure $T_{1,0}(M)$ possesses a symmetry group G_{2n+1}, Nurowski's scheme may produce local symmetric null solutions to (5). A first step toward the achievement of this goal is performed in Sec. III. Note that (3) is the pullback (via π) to $M\times\mathbb{R}$ of a field on M. It is then a natural question whether given a Yang–Mills field on $[C(M),F_\theta]$ of the form π^*D, it follows that D is a Yang–Mills field on (M,g_θ), where g_θ is the Webster metric. This question is answered in Sec. V, where we integrate along the fiber in the Yang–Mills functional $\widehat{\mathcal{YM}}$ on $C(M)$ and produce the new functional (7). As it turns out, D is a *pseudo Yang–Mills* field [i.e., a critical point of (7)] rather than a Yang–Mills field on (M,g_θ) (however, the two notions coincide in the special case $i_TR^D=0$). The converse [i.e., whether given a pseudo Yang–Mills field D on M its pullback π^*D is a Yang–Mills field on $C(M)$] is examined in Theorem 2. Solving (5) on $C(M)$ is therefore closely related to solving the pseudo Yang–Mills equations

$$\delta_b^D R^D = 0 \tag{6}$$

on M, and indeed (5) projects (under additional conditions, cf. Sec. V) on M to give (6). One of the main results in this paper is that solutions to (6) occur as boundary values of Yang–Mills fields on a strictly pseudoconvex bounded domain $\Omega \subset \mathbb{C}^n$ endowed with the Bergman metric g (cf. Theorem 1). For the proof of Theorem 1 we draw inspiration from Ref. 11 and make use of their canonical connection ∇ (the *Graham–Lee connection*) whose pointwise restriction to a level set (near $\partial\Omega$) of a defining function of Ω is the better known Tanaka–Webster connection of the level set. Using the fine asymptotic properties of the Bergman kernel of Ω we may choose a defining function allowing an explicit relationship among the Bergman metric g and the Webster metric of each level set, and therefore an explicit relationship among the Levi–Civita connection of (Ω, g) and the Graham–Lee connection. In the end, an elementary asymptotic analysis shows that boundary values D_b of Yang–Mills fields D on (Ω, g) satisfy (6) provided that D_b satisfy certain compatibility conditions along $\partial\Omega$ (cf. Sec. IV). In Secs. VI and VII we obtain the first and second variation formulae for the functional (7). The relevant operator occurring in the second variation formula is shown to be subelliptic of order $\frac{1}{2}$ (cf. Theorem 3). The problem of building an appropriate stability theory (along the lines of Ref. 4, yet relying on the subelliptic rather than on the elliptic theory) remains open. We feel that the importance of the Graham–Lee connection ∇ in applications deserves the Appendix: there we provide a new axiomatic description of ∇ together with a index-free proof.

II. STATEMENT OF MAIN RESULTS

Let $(M, T_{1,0}(M))$ be a compact strictly pseudoconvex CR manifold, of CR dimension n, and θ a contact form on M. Let $(E, \bar{\partial}_E) \to M$ be a CR-holomorphic vector bundle and h a Hermitian metric in E. Let $\mathcal{C}(E,h)$ be the affine space of all connections D in E such that $Dh=0$. We consider the functional

$$\mathcal{PYM}(D) = \frac{1}{2}\int_M \|\pi_H R^D\|^2 \theta \wedge (d\theta)^n. \tag{7}$$

Here $\pi_H : \Omega^2(\mathrm{Ad}\, E) \to \Omega^2(\mathrm{Ad}\, E)/\mathcal{J}_\theta^2$ is the natural projection and $\mathcal{J}_\theta^\bullet$ the ideal generated by θ in $\Omega^\bullet(\mathrm{Ad}\, E)$. A *pseudo Yang–Mills field* on M is a critical point of $\mathcal{PYM} : \mathcal{C}(E,h) \to [0, +\infty)$.

Let T be the characteristic direction of $(\partial\Omega, \theta)$, $\theta \equiv i/2(\bar{\partial} - \partial)\varphi$, and let $H(\partial\Omega)$ be the Levi distribution of (the CR manifold) $\partial\Omega$. Also we set $N = -JT$ (where J is the complex structure on $\mathbb{C}^n$). We shall show that:

Theorem 1: *Let $\Omega = [z \in U : \varphi(z) < 0]$ be a smoothly bounded strictly pseudoconvex domain in $\mathbb{C}^n$ and g its Bergman metric. Let $\pi : F \to U$ be a holomorphic vector bundle and h a Hermitian metric on F. Let $D_b \in \mathcal{C}(E,h)$ $[E = \pi^{-1}(\partial\Omega)]$ be the boundary values of a Yang–Mills field $D \in \mathcal{C}(F,h)$ on (Ω, g). Assume that $i_T R^{D_b} = 0$. Then D_b is a pseudo Yang–Mills field if and only if $i_N R^D = 0$ on $H(\partial\Omega)$.*

The proof relies on the explicit relationship among the Levi–Civita connection ∇^g of (Ω, g) and the Graham–Lee connection ∇ of φ (cf. Ref. 11 and our Appendix for the description and main properties of the Graham–Lee connection).

Urakawa 30–32 has started a study of Yang–Mills fields on M, that is of critical points of the functional

$$\mathcal{YM}(D) = \frac{1}{2}\int_M \|R^D\|^2 \mathrm{d\ vol}(g_\theta),$$

where $\mathrm{d\ vol}(g_\theta)$ is the canonical volume form associated to the Webster metric g_θ of (M, θ). As it will be shortly shown, $\mathcal{YM}$ and $\mathcal{PYM}$ are related. To motivate the definition of $\mathcal{PYM}$ let F_θ be the Fefferman metric of (M, θ) [a Lorentz metric on $C(M)$, the total space of the canonical circle bundle $\pi : C(M) \to M$ (cf. e.g., Lee,[18])]. By a result of Barletta *et al.*,[2] the base map $\phi : M \to N$

corresponding to any smooth S^1-invariant harmonic map $\Phi: C(M) \to N$ from $[C(M), F_\theta]$ into a Riemannian manifold (N, g_N) is locally a subelliptic harmonic map (in the sense of Jost and Xu[15]). Also ϕ is a critical point of the functional $E(\phi) = \frac{1}{2}\int_M \mathrm{trace}_{G_\theta}(\pi_H \phi^* g_N)\theta \wedge (d\theta)^n$, where G_θ is the Levi form. Here, if B is a bilinear form on $T(M)$, then $\pi_H B$ denotes the restriction of B to $H(M)$, the Levi distribution of $[M, T_{1,0}(M)]$. The functional E itself is obtained by integration along the fiber in the Dirichlet functional $\mathbb{E}(\Phi) = \frac{1}{2}\int_{C(M)} \mathrm{trace}_{F_\theta}(\Phi^* g_N)\mathrm{d\,vol}(F_\theta)$, where $\Phi = \phi \circ \pi$. Then perhaps subelliptic harmonic maps (rather than harmonic maps, with respect to the Webster metric) are the natural objects of study in CR geometry. Another example of the sort is the *CR Yamabe problem*, i.e., given a contact form θ on M such that G_θ is positive definite, find a contact form $\hat{\theta} = e^u \theta$, $u \in C^\infty(M)$, such that the pseudohermitian scalar curvature $\hat{\rho}$ of $(M, \hat{\theta})$ is a constant λ. By the result of Lee,[18] the Fefferman metric changes conformally $F_{\hat{\theta}} = e^{u \circ \pi} F_\theta$. Also the scalar curvature $K: C(M) \to \mathbb{R}$ of $[C(M), F_\theta]$ is S^1 invariant and the corresponding base function $\pi_* K: M \to \mathbb{R}$ is, up to a constant, the pseudohermitian scalar curvature ρ of (M, θ) [precisely $\pi_* K = (2n+1)/(n+1)\rho$]. Therefore, the CR Yamabe problem is nothing but the Yamabe problem for the Fefferman metric and the relevant equation (the Yamabe equation on $[C(M), F_\theta]$) projects on $c_n \Delta_b u + \rho u = \lambda u^{p-1}$ (the *CR Yamabe equation*), a nonlinear subelliptic equation on M (which may be analyzed with the techniques in Ref. 9, cf. Jerison and Lee,[13,14] and Gamara and Yacoub,[10] for a complete solution to the CR Yamabe problem). The common feature of the two examples above is that both provide natural objects on M, as projections of (S^1 invariant) geometric quantities on $C(M)$, associated to the Fefferman metric. A more refined statement is that both examples lead to nonlinear subelliptic problems on M. This has already been emphasized for the CR Yamabe problem. As to the example of S^1-invariant harmonic maps $\Phi: C(M) \to N$, the base map is a solution to $\Delta_b \phi^i + g^{\alpha\bar{\beta}} T_\alpha(\phi^j) T_{\bar{\beta}}(\phi^k)[(\Gamma_N)^i_{jk} \circ \phi] = 0$, where $(\Gamma_N)^i_{jk}$ are the Christoffel symbols of the second kind of g_N. On the same line of thought, we may state the following:

Theorem 2: *Let M be a compact strictly pseudoconvex CR manifold, of CR dimension n. Let θ be a contact form on M with G_θ positive definite. Let $(E, \bar{\partial}_E) \to M$ be a CR-holomorphic vector bundle and h a Hermitian metric in E. (i) There is a constant c_n depending only on the dimension and the orientation of M such that*

$$c_n \mathcal{YM}(D) = \mathcal{PYM}(D) + 2\int_M \|i_T R^D\|^2 \theta \wedge (d\theta)^n, \quad D \in \mathcal{C}(E,h). \tag{8}$$

Consequently, given a Hermitian connection D in E whose curvature R^D is of type $(1,1)$, D is a pseudo Yang–Mills field on M if and only if D is the Tanaka connection of $(E, \bar{\partial}_E, h)$. (ii) Let $\mathcal{Y}\hat{\mathcal{M}}(\mathbb{D}) = \frac{1}{2}\int_{C(M)} \langle R^{\mathbb{D}}, R^{\mathbb{D}} \rangle \mathrm{d\,vol}(F_\theta)$ be the Yang–Mills functional on $C(M)$, for $\mathbb{D} \in \mathcal{C}(\pi^* E, \pi^* h)$. Then

$$\mathcal{Y}\hat{\mathcal{M}}(\pi^* D) = 2\pi \mathcal{PYM}(D), \quad D \in \mathcal{C}(E,h). \tag{9}$$

Consequently, if $\pi^* D$ is a Yang–Mills field on $[C(M), F_\theta]$ then D is a pseudo Yang–Mills field on M. Vice versa, let D be a pseudo Yang–Mills field on M such that $i_T R^D = 0$. Then $\pi^* D$ is a Yang–Mills field on $C(M)$ if and only if

$$\left[R^{\alpha\bar{\beta}} - \frac{\rho}{2(n+1)} g^{\alpha\bar{\beta}} \right] R^D(T_\alpha, T_{\bar{\beta}}) u = 0, \tag{10}$$

for some local frame $\{T_\alpha : 1 \leqslant \alpha \leqslant n\}$ of $T_{1,0}(M)$ at any point $x \in M$, and

$$\Lambda_\theta R^D = 0. \tag{11}$$

In particular, if M is (pseudohermitian) Ricci flat then the pullback $\pi^* D$ of the canonical Tanaka connection D of (E,h) is a Yang–Mills field.

The main ingredients in the proof of Theorem 2 are a local coordinate calculation of the Fefferman metric of (M, θ), the explicit relationship among the Levi–Civita connection $\nabla^{C(M)}$ of

$[C(M), F_\theta]$, and the Tanaka–Webster connection ∇ of (M, θ) (cf. Lemma 2), and Theorem 2.3 in Ref. 30, p. 551. We may also state (delegating the definitions to Sec. II):

Theorem 3: *Let D be a pseudo Yang–Mills field and $D^t = D + A^t$, $|t| < \epsilon$, a smooth variation of D whose first order part $\varphi \equiv (\mathrm{d}A^t/\mathrm{d}t)_{t=0}$ satisfies $i_T\varphi = 0$ and $\delta_b^D \varphi = 0$. Then*

$$\frac{d^2}{dt^2}[\mathcal{PYM}(D^t)]_{t=0} = \int_M \langle \mathcal{S}_b^D(\varphi), \varphi \rangle \theta \wedge (\mathrm{d}\theta)^n \tag{12}$$

where $\mathcal{S}_b^D(\varphi) \equiv \Delta_b^D \varphi + \mathcal{R}_b^D(\varphi)$ and $\Delta_b^D \varphi \equiv d_b^D \delta_b^D \varphi + \delta_b^D d_b^D \varphi$ is the generalized sublaplacian. The operator $\mathcal{S}_b^D : \Omega^{0,1}[\mathrm{Ad}(E)] \to \Omega^{0,1}[\mathrm{Ad}(E)]$ is subelliptic of order $\frac{1}{2}$.

As $\mathcal{R}_b^D$ is a zero order operator, the crucial point in the proof of Theorem 3 is to show that

$$(\Delta_b^D \varphi) \otimes e_j = 2\{\Box_b \varphi_j^i + (n-1)(\nabla_T \varphi_j^i + \varphi_j^i \circ \tau) \circ J\} \otimes e_i + \textit{lower order terms}, \tag{13}$$

for any $\varphi \in \Omega^{0,1}[\mathrm{Ad}(E)]$, $\varphi e_j = \varphi_j^i \otimes e_i$, and then exploit the subellipticity of the Kohn–Rossi operator $\Box_b$ on scalar (0, 1) forms.

III. CR AND PSEUDOHERMITIAN GEOMETRY

A. Basic definitions and results

Let M be a C^∞ manifold, of real dimension $(2n+1)$. A complex subbundle $T_{1,0}(M) \subset T(M) \otimes \mathbb{C}$, of complex rank n, is a *CR structure* on M (of *CR dimension n*) if

$$T_{1,0}(M) \cap T_{0,1}(M) = (0),$$

$$Z, W \in \Gamma^\infty[T_{1,0}(M)] \Rightarrow (Z, W) \in \Gamma^\infty[T_{1,0}(M)].$$

Here $T_{0,1}(M) = \overline{T_{1,0}(M)}$ is the complex conjugate of $T_{1,0}(M)$. Also, if $E \to M$ is a vector bundle then $\Gamma^\infty(E)$ denotes the space of C^∞ sections in E (eventually defined on some open set $U \subseteq M$, to be understood from the context). The *tangential Cauchy–Riemann operator*

$$\bar{\partial}_b : C^\infty(M) \to \Gamma^\infty[T_{0,1}(M)^*]$$

is given by $(\bar{\partial}_b f)\bar{Z} = \bar{Z}(f)$, for any C^∞ function $f : M \to \mathbb{C}$ and any $Z \in T_{1,0}(M)$. Let $E \to M$ be a complex vector bundle over a CR manifold. A *pre-$\bar{\partial}$-operator* is a first-order differential operator

$$\bar{\partial}_E : \Gamma^\infty(E) \to \Gamma^\infty[T_{0,1}(M)^* \otimes E]$$

such that

$$\bar{\partial}_E(fu) = f\bar{\partial}_E u + (\bar{\partial}_b f) \otimes u,$$

for any $f \in C^\infty(M)$ and any $u \in \Gamma^\infty(E)$. A pair $(E, \bar{\partial}_E)$ consisting of a complex vector bundle and a pre-$\bar{\partial}$-operator is a *CR-holomorphic* vector bundle if $\bar{\partial}_E$ satisfies the *integrability condition*

$$(\bar{Z}, \bar{W}) \cdot u = \bar{Z} \cdot \bar{W} \cdot u - \bar{W} \cdot \bar{Z} \cdot u,$$

for any $u \in \Gamma^\infty(E)$, $Z, W \in T_{1,0}(M)$. Here $\bar{Z} \cdot u$ is short for $(\bar{\partial}_E u)\bar{Z}$.

Let $H(M) = \mathrm{Re}\{T_{1,0}(M) \oplus T_{0,1}(M)\}$ be the *Levi distribution* and $J : H(M) \to H(M)$, $J(Z + \bar{Z}) = i(Z - \bar{Z})$, $Z \in T_{1,0}(M)$, its complex structure $(i = \sqrt{-1})$. When M is oriented, which is assumed throughout this paper, the conormal bundle $H(M)_x^\perp = \{\omega \in T_x^*(M) : \mathrm{Ker}(\omega) \supseteq H(M)_x\}$, $x \in M$, is an oriented real line bundle, hence trivial [$H(M)^\perp \approx M \times \mathbb{R}$, a vector bundle isomorphism]. Therefore $H(M)^\perp \to M$ admits globally defined nowhere zero sections $\theta \in \Gamma^\infty[H(M)^\perp]$, each of which is referred to as a *pseudohermitian structure* on M. The *Levi form* is

$$L_\theta(Z,\bar{W}) = -i(\mathrm{d}\theta)(Z,\bar{W}),$$

for any $Z, W \in T_{1,0}(M)$. $[M, T_{1,0}(M)]$ is *nondegenerate* if L_θ is nondegenerate for some θ. If this is the case, each pseudohermitian structure θ is a *contact form*, i.e., $\theta \wedge (d\theta)^n$ is a volume form on M. Two pseudohermitian structures $\theta, \hat{\theta} \in \Gamma^\infty[H(M)^\perp]$ are related by $\hat{\theta} = f\theta$, for some C^∞ function $f: M \to \mathbb{R}\setminus\{0\}$. Then $L_{\hat{\theta}} = fL_\theta$, hence nondegeneracy is a CR invariant notion (i.e., invariant under a transformation $\theta \mapsto f\theta$ of the pseudohermitian structure). Let T be the unique nowhere zero globally defined tangent vector field on M, transverse to the Levi distribution, determined by $\theta(T) = 1$ and $i_T \mathrm{d}\theta = 0$ (the *characteristic direction* of $\mathrm{d}\theta$). Also, let us consider the semi-Riemannian metric g_θ [the *Webster metric* of (M, θ)] given by

$$g_\theta(X,Y) = G_\theta(X,Y), \quad g_\theta(X,T) = 0, \quad g_\theta(T,T) = 1,$$

where $G_\theta(X,Y) = (d\theta)(X, JY)$, $X, Y \in H(M)$, is the (real) *Levi form* (note that L_θ and [the $\mathbb{C}$-linear extension of) G_θ coincide on $T_{1,0}(M) \otimes T_{0,1}(M)$]. $[M, T_{1,0}(M)]$ is *strictly pseudoconvex* if L_θ is positive definite for some θ. For instance, if $M = \{(x,y,u) \in \mathbb{R}^3 : y \neq 0\}$ is endowed with the CR structure given by (4) in Sec. I then a calculation shows that the characteristic direction [corresponding to the contact form $\theta = (1/y)dx - ydz$] is

$$T = \frac{y(3+y^2)}{4(1+y^2)}\frac{\partial}{\partial x} - \frac{i}{8}y(1-y^2)\frac{\partial}{\partial y} - \frac{1+3y^2}{4y(1+y^2)}\frac{\partial}{\partial z}$$

so that

$$[T_1, T_{\bar{1}}] = \frac{i}{2}T_1 - \frac{i}{2}T_{\bar{1}} - \frac{2i}{1+y^2}T$$

(where $T_{\bar{1}} = \bar{T}_1$). Consequently,

$$L_\theta(T_1, T_{\bar{1}}) = (i/2)\theta[(T_1, T_{\bar{1}})] = 1/(1+y^2),$$

hence M is strictly pseudoconvex. A fundamental result in pseudohermitian geometry (established independently by Tanaka[29] and Webster[34]) is that on any nondegenerate CR manifold on which a contact form θ has been fixed there is a unique linear connection ∇ [the *Tanaka–Webster connection* of (M, θ)] such that (i) $H(M)$ is parallel with respect to ∇; (ii) $\nabla g_\theta = 0$, $\nabla J = 0$; and (iii) the torsion T_∇ of ∇ is *pure*, i.e.,

$$T_\nabla(Z,W) = 0, \quad T_\nabla(Z,\bar{W}) = 2iL_\theta(Z,\bar{W})T, \quad Z, W \in T_{1,0}(M),$$

$$\tau \circ J + J \circ \tau = 0,$$

where $\tau(X) = T_\nabla(T, X)$, $X \in T(M)$, is the *pseudohermitian torsion*. If M is three dimensional ($n = 1$) and T_1 is a local generator of the CR structure we set

$$\nabla_{T_1} T_1 = \Gamma^1_{11} T_1, \quad \nabla_{T_{\bar{1}}} T_1 = \Gamma^1_{\bar{1}1} T_1, \quad \nabla_T T_1 = \Gamma^1_{01} T_1.$$

A calculation [based on (i)-(iii)] shows that

$$\Gamma^1_{11} = g^{1\bar{1}}\{T_1(g_{1\bar{1}}) - g_\theta[T_1, (T_1, T_{\bar{1}})]\}, \tag{14}$$

$$\Gamma^1_{\bar{1}1} = g^{1\bar{1}} g_\theta[(T_{\bar{1}}, T_1), T_{\bar{1}}], \tag{15}$$

$$\Gamma_{01}^{1} = g^{1\bar{1}} g_{\theta}[(T,T_1),T_{\bar{1}}]. \tag{16}$$

Here $g_{1\bar{1}}=L_\theta(T_1,T_{\bar{1}})$ and $g^{1\bar{1}}=1/g_{1\bar{1}}$. Going back to the example $\mathbb{R}^3\backslash\{y=0\}$ with the CR structure (4) we have

$$(T,T_1) = \frac{i}{8}(1-y^2)T_1 + \frac{i}{8}(1+y^2)T_{\bar{1}}$$

hence [by (14)–(16)]

$$\Gamma_{11}^{1} = i\left(\frac{1}{2} + \frac{y^2}{1+y^2}\right), \quad \Gamma_{\bar{1}1}^{1} = -\frac{i}{2}(1+y^2), \quad \Gamma_{01}^{1} = \frac{i}{8}(1-y^2).$$

We assume from now on that, unless otherwise stated, M is strictly pseudoconvex. A complex valued differential p form η on M is *of type* $(p,0)$ [or a $(p,0)$ *form* on M] if $T_{0,1}(M)\rfloor\eta=0$. Let θ be a contact form on M and T the characteristic direction of $\mathrm{d}\theta$. Let $\{T_\alpha: 1\leqslant\alpha\leqslant n\}$ be a local frame in $T_{1,0}(M)$, defined on an open set $U\subseteq M$. Let $\{\theta^\alpha: 1\leqslant\alpha\leqslant n\}$ be the corresponding *admissible coframe*, i.e, the (locally defined) complex 1-forms determined by $\theta^\alpha(T_\beta)=\delta^\alpha_\beta$, $\theta^\alpha(T_{\bar{\beta}})=0$, and $\theta^\alpha(T)=0$. Here $T_{\bar{\beta}}=\overline{T_\beta}$. Then $\{\theta^\alpha,\theta^{\bar{\alpha}},\theta\}$ is a (local) frame of $T^*(M)\otimes\mathbb{C}$ on U and a $(p,0)$ form η on M may be locally expressed as sums of monomials of the form $\theta^{\alpha_1}\wedge\cdots\wedge\theta^{\alpha_p}$ or $\theta\wedge\theta^{\alpha_1}\wedge\cdots\wedge\theta^{\alpha_{p-1}}$ [with $C^\infty(U)$ coefficients]. Therefore, the top degree complex forms η such that $T_{1,0}(M)\rfloor\eta=0$ are (unlike the case of complex manifolds, where the top degree is the complex dimension) the forms of type $(n+1,0)$ (where n is the CR dimension). Let $K(M)=\Lambda^{n+1,0}(M)\to M$ be the bundle of $(n+1,0)$ forms on M (the *canonical line bundle*). There is a natural action of $\mathbb{R}^+=(0,+\infty)$ on $K(M)\backslash\{zero\ section\}$. Let $C(M)$ be the quotient space and $\pi: C(M)\to M$ the projection. Then $C(M)\to M$ is a principal S^1 bundle (the *canonical circle bundle*). Its locally trivial structure is described by

$$\pi^{-1}(U)\to U\times S^1, \quad [\omega]\mapsto(x,\lambda/|\lambda|),$$

$$\omega=\lambda(\theta\wedge\theta^1\wedge\cdots\wedge\theta^n)_x, \quad x\in U, \quad \lambda\in\mathbb{C}^*=\mathbb{C}\backslash\{0\}.$$

We shall need the local fiber coordinate

$$\gamma:\pi^{-1}(U)\to\mathbb{R}, \quad \gamma([\omega])=\arg(\lambda/|\lambda|),$$

where arg: $S^1\to[0,2\pi)$. Let $(E,\bar{\partial}_E)\to M$ be a CR holomorphic vector bundle. Let h be a Hermitian metric in E. Let $\mathcal{C}(E,h)$ be the affine space of all connections D in E such that $Dh=0$, i.e.

$$X[h(u,v)]=h(D_X u,v)+h(u,D_{\bar{X}}v),$$

for any $X\in T(M)\otimes\mathbb{C}$ and any $u,v\in\Gamma^\infty(E)$. A connection $D\in\mathcal{C}(E,h)$ is *Hermitian* if $D^{0,1}=\bar{\partial}_E$. Here $D^{0,1}u$ is the restriction of Du to $T_{0,1}(M)$. Let $\mathrm{Ad}(E)\to M$ be the subbundle of $\mathrm{End}(E)\to M$ consisting of all skew-symmetric endomorphisms S, i.e., $h(Su,v)+h(u,Sv)=0$, for any $u,v\in\Gamma^\infty(E)$. By a result in Ref. 6 p. 43, given a contact form θ and an endomorphism $S\in\Gamma^\infty[\mathrm{Ad}(E)]$ there is a unique Hermitian connection $D=D(h,\theta,S)$ in E (the *canonical Sconnection*) such that

$$\Lambda_\theta R^D = 2nS. \tag{17}$$

Here $R^D=D\circ D:\Omega^0(E)\to\Omega^2(E)$ is the curvature 2-form of D. Also we set $\Omega^k(E)=\Gamma^\infty[\Lambda^k T^*(M)\otimes E]$, $k\geqslant 0$. If $F\to M$ is a vector bundle and $\varphi\in\Gamma^\infty[T^*(M)\otimes T^*(M)\otimes F]$ the trace $\Lambda_\theta\varphi$ of φ is given by

$$i(\Lambda_\theta\varphi)_x = \sum_{\alpha=1}^{n} \varphi(Z_\alpha, Z_{\bar{\alpha}})_x,$$

where $\{Z_\alpha\}$ is a (local) orthonormal [i.e., $L_\theta(Z_\alpha, Z_{\bar{\beta}}) = \delta_{\alpha\beta}$] frame of $T_{1,0}(M)$ on $U \ni x$. Therefore $\Lambda_\theta\varphi \in \Gamma^\infty(F)$. When $S=0$ the canonical S connection is the *Tanaka connection* $D(h,\theta,0)$ in $E \to M$ (cf. Ref. 29). $D(h,\theta,0)$ is a CR invariant. Assume M to be compact. The *Yang–Mills functional* $\mathcal{YM}:\mathcal{C}(E,h)\to[0,+\infty)$ is given by

$$\mathcal{YM}(D) = \frac{1}{2}\int_M \|R^D\|^2 \theta \wedge (\mathrm{d}\theta)^n.$$

A *Yang–Mills field* on M is a critical point $D \in \mathcal{C}(E,h)$ of $\mathcal{YM}$, i.e., a solution to the Yang–Mills equations

$$\delta^D R^D = 0. \tag{18}$$

Let Ω be a differential 2-form on M. Then Ω is *of type* $(1,1)$ if $\Omega(Z,W)=0$, $\Omega(\bar{Z},\bar{W})=0$, for any $Z, W \in T_{1,0}(M)$, and $i_T\Omega=0$. Let $D \in \mathcal{C}(E,h)$ be a Hermitian connection such that its curvature R^D is a form of type $(1,1)$. By a result in Ref. 30, D is a Yang–Mills field if and only if D is the Tanaka connection $D(h,\theta,0)$. In general, canonical S connections solve the inhomogeneous Yang–Mills equations $\delta^D R^D = f$, in the presence of suitable compatibility conditions satisfied by f (cf. Theorem 2 in Ref. 6, pp. 44–45).

B. Symmetric CR structures

The CR structure $T_{1,0}(M)$ is *symmetric* if there is $X \in \mathcal{X}(M)$ such that

$$\mathcal{L}_X\theta = t\theta, \quad \mathcal{L}_X\theta^\alpha = w^\alpha_\beta\theta^\beta + \ell^\alpha\theta,$$

for some functions $t, w^\alpha_\beta, \ell^\alpha$ on M (t real valued) and X is a *symmetry* of $T_{1,0}(M)$. If

$$\hat{\theta} = e^u\theta, \quad \hat{\theta}^\alpha = U^\alpha_\beta\theta^\beta + v^\alpha\theta,$$

[where $[U^\alpha_\beta]$ is $\mathrm{GL}(n,\mathbb{C})$ valued] and X is a symmetry of the CR structure then

$$\mathcal{L}_X\hat{\theta} = \hat{t}\hat{\theta}, \quad \hat{t} \equiv t + X(u), \tag{19}$$

$$\mathcal{L}_X\hat{\theta}^\alpha = \hat{w}^\alpha_\beta\hat{\theta}^\beta + \hat{\ell}^\alpha\hat{\theta},$$

$$\hat{w}^\alpha_\beta \equiv (U^{-1})^\gamma_\beta[X(U^\alpha_\gamma) + U^\alpha_\rho w^\rho_\gamma],$$

$$\hat{\ell}^\alpha \equiv e^{-u}\{X(v^\alpha) + U^\alpha_\beta\ell^\beta + v^\alpha t - (U^{-1})^\gamma_\rho v^\rho[X(U^\alpha_\gamma) + U^\alpha_\beta w^\beta_\gamma]\}. \tag{20}$$

In particular (19) and (20) show that the notion of symmetric CR structure is globally defined. Assume from now on that the CR structure $T_{1,0}(M)$ admits $2n+1$ linearly independent symmetries $\widetilde{X}_1, \cdots, \widetilde{X}_{2n+1} \in \mathcal{X}(M)$ such that $[\widetilde{X}_i, \widetilde{X}_j] = c^k_{ij}\widetilde{X}_k$, for some $c^k_{ij} \in \mathbb{R}$.

Proposition 1: (Ref. 24) Let M *be a strictly pseudoconvex CR manifold with* $H^1(M;\mathbb{R})=0$. *There is a transformation* $\{\theta,\theta^\alpha\} \mapsto \{\Omega,\Omega^\alpha\}$ of the form

$$\Omega = e^u\theta, \quad \Omega^\alpha = U^\alpha_\beta\theta^\beta + v^\alpha\theta, \tag{21}$$

where $[U^\alpha_\beta]$ is $\mathrm{GL}(n,\mathbb{C})$ valued, such that

$$\mathcal{L}_{\widetilde{X}_i}\Omega = 0, \quad \mathcal{L}_{\widetilde{X}_i}\Omega^\alpha = 0, \quad 1 \leqslant i \leqslant 2n+1.$$

Here $H^1(M;\mathbb{R})$ is the first de Rham cohomology group. Its vanishing guarantees that the solution u to (22) is globally defined.

Proof of Proposition 2: As $\widetilde{X}_i$ are symmetries of the CR structure

$$\mathcal{L}_{\widetilde{X}_i}\theta = t_i\theta, \quad \mathcal{L}_{\widetilde{X}_i}\theta^\alpha = w_{i\beta}^\alpha\theta^\beta + \ell_i^\alpha\theta.$$

We must solve the system of first-order linear Partial different equations

$$t_i + \widetilde{X}_i(u) = 0, \tag{22}$$

$$\widetilde{X}_i(U_\beta^\alpha) + U_\gamma^\alpha w_{i\beta}^\gamma = 0, \tag{23}$$

$$\widetilde{X}_i(v^\alpha) + U_\beta^\alpha\ell_i^\beta + v^\alpha t_i = 0, \tag{24}$$

with the unknowns u, U_β^α, and v^α. Let $\eta \in \Omega^1(M)$ be defined by $\eta(\widetilde{X}_i) = t_i$, $1 \leqslant i \leqslant 2n+1$. Then (22) may be written $du + \eta = 0$. We have

$$\mathcal{L}_{\widetilde{X}_i}\mathcal{L}_{\widetilde{X}_j}\theta = \mathcal{L}_{\widetilde{X}_j}\mathcal{L}_{\widetilde{X}_i}\theta + \mathcal{L}_{[\widetilde{X}_i,\widetilde{X}_j]}\theta$$

hence

$$\widetilde{X}_i(t_j) - \widetilde{X}_j(t_i) - c_{ij}^k t_k = 0$$

that is $d\eta = 0$. Thus there is a globally defined real valued function $g \in C^\infty(M)$ such that $\eta = dg$ and $u \equiv -g$ solves (22). Next, we consider the (locally defined) 1-forms η_β^α and η^α given by

$$\eta_\beta^\alpha(\widetilde{X}_i) = w_{i\beta}^\alpha, \quad \eta^\alpha(\widetilde{X}_i) = \ell_i^\alpha, \quad 1 \leqslant i \leqslant 2n+1.$$

Then (23) and (24) may be written

$$dU_\beta^\alpha + U_\gamma^\alpha\eta_\beta^\gamma = 0, \tag{25}$$

$$dv^\alpha + v^\alpha\eta + U_\beta^\alpha\eta^\beta = 0. \tag{26}$$

Assuming that (25) has been solved in a neighborhood U of each point, let us solve (26). Multiplying in both sides by e^{-u} [where u is a solution to (22)] leads to

$$d(e^{-u}v^\alpha) + e^{-u}U_\beta^\alpha\eta^\beta = 0.$$

Therefore, to prove existence of a (local) solution v^α to (26) it suffices to show that $e^{-u}U_\beta^\alpha\eta^\beta$ is exact (in a neighborhood of a point). The identity

$$\mathcal{L}_{\widetilde{X}_i}\mathcal{L}_{\widetilde{X}_j}\theta^\alpha = \mathcal{L}_{\widetilde{X}_j}\mathcal{L}_{\widetilde{X}_i}\theta^\alpha + \mathcal{L}_{[\widetilde{X}_i,\widetilde{X}_j]}\theta^\alpha$$

yields

$$d\eta_\beta^\alpha = \eta_\gamma^\alpha \wedge \eta_\beta^\gamma, \tag{27}$$

$$d\eta^\alpha = \eta_\beta^\alpha \wedge \eta^\beta + \eta^\alpha \wedge \eta. \tag{28}$$

Let U_β^α be a solution to (25). Then [by (28)]

$$d(e^{-u}U^{\alpha}_{\beta}\eta^{\beta}) = e^{-u}(\mathrm{d}U^{\alpha}_{\beta}\wedge\eta^{\beta} + U^{\alpha}_{\beta}\mathrm{d}\eta^{\beta} - U^{\alpha}_{\beta}\mathrm{d}u\wedge\eta^{\beta}) = e^{-u}U^{\alpha}_{\beta}(\mathrm{d}\eta^{\beta} - \eta^{\beta}_{\gamma}\wedge\eta^{\gamma} - \eta^{\beta}\wedge\eta) = 0.$$

Thus there is a function $f^{\alpha}\in C^{\infty}(U)$ such that $e^{-u}U^{\alpha}_{\beta}\eta^{\beta}=\mathrm{d}f^{\alpha}$ and $v^{\alpha}\equiv -e^{u}f^{\alpha}$ solves (26). To solve (25) let (U,x^{i}) be a normal coordinate neighborhood at a point $x_0\in M$ (we think of M as a Riemannian manifold with the Webster metric g_{θ}). We shall show that for any $c^{\alpha}_{\beta}\in\mathbb{C}$ there is a unique solution to (25) with the initial condition $U^{\alpha}_{\beta}(x_0)=c^{\alpha}_{\beta}$. Let $a=(a^{1},\cdots,a^{2n+1})\in U$ be an arbitrary point and let us consider the geodesic $a_t=(a^{1}t,\cdots,a^{2n+1}t)$. Let $f^{\alpha}_{\beta}(t)$ be the solution to the Cauchy problem for the system of ordinary differential equations

$$\frac{df^{\alpha}_{\beta}}{dt} + f^{\alpha}_{\gamma}(t)\,\eta^{\gamma}_{\beta}(\dot{a}_t) = 0,$$

with the initial condition $f^{\alpha}_{\beta}(0)=c^{\alpha}_{\beta}$, where $\dot{a}_t$ is the tangent vector at a_t. We define $U^{\alpha}_{\beta}\in C^{\infty}(U)$ by setting $U^{\alpha}_{\beta}(a)=f^{\alpha}_{\beta}(1)$. Of course, if we start with $\det(c^{\alpha}_{\beta})\neq 0$ then $[U^{\alpha}_{\beta}]$ is $\mathrm{GL}(m,\mathbb{C})$ valued on a neighborhood of x_0. We wish to show that U^{α}_{β} satisfies (25), i.e.

$$Y(U^{\alpha}_{\beta}) + U^{\alpha}_{\gamma}(a)\,\eta^{\gamma}_{\beta,a}(Y) = 0, \tag{29}$$

for any $Y=b^{j}(\partial/\partial x^{j})_{a}\in T_a(M)$. We start by extending Y to the vector field $Y=b^{j}\partial/\partial x^{j}$ with constant components b^{j} on U. Similarly, let us extend the vector field $\dot{a}_t$ along the geodesic a_t to the vector field $X=a^{i}\partial/\partial x^{i}$. We shall show that along a_t

$$X[Y(U^{\alpha}_{\beta}) + U^{\alpha}_{\rho}\eta^{\rho}_{\beta}(Y)] + [Y(U^{\alpha}_{\gamma}) + U^{\alpha}_{\rho}\eta^{\rho}_{\gamma}(Y)]\eta^{\gamma}_{\beta}(X) = 0. \tag{30}$$

When this is done, we see that $Y(U^{\alpha}_{\beta})+U^{\alpha}_{\rho}\eta^{\rho}_{\beta}(Y)$, clearly satisfying $Y(U^{\alpha}_{\beta})+U^{\alpha}_{\rho}\eta^{\rho}_{\beta}(Y)=0$ at x_0, must be the zero function [which satisfies (30) with the same initial condition], i.e. (29) is verified. It remains that we prove (30). This follows from (27). Indeed (as $[X,Y]=0$)

$$X[\eta^{\alpha}_{\beta}(Y)] = Y[\eta^{\alpha}_{\beta}(X)] + \eta^{\alpha}_{\gamma}(X)\,\eta^{\gamma}_{\beta}(Y) - \eta^{\alpha}_{\gamma}(Y)\,\eta^{\gamma}_{\beta}(X)$$

and the proof of (30) is straightforward. Proposition 1 is a first step toward recovering the methods of Nurowski,[24] (eventually leading to local solutions of the Yang–Mills equations on $[C(M),F_{\theta}]$) as mentioned in Sec. I. The result in Proposition 1 may be refined to show that there is a coframe $\{\Omega,\Omega^{\alpha}\}$ such that

$$\mathcal{L}_{\tilde{X}_i}\Omega = 0, \quad \mathcal{L}_{\tilde{X}_i}\Omega^{\alpha} = 0, \quad d\Omega = 2i\sum_{\alpha=1}^{n}\Omega^{\alpha}\wedge\Omega^{\bar{\alpha}}$$

[compare to Eq. (2) in Sec. I]. The proof is illustrative of the local methods in pseudohermitian geometry. Let $\{\Omega,\Omega^{\alpha}\}$ be the 1-forms furnished by Proposition 21, given by a transformation of the form (21). If $\{T,T_{\alpha}\}$ is such that $\theta(T)=1$, $i_T\,\mathrm{d}\theta=0$, and $\theta^{\alpha}(T_{\beta})=\delta^{\alpha}_{\beta}$, $\theta^{\alpha}(T_{\bar{\beta}})=0$, $\theta^{\alpha}(T)=0$, let us set $W_{\alpha}=(U^{-1})^{\beta}_{\alpha}T_{\beta}$. One may easily show that

$$\mathrm{d}\Omega = 2iG_{\alpha\bar{\beta}}\Omega^{\alpha}\wedge\Omega^{\bar{\beta}} + \Phi\wedge\Omega, \tag{31}$$

where $G_{\alpha\bar{\beta}}=e^{u}(U^{-1})^{\gamma}_{\alpha}U^{\bar{\rho}}_{\bar{\beta}}g_{\gamma\bar{\rho}}$ and $\Phi=e^{-u}[W_{\alpha}(u)\Omega^{\alpha}+W_{\bar{\alpha}}(u)\Omega^{\bar{\alpha}}]$. By $\mathcal{L}_X=d\circ i_X+i_X\circ d$ it follows that $\mathcal{L}_{\tilde{X}_i}d\Omega=0$. Taking the Lie derivative of (31) gives

$$0 = \mathcal{L}_{\tilde{X}_i}\mathrm{d}\Omega = 2\sqrt{-1}\,\mathcal{L}_{\tilde{X}_i}(G_{\alpha\bar{\beta}})\Omega^{\alpha}\wedge\Omega^{\bar{\beta}} + (\mathcal{L}_{\tilde{X}_i}\Phi)\wedge\Omega$$

hence (as $\mathcal{L}_{\tilde{X}_i}\Phi\equiv 0$, mod Ω) on one hand $\tilde{X}_i(G_{\alpha\bar{\beta}})=0$, i.e., $G_{\alpha\bar{\beta}}=a_{\alpha\bar{\beta}}\in\mathbb{C}$, and on the other $\mathcal{L}_{\tilde{X}_i}\Phi=0$. The latter may be written $\mathrm{d}u_{\alpha}-u_{\alpha}\,\mathrm{d}u=0$ [where $u_{\alpha}=W_{\alpha}(u)$]. Hence $d(e^{-u}u_{\alpha})=0$, i.e., $u_{\alpha}=c_{\alpha}e^{u}$, for some $c_{\alpha}\in\mathbb{C}$. Therefore $\Phi=c_{\alpha}\Omega^{\alpha}+c_{\bar{\alpha}}\Omega^{\bar{\alpha}}$. Finally, let $[b^{\alpha}_{\beta}]$ be a square root of $[a_{\alpha\bar{\beta}}]$ (as $[a_{\alpha\bar{\beta}}]$ is positive definite) and consider the transformation

$$\hat{\Omega}^{\alpha} = b^{\alpha}_{\beta}\Omega^{\beta} + \frac{i}{2}c_{\bar{\beta}}(b^{-1})^{\bar{\beta}}_{\bar{\alpha}}\Omega.$$

Then $d\Omega = 2i\ \Sigma_{\alpha=1}^{n}\hat{\Omega}^{\alpha}\wedge\hat{\Omega}^{\bar{\alpha}}$ and $\mathcal{L}_{\tilde{X}_i}\hat{\Omega}^{\alpha}=0$. Q.E.D.

IV. BOUNDARY VALUES OF YANG–MILLS FIELDS

Let $\Omega\subset\mathbb{C}^n$ be a bounded domain with smooth boundary $\partial\Omega$, i.e., there is a neighborhood $U\supset\bar{\Omega}$ and a real valued function $\varphi\in C^{\infty}(U)$ such that $\Omega=[z\in U:\varphi(z)<0]$, $\partial\Omega=[z\in U:\varphi(z)=0]$, and $\nabla\varphi(z)\neq 0$, for any $z\in\partial\Omega$. We assume that Ω is strictly pseudoconvex, i.e., $\partial\Omega$ is a strictly pseudoconvex CR manifold (with the natural CR structure $T_{1,0}(\partial\Omega)=T^{1,0}(\mathbb{C}^n)\cap[T(\partial\Omega)\otimes\mathbb{C}]$ induced by the complex structure of the ambient space).

Let $\pi:F\to U$ be a holomorphic vector bundle. The portion $E=\pi^{-1}(\partial\Omega)$ of F over the boundary of Ω is CR holomorphic. Indeed, as F is holomorphic, there is a natural differential operator

$$\bar{\partial}_F:\Gamma^{\infty}(F)\to\Gamma^{\infty}[T^{0,1}(U)^{*}\otimes F]$$

where $T^{0,1}(U)$ is the antiholomorphic tangent bundle over U. Given $u\in\Gamma^{\infty}(E)$ let $\tilde{u}\in\Gamma^{\infty}(F)$ be a C^{∞} extension of u as a cross section in F and set $(\bar{\partial}_E u)_z=(\bar{\partial}_F\tilde{u})_z$ for any $z\in\partial\Omega$. The definition of $(\bar{\partial}_E u)_z$ does not depend upon the choice of extension $\tilde{u}$ of u because $(\bar{\partial}f)|_{T_{0,1}(\partial\Omega)}=\bar{\partial}_b(f|_{\partial\Omega})$ for any C^{∞} function $f:U\to\mathbb{C}$. Let $\{\Phi_{\alpha}:\pi^{-1}(\Omega_{\alpha})\to\Omega_{\alpha}\times\mathbb{C}^m:\alpha\in I\}$ be a trivialization atlas for F and $G_{\beta\alpha}:\Omega_{\beta}\cap\Omega_{\alpha}\to\mathrm{GL}(m,\mathbb{C})$ the corresponding transition functions. Set $U_{\alpha}=\Omega_{\alpha}\cap\partial\Omega$ and $g_{\beta\alpha}=G_{\beta\alpha}|_{U_{\alpha}\cap U_{\beta}}$. As $G_{\beta\alpha}$ are holomorphic, it follows that $E\to\partial\Omega$ is a peculiar type of CR-holomorphic vector bundle (called *locally trivial* by Le Brun[17]) in that its transition functions $g_{\beta\alpha}$ are matrix valued CR functions on $\partial\Omega$.

Let $K(\zeta,z)$ be the Bergman kernel of Ω. By a classical result in Ref. 8

$$K(\zeta,z)=c_{\Omega}|\nabla\varphi(z)|^2\cdot\det L_{\varphi}(z)\cdot\Psi(\zeta,z)^{-(n+1)}+H(\zeta,z), \tag{32}$$

(the *Fefferman asymptotic expansion formula* for the Bergman kernel) where $H\in C^{\infty}(\bar{\Omega}\times\bar{\Omega}\backslash\Delta)$, Δ is the diagonal of $\partial\Omega\times\partial\Omega$, and H satisfies the estimate

$$|H(\zeta,z)|\leqslant c'_{\Omega}|\Psi(\zeta,z)|^{-(n+1)+1/2}\cdot|\log|\Psi(\zeta,z)||. \tag{33}$$

Here $L_{\varphi}=\partial\bar{\partial}\varphi$. Also we set

$$\Psi(\zeta,z)=[F(\zeta,z)-\varphi(z)]\chi(|\zeta-z|)+[1-\chi(|\zeta-z|)]|\zeta-z|^2$$

where

$$F(\zeta,z)=-\sum_{j=1}^{n}\frac{\partial\varphi}{\partial z^j}(z)(\zeta^j-z^j)-\frac{1}{2}\sum_{j,k=1}^{n}\frac{\partial^2\varphi}{\partial z^j\partial z^k}(z)(\zeta^j-z^j)(\zeta^k-z^k)$$

and $\chi(t)$ is a C^{∞} cutoff function with $\chi(t)=1$ for $|t|<\epsilon_0/2$ and $\chi(t)=0$ for $|t|\geqslant 3\epsilon_0/4$. As a consequence of (32)

$$K(z,z)^{-1/(n+1)}=|\varphi(z)|[\Phi(z)+H(z,z)|\varphi(z)|^{n+1}]^{-1/(n+1)}$$

where $\Phi(z)\equiv c_{\Omega}|\nabla\varphi(z)|^2\det L_{\varphi}(z)$ stays finite near $\partial\Omega$ and [by (33)]

$$|H(z,z)||\varphi(z)|^{n+1}\leqslant c'_{\Omega}|\varphi(z)|^{1/2}|\log|\varphi(z)||\to 0,\quad as\ z\to\partial\Omega.$$

Therefore $K(z,z)^{-1/(n+1)}$ vanishes at $\partial\Omega$. Also, as $\Phi(z)\neq 0$ near the boundary, $\nabla K(z,z)^{-1/(n+1)}\neq 0$ along $\partial\Omega$, hence $K(z,z)^{-1/(n+1)}$ may be used as a defining function for Ω.

For the rest of this section we assume that $\varphi(z)\equiv -K(z,z)^{-1/(n+1)}$ and set $\theta\equiv(i/2)(\bar{\partial}-\partial)\varphi$. Then $\mathrm{d}\theta=i\partial\bar{\partial}\varphi$. Let us differentiate $\log|\varphi|=-[1/(n+1)]\log K$ [where K is short for $K(z,z)$] so that to obtain

$$\frac{1}{\varphi}\bar{\partial}\varphi=-\frac{1}{n+1}\bar{\partial}\log K.$$

Applying the operator $i\partial$ leads to

$$\frac{1}{\varphi}d\theta-\frac{i}{\varphi^2}\partial\varphi\wedge\bar{\partial}\varphi=-\frac{i}{n+1}\partial\bar{\partial}\log K. \tag{34}$$

We shall need the Bergman metric

$$g=\frac{\partial^2\log K}{\partial z^j\partial\bar{z}^k}\mathrm{d}z^j\odot\mathrm{d}\bar{z}^k.$$

As is well known, g is a Kähler metric on Ω (Kähler–Einstein when Ω is homogeneous). Here $\odot$ denotes the symmetric tensor product, i.e., $\alpha\odot\beta=\frac{1}{2}(\alpha\otimes\beta+\beta\otimes\alpha)$. Let us set $\omega(X,Y)=g(X,JY)$ [the Kähler 2-form of (Ω,J,g), where J is the underlying complex structure]. Then $\omega=-i\partial\bar{\partial}\log K$ and (34) may be written

$$g(X,Y)=\frac{n+1}{\varphi}\left[\frac{i}{\varphi}(\partial\varphi\wedge\bar{\partial}\varphi)(X,JY)-d\theta(X,JY)\right], \tag{35}$$

for any $X,Y\in\mathcal{X}(\Omega)$.

We denote by $M_\delta=\{z\in\Omega:\varphi(z)=-\delta\}$ ($\delta>0$) the level sets of φ. For δ sufficiently small M_δ is still a strictly pseudoconvex CR manifold (of CR dimension $n-1$). Therefore, there is a one-sided neighborhood V of $\partial\Omega$ which is foliated by the (strictly pseudoconvex) level sets of φ. Let $\mathcal{F}$ be the relevant foliation and let us denote by $H(\mathcal{F})\to V$ [respectively, by $T_{1,0}(\mathcal{F})\to V$] the bundle whose portion over M_δ is the Levi distribution $H(M_\delta)$ [respectively, the CR structure $T_{1,0}(M_\delta)$]. Note that

$$T_{1,0}(\mathcal{F})\cap T_{0,1}(\mathcal{F})=(0),$$

$$\{\Gamma^\infty[T_{1,0}(\mathcal{F})],\Gamma^\infty[T_{1,0}(\mathcal{F})]\}\subseteq\Gamma^\infty[T_{1,0}(\mathcal{F})].$$

Here $T_{0,1}(\mathcal{F})=\overline{T_{1,0}(\mathcal{F})}$. By a result in,[20] there is a unique complex vector field ξ on V, of type (1,0), such that $\partial\varphi(\xi)=1$ and ξ is orthogonal to $T_{1,0}(\mathcal{F})$ with respect to $\partial\bar{\partial}\varphi$, i.e., $\partial\bar{\partial}\varphi(\xi,\bar{Z})=0$, for any $Z\in T_{1,0}(\mathcal{F})$. We set $r\equiv 2\partial\bar{\partial}\varphi(\xi,\bar{\xi})$ (r is the *transverse curvature* of φ). Let $\xi=\frac{1}{2}(N-iT)$ be the real and imaginary parts of ξ. Then

$$(d\varphi)(N)=2,\quad (d\varphi)(T)=0,$$

$$\theta(N)=0,\quad \theta(T)=1,$$

$$\partial\varphi(N)=1,\quad \partial\varphi(T)=i.$$

In particular, T is tangent to (the leaves of) $\mathcal{F}$. $\mathcal{F}$ carries the tangential Riemannian metric g_θ [defined by (A1) in the Appendix]. Note that the pullback of g_θ to each leaf M_δ of $\mathcal{F}$ is the Webster metric of M_δ (associated to the contact form $j_\delta^*\theta$, where $j_\delta:M_\delta\subset V$). As a consequence of (35)

$$g(X,Y) = -\frac{n+1}{\varphi} g_\theta(X,Y), \quad X,Y \in H(\mathcal{F}). \tag{36}$$

Also (by $JT=-N$ and (A4))

$$g(X,T) = 0, \quad g(X,N) = 0, \quad X \in H(\mathcal{F}), \tag{37}$$

$$g(T,N) = 0, \quad g(T,T) = g(N,N) = \frac{n+1}{\varphi}\left(\frac{1}{\varphi} - r\right). \tag{38}$$

In particular $1-r\varphi>0$ everywhere in Ω. Using (36)–(38) we may relate the Levi–Civita connection ∇^g of (V,g) to the Graham–Lee connection ∇ (see the Appendix). By (36) [as $X(\varphi)=0$, $X \in T(\mathcal{F})$]

$$g(\nabla^g_X Y, Z) = g(\nabla_X Y, Z), \quad X,Y,Z \in H(\mathcal{F}). \tag{39}$$

Note that any tangent vector field $X \in T(V)$ decomposes as

$$X = \pi_H X + \theta(X)T + \frac{1}{2}(d\varphi)(X)N,$$

[$\pi_H : T(V) \to H(\mathcal{F})$ is the projection]. By (A3) $\theta([T,X])=0$, $X \in H(\mathcal{F})$. Also $[T,X] \in T(\mathcal{F})$, hence $[T,X] \in H(\mathcal{F})$, for any $X \in H(\mathcal{F})$. Taking into account the identity

$$2g(\nabla^g_X Y, Z) = X(g(Y,Z)) + Y[g(X,Z)] - Z(g(X,Y)) + g([X,Y],Z) + g([Z,X],Y) + g(X,[Z,Y]), \tag{40}$$

for any $X,Y,Z \in T(V)$, one has [by (37)]

$$2g(\nabla^g_X Y, T) = -T[g(X,Y)] + g[(X,Y),T] + g[(T,X),Y] + g[X,(T,Y)] = \frac{n+1}{\varphi}\{T[g_\theta(X,Y)]$$

$$- g_\theta[(T,X),Y] - g_\theta[X,(T,Y)]\} + \frac{n+1}{\varphi}\left(\frac{1}{\varphi} - r\right)\theta[(X,Y)],$$

for any $X,Y \in H(\mathcal{F})$. By (A13) and (A14) and $\nabla_X Y \in H(\mathcal{F})$ it follows that

$$T[g_\theta(X,Y)] - g_\theta[(T,X),Y] - g_\theta[X,(T,Y)] = 2g_\theta(\tau X, Y)$$

[note that one makes use of the fact that $\tau : H(\mathcal{F}) \to H(\mathcal{F})$ is self-adjoint, i.e., $g_\theta(\tau X, Y) = g_\theta(X, \tau Y)$, $X,Y \in H(\mathcal{F})$] hence

$$g(\nabla^g_X Y, T) = -g(\tau X, Y) - \frac{n+1}{\varphi}\left(\frac{1}{\varphi} - r\right)(\mathrm{d}\theta)(X,Y)$$

or

$$g(\nabla^g_X Y, T) = -g(\tau X, Y) - \left(\frac{1}{\varphi} - r\right)g(X, \phi Y), \tag{41}$$

for any $X,Y \in H(\mathcal{F})$. Exploiting again $\nabla^g g=0$ (and $g[(X,Y),N]=0$) we get

$$2g(\nabla^g_X Y, N) = -(\mathcal{L}_N g)(X,Y), X,Y \in H(\mathcal{F}).$$

Hence [by (A23) in Lemma 4]

$$2g(\nabla^g_X Y,N) = -\frac{n+1}{\varphi^2}N(\varphi)g_\theta(X,Y) + \frac{n+1}{\varphi}(\mathcal{L}_N g_\theta)(X,Y) = 2\left(\frac{1}{\varphi} - r\right)g(X,Y) + \frac{2(n+1)}{\varphi}(\mathrm{d}\theta)(X,\tau Y)$$

that is

$$g(\nabla^g_X Y,N) = \left(\frac{1}{\varphi} - r\right)g(X,Y) + g(X,\phi\tau Y), \tag{42}$$

for any $X,Y \in H(\mathcal{F})$. Note that (42) may be also derived from (41) by using the fact that g is a Kähler metric. Indeed

$$g(\nabla^g_X Y,N) = g(J\nabla^g_X Y,JN) = g(\nabla^g_X JY,T) = -g(\tau X,\phi Y) - \left(\frac{1}{\varphi} - r\right)g(X,\phi^2 Y),$$

etc. For further use, let us also remember that

$$(\mathcal{L}_N g)(X,Y) = -2\left(\frac{1}{\varphi} - r\right)g(X,Y) - 2g(X,\phi\tau Y), \tag{43}$$

for any $X,Y \in H(\mathcal{F})$. At this point, the identities (39) and (41) and (42) lead to

$$\nabla^g_X Y = \nabla_X Y + \left[\frac{\varphi}{1-\varphi r}g_\theta(\tau X,Y) + g_\theta(X,\phi Y)\right]T - \left[g_\theta(X,Y) + \frac{\varphi}{1-\varphi r}g_\theta(X,\phi\tau Y)\right]N, \tag{44}$$

for any $X,Y \in H(\mathcal{F})$. To compute $\nabla^g_X T$ we use (44) and

$$g(\nabla^g_X T,Y) = -g(T,\nabla^g_X Y)$$

so that

$$g(\nabla^g_X T,Y) = g(\tau X,Y) + \left(\frac{1}{\varphi} - r\right)g(X,\phi Y). \tag{45}$$

The component along T is $\frac{1}{2}X(\|T\|^2)$ hence

$$g(\nabla^g_X T,T) = -\frac{n+1}{2\varphi}X(r). \tag{46}$$

Moreover [by (A5) in the Appendix A]

$$2g(\nabla^g_X T,N) = g[X,(N,T)] = -g(X,\phi\nabla^H r)$$

that is

$$g(\nabla^g_X T,N) = -\frac{n+1}{2\varphi}(\phi X)(r). \tag{47}$$

Summing up [by (45)–(47)]

$$\nabla^g_X T = \tau X - \left(\frac{1}{\varphi} - r\right)\phi X - \frac{\varphi}{2(1-r\varphi)}[X(r)T + (\phi X)(r)N], \tag{48}$$

for any $X \in H(\mathcal{F})$. Again by (44) and

$$g(\nabla^g_X N,Y) = -g(N,\nabla^g_X Y)$$

we get

$$g(\nabla^g_X N, Y) = -\left(\frac{1}{\varphi} - r\right) g(X,Y) - g(X, \phi\tau Y). \tag{49}$$

Next [by (A5)]

$$g(\nabla^g_X N, T) = \frac{n+1}{2\varphi}(\phi X)(r). \tag{50}$$

Finally, the component along N is $\frac{1}{2}X(\|N\|^2)$ hence

$$g(\nabla^g_X N, N) = -\frac{n+1}{2\varphi} X(r). \tag{51}$$

Summing up [by (49)–(51)]

$$\nabla^g_X N = -\left(\frac{1}{\varphi} - r\right) X + \tau\phi X + \frac{\varphi}{2(1-r\varphi)}[(\phi X)(r) T - X(r) N], \tag{52}$$

for any $X \in H(\mathcal{F})$. We wish to compute $\nabla^g_T X$. To this end (by $\nabla g_\theta = 0$)

$$2g_\theta(\nabla_T X, Y) = T[g_\theta(X,Y)] + g_\theta[(T,X),Y] + g_\theta[(Y,T),X] + g_\theta[T,(Y,X)] + g_\theta(\tau X, Y) - g_\theta(\tau Y, X) - 2(\mathrm{d}\theta)(X,Y)$$

yielding [upon multiplication by $-(n+1)/\varphi$]

$$T[g(X,Y)] + g[(T,X),Y] + g[(Y,T),X] = 2g(\nabla_T X, Y).$$

Therefore (by $\nabla^g g = 0$)

$$2g(\nabla^g_T X, Y) = T[g(X,Y)] + g[(T,X),Y] + g[(Y,T),X] + g[T,(Y,X)] = 2g(\nabla_T X, Y) - \theta[(X,Y)]\|T\|^2$$

or

$$g(\nabla^g_T X, Y) = g(\nabla_T X, Y) + \left(\frac{1}{\varphi} - r\right) g(X, \phi Y). \tag{53}$$

Similar to the above

$$g(\nabla^g_T X, T) = -\frac{n+1}{2\varphi} X(r), \tag{54}$$

$$g(\nabla^g_T X, N) = -\frac{n+1}{2\varphi}(\phi X)(r). \tag{55}$$

Collecting the information in (53)–(55), we have proved

$$\nabla^g_T X = \nabla_T X - \left(\frac{1}{\varphi} - r\right)\phi X - \frac{\varphi}{2(1-r\varphi)}[X(r) T + (\phi X)(r) N], \tag{56}$$

for any $X \in H(\mathcal{F})$. Let us compute $\nabla^g_N X$. We have

$$2g(\nabla^g_N X, Y) = N[g(X,Y)] + g[(N,X),Y] + g[(Y,N),X] = 2g[(N,X),Y] + (\mathcal{L}_N g)(X,Y).$$

Using (43) and

$$(N,X) = \nabla_N X - rX - \tau(\phi X)$$

(see the Appendix) one shows that

$$g(\nabla^g_N X, Y) = g(\nabla_N X, Y) - \frac{1}{\varphi} g(X, Y). \tag{57}$$

Calculations similar to the above also furnish

$$g(\nabla^g_N X, T) = \frac{n+1}{2\varphi}(\phi X)(r), \tag{58}$$

$$g(\nabla^g_N X, N) = -\frac{n+1}{2\varphi} X(r). \tag{59}$$

Using (57)–(59) we may now conclude that

$$\nabla^g_N X = \nabla_N X - \frac{1}{\varphi} X + \frac{\varphi}{2(1-r\varphi)}[(\phi X)(r) T - X(r) N], \tag{60}$$

for any $X \in H(\mathcal{F})$. Moreover (omitting the details)

$$g(\nabla^g_N T, X) = -\frac{n+1}{2\varphi}(\phi X)(r),$$

$$g(\nabla^g_N T, T) = -\frac{n+1}{2\varphi}\left(N(r) + \frac{4}{\varphi^2} - \frac{2r}{\varphi}\right),$$

$$g(\nabla^g_N T, N) = -\frac{n+1}{2\varphi} T(r),$$

so that

$$\nabla^g_N T = -\frac{1}{2}\phi \nabla^H r - \frac{\varphi}{2(1-r\varphi)}\left[\left(N(r) + \frac{4}{\varphi^2} - \frac{2r}{\varphi}\right) T + T(r) N\right]. \tag{61}$$

Similarly we find

$$\nabla^g_T N = \frac{1}{2}\phi \nabla^H r - \frac{\varphi}{2(1-r\varphi)}\left[\left(N(r) + \frac{4}{\varphi^2} - \frac{6r}{\varphi} + 4r^2\right) T + T(r) N\right], \tag{62}$$

$$\nabla^g_T T = -\frac{1}{2}\nabla^H r - \frac{\varphi}{2(1-r\varphi)}\left[T(r) T - \left(N(r) + \frac{4}{\varphi^2} - \frac{6r}{\varphi} + 4r^2\right) N\right], \tag{63}$$

$$\nabla^g_N N = -\frac{1}{2}\nabla^H r + \frac{\varphi}{2(1-r\varphi)}\left[T(r) T - \left(N(r) + \frac{4}{\varphi^2} - \frac{2r}{\varphi}\right) N\right]. \tag{64}$$

Let us consider a holomorphic vector bundle $\pi: F \to U$, carrying the Hermitian metric h, and set $E_\delta = \pi^{-1}(M_\delta)$ (the portion of F over a leaf of $\mathcal{F}$). A connection $D \in \mathcal{C}(F, h)$ induces a connection $D^\delta \in \mathcal{C}(E_\delta, h_\delta)$ (where $h_{\delta,z} = h_z$, $z \in M_\delta$). D^δ is most easily described with respect to a local trivialization $\Phi: \pi^{-1}(O) \to O \times C^m$ of F, for some open subset $O \subseteq U$. Let us set $\sigma_i(z) = \Phi^{-1}(z, e_i)$, $z \in O$, $1 \leqslant i \leqslant m$, where $\{e_1, \cdots, e_m\}$ is the canonical linear basis in C^m. If $u_i \equiv \sigma_i|_{O \cap M_\delta}$ then D^δ is given by

$$(D_X^{\delta}u)_z = X(f^i)_z u_i(z) + f^i(z)(D_{(dj_{\delta})X}\sigma_i)_z, \quad z \in O \cap M_{\delta},$$

for any section $u=f^i u_i$, $f^i \in C^{\infty}(O \cap M_{\delta})$, and any $X \in \mathcal{X}(M_{\delta})$. It is easily shown that the definition of $(D_X^{\delta}u)_z$ doesn't depend upon the local trivialization chart Φ at z [i.e., if $g=[g_{ij}]: O \cap O' \to \mathrm{GL}(m,C)$, $g(z)=\Phi'_z \circ \Phi_z^{-1}$, are the transition functions of F then $(D_X^{\delta}u)_z$ is invariant under the transformation $\sigma_j(z)=g_j^i(z)\sigma'_i(z)$]. Let $R^D \in \Omega^2[\mathrm{Ad}(F)]$ and ω_j^i be the curvature tensor field and connection 1-forms of D ($D\sigma_j=\omega_j^i \otimes \sigma_i$), so that $R^D\sigma_j=2(d\omega_j^i-\omega_k^i \wedge \omega_j^k)\otimes\sigma_i$. Also, let $R^{\delta} \in \Omega^2[\mathrm{Ad}(E_{\delta})]$ and $(\omega_{\delta})_j^i$ be the curvature tensor field and the connection 1-forms of D^{δ}, respectively. Then $(\omega_{\delta})_j^i=j_{\delta}^*\omega_j^i$ yields

$$R^{\delta}u_i = (j_{\delta}^* R^D)\sigma_i, \quad 1 \leqslant i \leqslant m. \tag{65}$$

Let $\{W_{\alpha}\}$ be a local orthonormal $[g_{\theta}(W_{\alpha}, W_{\bar{\beta}})=\delta_{\alpha\beta}]$ frame of $T_{1,0}(\mathcal{F})$ and set

$$E_{\alpha} \equiv \sqrt{-\frac{\varphi}{n+1}}W_{\alpha}, \quad 1 \leqslant \alpha \leqslant n-1, \quad E_n \equiv \sqrt{\frac{2f\varphi}{n+1}}\xi,$$

where $f \equiv \varphi/(1-r\varphi)$. Then, given a connection D in $F \to U$, for any $X \in H(M_{\delta})$

$$(\delta^D R^D)X = -\sum_{a=1}^{n}[(D_{E_a}R^D)(E_{\bar{a}},X)+(D_{E_{\bar{a}}}R^D)(E_a,X)] = \frac{\varphi}{n+1}\sum_{\alpha=1}^{n-1}[(D_{W_{\alpha}}R^D)(W_{\bar{\alpha}},X)+(D_{W_{\bar{\alpha}}}R^D)$$
$$\times(W_{\alpha},X)] - \frac{2f\varphi}{n+1}[(D_{\xi}R^D)(\bar{\xi},X)+(D_{\bar{\xi}}R^D)(\xi,X)]$$

and

$$\sum_{\alpha=1}^{n-1}(D_{W_{\alpha}}R^D)(W_{\bar{\alpha}},X)\sigma_j = \sum_{\alpha}[D_{W_{\alpha}}(R^D(W_{\bar{\alpha}},X)\sigma_j) - R^D(W_{\bar{\alpha}},X)D_{W_{\alpha}}\sigma_j - R^D(\nabla^g_{W_{\alpha}}W_{\bar{\alpha}},X)\sigma_j$$
$$- R^D(W_{\bar{\alpha}},\nabla^g_{W_{\alpha}}X)\sigma_j] = [by\ (44)] = \sum_{\alpha}\{(D^{\delta}_{W_{\alpha}}R^{\delta})(W_{\bar{\alpha}},X)u_j - [fg_{\theta}(\tau W_{\alpha},W_{\bar{\alpha}})$$
$$+ g_{\theta}(W_{\alpha},\phi W_{\bar{\alpha}})]R^D(T,X)\sigma_j + [g_{\theta}(W_{\alpha},W_{\bar{\alpha}}) + fg_{\theta}(W_{\alpha},\phi\tau W_{\bar{\alpha}})]R^D(N,X)\sigma_j$$
$$- [fg_{\theta}(\tau W_{\alpha},X) + g_{\theta}(W_{\alpha},\phi X)]R^D(W_{\bar{\alpha}},T)\sigma_j + [g_{\theta}(W_{\alpha},X)$$
$$+ fg_{\theta}(W_{\alpha},\phi\tau X)]R^D(W_{\bar{\alpha}},N)\sigma_j\}.$$

Therefore [by the purity axiom (A6)]

$$\sum_{\alpha}(D_{W_{\alpha}}R^D)(W_{\bar{\alpha}},X) = \sum_{\alpha}(D^{\delta}_{W_{\alpha}}R^{\delta})(W_{\bar{\alpha}},X)u_j + i(n-1)R^D(T,X)\sigma_j + (n-1)R^D(N,X)\sigma_j$$
$$- fR^D(\pi_{0,1}\tau X,T) - R^D(\pi_{0,1}\phi X,T) + R^D(\pi_{0,1}X,N) + fR^D(\pi_{0,1}\phi\tau X,N).$$

We obtain

$$\sum_{\alpha}[(D_{W_{\alpha}}R^D)(W_{\bar{\alpha}},X)+(D_{W_{\bar{\alpha}}}R^D)(W_{\alpha},X)] = -(\delta_b^{D^{\delta}}R^{\delta})_X u_j + [R^D(N,(2n-3)X - f\phi\tau X)$$
$$+ R^D(T,\phi X + f\tau X)]\sigma_j \tag{66}$$

(cf. Sec. V for the definition of the operator $\delta_b^{D^{\delta}}$). Moreover

$$[(D_{\xi}R^D)(\bar{\xi},X)+(D_{\bar{\xi}}R^D)(\xi,X)]\sigma_j=\frac{1}{2}\{D_N[R^D(N,X)\sigma_j]+D_T[R^D(T,X)\sigma_j]-R^D(N,X)D_N\sigma_j$$
$$-R^D(T,X)D_T\sigma_j-R^D(\nabla^g_N N,X)\sigma_j-R^D(\nabla^g_T T,X)\sigma_j-R^D(N,\nabla^g_N X)\sigma_j$$
$$-R^D(T,\nabla^g_T X)\sigma_j\}.$$

Substitution from (56), (60), (63), and (64) gives

$$-R^D(\nabla^g_N N,X)-R^D(\nabla^g_T T,X)-R^D(N,\nabla^g_N X)-R^D(T,\nabla^g_T X)=R^D(\nabla^H r,X)-R^D(T,\nabla_T X)-R^D(N,\nabla_N X)$$
$$+\frac{1}{f}R^D(T,\phi X)+f(\phi X)(r)R^D(T,N)+\left(\frac{1}{\varphi}+2r\right)R^D(N,X).$$

We conclude that

$$[(D_{\xi}R^D)(\bar{\xi},X)+(D_{\bar{\xi}}R^D)(\xi,X)]\sigma_j=\frac{1}{2}\{(D_N i_N R^D)X\}+(D_T i_T R^D)X+R^D(\nabla^H r,X)+\frac{1}{f}R^D(T,\phi X)$$
$$+f(\phi X)(r)R^D(T,N)+\left(\frac{1}{\varphi}+2r\right)R^D(N,X) \tag{67}$$

[the covariant derivatives in the right hand member of (67) are defined with respect to D and ∇]. Finally [by (66) and (67)]

$$(\delta^D R^D)_X\sigma_j=\frac{\varphi}{n+1}\{-(\delta_b^{D^\delta}R^\delta)_X u_j+[R^D[N,(2n-3)X-f\phi\tau X]+R^D(T,\phi X+f\tau X)]\sigma_j\}$$
$$-\frac{f\varphi}{n+1}\left\{(D_N i_N R^D)X+(D_T i_T R^D)X+R^D(\nabla^H r,X)+R^D\left[T,\frac{1}{f}\phi X+f(\phi X)(r)N\right]\right.$$
$$\left.+\left(\frac{1}{\varphi}+2r\right)R^D(N,X)\right\}\sigma_j.$$

Assume that D is a Yang–Mills field on (Ω,g), i.e., $\delta^D R^D=0$ in Ω. Then, for $\varphi\to 0$ (as r and $\nabla^H r$ remain finite near $\partial\Omega$, (see Ref. 11, p. 164)

$$(\delta_b^{D_b}R^{D_b})_X u_j=2(n-2)R^D(N,X)\sigma_j, \tag{68}$$

where $D_b\equiv D^0$ is the boundary values of D. Therefore, if $i_T R^{D_b}=0$ then [cf. (86) in Sec. V] D_b is a pseudo Yang–Mills field on $\partial\Omega$ if and only if $i_N R^D=0$ on $H(\partial\Omega)$. Theorem 1 is proved. With the same techniques we may show that

Corollary 1: Let $D\in\mathcal{C}(F,h)$ be a Yang-Mills field on (Ω,g) such that $i_N R^D=0$. Then the boundary values D_b of D satisfy $\Lambda_\theta R^{D_b}=0$.

Corollary 1 shows that the axiom (17) (with $S=0$) in the description of the Tanaka connection, as well as (11) in Theorem 2, are rather natural occurrences. The proof is

$$0=(\delta^D R^D)_T\sigma_j=\frac{\varphi}{n+1}\sum_\alpha[(D_{W_\alpha}R^D)(W_{\bar{\alpha}},T)+(D_{W_{\bar{\alpha}}}R^D)(W_\alpha,T)]\sigma_j-\frac{2f\varphi}{n+1}\{D_N[R^D(N,T)\sigma_j]$$
$$-R^D(N,T)D_N\sigma_j-R^D(\nabla^g_N N,T)-R^D(N,\nabla^g_N T)\sigma_j\}$$

or [by (44), (48), (61), and (64)]

$$0=\varphi[(\delta^{D^\delta}R^\delta)_T u_j+2(n-1)R^D(T,N)\sigma_j]+\frac{1}{2}\varphi\{f[R^D(T,\nabla^H r)+R^D(N,\phi\nabla^H r)]+\text{trace }\pi_H R^D(\cdot,\tau\cdot)\}\sigma_j$$

$$+(n+1)f[2(D_N i_N R^D)T+R^D(N,\phi\nabla^H r)-R^D(T,\nabla^H r)]\sigma_j-\frac{2\varphi}{f}\Lambda_\theta R^D\sigma_j$$

$$-(n+1)f^2\left[N(r)+\frac{4}{\varphi^2}-\frac{2r}{\varphi}\right]R^D(T,N)\sigma_j.$$

When $\varphi\to 0$ one observes $\varphi/f\to 1$ and $f^2/\varphi^2\to 1$ hence

$$(\Lambda_\theta R^{D_b})u_j=-2(n+1)R^D(T,N)\sigma_j.$$

Q.E.D.

Summing up, in this section we considered the Dirichlet problem for the Yang–Mills equations

$$\delta^D R^D=0 \quad \text{in } \Omega$$

$$D=D^0 \quad \text{on } \partial\Omega \tag{69}$$

and dealt with the C^∞ regularity up to the boundary of a solution to (69). As a consequence of (68) we may also state:

Corollary 2: Let $\Omega\subset\mathbb{C}^2$ *be a smoothly bounded strictly pseudoconvex domain and* $D\in\mathcal{C}(F,h)$ *a solution to* (69) *for some* C^∞ *connection* $D^0\in\mathcal{C}(E,h)$. *Then* $D_b\equiv D^0$ *must satisfy the compatibility relations* $\delta_b^{D_b}R^{D_b}=0$. *If moreover* $i_T R^{D_b}=0$ *then* D_b *is a pseudo Yang–Mills field on* $\partial\Omega$.

The problem whether a given a pseudo Yang–Mills field D^0 on $\partial\Omega$ may be extended to a Yang–Mills field at the interior of Ω [i.e., the existence question for (69)] is open.

V. YANG–MILLS FIELDS AND THE FEFFERMAN METRIC

We wish to relate $\mathcal{PYM}$ to the Yang–Mills functional on $C(M)$. Given a contact form θ on M such that the Levi form L_θ is positive definite, let F_θ be the corresponding *Fefferman metric* [a Lorentz metric on $C(M)$]. We recall (cf. Ref. 18) that

$$F_\theta=\pi^*\widetilde{G}_\theta+2(\pi^*\theta)\odot\sigma, \tag{70}$$

$$\sigma=\frac{1}{n+2}\left\{d\gamma+\pi^*\left[i\omega_\alpha^\alpha-\frac{i}{2}g^{\alpha\bar\beta}dg_{\alpha\bar\beta}-\frac{\rho}{4(n+1)}\theta\right]\right\}. \tag{71}$$

Here ω_β^α are the connection 1-forms of the Tanaka–Webster connection of (M,θ), i.e., $\nabla T_\beta=\omega_\beta^\alpha\otimes T_\alpha$, and $g_{\alpha\bar\beta}=L_\theta(T_\alpha,T_{\bar\beta})$. Moreover $\rho=g^{\alpha\bar\beta}R_{\alpha\bar\beta}$ is the *pseudohermitian scalar curvature* (cf. e.g., Ref. 5, p. 229). The (0,2)-tensor field $\widetilde{G}_\theta$ is obtained by extending the Levi form G_θ to the whole of $T(M)$. Precisely, one requests that $\widetilde{G}_\theta=G_\theta$ on $H(M)\otimes H(M)$, while $\widetilde{G}_\theta(X,T)=0$, for any $X\in T(M)$ (obviously $\widetilde{G}_\theta$ is degenerate). Note that when M is compact $C(M)$ is compact, as well. It is noteworthy that σ [given by (71)] is a connection 1-form in $S^1\to C(M)\to M$. Let $T^\uparrow$ be the horizontal lift (with respect to σ) of the characteristic direction of $d\theta$ and S the tangent to the S^1 action. Then $T^\uparrow-S$ is timelike, hence $[C(M),F_\theta]$ is time oriented by $T^\uparrow-S$, i.e., $[C(M),F_\theta]$ is a space–time (see Ref. 3, p. 17). However, as M is compact $[C(M),F_\theta]$ is not chronological (cf. Proposition 2.6 in Ref. 3, p. 23).

Let $S\in\mathcal{X}[C(M)]$ be the tangent to the S^1 action {locally $S=[(n+2)/2]\partial/\partial\gamma$}. Then [by (70)] $F_\theta(S,S)=0$. Next (by Lemma 2) $\nabla_S^{C(M)}S=0$, i.e., the integral curves of S are (null) geodesics of $[C(M),F_\theta]$. Also $\mathcal{L}_S F_\theta=0$, hence [cf. (28) in Ref. 26 p. 185] S generates a *shear-free congruence* of null geodesics. The congruence is *symmetric* if there is a vector field $X\in\mathcal{X}[C(M)]$ such that

$$\mathcal{L}_X(\pi^*\theta) = t\pi^*\theta, \quad \mathcal{L}_X(\pi^*\theta^\alpha) = w^\alpha_\beta \pi^*\theta^\beta + \ell^\alpha \pi^*\theta,$$

where t is a real function and $w^\alpha_\beta, \ell^\alpha$ are complex functions on $C(M)$. We say that X is a *symmetry* of the congruence. We may look for $\mathcal{L}_X S$ in the form

$$\mathcal{L}_X S = a^\alpha T^\uparrow_\alpha + a^{\bar\alpha} T^\uparrow_{\bar\alpha} + bT^\uparrow + fS.$$

As X is a symmetry $a^\alpha = 0$, $b = 0$ and $f = -2(\mathcal{L}_X\sigma)S$. Therefore

$$\mathcal{L}_X S = fS. \tag{72}$$

Also one may easily check (by using the local frame $\{T^\uparrow_\alpha, T^\uparrow_{\bar\alpha}, T^\uparrow, S\}$ of $T[C(M)]\otimes\mathbb{C}$) that

$$\mathcal{L}_S(\pi^*\theta) = 0, \quad \mathcal{L}_S(\pi^*\theta^\alpha) = 0. \tag{73}$$

Using (72) and (73) and $\mathcal{L}_Y\mathcal{L}_Z\omega = \mathcal{L}_Z\mathcal{L}_Y\omega + \mathcal{L}_{[Y,Z]}\omega$ [for any $Y, Z \in \mathcal{X}(C(M))$, $\omega \in \Omega^1[C(M)]$] we obtain

$$S(t) = 0, \quad S(w^\alpha_\beta) = 0, \quad S(\ell^\alpha) = 0. \tag{74}$$

For instance

$$S(t)\pi^*\theta = \mathcal{L}_{[S,X]}\pi^*\theta = -f\mathcal{L}_S\pi^*\theta - (\pi^*\theta)(S)\mathrm{d}f = 0.$$

Our considerations draw inspiration from the calculations in Ref. 24 [which are both purely local and confined to the three-dimensional case $(n=1)$]. For this reason some of the results (e.g., Propositions 1 and 2) are attributed to Ref. 24 (the proofs are however new). (74) implies that $t, w^\alpha_\beta, \ell^\alpha$ are vertical lifts of functions on M. A vector field of the form ρS, for some function $\rho \neq 0$, is a *trivial* symmetry of the congruence.

Proposition 2: (Ref. 24) *Each nontrivial symmetry of the shear-free congruence* [*of null geodesics on* $C(M)$] *projects on a unique symmetry of the CR structure on* M.

Indeed, if X is a symmetry of S then $X - 2\sigma(X)S \in \mathrm{Ker}(\sigma)$, hence there is a unique vector field $\widetilde{X} \in \mathcal{X}(M)$ such that

$$\widetilde{X}^\uparrow = X - 2\sigma(X)S.$$

Then

$$\pi^*(t\theta) = \mathcal{L}_X(\pi^*\theta) = \mathcal{L}_{\widetilde{X}^\uparrow}(\pi^*\theta) + 2\mathcal{L}_{\sigma(X)S}(\pi^*\theta) = \mathcal{L}_{\widetilde{X}^\uparrow}(\pi^*\theta).$$

Consequently, for any $Z \in \mathcal{X}(M)$

$$t\theta(Z) = [\pi^*(t\theta)]Z^\uparrow = [\mathcal{L}_{\widetilde{X}^\uparrow}(\pi^*\theta)]Z^\uparrow = \widetilde{X}[\theta(Z)] - (\pi^*\theta)[\widetilde{X}^\uparrow, Z^\uparrow]$$

hence, as $[\widetilde{X}, Z]^\uparrow$ is the $\mathrm{Ker}(\sigma)$-component of $[\widetilde{X}^\uparrow, Z^\uparrow]$ [with respect to the decomposition $T[C(M)] = \mathrm{Ker}(\sigma)\oplus\mathbb{R}S$], we obtain $\mathcal{L}_{\widetilde{X}}\theta = t\theta$. It may be shown in a similar manner that $\mathcal{L}_{\widetilde{X}}\theta^\alpha = w^\alpha_\beta\theta^\beta + \ell^\alpha\theta$, i.e., $\widetilde{X}$ is a symmetry of the CR structure. Q.E.D.

Let $E \to M$ be a complex vector bundle and $\hat{E} = \pi^*E \to C(M)$ the pullback of E via π. The *natural lift* $\hat{u}: \pi^{-1}(U) \to \hat{E}$ of a section $u: U \to E$ is given by $\hat{u}(z) = \{x, u[\pi(z)]\}$, $z \in \pi^{-1}(U)$. If E carries a Hermitian metric h then so does $\hat{E}$. Indeed we may set $\hat{h}(\hat{e}_i, \hat{e}_j) = h_{i\bar{j}} \circ \pi$, where $h_{i\bar{j}} = h(e_i, e_j)$ and $\{e_1, \cdots, e_m\}$ is a (local) frame in E on U. There is a natural inner product $\langle,\rangle$ on $\Omega^2[\mathrm{Ad}(\hat{E})]$ induced by the inner product on scalar 2-forms

$$F_\theta^*(\alpha,\beta)d\,\mathrm{vol}(F_\theta)=\alpha\wedge *\beta,$$

$\alpha,\beta\in\Gamma^\infty\{\Lambda^2T^*[C(M)]\}$, and by the Killing–Cartan form of $\mathbf{u}(m)$, $m=\mathrm{rank}_{\mathbb{C}}E$, respectively. Here $*$ is the Hodge operator associated with the Fefferman metric F_θ. Precisely, if $S,T\in\Omega^0[\mathrm{Ad}(\hat{E})]$ then

$$\langle\alpha\otimes S,\beta\otimes T\rangle=F_\theta^*(\alpha,\beta)(S_j^i)\cdot(T_j^i),$$

where $S\hat{e}_j=S_j^i\hat{e}_i$, $T\hat{e}_j=T_j^i\hat{e}_i$ with respect to a (local) orthonormal $[h(e_i,e_j)=\delta_{ij}]$ frame $\{e_j\}$ in E, and $A\cdot B=-\mathrm{trace}(AB)$, $A,B\in\mathbf{u}(m)$. The Yang–Mills functional is given by

$$\mathcal{Y}\hat{\mathcal{M}}(\mathbb{D})=\frac{1}{2}\int_{C(M)}\langle R^{\mathbb{D}},R^{\mathbb{D}}\rangle d\,\mathrm{vol}(F_\theta),\quad \mathbb{D}\in\mathcal{C}(\hat{E},\hat{h}).$$

Any $D\in\mathcal{C}(E,h)$ induces a connection $\hat{D}=\pi^*D\in\mathcal{C}(\hat{E},\hat{h})$ which is described (in local coordinates) as follows. Let (U,x^A) be a local coordinate system on M. Then $[\pi^{-1}(U),\hat{x}^A:=x^A\circ\pi,\gamma]$ are local coordinates on $C(M)$. We set by definition

$$\hat{D}_{\partial/\partial\hat{x}^A}\hat{e}_j=(\Gamma_{Aj}^i\circ\pi)\hat{e}_i,\quad \hat{D}_{\partial/\partial\gamma}\hat{e}_j=0,$$

where $D_{\partial/\partial x^A}e_j=\Gamma_{Aj}^ie_i$. Our conventions as to the range of indices are $A,B,C,\cdots\in(1,\cdots,2n+1)$ and $i,j,k,\cdots\in(1,\cdots,m)$. We consider the linear map

$$\pi^*:\Gamma^\infty(U,\Lambda^kT^*(M)\otimes E)\to\Gamma^\infty\{\pi^{-1}(U),\Lambda^kT^*[C(M)]\otimes\hat{E}\}$$

given by

$$\pi^*(\omega^j\otimes e_j)=(\pi^*\omega^j)\otimes\hat{e}_j,\quad \omega^j\in\Omega^k(U),$$

(pullback and natural lifting). As $\{\hat{e}_j\}$ is a local frame in $\hat{E}\to C(M)$ it suffices to specify $\hat{D}$ on natural lifts of sections in $E\to M$. Then $\hat{D}$ admits the following coordinate-free description:

$$\hat{D}\hat{u}=\pi^*(Du),\quad u\in\Omega^0(E).$$

Clearly, if $Dh=0$ then $\hat{D}\hat{h}=0$. Let us consider the functional $\mathcal{PYM}:\mathcal{C}(E,h)\to[0,+\infty)$ given by

$$\mathcal{P}YM(D)=\frac{1}{2}\int_M\|\pi_HR^D\|^2\theta\wedge(\mathrm{d}\theta)^n.$$

Here $\pi_H:\Omega^2[\mathrm{Ad}(E)]\to\Omega^2[\mathrm{Ad}(E)]/\mathcal{J}_\theta^2$ is the projection described in Sec. II. Of course, when an admissible coframe $\{\theta^\alpha\}$ is fixed $\Omega^\cdot[\mathrm{Ad}(E)]/\mathcal{J}_\theta$ may be identified with the subalgebra $\Omega_H^\cdot[\mathrm{Ad}(E)]=\{\omega\in\Omega^\cdot[\mathrm{Ad}(E)]:i_T\omega=0\}$. Integration along the fiber in $\mathcal{Y}\hat{\mathcal{M}}(\pi^*D)$, $D\in\mathcal{C}(E,h)$, leads to (9) in Theorem 2. Indeed, let us set

$$R_{ABj}^ie_i=(R^De_j)(\partial/\partial x^A,\partial/\partial x^B).$$

Then

$$R^{\hat{D}}\hat{e}_j=[(R_{ABj}^i\circ\pi)d\hat{x}^A\wedge d\hat{x}^B]\otimes\hat{e}_i$$

hence

$$R^{\hat{D}}\hat{e}_j=\pi^*(R^De_j).\tag{75}$$

Given $\Omega=\Omega^j\otimes e_j\in\Omega^2(E)$, $\Omega^j=\Omega_{AB}^j\,\mathrm{d}x^A\wedge\mathrm{d}x^B$, we set

$$\langle \pi^*\Omega, \pi^*\Omega\rangle = F^*_\theta(\pi^*\Omega^j, \pi^*\Omega^{\bar{k}})(h_{j\bar{k}}\circ\pi). \tag{76}$$

Of course $\pi^*\Omega^j=(\Omega^j_{AB}\circ\pi)\mathrm{d}\hat{x}^A\wedge\mathrm{d}\hat{x}^B$ and the main technical difficulty in calculating (76) is the need for $F^{AB}=F^*_\theta(\mathrm{d}\hat{x}^A,\mathrm{d}\hat{x}^B)$, where $[F^{AB}]=[F_{AB}]^{-1}$ and $F_{AB}:=F_\theta(\partial/\partial\hat{x}^A,\partial/\partial\hat{x}^B)$. Let

$$F_\theta:\begin{bmatrix} F_{AB} & F_{A,2n+2} \\ F_{2n+2,B} & F_{2n+2,2n+2}\end{bmatrix}$$

be the components of the Fefferman metric with respect to $(\hat{x}^A,\gamma)$. Let us set $\partial/\partial x^A=\lambda^B_A T_B$, $\lambda^B_A\in C^\infty(U)$. Here one either adopts the convention $A,B,C,\cdots\in\{0,1,\cdots,n,\bar{1},\cdots,\bar{n}\}$ (with $T_0=T$) or relabels the vector fields $\{T,T_\alpha,T_{\bar{\alpha}}:1\leqslant\alpha\leqslant n\}$. Then [by (70)]

$$F_{AB}=\widetilde{G}_\theta\left(\frac{\partial}{\partial x^A},\frac{\partial}{\partial x^B}\right)+\theta\left(\frac{\partial}{\partial x^A}\right)\sigma\left(\frac{\partial}{\partial\hat{x}^B}\right)+\theta\left(\frac{\partial}{\partial x^B}\right)\sigma\left(\frac{\partial}{\partial\hat{x}^A}\right)=g_{\alpha\bar{\beta}}(\lambda^\alpha_A\lambda^{\bar{\beta}}_B+\lambda^\alpha_B\lambda^{\bar{\beta}}_A)+\lambda^0_A\sigma_B+\lambda^0_B\sigma_A$$

where $\sigma_A=\sigma(\partial/\partial\hat{x}^A)$. A calculation based on (71) shows that

$$\sigma_A=\frac{1}{n+2}\left\{i\lambda^B_A\left[\Gamma^\alpha_{B\alpha}-\frac{1}{2}g^{\alpha\bar{\beta}}T_B(g_{\alpha\bar{\beta}})\right]-\frac{\rho}{4(n+1)}\lambda^0_A\right\}\circ\pi$$

where $\Gamma^\beta_{B\alpha}$ are (among) the coefficients of the Tanaka–Webster connection of (M,θ) (i.e., $\nabla_{T_B}T_\alpha=\Gamma^\beta_{B\alpha}T_\beta$). Moreover [by (70)]

$$F_{A,2n+2}=2[(\pi^*\theta)\odot\sigma]\left(\frac{\partial}{\partial\hat{x}^A},\frac{\partial}{\partial\gamma}\right)=\frac{1}{n+2}\lambda^0_A,$$

$$F_{2n+2,2n+2}=0.$$

Next, using $F^{ab}F_{bc}=\delta^a_c$ (with $a,b,c,\cdots\in\{1,\cdots,2n+2\}$) we find

$$\begin{gathered} F^{AB}F_{BC}+\frac{\lambda^0_C}{n+2}F^{A,2n+2}=\delta^A_C \\ F^{AB}\lambda^0_B=0 \\ F^{2n+2,B}F_{BC}+\frac{\lambda^0_C}{n+2}F^{2n+2,2n+2}=0 \\ F^{2n+2,B}\lambda^0_B=n+2. \end{gathered} \tag{77}$$

Let us set

$$P_{AB}{}^i{}_j e_i=(R^D e_j)(T_A,T_B)$$

so that $R^i_{ABj}=\lambda^C_A\lambda^D_B P_{CD}{}^i{}_j$. In the sequel, for the sake of simplicity, we do not distinguish notationally between $f\in C^\infty(M)$ and its vertical lift $f\circ\pi$. Then

$$\begin{aligned}\langle R^{\hat{D}},R^{\hat{D}}\rangle &= h^{j\bar{k}}\langle R^{\hat{D}}\hat{e}_j,R^{\hat{D}}\hat{e}_k\rangle = h^{j\bar{k}}h_{r\bar{s}}F^*_\theta(R^r_{ABj}\,\mathrm{d}\hat{x}^A\wedge\mathrm{d}\hat{x}^B,R^s_{CDk}\,\mathrm{d}\hat{x}^C\wedge\mathrm{d}\hat{x}^D)\\ &= \frac{1}{2}h^{j\bar{k}}h_{r\bar{s}}R^r_{ABj}R^{\bar{s}}_{CD\bar{k}}(F^{AC}F^{BD}-F^{AD}F^{BC}),\end{aligned}$$

where $R^{\bar{i}}_{AB\bar{j}}=\overline{R^i_{ABj}}$. We obtain

$$\langle R^{\hat{D}}, R^{\hat{D}} \rangle = \frac{1}{2} h^{j\bar{k}} h_{r\bar{s}} \lambda_A^E \lambda_B^F \lambda_C^{\bar{G}} \lambda_D^{\bar{H}} P_{EF}{}^{r}{}_{j} P_{\bar{G}\bar{H}}{}^{\bar{s}}{}_{\bar{k}} (F^{AC} F^{BD} - F^{AD} F^{BC}), \tag{78}$$

where $\lambda_A^{\bar{B}} = \overline{\lambda_A^B}$ and $P_{\bar{A}\bar{B}}{}^{\bar{i}}{}_{\bar{j}} = \overline{P_{AB}{}^{i}{}_{j}}$. Note that λ_A^0 is real valued while $\lambda_A^{\bar{\alpha}} = \lambda_A^{\alpha+n}$. To calculate $\lambda_A^E \lambda_B^F \lambda_C^{\bar{G}} \lambda_D^{\bar{H}} (F^{AC} F^{BD} - F^{AD} F^{BC})$ we need the identities

$$F^{AB} \lambda_A^{\alpha} \lambda_B^{\bar{\beta}} = g^{\alpha\bar{\beta}}, \tag{79}$$

$$F^{AB} \lambda_A^{\alpha} \lambda_B^{\beta} = 0. \tag{80}$$

The proof of (79) and (80) follows from (77). Indeed (77) may be written

$$F^{AB} g_{\alpha\bar{\beta}} (\lambda_B^{\alpha} \lambda_C^{\bar{\beta}} + \lambda_C^{\alpha} \lambda_B^{\bar{\beta}}) + F^{AB} \lambda_C^0 \sigma_B + \frac{1}{n+2} F^{A,2n+2} \lambda_C^0 = \delta_C^A,$$

$$F^{AB} \lambda_B^0 = 0,$$

$$F^{2n+2,B} g_{\alpha\bar{\beta}} (\lambda_B^{\alpha} \lambda_C^{\bar{\beta}} + \lambda_C^{\alpha} \lambda_B^{\bar{\beta}}) + (n+2)\sigma_C + F^{2n+2,B} \lambda_C^0 \sigma_B + \frac{1}{n+2} F^{2n+2,2n+2} \lambda_C^0 = 0,$$

$$F^{2n+2,B} \lambda_B^0 = n+2.$$

If $\mu := = \lambda^{-1}$ then (by the first of the previous four identities)

$$\mu_D^A = \left(\frac{1}{n+2} F^{A,2n+2} + F^{AB} \sigma_B \right) \delta_D^0 + F^{AB} g_{\alpha\bar{\beta}} (\lambda_B^{\alpha} \delta_D^{\beta+n} + \lambda_B^{\bar{\beta}} \delta_D^{\alpha})$$

yielding

$$\mu_0^A = \frac{1}{n+2} F^{A,2n+2} + F^{AB} \sigma_B$$

$$\mu_{\alpha}^A = F^{AB} g_{\alpha\bar{\beta}} \lambda_B^{\bar{\beta}} \tag{81}$$

$$\mu_{\beta+n}^A = F^{AB} g_{\alpha\bar{\beta}} \lambda_B^{\alpha}.$$

The second and third of the identities (81) lead to (79) and (80), respectively. A calculation based on (79) and (80) shows that (78) may be written

$$\langle R^{\hat{D}}, R^{\hat{D}} \rangle = P^{\bar{\alpha}\bar{\beta}\bar{k}j} P_{\bar{\alpha}\bar{\beta}\bar{k}j} + P^{\alpha\beta\bar{k}j} P_{\alpha\beta\bar{k}j} + P^{\bar{\alpha}\bar{\beta}\bar{k}j} P_{\bar{\alpha}\beta\bar{k}j} + P^{\alpha\bar{\beta}\bar{k}j} P_{\alpha\bar{\beta}\bar{k}j} \tag{82}$$

where $P_{AB\bar{k}j} = h_{j\bar{s}} P_{AB\bar{k}}{}^{\bar{s}}$ and $P^{AB\bar{k}j} = h^{r\bar{k}} P^{AB}{}_{r}{}^{j}$. Also $P^{\alpha\beta}{}_{r}{}^{j} = g^{\alpha\bar{\lambda}} g^{\beta\bar{\mu}} P_{\bar{\lambda}\bar{\mu}r}{}^{j}$, etc. As $R^D e_j = (P_{AB}{}^{i}{}_{j} \theta^A \wedge \theta^B) \otimes e_i$ it follows that

$$\begin{aligned} \langle \pi_H R^D, \pi_H R^D \rangle &= h^{j\bar{k}} \langle (\pi_H R^D) e_j, (\pi_H R^D) e_k \rangle \\ &= h^{j\bar{k}} h_{r\bar{s}} G_{\theta}^{*} (P_{\alpha\beta}{}^{r}{}_{j} \theta^{\alpha} \wedge \theta^{\beta} + 2 P_{\alpha\bar{\beta}}{}^{r}{}_{j} \theta^{\alpha} \wedge \theta^{\bar{\beta}} + P_{\bar{\alpha}\bar{\beta}}{}^{r}{}_{j} \theta^{\bar{\alpha}} \wedge \theta^{\bar{\beta}}, \end{aligned}$$

$$P_{\lambda\mu}{}^{s}{}_{k}\theta^{\lambda}\wedge\theta^{\mu}+2P_{\lambda\bar{\mu}}{}^{s}{}_{k}\theta^{\lambda}\wedge\theta^{\bar{\mu}}+P_{\bar{\lambda}\bar{\mu}}{}^{s}{}_{k}\theta^{\bar{\lambda}}\wedge\theta^{\bar{\mu}})=\frac{1}{2}P_{\alpha\beta}{}^{\bar{k}j}P_{\bar{\lambda}\bar{\mu}\bar{k}j}(g^{\alpha\bar{\lambda}}g^{\beta\bar{\mu}}-g^{\alpha\bar{\mu}}g^{\beta\bar{\lambda}})$$
$$+2g^{\alpha\bar{\lambda}}g^{\bar{\beta}\mu}P_{\alpha\bar{\beta}}{}^{\bar{k}j}P_{\bar{\lambda}\mu\bar{k}j}+\frac{1}{2}P_{\bar{\alpha}\bar{\beta}}{}^{\bar{k}j}P_{\lambda\mu\bar{k}j}(g^{\bar{\alpha}\lambda}g^{\bar{\beta}\mu}$$
$$-g^{\bar{\alpha}\mu}g^{\bar{\beta}\lambda})=P^{\bar{\lambda}\bar{\mu}\bar{k}j}P_{\bar{\lambda}\bar{\mu}\bar{k}j}+2P^{\bar{\lambda}\mu\bar{k}j}P_{\bar{\lambda}\mu\bar{k}j}$$
$$+P^{\lambda\mu\bar{k}j}P_{\lambda\mu\bar{k}j}$$

hence [by (75) and (82)]

$$\langle R^{\hat{D}},R^{\hat{D}}\rangle=(\|\pi_{H}R^{D}\|\circ\pi)^{2}.$$

Finally we may integrate over $C(M)$ and use the identity

$$\int_{C(M)}(f\circ\pi)d\,\mathrm{vol}(F_{\theta})=2\pi\int_{M}f\theta\wedge(\mathrm{d}\theta)^{n},\quad f\in C^{\infty}(M).$$

The identity (9) in Theorem 1 is proved. (The symbol π on the right hand side denotes the irrational number $\pi\in\mathbb{R}$.) Assume now that $\hat{D}=\pi^{*}D$ is a Yang–Mills field on $C(M)$. Let $D^{t}=D+t\varphi$, $\varphi\in\Omega^{1}[\mathrm{Ad}(E)]$, be a variation of D. Then

$$\pi^{*}D^{t}=\hat{D}+t\pi^{*}\varphi.\tag{83}$$

A word on the conventions in (83). As seen earlier in this section, there is a natural map $\pi^{*}:\Omega^{1}[\mathrm{Ad}(E)]\to\Omega^{1}[\pi^{*}\mathrm{Ad}(E)]$. Yet $\mathrm{Ad}(\pi^{*}E)\approx\pi^{*}\,\mathrm{Ad}(E)$ (a vector bundle isomorphism) hence $\pi^{*}\varphi$ is an $\mathrm{Ad}(\pi^{*}E)$-valued 1-form on $C(M)$. Then [by (9)]

$$0=\frac{d}{dt}[\mathcal{Y}\hat{\mathcal{M}}(\hat{D}+t\pi^{*}\varphi)]_{t=0}=\frac{d}{dt}[\mathcal{Y}\hat{\mathcal{M}}(\pi^{*}D^{t})]_{t=0}=2\pi\frac{d}{dt}[\mathcal{P}YM(D^{t})]_{t=0},$$

i.e., D is a pseudo Yang–Mills field on M. The converse requires the first variation formula for the functional $\mathcal{PYM}$ [as well as the fact that the Yang–Mills equations on $C(M)$ project on M via π to give the Euler–Lagrange equations of the variational principle $\delta\mathcal{PYM}=0$, see Sec. IV]. To establish (8) we need the following:

Lemma 1: Let M be a nondegenerate CR manifold, θ a contact form on M, and $d\,\mathrm{vol}(g_{\theta})$ the canonical volume form associated to the Webster metric g_{θ}. Then $\theta\wedge(\mathrm{d}\theta)^{n}=\pm c_{n}d\,\mathrm{vol}(g_{\theta})$ where $c_{n}=(-1)^{s}2^{n}n!$, provided that the Levi form L_{θ} has s negative eigenvalues.

This corrects the constant c_{n} from Ref. 30, p. 546. If the Levi form L_{θ} has r positive and s negative eigenvalues $(r+s=n)$ then g_{θ} is a semi-Riemannian metric of signature $(2r+1,2s)$. Let $\mathcal{O}$ be a fixed orientation of M. To prove Lemma 1, let G_{AB} be the components of the Webster metric with respect to a chart $(U,x^{A})\in\mathcal{O}$, so that $d\,\mathrm{vol}(g_{\theta})=\sqrt{|\det(G_{AB})|}\mathrm{d}x^{1}\wedge\cdots\wedge\mathrm{d}x^{2n+1}$. Let $\{T_{\alpha}\}$ be a local frame of $T_{1,0}(M)$ and $\mu\in GL(2n+1,\mathbb{C})$ such that $T_{A}=\mu_{A}^{B}\partial/\partial x^{B}$. Then $d\,\mathrm{vol}(g_{\theta})=\sqrt{|\det(G_{AB})|}\det(\mu)\theta^{01\cdots n\bar{1}\cdots\bar{n}}$, where $\theta^{01\cdots n\bar{1}\cdots\bar{n}}$ is short for $\theta\wedge\theta^{1}\wedge\cdots\wedge\theta^{n}\wedge\theta^{\bar{1}}\wedge\cdots\wedge\theta^{\bar{n}}$, hence $\overline{\det(\mu)}=(-1)^{n^{2}}\det(\mu)$ [as $d\,\mathrm{vol}(g_{\theta})$ is a real form]. It follows that $\sqrt{|\det(G_{AB})|}=(-1)^{s}|\det(\mu)|^{-1}\det(g_{\alpha\bar{\beta}})$. A calculation shows that

$$\theta\wedge(d\theta)^{n}=2^{n}i^{n^{2}}n!\det(g_{\alpha\bar{\beta}})\theta^{01\cdots n\bar{1}\cdots\bar{n}}$$

(see also Ref. 19) and then $\theta\wedge(d\theta)^{n}=\pm c_{n}d\,\mathrm{vol}(g_{\theta})$. The sign is +1 if $\mathcal{O}$ and the orientation of $H(M)$ (induced by its complex structure J) agree. Lemma 1 is proved. Let us prove (8). As

$$R^{D}e_{j}=(\pi_{H}R^{D})e_{j}-2P_{0A}{}^{i}{}_{j}(\theta\wedge\theta^{A})\otimes e_{i}$$

it follows that

$$\|R^D\|^2 = \|\pi_H R^D\|^2 + 4g^{A\bar{B}} P_{0A}{}^i{}_j P_{0\bar{B}}{}^j{}_i.$$

Yet $i_T R^D = \theta^B \otimes [P_{0B}{}^i{}_j] \in \Omega^1[\mathrm{Ad}(E)]$ hence $\|R^D\|^2 = \|\pi_H R^D\|^2 + 4\|i_T R_D\|^2$. At this point we may integrate over M with respect to $\theta \wedge (d\theta)^n$ and use Lemma 1. The proof of the last statement in (i) of Theorem 2 is delegated to the next section.

VI. THE FIRST VARIATION FORMULA

Let $E \to M$ be a vector bundle and D a connection in E. We shall need the differential operator $d^D: \Omega^k(E) \to \Omega^{k+1}(E)$ given by

$$(d^D\varphi)(X_1, \cdots, X_{k+1}) = \sum_{i=1}^{k+1} (-1)^{i+1} D_{X_i}[\varphi(X_1, \cdots, \hat{X}_i, \cdots, X_{k+1})]$$
$$+ \sum_{1 \leqslant i < j \leqslant k+1} (-1)^{i+j} \varphi([X_i, X_j], X_1, \cdots, \hat{X}_i, \cdots, \hat{X}_j, \cdots, X_{k+1})$$

for any $\varphi \in \Omega^k(E)$ and any $X_i \in T(M)$, $1 \leqslant i \leqslant k$. Here a hat indicates, as usual, the suppression of a term. Let $D \in \mathcal{C}(E,h)$ and let us denote by the same symbol the connection induced by D in $\mathrm{Ad}(E) \to M$. The operator δ^D in (18) is the formal adjoint of $d^D: \Omega^1[\mathrm{Ad}(E)] \to \Omega^2[\mathrm{Ad}(E)]$ with respect to the inner product

$$(\varphi, \psi) = \int_M \langle \varphi, \psi \rangle \theta \wedge (\mathrm{d}\theta)^n, \quad \varphi, \psi \in \Omega^k(E). \tag{84}$$

Let $\varphi \in \Omega^1[\mathrm{Ad}(E)]$. A standard calculation shows that $R^{D+t\varphi} = R^D + td^D\varphi + t^2[\varphi \wedge \varphi]$ (where $[\varphi \wedge \psi]_{X,Y} = [\varphi_X, \psi_Y] - [\varphi_Y, \psi_X]$, $X, Y \in T(M)$, $\varphi, \psi \in \Omega^1[\mathrm{Ad}(E)]$) hence

$$\|\pi_H R^{D+t\varphi}\|^2 = \|\pi_H R^D\|^2 + 2t\langle \pi_H R^D, \pi_H d^D\varphi \rangle + O(t^2)$$

and

$$\frac{d}{dt}[\mathcal{PYM}(D + t\varphi)]_{t=0} = \frac{1}{2}\int_M \frac{d}{dt}(\|\pi_H R^{D+t\varphi}\|^2)_{t=0}\theta \wedge (\mathrm{d}\theta)^n = \int_M \langle \pi_H R^D, d^D\varphi \rangle \theta \wedge (\mathrm{d}\theta)^n$$
$$= \int_M \langle \delta^D \pi_H R^D, \varphi \rangle \theta \wedge (d\theta)^n.$$

Then $(d/dt)[\mathcal{PYM}(D+t\varphi)]_{t=0} = 0$ yields

$$\delta^D \pi_H R^D = 0. \tag{85}$$

Let $D \in \mathcal{C}(E,h)$ such that $i_T R^D = 0$. Then [by (18) and (85)] D is a pseudo Yang–Mills field if and only if D is a Yang–Mills field, and the last statement in part (i) of Theorem 2 follows from Theorem 2.3 in Ref. 30, p. 551.

Let us consider the operator $\delta_b^D: \Omega^{k+1}(E) \to \Omega^k(E)$ given by

$$(\delta_b^D\varphi)(X_1, \cdots, X_k) = -\sum_{a=1}^{2n} (D_{E_a}\varphi)(E_a, X_1, \cdots, X_k),$$

for any $\varphi \in \Omega^{k+1}(E)$ and $X_i \in T(M)$, $1 \leqslant i \leqslant k$, where $\{E_a : 1 \leqslant a \leqslant 2n\}$ is a local G_θ orthonormal frame of $H(M)$. Clearly, if $\varphi \in \Omega_H^k(E)$ then $\delta^D\varphi = \delta_b^D\varphi$ and $i_T\delta_b^D\varphi = 0$. Consequently, if $i_T R^D = 0$ then Eqs. (85) may also be written

$$\delta_b^D R^D = 0. \tag{86}$$

Now we attack the problem whether the pullback $\hat{D}=\pi^* D$ of a pseudo Yang–Mills field D on M is a Yang–Mills field on $C(M)$. As argued in the previous section, this doesn't follow directly from (9). In turn, the Yang–Mills equations on $C(M)$ are related to (85) due to

$$(\delta^{\hat{D}} R^{\hat{D}})(X^{\uparrow})\hat{u} = [(\delta_b^D R^D)(X)u + R^D(T,JX)u]\hat{}, \tag{87}$$

$$(\delta^{\hat{D}} R^{\hat{D}})(T^{\uparrow})\hat{u} = [(\delta_b^D R^D)(T)u]\hat{} - \frac{i}{n+2}\left[R^{\alpha\bar{\beta}} - \frac{\rho}{2(n+1)}g^{\alpha\bar{\beta}}\right][R^D(T_\alpha, T_{\bar{\beta}})u]\hat{}, \tag{88}$$

$$(\delta^{\hat{D}} R^{\hat{D}})(S)\hat{u} = 2[(\Lambda_\theta R^D)u]\hat{}, \tag{89}$$

for any $X \in H(M)$ and $u \in \Omega^0(E)$. Here $X^{\uparrow}$ is the horizontal lift of X with respect to the connection 1-form σ in $S^1 \to C(M) \to M$. Let $D \in \mathcal{C}(E,h)$ be a pseudo Yang–Mills field with $i_T R^D = 0$. Then [by (87)–(89)] $\delta^{\hat{D}} R^{\hat{D}} = 0$ if and only if (10) and (11) hold. This completes the proof of Theorem 2.

It remains that we prove (87)–(89). The formal adjoint $\delta^{\mathbb{D}}$ of $d^{\mathbb{D}}: \Omega^1[\mathrm{Ad}(\pi^* E)] \to \Omega^2[\mathrm{Ad}(\pi^* E)]$ is given by

$$(\delta^{\mathbb{D}}\psi)(Y)v = -\sum_{j=1}^{2n+2} \epsilon_j (\mathbb{D}_{X_j}\psi)(X_j, Y)v = -\sum_{j=1}^{2n+2} [\mathbb{D}_{X_j}\psi(X_j, Y)v - \psi(\nabla^{C(M)}_{X_j} X_j, Y)v - \psi(X_j, \nabla^{C(M)}_{X_j} Y)v - \psi(X_j, Y)\mathbb{D}_{X_j} v],$$

for any $\psi \in \Omega^2[\mathrm{Ad}(\pi^* E)]$, $Y \in T[C(M)]$, and $v \in \Omega^0(\pi^* E)$, where $\{X_j : 1 \leqslant j \leqslant 2n+2\}$ is a local orthonormal [i.e., $F_\theta(X_j, X_k) = \epsilon_j \delta_{jk}$, $\epsilon_1 = \cdots = \epsilon_{2n+1} = -\epsilon_{2n+2} = 1$] frame of $T[C(M)]$ and $\nabla^{C(M)}$ is the Levi–Civita connection of $[C(M), F_\theta]$. As $S^1 \to C(M) \to M$ is a principal bundle, the projection π is a submersion. However, if $S = [(n+2)/2]\partial/\partial\gamma$ then $F_\theta(S,S) = 0$, i.e., S is null, so that π is not a semi-Riemannian submersion [in the sense of Ref. 22, p. 212, as the fibers of π are degenerate submanifolds]. Nevertheless, we may relate $\nabla^{C(M)}$ to the Tanaka–Webster connection ∇ of (M, θ), very much in the spirit of Ref. 23. Precisely, we may state

Lemma 2: For any $X, Y \in H(M)$

$$\nabla^{C(M)}_{X^{\uparrow}} Y^{\uparrow} = (\nabla_X Y)^{\uparrow} - (d\theta)(X,Y)T^{\uparrow} - [A(X,Y) + (d\sigma)(X^{\uparrow}, Y^{\uparrow})]S,$$

$$\nabla^{C(M)}_{X^{\uparrow}} T^{\uparrow} = (\tau X + \phi X)^{\uparrow},$$

$$\nabla^{C(M)}_{T^{\uparrow}} X^{\uparrow} = (\nabla_T X + \phi X)^{\uparrow} + 2(d\sigma)(X^{\uparrow}, T^{\uparrow})S,$$

$$\nabla^{C(M)}_{X^{\uparrow}} S = \nabla^{C(M)}_S X^{\uparrow} = (JX)^{\uparrow},$$

$$\nabla^{C(M)}_{T^{\uparrow}} T^{\uparrow} = V^{\uparrow}, \quad \nabla^{C(M)}_S S = 0,$$

$$\nabla^{C(M)}_S T^{\uparrow} = \nabla^{C(M)}_{T^{\uparrow}} S = 0,$$

where $\phi: H(M) \to H(M)$ is given by $G_\theta(\phi X, Y) = (\mathrm{d}\sigma)(X^{\uparrow}, Y^{\uparrow})$, and $V \in H(M)$ is given by $G_\theta(V, Y) = 2(\mathrm{d}\sigma)(T^{\uparrow}, Y^{\uparrow})$.

Proof of Lemma 2: Let us recall that

$$2F_\theta(\nabla^{C(M)}_{\widetilde{X}}\widetilde{Y},\widetilde{Z}) = \widetilde{X}[F_\theta(\widetilde{Y},\widetilde{Z})] + \widetilde{Y}[F_\theta(\widetilde{X},\widetilde{Z})] - \widetilde{Z}[F_\theta(\widetilde{X},\widetilde{Y})] + F_\theta[(\widetilde{X},\widetilde{Y}),\widetilde{Z}] + F_\theta[(\widetilde{Z},\widetilde{X}),\widetilde{Y}] + F_\theta[\widetilde{X},(\widetilde{Z},\widetilde{Y})] \tag{90}$$

for any $\widetilde{X},\widetilde{Y},\widetilde{Z}\in T[C(M)]$. In particular for $\widetilde{X}=X^\uparrow$, $\widetilde{Y}=Y^\uparrow$, $\widetilde{Z}=Z^\uparrow$, for any $X,Y,Z\in H(M)$

$$F_\theta(\nabla^{C(M)}_{X^\uparrow}Y^\uparrow,Z^\uparrow) = g_\theta(\nabla^M_X Y,Z),$$

where ∇^M is the Levi–Civita connection of (M,g_θ). Here one used the fact that $[X,Y]^\uparrow$ is the horizontal component of $[X^\uparrow,Y^\uparrow]$, with respect to σ (cf., e.g., Ref. 16 Vol. I, p. 65). The Levi–Civita connection ∇^M and the Tanaka–Webster connection ∇ of (M,θ) are related by [cf. (1) in Ref. 1 p. 238)

$$\nabla^M = \nabla - (d\theta + A)\otimes T + \tau\otimes\theta + 2\theta\odot J, \tag{91}$$

where $A(X,Y)=g_\theta(X,\tau Y)$. Recall that A is symmetric and τ traceless (cf. Ref. 34). As $H(M)$ is ∇ parallel $\pi_H\nabla^M_X Y=\nabla_X Y$, where $\pi_H: T(M)\to H(M)$ is the projection associated with the direct sum decomposition $T(M)=H(M)\oplus\mathbb{R}T$. Therefore, by taking into account the decomposition $T[C(M)]=\mathrm{Ker}(\sigma)\oplus\mathrm{Ker}(d\pi)=H(M)^\uparrow\oplus\mathbb{R}T^\uparrow\oplus\mathbb{R}S$

$$\nabla^{C(M)}_{X^\uparrow}Y^\uparrow = (\nabla_X Y)^\uparrow + \lambda T^\uparrow + \mu S, \tag{92}$$

for some $\lambda,\mu\in C^\infty[C(M)]$, depending on X,Y. We may determine λ, μ by taking the inner product with S, $T^\uparrow$, respectively. To this end let us first observe that

$$F_\theta(\nabla^{C(M)}_{X^\uparrow}Y^\uparrow,S) = -(\mathrm{d}\theta)(X,Y).$$

Here we again used (90) together with the fact that $[X^\uparrow,S]=0$ (cf. e.g. Ref. 16 Vol. I, p. 79). Similarly

$$2F_\theta(\nabla^{C(M)}_{X^\uparrow}Y^\uparrow,T^\uparrow) = \sigma[(X^\uparrow,Y^\uparrow)] - T[g_\theta(X,Y)] + g_\theta[(T,X),Y] + g_\theta[X,(T,Y)]$$

and

$$2g_\theta(\nabla^M_X Y,T) = -T[g_\theta(X,Y)] + \theta[(X,Y)] + g_\theta[(T,X),Y] + g_\theta[X,(T,Y)]$$

hence

$$2F_\theta(\nabla^{C(M)}_{X^\uparrow}Y^\uparrow,T^\uparrow) = 2\theta(\nabla^M_X Y) - \theta[(X,Y)] + \sigma[(X^\uparrow,Y^\uparrow)]$$

or [by (91)]

$$F_\theta(\nabla^{C(M)}_{X^\uparrow}Y^\uparrow,T^\uparrow) = -A(X,Y) - (d\sigma)(X^\uparrow,Y^\uparrow).$$

Summing up, (92) leads to the first identity in Lemma 2. The proof of the remaining identities in Lemma 2 may be obtained in a similar manner. Let us go back to the proof of (87)–(89). Let $\{E_a: 1\leqslant a\leqslant 2n\}$ be a local orthonormal frame of the Levi distribution $H(M)$. Then $\{E^\uparrow_a, T^\uparrow\pm S\}$ is a local orthonormal frame of $T[C(M)]$ with respect to the Feferman metric F_θ. We make use of $i_S(\hat{D}\hat{u})=0$ and $i_S(\hat{R^D}\hat{u})=0$, for any $u\in\Omega^0(E)$. Then (by Lemma 2)

$$(\delta^{\hat{D}}R^{\hat{D}})(X^{\uparrow})\hat{u} = -\sum_{a=1}^{2n}(\hat{D}_{E_a^{\uparrow}}R^{\hat{D}})(E_a^{\uparrow},X^{\uparrow}) - (\hat{D}_{T^{\uparrow}+S}R^{\hat{D}})(T^{\uparrow}+S,X^{\uparrow}) + (\hat{D}_{T^{\uparrow}-S}R^{\hat{D}})(T^{\uparrow}-S,X^{\uparrow})$$

$$= [(\delta_b^D R^D)(X)u + 2R^D(T,JX)u] - \sum_{a=1}^{2n}[(\mathrm{d}\theta)(E_a,X)R^D(E_a,T)u]$$

and

$$\sum_{a=1}^{2n}(\mathrm{d}\theta)(E_a,X)E_a = -JX$$

hence (87) is proved. Similarly

$$(\delta^{\hat{D}}R^{\hat{D}})(T^{\uparrow})\hat{u} = [(\delta_b^D R^D)(T)u] + \sum_{a=1}^{2n}[R^D(E_a,\tau E_a + \phi E_a)u]. \tag{93}$$

Now, on one hand

$$\sum_{a=1}^{2n}R^D(E_a,\tau E_a)u = g^{\alpha\bar{\beta}}[R^D(T_\alpha,\tau T_{\bar{\beta}})u + R^D(T_{\bar{\beta}},\tau T_\alpha)u] = A^{\alpha\gamma}R^D(T_\alpha,T_\gamma)u + A^{\bar{\beta}\bar{\gamma}}R^D(T_{\bar{\beta}},T_{\bar{\gamma}})u = 0$$

(as $A_{\alpha\beta}=A_{\beta\alpha}$) with the corresponding simplification of (93). On the other hand

$$\sum_{a=1}^{2n}R^D(E_a,\phi E_a)u = \phi^{\alpha\gamma}R^D(T_\alpha,T_\gamma)u + \phi^{\alpha\bar{\gamma}}R^D(T_\alpha,T_{\bar{\gamma}})u + \phi^{\bar{\beta}\gamma}R^D(T_{\bar{\beta}},T_\gamma)u + \phi^{\bar{\beta}\bar{\gamma}}R^D(T_{\bar{\beta}},T_{\bar{\gamma}})u,$$

where $\phi T_\alpha = \phi_\alpha{}^\beta T_\beta + \phi_\alpha{}^{\bar{\beta}}T_{\bar{\beta}}$, $\phi^{\alpha\beta}=g^{\alpha\bar{\gamma}}\phi_{\bar{\gamma}}{}^{\beta}$, etc. Let us take the exterior derivative of (71) so that to obtain

$$(n+2)\mathrm{d}\sigma = \pi^*\left[i\mathrm{d}\omega_\alpha{}^\alpha - \frac{i}{2}\mathrm{d}g^{\alpha\bar{\beta}}\wedge\mathrm{d}g_{\alpha\bar{\beta}} - \frac{1}{4(n+1)}d(\rho\theta)\right].$$

Using the identities $\mathrm{d}g_{\alpha\bar{\beta}}=g_{\alpha\bar{\gamma}}\omega_{\bar{\beta}}{}^{\bar{\gamma}}+\omega_\alpha{}^\gamma g_{\gamma\bar{\beta}}$ (a consequence of $\nabla g_\theta=0$) and $\mathrm{d}g^{\alpha\bar{\beta}}=-g^{\gamma\bar{\beta}}g^{\alpha\bar{\rho}}\mathrm{d}g_{\bar{\rho}\gamma}$ (a consequence of $g^{\alpha\bar{\beta}}g_{\bar{\beta}\gamma}=\delta_\gamma^\alpha$) it follows that

$$\mathrm{d}g^{\alpha\bar{\beta}}\wedge\mathrm{d}g_{\alpha\bar{\beta}} = \omega_{\alpha\bar{\beta}}\wedge\omega^{\alpha\bar{\beta}} + \omega_{\bar{\alpha}\beta}\wedge\omega^{\bar{\alpha}\beta} = 0.$$

Also (cf. e.g., Ref. 34)

$$d\omega_\alpha{}^\alpha = R_{\lambda\bar{\mu}}\theta^\alpha\wedge\theta^{\bar{\mu}} + (W_{\alpha\lambda}^{\alpha}\theta^\lambda - W_{\alpha\bar{\mu}}^{\alpha}\theta^{\bar{\lambda}})\wedge\theta$$

where $R_{\lambda\bar{\mu}}$ is the pseudohermitian Ricci curvature and $W_{\alpha\lambda}^{\alpha}$ (respectively $W_{\alpha\bar{\mu}}^{\alpha}$) are certain contractions of the covariant derivatives of $A_{\bar{\beta}}^{\alpha}$. It follows that

$$(n+2)G_\theta(\phi X,Y) = i(R_{\alpha\bar{\beta}}\theta^\alpha\wedge\theta^{\bar{\beta}})(X,Y) - \frac{\rho}{4(n+1)}(\mathrm{d}\theta)(X,Y),$$

for any $X,Y\in H(M)$. Therefore

$$\phi^{\bar{\alpha}\beta} = \frac{i}{2(n+2)}\left(R^{\bar{\alpha}\beta} - \frac{\rho}{2(n+1)}g^{\bar{\alpha}\beta}\right), \quad \phi^{\alpha\beta}=0.$$

We may conclude that

$$\sum_{A=1}^{2n} R^D(E_a,\phi E_a)u = -\frac{i}{n+2}\left(R^{\alpha\bar{\beta}} - \frac{\rho}{2(n+1)}g^{\alpha\bar{\beta}}\right)R^D(T_\alpha,T_{\bar{\beta}})u$$

and (93) leads to (88). Finally (again by Lemma 2)

$$(\delta^{\hat{D}}R^{\hat{D}})(S)\hat{u} = \sum_{a=1}^{2n}[R^D(E_a,JE_a)u] = -2i[g^{\alpha\bar{\beta}}R^D(T_\alpha,T_{\bar{\beta}})u] = 2[(\Lambda_\theta R^D)u]$$

and (89) is proved.

The functional (7) may be generalized by considering $\mathcal{PYM}_p(D)=\int_M\|\pi_H R^D\|^p\theta\wedge(\mathrm{d}\theta)^n$ with $p\geqslant 0$. As well known, in Riemannian geometry there is a choice of p such that $\mathcal{YM}_p(D)=\int_M\|R^D\|^p d\,\mathrm{vol}(g)$ becomes a conformal invariant [precisely $2p$ should be the dimension of the given Riemannian manifold (M,g)] and it is a natural question (raised by the Referee) whether for an appropriate p the number $\mathcal{PYM}_p(D)$ is a CR invariant, i.e., invariant under a transformation $\tilde{\theta}=e^{2u}\theta$ with $u\in C^\infty(M)$. Unfortunately, unlike the Riemannian case beside from the norm and volume form the integrand $\pi_H R^D$ transforms as well according to the law

$$(\tilde{\pi}_H R^D)e_j = (\pi_H R^D)e_j + i[(2u^\beta\Omega^i_{j\alpha\beta} - u^{\bar{\beta}}\Omega^i_{j\alpha\bar{\beta}})\theta^\alpha\wedge\theta - (2u^{\bar{\beta}}\Omega^i_{j\bar{\alpha}\bar{\beta}} + u^\beta\Omega^i_{j\beta\bar{\alpha}})\theta^{\bar{\alpha}}\wedge\theta]\otimes e_i$$

where $R^D e_j=\Omega^i_j\otimes e_i$ and $\tilde{\pi}_H:\Omega^2[\mathrm{Ad}(E)]\to\Omega^2[\mathrm{Ad}(E)]/\mathcal{J}^2_{\tilde{\theta}}$ is the natural projection. The problem of building a CR invariant version of $\mathcal{PYM}(D)$ [an analog to $\mathcal{YM}_{n+1/2}(D)$, $g=g_\theta$] is open.

VII. THE SECOND VARIATION FORMULA

Let $\{D^t:|t|<\epsilon\}$ be a smooth family of connections in E, where $D=D^0$ is a pseudo Yang–Mills field. We write $D^t=D+A^t$, where $A^t\in\Omega^1[\mathrm{Ad}(E)]$ for each $|t|<\epsilon$. The curvature R^t of D^t is then given by

$$R^t = R^D + d^D A^t + \frac{1}{2}[A^t\wedge A^t]$$

(cf. e.g., (6.2) in Ref. 4, p. 212). Next, let us set $\varphi=\{dA^t/dt\}_{t=0}$ and $\psi=\{d^2A^t/dt^2\}_{t=0}$ and observe that

$$\|\pi_H R^t\|^2 = \|\pi_H R^D\|^2 + 2t\langle\pi_H R^D, d^D\varphi\rangle + t^2\{2\langle\pi_H R^D, d^D\psi\rangle + \langle\pi_H R^D,[\varphi\wedge\varphi]\rangle + \|\pi_H d^D\varphi\|^2\} + O(t^3).$$

Integrating by parts and using $\delta^D\pi_H R^D=0$ we obtain

$$\frac{d^2}{dt^2}[\mathcal{PYM}(D^t)]_{t=0} = \int_M(\|\pi_H d^D\varphi\|^2 + \langle\pi_H R^D,[\varphi\wedge\varphi]\rangle)\theta\wedge(\mathrm{d}\theta)^n. \tag{94}$$

We shall need the (zero order) operator $\mathcal{R}^D:\Omega^1[\mathrm{Ad}(E)]\to\Omega^1[\mathrm{Ad}(E)]$ given by

$$\mathcal{R}^D(\varphi)_X = \sum_{A=1}^{2n+1}[R^D_{E_A,X},\varphi_{E_A}],$$

for any $X\in T(M)$, $\varphi\in\Omega^1[\mathrm{Ad}(E)]$, where $\{E_A\}$ is a local orthonormal frame of $[T(M),g_\theta]$. Then (see (6.7) in Ref. 4, p. 213)

$$\langle[\varphi\wedge\varphi],R^D\rangle = \langle\varphi,\mathcal{R}^D(\varphi)\rangle. \tag{95}$$

Let us set

$$\mathcal{R}_b^D(\varphi)_X = \sum_{a=1}^{2n} [R^D_{E_a,X}, \varphi_{E_a}], \quad \mathcal{R}_0^D(\varphi)_X = [R^D_{T,X}, \varphi_T],$$

where $\{E_a\}$ is a local orthonormal frame of $(H(M), G_\theta)$, so that $\mathcal{R}^D = \mathcal{R}_b^D + \mathcal{R}_0^D$. Taking into account the identities

$$[\varphi \wedge \varphi] e_j = 4(\varphi_k^i \wedge \varphi_j^k) \otimes e_i,$$

$$(\theta \wedge i_T R^D) e_j = (P_{0A}{}^i{}_j \theta \wedge \theta^A) \otimes e_i,$$

$$\mathcal{R}_0^D(\varphi) e_j = [\varphi_j^k(T) P_{0A}{}^i{}_k - P_{0A}{}^k{}_j \varphi_k^i(T)] \theta^A \otimes e_i,$$

where $\varphi e_j = \varphi_j^i \otimes e_i$, $\varphi_j^i \in \Omega^1(U)$, we may conduct the calculations

$$\langle [\varphi \wedge \varphi], \theta \wedge i_T R^D \rangle = h^{j\bar{r}} \langle [\varphi \wedge \varphi] e_j, (\theta \wedge i_T R^D) e_r \rangle = 4 h^{j\bar{r}} h_{i\bar{s}} g_\theta^*(\varphi_k^i \wedge \varphi_j^k, P_{0A}{}^s{}_r \theta \wedge \theta^A)$$
$$= 2 h^{j\bar{r}} h_{i\bar{s}} g^{A\bar{B}} [\varphi_k^i(T) \varphi_j^k(T_A) - \varphi_k^i(T_A) \varphi_j^k(T)] P_{0\bar{B}}{}^{\bar{s}}{}_{\bar{r}},$$

and

$$\langle \varphi, \mathcal{R}_0^D(\varphi) \rangle = h^{j\bar{r}} h_{i\bar{s}} \varphi_j^i(T_A) [\varphi_{\bar{r}}^{\bar{k}}(T) P_{0\bar{B}}{}^{\bar{s}}{}_{\bar{k}} - P_{0\bar{B}}{}^{\bar{k}}{}_{\bar{r}} \varphi_{\bar{k}}^{\bar{s}}(T)] g^{A\bar{B}} = \varphi_j^i(T_A) g^{A\bar{B}} [h^{j\bar{k}} h_{i\bar{s}} \varphi_{\bar{k}}^{\bar{r}}(T) - h^{j\bar{r}} h_{i\bar{k}} \varphi_{\bar{s}}^{\bar{k}}(T)] P_{0\bar{B}}{}^{\bar{s}}{}_{\bar{r}}.$$

Assume now that $\{e_j\}$ is orthonormal ($h_{i\bar{j}} = \delta_{ij}$), so that $\varphi_{\bar{j}}^{\bar{i}} = -\varphi_i^j$ [as φ is Ad(E) valued]. Then

$$\langle [\varphi \wedge \varphi], \theta \wedge i_T R^D \rangle = 2 \sum_{i,j} [\varphi_k^i(T) \varphi_j^k(T_A) - \varphi_k^i(T_A) \varphi_j^k(T)] g^{A\bar{B}} P_{0\bar{B}}{}^{\bar{i}}{}_{\bar{j}}$$

$$\langle \varphi, \mathcal{R}_0^D(\varphi) \rangle = \sum_{r,s} [\varphi_i^s(T) \varphi_r^i(T_A) - \varphi_j^s(T_A) \varphi_r^j(T)] g^{A\bar{B}} P_{0\bar{B}}{}^{\bar{s}}{}_{\bar{r}}$$

hence

$$\langle [\varphi \wedge \varphi], \theta \wedge i_T R^D \rangle = 2 \langle \varphi, \mathcal{R}_0^D(\varphi) \rangle.$$

Finally, let us take into account (95) and the identity

$$R^D = \pi_H R^D + 2\theta \wedge i_T R^D.$$

We obtain

$$\langle [\varphi \wedge \varphi], \pi_H R^D \rangle = \langle \varphi, \mathcal{R}^D(\varphi) - 4\mathcal{R}_0^D(\varphi) \rangle,$$

so that (94) becomes

$$\frac{d^2}{dt^2} [\mathcal{P}YM(D^t)]_{t=0} = \int_M \langle \delta^D \pi_H d^D \varphi + \mathcal{R}^D(\varphi) - 4\mathcal{R}_0^D(\varphi), \varphi \rangle \theta \wedge (\mathrm{d}\theta)^n. \tag{96}$$

We now restrict our variations to those whose first-order part φ satisfies $i_T \varphi = 0$ and $\delta^D \varphi = 0$. Also, let us introduce the first-order differential operator $d_b^D : \Omega^1[\mathrm{Ad}(E)] \to \Omega_H^2[\mathrm{Ad}(E)]$ given by $d_b^D \equiv \pi_H \circ d^D$. Then $\delta^D \pi_H d^D \varphi = \delta_b^D d_b^D \varphi = \Delta_b^D \varphi$ and $\mathcal{R}_0^D(\varphi) = 0$, so that (96) yields (12) in Theorem 3. Here $\Delta_b^D \equiv d_b^D \delta_b^D + \delta_b^D d_b^D$ is the *generalized sublaplacian*. The Riemannian counterpart $\mathcal{S}^D = \Delta^D + \mathcal{R}^D$ (cf. Ref. 4, p. 213, where Δ^D is the generalized Hodge–de Rham laplacian) of $\mathcal{S}_b^D = \Delta_b^D + \mathcal{R}_b^D$ in Theorem 3 is an elliptic operator, hence its restriction to $\mathrm{Ker}(\delta^D) \subset \Omega^1[\mathrm{Ad}(E)]$ has a discrete spectrum tending to $+\infty$ and the eigenspace corresponding to each eigenvalue of $\mathcal{S}^D$ is finite dimensional. This allows one to employ concepts from Morse theory (cf. Definition 6.10 in

Ref. 4, p. 213) in order to discuss stability and weak stability of Yang–Mills fields (cf. Ref. 4, p. 214). The CR analog of this phenomenon is that $\Delta_b^D:\Omega^{0,1}[\mathrm{Ad}(E)]\to\Omega^{0,1}[\mathrm{Ad}(E)]$ is subelliptic of order $\frac{1}{2}$, where $\Omega^{0,q}[\mathrm{Ad}(E)]=\Gamma^\infty[\Lambda^{0,q}(M)\otimes\mathrm{Ad}(E)]$. A complex valued q-form η on M is of *type* $(0,q)$, or a $(0,q)$ *form*, if $T_{1,0}(M)\rfloor\eta=0$ and $i_T\eta=0$. We denote by $\Lambda^{0,q}(M)\to M$ the relevant bundle and set $\Omega^{0,q}(M)=\Gamma^\infty[\Lambda^{0,q}(M)]$. Let M be a strictly pseudoconvex CR manifold (not necessarily compact). It is the proper place to recall that a formally self-adjoint second-order differential operator $L:C^\infty(M)\to C^\infty(M)$ is *subelliptic* (of order $0<\epsilon\leqslant 1$) at a point $x\in M$ if there is a neighborhood U of x such that

$$\|u\|_\epsilon^2\leqslant C[(Lu,u)+\|u\|^2]$$

for any $u\in C_0^\infty(U)$, where $\|u\|_\epsilon$ is the Sobolev norm u of order ϵ, $\|u\|=(u,u)^{1/2}$, and

$$(u,v)=\int_M uv\,d\,\mathrm{vol}(g_\theta) \tag{97}$$

is the ordinary L^2 inner product. L is subelliptic (of order ϵ) if it is subelliptic at any $x\in M$. A typical example is the *sublaplacian*

$$\Delta_b u=-\operatorname{div}(\nabla^H u),\quad u\in C^\infty(M),$$

where $\nabla^H u\equiv\pi_H\nabla u$, ∇u is the gradient of u with respect to the Webster metric g_θ, and the divergence is defined with respect to the volume form $\omega\equiv\theta\wedge(d\theta)^n$, i.e.,

$$\mathcal{L}_X\omega=\operatorname{div}(X)\omega,$$

for any $X\in\mathcal{X}(M)$, where $\mathcal{L}_X$ is the Lie derivative. It is easily seen that $\Delta_b u=-\Sigma_{a=1}^{2n}E_a^*E_a u$, for any local orthonormal frame $\{E_a\}$ of $H(M)$ hence, by a well known lemma of Radkevic,[27] it follows that $\|u\|_{1/2}^2\leqslant C[(\Delta_b u,u)+\|u\|^2]$, for any $u\in C_0^\infty(U)$, i.e., Δ_b is subelliptic of order $\frac{1}{2}$. Here E_a^* is the formal adjoint of E_a with respect to the inner product (97). In the next section we relate Δ_b^D to the Kohn–Rossi operator $\Box_b$ and explain the subellipticity of $\Box_b$ on (0, 1) forms.

VIII. SUBELLIPTICITY OF Δ_b^D

Let $\{T_\alpha\}$ be a local frame of $T_{1,0}(M)$. We start by computing

$$(\delta_b^D d_b^D\varphi)T_\lambda=-\sum_{a=1}^{2n}(D_{E_a}d_b^D\varphi)(E_a,T_\lambda),$$

for any $\varphi\in\Omega_H^1[\mathrm{Ad}(E)]$. Let us take into account the identities

$$g^{\alpha\bar\beta}(D_{T_\alpha}d_b^D\varphi)(T_{\bar\beta},T_\lambda)=g^{\alpha\bar\beta}\{D_{T_\alpha}[(d_b^D\varphi)(T_{\bar\beta},T_\lambda)]-\Gamma_{\alpha\bar\beta}^{\bar\gamma}(d_b^D\varphi)(T_{\bar\gamma},T_\lambda)-\Gamma_{\alpha\lambda}^{\gamma}(d_b^D\varphi)(T_{\bar\beta},T_\gamma)\},$$

$$(d_b^D\varphi)(T_\alpha,T_{\bar\beta})e_j=[(\nabla_{T_\alpha}\varphi_j^i)T_{\bar\beta}-(\nabla_{T_{\bar\beta}}\varphi_j^i)T_\alpha+2(\omega_k^i\wedge\varphi_j^k+\varphi_k^i\wedge\omega_j^k)(T_\alpha,T_{\bar\beta})]e_i,$$

where ω_j^i are the connection 1-forms of D with respect to $\{e_i\}$. Also, let us set

$$\nabla_{\bar\mu}\nabla_\lambda\psi_{\bar\alpha}\equiv(\nabla_{T_{\bar\mu}}\nabla\psi)(T_\lambda,T_{\bar\alpha})=T_{\bar\mu}(\nabla_\lambda\psi_{\bar\alpha})-\Gamma_{\bar\mu\lambda}^{\rho}\nabla_\rho\psi_{\bar\alpha}-\Gamma_{\bar\mu\bar\alpha}^{\bar\rho}\psi_{\bar\rho},$$

for any $\psi=\psi_{\bar\alpha}\theta^{\bar\alpha}\in\Omega^{0,1}(M)$, where $\nabla_\alpha\psi_{\bar\beta}\equiv(\nabla_{T_\alpha}\psi)T_{\bar\beta}$. We obtain

$$g^{\alpha\bar{\beta}}(D_{T_\alpha}d_b^D\varphi)(T_{\bar{\beta}},T_\lambda)e_j = -g^{\alpha\bar{\beta}}\{\nabla_\alpha\nabla_\lambda\varphi^i_{j\bar{\beta}} - \nabla_\alpha\nabla_{\bar{\beta}}\varphi^i_{j\lambda} + \omega_j^k(T_{\bar{\beta}})A_k^i(T_\alpha,T_\lambda) - \omega_j^k(T_\lambda)A_k^i(T_\alpha,T_{\bar{\beta}})$$
$$+ \omega_k^i(T_\lambda)B_j^k(T_\alpha,T_{\bar{\beta}}) - \omega_k^i(T_{\bar{\beta}})B_j^k(T_\alpha,T_\lambda) + \omega_k^i(T_\alpha)[(\nabla_{T_\lambda}\varphi_j^k)T_{\bar{\beta}} - (\nabla_{T_{\bar{\beta}}}\varphi_j^k)T_\lambda]$$
$$+ \omega_j^k(T_\alpha)[(\nabla_{T_{\bar{\beta}}}\varphi_k^i)T_\lambda - (\nabla_{T_\lambda}\varphi_k^i)T_{\bar{\beta}}] + \varphi^k_{j\bar{\beta}}C_k^i(T_\alpha,T_\lambda) - \varphi^k_{j\lambda}C_k^i(T_\alpha,T_{\bar{\beta}})$$
$$+ \varphi^i_{k\lambda}D_j^k(T_\alpha,T_{\bar{\beta}}) - \varphi^i_{k\bar{\beta}}D_j^k(T_\alpha,T_{\bar{\beta}})\}\otimes e_i$$

where

$$A_j^i \equiv \nabla\varphi_j^i + \omega_k^i\otimes\varphi_j^k, \quad B_j^i \equiv \nabla\varphi_j^i - \omega_j^k\otimes\varphi_k^i,$$

$$C_j^i \equiv \nabla\omega_j^i + \omega_k^i\otimes\omega_j^k, \quad D_j^i \equiv \nabla\omega_j^i - \omega_j^k\otimes\omega_k^i,$$

and $\varphi^i_{jA}=\varphi_j^i(T_A)$, so that $\nabla_\alpha\nabla_{\bar{\beta}}\varphi^i_{j\lambda}$ (respectively, $\nabla_\alpha\nabla_\beta\varphi^i_{j\bar{\lambda}}$) is the second-order covariant derivative of the (1,0) form $\pi_{1,0}\varphi_j^i$ [respectively, of the (0,1)-form $\pi_{0,1}\varphi_j^i$] [$\pi_{1,0}:\Omega^1(M)\to\Omega^{1,0}(M)$ and $\pi_{0,1}:\Omega^1(M)\to\Omega^{0,1}(M)$ are the natural projections]. The previous identity is rather involved, yet one is interested in the second-order terms alone. Together with the similar expression for $g^{\alpha\bar{\beta}}(D_{T_{\bar{\beta}}}d_b^D\varphi)(T_\alpha,T_\lambda)e_j$ this leads to

$$(\delta_b^Dd_b^D\varphi)(T_\lambda)e_j = g^{\alpha\bar{\beta}}(\nabla_\alpha\nabla_\lambda\varphi^i_{j\bar{\beta}} + \nabla_{\bar{\beta}}\nabla_\lambda\varphi^i_{j\alpha} - \nabla_\alpha\nabla_{\bar{\beta}}\varphi^i_{j\lambda} - \nabla_{\bar{\beta}}\nabla_\alpha\varphi^i_{j\lambda})e_i + \textit{lower order terms}. \tag{98}$$

By *lower order terms* (l.o.t.) we mean a linear combination of $\nabla_A\varphi^i_{jB}$ and φ^i_{jB} [with $C^\infty(U)$ coefficients]. Next, we need to compute

$$(d_b^D\delta_b^D\varphi)T_\lambda = D_{T_\lambda}(\delta_b^D\varphi) = -\sum_{a=1}^{2n} D_{T_\lambda}[(D_{E_a}\varphi)E_a].$$

We have

$$\{D_{T_\lambda}[g^{\alpha\bar{\beta}}(D_{T_\alpha}\varphi)T_{\bar{\beta}}]\}e_j = g^{\alpha\bar{\beta}}[\nabla_\lambda\nabla_\alpha\varphi^i_{j\bar{\beta}} - \omega_j^k(T_\lambda)A_k^i(T_\alpha,T_{\bar{\beta}}) + \omega_k^i(T_\lambda)B_j^k(T_\alpha,T_{\bar{\beta}}) - \omega_k^j(T_\alpha)(\nabla_{T_\lambda}\varphi_k^i)T_{\bar{\beta}}$$
$$+ \omega_k^i(T_\alpha)(\nabla_{T_\lambda}\varphi_j^k)T_{\bar{\beta}} + \varphi^k_{j\bar{\beta}}C_k^i(T_\lambda,T_\alpha) - \varphi^i_{k\bar{\beta}}D_j^k(T_\lambda,T_\alpha)]e_i.$$

Together with a similar expression for $D_{T_\lambda}[g^{\alpha\bar{\beta}}(D_{T_{\bar{\beta}}}\varphi)T_\alpha]$ this yields

$$(d_b^D\delta_b^D\varphi)(T_\lambda)e_j = -g^{\alpha\bar{\beta}}(\nabla_\lambda\nabla_\alpha\varphi^i_{j\bar{\beta}} + \nabla_\lambda\nabla_{\bar{\beta}}\varphi^i_{j\alpha})e_i + l.o.t. \tag{99}$$

We shall need the commutation formulae

$$\nabla_\alpha\nabla_\beta\eta_{\bar{\gamma}} - \nabla_\beta\nabla_\alpha\eta_{\bar{\gamma}} = -\eta_{\bar{\rho}}R_{\bar{\gamma}\ \alpha\beta}^{\ \bar{\rho}},$$

$$\nabla_{\bar{\beta}}\nabla_\alpha\eta_\gamma - \nabla_\alpha\nabla_{\bar{\beta}}\eta_\gamma = 2ig_{\alpha\bar{\beta}}\nabla_0\eta_\gamma - \eta_\rho R_{\gamma\ \bar{\beta}\alpha}^{\ \rho},$$

where the convention for the curvature components (of the Tanaka–Webster connection) is $R(T_A,T_B)T_C = R_C^{\ D}{}_{AB}T_D$. Then [by (98) and (99)]

$$(\Delta_b^D\varphi)(T_\lambda)e_j = g^{\alpha\bar\beta}(\nabla_\alpha\nabla_\lambda\varphi^i_{j\bar\beta} - \nabla_\lambda\nabla_\alpha\varphi^i_{j\bar\beta} + \nabla_{\bar\beta}\nabla_\lambda\varphi^i_{j\alpha} - \nabla_\lambda\nabla_{\bar\beta}\varphi^i_{j\alpha} - \nabla_\alpha\nabla_{\bar\beta}\varphi^i_{j\lambda} - \nabla_{\bar\beta}\nabla_\alpha\varphi^i_{j\lambda})e_i + l.o.t.$$

$$= [-\varphi^i_j(T_{\bar\rho})g^{\alpha\bar\beta}R_{\bar\beta}{}^{\bar\rho}{}_{\alpha\lambda} + 2\sqrt{-1}\nabla_0\varphi^i_{j\lambda} - \varphi^i_j(T_\rho)g^{\alpha\bar\beta}R_\alpha{}^\rho{}_{\bar\beta\lambda} - 2g^{\alpha\bar\beta}\nabla_{\bar\beta}\nabla_\alpha\varphi^i_{j\lambda}$$

$$+ 2\sqrt{-1}n\nabla_0\varphi^i_{j\lambda} - \varphi^i_j(T_\rho)g^{\alpha\bar\beta}R_\lambda{}^\rho{}_{\bar\beta\alpha}]e_i + l.o.t.$$

At this point we need the Kohn–Rossi operator $\Box_b$ on $\Omega^{0,1}(M)$. We start by extending $\bar\partial_b$ (originally defined on functions, see Sec. III) to (0,1) forms. Precisely, if $\eta\in\Omega^{0,1}(M)$ then $\bar\partial_b\eta$ is the unique (0,2) form on M coinciding with $d\eta$ on $T_{0,1}(M)\otimes T_{0,1}(M)$. Next, let us set $\Box_b\equiv\bar\partial_b^*\bar\partial_b + \bar\partial_b\bar\partial_b^*$, where $\bar\partial_b^*$ is the formal adjoint of $\bar\partial_b$ with respect to the L^2 inner product $(\alpha,\beta) = \int_M g_\theta^*(\alpha,\bar\beta)\omega$. A straightforward calculation leads to

$$\Box_b\eta = (-g^{\alpha\bar\beta}\nabla_\alpha\nabla_{\bar\beta}\eta_{\bar\gamma} - 2i\nabla_0\eta_{\bar\gamma} + \eta_{\bar\rho}R^{\bar\rho}{}_{\bar\gamma})\theta^{\bar\gamma}, \tag{100}$$

for any $\eta=\eta_{\bar\gamma}\theta^{\bar\gamma}\in\Omega^{1,0}(U)$. Consequently

$$\bar\Box_b(\pi_{1,0}\varphi^i_j) = [\Box_b(\pi_{1,0}\varphi^i_j)^-]^- = [-g^{\alpha\bar\beta}\nabla_{\bar\beta}\nabla_\alpha\varphi^i_{j\lambda} + 2i\nabla_0\varphi^i_{j\lambda} + \varphi^i_j(T_\rho)R^\rho{}_\lambda]\theta^\lambda$$

hence

$$(\Delta_b^D\varphi)(T_\lambda)\theta^\lambda\otimes e_j = 2\bar\Box_b(\pi_{1,0}\varphi^i_j)e_i + \{2(n-1)\sqrt{-1}\nabla_0\varphi^i_{j\lambda} - \varphi^i_j(T_{\bar\rho})g^{\alpha\bar\beta}R_{\bar\beta}{}^{\bar\rho}{}_{\alpha\lambda} - \varphi^i_j(T_\rho)[2R^\rho{}_\lambda$$

$$+ g^{\alpha\bar\beta}(R_\alpha{}^\rho{}_{\bar\beta\lambda} + R_\lambda{}^\rho{}_{\bar\beta\alpha})]\}\theta^\lambda\otimes e_i + l.o.t.$$

To compute the curvature terms we need the identities

$$R_{\lambda\bar\mu} = R_\lambda{}^\alpha{}_{\alpha\bar\mu},$$

$$R_\alpha{}^\rho{}_{\lambda\mu} = 2i(A_{\mu\alpha}\delta^\rho_\lambda - A_{\lambda\alpha}\delta^\rho_\mu),$$

$$R_\alpha{}^\rho{}_{\bar\lambda\bar\mu} = 2i(g_{\alpha\bar\lambda}A^\rho_{\bar\mu} - g_{\alpha\bar\mu}A^\rho_{\bar\lambda}),$$

$$R_{\alpha\bar\beta\lambda\bar\mu} = R_{\lambda\bar\beta\alpha\bar\mu}, \quad R_{\alpha\bar\beta\lambda\bar\mu} = -R_{\bar\beta\alpha\lambda\bar\mu},$$

following essentially by the techniques developed in Ref. 34. Indeed we have

$$g^{\alpha\bar\beta}R_{\bar\beta}{}^{\bar\rho}{}_{\alpha\lambda} = -2i(n-1)A^{\bar\rho}_\lambda,$$

$$2R^\rho{}_\lambda + g^{\alpha\bar\beta}(R_\alpha{}^\rho{}_{\bar\beta\lambda} + R_\lambda{}^\rho{}_{\bar\beta\alpha}) = 0,$$

hence

$$(\Delta_b^D\varphi)(T_\lambda)\theta^\lambda\otimes e_j = 2\bar\Box_b(\pi_{1,0}\varphi^i_j)\otimes e_i + 2(n-1)\sqrt{-1}[(\nabla_T\varphi^i_j)T_\lambda + A^{\bar\rho}_\lambda\varphi^i_j(T_{\bar\rho})]\theta^\lambda\otimes e_i + l.o.t. \tag{101}$$

Recall that $\tau T_\alpha = A^{\bar\beta}_\alpha T_{\bar\beta}$. Then (101) together with the similar identity $(\Delta_b^D\varphi)(T_{\bar\lambda})e_j = 2[(\Box_b\pi_{0,1}\varphi^i_j)_{\bar\lambda} - (n-1)\sqrt{-1}(\nabla_0\varphi^i_{j\bar\lambda} + A^\rho_{\bar\lambda}\varphi^i_{j\rho})]e_i + l.o.t.$. leads to

$$(\Delta_b^D\varphi)\otimes e_j = 2[\Box_b(\pi_{0,1}\varphi_j^i) + \bar{\Box}_b(\pi_{1,0}\varphi_j^i) + (n-1)(\nabla_T\varphi_j^i + \varphi_j^i\circ\tau)\circ J]\otimes e_i + l.o.t.$$

and therefore to (13) when φ is a (0,1) form. Finally, let us show that $\Box_b$ is subelliptic on (scalar) (0,1) forms. As $\nabla\omega=0$, the sublaplacian may be computed as

$$\Delta_b f = -\operatorname{trace}\{T_A \mapsto \nabla_{T_A}\nabla^H f\} = -\nabla_\alpha f^\alpha - \nabla_{\bar\alpha} f^{\bar\alpha},$$

for any C^∞ function $f: M\to\mathbb{C}$, where $f^\alpha = g^{\alpha\bar\beta}T_{\bar\beta}(f)$. As $\nabla g_\theta = 0$

$$g^{\alpha\bar\beta}\nabla_\alpha\nabla_{\bar\beta}\eta_{\bar\lambda} = \nabla_\alpha(g^{\alpha\bar\beta}\nabla_{\bar\beta}\eta_{\bar\lambda}) = \nabla_\alpha(\eta_{\bar\lambda})^\alpha - \nabla_\alpha(g^{\alpha\bar\beta}\Gamma^{\bar\rho}_{\bar\beta\bar\lambda}\eta_{\bar\rho}).$$

A similar expression holds for $g^{\alpha\bar\beta}(\nabla_{\bar\beta}\nabla_\alpha\eta_{\bar\lambda})$. Adding up the two identities leads to

$$g^{\alpha\bar\beta}(\nabla_\alpha\nabla_{\bar\beta}\eta_{\bar\lambda} + \nabla_{\bar\beta}\nabla_\alpha\eta_{\bar\lambda}) = -\Delta_b\eta_{\bar\lambda} + l.o.t.$$

or [by the commutation formulae for the second order derivatives and (100)]

$$2(\Box_b\eta)_{\bar\lambda} - 2i(n-1)\nabla_0\eta_{\bar\lambda} - \eta_{\bar\rho}R^{\bar\rho}{}_{\bar\lambda} = \Delta_b\eta_{\bar\lambda} + g^{\alpha\bar\beta}[\nabla_\alpha(\Gamma^{\bar\rho}_{\bar\beta\bar\lambda}\eta_{\bar\rho}) + \nabla_{\bar\beta}(\Gamma^{\bar\rho}_{\alpha\bar\lambda}\eta_{\bar\rho})].$$

Hence $\Box_b$ is subelliptic on $\Omega^{0,1}(M)$, i.e., $\Box_b\eta$ is locally given by a subelliptic operator acting on the coefficients of η, plus lower order terms. In particular [by (13)] $(\Delta_b^D\varphi)\otimes e_j = \Delta_b[\varphi_j^i(T_{\bar\alpha})]\theta^{\bar\alpha}\otimes e_i$+l.o.t. Theorem 3 is completely proved.

APPENDIX: THE GRAHAM–LEE CONNECTION

Let $\Omega=\{\varphi<0\}\subset\mathbb{C}^n$ be a strictly pseudoconvex domain and $\mathcal{F}$ the foliation by level sets of φ of a one-sided neighborhood V of $\partial\Omega$ (as in Sec. III of this paper). Let $\{W_\alpha: 1\leqslant\alpha\leqslant n-1\}$ be a local frame of $T_{1,0}(\mathcal{F})$, so that $\{W_\alpha,\xi\}$ is a local frame of $T^{1,0}(V)$. Let g_θ be the tensor field given by

$$g_\theta(X,Y) = (d\theta)(X,JY),\quad g_\theta(X,T)=0,\quad g_\theta(T,T)=1, \tag{A1}$$

for any $X,Y\in H(\mathcal{F})$. Then g_θ is a tangential Riemannian metric for $\mathcal{F}$, i.e., a Riemannian metric in $T(\mathcal{F})\to V$. We consider as well

$$L_\theta(Z,\bar W) \equiv -i(d\theta)(Z,\bar W),\quad Z,W\in T_{1,0}(\mathcal{F}).$$

Note that L_θ and (the C-linear extension of) g_θ coincide on $T_{1,0}(\mathcal{F})\otimes T_{0,1}(\mathcal{F})$. We set $g_{\alpha\bar\beta} = g_\theta(W_\alpha, W_{\bar\beta})$. Let $\{\theta^\alpha: 1\leqslant\alpha\leqslant n-1\}$ be the (locally defined) complex 1 forms on V determined by

$$\theta^\alpha(W_\beta) = \delta^\alpha_\beta,\quad \theta^\alpha(W_{\bar\beta})=0,\quad \theta^\alpha(T)=0, \theta^\alpha(N)=0.$$

Then $(\theta^\alpha,\theta^{\bar\alpha},\theta,d\varphi)$ is a local frame of $T(V)\otimes\mathbb{C}$ and we may look for $\mathrm{d}\theta$ in the form

$$\mathrm{d}\theta = B_{\alpha\beta}\theta^\alpha\wedge\theta^\beta + B_{\alpha\bar\beta}\theta^\alpha\wedge\theta^{\bar\beta} + B_{\bar\alpha\bar\beta}\theta^{\bar\alpha}\wedge\theta^{\bar\beta} + (B_\alpha\theta^\alpha + B_{\bar\alpha}\theta^{\bar\alpha})\wedge\theta + (C_\alpha\theta^\alpha + C_{\bar\alpha}\theta^{\bar\alpha})\wedge\mathrm{d}\varphi + D\,\mathrm{d}\varphi\wedge\theta.$$

As $\mathrm{d}\theta = i\partial\bar\partial\varphi\in\Omega^{1,1}(U)$ it follows that $B_{\alpha\beta}=0$, $B_{\bar\alpha\bar\beta}=0$. Also

$$g_{\alpha\bar\beta} = g_\theta(W_\alpha,W_{\bar\beta}) = -i(d\theta)(W_\alpha,W_{\bar\beta}) = -\frac{i}{2}B_{\alpha\bar\beta}$$

i.e., $B_{\alpha\bar\beta}=2ig_{\alpha\bar\beta}$. Next

$$\frac{1}{2}B_\alpha = (d\theta)(W_\alpha, T) = i\partial\bar{\partial}\varphi(W_\alpha, T) = 0$$

as $T = i(\xi - \bar{\xi})$ [and ξ is orthogonal to $T_{1,0}(\mathcal{F})$ with respect to $\partial\bar{\partial}\varphi$], i.e., $B_\alpha = 0$, $B_{\bar{\alpha}} = 0$. Similarly $C_\alpha = 0$, $C_{\bar{\alpha}} = 0$. Finally

$$D = (\mathrm{d}\theta)(N, T) = i\partial\bar{\partial}\varphi(N, T) = 2\partial\bar{\partial}\varphi(\xi, \bar{\xi}) = r$$

i.e., $D = r$. We obtain the identity

$$\mathrm{d}\theta = 2ig_{\alpha\bar{\beta}}\theta^\alpha \wedge \theta^{\bar{\beta}} + r\,\mathrm{d}\varphi \wedge \theta. \tag{A2}$$

As an immediate consequence

$$i_T\,\mathrm{d}\theta = -\frac{r}{2}\mathrm{d}\varphi, \tag{A3}$$

$$i_N\,\mathrm{d}\theta = r\theta. \tag{A4}$$

For instance [by Eq. (A2)]

$$(\mathrm{d}\theta)(X, T) = \frac{r}{2}[(\mathrm{d}\varphi)(X) - (\mathrm{d}\varphi)(T)\,\theta(X)],$$

for any $X \in T(\mathcal{F})$, hence [as $(\mathrm{d}\varphi)(T) = 0$] one derives (A3). As an application of (A2) we decompose $[T, N]$ [according to $T(V) \otimes \mathbb{C} = T_{1,0}(\mathcal{F}) \oplus T_{0,1}(\mathcal{F}) \oplus \mathbb{C}T \oplus \mathbb{C}N$]. This is a bit trickier, as shown below. By (A3)

$$\theta([T, N]) = -2(\mathrm{d}\theta)(T, N) = r\,\mathrm{d}\varphi(N) = 2r.$$

Next

$$\begin{aligned} 2(\mathrm{d}\theta)[W_\alpha, (T, N)] &= 2W_\alpha(r) - \theta\{[W_\alpha, (T, N)]\} = (\textit{Jacobi's identity}) = 2W_\alpha(r) + \theta\{[T, (N, W_\alpha)]\} \\ &\quad + \theta\{[N, (W_\alpha, T)]\} = 2W_\alpha(r) + 2(\mathrm{d}\theta)[T, (W_\alpha, N)] - T\{\theta[(W_\alpha, N)]\} \\ &\quad + 2(\mathrm{d}\theta)[N, (T, W_\alpha)] - N\{\theta[(T, W_\alpha)]\} \end{aligned}$$

hence [by (A3) and (A4)]

$$(\mathrm{d}\theta)[W_\alpha, (T, N)] = W_\alpha(r).$$

We conclude that

$$(T, N) = iW^\alpha(r)W_\alpha - iW^{\bar{\alpha}}(r)W_{\bar{\alpha}} + 2rT, \tag{A5}$$

where $W^\alpha(r) = g^{\alpha\bar{\beta}}W_{\bar{\beta}}(r)$ and $W^{\bar{\alpha}}(r) = \overline{W^\alpha(r)}$.

Let ∇ be a linear connection on V. Let us consider the $T(V)$-valued 1 form τ on V defined by

$$\tau(X) = T_\nabla(T, X), \quad X \in T(V),$$

where T_∇ is the torsion tensor field of ∇. We say T_∇ is *pure* if

$$T_\nabla(Z, W) = 0, \quad T_\nabla(Z, \bar{W}) = 2iL_\theta(Z, \bar{W})T, \tag{A6}$$

$$T_\nabla(N, W) = rW + i\tau(W), \tag{A7}$$

for any $Z, W \in T_{1,0}(\mathcal{F})$, and

$$\tau[T_{1,0}(\mathcal{F})] \subseteq T_{0,1}(\mathcal{F}), \tag{A8}$$

$$\tau(N) = -J\nabla^H r - 2rT. \tag{A9}$$

Here $\nabla^H r$ is defined by $\nabla^H r = \pi_H \nabla r$ and $g_\theta(\nabla r, X) = X(r)$, $X \in T(\mathcal{F})$. Also $\pi_H : T(\mathcal{F}) \to H(\mathcal{F})$ is the projection associated to the direct sum decomposition $T(\mathcal{F}) = H(\mathcal{F}) \oplus \mathbb{R}T$. The Appendix is aimed at the following:

Theorem 4: (Ref. 11) *There is a unique linear connection* ∇ *on* V *such that:* (i) $T_{1,0}(\mathcal{F})$ *is parallel with respect to* ∇, (ii) $\nabla L_\theta = 0$, $\nabla T = 0$, $\nabla N = 0$, *and* (iii) T_∇ *is pure*.

∇ given by Theorem 4 is the *Graham–Lee connection*. Compare to Proposition 1.1 in Ref. 11, pp. 701–702. The axiomatic description in Theorem 4 is however new (cf. also Theorem 2 in Ref. 7). We first establish

Lemma 3: Let $\phi : T(\mathcal{F}) \to T(\mathcal{F})$ *be the bundle morphism given by* $\phi(X) = JX$, *for any* $X \in H(\mathcal{F})$, *and* $\phi(T) = 0$. *Then*

$$\phi^2 = -I + \theta \otimes T,$$

$$g_\theta(X, T) = \theta(X),$$

$$g_\theta(\phi X, \phi Y) = g_\theta(X, Y) - \theta(X)\theta(Y),$$

for any $X, Y \in T(\mathcal{F})$. *Moreover, if* ∇ *is a linear connection on* V *satisfying the axioms* (i)–(iii) *in Theorem* 4 *then*

$$\phi \circ \tau + \tau \circ \phi = 0 \tag{A10}$$

along $T(\mathcal{F})$. *Consequently* τ *may be computed as*

$$\tau(X) = -\frac{1}{2}\phi(\mathcal{L}_T \phi)X, \tag{A11}$$

for any $X \in H(\mathcal{F})$.

Proof: For any $X \in T(\mathcal{F})$

$$\phi(X) = \phi[\pi_H X + \theta(X)T] = J(\pi_H X) \in H(\mathcal{F}),$$

$$\phi^2(X) = J^2(\pi_H X) = -\pi_H X = -X + \theta(X)T.$$

The second statement in Lemma 112 follows from definitions [cf. (A1)]. The third identity follows from

$$g_\theta(\phi X, \phi Y) = (\mathrm{d}\theta)(\phi \pi_H X, \phi^2 \pi_H Y) = g_\theta(\pi_H Y, \pi_H X) = g_\theta(Y, X) - \theta(X) g_\theta(Y, T).$$

Let us prove (A10). As $\tau[T_{1,0}(\mathcal{F})] \subseteq T_{0,1}(\mathcal{F})$ [cf. axiom (A8)] there are complex valued functions $A_\alpha^{\bar{\beta}}$ such that $\tau(W_\alpha) = A_\alpha^{\bar{\beta}} W_{\bar{\beta}}$. Then

$$(\tau \circ \phi + \phi \circ \tau) W_\alpha = i\tau(W_\alpha) + A_\alpha^{\bar{\beta}} \phi(W_{\bar{\beta}}) = 0.$$

It remains that we check (A11). As $T_{1,0}(\mathcal{F})$ is parallel with respect to ∇ and ∇ is a real operator it follows that $T_{0,1}(\mathcal{F})$ is parallel, hence both $H(\mathcal{F})$ and its complex structure $J_{\mathcal{F}} \equiv J|_{H(\mathcal{F})}$ are parallel. Moreover, as $\nabla T = 0$, it follows that ϕ is parallel, as well. Let $X \in H(\mathcal{F})$. Then [by (A10)]

$$\phi \tau X = -T_\nabla(T, \phi X) = -\nabla_T \phi X + [T, \phi X].$$

Applying ϕ in both sides gives (as $\nabla \phi = 0$)

$$\tau X = -\nabla_T X - \phi[T,\phi X] = -[T,X] - \tau X - \phi[T,\phi X]$$

or

$$2\tau X = -\mathcal{L}_T X - \phi\mathcal{L}_T\phi X.$$

Q.E.D.

Proof of Theorem: To establish uniqueness, note first that, for any $X=X^{1,0}+X^{0,1}+\theta(X)T \in T(\mathcal{F})$ [with $X^{1,0}\in T_{1,0}(\mathcal{F})$, $X^{0,1}=\overline{X^{1,0}}$] one has (by $\nabla N=0$)

$$\nabla_N X = [N,X] + T_\nabla(N,X) = [by\ (A6)-(A7),\ (A9)] = [N,X] + rX^{1,0} + i\tau X^{1,0} + rX^{0,1} - i\tau X^{0,1} + \theta(X) \times (J\nabla^H r + 2rT)$$

that is

$$\nabla_N X = rX + \tau\phi X - [X,N] + \theta(X)(J\nabla^H r + rT), \tag{A12}$$

for any $X\in T(\mathcal{F})$. In view of (A11) $\nabla_N X$ is determined. As $\nabla N=0$, $\nabla T=0$ it remains that we compute $\nabla_X Z$, for $X\in T(\mathcal{F})$ and $Z\in T_{1,0}(\mathcal{F})$. Note that $\nabla T=0$, $\nabla L_\theta=0$ and $\nabla J_{\mathcal{F}}=0$ yield $\nabla g_\theta=0$, i.e.,

$$X[g_\theta(Y,Z)] = g_\theta(\nabla_X Y,Z) + g_\theta(Y,\nabla_X Z),$$

for any $X,Y,Z\in T(\mathcal{F})$. The well known Christoffel process then leads to

$$2g_\theta(\nabla_X Y,Z) = X[g_\theta(Y,Z)] + Y[g_\theta(X,Z)] - Z[g_\theta(X,Y)] + g_\theta[(X,Y),Z] + g_\theta[T_\nabla(X,Y),Z] + g_\theta[(Z,X),Y] + g_\theta[T_\nabla(Z,X),Y] + g_\theta[X,(Z,Y)] + g_\theta[X,T_\nabla(Z,Y)]. \tag{A13}$$

Note that (again by the purity axioms)

$$T_\nabla(X,Y) = 2(\mathrm{d}\theta)(X,Y)T + 2(\theta\wedge\tau)(X,Y), \tag{A14}$$

for any $X,Y\in T(\mathcal{F})$. Indeed [by (A6)]

$$T_\nabla(X,Y) = -2g_\theta(X,\phi Y)T + 2(\theta\wedge\tau)(X,Y).$$

Moreover

$$g_\theta(X,\phi Y) = g_\theta(\pi_H X,\phi\pi_H Y) + \theta(X)g_\theta(T,\phi\pi_H Y) = -(\mathrm{d}\theta)(\pi_H X,\pi_H Y) = -(\mathrm{d}\theta)(X,Y) + \theta(X)(\mathrm{d}\theta)(T,Y) + \theta(Y)(\mathrm{d}\theta)(X,T).$$

Finally [by (A3)] $(\mathrm{d}\theta)(X,T)=0$, $X\in T(\mathcal{F})$, and (A14) is proved. Replacing the torsion terms [from (A14) into (A13)] leads to

$$2g_\theta(\nabla_X Z,\bar{W}) = X[g_\theta(Z,\bar{W})] + Z[g_\theta(X,\bar{W})] - \bar{W}[g_\theta(X,Z)] + g_\theta[(X,Z),\bar{W}] + g_\theta[(\bar{W},X),Z] + g_\theta[X,(\bar{W},Z)], \tag{A15}$$

for any $X\in T(\mathcal{F})$ and $Z,W\in T_{1,0}(\mathcal{F})$, as [by (A8)]

$$\theta(X)[g_\theta(\tau Z,\bar{W}) - g_\theta(\tau\bar{W},Z)] = 0.$$

The uniqueness statement in Theorem 4 is proved. The following explicit expressions of (the various components of) ∇ are also available. By (A6)

$$\nabla_Z\bar{W} = \pi_{0,1}(Z,\bar{W}), \quad Z,W\in T_{1,0}(\mathcal{F}), \tag{A16}$$

where $\pi_{0,1}: T(\mathcal{F})\otimes\mathbb{C}\to T_{0,1}(\mathcal{F})$ is the projection. Of course

$$\nabla_{\bar{Z}}W = \overline{\nabla_Z \bar{W}}.$$

Moreover [by $\nabla L_\theta = 0$ and (A16)]

$$L_\theta(\nabla_Z W, \bar{V}) = Z[L_\theta(W,\bar{V})] - L_\theta[W, \pi_{0,1}(Z,\bar{V})],$$

for any $Z, W, V \in T_{1,0}(\mathcal{F})$, i.e.,

$$\nabla_Z W = g^{\alpha\bar{\beta}}\{Z[L_\theta(W, W_{\bar{\beta}})] - L_\theta[W, \pi_{0,1}(Z, W_{\bar{\beta}})]\}W_\alpha \tag{A17}$$

and

$$\nabla_{\bar{Z}}\bar{W} = \overline{\nabla_Z W}.$$

Next [by (A7) and (A8)]

$$\nabla_N Z = rZ + \pi_{1,0}[N,Z], \tag{A18}$$

for any $Z \in T_{1,0}(\mathcal{F})$, and

$$\nabla_N \bar{Z} = \overline{\nabla_N Z}.$$

Finally

$$\nabla_T Z = -\frac{1}{2}\phi(\mathcal{L}_T\phi)Z - [Z,T],$$

$$\nabla_T \bar{Z} = \overline{\nabla_T Z}, \quad Z \in T_{1,0}(\mathcal{F}). \tag{A19}$$

To establish the existence statement in Theorem 4 let ∇ be the linear connection on V defined by (A16)–(A19) and $\nabla T = 0$, $\nabla N = 0$. Let us check (i)–(iii) in Theorem 4. Clearly

$$\nabla_Z W, \quad \nabla_{\bar{Z}} W, \quad \nabla_N W \in T_{1,0}(\mathcal{F}),$$

for any $W \in T_{1,0}(\mathcal{F})$, by the very definitions [cf. (A16)–(A18). Moreover [by (A19)]

$$\nabla_T Z = \frac{1}{2}(\mathcal{L}_T Z - i\phi\mathcal{L}_T Z)$$

as [by (A3)] $\mathcal{L}_T Z \in H(\mathcal{F}) \otimes \mathbb{C}$. Therefore

$$\phi\nabla_T Z = i\nabla_T Z$$

that is [as $T_{1,0}(\mathcal{F})$ is the eigenspace corresponding to the eigenvalue i of [the $\mathbb{C}$-linear extension to $H(\mathcal{F})$ of] ϕ] $\nabla_T Z \in T_{1,0}(\mathcal{F})$. We conclude that ∇ obeys to (i). Let us check purity. By (A17)

$$L_\theta[\nabla_Z W - \nabla_W Z - (Z,W), \bar{V}] = Z[L_\theta(W,\bar{V})] - L_\theta[W, \pi_{0,1}(Z,\bar{V})] - W[L_\theta(Z,\bar{V})] + L_\theta[Z, \pi_{0,1}(W,\bar{V})]$$
$$- L_\theta[(Z,W),\bar{V}] = 3(\mathrm{d}^2\theta)(Z,W,\bar{V}) = 0.$$

Therefore $T_\nabla(Z,W) = 0$. Next [by (A16) and $\overline{\pi_{0,1}X} = \pi_{1,0}\bar{X}$, $X \in T(\mathcal{F}) \otimes \mathbb{C}$]

$$T_\nabla(Z,\bar{W}) = \pi_{0,1}[Z,\bar{W}] - \overline{\pi_{0,1}(W,\bar{Z})} - (Z,\bar{W}) = -\theta[(Z,\bar{W})]T = 2iL_\theta(Z,\bar{W})T.$$

Moreover [by (A18)]

$$T_\nabla(N,Z) = \nabla_N Z - (N,Z) = rZ - \pi_{0,1}(N,Z).$$

Also [by (A19)]

$$\tau(Z) = -\frac{1}{2}\phi(\mathcal{L}_T\phi)Z, \quad Z \in T_{1,0}(\mathcal{F}),$$

so that on one hand (A8) is satisfied, and on the other

$$\tau(Z) = -\frac{1}{2}[i\phi(T,Z) + (T,Z)] = -\pi_{0,1}(T,Z) = i[\pi_{0,1}(\bar{\xi},Z) - \pi_{0,1}(\xi,Z)] = i\pi_{0,1}(\bar{\xi},Z)$$

i.e.,

$$\tau(Z) = i\pi_{0,1}(N,Z), \quad Z \in T_{1,0}(\mathcal{F}). \tag{A20}$$

Here we made use of $T=i(\xi-\bar{\xi})$, $N=\xi+\bar{\xi}$, and $\pi_{0,1}(\xi,Z)=0$. Then (A20) yields (A7). Finally $\nabla T=\nabla N=0$ and (A5) yield (A9) and we conclude that ∇ obeys to (iii). It remains that we check $\nabla L_\theta=0$. Clearly $\nabla_Z L_\theta=0$, $Z\in T_{1,0}(\mathcal{F})$ [by (A16) and (A17)]. Next [by (A19) and (A8)]

$$(\nabla_T L_\theta)(Z,\bar{W}) = (\mathcal{L}_T L_\theta)(Z,\bar{W}), \quad Z,W \in T_{1,0}(\mathcal{F}),$$

and

$$(\mathcal{L}_T L_\theta)(Z,\bar{W}) = -i\{T[d\theta(Z,\bar{W})] - \mathrm{d}\theta[(T,Z),\bar{W}] - \mathrm{d}\theta[Z,(T,\bar{W})]\} = \frac{i}{2}(T\{\theta[(Z,\bar{W})]\} - \theta\{[(T,Z),\bar{W}]\}$$

$$- \theta\{[Z,(T,\bar{W})]\}) = (\text{by applying the Jacobi identity to the term } \theta\{[(T,Z),\bar{W}]\})$$

$$= \frac{i}{2}(T\{\theta[(Z,\bar{W})]\} + \theta\{[(Z,\bar{W}),T]\}) = i(\mathrm{d}\theta)[T,(Z,\bar{W})] = -\frac{ir}{2}(d\varphi)[(Z,\bar{W})] = 0$$

[by (A3) and $(Z,\bar{W})\in T(\mathcal{F})\otimes\mathbb{C}$]. Hence $\nabla_T L_\theta=0$. Finally [by (A18)]

$$(\nabla_N L_\theta)(Z,\bar{W}) = -2rg_\theta(Z,\bar{W}) + (\mathcal{L}_N g_\theta)(Z,\bar{W}), \quad Z,W \in T_{1,0}(\mathcal{F}),$$

and $\nabla_N L_\theta=0$ follows from (A23) in Lemma 124 below.

Lemma 4: *The following identities hold for any* $X\in T(\mathcal{F})$:

$$T_\nabla(N,X) = rX + \tau(\phi X) + \theta(X)(\phi\nabla^H r + rT), \tag{A21}$$

$$[N,\phi X] - \phi[N,X] = 2\tau(X) - \theta(X)\nabla^H r, \tag{A22}$$

Moreover

$$(\mathcal{L}_N g_\theta)(X,Y) = 2rg_\theta(X,Y) + 2(\mathrm{d}\theta)[X,\tau(Y)], \tag{A23}$$

for any $X,Y\in H(\mathcal{F})$.

Proof: (A21) follows from (A7). Let us replace X by ϕX in (A21)

$$\nabla_N\phi X - (N,\phi X) = r\phi X - \tau(X)$$

and subtract the identity got from (A21) by applying ϕ to both sides. Since $\nabla\phi=0$ we obtain (A22). The proof of (A23) is a consequence of (A4) and (A22), and the Jacobi identity

$$(\mathcal{L}_N g_\theta)(X,Y) = N[(\mathrm{d}\theta)(X,\phi Y)] - (\mathrm{d}\theta)[(N,X),\phi Y] + 2(\mathrm{d}\theta)[X,\tau(Y)] - (\mathrm{d}\theta)[X,(N,\phi Y)]$$

$$= -\frac{1}{2}N\{\theta[(X,\phi Y)]\} + \frac{1}{2}\theta\{[(N,X),\phi Y]\} + 2(\mathrm{d}\theta)[X,\tau(Y)] + \frac{1}{2}\theta\{[X,(N,\phi Y)]\}$$

$$= -\frac{1}{2}N\{\theta[(X,\phi Y)]\} - \frac{1}{2}\theta\{[(X,\phi Y),N]\} - \theta\{[X,\tau(Y)]\} = -(\mathrm{d}\theta)[N,(X,\phi Y)]$$

$$-\theta\{[X,\tau(Y)]\} = -r\theta[(X,\phi Y)] - \theta\{[X,\tau(Y)]\}$$

$$= 2r(\mathrm{d}\theta)(X,\phi Y) + 2(\mathrm{d}\theta)[X,\tau(Y)] = 2rg_\theta(X,Y) + 2(\mathrm{d}\theta)[X,\tau(Y)].$$

Theorem 4 is proved. Q.E.D.

As to the local calculations, if φ_β^α are the connection 1 forms of the Graham–Lee connection (i.e., $\nabla W_\beta = \varphi_\beta^\alpha \otimes W_\alpha$) then we may look for $\mathrm{d}\theta^\alpha$ in the form

$$\mathrm{d}\theta^\alpha = B_{\beta\gamma}^\alpha \theta^\beta \wedge \theta^\gamma + B_{\beta\bar{\gamma}}^\alpha \theta^\beta \wedge \theta^{\bar{\gamma}} + B_{\bar{\beta}\bar{\gamma}}^\alpha \theta^{\bar{\beta}} \wedge \theta^{\bar{\gamma}} + (B_\beta^\alpha \theta^\beta + B_{\bar{\beta}}^\alpha \theta^{\bar{\beta}}) \wedge \theta + (C_\beta^\alpha \theta^\beta + C_{\bar{\beta}}^\alpha \theta^{\bar{\beta}}) \wedge \mathrm{d}\varphi$$
$$+ D\,\mathrm{d}\varphi \wedge \theta. \tag{A24}$$

Indeed, applying this identity to the pair (W_β, W_γ) [respectively, to $(W_\beta, W_{\bar{\gamma}})$ and (W_β, T)] gives

$$B_{\beta\gamma}^\alpha - B_{\gamma\beta}^\alpha = \varphi_\beta^\alpha(W_\gamma) - \varphi_\gamma^\alpha(W_\beta), \quad B_{\beta\bar{\gamma}}^\alpha = \varphi_\beta^\alpha(W_{\bar{\gamma}}), \quad B_\beta^\alpha = \varphi_\beta^\alpha(T).$$

Similarly [applying (A24) to $(W_{\bar{\beta}}, T)$, (W_β, N), and $(W_{\bar{\beta}}, N)$ respectively]

$$B_{\bar{\beta}}^\alpha = -A_{\bar{\beta}}^\alpha, \quad C_\beta^\alpha = \frac{1}{2}[\varphi_\beta^\alpha(N) - r\delta_\beta^\alpha], \quad C_{\bar{\beta}}^\alpha = \frac{i}{2}A_{\bar{\beta}}^\alpha.$$

Finally [by (A5)]

$$D\,\mathrm{d}\varphi(N) = 2(\mathrm{d}\theta^\alpha)(N,T) = -\theta^\alpha[(N,T)] = iW^\alpha(r).$$

Summing up

$$\mathrm{d}\theta^\alpha = \theta^\beta \wedge \varphi_\beta^\alpha - i\partial\varphi \wedge \tau^\alpha + \frac{i}{2}W^\alpha(r)\mathrm{d}\varphi \wedge \theta + \frac{r}{2}\mathrm{d}\varphi \wedge \theta^\alpha, \tag{A25}$$

where $\tau^\alpha \equiv A_{\bar{\beta}}^\alpha \theta^{\bar{\beta}}$.

Given a linear connection ∇ on V we set $\alpha(X,Y) \equiv \Pi\nabla_X Y$, for any $X, Y \in T(\mathcal{F})$. If ∇ is the Graham–Lee connection then (by the proof of Theorem 4) $\alpha = 0$. One may identify, as usual, the normal bundle $\nu(\mathcal{F}) = T(V)/T(\mathcal{F})$ with $\mathbb{R}N$. If $\Pi^\perp : T(V) \to T(\mathcal{F})$ is the projection, let us set $\nabla^{\mathcal{F}} \equiv \Pi^\perp \nabla$. It is easily seen that $\nabla^{\mathcal{F}}$ is the Tanaka–Webster connection of each M_δ (i.e., the pointwise restriction of the Graham–Lee connection to a leaf of $\mathcal{F}$ is the Tanaka–Webster connection of the leaf). In particular $\tau : T(\mathcal{F}) \to T(\mathcal{F})$ is the pseudohermitian torsion of each leaf [hence $g_\theta(\tau X, Y) = g_\theta(X, \tau Y)$, for any $X, Y \in T(\mathcal{F})$].[9,20,31–33]

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The use of quadratic forms in the calculation of ground state electronic structures

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There are many examples in theoretical physics where a fundamental quantity can be considered a quadratic form $\rho=\Sigma_i\rho_i=|\Psi|^2$ and the corresponding linear form $\Psi=\Sigma_i\psi_i$ is highly relevant for the physical problem under study. This, in particular, is the case of the density and the wave function in quantum mechanics. In the study of N-identical-fermion systems we have the additional feature that Ψ is a function of the $3N$ configuration space coordinates and ρ is defined in three-dimensional real space. For many-electron systems in the ground state the wave function and the Hamiltonian are to be expressed in terms of the configuration space (CS), a replica of real space for each electron. Here we present a geometric formulation of the CS, of the wave function, of the density, and of the Hamiltonian to compute the electronic structure of the system. Then, using the new geometric notation and the indistinguishability and equivalence of the electrons, we obtain an alternative computational method for the ground state of the system. We present the method and discuss its usefulness and relation to other approaches. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2229423]

I. INTRODUCTION

Since the creation of wave quantum mechanics, in 1926, the calculation of the electronic structure of a many electron system, in its ground state, or near it, is an open subject. This central problem, with no exact analytic solution, has been studied from many points of view. When the study is to be used for the analysis of atoms, molecules, or condensed matter a first useful approximation is to solve the many electron Schrödinger equation for the system. This implies the use of the Coulomb potential of a configuration of nuclei as external potentials and of the electron-electron interaction potentials to a desired degree of accuracy. In this paper, after a brief review of the basic problem for a many electron system in a molecule, we start a systematic analysis of the problem using an accurate formulation, compatible with the initial conditions of the calculation, and through a systematic, geometric algebra based, definition of the configuration space, of the external potentials, of the one electron operators for a many electron system and of the electron-electron interaction terms, we arrive at a formal equation for the total energy. From this, using the fact that we are interested either in the ground state or in stationary states near the ground state, we formulate a variational problem from which a set of tractable equations, which self-consistently define the many electron wave function and density, is obtained. Finally we compare our resulting formalism with the more widely used procedures, showing that those methods are contained as special cases of ours.

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The basic approach for the calculation of the ground state electronic structures of atoms, molecules, and solids[1–3] considers the steady state Born-Oppenheimer approximation: a fixed given configuration of positively charged point-like nuclei, the so-called "structure" of the molecule, cluster, or crystal. The computational procedure involves the simultaneous calculation of: the N electron ground state electronic wave function Ψ_N a function of $3N$ coordinates, the (ground state) electronic density $\rho_N(x)$ a function of three coordinates, the total electronic energy E_N for the N electrons, a set of $M \geqslant N$ auxiliary spin-orbitals φ (called the SO), and the SO-energy eigenvalues ε_a. A minimum set of N auxiliary functions is required by Pauli's exclusion principle. The SO and the ε_a are important as far as they are related to the different type of response functions of the electronic system and as such to the set of its spectroscopic properties. The electronic density, wave function, SO, and ε_a are not observable in themselves but, through several spectroscopies, they can be studied as indirect observables. Point-contact spectroscopy and other recent techniques (see Ref. 4, and references therein) are good examples of such tools. The computational techniques can also be extended to time dependent[5,6] and to beyond Born-Oppenheimer[7] cases. In these approaches the electron is defined as a physical entity which obeys the Dirac equation for the electron's experimental mass and charge, the nonrelativistic limit of the Dirac equation is given by the Schrödinger equation if the spin of the electron is considered for magnetic interactions and for statistics.

Recently we have shown that there is a new, geometrical, starting point for formulating a mathematical theory for the density and for the related wave function,[8–12] we call KKW. There is a resulting methodology developed here.

In the calculation of the stationary ground state of the many electron (many indistinguishable equivalent fermions in general) wave function and densities a variational approach optimizes the solutions with respect to desirability criteria, in our case, the lowest ground state energy E. The variational procedure provides a suitable set of constants and a set of auxiliary functions. For computational method $\mathcal{M}$ of lowest ground state energy $E=\int \bar{\Psi}\hat{H}_{\mathcal{M}}\Psi dV$ we should consider the variation of a functional

$$\delta\left(\left[\int \bar{\Psi}\hat{H}_{\mathcal{M}}\Psi \mathrm{d}V - E\right] - \mu\left[\int \bar{\Psi}\Psi dV - N\right]\right) = 0, \tag{1}$$

where the second square parentheses impose the condition that this is an N electron system. Note that both $\bar{\Psi}\hat{H}_{\mathcal{M}}\Psi = \mathcal{E}(x)$ and $\bar{\Psi}\Psi = \rho_N(x)$ imply a projection into real space.

The basic formulation can be summarized as follows: to the N equivalent electron system, in real space $x \subset \mathbb{R}^3$, in volume V, obeying the Pauli's exclusion principle, corresponds an *analytical finite non-negative* total density function $\rho_N(x)$ such that the total electronic energy $E = \int \varepsilon \rho_N(x) \mathrm{d}V$ is well defined in the system's volume. To fulfill this condition there should exist a many electron *analytical square integrable* wave function $\Psi_N(\{x_n\}; n=1,\ldots,N)$ with $\{x_n\} \subset (\mathbb{R}^3)^N$ such that $\rho_N(x) \doteq |\Psi_N|^2 = \bar{\Psi}\Psi = \Sigma_{c=1}^{N}\rho_c(x) = \Sigma_{u=1}^{M\geqslant N}\rho_u(x)$.

Notice that two different expansions of the density are used simultaneously: one $(\Sigma_{c=1}^{N}\rho_c(x))$ is the description of the N equivalent electrons in the system, the second $(\Sigma_{u=1}^{M\geqslant N}\rho_u(x))$ describes the shell structure (M atomic or molecular orbitals). This generates a matrix of descriptions: one description, the shell structure, corresponds to the $M \geqslant N$ columns and the other, the per equivalent electron contribution, to the N rows of the matrix.

We have also indicated that this Hermitian square should be describable as either a sum of non-negative, finite analytical functions $\rho_c(x) = |\psi_c|^2$, one equivalent ψ_c for each electron in the system, or (to be able to agree with the Pauli's principle) as a sum of $M \geqslant N$, weighted by $w_u = |b_u|^2$, spin-orbital ϕ_u contributions $\rho_u(x) = |b_u\phi_u|^2$. This ensures that the physical conditions, which must be obeyed by the wave function itself and by the density, are fulfilled. In the case of the many electron (fermion) system *all N electrons* (*fermions*) *are equivalent*. The "system" to be studied is such that no electron can be distinguished by position. This equivalence requires that the density itself should be describable as a sum of N equal densities $\rho_{\text{one electron}}(x)$ which should be generated by equivalent contributions. That is $\rho_{\text{one electron}}(x) = 1/N\Sigma_u\rho_u(x)$. The many-electron

wave function $\Psi_N(\{x_n\};n=1,\ldots,N)$ should be used to compute the total energy and other properties of this ground state of the system. Historically the Hartree-Fock method (and its complement configuration interaction) fulfilled the conditions above.

What is needed is to find the analytical, possible complex, function $\mathbf{\Psi}(\{x_n\})$ of a set $\{x_n;n=1,\ldots,N\}$ of N coordinates which allows the factorization of a *finite non-negative* function

$$\rho(x)=\mathbf{\Psi}^{\dagger}(\{x_n\})\hat{N}(x,\{x_n\},\{x_n'\})\mathbf{\Psi}(\{x_n'\})\subset\mathbb{R}^{+}$$

(the real numbers $\mathbb{R}=\{\mathbb{R}^{-},0,\mathbb{R}^{+}\}$ are either negative, zero or positive). Here $\hat{N}(x,\{x_n\},\{x_{n'}\})=\Sigma_{nn'}\delta x_n x_n',\delta x x_n$ is a projector from configuration space X into the real space coordinates x.

In the KKW theory (all relevant points are presented in the following) the basic idea is that the density appears as a sum of densities and then the wave function Ψ_N should both be the square root of the total density function $\rho(x)=\Sigma_u\rho_u(x)$ and also provide the square root ϕ_u of each one of the contributions $\rho_u(x)$ to the total density. For this we require the use of geometric (multivector analysis) techniques. In fact the problem is similar to that of finding the linear form (geometric square root) $\mathbf{d}=a\mathbf{e}_1+b\mathbf{e}_2+c\mathbf{e}_3+\cdots$, which corresponds to the quadratic form $d^2=a^2+b^2+c^2+\cdots\subset\mathbb{R}^{+}$. Here $\mathbf{d}$ is the *geometric square root* of the scalar quantity d^2.

For a positive definite function $\rho(x)=\mathbf{d}^{\dagger}(x)\mathbf{d}(x)\subset\mathbb{R}^{+}$ an ordinary (scalar) square root $d(x)=\sqrt{\mathbf{d}^{\dagger}(x)\mathbf{d}(x)}=\sqrt{a^2(x)+b^2(x)+c^2(x)+\ldots}$ is not necessarily *analytical*, whereas the geometric square root function $\mathbf{d}(x)=a(x)\mathbf{e}_1+b(x)\mathbf{e}_2+c(x)\mathbf{e}_3+\cdots$, through the use of an *analytical* set ϕ of auxiliary complex functions $\phi=\{a(x),b(x),c(x),\ldots\}\subset\mathbb{C}$, can be demanded to be *analytical*. The Hermitian squares $\{a^2(x),b^2(x),c^2(x),\ldots\}\subset\mathbb{R}^{+}$. The analyticity property allows that a set of differential equations $\hat{D}a(x)=\epsilon_a a(x)$, $\hat{D}b(x)=\epsilon_b b(x),\ldots$, which incorporates physical and mathematical boundary conditions can be found.

The geometric square root. There is a freedom to choose for the description of the shell structure the most convenient anticommuting normalized basis set $\{\alpha_u,|\alpha_u|^2=1;$ and $\alpha_u\alpha_v=-\alpha_v\alpha_u,\ u\neq v,\ u,v=1,\ldots,M\geqslant N\}$.

Otherwise, as the electrons are equivalent, we will also need a symmetrized form of $\mathbf{d}$. For this purpose we will simultaneously introduce a second (one basis element per electron) anticommuting normalized basis set $\{\omega_i^S,|\omega_i^S|^2=1;$ and $\omega_i^S\omega^S j=-\omega_j^S\omega_i^S,\ j\neq i,\ i=1,\ldots,N\}$ and a normalized vector $\underline{\mathbf{S}}=\sqrt{1/N}(\omega_1^S+\omega_2^S+\omega_3^S+\cdots+\omega_N^S)$ where our definitions imply that $(\sqrt{1/N}(\omega_1^S+\omega_2^S+\omega_3^S+\cdots+\omega_N^S))^2=\underline{\mathbf{S}}^2=1$. The ω_i^S, therefore $\underline{\mathbf{S}}$, are defined to commute with the α_u. Consider $\mathbf{d}=(b_1\alpha_1+b_2\alpha_2+b_3\alpha_3+\cdots+b_M\alpha_M)\underline{\mathbf{S}}$, then $d^2=\Sigma_i|b_i|^2$. There is a double summation: over the basis set $\{\alpha_u\}$ and over the per electron in the system set $\{\omega_i^S\}$. The summations can be interchanged. This is what is called the geometric procedure as used in the following. The algebra of the $\{\alpha_u\}$ or of the $\{\omega_i^S\}$ is a Grassmann-Clifford algebra (see Refs. 10–12). Although there is no need to define a vector scalar-product we will define in the following an equivalent procedure to simplify the reading of the equations.

II. GEOMETRIC FORMULATION OF THE CALCULATION OF THE STATIONARY GROUND STATE OF A MANY-ELECTRON SYSTEM

Here we present the formalism for the calculation of the stationary ground state of the many electron (many equivalent fermions in general) wave function and densities and the corresponding variational approach.

A. Configuration space and real space

A basic concept in the study of a many-electron system (N interacting fermions) is, from the above-noted considerations, the simultaneous, repeated, use of real space (the space of the observer) for each one of the fermions of the system: configuration space. Then, if $\mathbf{x}$ represents a point in real space, it is customary to represent by $\mathbf{X}=\{\mathbf{x}_a;a=1,\ldots,N\}\}$ the set of points in the configuration space $\mathbf{X}$ for N fermions.

The volume integral $\int d\Omega$ when referred to the coordinates of fermion a is denoted by $\int d\Omega_a$. Also $\int d\Omega_N$ indicates the integration over all N space replicas $\int d\Omega_a$. In the formal notation to follow we introduce an integration operator $\int \widehat{d\Omega_N}$ to denote that repeated space integration for all N electrons is to be performed. Also $\int \widehat{d\Omega_{N-i}}$ to denote that the repeated space integration for all N electrons except the ith is to be performed. The absolute value of the distance between two fermion points $x_{ab}=|\mathbf{x}_b-\mathbf{x}_a|$.

Here and in the rest of our presentation we use a geometric notation

$$\mathbf{X}=\sum_a \omega_a \mathbf{x}_a;\{a=1,\ldots,N;\omega_a\omega_b=-\omega_b\omega_a, b\neq a\}, \tag{2}$$

introducing the per electron operator ω_a and, also, the projection operators $\bar{\omega}_a$ such that $\bar{\omega}_a\omega_b=\delta_{ab}$ selecting the part of the configuration space which corresponds to electron a; this is $\bar{\omega}_a\mathbf{X}=\mathbf{x}_a$.

This construction allows a clear formal definition of the electrons involved in each part of the calculation. Our geometric procedure introduces one feature of the statistics of the fermion system from the beginning because the interchange $\omega_a \leftrightarrow \omega_b$ in the products $\omega_a\omega_b$ for two electrons, in any given expression, will change the sign of the corresponding terms.

When the argument of a function is position, for $a=1$ for example, we will also use a nonbold notation or the fermion's numeral, say $\phi(\mathbf{x}_1)\doteq\phi(x_1)=\phi(1)$, as equivalent argument.

B. Basic principles

The Principles implied without further discussion in this paper are the same as those of the so-called *ab initio* approaches:[1]

- The total energy is a functional of the wave function.
- The possibility of using the Schrödinger equation for the N electron system. The kinetic energy is the sum of independent-electron-like kinetic energies for each electron.
- The ground state of the many electron system corresponds to the lowest total energy.
- The Pauli exclusion principle requires that the description for N electrons, included in the wave function, contains the occupancy of at least $M\geqslant N$ pseudo-electron orthonormal spin-orbitals ϕ_u.
- The equivalency and indistinguishability of the electrons require that all electrons are equivalently described.
- The operators acting on the ϕ_u are: multiplicative operators (constant, variable, and self-consistent variable functions, differential (the Laplace operator $\nabla^2_{(x_u)}$, in our case) and the integral operators $\int \widehat{d\Omega_u}$ defined earlier.
- A variational approach can be used.

The electronic structure calculation of a many electron system in the ground state requires then the simultaneous calculation of: the ground state electronic wave function Ψ_N, the (ground state) electronic density $\rho_N(x)$, the total electronic energy E_N for the N electrons, a set of $M\geqslant N$ auxiliary spin-orbitals (SO), and the SO-energy eigenvalues ϵ_a. A minimum set of N functions is required by Pauli's principle.

From $\rho(\mathbf{x})=\bar{\Psi}\Psi$ both quantities, wave function $\Psi(\mathbf{X})$ and density $\rho(\mathbf{x})$ could be considered as the fundamental variable, provided that derivatives of $\rho(\mathbf{x})$ are considered derivatives of $\bar{\Psi}\Psi$.

In our theory the density appears as a sum of densities and then the wave functions $\{\bar{\Psi},\Psi\}$ should together:

(1) be a factorization of the total density $\rho(x)=\Sigma_{n=1}^{N}\rho_{\text{one electron}}(x)=\Sigma_{i=1}^{M}\rho_i(x)=|\Psi|^2$, the first equality from the equivalence of the electrons, and
(2) provide the square root of each one of the M shell structure contributions $\rho_i(x)=|b_i\phi_i|^2$ to the total density.

C. The energy calculation

We rewrite the usual expression for the total nonrelativistic electronic energy operator or Hamiltonian $\hat{H}_0$ in correspondence with our formal definition of configuration space (an atomic electron structure is used in the following to simplify the notation, otherwise a summation Σ_A and the relative distances x_{aA} should be used in the electron-nucleus potential energy). We use the above-defined per electron geometric notation $\{\omega_b, \bar{\omega}_b\}$ to select, from the wave function Ψ_N^{KKW} and its conjugate $\overline{\Psi_N^{\mathrm{KKW}}}$, the corresponding contributions. A *per electron* operator is an *effective one-body* operator.

We consider first the per electron "a" kinetic energy operator

$$-\omega_a(\hbar^2\nabla^2_{(x_a)}/2m_e)\bar{\omega}_a$$

and the electron a to nucleus A (considered at the origin of coordinates) potential energy operator $-\omega_a(Z_Ae^2/|x_a|)\bar{\omega}_a$. The sum of the contributions of these two terms will be called "core" energy in the following.

Second, the pairwise Coulomb interaction $V^{\mathrm{Coul}}_{e-e,}$ between the electrons: a half of the sum over all a, of the for electron "a" in the pair a,b, electron-electron potential energy, we have

$$V^{\mathrm{Coul}}_{e-e} = \frac{1}{2}\sum\nolimits_{a=1}^{N} \omega_a \int \widehat{\mathrm{d}\Omega_{N-a}} \sum_{b\neq a} \left(\omega_b \frac{e^2}{|x_{ab}|}\bar{\omega}_b \right)\bar{\omega}_a$$

(notice that after performing the indicated $\int \widehat{\mathrm{d}\Omega_{N-a}}$ integration for all $b\neq a$ each term has been reduced to a per electron operator).

Then

$$\hat{H}_0 = \sum\nolimits_{a=1}^{N} \omega_a \left[-\frac{\hbar^2\nabla^2_{(x_a)}}{2m_e} - \frac{Z_Ae^2}{|x_a|} + \frac{1}{2}\int \widehat{\mathrm{d}\Omega_{N-a}} \sum_{b\neq a}^{N} \left(\omega_b \frac{e^2}{|x_{ab}|}\bar{\omega}_b \right) \right]\bar{\omega}_a. \tag{3}$$

Correspondingly, the wave function Ψ_N^{KKW} is (first in a per electron $n\subset N$ basis and second in a per orbital $i\subset M$ description, using the geometric operators α_i per auxiliary basis function ϕ_i (SO) with weight b_i, obeying $\alpha_i\alpha_j=-\alpha_j\alpha_i$, $j\neq i$, and the projection operators $\bar{\alpha}_i\alpha_j=\delta_{ij}$):

$$\Psi_N^{\mathrm{KKW}} = \sum_{n=1}^{N} (\omega\psi)_n, \tag{4}$$

$$\text{where } (\omega\psi)_n = \omega_n \left[\sum_{i=1}^{M\geqslant N} b_i\alpha_i\phi_i(x_n) \right], \tag{5}$$

$$\text{and} \quad \overline{\Psi_N^{\mathrm{KKW}}} = \sum_{n=1}^{N} (\bar{\psi}\varpi)_n, \tag{6}$$

$$\text{where } (\bar{\psi}\varpi)_n = \left[\sum_{i=1}^{M\geqslant N} b_i^*\bar{\alpha}_i\phi_i^*(x_n) \right]\varpi_n, \tag{7}$$

with normalization

$$N = \int \overline{\Psi_N^{\mathrm{KKW}}}\Psi_N^{\mathrm{KKW}}\mathrm{d}\Omega_N \doteq \sum_{c=1}^{N} \int \{\overline{\Psi_N^{\mathrm{KKW}}}\omega_c\bar{\omega}_c\Psi_N^{\mathrm{KKW}}\mathrm{d}\Omega_c\}, \tag{8}$$

and, when written in terms of the auxiliary spin-orbitals ϕ_i,

$$N = N \int \bar{\psi}\psi \mathrm{d}\Omega = N \sum_{i=1}^{M \geqslant N} \int \phi_i^* b_i^* \overline{\alpha_i} \alpha_i b_i \phi_i \mathrm{d}\Omega = N \sum_{i=1}^{M \geqslant N} |b_i|^2 \int |\phi_i|^2 \mathrm{d}\Omega \doteq N \sum_{i=1}^{M \geqslant N} |b_i|^2 \langle i|i\rangle. \quad (9)$$

In this paper we assume equal number of spin up and spin down electrons, the spin restricted case. The second line in (8), from the definition of $\int \mathrm{d}\Omega_N$ in Sec. II A is an identity. In (9) we use the orthonormality generated by $\overline{\alpha_i}\alpha_j = \delta_{ij}$.

Note that a double set of Grassmann (anticommuting) numbers $\{\omega_a; \alpha_i\}$ has been introduced, this has an analytical analogue in the determinants of the *ab initio* methods where either the exchange of columns or of rows change the sign of the determinant. Formally the wave function Ψ could be represented by a rectangular $M \times N$ matrix with entries $\alpha_i \omega_a$. The second line in (4) would correspond to the (real positive number) trace of $\bar{\Psi}\Psi$. Exchange terms will arise from (4) when used in (3). The ϕ_i's are defined to form an orthonormal set of spin-orbitals $\langle i|j\rangle \equiv \int \phi_i^* \phi_j \mathrm{d}\Omega = \delta_{ij}\delta_{s_i}^{s_j}$. The $\delta_{s_i}^{s_j}$ ensures that the spin of i and j are the same, this is superfluous here but will be used in the following. We introduce the normalization $\Sigma_i |b_i|^2 = 1$, then the one electron density $\rho_1(\mathbf{x}) = \bar{\psi}(\mathbf{x})\psi(\mathbf{x}) = \Sigma_i |b_i|^2 \phi_i^*(\mathbf{x})\phi_i(\mathbf{x})$.

In (3) the Hamiltonian $\hat{H}_0$ for electron n: $H^{\mathrm{core}}(x) + H^{\mathrm{interaction}}(x)$ where the second term is an effective local one-electron operator, even if the electron repulsion, being dependent on the inter-electron distance, is a two-electron (i for n, j for m) operator. The resulting potential is the same for all components of ψ.

D. Core energy

Rewrite the first two terms in (3) as $\Sigma_{c=1}^{N} \omega_c \hat{H}^{\mathrm{core}}(c)\bar{\omega}_c$, then

$$E_{\mathrm{core}} = \sum_{c=1}^{N} \int \bar{\Psi}\{\omega_c \hat{H}^{\mathrm{core}}(c)\bar{\omega}_c\}\Psi \mathrm{d}\Omega_c = \sum_{c=1}^{N} \int \sum_{d'} \bar{\omega}_{d'} \bar{\psi}_{d'}(\mathbf{x}_{d'})\{\omega_c \hat{H}^{\mathrm{core}}(c)\bar{\omega}_c\} \times \sum_{d} \omega_d \psi_d(\mathbf{x}_d)\mathrm{d}\Omega_c, \quad (10)$$

and from (5) and (7), orthonomality and equivalence:

$$E_{\mathrm{core}} = N \int \bar{\psi}_1(\mathbf{x}_1)\hat{H}^{\mathrm{core}}(1)\psi_1(\mathbf{x}_1)\mathrm{d}\Omega_1 = N \int \sum_i |b_i|^2 \phi_i^* \hat{H}^{\mathrm{core}} \phi_i \mathrm{d}\Omega. \quad (11)$$

The above-mentioned $\{\omega_c, \varpi_c\}$ and the $\{\alpha_i, \overline{\alpha_i}\}$ have selected the sum of the diagonal elements in (10). Note that the shell structure cannot be avoided.[8,9]

E. Electron-electron interaction energy

For the electron-electron interaction (e-e)

$$E^{e\text{-}e} = \int \overline{\Psi_N^{\mathrm{KKW}}} \sum\nolimits_a \omega_a \times \left[\frac{1}{2} \sum_{b \neq a}^{N} \int \left(\omega_b \frac{e^2}{|x_{ab}|} \bar{\omega}_b \right) \mathrm{d}\Omega_b \right] \bar{\omega}_a \Psi_N^{\mathrm{KKW}} \mathrm{d}\Omega_a. \quad (12)$$

Here, from the equivalence of the N electrons, we have N equal pairwise $\{1 \Leftrightarrow 2\}$ contributions which consider all spin-orbitals. Using the expansion of the ψ, we obtain

$$E^{e\text{-}e} = \frac{N}{2} \int \int \sum_i \phi_i^*(1) b_i^* \bar{\alpha}_i \sum_j \phi_i^*(2)\bar{\alpha}_j \frac{e^2}{|x_{12}|} \times \sum_k \phi_i(2)\alpha_k \sum_l \phi_i(1)\alpha_l \mathrm{d}\mathbf{\Omega}_1 \mathrm{d}\Omega_2. \quad (13)$$

Considering the property $\bar{\alpha}_i \alpha_j = \delta_{ij}$ there are three types of e-e terms:
(I) $j=k$ and $i=l$ which gives

$$\frac{N}{2}\int\left\{\sum_i \int\left[\sum_{j\neq i}|b_j|^2|\phi_j(2)|^2\frac{e^2}{|x_{12}|}\right]\mathbf{1}(x_2)\mathrm{d}\Omega_2\times|b_i|^2|\phi_i(1)|^2\right\}\mathbf{1}(x_1)\mathrm{d}\Omega_1$$
$$=\frac{N}{2}\sum_i\sum_{j\neq i}|b_j|^2|b_i|^2(ij,ij)=\frac{N}{2}E_{\mathrm{I}}, \tag{14}$$

where we have introduced the notation (ij,ij) for the integrals, as they are "Coulomb integrals" in the accepted electronic structure calculation language. Also the formal local unit factor $\mathbf{1}(x)=\bar{\psi}(x)\psi(x)/\rho_1(x)$ will be fundamental to perform the variational procedure in the following to find the effective equations for the $\psi(x)$. Note that the $\mathbf{1}(x)$ appear twice in this term, this will result in a factor 2 in the variational wave equation.

(II) $j=l\neq i$ and $i=k$ (the $\delta^{s_j}_{s_i}$ from spin orthonormality, and one change of sign from the interchange $\alpha_i\alpha_j=-\alpha_j\alpha_i$ is needed!)

$$-\frac{N}{2}\sum_{i,j\neq i}\delta^{s_j}_{s_i}|b_j|^2|b_i|^2\times\int\int\left[\phi^*_j(1)\phi^*_i(2)\frac{e^2}{|x_{12}|}\phi_i(1)\phi_j(2)\right]\mathrm{d}\Omega_2\mathbf{1}(x_1)\mathrm{d}\Omega_1$$
$$=-\frac{N}{2}\sum_{i,j\neq i}\delta^{s_j}_{s_i}|b_j|^2|b_i|^2(ji,ij)=\frac{N}{2}E_{\mathrm{II}}, \tag{15}$$

where we have used the notation $\delta^{s_j}_{s_i}(ji,ij)$ for the integrals, as they are "exchange integrals" corresponding to the $[i,j]$ pair of spin-orbitals in the accepted electronic structure calculation language; the $\delta^{s_j}_{s_i}$ requires $s_i=s_j$ and ensures that the product $\phi^*_j(1)\phi_i(1)$ of the SO, with spin s_i and s_j, respectively, is not null. We use again the formal local unit factor $\mathbf{1}(x)$.

(III) Null terms, all others, where $(i\neq l$ and $i\neq k)$ or $(j\neq l$ and $j\neq k)$.

E_{I} and E_{II} also contribute to the formal interpretation of the Pauli exclusion principle: first a given electron is not interacting with itself and, second, there is an "exchange" term for fermions, where from $\alpha_i\alpha_j=-\alpha_j\alpha_i$ a negative sign appears.

III. VARIATION OF THE TOTAL ENERGY WITH RESPECT TO THE $\bar{\psi}$

Here we consider the total energy in terms of the ψ as noted earlier. From the normalization (9) the per electron density is $\rho_{\text{one-electron}}(x)=\bar{\psi}(x)\psi(x)$ and the total density $N\rho_{\text{one-electron}}(x)$.

We write the total energy

$$E_{\text{total}}=E_{\text{core}}+\frac{N}{2}(E^{e\text{-}e}_{\mathrm{I}}+E^{e\text{-}e}_{\mathrm{II}}). \tag{16}$$

For the *core* term

$$E_{\text{core}}/N=\int\bar{\psi}_1(\mathbf{x}_1)\hat{H}^{\text{core}}(1)\psi_1(\mathbf{x}_1)\mathrm{d}\Omega_1, \tag{17}$$

the variation with respect to $\bar{\psi}_1(\mathbf{x}_1)$ gives

$$\hat{H}^{\text{core}}(1)\psi_1(\mathbf{x}_1)=\left\{-\frac{\hbar^2\nabla^2_{(1)}}{2m_e}-\frac{Z_Ae^2}{|\mathbf{x}_1|}\right\}\psi_1(\mathbf{x}_1). \tag{18}$$

For the variation of $E^{e\text{-}e}_{\mathrm{I}}/2$ with respect to $\bar{\psi}_1(\mathbf{x}_1)$ we obtain, defining

$$V_{\mathrm{I}}(\mathbf{x}_1)=\sum_i\left\{\frac{|b_i|^2|\phi_i(\mathbf{x}_1)|^2}{\rho_1(\mathbf{x}_1)}\times\int\left[\sum_{j\neq i}|b_j|^2|\phi_j(2)|^2\frac{e^2}{|x_{12}|}\right]\right\}\mathrm{d}\Omega_2, \tag{19}$$

and, considering that the factor $\mathbf{1}(\mathbf{x}_k)$ appears twice in (14), the repulsive electron-electron term

$$2\tfrac{1}{2}V_{\mathrm{I}}(\mathbf{x}_1)\bar{\psi}_1(\mathbf{x}_1) = V_{\mathrm{I}}(\mathbf{x}_1)\bar{\psi}_1(\mathbf{x}_1). \tag{20}$$

Finally for the variation of $E_{\mathrm{II}}^{e\text{-}e}/2$ with respect to $\bar{\psi}_1(\mathbf{x}_1)$ we obtain (assuming here, for simplicity not as a restriction in the method, to avoid introducing summations over spin coordinates, equal number of spins "up" and "down"), defining

$$V_{\mathrm{II}}(\mathbf{x}_1) = -\sum_{i,j\neq i}\frac{\delta_{s_i}^{s_j}|b_j|^2|b_i|^2}{2\rho_1(\mathbf{x}_1)} \times \int\left[\phi_j^*(1)\phi_i^*(2)\frac{e^2}{|x_{12}|}\phi_i(1)\phi_j(2)\right]\mathrm{d}\Omega_2, \tag{21}$$

the "attractive-like functions interchange" electron-electron term

$$V_{\mathrm{II}}(\mathbf{x}_1)\bar{\psi}_1(\mathbf{x}_1). \tag{22}$$

A. The KKW auxiliary equations

The variational procedure has been carried with respect to the $\bar{\psi}$'s, to obtain the formal equation which describes any electron n in the system (reminder ψ is a vectorial sum of functions ϕ_i). We collected the different terms of $\int\Psi_N^\dagger\hat{H}_0\Psi_N\mathrm{d}\Omega$ from (11) to (15) as in (16), and performed the variation with respect to $\bar{\psi}(x)$, as shown in the previous section. We obtain all together an effective Hamiltonian $\widehat{H^{\mathrm{KKW}}}$ eigenvalue equation

$$\widehat{H^{\mathrm{KKW}}}\psi(x) = \mu\psi(x),$$

$$\widehat{H^{\mathrm{KKW}}} \equiv \left\{-\frac{\hbar^2\nabla^2}{2m_e} - \frac{Ze^2}{|\mathbf{x}|} + V_{\mathrm{I}}(\mathbf{x}) + V_{\mathrm{II}}(\mathbf{x})\right\}. \tag{23}$$

This is not yet a practical equation. Use now the expansion of the ψ in terms of the ϕ for a further reduction. Write (23) as

$$\widehat{H^{\mathrm{KKW}}}\sum_{i=1}^{M\geqslant N} b_i\alpha_i\phi_i(x_n) = \mu\sum_{i=1}^{M\geqslant N} b_i\alpha_i\phi_i(x_n), \tag{24}$$

apply on both sides the projector $\bar{\alpha}_i$ to obtain the practical equations for the set of auxiliary orthonormal functions ϕ_i (from $\bar{\alpha}_i\psi=b_i\phi_i$),

$$\widehat{H^{\mathrm{KKW}}}\phi_i = \varepsilon_i\phi_i. \tag{25}$$

Finally we obtain, by left multiplication with $\bar{\psi}$ of (23), integration and the normalization $\langle\psi|\psi\rangle = 1$, $\langle\phi_i|\phi_i\rangle = 1$, a relation between the μ and the ε_i's given by $\mu=\Sigma_i\varepsilon_i|b_i|^2=\bar{\varepsilon}$, that is: μ in (23) is the weighted average eigenvalue.

B. A more familiar and practical form of the auxiliary wave equations

We can rewrite the electron-electron interaction energy in a computationally more practical form (related to the *ab initio* methods.[1]) Consider

$$E^{e\text{-}e} = \frac{N}{2}\{E_{\mathrm{I}} + E_{\mathrm{II}}\},$$

and rewrite as

$$\Rightarrow \frac{N}{2}\int \bar{\psi}(x_1)\{E_{\mathrm{Coul}}(\mathbf{x}_1)+E_{\mathrm{XC}}(\mathbf{x}_1)\}\psi(x_1)\mathrm{d}\Omega_1,$$

obtained if, in the above-presented definitions, the "self-Coulomb" integrals $|b_i|^2(ii,ii)$ are added to remove the condition $j\neq i$, to E_{I}. The "self-exchange" integrals $-|b_i|^2(ii,ii)$ are added to remove the condition $j\neq i$, to E_{II}. [The E_{II} is now as in the formally equivalent considerations of the first part of the Slater (1951) idea,[13] which here is no longer an approximation.] Then

$$\widehat{H^{\mathrm{KKW}}}\equiv\left\{-\frac{\hbar^2\nabla^2}{2m_e}-\frac{Ze^2}{|\mathbf{x}|}+V_{\mathrm{Coul}}(\mathbf{x})+V_{\mathrm{xc}}(\mathbf{x})\right\},$$

$$V_{\mathrm{Coul}}(\mathbf{x}_1)=N\int\left[\rho(2)\frac{e^2}{|x_{12}|}\right]\mathrm{d}\Omega_2,$$

$$V_{\mathrm{xc}}(\mathbf{x}_1)=-\frac{N}{\rho(\mathbf{x})}\sum_{i,j}\delta^{s_j}_{s_i}|b_j|^2|b_i|^2\times\int\left[\phi_j^*(1)\phi_i^*(2)\frac{e^2}{|x_{12}|}\phi_i(1)\phi_j(2)\right]\mathrm{d}\Omega_2. \tag{26}$$

By substitution of (26) in (25)

$$\left\{-\frac{\hbar^2\nabla^2}{2m_e}-\frac{Ze^2}{|\mathbf{x}|}+V_{\mathrm{Coul}}(\mathbf{x})+V_{\mathrm{xc}}(\mathbf{x})\right\}\phi_i(\mathbf{x})=\varepsilon_i\phi_i(\mathbf{x}). \tag{27}$$

Reminder $\widehat{H^{\mathrm{KKW}}}$ is the same for all ϕ_i's.

The total energy is obtained by direct integration of the set of equations (27) multiplied on the left by $\Sigma_i|b_i|^2\phi_i^*$ and comparing with (16):

$$E[\Psi]=\sum_i|b_i|^2\varepsilon_i-\frac{E_{\mathrm{Coul}}}{2}-\int V_{\mathrm{XC}}(\mathbf{x})\rho(\mathbf{x})\mathrm{d}\Omega+E_{\mathrm{XC}} \tag{28}$$

(we must remember that E_{Coul} and E_{XC} include the "self-Coulomb" and the "self-exchange," respectively).

With additional variational constants b_{ij} defined through $b_i=\sqrt{(1-\Sigma_{j>N}b_{ij})/N}$ for $i\leqslant N$ and $b_j=\sqrt{\Sigma_{i\leqslant N}b_{ij})/N}$ $j>N$, we obtain a (twice) variational procedure to obtain a set $\{b_{ij}\}$ and the ϕ_i. A secular determinant can be constructed and solved. If the basis $\{\phi_i\}$ is large enough a time-dependent formulation with $\Delta V(t)$ can be constructed where $b_i\Rightarrow b_i(t)$ and the $b_{ij}\Rightarrow b_{ij}(t)$ describe induced transitions.

Finally the basic definition for the total energy $E=E[\bar{\psi}(x)\psi(x)]$ of N ***equivalent*** carriers (electrons), can be *formally* written in terms of the density $N\bar{\psi}(x)\psi(x)$ defining

$$E_{\mathrm{core}}=N\int\left[\sum_i\frac{|b_i|^2\phi_i^*(\mathbf{x}_1)\hat{H}^{\mathrm{core}}\phi_i(\mathbf{x}_1)}{\rho_1(\mathbf{x}_1)}\right]\times\bar{\psi}(\mathbf{x}_1)\psi(\mathbf{x}_1)\mathrm{d}\Omega_1=N\int\varepsilon^{\mathrm{core}}(\mathbf{x}_1)\bar{\psi}(\mathbf{x}_1)\psi(\mathbf{x}_1)\mathrm{d}\Omega_1. \tag{29}$$

$$E=N\int\{\varepsilon^{\mathrm{core}}(\mathbf{x}_1)+\varepsilon^{\mathrm{inter}}(\mathbf{x}_1)\}\bar{\psi}(x)\psi(x)\mathrm{d}\Omega_1, \tag{30}$$

and, considering $E=N\int\varepsilon\bar{\psi}(x)\psi(x)\mathrm{d}\Omega_1$, we define

$$\varepsilon^{\mathrm{core}}(\mathbf{x}_1)+\varepsilon^{\mathrm{inter}}(\mathbf{x}_1)=\varepsilon.$$

IV. THE PROPERTIES OF THE WAVE FUNCTION: CONCLUSIONS

The KKW wave function describes a system of N electrons with an expansion based on $M \geqslant N$ auxiliary, mutually orthogonal functions, solutions of the same "KKW" Hamiltonian. The complete wave function, then the one density, is directly optimized and not each auxiliary function at a time.

From the many possibilities to construct the ψ it is useful to choose the one presented here because the eigenvalues ε_i, by construction the rate of change of the total energy with respect to occupation of the "i" spin-orbital, are an approximation to the removal energy of one electron, from that ϕ_i, in the system. Also because the SO functions, being related to the response function of the system, have become observables.

- The KKW method offers a complete variational solution to the problem of finding the wave function and simultaneously the energy of the ground state of the N electron system.
- To find the limit for the ground state energy of the system the number of auxiliary functions to be considered is $M > N$. The practical approach to this calculation will be twice variational, first in the sense that the auxiliary functions are found from the variation of a functional, and second because the weight of the contributions of the set of $M > N$ functions requires a set of variational parameters to be found.
- The new method systematically includes the kinetic and the potential energy for all the $M \geqslant N$ auxiliary functions. It has the advantage that all spin-orbitals are simultaneously optimized. An alternative would be to obtain $M' > N$ functions from the results for $M = N$ and, in a second step, the best possible b_{ij} for the M' case.
- The calculations can include the use in the Hamiltonian of selective pairwise interaction terms

$$(\Delta V_{e\text{-}e})_{ab} = \omega_a \omega_b (\Delta V_{mn}) \bar{\omega}_b \bar{\omega}_a,$$

  allowing the description of pair-correlations of any origin: magnetic, or electron-phonon or from any other indirect type. Also specific one spin-orbital cases $(\Delta V)_a = \omega_a (\Delta V_a) \bar{\omega}_a$. This being a further advantage of the geometric notation.
- The self-consistent solution requires, in general, numerical solutions. Nevertheless all analytic and computational methodologies in usual practice can be used without major changes.

Comparison with previous methodologies: Conclusions. In practice several features made the, now known as the Hartree-Fock method (HF[2,3]), the reference for atomic, molecular, and ground state condensed matter calculations: it is a formally correct variational procedure based on the use of a determinant of auxiliary functions for which a differential equation is deduced within the method. It includes (through the basic properties of the Slater determinant) the Pauli exclusion principle as well as the indistinguishability of equivalent fermions. HF is also a suitable starting calculation for establishing the procedure known as configuration interaction (CI), introducing a set of variational constants, when the spin-orbitals resulting from the HF calculation are used to construct a formally complete wave function as a sum of mutually orthogonal Slater determinants. The standard definition of "exchange energy" and of "correlation energy" is given in relation to the HF+CI procedures. In the determinants no two-electron-relative-coordinates functions are used, neither in these approaches nor in the one described earlier.

Another widely used methodology, based on the density functional theory (DFT) a correct formal procedure itself,[14,15] can be considered as related to HF+CI as the standard calculations include local density functionals for the exchange and correlation energies and potentials.

The methodology developed here shares both all the favorable features of the HF+CI method and the advantages of the DFT procedure. This suggests that there should be a relation among all three procedures HF+CI, DFT, and KKW.

- The KKW method ($M = N$) requires the self-consistent solution of N differential equations,

as in DFT, unlike the HF which is an $N\times N$ formulation. Compared to the *ab initio* techniques, our methodology employs a simpler set of equations.

- If, as in the HF method, using $M=N$, each auxiliary function were to be optimized separately one at a time in a self-consistent set, from our expressions (16) for the total energy, we go back to the HF procedure and results. Our method has the advantage that the complete set is optimized simultaneously to search for the lowest total energy.
- The KKW method in the minimum auxiliary functions procedure is equivalent to the Slater (1951) average exchange proposal (with the so-called "exact" exchange) and in fact transforms this Slater "approximation" into a nonapproximate procedure where all auxiliary functions are optimized simultaneously. This is independent of the DFT approximation for E_{XC}.
- The formal structure of the new method enriches the methodology of the DFT by showing that the Slater exchange and the Kohn-Sham procedures are formally integrated to the general scheme and also because an N-electron wave function Ψ, which is required in the theorems of the formal DFT theory, is constructed and used within the formalism.

The KKW approach also shows, from the different analysis presented here, DFT both as an *ab initio* and as a first principles method. This is an important formal contribution of our study.

In the following we quote standard use of the so called *ab initio* and DFT methods, see, for example Refs. 1, 16, and 17.

Computationally there is no need to consider a self-Coulomb energy. As all electrons have equivalent descriptions, with the same density per electron, there is an exact resultant factor $((N-1)/N)$ in the electron-electron Coulomb interaction. It is basic for the calculation of the hydrogen atom. It is dominant in the calculation of the helium atom where each of the two electrons interact with the other but not with itself, and progressively less important for larger systems where the interchange part of the interaction grows. Standard DFT programs[18,19] for atomic electronic structure calculations are easily modified, an $(N-1)/N$ factor in the Coulomb potential, replacement of the exchange-correlation and total energy subroutines, to solve the KKW equations (27). As a numerical test the relativistic program "David"[19] was adapted, the H atom calculation used as a first check of the numerical procedures, the He atom with $M=N$, the Hartree-Fock limit for the Coulomb interaction, and the He atom with $(1s,2s,2p)$ for the $M>N$ case, beryllium and krypton in the $M=N$ as further tests. All results are acceptable in the limit of the corresponding approximations (Hartree atomic units):

Atom	E_{total}	E_{HF}	E_{DFT}	E_{exp}
H	−0.5	−0.5	⋯	−0.5
He	−2.886	−2.864	−2.867	−2.90
Be	−14.603	−14.573	−14.592	−14.673
Ne	−128.87	−128.55	−128.62	−128.94
Kr	−2799.49	−2796.72	−2787.80	⋯

In our analysis we have gone beyond complex algebra and calculus, in fact we have gone to the more general domain of the Grassmann-Clifford algebra and analysis.

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Contractivity of positive and trace-preserving maps under L_p norms

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We provide a complete picture of contractivity of trace preserving positive maps with respect to p-norms. We show that for $p>1$ contractivity holds in general if and only if the map is unital. When the domain is restricted to the traceless subspace of Hermitian matrices, then contractivity is shown to hold in the case of qubits for arbitrary $p\geqslant 1$ and in the case of qutrits if and only if $p=1, \infty$. In all noncontractive cases best possible bounds on the p-norms are derived. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218675]

I. INTRODUCTION

This article addresses the following question: *Given a positive and trace preserving linear map T between matrix spaces, when is T contractive with respect to the p-norm, with* $1\leqslant p\leqslant\infty$.

This problem has come up in several contexts in recent years. For instance, Olkiewicz,[1] in his investigation of the superselection structure of dynamical semigroups, needs as a starting point the fact that a 2-positive map that is contractive with respect to both the trace and operator norm is also contractive with respect to the Hilbert-Schmidt norm. The same result is needed by Raginsky[2] in his study of entropy production of a quantum channel. In the context of quantum information this question arose again in Ref. 3, in the study of entanglement measures. It is shown there that any distance (in the space of matrices) that is contractive under completely positive trace preserving maps gives rise to a "suitable" entanglement measure. Their conjecture that the Hilbert-Schmidt norm is such a distance was disproved shortly thereafter by Ozawa in Ref. 4. In Ref. 5, Nielsen stated (without proof) that the Hilbert-Schmidt distance is contractive in the space of qubits, with respect to any completely positive trace preserving map. He also encouraged further study of this problem. Recently, the fact that a completely positive trace preserving map is contractive with respect to the trace norm was used in Ref. 6 in the context of condensed matter theory in a theoretical justification for the high accuracy of renormalization group algorithms.

Motivated by the appearance of the previous question in so many different areas of physics, we will try in this note to give a complete picture of the solution. We will first study the general case and then restrict the domain of the maps to the traceless hyperplane.

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II. THE GENERAL CASE

In the following $\mathcal{M}_n$ will denote the space of $n\times n$ matrices. A linear map $T:\mathcal{M}_n\to\mathcal{M}_r$ is called *positive* if it maps positive semidefinite matrices to positive semidefinite matrices, *trace preserving* if $\mathrm{tr}\,T(A)=\mathrm{tr}\,A$ for all $A\in\mathcal{M}_n$, and *unital* if $T(\mathbb{1})=\mathbb{1}$. It is easy to see that T is trace preserving if and only if its adjoint $T^*:\mathcal{M}_r\to\mathcal{M}_n$ is unital, and that T is positive if and only if T^* is positive.

The p-norm (we will assume always $1\leqslant p\leqslant\infty$) of a matrix A is defined as $(\mathrm{tr}|A|^p)^{1/p}=(\Sigma_i\lambda_i^p)^{1/p}$, where the λ_i are the singular values of A (i.e., the eigenvalues of $|A|\equiv\sqrt{A^*A}$). We write $\mathcal{S}_p^n$ for $\mathcal{M}_n$ endowed with the p-norm. For $T:\mathcal{M}_n\to\mathcal{M}_r$, we use $\|T\|_{p-p}$ to denote the operator norm of T when we consider the p-norm in both the original and the final space, i.e., $\|T\|_{p-p}=\sup_{A\in\mathcal{M}_n}(\|T(A)\|_p/\|A\|_p)$. T is called *contractive* under the p-norm if $\|T\|_{p-p}\leqslant 1$. Our first result is

Theorem 2.1: *If $T:\mathcal{M}_n\to\mathcal{M}_r$ is positive and trace preserving, then $\|T\|_{p-p}\leqslant n^{1-1/p}$.*

Moreover, the bound $n^{1-1/p}$ is attained when T is the the trace operator $\mathrm{tr}:\mathcal{M}_n\to\mathbb{C}$ (which is completely positive and trace preserving).

The main ingredient in the proof is a noncommutative version of the Riesz-Thorin theorem. (See Ref. 7 or Sec. IX.4 of Ref. 8.) We will also use a theorem of Russo and Dye (Ref. 9, Corollary 2.9).

Theorem 2.2 (Noncommutative Riesz-Thorin): *If $T:\mathcal{M}_n\to\mathcal{M}_r$ is a linear map, then*

$$\|T\|_{p-p}\leqslant\|T\|_{1-1}^{1/p}\|T\|_{\infty-\infty}^{1-1/p}.$$

Theorem 2.3 (Russo-Dye). *If $T:\mathcal{M}_n\to\mathcal{M}_r$ is positive, then $\|T\|_{\infty-\infty}=\|T(\mathbb{1})\|_\infty$.*

Proof. To prove Theorem 2.1, first note that under its hypotheses, T^* is positive and unital. Then Theorem 2.3 implies that $\|T^*\|_{\infty-\infty}=\|T^*(\mathbb{1})\|_\infty=\|\mathbb{1}\|_\infty=1$. Hence, using the duality $(S_1^n)^*=S_\infty^n$, we can conclude that $\|T\|_{1-1}=1$. Moreover, $\|T\|_{\infty-\infty}=\|T(\mathbb{1})\|_\infty\leqslant\|T(\mathbb{1})\|_1=\|\mathbb{1}\|_1=n$. Combining these bounds with Theorem 2.2 gives the claimed result. □

We used the fact that when T is trace preserving, then T positive implies $\|T\|_{1-1}=1$. In Ref. 9, Proposition 2.11 it is shown that for T trace preserving, T is positive if and only if $\|T\|_{1-1}=1$.

When T is positive, trace preserving and unital the argument used to prove Theorem 2.1 shows that $\|T\|_{1-1}=\|T\|_{\infty-\infty}=1$. Then Theorem 2.2 implies that T is contractive for all p-norms. The next Theorem shows that this is an equivalence.

Theorem 2.4: *If $T:\mathcal{M}_n\to\mathcal{M}_n$ is positive and trace preserving, the following are equivalent*:

(i) $\|T(\mathbb{1})\|_p\leqslant n^{1/p}$ *for some* $1<p\leqslant\infty$;
(ii) *T is unital*;
(iii) *T is contractive for the p-norm for every* $1\leqslant p\leqslant\infty$; and
(iv) *T is contractive for the p-norm for some* $1<p\leqslant\infty$.

Proof. It only remains to prove that (i)⇒(ii). To do this, let $(\lambda_i)_{i=1}^n$ denote the eigenvalues of $T(\mathbb{1})$. Since T is positive, $\lambda_i\geqslant 0$; and since T is trace-preserving, $\Sigma_i\lambda_i=\mathrm{tr}\,T(\mathbb{1})=\mathrm{tr}\,\mathbb{1}=n$. Hölder's inequality can then be used to conclude that $\Sigma_i\lambda_i^p\geqslant n$ with equality if and only if $\lambda_i=1$ for all i. But, by assumption, $\|T(\mathbb{1})\|_p\leqslant n^{1/p}$ for some $p>1$. Thus, we must have equality so that $T(\mathbb{1})=\mathbb{1}$.□

The hypothesis that T is both unital and trace preserving can only be satisfied when $r=n$. In that case, when T is trace preserving, but not unital, it follows that $\|T\|_{p-p}>1$. When $n\neq r$, this does not hold, i.e., there are non-unital trace-preserving completely positive maps $T:\mathcal{M}_n\to\mathcal{M}_r$ for which $\|T\|_{p-p}<1$. To see this one needs Jencova's result[10] that $\|T\|_{p-p}=\omega_p(T^C)$ where $\omega_p(T)$ is the completely bounded $1\to p$ norm studied in Ref. 11 and T^C denotes the conjugate or complementary channel defined in Refs. 12 and 13. From the results in Ref. 11 one can find depolarizing channels T_{dep} such that $\omega_p(T_{\mathrm{dep}})<1$. To see this let $\mu=1/(n+1)$ in Eq. (5.4) in Ref. 11. Since $\mu=1/(n+1)$ is the boundary between depolarizing channels which are entanglement breaking and those which are not, this yields examples in both classes. As the conjugate T_{dep}^C is *not* unital,[13] we have explicit examples of non-unital trace-preserving completely positive maps $T:\mathcal{M}_n\to\mathcal{M}_{n^2}$ for which $\|T\|_{p-p}<1$.

The implication (ii)⇒(iii) was proved using complex interpolation. For $p=2$, one can obtain

an elementary proof by using that $\|T\|_{2-2}^2$ is the largest eigenvalue of $T^*\circ T$ considered as an operator on the Hilbert space $\mathcal{M}_n$ with inner product $\langle A,B\rangle=\mathrm{tr}\,A^*B$. When T is both trace-preserving and unital, $\mathbb{1}$ is an eigenvector with eigenvalue 1, and the orthogonality of eigenvectors implies that $\mathrm{tr}\,G=\mathrm{tr}\,\mathbb{1}G=0$ for any other eigenvector G (which we can assume is Hermitian without loss of generality). Now let G be one of these eigenvectors and let ω be the largest real number for which $\mathbb{1}+\omega G$ is positive semi-definite. Since $T^*\circ T$ is also positive, $(T^*\circ T)(\mathbb{1}+\omega G)=\mathbb{1}+\lambda\omega G\geqslant 0$. But this implies that $\lambda\leqslant 1$ by the definition of ω so that $\|T^*\circ T\|_\infty=1$.

III. THE TRACELESS HYPERPLANE

Using the p-norm to measure the distance between density matrices, gives expressions of the form $\|\rho-\rho'\|_p$, where $\rho-\rho'$ is a Hermitian matrix with trace 0. In this section we investigate the behavior of such distances under positive and trace preserving maps. Let $T|_{\mathcal{H}_0}$ denote the restriction of T to the hyperplane $\mathcal{H}_0$ of traceless Hermitian matrices.

Theorem 3.1. *Let $T:\mathcal{M}_n\to\mathcal{M}_n$ be a positive trace preserving linear map. Then*

$$\|T|_{\mathcal{H}_0}\|_{p-p}\leqslant\begin{cases}\left(\dfrac{n}{2}\right)^{1-1/p}, & n \text{ even}\\ \left(\dfrac{2^{2-p}}{(n-1)^{1-p}+(n+1)^{1-p}}\right)^{1/p}, & n \text{ odd}\end{cases}.$$

Moreover, this bound is optimal, as there exists a completely positive trace preserving map that saturates the inequality.

Proof. We begin by proving the upper bound. For an arbitrary positive trace preserving map $T:\mathcal{M}_n\to\mathcal{M}_n$, consider A Hermitian, traceless and with $\|A\|_p\leqslant 1$. We can write $A=A_+-A_-$ with A_+ and A_- both positive semi-definite and $A_+A_-=0$. As T is positive, $[T(A)]_+\leqslant T(A_+)$ and $[T(A)]_-\leqslant T(A_-)$. Then,

$$\|T(A)\|_p^p=\mathrm{tr}|T(A)|^p=\mathrm{tr}([T(A)]_+)^p+\mathrm{tr}([T(A)]_-)^p=\|[T(A)]_+\|_p^p+\|[T(A)]_-\|_p^p\leqslant\|T(A_+)\|_p^p+\|T(A_-)\|_p^p.$$

Call $r=\mathrm{range}(A_+)$ and $s=\mathrm{range}(A_-)$ and denote the eigenvalues of A_+ and A_- by $\lambda_1,\ldots,\lambda_r$ and $\mu_1,\ldots,\mu_s$, respectively. It follows from Theorem 2.4 that $\|T(A_+)\|_p^p\leqslant r^{p-1}\|A_+\|_p^p$ and $\|T(A_-)\|_p^p\leqslant s^{p-1}\|A_-\|_p^p$. Using Lagrange multipliers in the problem

$$\text{maximize}\left\{r^{p-1}\sum_{i=1}^{r}\lambda_i^p+s^{p-1}\sum_{i=1}^{s}\mu_i^p\right\}$$

restricted to

$$\sum_{i=1}^{r}\lambda_i^p+\sum_{i=1}^{s}\mu_i^p=1,$$

$$\sum_{i=1}^{r}\lambda_i-\sum_{i=1}^{s}\mu_i=0$$

one finds that at least one of the following two conditions is satisfied: $\lambda_i=\lambda_j$ and $\mu_i=\mu_j$ for every i,j, or $s=r$.

In the first case we have that [assuming now without loss of generality that $\mathrm{tr}(A_+)=1$]

$$\frac{\|T(A)\|_p^p}{\|A\|_p^p}\leqslant\frac{2}{r^{1-p}+s^{1-p}}.$$

This is in turn maximized and leads to the inequality in Theorem 3.1 if $s=n-r$ and $r=n/2$ for even n, and $r=(n+1)/2$ for odd n respectively. In the second case $r=s$ we have that

$$\|T(A)\|_p^p \leqslant r^{p-1}(\|A_+\|_p^p + \|A_-\|_p^p),$$

yielding the sought inequality for $r=n/2$ (even n); whereas $r<n/2$ does not lead to a new inequality.

To prove optimality of the bound above, consider the completely positive and trace preserving map $T:\mathcal{M}_n\to\mathcal{M}_n$ given by

$$T(A) = |0\rangle\langle 0|\mathrm{tr}[PA] + |1\rangle\langle 1|\mathrm{tr}[(\mathbb{1}-P)A],$$

where P is a projector of dimension $d=\mathrm{tr}\,P$. If we apply this map to a traceless Hermitian operator of the form $A=P-(d/(n-d))(\mathbb{1}-P)$ we obtain

$$\frac{\|T(A)\|_p}{\|A\|_p} = \left(\frac{2d^p}{d+d^p(n-d)^{1-p}}\right)^{1/p}.$$

This achieves the above bound if $d=n/2[d=(n+1)/2]$ for n even (odd). □

Any trace-preserving map can be written uniquely in the form $T(A)=N\,\mathrm{tr}(A)+T_1(A)$ where $T_1(A)$ is a unital trace-preserving map and $N=(1/d)[T(\mathbb{1})-\mathbb{1}]$ is traceless. If T_1 is also positive, it follows from Theorem 2.4, that $\|T|_{\{\mathrm{tr}=0\}}\|_{p-p}\leqslant 1$ and we can drop the restriction to Hermitian matrices. Unfortunately, the previous results demonstrate that even when T is positive and trace preserving, T_1 need not be positive.

A. Maps on qubits

When $n=2$, Theorem 3.1 implies contractivity in the traceless subspace of Hermitian matrices, i.e., $\|T|_{\mathcal{H}_0}\|_{p-p}=1$. Here, however, there is no need to restrict to Hermitian matrices. For qubits, T positive and trace preserving implies that the previous map T_1 is always positive.

Theorem 3.2. *For any positive trace preserving linear map* $T:\mathcal{M}_2\to\mathcal{M}_2$ and $1\leqslant p\leqslant\infty$ *we have that*

$$\max_{\mathrm{tr}(A)=0,\|A\|_p=1} \|T(A)\|_p \leqslant 1.$$

Proof. The theorem is proved by showing that the T_1 defined above is indeed positive. Consider the action of T on a density operator $\rho=\frac{1}{2}(\mathbb{1}+w\cdot\sigma)$ represented as a vector $w\in\mathbb{R}^3$ on the Bloch sphere. Any trace preserving and positive linear map acts as

$$T(\mathbb{1}+w\cdot\sigma) = \mathbb{1} + [r+Rw]\cdot\sigma,$$

where $r\in\mathbb{R}^3$ and R is a real 3×3 matrix. T is positive iff $\|w\|_2\leqslant 1$ implies $\|r+Rw\|_2\leqslant 1$. Let λ be the largest singular value of R. Then there are unit vectors $u,w\in\mathbb{R}^3$ such that $Rw=\lambda u$. As $R(-w)=\lambda(-u)$, one can choose the sign of w such that $r\cdot u\geqslant 0$, and thus $1\geqslant\|r+\lambda u\|_2\geqslant\lambda$. This implies that the unital trace preserving map $T_1(\mathbb{1}+w\cdot\sigma):=\mathbb{1}+[Rw]\cdot\sigma$ is indeed positive, and the result follows from Theorem 2.4. □

B. The case of qutrits

Theorem 3.1 still implies contractivity in $\mathcal{H}_0$ for the case $n=3$ if $p=1$ or $p=\infty$ (whereas this fails for $1<p<\infty$). As in the case of qubits one might expect that the result for $p=\infty$ also extends to non Hermitian matrices. This is, however, not the case. A simple counterexample is given by the map

$$T(A) = \sum_{i=0}^{1}\langle i|A|i\rangle|0\rangle\langle 0| + \langle 2|A|2\rangle|1\rangle\langle 1|,$$

acting on $A=a_0|0\rangle\langle 0|+a_1|1\rangle\langle 1|+a_2|2\rangle\langle 2|$, where a_0,a_1,a_2 are the three complex cubic roots of unity. In this case we have that $\mathrm{tr}(A)=0$, $\|A\|_\infty=1$, but $\|T(A)\|_\infty>1$.

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Contraction of broken symmetries via Kac-Moody formalism

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I investigate contractions via Kac-Moody formalism. In particular, I show how the symmetry algebra of the standard two-dimensional Kepler system, which was identified by Daboul and Slodowy as an infinite-dimensional Kac-Moody loop algebra, and was denoted by $\mathbb{H}_2$, gets reduced by the symmetry breaking term, defined by the Hamiltonian $H(\beta)=(1/2m)(p_1^2+p_2^2)-\alpha/r-\beta r^{-1/2}\cos((\varphi-\gamma)/2)$. For this $H(\beta)$ I define two symmetry loop algebras $\mathfrak{L}_i(\beta)$, $i=1,2$, by choosing the "basic generators" differently. These $\mathfrak{L}_i(\beta)$ can be mapped isomorphically onto subalgebras of $\mathbb{H}_2$, of codimension two or three, revealing the reduction of symmetry. Both factor algebras $\mathfrak{L}_i(\beta)/I_i(E,\beta)$, relative to the corresponding energy-dependent ideals $I_i(E,\beta)$, are isomorphic to $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ for $E<0$ and $E>0$, respectively, just as for the pure Kepler case. However, they yield two different nonstandard contractions as $E\to 0$, namely to the Heisenberg-Weyl algebra $\mathfrak{h}_3=\mathfrak{tw}_1$ or to an Abelian Lie algebra, instead of the Euclidean algebra $\mathfrak{e}(2)$ for the pure Kepler case. The above-noted example suggests a general procedure for defining generalized contractions, and also illustrates the "*deformation contraction hysteresis*," where contraction which involves two contraction parameters can yield different contracted algebras, if the limits are carried out in different order. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2234726]

I. INTRODUCTION

In 1926 Pauli[1] obtained the energy levels of the relativistic hydrogen atom algebraically, by using the conserved angular-momentum $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ and the Hermitian form of the Laplace-Runge-Lenz vector

$$\mathbf{A}=\frac{1}{2}[\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p}]-m\alpha\hat{\mathbf{r}}. \tag{1}$$

The commutation relations among their components are given by

$$\begin{aligned}
&[L_i,L_j]=i\hbar\epsilon_{ijk}L_k, \quad i,j,k=1,2,3,\\
&[L_i,A_j]=i\hbar\epsilon_{ijk}A_k,\\
&[A_i,A_j]=-i2mH\hbar\epsilon_{ijk}L_k,
\end{aligned} \tag{2}$$

where H is the Hamiltonian of the nonrelativistic three-dimensional (3D) hydrogen atom. The commutation relations in (2) do not define a closed algebra, since the H on the right-hand side of (2) is an *operator* and not a number. To nevertheless obtain closed algebras physicists for 70 years

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have replaced the Hamiltonian H by its eigenvalues E, and thus obtained three different identifications of the symmetry algebra of the hydrogen atom, namely $\mathfrak{so}(4)$, $\mathfrak{so}(3,1)$ and $\mathfrak{e}(3)$, for $E<0$, $E>0$ and $E=0$, respectively.[2] The same conclusion can be reached by formally "normalizing" the Runge-Lenz vector $\mathbf{A}$ by dividing it by $\sqrt{2m|H|}$, but the resulting quotient vector becomes infinite for $H=0$.

Instead of the above-noted "conventional procedure," Daboul and Slodowy[3] showed that one can obtain a single closed algebra based on the commutation relations (2). This algebra is spanned by the following infinite set of generators:

$$\mathbb{H}_3 := \{h^n L_i, h^n A_i | i=1,2,3, n=0,1,\ldots\}, \quad \text{where } h := -2mH. \tag{3}$$

The algebra $\mathbb{H}_3$ and its generalizations $\mathbb{H}_N$, the symmetry algebras of the N-dimensional hydrogen atom, were identified[3,4] as positive loop algebras of twisted or untwisted Kac-Moody algebras,[5,6] for N odd or even, respectively. They were called the *hydrogen algebras*. The above-mentioned formalism will be reviewed in Sec. II, and applied to $\mathbb{H}_2$, the hydrogen algebra of the standard two-dimensional (2D) Kepler system, defined by the Hamiltonian H_0 of Eq. (5).

The algebras $\mathbb{H}_N$ depend on the Hamiltonian H, but *not* on its energy eigenvalues E. However, one can reproduce the usual three corresponding finite-dimensional algebras, $\mathfrak{so}(N+1)$, $\mathfrak{so}(N,1)$, and $\mathfrak{e}(N)$, as factor algebras $\mathbb{H}_N/I(E)$ relative to energy-dependent ideals $I(E)$; The ideals and factor-algebra formalism will be discussed and applied to $\mathbb{H}_2$ in Sec. II A.

In the present paper I investigate *what happens to the algebra* $\mathbb{H}_2$ *and its factor algebra, if the original symmetry of the 2D hydrogen atom is broken*. In particular, I shall study the following Hamiltonian:

$$H := H_0 - \beta r^{-1/2} \cos\left[\tfrac{1}{2}(\varphi-\gamma)\right] \quad (\gamma=0 \text{ in the present paper}), \tag{4}$$

where H_0 is the Hamiltonian of the two-dimensional Kepler problem

$$H_0 := \frac{1}{2m}(p_1^2+p_2^2) - \frac{\alpha}{r} = \frac{1}{2m}\left(p_r^2 + \frac{p_\varphi^2}{r^2}\right) - \frac{\alpha}{r}. \tag{5}$$

Throughout this paper I shall set the phase angle γ in (4) equal to zero, since it can always be removed by appropriate choice of the coordinate system (see, however, the discussion in Sec. V).

The Hamiltonian (4) has an interesting history: It was discovered by Winternitz *et al.*[7] already in 1967 in their systematic search for super-integrable systems. It was also derived in a more general complex form by Sen [Ref. 8, Eq. (3.14)] in 1987.

The symmetry of (4) was originally studied by Gorringe and Leach[9] in 1993 and recently reviewed by Leach and Flessas—Ref. 10, Sec. §3.3 (see also Ref. 11). The above-noted authors followed the conventional method and found that the symmetry algebras of (4) are $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ for $E<0$ and $E>0$, exactly as for the pure 2D Kepler problem (5). However, for $E=0$ they obtained the Heisenberg-Weyl algebra $\mathfrak{h}_3=\mathfrak{w}_1$ [which they denoted by $W(3,1)$],[9,10] instead of the Euclidean algebra $\mathfrak{e}(2)$ for the Kepler case (5).

This result was intriguing, since the symmetry breaking does not affect the symmetry for $E\neq 0$, and only affect it for $E=0$. And I wondered whether and how the above type of symmetry breaking can be treated via the Kac-Moody formalism. It turned out that the symmetry algebra of (4) can be treated, via the Kac-Moody formalism, similar to the pure Kepler case, with some important modifications. For example, it is possible to describe the symmetry algebra of (4) by two loop algebras, $\mathfrak{L}_1$ and $\mathfrak{L}_2$, depending on the choice of the "*basic generators*." It is remarkable that these two algebras can be mapped onto subalgebras of $\mathbb{H}_2$ of codimension two and three, i.e., $\mathbb{H}_2$ is larger than these image subalgebras by only two and three generators, out of infinitely many. The "missing" generators are manifestations of the symmetry breaking.

Moreover, I will show that the factor algebras $\mathfrak{L}_i/I_i(E,\beta)$ relative to the corresponding energy-

TABLE I. The three factor algebras $\mathbb{H}_2/I(E)$ and $\mathfrak{L}_i/I_i$ of the loop algebras $\mathbb{H}_2$ and $\mathfrak{L}_i$ relative to the corresponding energy-dependent ideals $I(E)$ and $I_i(E,\beta)$. For $E\neq 0$ all three factor algebras are isomorphic to $\mathfrak{so}(3)$ for $E<0$ and to $\mathfrak{so}(2,1)$ for $E>0$, but yield *different contractions* for $E\to 0$.

Hamiltonian	Factor algebra	$E<0$	$E=0$	$E<0$
H_0 in (5)	$\mathbb{H}_2/I(E)$	$\mathfrak{so}(3)$	$\mathfrak{e}(2)$	$\mathfrak{so}(2,1)$
H in (4)	$\mathfrak{L}_1(\beta)/I_1(E,\beta)$	$\mathfrak{so}(3)$	$\mathfrak{h}_3=\mathfrak{w}_1$	$\mathfrak{so}(2,1)$
H in (4)	$\mathfrak{L}_2(\beta)/I_2(E,\beta)$	$\mathfrak{so}(3)$	R^3	$\mathfrak{so}(2,1)$

dependent ideals yield different types of *contractions*,[12–14] which are included in Table I. This result is important, since the contraction procedure for the above-noted specific system can be generalized to other algebras, as discussed in Sec. VI.

In Sec. II I review Inönü-Wigner contraction and its generalization and in Sec. III I review the construction of the hydrogen algebra $\mathbb{H}_2$ for the pure 2D Kepler problem (5). In Secs. IV and V I construct two loop algebras $\mathfrak{L}_1$ and $\mathfrak{L}_2$ for the system (4) and their factor algebras $\mathfrak{L}_i/I_i(E,\beta)$. In Sec. VI I map the $\mathfrak{L}_i$ onto subalgebras $\mathbb{H}_2$, and as I already noted, I shall suggest a general procedure for defining contraction via Kac-Moody formalism and then give some conclusions.

II. REVIEW OF GENERALIZED INÖNÜ-WIGNER CONTRACTION

There are many formulations of contractions.[12,13] I shall give my own definition and notation:

Definition: Let $\mathfrak{g}:=\langle X_a, C_{ab}^c\rangle$ be a finite-dimensional Lie algebra with a basis X_a, $a=1,2,\ldots,N$ and structure constants C_{ab}^c, and let the parameter-dependent Lie algebra $\mathfrak{g}^\epsilon := \langle X_a^\epsilon, C_{ab}^c(\epsilon)\rangle$ be defined, such that the one-to-one linear map f_ϵ between $\mathfrak{g}$ and $\mathfrak{g}^\epsilon$,

$$f_\epsilon:\mathfrak{g}\mapsto\mathfrak{g}^\epsilon,\quad f_\epsilon(X_a)=\epsilon^{-n_a}X_a^\epsilon, \tag{6}$$

is an isomorphism of Lie algebras as long as $\epsilon\neq 0$. If the powers n_a satisfy the condition,

$$n_a+n_b\geqslant n_c \tag{7}$$

then the limit algebra $\mathfrak{g}^0=\langle X_a^0, C_{ab}^c(0)\rangle$ with the structure constants

$$C_{ab}^c(0):=\lim_{\epsilon\to 0} C_{ab}^c(\epsilon)$$

exists and it is called the *contracted algebra*. I shall refer to $\mathfrak{g}^\epsilon$ as the *contracting algebra* and to its generators X_a^ϵ as the *contracting generators*.

It is important to emphasize that X_a^ϵ and X_a^0 *denote the generators of the Lie algebras* $\mathfrak{g}^\epsilon$ *and* $\mathfrak{g}^0$ *which are defined via the structure constants* $C_{ab}^c(\epsilon)$ *and* $C_{ab}^c(0)$, *respectively*. Therefore, the X_a^0 *are not to be regarded as the limits of* X_a^ϵ *for* $\epsilon\to 0$. Thus, the X_a^0 *always* exist, by definition, as generators of the contracted algebra $\mathfrak{g}^0$, even though representations $r(X_a^\epsilon)$ of $\mathfrak{g}^\epsilon$ might exist with some of the generators having vanishing limits, i.e., $\lim_{\epsilon\to 0} r(X_b^\epsilon)=0$. Such representations could be called *not saved or unsaved*. Otherwise, they are called *saved representations*.[15] Actually in Sec. V I shall give a realization of a saved representation of an algebra whose contraction yields an Abelian algebra, i.e., $C_{ab}^c=0$ for all a,b,c. For this contraction even the adjoint representation[13] is not saved.

Usually X_a is used also to denote the contracting and contracted generators X_a^ϵ and X_a^0.[13] This convention is probably used to avoid confusing X_a^0 as the limit of X_a^ϵ for $\epsilon\to 0$. To distinguish the algebras $\mathfrak{g}^\epsilon$ from $\mathfrak{g}$ and $\mathfrak{g}^0$ one attaches an index ϵ to the commutators $[,]_\epsilon$, as it is done in Eq. (8) below. I find this usual notation confusing, since X_a^0 are the generators of a different algebra $\mathfrak{g}^0$. I prefer attaching the ϵ to the generators but keep the commutator symbol $[,]$ unchanged. This

notation is more useful and user-friendly, especially if matrix representations exist, since one uses $[A,B]=AB-BA$ and the standard matrix multiplication, whether the matrices A and B represent generators of the original or the contracted algebras.

In contrast to the formal definition of X_a^0, the limits $r(X_b^0) := \lim_{\epsilon\to 0} r(X_b^\epsilon)$ of *representations or realizations* $r(X_a^\epsilon)$, if they exist, should satisfy the commutation relations of $\mathfrak{g}^0$, although some of these representations may not be saved.

The condition (7) is necessary and sufficient to make the limit algebra $\mathfrak{g}^0$ well defined. It ensures that the *contracting structure constants* $C_{ab}^c(\epsilon)$, defined by

$$\sum_{c=1}^{N} C_{ab}^c(\epsilon) X_c^\epsilon := [X_a^\epsilon, X_b^\epsilon]_\epsilon = \epsilon^{n_a+n_b}[f_\epsilon(X_a), f_\epsilon(X_b)]_\epsilon = \epsilon^{n_a+n_b} f_\epsilon([X_a,X_b]) = \epsilon^{n_a+n_b} f_\epsilon\left(\sum_{c=1}^{N} C_{ab}^c X_c\right)$$
$$= \sum_{c=1}^{N} \epsilon^{n_a+n_b-n_c} C_{ab}^c X_c^\epsilon, \tag{8}$$

have finite limits for $\epsilon\to 0$.

The *Inönü-Wigner contraction* is a special case of the above-presented definition, where

$$\begin{aligned} n_i &= 0 \quad \text{for } i = 1,2,\ldots,M, \\ n_\alpha &= \text{const} > 0 \quad \text{for } \alpha = M+1, M+2, \ldots, N. \end{aligned} \tag{9}$$

In this case, and by choosing const$=1$ for convenience, we obtain for $\epsilon\to 0$:

$$\begin{aligned} [X_i^\epsilon, X_j^\epsilon] &= \sum_{k=1}^{M} C_{ij}^k X_k^\epsilon \Rightarrow \sum_{k=1}^{M} C_{ij}^k X_k^0, \\ \text{where } X_k^0 &:= \lim_{\epsilon\to 0} X_k^\epsilon, \end{aligned} \tag{10}$$

$$[X_i^\epsilon, X_\alpha^\epsilon] = \sum_{k=1}^{M} \epsilon C_{i\alpha}^k X_k^\epsilon + \sum_{\beta=M+1}^{N} C_{i\alpha}^\beta X_\beta^\epsilon \Rightarrow \sum_{\beta=M+1}^{N} C_{i\alpha}^\beta X_\beta^0, \tag{11}$$

$$[X_\alpha^\epsilon, X_\beta^\epsilon] = \sum_{k=1}^{M} \epsilon^2 C_{\alpha\beta}^k X_k^\epsilon + \sum_{\gamma=M+1}^{N} \epsilon C_{\alpha\beta}^\gamma X_\gamma^\epsilon \Rightarrow 0. \tag{12}$$

We see that the commutation relations (10) define a subalgebra $\mathfrak{g}_R := \langle X_i^0 \rangle \simeq \langle X_i \rangle$, because C_{ij}^α must vanish to satisfy the condition (7), as was originally concluded in Ref. 12. Note that (12) tells us that $I^0 = \langle X_\alpha^0 \rangle$ is an Abelian subalgebra, whereas (11) tells us that I^0 is an ideal of $\mathfrak{g}^0$.

The contractions which are not of the Inönü-Wigner type are called *generalized Inönü-Wigner contractions*. In the present paper we shall encounter one example of Inönü-Wigner contractions and two examples of generalized Inönü-Wigner contractions.

To give the reader an intuitive understanding of the above-presented definitions and notation, let us consider the famous example of contracting the Lorentz algebra to the Galilean algebra: Let e_{ij} denote a basis of 4×4 matrices, defined by $(e_{ij})_{kl} = \delta_{ik}\delta_{jl}$. They have the following commutation relations:

$$[e_{ij}, e_{st}] = \delta_{js} e_{it} - \delta_{it} e_{sj}, \quad i,j,s,t = 1,2,3,4. \tag{13}$$

We define the three contracting boosts by

$$B_i^\epsilon := \epsilon^2 e_{i4} + e_{4i} = \epsilon\left(\epsilon e_{i4} + \frac{1}{\epsilon} e_{4i}\right) =: \epsilon f_\epsilon(B_i), \quad i = 1,2,3. \tag{14}$$

These commute as follows:

$$[B_i^\epsilon, B_j^\epsilon] = \epsilon^2 [e_{i4}, e_{4j}] = \epsilon^2 (e_{ij} - e_{ji}) =: -\epsilon^2 L_{ij} \Rightarrow 0, \tag{15}$$

which shows how the Lorentz algebra $\mathfrak{so}(3,1)$ for $\epsilon=1$ is contracted to the Galilei algebra, which is the Euclidean algebra $\mathfrak{e}(3)$, in which the limits of the boosts $B_i^0 = e_{4i}$ generate an Abelian ideal.

III. THE HYDROGEN ALGEBRA $\mathbb{H}_2$ of H_0

Instead of the six generators **L** and **A** for the 3D Kepler problem, only three generators are conserved for the 2D Kepler problem.[10] These are the third component of angular momentum L_3 and two components of the Runge-Lenz vector **A**:

$$\begin{aligned} L \equiv L_3 &:= x p_y - y p_x = p_\varphi, \\ \mathbf{A} &:= (A_1, A_2) = L p_y \hat{\mathbf{x}} - L p_x \hat{\mathbf{y}} - m\alpha \hat{\mathbf{r}}. \end{aligned} \tag{16}$$

In the following I shall use the following notation:

$$h_0 \equiv -2mH_0, \quad h \equiv -2mH, \quad \varepsilon \equiv -2mE. \tag{17}$$

For simplicity and also in order to compare my results with those of Ref. 10, I shall use from now on *Poisson brackets* instead of commutation relations. But I shall nevertheless refer sometimes to these Poisson brackets as commutators.

The Poisson brackets of the above-mentioned generators are

$$\begin{aligned} \{L, A_1\} &= A_2, \\ \{A_2, L\} &= A_1, \\ \{A_1, A_2\} &= h_0 L, \end{aligned} \tag{18}$$

where $h_0 := -2mH_0$. The loop algebra $\mathbb{H}_2$ is spanned by the following generators:

$$L^{(2n)} := h_0^n L, \quad A_i^{(2n+1)} := h_0^n A_i \quad (i = 1,2), \quad n \geqslant 0. \tag{19}$$

I call the upper index the *grade* of the corresponding operator. According to the above-presented construction, every multiplication by h_0 raises the grade of the generators by 2. With the commutators (18) the set

$$\mathbb{H}_2 := \{A_1^{(2n+1)}, A_2^{(2n+1)}, L^{(2n)} | n \geqslant 0\} \tag{20}$$

becomes a closed Lie algebra, which is a subalgebra of the affine Kac-Moody algebra $A_1^{(1)}$.

A. The factor algebra $\mathbb{H}_2/I(E)$

The three standard finite-dimensional algebras, $\mathfrak{so}(3)$, $\mathfrak{so}(2,1)$, and $\mathfrak{e}(2)$ can be recovered from $\mathbb{H}_2$, as in Refs. 3 and 4, as follows: First we define an energy-dependent ideal of $\mathbb{H}_2$ by

$$\begin{aligned} I(E) &:= (H_0 - E)\mathbb{H}_2 = (h_0 - \varepsilon)\mathbb{H}_2, \\ &\text{where } \varepsilon := -2mE. \end{aligned} \tag{21}$$

Next, we define the *energy-dependent* factor algebra $\mathbb{H}_2/I(E)$ relative to the above-noted ideal. This factor algebra consists of three elements or classes,

$$\mathbb{H}_2/I(E) = \{\mathcal{A}_1^\varepsilon, \mathcal{A}_2^\varepsilon, \mathcal{L}^\varepsilon\}, \tag{22}$$

which obey the following commutation relations:

$$\{\mathcal{L}^\varepsilon, \mathcal{A}_1^\varepsilon\} = \mathcal{A}_2^\varepsilon, \quad \{\mathcal{A}_2^\varepsilon, \mathcal{L}^\varepsilon\} = \mathcal{A}_1^\varepsilon, \quad \{\mathcal{A}_1^\varepsilon, \mathcal{A}_2^\varepsilon\} = \varepsilon \mathcal{L}^\varepsilon. \tag{23}$$

The commutation relations (23) are exactly those of (18), except that the operator h_0 in (18) is now replaced by the numerical parameter ε. This is what physicists usually obtain by *directly* replacing the Hamiltonian H by its energy eigenvalue E.

The above-mentioned classes can be identified by their representatives as follows:

$$\mathcal{A}_1^\varepsilon = A_1 + I(E), \quad \mathcal{A}_2^\varepsilon = A_2 + I(E), \quad \mathcal{L}^\varepsilon = L + I(E). \tag{24}$$

To see why each "*basic element*" becomes a representative of its class, we recall that quite generally an ideal I of an algebra $\mathfrak{g}$ acts additively as the zero element of the factor algebra $\mathfrak{g}/I$. In our case, this fact yields the following equivalence relation in $\mathbb{H}_2/I(E)$:

$$h_0^n X_i \equiv \varepsilon^n X_i, \quad \text{mod } (I(E)), \tag{25}$$

where X_i is a basic generator, i.e., the element which generates the whole infinite "tower" $\{h_0^n X_i | n = 0, 1, \ldots\}$. The above-mentioned equivalence relation can be proved easily as follows:

$$h_0^n X_i - \varepsilon^n X_i = (h_0^n - \varepsilon^n) X_i = (h_0 - \varepsilon) \left(\sum_{k=0}^{n-1} \varepsilon^{n-1-k} h_0^k \right) X_i \in I(E). \tag{26}$$

Equation (25) tells us that in the factor algebra we can replace every element $h_0^n X_i \in \mathbb{H}_2$ by $\varepsilon^n X_i$, which is simply a numerical multiple of X_i. Hence, in $\mathbb{H}_2/I(E)$ we can replace every element in the tower $\{h_0^n X_i | n = 0, 1, \ldots\}$ by a single element X_i, so that $\mathbb{H}_2/I(E)$ is a finite-dimensional algebra generated by the X_i, which in our case are the three elements given in (24).

Note that *the Hamiltonian H_0 by itself is not an element of the ideal $I(E)$*.

B. Contraction of the factor algebra $\mathbb{H}_2/I(E)$

It is easy to check that the map

$$\begin{gathered} f_\varepsilon(\sqrt{\operatorname{sgn}(\varepsilon)} L_i) = \frac{1}{\sqrt{|\varepsilon|}} \mathcal{A}_i^\varepsilon, \quad i = 1, 2, \\ f_\varepsilon(L_3) = \mathcal{L}^\varepsilon, \end{gathered} \tag{27}$$

defines an isomorphism between the algebras $\mathfrak{so}(3)$, $\mathfrak{so}(2,1)$, and the factor algebra $\mathbb{H}_2/I(E)$ for $\varepsilon < 0$, $\varepsilon > 0$. Hence, by treating $\varepsilon = -2mE$ as a contraction parameter ϵ, the classes $\mathcal{A}_1^\varepsilon$, $\mathcal{A}_2^\varepsilon$, and $\mathcal{L}^\varepsilon$ with the commutation relations (23) can be regarded as the generators of a *contracting* algebra $\mathfrak{g}^\epsilon$ (see Sec. II), for $\varepsilon \neq 0$ (!).

For $\varepsilon \to 0$ the algebras $\mathbb{H}_2/I(\varepsilon)$ are contracted to $\mathbb{H}_2/I(0)$, whose commutation relations follow from (23)

$$\{\mathcal{L}^0, \mathcal{A}_1^0\} = \mathcal{A}_2^0, \quad \{\mathcal{A}_2^0, \mathcal{L}^0\} = \mathcal{A}_1^0, \quad \{\mathcal{A}_1^0, \mathcal{A}_2^0\} = 0. \tag{28}$$

Since these are the commutation relations of the Euclidean algebra $\mathfrak{e}(2)$, it follows that $\mathbb{H}_2/I(0) \simeq \mathfrak{e}(2)$. Since f_ϵ is an isomorphism for $\varepsilon \neq 0$, we conclude that a contraction of $\mathbb{H}_2/I(\varepsilon)$ for the nonbroken Hamiltonian H_0 in (5) is the same as the well-known contraction of $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ to the Euclidean algebra $\mathfrak{e}(2)$, as $\varepsilon \to 0$. Note that the number of generators remains the same after contraction. In the present case, the contraction is of the Inönü-Wigner type.

In the next two sections we shall see that the Factor algebras associated with the "broken Hamiltonian" H of (4) yield two contractions of the generalized Inönü-Wigner type.

IV. THE LOOP ALGEBRA $\mathfrak{L}_1(\beta)$ of H in (4)

For the Hamiltonian (4) there exist a generalized conserved Runge-Lenz vector,[10] which is given by

$$\mathbf{M} \equiv \mathbf{M}(\beta) := \mathbf{A} - m\beta\sqrt{r}\sin(\varphi/2)\hat{\boldsymbol{\phi}}(\varphi) = \left(\frac{p_\varphi^2}{r} - m\beta\right)\hat{\mathbf{r}}(\varphi) - (p_r p_\varphi + m\beta\sqrt{r}\sin(\varphi/2))\hat{\boldsymbol{\phi}}(\varphi). \tag{29}$$

Note that $\mathbf{M}(0)=\mathbf{A}$. The commutator of the two components of $\mathbf{M}$ in (29) yield a third conserved quantity, which I shall denote by S (It is called $-I$ in Ref. 10): It is defined by[10]

$$S := \{M_1, M_2\} = hp_\varphi - m\beta(p_r r^{1/2}\sin(\varphi/2) + p_\varphi r^{-1/2}\cos(\varphi/2)). \tag{30}$$

The commutators of S with M_i are[10]

$$\{S, M_1\} = hM_2, \quad N_1 := \{M_2, S\} = hM_1 - m^2\beta^2/2. \tag{31}$$

We can summarize the above-mentioned commutators as follows:

$$\{S, N_1\} = h^2 M_2, \quad \{M_2, S\} = N_1, \quad \{N_1, M_2\} = hS. \tag{32}$$

Therefore, I call the following three generators "*basic generators:*"

$$N_1, \quad M_2, \quad S, \tag{33}$$

because they can yield a closed algebra by multiplying them with powers of h as in (34). *The above-mentioned basic generators were chosen, such that none of them vanishes nor blows up for* $H=0$.

As before, since H commutes with the basic generators, we can close the algebra in (32) by including the following generators:

$$h^n M_2, \quad h^n N_1, \quad h^n S, \quad n \geqslant 0. \tag{34}$$

It is interesting to note that by commuting the basis generators N_1, M_2, and S, among themselves and with their commutators, we can never produce hM_2. This means that it is possible to obtain a closed algebra even without hM_2. Nevertheless, I included hM_2 in (34) in order to obtain a closed algebra which is generated by the basic generators over the polynomial ring $R[h]$.

A crucial step in identifying the algebra generated by the operators in (34) is to *assign grades* to each operator, because for Lie algebras of the Kac-Moody type the sum of the grades (which I am writing as upper indices) must be conserved under commutation. It is easy to check that the following identification of the grades is consistent:

$$M_2^{(2n+1)} := h^n M_2, \quad N_1^{(2n+3)} := h^n N_1, \quad S^{(2n+2)} := h^n S, \quad n \geqslant 0. \tag{35}$$

For example, using (32) we obtain

$$\{N_1^{(2m+3)}, M_2^{(2n+1)}\} = h^{m+n}\{N_1, M_2\} = h^{m+n+1}S = S^{(2m+2n+4)}.$$

Therefore the above-presented infinite generators span the following graded Loop algebra of the Kac-Moody type,

$$\mathfrak{L}_1(\beta) := \{M_2^{(2n+1)}, N_1^{(2n+3)}, S^{(2n+2)} | n \geqslant 0\}. \tag{36}$$

Note that the basic generators are graded as follows:

$$M_2 = M_2^{(1)}, \quad S = S^{(2)}, \quad N_1 = N_1^{(3)}.$$

A. The factor algebra $\mathfrak{L}_1(\beta)/I_1(E,\beta)$

As before, the factor algebra

$$\mathfrak{L}_1(\beta)/I_1(E,\beta) = \{\mathcal{M}_2^\varepsilon, \mathcal{N}_1^\varepsilon, \mathcal{S}^\varepsilon\}, \tag{37}$$

relative to the following energy-dependent ideal

$$I_1(E,\beta) \coloneqq (H-E)\mathfrak{L}_1(\beta) = (h-\varepsilon)\mathfrak{L}_1(\beta), \tag{38}$$

where $\varepsilon = -2mE$, has three classes, which commute as follows:

$$\{\mathcal{S}^\varepsilon, \mathcal{N}_1^\varepsilon\} = \varepsilon^2 \mathcal{M}_2^\varepsilon, \quad \{\mathcal{M}_2^\varepsilon, \mathcal{S}^\varepsilon\} = \mathcal{N}_1^\varepsilon, \quad \{\mathcal{N}_1^\varepsilon, \mathcal{M}_2^\varepsilon\} = \varepsilon \mathcal{S}^\varepsilon. \tag{39}$$

B. Contraction of the factor algebra $\mathfrak{L}_1/I_1(E,\beta)$

In the present case we need a different map

$$\begin{aligned} f_\varepsilon(\sqrt{\mathrm{sgn}(\varepsilon)}L_1) &= \mathcal{N}_1^\varepsilon/|\varepsilon|^{3/2} =: \hat{\mathcal{N}}_1{}^\varepsilon, \\ f_\varepsilon(\sqrt{\mathrm{sgn}(\varepsilon)}L_2) &= \mathcal{M}_2^\varepsilon/|\varepsilon|^{1/2} =: \hat{\mathcal{M}}_2{}^\varepsilon, \\ f_\varepsilon(L_3) &= \mathcal{S}^\varepsilon/|\varepsilon| =: \hat{\mathcal{S}}^\varepsilon, \end{aligned} \tag{40}$$

which again defines an isomorphism between the algebras $\mathfrak{so}(3)$, $\mathfrak{so}(2,1)$ and the factor algebra $\mathfrak{L}_1/I_1(E,\beta)$ for $\varepsilon<0$, $\varepsilon>0$. The three generators $\hat{\mathcal{N}}_1^\varepsilon$, $\hat{\mathcal{M}}_2^\varepsilon$, and $\hat{\mathcal{S}}^\varepsilon$ may be called "normalized" generators.

The contraction of the factor algebras $\mathfrak{L}_1/I_1(E,\beta)$ yields $\mathfrak{L}_1/I_1(0,\beta)$, whose commutation relations follow from (39). They are given by

$$\begin{aligned} [\mathcal{N}_1^0, \mathcal{M}_2^0] &= \lim_{\varepsilon\to 0} \varepsilon^{3/2+1/2-1}\mathcal{S}^\varepsilon = 0, \\ [\mathcal{S}^0, \mathcal{N}_1^0] &= \lim_{\varepsilon\to 0} \varepsilon^{1+3/2-1/2}\mathcal{M}_2^\varepsilon = 0, \end{aligned} \tag{41}$$

$$[\mathcal{M}_2^0, \mathcal{S}^0] = \lim_{\varepsilon\to 0} \varepsilon^{1/2+1-3/2}\mathcal{N}_1^\varepsilon = \mathcal{N}_1^0. \tag{42}$$

These are the commutation relations of the Heisenberg-Weyl algebra $\mathfrak{h}_3 = \mathfrak{w}_1$, as we can see by using the following map:

$$\mathcal{M}_2^0 \to \partial_x, \quad \mathcal{S}^0 \to x, \quad \mathcal{N}_1^0 \to 1.$$

It is important to note that in the factor algebra $\mathfrak{L}_1(\beta)/I_1(E,\beta)$ we are *not* allowed to replace the h in N_1 of (31) by ε, since neither h nor $(h-\varepsilon)M_1$ are elements of the ideal $I_1(E,\beta)$. Hence, N_1 is independent of E and thus it should *not* be replaced by the constant $-m^2\beta^2/2$ for $E=0$.

V. A SECOND LOOP ALGEBRA $\mathfrak{L}_2(\beta)$ OF H IN (4)

In this section I show that a different choice of the basic generators yields different contractions. Instead of the three generators in (33) I now choose the basic generators as follows:

$$N_1, \quad N_2 \coloneqq hM_2, \quad S. \tag{43}$$

The choice of N_2 in (43) may seem unjustified. But I chose it nevertheless in order to illustrate

how we can obtain different contractions by simply removing some generators from the *same* loop algebra.

The choice (43) would seem less strange, had I kept the phase angle γ in (4) arbitrary: In this case I would have obtained

$$\begin{aligned}\widetilde{N}_1 &:= \{\widetilde{M}_2, \widetilde{S}\} = \widetilde{h}\widetilde{M}_1 - \tfrac{1}{2}m^2\beta^2 \cos\,\gamma,\\ \widetilde{N}_2 &:= \{\widetilde{S}_1, \widetilde{M}_1\} = \widetilde{h}\widetilde{M}_2 - \tfrac{1}{2}m^2\beta^2 \sin\,\gamma,\end{aligned} \tag{44}$$

where the tilde over the quantities denotes the quantities of the previous section, but with $\gamma \neq 0$. Hence, for γ arbitrary, the $\widetilde{N}_1$, $\widetilde{N}_2$, and $\widetilde{S}$ would have seemed to be the natural choice for the basic generators. In fact, these generators were originally chosen by Leach and Flessas [Ref. 10, Eq. (3.4.5)] as the symmetry generators of the Hamiltonian (4) for $E \neq 0$. However, for $E=0$ they made a different choice, and chose the following linear combinations of $\widetilde{N}_1$ and $\widetilde{N}_2$:

$$\begin{aligned}N_1 &= \cos\,\gamma\widetilde{N}_1 + \sin\,\gamma\widetilde{N}_2 = hM_1 - \tfrac{1}{2}m^2\beta^2,\\ M_2 &= \frac{1}{h}(\sin\,\gamma\widetilde{N}_1 - \cos\,\gamma\widetilde{N}_2).\end{aligned} \tag{45}$$

We see that their second choice (45) corresponds exactly to the generators which I used in Sec. IV, by setting $\gamma=0$ from the beginning. This explains why they were able to obtain the algebra $\mathfrak{w}_1$ as the symmetry algebra for $E=0$; for $E \neq 0$ it does not matter which linear combinations one chooses: one always obtains $\mathfrak{so}(3)$ or $\mathfrak{so}(2,1)$.

The generators in (43) commute as follows:

$$\{N_1, N_2\} = h^2 S, \quad \{N_2, S\} = hN_1, \quad \{S, N_1\} = hN_2. \tag{46}$$

Following the same procedure as before, the following operators

$$\begin{aligned}N_1^{(2n+3)} &:= h^n N_1,\\ N_2^{(2n+3)} &:= h^n N_2.\\ S^{(2n+2)} &:= h^n S,\end{aligned} \tag{47}$$

for $n \geqslant 0$, yield the following Loop algebra, provided one uses the grading in (47)

$$\mathfrak{L}_2 := \{N_1^{(2n+3)}, N_2^{(2n+3)}, S^{(2n+2)} | n \geqslant 0\}. \tag{48}$$

The factor algebra $\mathfrak{L}_2(\beta)/I_2(E,\beta)$. The factor algebra in this case consists also of three classes, namely

$$\mathfrak{L}_2(\beta)/I_2(E,\beta) = \{\mathcal{N}_1^\varepsilon, \mathcal{N}_2^\varepsilon, \mathcal{S}^\varepsilon\}, \tag{49}$$

where

$$I_2(E,\beta) := (H-E)\mathfrak{L}_2(\beta) = (h-\varepsilon)\mathfrak{L}_2(\beta). \tag{50}$$

These classes commute as follows:

$$\{\mathcal{N}_1^\varepsilon, \mathcal{N}_2^\varepsilon\} = \varepsilon^2 \mathcal{S}^\varepsilon, \quad \{\mathcal{N}_2^\varepsilon, \mathcal{S}^\varepsilon\} = \varepsilon \mathcal{N}_1^\varepsilon, \quad \{\mathcal{S}^\varepsilon, \mathcal{N}_1^\varepsilon\} = \varepsilon \mathcal{N}_2^\varepsilon. \tag{51}$$

Hence, in this case we obtain for $\varepsilon \to 0$ a contraction of $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ to an Abelian algebra, which I denote by R^3. This is a generalized Inönü-Wigner contraction.

Note that if $N_2=hM_2$, as defined in (43), then $N_2^{(2n+3)}=M_2^{(2n+3)}$, so that $\mathfrak{L}_2$ is just a subalgebra of $\mathfrak{L}_1$, with just the element M_2 removed, i.e.,

$$\mathfrak{L}_2 = \mathfrak{L}_1 \setminus M_2^{(1)} = \mathfrak{L}_1 \setminus M_2. \tag{52}$$

Again note that in the factor algebra $\mathfrak{L}_2(\beta)/I_2(E,\beta)$ we are *not* allowed to replace $N_2=hM_2$ by εM_2, since $(h-\varepsilon)M_2$ is NOT an element of the ideal $I_2(E,\beta)$, because (52) tells us that $M_2 \notin \mathfrak{L}_2$. Thus, the class $\mathcal{N}_2^0=N_2+I_2(0)\neq I_2(0)$, which means that the contracted factor algebra $\mathfrak{L}_2(\beta)/I_2(0,\beta)$ remains 3D, as it should. Note that with the formal factor-algebra construction every one of the three generators is well defined and will not vanish in the limit $\varepsilon\to 0$, so that this realization is *saved.*[15] *In contrast, if instead we follow the standard procedure and work directly with the generators* N_1, N_2, *and* S *and just replace the* h *by* ε, *then* $N_2=hM_2$ *will become* $N_2=\varepsilon M_2$ *and thus it will vanish in the limit* $\varepsilon\to 0$, so that N_2 will not be saved.

VI. SUMMARY AND CONCLUSIONS

In the present paper I constructed two Kac-Moody loop algebras $\mathfrak{L}_1(\beta)$ and $\mathfrak{L}_2(\beta)$. The second algebra $\mathfrak{L}_2(\beta)$ was studied simply to show that one has the freedom of constructing more than one loop algebra from the conserved constants of motion, M_1, M_2, S, and H. These two infinite-dimensional algebras are operator-valued and thus do *not* depend on energy E.

To study contractions I first constructed E-dependent factor algebras, in order to obtain finite-dimensional algebras out of the infinite-dimensional ones. As I explained in Eq. (25), this construction enables us to replace all the higher generations $X_i^n := h^n X_i$ by $\varepsilon^n X_i$, so that within the factor algebras all the generators X_i^n become numerical multiples of the basic generators $X_i=X_i^0$. In particular, for $E=0$ we obtain $\varepsilon^n X_i=0$ for $n\geqslant 1$.

To avoid any misunderstanding, I want to emphasize again that I am *not* contracting the infinite-dimensional Kac-Moody loop algebras, $\mathbb{H}_2$, $\mathfrak{L}_1(\beta)$ and $\mathfrak{L}_2(\beta)$; *I am only contracting their (3D) factor algebras*, $\mathbb{H}_2/I(E)$, $\mathfrak{L}_1(\beta)/I_1(E,\beta)$, and $\mathfrak{L}_2(\beta)/I_2(E,\beta)$, by using the energy E as the contraction parameter. It is interesting that although all three factor algebras are isomorphic to $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$ for $E<0$ and $E>0$, they contract for $E\to 0$ to three different algebras $\mathfrak{e}(2)$, $\mathfrak{w}_1$, and R^3, which are also 3D. The first contraction is of the Inönü-Wigner type while the other two are of the generalized Inönü-Wigner type. In all these contractions the dimension of the algebras is preserved, since the factor algebras do not change their dimensions as $E\to 0$. These contractions are summarized in Table I.

The effect of symmetry breaking in $H(\beta)$ manifests itself differently in the standard and the Kac-Moody treatments: In the standard procedure, which was followed by Leach *et al.*,[9,10] the symmetry algebras for H_0 and $H(\beta)$ are exactly the same, namely $\mathfrak{so}(3)$ and $\mathfrak{so}(2,1)$. The effect of symmetry breaking manifests itself only for $E\neq 0$.

In contrast, as we shall now see, the Loop algebras $\mathfrak{L}_1$ and $\mathfrak{L}_2$ for the "broken Hamiltonian" $H(\beta)$ are *smaller* than the hydrogen algebra $\mathbb{H}_2$ for H_0 (irrespective of the energy !). They are smaller by two and three elements, respectively, thereby revealing the symmetry breaking:

To compare $\mathfrak{L}_1$ and $\mathfrak{L}_2$ with $\mathbb{H}_2$, I define two maps, as follows: $f_1:\mathfrak{L}_1\mapsto\mathbb{H}_2$, defined by

$$f_1(N_1^{(2n+3)}(\beta)) := A_1^{(2n+3)},$$

$$f_1(M_2^{(2n+1)}(\beta)) := A_2^{(2n+1)},$$

$$f_1(S^{(2n+2)}(\beta)) := L^{(2n+2)}, \tag{53}$$

for $n\geqslant 0$, and $f_2:\mathfrak{L}_2\mapsto\mathbb{H}_2$, defined by

$$f_2(N_1^{(2n+3)}(\beta)) := A_1^{(2n+3)},$$

$$f_2(N_2^{(2n+3)}(\beta)) := A_2^{(2n+3)}, \tag{54}$$

$$f_2(S^{(2n+2)}(\beta)) := L^{(2n+2)},$$

for $n \geqslant 0$. It is easy to check that these two maps, which keep the grades of the generators unchanged, define isomorphisms from $\mathfrak{L}_1$ and $\mathfrak{L}_2$ onto subalgebras of $\mathbb{H}_2$ of codimension two and three, respectively. Hence,

$$\mathbb{H}_2 = \begin{cases} f_1(\mathfrak{L}_1(\beta)) \cup \{L, A_1\} \\ f_2(\mathfrak{L}_2(\beta)) \cup \{L, A_1, A_2\}. \end{cases} \tag{55}$$

Thus, we can conclude that symmetry breaking of the type (4) reduces the loop algebra $\mathbb{H}_2$ of the original system H_0 by only finite number of generators. By constructing the corresponding factor algebras, I obtained different contractions depending on the missing terms (see Table I).

By defining the ε-dependent ideals and constructing the factor algebras, we are essentially replacing each infinite-dimensional "*tower*" $\{X_i^n\}$ by one element $X_i^{n_i^{\min}}$ which has the *lowest grade*. *By removing generators from the original loop algebra, we increase the grade of the corresponding basic generators*. This in turn increases the powers of the contraction parameter ε which multiply the structure constants of the original algebra $\mathfrak{g}$, which is being contracted.

The results obtained in the present paper suggest a *general procedure for defining contractions via Kac-Moody formalism* as follows:

- Start with of a finite dimensional Lie algebra $\mathfrak{g}$, which may be graded, via s-dimensional automorphism, as follows:

$$\mathfrak{g} = \bigoplus_{k=0}^{s-1} \mathfrak{g}_k \quad \text{with } [\mathfrak{g}_i, \mathfrak{g}_j] \subseteq \mathfrak{g}_{i+j}, \tag{56}$$

  where the indices are modulo s.
- Then consider the *positive* subalgebra of a general (twisted or untwisted) loop algebra of a finite dimensional algebra $\mathfrak{g}$,

$$\mathfrak{L} = \{ \bigoplus_{k=0}^{s-1} z^{sn+k} \otimes \mathfrak{g}_k | n \geqslant 0 \}, \tag{57}$$

  where z may be a scalar or an operator which commutes with all the generators of $X_i \in \mathfrak{g}$.
- Then remove some generators from $\mathfrak{L}$, and make sure that the *remaining set* $\mathfrak{L}_R$ yields a subalgebra of $\mathfrak{L}$. This is not automatic: see, for example, the conditions in (60). Then make sure that the set

$$I_R(\varepsilon) = (z - \varepsilon)\mathfrak{L}_R \tag{58}$$

  is an ideal of $\mathfrak{L}_R$, since for some choices $(z-\varepsilon)\mathfrak{L}_R$ is not a subalgebra of $\mathfrak{L}_R$.
- Finally, define the factor algebras $\mathfrak{L}_R / I_R(\varepsilon)$, which will be isomorphic to one or two real forms of $\mathfrak{g}$, depending on the sign of parameter ε. The ε can be used as a contraction parameter. One may get different contractions for the same original algebra $\mathfrak{g}$ as $\varepsilon \to 0$, depending on the removed generators.

For example, we can define subalgebras of $\mathbb{H}_2$ by

$$\mathbb{H}_2(n_1, n_2, n_3) := \langle h^{n_1+n} A_1, h^{n_2+n} A_2, h^{n_3+n} L_3, n \geqslant 0 \rangle \tag{59}$$

if the n_i satisfy the following conditions:

$$n_1 + n_2 - n_3 + 1 \geqslant 0, \quad n_3 + n_1 - n_2 \geqslant 0, \quad n_3 + n_2 - n_1 \geqslant 0. \tag{60}$$

In particular, as I showed explicitly in (53) and (54), the loop algebras $\mathfrak{L}_i$ are isomorphic to the following subalgebras of $\mathbb{H}_2$, and thus give us intuitive physical realizations of the formal definition in (59):

$$\mathfrak{L}_1 \simeq \mathbb{H}_2(1,0,1), \quad \mathfrak{L}_2 \simeq \mathbb{H}_2(1,1,1). \tag{61}$$

In these subalgebras of $\mathbb{H}_2$ the conditions (60) are clearly satisfied.

The conditions (60) follow from two different arguments:

(1) The generators of the subalgebra $\mathbb{H}_2(n_1,n_2,n_3)$ commute as follows:

$$\begin{aligned}
&[h^{n_1}A_1, h^{n_2}A_2] = h^{n_1+n_2+1}L_3, \quad \text{hence } n_3 \leqslant n_1+n_2+1,\\
&[h^{n_3}L_3, h^{n_1}A_1] = h^{n_3+n_1}A_2, \quad \text{hence } n_2 \leqslant n_3+n_1,\\
&[h^{n_3}L_3, h^{n_2}A_2] = -h^{n_3+n_2}A_1, \quad \text{hence } n_1 \leqslant n_3+n_2.
\end{aligned} \tag{62}$$

The conditions (60) are necessary to ensure that the right-hand side of the above-mentioned commutators are elements of $\mathbb{H}_2(n_1,n_2,n_3)$.

(2) In the factor algebra $\mathbb{H}_2(n_1,n_2,n_3)/((h-\varepsilon)\mathbb{H}_2(n_1,n_2,n_3))$ only the generators with lowest grade are linearly independent. Their commutators are

$$\begin{aligned}
&[\epsilon^{n_1}A_1, \epsilon^{n_2}A_2] = \epsilon^{n_1+n_2-n_3+1}(\epsilon^{n_3}L_3),\\
&[\epsilon^{n_3}L_3, \epsilon^{n_1}A_1] = \epsilon^{n_3+n_1-n_2}(\epsilon^{n_2}A_2),\\
&[\epsilon^{n_3}L_3, \epsilon^{n_2}A_2] = -\epsilon^{n_3+n_2-n_1}(\epsilon^{n_1}A_1).
\end{aligned} \tag{63}$$

Hence, in order for the right-hand side of the above three equations to exist as $\epsilon \to 0$, the exponents of ϵ must be non-negative. This requirement yields exactly the same conditions on the n_i as those given in (62), which were necessary for the existence of subalgebras of $\mathbb{H}_2$.

- More generally, given an N-dimensional semisimple algebra $\mathfrak{g}$, we can define subalgebras $\mathfrak{g}_n$ by

$$\mathfrak{g}_n := \langle h^{n_i}X_i | n \geqslant 0 \text{ and } i = 1,2,\ldots,N\rangle. \tag{64}$$

  Instead of an operator h, with $[h,X_i]=0$, we can also use a formal variable z.

  These subalgebras yield well-defined contractions via the factor-algebra $\mathfrak{g}_n/((h-\epsilon)\mathfrak{g}_n)$, provided the n_i satisfy the general condition (7), namely $\epsilon^{n_i+n_j-n_k}C_{ij}^k < \infty$.

Finally, we note that by taking the limit $\beta \to 0$ in the "*deformed Hamiltonian*" $H(\beta)$ of (4) we recover the original Hamiltonian H_0 and thus obtain the symmetry algebra $\mathbb{H}_2$. In contrast, for as $\beta \to 0$ the loop symmetry algebras $\mathfrak{L}_i(\beta)$ (and thus also their factor algebras) remain unchanged and do *not* go back to $\mathbb{H}_2$ (and its factor algebras). I call this phenomenon the *DC (deformation-contraction) hysteresis*, since *we obtain different contractions depending on the order of taking the limits* $E \to 0$ *and* $\beta \to 0$. The subtlety of the DC hysteresis, which yields $\mathfrak{w}_1$ instead of $\mathfrak{e}_2$, is illustrated in Fig. 1.

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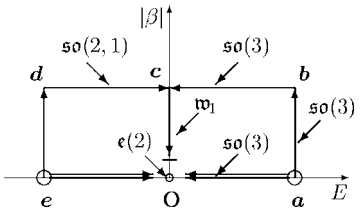

FIG. 1. The "*DC hysteresis*" in the (E,β) parameter plane, by comparing the contraction limits $E\to 0$ of the factor algebras $\mathbb{H}_2/I(E)$ and $\mathfrak{L}_1/I_1(E,\beta)$, is illustrated: If we contract the factor algebras $\mathbb{H}_2/I(E)$ of H_0 along the horizontal energy E-axis, which corresponds to $\beta=0$, we obtain $\mathfrak{e}(2)$. This contraction is indicated by the double arrows ($\mathbf{e}\Rightarrow\mathbf{O}\Leftarrow\mathbf{a}$). In contrast, for $\beta\neq 0$ the contraction of $\mathfrak{L}_1/I_1(E,\beta)$ of H yields the Weyl algebra $\mathfrak{L}_1/I_1(0,\beta)=\mathfrak{w}_1$, as illustrated by $\mathbf{d}\to\mathbf{c}\leftarrow\mathbf{b}$. Finally, taking the limit of $\mathfrak{L}_1/I_1(0,\beta)$ as $\beta\to 0$ downwards along the vertical $|\beta|$-axis to the origin $(E,\beta)=(0,0)$ leaves the algebra $\mathfrak{w}_1$ unchanged. Thus, the two paths originating in **a** yield different limits: $\mathfrak{so}(3)\simeq\mathbb{H}_2/I(E)\simeq\mathfrak{L}_1(\beta)/I_1(E,\beta)\to\mathfrak{L}_1(\beta)/I_1(0,\beta)\simeq\mathfrak{L}_1(0)/I_1(0,0)\simeq\mathfrak{w}_1\neq\mathfrak{e}(2)\simeq\mathbb{H}_2/I(0)\Leftarrow\mathbb{H}_2/I(E)$.

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Existence of weak solutions and trajectory attractors for the moist atmospheric equations in geophysics

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In this paper, we consider the initial boundary value problem for the primitive equations of moist atmospheric dynamics that are used to describe the turbulent behavior of long-term weather prediction and climate changes. By the Faedo-Galerkin method, we obtain the existence of global weak solutions to the problem in a large-scale atmosphere. By studying the long-time behavior of solutions, we obtain trajectory and global attractors for the primitive equations of moist atmosphere. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2245207]

I. INTRODUCTION

There are two ways to describe the mechanism of long-term weather prediction and climate changes. First, one can use history records and numerical computations to predict the future weather and possible global changes. Second, since the atmosphere is a specific compressible fluid, one can study the mathematical equations and models governing the motion of the atmosphere. Bjerkness, one of the pioneers of meteorology, said that the weather forecasting can be thought of as an initial boundary value problem in mathematical physics. In 1922, Richardson introduced the so-called primitive atmospheric equations that consisted of the hydrodynamic, thermodynamic, and state equations with Coriolis force; cf. Ref. 1. At that time, the primitive atmospheric equations were too complicated to be studied theoretically or to be solved numerically. However, there were some simple numerical models, such as the barotropic model formulated by Neumann, etc. in Ref. 2 and the quasigeostrophic model introduced by Charney and Philips in Ref. 3.

In recent years, due to the considerable improvement in computer capacity and the development of atmospheric science, there were some mathematicians who began to consider the primitive equations of atmosphere. Since the momentum conservation equation in the vertical direction can be replaced by the hydrostatic equation given later, which satisfies meteorological observations and history data in a large-scale atmosphere, the fundamental equations governing the motion of the atmosphere can be reduced to the primitive equations of large-scale atmosphere; cf. Ref. 1. In Ref. 4, introducing the viscosity terms and some technical treatment, Lions, Temam, and Wang obtained a new formulation of the primitive equations of large-scale dry atmosphere that was amenable to mathematical treatment. In a p-coordinate system (the definition will be given later), the new formulation of the primitive equations is similar to but more complicated than Navier-Stokes equations of incompressible fluid. By the methods used to solve Navier-Stokes system in Ref. 5, they obtained the existence of global weak solutions of the initial boundary value problem for the new formulation of the primitive equations. And under the hypothesis that there exist global strong solutions for the problem, they established some physically relevant estimates for the Hausdorff and fractal dimensions of attractors for the primitive equations. By the same methods, in Ref. 6 they established some mathematical theory for the models of the coupled

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atmosphere and ocean introduced in Ref. 7. In Refs. 8 and 9, under the hypothesis of the existence of the global strong solutions for the initial boundary value problem of the dry and moist atmospheric fundamental equations, Li and Chou studied asymptotic behavior of solutions for the problem. By taking advantage of the geostrophic balance and other geophysical consideration, several intermediate models have been the subject of studying the long-time dynamics and global attractors in order to describe the mechanism of weather prediction and climate dynamics (see, e.g., Refs. 10–13).

In the present paper, we are interested in finding the existence of global weak solutions, trajectory, and global attractors for the large-scale moist atmospheric primitive equations. Our main results are Theorem 3.8 and Theorem 4.15. Without the hypothesis that there exist global strong solutions for the initial boundary problem of the new formulation of large-scale moist atmospheric primitive equations (IBVP), which will be given in Sec. II, we obtain global attractors for the moist atmospheric primitive equations in some weak sense (the details will be given in Sec. IV). (IBVP) generalizes the work in Ref. 4, where the authors considered the dry atmospheric primitive equations. Since the moist atmospheric equations are more complicated than the dry atmospheric primitive equations, we must study more nonlinear terms than those in Ref. 4. Under some technical treatment, (IBVP) is corresponding to Problem 3.1 given in the Sec. III C. Using the methods in Ref. 4, we can make full use of the hydrostatic equation, which provides a relation between pressure and density to obtain the existence of global weak solutions for Problem 3.1. Problem 3.1 is similar to but more complicated than Navier-Stokes systems of incompressible fluids. In particular, the nonlinear terms in Problem 3.1 is more complicated than those in the Navier-Stokes system. Since the existence of global strong solutions of Problem 3.1 remains unproved (recently, in Ref. 14, Cao and Titi have proved the global existence and uniqueness of strong solutions to a three-dimensional viscous primitive equations in a cylindrical domain), we cannot use the well-known methods based on the analysis of global attractors of the corresponding semigroup. Our approach to finding the existence of trajectory and global attractors for the moist atmospheric equations is inspired by Refs. 15 and 16. In those papers, Vishik and Chepyzhov obtained the trajectory and global attractors of three-dimensional Navier-Stokes system without the assumption that there exist global strong solutions for the system. Here, the trajectory and global attractors is related to the time translation semigroup $\{T(t)\}$ given in the subsection IV A.

The paper is organized as follows: In Sec. II, we shall pose the new formulation of the primitive equations of a large-scale moist atmosphere. In Sec. III, we shall give a mathematical setting for the initial boundary value problem for the new formulation of primitive equations of large-scale moist atmosphere and obtain the existence of global weak solutions to Problem 3.1. In Sec. IV, we shall prove the existence of trajectory and global attractors of the moist atmospheric primitive equations.

II. THE PRIMITIVE EQUATIONS OF LARGE-SCALE MOIST ATMOSPHERE

Inspired by the methods used by Lions, Temam, and Wang introduced in Refs. 4 and 7, we shall give the new formulation of the primitive equations of large-scale moist atmosphere in this section.

In a noninertial coordinate system, the atmosphere motion is described by the following equations (see, e.g., Refs. 17, 9, and 18):

The momentum conservation equation,

$$\frac{dV_3}{dt} = -\frac{1}{\rho}\,\mathrm{grad}_3\, p + G - 2\Omega \times V_3 + D. \tag{2.1}$$

The continuity equation;

$$\frac{d\rho}{dt} + \rho\,\mathrm{div}_3\, V_3 = 0. \tag{2.2}$$

The first law of thermodynamics,

$$c_p\frac{dT}{dt}-\frac{RT}{p}(1+cq)\frac{dp}{dt}=\frac{dQ}{dt}. \tag{2.3}$$

The equation of state,

$$p=R\rho T(1+cq). \tag{2.4}$$

The conservation equation of water vapor in the air,

$$\frac{dq}{dt}=\frac{1}{\rho}W_1+W_2, \tag{2.5}$$

where the unknown functions are V_3, ρ, q, p, T. V_3 is the three-dimensional velocity, ρ density, p pressure, $q=\rho_1/\rho$ the mixing ratio of water vapor in the air, ρ_1 density of water vapor in the air, T temperature, G gravity, $-2\Omega\times V_3$ Coriolis force, Ω angular velocity of the earth, D the viscosity terms (which include the diabatic heating and the friction of the atmosphere), dQ/dt the heat flux per unit density in a unit time interval, W_1 the rate of condensation of water vapor per unit volume, W_2 the time rate of change of water vapor content per unit mass due to the vertical and horizontal diffusion of water vapor, R gas constants for dry air, c_p specific heat of air at constant pressure, c is a positive constant ($c\approx 0.618$), grad_3 and div_3 gradient and divergence in the three-dimensional atmosphere, respectively.

Remark 2.1: The equations (2.1)–(2.5) are different from the atmospheric equations in Ref. 7, where the authors only considered the equations (2.1), (2.2), (2.5) with (2.3) and (2.4) when $c=0$.

In the spherical coordinate system, let $\theta(0\le\theta\le\pi)$ denote the colatitude of the earth, $\varphi(0\le\varphi\le 2\pi)$ the longitude of the earth, r the radial distance, $z=r-a$ the height above sea level, a the radius of the earth,

$$V_3=v_\theta e_\theta+v_\varphi e_\varphi+v_r e_z,$$

where e_θ, e_φ and e_z are unit vectors in the θ, φ, z direction, and

$$e_\theta=\frac{1}{a}\frac{\partial}{\partial\theta},\quad e_\varphi=\frac{1}{a\sin\theta}\frac{\partial}{\partial\varphi},\quad e_z=\frac{\partial}{\partial z}.$$

Then the equations (2.1)–(2.5) can be written as the following fundamental equations of the moist atmosphere (see, for details, Ref. 17)

$$\frac{dv_\theta}{dt}+\frac{1}{r}(v_r v_\theta-v_\varphi^2\cot\theta)=-\frac{1}{\rho r}\frac{\partial p}{\partial\theta}+2\Omega\cos\theta v_\varphi+D_\theta, \tag{2.6}$$

$$\frac{dv_\varphi}{dt}+\frac{1}{r}(v_r v_\varphi+v_\theta v_\varphi\cot\theta)=-\frac{1}{\rho r\sin\theta}\frac{\partial p}{\partial\varphi}-2\Omega\cos\theta v_\theta-2\Omega\sin\theta v_r+D_\varphi, \tag{2.7}$$

$$\frac{dv_r}{dt}-\frac{1}{r}(v_\theta^2+v_\varphi^2)=-\frac{1}{\rho}\frac{\partial p}{\partial r}-g+2\Omega\sin\theta v_\varphi+D_r, \tag{2.8}$$

$$\frac{d\rho}{dt}+\rho\left(\frac{1}{r\sin\theta}\frac{\partial v_\theta\sin\theta}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial v_\varphi}{\partial\varphi}+\frac{1}{r^2}\frac{\partial r^2 v_r}{\partial r}\right)=0, \tag{2.9}$$

$$c_p\frac{dT}{dt}-\frac{RT}{p}(1+cq)\frac{dp}{dt}=\frac{dQ}{dt}, \tag{2.10}$$

$$p = R\rho T(1 + cq), \tag{2.11}$$

$$\frac{dq}{dt} = \frac{1}{\rho} W_1 + W_2, \tag{2.12}$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{v_\theta}{r}\frac{\partial}{\partial \theta} + \frac{v_\varphi}{r \sin\theta}\frac{\partial}{\partial \varphi} + v_r \frac{\partial}{\partial r},$$

and $D=(D_\theta, D_\varphi, D_r)$ are the viscosity terms.

Under the coordinate transformation $(t, \theta, \varphi, z) \to (t, \theta, \varphi, p)$ (p denotes pressure) and some technical treatment, Eq. (2.8) being replaced by the hydrostatic equation

$$\frac{\partial p}{\partial r} = -\rho g,$$

and the specific viscosity terms being introduced, Eqs. (2.6)–(2.12) can be written as the following nondimensional form (for details, we refer the readers to Refs. 4 and 7 and references therein),

$$\frac{\partial v}{\partial t} + \nabla_v v + \omega \frac{\partial v}{\partial \xi} + \frac{f}{R_0} k \times v + \operatorname{grad} \Phi - \frac{1}{\mathrm{Re}_1}\Delta v - \frac{1}{\mathrm{Re}_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2 \frac{\partial v}{\partial \xi}\right] = f_1, \tag{2.13}$$

$$\operatorname{div} v + \frac{\partial \omega}{\partial \xi} = 0, \tag{2.14}$$

$$\frac{\partial \Phi}{\partial \xi} + \frac{bP}{p}(1 + cq)T = 0, \tag{2.15}$$

$$a_1\left(\frac{\partial T}{\partial t} + \nabla_v T + \omega \frac{\partial T}{\partial \xi}\right) - \frac{bP}{p}(1 + cq)\omega - \frac{1}{Rt_1}\Delta T - \frac{1}{Rt_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2 \frac{\partial T}{\partial \xi}\right] = f_2, \tag{2.16}$$

$$\frac{\partial q}{\partial t} + \nabla_v q + \omega \frac{\partial q}{\partial \xi} - \frac{1}{Rt_3}\Delta q - \frac{1}{Rt_4}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2 \frac{\partial q}{\partial \xi}\right] = f_3, \tag{2.17}$$

where the unknown functions are v, ω, Φ, q, T. $v=(v_\theta, v_\varphi)$ the horizontal velocity, $\Phi = gz$ the geopotential, $\omega = dp/dt$ vertical velocity in the $p-$ coordinate system, $f = 2\cos\theta$ Coriolis parameter, k vertical unit vector, P an approximate value of pressure at the surface of the earth, Re_1, Re_2, Rt_1, Rt_2, Rt_3, Rt_4 Reynolds numbers, $\bar{T}$ a given vertical distribution of the standard temperature on the interval $[p_0, P]$, $\overline{T_0}$ reference value of the temperature T, p_0 pressure of the upper atmosphere, and $p_0 > 0$, the variable ξ satisfying $p=(P-p_0)\xi + p_0$, f_1, f_2, f_3 given functions on $S^2 \times (0,1)$, a_1, b positive constants. The definitions of operators $\nabla_v v$, Δv, ΔT, Δq, $\nabla_v q$, $\nabla_v T$, $\operatorname{div} v$, $\operatorname{grad}\Phi$ will be given in the Sec. III A. Equations (2.13)–(2.17) are called the primitive equations of the large-scale moist atmosphere.

Remark 2.2: In the real physical situation, f_1, f_2, f_3 are taken as zero. However, from the mathematical point of view, we can consider the general case that f_1, f_2, f_3 are not always equal to zero.

The space domain of the equations is

$$M = S^2 \times (0,1),$$

where S^2 is two-dimensional unit sphere. The boundary value conditions are given by

$$\xi = 1(p = P):(v, \omega) = 0, \frac{\partial T}{\partial \xi} = \alpha_s(\overline{T_s} - T), \quad \frac{\partial q}{\partial \xi} = \beta_s(\overline{q_s} - q), \tag{2.18}$$

$$\xi = 0(p = p_0):(v, \omega) = 0, \quad \frac{\partial T}{\partial \xi} = 0, \frac{\partial q}{\partial \xi} = 0, \tag{2.19}$$

where α_s, β_s are constants, $\overline{T_s}$ the given temperature on the surface of the earth, $\overline{q_s}$ the given mixing ratio of water vapor on the surface of the earth.

Integrating (2.14) and using the boundary conditions (2.18), (2.19), we have

$$\omega(t; \theta, \varphi, \xi) = W(v)(t; \theta, \varphi, \xi) = \int_{\xi}^{1} \operatorname{div} v(t; \theta, \varphi, \xi') d\xi', \tag{2.20}$$

$$\int_0^1 \operatorname{div} v \, d\xi = 0. \tag{2.21}$$

Suppose that Φ_s is a certain unknown function at the isobaric surface $p=P$. Integrating (2.15), we obtain

$$\Phi(t; \theta, \varphi, \xi) = \Phi_s(t; \theta, \varphi, \xi) + \int_{\xi}^{1} \frac{bP}{p}(1 + cq)T \, d\xi'. \tag{2.21'}$$

Then Eqs. (2.13)–(2.17) can be written as

$$\frac{\partial v}{\partial t} + \nabla_v v + W(v)\frac{\partial v}{\partial \xi} + \frac{f}{R_0}k \times v + \operatorname{grad} \Phi_s + \int_{\xi}^{1} \frac{bP}{p} \operatorname{grad}(1 + cq)T \, d\xi' - \frac{1}{\mathrm{Re}_1}\Delta v - \frac{1}{\mathrm{Re}_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial v}{\partial \xi}\right] = f_1, \tag{2.22}$$

$$a_1\left(\frac{\partial T}{\partial t} + \nabla_v T + W(v)\frac{\partial T}{\partial \xi}\right) - \frac{bP}{p}(1 + cq)W(v) - \frac{1}{\mathrm{Rt}_1}\Delta T - \frac{1}{\mathrm{Rt}_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial T}{\partial \xi}\right] = f_2, \tag{2.23}$$

$$\frac{\partial q}{\partial t} + \nabla_v q + W(v)\frac{\partial q}{\partial \xi} - \frac{1}{\mathrm{Rt}_3}\Delta q - \frac{1}{\mathrm{Rt}_4}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial q}{\partial \xi}\right] = f_3, \tag{2.24}$$

$$\int_0^1 \operatorname{div} v \, d\xi = 0, \tag{2.25}$$

where the definitions of grad T, grad Φ_s will be given in the Sec. III A. The boundary value conditions of Eqs. (2.22)–(2.25) are given by

$$\xi = 1(p = P):v = 0, \quad \frac{\partial T}{\partial \xi} = \alpha_s(\overline{T_s} - T), \quad \frac{\partial q}{\partial \xi} = \beta_s(\overline{q_s} - q), \tag{2.26}$$

$$\xi = 0(p = p_0):v = 0, \quad \frac{\partial T}{\partial \xi} = 0, \quad \frac{\partial q}{\partial \xi} = 0; \tag{2.27}$$

the initial value conditions can be given as

$$U_0 = (v_0, T_0, q_0). \tag{2.28}$$

We call (2.22)–(2.28) as the initial boundary problem of the new formulation of the primitive equations of large-scale moist atmosphere, denoted by (IBVP).

Remark 2.3: In this paper, we only study the primitive equations of large-scale moist atmosphere with viscosity terms given for horizontal velocity. In the future work, we can consider the equations with viscosity terms for the three-dimensional velocity.

III. EXISTENCE OF GLOBAL WEAK SOLUTIONS FOR THE PROBLEM (IBVP)

The section is divided into four subsections. In Sec. III A, some function spaces for the problem (IBVP) will be given. In Sec. III B, we shall give properties of some functionals corresponding to Eqs. (2.22)–(2.25). In Sec. III C, we shall introduce weak formulation for the problem (IBVP). The proof of the existence of global weak solutions to the problem (IBVP) will be given in Sec. III D.

A. Some function spaces

Let e_θ, e_φ, e_ξ be the unit vectors in θ, φ, and ξ directions of the space domain M, respectively,

$$e_\theta = \frac{\partial}{\partial \theta}, \quad e_\varphi = \frac{1}{\sin\theta}\frac{\partial}{\partial \varphi}, \quad e_\xi = \frac{\partial}{\partial \xi}.$$

The inner product and norm on $T_{(\theta,\varphi,\xi)}M$ [the tangent space of M at the point (θ,φ,ξ)] are given by

$$(X,Y)_T = X \cdot Y = X_1Y_1 + X_2Y_2 + X_3Y_3, |X|_T = (X,X)^{1/2}$$

for

$$X = X_1e_\theta + X_2e_\varphi + X_3e_\xi, \quad Y = Y_1e_\theta + Y_2e_\varphi + Y_3e_\xi \in T_{(\theta,\varphi,\xi)}M.$$

$L^2(M) := \{h; h: M \to \mathbb{R}, \int_M |h|^2\, dM < +\infty\}$ with the norm $|h|_2 = (\int_M |h|^2\, dM)^{1/2}$. $|\cdot|_p$ is the usual norm in $L^p(M)$. $L^2(TM|TS^2) = \{v; v: M \to TS^2\}$ is the first two components of L^2 vector fields on M with the norm $|v|_2 = (\int_M (|v_\theta|^2 + |v_\varphi|^2) dM)^{1/2}$, where TM, TS^2 are the tangent space of M and S^2, respectively, $v = (v_\theta, v_\varphi)$. $C^\infty(S^2)$ is the function space for all smooth functions from S^2 to $\mathbb{R}$. $C^\infty(M)$ is the function space for all smooth functions from M to $\mathbb{R}$. $C^\infty(\mathrm{TM}|\mathrm{TS}^2)$ is the first two components of smooth vector fields on M. $C_0^\infty(M) := \{u; u \in C^\infty(M), \mathrm{supp}\, u$ is a compact subset in $M\}$. $C_0^\infty(\mathrm{TM}|\mathrm{TS}^2) := \{u; u \in C^\infty(\mathrm{TM}|\mathrm{TS}^2), \mathrm{supp}\, u$ is a compact subset in $M\}$. $H^m(M)$ is the Sobolev space of functions that are in L^2,together with all their covariant derivatives with respect to e_θ, e_φ, e_ξ of order $\leq m$, with the norm

$$\|h\|_m = \left(\int_M \left(\sum_{1 \leq k \leq m} \sum_{i_j = 1,2,3; j = 1,\ldots,k} |\nabla_{i_1} \cdots \nabla_{i_k} h| + |h|^2 \right) dM \right)^{1/2},$$

where $\nabla_1 = \nabla_{e_\theta}$, $\nabla_2 = \nabla_{e_\varphi}$, $\nabla_3 = \nabla_{e_\xi} = \partial/\partial\xi$ (the definitions of $\nabla_{e_\theta}, \nabla_{e_\varphi}$ will be given later). $H^m(\mathrm{TM}|\mathrm{TS}^2) = \{v; v = (v_\theta, v_\varphi): M \to TS^2, v_\theta, v_\varphi \in H^m(M)\}$, the norm of which is similar to that of $H^m(M)$, that is, in the above formula of norm, we can let $h = (v_\theta, v_\varphi) = v_\theta e_\theta + v_\varphi e_\varphi$.

The horizontal divergence div, the horizontal gradient $\nabla = \mathrm{grad}$, the horizontal covariant derivative ∇_v and horizontal Laplace-Beltrami operator Δ for scalar and vector functions are defined by

$$\mathrm{div}\, v = \mathrm{div}(v_\theta e_\theta + v_\varphi e_\varphi) = \frac{1}{\sin\theta}\left(\frac{\partial v_\theta \sin\theta}{\partial\theta} + \frac{\partial v_\varphi}{\partial\varphi} \right), \tag{3.1}$$

$$\nabla T = \operatorname{grad} T = \frac{\partial T}{\partial \theta} e_\theta + \frac{1}{\sin\theta}\frac{\partial T}{\partial \varphi} e_\varphi, \tag{3.2}$$

$$\operatorname{grad} \Phi_s = \frac{\partial \Phi_s}{\partial \theta} e_\theta + \frac{1}{\sin\theta}\frac{\partial \Phi_s}{\partial \varphi} e_\varphi, \tag{3.3}$$

$$\nabla_v \tilde{v} = \left(v_\theta \frac{\partial \tilde{v}_\theta}{\partial \theta} + \frac{v_\varphi}{\sin\theta}\frac{\partial \tilde{v}_\theta}{\partial \varphi} - v_\varphi \tilde{v}_\varphi \cot\theta \right) e_\theta + \left(v_\theta \frac{\partial \tilde{v}_\varphi}{\partial \theta} + \frac{v_\varphi}{\sin\theta}\frac{\partial \tilde{v}_\varphi}{\partial \varphi} + v_\varphi \tilde{v}_\theta \cot\theta \right) e_\varphi, \tag{3.4}$$

$$\nabla_v T = v_\theta \frac{\partial T}{\partial \theta} + \frac{v_\varphi}{\sin\theta}\frac{\partial T}{\partial \varphi}, \tag{3.5}$$

$$\nabla_v q = v_\theta \frac{\partial q}{\partial \theta} + \frac{v_\varphi}{\sin\theta}\frac{\partial q}{\partial \varphi}, \tag{3.6}$$

$$\Delta T = \frac{1}{\sin\theta}\left[\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial T}{\partial \theta} \right) + \frac{1}{\sin\theta}\frac{\partial^2 T}{\partial \varphi^2} \right], \tag{3.7}$$

$$\Delta q = \frac{1}{\sin\theta}\left[\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial q}{\partial \theta} \right) + \frac{1}{\sin\theta}\frac{\partial^2 q}{\partial \varphi^2} \right], \tag{3.8}$$

$$\Delta v = \left(\Delta v_\theta - \frac{2\cos\theta}{\sin^2\theta}\frac{\partial v_\varphi}{\partial \varphi} - \frac{v_\theta}{\sin^2\theta} \right) e_\theta + \left(\Delta v_\varphi + \frac{2\cos\theta}{\sin^2\theta}\frac{\partial v_\theta}{\partial \varphi} - \frac{v_\varphi}{\sin^2\theta} \right) e_\varphi, \tag{3.9}$$

where $v = v_\theta e_\theta + v_\varphi e_\varphi$, $\tilde{v} = \tilde{v}_\theta e_\theta + \tilde{v}_\varphi e_\varphi \in C^\infty(\mathrm{TM}|\mathrm{TS}^2)$, T, $q \in C^\infty(M)$, $\Phi_s \in C^\infty(S^2)$.

Now we can define our working spaces for the problem (IBVP). Let

$$\tilde{V} := \left\{ v; v \in C_0^\infty(\mathrm{TM}|\mathrm{TS}^2),\ \int_0^1 \operatorname{div} v \, d\xi = 0 \right\},$$

V_1 = the closure of $\tilde{V}$ with respect to the norm $\|\cdot\|_1$,

$$V_2 = H^1(M),$$

H_1 = the closure of $\tilde{V}$ with respect to the norm $|\cdot|_2$,

$$H_2 = L^2(M),$$

$$V = V_1 \times V_2 \times V_2,$$

$$H = H_1 \times H_2 \times H_2,$$

$V_1^{(3)}$ = the closure of $\tilde{V}$ with respect to the norm $\|\cdot\|_3$,

$$V_2^{(3)} = H^3(M),$$

$$V^{(3)} = V_1^{(3)} \times V_2^{(3)} \times V_2^{(3)},$$

$$V^{(-3)} = (V^{(3)})',$$

where $(V^{(3)})'$ is the dual space of $V^{(3)}$. In order to study the nonlinear terms of the equations (2.22)–(2.24), we have to introduce the spaces $V^{(3)}$ and $V^{(-3)}$. The inner product and norm on V, V_1, V_2 are given by

$$(v,v_1)_{V_1} = \int_M \left(\nabla_{e_\theta} v \cdot \nabla_{e_\theta} v_1 + \nabla_{e_\varphi} v \cdot \nabla_{e_\varphi} v_1 + \frac{\partial v}{\partial \xi} \frac{\partial v_1}{\partial \xi} + v \cdot v_1 \right) dM,$$

$$\|v\|_{V_1} = (v,v)_{V_1}^{1/2}, \quad \forall\, v,v_1 \in V_1,$$

$$(T,T_1)_{V_2} = \int_M \left(\operatorname{grad} T \cdot \operatorname{grad} T_1 + \frac{\partial T}{\partial \xi} \frac{\partial T_1}{\partial \xi} + T T_1 \right) dM,$$

$$\|T\|_{V_2} = (T,T)_{V_2}^{1/2}, \quad \forall\, T,\ T_1 \in V_2,$$

$$(q,q_1)_{V_2} = \int_M \left(\operatorname{grad} q \cdot \operatorname{grad} q_1 + \frac{\partial q}{\partial \xi} \frac{\partial q_1}{\partial \xi} + q q_1 \right) dM,$$

$$\|q\|_{V_2} = (q,q)_{V_2}^{1/2}, \quad \forall\, q,\ q_1 \in V_2,$$

$$(U,U_1)_H = (v,v_1) + (a_1 T, T_1) + (q,q_1),$$

$$(U,U_1)_V = (v,v_1)_{V_1} + (T,T_1)_{V_2} + (q,q_1)_{V_2},$$

$$\|U\| = (U,U)_V^{1/2}, \quad |U|_2 = (U,U)_H^{1/2}, \quad \forall\, U = (v,T,q), \quad U_1 = (v_1,T_1,q_1) \in V,$$

$$\|U\|_{(3)} = (\|v\|_3^3 + \|T\|_3^3 + \|q\|_3^3)^{1/3}, \quad \forall\, U \in V^{(3)},$$

$$(T,T_1)_{H_2} = (a_1 T, T_1), \quad |T|_2 = (T,T)_{H_2}^{1/2}, \quad |v|_2 = (v,v)^{1/2},$$

where $(\cdot,\cdot)$ denotes the L^2 inner products in H_1, H_2. By the definitions of V, H, we can obtain

$$V \subset H = H' \subset V' \subset V^{(-3)},$$

where V' is the dual space of V.

B. Properties of some functionals and their associated operators

In this section, we shall define some functionals and their corresponding operators that are related to the equations (2.22)–(2.25) and give some estimates about those functionals.

Now, we define the functionals $\tilde{a}: V \times V \to \mathbb{R}$, $\tilde{a}_1: V_1 \times V_1 \to \mathbb{R}$, $\tilde{a}_2: V_2 \times V_2 \to \mathbb{R}$, $\tilde{a}_3: V_2 \times V_2 \to \mathbb{R}$, and their corresponding linear operators $A: V \to V'$, $A_1: V_1 \to V_1'$, $A_2: V_2 \to V_2'$, $A_3: V_2 \to V_2'$ by

$$\tilde{a}(U,U_1) = (AU,U_1) = \tilde{a}_1(v,v_1) + \tilde{a}_2(T,T_1) + \tilde{a}_3(q,q_1),$$

where

$$\tilde{a}_1(v,v_1)=(A_1v,v_1)=\int_M\left[\frac{1}{\mathrm{Re}_1}(\nabla_{e_\theta}v\cdot\nabla_{e_\theta}v_1+\nabla_{e_\varphi}v\cdot\nabla_{e_\varphi}v_1+v\cdot v_1)+\frac{1}{\mathrm{Re}_2}\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2\frac{\partial v}{\partial\xi}\frac{\partial v_1}{\partial\xi}\right]dM,$$

$$\tilde{a}_2(T,T_1)=(A_2T,T_1)=\int_M\left[\frac{1}{\mathrm{Rt}_1}\,\mathrm{grad}\,T\cdot\mathrm{grad}\,T_1+\frac{1}{\mathrm{Rt}_2}\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2\frac{\partial T}{\partial\xi}\frac{\partial T_1}{\partial\xi}\right]dM+\int_{\Gamma_1}\frac{\alpha_s}{\mathrm{Rt}_2}\left(\frac{p\overline{T_0}}{P\bar{T}}\right)^2TT_1\,dS^2,$$

$$\tilde{a}_3(q,q_1)=(A_3q,q_1)=\int_M\left[\frac{1}{\mathrm{Rt}_3}\,\mathrm{grad}\,q\cdot\mathrm{grad}\,q_1+\frac{1}{\mathrm{Rt}_4}\left(\frac{p\overline{q_0}}{P\bar{q}}\right)^2\frac{\partial q}{\partial\xi}\frac{\partial q_1}{\partial\xi}\right]dM+\int_{\Gamma_1}\frac{\beta_s}{Rt_4}\left(\frac{p\overline{q_0}}{P\bar{q}}\right)^2qq_1\,dS^2,$$

$$\Gamma_1=S^2\times 1.$$

Lemma 3.1:

(1) a is coercive and continuous. $A:V\to V'$ is an isomorphism. Moreover,

$$a(U,U_1)\le c_1\max\left\{\frac{1}{\mathrm{Re}_1},\frac{1}{\mathrm{Re}_2}\right\}\|v\|_{V_1}\|v_1\|_{V_1}+c_2\max\left\{\frac{1}{\mathrm{Rt}_1},\frac{1}{\mathrm{Rt}_2},\frac{\alpha_s}{\mathrm{Rt}_2}\right\}\|T\|_{V_2}\|T_1\|_{V_2}+c_3\max\left\{\frac{1}{\mathrm{Rt}_3},\frac{1}{\mathrm{Rt}_4},\frac{\beta_s}{\mathrm{Rt}_4}\right\}\|q\|_{V_2}\|q_1\|_{V_2}\le\frac{1}{R_{\min}}\|U\|\|U_1\|,\tag{3.10}$$

$$a(U,U)\ge c_4\min\left\{\frac{1}{\mathrm{Re}_1},\frac{1}{\mathrm{Re}_2}\right\}\|v\|_{V_1}^2+c_5\min\left\{\frac{1}{\mathrm{Rt}_1},\frac{1}{\mathrm{Rt}_2},\frac{\alpha_s}{\mathrm{Rt}_2}\right\}\|T\|_{V_2}^2+c_6\min\left\{\frac{1}{\mathrm{Rt}_3},\frac{1}{\mathrm{Rt}_4},\frac{\beta_s}{\mathrm{Rt}_4}\right\}\|q\|_{V_2}^2\ge\frac{1}{R_{\max}}\|U\|^2,\tag{3.11}$$

where

$$R_{\min}=\frac{1}{\min\{c_1,c_2,c_3\}}\min\left\{\mathrm{Re}_1,\mathrm{Re}_2,\mathrm{Rt}_1,\mathrm{Rt}_2,\mathrm{Rt}_3,\mathrm{Rt}_4,\frac{\mathrm{Rt}_2}{\alpha_s},\frac{\mathrm{Rt}_4}{\beta_s}\right\},$$

$$R_{\max}=\frac{1}{\max\{c_4,c_5,c_6\}}\min\left\{\mathrm{Re}_1,\mathrm{Re}_2,\mathrm{Rt}_1,\mathrm{Rt}_2,\mathrm{Rt}_3,\mathrm{Rt}_4,\frac{\mathrm{Rt}_2}{\alpha_s},\frac{\mathrm{Rt}_4}{\beta_s}\right\}.$$

In this paper, c_i will denote positive constants and can be determined in concrete conditions.

(2) The isomorphism $A:V\to V'$ can be extended to a self-adjoint unbounded linear operator on H with a compact inverse $A^{-1}:H\to H$ and with the domain of definition of the operator $D(A)=V\cap(H^2(TM\,|\,TS^2)\times H^2(M)\times H^2(M))$.

Proof: The operator A is similar to the usual positive symmetric operator $-\Delta$ on H_0^1. Therefore we omit the details of the proof. For details, the readers can refer to [Ref. 4 Lemma 2.3].

Concerning the nonlinear terms of the equations (2.22)–(2.24), we can define the functional $\tilde{b}:V\times V\times V\to\mathbb{R}$ and its corresponding operator $B:H\times H\to H$ by

$$\tilde{b}(U,U_1,U_2)=(B(U,U_1),U_2)_H=b_1(v,v_1,v_2)+b_2(v,T_1,T_2)+b_3(v,q_1,q_2),$$

where

$$b_1(v,v_1,v_2)=\int_M\left[\nabla_v v_1+\left(\int_\xi^1 \operatorname{div} v\, d\xi'\right)\frac{\partial v_1}{\partial \xi}\right]\cdot v_2\, dM,$$

$$b_2(v,T_1,T_2)=\int_M\left[\nabla_v T_1+\left(\int_\xi^1 \operatorname{div} v\, d\xi'\right)\frac{\partial T_1}{\partial \xi}\right]T_2\, dM,$$

$$b_3(v,q_1,q_2)=\int_M\left[\nabla_v q_1+\left(\int_\xi^1 \operatorname{div} v\, d\xi'\right)\frac{\partial q_1}{\partial \xi}\right]q_2\, dM.$$

Let

$$b_4(U,U,U_2)=\int_M\left[\left(\int_\xi^1 \frac{bP}{p}\operatorname{grad}(Tcq)d\xi'\right)\cdot v_2-\frac{bP}{p}cqW(v)T_2\right]dM$$

and

$$b(U,U_1,U_2)=\tilde{b}(U,U_1,U_2)+b_4(U,U,U_2).$$

Lemma 3.2:
(1) For any $U,\ U_1\in D(A)$,

$$b_1(v,v_1,v_1)=b_2(v,T_1,T_1)=b_3(v,q_1,q_1)=0,\quad b_4(U,U,U)=0.$$

(2) For any $U\in D(A),\ U_2\in D(A)\cap V^{(3)}$,

$$|b(U,U,U_2)|\le c_7\|U\||U|_2\|U_2\|_{(3)}. \tag{3.12}$$

Proof: (1) By (3.4), for any $U=(v,T,q),\ U_1=(v_1,T_1,q_1)\in D(A)$, we can obtain

$$\nabla_v|v_1|^2=\nabla_v v_1\cdot v_1+v_1\cdot\nabla_v v_1=2\nabla_v v_1\cdot v_1.$$

Then

$$\begin{aligned}
b_1(v,v_1,v_1)&=\int_M\left[\nabla_v v_1\cdot v_1+\frac{1}{2}\left(\int_\xi^1 \operatorname{div} v d\xi'\right)\frac{\partial|v_1|^2}{\partial\xi}\right]dM\\
&=\int_M\left[\frac{1}{2}\nabla_v|v_1|^2+\frac{1}{2}\left(\int_\xi^1 \operatorname{div} v d\xi'\right)\frac{\partial|v_1|^2}{\partial\xi}\right]dM\\
&=\frac{1}{2}\int_M\left[\operatorname{div}(v|v_1|^2)-|v_1|^2\operatorname{div} v+\left(\int_\xi^1 \operatorname{div} v\, d\xi'\right)\frac{\partial|v_1|^2}{\partial\xi}\right]dM\\
&=\frac{1}{2}\int_M\left[-|v_1|^2\operatorname{div} v+\left(\int_\xi^1 \operatorname{div} v\, d\xi'\right)\frac{\partial|v_1|^2}{\partial\xi}\right]dM\\
&=-\frac{1}{2}\int_M\left[|v_1|^2\left(\operatorname{div} v+\frac{\partial W(v)}{\partial\xi}\right)\right]dM+\int_M|v_1|^2\left(\int_\xi^1 \operatorname{div} v d\xi'\right)\Bigg|_{\xi=0,1}dM=0.
\end{aligned}$$

Similarly, we prove $b_2(v,T_1,T_1)=b_3(v,q_1,q_1)=0$,

$$b_4(U,U,U)=\int_M\left[\left(\int_\xi^1\frac{bP}{p}\,\mathrm{grad}(Tcq)d\xi'\right)\cdot v-\frac{bP}{p}cqW(v)T\right]dM,$$

$$=\int_M\left[\left(-\int_\xi^1\frac{bP}{p}(Tcq)d\xi'\right)\cdot \mathrm{div}\,v-\frac{bP}{p}cqW(v)T\right]dM,$$

$$=\int_M\left[\left(-\int_\xi^1\frac{bP}{p}(Tcq)d\xi'\right)\cdot\frac{\partial\left(\int_\xi^1\mathrm{div}\,vd\xi'\right)}{\partial\xi}-\frac{bP}{p}cqW(v)T\right]dM,$$

$$=\int_M\left(\frac{bP}{p}TcqW(v)-\frac{bP}{p}cqW(v)T\right)dM=0.$$

(2) For any $U=(v,T,q),U_1=(v_1,T_1,q_1)\in D(A),\ U_2=(v_2,T_2,q_2)\in D(A)\cap V^{(3)}$,

$$\left|\int_M\left[\left(\int_\xi^1\mathrm{div}\,vd\xi'\right)\frac{\partial v_1}{\partial\xi}\right]\cdot v_2\,dM\right|\le\int_M\left|v_1\cdot\left(\frac{\partial v_2}{\partial\xi}\int_\xi^1\mathrm{div}\,vd\xi'+v_2\,\mathrm{div}\,v\right)\right|dM$$

$$\le\|v\|_{V_1}|v_1|_2\left|\frac{\partial v_2}{\partial\xi}\right|_{L^\infty}\le\|U\||U_1|_2\left|\frac{\partial U_2}{\partial\xi}\right|_{L^\infty}$$

$$\le C\|U\||U_1|_2\|U_2\|_{(3)},$$

where C is a positive constant. Similarly, we derive

$$|b(U,U,U_2)|\le c_7\|U\||U|_2\|U_2\|_{(3)}.$$

Related to the linear terms, we can define a bilinear functional $e:V\times V\to\mathbb{R}$ and its corresponding operator $\tilde{E}:H\to H$ by

$$e(U,U_1)=(\tilde{E}U,U_1)_H$$

$$=\int_M\left[\frac{f}{R_0}(k\times v)\cdot v_1+\left(\int_\xi^1\frac{bP}{p}\,\mathrm{grad}\,T\,d\xi'\right)\cdot v_1-\frac{bP}{p}W(v)T_1\right]dM.$$

Lemma 3.3:
(1) For any $U,\ U_1\in V$,

$$|e(U,U_1)|\le C\|U\|\|U_1\|,\tag{3.13}$$

where C is a positive constant.
(2) For any $U,\ U\in V$,

$$|e(U,U)|=0.$$

Proof: The first part of the Lemma is obvious, so we omit the details of the proof. The proof of the second part is similar to the proof of $b_4(U,U,U)=0$.

C. Weak formulation for the problem (IBVP)

In this section, we will introduce a weak formulation for the problem (IBVP) by eliminating the geopotential Φ_s in the equation (2.22). The method is similar to eliminating the pressure in obtaining the existence of global weak solutions for the Navier-Stokes system.

First, we shall homogenize the boundary value condition (2.26) for T, q. By

$$\frac{\partial T'}{\partial \xi} = \alpha_s(\overline{T_s} - T'), \quad \frac{\partial q'}{\partial \xi} = \beta_s(\overline{q_s} - q'),$$

we obtain

$$T' = \overline{T_s}(1 - \exp(-\alpha_s \xi)), \quad q' = \overline{q_s}(1 - \exp(-\beta_s \xi)).$$

Let

$$T'_\varepsilon = T' \psi_\varepsilon(\xi), \quad q'_\varepsilon = q' \psi_\varepsilon(\xi),$$

where $0 < \varepsilon < \frac{1}{2}$,

$$\psi_\varepsilon(\xi) := \begin{cases} 1, & 1-\varepsilon \le \xi \le 1, \\ \text{increasing}, & 1-2\varepsilon \le \xi \le 1-\varepsilon, \\ 0, & 0 \le \xi \le 1-2\varepsilon. \end{cases}$$

Then, by letting $\widetilde{U} = (v, \widetilde{T}, \widetilde{q}) = U - U'_\varepsilon = (v, T, q) - (0, T'_\varepsilon, q'_\varepsilon)$, the problem (IBVP) can be rewritten as the following equations:

$$\begin{aligned} &\frac{\partial v}{\partial t} + \nabla_v v + W(v)\frac{\partial v}{\partial \xi} + \frac{f}{R_0} k \times v + \operatorname{grad} \Phi_s + \int_\xi^1 \frac{bP}{p} \operatorname{grad}(1 + c\widetilde{q})\widetilde{T}\, d\xi' + \int_\xi^1 \frac{bP}{p} \operatorname{grad}(cq'_\varepsilon \widetilde{T} \\ &\quad + cT'_\varepsilon \widetilde{q}) d\xi' - \frac{1}{\mathrm{Re}_1}\Delta v - \frac{1}{\mathrm{Re}_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial v}{\partial \xi}\right] = \widetilde{f_1} = f_1 - \int_\xi^1 \frac{bP}{p} \operatorname{grad}(1 + cq'_\varepsilon) T'_\varepsilon \, d\xi', \end{aligned} \tag{3.14}$$

$$\begin{aligned} &a_1\left(\frac{\partial \widetilde{T}}{\partial t} + \nabla_v \widetilde{T} + W(v)\frac{\partial \widetilde{T}}{\partial \xi}\right) + a_1\left(\nabla_v T'_\varepsilon + W(v)\frac{\partial T'_\varepsilon}{\partial \xi}\right) - \frac{bP}{p}(1 + c\widetilde{q})W(v) - \frac{bP}{p}(cq'_\varepsilon)W(v) - \frac{1}{Rt_1}\Delta \widetilde{T} \\ &\quad - \frac{1}{Rt_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial \widetilde{T}}{\partial \xi}\right] = \widetilde{f_2} = f_2 + \frac{1}{\mathrm{Rt}_1}\Delta T'_\varepsilon + \frac{1}{\mathrm{Rt}_2}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial T'_\varepsilon}{\partial \xi}\right], \end{aligned} \tag{3.15}$$

$$\begin{aligned} &\frac{\partial \widetilde{q}}{\partial t} + \nabla_v \widetilde{q} + W(v)\frac{\partial \widetilde{q}}{\partial \xi} + \nabla_v q'_\varepsilon + W(v)\frac{\partial q'_\varepsilon}{\partial \xi} - \frac{1}{\mathrm{Rt}_3}\Delta \widetilde{q} - \frac{1}{\mathrm{Rt}_4}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial \widetilde{q}}{\partial \xi}\right] \\ &\quad = \widetilde{f_3} = f_3 + \frac{1}{\mathrm{Rt}_3}\Delta q'_\varepsilon + \frac{1}{\mathrm{Rt}_4}\frac{\partial}{\partial \xi}\left[\left(\frac{p\overline{T_0}}{P\overline{T}}\right)^2 \frac{\partial q'_\varepsilon}{\partial \xi}\right], \end{aligned} \tag{3.16}$$

$$\int_0^1 \operatorname{div} v \, d\xi = 0, \tag{3.17}$$

with the initial and boundary value conditions

$$\xi = 1 (p = P): v = 0, \quad \frac{\partial \widetilde{T}}{\partial \xi} + \alpha_s \widetilde{T} = 0, \quad \frac{\partial \widetilde{q}}{\partial \xi} + \beta_s \widetilde{q} = 0, \tag{3.18}$$

$$\xi = 0 (p = p_0): v = 0, \quad \frac{\partial \widetilde{T}}{\partial \xi} = 0, \quad \frac{\partial \widetilde{q}}{\partial \xi} = 0. \tag{3.19}$$

$$\tilde{U}_0 = (v_0, \widetilde{T_0}, \widetilde{q_0}). \tag{3.20}$$

Now we can introduce the weak formulation for the problem (IBVP).

Problem 3.1: For $\tilde{f}=(\widetilde{f_1}, \widetilde{f_2}, \widetilde{f_3})$, $\tilde{U}_0=(v_0, \widetilde{T_0}, \widetilde{q_0}) \in H$ given, find $\tilde{U}=(v, \tilde{T}, \tilde{q})$ such that

$$\tilde{U} \in L^2(0,\mathcal{T};V) \cap L^\infty(0,\mathcal{T};H), \quad \forall\, \mathcal{T}>0, \tag{3.21}$$

$$\frac{d}{dt}(\tilde{U}, U_1)_H + (A\tilde{U}, U_1)_H + ((B\tilde{U}, \tilde{U}), U_1)_H + ((B\tilde{U}, U_\varepsilon'), U_1)_H + ((F\tilde{U}, U_\varepsilon'), U_1)_H + (\tilde{E}\tilde{U}, U_1)_H$$
$$= (\tilde{f}, U_1)_H, \quad \text{in } (C_0^\infty(0,\mathcal{T}))', \quad \forall\, U_1 \in D(A) \tag{3.22}$$

$$\tilde{U}|_{t=0} = \tilde{U}_0, \quad \text{in } V^{(-3)}, \tag{3.23}$$

where

$$((F\tilde{U}, U_\varepsilon'), U_1)_H = \int_M \left[\left(\int_\xi^1 \frac{bP}{p} \operatorname{grad}(cq_\varepsilon' \tilde{T} + cT_\varepsilon' \tilde{q}) d\xi' \right) \cdot v_1 - \frac{bP}{p}(cq_\varepsilon') W(v) T_1 \right] dM.$$

D. Proof of the existence of global weak solutions

In this section, we shall prove the existence of global weak solutions for the problem (IBVP) by proving the existence of global weak solutions for Problem 3.1. In order to do this, we need some lemmas.

Lemma 3.4: (cf. Ref. 4 Lemma 2.1):

(1) If $v \in H_1$, $\int_M v v_1\, dM = 0$, $\forall v_1 \in C_0^\infty(\mathrm{TM}|\mathrm{TS}^2)$, then

$$v = \operatorname{grad} \Phi_s, \quad \Phi_s \in (C_0^\infty(S^2))'.$$

(2) Let $H_1^\perp$ be the orthogonal complement of H_1 in $L^2(\mathrm{TM}|\mathrm{TS}^2)$. Then

$$H_1^\perp = \{v; v \in L^2(\mathrm{TM}|\mathrm{TS}^2), \quad v = \operatorname{grad} l,\ l \in H^1(S^2)\}, \tag{3.24}$$

$$H_1 = \left\{ v; v \in L^2(\mathrm{TM}|\mathrm{TS}^2), \quad \int_0^1 \operatorname{div} v\, d\xi = 0 \right\}, \tag{3.25}$$

$$V_1 = \left\{ v; v \in H_0^1(\mathrm{TM}|\mathrm{TS}^2), \quad \int_0^1 \operatorname{div} v\, d\xi = 0 \right\}. \tag{3.26}$$

By this lemma, we know that if there is a solution $\tilde{U}=(v, \tilde{T}, \tilde{q})$ for Problem 3.1, then there is a unique $\Phi_s \in (C_0^\infty(S^2))'$ (up to a constant) such that (v, T, q, Φ_s) is a solution for the problem (IBVP). On other hand, if (v, T, q, Φ_s) is a solution for the problem (IBVP) [(v, T, q, Φ_s) is sufficiently smooth], then $\tilde{U}=(v, \tilde{T}, \tilde{q})$ is a solution to Problem 3.1.

In order to solve Problem 3.1 by the Faedo-Galerkin method, we need the following three lemmas.

Lemma 3.5: The eigenvalue problem,

$$AU = \mu U, \quad U \in V,$$

exists a sequence of eigenvalues, $0 < \mu_1 < \mu_2 \le \mu_3 \le \cdots \le \mu_n \le \cdots$, of finite multiplicity and going to infinity, with the first eigenvalue being simple, having a positive eigenfunction. Moreover, the eigenfunction sequence $\{\phi_n\}$ is an orthonormal basis of V.

Proof: This lemma is a corollary of Lemma 3.1.

Lemma 3.6: For any $\delta>0$, there is $0<\varepsilon<1/2$ such that

$$|((F\widetilde{U},U_\varepsilon'),\widetilde{U})_H|\le\delta\|\widetilde{U}\|^2, \tag{3.27}$$

$$|((B\widetilde{U},U_\varepsilon'),\widetilde{U})_H|\le\delta\|\widetilde{U}\|^2,\quad \forall\ \widetilde{U}\in V. \tag{3.28}$$

Proof: By the definition, for any $U_1\in V$,

$$\begin{aligned}
|((F\widetilde{U},U_\varepsilon'),U_1)_H| &= \left|\int_M\left[\left(\int_\xi^1\frac{bP}{p}\,\mathrm{grad}(cq_\varepsilon'\widetilde{T}+cT_\varepsilon'\widetilde{q})d\xi'\right)\cdot v_1-\frac{bP}{p}(cq_\varepsilon')W(v)T_1\right]dM\right| \\
&\le \left|\int_M\left(\int_\xi^1\frac{bP}{p}cq_\varepsilon'\,\mathrm{grad}\,\widetilde{T}\,d\xi'\right)\cdot v_1\,dM\right| \\
&\quad+\left|\int_M\left(\int_\xi^1\frac{bP}{p}c\widetilde{T}\,\mathrm{grad}\,q_\varepsilon'\,d\xi'\right)\cdot v_1\,dM\right| \\
&\quad+\left|\int_M\left(\int_\xi^1\frac{bP}{p}cT_\varepsilon'\,\mathrm{grad}\,\widetilde{q}\,d\xi'\right)\cdot v_1\,dM\right| \\
&\quad+\left|\int_M\left(\int_\xi^1\frac{bP}{p}c\widetilde{q}\,\mathrm{grad}\,T_\varepsilon'\,d\xi'\right)\cdot v_1 dM\right| \\
&\quad+\left|\int_M\frac{bP}{p}cq_\varepsilon'\left(\int_\xi^1\mathrm{div}\,v\,d\xi'\right)T_1\,dM\right|\le I_1+I_2+I_3+I_4+I_5.
\end{aligned}$$

By the definition of q_ε',

$$\begin{aligned}
I_1 &= \left|\int_M\left(\int_\xi^1\frac{bP}{p}cq_\varepsilon'\,\mathrm{grad}\,\widetilde{T}\,d\xi'\right)\cdot v_1\,dM\right|\le\left|\int_{S^2\times[1-2\varepsilon]}\left(\int_{1-2\varepsilon}^1\frac{bP}{p}cq_\varepsilon'\,\mathrm{grad}\,\widetilde{T}\,d\xi'\right)\cdot v_1\,dM\right| \\
&\le c_8|q_\varepsilon'|_{L^\infty(S^2)}\left|\int_{S^2\times[1-2\varepsilon]}\left(\int_{1-2\varepsilon}^1\mathrm{grad}\,\widetilde{T}\,d\xi'\right)\cdot v_1\,dM\right|\le 4c_8\varepsilon^2|q_\varepsilon'|_{L^\infty(S^2)} \\
&\quad\times\left|\int_{S^2}\left(\int_{1-2\varepsilon}^1|\mathrm{grad}\,\widetilde{T}|^2\,d\xi'\right)^{1/2}\left(\int_{1-2\varepsilon}^1|v_1|^2\,d\xi'\right)^{1/2}dS^2\right|\le 4c_8\varepsilon^2|q_\varepsilon'|_{L^\infty(S^2)}\|\|T\|_{V_2}\|v_1\|_{V_1} \\
&\le c_9\varepsilon\|U\|\|U_1\|.
\end{aligned}$$

Similarly, we can prove

$$I_i\le c_{8+i}\varepsilon\|U\|\|U_1\|,\quad i=2,3,4,5.$$

So

$$|((F\widetilde{U},U_\varepsilon'),\widetilde{U})_H|\le\delta\|\widetilde{U}\|^2.$$

Since the proof of (3.28) is similar to the proof of $I_1\le c_9\varepsilon\|U\|\|U_1\|$, we omit the details of the proof.

Lemma 3.7 (Lions-Magenes) (Ref. 19): Suppose that $g\in L^\infty(0,\mathcal{T};E)$ and the function $g(t)$ is weakly continuous in E_0: $g\in C_\omega(0,\mathcal{T};E_0)$, that is, for any function $\phi\in(E_0)'$ the function $\langle g(t),\phi\rangle$ belongs to $C[0,\mathcal{T}]$, where E, $E_0(E\subset E_0)$ are Banach spaces. Then $g(t)\in E$ for all $0\le t\le\mathcal{T}$ and $g(t)$ is weakly continuous in E.

Now we can state one of our main results.

Theorem 3.8: Under the assumptions of Problem 3.1 and for any $\mathcal{T}>0$, there is at least one solution $\tilde{U}=(v,\tilde{T},\tilde{q})$ on the time interval $[0,\mathcal{T}]$ to Problem 3.1, and $\tilde{U}=(v,\tilde{T},\tilde{q})$ satisfies

$$\widetilde{U_t} \in L^2(0,\mathcal{T};V^{(-3)}), \tag{3.29}$$

$$\tilde{U} \in C_\omega(0,\mathcal{T};H). \tag{3.30}$$

Moreover, $\tilde{U}$ satisfies the energy inequality

$$-\int_0^\infty |\tilde{U}(t)|_2^2\psi'(s)ds + \frac{1}{R_{\max}}\int_0^\infty \|\tilde{U}(s)\|^2\psi(s)ds \le 2\int_0^\infty (\tilde{f},\tilde{U}(s))_H\psi(s)ds, \tag{3.31}$$

where $\psi(s)\in C_0^\infty(]0,\mathcal{T}[), \psi(s)\ge 0$.

Proof: We shall prove Theorem 3.8 by the Faedo-Galerkin method. Since the procedure is similar to the proof of the existence of Leray-Hopf weak solutions to the Navier-Stokes system in Ref. 5, Theorem 6.1, we only give the outline of the proof. First, we can look for an approximate solution $\tilde{U}_m(x,t)$ for Problem 3.1, where $\tilde{U}_m(x,t)=\Sigma_{i=1}^m \alpha_{i,m}(t)\phi_i(x)$ and $\phi_i(x)$ is defined in Lemma 3.5. The function $\tilde{U}_m$ satisfies

$$\frac{d}{dt}(\tilde{U}_m,\phi_i(x))_H + (A\tilde{U}_m,\phi_i(x))_H + ((B\tilde{U}_m,\tilde{U}_m),\phi_i(x))_H + ((B\tilde{U}_m,U_\varepsilon'),\phi_i(x))_H + ((F\tilde{U}_m,U_\varepsilon'),\phi_i(x))_H$$
$$+ (\tilde{E}\tilde{U}_m,\phi_i(x))_H = (\tilde{f},\phi_i(x))_H, \quad i=1,2,\ldots,m, \tag{3.32}$$

$$\tilde{U}_m|_{t=0} = \tilde{U}_{0,m}, \tag{3.33}$$

where $\tilde{U}_{0,m}\to\tilde{U}_0$ in H. As usually, it is straightforward (see Ref. 5) from (3.32) and Lemma 3.6 that

$$\frac{1}{2}\frac{d}{dt}|\tilde{U}_m(s)|_2^2 + \frac{1}{R_{\max}}\|\tilde{U}_m(s)\|^2 \le \frac{1}{2R_{\max}}\|\tilde{U}_m(s)\|^2 + (\tilde{f},\tilde{U}_m(s))_H. \tag{3.34}$$

Integrating (3.34) from 0 to t, $t\in]0,\mathcal{T}]$, we can obtain

$$|\tilde{U}_m(t)|_2^2 + \frac{1}{R_{\max}}\int_0^t \|\tilde{U}_m(s)\|^2\,ds \le |\tilde{U}_{0,m}|_2^2 + 2\int_0^t (\tilde{f},\tilde{U}_m(s))_H\,ds, \quad t\in 0,\mathcal{T}. \tag{3.35}$$

By the Gronwall inequality and (3.34), we have

$$|\tilde{U}_m(t)|_2^2 + c_{14}\int_0^t \|\tilde{U}_m(t)\|^2\,ds \le |\tilde{U}_{0,m}|_2^2 + c_{15}\int_0^t \|\tilde{f}(s)\|_{V'}\,ds, \quad t\in 0,\mathcal{T}. \tag{3.36}$$

So $\{\tilde{U}_m\}$ is bounded in the space $L^2(0,\mathcal{T};V)\cap L^\infty(0,\mathcal{T};H)$. Going if necessary to a subsequence $\{\tilde{U}_m\}$ (that we label the same), $\tilde{U}_m\to\tilde{U}$ $(m\to\infty)$ weakly in $L^2(0,\mathcal{T};V)$ and * weakly in $L^\infty(0,\mathcal{T};H)$. Due to a compactness theorem (see Ref. 5), we can extract a subsequence $\{\tilde{U}_m\}$ denoted by the same such that $\tilde{U}_m\to\tilde{U}$ $(m\to\infty)$strongly in $L^2(0,\mathcal{T};H)$. By passing to the limit in (3.32), we conclude that $\tilde{U}$ is a weak solution to Problem 3.1. By Lemmas 3.1, 3.2, 3.3, we know that

$$\{(\tilde{U}_m)_t\} \text{ is bounded set of } L^2(0,\mathcal{T};V^{(-3)}).$$

Therefore, $\tilde{U}_t \in L^2(0,\mathcal{T};V^{(-3)})$. Finally, by Lemma 3.7 and $\tilde{U} \in C(0,\mathcal{T};V^{(-3)})$, we have $\tilde{U} \in C_\omega(0,\mathcal{T};H)$.

Now let us prove the energy inequality. From $\tilde{U}_m \to \tilde{U}$ $(m\to\infty)$ strongly in $L^2(0,\mathcal{T};H)$, it follows that $|\tilde{U}_m|_2 \to |\tilde{U}|_2$ $(m\to\infty)$ strongly in $L^2(0,\mathcal{T})$. Going if necessary to a subsequence, $|\tilde{U}_m|_2 \to |\tilde{U}|_2$ $(m\to\infty)$, a.e. in $[0,\mathcal{T}]$. Let $\psi(s) \in C_0^\infty(]0,\mathcal{T}[)$, $\psi(s)\geq 0$. By (3.31) and the Lebesgue Dominated Theorem, we have

$$\int_0^\infty |\tilde{U}_m(t)|_2^2 \psi'(s)ds \to \int_0^\infty |\tilde{U}(t)|_2^2 \psi'(s)ds, \quad m\to\infty. \tag{3.37}$$

$\tilde{U}_m \to \tilde{U}$ $(m\to\infty)$ weakly in $L^2(0,\mathcal{T};V)$ implies that $\tilde{U}_m\psi^{1/2}(s) \to \tilde{U}\psi^{1/2}(s)$ $(m\to\infty)$ weakly in $L^2(0,\mathcal{T};V)$. By the lower weak semicontinuity of the norm, we get

$$\int_0^\infty \|\tilde{U}(s)\|^2 \psi(s)ds \leq \liminf_{m\to\infty} \int_0^\infty \|\tilde{U}_m(s)\|^2 \psi(s)ds. \tag{3.38}$$

Using (3.32) and (3.33), we have

$$-\int_0^\infty |\tilde{U}_m(t)|_2^2 \psi'(s)ds + \frac{1}{R_{\max}} \int_0^\infty \|\tilde{U}_m(s)\|^2 \psi(s)ds \leq 2\int_0^\infty (\tilde{f}, \tilde{U}_m(s))_H \psi(s)ds. \tag{3.39}$$

Combining (3.37) with (3.38), we pass to the limit in (3.39) and obtain the energy inequality. The proof is complete.

IV. TRAJECTORY AND GLOBAL ATTRACTORS FOR THE MOIST ATMOSPHERIC EQUATIONS

This section is divided into two subsections. In Sec. IV A, we give some preliminaries about trajectory and global attractors. In Sec. IV B, we shall prove the existence of trajectory and global attractors for the system (2.22)–(2.27).

A. Preliminaries

We recall the Trajectory Attractors Theory of Vishik and Chepyzhov; cf. Refs. 15 and 16.

Let E, E_0 be two Banach spaces such that $E\subseteq E_0$. An autonomous evolution equation,

$$\frac{\partial u}{\partial t} = G(u), \tag{4.1}$$

where G is a differential operator. Denote a specific family of solutions to the equation (4.1) by $\mathcal{K}^+$, $\mathcal{K}^+ \subset C(\mathbb{R}_+;\, E_0)\cap L^\infty(\mathbb{R}_+;\, E)$. $\mathcal{K}^+$ will be called the *trajectory space* of the equation (4.1) and its elements are *trajectories* of (4.1). $\mathcal{K}^+$ is *translation invariant* in the following sense: if $\forall u(s) \in \mathcal{K}^+$, $h\in\mathbb{R}_+$, then $u(s+h)\in\mathcal{K}^+$.

The action of translation operators $T(t)(t\geq 0)$ on the space $C(\mathbb{R}_+;E_0)\cap L^\infty(\mathbb{R}_+;E)$ is defined by

$$T(t)u(s) = u(t+s), \quad \forall\, t\geq 0, \quad u\in C(\mathbb{R}_+;E_0)\cap L^\infty(\mathbb{R}_+;E).$$

By the definition, we have $T(t_1+t_2)=T(t_1)T(t_2)$ for $t_1,t_2\geq 0$, and $T(0)$ is the identity operator on the space $C(\mathbb{R}_+;E_0)\cap L^\infty(\mathbb{R}_+;E)$. The semigroup $\{T(t)\}=\{T(t);t\geq 0\}$ is known as the *time translation group* on $C(\mathbb{R}_+;\, E_0)\cap L^\infty(\mathbb{R}_+;E)$.

We shall introduce a topology in the trajectory space $\mathcal{K}^+$. We call that the sequence $\{f_n(s)\}$ **(**$\{f_n(s)\}\subset C(\mathbb{R}_+;E_0)$**)** converges to $f(s)$**(**$f(s)\in C(\mathbb{R}_+;E_0)$**)** in the topology space $C_{\text{loc}}(\mathbb{R}_+;E_0)$ if

$$\max_{s\in[0,\mathcal{T}]}\|f_n(s)-f(s)\|_{E_0}\to 0,\quad \text{as } n\to\infty,\quad \forall\,\mathcal{T}>0. \tag{4.2}$$

The topology in $\mathcal{K}^+$ is induced by the topological space $C_{\text{loc}}(\mathbb{R}_+;E_0)$. It is clear that the translation semigroup $\{T(t)\}$ is continuous in the space $C_{\text{loc}}(\mathbb{R}_+;E_0)$, in particular, it is continuous in $\mathcal{K}^+$. A set Ξ is said to be bounded in $\mathcal{K}^+$ if

$$\|u\|_{L^\infty(\mathbb{R}_+;E)}=\operatorname{ess\,sup}_{s\ge 0}\|u(s)\|_E\le c_{16},\quad \forall\, u\in\Xi. \tag{4.3}$$

Definition 4.1: A set $\Lambda\subset C(\mathbb{R}_+;E_0)\cap L^\infty(\mathbb{R}_+;\,E)$ is said to be attracting for the trajectory space $\mathcal{K}^+$ of the equation (4.1) in the topology of $C_{\text{loc}}(\mathbb{R}_+;E_0)$, if for any bounded [in $L^\infty(\mathbb{R}_+;E)$] set $\Xi\subseteq\mathcal{K}^+$ and any number $\mathcal{T}\ge 0$, the following relation holds:

$$\operatorname{dist}_{C(0,\mathcal{T};E_0)}(\Pi_{\mathcal{T}}T(t)\Xi,\Pi_{\mathcal{T}}\Lambda)\to 0,\quad \text{as } t\to\infty, \tag{4.4}$$

where $\Pi_{\mathcal{T}}$ is the restriction operator to the interval $[0,\mathcal{T}]$: if $u\in C(\mathbb{R}_+;E_0)\cap L^\infty(\mathbb{R}_+;E)$, then

$$\Pi_{\mathcal{T}}u\in C(0,\mathcal{T};E_0)\cap L^\infty(0,\mathcal{T};E),\quad \Pi_{\mathcal{T}}u(s)=u(s),\quad \text{for } s\in[0,\mathcal{T}];$$

and

$$\operatorname{dist}_{C(0,\mathcal{T};E_0)}(\Pi_{\mathcal{T}}T(t)\Xi,\Pi_{\mathcal{T}}\Lambda)=\sup_{a\in\Xi}\inf_{b\in\Lambda}\max_{s\in[0,\mathcal{T}]}\|a(s+t)-b(s)\|_{E_0}.$$

Definition 4.2: A set $\mathcal{H}\subseteq\mathcal{K}^+$ is called the **trajectory attractor** in the trajectory space $\mathcal{K}^+$ with respect to the topology $C_{\text{loc}}(\mathbb{R}_+;E_0)$ if we have the following.

(1) $\mathcal{H}$ is a compact set in $C_{\text{loc}}(\mathbb{R}_+;\,E_0)$ and bounded in $L^\infty(\mathbb{R}_+;\,E)$;

(2) $\mathcal{H}$ is strictly invariant with respect to $\{T(t)\}$, i.e.,

$$T(t)\mathcal{H}=\mathcal{H},\quad \forall\, t\ge 0;$$

(3) $\mathcal{H}$ is an attracting set in $\mathcal{K}^+$ in the topology of $C_{\text{loc}}(\mathbb{R}_+;E_0)$.

Theorem 4.3: (cf. Ref. 16): Suppose that the trajectory space $\mathcal{K}^+$ is translation invariant. Assume also that for $\mathcal{K}^+$ there exists an attracting set Λ such that $\Lambda\subseteq\mathcal{K}^+$, Λ is compact set in $C_{\text{loc}}(\mathbb{R}_+;E_0)$ and bounded in $L^\infty(\mathbb{R}_+;E)$. Then in $\mathcal{K}^+$ there exists a trajectory attractor $\mathcal{H}\subseteq\Lambda$ and $\mathcal{H}$ is unique in $\mathcal{K}^+$, moreover,

$$\mathcal{H}=\bigcap_{\mathcal{T}\ge 0}\overline{\bigcup_{t\ge\mathcal{T}}T(t)\Lambda}, \tag{4.5}$$

where $\overline{\cup_{t\ge\mathcal{T}}T(t)\Lambda}$ is the closure of the set $\cup_{t\ge\mathcal{T}}T(t)\Lambda$ in the space $C_{\text{loc}}(\mathbb{R}_+;E_0)$.

Now we shall recall the definition of global attractors. First, we introduce some notations. For a set $\Xi\subseteq E$, we define $\Xi(t)\subseteq E$ for $t\ge 0$ as follows:

$$\Xi(t)=\{u(t);\ u\in\Xi\}\subseteq E.$$

In a similar way, for the trajectory attractor $\mathcal{H}$ we define the set

$$\mathcal{H}(t)=\{u(t);\ u\in\mathcal{H}\}\subseteq E,\quad \text{for } t\ge 0.$$

We note that $\mathcal{H}(t)$ is independent of time t.

Definition 4.4: A set $\mathcal{A}\subseteq E$ is called the *global attractor* in E_0 of the equation (4.1) if we have the following:

(1) $\mathcal{A}$ is a compact set in E_0 and bounded in E;

(2) any bounded [in $L^\infty(\mathbb{R}_+;E)$] set of trajectories $\Xi\subset\mathcal{K}^+$ satisfies the property that the section $\Xi(t)$ are attracted to $\mathcal{A}$ as $t\to\infty$ with respect to the norm of E_0:

$$\operatorname{dist}_{E_0}(\Xi(t),\mathcal{A})\to 0,\ \text{as } t\to\infty; \tag{4.6}$$

(3) $\mathcal{A}$ is the minimal set satisfying (1) and (2), that is, $\mathcal{A}$ belongs to any attracting set compact in E_0 and bounded in E.

Theorem 4.5: (cf. Ref. 16): If the assumptions of Theorem 4.3 are satisfied, then the global attractor (in E_0) $\mathcal{A}$ of the equation (4.1) exists and $\mathcal{A}=\mathcal{H}(0)$.

Remark 4.6: Definition 4.4 generalizes the well-known notion of global (E,E_0)—the attractor of the semigroup corresponding to the Cauchy problem for the equation (4.1) under the assumption that the solution for the problem is unique (see Refs. 20–22). Assume that for any u_0, there exists a unique trajectory $u\in\mathcal{K}^+$ such that $u(0)=u_0$. Then the global attractor (in E_0) is identical to the usual global (E,E_0)—attractor of the semigroup. We shall explain the point in Theorem 4.8.

Under the assumption that there is a unique solution for the Cauchy problem,

$$\frac{\partial u}{\partial t}=G(u),\quad u(0)=u_0, \tag{4.7}$$

following the standard approach, we can introduce an operator semigroup $\{S(t);t\geq 0\}$ in the space E corresponding to the problem (4.7) by the formula

$$S(t)u_0=u(t),\quad t\geq 0. \tag{4.8}$$

Definition 4.7: A set $\mathcal{A}_1\subseteq E$ is called the global (E,E_0) attractor of the semigroup $\{S(t)\}$ acting in E if we have the following:

(1) $\mathcal{A}_1$ is a compact set in E_0 and bounded in E;
(2) $S(t)\mathcal{A}_1=\mathcal{A}_1,\ \forall t\geq 0$;
(3) any bounded (in E) set $\Xi_0\subset E$ satisfies

$$\mathrm{dist}_{E_0}(S(t)\Xi_0,\mathcal{A}_1)\to 0,\quad \text{as } t\to\infty. \tag{4.9}$$

Theorem 4.8. (cf. Ref. 16): Suppose that the assumptions of Theorem 4.5 are satisfied and the semigroup $\{S(t)\}$ is bounded [for any bounded (in E) set $\Xi_0\subset E$, the set $\overline{\cup_{t\geq 0}S(t)\Xi_0}$ is bounded in E]. Then the global (E_0,E) attractor $\mathcal{A}_1$ of the equation (4.1) exists and $\mathcal{A}_1=\mathcal{A}=\mathcal{H}(0)$, where $\mathcal{A}$ is the global attractor (in E_0) of the equation (4.1).

B. Existence of trajectory and global attractors

At first, we shall construct the trajectory space $\mathcal{K}^+$ of the system (2.22)–(2.27). By Theorem 3.8, if $\tilde{U}$ is a weak solution to Problem 3.1, then $\tilde{U}\in L^2(0,\mathcal{T};V)\cap L^\infty(0,\mathcal{T};H)$ and $\tilde{U}$ satisfies the energy inequality

$$-\int_0^\infty |\tilde{U}(t)|_2^2\psi'(s)ds+\frac{1}{R_{\max}}\int_0^\infty \|\tilde{U}(s)\|^2\psi(s)ds\leq 2\int_0^\infty (\tilde{f},\tilde{U}(s))_H\psi(s)ds, \tag{4.10}$$

where $\psi(s)\in C_0^\infty(]0,\mathcal{T}[),\psi(s)\geq 0$. The inequality can be interpreted as follows:

$$\frac{1}{2}\frac{d}{dt}|\tilde{U}(s)|_2^2+\frac{1}{R_{\max}}\|\tilde{U}(s)\|^2\leq\frac{1}{2R_{\max}}\|\tilde{U}(s)\|^2+(\tilde{f},\tilde{U}(s))_H,\quad s\in]0,\mathcal{T}]. \tag{4.11}$$

Definition 4.9: The trajectory space $\mathcal{K}^+$ of the system (2.22)–(2.27) consists of all functions,

$$\tilde{U}\in L^2_{\mathrm{loc}}(\mathbb{R}_+;V)\cap L^\infty(\mathbb{R}_+;H),$$

where $\tilde{U}$ satisfies the condition: for any $\mathcal{T}>0$; the function $\Pi_{\mathcal{T}}\tilde{U}$ is a weak solution for Problem 3.1 on the time interval $[0,\mathcal{T}]$ satisfying the energy inequality (4.10).

Lemma 4.10 (cf. Ref. 23): If Y is a Banach space and $E\subset\subset E_0\subset Y$, where $\subset\subset$ denotes compact embedding, then we have the following embedding:

$$W^{\infty,p}(0,\mathcal{T};E,Y) \subset\subset C(0,\mathcal{T};E_0),$$

where $W^{\infty,p}(0,\mathcal{T};E,Y)=\{u(s);\ s\in(0,\mathcal{T}),u\in L^{\infty}(0,\mathcal{T};E),\ u_t\in L^p(0,\mathcal{T};Y)\}$, $p>1$, with the norm

$$\|u\|_{W^{\infty,p}}=\operatorname{ess}\sup_{\mathcal{T}\geq s\geq 0}\|u\|_E+\left(\int_0^{\mathcal{T}}\|u_t(s)\|_Y^p ds\right)^{1/p}.$$

Proposition 4.11: If $\mathcal{K}^+$ is a trajectory space in Definition 4.9, then we have the following.

(1) For any $\tilde{U}_0\in H$, there exists a trajectory $\tilde{U}(t)\in\mathcal{K}^+$ such that $\tilde{U}(0)=\tilde{U}_0$;

(2) $\mathcal{K}^+\subset C(\mathbb{R}_+;V^{(-3)})\cap L^{\infty}(\mathbb{R}_+;H)$;

(3) $\mathcal{K}^+$ is trajectory invariant, i.e., $T(t)\mathcal{K}^+\subseteq\mathcal{K}^+$.

Proof: By Definition 4.9, we can know that (1), (2) are corollaries of Theorem 3.8 and Lemma 4.10. Since the equations (3.14)–(3.16) are autonomous, $\mathcal{K}^+$ is trajectory invariant for the time translation semigroup $\{T(t)\}$.

Proposition 4.12: For any $\tilde{U}\in\mathcal{K}^+$, the following inequality holds:

$$\begin{aligned}\|T(t)\tilde{U}\|_{L^{\infty}(\mathbb{R}_+;H)}+\|T(t)\tilde{U}\|_{L^2(0,1;V)}+\|T(t)\tilde{U}_t\|_{L^2(0,1;V^{(-3)})}&=\operatorname{ess}\sup_{s\geq t}|\tilde{U}(s)|+\left(\int_t^{t+1}\|\tilde{U}(s)\|^2 ds\right)^{1/2}\\&+\left(\int_t^{t+1}\|\tilde{U}_t(s)\|_{V^{(-3)}}^2\,ds\right)^{1/2}\leq c_{22}\|\tilde{U}\|_{L^{\infty}(0,1;H)}^2\exp(-c_{23}t)+c_{24}\|\tilde{U}\|_{L^{\infty}(0,1;H)}\exp(-c_{23}t)\\&+c_{25},\quad\forall\, t\geq 0.\end{aligned}\tag{4.12}$$

In order to prove Proposition 4.12, we need the following general Gronwall Lemma.

Lemma 4.13. (cf. Ref. 15): Let $y(s)$, $\varphi(s)\in L^1_{\mathrm{loc}}(0,\infty)$, and

$$-\int_0^{\infty}y(s)\psi'(s)ds+\alpha\int_0^{\infty}y(s)\psi(s)ds\leq\int_0^{\infty}\varphi(s)\psi(s)ds,\tag{4.13}$$

for any $\psi(s)\in C_0^{\infty}(\mathbb{R}_+)$, $\psi(s)\geq 0$, where $\alpha\in\mathbb{R}$; then

$$y(t)e^{\alpha t}-y(\tau)e^{\alpha\mathcal{T}}\leq\int_{\mathcal{T}}^{t}\varphi(s)e^{\alpha s}\,ds,$$

for any t, $\mathcal{T}\in\mathbb{R}_+\backslash\tilde{Q}$, $t\geq\mathcal{T}$, where $\mu(\tilde{Q})=0$, and the Lebesgue measure of $\tilde{Q}$ is equal to zero.

Proof of Proposition 4.12: (1) By the definitions of the spaces V, H, $\mathcal{K}^+$, we have

$$c_{17}|\tilde{U}(s)|_2^2\leq\|\tilde{U}(s)\|^2,\quad\forall\,\tilde{U}\in\mathcal{K}^+,\quad s\geq 0.\tag{4.14}$$

By (4.10), we obtain

$$\begin{aligned}-\int_0^{\infty}|\tilde{U}(s)|_2^2\psi'(s)ds+\frac{c_{17}}{2R_{\max}}\int_0^{\infty}|\tilde{U}(s)|_2^2\psi(s)ds\leq\int_0^{\infty}\Bigg(&2R_{\max}\|\tilde{f}\|_{V'}^2-\frac{1}{2R_{\max}}(\|\tilde{U}(s)\|^2\\&-c_{17}|\tilde{U}(s)|_2^2)\Bigg)\psi(s)ds.\end{aligned}\tag{4.15}$$

Applying Lemma 4.13, we get the following inequality:

$$|\widetilde{U}(t)|_2^2 e^{c_{18}t} - |\widetilde{U}(\mathcal{T})|_2^2 e^{c_{18}\mathcal{T}} \le \int_{\mathcal{T}}^{t} \left(2R_{\max}\|\widetilde{f}\|_{V'}^2 - \frac{1}{2R_{\max}}(\|\widetilde{U}(s)\|^2 - c_{17}|\widetilde{U}(s)|_2^2) \right) e^{c_{18}s}\, ds, \tag{4.16}$$

for any t, $\mathcal{T} \in \mathbb{R}_+ \backslash \widetilde{Q}$, $t \ge \mathcal{T}$, $c_{18} = c_{17}/2R_{\max}$, where $\mu(\widetilde{Q}) = 0$. Combining (4.14) with (4.16), we obtain

$$|\widetilde{U}(t)|_2^2 e^{c_{18}t} - |\widetilde{U}(\mathcal{T})|_2^2 e^{c_{18}\mathcal{T}} \le \int_{\mathcal{T}}^{t} 2R_{\max}\|\widetilde{f}\|_{V'} e^{c_{18}s}\, ds. \tag{4.17}$$

By (4.17), we get

$$\|T(t)\widetilde{U}\|_{L^\infty(\mathbb{R}_+;H)} \le \|\widetilde{U}\|_{L^\infty(0,1;H)} \exp(-c_{18}t) + c_{19}, \quad \forall\, t \ge 0. \tag{4.18}$$

(2) Combining (4.16) with (4.18), we get

$$\frac{1}{2R_{\max}} \int_t^{t+1} (\|\widetilde{U}(s)\|^2 - c_{17}|\widetilde{U}(s)|_2^2) e^{c_{18}s}\, ds \le c_{19}(e^{c_{18}(t+1)} - e^{c_{18}t}) + |\widetilde{U}(t)|_2^2 e^{c_{18}t} \le c_{19}(e^{c_{18}(t+1)} - e^{c_{18}t}) + \|\widetilde{U}\|_{L^\infty(0,1;H)}^2 + c_{19}e^{c_{18}t} \le \|\widetilde{U}\|_{L^\infty(0,1;H)}^2 + c_{19}e^{c_{18}(t+1)},$$

i.e.,

$$\frac{1}{2R_{\max}} \int_t^{t+1} \|\widetilde{U}(s)\|^2 e^{c_{18}s}\, ds \le c_{18} \int_t^{t+1} |\widetilde{U}(s)|_2^2 e^{c_{18}s}\, ds + \|\widetilde{U}\|_{L^\infty(0,1;H)}^2 + c_{19}e^{c_{18}(t+1)}. \tag{4.19}$$

By (4.18), we have

$$c_{18} \int_t^{t+1} |\widetilde{U}(s)|_2^2 e^{c_{18}s}\, ds \le c_{18}\|\widetilde{U}\|_{L^\infty(0,1;H)}^2 + c_{19}(e^{c_{18}(t+1)} - e^{c_{18}t}). \tag{4.20}$$

Combining (4.19) with (4.20), we obtain

$$\frac{1}{2R_{\max}} \int_t^{t+1} \|\widetilde{U}(s)\|^2 e^{c_{18}s}\, ds \le (c_{18}+1)\|\widetilde{U}\|_{L^\infty(0,1;H)}^2 + c_{19}(2e^{c_{18}(t+1)} - e^{c_{18}t}).$$

Therefore

$$\frac{1}{2R_{\max}} \int_t^{t+1} \|\widetilde{U}(s)\|^2\, ds \le (c_{18}+1)\|\widetilde{U}\|_{L^\infty(0,1;H)}^2 e^{-c_{18}t} + c_{19}(2e^{c_{18}} - 1). \tag{4.21}$$

(3) By Lemma 3.2, Lemma 3.3, Lemma 3.6, assumptions of Problem 3.1 and (3.22), we obtain

$$\|\widetilde{U}_t(s)\|_{V^{(-3)}} \le \|\widetilde{U}(s)\|\,|\widetilde{U}(s)|_2 + c_{20}\|\widetilde{U}(s)\| + \|\widetilde{f}\|_{V'}.$$

So

$$\left(\int_t^{t+1}\|\widetilde{U}_t(s)\|^2_{V^{(-3)}}\,ds\right)^{1/2}\le\left(\int_t^{t+1}\|\widetilde{U}(s)\|^2|\widetilde{U}(s)|_2^2\,ds\right)^{1/2}+c_{21}+c_{21}\left(\int_t^{t+1}\|\widetilde{U}(s)\|^2\,ds\right)^{1/2}$$
$$\le c_{21}\|\widetilde{U}\|_{L^\infty(t,t+1;H)}\left(\int_t^{t+1}\|\widetilde{U}(s)\|^2\,ds\right)^{1/2}+c_{21}$$
$$+c_{21}\left(\int_t^{t+1}\|\widetilde{U}(s)\|^2\,ds\right)^{1/2},\quad\forall\, t\ge 0. \tag{4.22}$$

Therefore, by (4.18), (4.21), (4.22), there exist two positive constants c_{20},c_{21}, such that

$$\|T(t)\widetilde{U}\|_{L^\infty(\mathbb{R}_+;H)}+\|T(t)\widetilde{U}\|_{L^2(0,1;V)}+\|T(t)\widetilde{U}_t\|_{L^2(0,1;V^{(-3)})}\le c_{22}\|\widetilde{U}\|^2_{L^\infty(0,1;H)}\exp(-c_{23}t)$$
$$+c_{24}\|\widetilde{U}\|_{L^\infty(0,1;H)}\exp(-c_{23}t)+c_{25},\quad\forall\, t\ge 0.$$

The proof is complete.

Proposition 4.14: If $\{\widetilde{U}_n\}\subset\mathcal{K}^+$ is a bounded sequence in $L^\infty(\mathbb{R}_+;H)$, and for some $\widetilde{U}\in C(\mathbb{R}_+;V^{(-3)})$ the following relation holds:

$$\widetilde{U}_n\to\widetilde{U}\quad\text{in } C_{\mathrm{loc}}(\mathbb{R}_+;V^{(-3)}),\quad\text{as } n\to\infty.$$

Then $\widetilde{U}\in\mathcal{K}^+$.

Proof: We only give the outline of the proof. Since $\{\widetilde{U}_n\}\subset\mathcal{K}^+$ is bounded in $L^\infty(\mathbb{R}_+;H)$, by Proposition 4.12, we know, if necessary going to the subsequence of $\{\widetilde{U}_n\}$,

$$(\widetilde{U}_n)_t+A\widetilde{U}_n+(B\widetilde{U}_n,\widetilde{U}_n)+(B\widetilde{U}_n,U')+(F\widetilde{U}_n,U')+\widetilde{E}\widetilde{U}_n-\widetilde{f}\rightharpoonup(\widetilde{U})_t+A\widetilde{U}+(B\widetilde{U},\widetilde{U})+(B\widetilde{U},U')$$
$$+(F\widetilde{U},U')+\widetilde{E}\widetilde{U}-\widetilde{f},$$

weakly in $L^2(0,\mathcal{T};V^{(-3)})$, for any $\mathcal{T}>0$. Hence $\widetilde{U}$ is a weak solution for Problem 3.1.

In order to prove that $\widetilde{U}\in\mathcal{K}^+$, we should check that $\widetilde{U}$ satisfies the energy inequality (4.10). By $\{\widetilde{U}_n\}\subset\mathcal{K}^+$, for every n, $\widetilde{U}_n$ satisfies

$$-\int_0^\infty|\widetilde{U}_n(t)|_2^2\psi'(s)ds+\frac{1}{R_{\max}}\int_0^\infty\|\widetilde{U}_n(s)\|^2\psi(s)ds\le 2\int_0^\infty(\widetilde{f},\widetilde{U}_n(s))_H\psi(s)ds,$$

where $\psi(s)\in C_0^\infty(]0,\mathcal{T}[)$, $\psi(s)\ge 0$. Since $\{\widetilde{U}_n\}\subset\mathcal{K}^+$ is bounded in $L^\infty(\mathbb{R}_+;H)$, by Proposition 4.12, going if necessary to a subsequence, we obtain that $\widetilde{U}_m\to\widetilde{U}$ $(m\to\infty)$ weakly in $L^2(0,\mathcal{T};V)$ and * weakly in $L^\infty(0,\mathcal{T};H)$. Similarly to prove (3.39), we can take a limit in the above inequality and get the energy inequality

$$-\int_0^\infty|\widetilde{U}(t)|_2^2\psi'(s)ds+\frac{1}{R_{\max}}\int_0^\infty\|\widetilde{U}(s)\|^2\psi(s)ds\le 2\int_0^\infty(\widetilde{f},\widetilde{U}(s))_H\psi(s)ds.$$

Now we can state the main result of this section.

Theorem 4.15: Under the assumptions of Problem 3.1, there is a trajectory attractor $\mathcal{H}\subseteq\mathcal{K}^+$ for the system (2.22)–(2.27) and $\mathcal{H}$ is unique in $\mathcal{K}^+$. Moreover $\mathcal{A}=\mathcal{H}(0)$ is the global attractor for the system (2.22)–(2.27) in the space $V^{(-3)}$.

Proof: In order to apply Theorem 4.3 and Theorem 4.5, we have to construct an attracting set Λ for the time translation semigroup $\{T(t)\}$, where $\Lambda\subseteq\mathcal{K}^+$ and Λ is a compact set in $C_{\mathrm{loc}}(\mathbb{R}_+;V^{(-3)})$ and bounded in $L^\infty(\mathbb{R}_+;H)$. Let

$$\Lambda = \left\{ \widetilde{U} \in \mathcal{K}^+;\ \operatorname*{ess\,sup}_{t\geq 0}\{\|\widetilde{U}\|_{L^\infty(t,t+1;H)} + \|\widetilde{U}_t\|_{L^2(t,t+1;V^{(-3)})}\} \leq 3c_{25} \right\}. \tag{4.23}$$

We claim that Λ is an attracting set that satisfies the conditions in Theorem 4.3. Indeed, assume $\Xi \subseteq \mathcal{K}^+$ and Ξ is a bounded in $L^\infty(\mathbb{R}_+;\ H)$, i.e.,

$$\|\widetilde{U}\|_{L^\infty(\mathbb{R}_+;\ H)} = \operatorname*{ess\,sup}_{s\geq 0}\|\widetilde{U}\|_E \leq c_{26}, \quad \forall\ u \in \Xi.$$

By Proposition 4.12, there exists $t_1 > 0$ such that $T(t)\Xi \subseteq \Lambda$ for $t \geq t_1$. By the definition of Λ, we can know that Λ is bounded in $L^\infty(\mathbb{R}_+;\ H)$. By (4.23), for any $\mathcal{T} > 0$, $\Pi_{\mathcal{T}}\Lambda$ is bounded in $W^{\infty,2}(0,\mathcal{T};H,V^{(-3)})$. Applying Lemma 4.10, we can obtain that the closure of $\Pi_{\mathcal{T}}\Lambda$ is compact in $C(0,\mathcal{T};\ V^{(-3)})$, that is, the closure of Λ is compact in $C_{\mathrm{loc}}(\mathbb{R}_+;V^{(-3)})$. Now, we shall prove that Λ is closed in $C_{\mathrm{loc}}(\mathbb{R}_+;V^{(-3)})$. Suppose that there is a sequence $\{\widetilde{U}_n\} \subset \Lambda$ that satisfies

$$\widetilde{U}_n \to \widetilde{U} \quad \text{in } C_{\mathrm{loc}}(\mathbb{R}_+;V^{(-3)}), \quad \text{as } n \to \infty .$$

On the other hand, by (4.23), $\{\widetilde{U}_n\}$ is bounded in $L^\infty(\mathbb{R}_+;H)$. Applying Proposition 4.14, we get that $\widetilde{U} \in \mathcal{K}^+$. By the lower weak continuity of the norm and

$$\|\widetilde{U}_n\|_{L^\infty(t,t+1;H)} + \|(\widetilde{U}_n)_t\|_{L^2(t,t+1;V^{(-3)})} \leq 3c_{25},$$

we can have

$$\|\widetilde{U}\|_{L^\infty(t,t+1;H)} + \|\widetilde{U}_t\|_{L^2(t,t+1;V^{(-3)})} \leq 3c_{25}.$$

Therefore, $\widetilde{U} \in \Lambda$, that is, Λ is compact in $C_{\mathrm{loc}}(\mathbb{R}_+;\ V^{(-3)})$. Applying Theorem 4.3 and Theorem 4.5, we obtain Theorem 4.15 and the trajectory attractor

$$\mathcal{H} = \cap_{\mathcal{T}\geq 0}\overline{\cup_{t\geq \mathcal{T}} T(t)\Lambda},$$

where $\overline{\cup_{t\geq \mathcal{T}} T(t)\Lambda}$ is the closure of the set $\cup_{t\geq \mathcal{T}} T(t)\Lambda$ in the space $C_{\mathrm{loc}}(\mathbb{R}_+;\ V^{(-3)})$. The proof is complete.

Remark 4.16: In Lemma 4.10, we can let $E_0 = V^{(-\delta)}$, $0 < \delta \leq 3$, $E = H$, $Y = V^{(-3)}$, where E_0 is in Theorem 4.8, $V^{(-\delta)} = (V^{(\delta)})'$ and the definition of $V^{(\delta)}$ is similar to $V^{(3)}$. Thus, we can replace $V^{(-3)}$ in Propositions 4.11, 4.14 by $V^{(-\delta)}$. Therefore, we obtain the trajectory attractor $\mathcal{H} \subseteq \mathcal{K}^+ \subset C(\mathbb{R}_+;V^{(-\delta)}) \cap L^\infty(\mathbb{R}_+;H)$ and the global attractor of the system (2.22)–(2.27) in the space $V^{(-\delta)}$.

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Waves, particles, and field dynamics

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The idea of associating particle trajectories with wave propagation rays is examined in the context of general relativity. The additional assumption that also Hamilton-Jacobi particle equation and wave front equation of motion can be identified in an $n>3$ coordinate space leads to a Kaluza-Klein type theory involving Klein-Gordon and Dirac equations. Moreover de Broglie and Einstein-Planck quantum relations can be deduced in a natural way. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In the present paper we attempt to suggest a new point of view on the intriguing problems of wave-particle duality and the relationship between general relativity and quantum mechanics.[1]

A. Historical context

In 1970, Boillat[2] proposed the idea that the trajectories of motion of (*stable*) *particles* could be identified with the rays of propagation of (*exceptional*) *waves* across the physical space. Such an idea somehow reminds one of the concept of *pilot wave* earlier introduced by de Broglie[3] and also the so-called "realistic" interpretation of Schrödinger equation given by Bohm.[4] Boillat's approach is significantly different with respect to previous ones since he operates in the context of a quite general *nonlinear* wave propagation theory[5] obtaining the well-known Born-Infeld electrodynamics[6] and some other relevant results (for interesting physical applications see, e.g., Refs. 7 and 8).

B. Our contribution

Here we will come back to the idea of identifying *wave rays* and *particle trajectories* but we add a further assumption by also requiring that the *evolution equation*, along wave rays (provided by wave kinematics), and the *Hamilton-Jacobi equation* (governing the particles dynamics) must be identified. As we shall see, we will be able to tune wave and particle motions provided that the *normal speeds* of waves are equal to the speed of light c across an *n-dimensional* coordinate space. This condition leads to the dynamics of a zero rest mass particle across the same *n-dimensional* space, the projection of which onto the physical *three-dimensional* subspace embedded into it can be interpreted as the motion of a massive relativistic particle.[9] (For models treating mass as related to higher dimensional space-time see, e.g., Refs. 10–18). We look also for the Lagrangian governing the *field* candidate to fit the conditions arising from the previous assumptions and we obtain Klein-Gordon and Dirac equations arising in the embedded physical space from a D'Alembert equation holding in the embedding space.

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II. WAVES AND PARTICLE DYNAMICS

Let us consider an $n+1$ dimensional real differentiable manifold V^{n+1}, representing a space-time endowed with a symmetric metric g of signature $(+,-,\cdots,-)$ and a torsionless connection Γ. On V^{n+1} we represent any system of curvilinear coordinates with $x^{\mu},\mu=0,I$, with $I=1,2,\ldots,n$. The phyisically observable space-time is then described by a four-dimensional sub-manifold V^4 on which the observable coordinates are labeled by the indices $0,i$, where $i=1,2,3$, while we will label the remaining coordinates $x^4,x^5,\ldots,x^n$ by underlined Latin indices $\underline{i}=4,5,\ldots,n$. (We point out that the signature relative to the extra dimensions seems to be relevant for our purposes and cannot be taken otherwise.) For our purposes it proves convenient to adopt the synchronous gauge which requires the following $n+1$ conditions on the metric tensor:

$$g_{00}=1, \quad g_{0I}=g_{I0}=0, \tag{1}$$

implying the synchronization of time:

$$x^0=ct. \tag{2}$$

Let us now consider any differentiable real valued function $\varphi(t,x^I)$, which we can always assume to be dimensionless, such that

$$g^{\mu\nu}\frac{\partial\varphi}{\partial x^{\mu}}\frac{\partial\varphi}{\partial x^{\nu}}\leqslant 0, \tag{3}$$

$g^{\mu\nu}$ being the contravariant components of the metric tensor defined as usual by the relation

$$g^{\mu\nu}g_{\nu\rho}=\delta^{\mu}_{\rho}. \tag{4}$$

Then

$$\varphi(t,x^I)=0 \tag{5}$$

may be interpreted as the world sheet of a wave front traveling across the n-space. We point out that φ is determined by (5) except for an arbitrary nonvanishing factor. The trajectory (*ray*) of each point of the wave front can be described by its parametric equations:

$$x^I\equiv x^I(t). \tag{6}$$

Substituting (6) into (5) and differentiating with respect to t we obtain the differential equation governing the wave kinematics:

$$\frac{\partial\varphi}{\partial t}+V^I\frac{\partial\varphi}{\partial x^I}=0, \tag{7}$$

where

$$V^I=\frac{\mathrm{d}}{\mathrm{d}t}x^I(t) \tag{8}$$

is the ray velocity of the point of the wave front. Assuming $\varphi_{,I}\neq 0$, Eq. (7) can be written also in the equivalent form:

$$\frac{\partial\varphi}{\partial t}+V|\nabla\varphi|=0, \quad |\nabla\varphi|=\sqrt{-g^{IK}\varphi_{,I}\varphi_{,K}}, \tag{9}$$

where the contravariant components of the metric tensor, in the gauge (1), result to be

$$g^{00}=1, \quad g^{0I}=g^{I0}=0, \quad g^{IJ}g_{JK}=\delta^I_K. \tag{10}$$

Then the normal wave speed is given by

$$V = V^I n_I, \quad n_I = \frac{\varphi_{,I}}{|\nabla\varphi|}, \quad g^{IK} n_I n_K = -1, \tag{11}$$

the comma denoting partial derivative, as usual. The first step of our work consists in asking whether and at which conditions the first equation in Eq. (9)—the wave front equation—can be interpreted also as a Hamilton-Jacobi equation:

$$\frac{\partial S}{\partial t} + H = 0, \tag{12}$$

governing the motion of some particle. In order to make possible such interpretation we may think of the function φ as proportional to the Hamilton generating function of the particle dynamics according to

$$S = \alpha\varphi, \tag{13}$$

where α is a suitable dimensional (positive) constant which will be specified later coherently with a physical interpretation of the theory. Then we can write the first equation in (9) in the form (12) provided that the Hamiltonian of the particle is given by

$$H = V|\nabla S|, \quad |\nabla S| = \sqrt{-g^{IK} S_{,I} S_{,K}}. \tag{14}$$

Since, according to Hamilton-Jacobi's theory,

$$p_I = S_{,I}, \quad E = H \tag{15}$$

(where p_I is the canonical momentum of the particle, and the Hamiltonian H is the generalized energy) from (14) it results:

$$E = V\sqrt{-g^{IK} p_{,I} p_{,K}}. \tag{16}$$

It is immediate to see that (16) is compatible with relativity if and only if

$$V = c, \tag{17}$$

and the particle has zero rest mass. In fact at those conditions it results:

$$E = cp, \quad p = \sqrt{-g^{IK} p_I p_K}. \tag{18}$$

The Hamilton equations,

$$\frac{\mathrm{d}p_I}{\mathrm{d}t} = -\frac{\partial H}{\partial x^I}, \quad \frac{\mathrm{d}x^I}{\mathrm{d}t} = \frac{\partial H}{\partial p_I}, \tag{19}$$

result:

$$\frac{\mathrm{d}p_I}{\mathrm{d}t} = g^{JK}{}_{,I} \frac{c p_J p_K}{2p}, \tag{20}$$

$$\frac{\mathrm{d}x^I}{\mathrm{d}t} = -c\frac{p^I}{p}. \tag{21}$$

One realizes that (20) is also equivalent to the geodesic condition:

$$\frac{\mathrm{d}p_I}{\mathrm{d}t} - \Gamma^K_{IJ} p_K \frac{\mathrm{d}x^J}{\mathrm{d}t} = 0, \tag{22}$$

which, thanks to (21), becomes

$$\frac{\mathrm{d}p_I}{\mathrm{d}t} + \Gamma^K_{IJ}\frac{cp^J p_K}{p} = 0. \tag{23}$$

In fact,

$$\tfrac{1}{2}g^{JK}{}_{,I}p_J p_K \equiv -\Gamma^K_{JI}p_K p^J,$$

being

$$g^{JK}{}_{;I} \equiv g^{JK}{}_{,I} + \Gamma^J_{IM}g^{MK} + \Gamma^K_{IM}g^{JM} = 0, \tag{24}$$

because of the metricity of g^{JK}, where

$$\Gamma^K_{JI} = \tfrac{1}{2}g^{KM}(g_{JM,I} + g_{IM,J} - g_{JI,M}). \tag{25}$$

Therefore we may conclude that the differential equation governing wave kinematics may be identified with the Hamilton-Jacobi equation governing the motion of a massless particle traveling at the speed of light across the *n-dimensional* space, provided that the wave itself travels at the speed of light. Now we can split the n-vectors $(p_I),(x^I)$ into their components onto the physical space and p_i,x^i and the extra components $p_{\underline{i}},x^{\underline{i}}$ and write

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = g^{jk}{}_{,i}\frac{cp_j p_k}{2p} + g^{\underline{jk}}{}_{,i}\frac{cp_{\underline{j}}p_{\underline{k}}}{2p} + g^{j\underline{k}}{}_{,i}\frac{cp_j p_{\underline{k}}}{p}, \quad \frac{\mathrm{d}x^i}{\mathrm{d}t} = -c\frac{p^i}{p}, \tag{26}$$

$$\frac{\mathrm{d}p_{\underline{i}}}{\mathrm{d}t} = g^{jk}{}_{,\underline{i}}\frac{cp_j p_k}{2p} + g^{\underline{jk}}{}_{,\underline{i}}\frac{cp_{\underline{j}}p_{\underline{k}}}{2p} + g^{j\underline{k}}{}_{,\underline{i}}\frac{cp_j p_{\underline{k}}}{p}, \quad \frac{\mathrm{d}x^{\underline{i}}}{\mathrm{d}t} = -c\frac{p^{\underline{i}}}{p}. \tag{27}$$

Moreover we can interpret

$$m = \frac{1}{c}\sqrt{-(2g^{\underline{ik}}p_k + g^{\underline{ik}}p_{\underline{k}})p_{\underline{i}}}, \tag{28}$$

as a constant rest mass of some particle provided that we assume

$$(2g^{\underline{ik}}p_k + g^{\underline{ik}}p_{\underline{k}})p_{\underline{i}} = \text{const}. \tag{29}$$

Such a choice is always possible since $p_I = \alpha\varphi_{,I}$ and φ is defined except for a nonvanishing factor according to (5). Then we gain the Hamiltonian of a massive particle:

$$H = c\sqrt{m^2c^2 + \vec{p}^2}, \quad \vec{p}^2 = -g^{ik}p_i p_k. \tag{30}$$

We point out that when

$$\tfrac{1}{2}g^{\underline{jk}}{}_{,i}p_j p_{\underline{k}} + g^{j\underline{k}}{}_{,i}p_j p_{\underline{k}} = 0, \tag{31}$$

and g_{jk} depends only on the observable variables t,x^i, the first equation in (26) becomes the equation of the geodesic trajectory of a particle of rest mass m crossing the physical 3D space in the presence of a gravitational field. More (nongravitational fields) described by $g_{\underline{jk}},g_{j\underline{k}}$, can be introduced in a Kaluza-Klein type theory (see Sec. VII).

III. dE BROGLIE AND EINSTIEN-PLANCK RELATIONS

The Hamilton generating function S, proportional to the function φ, can easily be evaluated by integration of Eq. (7), in which the ray velocity V^I has the direction of the normal vector n^I, resulting in

$$V^I = -cn^I. \tag{32}$$

Then the equation to be integrated becomes

$$\frac{\partial S}{\partial t} - cn^I \frac{\partial S}{\partial x^I} = 0, \tag{33}$$

or

$$\frac{\partial S}{\partial t} + c\frac{\partial S}{\partial x_n} = 0, \tag{34}$$

since

$$n^I S_{,I} = -\frac{\partial S}{\partial x_n}, \quad x_n = x^I n_I.$$

The solution is

$$S = f(x_n - ct) \equiv f(x^I n_I - ct) \equiv f(x^i n_i + x^{\underline{i}} n_{\underline{i}} - ct), \tag{35}$$

where f may be any differentiable function of its argument $x_n - ct$. Such kind of solution is what in wave propagation theory is called a *simple wave*.[19–21] Since $S = \alpha\varphi$, it results also that

$$\varphi = \frac{1}{\alpha} f(x^i n_i + x^{\underline{i}} n_{\underline{i}} - ct). \tag{36}$$

Then the canonical momenta, evaluated during the wave-particle motion, become

$$p_I = \alpha\varphi' n_I, \Leftrightarrow p_i = \alpha\varphi' n_i, \quad p_{\underline{i}} = \alpha\varphi' n_{\underline{i}}, \tag{37}$$

and the Hamiltonian:

$$H \equiv E = \alpha c \varphi'. \tag{38}$$

It proves convenient to introduce the following quantities related to wave propagation:

$$k_I = \varphi' n_I, \Leftrightarrow k_i = \varphi' n_i, \quad k_{\underline{i}} = \varphi' n_{\underline{i}}, \tag{39}$$

$$\omega = c\varphi'. \tag{40}$$

On identifying the constant α with Planck's constant the following well-known relations arise naturally:

$$p_I = \hbar\, k_I \Leftrightarrow p_i = \hbar\, k_i, \quad p_{\underline{i}} = \hbar\, k_{\underline{i}} \text{ (de Broglie)}, \tag{41}$$

$$E = \hbar\, \omega \text{ (Einstien-Planck)}. \tag{42}$$

In the special case of a periodic wave it is immediate to recognize in the quantities $\omega, (k_I) \equiv (k_i, k_{\underline{i}})$, the frequency and the wave number vectors.

IV. WAVE DYNAMICS AND FIELD EQUATIONS

The problem of wave dynamics consists in determining a class of field equation candidates to explain the wave kinematics equivalent to Hamilton-Jacobi particle mechanics, as examined in the previous sections. Of course the main condition required by the system of field equations is that it must provide waves traveling with the speed of light across an *n-dimensional* space, but that condition alone is too wide to characterize a physically meaningful class of field equations. So we need some other reasonable assumptions. Therefore we will require the following ones:

(i) The system of field equations must be Lagrangian. This condition is usual for physical fields and needs no special explanation.
(ii) The production term of the system must be zero (at least in correspondence to the simple wave solutions). This second assumption is required in order to provide regular solutions to the system as simple waves,[19–21] ensuring that the particles travel along the rays at characteristic speeds. In principle also discontinuity waves[22] could be considered, but if we want to be able to compare the results with quantum mechanical ones we need regular solutions which can be expanded into Fourier series.
(iii) The normal speed of all simple waves must be equal to the speed of light c. This is the true kinematic condition we have previously examined.

The Lagrangian system. Let us consider a candidate field $\boldsymbol{\psi}$, which in general may be a complex column vector belonging to an N-dimensional Euclidean complex space, and is assumed to be a set of regular functions of x^I,t, invariant with respect to any regular coordinate transformation; and let

$$L \equiv \sqrt{|g|}\mathcal{L}(\boldsymbol{v},\boldsymbol{v}^+,\boldsymbol{w}_I,\boldsymbol{w}_I^+), \quad \boldsymbol{v} = \frac{\partial \boldsymbol{\psi}}{\partial t}, \quad \boldsymbol{w}_I = \frac{\partial \boldsymbol{\psi}}{\partial x^I} \tag{43}$$

be a Lagrangian density governing the field dynamics (where $^+$ denotes the transposed complex conjugation). Such Lagrangian is supposed to depend only on $\boldsymbol{v},\boldsymbol{w}_I$, in order to fulfill assumption (ii). Then the system of first-order field equations is

$$\frac{\partial}{\partial t}\left(\sqrt{|g|}\frac{\partial \mathcal{L}}{\partial \boldsymbol{v}^+}\right) + \frac{\partial}{\partial x^I}\left(\sqrt{|g|}\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}_I^+}\right) = 0, \tag{44}$$

$$\frac{\partial \boldsymbol{w}_I}{\partial t} - \frac{\partial \boldsymbol{v}}{\partial x^I} = 0 \tag{45}$$

(together with its complex conjugate). On applying the correspondence rules,[19]

$$\frac{\partial}{\partial t}(\cdot) \to -\lambda\frac{\partial}{\partial \varphi}(\cdot) \equiv -\lambda(\cdot)', \quad \frac{\partial}{\partial x^I}(\cdot) \to n_I\frac{\partial}{\partial \varphi}(\cdot) \equiv n_I(\cdot)', \tag{46}$$

prime denoting differentiation respect to φ, we obtain, according to wave propagation theory, the algebraic system for the simple waves:

$$-\lambda\left(\sqrt{|g|}\frac{\partial \mathcal{L}}{\partial \boldsymbol{v}^+}\right)' + n_I\left(\sqrt{|g|}\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}_I^+}\right)' = 0, \tag{47}$$

$$-\lambda \boldsymbol{w}_I' - n_I \boldsymbol{v}' = 0, \tag{48}$$

in which λ is the characteristic normal speed of the simple waves and the unknown field variables $\boldsymbol{v},\boldsymbol{w}_I$ are functions of φ. We point out that even if the wave propagation theory we are applying here was originally carried out in the context of real valued fields, its extension to complex fields is straightforward (see, e.g., Ref. 23). Simple manipulations on (47) and (48), after eliminating $\boldsymbol{w}_I$ by direct substitution, lead to

$$n_I\left\{\lambda^2\frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{v}^+\,\partial \boldsymbol{v}}g^{IJ} - \lambda\left(n^I\frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{v}^+\,\partial \boldsymbol{w}_J} + \frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{w}_I^+\,\partial \boldsymbol{v}}n^J\right) - \frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{w}_I^+\,\partial \boldsymbol{w}_J}\right\}n_J\boldsymbol{v}' = 0. \tag{49}$$

Since the Lagrangian density cannot depend on the wave front geometry, i.e., on n_I, the following conditions must hold:

$$\lambda^2 \frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{v}^+ \partial \boldsymbol{v}} g^{IJ} - \frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{w}_I^+ \partial \boldsymbol{w}_J} = 0, \tag{50}$$

$$\frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{v}^+ \partial \boldsymbol{w}_J} = 0 \Leftrightarrow \frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{w}_I^+ \partial \boldsymbol{v}} = 0. \tag{51}$$

The latter condition implies that

$$\mathcal{L} = \mathcal{L}_1(\boldsymbol{v}, \boldsymbol{v}^+) + \mathcal{L}_2(\boldsymbol{w}_I, \boldsymbol{w}_I^+), \tag{52}$$

which introduced into the former yields

$$\lambda^2 \frac{\partial^2 \mathcal{L}_1}{\partial \boldsymbol{v}^+ \partial \boldsymbol{v}} g^{IJ} - \frac{\partial^2 \mathcal{L}_2}{\partial \boldsymbol{w}_I^+ \partial \boldsymbol{w}_J} = 0. \tag{53}$$

Thanks to our assumption (iii), the normal speeds of simple wave propagation must equal the speed of light, and therefore (53) becomes

$$c^2 \frac{\partial^2 \mathcal{L}_1}{\partial \boldsymbol{v}^+ \partial \boldsymbol{v}} g^{IJ} = \frac{\partial^2 \mathcal{L}_2}{\partial \boldsymbol{w}_I^+ \partial \boldsymbol{w}_J}. \tag{54}$$

The Hessian matrices of $\mathcal{L}_1, \mathcal{L}_2$ are manifestly independent of the fields $\boldsymbol{v}, \boldsymbol{w}_I$, so we may write them as

$$\frac{\partial^2 \mathcal{L}_1}{\partial \boldsymbol{v}^+ \partial \boldsymbol{v}} = \frac{1}{c^2} \mathsf{a}, \tag{55}$$

$$\frac{\partial^2 \mathcal{L}_2}{\partial \boldsymbol{w}_I^+ \partial \boldsymbol{w}_J} = g^{IJ} \mathsf{a}, \tag{56}$$

where a is a nonsingular Hermitian matrix, independent of the fields. From those conditions the form of Lagrangian density is determined as

$$L = \tfrac{1}{2} \sqrt{|g|} \left(g^{IJ} \boldsymbol{w}_I^+ \mathsf{a} \boldsymbol{w}_J + \frac{1}{c^2} \boldsymbol{v}^+ \mathsf{a} \boldsymbol{v} \right). \tag{57}$$

The Euler-Lagrange equations are given by

$$\frac{\partial}{\partial t} (\sqrt{|g|} \mathsf{a} \boldsymbol{v}) + \frac{\partial}{\partial x^J} (c^2 \sqrt{|g|} g^{IJ} \mathsf{a} \boldsymbol{w}_J) = 0, \tag{58}$$

or

$$(\mathsf{a} \boldsymbol{v})_{;0} + (c g^{IJ} \mathsf{a} \boldsymbol{w}_J)_{;I} = 0. \tag{59}$$

We observe that a, beside being independent of the fields $\boldsymbol{v}, \boldsymbol{w}_I$, must be independent also of x^I, t, otherwise a nonvanishing production term will arise into the field equations. Then, since a is a nonsingular matrix, taking account of the metricity condition ($g^{IJ}{}_{;K}=0$), the field equations result simply:

$$\boldsymbol{v}_{;0} + c g^{IJ} \boldsymbol{w}_{J;I} = 0, \quad c \boldsymbol{w}_{I;0} - \boldsymbol{v}_{;I} = 0. \tag{60}$$

The coefficient matrix a disappears from the equations and its role becomes irrelevant in the Lagrangian; so it is not a restriction to choose:

$$\mathsf{a} = k\mathsf{I}, \tag{61}$$

with k the dimensional constant and I the identity matrix in the field space. Then the scalar Lagrangian density becomes

$$\mathcal{L} = \frac{1}{2}k\left(g^{IJ}\boldsymbol{w}_I^+\boldsymbol{w}_J + \frac{1}{c^2}\boldsymbol{v}^+\boldsymbol{v}\right). \tag{62}$$

We point out that the algebraic system which determines the simple waves, arising from (60), which is given by

$$\frac{1}{c}\lambda\boldsymbol{v}' - cn^I\boldsymbol{w}_I' = 0, \quad \lambda\boldsymbol{w}_I' + n_I\boldsymbol{v}' = 0, \tag{63}$$

yields, through direct substitution,

$$(\lambda^2 - c^2)\boldsymbol{v}' = 0, \tag{64}$$

from which the characteristic speeds become

$$\lambda = \pm c. \tag{65}$$

Such values imply, significantly, that the energy of the particle associated to wave propagation, thanks to (16), taking into account that $V=\lambda$, results to be

$$E = \pm\sqrt{m^2c^4 + c^2\vec{p}^2}. \tag{66}$$

The latter result states that, corresponding to any simple wave front traveling at normal speed $+c$, there exists an identical wave front traveling in the opposite sense at speed $-c$; that is usual in wave propagation. And, corresponding to a particle of energy $+|E|$, associated with the former wave, there exists another particle of negative energy $-|E|$, associated to the latter wave. Such circumstance, as it is well known, was noticed for the first time by Dirac, examining the solutions of his famous equation. According to our present approach the result arises naturally as a consequence of wave particle correlation expressed by (16), being $V=\lambda$, and the assumption that the system of field equations is Lagrangian.

V. THE KLEIN-GORDON EQUATION

Let us now study in more detail the system of field equations (60).

A. Second-order formulation

First of all we point out that we can always replace the fields $\boldsymbol{v}, \boldsymbol{w}_I$, with their original definitions in terms of derivatives of the field $\boldsymbol{\psi}$, according to (43), obtaining a system of N second-order equations, instead of the original system of $2N$ first-order equations:

$$\boldsymbol{\psi}_{;0;0} + g^{IJ}\boldsymbol{\psi}_{;I;J} = 0. \tag{67}$$

This generalized D'Alembert equation governing the propagation of the field $\boldsymbol{\psi}$ across the *n-dimensional* space is equivalent to a generalized Klein-Gordon equation for the propagation of the same field across the physical *three-dimensional* space. In fact the solutions of the field, being simple waves, depend on the argument $x_n - ct$ being composite functions through φ of the same argument. Now:

$$x_n - ct \equiv \frac{1}{p}(p_I x^I - cpt) \equiv \frac{c}{E}(p_I x^I - Et). \tag{68}$$

Therefore we can consider the field $\boldsymbol{\psi}$ as a function of the form:

$$\boldsymbol{\psi} \equiv \boldsymbol{\psi}(p_i x^i + p_{\underline{i}} x^{\underline{i}} - Et). \tag{69}$$

Without affecting time we may choose the space coordinates $x^{\underline{i}}$ in such a way that

$$x^n = x^i N_{\underline{i}}, \quad g^{nn} \equiv g^{\underline{jk}} N_{\underline{j}} N_{\underline{k}} = -1, \quad g^{ij} = g^{j\underline{i}} = 0, \tag{70}$$

with

$$p_{\underline{i}} = -mcN_{\underline{i}}, \quad N_{\underline{i}} = \frac{p_{\underline{i}}}{\sqrt{-g^{\underline{jk}} p_{\underline{j}} p_{\underline{k}}}}. \tag{71}$$

Then the simple wave will travel across a five-dimensional sub-space-time, resulting in (69)

$$\boldsymbol{\psi} \equiv \boldsymbol{\psi}(p_i x^i + mcx^n - Et). \tag{72}$$

If we require the additional assumption that $\boldsymbol{\psi}$ belongs to the Hilbert space L^2, so that it can be expanded into Fourier series, we can write

$$\boldsymbol{\psi} = \sum_{r=-\infty}^{+\infty} \boldsymbol{c}_r e^{(i/\hbar)(p_{ri}x^i + mcx^n - E_r t)} \equiv e^{(i/\hbar)mcx^n} \sum_{r=-\infty}^{+\infty} \boldsymbol{c}_r e^{(i/\hbar)(p_{ri}x^i - E_r t)}, \tag{73}$$

where the energies result to be

$$E_r = c\sqrt{\vec{p}_r^{\,2} + m^2c^2}. \tag{74}$$

Then we are able to evaluate the Laplacian:

$$g^{\underline{ij}} \boldsymbol{\psi}_{;\underline{i};\underline{j}} = \frac{m^2c^2}{\hbar^2} \boldsymbol{\psi}.$$

Then the field equation (67) leads to the Klein-Gordon equation in generalized coordinates:

$$\boldsymbol{\psi}_{;0;0} + g^{ij} \boldsymbol{\psi}_{;i;j} + \frac{m^2c^2}{\hbar^2} \boldsymbol{\psi} = 0. \tag{75}$$

B. First-order formulation

A further relevant consideration arises on evaluating the divergence of $\boldsymbol{w}_I$ in terms of the field variables $\boldsymbol{w}_i, \boldsymbol{w}_{\underline{i}}$. Taking account of the previous results we have

$$\boldsymbol{w}_{\underline{j}} = \boldsymbol{w}_n \delta_{\underline{jn}}, \quad \boldsymbol{w}_{\underline{j};\underline{i}} = \frac{imc}{\hbar} \boldsymbol{w}_n \delta_{\underline{jn}}. \tag{76}$$

It follows into the system (60):

$$\boldsymbol{v}_{;0} + cg^{ij} \boldsymbol{w}_{j;i} + i\frac{mc^2}{\hbar} \boldsymbol{w} = 0, \tag{77}$$

$$c\boldsymbol{w}_{i;0} - \boldsymbol{v}_{;i} = 0, \quad c\boldsymbol{w}_{n;0} - \boldsymbol{v}_{;n} = 0. \tag{78}$$

That result is equivalent to saying that we need only *one* extra space dimension to introduce the rest mass. Then the space-time needs to have five dimensions if the particle travels across a gravitational field or six if the electromagnetic field is added or more if other fundamental fields are present (Kaluza-Klein type theories).

VI. THE DIRAC EQUATION

In the *N-dimensional* linear space of the field variables $\boldsymbol{v}, \boldsymbol{w}_I$ it is always possible to find a set of n nonsingular matrices α^I relating the n vectors $(\boldsymbol{w}_I)$ with the vector $\boldsymbol{v}$ in such a way that

$$\boldsymbol{v} = c\alpha^I \boldsymbol{w}_I. \tag{79}$$

Thanks to (79), the field equations (60) may be written only in terms of $\boldsymbol{w}_I$ as

$$\alpha^I_{;0}\boldsymbol{w}_I + \alpha^I \boldsymbol{w}_{I;0} + g^{IJ}\boldsymbol{w}_{J;I} = 0, \tag{80}$$

$$\boldsymbol{w}_{I;0} - \alpha^J_{;I}\boldsymbol{w}_J - \alpha^J \boldsymbol{w}_{J;I} = 0. \tag{81}$$

On taking the scalar product of (81) by α^I we have

$$\alpha^I \boldsymbol{w}_{I;0} - \alpha^I \alpha^J_{;I}\boldsymbol{w}_J - \alpha^I \alpha^J \boldsymbol{w}_{J;I} = 0. \tag{82}$$

Now we need to remember that $\boldsymbol{w}_J$ is a gradient of a field which is scalar with respect to any regular coordinate transformation, being by its definition given by the third equation in (43):

$$\boldsymbol{w}_J = \boldsymbol{\psi}_{;J} \equiv \boldsymbol{\psi}_{,J}.$$

Then,

$$\boldsymbol{w}_{J;I} \equiv \boldsymbol{\psi}_{;J;I} \equiv \boldsymbol{\psi}_{,J,I} - \Gamma^K_{IJ}\boldsymbol{\psi}_K$$

is symmetric with respect to I, J. Therefore (82) becomes

$$\alpha^I \boldsymbol{w}_{I;0} - \alpha^I \alpha^J_{;I}\boldsymbol{w}_J - \tfrac{1}{2}(\alpha^I \alpha^J + \alpha^J \alpha^I)\boldsymbol{w}_{J;I} = 0. \tag{83}$$

Subtraction of (83) from (80), after few manipulations, leads to

$$(\alpha^J_{;0} + \alpha^I \alpha^J_{;I})\boldsymbol{w}_J + \tfrac{1}{2}(\alpha^I \alpha^J + \alpha^J \alpha^I - 2g^{IJ}\mathrm{I})\boldsymbol{w}_{J;I} = 0. \tag{84}$$

The last condition (84) holds for any value of the field $\boldsymbol{w}_J$ and its derivatives $\boldsymbol{w}_{J;I}$, iff

$$\alpha^J_{;0} + \alpha^I \alpha^J_{;I} = 0, \tag{85}$$

$$\alpha^I \alpha^J + \alpha^J \alpha^I = -2g^{IJ}\mathrm{I}. \tag{86}$$

It is easy to recognize in the last relation a general relativistic extension of the same anticommutation rule holding for the Dirac matrices.[24] The matrices α^I must also fulfill condition (85). Equations (60) are now dependent and lead to a field equation of the form:

$$\boldsymbol{v}_{;0} - \alpha^I \boldsymbol{v}_{;I} + c\alpha^I \alpha^J_{;I} w_J = 0, \tag{87}$$

which represents a generalized form of the Dirac equation.

We point out that each matrix α^J, when multiplied by itself, becomes equal to the identity matrix. Then its eigenvalues are ± 1. With a suitable choice of a locally flat coordinate system we can always diagonalize one of such matrices. When $N=4$ the last choice, together with the anticommutation rule (86) and the assumption that the matrices are constant, yields to the known Dirac matrices. Moreover the field equation (87) becomes the usual Dirac equation:

$$\frac{\partial \boldsymbol{v}}{\partial t} + c\vec{\alpha}\cdot\vec{\nabla}\boldsymbol{v} + i\frac{mc^2}{\hbar}\beta\boldsymbol{v} = 0. \tag{88}$$

VII. KALUZA-KLEIN TYPE THEORIES

Starting from the previous results, having arisen in the context of wave propagation theory versus Hamiltonian mechanics, we are naturally led to include the field $\boldsymbol{\psi} \equiv (\psi^{(\bar{h})}), \bar{h} = 1, 2, \ldots, N$ among the components of the metric tensor of the manifold V^{n+1} following a Kaluza-Klein type scheme.[25] Some authors proposed different methods to deduce the Klein-Gordon equation, for a scalar field, from a Kaluza-Klein theory, dealing with the physical space-time (V^4) filled by matter, as embedded into a higher dimensional empty space-time: see, e.g., Refs. 10–18. Here we propose a way to involve even more fields $\psi^{(\bar{h})}$.

A. Particle traveling across a gravitational field

In the absence of electromagnetic and Yang-Mills fields we suppose to work in a V^{5+N} space-time manifold on which we represent the metric tensor and its inverse as,

$$(g_{AB}) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & g_{ij} & 0 & 0 \\ 0 & 0 & -(\psi^{(\bar{h})})^2 \delta_{\bar{h}\bar{k}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{89}$$

$$(g^{AB}) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & g^{ij} & 0 & 0 \\ 0 & 0 & -\dfrac{1}{(\psi^{(\bar{h})})^2} \delta^{\bar{h}\bar{k}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{90}$$

where no summation is intended under the repeated couples $(\bar{h})$-$\bar{h}$ or $(\bar{k})$-$\bar{k}$.

If we assume that $g_{jk}(t, x^i), \psi^{(\bar{h})}(t, x^i, x^n)$, according to the coordinate choice (70), the non-null field equations become

$$\tilde{R}_{00} - \tfrac{1}{2}\tilde{R} = \kappa T_{00}, \tag{91}$$

$$\tilde{R}_{jk} - \tfrac{1}{2}\tilde{R} g_{jk} = \kappa T_{jk}, \tag{92}$$

$$\psi^{(\bar{h})}_{;0;0} + g^{jk} \psi^{(\bar{h})}_{;j;k} = \psi^{(\bar{h})}_{;n;n}, \tag{93}$$

where $\tilde{R}_{00}, \tilde{R}_{jk}$ denote the non-null components of the Ricci tensor related to the V^4 physical space-time, and

$$\kappa T_{00} = -\sum_{\bar{h}=1}^{N} \frac{\psi^{(\bar{h})}_{;0;0}}{\psi^{(\bar{h})}}, \quad \kappa T_{jk} = -\sum_{\bar{h}=1}^{N} \frac{\psi^{(\bar{h})}_{;j;k}}{\psi^{(\bar{h})}}, \tag{94}$$

are the nonvanishing energy-momentum tensor components arising on V^4.

Moreover it results that

$$p_{\underline{j}} \equiv \hbar\, \varphi_{,\underline{j}} = \hbar\, \delta_{\underline{j}n} \varphi_{,n} \equiv \delta_{\underline{j}n} p_n. \tag{95}$$

Then the particle equation of motion [the first equation in (26)] becomes

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = g^{jk}{}_{,i}\frac{cp_jp_k}{2p} + g^{nn}{}_{,i}\frac{cp_n^2}{2p}, \tag{96}$$

since $g^{nn}=-1$, the previous equation becomes the geodesic condition on the physical space:

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = g^{jk}{}_{,i}\frac{cp_jp_k}{2p}. \tag{97}$$

B. Adding the electromagnetic field

The electromagnetic field can be added according to a Kaluza-Klein scheme, by the metric tensor:

$$(g_{AB}) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \bar{g}_{ij} & \kappa\phi^2 A_k & 0 & 0 \\ 0 & \kappa\phi^2 A_j & -\phi^2 & 0 & 0 \\ 0 & 0 & 0 & -(\psi^{(\bar{h})})^2\delta_{\bar{h}\bar{k}} & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \tag{98}$$

with

$$\bar{g}_{ij} = g_{ij} - \kappa^2\phi^2 A_jA_k, \tag{99}$$

ϕ being the Kaluza-Klein dilaton scalar field and A_j the electromagnetic vector potential.

We emphasize that we need to choose the *radiation gauge* $g_{40}\equiv A_0=0$ in order to preserve the synchronization assumption (1).

C. Adding the Yang-Mills fields

In a similar way one can introduce also Yang-Mills fields into the metric tensor:[26–28]

$$(g_{AB}) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \hat{g}_{ij} & \kappa\phi^2 A_k & \kappa(\phi^{(a)})^2 A_k^b & 0 \\ 0 & \kappa\phi^2 A_j & -\phi^2 & 0 & 0 \\ 0 & \kappa\phi^2 A_j & \kappa(\phi^{(a)})^2 A_j^a & -(\phi^{(a)})^2\delta^{ab} & 0 \\ 0 & 0 & 0 & 0 & -(\psi^{(\bar{h})})^2\delta_{\bar{h}\bar{k}} \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\hat{g}_{ij} = g_{ij} - \kappa^2\{\phi^2 A_jA_k + (\phi^{(a)})^2\delta_{ab}A_j^aA_k^b\}, \tag{100}$$

with the gauge choices $A_0=0, A_0^a=0$.

VIII. CONCLUSION

We have examined in some detail, in the context of general relativity, in a synchronous gauge, the idea that particle trajectories of motion can be the same as the rays of suitable waves propagating across the space. Moreover we have suggested that the wave front propagation equation and the Hamilton-Jacobi equation of some particle motion could represent two ways of interpreting the same differential equation. Such assumption has led us to the condition that the wave normal speed must be equal to the speed of light in empty space and the consequence that massive free particles can exist only if the space has more than three dimensions. In order to establish a Lagrangian complex field theory capable of generating the waves we need, we found that the field equation needs to be linear with respect to the new field variables and assume the form of a

D'Alembert equation in general coordinates. We have also shown that the field equations we obtained can be written either in the form of Klein-Gordon equation (second-order formulation) or as Dirac equation (first-order formulation) when $N=4$. Moreover we have shown how to include the new additional field ψ into the frame of Kaluza-Klein type theories.

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Separation of unistochastic matrices from the double stochastic ones: Recovery of a 3×3 unitary matrix from experimental data

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The aim of the paper is to provide a constructive method for recovering a unitary matrix from experimental data. Since there is a natural immersion of unitary matrices within the set of double stochastic ones, the problem to solve is to find necessary and sufficient criteria that separate the two sets. A complete solution is provided for the three-dimensional case, accompanied by a χ^2 test necessary for the reconstruction of a unitary matrix from error affected data. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2229424]

I. INTRODUCTION

An $n\times n$ matrix M is said to be double stochastic if its elements satisfy the relations

$$m_{ij}\geqslant 0,\quad \sum_{i=1}^{n} m_{ij}=1,\quad \sum_{j=1}^{n} m_{ij}=1. \tag{1}$$

All such matrices form a convex set called the Birkhoff's polytope.[1] The unistochastic matrices are a subset of the double stochastic ones defined by

$$m_{ij}=|U_{ij}|^2, \tag{2}$$

where U is a unitary matrix, i.e., satisfies the relation

$$UU^{\dagger}=U^{\dagger}U=I_n, \tag{3}$$

where † denotes the adjoint, and I_n is the n-dimensional unit matrix.

It is well known that for $n\geqslant 3$ there are double stochastic matrices that are not unistochastic,[2] and from a mathematical point of view there are a few interesting problems that deserve to be solved:

(i) Given a double stochastic matrix, $M=(m_{ij})$, $i,j=1,\ldots,n$, what are the necessary and sufficient conditions for M to be unistochastic?
(ii) Supposing M unistochastic, to what extent the matrix U is determined by M, i.e., how many solutions one could get.
(iii) If M is unistochastic, how one can reconstruct the unitary U from the given data.

The problem (i) was completely solved only for the three-dimensional case.[3] A characterization of the subset of double stochastic matrices that come from unistochastic ones, Eq. (2), for $n=3$, was given in Refs. 3 and 4. For $n\geqslant 4$ only partial results are known, see, e.g., Refs. 5–12. In general the theoretical physicists working on this problem were not aware of the embedding of the unitary matrices into the double stochastic ones, Eq. (2), hence there was not an intrinsic pressure for solving problem (i). In this respect see Ref. 9, Introduction, where it is said: "*We are not*

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concerned here with the **consistency** *problem, which amounts to obtaining necessary and sufficient conditions on the set of numbers* $|U_{jk}|$ *for this set to represent the moduli of a unitary matrix*."

In this paper we will provide necessary and sufficient conditions for the separation of the two sets, conditions expressed in terms of the entries of a double stochastic matrix on the independent parameters entering the unitary matrix. We mention also that the Theorem 1 in Ref. 3, which provides necessary and sufficient conditions in the $n=3$ case, is only an existence theorem, and it does not provide a constructive method for recovering a unitary matrix from a double stochastic one.

Concerning problem (ii) it was shown that the generic situation, for $n \geqslant 4$ is the existence of a continuum of solutions, see Refs. 6–9 and 11 and 12. In particular complex Hadamard matrices, i.e., unitary matrices with equal moduli, $|U_{ij}|=1/\sqrt{n}$, have been found that depend on arbitrary phases, see Refs. 13–17.

The solution of the mathematical problem (iii) for $n=3$ can be easily obtained, as we show in the following, but its applications in high energy physics presented some challenges since the measured numbers are affected by errors. Usually one starts with a theoretical model formalized by a unitary matrix, and the problem is to recover the unitary matrix from measurements of its moduli, or of some "angular looking objects," $U_{ij}U_{lk}U_{ik}^{*}U_{lj}^{*}$, where * means complex conjugation. When $|U_{ij}|^2$ are measured one gets a numerical matrix as

$$V=(V_{ij}^2), \tag{4}$$

where every V_{ij} is affected by errors, so we do not know how far from $|U_{ij}|$ are the measured values V_{ij}, and by consequence the double stochasticity relations (1) are only approximately satisfied, if any. More generally, that means that we have to test the full compatibility between the data and the unistochastic property. Second, by supposing the data are compatible with the existence of a unitary matrix we need a reliable algorithm for an explicit recovery of a unitary matrix from data, because some parameters entering the unitary matrix may have a physical significance, and we want to know them, an example being the CP-violating phase from the Cabibbo-Kobayashi-Maskawa (CKM) matrix.

Indeed the recovery of a unitary matrix from experimental data is a central problem in the electro-weak interactions[18] where the (assumed) unitary CKM matrix[19] plays a fundamental role. Hence the recovery problem of a unitary matrix from experimental data is not an academic problem, it has many practical consequences. Let us recall that there are two big collaborations, BaBar in the United States, and Belle in Japan whose efforts are to measure as exact as possible the b-quark related entries of the CKM matrix. In Europe, at CERN, there is under construction the LHC machine, one of its main aims being a better understanding of the so called B-physics. Thus a reliable algorithm for recovery of unitary matrices, able to obtain the independent parameters of the CKM matrix, could have consequences on both the design of future experiments, as well as on the design of future high energy machines, including neutrino factories.

The main goal of the paper is to provide a reliable algorithm for the reconstruction of a unitary matrix from experimental data, when these ones are compatible with the theoretical model. We mention that nowadays the algorithm for reconstruction of a 3×3 unitary matrix from experimental data does not make use of the double stochasticity relations (1), and the phenomenological model used to describe the data and to reconstruct a unitary matrix from them is mainly based on the use of a *single* orthogonality relation, expressed as a triangle in the complex plane,[20–29] although the proof of Theorem 1 from Ref. 3 explicitly stresses the necessity of using at least *two* orthogonality relations.

The paper is organized as follows. In Sec. II starting from the properties of double stochastic matrices and the embedding relation (2) of unitary matrices within that set, we describe the gauge group of unitary matrices, i.e., the group of the most elementary transformations whose action on the unitary matrices does not change the unitarity property, or the physical content. In Sec. III we provide a parametrization of unitary matrices that is essential in devising a reconstruction algorithm in terms of physically relevant quantities. In Sec. IV we define two phenomenological

models, unitarity condition method, and unitarity triangles method, by using the embedding (2) and the double stochasticity properties (1). We find the necessary and sufficient conditions the data have to satisfy in each model in order to be consistent with the unitarity properties, and give the reconstruction algorithm of unitary matrices from double stochastic matrices. In Sec. V we show that both approaches are completely equivalent, then and only then, when they are formulated in terms of *four* independent moduli; a consequence will be that the second model has to use at least *two* orthogonality relations. In Sec. VI we describe the reconstruction algorithm of unitary matrices from experimental data that are compatible with the double stochasticity property. With this aim in view we define χ^2-tests that allow the recovery of unitary matrices from error affected data, including a method for doing statistics on moduli of unitary matrices. The paper ends with conclusions.

II. UNITARY MATRICES AND THEIR GAUGE SUBGROUP

It is well known that an $n\times n$ unitary matrix depends on n^2 parameters,[30,31] that are usually taken as $n(n-1)/2$ angles and $n(n+1)/2$ phases, each set taking values within $[0,\pi/2]$, and, respectively, $[0,2\pi)$. Equation (2) tells us that, given a definite unitary matrix, all the unitary matrices obtained by multiplying it at left and/or at right by diagonal phase matrices, $D=\mathrm{diag}(e^{i\phi_1},\ldots,e^{i\phi_n})$, with arbitrary real ϕ_i, $i=1,\ldots,n$, generate a single double stochastic matrix. That means that we can simplify a little bit the form of a unitary matrix since the values of $2n-1$ phases are at our disposal, and a common choice for them is 0 and/or π. In high energy physics this property is known as phase invariance.[32–36] Thus we can take the entries from the first row and the first column as non-negative quantities, such that the number of independent parameters entering a unitary matrix gets $n^2-(2n-1)=(n-1)^2$, and it is equal to the number of independent parameters entering a double stochastic matrix. Hence we could say that the embedding (2) suggests that the "natural" coordinates to parametrize a unitary matrix could be the moduli of its entries. Unfortunately that can be done only for 3×3 matrices, but even in this case there are supplementary relations that have to be fulfilled by the moduli in order to get from them a unitary matrix.

Besides these transformations there are other transformations: multiplication at left and/or right by permutation matrices. Permutation matrices are matrices whose elements on each row and each column are zero, but that equal unity. They interchange rows, and, respectively, columns between themselves. Both diagonal phase matrices and permutation matrices are subgroups of unitary matrices. If D denotes a diagonal phase matrix and P a permutation matrix then

$$DD^\dagger = PP^\dagger = I_n.$$

Other equivalent unitary matrices can be obtained by taking the complex conjugate matrix, and/or the transpose of the original one. If we denote the transpose operator by T, and by C the complex conjugation, both these transforms form a subgroup because

$$T^2 = C^2 = \mathrm{Identity}.$$

Thus the product group

$$K = D\times P\times T\times C$$

is the gauge invariance subgroup of unitary matrices, and, in the following, we work only with the coset defined by

$$X \cong U(n)/K, \tag{5}$$

where $U(n)$ denotes the n-dimensional unitary group. The C invariance has an important consequence: the range of all independent phases entering $U(n)$ is $[0,\pi]$. The multiplicity of solutions appearing in the recovery problem of a unitary matrix from a double stochastic one will be given modulo the above-noted simplest transformations of unitary matrices.

III. PARAMETRIZATION OF UNITARY MATRICES

For devising a recovery algorithm of unitary matrices from double stochastic ones, or from experimental data, we need an explicit parametrization of them. That will lead us easily to the necessary and sufficient conditions a double stochastic matrix has to satisfy for also being unistochastic, even if a complete explicit solution is found only for $n=3$. These conditions will lead to separation criteria between the double stochastic and unistochastic matrices.

There are essentially two types of parametrizations: first the classical result by Murnagham,[30] which states that the matrices from the unitary group $U(n)$ are products of a diagonal phase matrix containing n phases, and $n(n-1)/2$ matrices whose main building block has the form

$$U=\begin{pmatrix} \cos\theta & -\sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & \cos\theta \end{pmatrix}, \tag{6}$$

i.e., a parametrization in terms of $n(n-1)/2$ angles θ_i, and $n(n+1)/2$ phases φ_i. The usual parametrization of the CKM matrix[37] used in high energy physics is of this type. A second parametrization, also through factorization, is that given in Ref. 38. The idea behind such a parametrization comes from the following sequence:

$$U(n)\cong\frac{U(n)}{U(n-1)}\times\frac{U(n-1)}{U(n-2)}\times\cdots\times\frac{U(2)}{U(1)}\times U(1)\cong S^{2n-1}\times S^{2n-3}\times\cdots\times S^3\times S^1. \tag{7}$$

This sequence shows that each factor can be parametrized by an arbitrary point on the corresponding complex sphere, i.e., by a single complex $(n-k)$-dimensional unit vector. Such a parametrization could be appealing for high energy physicists since it shows that the information brought by each generation of quarks, or leptons is contained in a single complex unit vector. The first parametrization of CKM matrix, Ref. 19, is of this form. The explicit realization of this parametrization, which is the main result in Ref. 38, is given by

Theorem 1: *Any element $U_n\in U(n)$ can be factored into an ordered product of n matrices of the following form*

$$U_n=B_n^0\cdots B_{n-1}^1\ldots B_1^{n-1}, \tag{8}$$

where

$$B_{n-k}^k=\begin{pmatrix} I_k & 0 \\ 0 & B_{n-k} \end{pmatrix}$$

and $B_{n-k}\in U(n-k)$ are special unitary matrices, each one generated by a single complex $(n-k)$-dimensional unit vector, $b_{n-k}\in S^{2(n-k)-1}$. For example, $B_1=e^{i\varphi}$, where φ is an arbitrary phase.

If $y_m\in S^{2m-1}$, $m=1,\ldots,n$, is parametrized by

$$y_m=(e^{i\varphi_1}\cos\theta_1,e^{i\varphi_2}\sin\theta_1\cos\theta_2,\ldots,e^{i\varphi_m}\sin\theta_1\cdots\sin\theta_{m-1})^t,$$

where t means transpose, then the m columns of B_m are given by

$$v_1=y_m=\begin{pmatrix} e^{i\varphi_1}\cos\theta_1 \\ e^{i\varphi_2}\sin\theta_1\cos\theta_2 \\ \vdots \\ e^{i\varphi_m}\sin\theta_1\cdots\sin\theta_{m-1} \end{pmatrix}$$

and

$$v_{k+1}=\frac{\mathrm{d}}{\mathrm{d}\theta_k}v_1(\theta_1=\cdots=\theta_{k-1}=\pi/2),\quad k=1,\ldots,m-1,$$

where in the above-mentioned formula one calculates first the derivative and afterwards the restriction to $\pi/2$.

In what follows we need an explicit parametrization of B_{n-k}, $k=0,\ldots,n-1$, and by taking into account that we work with representatives from the X coset, Eq. (5), we choose the corresponding n generating vectors as follows:

$$y_n = (\cos a_1, \sin a_1 \cos a_2, \ldots, \sin a_1 \ldots \sin a_{n-1})^t,$$

$$y_{n-1} = (-\cos b_1, e^{i\beta_1} \sin b_1 \cos b_2, \ldots, e^{i\beta_{n-2}} \sin b_1 \ldots \sin b_{n-2})^t,$$

$$\vdots \tag{9}$$

$$y_2 = (-\cos z_1, e^{i\psi_1} \sin z_1)^t,$$

$$y_1 = -1.$$

With this choice the first row of U_n has the form

$$U_{11} = \cos a_1, \quad U_{12} = \cos b_1 \sin a_1, \cdots U_{1n} = \sin a_1 \ldots \sin z_1 \tag{10}$$

and the first column is given by y_n. In the following we will assume that U_n, Eq. (8), has its first column given by y_n, and its first row given by (10), and this is our standard form in the rest of the paper for a unitary matrix. A similar parametrization was obtained recently, see Ref. 39; for the case $n=3$ see also Refs. 40 and 41.

IV. PHENOMENOLOGICAL MODELS

By "phenomenological model" we will understand in the following a relationship between the entries of a double stochastic matrix and the entries of a unitary matrix, the main goal being the finding of the necessary and sufficient conditions that separate the two sets. Depending on the context the "experimental data" will denote either the entries of a double stochastic matrix, or the numbers, affected by errors, measured in an experiment. Usually the experimental data on the 3×3 CKM matrix entries from the quark sector are given in terms of moduli of the unitary matrix that define the theoretical model, $|U_{ij}|$, or angular looking objects $U_{\alpha j}U_{\beta k}U^*_{\alpha k}U^*_{\beta j}$, which are equivalent to the angles of the triangles generated by the orthogonality relations. For the beginning we assume that the data have no errors, which is the current mathematical setting, i.e., the moduli are the entries of a double stochastic matrix, and we want to solve problems (i)–(iii) from Sec. I. For doing that we have at our disposal an explicit parametrization of unitary matrices, (8) and (9), and the unitarity property

$$UU^\dagger = U^\dagger U = I_n.$$

This concise form is equivalent to $2n$ relations

$$\sum_{i=1}^{i=n} |U_{ji}|^2 - 1 = 0, \quad j = 1, \ldots, n,$$

$$\sum_{i=1}^{i=n} |U_{ij}|^2 - 1 = 0, \quad j = 1, \ldots, n \tag{11}$$

showing that the numbers $m_{ij}=|U_{ij}|^2$ define a double stochastic matrix, which implies that only $2n-1$ relations from the set (11) are independent, and by $n(n-1)$ orthogonality relations

$$\sum_{i=1}^{i=n} U_{ji}U_{ki}^{*}=0, \quad j<k, \quad i=1,\ldots,n,$$
$$\sum_{i=1}^{i=n} U_{ij}U_{ik}^{*}=0, \quad j<k, \quad i=1,\ldots,n, \tag{12}$$

which can be visualized as polygons in the complex plane. The last relations are the supplementary relations the numbers U_{ij} have to satisfy in order that the corresponding matrix should be unitary. The number of relations (11) and (12) is greater than n^2, but we have written all of them since they could be useful in over-constraining the experimental data, which usually are affected by errors.

The relations (11) and, respectively, (12) can be used to define two different phenomenological models. The first model is given by the relations (11) together with

$$m_{ij}=|U_{ij}|^2, \quad i,j=1,\ldots,n-1, \tag{13}$$

where m_{ij} are the entries of a double stochastic matrix, and U_{ij} are the entries of a unitary matrix parametrized as in Theorem 1. The last relation is equivalent to the following:

$$m_{11}=\cos^2 a_1, \quad m_{12}=\sin^2 a_1\cos^2 b_1,\ldots,m_{1n}=\sin^2 a_1\cdots\sin^2 z_1,$$
$$m_{21}=\cos^2 a_2\sin^2 a_1,\ldots,m_{nn-1}=\sin^2 a_1\cdots\sin^2 a_{n-1}, \tag{14}$$

$$m_{22}=\cos^2 a_1\cos^2 a_2\cos^2 b_1+\cos^2 b_2\sin^2 a_2\sin^2 b_1$$
$$+2\cos a_1\cos a_2\cos b_1\cos b_2\sin a_2\sin b_1\cos\beta_1, \tag{15}$$

$$m_{32}=\cos^2 a_1\cos^2 a_3\cos^2 b_1\sin^2 a_2+\cos^2 a_2\cos^2 a_3\cos^2 b_2\sin^2 b_1+\sin^2 a_3\sin^2 b_1\sin^2 b_2$$
$$-2\cos a_1\cos a_2\cos^2 a_3\cos b_1\cos b_2\sin a_2\sin b_1\cos\beta_1$$
$$+2\cos a_1\cos a_3\cos b_1\sin a_2\sin a_3\sin b_1\sin b_2\cos\beta_2$$
$$-2\cos a_2\cos a_3\cos b_2\sin a_3\sin^2 b_1\sin b_2\cos(\beta_1-\beta_2),\ \text{etc}\,., \tag{16}$$

where we have written only the simplest equations. It is easily seen from the above-noted equations that, since m_{1i} and m_{i1}, $i=1,\ldots,n-1$, are entries of a double stochastic matrix, there is a unique solution for $\cos a_i\in(0,1)$, $i=1,\ldots,n-1$, of the form

$$\cos^2 a_1=m_{11}, \quad \cos^2 a_k=\frac{m_{k1}}{1-\sum_{i=1}^{k-1} m_{i1}}, \quad k=2,\ldots,n-1 \tag{17}$$

and similarly for $\cos b_1$, $\cos c_1,\ldots,\cos z_1$. Hence the number of angles that have to be found is $(n-1)(n-2)/2-(2n-3)=(n-2)(n-3)/2$. In that way the number of equations of the form (15) and (16) we have to solve is only $(n-2)^2$. We substitute the forms for $\cos a_i$, $\sin a_i$, and similar ones, from the first column and the first row, in Eqs. (15) and (16), such that we get $(n-2)^2$ equations that depend on $(n-1)^2$ moduli m_{ij}, $i,j=1,\ldots,n-1$. We now do a relabeling of the angles, $b_i\to b_{i-1}$, $i=2,\ldots,n-2$, $c_2\to b_{n-1},\ldots$, etc., and similarly for the phases. With this notation the necessary and sufficient conditions for a double stochastic matrix to be also unistochastic are given by the relations

$$0\leqslant\cos b_i\leqslant 1, \quad i=1,\ldots,\frac{(n-2)(n-3)}{2}, \tag{18}$$

$$-1 \leqslant \cos \beta_i \leqslant 1, \quad i = 1, \ldots, \frac{(n-1)(n-2)}{2}, \tag{19}$$

where $\cos b_i$ and $\cos \beta_i$ are the solutions in terms of m_{ij} of the $(n-2)^2$ equations of the form (15) and (16). The above-noted relations are at the same time the separation criteria between the double stochastic and unistochastic matrices, and their fulfillment is equivalent to the existence of at least one unitary matrix compatible with the m_{ij}. To check them we have to solve analytically or numerically the $(n-2)^2$ equations (15) and (16). Numerically this can be done when m_{ij} are the elements of a double stochastic matrix, but for the real case of experimental data with errors we need an analytic solution to be used in a χ^2-test, and until now this was found only for the case $n=3$. In conclusion for 3×3 data coming from an exact double stochastic matrix we have only one constraint, namely, $-1 \leqslant \cos \beta_1 \leqslant 1$. If the data come from an experiment we have to check also the compatibility of the entries from the first row and first column with the relations (17), i.e., to see if the conditions $0 \leqslant \cos^2 a_i \leqslant 1$ are satisfied.

Taking into account the relation (13), $m_{ij}=|U_{ij}|^2$, which shows how the unitary matrices are embedded into the double stochastic ones, the parametrization of unitary matrices by their moduli seems to be very appealing in this case, although it is not a natural one in the general case. A natural parametrization would be one whose parameters are free, i.e., there are no supplementary constraints upon them, as Eqs. (18) and (19), to enforce unitarity.

The problem we addressed in Ref. 11 was to what extent the knowledge of the moduli, $m_{ij} = |U_{ij}|$, of an $n\times n$ unitary matrix U determines U. If we identify the parameters to the moduli, they will be lying within the simple domain

$$D = (0,1) \times \cdots \times (0,1) \equiv (0,1)^{(n-1)^2},$$

where the above-presented notation means that the number of factors entering the topological product is $(n-1)^2$. We excluded only the extremities of each interval, i.e., the points 0 and 1 that is a zero measure set within $U(n)$ and has no relevance to the problem of recovery of a unitary matrix from a double stochastic one.

Nothing remains but to check if the new parametrization is one-to-one. A solution to the last problem is the following: start with a one-to-one parametrization of $U(n)$, such as that given in the preceding section, and then change the coordinates taking as new coordinates the moduli of the $(n-2)^2$ entries; these ones are obtained by deleting the first and the last row, respectively, the first and the last column. The moduli of the first row and the first column are in one-to-one correspondence with the parameters entering the unitary matrix, see, e.g., Eq. (17), and the moduli entering the last row and the last column are uniquely determined by the double stochasticity property. Afterwords use the implicit function theorem to find the points where the new parametrization fails to be one-to-one. The corresponding variety upon which the application is not a bijective one is given by setting to zero the Jacobian of the transformation, i.e.,

$$J = \frac{\partial(m_{22}, \ldots, m_{2n-1}, \ldots, m_{n-1n-1})}{\partial(b_1, \ldots, b_{(n-2)(n-3)/2}, \beta_1, \ldots, \beta_{(n-1)(n-2)/2})} = 0. \tag{20}$$

One gets that, generically, for $n \geqslant 4$ the unitary group $U(n)$ cannot be fully parametrized by the moduli of its entries,[6–17] i.e., for a given set of moduli there exists a continuum of solutions, the simplest example being the case of complex Hadamard matrices.[13–17] The maximum dimension of the above-mentioned variety is $(n-2)^2-1=(n-3)(n-1)$. For $n=3$, $J\neq 0$, and only in this case the parametrization of a unitary matrix through the moduli could be one-to-one. If the moduli are outside of the above-mentioned variety an upper bound for the multiplicity is $2^{[n(n-3)]/2}$, bound that is saturated for $n=3$, when there is essentially only one complex matrix, if we take into account the gauge invariance of unitary matrices.

In the case of exact double stochastic matrices, as we showed before, only $(n-2)^2$ moduli

enter the game since the angles entering the first column and the first row are uniquely determined. To have a flavor of the problem we consider more in detail the case $n=4$, when there are four equations, two of them being Eqs. (15) and (16), and the last two are

$$\begin{aligned} m_{23} = {} & \cos^2 b_1 \cos^2 b_2 \cos^2 c_1 \sin^2 a_2 + \cos^2 a_1 \cos^2 a_2 \cos^2 c_1 \sin^2 b_1 + \sin^2 a_2 \sin^2 b_2 \sin^2 c_1 \\ & - 2 \cos a_1 \cos a_2 \cos b_1 \cos b_2 \cos^2 c_1 \sin a_2 \sin b_1 \cos \beta_1 \\ & + 2 \cos b_1 \cos b_2 \cos c_1 \sin^2 a_2 \sin b_2 \sin c_1 \cos \gamma_1 \\ & - 2 \cos a_1 \cos a_2 \cos c_1 \sin a_2 \sin b_1 \sin b_2 \sin c_1 \cos(\beta_1 + \gamma_1), \end{aligned} \tag{21}$$

$$\begin{aligned} m_{33} = {} & \cos^2 a_2 \cos^2 a_3 \cos^2 b_1 \cos^2 b_2 \cos^2 c_1 + \cos^2 a_1 \cos^2 a_3 \cos^2 c_1 \sin^2 a_2 \sin^2 b_1 \\ & + \cos^2 b_1 \cos^2 c_1 \sin^2 a_3 \sin^2 b_2 + \cos^2 b_2 \sin^2 a_3 \sin^2 c_1 + \cos^2 a_2 \cos^2 a_3 \sin^2 b_2 \sin^2 c_1 \\ & + 2 \cos a_1 \cos a_2 \cos^2 a_3 \cos b_1 \cos b_2 \cos^2 c_1 \sin a_2 \sin b_1 \cos \beta_1 \\ & - 2 \cos a_2 \cos a_3 \cos^2 b_1 \cos b_2 \cos^2 c_1 \sin a_3 \sin b_2 \cos(\beta_1 - \beta_2) \\ & - 2 \cos a_1 \cos a_3 \cos b_1 \cos^2 c_1 \sin a_2 \sin a_3 \sin b_1 \sin b_2 \cos \beta_2 \\ & + 2 \cos a_2 \cos a_3 \cos b_1 \cos^2 b_2 \cos c_1 \sin a_3 \sin c_1 \cos(\beta_1 - \beta_2 - \gamma_1) \\ & + 2 \cos a_1 \cos a_3 \cos b_2 \cos c_1 \sin a_2 \sin a_3 \sin b_1 \sin c_1 \cos(\beta_2 + \gamma_1) \\ & + 2 \cos^2 a_2 \cos^2 a_3 \cos b_1 \cos b_2 \cos c_1 \sin b_2 \sin c_1 \cos \gamma_1 \\ & - 2 \cos b_1 \cos b_2 \cos c_1 \sin^2 a_3 \sin b_2 \sin c_1 \cos \gamma_1 \\ & + 2 \cos a_1 \cos a_2 \cos^2 a_3 \cos c_1 \sin a_2 \sin b_1 \sin b_2 \sin c_1 \cos(\beta_1 + \gamma_1) \\ & - 2 \cos a_2 \cos a_3 \cos b_1 \cos c_1 \sin a_3 \sin^2 b_2 \sin c_1 \cos(\beta_1 - \beta_2 + \gamma_1) \\ & + 2 \cos a_2 \cos a_3 \cos b_2 \sin a_3 \sin b_2 \sin^2 c_1 \cos(\beta_1 - \beta_2). \end{aligned} \tag{22}$$

From Eq. (14) we get

$$\cos a_1 = \sqrt{m_{11}}, \quad \sin a_1 = \sqrt{1 - m_{11}},$$

$$\cos a_2 = \sqrt{\frac{m_{21}}{1 - m_{11}}}, \quad \sin a_2 = \sqrt{\frac{1 - m_{11} - m_{21}}{1 - m_{11}}},$$

$$\cos a_3 = \sqrt{\frac{m_{31}}{1 - m_{11} - m_{21}}}, \quad \sin a_3 = \sqrt{\frac{1 - m_{11} - m_{21} - m_{31}}{1 - m_{11} - m_{21}}}, \tag{23}$$

$$\cos b_1 = \sqrt{\frac{m_{12}}{1 - m_{11}}}, \quad \sin b_1 = \sqrt{\frac{1 - m_{11} - m_{12}}{1 - m_{11}}},$$

$$\cos c_1 = \sqrt{\frac{m_{13}}{1 - m_{11} - m_{12}}}, \quad \sin c_1 = \sqrt{\frac{1 - m_{11} - m_{12} - m_{13}}{1 - m_{11} - m_{12}}}.$$

By substituting relations (23) into Eqs. (15) and (16) and (21) and (22) we obtain four equations that depend on nine moduli m_{ij}, $i,j=1,2,3$, and on the nonrelabeled parameters b_2, β_1, β_2, γ_1,

$$f_{22}-m_{22}=0,\quad f_{23}-m_{23}=0,$$
$$f_{32}-m_{32}=0,\quad f_{33}-m_{33}=0. \tag{24}$$

In general the rank of the Jacobian matrix

$$J=\frac{\partial(f_{22},f_{23},f_{32},f_{33})}{\partial(b_2,\beta_1,\beta_2,\gamma_1)} \tag{25}$$

will be less than $(n-2)^2$ since we know that there are particular solutions that depend on an arbitrary phase. If we look at the Jacobian (25) as a function on the Birkoff's polytope, i.e., depending on $(n-1)^2=9$ independent moduli m_{ij}, it could be possible to find a domain where rank $(J)=4$, i.e., in this case we have only one solution. Then the compatibility relations between the double stochastic matrix entries $(m_{ij})_{i,j=1}^{3}$, and the unitarity property, or in other words, the separation criteria between the two sets, are four, and they have the form

$$0\leqslant \cos b_2\leqslant 1,\quad -1\leqslant \cos\beta_1\leqslant 1,\quad -1\leqslant \cos\beta_2\leqslant 1,\quad -1\leqslant \cos\gamma_1\leqslant 1. \tag{26}$$

The above-presented relations are the necessary and sufficient conditions the moduli of a 4×4 double stochastic matrix have to satisfy in order for there to be a unitary matrix whose moduli coincide with m_{ij}, and their intersection gives the maximal domain within the m_{ij} simplex that is compatible to the existence of unitary matrices.

In the case when for a given numerical matrix, rank $(J)<4$, there is no one-to-one correspondence between the entries m_{ij} of a double stochastic matrix and the independents parameters entering a unitary matrix, i.e., there is at least one solution that depends on an arbitrary parameter, phase, or, angle.

The checking of criteria (26) requires explicit analytic solutions for

$$\cos b_2,\quad \cos\beta_1,\quad \cos\beta_2,\quad \cos\gamma_1$$

in terms of m_{ij}, and when these ones are not numbers, solving Eq. (24), is not a simple problem even with the symbolic calculation software packages nowadays available. The only results in this direction are those obtained in Ref. 9 however they have to be used with caution since the authors assumed that no matter how the numbers entering a double stochastic matrix are, Eq. (24) has a physical solution.

By taking into account the above-noted considerations the following result holds.

Theorem 2: *Suppose we have a generalized spherical coordinate system on the unitary group* $U(n)$, *and let* $U\in U(n)$ *be a given matrix parametrized as in Theorem 1*, *through* $n(n-l)/2$ *angles*, *each one taking values in* $[0,\pi/2]$, *and* $(n-1)(n-2)/2$ *phases taking values in* $[0,\pi]$, *and let* $M=(m_{ij})$ *be an* $n\times n$ *double stochastic matrix*, *whose entries are supposed to come from a unistochastic matrix U by the embedding*

$$m_{ij}=|U_{ij}|^2,\quad i,j=1,\ldots,n-1. \tag{27}$$

From Eq. (14) *we get a unique solution for the angles entering the first column and the first row of U as follows:*

$$\cos^2 a_1=m_{11},\quad \cos^2 a_2=\frac{m_{21}}{1-m_{11}},\ldots,\cos^2 a_{n-1}=\frac{m_{n-11}}{1-m_{11}-\sum_{i=2}^{n-1}m_{i1}},$$
$$\cos^2 b_1=\frac{m_{12}}{1-m_{11}},\ldots,\cos^2 z_1=\frac{m_{1n-1}}{1-m_{11}-\sum_{i=2}^{n-1}m_{1i}}. \tag{28}$$

We substitute them in Eq. (27) *obtaining a set of* $(n-2)^2$ *equations that*, *after relabeling of the angles and phases*, *is of the form*

$$f_{ij}(b_1,\ldots,b_{\frac{(n-2)(n-3)}{2}},\beta_1,\ldots,\beta_{\frac{(n-1)(n-2)}{2}})=m_{ij},\quad i,j=2,\ldots,n-1. \tag{29}$$

The solutions of the above equations are compatible with the existence of a unitary matrix, if and only if, all the angles and phases satisfy the unitarity constraints (18) and (19). *For* $n\geqslant 4$ *the solutions of Eq.* (29) *could depend on arbitrary angles and/or phases on the variety obtained by setting to zero the determinant of Jacobian matrix of the transformation* (29)

$$J=\frac{\partial(f_{22},\ldots,f_{2n-1},f_{n-12}\ldots,f_{n-1n-1})}{\partial(b_1,\ldots,b_{[(n-2)(n-3)]/2},\beta_1,\ldots,\beta_{[(n-1)(n-2)]/2})}. \tag{30}$$

If p *is the rank of the Jacobian matrix* (30) *the solution of* (29) *depends upon* $(n-2)^2-p$ *arbitrary parameters, angles and/or phases. Outside this variety the number of discrete solutions* N_s *satisfies* $1\leqslant N_s\leqslant 2^{[n(n-3)]/2}$.

Proof: Since we use a spherical coordinate system, (29) are trigonometric equations in our parametrization, as the example of case $n=4$ shows, and consequently the multiplicity of the solutions may arise from the two possible phase solutions for all values of sine or cosine functions that satisfy Eq. (29) and the constraints (18) and (19). The number of independent phases is $(n-1)(n-2)/2$ and, since we do not make any distinction between U and its complex conjugate U^*, condition that halves the number of solutions, the above bound for N_s follows.

For $n=3$ the Jacobian does not vanish and one gets $1\leqslant N_s\leqslant 1$, and this bound implies the existence of a complex unitary matrix, if and only if, when the values m_{ij}, coming from a double stochastic matrix satisfy the relation $-1\leqslant\cos\beta_1\leqslant 1$. □

An example of a unitary matrix that cannot be recovered from its moduli is the following. If P and $Q_i, i=1,\ldots,m$, are $m\times m$ and, respectively, $n\times n$ unitary matrices whose first rows and first columns are positive numbers and depend on p and, respectively, q_i arbitrary phases, then the following $m\times n$ array

$$M=\begin{pmatrix} p_{11}Q_1 & \cdot & \cdot & p_{1m}Q_m \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ p_{1m}Q_1 & \cdot & \cdot & p_{mm}Q_m \end{pmatrix} \tag{31}$$

defines a unitary matrix that could depend on

$$p+q_1+(m-1)\sum_{i=2}^{n}q_i \tag{32}$$

arbitrary phases.

Indeed it is easily seen that we can multiply at left all the matrices $Q_2,\ldots,Q_m$ by diagonal phase matrices $D_j=\mathrm{diag}(1,e^{\imath\varphi_{1,j}},\ldots,,e^{\imath\varphi_{n-1,j}}), j=2,\ldots,m$, by preserving the entries from the first row and column of M positive numbers, obtaining a set of unitary matrices that are all applied in the same double stochastic matrix. Thus their recovery from the moduli cannot be done because all the arbitrary phases φ_{ij} disappear when one computes their moduli, and as a consequence they do not appear in equations such as (15) and (16).

A second phenomenological model can be defined by starting from the orthogonality relations (12), but since in this case the polygons angles enter the game its formulation for arbitrary n is more difficult. Thus in the following we will discuss the case $n=3$ for both the models, which has applications in high energy physics.

A. Unitarity condition method

In the $n=3$ case the unitary (CKM) matrix is parametrized by *four* independent parameters given by the so-called mixing angles, θ_{12}, θ_{13}, θ_{23}, and the *CP*-violating phase δ. Hence in the following we will change the notation from Sec. III to another notation that is more familiar to

experimenters and phenomenologists. That means that in Eq. (9) defining the generating vectors we make the substitution: $(a_1 \to \theta_{12}, a_2 \to \theta_{23}, b_1 \to \theta_{13}, \beta_1 \to \delta)$; after that we make the notation

$$\cos\,\theta_{ij} = c_{ij}, \quad \sin\,\theta_{ij} = s_{ij}, \quad ij = 12,13,23$$

and by using Theorem 1 we get the following form

$$U = \begin{pmatrix} c_{12} & c_{13}s_{12} & s_{12}s_{13} \\ c_{23}s_{12} & -c_{12}c_{13}c_{23} - e^{i\delta}s_{13}s_{23} & -c_{12}c_{23}s_{13} + e^{i\delta}c_{13}s_{23} \\ s_{13}s_{23} & c_{23}s_{13}e^{i\delta} - c_{12}c_{13}s_{23} & -c_{13}c_{23}e^{i\delta} - c_{12}s_{13}s_{23} \end{pmatrix}. \tag{33}$$

The theoretical model (33) is supplemented by the experimental data supplied by experimenters. In the quark sector one measures two kinds of parameters: the moduli of the unitary matrix (33), see Ref. 18, under the form of a positive entries matrix, written with the physicists notation

$$V = \begin{pmatrix} V_{ud}^2 & V_{us}^2 & V_{ub}^2 \\ V_{cd}^2 & V_{cs}^2 & V_{cb}^2 \\ V_{td}^2 & V_{ts}^2 & V_{tb}^2 \end{pmatrix}, \tag{34}$$

where u, s, b, etc., are names for quarks, and the angles of the so-called standard unitarity triangle,[20] denoted by α/ϕ_1, β/ϕ_2, γ/ϕ_3.[42] In this paper V denotes either a double stochastic matrix, or a set of numbers affected by errors, when V_{ij} are measured in experiments. More generally the experimental data are given in terms of some functions $f_k(V_{ij})$, $k=1,\ldots,N$, that depend on the V entries, or the theoretical parameters s_{ij} and δ.

Similar to the general case treated in the previous section, we define our phenomenological model as a relationship between the theoretical object (33) and the experimental data (34). It is given by the double stochasticity relations (11), which now take the form

$$\begin{aligned} &\sum_{i=d,s,b} V_{ji}^2 - 1 = 0, \quad j = u,c,t, \\ &\sum_{i=u,c,t} V_{ij}^2 - 1 = 0, \quad j = d,s,b \end{aligned} \tag{35}$$

and by the embedding relation of a unitary matrix into the double stochastic set

$$V = |U|^2,$$

which leads to the following relations:

$$\begin{aligned} &V_{ud}^2 = c_{12}^2, V_{us}^2 = s_{12}^2 c_{13}^2, V_{ub}^2 = s_{12}^2 s_{13}^2, \\ &V_{cd}^2 = s_{12}^2 c_{23}^2, V_{td}^2 = s_{12}^2 s_{23}^2, \\ &V_{cs}^2 = c_{12}^2 c_{13}^2 c_{23}^2 + s_{13}^2 s_{23}^2 + 2c_{12}c_{13}c_{23}s_{13}s_{23}\cos\,\delta, \\ &V_{cb}^2 = c_{12}^2 c_{23}^2 s_{13}^2 + c_{13}^2 s_{23}^2 - 2c_{12}c_{13}c_{23}s_{13}s_{23}\cos\,\delta, \\ &V_{ts}^2 = c_{23}^2 s_{13}^2 + c_{12}^2 c_{13}^2 s_{23}^2 - 2c_{12}c_{13}c_{23}s_{13}s_{23}\cos\,\delta, \\ &V_{tb}^2 = c_{13}^2 s_{23}^2 + c_{12}^2 c_{13}^2 s_{23}^2 + 2c_{12}c_{13}c_{23}s_{13}s_{23}\cos\,\delta. \end{aligned} \tag{36}$$

The above-noted phenomenological model was introduced in Ref. 43. The relations (36) depend only on $\cos\,\delta$, which has the consequence that we can restrict δ to the interval $[0,\pi]$, this property

being equivalent to the CKM matrix invariance under the complex conjugation, as was shown in Sec. II.

Especially for physicists we want to make a few remarks. First we stress that in any phenomenological analysis one works with *two* distinct objects: the first is the theoretical one, that in our case coincides with the matrix U, Eq. (33), which is *assumed and built as a unitary matrix*; the second object is provided by the *experimental data*, $V=(V_{ij}^2)$, Eq. (34). The aim of any phenomenological analysis is twofold: (a) *checking the consistency of data with the theoretical model*, and (b) *determination of parameters entering the theoretical model from the experimental data, if these ones are consistent with it*. That is the reason for making a clear distinction between the theoretical quantities and the experimental ones, by using different symbols for denoting them. The second remark concerns the double stochasticity relations, Eq. (35), which are considered by (many) high energy physicists as testing the *unitarity*, statement which is wrong, since it is well known that for $n\geqslant 3$ there exist double stochastic matrices which are not unistochastic.[2] Checking the consistency, of the data with the theoretical model means checking the consistency of relations (36), i.e., we have to see if the solutions of Eq. (36) lead to physical values for the mixing parameters θ_{ij} and δ; and only in this case Eq. (35) *together* with Eq. (36) prove the unitarity property of the data.

Let us assume for a moment that relations (35) are exactly satisfied. Then it is an easy matter to find from the first five relations (36) three independent ones which give a unique solution for the c_{ij}, $ij=12,13,23$. In other words, if the experimental numbers satisfy the relations

$$V_{ud}^2+V_{us}^2+V_{ub}^2=1,$$

$$V_{ud}^2+V_{cd}^2+V_{td}^2=1,$$

we always get a solution for c_{ij} that is unique and depends on the three chosen independent parameters. Substituting this solution in the last equations one gets four equations for $\cos\delta$, which lead to a unique solution for it. But nobody guarantees us that the solution will satisfy the physical constraint

$$-1\leqslant\cos\delta\leqslant 1. \tag{37}$$

The last relation gives the necessary and sufficient condition the data have to satisfy in order that the 3×3 matrix (34) comes from a unitary matrix, i.e., it is the consistency condition between the data and the theoretical model.

To better understand the above-noted considerations and see the power of the found criterion (37) and how it works, we will give a few numerical examples, and for that we will use moduli entering the first two rows. We make the following notation:

$$V_{ud}=a,\quad V_{us}=b,\quad V_{ub}=c,\quad V_{cd}=d,\quad V_{cs}=e,\quad \text{and}\quad V_{cb}=f.$$

First we choose as independent moduli a, b, d, and e and with them form the square root of a double stochastic matrix

$$S_1=\begin{pmatrix} a & b & \sqrt{1-a^2-b^2} \\ d & e & \sqrt{1-d^2-e^2} \\ \sqrt{1-a^2-d^2} & \sqrt{1-b^2-e^2} & \sqrt{-1+a^2+b^2+d^2+e^2} \end{pmatrix}, \tag{38}$$

i.e., S_1^2 is an exact doubly stochastic matrix, where the square is taken entry-wise, by using the Hadamard product from linear algebra. From the relations (36) we get the solution

$$c_{12}=V_{ud}=a,\quad c_{13}=\frac{V_{us}}{\sqrt{1-V_{ud}^2}}=\frac{b}{\sqrt{1-a^2}},\quad c_{23}=\frac{V_{cd}}{\sqrt{1-V_{ud}^2}}=\frac{d}{\sqrt{1-a^2}}. \tag{39}$$

$$\cos\,\delta_1 = \frac{-(1-a^2)^2(1-e^2)+(1-a^2)(b^2+d^2)-b^2d^2(1+a^2)}{2abd\sqrt{1-a^2-b^2}\sqrt{1-a^2-d^2}}. \tag{40}$$

In the second case we take b, c, d, and, f as independent moduli, and get

$$S_2 = \begin{pmatrix} \sqrt{1-b^2-c^2} & b & c \\ d & \sqrt{1-d^2-f^2} & f \\ \sqrt{b^2+c^2-d^2} & \sqrt{d^2+f^2-b^2} & \sqrt{1-c^2-f^2} \end{pmatrix}, \tag{41}$$

$$c_{12} = \sqrt{1-b^2-c^2}, \quad c_{13} = \frac{b}{\sqrt{b^2+c^2}}, \quad c_{23} = \frac{d}{\sqrt{b^2+c^2}}, \tag{42}$$

$$\cos\,\delta_2 = \frac{b^2(b^2+c^2)-d^2(b^2-c^2+c^2(b^2+c^2))-f^2(b^2+c^2)^2}{2bcd\sqrt{1-b^2-c^2}\sqrt{b^2+c^2-d^2}}. \tag{43}$$

If the data are the entries of the following double stochastic matrix

$$V = \begin{pmatrix} \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{4} & \frac{2}{5} & \frac{7}{20} \\ \frac{5}{12} & \frac{1}{10} & \frac{29}{60} \end{pmatrix} \tag{44}$$

we get from Eqs. (39) and (40) and (42) and (43),

$$c_{12} = \frac{1}{\sqrt{3}}, \quad c_{13} = \frac{\sqrt{3}}{2}, \quad c_{23} = \frac{\sqrt{6}}{4}, \quad \cos\,\delta_1 = \cos\,\delta_2 = \frac{4\sqrt{15}}{25} \tag{45}$$

and the results show that the data are compatible to the existence of a unitary matrix. We remark that no matter how the independent moduli are chosen, c_{ij} and $\cos\,\delta$ take the same value, and this is a consequence of the fact that the properties of a double stochastic matrix do not change by multiplying it at left and/or right by permutation matrices. From a mathematical point of view the story ends here, because we can easily reconstruct the unitary matrix whose moduli are given in (44), by using the results (45) in the unitary matrix (33). We get

$$U = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{2} & -\frac{9}{20}\sqrt{\frac{3}{2}} - \frac{1}{20}\sqrt{\frac{77}{2}}i & \frac{7}{20\sqrt{2}} + \frac{1}{20}\sqrt{\frac{231}{2}}i \\ \frac{1}{2}\sqrt{\frac{5}{3}} & -\frac{13}{20\sqrt{10}} + \frac{1}{20}\sqrt{\frac{231}{10}}i & -\frac{61}{20\sqrt{30}} - \frac{3}{20}\sqrt{\frac{77}{10}}i \end{pmatrix}. \tag{46}$$

Hence the reconstruction algorithm of unitary matrices from the double stochastic ones is the following: *Start with a double stochastic matrix such as* (44) *and solve the system of equations* (36). *If the numerical value for* $\cos\,\delta$ *satisfies the inequalities* (37), *then with the values for* c_{ij} *and* $\cos\,\delta$ *go to* (33) *and find the corresponding unitary matrix.*

When the matrices S_1 and S_2, Eqs. (38) and (41), do not lead to the same double stochastic matrix, as for experimental data recommended in Ref. 18, the situation changes. For example, by using the numbers: $a=0.9738\pm0.0005$, $b=0.22\pm0.0026$, $c=0.00367\pm0.00047$, $d=0.224\pm0.012$, $e=0.996\pm0.013$, $f=0.0423\pm0.0015$, to define two doubly stochastic matrices S_1^2 and S_2^2 one gets

$$\cos\delta_1^+ = -0.03i, \quad \cos\delta_1^c = 1.59, \quad \cos\delta_1^- = 1.08, \tag{47}$$

$$\cos\delta_2^+ = 8.95i, \quad \cos\delta_2^c = 5.985i, \quad \cos\delta_2^- = 7.699, \tag{48}$$

where the indexes $+$, c, $-$ denote the $\cos\delta$ values obtained from central values $+1\sigma$, the central values, and, respectively, central values -1σ. The above results show that our criterion (37) is very sensitive to small variations of the parameters of the order of errors, and, on the other hand, one sees that the fulfillment of unitarity for experimental data is not an easy problem. We remark that $\cos\delta_1 \neq \cos\delta_2$, although by construction both the matrices S_1^2 and S_2^2 are double stochastic. But these ones are different because numerically, e.g., $e \neq \sqrt{1-d^2-f^2}$. Hence in the case of experimental data we have to take care and try to find how the necessary and sufficient conditions for the existence of a unitary matrix could be implemented. In this case also the relations (35) are not exactly fulfilled. Consequently the numbers c_{ij} obtained from relations (39) and (42) could be different, depending on the independent parameters we use for their determination. On the other hand the last four relations (36) provide us formulas for $\cos\delta$ and these formulas have to give the same number when comparing theory with experiment, by supposing the data come from a unitary matrix. Their explicit form depends on the independent four parameters we choose to parametrize the data. In fact there are 58 independent groups of four independent moduli that lead to 165 different expressions for $\cos\delta$. Depending on the explicit choice of the four independent parameters we get one, two, three, or four different expressions for $\cos\delta$.

Looking at Eqs. (39) and (40) and (42) and (43) we see that the expressions defining the mixing angles and phase δ are quite different. Thus if the data are compatible to the existence of a unitary matrix these angles c_{ij} and phases $\delta^{(i)}$ have to be equal, and these are the most general necessary conditions for unitarity; they can be written as

$$0 \leqslant c_{ij}^{(m)} \leqslant 1, \quad c_{ij}^{(m)} = c_{ij}^{(n)}, \quad m,n = 1, \ldots, 58, \quad \cos\delta^{(i)} = \cos\delta^{(j)}, \quad i,j = 1, \ldots, 165.$$

The above-presented relations are also satisfied by the double stochastic matrices, and the condition that separates the unitary matrices from the double stochastic ones is given by relation (37), i.e., $-1 \leqslant \cos\delta^{(i)} \leqslant 1$.

The formulas such as (40) and (43), together with the condition $-1 \leqslant \cos\delta \leqslant 1$, give the description of the physical region in terms of the four independent moduli we have chosen. Indeed the physical region is given by

$$1 - \cos^2\delta_1 = \sin^2\delta_1 \geqslant 0$$

so we get

$$-(1-a^2-b^2-d^2+b^2d^2-2abde-e^2+a^2e^2)(1-a^2-b^2-d^2+b^2d^2+2abde-e^2+a^2e^2)$$
$$\times(a^2+b^2)^2/(4a^2b^2(-1+a^2+b^2)(-1+d^2+e^2)(-1+a^2+b^2+d^2+e^2)) \geqslant 0, \tag{49}$$

where on the last row we separated a positive factor. Thus the physical region is given by

$$-(1-a^2-b^2-d^2+b^2d^2-2abde-e^2+a^2e^2)(1-a^2-b^2-d^2+b^2d^2+2abde-e^2+a^2e^2) \geqslant 0. \tag{50}$$

If we denote by

$$l_1 = ab, \quad l_2 = de, \quad l_3 = \sqrt{1-a^2-d^2}\sqrt{1-b^2-e^2}$$

the lengths of the unitarity triangle generated by the first and the second columns of the S_1 matrix, from Heron's formula

$$A=\sqrt{p(p-l_1)(p-l_2)(p-l_3)},\quad \text{where } p=(l_1+l_2+l_3)/2$$

is the semiperimeter, we get the area, A, of the unitarity triangle, which according to Ref. 33 is the same for all the six unitarity triangles. We write it as

$$\begin{aligned}16A^2=&-(1-a^2-b^2-d^2+b^2d^2-2abde-e^2+a^2e^2)\\&\times(1-a^2-b^2-d^2+b^2d^2-2abde-e^2+a^2e^2)\geqslant 0\end{aligned}\tag{51}$$

and see that formulas (50) and (51) are the same up to a multiplicative factor, i.e., they are perfectly equivalent. This area is the geometric invariant of the 3×3 CKM matrix describing the CP-violation.[33] We remark that the positivity of A^2 is the key ingredient used to characterize the set of orthostochastic matrices and its boundary, within the double stochastic set, see Proposition 2.2 in Ref. 4.

B. Unitarity triangle method

The second phenomenological model is defined by the orthogonality relations of rows, and, respectively, columns of a unitary matrix, and by the double stochastic relations (35). Although there are six such relations, see Eq. (12), usually one considers only the orthogonality of the first and the third columns of U, a relation that is written as

$$U_{ud}U_{ub}^*+U_{cd}U_{cb}^*+U_{td}U_{tb}^*=0.\tag{52}$$

The above-presented equation can be visualized as a triangle in the complex plane. Usually (52) is scaled by dividing it through the middle term such that the length of one side is 1. Taking into account that our parametrization, Eq. (33), of a unitary matrix has the entries of the first column and the first row positive quantities, we divide by the first term, $U_{ud}U_{ub}^*$, which is positive. In fact, what matters are the angles of the triangle, and our choice has the advantage that the triangle generated by Eq. (52) has two angles which numerically coincide, modulo π, with the phases of U_{23} and U_{33}; together with the phases of U_{22} and U_{32} they can be used for the determination of the unitary matrix U, since all these angles are measurable quantities in experiments, see, e.g., Ref. 20, or 44.

The other sides have the lengths

$$\begin{aligned}R_{db,c}^{(1)}&=\left|\frac{U_{cd}U_{cb}^*}{U_{ud}U_{ub^*}}\right|=\frac{d\sqrt{1-d^2-e^2}}{a\sqrt{1-a^2-b^2}},\\R_{db,t}^{(1)}&=\left|\frac{U_{td}U_{tb}^*}{U_{ud}U_{ub}^*}\right|=\frac{\sqrt{1-a^2-d^2}\sqrt{a^2+b^2+d^2+e^2-1}}{a\sqrt{1-a^2-b^2}},\end{aligned}\tag{53}$$

where we have written on the right-hand side the R-values in our choice of the four independent parameters by using the matrix (38). The physical condition takes the form

$$|R_{db,c}^{(1)}-R_{db,t}^{(1)}|\leqslant 1\leqslant R_{db,c}^{(1)}+R_{db,t}^{(1)},\tag{54}$$

which says that with the lengths 1, $R_{db,c}$ and $R_{db,t}$ one can construct a triangle. The above noted condition is equivalent to the positivity of the squared area A^2 given by relation (51), see Ref. 4. If we use the matrix (41) we find

$$\begin{aligned}R_{db,c}^{(2)}&=\left|\frac{U_{cd}U_{cb}^*}{U_{ud}U_{ub}^*}\right|=\frac{df}{c\sqrt{1-b^2-c^2}},\\R_{db,t}^{(2)}&=\left|\frac{U_{td}U_{tb}^*}{U_{ud}U_{ub}^*}\right|=\frac{\sqrt{1-c^2-f^2}\sqrt{b^2+c^2-d^2}}{c\sqrt{1-b^2-c^2}}.\end{aligned}\tag{55}$$

We remark that in Eqs. (53)–(55) the left side is the same, and only the right side differs, because the four independent moduli we use are different. Since there are 58 different groups of independent moduli there will be 58 different expressions $R^{(i)}_{db,j}$, $j=c,t$, and $i=1,\ldots,58$.

If now we use the orthogonality between the first and the second columns, i.e.,

$$U_{ud}U^*_{us}+U_{cd}U^*_{cs}+U_{td}U^*_{ts}=0 \tag{56}$$

one gets similarly

$$\begin{aligned} R^{(1)}_{ds,c}&=\left|\frac{U_{cd}U^*_{cs}}{U_{ud}U^*_{us}}\right|=\frac{de}{ab},\\ R^{(1)}_{ds,t}&=\left|\frac{U_{td}U^*_{ts}}{U_{ud}U^*_{us}}\right|=\frac{\sqrt{1-a^2-d^2}\sqrt{1-b^2-e^2}}{ab}, \end{aligned} \tag{57}$$

and, respectively,

$$\begin{aligned} R^{(2)}_{ds,c}&=\left|\frac{U_{cd}U^*_{cs}}{U_{ud}U^*_{us}}\right|=\frac{d\sqrt{1-d^2-f^2}}{b\sqrt{1-b^2-c^2}},\\ R^{(2)}_{ds,t}&=\left|\frac{U_{td}U^*_{ts}}{U_{ud}U^*_{us}}\right|=\frac{\sqrt{b^2+c^2-d^2}\sqrt{d^2+f^2-b^2}}{b\sqrt{1-b^2-c^2}}. \end{aligned} \tag{58}$$

If as in the preceding case we compute the expressions on the right-hand side using the data (44) we find

$$R^{(1)}_{db,c}=R^{(2)}_{db,c}=\frac{3}{2}\sqrt{\frac{7}{10}},\quad R^{(1)}_{db,t}=R^{(2)}_{db,t}=\frac{1}{2}\sqrt{\frac{29}{2}} \tag{59}$$

and, respectively,

$$R^{(1)}_{ds,c}=R^{(2)}_{ds,c}=\sqrt{\frac{3}{5}},\quad R^{(1)}_{ds,t}=R^{(2)}_{ds,t}=\frac{1}{2}, \tag{60}$$

which both satisfy the inequalities of the form (54).

With the central values from Ref. 18 one gets

$$\begin{aligned} &R^{(1)}_{db,c}=0.8i,\quad R^{(1)}_{db,t}=0.71,\quad R^{(1)}_{ds,c}=1.04,\quad R^{(1)}_{ds,t}=0.037i,\\ &R^{(2)}_{db,c}=2.58,\quad R^{(2)}_{db,t}=11.72i,\quad R^{(2)}_{ds,c}=1.016,\quad R^{(2)}_{ds,t}=0.012i, \end{aligned} \tag{61}$$

a result that sends the same signal of incompatibility as in Sec. IV, see Eq. (48).

From the above-presented equations we can obtain the angles of the triangles generated by relations (52) and, respectively, (56). For each triangle we denote by φ_3 the angle of the triangle associated to the vertex $(0,0)$, the other two, φ_1 and φ_2, being associated, respectively, to the vertexes (ρ,η) and $(1,0)$, where (ρ,η) are the coordinates of the triangle apex. For the second triangle we make the substitution $\varphi_i\to\psi_i$, $i=1,2,3$, and find

$$\cos\varphi_1=4\sqrt{\frac{7}{145}}\approx 0.8,\quad \cos\varphi_2=\frac{61}{10\sqrt{58}}\approx 0.88,\quad \cos\varphi_3=-\frac{1}{2}\sqrt{\frac{7}{10}}\approx -0.42 \tag{62}$$

and, respectively,

$$\cos\psi_1 = -\frac{1}{4}\sqrt{\frac{3}{5}} \approx -0.19, \quad \cos\psi_2 = \frac{13}{20} \approx 0.65, \quad \cos\psi_3 = \frac{9}{8}\sqrt{\frac{3}{5}} \approx 0.87. \tag{63}$$

Similar to the preceding case the necessary and sufficient conditions for unitarity are the constraints: all $R^{(j)} \geqslant 0$, and

$$R^{(i)}_{db,c} = R^{(j)}_{db,c}, \quad R^{(i)}_{db,t} = R^{(j)}_{db,t}, \quad i,j = 1, \ldots, 58, \tag{64}$$

$$R^{(i)}_{ds,c} = R^{(j)}_{ds,c}, \quad R^{(i)}_{ds,t} = R^{(j)}_{ds,t}, \quad i,j = 1, \ldots, 58, \tag{65}$$

$$|R^{(i)}_{db,c} - R^{(j)}_{db,c}| \leqslant 1 \leqslant R^{(i)}_{db,c} + R^{(j)}_{db,c}, \quad j = 1, \ldots, 58, \tag{66}$$

$$|R^{(i)}_{ds,t} - R^{(j)}_{ds,t}| \leqslant 1 \leqslant R^{(i)}_{ds,t} + R^{(j)}_{ds,t}, \quad j = 1, \ldots, 58, \tag{67}$$

where in the last equations we have written only the conditions implied by two orthogonality relations, although for applications we must calculate the constraints for all six orthogonality relations.

The first remark is that this approach, in the variant used by physicists, does not make use of the double stochasticity relations, Eq. (35), the physicists implicitly assuming that these relations are satisfied by the numbers obtained from experiments. With the above notation, (ρ, η), for the apex of the triangle, Eq. (53) is written under the form, see, e.g., Refs. 20–29

$$\begin{aligned} R^{(1)}_{db,c} &= \left| \frac{U_{cd}U^*_{cb}}{U_{ud}U_{ub}} \right| = \sqrt{\rho^2 + \eta^2}, \\ R^{(1)}_{db,t} &= \left| \frac{U_{td}U^*_{tb}}{U_{ud}U_{ub}} \right| = \sqrt{(1-\rho)^2 + \eta^2}. \end{aligned} \tag{68}$$

The second remark is that in contradistinction to what physicists believe, ρ and η have no special relationship with a parametrization of the CKM matrix, in particular that provided by Wolfenstein.[45] Indeed on the right-hand side, Eq. (68), are the lengths of two sides of the above-defined triangle, those $\neq 1$. Physical meaning have only the angles of that triangle which can be measured.[20,44] The third remark is that in this approach there is no relationship between the CP-violating phase δ and the angles of the unitarity triangles. Because the phase is interesting from a physical point of view, the phenomenologists make the identification

$$\delta = \varphi_3 \quad \text{or} \quad \delta \approx \varphi_3 \tag{69}$$

see, e.g., Refs. 21–29. Looking at the numerical values obtained for $\cos\delta = (4/25)\sqrt{15}$, relation (45), and for the angles of the unitarity triangles, (62) and (63), computed by using an exact unitary matrix, we obtained a numerical proof that the claim (69) is wrong. A simpler contra example is the following: take all $V^2_{ij} = 1/3$. Then all six triangles are equilateral and by consequence we have $\phi_1 = \phi_2 = \phi_3 = 60°$, and from the first phenomenological model we get $\delta = 90°$.

Although this model in the form (68) is currently used in many phenomenological analyses, see, e.g., Refs. 25 and 26, it cannot directly provide numbers for the parameters c_{ij} and δ such that there is no (reliable) recovery algorithm for unitary matrices from double stochastic matrices. The positive thing is that, if properly used, this phenomenological model allows the determination of all the angles of all six unitarity triangles, which are measurable quantities. Hence the real problem is to find a recovery algorithm for unitary matrices starting with measured values for all these angles. This problem was first raised by Aleksan *et al.*[44] and in the next section we will solve it.

V. EQUIVALENCE OF THE TWO APPROACHES

Relations (48) and (61), as well as (45) and (62), have shown that the unitarity sends the same signal of (in)consistency between the data and the theoretical model, although each one in a specific way. This is natural since both models are based on the unitarity property of matrices modeling the CP-violation. In the following we will prove that from a theoretical point of view the above-presented phenomenological models are only *partially* equivalent in the following sense: if we start with four independent angles we can reconstruct more than a unitary matrix, the multiplicity being equal to five, *and the solutions given by the two models are the same if and only if four moduli take the same values*. This opens the possibility to define new phenomenological models, in terms of moduli and phases, by taking into account all the experimental data. In particular we provide an expression for the phase δ in the second phenomenological model.

The starting point is the relation (53) that we write in a complex form. For that we define the four independent angles that enter the CKM matrix (33), namely $U_{ij}=|U_{ij}|e^{\iota\omega_{ij}}$, $i,j=2,3$. With this notation we write the complex form of (53) as

$$R_{db,c}(\cos\omega_{23}+i\sin\omega_{23})=\frac{U_{cd}^{*}U_{cb}}{U_{ud}^{*}U_{ub}}, \tag{70}$$

$$R_{db,t}(\cos\omega_{33}+i\sin\omega_{33})=-\frac{U_{td}^{*}U_{tb}}{U_{ud}^{*}U_{ub}} \tag{71}$$

by using the fact that in our parametrization the elements of the first row and first column are positive. In the above second relation we put a minus sign since U_{33}, as well as U_{22}, has an overall phase equal to π. In fact the angles of the triangle are defined up to an integer multiple of π. From (70) we get

$$\sin\omega_{23}=\frac{c_{13}c_{23}s_{23}\sin\delta}{c_{12}s_{13}R_{db,c}}, \tag{72}$$

$$\cos\omega_{23}=-\frac{c_{23}(c_{12}c_{23}s_{13}-c_{13}s_{23}\cos\delta)}{c_{12}s_{13}R_{db,c}}. \tag{73}$$

The above-noted relations are equivalent to

$$\tan\omega_{23}=\frac{c_{13}s_{23}\sin\delta}{-c_{12}c_{23}s_{13}+c_{13}s_{23}\cos\delta}. \tag{74}$$

The last formula depends only on theoretical parameters entering (33), and does not depend on the lengths of the unitarity triangle. If in (74) we substitute values for c_{ij} and $\cos\delta$ taken for example from the phenomenological model, Eqs. (39) and (40), we get a formula for $\tan\omega_{23}$ in terms of moduli that are measurable quantities.

Conversely, from relations (72) and (73) we get a formula for $\cos\delta$. Indeed, from the identity $\sin^2\omega_{23}+\cos^2\omega_{23}=1$ we find

$$\cos\delta=\frac{c_{12}^2c_{23}^4s_{13}^2+c_{13}^2c_{23}^2s_{23}^2-c_{12}^2s_{13}^2R_{db,c}^2}{2c_{12}c_{13}c_{23}^3s_{13}s_{23}}. \tag{75}$$

If in it we substitute the formulas (39) and $R_{db,c}$ from Eq. (53) we find Eq. (40) for $\cos\delta$. If instead of (53) we use the corresponding form for $R_{db,c}$, which comes from the relation (55), one gets Eq. (43), and so on.

In the same way from relation (71) one gets

$$\tan \omega_{33} = \frac{c_{13}c_{23} \sin \delta}{c_{12}s_{13}s_{23} + c_{13}c_{23} \cos \delta} \tag{76}$$

and

$$\cos \delta = \frac{c_{12}^2 s_{13}^2 R_{db,t}^2 - c_{13}^2 c_{23}^2 s_{23}^2 - c_{12}^2 s_{13}^2 s_{23}^4}{2c_{12}c_{13}c_{23}s_{13}s_{23}^3}. \tag{77}$$

From relations (70) and (71) we find

$$\frac{R_{db,t}}{R_{db,c}}(\cos(\omega_{33} - \omega_{23}) + i \sin(\omega_{33} - \omega_{23})) = -\frac{U_{td}^* U_{tb}}{U_{cd}^* U_{cb}} \tag{78}$$

and from it we can obtain a similar formula for $\tan(\omega_{33} - \omega_{23})$.

Similarly the complex form of the second triangle, Eq. (57), is

$$R_{ds,c}(\cos \omega_{22} + i \sin \omega_{22}) = -\frac{U_{cd}^* U_{cs}}{U_{ud}^* U_{us}}, \tag{79}$$

$$R_{ds,t}(\cos \omega_{32} + i \sin \omega_{32}) = \frac{U_{td}^* U_{ts}}{U_{ud}^* U_{us}}, \tag{80}$$

wherefrom we get

$$\tan \omega_{22} = \frac{s_{13}s_{23} \sin \delta}{c_{12}c_{13}c_{23} + s_{13}s_{23} \cos \delta}, \tag{81}$$

$$\tan \omega_{32} = \frac{c_{23}s_{13} \sin \delta}{-c_{12}c_{13}s_{23} + c_{23}s_{13} \cos \delta}. \tag{82}$$

From the above-noted calculations one sees that one orthogonality relation determines only two independent angles, and from them one cannot reconstruct the unitary matrix because each angle depends on the *four* independent parameters entering the generic form (33) of a 3×3 unitary matrix.

Similar to relations (75) and (77) one can find two other independent formulas for $\cos \delta$. Since all four expressions are independent and depend on four parameters, they can be inversed to find c_{ij} and $\cos \delta$ as functions of the ratios $R_{ij,k}$, obtaining the correct formula for $\cos \delta$ in this approach. However the formulas for some c_{ij} contains more than a hundred terms, and we will not give them here.

From a mathematical point of view the angles ω_{ij}, $i, j = 2, 3$ are not very interesting, although their existence was the essential ingredient for obtaining the necessary and sufficient conditions for the existence of a unitary matrix from the entries of a double stochastic matrix, see Ref. 3. From a physical point of view they are very interesting because they are measurable quantities. Similar to the preceding cases we have to use all six orthogonality relations, although for a double stochastic matrix all the angles ω_{ij}, $i, j = 2, 3$ have the same numerical values, irrespective of the orthogonality property we use. However irrespective of what triangles we use we get the same functions $\tan \omega_{22}$, $\tan \omega_{23}$, $\tan \omega_{32}$, and $\tan \omega_{33}$. If we use the orthogonality of the second and the third columns, respectively, of the second and the third rows, we get the angles of the corresponding triangles as linear functions of ω_{22}, ω_{23}, ω_{32}, ω_{33}, modulo π, see Ref. 44. For example, the angles of the unitarity triangle generated by relation (52), or (53), are given by ω_{33}, $\pi - \omega_{23}$, and $\omega_{23} - \omega_{33}$, etc.

In the following we give the necessary and sufficient conditions for recovery of a unitary matrix when we know the angles ω_{ij}, $i, j = 2, 3$, solving the problem first raised by Aleksan *et al.*[44] In the following we make the notation

$$\tan \omega_{22} = t_{22}, \quad \tan \omega_{23} = t_{23}, \quad \tan \omega_{32} = t_{32}, \quad \tan \omega_{33} = t_{33} \tag{83}$$

and from Eqs. (74) and (76), and (81) and (82) we get

$$c_{13}^2 = \frac{t_{23}t_{33}(t_{22} - t_{32})}{t_{22}t_{23}(t_{33} - t_{32}) + t_{32}t_{33}(t_{22} - t_{23})},$$

$$c_{23}^2 = \frac{t_{32}t_{33}(t_{22} - t_{23})}{t_{22}t_{23}(t_{33} - t_{32}) + t_{32}t_{33}(t_{22} - t_{23})}, \tag{84}$$

$$c_{12}^2 = \frac{N_1}{N_2},$$

where

$$\begin{aligned} N_1 &= (t_{22} - t_{23})(t_{22} - t_{32})(t_{23} - t_{33})(t_{32} - t_{33}), \\ N_2 &= t_{23}^2 t_{32}^2 + t_{22}^2 t_{33}^2 + t_{23}^2 t_{32}^2 (t_{22}^2 + t_{33}^2) + t_{22}^2 t_{33}^2 (t_{23}^2 + t_{32}^2) \\ &\quad - 2t_{22}t_{23}t_{32}t_{33}[1 + (t_{23} + t_{32})(t_{22} + t_{33}) - t_{23}t_{32} - t_{22}t_{33}]. \end{aligned} \tag{85}$$

Substituting the values for c_{ij} from relations (84) and (85) in any equation (74), (76), (81), (82), or a combination of them, we get a formula for $\cos \delta$, that is too long to be written down here. Hence the necessary and sufficient conditions for the existence of a unitary matrix coming from the angles ω_{ij} are

$$0 \leqslant c_{12}^2 \leqslant 1, \quad 0 \leqslant c_{13}^2 \leqslant 1, \quad 0 \leqslant c_{23}^2 \leqslant 1, \quad -1 \leqslant \cos \delta \leqslant 1. \tag{86}$$

By using the numerical values

$$t_{22} = \frac{1}{9}\sqrt{\frac{77}{3}}, \quad t_{23} = \sqrt{\frac{33}{7}}, \quad t_{32} = -\frac{\sqrt{231}}{13}, \quad t_{33} = \frac{3\sqrt{231}}{61} \tag{87}$$

obtained from the matrix (46) we get by using relations (84) and (85)

$$c_{12} = \frac{1}{\sqrt{3}}, \quad c_{13} = \frac{\sqrt{3}}{2}, \quad c_{23} = \frac{\sqrt{6}}{4} \tag{88}$$

showing that Eqs. (84) and (85) uniquely define the parameters c_{ij}, in perfect accord with (45).

If in Eqs. (74) and (76), and (81) and (82) we substitute the mixing angles as given by (84) and (85) we get equations for $\cos \delta$ that lead to the solutions

$$\cos \delta = \frac{4}{5}\sqrt{\frac{3}{5}}, \quad \cos \delta = -\frac{139}{116}\sqrt{\frac{3}{5}}, \quad \cos \delta = \frac{9}{8}\sqrt{\frac{3}{5}}, \tag{89}$$

$$\cos \delta = -\frac{1}{4}\sqrt{\frac{3}{5}}, \quad \cos \delta = -\frac{41}{32}\sqrt{\frac{3}{5}}. \tag{90}$$

In fact from each equation (74)–(76) and (81) and (82) one gets two solutions for $\cos \delta$, and only one of them coincides with that found in the first phenomenological model, see (45). Hence the problem of recovering a unitary matrix when we know four independent angles ω_{ij} is not unique, and the finite multiplicity is at least five. However this result does not contradict the general result stated in Theorem 2, a theorem which gives uniqueness if and only if we use four independent moduli. To see what happens in the above-noted case, we recover the unitary matrix by using c_{ij} taken from relations (88), and the second value for $\cos \delta$,

$$\cos\delta = -\frac{139}{116}\sqrt{\frac{3}{5}}.$$

The moduli matrix has the form

$$V_1 = \begin{pmatrix} \frac{1}{3} & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{4} & \frac{47}{1856} & \frac{1345}{1856} \\ \frac{5}{12} & \frac{881}{1856} & \frac{605}{5568} \end{pmatrix}. \tag{91}$$

By comparing the matrix V_1 with the original one, Eq. (44), we see that the elements of the first row and column coincide, the others are different. In order to obtain a unique solution we can use relation (77), or any other equivalent to, which make use of one of the lengths of unitarity triangle sides, which depends on the fourth independent moduli. Hence by using information coming only from triangles angles we have a finite multiplicity solution. The uniqueness is obtained if and only if the information is supplemented by an independent modulus, e.g., in the above-mentioned case $V(2,2)$, or a length of a unitarity triangle. The phenomenological implications of the above-noted results on the global fit methods for recovering a unitary matrix from moduli and angles will be treated elsewhere.

VI. RECOVERY OF UNITARY MATRICES FROM EXPERIMENTAL DATA

If the data come from an exact numerical matrix the problem to solve is quite simple: we have to test the stochasticity property, and, afterwards, the unitarity constraints, i.e., the condition, $-1 \leqslant \cos\delta \leqslant 1$, in the unitarity condition method, or the inequalities, $|R_{\alpha\beta,\gamma} - R_{\alpha\beta,\gamma}| \leqslant 1 \leqslant R_{\alpha\beta,\gamma} + R_{\alpha\beta,\gamma}$, coming from two orthogonality relations in the case of the standard unitarity triangles approach. If the data pass any one of the tests, one can easily reconstruct the unitary matrix Eq. (33) from the data (34), as the numerical examples from the previous sections have shown. If the physical conditions are violated, there is no compatibility and the discussion ends here. The real problem, from a physical point of view, is when the data come from experiment, i.e., are numbers affected by errors, and the problem is how we proceed in this situation, because neither the double stochasticity relations, nor the unitarity constraints are exactly satisfied.

There is the place where the gauge invariance subgroup K of unitary matrices enters the game, and its implications are the following. We have to find all *four* independent moduli groups and find all the possible forms for $\cos\delta$, and, respectively, the lengths of the unitarity triangles. And we have to impose that the numerical values for them should be approximately equal. The usual case with the present data is that the numerical values obtained for moduli are such that $\cos\delta^{(i)} \neq \cos\delta^{(j)}$, and/or $R^{(i)}_{\alpha\beta,\gamma} \neq R^{(j)}_{\alpha\beta,\gamma}$, $i \neq j$. Even more $\cos\delta^{(i)}$ could be outside the physical region, or the lengths of unitarity triangles are imaginary, or if they are real are not compatible with the existence of a triangle, as the numerical examples provided in the paper show. Hence, in contradistinction with the usage nowadays, see Ref. 20, we have to devise a fitting model that should implement the fulfillment of the above-noted theoretical constraints, and which should take into account the experimental data.

The method we expose here is discussed in more detail in Ref. 46. It is a least-squares method for checking the compatibility of the data with the theoretical models in both approaches, and if the data pass the physical conditions imposed by unitarity, from the fits one gets values for the parameters entering the theoretical model that by assumption gives a reliable description of the physical reality that is investigated by experiment.

It follows that in both approaches the χ^2-function must contain two separate terms, the first have to impose the fulfillment of the unitarity constraints by the free parameters entering the

physical model, and their best determination from the data, and the second one should depend on physical quantities that are measured in (different) experiments. Thus our proposal for the first terms is

$$\chi_1^2 = \sum_{i<j} (\cos \delta^{(i)} - \cos \delta^{(j)})^2 + \sum_{j=u,c,t} \left(\sum_{i=d,s,b} V_{ji}^2 - 1 \right)^2 + \sum_{j=d,s,b} \left(\sum_{i=u,c,t} V_{ij}^2 - 1 \right)^2, \quad -1 \leqslant \cos \delta^{(i)} \leqslant 1 \tag{92}$$

for the unitarity condition method, and, respectively,

$$\chi_2^2 = \sum_{\substack{\alpha\beta,\gamma \\ i<j}} (R_{\alpha\beta,\gamma}^{(i)} - R_{\alpha\beta,\gamma}^{(j)})^2 + \sum_{j=u,c,t} \left(\sum_{i=d,s,b} V_{ji}^2 - 1 \right)^2 + \sum_{j=d,s,b} \left(\sum_{i=u,c,t} V_{ij}^2 - 1 \right)^2,$$
$$R_{\alpha\beta,\gamma}^{(i)} \geqslant 0, \quad |R_{\alpha\beta,\gamma}^{(i)} - R_{\alpha\beta,\gamma}^{(i)}| \leqslant 1 \leqslant R_{\alpha\beta,\gamma}^{(i)} + R_{\alpha\beta,\gamma}^{(i)} \tag{93}$$

for the unitarity triangles method. Both the $\chi_{1,2}^2$ formulas test the double stochasticity property and the unitarity; from the point of view of numerical computation the unitarity property is the most difficult to satisfy.

Concerning the second component of χ^2-test it is of the form

$$\chi_3^2 = \sum_{i=1} \left(\frac{d_i - \tilde{d}_i}{\sigma_i} \right)^2, \tag{94}$$

where d_i are theoretical functions depending on the theoretical parameters s_{ij} and δ, or on V_{kl}, and/or the angles ϕ_i, ψ_i which are given by the phenomenological model one works with, while $\tilde{d}_i$ are the measured experimental data for d_i, and σ is the vector of errors associated to $\tilde{d}_i$. The formulas

$$\chi_u^2 = \chi_1^2 + \chi_3^2$$

and, respectively,

$$\chi_t^2 = \chi_2^2 + \chi_3^2$$

are our proposals for χ^2-tools necessary in analyzing the experimental data.

A remark is the following: as we have seen the second phenomenological model does not yet provide an explicit formula for cos δ, although our results have shown that it is possible to obtain it. In any case a global fit done by using either χ_u^2 or χ_t^2 will give values for all the moduli. Hence for the reconstruction of a unitary matrix in the second phenomenological model we have to use formulas such as (77). A true global fit will be that which will use all the experimental data by merging the above-mentioned two phenomenological models. The fulfillment of constraints (92) and (93) can be enforced by penalty functions that are equivalent to defining at least two Lagrange multipliers, etc.; but these are technical details depending on the concrete problem.

The convexity property of the double stochastic matrices allows us to devise a method for doing statistics on unitary matrices that is still an open problem in the physical literature, see, e.g., Ref. 47. Let us suppose that by doing a fit with the above-noted methods we got n moduli matrices that are consistent with n (approximate) unitary matrices, $U_1, U_2, \ldots, U_n$. The convexity property together with the embedding (2) tell us that the matrix

$$M^2 = \sum_{i=1}^{n} x_i |U_i|^2, \quad \sum_{i=1}^{n} x_i = 1, \quad 0 \leqslant x_i \leqslant 1, \ i = 1, \ldots, n$$

is double stochastic, where as usual in this paper we use the Hadamard product to define the above relation. Then the correct formulas for the mean value $\langle M \rangle$, and the error matrix σ_M are given by

$$\langle M\rangle = \sqrt{\left(\sum_{i=1}^{n} |U_i|^2\right) \Big/ n},$$
$$\sigma_M = \sqrt{\left(\sum_{i=1}^{n} |U_i|^4\right) \Big/ n - \langle M\rangle^4}. \tag{95}$$

If the entries of the mean value matrix, $\langle M\rangle$, obtained in this way are not too far from the entries coming from a unitary matrix, one can reconstruct from $\langle M\rangle$ an (approximate) unitary matrix by using the technique developed in the paper.

VII. CONCLUSIONS

Our main reason for studying the separation criteria between the double stochastic matrices and the unistochastic ones was their importance in high energy physics, where the present algorithms for reconstruction of unitary matrices from experimental data are not yet reliable in our opinion. Fortunately for the 3×3 matrices, which seem to be the physical choice in the electroweak interaction, there are explicit formulas for the independent parameters entering a unitary matrix in terms of four independent elements of a double stochastic one. That allows us to check the unitarity properties of exact double stochastic matrices, and an easy reconstruction of the unitary one from the entries of the double stochastic matrix when the compatibility conditions are fulfilled. These formulas can be used to define χ^2-functions for checking the compatibility between the experimental data and the unitarity property of the CKM matrix, and to recover a unitary matrix from error affected data. More important, starting from the convexity of the Birkhoff's polytope, we found a method for doing statistics on the (moduli of) unitary matrices.

We have also shown that, because the unitarity triangles method[20] and the unitarity condition method,[43] both being consequences of the unitarity property, are completely equivalent if and only if they are formulated in terms of four independent moduli. In the same time we have shown that the unitarity triangles method has to make effective use of the double stochasticity relations in order to obtain reliable results. Writing the unitarity triangles method in complex form we have obtained formulas for the four independent phases entering a unitary matrix, these phases being the angles of the unitarity triangles, modulo π. This opens the possibility to treat coherently all the experimental data available on moduli and angles by merging the above-mentioned phenomenological models into a true global one, the aim in view being a precise determination of the phase δ that is the key parameter in understanding the CP-violation.

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Diamagnetic expansions for perfect quantum gases

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In this work we study the diamagnetic properties of a perfect quantum gas in the presence of a constant magnetic field of intensity B. We investigate the Gibbs semigroup associated with the one particle operator at finite volume, and study its Taylor series with respect to the field parameter $\omega := eB/c$ in different topologies. This allows us to prove the existence of the thermodynamic limit for the pressure and for all its derivatives with respect to ω (the so-called generalized susceptibilities). © *2006 American Institute of Physics.* [DOI: 10.1063/1.2259582]

I. INTRODUCTION

This paper is motivated by the study of the diamagnetic properties of a perfect quantum gas interacting with a constant magnetic field, $\mathbf{B} := B\mathbf{e}_3$, $B > 0$, $\mathbf{e}_3 := (0,0,1)$. The system obeys either the Bose or the Fermi statistics. Since we are only studying orbital diamagnetic effects, we consider a gas of spinless and charged particles.

We are mainly interested in the bulk response, i.e., the thermodynamic limit of the pressure and its derivatives w.r.t. cyclotron frequency $\omega := eB/c$. As in Briet *et al.* (2005) we use the term *generalized susceptibilities* to designate such quantities.

This question has been already addressed by several authors. Thus, one finds results concerning the existence of the large volume limit of pressure for both Fermi and Bose gases (Angelescu and Corciovei, 1975; Angelescu *et al.*, 1975b), the magnetization for a Bose gas (Cornean, 2000; Macris *et al.*, 1997) and the magnetic susceptibility for a Fermi gas (Angelescu *et al.*, 1975b). In (Briet *et al.*, 2005), extensions of these results to the case of generalized susceptibilities were announced.

This paper is the first in a series of two devoted to the rigorous proof of the results announced in (Briet *et al.*, 2005). Here we consider the regime in which the inverse temperature $\beta := 1/(kT)$ is positive and finite and the fugacity $z = e^{\beta\mu}$ belongs to the unit complex disk. Such conditions were also used in (Angelescu and Corciovei, 1975; Angelescu *et al.*, 1975b; Macris *et al.*, 1997). But here we also allow any positive value of the cyclotron frequency $\omega := e/cB$. In a forthcoming, paper, we will extend these results to some larger z-complex domains (in fact, to $\mathbf{D}_\epsilon$ defined below). One can also find different aspects of this problem in (Macris *et al.*, 1997; Combescure and Robert, 1990; Helffer and Sjöstrand, 1990).

The main part of this work is concerned with a new approach to the magnetic perturbation theory for a semigroup generated by a magnetic Schrödinger operator. It extends the results given

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in (Angelescu *et al.*, 1975a; Cornean, 2000) and heavily relies on the use of the magnetic phase factor. This allows us to have good control on the magnetic perturbation wrt the size of the volume (Briet and Cornean, 2002; Cornean and Nenciu, 1998; Nenciu, 2002) in which the gas is confined.

Let us now describe our results. Let Λ be an open, bounded, and connected subset of $\mathbb{R}^3$ containing the origin of $\mathbb{R}^3$ and with smooth boundary $\partial\Lambda$. Set

$$\Lambda_L := \{\mathbf{x} \in \mathbb{R}^3, \mathbf{x}/L \in \Lambda\}; \quad L > 1. \tag{1.1}$$

Here we use the transverse gauge, i.e., the magnetic potential is defined as $B\mathbf{a} := (B/2)\mathbf{e}_3 \wedge \mathbf{x}$. The one particle Hamiltonian,

$$H_L(\omega) = \frac{1}{2}(-i\boldsymbol{\nabla} - \omega\mathbf{a})^2, \tag{1.2}$$

is first defined in the form sense on $H_0^1(\Lambda_L)$, and then one considers its Friedrichs extension (Reed and Simon, 2003). Thus we work with Dirichlet boundary conditions (DBC).

It is well-known that $H_L(\omega)$, $\omega \in \mathbb{R}$, generates a Gibbs semigroup,

$$\{W_L(\beta,\omega) = e^{-\beta H_L(\omega)} : \beta \geq 0\}, \tag{1.3}$$

i.e., for all $\beta > 0$, $W_L(\beta,\omega) \in B_1(L^2(\mathbb{R}^3)$, the set of trace class operators on $\mathcal{H}_L$ (Angelescu and Corciovei, 1975; Zagrebnov, 1978)

Then for $\beta > 0$, $\omega \in \mathbb{R}$, the grand canonical pressure of a quantum gas at finite volume is defined as (Huang, 1987; Angelescu and Corciovei, 1975; Angelescu *et al.*, 1975b)

$$P_L(\beta,\omega,z,\epsilon) = \frac{\epsilon}{\beta|\Lambda_L|} \cdot \mathrm{Tr}\{\ln(1 + \epsilon z W_L(\beta,\omega)\}, \tag{1.4}$$

where $\epsilon = -1 (\epsilon = 1)$ for Bose (Fermi) statistics. Since $\omega/2 = \inf \sigma(H_\infty(\omega))$, then the pressure is an analytic function wrt z on the complex domain $\mathbf{D}_\epsilon$ with

$$\mathbf{D}_{+1} := \mathbb{C} \setminus (-\infty, -e^{\beta\omega/2}], \quad \mathbf{D}_{-1} := \mathbb{C} \setminus [e^{\beta\omega/2}, \infty).$$

Let $n \geq 1$ and define the susceptibility of order n at finite volume by

$$\chi_L^{(n)}(\beta,\omega,z,\epsilon) := \frac{\partial^n P_L}{\partial \omega^n}(\beta,\omega,z,\epsilon). \tag{1.5}$$

If $n = 0$ we set $\chi_L^{(0)}(\beta,\omega,z,\epsilon) := P_L(\beta,\omega,z,\epsilon)$.

A. Results

Our first result describes the properties of the above defined quantities at finite volume, and it is given by the following theorem.

Theorem 1.1: *Let $\beta > 0$. Then the map $\mathbb{R} \ni \omega \to W_L(\beta,\omega) \in B_1(L^2(\mathbb{R}^3))$ is real analytic and admits an entire extension. For each open and bounded set $\mathcal{K}$ that obeys $\bar{\mathcal{K}} \subset \mathbf{D}_\epsilon$, $\epsilon = -1, +1$, there exists an open neighborhood $\mathcal{N}$ of the real axis such that the pressure at finite volume $P_L(\beta,\omega,z,\epsilon)$ is analytic* wrt (ω,z) *on $\mathcal{N} \times \mathcal{K}$. Let $\omega \in \mathbb{R}$, and $|z| < 1$. Then for $n \geq 0$ we have* [*see* (1.3)]:

$$\chi_L^{(n)}(\beta,\omega,z,\epsilon) = \frac{\epsilon}{\beta|\Lambda_L|} \sum_{k \geq 1} \frac{(-\epsilon z)^k}{k} \mathrm{Tr}\left\{\frac{\partial^n W_L(k\beta,\omega)}{\partial \omega^n}\right\}. \tag{1.6}$$

We now discuss the limit $L = \infty$. First, we define the candidates, $\chi_\infty^{(n)}$, for these limits. Recall that the one particle operator $H_\infty(\omega) = \frac{1}{2}(-i\boldsymbol{\nabla} - \omega\mathbf{a})^2$ on $L^2(\mathbb{R}^3)$, $\omega \in \mathbb{R}$, is positive and essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Denote by $W_\infty(\beta,\omega)$, $\beta \geq 0$ the semigroup generated by $H_\infty(\omega)$. Then $W_\infty(\beta,\omega)$ has an explicit integral kernel satisfying (see Sec. III):

$$G_\infty(\mathbf{x},\mathbf{x};\beta,\omega)=\frac{1}{(2\pi\beta)^{3/2}}\frac{\omega\beta/2}{\sinh(\omega\beta/2)},\quad \forall\,\mathbf{x}\in\mathbb{R}^3. \tag{1.7}$$

Note that the right hand side is independent of $\mathbf{x}$. Let $\beta>0$, $\omega\geq 0$ and $|z|<1$.

In view of (1.6), define

$$P_\infty(\beta,\omega,z,\epsilon):=\frac{\epsilon}{\beta}\sum_{k\geq 1}\frac{(-\epsilon z)^k}{k}G_\infty(\mathbf{0},\mathbf{0};k\beta,\omega), \tag{1.8}$$

which is well defined because of the estimate $\sinh(t)\geq t$ if $t\geq 0$. Then by the results of (Angelescu and Corciovei, 1975; Angelescu *et al.*, 1975b), we know that

$$\lim_{L\to\infty}P_L(\beta,\omega,z,\epsilon)=P_\infty(\beta,\omega,z,\epsilon).$$

It is quite natural to choose $\chi_\infty^{(n)}:=\partial^n P_\infty/\partial\omega^n$ provided that this last quantity exists. Note that it is not very easy to see this just from (1.8) and (1.7).

We then prove the following.

Theorem 1.2: *Let* $\beta>0$, $\omega\geq 0$ *and* $|z|<1$. *Fix* $n\geq 1$ *and define*

$$\chi_\infty^{(n)}(\beta,\omega,z,\epsilon):=\frac{\partial^n P_\infty}{\partial\omega^n}(\beta,\omega,z,\epsilon). \tag{1.9}$$

Then we have the equality:

$$\chi_\infty^{(n)}(\beta,\omega,z,\epsilon)=\frac{\epsilon}{\beta}\sum_{k\geq 0}\frac{(-\epsilon z)^k}{k}\frac{\partial^n G_\infty}{\partial\omega^n}(\mathbf{0},\mathbf{0};k\beta,\omega). \tag{1.10}$$

Moreover,

$$\lim_{L\to\infty}\chi_L^{(n)}(\beta,\omega,z,\epsilon)=\chi_\infty^{(n)}(\beta,\omega,z,\epsilon) \tag{1.11}$$

uniformly on $[\beta_0,\beta_1]\times[\omega_0,\omega_1]$, $0<\beta_0<\beta_1<\infty$, *and* $0<\omega_0<\omega_1<\infty$.

B. Relation with the de Haas-van Alphen (dHvA) effect

Our results can be easily extended to the case of more general Bloch electrons, that is, when one has a background smooth and periodic electric potential V. More precisely, let us assume that $V\in C^\infty(\mathbb{R}^3)$, $V\geq 0$, and if Γ is a periodic lattice in $\mathbb{R}^3$, then $V(\cdot)=V(\cdot+\gamma)$ for all $\gamma\in\Gamma$. Denote by Ω the elementary cell of Γ. In this case, the grand canonical pressure at the thermodynamic limit will be given by (we work with fermions; thus $\epsilon=1$)

$$P_\infty(\beta,\omega,z)=\frac{1}{\beta}\sum_{k\geq 1}\frac{(-z)^k}{k}\frac{1}{|\Omega|}\int_\Omega G_\infty(\mathbf{x},\mathbf{x};k\beta,\omega)d\mathbf{x}, \tag{1.12}$$

where $G_\infty(\mathbf{x},\mathbf{x}';k\beta,\omega)$ is the smooth integral kernel of the semigroup generated by $\frac{1}{2}(-i\nabla+\omega\mathbf{a})^2+V$. This formula only holds for $|z|<1$, but it can be analytically continued to $\mathbb{C}\backslash(-\infty,-1]$; see Angelescu and Corciovei (1975) or Helffer and Sjöstrand (1990).

Now one can start looking at the behavior of $P_\infty(\beta,\omega,z)$ as a function of ω, in particular, around the point $\omega_0=0$. Working in canonical conditions, that is when z is a function of β, ω and the fixed particle density ρ, then one is interesting in the object

$$p_\infty(\beta,\omega,\rho):=P_\infty(\beta,\omega,z(\beta,\omega,\rho)).$$

A thorough analysis of the ω behavior near 0, involving derivatives with respect to ω of the above quantity, has been already given by Helffer and Sjöstrand in 1990.

Alternatively, one can start from the finite volume quantities, and define a $z_L(\beta,\omega,\rho)$ as the unique solution of the equation $\rho_L := \beta z\, \partial_z P_L(\beta,\omega,z_L)=\rho$ and $p_L(\beta,\omega,\rho) := P_\infty(\beta,\omega,z_L(\beta,\omega,\rho))$. Is it still true that at large volumes we have, for example, that

$$\partial_\omega^n p_L(\beta,\omega,\rho) \sim \partial_\omega^n p_\infty(\beta,\omega,\rho), \quad n \geq 1\,?$$

The main achievement of our paper is that at least for small densities (which fix $|z|<1$) the answer is yes. In a companion paper we will prove that this is true for all $z \in \mathbb{C}\backslash(-\infty,-1]$.

We end the introduction by giving the plan of this paper. In Sec. II we discuss the analyticity of the Gibbs semigroup with respect to ω in the trace class sense. The trace norm estimates we obtain depend on the size of the domain, due to the linear growth of the magnetic potential. Using magnetic perturbation theory we manage to regularize the trace expansions and to extend these results to the infinite volume case in Secs. III and IV. Finally, we prove the existence of thermodynamic limits in Sec. V.

II. ANALYTICITY OF GIBBS SEMIGROUPS

A. B_1 analyticity

Let Λ_L, $L \geq 1$ be domains of $\mathbb{R}^3$ as defined in (1.1). In the following we will denote, respectively, by $\|T\|_1$, $\|T\|_2$, and $\|T\|$, the trace norm in $B_1(L^2(\Lambda_L))$, the Hilbert-Schmidt norm in $B_2(L^2(\Lambda_L))$ and the operator norm in $B(L^2(\Lambda_L))$ of T.

In this section we study, the ω expansion of $W_L(\beta,\omega)$. This question has been already considered (Hille and Phillips, 1957; Angelescu *et al.*, 1975b; Zagrebnov, 1978) in connection with the B_1 analyticity of $W_L(\beta,\omega)$. Combining their result with our analysis below, this gives the following. Define the operators

$$\hat{R}_{1,L}(\beta,\omega) := \mathbf{a}\cdot(i\boldsymbol{\nabla}_{\mathbf{x}} + \omega\mathbf{a})W_L(\beta,\omega), \tag{2.1}$$

$$\hat{R}_{2,L}(\beta,\omega) := \frac{1}{2}\mathbf{a}^2 W_L(\beta,\omega). \tag{2.2}$$

Both operators $\hat{R}_{1,L}(\beta,\omega)$ and $\hat{R}_{2,L}(\beta,\omega)$ belong to $B(\Lambda_L)$ and we have the following estimate on their norm.

Lemma 2.1: *For all* $\beta>0$, $\omega\geq 0$, *and* $L>1$, *there exists a positive constant* C *such that*

$$\|\hat{R}_{1,L}\| \leq \frac{CL}{\sqrt{\beta}} \quad \text{and} \quad \|\hat{R}_{2,L}\| \leq CL^2. \tag{2.3}$$

Proof: Let $\varphi \in L^2(\Lambda_L)$. Since $W_L(\beta,\omega)L^2(\Lambda_L) \subset \mathrm{Dom}(H_L(\omega))$ (Kato, 1966) after a standard argument [note that the absolute value of the components of $\mathbf{a}$ are bounded from above by $\mathrm{diam}(\Lambda_1)\cdot L$]:

$$\|\mathbf{a}\cdot(i\boldsymbol{\nabla}_{\mathbf{x}} + \omega\mathbf{a})W_L(\beta,\omega)\varphi\|^2 \leq CL^2\langle H_L(\omega)W_L(\beta,\omega)\varphi, W_L(\beta,\omega)\varphi\rangle \leq \frac{C\cdot L^2}{\beta}\|\varphi\|^2, \tag{2.4}$$

where the last estimate is given by the spectral theorem. The second bound of (2.3) is obvious.□

Remark 2.2: *Due to the diamagnetic inequality* [*see* (2.30)], *we have for all* $\beta>0$ *and* $\omega \in \mathbb{R}$,

$$\|W_L(\beta,\omega)\|_1 = \mathrm{Tr}(W_L(\beta,\omega)) \leq \frac{L^3}{(2\pi\beta)^{3/2}}. \tag{2.5}$$

Then both operators $\hat{R}_{1,L}, \hat{R}_{2,L}$ *are trace class*, *since we can factorize the operator* $\hat{R}_{1,L}(\beta,\omega) = \hat{R}_{1,L}(\beta/2,\omega)W_L(\beta/2,\omega)$.

For $n \geq 1$, define

$$\mathcal{D}_n(\beta) := \{0 < \tau_n < \tau_{n-1} < \ldots \tau_1 < \beta\} \subset \mathbb{R}^n. \tag{2.6}$$

Let $(i_1, \ldots, i_n) \in \{1,2\}^n$. Lemma 2.1 allows us to define the following family of bounded operators:

$$\hat{I}_{n,L}(i_1, \ldots, i_n)(\beta,\omega) := \int_{\mathcal{D}_n(\beta)} W_L(\beta - \tau_1, \omega)\hat{R}_{i_1,L}(\tau_1 - \tau_2, \omega) \times \hat{R}_{i_2,L}(\tau_2 - \tau_3, \omega) \ldots \hat{R}_{i_{n-1},L}(\tau_{n-1} - \tau_n, \omega)\hat{R}_{i_n,L}(\tau_n, \omega) d\tau, \tag{2.7}$$

where dr is the n-dimensional Lebesgue measure. These operators are in fact trace class, and we will estimate their trace norm later. Let $n \geq 1$, $(i_1, \ldots, i_n) \in \{1,2\}^n$ and χ_k^n be the characteristic function,

$$\chi_k^n(i_1, \ldots, i_k) := \begin{cases} 1, & \text{if } i_1 + \ldots + i_k = n, \\ 0, & \text{otherwise.} \end{cases} \tag{2.8}$$

Then we have the following.

Theorem 2.3: *Fix $\beta > 0$. Then the operator-valued function $\mathbb{R} \ni \omega \mapsto W_L(\beta,\omega) \in B_1$ admits an entire extension to the whole complex plane. Fix $\omega_0 \geq 0$. For all $\omega \in \mathbb{C}$ we have*

$$W_L(\beta,\omega) = \sum_{n=0}^{\infty} \frac{(\omega - \omega_0)^n}{n!} \frac{\partial^n W_L}{\partial \omega^n}(\beta,\omega_0), \tag{2.9}$$

$$\frac{1}{n!}\frac{\partial^n W_L}{\partial \omega^n}(\beta,\omega_0) = \sum_{k=1}^{n} (-1)^k \sum_{i_j \in \{1,2\}} \chi_k^n(i_1, \ldots, i_k)\hat{I}_{k,L}(i_1, \ldots, i_k)(\beta,\omega_0). \tag{2.10}$$

Moreover, there exists a positive constant C independent of $n \geq 1$, $\beta > 0$, and L such that

$$\left\| \frac{1}{n!}\frac{\partial^n W_L}{\partial \omega^n}(\beta,\omega_0) \right\|_1 \leq C^n \frac{(1+\beta)^n}{\beta^{3/2}} L^{n+3} \frac{1}{[(n-1)/4]!}. \tag{2.11}$$

For all $\omega \in \mathbb{C}$, $\{W_L(\beta,\omega), \beta > 0\}$ is a Gibbs semigroup with its generator given by the closed operator $H_L(\omega)$.

Remark 2.4: This theorem implies that the trace of the semigroup W_L is an entire function of ω, and by (2.9),

$$\mathrm{Tr}(W_L(\beta,\omega)) = \sum_{n=0}^{\infty} \frac{(\omega - \omega_0)^n}{n!} \mathrm{Tr}\left(\frac{\partial^n W_L}{\partial \omega^n}(\beta,\omega_0) \right). \tag{2.12}$$

Proof of Theorem 2.3: We will use here some results from Hille and Phillips (1957) and Angelescu *et al.* (1975b), which we briefly recall. Let $\omega_0 \geq 0$. For $\omega \in \mathbb{C}$ set $\delta\omega := \omega - \omega_0$. Then the operator

$$H_L(\omega) - H_L(\omega_0) = (\delta\omega)\mathbf{a} \cdot (i\nabla_{\mathbf{x}} + \omega_0 \mathbf{a}) + \frac{(\delta\omega)^2}{2}\mathbf{a}^2 \tag{2.13}$$

is relatively bounded to $H_L(\beta,\omega_0)$ with relative bound zero. Note that for $\beta > 0$ from (2.13) we have, in the operator sense on $\mathcal{H}_L$,

$$\hat{R}_L(\beta,\omega) := (H_L(\omega) - H_L(\omega_0))W_L(\beta,\omega_0) = \delta\omega \hat{R}_{1,L}(\beta,\omega_0) + (\delta\omega)^2 \hat{R}_{2,L}(\beta,\omega_0). \tag{2.14}$$

For every compact subset $K \subset \mathbb{C}$, and due to the estimates (2.3), this operator satisfies

$$\int_0^1 d\tau \sup_{\omega\in K}\|\hat{R}_L(\tau,\omega)\| < \infty .$$

Let $0<\beta_1\leq\beta_0<\infty$. Then the series

$$W_L(\beta,\omega,\omega_0)=\sum_{n=0}^{\infty}(-1)^n W_L^{(n)}(\beta,\omega,\omega_0), \tag{2.15}$$

where $W_L^{(0)}(\beta,\omega,\omega_0)=W_L(\beta,\omega_0)$, and for $n\geq 1$,

$$W_L^{(n)}(\beta,\omega,\omega_0)=\int_0^\beta d\tau\, W_L(\beta-\tau,\omega_0)(H_L(\omega)-H_L(\omega_0))W_L^{(n-1)}(\tau,\omega_0) \tag{2.16}$$

is uniformly B_1 convergent on $K\times[\beta_1,\beta_0]$. This result was obtained in Angelescu *et al.* (1975b). Since $W_L(\beta,\omega,\omega_0)$ is the uniform limit of a sequence of entire B_1-valued functions, it follows via the Cauchy integral formula that $W_L(\beta,\omega,\omega_0)$ is also B_1 entire in ω. Moreover, for real ω it coincides with the operator $e^{-\beta H_L(\omega)}, \beta>0$.

What we do here is to identify its nth order derivative with respect to ω. From (2.16) and (2.14), a simple induction argument yields the following finite rearranging:

$$\sum_{n=0}^{N}(-1)^n W_L^{(n)}(\beta,\omega,\omega_0)=W_L(\beta,\omega_0)+\sum_{n=1}^{N}(\delta\omega)^n\sum_{k=1}^{n}(-1)^k\sum_{i_j\in\{1,2\}}\chi_k^n(i_1,\ldots,i_k)\hat{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega_0)$$
$$+\mathcal{R}_{N+1,L}(\beta,\omega,\omega_0), \tag{2.17}$$

where

$$\mathcal{R}_{N+1,L}(\beta,\omega,\omega_0)=\sum_{n=N+1}^{2N}(\delta\omega)^n\sum_{k=1}^{N}(-1)^k\sum_{i_j\in\{1,2\}}\chi_k^n(i_1,\ldots,i_k)\hat{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega_0). \tag{2.18}$$

Now differentiation with respect to ω commutes with the limit $N\to\infty$, again due to the uniform convergence and the Cauchy integral formula. Hence (2.9) is proved, since the nth order derivative of $\Sigma_{j=0}^{N}(-1)^j W_L^{(j)}(\beta,\omega,\omega_0)$ at $\omega=\omega_0$ equals the right hand side of (2.10) if $N\geq n$.

In the second part of the proof, we use the methods of Angelescu *et al.* (1975b) in order to estimate the B_1 norm of the operators $I_{k,L}(i_1,\ldots,i_k)$ as claimed in (2.11). We first have

$$\|\hat{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega_0)\|_1\leq\int_{\mathcal{D}_k(\beta)}d\tau\|W_L(\beta-\tau_1,\omega_0)\hat{R}_{i_1,L}(\tau_1-\tau_2,\omega_0)\ldots\hat{R}_{i_k,L}(\tau_k,\omega_0)\|_1. \tag{2.19}$$

Recall that the Ginibre-Gruber inequality reads as Angelescu *et al.* (1975b),

$$\left\|\prod_{l=0}^{k}A_l T(t_l)\right\|_1\leq\left(\prod_{l=0}^{k}\|A_l\|\right)\mathrm{Tr}\,T(t_0+t_1+\cdots+t_k), \tag{2.20}$$

where $\{A_l, 0\leq l\leq k\}$ are bounded operators and $T(t), t>0$ is a Gibbs semigroup. Then taking $A_0 := W_L((\beta-\tau_1)/2,\omega_0)$, $A_l := \hat{R}_{i_l,L}((\tau_l-\tau_{l+1})/2,\omega_0)$ if $l\geq 1$ (we put $\tau_{k+1}\equiv 0$) and $T(t)=W_L(t/2,\omega_0)$. On $D_k(\beta)$, we have the estimate $\|A_0\|\leq 1\leq\sqrt{(1+\beta)/(\beta-\tau_1)}$ and by the Lemma 2.1 for $l\geq 1$,

$$\|A_l\|=\left\|\hat{R}_{i_l,L}\left(\frac{\tau_l-\tau_{l+1}}{2},\omega_0\right)\right\|\leq\mathrm{const}\cdot L^{i_l}\frac{\sqrt{1+\beta}}{\sqrt{\tau_l-\tau_{l+1}}}. \tag{2.21}$$

Let $f_k:\mathcal{D}_k(\beta)\to\mathbb{R}$ be defined as

$$f_k(\tau) := \frac{1}{\sqrt{(\beta-\tau_1)(\tau_1-\tau_2)\cdots(\tau_{k-1}-\tau_k)\tau_k}}, \tag{2.22}$$

and it satisfies

$$\int_{\mathcal{D}_k(\beta)} f_k(\tau)d\tau = \frac{\beta^{(k-1)/2}\pi^{(k+1)/2}}{\Gamma\left(\frac{k+1}{2}\right)}. \tag{2.23}$$

Let $i_1+\cdots+i_k=n$. Then from (2.5), (2.20), (2.21), and (2.23), we obtain the existence of a numerical constant C, such that for every $\beta>0$:

$$\|\hat{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega_0)\|_1 \leq \frac{L^{n+3}C^k(1+\beta)^k}{\beta^{3/2}\Gamma\left(\frac{k+1}{2}\right)}. \tag{2.24}$$

Thus, we have the estimate [see (2.10)]:

$$\frac{1}{n!}\|(\partial_\omega^n W_L)(\beta,\omega_0)\|_1 \leq C^n L^{n+3}\frac{(1+\beta)^n}{\beta^{3/2}}\sum_{k=1}^{n}\sum_{i_j\in\{1,2\}}\frac{\chi_k^n(i_1,\ldots,i_k)}{\Gamma\left(\frac{k+1}{2}\right)}. \tag{2.25}$$

But a lot of terms in the above sum are zero, since $\chi_k^n(i_1,\ldots,i_k)=0$ if $k<[(n+1)/2]$. Since Γ is increasing, we can give a rough estimate of the form

$$\sum_{k=1}^{n}\sum_{i_j\in\{1,2\}}\frac{\chi_k^n(i_1,\ldots,i_k)}{\Gamma\left(\frac{k+1}{2}\right)} \leq n2^n\frac{1}{\Gamma\left(\frac{[(n+1)/2]+1}{2}\right)} \leq n2^n\frac{1}{[(n-1)/4]!}. \tag{2.26}$$

□

B. Proof of Theorem 1.1

The analyticity properties of the pressure are now easy to prove once we have the B_1 analyticity of the Gibbs semigroup. See Angelescu *et al.* (1975a) for details.

Now let $\beta>0, \omega\geq 0$ and $|z|<1$. Since $\|zW_L(\beta,\omega)\|<1$, the logarithm in the pressure at finite volume can be expanded, and then

$$P_L(\beta,\omega,z,\epsilon) = \epsilon/(\beta|\Lambda_L|)\sum_{k\geq 1}(-\epsilon z)^k/k \operatorname{Tr} W_L(k\beta,\omega). \tag{2.27}$$

Starting from Definition (1.5), and using Theorem 2.3, we obtain

$$\chi_L^{(n)}(\beta,\omega,z,\epsilon) = \epsilon/(\beta|\Lambda_L|)\sum_{k\geq 0}(-\epsilon z)^k/k \operatorname{Tr}\left(\frac{\partial^n W_L(k\beta,\omega)}{\partial\omega^n}\right). \tag{2.28}$$

Note that (2.11) ensures that the growth in k that comes from the trace of the nth derivative of $W_L(k\beta,\omega)$ is not faster than some polynomial, but since $|z|<1$, the series in k is convergent. This finishes the proof of the theorem. □

C. Analyticity of the semigroup's integral kernel

In the rest of this paper we will only consider $\Lambda_L=(-L/2,L/2)^3, L\geq 1$. For $\omega\in\mathbb{R}$, $H_L(\omega)$ is essentially self-adjoint on

$$\left\{\phi \in C^1(\bar{\Lambda}_L) \cup C^2(\Lambda_L), \phi\big|_{\partial\Lambda_L} = 0, \Delta\phi \in L^2(\Lambda_L)\right\}.$$

Let $G_L(\mathbf{x},\mathbf{x}';\beta,\omega)$ be the integral kernel of $W_L(\beta,\omega)$ [see, e.g., Angelescu and Corciovei (1975)]. Standard elliptic estimates for the eigenfunctions of $H_L(\omega)$, together with the fact that $e^{-\beta H_L(\omega)}$ is trace class, imply that $G_L(\mathbf{x},\mathbf{x}';\beta,\omega)$ is smooth in $(\mathbf{x},\mathbf{x}') \in \Lambda_L \times \Lambda_L$. Moreover, $G_L(\mathbf{x},\mathbf{x}';\beta,\omega)=0$ if either $\mathbf{x}$ or $\mathbf{x}'$ are on the boundary.

To prove the next theorem, we need the following result from Cornean (2000), concerning the C^1 regularity up to the boundary of the integral kernel. Let $\beta>0$ and let $G_\infty(\mathbf{x},\mathbf{x}',\beta) := G_\infty(\mathbf{x},\mathbf{x}',\beta,\omega=0)$ be the heat kernel on the whole space, i.e.,

$$G_\infty(\mathbf{x},\mathbf{x}';\beta) = \frac{1}{(2\pi\beta)^{3/2}} e^{-|\mathbf{x}-\mathbf{x}'|^2/2\beta}. \tag{2.29}$$

Recall that the diamagnetic estimate reads as Angelescu and Corciovei (1975):

$$|G_L(\mathbf{x},\mathbf{x}';\beta,\omega)| \leq G_\infty(\mathbf{x},\mathbf{x}';\beta), \quad (\mathbf{x},\mathbf{x}') \in \Lambda_L \times \Lambda_L, \quad \omega \geq 0. \tag{2.30}$$

Then we have the following.

Lemma 2.5: Let $\beta>0$ and $\omega\geq 0$. Then on $\Lambda_L\times\Lambda_L$, we have

$$|(i\nabla_{\mathbf{x}} + \omega\mathbf{a}(\mathbf{x}))G_L(\mathbf{x},\mathbf{x}';\beta,\omega)| \leq \frac{\mathcal{C}}{\sqrt{\beta}} G_\infty(\mathbf{x},\mathbf{x}',8\beta), \tag{2.31}$$

where $\mathcal{C}=\mathcal{C}(\beta,\omega)=c\cdot(1+\beta)^5(1+\omega)^3$ and $c>1$ is a numerical constant.

This estimate allows us to define the integral kernels of the operators defined in (2.2); more precisely, for $(\mathbf{x},\mathbf{x}') \in \Lambda_L\times\Lambda_L$, we have

$$\hat{R}_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega) := \mathbf{a}(\mathbf{x}) \cdot (i\nabla_{\mathbf{x}} + \omega\mathbf{a}(\mathbf{x}))G_L(\mathbf{x},\mathbf{x}';\beta,\omega),$$

$$\hat{R}_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega) := \frac{1}{2}\mathbf{a}^2(\mathbf{x})G_L(\mathbf{x},\mathbf{x}';\beta,\omega). \tag{2.32}$$

Consider the operator $W_L(\beta,\omega)$ for complex ω, defined by a B_1-convergent complex power series in Theorem 2.3. We will now prove that it has an integral kernel analytic in ω.

Theorem 2.6: *Let $\beta>0$ and fix $\omega_0\geq 0$.*

(i) *The operator $(\partial_\omega^n W_L)(\beta,\omega_0)$* defined in (2.10) *has an integral kernel denoted by $(\partial_\omega^n W_L)\times(\mathbf{x},\mathbf{x}';\beta,\omega_0)$, which is jointly continuous on $(\mathbf{x},\mathbf{x}') \in \bar{\Lambda}_L\times\bar{\Lambda}_L$, and obeys the estimate*

$$\frac{1}{n!}\left|\frac{\partial^n W_L}{\partial\omega^n}(\mathbf{x},\mathbf{x}';\beta,\omega_0)\right| \leq c^n \frac{(1+\omega_0)^{3n}(1+\beta)^{6n}L^n}{\beta^{3/2}\left[\frac{n-1}{4}\right]!}, \quad n\geq 1, \tag{2.33}$$

for some numerical constant $c\geq 1$.

(ii) *For $\omega\in\mathbb{C}$, the operator $W_L(\beta,\omega)$ has an integral kernel $G_L(\mathbf{x},\mathbf{x}';\beta,\omega)$ given by*

$$G_L(\mathbf{x},\mathbf{x}';\beta,\omega) = \sum_{n=0}^{\infty} \frac{(\omega-\omega_0)^n}{n!}\left(\frac{\partial^n W_L}{\partial\omega^n}\right)(\mathbf{x},\mathbf{x}';\beta,\omega_0), \tag{2.34}$$

where the above series is uniformly convergent on $\bar{\Lambda}_L\times\bar{\Lambda}_L$. Thus G_L is jointly continuous on $\bar{\Lambda}_L\times\bar{\Lambda}_L$ and is an entire function of ω.

Proof of Theorem 2.6: Lemma 2.5 obviously implies for $\beta>0$ and $\omega\geq 0$ the estimate

$$|\hat{R}_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega)| \leq L\frac{\mathcal{C}}{\sqrt{\beta}}G_\infty(\mathbf{x},\mathbf{x}';8\beta). \tag{2.35}$$

We also have

$$|\hat{R}_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega)| \leq \frac{L^2}{4}G_\infty(\mathbf{x},\mathbf{x}';\beta). \tag{2.36}$$

In the following, we will often use the uniform estimate with respect to the index $i=1,2$:

$$|\hat{R}_{i,L}(\mathbf{x},\mathbf{x}';t,\omega)| \leq L^i\mathcal{C}_1\sqrt{\frac{(1+\beta)}{t}}G_\infty(\mathbf{x},\mathbf{x}';8t), \quad 0<t\leq\beta, \tag{2.37}$$

where $\mathcal{C}_1 := \mathcal{C}_1(\beta,\omega)=2\sqrt{2}\mathcal{C}(\beta,\omega)$.

Let us start by proving (i). Fix $\beta>0,\omega_0\geq 0, L\geq 1$, and consider the operator $\hat{I}_{k,L}(i_1,\ldots,i_k)\times(\beta,\omega_0)$, $k\geq 1$ defined in (2.7). It admits a continuous integral kernel, $\hat{I}_{k,L}(\mathbf{x},\mathbf{x}';\beta,\omega_0) := \hat{I}_{k,L}(i_1,\ldots,i_k)(\mathbf{x},\mathbf{x}';\beta,\omega_0)$ on $\Lambda_L\times\Lambda_L$ given by

$$\begin{aligned}\hat{I}_{k,L}(\mathbf{x},\mathbf{x}';\beta,\omega_0) = \int_{D_k(\beta)} d\tau \int_{\Lambda_L^k} d\mathbf{y}\, G_L(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega_0)\hat{R}_{i_1,L}(\mathbf{y}_1,\mathbf{y}_2;\tau_1 \\ -\tau_2,\omega_0)\cdots\cdots \hat{R}_{i_{k-1},L}(\mathbf{y}_{k-1},\mathbf{y}_n;\tau_{k-1}-\tau_k,\omega_0)\hat{R}_{i_k,L}(\mathbf{y}_k,\mathbf{x}';\tau_k,\omega_0),\end{aligned} \tag{2.38}$$

where $d\mathbf{y}$ denotes the Lebesgue measure on $\mathbb{R}^{3k}$ and $D_k(\beta)$ is defined in (2.6). Let $i_1+i_2+\cdots+i_k=n$. Then by using the Lemma 2.5, the estimate

$$|G_L(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega_0)| \leq 8^{3/2}\sqrt{\frac{\beta}{\beta-\tau_1}}G_\infty(\mathbf{x},\mathbf{y}_1;8(\beta-\tau_1)), \quad 0<\tau_1<\beta,$$

and (2.37), the following estimate holds on $\Lambda_L\times\Lambda_L$:

$$\begin{aligned}|\hat{I}_{k,L}(\mathbf{x},\mathbf{x}';\beta,\omega_0)| \leq 8^{3/2}(1+\beta)^{(k+1)/2}\mathcal{C}_1^k L^n \\ \times\int_{D_k(\beta)} f_k(\tau)d\tau\int_{\Lambda_L^k} d\mathbf{y}G_\infty(\mathbf{x},\mathbf{y}_1;8(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_k,\mathbf{x}';8\tau_k),\end{aligned} \tag{2.39}$$

where the function f_k is defined in (2.22). Notice that by using the semigroup property,

$$\begin{aligned}\int_{\Lambda_L^k} d\mathbf{y}\, G_\infty(\mathbf{x},\mathbf{y}_1;t_1)\ldots G_\infty(\mathbf{y}_k,\mathbf{x}';t_k) \leq \int_{\mathbb{R}^k} d\mathbf{y}\, G_\infty(\mathbf{x},\mathbf{y}_1;t_1)\ldots G_\infty(\mathbf{y}_k,\mathbf{x}';t_k) \\ = G_\infty(\mathbf{x},\mathbf{x}';t_1+\cdots+t_k).\end{aligned} \tag{2.40}$$

Therefore from (2.39) we get

$$|\hat{I}_{k,L}(\mathbf{x},\mathbf{x}';\beta,\omega_0)| \leq 8^{3/2}(1+\beta)^{(k+1)/2}\mathcal{C}_1^k L^n G_\infty(\mathbf{x},\mathbf{x}';8\beta)\int_{D_k(\beta)} f_k(\tau)d\tau. \tag{2.41}$$

Then Theorem 2.3 together with (2.23) and (2.41) show that the operator $(\partial^n W_L/\partial\omega^n)(\beta,\omega_0)$, $n\geq 1$ given by (2.9), admits a continuous integral kernel satisfying

$$\left|\frac{\partial^n W_L}{\partial \omega^n}(\mathbf{x},\mathbf{x}';\beta,\omega_0)\right| \leq (8^3\pi)^{1/2}\mathcal{C}_2^n n!\, L^n G_\infty(\mathbf{x},\mathbf{x}';8\beta)\sum_{k=1}^{n}\sum_{i_j\in\{1,2\}}\frac{\chi_k^n(i_1,\ldots,i_k)}{\Gamma\left(\frac{k+1}{2}\right)},$$

for a new constant $\mathcal{C}_2=\mathcal{C}_2(\beta,\omega_0):=\pi^{1/2}(1+\beta)\mathcal{C}_1(\beta,\omega_0)$. Then by mimicking the proof of (2.26) we get from the last inequality

$$\frac{1}{n!}\left|\frac{\partial^n W_L}{\partial \omega^n}(\mathbf{x},\mathbf{x}';\beta,\omega_0)\right| \leq \frac{c^n(1+\beta)^{6n}(1+\omega_0)^{3n}L^n}{[(n-1)/4]!}G_\infty(\mathbf{x},\mathbf{x}';8\beta), \tag{2.42}$$

where c is a numerical constant. Since $G_\infty(\mathbf{x},\mathbf{x}';8\beta)\leq(16\pi\beta)^{-3/2}$, (2.42) implies the estimate (2.33) and proves (i). Then (ii) follows easily from the previous estimate since $1/[(n-1)/4]!$ has a superexponential decay in n. □

III. REGULARIZED EXPANSION

The bounds obtained in the previous section are not convenient for the proof of the existence of the thermodynamic limit of the magnetic susceptibilities. In particular, the bound on $(\partial^n W_L/\partial\omega^n)(\mathbf{x},\mathbf{x}',\beta,\omega_0)$ given by (2.42) is of order L^n. Then this gives a bound on its trace of order L^{3+n}, while in view of (1.6) we need a bound that goes like L^3.

In this section, we give an improvement of these estimates. In order to do that, we need to introduce the magnetic phase ϕ and the magnetic flux fl defined as [here $\mathbf{x},\mathbf{y},\mathbf{z}\in\Lambda_L$ and $\mathbf{e}=(0,0,1)$]:

$$\phi(\mathbf{x},\mathbf{y}) := \frac{1}{2}\mathbf{e}\cdot(\mathbf{y}\wedge\mathbf{x}) = -\phi(\mathbf{y},\mathbf{x}), \tag{3.1}$$

$$\mathrm{fl}(\mathbf{x},\mathbf{y},\mathbf{z}) := \phi(\mathbf{x},\mathbf{y})+\phi(\mathbf{y},\mathbf{z})+\phi(\mathbf{z},\mathbf{x}) = \frac{1}{2}\mathbf{e}\cdot\{(\mathbf{x}-\mathbf{y})\wedge(\mathbf{z}-\mathbf{y})\}. \tag{3.2}$$

Note that fl is really the magnetic flux through the triangle defined by the three vectors, and we have

$$|\mathrm{fl}(\mathbf{x},\mathbf{y},\mathbf{z})| \leq |\mathbf{x}-\mathbf{y}||\mathbf{y}-\mathbf{z}|. \tag{3.3}$$

For $n\geq 1$ and $\mathbf{x}=\mathbf{y}_0,\mathbf{y}_1,\ldots,\mathbf{y}_n$, some arbitrary vectors in Λ_L, define

$$\mathrm{Fl}_n(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_n) := \phi(\mathbf{y}_n,\mathbf{x})+\sum_{k=0}^{n-1}\phi(\mathbf{y}_k,\mathbf{y}_{k+1}) = \sum_{k=1}^{n-1}\mathrm{fl}(\mathbf{x},\mathbf{y}_k,\mathbf{y}_{k+1}), \quad \text{if } n\geq 2 \tag{3.4}$$

and

$$\mathrm{Fl}_1(\mathbf{x},\mathbf{y}_1)=0.$$

Notice that due to (3.3), we have

$$|\mathrm{Fl}_n(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_n)| \leq \sum_{k=1}^{n-1}\sum_{l=1}^{k}|\mathbf{y}_{l-1}-\mathbf{y}_l||\mathbf{y}_k-\mathbf{y}_{k+1}|. \tag{3.5}$$

Let $\omega\geq 0$. Consider now the bounded operators given by their integral kernels on $\Lambda_L\times\Lambda_L$,

$$R_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega) := \mathbf{a}(\mathbf{x}-\mathbf{x}')\cdot(i\nabla_{\mathbf{x}}+\omega\mathbf{a}(\mathbf{x}))G_L(\mathbf{x},\mathbf{x}';\beta,\omega).$$

$$R_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega) := \frac{1}{2}\mathbf{a}^2(\mathbf{x}-\mathbf{x}')G_L(\mathbf{x},\mathbf{x}';\beta,\omega). \tag{3.6}$$

Then by the Lemma 2.5, a straightforward estimate yields to

$$|R_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega)| \le \frac{\mathcal{C}|\mathbf{x}-\mathbf{x}'|}{2\sqrt{\beta}}G_\infty(\mathbf{x},\mathbf{x}',8\beta) \le 4\mathcal{C}_1 G_\infty(\mathbf{x},\mathbf{x}',16\beta), \tag{3.7}$$

for all $(\mathbf{x},\mathbf{x}')\in\Lambda_L\times\Lambda_L$. Similarly, by (2.30) we have

$$|R_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega)| \le \frac{|\mathbf{x}-\mathbf{x}'|^2}{8}G_\infty(\mathbf{x},\mathbf{x}',\beta) \le \frac{\beta}{\sqrt{2}}G_\infty(\mathbf{x},\mathbf{x}',2\beta). \tag{3.8}$$

In the sequel for $i=1,2$, we will use the estimate on $\Lambda_L\times\Lambda_L$,

$$|R_{i,L}(\mathbf{x},\mathbf{x}';\beta,\omega)| \le \mathcal{C}_3 G_\infty(\mathbf{x},\mathbf{x}',16\beta), \tag{3.9}$$

where $\mathcal{C}_3=\mathcal{C}_3(\beta,\omega) := 16\mathcal{C}_1(\beta,\omega)$ and $\mathcal{C}_1$ is given in (2.37).

Notice that (3.9) provides a uniform bound wrt. L and β near $\beta=0$ on the operator kernels. This in contrast with the bound on the norm operator of $\hat{R}_{i,L}; i=1,2$ [see Sec. II B, (2.35) and (2.36)]. Using the Schur-Holmgren estimate for the operator norm of an integral operator, (3.9) eventually implies

$$\|R_{i,L}\| \le \mathcal{C}_3, \quad i=1,2. \tag{3.10}$$

Let $\mathbf{x}\in\Lambda_L$. For $k\ge 1$, $m\ge 0$, $\omega\ge 0$, and $\beta>0$, define the continuous function,

$$\begin{aligned} W^m_{k,L}(\mathbf{x};\beta,\omega) := \sum_{j=1}^{k}(-1)^j \sum_{(i_1,\ldots,i_j)\in\{1,2\}^j} \chi^k_j(i_1,\ldots,i_j)\int_{D_j(\beta)} d\tau \int_{\Lambda^j} d\mathbf{y}\frac{(i(\mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j)))^m}{m!} \\ \times G_L(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega)R_{i_1,L}(\mathbf{y}_1,\mathbf{y}_2;\tau_1-\tau_2,\omega)\ldots R_{i_{j-1},L}(\mathbf{y}_{j-1},\mathbf{y}_j;\tau_{j-1}-\tau_j,\omega) \\ \times R_{i_j,L}(\mathbf{y}_j,\mathbf{x};\tau_j,\omega), \end{aligned} \tag{3.11}$$

where in the case of $m=0$ we set $0^0\equiv 1$.

The main result of this section gives a new expression for the diagonal of kernel's nth derivative with respect to ω at finite volume.

Theorem 3.1: *Let $\beta>0$ and $\omega\ge 0$. Then for all $\mathbf{x}\in\Lambda_L$, and for all $n\ge 1$, one has*

$$\frac{1}{n!}\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x},\beta,\omega) = \sum_{k=1}^{n} W^{n-k}_{k,L}(\mathbf{x};\beta,\omega), \tag{3.12}$$

and, moreover, uniformly in $L>1$:

$$|W^m_{k,L}(\mathbf{x};\beta,\omega)| \le c(m,k)\frac{(1+\beta)^{7(m+k)+3}}{\beta^{3/2}}(1+\omega)^{3(m+k)+2}, \tag{3.13}$$

where $c(m,k)=c^{m+k}(m^m/m!)\Sigma_{j=1}^{k}\frac{j^{2m}}{j!}$ and c is again a numerical factor.

Proof: We first need to introduce some new notation. Fix $\omega_0\ge 0$. Let $\omega\in\mathbb{C}$, $\delta\omega=\omega-\omega_0$ and $\tilde{R}_{i,L}(\beta,\omega,\omega_0)$, $i=1,2$, $\tilde{W}_L(\beta,\omega,\omega_0)$ be the operators on $\mathcal{H}_L$ defined via their respective integral kernel given on $\Lambda_L\times\Lambda_L$, by

$$\widetilde{R}_{i,L}(\mathbf{x},\mathbf{x}';\beta,\omega,\omega_0) = e^{i\ \delta\omega\ \phi(\mathbf{x},\mathbf{x}')}R_{i,L}(\mathbf{x},\mathbf{x}';\beta,\omega_0), \quad i=1,2,$$

$$\widetilde{W}_L(\mathbf{x},\mathbf{x}';\beta,\omega,\omega_0) = e^{i\delta\omega\phi(\mathbf{x},\mathbf{x}')}G_L(\mathbf{x},\mathbf{x}';\beta,\omega_0), \tag{3.14}$$

where ϕ is defined in (3.1). We also set

$$\widetilde{R}_L(\mathbf{x},\mathbf{x}';\beta,\omega,\omega_0) := \delta\omega\,\widetilde{R}_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega,\omega_0) + (\delta\omega)^2\widetilde{R}_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega,\omega_0).$$

Except for a phase factor, the kernel of $\widetilde{W}_L$ and $\widetilde{R}_{i,L}$, $i=1,2$ is the same as the one of W_L, $R_{i,L}$, $i=1,2$, respectively. Then they satisfy (2.30) and (3.9), respectively. Hence, by the same arguments as above, they are bounded operators and

$$\|\widetilde{W}_L\| \leq 1, \|\widetilde{R}_{i,L}\| \leq \mathcal{C}_3 \tag{3.15}$$

[see (3.10)]. Notice also that since $\|\widetilde{W}_L\|_{\mathcal{I}_2} = \|W_L\|_{\mathcal{I}_2} \leq L^{3/2}/(2\pi\beta)^{3/4}$, then by (3.9), $R_{i,L}$, $i=1,2$ as well as $\widetilde{R}_{i,L}$, $i=1,2$ are in the Hilbert-Schmidt class and for $\beta>0$, $\omega_0\geq 0$ and $\omega\in\mathbb{C}$,

$$\|R_{i,L}(\beta,\omega)\|_{\mathcal{I}_2}, \|\widetilde{R}_{i,L}\|_{\mathcal{I}_2}(\beta,\omega,\omega_0) \leq \mathcal{C}_3\|W_L(16\beta,\omega)\|_{\mathcal{I}_2} \leq \mathcal{C}_3\frac{L^{3/2}}{(2\pi\beta)^{3/4}}, \tag{3.16}$$

where $\mathcal{C}_3 = \mathcal{C}_3(\beta,\omega_0)$ was first introduced in (3.9). We now define the following family of bounded operators on $\mathcal{H}_L$. Let $k\geq 1$, $\{i_1,\ldots,i_k\}\in\{1,2\}^k$, $\beta>0$, $\omega_0\geq 0$. For all $\omega\in\mathbb{C}$, set

$$\widetilde{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega,\omega_0) := \int_{D_k(\beta)} d\tau\,\widetilde{W}_L(\beta-\tau_1,\omega,\omega_0)\widetilde{R}_{i_1,L}(\tau_1-\tau_2,\omega,\omega_0)\ldots\widetilde{R}_{i_{k-1},L}(\tau_{k-1} - \tau_k,\omega,\omega_0)\widetilde{R}_{i_k,L}(\tau_k,\omega,\omega_0), \tag{3.17}$$

and for $n\geq 1$,

$$W_{n,L}(\beta,\omega,\omega_0) := \sum_{k=1}^{n}(-1)^k\sum_{i_j\in\{1,2\}}\chi_k^n(i_1,\ldots,i_k)\widetilde{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega,\omega_0), \tag{3.18}$$

where χ_k^n is defined in (2.8).

Lemma 3.2: Let $N\geq 1$, $\beta>0$, $\omega_0\geq 0$. For all $\omega\in\mathbb{C}$, set $\delta\omega=\omega-\omega_0$. Then as bounded operators we can write

$$W_L(\beta,\omega) = \widetilde{W}_L(\beta,\omega,\omega_0) + \sum_{n=1}^{n}(\delta\omega)^n W_{n,L}(\beta,\omega,\omega_0) + \widetilde{\mathcal{R}}^{(1)}_{N+1,L}(\beta,\omega,\omega_0) + \widetilde{\mathcal{R}}^{(2)}_{N+1,L}(\beta,\omega,\omega_0), \tag{3.19}$$

where $\widetilde{\mathcal{R}}^{(1)}_{N+1,L}(\beta,\omega,\omega_0)$ and $\widetilde{\mathcal{R}}^{(2)}_{N+1,L}(\beta,\omega,\omega_0)$ are the following bounded operators on $\mathcal{H}_L$:

$$\widetilde{\mathcal{R}}^{(1)}_{N+1,L}(\beta,\omega,\omega_0) := (-1)^{N+1}\sum_{n=N+1}^{2N+2}(\delta\omega)^n\sum_{i_j\in\{1,2\}}\chi_{N+1}^n(i_1,\ldots,i_n) \times\int_{D_{N+1}(\beta)} d\tau\,W_L(\beta-\tau_1,\omega)\widetilde{\mathcal{R}}_{i_1,L}(\tau_1-\tau_2,\omega,\omega_0)\ldots\widetilde{\mathcal{R}}_{i_{N+1},L}(\tau_{N+1},\omega,\omega_0), \tag{3.20}$$

where $D_{N+1}(\beta)$ is given in (2.6) *and*

$$\tilde{\mathcal{R}}^{(2)}_{N+1,L}(\beta,\omega,\omega_0)=\sum_{n=N+1}^{2N}(\delta\omega)^n\sum_{k=1}^{N}(-1)^k\sum_{i_j\in\{1,2\}}\chi^n_k(i_1,\ldots,i_k)\cdot\tilde{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega,\omega_0). \tag{3.21}$$

Proof of lemma: In this proof we fix $\omega_0\geq 0$ and omit everywhere the ω_0 dependence. We first note that $\tilde{W}_L(\beta,\omega)$ is strongly differentiable with respect to $\beta>0$ [see Cornean (2000)] and satisfies

$$\frac{\partial\tilde{W}_L(\beta,\omega)}{\partial\beta}+H_L(\omega)\tilde{W}_L(\beta,\omega)=\tilde{R}_L(\beta,\omega).$$

By using Proposition 3 from Cornean (2000), we can write the following Dyson-type integral equation:

$$W_L(\beta,\omega)=\tilde{W}_L(\beta,\omega)-\int_0^\beta d\tau\, W_L(\beta-\tau,\omega)\tilde{R}_L(\tau,\omega). \tag{3.22}$$

The above integral is a Riemann integral and converges in the operator norm sense. By iterating (3.22), we obtain

$$\begin{aligned}W_L(\beta,\omega)=\tilde{W}_L(\beta,\omega)+\sum_{n=1}^{N}(-1)^n\int_0^\beta d\tau_1\int_0^{\beta-\tau_1}d\tau_2\ldots\int_0^{\beta-\tau_1-\ldots-\tau_{n-1}}d\tau_n\\ \times\tilde{W}_L(\beta-\tau_1-\ldots-\tau_n,\omega)\tilde{R}_L(\tau_n,\omega)\ldots\tilde{R}_L(\tau_1,\omega)+\tilde{R}^{(1)}_{N+1,L}(\beta,\omega),\end{aligned} \tag{3.23}$$

where

$$\begin{aligned}\tilde{\mathcal{R}}^{(1)}_{N+1,L}(\beta,\omega)=(-1)^{N+1}\int_0^\beta d\tau_1\int_0^{\beta-\tau_1}d\tau_2\cdots\int_0^{\beta-\tau_1-\ldots-\tau_N}d\tau_{N+1}\\ \times W_L(\beta-\tau_1-\ldots-\tau_{N+1},\omega)\cdot\tilde{R}_L(\tau_{N+1},\omega)\ldots\tilde{R}_L(\tau_1,\omega).\end{aligned} \tag{3.24}$$

Then a straightforward change of variables in the integrals of the rhs of the last two formulas yields

$$\begin{aligned}W_L(\beta,\omega)=\tilde{W}_L(\beta,\omega)+\sum_{n=1}^{N}(-1)^n\int_{D_n(\beta)}d\tau\,\tilde{W}_L(\beta-\tau_1,\omega)\tilde{R}_L(\tau_1-\tau_2,\omega)\cdots\tilde{R}_L(\tau_{n-1}-\tau_n,\omega)\tilde{R}_L(\tau_n,\omega)\\ +\tilde{R}^{(1)}_{N+1,L}(\beta,\omega),\end{aligned}$$

with

$$\tilde{\mathcal{R}}^{(1)}_{N+1,L}(\beta,\omega)=(-1)^{N+1}\int_{D_{N+1}(\beta)}d\tau\,W_L(\beta-\tau_1,\omega)\cdot\tilde{R}_L(\tau_1,\omega)\ldots\tilde{R}_L(\tau_{N+1},\omega), \tag{3.25}$$

where $D_n(\beta)$ is defined in (2.6). Recall that $\tilde{R}_L=\delta\omega\tilde{R}_{1,L}+(\delta\omega)^2\tilde{R}_{2,L}$. So (3.25) gives (3.20) and a simple induction argument finishes the proof of the lemma. □

Continuing the proof of Theorem 3.1: From Theorem 2.6, we know that for $\mathbf{x}\in\Lambda_L$, and $\beta>0$, $\mathbb{C}\ni\omega\to G_L(\mathbf{x},\mathbf{x};\beta,\omega)$ is an entire function.

In order to prove (3.12), we will show that for all $\mathbf{x}\in\Lambda_L$, we have

$$G_L(\mathbf{x},\mathbf{x};\beta,\omega) = G_L(\mathbf{x},\mathbf{x};\beta,\omega_0) + \sum_{n=1}^{N} (\delta\omega)^n \sum_{k=1}^{n} W_{k,L}^{n-k}(\mathbf{x};\beta,\omega_0) + \widetilde{\mathcal{R}}_{N+1,L}(\mathbf{x};\beta,\omega,\omega_0), \quad (3.26)$$

where the remainder term satisfies the property that its first N derivatives at ω_0 are zero.

By rewriting Lemma 3.2 in terms of the corresponding integral kernels, and looking at the diagonal of these kernels, we have [remember that $\phi(\mathbf{x},\mathbf{x})=0$]

$$G_L(\mathbf{x},\mathbf{x};\beta,\omega) = G_L(\mathbf{x},\mathbf{x};\beta,\omega_0) + \sum_{n=1}^{N} (\delta\omega)^n W_{n,L}(\mathbf{x},\mathbf{x};\beta,\omega,\omega_0) + \widetilde{\mathcal{R}}^{(1)}_{N+1,L}(\mathbf{x},\mathbf{x};\beta,\omega,\omega_0)$$
$$+ \widetilde{\mathcal{R}}^{(2)}_{N+1,L}(\mathbf{x},\mathbf{x};\beta,\omega,\omega_0). \quad (3.27)$$

By construction, the two remainders are smooth functions that remain smooth, even if they are divided by $(\delta\omega)^{N+1}$; see formulas (3.20) and (3.21). This means that their first N derivatives at ω_0 are all zero. Thus the Nth derivative of $G_L(\mathbf{x},\mathbf{x};\beta,\cdot)$ at ω_0 can only come from the W's.

What we still have to do is to remove the ω dependence from W's. Let us show that for $1 \leq n \leq N$, $\mathbf{x} \in \Lambda_L$ and $|\delta\omega| < 1$,

$$W_{n,L}(\mathbf{x},\mathbf{x};\beta,\omega,\omega_0) = \sum_{m=0}^{N} (\delta\omega)^m W_{n,L}^m(\mathbf{x};\beta,\omega_0) + \widetilde{\mathcal{R}}^{(3)}_{n,N+1}(\mathbf{x};\beta,\omega,\omega_0), \quad (3.28)$$

where $W_{n,L}^m$ were introduced in (3.11), and $\widetilde{\mathcal{R}}^{(3)}_{n,N+1}(\mathbf{x};\beta,\omega,\omega_0)$ has its first N derivatives at ω_0 equal to 0. Indeed, if we replace the integral kernel of $\widetilde{I}_{k,L}$ from (3.17) in the expression of $W_{N,L}$ from (3.18), we see that we can add up all the magnetic phases, and obtain a factor of the type

$$\exp\{\phi(\mathbf{x},\mathbf{y}_1) + \phi(\mathbf{y}_1,\mathbf{y}_2) + \cdots + \phi(y_{k-1},\mathbf{y}_k) + \phi(y_k,\mathbf{x})\}.$$

Then this exponent will equal the magnetic flux defined in (3.4), plus an additional contribution $\phi(\mathbf{x},\mathbf{x})$ *that is zero due to the antisymmetry of the magnetic phase*. Now if we expand $e^{i(\delta\omega)\mathrm{Fl}_j(\mathbf{x},\ldots,\mathbf{y}_j)}$ in Taylor series up to the Nth order we obtain (3.28), where the remainder has again the property that its first N derivatives at ω_0 are zero. Now introduce (3.28) in (3.27), and after some algebra involving the multiplication of two series, we eventually get (3.26). Then we can identify the Nth derivative at ω_0 of the kernel's diagonal as the coefficient multiplying the Nth power of $\delta\omega$. The identity (3.12) is proved.

Now let us prove the second part of the theorem, i.e., the estimate (3.13), which is also linked to the natural question "why is formula (3.12) better than the one from (2.34)?" The answer is that $W_{k,L}^m(\mathbf{x};\beta,\omega_0)$ *does not grow with* L, and we will see in the next section that it even converges when L tends to infinity. Let us show here its uniform boundedness in L.

Looking at its definition given (3.11) and using the estimates from (3.9) together with the diamagnetic inequality, we see that we need to estimate

$$|W_{k,L}^m(\mathbf{x};\beta,\omega)| \leq \mathcal{C}_3^k \sum_{j=1}^{k} (-1)^j \sum_{(i_1,\ldots,i_j)\in\{1,2\}^j} \chi_j^k(i_1,\ldots,i_j) \int_{D_j(\beta)} d\tau \int_{\Lambda^j} d\mathbf{y} \frac{|\mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j)|^m}{m!}$$
$$\times G_\infty(\mathbf{x},\mathbf{y}_1;16(\beta-\tau_1)) G_\infty(\mathbf{y}_1,\mathbf{y}_2;16(\tau_1-\tau_2)) \ldots G_\infty(\mathbf{y}_{j-1},\mathbf{y}_j;16(\tau_{j-1}-\tau_j))$$
$$\times G_\infty(\mathbf{y}_j,\mathbf{x};16\tau_j). \quad (3.29)$$

Let $\alpha = 16m$, and identify $\mathbf{x}=\mathbf{y}_0$. In view of (3.5) and the explicit form (2.29) of the heat kernel, for $1 \leq l \leq j-1, 1 \leq l' \leq l$; $\mathbf{y}_0,\mathbf{y}_1,\ldots,\mathbf{y}_j \in \Lambda_L^{j+1}$ and $\{\tau_1,\tau_2,\ldots\tau_j\} \in D_j(\beta)$, we need the straightforward estimate

$$|\mathbf{y}_{l'-1}-\mathbf{y}_{l'}||\mathbf{y}_l-\mathbf{y}_{l+1}|\exp\left(-\frac{|\mathbf{x}-\mathbf{y}_1|^2}{2\alpha(\beta-\tau_1)}\right)\ldots\exp\left(\frac{|\mathbf{y}_k-\mathbf{x}|^2}{2\alpha\tau_k}\right)$$
$$\leq 2\alpha\beta\exp\left(-\frac{|\mathbf{x}-\mathbf{y}_1|^2}{4\alpha(\beta-\tau_1)}\right)\ldots\exp\left(-\frac{|\mathbf{y}_k-\mathbf{x}|^2}{4\alpha\tau_k}\right). \tag{3.30}$$

Thus (3.5) and (3.30) imply

$$|\mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j)|^m G_\infty(\mathbf{x},\mathbf{y}_1;16(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_j,\mathbf{x};16\tau_j)$$
$$\leq\left(\sum_{l=1}^{j-1} l\alpha\beta\right)^{m_2 3(j+1)/2} G_\infty(\mathbf{x},\mathbf{y}_1;32(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_j,\mathbf{x};32\tau_j)$$
$$\leq(8j^2m\beta)^{m_2 3(j+1)/2} G_\infty(\mathbf{x},\mathbf{y}_1;32(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_j,\mathbf{x};32\tau_j). \tag{3.31}$$

Integrating over the spatial coordinates, using the semigroup property (2.40), and then integrating over τ variables, one eventually obtains the uniform upper bound in L given in (3.13). □

Remark 3.3: *Theorem 3.1 gives us what we need for the purpose of this paper. One can show that our analysis can be applied in order to get the off-diagonal terms of the integral kernel, i.e.,* $\partial^n G_L/\partial\omega^n(\mathbf{x},\mathbf{x}';\beta,\omega)(\mathbf{x},\mathbf{x}')\in\Lambda_L\times\Lambda_L$, *and* $\beta>0,\omega>0$. *In that case we get*

$$\frac{1}{n!}\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x}';\beta,\omega)=\frac{i^n\phi^n(\mathbf{x},\mathbf{x}')}{n!}G_L(\mathbf{x},\mathbf{x}';\beta,\omega)$$
$$+\sum_{k=1}^{n}\sum_{j=1}^{k}(-1)^j\int_{D_j(\beta)}d\tau\sum_{(i_1,\ldots,i_j)\in\{1,2\}^j}\chi_j^k(i_1,\ldots,i_j)$$
$$\times\int_{\Lambda^j}d\mathbf{y}\frac{(i(\sum_{l=1}^{j-1}\mathrm{fl}(\mathbf{x},\mathbf{y}_l,y_{l+1})+\mathrm{fl}(\mathbf{x},\mathbf{y}_j,\mathbf{x}')+\phi(\mathbf{x},\mathbf{x}')))^{n-k}}{(n-k)!}$$
$$\times G_L(\mathbf{x},\mathbf{y}_1,\beta-\tau_1,\omega)R_{i1,L}(\mathbf{y}_1,\mathbf{y}_2,\tau_1-\tau_2,\omega)\ldots R_{ij,L}(\mathbf{y}_j,\mathbf{x}',\tau_j,\omega). \tag{3.32}$$

Remark 3.4: *Let* $\beta>0$ *and* $\omega_0\geq 0$ *and* $\omega\in\mathbb{C}$. *From* (3.16) *we have* $\|W_L(\beta-\tau,\omega,\omega_0)\widetilde{R}_L(\tau,\omega,\omega_0)\|_1\leq\|W_L(\beta-\tau,\omega,\omega_0)\|_2\|\widetilde{R}_L(\tau,\omega,\omega_0)\|_2$

$$\leq\frac{C(\beta,\omega,\omega_0)L^3}{(\beta-\tau)^{3/4}\tau^{3/4}},$$

where $C(\beta,\omega,\omega_0)=\mathcal{C}_3(\beta,\omega_0)(|\delta\omega|+|(\delta\omega)|^2)$ *and* $\mathcal{C}_3(\beta,\omega_0)$ *is given in* (3.9) *Then the* B_1*-operator valued function* $\tau\in(0,\beta)\to W_L(\beta-\tau,\omega)\widetilde{R}_L(\tau,\omega,\omega_0)$ *is* B_1 *integrable. Denote by* $U_L(\beta,\omega,\omega_0)=\int_0^\beta W_L(\beta-\tau,\omega)\widetilde{R}_L(\tau,\omega,\omega_0)$,

$$\|U_L(\beta,\omega,\omega_0)\|_1\leq CL^3\int_0^\beta\frac{1}{(\beta-\tau)^{3/4}\tau^{3/4}}\leq\frac{16CL^3}{\sqrt{\beta}}. \tag{3.33}$$

The Duhamel-type formula (3.22) *then implies that* $\widetilde{W}_L(\beta,\omega)$ *is of trace class as a sum of the two trace class operators,* W_L *and* U_L. *Consequently, the operators* $\tilde{I}_{k,L}(i_1,\ldots,i_k)(\beta,\omega,\omega_0)$ *defined in* (3.17) *are of trace class because the integrals only involve* B_1*-integrable functions.*

IV. LARGE VOLUME BEHAVIOR

For further applications in Sec. IV, we need to have a similar result as in Theorem 3.1, but with $L=\infty$. The results of Sec. II cannot be applied to this situation. On the contrary, we will show in this section that Theorem 3.1 remains true even if we take $L=\infty$, and the quantities at finite volume converge pointwise to the ones defined on the whole space.

Recall first that the explicit form of the integral kernel of $e^{-\beta H_\infty(\omega)};\beta>0,\omega\geq 0$ is given by

$$G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)=\frac{1}{(2\pi\beta)^{3/2}}\frac{\omega\beta/2}{\sinh(\omega\beta/2)}e^{i\omega\phi(\mathbf{x},\mathbf{x}')}\times\exp\left\{-\frac{1}{2\beta}\left(\frac{\omega\beta/2}{\tanh(\omega\beta/2)}[(x_1-x_1')^2+(x_2-x_2')^2]+(x_3-x_3')^2\right)\right\},\tag{4.1}$$

where the phase ϕ is defined in (3.1).

We start with a technical result. For any $\mathbf{x}\in\Lambda_L$, we denote with $d(\mathbf{x}):=\mathrm{dist}(\mathbf{x},\partial\Lambda_L)$. Let $M:=\{(\mathbf{x},\mathbf{x}')\in\Lambda_L\times\Lambda_L: d(\mathbf{x})\leq 1 \text{ or } d(\mathbf{x}')\leq 1\}$, and denote with χ_M the characteristic function of M.

Theorem 4.1: *Let $\beta>0$ and $\omega\geq 0$. Then for any $(\mathbf{x},\mathbf{x}')\in\Lambda_L\times\Lambda_L$, we have*

$$|G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)|\leq 2\chi_M(\mathbf{x},\mathbf{x}')G_\infty(\mathbf{x},\mathbf{x}';\beta)+\mathcal{C}_4(1-\chi_M)\times(\mathbf{x},\mathbf{x}')G_\infty(\mathbf{x},\mathbf{x}';16\beta)e^{-(d^2(\mathbf{x})/64\beta+d^2(\mathbf{x}')/64\beta)},\tag{4.2}$$

and

$$|(-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(\mathbf{x}))[G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)]|\leq\frac{\mathcal{C}_5}{\sqrt{\beta}}\chi_M(\mathbf{x},\mathbf{x}')G_\infty(\mathbf{x},\mathbf{x}';8\beta)+\mathcal{C}_6(1-\chi_M)G_\infty(\mathbf{x},\mathbf{x}';16\beta)e^{-(d^2(\mathbf{x})/64\beta+d^2(\mathbf{x}')/64\beta)},\tag{4.3}$$

where $\mathcal{C}_4=\mathcal{C}_4(\beta,\omega)=c(1+\beta)^6(1+\omega)^4$, $\mathcal{C}_5=\mathcal{C}_5(\beta,\omega)=c(1+\beta)^5(1+\omega)^3$, $\mathcal{C}_6=\mathcal{C}_6(\beta,\omega)=c(1+\beta)^8(1+\omega)^5$, *and $c>1$ is a numerical constant.*

To prove the theorem, we need the following lemma.

Lemma 4.2: Let $\beta>0$, $\omega\geq 0$ and $\alpha\in\{0,1\}$. Then for every $(\mathbf{x},\mathbf{x}')\in\Lambda_L\times\Lambda_L$ we have

$$\partial_{x_i}^\alpha G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-\partial_{x_i}^\alpha G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)$$

$$\frac{1}{2}\int_0^\beta d\tau\int_{\partial\Lambda_L}d\sigma(\mathbf{y})\partial_{x_i}^\alpha G_\infty(\mathbf{x},\mathbf{y};\tau,\omega)[\mathbf{n}_{\mathbf{y}}\cdot\nabla_{\mathbf{y}}G_L(\mathbf{y},\mathbf{x}';\beta-\tau,\omega)],\tag{4.4}$$

where $d\sigma(\mathbf{y})$ is the measure on $\partial\Lambda_L$ and $\mathbf{n}_{\mathbf{y}}$ is the outer normal to $\partial\Lambda_L$ at $\mathbf{y}$.

Proof: Let $\beta>0$, $\omega\geq 0$. Recall that both Green's functions $G_\infty(\mathbf{x},\mathbf{x}';\tau,\omega)$ and $G_L(\mathbf{x},\mathbf{x}';\tau,\omega)$ satisfy in $\Lambda_L\times\Lambda_L$ in a distributional sense, the equation

$$\text{(i) } \partial_\tau G(\mathbf{x},\mathbf{x}';\tau)=-\frac{1}{2}[-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(\mathbf{x})]^2G(\mathbf{x},\mathbf{x}';\tau);\quad \tau>0,\tag{4.5}$$

$$\text{(ii) } G(\mathbf{x},\mathbf{x}';\tau=0_+)=\delta(\mathbf{x}-\mathbf{x}').\tag{4.6}$$

For $0<\tau<\beta$ and on $\Lambda_L\times\Lambda_L$, define the following quantity:

$$Q(\mathbf{x},\mathbf{x}';\beta,\tau):=\int_{\Lambda_L}d\mathbf{y}\,\overline{G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)}G_\infty(\mathbf{y},\mathbf{x}';\tau,\omega).\tag{4.7}$$

Then by (4.5), it is easy to see that

$$\partial_\tau Q(\mathbf{x},\mathbf{x}';\beta,\tau)=\frac{1}{2}\int_{\Lambda_L} d\mathbf{y}\,\{\overline{(-i\nabla_{\mathbf{y}}-\omega\mathbf{a}(\mathbf{y}))^2 G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)}G_\infty(\mathbf{y},\mathbf{x}';\tau,\omega)$$
$$-\overline{G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)}(-i\nabla_{\mathbf{y}}-\omega\mathbf{a}(\mathbf{y}))^2 G_\infty(\mathbf{y},\mathbf{x}';\tau,\omega)\}. \tag{4.8}$$

Since $G_L(\mathbf{x},\mathbf{x}';\tau,\omega)=0$ if $\mathbf{x}\in\partial\Lambda_L$ or $\mathbf{x}'\in\partial\Lambda_L$, integration by parts gives

$$\partial_\tau Q(\mathbf{x},\mathbf{x}';\beta,\tau)=\frac{1}{2}\int_{\partial\Lambda_L} d\sigma(\mathbf{y})\overline{\mathbf{n}_{\mathbf{y}}\cdot\nabla_{\mathbf{y}}G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)}G_\infty(\mathbf{y},\mathbf{x}';\tau,\omega). \tag{4.9}$$

Now, by integrating with respect to τ from 0_+ to β_-, and using (4.6), we obtain

$$G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)=\frac{1}{2}\int_0^\beta d\tau\int_{\partial\Lambda_L} d\sigma(\mathbf{y})\overline{\mathbf{n}_{\mathbf{y}}\cdot\nabla_{\mathbf{y}}G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)}G_\infty(\mathbf{y},\mathbf{x}';\tau,\omega). \tag{4.10}$$

Now, using the self-adjointness property of the semigroup, we obtain $G(\mathbf{x},\mathbf{y};\tau)=\overline{G(\mathbf{y},\mathbf{x};\tau)}$; thus, we can rewrite (4.10) as

$$G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)=\frac{1}{2}\int_0^\beta d\tau\int_{\partial\Lambda_L} d\sigma(\mathbf{y})G_\infty(\mathbf{x},\mathbf{y};\tau,\omega)[\mathbf{n}_{\mathbf{y}}\cdot\nabla_{\mathbf{y}}G_L(\mathbf{y},\mathbf{x}';\beta-\tau,\omega)]. \tag{4.11}$$

The lemma now follows from (4.11). □

Proof of Theorem 4.1: Let $\beta>0$, $\omega\geq 0$, and suppose first that $(\mathbf{x},\mathbf{x}')\in M$. Then (4.2) follows from the diamagnetic inequality (2.30). Let us show (4.3) in the same case. We know from (2.31) that

$$|(-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(\mathbf{x}))G_L(\mathbf{x},\mathbf{x}';\beta,\omega)|\leq\frac{\mathcal{C}}{\sqrt{\beta}}G_\infty(\mathbf{x},\mathbf{x}';8\beta). \tag{4.12}$$

On the other hand, using the observation that $-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(\mathbf{x})$ is transformed into $-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(\mathbf{x}-\mathbf{x}')$ after commutation with $e^{i\phi(\mathbf{x},\mathbf{x}')}$; then, by direct computation from (4.1), we get that for all $\eta>0$,

$$|(-i\nabla\mathbf{x}-\omega\mathbf{a}(\mathbf{x}))G_\infty(\mathbf{x},\mathbf{x}';\eta\beta,\omega)|\leq\frac{\mathcal{C}_1'}{\sqrt{\eta\beta}}G_\infty(\mathbf{x},\mathbf{x}';2\eta\beta), \tag{4.13}$$

where $\mathcal{C}_1'=\mathcal{C}_1'(\beta,\omega)=2(1+\eta)(1+\omega)(1+\beta)$. Then (4.12) and (4.13) for $\eta=1$ imply (4.3).

Now suppose that $(\mathbf{x},\mathbf{x}')\notin M$. This means that neither points are near the boundary. For $\mathbf{y}\in\partial\Lambda$ then by (2.31), we have

$$|\nabla_{\mathbf{y}}G_L(\mathbf{y},\mathbf{x};\beta-\tau,\omega)|\leq\frac{\mathcal{C}_1}{\sqrt{\beta-\tau}}G_\infty(\mathbf{y},\mathbf{x},8(\beta-\tau)). \tag{4.14}$$

By applying the estimates (4.14), (2.30), and the Lemma 4.2, we get

$$|G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)|\leq 2^{7/2}\mathcal{C}_1\int_0^\beta d\tau\int_{\partial\Lambda_L} d\sigma(\mathbf{y})\frac{G_\infty(\mathbf{y},\mathbf{x};8(\beta-\tau))}{\sqrt{\beta-\tau}}G_\infty(\mathbf{y},\mathbf{x}';8\tau). \tag{4.15}$$

But if $\mathbf{y}\in\partial\Lambda_L$, $|\mathbf{x}-\mathbf{y}|\geq d(\mathbf{x})$, then a straightforward estimate shows that for $0<t<\beta$, we have $G_\infty(\mathbf{y},\mathbf{x};8t)\leq e^{-d^2(x)/32\beta}G_\infty(\mathbf{y},\mathbf{x};16t)$. Thus, we get the rhs of (4.15),

$$\leq 2^5 \mathcal{C}_1 \int_0^\beta d\tau \frac{e^{-(d^2(x)/32(\beta-\tau)+d^2(x')/32\tau)}}{\sqrt{\beta-\tau}} \int_{\partial\Lambda_L} d\sigma(\mathbf{y}) G_\infty(\mathbf{y},\mathbf{x};16(\beta-\tau)) G_\infty(\mathbf{y},\mathbf{x}';16\tau). \tag{4.16}$$

For any t, $t'>0$, let us look at the integral

$$\int_{\partial\Lambda_L} d\sigma(\mathbf{y}) G_\infty(\mathbf{y},\mathbf{x};t) G_\infty(\mathbf{y},\mathbf{x}';t'). \tag{4.17}$$

Using the convexity of Λ_L, replacing the integrals on the sides of $\partial\Lambda_L$ by integrals on $\mathbb{R}^2$ (thus getting an upper bound), and using the semigroup property in two dimensions, we can show that there exists a numerical constant $C>0$, such that

$$\int_{\partial\Lambda_L} d\sigma(\mathbf{y}) G_\infty(\mathbf{y},\mathbf{x};t) G_\infty(\mathbf{y},\mathbf{x}';t') \leq C \frac{\sqrt{t+t'}}{\sqrt{t}\sqrt{t'}} G_\infty(\mathbf{x},\mathbf{x}';t+t'). \tag{4.18}$$

To be more precise, let us look at the integral on the hyperplane defined by $H := \mathbb{R}^2 + (L/2,0,0)$:

$$\int_H d\sigma(\mathbf{y}) G_\infty(\mathbf{y},\mathbf{x};t) G_\infty(\mathbf{y},\mathbf{x}';t'), \tag{4.19}$$

where $\mathbf{x}$ and $\mathbf{x}'$ are on the same side of $\mathbb{R}^3$ with respect to H. Decompose $\mathbf{x}=\mathbf{x}_1+\mathbf{x}_2$ and $\mathbf{x}'=\mathbf{x}_1'+\mathbf{x}_2'$, where $\mathbf{x}_1$ and $\mathbf{x}_1'$ are the parallel components with H, while $\mathbf{x}_2$ and $\mathbf{x}_2'$ are the orthogonal components on H. Note that here $|\mathbf{x}_2|^2+|\mathbf{x}_2'|^2 \geq |\mathbf{x}_2-\mathbf{x}_2'|^2$. Since $|\mathbf{x}-\mathbf{y}|^2=|\mathbf{x}_1-\mathbf{y}|^2+|\mathbf{x}_2|^2$ if $\mathbf{y}\in H$, we can explicitly integrate with respect to $\mathbf{y}$ and eventually get (4.18).

Then we can write

$$\int_{\partial\Lambda_L} d\sigma(\mathbf{y}) G_\infty(\mathbf{y},\mathbf{x};16(\beta-\tau)) G_\infty(\mathbf{y},\mathbf{x}';16\tau) \leq \mathcal{C}_1' \frac{\sqrt{\beta}}{\sqrt{(\beta-\tau)\tau}} G_\infty(\mathbf{x},\mathbf{x}';16\beta).$$

Therefore, since $\mathbf{x},\mathbf{x}'$ satisfy $d(\mathbf{x})$, $d(\mathbf{x}')\geq 1$, we get

$$\begin{aligned} |G_L(\mathbf{x},\mathbf{x}';\beta,\omega) - G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)| &\leq 2^4 \mathcal{C}_1 \mathcal{C}_1' G_\infty(\mathbf{x},\mathbf{x}';16\beta) e^{-(d^2(\mathbf{x})/64\beta + d^2(\mathbf{x}')/64\beta)} \\ &\quad \times \int_0^\beta d\tau \frac{e^{-(1/64(\beta-\tau)+1/64\tau)}}{\sqrt{\beta-\tau}} \frac{\sqrt{\beta}}{\sqrt{(\beta-\tau)\tau}}. \end{aligned} \tag{4.20}$$

Due the exponential decay, there are no singularities in this integral, and a straightforward estimate gives (4.2).

We now use the same method as above to prove (4.3) in the case when $(\mathbf{x},\mathbf{x}') \notin M$. We know from Lemma 4.2 that

$$\begin{aligned} &(-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(x))(G_L(\mathbf{x},\mathbf{x}';\beta,\omega) - G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)) \\ &\quad = \frac{1}{2}\int_0^\beta d\tau \int_{\partial\Lambda_L} d\sigma(\mathbf{y}) \cdot (-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(x)) G_\infty(\mathbf{x},\mathbf{y};\tau,\omega)[\mathbf{n}_{\mathbf{y}} \cdot \nabla_{\mathbf{y}} G_L(\mathbf{y},\mathbf{x}';\beta-\tau,\omega)]. \end{aligned} \tag{4.21}$$

Then by (4.12) and (4.13),

$$\begin{aligned}&\left|(-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(x))(G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta\omega))\right|\\&\quad\le 4\mathcal{C}_1\mathcal{C}_1'\int_0^\beta d\tau\int_{\partial\Lambda_L}d\sigma(\mathbf{y})\frac{G_\infty(\mathbf{y},\mathbf{x};8(\beta-\tau))}{\sqrt{\beta-\tau}}\frac{G_\infty(\mathbf{y},\mathbf{x}';8\tau)}{\sqrt{\tau}}.\end{aligned}\tag{4.22}$$

Then, by using the same arguments leading to (4.20), we get

$$\begin{aligned}&\left|(-i\nabla_{\mathbf{x}}-\omega\mathbf{a}(x))(G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta\omega))\right|\\&\quad\le 16\sqrt{\beta}\mathcal{C}_1\mathcal{C}_1'^2G_\infty(\mathbf{x},\mathbf{x}';16\beta)e^{-(d^2(x)/64\beta+d^2(x')/64\beta)}\int_0^\beta d\tau\frac{e^{-(1/64(\beta-\tau)+1/64\tau)}}{\tau(\beta-\tau)},\end{aligned}\tag{4.23}$$

from which (4.3) follows. Theorem 4.1 is proved.

We now want to prove that the equality (3.12) stated in Theorem 3.1 remains true, even if L tends to infinity. It is well known (see, e.g., Angelescu and Corciovei (1975)) that for $\beta>0,\omega\ge 0$ and $(\mathbf{x},\mathbf{x}')\in\mathbb{R}^3\times\mathbb{R}^3$,

$$G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)=\lim_{L\to\infty}G_L(\mathbf{x},\mathbf{x}';\beta,\omega).\tag{4.24}$$

Our main goal now is to show that this pointwise convergence holds true for all the derivatives $\partial^n G_L/\partial\omega^n, n\ge 1$.

We need to introduce some notation. Let $\beta>0$ and $\omega\ge 0$. For $(\mathbf{x},\mathbf{x}')\in\mathbb{R}^3\times\mathbb{R}^3$, define

$$R_{1,\infty}(\mathbf{x},\mathbf{x}';\beta,\omega):=\mathbf{a}(\mathbf{x}-\mathbf{x}')\cdot(i\nabla_{\mathbf{x}}+\omega\mathbf{a}(\mathbf{x}))G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega),$$

$$R_{2,\infty}(\mathbf{x},\mathbf{x}';\beta,\omega):=\frac{1}{2}\mathbf{a}^2(\mathbf{x}-\mathbf{x}')G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega).\tag{4.25}$$

Let us note that we again have the same type of estimates as in (3.7), (3.8), and (3.9), i.e., Gaussian localization in the difference of the spatial arguments. The linear growth of the magnetic potential disappears when one commutes $-i\nabla_{\mathbf{x}}$ with the magnetic phase, as we have already seen in (4.13).

Now define for $\mathbf{x}\in\mathbb{R}^3$, $k\ge 1, m\ge 0$:

$$\begin{aligned}W_{k,\infty}^m(\mathbf{x};\beta,\omega):=&\sum_{j=1}^k(-1)^j\sum_{(i_1,\ldots,i_j)\in\{1,2\}^j}\chi_j^k(i_1,\ldots,i_j)\int_{D_j(\beta)}d\tau\int_{\mathbb{R}^{3j}}d\mathbf{y}\\&\times\frac{(i(\mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j)))^m}{m!}G_\infty(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega)R_{i_1,\infty}(\mathbf{y}_1,\mathbf{y}_2;\tau_1-\tau_2,\omega)\ldots R_{i_{j-1},\infty}\\&\times(\mathbf{y}_{j-1},\mathbf{y}_k;\tau_{j-1}-\tau_j,\omega)R_{i_j,\infty}(\mathbf{y}_j,\mathbf{x};\tau_j,\omega).\end{aligned}\tag{4.26}$$

Since every integrand is bounded by a free heat kernel and because the flux Fl_j can be bound by *differences* of its arguments [see (3.5)], then the above multiple integrals are absolutely convergent. Also note the important thing that multiplication by $|\mathbf{y}-\mathbf{y}'|^m$ of the free heat kernel only improves the singularity in the time variable due to the estimate

$$|\mathbf{y}-\mathbf{y}'|^m\mathbf{e}^{-|\mathbf{y}-\mathbf{y}'|^2/t}\le\mathrm{const}\cdot t^{m/2}\mathbf{e}^{-|\mathbf{y}-\mathbf{y}'|^2/(2t)}.\tag{4.27}$$

The last important remark about $W_{k,\infty}^m(\mathbf{x};\beta,\omega)$ is that *it does not depend on* $\mathbf{x}$. This can be seen by factorizing all the magnetic phases that enter in the various factors of the integrand, and see that they add up to give another Fl_j, which only depends on differences of variables. The remaining factors are also just functions of differences of variables. Therefore by changing $\mathbf{x}$ we get the same value for $W_{k;\infty}^m$ after a change of variables (a translation) in all integrals, since $W_{k,\infty}^m$ only involves integrals defined on the whole space.

Then we have the following.

Theorem 4.3: *Let* $\beta>0$ *and* $\omega\geq 0$. *Fix* $\mathbf{x}\in\mathbb{R}^3$ *and* $n\geq 1$. *Then we have*

$$\frac{1}{n!}\frac{\partial^n G_\infty}{\partial\omega^n}(\mathbf{x},\mathbf{x};\beta,\omega)=\lim_{L\to\infty}\frac{1}{n!}\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x};\beta,\omega)=\sum_{k=1}^{n}W_{k,\infty}^{n-k}(\mathbf{x};\beta,\omega). \tag{4.28}$$

Proof: Fix $\beta>0$ and $\omega\geq 0$. Let $n\geq 1$ and $(\mathbf{x},\mathbf{x}')\in\mathbb{R}^3$. Choose L large enough such that $\mathbf{x}\in\Lambda_L$. Then from (4.2) and (4.3), we have

$$\left|G_L(\mathbf{x},\mathbf{x}';\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)\right|\leq \mathcal{C}_4\beta^{-3/2}e^{-(d^2(\mathbf{x})/64\beta+d^2(\mathbf{x}')/64\beta)},$$

$$\left|R_{1,L}(\mathbf{x},\mathbf{x}';\beta,\omega)-R_{1,\infty}(\mathbf{x},\mathbf{x}';\beta,\omega)\right|\leq \mathcal{C}_6\beta^{-1}e^{-(d^2(\mathbf{x})/64\beta+d^2(\mathbf{x}')/64\beta)},$$

$$\left|R_{2,L}(\mathbf{x},\mathbf{x}';\beta,\omega)-R_{2,\infty}(\mathbf{x},\mathbf{x}';\beta,\omega)\right|\leq \mathcal{C}_4\beta^{-1/2}e^{-(d^2(\mathbf{x})/64\beta+d^2(\mathbf{x}')/64\beta)}, \tag{4.29}$$

Then, for all $(\mathbf{x},\mathbf{x}')\in\mathbb{R}^3\times\mathbb{R}^3$, estimates (4.29) show, respectively, that

$$\lim_{L\to\infty}G_L(\mathbf{x},\mathbf{x}',\beta,\omega)=G_\infty(\mathbf{x},\mathbf{x}',\beta,\omega),$$

$$\lim_{L\to\infty}R_{i,L}(\mathbf{x},\mathbf{x}',\beta,\omega)=R_{i,\infty}(\mathbf{x},\mathbf{x}',\beta,\omega),$$

for $i=1,2$. Then

$$\begin{aligned}&\lim_{L\to\infty}G_L(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega)R_{i_1,L}(\mathbf{y}_1,\mathbf{y}_2;\tau_1-\tau_2,\omega)\ldots R_{i_j,L}(\mathbf{y}_j,\mathbf{x};\tau_j,\omega)\\&\quad=G_\infty(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega)R_{i_1,\infty}(\mathbf{y}_1,\mathbf{y}_2;\tau_1-\tau_2,\omega)\ldots R_{i_j,L}(\mathbf{y}_j,\mathbf{x};\tau_j,\omega).\end{aligned}$$

Furthermore, by (3.9) and (2.30), we have

$$\begin{aligned}&\left|G_L(\mathbf{x},\mathbf{y}_1;\beta-\tau_1,\omega)R_{i_1,L}(\mathbf{y}_1,\mathbf{y}_2;\tau_1-\tau_2,\omega)\ldots R_{i_j,L}(\mathbf{y}_j,\mathbf{x};\tau_j,\omega)\right|\\&\quad\leq 4^3C_3^jG_\infty(\mathbf{x},\mathbf{y}_1;16(\beta-\tau_1))G_\infty(\mathbf{y}_1,\mathbf{y}_2;16(\tau_1-\tau_2))\ldots G_\infty(\mathbf{y}_j,\mathbf{x};16\tau_j),\end{aligned}$$

this last quantity is L independent and $\mathbb{R}^3$ integrable by the semigroup property since

$$\int_{\mathbb{R}^{3j}}d\mathbf{y}\;G_\infty(\mathbf{x},\mathbf{y}_1;16(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_j,\mathbf{x};16\tau_j)=G_\infty(\mathbf{x},\mathbf{y}_1;16\beta).$$

Note that the flux Fl_j does not influence anything, since it can be bound by powers of differences between spatial variables, which will meet the Gaussian decay of the free heat kernels. Thus, they will only affect the time integrals (by making them even less singular).

Then, by applying Lebesgue's dominated convergence theorem, we get from (3.11) and (3.12),

$$\lim_{L\to\infty}\frac{1}{n!}\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x},\beta,\omega)=\sum_{k=1}^{n}W_{k,\infty}^{n-k}(\mathbf{x};\beta,\omega). \tag{4.30}$$

Now the remaining thing is to show that this also equals $(1/n!)\,(\partial^n G_\infty/\partial\omega^n)\,(\mathbf{x},\mathbf{x},\beta,\omega)$. Fix $\omega_0\geq 0$ and choose $\omega\in\mathbb{R}$ such that $|\delta\omega|=|\omega-\omega_0|\leq 1$. From the usual Taylor formula, we can write

$$G_L(\mathbf{x},\mathbf{x},\beta,\omega)=\sum_{n=0}^{N}(\delta\omega)^n\frac{1}{n!}\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x},\beta,\omega_0)+(\delta\omega)^{N+1}\frac{1}{(N+1)!}\frac{\partial^{N+1}G_L}{\partial\omega^{N+1}}(\mathbf{x},\mathbf{x},\beta,\omega_1), \tag{4.31}$$

where ω_1 is between ω_0 and ω. Then by taking L to infinity, we easily get the estimate [note that $\Sigma_{k=1}^{N+1}W_{k,L}^{N+1-k}(\mathbf{x};\beta,\omega_1)$ is bounded by a constant independent of L; see the estimate from (3.13)]:

$$\left|G_\infty(\mathbf{x},\mathbf{x},\beta,\omega)-G_\infty(\mathbf{x},\mathbf{x},\beta,\omega_0)-\sum_{n=1}^{N}(\delta\omega)^n\sum_{k=1}^{n}W_{k,\infty}^{n-k}(\mathbf{x};\beta,\omega_0)\right|\le C(N,\beta)|\delta\omega|^{N+1}. \tag{4.32}$$

Since $G_\infty(\mathbf{x},\mathbf{x};\beta,\omega)$ is smooth in ω [see (1.7)], it follows that the coefficient of $(\delta\omega)^n$ must equal $(1/n!)\ (\partial^n G_\infty/\partial\omega^n)(\mathbf{x},\mathbf{x},\beta,\omega_0)$ and we are done. □

V. THERMODYNAMIC LIMIT FOR MAGNETIC SUSCEPTIBILITIES

As a consequence of the analysis of the previous section we are now able to prove the main technical result of this paper.

Theorem 5.1: *Let* $n\ge 1$, $\beta>0$, *and* $w>0$,

$$\int_{\Lambda_L}d\mathbf{x}\left|\frac{\partial^n G_\infty}{\partial\omega^n}(\mathbf{x},\mathbf{x};\beta,\omega)-\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x};\beta,\omega)\right|\le L^2\mathcal{C}(n,\beta,\omega), \tag{5.1}$$

where $\mathcal{C}(n,\beta,\omega):=c(n)[(1+\beta)^{7n+8}/\sqrt{\beta}](1+\omega)^{3n+5}$, *where* $c(n)$ *only depends on* n.

Proof: Let $1\le j\le k$, $1\le k\le n$, $1\le m\le n-k$, and denote the integrand in (4.26) with:

$$\begin{aligned}F_{j,\infty}^m&=F_{j,\infty}^m(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega)\\&=\frac{(i\mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j))^m}{m!}G_\infty(\mathbf{x},\mathbf{y}_1,\beta-\tau_1,\omega)\ldots R_{i_j,\infty}(\mathbf{y}_j,\mathbf{x},\tau_j,\omega).\end{aligned} \tag{5.2}$$

Denote also by

$$F_{j,L}^m=F_{j,L}^m(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega)=\frac{(i\ \mathrm{Fl}_j(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j))^m}{m!}G_L(\mathbf{x},\mathbf{y}_1,\beta-\tau_1,\omega)\ldots R_{i_j,L}(\mathbf{y}_j,\mathbf{x},\tau_j,\omega). \tag{5.3}$$

Let $n\ge 1$, $\beta\ge 0$, $\omega\ge 0$, and fix $\mathbf{x}\in\mathbb{R}^3$. Then by applying the Theorem 4.3, we can split the integrals from W's in "inner" and "outer" regions:

$$\frac{\partial^n G_\infty}{\partial\omega^n}(\mathbf{x},\mathbf{x},\beta,\omega)=f_L^n(\mathbf{x},\beta,\omega)+g_L^n(\mathbf{x},\beta,\omega), \tag{5.4}$$

where

$$f_L^n(\mathbf{x},\beta,\omega):=n!\sum_{k=1}^{n}\sum_{j=1}^{k}(-1)^j\sum_{(i_1,\ldots,i_j)\in\{1,2\}^j}\chi_j^k(i_1,\ldots,i_j)\int_{D_j(\beta)}d\tau\int_{\Lambda_L^j}d\mathbf{y}$$

$$F_{j,\infty}^{n-k}(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega), \tag{5.5}$$

$$g_L^n(\mathbf{x},\beta,\omega) := n!\sum_{k=1}^{n}\sum_{j=1}^{k}(-1)^j \sum_{(i_1,\ldots,i_j)\in\{1,2\}^j} \chi_j^k(i_1,\ldots,i_j)\sum_{l=1}^{j}\int_{D_j(\beta)} d\tau \int_{\mathbb{R}^3} d\mathbf{y}_1 \cdots \int_{\mathbb{R}^3\setminus\Lambda_L} \times d\mathbf{y}_l \int_{\mathbb{R}^3} d\mathbf{y}_{l+1}\cdots\int_{\mathbb{R}^3} d\mathbf{y}_j F_{j,\infty}^{n-k}(\mathbf{x},\mathbf{y}_1,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega). \tag{5.6}$$

Let us now show that

$$\int_\Lambda d\mathbf{x}\left| f_L^n(\mathbf{x},\beta,\omega) - \frac{\partial^n G_L}{\partial\omega^n}(\mathbf{x},\mathbf{x};\beta,\omega)\right| \le L^2 f(n,\beta,\omega), \tag{5.7}$$

where $f(n,\beta,\omega) := c(n)[(1+\beta)^{7n+3}/\sqrt{\beta}](1+\omega)^{3n+2}$, $c(n)$ depending only on n.

From now, for the sake of simplicity we often omit the explicit dependence of all variables. In view of (3.11), (3.12), (4.26), and (4.28), we need to estimate

$$F_{j,\infty}^m - F_{j,L}^m = \frac{(i\mathrm{Fl}_j)^m}{m!}\left\{(G_\infty - G_L)R_{i_1,\infty}\ldots R_{i_j,\infty} + \sum_{l=1}^{j} G_L R_{i_1,L}\ldots R_{i_{l-1},L}(R_{i_l,\infty} - R_{i_l,L})R_{i_{l+1},\infty}\ldots R_{i_j,\infty}\right\}. \tag{5.8}$$

Denote by $\chi(\mathbf{x})$ the characteristic of $\{\mathbf{x}\in\Lambda, d(\mathbf{x})\le 1\}$. Thanks to the Theorem 4.1, we have

$$\begin{aligned}|(R_{1,\infty} - R_{1,L})(\mathbf{x},\mathbf{x}';\beta,\omega)| &\le |\mathbf{a}(\mathbf{x}-\mathbf{x}')(i\nabla_{\mathbf{x}} + \omega\mathbf{a})(G_\infty - G_L)(\mathbf{x},\mathbf{x}';\beta,\omega)| \\ &\le \mathcal{C}_7 G_\infty(\mathbf{x},\mathbf{x}';32\beta)(\chi(\mathbf{x}) + \chi(\mathbf{x}') + e^{-(d^2(x)/64\beta + d^2(x')/64\beta)}),\end{aligned} \tag{5.9}$$

where $\mathcal{C}_7 = \mathcal{C}_7(\beta,\omega) = c(1+\beta)^9(1+\omega)^5$ for some numerical constant $c>1$. But again by Theorem 4.1, we may use the bound

$$\begin{aligned}|(G_\infty - G_L)(\mathbf{x},\mathbf{x}';\beta,\omega)|, |(R_{2,\infty} - R_{2,L})(\mathbf{x},\mathbf{x}';\beta,\omega)| &\le \mathcal{C}_7 G_\infty(\mathbf{x},\mathbf{x}';32\beta)(\chi(\mathbf{x}) + \chi(\mathbf{x}') \\ &\quad + e^{-(d^2(\mathbf{x})/64\beta + d^2(\mathbf{x}')/64\beta)}).\end{aligned} \tag{5.10}$$

On the other hand, by (3.9), (4.13), and (4.25), the kernel of $R_{i,\infty}$, $i=1,2$ and of $R_{i,L}$, $i=1,2$ satisfy the inequality

$$\max\{|(R_{i,\infty}(\mathbf{x},\mathbf{x}';\beta,\omega)|, |R_{i,L}(\mathbf{x},\mathbf{x}';\beta,\omega)|\} \le \mathcal{C}_3' G_\infty(\mathbf{x},\mathbf{x}';16\beta), \tag{5.11}$$

where $\mathcal{C}_3' = \mathcal{C}_3'\beta,\omega) = c\cdot\mathcal{C}_1$, $\mathcal{C}_1$ is defined in (2.37), and $c>1$ is a numerical constant that is chosen large enough such that we have $G_\infty(\mathbf{x},\mathbf{x}';\beta) \le \mathcal{C}_3' G_\infty(\mathbf{x},\mathbf{x}';16\beta)$.

Set $\mathbf{y}_0 := \mathbf{x}$. Then (2.30), (5.11), together with (5.9) and (5.10), give

$$|F_{j,\infty}^m - F_{j,L}^m| \le \mathcal{C}_7\mathcal{C}_3'^{j-1}\frac{|\mathrm{Fl}_j|^m}{m!} G_\infty(\mathbf{y}_0,\mathbf{y}_1;32(\beta-\tau_1))\cdots G_\infty(\mathbf{y}_j,\mathbf{y}_0;32\tau_j)\sum_{l=0}^{j}(2\chi(\mathbf{x}_l) + e^{-d^2(x_l)/64\beta}). \tag{5.12}$$

Thus, from this inequality and (3.5), we need to estimate the quantity

$$Q := \left(\sum_{l=1}^{j-1}\sum_{l'=1}^{l}|\mathbf{y}_{l'-1} - \mathbf{y}_{l'}||\mathbf{y}_l - \mathbf{y}_{l+1}|\right)^m G_\infty(\mathbf{y}_0,\mathbf{y}_1;32(\beta-\tau_1))\ldots G_\infty(\mathbf{y}_j,\mathbf{y}_0;32\tau_j).$$

By using (4.27), we have

$$Q \le (8\beta j^2)^m m^m 2^{3(j+1)/2} G_\infty(\mathbf{y}_0;\mathbf{y}_1;64(\beta-\tau_1))\cdots, G_\infty(\mathbf{y}_j,\mathbf{y}_0;64\tau_j),$$

and then for $j\le n$,

$$|F^m_{j,\infty} - F^m_{j,L}| \leq 2^{3(n+1)/2}\mathcal{C}_7\mathcal{C}_3'^{n-1}\frac{(8\beta j^2)^m m^m}{m!}G_\infty(\mathbf{y}_0,\mathbf{y}_1;64(\beta-\tau_1))\cdots G_\infty(\mathbf{y}_j,\mathbf{y}_0;64\tau_j)$$
$$\times\sum_{l=0}^{j}(2\chi(\mathbf{x}_l)+e^{-d^2(x_l)/64\beta}). \tag{5.13}$$

By extending the integration with respect to $\mathbf{y}_0,\ldots\mathbf{y}_{l-1},\mathbf{y}_{l+1}\ldots\mathbf{y}_j$ on the whole $\mathbb{R}^3$ space, and using the semigroup property (2.40) and the fact that $G_\infty(\mathbf{x},\mathbf{x};t)=1/(2\pi t)^{3/2}$, we get

$$\left|\int_{\Lambda_L^{j+1}} d\mathbf{y}(F^{n-k}_{j,\infty}-F^{n-k}_{j,L})\right| \leq c^n\mathcal{C}_7\mathcal{C}_3'^{n-1}(j+1)\frac{(\beta_j^2)^{(n-k)}(n-k)^{n-k}}{\beta^{3/2}(n-k)!}\int_{\Lambda_L} d\mathbf{x}(2\chi(\mathbf{x})+e^{-d^2(x)/64\beta}), \tag{5.14}$$

for some positive constant c. Moreover, simple estimates show that

$$\int_{\Lambda_L} d\mathbf{x}(2\chi(\mathbf{x})+e^{-d^2(\mathbf{x})/64\beta}) \leq cL^2(1+\sqrt{\beta}),$$

where c is also some positive numerical constant. From (5.5) and Theorem 3.1,

$$\int_{\Lambda_L} d\mathbf{y}_0\left\{\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{y}_0,\mathbf{y}_0;\beta,\omega)-f_L^n(\mathbf{y}_0,\beta,\omega)\right\} = n!\sum_{k=1}^{n}\sum_{j=1}^{k}(-1)^j\sum_{(i_1,\ldots,i_j)\in\{1,2\}j}\chi_j^k(i_1,\ldots,i_j)\int_{D_j(\beta)}d\tau$$
$$\times\int_{\Lambda^{j+1}} d\mathbf{y}(F^{n-k}_{j,\infty}-F^{n-k}_{j,L})(\mathbf{y}_0,\mathbf{y}_1,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega). \tag{5.15}$$

Then (5.14), together with (5.15), lead to

$$\left|\int_{\Lambda_L} d\mathbf{y}_0\left(\frac{\partial^n G_L}{\partial\omega^n}(\mathbf{y}_0,\mathbf{x};\beta,\omega)-f_L^n(\mathbf{y}_0,\beta,\omega)\right)\right| \leq L^2c(n)\frac{(1+\beta)^{7n+3}}{\sqrt{\beta}}(1+\omega)^{3n+2},$$

where $c(n)=(n+1)!\,c^n\Sigma_{k=1}^n\,[(n-k)^{n-k}/(n-k)!\,]\,\Sigma_{j=1}^k\,[j^{2(n-k)}/j!\,]$ and c is again a numerical factor. This last estimate clearly implies (5.7).

Let us now prove that for all $\beta>0$ and $\omega\geq 0$, $g_L^n(\mathbf{y}_0,\beta,\omega)$ given in (5.6) satisfies

$$\left|\int_{\Lambda_L} d\mathbf{y}_0\, g_L^n(\mathbf{y}_0,\beta,\omega)\right| \leq L^2 g(n,\beta,\omega), \tag{5.16}$$

where $g(n,\beta,\omega):=c(n)(1+\beta)^{7n+2}(1+\omega)^{3n+2}$ and $c(n)$ is a positive constant depending only on n. The same arguments as above leading to the estimate (5.13) imply

$$|F^m_{j,\infty}(\mathbf{y}_0,\ldots,\mathbf{y}_j,\tau_1,\ldots,\tau_j,\beta,\omega)| \leq \mathcal{C}_7\mathcal{C}_3'^{j-1}\frac{|\mathrm{Fl}_j|^m}{m!}G_\infty(\mathbf{y}_0,\mathbf{y}_1;32(\beta-\tau_1))\cdots G_\infty(\mathbf{y}_j,\mathbf{y}_0;32\tau_j)$$
$$\leq \mathcal{C}_7\mathcal{C}_3'^{j-1}\frac{(8\beta j^2)^m m^m 2^{3(j+1)/2}}{m!}$$
$$\times G_\infty(\mathbf{y}_0,\mathbf{y}_1;64(\beta-\tau_1))\cdots G_\infty(\mathbf{y}_j,\mathbf{y}_0;64\tau_j). \tag{5.17}$$

On the other hand, by the semigroup property (put $\Lambda_L^c:=\mathbb{R}^3\backslash\Lambda_L$),

$$\int_{\mathbb{R}^3} d\mathbf{y}_1 \dots \int_{\Lambda_L^c} d\mathbf{y}_l \int_{\mathbb{R}^3} d\mathbf{y}_{l+1\dots} \int_{\mathbb{R}^3} d\mathbf{y}_j \, G_\infty(\mathbf{y}_0,\mathbf{y}_1;64(\beta-\tau_1)) \cdots G_\infty(\mathbf{y}_j,\mathbf{y}_0;64\tau_j)$$

$$= \int_{\Lambda_L^c} d\mathbf{y}_l \, G_\infty(\mathbf{y}_0,\mathbf{y}_l;64(\beta-\tau_1)) G_\infty(\mathbf{y}_l,\mathbf{y}_0;64_{\tau l}). \tag{5.18}$$

Then (5.6), (5.17), and (5.18) imply

$$\left| \int_{\Lambda_L} d\mathbf{y}_0 \, g_L^n(\mathbf{y}_0,\beta,\omega) \right| \leq n! \sum_{k=1}^{n} \sum_{j=1}^{k} \mathcal{C}_7 \mathcal{C}_3'^{j-1} 2^{(5j+3)/2} \frac{(8\beta j^2)^{(n-k)}(n-k)^{n-k}}{(n-k)!}$$

$$\times \int_{D_j(\beta)} d\tau \sum_{l=1}^{j} \int_{\Lambda_L} d\mathbf{y}_0 \int_{\Lambda_L^c} d\mathbf{y}_l \, G_\infty(\mathbf{y}_0,\mathbf{y}_l;64(\beta-\tau_l)) G_\infty(\mathbf{y}_l,\mathbf{y}_0;64\tau_l). \tag{5.19}$$

By using the explicit form of the heat kernel given in (2.29), a straightforward computation shows that

$$\int_{\Lambda_L} d\mathbf{y}_0 \int_{\Lambda_L^c} d\mathbf{y}_l \, G_\infty(\mathbf{y}_0,\mathbf{y}_l;64(\beta-\tau_l)) G_\infty(\mathbf{y}_l,\mathbf{y}_0;64\tau_l) \leq c\frac{L^2}{\beta},$$

for some positive constant c. Hence, we get

$$\left| \int_{\Lambda} d\mathbf{y}_0 \, g_L^n(\mathbf{y}_0,\beta,\omega) \right| \leq L^2 c(n)(1+\beta)^{7n+2}(1+\omega)^{3n+2},$$

where $c(n)=n!\,c^n\Sigma_{k=1}^n\Sigma_{j=1}^k[j^{2(n-k)}(n-k)^{n-k}/(n-k)!\,(j-1)!]$ and c is a positive numerical factor. This shows (5.16). Then (5.16) and (5.7) imply the theorem. □

The proof of Theorem 1.2

We are now ready to prove the thermodynamic limit of generalized susceptibilities in the grand-canonical ensemble, when the chemical potential is negative (fugacity z less than one).

Let $L\geq 1$, $\beta>0$, $\omega\geq 0$ and $|z|<1$. We know from (1.8) and (2.27) that

$$P_L(\beta,\omega,z,\epsilon) - P_\infty(\beta,\omega,z,\epsilon) = \frac{\epsilon}{\beta|\Lambda_L|} \sum_{k\geq 1} \frac{(-\epsilon z)^k}{k} \int_{\Lambda_L} d\mathbf{x}\{G_L(\mathbf{x},\mathbf{x};k\beta,\omega) - G_\infty(\mathbf{x},\mathbf{x};k\beta,\omega)\}. \tag{5.20}$$

Then by applying the Theorem 5.1 we get

$$\frac{\partial^n(P_L-P_\infty)}{\partial\omega^n} = \frac{\epsilon}{\beta|\Lambda_L|} \sum_{k\geq 1} \frac{(-\epsilon z)^k}{k} \int_{\Lambda_L} d\mathbf{x} \left(\frac{\partial^n G_L}{\partial\omega^n} - \frac{\partial^n G_\infty}{\partial\omega^n} \right)(\mathbf{x},\mathbf{x};k\beta,\omega).$$

In particular, this also shows that the series from (1.10) must converge. Moreover, by using again the bound (5.1) in the last formula, we have

$$|\chi_L^{(n)} - \chi_\infty^{(n)}| \leq c(n)(1+\omega)^{3n+5} \frac{1}{\beta L} \sum_{k\geq 1} \frac{|z|^k}{k} \frac{(1+k\beta)^{7n+8}}{\sqrt{k\beta}}.$$

Since the series on the rhs of this last inequality is finite and L independent, this proves (1.11).□

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String equations in Whitham hierarchies: τ-functions and Virasoro constraints

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A scheme for solving Whitham hierarchies satisfying a special class of string equations is presented. The τ-function of the corresponding solutions is obtained and the differential expressions of the underlying Virasoro constraints are characterized. Illustrative examples of exact solutions of Whitham hierarchies are derived and applications to conformal maps dynamics are indicated. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2218982]

I. INTRODUCTION

Nonlinear integrable models of dispersionless type[1–4] arise in several branches of physics and applied mathematics. They have gained prominence after the discovery of their relevance in the formalism of quantum topological fields,[5,6] and of their role in the theory of deformations of conformal and quasiconformal maps on the complex plane.[7–9] Recently, new applications have been found[10–16] which include dynamics of conformal maps, growth processes of Laplacian type and large N limits of random matrix partition functions.

From the point of view of the theory of integrable systems, these models turn to be furnished by members of the so called *universal Whitham hierarchies* introduced by Krichever in Refs. 4 and 5. A particularly important example of these hierarchies is the dispersionless Toda (dToda) hierarchy.[10–13,17,18] The solutions of dispersionless integrable models underlying many of their applications satisfy special systems of constraints called *string equations*, which posses attractive mathematical properties and interesting physical meaning. Takasaki and Takebe[19–22] showed the relevance of string equations for studying the dispersionless Kadomtsev-Petviashvilii (KP) and Toda hierarchies and, in particular, for characterizing their associated symmetry groups. Nevertheless, although some schemes for solving string equations in the dispersionless KP and Toda hierarchies were provided in Refs. 23–25, general efficient methods of solution for string equations are still lacking.

In a recent work[26] a general formalism of Whitham hierarchies based on a factorization problem on a Lie group of canonical transformations has been proposed. It leads to a natural formulation of string equations in terms of dressing transformations. The present article is concerned with the analysis of these string equations and, in particular, their applications for characterizing exact solutions of Whitham hierarchies. Thus, we provide a solution scheme for a special class of string equations which determines not only the solutions of the algebraic orbits of the Whitham hierarchy,[5] but also the solutions arising in the above-mentioned applications of dispersionless integrable models.[24,25] We characterize the τ-function corresponding to these solutions and, by taking advantage of the string equations, we also derive the differential expressions of the underlying Virasoro constraints.

The elements of the phase space for a zero genus Whitham hierarchy are characterized by a finite set

$$(q_\alpha, z_\alpha^{-1}(p)), \quad \alpha = 0, \ldots, M,$$

of *punctures* q_α, where $q_0 := \infty$, of the complex p-plane and an associated set of local coordinates of the form

$$z_\alpha = \begin{cases} p + \sum_{n=1}^{\infty} \frac{d_{0n}}{p^n}, & \alpha = 0, \\ \frac{d_i}{p - q_i} + \sum_{n=0}^{\infty} d_{in}(p - q_i)^n, & \alpha = i = 1, \ldots, M. \end{cases} \tag{1}$$

The set of flows of the Whitham hierarchy can be formulated as the following infinite system of quasiclassical Lax equations:

$$\frac{\partial z_\alpha}{\partial t_{\mu n}} = \{\Omega_{\mu n}, z_\alpha\}, \tag{2}$$

where the Poisson bracket is defined as

$$\{F, G\} := \frac{\partial F}{\partial p}\frac{\partial G}{\partial x} - \frac{\partial F}{\partial x}\frac{\partial G}{\partial p}$$

and the Hamiltonian functions are

$$\Omega_{\mu n} := \begin{cases} (z_\mu^n)_{(\mu,+)}, & n \geqslant 1, \\ -\log_i(p - q_i), & n = 0, \quad \mu = i = 1, \ldots, M. \end{cases} \tag{3}$$

Here $(\cdot)_{(i,+)}$ and $(\cdot)_{(0,+)}$ stand for the projectors on the subspaces generated by $\{(p-q_i)^{-n}\}_{n=1}^{\infty}$ and $\{p^n\}_{n=0}^{\infty}$ in the corresponding spaces of Laurent series. Henceforth, it will be assumed that appropriate nonintersecting cuts connecting $p=\infty$ with the points q_i are made which allow us to define the logarithmic branches associated with Ω_{i0}. As several of these branches will appear simultaneously in certain equations, to avoid possible misunderstanding we introduce the notation convention $\log_i(p-q_i)$. For $M=0$ and $M=1$ these systems represent the dispersionless versions of the KP and Toda hierarchies, respectively.

In what follows Greek and Latin suffixes will be used to label indices of the sets $\{0, \ldots, M\}$ and $\{1, \ldots, M\}$, respectively. In our analysis we use an extended Lax formalism with Orlov functions

$$m_\alpha(z, \mathbf{t}) = \sum_{n=1}^{\infty} n t_{\alpha n} z_\alpha^{n-1} + \frac{t_{\alpha 0}}{z_\alpha} + \sum_{n \geqslant 2} \frac{v_{\alpha n}}{z_\alpha^n}, \quad t_{00} := -\sum_{i=1}^{M} t_{i0}, \tag{4}$$

such that

$$\{z_\alpha, m_\alpha\} = 1, \quad \forall\, \alpha,$$

and verifying the same Lax equations (2) as the variables z_α.

The basic notions about the Whitham hierarchy which are necessary for the subsequent discussion are introduced in Sec. II. String equations and symmetries are discussed in Sec. III, where the main results concerning the construction of solutions from meromorphic string equations and their Virasoro invariance are proved. Section IV presents a scheme for solving an special class of string equations, which is illustrated with several explicit examples. A formula for the correspond-

ing τ-function is given which generalizes the expression of the τ-function of analytic curves found in Ref. 10. Finally, we analyze the Virasoro symmetries associated to the string equations and obtain the corresponding Virasoro constraints in differential form.

II. THE WHITHAM HIERARCHY

In order to display the main features of the Whitham hierarchy it is convenient to use the following concise formulation in terms of the system of equations:

$$\mathrm{d}z_\alpha \wedge \mathrm{d}m_\alpha = \mathrm{d}\omega, \quad \forall\ \alpha, \tag{5}$$

where ω is the one-form defined by

$$\omega := \sum_{\mu,n} \Omega_{\mu n} \mathrm{d}t_{\mu n}. \tag{6}$$

To see how to get from system (5) to the Whitham hierarchy, note that by identifying the coefficients of $dp \wedge dt_{\mu n}$ and $dx \wedge dt_{\mu n}$ in (5) we obtain

$$\begin{aligned} \frac{\partial z_\alpha}{\partial p}\frac{\partial m_\alpha}{\partial t_{\mu n}} - \frac{\partial m_\alpha}{\partial p}\frac{\partial z_\alpha}{\partial t_{\mu n}} &= \frac{\partial \Omega_{\mu n}}{\partial p}, \\ \frac{\partial z_\alpha}{\partial x}\frac{\partial m_\alpha}{\partial t_{\mu n}} - \frac{\partial m_\alpha}{\partial x}\frac{\partial z_\alpha}{\partial t_{\mu n}} &= \frac{\partial \Omega_{\mu n}}{\partial x}. \end{aligned} \tag{7}$$

and, in particular, a $\Omega_{01}=p$, for $(\mu,n)=(0,1)$, system (7) implies

$$\{z_\alpha, m_\alpha\} = 1.$$

Thus, using this fact and solving (7) for $\partial z_\alpha/\partial t_{\mu n}$ and $\partial m_\alpha/\partial t_{\mu n}$, we deduce

$$\frac{\partial z_\alpha}{\partial t_{\mu n}} = \{\Omega_{\mu n}, z_\alpha\}, \quad \frac{\partial m_\alpha}{\partial t_{\mu n}} = \{\Omega_{\mu n}, m_\alpha\}.$$

It is now natural to introduce the S-functions of the Whitham hierarchy. Indeed as a consequence of (5) we find

$$\mathrm{d}\left(m_\alpha \mathrm{d}z_\alpha + \sum_{\mu,n} \Omega_{\mu n} \mathrm{d}t_{\mu n} \right) = 0, \quad \forall\ \alpha,$$

so that there exist functions $S_\alpha(z_\alpha, \boldsymbol{t})$ such that

$$\mathrm{d}S_\alpha = m_\alpha \mathrm{d}z_\alpha + \sum_{\mu,n} \Omega_{\mu n} \mathrm{d}t_{\mu n}, \quad \forall\ \alpha, \tag{8}$$

and from (4) we see that they admit expansions of the form

$$S_\alpha = \sum_{n\geqslant 1} z_\alpha^n t_{\alpha n} + \log z_\alpha t_{\alpha 0} - v_\alpha(\mathbf{t}) - \sum_{n\geqslant 1} \frac{v_{\alpha n+1}}{n}\frac{1}{z_\alpha^n}, \quad z_\alpha \to \infty. \tag{9}$$

It is important to notice that from (1)–(4) and (8) it follows that

$$\mathrm{d}S_0 = \sum_{n\geqslant 1} (n z_0^{n-1} t_{0n} \mathrm{d}z_0 + (z_0^n)_{(0,+)} \mathrm{d}t_{0n}) + \frac{t_{00}}{z_0}\mathrm{d}z_0 + \mathcal{O}\left(\frac{1}{z_0^2}\right)\mathrm{d}z_0, \quad z_0 \to \infty,$$

and consequently we may take

$$v_0(\mathbf{t}) \equiv 0.$$

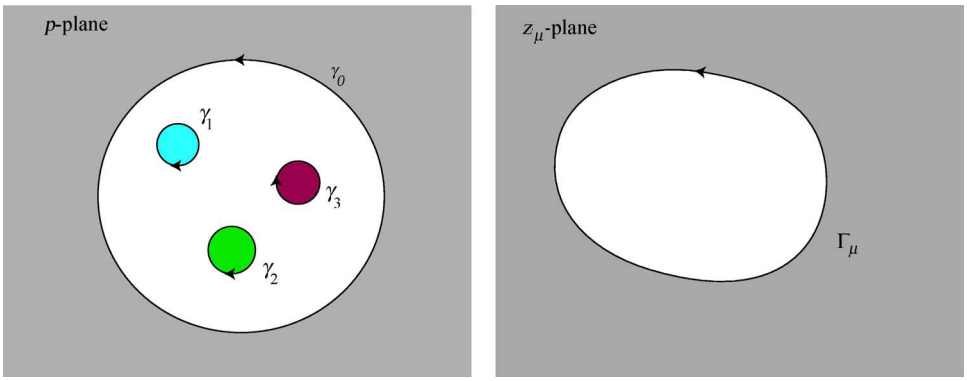

FIG. 1. (Color online) Right exteriors of γ_μ and Γ_μ.

To proceed further some analytic properties of the dynamical variables of the Whitham hierarchy are required. Thus we will henceforth suppose that there exist positively oriented closed curves Γ_μ in the complex planes of the variables z_μ such that each function $z_\mu(p)$ determines a conformal map of the right exterior of a circle $\gamma_\mu := z_\mu^{-1}(\Gamma_\mu)$ on the exterior of Γ_μ. We will assume that the circle γ_0 encircles all the $\gamma_i, (i=1,\ldots M)$ (see Fig. 1). Moreover, for each α the functions S_α and m_α will be assumed to be analytic in the exterior of Γ_α.

Under the previous conditions one can prove that

$$\partial_{\beta,m} v_{\alpha,n+1} = \partial_{\alpha,n} v_{\beta,m+1}, \quad \forall\, \alpha,\beta, \quad n,m \geqslant 0. \tag{10}$$

Here the functions v_{i1} are defined by

$$v_{i1} := v_i - \sum_{j<i} \log_{ji}(-1) t_{j0}, \tag{11}$$

and we are denoting

$$\log_{ji}(-1) := \log_j(q_i - q_j) - \log_i(q_j - q_i) = -\log_{ij}(-1).$$

In other words, it is ensured the existence of a *free-energy function* $F=F(\boldsymbol{t})$, the logarithm $F=\log \tau$ of the *dispersionless* τ-function, verifying

$$\mathrm{d}F = \sum_{(\alpha,n)\neq(0,0)} v_{\alpha n+1} \mathrm{d}t_{\alpha n}. \tag{12}$$

Let us first prove (10) for the case $(\alpha,n)=(i,0),(\beta,m)=(j,0)$. From the equations

$$\partial_{l0} S_k = -\log_l(p - q_l),$$

it follows that

$$\partial_{i0} v_j = \log_i(q_j - q_i), \quad \partial_{j0} v_i = \log_j(q_i - q_j),$$

so that the functions defined in (11) satisfy

$$\partial_{i0} v_{j1} = \partial_{j0} v_{i1}.$$

We indicate the strategy for proving the remaining cases of (10) by considering the choice $\alpha=i,\beta=j\geqslant 1,n,m\geqslant 1$ of (10). From (4) and (8) it follows that

$$v_{i,n+1} = \frac{1}{2\pi i}\oint_{\Gamma_i} z_i^n m_i \mathrm{d}z_i, \quad \partial_{j,m} S_i = (z_j^m)_{(j,+)},$$

so that

$$\partial_{j,m} v_{i,n+1} = \frac{1}{2\pi i}\oint_{\gamma_i} z_i^n \mathrm{d}(z_j^m)_{(j,+)} = \frac{1}{2\pi i}\oint_{\gamma_i} (z_i^n)_{(i,+)} \mathrm{d}(z_j^m)_{(j,+)} = \frac{1}{2\pi i}\oint_{\gamma_j} (z_j^m)_{(j,+)} \mathrm{d}(z_i^n)_{(i,+)} = \partial_{i,n} v_{j,m+1}, \tag{13}$$

where we have taken into account that $(z_i^n)_{(i,+)}\partial_p(z_j^m)_{(j,+)}$ is a rational function of p which has finite poles at q_i and q_j only and a zero residue at ∞.

III. STRING EQUATIONS AND SYMMETRIES

As it was shown in Ref. 26, the analysis of the factorization problem for the Whitham hierarchy shows that this hierarchy admits a natural formulation in terms of systems of string equations of the form

$$\begin{aligned} P_i(z_i,m_i) &= P_0(z_0,m_0), \\ Q_i(z_i,m_i) &= Q_0(z_0,m_0), \end{aligned} \quad i = 1,2,\ldots,M, \tag{14}$$

where $\{P_\alpha, Q_\alpha\}_{\alpha=0}^M$ are pairs of canonically conjugate variables

$$\{P_\alpha(p,x), Q_\alpha(p,x)\} = 1, \quad \forall\ \alpha. \tag{15}$$

In what follows we consider the problem of finding systems of form (14) which are appropriate to generate exact solutions of the Whitham hierarchy.

Given a solution $(z_\alpha(p,\boldsymbol{t}), m_\alpha(p,\boldsymbol{t}))$ of system (14), if we denote

$$\mathcal{P}_\alpha(p,\mathbf{t}) \coloneqq P_\alpha(z_\alpha(p,\mathbf{t}), m_\alpha(p,\mathbf{t})), \quad \mathcal{Q}_\alpha(p,\mathbf{t}) \coloneqq Q_\alpha(z_\alpha(p,\mathbf{t}), m_\alpha(p,\mathbf{t})),$$

then (14) and (15) imply

$$\mathrm{d}\mathcal{P}_\alpha \wedge \mathrm{d}\mathcal{Q}_\alpha = \mathrm{d}\mathcal{P}_\beta \wedge \mathrm{d}\mathcal{Q}_\beta, \quad \forall\ \alpha,\beta \tag{16}$$

and

$$\mathrm{d}\mathcal{P}_\alpha \wedge \mathrm{d}\mathcal{Q}_\alpha = \mathrm{d}z_\alpha \wedge \mathrm{d}m_\alpha, \quad \forall\ \alpha, \tag{17}$$

respectively. Hence solutions of the system of string equations verify

$$\mathrm{d}\mathcal{P}_\alpha \wedge \mathrm{d}\mathcal{Q}_\alpha = \mathrm{d}z_\beta \wedge \mathrm{d}m_\beta, \quad \forall\ \alpha,\beta. \tag{18}$$

The next result provides a convenient framework for our subsequent discussion of solutions of (14).

Theorem 1: *Let* $(z_\alpha(p,\boldsymbol{t}), m_\alpha(p,\boldsymbol{t}))$ *be a solution of* (14) *which admits expansions of forms* (1)–(4) *and such that the coefficients of the two-forms* (18) *are meromorphic functions of the complex variable p with finite poles at* $\{q_1,\ldots,q_M\}$ *only. Then* $(z_\alpha(p,\boldsymbol{t}), m_\alpha(p,\boldsymbol{t}))$ *is a solution of the Whitham hierarchy*.

Proof: In view of the hypothesis of the theorem the coefficients of the two-forms (18) with respect to the basis

$$\{\mathrm{d}p \wedge \mathrm{d}t_{\alpha n}, \quad \mathrm{d}t_{\alpha n} \wedge \mathrm{d}t_{\beta m}\}$$

are determined by their principal parts at $q_\mu, (\mu = 0,\ldots,M)$, so that by taking (18) into account we may write

$$\mathrm{d}z_\alpha \wedge \mathrm{d}m_\alpha = \sum_{\mu=0}^{M} (\mathrm{d}z_\mu \wedge \mathrm{d}m_\mu)_{(\mu,+)}, \quad \forall\, \alpha.$$

Moreover the terms in these decompositions can be found by using expansions (4) of the functions m_μ as follows:

$$\begin{aligned}\mathrm{d}z_\mu \wedge \mathrm{d}m_\mu &= \mathrm{d}z_\mu \wedge \left(\sum_{n=1}^{\infty} n z_\mu^{n-1} \mathrm{d}t_{\mu n} + \frac{\mathrm{d}t_{\mu 0}}{z_\mu} + \sum_{n\geqslant 2} \frac{\mathrm{d}v_{\mu n}}{z_\mu^n} \right) \\ &= \mathrm{d}\left(\sum_{n=1}^{\infty} z_\mu^n \mathrm{d}t_{\mu n} + \log z_\mu \mathrm{d}t_{\mu 0} - \sum_{n\geqslant 2} \frac{1}{n-1} \frac{\mathrm{d}v_{\mu n}}{z_\mu^{n-1}} \right),\end{aligned}$$

so that

$$(\mathrm{d}z_\mu \wedge \mathrm{d}m_\mu)_{(\mu,+)} = \mathrm{d}\left(\sum_{n=1}^{\infty} (z_\mu^n)_{(\mu,+)} \mathrm{d}t_{\mu n} - (1-\delta_{\mu 0}) \log(p - q_\mu) \mathrm{d}t_{\mu 0} \right) = \mathrm{d}\left(\sum_n \Omega_{\mu n} \mathrm{d}t_{\mu n} \right).$$

Thus we find

$$\mathrm{d}z_\alpha \wedge \mathrm{d}m_\alpha = \mathrm{d}\omega = \mathrm{d}\left(\sum_{\mu,n} \Omega_{\mu n} \mathrm{d}t_{\mu n} \right), \quad \forall\, \alpha,$$

and, consequently, this proves that the functions $(z_\alpha(p,\boldsymbol{t}), m_\alpha(p,\boldsymbol{t}))$ determine a solution of the Whitham hierarchy. ■

Following the dressing scheme of Refs. 19–22 it can be shown[26] that each solution of the Whitham hierarchy is determined by an associated system of string equations.

As it was shown in Ref. 26 a complete formulation of the symmetry group of the Whitham hierarchy is obtained by considering deformations of the associated factorization problem. On the other hand, a natural representation of this group is provided by the following symmetries of string equations implemented by Hamiltonian vector fields.

Theorem 2. *Given a vector function*

$$\mathbb{F} := (F_0(z_0,m_0), \ldots, F_M(z_M,m_M)), \tag{19}$$

the infinitesimal deformation

$$\begin{aligned}&\delta_{\mathbb{F}} P_\alpha := \{F_\alpha, P_\alpha\}, \quad \delta_{\mathbb{F}} Q_\alpha := \{F_\alpha, Q_\alpha\}, \\ &\delta_{\mathbb{F}} z_\alpha := \{z_\alpha, (F_\alpha)_-\}, \quad \delta_{\mathbb{F}} m_\alpha := \{m_\alpha, (F_\alpha)_-\},\end{aligned} \tag{20}$$

where

$$(F_\alpha)_- := F_\alpha - \sum_\beta (F_\beta)_{(\beta,+)},$$

determines a symmetry of the system of string equations (14).

Proof: We have to prove that given a solution (z_α, m_α) of (14), then at first order in ϵ

$$\begin{aligned}&(P_i + \epsilon\delta_{\mathbb{F}} P_i)(z_i + \epsilon\delta_{\mathbb{F}} z_i, m_i + \epsilon\delta_{\mathbb{F}} m_i) = (P_0 + \epsilon\delta_{\mathbb{F}} P_0)(z_0 + \epsilon\delta_{\mathbb{F}} z_0, m_0 + \epsilon\delta_{\mathbb{F}} m_0), \\ &(Q_i + \epsilon\delta_{\mathbb{F}} Q_i)(z_i + \epsilon\delta_{\mathbb{F}} z_i, m_i + \epsilon\delta_{\mathbb{F}} m_i) = (Q_0 + \delta_{\mathbb{F}} Q_0)(z_0 + \epsilon\delta_{\mathbb{F}} z_0, m_0 + \epsilon\delta_{\mathbb{F}} m_0),\end{aligned} \tag{21}$$

for all $i = 1, \ldots, M$. Let us consider the first group of equations of (21), they can be rewritten as

$$\frac{\partial P_i}{\partial z_i}\delta_{\mathbb{F}} z_i + \frac{\partial P_i}{\partial m_i}\delta_{\mathbb{F}} m_i + \{F_i, P_i\} = \frac{\partial P_0}{\partial z_0}\delta_{\mathbb{F}} z_0 + \frac{\partial P_0}{\partial m_0}\delta_{\mathbb{F}} m_0 + \{F_0, P_0\},$$

or, equivalently, by taking (20) into account, as

$$\{F_i - (F_i)_-, P_i\} = \{F_0 - (F_0)_-, P_0\}, \quad \forall\, i. \tag{22}$$

By hypothesis $P_i(z_i, m_i) = P_0(z_0, m_0)$. On the other hand

$$F_i - (F_i)_- = F_0 - (F_0)_- = \sum_\beta (F_\beta)_{(\beta,+)},$$

so that (22) is satisfied. The proof for the second group of equations of (21) is identical. □

We note that the condition for a solution (z_α, m_α) of the string equations (14) to be invariant under a symmetry (20) is

$$(F_\alpha(z_\alpha, m_\alpha))_- = 0, \quad \forall\, \alpha, \tag{23}$$

or equivalently

$$F_\alpha = \sum_\mu (F_\mu)_{(\mu,+)}, \quad \forall\, \alpha. \tag{24}$$

In other words, the functions $F_\alpha(z_\alpha, m_\alpha)$ must reduce to a unique meromorphic function of p with finite poles at the punctures q_i only. As a consequence it follows that, under the hypothesis of Theorem 1, solutions of the Whitham hierarchy satisfying a system of string equations (14) are invariant under the symmetries generated by

$$\mathbb{P} = (P_0(z_0, m_0), \ldots, P_M(z_M, m_M)), \quad \mathbb{Q} = (Q_0(z_0, m_0), \ldots, Q_M(z_M, m_M)),$$

and, more generally, they are invariant under the symmetries generated by

$$\mathbb{V}_{rs} = (P_0^{r+1} Q_0^{s+1}, \ldots, P_M^{r+1} Q_M^{s+1}), \quad r \geqslant -1, \quad s \geqslant 0, \tag{25}$$

which determine a Poisson Lie algebra $\mathcal{W}$ of symmetries

$$\{\mathbb{V}_{rs}, \mathbb{V}_{r's'}\} = ((r+1)(s'+1) - (r'+1)(s+1))V_{r+r's+s'}.$$

In particular the functions $\mathbb{V}_r := \mathbb{V}_{r0}$ and $\widetilde{\mathbb{V}}_s := -\mathbb{V}_{0s}$ generate two Virasoro algebras.

$$\{\mathbb{V}_r, \mathbb{V}_{r'}\} = (r - r')\mathbb{V}_{r+r'}, \quad \{\widetilde{\mathbb{V}}_s, \widetilde{\mathbb{V}}_{s'}\} = (s - s')\widetilde{\mathbb{V}}_{s+s'}.$$

IV. A SOLVABLE CLASS OF STRING EQUATIONS

In Ref. 26 a class of string equations was introduced which manifests special properties with respect to the group of dressing transformations. We next provide a scheme of solution for this class.

Let us consider systems of string equations associated to splittings

$$\{1, \ldots, M\} = I \cup J, \quad I \cap J = \emptyset$$

of the form

$$i \in I \begin{cases} z_i^{n_i} = z_0^{n_0} \\ \dfrac{1}{n_i}\dfrac{m_i}{z_i^{n_i-1}} = \dfrac{1}{n_0}\dfrac{m_0}{z_0^{n_0-1}}, \end{cases} \qquad j \in J \begin{cases} -\dfrac{n_0}{n_j}\dfrac{m_j}{z_j^{n_j-1}} = z_0^{n_0} \\ \dfrac{1}{n_0} z_j^{n_j} = \dfrac{1}{n_0}\dfrac{m_0}{z_0^{n_0-1}}, \end{cases} \tag{26}$$

where n_α are arbitrary positive integers. For $J=\emptyset$ these systems furnish the solutions describing the algebraic orbits of the Whitham hierarchy,[5] while the case $I=\emptyset$ includes the systems of string equations considered by Takasaki[18] and Wiegmann-Zabrodin[10–14] in their applications of the dToda hierarchy. The discussion of our scheme for solving (26) requires the consideration of the two cases $J=\emptyset$ and $J\neq\emptyset$ separately. In what follows we consider solutions with only a finite number of times $t_{\mu n}$ different from zero.

A. The case $J=\emptyset$

The corresponding system is given by

$$\begin{aligned} & z_i^{n_i} = z_0^{n_0}, \\ & \frac{1}{n_i}\frac{m_i}{z_i^{n_i-1}} = \frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}}, \qquad i = 1, \dots, M. \end{aligned} \tag{27}$$

The first group of equations (27) is satisfied by setting

$$z_i^{n_i} = z_0^{n_0} = E(p) := p^{n_0} + u_{n_0-2}p^{n_0-2} + \cdots + u_0 + \sum_{i=1}^{M}\sum_{s=1}^{n_i}\frac{v_{is}}{(p-q_i)^s}, \tag{28}$$

and, obviously, appropriate branches of z_μ can be defined which are compatible with the required asymptotic expansions (1). On the other hand, notice that the remaining string equations in (27) can be rewritten as

$$m_i = m_0\frac{\mathrm{d}z_0}{\mathrm{d}z_i}, \tag{29}$$

so that they are verified by taking

$$m_\alpha = \frac{\partial S}{\partial z_\alpha}, \qquad \forall\ \alpha, \tag{30}$$

for a given function $S(p,\mathbf{t})$, which means that all the S_α are equal to S. Moreover, it is straightforward to prove that the expansions (4) are satisfied if we set

$$S = \sum_{n=1}^{N_0} t_{0n}(z_0^n)_{(0,+)} + \sum_{j=1}^{M}\left(\sum_{n=1}^{N_j} t_{jn}(z_j^n)_{(j,+)} - t_{j0}\ln_j(p-q_j)\right). \tag{31}$$

In order to satisfy the hypothesis of Theorem 1, the functions $z_0^{n_0}$ and $m_0/z_0^{n_0-1}$ must be rational functions of p with possible finite poles at the points q_i only. In view of (28) this condition is verified by z_0^n. On the other hand, (27) and (30) imply that

$$\frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}} = \frac{\partial_p S}{\partial_p E}.$$

Therefore, the requirements of Theorem 1 are satisfied provided that

$$\partial_p S(p_r) = 0, \tag{32}$$

where p_r are the zeros of

$$\partial_p E(p_r) = 0.$$

We observe that the number of zeros p_r is

$$M + n_0 - 1 + \sum_{i=1}^{M} n_i,$$

which equals the number of unknowns $\{q_i, u_0, \ldots, u_{n_0-2}, v_{is}\}$. Equation (32) coincides with those formulated by Krichever in Ref. 5 for determining the algebraic orbits of the Whitham hierarchy.

Example: $M=2$, $n_0=n_1=n_2=1$, $N_0=2$, $N_1=N_2=1$.

In this case (28) reads

$$z_\alpha = E(p) = p + \frac{v_1}{p-q_1} + \frac{v_2}{p-q_2}, \quad 0 \leqslant \alpha \leqslant 2,$$

and (32) leads to

$$-t_{10} - t_{20} + 2t_{02}v_1 + 2t_{02}v_2 = 0,$$

$$q_1 t_{10} + 2q_2 t_{10} + 2q_1 t_{20} + q_2 t_{20} + t_{01}v_1 - 4q_2 t_{02}v_1 - t_{11}v_1 + t_{01}v_2 - 4q_1 t_{02}v_2 - t_{21}v_2 = 0,$$

$$-2q_1 q_2 t_{10} - {q_2}^2 t_{10} - {q_1}^2 t_{20} - 2q_1 q_2 t_{20} - 2q_2 t_{01}v_1 + 2{q_2}^2 t_{02}v_1 + 2q_2 t_{11}v_1 - 2q_1 t_{01}v_2 + 2{q_1}^2 t_{02}v_2 + 2q_1 t_{21}v_2 = 0,$$

$$q_1 {q_2}^2 t_{10} + {q_1}^2 q_2 t_{20} + {q_2}^2 t_{01}v_1 - {q_2}^2 t_{11}v_1 + {q_1}^2 t_{01}v_2 - {q_1}^2 t_{21}v_2 = 0.$$

By solving this system we obtain

$$z_\alpha = E(p) = p + \frac{2t_{10} + t_{20}}{4t_{02}\left(p + \dfrac{2t_{01}t_{10} - 2t_{10}t_{11} + 2t_{01}t_{20} - t_{11}t_{20} - t_{20}t_{21}}{4t_{02}(t_{10}+t_{20})}\right)} + \frac{t_{20}}{4t_{02}\left(p - \dfrac{-2t_{01}(t_{10}+t_{20}) + 2t_{20}t_{21} + t_{10}(t_{11}+t_{21})}{4t_{02}(t_{10}+t_{20})}\right)}, \quad 0 \leqslant \alpha \leqslant 2.$$

B. The case $J \neq \emptyset$

Now we consider system (26) for the generic case $J \neq \emptyset$. We look for functions m_α of the form

$$m_\alpha(z,t) = \sum_{n=1}^{N_\alpha} n t_{\alpha n} z_\alpha^{n-1} + \frac{t_{\alpha 0}}{z_\alpha} + \sum_{n \geqslant 2} \frac{v_{\alpha n}}{z_\alpha^n}, \quad t_{00} = -\sum_{i=1}^{M} t_{i0}, \tag{33}$$

for arbitrary positive integers N_α. In order to verify the hypothesis of Theorem 1 and expansions (1), we set

$$z_0^{n_0} = z_i^{n_i} = E_1(p) := p^{n_0} + u_{n_0-2}p^{n_0-2} + \cdots + u_0 + \sum_{l \in I}\sum_{n=1}^{n_l} \frac{a_{ln}}{(p-q_l)^n} + \sum_{k \in J}\sum_{n=1}^{n_{0k}} \frac{b_{kn}}{(p-q_k)^n}, \quad \forall\, i \in I, \tag{34}$$

$$z_j^{n_j} = E_2(p) := \sum_{n=0}^{n_{00}} c_n p^n + \sum_{l\in I}\sum_{n=1}^{n_{0l}} \frac{\widetilde{a}_{ln}}{(p-q_l)^n} + \sum_{k\in J}\sum_{n=1}^{n_k} \frac{\widetilde{b}_{kn}}{(p-q_k)^n}, \quad \forall\, j \in J, \tag{35}$$

where n_{00}, n_{0l}, n_{0k} $(l \in I, k \in J)$, the poles q_i and the coefficients of E_1 and E_2 are to be determined.

By introducing the functions

$$\mathcal{M}_\alpha := m_\alpha z_\alpha, \tag{36}$$

and taking (34) and (35) into account it follows that the system of string equations (26) reduces to

$$\mathcal{M}_0 = \frac{n_0}{n_i}\mathcal{M}_i = -\frac{n_0}{n_j}\mathcal{M}_j = E_1(p)E_2(p), \quad \forall\, i \in I, \quad j \in J. \tag{37}$$

On the other hand, due to their rational character, the functions $\mathcal{M}_\alpha$ can be written in terms of their principal parts at the poles q_β

$$\mathcal{M}_\alpha = \sum_{\beta=0}^{M} (\mathcal{M}_\alpha)_{(\beta,+)},$$

and by taking (4) into account we get

$$(\mathcal{M}_0)_{(0,+)} = \sum_{n=1}^{N_0} n t_{0n} (z_0^n)_{(0,+)} + t_{00}, \quad t_{00} = -\sum_{i=1}^{M} t_{i0},$$

$$(\mathcal{M}_i)_{(i,+)} = \sum_{n=1}^{N_i} n t_{in} (z_i^n)_{(i,+)}.$$

Therefore (37) is satisfied by

$$\begin{gathered}\mathcal{M}_0 = \sum_{n=1}^{N_0} n t_{0n} (z_0^n)_{(0,+)} + t_{00} + \sum_{i\in I} \frac{n_0}{n_i} \sum_{n=1}^{N_i} n t_{in} (z_i^n)_{(i,+)} - \sum_{j\in J} \frac{n_0}{n_j} \sum_{n=1}^{N_j} n t_{jn} (z_j^n)_{(j,+)}, \quad t_{00} = -\sum_{j=1}^{M} t_{j0} \\ \mathcal{M}_i = \frac{n_i}{n}\mathcal{M}_0, \quad \mathcal{M}_j = -\frac{n_j}{n}\mathcal{M}_0, \quad \forall\, i \in I, \quad j \in J,\end{gathered} \tag{38}$$

provided $\mathcal{M}_0$ verifies the equation

$$\mathcal{M}_0 = E_1(p)E_2(p). \tag{39}$$

At this point notice that from (34), (35), and (37) it follows that (39) is the only equation to be satisfied in order to solve the system of string equations (26). Both sides of (39) are rational functions of p with finite poles at $\{q_1, \ldots, q_M\}$ only, so that (39) holds if and only if the principal parts of both members at $\{q_0, q_1, \ldots, q_M\}$ coincide. Now we have that:

(i) At $q_0 = \infty$, the function $\mathcal{M}_0$ has a pole of order N_0, while $E_1(p)E_2(p)$ has a pole of order $n_{00}+n_0$, consequently (39) requires that $n_{00} = N_0 - n_0$, so that identifying the principal parts at q_0 represents $N_0 + 1$ equations.

(ii) At q_i, $(i \in I)$, the function $\mathcal{M}_0$ has a pole of order N_i and $E_1(p)E_2(p)$ has a pole of order $n_i + n_{0i}$. Hence $n_{0i} = N_i - n_i$ and identifying the corresponding principal parts leads to N_i equations.

(iii) At q_j, $(j \in J)$, the function $\mathcal{M}_0$ has a pole of order N_j and $E_1(p)E_2(p)$ has a pole of order $n_{0j} + n_j$. Hence $n_{0j} = N_j - n_j$ and identifying the corresponding principal parts leads to N_j equations.

Thus, Eq. (39) leads to $N_0+\Sigma_{i=1}^{M}N_i+1$ equations. On the other hand we have $N_0+\Sigma_{i=1}^{M}N_i+M$ unknown coefficients given by

$$q_i, \quad i=1,2,\ldots,M,$$

$$a_{i1},\ldots,a_{in_i}, \quad \tilde{a}_{i1},\ldots,\tilde{a}_{iN_i-n_i}, \quad i\in I,$$

$$b_{j1},\ldots,b_{jN_j-n_j}, \quad \tilde{b}_{j1},\ldots,\tilde{b}_{jn_j}, \quad j\in J, \tag{40}$$

$$u_0,\ldots,u_{n_0-2},$$

$$c_0,\ldots,c_{N_0-n_0}.$$

The additional $M-1$ equations required for determining these coefficients arise by imposing the asymptotic behavior (1)–(4) to (z_α,m_α). Note that (34) and (35) imply that the functions z_α have the asymptotic form (1). In what concerns the functions m_α, from the expression (38) for $\mathcal{M}_0$ it follows that

$$\mathcal{M}_0=\sum_{n=1}^{N_0} nt_{0n}z_0^n+t_{00}+\mathcal{O}\left(\frac{1}{z_0}\right), \quad z_0\to\infty,$$

so that m_0 satisfies an expansion of form (4). But in order for m_i $(i=1,2,\ldots,M)$ to satisfy (4) we must impose that

$$\mathrm{Res}(m_i,z_i=\infty)=t_{i0}, \quad i=1,2,\ldots,M. \tag{41}$$

However, let us see that as a consequence of the string equations (26) it follows that

$$\sum_{\alpha=0}^{M}\mathrm{Res}(m_\alpha,z_\alpha=\infty)=0, \tag{42}$$

and, consequently, only $M-1$ of Eq. (41) need to be imposed. Indeed, we have

$$2\pi i\sum_{\alpha=0}^{M}\mathrm{Res}(m_\alpha,z_\alpha=\infty)=\sum_{\alpha=0}^{M}\oint_{\Gamma_\alpha}m_\alpha \mathrm{d}z_\alpha=\sum_{\alpha=0}^{M}\oint_{\gamma_\alpha}m_\alpha\partial_p z_\alpha \mathrm{d}p.$$

On the other hand (34), (35), and (37) imply

$$m_i\partial_p z_i=m_0\partial_p z_0, \quad i\in I,$$

$$m_j\partial_p z_j=m_0\partial_p z_0-\frac{1}{n_0}\partial_p(E_1(p)E_2(p)), \quad j\in J,$$

so that

$$2\pi i\sum_{\alpha=0}^{M}\mathrm{Res}(m_\alpha,z_\alpha=\infty)=\oint_{\gamma}m_0\partial_p z_0\mathrm{d}p=0, \quad \gamma:=\sum_{\alpha=0}^{M}\gamma_\alpha,$$

where we have taken into account that

$$m_0\partial_p z_0 = \frac{1}{n_0}E_2(p)\partial_p E_1(p),$$

is a rational function of p with finite poles at q_i only, and the fact that

$$\gamma \sim 0 \quad \text{in} \quad \mathbb{C}\setminus\{q_1,\ldots,q_M\}.$$

In this way we have a system of

$$N_0 + \sum_{i=1}^{M} N_i + M,$$

equations to determine the same number of unknown coefficients. Therefore, according to Theorem 1, this method furnishes solutions of the Whitham hierarchy.

C. Examples

(1) $M=1$, $I=\emptyset$, $n_0=2$, $n_1=1$, $N_0=N_1=3$. Note that in this case all the equations come from (39). We set

$$z_0^2 = p^2 + u_0 + \frac{a_1}{p-q} + \frac{a_2}{(p-q)^2}, \quad z_1 = \frac{b_1}{p-q} + c_0 + c_1 p.$$

From (39) one obtains the system

$$p^3: \quad 3t_{03} = c_1,$$

$$p^2: \quad 2t_{02} = c_0,$$

$$p^1: \quad t_{01} + \frac{9t_{03}u_0}{2} = b_1 + c_1 u_0,$$

$$p^0: \quad \frac{9a_1 t_{03}}{2} - t_{10} + 2t_{02}u_0 = a_1 c_1 + b_1 q + c_0 u_0,$$

$$(p-q)^{-3}: \quad -6{b_1}^2 t_{13} = a_2,$$

$$(p-q)^{-2}: \quad -2{b_1}^2(2t_{12} + 9(c_0 + c_1 q)t_{13}) = a_1 b_1 + a_2(c_0 + c_1 q),$$

$$\begin{aligned}(p-q)^{-1}: \quad & -2b_1(t_{11} + 4(c_0 + c_1 q)t_{12} + 9(c_0^2 + 2c_0 c_1 q + c_1 b_1 + c_1^2 q^2)t_{13}) \\ & = a_2 c_1 + a_1(c_0 + c_1 q) + b_1(q^2 + u_0),\end{aligned}$$

and by solving these equations we find

$$\begin{aligned}z_0^2 = p^2 & - \frac{2(qt_{01} + t_{10} + 6t_{01}t_{03}t_{12} + 36t_{01}t_{02}t_{03}t_{13} + 54qt_{01}{t_{03}}^2 t_{13})}{3t_{03}(q + 6t_{03}t_{12} + 36t_{02}t_{03}t_{13} + 54q{t_{03}}^2 t_{13})} \\ & + \frac{4t_{10}(t_{12} + 6t_{02}t_{13} + 9qt_{03}t_{13})}{(p-q)(q + 54q{t_{03}}^2 t_{13} + 6t_{03}(t_{12} + 6t_{02}t_{13}))} - \frac{6{t_{10}}^2 t_{13}}{(p-q)^2(q + 54q{t_{03}}^2 t_{13} + 6t_{03}(t_{12} + 6t_{02}t_{13}))^2},\end{aligned}$$

$$z_1 = -\frac{t_{10}}{(p-q)(q+6t_{03}t_{12}+36t_{02}t_{03}t_{13}+54q{t_{03}}^2t_{13})} + 2t_{02} + 3pt_{03},$$

where q is determined by the implicit equation

$$\begin{aligned}
&-2qt_{01}+3q^3t_{03}-2t_{10}+6qt_{03}t_{11}-12t_{01}t_{03}t_{12}+24qt_{02}t_{03}t_{12}+54q^2{t_{03}}^2t_{12}+36{t_{03}}^2t_{11}t_{12}\\
&\quad+144t_{02}{t_{03}}^2{t_{12}}^2+216q{t_{03}}^3{t_{12}}^2-72t_{01}t_{02}t_{03}t_{13}+72q{t_{02}}^2t_{03}t_{13}-108qt_{01}{t_{03}}^2t_{13}+324q^2t_{02}{t_{03}}^2t_{13}\\
&\quad+324q^3{t_{03}}^3t_{13}-108{t_{03}}^2t_{10}t_{13}+216t_{02}{t_{03}}^2t_{11}t_{13}+324q{t_{03}}^3t_{11}t_{13}+1296{t_{02}}^2{t_{03}}^2t_{12}t_{13}\\
&\quad+3888q{t_{02}}{t_{03}}^3t_{12}t_{13}+2916q^2{t_{03}}^4t_{12}t_{13}+2592{t_{02}}^3{t_{03}}^2{t_{13}}^2+11664q{t_{02}}^2{t_{03}}^3{t_{13}}^2\\
&\quad+17496q^2t_{02}{t_{03}}^4{t_{13}}^2+8748q^3{t_{03}}^5{t_{13}}^2=0.
\end{aligned}$$

(2) $M=2$, $I=\emptyset$, $n_0=n_1=n_2=1$, $N_0=N_1=2$, $N_2=1$. In this case there are three punctures $\{q_0=\infty, q_1, q_2\}$ and we have to impose Eq. (41) for $i=1$. We take

$$z_0 = p + \frac{a_1}{p-q_1}, \quad z_1 = z_2 = \frac{b_1}{p-q_1} + \frac{b_2}{p-q_2} + c_0 + c_1p.$$

Then, by identifying powers of p, $(p-q_1)^{-1}$ and $(p-q_2)^{-1}$ in (39) the following system of equations arises

$$p^2: \quad 2t_{02} = c_1,$$

$$p^1: \quad t_{01} = c_0,$$

$$p^0: \quad 4a_1t_{02} - t_{10} - t_{20} = b_1 + b_2 + a_1c_1,$$

$$(p-q_1)^{-2}: \quad -2b_1t_{12} = a_1,$$

$$(p-q_1)^{-1}: \quad -b_1t_{11} - 4b_1\left(c_0 + c_1q_1 + \frac{b_2}{q_1-q_2}\right)t_{12} = b_1q_1 + a_1\left(c_0 + c_1q_1 + \frac{b_2}{q_1-q_2}\right),$$

$$(p-q_2)^{-1}: \quad -t_{21} = q_2 - \frac{a_1}{q_1-q_2}.$$

Moreover, by taking (38) into account, from (41) we get

$$\begin{aligned}
&-q_1t_{01} - 2(2a_1+{q_1}^2)t_{02} - \left(c_0 + c_1q_1 + \frac{b_2}{q_1-q_2}\right)t_{11}\\
&\quad -2\left(2b_1\left(c_1 - \frac{b_2}{(q_1-q_2)^2}\right) + \left(c_0 + c_1q_1 + \frac{b_2}{q_1-q_2}\right)^2\right)t_{12} + t_{20} + \frac{b_2t_{21}}{q_1-q_2} = 0.
\end{aligned}$$

These equations lead to

$$z_0 = p - \frac{1}{2(1+4t_{02}t_{12})(p-q_1)}(r^2(1+4t_{02}t_{12}) - 2t_{12}(t_{10}+t_{20}) + r(t_{11}+2t_{01}t_{12}-t_{21}-4t_{02}t_{12}t_{21})),$$

$$z_1 = \frac{1}{4t_{12}(1+4t_{02}t_{12})(p-q_1)}(r^2(1+4t_{02}t_{12}) - 2t_{12}(t_{10}+t_{20}) + r(t_{11}+2t_{01}t_{12} - t_{21} - 4t_{02}t_{12}t_{21}))$$
$$+ \frac{1}{4t_{12}(p-q_2)}(-r^2(1+4t_{02}t_{12}) - 2t_{12}(t_{10}+t_{20}) + r(-t_{11} - 2t_{01}t_{12} + t_{21} + 4t_{02}t_{12}t_{21}))$$
$$+ t_{01} + 2pt_{02},$$

where

$$q_1 = \frac{1}{2r(1+4t_{02}t_{12})}(r^2(1+4t_{02}t_{12}) + 2t_{12}(t_{10}+t_{20}) - r(t_{11}+2t_{01}t_{12}+t_{21}+4t_{02}t_{12}t_{21})),$$

$$q_2 = -\frac{1}{2r(1+4t_{02}t_{12})}(r^2(1+4t_{02}t_{12}) - 2t_{12}(t_{10}+t_{20}) + r(t_{11}+2t_{01}t_{12}+t_{21}+4t_{02}t_{12}t_{21})),$$

and r is determined by

$$3r^4(1+4t_{02}t_{12})^2 - 4{t_{12}}^2(t_{10}+t_{20})^2 + 4r^3(1+4t_{02}t_{12})(t_{11}+2t_{01}t_{12} - (1+4t_{02}t_{12})t_{21}) + r^2({t_{11}}^2$$
$$+ 4{t_{01}}^2{t_{12}}^2 + 4t_{10}t_{12}(1+4t_{02}t_{12}) - 4t_{12}t_{20} - 16t_{02}{t_{12}}^2t_{20} - 4t_{01}t_{12}t_{21} - 16t_{01}t_{02}{t_{12}}^2t_{21} + {t_{21}}^2$$
$$+ 8t_{02}t_{12}{t_{21}}^2 + 16{t_{02}}^2{t_{12}}^2{t_{21}}^2 + 2t_{11}(2t_{01}t_{12} - (1+4t_{02}t_{12})t_{21})) = 0.$$

(3) $M=2$, $I=\{1\}$, $J=\{2\}$, $n_0=n_1=n_2=N_0=1$, $N_1=N_2=2$. In this case we take

$$z_0 = z_1 = E_1(p) = p + \frac{v_{11}}{p-q_1} + \frac{v_{21}}{p-q_2}, \quad z_2 = E_2(p) = \frac{w_{21}}{p-q_2} + \frac{w_{11}}{p-q_1} + c_0.$$

By equating the coefficients of p^1, p^0, $(p-q_i)^{-j}$, $i,j=1,2$ in (39) one finds

$$p^1: \quad t_{01} = c_0,$$

$$p^0: \quad -t_{10} - t_{20} = w_{11} + w_{21},$$

$$(p-q_1)^{-2}: \quad 2t_{12}{v_{11}}^2 = v_{11}w_{11},$$

$$(p-q_1)^{-1}: \quad v_{11}\left(t_{11} + 4t_{12}\left(q_1 + \frac{v_{21}}{q_1-q_2}\right)\right) = \left(q_1 + \frac{v_{21}}{q_1-q_2}\right)w_{11} + v_{11}\left(c_0 + \frac{w_{21}}{q_1-q_2}\right),$$

$$(p-q_2)^{-2}: \quad -2t_{22}{w_{21}}^2 = v_{21}w_{21},$$

$$(p-q_2)^{-1}: \quad -(t_{21}w_{21}) - 4t_{22}\left(c_0 + \frac{w_{11}}{-q_1+q_2}\right)w_{21} = c_0v_{21} + \frac{v_{21}w_{11} + (-(q_1q_2) + {q_2}^2 + v_{11})w_{21}}{-q_1+q_2},$$

and (41) leads to

$$-q_2t_{01} + t_{10} - \frac{t_{11}v_{11}}{-q_1+q_2} - 2t_{12}\left(\frac{{v_{11}}^2}{(-q_1+q_2)^2} + \frac{2v_{11}\left(q_1 + \frac{v_{21}}{q_1-q_2}\right)}{-q_1+q_2}\right) - t_{21}\left(c_0 + \frac{w_{11}}{-q_1+q_2}\right)$$
$$- 2t_{22}\left(\left(c_0 + \frac{w_{11}}{-q_1+q_2}\right)^2 - \frac{2w_{11}w_{21}}{(q_1-q_2)^2}\right) = 0.$$

By solving these equations one obtains

$$E_1(p) = p - \frac{2r_1{}^2 t_{12} + (t_{10}+t_{20})(1+4t_{12}t_{22}) - r_1(t_{01}-t_{11}+2t_{12}t_{21}+4t_{01}t_{12}t_{22})}{4(p-q_1)t_{12}(1+4t_{12}t_{22})}$$
$$- \frac{t_{22}(2r_1{}^2 t_{12} - (t_{10}+t_{20})(1+4t_{12}t_{22}) - r_1(t_{01}-t_{11}+2t_{12}t_{21}+4t_{01}t_{12}t_{22}))}{(p-q_2)(1+4t_{12}t_{22})},$$

$$E_2(p) = t_{01} - \frac{2r_1{}^2 t_{12} + (t_{10}+t_{20})(1+4t_{12}t_{22}) - r_1(t_{01}-t_{11}+2t_{12}t_{21}+4t_{01}t_{12}t_{22})}{2(p-q_1)(1+4t_{12}t_{22})}$$
$$+ \frac{2r_1{}^2 t_{12} - (t_{10}+t_{20})(1+4t_{12}t_{22}) - r_1(t_{01}-t_{11}+2t_{12}t_{21}+4t_{01}t_{12}t_{22})}{2(p-q_2)(1+4t_{12}t_{22})},$$

where

$$q_1 = \frac{r_1}{2} - \frac{(t_{10}+t_{20})(1+4t_{12}t_{22}) + r_1(t_{11}+2t_{12}t_{21}+t_{01}(-1+4t_{12}t_{22}))}{4r_1 t_{12}},$$

$$q_2 = -\frac{r_1}{2} - \frac{(t_{10}+t_{20})(1+4t_{12}t_{22}) + r_1(t_{11}+2t_{12}t_{21}+t_{01}(-1+4t_{12}t_{22}))}{4r_1 t_{12}},$$

and r_1 satisfies

$$-12r_1{}^4 t_{12}{}^2 + (t_{10}+t_{20})^2(1+4t_{12}t_{22})^2 + 8r_1{}^3 t_{12}(t_{01}-t_{11}+2t_{12}t_{21}+4t_{01}t_{12}t_{22}) - r_1{}^2(t_{11}{}^2 - 4t_{11}t_{12}t_{21}$$
$$- 2t_{01}(t_{11}-2t_{12}t_{21})(1+4t_{12}t_{22}) + (t_{01}+4t_{01}t_{12}t_{22})^2 + 4t_{12}(-t_{10}+t_{20}+t_{12}t_{21}{}^2 - 4t_{10}t_{12}t_{22}$$
$$+ 4t_{12}t_{20}t_{22})) = 0.$$

D. *S*-functions

According to the identities

$$\partial_p S_\alpha = \mathcal{M}_\alpha \partial_p \log z_\alpha, \quad \mathcal{M}_\alpha = m_\alpha z_\alpha,$$

it follows at once from (34), (35), and (37) that the functions $\partial_p S_\alpha$ are rational functions of p with finite poles at the points q_i $(i=1,\ldots,M)$ only. Thus we may decompose the functions $\partial_p S_\alpha$ into their principal parts

$$\partial_p S_\alpha = \sum_\beta (\partial_p S_\alpha)_{(\beta,+)}, \tag{43}$$

and, in view of asymptotic behavior (9), we may write

$$(\partial_p S_\alpha)_{(\alpha,+)} = \partial_p R_\alpha, \tag{44}$$

where

$$R_\alpha := \sum_{n\geqslant 1} (z_\alpha^n)_{(\alpha,+)} t_{\alpha n} - (1-\delta_{\alpha 0}) t_{\alpha 0} \log_\alpha (p-q_\alpha). \tag{45}$$

Further, from (34), (35), and (37) we obtain

$$\partial_p S_i = \partial_p S_0, \quad \forall\, i \in I,$$

$$\partial_p S_j = \partial_p S_0 - \frac{1}{n_0}\partial_p(E_1E_2), \quad \forall\, j \in J, \tag{46}$$

which leads to

$$S_\alpha = \begin{cases} \displaystyle\sum_\beta R_\beta + \frac{1}{n_0}\sum_{j\in J}(E_1E_2)_{(j,+)}, & \alpha \in \{0\}\cup I \\ \displaystyle\sum_\beta R_\beta - \frac{1}{n_0}(E_1E_2)_{(0,+)} - \frac{1}{n_0}\sum_{i\in I}(E_1E_2)_{(i,+)}, & \alpha \in J. \end{cases} \tag{47}$$

In principle, (46) implies the expressions (47) plus additional p-independent terms $w_\alpha(t)$. However these terms can be removed by using (8) and (9). Indeed, assymptotic behavior (9) for S_0 requires $w_0=0$. On the other hand, (8) says that

$$\mathrm{d}S_i - \mathrm{d}S_0 = m_i \mathrm{d}z_i - m_0 \mathrm{d}z_0,$$

so that by using the string equations (26) we deduce

$$\mathrm{d}w_i = \begin{cases} \mathrm{d}S_i - \mathrm{d}S_0 = 0, & i \in I \\ \mathrm{d}S_i - \mathrm{d}S_0 + \dfrac{1}{n_0}\mathrm{d}(E_1E_2) = 0, & i \in J. \end{cases}$$

E. τ-functions

Theorem 3: *The τ-function for the solutions of the Whitham hierarchy associated with the class of string equations* (26) *is given by*

$$\begin{aligned} 2\log\tau &= \sum_\alpha \frac{1}{2\pi i}\oint_{\Gamma_\alpha}\left(\sum_{n\geqslant 1} z_\alpha^n t_{\alpha n}\right) m_\alpha \mathrm{d}z_\alpha - \sum_{j\in J}\frac{1}{4\pi i n_j}\oint_{\Gamma_j} z_j m_j^2 \mathrm{d}z_j + \sum_i t_{i0}v_{i1} \\ &= \sum_\alpha \sum_{n\geqslant 0} t_{\alpha n} v_{\alpha n+1} - \sum_{j\in J}\frac{1}{n_j}\sum_{n\geqslant 1} n t_{jn} v_{jn+1} - \sum_{j\in J}\frac{t_{j0}^2}{2n_j} \end{aligned} \tag{48}$$

Proof: Our strategy to prove (48) is to start from the free-energy function for the algebraic orbits of the Whitham hierarchy[5]

$$F_0 := \sum_\alpha \frac{1}{4\pi i}\oint_{\Gamma_\alpha}\left(\sum_{n\geqslant 1} z_\alpha^n t_{\alpha n}\right) m_\alpha \mathrm{d}z_\alpha + \frac{1}{2}\sum_i t_{i0}v_{i1}, \tag{49}$$

and determine the appropriate modifications to get the free-energy function for the solutions of the class of string equations (26).

By differentiating F_0 with respect to t_{ln}, $n\geqslant 1$ we get

$$\partial_{l,n}F_0 = \frac{1}{4\pi i}\oint_{\Gamma_l} z_l^n m_l \mathrm{d}z_l + \sum_\alpha \frac{1}{4\pi i}\oint_{\gamma_\alpha}\left(\sum_{m\geqslant 1} z_\alpha^m t_{\alpha m}\right)\partial_p((z_l^n)_{(l,+)})\mathrm{d}p + \frac{1}{2}\sum_i t_{i0}\partial_{l,n}v_{i1}, \tag{50}$$

and arguing as in the derivation of (13), we find that

$$\oint_{\gamma_\alpha}\left(\sum_{m\geqslant 1} z_\alpha^m t_{\alpha m}\right)\partial_p((z_l^n)_{(l,+)})\mathrm{d}p = \oint_{\gamma_l} z_l^n \partial_p\left(\sum_{m\geqslant 1}(z_\alpha^m)_{(\alpha,+)} t_{\alpha m}\right)\mathrm{d}p.$$

On the other hand, for $i\neq l$ we have

$$\partial_{l,n}S_i = (z_l^n)_{(l,+)} = -\partial_{l,n}v_{i1} + \mathcal{O}\left(\frac{1}{z_i}\right), \quad p \to q_i,$$

so that

$$\begin{aligned}\partial_{l,n}v_{i1} &= -(z_l^n)_{(l,+)}(q_i)\\ &= \frac{1}{2\pi i}\oint_{\gamma_i}\frac{(z_l^n)_{(l,+)}}{p-q_i}\mathrm{d}p = -\frac{1}{2\pi i}\oint_{\gamma_l}(z_l^n)_{(l,+)}\partial_p\log(p-q_i)\mathrm{d}p\\ &= -\frac{1}{2\pi i}\oint_{\gamma_l} z_l^n\partial_p\log(p-q_i)\mathrm{d}p, \quad i\neq l,\end{aligned}$$

and the same expression turns out to hold for $i=l$. Hence, (50) can be rewritten as

$$\begin{aligned}\partial_{l,n}F_0 &= \frac{1}{2}v_{ln+1} + \frac{1}{4\pi i}\oint_{\gamma_l} z_l^n\sum_\alpha\partial_p\left(\sum_{m\geqslant 1}(z_\alpha^m)_{(\alpha,+)}t_{\alpha m} - (1-\delta_{\alpha 0})t_{\alpha 0}\log(p-q_\alpha)\right)\mathrm{d}p\\ &= v_{ln+1} + \frac{1}{4\pi i}\oint_{\gamma_l} z_l^n\left(\sum_\alpha\partial_p R_\alpha - \partial_p S_l\right)\mathrm{d}p\\ &= v_{ln+1} + \sum_\alpha\frac{1}{4\pi i}\oint_{\gamma_l}(z_l^n)_{(l,+)}(\partial_p R_\alpha - (\partial_p S_l)_{(\alpha,+)})\mathrm{d}p. \end{aligned} \tag{51}$$

Further, we have that

$$\begin{aligned}\frac{1}{4\pi i}\oint_{\gamma_l}(z_l^n)_{(l,+)}(\partial_p R_\alpha - (\partial_p S_l)_{(\alpha,+)})\mathrm{d}p &= -\frac{1}{4\pi i}\oint_{\gamma_\alpha}(z_l^n)_{(l,+)}(\partial_p R_\alpha - (\partial_p S_l)_{(\alpha,+)})\mathrm{d}p\\ &= -\frac{1}{4\pi i}\oint_{\gamma_\alpha}(z_l^n)_{(l,+)}(\partial_p S_\alpha - \partial_p S_l)\mathrm{d}p,\end{aligned}$$

so that from (46) and by taking into account

$$\oint_{\gamma_0}(z_l^n)_{(l,+)}\partial_p(E_1E_2)\mathrm{d}p = -\sum_{i=1}^M\oint_{\gamma_i}(z_l^n)_{(l,+)}\partial_p(E_1E_2)\mathrm{d}p,$$

we get

$$\begin{aligned}\partial_{l,n}F_0 &= v_{ln+1} + \frac{1}{n_0}\sum_{j\in J}\frac{1}{4\pi i}\oint_{\gamma_j}(z_l^n)_{(l,+)}\partial_p(E_1E_2)\mathrm{d}p = v_{ln+1} + \sum_{j\in J}\frac{1}{4\pi i n_j}\oint_{\Gamma_j} z_j m_j\partial_{l,n}m_j\mathrm{d}z_j\\ &= v_{ln+1} + \partial_{l,n}\left(\sum_{j\in J}\frac{1}{8\pi i n_j}\oint_{\Gamma_j} z_j m_j^2\mathrm{d}z_j\right),\end{aligned} \tag{52}$$

which shows that

$$\partial_{l,n}\log\tau = v_{ln+1}.$$

By a similar procedure one finds

$$\partial_{0,n}\log\tau = v_{0n+1}, \quad n\geqslant 1.$$

Nevertheless, proving that

$$\partial_{l,0}\log\tau = v_{l1}, \quad l = 1, \ldots, M \tag{53}$$

requires a more involved analysis. First we differentiate F_0 with respect to t_{l0}

$$\partial_{l,0}F_0 = \sum_\alpha \frac{1}{4\pi i}\oint_{\gamma_\alpha}\left(\sum_{m\geqslant 1} z_\alpha^m t_{\alpha m}\right)\partial_p(-\log(p-q_l))\mathrm{d}p + \frac{1}{2}\sum_i t_{i0}\partial_{l,0}v_{i1} + \frac{1}{2}v_{l1}, \tag{54}$$

and use the following relations:

$$\oint_{\gamma_\alpha}\left(\sum_{m\geqslant 1} z_\alpha^m t_{\alpha m}\right)\frac{1}{p-q_l}\mathrm{d}p = -\oint_{\gamma_l}\left(\sum_{m\geqslant 1}(z_\alpha^m)_{(\alpha,+)}t_{\alpha m}\right)\frac{1}{p-q_l}\mathrm{d}p, \quad \alpha \neq l,$$

$$\oint_{\gamma_l}\left(\sum_{m\geqslant 1} z_l^m t_{lm}\right)\frac{1}{p-q_l}\mathrm{d}p = -2\pi i\lim_{p\to q_l}\left(\sum_{m\geqslant 1}(z_l^m - (z_l^m)_{(l,+)})t_{lm}\right),$$

$$\sum_{i\neq l} t_{i0}\partial_{l0}v_{i1} = \sum_{i\neq l} t_{i0}\log_l(q_i - q_l) - \sum_{i>l} t_{i0}\log_{li}(-1) = \sum_{i\neq l} t_{i0}\log_i(q_l - q_i) - \sum_{i<l} t_{i0}\log_{il}(-1),$$

$$\partial_{l,0}v_{l1} = \lim_{p\to q_l}\log(z_l(p-q_l)).$$

Then (54) becomes

$$\begin{aligned}\partial_{l,0}F_0 = {} & \frac{1}{2}v_{l1} + \frac{1}{4\pi i}\oint_{\gamma_l}\frac{\mathrm{d}p}{p-q_l}\sum_{\alpha\neq l}\left(\sum_{m\geqslant 1}(z_\alpha^m)_{(\alpha,+)}t_{\alpha m} - (1-\delta_{\alpha 0})t_{\alpha 0}\log_\alpha(p-q_\alpha)\right) \\ & + \frac{1}{2}\lim_{p\to q_l}\left(\sum_{m\geqslant 1}(z_l^m - (z_l^m)_{(l,+)})t_{lm} + t_{l0}\log z_l + \ t_{l0}\log_l(p-q_l)\right) - \frac{1}{2}\sum_{i<l} t_{i0}\log_{il}(-1).\end{aligned} \tag{55}$$

Further, from asymptotic expansion (9) of S_l we have that

$$v_l = \lim_{p\to q_l}\left(\sum_{m\geqslant 1} z_l^m t_{lm} + t_{l0}\log z_l - S_l\right),$$

which allows us to rewrite (55) in the form

$$\partial_{l,0}F_0 = v_{l1} + \frac{1}{4\pi i}\oint_{\gamma_l}\frac{\mathrm{d}p}{p-q_l}\sum_{\alpha\neq l} R_\alpha + \frac{1}{2}\lim_{p\to q_l}(S_l - R_l) = v_{l1} + \frac{1}{4\pi i}\oint_{\gamma_l}\frac{\mathrm{d}p}{p-q_l}\left(\sum_\alpha R_\alpha - S_l\right). \tag{56}$$

Now by using (47) it is straightforward to see that

$$\frac{1}{4\pi i}\oint_{\gamma_l}\frac{\mathrm{d}p}{p-q_l}\left(\sum_\alpha R_\alpha - S_l\right) = \frac{1}{n_0}\sum_{j\in J}\frac{1}{4\pi i}\oint_{\gamma_j}\frac{\mathrm{d}p}{p-q_l}E_1E_2 = \sum_{j\in J}\frac{1}{4\pi i n_j}\oint_{\Gamma_j} z_j m_j\partial_{l,0}m_j\mathrm{d}z_j, \tag{57}$$

which shows that (56) is equivalent to (53). □

F. Conformal maps dynamics

We will outline how our scheme applies for characterizing dToda dynamics of conformal maps, and, in particular, how (48) gives rise to the expression of the τ-function of analytic curves found in Ref. 10.

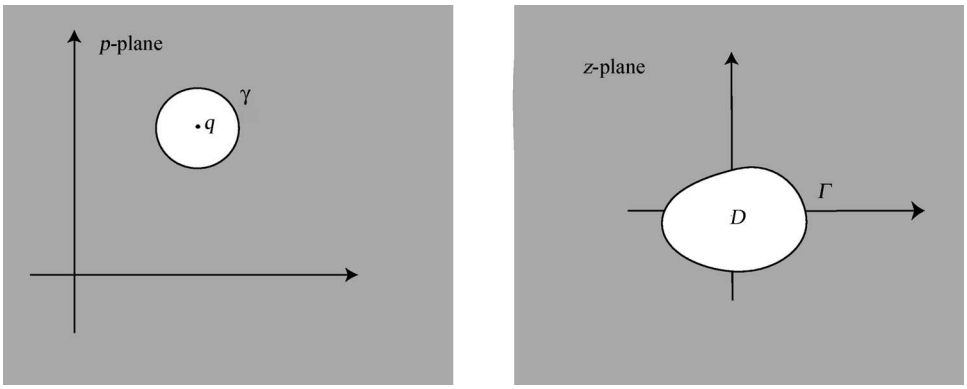

FIG. 2. Conformal map $z=z(p)$.

Given a simply connected domain D bounded by a closed path Γ in the z-plane, there exists[27] a unique circle γ in the p-plane and a unique conformal map $z=z(p)$ satisfying

$$z(p) = p + \sum_{n=1}^{\infty} \frac{d_n}{p^n}, \quad z \to \infty, \tag{58}$$

such that $z=z(p)$ transforms the exterior of γ into the exterior of Γ (see Fig. 2). Note that the conformal map used by Wiegmann-Zabrodin[10] is given by $z(rp+q)$, where q and r are the center and the radius of γ, respectively.

Let us define the function

$$\bar{z}(p) = \overline{z(\mathcal{I}_\gamma(p))}, \tag{59}$$

where $\mathcal{I}_\gamma$ denotes the inversion with respect to the circle γ

$$\mathcal{I}_\gamma(p) := q + \frac{r^2}{\bar{p} - \bar{q}}.$$

It is clear that

$$\bar{z}(p) = \overline{z(p)}, \quad \forall\, p \in \gamma.$$

If Γ is asssumed to be an analytic curve, then it can be described by an equation of the form

$$\bar{z} = \mathcal{S}(z), \tag{60}$$

where $\mathcal{S}(z) := \bar{z}(p(z))$ (the Schwarz function) is analytic in a neigborhood of γ. Thus, if Γ encircles the origin, $\mathcal{S}(z)$ can be expanded as

$$\mathcal{S}(z) = \sum_{n\geqslant 1} n t_n z^{n-1} + \frac{t_0}{z} + \sum_{n\geqslant 1} \frac{v_n(t)}{z^{n+1}}, \tag{61}$$

where the coefficients t_n $(n \geqslant 0)$, the exterior harmonic moments of Γ, determine the curve Γ and conformal map (58). Note, in particular, that the coefficient t_0,

$$t_0 = \frac{1}{2\pi i} \oint_\Gamma \bar{z} \mathrm{d}z = \frac{1}{\pi} \int_D \mathrm{d}x\mathrm{d}y,$$

represents the area of D.

In this way, by considering the harmonic moments as independent complex parameters, if we define

$$q_1 = q, \quad z_0(p) = z(p), \quad z_1(p) = \bar{z}(p),$$

$$t_{0n} := t_n, \quad t_{1n} = -\bar{t}_n, \quad n \geqslant 0,$$

$$m_0 = \mathcal{S}(z_0), \quad m_1 = -z(p(z_1)),$$

we obtain a solution of the system of string equations

$$-m_1 = z_0, \quad z_1 = m_0. \tag{62}$$

Further, by taking into account that

$$v_{1n+1} = -\bar{v}_{0n+1} = -\bar{v}_n, \quad n \geqslant 1,$$

and the identity

$$t_0^2 + 2\sum_{n\geqslant 1} n t_n v_n = \frac{1}{2\pi i}\oint_\Gamma z\mathcal{S}(z)^2 \mathrm{d}z = \frac{1}{2\pi i}\oint_\Gamma z\bar{z}^2 \mathrm{d}z = \frac{1}{\pi}\int_D |z|^2 \mathrm{d}x\mathrm{d}y = \bar{t}_0^2 + 2\sum_{n\geqslant 1} n\bar{t}_n\bar{v}_n,$$

we see that (48) reduces to

$$2\log\tau = \frac{1}{2}\sum_{n\geqslant 1}(2-n)(t_n v_n + \bar{t}_n\bar{v}_n) + t_0 v_0 - \frac{t_0^2}{2}, \tag{63}$$

where $v_0 := -v_{11}$, which is the expression for the τ-function associated to analytic curves obtained in Ref. 10. Notice that (62) is the simplest nontrivial case ($I=\emptyset$, $J=\{1\}$, $n_0=n_1=1$) of the class of string equations (26).

G. Symmetry constraints

As we proved earlier, solutions (z_α, m_α) of systems of string equations (14) are invariant under the symmetries

$$\mathbb{V}_{rs} = (P_0^{r+1}Q_0^{s+1}, \ldots, P_M^{r+1}Q_M^{s+1}), \quad r \geqslant -1, s \geqslant 0.$$

Moreover, as a consequence of (14) we have that the following identities hold:

$$P_0^{r+1}Q_0^{s+1} = P_i^{r+1}Q_i^{s+1} = P_j^{r+1}Q_j^{s+1} = P_0^{r+1}Q_j^{s+1}, \quad \forall\, i \in I, j \in J, \tag{64}$$

for the values of the functions P_μ and Q_μ at a solution (z_α, m_α). In particular these identities lead to the following expressions for the constraints arising from the invariance of (26) under the action of $\mathbb{V}_{rs}$.

Theorem 4: *If* (z_α, m_α) *is a solution of the string equations* (26) *then it satisfies the identities*

$$\sum_{\alpha\in\{0\}\cup I}\oint_{\Gamma_\alpha}\left(\frac{z_\alpha}{n_\alpha}\right)^s z_\alpha^{(r-s)n_\alpha} m_\alpha^{s+1}\mathrm{d}z_\alpha + (-1)^r\frac{s+1}{r+1}n_0^{r-s}\sum_{j\in J}\oint_{\Gamma_j}\left(\frac{z_j}{n_j}\right)^r z_j^{(s-r)n_j} m_j^{r+1}\mathrm{d}z_j = 0, \tag{65}$$

for all $r, s \geqslant 0$.

Proof: From (34)–(37) we find that (64) takes the form

$$z_0^{n_0(r+1)}\left(\frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}}\right)^{s+1}=z_i^{n_i(r+1)}\left(\frac{1}{n_i}\frac{m_i}{z_i^{n_i-1}}\right)^{s+1}=\left(\frac{z_j^{n_j}}{n_0}\right)^{s+1}\left(-\frac{n_0}{n_j}\frac{m_j}{z_j^{n_j-1}}\right)^{r+1}$$

$$=\frac{1}{n_0^{s+1}}E_1^{r+1}E_2^{s+1},\quad \forall\, i\in I, j\in J, \tag{66}$$

and we have that

$$z_0^{n_0(r+1)}\left(\frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}}\right)^{s+1}\partial_p\log E_1=z_i^{n_i(r+1)}\left(\frac{1}{n_i}\frac{m_i}{z_i^{n_i-1}}\right)^{s+1}\partial_p\log E_1=\frac{(\partial_p E_1^{r+1})E_2^{s+1}}{(r+1)n_0^{s+1}}, \tag{67}$$

$$\left(\frac{z_j^{n_j}}{n_0}\right)^{s+1}\left(-\frac{n_0}{n_j}\frac{m_j}{z_j^{n_j-1}}\right)^{r+1}\partial_p\log E_2=-\frac{r+1}{s+1}z_0^{n_0(r+1)}\left(\frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}}\right)^{s+1}\partial_p\log E_1+\partial_p\left(\frac{E_1^{r+1}E_2^{s+1}}{(s+1)n_0^{s+1}}\right),$$

for all $r,s\geqslant 0$ and $i\in I$, $j\in J$. Hence if we proceed as in the proof of (42) and take into account that

$$\partial_p\log E_1=n_0\partial_p\log z_0=n_i\partial_p\log z_i,\quad \forall\, i\in I,$$

$$\partial_p\log E_2=n_j\partial_p\log z_j,\quad \forall\, j\in J,$$

it is straightforward to prove that

$$\sum_{\alpha\in\{0\}\cup I}\oint_{\Gamma_\alpha}z_\alpha^{n_\alpha(r+1)}\left(\frac{1}{n_\alpha}\frac{m_\alpha}{z_\alpha^{n_\alpha-1}}\right)^{s+1}n_\alpha\frac{\mathrm{d}z_\alpha}{z_\alpha}-\sum_{j\in J}\frac{s+1}{r+1}\oint_{\Gamma_j}\left(\frac{z_j^{n_j}}{n_0}\right)^{s+1}\left(-\frac{n_0}{n_j}\frac{m_j}{z_j^{n_j-1}}\right)^{r+1}n_j\frac{\mathrm{d}z_j}{z_j}$$

$$=\oint_\gamma z_0^{n_0(r+1)}\left(\frac{1}{n_0}\frac{m_0}{z_0^{n_0-1}}\right)^{s+1}\partial_p\log E_1\mathrm{d}p=\oint_\gamma\frac{(\partial_p E_1^{r+1})E_2^{s+1}}{(r+1)n_0^{s+1}}\mathrm{d}p=0, \tag{68}$$

where $\gamma:=\Sigma_{\alpha=0}^M\gamma_\alpha$. This proves that the identities (65) hold. □

By evaluating the integrals of the left-hand side we obtain the symmetry constraints in terms of differential equations for the free-energy function $F=\log\tau$.

Examples: For $r=s=0$, Eq. (68) reduces to (42), so that it implies

$$\sum_\alpha t_{\alpha 0}=0.$$

The cases $(r,s)=(1,0)$ and $(r,s)=(2,0)$ correspond to the Virasoro constraints induced by $\mathbb{V}_1$ and $\mathbb{V}_2$, respectively, and lead to the identities

$$\sum_{\alpha\in\{0\}\cup I}\partial_{\alpha,n_\alpha}F-\sum_{j\in J}\frac{n_0}{n_j}\left(\sum_{n-n'=n_j-1}nt_{jn}\partial_{j,n'-1}F+n_jt_{jn_j}t_{j0}+\frac{1}{2}\sum_{n+n'=n_j}nn't_{jn}t_{jn'}\right)=0,$$

$$\sum_{\alpha\in\{0\}\cup I}\partial_{\alpha,2n_\alpha}F+\sum_{j\in J}\left(\frac{n_0}{n_j}\right)^2\left(\sum_{n-n'-n''=2n_j-2}nt_{jn}(\partial_{j,n'-1}F)(\partial_{j,n''-1}F)+2\sum_{n-n'=2n_j-1}nt_{jn}t_{j0}\partial_{j,n'-1}F\right.$$

$$+\sum_{n+n'-n''=2n_j-1}nn't_{jn}t_{jn'}\partial_{j,n''-1}F+2n_jt_{j2n_j}t_{j0}^2+\sum_{n+n'=2n_j}nn't_{jn}t_{jn'}t_{j0}$$

$$\left.+\frac{1}{3}\sum_{n+n'+n''=2n_j}nn'n''t_{jn}t_{jn'}t_{jn''}\right)=0.$$

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On solutions of the two-component Camassa-Holm system

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Following the approach of [Chen *et al.*Lett. Math. Phys. **75**, 1–15 (2006)], we continue the study of the two-component Camassa-Holm system by using its relation with the first negative flow of the AKNS hierarchy. We obtain a more general class of particular solutions including the multisoliton ones. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2234729]

I. INTRODUCTION

The Camassa-Holm equation

$$u_t - u_{xxt} + \kappa u_x + 3uu_x - 2u_x u_{xx} - uu_{xxx} = 0 \tag{1.1}$$

is an integrable system that was derived in Refs. 5 and 6 as a shallow water wave equation. Here κ is a constant, $u=u(x,t)$ and u_x, u_t, etc., denote the partial derivatives of the function u with respect to the variables of the subscripts. Equation (1.1) first appeared in the work of Fuchssteiner and Fokas[10] when they studied the hereditary symmetries of soliton PDEs. Due to its physical background and its special features such as the existence of peakon solutions, the Camassa-Holm equation has drawn much attention among experts in soliton theory during the last ten years. See Refs. 1, 2, 9, 11, 12, and 14–17, and references therein.

Recently a two-component generalization of the Camassa-Holm equation, called the two-component Camassa-Holm (2-CH) system, was proposed by Liu and Zhang in Ref. 15 (see also Ref. 8). It takes the form

$$m_t + um_x + 2mu_x - \rho\rho_x = 0, \tag{1.2}$$

$$\rho_t + (\rho u)_x = 0, \tag{1.3}$$

where $m=u-u_{xx}+\frac{1}{2}\kappa$. This system is reduced to the Camassa-Holm equation when we set $\rho=0$. In Ref. 7, Chen *et al.* proved that the 2-CH system is related to the first negative flow of the AKNS hierarchy through an appropriate reciprocal transformation. By using this relation, they obtained multikink solutions and traveling peakon solutions of the 2-CH system. Some recent works on the properties of the 2-CH system can be found in Refs. 3, 4, 8, and 18.

In this note, we consider the special solutions of the 2-CH system. We obtain a more general class of peakon and multikink solutions and, in particular, its multisoliton solutions by using a relation between the 2-CH system and the first negative flow of the AKNS hierarchy. This relation was first found by Li[13] following the idea of Ref. 7 and is simpler than the one given there. In Sec. II, we explain the relations between the 2-CH system and the first negative flow of the AKNS hierarchy; in Sec. III, we derive the traveling wave solutions of the 2-CH system; in Sec. IV we construct its multikink and multisoliton solutions.

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II. RELATIONS TO THE FIRST NEGATIVE FLOW OF THE AKNS HIERARCHY

Let us first recall some results of Ref. 7. Since the parameter κ in (1.2) can be canceled through a Galilean transformation, we assume henceforth that κ vanishes unless otherwise stated. Then the 2-CH system (1.2), (1.3) is equivalent to the compatibility condition of the spectral problem

$$\phi_{xx} + \left(-\tfrac{1}{4} + m\lambda - \rho^2\lambda^2\right)\phi = 0, \tag{2.1}$$

$$\phi_t + \left(\frac{1}{2\lambda} + u\right)\phi_x - \frac{u_x}{2}\phi = 0 \tag{2.2}$$

with the spectral parameter λ. Assume $\rho \neq 0$ and denote $\varphi = \sqrt{\rho}\phi$. Through the reciprocal transformation

$$\mathrm{d}y = \rho \mathrm{d}x - \rho u \mathrm{d}t, \quad \mathrm{d}s = \mathrm{d}t, \tag{2.3}$$

the linear system (2.1), (2.2) is converted to

$$\varphi_{yy} + (Q + P\lambda - \lambda^2)\varphi = 0, \tag{2.4}$$

$$\varphi_s + \frac{\rho}{2\lambda}\varphi_y - \frac{\rho_y}{4\lambda}\varphi = 0 \tag{2.5}$$

with

$$P = \frac{m}{\rho^2}, \quad Q = -\frac{1}{4\rho^2} - \frac{\rho_{yy}}{2\rho} + \frac{\rho_y^2}{4\rho^2}. \tag{2.6}$$

The linear system (2.4), (2.5) is compatible iff there exists a function $f = f(y,s)$ satisfying the following:

$$P = f_y, \quad \rho = f_s, \tag{2.7}$$

$$\partial_y(f_y f_s) + \partial_s\left(\frac{f_y^2}{2} + \frac{f_{ys}^2 - 1}{2f_s^2} - \frac{f_{yys}}{f_s}\right) = 0. \tag{2.8}$$

Any function $f(y,s)$ satisfying Eq. (2.8) is called a *primary solution*[7] of the 2-CH system (1.2), (1.3). It plays a crucial role in constructing parametric solutions of the 2-CH system.

Theorem 2.1 (Ref. 7): *Let $f(y,s)$ be a solution of Eq.* (2.8), *then the functions $x(t,s)$, $u(t,s)$, $\rho(t,s)$ defined by*

$$x = f(t,s), \quad u = \frac{\partial x}{\partial t}, \quad \frac{1}{\rho} = \frac{\partial x}{\partial s} \tag{2.9}$$

give a parametric solution of the 2-CH system (1.2), (1.3).

The first negative flow of the AKNS hierarchy is equivalent to the compatibility condition of the spectral problem

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_y = \begin{pmatrix}\lambda & -q\\ r & -\lambda\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{2.10}$$

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_s = \frac{1}{4\lambda}\begin{pmatrix}a & b\\ c & -a\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{2.11}$$

where λ is the spectral parameter. This flow is expressed as

$$q_s = \tfrac{1}{2}b, \quad r_s = \tfrac{1}{2}c, \quad b_y = 2aq, \quad c_y = 2ar, \quad a_y + br + cq = 0. \tag{2.12}$$

The 2-CH system is related to it under the constraint

$$a^2 + bc = 1. \tag{2.13}$$

Theorem 2.2 (Ref. 7): *Suppose the functions q,r,a,b,c satisfy the system* (2.12), (2.13). *Then any solution $f(y,s)$ of*

$$2a = be^{-f} - ce^{f} \tag{2.14}$$

is a primary solution of the 2-CH system.

Theorem 2.3 (Ref. 7): *If $f(y,s)$ is a primary solution of the 2-CH system, then a solution (q,r,a,b,c) of the system* (2.12), (2.13) *is given by*

$$q = \frac{e^f}{2}\left(f_y + \frac{\varepsilon - f_{ys}}{f_s}\right), \quad r = \frac{e^{-f}}{2}\left(f_y - \frac{\varepsilon - f_{ys}}{f_s}\right),$$

$$b = 2q_s, \quad c = 2r_s, \quad a = \tfrac{1}{2}(be^{-f} - ce^{f}), \tag{2.15}$$

where $\varepsilon = 1$ or $\varepsilon = -1$.

The above-presented theorems establish an explicit relation between the 2-CH system and the first negative flow of the AKNS hierarchy satisfying (2.13). The following theorem, obtained by Li,[13] gives another relation between these two systems.

Theorem 2.4: *Let the functions $q(y,s)$, $r(y,s)$, $a(y,s)$, $b(y,s)$, $c(y,s)$ give a solution of the system* (2.12), (2.13). *If neither of q, q_s (respectively, r, r_s) vanishes at any point, then the function $f(y,s)$ defined by*

$$f = \ln q \quad (\textit{respectively}, \ f = \ln r) \tag{2.16}$$

is a primary solution of the 2-CH system.

Proof: The functions q,r,a,b,c satisfying the conditions of the theorem determine a compatible linear system (2.10), (2.11). Since the system (2.12), (2.13) is invariant under the transformation $(q,r,a,b,c) \mapsto (r,q,a,c,b)$, we only need to prove the case $f = \ln q$. For this, let

$$\varphi = e^{-f/2}\psi_1, \quad P = f_y = \frac{q_y}{q}, \quad \rho = f_s = \frac{q_s}{q}, \quad Q = \frac{1}{\rho^2}\left(\frac{1}{4}\rho_y^2 - \frac{1}{2}\rho\rho_{yy} - \frac{1}{4}\right). \tag{2.17}$$

With the help of (2.12), (2.13) we can simplify the expression of Q to the form

$$Q = \frac{1}{2}\frac{q_{yy}}{q} - \frac{3}{4}\frac{q_y^2}{q^2} + qr. \tag{2.18}$$

To prove the theorem, we need to check that (2.17) transforms the linear system (2.10), (2.11) to (2.4), (2.5). From (2.10), (2.11) it follows that

$$\varphi_s = -\frac{f_s}{2}e^{-f/2}\psi_1 + e^{-f/2}\left(\frac{a}{4\lambda}\psi_1 + \frac{b}{4\lambda}\psi_2\right) = \left(\left(-\frac{q_s}{2q} + \frac{a}{4\lambda}\right)\psi_1 + \frac{b}{4\lambda}\psi_2\right)e^{-f/2}, \tag{2.19}$$

$$\varphi_y = -\frac{f_y}{2}e^{-f/2}\psi_1 + e^{-f/2}(\lambda\psi_1 - q\psi_2) = \left(\left(-\frac{q_y}{2q} + \lambda\right)\psi_1 - q\psi_2\right)e^{-f/2}. \tag{2.20}$$

They yield the needed result

$$4\lambda\left(\varphi_s + \frac{\rho}{2\lambda}\varphi_y - \frac{\rho_y}{4\lambda}\varphi\right) = \left(-2\lambda\frac{q_s}{q} + a + 2\frac{q_s}{q}\left(-\frac{q_y}{2q} + \lambda\right) - \frac{q_{ys}}{q} + \frac{q_y q_s}{q^2}\right)\psi_1 e^{-f/2} + (b - 2q_s)\psi_2 e^{-f/2} = 0,$$

$$\varphi_{yy} = \left(-\frac{f_y}{2}\left(-\frac{q_y}{2q} + \lambda\right) - \frac{1}{2}\left(\frac{q_{yy}}{q} - \frac{q_y^2}{q^2}\right)\right)\psi_1 e^{-f/2} + \left(\frac{f_y}{2}q - q_y\right)\psi_2 e^{-f/2}$$
$$+ \left(-\frac{q_y}{2q} + \lambda\right)(\lambda\psi_1 - q\psi_2)e^{-f/2} - q(r\psi_1 - \lambda\psi_2)e^{-f/2}$$

$$= \left(\frac{q_y^2}{4q^2} - \frac{q_{yy}}{2q} + \frac{q_y^2}{2q^2} - qr - \frac{q_y}{q}\lambda + \lambda^2\right)\psi_1 e^{-f/2} = -(Q + \lambda P - \lambda^2)\varphi.$$

The theorem is proved. □

Note that the transformation $(q,r,a,b,c) \mapsto (-q,-r,a,-b,-c)$ keeps (2.12), (2.13) invariant, hence without loss of generality we can take q to be always positive. Then by using Theorem 2.3 and Theorem 2.4, the following two corollaries are easily obtained.

Corollary 2.5: Equation (2.8) *is invariant under the following Bäcklund transformations*:

$$\mathcal{Q}_\varepsilon : f \mapsto f + \ln\left(\frac{f_y f_s - f_{ys} + \varepsilon}{2f_s}\right), \quad \varepsilon = 1 \text{ or } \varepsilon = -1. \tag{2.21}$$

Corollary 2.6: For $\varepsilon = 1$ *or* $\varepsilon = -1$, *the system* (2.12), (2.13) *is invariant under the transformation*

$$q \mapsto \tilde{q} = q_y + \frac{q(\varepsilon q - q_{ys})}{2q_s}, \quad r \mapsto \tilde{r} = \frac{1}{2q_s}\left(-\varepsilon + \frac{q_{ys}}{q}\right),$$

$$b \mapsto \tilde{b} = 2\tilde{q}_s, \quad c \mapsto \tilde{c} = 2\tilde{r}_s, \quad a \mapsto \tilde{a} = \frac{\tilde{q}_s}{q} - q\tilde{r}_s. \tag{2.22}$$

Remark 2.7: The Bäcklund transformations (2.21) of Eq. (2.8) correspond to the relation $f = \ln q$ in Theorem 2.4. The Bäcklund transformations of (2.8) corresponding to $f = \ln r$ also take the form (2.21) modulo the trivial Bäcklund transformations: $f \mapsto -f$ and $f \mapsto f + c_0$ (c_0 is any constant).

Proposition 2.8: If $f(y,s)$ *is a primary solution of the 2-CH system*, *then the functions* q,r,a,b,c *defined by*

$$q = e^f, \quad r = \frac{1}{2}\left(\frac{f_y^2}{2} - f_{yy} - \frac{f_{yys}}{f_s} + \frac{f_{ys}^2 - 1}{2f_s^2}\right)e^{-f},$$

$$a = f_{ys} + f_y f_s, \quad b = 2f_s e^f, \quad c = \frac{1 - (f_{ys} + f_y f_s)^2}{2f_s}e^{-f} \tag{2.23}$$

satisfy (2.12), (2.13).

Proof: We only need to check $r_s = \frac{1}{2}c$. It holds true because

$$2r_s = \partial_s\left(\frac{f_y^2}{2} - \frac{f_{yys}}{f_s} + \frac{f_{ys}^2 - 1}{2f_s^2}\right)e^{-f} - f_{yys}e^{-f} - f_s\left(\frac{f_y^2}{2} - f_{yy} - \frac{f_{yys}}{f_s} + \frac{f_{ys}^2 - 1}{2f_s^2}\right)e^{-f}$$

$$=\left(\partial_y(f_y f_s)+\partial_s\left(\frac{f_y^2}{2}+\frac{f_{ys}^2-1}{2f_s^2}-\frac{f_{yys}}{f_s}\right)\right)e^{-f}+\left(-f_y f_{ys}-\frac{f_y^2 f_s}{2}-\frac{f_{ys}^2-1}{2f_s}\right)e^{-f}=c.$$

Here the last equality follows from Eq. (2.8). The proposition is proved. □

Theorem 2.4 together with Theorem 2.1 provides a simple method to construct parametric solutions of the 2-CH system. For example, the multikink solutions like those given in Ref. 7 can be found immediately. This method will be used in Sec. IV to get a more general class of solutions including multisoliton ones.

III. TRAVELING WAVE SOLUTIONS

In this section we keep the parameter κ in the 2-CH system (1.2), (1.3) to be an arbitrary constant. Suppose the 2-CH system has a solution of the form

$$u(x,t)=h(z),\quad \rho(x,t)=g(z)$$

where $z=x+vt$ with v being a constant. Then the 2-CH system (1.2), (1.3) is reduced to

$$v(h'-h''')+3hh'-2h'h''-hh'''+\kappa h'-gg'=0, \tag{3.1}$$

$$vg'+gh'+hg'=0. \tag{3.2}$$

Assume that there exists a constant θ such that as $z\to\pm\infty$,

$$h\to\theta-v,\quad \frac{\mathrm{d}^i h}{\mathrm{d}z^i}\to 0\quad \text{for } i=1,2,\ldots\ . \tag{3.3}$$

Then by integrating Eqs. (3.1), (3.2) we obtain

$$g=\frac{A}{h+v},\quad h'^2=\frac{A^2}{(h+v)^2}-\frac{C}{h+v}+B-(2v-\kappa)(h+v)+(h+v)^2. \tag{3.4}$$

Here A,B,C are constants and because of (3.3) we have

$$B=\frac{A^2}{\theta^2}+2(2v-\kappa)\theta-3\theta^2,\quad C=\frac{2A^2}{\theta}+(2v-\kappa)\theta^2-2\theta^3. \tag{3.5}$$

Denote $\tilde{h}=h+v-\theta$, $\alpha=v-\frac{1}{2}\kappa-2\theta$ and assume

$$\beta^2=\frac{A^2}{\theta^2}-(2v-\kappa)\theta+3\theta^2>0. \tag{3.6}$$

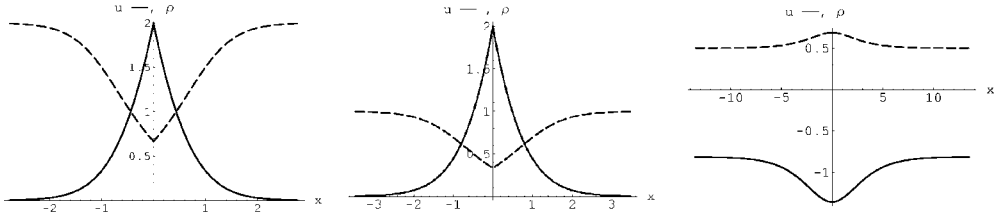
Then we rewrite the second equation in (3.4) to

$$\tilde{h}'^2=\frac{\tilde{h}^2(\tilde{h}^2-2\alpha\tilde{h}+\beta^2)}{(\tilde{h}+\theta)^2} \tag{3.7}$$

with

$$\alpha^2-\beta^2=\left(v-\theta-\frac{1}{2}\kappa\right)^2-\frac{A^2}{\theta^2}. \tag{3.8}$$

From (3.7) we get



(a) $x_0=0, u_0=2, \theta=1, v=1, \kappa=2, A=2, \alpha=-2, \beta=\sqrt{7}, \alpha^2-\beta^2<0$;
(b) $\varepsilon_1=\varepsilon_2=1, x_0=0, u_0=2, \theta=1, v=1, \kappa=2, A=1, \alpha=-2, \beta=2, \alpha^2-\beta^2=0$;
(c) $\varepsilon_3=1, \varepsilon_4=-1, \theta=2, v=45/16, \kappa=0, A=1, \alpha=-19/16, \beta=1, \alpha^2-\beta^2>0$.

FIG. 1. Traveling wave solution (3.10) at $t=0$.

$$\varepsilon z+c_\varepsilon=\begin{cases}\sinh^{-1}\left(\dfrac{\tilde{h}-\alpha}{\sqrt{\beta^2-\alpha^2}}\right)-\dfrac{\theta}{\beta}\sinh^{-1}\left(\dfrac{\beta^2/\tilde{h}-\alpha}{\sqrt{\beta^2-\alpha^2}}\right), & \alpha^2-\beta^2<0\\ \ln(\varepsilon_1(\tilde{h}-\alpha))-\dfrac{\theta}{\beta}\ln\left(\varepsilon_2\left(\dfrac{1}{\tilde{h}}-\dfrac{\alpha}{\beta^2}\right)\right), & \alpha^2-\beta^2=0\\ \cosh^{-1}\left(\varepsilon_3\dfrac{\tilde{h}-\alpha}{\sqrt{\alpha^2-\beta^2}}\right)-\dfrac{\theta}{\beta}\cosh^{-1}\left(\varepsilon_4\dfrac{\beta^2/\tilde{h}-\alpha}{\sqrt{\alpha^2-\beta^2}}\right), & \alpha^2-\beta^2>0.\end{cases} \tag{3.9}$$

Here $\varepsilon, \varepsilon_1, \ldots, \varepsilon_4=1$ or -1; c_{-1}, c_1 are constants.

Since $\tilde{h}$ tends to zero when $z\to\pm\infty$, formula (3.9) shows that

$$|h-(\theta-v)|\sim e^{-\gamma z}$$

for certain $\gamma>0$ as $z\to+\infty$. Thus any traveling wave solution of the 2-CH system satisfying the conditions (3.3), (3.6) decades exponentially at infinity. Whether $\tilde{h}$ in (3.9) can be expressed as an explicit function with respect to z depends on the value of θ/β. For example, the peakon solutions given in Ref. 7 correspond to the special cases $\beta=\theta$ and $\beta=2\theta$, respectively.

Example 3.1: We construct a continuous traveling wave solution of the 2-CH system as

$$x+vt-x_0=\begin{cases}F(u)-F(u_0), & x+vt-x_0<0\\ -F(u)+F(u_0), & x+vt-x_0>0,\end{cases}\qquad \rho=\frac{A}{u+v}. \tag{3.10}$$

Here $F(h)$ is the right-hand side of (3.9) with $\tilde{h}$ replaced by $h+v-\theta$. Formulas (3.10) yield peakon solutions of the 2-CH system whenever $\alpha^2-\beta^2\le 0$. In the case $\alpha^2-\beta^2>0$, let $\tilde{h}$ take its value on either interval

$$\left[\max\left\{\alpha+\sqrt{\alpha^2-\beta^2}, \frac{\beta^2}{\alpha+\sqrt{\alpha^2-\beta^2}}\right\}, 0\right)$$

for $\alpha<0, \varepsilon_3=1, \varepsilon_4=-1$, or

$$\left(0, \min\left\{\alpha+\sqrt{\alpha^2-\beta^2}, \frac{\beta^2}{\alpha+\sqrt{\alpha^2-\beta^2}}\right\}\right]$$

for $\alpha>0, \varepsilon_3=-1, \varepsilon_4=1$, then (3.10) gives a smooth solitary wave solution. See Fig. 1.

IV. MULTIKINK AND MULTISOLITON SOLUTIONS

In this section, we employ the results of Sec. II to look for particular solutions of the 2-CH system. To this end, let us first consider the particular solutions of the system (2.12), (2.13) by using the Darboux transformation of the associated linear system (2.10), (2.11).

In the notations

$$\psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\quad J=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad M=\lambda J+\begin{pmatrix}0 & -q\\ r & 0\end{pmatrix},\quad N=\begin{pmatrix}a & b\\ c & -a\end{pmatrix} \tag{4.1}$$

we can rewrite (2.10), (2.11) in matrix form. It is straightforward to verify the following.

Proposition 4.1: Suppose $\Lambda=\mathrm{diag}(\lambda_1,\lambda_2)$ *with* λ_1,λ_2 *being nonzero constants, and there is given a nondegenerate matrix* $H=(h_{ij})_{2\times 2}$ *satisfying*

$$H_y=JH\Lambda+\begin{pmatrix}0 & -q\\ r & 0\end{pmatrix}H,$$

$$H_s=\frac{1}{4}NH\Lambda^{-1}. \tag{4.2}$$

Let $S=H\Lambda H^{-1}$ *and* I *be the unit matrix of order two, then the linear system* (2.10), (2.11) *has the following Darboux transformation*:

$$\psi\mapsto\tilde{\psi}=(\lambda I-S)\psi,\quad M\mapsto\tilde{M}=M+[J,S],\quad N\mapsto\tilde{N}=SNS^{-1}, \tag{4.3}$$

where $[J,S]=JS-SJ$. *Particularly,* q,r *are transformed to*

$$\tilde{q}=q+\frac{2(\lambda_1-\lambda_2)h_{11}h_{12}}{\det H},\quad \tilde{r}=r-\frac{2(\lambda_1-\lambda_2)h_{21}h_{22}}{\det H}. \tag{4.4}$$

The two columns of H in the proposition are solutions of the linear systems (2.10), (2.11) with $\lambda=\lambda_1$ and $\lambda=\lambda_2$, respectively. Note that $\lambda I-S$ is nondegenerate for general λ. Given a fundamental solution matrix Ψ of the system (2.10), (2.11), then $\tilde{\Psi}=(\lambda I-S)\Psi$ is a fundamental solution matrix of this system with M,N replaced by $\tilde{M},\tilde{N}$. And from $\tilde{\Psi}$ we can find a solution $\tilde{H}$ of (4.2) corresponding to $\tilde{\Lambda}=\mathrm{diag}(\tilde{\lambda}_1,\tilde{\lambda}_2)$. In this way the Darboux transformation can be continued to generate a sequence of solutions of the system (2.12), (2.13) starting from an initial solution of it.

Let us take an initial solution of the system (2.12), (2.13) as

$$q^{(0)}=r^{(0)}=b^{(0)}=c^{(0)}=0,\quad a^{(0)}=1. \tag{4.5}$$

It gives a diagonal system (2.10), (2.11), which has a fundamental solution matrix

$$\Psi^{(0)}(\lambda)=\begin{pmatrix}e^{\omega(\lambda)} & 0\\ 0 & e^{-\omega(\lambda)}\end{pmatrix} \tag{4.6}$$

with $\omega(\lambda)=\lambda y+s/4\lambda$.

The Darboux transformation in Proposition 4.1 yields

$$\Lambda^{(i)}=\mathrm{diag}(-\lambda_i,\lambda_i),\quad \lambda_i>0, \tag{4.7}$$

$$H^{(i)}=\left(\Psi^{(i-1)}(-\lambda_i)\begin{pmatrix}1\\ 0\end{pmatrix},\Psi^{(i-1)}(\lambda_i)\begin{pmatrix}\alpha_i\\ 1\end{pmatrix}\right), \tag{4.8}$$

$$S^{(i)}=H^{(i)}\Lambda^{(i)}(H^{(i)})^{-1}, \tag{4.9}$$

$$\Psi^{(i)}(\lambda) = (\lambda I - S^{(i)})\Psi^{(i-1)}(\lambda), \tag{4.10}$$

where α_i's are nonzero constants for $i=1,2,3,\ldots$. The first formula in (4.4) takes the form

$$q^{(i)} = q^{(i-1)} - 4\lambda_i \frac{h_{12}^{(i)}}{h_{22}^{(i)}}. \tag{4.11}$$

By a direct calculation, we get the results of the first three steps as

$$q^{(1)} = -4\alpha_1\lambda_1 e^{2\omega(\lambda_1)}, \tag{4.12}$$

$$q^{(2)} = 4\frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}(\alpha_1\lambda_1 e^{2\omega(\lambda_1)} - \alpha_2\lambda_2 e^{2\omega(\lambda_2)}), \tag{4.13}$$

$$q^{(3)} = 4\frac{\lambda_1+\lambda_3}{\lambda_3-\lambda_1}\left(\frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}(-\alpha_1\lambda_1 e^{2\omega(\lambda_1)} + \alpha_2\lambda_2 e^{2\omega(\lambda_2)}) - \frac{\lambda_1+\lambda_3}{\lambda_3-\lambda_1}\alpha_3\lambda_3 e^{2\omega(\lambda_3)}\right). \tag{4.14}$$

Here we can always choose λ_j's pairwise distinct and α_j's with the right signs to make both $q^{(i)}, q_s^{(i)}$ identically positive. Due to Theorem 2.4 and Theorem 2.1 $q^{(i)}$ yield multikink solutions of the 2-CH system when $i \geq 2$. Multikink solutions of this kind were deduced in another way in Ref. 7.

Now let us look for particular solutions of the system (2.12), (2.13) that correspond to multisoliton solutions of the 2-CH system. For this, we denote

$$\xi = \frac{s}{\mu} + \nu y,$$

where μ, ν are constants and $\mu \neq 0$. It is easy to check that

$$q = e^{\xi}, \quad r = \frac{1}{4}(\nu^2 - \mu^2)e^{-\xi}, \quad a = \frac{\nu}{\mu}, \quad b = \frac{2}{\mu}e^{\xi}, \quad c = \frac{\mu^2-\nu^2}{2\mu}e^{-\xi} \tag{4.15}$$

satisfy (2.12), (2.13). The linear system (2.10), (2.11) determined by (4.15) has a fundamental solution matrix

$$\Psi(\lambda) = \begin{pmatrix} e^{\frac{\xi+\zeta(\lambda)}{2}} & e^{\frac{\xi-\zeta(\lambda)}{2}} \\ \frac{2\lambda-\nu-\sqrt{\Delta(\lambda)}}{2}e^{\frac{-\xi+\zeta(\lambda)}{2}} & \frac{2\lambda-\nu+\sqrt{\Delta(\lambda)}}{2}e^{-\frac{\xi+\zeta(\lambda)}{2}} \end{pmatrix} \tag{4.16}$$

with

$$\Delta(\lambda) = 4\lambda^2 - 4\nu\lambda + \mu^2, \quad \zeta(\lambda) = \sqrt{\Delta(\lambda)}\left(y - \frac{1}{2\mu\lambda}s\right).$$

We carry out the Darboux transformation in Proposition 4.1 as

$$\Lambda = \mathrm{diag}(\lambda_1, \lambda_2), \tag{4.17}$$

$$H = \left(\Psi(\lambda_1)\begin{pmatrix}1\\ \beta_1\end{pmatrix}, \Psi(\lambda_2)\begin{pmatrix}1\\ \beta_2\end{pmatrix}\right), \tag{4.18}$$

$$S = H\Lambda H^{-1}, \tag{4.19}$$

$$\tilde{\Psi}(\lambda) = (\lambda I - S)\Psi(\lambda), \tag{4.20}$$

$$\tilde{\Lambda} = \mathrm{diag}(\lambda_3, \lambda_4), \tag{4.21}$$

$$\tilde{H} = \left(\tilde{\Psi}(\lambda_3)\begin{pmatrix}1\\ \beta_3\end{pmatrix}, \tilde{\Psi}(\lambda_4)\begin{pmatrix}1\\ \beta_4\end{pmatrix}\right). \tag{4.22}$$

Here λ_i's are pairwise distinct and β_i's are constants. For the convenience of the straightforward computations, we introduce the following notation:

$$\Delta_j = \Delta(\lambda_j), \quad \zeta_j = \zeta(\lambda_j),$$

$$g_{1j} = e^{\zeta_j/2} + \beta_j e^{-\zeta_j/2}, \quad g_{2j} = \frac{2\lambda_j - \nu - \sqrt{\Delta_j}}{2} e^{\zeta_j/2} + \beta_j \frac{2\lambda_j - \nu + \sqrt{\Delta_j}}{2} e^{-\zeta_j/2},$$

$$K_j = \frac{g_{2j}}{g_{1j}} = \left(\lambda_j - \frac{\nu + \sqrt{\Delta_j}}{2}\right) + \frac{\beta_j \sqrt{\Delta_j}}{e^{\zeta_j} + \beta_j},$$

where $j = 1, 2, 3, 4$. By using the first formula in (4.4) we get

$$\tilde{q} = q + \frac{2(\lambda_1 - \lambda_2)}{\dfrac{h_{22}}{h_{12}} - \dfrac{h_{21}}{h_{11}}} = e^{\xi}\left(1 + \frac{2(\lambda_2 - \lambda_1)}{K_1 - K_2}\right), \tag{4.23}$$

$$\tilde{\tilde{q}} = \tilde{q} + \frac{2(\lambda_3 - \lambda_4)}{\dfrac{\tilde{h}_{22}}{\tilde{h}_{12}} - \dfrac{\tilde{h}_{21}}{\tilde{h}_{11}}} = e^{\xi}\left(1 + \frac{2(\lambda_2 - \lambda_1)}{K_1 - K_2} + \frac{2(\lambda_4 - \lambda_3)}{R_3 - R_4}\right), \tag{4.24}$$

where

$$R_j = \frac{(\lambda_2 - \lambda_1) g_{21} g_{22} g_{1j} + (\lambda_j - \lambda_2) g_{11} g_{22} g_{2j} - (\lambda_j - \lambda_1) g_{12} g_{21} g_{2j}}{(\lambda_j - \lambda_1) g_{11} g_{22} g_{1j} - (\lambda_j - \lambda_2) g_{12} g_{21} g_{1j} + (\lambda_1 - \lambda_2) g_{11} g_{12} g_{2j}}$$

$$= \frac{(\lambda_2 - \lambda_1) K_1 K_2 + (\lambda_j - \lambda_2) K_2 K_j + (\lambda_1 - \lambda_j) K_j K_1}{(\lambda_j - \lambda_1) K_2 + (\lambda_2 - \lambda_j) K_1 + (\lambda_1 - \lambda_2) K_j}, \quad j = 3, 4.$$

Due to Theorem 2.4 and Theorem 2.1, formulas (4.23), (4.24) yield solutions of the 2-CH system. When the parameters involved are chosen appropriately we can get multisoliton solutions.

Example 4.2: Formula (4.23) is written as

$$\tilde{q} = e^{\xi}\left(1 + \frac{2(\lambda_2 - \lambda_1)}{\lambda_1 - \lambda_2 - \dfrac{1}{2}(\sqrt{\Delta_1} - \sqrt{\Delta_2}) + \dfrac{\beta_1 \sqrt{\Delta_1}}{e^{\zeta_1} + \beta_1} - \dfrac{\beta_2 \sqrt{\Delta_2}}{e^{\zeta_2} + \beta_2}}\right). \tag{4.25}$$

By a careful analysis of the parameters, we know that

$$\nu > \mu > 0, \quad \lambda_1 > \lambda_2 > \frac{1}{2}(\nu + \sqrt{\nu^2 - \mu^2}), \quad \beta_1 < 0, \quad \beta_2 > 0 \tag{4.26}$$

is a sufficient condition for both $\tilde{q}$ and $\tilde{q}_s$ being identically positive. Under this condition formula (4.25) gives a 2-soliton solution of the 2-CH system. If we change (4.26) by setting $\beta_2 = 0$, then

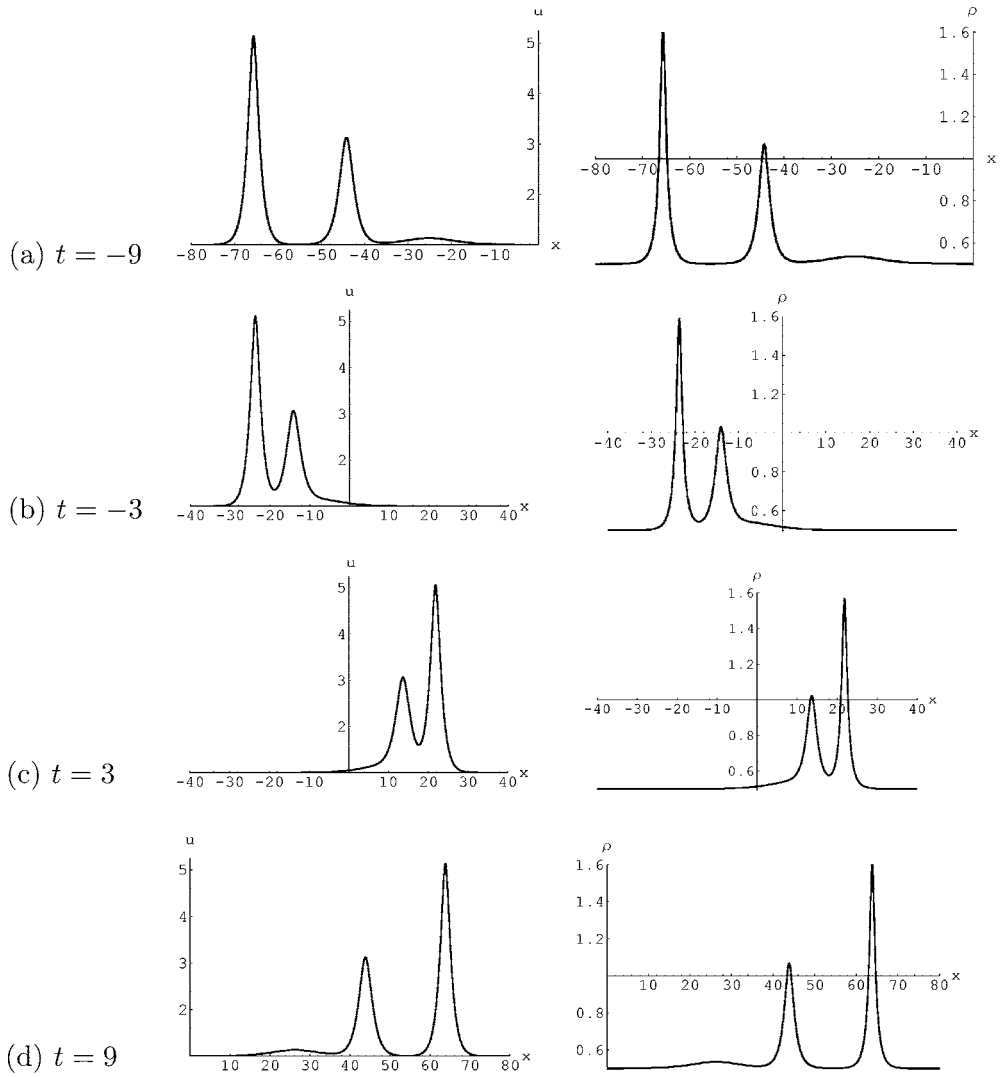


FIG. 2. 3-soliton solution of 2-CH by (4.24) with $\mu=1/2, \nu=1, \lambda_1=2, \lambda_2=1, \lambda_3=5, \lambda_4=3, \beta_1=-1, \beta_2=1, \beta_3=0, \beta_4=1$.

$$\tilde{q}|_{\beta_2=0} = e^{\xi}\left(1 + \frac{4(\lambda_2-\lambda_1)(e^{\zeta_1}+\beta_1)}{(2(\lambda_1-\lambda_2)-(\sqrt{\Delta_1}-\sqrt{\Delta_2}))e^{\zeta_1}+\beta_1(2(\lambda_1-\lambda_2)+\sqrt{\Delta_1}+\sqrt{\Delta_2})}\right) \tag{4.27}$$

gives a solitary wave solution of the 2-CH system. With a little further argument, we know that formula (4.27) yields a traveling wave solution of the 2-CH system. It corresponds to the case $\alpha^2-\beta^2>0$ of (3.9). This also implies that the solitary wave solutions given by (3.10) are smooth.

From formula (4.24) we can obtain 3-soliton or 4-soliton solutions of the 2-CH system whenever the parameters are appropriately chosen. See Fig. 2.

V. CONCLUSION

Theorem 2.1 and Theorem 2.4 provide a simple method to find parametric solutions of the 2-CH system (1.2), (1.3) from solutions of the first negative flow (2.12), (2.13) of the AKNS hierarchy. We have shown that apart from the peakon and multikink solutions, the 2-CH system also possesses n-soliton solutions for $n\leqslant 4$. We expect that for any positive integer n, the n-soliton

solution of the 2-CH system can also be obtained by using the Darboux transformation given in Proposition 4.1, with the seed solution (4.15), (4.16) and appropriately chosen parameters involved in the Darboux transformation.

ACKNOWLEDGMENTS

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Evaluation representations of quantum affine algebras at roots of unity

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The purpose of this paper is to compute the Drinfel'd polynomials for two types of evaluation representations of quantum affine algebras at roots of unity and construct those representations as the submodules of evaluation Schnizer modules. Moreover, we obtain the necessary and sufficient condition for that the two types of evaluation representations are isomorphic to each other. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2235047]

I. INTRODUCTION

For a generic q, let $U_q(\mathfrak{g})$ be the quantum algebra associated with a simple Lie algebra $\mathfrak{g}$ and $U_q(\tilde{\mathfrak{g}})$ be the nontwisted quantum loop algebra of $\mathfrak{g}$. It is known that every finite-dimensional irreducible $U_q(\mathfrak{g})$ (respectively, $U_q(\tilde{\mathfrak{g}})$) modules are highest-weight module and classified by highest weights. Moreover, there exists one to one correspondence from the set of their highest weights to $\mathbb{Z}_+^n$ (respectively, polynomials $\mathbb{C}_0[t]^n$), where $\mathbb{Z}_+ := \{0,1,2,\ldots\}$ (respectively, $\mathbb{C}_0[t] := \{P \in \mathbb{C}[t] | P$ is monic and $P(0) \neq 0\}$). The theory of finite-dimensional $U_q(\tilde{\mathfrak{g}})$-modules is introduced in Ref. 10. We denote the $U_q(\mathfrak{g})$ (respectively, $U_q(\tilde{\mathfrak{g}})$) module corresponding to $\lambda \in \mathbb{Z}_+^n$ (respectively, $\mathbf{P} \in \mathbb{C}_0[t]^n$) by $V_q(\lambda)$ (respectively, $V_q(\mathbf{P})$), where the polynomial $\mathbf{P}$ of $\tilde{V}_q(\mathbf{P})$ is called "Drinfel'd polynomial."

In the case $\mathfrak{g} = \mathfrak{sl}_{n+1}$, there exist $\mathbb{C}$-algebra homomorphisms $ev_{\mathbf{a}}^+$, $ev_{\mathbf{a}}^-$: $U_q(\widetilde{\mathfrak{sl}_{n+1}}) \to U_q(\mathfrak{sl}_{n+1})$ for $\mathbf{a} \in \mathbb{C}^\times$ (see Refs. 17 and 8). By using these homomorphisms, we can regard $V_q(\lambda)$ as a $U_q(\widetilde{\mathfrak{sl}_{n+1}})$-module, which are called "evaluation representations" and denoted by $V_q(\lambda)_{\mathbf{a}}^{\pm}$. By the classification theorem of finite-dimensional $U_q(\widetilde{\mathfrak{sl}_{n+1}})$-modules, (Ref. 10) there exists a unique polynomial $\mathbf{P}_{\mathbf{a}}^{\pm} \in \mathbb{C}_0[t]^n$ such that $V_q(\lambda)_{\mathbf{a}}^{\pm}$ is isomorphic to $\tilde{V}_q(\mathbf{P}_{\mathbf{a}}^{\pm})$ as a $U_q(\widetilde{\mathfrak{sl}_{n+1}})$-module. The Drinfel'd polynomials $\mathbf{P}_{\mathbf{a}}^{\pm}$ are computed by Chari and Pressley in Ref. 8. In this paper we shall consider evaluation representations at roots of unity.

Let ε be a primitive lth root of unity. The representation theory of quantum algebras at roots of unity is divided into two types. One is for $U_\varepsilon(\mathfrak{g})$, $U_\varepsilon(\tilde{\mathfrak{g}})$ defined by De Concini-Kac (=nonrestricted type) in Ref. 13 and the other is for $U_\varepsilon^{\mathrm{res}}(\mathfrak{g})$, $U_\varepsilon^{\mathrm{res}}(\tilde{\mathfrak{g}})$ defined by Lusztig (=restricted type) in Ref. 18.

$U_\varepsilon^{\mathrm{res}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{res}}(\tilde{\mathfrak{g}})$ has the $\mathbb{C}$-subalgebra $U_\varepsilon^{\mathrm{fin}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{fin}}(\tilde{\mathfrak{g}})$) which is called "small quantum algebra." By the tensor product theorem (see Refs. 18 and 11), in order to understand the representation theory of $U_\varepsilon^{\mathrm{res}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{res}}(\tilde{\mathfrak{g}})$), we may consider the one of $U_\varepsilon^{\mathrm{fin}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{fin}}(\tilde{\mathfrak{g}})$). Indeed, every finite-dimensional irreducible $U_\varepsilon^{\mathrm{fin}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{fin}}(\tilde{\mathfrak{g}})$) module is a highest-weight module and classified by highest weight. Moreover, there exists one to one correspondence from the set of their highest weights to $\mathbb{Z}_l^n$ (respectively, polynomials $\mathbb{C}_l[t]^n$), where $\mathbb{Z}_l := \{0,1,\cdots,l-1\}$ (respectively, $\mathbb{C}_l[t] := \{P \in \mathbb{C}_0[t] | P$ is not divisible by $(1-ct^l)$ for any $c \in \mathbb{C}^\times\}$). We denote the $U_\varepsilon^{\mathrm{fin}}(\mathfrak{g})$ (respectively, $U_\varepsilon^{\mathrm{fin}}(\tilde{\mathfrak{g}})$) module corresponding to $\lambda \in \mathbb{Z}_l^n$ (respectively, $\mathbf{P} \in \mathbb{C}_l[t]^n$) by $V_\varepsilon^{\mathrm{fin}}(\lambda)$ (respectively, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$).

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We also obtain the evaluation representations of $V_\varepsilon^{\mathrm{fin}}(\lambda)$ in the case of $U_\varepsilon^{\mathrm{fin}}(\widetilde{\mathfrak{sl}}_{n+1})$. We denote them by $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}}^{\pm}$. We can compute the Drinfel'd polynomials of $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}}^{\pm}$ by a similar method to Ref. 8 (see Theorem 4.13 in this paper). Moreover, for $\mathbf{a}_\pm \in \mathbb{C}^\times$, we shall show that $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_+}^{+}$ is isomorphic to $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_-}^{-}$ if and only if

$$\mathbf{a}_+ = \mathbf{a}_- \varepsilon^{2(\sum_{k=1}^{i-1}\lambda_k - \sum_{k=i+1}^{n}\lambda_{k+i})} \text{ for all } i \in \mathrm{supp}(\lambda), \tag{1.1}$$

where $\mathrm{supp}(\lambda) := \{1 \leqslant i \leqslant n \,|\, \lambda_i \neq 0\}$. If q is generic, condition (1.1) never occurs for $\#(\mathrm{supp}(\lambda)) > 1$. But, in this case, there exists $\lambda \in \mathbb{Z}_l^n$ which satisfies (1.1) for $\#(\mathrm{supp}(\lambda)) > 1$ (see Propositions 4.14, 4.15).

On the other hand, many finite-dimensional irreducible $U_\varepsilon(\mathfrak{g})$ (respectively, $U_\varepsilon(\widetilde{\mathfrak{g}})$) modules are no longer highest- or lowest-weight modules and they are characterized by several continuous parameters (see Refs. 13 and 6). For $\mathfrak{g} = \mathfrak{sl}_{n+1}$, such $U_\varepsilon(\mathfrak{sl}_{n+1})$-modules are constructed explicitly in Ref. 12, which are called "maximal cyclic representation." For an arbitrary simple Lie algebra $\mathfrak{g}$, Schnizer introduced an alternative construction of such $U_\varepsilon(\mathfrak{g})$-modules in Refs. 23 and 24, which we call "Schnizer modules."

By using the theory of the quantum algebra of restricted type, we obtain that every finite-dimensional irreducible "nilpotent" $U_\varepsilon(\mathfrak{sl}_{n+1})$-modules are highest-weight module and classified by highest weight (see Secs. III D and V B). Moreover, there exists one to one correspondence from the set of their highest weights to $\mathbb{Z}_l^n$ (respectively, $\mathbb{C}_l[t]^n$). We denote the $U_\varepsilon(\mathfrak{sl}_{n+1})$ (respectively, $U_\varepsilon(\widetilde{\mathfrak{sl}}_{n+1})$) module corresponding to $\lambda \in \mathbb{Z}_l^n$ (respectively, $\mathbf{P} \in \mathbb{C}_l[t]^n$) by $V_\varepsilon^{\mathrm{nil}}(\lambda)$ (respectively, $\widetilde{V}_\varepsilon^{\mathrm{nil}}(\mathbf{P})$). We also obtain the evaluation representations of $V_\varepsilon^{\mathrm{nil}}(\lambda)$, which are denoted by $V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}}^{\pm}$. The module $V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}}^{\pm}$ is regraded as a $U_\varepsilon^{\mathrm{fin}}(\widetilde{\mathfrak{sl}}_{n+1})$-module and $V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}}^{\pm}$ is isomorphic to $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}}^{\pm}$ as a $U_\varepsilon^{\mathrm{fin}}(\widetilde{\mathfrak{sl}}_{n+1})$-module (see Sec. V B). Therefore, for $\mathbf{a}_\pm \in \mathbb{C}^\times$, we obtain

$$V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_+}^{+} \text{ is isomorphic to } V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_-}^{-} \text{ if and only if (1.1) holds.} \tag{1.2}$$

We can also prove (1.2) without using the theory of the quantum algebra of restricted type. In Ref. 22, T.N. showed that one can construct $V_\varepsilon^{\mathrm{nil}}(\lambda)$ as the subrepresentation of a maximal cyclic representation by specializing their parameters properly for type A. Similarly, in Ref. 2, we found that we can construct $V_\varepsilon^{\mathrm{nil}}(\lambda)$ as a submodule of a Schnizer module if $\mathfrak{g} = A$, B, C, or D, and then we can construct $V_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}}^{\pm}$ as the submodule of evaluation of a Schnizer module. By using this fact, we can prove (1.2) (see Sec. V alternative proof of Proposition 5.11(b)).

The organization of this paper is as follows. In Sec. II, we introduce basic properties of quantum algebras for generic q. In Sec. III, we introduce quantum algebras at roots of unity of nonrestricted type and restricted type. Moreover, we prove the isomorphisn theorem of these algebras. In Sec. IV (respectively, Sec. V), we discuss the evaluation representations of restricted (respectively, nonrestricted) type.

II. QUANTUM ALGEBRAS (GENERIC CASE)

A. Notations

We fix the following notations (see Refs. 3 and 6). Let $\mathfrak{sl}_{n+1}$ be the finite-dimensional simple Lie algebra over $\mathbb{C}$ of type A_n and $\widetilde{\mathfrak{sl}}_{n+1} = \mathfrak{sl}_{n+1} \otimes \mathbb{C}[t, t^{-1}]$ be the loop algebra of $\mathfrak{sl}_{n+1}$. We set $I := \{1, 2, \ldots, n\}$ and $\widetilde{I} := I \sqcup \{0\}$. Let $(\mathfrak{a}_{i,j})_{i,j\in\widetilde{I}}$ be the generalized Cartan matrix of $\widetilde{\mathfrak{sl}}_{n+1}$, that is, $\mathfrak{a}_{i,i} = 2$, $\mathfrak{a}_{i,j} = -1$ if $|i-j| = 1$ or n, and $\mathfrak{a}_{i,j} = 0$ otherwise. Then $(\mathfrak{a}_{i,j})_{i,j\in I}$ is the Cartan matrix of $\mathfrak{sl}_{n+1}$. Let $\Pi := \{\alpha_i\}_{i\in I}$ (respectively, $\widetilde{\Pi} := \{\alpha_i\}_{i\in\widetilde{I}}$) be the set of the simple roots of $\mathfrak{sl}_{n+1}$ (respectively, $\widetilde{\mathfrak{sl}}_{n+1}$) and $\Pi^\vee := \{\alpha_i^\vee\}_{i\in I}$ (respectively, $\widetilde{\Pi}^\vee := \{\alpha_i^\vee\}_{i\in\widetilde{I}}$) be the set of the simple coroots of $\mathfrak{sl}_{n+1}$ (respectively, $\widetilde{\mathfrak{sl}}_{n+1}$). Let $\mathfrak{h}$ be the Cartan subalgebra of $\mathfrak{sl}_{n+1}$ and $\mathfrak{h}^*$ be the $\mathbb{C}$-dual space of $\mathfrak{h}$. Then $\Pi^\vee$ (respectively, Π) is a $\mathbb{C}$-basis of $\mathfrak{h}$ (respectively, $\mathfrak{h}^*$). We have a $\mathbb{C}$-bilinear map $\langle , \rangle : \mathfrak{h}^* \times \mathfrak{h} \to \mathbb{C}$ such that $\langle \alpha_j, \alpha_i^\vee \rangle = \mathfrak{a}_{i,j}$ for any $i, j \in I$. Define the root lattice $Q := \oplus_{i\in I}\mathbb{Z}\alpha_i$ (respectively,

the coroot lattice $Q^\vee := \oplus_{i\in I}\mathbb{Z}\alpha_i^\vee$) and the affine root lattice $\widetilde{Q} := \mathbb{Z}\alpha_0 \oplus Q$ (respectively, the affine coroot lattice $\widetilde{Q}^\vee := \mathbb{Z}\alpha_0^\vee \oplus Q^\vee$). For $i \in I$, we define the fundamental weights $\{\Lambda_i\}_{i\in I} \subset \mathfrak{h}^*$ by

$$\Lambda_i := \frac{1}{n+1}\left\{(n-i+1)\sum_{k=1}^{i} k\alpha_k + i\sum_{k=i+1}^{n}(n-k+1)\alpha_k\right\}. \tag{2.1}$$

Similarly, we define the fundamental coweights $\{\Lambda_i^\vee\}_{i\in I} \subset \mathfrak{h}$ by replacing α in Λ_i with $\alpha^\vee$. Then we have $\langle \Lambda_i, \alpha_j^\vee\rangle = \delta_{i,j}$ (respectively, $\langle \alpha_j, \Lambda_i^\vee\rangle = \delta_{i,j}$) for any $i,j \in I$. Define the weight lattice $P := \oplus_{i\in I}\mathbb{Z}\Lambda_i$ (respectively, the coweight lattice $P^\vee := \oplus_{i\in I}\mathbb{Z}\Lambda_i^\vee$) and define a symmetric bilinear form $(,)$: $\mathfrak{h}^* \times \mathfrak{h}^* \to \mathbb{C}$ determined by $(\alpha_i, \alpha_j) = \mathfrak{a}_{i,j}$ for any $i,j \in I$.

Let Δ (respectively, Δ_+) be the set of roots (respectively, positive roots) of $\widetilde{\mathfrak{sl}_{n+1}}$ and $\theta := \Sigma_{i\in I}\alpha_i$ be the highest root in Δ. We set $\delta := \alpha_0 + \theta$. Let $\widetilde{\Delta}$ be the affine root system of $\widetilde{\mathfrak{sl}_{n+1}}$. Then we have $\widetilde{\Delta} = \widetilde{\Delta}^{\mathrm{re}} \sqcup \widetilde{\Delta}^{\mathrm{im}}$, where

$$\widetilde{\Delta}^{\mathrm{re}} := \{\alpha + n\delta | \alpha \in \Delta, n \in \mathbb{Z}\}, \quad \Delta^{\mathrm{im}} := \{n\delta | n \in \mathbb{Z}^\times := (\mathbb{Z}\setminus\{0\})\},$$

and $\widetilde{\Delta} = \widetilde{\Delta}_+ \sqcup (-\widetilde{\Delta}_+)$, where

$$\widetilde{\Delta}_+ := \widetilde{\Delta}_+^{\mathrm{re}} \sqcup \widetilde{\Delta}_+^{\mathrm{im}}, \quad \widetilde{\Delta}_+^{\mathrm{re}} := \{\alpha + n\delta | \alpha \in \Delta, n \in \mathbb{N} := \{1,2,\dots\}\} \sqcup \Delta_+, \quad \widetilde{\Delta}_+^{\mathrm{im}} := \{n\delta | n \in \mathbb{N}\}.$$

Moreover, we set

$$\widetilde{\Delta}_+^{\mathrm{im}}(I) := I \times \widetilde{\Delta}_\times^{\mathrm{im}} = \{(i,n\delta) | i \in I, n \in \mathbb{N}\}, \quad \widetilde{\Delta}_+(I) := \widetilde{\Delta}_+^{\mathrm{re}} \sqcup \widetilde{\Delta}_+^{\mathrm{im}}(I),$$

$$\widetilde{\Delta}^{\mathrm{im}}(I) := \{(i,n\delta) | i \in I, n \in \mathbb{Z}^\times\}, \quad \widetilde{\Delta}(I) := \widetilde{\Delta}^{\mathrm{re}} \sqcup \widetilde{\Delta}^{\mathrm{im}}(I).$$

For $i \in \widetilde{I}$, let s_i be the simple reflection on $\mathfrak{h}^*$, that is, $s_i(\lambda) = \lambda - \langle \lambda, \alpha_i^\vee\rangle\alpha_i$ for any $\lambda \in \mathfrak{h}^*$. The affine Weyl group $\widetilde{\mathcal{W}}$ of $\widetilde{\mathfrak{sl}_{n+1}}$ (respectively, Weyl group $\mathcal{W}$ of $\mathfrak{sl}_{n+1}$) is generated by $\{s_i\}_{i\in\widetilde{I}}$ (respectively, $\{s_i\}_{i\in I}$). For $x \in \mathfrak{h}$, we define $t_x: \mathfrak{h}^* \to \mathfrak{h}^*$ by $t_x(\lambda) = \lambda - \langle \lambda, x\rangle\delta$ and set $T_{P^\vee} := \{t_x | x \in P^\vee\}$, $T_{Q^\vee} := \{t_x | x \in Q^\vee\}$. Consider the extended affine Weyl group $\hat{\mathcal{W}} := \mathcal{W}\widetilde{\times}T_{P^\vee}$, where the structure of the semi-direct product is given by $(s,t_x)(s',t_y) = (ss', t_{s'^{-1}x}t_y)$ for any $s,s' \in \mathcal{W}$, and $x,y \in P^\vee$. We set $\mathcal{T} := \{\tau: \widetilde{I} \to \widetilde{I}; \text{permutation} \,|\, \mathfrak{a}_{\tau(i),\tau(j)} = \mathfrak{a}_{i,j} \text{ for any } i,j \in \widetilde{I}\}$ and define the semi-direct product $\mathcal{T}\widetilde{\times}\widetilde{\mathcal{W}}$ by $\tau s_i \tau^{-1} = s_{\tau(i)}$ for $\tau \in \mathcal{T}$, $i \in \widetilde{I}$. It is known that $\hat{\mathcal{W}} \cong \mathcal{T}\widetilde{\times}\widetilde{\mathcal{W}}$ and $\widetilde{\mathcal{W}} \cong \mathcal{W}\widetilde{\times}T_{Q^\vee}$. In particular, the latter isomorphism is given by $s_i \mapsto (s_i, id_{\mathfrak{h}^*})$ for $i \in I$ and $s_0 \mapsto (s_\theta, t_{\theta^\vee})$, where $\theta^\vee := \Sigma_{i\in I}\alpha_i^\vee$. The length of an element $\tau w \in \hat{\mathcal{W}}$ ($\tau \in \mathcal{T}, w \in \widetilde{\mathcal{W}}$) is given by $l_{\widetilde{\mathcal{W}}}(\tau w) := l_{\widetilde{\mathcal{W}}}(w)$, where $l_{\widetilde{\mathcal{W}}}$ is the length function of $\widetilde{\mathcal{W}}$.

Let q be an indeterminate. For $r \in \mathbb{Z}$, $m \in \mathbb{N}$, we define q-integers and Gaussian binomial coefficients in the rational function field $\mathbb{C}(q)$ by

$$[r] := \frac{q^r - q^{-r}}{q - q^{-1}}, \quad [m]! := [m][m-1]\cdots[1], \quad \begin{bmatrix} r \\ m \end{bmatrix} := \frac{[r][r-1]\cdots[r-m+1]}{[1][2]\cdots[m]}.$$

Similarly, for $c \in \mathbb{C}$ ($c \neq 0, \pm 1$), we define

$$[r]_c := \frac{c^r - c^{-r}}{c - c^{-1}}, \quad [m]_c! := [m]_c[m-1]_c\cdots[1]_c, \quad \begin{bmatrix} r \\ m \end{bmatrix}_c := \frac{[r]_c[r-1]_c\cdots[r-m+1]_c}{[1]_c[2]_c\cdots[m]_c}.$$

We set $[0]! := [0]_c! := 1$.

B. Definitions

Definition 2.1: The quantum loop algebra $\widetilde{U}_q := U_q(\widetilde{\mathfrak{sl}_{n+1}})$ (respectively, the quantum algebra $U_q := U_q(\mathfrak{sl}_{n+1})$, the extended quantum algebra $U_q' := U_q'(\mathfrak{sl}_{n+1})$) is an associative $\mathbb{C}(q)$-algebra generated by $\{E_i, F_i, K_\mu | i \in \widetilde{I}$ (respectively, $i \in I$, $i \in I$), $\mu \in \widetilde{Q}$ (respectively, $\mu \in Q$, $\mu \in P$)$\}$ with the relations

$$K_\mu K_\nu = K_{\mu+\nu}, \quad K_0 = 1, \quad K_{\alpha_0} = K_\theta^{-1},$$

$$K_\mu E_j K_\mu^{-1} = q^{(\mu,\alpha_j)} E_j, \quad K_\mu F_j K_\mu^{-1} = q^{-(\mu,\alpha_j)} F_j,$$

$$E_i F_j - F_j E_i = \delta_{i,j} \frac{K_{\alpha_i} - K_{\alpha_i}^{-1}}{q - q^{-1}},$$

$$\sum_{r=0}^{1-\mathfrak{a}_{ij}} (-1)^r E_i^{(r)} E_j E_i^{(1-\mathfrak{a}_{i,j}-r)} = \sum_{r=0}^{1-\mathfrak{a}_{ij}} (-1)^r F_i^{(r)} F_j F_i^{(1-\mathfrak{a}_{i,j}-r)} = 0, \quad i \neq j,$$

where

$$E_i^{(r)} := \frac{1}{[r]!} E_i^r, \quad F_i^{(r)} := \frac{1}{[r]!} F_i^r \quad (r \in \mathbb{Z}_+ := \{0,1,2,\dots\}).$$

Let $\widetilde{U}_q^+$ (respectively, $\widetilde{U}_q^-$, $\widetilde{U}_q^0$) be the $\mathbb{C}(q)$-subalgebra of $\widetilde{U}_q$ generated by $\{E_i\}_{i\in\widetilde{I}}$ (respectively, $\{F_i\}_{i\in\widetilde{I}}$, $\{K_\mu\}_{\mu\in Q}$). Similarly, let U_q^+ (respectively, U_q^-, U_q^0) be the $\mathbb{C}(q)$-subalgebra of U_q generated by $\{E_i\}_{i\in I}$ (respectively, $\{F_i\}_{i\in I}$, $\{K_\mu\}_{\mu\in Q}$).

It is well known that $\widetilde{U}_q$ (respectively, U_q) have a Hopf algebra structure and its comultiplication is given by

$$\Delta(E_i) = E_i \otimes 1 + K_{\alpha_i} \otimes E_i, \quad \Delta(F_i) = F_i \otimes K_{\alpha_i}^{-1} + 1 \otimes F_i, \quad \Delta(K_\mu) = K_\mu \otimes K_\mu,$$

where $i \in \widetilde{I}$ (respectively, I), $\mu \in Q$.

We have a $\mathbb{C}$-algebra anti-automorphism $\Omega : \widetilde{U}_q \to \widetilde{U}_q$ and a $\mathbb{C}(q)$-algebra anti-automorphism $\Phi : \widetilde{U}_q \to \widetilde{U}_q$ such that

$$\Omega(q) = q^{-1}, \quad \Omega(E_i) = F_i, \quad \Omega(F_i) = E_i, \quad \Omega(K_\mu) = K_\mu^{-1}, \tag{2.2}$$

$$\Phi(E_i) = E_i, \quad \Phi(F_i) = F_i, \quad \Phi(K_\mu) = K_\mu^{-1}, \tag{2.3}$$

for $i \in \widetilde{I}$, $\mu \in Q$. Let T_i be the $\mathbb{C}(q)$-algebra automorphism of $\widetilde{U}_q$ introduced by Lusztig (Ref. 21, Chap. 37):

$$T_i(E_i^{(m)}) = (-1)^m q^{-m(m-1)} F_i^{(m)} K_{\alpha_i}^m, \quad T_i(F_i^{(m)}) = (-1)^m q^{m(m-1)} K_{\alpha_i}^{-1} E_i^{(m)},$$

$$T_i(E_j^{(m)}) = \sum_{r=0}^{-m\mathfrak{a}_{i,j}} (-1)^{r-m\mathfrak{a}_{i,j}} q^{-r} E_i^{(-m\mathfrak{a}_{i,j}-r)} E_j^{(m)} E_i^{(r)} \quad (i \neq j),$$

$$T_i(F_j^{(m)}) = \sum_{r=0}^{-m\mathfrak{a}_{i,j}} (-1)^{r-m\mathfrak{a}_{i,j}} q^{r} F_i^{(r)} F_j^{(m)} F_i^{(-m\mathfrak{a}_{i,j}-r)} \quad (i \neq j),$$

$$T_i(K_\mu) = K_{s_i(\mu)}, \tag{2.4}$$

where $i \in \widetilde{I}$, $m \in \mathbb{N}$, $\mu \in Q$. For $\tau \in \mathcal{T}$, we define $\widetilde{U}_q$-automorphism T_τ by

$$T_\tau(E_i) := E_{\tau(i)}, \quad T_\tau(F_i) := F_{\tau(i)}, \quad T_\tau(K_{\alpha_i}^{\pm 1}) := K_{\alpha_{\tau(i)}}^{\pm 1} \quad (i \in \widetilde{I}). \tag{2.5}$$

We obtain that

$$T_i^{-1} = \Phi T_i \Phi^{-1}, \quad T_i \Omega = \Omega T_i, \quad T_\tau \Omega = \Omega T_\tau. \tag{2.6}$$

Let $w \in \hat{\mathcal{W}}$ and $w = \tau s_{i_1} \cdots s_{i_m}$ ($\tau \in \mathcal{T}, i_1, \ldots, i_m \in \widetilde{I}, m \in \mathbb{N}$) be a reduced expression of w. Then $T_w := T_\tau T_{i_1} \cdots T_{i_m}$ is a well-defined $\widetilde{U}_q$-automorphism, that is, T_w does not depend on the choice of reduced expression of w.

C. Drinfel'd realization

It is known that $\widetilde{U}_q$ has another realization which is called Drinfel'd realization.

Definition 2.2 (Ref. 14): Let $\mathcal{D}_q$ be an associative $\mathbb{C}(q)$-algebra generated by $\{X_{i,r}^{\pm}, H_{i,s}, K_\mu | i \in I, r, s \in \mathbb{Z}, s \neq 0, \mu \in Q\}$ with the relations

$$K_\mu K_\nu = K_{\mu+\nu}, \quad K_0 = 1, \quad [K_\mu, H_{j,s}] = [H_{i,r}, H_{j,s}] = 0,$$

$$K_\mu X_{i,r}^{\pm} K_\mu^{-1} = q^{\pm(\mu,\alpha_i)} X_{i,r}^{\pm}, \quad [H_{j,s}, X_{i,r}^{\pm}] = \pm \frac{[r\mathfrak{a}_{i,j}]}{r} X_{i,r+s},$$

$$X_{i,r+1}^{\pm} X_{j,s}^{\pm} - q^{\pm \mathfrak{a}_{i,j}} X_{j,s}^{\pm} X_{i,r+1}^{\pm} = q^{\pm \mathfrak{a}_{i,j}} X_{i,r}^{\pm} X_{j,s+1}^{\pm} - X_{j,s+1}^{\pm} X_{i,r}^{\pm},$$

$$[X_{i,r}^{+}, X_{j,s}^{-}] = \delta_{i,j} \frac{\Psi_{i,r+s}^{+} - \Psi_{i,r+s}^{-}}{q - q^{-1}},$$

$$\sum_{\pi \in \mathcal{S}_m} \sum_{k=0}^{\mathbf{m}} (-1)^k \begin{bmatrix} \mathbf{m} \\ k \end{bmatrix} X_{i,r_{\pi}(1)}^{\pm} \cdots X_{i,r_{\pi(1)}}^{\pm} X_{j,s}^{\pm} X_{i,r_{\pi(k+1)}}^{\pm} \cdots X_{i,r_{\pi(\mathbf{m})}}^{\pm} = 0 \quad (i \neq j),$$

for $r_1, \ldots, r_{\mathbf{m}} \in \mathbb{Z}$, where $\mathbf{m} := 1 - \mathfrak{a}_{i,j}$, $\mathcal{S}_{\mathbf{m}}$ is the symmetric group on $\mathbf{m}$ letters, and $\Psi_{i,r}^{\pm}$ are determined by

$$\sum_{r=0}^{\infty} \Psi_{i,\pm r}^{\pm} u^{\pm r} := K_{\alpha_i}^{\pm 1} \exp\left(\pm (q - q^{-1}) \sum_{s=1}^{\infty} H_{i,\pm s} u^{\pm s} \right),$$

and $\Psi_{i,\pm r}^{\pm} := 0$ if $r < 0$.

For $i \in I$, let $t_{\Lambda_i^\vee} = \tau s_{j_1} \cdots s_{j_r}$ ($\tau \in \mathcal{T}, j_1, \cdots j_r \in \widetilde{I}$) be a reduced expression of $t_{\Lambda_i^\vee}$ (see Sec. II A). Then we set $T_{\Lambda_i^\vee} := T_\tau T_{j_1} \cdots T_{j_r}$.

Theorem 2.3 (Ref. 3): *There exists a $\mathbb{C}(q)$-algebra isomorphism $T: \mathcal{D}_q \to \widetilde{U}_q$ such that*

$$T(X_{i,r}^{+}) = (-1)^{ir} T_{\Lambda_i^\vee}^{-r}(E_i), \quad T(X_{i,r}^{-}) = (-1)^{ir} T_{\Lambda_i^\vee}^{r}(F_i) \quad (i \in I, r \in \mathbb{Z}). \tag{2.7}$$

In particular, by Ref. 3, Sec. 4 Remark and Ref. 8, Sec. 2.5, we obtain the inverse map of T:

$$T^{-1}(E_i) = X_{i,0}^{+}, \quad T^{-1}(F_i) = X_{i,0}^{-}, \quad T^{-1}(K_\mu) = K_\mu,$$

$$T^{-1}(E_0) = (-1)^{m+1} q^{n+1} [X_{n,0}^{-}, \cdots [X_{m+1,0}^{-}, [X_{i,0}^{-}, \cdots [X_{m-1,0}^{-} X_{m,1}^{-}]_{q^{-1}} \cdots]_{q^{-1}} \quad K_\theta^{-1},$$

$$T^{-1}(F_0) = (-1)^{m+n}[X^+_{n,0}, \cdots [X^+_{m+1,0}, [X^+_{1,0}, \cdots [X^+_{m-1,0}, X^+_{m,-1}]_{q^{-1}} \cdots]_{q^{-1}} \quad K_\theta, \tag{2.8}$$

for $m, i \in I$, where $[u,v]_{q^{\pm 1}} := uv - q^{\pm 1}vu$ for $u, v \in \widetilde{U}_q$ (T is independent of the choice of m). We identify $\mathcal{D}_q$ with $\widetilde{U}_q$ by this isomorphism T.

D. PBW basis

Let w_0 be the longest element in $\mathcal{W}$ and $w_0 = s_{i_1} \cdots s_{i_N}$ be a reduced expression of w_0. We set $\gamma_1 := \alpha_{i_1}$, $\gamma_2 := s_{i_1}(\alpha_{i_2}), \ldots, \gamma_N := s_{i_1} \cdots s_{i_{N-1}}(\alpha_{i_N})$. By the theory of the classical Lie algebra, we have $\Delta_+ = \{\gamma_1, \ldots, \gamma_N\}$. Define the root vectors in U_q by

$$\bar{E}_{\gamma_k} := T_{i_1}, \cdots T_{i_{k-1}}(E_{\alpha_{i_k}}), \quad \bar{F}_{\gamma_k} := \Omega(E_{\gamma_k}), \tag{2.9}$$

for $1 \leqslant k \leqslant N$, where $E_{\alpha_i} := E_i$, $F_{\alpha_i} := F_i (i \in I)$. We set

$$\mathbb{Z}_+^{\Delta_+} := \{c : \Delta_+ \to \mathbb{Z}_+; \text{map}\}, \quad B_q^0 := \{K_\mu | \mu \in Q\},$$

$$B_q^+ := \left\{ \prod_{\gamma \in \Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)} | c \in \mathbb{Z}_+^{\Delta_+} \right\}, \quad B_q^- := \Omega(B_q^+), \quad B_q := B_q^- B_q^0 B_q^+, \tag{2.10}$$

where $<$ means that the product is ordered by $\gamma_1 < \cdots < \gamma_N$.

Theorem 2.4 (Ref. 19, Sec. 1): *$B_q^\star$ (respectively, B_q) is a $\mathbb{C}(q)$-basis of $U_q^\star$ (respectively, U_q) for $\star \in \{-, 0, +\}$.*

The following notations and facts are given in Ref. 5. Let $\rho^\vee := \frac{1}{2}\sum_{\alpha \in \Delta_+} \alpha^\vee (\in P^\vee)$ and $t_{2\rho^\vee} = s_{j_1} \cdots s_{j_{\tilde{N}}}$ be a reduced expression of $t_{2\rho^\vee} (2\rho^\vee \in Q^\vee)$. Define the doubly infinite sequence $(\ldots, i_{-1}, i_0, i_1, \ldots)$ by $i_k := j_{k'}$ if $k \equiv k' \pmod{\tilde{N}}$ for all $k \in \mathbb{Z}$, $1 \leqslant k' \leqslant \tilde{N}$. We set

$$\beta_k := s_{i_0} s_{i_{-1}} \cdots s_{i_{k+1}}(\alpha_{i_k}) \quad (k \leqslant 0) \quad \beta_k := s_{i_1} s_{i_2} \cdots s_{i_{k-1}}(\alpha_{i_k}) \quad (k > 0).$$

Then we have $\widetilde{\Delta}_+^{\text{re}} = \{\beta_k\}_{k \in \mathbb{Z}}$. Define a total order on $\widetilde{\Delta}_+(I)$ by

$$\beta_0 < \beta_{-1} < \beta_{-2} < \cdots < (1, \delta) < \cdots < (n, \delta) < (1, 2\delta) < \cdots < (n, 2\delta) < \cdots < \beta_2 < \beta_1. \tag{2.11}$$

We set $E_{\alpha_i} := E_i$, $F_{\alpha_i} := F_i$ $(i \in \widetilde{I})$. Define the positive real root vectors in $\widetilde{U}_q$ by

$$E_{\beta_k} := T_{i_0}^{-1} T_{i_{-1}}^{-1} \cdots T_{i_{k+1}}^{-1}(E_{\alpha_{i_k}}) \quad (k \leqslant 0) \quad E_{\beta_k} := T_{i_1} T_{i_2} \cdots T_{i_{k-1}}(E_{\alpha_{i_k}}) \quad (k > 0), \tag{2.12}$$

and the positive imaginary root vectors $E_{(i,r\delta)}$ by

$$\exp\left((q - q^{-1}) \sum_{s=1}^{\infty} E_{(i,s\delta)} u^k \right) := 1 + \sum_{s=1}^{\infty} (q - q^{-1}) \hat{E}_{(i,s\delta)} u^k, \tag{2.13}$$

where $\hat{E}_{(i,s\delta)} := E_{-\alpha_i + s\delta} E_i - q^{-2} E_i E_{-\alpha_i + s\delta}$ for $i \in I$, $s \in \mathbb{N}$. Define the negative root vectors by $F_\beta := \Omega(E_\beta)$ for $\beta \in \widetilde{\Delta}_+(I)$. We set

$$\mathbb{Z}_+^{\widetilde{\Delta}_+(I)} := \{c : \widetilde{\Delta}_+(I) \to \mathbb{Z}_+; \text{map} | \, \#\{c(\beta) \neq 0\} < \infty\}, \quad \widetilde{B}_q^0 := \{K_\mu | \mu \in Q\},$$

$$\widetilde{B}_q^+ := \left\{ \prod_{\beta \in \widetilde{\Delta}_+(I)}^{<} E_\beta^{c(\beta)} | c \in \mathbb{Z}_+^{\widetilde{\Delta}_+(I)} \right\}, \quad \widetilde{B}_q^- := \Omega(\widetilde{B}_q^+), \quad \widetilde{B}_q := \widetilde{B}_q^- \widetilde{B}_q^0 \widetilde{B}_q^+, \tag{2.14}$$

where $<$ is the total order as in (2.11).

Theorem 2.5 (Ref. 4): $\widetilde{B}_q^{\star}$ (*respectively*, $\widetilde{B}_q$) *is a* $\mathbb{C}(q)$*-basis of* $\widetilde{U}_q^{\star}$ (*respectively*, $\widetilde{U}_q$) *for* $\star \in \{-,0,+\}$.

By Ref. 5 Lemma 1.5, we obtain

$$X_{i,r}^{+} = (-1)^{ir} E_{\alpha_i + r\delta} \quad (r \geqslant 0), \quad X_{i,r}^{+} = (-1)^{ir-1} F_{-\alpha_i - r\delta} K_i^{-1} \quad (r < 0),$$

$$X_{i,r}^{-} = (-1)^{ir-1} K_i E_{-\alpha_i + r\delta} \quad (r > 0), \quad X_{i,r}^{-} = (-1)^{ir} F_{\alpha_i - r\delta} \quad (r \leqslant 0),$$

$$H_{i,s} = (-1)^{is} E_{(i,s\delta)}, \quad \Psi_{i,s}^{+} = (-1)^{is}(q - q^{-1}) K_i \hat{E}_{(i,s\delta)}, \tag{2.15}$$

for $i \in I$, $r \in \mathbb{Z}$, $s \in \mathbb{N}$.

E. Evaluation homomorphisms

There exists a $\mathbb{C}(q)$-algebra homomorphism $U_q(\mathfrak{sl}_{n+1}) \to U_q(\widetilde{\mathfrak{sl}_{n+1}})$ such that

$$E_i \mapsto X_{i,0}^{+}, \quad F_i \mapsto X_{i,0}^{-}, \quad K_\mu \mapsto K_\mu, \tag{2.16}$$

for $i \in I$, $\mu \in Q$. Moreover, for $m \in I$, $0 \leqslant k \leqslant n-m$, there exists a $\mathbb{C}(q)$-algebra homomorphism $U_q(\widetilde{\mathfrak{sl}_{m+1}}) \to U_q(\widetilde{\mathfrak{sl}_{n+1}})$ such that

$$X_{i,r}^{\pm} \mapsto X_{i+k,r}^{\pm}, \quad H_{i,s} \mapsto H_{i+k,s}, \quad K_{\alpha_i} \mapsto K_{\alpha_{i+k}}, \tag{2.17}$$

for $1 \leqslant i \leqslant m$, r, $s \in \mathbb{Z}(s \neq 0)$. Hence we can regard any $U_q(\widetilde{\mathfrak{sl}_{n+1}})$-module as a $U_q(\mathfrak{sl}_{n+1})$-module and $U_q(\widetilde{\mathfrak{sl}_{m+1}})$-module. Let $U_q'(\mathfrak{sl}_{n+1})$ be the extended quantum algebra in Definition 2.1. By the following proposition, we can regard any $U_q'(\mathfrak{sl}_{n+1})$-module as a $U_q(\widetilde{\mathfrak{sl}_{n+1}})$- module.

Proposition 2.6: (Ref. 17, Sec. 2, Ref. 8, Proposition 3.4): For any $\mathbf{a} \in \mathbb{C}^{\times}$, *there exist* $\mathbb{C}(q)$*- algebra homomorphisms* $\mathrm{ev}_{\mathbf{a}}^{\pm}$: $U_q(\widetilde{\mathfrak{sl}_{n+1}}) \to U_q'(\mathfrak{sl}_{n+1})$ *such that*

$$\mathrm{ev}_{\mathbf{a}}^{\pm}(E_i) = E_i, \quad \mathrm{ev}_{\mathbf{a}}^{\pm}(F_i) = F_i, \quad \mathrm{ev}_{\mathbf{a}}^{\pm}(K_\mu) = K_\mu,$$

$$\mathrm{ev}_{\mathbf{a}}^{+}(E_0) = q^{-1}\mathbf{a} K_{\Lambda_1} K_{\Lambda_n}^{-1} [F_n, [F_{n-1}, \ldots, [F_2, F_1]_{q^{-1}} \cdots]_{q^{-1}},$$

$$\mathrm{ev}_{\mathbf{a}}^{-}(E_0) = q^{-1}\mathbf{a} K_{\Lambda_1}^{-1} K_{\Lambda_n} [F_1, [F_2, \ldots, [F_{n-1}, F_n]_{q^{-1}} \cdots]_{q^{-1}},$$

$$\mathrm{ev}_{\mathbf{a}}^{+}(F_0) = (-1)^{n-1} q^n \mathbf{a}^{-1} K_{\Lambda_1}^{-1} K_{\Lambda_n} [E_n, [E_{n-1}, \ldots, [E_2, E_1]_{q^{-1}} \cdots]_{q^{-1}},$$

$$\mathrm{ev}_{\mathbf{a}}^{-}(F_0) = (-1)^{n-1} q^n \mathbf{a}^{-1} K_{\Lambda_1} K_{\Lambda_n}^{-1} [E_1, [E_2, \ldots, [E_{n-1}, E_n]_{q^{-1}} \cdots]_{q^{-1}},$$

for $i \in I$ and $\mu \in P$. By (2.4) and (2.6), we obtain

$$\mathrm{ev}_{\mathbf{a}}^{+}(E_0) = q^{-n}\mathbf{a} K_{\Lambda_1} K_{\Lambda_n}^{-1} T_1^{-1} \cdots T_{n-1}^{-1}(F_n), \quad \mathrm{ev}_{\mathbf{a}}^{-}(E_0) = q^{-n}\mathbf{a} K_{\Lambda_1}^{-1} K_{\Lambda_n} T_n^{-1} \cdots T_2^{-1}(F_1),$$

$$\mathrm{ev}_{\mathbf{a}}^{+}(F_0) = q^{n}\mathbf{a}^{-1} K_{\Lambda_1}^{-1} K_{\Lambda_n} T_1^{-1} \cdots T_{n-1}^{-1}(E_n), \quad \mathrm{ev}_{\mathbf{a}}^{-}(F_0) = q^{n}\mathbf{a}^{-1} K_{\Lambda_1} K_{\Lambda_n}^{-1} T_n^{-1} \cdots T_2^{-1}(E_1). \tag{2.18}$$

III. QUANTUM ALGEBRAS AT ROOTS OF UNITY

In the rest of this paper, we fix the following notations. Let l be an odd integer greater than 2 and ε be a primitive lth root of unity. Moreover, we assume $\gcd(l, n+1) = 1$. By Ref. 6 Lemma 2.1 and Corollary 2.1, we obtain that $\gcd(l, n+1) = 1$ if and only if $\det([k\mathfrak{a}_{i,j}])_{i,j \in I} \neq 0$ for any $k \in \mathbb{Z}$ such that $k \not\equiv 0 \bmod l$.

A. Quantum algebras of nonrestricted type

Let $\mathcal{A}:=\mathbb{C}[q,q^{-1}]$ be the Laurent polynomial ring and $\widetilde{U}_{\mathcal{A}}$ (respectively, $U_{\mathcal{A}}$) be the $\mathcal{A}$-subalgebra of $\widetilde{U}_q$ (respectively, U_q) generated by $\{E_i,F_i,K_{\alpha_j},[K_{\alpha_j};0]\,|\,i\in\widetilde{I}$ (respectively, $i\in I),j\in I\}$, where $[K_{\alpha_j};0]:=(K_{\alpha_j}-K_{\alpha_j}^{-1})/(q-q^{-1})$ for $j\in I$. Let $\widetilde{U}_{\mathcal{A}}^+$ (respectively, $\widetilde{U}_{\mathcal{A}}^-$, $\widetilde{U}_{\mathcal{A}}^0$) be the $\mathcal{A}$-subalgebra of $\widetilde{U}_{\mathcal{A}}$ generated by $\{E_i\}_{i\in\widetilde{I}}$ (respectively, $\{F_i\}_{i\in\widetilde{I}}$, $\{K_{\alpha_i},[K_{\alpha_i};0]\}_{i\in I}$) and $U_{\mathcal{A}}^+$ (respectively, $U_{\mathcal{A}}^-$, $U_{\mathcal{A}}^0$) be the $\mathcal{A}$-subalgebra of $U_{\mathcal{A}}$ generated by $\{E_i\}_{i\in I}$ (respectively, $\{F_i\}_{i\in I}$, $\{K_{\alpha_i},[K_{\alpha_i};0]\}_{i\in I}$). We have triangular decompositions $\widetilde{U}_{\mathcal{A}}=\widetilde{U}_{\mathcal{A}}^-\widetilde{U}_{\mathcal{A}}^0\widetilde{U}_{\mathcal{A}}^+$ and $U_{\mathcal{A}}=U_{\mathcal{A}}^-U_{\mathcal{A}}^0U_{\mathcal{A}}^+$. We set

$$\widetilde{B}_{\mathcal{A}}^+:=\widetilde{B}_q^+,\quad \widetilde{B}_{\mathcal{A}}^-:=\widetilde{B}_q^-,\quad \widetilde{B}_{\mathcal{A}}^0:=\left\{\prod_{i\in I}K_{\alpha_i}^{\delta_i}[K_{\alpha_i};0]^{m_i}\,|\,m_i\in\mathbb{Z}_+,\delta_i=0\text{ or }1\right\},\quad \widetilde{B}_{\mathcal{A}}:=\widetilde{B}_{\mathcal{A}}^-\widetilde{B}_{\mathcal{A}}^0\widetilde{B}_{\mathcal{A}}^+,$$

$$B_{\mathcal{A}}^+:=B_q^+,\quad B_{\mathcal{A}}^-=B_q^-,\quad B_{\mathcal{A}}^0:=\left\{\prod_{i\in I}K_{\alpha_i}^{\delta_i}[K_{\alpha_i};0]^{m_i}\,|\,m_i\in\mathbb{Z}_+,\delta_i=0\text{ or }1\right\},\quad B_{\mathcal{A}}:=B_{\mathcal{A}}^-B_{\mathcal{A}}^0B_{\mathcal{A}}^+.$$

We have $T_i(\widetilde{U}_{\mathcal{A}})\subset\widetilde{U}_{\mathcal{A}}$ by (2.4) and $T_i^{-1}(\widetilde{U}_{\mathcal{A}})\subset\widetilde{U}_{\mathcal{A}}$ by (2.6) for $i\in I$. Hence, by (2.12) and (2.15), we have E_β, F_β, $X_{i,r}^\pm$, $H_{i,s}\in\widetilde{U}_{\mathcal{A}}$ for all $\beta\in\widetilde{\Delta}_+(I)$, $i\in I$, r, $s\in\mathbb{Z}(s\neq 0)$. Similarly, we obtain $T_i^{\pm 1}(U_{\mathcal{A}})\subset U_{\mathcal{A}}$ and $\bar{E}_\gamma$, $\bar{F}_\gamma\in U_{\mathcal{A}}$ for all $\gamma\in\Delta_+$ by (2.9). Thus we obtain $\widetilde{B}_{\mathcal{A}}^\star$, $\widetilde{B}_{\mathcal{A}}\subset\widetilde{U}_{\mathcal{A}}$ and $B_{\mathcal{A}}^\star$, $B_{\mathcal{A}}\subset U_{\mathcal{A}}$ ($\star\in\{-,0,+\}$).

Proposition 3.1: $B_{\mathcal{A}}^\star$ (respectively, $B_{\mathcal{A}}$) is an $\mathcal{A}$-basis of $U_{\mathcal{A}}^\star$ (respectively, $U_{\mathcal{A}}$) for $\star\in\{-,0,+\}$.

Proof: By Theorem 2.4, $B_q^\star$ (respectively, B_q) is $\mathbb{C}$-linearly independent in $U_q^\star$ (respectively, U_q) for $\star\in\{-,0,+\}$. Thus $B_{\mathcal{A}}^\star$ (respectively, $B_{\mathcal{A}}$) is $\mathcal{A}$-linearly independent in $U_{\mathcal{A}}^\star$ (respectively, $U_{\mathcal{A}}$). Let $V_{\mathcal{A}}^\star$ (respectively, $V_{\mathcal{A}}$) be the $\mathcal{A}$-subalgebra of $U_{\mathcal{A}}^\star$ (respectively, $U_{\mathcal{A}}$) generated by $B_{\mathcal{A}}^\star$ (respectively, $B_{\mathcal{A}}$). It is enough to prove that $U_{\mathcal{A}}^\star V_{\mathcal{A}}^\star\subset V_{\mathcal{A}}^\star$ for all $\star\in\{-,0,+\}$. Indeed, if we can prove this claim, then we obtain $U_{\mathcal{A}}^\star=V_{\mathcal{A}}^\star$ and $U_{\mathcal{A}}=U_{\mathcal{A}}^-U_{\mathcal{A}}^0U_{\mathcal{A}}^+=V_{\mathcal{A}}^-V_{\mathcal{A}}^0V_{\mathcal{A}}^+=V_{\mathcal{A}}$. So $U_{\mathcal{A}}^\star$ (respectively, $U_{\mathcal{A}}$) is generated by $B_{\mathcal{A}}^\star$ (respectively, $B_{\mathcal{A}}$) as $\mathcal{A}$-module.

By the following formula, we have $K_{\alpha_i}^{\pm 1}(\Pi_{i\in I}K_{\alpha_i}^{\delta_i}[K_{\alpha_i};0]^{m_i})\in V_{\mathcal{A}}^0$ for all $i\in I$, $m_i\in\mathbb{Z}_+$:

$$K_{\alpha_i}^2=K_{\alpha_i}(K_{\alpha_i}-K_{\alpha_i}^{-1})+1=(q-q^{-1})K_{\alpha_i}[K_{\alpha_i};0]+1\in V_{\mathcal{A}}^0,$$

$$K_{\alpha_i}^{-1}=K_{\alpha_i}-(K_{\alpha_i}-K_{\alpha_i}^{-1})=K_{\alpha_i}-(q-q^{-1})[K_{\alpha_i};0]\in V_{\mathcal{A}}^0.$$

Thus we obtain $U_{\mathcal{A}}^0V_{\mathcal{A}}^0\subset V_{\mathcal{A}}^0$. By Ref. 13 Lemma 1.7, we get the following formula: for α, $\beta\in\Delta_+$ such that $\beta>\alpha$,

$$E_\beta E_\alpha=\sum_{c\in\mathbb{Z}_+^{\Delta_+}}a_c\prod_{\gamma\in\Delta_+}^{<}E_\gamma^{c(\gamma)},$$

where $a_c\in\mathcal{A}$. So we obtain the case of $\star=+$. Similarly, by using the automorphism Ω (see (2.2)), we obtain the case of $\star=-$. □

By Ref. 6 Proposition 1.7(c), we obtain the following formula: for $\alpha,\beta\in\widetilde{\Delta}_+(I)$ such that $\beta>\alpha$,

$$E_\beta E_\alpha=q^{(\alpha,\beta)}E_\alpha E_\beta+\sum_{\alpha<\gamma_1<\cdots<\gamma_m<\beta}c_\gamma E_{\gamma_1}^{a_1}\cdots E_{\gamma_m}^{a_m},$$

where $c_\gamma\in\mathcal{A}$ for $\gamma=(\gamma_1,\ldots,\gamma_m)\in\widetilde{\Delta}_+(I)^m$. So, in a similar way to the proof of Proposition 3.1, we obtain the following proposition.

Proposition 3.2: $\widetilde{B}_{\mathcal{A}}^\star$ (respectively, $\widetilde{B}_{\mathcal{A}}$) is an $\mathcal{A}$-basis of $\widetilde{U}_{\mathcal{A}}^\star$ (respectively, $\widetilde{U}_{\mathcal{A}}$) for $\star\in\{-,0,+\}$.

Now we define the quantum algebras of nonrestricted type. We regard $\mathbb{C}$ as $\mathcal{A}$-module by $g(q).c := g(\varepsilon)c$ for $g(q) \in \mathcal{A}$, $c \in \mathbb{C}$ and denote it by $\mathbb{C}_\varepsilon$. We define

$$\widetilde{U}_\varepsilon := \widetilde{U}_\mathcal{A} \otimes_\mathcal{A} \mathbb{C}_\varepsilon \quad (\text{respectively, } U_\varepsilon := U_\mathcal{A} \otimes_\mathcal{A} \mathbb{C}_\varepsilon).$$

Then we call $\widetilde{U}_\varepsilon$ (respectively, U_ε) "quantum loop algebra (respectively, quantum algebra) of nonrestricted type (or De Concini-Kac type)" (see Refs. 6 and 13). For $\star \in \{-,0,+\}$, we set $\widetilde{U}^\star_\varepsilon := \widetilde{U}^\star_\mathcal{A} \otimes_\mathcal{A} 1$ (respectively, $U^\star_\varepsilon := U^\star_\mathcal{A} \otimes_\mathcal{A} 1$). We simply denote $u \otimes 1$ by u for $u \in \widetilde{U}_\mathcal{A}$ (respectively, $U_\mathcal{A}$).

Remark 3.3: (a) In Ref. 6 (respectively, Ref. 13), $\widetilde{U}_\varepsilon$ (respectively, U_ε) is defined by $\widetilde{U}_\varepsilon := \widetilde{U}_{\mathcal{A}^\varepsilon}/(q-\varepsilon)\widetilde{U}_{\mathcal{A}^\varepsilon}$ (respectively, $U_\varepsilon := U_\mathcal{A}/(q-\varepsilon)U_\mathcal{A}$), where $\mathcal{A}^\varepsilon := \{g(q) \in \mathbb{C}(q) \,|\, g(q) \text{ has no poles at } q=\varepsilon\} (\supset \mathcal{A})$ and $(q-\varepsilon)\widetilde{U}_{\mathcal{A}^\varepsilon}$ (respectively, $(q-\varepsilon)U_\mathcal{A}$) is the two-sided ideal of $\mathbb{C}$-algebra $\widetilde{U}_{\mathcal{A}^\varepsilon}$ (respectively, $U_\mathcal{A}$) generated by $(q-\varepsilon)$. But, by the universality of tensor product, we obtain

$$\widetilde{U}_\mathcal{A} \otimes_\mathcal{A} \mathbb{C}_\varepsilon \cong \widetilde{U}_\mathcal{A}/(q-\varepsilon)\widetilde{U}_\mathcal{A} \cong \widetilde{U}_{\mathcal{A}^\varepsilon}/(q-\varepsilon)\widetilde{U}_{\mathcal{A}^\varepsilon} \quad (\text{as } \mathbb{C}\text{-algebra}),$$

$$U_\mathcal{A} \otimes_\mathcal{A} \mathbb{C}_\varepsilon \cong U_\mathcal{A}/(q-\varepsilon)U_\mathcal{A} \cong U_{\mathcal{A}^\varepsilon}/(q-\varepsilon)U_{\mathcal{A}^\varepsilon} \quad (\text{as } \mathbb{C}\text{-algebra}).$$

(b) $\widetilde{U}_\varepsilon$ (respectively, U_ε) is the associative algebra over $\mathbb{C}$ on generators $\{E_i, F_i, K_\mu \,|\, i \in \widetilde{I}$ (respectively, I), $\mu \in \widetilde{Q}$ (respectively, $Q)\}$ and defining relations in Definition 2.1 replaced q by ε (see Ref. 6, Sec. 1.9 and Ref. 13, Sec. 1.5).

We set $\widetilde{B}^\star_\varepsilon := \widetilde{B}_\mathcal{A} \otimes_\mathcal{A} 1$ ($\star \in \{-,0,+\}$). Similarly, we define $\widetilde{B}_\varepsilon$, $B^\star_\varepsilon$ and B_ε.

Lemma 3.4: Let $\{v_j\}_j$ be an $\mathcal{A}$-basis in $\widetilde{U}_\mathcal{A}$ (respectively, $U_\mathcal{A}$). Then $\{v_j + (q-\varepsilon)\widetilde{U}_\mathcal{A}\}_j$ (respectively, $\{v_j + (q-\varepsilon)U_\mathcal{A}\}_j$) is a $\mathbb{C}$-basis of $\widetilde{U}_\mathcal{A}/(q-\varepsilon)\widetilde{U}_\mathcal{A}$ (respectively, $U_\mathcal{A}/(q-\varepsilon)U_\mathcal{A}$).

Proof: $\widetilde{U}_\mathcal{A}/(q-\varepsilon)\widetilde{U}_\mathcal{A}$ is spanned by $\{v_j + (q-\varepsilon)\widetilde{U}_\mathcal{A}\}_j$ as $\mathbb{C}$-vector space. So we shall prove that $\{v_j + (q-\varepsilon)\widetilde{U}_\mathcal{A}\}_j$ is linearly independent over $\mathbb{C}$ in $\widetilde{U}_\mathcal{A}/(q-\varepsilon)\widetilde{U}_\mathcal{A}$. We assume that $\Sigma_j c_j (v_j + (q-\varepsilon)\widetilde{U}_\mathcal{A}) = 0$ ($c_j \in \mathbb{C}, \#\{j \,|\, c_j \neq 0\} < \infty$). Then $\Sigma_j c_j v_j \in (q-\varepsilon)\widetilde{U}_\mathcal{A}$. Since $\widetilde{U}_\mathcal{A}$ is generated by $\{v_j\}_j$ as an $\mathcal{A}$-module, there exist $c_{j,m} \in \mathbb{C} (m \in \mathbb{Z}, \#\{(j,m) \,|\, c_{j,m} \neq 0\} < \infty)$ such that $\Sigma_j c_j v_j = (q-\varepsilon)\Sigma_{j,m} c_{j,m} q^m v_j$ in $\widetilde{U}_\mathcal{A}$. Since $\{v_j\}_j$ is linearly independent over $\mathcal{A}$ in $\widetilde{U}_\mathcal{A}$, we obtain $c_j = (q-\varepsilon)\Sigma_{m \in \mathbb{Z}} c_{j,m} q^m$ for all j. Therefore we obtain $c_j = c_{j,m} = 0$ for any j and m. Similarly, we obtain the case of $U_\mathcal{A}$. □

By this lemma, Proposition 3.2, and Remark 3.3(a), we obtain the following proposition.

Proposition 3.5: $\widetilde{B}^\star_\varepsilon$ (respectively, $\widetilde{B}_\varepsilon$) is a $\mathbb{C}$-basis of $\widetilde{U}^\star_\varepsilon$ (respectively, $\widetilde{U}_\varepsilon$) for $\star \in \{-,0,+\}$.

The classical case of this proposition is given in Ref. 13, Sec. 1.7.

Proposition 3.6: $B^\star_\varepsilon$ (respectively, B_ε) is a $\mathbb{C}$-basis of $U^\star_\varepsilon$ (respectively, U_ε) for $\star \in \{-,0,+\}$.

Let $Z(\widetilde{U}_\varepsilon)$ (respectively $Z(U_\varepsilon)$) be the center of $\widetilde{U}_\varepsilon$ (respectively, U_ε) and $\widetilde{Z}_0$ (respectively, Z_0) be the $\mathbb{C}$-subalgebra of $\widetilde{U}_\varepsilon$ (respectively, U_ε) generated by $\{E^l_\beta, F^l_\beta, E_{(i,sl\delta)}, F_{(i,sl\delta)}, K^l_\mu \,|\, \beta \in \widetilde{\Delta}^{\mathrm{re}}_+, i \in I, s \in \mathbb{N}, \mu \in Q\}$ (respectively, $\{\bar{E}^l_\gamma, \bar{F}^l_\gamma, K^l_\mu \,|\, \gamma \in \Delta_+, \mu \in Q\}$).

Proposition 3.7 (Ref. 6, Lemma 2.2, Proposition 2.3): $\widetilde{Z}_0 = Z(\widetilde{U})$.

Proposition 3.8 (Ref. 13, Corollary 3.1): $Z_0 \subset Z(U_\varepsilon)$.

For $m \in \mathbb{N}$, we set $\mathbb{Z}_m := \{0,1,\ldots,m-1\} \subset \mathbb{Z}_+$ and $Q_m := \oplus_{i \in I} \mathbb{Z}_m \alpha_i$. Let I_ε be the two-sided ideal of U_ε generated by $\{\bar{E}^l_\gamma, \bar{F}^l_\gamma, K^{2l}_\mu - 1 \,|\, \gamma \in \Delta_+, \mu \in Q\}$ and set $(U_\varepsilon/I_\varepsilon)^\star := \{u + I_\varepsilon \,|\, u \in U^\star_\varepsilon\} \subset U_\varepsilon/I_\varepsilon$ for $\star \in \{-,0,+\}$. We set

$$\mathbb{Z}_l^{\Delta_+} := \{c : \Delta_+ \to \mathbb{Z}_l; \text{map}\}, \quad B^+_l := \left\{ \left(\prod_{\gamma \in \Delta_+}^{<} \bar{E}_\gamma \right) + I_\varepsilon \,|\, \gamma \in \mathbb{Z}_l^{\Delta_+} \right\},$$

$$B^-_l := \Omega(B^+_l), \quad B^0_l := \{K_\mu + I_\varepsilon \,|\, \mu \in Q_{2l}\}, \quad B_l := B^-_l B^0_l B^+_l. \tag{3.1}$$

Proposition 3.9: $B_l^\star$ (*respectively*, B_l) *is a* $\mathbb{C}$*-basis of* $(U_\varepsilon/I_\varepsilon)^\star$ (*respectively*, $U_\varepsilon/I_\varepsilon$) *for* $\star \in \{-,0,+\}$.

Proof: We shall prove that B_l^+ is a $\mathbb{C}$-basis of $(U_\varepsilon/I_\varepsilon)^+$. We can also prove the other cases similarly. Let V_l^+ be the $\mathbb{C}$-subspace of $(U_\varepsilon/I_\varepsilon)^+$ spanned by B_l^+ and $u+I_\varepsilon \in (U_\varepsilon/I_\varepsilon)^+$. By Theorem 2.4, there exist $a_c \in \mathbb{C}(c \in \mathbb{Z}_+^{\Delta_+})$ such that $u+I_\varepsilon=\Sigma_{c\in\mathbb{Z}_+^{\Delta_+}} a_c \Pi_{\gamma\in\Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)}+I_\varepsilon$. If c is an element in $\mathbb{Z}_+^{\Delta_+}\backslash\mathbb{Z}_l^{\Delta_+}$, then there exists $\gamma_0 \in \Delta_+$ such that $c(\gamma_0) \geqslant l$. Then we have $\Pi_{\gamma\in\Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)} \in I_\varepsilon$. Hence $u+I_\varepsilon=\Sigma_{c\in\mathbb{Z}_l^{\Delta_+}} a_c \Pi_{\gamma\in\Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)}+I_\varepsilon \in V_l^+$. So $(U_\varepsilon/I_\varepsilon)^+$ is spanned by B_l^+.

Let $u=\Sigma_{c\in\mathbb{Z}_l^{\Delta_+}} a_c \Pi_{\gamma\in\Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)} \in U_\varepsilon^+(a_c \in \mathbb{C}, c \in \mathbb{Z}_l^{\Delta_+})$. We assume $u+I_\varepsilon=0$ in $(U_\varepsilon/I_\varepsilon)^+$. Then we have $u \in I_\varepsilon \cap U_\varepsilon^+$. By Theorem 2.4, we obtain

$$I_\varepsilon \cap U_\varepsilon^+ = \left(\sum_{\gamma\in\Delta_+} U_\varepsilon \bar{E}_\gamma^l + \sum_{\mu\in Q} U_\varepsilon (K_\mu^{2l}-1) + \sum_{\gamma\in\Delta_+} U_\varepsilon \bar{F}_\gamma^l \right) \cap U_\varepsilon^+ = \sum_{\gamma\in\Delta_+} U_\varepsilon^+ \bar{E}_\gamma^l.$$

Hence there exists $u'=\Sigma_{c'\in\mathbb{Z}_+^{\Delta_+}} b_{c'} \Pi_{\gamma\in\Delta_+}^{<} \bar{E}_\beta^{c'(\beta)} \in U_\varepsilon^+(b_{c'} \in \mathbb{C}, c' \in \mathbb{Z}_l^{\Delta_+})$ such that $u=\Sigma_{\gamma\in\Delta_+} u' \bar{E}_\gamma^l$. Since $\bar{E}_\gamma^l$ is a central element in U_ε (see Proposition 3.8), we have

$$\sum_{\gamma\in\Delta_+} u' \bar{E}_\gamma^l \in \sum_{c\in\mathbb{Z}_+^{\Delta_+}\backslash\mathbb{Z}_l^{\Delta_+}} \mathbb{C}\left(\prod_{\gamma\in\Delta_+}^{<} \bar{E}_\gamma^{c(\gamma)} \right).$$

Thus, by Proposition 3.6, we get $a_c=0$ for any $c \in \mathbb{Z}_l^{\Delta_+}$. Therefore B_l^+ is linearly independent in $(U_\varepsilon/I_\varepsilon)^+$.

Let $\tilde{I}_\varepsilon$ be the two-sided ideal of $\tilde{U}_\varepsilon$ generated by $\{E_\beta^l, F_\beta^l, E_{(i,sl\delta)}, F_{(i,sl\delta)}, K_\mu^{2l}-1 \,|\, \beta \in \tilde{\Delta}_+^{\mathrm{re}}, i \in I, s \in \mathbb{N}, \mu \in Q\}$ and set $(\tilde{U}_\varepsilon/\tilde{I}_\varepsilon)^\star := \{u+\tilde{I}_\varepsilon \,|\, u \in \tilde{U}_\varepsilon^\star\}$ for $\star \in \{-,0,+\}$. We define

$$\mathbb{Z}_l^{\tilde{\Delta}_+(I)} := \{c \in \mathbb{Z}_+^{\tilde{\Delta}_+(I)} | c(\beta) \in \mathbb{Z}_l, c((i,sl\delta))=0 (\beta \in \tilde{\Delta}_+^{\mathrm{re}}, i \in I, s \in \mathbb{N})\},$$

$$\tilde{B}_l^+ := \left\{ \prod_{\beta\in\tilde{\Delta}_+(I)}^{<} E_\beta^{c(\beta)} + \tilde{I}_\varepsilon | c \in \mathbb{Z}_l^{\tilde{\Delta}_+(I)} \right\}, \quad \tilde{B}_l^- := \Omega(\tilde{B}_l^+),$$

$$\tilde{B}_l^0 := \{K_\mu + \tilde{I}_\varepsilon | \mu \in Q_{2l}\}, \quad \tilde{B}_l := \tilde{B}_l^- \tilde{B}_l^0 \tilde{B}_l^+. \tag{3.2}$$

Then, by Theorem 2.5 and Proposition 3.7, we obtain the following proposition.

Proposition 3.10: $\tilde{B}_l^\star$ (*respectively*, $\tilde{B}_l$) *is a* $\mathbb{C}$*-basis of* $(\tilde{U}_\varepsilon/\tilde{I}_\varepsilon)^\star$ (*respectively*, $(\tilde{U}_\varepsilon/\tilde{I}_\varepsilon)$) *for* $\star \in \{-,0,+\}$.

The proof of this proposition is similar to the one of Proposition 3.9.

B. Quantum algebras of restricted type

Let $\tilde{U}_{\mathcal{A}}^{\mathrm{res}}$ (respectively, $U_{\mathcal{A}}^{\mathrm{res}}$) be the $\mathcal{A}$-subalgebra of $\tilde{U}_q$ (respectively, U_q) generated by $\{E_i^{(m)}, F_i^{(m)}, K_\mu | i \in \tilde{I}$ (respectively, I), $m \in \mathbb{N}, \mu \in Q\}$. We set

$$\begin{bmatrix} K_{\alpha_i}; r \\ m \end{bmatrix} := \prod_{s=1}^{m} \frac{K_{\alpha_i} q^{r-s+1} - K_{\alpha_i}^{-1} q^{-r+s-1}}{q^s - q^{-s}},$$

for $m \in \mathbb{N}$, $r \in \mathbb{Z}$, $i \in I$. It is known that $\begin{bmatrix} K_{\alpha_i}; r \\ m \end{bmatrix} \in U_{\mathcal{A}}^{\mathrm{res}}$ (see Ref. 9, Sec. 9.3A). By (2.4) and (2.6), we have $T_i^{\pm 1}(\tilde{U}_{\mathcal{A}}^{\mathrm{res}}) \subset \tilde{U}_{\mathcal{A}}^{\mathrm{res}}$ (respectively, $T_{\mathbf{i}}^{\pm 1}(U_{\mathcal{A}}^{\mathrm{res}}) \subset U_{\mathcal{A}}^{\mathrm{res}}$) for any $i \in \tilde{I}$ (respectively, I). Hence we obtain $E_\beta, F_\beta, X_{i,r}^\pm, H_{i,s} \in \tilde{U}_{\mathcal{A}}^{\mathrm{res}}$ for $\beta \in \tilde{\Delta}_+(I)$, $i \in I$, $r, s \in \mathbb{Z}(s \neq 0)$ by (2.12) and (2.15). Similarly, we obtain $\bar{E}_\gamma, \bar{F}_\gamma \in U_{\mathcal{A}}^{\mathrm{res}}$ for any $\gamma \in \Delta_+$ by (2.9). We define

$$\widetilde{U}_{\varepsilon}^{\mathrm{res}} := \widetilde{U}_{\mathcal{A}}^{\mathrm{res}} \otimes_{\mathcal{A}} \mathbb{C}_{\varepsilon} \quad (\text{respectively, } U_{\varepsilon}^{\mathrm{res}} := U_{\mathcal{A}}^{\mathrm{res}} \otimes_{\mathcal{A}} \mathbb{C}_{\varepsilon}).$$

Then we call $\widetilde{U}_{\varepsilon}^{\mathrm{res}}$ (respectively, $U_{\varepsilon}^{\mathrm{res}}$) "quantum loop algebra (respectively, quantum algebra) of restricted type (or Lusztig type)" (see Refs. 18 and 11). We denote $E_{\beta} \otimes 1$ by e_{β} for $\beta \in \widetilde{\Delta}_{+}(I)$. Similarly, we set $f_{\beta} := F_{\beta} \otimes 1$, $k_{\mu} := K_{\mu} \otimes 1$, $x_{i,r} := X_{i,r} \otimes 1, \ldots$. Moreover, we set

$$\dot{e}_{\beta} := e_{\beta}, \quad \dot{f}_{\beta} := \Omega(\dot{e}_{\beta}), \quad \dot{e}_{(i,m\delta)} := \left(\frac{1}{[m]} E_{(i,m\delta)} \right) \otimes 1, \quad \dot{f}_{(i,m\delta)} := \Omega(\dot{e}_{(i,m\delta)}),$$

$$\dot{h}_{i,s} := \left(\frac{1}{[s]} H_{i,s} \right) \otimes 1, \quad \begin{bmatrix} k_{\alpha_i}; r \\ m \end{bmatrix} := \begin{bmatrix} K_{\alpha_i}; r \\ m \end{bmatrix} \otimes 1,$$

for $\beta \in \widetilde{\Delta}_{+}^{\mathrm{re}}$, $i \in I$, $m \in \mathbb{N}$, $r, s \in \mathbb{Z}(s \neq 0)$. Let $(\widetilde{U}_{\varepsilon}^{\mathrm{res}})^{\pm}$ (respectively, $(\widetilde{U}_{\varepsilon}^{\mathrm{res}})^{0}$) be the $\mathbb{C}$-subalgebra of $\widetilde{U}_{\varepsilon}^{\mathrm{res}}$ generated by $\{(x_{i,r}^{\pm})^{(m)} | i \in I, r \in \mathbb{Z}, m \in \mathbb{N}\}$ (respectively, $\left\{ k_{\mu}, \begin{bmatrix} k_{\alpha_i}; r \\ m \end{bmatrix}, \dot{h}_{i,s} \middle| \mu \in Q, i \in I, r \in \mathbb{Z}, m \in \mathbb{N}, s \in \mathbb{Z}^{\times} \right\}$) and $(U_{\varepsilon}^{\mathrm{res}})^{+}$ (respectively, $(U_{\varepsilon}^{\mathrm{res}})^{-}, (U_{\varepsilon}^{\mathrm{res}})^{0}$) be the $\mathbb{C}$-subalgebra of $U_{\varepsilon}^{\mathrm{res}}$ generated by $\{e_i^{(m)} | i \in I, m \in \mathbb{N}\}$ (respectively, $\{f_i^{(m)} | i \in I, m \in \mathbb{N}\}$, $\left\{ k_{\mu}, \begin{bmatrix} k_{\alpha_i}; r \\ m \end{bmatrix} \middle| \mu \in Q, i \in I, r \in \mathbb{Z}, m \in \mathbb{N} \right\}$). We obtain that $\begin{bmatrix} k_{\alpha_i}; r \\ m \end{bmatrix}$ is generated by $\left\{ k_{\alpha_i}, \begin{bmatrix} k_{\alpha_i}; 0 \\ l \end{bmatrix} \right\}$ for $i \in I$, $r \in \mathbb{Z}$, $m \in \mathbb{N}$. It is known that $U_{\varepsilon}^{\mathrm{res}}$ has the triangular decomposition, that is, the multiplication map defines an isomorphism of $\mathbb{C}$-vector spaces:

$$(U_{\varepsilon}^{\mathrm{res}})^{-} \otimes (U_{\varepsilon}^{\mathrm{res}})^{0} \otimes (U_{\varepsilon}^{\mathrm{res}})^{+} \xrightarrow{\sim} U_{\varepsilon}^{\mathrm{res}} \quad (u^{-} \otimes u^{0} \otimes u^{+} \mapsto u^{-} u^{0} u^{+}). \tag{3.3}$$

Moreover, by Ref. 11, Proposition 6.1, we have

$$(\widetilde{U}_{\varepsilon}^{\mathrm{res}})^{-} \otimes (\widetilde{U}_{\varepsilon}^{\mathrm{res}})^{0} \otimes (\widetilde{U}_{\varepsilon}^{\mathrm{res}})^{+} \xrightarrow{\sim} \widetilde{U}_{\varepsilon}^{\mathrm{res}} \quad (\widetilde{u}^{-} \otimes \widetilde{u}^{0} \otimes \widetilde{u}^{+} \mapsto \widetilde{u}^{-} \widetilde{u}^{0} \widetilde{u}^{-}). \tag{3.4}$$

We set

$$(\widetilde{B}_{\varepsilon}^{\mathrm{res}}) := \left\{ \prod_{\beta \in \widetilde{\Delta}_{+}(I)}^{<} \dot{e}_{\beta}^{(c(\beta))} | c \in \mathbb{Z}_{l}^{\widetilde{\Delta}_{+}(I)} \right\}, \quad (\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{-} := \Omega((\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{+}),$$

$$(\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{0} := \left\{ \prod_{i \in I} k_{\alpha_i}^{\delta_i} \begin{bmatrix} k_{\alpha_i}; 0 \\ m_i \end{bmatrix} | m_i \in \mathbb{N}, \delta_i = 0 \text{ or } 1 \right\}, \quad \widetilde{B}_{\varepsilon}^{\mathrm{res}} := (\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{-} (\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{0} (\widetilde{B}_{\varepsilon}^{\mathrm{res}})^{+},$$

(see (2.14)). By Ref. 16, we obtain the following theorem.

Theorem 3.11: *$\widetilde{B}_{\varepsilon}^{\mathrm{res}}$ is a $\mathbb{C}$-basis of $\widetilde{U}_{\varepsilon}^{\mathrm{res}}$.*

Proof: By Ref. 16, we obtain a PBW basis of $\widetilde{U}_{\mathcal{A}}^{\mathrm{res}}$. Since any $\mathcal{A}$-basis of $\widetilde{U}_{\mathcal{A}}^{\mathrm{res}}$ becomes $\mathbb{C}$-basis of $\widetilde{U}_{\mathcal{A}}^{\mathrm{res}} \otimes_{\mathcal{A}} \mathbb{C}_{\varepsilon}$ canonically (see Lemma 3.4), we obtain this theorem. □

C. Small quantum algebras

Let $\widetilde{U}_{\varepsilon}^{\mathrm{fin}}$ (respectively, $U_{\varepsilon}^{\mathrm{fin}}$) be the $\mathbb{C}$-subalgebra of $\widetilde{U}_{\varepsilon}^{\mathrm{res}}$ (respectively, $U_{\varepsilon}^{\mathrm{res}}$) generated by $\{e_i, f_i, k_{\mu} | i \in \widetilde{I}$ (respectively, I), $\mu \in Q\}$). Then we call $\widetilde{U}_{\varepsilon}^{\mathrm{fin}}$ (respectively, $U_{\varepsilon}^{\mathrm{fin}}$) "small quantum loop algebra (respectively, small quantum algebra)." Let $\mathcal{D}_{\varepsilon}^{\mathrm{fin}}$ be the $\mathbb{C}$-subalgebra of $\widetilde{U}_{\varepsilon}^{\mathrm{res}}$ generated by $\{x_{i,r}^{\pm}, h_{i,s}, k_{\mu} | i \in I, r, s \in \mathbb{Z}(s \neq 0), \mu \in Q\}$. By (2.8), we obtain $e_0, f_0 \in \mathcal{D}_{\varepsilon}^{\mathrm{fin}}$. So we have $\mathcal{D}_{\varepsilon}^{\mathrm{fin}} = \widetilde{U}_{\varepsilon}^{\mathrm{fin}}$. Let $(\widetilde{U}_{\varepsilon}^{\mathrm{fin}})^{\pm}$ (respectively, $(\widetilde{U}_{\varepsilon}^{\mathrm{fin}})^{0}$) be the $\mathbb{C}$-subalgebra of $\widetilde{U}_{\varepsilon}^{\mathrm{fin}}$ generated by $\{x_{i,r}^{\pm} | i \in I, r \in \mathbb{Z}\}$ (respectively, $\{h_{i,s}, k_{\mu} | i \in I, s \in \mathbb{Z}^{\times}, \mu \in Q\}$) and $(U_{\varepsilon}^{\mathrm{fin}})^{+}$ (respectively, $(U_{\varepsilon}^{\mathrm{fin}})^{-}, (U_{\varepsilon}^{\mathrm{fin}})^{0}$) be the $\mathbb{C}$-subalgebra of $U_{\varepsilon}^{\mathrm{fin}}$ generated by $\{e_i\}_{i \in I}$ (respectively, $\{f_i\}_{i \in I}$, $\{k_{\mu}\}_{\mu \in Q}$). Let $\mathbb{Z}_{l}^{\Delta_{+}}$ be as in (3.1). We set

$$(B_\varepsilon^{\mathrm{fin}})^+ := \left\{ \prod_{\gamma\in\Delta_+}^{<} \overline{e}_\gamma^{c(\gamma)} | c \in \mathbb{Z}_l^{\Delta_+} \right\}, \quad (B_\varepsilon^{\mathrm{fin}})^- := \Omega((B_\varepsilon^{\mathrm{fin}})^+),$$

$$(B_\varepsilon^{\mathrm{fin}})^0 := \{k_\mu | \mu \in Q_{2l}\}, \quad B_\varepsilon^{\mathrm{fin}} := (B_\varepsilon^{\mathrm{fin}})^-(B_\varepsilon^{\mathrm{fin}})^0(B_\varepsilon^{\mathrm{fin}})^+. \tag{3.5}$$

Theorem 3.12 (Ref. 19, Sec. 5, Ref. 20, Sec. 8): $(B_\varepsilon^{fin})^\star$ *(respectively,* B_ε^{fin}*) is a* $\mathbb{C}$*-basis of* $(U_\varepsilon^{\mathrm{fin}})^\star$ *(respectively,* $U_\varepsilon^{\mathrm{fin}}$*) for* $\star \in \{-,0,+\}$.

Since e_β, f_β are generated by $\{e_i\}_{i\in\tilde{I}}, \{f_i\}_{i\in\tilde{I}}$, respectively, we get e_β, $f_\beta \in \tilde{U}_\varepsilon^{\mathrm{fin}}$ for any $\beta \in \tilde{\Delta}_+(I)$. For $\beta \in \tilde{\Delta}_+^{\mathrm{re}}$, $i \in I$, $m \in \mathbb{N}$, we have

$$e_\beta^l = [l]_\varepsilon! \dot{e}_\beta^{(l)}, \quad f_\beta^l = [l]_\varepsilon! \dot{f}_\beta^{(l)}, \quad e_{(i,ml\delta)} = [l]_\varepsilon \dot{e}_{(i,ml\delta)}, \quad f_{(i,ml\delta)} = [l]_\varepsilon \dot{f}_{(i,ml\delta)},$$

$$\prod_{r=1}^{l} (k_{\alpha_i}\varepsilon^{1-r} - k_{\alpha_i}\varepsilon^{r-1}) = \prod_{r=1}^{l} (\varepsilon^r - \varepsilon^{-r}) \begin{bmatrix} k_{\alpha_i}; 0 \\ l \end{bmatrix},$$

(see Ref. 18, Lemma 4.4). So we obtain

$$e_\beta^l = f_\beta^l = e_{(i,sl\delta)} = f_{(i,sl\delta)} = k_{\alpha_i}^{2l} - 1 = 0, \tag{3.6}$$

for any $\beta \in \tilde{\Delta}_+^{\mathrm{re}}$, $s \in \mathbb{N}$, $i \in I$. Let $\mathbb{Z}_l^{\tilde{\Delta}_+(I)}$ be as in (3.2). Define

$$(\tilde{B}_\varepsilon^{\mathrm{fin}})^+ := \left\{ \prod_{\beta\in\tilde{\Delta}_+(I)}^{<} e_\beta^{c(\beta)} | c \in \mathbb{Z}_l^{\tilde{\Delta}_+(I)} \right\}, \quad (\tilde{B}_\varepsilon^{\mathrm{fin}})^- := \Omega((\tilde{B}_\varepsilon^{\mathrm{fin}})^+),$$

$$(\tilde{B}_\varepsilon^{\mathrm{fin}})^0 := \{k_\mu | \mu \in Q_{2l}\}, \quad \tilde{B}_\varepsilon^{\mathrm{fin}} := (\tilde{B}_\varepsilon^{\mathrm{fin}})^-(\tilde{B}_\varepsilon^{\mathrm{fin}})^0(\tilde{B}_\varepsilon^{\mathrm{fin}})^+.$$

Since $e_\beta, f_\beta \in \tilde{U}_\varepsilon^{\mathrm{fin}}$ for any $\beta \in \tilde{\Delta}_+(I)$, we have $\tilde{B}_\varepsilon^{\mathrm{fin}} \subset \tilde{U}_\varepsilon^{\mathrm{fin}}$. Therefore, by Theorem 3.11, we obtain the following lemma.

Proposition 3.13: $\tilde{B}_\varepsilon^{\mathrm{fin}}$ *is linearly independent in* $\tilde{U}_\varepsilon^{\mathrm{fin}}$.

D. Isomorphism theorem

Proposition 3.14 (Ref. 2, Lemma 4.8): There exists a $\mathbb{C}$*-algebra isomorphism* $\bar{\phi}: U_\varepsilon/I_\varepsilon \to U_\varepsilon^{\mathrm{fin}}$ *such that* $\bar{\phi}(E_i+I_\varepsilon)=e_i$, $\bar{\phi}(F_i+I_\varepsilon)=f_i$ and $\bar{\phi}(K_\mu+I_\varepsilon)=k_\mu$ *for* $i \in I$, $\mu \in Q$.

We obtain an affine version of the above-noted result:

Theorem 3.15: *There exists a* $\mathbb{C}$*-algebra isomorphism* $\tilde{\phi}: \tilde{U}_\varepsilon/\tilde{I}_\varepsilon \to \tilde{U}_\varepsilon^{\mathrm{fin}}$ *such that* $\tilde{\phi}(E_i+\tilde{I}_\varepsilon) = e_i$, $\tilde{\phi}(F_i+\tilde{I}_\varepsilon)=f_i$ *and* $\tilde{\phi}(K_\mu+\tilde{I}_\varepsilon)=k_\mu$ *for* $i \in \tilde{I}$, $\mu \in Q$. *In particular,* $\tilde{B}_\varepsilon^{\mathrm{fin}}$ *is a* $\mathbb{C}$*-basis of* $\tilde{U}_\varepsilon^{\mathrm{fin}}$.

Proof: Elements in $\{e_i, f_i, k_\mu | i \in \tilde{I}, \mu \in Q\} (\subset \tilde{U}_\varepsilon^{\mathrm{fin}})$ satisfy the relations of Definition 2.1. So, by the universality of $\tilde{U}_\varepsilon$ (see Remark 3.3 (b)), there exists a surjective $\mathbb{C}$-algebra homomorphism $\phi: \tilde{U}_\varepsilon \to \tilde{U}_\varepsilon^{\mathrm{fin}}$ such that $E_i \mapsto e_i$, $F_i \mapsto f_i$, $K_\mu \mapsto k_\mu$ for $i \in \tilde{I}$, $\mu \in Q$. Since $e_\beta = E_\beta \otimes 1$ and $f_\beta = F_\beta \otimes 1$ $(\beta \in \tilde{\Delta}_+(I))$, we obtain $\phi(E_\beta)=e_\beta$ and $\phi(F_\beta)=f_\beta$. Then, by (3.6), we have $\phi(\tilde{I}_\varepsilon)=0$. Hence there exists a surjective $\mathbb{C}$-algebra homomorphism $\tilde{\phi}: \tilde{U}_\varepsilon/\tilde{I}_\varepsilon \to \tilde{U}_\varepsilon^{\mathrm{fin}}$ such that $\tilde{\phi}(E_\beta+\tilde{I}_\varepsilon)=e_\beta$, $\tilde{\phi}(F_\beta+\tilde{I}_\varepsilon) = f_\beta$ and $\tilde{\phi}(K_\mu+\tilde{I}_\varepsilon)=k_\mu$ for $\beta \in \tilde{\Delta}_+(I)$, $\mu \in Q$.

Let $u \in \mathrm{Ker}(\tilde{\phi})$. By Proposition 3.10, we have

$$u = \sum_{\mu\in Q_{2l}} \sum_{c,c' \in \mathbb{Z}_l^{\tilde{\Delta}_+(I)}} a(c,\mu,c') \left(\prod_{\beta\in\tilde{\Delta}_+(I)}^{<} E_\beta^{c(\beta)} + \tilde{I}_\varepsilon \right) (K_\mu + \tilde{I}_\varepsilon) \left(\prod_{\beta\in\tilde{\Delta}_+(I)}^{<} F_\beta^{c'(\beta)} + \tilde{I}_\varepsilon \right),$$

where $a(c,\mu,c') \in \mathbb{C}$. Then we get

$$0=\tilde{\phi}(u)=\sum_{\mu\in Q_{2l}}\sum_{c,c'\in\mathbb{Z}_l^{\tilde{\Delta}_+(I)}}a(c,\mu,c')\left(\prod_{\beta\in\tilde{\Delta}_+(I)}^{<}e_\beta^{c(\beta)}\right)k_\mu\left(\prod_{\beta\in\tilde{\Delta}_+(I)}^{<}f_\beta^{c'(\beta)}\right).$$

Hence, by Lemma 3.13, we obtain $a(c,\mu,c')=0$ for any $c,c'\in\mathbb{Z}_l^{\tilde{\Delta}_+(I)}$, $\mu\in Q_{2l}$. Thus $\tilde{\phi}$ is injective. Therefore $\tilde{\phi}$ is an isomorphism and $\tilde{B}_\varepsilon^{\mathrm{fin}}$ is a $\mathbb{C}$-basis of $\tilde{U}_\varepsilon^{\mathrm{fin}}$. □

IV. EVALUATION REPRESENTATIONS OF RESTRICTED TYPE

A. Representation theory of restricted type

We call a $\tilde{U}_\varepsilon^{\mathrm{res}}$-module (respectively, $U_\varepsilon^{\mathrm{res}}$-module) V "type **1**" if $k_\mu^l=1$ on V for any $\mu\in Q$. In general, finite-dimensional irreducible $\tilde{U}_\varepsilon^{\mathrm{res}}$-modules (respectively, $U_\varepsilon^{\mathrm{res}}$-modules) are classified into 2^n types according to $\{\sigma:Q\to\{\pm1\};$ group homomorphism$\}$. It is known that for any $\sigma:Q\to\{\pm1\}$, the category of finite-dimensional $\tilde{U}_\varepsilon^{\mathrm{res}}$-modules (respectively, $U_\varepsilon^{\mathrm{res}}$-modules) of type σ is essentially equivalent to the category of the finite-dimensional $\tilde{U}_\varepsilon^{\mathrm{res}}$-modules (respectively, $U_\varepsilon^{\mathrm{res}}$-modules) of type **1**.

Let $U=U_\varepsilon^{\mathrm{res}}$, $U_\varepsilon^{\mathrm{fin}}$, $\tilde{U}_\varepsilon^{\mathrm{res}}$, or $\tilde{U}_\varepsilon^{\mathrm{fin}}$.

Definition 4.1: Let V be a U-module and v be a nonzero vector in V. Suppose that v satisfies

$$e_i^{(m)}v=0 \text{ for any } i\in I,\quad m\in\mathbb{N} \text{ if } U=U_\varepsilon^{\mathrm{res}},\quad e_iv=0 \text{ for any } i\in I \text{ if } U=U_\varepsilon^{\mathrm{fin}},$$

$$(x_{i,r}^+)^{(m)}v=0 \text{ for any } i\in I,\quad m\in\mathbb{N},\quad r\in\mathbb{Z} \text{ if } U=\tilde{U}_\varepsilon^{\mathrm{res}},$$

$$x_{i,r}^+v=0 \text{ for any } i\in I,\quad r\in\mathbb{Z} \text{ if } U=\tilde{U}_\varepsilon^{\mathrm{fin}}.$$

We call v a "primitive vector" in V.

Definition 4.2: Let V be a U-module and $\Lambda:U^0\to\mathbb{C}$ be a $\mathbb{C}$-algebra homomorphism. We assume that V is generated as a U-module by a primitive vector $v_\Lambda\in V$ such that

$$u_0v_\Lambda=\Lambda(u_0)v_\Lambda,$$

for any $u_0\in U^0$. Then we call V a "highest-weight U-module" generated by a "highest-weight vector" v_Λ with "highest weight Λ."

Proposition 4.3: For any $\mathbb{C}$-algebra homomorphism $\Lambda:U^0\to\mathbb{C}$, there exists a unique (up to isomorphism) irreducible highest-weight U-module V with highest weight Λ.

Proof: For any $U_\varepsilon^{\mathrm{res}}$-module (respectively, $\tilde{U}_\varepsilon^{\mathrm{res}}$-module) V, we can define the weight spaces on V by

$$V_\mu:=\left\{v\in V\,|\,k_\alpha v=\varepsilon^{\langle\mu,\alpha_i^\vee\rangle}v,\quad \begin{bmatrix}k_{\alpha_i};0\\ l\end{bmatrix}v=\begin{bmatrix}\langle\mu,\alpha_i^\vee\rangle\\ l\end{bmatrix}_\varepsilon v \text{ for any } i\in I\right\},\tag{4.1}$$

where $\mu\in P$ (see Refs. 18 and 11). Then, by the theory of highest-weight modules, we obtain this proposition in the case of $U=U_\varepsilon^{\mathrm{res}}$ or $\tilde{U}_\varepsilon^{\mathrm{res}}$ (see Ref. 11, Proposition 7.3). So we shall prove the case of $\tilde{U}_\varepsilon^{\mathrm{fin}}$. We can prove the case of $U_\varepsilon^{\mathrm{fin}}$ similarly.

Let $\hat{U}_\varepsilon^{\mathrm{fin}}$ be the $\mathbb{C}$-subalgebra of $\tilde{U}_\varepsilon^{\mathrm{res}}$ generated by $\tilde{U}_\varepsilon^{\mathrm{fin}}\cup\left\{\begin{bmatrix}k_{\alpha_i};0\\ l\end{bmatrix}\,\middle|\, i\in I\right\}$. For any $\mathbb{C}$-algebra homomorphism $\Lambda:(\tilde{U}_\varepsilon^{\mathrm{fin}})^0\to\mathbb{C}$, let $\hat{I}_\varepsilon^{\mathrm{fin}}(\Lambda)$ (respectively, $\tilde{I}_\varepsilon^{\mathrm{fin}}(\Lambda)$) be the left ideal of $\hat{U}_\varepsilon^{\mathrm{fin}}$ (respectively, $\tilde{U}_\varepsilon^{\mathrm{fin}}$) generated by $\left\{x_{i,r}^+,u_0-\Lambda(u_0),\begin{bmatrix}k_{\alpha_i};0\\ l\end{bmatrix}\,\middle|\, i\in I,r\in\mathbb{Z},u_0\in(\tilde{U}_\varepsilon^{\mathrm{fin}})^0\right\}$ (respectively, $\{x_{i,r}^+,u_0-\Lambda(u_0)\,|\,i\in I,r\in\mathbb{Z},u_0\in(\tilde{U}_\varepsilon^{\mathrm{fin}})^0\}$). We define a $\hat{U}_\varepsilon^{\mathrm{fin}}$-module $\hat{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ and a $\tilde{U}_\varepsilon^{\mathrm{fin}}$-module $\tilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$, respectively, by

$$\hat{M}_\varepsilon^{\mathrm{fin}}(\Lambda) := \hat{U}_\varepsilon^{\mathrm{fin}}/\hat{I}_\varepsilon^{\mathrm{fin}}(\Lambda), \quad \widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda) := \widetilde{U}_\varepsilon^{\mathrm{fin}}/\widetilde{I}_\varepsilon^{\mathrm{fin}}(\Lambda).$$

We set $\hat{v}_\Lambda := 1+\hat{I}_\varepsilon^{\mathrm{fin}}(\Lambda) \in \hat{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ and $\tilde{v}_\Lambda := 1+\widetilde{I}_\varepsilon^{\mathrm{fin}}(\Lambda) \in \widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$. Let $\hat{N}_\varepsilon^{\mathrm{fin}}(\Lambda)$ be the $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-submodule of $\hat{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ generated by $\hat{v}_\Lambda$. Then, by the universality of the $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module $\widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$, there exists a surjective $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module homomorphism $\phi: \widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda) \to \hat{N}_\varepsilon^{\mathrm{fin}}(\Lambda)$ such that $\phi(\tilde{v}_\Lambda) = \hat{v}_\Lambda$. Let B be a $\mathbb{C}$-basis of $(\widetilde{U}_\varepsilon^{\mathrm{fin}})^-$. Then, by (3.4), we obtain that $\{u\hat{v}_\Lambda \,|\, u \in B\}$ (respectively, $\{u\tilde{v}_\Lambda \,|\, u \in B\}$) is a $\mathbb{C}$-basis of $\hat{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ (respectively, $\widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$). Hence ϕ is an isomorphism of $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module. So we can regard $\widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ as $\hat{U}_\varepsilon^{\mathrm{fin}}$-module. In a similar way to (4.1), we can define the weight spaces on this module. Then, by the theory of the highest-weight module, $\widetilde{M}_\varepsilon^{\mathrm{fin}}(\Lambda)$ has a unique simple quotient of $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module and it is the unique irreducible highest-weight $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module with highest weight Λ. □

For any $\mathbb{C}$-algebra homomorphism $\Lambda: U^0 \to \mathbb{C}$, we denote the unique irreducible highest weight U-module with highest weight Λ by $V_\varepsilon^{\mathrm{res}}(\Lambda)$ if $U = U_\varepsilon^{\mathrm{res}}$, $V_\varepsilon^{\mathrm{fin}}(\Lambda)$ if $U = U_\varepsilon^{\mathrm{fin}}$, $\widetilde{V}_\varepsilon^{\mathrm{res}}(\Lambda)$ if $U = \widetilde{U}_\varepsilon^{\mathrm{res}}$, and $\widetilde{V}_\varepsilon^{\mathrm{fin}}(\Lambda)$ if $U = \widetilde{U}_\varepsilon^{\mathrm{fin}}$. Then, by Proposition 4.3 and the uniqueness of the primitive vectors, we obtain the following proposition.

Proposition 4.4: Let Λ and $\Lambda': U^0 \to \mathbb{C}$ be $\mathbb{C}$-algebra homomorphisms. Then $V_\varepsilon^{res}(\Lambda)$ (respectively, $V_\varepsilon^{fin}(\Lambda)$, $\widetilde{V}_\varepsilon^{res}(\Lambda)$, $\widetilde{V}_\varepsilon^{fin}(\Lambda)$) is isomorphic to $V_\varepsilon^{res}(\Lambda')$ (respectively, $V_\varepsilon^{fin}(\Lambda')$, $\widetilde{V}_\varepsilon^{res}(\Lambda')$, $\widetilde{V}_\varepsilon^{fin}(\Lambda')$) if and only if $\Lambda = \Lambda'$.

Now, we define $\mathcal{P}_{i,m} \in \widetilde{U}_q$ inductively by

$$\mathcal{P}_{i,0} := 1, \quad \mathcal{P}_{i,m} := -\frac{K_{\alpha_i}^{-1}}{1-q^{-2m}} \sum_{s=1}^{m} \Psi_{i,s}^{+} \mathcal{P}_{i,m-s}, \quad \mathcal{P}_{i,-m} := \Omega(\mathcal{P}_{i,m}),$$

where Ω as in (2.2). We have $\Omega(\Psi_{i,s}^{+}) = \Psi_{i,-s}^{-}$.

Proposition 4.5 (Ref. 11, Sec. 3): For any $i \in I$, $r \in \mathbb{Z}$, we have $\mathcal{P}_{i,r} \in \widetilde{U}_{\mathcal{A}}^{res}$. Moreover, $(\widetilde{U}_\varepsilon^{\mathrm{res}})^0$ is generated by $\left\{k_{\alpha_i}, \begin{bmatrix} k_{\alpha_i};0 \\ l \end{bmatrix}, \mathcal{P}_{i,r} \otimes 1 \,\middle|\, i \in I, r \in \mathbb{Z}\right\}$ as a $\mathbb{C}$-algebra.

We simply denote $\mathcal{P}_{i,r} \otimes 1 \in \widetilde{U}_\varepsilon^{\mathrm{res}}$ by $\mathcal{P}_{i,r}$. We set

$$\mathbb{C}_0[t] := \{P \in \mathbb{C}_0[t] \,|\, P \text{ is monic, } P(0) \neq 0\}.$$

We call a polynomial $P \in \mathbb{C}[t]$ "l-acyclic" if it is not divisible by $(1-ct^l)$ for any $c \in \mathbb{C}^\times$ (see Ref. 15) and set

$$\mathbb{C}_l[t] := \{P \in \mathbb{C}_0[t] \,|\, P \text{ is } l\text{-acyclic}\}.$$

Definition 4.6: (a) For $\lambda = (\lambda_i)_{i\in I} \in \mathbb{Z}_+^n$, let $\lambda_i^{(0)} \in \mathbb{Z}_l$ and $\lambda_i^{(1)} \in \mathbb{Z}_+$ such that $\lambda_i = \lambda_i^{(0)} + l\lambda_i^{(1)}$ ($i \in I$). We define a $\mathbb{C}$-algebra homomorphism $\Lambda_\lambda^{\mathrm{res}}: (U_\varepsilon^{\mathrm{res}})^0 \to \mathbb{C}$ by

$$\Lambda_\lambda^{\mathrm{res}}(k_{\alpha_i}) := \varepsilon^{\lambda_i^{(0)}}, \quad \Lambda_\lambda^{\mathrm{res}}\left(\begin{bmatrix} k_{\alpha_i};0 \\ l \end{bmatrix}\right) := \lambda_i^{(1)} \quad (i \in I).$$

(b) For $\lambda = (\lambda_i)_{i\in I} \in \mathbb{Z}_l^n$, we define a $\mathbb{C}$-algebra homomorphism $\Lambda_\lambda^{\mathrm{fin}}: (U_\varepsilon^{\mathrm{fin}})^0 \to \mathbb{C}$ by

$$\Lambda_\lambda^{\mathrm{fin}}(k_{\alpha_i}) := \varepsilon^{\lambda_i} \quad (i \in I).$$

(c) For $\mathbf{P} = (P_i)_{i\in I} \in \mathbb{C}_0[t]^n$, let $p_i^{(0)} \in \mathbb{Z}_l$ and $p_i^{(1)} \in \mathbb{Z}_+$ such that $\deg(P_i) = p_i^{(0)} + lp_i^{(1)}$ ($i \in I$). We define a $\mathbb{C}$-algebra homomorphism $\widetilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}: (\widetilde{U}_\varepsilon^{\mathrm{res}})^0 \to \mathbb{C}$ by

$$\widetilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}(k_{\alpha_i}) := \varepsilon^{p_i^{(0)}}, \quad \widetilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}\left(\begin{bmatrix} k_{\alpha_i};0 \\ l \end{bmatrix}\right) := p_i^{(1)} \quad (i \in I),$$

$$\sum_{m=0}^{\infty} \tilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}(\mathcal{P}_{i,m})t^m := \frac{P_i(t)}{P_i(0)}, \quad \sum_{m=0}^{\infty} \tilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}(\mathcal{P}_{i,-m})t^m := t^{\deg(P_i)}P_i(t^{-1}),$$

(see Ref. 11, Sec. 8).

(d) For $\mathbf{P}=(P_i)_{i\in I}\in \mathbb{C}_l[t]^n$, we define a $\mathbb{C}$-algebra homomorphism $\tilde{\Lambda}_{\mathbf{P}}^{\mathrm{fin}}:(\tilde{U}_\varepsilon^{\mathrm{fin}})^0\to\mathbb{C}$ by

$$\sum_{m=0}^{\infty} \tilde{\Lambda}_{\mathbf{P}}^{\mathrm{fin}}(\psi_{i,m}^{+})t^m := \varepsilon^{\deg(P_i)}\frac{P_i(\varepsilon^{-2}t)}{P_i(t)} := \sum_{m=0}^{\infty} \tilde{\Lambda}_{\mathbf{P}}^{\mathrm{fin}}(\psi_{i,-m}^{-})t^{-m},$$

in the sense that the left- and right-hand sides are the Laurent expansions of the middle term about $t=0$ and $t=\infty$, respectively (see Ref. 11, Sec. 8).

By Ref. 11, Sec. 8, we obtain $\tilde{\Lambda}_{\mathbf{P}}^{\mathrm{fin}}=\tilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}}|_{(\tilde{U}_\varepsilon^{\mathrm{fin}})^0}$ ($\mathbf{P}\in\mathbb{C}_l[t]^n$). For $\lambda\in\mathbb{Z}_+^n$ (respectively, $\mathbb{Z}_l^n$), we set $V_\varepsilon^{\mathrm{res}}(\lambda):=V_\varepsilon^{\mathrm{res}}(\Lambda_\lambda^{\mathrm{res}})$ (respectively, $V_\varepsilon^{\mathrm{fin}}(\lambda):=V_\varepsilon^{\mathrm{fin}}(\Lambda_\lambda^{\mathrm{fin}})$). Similarly, for $\mathbf{P}\in\mathbb{C}_0[t]^n$ (respectively, $\mathbb{C}_l[t]^n$), we set $\tilde{V}_\varepsilon^{\mathrm{res}}(\mathbf{P}):=\tilde{V}_\varepsilon^{\mathrm{res}}(\tilde{\Lambda}_{\mathbf{P}}^{\mathrm{res}})$ (respectively, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P}):=\tilde{V}_\varepsilon^{\mathrm{fin}}(\tilde{\Lambda}_{\mathbf{P}}^{\mathrm{fin}})$) and call $\mathbf{P}$ "Drinfel'd polynomial" of $\tilde{V}_\varepsilon^{\mathrm{res}}(\mathbf{P})$ (respectively, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$).

Theorem 4.7 (Refs. 18 and 9, Proposition 11.2.10): *For any* $\lambda\in\mathbb{Z}_+^n$ (*respectively*, $\mathbb{Z}_l^n$), $V_\varepsilon^{\mathrm{res}}(\lambda)$ (*respectively*, $V_\varepsilon^{\mathrm{fin}}(\lambda)$) *is a finite-dimensional irreducible* $U_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $U_\varepsilon^{\mathrm{fin}}$*-module*) *of type* **1**. *Conversely, for any finite-dimensional irreducible* $U_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $U_\varepsilon^{\mathrm{fin}}$*-module*) *V of type* **1**, *there exists a unique* $\lambda\in\mathbb{Z}_+^n$ (*respectively*, $\mathbb{Z}_l^n$) *such that V is isomorphic to* $V_\varepsilon^{\mathrm{res}}(\lambda)$ (*respectively*, $V_\varepsilon^{\mathrm{fin}}(\lambda)$) *as a* $U_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $U_\varepsilon^{\mathrm{fin}}$*-module*). *In particular, for any* $\lambda\in\mathbb{Z}_l^n$, $V_\varepsilon^{\mathrm{fin}}(\lambda)$ *is isomorphic to* $V_\varepsilon^{\mathrm{res}}(\lambda)$ *as a* $U_\varepsilon^{\mathrm{fin}}$*-module*.

Theorem 4.8 (Ref. 11, Theorem 8.2, 9.2, Ref. 15, Theorem 2.6): *For any* $\mathbf{P}\in\mathbb{C}_0[t]^n$ (*respectively*, $\mathbb{C}_l[t]^n$), $\tilde{V}_\varepsilon^{\mathrm{res}}(\mathbf{P})$ (*respectively*, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$) *is a finite-dimensional irreducible* $\tilde{U}_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module*) *of type* **1**. *Conversely, for any finite-dimensional irreducible* $\tilde{U}_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module*) *V of type* **1**, *there exists a unique* $\mathbf{P}\in\mathbb{C}_0[t]^n$ (*respectively*, $\mathbb{C}_l[t]^n$) *such that V is isomorphic to* $\tilde{V}_\varepsilon^{\mathrm{res}}(\mathbf{P})$ (*respectively*, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$) *as a* $\tilde{U}_\varepsilon^{\mathrm{res}}$*-module* (*respectively*, $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module*). *In particular, for any* $\mathbf{P}\in\mathbb{C}_l[t]^n$, $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$ *is isomorphic to* $\tilde{V}_\varepsilon^{\mathrm{res}}(\mathbf{P})$ *as a* $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module*.

By the tensor product theorem, in order to understand the representation theory of $\tilde{U}_\varepsilon^{\mathrm{res}}$ (respectively, $U_\varepsilon^{\mathrm{res}}$), it is sufficient to consider $\tilde{U}_\varepsilon^{\mathrm{fin}}$ (respectively $U_\varepsilon^{\mathrm{fin}}$) (see Refs. 11 and 18).

B. Drinfel'd polynomials of evaluation representations

For $m\in\mathbb{Z}_+$, let $V_\varepsilon^{\mathrm{fin}}(m)$ be the $(m+1)$-dimensional irreducible $U_\varepsilon^{\mathrm{fin}}(\mathfrak{sl}_2)$-module. By (2.16), we can regard $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$ as a $U_\varepsilon^{\mathrm{fin}}(\mathfrak{sl}_{n+1})$-module ($\mathbf{P}\in\mathbb{C}_l[t]^n$). Then, by Ref. 11, Secs. 7–9 (in particular, p. 321), we obtain the following theorem.

Theorem 4.9 (Ref. 11): *For any* $P\in\mathbb{C}_l[t](P\neq 1)$, *there exist* r, $m_s\in\mathbb{N}$ *and* $c_s\in\mathbb{C}^\times(1\leqslant s\leqslant r)$ *such that*

$$\tilde{V}_\varepsilon^{fin}(P)\cong\tilde{V}_\varepsilon^{fin}(P_1)\otimes\cdots\otimes\tilde{V}_\varepsilon^{fin}(P_r)\quad(\textit{as a } U_\varepsilon^{\mathrm{fin}}(\widetilde{\mathfrak{sl}_2})-\textit{module}),$$

where $P=\prod_{s=1}^r P_s$, $P_s(t)=\prod_{p=1}^{m_s}(t-c_s\varepsilon^{m_s+1-2p})\in\mathbb{C}_l[t]$ $(1\leqslant s\leqslant r)$. *In particular,* $\tilde{V}_\varepsilon^{fin}(P_s)$ *is isomorphic to* $V_\varepsilon^{fin}(m_s)$ *as a* $U_\varepsilon^{\mathrm{fin}}(\mathbf{sl}_2)$*-module*.

By this theorem, we obtain the following lemma.

Lemma 4.10: Let $P\in\mathbb{C}_l[t]$, $m\in\mathbb{N}$. *If* $\tilde{V}_\varepsilon^{fin}(P)$ *is isomorphic to* $V_\varepsilon^{fin}(m)$ *as a* $U_\varepsilon^{\mathrm{fin}}(\mathbf{sl}_2)$*-module, then there exists* $c\in\mathbb{C}^\times$ *such that* $P(t)=\prod_{p=1}^m(t-c\varepsilon^{m+1-2p})$.

By using this lemma, we can prove the following lemma.

Lemma 4.11: Let $\mathbf{P}=(P_i)_{i\in I}\in\mathbb{C}_l[t]^n$, $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_l^n$. *We assume* $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$ *is isomorphic to* $V_\varepsilon^{\mathrm{fin}}(\lambda)$ *as a* $U_\varepsilon^{\mathrm{fin}}$*-module. Then, for any* $i\in I(P_i\neq 1)$, *there exists* $c_i\in\mathbb{C}^\times$ *such that* $P_i(t)=\prod_{p=1}^{\lambda_i}(t-c_i\varepsilon^{\lambda_i+1-2p})$.

Proof: Let $v_{\mathbf{P}}$ be a highest-weight vector in $\tilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P})$. Then $v_{\mathbf{P}}$ is also a highest-weight vector in $V_\varepsilon^{\mathrm{fin}}(\lambda)$. For $i\in I$, let $(\tilde{U}_\varepsilon^{\mathrm{fin}})_i$ (respectively, $(U_\varepsilon^{\mathrm{fin}})_i$) be the $\mathbb{C}$-subalgebra of $\tilde{U}_\varepsilon^{\mathrm{fin}}$ (respectively, $U_\varepsilon^{\mathrm{fin}}$)

generated by $\{x^{\pm}_{i,r}, h_{i,s}, k_{\alpha_i} | r,s \in \mathbb{Z}, s \neq 0\}$ (respectively, $\{e_i, f_i, k_{\alpha_i}\}$) and $\widetilde{W}_i$ (respectively, W_i) be the $(\widetilde{U}^{\mathrm{fin}}_{\varepsilon})_i$-submodule (respectively, $(U^{\mathrm{fin}}_{\varepsilon})_i$-submodule) of $\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P})$ generated by $v_{\mathbf{P}}$. By (2.17) (respectively, (2.16)), we can regard $\widetilde{W}_i$ (respectively W_i) as a $U^{\mathrm{fin}}_{\varepsilon}(\widetilde{\mathfrak{sl}}_2)$-module (respectively, $U^{\mathrm{fin}}_{\varepsilon}(\widetilde{\mathfrak{sl}}_2)$-module). Then, by Lemma 7.6 in Ref. 11, we obtain $\widetilde{W}_i \cong \widetilde{V}^{\mathrm{fin}}_{\varepsilon}(P_i)$ as a $U^{\mathrm{fin}}_{\varepsilon}(\widetilde{\mathfrak{sl}}_2)$-module. Similarly (more easily), we obtain $W_i \cong V^{\mathrm{fin}}_{\varepsilon}(\lambda_i)$ as a $U^{\mathrm{fin}}_{\varepsilon}(\mathfrak{sl}_2)$-module. So, by Lemma 4.10, it is enough to prove $\widetilde{W}_i = W_i$ for $i \in I$ such that $P_i \neq 1$.

By (3.4), $\widetilde{W}_i$ is spanned by $\{x^{-}_{i,r_1} \cdots x^{-}_{i,r_m} v_{\mathbf{P}} | r_1, \cdots r_m \in \mathbb{Z}, m \in \mathbb{Z}_+\}$ as a $\mathbb{C}$-vector space. By Theorem 4.8, we can regard $\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P})$ as a $\widetilde{U}^{\mathrm{res}}_{\varepsilon}$-module and define the weight spaces on $\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P})$ in a similar way to (4.1). Then, by the relations of Drinfel'd realization, we have $x^{-}_{i,r_1} \cdots x^{-}_{i,r_m} v_{\mathbf{P}} \in (\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P}))_{\lambda - m\alpha_i}$ for any $m \in \mathbb{N}, r_1, \cdots r_m \in \mathbb{Z}$. So we obtain $\widetilde{W}_i \subset \oplus_{m \geqslant 0} (\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P}))_{\lambda - m\alpha_i}$. On the other hand, by the assumption of this lemma, $\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P})$ is isomorphic to $V^{\mathrm{fin}}_{\varepsilon}(\lambda)$ as a $U^{\mathrm{fin}}_{\varepsilon}$-module. Hence, by (3.3), $\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P})$ is spanned by $\{\Pi^{<}_{\gamma \in \Delta_+} \overline{f}^{c(\gamma)}_{\gamma} v_{\mathbf{P}} | c \in \mathbb{Z}_l^{\Delta_+}\}$. Since $\Pi^{<}_{\gamma \in \Delta_+} \overline{f}^{c(\gamma)}_{\gamma} v_{\mathbf{P}} \in (\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P}))_{\Sigma_{\gamma \in \Delta_+} c(\gamma)\gamma}$, we have

$$\bigoplus_{m \geqslant 0} (\widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P}))_{\lambda - m\alpha_i} = \bigoplus_{m \in \mathbb{Z}_l} \mathbb{C} f_i^m v_{\mathbf{P}} \subset W_i.$$

Then we have $\widetilde{W}_i = W_i$. □

Let $(U^{\mathrm{res}}_{\mathcal{A}})'$ (respectively, $(U^{\mathrm{fin}}_{\varepsilon})'$) be the extended algebra of $U^{\mathrm{res}}_{\mathcal{A}}$ (respectively, $U^{\mathrm{fin}}_{\varepsilon}$) defined by replacing $\{K_\mu | \mu \in Q\}$ with $\{K_\mu | \mu \in P\}$ (see Definition 2.1). By (2.18), we obtain $\mathrm{ev}^{\pm}_{\mathbf{a}}(\widetilde{U}^{\mathrm{res}}_{\mathcal{A}}) \subset (U^{\mathrm{res}}_{\mathcal{A}})'$ $(\mathbf{a} \in \mathbb{C}^{\times})$. Hence, by Proposition 2.6, we obtain the evaluation $\widetilde{U}^{\mathrm{fin}}_{\varepsilon}$-homomorphisms $(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{\pm}: \widetilde{U}^{\mathrm{fin}}_{\varepsilon} \to (U^{\mathrm{fin}}_{\varepsilon})'$ defined by

$$(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{\pm}(e_i) := e_i, \quad (\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{\pm}(f_i) := f_i \quad (\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{\pm}(k_\mu) := k_\mu,$$

$$(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{+}(e_0) := \mathbf{a}\varepsilon^{-1} k_{\Lambda_1} k^{-1}_{\Lambda_n} [f_n, [f_{n-1}, \ldots, [f_2 f_1]_{\varepsilon^{-1}} \cdots]_{\varepsilon^{-1}},$$

$$(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{+}(f_0) := \mathbf{a}^{-1}(-1)^{n-1} \varepsilon^n k^{-1}_{\Lambda_1} k_{\Lambda_n} [e_n, [e_{n-1}, \ldots, [e_2, e_1]_{\varepsilon^{-1}} \cdots]_{\varepsilon^{-1}},$$

$$(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{-}(e_0) := \mathbf{a}\varepsilon^{-1} k^{-1}_{\Lambda_1} k_{\Lambda_n} [f_1, [f_2, \ldots, [f_{n-1}, f_n]_{\varepsilon^{-1}} \cdots]_{\varepsilon^{-1}},$$

$$(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}})^{-}(f_0) := \mathbf{a}^{-1}(-1)^{n-1} \varepsilon^n k_{\Lambda_1} k^{-1}_{\Lambda_n} [e_1, [e_2, \ldots, [e_{n-1}, e_n]_{\varepsilon^{-1}} \cdots]_{\varepsilon^{-1}}, \tag{4.2}$$

for $i \in I$, $\mu \in Q$. For any $\lambda \in \mathbb{Z}_l^n$, we regard $V^{\mathrm{fin}}_{\varepsilon}(\lambda)$ as a $(U^{\mathrm{fin}}_{\varepsilon})'$-module through these homomorphisms. Then the evaluation $\widetilde{U}^{\mathrm{fin}}_{\varepsilon}$-representations are defined by the following method.

Definition 4.12: Let $\mathbf{a} \in \mathbb{C}^{\times}$, $\lambda = (\lambda_i)_{i \in I} \in \mathbb{Z}_l^n$. We set

$$\lambda_{\Lambda_i} := \sum_{j \in I} \lambda_j (\Lambda_i, \Lambda_j) \quad (i \in I), \tag{4.3}$$

$$\mathbf{a}^{\lambda}_{+} := \mathbf{a}\varepsilon^{-\lambda_{\Lambda_1} + \lambda_{\Lambda_n} + n}, \quad \mathbf{a}^{\lambda}_{-} := \mathbf{a}(-1)^{n+1} \varepsilon^{\lambda_{\Lambda_1} - \lambda_{\Lambda_n} + 2n + 1}. \tag{4.4}$$

We regard $V^{\mathrm{fin}}_{\varepsilon}(\lambda)$ as a $\widetilde{U}^{\mathrm{fin}}_{\varepsilon}$-module by using $(\mathrm{ev}^{\mathrm{fin}}_{\mathbf{a}^{\lambda}_{\pm}})^{\pm}$ and denote it by $V^{\mathrm{fin}}_{\varepsilon}(\lambda)^{\pm}_{\mathbf{a}}$.

Since $V^{\mathrm{fin}}_{\varepsilon}(\lambda)$ is irreducible as a $U^{\mathrm{fin}}_{\varepsilon}$-module, $V^{\mathrm{fin}}_{\varepsilon}(\lambda)^{\pm}_{\mathbf{a}}$ is a finite-dimensional irreducible $\widetilde{U}^{\mathrm{fin}}_{\varepsilon}$-module of type **1**. Thus, by Theorem 4.8, there exists a unique $\mathbf{P}^{\pm}_{\mathbf{a}} = (P^{\pm}_{i,\mathbf{a}})_{i \in I} \in \mathbb{C}_l[t]^n$ such that $V^{\mathrm{fin}}_{\varepsilon}(\lambda)^{\pm}_{\mathbf{a}} \cong \widetilde{V}^{\mathrm{fin}}_{\varepsilon}(\mathbf{P}^{\pm}_{\mathbf{a}})$ as a $\widetilde{U}^{\mathrm{fin}}_{\varepsilon}$-module. Let $i \in I$ such that $P^{\pm}_{i,\mathbf{a}} \neq 1$. Then, by Lemma 4.11, there exist $\mathbf{a}_{(\pm,i)} \in \mathbb{C}^{\times}$ such that $P^{(\pm)}_{i,\mathbf{a}}(t) = \Pi^{\lambda_i}_{p=1}(t - \mathbf{a}_{(\pm,i)} \varepsilon^{\lambda_i + 1 - 2p})$. Around $t = 0$, we have

$$\varepsilon^{\lambda_i}+(\varepsilon^{\lambda_i}-\varepsilon^{-\lambda_i})\sum_{m=1}^{\infty}(\mathbf{a}_{(\pm,i)}^{-1}\varepsilon^{\lambda_i-1}t)^m=\frac{\varepsilon^{\lambda_i}-\mathbf{a}_{(\pm,i)}^{-1}\varepsilon^{-1}t}{1-\mathbf{a}_{(\pm,i)}^{-1}\varepsilon^{\lambda_i-1}t}=\varepsilon^{\lambda_i}\frac{\varepsilon^{-2\lambda_i}(t-\mathbf{a}_{(\pm,i)}\varepsilon^{\lambda_i+1})}{t-\mathbf{a}_{(\pm,i)}\varepsilon^{-\lambda_i+1}}=\varepsilon^{\deg(P_{i,\mathbf{a}}^{\pm})}\frac{P_{i,\mathbf{a}}^{\pm}(\varepsilon^{-2}t)}{P_{i,\mathbf{a}}^{\pm}(t)}$$

(see Ref. 7, Corollary 4.2). Thus, by Definition 4.6(d), we obtain

$$\sum_{m=0}^{\infty}\tilde{\Lambda}_{\mathbf{P}_{\mathbf{a}}^{\pm}}^{\mathrm{fin}}(\psi_{i,m}^{+})t^m=\varepsilon^{\deg}(P_{i,\mathbf{a}}^{\pm})\frac{P_{i,\mathbf{a}}^{\pm}(\varepsilon^{-2}t)}{P_{i,\mathbf{a}}^{\pm}(t)}=\varepsilon^{\lambda_i}+(\varepsilon^{\lambda_i}-\varepsilon^{-\lambda_i})\sum_{m=1}^{\infty}(\mathbf{a}_{(\pm,i)}^{-1}\varepsilon^{\lambda_i-1}t)^m. \tag{4.5}$$

Hence we can calculate $\mathbf{a}_{(\pm,i)}$ explicitly by the computation of $\tilde{\Lambda}_{\mathbf{P}_{\mathbf{a}}^{\pm}}^{\mathrm{fin}}(\psi_{i,1}^{+})$. Therefore, in a similar way to the proof of Ref. 8, Theorem 3.5, we obtain the following theorem.

Theorem 4.13: *For* $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_{l}^{n}$, $\mathbf{a}\in\mathbb{C}^{\times}$, *let* $\mathbf{P}_{\mathbf{a}}^{\pm}=(P_{i,\mathbf{a}}^{\pm})_{i\in I}\in\mathbb{C}_l[t]^n$ *such that* $\tilde{V}_{\varepsilon}^{\mathrm{fin}}(\mathbf{P}_{\mathbf{a}}^{\pm})\cong V_{\varepsilon}^{\mathrm{fin}}(\lambda)_{\mathbf{a}}^{\pm}$. *Then, for any* $i\in I$ *such that* $P_{i,\mathbf{a}}^{\pm}\neq 1$, *we obtain*

$$P_{i,\mathbf{a}}^{\pm}=\prod_{p=1}^{\lambda_i}(t-\varepsilon^{\lambda_i-2p+1}\mathbf{a}_{(\pm,i)}), \tag{4.6}$$

where

$$\mathbf{a}_{(\pm,i)}:=\mathbf{a}^{-1}\varepsilon^{\pm(\lambda^{(i)}+i)}, \tag{4.7}$$

$$\lambda^{(i)}:=\sum_{k=1}^{i-1}\lambda_k-\sum_{k=i+1}^{n}\lambda_k. \tag{4.8}$$

Proof: We shall prove the case of $P_{i,\mathbf{a}}^{+}$. We can also prove the case of $P_{i,\mathbf{a}}^{-}$ similarly. Let v_+ be the highest-weight vector in $\tilde{V}_{\varepsilon}^{\mathrm{fin}}(\mathbf{P}_{\mathbf{a}}^{+})$. By (2.8), for any $i\in I$, we have

$$e_0v_+=(-1)^{i+1}\varepsilon^{n+1}[f_n,\cdots[f_{i+1},[f_1,\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}k_{\theta}^{-1}v_+.$$

Then we get

$$\begin{aligned}
e_ne_0v_+&=(-1)^{i+1}\varepsilon^{-\sum_{k\in I}\lambda_k+n+1}\{e_nf_n[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}\\
&\quad-\varepsilon^{-1}[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}e_nf_n\}v_+\\
&=(-1)^{i+1}\varepsilon^{-\sum_{k\in I}\lambda_k+n+1}\left\{\left(\frac{k_{\alpha_n}-k_{\alpha_n}^{-1}}{\varepsilon-\varepsilon^{-1}}\right)[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}\right.\\
&\quad\left.-\varepsilon^{-1}[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}\left(\frac{k_{\alpha_n}-k_{\alpha_n}^{-1}}{\varepsilon-\varepsilon^{-1}}\right)\right\}v_+\\
&=(-1)^{i+1}\varepsilon^{-\sum_{k\in I}\lambda_k+n+1}([\lambda_n+1]_{\varepsilon}-\varepsilon^{-1}[\lambda_n]_{\varepsilon})[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}v_+\\
&=(-1)^{i+1}\varepsilon^{\lambda_n-\sum_{k\in I}\lambda_k+n+1}[f_{n-1},[\cdots[f_{i-1},x_{i,1}^{-}]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}v_+.
\end{aligned}$$

By repeating this, we obtain

$$e_i\cdots e_1e_{i+1}\cdots e_ne_0v_+=e_i\{(-1)^{i+1}\varepsilon^{-\lambda_i+n+1}x_{i,1}^{-}v_+\}=(-1)^{i+1}\varepsilon^{-\lambda_i+n+1}x_{i,0}^{+}x_{i,1}^{-}v_+. \tag{4.9}$$

On the other hand, by (4.2), we have

$$e_0v_+=(\mathrm{ev}_{\mathbf{a}_+^{\lambda}}^{\mathrm{fin}})^{+}(e_0)v_+=\mathbf{a}_+^{\lambda}\varepsilon^{-1}k_{\Lambda_1}k_{\Lambda_n}^{-1}[f_n,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]\ {}_{\varepsilon^{-1}}v_+.$$

Since $(\Lambda_1-\Lambda_n,\theta)=0$, we have

$$k_{\Lambda_1}k_{\Lambda_n}^{-1}[f_n,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}=[f_n,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}k_{\Lambda_1}k_{\Lambda_n}^{-1}.$$

Moreover, we have $k_{\Lambda_1}v_+=\varepsilon^{\lambda_{\Lambda_1}}v_+$, $k_{\Lambda_n}v_+=\varepsilon^{\lambda_{\Lambda_n}}v_+$. So, by (4.4), we obtain

$$e_0v_+=\mathbf{a}\varepsilon^{n-1}[f_n,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}v_+.$$

In a similar way to the above-noted proof, we have

$$e_{i+1}\cdots e_ne_0v_+=\mathbf{a}\varepsilon^{\sum_{k=i+1}\lambda_k+n-1}[f_i,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}v_+.$$

Here, we obtain

$$\begin{aligned}e_1[f_i,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}v_+&=[f_i,[\cdots[f_2,e_1f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}v_+=\left\{[f_i,[\cdots[f_2,f_1e_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}\right.\\&\quad\left.+\left[f_{i,}\left[\cdots\left[f_2,\frac{k_{\alpha_1}-k_{\alpha_1}^{-1}}{\varepsilon-\varepsilon^{-1}}\right]_{\varepsilon^{-1}}\cdots\right]_{\varepsilon^{-1}}\right\}v_+\right.\\&=\{[f_i,[\cdots[f_2,f_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}e_1+[f_i,[\cdots[f_3,f_2]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}(-\varepsilon^{-1}k_{\alpha_1}^{-1})\}v_+\\&=\varepsilon^{-\lambda_1-1}[f_i,[\cdots[f_3,f_2]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}v_+.\end{aligned}$$

By repeating this, we get

$$e_i\cdots e_1e_{i+1}\cdots e_ne_0v_+=(-1)^{i-1}\mathbf{a}\varepsilon^{-\sum_{k=1}^{i-1}\lambda_k-(i-1)+\sum_{k=i+1}^{n}\lambda_k+n-1}e_if_iv_+=(-1)^{i-1}\mathbf{a}\varepsilon^{-\lambda^{(i)}-i+n}[\lambda_i]_\varepsilon v_+. \tag{4.10}$$

Thus, by (4.9) and (4.10), we obtain

$$\psi_{i,1}v_+=(\varepsilon-\varepsilon^{-1})x_{i,0}^+x_{i,1}^-v_+=\mathbf{a}\varepsilon^{\lambda_i-\lambda^{(i)}-i-1}(\varepsilon^{\lambda_i}-\varepsilon^{-\lambda_i})v_+.$$

On the other hand, by (4.5), we have $\psi_{i,1}^+v_+=\tilde{\Lambda}_{\mathbf{P}_\mathbf{a}^+}^{\mathrm{fin}}(\psi_{i,1}^+)v_+=\mathbf{a}_{(+,i)}^{-1}\varepsilon^{\lambda_i-1}(\varepsilon^{\lambda_i}-\varepsilon^{-\lambda_i})$. Therefore we obtain $\mathbf{a}_{(+,i)}=\mathbf{a}^{-1}\varepsilon^{\lambda^{(i)}+i}$.

For $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_l^n$, we set $\mathrm{supp}(\lambda):=\{i\in I\,|\,\lambda_i\neq 0\}$.

Proposition 4.14: Let $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_l^n$, $\mathbf{a}_\pm\in\mathbb{C}^\times$.

(*a*) *If* $\lambda=0$, *then* $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_+}^+$ *is isomorphic to* $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_-}^-$ *as a* $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module*.

(*b*) *In the case of* $\lambda\neq 0$, $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_+}^+$ *is isomorphic to* $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_-}^-$ *as a* $\tilde{U}_\varepsilon^{\mathrm{fin}}$*-module if and only if* $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ *for any* $i\in\mathrm{supp}(\lambda)$.

Proof: (a) is obvious. So we shall prove (b). By Theorem (4.8), $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_+}^+$ is isomorphic to $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_-}^-$ if and only if $\mathbf{P}_{\mathbf{a}_+}^+=\mathbf{P}_{\mathbf{a}_-}^-$. By (4.5) and Theorem 4.13, we obtain $\mathbf{P}_{\mathbf{a}_+}^+=\mathbf{P}_{\mathbf{a}_-}^-$ if and only if $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ for any $i\in\mathrm{supp}(\lambda)$.

Proposition 4.15: Let $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_l^n(\lambda\neq 0)$, $\mathbf{a}_\pm\in\mathbb{C}^\times$. *Let* $i_1,\ldots,i_m\in I$ *such that* $\mathrm{supp}(\lambda)=\{i_1,\ldots,i_m\}$ *and* $i_1<\ldots<i_m$. *Then* $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ *for any* $i\in\mathrm{supp}(\lambda)$ *if and only if the following conditions* (*a*) *and* (*b*) *hold*.

(*a*) *For any* $2\leqslant r\leqslant m$,

$$\lambda_{i_r}\equiv(-1)^{r-1}\lambda_{i_1}+(-1)^ri_1-i_r+2\sum_{k=2}^{r-1}(-1)^{r-1+k}i_k\equiv 0\quad(mod\ l).$$

(*b*)

$$\mathbf{a}_+=\begin{cases}\mathbf{a}_-\varepsilon^{2\sum_{k=1}^m(-1)^{k-1}i_k} & \text{if } m \text{ is odd}\\ \mathbf{a}_-\varepsilon^{2(\lambda_{i_1}+\sum_{k=2}^m(-1)^ki_k)} & \text{if } m \text{ is even}.\end{cases}$$

Proof: We assume $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ for any $i\in\mathrm{supp}(\lambda)$. Then $\varepsilon^{2(\lambda^{(i)}+i)}=\varepsilon^{2(\lambda^{(j)}+j)}$ for any $i,j\in\mathrm{supp}(\lambda)$. Hence, for $2\leqslant r\leqslant m$, we have $\lambda^{(i_r)}-\lambda^{(i_{r-1})}+i_r-i_{r-1}\equiv 0(\mathrm{mod}\, l)$. By (4.8), for $1\leqslant r\leqslant m$, we obtain

$$\lambda^{(i_r)}=\sum_{k=1}^{i_r-1}\lambda_k-\sum_{k=i_r+1}^{n}\lambda_k=\sum_{k=1}^{r-1}\lambda_{i_k}-\sum_{k=r+1}^{m}\lambda_{i_k}.$$

Thus, for $2\leqslant r\leqslant m$, we get

$$\lambda^{(i_r)}-\lambda^{(i_{r-1})}+i_r-i_{r-1}=\lambda_{i_r}+\lambda_{i_{r-1}}+i_r-i_{r-1}\equiv 0 \pmod{l}.$$

Hence $(-1)^r\lambda_{i_r}-(-1)^{r-1}\lambda_{i_{r-1}}\equiv(-1)^{r-2}i_{r-1}+(-1)^{r-1}i_r$. Therefore, we obtain

$$\begin{aligned}(-1)^r\lambda_{i_r}&\equiv-\lambda_{i_1}+\sum_{k=2}^{r}\{(-1)^k\lambda_{i_k}-(-1)^{k-1}\lambda_{i_{k-1}}\}\\&\equiv-\lambda_{i_1}+\sum_{k=2}^{r}\{(-1)^{k-1}i_k+(-1)^{k-2}i_{k-1}\}\\&\equiv-\lambda_{i_1}+i_1+(-1)^{r-1}i_r+2\sum_{k=2}^{r-1}(-1)^{k-1}i_k\quad(2\leqslant r\leqslant m).\end{aligned}$$

Thus we have (a). In particular, if λ_{i_r} is as in (a), then $\lambda_{i_{r-1}}+\lambda_{i_r}\equiv i_{r-1}-i_r$ for any $2\leqslant r\leqslant m$ and $\lambda^{(i)}+i\equiv\lambda^{(j)}+j$ for any $i,j\in\mathrm{supp}(\lambda)$. Hence, for $1\leqslant r\leqslant m$, we have $\lambda^{(i_r)}+i_r\equiv\lambda^{(1)}+i_1\equiv-\sum_{k=2}^{m}\lambda_{i_k}+i_1$. If m is odd, then we get

$$\begin{aligned}-\sum_{k=2}^{m}\lambda_{i_k}+i_1&\equiv-(\lambda_{i_2}+\lambda_{i_3})-\cdots-(\lambda_{i_{m-1}}+\lambda_{i_m})+i_1\\&\equiv(-i_2+i_3)+\cdots+(-i_{m-1}+i_m)+i_1\\&\equiv\sum_{k=1}^{m}(-1)^{k-1}i_k.\end{aligned}$$

Similarly, we have the case that m is even. Therefore we obtain (b). So we can prove "only if part" of this proposition. The proof of "if part" follows the proof of "only if part." □

Remark 4.16: For $\lambda=(\lambda_i)_{i\in I}\in\mathbb{Z}_+^n$, let $V_q(\lambda)$ be the finite-dimensional irreducible U_q-module with highest weight λ of type **1**. For $\mathbf{a}\in\mathbb{C}^\times$, let $V_q(\lambda)_{\mathbf{a}}^{\pm}$ be the evaluation representation of $V_q(\lambda)$ arising from $\mathrm{ev}_{\mathbf{a}}^{\pm}$ (see Ref. 8). In the case that q is not a root of unity, for any $\mathbf{a}_\pm\in\mathbb{C}^\times$, $V_q(\lambda)_{\mathbf{a}_+}^{+}$ is not isomorphic to $V_q(\lambda)_{\mathbf{a}_-}^{-}$ if $\#(\mathrm{supp}(\lambda))>1$. But, in the case that q is a root of unity, there exist $\lambda\in\mathbb{Z}_l^n$ and $\mathbf{a}_\pm\in\mathbb{C}^\times$ such that $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_+}^{+}$ is isomorphic to $V_\varepsilon^{\mathrm{fin}}(\lambda)_{\mathbf{a}_-}^{-}$ even if $\#(\mathrm{supp}(\lambda))>1$ by Propositions 4.14, 4.15.

V. EVALUATION REPRESENTATIONS OF NONRESTRICTED TYPE

A. Schnizer modules and evaluation representations

We fix the following notations. Let $N:=\frac{1}{2}n(n+1)$ be the number of the positive roots of $\mathfrak{sl}_{n+1}$. Let V_N be an l^N-dimensional $\mathbb{C}$-vector space and $\{v(m)\in V_N|m=(m_{i,j})_{1\leqslant i\leqslant j\leqslant n}\in\mathbb{Z}_l^N\}$ be a $\mathbb{C}$-basis of V_N. For $m\in\mathbb{Z}_l^N$, $m'\in\mathbb{Z}^N$, we set $v(m+lm'):=v(m)$. For $i,j\in I$, we define $\epsilon_{i,j}$, $\alpha_{i,j}\in\mathbb{Z}_l^N$ by

$$\epsilon_{i,j} := (\delta_{i,r}\delta_{j,s})_{1\leqslant r\leqslant s\leqslant n} \quad (i \leqslant j), \quad \alpha_{i,j} := \sum_{k=j+1}^{i} \epsilon_{k-1,n-i+k} - \sum_{k=j}^{i} \epsilon_{k,n-i+k} \quad (j \leqslant i), \tag{5.1}$$

where $\delta_{i,j}$ is Kronecker's symbol. For $i,j \in I$, $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^{\times})^N$, $c=(c_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^N$, we define

$$M_{i,j}(c) := \sum_{k=i-1}^{j-1} (c_{i,k} - c_{i-1,k}) + \sum_{k=i}^{j} (c_{i,k} - c_{i+1,k}) \quad (i \leqslant j), \tag{5.2}$$

$$N_{i,j}(c) := c_{j-1,n-i+j} - c_{j,n-i+j} \quad (j \leqslant i), \tag{5.3}$$

$$\mu_i(c) := \sum_{k=i-1}^{n} c_{i-1,k} - 2\sum_{k=i}^{n} c_{i,k} + \sum_{k=i+1}^{n} c_{i+1,k}, \tag{5.4}$$

$$a(c) := \prod_{1\leqslant i\leqslant j\leqslant n} a_{i,j}^{c_{i,j}}, \tag{5.5}$$

where $c_{i,j}=0$ if the index (i,j) is out of the range.

Theorem 5.1 (Ref. 24, Theorem 3.2, Ref. 23). *Let* $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^{\times})^N$, $b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^n$, and $\lambda=(\lambda_i)_{i\in I} \in \mathbb{C}^n$. Then there exists a $\mathbb{C}$ algebra homomorphism $\rho:=\rho(a,b,\lambda)$: $U_\varepsilon \to End(V_N)$ *such that for* $i \in I$ *and* $m \in \mathbb{Z}_l^N$,

$$\rho(E_i)(v(m)) = \sum_{j=1}^{i} a(\alpha_{i,j})[N_{i,j}(m+b)]_\varepsilon v(m+\alpha_{i,j}), \tag{5.6}$$

$$\rho(F_i)(v(m)) = \sum_{j=i}^{n} a_{i,j}[M_{i,j}(m+b) - \lambda_i]_\varepsilon v(m+\epsilon_{i,j}), \tag{5.7}$$

$$\rho(K_{\alpha_i})(v(m)) = \varepsilon^{\mu_i(m+b)+\lambda_i} v(m). \tag{5.8}$$

We denote the l^N-dimensional U_ε-module associated with $(\rho(a,b,\lambda),V_N)$ by $V_\varepsilon(a,b,\lambda)$. We call $V_\varepsilon(a,b,\lambda)$ a "Schnizer module."

Now, for $i \in I$ and $r=(r_1,\ldots,r_i) \in I^i$, we set

$$F_{\theta_i} := [F_i,[\cdots[F_2,F_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}, \quad E_{\theta_i} := [E_i,[\cdots[E_2,E_1]_{\varepsilon^{-1}}\cdots]_{\varepsilon^{-1}}, \tag{5.9}$$

$$\epsilon_r := \sum_{k=1}^{i} \epsilon_{k,r_k}, \quad \alpha_r := \sum_{k=1}^{i} \alpha_{k,r_k}. \tag{5.10}$$

For $1 \leqslant s \leqslant i$, we set

$$R_{s,i} := \{r_i^s = (r_{1,i}^s,\ldots,r_{i,i}^s) \in I^i | r_{1,i}^s \geqslant \cdots \geqslant r_{s-1,i}^s \geqslant r_{s,i}^s < r_{s+1,i}^s < \cdots < r_{i,i}^s\},$$

$$R_{s,i}^F := \{r_i^s = (r_{1,i}^s,\ldots,r_{i,i}^s) \in R_{s,i} | k \leqslant r_{k,i}^s \text{ for } 1 \leqslant k \leqslant i\},$$

$$R_{s,i}^E := \{r_i^s = (r_{1,i}^s,\ldots,r_{i,i}^s) \in R_{s,i} | r_{k,i}^s \leqslant k \text{ for } 1 \leqslant k \leqslant i\},$$

$$R_i^F := \bigsqcup_{s=1}^{i} R_{s,i}^F, \quad R_i^E := \bigsqcup_{s=1}^{i} R_{s,i}^E. \tag{5.11}$$

Moreover, for $c \in \mathbb{C}^N$, set

$$C_i(c, r_i^s) := \sum_{k=1}^{s-1} M_{k,r_{k,i}^s}(c) - \sum_{k=s+1}^{i} M_{k,r_{k,i}^s}(c) \quad (r_i^s \in R_{i,s}^F).$$

$$D_i(c, r_i^s) := \sum_{k=1}^{s-1} N_{k,r_{k,i}^s}(c) - \sum_{k=s+1}^{i} N_{k,r_{k,i}^s}(c) \quad (r_i^s \in R_{i,s}^E). \tag{5.12}$$

Lemma 5.2: Let $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^\times)^N$, $b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^N$, $\lambda=(\lambda_i)_{i\in I} \in \mathbb{C}^n$, $i \in I$, *and* $m=(m_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{Z}_l^N$. *We have*

$$F_{\theta_i} v(m) = \sum_{r_i^s \in R_i^F} (-1)^{i+s} a(\epsilon_{r_i^s}) \varepsilon^{C_i(m+b, r_i^s) - \lambda^{(s,i)} + 1 - s} [M_{s,r_{s,i}^s}(m+b) - \lambda_s]_\varepsilon v(m + \epsilon_{r_i^s}),$$

$$E_{\theta_i} v(m) = \sum_{r_i^s \in R_i^E} (-1)^{i+s} a(\alpha_{r_i^s}) \varepsilon^{D_i(m+b, r_i^s) + 1 - s} [N_{s,1}(m+b) - \lambda_s]_\varepsilon v(m + \alpha_{r_i^s}),$$

in $V_\varepsilon(a,b,\lambda)$, *where* $\lambda^{(s,i)} := \Sigma_{k=1}^{s-1} \lambda_k - \Sigma_{k=s+1}^{i} \lambda_k$.

Proof: We shall prove the F_{θ_i}-case by the induction on i. We can prove the E_{θ_i}-case similarly. If $i=1$, then we have

$$F_{\theta_1} v(m) = \sum_{r_1^1 \in R_1^F} a(\epsilon_{1,r_{1,1}^1}) [M_{1,r_{1,1}^1}(m+b) - \lambda_1]_\varepsilon v(m + \epsilon_{1,r_{1,1}^1}).$$

We replace $r_{1,1}^1$ with j. Then we obtain

$$F_{\theta_1} v(m) = \sum_{j=1}^{n} a(\epsilon_{1,j}) [M_{1,j}(m+b) - \lambda_1]_\varepsilon v(m + \epsilon_{1,j}) = F_1 v(m).$$

Now we assume that $i>1$ and the case of $(i-1)$ holds. For $i \leqslant j \leqslant n$, $r_{i-1}^s \in R_{i-1}^F$, we set

$$\begin{aligned} \mathbf{M}(r_{i-1}^s, j) := {} & [M_{s,r_{s,i-1}^s}(m+b) - \lambda_s]_\varepsilon [M_{i,j}(m+b) - \lambda_i + M_{i,j}(\epsilon_{r_{i-1}^s})]_\varepsilon - \varepsilon^{C_{i-1}(\epsilon_{i,j}, r_{i-1}^s) - 1} [M_{s,r_{s,i-1}^s}(m+b) \\ & - \lambda_s + M_{s,r_{s,i-1}^s}(\epsilon_{i,j})]_\epsilon [M_{i,j}(m+b) - \lambda_i]_\varepsilon. \end{aligned}$$

Then, by the assumption of the induction, we have

$$\begin{aligned} F_{\theta_i} v(m) &= [F_i, F_{\theta_{i-1}}]_{\varepsilon^{-1}} v(m) \\ &= \sum_{j=i}^{n} \sum_{r_{i-1}^s \in R_{i-1}^F} (-1)^{i+s-1} a_{i,j} a(\epsilon_{r_{i-1}^s}) \varepsilon^{C_{i-1}(m+b, r_{i-1}^s) - \lambda^{(s,i-1)} + 1 - s} \mathbf{M}(r_{i-1}^s, j) v(m + \epsilon_{r_{i-1}^s} + \epsilon_{i,j}). \end{aligned}$$

Now we set

$$\xi(j > j') := \begin{cases} 1 & \text{if } j > j' \\ 0 & \text{if } j \leqslant j', \end{cases} \qquad \xi(j \leqslant j') := \begin{cases} 1 & \text{if } j \leqslant j' \\ 0 & \text{if } j > j'. \end{cases}$$

Then, for any $1 \leqslant i \leqslant j \leqslant n$, $1 \leqslant i' \leqslant j' \leqslant n$, we get

$$M_{i,j}(\epsilon_{i',j'}) = -\delta_{i-1,i'}\xi(j > j') + \delta_{i,i'}\xi(j > j') + \delta_{i,i'}\xi(j \geqslant j') - \delta_{i+1,i'}\xi(j \geqslant j'),$$

Hence, for any $i \leqslant j \leqslant n$, $1 \leqslant s \leqslant i-1$, $r^s_{i-1} \in R^F_{i-1}$, we have

$$M_{i,j}(\epsilon_{r^s_{i-1}}) = -\xi(j > r^s_{i-1,i-1}), \quad M_{s,r^s_{s,i-1}}(\epsilon_{i,j}) = -\delta_{s,i-1}\xi(r^{i-1}_{i-1,i-1} \geqslant j),$$

$$C_{i-1}(\epsilon_{i,j}, r^s_{i-1}) = \xi(i-1 > s)\xi(r^s_{i-1,i-1} \geqslant j).$$

Thus, we have

$$\begin{aligned}\mathbf{M}(r^s_{i-1}, j) = {} & [M_{s,r^s_{s,i-1}}(m+b) - \lambda_s]_\varepsilon [M_{i,j}(m+b) - \lambda_i - \xi(j > r^s_{i-1,i-1})]_\varepsilon \\ & - \varepsilon^{\xi(i-1>s)\xi(r^s_{i-1,i-1} \geqslant j)-1}[M_{s,r^s_{s,i-1}}(m+b) - \lambda_s - \delta_{s,i-1}\xi(r^{i-1}_{i-1,i-1} \geqslant j)]_\varepsilon [M_{i,j}(m+b) - \lambda_i]_\varepsilon.\end{aligned}$$

Since $[c]_\varepsilon - \varepsilon^{-1}[c-1]_\varepsilon = \varepsilon^{c-1}$ and $[c-1]_\varepsilon - \varepsilon^{-1}[c]_\varepsilon = -\varepsilon^{-c}$ for any $c \in \mathbb{C}$, we have

$$\mathbf{M}(r^s_{i-1}, j) = -\varepsilon^{M_{i,j}(m+b)+\lambda_i}[M_{s,r^s_{s,i-1}}(m+b) - \lambda_s]_\varepsilon \quad (s \leqslant i-1, r^s_{i-1,i-1} < j),$$

$$\mathbf{M}(r^s_{i-1}, j) = 0 \quad (s < i-1, j \leqslant r^s_{i-1,i-1}),$$

$$\mathbf{M}(r^{i-1}_{i-1}, j) = \varepsilon^{\tilde{M}(r^{i-1}_{i-1},j)}[M_{i,j}(m+b) - \lambda_i]_\varepsilon \quad (j \leqslant r^{i-1}_{i-1,i-1}),$$

where $\tilde{M}(r^{i-1}_{i-1}, j) := M_{i-1,r^{i-1}_{i-1,i-1}}(m+b) - \lambda_{i-1} - 1$. Therefore we obtain

$$\begin{aligned}F_{\theta_i} v(m) = {} & \sum_{j > r^s_{i-1,i-1}} \sum_{r^s_{i-1} \in R^F_{i-1}} (-1)^{i+s} a(\epsilon_{r^s_{i-1}} + \epsilon_{i,j}) \varepsilon^{C_{i-1}(m+b, r^s_{i-1}) - M_{i,j}(m+b) - \lambda^{(s,i)} + 1 - s}[M_{s,r^s_{s,i-1}}(m+b) \\ & - \lambda_s]_\varepsilon v(m + \epsilon_{r^s_{i-1}} + \varepsilon_{i,j}) + \sum_{j \leqslant r^s_{i-1,i-1}} \sum_{r^{i-1}_{i-1} \in R^F_{i-1,i-1}} (-1)^{i+i} a(\epsilon_{r^{i-1}_{i-1}} \\ & + \epsilon_{i,j}) \varepsilon^{C_{i-1}(m+b, r^{i-1}_{i-1}) - M_{i,j}(m+b) - \lambda^{(i,i)} + 1 - i}[M_{i,j}(m+b) - \lambda_i]_\varepsilon v(m + \epsilon_{r^{i-1}_{i-1}} + \varepsilon_{i,j}).\end{aligned}$$

Here, if we set

$$r^s_i = (r^s_{1,i}, \ldots, r^s_{i,i}) := \begin{cases} (r^s_{1,i-1}, \ldots, r^s_{i-1,i-1}, j) & \text{if } s \leqslant i-1 \text{ and } j > r^s_{i-1,i-1} \\ (r^{i-1}_{1,i-1}, \ldots, r^{i-1}_{i-1,i-1}, j) & \text{if } s = i \text{ and } j \leqslant r^{i-1}_{i-1,i-1}, \end{cases}$$

then we have F_{θ_i}-case. □

For $s \in I$, we set

$$R_s := \{r^s = (r^s_k)_{k \in I} \in I^n \,|\, r^s_1 \geqslant \cdots \geqslant r^s_{s-1} \geqslant r^s_s < r^s_{s+1} < \cdots < r^s_n\},$$

$$R^F_s := \{r^s = (r^s_i)_{i \in I} \in R_s \,|\, k \leqslant r^s_k \text{ for any } k \in I\},$$

$$R^E_s := \{r^s = (r^s_i)_{i \in I} \in R_s \,|\, r^s_k \leqslant k \text{ for any } k \in I\},$$

$$R^F := \bigsqcup_{s=1}^{n} R^F_s, \quad R^E := \bigsqcup_{s=1}^{n} R^E_s. \tag{5.13}$$

Note if $r^s = (r^s_k)_{k \in I} \in R^F_s$ (respectively, R^E_s), then $r^s_k = k$ for any $s \leqslant k \leqslant n$ (respectively, $r^s_k = 1$ for any $1 \leqslant k \leqslant s$). Moreover, for $c \in \mathbb{C}^N$, we set

$$C(c,r^s) := c_{s-1,s-1} - c_{n,n} + \sum_{k=1}^{n} c_{1,k} + \sum_{k=1}^{s-1} \sum_{p=r_{k+1}^s}^{r_k^s - 1} c_{k,p} - \sum_{k=1}^{s} \sum_{p=r_k^s+1}^{r_{k-1}^s} c_{k,p} \quad (r^s \in R_s^F),$$

$$D(c,r^s) := - \sum_{k=n-s+2}^{n} c_{1,k} - \sum_{k=s+1}^{n} (c_{r_k^s-1,n-k+r_k^s} - c_{r_k^s,n-k+r_k^s}) \quad (r^s \in R_s^E), \tag{5.14}$$

where $r_0^s := n$. Then, by Lemma 5.2, we obtain the following lemma.

Lemma 5.3: Let $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^\times)^N$, $b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^N$, $\lambda=(\lambda_i)_{i\in I} \in \mathbb{C}^n$, *and* $m=(m_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{Z}_l^N$. *We have*

$$F_{\theta_n} v(m) = \sum_{r^s \in R^F} (-1)^{s+n} a(\epsilon_{r^s}) \varepsilon^{C(m+b,r^s)-\lambda^{(s)}+1-s} [-m_{s-1,s-1} + m_{s,s} - b_{s-1,s-1} + b_{s,s} - \lambda_s]_\varepsilon v(m+\epsilon_{r^s}),$$

$$E_{\theta_n} v(m) = \sum_{r^s \in R^E} (-1)^{s+n} a(\alpha_{r^s}) \varepsilon^{D(m+b,r^s)+1-s} [-m_{1,n-s+1} - b_{1,n-s+1}]_\varepsilon v(m+\alpha_{r^s}),$$

in $V_\varepsilon(a,b,\lambda)$, *where* $\lambda^{(s)}$ *as in (4.8).*

Let $U'_{\mathcal{A}}$ (respectively, U'_ε) be the extended algebra of $U_{\mathcal{A}}$ (respectively, U_ε) defined by replacing $\{K_\mu | \mu \in Q\}$ with $\{K_\mu | \mu \in P\}$ (see Definition 2.1). By (2.18), we have $\mathrm{ev}_{\mathbf{a}}^{\pm}(\widetilde{U}_{\mathcal{A}}) \subset U'_{\mathcal{A}}(\mathbf{a} \in \mathbb{C}^\times)$. So we obtain the evaluation homomorphisms $\mathrm{ev}_{\mathbf{a}}^{\pm}: \widetilde{U}_\varepsilon \to U'_\varepsilon$ as in Proposition 2.6. On the other hand, by (2.1), we can regard an arbitrary Schnizer module $V_\varepsilon(a,b,\lambda)$ as a U'_ε-module if we define

$$K_{\Lambda_i} v(m) := \varepsilon^{-\sum_{k=i}^{n} (m_{i,k}+b_{i,k})+\lambda_{\Lambda_i}} v(m), \tag{5.15}$$

for any $i \in I$, $m \in \mathbb{Z}_l^N$, where λ_{Λ_i} as in (4.3).

Definition 5.4: Let $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^\times)^N$, $b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^N$, $\lambda=(\lambda_i)_{i\in I} \in \mathbb{C}^n$, and $\mathbf{a} \in \mathbb{C}^\times$. Then we define $\widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm} := \widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm}(a,b,\lambda) := \rho(a,b,\lambda) \circ \mathrm{ev}_{\mathbf{a}_\pm^\lambda}^{\pm}: \widetilde{U}_\varepsilon \to \mathrm{End}(V_N)$, where $\rho=\rho(a,b,\lambda)$ is as in Theorem 5.1 and $\mathbf{a}_\pm^\lambda$ are as in (4.4). We denote the l^N-dimensional $\widetilde{U}_\varepsilon$-module associated with $(\widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm}, V_N)$ by $V_\varepsilon(a,b,\lambda)_{\mathbf{a}}^{\pm}$.

For $c \in C^N$, we set

$$C_E(c,r^s) := c_{s-1,s-1} + \sum_{k=1}^{s-1} \sum_{p=r_{k+1}^s}^{r_k^s - 1} c_{k,p} - \sum_{k=1}^{s} \sum_{p=r_k^s+1}^{r_{k-1}^s} c_{k,p} \quad (r^s \in R_s^F),$$

$$D_F(c,r^s) := - c_{n,n} + \sum_{k=1}^{n-s+1} c_{1,k} - \sum_{k=s+1}^{n} (c_{r_k^s-1,n-k+r_k^s} - c_{r_k^s,n-k+r_k^s}) \quad (r^s \in R_s^E). \tag{5.16}$$

Proposition 5.5: Let $a=(a_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in (\mathbb{C}^\times)^N$, $b=(b_{i,j})_{1\leqslant i\leqslant j\leqslant n} \in \mathbb{C}^N$, $\lambda=(\lambda_i)_{i\in I} \in \mathbb{C}^n$, *and* $\mathbf{a} \in \mathbb{C}^\times$. *Then, for any* $i \in I$ *and* $m \in \mathbb{Z}_l^N$, *we obtain*

$$\widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm}(E_i)(v(m)) = \rho(E_i)(v(m)), \quad \widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm}(F_i)(v(m)) = \rho(F_i)(v(m)),$$

$$\widetilde{\mathrm{ev}}_{\mathbf{a}}^{\pm}(K_{\alpha_i})(v(m)) = \rho(K_{\alpha_i})(v(m)),$$

$$\widetilde{\mathrm{ev}}^{\pm}_{\mathbf{a}}(E_0)(v(m)) = \mathbf{a} \sum_{r^s \leqslant R^F} (-1)^{s+n} a(\epsilon_{r^s}) \varepsilon^{\pm(C_E(m+b,r^s)-\lambda^{(s)}-s)+n}[-m_{s-1,s-1}+m_{s,s}-b_{s-1,s-1}+b_{s,s}-\lambda_s]_\varepsilon \times v(m+\epsilon_{r^s}),$$

$$\widetilde{\mathrm{ev}}^{\pm}_{\mathbf{a}}(F_0)(v(m)) = \mathbf{a}^{-1} \sum_{r^s \leqslant R^E} (-1)^{s-1} a(\alpha_{r^s}) \varepsilon^{\pm(D_F(m+b,r^s)-s+n+1)-n}[-m_{1,n-s+1}-b_{1,n-s}]_\varepsilon v(m+\alpha_{r^s}),$$

where ϵ_{r^s}, α_{r^s} *are as in (5.10),* R^F, R^E *are as in (5.13), and* $C_E(m+b,r^s)$, $D_F(m+b,r^s)$ *are as in (5.16).*

Proof: By Proposition 2.6, Theorem 5.1, Lemma 5.3, and (5.15), we obtain the $\widetilde{\mathrm{ev}}^{+}_{\mathbf{a}}$-case. Similarly, we obtain the $\widetilde{\mathrm{ev}}^{-}_{\mathbf{a}}$-case. □

B. Nilpotent modules

Definition 5.6: Let V be a $\widetilde{U}_\varepsilon$-module (respectively, U_ε-module). We assume $E^l_\beta = F^l_\beta = E_{(i,sl\delta)} = F_{(i,sl\delta)} = 0$ on V for any $\beta \in \widetilde{\Delta}^{\mathrm{re}}_+$, $i \in I$, $s \in \mathbb{N}$ (respectively, $\bar{E}^l_\gamma = \bar{F}^l_\gamma = 0$ on V for any $\gamma \in \Delta_+$). Then we call V a "nilpotent" $\widetilde{U}_\varepsilon$-module (respectively, U_ε-module). In particular, if $K^l_\mu = 1$ on V for any $\mu \in Q$, then we call V a nilpotent $\widetilde{U}_\varepsilon$-module (respectively U_ε-module) of "type **1**."

For $\lambda \in \mathbb{Z}^n_l$, let $V^{\mathrm{fin}}_\varepsilon(\lambda)$ be the $U^{\mathrm{fin}}_\varepsilon$-module in Sec. IV A. By Proposition 3.14, we can regard $V^{\mathrm{fin}}_\varepsilon(\lambda)$ as a nilpotent U_ε-module. We denote U_ε-module $V^{\mathrm{fin}}_\varepsilon(\lambda)$ by $V^{\mathrm{nil}}_\varepsilon(\lambda)$. By Proposition 3.14 and Theorem 4.7, we obtain the following proposition.

Proposition 5.7: For any $\lambda \in \mathbb{Z}^n_l$, $V^{\mathrm{nil}}_\varepsilon(\lambda)$ *is a finite-dimensional irreducible nilpotent* U_ε*-module of type* **1**. *Conversely, for any finite-dimensional irreducible nilpotent* U_ε*-module* V *of type* **1**, *there exists a unique* $\lambda \in \mathbb{Z}^n_l$ *such that* V *is isomorphic to* $V^{\mathrm{nil}}_\varepsilon(\lambda)$.

We can construct $V^{\mathrm{nil}}_\varepsilon(\lambda)$ as a U_ε-submodule of Schnizer module $V_\varepsilon(a,b,\lambda)$ as follows (Refs. 1, 2, and 22). For $i,j \in I (i \leqslant j)$, $\lambda \in \mathbb{Z}^n_l$, we set

$$a^{(0)}_{i,j} := 1, \quad b^{(0)}_{i,j} := 0, \quad a^{(0)} := (a^{(0)}_{i,j})_{1 \leqslant i \leqslant j \leqslant n}, \quad b^{(0)} := (b^{(0)}_{i,j})_{1 \leqslant i \leqslant j \leqslant n}, \tag{5.17}$$

$$\rho^0_\lambda := \rho(a^{(0)}, b^{(0)}, \lambda), \quad V^0_\varepsilon(\lambda) := V_\varepsilon(a^{(0)}, b^{(0)}, \lambda). \tag{5.18}$$

We denote $v(0)$ in $V^0_\varepsilon(\lambda)$ by $v_\lambda(0)$. For $\lambda = (\lambda_i)_{i \in I} \in \mathbb{Z}^n_l$, we define $m^\lambda = (m^\lambda_{i,j})_{1 \leqslant i \leqslant j \leqslant n} \in \mathbb{Z}^n_l$ by

$$m^\lambda_{i,j} \equiv \sum_{k=1}^{i} \lambda_{j-k+1} \pmod{l} \quad 1 \leqslant i \leqslant j \leqslant n. \tag{5.19}$$

Proposition 5.8: Let $\lambda \in \mathbb{Z}^n_l$ *and* $v \in V^0_\varepsilon(\lambda)$.
(*a*) $E_i v = 0$ *for any* $i \in I$ *if and only if* $v \in \mathbb{C} v_\lambda(0)$.
(*b*) $F_i v = 0$ *for any* $i \in I$ *if and only if* $v \in \mathbb{C} v(m^\lambda)$.

Proof: By Ref. 2, we obtain (a). So we shall prove (b). "If part." By (5.19), we have

$$m^\lambda_{i,i} - m^\lambda_{i-1,i-1} = \lambda_i, \quad m^\lambda_{i,j} - m^\lambda_{i-1,j} = \lambda_{j-i+1}, \quad m^\lambda_{i,j} - m^\lambda_{i+1,j} = -\lambda_{j-i}, \tag{5.20}$$

for any $1 \leqslant i \leqslant j \leqslant n$. Hence, by (5.2), we get

$$M_{i,j}(m^\lambda) = m^\lambda_{i,i} - m^\lambda_{i-1,i-1} + \sum_{k=i}^{j-1} (m^\lambda_{i,k} - m^\lambda_{i-1,k}) + \sum_{k=i+1}^{j} (m^\lambda_{i,k} - m^\lambda_{i+1,k})$$
$$= \lambda_i + \left(\sum_{k=i}^{j-1} \lambda_{k-i+1} - \sum_{k=i+1}^{j} \lambda_{k-i} \right) = \lambda_i,$$

for any $1 \leqslant i \leqslant j \leqslant n$. Therefore, by (5.7), we obtain

$$F_i v(m^\lambda) = \sum_{j=i}^{n} [M_{i,j}(m^\lambda) - \lambda_i]_\varepsilon v(m^\lambda + \epsilon_{i,j}) = \sum_{j=i}^{n} [\lambda_i - \lambda_i]_\varepsilon v(m^\lambda + \epsilon_{i,j}) = 0 \quad (i \in I).$$

"Only if part." Let $v = \Sigma_{m \in \mathbb{Z}_l^n} c_m v(m) \in V(\lambda) (c_m \in \mathbb{C})$. We assume that $F_i v = 0$ for any $i \in I$. Set

$$\mathbb{Z}_l^n(r) := \{m = (m_{i,j})_{1 \leqslant i \leqslant j \leqslant n} \in \mathbb{Z}_l^n | m_{i,j} = m_{i,j}^\lambda \text{ if } j - i < r\} \ (r = 1, \ldots, n), \quad \mathbb{Z}_l^n(0) := \mathbb{Z}_l^n.$$

Then we have

$$\mathbb{Z}_l^n = \mathbb{Z}_l^n(0) \supset \mathbb{Z}_l^n(1) \supset \cdots \supset \mathbb{Z}_l^n(n) = \{m^\lambda\}.$$

We shall prove that $v = \Sigma_{m \in \mathbb{Z}_l^n(r)} c_m v(m)$ for all $0 \leqslant r \leqslant n$ by the induction on r. Indeed, if we can prove this claim, then we obtain $v = c_{m^\lambda} v(m^\lambda) \in \mathbb{C} v(m^\lambda)$. If $r = 0$, then there is nothing to prove. So we assume that $r > 0$ and the case of $(r-1)$ holds.

In a similar way to the proof of "if part," for any $m \in \mathbb{Z}_l^n(r-1)$, we have $M_{i,j}(m) = \lambda_i$ if $j - i < r - 1$. Moreover, for any $m \in \mathbb{Z}_l^n(r-1)$ and $i \in I$ such that $i + r - 1 \leqslant n$, we get

$$M_{i,i+r-1}(m) = \sum_{k=i}^{i+r-2} m_{i,k} - \sum_{k=i-1}^{i+r-2} m_{i-1,k} + \sum_{k=i}^{i+r-1} m_{i,k} - \sum_{k=i+1}^{i+r-1} m_{i+1,k} = M_{i,i+r-1}(m^\lambda) - m_{i-1,i+r-2} + m_{i,i+r-1}$$
$$+ m_{i-1,i+r-2}^\lambda - m_{i,i+r-1}^\lambda = \lambda_i - m_{i-1,i+r-2} + m_{i,i+r-1} - \lambda_{i+r-1}.$$

Therefore, by (5.7), we get

$$F_i v = \sum_{m \in \mathbb{Z}_l^n(r-1)} c_m [m_{i,i+r-1} - m_{i-1,i+r-2} - \lambda_{i+r-1}]_\varepsilon v(m + \epsilon_{i,i+r-1})$$
$$+ \sum_{j=i+r}^{n} \sum_{m \in \mathbb{Z}_l^n(r-1)} c_m [M_{i,j}(m) - \lambda_i]_\varepsilon v(m + \epsilon_{i,j}) = 0 \quad (i \leqslant n - r + 1). \tag{5.21}$$

Now, for $1 \leqslant s \leqslant n - r + 1$, we set

$$\mathbb{Z}_l^n(r-1, s) := \{m = (m_{i,j})_{1 \leqslant i \leqslant j \leqslant n} \in \mathbb{Z}_l^n(r-1) | m_{i,i+r-1} - m_{i-1,i+r-2} \equiv \lambda_{i+r-1} \pmod{l} \text{ if } s \leqslant i \leqslant n - r + 1\}.$$

We have $m_{i,i+r-1} - m_{i-1,i+r-2} \equiv \lambda_{i+r-1}$ for any $1 \leqslant i \leqslant n - r + 1$ if and only if $m_{i,i+r-1} = m_{i,i+r-1}^\lambda$ for any $1 \leqslant i \leqslant n - r + 1$. Hence we get

$$\mathbb{Z}_l^n(r-1) \supset \mathbb{Z}_l^n(r-1, n-r+1) \supset \cdots \supset \mathbb{Z}_l^n(r-1, 1) = \mathbb{Z}_l^n(r).$$

So it is enough to prove that $v = \Sigma_{m \in \mathbb{Z}_l^n(r-1,s)} c_m v(m)$ for all $1 \leqslant s \leqslant n - r + 1$. We shall prove this claim by the induction on s. By (5.21), we obtain

$$F_{n-r+1} v = \sum_{m \in \mathbb{Z}_l^n(r-1)} c_m [m_{n-r+1,n} - m_{n-r,n-1} - \lambda_n]_\varepsilon v(m + \epsilon_{n-r+1,n}) = 0.$$

Thus, $c_m [m_{n-r+1,n} - m_{n-r,n-1} - \lambda_n]_\varepsilon = 0$ for any $m \in \mathbb{Z}_l^n(r-1)$. So if $c_m \neq 0$ for any $m \in \mathbb{Z}_l^n(r-1)$, then $m_{n-r+1,n} - m_{n-r,n-1} \equiv \lambda_n$. Hence $v = \Sigma_{m \in \mathbb{Z}_l^n(r-1,n-r+1)} c_m v(m)$.

Now we assume that $s < n - r + 1$ and the case of $(s+1)$ holds. By (5.21), we get

$$F_s v = \sum_{m \in \mathbb{Z}_l^n(r-1,s+1)} c_m [m_{s,s+r-1} - m_{s-1,s+r-2} - \lambda_{s+r-1}]_\varepsilon v(m + \epsilon_{s,s+r-1}) + \sum_{j=s+r}^{n} \sum_{m \in \mathbb{Z}_l^n(r-1,s+1)} c_m [M_{s,j}(m)$$
$$- \lambda_s]_\varepsilon v(m + \epsilon_{s,j}) = 0.$$

Here, for $m = (m_{i,j})_{1 \leqslant i \leqslant j \leqslant n} \in \mathbb{Z}_l^n(r-1, s+1)$, we obtain

$$(m+\epsilon_{s,s+r-1})_{s+1,s+r}-(m+\epsilon_{s,s+r-1})_{s,s+r-1}\equiv(m_{s+1,s+r}-m_{s,s+r-1})-1\equiv\lambda_{s+r}-1,$$

$$(m+\epsilon_{s,j})_{s+1,s+r}-(m+\epsilon_{s,j})_{s,s+r-1}\equiv m_{s+1,s+r}-m_{s,s+r-1}\equiv\lambda_{s+r}\ (s+r\leqslant j\leqslant n).$$

Hence, by the linear independence, we obtain $c_m[m_{s,s+r-1}-m_{s-1,s+r-2}-\lambda_{s+r-1}]_\varepsilon=0$ for any $m\in\mathbb{Z}_l^n(r-1,s+1)$. So if $c_m\neq 0$, then $m_{s,s+r-1}-m_{s-1,s+r-2}\equiv\lambda_{s+r-1}$ for any $m\in\mathbb{Z}_l^n(r-1,s+1)$. Then we have $v=\Sigma_{m\in\mathbb{Z}_l^n(r-1,s)}c_m v(m)$. □

For $\lambda\in\mathbb{Z}_l^n$, let $V_\varepsilon^0(\lambda)$ be as in (5.18) and $L_\varepsilon^{\mathrm{nil}}(\lambda)$ be the U_ε-submodule of $V_\varepsilon^0(\lambda)$ generated by $v_\lambda(0)$.

Proposition 5.9 (Refs. 2 and 22): For any $\lambda\in\mathbb{Z}_l^n$, $L_\varepsilon^{\mathrm{nil}}(\lambda)$ *is isomorphic to* $V_\varepsilon^{\mathrm{nil}}(\lambda)$ *as a* U_ε*-module*.

For $\mathbf{a}\in\mathbb{C}^\times$, $\lambda\in\mathbb{Z}_l^n$, let $V_\varepsilon^0(\lambda)_\mathbf{a}^\pm$ (respectively, $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^\pm$) be the evaluation representation of $V_\varepsilon^0(\lambda)$ (respectively, $L_\varepsilon^{\mathrm{nil}}(\lambda)$) (see Definition 5.4). Then $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^\pm$ is the $\widetilde{U}_\varepsilon$-submodule of $V_\varepsilon^0(\lambda)_\mathbf{a}^\pm$ generated by $v_\lambda(0)$, respectively.

Now, let $\widetilde{\phi}:\widetilde{U}_\varepsilon/\widetilde{I}_\varepsilon\to\widetilde{U}_\varepsilon^{\mathrm{fin}}$ (respectively, $\bar{\phi}:U_\varepsilon/I_\varepsilon\to U_\varepsilon^{\mathrm{fin}}$) be the isomorphism in Theorem 3.15 (respectively, Proposition 3.14). Let I_ε' be the two-sided ideal of U_ε' generated by $\{\widetilde{E}_\gamma^l,\widetilde{F}_\gamma^l,K_\mu^{2l}-1\,|\,\gamma\in\Delta_+,\mu\in P\}$. Then we can regard $\bar{\phi}$ as an isomorphism from $U_\varepsilon'/I_\varepsilon'$ to $(U_\varepsilon^{\mathrm{fin}})'$. Let $\widetilde{\pi}:\widetilde{U}_\varepsilon\to\widetilde{U}_\varepsilon/\widetilde{I}_\varepsilon$ (respectively, $\pi:U_\varepsilon'\to U_\varepsilon'/I_\varepsilon'$) be the projection and $\mathrm{ev}_\mathbf{a}^\pm:\widetilde{U}_\varepsilon\to U_\varepsilon'$ (respectively, $(\mathrm{ev}_\mathbf{a}^{\mathrm{fin}})^\pm:\widetilde{U}_\varepsilon^{\mathrm{fin}}\to(U_\varepsilon^{\mathrm{fin}})'$) be the evaluation homomorphism in Proposition 2.6 (respectively, (4.2))). Then, by the definition of these maps, the following diagram commutes:

$$\begin{array}{ccc}
\widetilde{U}_\varepsilon & \xrightarrow{\mathrm{ev}_\mathbf{a}^\pm} & U_\varepsilon' \\
\widetilde{\pi}\downarrow & & \downarrow\pi \\
\widetilde{U}_\varepsilon/\widetilde{I}_\varepsilon & & U_\varepsilon'/I_\varepsilon' \\
\widetilde{\phi}\downarrow & & \uparrow\widetilde{\phi}^{-1} \\
\widetilde{U}_\varepsilon^{\mathrm{fin}} & \xrightarrow{(\mathrm{ev}_\mathbf{a}^{\mathrm{fin}})^\pm} & (U_\varepsilon^{\mathrm{fin}})'
\end{array} \tag{5.22}$$

Proposition 5.10: For any $\mathbf{a}\in\mathbb{C}^\times$ *and* $\lambda\in\mathbb{Z}_l^n$, $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^\pm$ *is a finite-dimensional irreducible nilpotent* $\widetilde{U}_\varepsilon$*-module of type* **1**.

Proof: We shall prove the case of $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$. Since we can prove the case of $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^-$ similarly. By Theorem 5.9, $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$ is a finite-dimensional irreducible $\widetilde{U}_\varepsilon$-module of type **1**. So we shall prove, that $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$ is a nilpotent $\widetilde{U}_\varepsilon$-module.

For $\lambda\in\mathbb{Z}_l^n$, let ρ_λ^0 as in (5.18). We define $\bar{\rho}_\lambda^0:U_\varepsilon'/I_\varepsilon'\to\mathrm{End}(L_\varepsilon^{\mathrm{nil}}(\lambda))$ by $\bar{\rho}_\lambda^0(u+I_\varepsilon):=\rho_\lambda^0(u)$ for any $u\in U_\varepsilon'$. Since $L_\varepsilon^{\mathrm{nil}}(\lambda)$ is a nilpotent U_ε-module, $\bar{\rho}_\lambda^0$ is well-defined. Then, for any $u\in U_\varepsilon'$, $v\in L_\varepsilon^{\mathrm{nil}}(\lambda)$, we have $u.v=\bar{\rho}_\lambda^0\circ\pi(u)(v)$ on $L_\varepsilon^{\mathrm{nil}}(\lambda)$. Hence, for any $u\in\widetilde{U}_\varepsilon$ and $v\in L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$, we get

$$u.v=\bar{\rho}_\lambda^0\circ\pi\circ\mathrm{ev}_\mathbf{a}^+(u)(v)=\bar{\rho}_\lambda^0\circ(\bar{\phi}')^{-1}\circ(\mathrm{ev}_\mathbf{a}^{\mathrm{fin}})^+\circ\widetilde{\phi}\circ\widetilde{\pi}(u)(v)\ \text{on}\ L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+,$$

by (5.22). Since $\widetilde{\pi}(\widetilde{I}_\varepsilon)=0$, we obtain $\widetilde{I}_\varepsilon=0$ on $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$. Therefore $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^+$ is a nilpotent $\widetilde{U}_\varepsilon$-module. □

By Theorem 3.15 and Proposition 5.10, we can regard $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^\pm$ as a $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module. We denote $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module $L_\varepsilon^{\mathrm{nil}}(\lambda)_\mathbf{a}^\pm$ by $L_\varepsilon^{\mathrm{fin}}(\lambda)_\mathbf{a}^\pm$. Let $\mathbf{P}_\mathbf{a}^\pm$ be as in (4.6) and $\widetilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P}_\mathbf{a}^\pm)$ be the evaluation representation of $\widetilde{U}_\varepsilon^{\mathrm{fin}}$ in Sec. IV. Then, by Theorem 4.13, 5.9, $L_\varepsilon^{\mathrm{fin}}(\lambda)_\mathbf{a}^\pm$ is isomorphic to $\widetilde{V}_\varepsilon^{\mathrm{fin}}(\mathbf{P}_\mathbf{a}^\pm)$ as a $\widetilde{U}_\varepsilon^{\mathrm{fin}}$-module. Hence, by Proposition 4.14, we obtain the following proposition.

Proposition 5.11: Let $\lambda=(\lambda_i)_{i\in l}\in\mathbb{Z}_l^n$, $\mathbf{a}_\pm\in\mathbb{C}^\times$.

(*a*) *If* $\lambda=0$, *then* $L_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_+}^+$ *is isomorphic to* $L_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_-}^-$ *as a* $\widetilde{U}_\varepsilon$*-module*.

(*b*) *In the case of* $\lambda\neq 0$, $L_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_+}^+$ *is isomorphic to* $L_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_-}^-$ *as a* $\widetilde{U}_\varepsilon$*-module if and only if* $\mathbf{a}_+$

$=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ *for any* $i\in\mathrm{supp}(\lambda)$.

C. Alternative proof of Proposition 5.11(b)

We can also prove Proposition 5.11(b) without using the theory of restricted type. We give here the alternative proof.

"*Proof of only if part:*" We assume that $L_\varepsilon^{\mathrm{nil}}(\lambda)^+_{\mathbf{a}_+}\cong L_\varepsilon^{\mathrm{nil}}(\lambda)^-_{\mathbf{a}_-}$. Then there exists a $\widetilde{U}_\varepsilon$-module isomorphism $\phi: L_\varepsilon^{\mathrm{nil}}(\lambda)^+_{\mathbf{a}_+}\to L_\varepsilon^{\mathrm{nil}}(\lambda)^-_{\mathbf{a}_-}$. By Proposition 5.8(a), there exists $d\in\mathbb{C}^\times$ such that $\phi(v_\lambda(0))=dv_\lambda(0)$. Since $L_\varepsilon^{\mathrm{nil}}(\lambda)^+_{\mathbf{a}_+}$ is generated by $v_\lambda(0)$ as a $\widetilde{U}_\varepsilon$-module, we obtain $\phi(v)=dv$ for any $v\in L_\varepsilon^{\mathrm{nil}}(\lambda)_{\mathbf{a}_+}$. Hence we have

$$\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)v_\lambda(0)=d^{-1}\phi(\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)v_\lambda(0))=d^{-1}\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)\phi(v_\lambda(0))=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)v_\lambda(0). \tag{5.23}$$

For $c=(c_{i,j})_{1\leqslant i\leqslant j\leqslant n}\in\mathbb{C}^N$, $r^s\in R^F$, let $C_E(c,r^s)$ be as in (5.16). Then $C_E(0,r^s)=0$ for $r^s\in R^F$. By Theorem 5.5, we obtain

$$\widetilde{\mathrm{ev}}^\pm_{\mathbf{a}_\pm}(E_0)v_\lambda(0)=\mathbf{a}_\pm\sum_{r^s\in R^F}(-1)^{s+n}\varepsilon^{\mp(\lambda^{(s)}+s)+n}[-\lambda_s]_\varepsilon v(\epsilon_{r^s}). \tag{5.24}$$

Since $\{v(\epsilon_{r^s})\,|\,r^s\in R^F\}$ is linearly independent, by (5.23) and (5.24), we have $\mathbf{a}_+\varepsilon^{-\lambda^{(s)}-s}[\lambda_s]_\varepsilon=\mathbf{a}_-\varepsilon^{\lambda^{(s)}+s}[\lambda_s]_\varepsilon$ for any $s\in I$. Hence $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ for any $i\in\mathrm{supp}(\lambda)$.

"*Proof of if part:*" We assume that $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(i)}+i)}$ for any $i\in\mathrm{supp}(\lambda)$. By the definition of $\widetilde{\mathrm{ev}}^\pm_{\mathbf{a}_\pm}$, we have $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_i)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_i)$, $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(F_i)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(F_i)$, and $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(K_{\alpha_i})=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(K_{\alpha_i})$ on $V_\varepsilon^{\mathrm{nil}}(\lambda)$ for any $i\in I$. So it is enough to prove that $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)$ and $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(F_0)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(F_0)$ on $V_\varepsilon^{\mathrm{nil}}(\lambda)$. By (5.24), we obtain $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)v_\lambda(0)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)v_\lambda(0)$. On the other hand, for any $j_1,\cdots j_r\in I(r\in\mathbb{N})$, we get

$$\begin{aligned}\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)(F_{j_1}\cdots F_{j_r}v_\lambda(0))&=\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(F_{j_1}\cdots F_{j_r})(\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)v_\lambda(0))=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(F_{j_1}\cdots F_{j_r})(\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)v_\lambda(0))\\&=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)(F_{j_1}\cdots F_{j_r}v_\lambda(0)).\end{aligned}$$

Since $L_\varepsilon^{\mathrm{nil}}(\lambda)$ is spanned by $U_\varepsilon^-v_\lambda(0)$ as a $\mathbb{C}$-vector space, we obtain $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(E_0)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(E_0)$ on $V_\varepsilon^{\mathrm{nil}}(\lambda)$.

Now, for $c=(c_{i,j})_{1\leqslant i\leqslant j\leqslant n}\in\mathbb{C}^N$, $r^s\in R^E$, let $D_F(c,r^s)$ be as in Proposition 5.5 and m^λ be as in (5.19). Then, for any $r^s\in R^E$, we have

$$\begin{aligned}D_F(m^\lambda,r^s)&=-m^\lambda_{n,n}+\sum_{k=1}^{n-s+1}m^\lambda_{1,k}-\sum_{k=s+1}^{n}(m^\lambda_{r^s_k-1,n-k+r^s_k}-m^\lambda_{r^s_k,n-k+r^s_k})\\&=-\sum_{k=1}^{n}\lambda_{n-k+1}+\sum_{k=1}^{n-s+1}\lambda_k+\sum_{k=s+1}^{n}\lambda_{n-k+1}=\lambda^{(n-s+1)},\end{aligned}$$

(see (5.20)). Hence, by Theorem 5.5, we get

$$\widetilde{\mathrm{ev}}^\pm_{\mathbf{a}_\pm}(F_0)v(m^\lambda)=\mathbf{a}_\pm^{-1}\sum_{r^s\in R^E}(-1)^{s-1}\varepsilon^{\pm(\lambda^{(n-s+1)}-s+n+1)-n}[-\lambda_{n-s+1}]_\varepsilon v(m^\lambda+\alpha_{r^s}).$$

By the assumption, if $\lambda_{n-s+1}\neq 0$, then we have $\mathbf{a}_+=\mathbf{a}_-\varepsilon^{2(\lambda^{(n-s+1)}+(n-s+1))}$. So we obtain

$$\mathbf{a}_+^{-1}\varepsilon^{\lambda^{(n-s+1)}-s+n+1}=\mathbf{a}_-^{-1}\varepsilon^{-2\lambda^{(n-s+1)}-2(n-s+1)+\lambda^{(n-s+1)}-s+n+1}=\mathbf{a}_-^{-1}\varepsilon^{-(\lambda^{(n-s+1)}-s+n+1)}.$$

We have that $\widetilde{\mathrm{ev}}^+_{\mathbf{a}^+}(F_0)v(m^\lambda)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(F_0)v(m^\lambda)$.

On the other hand, in a similar way to the proof of Proposition 5.6 in Ref. 22, we obtain that there exists a nonzero vector $v_L\in L_\varepsilon^{\mathrm{nil}}(\lambda)$ such that $F_iv_L=0$ for any $i\in I$. Hence, by Proposition 5.8(b), we obtain $v(m^\lambda)\in L_\varepsilon^{\mathrm{nil}}(\lambda)$. Then $L_\varepsilon^{\mathrm{nil}}(\lambda)$ is spanned by $U_\varepsilon^+v(m^\lambda)$ as a $\mathbb{C}$-vector space. Therefore, in a similar way to the proof of E_0-case, we obtain $\widetilde{\mathrm{ev}}^+_{\mathbf{a}_+}(F_0)=\widetilde{\mathrm{ev}}^-_{\mathbf{a}_-}(F_0)$ on $L_\varepsilon^{\mathrm{nil}}(\lambda)$.

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On Miura transformations among nonlinear partial differential equations*

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In this paper, we study Miura transformations $u \mapsto v$ from partial differential equations $u_{xxx}=\mathcal{F}(u,u_x,u_t)$ to nonlinear partial differential equations $\mathcal{G}(v,v_x,v_t,\ldots,\partial_x^l v,\ldots,\partial_t^l v)=0$ defined using integrable systems on v. We classify all such Miura transformations under some restrictions, and hence generalize the classical Miura transformation to a large class of nonlinear partial differential equations. For some examples, by applying Miura transformations found in this paper, we derive exact solutions v from known solutions u. In particular, kink and soliton-kink solutions of $v_t=\frac{3}{2}v_x \sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$ are obtained from constant solutions and soliton solutions of the MKdV equation. As another application of Miura transformations of this paper, we deduce a new Bäcklund transformation for each of $v_t=\frac{3}{2}v_x \sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$ and $v_t=-\frac{3}{2}v_x \sinh^2 v-\frac{1}{2}v_x^3+v_{xxx}$ from the known Bäcklund transformations for the MKdV equations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

It is now well known that if v is a solution of the negative MKdV equation

$$v_t = v_{xxx} - 6v^2 v_x, \tag{1.1}$$

then $u=v_x-v^2$ is a solution of the KdV equation

$$u_t = u_{xxx} + 6uu_x. \tag{1.2}$$

The transformation $v \mapsto u=v_x-v^2$ from solutions of the negative MKdV equation to solutions of the KdV equation is the classical Miura transformation.[6]

On the other hand, if u is a solution of the KdV equation, then the system

$$\begin{aligned} v_x &= v^2 + u, \\ v_t &= 2v^2 u + 2u^2 + 2vu_x + u_{xx} \end{aligned} \tag{1.3}$$

on v is integrable and yields a solution v (with a constant of integration) of the negative MKdV equation.

*Dedicated to the memory of our great mentor, Professor Shiing-Shen Chern.

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So, the classical Miura transformation $v \mapsto u = v_x - v^2$ and this second transformation $u \mapsto v$ defined using (1.3) together give a local equivalence between the negative MKdV equation and the KdV equation.

Motivated by this example, we give the following general definition of Miura transformations of the type $u \mapsto v$ above.

Let $n > 0$ and $k \geqslant 0$ be integers. Consider a system

$$\begin{aligned} \Phi_x &= \Omega(\phi_1, \ldots, \phi_n, u, u_x, u_t, \ldots, \partial_x^k u, \ldots, \partial_t^k u), \\ \Phi_t &= \Theta(\phi_1, \ldots, \phi_n, u, u_x, u_t, \ldots, \partial_x^k u, \ldots, \partial_t^k u) \end{aligned} \tag{1.4}$$

on the (row) vector Φ of n functions $\phi_1, \ldots, \phi_n$. Following Ref. 6, we say that (1.4) is an *integrable system* associated with a partial differential equation (PDE)

$$\mathcal{F}(u, u_x, u_t, \ldots, \partial_x^l u, \ldots, \partial_t^l u) = 0 \tag{1.5}$$

if it is integrable on a nonempty open subset of the Φ space when and only when u is a solution to a fixed set of PDEs implied by (1.5).

The functions defined by integrable systems associated with a PDE were called *pseudopotentials* of the equation by Wahlquist and Estabrook in Ref. 13, and they have been studied extensively in the literature.

Let (1.4) be an integrable system associated with (1.5). A map

$$u \mapsto v = F(\phi_1, \ldots, \phi_n, u, u_x, u_t, \ldots, \partial_x^k u, \ldots, \partial_t^k u) \tag{1.6}$$

is called a *Miura-transformation* (MT) from (1.5) to a nonlinear PDE

$$\mathcal{G}(v, v_x, v_t, \ldots, \partial_x^l v, \ldots, \partial_t^l v) = 0 \tag{1.7}$$

defined using (1.4) if it is nonconstant with respect to at least one of $\phi_1, \ldots, \phi_n$, and v is always a solution of (1.7) for each solution u of (1.5) and every solution $\Phi = (\phi_1, \ldots, \phi_n)$ of the corresponding system (1.4).

In general, given a solution u of (1.5), investigating (1.4) is much easier than solving (1.7). This is the reason for why MTs are useful. When (1.5) and (1.7) are the same equation, a MT is then called a *Bäcklund transformation* (BT) for the equation. There is a huge literature on such transformations (see, e.g., Refs. 8, 5, 14, 10, and 7).

In this paper, we explicitly determine all MTs $u \mapsto v$ from PDEs of the form

$$u_{xxx} = \mathcal{F}(u, u_x, u_t) \tag{1.8}$$

to nonlinear PDEs of the form

$$\mathcal{G}(v, v_x, v_t, \ldots, \partial_x^l v, \ldots, \partial_t^l v) = 0 \tag{1.9}$$

defined using integrable systems of the form

$$\begin{aligned} v_x &= \omega(v) + u, \\ v_t &= \Theta(v, u, u_x, u_{xx}) \end{aligned} \tag{1.10}$$

associated with (1.8). For the main classification results of this paper, see Theorems 2.4 and 2.6.

In each of such situations, the map $v \mapsto u = v_x - \omega(v)$ is a MT from (1.9) to (1.8), and the transformations $u \mapsto v$ and $v \mapsto u = v_x - \omega(v)$ together give a local equivalence between (1.8) and (1.9). This motivates our choice of the special format of the associated integrable system (1.10).

This work is a continuation of Ref. 14. Our method originated from the work[2] of Chern and Tenenblat and relies on the requirement that *the source* PDE $u_{xxx} = \mathcal{F}(u, u_x, u_t)$ *in question has enough solutions so that at each point in a nonempty open subset of the xt space, the values of u*,

u_x, u_t, and u_{xx} are independent from each other; *hence*, *we can treat them as independent variables in the functions* $\mathcal{F}$, $\mathcal{G}$, ω, *and* Θ *when we want to determine these functions*. We will always omit this requirement from the statements of our results.

Most papers in this area are about constructions of BTs, MTs, and solutions, and there are several results on classifications of such transformations. However, all these classification results (see, e.g., Ref. 9) assume that the PDEs considered satisfy certain integrability conditions, such as Lax pairs, symmetries, or high order conservation laws; moreover, some authors allow transformations that are more general than those which we use. As a feature of this paper, we do not assume that the PDEs studied have any structures.

The organization of this paper is as follows. In Sec. II, we prove this paper's classification of MTs. Section III is devoted to exact solutions obtained using MTs of this paper, with soliton-kink solutions presented in Examples 3.7 and 3.8; while Sec. IV deals with BTs deduced in terms of such MTs, with two new BTs given in Examples 4.6 and 4.7.

II. MIURA TRANSFORMATIONS

First, we have the following complete classification of all the integrable systems of the form (1.10) associated with PDEs of the form (1.8). Recall that a linear coordinate change of the xt space has the form $\tilde{x}=a_1x+b_1t+c_1$ and $\tilde{t}=a_2x+b_2t+c_2$ with $a_1b_2\neq a_2b_1$, while a linear coordinate change of the u axis can be written as $u\mapsto au+b$ with $a\neq 0$.

Theorem 2.1: *Up to linear coordinate changes of the* xt, u, *and* v *spaces*, (1.10) *is an integrable system associated with* (1.8) *if and only if*: *when* ω *is linear*,

$$\mathcal{F}(u,u_x,u_t)=p(u)+q(u)u_x+\frac{3\delta Q'(u)}{2Q(u)}u_x^2+s(u)u_x^3+Q(u)u_t, \tag{2.1}$$

$$\omega(v)=\delta v, \tag{2.2}$$

$$\Theta(v,u,u_x,u_{xx})=\widetilde{\Theta}(v,u)+\frac{\delta}{Q(u)}u_x+\frac{Q'(u)}{2Q(u)^2}u_x^2+\frac{1}{Q(u)}u_{xx} \tag{2.3}$$

for some smooth functions q *and* Q *such that* $Q\neq 0$, *where* $\delta=0$ *or* 1,

$$p(u)=Q(u)\left(\delta\theta_0-\theta_1u+\delta\int\frac{\delta-q(u)}{Q(u)}\mathrm{d}u\right), \tag{2.4}$$

$$s(u)=\frac{Q'(u)^2}{Q(u)^2}-\frac{Q''(u)}{2Q(u)}, \tag{2.5}$$

$$\widetilde{\Theta}(v,u)=\theta_0+\theta_1v+\int\frac{\delta-q(u)}{Q(u)}\mathrm{d}u \tag{2.6}$$

for some constants θ_0 *and* θ_1; *when* ω *is nonlinear*,

$$\mathcal{F}(u,u_x,u_t)=-6uu_x+u_t, \tag{2.7}$$

$$\omega(v)=v^2, \tag{2.8}$$

$$\Theta(v,u,u_x,u_{xx})=2v^2u+2u^2+2vu_x+u_{xx}, \tag{2.9}$$

or

$$\mathcal{F}(u,u_x,u_t)=-\tfrac{3}{2}u^2u_x+u_t, \tag{2.10}$$

$$\omega(v) = \sin v, \tag{2.11}$$

$$\Theta(v,u,u_x,u_{xx}) = \sin v + u + \tfrac{1}{2}u^2\sin v + \tfrac{1}{2}u^3 + u_x\cos v + u_{xx}, \tag{2.12}$$

or

$$\mathcal{F}(u,u_x,u_t) = \tfrac{3}{2}u^2u_x + u_t, \tag{2.13}$$

$$\omega(v) = \sinh v, \tag{2.14}$$

$$\Theta(v,u,u_x,u_{xx}) = \sinh v + u - \tfrac{1}{2}u^2\sinh v - \tfrac{1}{2}u^3 + u_x\cosh v + u_{xx}. \tag{2.15}$$

Proof: If (1.10) is an integrable system associated with (1.8), then by Lemma 2.11 of Ref. 14,

$$\Theta(v,u,u_x,u_{xx}) = \check{\Theta}(v,u,u_x) + \hat{\Theta}(v,u)u_{xx}, \tag{2.16}$$

$$\mathcal{F}(u,u_x,u_t) = P(u,u_x) + Q(u)u_t \tag{2.17}$$

for some smooth functions $\check{\Theta}$, $\hat{\Theta}$, P, and Q satisfying $\hat{\Theta}(v,u)Q(u)\equiv 1$. Hence, $\hat{\Theta}$ does not depend on v, $Q\neq 0$, and $\hat{\Theta}=1/Q$. Applying Lemma 2.11 of Ref. 14 again, (1.10) is an integrable system associated with (1.8) if and only if

$$\mathcal{F}(u,u_x,u_t) = p(u) + q(u)u_x + r(u)u_x^2 + s(u)u_x^3 + Q(u)u_t, \tag{2.18}$$

$$\Theta(v,u,u_x,u_{xx}) = \widetilde{\Theta}(v,u) + \frac{\omega'(v)}{Q(u)}u_x + \frac{Q'(u)}{2Q(u)^2}u_x^2 + \frac{1}{Q(u)}u_{xx} \tag{2.19}$$

for some smooth functions p, q, r, s, and $\widetilde{\Theta}$ satisfying

$$-Q''(u)Q(u) + 2Q'(u)^2 = 2s(u)Q(u)^2, \tag{2.20}$$

$$3\omega'(v)Q'(u) = 2r(u)Q(u), \tag{2.21}$$

$$\omega'^2(v) = (\omega(v)+u)\omega''(v) + Q(u)\frac{\partial\widetilde{\Theta}(v,u)}{\partial u} + q(u), \tag{2.22}$$

$$\omega'(v)\widetilde{\Theta}(v,u) = (\omega(v)+u)\frac{\partial\widetilde{\Theta}(v,u)}{\partial v} + p(u)/Q(u). \tag{2.23}$$

From (2.21) we see that either ω is linear, or Q is (nonzero and) constant.

Case 1: *ω is linear*. Then, $\omega(v)=\omega_0+\omega_1 v$ for some constants ω_0 and ω_1. Replacing u by $u-\omega_0$ if necessary, we can assume that $\omega_0=0$. When $\omega_1\neq 0$, after replacing x by x/ω_1 and u by $\omega_1 u$, we have that $\omega_1=1$. So, up to a shift in the u direction and a rescaling of the x and u directions, we can always assume that $\omega(v)=\delta v$, where $\delta=0$ or 1. Then, from (2.20)–(2.22) we deduce (2.5) and that $r=3\delta Q'/(2Q)$,

$$\widetilde{\Theta}(v,u) = \theta(v) + \int\frac{\delta - q(u)}{Q(u)}\mathrm{d}u \tag{2.24}$$

for some smooth function θ. Differentiating (2.23) with respect to v yields that $(\omega+u)\theta''=0$, and hence $\theta(v)=\theta_0+\theta_1 v$ for some constants θ_0 and θ_1. Then, (2.23) and (2.24) imply (2.4) and (2.6), respectively.

Case 2: Q is constant. Replacing t by Qt, we can assume that $Q=1$. Then $\widehat{\Theta}=1$. Now, (2.20) and (2.21) are equivalent to $s=0$ and $r=0$, respectively. So, (2.18), (2.19), (2.22), and (2.23) can be rewritten as

$$\mathcal{F}(u,u_x,u_t)=p(u)+q(u)u_x+u_t, \tag{2.25}$$

$$\Theta(v,u,u_x,u_{xx})=\widetilde{\Theta}(v,u)+\omega'(v)u_x+u_{xx}, \tag{2.26}$$

$$\frac{\partial\widetilde{\Theta}(v,u)}{\partial u}=\omega'(v)^2-\omega(v)\omega''(v)-\omega''(v)u-q(u), \tag{2.27}$$

$$p(u)=\omega'(v)\widetilde{\Theta}(v,u)-(\omega(v)+u)\frac{\partial\widetilde{\Theta}(v,u)}{\partial v}, \tag{2.28}$$

respectively. From (2.27) we have that

$$\widetilde{\Theta}(v,u)=\theta(v)+(\omega'(v)^2-\omega(v)\omega''(v))u-\tfrac{1}{2}\omega''(v)u^2-\int q(u)\mathrm{d}u \tag{2.29}$$

for some smooth function θ. In particular, $\partial\widetilde{\Theta}(v,u)/\partial v$ is polynomial in u of degree $\leqslant 2$. Taking the v derivative of (2.28) yields that

$$(\omega(v)+u)\frac{\partial^2\widetilde{\Theta}(v,u)}{\partial v^2}=\omega''(v)\widetilde{\Theta}(v,u). \tag{2.30}$$

Since ω is not linear, from (2.30) and (2.29) one then deduces that q is a polynomial of degree $\leqslant 2$, i.e., $q(u)=q_0+q_1u+q_2u^2$ for some constants q_0, q_1, and q_2. When $q_2\neq 0$, using a shift in the u direction, we can always have that $q_1=0$. By applying the coordinate change $\tilde{x}=x-q_0t$ and $\tilde{t}=t$ if necessary, we can assume that $q_0=0$. Thus,

$$q(u)=q_1u+q_2u^2, \tag{2.31}$$

and hence (2.27) is equivalent to that

$$\widetilde{\Theta}(v,u)=\theta(v)+(\omega'(v)^2-\omega(v)\omega''(v))u-\tfrac{1}{2}(\omega''(v)+q_1)u^2-\frac{q_2}{3}u^3 \tag{2.32}$$

for some smooth function θ. By (2.28), p is a polynomial of degree $\leqslant 3$, i.e., $p(u)=p_0+p_1u+p_2u^2+p_3u^3$ for some constants p_0, p_1, p_2, and p_3. So, (2.28) can be rewritten as

$$p_3=-\frac{q_2}{3}\omega'(v)+\frac{1}{2}\omega'''(v), \tag{2.33}$$

$$p_2=-\frac{q_1}{2}\omega'(v)-\frac{3}{2}\omega'(v)\omega''(v)+\frac{3}{2}\omega(v)\omega'''(v), \tag{2.34}$$

$$p_1=\omega'(v)^3-2\omega(v)\omega'(v)\omega''(v)+\omega(v)^2\omega'''(v)-\theta'(v), \tag{2.35}$$

$$p_0=\omega'(v)\theta(v)-\omega(v)\theta'(v). \tag{2.36}$$

By taking the v derivative of (2.33) we obtain that

$$\omega''''(v) = \frac{2q_2}{3}\omega''(v). \tag{2.37}$$

If $q_2<0$ (and hence one can assume that $q_1=0$), by a rescaling in the u direction, one has that $q_2=-3/2$. So, $q(u)=-3u^2/2$. Thus, (2.37) implies that up to a shift in the v direction, $\omega''(v)=-c\sin v$ for some constant $c\neq 0$, and hence $\omega(v)=a+bv+c\sin v$ for some constants a and b. After replacing x by x/c, t by t/c^3 and u by cu, the PDE on u stays invariant, while in the new system on ϕ, $\omega(v)=a/c+bv/c+\sin v$. So, we can assume that $c=1$. Then, (2.33)–(2.36) together are equivalent to $a=b=0$ and $p=\theta=0$. Therefore, in this subcase, up to linear coordinate changes of the xt, u, and v spaces, (2.25)–(2.28) can be rewritten as (2.7)–(2.9).

If $q_2=0$, then (2.33) implies that $\omega(v)=a+bv+cv^2+p_3v^3/3$ for some constants a, b, and c. By comparing the v^3 coefficients in (2.34) one gets that $p_3=0$. Hence, $c\neq 0$. By rescaling the x and u variables, we can assume that $c=1$; then after a shift in the v direction, one can reach the situation where $b=0$; and finally a shift in the u direction can make $\omega(v)=v^2$. Then, (2.33)–(2.36) together are equivalent to $q_1=-6$, i.e., $q(u)=-6u$, and $p=\theta=0$. Therefore, in this subcase, up to linear coordinate changes of the xt, u, and v spaces, (2.25)–(2.28) can be rewritten as (2.10)–(2.12).

If $q_2>0$, one can show similarly that up to linear coordinate changes of the xt, u, and v spaces, (2.25)–(2.28) can be rewritten as (2.13)–(2.15). This finishes the proof. ■

The case of a linear ω in Theorem 2.1 includes the following class of examples.

Example 2.2: Let $\delta=0$ or 1, and $n\in\mathbb{N}$. For any real constants θ_0, θ_1, $q_1,\ldots,q_n$ satisfying $q_n\neq 0$, the nonlinear PDE

$$u_{xxx} = \delta\theta_0 + (\delta-\theta_1)u - \frac{\delta q_1}{2}u^2 - \cdots - \frac{\delta q_n}{n+1}u^{n+1} + (q_1u+\cdots+q_nu^n)u_x + u_t \tag{2.38}$$

has the associated integrable system

$$\begin{aligned} v_x &= \delta v + u,\\ v_t &= \theta_0 + \theta_1 v + \delta u - \frac{q_1}{2}u^2 - \cdots - \frac{q_n}{n+1}u^{n+1} + \delta u_x + u_{xx}. \end{aligned} \tag{2.39}$$

The following principle gives a general way for obtaining Miura transformations among PDEs from associated integrable systems of forms similar to that of (1.10).

Principle 2.3: *If*

$$\begin{aligned} v_x &= \omega(v) + u,\\ v_t &= \Theta(v,u,u_x,u_t,\ldots,\partial_x^k u,\ldots,\partial_t^k u) \end{aligned} \tag{2.40}$$

is an integrable system associated with a partial differential equation

$$\mathcal{F}(u,u_x,u_t,\ldots,\partial_x^l u,\ldots,\partial_t^l u) = 0, \tag{2.41}$$

then $u\mapsto v$ *is a Miura transformation from* (2.41) *to the partial differential equation*

$$v_t = \Theta(v,v_x-\omega(v),\ldots,\partial_x^l(v_x-\omega(v)),\ldots,\partial_t^l(v_x-\omega(v))) \tag{2.42}$$

defined using (2.40).

In this case, the Miura transformations $u\mapsto v$ *and* $v\mapsto u=v_x-\omega(v)$ *together give a local equivalence between* (2.41) and (2.42).

Applying Principle 2.3 to the case in Theorem 2.1 with a linear ω immediately yields the following classification.

Theorem 2.4: *Assume that* ω *in* (1.10) *is linear. Then,* $u\mapsto v$ *is a Miura transformation from a partial differential equation* (1.8) *to a nonlinear partial differential equation* (1.9) *defined using an integral system* (1.10) *associated with* (1.8) *if and only if up to linear coordinate changes of the*

xt, *u*, *and v spaces*, (1.8)–(1.10) *can be written as*

$$u_{xxx} = p(u) + q(u)u_x + \frac{3\delta Q'(u)}{2Q(u)}u_x^2 + s(u)u_x^3 + Q(u)u_t, \tag{2.43}$$

$$v_t = \widetilde{\Theta}(v, v_x - \delta v) + \frac{\delta}{Q(v_x - \delta v)}(v_{xx} - \delta v_x) + \frac{Q'(v_x - \delta v)}{2Q(v_x - \delta v)^2}(v_{xx} - \delta v_x)^2 + \frac{1}{Q(v_x - \delta v)}(v_{xxx} - \delta v_{xx}) \tag{2.44}$$

and

$$\begin{aligned} v_x &= \delta v + u, \\ v_t &= \widetilde{\Theta}(v, u) + \frac{\delta}{Q(u)}u_x + \frac{Q'(u)}{2Q(u)^2}u_x^2 + \frac{1}{Q(u)}u_{xx} \end{aligned} \tag{2.45}$$

for some smooth functions q and Q such that $Q \neq 0$ *and one of them is nonconstant*, *where* $\delta = 0$ *or* 1, *and p*, *s*, *and* $\widetilde{\Theta}$ *are given by* (2.4)–(2.6).

Example 2.5: When (2.43) is (2.38), (2.44) becomes

$$v_t = \theta_0 + (\theta_1 - \delta)v - \frac{q_1}{2}(v_x - \delta v)^2 - \cdots - \frac{q_n}{n+1}(v_x - \delta v)^{n+1} + v_{xxx}, \tag{2.46}$$

which also does not involve the second-order *x* derivative.

From Principle 2.3 and the case of Theorem 2.1 with a nonlinear ω, we immediately obtain the following classification.

Theorem 2.6: *Assume that* ω *in* (1.10) *is nonlinear. Then*, $u \mapsto v$ *is a Miura transformation from a partial differential equation* (1.8) *to a nonlinear partial differential equation* (1.9) *defined using an integrable system* (1.10) *associated with* (1.8) *if and only if up to linear coordinate changes of the xt*, *u*, *and v spaces*, *either* (1.8)–(1.10) *are the KdV equation* (1.2), *the negative MKdV equation* (1.1), *and the integrable system* (1.3), *respectively*, *or they form one of the following two cases*:

Case 1.

$$u_t = \tfrac{3}{2}u^2u_x + u_{xxx}, \tag{2.47}$$

$$v_t = \tfrac{3}{2}v_x\sin^2 v + \tfrac{1}{2}v_x^3 + v_{xxx}, \tag{2.48}$$

and

$$\begin{aligned} v_x &= \sin v + u, \\ v_t &= \sin v + u + \tfrac{1}{2}u^2 \sin v + \tfrac{1}{2}u^3 + u_x \cos v + u_{xx}. \end{aligned} \tag{2.49}$$

Case 2.

$$u_t = -\tfrac{3}{2}u^2u_x + u_{xxx}, \tag{2.50}$$

$$v_t = -\tfrac{3}{2}v_x \sinh^2 v - \tfrac{1}{2}v_x^3 + v_{xxx}, \tag{2.51}$$

and

$$v_x = \sinh v + u, \tag{2.52}$$

$$v_t = \sinh v + u - \tfrac{1}{2}u^2 \sinh v - \tfrac{1}{2}u^3 + u_x \cosh v + u_{xx}.$$

Remark 2.7: Note that (2.48) is a real form of

$$u_t + u_{xxx} - \tfrac{1}{8}u_x^3 + u_x(ae^u + be^{-u}) + c = 0, \tag{2.53}$$

which was found by Fokas in Ref. 3, and by Calogero and Degasperis in Ref. 1. In Ref. 14, a BT for (2.48) was found.

III. EXACT SOLUTIONS

If $u \mapsto v$ is a MT from a PDE (1.8) to a nonlinear PDE (1.9) defined using an integrable system (1.10), then from a solution u of (1.8), by solving the integrable system (1.10), one gets a one-parameter family of solutions v of (1.9). In the following, we give eight examples, the first two of which correspond to the case of a linear ω, and the others the case of a nonlinear ω.

In general, it is not easy (if possible) to get explicit formulas for the solutions v of (1.10) when a solution u of (1.8) is given, even though u can be explicit and simple. In such a situation, using an ordinary differential equation (ODE) solver, one can usually obtain numerical approximations of these solutions of (1.10), and hence of exact solutions of (1.9). Sometimes, even u can be given via an ODE. We will use this method whenever needed.

Example 3.1: In Example 2.2, let $\delta=1$ and $n=1$. Using a linear coordinate change of the u axis and one of the xt plane we can bring (2.38) into the form

$$u_{xxx} = \theta_0 - u^2 + 2uu_x + u_t. \tag{3.1}$$

Then, the associated integrable system (2.39) becomes

$$\begin{aligned} v_x &= v + u, \\ v_t &= \theta_0 + v + u - u^2 + u_x + u_{xx}, \end{aligned} \tag{3.2}$$

while the corresponding PDE (2.46) on v takes the form

$$v_t = \theta_0 - (v_x - v)^2 + v_{xxx}. \tag{3.3}$$

The x-independent solution of (3.1) are

$$u(x,t) = c_1 \tan(c_1 t + \alpha) \tag{3.4}$$

if $\theta_0 < 0$,

$$u(x,t) = -\frac{1}{t+\alpha}, \quad u = 0 \tag{3.5}$$

if $\theta_0 = 0$, and

$$u(x,t) = -c_2 \tanh(c_2 t + \alpha), \quad u(x,t) = -c_2 \coth(c_2 t + \alpha), \quad u = \pm c_2 \tag{3.6}$$

if $\theta_0 > 0$, where $c_1 = \sqrt{-\theta_0}$, $c_2 = \sqrt{\theta_0}$, and α is an arbitrary real constant. Note that the tanh solutions are x-steady solutions *antikink* in the t variable, starting from (the constant solution) c_2 at $t=-\infty$ and strictly decreasing to (the constant solution) $-c_2$ at $t=+\infty$. Moreover, the tanh solutions have exactly one inflection point.

For such a u, the solutions of (3.2), i.e., the corresponding solutions of (3.3), are

$$v(x,t) = ce^{x+t} - u(x,t), \tag{3.7}$$

where c is also an arbitrary real constant. We mention that when u is one of the tanh-solutions above, the corresponding v with $c=0$ is an x-steady solution *kink* in the t variable. Figure 1 shows the u with $\theta_0=1$ and $\alpha=0$ together with the corresponding v with $c=0$.

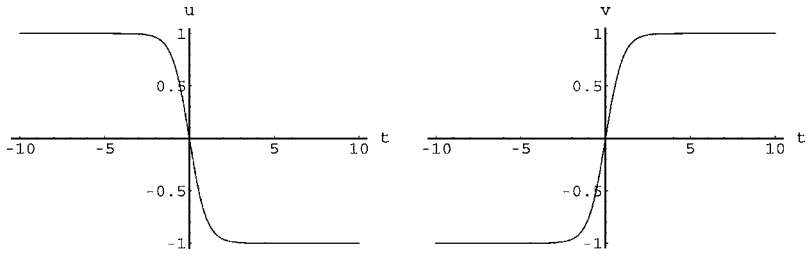

FIG. 1. Solutions antikink and kink in the t variable.

The following example generalizes the main parts of Example 3.1 to the case with an $n \geqslant 2$.

Example 3.2: Let $\delta=1$ and $n \in \mathbb{N}$ such that $n \geqslant 2$. Then, (2.38), (2.39), and (2.46) become

$$u_{xxx} = \theta_0 + (1-\theta_1)u - \frac{q_1}{2}u^2 - \cdots - \frac{q_n}{n+1}u^{n+1} + (q_1 u + \cdots + q_n u^n)u_x + u_t, \tag{3.8}$$

$$\begin{aligned} v_x &= v + u, \\ v_t &= \theta_0 + \theta_1 v + u - \frac{q_1}{2}u^2 - \cdots - \frac{q_n}{n+1}u^{n+1} + u_x + u_{xx}, \end{aligned} \tag{3.9}$$

$$v_t = \theta_0 + (\theta_1 - 1)v - \frac{q_1}{2}(v_x - v)^2 - \cdots - \frac{q_n}{n+1}(v_x - v)^{n+1} + v_{xxx}, \tag{3.10}$$

respectively. The x-steady solutions $u(x,t)=f(t)$ of (3.8) are given by the ODE

$$f'(t) = \frac{q_n}{n+1}f(t)^{n+1} + \cdots + \frac{q_1}{2}f(t)^2 + (\theta_1 - 1)f(t) - \theta_0. \tag{3.11}$$

For each such u, the solutions of (3.9), i.e., the corresponding solutions of (3.10), are

$$v(x,t) = c\mathrm{e}^{x+\theta_1 t} - f(t), \tag{3.12}$$

where c is an arbitrary real constant.

Assume that the polynomial on the right-hand side of (3.11) has $k \geqslant 2$ distinct real roots. Then, (3.8) has $k-1$ one-parameter families of x-steady solutions between these roots and kink or antikink in the t variable. For each such u, the corresponding v with $c=0$ is also an x-steady solution kink or antikink in the t variable; and when $\theta_1=0$, the corresponding v's with $c<0$ are solutions kink or antikink in the t variable and moving down in the x direction, and those v's with $c>0$ are solutions kink or antikink in the t variable and moving up in the x direction.

As a particular example, if we let $n=3$, $\theta_0=(1.42^2-1)^2-1$, $\theta_1=1$, $q_1=-4$, $q_2=0$ and $q_3=4$, then (3.8)–(3.10) take the form

$$u_{xxx} = \theta_0 + 2u^2 - u^4 + (-4u + 4u^3)u_x + u_t, \tag{3.13}$$

$$\begin{aligned} v_x &= v + u, \\ v_t &= \theta_0 + v + u + 2u^2 - u^4 + u_x + u_{xx}, \end{aligned} \tag{3.14}$$

$$v_t = \theta_0 + 2(v_x - v)^2 - (v_x - v)^4 + v_{xxx}, \tag{3.15}$$

respectively. In this case, the real constant solutions of (3.13) are $u=\pm 1.42$, the x-steady solution

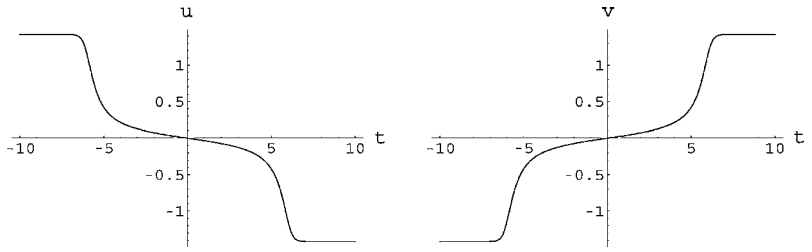

FIG. 2. A 2-antikink and a 2-kink.

u satisfying $u(0,0)=0$ is a *2-antikink*, i.e., an antikink having exactly $2(2)-1=3$ infection points, and the corresponding v with $c=0$ is a *2-kink*. Figure 2 indicates them.

Multikink and *multi-antikink* solutions with more than two "steps" can be obtained similarly. We omit the details.

Next, we discuss the solution of the nonlinear PDE (2.48) obtained from known solutions of the MKdV equation (2.47) and in terms of the MT from (2.47) to (2.48) defined using (2.49). We divide our discussion into several parts according to the complexity of the known solutions of the MKdV equation used. Note that v *is a solution of* (2.49) *if and only if* $v+2\pi$ *is*.

Example 3.3: The MKdV equation (2.47) has the trivial solution $u=0$. Substituting this solution into (2.49) gives that

$$\begin{aligned} v_x &= \sin v, \\ v_t &= \sin v. \end{aligned} \tag{3.16}$$

Solving this system yields the solutions $v=n\pi$ and

$$v(x,t) = 2n\pi + 2\arctan(\alpha e^{x+t}) = (2n+1)\pi \pm \arccos\tanh(x+t+\beta) \tag{3.17}$$

of (2.48), where $n \in \mathbb{Z}$, α is a nonzero real constant, and β is an arbitrary real constant. The above-mentioned nonconstant solutions are kink or antikink solutions, whose profiles are illustrated in Fig. 3.

Example 3.4: Let $c \in (-1,1)$ be nonzero. Substituting the constant solution $u=c$ of (2.47) into (2.49) gives that

$$\begin{aligned} v_x &= \sin v + c, \\ v_t &= (1 + c^2/2)(\sin v + c). \end{aligned} \tag{3.18}$$

Solving this system yields the solutions

$$v = 2n\pi + \arcsin(-c), \quad v = (2n+1)\pi - \arcsin(-c), \tag{3.19}$$

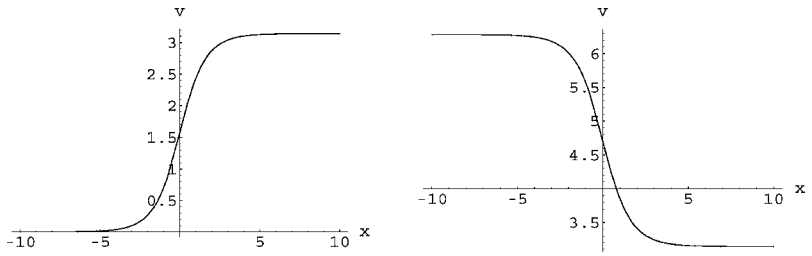

FIG. 3. Profiles of kink and antikink solutions of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

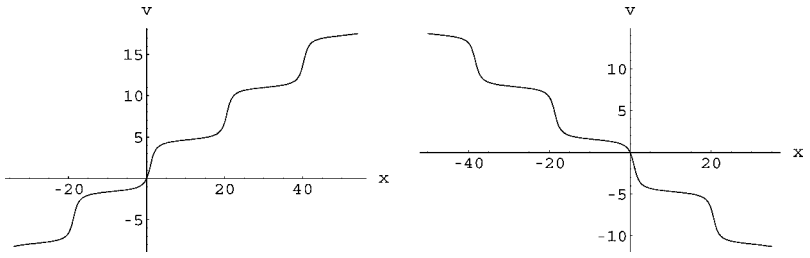

FIG. 4. Profiles of up- and down-stair solutions of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

$$v(x,t)=2n\pi+2\arctan\frac{c_1+c_2\alpha\exp\left((\operatorname{sgn}c)\sqrt{1-c^2}(x+c_3t)\right)}{1+\alpha\exp((\operatorname{sgn}c)\sqrt{1-c^2}(x+c_3t))} \tag{3.20}$$

of 2.48, where $n\in\mathbb{Z}$, α is a nonzero real constant, and

$$c_1=-1/c+\sqrt{1/c^2-1},\quad c_2=-1/c-\sqrt{1/c^2-1},\quad c_3=1+c^2/2. \tag{3.21}$$

The above-noted nonconstant solutions are also kink or antikink solutions.

Example 3.5: Substituting the constant solution $u=\pm1$ of (2.47) into (2.49) gives the system (3.18) with $c=\pm1$. Solving this system yields the solutions

$$v=(2n\mp1/2)\pi,\quad v(x,t)=(2n\mp1/2)\pi-2\operatorname{arccot}(\alpha\pm x\pm3t/2) \tag{3.22}$$

of (2.48), where $n\in\mathbb{Z}$, and α is a real constant. The above-noted nonconstant solutions are also kink or antikink solutions.

Therefore, from constant solutions of the MKdV equation (2.47), one gets three classes of kink and antikink solutions of (2.48).

Example 3.6: From the constant solution $u=c$ of the MKdV equation (2.47) satisfying $|c|>1$, we get the solution

$$v(x,t)=2n\pi+2\arctan\left(\frac{\sqrt{c^2-1}}{c}\tan\left(\frac{\sqrt{c^2-1}}{2}\left[x+\left(1+\frac{c^2}{2}\right)t+\alpha\right]\right)-\frac{1}{c}\right) \tag{3.23}$$

of (2.48), where $n\in\mathbb{Z}$, and α is a real constant. Note that v is smooth on $\mathbb{R}^2$, and the formula (3.23) should be understood as its continuous extension to $\mathbb{R}^2$. When $c>1$ (respectively, $c<-1$), the profiles of these solutions look like stairs going up (respectively, down) in the x increasing direction, and hence we call these solutions *up-stair solutions* (respectively, *down-stair solutions*), see Fig. 4 for illustrations with $c=\pm1.05$.

Example 3.7: The MKdV equation (2.47) has one-soliton solutions

$$u(x,t)=\pm2k\operatorname{sech}(kx+k^3t+\alpha), \tag{3.24}$$

where k and α are arbitrary real constants satisfying $k>0$. Figure 5 shows a profile of the positive one-soliton solution with $k=1$ and $\alpha=0$.

From this one-soliton solution, we obtain two types of solutions of (2.49), i.e., solutions of (2.48): the majority of these solutions are kink-like solutions carrying a one-soliton and hence are called *one-soliton-kink* solutions, and the remaining ones are countably many kink solutions between the one-soliton-kink solutions and given by

$$v(x,t)=2n\pi-\arccos\tanh(x+t), \tag{3.25}$$

where $n\in\mathbb{Z}$. Figure 6 illustrates these solutions at $t=0$, while Fig. 7 consists of the wave forms of the one-soliton-kink solution v with $v(0,0)=\pi/2$ at $t=-4$, -2, -1 (first row) and at $t=0$, 1, 3 (second row).

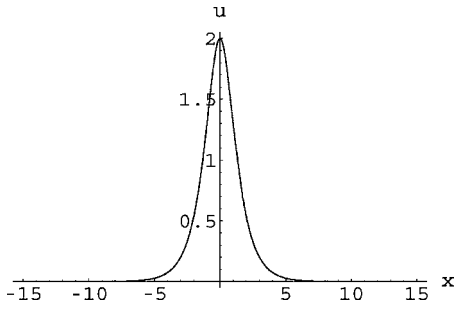

FIG. 5. Profile of a one-soliton solution of $u_t=\frac{3}{2}u^2u_x+u_{xxx}$.

The solutions v satisfying $v(0,0)=(2n+1)\pi$ with $n\in\mathbb{Z}$ are x-attractors, i.e., all nearby solutions approach these solutions as $x\to\pm\infty$; while the kink solutions are unstable in the x direction. Note that when t is sufficiently negative, the effect of the one-soliton u is a solitary valley in v; and when t is sufficiently large, the effect is a solitary peak. Moreover, if a negative soliton solution is used, then the solutions v so obtained are *one-soliton-antikink* solutions and antikink solutions.

Example 3.8: The MKdV equation (2.47) has two-soliton solutions

$$u(x,t)=\frac{2(k_1^2-k_2^2)(k_1\cosh g(x,t)+k_2\cosh f(x,t))}{(k_1^2+k_2^2)\cosh f(x,t)\cosh g(x,t)-2k_1k_2(\sinh f(x,t)\sinh g(x,t)-1)}, \tag{3.26}$$

where

$$f(x,t)=k_1x+k_1^3t+\alpha,\quad g(x,t)=k_2x+k_2^3t+\beta, \tag{3.27}$$

and k_1, k_2, α, and β are arbitrary real constants such that $k_1\neq 0\neq k_2$ and $|k_1|\neq|k_2|$ (either $k_1=0$ or $k_2=0$ for one-soliton solutions). Figure 8 shows the profiles of the two-soliton solution with $k_1=2$, $k_2=1$, $\alpha=-10$, and $\beta=0$ at $t=-2$, 0, 1 (first row) and at $t=2$, 3, 5 (second row).

From this two-soliton solution, we obtain two types of solutions of (2.49), i.e., solutions of (2.48): the majority of these solutions are two-kink-like solutions carrying a one-soliton and hence are called *one-soliton-two-kink* solutions, and the remaining ones are countably many two-kink solutions between the one-soliton-two-kink solutions (no formula for them). Figure 9 illustrates these solutions at $t=0$; while Fig. 10 consists of the wave forms of the one-soliton-two-kink solution v with $v(0,0)=\pi/2$ at $t=-3$, -1, 0 (first row), at $t=1$, 2, 3 (second row), and at $t=4$, 5, 7 (third row).

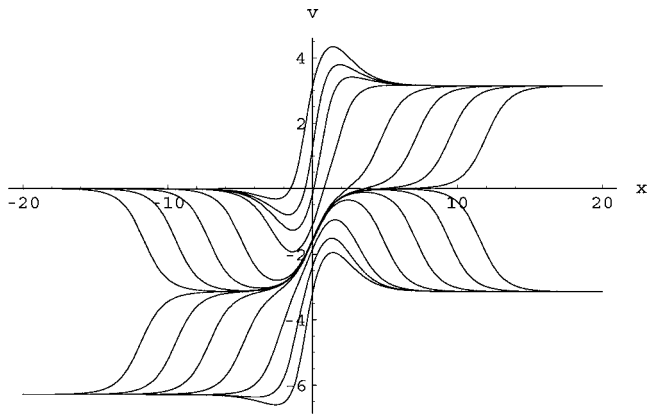

FIG. 6. Profiles of one-soliton-kink and kink solutions of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

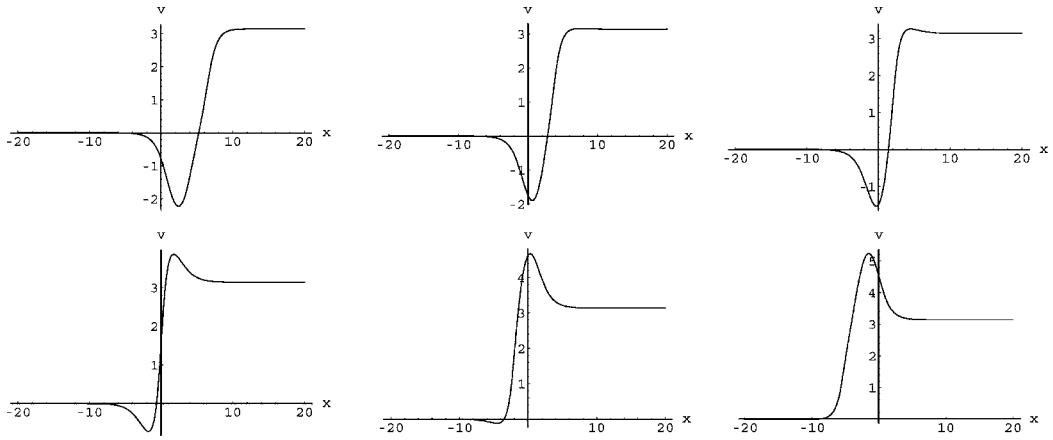

FIG. 7. Profiles of a one-soliton-kink solution of $v_t=\frac{3}{2}v_x \sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

When $k_1=k_2$ and $\alpha=\beta$, the countably many two-kink solutions look almost like kink solutions. Figure 11 shows such a solution together with nearby one-soliton-two-kink solutions at $t=0$ for the situation of $k_1=k_2=1$ and $\alpha=\beta=0$.

Again, the solutions v satisfying $v(0,0)=(2n+1)\pi$ with $n\in\mathbb{Z}$ are x-attractors; while the two-kink solutions are unstable in the x direction. Note that when t is sufficiently negative, the effects of the wider soliton and the narrower one in u are a solitary valley in v and a step in v, respectively; and when t is sufficiently large, the effects are a solitary peak and a step, respectively. Moreover, if a negative two-soliton solution is used, then the solutions v so obtained are *one-soliton-two-antikink* solutions and two-antikink solutions.

In general, an n-soliton solution u of the MKdV equation (2.47) gives countably many one-parameter families of *one-soliton-n-kink* or *one-soliton-n-antikink* solutions and countably many *n-kink* or *n-antikink* solutions of (2.48).

The exact solutions of (2.51) obtained from known solutions of the negative MKdV equation (2.50) and via the integrable system (2.52) can be discussed similarly. However, all the solutions v so defined seem to blow up, even for the ones deduced from $u=0$. So, we omit the details.

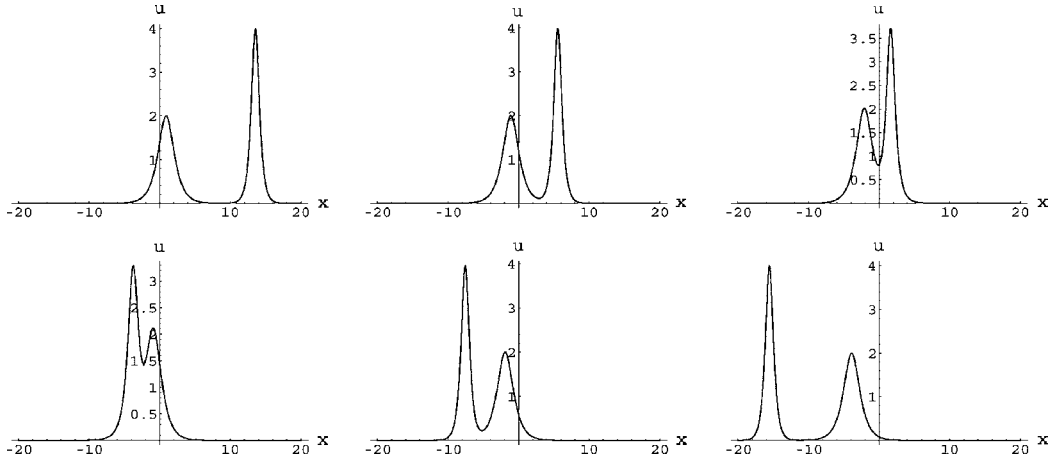

FIG. 8. Profiles of a two-soliton solution of $u_t=\frac{3}{2}u^2u_x+u_{xxx}$.

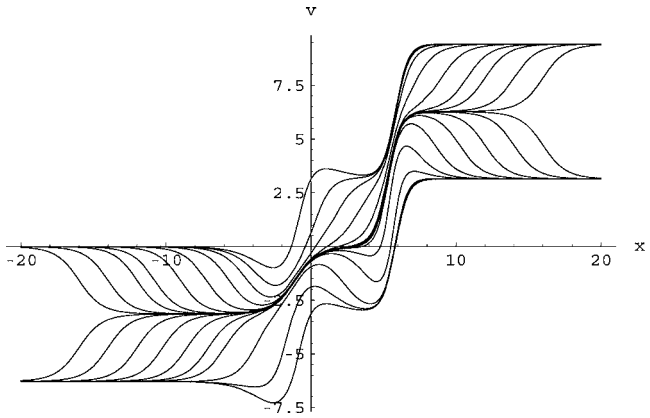

FIG. 9. Profiles of one-soliton-two-kinks and a two-kink of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

IV. BÄCKLUND TRANSFORMATIONS

In this section, we present a general method for obtaining new BTs from known ones using MTs, and apply the method to deduce BTs for PDEs in Theorems 2.4 and 2.6.

Theorem 4.1: *Assume that there is a local equivalence between a partial differential equation*

$$\mathcal{F}(u,u_x,u_t,\ldots,\partial_x^j u,\ldots,\partial_t^j u)=0 \tag{4.1}$$

and another partial differential equation

$$\mathcal{G}(v,v_x,v_t,\ldots,\partial_x^j v,\ldots,\partial_t^j v)=0 \tag{4.2}$$

given by Miura transformations $u\mapsto v$, defined using an integrable system

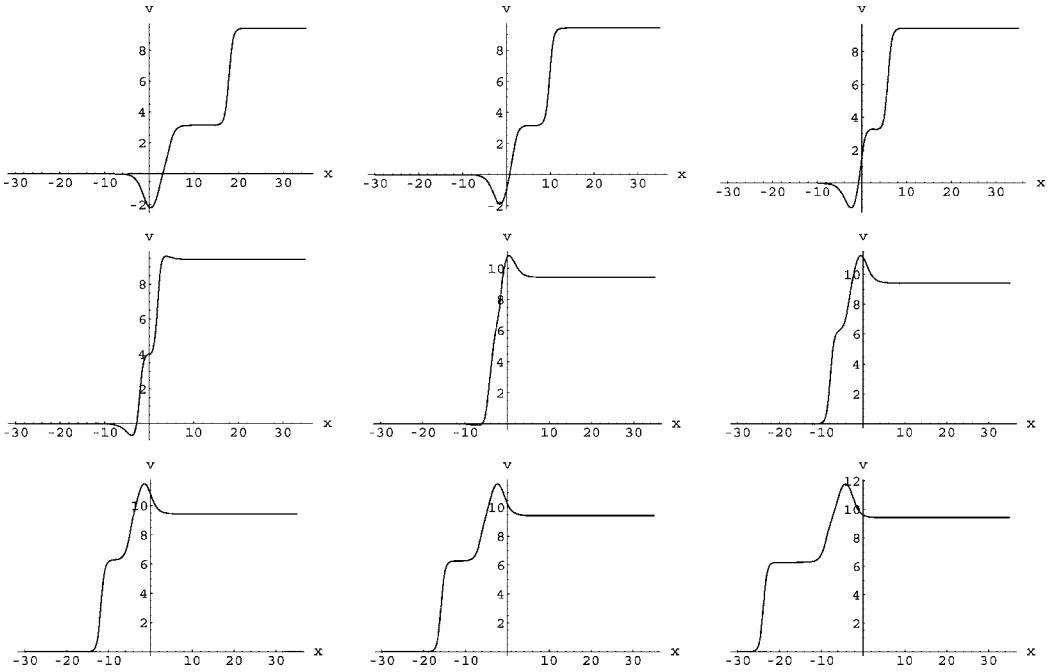

FIG. 10. Profiles of a one-soliton-two-kink solution of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

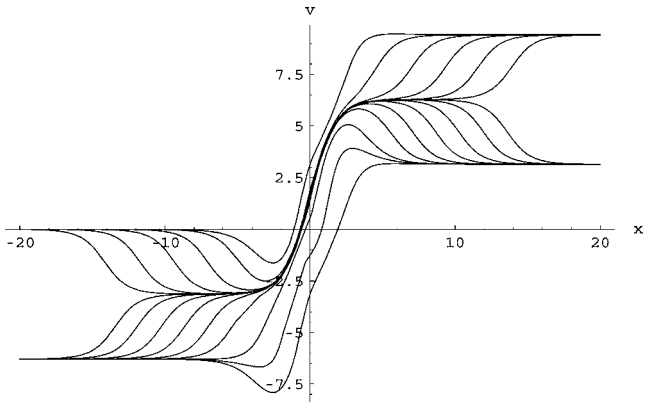

FIG. 11. Profiles of one-soliton-two-kinks and an almost kink of $v_t=\frac{3}{2}v_x\sin^2 v+\frac{1}{2}v_x^3+v_{xxx}$.

$$\begin{aligned} v_x &= \omega(v)+u,\\ v_t &= \Theta(v,u,u_x,u_t,\ldots,\partial_x^k u,\ldots,\partial_t^k u) \end{aligned} \tag{4.3}$$

associated with (4.1), *and* $v\mapsto u=v_x-\omega(v)$.

(i) *If* (4.1) *has a Bäcklund transformation*

$$u\mapsto \tilde{u}=F(\phi_1,\ldots,\phi_n,u,u_x,u_t,\ldots,\partial_x^k u,\ldots,\partial_t^k u) \tag{4.4}$$

defined using its associated integrable system

$$\begin{aligned} \Phi_x &= \Gamma(\phi_1,\ldots,\phi_n,u,u_x,u_t,\ldots,\partial_x^k u,\ldots,\partial_t^k u),\\ \Phi_t &= \Delta(\phi_1,\ldots,\phi_n,u,u_x,u_t,\ldots,\partial_x^k u,\ldots,\partial_t^k u), \end{aligned} \tag{4.5}$$

then (4.2) *also has a Bäcklund transformation*, *i.e.*,

$$v\mapsto u=v_x-\omega(v)\mapsto \tilde{u}=F(\phi_1,\ldots,\partial_t^k(v_x-\omega(v)))\mapsto \tilde{v} \tag{4.6}$$

defined using its associated integrable system

$$\begin{aligned} \Phi_x &= \Gamma(\phi_1,\ldots,\phi_n,v_x-\omega(v),\ldots,\partial_t^k(v_x-\omega(v))),\\ \tilde{v}_x &= w(\tilde{v})+F(\phi_1,\ldots,\partial_t^k(v_x-\omega(v))),\\ \Phi_t &= \Delta(\phi_1,\ldots,\phi_n,v_x-\omega(v),\ldots,\partial_t^k(v_x-\omega(v))),\\ \tilde{v}_t &= \Theta(\tilde{v},\ldots,\partial_t^k F(\phi_1,\ldots,\partial_t^k(v_x-\omega(v)))). \end{aligned} \tag{4.7}$$

(ii) *If* (4.2) *has a Bäcklund transformation*

$$v\mapsto \tilde{v}=F(\phi_1,\ldots,\phi_n,v,v_x,v_t,\ldots,\partial_x^k v,\ldots,\partial_t^k v) \tag{4.8}$$

defined using its associated integrable system

$$\begin{aligned} \Phi_x &= \Gamma(\phi_1,\ldots,\phi_n,v,v_x,v_t,\ldots,\partial_x^k v,\ldots,\partial_t^k v),\\ \Phi_t &= \Delta(\phi_1,\ldots,\phi_n,v,v_x,v_t,\ldots,\partial_x^k v,\ldots,\partial_t^k v), \end{aligned} \tag{4.9}$$

then (4.1) *also has a Bäcklund transformation*, *i.e.*,

$$u \mapsto v \mapsto \tilde{v} = F(\phi_1, \ldots, \partial_t^k v) \mapsto \tilde{u} = \tilde{v}_x - \omega(\tilde{v}) \tag{4.10}$$

defined using its associated integrable system

$$\begin{gathered} v_x = \omega(v) + u, \\ \Phi_x = \Gamma(\phi_1, \ldots, \phi_n, v, v_x, v_t, \ldots, \partial_x^k v, \ldots, \partial_t^k v), \\ v_t = \Theta(v, u, u_x, u_t, \ldots, \partial_x^k u, \ldots, \partial_t^k u), \\ \Phi_t = \Delta(\phi_1, \ldots, \phi_n, v, v_x, v_t, \ldots, \partial_x^k v, \ldots, \partial_t^k v). \end{gathered} \tag{4.11}$$

Note that the new BT is defined using $n+1$ pseudopotentials, i.e., $\phi_1, \ldots, \phi_n$, $\tilde{v}$ in (i) and v, $\phi_1, \ldots, \phi_n$ in (ii). Sometimes, the new BT can be equivalently defined using an associated integrable system of a lower degree (i.e., with less pseudopotentials, see Sec. I in Ref. 14 for the definition of degree).

Combining Theorems 4.1 and (2.4) we immediately get the following fact.

Corollary 4.2: *If one of the nonlinear partial differential equations* (2.43) and (2.44) *has a Bäcklund transformation*, *then the other one also has a Bäcklund transformation*.

A special case of Corollary 4.2 is the following classical example.

Example 4.3: In Ref. 12, Wahlquist and Estabrook found a BT $v \mapsto \tilde{v}$ for the potential KdV equation

$$v_t = 3v_x^2 + v_{xxx} \tag{4.12}$$

defined by

$$\begin{gathered} \tilde{v}_x = \lambda - v_x - \tfrac{1}{2}(v - \tilde{v})^2, \\ \tilde{v}_t = -v_t + (v - \tilde{v})(v_{xx} - \tilde{v}_{xx}) - 2(v_x^2 + v_x \tilde{v}_x + \tilde{v}_x^2), \end{gathered} \tag{4.13}$$

where λ is an arbitrary constant. From this BT, they deduced the now well-known BT $u \mapsto \tilde{u}$ for the KdV equation (1.2) defined by

$$u \mapsto v = \int u \, \mathrm{d}x \mapsto \tilde{v} \mapsto \tilde{u} := \tilde{v}_x. \tag{4.14}$$

So, the BT $u \mapsto \tilde{u} = \tilde{v}_x$ for the KdV equation is defined using the integrable system

$$\begin{gathered} v_x = u, \\ \tilde{v}_x = \lambda - u - \tfrac{1}{2}(v - \tilde{v})^2, \\ v_t = 2v^2 u + 2u^2 + 2v u_x + u_{xx}, \\ \tilde{v}_t = -3u^2 - u_{xx} + (v - \tilde{v})(u_x - \tilde{v}_{xx}) - 2(u^2 + u\tilde{v}_x + \tilde{v}_x^2) \end{gathered} \tag{4.15}$$

associated with the KdV equation.

Note that the transformation $u \mapsto v$ from the KdV equation (1.2) to the potential KdV equation (4.12) defined using $v_x = u$ and $v_t = 3u^2 + u_{xx}$ is an easy example of the MT given by Theorem 2.4 with $\delta = 0$, $Q = 1$ and $\tilde{\Theta}(v, u) = 3u^2$.

In Ref. 11, it is shown that the above BT $u \mapsto \tilde{u}$ for the KdV equation can also be defined as follows. Let ϕ be the solution of the associated integrable system

$$\phi_x = -\lambda + \phi^2 + u,$$
$$\phi_t = 4\lambda(-\lambda + \phi^2) + 2(\lambda + \phi^2)u + 2u^2 + 2\phi u_x + u_{xx}, \tag{4.16}$$

where λ is an arbitrary constant, then

$$u \mapsto \tilde{u} = 2\lambda - 2\phi^2 - u \tag{4.17}$$

is the BT.

Generalizing the above-presented example, we have the following fact.

Corollary 4.4: If one of a partial differential equation

$$u_t = \partial_x f(u, u_x, u_t, \ldots, \partial_x^j u, \ldots, \partial_t^j u) \tag{4.18}$$

and its potential equation

$$v_t = f(v_x, v_{xx}, v_{xt}, \ldots, \partial_x^j v_x, \ldots, \partial_t^j v_x) \tag{4.19}$$

has a Bäcklund transformation, then the other one also has a Bäcklund transformation.

Proof: This is because that there is a MT $u \mapsto v$ from (4.18) to (4.19) defined using the integrable system

$$v_x = u,$$
$$v_t = f(u, u_x, u_t, \ldots, \partial_x^j u, \ldots, \partial_t^j u) \tag{4.20}$$

associated with (4.18). ■

Example 4.5: Using Theorem 4.1 and the local equivalence between the KdV equation and the MKdV equation mentioned at the beginning of this paper, one can get the known BT for the KdV equation from that for the MKdV equation, and vis versa. We omit the details.

Example 4.6: In Ref. 4, Lamb obtained the following BT

$$u \mapsto \tilde{u} = \frac{4\lambda\phi}{1 + \phi^2} + u \tag{4.21}$$

for the MKdV equation (2.47), where λ is an arbitrary nonzero constant, and ϕ is the solution of the associated integrable system

$$\phi_x = \lambda\phi + \tfrac{1}{2}(1 + \phi^2)u,$$
$$\phi_t = \lambda^3 + \tfrac{1}{2}\lambda^2(1 + \phi^2)u + \tfrac{1}{2}\lambda\phi u^2 + \tfrac{1}{4}(1 + \phi^2)u^3 + \tfrac{1}{2}\lambda(1 - \phi^2)u_x + \tfrac{1}{2}(1 + \phi^2)u_{xx}. \tag{4.22}$$

Using this BT together with the MTs $u \mapsto v$ from (2.47) to (2.48), defined using (2.49), and $v \mapsto u = v_x - \sin v$ from (2.48) to (2.47), we deduce a BT $v \mapsto \tilde{v}$ for the nonlinear PDE (2.48):

$$v \mapsto u = v_x - \sin v \mapsto \tilde{u} = \frac{4\lambda\phi}{1 + \phi^2} + (v_x - \sin v) \mapsto \tilde{v} \tag{4.23}$$

defined using the integrable system

$$\phi_x = \lambda\phi + \tfrac{1}{2}(1 + \phi^2)u,$$
$$\tilde{v}_x = \sin\tilde{v} + \tilde{u},$$
$$\phi_t = \lambda^3 + \tfrac{1}{2}\lambda^2(1 + \phi^2)u + \tfrac{1}{2}\lambda\phi u^2 + \tfrac{1}{4}(1 + \phi^2)u^3 + \tfrac{1}{2}\lambda(1 - \phi^2)u_x + \tfrac{1}{2}(1 + \phi^2)u_{xx},$$

$$\tilde{v}_t = \sin\tilde{v} + \tilde{u} + \tfrac{1}{2}\tilde{u}^2 \sin\tilde{v} + \tfrac{1}{2}\tilde{u}^3 + \tilde{u}_x \cos\tilde{v} + \tilde{u}_{xx} \tag{4.24}$$

associated with (2.48). Note that u and $\tilde{u}$ in (4.24) are expressions in ϕ and v and are given by (4.23).

In Ref. 14, a BT for (2.48) using one pseudopotential was found. Now, (4.23) is another BT for (2.48), using two pseudopotentials. Moreover, a new BT for the MKdV equation can be deduced similarly, see Ref. 15.

Example 4.7: In Ref. 14, the BT

$$u \mapsto \tilde{u} = 2\sinh\phi + u \tag{4.25}$$

for the negative MKdV equation (2.50) defined using its associated integrable system

$$\begin{aligned} \phi_x &= \sinh\phi + u, \\ \phi_t &= \sinh\phi + u - \tfrac{1}{2}u^2 \sinh\phi - \tfrac{1}{2}u^3 + u_x \cosh\phi + u_{xx} \end{aligned} \tag{4.26}$$

has been deduced. From this BT for (2.50) and the local equivalence between (2.50) and (2.51) given in Theorem 2.6, we obtain the BT

$$v \mapsto u = v_x - \sinh v \mapsto \tilde{u} = 2\sinh\phi - \sinh v + v_x \mapsto \tilde{v} \tag{4.27}$$

for (2.51) defined using the integrable system

$$\begin{aligned} \phi_x &= \sinh\phi + u, \\ \tilde{v}_x &= \sinh\tilde{v} + \tilde{u}, \\ \phi_t &= \sinh\phi + u - \tfrac{1}{2}u^2 \sinh\phi - \tfrac{1}{2}u^3 + u_x \cosh\phi + u_{xx}, \\ \tilde{v}_t &= \sinh\tilde{v} + \tilde{u} - \tfrac{1}{2}\tilde{u}^2 \sinh\tilde{v} - \tfrac{1}{2}\tilde{u}^3 + \tilde{u}_x \cosh\tilde{v} + \tilde{u}_{xx} \end{aligned} \tag{4.28}$$

associated with (2.51).

We believe that this is the first time that a BT for (2.51) is found. By Theorem 2.43 in Ref. 14 this BT cannot be defined using an associated integrable system of the form

$$\begin{aligned} \phi_x &= \Gamma(\phi, u, u_x, u_{xx}), \\ \phi_t &= \Delta(\phi, u, u_x, u_{xx}). \end{aligned} \tag{4.29}$$

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Heat-kernel expansion on noncompact domains and a generalized zeta-function regularization procedure

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Heat-kernel expansion and zeta function regularization are discussed for Laplace-type operators with discrete spectrum in noncompact domains. Since a general theory is lacking, the heat-kernel expansion is investigated by means of several examples. It is pointed out that for a class of exponential (analytic) interactions, generically the noncompactness of the domain gives rise to logarithmic terms in the heat-kernel expansion. Then, a meromorphic continuation of the associated zeta function is investigated. A simple model is considered, for which the analytic continuation of the zeta function is not regular at the origin, displaying a pole of higher order. For a physically meaningful evaluation of the related functional determinant, a generalized zeta function regularization procedure is proposed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2259580]

I. INTRODUCTION

Within the so-called one-loop approximation in quantum field theory, the Euclidean one-loop effective action can be expressed in terms of the sum of the classical action and a contribution depending on a functional determinant of an elliptic differential operator, the so-called fluctuation operator. The ultraviolet one-loop divergences which are present need to be regularized by means of a suitable technique (for recent reviews, see Refs. 1–5).

In general, one works in Euclidean spacetime and deals with a self-adjoint, non-negative, second-order differential operator of the form

$$L = -\Delta + V, \tag{1.1}$$

where Δ is the Laplace-Beltrami operator and V a potential depending on the classical background solution and containing, in general, a mass term. It is well known that the one-loop effective action $W \equiv W[\Phi]$, is related to the functional determinant of the field operator L by

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$$W = -\ln Z = S + \frac{1}{2}\ln\det\frac{L}{\mu^2}, \tag{1.2}$$

S being the classical action and μ^2 a renormalization parameter, which appears for dimensional reasons.

The one-loop divergences may be dealt with by using a variant of the zeta-function regularization method.[6–8] One namely introduces the regularization parameter ε and considers

$$W(\varepsilon) = S - \frac{1}{2}\int_0^\infty \mathrm{d}t\,\frac{t^{\varepsilon-1}}{\Gamma(1+\varepsilon)}\mathrm{Tr}\,e^{-tL/\mu^2} = S - \frac{1}{2\varepsilon}\zeta(\varepsilon|L/\mu^2), \tag{1.3}$$

where, as usual, for the elliptic operator L the zeta function is defined by means of the Mellin-type transform

$$\zeta(s|L) = \frac{1}{\Gamma(s)}\int_0^\infty \mathrm{d}t\,t^{s-1}\mathrm{Tr}\,e^{-tL}, \quad \zeta(s|L/\mu^2) = \mu^{2s}\zeta(s|L). \tag{1.4}$$

Here the heat trace $\mathrm{Tr}\,e^{-tL}$ plays a preeminent role. Recall that, for a second-order elliptic nonnegative operator L in a *compact* d-dimensional manifold without boundary, one has the small-t asymptotic expansion

$$\mathrm{Tr}\,e^{-tL} \simeq \sum_{j=0}^{\infty} A_j(L)t^{j-d/2}, \tag{1.5}$$

where $A_j(L)$ are the Seeley-DeWitt coefficients.[9,10] As a result, for a second-order differential operator in d-dimensions, the integral (1.4) is convergent in the domain $\mathrm{Re}\,s > d/2$.

In the compact case, $\zeta(s|L)$ is regular at the origin and one has the well-known result $\zeta(0|L) = A_{d/2}(L)$. The latter quantity is computable (see, for example, the recent reviews (Refs. 11 and 12) and depends on the potential and on geometric invariants. In particular, for odd dimensional manifolds without boundaries, $\zeta(0|L) = 0$. Performing a Taylor expansion of the zeta function we obtain

$$W(\varepsilon) = S - \frac{1}{2\varepsilon}\zeta(0|L) + \frac{\zeta(0|L)}{2}\ln\mu^2 + \frac{\zeta'(0|L)}{2} + O(\varepsilon). \tag{1.6}$$

Thus, the one-loop divergences as well as finite contributions to the one-loop effective action are expressed in terms of the zeta function and its derivative evaluated at the origin.

In this paper, we would like to discuss a more general situation where *logarithmic terms* in the heat-trace asymptotics are present. First, we recall a well-known but crucial fact concerning the local heat-kernel expansion associated with a Laplace type operator in R^d of the kind

$$H = -\Delta + V(x). \tag{1.7}$$

If the potential is real and non-negative, with an additional, rather mild hypothesis, the operator H is essentially self-adjoint in $C_0^\infty(R^d)$. We will be interested in confining potentials which, with the additional hypothesis of being also smooth functions, give rise to a discrete spectrum. As has been shown in Refs. 13 and 14, the local heat-kernel expansion can be partially summed over and rewritten under the form

$$K_t(x,x) = \frac{1}{(4\pi t)^{d/2}}e^{-tV(x)}\sum_{n=0}^{\infty} b_n(x)t^n, \tag{1.8}$$

where the new coefficients $b_n(x)$ can easily be computed and depend only on the derivatives of the potential $V(x)$. The first few read

$$b_0(x) = 1, \quad b_1(x) = 0,$$

$$b_2(x) = -\frac{1}{6}\Delta V, \quad b_3(x) = -\frac{\Delta^2 V}{60} + \frac{\nabla_k V \nabla_k V}{12}, \tag{1.9}$$

$$b_4(x) = -\frac{\Delta^3 V}{840} + \frac{(\Delta V)^2}{72} + \frac{\nabla_i \nabla_j V \nabla_i \nabla_j V}{90} + \frac{\nabla_k V \nabla_k \Delta V}{30}. \tag{1.10}$$

We will make use of such a resummation for obtaining the heat-kernel trace asymptotics in Sec. II.

If one is dealing with smooth compact manifolds, the passage to the heat-kernel trace is accomplished by integrating term by term over the coordinates, and no logarithmic contribution in the heat-trace expansion appears. However, in the case of nonsmooth manifolds one may get logarithmic terms in the heat-kernel trace, e.g., when one considers the Laplace operator on higher-dimensional cones,[15,16] but also in four-dimensional spacetimes with a three-dimensional, noncompact, hyperbolic spatial section of finite volume,[17] and in the case of general pseudo-differential operators.[18] More recently, the presence of logarithmic terms in self-interacting scalar field theory defined on manifolds with noncommutative coordinates has also been pointed out.[19–21] This goes together with a nontypical behavior of the corresponding zeta function: possibly a simple pole at the origin and higher-order poles at other places.

Here we would like to investigate the case of Laplace-type self-adjoint operators defined on *noncompact* manifolds. To our knowledge, for the general case of a confining potential and discrete spectrum, a systematic theory has yet to be formulated. A pioneering investigation along this line can be found in Ref. 22. Other studies involve one-dimensional problems on the real half-line[23] and the Barnes zeta functions.[24] With regard to the presence of logarithmic terms in heat-trace asymptotics, one should note that they have been considered in the abstract context of regularized products in many places.

Recall that, under certain conditions, the regularized product associated with an infinite sequence of nonzero complex numbers $\{\lambda_n\}$ has a related Dirichlet series $\Sigma_n \lambda_n^{-s}$ (the zeta-function). In this paper, we are only interested in the case when the λ_n are eigenvalues of *non-negative* differential operators and the zeta function converges absolutely for Re s sufficiently large. When this zeta-function is holomorphic at the origin, the regularized product is defined as $\exp[-\zeta'(0)]$. A general theory is presented in Refs. 27 and 28 and other relevant papers are Refs. 29–31 and references quoted therein. It is worth mentioning that the case of noncompact domains but with scattering potentials, namely the ones for which a continuous spectrum exists, is well understood and the S-matrix or the phase shift function then enter the game (see, for instance, Ref. 32). In this context, delta-like potentials have also been considered (see, e.g., Refs. 33–35, and references therein). If the potential is singular, for instance, proportional to $1/x^2$, the presence of logarithmic terms in the local heat-kernel expansion is also possible, their coefficients becoming distributions[25] (see also the recent paper (Ref. 26) and references therein). Here, we will not deal with situations of this kind. Moreover, for the sake of simplicity, we will limit ourselves to the R^d flat case.

The content of the paper is as follows. In Sec. II, local heat-kernel asymptotics are reviewed for the simple case we are going to deal with. In Sec. III, the heat-trace asymptotics are investigated and the possibility for the presence of logarithmic terms is pointed out explicitly. The consequences of such unusual terms are discussed in Sec. IV in some detail. Finally, in Sec. V, a simple model of confinement is proposed and a generalization of the zeta-function regularization method is constructed to deal with this case. The paper ends with some conclusions and an Appendix.

II. HEAT-KERNEL TRACE ASYMPTOTICS IN NONCOMPACT DOMAINS

In this section we will show that, for suitable classes of potentials in noncompact domains, logarithmic terms can actually be present in the heat-trace expansion. Under the usual hypothesis

concerning the potential $V(x)$—namely $V(x)$ smooth enough, non-negative, and going to infinity for $|x|\to\infty$—the heat trace can be shown to exist and the heat kernel asymptotics is given by

$$\mathrm{Tr}\, e^{-tH} = \int_{R^d} \mathrm{d}x\, K_t(x,x) = \frac{1}{(4\pi t)^{d/2}} \int_{R^d} \mathrm{d}x\, e^{-tV(x)}[1 + t^2 b_2(x) + t^3 b_3(x) + \cdots]. \tag{2.1}$$

In particular we shall focus our attention on the class of spherical potentials, $V(x)=V(r)$, $r \in [0,\infty)$, and thus

$$\mathrm{Tr}\, e^{-tH} = \frac{\Omega_d}{(4\pi t)^{d/2}} \int_0^\infty \mathrm{d}r\, r^{d-1} e^{-tV(r)}[1 + O(t^2)], \tag{2.2}$$

where $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$. The latter expression will be our starting point for further discussions.

As a first family of potentials, let us consider $V(r)$ to be a positive polynomial of degree Q. In this case, we will show that logarithmic terms are absent, but the leading term goes as $O(t^{-d/2-d/Q})$, in contrast to the leading behavior $O(t^{-d/2})$ associated with the compact case. To prove this, since we are interested in the short-t leading term, it is sufficient to consider the leading term of the potential, namely $V(r)=r^Q+\cdots$. Thus, the leading term in the heat trace reads

$$\mathrm{Tr}\, e^{-tH} \simeq \frac{\Omega_d}{(4\pi t)^{d/2}} \int_0^\infty \mathrm{d}r\, r^{d-1} e^{-tr^Q} = \frac{2^{1-d}\Gamma(d/Q)}{Q\Gamma(d/2)t^{d/2+d/Q}}. \tag{2.3}$$

One can check that this result holds true for the case $Q=2$, for which the heat trace is well known, since it corresponds to the partition function of a harmonic oscillator in d-dimensions. In fact one has eigenvalues $2n+1$ for each dimension and then

$$\mathrm{Tr}\, e^{-tH} = \left(\sum_0^\infty e^{-t(2n+1)}\right)^d = \frac{1}{(2\sinh t)^d} \simeq \frac{1}{(2t)^d} + \cdots, \tag{2.4}$$

in agreement with Eq. (2.3) (note that here $m=1/2$ and $\omega=2$). Our results also agree with those for the one-dimensional case investigated in Ref. 23.

The situation drastically changes if one considers exponential confining potentials which, for large r, go asymptotically as $V(r)\simeq e^{r^Q}$. We will show that in these cases logarithmic terms are present. In fact, we have

$$\mathrm{Tr}\, e^{-tH} \simeq \frac{\Omega_d}{(4\pi)^{d/2}t^{d/2}} \int_0^\infty \mathrm{d}r\, r^{d-1} e^{-te^{r^Q}} = \frac{\Omega_d}{(4\pi)^{d/2}t^{d/2}Q} \int_1^\infty \mathrm{d}y\, y^{-1} e^{-ty} (\ln y)^{d/Q-1}. \tag{2.5}$$

For simplicity, let us now assume d/Q to be an integer. In such case we can use (A4) and (A6), thus obtaining the leading term in the form

$$\mathrm{Tr}\, e^{-tH} \simeq \frac{(-1)^{d/Q}}{2^d Q\Gamma(d/2+1)t^{d/2}} (\ln t)^{d/Q}. \tag{2.6}$$

It has to be noted that with respect to the compact case, for such class of potentials on noncompact manifolds, the leading term in the trace is modified by the presence of the logarithmic factor $(\ln t)^{d/Q}$. We also note that, for $Q=1$, (2.6) yields the same result obtained by Nash in Ref. 22 using a different method. Let us emphasize that those comparisons are essential both for consistency reasons and in view of its application to real situations in physics.

Equations (2.3) and (2.5) give only the leading term in the trace of the heat kernel, but in principle it is possible to go on in the expansion by integrating other terms of the local asymptotics. However it should be stressed that more terms in the local expansion can give contributions of the same order to the trace asymptotics. This can be easily seen by considering, for instance, the one-dimensional harmonic oscillator described by the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\omega^2 x^2}{4}, \quad \hbar = 1, \quad m = \frac{1}{2}. \tag{2.7}$$

For this model, one has

$$\mathrm{Tr}\, e^{-tH} = \frac{1}{2\sinh(\omega t/2)} = \frac{1}{\omega t} - \frac{\omega t}{24} + O(t^3), \tag{2.8}$$

$$K_t(x,x) = \sqrt{\frac{\omega}{4\pi \sinh \omega t}} e^{-\omega x^2(\cosh \omega t - 1)/2 \sinh \omega t} = \frac{e^{-tV}}{\sqrt{4\pi t}}(1 + b_2 t^2 + b_3 t^3 + \cdots),$$

$$b_2 = -\frac{\omega^2}{12}, \quad b_3 = \frac{\omega^4 x^2}{48}. \tag{2.9}$$

In order to get the expansion (2.8) up to order t, one needs to integrate the local expansion up to order $t^{5/2}$. This means that both b_2 and b_3 give a contribution of order t in the trace asymptotics. To obtain the subsequent term t^3, one has to consider all b_n coefficients up to b_6.

III. MEROMORPHIC EXTENSION OF THE ZETA-FUNCTION

With respect to the compact case, the meromorphic structure of the zeta-function associated with the operator H is generically quite complicated and it is strictly related to the form of the potential. In order to show this, we first consider the polynomial case $V(r)=r^Q$ and assume $Q=2P$ to be an even number. Under such assumption all b_n coefficients are polynomials in r and the heat-trace asymptotics are of the form

$$\mathrm{Tr}\, e^{-tH} = \sum_n C_n t^{\alpha_n - (d/2 + d/Q)}, \quad C_0 = \frac{\Gamma(d/Q)}{2^{d-1} Q \Gamma(d/2)}, \quad \alpha_0 = 1 < \alpha_1 < \alpha_2 < \cdots, \tag{3.1}$$

where the C_n are numerical coefficients obtained by integrating the local expansion, and the α_n are rational numbers. Making use of (1.4) and splitting the integration over t into $(0,1]$ and $[1,\infty)$, we get

$$\zeta(s|H) = \frac{1}{\Gamma(s)} \sum_n \frac{C_n}{s + \alpha_n - \left(\frac{d}{2} + \frac{d}{Q}\right)} + \frac{J(s)}{\Gamma(s)}, \tag{3.2}$$

where $J(s)$ is an analytic function. It follows that for such class of potentials the zeta function admits only simple poles—as it happens in the compact case—but whose location strictly depends on the form of the potential, since the α_n are not universal powers. Moreover, we see that $\zeta(0|H)$ is not vanishing if and only if $\alpha_n = d/2 + d/Q$ for some n and the corresponding coefficient C_n is different from zero (note that if this coefficient $C_n=0$, then the corresponding term is absent from the sum, for any s).

The situation becomes more complicated for the class of exponential potentials we have considered in Sec. II. In fact, in such case one obtains in general an asymptotic expansion with terms of the kind $t^\alpha (\ln t)^\beta$, α and β being rational numbers which depend on the potential, and this means that the meromorphic extension of the zeta function will have poles or branch points of order β at $s=-\alpha$ (see (A8)).

In order to compute the nonholomorphic structure of the zeta function for this class of potentials it is convenient to proceed as follows. We use the general expression (1.8) in (1.4) and thus, for $\mathrm{Re}\, s$ sufficiently large and $V(x)=V(r)>0$, we can write

$$\zeta(s|H) \sim \frac{1}{(4\pi)^{d/2}\Gamma(s)}\sum_n \int_0^\infty \mathrm{d}t\, t^{s+n-d/2-1}\int_{R^d}\mathrm{d}x\, b_n(x)e^{-tV(x)} = \sum_n \frac{\Gamma(s+n-d/2)}{(4\pi)^{d/2}\Gamma(s)}\int_{R^d}\mathrm{d}x\, b_n(x) \times [V(x)]^{-(s+n-d/2)}, \tag{3.3}$$

which is well defined for even Q, since in such case all coefficients $b_n(x)$ are regular everywhere. Since $V(r)$ is exponential like and spherically symmetric, we may assume that

$$b_n = \sum_{pq} C_{pq}^n r^p V^q, \quad 0 \leqslant p \leqslant 2(n-1)(Q-1), \quad 1 \leqslant q < n, \quad n \geqslant 2. \tag{3.4}$$

Now, the integration can be performed and we obtain for the nonholomorphic part

$$\zeta(s|H) \sim \frac{\Omega_d}{(4\pi)^{d/2}\Gamma(s)}\left[\Gamma(s-d/2)\int_0^\infty \mathrm{d}r\, r^{d-1}e^{-(s-d/2)r^Q} + \sum_{n\geqslant 2;pq} C_{pq}^n \Gamma(s+n-d/2)\int_0^\infty \mathrm{d}r\, r^{d+p-1}e^{-(s+n-q-d/2)r^Q}\right] = \frac{\Omega_d}{(4\pi)^{d/2}Q\Gamma(s)}\left[\frac{\Gamma(s-d/2)\Gamma(d/Q)}{(s-d/2)^{d/Q}} + \sum_{n\geqslant 2;pq} C_{pq}^n \frac{\Gamma(s+n-d/2)\Gamma((d+p)/Q)}{(s+n-q-d/2)^{(d+p)/Q}}\right]. \tag{3.5}$$

As a consequence, it follows that generically the zeta function may have poles and branch points of any order. It should also be noted that in the case of even dimension it is not holomorphic at the origin.

For example, in the simplest case $d=Q=2$, $V(r)=e^{r^2}$, by straightforward dimensional analysis one can see that only the term proportional to C_{21}^2 contributes to the singularity at the origin and we get (see Sec. IV)

$$\zeta(s|H) = \frac{C_{21}^2}{4s} + \cdots, \quad C_{21}^2 = -\frac{2}{3}. \tag{3.6}$$

We conclude this section by studying the asymptotics of the spectral density associated with the operator H. We can define the spectral density via the spectral representation of the heat trace, namely

$$\mathrm{Tr}\, e^{-tH} = \int_0^\infty e^{-t\lambda}\mathrm{d}N(\lambda) = \int_0^\infty \mathrm{d}\lambda e^{-t\lambda}\rho(\lambda). \tag{3.7}$$

For the polynomial interaction, the Tauberian theorems (see the Appendix) and the short-t leading terms of the heat-trace expansion give

$$N(\lambda) \simeq \lambda^{(dQ+2d)/2Q}, \quad \rho(\lambda) \simeq \lambda^{(dQ+2d)/2Q-1}, \quad \lambda \to \infty, \tag{3.8}$$

while for the exponential interaction, with d/Q an integer,

$$N(\lambda) \simeq \lambda^{d/Q}(\ln\lambda)^{d/Q}, \quad \rho(\lambda) \simeq \lambda^{d/Q-1}(\ln\lambda)^{d/Q}, \quad \lambda \to \infty. \tag{3.9}$$

In particular, when $Q=d$, one has

$$N(\lambda) \simeq \lambda(\ln\lambda), \quad \rho(\lambda) \simeq \ln\lambda, \quad \lambda \to \infty. \tag{3.10}$$

In this last case the distribution of the eigenvalues of the operator H resembles the asymptotic behavior which one meets in number theory, namely the asymptotic distribution of the nontrivial zeroes of the Riemann zeta function.[22] With regard to this important issue we refer the reader to the literature, mentioning the relevance of the method based on Cramer's V-function (Ref. 36 and references therein). Other related papers are Refs. 37 and 38.

IV. A SIMPLE MODEL OF CONFINEMENT

In this section we investigate an explicit model, namely a massive scalar field defined on a flat spacetime $R\times R^3$ in an external static field described by a confining potential which is asymptotically exponential in two dimensions. In the Euclidean version, we may compactify the "time" coordinate and the *zeta* spatial coordinate, assuming periodic boundary conditions with periods β and l, respectively. As a result, the relevant operator reads

$$L=-\frac{\mathrm{d}^2}{\mathrm{d}^2\tau}-\frac{\mathrm{d}^2}{\mathrm{d}z^2}+H_2+M^2,\quad H_2=-\Delta_2+V(r),\quad V(r)=g^2e^{\alpha^2r^2}, \tag{4.1}$$

g and α being dimensional parameters. Making use of Poisson's resummation formula, the heat trace can be written as

$$\mathrm{Tr}\, e^{-tL}=\frac{Se^{-tM^2}}{4\pi t}\mathrm{Tr}\, e^{-tH_2}+\ldots, \tag{4.2}$$

where $S=\beta l$ and the dots stand for exponentially small terms in the parameter t.

In this model, the zeta function can be computed by using the method described in Sec. III, but one now obtains an expression which is different from (3.3), since the potential is defined only on R^2 and one needs to take the factor $e^{-tM^2/t}$ into account. As a result, we get

$$\zeta(s|L)\sim\frac{S}{(4\pi)^2\Gamma(s)}\sum_n\int_0^\infty \mathrm{d}t\, t^{s+n-3}\int_{R^2}\mathrm{d}x\,\tilde{b}_n(x)e^{-tV(r)}=\sum_n\frac{\Gamma(s+n-2)}{(4\pi)^2\Gamma(s)}\int_{R^2}\mathrm{d}x\,\tilde{b}_n(x)[V(r)]^{-(s+n-2)}, \tag{4.3}$$

where the $\tilde{b}_n$ are related to the b_n in (3.4) by

$$\tilde{b}_n=\sum_{j+k=n}\frac{(-1)^kb_jM^{2k}}{k!},\quad n\geqslant 2,\quad \tilde{b}_0=1,\quad \tilde{b}_1=-M^2. \tag{4.4}$$

The $\tilde{b}_n$ have again the same structure as in Eq. (3.4), but now q can vanish, namely

$$\tilde{b}_n=\sum_{pq}\tilde{C}^n_{pq}r^pa^qe^{qbr^2},\quad 0\leqslant p\leqslant 2(n-1),\quad 0\leqslant q<n,\quad n\geqslant 0, \tag{4.5}$$

$$\tilde{C}^n_{00}=\frac{(-1)^nM^{2n}}{n!}. \tag{4.6}$$

The b_n coefficients which appear in Eq. (4.5) can be evaluated by making use of (1.9) and (1.10); the first nontrivial ones read

$$b_2=-\frac{2g\alpha e^{\alpha r^2}}{3}(1+\alpha r^2),$$

$$b_3=-\frac{4g\alpha^2e^{\alpha r^2}}{15}(2+4\alpha r^2+\alpha^2r^4)+\frac{g^2\alpha^2e^{2\alpha r^2}}{3},$$

$$b_4=-\frac{8g\alpha^3e^{\alpha r^2}}{105}(6+18\alpha r^2+9\alpha^2r^4+\alpha^3r^6)+\frac{2g^2\alpha^2e^{2\alpha r^2}}{45}(7+38\alpha r^2+21\alpha^2r^4), \tag{4.7}$$

from which we can read off the C^n_{pq} coefficients up to $n=4$.

By integrating (4.3), the nonholomorphic contribution to the zeta function reads

$$\zeta(s|L) = \frac{S}{16\pi\Gamma(s)} \sum_{n\geqslant 0;pq} \tilde{C}^n_{pq} \frac{\Gamma(s+n-2)\Gamma(1+p/2)a^{-(s+n-q-2)}}{b^{1+p/2}(s+n-q-2)^{1+p/2}}. \tag{4.8}$$

Since in our specific example p is even, the zeta function has only poles of oder $p/2$. In particular, in a neighborhood of $s=0$ the pole structure is

$$\zeta(s|L) = \frac{S}{16\pi\alpha}\left[\frac{M^4}{2s} + \sum_{n=3}^{6} \frac{\tilde{C}^n_{2,n-2}\Gamma(n-2)}{\alpha s} + 2\sum_{n=3}^{6} \frac{\tilde{C}^n_{4,n-2}\Gamma(n-2)}{\alpha^2 s^2}\right] + \cdots . \tag{4.9}$$

Thus, the zeta function $\zeta(s|L)$ is *not* regular at the origin: a pole of second-order appears. Within a physical context (restricted most of the time to the realm of pseudodifferential operators in compact domains), this is a very unusual behavior for the zeta function.[19–21] In these cases, as far as the one-loop effective action is concerned, the otherwise well-established zeta function regularization procedure needs to be modified.[5,39]

Our proposal, which extends in a natural way the one formulated in Refs. 19–21, consists in the introduction of an additional spectral function which depends on the order of the pole at the origin of the initial zeta function. Thus, in the case of a pole of order N, the auxiliary spectral function reads

$$\omega(s) = s^N \zeta(s|L), \tag{4.10}$$

and the definition of the regularized determinant is generalized as

$$\ln\det\frac{L}{\mu^2} = -\frac{1}{(N+1)!}\lim_{s\to 0}\frac{\mathrm{d}^{N+1}}{\mathrm{d}s^{N+1}}[\mu^{2s}\omega(s)], \tag{4.11}$$

with the normalization chosen in such a way that when $\zeta(s|L)$ is regular at the origin, one does recover the ordinary definition of regularized functional determinant. This is an essential condition in order to preserve the well-established properties defining the zeta function regularization procedure.

Recalling our example before, we have seen that in this model a second-order pole will generically appear. Then, the new spectral function, which is regular at the origin, will be given by

$$\omega(s) = s^2 \zeta(s|L). \tag{4.12}$$

We correspondingly define

$$\ln\det\frac{L}{\mu^2} = -\frac{1}{3!}\lim_{s\to 0}\frac{\mathrm{d}^3}{\mathrm{d}s^3}[\mu^{2s}\omega(s)]. \tag{4.13}$$

It has to be mentioned here that, within the context of a general theory of regularized products (see, e.g., Ref. 27), in the case when the related zeta function is not holomorphic at the origin but has a first-order pole—and we have stressed this to happen when logarithmic terms are present in the heat-trace asymptotics—a new definition of regularized product was proposed recently.[40] It reads

$$\prod_{k=1}^{\infty}\lambda_k \equiv \exp\left[-\mathrm{Res}\left(\frac{\zeta(s)}{s^2}\right)_{s=0}\right], \quad \zeta(s) = \sum_{k=1}^{\infty}\lambda_k^{-s}. \tag{4.14}$$

Recalling the definition of residue, it is straightforward to conclude that this prescription is equivalent to ours, Eq. (4.11). This is a further consistency check and inscribes our result in a very general context.

We conclude with the following remark. The one-loop renormalization group equations associated with the presence of the renormalization scale μ can be treated along the same lines as in Ref. 39. This shows both the power and flexibility of the zeta-function method to easily cope with

nonstandard and unexpected situations, without ever losing contact with the fundamental issue of its applicability to actual physical problems. This means, in particular, that the results obtained with the method must be checked to be physically meaningful and to reproduce measured experimental values.

V. CONCLUSION

In this paper we have considered several examples of the determination of heat-kernel traces associated with operators of Laplace type defined on noncompact domains. For the sake of simplicity, we have restricted our analysis to R^d and to analytic but confining potentials, thus dealing with discrete spectra only. However, the adequacy of the procedure to treat more general settings has been exhibited. In particular, although for the sake of simplicity we have postponed the treatment of the case when d/Q is noninteger, with some extra effort this can be dealt with along the same lines. New branching points appear there.

We have shown that for confining potentials of exponential behavior at infinity, the asymptotics of the heat-kernel trace contain generically logarithmic terms. As a consequence, the meromorphic structure of the associated zeta function develops higher-order poles as well as branching points. In particular, we have exhibited some cases where the zeta function is not regular at the origin.

In these situations, one is confronted with the nontrivial task of having to define the corresponding regularized functional determinant or the one-loop effective potential. In fact, in the example of an apparently reasonable model of confinement, constructed by means of an asymptotically exponential potential, we have proven that the meromorphic continuation of the zeta function already develops a higher-order pole at the origin. This, as far as we know, is an absolutely novel finding in the field, even more since it comes from such an apparently harmless model.

In order to deal with these special cases, we have proposed a generalization of the zeta function regularization procedure, consisting in the introduction of a new, auxiliary zeta function which is still regular at the origin, together with a correspondingly new definition for the zeta-regularized determinant (thus extending Ray and Singer's definition). This general prescription—which naturally extends particular cases already considered by some of us before[19–21]—turns out to be equivalent to the one recently proposed by Hirano *et al.*[40] in a more generic context of a theory of regularized products. In accordance with our fundamental aim never to abandon the already established connections with the physical world (e.g., the many uses of zeta regularization in experimental physics), all the new quantities have been defined in such a way as to recover the celebrated results of zeta-function regularization in the absence of poles at the origin.

Still pending is the task to construct an explicit general theory to deal with the whole class of Laplacian-type operators in noncompact domains, which we leave for further work.

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APPENDIX: SOME USEFUL FORMULAS

Here we list some expressions that have been employed in the text. We start with the incomplete gamma function, useful in order to reveal the presence of logarithmic terms in the heat-kernel trace expansion. Its definition reads

$$\Gamma(s,t) = \int_t^\infty \mathrm{d}y\, y^{s-1}e^{-y} = \Gamma(s) - \frac{t^s}{s} - t^s\sum_{r=1}^{\infty}\frac{t^n}{n!(s+n)}, \tag{A1}$$

and thus

$$\Gamma(0,t) = -\ln t - \gamma - t - \frac{t^2}{4} + O(t^3), \tag{A2}$$

γ being Euler's constant. Taking the derivative of order n of $\Gamma(s,t)$ with respect to s, one gets

$$\frac{\mathrm{d}^n}{\mathrm{d}s^n}\Gamma(s,t) = \int_t^\infty \mathrm{d}y(\ln y)^n y^{s-1}e^{-y}, \tag{A3}$$

from which it follows that

$$\int_1^\infty \mathrm{d}y(\ln y)^n y^{s-1}e^{-ty} = \frac{\mathrm{d}^n}{\mathrm{d}s^n}\frac{\Gamma(s,t)}{t^s} = \sum_{k=0}^{n} f_k(s)\Gamma(s)\frac{(\ln t)^k}{t^s} - \frac{(-1)^n n!}{s^{n+1}} + O(t), \tag{A4}$$

where the $f_k(s)$ are computable functions. In particular,

$$f_n(s) = (-1)^n, \quad f_{n-1}(s) = (-1)^{n+1}\psi(s), \tag{A5}$$

$\psi(s)$ being the digamma function. In the limit $s\to 0$ we finally have

$$\int_1^\infty \mathrm{d}y(\ln y)^n y^{-1}e^{-ty} = \sum_{k=0}^{n+1} c_k(\ln t)^k + O(t), \tag{A6}$$

where

$$c_{n+1} = \frac{(-1)^{n+1}}{n+1}, \quad c_n = (-1)^{n+1}\gamma. \tag{A7}$$

With a view to the analytic continuation of zeta functions, the following formulas are useful too. If α is a complex number with positive real part, and β such that Re $\beta > -1$, one has

$$\int_0^1 \mathrm{d}t\, t^{\alpha-1}(\ln t)^\beta = \frac{(-1)^\beta\Gamma(\beta+1)}{\alpha^{\beta+1}}. \tag{A8}$$

To prove this, it is sufficient to perform the change of variable $u=-\ln t$ and recall the definition of the Euler gamma function.

Furthermore, for the asymptotics of the spectral density for large λ, one has

$$t^{-s} = \int_0^\infty e^{-t\lambda}\frac{\lambda^{s-1}}{\Gamma(s)}. \tag{A9}$$

Taking the derivative with respect to s,

$$\ln t t^{-s} = \int_0^\infty e^{-t\lambda}\lambda^{s-1}\left[-\frac{\ln\lambda}{\Gamma(s)} + \frac{\Gamma'(s)}{\Gamma(s)}\right], \tag{A10}$$

and

$$\ln^2 tt^{-s} = \int_0^\infty e^{-t\lambda}\lambda^{s-1}\left[\frac{\ln^2\lambda}{\Gamma(s)} + 2\frac{\Gamma'(s)}{\Gamma^2(s)}\ln\lambda - \frac{\Gamma''(s)}{\Gamma(s)} - \frac{\Gamma'(s)}{\Gamma^2(s)}\right]. \tag{A11}$$

The above-noted identities are compatible with the Karamata Tauberian theorems, which can be stated as follows. Suppose we deal with

$$\int_0^\infty e^{-t\lambda} dN(\lambda) = K(t). \tag{A12}$$

(i) If

$$K(t) \simeq At^{-r}, \quad t \to 0, \tag{A13}$$

then

$$N(\lambda) \simeq A\frac{\lambda^r}{\Gamma(r+1)}, \quad \lambda \to \infty. \tag{A14}$$

(ii) If

$$K(t) \simeq At^{-r}\ln^N t, \quad t \to 0, \tag{A15}$$

then

$$N(\lambda) \simeq A\frac{\lambda^r \ln^N \lambda}{\Gamma(r+1)}, \quad \lambda \to \infty. \tag{A16}$$

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Is weak pseudo-Hermiticity weaker than pseudo-Hermiticity?

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For a weakly pseudo-Hermitian linear operator, we give a spectral condition that ensures its pseudo-Hermiticity. This condition is always satisfied whenever the operator acts in a finite-dimensional Hilbert space. Hence weak pseudo-Hermiticity and pseudo-Hermiticity are equivalent in finite-dimensions. This equivalence extends to a much larger class of operators. Quantum systems whose Hamiltonian is selected from among these operators correspond to pseudo-Hermitian quantum systems possessing certain symmetries. © *2006 American Institute of Physics.*
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I. INTRODUCTION

References 1 and 2 discuss a notion of a pseudo-Hermitian operator that has proven to be a convenient tool in the study of $\mathcal{PT}$-symmetric Hamiltonians.[3–7] It also plays a central role in solving some of the basic problems of relativistic quantum mechanics and quantum cosmology[8] and revealing some interesting analogies between quantum mechanics and general relativity.[9] The following is a mathematically precise description of this notion.[1]

Definition 1: A densely defined linear operator $H:\mathcal{H}\to\mathcal{H}$ acting in a separable Hilbert space $\mathcal{H}$ is said to be *pseudo-Hermitian* if there exists a Hermitian automorphism $\eta:\mathcal{H}\to\mathcal{H}$ satisfying

$$H^\dagger = \eta H \eta^{-1}, \tag{1}$$

where $H^\dagger$ denotes the adjoint of H. (Throughout this paper, "Hermitian" means "self-adjoint," e.g., $\eta^\dagger=\eta$.)

For a discussion of the earlier uses of the term pseudo-Hermitian in the context of indefinite-metric theories see Ref. 10.

Note that an automorphism is by definition an everywhere-defined, one-to-one, and onto linear operator. Moreover, an everywhere-defined Hermitian linear operator is necessarily bounded (this is known as the Hellinger-Toeplitz theorem[11]), and a bounded one-to-one onto linear map has a bounded inverse (this is known as the inverse mapping theorem[11] or Banach's theorem[12]). As a result, if one adopts the definition of an invertible operator that identifies the latter with a one-to-one, onto linear map with a bounded inverse,[13–15] then *a linear operator is everywhere-defined, Hermitian, and invertible if and only if it is a Hermitian automorphism*. Usually in physics literature one ignores the technical issues associated with the domain of the operators and uses "Hermitian automorphism" and "Hermitian invertible linear map" synonymously. Another more familiar term used for such an operator particularly in the context of pseudo-Hermitian operators is "*pseudo-metric*."

The operator equation (1) in particular implies that the domain of its both sides must coincide. In light of the fact that η is everywhere-defined, this means

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$$\eta(\mathcal{D}(H)) = \mathcal{D}(H^\dagger), \tag{2}$$

where $\mathcal{D}(L)$ denotes the domain of a linear operator $L:\mathcal{H}\to\mathcal{H}$, and $L(\mathcal{S})$ stands for the image of a subset $\mathcal{S}\subseteq\mathcal{H}$ under L.

Definition 1 is a direct generalization of the notion of a self-adjoint operator, for the latter corresponds to a pseudo-Hermitian operator admitting the identity operator $I:\mathcal{H}\to\mathcal{H}$ as a pseudo-metric. (We may similarly generalize the notion of a *symmetric operator*[11] by replacing (2) with $\eta(\mathcal{D}(H))\subseteq\mathcal{D}(H^\dagger)$ and requiring that (1) holds in $\eta(\mathcal{D}(H))$.)

In Ref. 4, Solombrino has slightly weakened the defining condition of a pseudo-Hermitian operator by relaxing the requirement of the Hermiticity of η. This leads to the following notion of weak pseudo-Hermiticity.

Definition 2: A linear operator $H:\mathcal{H}\to\mathcal{H}$ acting in a separable Hilbert space $\mathcal{H}$ is said to be *weakly pseudo-Hermitian* if there exists an everywhere-defined, bounded, invertible, linear map (i.e., a bounded automorphism) $\eta_w:\mathcal{H}\to\mathcal{H}$ satisfying

$$H^\dagger = \eta_w H \eta_w^{-1}. \tag{3}$$

Again (3) implies

$$\eta_w(\mathcal{D}(H)) = \mathcal{D}(H^\dagger). \tag{4}$$

The basic motivation for introducing weak pseudo-Hermiticity is that the Hermiticity of η in (1) does not play any significant role in establishing the spectral characterization theorem(s) for diagonalizable pseudo-Hermitian operators with a discrete spectrum.[1,2,4] This suggests, at least for diagonalizable operators with a discrete spectrum, that pseudo-Hermiticity and weak pseudo-Hermiticity are equivalent conditions.[4] In Ref. 5 Bagchi and Quesne explore the relationship between these two concepts and use the term "complementary" to describe it. Though it is not made explicit in their analysis, their approach can be consistently applied only to a restricted class of bounded automorphisms η, namely to those for which $\eta+\eta^\dagger$ is also an automorphism. More recently, Znojil[7] has suggested that considering weak-pseudo-Hermitian Hamiltonians may provide further insight into the current search for potential applications of non-Hermitian Hamiltonians in quantum mechanics.

The purpose of this paper is to conduct a careful reexamination of the relationship between weak pseudo-Hermiticity and pseudo-Hermiticity for a general not necessarily diagonalizable linear operator. We will establish the equivalence of these concepts for a large class of linear operators including all linear operators that act in a finite-dimensional Hilbert space, i.e., matrix Hamiltonians.

Before starting our analysis we introduce our conventions and notation.

- $\mathcal{H}$ denotes a separable Hilbert space.
- For any linear operator $H:\mathcal{H}\to\mathcal{H}$, $\mathfrak{U}_H$ stands for the set of all bounded automorphisms $\eta_w:\mathcal{H}\to\mathcal{H}$ satisfying (3). Therefore, H is weakly pseudo-Hermitian if $\mathfrak{U}_H\neq\emptyset$. It is pseudo-Hermitian if $\mathfrak{U}_H$ contains a Hermitian element.
- For any bounded operator $B:\mathcal{H}\to\mathcal{H}$, $\|B\|$ denotes the norm of B.

II. A CAREFUL LOOK AT WEAK PSEUDO-HERMITICITY

First we present some useful facts.

Proposition 1: Let $H:\mathcal{H}\to\mathcal{H}$ be a weakly pseudo-Hermitian linear operator. Then for all η_w, $\eta_w'\in\mathfrak{U}_H$, $\eta_w^{-1}\eta_w'$ is a bounded automorphism commuting with H.

Proof: Let η_w, $\eta_w'\in\mathfrak{U}_H$. Because both η_w and η_w' are bounded, one-to-one, and onto, so are η_w^{-1} and $\eta_w^{-1}\eta_w'$. Furthermore, as shown in Ref. 1, in view of (3) and its analog satisfied by η_w', we have $[\eta_w^{-1}\eta_w', H]=0$. □

Proposition 2: Let $H:\mathcal{H}\to\mathcal{H}$ be a closed weakly pseudo-Hermitian linear operator and $\eta_w\in\mathfrak{U}_H$. Then $\eta_w^\dagger\in\mathfrak{U}_H$ provided that $\eta_w^\dagger\mathcal{D}(H)=\mathcal{D}(H^\dagger)$. In this case

$$A := \eta_w^{-1}\eta_w^\dagger \tag{5}$$

is a bounded automorphisms commuting with H. (Although Definitions 1 and 2 do not require H to be a closed operator, this requirement is necessary to derive many of the useful properties of pseudo-Hermitian and weakly pseudo-symmetric operators. Here we need it to assure that $H^{\dagger\dagger}=H$.[16])

Proof: Let $\eta_w \in \mathfrak{U}_H$ be such that $\eta_w^\dagger \mathcal{D}(H)=\mathcal{D}(H^\dagger)$. η_w satisfies (3) or equivalently

$$\eta_w H = H^\dagger \eta_w. \tag{6}$$

This in particular implies

$$\eta_w^{-1}\mathcal{D}(H^\dagger) = \mathcal{D}(H^\dagger \eta_w) = \mathcal{D}(\eta_w H) = \mathcal{D}(H). \tag{7}$$

Now, take the adjoint of both sides of this equation. [Note that for a pair of (densely defined) linear operators $A,B:\mathcal{H}\to\mathcal{H}$ that are not bounded and everywhere-defined, the relation $(AB)^\dagger=B^\dagger A^\dagger$ does not hold in general (Ref. 14, Sec. 7.7).] Because $\mathcal{D}(\eta_w H)=\mathcal{D}(H)$ is dense and η_w is bounded and everywhere-defined, we have (Ref. 14, Sec. 7.7)

$$(\eta_w H)^\dagger = H^\dagger \eta_w^\dagger, \tag{8}$$

or alternatively

$$H^\dagger = (\eta_w H)^\dagger \eta_w^{\dagger -1}. \tag{9}$$

Furthermore, as explained in Ref. 14, Sec. 7.7, because $\mathcal{D}(H^\dagger \eta_w)=\eta_w^{-1}\mathcal{D}(H^\dagger)=\mathcal{D}(H)$ is dense, $\mathcal{D}(\eta_w^\dagger H)\subseteq\mathcal{D}((H^\dagger\eta_w)^\dagger)$ and

$$(H^\dagger\eta_w)^\dagger\psi = \eta_w^\dagger H\psi \quad \text{for all } \psi\in\mathcal{D}(\eta_w^\dagger H)=\mathcal{D}(H). \tag{10}$$

This in turn means that

$$(H^\dagger\eta_w)^\dagger\eta_w^{\dagger -1}\phi = \eta_w^\dagger H\eta_w^{\dagger -1}\phi \quad \text{for all } \phi\in\eta_w^\dagger\mathcal{D}(H). \tag{11}$$

Therefore, in view of the hypothesis: $\eta_w^\dagger\mathcal{D}(H)=\mathcal{D}(H^\dagger)$ and Eqs. (6), (9), and (10) (as envisaged in Ref. 5)

$$H^\dagger = \eta_w^\dagger H \eta_w^{\dagger -1}. \tag{12}$$

This together with the fact that the adjoint $(\eta_w^\dagger)$ of a bounded automorphism (η_w) is a bounded automorphism establish $\eta_w^\dagger\in\mathfrak{U}_H$. The fact that $[A,H]=0$ follows from Proposition 1. □

Proposition 3: Let H and A be as in Proposition 2 and $r_A := \lim_{n\to\infty}\|A^n\|^{1/n}$ be the spectral radius[17] of A. Then the spectrum σ_A of A lies in the annulus centered at $0\in\mathbb{C}$ and having as its inner and outer radii r_A^{-1} and r_A, respectively, i.e.,

$$\sigma_A \subseteq \{z\in\mathbb{C}\,|\,r_A^{-1}\leqslant|z|\leqslant r_A\}. \tag{13}$$

In particular, $\|A\|\geqslant r_A\geqslant 1$.

Proof: According to Proposition 2, A is a bounded invertible linear map. This implies that $A^\dagger$ and A^{-1} are bounded operators, and the following identities are satisfied:[17,14]

$$\sigma_{A^\dagger}=\{\lambda\in\mathbb{C}\,|\,\lambda^*\in\sigma_A\},\quad \sigma_{A^{-1}}=\{\lambda\in\mathbb{C}\,|\,\lambda^{-1}\in\sigma_A\}. \tag{14}$$

Furthermore, because $A^{-1}=\eta_w^{\dagger -1}\eta_w$, $A^\dagger=\eta_w\eta_w^{-1\dagger}=\eta_w A^{-1}\eta_w^{-1}$, and η_w is invertible, we have $\sigma_{A^\dagger}=\sigma_{A^{-1}}$.[15] Combining this result with (14), we find that for all $\lambda\in\sigma_A$, $1/\lambda^*\in\sigma_A$. Next, we recall that for all $\mu\in\sigma_A$, $|\mu|\leqslant r_A$. Applying this inequality for $\mu=\lambda$ and $1/\lambda^*$, we then find $r_A^{-1}\leqslant|\lambda|\leqslant r_A$ for all $\lambda\in\sigma_A$. (Because there is always $\Lambda\in\sigma_A$ such that $|\Lambda|=r_A$ and $1/\Lambda^*\in\sigma_A$, σ_A intersects both the circles $|z|=r_A$ and $|z|=r_A^{-1}$.) This establishes (13). Finally, because the spectrum of every bounded operator is nonempty, we must have $r_A^{-1}\leqslant r_A$, which in turn implies $r_A\geqslant 1$. The fact that

$r_A \leqslant \|A\|$ is well-known.[17] □

The following is our main result. It links the equivalence of weak pseudo-Hermiticity and pseudo-Hermiticity of a large class of linear operators H with the existence of an $\eta_w \in \mathfrak{U}_H$ such that the unit circle $S^1 := \{e^{i\varphi} \in \mathbb{C} \,|\, \varphi \in [0, 2\pi)\}$ is not a subset of σ_A. Note that Proposition 3 does not rule out this possibility.

Theorem 1: Let $H: \mathcal{H} \to \mathcal{H}$ be a closed weakly pseudo-Hermitian linear operator acting in a separable Hilbert space $\mathcal{H}$. Then H is pseudo-Hermitian, if there is $\eta_w \in \mathfrak{U}_H$ such that $\eta_w^\dagger \mathcal{D}(H) = \mathcal{D}(H^\dagger)$ and the unit circle S^1 is not a subset of the spectrum σ_A of $A := \eta_w^{-1} \eta_w^\dagger$.

Proof: Let $\eta_w \in \mathfrak{U}_H$ be such that $\eta_w^\dagger \mathcal{D}(H) = \mathcal{D}(H^\dagger)$, and $\vartheta \in [0, 2\pi)$ be arbitrary. Then according to Proposition 2, $\eta_w^\dagger \in \mathfrak{U}_H$, and both (3) and (12) hold. Expressing these equations in the form

$$\eta_w H = H^\dagger \eta_w, \tag{15}$$

$$\eta_w^\dagger H = H^\dagger \eta_w^\dagger, \tag{16}$$

multiplying both sides of (15) and (16), respectively, by $ie^{i\vartheta}$ and $-ie^{-i\vartheta}$, and adding the resulting equations side by side, we find

$$\eta(\vartheta) H = H^\dagger \eta(\vartheta), \tag{17}$$

where

$$\eta(\vartheta) := i(e^{i\vartheta} \eta_w - e^{-i\vartheta} \eta_w^\dagger) \quad \text{for all } \vartheta \in [0, 2\pi). \tag{18}$$

The operator $\eta(\vartheta)$ is manifestly Hermitian. It is also everywhere-defined and bounded, because both η_w and $\eta_w^\dagger$ share these properties. But it need not be invertible. We can express $\eta(\vartheta)$ in the form

$$\eta(\vartheta) = -ie^{-i\vartheta} \eta_w (A - e^{2i\vartheta} I), \tag{19}$$

where I stands for the identity operator acting on $\mathcal{H}$. Clearly because η_w is invertible, $\eta(\vartheta)$ is invertible if and only if $A - e^{2i\vartheta} I$ is invertible. By the definition of the spectrum of a linear operator,[11–17] the latter condition is equivalent to $e^{2i\vartheta} \notin \sigma_A$. If $S^1 \subseteq \sigma_A$, there is $\vartheta_\star \in [0, \pi)$ such that $e^{2i\vartheta_\star} \notin \sigma_A$. Therefore, $\eta_\star := \eta(\vartheta_\star)$ is invertible; $\mathfrak{U}_H$ includes a Hermitian operator $\eta_\star$; and H is pseudo-Hermitian. □

Corollary: A linear operator acting in a finite-dimensional Hilbert space is weakly pseudo-Hermitian if and only if it is pseudo-Hermitian. (As pointed out by the referee, this is a known result.[18])

Proof: According to Definitions 1 and 2, every pseudo-Hermitian operator is weakly pseudo-Hermitian. The converse holds for an operator acting in a finite-dimensional Hilbert space, because in this case all the operators are everywhere-defined (bounded and hence closed) and σ_A of Theorem 1 is a finite set. Hence, it cannot include S^1 as a subset. □

In summary, a weakly pseudo-Hermitian linear operator may fail to be pseudo-Hermitian, if it acts in an infinite-dimensional space and for every $\eta_w \in \mathfrak{U}_H$ either $\eta_w^\dagger \mathcal{D}(H) \neq \mathcal{D}(H^\dagger)$ or $S^1 \subseteq \sigma_A$ where $A := \eta_w^{-1} \eta_w^\dagger$. The latter condition seems to be very difficult to satisfy.

III. EXAMPLES

Consider the following bounded automorphism that is employed in Ref. 7:

$$\eta_w = \begin{pmatrix} 0 & 0 & \mathcal{P} \\ \mathcal{P} & 0 & 0 \\ 0 & \mathcal{P} & 0 \end{pmatrix}, \tag{20}$$

where $\mathcal{P}$ is the usual parity operator acting in $L^2(\mathbb{R})$, the Hilbert space is $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$, a three-component representation of the state vectors is used, and $H = (H_{ij})$ is a 3×3 matrix of

differential operators H_{ij} such that $\mathcal{P}\mathcal{D}(H)=\mathcal{D}(H)=\mathcal{D}(H^\dagger)$. It is not difficult to see that $\vartheta_\star=3\pi/2$ fulfills the conditions of Theorem 1, and

$$\eta_\star := \eta\left(\frac{3\pi}{2}\right) = \eta_w + \eta_w^\dagger = \begin{pmatrix} 0 & \mathcal{P} & \mathcal{P} \\ \mathcal{P} & 0 & \mathcal{P} \\ \mathcal{P} & \mathcal{P} & 0 \end{pmatrix} \tag{21}$$

is a genuine pseudo-metric belonging to $\mathfrak{U}_H$. Indeed, it is not only everywhere-defined, bounded, Hermitian, and one-to-one, but it is also onto and its inverse is bounded. This can be directly checked. Alternatively, we may apply Theorem 1 and show that $S^1 \nsubseteq \sigma_A$. It is very easy to compute the symmetry generator (5):

$$A = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{22}$$

where 1 is viewed as the identity operator acting in $L^2(\mathbb{R})$. Clearly, $\sigma_A=\{1, e^{2i\pi/3}, e^{4i\pi/3}\}$. Hence $S^1 \nsubseteq \sigma_A$ and $\eta_\star$ is invertible.

This calculation shows that the systems considered in Ref. 7 can be identified with $\eta_\star$-pseudo-Hermitian Hamiltonians acting in $L^2(\mathbb{R})\oplus L^2(\mathbb{R})\oplus L^2(\mathbb{R})$ and commuting with A, where $\eta_\star$ and A are, respectively, given by (21) and (22). *These systems can be studied without any reference to weak pseudo-Hermiticity*.

Another probably more interesting example is $\eta_w:\mathbb{C}^2\to\mathbb{C}^2$ that is defined by its standard matrix representation according to

$$\eta_w = \begin{pmatrix} 1 & 1 \\ -1 & i \end{pmatrix}. \tag{23}$$

The symmetry generator (5) and the most general Hamiltonian $H:\mathbb{C}\to\mathbb{C}$ satisfying (6) have the following standard matrix representations:

$$A = \begin{pmatrix} i & 0 \\ 1-i & -1 \end{pmatrix} = -iM_1 - M_2, \tag{24}$$

$$H = \begin{pmatrix} a & 0 \\ ib & a+b \end{pmatrix} = aI + bM_1, \tag{25}$$

where

$$M_1 := \begin{pmatrix} 0 & 0 \\ i & 1 \end{pmatrix}, \quad M_2 := \begin{pmatrix} 1 & 0 \\ -i & 0 \end{pmatrix},$$

I is the identity matrix, and $a,b\in\mathbb{R}$ are arbitrary. Clearly, A and H commute for all $a,b\in\mathbb{R}$.

We can also easily compute $A-e^{2i\vartheta}I$. It turns out to be noninvertible only for $\vartheta=\pi/4,\pi/2,5\pi/4,3\pi/2$. This in turn means that $\eta(\vartheta)$ is noninvertible for these four values of ϑ. In particular, $\eta(3\pi/2)=\eta_w+\eta_w^\dagger$ that is considered in Ref. 5 is not invertible. (The possibility that given an invertible operator η_w the operators $\eta_w\pm\eta_w^\dagger$ may fail to be invertible seems to be overlooked in Ref. 5.)

In general, $\eta(\vartheta)$ has the following explicit form:

$$\eta(\vartheta)=2c\begin{pmatrix}-t & i\\ -i & -1\end{pmatrix}, \tag{26}$$

where $c:=\cos\vartheta$ and $t:=\tan\vartheta$. In terms of c and t the invertibility condition: $\vartheta\notin\{\pi/4,\pi/2,5\pi/4,3\pi/2\}$, takes the simple form: $c\neq 0$ and $t\neq 1$.

Having obtained an infinite class of pseudo-metric operators $\eta(\vartheta)$ that render the Hamiltonians of the form (25) pseudo-Hermitian, we can construct the following family of symmetry generators:[1,6]

$$A(r,t_1,t_2):=\eta(\vartheta_2)^{-1}\eta(\vartheta_1)=r\begin{pmatrix}1-t_1 & 0\\ i(t_1-t_2) & 1-t_2\end{pmatrix}=r(I-t_2M_1-t_1M_2), \tag{27}$$

where $r:=\cos\vartheta_1/(\cos\vartheta_2-\sin\vartheta_2)\neq 0$ and $t_i:=\tan\vartheta_i\neq 1$ for $i=1,2$. Comparing (25) and (27), we see that the only nontrivial symmetry generator for the system is M_2. We could reach the same conclusion using (24).

Finally, we note that $\eta(\alpha)$ is positive-definite whenever $c<0$ and $t>1$ which corresponds to $5\pi/4<\vartheta<3\pi/2$. In particular, H is pseudo-Hermitian with respect to a set of positive-definite metric operators. According to Ref. 2, this implies that it is quasi-Hermitian[19] and has real eigenvalues. The latter is easily seen from (25) where the eigenvalues appear as diagonal entries.

IV. CONCLUDING REMARKS

In this paper, we have examined the relation between the notions of pseudo-Hermiticity and weak pseudo-Hermiticity. We have found a sufficient spectral condition that ensures whether a given weakly pseudo-Hermitian operator is pseudo-Hermitian. This condition which is not sensitive to the diagonalizability of the operator in question is trivially satisfied in finite-dimensional Hilbert spaces. Hence weak pseudo-Hermiticity and pseudo-Hermiticity are equivalent in finite dimensions. This equivalence extends to a large class of operators acting in infinite-dimensional Hilbert spaces. Our general results seem to indicate that further investigation of weak pseudo-Hermiticity is not likely to produce any substantial insight into the current study of the possible applications of non-Hermitian Hamiltonians in quantum mechanics.

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On the optimality of quantum encryption schemes

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It is well known that n bits of entropy are necessary and sufficient to perfectly encrypt n bits (one-time pad). Even if we allow the encryption to be approximate, the amount of entropy needed does not asymptotically change. However, this is not the case when we are encrypting quantum bits. For the perfect encryption of n quantum bits, $2n$ bits of entropy are necessary and sufficient (quantum one-time pad), but for approximate encryption one asymptotically needs only n bits of entropy. In this paper, we provide the optimal trade-off between the approximation measure ϵ and the amount of classical entropy used in the encryption of single quantum bits. Then, we consider n-qubit encryption schemes which are a composition of independent single-qubit ones and provide the optimal schemes both in the 2- and the ∞-norm. Moreover, we provide a counterexample to show that the encryption scheme of Ambainis-Smith [Proceedings of RANDOM '04, pp. 249–260] based on small-bias sets does not work in the ∞-norm. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2339014]

I. INTRODUCTION

Secure transmission of information is a subject that has been studied extensively. In this model, Alice wants to securely transmit a message to Bob using a secret key that they both share, in such a way that any eavesdropper gets absolutely no information about the message sent. In the classical world, Shannon[11,12] has shown that for the perfect encryption of n classical bits, it is necessary and sufficient to use n bits of classical entropy (one-time pad). By performing a bitwise XOR between the n-bit message and the n-bit secret key, the view of any eavesdropper that has no knowledge of the key is just a uniformly random n-bit string. Ambainis *et al.*[2] showed that $2n$ classical bits of entropy are necessary and sufficient for the transmission of n quantum bits.

Let us briefly sketch how one can perfectly encrypt a quantum bit. Let ρ be the state of an arbitrary qubit and let I,X,Y,Z be the four Pauli matrices. Then, by using two bits of classical entropy we can uniformly pick one of the four matrices and apply it to our qubit. The state of the qubit after the encryption is

$$\mathcal{E}(\rho) = \tfrac{1}{4}(\rho + X\rho X + Y\rho Y + Z\rho Z).$$

It is easy to verify that for all states $\rho, \mathcal{E}(\rho) = \frac{1}{2}\mathbb{I}$ and hence the view of the eavesdropper is the completely mixed state, i.e., she gets no information about the encrypted state ρ. The scheme easily generalizes to n-qubit states by using $2n$ classical bits of entropy.

The entropy needed for the perfect encryption of quantum states is two times what is needed for the perfect encryption of classical bits. Interestingly, this is no longer true, when we look at *approximate encryption*. Let $\rho \in \mathbb{C}^{d\times d}$ be the state of a $(\log d)$-qubit message, $\{U_k \in \mathbb{C}^{d\times d} | k \in [N]\}$ be a set of N unitary operations acting on $\log d$ qubits and $\mathcal{D}=\{w_1,\ldots,w_N\}$ be a distribu-

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tion on $[N]$. Imagine the encryption scheme, where Alice picks a unitary U_k with probability w_k and applies it to the message. The ciphertext can be written as

$$\mathcal{E}(\rho) = \sum_{k\epsilon[N]} w_k \rho U_k^\dagger$$

and the entropy of the scheme is defined as the Shannon entropy $H(\mathcal{D})$.

Definition 1: The map $\mathcal{E}$ is an (ϵ,H)-approximate encryption scheme for the ∞-norm, if the entropy of the scheme is H and for all states ρ

$$\left\| \mathcal{E}(\rho) - \frac{\mathbb{I}}{d} \right\|_\infty \leqslant \frac{\epsilon}{d}.$$

Similarly, the map $\mathcal{E}$ is an (ϵ,H)-approximate encryption scheme for the 2-norm, if the entropy of the scheme is H and for all states ρ

$$\left\| \mathcal{E}(\rho) - \frac{\mathbb{I}}{d} \right\|_2 \leqslant \frac{\epsilon}{\sqrt{d}}.$$

Hayden, *et al.*[5] found an $(\epsilon, n+o(n))$-approximate encryption scheme for n qubits. Specifically, they showed that an encryption scheme that applies a unitary on ρ picked uniformly from a random set of unitaries of size $2^{n+o(n)}$ achieves ϵ-approximation. Ambainis and Smith[3] derandomized this construction using small-bias sets and constructed deterministically a set of $2^{n+o(n)}$ unitaries that achieves an $(\epsilon, n+o(n))$-approximation for the 2-norm.

On the other hand, it is not hard to see that for the classical case, one needs at least $n - \log(1-\epsilon/2)$ bits of entropy for an ϵ-approximation scheme. Hence, the entropy needed for the approximate encryption of classical and quantum states is asymptotically equal.

In this paper, we start by investigating the approximate encryption of single qubits and find the optimal trade-off between the approximation measure ϵ and the amount of classical entropy H, i.e., we calculate the least amount of classical entropy which is necessary and sufficient to achieve an ϵ-approximation. Our proof is constructive in the sense that for any given ϵ we describe the encryption scheme that achieves the optimal H and vice versa. The following theorem holds both for the ∞- and 2-norm. Note the weights in the distributions are in decreasing order.

Theorem 1: *Let $\mathcal{E}(\rho)$ be the optimal (ϵ,H)-approximate encryption scheme for a qubit. Then,*

1. The encryption is of the form $\mathcal{E}(\rho)=w\rho+xX\rho X+yY\rho Y+zZ\rho Z$.
2. For any fixed ϵ, the optimal distribution $\mathcal{D}$ (and hence the minimum entropy H) is:

(i) $\epsilon \leqslant 1/6 : \mathcal{D} = \left\{\frac{1}{4}+\frac{\epsilon}{2}, \frac{1}{4}+\frac{\epsilon}{2}, \frac{1}{4}+\frac{\epsilon}{2}, \frac{1}{4}-\frac{3\epsilon}{2}\right\}$,
(ii) $1/6 \leqslant \epsilon \leqslant 0.287 : \mathcal{D} = \left\{2\epsilon, \frac{1}{2}-\epsilon, \frac{1}{2}-\epsilon, 0\right\}$,
(iii) $\epsilon \geqslant 0.287 : \mathcal{D} = \left\{\frac{1}{4}+\frac{3\epsilon}{2}, \frac{1}{4}-\frac{\epsilon}{2}, \frac{1}{4}-\frac{\epsilon}{2}, \frac{1}{4}-\frac{\epsilon}{2}\right\}$.

In Sec. II we find the optimal Pauli encryption scheme for a qubit and in Sec. III we show that Pauli encryption schemes are no worse than general encryption schemes.

Next, in Sec. IV we consider n-qubit encryption schemes which are a composition of independent single-qubit schemes that each use entropy H. In general, such questions are not easy to tackle, since they hinge on notoriously hard questions on the additivity of quantum channels. However, in this case we only consider unitary operations and hence we can use a result of King[6] in order to find the optimal schemes.

Theorem 2: *Let P be the single-qubit Pauli encryption scheme, which achieves the optimal approximation ϵ for the given entropy H. Then, the optimal n-qubit independent encryption scheme $R(\rho)$ is the same for both the 2- and the ∞-norm and has the following properties*:

1. $R(\rho)=P^{\otimes n}(\rho)$.
2. $\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_2 \leqslant \sqrt{n}\frac{\epsilon}{2^{n/2}}+\frac{o(\epsilon\sqrt{n})}{2^{n/2}}$.
3. $\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_\infty \leqslant n\frac{\epsilon}{2^n}+\frac{o(n\epsilon)}{2^n}$.

The above-mentioned bounds are tight and hence for any encryption scheme that acts independently on each qubit, $2n-o(n)$ bits of entropy are necessary for approximate encryption.

Finally, in Sec. V we discuss nonindependent n-qubit encryption schemes. In particular, we are interested in the Ambainis-Smith small-bias set based scheme. In Ref. 3, they found an $(\epsilon, n+o(n))$-approximate encryption scheme for the 2-norm. Their scheme uses a deterministically constructed small-bias set of $2n$-bit strings of size $2^{n+o(n)}$, where each string corresponds to a unitary which is a tensor product of n Pauli matrices. The message is encrypted by picking uniformly a unitary from this set. One of the open questions in their paper is whether this scheme is also an $(\epsilon, n+o(n))$-approximate encryption scheme for the ∞-norm. We resolve this by finding an example of an asymptotically optimal small-bias set, for which the encryption scheme of Ambainis-Smith fails in the ∞-norm. However, it is possible that an $(\epsilon, n+o(n))$-approximate encryption scheme for the ∞-norm can be constructed in a different way, for example by using a small-bias set with some extra properties.

II. THE OPTIMAL PAULI ENCRYPTION SCHEME

The input state to our encryption scheme is a quantum bit which can be described by a density matrix ρ, i.e., a Hermitian matrix with unit trace

$$\rho = \tfrac{1}{2}(\mathbb{I} + r_x X + r_y Y + r_z Z), \tag{1}$$

where $(\vec{r}=r_x, r_y, r_z)$ is a unit vector, and the four Pauli matrices are

$$\mathbb{I}=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \quad X=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad Y=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}, \quad Z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}.$$

Let us denote +1 eigenvectors of the matrices X, Y and Z by $|x+\rangle, |y+\rangle$, and $z+\rangle$.

A *Pauli encryption scheme* for single qubits is described by a probability distribution on the four Pauli matrices, i.e., by a probability vector $\mathcal{D}=(w,x,y,z)$, such that the encryption of a qubit ρ is given by

$$\mathcal{E}_{IXYZ}(\rho) = w\rho + xX\rho X + yY\rho Y + zZ\rho Z. \tag{2}$$

Without loss of generality, we can assume the weights $\{w,x,y,z\}$ obey $w \geqslant z \geqslant x \geqslant y \geqslant 0$. The reason for this is that these four unitaries are freely interchangeable by picking a suitable $\rho = U\rho' U^\dagger$. If the original qubit ρ was encoded by $\mathcal{E}(\rho)$, with weights $\{w,x,y,z\}$, we can achieve the same encoding $E'(\rho')$ on the transformed qubit ρ', just with $\{w,x,y,z\}$ permuted.

The classical entropy used by the encryption scheme is the entropy of the probability distribution, i.e., $H(\{p_i\})=-\Sigma_i p_i \log_2 p_i = -w \log w - x \log x - y \log y - z \log z$.

To test how good the encryption scheme is, we want to know how much the encrypted state differs from the completely mixed state in the 2- and the operator norm. For any d-dimensional matrix A, the 2- and operator norm are related to the eigenvalues of the matrix, namely

$$\|A\|_2^2 = \sum_{k=1}^{d} \lambda_k^2, \quad \|A\|_\infty = \max_k |\lambda_k|.$$

Thus, for the operator norm we need to examine the maximum of the absolute value of the eigenvalues of

$$I(\rho) = \mathcal{E}_{IXYZ}(\rho) - \tfrac{1}{2}\mathbb{I}.$$

Note, that since the matrix $I(\rho)$ has trace equal to 0, the two eigenvalues are of the form $\pm\lambda$ and hence, the 2-norm is maximized simultaneously with the operator norm.

A. The maximum eigenvalue of $I(\rho)$

After applying the channel (2) to the density matrix described by (1), we obtain

$$\mathcal{E}_{IXYZ}(\rho) = \tfrac{1}{2}(\mathbb{I} + r'_x X + r'_y Y + r'_z Z),$$

where the new parameters can be easily determined from (2) using the anticommutation relations for Pauli matrices,

$$r'_x = (w + x - z - y)r_x = (2(w + x) - 1)r_x,$$

$$r'_y = (w + y - z - x)r_y = (2(w + y) - 1)r_y,$$

$$r'_z = (w + z - x - y)r_z = (2(w + z) - 1)r_z.$$

This shows that the parameters r_x, r_y, and r_z shrink according to the above-presented relations. The factors can be negative, but because have $w \geqslant z \geqslant x \geqslant y$ and $w+z+x+y=1$, with a little work one can verify that the magnitude of the shrinking factor $|2(w+z)-1|$ in front of r_z is the largest of the three.

Using the geometric description (1) of ρ, we can express the matrix $I(\rho)$ as

$$I(\rho) = \mathcal{E}(\rho) - \tfrac{1}{2}\mathbb{I} = \tfrac{1}{2}(r'_x X + r'_y Y + r'_z Z).$$

Its eigenvalues are then simply

$$\lambda_{I(\rho)} = \pm\tfrac{1}{2}|\vec{r}'|.$$

Our goal is to find the maximum eigenvalue $|\lambda_{I(\rho)}|$ over all states ρ as a function of the probability distribution $\mathcal{D}=(w,z,x,y)$ and then pick the distribution that minimizes it. Already knowing that the shrinking factor in front of r_z is the largest, we can maximize $|\lambda_{I(\rho)}| = \frac{1}{2}(1+|\vec{r}'|)$ by picking ρ with $\vec{r}=(0,0,1)$. This gives us $\vec{r}'=(0,0,2(w+z)-1)$, and

$$\max_\rho |\lambda_{I(\rho)}| = \left|w + z - \tfrac{1}{2}\right|. \tag{3}$$

Note that w and z are the two largest weights and therefore we always have $w+z \geqslant \frac{1}{2}$.

B. The optimal trade-off between approximation and entropy

In Sec. II A, we found an upper bound on the maximum eigenvalue of $I(\rho)$ as a function of the probability distribution used by the Pauli encryption scheme. Note also that Eq. (3) shows that for a perfect encryption the only possible scheme is the one that uses a uniform distribution over the four Pauli matrices.

The natural question is to find the optimal Pauli encryption scheme when we can only use a fixed amount H of classical entropy. Turning the question around, we fix the approximation parameter ϵ and calculate the necessary entropy to achieve it.

Let us fix $\epsilon = \max_\rho |\lambda| = w+z-1/2$. In addition, the condition $w \geqslant z$ implies that $1/4+\epsilon/2 \geqslant z$. Our goal is to minimize the classical entropy needed to achieve approximation ϵ:

$$H(\epsilon) = \min_{\mathcal{D}}(-w \log w - z \log z - x \log x - y \log y).$$

Keeping x, y, and ϵ fixed, the entropy as a function of z is concave, with a maximum at $z=w$. Because $z \leqslant w$, the entropy decreases with decreasing z. Specifically, if $z > x+y$, one can decrease

the entropy by setting $z=x+y$ (and increasing w accordingly, to keep ϵ fixed). Without loss of generality, one can then assume that $z \leqslant x+y$ for the optimal $\mathcal{D}$. Now, let us minimize the entropy as a function of x. It is concave in x, with a maximum at $x=y=(1-w-z)/2$ and possible minima at the end points. Because $x \geqslant y$, we want to pick x as large as possible. Because $x \leqslant z$ and $z \leqslant x+y$, this results in $x=z$. The weights that minimize the entropy for a fixed ϵ thus are (as a function of z)

$$w = 1/2 + \epsilon - z, \quad x = z, \quad y = 1/2 - \epsilon - z.$$

To find the optimal $H(\epsilon)$, one thus needs to minimize

$$H(\epsilon,z) = -\left(\tfrac{1}{2}+\epsilon-z\right)\log\left(\tfrac{1}{2}+\epsilon-z\right) - 2z\log z - \left(\tfrac{1}{2}-\epsilon-z\right)\log\left(\tfrac{1}{2}-\epsilon-z\right)$$

with respect to z, remembering the constraints collected so far ($w \geqslant z \geqslant x \geqslant y \geqslant 0, x+y \geqslant z$):

$$\frac{1}{4}+\frac{\epsilon}{2} \geqslant z \geqslant \frac{1}{4}-\frac{\epsilon}{2}, \tag{4}$$

$$\tfrac{1}{2}-\epsilon \geqslant z. \tag{5}$$

We perform this minimization in the first section of the Appendix and conclude that for $\epsilon \leqslant 1/6$, picking the three larger weights to be equal is the entropy-minimizing strategy. For $1/6 \leqslant \epsilon \leqslant \epsilon_0$, picking only three unitaries, with two of the lower weights equal is the best choice. For $\epsilon_0 \leqslant \epsilon \leqslant 1/2$, it is optimal to pick the three smaller weights to be equal.

Turning the argument around—given entropy H, what is the optimal Pauli encryption scheme? There is a unique way to pick the probability distribution with the given entropy that minimizes the parameter ϵ,

$$(i) H \geqslant \log_2 3 : \mathcal{D} = (z,z,z,1-3z),$$

$$(ii) \log_2 3 \geqslant H \geqslant H_0 : \mathcal{D} = (1-2z,z,z,0),$$

$$(iii) H_0 \geqslant H : \mathcal{D} = (1-3z,z,z,z). \tag{6}$$

Note that the weights are in descending order and that the approximation ϵ is given by the sum of the largest two weights minus $\frac{1}{2}$. Also, one should not expect the optimal distribution parameters to be continuous at H_0. These two ways of picking the weights come from different regions in the parameter space $\{w,z,x,y\}$, and the choice of the optimal distribution is simply a numerical minimum of these two functions. The point H_0 (or equivalently ϵ_0) does not have an obvious special meaning.

III. THE OPTIMALITY OF PAULI ENCRYPTION SCHEMES

In this section we give an elementary constructive proof that the Pauli encryption schemes are no worse than any general encryption scheme. For any encryption scheme $\mathcal{E}(\rho)=\Sigma_k p_k U_k \rho U_k^\dagger$ with arbitrary unitaries and weights, we give a Pauli encryption scheme with weights $\{w,z,x,y\}$ that has lower entropy, and is no worse than $\mathcal{E}(\rho)$. We show this by finding a density matrix ρ_0, for which the maximum eigenvalue of $I(\rho_0)$ is the same as in (3), which is the worst case for the newly found Pauli scheme. Hence, the Pauli encryption scheme of Sec. II is optimal amongst all possible encryption schemes.

After completion of this work, we learned of an alternative proof of optimality of Pauli encryption for a single qubit by Bouda and Ziman.[4] They investigated perfect encryption of a subspace of the Bloch sphere, while we are interested in approximate encryption of the whole Bloch sphere. Their proof uses the Kraus representation of the quantum channel, showing that the representation of a channel using orthogonal matrices requires the least amount of entropy.

Using the fact that every channel can be expressed also as a Pauli channel,[10] we can utilize a clever trick by Nielsen[8] to prove that the weights of this Pauli channel majorize the weights of the original channel. Knowing that the entropy is concave, we can conclude that the Pauli realization of the channel requires the least amount of entropy. The details of this proof are given in the second section of Appendix. Let us now continue with our proof.

Let T be an encryption scheme with distribution $\{w_1, w_2, \ldots, w_N\}$ over N unitaries U_k, where the weights are in decreasing order. We parametrize the unitaries as $U_k = e^{i\alpha_k} e^{i\phi_k(\vec{n}_k \cdot \vec{\sigma})}$, where $(\vec{n}_k = x_k, y_k, z_k)$ and $\vec{\sigma} = (X, Y, Z)$. The phases α_k are not important in our analysis and hence, we denote the parametrization of U_k only as $U(\phi_k, \vec{n}_k)$.

We have the following three cases:

Case 1: $w_1 + w_2 - 1/2 \leqslant 0$. We show that the entropy H of the encryption scheme T is greater or equal to 2, and for $H = 2$, we already know a perfect encoding with four unitaries and $w_k = 1/4$. It is clear that if $w_1 < 1/4$ then the entropy is larger than 2. Let us assume that $w_1 \geqslant 1/4$. From the concavity of the Shannon entropy, we know that the entropy of a distribution that contains two weights (w_k, w_l) with $w_k \geqslant w_l$ decreases if we change them into $(w_k + \Delta, w_l - \Delta)$.

Hence we can decrease the entropy of the initial distribution $\{w_1, w_2, \ldots, w_N\}$ by increasing the weight w_2 to make it equal to $w_2' = 1/2 - w_1$ and decreasing some of the smaller weights. We can further decrease the entropy by making the middle weights all equal, i.e. $\{w_1, w_2', w_2', \ldots, w_2', w_N\}$. Picking $w_1 = x$ fully determines the distribution, giving $w_2' = 1/2 - x$ and $w_N = (4 - N)/2 + (N - 3)x$. The constraints $1/2 \geqslant w_1 \geqslant w_2 \geqslant w_N \geqslant 0$ give us

$$\frac{N-3}{2(N-2)} \geqslant x \geqslant \frac{N-4}{2(N-3)}. \tag{7}$$

The entropy as a function of x is concave (the second derivative is negative) and therefore, we look for the minimum entropy at the end points, given in (7). These end points correspond to choosing the distribution as $\{w_1, w_2, \ldots, w_2\}$ with $w_2 = (1 - w_1)/(N - 1)$. The entropy of such distributions as a function of N is

$$H(N) = -w_1 \log w_1 - (N-1) w_2 \log w_2 = -\frac{N-3}{2(N-2)} \log(N-3) + 1 + \log(N-2).$$

It is easy to see that this function is a monotone, growing function of N with a minimum for $H(4) = 2$. We conclude that any encryption scheme with $n \geqslant 5$ unitaries and $w_1 + w_2 - 1/2 < 0$ uses entropy $H \geqslant 2$ and hence is worse than the perfect encryption scheme with four unitaries.

Case 2: $w_1 + w_2 - 1/2 \geqslant 0$ and $\Sigma_{k=3}^{n} w_k \leqslant 2w_2$. We show that there exists a Pauli encryption scheme that is no worse than T and uses less entropy. Let P be the Pauli scheme that uses the distribution $\{w_1, w_2, w_2, w_3'\}$. This is possible by the constraint $\Sigma_{k=3}^{n} w_k \leqslant 2w_2$ and from the concavity of the entropy, P uses less entropy. We also know from Eq. (3) that for the encryption scheme P,

$$\max_\rho |\lambda_{I(\rho)}| = \left| w_1 + w_2 - \tfrac{1}{2} \right|.$$

Without loss of generality, when encoding an input density matrix ρ with the set of unitaries

$$U(\phi_1, \vec{n}_1), U(\phi_2, \vec{n}_2), U(\phi_3, \vec{n}_3), \ldots, U(\phi_n, \vec{n}_n)$$

one can equivalently analyze the encoding of the density matrix $\rho' = U_1^\dagger \rho U_1$ with a related set of unitaries:

$$\mathbb{I}, U(\phi_2', \vec{n}_2'), U(\phi_3', \vec{n}_3'), \ldots, U(\phi_n', \vec{n}_n').$$

The approximation parameter ϵ of the encoding scheme is basis independent, it is now convenient to pick a basis in which the unitaries are of the form

$$\mathbb{I}, Z_{\alpha_2}, (z_3 Z + x_3 X + y_3 Y)_{\alpha_3}, \ldots, (z_n Z + x_n X + y_n Y)_{\alpha_n},$$

where $x_k^2 + y_k^2 + z_k^2 = 1$, and Z_{α_2} denotes a rotation about the z-axis, namely $Z_{\alpha_2} = e^{-i\alpha_2 Z} = (\cos \alpha_2)\mathbb{I} - i(\sin \alpha_2)Z$.

Let us now check how well the $|z+\rangle$ state is encoded,

$$\rho = |z+\rangle\langle z+| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

Note that since ρ is an eigenstate of Z, it commutes with Z_{α_2}. After some algebraic manipulations, we have

$$I(\rho) = \mathcal{E}(\rho) - \frac{1}{2}\mathbb{I} = \begin{bmatrix} \left(w_1 + w_2 - \frac{1}{2}\right) + \left(\sum_{k=3}^n w_k A_k\right) & \left(\sum_{k=3}^n w_k B_k\right)^* \\ \left(\sum_{k=3}^n w_k B_k\right) & -\left(w_1 + w_2 - \frac{1}{2}\right) - \left(\sum_{k=3}^n w_k A_k\right) \end{bmatrix},$$

where

$$A_k = \cos^2 \alpha_k + z_k^2 \sin^2 \alpha_k,$$

$$B_k = (\cos \alpha_k + i z_k \sin \alpha_k)(x_k - i y_k) i \sin \alpha_k.$$

The eigenvalues of $I(\rho)$ are now

$$\lambda_{I(\rho)}^2 = \left[\left(w_1 + w_2 - \frac{1}{2}\right) + \left(\sum_{k=3}^n w_k A_i\right)\right]^2 + \left|\sum_{k=3}^n w_k B_k\right|^2.$$

We know that $w_1 + w_2 - 1/2 \geq 0$ and $A_k \geq 0$. Thus we can bound the eigenvalues as

$$\lambda_{I(\rho)}^2 \geq \left(w_1 + w_2 - \tfrac{1}{2}\right)^2,$$

with w_1 and w_2 the two largest weights. The equality is achieved if we pick our unitaries with $z_k = 0$ and $\cos \alpha_k = 0$, which imply $A_k = B_k = 0$.

This is the same result as in Eq. (3) and hence no matter how we pick the unitaries, the encryption cannot be better than in the Pauli encryption scheme.

Case 3: $w_1 + w_2 - 1/2 \geq 0$ and $\Sigma_{k=3}^n w_k \geq 2w_2$. Since $w_1 + w_2 \geq 1/2$, we conclude that $w_1 \geq 1/4 \geq \frac{1}{3}(w_2 + \Sigma_{k=3}^n w_k)$ and so, it is possible to consider the Pauli scheme P that uses the distribution $\left\{w_1, \frac{1}{3}(w_2 + \Sigma_{k=3}^n w_k), \frac{1}{3}(w_2 + \Sigma_{k=3}^n w_k), \frac{1}{3}(w_2 + \Sigma_{k=3}^n w_k)\right\}$. Moreover, the constraint $\Sigma_{k=3}^n w_k \geq 2w_2$ implies that $\frac{1}{3}(w_2 + \Sigma_{k=3}^n w_k) \geq w_2$ and hence from the concavity of the entropy, P uses less entropy than T. From Eq. (3), we know that for the encryption scheme P,

$$\max_\rho |\lambda_{I(\rho)}| = \left| w_1 + \frac{1}{3}\left(w_2 + \sum_{k=3}^n w_k\right) - \frac{1}{2} \right|. \tag{8}$$

In what follows, we calculate how well the states $|z+\rangle, |x+\rangle$ and $|y+\rangle$ are encrypted by T and prove that at least one of them is encoded worse than in the Pauli scheme P.

We pick the unitaries of T to be

$$\mathbb{I}, Z_{\alpha_2}, (z_3 Z + x_3 X + y_3 Y)_{\alpha_3}, \ldots, (z_n Z + x_n X + y_n Y)_{\alpha_n}.$$

Similar to Case 2, the $|z+\rangle$ state is encoded no better than with

$$\lambda_z^2 \geqslant \left(w_1 + w_2 + \sum_{k=3}^{n} w_k(\cos^2 \alpha_k + \sin^2 \alpha_k \cos^2 \beta_k) - \frac{1}{2} \right)^2,$$

where we named $z_k = \cos \beta_k$, $x_k = \sin \beta_k \cos \gamma_k$, and $y_k = \sin \beta_k \sin \gamma_k$. Let us now check how well the $|x+\rangle$ state is encoded,

$$\rho_x = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

$$Z_{\alpha_2} \rho_x Z_{\alpha_2}^\dagger = \frac{1}{2}\begin{bmatrix} 1 & e^{-2i\alpha_2} \\ e^{2i\alpha_2} & 1 \end{bmatrix},$$

$$U_k \rho_x U_k^\dagger = \frac{1}{2}\begin{bmatrix} 1 + C_k & D_k - iE_k \\ D_k + iE_k & 1 - C_k \end{bmatrix},$$

where $D_k = (-1 + 2\cos^2 \alpha_k + 2 \sin^2 \alpha_k \sin^2 \beta_k \cos^2 \gamma_k)$ and C_k, E_k are functions of $\alpha_k, \beta_k, \gamma_k$ which do not affect the bounds. The encoding of ρ_x becomes

$$I(\rho_x) = \mathcal{E}(\rho_x) - \frac{\mathbb{I}}{2} = w_1 \mathbb{I} \rho_x \mathbb{I} + w_2 Z_{\alpha_2} \rho_x Z_{\alpha_2} + \sum_{k \geqslant 3} w_k U_k \rho_x U_i^\dagger - \frac{\mathbb{I}}{2}$$

$$= \frac{1}{2}\begin{bmatrix} \sum_{k \geqslant 3} w_k C_k & F - iG \\ F + iG & -\sum_{k \geqslant 3} w_k C_k \end{bmatrix},$$

where $F = w_1 - w_2 + 2w_2 \cos^2 \alpha_2 + \Sigma_{k \geqslant 3} w_k D_k$ and $G = w_1 \sin 2\alpha + \Sigma_{k \geqslant 3} w_k E_k$. We are ready to bound the eigenvalue:

$$\lambda_x^2 = \frac{1}{4}\left(\sum_{k \geqslant 3} w_k C_k \right)^2 + \frac{1}{4} G^2 + \frac{1}{4} F^2 \geqslant \frac{1}{4} F^2 = \frac{1}{4}\Big(w_1 - w_2 + 2w_2 \cos^2 \alpha_2 + \sum_{k \geqslant 3} w_k (-1 + 2\cos^2 \alpha_k$$
$$+ 2 \sin^2 \alpha_k \sin^2 \beta_k \cos^2 \gamma_k) \Big)^2 = \left(w_1 + w_2 \cos^2 \alpha_2 + \sum_{k \geqslant 3} w_k \cos^2 \alpha_k \right.$$
$$\left. + \sum_{k=3}^{n} w_k \sin^2 \alpha_k \sin^2 \beta_k \cos^2 \gamma_k - \frac{1}{2} \right)^2.$$

Using the same type of computation as above, we encode the $|y+\rangle$ state and obtain a bound for the eigenvalues of $I(\rho_y) = \mathcal{E}(\rho_y) - \mathbb{I}/2$:

$$\lambda_y^2 \geqslant \left(w_1 + w_2 \cos^2 \alpha_2 + \sum_{k \geqslant 3} w_k \cos^2 \alpha_k + \sum_{k=3}^{n} w_k \sin^2 \alpha_k \sin^2 \beta_k \sin^2 \gamma_k - \frac{1}{2} \right)^2.$$

Summing the three inequalities of the eigenvalues, we obtain that

$$|\lambda_x| + |\lambda_y| + |\lambda_z| \geqslant \left(3w_1 + w_2 + \sum_{k=3}^{n} w_k + \left(2 \sum_{k \geqslant 2} w_k \cos^2 \alpha_k \right) - \frac{3}{2} \right) \geqslant \left(3w_1 + w_2 + \sum_{k=3}^{n} w_k - \frac{3}{2} \right),$$

which implies that at least one of the three λ is greater or equal to (8). This means the Pauli encryption scheme P is no worse than T, while using less entropy.

This concludes the proof that Pauli encryption schemes are no worse than general encryption schemes. This also concludes the proof of Theorem 1.

IV. *N*-QUBIT INDEPENDENT ENCRYPTION SCHEMES

In this section we consider n-qubit encryption schemes which are composed of independent single-qubit schemes, each using H amount of classical entropy. For clarity of exposition, we assume that for each qubit we use the same amount of classical entropy. All the results go through in the more general case where for each qubit k we use entropy H_k. By independent we mean that the encryption has the form $R(\rho)=(R_1\otimes\cdots\otimes R_n)(\rho)$.

Theorem 2: *Let P be the single-qubit Pauli encryption scheme, which achieves the optimal approximation* ϵ *for the given entropy H. Then, the optimal n-qubit independent encryption scheme* $R(\rho)$ *is the same for both the 2- and the* ∞*-norm and has the following properties*:

1. $R(\rho)=P^{\otimes n}(\rho)$.
2. $\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_2\leqslant\sqrt{n}\frac{\epsilon}{2^{n/2}}+\frac{o(\epsilon\sqrt{n})}{2^n/2}$.
3. $\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_\infty\leqslant n\frac{\epsilon}{2^n}+\frac{o(n\epsilon)}{2^n}$.

Proof: We first employ a result by King[6] to show that product states are the worst encoded states for independent encryption schemes. King proved that the p-norm of a product of unital channels is multiplicative, i.e., for $p\geqslant 1$,

$$\max_\rho\|R(\rho)\|_p=\prod_{i=1}^n\left(\max_{\xi_i}\|R_i(\xi_i)\|_p\right). \tag{9}$$

A quantum channel Φ is *unital* if it preserves unity, i.e., $\Phi(\mathbb{I})=\mathbb{I}$. The encryption schemes we consider here are unital. The p-norm of a channel R is the maximum of $\|R(\rho)\|_p$ over all input states ρ. Note that the multiplicativity of the p-norms, and hence the additivity of the capacities of nonunital channels is a main open question.[13] This shows that the norm $\|R(\rho)\|_p$ is maximized by a product state $\rho=\xi_1\otimes\cdots\otimes\xi_n$, where ξ_i is the state of the ith qubit. In our encryption schemes we measure the quality of the approximation by the maximum of the norm $\|R(\rho)-\mathbb{I}/2^n\|_p$, for $p=2$ and $p=\infty$. Let λ_k be the eigenvalues of $R(\rho)$; then, the eigenvalues of $R(\rho)-\mathbb{I}/2^n$ are $(\lambda_k-1/2^n)$ and we have

$$\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_2^2=\sum_{k=1}^{2^n}\left(\lambda_k-\frac{1}{2^n}\right)^2=\sum_{k=1}^{2^n}\left(\lambda_k^2-2\frac{\lambda_k}{2^n}+\frac{1}{2^{2n}}\right)=\|R(\rho)\|_2^2-\frac{1}{2^n}, \tag{10}$$

$$\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_\infty=\max_k\left(\lambda_k-\frac{1}{2^n}\right)=\|R(\rho)\|_\infty-\frac{1}{2^n}. \tag{11}$$

It is clear that the norm of $R(\rho)-\mathbb{I}/2^n$ is maximized when the norm of $R(\rho)$ is maximized and, therefore, for any independent encryption scheme the worst encoded state is a product state.

Hence, in order to find the optimal independent encryption scheme, one needs to find the scheme that encrypts product states optimally. The encryption of a product state $R(\xi_1\otimes\cdots\otimes\xi_n)=R_1(\xi_1)\otimes\cdots\otimes R_n(\xi_n)$ is also a product state and the eigenvalues of $R(\xi_1\otimes\cdots\otimes\xi_n)$ are simply products of the eigenvalues of $R_k(\xi_k)$. Without loss of generality, let us now encrypt a state $\xi_1\otimes\rho_{2\ldots n}$ using $R=R_1\otimes R_{2\ldots n}$. The eigenvalues of the single-qubit encryption $R_1(\xi_1)$ can be expressed as $\mu_{1,2}=(1\pm\epsilon_1)/2$ and the eigenvalues of $R_{2\ldots n}(\rho_{2\ldots n})$ as $\nu_{k=1,\ldots,2^{n-1}}=(1+\delta_k)/2^{n-1}$. Hence, the eigenvalues and 2-norm of $R(\xi_1\otimes\rho_{2\ldots n})-\mathbb{I}/2^n$ are

$$\lambda_{i,k}=\mu_i\nu_k-\frac{1}{2^n}=\frac{\delta_k\pm\epsilon_1(1+\delta_k)}{2^n},$$

$$\left\| R(\xi_1 \otimes \rho_{2\ldots n}) - \frac{\mathbb{I}}{2^n} \right\|_2^2 = \sum_{k=1}^{2^{n-1}} \sum_{i=1}^{2} \lambda_{i,k}^2 = \sum_{k=1}^{2^{n-1}} \frac{\delta_k^2 + \epsilon_1^2 (1+\delta_k)^2}{2^{2n}}. \tag{12}$$

The last expression is a growing function of ϵ_1 and, therefore, the optimal n-qubit encryption scheme has to be optimal (i.e., Pauli) on the first qubit, giving the smallest possible upper bound ϵ_1. After going through this procedure for all qubits, we see that the optimal encryption scheme for product states in the 2-norm is the Pauli scheme $P^{\otimes n}$. It is straightforward to obtain the same statement for the ∞-norm using (12). This concludes the proof that the optimal n-qubit independent encryption scheme for both the 2- and the operator norm is the Pauli scheme $P^{\otimes n}(\rho)$.

We now prove tight upper bounds for the quality of the approximation of the Pauli encryption scheme. For the 2-norm, Eq. (9) and induction imply

$$\max_{\rho} \|P^{\otimes n}(\rho)\|_2 = \left(\max_{\xi} \|P(\xi)\|_2 \right)^n.$$

Let us pick ξ to be the worst encoded single-qubit state for P. The eigenvalues of $P(\xi)$ are $(1 \pm \epsilon)/2$ and therefore:

$$\|P^{\otimes n}(\rho)\|_2 \leq \max_{\rho} \|P^{\otimes n}(\rho)\|_2 = \left(\left(\frac{1+\epsilon}{2} \right)^2 + \left(\frac{1-\epsilon}{2} \right)^2 \right)^{n/2} = \left(\frac{1+\epsilon^2}{2} \right)^{n/2}.$$

From Eq. (10), we bound the 2-norm of $P^{\otimes n}(\rho) - \mathbb{I}/2^n$ as

$$\left\| P^{\otimes n}(\rho) - \frac{\mathbb{I}}{2^n} \right\|_2 = \left[\|P^{\otimes n}(\rho)\|_2^2 - \frac{1}{2^n} \right]^{1/2} \leq \left[\left(\frac{1+\epsilon^2}{2} \right)^n - \frac{1}{2^n} \right]^{1/2} = \frac{\epsilon\sqrt{n}}{2^{n/2}} + \frac{o(\epsilon\sqrt{n})}{2^{n/2}}.$$

For the ∞-norm, multiplicativity of norms (9) implies

$$\|P^{\otimes n}(\rho)\|_\infty \leq \max_{\rho} \|P^{\otimes n}(\rho)\|_\infty = \max_{\xi} \|P(\xi)\|_\infty^n = \left(\frac{1+\epsilon}{2} \right)^n,$$

and therefore Eq. (11) gives us

$$\left\| P^{\otimes n}(\rho) - \frac{\mathbb{I}}{2^n} \right\|_\infty = \|P^{\otimes n}(\rho)\|_\infty - \frac{1}{2^n} \leq \left(\frac{1+\epsilon}{2} \right)^n - \frac{1}{2^n} = \frac{n\epsilon}{2^n} + \frac{o(n\epsilon)}{2^n}.$$

Note that both bounds are tight and achieved for product states. □

Since the bounds in Theorem 2 are tight, any good independent encryption scheme requires that the approximation parameter for each single qubit is $\epsilon = O(1/\sqrt{n})$ for the 2-norm and $\epsilon = O(1/n)$ for the ∞-norm. Hence, from Eq. (15) we conclude that the amount of entropy needed for the encryption of n-qubit states is $2n - o(n)$.

V. GENERAL *N*-QUBIT ENCRYPTION SCHEMES

In Sec. IV, we found the optimal way to independently compose single-qubit encryption schemes in order to encrypt n-qubit states. However, one can do better with encryption schemes that do not act independently on each qubit. For example, the encryption scheme in Ref. 5 uniformly picks an n-qubit unitary from a set of $O(n2^n)$ random ones and hence it is not an independent encoding. Note also that it only uses $n + \log n + O(1)$ bits of entropy.

Ambainis and Smith[3] managed to derandomize the encryption scheme of Ref. 5 by explicitly describing the set of unitaries. In particular, they use a set of $2n$-bit strings, where each string corresponds to a product of n Pauli matrices (the bits $\{2j-1, 2j\}$ define the Pauli matrix for the jth qubit). They prove that if the set of strings is a small-bias set of size $O(n2^n)$, then picking a random unitary from this set gives an $(\epsilon, n + 2\log n + 2\log(1/\epsilon))$ encryption scheme in the 2-norm.

A δ-biased set is a set of k-bit strings such that for all possible subsets of bits, the probability over the set that the parity of the subset is 0, is $\left[\frac{1}{2}-\delta,\frac{1}{2}+\delta\right]$. Naor and Naor[7] gave the first such construction with size polynomial in k and $1/\delta$. Alon *et al.*[1] showed a lower bound on the size of a δ-biased set

$$N(k,\delta)\geqslant\Omega\left(\min\left\{\frac{k}{\delta^2\log(1/\delta)},2^k\right\}\right).$$

Since we are interested in encryption schemes which use less than 2n bits of entropy, we only consider δ-biased sets of size $o(2^{2n})$ and hence $\delta=\omega(1/2^n)$. Ambainis and Smith showed the following:

There exists a function $\delta(n)=\omega(1/2^n)$ such that any $O(\delta(n))$-biased set gives rise to a good encryption scheme in the 2-norm and moreover it has size $N=o(2^{2n})$.

In fact, their result holds for any $\delta(n)=1/\alpha(n)2^{n/2}$, where $\alpha(n)$ is any slowly growing function of n (e.g., $\log n$). Note that there are explicit constructions of such small-bias sets of size $N=\mathrm{poly}(\alpha(n),n)2^n$. However, it was an open question whether the same holds for the case of ∞-norm. Here, we resolve this question by providing a counterexample. We show that

For any $\delta(n)=\omega(1/2^n)$ there exists a $O(\delta(n))$-biased set of size $N=o(2^{2n})$ which is not good in the ∞-norm.

Let us, first, compute the norm $\|R(\rho)-\mathbb{I}/2^n\|_\infty$, where R is a Pauli encryption scheme and $\rho=|z+\rangle^{\otimes n}\langle z+|^{\otimes n}$. The density matrix of this state in the z-basis is

$$\rho=\left(\frac{\mathbb{I}+Z}{2}\right)^{\otimes n}=\begin{pmatrix}1&0&\cdots\\0&0&\cdots\\\vdots&\vdots&\ddots\end{pmatrix}.$$

The unitaries in the encryption scheme can be written as $U^k=U_1^k\otimes\cdots\otimes U_n^k$ with $U_i^k\in\{\mathbb{I},X,Y,Z\}$. For each unitary U^k we define a string $\chi^k\in\{0,1\}^n$ with $\chi_i^k=0$ if $U_i^k\in\{\mathbb{I},Z\}$, and $\chi_i^k=1$ if $U_i^k\in\{X,Y\}$. Note that $XZX=YZY=-Z$ and $ZZZ=\mathbb{I}Z\mathbb{I}=Z$, and hence

$$R(\rho)=\frac{1}{N}\sum_{k=1}^{N}\left(\frac{\mathbb{I}+(-1)^{\chi_1^k}Z}{2}\right)\otimes\cdots\otimes\left(\frac{\mathbb{I}+(-1)^{\chi_n^k}Z}{2}\right).$$

The density matrix of the encrypted state is again diagonal in the z-basis and therefore its eigenvalues are simply its diagonal elements. The size of each eigenvalue λ_χ is exactly the number of unitaries U^k with the same corresponding string χ divided by N. Thus,

$$\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_\infty=\max_\chi\left|\lambda_\chi-\frac{1}{2^n}\right|=\max_\chi\left|\frac{1}{N}(\#\textit{of unitaries with the same }\chi)-\frac{1}{2^n}\right|.$$

It is easy to see that starting from any small-bias set we can create a set which is asymptotically as good as the initial one and it has the extra property that it contains at least a $\delta(n)$ fraction of the unitaries with $\chi=0$. We start with a $O(\delta(n))$-biased set of size N and add $\delta(n)N$ unitaries with $\chi=0$ to the initial set. The new set has size $N'=O(N)$ and bias $O(\delta(n))$, and therefore, it is asymptotically as good as the original set. Hence

$$\left\|R(\rho)-\frac{\mathbb{I}}{2^n}\right\|_\infty=\max_\chi\left|\frac{1}{N'}(\#\textit{of unitaries with the same }\chi)-\frac{1}{2^n}\right|\geqslant O(\delta(n))-\frac{1}{2^n}=w\left(\frac{1}{2^n}\right),$$

which means that the encryption scheme R is not good in the ∞-norm. In other words, we show that although a δ-biased set encryption scheme is always good for the 2-norm, this is not the case for the ∞-norm. However, it is still conceivable that one might be able to use δ-biased sets with some extra properties in order to achieve good encryption for the ∞-norm.

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APPENDIX

1. Minimization of the entropy $H(\epsilon,z)$

Here, we provide details for the minimization of the function $H(\epsilon,z)$ with respect to z that concludes the proof of the optimal trade-off between approximation and entropy. Recall that

$$H(\epsilon,z) = -\left(\tfrac{1}{2}+\epsilon-z\right)\log\left(\tfrac{1}{2}+\epsilon-z\right) - 2z\log z - \left(\tfrac{1}{2}-\epsilon-z\right)\log\left(\tfrac{1}{2}-\epsilon-z\right)$$

and the constraints are

$$\frac{1}{4}+\frac{\epsilon}{2} \geqslant z \geqslant \frac{1}{4}-\frac{\epsilon}{2}, \tag{A1}$$

$$\frac{1}{2}-\epsilon \geqslant z. \tag{A2}$$

The entropy as a function of z is again a concave function and hence, in order to find the minimum we investigate the end points of the allowed interval for z. There are two cases:

Case 1: for $\epsilon \leqslant 1/6$, the constraint (4) is tighter. The left end point is $\{\frac{1}{4}+\epsilon/2, \frac{1}{4}+\epsilon/2, \frac{1}{4}+\epsilon/2, \frac{1}{4}-3\epsilon/2\}$, giving

$$H_1(\epsilon) = -3\left(\frac{1}{4}+\frac{\epsilon}{2}\right)\log\left(\frac{1}{4}+\frac{\epsilon}{2}\right) - \left(\frac{1}{4}-\frac{3\epsilon}{2}\right)\log\left(\frac{1}{4}-\frac{3\epsilon}{2}\right) = 2 - \frac{6}{\ln 2}\epsilon^2 + O(\epsilon^3).$$

The right end point is $\{\frac{1}{4}+3\epsilon/2, \frac{1}{4}-\epsilon/2, \frac{1}{4}-\epsilon/2, \frac{1}{4}-\epsilon/2\}$, giving

$$H_2(\epsilon) = -\left(\frac{1}{4}+\frac{3\epsilon}{2}\right)\log\left(\frac{1}{4}+\frac{3\epsilon}{2}\right) - 3\left(\frac{1}{4}-\frac{\epsilon}{2}\right)\log\left(\frac{1}{4}-\frac{\epsilon}{2}\right).$$

At $\epsilon=0$, $H_1=H_2=2$. At $\epsilon=1/6$, $H_1 \leqslant H_2$. The derivative of H_2-H_1 is always negative,

$$\frac{\mathrm{d}(H_2-H_1)}{\mathrm{d}\epsilon} = \frac{3}{2}\log\frac{(1-2\epsilon)(1-6\epsilon)}{(1+2\epsilon)(1+6\epsilon)} \leqslant 0,$$

so we conclude that H_1 is the best choice for $\epsilon \leqslant 1/6$. At $\epsilon=1/6$, H_1 achieves the value of $\log_2 3$, which means only three equally weighed unitaries are used.

Case 2: for $\epsilon \geqslant 1/6$, the constraint (5) is tighter, changing the left end point of z to $z=1/2-\epsilon$. This sets $y=0$, which is the regime of using only three unitaries, i.e., the distribution is $\{2\epsilon, \frac{1}{2}-\epsilon, \frac{1}{2}-\epsilon, 0\}$ and the entropy

$$H_3(\epsilon) = -2\epsilon\log 2\epsilon - 2\left(\tfrac{1}{2}-\epsilon\right)\log\left(\tfrac{1}{2}-\epsilon\right).$$

The second derivative of H_3-H_2 is always negative,

$$\frac{\mathrm{d}^2}{\mathrm{d}\epsilon^2}(H_3 - H_2) = -2[\epsilon(1-2\epsilon)(1+6\epsilon)\ln 2]^{-1},$$

so the function $H_3 - H_2$ is concave. That allows for only two points where $H_3 = H_2$. One of them is at $\epsilon = 1/2$, the other is found numerically to be $\epsilon_0 \approx 0.287$ with $H_0 \approx 1.41$. We conclude that for $1/6 \leqslant \epsilon \leqslant \epsilon_0$, the choice of H_3 is optimal, whereas for $\epsilon_0 \leqslant \epsilon \leqslant 1/2$, the best choice is H_2.

2. Another proof of optimality of Pauli encryption schemes

It is known[10] that every unital channel $\mathcal{E}$ with weights $\{w_k\}$ and unitaries U_k is equivalent to a Pauli channel with some other weights $\{x_m\}$, that is

$$\mathcal{E}(\rho) = \sum_k w_k U_k \rho U_k^\dagger, \tag{A3}$$

$$\mathcal{E}(\rho) = x_1\rho + x_2 X\rho X + x_3 Y\rho Y + x_4 Z\rho Z. \tag{A4}$$

This channel is an ϵ-randomizing map. We will prove that the Pauli realization of it has smaller entropy.

Suppose we act with this channel on one half of the Bell state $|\psi^+\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$. The first definition of $\mathcal{E}$ will give us

$$\rho' = \mathcal{E}(\rho) = \sum_k w_k (U_k \otimes \mathbb{I})|\psi^+\rangle\langle\psi^+|(U_k \otimes \mathbb{I})^\dagger = \sum_k w_k |\psi_k\rangle\langle\psi_k|, \tag{A5}$$

where $|\psi_k\rangle = (U_k \otimes \mathbb{I})|\psi^+\rangle$ are pure states. On the other hand, the second realization of $\mathcal{E}$ (with Pauli operations) acting on one half of the state $|\psi^+\rangle$ will transform it into a state with density matrix diagonal in the Bell basis, $\rho' = \mathrm{diag}(x_1, x_2, x_3, x_4)$.

In Ref. 8, Nielsen showed that when a density matrix can be expressed as $\rho' = \Sigma_k w_k |\varphi_k\rangle\langle\varphi_k|$, where $|\varphi_k\rangle$ are normalized states, the (ordered) vector of probabilities w_k is majorized by the vector of eigenvalues of ρ', that is $(w_k) \prec \lambda(\rho')$.

In our case, the vector of eigenvalues of ρ' is (x_m), and the majorization $(w_k) \prec (x_m)$ means $\Sigma_{m=1}^n w_m \leqslant \Sigma_{m=1}^n x_m$ for any $n \geqslant 1$. Note that if the length of (w_k) is greater than four, we pad the vector (x_m) by zero entries to make the lengths of the vectors equal.

The entropy function is concave. Because the vector of weights for the Pauli realization (x_k) majorizes the vector of weights for the original realization (w_k), the Pauli realization of the channel has smaller entropy, $S(\{x_k\}) \leqslant S(\{w_k\})$. This means the Pauli channel is the optimal (entropy-wise) realization of any unital channel.

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Sheaf-theoretic representation of quantum measure algebras

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We construct a sheaf-theoretic representation of quantum probabilistic structures, in terms of covering systems of Boolean measure algebras. These systems coordinatize quantum states by means of Boolean coefficients, interpreted as Boolean localization measures. The representation is based on the existence of a pair of adjoint functors between the category of presheaves of Boolean measure algebras and the category of quantum measure algebras. The sheaf-theoretic semantic transition of quantum structures shifts their physical significance from the orthoposet axiomatization at the level of events, to the sheaf-theoretic gluing conditions at the level of Boolean localization systems. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The groundbreaking 1936 paper by von Neumann and Birkhoff entitled "The Logic of Quantum Mechanics" introduced for the first time the notion of logic of a physical theory. For classical theories the appropriate logic is a Boolean algebra; but for quantum theories a non-Boolean logical structure is necessary, which can be an orthocomplemented lattice, or a partial Boolean algebra, or some other structure of a related form. The logic of a physical theory reflects the structure of the propositions describing the behavior of a physical system in the domain of the corresponding theory.

Naturally, the typical mathematical structure associated with logic is an ordered structure. The original quantum logical formulation of quantum theory[1,2] depends in an essential way on the identification of propositions with projection operators on a complex Hilbert space. A nonclassical, non-Boolean logical structure is effectively induced which has its origins in quantum theory. More accurately, the Hilbert space quantum logic has been initially axiomatized as a complete, atomic, orthomodular lattice. Equivalently, it could be cast isomorphic to the partial Boolean algebra of closed subspaces of the Hilbert space associated with the quantum system, or alternatively the partial Boolean algebra of projection operators of the system. On the contrary, the propositional logic of classical mechanics is Boolean logic, meaning that the class of models over which validity and associated semantic notions are defined for the propositions of classical mechanics is the class of Boolean logic structures.

The notion of logic of a physical theory essentially reflects the structure of events being observed in the context of that theory. Associated with such an events structure, there always exists a corresponding probabilistic structure, defined by means of convex sets of measures on that logic. In this sense, the probabilistic structure of a classical system is described by convex sets of probability measures on the Boolean algebra of events of the system, whereas the probabilistic structure of a quantum system is described by convex sets of probability measures on the quantum logic structure of that system. More accurately, in the case of quantum systems, if the quantum events logic is denoted by L, each quantum probability measure, called quantum state, is defined by a mapping;

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$$p:L \to [0,1]$$

such that the following conditions are satisfied: $p(1)=1$ and $p(x\vee y)=p(x)+p(y)$, if $x\perp y$, where, $x, y \in L$. In the Hilbert space formulation of quantum theory, L denotes the Hilbert space quantum logic, whereas a quantum state is defined by the Hilbert space inner product,

$$\langle \varphi, Px\varphi \rangle,$$

where $x \in L$, φ is a normalized vector in the Hilbert space, and Px is the orthogonal projection operator corresponding to $x \in L$. We remind that there exists a bijective correspondence between elements of L, or equivalently closed subspaces of the Hilbert space, and orthogonal projection operators.

In this work we will develop the idea that in quantum theory, Boolean localization measures can be understood as providing a coordinatization of a quantum probabilistic structure by establishing a principle of contextuality. More concretely, we shall argue that the covering coordinatization process induced by Boolean localization systems, being formed from families of collated compatible local Boolean measures, leads naturally to a contextual description of quantum events, and their associated quantum probabilities of a corresponding global quantum structure, with respect to local Boolean reference frames of measurement.

An intuitive flavor of this insight is provided by Kochen-Specker theorem,[3] according to which the complete comprehension of a quantum mechanical system is impossible, in case that a single system of Boolean devices is only used globally. On the other side, in every concrete measurement context, the set of events that have been actualized in this context form a Boolean algebra. This fact motivates the assertion that a Boolean algebra in the lattice of quantum events serves as a local reference frame, conceived in a precise category-theoretical sense, relative to which a measurement result is being coordinatized. The conceptual meaning of the proposed scheme implies that a quantum logical or quantum probabilistic structure is being construed by means of covering Boolean reference frames, regulated by our measurement localization procedures, which interlock to form a global coherent picture in a nontrivial way. Hence Boolean descriptive contexts are not abandoned once and for all, but instead are used locally, accomplishing the task of providing partial congruent relations with globally non-Boolean objects, the internal structure and functioning of which are being hopefully recovered by the interconnecting machinery governing the local objects. In this work we propose a mathematical scheme for the implementation of the above-mentioned assertion, in relation to quantum measure algebras, based on categorical and sheaf-theoretic methods.[4–8] Contextual category theoretical approaches to quantum structures have also been considered, from a different viewpoint in Refs. 9 and 10, and discussed in Refs. 11 and 12. A remarkable conceptual affinity to the viewpoint of the present paper, although not based on categorical methods, can be found in Refs. 13 and 14. For a general mathematical and philosophical discussion of sheaves, variable sets, and related structures, the interested reader should consult Ref. 15. Recently, there has also appeared in the literature a complete treatment of the dynamical aspects of physical theories, and in particular gauge theories, along topological sheaf-theoretic lines,[16,17] as an application of the framework of Mallios's abstract differential geometry.[18] Finally, it is worth mentioning that a sheaf-theoretic approach to quantum structures has been initiated independently by de Groote in a series of preprints.[19–22] In a general setting, de Groote constructs a theory of presheaves on the quantum lattice of closed subspaces of a complex Hilbert space, by transposing literally and generalizing the corresponding constructions from the lattice of open sets of a topological space to the quantum lattice. In comparison, our approach emphasizes the crucial role of Boolean localization systems in the global formation of quantum structures, and, thus, shifts the focus of relevant constructions to sheaves over suitable Grothendieck topologies on a base category of Boolean subalgebras of global quantum algebras.

The development of the conceptual and technical machinery of localization systems for generating a nontrivial global event and observable structures, as has been recently demonstrated in Refs. 23 and 24, effectuates a transition in the semantics of events and observables from a

set-theoretic to a sheaf-theoretic one. This is a crucial semantic difference that characterizes the present approach in comparison to the vast literature on quantum measurement and quantum logic. In Sec. II we will attempt to motivate physically the necessity of this transition on the basis of appropriate requirements that generalized procedures of physical measurement should respect, referring to the apprehension of physical information in terms of observables.

II. PHYSICAL MOTIVATION AND GENERAL CONCEPTUAL FRAMEWORK

Procedures of physical measurement presuppose, at the fundamental level, the existence of a localization process for extracting information related with the local behavior of a physical system, and, thus, discerning observable events. In a general setting, a localization process is usually being implemented physically by the preparation of suitable local reference domains for measurement of observable attributes. Subsequently, these reference domains instantiate local physical contexts for observation of events, which takes place by means of events-registering measurement devices, operating locally within these contexts. In a broad perspective, it is important to notice that registering an event, which has been observed in the context of a prepared reference domain, is not always equivalent to conferring a numerical identity to it, expressed in terms of some real value corresponding to a physical attribute. On the contrary, the latter is only a limited case of the localization process, when, in particular, it is assumed that all local reference contexts can be contracted to points, meaning that points are considered as unique measures of localization in the physical "continuum."

This is exactly the crucial assumption underlying the employment of the set-theoretic structure of the real line as a model of the physical continuum. The semantics of the physical continuum in the standard interpretation of physical theories is associated with the codomain of valuation of physical attributes. Usually the notion of continuum is tied to the attribute of position, serving as the range of values characterizing this particular attribution. In this sense, the model adopted to represent these values is the real line, specified as a set-theoretic structure of points that are independent and possess the property of infinite distinguishability with absolute precision. The adoption of the set theoretical real line model is usually justified on the basis of arguments, stipulating that quantities admissible as measured results must be real numbers, since the resort to real numbers has the advantage of securing our empirical access to the external world. Essentially, the basic semantic assumption underlying the employment of the set theoretic structure of the real line for the modeling of the localization structure of the physical continuum is that real number representability constitutes our global form of observation.

The success of this localizing philosophy for classical theories is due to the association of the notion of physical continuum with the attribute of position and the theoretical fact that all classical observables can be determined precisely and simultaneously at the unique measure of localization of that attribute, viz., at a spatial point, parametrized by the field of real numbers. Nevertheless, the major foundational difference between classical and quantum physical systems from the perspective of the modeling scheme by observables is a consequence of a single principle that can be termed principle of simultaneous observability. According to this, in the classical description of physical systems all their observables are theoretically compatible, or else they can be simultaneously specified in a single local measurement context. On the other side, the quantum description of physical systems is based on the assertion of incompatibility of all theoretical observables in a single local measurement context, and as a consequence quantum-theoretically the simultaneous specification of all observables is not possible. The conceptual roots of the violation of the principle of simultaneous observability in the quantum regime is tied with Heisenberg's uncertainty principle and Bohr's principle of complementarity of physical descriptions.

In this train of thought, a fruitful fundamental strategy implied by quantum theory would ideally fulfill the following objectives: First, it should disassociate the physical meaning of the notion of localization from its restricted spatial connotation reference context. Second, it should allow the functional dependence of observables on generalized localization measures induced by the preparation of suitably structured domains of measurement, not necessarily based on the existence of an underlying set-theoretic structure of points on the real line. Regarding the imple-

mentation of this strategy, it should be essential to interpret any local observable as a relational information algebraic number-like object with respect to the corresponding local context of measurement. At a further stage, it should be necessary to establish appropriate compatibility conditions for gluing the information content of local observables globally. Mathematically, the implementation of this strategy is being precisely captured by the concept of a sheaf-theoretic fibered structure, explained in the sequel. The primary physical motivation of this paper concerns the possibility of constructing explicitly an appropriate localization process suited to quantum physical observation, along the objectives of the above-stated strategy, and study in particular its consequences referring to the interpretation of quantum probabilistic structures. For this purpose, the focus is shifted from point-set to topological localization models of partially ordered global quantum event structures.

Before embarking on a qualitative discussion of the relevance of the concept of sheaf for this endeavor, it is initially instructive to clarify that the functioning of a localization process amounts to filtering the information content of a global structure of partially ordered physical events, through a concretely specified structure of observation domains determined by a homologous operational physical procedure. The latter is defined by the requirement that the reference contexts of measurement, together with their structural transformations, should form a mathematical category. Thus, the localization process should be implemented in terms of an action of the category of reference contexts on a set-theoretic global structure of physical events. The latter is then partitioned into sorts parametrized by the objects of the category of contexts. In this sense, the functioning of a localization process can be represented by means of a fibered construct, understood geometrically as a presheaf, or equivalently, as a variable set over the base category of contexts. The fibers of this construct may be thought of, in analogy to the case of the action of a group on a set of points, as the "generalized orbits" of the action of the category of contexts. The notion of functional dependence incorporated in this action, forces the ordered structure of physical events to fiber over the base category of reference contexts. Most important, the presheaf fibered construct incorporates the physical requirement of uniformity of observed events. More concretely, for any two events observed over the same domain of measurement, the structure of all reference contexts that relate to the first cannot be distinguished in any possible way from the structure of contexts relating to the second. Consequently, all the events observed within any particular reference context, implementing a localization process, are uniformly equivalent to each other. Equivalently stated, the compatibility of the localization process with the physical requirement of uniformity, demands that the relation of (partial) order in a global set-theoretic universe of events is induced by lifting appropriately a structured family of arrows from the base category of reference contexts to the fibers. It is precisely that condition of compatibility being formalized by the construction of the category of elements of the corresponding presheaf.

The disassociation of the physical meaning of a localization process from its restricted spatial connotation reference context requires, first of all, the abstraction of the constitutive properties of localization in appropriate categorical terms, and then, the effectuation of these properties for the definition of localization systems of global event structures. Regarding these objectives, the sought abstraction is being implemented by means of covering devices on the base category of reference contexts, called in categorical terminology covering sieves. The constitutive properties of localization being abstracted categorically in terms of sieves, being qualified as covering ones, satisfy the following basic requirements:

(i) The covering sieves are covariant under pullback operations, viz. they are stable under change of a base reference context. Most important, the stability conditions are functorial. This requirement means, in particular, that the intersection of covering sieves is also a covering sieve, for each reference context in the base category.
(ii) The covering sieves are transitive, such that, intuitively stated, covering sieves of figures of a context in covering sieves of this context are also covering sieves of the context themselves.

From a physical perspective, the consideration of covering sieves as generalized measures of localization of events in a global partially ordered structure of events gives rise to localization systems of the latter. More specifically, the operation which assigns to each reference context of the base category a collection of covering sieves satisfying the closure conditions stated previously gives rise to the notion of a Grothendieck topology on the category of contexts. The construction of a suitable Grothendieck topology on the base category of contexts is significant for the following reasons: First, it elucidates precisely and unquestionably the conception of local in a categorical measurement environment, such that this conception becomes detached from its restricted spatial connotation, and thus, expressed exclusively in relational information terms. Second, it permits the collation of local observable information into global ones by utilization of the notion of sheaf for that Grothendieck topology. The definition of sheaf essentially expresses gluing conditions, providing the means for studying the global consequences of locally defined properties. The transition from locally defined observable information into global ones is being effectuated via a compatible family of elements over a localization system of a global event structure. A sheaf assigns a set of elements to each reference context of a localization system, representing local observable data colected within that context. A choice of elements from these sets, one for each context, forms a compatible family if the choice respects the mappings induced by the restriction functions among contexts, and moreover, if the elements chosen agree whenever two contexts of the localization system overlap. If such a locally compatible choice induces a unique choice for a global event structure being localized, viz. a global choice, then the condition for being a sheaf is satisfied. We note that, in general, there will be more locally defined or partial choices than globally defined ones, since not all partial choices need be extendible to global ones, but a compatible family of partial choices uniquely extends to a global one, or in other words, any presheaf uniquely defines a sheaf.

Having explained in detail the physical motivation, as well as the key conceptual prerequisites and ideas underlying the modeling of localization processes for acquisition and efficient handling of observable information related with the behavior of physical systems in a broad perspective, in the sequel, we focus our attention on the implementation of a concrete localization process of quantum probabilistic structures effectuated by Boolean localization systems of quantum measurement.

III. CATEGORICAL PROBABILISTIC STRUCTURES

According to the category-theoretic approach to each kind of mathematical structure, there corresponds a *category* whose objects have that structure, and whose morphisms preserve it. Moreover to any natural construction on structures of one kind, yielding structures of another kind, there corresponds a *functor* from the category of the first kind to the category of the second.

A *classical event structure* is a small category, denoted by $\mathcal{B}$, which is called the category of Boolean event algebras. Its objects are Boolean algebras of events, and its arrows are Boolean algebraic morphisms.

A *quantum event structure* is a small category, denoted by $\mathcal{L}$, which is called the category of quantum event algebras.

Its objects, denoted by L, are quantum algebras of events, that is orthomodular σ-orthoposets. More concretely, each object L in $\mathcal{L}$ is considered as a partially ordered set of quantum events, endowed with a maximal element 1, and with an operation of orthocomplementation $[-]^*: L \to L$, which satisfy, for all $l \in L$, the following conditions: (a) $l \leqslant 1$, (b) $l^{**} = l$, (c) $l \vee l^* = 1$, (d) $l \leq \acute{l} \Rightarrow \acute{l}^* \leq l^*$, (e) $l \perp \acute{l} \Rightarrow l \vee \acute{l} \in L$, (f) for $l, \acute{l} \in L$, $l \leqslant \acute{l}$ implies that l and $\acute{l}$ are compatible, where $0 := 1^*$, $l \perp \acute{l} := l \leqslant \acute{l}^*$, and the operations of meet $\wedge$ and join $\vee$ are defined as usually. We also recall that $l, \acute{l} \in L$ are compatible if the sublattice generated by $\{l, l^*, \acute{l}, \acute{l}^*\}$ is a Boolean algebra, namely if it is a Boolean sublattice. The σ-completeness condition, namely that the join of countable families of pairwise orthogonal events must exist, is also required in order to have a well-defined theory of observables over L.

Its arrows are quantum algebraic morphisms, that is maps $L \xrightarrow{H} K$, which satisfy, for all $k \in K$, the following conditions: (a) $H(1)=1$, (b) $H(k^*)=[H(k)]^*$, (c) $k \leq \acute{k} \Rightarrow H(k) \leq H(\acute{k})$, (d) $k \perp \acute{k} \Rightarrow H(k \vee \acute{k}) \leq H(k) \vee H(\acute{k})$.

Next we introduce the categories associated with probabilistic structures.

A *quantum convex measure structure* is a small category, denoted by Σ, which is called the category of convex sets of quantum probability measures.

Its objects are the convex sets Θ of quantum states or quantum probability measures on a quantum event algebra L. Each quantum probability measure, or quantum state, is defined by a mapping;

$$p: L \to [0,1]$$

such that the following conditions are satisfied: $p(1)=1$ and $p(x \vee y)=p(x)+p(y)$, if $x \perp y$, where x, $y \in L$. On each set Θ, there is defined the operation of convex mixing by means of the mappings,

$$\sigma^n: E^n \times \Theta^n \to \Theta$$

for each natural number n, such that

$$\sigma^n(\underline{e},\underline{p}) := \sum_i e_i p_i,$$

where $\underline{e}=\langle e_1, \ldots, e_n \rangle$, is a vector of real numbers, with $e_i \geq 0$ and $\Sigma_i e_i = 1$, and also, $\underline{p}=\langle p_1 \ldots p_n \rangle$ is a vector of quantum states. The unique quantum state $\Sigma_i e_i p_i$ is called the convex mixture of $\underline{p}$. The convex mixture of $\underline{p}$, evaluated at $x \in L$, is the superposition of probabilities $\Sigma_i e_i p_i(x)$. For a quantum state p_i and an event $x \in L$, $p_i(x)$ denotes the probability of occurrence of x in state p_i.

The arrows in the category Σ are morphisms of convex sets of probability measures, that is morphisms of sets $[\,]^h: \Theta \to \Phi$ which commute with the operation of convex mixing, that is,

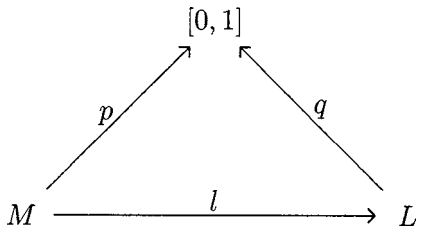
$$[\sigma^n(\underline{e},\underline{p})]^h = \sigma^n(\underline{e},\underline{p}^h).$$

We note that Θ and Φ are regarded as defined over the same quantum event algebra L, otherwise we have to take into account the quantum algebraic morphisms as well.

Using the information encoded in the categories of quantum event algebras $\mathcal{L}$, and quantum probabilistic structures Σ, it is possible to construct a new category, called the category of quantum probabilities, constructed as a category fibered in groupoids over the category of quantum event algebras $\mathcal{L}$, as follows:

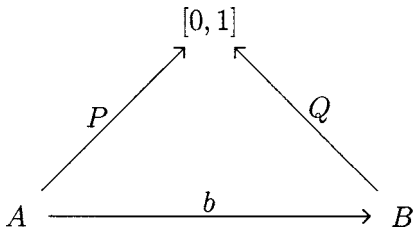
A *quantum probabilistic structure* is a small category, denoted by $\mathcal{Q}$, which is called the category of quantum states or quantum probabilities.

Its objects are the quantum measure algebras $\langle M,p \rangle := {}^pM$, where M is a quantum event algebra and p is a quantum probability measure on M, defined by the measurable mapping $p: M \to [0,1]$. The arrows in $\mathcal{Q}$, denoted by ${}^pM \xrightarrow{l} {}^qL$, are commutative triangles, or equivalently, are those quantum logic morphisms $M \xrightarrow{l} L$ in $\mathcal{L}$, such that $p=q \circ l$ in the diagram to follow is again a quantum probability measure.



Correspondingly, a *Boolean probabilistic structure* is a small category, denoted by $\mathcal{C}$, which is called the category of Boolean probability measures, or classical states.

Its objects are the Boolean measure algebras $\langle A,P\rangle := {}^{P}A$, where A is a Boolean event algebra and P is a Boolean probability measure on M, defined by the measurable mapping $P:A\to[0,1]$. The arrows in $\mathcal{C}$, denoted by ${}^{P}A\xrightarrow[b]{}{}^{Q}B$, are commutative triangles, or equivalently, are those Boolean logic morphisms $A\to B$ in $\mathcal{B}$, such that $P=Q\circ b$ in the diagram to follow is again a classical state.



IV. PRESHEAF AND COEFFICIENTS BOOLEAN FUNCTORS

A. Presheaves of Boolean probability measures

If $\mathcal{C}^{\mathrm{op}}$ is the opposite category of $\mathcal{C}$, then $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$ denotes the functor category of presheaves on Boolean measure algebras. Its objects are all functors $\mathbf{X}:\mathcal{C}^{\mathrm{op}}\to\mathbf{Sets}$, and its morphisms are all natural transformations between such functors. Each object $\mathbf{X}$ in this category is a contravariant set-valued functor on $\mathcal{C}$, called a presheaf of Boolean probability measures on $\mathcal{C}$.

A functor $\mathbf{X}$ is a structure-preserving morphism of these categories, that it preserves composition and identities. A functor in the category $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$ can be understood as a contravariant translation of the language of $\mathcal{C}$ into that of **Sets**. Given another such translation (contravariant functor) $\acute{\mathbf{X}}$ of $\mathcal{C}$ into **Sets** we need to compare them. This can be done by giving, for each object ${}^{P}A$ in $\mathcal{C}$ a transformation $\tau_{{}^{P}A}:\mathbf{X}({}^{P}A)\to\acute{\mathbf{X}}({}^{P}A)$ which compares the two images of the object ${}^{P}A$. Not any morphism will do, however, as it would be necessary for the construction to be parametric in ${}^{P}A$, rather than ad hoc. Since ${}^{P}A$ is an object in $\mathcal{C}$ while $\mathbf{X}({}^{P}A)$ is in **Sets** we cannot link them by a morphism. Rather the goal is that the transformation should respect the morphisms of $\mathcal{C}$, or in other words the interpretations of $v:{}^{P}A\to{}^{Q}B$ by $\mathbf{X}$ and $\acute{\mathbf{X}}$ should be compatible with the transformation under τ. Then τ is a natural transformation in the category of presheaves $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$.

For each Boolean measure algebra ${}^{P}A$ of $\mathcal{C}$, $\mathbf{X}({}^{P}A)$ is a set, and for each arrow $f:{}^{Q}B\to{}^{P}A$, $\mathbf{X}(f):\mathbf{X}({}^{P}A)\to\mathbf{X}({}^{Q}B)$ is a set function. If $\mathbf{X}$ is a presheaf on $\mathcal{C}$ and $x\in\mathbf{X}(O)$, the value $\mathbf{X}(f)(x)$ for an arrow $f:{}^{Q}B\to{}^{P}A$ in $\mathcal{C}$ is called the restriction of x along f and is denoted by $\mathbf{X}(f)(x)=x\cdot f$.

Each object ${}^{P}A$ of $\mathcal{C}$ gives rise to a contravariant Hom-functor $y[{}^{P}A]:=\mathrm{Hom}_{\mathcal{C}}(-,{}^{P}A)$. This functor defines a presheaf on $\mathcal{C}$. Its action on an object ${}^{Q}B$ of $\mathcal{C}$ is given by

$$y[{}^{P}A]({}^{Q}B) := \mathrm{Hom}_{\mathcal{C}}({}^{Q}B,{}^{P}A)$$

whereas its action on a morphism ${}^{R}C\xrightarrow{w}{}^{Q}B$, for $v:{}^{Q}B\to{}^{P}A$ is given by

$$y[{}^{P}A](w):\quad \mathrm{Hom}_{\mathcal{C}}({}^{Q}B,{}^{P}A)\to\mathrm{Hom}_{\mathcal{C}}({}^{R}C,{}^{P}A),$$

$$y[{}^{P}A](w)(v)=v\circ w.$$

Furthermore y can be made into a functor from $\mathcal{C}$ to the contravariant functors on $\mathcal{C}$,

$$y:\quad \mathcal{C}\to\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}},$$

such that ${}^{P}A\mapsto\mathrm{Hom}_{\mathcal{C}}(-,{}^{P}A)$. This is an embedding, called the Yoneda embedding,[5] and it is a full and faithful functor.

The functor category of presheaves on Boolean measure algebras $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$, provides an instantiation of a structure known as topos.[6–8] A topos exemplifies a well-defined notion of a categorical universe of variable sets. It can be conceived as a local mathematical framework corresponding to a generalized model of set theory or as a generalized space. Moreover it provides a natural example of a many-valued truth structure, which remarkably is not ad hoc, but reflects genuine constraints of the surrounding universe.

B. Boolean measure algebras fibrations

Since $\mathcal{C}$ is a small category, there is a set consisting of all the elements of all the sets $\mathbf{X}({}^{P}A)$, and similarly there is a set consisting of all the functions $\mathbf{X}(f)$. This observation regarding $\mathbf{X}:\mathcal{C}^{\mathrm{op}}\rightarrow\mathbf{Sets}$ permits us to take the disjoint union of all the sets of the form $\mathbf{X}({}^{P}A)$ for all objects ${}^{P}A$ of $\mathcal{C}$. The elements of this disjoint union can be represented as pairs $({}^{P}A,\chi)$ for all objects ${}^{P}A$ of $\mathcal{C}$ and elements $\chi\in\mathbf{X}({}^{P}A)$. Thus the disjoint union of sets is made by labeling the elements. Now we can construct a category whose set of objects is the disjoint union just mentioned. This structure is called the category of elements of the presheaf $\mathbf{X}$, denoted by $\int(\mathbf{X},\mathcal{C})$. Its objects are all pairs $({}^{P}A,\chi)$, and its morphisms $({}^{R}C,\acute{\chi})\rightarrow({}^{P}A,\chi)$ are those morphisms $u:{}^{R}C\rightarrow{}^{P}A$ of $\mathcal{C}$ for which $\chi\cdot u=\acute{\chi}$. Projection on the second coordinate of $\int(\mathbf{X},\mathcal{C})$, defines a functor $\int_{\mathbf{X}}:\int(\mathbf{X},\mathcal{C})\rightarrow\mathcal{C}$. $\int(\mathbf{X},\mathcal{C})$ together with the projection functor $\int_{\mathbf{X}}$ is equivalent to the discrete fibration induced by $\mathbf{X}$, and $\mathcal{C}$ is the base category of the fibration. We note that the fibration is discrete because the fibers are categories in which the only arrows are identity arrows. If ${}^{P}A$ is a Boolean measure algebra of $\mathcal{C}$, the inverse image under $\int_{\mathbf{X}}$ of ${}^{P}A$ is simply the set $\mathbf{X}({}^{P}A)$, although its elements are written as pairs so as to form a disjoint union. The instantiation of the fibration induced by $\mathbf{X}$ is an application of the general Grothendieck construction.[8]

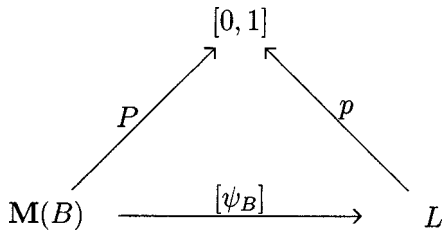
$$\begin{array}{ccc} \int(\mathbf{X},\mathcal{C}) & & \\ \Big\downarrow{\scriptstyle \int_{\mathbf{X}}} & & \\ \mathcal{C} & \xrightarrow{\ \mathbf{X}\ } & \mathbf{Sets} \end{array}$$

The split discrete fibration induced by $\mathbf{X}$, where $\mathcal{C}$ is the base category of the fibration, provides a well-defined notion of a uniform homologous fibered structure in the following sense: First, by the arrows specification defined in the category of elements of $\mathbf{X}$, any element χ, determined over the measure algebra ${}^{P}A$, is homologously related with any other element $\acute{\chi}$ over the measure algebra ${}^{R}C$, and so on, by variation over all the contexts of the base category. Second, all the elements χ of $\mathbf{X}$, of the same sort ${}^{P}A$, viz. determined over the same measure algebra ${}^{P}A$, are uniformly equivalent to each other, since all the arrows in $\int(\mathbf{X},\mathcal{C})$ are induced by lifting arrows from the base category $\mathcal{C}$.

C. Functor of Boolean measure coefficients

We define a modeling Boolean coefficients functor, $\mathbf{M}:\mathcal{C}\rightarrow\mathcal{Q}$, which assigns to Boolean measure algebras in $\mathcal{C}$, that instantiates a model category, the underlying quantum measure algebras from $\mathcal{Q}$, and to Boolean measurable morphisms the underlying quantum measurable morphisms. Hence $\mathbf{M}$ acts as a forgetful functor, forgetting the extra Boolean structure of $\mathcal{C}$.

Equivalently the Boolean coefficients functor can be characterized as $\mathbf{M}:\mathcal{B}\rightarrow\mathcal{L}$, which assigns to Boolean event algebras in $\mathcal{B}$ the underlying quantum event algebras from $\mathcal{L}$, and to Boolean morphisms the underlying quantum algebraic morphisms, such that the following diagram commutes:



V. ADJOINT FUNCTORIAL RELATION

We consider the category of quantum measure algebras $\mathcal{Q}$ and the modeling functor **M**, and we define the functor **R** from $\mathcal{Q}$ to the topos of presheaves on Boolean measure algebras $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$, given by

$$\mathbf{R}({}^{p}L):{}^{P}A \mapsto \mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{p}L).$$

A natural transformation τ in the topos of presheaves on Boolean measure algebras $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$ between **X** and $\mathbf{R}({}^{p}L)$, $\tau:\mathbf{X}\to\mathbf{R}({}^{p}L)$ is a family $\tau_{{}^{p}A}$ indexed by Boolean measure algebras ${}^{P}A$ of $\mathcal{C}$ for which each $\tau_{{}^{p}A}$ is a map

$$\tau_{{}^{p}A}:\mathbf{X}({}^{P}A) \to \mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{p}L)$$

of sets, such that the diagram of sets to follow, commutes for each Boolean morphism $u:{}^{R}\mathcal{C} \to {}^{P}A$ of $\mathcal{C}$,

$$\begin{array}{ccc} \mathbf{X}({}^{P}A) & \xrightarrow{\tau_{{}^{P}A}} & Hom_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{p}L) \\ \Big\downarrow{\scriptstyle \mathbf{X}(u)} & & \Big\downarrow{\scriptstyle \mathbf{M}(u)} \\ \mathbf{X}({}^{R}C) & \xrightarrow{\tau_{{}^{R}C}} & Hom_{\mathcal{Q}}(\mathbf{M}({}^{R}C),{}^{p}L) \end{array}$$

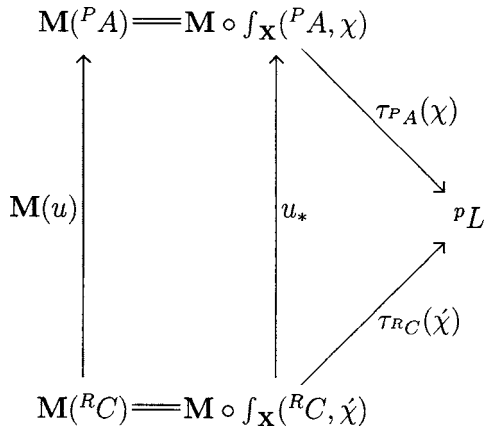
If we make use of the category of elements of the Boolean measure algebras-variable set X, being an object in the topos of presheaves $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$, then the map $\tau_{{}^{p}A}$, defined earlier, can be characterized as

$$\tau_{{}^{p}A}:({}^{P}A,\chi) \to \mathrm{Hom}_{\mathcal{Q}}\left(\mathbf{M}\circ\int_{\mathbf{X}}({}^{P}A,\chi),{}^{p}L\right).$$

Equivalently such a τ can be seen as a family of arrows of $\mathcal{Q}$ which is being indexed by objects $({}^{P}A,\chi)$ of the category of elements of the presheaf of Boolean measure algebras **X**, namely

$$\{\tau_{{}^{p}A}(\chi):\mathbf{M}({}^{P}A) \to {}^{p}L\}_{({}^{P}A,\chi)}.$$

From the perspective of the category of elements of **X**, the condition of the commutativity of the above-presented diagram is equivalent to the condition that for each Boolean morphism $u:{}^{R}\mathcal{C} \to {}^{P}A$ of $\mathcal{C}$, the following diagram commutes.



From the diagram above-presented, we conclude that the arrows $\tau^{P}{}_{A}(\chi)$ form a cocone from the functor $\mathbf{M}\circ\int_{\mathbf{X}}$ to the quantum measure algebra ${}^{P}L$. Making use of the definition of the colimit, we conclude that each such cocone emerges by the composition of the colimiting cocone with a unique arrow from the colimit $\mathbf{LX}$ to the quantum measure algebra object ${}^{P}L$. In other words, there is a bijection which is natural in $\mathbf{X}$ and ${}^{P}L$,

$$\mathrm{Nat}(\mathbf{X},\mathbf{R}({}^{P}L)) \cong \mathrm{Hom}_{\mathcal{Q}}(\mathbf{LX},{}^{P}L).$$

From the above-noted bijection we are driven to the conclusion that the functor $\mathbf{R}$ from $\mathcal{Q}$ to the topos of presheaves $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$, given by

$$\mathbf{R}({}^{P}L):{}^{P}A \mapsto \mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{P}L),$$

has a left adjoint $\mathbf{L}:\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}\to\mathcal{Q}$, which is defined for each presheaf of Boolean measure algebras $\mathbf{X}$ in $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$ as the colimit

$$\mathbf{L}(\mathbf{X}) = \mathrm{Colim}\left\{\int (\mathbf{X},\mathcal{C}) \xrightarrow{\int_{\mathbf{X}}} \mathcal{C} \xrightarrow{\mathbf{M}} \mathcal{Q}\right\}.$$

Consequently there is a *pair of adjoint functors* $\mathbf{L}\dashv\mathbf{R}$ as follows:

$$\mathbf{L}:\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}} \leftrightarrows \mathcal{Q}:\mathbf{R}.$$

Thus we have constructed an adjunction which consists of the functors $\mathbf{L}$ and $\mathbf{R}$, called left and right adjoints with respect to each other, respectively, as well as the natural bijection:

$$\begin{array}{ccc} Nat(\mathbf{X},\mathbf{R}({}^{p}L)) & \xrightarrow{\ \mathbf{r}\ } & Hom_{\mathcal{Q}}(\mathbf{LX},{}^{p}L) \\ \| & & \| \\ Nat(\mathbf{X},\mathbf{R}({}^{p}L)) & \xleftarrow{\ \mathbf{l}\ } & Hom_{\mathcal{Q}}(\mathbf{LX},{}^{p}L) \end{array}$$

$$\mathrm{Nat}(\mathbf{X},\mathbf{R}({}^{p}L)) \cong \mathrm{Hom}_{\mathcal{Q}}(\mathbf{LX},{}^{p}L).$$

In the above-described adjunction, between the topos of presheaves of Boolean measure algebras and the category of quantum measure algebras, the map $\mathbf{r}$ is called the right adjoint operator and the map $\mathbf{l}$ the left adjoint operator.

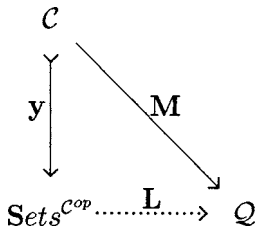
If in the bijection defining the adjunction we use as $\mathbf{X}$ the representable presheaf of the topos of Boolean measure algebras $\mathbf{y}[{}^{P}A]$, it takes the form:

$$\mathrm{Nat}(\mathbf{y}[{}^{P}A],\mathbf{R}({}^{p}L)) \cong \mathrm{Hom}_{\mathcal{Q}}(\mathbf{Ly}[{}^{P}A],{}^{p}L).$$

We note that when $\mathbf{X}=\mathbf{y}[{}^{P}A]$ is representable, then the corresponding category of elements $\int(\mathbf{y}[{}^{P}A],\mathcal{C})$ has a terminal object, namely the element $1:{}^{P}A\to{}^{P}A$ of $\mathbf{y}[{}^{P}A]({}^{P}A)$. Therefore the colimit of the composite $\mathbf{M}\circ\int_{\mathbf{y}[{}^{P}A]}$ is going to be just the value of $\mathbf{M}\circ\int_{\mathbf{y}[{}^{P}A]}$ on the terminal object. Thus we have

$$\mathbf{Ly}[{}^{P}A]({}^{P}A) \cong \mathbf{M}\circ\int_{\mathbf{y}[{}^{P}A]}({}^{P}A,1) = \mathbf{M}({}^{P}A).$$

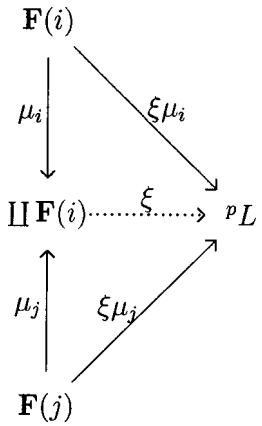
Thus we can characterize $\mathbf{M}({}^{P}A)$ as the colimit of the representable presheaf on the category of Boolean measure algebras,



VI. TENSOR PRODUCT REPRESENTATION OF THE COLIMIT

The content of the adjunction between the topos of presheaves of Boolean measure algebras and the category of quantum measure algebras can be analyzed if we make use of the categorical construction of the above-defined colimit, as a coequalizer of a coproduct. We consider the colimit of any functor $\mathbf{F}:\mathcal{I}\to\mathcal{Q}$ from some index category $\mathcal{I}$ to $\mathcal{Q}$. Let $\mu_i:\mathbf{F}(i)\to\amalg_i\mathbf{F}(i)$, $i\in I$, be the injections into the coproduct. A morphism from this coproduct, $\xi:\amalg_i\mathbf{F}(i)\to{}^{p}L$, is determined uniquely by the set of its components $\xi_i=\xi\mu_i$. These components ξ_i are going to form a cocone over $\mathbf{F}$ to the quantum measure algebra vertex ${}^{p}L$ only when for all arrows $v:i\to j$ of the index category $\mathcal{I}$ the following conditions are satisfied:

$$(\xi\mu_j)\mathbf{F}(v) = \xi\mu_i$$

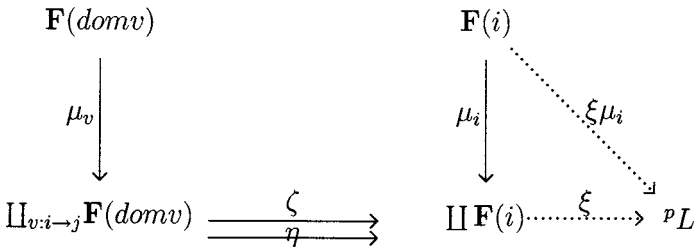


So we consider all $\mathbf{F}(\mathrm{dom}\,v)$ for all arrows v with its injections ν_v and obtain their coproduct $\amalg_{v:i\to j}\mathbf{F}(\mathrm{dom}\,v)$. Next we construct two arrows ζ and η, defined in terms of the injections ν_v and μ_i, for each $v:i\to j$ by the conditions

$$\zeta\nu_v = \mu_i,$$

$$\eta\nu_v = \mu_j \mathbf{F}(v)$$

as well as their coequalizer ξ;



The coequalizer condition $\xi\zeta = \xi\eta$ tells us that the arrows $\xi\mu_i$ form a cocone over $\mathbf{F}$ to the quantum measure algebra vertex ${}^{P}L$. We further note that since ξ is the coequalizer of the arrows ζ and η this cocone is the colimiting cocone for the functor $\mathbf{F}: I \to \mathcal{Q}$ from some index category $\mathcal{I}$ to $\mathcal{Q}$. Hence the colimit of the functor $\mathbf{F}$ can be constructed as a coequalizer of coproduct according to the following diagram:

$$\coprod_{v:i\to j} \mathbf{F}(domv) \underset{\eta}{\overset{\zeta}{\rightrightarrows}} \coprod \mathbf{F}(i) \xrightarrow{\xi} Colim\mathbf{F}$$

In the case considered the index category is the category of elements of the presheaf of Boolean measure algebras $\mathbf{X}$ and the functor $\mathbf{M} \circ G_{\mathbf{X}}$ plays the role of the functor $\mathbf{F}: \mathcal{I} \to \mathcal{Q}$. In the above-presented diagram the second coproduct is over all the objects $({}^{P}A, \chi)$ with $\chi \in \mathbf{X}({}^{P}A)$ of the category of elements, while the first coproduct is over all the maps $v: ({}^{R}C, \acute{\chi}) \to ({}^{P}A, \chi)$ of that category, so that $v: {}^{R}C \to {}^{P}A$ and the condition $\chi v = \acute{\chi}$ is satisfied. We conclude that the colimit $\mathbf{L}_M(\mathbf{X})$ can be equivalently presented as the following coequalizer:

$$\coprod_{v:{}^{R}C\to{}^{P}A} \mathbf{M}({}^{R}C) \underset{\eta}{\overset{\zeta}{\rightrightarrows}} \coprod_{({}^{P}A,\chi)} \mathbf{M}({}^{P}A) \xrightarrow{\xi} \mathbf{X}\otimes_{\mathcal{C}}\mathbf{M}$$

The coequalizer presentation of the colimit shows that the Hom-functor $\mathbf{R}$ has a left adjoint which can be characterized categorically as the tensor product $-\otimes_{\mathcal{C}}\mathbf{M}$.

In order to clarify the above-presented observation, we forget for the moment that the discussion concerns the category of quantum measure algebras $\mathcal{Q}$, and we consider instead the category **Sets**. Then the coproduct $\coprod_p \mathbf{M}({}^{P}A)$ is a coproduct of sets, which is equivalent to the product $\mathbf{X}({}^{P}A) \times \mathbf{M}({}^{P}A)$ for ${}^{P}A \in \mathcal{C}$. The coequalizer is thus the definition of the tensor product $\mathbf{X}\otimes_{\mathcal{C}}\mathbf{M}$ of the set valued functors:

$$\mathbf{X}: \mathcal{C}^{\mathrm{op}} \to \mathbf{Sets}, \quad \mathbf{M}: \mathcal{C} \to \mathbf{Sets}$$

$$\mathbf{X}: \mathcal{C}^{op} \longrightarrow \mathbf{Sets}, \qquad \mathbf{M}: \mathcal{C} \longrightarrow \mathbf{Sets}$$

$$\coprod_{{}^{P}A,{}^{R}C} \mathbf{X}({}^{P}A) \times Hom({}^{R}C, {}^{P}A) \times \mathbf{M}({}^{R}C) \underset{\eta}{\overset{\zeta}{\rightrightarrows}} \coprod_{{}^{P}A} \mathbf{X}({}^{P}A) \times \mathbf{M}({}^{P}A) \xrightarrow{\xi} \mathbf{X}\otimes_{\mathcal{C}}\mathbf{M}$$

According to the above-presented diagram for elements $\chi \in \mathbf{X}({}^{P}A)$, $v: {}^{R}C \to {}^{P}A$ and $\acute{y} \in \mathbf{M}({}^{R}C)$ the following equations hold:

$$\zeta(\chi, v, \acute{y}) = (\chi v, \acute{y}), \quad \eta(\chi, v, \acute{y}) = (\chi, v\acute{y})$$

symmetric in $\mathbf{X}$ and $\mathbf{M}$. Hence the elements of the set $\mathbf{X}\otimes_{\mathcal{C}}\mathbf{M}$ are all of the form $\xi(\chi, y)$. This element can be written as

$$\xi(\chi, y) = \chi \otimes y, \quad \chi \in \mathbf{X}({}^{P}A), y \in \mathbf{M}({}^{P}A).$$

Thus if we take into account the above-presented definitions of ζ and η, we obtain

$$\chi v \otimes \acute{y} = \chi \otimes v\acute{y}.$$

Furthermore if we define the arrows

$$k_{^PA}:\mathbf{X}\otimes_{\mathcal{C}}\mathbf{M} \to {}^{p}L, \quad l_{^PA}:\mathbf{X}({}^{P}A) \to \mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{p}L)$$

they are related under the fundamental adjunction by

$$k_{^PA}(\chi,y) = l_{^PA}(\chi)(y), \quad {}^{P}A \in \mathcal{C}, \chi \in \mathbf{X}({}^{P}A), y \in \mathbf{M}({}^{P}A).$$

Here we consider k as a function on $\amalg_{^PA}\mathbf{X}({}^{P}A)\times\mathbf{M}({}^{P}A)$ with components $k_{^PA}:\mathbf{X}({}^{P}A)\times\mathbf{M}({}^{P}A) \to {}^{p}L$ satisfying

$$k_{^RC}(\chi v, y) = k_{^PA}(\chi, vy)$$

in agreement with the above-defined equivalence relation.

Now we replace the category **Sets** by the category of quantum measure algebras $\mathcal{Q}$ under study. The element y in the set $\mathbf{M}({}^{P}A)$ is replaced by a generalized element $y:\mathbf{M}({}^{R}C)\to\mathbf{M}({}^{P}A)$ from some modeling object $\mathbf{M}({}^{R}C)$ of $\mathcal{Q}$. Then we consider k as a function $\amalg_{({}^{P}A,\chi)}\mathbf{M}({}^{P}A)\to{}^{p}L$ with components $k_{({}^{P}A,\chi)}:\mathbf{M}({}^{P}A)\to{}^{p}L$ for each $\chi\in\mathbf{X}({}^{P}A)$, that for all arrows $v:{}^{R}C\to{}^{P}A$ satisfy

$$k_{({}^{R}C,\chi v)} = k_{({}^{P}A,\chi)} \circ \mathbf{M}(v).$$

Then the condition defining the bijection holding by virtue of the fundamental adjunction is given by

$$k_{({}^{P}A,\chi)} \circ y = l_{^PA}(\chi) \circ y:\mathbf{M}({}^{R}C) \to {}^{p}L.$$

This argument, being natural in the object $\mathbf{M}({}^{R}C)$, is determined by setting $\mathbf{M}({}^{R}C)=\mathbf{A}({}^{P}A)$ with y being the identity map. Hence the bijection takes the form $k_{({}^{P}A,\chi)}=l_{^PA}(\chi)$, where $k:\amalg_{({}^{P}A,\chi)}\mathbf{M}({}^{P}A)\to{}^{p}L$, and $l_{^PA}:\mathbf{X}({}^{P}A)\to\mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),{}^{p}L)$.

VII. SYSTEM OF LOCALIZATIONS FOR QUANTUM MEASURE ALGEBRAS

The notion of a system of localizations for a quantum measure algebra, which will be defined in the sequel, is conceptually based on the expectation that a quantum measure algebra ${}^{p}L$ in $\mathcal{Q}$ is possible to be comprehended by means of certain structure preserving maps $\mathbf{M}({}^{P}A)\to{}^{p}L$ with local or modeling objects Boolean measure algebras ${}^{P}A$ in $\mathcal{C}$ as their domains. It is obvious that any single map from any modeling Boolean measure algebra to a quantum measure algebra is not adequate to determine it entirely, and hence, it contains only a fraction of the total information content included in it. This problem may be tackled, only if we employ many appropriate structure preserving maps from the modeling Boolean measure algebras to a quantum measure algebra simultaneously, so as to cover it completely. In turn the information available about each map of the specified kind may be used to determine the quantum measure algebra itself. In this case we conceive the family of such maps as the generator of a system of localizations for a quantum measure algebra. The notion of local is characterized using a notion of topology on $\mathcal{C}$, the axioms of which express closure conditions on the collection of modeling algebras of Boolean coefficient probability measures.

A. The notion of Grothendieck topology on $\mathcal{C}$

We start our discussion by explicating the notion of a topology on the category of Boolean measure algebras $\mathcal{C}$. A topology on $\mathcal{C}$ is a system of arrows $\mathbf{\Lambda}$, where for each object ${}^{P}A$ there is a set $\mathbf{\Lambda}({}^{P}A)$ that contains indexed families of $\mathcal{C}$-morphisms,

$$\mathbf{\Lambda}({}^{P}A) = \{\psi_i : {}^{R}C_i \to {}^{P}A, i \in I\}$$

that is, Boolean homomorphisms to ${}^{P}A$, such that certain appropriate conditions are satisfied.

The notion of a topology on the category of Boolean measure algebras $\mathcal{C}$ is a categorical generalization of a system of set-theoretical covers on a topology $\mathbf{T}$, where a cover for $U \in \mathbf{T}$ is a set $\{U_i : U_i \in \mathbf{T}, \mathbf{i} \in \mathbf{I}\}$ such that $\cup U_i = U$. The generalization is achieved by noting that the topology ordered by inclusion is a poset category and that any cover corresponds to a collection of inclusion arrows $U_i \to U$. Given this fact, any family of arrows contained in $\mathbf{\Lambda}({}^{P}A)$ of a topology is a cover as well.

The specification of a categorial or Grothendieck topology on the category of Boolean measure algebras takes place through the introduction of appropriate covering devices, called covering sieves. For an object ${}^{P}A$ in $\mathcal{C}$, a ${}^{P}A$-sieve is a family ϱ of $\mathcal{C}$-morphisms with codomain ${}^{P}A$, such that if ${}^{R}C \to {}^{P}A$ belongs to ϱ and ${}^{Q}D \to {}^{R}C$ is any $\mathcal{C}$-morphism, then the composite ${}^{Q}D \to {}^{R}C \to {}^{P}A$ belongs to ϱ.

A Grothendieck topology on the category of Boolean measure algebras $\mathcal{C}$ is a system J of sets, $J({}^{P}A)$ for each ${}^{P}A$ in $\mathcal{C}$, where each $J({}^{P}A)$ consists of a set of ${}^{P}A$-sieves (called the covering sieves), which satisfy the following conditions:

1. For any ${}^{P}A$ in $\mathcal{C}$ the maximal sieve $\{g : \mathrm{cod}(g) = {}^{P}A\}$ belongs to $J({}^{P}A)$ (maximality condition).
2. If ϱ belongs to $J({}^{P}A)$ and $f : {}^{R}C \to {}^{P}A$ is a $\mathcal{C}$-morphism, then $f^{*}(\varrho) = \{h : {}^{R}C \to {}^{P}A, f \cdot h \in \varrho\}$ belongs to $J({}^{R}C)$ (stability condition).
3. If ϱ belongs to $J({}^{P}A)$ and S is a sieve on ${}^{R}C$, where for each $f : {}^{R}C \to {}^{P}A$ belonging to ϱ, we have $f^{*}(S)$ in $J({}^{R}C)$, then S belongs to $J({}^{P}A)$ (transitivity condition).

The small category $\mathcal{C}$ together with a Grothendieck topology $\mathbf{J}$ is called a Boolean measure algebras site.

B. The Grothendieck topology of epimorphic families

We consider $\mathcal{C}$ as a model category, whose set of objects $\{{}^{P_i}A_i : i \in I\}$, I: index set, generate $\mathcal{Q}$, in the sense that

$$\mathbf{M}({}^{P_i}A_i) \xrightarrow{w_i} {}^{p}L \underset{u}{\overset{v}{\rightrightarrows}} {}^{t}K$$

the identity $v \circ w_i = u \circ w_i$, for every arrow $w_i : \mathbf{M}({}^{P_i}A_i) \to {}^{p}L$, and every ${}^{P_i}A_i$, implies that $v = u$. Equivalently we can say that the set of all arrows $w_i : \mathbf{M}({}^{P_i}A_i) \to {}^{p}L$, constitute an epimorphic family.

The consideration that $\mathcal{C}$ is a generating model category of $\mathcal{Q}$ points exactly to the depiction of the appropriate Grothendieck topology on $\mathcal{C}$.

We assert that a sieve S on a Boolean measure algebra ${}^{P}A$ in $\mathcal{C}$ is to be a covering sieve of ${}^{P}A$, when the arrows $s : {}^{R}C \to {}^{P}A$ belonging to the sieve S together form an epimorphic family in $\mathcal{Q}$. This requirement may be equivalently expressed in terms of a map

$$\Phi_S : \amalg_{(s:{}^{R}C \to {}^{P}A) \in S} {}^{R}C \to {}^{P}A$$

being an epi in $\mathcal{Q}$.

We will show that the choice of covering sieves on Boolean measure algebras ${}^{P}A$ in $\mathcal{C}$, as being epimorphic families in $\mathcal{Q}$, does indeed define a Grothendieck topology on $\mathcal{C}$.

First of all we notice that the maximal sieve on each Boolean measure algebra ${}^{P}A$ includes the identity ${}^{P}A \to {}^{P}A$, thus it is a covering sieve. Next, the transitivity property of the depicted covering sieves is obvious. It remains to demonstrate that the covering sieves remain stable under pullback. For this purpose we consider the pullback of such a covering sieve S on ${}^{P}A$ along any arrow $h : {}^{Q}D \to {}^{P}A$ in $\mathcal{C}$

$$\begin{array}{ccc} \amalg_{s\in S}{}^{R}C\times_{P_A}{}^{Q}D & \longrightarrow & {}^{Q}D \\ \downarrow & & \downarrow h \\ \amalg_{s\in S}{}^{R}C & \xrightarrow{\Phi} & {}^{P}A \end{array}$$

The Boolean measure algebras ${}^{P}A$ in $\mathcal{C}$ generate the category of quantum measure algebras $\mathcal{Q}$, hence, there exists for each arrow $s:{}^{R}C\to{}^{P}A$ in S, an epimorphic family of arrows $\amalg[{}^{T}E]^{s}\to{}^{R}C\times_{P_A}{}^{Q}D$, or equivalently $\{[{}^{T}E]^{s}_{j}\to{}^{R}C\times_{P_A}{}^{Q}D\}_{j}$, with each domain $[{}^{T}E]^{s}$ a Boolean measure algebra.

Consequently the collection of all the composites:

$$[{}^{T}E]^{s}_{j}\to{}^{R}C\times_{P_A}{}^{Q}D\to{}^{Q}D$$

for all $s:{}^{R}C\to{}^{P}A$ in S, and all indices j together form an epimorphic family in $\mathcal{Q}$, that is contained in the sieve $h^{*}(S)$, being the pullback of S along $h:{}^{Q}D\to{}^{P}A$. Therefore the sieve $h^{*}(S)$ is a covering sieve.

C. Covering sieves as localization systems

If we consider a quantum measure algebra ${}^{p}L$, and all quantum algebraic morphisms of the form $\psi_{P_A}:\mathbf{M}({}^{P}A)\to{}^{p}L$, with domains ${}^{P}A$, in the generating model category of Boolean measure algebras $\mathcal{C}$, then the family of all these maps ψ_{P_A}, constitute an epimorphism:

$$S:\amalg_{({}^{P}A\in\mathcal{C},\psi_{P_A}:\mathbf{M}({}^{P}A)\to{}^{p}L)}\mathbf{M}({}^{P}A)\to{}^{p}L.$$

We say that a sieve on a quantum measure algebra defines a covering sieve by objects of its generating model category $\mathcal{C}$, when the quantum algebraic morphisms belonging to the sieve define the preceding epimorphism.

From a physical perspective covering sieves by Boolean measure algebras are equivalent to Boolean localization systems of quantum measure algebras. These localization systems filter the information of a quantum measure algebra through Boolean domains, associated with procedures of localization in measurement environments. We will discuss localizations systems in detail, in order to unravel the physical meaning of the requirements underlying the notion of Grothendieck topology, and subsequently, the notion of covering sieves defined previously. It is instructive to begin with the notion of a system of prelocalizations for a quantum measure algebra.

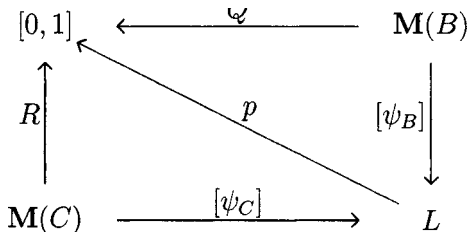
A *system of prelocalizations* for a quantum measure algebra ${}^{p}L$ in $\mathcal{Q}$ is a subfunctor of the Hom-functor $\mathbf{R}({}^{p}L)$ of the form $\mathbf{S}:\mathcal{C}^{\mathrm{op}}\to\mathbf{Sets}$, namely for all ${}^{P}A$ in $\mathcal{C}$ it satisfies $\mathbf{S}({}^{P}A)\subseteq[\mathbf{R}({}^{p}L)]({}^{P}A)$. Hence a system of prelocalizations for quantum measure algebra ${}^{p}L$ in $\mathcal{Q}$ is an ideal $\mathbf{S}({}^{P}A)$ of quantum algebraic morphisms of the form

$$\psi_{P_A}:\mathbf{M}({}^{P}A)\to{}^{p}L,\quad {}^{P}A\in\mathcal{C},$$

such that $\{\psi_{P_A}:\mathbf{M}({}^{P}A)\to{}^{p}L$ in $\mathbf{S}({}^{P}A)$, and $\mathbf{A}(v):\mathbf{M}({}^{R}C)\to\mathbf{M}({}^{P}A)$ in $\mathcal{Q}$ for $v:{}^{R}C\to{}^{P}A$ in $\mathcal{C}$, implies $\psi_{P_A}\circ\mathbf{M}(v):\mathbf{M}({}^{R}C)\to\mathcal{Q}$ in $\mathbf{S}({}^{P}A)\}$.

The introduction of the notion of a system of prelocalizations is forced on the basis of operational physical arguments. According to Kochen-Specker theorem it not possible to understand completely a quantum mechanical system with the use of a single system of Boolean devices. On the other side, in every concrete experimental context, the set of events that have been actualized in this context forms a Boolean algebra. In light of this we can say that any Boolean domain object $(B,[\psi_{B}]:\mathbf{M}(B)\to L)$ in a system of prelocalizations for a quantum event algebra L, making the diagram below commutative, corresponds to a set of Boolean classical events that

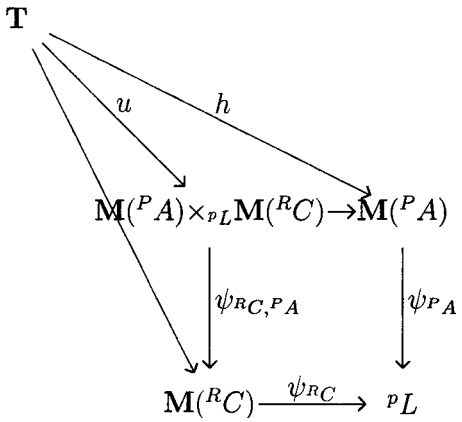
become actualized in the experimental context of B. These Boolean domains play the role of localizing devices in a quantum event structure, which are induced by measurement situations. The above-noted observation is equivalent to the statement that a measurement-induced Boolean algebra serves as a reference frame, in a topos-theoretical environment, relative to which a measurement result is being coordinatized. Correspondingly, by commutativity of the diagram to follow, we obtain naturally the notion of coordinatizing Boolean measure algebras in a system of prelocalizations for a quantum measure algebra over a quantum event algebra L. The same notion suggests an effective way of comprehending quantum theory in a contextual perspective, pointing to a relativity principle of a topos-theoretical origin. Concretely it supports the assertion that the quantum world is the universe of varying Boolean reference frames, which interconnect to form a coherent picture in a nontrivial way.



Adopting the aforementioned perspective on quantum measure algebraic structures, the operation of the Hom-functor $\mathbf{R}({}^{p}L)$ is equivalent to depicting an ideal of morphisms which are to play the role of local coverings of a quantum measure algebra by modeling objects. The notion of a system of prelocalizations formalizes an intuitive idea, according to which, if we sent many coordinatizing Boolean measure algebras into the quantum measure algebra homomorphically, then we would expect that these modeling objects would prove to be enough for the complete determination of the quantum measure algebra. If we consider a geometrical viewpoint, we may legitimately characterize metaphorically the maps $\psi^{p}{}_{A}:\mathbf{M}({}^{P}A)\rightarrow{}^{p}L$, where ${}^{P}A$ in $\mathcal{C}$, in a system of prelocalizations for quantum measure algebra ${}^{p}L$ as Boolean measure algebra charts. Correspondingly the modeling Boolean domain objects $(A,[\psi_A]:\mathbf{M}(A)\rightarrow L)$ in a system of prelocalizations for a quantum event algebra, making the above-presented diagram commutative, may be characterized as measurement charts. Subsequently, their domains A may be called Boolean coefficient domains induced by measurement, the elements of A measured local Boolean coefficients, and the elements of L quantum events (or quantum propositions in a logical interpretation), coordinatized by Boolean coefficients. Finally, the Boolean morphisms $\upsilon:D\rightarrow A$ in $\mathcal{B}$ play the equivalent role of transition maps.

Under these intuitive identifications, we say that a family of Boolean measure algebra charts $\psi^{p}{}_{A}:\mathbf{M}({}^{P}A)\rightarrow{}^{p}L$, ${}^{P}A$ in $\mathcal{C}$ (or correspondingly a family of Boolean measurement charts $[\psi_A]:\mathbf{M}(A)\rightarrow L$ making the above-presented diagram commutative), is the generator of the system of prelocalization $\mathbf{S}$ iff this system is the smallest among all that contains that family. It is evident that a quantum measure algebra, and correspondingly the quantum event algebra over which it is defined, can have many systems of measurement prelocalizations, that, remarkably, form an ordered structure. More specifically, systems of prelocalization constitute a partially ordered set under inclusion. Furthermore, the intersection of any number of systems of prelocalization is again a system of prelocalizations. We emphasize that the minimal system is the empty one, namely $\mathbf{S}({}^{P}A)=\emptyset$, for all ${}^{P}A$ in $\mathcal{C}$, whereas the maximal system is the Hom-functor $\mathbf{R}({}^{p}L)$ itself, or equivalently, all quantum algebraic morphisms $\psi^{p}{}_{A}:\mathbf{M}({}^{P}A)\rightarrow{}^{p}L$, for all ${}^{P}A$ in $\mathcal{C}$.

The transition from a system of prelocalizations to a system of localizations for a quantum measure algebra can be effected under the restriction that certain compatibility conditions have to be satisfied on the overlap of the modeling Boolean coefficient domains covering the quantum measure algebra under investigation. In order to accomplish this we use a pullback diagram in $\mathcal{Q}$ as follows:



The pullback of the Boolean charts $\psi_{^PA}:\mathbf{M}(^PA)\to{}^pL$, ^PA in $\mathcal{C}$, and $\psi_{^RC}:\mathbf{M}(^RC)\to{}^pL$, $^RC\in\mathcal{C}$ with common codomain the quantum measure algebra ^pL consists of the object $\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC)$ and two arrows $\psi_{^PA^RC}$ and $\psi_{^RC^PA}$, called projections, as shown in the above-presented diagram. The square commutes and for any object T and arrows h and g that make the outer square commute, there is a unique $u:T\to\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC)$ that makes the whole diagram commutative. Hence we obtain the condition:

$$\psi_{^RC}\circ g=\psi_{^PA}\circ h.$$

The pullback of the Boolean measure algebra charts $\psi_{^PA}:\mathbf{A}(^PA)\to{}^pL$, ^PA in $\mathcal{C}$, and $\psi_{^RC}:\mathbf{M}(^RC)\to{}^pL$, ^RC in $\mathcal{C}$, is equivalently characterized as their fiber product, because $\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC)$ is not the whole product $\mathbf{A}(^PA)\times\mathbf{M}(^RC)$ but the product taken fiber by fiber. We notice that if $\psi_{^PA}$ and $\psi_{^RC}$ are injective, then their pullback is isomorphic with the intersection $\mathbf{M}(^PA)\cap\mathbf{M}(^{P'}A)$. Then we can define the pasting map, which is an isomorphism, as follows:

$$\Omega_{^PA,^RC}:\psi_{^RC^PA}(\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC))\to\psi_{^PA^RC}(\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC))$$

by putting

$$\Omega_{^PA,^RC}=\psi_{^PA^RC}\circ\psi^RC^PA^{-1}.$$

Then we have the following cocycle conditions:

$$\Omega_{^PA,^PA}=1_{^PA},\quad 1_{^PA}:=id_{^PA}$$

$$\Omega_{^PA,^RC}\circ\Omega_{^RC,^TE}=\Omega_{^PA,^TE}\quad if\ \mathbf{M}(^PA)\cap\mathbf{M}(^RC)\cap\mathbf{M}(^TE)\neq 0,$$

$$\Omega_{^PA,^RC}=\Omega^{-1}_{^RC,^PA}\quad if\ \mathbf{M}(^PA)\cap\mathbf{M}(^RC)\neq 0.$$

The pasting map assures that the mapping $\psi_{^RC^PA}(\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC))$ and also $\psi_{^PA^RC}(\mathbf{M}(^PA)\times_{^pL}\mathbf{M}(^RC))$ are going to cover the same part of the quantum measure algebra in a compatible way. It is obvious that the above-mentioned compatibility conditions are translated immediately to corresponding compatibility conditions concerning Boolean measurement charts on the quantum event structure.

Given a system of prelocalizations for a quantum measure algebra ^pL in $\mathcal{Q}$, and correspondingly for the quantum event algebra over which it is defined, we call it a *system of localizations* iff the above-noted compatibility conditions are satisfied and moreover the quantum algebraic structure is preserved.

We assert that the above-noted compatibility conditions provide the necessary relations for understanding a system of localizations for a quantum measure algebra as a structure sheaf or sheaf of Boolean coefficients, consisting of local Boolean measure algebras. This is related to the observation that systems of localizations are actually subfunctors of the representable Hom-functor $\mathbf{R}({}^{p}L)$ of the form $\mathbf{S}:\mathcal{C}^{\mathrm{op}}\rightarrow\mathbf{Sets}$, namely for all ${}^{P}A$ in $\mathcal{C}$ satisfy $\mathbf{S}({}^{P}A)\subseteq[\mathbf{R}({}^{p}L)]({}^{P}A)$. In this sense the pullback compatibility conditions express gluing relations on overlaps of Boolean measure algebra charts and convert a presheaf subfunctor of the Hom-functor into a sheaf for the Grothendieck topology specified. The concept of sheaf expresses exactly the pasting conditions that local Boolean coefficients algebras have to satisfy, namely, the way by which local data can be collated together into global ones. We stress the point that the transition from locally defined properties to global consequences happens via a compatible family of elements over a cover of the global object. A cover, or equivalently a localization system of the global, object, being a quantum measure algebra structure in the present scheme, can be viewed as providing a decomposition of that object into simpler modeling objects.

The comprehension of a localization system as a sheaf of Boolean coefficients permits the conception of a quantum measure algebra (or of its associated quantum event algebra) as a generalized Boolean manifold, obtained by pasting the $\psi_{{}^{R}C{}^{P}A}(\mathbf{M}({}^{P}A)\times_{{}^{p}L}\mathbf{M}({}^{R}C))$ and $\psi_{{}^{P}A{}^{P'}A}(\mathbf{M}({}^{P}A)\times_{{}^{p}L}\mathbf{M}({}^{R}C))$ covers together by the transition functions $\Omega_{{}^{P}A,{}^{R}C}$.

More specifically, the equivalence relations in the category of elements of such a structure sheaf, represented by a Boolean system of Boolean probabilities coefficients, have to be taken into account according to the analysis of the adjoint relation presented in Sec. VI. Equivalence relations of this form give rise to congruences in the structure sheaf of Boolean coefficients, which are expressed categorically as a colimit in the category of elements of such a structure sheaf. In this perspective the generalized manifold, which represents categorically a quantum measure algebra, is understood as a colimit in a sheaf of Boolean coefficients, which contains compatible families of modeling Boolean measure algebras. It is instructive to emphasize that the organization of Boolean coordinatizing objects in localization systems takes the form of interconnection of these modeling objects through the categorical construction of colimit, the latter being the means to comprehend an object of complex structure (quantum measure algebra) from simpler coefficient objects (Boolean measure algebras).

The above-noted ideas provide the basis for the formulation of a sheaf-theoretic representation theorem concerning quantum measure algebras as we shall present in the following section.

VIII. REPRESENTATION OF QUANTUM MEASURE ALGEBRAS

A. Unit and counit of the adjoint relation

We again focus our attention on the fundamental adjoint relation established, and investigate the unit and the counit of it. For any presheaf $\mathbf{X}$ in the topos $\mathbf{Sets}^{\mathcal{C}^{\mathrm{op}}}$, the **unit** $\delta_{\mathbf{X}}:\mathbf{X}\rightarrow\mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}(\_),\mathbf{X}\otimes_{\mathcal{C}}\mathbf{M})$ has components:

$$\delta_{\mathbf{X}}({}^{P}A):\mathbf{X}({}^{P}A)\rightarrow\mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}({}^{P}A),\mathbf{X}\otimes_{\mathcal{C}}\mathbf{M})$$

for each Boolean measure algebra ${}^{P}A$ in $\mathcal{C}$.

If we make use of the representable presheaf $y[{}^{P}A]$ we obtain

$$\delta_{\mathbf{y}[{}^{P}A]}:\mathbf{y}[{}^{P}A]\rightarrow\mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}(\_),\mathbf{y}[{}^{P}A]\otimes_{\mathcal{C}}\mathbf{M}).$$

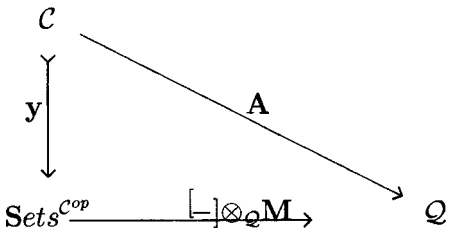
Hence for each object ${}^{P}A$ of $\mathcal{C}$ the unit, in the case considered, corresponds to a map

$$\mathbf{M}({}^{P}A)\rightarrow\mathbf{y}[{}^{P}A]\otimes_{\mathcal{C}}\mathbf{M}.$$

But since

$$\mathbf{y}[{}^{P}A]\otimes_{\mathcal{C}}\mathbf{M}\cong\mathbf{M}({}^{P}A)$$

the unit for the representable presheaf of Boolean measure algebras is clearly an isomorphism. By the preceding discussion we conclude that the following diagram commutes:

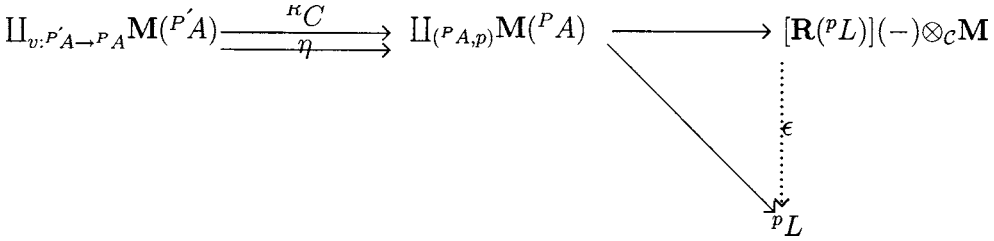


Thus the unit of the fundamental adjunction referring to the representable presheaf of the category of Boolean measure algebras provides a quantum algebraic morphism, $\mathbf{M}({}^{P}A)\rightarrow\mathbf{y}[{}^{P}A]\otimes_{\mathcal{C}}\mathbf{M}$, which is an isomorphism.

On the other side, for each quantum measure algebra ${}^{p}L$ in $\mathcal{Q}$ the *counit* is defined as follows:

$$\epsilon_{{}^{p}L}:\mathrm{Hom}_{\mathcal{Q}}(\mathbf{M}(\_),{}^{p}L)\otimes_{\mathcal{C}}\mathbf{M}\rightarrow{}^{p}L.$$

The counit corresponds to the vertical map in the following diagram:

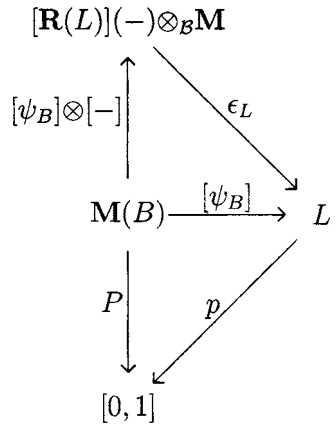


B. Boolean representation

The sheaf-theoretic representation of a quantum measure algebra in terms of Boolean measure localization systems is formulated in terms of the following proposition, effectuated by means of the vertical counit map in the preceding diagram.

The representation of a quantum measure algebra ${}^{p}L$ in $\mathcal{Q}$, in terms of a coordinatization system of Boolean measure algebra localizations **S**, consisting of Boolean probability coefficients, is full and faithful, if and only if the counit of the established adjoint relation, restricted to that system, is an isomorphism, that is, structure-preserving, 1-1 and onto.

It is easy to see that the counit of the adjunction, restricted to a system of Boolean measure algebra localizations is a quantum algebraic isomorphism, iff the right adjoint functor is full and faithful, or equivalently, iff the cocone from the functor $\mathbf{M}\circ\int_{\mathbf{R}({}^{p}L)}$ to the quantum measure algebra ${}^{p}L$ is universal for each ${}^{p}L$ in $\mathcal{Q}$. In the latter case we characterize the Boolean measure coefficients functor $\mathbf{M}:\mathcal{C}\rightarrow\mathcal{Q}$, a proper modeling functor. As a consequence if we consider as $\mathcal{B}$ the category of Boolean subalgebras of a quantum event algebra L of ordinary quantum mechanics, that is an orthomodular σ-orthoposet of orthogonal projections of a Hilbert space, together with a proper modeling inclusion functor $\mathbf{M}:\mathcal{B}\rightarrow\mathcal{L}$, such that the diagram to follow commutes, the counit of the established adjunction restricted to a system of Boolean localizations is an isomorphism



$$\epsilon_L : \mathbf{R}(L)\otimes_{\mathcal{B}}\mathbf{M}\rightarrow^{\cong}L$$

$$\epsilon_L{:}\mathbf{R}(L)\otimes_{\mathcal{B}}\mathbf{M}\rightarrow^{\cong}L$$

such that

$$[\psi_B] = \epsilon_L \circ ([\psi_B] \otimes \_)$$

or in the notation of elements equivalently:

$$\epsilon_L([\psi_B] \otimes a) = [\psi_B](a), \quad a \in \mathbf{M}(B),$$

where $p([\psi_B](a))=(P(a))$, for all $[\psi_B]{:}\mathbf{M}(B)\rightarrow L$ according to the above-presented commutative diagram.

IX. CONCLUSIONS

The primary physical motivation of this paper has been the implementation and explicit construction of an appropriate localization process suited to quantum physical observation, and in particular, the study of its consequences referring to the interpretation of quantum probabilistic structures. The crucial ideas and techniques related to the objective of interpreting quantum measure algebras sheaf-theoretically in the topos-theoretic environment of Grothendieck sites are based on extension and elaboration of previous works of the author, communicated, both conceptually and technically, in the literature.[23–27] The defining characteristic of the topos-theoretic perspective enunciated by the author in this endeavor has been the change of resolution focus form point-set to variable topological localization models of quantum algebraic structures, which effectively induce a transition in the semantics of global quantum event observable and probability algebras from a set-theoretic to a sheaf-theoretic one. The significance and semantic differentiation of this work in relation to the foundations of quantum theory can be cast in the form of the following statements:

1. Conceptually, the physical meaning of the notion of localization is being disassociated from its restricted spatial connotation reference context. We have argued that this is an essential and necessary reconceptualization of the meaning of locality in relational information terms forced by the quantum description of physical systems.
2. A suitable localization process of global quantum event and probabilistic structures that respects the premises of the quantum theory of measurement is being formulated in terms of Boolean localization systems, described categorically in terms of an appropriate Grothendieck topology, which incorporate the constitutive requirements of the notion of Boolean localization in functorial relational terms.

3. Global quantum event and probabilistic structures are being functionally and functorially dependent on generalized topological localization measures induced by the preparation of Boolean structured domains of measurement, not necessarily based on the existence of an underlying set-theoretic structure of points on the real line.
4. The sheaf-theoretic semantic transition of quantum measure algebras has been forced by means of gluing cocycle conditions over an explicitly constructed uniform and homologous fibered representation of quantum states with respect to local Boolean reference frames for the Grothendieck topology of epimorphic families. According to this representation, quantum states have been conceptualized as equivalence classes of local Boolean coordinates with respect to those reference frames. Subsequently, an isomorphic representation of quantum measure algebras with colimits taken in the categories of elements of sheaves of Boolean reference frames has been constructed.
5. The physical significance of the sheaf-theoretic representation of quantum measure algebras is encapsulated in the realization that the whole information content of a quantum measure algebra is preserved by the action of some covering system, if and only if that system forms a Boolean localization system. Hence, the significance of a quantum measure algebra is shifted from the orthoposet axiomatization at the level of events, to the sheaf-theoretic gluing conditions at the level of Boolean localization systems.
6. The preservation of quantum information property according to the above is being formally established by the counit of the related adjunction isomorphism. More specifically, the surjective property of the counit guarantees that the Boolean localization measures, representing objects in the category of elements of the sheaf $\int(\mathbf{R}(^{p}L),\mathcal{C})$, cover entirely a quantum measure algebra ^{p}L, whereas its injective property guarantees that any two covers are compatible in a system of localizations. Moreover, since the counit is also a homomorphism, it preserves the algebraic structure.
7. The physical content of the sheaf-theoretic representation of quantum events algebras can be formulated in terms of a functoriality property. According to this, the information content of a quantum measure algebra is covariant under the groupoid of gluing isomorphisms between overlapping local Boolean reference frames, along their intersections, in a Boolean localization system.
8. In the physical state of affairs, each cover corresponds to a Boolean measure algebra of events realized locally (with respect to the Grothendieck topology of epimorphic families) in a measurement situation. The equivalence classes of local Boolean measure coefficients represent quantum states in ^{p}L, via the sheaf-theoretic pullback compatibility conditions. In this sense, the notion of quantum probability is basically classical when interpreted locally *à la Grothendieck*. Moreover, the probabilities of actualization of events in equivalent local measurement environments are equal.
9. Conclusively, the structure of a quantum measure algebra is being generated by the information that its structure preserving morphims, encoded as Boolean covers in localization systems carry, as well as their compatibility relations. Most significantly, the same compatibility conditions provide the necessary relations for understanding a system of localizations for a quantum probabilistic structure, as a structure sheaf of Boolean measure coefficients associated with local contexts of measurement.

Finally, it would be instructive to comment briefly on the possible implications of the proposed topos-theoretic interpretation schema of quantum structures, based on a reconceptualization of the notion of physical localization, in relation to the ongoing research on quantum relativity and quantum gravity. A preliminary account of the attempt to establish a connective link with the conception of a categorical theory of covariant quantum gravitational dynamics based on the utilization of topological localization systems in the physical "continuum" is in the phase of intense development, while some basic ideas and results related with this program have already been communicated.[28] In the context of that work we initiate a sheaf-theoretic dynamical analysis of quantum observable structures by synthesizing the flexible categorical machinery of Grothendieck topoi, together with the powerful sheaf-theoretic methodology of Mallios's abstract differential geometry.[18]

The crucial physical issue incorporated in the idea of generalized topological localization processes, conceived in the sense of Grothendieck topologies on a base category of structured reference contexts, is related to a novel topos-theoretic conception of the physical "continuum." According to this conception the quantum regime of observable dynamical phenomena should be understood in functorial terms of categorically localized information, and not in the restricted classical localization terms conceived by means of metrical properties on a pre-existing smooth set-theoretic spacetime manifold. Subsequently, that semantic transition can be implemented conceptually and technically by the replacement of the classical variable metrical ruler of localization on a smooth background spacetime manifold, with a variable sheaf-cohomological ruler of categorical localization in a Grothendieck topos, that captures the relational information of observables in the quantum regime, filtered through local reference frames in that topos. Then, the dynamical properties of quantum structures can be addressed to the global topos-theoretic dynamics generated by interlocking diagrams of local frames in that topos, giving rise to generalized De Rham complexes of sheaves encapsulating cohomologically the corresponding dynamical behavior.

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Galois quantum systems, irreducible polynomials and Riemann surfaces

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Finite quantum systems in which the position and momentum take values in the Galois field GF(p^ℓ), are studied. Ideas from the subject of field extension are transferred in the context of quantum mechanics. The Frobenius automorphisms in Galois fields lead naturally to the "Frobenius formalism" in a quantum context. The Hilbert space splits into "Frobenius subspaces" which are labeled with the irreducible polynomials associated with the $y^{p^\ell}-y$. The Frobenius maps transform unitarily the states of a Galois quantum system and leave fixed all states in some of its Galois subsystems (where the position and momentum take values in subfields of GF(p^ℓ)). An analytic representation of these systems in the ℓ-sheeted complex plane shows deeper links between Galois theory and Riemann surfaces. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2345111]

I. INTRODUCTION

Quantum systems with finite-dimensional Hilbert spaces were studied originally by Weyl[1] and Schwinger,[2] and later by many authors (for a review with an extensive list of references see Ref. 3). In this case the position and momentum take values in the ring $\mathcal{Z}_d$ (the integers modulo d) and the phase space of the system is the toroidal lattice $\mathcal{Z}_d\times\mathcal{Z}_d$. We can try to develop a phase space formalism which is similar to the one for the harmonic oscillator. For example, we can define displacements and show that they form a Heisenberg-Weyl group.

An important class of transformations in the harmonic oscillator $R\times R$ phase space are the symplectic Sp$(2,R)$ transformations. Apart from their theoretical importance, they are intimately related to more practical areas like squeezing and quantum tomography in quantum optics. In finite quantum systems, the $\mathcal{Z}_d\times\mathcal{Z}_d$ phase space is in general a collection of points with no geometrical structure and we cannot define symplectic transformations. The root of these difficulties is that $\mathcal{Z}_d$ is a ring. However when d is the power of a prime number p (i.e., $d=p^\ell$) the $\mathcal{Z}_d$ (with appropriate multiplication rule) becomes the Galois field GF(p^ℓ). We call them Galois quantum systems. In this case the phase space is a finite geometry[4] and we can define the group of symplectic transformations Sp$(2,GF(p^\ell))$.[5–7]

There are some other remarkable properties of the Galois quantum systems. Mutually unbiased bases are important in quantum information processing and have been studied extensively in the last few years.[8–18] It is known that the number of such bases cannot exceed $d+1$; and it is also known that for systems where d is the power of a prime, the number of such bases is indeed $d+1$. Similar ideas appear in the so-called "mean king's problem."[19–21] Applications of these ideas to quantum coding have been discussed in Refs. 22 and 23.

A central concept in a Galois field is the Frobenius automorphisms which leave fixed all elements in some of its subfields. Galois quantum systems inherit the properties of Galois fields and in this paper we develop a "Frobenius formalism" in a quantum context. Preliminary work in this direction has been presented in Ref. 7 for the case where ℓ is a prime number. In this simple case there is only one proper subfield of GF(p^ℓ) which is the $\mathcal{Z}_p$ and we get a two layer structure.

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Here we consider the more complicated case of general ℓ and get a multilayer structure. In order to do this we first construct a labeling method for the irreducible polynomials associated with the $y^{p^\ell}-y$. To each irreducible polynomial corresponds a Frobenius subspace comprised of position states labeled with the Galois conjugates corresponding to this polynomial. We then introduce the Frobenius transformations $\mathcal{G}$ which leave these subspaces invariant. The powers of $\mathcal{G}$ form a cyclic group of order ℓ. We explain how the Frobenius transformations leave fixed all states in Galois subsystems (where the position and momentum take values in subfields of GF(p^ℓ)).

There are deep connections between Riemann surfaces and Galois theory. Roughly speaking, the multivaluedness in coverings of Riemann surfaces can be related to the Galois conjugates. An example of this relationship has been discussed in Ref. 24, in a very different context from ours. Here we introduce an analytic representation of Galois quantum systems in the ℓ-sheeted complex plane. We show how various aspects of the Frobenius transformations are elegantly expressed in the language of analytic functions.

II. GALOIS FIELDS

We consider the Galois field GF(p^ℓ). The elements of the Galois field GF(p^ℓ) can be written as polynomials

$$\alpha=\alpha_0+\alpha_1\epsilon+\cdots+\alpha_{\ell-1}\epsilon^{\ell-1},\quad \alpha_0,\alpha_1,\ldots,\alpha_{\ell-1}\in\mathcal{Z}_p. \tag{1}$$

These polynomials are defined modulo an irreducible polynomial of degree ℓ:

$$P(\epsilon)\equiv c_0+c_1\epsilon+\cdots+c_{\ell-1}\epsilon^{\ell-1}+\epsilon^{\ell},\quad c_0,c_1,\ldots,c_{\ell-1}\in\mathcal{Z}_p. \tag{2}$$

Different irreducible polynomials of the same degree ℓ lead to isomorphic finite fields.

The α, $\alpha^p,\ldots,\alpha^{p^{\ell-1}}$ are Galois conjugates. The trace of α is defined as

$$\mathrm{Tr}(\alpha)=\alpha+\alpha^p+\cdots+\alpha^{p^{\ell-1}},\quad \mathrm{Tr}(\alpha)\in\mathcal{Z}_p. \tag{3}$$

All conjugates have the same trace. Elements of the base field $\mathcal{Z}_p$ are Galois self-conjugates.

As in Ref. 7, for practical calculations we introduce the $\ell\times\ell$ matrices

$$g_{\lambda\kappa}\equiv\mathrm{Tr}(\epsilon^{\lambda+\kappa}),\quad G\equiv g^{-1},\quad g_{\lambda\kappa},G_{\lambda\kappa}\in\mathcal{Z}_p. \tag{4}$$

We also introduce a dual basis $E_0,E_1,\ldots,E_{\ell-1}$, as follows:

$$E_\kappa=\sum_\lambda G_{\kappa\lambda}\epsilon^\lambda,\quad \mathrm{Tr}(\epsilon^\kappa E_\lambda)=\delta_{\kappa\lambda}. \tag{5}$$

A number $\alpha\in\mathrm{GF}(p^\ell)$ can be expressed in the two bases as

$$\begin{gathered}\alpha=\sum_{\lambda=0}^{\ell-1}\alpha_\lambda\epsilon^\lambda=\sum_{\lambda=0}^{\ell-1}\overline{\alpha_\lambda}E_\lambda,\\ \alpha_\lambda=\mathrm{Tr}[\alpha E_\lambda];\quad \overline{\alpha_\lambda}=\mathrm{Tr}[\alpha\epsilon^\lambda].\end{gathered} \tag{6}$$

We refer to α_λ and $\overline{\alpha_\lambda}$ as the components and dual components of α, correspondingly. They are related as follows:

$$\alpha_\lambda=\sum_\kappa G_{\lambda\kappa}\overline{\alpha_\kappa},\quad \overline{\alpha_\lambda}=\sum_\kappa g_{\lambda\kappa}\alpha_\kappa. \tag{7}$$

The trace of the product $\alpha\beta$ is given in terms of the components of these numbers as

$$\mathrm{Tr}(\alpha\beta)=\sum_{\lambda,\kappa}g_{\lambda\kappa}\alpha_\lambda\beta_\kappa=\sum_{\lambda,\kappa}G_{\lambda\kappa}\overline{\alpha_\lambda}\overline{\beta_\kappa}=\sum_\lambda\alpha_\lambda\overline{\beta_\lambda}=\sum_\lambda\overline{\alpha_\lambda}\beta_\lambda. \tag{8}$$

We also introduce the $\ell \times \ell$ matrix $\mathcal{C}$ with elements in $\mathcal{Z}_p$, through the relations:

$$\epsilon^{\mu p} = \sum_{\kappa=0}^{\ell-1} \epsilon^{\kappa} \mathcal{C}_{\kappa\mu}. \tag{9}$$

κ, μ take values from 0 to $\ell-1$. We can show that

$$\mathcal{C}^{\ell} = \mathbf{1}, \quad \mathcal{C}_{\kappa 0} = \delta(\kappa, 0), \tag{10}$$

where δ is the Kronecker delta. The conjugates of an arbitrary number α can now be written in terms of its components as

$$\alpha^{p^{\lambda}} = \sum_{\kappa,\mu} \epsilon^{\kappa} (\mathcal{C}^{\lambda})_{\kappa\mu} \alpha_{\mu}. \tag{11}$$

A. Characters

We consider the following complex-valued function which is an additive character in GF(p^{ℓ}):

$$\chi(\alpha) = \omega[\mathrm{Tr}(\alpha)], \quad \chi(\alpha)\chi(\beta) = \chi(\alpha + \beta), \tag{12}$$

where

$$\omega = \exp\left(i\frac{2\pi}{p}\right), \quad \omega(m) \equiv \omega^{m}, \quad m \in \mathcal{Z}_p. \tag{13}$$

We can easily show that for $n, m, r \in \mathrm{GF}(p^{\ell})$:

$$\frac{1}{p^{\ell}} \sum_{n} \omega[\mathrm{Tr}(nm - nr)] = \delta(m, r). \tag{14}$$

A more general relation is

$$\frac{1}{p^{\ell}} \sum_{n} \omega[\mathrm{Tr}(nm - n^{p^{\lambda}} r)] = \delta(m, r^{p^{\ell-\lambda}}) = \delta(m^{p^{\lambda}}, r). \tag{15}$$

We can also rewrite this in terms of the components of the $m^{p^{\lambda}}, r$:

$$\delta(m^{p^{\lambda}}, r) = \prod_{\kappa=0}^{\ell-1} \delta\left(\sum_{\mu} (\mathcal{C}^{\lambda})_{\kappa\mu} m_{\mu}, r_{\kappa}\right). \tag{16}$$

B. Labeling of the irreducible polynomials

The Frobenius map

$$\sigma: \alpha \to \alpha^{p}, \quad \sigma^{\ell} = \mathbf{1} \tag{17}$$

defines an automorphism in GF(p^{ℓ}). It maps the Galois conjugates to each other and leave all elements of the base field $\mathcal{Z}_p$ fixed. The Frobenius map can be written in terms of the components of α and α^{p} as

$$\sigma: \alpha_{\kappa} \to \sum_{\mu} \mathcal{C}_{\kappa\mu} \alpha_{\mu}. \tag{18}$$

The

$$\Sigma_1 = \{\mathbf{1}, \sigma, \ldots, \sigma^{\ell-1}\} \tag{19}$$

form the Galois group which is a cyclic group of order ℓ. It comprises all automorphisms of GF(p^ℓ) which leaves the elements of the subfield $\mathcal{Z}_p$ fixed.

The product

$$f(y) \equiv (y-\alpha)(y-\alpha^p)\cdots(y-\alpha^{p^{d-1}}) \tag{20}$$

involves all the Galois conjugates and is an irreducible polynomial of degree d in $\mathcal{Z}_p[y]$ (the polynomials with coefficients in $\mathcal{Z}_p$). It is known that the number of such irreducible polynomials of degree d is given in terms of the Möbius μ-function as

$$n(d,p) = \frac{1}{d}\sum_{e|d} \mu(e) p^{d/e}, \tag{21}$$

where the summation is over all e which are divisors of d (we denote this as $e|d$). It is easily seen that

$$n(1,p) = p. \tag{22}$$

We label the various irreducible polynomials of degree d as $f_{d\kappa}(y)$ where κ takes values from 1 to $n(d,p)$. The product of all distinct irreducible polynomials in $\mathcal{Z}_p[y]$ of degree d, where d is a divisor of ℓ, is

$$\prod_{d|\ell} \prod_{\kappa=1}^{n(d,p)} f_{d\kappa}(y) = y^{p^\ell} - y. \tag{23}$$

From the degrees of these polynomials we easily show that

$$\sum_{d|\ell} d n(d,p) = p^\ell. \tag{24}$$

We call $\mathfrak{q}_\ell$ the number of divisors of ℓ and we write them in ascending order as

$$d_1 = 1 < d_2 < \cdots < d_{\mathfrak{q}_{\ell-1}} < d_{\mathfrak{q}_\ell} = \ell\ . \tag{25}$$

We introduce the

$$w(\ell,d,p) = \sum_{d_i<d} n(d_i,p). \tag{26}$$

Here the summation is over all divisors d_i of ℓ (given in Eq. (25)), which are smaller than d.

The total number of irreducible polynomials entering in the factorization of $y^{p^\ell}-y$ in Eq. (29) is

$$\mathfrak{M}(\ell,p) = \sum_{d|\ell} n(d,p). \tag{27}$$

Therefore an alternative labeling system for these polynomials is to use a single index $\mathfrak{N}$:

$$f_{\mathfrak{N}}(y) \equiv f_{d\kappa}(y), \quad \mathfrak{N} = 1, \ldots, \mathfrak{M}(\ell,p). \tag{28}$$

There is one-to-one map between the (d,κ) and $\mathfrak{N}$. When (d,κ) are given we calculate the corresponding $\mathfrak{N}$ as

$$\mathfrak{N} = w(\ell,d,p) + \kappa. \tag{29}$$

When the $\mathfrak{N}$ is given we can calculate the corresponding (d,κ) by finding the *largest* d_i among the divisors of ℓ (in Eq. (25)), such that the $w(\ell,d_i,p)$ is smaller than $\mathfrak{N}$ and then

$$d = d_{i+1}, \quad \kappa = \mathfrak{N} - w(\ell, d_i, p). \tag{30}$$

We introduce a notation which indicates for each number m in the Galois field GF(p^ℓ) the corresponding irreducible polynomial $f_{d\kappa}(y)$. We stress that this depends on the choice of the irreducible polynomial $P(\epsilon)$ in Eq. (2); but different choices lead to isomorphic results. We first take any of the d Galois conjugates corresponding to $f_{d\kappa}(y)$, and denote it as $m(d,\kappa,1)$. We then denote the rest of them as

$$m(d,\kappa,\nu) = [m(d,\kappa,1)]^{p^{\nu-1}}, \quad \kappa = 1, \ldots, n(d,p), \quad \nu = 1, \ldots, d. \tag{31}$$

The index ν labels the various Galois conjugates corresponding to a given irreducible polynomial $f_{d\kappa}(y)$. In the special case $d=1$ it is easily seen that $m(1,\kappa,1)=\kappa$ where $\kappa \in \mathcal{Z}_p$.

It is clear from our above-presented discussion that an alternative labeling system for these numbers is

$$m(d,\kappa,\nu) = m(\mathfrak{N},\nu), \tag{32}$$

where the relation between (d,κ) and $\mathfrak{N}$ has been given in Eqs. (29) and (30).

C. Subfields

When d is a divisor of ℓ the GF(p^d) is a subfield of GF(p^ℓ). The GF(p^d) contains the Galois conjugates corresponding to all irreducible polynomials $f_{e\kappa}(y)$ where e is a divisor of d. Then:

$$\prod_{e|d} \prod_{\kappa=1}^{n(e,p)} f_{e\kappa}(y) = y^{p^d} - y. \tag{33}$$

The $y^{p^d}-y$ is a divisor of $y^{p^\ell}-y$.

Using the other labeling method of the irreducible polynomials we rewrite Eq. (33) as

$$\prod_{\mathfrak{N}=1}^{\mathfrak{M}(d,p)} f_{\mathfrak{N}}(y) = y^{p^d} - y. \tag{34}$$

When the label $\mathfrak{N}$ takes all values from 1 to $\mathfrak{M}(d,p)$, we get all the irreducible polynomials $f_{\mathfrak{N}}(y)$ contained in $y^{p^d}-y$.

The

$$\Sigma_d = \{\mathbf{1}, \sigma^d, \ldots, \sigma^{\ell-d}\} \tag{35}$$

form a cyclic group of order ℓ/d. It is a subgroup of Σ_1 and comprises all automorphisms of GF(p^ℓ) which leave the elements of the subfield GF(p^d) fixed.

D. Example

We consider the field GF(16). Practical calculations depend on the choice of the irreducible polynomial and we choose $P(\epsilon)=\epsilon^4+\epsilon+1$. The matrices g, G, and $\mathcal{C}$ are in this example:

$$g = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad G = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{C} = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{36}$$

The irreducible polynomials are

$$f_{11}(y)=y,$$

$$f_{12}(y)=y-1,$$

$$\begin{aligned} f_{21}(y)&=y^2+y+1=(y-\epsilon-\epsilon^2)(y-1-\epsilon-\epsilon^2),\\ f_{41}(y)&=y^4+y+1=(y-\epsilon)(y-\epsilon^2)(y-1-\epsilon)(y-1-\epsilon^2),\end{aligned} \tag{37}$$

$$f_{42}(y)=y^4+y^3+y^2+y+1=(y-\epsilon^3)(y-\epsilon^2-\epsilon^3)(y-1-\epsilon-\epsilon^2-\epsilon^3)(y-\epsilon-\epsilon^3),$$

$$f_{43}(y)=y^4+y^3+1=(y-1-\epsilon^3)(y-1-\epsilon^2-\epsilon^3)(y-\epsilon-\epsilon^2-\epsilon^3)(y-1-\epsilon-\epsilon^3).$$

In this case the labeling of the elements of this field introduced in Eq. (31) is as follows:

$$m(1,1,1)=0,\quad m(1,2,1)=1,$$

$$m(2,1,1)=\epsilon+\epsilon^2,\quad m(2,1,2)=1+\epsilon+\epsilon^2,$$

$$m(4,1,1)=\epsilon,\quad m(4,1,2)=\epsilon^2,\quad m(4,1,3)=1+\epsilon,\quad m(4,1,4)=1+\epsilon^2, \tag{38}$$

$$m(4,2,1)=\epsilon^3,\quad m(4,2,2)=\epsilon^2+\epsilon^3,\quad m(4,2,3)=1+\epsilon+\epsilon^2+\epsilon^3,\quad m(4,2,4)=\epsilon+\epsilon^3,$$

$$m(4,3,1)=1+\epsilon^3,\quad m(4,3,2)=1+\epsilon^2+\epsilon^3,\quad m(4,3,3)=\epsilon+\epsilon^2+\epsilon^3,\quad m(4,3,4)=1+\epsilon+\epsilon^3.$$

It is easy to check that the four elements $m(1,1,1)$, $m(1,2,1)$, $m(2,1,1)$, $m(2,1,2)$ associated to the irreducible polynomials $f_{11}(y)$, $f_{12}(y)$, $f_{21}(y)$, form a subfield which is the GF(4).

III. GALOIS QUANTUM SYSTEMS

A. Finite quantum systems with phase space $\mathcal{Z}_d\times\mathcal{Z}_d$

We consider a quantum system with a d-dimensional Hilbert space $\mathcal{H}$ and an orthonormal basis of "position states" $|\mathcal{X};m\rangle$ where m takes values in the ring $\mathcal{Z}_d$. The Fourier operator is defined as

$$\mathcal{F}=d^{-1/2}\sum_{m=0}^{d-1}\sum_{n=0}^{d-1}\Omega_d(mn)|\mathcal{X};m\rangle\langle\mathcal{X};n|,\quad \mathcal{F}^4=\mathbf{1}, \tag{39}$$

where we use the notation

$$\Omega_d=\exp\left[i\frac{2\pi}{d}\right],\quad \Omega_d(m)\equiv\Omega_d^m,\quad m\in\mathcal{Z}_d. \tag{40}$$

Acting with the Fourier operators on the position states we get the momentum states

$$|\mathcal{P};m\rangle=\mathcal{F}|\mathcal{X};m\rangle=d^{-1/2}\sum_n\Omega_d(mn)|\mathcal{X};n\rangle. \tag{41}$$

Position and momentum operators $\hat{x}$ and $\hat{p}$ are defined as

$$\mathfrak{x} = \sum_{n=0}^{d-1} n|\mathcal{X};n\rangle\langle\mathcal{X};n|, \quad \mathfrak{p} = \mathcal{F}\hat{x}\mathcal{F}^{\dagger} = \sum_{n=0}^{d-1} n|\mathcal{P};n\rangle\langle\mathcal{P};n|. \tag{42}$$

All numbers in $\mathcal{Z}_p$ obey the relation $m^p = m$ and the Cayley-Hamilton theorem can be used to prove that::

$$\mathfrak{x}^p = \mathfrak{x}; \quad \mathfrak{p}^p = \mathfrak{p}. \tag{43}$$

The position-momentum phase space is the toroidal lattice $\mathcal{Z}_d \times \mathcal{Z}_d$ and in it we define displacement operators which form the Heisenberg-Weyl group:

$$\mathcal{Z} = \Omega_d^{\mathfrak{x}} = \sum_{n=0}^{d-1} \Omega_d(n)|\mathcal{X};n\rangle\langle\mathcal{X};n|,$$

$$\mathcal{X} = \Omega_d^{-\mathfrak{p}} = \sum_{n=0}^{d-1} \Omega_d(-n)|\mathcal{P};n\rangle\langle\mathcal{P};n|, \tag{44}$$

$$\mathcal{X}^d = \mathcal{Z}^d = \mathbf{1}, \quad \mathcal{X}^\beta\mathcal{Z}^\alpha = \mathcal{Z}^\alpha\mathcal{X}^\beta\Omega_d(-\alpha\beta), \quad \alpha,\beta \in \mathcal{Z}_d.$$

General displacement operators are defined as

$$\mathcal{D}(\alpha,\beta) = \mathcal{Z}^\alpha\mathcal{X}^\beta\Omega_d(-2^{-1}\alpha\beta). \tag{45}$$

B. Galois quantum systems with phase space GF(p^ℓ)×GF(p^ℓ)

We next consider the case that d is a prime p in which case $\mathcal{Z}_p$ is a Galois field and the phase space $\mathcal{Z}_p \times \mathcal{Z}_p$ is a finite geometry. This is an example of a Galois quantum system. Following Ref. 7 we construct bigger Galois quantum systems with dimension p^ℓ by considering the tensor product

$$H = \mathcal{H} \otimes \cdots \otimes \mathcal{H} \tag{46}$$

of ℓ such spaces. We use calligraphic letters for operators and states on the various p-dimensional Hilbert spaces $\mathcal{H}$; and ordinary letters for operators and states on the p^ℓ-dimensional Hilbert space H.

The position states in H are labeled with $m \in \mathrm{GF}(p^\ell)$:

$$|X;m\rangle \equiv |\mathcal{X};m_0\rangle \otimes \cdots \otimes |\mathcal{X};m_{\ell-1}\rangle. \tag{47}$$

The system is in the position state $m = m_0 + m_1\epsilon + \cdots + m_{\ell-1}\epsilon^{\ell-1}$ when its first component is in the position state m_0, its second component in the position state m_1, etc.

The Fourier transform is given by

$$F = (p^\ell)^{-1/2}\sum_{m,n} \omega[\mathrm{Tr}(mn)]|X;m\rangle\langle X;n|, \quad F^4 = \mathbf{1}, \tag{48}$$

where $\omega = \Omega_p$ (see also Eq. (13)). We note that F is different from the operator $\mathcal{F}\otimes\cdots\otimes\mathcal{F}$ which performs independent Fourier transforms on each of the component systems. A Galois quantum system with Hilbert space H, Fourier transform F, and positions (and momenta) in GF(p^ℓ) has much more structure than a "simple" tensor product system which has the same Hilbert space H, Fourier transform $\mathcal{F}\otimes\cdots\otimes\mathcal{F}$ and positions (and momenta) in $\mathcal{Z}_p \times \cdots \times \mathcal{Z}_p$. An element m of the Galois field GF(p^ℓ) is *not* just an ℓ-dimensional vector $(m_0,\ldots,m_{\ell-1})$; there is a lot of extra structure related to the Galois multiplication. And this enters in the Fourier transform Fwhich uses

the trace of the Galois product mn and which according to Eq. (8) is $\Sigma g_{\lambda\kappa} m_\lambda n_\kappa$. In contrast, the Fourier transform $\mathcal{F}\otimes\cdots\otimes\mathcal{F}$ uses the $\Sigma m_\lambda n_\lambda$:

$$F=(p^\ell)^{-1/2}\sum_{m,n}\omega\Big[\sum g_{\lambda\kappa}m_\lambda n_\kappa\Big]|\mathcal{X};m_0\rangle\langle\mathcal{X};n_0|\otimes\cdots\otimes|\mathcal{X};m_{\ell-1}\rangle\langle\mathcal{X};n_{\ell-1}|,$$
$$\mathcal{F}\otimes\cdots\otimes\mathcal{F}=(p^\ell)^{-1/2}\sum_{m,n}\omega\Big[\sum m_\lambda n_\lambda\Big]|\mathcal{X};m_0\rangle\langle\mathcal{X};n_0|\otimes\cdots\otimes|\mathcal{X};m_{\ell-1}\rangle\langle\mathcal{X};n_{\ell-1}| \tag{49}$$

Momentum states are defined as

$$|P;m\rangle=F|X;m\rangle=(p^\ell)^{-1/2}\sum_n\omega[\mathrm{Tr}(mn)]|X;n\rangle=|\mathcal{P};\overline{m_0}\rangle\otimes\cdots\otimes|\mathcal{P};\overline{m}_{\ell-1}\rangle. \tag{50}$$

The dual components $\overline{m_i}$ of m enter in the momentum states, while the components m_i enter in the position states.

The position and momentum operators are given by

$$\hat{x}=\sum_m m|X;m\rangle\langle X;m|,\quad \hat{p}=F\hat{x}F^\dagger=\sum_m m|P;m\rangle\langle P;m|. \tag{51}$$

All numbers in $\mathrm{GF}(p^\ell)$ obey the relation $m^{p^\ell}=m$ and the Cayley–Hamilton theorem can be used to prove that

$$\hat{x}^{p^\ell}=\hat{x},\quad \hat{p}^{p^\ell}=\hat{p}. \tag{52}$$

C. Displacements in Galois quantum systems

Displacement operators in Galois quantum systems have been discussed in Ref. 7. They are given by

$$Z^\alpha=\sum_n\omega[\mathrm{Tr}(\alpha n)]|X;n\rangle\langle X;n|,$$
$$X^\beta=\sum_n\omega[-\mathrm{Tr}(\beta n)]|P;n\rangle\langle P;n|, \tag{53}$$

where $\alpha,\beta\in\mathrm{GF}(p^\ell)$. We can show that

$$Z^\alpha|P;m\rangle=|P;m+\alpha\rangle,\quad Z^\alpha|X;m\rangle=\omega[\mathrm{Tr}(\alpha m)]|X;m\rangle, \tag{54}$$

$$X^\beta|P;m\rangle=\omega[-\mathrm{Tr}(m\beta)]|P;m\rangle,\quad X^\beta|X;m\rangle=|X;m+\beta\rangle, \tag{55}$$

and also that

$$X^\beta Z^\alpha=Z^\alpha X^\beta\omega[-\mathrm{Tr}(\alpha\beta)]. \tag{56}$$

The displacement operators form a Heisenberg-Weyl group.

General displacement in the $\mathrm{GF}(p^\ell)\times\mathrm{GF}(p^\ell)$ phase space is defined as

$$D(\alpha,\beta)=Z^\alpha X^\beta\omega\Big[-\tfrac{1}{2}\,\mathrm{Tr}(\alpha\beta)\Big]. \tag{57}$$

The displacement operators acting on H are expressed in terms of the displacement operators $\mathcal{D}$ acting on the various components of the system as

$$D(\alpha,\beta)=\mathcal{D}(\overline{\alpha_0},\beta_0)\otimes\cdots\otimes\mathcal{D}(\overline{\alpha}_{\ell-1},\beta_{\ell-1}). \tag{58}$$

Here $\overline{\alpha_i}$ are the dual components of α and β_i are the components of β as in Eq. (6).

IV. FROBENIUS FORMALISM

A. Frobenius subspaces

We split the Hilbert space H into subspaces, each of which is spanned by conjugate position states, i.e., position states labeled with Galois conjugate numbers. All Galois conjugates correspond to a particular irreducible polynomial and we label each of these subspaces with the indices of the corresponding irreducible polynomial. For the irreducible polynomial $f_{d\kappa}(y)$ we consider the d-dimensional space

$$\mathfrak{H}_{d\kappa} = \text{span}\{|X;m(d,\kappa,1)\rangle, |X;m(d,\kappa,2)\rangle, \ldots, |X;m(d,\kappa,d)\rangle\}. \tag{59}$$

We have explained earlier that d is a divisor of ℓ and takes $\mathfrak{q}_\ell$ values; and that κ takes $n(d,p)$ values. An alternative to the indices (d,κ) is the index $\mathfrak{N}$ as explained in Eqs. (29) and (30). Therefore Eq. (59) can be rewritten as

$$\mathfrak{H}_{\mathfrak{N}} = \text{span}\{|X;m(\mathfrak{N},1)\rangle, |X;m(\mathfrak{N},2)\rangle, \ldots, |X;m(\mathfrak{N},d)\rangle\}. \tag{60}$$

We call $\pi_{d\kappa}$ (or $\pi_{\mathfrak{N}}$) the projection operators to the spaces $\mathfrak{H}_{d\kappa}$. In the special case $d=1$ we have p one-dimensional spaces $\mathfrak{H}_{1\kappa}$ and

$$\pi_{1\kappa} = |X;\kappa\rangle\langle X;\kappa|, \quad \kappa \in \mathcal{Z}_p. \tag{61}$$

The spaces $\mathfrak{H}_{d\kappa}$ have been defined with respect to position states. If we use the states $U|X;m\rangle$ where U is any unitary operator we will get different Frobenius subspaces which we denote as $U\mathfrak{H}_{d\kappa}$. For example, the Frobenius subspaces with respect to momentum states are $F\mathfrak{H}_{d\kappa}$ and they are different from $\mathfrak{H}_{d\kappa}$. Only in the special case the U commutes with $\pi_{d\kappa}$, the spaces $U\mathfrak{H}_{d\kappa}$ and $\mathfrak{H}_{d\kappa}$ are the same:

$$[U,\pi_{d\kappa}] = 0 \rightarrow U\mathfrak{H}_{d\kappa} = \mathfrak{H}_{d\kappa}. \tag{62}$$

We call $\overline{\mathfrak{H}}_d$ the Hilbert space which is the direct sum of all $\mathfrak{H}_{d\kappa}$:

$$\overline{\mathfrak{H}}_d = \bigoplus_{\kappa=1}^{n(d,p)} \mathfrak{H}_{d\kappa} = \bigoplus_{\mathfrak{N}=w(\ell,d,p)+1}^{w(\ell,d,p)+n(d,p)} \mathfrak{H}_{\mathfrak{N}}, \tag{63}$$

where $w(\ell,d,p)$ has been defined in Eq. (26). The dimension of $\overline{\mathfrak{H}}_d$ is $dn(d,p)$. We call $\overline{\pi}_d$ the projection operators to the spaces $\overline{\mathfrak{H}}_d$.

The Frobenius subspace $\mathfrak{H}_{d\kappa}$ is the null space of the corresponding irreducible polynomial operator $f_{d\kappa}(\hat{x})$,

$$f_{d\kappa}(\hat{x})\,\pi_{d\kappa} = 0. \tag{64}$$

B. Galois subsystems

Let d be a divisor of ℓ. We call H_d the Hilbert space which is the direct sum of all $\overline{\mathfrak{H}}_e$ where e is any of the $\mathfrak{q}_d$ divisors of d:

$$H_d = \bigoplus_{e|d} \overline{\mathfrak{H}}_e. \tag{65}$$

This space is spanned by position states labeled with numbers in the subfield $\text{GF}(p^d)$. Indeed we have included here position states labeled with Galois numbers corresponding to all irreducible polynomials $f_{e\kappa}(y)$ where e is a divisor of d; and we have seen in Eq. (33) that they form the subfield $\text{GF}(p^d)$. Therefore the space H_d describes a Galois subsystem. In the special case $d=1$ the space H_1 is p-dimensional and is spanned by position states labeled with integers in $\mathcal{Z}_p$. In the other extreme special case $d=\ell$ it is easily seen that $H_\ell = H$.

We note that the spaces $\mathfrak{H}_{d\kappa}$ and $\overline{\mathfrak{H}}_d$ describe subsystems which are *not* Galois subsystems because the position does not take all values in a Galois subfield.

We call Π_d the projection operator to the space H_d. Then:

$$\Pi_d = \sum_{e|d} \sum_{\kappa=1}^{n(e,p)} \pi_{e\kappa} = \sum_{e|d} \overline{\pi}_e. \tag{66}$$

In the special cases $d=1$ and $d=\ell$ we get

$$\Pi_1 = \sum_{\kappa \in \mathcal{Z}_p} |X;\kappa\rangle\langle X;\kappa|, \quad \Pi_\ell = \mathbf{1}. \tag{67}$$

C. Frobenius transformations

Frobenius transformations in $\mathfrak{H}_{d\kappa}$ are the following unitary transformations:

$$\mathcal{G}_{d\kappa} = \sum_{\nu \in \mathcal{Z}_d} |X;m(d,\kappa,\nu+1)\rangle\langle X;m(d,\kappa,\nu)|,$$
$$\mathcal{G}_{d\kappa}^d = \pi_{d\kappa}. \tag{68}$$

The summation is over all the Galois conjugates corresponding to the irreducible polynomial $f_{d\kappa}$. In the special case $d=1$ we get

$$\mathcal{G}_{1\kappa} = \pi_{1\kappa} = |X;\kappa\rangle\langle X;\kappa|, \quad \kappa \in \mathcal{Z}_p. \tag{69}$$

The $\{\mathbf{1}, \mathcal{G}_{d\kappa}, \mathcal{G}_{d\kappa}^2, \ldots, \mathcal{G}_{d\kappa}^{d-1}\}$ form a cyclic group of order d.

We sum all the transforms $\mathcal{G}_{d\kappa}$ and we get the following unitary transformations in H:

$$\mathcal{G} = \sum_{d,\kappa} \mathcal{G}_{d\kappa}, \quad \mathcal{G}^\ell = \mathbf{1}, \quad [\mathcal{G}, \pi_{d\kappa}] = 0, \quad \mathcal{G}\pi_{d\kappa} = \mathcal{G}_{d\kappa}. \tag{70}$$

As above, d are the divisors of ℓ; and κ takes values from 1 to $n(d,p)$. These transformations are the analogue in the present context of the transformations σ in Eq. (17) for Galois fields, and we call them Frobenius transformations. More general relations than $\mathcal{G}^\ell = \mathbf{1}$ are the following:

$$\mathcal{G}^d \overline{\pi}_d = \overline{\pi}_d, \quad \mathcal{G}^d \Pi_d = \Pi_d. \tag{71}$$

We have explained earlier that the spaces $\mathfrak{H}_{d\kappa}$ have been defined with respect to position states; and that if we use more general states $U|X;m\rangle$ we get different Frobenius subspaces $U\mathfrak{H}_{d\kappa}$. The corresponding Frobenius transformations in these spaces, are $U\mathcal{G}U^\dagger$. Only in the special case

$$[\mathcal{G}, U] = 0 \tag{72}$$

the Frobenius transformations are the same in both sets of Frobenius subspaces $\mathfrak{H}_{d\kappa}$ and $U\mathfrak{H}_{d\kappa}$. An example of this is the Frobenius subspaces $F\mathfrak{H}_{d\kappa}$, with respect to momentum states. Using Eq. (16) we prove that in this case

$$[\mathcal{G}, F] = 0. \tag{73}$$

Therefore the Frobenius transformations are the same in both $F\mathfrak{H}_{d\kappa}$ and $\mathfrak{H}_{d\kappa}$. Acting with $\mathcal{G}^\lambda$ on position and momentum states we get

$$\mathcal{G}^\lambda |X;m\rangle = |X;m^{p^\lambda}\rangle, \quad \mathcal{G}^\lambda |P;m\rangle = |P;m^{p^\lambda}\rangle, \tag{74}$$

where $\lambda \in \mathcal{Z}_\ell$. We can also show that

$$\mathcal{G}^{\lambda}X^{\beta}(\mathcal{G}^{\dagger})^{\lambda}=X^{\beta^{p^{\lambda}}},\quad \mathcal{G}^{\lambda}Z^{\alpha}(\mathcal{G}^{\dagger})^{\lambda}=Z^{\alpha^{p^{\lambda}}} \tag{75}$$

and more generally that

$$\mathcal{G}^{\lambda}D(\alpha,\beta)(\mathcal{G}^{\dagger})^{\lambda}=D(\alpha^{p^{\lambda}},\beta^{p^{\lambda}}). \tag{76}$$

When $m,\alpha,\beta\in\mathcal{Z}_p$ we get

$$\begin{gathered} m\in\mathcal{Z}_p\rightarrow\mathcal{G}^{\lambda}|X;m\rangle=|X;m\rangle,\quad \mathcal{G}^{\lambda}|P;m\rangle=|P;m\rangle,\\ \alpha,\beta\in\mathcal{Z}_p\rightarrow\mathcal{G}^{\lambda}D(\alpha,\beta)(\mathcal{G}^{\dagger})^{\lambda}=D(\alpha,\beta). \end{gathered} \tag{77}$$

From Eqs. (74)–(76) it is tempting to interpret Frobenius transformations as magnifying the "area" of the phase space by a power (from A to $A^{p^{\lambda}}$). We note that the phase space here is *not* a continuum; that magnification is simply one-to-one relabeling; and that $\mathcal{G}^{\ell}=\mathbf{1}$.

The

$$\mathfrak{G}_1=\{\mathbf{1},\mathcal{G},\mathcal{G}^2,\ldots,\mathcal{G}^{\ell-1}\} \tag{78}$$

form a cyclic group of order ℓ whose elements leave fixed all the states in the Galois subsystem described with the space H_1. This is the analogue of the Galois group of Eq. (19) in the present context. If d is a divisor of ℓ the

$$\mathfrak{G}_d=\{\mathbf{1},\mathcal{G}^d,\mathcal{G}^{2d},\ldots,\mathcal{G}^{\ell-d}\} \tag{79}$$

form a cyclic subgroup of $\mathfrak{G}_1$ of order ℓ/d. Its elements leave fixed all states in the Galois subsystem described with the space H_d. This is the analogue of the group Σ_d in Eq. (35). We consider the subfield GF(p^d) of GF(p^{ℓ}). For m,α,β in the subfield GF(p^d) of GF(p^{ℓ}), we get

$$\begin{gathered} m\in GF(p^d)\rightarrow\mathcal{G}^{\lambda d}|X;m\rangle=|X;m\rangle,\quad \mathcal{G}^{\lambda d}|P;m\rangle=|P;m\rangle,\\ \alpha,\beta\in GF(p^d)\rightarrow\mathcal{G}^{\lambda d}D(\alpha,\beta)(\mathcal{G}^{\dagger})^{\lambda d}=D(\alpha,\beta). \end{gathered} \tag{80}$$

V. ANALYTIC REPRESENTATION OF GALOIS QUANTUM SYSTEMS IN RIEMANN SURFACES

Various analytic representations have been used in quantum mechanics (for a review see Ref. 25). Here we show that an analytic representation of quantum states in the space H can be defined in the ℓ-sheeted complex plane. This analytic representation is related to the one discussed in Ref. 26, which was introduced from a Riemann surfaces point of view and did not involve Galois theory. The aim here is to show the conceptual link between the multivaluedness in coverings of Riemann surfaces and the multivaluedness related to the conjugates in Galois theory.

A. Bargmann representation of a harmonic oscillator in the ℓ-sheeted complex plane

We consider a harmonic oscillator described with the infinite-dimensional Hilbert space h. In the number state basis $\{|N\rangle\}$, a general state $|f\rangle$ can be written as

$$|s\rangle=\sum_{N=0}^{\infty}s(N)|N\rangle,\quad \sum_{N=0}^{\infty}|s(N)|^2=1. \tag{81}$$

In the Bargmann representation this state is represented with the function

$$S_1(z) = \sum_{N=0}^{\infty} s(N) z^N (N!)^{-1/2}, \tag{82}$$

which is analytic in the complex plane C. The scalar product of two states $|s\rangle$ and $|q\rangle$ represented with the functions $S_1(z)$ and $Q_1(z)$ is given by

$$\langle q|s\rangle = \int_C d\mu_1(z) \exp(-|z|^2)[Q_1(z)]^* S_1(z), \quad d\mu_1(z) = \frac{dz_R dz_I}{\pi}, \tag{83}$$

where z_R, z_I are the real and imaginary parts of z, correspondingly.

Following Ref. 26 we consider the Riemann surface $C^*/\mathcal{Z}_\ell$ associated with the map $z^{1/\ell}$. Here $C^* = C - \{0\}$ is the punctured complex plane and $\mathcal{Z}_\ell$ the discrete group of transformations

$$z \to \Omega_\ell z, \tag{84}$$

which is isomorphic to the integers modulo ℓ. The covering surface of this Riemann surface is the ℓ-sheeted complex plane with the following cuts T_m and sheets Ξ_m:

$$\begin{aligned} T_m &= \{z = r\Omega_\ell^m; r \geqslant 0\}, \quad m = 0, \ldots, \ell - 1, \\ \Xi_m &= \left\{ z = r \exp(i\phi); r \geqslant 0; \frac{2\pi m}{\ell} < \phi < \frac{2\pi(m+1)}{\ell} \right\}. \end{aligned} \tag{85}$$

The sheet number of a complex number z is defined as

$$\tau(z) = \mathrm{IP}\left(\frac{\ell \arg(z)}{2\pi} \right), \quad \tau(z) \in \mathcal{Z}_\ell, \tag{86}$$

where IP stands for the integer part of the number. We split the Hilbert space h into ℓ subspaces as follows:

$$h = \bigoplus_{m=0}^{\ell-1} h_m, \quad h_m = \mathrm{span}\{|m\rangle, |m + \ell\rangle, |m + 2\ell\rangle, \ldots\}. \tag{87}$$

We call ϖ_m the projection operator to the space h_m. We introduce an analytic representation in the ℓ-sheeted complex plane where the general state $|s\rangle$ of Eq. (81) is represented with the function

$$S_\ell(z) = \sum_{N=0}^{\infty} s(\tau(z) + N\ell) z^{N\ell} (N!)^{-1/2}. \tag{88}$$

We note that in the m-sheet Ξ_m, this function represents only the projection $\varpi_m|s\rangle$ of the state $|s\rangle$ in the subspace h_m. But when we consider the function $S_\ell(z)$ in all the ℓ sheets we get all the projections $\varpi_m|s\rangle$ and therefore the full state $|s\rangle$.

The function $S_\ell(z)$ is analytic in the interior of all sheets Ξ_m and has discontinuities across the cuts T_m given by

$$\Delta_m(z) = \sum_{N=0}^{\infty} [s(m + N\ell) - s(m + N\ell - 1)] z^{\ell N} (N!)^{-1/2}. \tag{89}$$

The scalar product of two states $|s\rangle$ and $|q\rangle$ represented with the functions $S_\ell(z)$ and $Q_\ell(z)$ is given by

$$\langle q|s\rangle = \int_C d\mu_\ell(z)\exp(-|z|^{2\ell})[Q_\ell(z)]^* S_\ell(z), \quad d\mu_\ell(z) = \ell^2|z|^{2(\ell-1)}\frac{dz_R dz_I}{\pi}. \tag{90}$$

More details about this formalism are given in Ref. 26.

B. Analytic representation of Galois quantum systems in the ℓ-sheeted complex plane

We now apply the general formalism of the previous section in our context. We consider a Galois quantum system described with the Hilbert space H. Using the orthonormal basis $|X;m(\mathfrak{N},\nu)\rangle$ which we introduced earlier, we express the general state of this system as

$$|s\rangle = \sum_{\mathfrak{N}=1}^{\mathfrak{M}(\ell,p)} \sum_{\nu=1}^{d} s(\mathfrak{N},\nu)|X;m(\mathfrak{N},\nu)\rangle. \tag{91}$$

In the summation ν takes values from 1 to d (which is given in terms of $\mathfrak{N}$ in Eq. (30)). We will describe how this state is represented by an analytic function, in three steps.

In the first step we consider the projection of this state to the d-dimensional space $\mathfrak{H}_\mathfrak{N}$,

$$\pi_\mathfrak{N}|s\rangle = \sum_{\nu=1}^{d} s(\mathfrak{N},\nu)|X;m(\mathfrak{N},\nu)\rangle. \tag{92}$$

This is represented in the ℓ-sheeted complex plane with the function

$$\mathfrak{S}_\mathfrak{N}(z) = s[\mathfrak{N},\nu=\tau(z)(\mathrm{mod}\ d)]z^{\ell\mathfrak{N}}(\mathfrak{N}\,!\,)^{-1/2}. \tag{93}$$

In the first d sheets we have d functions which represent the d components of this state (for ν equal 1 to d). The fact that $\nu=\tau(z)$ modulo d, implies that there is periodicity in the next d sheets, which continues up to the last d sheets (the d is a divisor of ℓ). Therefore

$$\mathfrak{S}_\mathfrak{N}(z\Omega_\ell^d) = \mathfrak{S}_\mathfrak{N}(z). \tag{94}$$

In the second step we consider the projection of the state $|s\rangle$ to the $dn(d,p)$-dimensional space $\overline{\mathfrak{H}}_d$:

$$\overline{\pi}_d|s\rangle = \sum_{\mathfrak{N}=w(\ell,d,p)+1}^{w(\ell,d,p)+n(d,p)} \sum_{\nu} s(\mathfrak{N},\nu)|X;m(\mathfrak{N},\nu)\rangle, \tag{95}$$

where $w(\ell,d,p)$ has been defined in Eq. (26). This is represented in the ℓ-sheeted complex plane with the function

$$\overline{\mathfrak{S}}_d(z) = \sum_{\mathfrak{N}=w(\ell,d,p)+1}^{w(\ell,d,p)+n(d,p)} \mathfrak{S}_\mathfrak{N}(z) = \sum_{\mathfrak{N}=w(\ell,d,p)+1}^{w(\ell,d,p)+n(d,p)} s[\mathfrak{N},\nu=\tau(z)(\mathrm{mod}\ d)]z^{\ell\mathfrak{N}}(\mathfrak{N}\,!\,)^{-1/2}. \tag{96}$$

As above, d different functions in the first d sheets represent this state and there is periodicity in the rest of the sheets:

$$\overline{\mathfrak{S}}_d(z\Omega_\ell^d) = \overline{\mathfrak{S}}_d(z). \tag{97}$$

We note that Frobenius transformations on the state $\overline{\pi}_d|s\rangle$ are easily implemented in this representation as

$$\mathcal{G}^\kappa\overline{\pi}_d|s\rangle \to \overline{\mathfrak{S}}_d(z\Omega_\ell^\kappa). \tag{98}$$

Then Eq. (97) expresses in this representation the relation $\mathcal{G}^d\overline{\pi}_d=\overline{\pi}_d$ given in Eq. (71).

In the third step we consider the full state $|s\rangle$. It is represented with the function

$$S(z)=\sum_d \overline{\mathfrak{S}}_d(z)=\sum_{\mathfrak{N}=1}^{\mathfrak{M}(\ell,,p)} s[\mathfrak{N},\nu=\pi(z)(\mathrm{mod}\ d)]z^{\ell\mathfrak{N}}(\mathfrak{N}\,!\,)^{-1/2}. \tag{99}$$

The function $S(z)$ is analytic in the interior of all sheets Ξ_m and has discontinuities across the cuts T_m given by

$$\Delta_m(z)=\sum_{\mathfrak{N}=1}^{\mathfrak{M}(\ell,,p)} \{s[\mathfrak{N},\nu=m(\mathrm{mod}\ d)]-s[\mathfrak{N},\nu=m-1(\mathrm{mod}\ d)]\}z^{\ell\mathfrak{N}}(\mathfrak{N}\,!\,)^{-1/2}. \tag{100}$$

The scalar product of two states is given by Eq. (90).

Frobenius transformations on the state $|s\rangle$ are easily implemented in this representation as

$$\mathcal{G}^\kappa|s\rangle\rightarrow S(z\Omega_\ell^\kappa). \tag{101}$$

The relation $\mathcal{G}^\ell=\mathbf{1}$ of Eq. (70), is seen in this representation through the fact that $\Omega_\ell^\ell=1$.

The projection $\Pi_d|s\rangle$ of the state $|s\rangle$ in the space H_d is represented with the function

$$S_d(z)=\sum_{e|d} \overline{\mathfrak{S}}_e(z). \tag{102}$$

The summation is over all divisors e of d. Using Eq. (97) we easily show that

$$S_d(z\Omega_\ell^d)=S_d(z). \tag{103}$$

This expresses in this representation the relation $\mathcal{G}^d\Pi_d=\Pi_d$ given in Eq. (71) which expresses the fact that the transformations of Eq. (79) leave fixed all the states in the Galois subsystem described with the space H_d.

VI. DISCUSSION

In this paper we brought ideas from the subject of field extension in the context of finite quantum systems. Field extension constructs large fields from smaller ones. We have constructed the Hilbert space H as the tensor product of ℓ Hilbert spaces $\mathcal{H}$ and used the Fourier transform of Eq. (48) which contains the trace of the Galois product, and this provides the system with Galois structure.

One important aspect of a Galois theory is the Frobenius automorphisms σ of $\mathrm{GF}(p^\ell)$ which are given in Eq. (17). Powers of these automorphisms leave fixed the elements of the subfield $\mathcal{Z}_p$ and form the cyclic group Σ_1 of Eq. (19) of order ℓ. More generally the powers of σ in Eq. (35) leave fixed the elements of the subfield $\mathrm{GF}(p^d)$ and form the cyclic group Σ_d of order ℓ/d. We have studied in detail the implications of this in our context. We have introduced the Frobenius transformations $\mathcal{G}$ of Eq. (70) and shown that its powers in Eq. (78) leave fixed all the states in the Galois subsystem described with the space H_1 and form the cyclic group $\mathfrak{G}_1$ of order ℓ. More generally the powers of $\mathcal{G}$ in Eq. (79) leave fixed all the states in the Galois subsystem described with the space H_d and form the cyclic group $\mathfrak{G}_d$ of order ℓ/d.

We have also studied an analytic representation of Galois quantum systems in the ℓ-sheeted complex plane. The purpose is to show connections between Riemann surfaces and Galois theory. The basic idea is that multivaluedness in Riemann surfaces can be related to the Galois conjugates. We have seen in Eq. (101) how the Frobenius transformations are implemented in this language; and how the fact that the transformations of Eq. (79) leave fixed all the states in the Galois subsystem described with the space H_d is easily proved using Eq. (103).

Galois fields have previously been used in quantum mechanics with a physical motivation: in order to have well-defined symplectic transformations; or in the context of mutually unbiased bases; or in the context of quantum coding. The present paper studied more mathematical aspects

of this structure and in particular the Frobenius formalism and its links to Riemann surfaces. Potential applications include quantum coding, quantum information processing, the magnetic translation group in condensed matter, quantum chaos, etc.

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Magnetic monopoles in quantum adiabatic dynamics and the immersion property of the control manifold

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It is well known that the Berry phase of a cyclic adiabatic dynamical system appears formally as the flux of a magnetic field in the control parameter manifold. In this electromagnetic picture a level crossing appears as a Dirac magnetic monopole in this manifold. We make an extensive study of the magnetic monopole model of eigenvalue crossings. We show that the properties of the monopole magnetic field in the control manifold are determined by the immersion of the control manifold in a space given by the universal classifying theorem of fiber bundles. We give a detailed illustrative study of the simple but instructive case of a two level crossing of a system controlled by a two-dimensional manifold. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2345473]

I. INTRODUCTION

In 1984, Berry Ref. 1 proved, in the context of the standard adiabatic approximation, that the wave function of a quantum dynamical system takes the form

$$\psi(t) = \exp\left(- i\hbar^{-1} \int_0^t E_a(\vec{R}(t'))\mathrm{d}t' - \int_0^t \langle a,\vec{R}(t')|\partial_{t'}|a,\vec{R}(t')\rangle \mathrm{d}t' \right) |a,\vec{R}(t)\rangle, \tag{1}$$

where E_a is a nondegenerate instantaneous eigenvalue which is isolated from the rest of the Hamiltonian spectrum and has the instantaneous eigenvector $|a,\vec{R}(t)\rangle$. $\vec{R}$ is a set of classical control parameters used to model the time-dependent environment of the system. The set of all configurations of $\vec{R}$ is assumed to form a $\mathcal{C}^\infty$-manifold $\mathcal{M}$. The important result is the presence of an extra phase term $\exp(-\int_0^t \langle a,\vec{R}(t')|\partial_{t'}|a,\vec{R}(t')\rangle \mathrm{d}t')$ called the Berry phase. Simon[2] later found that the mathematical structure which models the Berry phase phenomenon is a principal bundle with base space $\mathcal{M}$ and with structure group U(1). If we eliminate the dynamical phase by a gauge transformation, which involves redefining the eigenvector at each time, then the expression [Eq. (1)) is the horizontal lift of the curve $\mathcal{C}$ described by $t \mapsto \vec{R}(t)$ with gauge potential $A = \langle a,\vec{R}|d_{\mathcal{M}}|a,\vec{R}\rangle$. If $\mathcal{C}$ is closed then the Berry phase $\exp(-\oint_{\mathcal{C}} A) \in \mathrm{U}(1)$ is the holonomy of the horizontal lift.

In 1984, Wilczek and Zee[3] introduced the concept of a non-Abelian Berry phase in the context of the adiabatic approximation. Let $E_a(\vec{R}(t))$ be an M-fold degenerate instantaneous eigenvalue isolated from the rest of the spectrum and $\{|a,i,\vec{R}(t)\rangle\}_{i=1,\ldots,M}$ be an orthonormal basis for the associated eigensubspace. If the initial state is $\psi(0)=|a,i,\vec{R}(0)\rangle$, then the wave function is

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$$\psi(t) = \sum_{j=1}^{M} \exp\left(-i\hbar^{-1} \int_0^t E_a(\vec{R}(t'))\mathrm{d}t' \right) \left[\mathbb{T} e^{-\int_0^t A(\vec{R}(t'))} \right]_{ji} |a, j, \vec{R}(t)\rangle, \tag{2}$$

where the matricial one-form A has the elements $A_{ij} = \langle a, i, \vec{R} | d_{\mathcal{M}} | a, j, \vec{R} \rangle$, and $\mathbb{T}$ is the time-ordering operator. By elimination of the dynamical phase this expression becomes a horizontal lift of the curve $\mathcal{C}$ described by $t \mapsto \vec{R}(t)$ into a principal bundle with base space $\mathcal{M}$ and structure group $\mathrm{U}(M)$. If $\mathcal{C}$ is closed then $\mathbb{P} \exp(-\oint_{\mathcal{C}} A(\vec{R})) \in \mathrm{U}(M)$ is the holonomy of the horizontal lift, $\mathbb{P}$ being the path-ordering operator.

More generally for a quantum dynamical system, let $\{E_a(\vec{R}(t))\}_{a \in I}$ be a set of eigenvalues indexed by I, and isolated from the rest of the spectrum. Suppose that $\psi(0) = |a, \vec{R}(0)\rangle$; the wave function is then

$$\psi(t) = \sum_{b \in I} \left[\mathbb{T} e^{-i\hbar^{-1} \int_0^t E(\vec{R}(t'))\mathrm{d}t' - \int_0^t A(\vec{R}(t'))} \right]_{ba} |b, \vec{R}(t)\rangle, \tag{3}$$

where we have the matrices $E(\vec{R}(t))_{ab} = E_a(\vec{R}(t))\,\delta_{ab}$ and $A(\vec{R})_{ab} = \langle a, \vec{R} | d_{\mathcal{M}} | b, \vec{R} \rangle$. When the matrices E and A do not commute then the mathematical structure which models the non-Abelian phase phenomenon is a principal composite bundle with base space $\mathcal{M} \times \mathbb{R}$, where $\mathbb{R}$ models the time (see Ref. 4).

For each of the three preceding cases, an appropriate gauge potential $A \in \Omega^1(\mathcal{M}, \mathfrak{u}(M))$ has been defined, to be associated with the principal bundle $\mathcal{P}$ with base space $\mathcal{M}$ and with structure group $\mathrm{U}(M)$ (where $M = 1$ for the Berry's orginal case; M is the degenerate order for Wilczek's case, and $M = \mathrm{card} I$ for the general case). In the one-dimensional case, the bundle curvature is defined by $B = d_{\mathcal{M}} A$ and it satisfies the equation $d_{\mathcal{M}} B = 0$. It is easy to prove that this equation is the analog in $\mathcal{M}$ to half of the Maxwell equations. We can then identify B with a magnetic field existing in $\mathcal{M}$ and A with its magnetic potential. In this picture, for any closed curve $\mathcal{C}$ for which there exists a surface $\mathcal{S} \subset \mathcal{M}$ such that $\partial_{\mathcal{M}} \mathcal{S} = \mathcal{C}$, the holonomy term can be written (using the Stokes theorem) as the flux of the magnetic field B through $\mathcal{S}$: $\oint_{\mathcal{C}} A = \int_{\mathcal{S}} B$. By using the expression for A, it is easy to show that

$$B = \mathrm{d}_{\mathcal{M}} A = 2i\mathfrak{I} \frac{\partial \langle a, \vec{R}|}{\partial R^\mu} \frac{\partial |a, \vec{R}\rangle}{\partial R^\nu} \mathrm{d}R^\mu \wedge \mathrm{d}R^\nu. \tag{4}$$

By using the closure relation one can write

$$B = i\mathfrak{I} \sum_{b \neq a} \frac{\langle a, \vec{R} | \partial_\mu H(\vec{R}) | b, \vec{R} \rangle \langle b, \vec{R} | \partial_\nu H(\vec{R}) | a, \vec{R} \rangle}{(E_b(\vec{R}) - E_a(\vec{R}))^2} \mathrm{d}R^\mu \wedge \mathrm{d}R^\nu, \tag{5}$$

where $H(\vec{R})$ is the system Hamiltonian. We cannot strictly apply the one-dimensional adiabatic approximation if the eigenvalue E_a is not isolated from the rest of the spectrum. Nevertheless, the formal use of this approximation in the case where two eigenvalues E_a and E_c cross at $\vec{R}_{ac} \in \mathcal{M}$, produces the result $B(\vec{R}_{ac}) = +\infty$. This magnetic field divergence must be interpreted as a magnetic monopole at $\vec{R}_{ac}$ in $\mathcal{M}$. In the M-dimensional case the field defined by the Cartan structure equation $F = d_{\mathcal{M}} A + \frac{1}{2}[A, A]$ satisfies the Bianchi identity $d_{\mathcal{M}} F + [A, F] = 0$. The Bianchi identity is analogous in $\mathcal{M}$ to half of the Yang-Mills equations. The eigenvalue crossings then appear as non-Abelian monopoles (so-called colored monopoles in the case where the structure group is SU(3), see Refs. 5 and 6), as has already been pointed by Wilczek and Zee.[3]

This paper studies the properties of the adiabatic magnetic monopoles, with special attention to the monopole magnetic field distribution in $\mathcal{M}$ and on the apparent charge of the monopole. We show that these properties are determined by the immersion of $\mathcal{M}$ in a universal space associated with the topology of the adiabatic bundle.

The concept of the virtual magnetic monopole is today very important for nonrelativistic quantum physics. In 1986, Moody *et al.*[7] showed the possibility of realizing a magnetic monopole via the precession of a diatomic molecule. Fang *et al.*[8] showed that a trapped Λ-type atom induced a magnetic monopole. Recently Zhong *et al.*[9,10] observed experimentally a magnetic monopole in the crystal momentum space related to the anomalous Hall effect in the $SrRuO_3$ crystal. These examples show the importance of understanding the properties of the adiabatic magnetic monopoles.

Section II recalls the definition and the properties of the universal classifying space for the general case. Section III is devoted to the Dirac magnetic monopole theory, in particular its link with Berry's original example of a geometric phase. A more complete discussion of the results reviewed in these sections can be found in Ref. 11. Originally $\mathcal{M}$ is a soft manifold (i.e., one without a natural metric), because it is a set of classical control parameters of the environment which do not necessarily have the same physical nature. Section IV shows that $\mathcal{M}$ can be rigidified (endowed with a metric) by an appropriate immersion. This rigidification is needed to describe the monopole magnetic field distribution in $\mathcal{M}$. Section V is devoted to the analysis of the apparent monopole charge in $\mathcal{M}$. Section VI generalizes the discussion to the case of the non-Abelian monopoles. In most of this paper we suppose that $\dim \mathcal{M}=2$ and restrict our attention to the monopole (level crossing) neighborhood. We discuss the effect of these assumptions in the last section.

II. THE UNIVERSAL SPACE OF QUANTUM ADIABATIC DYNAMICS

Bohm and Mostafazadeh showed in Refs. 12 and 13 that the Berry phase phenomena are related to the nonadiabatic geometric phases of cyclic dynamical quantum systems discovered by Aharonov and Anandan.[14] This relationship is given by the universal classifying theorem of principal bundles (see Refs. 15 and 16). Here we recall this theorem, and the associated induced geometric structure of quantum mechanics.

A. The universal classifying theorem

Let $\mathcal{B}=(B,X,G,\pi_B)$ be a principal bundle with base space X, total space B, structure group G, and projection π_B. We say that $\mathcal{B}$ is n-universal if for every cell n-complex K (see Refs. 15 and 16), for every cell subcomplex $L\subset K$, for every principal bundle $\mathcal{B}'=(B',K,G,\pi_{B'})$ and for every map $h:(\pi_{B'}^{-1}(L),L,G,\pi_{B'})\to(B,X,G,\pi_B)$, there exists an extension of h to $(B',K,G,\pi_{B'})\to(B,X,G,\pi_B)$.

If $\mathcal{B}=(B,X,G,\pi_B)$ is $(n+1)$-universal and if K is a cell n-complex then there exists a map $f:K\to X$ such that the following diagram commutes

$$\begin{array}{ccc} f^*B & \overset{f^*}{\leftarrow} & B \\ \pi_{f^*B}\downarrow & & \downarrow\pi_B \\ K & \overset{f}{\rightarrow} & X \end{array},$$

where $f^*\mathcal{B}$ is the bundle induced by f. X is called the universal manifold of K and f is called the universal map. In the case of the adiabatic bundle $\mathcal{P}$, the situation is as follows. Suppose that the Hilbert space is n-dimensional. In the case of the one-dimensional adiabatic approximation, the universal manifold of $\mathcal{P}$ is the projective space $\mathbb{C}P^{n-1}$, and the universal map can be written:

$$f:\begin{array}{c}\mathcal{M}\to\mathbb{C}P^{n-1}\\ \vec{R}\mapsto|a,\vec{R}\rangle\langle a,\vec{R}|\end{array}.$$

In the m-dimensional adiabatic approximation, the universal manifold is the Grassmanian manifold $G_m(\mathbb{C}^n)=U(n)/(U(m)\times U(m-n))$ and the universal map is

$$\mathcal{M} \to G_m(\mathbb{C}^n)$$
$$f: \vec{R} \mapsto \sum_{a \in I} |a,\vec{R}\rangle\langle a,\vec{R}|$$

(see Ref. 13). In the following we will restrict our attention to $\mathbb{C}P^{n-1}$ and will analyze its structure.

B. The Kählerian structure of quantum dynamics

The physical reason which explains why $\mathbb{C}P^{n-1}$ is the universal space of quantum mechanics is the following. We know that the mathematical structure of quantum mechanics is a separable $\mathbb{C}$-Hilbert space $\mathcal{H}$ which models the state space. The probabilistic interpretation of quatum mechanics states that a physical state ψ is a probability amplitude, and so we must have $\|\psi\|=1$. In this way two proportional vectors represent the same physical state. Moreover, the phase of a vector does not give physical information; only the phase difference between two vectors has a physical meaning (quantum interference theory). We then see that the Hilbert space $\mathcal{H}$ contains a lot of "nonphysical" information, so that it is not the most efficient structure to describe quantum mechanics. To define the "true" space of quantum mechanics we first consider $\mathcal{H}$. If $\psi=\alpha\phi$ with $\alpha \in \mathbb{R}^+$ and $\alpha \neq 0$ then the two vectors ψ and ϕ define the same physical state (they have only a different norm). This previous relation is an equivalence relation $\sim$, which signifies that a physical state is an equivalence class. So the physical space is

$$\mathcal{N} = (\mathcal{H} \setminus \{0\})/\sim, \tag{6}$$

which is called the space of normed rays. Suppose that the question of interference is ignored; then two vectors which are only different by a phase factor represent the same physical state. We define the group action of U(1) on $\mathcal{N}$ by

$$\forall e^{i\varphi} \in U(1), \forall [\psi] \in \mathcal{N}, \quad e^{i\varphi}[\psi] = [e^{i\varphi}\psi]. \tag{7}$$

Since two vectors represent the same state if they belong to the same orbit, then the physical space is the homogeneous space of the orbits

$$\mathcal{R} = \mathcal{N}/U(1), \tag{8}$$

which is called the complex projective space. If $\mathcal{H}$ is finite dimensional, $\dim \mathcal{H}=n$, we have $\mathcal{R}=\mathbb{C}P^{n-1}$ (it is a $(n-1)$-dimensional $\mathbb{C}^\infty$-differential complex manifold). In the case $n=2$ there exists an exceptional diffeomorphism

$$\mathbb{C}P^1 \simeq S^3/S^1 \simeq S^2. \tag{9}$$

Thus the space of a quantum two-level system (a spin for example) is the sphere.

Let $\psi \in \mathcal{H}$, with $\psi=(\psi^0,\psi^1,\ldots,\psi^{n-1})$. We set $w^i=\psi^i/\psi^0$ for all $i=1,\ldots,n-1$. The complex numbers $\{w^i\}_i$ are called the homogeneous coordinates of ψ in $\mathbb{C}P^{n-1}$. We can write the gauge potential by using these coordinates:

$$A = \frac{\psi^\dagger \mathrm{d}\psi}{\psi^\dagger\psi} = \frac{i}{2}\frac{\psi^\dagger \mathrm{d}\psi - \psi \mathrm{d}\psi^\dagger}{\psi^\dagger\psi} \tag{10}$$

$$= \frac{i}{2}\frac{\bar{\psi}_\alpha \mathrm{d}\psi^\alpha - \psi^\alpha \mathrm{d}\bar{\psi}_\alpha}{\bar{\psi}_\gamma\psi^\gamma} \tag{11}$$

$$= \frac{i}{2} \frac{\bar{w}_i \mathrm{d}w^i - w^i \mathrm{d}\bar{w}_i}{1 + \bar{w}_j w^j}. \tag{12}$$

Einstein's notation has been adopted for the sum, with the convention that the Greek indices take the values $0, \ldots, n-1$ and that the Latin indices take the values $1, \ldots, n-1$. The magnetic field (the curvature of the universal bundle) can be written

$$F = \mathrm{d}A = i \frac{\bar{w}_i w^j - (1 + \bar{w}_k w^k)\delta_i^j}{(1 + \bar{w}_l w^l)^2} \mathrm{d}w^i \wedge \mathrm{d}\bar{w}_j. \tag{13}$$

We introduce the function

$$K = \tfrac{1}{2} \mathrm{Ln}(1 + \bar{w}_k w^k), \tag{14}$$

where Ln is the multivalued complex logarithm. We also introduce the Dolbeault operators of the complex manifold ∂ and $\bar{\partial}$ ($\bar{\partial} + \partial = d$) (a presentation of complex differential geometry can be found in Ref. 17). It is easy to see that

$$\bar{\partial}\partial K = \frac{1}{2} \frac{\bar{w}_i w^j - (1 + \bar{w}_k w^k)\delta_i^j}{(1 + \bar{w}_l w^l)^2} \mathrm{d}w^i \wedge \mathrm{d}\bar{w}_j \tag{15}$$

and we then have $F = 2i\bar{\partial}\partial K$. We recognize here the structure of a Kählerian geometry (see Ref. 17); K is the Kähler potential and F is the Kähler form of $\mathbb{C}P^{n-1}$. We know that a Kählerian manifold is endowed with a natural metric, which in this case is the Fubini-Study metric

$$\eta = \mathrm{d}l^2 = \frac{(1 + \bar{w}_k w^k)\delta_i^j - \bar{w}_i w^j}{(1 + \bar{w}_l w^l)^2} \mathrm{d}w^i \mathrm{d}\bar{w}_j. \tag{16}$$

This Kählerian structure of quantum mechanics was indicated by Anandan and Aharonov in Ref. 18.

III. MAGNETIC MONOPOLE

We have seen that the divergence of the magnetic field of $\mathcal{M}$ relates a level crossing to the presence of a magnetic monopole in the electromagnetic picture. We recall here the theory of the Dirac magnetic monopole[19] and also the direct relationship between this theory and the Berry phase phenomenon.

A. The Dirac magnetic monopole theory

We consider a magnetic monopole with magnetic charge g, at the position (0, 0, 0) in a three-dimensional space. The first aspect of the Dirac model is that we do not consider $\mathbb{R}^3$ as being the fundamental manifold, but as a foliation $(S^2, \mathbb{R}^+)$, where S^2 is a sphere centered on the monopole and $\mathbb{R}^+$ is the foliation parameter space which describes the radius of the sphere. We consider the $U(1)$-principal bundle with base space S^2. We know that an atlas of S^2 must have at least two local charts. We choose the following charts:

$$U^N = \{(\theta, \varphi), \theta \in [0, \pi/2 + \epsilon], \varphi \in [0, 2\pi[\},$$

$$U^S = \{(\theta, \varphi), \theta \in [\pi/2 - \epsilon, \pi], \varphi \in [0, 2\pi[\}.$$

In these charts of the north and south hemispheres (the choice of the equator S^1 being arbitrary) ϵ is a small parameter which is used to ensure the nonvanishing intersection of the charts. On S^2 we introduce the local potential

$$A^N = ig(1 - \cos\theta)\mathrm{d}\varphi, \tag{17}$$

$$A^S = -ig(1+\cos\theta)\mathrm{d}\varphi. \tag{18}$$

By using the vector formalism of $\mathbb{R}^3$ we have

$$\vec{A}^N = \frac{g(1-\cos\theta)}{r\sin\theta}\vec{e}_\varphi, \tag{19}$$

$$\vec{A}^S = -\frac{g(1+\cos\theta)}{r\sin\theta}\vec{e}_\varphi. \tag{20}$$

(We should note that A^N is singular if we extend it at $\theta=\pi$ and A^S is singular if we extend it at $\theta=0$.)

The magnetic field (the curvature) is then $F=\mathrm{d}A$. We compute the magnetic flux through S^2; by using Stokes theorem we find

$$\Phi = \int_{S^2} F \tag{21}$$

$$= \lim_{\epsilon\to 0}\left(\int_{U^N}\mathrm{d}A^N + \int_{U^S}\mathrm{d}A^S\right) \tag{22}$$

$$= \lim_{\epsilon\to 0}\left(\int_{\partial U^N}A^N + \int_{\partial U^S}A^S\right) \tag{23}$$

$$= \int_{S^1} A^N - A^S \tag{24}$$

$$= \int_{S^1} 2g\mathrm{d}\varphi \tag{25}$$

$$= 4\pi g. \tag{26}$$

This is, effectively, the flux of a central field with charge g. We introduce the transition function $g^{NS}=e^{2ig\varphi}$, and we then have

$$A^N = A^S + (g^{NS})^{-1}\mathrm{d}g^{NS}. \tag{27}$$

To have a single transition one should require that $g^{NS}(\varphi=0)=g^{NS}(\varphi=\pi)\Leftrightarrow 2g\in\mathbb{Z}$. This is the Dirac quantization condition.

By the foliation we extend this result to all of $\mathbb{R}^3$ and we have

$$A^N = -ig\frac{y\mathrm{d}x - x\mathrm{d}y}{r(r+z)}, \tag{28}$$

$$A^S = ig\frac{y\mathrm{d}x - x\mathrm{d}y}{r(r-z)}, \tag{29}$$

$$F = ig\frac{x\mathrm{d}y \wedge \mathrm{d}z + y\mathrm{d}z \wedge \mathrm{d}x + z\mathrm{d}x \wedge \mathrm{d}y}{r^3} \tag{30}$$

with $r=\sqrt{x^2+y^2+z^2}$. By using the Hodge duality we find the correct expression in the vector formalism for the magnetic field: $\vec{F}=g\vec{r}/r^3$.

On the z axis A^N is singular at $z\leqslant 0$ and A^S is singular at $z\geqslant 0$. We call these two semilines the Dirac strings. We note that by a gauge transformation (with another choice of equator) the Dirac strings rotate in the space.

B. The magnetic monopole of a simple two-level system

We consider the system originally considered by Berry a spin $\frac{1}{2}$ particle interacting with a magnetic field, described by the Hamiltonian

$$H(\vec{x}) = x^i\sigma_i = \begin{pmatrix} x^3 & x^1 - ix^2 \\ x^1 + ix^2 & -x^3 \end{pmatrix}. \tag{31}$$

The eigenvalues of $H(\vec{x})$ are $E_\pm(\vec{x})=\pm r=\pm\sqrt{(x^1)^2+(x^2)^2+(x^3)^2}$. We thus have a level crossing at $\vec{x}=\vec{0}$. The eigenvector associated with E_+ is

$$|+,\vec{x}\rangle^N = \frac{1}{\sqrt{2r(r+x^3)}}\begin{pmatrix} r+x^3 \\ x^1+ix^2 \end{pmatrix} = \begin{pmatrix} \cos\dfrac{\theta}{2} \\ e^{i\varphi}\sin\dfrac{\theta}{2} \end{pmatrix}, \tag{32}$$

where $\theta=\arctan\sqrt{(x^1)^2+(x^2)^2}/x^3$ and $\varphi=\arctan x^2/x^1$ are, together with r, the spherical coordinates of $\mathbb{R}^3$. With another convention for the matrix representation, the eigenstate is

$$|+,\vec{x}\rangle^S = \frac{1}{\sqrt{2r(r-x^3)}}\begin{pmatrix} x^1-ix^2 \\ r-x^3 \end{pmatrix} = \begin{pmatrix} e^{-i\varphi}\cos\dfrac{\theta}{2} \\ \sin\dfrac{\theta}{2} \end{pmatrix}. \tag{33}$$

We compute the adiabatic gauge potential

$$A^N = {}^N\langle +,\vec{x}|\mathrm{d}|+,\vec{x}\rangle^N = -\frac{i}{2}\frac{x^2\mathrm{d}x^1 - x^1\mathrm{d}x^2}{r(r+x^3)} = \frac{i}{2}(1-\cos\theta)\mathrm{d}\varphi, \tag{34}$$

$$A^S = {}^S\langle +,\vec{x}|\mathrm{d}|+,\vec{x}\rangle^S = \frac{i}{2}\frac{x^2\mathrm{d}x^1 - x^1\mathrm{d}x^2}{r(r-x^3)} = -\frac{i}{2}(1+\cos\theta)\mathrm{d}\varphi. \tag{35}$$

We recognize here the magnetic potential associated with a magnetic monopole of charge $\frac{1}{2}$ at $\vec{x}=\vec{0}\in\mathbb{R}^3$. We see that a level crossing leads to the equations appropriate to a Dirac magnetic monopole. Let us consider that r is constant; the manifold describing the system is the sphere $S^2=\mathbb{C}P^1$ with coordinate system (θ,φ). We see that the present representation is in fact the universal model of quantum mechanics. We designate S^2 by the term "universal manifold," and $\mathbb{R}^3$ foliated by S^2 by the term "generalized universal space."

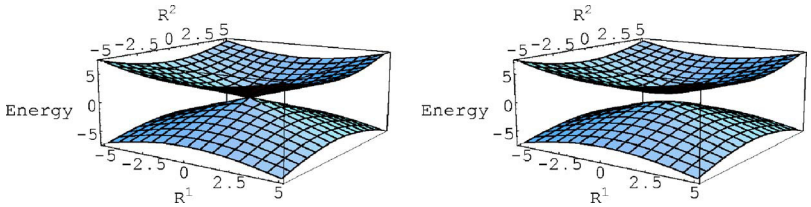

FIG. 1. (Color online) Representations of two levels with respect to the control manifold $\mathcal{M}$, the immersions being defined by, left: $f^1(\vec{R})=R^1$, $f^2(\vec{R})=R^2$, $f^3(\vec{R})=0$, right: $f^1(\vec{R})=R^1$, $f^2(\vec{R})=R^2$, $f^3(\vec{R})=1$. For the left panel, the monopole is in $f(\mathcal{M})$, and we have a crossing for $f(\vec{R})=0$. In the right panel, the monopole is not in $f(\mathcal{M})$, but $f(\mathcal{M})$ passes by the neighborhood of the monopole for $\vec{R}=0$; at this position we see an avoided crossing.

IV. THE ADIABATIC MAGNETIC MONOPOLE FIELD ASSOCIATED WITH A TWO LEVEL CROSSING

A. Immersion of the control manifold, level crossings, and avoided level crossings

We consider an adiabatic quantum dynamical system described by the Hamiltonian $H(\vec{R})$, with $\vec{R}\in\mathcal{M}$. The control manifold $\mathcal{M}$ is supposed to be two dimensional. We consider a crossing between two nondegenerate eigenvalues E_1 and E_2 of $H(\vec{R})$. In the neighborhood $\mathcal{U}$ of this crossing we consider the effective Hamiltonian associated with this crossing:

$$\forall \vec{R}\in\mathcal{U},\quad H^{\text{eff}}(\vec{R})=\begin{pmatrix} f^3(\vec{R}) & f^1(\vec{R})-if^2(\vec{R}) \\ f^1(\vec{R})+if^2(\vec{R}) & -f^3(\vec{R}) \end{pmatrix}. \tag{36}$$

H^{eff} is obtained by a partitioning technique,[20] arising from a quantum KAM method,[21] an adiabatic elemination method,[21] or a Bloch wave operator method.[20,22] Comparing the Hamiltonian [Eq. (36)] with the Hamiltonian Eq. (31) of the universal model, we see that we have a map f from the control manifold $\mathcal{M}$ to the generalized universal space $\mathbb{R}^3$, with $f(\vec{R})=(f^1(\vec{R}),f^2(\vec{R}),f^3(\vec{R}))\in\mathbb{R}^3$. In order to respect the geometric framework we suppose that f is a $\mathcal{C}^\infty$-map. Let $f_*:T_{\vec{R}}\mathcal{M}\to T_{f(\vec{R})}\mathbb{R}^3$ be the push-forward map (which is a linear map between two vector spaces for a fixed $\vec{R}$). We suppose that $\ker f_*=\{0\}$ (f_* is an injective map), and f is then an immersion of $\mathcal{M}$ in $\mathbb{R}^3$ (we will discuss this assumption later). There is no reason to suppose that f is an embedding; several points of $\mathcal{M}$ can be associated with the same point in the universal space and we will use this possibility in the later discussion.

We have a level crossing at $\vec{R}_0\in\mathcal{M}$ if and only if $f(\vec{R}_0)=0$. Although only one magnetic monopole is present in the generalized universal space $\mathbb{R}^3$, it is possible that several monopoles (crossings between E_1 and E_2) exist at several points $\{\vec{R}_i\}_{i=1,\ldots,n}$ if $f(\vec{R}_1)=f(\vec{R}_2)=\cdots=f(\vec{R}_n)=0$.

An avoided crossing manifests itself in this geometric analysis by virtue of the fact that the immersed manifold $f(\mathcal{M})$ does not include 0 but passes through a neighborhood of 0, i.e., $\forall\vec{R}\in\mathcal{U}$, $f(\vec{R})\neq 0$, but $\exists\vec{R}_0$ and $\exists\epsilon$ a small positive constant such that $\|f(\vec{R}_0)\|=\sqrt{(f^1(\vec{R}_0))^2+(f^2(\vec{R}_0))^2+(f^3(\vec{R}_0))^2}=\epsilon$ and $\forall\vec{R}\in\mathcal{U}$, $\vec{R}\neq\vec{R}_0$, $\|f(\vec{R}_0)\|>\epsilon$ ($\vec{R}_0$ is a local minimum of the vector norm). Note that 2ϵ is the energy gap of the avoided crossing (Fig. 1).

B. The Riemannian structure of the control manifold

The control manifold $\mathcal{M}$ is not endowed with a natural metric. The Euclidian metric defined by the scalar product $\vec{R}\cdot\vec{Q}=R^\mu Q^\nu\delta_{\mu\nu}$ does not have a physical meaning, because the control parameters can have different physical natures. However, we know that the universal manifold is endowed with a metric which is natural for the quantum mechanics, the Fubini-Study metric. We will use this metric and the immersion f to rigidify the manifold $\mathcal{M}$.

The universal manifold is a sphere $S^2 \simeq \mathbb{C}P^1$ considered as a sheaf of the foliation of $\mathbb{R}^3$. Let $\psi=(\psi^0,\psi^1)=\psi^0(1,w^1)$ be a vector of the space spanned by the eigenvectors of the Hamiltonian [Eq. (36)]. $w^1 \in \mathbb{C}$ is the coordinate on $\mathbb{C}P^1$. The Fubini-Study metric of $\mathbb{C}P$ (to be closer to the usual electromagnetic formalism, we have removed the factor i in order to have real fields in place of purely imaginary fields) is

$$\eta = \frac{(1+\bar{w}_1 w^1)-\bar{w}_1 w^1}{(1+\bar{w}_1 w^1)^2} \mathrm{d}\bar{w}_1 \mathrm{d}w^1 = \frac{\mathrm{d}\bar{w}_1 \mathrm{d}w^1}{(1+\bar{w}_1 w^1)^2}. \tag{37}$$

This expression is precisely the conformal representation of the Riemannian metric of the sphere (see Ref. 23). The Kählerian structure of $\mathbb{C}P^1$ is equivalent to the Riemannian structure of S^2. We can then write, with the standard coordinate system of S^2,

$$\eta = r^2 \sin^2 \varphi \mathrm{d}\theta^2 + r^2 \mathrm{d}\varphi^2. \tag{38}$$

We know that the Riemannian metric of S^2 centered on 0 in $\mathbb{R}^3$ is obtained as being the metric induced by the Euclidian metric of $\mathbb{R}^3$. We write δ for this metric ($\delta_{ij}=0$ if $i \neq j$ or $=1$ if $i=j$). We see that the rigidification of $\mathcal{M}$ is obtained by the metric induced by the immersion of $\mathcal{M}$ in $\mathbb{R}^3$ endowed with δ. The natural metric of $\mathcal{M}$ is then

$$g = g_{\mu\nu} \mathrm{d}R^\mu \mathrm{d}R^\nu = \delta_{ij} \frac{\partial f^i}{\partial R^\mu} \frac{\partial f^j}{\partial R^\nu} \mathrm{d}R^\mu \mathrm{d}R^\nu. \tag{39}$$

Moreover, we can write $H^{\mathrm{eff}}(\vec{R})=f^i(\vec{R})\sigma_i$ where $\{\sigma_1,\sigma_2,\sigma_2\}$ are the Pauli matrices. Since $\frac{1}{2}\mathrm{tr}(\sigma_i\sigma_j)=\delta_{ij}$ we obtain

$$g_{\mu\nu} = \frac{1}{2}\mathrm{tr}\left(\frac{\partial H^{\mathrm{eff}}}{\partial R^\mu} \frac{\partial H^{\mathrm{eff}}}{\partial R^\nu} \right). \tag{40}$$

We have supposed that f is an immersion, i.e., that f_* is injective. If this is not the case, then the bilinear form g defined by Eq. (39) is not a metric in a rigorous mathematical sense. g is then not positively defined (if f_* is not injective, then there exists an isotropic tangent vector of $\mathcal{M}$, i.e., $\exists X^\mu \partial_\mu \in T\mathcal{M}$ such that $g_{\mu\nu}X^\mu X^\nu=0$). In this case, by an abuse of language, we will continue to call g a metric, and we will continue to consider that

$$\int_{\mathcal{C}} \sqrt{g_{\mu\nu} \frac{\mathrm{d}\eta^\mu}{\mathrm{d}s} \frac{\mathrm{d}\eta^\nu}{\mathrm{d}s}} \mathrm{d}s$$

is the length of $\mathcal{C}$ parametrized by $s \mapsto \eta(s)$ in $\mathcal{M}$. This abuse of language is standard in physics; for example, in the context of special relativity we call a metric the bilinear form defined by $\eta_{\mu\nu}=0$ if $\mu \neq \nu$, $\eta_{ii}=1$ if $i=1,2,3$ and $\eta_{00}=-1$. The Minkwoski metric η is also not positively defined and is not a metric in the mathematical sense.

C. Magnetic field of the control manifold

In the universal space $\mathbb{R}^3$ we have the gauge potential (we choose one of the two conventions) (to be closer to the usual electromagnetic formalism, we have removed the factor i in order to have real fields in place of purely imaginary fields)

$$A = \frac{1}{2} \frac{x^2 \mathrm{d}x^1 - x^1 \mathrm{d}x^2}{r(r-x^3)} \in \Omega^1 \mathbb{R}^3 \tag{41}$$

and the magnetic monopole field is

$$B = \mathrm{d}A = \frac{1}{2} \frac{x^1 \mathrm{d}x^2 \wedge \mathrm{d}x^3 + x^2 \mathrm{d}x^3 \wedge \mathrm{d}x^1 + x^3 \mathrm{d}x^1 \wedge \mathrm{d}x^2}{r^3} \in \Omega^2 R^3 \tag{42}$$

By using the identity

$$\mathrm{d}x^i \leftrightarrow \begin{pmatrix} \delta_{1i} \\ \delta_{2i} \\ \delta_{3i} \end{pmatrix},$$

we can write $A \in \Omega^1\mathbb{R}^3$ as being a vector field of $\mathbb{R}^3$:$\vec{A}$. We recall the definition of the Hodge star operator associated with a metric q in a n-dimensional manifold X:

$$*_q : \Omega^r X \to \Omega^{n-r} X$$

$$*_q(\mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_r}) = \frac{\sqrt{|\det q|}}{(n-r)!} q^{i_1 j_1} \cdots q^{i_r j_r} \epsilon_{j_1,\ldots,j_n} \mathrm{d}x^{j_{r+1}} \wedge \cdots \wedge \mathrm{d}x^{j_n},$$

where ϵ is the Levi-Civita symbol, $q^{ij}q_{jk} = \delta^i_k$ and $\det q = q_{1i_1}q_{2i_2}\ldots q_{ni_n}\epsilon^{i_1 i_2 \ldots i_n}$.

In $\mathbb{R}^3$ we have simply $*_\delta : \Omega^2\mathbb{R}^3 \to \Omega^1\mathbb{R}^3$, with $*_\delta(\mathrm{d}x^1 \wedge \mathrm{d}x^2) = \mathrm{d}x^3$. Then $*_\delta B \in \Omega^1\mathbb{R}^3$ and we can consider it as being a magnetic vector field $\vec{B}$. The relation $B = \mathrm{d}A$ is then $\vec{B} = \vec{\mathrm{curl}}\vec{A}$.

Consider the pullback $f^* : \Omega^*\mathbb{R}^3 \to \Omega^*\mathcal{M}$. The gauge potential in $\mathcal{M}$ is

$$f^*A = A_i \frac{\partial f^i}{\partial R^\mu} \mathrm{d}R^\mu. \tag{43}$$

Note that we can compute f^*A directly with the eigenvector of [Eq. (36)]:

$$f^*A = \langle 1, \vec{R} | \mathrm{d}_{\mathcal{M}} | 1, \vec{R} \rangle = f^*(\langle +, \vec{x} | \mathrm{d} | + \vec{x} \rangle)_{\vec{x}=f(\vec{R})}. \tag{44}$$

As f^* is a chain map for the exterior differential, then the magnetic field is

$$f^*B = f^*\mathrm{d}A = \mathrm{d}_{\mathcal{M}} f^*A = B_{ij} \frac{\partial f^i}{\partial R^\mu} \frac{\partial f^j}{\partial R^\nu} \mathrm{d}R^\mu \wedge \mathrm{d}R^\nu = 2B_{ij} \frac{\partial f^i}{\partial R^1} \frac{\partial f^j}{\partial R^2} \mathrm{d}R^1 \wedge \mathrm{d}R^2. \tag{45}$$

In the same way that in $\mathbb{R}^3$ the field associated with the usual electromagnetic formalism is not $f^*B \in \Omega^2\mathcal{M}$ but $*_g f^*B \in \Omega^0\mathcal{M}$, we see that

$$*_g(\mathrm{d}R^1 \wedge \mathrm{d}R^2) = \sqrt{|\det g|} g^{1\mu} g^{2\nu} \epsilon_{\mu\nu} \tag{46}$$

$$= \sqrt{|\det g|}(g^{11}g^{22} - g^{12}g^{21}) \tag{47}$$

$$= \sqrt{|\det g|} \det g^{-1} \tag{48}$$

$$= \frac{\sqrt{|\det g|}}{\det g} \tag{49}$$

$$= \frac{\mathrm{sgn}(\det g)}{\sqrt{|\det g|}}. \tag{50}$$

As g is a Riemannian metric (because it is induced by the Euclidian metric) $\det g > 0$, and then

$$*_g f^*B = 2B_{ij} \frac{\partial f^i}{\partial R^1} \frac{\partial f^j}{\partial R^2} \frac{1}{\sqrt{\det g}}. \tag{51}$$

Consider the two-coform

$$N = \frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\frac{\partial}{\partial x^i} \wedge \frac{\partial}{\partial x^j}. \tag{52}$$

It is clear that $\vec{N} = *_{\delta} N$ is a vector normal to the immersed manifold $f(\mathcal{M})$. We compute the norm of $\vec{N}$:

$$\|\vec{N}\|^2 = \delta_{kl}(*_{\delta}N)^k(*_{\delta}N)^l \tag{53}$$

$$= \delta_{kl}\frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\epsilon_{ij}{}^{k}\frac{\partial f^n}{\partial R^1}\frac{\partial f^m}{\partial R^2}\epsilon_{nm}{}^{l} \tag{54}$$

$$= (\delta_{in}\delta_{jm} - \delta_{im}\delta_{jn})\frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\frac{\partial f^n}{\partial R^1}\frac{\partial f^m}{\partial R^2}, \tag{55}$$

where we have used the following property of the Levi-Civita symbol: $\epsilon_{ij}{}^{k}\epsilon_{nm}{}^{l}\delta_{kl} = \delta_{in}\delta_{jm} - \delta_{im}\delta_{jn}$ (see Ref. 24). We also have the result:

$$\det g = g_{1\mu}g_{2\nu}\epsilon^{\mu\nu} \tag{56}$$

$$= \delta_{in}\frac{\partial f^i}{\partial R^1}\frac{\partial f^n}{\partial R^\mu}\delta_{jm}\frac{\partial f^j}{\partial R^2}\frac{\partial f^m}{\partial R^\nu}\epsilon^{\mu\nu} \tag{57}$$

$$= \delta_{in}\delta_{jm}\frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\left(\frac{\partial f^n}{\partial R^1}\frac{\partial f^m}{\partial R^2} - \frac{\partial f^m}{\partial R^1}\frac{\partial f^n}{\partial R^2}\right) \tag{58}$$

$$= (\delta_{in}\delta_{jm} - \delta_{im}\delta_{jn})\frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\frac{\partial f^n}{\partial R^1}\frac{\partial f^m}{\partial R^2}. \tag{59}$$

We see that $\|\vec{N}\| = \sqrt{\det g}$. Let $\vec{u}_N = (1/\sqrt{\det g})\vec{N}$ be the unit normal vector to $f(\mathcal{M})$. The density of the flux of $\vec{B}$ through $f(\mathcal{M})$ is then

$$\vec{B}\cdot\vec{u}_N = \frac{1}{\sqrt{\det g}}\langle B, N\rangle = 2B_{ij}\frac{\partial f^i}{\partial R^1}\frac{\partial f^j}{\partial R^2}\frac{1}{\sqrt{\det g}}. \tag{60}$$

Here $\langle .,. \rangle$ is the duality product between tangent and cotangent spaces (i.e. $\langle dx^i, \partial/\partial x^j\rangle = \delta^i_j$). To summarize, we have the results

$$*_g f^* dA = *_g f^* B = *_g d_{\mathcal{M}} f^* A = \vec{B}\cdot\vec{u}_N. \tag{61}$$

The magnetic field in $\mathcal{M}(*_g f^* B)$ is equal to the density of the flux of the magnetic field of $\mathbb{R}^3$ through the immersed manifold $f(\mathcal{M})$.

D. Examples

The charts of the magnetic field $d_{\mathcal{M}} f^* A$ can be used to analyze the adiabatic properties of a quantum dynamical system, since this field makes monopoles appear at the eigenvalue crossings and since it is proportional to the nonadiabatic transitions. It is sometimes difficult to interpret these charts; the immersion property of the control manifold can help us with that interpretation.

In order to illustrate the effects of the control manifold immersion we consider three simple examples of three level systems. To simplify the analysis our chosen method of producing an effective Hamiltonian is the partioning method by adiabatic elimination.[21] Let H be the total Hamiltonian matrix with the form

$$H = \begin{pmatrix} H_{00} & H_{10} \\ H_{01} & H_{11} \end{pmatrix}, \tag{62}$$

where H_{ij} are matrix blocs, H_{00} being the bloc corresponding to the considered crossing. The effective Hamiltonian after the adiabatic elimination process is

$$H^{\text{eff}} = H_{00} - H_{01}H_{11}^{-1}H_{10}. \tag{63}$$

Moreover we can redefine $H^{\text{eff}} \to H^{\text{eff}} - (\text{tr}H^{\text{eff}}/\text{tr}I)I$ (I is the identity matrix) in order to have a traceless effective Hamiltonian.

The first example we study is the Hamiltonian

$$H_1(u,\theta) = \begin{pmatrix} 0 & 0 & ue^{i\theta} \\ 0 & 1 & 1 \\ ue^{-i\theta} & 1 & 1 \end{pmatrix}. \tag{64}$$

This Hamiltonian corresponds to the RWA description of a three level atom interacting with two lasers such that the first laser is quasiresonant with the transition $|1\rangle$ to $|3\rangle$ and the second laser is quasiresonant with the transition $|2\rangle$ to $|3\rangle$ ($|i\rangle$ is the bare atom basis, the basis in which the matrix (Eq. (64) is written). u and ϕ are the amplitude and the phase of the first laser and constitute the control parameters; its polarization is constant. The second laser is constant with an amplitude equal to 1 in reduced units. For $u=0$,

$$H_1(0,\theta) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

has the eigenvalues {0,0,2}. In the neighborhood of the crossing the effective Hamiltonian (with adiabatic elimination of the state 3) is

$$H_1^{\text{eff}} = \begin{pmatrix} -\dfrac{u^2}{2} & ue^{i\theta} \\ ue^{-i\theta} & \dfrac{u^2}{2} \end{pmatrix}. \tag{65}$$

The immersion of the control manifold is then

$$f_1(u,\theta) = \begin{pmatrix} u\cos\theta \\ u\sin\theta \\ -\dfrac{u^2}{2} \end{pmatrix}. \tag{66}$$

The first immersed manifold is then diffeomorphic to an elliptic paraboloid.

The second example is the Hamiltonian

$$H_2(\theta,\phi) = \begin{pmatrix} 0 & 2(e^{i\phi}-1) & \cos\theta \\ 2(e^{-i\phi}-1) & 1 & e^{-i\phi} \\ \cos\theta & e^{i\phi} & 1 \end{pmatrix}. \tag{67}$$

This Hamiltonian corresponds to the RWA description of a three level atom interacting with four lasers such that the first and the second laser are quasiresonant with the transition $|1\rangle$ to $|2\rangle$, the third laser is quasiresonant with the transition $|1\rangle$ to $|3\rangle$ and the fourth laser is quasiresonant with the transition $|2\rangle$ to $|3\rangle$. The second laser is constant with an amplitude equal to 2 in reduced units, the first laser presents a phase modulation with a constant amplitude equal to 2, the third laser

presents a polarization modulation with a constant amplitude equal to 1, and the fourth laser presents a phase modulation synchronized with the phase modulation of the second laser. The control parameters are ϕ (the phase of the second and of the fourth lasers) and θ (the angle between the polarization of the third laser and the atom electric dipole moment). For $(\theta,\phi)=(\pi/2,0)$,

$$H_2\left(\frac{\pi}{2},0\right)=\begin{pmatrix}0&0&0\\0&1&1\\0&1&1\end{pmatrix}$$

and in the neighborhood of the crossing, the effective Hamiltonian (with adiabatic elimination of the state 3) is

$$H_2^{\text{eff}}(\theta,\phi)=\begin{pmatrix}-\dfrac{\sin^2\theta}{2} & 2(e^{i\phi}-1)-\cos\theta e^{i\phi}\\ 2(e^{-i\phi}-1)-\cos\theta e^{-i\phi} & \dfrac{\sin^2\theta}{2}\end{pmatrix}. \tag{68}$$

The immersion of the control manifold is then

$$f_2(\theta,\phi)=\begin{pmatrix}(2-\cos\theta)\cos\phi-2\\(2-\cos\theta)\sin\phi\\-\dfrac{\sin^2\theta}{2}\end{pmatrix}. \tag{69}$$

The second immersed manifold is then diffeormorphic to a half torus.

The third example is the Hamiltonian

$$H_3(u,\theta)=\begin{pmatrix}0 & 2(e^{i\theta}-1) & u\cos\dfrac{\theta}{2}\\ 2(e^{-i\theta}-1) & 0 & ue^{-i\theta}\\ u\cos\dfrac{\theta}{2} & ue^{i\theta} & 1\end{pmatrix}. \tag{70}$$

This Hamiltonian corresponds to the RWA description of a three level atom interacting with four lasers such that the first and the second laser are quasiresonant with the transition $|1\rangle$ to $|2\rangle$, the third laser is quasiresonant with the transition $|1\rangle$ to $|3\rangle$, and the fourth laser is quasiresonant with the transition $|2\rangle$ to $|3\rangle$. The second laser is constant with an amplitude equal to 2 in reduced units, the first laser presents a phase modulation with a constant amplitude equal to 2, the third laser presents a polarization modulation synchronized with the phase modulation of the first laser and it presents an amplitude modulation; finally, the fourth laser presents a phase modulation synchronized with the phase modulation of the second laser. The control parameters are u (the amplitude of the third laser) and θ (the phase of the second and of the fourth lasers, $\theta/2$ being the angle between the synchronized polarization of the third laser and the atom electric dipole moment). For $(u,\theta)=(0,0)$,

$$H_3(0,0)=\begin{pmatrix}0&0&0\\0&0&0\\0&0&1\end{pmatrix},$$

and in the neighborhood of the crossing, the effective Hamiltonian (with adiabatic elimination of the state 3) is

$$H_3^{\text{eff}}(u,\theta)=\begin{pmatrix} \dfrac{u^2\sin^2\dfrac{\theta}{2}}{2} & 2(e^{i\theta}-1)-u^2\cos\dfrac{\theta}{2}e^{i\theta} \\ 2(e^{-i\theta}-1)-u^2\cos\dfrac{\theta}{2}e^{-i\theta} & -\dfrac{u^2\sin^2\dfrac{\theta}{2}}{2} \end{pmatrix}. \tag{71}$$

The immersion of the control manifold is then

$$f_3(u,\theta)=\begin{pmatrix} \left(2-u^2\cos\dfrac{\theta}{2}\right)\cos\theta-2 \\ \left(2-u^2\cos\dfrac{\theta}{2}\right)\sin\theta \\ \dfrac{u^2\sin^2\dfrac{\theta}{2}}{2} \end{pmatrix}. \tag{72}$$

The third immersed manifold is then diffeomorphic to a half Moebius strip.

For these three examples we have computed $\langle 1,\vec{R}|d_{\mathcal{M}}|1,\vec{R}\rangle$, which is equal to f^*A, and we have drawn the magnetic field of the control manifold $d_{\mathcal{M}}f^*A$. We have moreover drawn the flux density of a monopole magnetic field through the immersed surfaces. The results are represented in Fig. 2.

We see with these figures that the immersion can be used to interpret the magnetic field chart, particularly for the third example, where the sign inversion of the field is explained by the nonorientability (the twist) of the Moebius strip, and for the second example, where the existence of the two lobes of the field is explained.

V. THE APPARENT CHARGE OF A TWO LEVEL CROSSING MAGNETIC MONOPOLE IN THE CONTROL MANIFOLD

In the universal model the monopole has a charge equal to $\frac{1}{2}$. Experimentally, it is the magnetic field on $\mathcal{M}$ that we see, and the apparent charge of the monopole in $\mathcal{M}$ can be different from $\frac{1}{2}$. Leboeuf and Mouchet[25] proposed a physical realization of nonelementary magnetic monopoles in quantum adiabatic dynamics by introducing constraint parameters. They explored the properties of their nonelementary monopoles by an analysis of Dirac strings. In this paper we want to exhibit nonelementary monopoles in a different way, using the immersion of the control manifold in the generalized universal space. Although our analysis is similar to the method followed by Leboeuf and Mouchet, we present it briefly, without repeating the discussion about Dirac strings. The interested reader can see Ref. 25

A. The geometry of a level crossing

In the universal model the single monopole has a magnetic charge equal to $\frac{1}{2}$. For the Hamiltonian [Eq. (31)] that corresponds to the conical crossing of the eigenvalues $\pm\sqrt{(x^1)^2+(x^2)^2+(x^3)^2}$, a conical crossing being a zero-order contact between the energy surfaces. We recall that a contact at $\vec{R}_0$ between two surfaces defined by the equations $z=E_+(R^1,R^2)$ and $z=E_-(R^1,R^2)$ in the space (R_1,R_2,z) is said to be of order r if and only if the function $E_+(\vec{R})-E_-(\vec{R})$ and each of its derivatives of order $\leqslant r$ vanish at $\vec{R}_0$. We know that the concept of contact order is invariant under diffeomorphism, so this notion is well defined even without endowing $\mathcal{M}$ with a metric (Fig. 2). To have a complete exposition of contact manifold theory, the reader can see Ref. 26.

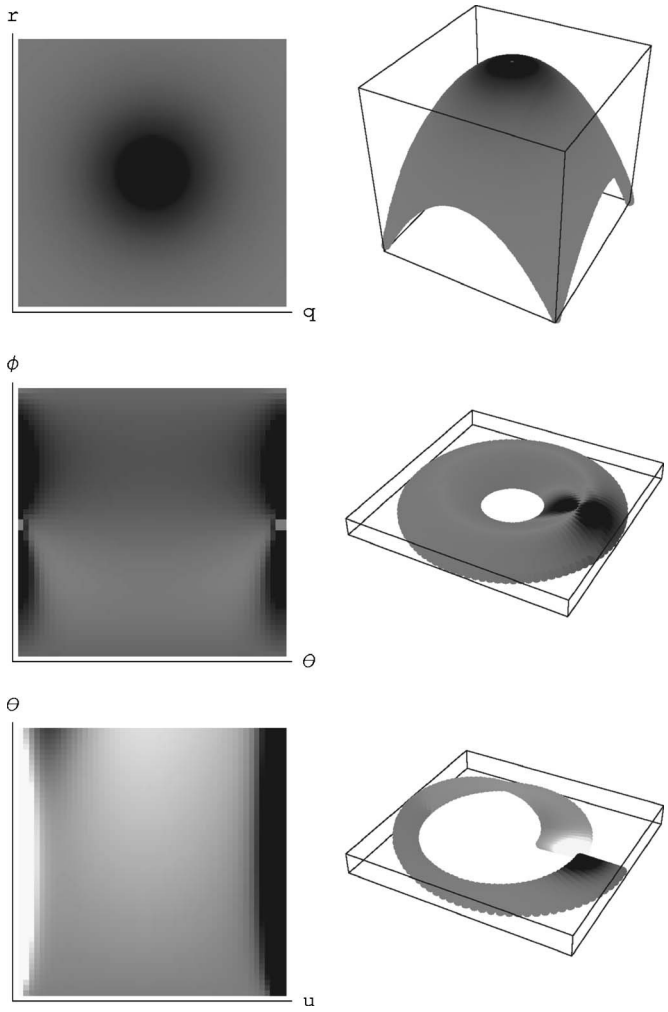

FIG. 2. Left: the magnetic field of the control manifold $d_{\mathcal{M}}\langle 1,\vec{R}|d_{\mathcal{M}}|1,\vec{R}\rangle$, Right: the immersed manifold and the flux density of a central field centered on (0, 0, 0), from top to bottom: the first example [Eq. (64)], the second example [Eq. (67)], and the third example [Eq. (70)]. The colors of the fields density are such that a strong positive field (or a strong positive flux) is black, a strong negative field (or a strong negative flux) is white, a vanishing field is gray. For the first example: $q=u\cos\theta$ and $r=u\sin\theta$.

For the generic Hamiltonian [Eq. (36)], the contact order between the energy surfaces (the order of the intersection) depends of the immersion f. Let $E_{\pm}=\pm\sqrt{f^i(\vec{R})f^j(\vec{R})\delta_{ij}}$ be the eigenvalues of the effective Hamiltonian. Let $\epsilon(\vec{R})=[E_+(\vec{R})-E_-(\vec{R})]/2$. By definition if $\vec{R}_0$ is the position of a level crossing then $\epsilon(\vec{R}_0)=0$ (i.e., $\forall i$, $f^i(\vec{R}_0)=0$). We have:

$$\frac{\partial\epsilon}{\partial R^\mu}=\frac{\frac{\partial f^i}{\partial R^\mu}f^j\delta_{ij}}{\sqrt{f^if^j\delta_{ij}}} \tag{73}$$

$$=\frac{\frac{\partial f^1}{\partial R^\mu}f^1}{\sqrt{(f^1)^2+(f^2)^2+(f^3)^2}}+\frac{\frac{\partial f^2}{\partial R^\mu}f^2}{\sqrt{(f^1)^2+(f^2)^2+(f^3)^2}}+\frac{\frac{\partial f^3}{\partial R^\mu}f^3}{\sqrt{(f^1)^2+(f^2)^2+(f^3)^2}}. \tag{74}$$

It is then clear that

$$\forall i, \quad \left.\frac{\partial f^i}{\partial R^\mu}\right]_{\vec{R}=\vec{R}_0} = 0 \Rightarrow \left.\frac{\partial \epsilon}{\partial R^\mu}\right]_{\vec{R}=\vec{R}_0} = 0. \tag{75}$$

The contact order between the energy surfaces is $\geqslant 1$ if $\forall i$, $\forall \mu$ $\partial f^i/\partial R^\mu]_{\vec{R}=\vec{R}_0}=0$. More generally, we can prove that

$$\frac{\partial^n \epsilon}{\partial R^{\mu_1} \dots \partial R^{\mu_n}} = \frac{1}{2}\sum_{p=0}^{n-1} \sum_{\sigma \in S_n} \frac{1}{(n-p)!p!} \frac{\partial^{n-p} f^i}{\partial R^{\mu_{\sigma(1)}} \dots \partial R^{\mu_{\sigma(n-p)}}} \frac{\partial^p f^j}{\partial R^{\mu_{\sigma(n-p+1)}} \dots \partial R^{\mu_{\sigma(n)}}} \delta_{ij}$$
$$- \frac{1}{2\epsilon}\sum_{p=1}^{n-1} \sum_{\sigma \in S_n} \frac{1}{(n-p)!p!} \frac{\partial^{n-p} \epsilon}{\partial R^{\mu_{\sigma(1)}} \dots \partial R^{\mu_{\sigma(n-p)}}} \frac{\partial^p \epsilon}{\partial R^{\mu_{\sigma(n-p+1)}} \dots \partial R^{\mu_{\sigma(n)}}}, \tag{76}$$

where S_n is the nth group of permutations. Then, the order of the crossing is greater than or equal to r if $\forall n \leqslant r$, $\forall i$, $\forall \mu_1, \dots, \mu_n$ $\partial^n f^i/\partial R^{\mu_1} \dots \partial R^{\mu_n}]_{\vec{R}=\vec{R}_0}=0$.

B. Perturbative analysis

We will see that the apparent charge of the magnetic monopole in $\mathcal{M}$ is related to the order of the eigenvalue crossing and thereby is related to the number of zero derivatives of f at $\vec{R}_0$. We consider a neighborhood $\mathcal{U}$ of $\vec{R}_0$. We suppose that $f(\mathcal{U})$ is tangent to the plane $x^3=0$ in $\mathbb{R}^3$, i.e., that the Dirac strings are orthogonal to $f(\mathcal{U})$. If this is not the case, we can always use a gauge transformation such that the Dirac strings rotate to be orthogonal to $f(\mathcal{U})$; in other words we change the coordinates system such that the x^3 axis coincides with the Dirac strings. In agreement with this hypothesis, and with $\mathcal{U}$ sufficiently small, we can consider that $\forall \vec{R} \in \mathcal{U} f^3(\vec{R}) \simeq 0$. In the plane $x^3=0$ we have the gauge potential

$$A = \frac{i}{2}\frac{x^2 \mathrm{d}x^1 - x^1 \mathrm{d}x^2}{(x^1)^2 + (x^2)^2} = \frac{i}{2}\frac{x^i \mathrm{d}x^j \epsilon_{ij}}{x^i x^j \delta_{ij}}. \tag{77}$$

Note that in this expression the Kronecker symbol δ_{ij} plays the role of the metric tensor of the Euclidian plane and the Levi-Civita symbol ϵ_{ij} plays the role of the vector cross product in the Euclidian space. They are then metric dependent tensors (contrary to the previous parts of this paper where the Levi-Civita symbol has been used to represent the sum over the permutations).

The gauge potential in $\mathcal{M}$ in the neighborhood of $\vec{R}_0$ is

$$f^* A = \frac{i}{2}\frac{f^i(\vec{R})\dfrac{\partial f^j}{\partial R^\mu}\epsilon_{ij}\mathrm{d}R^\mu}{f^i(\vec{R}) f^j(\vec{R})\delta_{ij}}. \tag{78}$$

But in the neighborhood of $\vec{R}_0$ we can use a Taylor expansion:

$$f^i(\vec{R}) = f^i(\vec{R}_0) + (R^\mu - R_0^\mu) \left.\frac{\partial f^i}{\partial R^\mu}\right]_{\vec{R}=\vec{R}_0} + \left.\frac{(R^\mu - R_0^\mu)(R^\nu - R_0^\nu)}{2}\frac{\partial^2 f^i}{\partial R^\mu \partial R^\nu}\right]_{\vec{R}_0}$$
$$+ \dots + \frac{(R^{\mu_1} - R_0^{\mu_1}) \dots (R^{\mu_n} - R_0^{\mu_n})}{n!} \left.\frac{\partial^n f^i}{\partial R^{\mu_1} \dots \partial R^{\mu_n}}\right]_{\vec{R}_0} + \mathcal{O}(((R^\mu - R_0^\mu)(R^\nu - R_0^\nu)\delta_{\mu\nu})^{n/2}). \tag{79}$$

Now we suppose that $\forall r \leqslant n-1$, $\forall i$, $\forall \mu_1, \dots, \mu_r$ $\partial^r f^i/\partial R^{\mu_1} \dots \partial R^{\mu_r}]_{\vec{R}=\vec{R}_0}=0$; the contact order of the level crossing is then equal to $n-1$. It is clear that any Taylor expansion must be of an order equal to n. $\forall \vec{R}$ in the neighborhood of $\vec{R}_0$ we have

$$f^i(\vec{R}) \simeq \frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_n} - R_0^{\mu_n})}{n!} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_n}} \right]_{\vec{R}_0}, \tag{80}$$

$$\frac{\partial f^i}{\partial R^\nu} \simeq \frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_{n-1}} - R_0^{\mu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_{n-1}} \partial R^\nu} \right]_{\vec{R}_0}, \tag{81}$$

$$g_{\mu\nu}(\vec{R}) = \frac{\partial f^i}{\partial R^\mu} \frac{\partial f^j}{\partial R^\nu} \delta_{ij} \tag{82}$$

$$\simeq \frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_{n-1}} - R_0^{\mu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_{n-1}} \partial R^\mu} \right]_{\vec{R}_0} \times \frac{(R^{\nu_1} - R_0^{\nu_1}) \ldots (R^{\nu_{n-1}} - R_0^{\nu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^i}{\partial R^{\nu_1} \ldots \partial R^{\nu_{n-1}} \partial R^\nu} \right]_{\vec{R}_0} \delta_{ij}, \tag{83}$$

$$f^i f^j \delta_{ij} \simeq \frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_n} - R_0^{\mu_n})(R^{\nu_1} - R_0^{\nu_1}) \ldots (R^{\nu_n} - R_0^{\nu_n})}{(n!)^2} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_n}} \right]_{\vec{R}_0} \times \left. \frac{\partial^n f^j}{\partial R^{\nu_1} \ldots \partial R^{\nu_n}} \right]_{\vec{R}_0} \delta_{ij} \tag{84}$$

$$\simeq \frac{(R^{\mu_n} - R_0^{\mu_n})(R^{\nu_n} - R_0^{\nu_n})}{n^2} g_{\mu_n \nu_n} \tag{85}$$

$$\simeq \frac{\mathcal{N}}{n^2}. \tag{86}$$

We then have

$$f^* A \simeq \frac{in^2}{2\mathcal{N}} \left(\frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_n} - R_0^{\mu_n})}{n!} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_n}} \right]_{\vec{R}_0} \times \frac{(R^{\nu_1} - R_0^{\nu_1}) \ldots (R^{\nu_{n-1}} - R_0^{\nu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^j}{\partial R^{\nu_1} \ldots \partial R^{\nu_n}} \right]_{\vec{R}_0} \epsilon_{ij} \right). \tag{87}$$

However, the cross product in $\mathcal{M}$ induced by the Euclidian cross product is defined by

$$(R^\mu - R_0^\mu) \mathrm{d}R^\nu \epsilon^g_{\mu\nu} = (R^\mu - R_0^\mu) \mathrm{d}R^\nu \frac{\partial f^i}{\partial R^\mu} \frac{\partial f^j}{\partial R^\nu} \epsilon_{ij} \tag{88}$$

$$\simeq (R^\mu - R_0^\mu) \mathrm{d}R^\nu \frac{(R^{\mu_1} - R_0^{\mu_1}) \ldots (R^{\mu_{n-1}} - R_0^{\mu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^i}{\partial R^{\mu_1} \ldots \partial R^{\mu_{n-1}} \partial R^\mu} \right]_{\vec{R}_0} \times \frac{(R^{\nu_1} - R_0^{\nu_1}) \ldots (R^{\nu_{n-1}} - R_0^{\nu_{n-1}})}{(n-1)!} \left. \frac{\partial^n f^j}{\partial R^{\nu_1} \ldots \partial R^{\nu_{n-1}} \partial R^\nu} \right]_{\vec{R}_0} \epsilon_{ij}. \tag{89}$$

In summary, we have the result

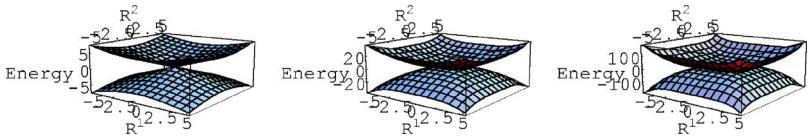

FIG. 3. (Color online) The energy surfaces drown with respect to the coordinates of $\mathcal{M}$ for (from left to right): the immersion $f(\vec{R})=(R^1,R^2,0)$ (a monopole with charge $\frac{1}{2}$), the immersion $f(\vec{R})=((R^1)^2,(R^2)^2,0)$ (a monopole with charge 1), and the immersion $f(\vec{R})=((R^1)^3,(R^2)^3,0)$ (a monopole with charge $\frac{3}{2}$).

$$f^*A \simeq \frac{ni}{2}\frac{(R^\mu - R_0^\mu)\mathrm{d}R^\nu \epsilon^g_{\mu\nu}}{(R^\lambda - R_0^\lambda)(R^\rho - R_0^\rho)g_{\lambda\rho}}. \tag{90}$$

By comparing this expression with Eq. (77), we see that f^*A is the gauge potential of a monopole with magnetic charge equal to $n/2$ in the curved space $\mathcal{M}$ with metric g. We conclude that if the magnetic monopole in $\mathcal{M}$ has a charge equal to n then the contact order of the energy surface crossing is equal to $n-1$ (Fig. 3).

C. Topological analysis

The previous analysis has the advantage that it exhibits the monopole gauge potential in $\mathcal{M}$, but a shorter analysis is possible using a topological result. Let S^1 be a circle in the plane $x^3=0$ centered over 0. We have (see Ref. 27, p. 152)

$$\frac{-i}{2\pi}\oint_{S^1} A = \frac{1}{4\pi}\oint_{S^1}\frac{x^2\mathrm{d}x^1 - x^1\mathrm{d}x^2}{(x^1)^2+(x^2)^2} = \frac{1}{2} \tag{91}$$

more generally for any loop $\mathcal{C}$ in the plane $\mathcal{M}$ (a loop is a closed path) we have

$$\frac{1}{2\pi}\oint_{\mathcal{C}}\frac{x^2\mathrm{d}x^1 - x^1\mathrm{d}x^2}{(x^1)^2+(x^2)^2} = n, \tag{92}$$

where n is the number of oriented turns of $\mathcal{C}$ around 0. This number is a topological character of the loop in $\mathbb{R}^2\backslash\{0\}$: it is invariant by homotopy and is called the winding number. We can use this invariant to characterize the monopole charge. Let S^1 be a circle on $\mathcal{M}$ centered on $\vec{R}_0$. $f(\mathcal{M})$ is not a plane, but if the radius of S^1 is sufficiently small we can consider that $f(\mathcal{M})$ is approximately flat in the neighborhood of $f(S^1)$. We use the complex coordinate of $\mathcal{M}$, $z=R^1+iR^2$,

$$f(z) = \sqrt{(f^1(z))^2+(f^2(z))^2}\exp\left(i\arctan\frac{f^2(z)}{f^1(z)}\right) \tag{93}$$

$$= \epsilon(z)\exp\left(i\arctan\frac{f^2(z)}{f^1(z)}\right). \tag{94}$$

If the contact order is equal to $n-1$, then ϵ has a zero of order n at z_0. We can then write $f(z)=(z-z_0)^n h(z)$, where $h(z)$ is a holomorphic function and where $(z-z_0)^n=r^n e^{in\theta}$. We have:

$$\arg f(z) = \arg(z-z_0)^n + \arg h(z) = n\theta + \arg h(z), \tag{95}$$

$$\frac{1}{2\pi}\oint_{S^1} \mathrm{d}\arg f = \frac{1}{2\pi}\oint_{S^1} n\mathrm{d}\theta + \frac{1}{2\pi}\mathrm{d}\arg h(z) \tag{96}$$

$$= n + \underbrace{\frac{1}{2\pi}\oint_{S^1} \frac{\partial h(z)}{\partial z}\mathrm{d}z}_{=0 \text{ by the residus lemma}} \tag{97}$$

$$= n. \tag{98}$$

We also have

$$\mathrm{d}\arg f = \mathrm{d}\arctan\frac{f^2}{f^1} = \frac{f^1\mathrm{d}f^2 - f^2\mathrm{d}f^1}{(f^1)^1 + (f^2)^2} = -i2f^*A \tag{99}$$

and so conclude that

$$\frac{-i}{2\pi}\oint_{S^1} f^*A = \frac{-i}{2\pi}\oint_{f(S^1)} A = \frac{n}{2}. \tag{100}$$

The monopole in $\mathcal{M}$ thus has an apparent charge equal to $n/2$.

VI. NON-ABELIAN MONOPOLE ASSOCIATED WITH A MULTILEVEL CROSSING

In the previous parts we have considered only two-level crossings between nondegenerate states. Now we consider multilevel crossings, for example the crossing of three nondegenerate states or the crossing of a doubly degenerate state with a nondegenerate state.

A. Immersion of the control manifold

By elimination of the other states, we suppose that the Hamiltonian can be written in the neighborhood of the multilevel crossing as

$$H^{\mathrm{eff}}(\vec{R}) = f^i(\vec{R})J_i, \tag{101}$$

where $\{J_i\}$ is a set of generators of a real Lie algebra $\mathfrak{g}$ associated with a Lie group G (the Hamiltonian symmetry group). Usually we have $G=\mathrm{U}(m)$, where m is the number of levels involved in the crossing (or the sum of the degeneracy degrees of the levels involved in the crossing). But we know that the physics of an m-level system can be described simply by $G=\mathrm{SU}(m)$ (see Refs. 28 and 29). Let d be the number of generators of G ($d=\dim\mathfrak{g}$). The immersion f defined by $f(\vec{R})=(f^1(\vec{R}),\ldots,f^d(\vec{R}))$ is then a map from $\mathcal{M}$ to $\mathbb{R}^d$. $\mathbb{R}^d$ plays the role of the generalized universal space in place of $\mathbb{R}^3$. Let $\{H_i,E_\alpha\}_{i,\alpha}$ be the Cartan basis of $\mathfrak{g}$. The Cartan subalgebra (the algebra generated by $\{H_i\}_i$) is the Lie algebra of the maximal torus T of G. Let $E(\vec{R})$ be the diagonal matrix of the eigenvalues of $H(\vec{R})$ (the matrix of levels involved in the crossing). As the diagonal matrix group is Abelian, we have $E(\vec{R})=b^i(\vec{R})H_i$. Then the diagonalization of H^{eff} can be written

$$H^{\text{eff}}(\vec{R}) = e^{i\chi^{\alpha}(\vec{R})E_{\alpha}} E(\vec{R}) e^{-i\chi^{\alpha}(\vec{R})E_{\alpha}} \tag{102}$$

$$= \exp\left(i \sum_{\alpha>0} (z^{\alpha}(\vec{R})E_{\alpha} + \overline{z}^{\alpha}(\vec{R})E_{-\alpha}) \right) E(\vec{R})$$
$$\times \exp\left(- i \sum_{\alpha>0} (\overline{z}^{\alpha}(\vec{R})E_{\alpha} + z^{\alpha}(\vec{R})E_{-\alpha}) \right), \tag{103}$$

where $T(\vec{R}) = e^{i\chi^{\alpha}(\vec{R})E_{\alpha}}$ is the diagonalizing matrix for $H^{\text{eff}}(\vec{R})$. The Berry phase depends only on $z^{\alpha}(\vec{R})$ or equivalently on $\chi^{\alpha}(\vec{R})$. Moreover it is clear that $\{\chi^{\alpha}\}_{\alpha}$ and $\{z^{\alpha}\}_{\alpha}$ are, respectively, real and complex coordinates systems for the manifold G/T. This manifold is called a flag manifold, Mostafazadeh[30] has shown that it is also the universal manifold for the system with symmetry group G, and $\chi: \mathcal{M} \to G/T$ defined by $\chi(\vec{R}) = (\chi^{\alpha}(\vec{R}))_{\alpha}$ is the universal map. Clearly the flag manifold G/T is a complex manifold which has a Riemannian structure induced by the embedding $G/T \hookrightarrow \mathbb{C}P^{n-1}$ (see Ref. 30), where n is the dimension of the original Hilbert space. The Kählerian structure of $\mathbb{C}P^{n-1}$ induces the Riemannian structure of G/T considered as a real manifold. Let r be the rank of $\mathfrak{g}$ (the dimension of the Cartan subalgebra). $\mathbb{R}^d$ is foliated with leafs which are diffeomorphic to G/T and with the foliation parameters $\{b^i(\vec{R})\}_{i=1,\ldots,r}$, $(G/T, \mathbb{R}^r) \simeq \mathbb{R}^d$. Considering a particular leaf G/T, we have the following commutative diagram:

$$\begin{array}{ccc} \mathcal{M} & \overset{\chi^{\alpha}}{\to} & G/T \\ f^i \downarrow & \Phi^{\alpha} \swarrow & \downarrow \hookrightarrow \\ \mathbb{R}^d & \underset{\hookrightarrow}{\to} & \mathbb{C}P^{n-1} \end{array}$$

where Φ is defined by

$$H^{\text{eff}}(\vec{R}) = \text{Ad}(e^{i\chi^{\alpha}(\vec{R})E_{\alpha}}) b^i(\vec{R}) H_i = e^{i\chi^{\alpha}(\vec{R})\text{ad}(E_{\alpha})} b^i(\vec{R}) H_i = \Phi^i(\vec{R}) H_i + \Phi^{\beta}(\chi(\vec{R})) E_{\beta}., \tag{104}$$

Here Ad is the adjoint action of the Lie group on its Lie algebra, and ad is the adjoint action of the Lie algebra on itself. We suppose that G is compact and semisimple; then the Killing form of its *complex* Lie algebra $\mathfrak{g}_{\mathbb{C}}$ is positively defined. Following the commutativity structure of the previous diagram, the Riemannian structure of G/T is also induced by the Killing form of $\mathfrak{g}_{\mathbb{C}}$ considered as a scalar product on $\mathbb{R}^d$. If $G = \text{SU}(N)$ then $2NK$ is the Euclidian metric of $\mathbb{R}^d$ (where K is the Killing form of $\text{SU}(N)$).

In the case of a two-level crossing, $G = \text{SU}(2)$, $d = 3$ and the maximal torus is $\text{U}(1)$; the flag manifold is then $\text{SU}(2)/\text{U}(1) \simeq S^2$ in agreement with the discussion in previous sections. In the case of a three-level crossing, $G = \text{SU}(3)$, the universal space is $\mathbb{R}^8$, the maximal torus is $T^2 = \text{U}(1) \times \text{U}(1)$ and the flag manifold is $\text{SU}(3)/(\text{U}(1) \times \text{U}(1))$. For the generic case of an N-level crossing, the symmetry group is $\text{SU}(N)$, its dimension is $d = N^2 - 1$, and the standard monopole exists in the universal space $\mathbb{R}^{N^2-1}$. The flag manifold (the universal manifold) is $\text{SU}(N)/T^{N-1} \simeq \mathbb{C}P^{N-1} \ltimes \mathbb{C}P^{N-2} \ltimes \ldots \ltimes \mathbb{C}P^1$ where T^{N-1} is the $(N-1)$-torus:

$$T^{N-1} = \underbrace{\text{U}(1) \times \cdots \times \text{U}(1)}_{N-1 \text{ times}}$$

and where $\ltimes$ denotes a possible nontrivial topological product. The induced metric on $\mathcal{M}$ is

$$g_{\mu\nu} = \delta_{ij} \frac{\partial f^i}{\partial R^{\mu}} \frac{\partial f^j}{\partial R^{\nu}} \tag{105}$$

with $i = 1, \ldots, N^2 - 1$ and $\mu = 1, 2$.

B. An analogy with the field theory

The monopole gauge potential is $A \in \Omega^1(\mathbb{R}^{N^2-1}, \mathfrak{su}(N))$. The monopole field is obtained by the Cartan structure equation $F = \mathrm{d}A + \frac{1}{2}[A,A] \in \Omega^2(\mathbb{R}^{N^2-1}, \mathfrak{su}(N))$ and satisfies half of the Yang-Mills equations, i.e., the Bianchi identity $\mathrm{d}F + [A,F] = 0$. In $\mathcal{M}$, $f^*A \in \Omega^1(\mathcal{M}, \mathfrak{su}(N))$ and $f^*F \in \Omega^2(\mathcal{M}, \mathfrak{su}(N))$ satisfy similar equations. Consider the Abelian case of a pure adiabatic transport. We suppose that the evolution of the system is a path $\mathcal{C}$ on $\mathcal{M}$ which passes in the neighborhood of a two-level crossing but is sufficiently far away or is traversed at such a speed that no population transfer occurs. The path $\mathcal{C}$ is parametrized by a function $t \mapsto \vec{R}(t)$. Let $\{|+,\vec{R}\rangle^N, |-,\vec{R}\rangle^N\}$ be the two eigenvectors. If we suppose that $\psi(0) = |+,\vec{R}(0)\rangle^N$ then we have

$$\psi(t) = \exp\left(- i\hbar^{-1} \int_0^t E_+(\vec{R}(t'))\mathrm{d}t' - \int_{\vec{R}(0)}^{\vec{R}(t)} A_+^N(\vec{R}) \right) |+,\vec{R}(t)\rangle^N, \tag{106}$$

where $A_+^N = {}^N\langle +,\vec{R}|d_{\mathcal{M}}|+,\vec{R}\rangle^N$. The gauge group associated with this situation is U(1). We have a complete analogy with electrodynamics, where ψ is the matter field of a charged particle which is moving on the path $\mathcal{C}$ in $\mathcal{M}$ and which is subject to the monopole magnetic field. Indeed, Ezawa[31] notes that a single matter field $\phi(x)$ cannot be used in the whole space-time in the presence of a magnetic monopole. He uses a path-dependent formalism with $\phi(x,\mathcal{P}) = \exp(\int_\infty^x A)\phi(x)$ where $\mathcal{P}$ is a path from infinity to x. This new field is gauge invariant. In the same way, in the generalized universal space $\mathbb{R}^3$ we cannot use a single field $|+,\vec{x}\rangle$ as a matter field because

$$|+,\vec{x}\rangle^N = \frac{1}{\sqrt{2r(r+x^3)}} \begin{pmatrix} r + x^3 \\ x^1 + ix^2 \end{pmatrix}$$

is not defined for $x^3 \leqslant 0$ and

$$|+,\vec{x}\rangle^S = \frac{1}{\sqrt{2r(r-x^3)}} \begin{pmatrix} x^1 - ix^2 \\ r - x^3 \end{pmatrix}$$

is not defined for $x^3 \geqslant 0$. Following Ezawa, by elimination of the dynamical phase, we set $\tilde{\psi}(\vec{x},\mathcal{C}) = \exp(-\int_{\vec{x}_0}^{\vec{x}} A_+)|+,\vec{x}\rangle$ where $\mathcal{C}$ is a path from an arbitrary point $\vec{x}_0$ to $\vec{x}$. Let U_S and U_N be the charts for which A_+^S and A_+^N, respectively, are well defined. Suppose that $\vec{x}_0 \in U_S$. Then

$$\tilde{\phi}(\vec{x},\mathcal{C}) = \begin{cases} \exp\left(- \int_{\vec{x}_0}^{\vec{x}} A_+^S \right) |+,\vec{x}\rangle^S \text{if } \vec{x} \in U_S \\ \exp\left(- \int_{\vec{x}_0}^{\vec{x}_1} A_+^S \right) \exp\left(- \int_{\vec{x}_1}^{\vec{x}} A^N \right) |+,\vec{x}\rangle^N \quad \text{if } \vec{x} \in U_N, \text{ with } \vec{x}_1 \in U_N \cap U_S. \end{cases} \tag{107}$$

We see that the formalism used by Ezawa to define a matter field in the presence of a magnetic monopole is similar to the adiabatic transport formula. Then we can say that the quantum system driven along a path $\mathcal{C}$ in the control parameter manifold $\mathcal{M}$ is similar to, for example, an electron which is forced to follow $\mathcal{C}$ in presence of a monopole magnetic field.

Now consider the case of a crossing of three nondegenerate states. The wave function is

$$\psi(t) = \sum_{b=1}^{3} \left[\mathbb{T} \exp\left(- i\hbar^{-1} \int_0^t E(\vec{R}(t'))\mathrm{d}t' - \int_{\vec{R}(0)}^{\vec{R}(t)} A(\vec{R}) \right) \right]_{ba} |b,\vec{R}(t)\rangle \tag{108}$$

and the gauge group is SU(3). SU(3) is represented on the space spanned by $\{|1,\vec{R}\rangle, |2,\vec{R}\rangle, |3,\vec{R}\rangle\}$ by the irreducible representation $D^{1,0}$ (see Refs. 32). The situation is completely analogous to that of a quark field ψ in the presence of a colored monopole, see Ref. 5, 6, and 31,

$\{|1,\vec{R}\rangle,|2,\vec{R}\rangle,|3,\vec{R}\rangle\}$ being a color triplet. As is the case in chromodynamics, *"since SU(3) is unbroken symmetry, (…) the specification of the colour of a quark field depends on an arbitray choice of basis for the three-dimensional space of colours at each point in space-time"* (see Ref. 33), the basis $\{|1,\vec{R}\rangle,|2,\vec{R}\rangle,|3,\vec{R}\rangle\}$ defined the colors at each point $\vec{R}$ of $\mathcal{M}$, the color operators being

$$J_3=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix},\quad \sqrt{3}J_8=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix} \tag{109}$$

the matrices being written in the $\vec{R}$-dependent basis $\{|1,\vec{R}\rangle,|2,\vec{R}\rangle,|3,\vec{R}\rangle\}$. The initial point of the dynamics $\vec{R}(0)$ can be considered as being a privileged point and consitutes a symmetry breaking. For example, in the case of an atom or a molecule driven by a pulse chirped laser, the initial point is the position in $\mathcal{M}$ for which the laser is off. In this case the basis $\{|1,\vec{R}(0)\rangle,|2,\vec{R}(0)\rangle,|3,\vec{R}(0)\rangle\}$ is privileged as the basis for the bare atom or molecule unperturbed by the field. The two possible descriptions of the color using "the symmetry breaking basis" and using "the $\vec{R}$-dependent basis," are associated with the choice of the molecular time-dependent description of population transfers, using "the unperturbed basis" or using "the instantaneous dressed basis."

VII. FINAL REMARKS AND CONCLUSION

A. Global description versus local description

All of the previous discussion has concerned the neighborhood of a crossing, and has thus given a local analysis. If we consider $\mathcal{M}$ globally these might be several crossings (monopoles) on $\mathcal{M}$. Let n be the dimension of the original Hilbert space and m be the dimension of the adiabatic subspace. We know that the universal manifold of the gobal description is the Grassmanian manifold $G_m(\mathbb{C}^n)$. The relation between global and local description is the following. Let f be the global universal map from $\mathcal{M}$ to $G_m(\mathbb{C}^n)$. Let $\vec{R}_0$ be a point where there exists a level crossing. Let G/T be the flag manifold of this level crossing (the local universal manifold) and χ be the local universal map from $\mathcal{M}$ to G/T. $G_m(\mathbb{C}^n)=\mathrm{U}(n)/(\mathrm{U}(n-m)\times\mathrm{U}(m))$ where $\mathrm{U}(n)$ is the group of unitary tranformations of the original space, $\mathrm{U}(m)$ is the group of unitary transformations of the adiabatic space and $\mathrm{U}(n-m)$ characterizes the adiabatic independence of the quantum system from the exterior of the adiabatic space. It is clear that G is a subgroup of $\mathrm{U}(n)$ and T is a subgroup of $\mathrm{U}(m)$, and then G/T is a submanifold of $G_m(\mathbb{C}^n)$ which is localized with the point $f(\vec{R}_0)=\chi(\vec{R}_0)$.

The local description depends on the choice of the effective Hamiltonian technique. Indeed, H^{eff} does not have the same expression in the different partitioning methods.[20–22] The geometric local description will be relevant if and only if $H^{\mathrm{eff}}(\vec{R})$ is good approximation of $H(\vec{R})$ for the crossing, i.e., if the behaviors of the eigenvalues and of the overlaps of the eigenvectors of $H^{\mathrm{eff}}(\vec{R})$ (and their first derivatives) are close to the behaviors of the associated quantities of $H(\vec{R})$. In general the problem of finding an efficient effective Hamiltonian associated with a crossing is not a simple one.

B. The control manifold

All of the discussion can be generalized to a control manifold with dimension greater than two, exept for the links between $*_g f^* B$ and the monopole magnetic flux, which is the most interesting aspect of the monopole magnetic field in the two-dimensional case. Note that for a two-level crossing, the map $f:\mathcal{M}\to\mathbb{R}^3$ cannot be an immersion if $\dim\mathcal{M}>2$.

We can remark that in a theoretical study, the choice of the control manifold can be arbitrary; in order to have a physical meaning for $\mathcal{M}$ and its virtual magnetic monopoles, we can choose $\mathcal{M}$

to be closely appropriate to the experimental situation. The two parameters of $\mathcal{M}$ must be two "control levers" of the experimentalist, in order that the monopole effects can appear naturally in the experimental results

C. The charge of non-Abelian monopoles

The definition of the charge of a non-Abelian monopole, for example, for a three level crossing, is not clear. In the Abelian case the generalized universal space is $\mathbb{R}^3$ and we can apply the method followed in field theory. In the non-Abelian cases the generalized universal space is $\mathbb{R}^d$ with $d>3$, which cannot be identified with the usual physical space. The topological methods usually followed must be adapted and more subtle studies are needed to find a relevant definition of the charge of the non-Abelian adiabatic monopoles.

D. About nonadiabatic evolutions

The adiabatic assumption states that the quantum dynamical system can be described at each time by a little set of instantaneous eigenvectors. In the nonadiabatic cases, there exist some techniques to describe the quantum system with a time-dependent non-eigenbasis (see, for example, the time-dependent wave operator theory).[34] In this case, the dynamics can be represented by a finite dimensional effective Hamiltonian. We can suppose that these time-dependent vectors can be expressed as control parameter-dependent vectors (in fact this is a strong assumption because in general these vectors depend not only on the instantaneous time but also on the past evolution). In this case the wave function takes the form of Eq. (3) but where $|a,\vec{R}(t)\rangle$ is not an eigenvector and where $E(\vec{R}(t))_{ab}=\langle a,\vec{R}(t)|H^{\text{eff}}(\vec{R}(t))|b,\vec{R}(t)\rangle$ is not a diagonal matrix. Following the works of Mostafazadeh and Bohm[35,36] we can suppose that there exists a smooth map $\mathcal{F}:\mathcal{M}\to\mathcal{M}$ such that $\{|a,\vec{R}(t)\rangle\}_a$ are the eigenvectors of $\tilde{H}^{\text{eff}}(\vec{R})=H^{\text{eff}}(F(\vec{R}))$. Let f be the immersion map associated with $\tilde{H}^{\text{eff}}$, we can consider $f\circ F$ as the immersion map of H^{eff}, this map is well associated with the properties of magnetic monopoles since $\{|a,\vec{R}\rangle\}_a$ are the eigenvectors of $\tilde{H}^{\text{eff}}$. Nevertheless the physical significance of these monopoles is not clear because they are not associated with an eigenlevel crossing. Moreover the assumption of the existence of F and above all the assumption of the control parameters dependence of the basis are important limitations on the class of nonadiabatic quantum systems for which we can apply the theory presented in this paper.

E. Conclusion

The knowledge of the magnetic field in the control manifold can be very important for the numerical simulations of quantum adiabatic dynamics. By computing this field, which is equal to the monopole field density of $f(\mathcal{M})$, we can localize the level crossings. It is well known that the variations of the wave function are more important in the neighborhood of the level crossings. If we model the control manifold by using a discrete numerical lattice X, then we need more vertices in the neighborhood of the level crossings in order to have a minimal data storage requirement, together with a good description of the wave function. We must then employ a nonhomogeneous lattice with small cells in the neighborhood of the crossing and with larger cells elsewhere. We can use the field $*_g f^* B$ to obtain a criterion about the local choice of cell sizes.

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Phase space quantum mechanics - Direct

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Conventional approach to quantum mechanics in phase space, (q,p), is to take the operator based quantum mechanics of Schrödinger, or an equivalent, and assign a c-number function in phase space to it. We propose to begin with a higher level of abstraction, in which the independence and the symmetric role of q and p is maintained throughout, and at once arrive at phase space state functions. Upon reduction to the q- or p-space the proposed formalism gives the conventional quantum mechanics, however, with a definite rule for ordering of factors of noncommuting observables. Further conceptual and practical merits of the formalism are demonstrated throughout the text. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Wigner's 1932 initiative[1] is a reformulation of the operator based quantum theory of Schrödinger in the language of c-number distribution functions in a phase space. His prescription, however, turns out to have a feature extra to what one finds in Schrödinger's theory. There is nothing in the founding principles of the operator based theory to prescribe a rule for ordering of the factors of noncommuting operators in a product. In contrast, Wigner's formalism, upon reduction from phase space to the configuration space, acquires Weyl's ordering,[2,3] How and at what stage, in going from Schrödinger's state functions in configuration space to those of Wigner in phase space and again coming back to the configuration space, acquires Weyl's ordering creep in? This feature is not unique to Wigner's functions. Other distributions exist in the literature, e.g., Kirkwood,[4] Husimi,[5] Margenau and Hill,[6] Torres-Vega and Frederick,[7–9] Li *et al.*,[10] de Gosson,[11,12] etc. Each of them carries its own ordering rule, with no precedence in the configuration space formalism. Can one conjecture that the phase space formulations of quantum mechanics are more complete than their configuration space counterpart, because of their built-in ordering rules? If so, there should be a way to arrive at phase space formulations without reference to the conventional operator based theory. Here we argue that in the classical dynamics and classical statistical dynamics (Liouville's equation) the generalized coordinates and momenta, q and p, respectively, play symmetric and more importantly, independent roles. In the operator based quantum theory one or the other loses its identity at the expense of the other and the formalism reduces to one in either q or p space. One could avoid this by carrying the q and p formalisms concomitantly and at once arrive at state functions in qp spaces. The so-obtained state functions are the qp representa-

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tion of the mixed states of quantum statistical mechanics. The operator based theory emerges as a special case of this general one, but this time with a definite ordering rule for noncommutative operators. The rule depends on the nature of the q and p variables, adopted initially.

II. EXTENSION OF THE CLASSICAL DYNAMICS

Let $q=\{q_i(t), i=1,\ldots,N\}$ be the collection of the generalized coordinates describing the state of motion of a dynamical system. It is customary to assign a Lagrangian, $L^q(q,\dot{q})$, to the system, define the conjugate momenta, $p=\partial L^q/\partial\dot{q}$, and construct the $H(q,p)=\dot{q}p-L^q$. One may do this the other way around. Begin with a given $H(q,p)$ and find $L^q(q,\dot{q})$ as a solution of the following differential equation;

$$H\left(q,\frac{\partial L^q}{\partial\dot{q}}\right)-\dot{q}\frac{\partial L^q}{\partial\dot{q}}+L^q=0. \tag{1}$$

One may, however, carry out the same procedure with q replaced by p and arrive at a $L^p(p,\dot{p})$ satisfying the differential equation

$$H\left(\frac{\partial L^p}{\partial\dot{p}},p\right)+\dot{p}\frac{\partial L^p}{\partial\dot{p}}-L^p=0. \tag{2}$$

The use of L^p to study the evolution of a dynamical system is not a common practice. But it is a possibility and has precedence.[13] There is no bar to employing the two alternatives simultaneously. We follow Sobouti and Nasiri[14] (hereafter, paper I) and define the "extended Lagrangian"

$$\mathcal{L}(q,\dot{q};p,\dot{p})=-\dot{q}p-q\dot{p}+L^q(q,\dot{q})+L^p(p,\dot{p}). \tag{3}$$

The first two terms on the right-hand side constitute a total time derivative and are introduced for later convenience. One may now write down the Euler-Lagrange equations for q and p,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}}-\frac{\partial\mathcal{L}}{\partial q}=\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L^q}{\partial\dot{q}}-\frac{\partial L^q}{\partial q}=0, \tag{4a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{p}}-\frac{\partial\mathcal{L}}{\partial p}=\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L^p}{\partial\dot{p}}-\frac{\partial L^p}{\partial p}=0. \tag{4b}$$

Equation (4a) is the conventional equation of motion in q space. With preassigned initial values $q(t_0)$ and $\dot{q}(t_0)$ at t_0 it can be solved for the orbits $q(t)$ in q space. Similarly, with given initial values $p(t_0)$ and $\dot{p}(t_0)$, Eq. (4b) can be solved for the orbits $p(t)$ in the p space. The conditions for q and p orbits to represent the same state of motion of the system are $p(t_0)=\partial L^q/\partial\dot{q}|_{t_0}$ and $q(t_0)=\partial L^p/\partial\dot{p}|_{t_0}$. Such a state of motion will be referred to as a "pure state." Otherwise it will be called a "mixed state" of motion. The nomenclature is from the statistical quantum mechanics and it will be seen later that they imply the same notions as therein. On a pure state p and q are initially canonically conjugate pairs and it is shown in paper I that once they are canonically conjugate at one time they remain so for all times. On the other hand there are no restrictions on the initial values of q and p on mixed states. Therefore, $q(t)$ and $p(t)$ remain unrelated and evolve independently. The existence of the extended Lagrangian $\mathcal{L}(q,\dot{q};p,\dot{p})$, however, permits the following "extended momenta" to be defined:

$$\pi_q=\frac{\partial\mathcal{L}}{\partial\dot{q}}=\frac{\partial L^q}{\partial\dot{q}}-p, \tag{5a}$$

$$\pi_p = \frac{\partial \mathcal{L}}{\partial \dot{p}} = \frac{\partial L^p}{\partial \dot{p}} - q. \tag{5b}$$

These in turn allow an "extended Hamiltonian" to be defined through the following Legendre transformation;

$$\mathcal{H}(q,\pi_q;p,\pi_p) = \dot{q}\pi_q + \dot{p}\pi_p - \mathcal{L}(q,\dot{q};p,\dot{p}). \tag{6}$$

To eliminate $\dot{q}$ and $\dot{p}$ from $\mathcal{H}$ one substitutes (a) for $\mathcal{L}$ from Eq. (3), (b) for L^q and L^p from Eqs. (1) and (2), and (c) for $\partial L^q/\partial \dot{q}$ and $\partial L^p/\partial \dot{p}$ from Eqs. (5a) and (5b). One arrives at

$$\mathcal{H}(q,\pi_q;p,\pi_p) = H(q,p+\pi_q) - H(q+\pi_p,p) = \sum_{n=0} \frac{1}{n!}\left[\frac{\partial^n H}{\partial p^n}\pi_q^n - \frac{\partial^n H}{\partial q^n}\pi_p^n\right], \tag{7}$$

where the derivatives are to be evaluated at (q,p). We leave it to the reader to familiarize him/herself with $\mathcal{H}$ by writing down four Hamilton's equations for $\dot{q}, \dot{\pi}_q, \dot{p}$, and $\dot{\pi}_p$. Here, the condition for pure state motions is $\pi_q(t_0)=\pi_p(t_0)=0$, and once they are initially zero they remain so for all times. Then by Eqs. (5a) and (5b) q and p turn into canonically conjugate pairs for all times (paper I). To summarize, for any dynamical system we introduce an extended phase space, $(q,\pi_q;p,\pi_P)$, extended momenta, Lagrangians, and Hamiltonians. All concepts and procedures of the conventional dynamics are extendible to this extended dynamics. Of particular relevance to this paper, which will be referred to shortly, are: (1) canonical transformations from one set of variables $(q,\pi_q;p,\pi_p)$ to another, and (2) Poisson's brackets extended as

$$\{F,G\} = \frac{\partial F}{\partial q}\frac{\partial G}{\partial \pi_q} - \frac{\partial F}{\partial \pi_q}\frac{\partial G}{\partial q} + \frac{\partial F}{\partial p}\frac{\partial G}{\partial \pi_p} - \frac{\partial F}{\partial \pi_p}\frac{\partial G}{\partial p}. \tag{8}$$

III. QUANTUM DYNAMICS IN *qp* SPACE

Now that we have the extended the Hamiltonian of Eq. (7) we may construct a quantum mechanics in qp space. We do this on the following premises.

(1) Let $\mathcal{X}$ be the function space of all integrable complex functions $\chi(q,p)$. Let q,π_q,p, and, π_p be operators on $\mathcal{X}$, satisfying the commutation rules

$$[q,\pi_q] = [p,\pi_p] = i\hbar\,, \quad [q,p] = [\pi_q,\pi_p] = [q,\pi_p] = [p,\pi_q] = 0. \tag{9}$$

These are the fundamental Poisson brackets of Eq. (8), promoted to commutation brackets by Dirac's prescription. Note the manifest independence of q and p in the vanishing of their commutation brackets.

(2) By virtue of Eq. (9), $\mathcal{H}$ is now an operator on $\mathcal{X}$. Let $\chi(q,p,t) \in \mathcal{X}$ be a state function satisfying the Schrödinger-type equation

$$i\hbar\frac{\partial \chi}{\partial t} = \mathcal{H}\chi = \left[H\left(q,p - i\hbar\frac{\partial}{\partial q}\right) - H\left(q - i\hbar\frac{\partial}{\partial p},p\right)\right]\chi. \tag{10}$$

(3) Let the rule to evaluate the expectation values of an observable $O(q,p)$, a real c-number operator on $\mathcal{X}$, be

$$\langle O(q,p)\rangle = \int O(q,p)\mathrm{Re}\,\chi \mathrm{d}q\mathrm{d}p = \frac{1}{2}\int O(q,p)(\chi+\chi^*)\mathrm{d}q\mathrm{d}p. \tag{11}$$

We will return to this averaging rule shortly, and revise it. The logic behind it, however, is to be noted, the averages of observables should be real. In what follows we demonstrate that (1) the formalism so designed is a theory of quantum ensembles in phase space. Its pure state case is the conventional quantum mechanics, however, with a definite ordering rule accompanying it. (2) It

can be transformed to other phase space formalisms, including to that of Wigner, by suitable unitary or similarity transformations on $\mathcal{X}$. The latter in turn originates from suitable canonical transformations from one extended phase space coordinate to another.

A. Solutions of Eq. (10)

To begin with, χ is of the form

$$\chi(q,p) = F(q,p)e^{-ipq/\hbar}. \tag{12}$$

The exponential factor is a consequence of the total time derivative, $-\mathrm{d}(qp)/\mathrm{d}t$ in Eq. (3). It is easily verified that

$$\left(p - i\hbar\frac{\partial}{\partial q}\right)\chi = i\hbar\frac{\partial F}{\partial q}e^{-ipq/\hbar}, \tag{13a}$$

$$\left(q - i\hbar\frac{\partial}{\partial p}\right)\chi = i\hbar\frac{\partial F}{\partial p}e^{-ipq/\hbar}. \tag{13b}$$

Substitution of Eqs. (13) and (12) in Eq. (10) gives

$$i\hbar\frac{\partial F}{\partial t} = \left[H\left(q, -i\hbar\frac{\partial}{\partial q}\right) - H\left(-i\hbar\frac{\partial}{\partial p}, p\right)\right]F. \tag{14}$$

The operators on the right-hand side of Eq. (14) are recognized as the Hamiltonians of the conventional quantum mechanics, the first in q and the second in p representation. Thus, one obtains the superposition of the separable solutions

$$\chi(q,p,t) = \sum_{\alpha,\beta} A_{\alpha\beta}\psi_\alpha(q,t)\phi^*_\beta(p,t)e^{-ipq/\hbar}, \tag{15}$$

where

$$i\hbar\frac{\partial\psi_\alpha}{\partial t} = H\left(q, -i\hbar\frac{\partial}{\partial q}\right)\psi_\alpha, \tag{16a}$$

$$i\hbar\frac{\partial\phi_\beta}{\partial t} = H\left(i\hbar\frac{\partial}{\partial p}, p\right)\phi_\beta. \tag{16b}$$

To each $\psi_\alpha(q)$ there corresponds a $\phi_\alpha(p)$ that are Fourier transforms of each other,

$$\psi_\alpha(q) = \frac{1}{(2\pi\hbar)^{N/2}}\int \phi_\alpha(p)e^{ipq/\hbar}\mathrm{d}p, \tag{17}$$

where N is the number of degrees of freedom of the system.

B. The averaging rule revisited: Acceptable state functions

Let $Q(q)$ be an observable represented by a real polynomial or series in q. Its matrix representation, $\hat{Q}$, in either $\chi-$, $\psi-$, or ϕ-basis is Hermitian. Thus

$$Q_{\beta\alpha} = \int \psi_\alpha(q) Q(q) \psi^*_\beta(p) e^{-ipq/\hbar} \mathrm{d}p\mathrm{d}q$$

$$= \int \psi^*_\beta(q) Q(q) \psi_\alpha(q) \mathrm{d}q = \int \phi^*_\beta(p) Q\left(i\hbar \frac{\partial}{\partial p}\right) \phi_\alpha(p) \mathrm{d}p = Q^*_{\alpha\beta}, \tag{18}$$

where we have used the fact that ψ and ϕ bases are the Fourier transforms of each other. The coefficient $(2\pi\hbar)^{-N/2}$ is suppressed for brevity. The expectation value of Q, by Eq. (11), now becomes

$$\langle Q \rangle = \frac{1}{2} \int Q(\chi + \chi^*) \mathrm{d}p\mathrm{d}d = \frac{1}{2} \mathrm{tr}[\hat{\mathrm{Q}}(\hat{\mathrm{A}} + \hat{\mathrm{A}}^\dagger)], \tag{19}$$

where $\hat{A}$ is the matrix of $A_{\alpha\beta}$ of Eq. (15). This gives the freedom of choosing $\hat{A} = \hat{A}^\dagger$ and of simplifying Eq. (11) to read $\langle Q \rangle = \int Q\chi \mathrm{d}p\mathrm{d}q = \mathrm{tr}(\hat{Q}\hat{A})$. Choosing $Q(q) = 1$, imposes the further restriction $\mathrm{tr}\,\hat{A} = 1$. Requiring the averages of all positive definite functions of q to be positive still restricts $\hat{A}$ to be a positive definite matrix. Had one chosen a differentiable function $P(p)$ instead of $Q(q)$, one still would have arrived at the same requirements for $\hat{A}$.To summarize, χ of Eq. (15) is a physically acceptable solution if

$$\hat{A} = \hat{A}^\dagger, \text{ positive definite,} \quad \text{and} \quad \mathrm{tr}\hat{A} = 1. \tag{20}$$

With this provision the averaging rule of Eq. (11) for $Q(q) + P(p)$ reduces to

$$\langle Q(q) + P(p) \rangle = \int (Q + P) \chi \mathrm{d}p\mathrm{d}q. \tag{21}$$

For a product $Q(q)P(p)$, by the prescription of Eq. (11) and with the restrictions of Eq. (20) on $\hat{A}$, one has

$$\langle QP \rangle = \mathrm{Re}\ \mathrm{tr}(\hat{Q}\hat{P}\hat{A}) = \frac{1}{2}\ \mathrm{tr}(\hat{Q}\hat{P}\hat{A} + \hat{A}\hat{P}\hat{Q}) = \mathrm{tr}\left[\frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})\hat{A}\right], \tag{22}$$

where $\hat{Q}$ and $\hat{P}$ are the matrix representations of $Q(q)$ and $P(p)$ as in Eq. (18). Translation of this to the q space language, say, is

$$\langle QP \rangle = \frac{1}{2} A_{\alpha\beta} \int \psi^*_\beta(q) \left[Q(q) P\left(-i\hbar \frac{\partial}{\partial q}\right) + P\left(-i\hbar \frac{\partial}{\partial q}\right) Q(q) \right] \psi_\alpha \mathrm{d}p. \tag{23}$$

Thus, upon reduction of the formalism of the present paper to that of the q-space, the ordering rule associated with a product $Q(q)P(p)$ is the symmetric ordering. It has emerged from the formalism itself, unlike the ad hoc ordering rules of the conventional quantum mechanics.

IV. MORE ABOUT EQ. (10)

It was stated earlier that the proposed dynamics is essentially that of the ensembles. Here we elaborate on this, and show that (1) the classical limit of the theory is Liouville's equation that governs the dynamics of classical ensembles. (2) Its pure state case is Schrödinger's operator based theory. (3) In its full generality the theory gives von Neumann's density matrix and the evolution equation associated with it.

A. Classical correspondence

In Eq. (10) expanding the Hamiltonian operators about (q,p), and retaining only the first terms in the expansion, gives

$$\frac{\partial \chi}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial \chi}{\partial q} - \frac{\partial H}{\partial p}\frac{\partial \chi}{\partial p} = \frac{\mathrm{d}\chi}{\mathrm{d}t} = 0. \tag{24}$$

This is the Liouville equation for the distribution function of classical ensembles. Its most general solutions are $\chi[q(t),p(t)]$, where $q(t)$ and $p(t)$ are the classical trajectories in q and p spaces. The two trajectories may represent the same state of motion if they satisfy the conditions of initial canonical conjugacy narrated below Eq. (4). Otherwise, they remain independent and evolve independently. It is this classical notion of independence that we have carried through to the quantum formalism. Let us also note that the reduction of the phase space evolution equation to the classical Liouville's equation is a common feature of all such formalisms.

B. Schrödinger's case

Allowance for only one term in Eq. (15) reproduces the conventional quantum mechanics in all its details. Thus

$$\chi = \psi(q)\phi^*(p)e^{-ipq/\hbar}, \tag{25a}$$

$$i\hbar\frac{\partial \psi}{\partial t} = H\left(q, -i\hbar\frac{\partial}{\partial q}\right)\psi, \tag{25b}$$

$$\psi \text{ and } \phi \text{ Fourier transforms of each other}, \tag{25c}$$

$$\int \chi \mathrm{d}p\mathrm{d}q = \int \psi^*\psi \mathrm{d}q = \int \phi^*\phi \mathrm{d}p = 1, \tag{25d}$$

$$\langle Q(q)P(p)\rangle = \frac{1}{2}\int \psi^*\left[p\left(-i\hbar\frac{\partial}{\partial q}\right)Q(q) + Q(q)P\left(-i\hbar\frac{\partial}{\partial q}\right)\right]\psi \mathrm{d}q. \tag{25e}$$

Heisenberg's uncertainty principle follows immediately from Eq. (25) that one may find in standard texts in quantum mechanics. The ordering rule of Eq. (25e) is, however, the added feature of the theory.

C. Density matrix and von Neumann's equation

The state function of Eq. (15), as it stands represents the state of an ensemble in a mixed state. If the matrix $\hat{A}$ is diagonalized to $A_{\alpha\beta}=A_\alpha\delta_{\alpha\beta}$, χ reduces to $\chi=\Sigma A_\alpha\psi_\alpha\phi_\alpha^* e^{-ipq/\hbar}$. Upon integration over q or p one immediately recognizes A_α as the probability of the system to be in the state $\psi_\alpha(q,t)$ or $\phi_\alpha(p,t)$. One may, however, do better. Let $\{\phi_n(q)\}$ be a complete orthonormal time independent basis set, and $\{\phi_n(p)\}$ be its Fourier replica. These basis sets are not required to be the eigenstates of $H(q,p)$, though this is a possibility. Hereafter, to avoid the ambiguity, we use the Latin subscripts to denote the members of the basis set and reserve Greek subscripts to denote the solutions of Eqs. (16a) and (16b). Expansion of χ in these bases assumes the form $\chi(q,p,t)=A_{mn}(t)\psi_n(q)\phi_m^*(p)e^{-ipq/\hbar}$. Substituting this form in Eq. (10), multiplying the resulting equation by $\psi_n^*(q)\phi_m(p)e^{ipq/\hbar}$, and integrating over q and p gives

$$i\hbar\frac{d\hat{A}}{dt}=[\hat{A},\hat{H}],\quad \hat{A}=\hat{A}^{\dagger}\quad \text{positive definite and tr}\,\hat{A}=1, \tag{26}$$

where $\hat{A}$ is the matrix of the expansion coefficients and $\hat{H}$ that of the $H(q,p)$ in either $\chi-$, $\psi-$, or $\phi-$ basis. Equation (26) is von Neumann's equation for the evolution of the density matrix. As is known the case $\text{tr}(\hat{A}^2)=\text{tr}\,\hat{A}=1$ represents an ensemble in a pure state. If $\text{tr}(\hat{A}^2)<1$, the ensemble is in a mixed state.

V. CANONICAL TRANSFORMATIONS

All machinery of the canonical transformations from one extended coordinate system to another and their associated unitary or similarity transformations in the function space are available for a forage of deliberations. Except for a passing remark on the prospects of fuller uses of this approach at the end of this section, here we confine ourselves to one one-parameter family of transformations of which Wigner's state function emerges as a special case. Husimi's all positive distribution functions are also briefly mentioned.

Consider the infinitesimal transformations

$$q=Q-\delta\alpha\Pi_P,\quad \pi_q=\Pi_Q;\quad p=P-\delta\alpha\Pi_Q,\quad \pi_p=\Pi_P, \tag{27}$$

The generator of the transformation is $G=\pi_p\pi_q$. To this (and for a finite α) there corresponds the unitary operator

$$U_\alpha=e^{-i\alpha G/\hbar}=e^{i\hbar\alpha\partial^2/\partial_q\partial_p},\quad U_\alpha^{\dagger}U_\alpha=1, \tag{28}$$

in the function space. Operating by U_α on a pure state function $\chi(q,p,t)=\psi(q)\phi^*(p)\times\exp(-ipq/\hbar)$ generates another state function (let us call it α-representation)

$$\chi(q,p,t)=U_\alpha\chi=\left(\frac{1}{2\pi\hbar}\right)^N\int\psi(q-\alpha\tau)\psi^*(q+(1-\alpha)\tau)e^{ip\tau/\hbar}d\tau. \tag{29}$$

See the Appendix for proof of Eq. (29). For $\alpha=1/2$, Eq. (29) gives Wigner's standard function,[15,16] $\chi_{1/2}=W(q,p,t)$. The cases $\alpha=0$ and 1 simply give back χ and χ^* of this paper, respectively. Similarly, operation by U_α on Eq. (10) gives the evolution equation for χ_α,

$$\begin{aligned}
&i\hbar\frac{\partial\chi_\alpha(q,p,t)}{\partial t}=i\hbar\frac{\partial}{\partial t}(U_\alpha\chi)=(U_\alpha\mathcal{H}U_\alpha^{\dagger})U_\alpha\chi,\\
&i\hbar\frac{\partial\chi_\alpha(q,p,t)}{\partial t}=\mathcal{H}_\alpha\chi_\alpha=-\frac{\hbar^2(1-2\alpha)}{2m}\frac{\partial^2}{\partial q^2}\chi_\alpha-i\hbar\frac{p}{m}\frac{\partial}{\partial_q}\chi_\alpha\\
&\qquad+\sum_{n=0}\frac{(-\alpha)^n-(1-\alpha)^n}{n!}(-i\hbar)^n\frac{\partial^n V}{\partial q^n}\frac{\partial^n}{\partial p^n}\chi_\alpha.
\end{aligned} \tag{30}$$

See the Appendix for proof of Eq. (30). For $\alpha=1/2$, even n terms in Eq. (30) cancel out and one again recovers Wigner's evolution equation.[3] See Eq. (A7).

A. Assigning *q*-space operators to phase space functions: Ordering rule

The phase space state functions are devised to evaluate the expectation values of a c-number observable, $F(q,p)$, by integrations over the phase space. Upon reduction to the q space, say, $f(q,p)$ turns into a differential operator in terms of q and π_q. The questions are: (l) how are different factors of noncommuting q and π_q ordered in a given α-representation? (2) Averaging a given $F(q,p)$ with different χ_α's gives different values, how do such averages change from one

α-representation to another? Let $\hat{F}_\alpha(q,\pi_q)$ be the q space operator corresponding to the c-number monomial $q^n p^m$ in phase space when averaged by χ_α. The defining equation for$\hat{F}_\alpha(q,\pi_q)$ is

$$\langle q^n p^m\rangle_\alpha = \int q^n p^m \chi_\alpha \mathrm{d}p\mathrm{d}q = \int \psi^*(q)\hat{F}_\alpha(q,\pi_q)\psi(q)\mathrm{d}q. \tag{31}$$

For the combination of $\alpha=0$ and 1 corresponding to $(\chi+\chi^*)$ of Eq. (11) this is already worked out in Eq. (25e) and is the symmetric ordering

$$q^n p^m \to \tfrac{1}{2}(q^n \pi_q^m + \pi_q^m q^n). \tag{32}$$

For a general α, it is given in Eq. (A10),

$$q^n p^m \to \sum_{r=0}^{m} \binom{m}{r} ((1-\alpha)\pi_q)^r q^n (\alpha\pi_q)^{m-r}. \tag{33}$$

For $\alpha=1/2$ this reduces to Weyl's ordering,[2,3] which is known to go with Wigner's functions. To answer the second question we note the following:

$$\langle q^n p^m\rangle_{\alpha=0} = \int q^n p^m \chi \mathrm{d}q\mathrm{d}p = \int q^n p^m U_\alpha^\dagger \chi_\alpha \mathrm{d}q\mathrm{d}p = \int U_\alpha(q^n p^m)\chi_\alpha \mathrm{d}q\mathrm{d}p = \langle U_\alpha(q^n p^m)\rangle_\alpha, \tag{34}$$

where by Eq. (29) we have used $\chi=U^\dagger\chi_\alpha$. The conclusion is that $q^n p^m$ averaged by χ is the same as $U_\alpha(q^n p^m)$ averaged by χ_α. Upon adoption of

$$U_\alpha = \sum \frac{(-i\alpha\hbar)^k}{k!}\frac{\partial^k}{\partial q^k}\frac{\partial^k}{\partial p^k}$$

and operation by it on $q^n p^m$ one finds

$$\begin{aligned} U_\alpha(q^n p^m) &= \sum_{k=0}^{\text{smaller of } n \text{ or } m} (-i\hbar\alpha)^k k! \binom{n}{k}\binom{m}{k} q^{q^{n-k}} p^{m-k} \\ &= q^n p^m + (-i\hbar\alpha)mnq^{n-1}p^{m-1} + \frac{1}{2}(-i\hbar\alpha)^2 n(n-1)m(m-1)q^{n-2}p^{m-2} + \cdots . \end{aligned} \tag{35}$$

B. Assigning phase space functions to *q* space operators

To a given operator $\hat{F}(q,\pi_q)$, a Taylor-expanded series in whatever order of powers of q and π_q, we associate the following c-number function:

$$F(q,p) = \sum_{n,m} F_{mn}\chi_{nm} = \langle q|\hat{F}|p\rangle e^{-ipq/\hbar}, \tag{36}$$

where $F_{mn}=\langle n|\hat{F}|m\rangle$ is the matrix element of $\hat{F}$ in the basis of the eigenstates of $\hat{H}(q,\pi_g)$. This is actually the inverse of the procedure that we used in Eq. (31) to associate an operator with a c-number function (let $\alpha=0$ and replace $q^n p^m$ by $F(q,p)$ in Eq. (33) to see the analogy). The second equality in Eq. (36) expresses the same in the ket- and bra- notation of Dirac.

The corresponding function in α-representation is simply

$$F_\alpha(q,p) = U_\alpha F(q,p) = \sum_{n,m} F_{mn} U_\alpha \chi_{nm} = \int \langle q - \alpha\tau|\hat{F}|q + 1(1-\alpha)\tau\rangle e^{ip\tau/\hbar} \mathrm{d}\tau. \tag{37}$$

This is actually the generalization of Eq. (29) for a general operator $\hat{F}(q,\pi_q)$. The rule for the product $\hat{F}=\hat{A}\hat{B}$ is worked out in Eq. (A13):

$$F(q,p=)\langle q|\hat{A}(q,\pi_q)\hat{B}(q,\pi_q)|p\rangle e^{-ipq/\hbar} = \sum_{n=0}^{\infty} \frac{(-i\hbar)^n}{n!} \frac{\partial^n A(q,p)}{\partial p^n} \frac{\partial^n B(q,p)}{\partial q^n}. \tag{38}$$

One may also work out the α-representation of Eq. (38):

$$\begin{aligned} F_\alpha(q,p) = U_\alpha F(q,p) &= A_\alpha\left[q + i\hbar\,\alpha\frac{\partial}{\partial p}, p - i\hbar\,\alpha(1-\alpha)\frac{\partial}{\partial q}\right] B_\alpha(q,p) \\ &= \sum_{n=0}^{\infty} \frac{(i\hbar)^n}{n!}\left[\alpha\frac{\partial}{\partial_{qA}}\frac{\partial}{\partial_{pB}} - (1-\alpha)\frac{\partial}{\partial_{pA}}\frac{\partial}{\partial_{qB}}\right]^n A_\alpha(q,p)B_\alpha(q,p). \end{aligned} \tag{39}$$

See Eq. (A17) for details of the derivation. In Sec. VII, we analyze Bloch's problem as an illustration of the use of the developments of the last two subsections.

C. A remark on general transformations

An economical way of treating canonical transformations is the symplectic formalism. Let $\boldsymbol{\eta}$ be the column vector $(q,\ \pi_q;\ p,\ \pi_p)$. The equations of the classical dynamics assume the following form

$$\dot{\boldsymbol{\eta}} = \mathbf{J}\frac{\partial \mathcal{H}}{\partial \boldsymbol{\eta}}, \tag{40}$$

where $\mathcal{H}(\boldsymbol{\eta})$ is the extended Hamiltonian of Eq. (7) and $\mathbf{J}$ is the symplectic metric

$$\mathbf{J} = \begin{pmatrix} j & 0 \\ 0 & j \end{pmatrix}, \quad j = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{41}$$

An infinitesimal canonical transformation from $\boldsymbol{\eta}$ to $\boldsymbol{\eta}+\delta\boldsymbol{\eta}$ is of the form

$$\boldsymbol{\eta} + \delta\boldsymbol{\eta} = \boldsymbol{\eta} - \boldsymbol{\epsilon}\frac{\partial G(\boldsymbol{\eta})}{\partial \boldsymbol{\eta}}, \tag{42}$$

where G is the generator of the transformation and $\boldsymbol{\epsilon}$ indicates its infinitesimal character. The matrix of the transformation is

$$M_{ij} = \delta_{ij} - \boldsymbol{\epsilon}\frac{\partial^2 G}{\partial \eta_i \eta_j}. \tag{43}$$

The condition for canonicity is

$$\mathbf{M}\mathbf{J}\mathbf{M}^\dagger = \mathbf{J} + O(\boldsymbol{\epsilon}^2). \tag{44}$$

This imposes the condition on G to be either linear in η_j or quadratic and symmetric in η_i, η_j or both. For clarity, hereafter we confine our discussion to a system of one degree of freedom, $N=1$. The most general form of G with the restriction just mentioned is

$$G(\boldsymbol{\eta}) = a_i\eta_i + \alpha_{ij}\eta_i\eta_j, \quad i,j = 1,2,3,4 \text{ correspond to } q,\ \pi_q;\ p,\ \pi_p, \tag{45}$$

where the four parameters a_i initiate translations and the ten symmetric α_{ij} cause rotations, boosts, squeezes, scale changes, etc. The ten transformations α_{ij} constitute a symplectic group $SP(4)$, and

is locally isomorphic to the (3+2)-dimensional Lorentz group. This is the group that Kim and Noz[17] encounter in their study of four-dimensional phase space consisting of two oscillators representation of $O(3+2)$, and proves to be a useful mathematical tool in quantum optics. To each of the fourteen transformations of Eq. (45) there corresponds a unitary or similarity transformation in the function space. That of Eq. (27) it is unitary. An example of nonunitary operators is the following. To the canonical coordinate transformation

$$q = Q + \frac{i\epsilon}{2\hbar}\Pi_Q + \frac{1}{2}\Pi_P, \quad \pi_q = \Pi_Q,$$
$$p = P + \frac{i\hbar}{2\epsilon}\Pi_P + \frac{1}{2}\Pi_Q, \quad \pi_p = \Pi_P, \tag{46}$$

there corresponds the complex similarity operator

$$S_\varepsilon = \exp\left[\left(\frac{\varepsilon}{4}\frac{\partial^2}{\partial q^2} + \frac{\hbar^2}{4\varepsilon}\frac{\partial^2}{\partial p^2}\right) + \frac{i\hbar}{2}\frac{\partial^2}{\partial q\,\partial p}\right], \tag{47}$$

where ε is a finite parameter of the transformation. Husimi's[5] all positive distribution in terms of χ is

$$\chi_{\mathrm{Hus}}(q,p,\varepsilon) = S_\varepsilon \chi(q,p). \tag{48}$$

VI. BLOCK'S EQUATION IN PHASE SPACE

In this section we intend to illustrate some usage of the formalism developed so far. In any discussion of statistical mechanics, the partition function, $Z(\beta)=\mathrm{tr}\,\hat{\Omega}$, $\hat{\Omega}(q,\pi_q)=\exp(-\beta\hat{H})$, plays a pivotal role. Its calculation, however, is often cumbersome. One practice is to translate $\hat{\Omega}$ and the corresponding Bloch's differential equation[18] into a phase space language,[3,16] solve the equation for a c-number $\Omega(q,p,\beta)$ and calculate $Z(\beta)=\int\Omega(p,q,\beta)\mathrm{d}q\mathrm{d}p$. The ease of doing the job depends on the choice of the c-number assigned to $\hat{\Omega}$. Our suggestion is that of Eq. (36) Bloch's equation for $\hat{\Omega}$ is

$$\frac{\partial\hat{\Omega}}{\partial\beta} = -\hat{H}\hat{\Omega} = -\hat{\Omega}\hat{H}. \tag{49}$$

We apply the rule of Eq. (36) to Eq. (49). Noting that $\hat{H}(q,\pi_q)\rightarrow H(q,p)=p^2/2m+V(q)$ and using the product rule of Eq. (38) gives

$$-\frac{\partial\Omega(q,p;\beta)}{\partial\beta} = \left\{H(q,p) - \frac{ip\hbar}{m}\frac{\partial}{\partial q} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\right\}\Omega(p,q). \tag{50}$$

This same result is obtained in Ref. 19, however, by a totally different approach and through much lengthier calculations using Moyal's characteristic technique. Equation (49) in Wigner's representation is obtained by replacing $\hat{\Omega}$ with $\Omega_W(q,p;\beta)$, $\hat{H}$ with $p^2/2m+V(q)$ and using Eq. (A17) with $\alpha=1/2$ to find the expression corresponding to $\hat{H}\hat{\Omega}$. In agreement with Refs. 3 and 16 one finds

$$-\frac{\partial\Omega_W(q,p;\beta)}{\partial\beta} = \left\{\frac{p^2}{2m} - \frac{\hbar^2}{8m}\frac{\partial^2}{\partial q^2} + \sum_{n=0}^{n=\infty}\frac{(i\hbar/2)^n}{n!}\frac{\partial^n}{\partial q^n}V(q)\frac{\partial^n}{\partial p^n}\right\}\Omega_W(q,p;\beta). \tag{51}$$

The contrast between the two, Eqs. (50) and (51), is striking. The former is a second-order differential equation in q and the exact quantum effects in it appear as $\hbar$ and $\hbar^2$ only, while the latter in addition to $\partial^2/\partial q^2$ is an nth-order differential equation in p and has all powers of $\hbar$ in it.

In the following we solve Eq. (50) and give the partition functions for the simple harmonic and linear potentials.

A. Simple harmonic potential

For $H(q,p)=l/2(p^2/m+m\omega^2q^2)$ the solution is of the form

$$\Omega = \exp\left[- A(\beta)H(q,p) - iB(\beta)\frac{pq}{\hbar} - C(\beta) \right]. \tag{52}$$

Substituting this in Eq. (50) and letting the coefficients of different powers of q and p vanish, gives

$$\frac{\mathrm{d}A}{\mathrm{d}\beta} = 1 - \hbar^2\omega^2A^2, \tag{53a}$$

$$\frac{\mathrm{d}B}{\mathrm{d}\beta} = \hbar^2\omega^2A(1-B), \tag{53b}$$

$$\frac{\mathrm{d}C}{\mathrm{d}\beta} = \frac{1}{2}\hbar^2\omega^2A. \tag{53c}$$

The condition $\Omega(q,p,0)=1$ imposes the boundary conditions $A(0)=B(0)=C(0)=0$. With these provisions one finds

$$A(\beta) = \frac{1}{\hbar\,\omega}\tanh\beta\hbar\,\omega, \tag{54a}$$

$$B(\beta) = \tanh\beta\hbar\,\omega\tanh\frac{\beta\hbar\,\omega}{2}, \tag{54b}$$

$$C(\beta) = -\frac{1}{2}\ln\cosh\beta\hbar\,\omega. \tag{54c}$$

The partition function is

$$Z(\beta) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\Omega(q,p,\beta)\mathrm{d}q\mathrm{d}p = \left[2\sinh\frac{\beta\hbar\,\omega}{2} \right]^{-1}. \tag{55}$$

The normalized density function is $\chi(q,p,\beta)=\Omega(q,p,\beta)/2\pi\hbar Z(\beta)$, with low and high temperature limits

$$\chi = \frac{\sqrt{2}}{\pi\hbar}\exp\left[- H(q,p) - \frac{ipq}{\hbar} \right], \quad \beta\hbar\,\omega \gg 1,$$

$$\chi = \frac{\beta\omega}{2\pi}\exp[-\beta H(q,p)], \quad \beta\hbar\,\omega \ll 1, \tag{56}$$

in agreement with the quantum and classical limits, respectively.

B. Linear potential

The case is of interest for quark model,[20] where a sea of semi-infinite matter creates a linear potential $V(q)=kq$, $0\leq q<\infty$, and $k>0$. By the same procedure above one obtains

$$\Omega(q,p,\beta) = \exp\left[-\beta H - \frac{i\beta^2 p\hbar k}{2m} + \frac{\beta^3\hbar^2 k^2}{6m}\right], \tag{57}$$

$$Z(\beta) = \sqrt{\frac{2\pi m}{\beta^3 k^2}}\exp\left[\frac{\beta^3\hbar^2 k^2}{24m}\right]. \tag{58}$$

$$\chi(q,p;\beta) = \sqrt{\frac{\beta^3 k^2}{2\pi m}}\exp\left[-\beta H - \frac{i\beta^2 p\hbar k}{2m} + \frac{\beta^3\hbar^2 k^2}{8m}\right]. \tag{59}$$

The corresponding Wigner's function[21] can be obtained by letting $U_{1/2}$ operate on Eq. (59).

VII. CONCLUSION

We have developed a quantum mechanics in phase space by carrying the independent and symmetric roles of q and p, so eminent in the Hamiltonian formulation of the classical mechanics, to quantum domain. This is done through the extension of the phase space by introducing the momenta π_q and π_p conjugate to q and p, respectively, and the subsequent extensions of the Lagrangians, Hamiltonians, Poisson's brackets, etc. In its full generality, the theory describes the dynamics of the quantum ensembles. Its pure state case is reducible to the conventional quantum mechanics in q- or p-spaces, however, with a definite rule for ordering of the factors of noncommuting operators. The latter feature is a direct consequence of the independence of q and p that is maintained at all stages of the formalism. Simple rules for assigning an operator $\hat{F}(q,\pi_q)$ in q-space to a function $F(q,p)$ in phase space and vice versa are prescribed. Extended canonical transformations enable one to go from one extended phase space to another. Correspondingly the associated unitary or similarity transformations in the function space enable one to generate further state functions from a given one. This unifying feature of the theory makes the comparison of the various functions existing in the literature possible and transparent.

To demonstrate the simplicity and the power of the formalism certain examples are worked out. Treatment of Bloch's equation, partition functions for simple harmonic and linear potentials, and the mathematical lemmas of the Appendix serve this end. Nasiri and Safari[22] and Razavi[23] have found the presented formalism of considerable assistance in their study of dissipative quantum systems.

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APPENDIX

Evaluation of $\chi_\alpha = U_\alpha\chi$: By three Fourier and inverse Fourier transformations we convert $\chi = \psi(q)\phi^*(p)\exp(-ipq/\hbar)$ into the following forms;

$$\chi = \int \phi(p')\phi^*(p'')\exp\frac{iq(p'-p'')}{\hbar}\exp\frac{ip\tau}{\hbar}\exp\frac{-ip''}{\hbar}\mathrm{d}p'\mathrm{d}p''\mathrm{d}\tau. \tag{A1}$$

By this provision we have moved both q and p variables to the exponent. Next we expand U_α of Eq. (28) in power series, operate by it on the q and p exponents, and arrive at

$$\sum_{k=0}^{k=\infty}\frac{(i\alpha\hbar)^k}{k!}\frac{\partial^k}{\partial p^k}\frac{\partial^k}{\partial q^k}\exp\frac{iq(p'-p'')}{\hbar}\exp\frac{ip\tau}{\hbar} = \exp\frac{-i\alpha\tau(p'-p'')}{\hbar}\exp\frac{iq(p'-p'')}{\hbar}\exp\frac{ip\tau}{\hbar}. \tag{A2}$$

Using Eqs. (A1) and (A2) in the expression $\chi_\alpha = U_\alpha\chi$, and inverting ϕ's back to ψ's gives Eq. (29),

$$\chi_\alpha(p,q,t) = U_\alpha \chi = \left(\frac{1}{2\pi\hbar}\right)^N \int \psi(q-\alpha\tau)\psi^*(q+(1-\alpha)\tau)e^{ip\tau/\hbar}\mathrm{d}\tau. \tag{A3}$$

As mentioned earlier, for $\alpha=1/2$ one recovers Wigner's standard state functions.

Evolution equation for χ_α: To prove Eq. (30), it is sufficient to evaluate $\mathcal{H}_\alpha = U_\alpha \mathcal{H} U_\alpha^\dagger$, where $\mathcal{H}$ is the extended Hamiltonian of Eq. (10). It is easy to show that $Q = U_\alpha q U_\alpha^\dagger = q - \alpha\pi_P$ and $P = U_{\alpha p} U_\alpha^\dagger = p - \alpha\pi_q$, which is the essence of the transformations of Eq. (27). We also note that

$$U_\alpha q^n p^m U_\alpha^\dagger = (q-\alpha\pi_p)^n (p-\alpha\pi_q)^m = (p-\alpha\pi_q)^m (q-\alpha\pi_p)^n. \tag{A4}$$

We leave it to the reader to verify Eq. (A4) for him/herself for some small n and m. It is needless to say that $[Q,P]=0$, because the transformation is unitary. With these provisions one finds

$$\mathcal{H}_\alpha = H[q-\alpha\pi_p, p+(1-\alpha)\pi_q] - H[q-(1-\alpha)\pi_p, p-\alpha\pi_q). \tag{A5}$$

Expansion of the Hamiltonian about (q,p) gives

$$\mathcal{H}_\alpha = -\frac{\hbar^2(1-2\alpha)}{2m}\frac{\partial^2}{\partial q^2} - i\hbar\frac{p}{m}\frac{\partial}{\partial q} + \sum_{n=0}\frac{(-\alpha)^n - (1-\alpha)^n}{n!}(-i\hbar)^n \frac{\partial^n V}{\partial q^n}\frac{\partial^n}{\partial p^n}. \tag{A6}$$

The Wigner case is for $\alpha=1/2$,

$$\mathcal{H}_W = -i\hbar\frac{p}{m}\frac{\partial}{\partial q} + \sum_{n=0}\frac{1}{(2n+1)!}\left(\frac{\hbar}{2i}\right)^{2n+1}\frac{\partial^{2n+1}V}{\partial q^{2n+1}}\frac{\partial^{2n+1}}{\partial p^{2n+1}}. \tag{A7}$$

Ordering rule in α*-representation, proof of Eq.* (33): With Eqs. (31) and (A3) we have

$$\langle q^n p^m\rangle_\alpha = \int_{-\infty}^{+\infty} q^n \psi(q-\alpha\tau)\psi^*(q+(1-\alpha)\tau)p^m e^{ip\tau/\hbar}\mathrm{d}q\mathrm{d}p\mathrm{d}\tau. \tag{A8}$$

Writing p^m as $(i\hbar)^m\partial^m/\partial\tau^m$, integrating by parts m times with respect to τ frees the integrand from the p^m factor. Then integration with respect to p gives $\delta(\tau)$. Thus

$$\langle q^n p^m\rangle_\alpha = \int_{-\infty}^{+\infty} q^n(-i\hbar)^m\frac{\partial^m}{\partial\tau^m}[\psi(q-\alpha\tau)\psi^*(q+(1-\alpha)\tau)]\delta(\tau)\mathrm{d}q\mathrm{d}\tau. \tag{A9}$$

Next we substitute $\partial/\partial\tau$ by $\partial/\partial q$ with appropriate adjustments and carry out integrations by parts over q whereever necessary to free ψ^* and arrive at

$$\langle q^n p^m\rangle_\alpha = \int_{-\infty}^{+\infty}\psi^*(q)\left[\sum_{r=0}^{m}\binom{m}{r}((1-\alpha)\pi_q)^r q^n(\alpha\pi_q)^{m-r}\right]\psi(q)\mathrm{d}q. \tag{A10}$$

The expression in the integrand is the desired ordering of Eq. (33), corresponding to $q^n p^m$ in α-representation. For $\alpha=1/2$ one recovers Weyl's ordering

$$q^n p^m \to \left(\frac{1}{2}\right)^m \sum_{r=0}^{m}\binom{m}{r}\pi_q^r q^n \pi_q^{m-r}. \tag{A11}$$

The combination of $\alpha=0$ and 1, corresponding to averaging by $x+\chi^*$, is the symmetric ordering of Eq. (32). □

The product rule, proof of Eqs. (38) *and* (39): The phase space function corresponding to the product of two operators $\hat{F}=\hat{A}\hat{B}$, by the definition of Eq. (36), is

$$F(q,p)=\langle q|\hat{A}\hat{B}|p\rangle e^{-ipq/\hbar}=\int\langle q|\hat{A}|p'\rangle\langle p'|\hat{B}|p\rangle e^{-ipq/\hbar}\mathrm{d}q\mathrm{d}p$$

$$=\int A(q,p')B(q',p)\exp\frac{-i(q'-q)(p'-p)}{\hbar}\mathrm{d}q\mathrm{d}q, \tag{A12}$$

where by Eq. (36), we have substituted $\langle q|\hat{A}|p'\rangle=A(q,p')\exp(ip'q/\hbar)$ and similarly for $\langle q'|\hat{B}|p\rangle$. With further change of variables $q'-q=q''$ and $p'-p=p''$, we obtain

$$F(q,p)=\int A(q,p''+p)B(q''+q,p)e^{-iq''p''/\hbar}\mathrm{d}q''\mathrm{d}p''=\sum_{n=0}^{\infty}\frac{(-i\hbar)^n}{n!}\frac{\partial^n A(q,p)}{\partial p^n}\frac{\partial^n B(q,p)}{\partial q^n}, \tag{A13}$$

where we have Taylor-expanded $A(q,p+p'')$ and $B(q+q'',p)$ about (q,p) and carried out the required integration by parts.

To deduce Eq. (39), we first Fourier-transform $A(q,p)$ to $a(p',q')$ and $B(q,p)$ to $b(p'',q'')$ in Eq. (A13) and carry out the necessary differentiations:

$$F(q,p)=\sum_{n=0}^{\infty}\frac{(-i\hbar)^n}{n!}\frac{\partial^n}{\partial p^n}\int a(p',q')\exp\frac{-ip'q+iq'p}{\hbar}\mathrm{d}p'\mathrm{d}q'\frac{\partial^n}{\partial q^n}$$

$$\times\int b(p'',q'')\exp\frac{-ip''q+iq''p}{\hbar}\mathrm{d}q''\mathrm{d}p''$$

$$=\int a(p',q')\exp\frac{-ip'q+iq'p}{\hbar}b(p'',q'')\exp\frac{-ip'',q''p}{\hbar}e^{-iq'p''/\hbar}\mathrm{d}q'\mathrm{d}p'\mathrm{d}q''\mathrm{d}p''. \tag{A14}$$

Next we operate on Eq. (A14) by a Taylor-expanded form of U_α as in Eq. (A2) and perform the required differentiations:

$$F_\alpha(q,p)=U_\alpha F(q,p)=\int e^{i\alpha q'p'/\hbar}\exp\frac{-ip'q+iq'p-(1-\alpha)q'p''+\alpha q''p'}{\hbar}a(q',p')$$

$$\times e^{i\alpha q''p''/\hbar}\exp\frac{-ip''q+iq''p}{\hbar}b(p'',q'')\mathrm{d}q'\mathrm{d}p'\mathrm{d}q''\mathrm{d}p''. \tag{A15}$$

The exponentials preceding $a(p',q')$ can be written as

$$e^{i\hbar\alpha\partial^2/\partial p\partial q}\exp\frac{-ip'(q+\alpha q'')+iq'(p-(1-\alpha)p'')}{\hbar},$$

where the first factor is simply $U_\alpha(q,p)$ independent of the integration variables (q',p',q'',p''). With this provision integrations over q' and p' can now be carried out and $a(p',q')$ inverse-Fourier transformed. One finds

$$F_\alpha(q,p)=\int\{U_\alpha A[q+\alpha q'',p-(1-\alpha)p'']\}e^{i\alpha q''p''/\hbar}e^{(-ip''q+iq''p)/\hbar}b(p'',q'')\mathrm{d}q''\mathrm{d}p''. \tag{A16}$$

We again apply the same trick. To the left of the rightmost exponential we replace, everywhere, q'' by $(-i\hbar\partial/\partial p)$ and p'' by $(i\hbar\partial/\partial q)$, perform the inverse Fourier transform of $b(p'',q'')$ and find

$$F_\alpha(q,p) = U_\alpha F(q,p) = A_\alpha\left[q + i\hbar\,\alpha\frac{\partial}{\partial p}, p - i\hbar\,\alpha(1-\alpha)\frac{\partial}{\partial q}\right]B_\alpha(q,p)$$

$$= \sum_{n=0}^{\infty}\frac{(i\hbar)^n}{n!}\left[\alpha\frac{\partial}{\partial q_A}\frac{\partial}{\partial p_B} - (1-\alpha)\frac{\partial}{\partial p_A}\frac{\partial}{\partial q_B}\right]^n A_\alpha(q,p)B_\alpha(q,p). \tag{A17}$$

where $\partial/\partial p_A$ indicates a differentiation on $A(q,p)$ only, similarly the other differential operators.□

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Extremal covariant measurements

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We characterize the extremal points of the convex set of quantum measurements that are covariant under a finite-dimensional projective representation of a compact group, with action of the group on the measurement probability space which is generally nontransitive. In this case the POVM density is made of multiple orbits of positive operators, and, in the case of extremal measurements, we provide a bound for the number of orbits and for the rank of POVM elements. Two relevant applications are considered, concerning state discrimination with mutually unbiased bases and the maximization of the mutual information. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2349481]

I. INTRODUCTION

A fundamental issue in the theory of quantum information[1] is the investigation of the ultimate precision limits for extracting classical information from a quantum system. Indeed, when the information is encoded on quantum states, its read-out suffers the intrinsically quantum limitation of discriminating among nonorthogonal states. One then needs to optimize the discrimination with respect to a given optimality criterion, which is dictated by the particular task for which the measurement is designed, or by the particular way the information is encoded over states. The good news is that, although the position of the problem has a limited generality due to the specific form of the optimality criterion, nevertheless for a large class of criteria the optimization method is given by a standard procedure. In such approach all possible measurements form a convex set (the convex combination of two measurements corresponding to the random choice between their apparatuses), and the optimization consists in maximizing a convex functional, e.g., the mutual information,[2,3] or to minimizing a concave functional, e.g., a Bayes cost,[4,5] over the convex set of measurements. Since the global maximum of a convex functional (or the minimum of a concave functional) is achieved over extremal points, the optimization can be restricted to the extremal elements of the set only.

In most situations of interest, the set of signal states on which the information is encoded is invariant under the unitary action of some group of physical transformations. The symmetry of the set of signal states is then reflected in a symmetry of the optimal measurements, which without loss of generality can be assumed to be *covariant*[5] with respect to the same group of transformations.

The problem of charactering extremal covariant measurements has been addressed in Refs. 6 and 7, however restricting the analysis to the case of group-action that is *transitive* on the probability space of measurement outcomes, namely any two points in the probability space are connected by some group element. The present paper completes the investigation by generalizing all results to the case of nontransitive group actions. Indeed the discrimination of states belonging to disjoint group orbits occurs in actual applications, and this situation has received little attention in the literature. Moreover, when classical information is encoded on quantum states it can be

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convenient to decode it with a measurement having outcomes that are not in one-to-one correspondence with the encoding states. This typically happens when the optimality criterion is nonlinear in the probabilities of measurement outcomes, as in the case of the mutual information.[8] In the presence of group symmetry, as recently noted by Decker,[9] even if the encoding states form a single group orbit, the maximization of the mutual information often selects covariant measurements with probability space that splits into disjoint orbits. It is then interesting to quantify the number of orbits needed for the maximization of the mutual information, or at least to give an upper bound for it. Indeed, as we will see in the present paper, the characterization of extremal covariant measurements also provides as a by-product an alternative and simpler derivation of the bound given in Ref. 9.

II. STATEMENT OF THE PROBLEM

In the general framework of quantum mechanics the state of a system is represented by a density operator ρ on a given Hilbert space $\mathcal{H}$, whereas the statistics of a measurement is described by a positive operator valued measure (POVM), which associates a positive semidefinite operator $P(B) \in \mathcal{B}(\mathcal{H})$ to any subset $B \in \sigma(\mathfrak{X})$ of the σ-algebra of events in the probability space $\mathfrak{X}$. The defining properties for a POVM are

$$0 \leqslant P(B) \leqslant \mathbb{1}, \quad \forall\, B \in \sigma(\mathfrak{X}), \tag{1}$$

$$P(\cup_{k=1}^{\infty} B_k) = \sum_{k=1}^{\infty} P(B_k), \quad \forall\, \{B_k\} \text{ disjoint} \tag{2}$$

$$P(\mathfrak{X}) = \mathbb{1}. \tag{3}$$

The probability of the event $B \in \sigma(\mathfrak{X})$ is then given by the Born rule

$$p(B) = \mathrm{Tr}[\rho P(B)]. \tag{4}$$

In this paper we will consider the case where the probability space $\mathfrak{X}$ supports the action of a compact group $\mathbf{G}$, namely any group element $g \in \mathbf{G}$ acts as a measurable automorphism of the probability space $\mathfrak{X}$, which maps $x \in \mathfrak{X}$ to $gx \in \mathfrak{X}$. If any two points $x_1, x_2 \in \mathfrak{X}$ are connected by some group element, i.e., $x_2 = g x_1$ for some $g \in \mathbf{G}$, the group action is called *transitive*. In this case, which is the most studied in the literature,[4,5] the whole probability space is the group orbit of an arbitrary point $x_0 \in \mathfrak{X}$, namely $\mathfrak{X} = \{g x_0 \,|\, g \in \mathbf{G}\}$. In this paper we will study the more general case where the group action is not transitive, and, accordingly, the probability space is not a single group orbit, but the union of a set of disjoint orbits, each one being labeled by an index $i \in \mathcal{I}$ for some set $\mathcal{I}$. For simplicity, we will assume the index set $\mathcal{I}$ to be finite.

The simplest case of the nontransitive group action then arises when the probability space is the Cartesian product of the index set $\mathcal{I}$ with the compact group $\mathbf{G}$, i.e., $\mathfrak{X} = \mathcal{I} \times \mathbf{G}$. In this case, the action of a group element $h \in \mathbf{G}$ on a point $x = (i, g) \in \mathcal{I} \times \mathbf{G}$ is given by $hx = (i, hg)$. Measurements with outcomes in $\mathcal{I} \times \mathbf{G}$ naturally arise in the discrimination of a set of signal states which is the union of a certain number of disjoint group orbits, each orbit $\mathcal{O}_i$ being generated by the action of the group on a given initial state ρ_i, namely $\mathcal{O}_i = \{U_g \rho_i U_g^\dagger \,|\, g \in \mathbf{G}\}$ for some unitary representation $\mathsf{R}(\mathbf{G}) = \{U_g \,|\, g \in \mathbf{G}\}$. Precisely, if the *stability group* $\mathbf{G}_i = \{h \in \mathbf{G} \,|\, U_h \rho_i U_h^\dagger = \rho_i\}$ associated to any state ρ_i consists only of the identity element e, then there is a one-to-one correspondence between signal states and points of the probability space $\mathfrak{X} = \mathcal{I} \times \mathbf{G}$. In Sec. IV we will study in detail the case of POVMs with probability space $\mathfrak{X} = \mathcal{I} \times \mathbf{G}$.

If the stability groups associated to the initial states $\{\rho_i \,|\, i \in \mathcal{I}\}$ are nontrivial, namely $\mathbf{G}_i \neq \{e\}$ for some $i \in \mathcal{I}$, in order to have a one-to-one correspondence between signal states and measurement outcomes, one must consider the probability space $\mathfrak{X} = \cup_{i \in \mathcal{I}} \mathbf{G}/\mathbf{G}_i$, where $\mathbf{G}/\mathbf{G}_i$ denotes the quotient of $\mathbf{G}$ with respect to the equivalence relation "$g \sim g'$ if $g' = g \cdot h$ for some $h \in \mathbf{G}_i$." This more general case will be treated in Sec. V.

Definition 1 (*covariant POVMs*): *Let* $\mathfrak{X}$ *be a probability space supporting the group action* $g: x \in \mathfrak{X} \mapsto gx \in \mathfrak{X}$. *A POVM is covariant*[5] *if it satisfies the property*

$$P(B) = U_g^\dagger P(gB) U_g, \quad \forall\, B \in \sigma(\mathfrak{X}),\ \forall\, g \in \mathbf{G}, \tag{5}$$

where $gB \doteq \{gx | x \in B\}$.

In the case $\mathfrak{X} = \mathcal{I} \times \mathbf{G}$, it is simple to prove[10] that any covariant POVM admits an operator density $M(i,g)$ with respect to the (normalized) Haar measure $\mathrm{d}g$ on the group $\mathbf{G}$, namely, if $B = (i,A)$, where $A \subseteq \mathbf{G}$ is a measurable subset, then $P(B) = \int_A \mathrm{d}g M(i,g)$. Moreover, such an operator density has necessarily the form[10]

$$M(i,g) = U_g A_i U_g^\dagger, \tag{6}$$

where $A_i \in \mathcal{B}(\mathcal{H})$ are Hermitian operators satisfying the constraints

$$A_i \geqslant 0, \quad \forall\, i \in \mathcal{I}, \tag{7}$$

$$\sum_{i \in \mathcal{I}} \int_{\mathbf{G}} \mathrm{d}g\, U_g A_i U_g^\dagger = \mathbb{1}. \tag{8}$$

Here and throughout the paper we adopt for the Haar measure the normalization

$$\int_{\mathbf{G}} \mathrm{d}g = 1. \tag{9}$$

According to the above discussion, any covariant POVM with probability space $\mathfrak{X} = \mathcal{I} \times \mathbf{G}$ is completely specified by a set of operators $\{A_i | i \in \mathcal{I}\}$, such that both constraints in Eqs. (7) and (8) are satisfied. Moreover, it turns out that it is very useful to represent such a vector of operators as a single block operator $A = \oplus_{i \in I} A_i$, acting on an auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}} \doteq \oplus_{i \in I} W_i$, where $\mathcal{W}_i \simeq \mathcal{H}\, \forall\, i \in \mathcal{I}$. In terms of the block operator $A \in \oplus_{i \in I} B(W_i)$ the two constraints Eq. (7) and Eq. (8) become

$$A \geqslant 0, \tag{10}$$

and

$$\mathcal{L}(A) = \mathbb{1}, \tag{11}$$

where $\mathcal{L}: \oplus_{i \in I} B(W_i) \to B(H)$ is the linear map

$$\mathcal{L}(A) \doteq \sum_{i \in \mathcal{I}} \int_{\mathbf{G}} \mathrm{d}g\, U_g A_i U_g^\dagger. \tag{12}$$

The two constraints (10) and (11) define such a convex subset of the space of block operators $\oplus_{i \in I} B(W_i)$, which is in one-to-one affine correspondence with the convex set of covariant POVMs. In the following, the convex set of block operators will be denoted by C.

Proposition 1: *The convex set* C, *defined by the constraints* (10) and (11) *is compact in the operator norm.*

Proof: Since C is a subset of a finite dimensional vector space, it enough to show that C is bounded and closed. C is bounded, since for any $A \in \mathsf{C}$, one has $||A|| \leqslant \mathrm{Tr}[A] = \Sigma_{i \in \mathcal{I}} \mathrm{Tr}[A_i] = \mathrm{Tr}[\mathcal{L}(A)] = d$ (using Eqs. (10) and (11)). Moreover, C is closed. In fact, if $\{A_n\}$ is a Cauchy sequence of points in C, then A_n converges to some block operator $A \in \oplus_{i \in I} B(W_i)$. We claim that A belongs to C. Of course, A satisfies condition (10). As regards condition (11), just notice that the $\mathcal{L}$ is continuous, being linear. Therefore, we have $||\mathcal{L}(A) - \mathbb{1}|| = ||\mathcal{L}(A - A_n)|| \to 0$, namely A satisfies condition (11). ■

Observation 1: Since the convex set C is compact, it coincides with the convex hull of its extreme points, i.e., any element $A \in \mathsf{C}$ can be written as convex combination of extreme points. The classification of the extreme points of C will be given in Sec. IV.

Observation 2: In this section and all throughout the paper, $\mathbf{G}$ is assumed to be a compact Lie group. Nevertheless, all results clearly hold also if $\mathbf{G}$ is a finite group, with cardinality $|\mathbf{G}|$. In this case, one only has to make the substitution $\int_{\mathbf{G}} \mathrm{d}g \to (1/|\mathbf{G}|)\Sigma_{g\in\mathbf{G}}$. Moreover, since now the probability space $\mathfrak{X}=\mathcal{I}\times\mathbf{G}$ is discrete, there is no need of introducing any operator density, and we simply have

$$P(i,g) = \frac{1}{|\mathbf{G}|} U_g A_i U_g^\dagger. \tag{13}$$

An example of covariant POVM with a finite symmetry group will be given in Sec. VI.

III. SOME RESULTS OF ELEMENTARY GROUP THEORY

Let $\mathbf{G}$ be a compact Lie group and let $\mathrm{d}g$ be the invariant Haar measure on $\mathbf{G}$, normalized such that $\int_{\mathbf{G}} \mathrm{d}g = 1$. Consider a finite dimensional Hilbert space $\mathcal{H}$ and represent $\mathbf{G}$ on $\mathcal{H}$ by a unitary (generally projective) representation $\mathsf{R}(\mathbf{G})=\{U_g \,|\, g\in\mathbf{G}\}$. The collection of equivalence classes of irreducible representations which show up in the decomposition of $\mathsf{R}(\mathbf{G})$ will be denoted by S. Then $\mathcal{H}$ can be decomposed into the direct sum of orthogonal irreducible subspaces:

$$\mathcal{H} = \bigoplus_{\mu\in S} \bigoplus_{k=1}^{m_\mu} \mathcal{H}_k^\mu, \tag{14}$$

where the index μ labels equivalence classes of irreducible representations (irreps), while the index i is a degeneracy index labeling m_μ different equivalent representations in the class μ. Subspaces carrying equivalent irreps have all the same dimension d_μ and are connected by invariant isomorphisms, namely for any $k,l=1,\ldots,m_\mu$ there is an operator $T_{kl}^\mu \in \mathcal{B}(\mathcal{H})$ such that $\mathsf{Supp}(T_{kl}^\mu)=\mathcal{H}_l^\mu$, $\mathsf{Rng}(T_{kl}^\mu)=\mathcal{H}_k^\mu$, and $[T_{kl}^\mu, U_g]=0\ \forall g\in\mathbf{G}$. Due to Schur lemmas, any operator O in the commutant of the representation $\mathsf{R}(\mathbf{G})$ has the form:

$$O = \sum_\mu \sum_{k,l=1}^{m_\mu} \frac{\mathrm{Tr}[T_{lk}^\mu O]}{d_\mu} T_{kl}^\mu. \tag{15}$$

Using the above-presented formula, the normalization of a covariant POVM, given by Eq. (11), can be rewritten in a simple form. In fact, due to the invariance of the Haar measure $\mathrm{d}g$, we have $[\mathcal{L}(A), U_g]=0\ \forall g\in\mathbf{G}$, i.e., $\mathcal{L}(A)$ belongs to the commutant of $\mathsf{R}(\mathbf{G})$. Then, by exploiting Eq. (15), we rewrite the normalization constraint (11) as

$$\sum_{i\in\mathcal{I}} \mathrm{Tr}[T_{kl}^\mu A_i] = d_\mu \delta_{kl}, \quad \forall\, \mu\in S, \quad \forall\, k,l=1,\ldots,m_\mu, \tag{16}$$

δ_{kl} denoting the Kronecker delta.

Again, this condition can be recast into a compact form by introducing the auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}}=\oplus_{i\in I} W_i$, with $\mathcal{W}_i \simeq \mathcal{H}\ \forall i\in\mathcal{I}$, and constructing a block operator with a repeated direct sum of the same operator T_{kl}^μ, i.e.,

$$S_{kl}^\mu = \bigoplus_{i\in\mathcal{I}} S_{kli}^\mu, \quad S_{kli}^\mu = T_\mu^{kl}, \quad \forall\, i\in\mathcal{I}. \tag{17}$$

With this definition, Eq. (16) becomes

$$\mathrm{Tr}[S_{kl}^\mu A] = d_\mu \delta_{kl}, \quad \forall\, \mu\in S, \quad \forall\, k,l=1,\ldots,m_\mu, \tag{18}$$

where A is the block operator $A=\oplus_{i\in I} A_i$.

IV. EXTREMAL COVARIANT POVMs

This section contains the main result of the paper, namely the characterization of the extremal covariant POVMs with probability space $\mathcal{I}\otimes\mathbf{G}$. Such a characterization will be given by exploiting the one-to-one affine correspondence between the convex set of covariant POVMs and the convex set C of block operators defined by the constraints (10) and (11), or, equivalently, by (10) and (18).

Definition 2: *An Hermitian block operator* $P=\oplus_{i\in I}P_i$ *is a perturbation of* $A\in\mathsf{C}$ *if there exists an* $\epsilon>0$ *such that* $A+tP\in\mathsf{C}$ *for any* $t\in[-\epsilon,\epsilon]$.

Clearly, a point $A\in\mathsf{C}$ is extreme if and only if it admits only the trivial perturbation $P=0$.

Lemma 1: *A block operator* $P=\oplus_{i\in I}P_i$ *is a perturbation of* $A\in\mathsf{C}$ *if and only if*

$$\mathsf{Supp}(P)\subseteq\mathsf{Supp}(A), \tag{19}$$

$$\mathrm{Tr}[S_{kl}^{\mu}P]=0,\quad \forall\,\mu\in S,\quad \forall\,k,l=1,\ldots,m_{\mu}. \tag{20}$$

Proof: Condition (19) is equivalent to the existence of an $\epsilon>0$ such that $A+tP\geqslant 0$ for all $t\in[-\epsilon,\epsilon]$ (see Lemma 1 of Ref. 7). On the other hand, condition (20) is equivalent to require that $A+tP$ satisfies the normalization constraint (16) for all $t\in[-\epsilon,\epsilon]$. ■

Observation: Note that, due to the block form of both P and A, condition (19) is equivalent to

$$\mathsf{Supp}(P_i)\subseteq\mathsf{Supp}(A_i),\quad \forall\,i\in\mathcal{I}. \tag{21}$$

Using the previous lemma, we can obtain a first characterization of extremality:

Theorem 1 (Minimal support condition): *A point* $A\in\mathsf{C}$ *is extremal if and only if for any* $B\in\mathsf{C}$,

$$\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)=\Rightarrow A=B. \tag{22}$$

Proof: Suppose A extremal. Then, if $\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)$, according to Lemma 1, $P=A-B$ is a perturbation of $A\in\mathsf{C}$. Hence, P must be zero. Conversely, if P is a perturbation of A, then $B=A+tP$ is an element of C for some $t\neq 0$. Due to Lemma 1, we have $\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)$. Then, condition (22) implies $B=A+tP=A$, i.e., $P=0$. Therefore, A is extremal. ■

Corollary 1: *If* $A\in\mathsf{C}$ *and* $\mathrm{rank}(A)=1$, *then* A *is extremal*.

Proof: Since $\mathrm{rank}(A)=1$, then, for any $B\in\mathsf{C}$, the condition $\mathsf{Supp}(B)\subseteq\mathsf{Supp}(A)$ implies $B=\lambda A$ for some $\lambda>0$. Moreover, since both A and B are in C, from Eq. (18) we have $d_{\mu}=\mathrm{Tr}[S_{kk}^{\mu}B]=\lambda\,\mathrm{Tr}[S_{kk}^{\mu}A]=\lambda d_{\mu}$, whence necessarily $\lambda=1$. Condition (22) then ensures that A is extremal. ■

A deeper characterization of extremal covariant POVMs can be obtained by using the following lemma.

Lemma 2: *Let* A *be a point of* C, *represented as*

$$A=\bigoplus_{i\in\mathcal{I}}X_i^{\dagger}X_i, \tag{23}$$

and define $\mathcal{H}_i=\mathsf{Rng}(X_i)$ *the range of* X_i. *A block operator* $P=\oplus_{i\in I}P_i$ *is a perturbation of* A *if and only if*

$$P_i=X_i^{\dagger}Q_iX_i,\quad \forall\,i\in\mathcal{I}, \tag{24}$$

for some Hermitian $Q_i\in\mathcal{B}(\mathcal{H}_i)$, *and*

$$\sum_{i\in\mathcal{I}}\mathrm{Tr}[S_{kli}^{\mu}X_i^{\dagger}Q_iX_i]=0. \tag{25}$$

Proof: First of all, the form (24) is equivalent to condition (19). In fact, if P has the form (24), then clearly $\mathsf{Supp}(P)\subseteq\mathsf{Supp}(A)$. Conversely, if we assume condition (19) and write

$P=\oplus_{i\in I}P_i$, we have necessarily $\mathsf{Supp}(P_i)\subseteq\mathsf{Supp}(X_i^\dagger X_i)=\mathsf{Supp}(X_i)$. Exploiting the singular value decomposition $X_i=\Sigma_{n=1}^{r_i}\lambda_n^{(i)}|w_n^i\rangle\langle v_n^i|$, where $\{|v_n^i\rangle\}$ and $\{|w_n^i\rangle\}$ are orthonormal bases for $\mathsf{Supp}(X_i)$ and $\mathsf{Rng}(X_i)$ respectively, we have that any Hermitian operator P_i satisfying $\mathsf{Supp}(P_i)\subseteq\mathsf{Supp}(X_i)$ has the form $P_i=\Sigma_{m,n}p_{mn}^{(i)}|v_m\rangle\langle v_n|$, whence it can be written as $P_i=X_i^\dagger Q_i X_i$, for some suitable Hermitian operator $Q_i\in\mathcal{B}(\mathsf{Rng}(X))$. Once the equivalence between the form (24) and condition (19) is established, relation (25) follows directly from Eq. (20). ■

Observation: According to the previous lemma, a perturbation of A is completely specified by a set of Hermitian operators $\{Q_i\in\mathcal{B}(\mathcal{H}_i)|i\in\mathcal{I}\}$, where $\mathcal{H}_i=\mathsf{Rng}(X_i)$. Such operators can be cast into a single block operator $Q\in\oplus_{i\in I}\mathcal{B}(H_i)$ by defining

$$Q=\bigoplus_{i\in\mathcal{I}}Q_i. \tag{26}$$

In terms of the block operator Q we have the following:

Lemma 3: *Let* $A=\oplus_{i\in I}X_i^\dagger X_i$ *be a point of* C. *Define the block operators*

$$F_{kl}^\mu=\bigoplus_{i\in\mathcal{I}}X_i S_{kli}^\mu X_i^\dagger. \tag{27}$$

Then A admits a perturbation if and only if there exists an Hermitian block operator $Q\in\oplus_{i\in I}\mathcal{B}(H_i)$ *such that*

$$\mathrm{Tr}[F_{kl}^\mu Q]=0,\quad \forall\,\mu\in\mathsf{S},\quad \forall\,k,l=1,\ldots,m_\mu. \tag{28}$$

Proof: Using the definition of F_{kl}^μ and the cyclic property of the trace, it is immediate to see that Eq. (28) is equivalent to Eq. (25). ■

The previous lemma enables us to characterize the extremal points of C.

Theorem 2 (Spanning set condition): *Let* $A=\oplus_{i\in I}X_i^\dagger X_i$ *be a point of* C, *and* $\mathsf{F}=\{F_{kl}^\mu|\mu\in\mathsf{S},k,l=1,\ldots,m_\mu\}$ *be the set of block operators defined in Lemma 3*. *Then*, *A is extremal if and only if*

$$\mathsf{Span}(\mathsf{F})=\bigoplus_{i\in\mathcal{I}}\mathcal{B}(\mathcal{H}_i), \tag{29}$$

where $\mathcal{H}_i=\mathsf{Rng}(X_i)$.

Proof: A is extremal iff it admits only the trivial perturbation $P=0$. Equivalently, due to Lemma 3, A is extremal iff the only Hermitian operator $Q\in\oplus_{i\in I}\mathcal{B}(H_i)$ that satisfies Eq. (28) is the null operator $Q=0$. Let us decompose the Hilbert space $\mathcal{K}=\oplus_{i\in I}\mathcal{B}(H_i)$, as $\mathcal{K}=\mathsf{Span}(\mathsf{F})\oplus\mathsf{Span}(\mathsf{F})^\perp$, where $\perp$ denotes the orthogonal complement with respect to the Hilbert-Schmidt product $(A,B)=\mathrm{Tr}[A^\dagger B]$. Then, A is extremal iff the only Hermitian operator in $\mathsf{Span}(\mathsf{F})^\perp$ is the null operator. This is equivalent to the condition $\mathsf{Span}(\mathsf{F})^\perp=\{0\}$, i.e., $\mathcal{K}=\mathsf{Span}(\mathsf{F})$. ■

Corollary 2: *Let* $A=\oplus_{i\in I}X_i^\dagger X_i$ *be a point of* C, *and let define* $r_i=\mathrm{rank}(X_i)$. *If A is extremal*, *then the following relation holds*

$$\sum_{i\in\mathcal{I}}r_i^2\leqslant\sum_{\mu\in\mathsf{S}}m_\mu^2. \tag{30}$$

Proof: For an extreme point of C, relation (29) implies that the cardinality of the set F is greater than the dimension of $\mathcal{K}=\oplus_{i\in I}\mathcal{B}(H_i)$. Then, the upper bound (30) follows from $\dim\mathcal{K}=\Sigma_{i\in\mathcal{I}}r_i^2$ and from the fact that $|\mathsf{F}|=\Sigma_{\mu\in\mathsf{S}}m_\mu^2$. ■

Observation: If the group-representation $\mathsf{R}(\mathbf{G})$ is irreducible, then its Clebsch-Gordan decomposition contains only one term $\bar{\mu}$ with multiplicity $m_{\bar{\mu}}=1$. Then, bound (30) becomes $\Sigma_{i\in\mathcal{I}}r_i^2\leqslant 1$, namely for an extremal $A=\oplus_{i\in I}A_i$, one has necessarily $\mathrm{rank}(A_{i_0})=1$ for some $i_0\in\mathcal{I}$, and $A_i=0$ for any $i\neq i_0$ (this is also a sufficient condition, due to Corollary 1). In terms of the corresponding covariant POVM $M(i,g)=U_g A_i U_g^\dagger$, one has $M(i,g)=0$ for any $i\neq i_0$, i.e., corresponding to events in the probability space that never occur.

V. EXTREMAL COVARIANT POVMs IN THE PRESENCE OF NONTRIVIAL STABILITY GROUPS

In Sec. IV, we obtained a characterization of extremal covariant POVMs whose probability space is $\mathfrak{X}=\mathcal{I}\times\mathbf{G}$ for some finite index set $\mathcal{I}$. The framework we outlined is suitable for a straightforward generalization to the case $\mathfrak{X}=\cup_{i\in\mathcal{I}}\mathbf{G}/\mathbf{G}_i$, where $\mathbf{G}_i$ are compact subgroups of $\mathbf{G}$.

In this case, it is possible to show that a covariant POVM P admits a density $M(x_i)$ such that for any measurable subset $B\subseteq\mathbf{G}/\mathbf{G}_i$ one has $P(B)\equiv P_i(B)\doteq\int_{B_i}\mathrm{d}x_i M(x_i)$, where $\mathrm{d}x_i$ is the group invariant measure on $\mathbf{G}/\mathbf{G}_i$. The form of the operator density is now

$$M(x_i)=U_{g_i(x_i)}A_iU^\dagger_{g_i(x_i)}, \tag{31}$$

where $A_i\geqslant 0$, and $g_i(x_i)\in\mathbf{G}$ is any representative element of the equivalence class $x_i\in\mathbf{G}/\mathbf{G}_i$. The normalization of the POVM is still given by Eq. (16). In addition, in order to remove the dependence of $M(x_i)$ from the choice of the representative $g_i(x_i)$, each operator A_i must satisfy the relation

$$[A_i,U_h]=0,\quad \forall\, h\in\mathbf{G}_i. \tag{32}$$

The commutation constraint (32) can be simplified by decomposing each representation $\mathsf{R}(\mathbf{G}_i)=\{U_h|h\in\mathbf{G}_i\}$ into irreps

$$U_h=\bigoplus_{\nu\in\mathsf{S}_i}U_h^{\nu_i}\otimes\mathbb{1}_{m_{\nu_i}}, \tag{33}$$

where m_{ν_i} denotes the multiplicity of the irrep ν_i, and S_i denotes the collection of all irreps contained in the decomposition of $\mathsf{R}(\mathbf{G}_i)$. This corresponds to the decomposition of the Hilbert space $\mathcal{H}$ as

$$\mathcal{H}=\bigoplus_{\nu_i\in\mathsf{S}_i}\mathcal{H}_{\nu_i}\otimes\mathbb{C}^{m_{\nu_i}}, \tag{34}$$

where $\mathcal{H}_{\nu_i}$ is a representation space, supporting the irrep ν_i, and $\mathbb{C}^{m_{\nu_i}}$ is a multiplicity space. In this decomposition, the commutation relation (32) is equivalent to the block form

$$A_i=\bigoplus_{\nu_i\in\mathsf{S}_i}\mathbb{1}_{\nu_i}\otimes A_{i,\nu_i}, \tag{35}$$

where $A_{i,\nu_i}\geqslant 0$ are operators acting on the multiplicity space $\mathbb{C}^{m_{\nu_i}}$.

By defining $\omega=(i,\nu_i)$ and $\Omega=\cup_{i\in\mathcal{I}}S_i$, we can introduce an auxiliary Hilbert space, and associate to a covariant POVM the block operator

$$A=\bigoplus_{\omega\in\Omega}A_\omega, \tag{36}$$

where $A_\omega\doteq A_{i,\nu_i}$. Furthermore, we define the block operators

$$S^\mu_{kl}=\bigoplus_{\omega\in\Omega}S^\mu_{kl\omega}, \tag{37}$$

where now $S_{kl\omega}=\mathrm{Tr}_{\mathcal{H}_{\nu_i}}[\Pi_{\nu_i}T^\mu_{kl}]$. Here Π_{ν_i} denotes the projector onto $\mathcal{H}_{\nu_i}\otimes\mathbb{C}^{m_{\nu_i}}$, and $\mathrm{Tr}_{\mathcal{H}_{\nu_i}}$ denotes the partial trace over $\mathcal{H}_{\nu_i}$. With these definitions, the normalization of the POVM, given by Eq. (16), becomes equivalent to

$$\mathrm{Tr}[S^\mu_{kl}A]=\delta_{kl}d_\mu. \tag{38}$$

Now we call D the convex set of block operators $A=\oplus_{\omega\in\Omega}A_\omega$, defined by the two conditions $A\geqslant 0$ and Eq. (38). Such a convex set is in one-to-one affine correspondence with the convex set of covariant POVMs with probability space $\mathfrak{X}=\cup_{i\in\mathcal{I}}\mathbf{G}/\mathbf{G}_i$. Since the constraints defining D are formally the same defining the convex set C, we can exploit the characterization of extremal points of the previous section. In particular, Corollary 2 becomes

Corollary 3: *Let* $A=\oplus_{\omega\in\Omega}X_\omega^\dagger X_\omega$ *be a point of* D, *and define* $r_{i,\nu_i}\equiv r_\omega=\mathrm{rank}(X_\omega)$. *If* A *is extremal*, *then the following relation holds:*

$$\sum_{i\in\mathcal{I}}\sum_{\nu_i\in\mathsf{S}_i} r_{i,\nu_i}^2 \leqslant \sum_{\mu\in\mathsf{S}} m_\mu^2. \tag{39}$$

Observation: As in the case of Corollary 2, if the representation $\mathsf{R}(\mathbf{G})$ is irreducible, as a consequence of the bound about ranks, one obtains $\mathrm{rank}(A_{\omega_0})=1$ for some $\omega_0\in\Omega$, and $A_\omega=0$ for any $\omega\neq\omega_0$.

VI. APPLICATIONS

Here we give two examples of the use of the characterization of extremal POVMs in the solution of concrete optimization problems.

A. State discrimination with mutually unbiased bases

1. Two Fourier transformed bases

Here we consider a case of state discrimination where the set of signal states is the union of two mutually unbiased bases (MUBs),[11] related by Fourier transform. Precisely, let $\mathcal{H}$ be a d-dimensional Hilbert space, and consider the orthornormal bases $\mathcal{B}_1=\{|n\rangle\,|\,n=0,\ldots,d-1\}$ and $\mathcal{B}_2=\{|e_n\rangle\,|\,n=0,\ldots,d-1\}$, where $|e_n\rangle=(1/\sqrt{d})\Sigma_{m=0}^{d-1}\omega^{mn}|m\rangle$, $\omega=\exp(2\pi i/d)$. $\mathcal{B}_1$ and $\mathcal{B}_2$ are mutually unbiased, namely $|\langle m|e_n\rangle|^2=1/d$ for any m,n. Consider the two sets of states defined by $\mathcal{S}_1=\{\rho_{1n}=|n\rangle\langle n|\,|n=0,\ldots,d-1\}$ and $\mathcal{S}_2=\{\rho_{2n}=|e_n\rangle\langle e_n|\,|n=0,\ldots,d-1\}$. Now the problem is to determine with minimum error probability the state of the system, which is randomly prepared either in a state of $\mathcal{S}_1$ with probability p/d, or in a state of $\mathcal{S}_2$ with probability $(1-p)/d$.

Exploiting the results of the present paper it is immediate to find the measurement that minimizes the error probability. In fact, let us consider the irreducible representation of the group $\mathbf{G}=\mathbb{Z}_d\times\mathbb{Z}_d$ given by

$$\mathsf{R}(\mathbf{G})=\left\{U_{pq}=\sum_{n=0}^{d-1}\omega^{qn}|n\oplus p\rangle\langle n|,(p,q)\in\mathbb{Z}_d\times\mathbb{Z}_d\right\}, \tag{40}$$

where $\oplus$ denotes addition modulo d. Then, the sets $\mathcal{S}_1$ and $\mathcal{S}_2$ are the group orbits of the initial states ρ_{10} and ρ_{20}, respectively. Moreover, the states ρ_{10} and ρ_{20} have nontrivial stability groups $\mathbf{G}_1$ and $\mathbf{G}_2$, defined by the unitaries $\mathsf{R}(\mathbf{G}_1)=\{U_{0q}\,|\,q\in\mathbb{Z}_d\}$ and $\mathsf{R}(\mathbf{G}_2)=\{U_{p0}\,|\,p\in\mathbb{Z}_d\}$. Therefore, signal states are in one-to-one correspondence with points of the probability space $\mathcal{X}=\mathbf{G}/\mathbf{G}_1\cup\mathbf{G}/\mathbf{G}_2$, such points being denoted by couples (i,n) where $i\in\{1,2\}$ and $n\in\mathbb{Z}_d$. For the discrimination we can consider without loss of generality a covariant POVM, of the form of Eq. (31), where now the group element g is the couple $(p,q)\in\mathbb{Z}_d\times\mathbb{Z}_d$. Moreover, since the probabilities are linear in the POVM, in the minimization of the error probability we can restrict the attention to extremal covariant POVMs. Now, the representation $\mathsf{R}(\mathbf{G})$ is irreducible, whence Corollary 3 requires either $A_1=0$ or $A_2=0$ in Eq. (31). This means that either the states in $\mathcal{S}_1$ or the states in $\mathcal{S}_2$ are never detected. Moreover, since the states within a given set, either $\mathcal{S}_1$ or $\mathcal{S}_2$, are orthogonal, they can be perfectly distinguished among themselves. Therefore, the optimal POVM is $P^{(1)}(i,n)=\delta_{i1}|n\rangle\langle n|$ if $p\geqslant 1/2$, and $P^{(2)}(i,n)=\delta_{i2}|e_n\rangle\langle e_n|$ otherwise. In particular, if $p=1/2$, an experimenter who tries to discriminate states of two Fourier transformed bases cannot do anything better than randomly choosing one of the orthogonal measurements $P^{(1)}$ and $P^{(2)}$. This is the working principle of the BB84 crypthographic protocol.[13]

2. Mutually unbiased bases in prime dimension

If the dimension of the Hilbert space $\mathcal{H}$ is a prime number, then there are $d+1$ MUBs that are generated by the irreducible representation

$$\mathsf{R}(\mathbf{G}) = \left\{ U_{pq} = \sum_{n=0}^{d-1} \omega^{qn} |n \oplus p\rangle\langle n|, (p,q) \in \mathbb{Z}_d \times \mathbb{Z}_d \right\}$$

via the construction by Wootters and Fields[11] (see also Ref. 12).

In this case, the result of the previous paragraph can be immediately generalized to a case of state discrimination with more than two MUBs. Again, due to the irreducibility of the representation $\mathsf{R}(\mathbf{G})$, an extremal POVM is the group orbit of a single operator. Therefore, denoting by $\mathcal{S}_i$ the set of states associated to the basis $\mathcal{B}_i$, and by p_i/d the probability of extracting a state from $\mathcal{S}_i$ ($\Sigma_{i\in\mathcal{I}} p_i = 1$), we have that the covariant POVM which discriminates the signal states with minimum error probability is the orthogonal measurement onto the basis $\mathcal{B}_{\bar{l}}$ such that $p_{\bar{l}} = \max_{l\in\mathcal{I}}\{p_l\}$.

3. Mutually unbiased bases in dimension p^r

In the case of Hilbert space dimension $d = p^r$, where p is prime number, $d+1$ MUBs can be constructed by introducing a projective representation of the Abelian group $\tilde{\mathbf{G}} = \mathbb{F}_d \times \mathbb{F}_d$, where $\mathbb{F}_d$ is the finite field of cardinality d, considered here as an additive group. In order to apply the results of the paper to this case, we first outline the method for constructing MUBs presented in Ref. 12, to which we refer for details and for the explicit proofs.

Consider an orthonormal basis for $\mathcal{H}$, denoted as $\{|n\rangle \,|\, n \in \mathbb{F}_d\}$, in which basis elements are labeled by elements of the field. Then, introduce the projective representation

$$\mathsf{R}(\tilde{\mathbf{G}}) = \{U_p V_q | (p,q) \in \mathbb{F}_d \times \mathbb{F}_d\}, \tag{41}$$

where U_p, V_q are the unitary operators uniquely defined by the relations

$$U_p |n\rangle = |n+p\rangle,$$

$$V_q |n\rangle = \langle q,n\rangle |n\rangle. \tag{42}$$

Here, $\langle a,b\rangle \doteq \chi(a\cdot b)$, where $\chi(x)$ is any nontrivial character of the additive group $\mathbb{F}_d$, and $a+b$ ($a\cdot b$) denote the addition (product) in the finite field $\mathbb{F}_d$. With the above definition $\langle a,b\rangle$ is a symmetric bicharacter for the additive group $\mathbb{F}_d$, namely $|\langle a,b\rangle| = 1, \langle a,b\rangle = \langle b,a\rangle$, and $\langle a,b+c\rangle = \langle a,b\rangle\langle a,c\rangle$, for any $a,b,c \in \mathbb{F}_d$. By definition (42), the operators U_p, V_q commute up to a phase, namely

$$V_q U_p = \langle p,q\rangle U_p V_q. \tag{43}$$

To construct $d+1$ MUBs, it is useful to introduce $d+1$ sets of the unitary operators, each set being labeled by an index $i \in \mathbb{F}_d \cup \{\infty\}$ (∞ is just a label which denotes an additional value, not in $\mathbb{F}_d$, of the index i). The $d+1$ sets of unitary operators are defined by

$$W(i,j) \doteq \begin{cases} \alpha(i,j) U_j V_{i\cdot j}, & i \in \mathbb{F}_d \\ V_j, & i = \infty, \end{cases} \tag{44}$$

where $\alpha(i,j)$ are suitable phase factors (see Ref. 12), chosen in such a way that, for any fixed i, the operators $W(i,j)$ form a unitary representation of the additive group $\mathbb{F}_d$, namely

$$W(i,j)W(i,l) = W(i,j+l), \quad \forall\, j,l \in \mathbb{F}_d. \tag{45}$$

Since the group $\mathbb{F}_d$ is Abelian, for fixed i the operators $W(i,j)$ can be diagonalized on the same basis, denoted by $\mathcal{B}_i$. The above construction guarantees that the bases $\{\mathcal{B}_i | i \in \mathbb{F}_d \cup \{\infty\}\}$ are all mutually unbiased. Moreover, the one-dimensional projector $P(i,k)$ onto the kth element of the basis $\mathcal{B}_i$ can be written as[12]

$$P(i,k) = d^{-1} \sum_{j\in\mathbb{F}_d} \overline{\langle j,k\rangle} W(i,j). \tag{46}$$

Now we exploit the above-noted construction to show that, for any $i \in \mathbb{F}_d \cup \{\infty\}$, the set of states $\mathcal{S}_i = \{\rho_{ik} = P_{ik} | k \in \mathbb{F}_d\}$ is the orbit of the initial state $\rho_{i0} = P_{i0}$ under the action of the representation $\mathsf{R}(\tilde{G})$.

For $i \in \mathbb{F}_d$, we have indeed

$$\begin{aligned} U_p V_q P(i,k) V_q^\dagger U_p^\dagger &= d^{-1} \sum_{j \in \mathbb{F}_d} \overline{\langle j,k \rangle} \alpha(i,j) U_p V_q U_j V_{k \cdot j} V_{-q} U_{-p} \\ &= d^{-1} \sum_{j \in \mathbb{F}_d} \overline{\langle j,k \rangle} \langle j,q \rangle \langle i \cdot j, -p \rangle \alpha(i,j) U_j V_{i \cdot j} \\ &= d^{-1} \sum_{j \in \mathbb{F}_d} \overline{\langle j,k-q+i \cdot p \rangle} W(i,j) = P(i,k-q+i \cdot p), \end{aligned} \tag{47}$$

where we used Eqs. (46), (44), (43), and the properties $\langle a,-b \rangle = \overline{\langle a,b \rangle}$, $\langle a,b+c \rangle = \langle a,b \rangle \langle a,c \rangle$, and $\langle a,b \cdot c \rangle = \langle a \cdot b,c \rangle$. Similarly, for $i = \infty$ we obtain

$$U_p V_q P(\infty,k) V_q^\dagger U_p^\dagger = P(\infty,k+p). \tag{48}$$

Notice that from Eqs. (47), (48) it also follows that for any $i \in \mathbb{F}_d \cup \{\infty\}$, the stability group of $\rho_{i0} = P_{i0}$ is the additive group $\mathbb{F}_d$, which is projectively represented by the unitaries $\{U_p V_{i \cdot p} | p \in \mathbb{F}_d\}$ for $i \in \mathbb{F}_d$, and by the unitaries $\{V_q | q \in \mathbb{F}_d\}$ for $i = \infty$.

In the problem of state discrimination where the state ρ_{ik} is randomly drawn from the set $\mathcal{S}_i$ with probability p_i/d, we can then use the results about extremal covariant POVMs with nontrivial stability group to find the minimum error POVM. Again, since the representation $\mathsf{R}(\tilde{\mathbf{G}})$ is irreducible,[14] an extremal POVM must be the group orbit of a single operator. The optimal POVM for state discrimination is then the orthogonal measurement onto the basis $\mathcal{B}_{\bar{l}}$ which occurs with highest probability $p_{\bar{l}} = \max_i \{p_i\}$.

B. Maximization of the mutual information

A frequent problem in quantum communication is to find the POVM $P_i, i \in \mathcal{I}$, that maximizes the mutual information with a given set of signal states $\mathcal{S} = \{\rho_j | j \in \mathcal{J}\}$. Denoting by p_j the probability of the signal state ρ_j, by $q_i = \Sigma_{j \in \mathcal{J}} p_j \mathrm{Tr}[M_i \rho_j]$ the overall probability of the outcome i, and by $p_{ij} = p_j \mathrm{Tr}[M_i \rho_j]$ the joint probability of the outcome j with the state ρ_i, the mutual information is defined as

$$I = H(\{p_{ij}\}) - H(\{p_i\}) - H(\{q_j\}), \tag{49}$$

where $H(\{p_i\}) \doteq \Sigma_i - p_i \log(p_i)$ is the Shannon entropy. As in the minimization of a Bayes cost,[4,5] when the set of signal states is invariant under the action of some finite group $\mathbf{G}$ and all states in the same group orbit have the same probability, one can without loss of generality restrict the search for the optimal POVM among covariant POVMs with probability space $\mathcal{X} = \mathcal{I} \otimes \mathbf{G}$, for some finite index set $\mathcal{I}$.[15,9] However, differently from the case of state discrimination, the points of the probability space do not need to be in one-to-one correspondence with the signal states. Therefore, the set $\mathcal{I}$ is not specified *a priori*.

Combining our characterization of extremal covariant POVMs with the following basic properties of the mutual information (for the proofs, see Ref. 15), we can readily obtain a bound about the cardinality of the index set $\mathcal{I}$.

Property 1: *The mutual information is a convex functional of the POVM.*

Property 2: *In the maximization of the mutual information, one can consider without loss of generality POVMs made of rank-one operators.*

Consider a covariant POVM $P(i,g) = (1/(|\mathbf{G}|) U_g A_i U_g^\dagger$. Due to Property 1, in the maximization of the mutual information we can consider extremal covariant POVMs. Then, from Corollary 2,

we have the bound $\Sigma_{i\in\mathcal{I}}\mathrm{rank}(A_i)^2 \leqslant \Sigma_{\mu\in\mathsf{S}} m_\mu^2$. Due to Property 2, this also implies that the number of (rank-one) operators A_i must be smaller than $\Sigma_{\mu\in\mathsf{S}} m_\mu^2$. Therefore, we can assume without loss of generality

$$|\mathcal{I}| \leqslant \sum_{\mu\in\mathsf{S}} m_\mu^2. \tag{50}$$

This provides an alternative derivation of the bound given in Ref. 9. Finally, if the representation $\mathsf{R}(\mathbf{G})$ is irreducible, the bound gives $|\mathcal{I}|=1$, namely the probability space is $\mathcal{X}\simeq\mathbf{G}$, according to the classic result of Ref. 15.

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Pointwise analysis of scalar fields: A nonstandard approach

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A new nonstandard-analytical approach to quantum fields is presented, which gives a mathematical foundation for manipulating pointwise-defined quantum fields. In our approach, a field operator $\phi(x)$ is not a standard operator-valued distribution, but a nonstandard operator-valued function. Then formal expressions containing, e.g., $\phi(x)^2$ can be understood literally, and shown to be well defined. In the free field cases, we show that the Wightman functions are explicitly calculated with the pointwise field, without any regularization, e.g., Wick product. Our notion of pointwise fields is applied also to the path integral formalisms of scalar fields. We show that some of physicists' naive expressions of Lagrangian path integral formulas can be rigorously justified. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The main object of *nonstandard mathematics*,[1–3] originated by A. Robinson, is to give a rigorous foundation for the notions of infinities and infinitesimals, e.g., infinite real numbers and infinitesimal real numbers. *Nonstandard approaches to quantum physics*[4–12] are those which use nonstandard mathematics as a fundamental tool of quantum physics.

In this paper, we give a new nonstandard approach which gives a rigorous foundation for manipulating *pointwise-defined* quantum fields. For example, consider the physicist's naive expression of the Hamiltonian of a free scalar field with mass m:

$$H_m = \frac{1}{2}\int \left[\hat{\pi}(\boldsymbol{x})^2 + \sum_{k=1}^{\mathbf{d}} (\partial_k \hat{\phi}(\boldsymbol{x}))^2 + m^2 \hat{\phi}(\boldsymbol{x})^2 \right] \mathrm{d}\boldsymbol{x}.$$

In the standard approach, the field operators $\hat{\phi}$ and $\hat{\pi}$ are considered as operator-valued distributions, which are not pointwise-defined functions. So expressions like $\hat{\phi}(\boldsymbol{x})^2$ are mathematically meaningless, and hence the right-hand side must be regarded as nothing more than a formal expression. On the other hand, in our approach, the above-noted right-hand side can be understood *literally*, and shown to be well defined.

Our notion of pointwise fields is applicable also to the path integral formalisms. Standard justifications of path integrals for scalar fields are based on the theorems of Feynman–Kac–Nelson and Minlos, where the path space is taken to be the space $\mathcal{S}'$ of tempered distributions. Thus ϕ^2 and $(\partial_k \phi)^2$ are not always meaningful for a path $\phi \in \mathcal{S}'$. However, physicists use the path integral expression like

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$$\int e^{\alpha \int L(\phi, \partial_k \phi) \mathrm{d}x} \mathrm{d}\phi,$$

where L is the Lagrangian, and $\alpha \in \mathbf{C}$ is a constant. Usually L contains ϕ^2 and $(\partial_k \phi)^2$. Thus in the standard approach, the above-presented expression must be regarded as merely a formal one. On the other hand, our approach enables one to justify the expression *literally.*

Our approach is based on the notion of hyperfinite-dimensional Schrödinger representations of fields. A *Schrödinger representation of a quantum field* is a representation where the state space is a function space $\mathcal{H}$, typically $\mathcal{H}=L^2(M,\mu)$ with a measure space (M,μ), and the field operators at $t=0$, called *time zero field operators*, are represented as the multiplication operators on $\mathcal{H}$. A *hyperfinite-dimensional (or ⋆finite-dimensional) Schrödinger representation* is a Schrödinger representation where M is taken to be a hyperfinite-dimensional linear space, i.e., $M \cong {}^\star\mathbf{R}^\nu$ for a infinite ⋆natural number $\nu \in {}^\star\mathbf{N}$.

II. NONSTANDARD ANALYSIS

There are several different formulations of nonstandard analysis. This paper adopts the set-theoretical approach based on superstructures instituted by Robinson and Zakon[13] and follows the up-to-date description by Chang and Keisler.[14] For the introductory purpose, see Hurd and Loeb.[2]

In this paper, we always work with a nonstandard universe $\langle V(X), V(Y), \star \rangle$ which is κ-saturated with $\mathrm{card}(V(X)) < \kappa$; such a nonstandard universe is said to be *polysaturated*. We also assume that the base X includes the complex numbers $\mathbf{C}$ and any other structures under consideration such as given groups and Hilbert spaces.

For a set S, let ${}^\sigma S = \{{}^\star s \,|\, s \in S\}$. We identify ${}^\star z$ with z for all $z \in \mathbf{C}$. Hence, ${}^\sigma S = S$ if S is a subset of $\mathbf{C}$, e.g., ${}^\sigma\mathbf{C}=\mathbf{C}$, ${}^\sigma\mathbf{R}=\mathbf{R}$ (the real numbers), ${}^\sigma\mathbf{Z}=\mathbf{Z}$ (the integers), and ${}^\sigma\mathbf{N}=\mathbf{N}$. Let $\mathbf{R}^+$, ${}^\star\mathbf{R}_0$, ${}^\star\mathbf{R}_0^+$, ${}^\star\mathbf{R}_\infty^+$, and ${}^\star\mathbf{N}_\infty$ denote the sets of positive real numbers, infinitesimal hyper-real numbers, positive infinitesimal hyper-real numbers, positive infinite hyper-real numbers, and infinite hypernatural numbers, respectively. It is shown that ${}^\star\mathbf{N}_\infty = {}^\star\mathbf{N} \backslash \mathbf{N}$. We write $x \sim \infty$ if $x \in {}^\star\mathbf{R}_\infty^+$, and $0 < x < \infty$ if $x \in \mathrm{fin}\ {}^\star\mathbf{R}^+ = {}^\star\mathbf{R}^+ \backslash {}^\star\mathbf{R}_\infty^+$. If $r \in {}^\star\mathbf{R}$ and $|r| < \infty$, the standard part of r is denoted by ${}^\circ r$. If $r \sim \infty$, we write ${}^\circ r = \infty$. Let $x, y \in {}^\star\mathbf{R}^+$. We say that x is of the *order* of y, in symbols $x \asymp y$, iff $0 < x/y < \infty$ and $0 < y/x < \infty$. We write $x \ll y$ if $x/y \approx 0$. For a hyperfinite (⋆-finite) set F, let $|F|$ denote the internal cardinal number of F.

Let $(X, \mathcal{O})$ be a topological space. Let $\mathcal{O}_x$ denote the system of open neighborhoods of $x \in X$. The *monad* of $x \in X$ is the subset of ${}^\star X$ defined by $\mathrm{mon}_\mathcal{O}(x) = \cap \{{}^\star O \,|\, O \in \mathcal{O}_x\}$. The set of *near standard* points is the subset of ${}^\star X$ defined by $\mathrm{ns}({}^\star X) = \cup \{\mathrm{mon}_\mathcal{O}(x) \,|\, x \in X\}$. It is shown that $(X, \mathcal{O})$ is Hausdorff if and only if $x \neq y$ implies $\mathrm{mon}_\mathcal{O}(x) \cap \mathrm{mon}_\mathcal{O}(y) = \emptyset$. Thus for any Hausdorff space $(X, \mathcal{O})$, we can define the equivalence relation $\approx_\mathcal{O}$ on $\mathrm{ns}{}^\star X$ so that $a \approx_\mathcal{O} b$ iff $a \in \mathrm{mon}_\mathcal{O}(x)$ and $b \in \mathrm{mon}_\mathcal{O}(x)$ for some $x \in X$.

Let f and g be functions from ${}^\star\mathbf{R}^n$ to ${}^\star\mathbf{C}$. When we consider the approximation $f \approx g$, we must make clear what topology is considered. For example,

1. pointwise topology: $f \approx g \Leftrightarrow (\forall x \in \mathbf{R}) f(x) \approx g(x)$.
2. L^p topology: $f \approx g \Leftrightarrow \|f-g\|_p \approx 0$.
3. topology of Schwartz distributions:

$$f \approx g \Leftrightarrow (\forall h \in \mathcal{D}(\mathbf{R}^n))(f,h) \approx (g,h).$$

In this paper we frequently use the approximations with respect to L^2 topology and that of Schwartz distributions.

For further information on nonstandard real analysis, we refer to Stroyan and Luxemburg[3] and Hurd and Loeb.[2]

III. NONSTANDARD DISTRIBUTIONS

There are several approaches to nonstandard distribution theory. In this paper, we use the following framework.

Let $\mathbf{d} \in \mathbf{N}$. Let M be a $\mathbf{d}$-dimensional possibly noncompact Riemannian manifold. Let $\mathcal{D} = \mathcal{D}(M)$ be the space of smooth functions from M to $\mathbf{R}$ whose support is compact. $\mathcal{D}$ is furnished with the inner product

$$(f,g) = \int_M f(x)g(x)\mathrm{d}x.$$

The nonstandard extension ${}^\star\mathcal{D}$ has the transferred ${}^\star\mathbf{R}$-valued inner product

$${}^\star(f,g) = {}^\star\int_{{}^\star M} f(x)g(x)\mathrm{d}x.$$

We abbreviate ${}^\star(f,g)$ simply as (f,g).

Let $\mathcal{F}$ be a $\star$finite-dimensional subspace of ${}^\star\mathcal{D}$ such that

$${}^\sigma\mathcal{D} \subset \mathcal{F} \subset {}^\star\mathcal{D}.$$

The existence of such $\mathcal{F}$ is shown by the saturation principle in nonstandard analysis. Note that there is $\nu \in {}^\star\mathbf{N}$ satisfying $\mathcal{F} \cong {}^\star\mathbf{R}^\nu$ (isomorphism of *linear spaces).

Since $\mathcal{F}$ is $\star$finite-dimensional, its *internal* algebraic dual

$$\mathcal{F}_1^* = \{f | f:\mathcal{F} \to {}^\star\mathbf{R},\ {}^\star\text{linear}\}$$

is equal to its *internal* topological dual

$$\mathcal{F}_2^* = \{f | f:\mathcal{F} \to {}^\star\mathbf{R},\ {}^\star\text{continuous}\}.$$

Let $\mathcal{F}^*$ denote the internal dual space of $\mathcal{F}$, that is, $\mathcal{F}^* = \mathcal{F}_1^* = \mathcal{F}_2^*$. Note that the inner product $(\cdot,\cdot)$ naturally determines an isomorphism $e:\mathcal{F}^* \cong \mathcal{F}$. Since $\mathbf{R}$ is a subfield of ${}^\star\mathbf{R}$, the internal linear spaces $\mathcal{F}$ and $\mathcal{F}^*$ over ${}^\star\mathbf{R}$ can also be regarded as external linear spaces over $\mathbf{R}$, i.e., as real linear spaces in the usual (standard-mathematical) sense. Thus such a phrase as "linear map from $\mathcal{D}$ to $\mathcal{F}$" makes sense.

Let $\mathcal{D}^*$ denote the algebraic dual of $\mathcal{D}$ in the usual sense.

Lemma 3.1: *There is an injective linear map* $\pi:\mathcal{D}^* \to \mathcal{F}$ *such that*

$$(\forall f \in \mathcal{F})(\pi(F),f) = ({}^\star F)(f) \tag{1}$$

for all $F \in \mathcal{D}^*$.

Proof: Let $F \in \mathcal{D}^*$. The map $\alpha_F:\mathcal{F} \to {}^\star\mathbf{R}$ defined by $\alpha_F(f) = ({}^\star F)(f)$ is a *linear functional on $\mathcal{F}$, that is, $\alpha_F \in \mathcal{F}^*$. Define π by $\pi(F) = e(\alpha_F)$, where e denotes the natural isomorphism $e:\mathcal{F}^* \cong \mathcal{F}$. Then we can check that (1) holds. We will show that π is injective. Since π is linear, it suffices to show that

$$\pi(F) = 0 \Rightarrow F = 0 \text{ for any } F \in \mathcal{D}^*.$$

Suppose $\pi(F) = 0$. Then by (1), we have

$$(\forall f \in \mathcal{F})({}^\star F)(f) = 0.$$

Since ${}^\sigma\mathcal{D} \subset \mathcal{F}$, we have

$$(\forall f \in \mathcal{D})({}^\star F)({}^\star f) = 0.$$

By the transfer principle, this is equivalent to

$$(\forall f \in \mathcal{D})F(f) = 0.$$

This means $F=0$. *QED*

By the above Lemma, we have the relation

$$\mathcal{D} \overset{a}{\hookrightarrow} \mathcal{D}' \subset \mathcal{D}^* \overset{\pi}{\hookrightarrow} \mathcal{F} \subset {}^\star\mathcal{D} \subset {}^\star L^2(M),$$

where $\mathcal{D} \overset{a}{\hookrightarrow} \mathcal{D}'$ denotes the natural embedding $a: f \mapsto (\cdot, f)$. The embedding $\mathcal{D}' \subset \mathcal{D}^* \overset{\pi}{\hookrightarrow} \mathcal{F}$ permits us to consider a Schwartz distribution as an element of $\mathcal{F}$, a space of *pointwise-defined* functions on ${}^\star M$.

For $x \in {}^\star M$, define $\delta_x \in \mathcal{F}$ by

$$(\forall f \in \mathcal{F})(\delta_x, f) = f(x).$$

The nth derivatives of δ_x are already defined because $\delta_x \in {}^\star\mathcal{D}$. In the case where $M=\mathbf{R}^n$, clearly we have

$$((\partial/\partial x_k)\delta_x, f) = -(\delta_x, (\partial/\partial x_k)f).$$

But note that a derivative of δ_x may not be in $\mathcal{F}$. In the case where $M=\mathbf{R}^n$, $(\partial^l/\partial x_k^l)\delta_x (1 \leqslant k \leqslant n)$ is well-defined for any $l \in {}^\star\mathbf{N}$, but $(\partial^l/\partial x_k^l)\delta_x \notin \mathcal{F}$ can occur even if $l < \infty$. However we can define a "derivative" $\delta_x^k \in \mathcal{F}$ such that

$$(\delta_x^k, f) = -(\partial/\partial x_k)f(x), \quad f \in \mathcal{F}.$$

Clearly we see the relation $\delta_x^k = E_{\mathcal{F}}(\partial/\partial x_k)\delta_x$ where $E_{\mathcal{F}}$ is the orthogonal projection from ${}^\star L^2(\mathbf{R}^n)$ to $\mathcal{F}$. So δ_x^k is called a *projected derivative.*

Also note that the following relations do *not* hold:

$$x \neq y \Rightarrow \delta_x(y) = 0,$$

$$\delta_x(y) = \delta_0(y-x)(M = \mathbf{R}^n).$$

On the other hand, since our nonstandard delta functions are pointwise-defined, the product of delta functions such as $f(x) = \delta_a(x)^2$ are well defined. An inner product of delta functions such as (δ_x, δ_y) is also well defined. Thus we can directly justify the physicists' *trace formula* as follows.

Proposition 3.2: *The following properties hold.*

(*i*) $\delta_x(y) = \delta_y(x)$.

(*ii*) $\int_{{}^\star M} f(x)\delta_x \mathrm{d}x = f$ *for any* $f \in \mathcal{F}$.

(*iii*) (*Trace formula*) *Let* $A: \mathcal{F} \to \mathcal{F}$ *be an internal linear operator. Then*

$$\mathrm{Tr}\, A = \int_{{}^\star M} (\delta_x, A\delta_x)\mathrm{d}x. \tag{2}$$

(*iv*) *Let* $e_1, \ldots, e_\nu \in \mathcal{F}$ *be an orthonormal basis of* $\mathcal{F}$. *Then*

$$\delta_x(y) = \sum_{k=1}^{\nu} e_k(x)e_k(y). \tag{3}$$

Proof: (i) holds because $\delta_x(y) = (\delta_x, \delta_y) = \delta_y(x)$.

(ii) For any $g \in \mathcal{F}$,

$$\left(\int_{\star_M} f(x)\,\delta_x dx, g\right) = \int\int_{\star_M} f(x)\,\delta_x(y)\mathrm{d}x g(y)\mathrm{d}y = \int\int_{\star_M} \delta_x(y) g(y)\mathrm{d}y f(x)\mathrm{d}x = \int_{\star_M} (\delta_x, g) f(x)\mathrm{d}x$$

$$= \int_{\star_M} g(x) f(x)\mathrm{d}x = (f,g).$$

Thus (ii) holds.

(iii) Since (ii) and

$$(\delta_x, A\,\delta_y) = \int \delta_x(s)(A\,\delta_y)(s)\mathrm{d}s = (A\,\delta_y)(x),$$

we have

$$\mathrm{Tr}\,A = \sum_i (e_i, Ae_i) = \sum \left(\int_{\star_M} e_i(x)\,\delta_x \mathrm{d}x, A\int_{\star_M} e_i(x)\,\delta_x \mathrm{d}x\right) = \sum \int\int_{\star_M} e_i(x) e_i(y)(\delta_x, A\,\delta_y)\mathrm{d}x\mathrm{d}y$$

$$= \int\int_{\star_M} \delta_x(y)(\delta_x, A\,\delta_y)\mathrm{d}x\mathrm{d}y = \int\int_{\star_M} \delta_y(x)(\delta_x, A\,\delta_y)\mathrm{d}x\mathrm{d}y = \int\int_{\star_M} \delta_y(x)(A\,\delta_y)(x)\mathrm{d}x\mathrm{d}y$$

$$= \int_{\star_M} (\delta_y, A\,\delta_y)\mathrm{d}y.$$

(iv) For any $g \in \mathcal{F}$, we have

$$\left(\sum_{k=1}^{\nu} e_k(x) e_k(\cdot), g\right) = \sum_{k=1}^{\nu} e_k(x)(e_k, g) = g(x).$$

Thus Eq. (3) holds. *QED*

IV. HAMILTONIAN FORMALISM

Let $\mathbf{d} \in \mathbf{N}$, and M be a $\mathbf{d}$-dimensional Riemannian manifold. We work in $(\mathbf{d}+1)$-dimensional space-time ${}^\star M \times {}^\star\mathbf{R}$.

Since $\mathcal{F} \cong {}^\star\mathbf{R}^\nu$, $\mathcal{F}$ is equipped with the natural $\star$Lebesgue measure. Let $L^2(\mathcal{F})$ denote the $\star$Hilbert space of functions on $\mathcal{F}$ square integrable with respect to the $\star$Lebesgue measure:

$$L^2(\mathcal{F}) = \left\{ F | F: \mathcal{F} \to {}^\star\mathbf{C}, \text{internal}, \int_{\mathcal{F}} |F(f)|^2 \mathrm{d}f < {}^\star\infty \right\}.$$

The L^2 inner product is denoted by $\langle \cdot | \cdot \rangle$:

$$\langle F | G \rangle \equiv \int_{\mathcal{F}} \overline{F(f)} G(f)\mathrm{d}f.$$

On the other hand, the real inner product on $\mathcal{D}(M)$ is denoted by

$$(f,g) = \int_M f(\boldsymbol{x}) g(\boldsymbol{x})\mathrm{d}\boldsymbol{x}.$$

For $\boldsymbol{x} \in {}^\star M$, define the $\star$unbounded self-adjoint operator $\hat{\phi}(\boldsymbol{x})$ on $L^2(\mathcal{F})$ by

$$(\hat{\phi}(\boldsymbol{x}) F)(f) = f(\boldsymbol{x}) F(f).$$

For $f \in \mathcal{F}$, define the $\star$unbounded self-adjoint operator $\hat{\phi}(f)$ on $L^2(\mathcal{F})$ by

$$\hat{\phi}(f) = \int_{{}^\star M} f(\boldsymbol{x})\hat{\phi}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}.$$

Evidently $\hat{\phi}(f)$ operates as follows:

$$(\hat{\phi}(f)F)(g) = (f,g)F(g).$$

Note that the relation $\hat{\phi}(\boldsymbol{x}) = \hat{\phi}(\delta_{\boldsymbol{x}})$ holds.

For $f \in \mathcal{F}$, define the $\star$unbounded self-adjoint operator $\hat{\pi}(f)$ on $L^2(\mathcal{F})$ by

$$(e^{it\hat{\pi}(f)}F)(g) = F(tf+g), \quad t \in {}^\star\mathbf{R}.$$

In other words, $i\hat{\pi}(f)$ is the internal differential operator in the direction of f. For $x \in {}^\star M$, define the $\star$unbounded self-adjoint operator $\hat{\pi}(\boldsymbol{x})$ on $L^2(\mathcal{F})$ by $\hat{\pi}(\boldsymbol{x}) = \hat{\pi}(\delta_{\boldsymbol{x}})$.

We can check the canonical commutation relations:

$$[\hat{\phi}(f),\hat{\phi}(g)] = [\hat{\pi}(f),\hat{\pi}(g)] = 0, \quad [\hat{\phi}(f),\hat{\pi}(g)] = i(f,g).$$

In other words,

$$[\hat{\phi}(\boldsymbol{x}),\hat{\phi}(\boldsymbol{y})] = [\hat{\pi}(\boldsymbol{x}),\hat{\pi}(\boldsymbol{y})] = 0, \quad [\hat{\phi}(\boldsymbol{x}),\hat{\pi}(\boldsymbol{y})] = i\delta_{\boldsymbol{x}}(\boldsymbol{y}).$$

But note that the following does *not* hold:

$$\boldsymbol{x} \neq \boldsymbol{y} \Rightarrow [\hat{\phi}(\boldsymbol{x}),\hat{\pi}(\boldsymbol{y})] = 0.$$

Let the *Hamiltonian H* be an internal positive operator on $L^2(\mathcal{F})$ with a nondegenerate ground state $\Omega \in L^2(\mathcal{F})$, called the *vacuum*. For $x \in {}^\star\mathbf{R} \times {}^\star M$, the field operator $\hat{\phi}(x)$ is determined by H:

$$\hat{\phi}(x) = \hat{\phi}(x_0,\boldsymbol{x}) \equiv e^{-ix_0H}\hat{\phi}(\boldsymbol{x})e^{ix_0H}, \quad \boldsymbol{x} \in {}^\star M.$$

For $f \in {}^\star\mathcal{D}(\mathbf{R}\times M)$, define $\hat{\phi}(f)$ by

$$\hat{\phi}(f) = \int_{{}^\star\mathbf{R}\times{}^\star M} f(x)\hat{\phi}(x)\mathrm{d}x.$$

For $f_1,\ldots,f_n \in \mathcal{D}(\mathbf{R}\times M)$, define $w_n(f_1,\ldots,f_n) \in \mathbf{C}\cup\{\infty\}$ by

$$w_n(f_1,\ldots,f_n) = {}^\circ\langle\Omega|\hat{\phi}({}^\star f_1)\cdots\hat{\phi}({}^\star f_n)\Omega\rangle.$$

If $\{w_n\}_{n\in\mathbf{N}}$ are Schwartz distributions, the Hamiltonian H is called *Schwartz*. If $M=\mathbf{R}^{\mathbf{d}}$ and if $\{w_n\}_{n\in\mathbf{N}}$ satisfy the Wightman axioms for scalar fields, H is called *Wightman.*

If the vacuum expectations $\{w_n\}_{n\in\mathbf{N}}$ characterize a (standard) quantum field theory $\mathcal{A}$, the triple $(L^2(\mathcal{F}),\hat{\phi},H)$ is called a *hyperfinite(-dimensional) Schrödinger representation* of $\mathcal{A}$.

The following problem is still open:

Question: Does every scalar field theory satisfying the Wightman axioms have a hyperfinite Schrödinger representation?

Let $e_1,\ldots,e_\nu$ be an orthonormal basis of $\mathcal{F}$. Define the $\star$unbounded self-adjoint operator $\Delta_{\mathcal{F}}$ on $L^2(\mathcal{F})$ to be the ν-dimensional Laplacian, that is,

$$\Delta_{\mathcal{F}} = -\sum_{k=1}^{\nu}\hat{\pi}(e_k)^2,$$

which is determined independent from the basis $\{e_k\}$.

Let $\Xi_{\mathcal{F}}$ be the positive operator on $L^2(\mathcal{F})$ defined by

$$(\Xi_{\mathcal{F}}F)(f) = (f,f)F(f), \quad f \in \mathcal{F}.$$

We see the following relation:

$$\Xi_{\mathcal{F}} = \sum_{k=1}^{\nu} \hat{\phi}(e_k)^2.$$

Proposition 4.1: *The following equations hold*:

$$\Delta_{\mathcal{F}} = -\int_{^\star\mathbf{R}^{\mathbf{d}}} \hat{\pi}(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}, \tag{4}$$

$$\Xi_{\mathcal{F}} = \int_{^\star\mathbf{R}^{\mathbf{d}}} \hat{\phi}(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}. \tag{5}$$

Proof: The first equation is shown as follows:

$$\begin{aligned}
\Delta_{\mathcal{F}} &= -\sum_{k=1}^{\nu} \hat{\pi}(e_k)^2 = -\sum_{k=1}^{\nu} \left[\int_{^\star\mathbf{R}^{\mathbf{d}}} e_k(\boldsymbol{x}) \hat{\pi}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \right]^2 = -\sum_{k=1}^{\nu} \int_{^\star\mathbf{R}^{\mathbf{d}}} \int_{^\star\mathbf{R}^{\mathbf{d}}} e_k(\boldsymbol{x}) \hat{\pi}(\boldsymbol{x}) e_k(\boldsymbol{y}) \hat{\pi}(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \\
&= -\int_{^\star\mathbf{R}^{\mathbf{d}}} \int_{^\star\mathbf{R}^{\mathbf{d}}} \sum_{k=1}^{\nu} e_k(\boldsymbol{x}) e_k(\boldsymbol{y}) \hat{\pi}(\boldsymbol{x}) \hat{\pi}(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \\
&= -\int_{^\star\mathbf{R}^{\mathbf{d}}} \int_{^\star\mathbf{R}^{\mathbf{d}}} \delta_{\boldsymbol{x}}(\boldsymbol{y}) \hat{\pi}(\boldsymbol{x}) \hat{\pi}(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} = -\int_{^\star\mathbf{R}^{\mathbf{d}}} \hat{\pi}(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}.
\end{aligned}$$

The second is shown similarly. *QED*

Let $A : \mathcal{F} \to \mathcal{F}$ be invertible internal linear operators. Define the operator T_A on $L^2(\mathcal{F})$ by

$$(T_A F)(f) = F(A^{-1}f).$$

Clearly, T_A is unitary if $A \in SL(\mathcal{F})$.

The most general form of the free Hamiltonian will be

$$H = -\alpha T_A \Delta_{\mathcal{F}} T_A^{-1} + \beta T_B \Xi_{\mathcal{F}} T_B^{-1},$$

where A and B are invertible internal linear operators on $\mathcal{F}$.

We assume that A and B are positive without loss of generality. Let $F \in L^2(\mathcal{F})$. Then we have

$$(T_A^{-1} H T_A F)(f) = -\alpha(\Delta_{\mathcal{F}} F)(f) + \beta(f, B^{-1}A^2B^{-1}f)F(f).$$

Since $B^{-1}A^2B^{-1}$ is a ν-dimensional positive matrix, it has positive eigenvalues $\lambda_1, \ldots, \lambda_\nu \in {}^\star\mathbf{R}$ and corresponding eigenvectors $v_1, \ldots, v_\nu \in \mathcal{F}$:

$$B^{-1}A^2B^{-1}v_k = \lambda_k v_k, \quad (v_k, v_l) = \delta_{kl}, \quad k,l = 1, \ldots, \nu.$$

Thus we have

$$T_A^{-1} H T_A = \sum_{k=1}^{\nu} \alpha \hat{\pi}(v_k)^2 + \beta \lambda_k \hat{\phi}(v_k)^2,$$

and hence

$$H=\sum_{k=1}^{\nu}\left[\alpha T_A\hat{\pi}(v_k)^2T_A^{-1}+\beta\lambda_k T_A\hat{\phi}(v_k)^2T_A^{-1}\right]=\sum_{k=1}^{\nu}\left[\alpha\hat{\pi}(Av_k)^2+\beta\lambda_k\hat{\phi}(A^{-1}v_k)^2\right].$$

This is the decomposition of H into independent harmonic oscillators, because the following canonical commutation relations hold:

$$[\hat{\phi}(A^{-1}v_k),\hat{\pi}(Av_l)]=i(A^{-1}v_k,Av_l)=i\delta_{kl}.$$

V. FREE MASSIVE SCALAR FIELDS

The Hamiltonian of a free scalar field (Klein-Gordon field) with mass m is given by

$$H_m=\frac{1}{2}\int_{{}^\star\mathbf{R}^{\mathbf{d}}}\left[\hat{\pi}(\boldsymbol{x})^2+\sum_{k=1}^{\mathbf{d}}(\partial_k\hat{\phi}(\boldsymbol{x}))^2+m^2\hat{\phi}(\boldsymbol{x})^2\right]\mathrm{d}\boldsymbol{x}.$$

In this section, we show that the right-hand side can be interpreted *literally*, and is well-defined, and that it has the following property.

Theorem 5.1: *H_m is Wightman. The vacuum expectation values $\{w_n\}$ characterize the free scalar field of mass m.*

Let $E_{\mathcal{F}}$ denote the internal orthogonal projection from ${}^\star L^2(M)$ to $\mathcal{F}$. For an internal operator X on ${}^\star L^2(M)$, define the operator $(X)_{\mathcal{F}}:\mathcal{F}\to\mathcal{F}$ by

$$(X)_{\mathcal{F}}=E_{\mathcal{F}}X\restriction\mathcal{F}.$$

Set

$$H_m=-\alpha T_A\Delta_{\mathcal{F}}T_A^{-1}+\beta T_B\Xi_{\mathcal{F}}T_B^{-1},$$

and we find

$$\alpha=\beta=\tfrac{1}{2},\quad A=I.$$

To give the explicit form of the positive operator B, we must solve

$$T_B\Xi_{\mathcal{F}}T_B^{-1}=\int_{{}^\star\mathbf{R}^{\mathbf{d}}}\left[\sum_{k=1}^{\mathbf{d}}(\partial_k\hat{\phi}(\boldsymbol{x}))^2+m^2\hat{\phi}(\boldsymbol{x})^2\right]\mathrm{d}\boldsymbol{x}.$$

Let $F\in L^2(\mathcal{F})$. Then for any $f\in\mathcal{F}$,

$$\left(\int_{{}^\star\mathbf{R}^{\mathbf{d}}}\left[\sum_{k=1}^{\mathbf{d}}(\partial_k\hat{\phi}(\boldsymbol{x}))^2+m^2\hat{\phi}(\boldsymbol{x})^2\right]\mathrm{d}\boldsymbol{x}F\right)(f)$$

$$=\int_{{}^\star\mathbf{R}^{\mathbf{d}}}\left[\sum_{k=1}^{\mathbf{d}}(\partial_k f(\boldsymbol{x}))^2+m^2f(\boldsymbol{x})^2\right]\mathrm{d}\boldsymbol{x}F(f)$$

$$=(f,(-\Delta+m^2)f)F(f)=(f,(-\Delta+m^2)_{\mathcal{F}}f)F(f),$$

where Δ is the Laplacian on ${}^\star\mathbf{R}^{\mathbf{d}}$.

On the other hand,

$$(T_B\Xi_{\mathcal{F}}T_B^{-1}F)(f)=(\Xi_{\mathcal{F}}T_B^{-1}F)(B^{-1}f)=(B^{-1}f,B^{-1}f)F(f)=(f,B^{-2}f)F(f).$$

Thus we have

$$B^{-2}=(-\Delta+m^2)_{\mathcal{F}},$$

$$H = (-1/2)\Delta_{\mathcal{F}} + (1/2)T_B \Xi_{\mathcal{F}} T_B^{-1}.$$

Let $e_k \in \mathcal{F}$ be an orthonormal basis of $\mathcal{F}$ such that

$$B^{-2} e_k = \lambda_k e_k, \quad \lambda_k \in {}^{\star}\mathbf{C}.$$

Then

$$H_k = (1/2)[\hat{\pi}(e_k)^2 + \lambda_k \hat{\phi}(e_k)^2] = \lambda_k^{1/2}(a^+(e_k)a(e_k) + (1/2))$$

where

$$a(e_k) \equiv 2^{-1/2}\lambda_k^{1/4}(\hat{\phi}(e_k) + \lambda_k^{-1/2} i\hat{\pi}(e_k)),$$

$$a^+(e_k) \equiv 2^{-1/2}\lambda_k^{1/4}(\hat{\phi}(e_k) - \lambda_k^{-1/2} i\hat{\pi}(e_k)).$$

Thus their time evolutions are given by

$$a_t(e_k) \equiv e^{itH} a(e_k) e^{-itH} = e^{itH_k} a(e_k) e^{-itH_k} = a(e_k) e^{-i\lambda_k^{1/2} t},$$

$$a_t^+(e_k) \equiv e^{itH} a^+(e_k) e^{-itH} = e^{itH_k} a^+(e_k) e^{-itH_k} = a^+(e_k) e^{i\lambda_k^{1/2} t}.$$

Since we have

$$\hat{\phi}(e_k) = 2^{-1/2}\lambda_k^{-1/4}[a(e_k) + a^+(e_k)], \quad \hat{\pi}(e_k) = -i2^{-1/2}\lambda_k^{1/4}[a(e_k) - a^+(e_k)],$$

the time evolutions of field operators are given by

$$\hat{\phi}_t(e_k) \equiv e^{itH_k}\hat{\phi}(e_k)e^{-itH_k} = 2^{-1/2}\lambda_k^{-1/4}[e^{-i\lambda_k^{1/2}t}a(e_k) + e^{i\lambda_k^{1/2}t}a^+(e_k)],$$

$$\hat{\pi}_t(e_k) \equiv e^{itH_k}\hat{\pi}(e_k)e^{-itH_k} = -i2^{-1/2}\lambda_k^{1/4}[e^{-i\lambda_k^{1/2}t}a(e_k) - e^{i\lambda_k^{1/2}t}a^+(e_k)].$$

For $x=(x_0,\boldsymbol{x}) \in {}^{\star}\mathbf{R}^{\mathbf{d}+1}$, let $\hat{\phi}(x) \equiv e^{ix_0 H_k}\hat{\phi}(\boldsymbol{x})e^{-ix_0 H_k}$. Then we have the following representation of $\hat{\phi}(x)$:

$$\hat{\phi}(x) = \sum_k e_k(\boldsymbol{x})\hat{\phi}(x_0, e_k) = 2^{-1/2}\sum_k e_k(x)\lambda_k^{-1/4}[e^{-i\lambda_k^{1/2}x_0}a(e_k) + e^{i\lambda_k^{1/2}x_0}a^+(e_k)].$$

Thus the two-point Wightman function is calculated as follows:

$$\begin{aligned}
\langle\Omega|\hat{\phi}(x)\hat{\phi}(y)\Omega\rangle &= \langle\Omega|2^{-1}\sum_{jk}[e_k(\boldsymbol{x})e_j(\boldsymbol{y})\lambda_k^{-1/2}e^{-i\lambda_k^{1/2}x_0}a(e_k)e^{i\lambda_j^{1/2}y_0}a^+(e_j)]\Omega\rangle \\
&= \langle\Omega|2^{-1}\sum_{jk}[e_k(\boldsymbol{x})e_j(\boldsymbol{y})\lambda_k^{-1/2}e^{-i\lambda_k^{1/2}(x_0-y_0)}a(e_k)a^+(e_j)]\Omega\rangle \\
&= \langle\Omega|2^{-1}\sum_{k}[e_k(\boldsymbol{x})e_k(\boldsymbol{y})\lambda_k^{-1/2}e^{-i\lambda_k^{1/2}(x_0-y_0)}a(e_k)a^+(e_k)]\Omega\rangle \\
&= 2^{-1}\sum_k [e_k(\boldsymbol{x})e_k(\boldsymbol{y})\lambda_k^{-1/2}e^{-i\lambda_k^{1/2}(x_0-y_0)}].
\end{aligned}$$

Let $\Lambda = -\Delta + m^2$ and $\Lambda_{\mathcal{F}} = (\Lambda)_{\mathcal{F}}$. Then by the relation

$$\delta_{\boldsymbol{x}} = \sum_k e_k(\boldsymbol{x})e_k,$$

we find

$$\langle\Omega|\hat{\phi}(x)\hat{\phi}(y)\Omega\rangle = (1/2)(\delta_x, \Lambda_{\mathcal{F}}^{-1/2} e^{-i\Lambda_{\mathcal{F}}^{1/2}(x_0-y_0)}\delta_y).$$

To show that H is Wightman, we evaluate the smeared two-point function $\langle\Omega|\hat{\phi}(x_0,f)\hat{\phi}(y_0,g)\Omega\rangle$ for $f,g\in\mathcal{D}(\mathbf{R}^{\mathbf{d}})$.

Notice that the following relations hold for Λ and $\Lambda_{\mathcal{F}}$:

$$(\forall r\in\mathbf{R})\Lambda^r({}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}})) = {}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}}), \tag{6}$$

$$(\forall n\in\mathbf{Z})(\Lambda_{\mathcal{F}})^n({}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}})) = {}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}}), \tag{7}$$

$$(\forall n\in\mathbf{Z})(\forall f\in {}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}}))\Lambda^n f = (\Lambda_{\mathcal{F}})^n f. \tag{8}$$

These imply that

$$(\forall r\in\mathbf{R})(\forall f\in {}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}}))e^{ir\Lambda}f \approx e^{ir\Lambda_{\mathcal{F}}}f, \tag{9}$$

$$(\forall r\in\mathbf{R})(\forall f\in {}^{\sigma}\mathcal{D}(\mathcal{R}^{\mathbf{d}}))\Lambda^r f \approx (\Lambda_{\mathcal{F}})^r f. \tag{10}$$

Therefore we conclude that for $f,g\in\mathcal{D}(\mathcal{R}^{\mathbf{d}})$,

$$\begin{aligned}\langle\Omega|\hat{\phi}(x_0,f)\hat{\phi}(y_0,g)\Omega\rangle &= (f,\Lambda_{\mathcal{F}}^{-1/2}e^{-i\Lambda_{\mathcal{F}}^{1/2}(x_0-y_0)}g) \approx (f,\Lambda^{-1/2}e^{-i\Lambda^{1/2}(x_0-y_0)}g)\\ &= \left(\hat{f},\left(\sum p_i^2+m^2\right)^{-1/2}e^{-i(\Sigma\, p_i^2+m^2)^{1/2}(x_0-y_0)}\hat{g}\right) = (\hat{f},\omega_{\boldsymbol{p}}^{-1}e^{-i\omega_{\boldsymbol{p}}(x_0-y_0)}\hat{g})\\ &= \int_{{}^{\star}\mathbf{R}^{\mathbf{d}}}\overline{\widetilde{f}(\boldsymbol{p})}\frac{e^{-i\omega_{\boldsymbol{p}}(x_0-y_0)}}{\omega_{\boldsymbol{p}}}\widetilde{g}(\boldsymbol{p})\mathrm{d}\boldsymbol{p},\end{aligned} \tag{11}$$

where $\widetilde{f}$ is the Fourier transform of f, and

$$\omega_{\boldsymbol{p}} = \left(\sum_{k=1}^{\mathbf{d}} p_k^2 + m^2\right)^{1/2}.$$

The last formula (11) is the same as the standard two-point function of a free scalar field. This means that all the vacuum expectations of our nonstandard field operators $\hat{\phi}(f_1)\cdots\hat{\phi}(f_n)$ are infinitesimally near to the standard ones, and hence H is Wightman.

VI. LAGRANGIAN PATH INTEGRAL

Consider the Hamiltonian

$$H = -\Delta_{\mathcal{F}} + V,$$

where the potential $V:\mathcal{F}\to{}^{\star}\mathbf{R}$ is such that H is self-adjoint. We examine a nonstandard path integral representation of the time evolution with respect to H.

Let $0\leqslant\theta<\pi/2$, $t\geqslant 0$ and $\tau=e^{i\theta}t$. For $f_0,\ldots,f_n\in\mathcal{F}$, define $R_n(f_0,\ldots,f_n,\tau)\in{}^{\star}\mathbf{C}$ by

$$R_n(f_0,\ldots,f_n,\tau) = \sum_{j=1}^{n}\frac{\tau}{n}\left[\frac{1}{2}\left(\frac{|f_j-f_{j-1}|}{\tau/n}\right)^2 + V(f_j)\right].$$

For $f_{\mathrm{ini}},f_{\mathrm{fin}}\in\mathcal{F}$, define $K_n(f_{\mathrm{ini}},f_{\mathrm{fin}};\tau)\in{}^{\star}\mathbf{C}$ by

$$K_n(f_{\mathrm{ini}},f_{\mathrm{fin}};\tau) \equiv (2\pi\tau/n)^{-\nu n/2}\int_{\mathcal{F}}\cdots\int_{\mathcal{F}} e^{-R_n(f_0,\ldots,f_n,\tau)}\mathrm{d}f_{n-1}\cdots df_1,$$

where $f_0=f_{\mathrm{ini}}$, $f_n=f_{\mathrm{fin}}$. For $F\in L^2(\mathcal{F})$, define $\hat{K}_n(\tau)F\in L^2(\mathcal{F})$ by

$$(\hat{K}_n(\tau)F)(f) \equiv \int_{\mathcal{F}} K_n(g,f;\tau)F(g)\mathrm{d}g.$$

By transferring the standard Trotter formula, we find

$$e^{-\tau(-\Delta_{\mathcal{F}}+V)}F = \lim_{n\to{}^\star\infty} \hat{K}_n(\tau)F.$$

The exact expression of this equation is the following:

$$(\forall \epsilon \in {}^\star\mathbf{R}^+)(\exists k \in {}^\star\mathbf{N})(\forall n \in {}^\star\mathbf{N})(n > k \Rightarrow \|\hat{K}_n(\tau)F - e^{-\tau(-\Delta_{\mathcal{F}}+V)}F\| < \epsilon),$$

where $\|\cdot\|$ denotes the ${}^\star\mathbf{R}$-valued norm on $L^2(\mathcal{F})$.

By the saturation principle, we find the following.

Theorem 6.1: *Let* $S \subset L^2(\mathcal{F})$ *satisfy* $\mathrm{card}(S) < \kappa$. *Then there exists* $n \sim \infty$ *such that for any* $F \in S$,

$$e^{-\tau(-\Delta_{\mathcal{F}}+V)}F \approx \hat{K}_n(\tau)F.$$

Let $\epsilon = t/n$ $(=|\tau|/n)$. For $\Phi = (f_0, \ldots, f_n) \in \mathcal{F}^{n+1}$, define the $\mathcal{F}$-valued path $\tilde{\Phi}:[0,t]\to\mathcal{F}$ by

$$\tilde{\Phi}(t) = (((k+1)\epsilon - t)f_k + (t - k\epsilon)f_{k+1})/\epsilon$$

if $k\epsilon \leqslant t \leqslant (k+1)\epsilon$ $(k=0,\ldots,n)$. That is, $\tilde{\Phi}$ is the piecewise linear path such that $\tilde{\Phi}(k\epsilon) = f_k$ for $k = 0, \ldots, n$.

Define the set of paths $\mathcal{L}_n$ by

$$\mathcal{L}_n = \{\tilde{\Phi} | \Phi \in \mathcal{F}^{n+1}\}.$$

For $f, g \in \mathcal{F}$, define $\mathcal{L}_n[f,g] \subset \mathcal{L}_n$ by

$$\mathcal{L}_n[f,g] = \{\phi \in \mathcal{L}_n | \phi(0) = f, \phi(t) = g\}.$$

The $\star$Lebesgue measures on $\mathcal{L}_n$ and $\mathcal{L}_n[f,g]$ are naturally defined by those of $\mathcal{F}^{n+1}$ and $\mathcal{F}^{n-1}$, respectively, i.e., for any function $h:\mathcal{L}_n \to {}^\star\mathbf{C}$,

$$\int_{\mathcal{L}_n} F(\phi)\mathrm{d}\phi \equiv \int_{\mathcal{F}^{n+1}} h(\tilde{\Phi})\mathrm{d}\Phi = \int_{\mathcal{F}} \cdots \int_{\mathcal{F}} h(\tilde{\Phi})\mathrm{d}\phi_0 \cdots \mathrm{d}\phi_n.$$

$$\int_{\mathcal{L}_n[f,g]} h(\phi)\mathrm{d}\phi \equiv \int_{\mathcal{F}} \cdots \int_{\mathcal{F}} h((f,\phi_1,\ldots,\phi_{n-1},g)^\sim)\mathrm{d}\phi_1 \cdots \mathrm{d}\phi_{n-1}.$$

For a path $\phi:[0,t]\to\mathcal{F}$, define the generalized action integral $S(\phi,\tau)$ by

$$S(\phi,\tau) \equiv \int_0^t \left[\frac{e^{-i\theta}}{2}\|\dot{\phi}(s)\|^2 + e^{i\theta}V(\phi(s))\right]\mathrm{d}s.$$

Of course, if $\tau > 0$ (equivalently $\theta = 0$) then $S(\phi,\tau)$ is the Euclidean action of the path ϕ, and if τ is pure imaginary (equivalently $\theta = \pi/2$) then $-iS(\phi,\tau)$ is the Minkowskian action of the path ϕ.

For $f_{\mathrm{ini}}, f_{\mathrm{fin}} \in \mathcal{F}$, let

$$K'_n(\tau; f_{\mathrm{ini}}, f_{\mathrm{fin}}) \equiv (2\pi\tau/n)^{-\nu n/2} \int_{\mathcal{L}_n[f_{\mathrm{ini}},f_{\mathrm{fin}}]} e^{-S(\phi,t,\theta)}\mathrm{d}\phi.$$

For $F \in L^2(\mathbf{R}^N)$, define $\hat{K}'_n(\tau)F \in L^2(\mathcal{F})$ by

$$(\hat{K}'_n(\tau)F)(f) \equiv \int_{\mathcal{F}} K'_n(\tau;g,f)F(g)\mathrm{d}g.$$

Note that

$$\left|\exp\left(-\frac{\tau}{2n}\sum_{j=1}^{n}\left(\frac{\|\phi_j-\phi_{j-1}\|}{\tau/n}\right)^2\right)\right| = \left|\exp\left(-\frac{e^{-i\theta}t}{2n}\sum_{j=1}^{n}\left(\frac{\|\phi_j-\phi_{j-1}\|}{t/n}\right)^2\right)\right|$$
$$= \exp\left(-\frac{n\cos\theta}{2t}\sum_{j=1}^{n}\|\phi_j-\phi_{j-1}\|^2\right).$$

This implies that the paths which effectively contribute to the path integral satisfy

$$\|\phi_{k+1}-\phi_k\|^2 \leqslant O\left(\frac{t}{n\cos\theta}\right) = O\left(\frac{t}{n(\pi/2-\theta)}\right)$$

as $n \to {}^\star\infty$ when $0 \leqslant \theta < \pi/2$. Therefore it follows that

$$R_n(\Phi,\tau) - S(\tilde{\Phi}) \to 0 \quad \text{as } n \to {}^\star\infty$$

and

$$(\hat{K}_n(\tau) - \hat{K}'_n(\tau))F \to 0 \quad \text{as } n \to {}^\star\infty$$

when $0 \leqslant \theta < \pi/2$. Thus

$$e^{-\tau(-\Delta_{\mathcal{F}}+V)}F = \lim_{n\to{}^\star\infty} \hat{K}'_n(\tau)F.$$

By the saturation principle, we have

Theorem 6.2 (Lagrangian path integral): *Let* $S \subset L^2(\mathcal{F})$ *and* $\mathrm{card}S < \kappa$. *Suppose* $0 \leqslant \theta < \pi/2$. *Then there exists* $n \in {}^\star\mathbf{N}$ *such that for any* $F \in S$,

$$(e^{-\tau(-\Delta_{\mathcal{F}}+V)}F)(f) \approx (\hat{K}'_n(\tau)F)(f) = (2\pi\tau/n)^{-\nu n/2}\int_{\mathcal{F}}\int_{\mathcal{L}_n[g,f]} e^{-S(\phi,\tau)}F(g)\mathrm{d}\phi\mathrm{d}g.$$

where $\tau = e^{i\theta}t$, $t \in {}^\star\mathbf{R}$. *The above approximation "*$\approx$*" is with respect to the* $\star$ *norm of* $L^2(\mathcal{F})$.

Next we consider the case of free scalar field Hamiltonian:

$$H_m = \frac{1}{2}\int_{{}^\star\mathbf{R}^{\mathbf{d}}}\left[\hat{\pi}(\boldsymbol{x})^2 + \sum_{k=1}^{\mathbf{d}}(\partial_k\hat{\phi}(\boldsymbol{x}))^2 + m^2\hat{\phi}(\boldsymbol{x})^2\right]\mathrm{d}\boldsymbol{x}.$$

The infinite energy of vacuum is not regularized on H_m:

$$H_m\Omega = E_0\Omega, \quad E_0 = \nu/2 \sim \infty.$$

Let H'_m be the vacuum-energy regularization of H_m, i.e.,

$$H'_m = H_m - E_0.$$

Set

$$H'_m = \tfrac{1}{2}\Delta_{\mathcal{F}} + V,$$

then as shown in Sec. V, we have for $f \in \mathcal{F}$,

$$V(f) = (1/2)(f,(-\Delta + m^2)f) - E_0 = \frac{1}{2}\int_{{}^\star\mathbf{R}^\mathbf{d}} \left[\sum_{k=1}^{\mathbf{d}} (\partial_k f(\boldsymbol{x}))^2 + m^2 f(\boldsymbol{x})^2 \right] \mathrm{d}\boldsymbol{x} - E_0.$$

Hence we have

$$\begin{aligned} S(\phi,\tau) &\equiv \int_0^t \left[\frac{e^{-i\theta}}{2} \|\dot{\phi}(s)\|^2 + \int_{{}^\star\mathbf{R}^\mathbf{d}} \frac{e^{i\theta}}{2} \left[\sum_{k=1}^{\mathbf{d}} (\partial_k \phi(s)(\boldsymbol{x}))^2 + m^2 \phi(s)(\boldsymbol{x})^2 \right] \mathrm{d}\boldsymbol{x} - E_0 \right] \mathrm{d}s \\ &= \int_0^t \left[\int_{{}^\star\mathbf{R}^\mathbf{d}} \frac{e^{-i\theta}}{2} \dot{\phi}(s)(\boldsymbol{x})^2 + \frac{e^{i\theta}}{2} \left[\sum_{k=1}^{\mathbf{d}} (\partial_k \phi(s)(\boldsymbol{x}))^2 + m^2 \phi(s)(\boldsymbol{x})^2 \right] \mathrm{d}\boldsymbol{x} - E_0 \right] \mathrm{d}s \\ &= \int_0^t \int_{{}^\star\mathbf{R}^\mathbf{d}} \frac{e^{-i\theta}}{2} \dot{\phi}(s)(\boldsymbol{x})^2 + \frac{e^{i\theta}}{2} \sum_{k=1}^{\mathbf{d}} (\partial_k \phi(s)(\boldsymbol{x}))^2 + \frac{e^{i\theta}}{2} m^2 \phi(s)(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}\mathrm{d}s - tE_0 \\ &= \frac{e^{i\theta}}{2} \int_{[0,t]\times{}^\star\mathbf{R}^\mathbf{d}} \left(\mathcal{E}_\theta \partial^k \phi \partial_k \phi + m^2 \phi^2 \right) \mathrm{d}x - tE_0, \end{aligned}$$

where $\mathcal{E}_\theta$ denotes the θ-parametrized Einstein convention:

$$\mathcal{E}_\theta A^k B_k = e^{-2i\theta} A_0 B_0 + \sum_{k=1}^{\mathbf{d}} A_k B_k,$$

which is the Euclidean inner product if $\theta=0$, and is the Minkowskian inner product if $\theta=\pi/2$. Evidently

$$L = \tfrac{1}{2}(\mathcal{E}_\theta \partial^k \phi \partial_k \phi + m^2 \phi^2)$$

is the θ-parametrized Lagrangian for a free scalar field. Thus we can write

$$S(\phi,\tau) = e^{i\theta} \int_{[0,t]\times{}^\star\mathbf{R}^\mathbf{d}} L\mathrm{d}x - tE_0.$$

Then we have the following theorem:

Theorem 6.3 (Lagrangian path integral for free scalar fields): *Let* $S \subset L^2(\mathcal{F})$ *and* $\mathrm{card}S < \kappa$. *Suppose* $0 \leqslant \theta < \pi/2$. *Then there exists* $n \in {}^\star\mathbf{N}$ *such that for any* $F \in S$,

$$(e^{-\tau H'_m} F)(f) \approx (2\pi\tau/n)^{-\nu n/2} e^{tE_0} \int_{\mathcal{F}} \int_{\mathcal{L}_n[g,f]} e^{-e^{i\theta}\int_{[0,t]\times{}^\star\mathbf{R}^\mathbf{d}} L\mathrm{d}x} F(g)\mathrm{d}\phi\mathrm{d}g,$$

where $\tau = e^{i\theta}t$, $t \in {}^\star\mathbf{R}$. *The above approximation* "$\approx$" *is with respect to the* $\star$*norm of* $L^2(\mathcal{F})$.

VII. GENERATING FUNCTIONAL

In the physical literature, the *generating functional* of a scalar field $\hat{\phi}$ is "defined" by

$$Z[J] = \langle \Omega | \mathrm{T} \exp\left[i \int J(x)\hat{\phi}(x)\mathrm{d}x \right] \Omega \rangle, \tag{12}$$

where T denotes the time-ordered product (T-product).

However, if $\hat{\phi}$ is regarded as a standard operator-valued distribution, the T-product is not well-defined. On the other hand, if $\hat{\phi}$ is regarded as a nonstandard pointwise field operator instead of a standard operator-valued distribution, the T-product can be defined rigorously. Let us call it a *nonstandard T-product.* However the problem of uniqueness of the nonstandard T-product still remains unsolved; we supposed $\mathcal{F}$ to be an *arbitrary* hyperfinite-dimensional subspace such that

$\mathcal{D}\subset\mathcal{F}\subset{}^{\star}\mathcal{D}$. The definition of the T-product can be sensitive to the selection of $\mathcal{F}$. This problem is open:

Question: Does a nonstandard T-product depend on $\mathcal{F}$? If so, what selection of $\mathcal{F}$ defines physically meaningful T-products?

In this paper, we do not examine this problem further. Instead we consider the path integral representation of a generating functional. In the physical literature, the following formula is given:

$$Z[J]=\frac{\int \exp i\int_{\mathbf{R}^{\mathbf{d}+1}}[L(\phi,\partial\phi)+J(x)\phi(x)]\mathrm{d}x\mathrm{d}\phi}{\int \exp i\int_{\mathbf{R}^{\mathbf{d}+1}}[L(\phi,\partial\phi)]\mathrm{d}x\mathrm{d}\phi}. \tag{13}$$

In our approach, to examine the right-hand side of this formula seems easier than to examine T-products.

In Sec. VI, the path space $\mathcal{L}$ was defined to be a set of paths $\phi:[0,t]\to\mathcal{F}$. Let $T\in{}^{\star}\mathbf{R}_{\infty}^{+}$. In this section, we consider the path space $\mathcal{L}_T$ is a set of the paths $\phi:{}^{\star}R\to\mathcal{F}$, where $\phi(t)=0$ if $|t|>T$. For $\phi_1,\phi_2\in\mathcal{L}_T$, the inner product (ϕ_1,ϕ_2) is given by

$$(\phi_1,\phi_2)=\int_{{}^{\star}\mathbf{R}}(\phi_1(x_0),\phi_2(x_0))\mathrm{d}x_0=\int_{{}^{\star}\mathbf{R}^{\mathbf{d}+1}}\phi_1(x)\phi_2(x)\mathrm{d}x,$$

where $\phi_j(x)\equiv\phi_j(x_0)(x_1,\ldots,x_{\mathbf{d}})$. Thus $\mathcal{L}_T$ is naturally embedded into ${}^{\star}L(\mathbf{R}^{\mathbf{d}+1})$. We can suppose ${}^{\sigma}\mathcal{D}(\mathbf{R}^{\mathbf{d}+1})\subset\mathcal{L}_T$ by the saturation principle.

Equation (13) is rewritten in our notations parallel to Theorem 6.3 as

$$Z[J]=\frac{\int_{\mathcal{L}_T}\exp-\int_{{}^{\star}\mathbf{R}^{\mathbf{d}+1}}[e^{i\theta}L(\phi,\partial\phi)+J(x)\phi(x)]\mathrm{d}x\mathrm{d}\phi}{\int_{\mathcal{L}_T}\exp-\int_{{}^{\star}\mathbf{R}^{\mathbf{d}+1}}e^{i\theta}L(\phi,\partial\phi)\mathrm{d}x\mathrm{d}\phi}. \tag{14}$$

Here we confine ourselves to the case of free massive scalar fields:

$$L=\tfrac{1}{2}(\mathcal{E}_{\theta}\partial^{k}\phi\partial_{k}\phi+m^{2}\phi^{2}).$$

Thus for any $\phi\in\mathcal{L}_T$ we have

$$\begin{aligned}\int_{\mathbf{R}^{\mathbf{d}+1}}[L(\phi,\partial\phi)+J(x)\phi(x)]\mathrm{d}x\mathrm{d}\phi&=\int_{\mathbf{R}^{\mathbf{d}+1}}\left[\frac{1}{2}(-\mathcal{E}_{\theta}\phi\partial^{k}\partial_{k}\phi+m^{2}\phi^{2})+J(x)\phi(x)\right]\mathrm{d}x\mathrm{d}\phi\\&=\frac{1}{2}(\phi,(-\mathcal{E}_{\theta}\partial^{k}\partial_{k}+m^{2})\phi)+(J,\phi).\end{aligned}$$

Note that

$$\begin{aligned}\mathrm{Re}\left[e^{i\theta}\int_{{}^{\star}\mathbf{R}^{\mathbf{d}+1}}L(\phi,\partial\phi)\mathrm{d}x\mathrm{d}\phi\right]&=\mathrm{Re}\left[e^{i\theta}\frac{1}{2}(\phi,(-\mathcal{E}_{\theta}\partial^{k}\partial_{k}+m^{2})\phi)\right]\\&=\mathrm{Re}\left[e^{i\theta}\frac{1}{2}\left(\phi,\left(-e^{-2i\theta}\partial_{0}^{2}-\sum_{k=1}^{\mathbf{d}}\partial_{k}^{2}+m^{2}\right)\phi\right)\right]\\&=\cos\theta\frac{1}{2}\left(\phi,\left(-\sum_{k=0}^{\mathbf{d}}\partial_{k}^{2}+m^{2}\right)\phi\right)\geqslant 0.\end{aligned}$$

Therefore if $0\leqslant\theta<\pi/2$ then the real part of the exponent is strictly negative, and hence the

above-mentioned path integral is well-defined. (In the purely Minkowskian case $\theta=\pi/2$, it is unclear whether it can be well-defined.) Since $\mathcal{L}$ is hyperfinite-dimensional, the integral can be calculated by transferring the finite-dimensional standard Gaussian integral formula:

Proposition 7.1: *Let $\tilde{\mathcal{L}}_T=\mathcal{L}_T+i\mathcal{L}_T$ be the internal complexification of $\mathcal{L}_T$. Let $A:\tilde{\mathcal{L}}_T\to\tilde{\mathcal{L}}_T$ be an internal linear operator such that*

1. *A is symmetric in the sense of*

$$(\forall\phi,\psi\in\mathcal{L}_T)\quad(\phi,A\psi)=(\psi,A\phi), \tag{15}$$

2. $(\forall\phi\in\mathcal{L}_T)\quad\phi\neq 0\Rightarrow \mathrm{Re}(\phi,A\phi)>0.$

Then the following holds:

$$\int_{\mathcal{L}_T}\exp\left[-\frac{1}{2}(\phi,A\phi)+(\phi,\psi)\right]d\phi=\left(\det\frac{A}{2\pi}\right)^{-1/2}\exp\frac{1}{2}(\psi,A^{-1}\psi). \tag{16}$$

Let $\Lambda_\theta=e^{i\theta}(-\mathcal{E}_\theta\partial^k\partial_k+m^2)$ be an ($\star$unbounded) operator on $L^2(\mathbf{R}^{\mathbf{d}+1})$, and E be the orthogonal projection from $L^2(\mathbf{R}^{\mathbf{d}+1})$ to $\tilde{\mathcal{L}}_T$. Let $\Lambda_\theta^E=E\Lambda_\theta\restriction\tilde{\mathcal{L}}_T$. We can check that Λ_θ^E is symmetric in the sense of (15).

Applying the above-mentioned formula, we find for any $J\in{}^\star L^2(\mathbf{R}^{\mathbf{d}+1})$,

$$Z[J]=\frac{\displaystyle\int_{\mathcal{L}_T}\exp-\left[e^{i\theta}\frac{1}{2}(\phi,(-\mathcal{E}_\theta\partial^k\partial_k+m^2)\phi)+(J,\phi)\right]\mathrm{d}\phi}{\displaystyle\int_{\mathcal{L}_T}\exp-e^{i\theta}\frac{1}{2}(\phi,(-\mathcal{E}_\theta\partial^k\partial_k+m^2)\phi)\mathrm{d}\phi}=\frac{\displaystyle\int_{\mathcal{L}_T}\exp\left[-\tfrac{1}{2}(\phi,\Lambda_\theta^E\phi)-(J,\phi)\right]\mathrm{d}\phi}{\displaystyle\int_{\mathcal{L}_T}\exp-\tfrac{1}{2}(\phi,\Lambda_\theta^E\phi)\mathrm{d}\phi}$$

$$=\exp\frac{1}{2}(J,(\Lambda_\theta^E)^{-1}J).$$

In the case where $0\leqq\theta<\pi/2$, and $\theta\in\mathbf{R}$ (and hence $\theta\neq\pi/2$), the properties parallel to Eqs. (6)–(10) hold for Λ_θ; especially we see

$$(\forall n\in\mathbf{Z})(\forall f\in{}^\sigma\mathcal{D}(\mathcal{R}^{\mathbf{d}}))\quad\Lambda_\theta^n f=(\Lambda_\theta^E)^n f. \tag{17}$$

Thus we have for any $f\in{}^\sigma\mathcal{D}(\mathcal{R}^{\mathbf{d}})$,

$$Z[J]=\exp\tfrac{1}{2}(J,(\Lambda_\theta^E)^{-1}J)=\exp\tfrac{1}{2}(J,\Lambda_\theta^{-1}J). \tag{18}$$

By the principle of eternity in nonstandard analysis, there exists $\epsilon\approx 0$, $\epsilon>0$ such that

$$Z[J]=\exp\tfrac{1}{2}(J,\Lambda_{(\pi/2)-\epsilon}^{-1}J). \tag{19}$$

This means that our nonstandard method permits us to consider some "almost Minkowskian" cases in manipulating path integrals. Purely Minkowskian path integrals seem difficult to be justified even if we use nonstandard methods, but the "almost Minkowskian" path integrals can be used as a substitute for them.

By the Fourier transformation, Λ_θ^{-1} is represented as the multiplication operator

$$\tilde{\Lambda}_\theta^{-1}(p)=\frac{e^{i\theta}}{p_0^2+e^{2i\theta}\sum_k p_k^2+e^{2i\theta}m^2}.$$

In the "almost Minkowskian" case $\theta=(\pi/2)-\epsilon$, we find

$$\tilde{\Lambda}_{\theta}^{-1}(p) \approx \frac{i}{p_0^2 - \sum_k p_k^2 - m^2 + i\epsilon},$$

where the approximation is in the sense of Schwartz distribution. Since the right-hand side is the Fourier transform of the Feynman Green function $\Delta_F(x)$, we have

$$Z[J] \approx \exp \tfrac{1}{2}(J, \Delta_F J),$$

for any $J \in \mathcal{D}(\mathbf{R}^{\mathbf{d}+1})$. Thus a rigorous justification of physicists' path-integral calculation of the generating functional has been given.

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Analyticity of the scattering amplitude, causality, and high-energy bounds in quantum field theory on noncommutative space–time

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In the framework of quantum field theory on noncommutative space–time with the symmetry group $O(1,1)\times SO(2)$, we prove that the Jost-Lehmann-Dyson representation, based on the causality condition taken in connection with this symmetry, leads to the mere impossibility of drawing any conclusion on the analyticity of the $2\rightarrow 2$-scattering amplitude in $\cos\Theta$, Θ being the scattering angle. Discussions on the possible ways of obtaining high-energy bounds analogous to the Froissart-Martin bound on the total cross section are also presented. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2338761]

I. INTRODUCTION

The development of quantum field theory (QFT) on noncommutative (NC) space–time, especially after the seminal work of Seiberg and Witten,[1] which showed that the NC QFT arises from string theory, has lately triggered interest also towards the formulation of an axiomatic approach to the subject. The power of the axiomatic approach is that that the results are rigorously derived, with no reference to the specific form of interaction or to perturbation theory. Consequently, in the framework of noncommutative spaces, the analytical properties of scattering amplitude in energy E and forward dispersion relations have been considered,[2,3] Wightman functions have been introduced and the CPT theorem has been proven,[4,5] and as well attempts towards a proof of the spin-statistics theorem have been made.[5] [In the context of the Lagrangian approach to NC QFT, the CPT and spin-statistics theorems have been proven in general in Ref. 6; for CPT invariance in NC QED, see Refs. 7 and 8, and in NC standard model.[9]]

In the axiomatic approach to commutative QFT, one of the fundamental results consisted of the rigorous proof of the Froissart bound on the high-energy behavior of the scattering amplitude, based on its analyticity properties.[10,11] In this paper we aim at obtaining the analog of this bound when the space–time is noncommutative. Such an undertaking, besides being topical in itself, would also prove fruitful in the conceptual understanding of subtle issues, such as causality, in nonlocal theories to which the NC QFTs belong.

In the following, we shall consider NC QFT on a space–time with the commutation relation

$$[x_\mu, x_\nu] = i\theta_{\mu\nu}, \tag{1.1}$$

where $\theta_{\mu\nu}$ is an antisymmetric constant matrix (for a review, see, e.g., Refs. 12 and 13). Such NC theories violate Lorentz invariance, while translational invariance still holds. We can always choose the system of coordinates such that $\theta_{13}=\theta_{23}=0$ and $\theta_{12}=-\theta_{21}\equiv\theta$. Then, for the particular case of space–space noncommutativity, i.e., $\theta_{0i}=0$, the theory is invariant under the subgroup $O(1,1)\times SO(2)$ of the Lorentz group. The requirement that time be commutative ($\theta_{0i}=0$) discards the well-known problems with the unitarity[14] of the NC theories and with causality[15,16] (see also Ref. 6). As well, the $\theta_{0i}=0$ case allows a proper definition of the S-matrix.[3]

In the conventional (commutative) QFT, the Froissart bound was first obtained[10] using the conjectured Mandelstam representation (double dispersion relation),[17] which assumes analyticity in the entire E and $\cos\Theta$ complex planes. The Froissart bound,

$$\sigma_{\text{tot}}(E) \leqslant c \ln^2 \frac{E}{E_0}, \tag{1.2}$$

expresses the upper limit of the total cross section σ_{tot} as a function of the center-of-mass system (CMS) energy E, when $E \to \infty$. However, such an analyticity or equivalently the double dispersion relation has not been proven, while smaller domains of analyticity in $\cos\Theta$ were already known.[18]

One of the main ingredients in rigorously obtaining the Froissart bound is the Jost-Lehmann-Dyson representation[19,20] of the Fourier transform of the matrix element of the commutator of currents, which is based on the causality as well as the spectral conditions (for an overall review, see Ref. 21). Based on this integral representation, one obtains the domain of analyticity of the scattering amplitude in $\cos\Theta$. This domain proves to be an ellipse—the so-called Lehmann's ellipse.[18]

However, this domain of analyticity in $\cos\Theta$ can be enlarged to the so-called Martin's ellipse by using the dispersion relations satisfied by the scattering amplitude and the unitarity constraint on the partial-wave amplitudes. Using this larger domain of analyticity, the Froissart bound (1.2) was rigorously proven in QFT (Ref. 11) (for a review, see Ref. 22).

Further on, the analog of the Froissart-Martin bound was rigorously obtained for the $2 \to 2$-particle scattering in a space–time of arbitrary dimension D.[23,24]

In NC QFT with $\theta_{0i}=0$, we shall follow the same path for the derivation of the high-energy bound on the scattering amplitude, starting from the Jost-Lehmann-Dyson representation and adapting the derivation to the new symmetry $O(1,1)\times SO(2)$ and to the nonlocality of the NC theory. [A preliminary work along this line with stronger claims, based on a conjecture, has been previously reported in Ref. 25.] In Sec. II we derive the Jost-Lehmann-Dyson representation satisfying the light-wedge (instead of light-cone) causality condition, inspired by the above symmetry. We show that no analyticity of the scattering amplitude in $\cos\Theta$ can be obtained in such a case. Since the causality condition is the key ingredient for the analyticity of the scattering amplitude, in Sec. III we discuss possible causality postulates in the noncommutative case, in relation both with the maximal symmetry of the theory (twisted Poincaré[26]) and with the scale of nonlocality as obtained so far in perturbative calculations. It turns out that by postulating a *finite range of nonlocality*, compatible with the twisted Poincaré symmetry, and by using the global nature of local commutativity, we can obtain from the Jost-Lehmann-Dyson representation a domain of analyticity in $\cos\Theta$, which coincides with the Lehmann ellipse. Further, the extension of this analyticity domain to Martin's ellipse is possible in the case of the incoming particles' momenta orthogonal to the NC plane (x_1, x_2), which eventually enables us to derive the analog of the Froissart-Martin bound (1.2) for the total cross section. The general configuration of incoming particles' momenta is also discussed, together with the problems which arise in such a case. However, the perturbative calculations performed so far seem to indicate an *infinite range of nonlocality*, in which case the initial causality condition involving the light wedge should be postulated, leading to the lack of analyticity of the scattering amplitude. The situation is discussed in connection with the perturbative problem of UV/IR mixing in NC QFT. Section 6 is devoted to conclusion and discussions.

II. JOST-LEHMANN-DYSON REPRESENTATION

The Jost-Lehmann-Dyson representation[19,20] is the integral representation for the Fourier transform of the matrix elements of causal commutators, satisfying the causality and spectral conditions. For definiteness and simplicity, we shall obtain it below for a particular matrix element of the commutator of currents

$$f(q) = \int d^4x e^{iqx} f(x), \tag{2.1}$$

where

$$f(x) = \left\langle p' \left| \left[j\left(\frac{x}{2}\right), j'\left(-\frac{x}{2}\right) \right] \right| p \right\rangle. \tag{2.2}$$

The process considered is the $2 \to 2$ scalar particles scattering, $k+p \to k'+p'$, and j and j' are the scalar currents corresponding to the incoming and outgoing particles with momenta k and k' (see also Refs. 21 and 27). We emphasize that the (form of the) integral representation eventually obtained is, however, valid for *any* other matrix element of any commutator of currents.

For NC QFT with $O(1,1) \times SO(2)$ symmetry, in Ref. 28 a new causality condition was proposed, involving (instead of the light cone) the light wedge corresponding to the coordinates x_0 and x_3, which form a two-dimensional space with the $O(1,1)$ symmetry. Accordingly, we shall require the vanishing of the commutator of two currents (in general, observables) at spacelike separations in the sense of $O(1,1)$ as

$$\left[j\left(\frac{x}{2}\right), j'\left(-\frac{x}{2}\right) \right] = 0, \quad \text{for } \tilde{x}^2 \equiv x_0^2 - x_3^2 < 0. \tag{2.3}$$

The spectral condition compatible with (2.3) would require now that the physical momenta be in the forward light wedge,

$$\tilde{p}^2 \equiv p_0^2 - p_3^2 > 0 \quad \text{and} \quad p_0 > 0. \tag{2.4}$$

The standard spectral condition

$$p_0^2 - p_1^2 - p_2^2 - p_3^2 \geqslant 0, \quad p_0 > 0,$$

based on Poincaré symmetry or twisted Poincaré symmetry,[26] implies the forward light-wedge condition (2.4) as well.

The spectral condition (2.4) will impose restrictions on $f(q)$. Using the translational invariance in (2.2), one can express the matrix element of the commutator of currents, $f(x)$, in the form

$$\begin{aligned} f(x) &= \int dq e^{-iqx + i(p+p')(x/2)} G_1(q) - \int dq e^{iqx - i(p+p')(x/2)} G_2(q) \\ &= \int dq e^{-iqx} \left[G_1\left(q + \frac{1}{2}(p+p')\right) - G_2\left(-q + \frac{1}{2}(p+p')\right) \right], \end{aligned} \tag{2.5}$$

where

$$\begin{aligned} G_1(q) &= \langle p' | j(0) | q \rangle \langle q | j'(0) | p \rangle, \\ G_2(q) &= \langle p' | j'(0) | q \rangle \langle q | j(0) | p \rangle. \end{aligned} \tag{2.6}$$

Comparing (2.5) with the inverse Fourier transformation, $f(x) = \int dq e^{-iqx} f(q)$, it follows that

$$f(q) = f_1(q) - f_2(q) = G_1\left(q + \frac{1}{2}(p+p')\right) - G_2\left(-q + \frac{1}{2}(p+p')\right). \tag{2.7}$$

[Throughout the paper we omit all the inessential factors of $(2\pi)^n$, which are irrelevant for the analyticity considerations.] Given the way the functions G_1 and G_2 are defined in (2.6), one finds that $f(q)=0$ in the region where the momenta $q+1/2(p+p')$ and $-q+1/2(p+p')$ are simultaneously nonphysical, i.e., when they are out of the future light wedge (2.4).

In order to express the condition for $f(q)=0$, we shall define the $O(1,1)$-invariant $\tilde{m}^2=k_0^2-k_3^2=f(m^2,k_1^2+k_2^2)$, where k is the momentum of an arbitrary state and m is its mass. However, we have to point out that $\tilde{m}$ is only a kinematical variable, invariant with respect to $O(1,1)$ (but not the mass).

For the *physical* states with momentum $q+1/2(p+p')$, we take $\tilde{m}_1$ to be the minimal value of the $O(1,1)$-invariant quantity above. Then, in the Breit frame, where $1/2(p+p')=(p_0,0,0,0)$, one finds that $f_1(q)\neq 0$ for all the q values, satisfying the spectral condition $q_0+p_0\geqslant 0$ and $(q_0-p_0)^2-q_3^2\geqslant 0$. In other words, $f_1(q)=0$ for $q_0<-p_0+\sqrt{q_3^2+\tilde{m}_1^2}$. Similarly, one finds that $f_2(q)=0$ for $p_0-\sqrt{q_3^2+\tilde{m}_2^2}<q_0$ [where $\tilde{m}_2$ has a meaning analogous to that of $\tilde{m}_1$, but for the states with the momentum $-q+1/2(p+p')$].

As a result, due to the spectral condition (2.4), $f(q)=0$ in the region outside the hyperbola

$$p_0-\sqrt{q_3^2+\tilde{m}_2^2}<q_0<-p_0+\sqrt{q_3^2+\tilde{m}_1^2}. \tag{2.8}$$

To derive the Jost-Lehmann-Dyson representation, further we consider the six-dimensional space–time with the Minkowskian metric $(+,-,-,-,-,-)$. On this space, we define the vector $z=(x_0,x_1,x_2,x_3,y_1,y_2)$. For practical purposes we introduce also the notations for the two-dimensional vector $\tilde{x}=(x_0,x_3)$ and the four-dimensional vector $\tilde{z}=(z_0,z_3,z_4,z_5)\equiv(x_0,x_3,y_1,y_2)$. On the six-dimensional space we define the function

$$F(z)=f(x)\delta(\tilde{x}^2-y^2)=f(x)\delta(\tilde{z}^2), \tag{2.9}$$

depending on all six coordinates.

When the causality condition (2.3) is fulfilled, i.e., for the physical region, $f(x)$ and $F(z)$ determine each other, since

$$\int dy_1dy_2F(z)=f(x)\theta(\tilde{x}^2)=\begin{cases}f(x) & \text{for} \quad \tilde{x}^2>0,\\ 0 & \text{for} \quad \tilde{x}^2<0.\end{cases} \tag{2.10}$$

The Fourier transform of $F(z)$,

$$F(r)=\int d^6z e^{izr}F(z), \tag{2.11}$$

can be expressed, using (2.9) and (2.10), as

$$F(r)=\int d^4qD_1(r-\hat{q})f(q). \tag{2.12}$$

Denoting the remaining four-dimensional vector $\tilde{r}=(r_0,r_3,r_4,r_5)$, we have

$$D_1(r)=\int d^6z e^{izr}\delta(\tilde{z}^2)=\frac{\delta(r_1)\delta(r_2)}{\tilde{r}^2}=\delta(r_1)\delta(r_2)D_1(\tilde{r}), \tag{2.13}$$

with $D_1(\tilde{r})=1/\tilde{r}^2$.

We define now the "subvector" of a six-dimensional vector as $\hat{q}=(q_0,q_1,q_2,q_3,0,0)$ and we find the relation between $F(\hat{q})$ and $f(q)$ in view of the causality condition (2.3),

$$F(\hat{q})=\int d^4xf(x)\theta(\tilde{x}^2)e^{iqx}=f(q). \tag{2.14}$$

$D_1(\tilde{r})$ satisfies the four-dimensional wave equation,

$$\Box_4D_1(\tilde{r})=0, \tag{2.15}$$

where the d'Alembertian is defined with respect to the coordinates r_0,r_3,r_4,r_5. Then, due to (2.12), it follows that $F(r)$ satisfies the same equation,

$$\Box_4 F(r) = 0. \tag{2.16}$$

It is crucial to note that $F(r)$ depends on all six variables $r_0, \ldots, r_5$

$$F(r) = \int d^4q f(q) D_1(\tilde{r} - \tilde{q}) \delta(r_1 - q_1) \delta(r_2 - q_2),$$

where $\tilde{q} = (q_0, q_3, 0, 0)$.

The solution of (2.16) can be written in the form:[31]

$$F(r') = \int d^3\Sigma_\alpha \int\int dr_1 dr_2 \left[F(r) \frac{\partial D(\tilde{r} - \tilde{r}')}{\partial \tilde{r}_\alpha} - D(\tilde{r} - \tilde{r}') \frac{\partial F(r)}{\partial \tilde{r}_\alpha} \right] \delta(r_1) \delta(r_2),$$

where $D(\tilde{r})$ satisfies the homogeneous differential equation $\Box_4 D(\tilde{r}) = 0$, with the initial conditions

$$D(\vec{r}) \Big|_{r_0=0} = 0 \quad \text{and} \quad \frac{\partial D}{\partial r_0}(\vec{r}) \Big|_{r_0=0} = \prod_{i=1}^{3} \delta(r_i).$$

The first condition implies that $D(\tilde{r})$ is an odd function, with the result that

$$D(\tilde{r}) = \int d^4z e^{-i\tilde{z}\tilde{r}} \epsilon(z_0) \delta(\tilde{z}^2) = \epsilon(r_0) \delta(\tilde{r}^2). \tag{2.17}$$

We note here that the surface Σ is three-dimensional and not five-dimensional as it is in the commutative case with light-cone causality condition. Now we can express $f(q)$ using (2.14) as

$$f(q) = F(\hat{q}) = \int dr_1 dr_2 \delta(r_1 - q_1) \delta(r_2 - q_2) \int d^3\Sigma_\alpha \left[F(r) \frac{\partial D(\tilde{r} - \tilde{q})}{\partial \tilde{r}_\alpha} - D(\tilde{r} - \tilde{q}) \frac{\partial F(r)}{\partial \tilde{r}_\alpha} \right]. \tag{2.18}$$

Due to the arbitrariness of the surface Σ, one can reduce the integration over r_4 and r_5, using the cylindrical symmetry, to the integral over $\kappa^2 = r_4^2 + r_5^2$. Subsequently, we change the notation of variables r_i to u_i and use the explicit form of $D(\tilde{r})$ from (2.17) to obtain

$$\begin{aligned} f(q) = & \int du_1 du_2 \delta(u_1 - q_1) \delta(u_2 - q_2) \int d^1\Sigma_j d\kappa^2 \\ & \times \left\{ F(u, \kappa^2) \frac{\partial}{\partial \tilde{u}_j} [\epsilon(u_0 - q_0) \delta((\tilde{u} - \tilde{q})^2 - \kappa^2)] - \epsilon(u_0 - q_0) \delta((\tilde{u} - \tilde{q})^2 - \kappa^2) \frac{\partial F(u, \kappa^2)}{\partial \tilde{u}_j} \right\}. \end{aligned} \tag{2.19}$$

Using the standard mathematical procedure[31] for performing the integration in (2.19), we obtain the Jost-Lehmann-Dyson representation in NC QFT, satisfying the light-wedge causality condition (2.3),

$$f(q) = \int d^4u d\kappa^2 \epsilon(q_0 - u_0) \delta[(q_0 - u_0)^2 - (q_3 - u_3)^2 - \kappa^2] \times \delta(q_1 - u_1) \delta(q_2 - u_2) \phi(u, \kappa^2), \tag{2.20}$$

where $\phi(u, \kappa^2) = -[\partial F(u, \kappa^2)] / \partial \tilde{u}_0$.

Equivalently, denoting $\tilde{u} = (u_0, u_3)$, (2.20) can be written as

$$f(q) = \int d^2\tilde{u} d\kappa^2 \epsilon(q_0 - u_0) \delta[(\tilde{q} - \tilde{u})^2 - \kappa^2] \phi(\tilde{u}, q_1, q_2, \kappa^2). \tag{2.21}$$

The function $\phi(\tilde{u},q_1,q_2,\kappa^2)$ is an arbitrary function, except that the requirement of spectral condition determines a domain in which $\phi(\tilde{u},q_1,q_2,\kappa^2)=0$. This domain is outside the region where the δ function in (2.21) vanishes, i.e.,

$$(\tilde{q}-\tilde{u})^2-\kappa^2=0, \tag{2.22}$$

but with $\tilde{q}$ in the region given by (2.8), where $f(q)=0$. Putting together (2.22) and (2.8), we obtain the domain out of which $\phi(\tilde{u},q_1,q_2,\kappa^2)=0$,

$$\begin{aligned} &\text{a)} \quad \tfrac{1}{2}(\tilde{p}+\tilde{p}')\pm\tilde{u} \text{ are in the forward lightwedge (cf. (2.4));} \\ &\text{b)} \quad \kappa \geqslant \max\left\{0,\tilde{m}_1-\sqrt{\left(\frac{\tilde{p}+\tilde{p}'}{2}+\tilde{u}\right)^2},\tilde{m}_2-\sqrt{\left(\frac{\tilde{p}+\tilde{p}'}{2}-\tilde{u}\right)^2}\right\}. \end{aligned} \tag{2.23}$$

For the purpose of expressing the scattering amplitude, we actually need the Fourier transform $f_R(q)$ of the retarded commutator,

$$f_R(x)=\theta(x_0)f(x)=\left\langle p'\left|\,\theta(x_0)\left[j\left(\frac{x}{2}\right),j'\left(-\frac{x}{2}\right)\right]\right|p\right\rangle. \tag{2.24}$$

Using (2.24) and the Fourier transformation $f(x)=\int dq' e^{-iq'x}f(q')$, we can express $f_R(q)$ as follows:

$$f_R(q)=\int dx e^{iqx}f_R(x)=\int dx e^{iqx}\theta(x_0)f(x)=\int dq' f(q')\int dx e^{i(q-q')x}\theta(x_0). \tag{2.25}$$

Taking into account that

$$\int dx_0 e^{i(q-q')x}\theta(x_0)=-i\frac{e^{i(\vec{q}-\vec{q}')\vec{x}}}{q_0-q_0'},$$

Eq. (2.25) becomes

$$f_R(q)=i\int dq_0'\frac{f(q_0',\vec{q})}{q_0'-q_0}.$$

Now, in the above formula we introduce the Jost-Lehmann-Dyson representation (2.21), with the result

$$f_R(q)=i\int\frac{dq_0'}{q_0'-q_0}\int d^2\tilde{u}d\kappa^2\epsilon(q_0'-u_0)\delta[(q_0'-u_0)^2-(q_3-u_3)-\kappa^2]\phi(\tilde{u},q_1,q_2,\kappa^2). \tag{2.26}$$

In (2.26) one can integrate over q_0', using the known formula of integration with a δ-function, $\int G(x)\delta(g(x))dx=\Sigma_i G(x_{0i})/\partial g/\partial x|_{x=x_{0i}}$, where x_{0i} are the simple roots of the function $g(x)$. We identify in (2.26) $G(q_0')=[\epsilon(q'0-u_0)]/(q_0'-q_0)$ and $g(q_0')=(q_0'-u_0)^2-(q_3-u_3)-\kappa^2$ (with the roots $q_0'=u_0\pm[(q_3-u_3)^2+\kappa^2]^{1/2}$).

With these considerations, from (2.26) we obtain the NC version of the Jost-Lehmann-Dyson representation for the retarded commutator,

$$f_R(q)=\int d^2\tilde{u}d\kappa^2\frac{\phi(\tilde{u},q_1,q_2,\kappa^2)}{(q_0-u_0)^2-(q_3-u_3)^2-\kappa^2}. \tag{2.27}$$

Compared to the usual Jost-Lehmann-Dyson representation,

$$f_R^{\text{comm}}(q) = \int d^4u d\kappa^2 \frac{\phi(u,\kappa^2)}{(q_0-u_0)^2-(\vec{q}-\vec{u})^2-\kappa^2}, \tag{2.28}$$

the expression (2.27) is essentially different in the sense that the arbitrary function ϕ now depends on q_1 and q_2. This feature will have further crucial implications in the discussion of analyticity of the scattering amplitude in $\cos\Theta$.

A. (Non-)Analyticity of the scattering amplitude in $\cos\Theta$

In the center-of-mass system (CMS) and in a set in which the incoming particles are along the vector $\vec{\beta}=(0,0,\theta)$, the scattering amplitude in NC QFT depends still on only two variables, the CM energy E and the cosine of the scattering angle, $\cos\Theta$ (for a discussion about the number of variables in the scattering amplitude for a general type of noncommutativity, see Ref. 29). [The 'magnetic' vector $\vec{\beta}$ is defined as $\beta_i = 1/2\,\epsilon_{ijk}\theta_{jk}$. The terminology stems from the antisymmetric background field $B_{\mu\nu}$ (analogous to $F_{\mu\nu}$ in QED), which gives rise to noncommutativity in string theory, with $\theta_{\mu\nu}$ essentially proportional to $B_{\mu\nu}$ (see, e.g., Ref. 1).]

Depending on the variable in which the analyticity is considered, one chooses an appropriate reduction formula for the scattering amplitude, such that in a given frame all the dependence on the considered variable is contained only in the exponent. Since we are interested in the analyticity in $\cos\Theta$, it is natural to take the reduction

$$M(E,\cos\Theta) = i\int d^4x e^{i(k'-p')\cdot(x/2)}\theta(x)\left\langle 0\left|\left[j_1\left(\frac{x}{2}\right),j_2\left(-\frac{x}{2}\right)\right]\right|p,k\right\rangle,$$

where $-1/2(k'-p')=q$, such that in the center-of-mass frame the whole dependence on $\cos\Theta$ is contained in q (j_1 and j_2 are the appropriate currents, corresponding to the outgoing particles of momenta p' and k'). The previous expression of the scattering amplitude $M(E,\cos\Theta)$ considered as a function of the complex vector $q=-1/2(k'-p')$ can be treated along the same lines as the retarded matrix element $f_R(q)$ between one-particle states introduced above in Eq. (2.25). This treatment results in a Jost-Lehmann-Dyson representation similar to (2.27), which therefore allows one to write the scattering amplitude as follows (compare with the expression given in Ref. 21 for the commutative case):

$$M(E,\cos\Theta) = i\int d^2\tilde{u} d\kappa^2 \frac{\phi(\tilde{u},\kappa^2,k+p,(k'-p')_{1,2})}{\left[\frac{1}{2}(\tilde{k}'-\tilde{p}')+\tilde{u}\right]^2-\kappa^2}, \tag{2.29}$$

where $\phi(\tilde{u},\kappa^2,\ldots)$ is a function of its $O(1,1)$- and $SO(2)$-invariant variables: $u_0^2-u_3^2$, $(k_0+p_0)^2-(k_3-p_3)^2$, $(k_1+p_1)^2+(k_2+p_2)^2$, $(k_1'-p_1')^2+(k_2'-p_2')^2,\ldots$. The function ϕ is zero in a certain domain, determined by the causal and spectral conditions, but otherwise arbitrary.

For the discussion of analyticity of $M(E,\cos\Theta)$ in $\cos\Theta$, it is of crucial importance that all dependence on $\cos\Theta$ be contained in the denominator of (2.29). But, since the *arbitrary* function ϕ depends now on $(k'-p')_{1,2}$, it also depends on $\cos\Theta$. This makes impossible the mere consideration of any analyticity property of the scattering amplitude in $\cos\Theta$.

Since the Jost-Lehmann-Dyson representation reflects the effect of the causal and spectral axioms, we notice that the hypotheses (2.3) and (2.4) used for the present derivation allow for a much larger physical region, by not taking into account at all the effect of the NC coordinates x_1 and x_2. One might wonder now whether in the above derivation there is any condition which could be subject to challenge. In that case there might also appear the possibility that an analyticity domain can be obtained, leading to some high-energy upper bound on the scattering amplitude.

III. CAUSALITY IN NC QFT

A. Causality and symmetry in NC QFT

In the following, we shall challenge the causality condition (2.3):

$$f(x)=0, \quad \text{for } \tilde{x}^2 \equiv x_0^2 - x_3^2 < 0, \tag{3.1}$$

which takes into account *only* the variables connected with the $O(1,1)$ symmetry.

This causality condition is suitable in the case when the nonlocality in the NC variables x_1 and x_2 is *infinite*. The fact that in the causality condition (3.1) the coordinates x_1 and x_2 do not enter means that the propagation of a signal in this plane is instantaneous: *no matter how far apart in the noncommutative coordinates two events are*, the allowed region for correlation is given by only the condition $x_0^2 - x_3^2 > 0$, which involves the propagation of a signal only in the x_3-direction, while the time for the propagation along x_1- and x_2-directions is totally ignored.

Recall that we are using an axiomatic approach, in whose commutative counterpart the assumption of locality was a postulate. In our noncommutative case, the postulate of locality has to be replaced by a postulate prescribing the scale of nonlocality. Postulating that the scale of nonlocality in x_1 and x_2 is $l \sim \sqrt{\theta}$, then the propagation of the interaction in the noncommutative coordinates is instantaneous *only within this distance l*. It follows then that two events are correlated, i.e., $f(x) \neq 0$, when $x_1^2 + x_2^2 \leqslant l^2$ (where $x_1^2 + x_2^2$ is the distance in the NC plane with $SO(2)$ symmetry), provided also that $x_0^2 - x_3^2 \geqslant 0$ (the events are timelike separated in the sense of $O(1,1)$). Adding the two conditions, we obtain that

$$f(x) \neq 0, \quad \text{for } x_0^2 - x_3^2 - (x_1^2 + x_2^2 - l^2) \geqslant 0. \tag{3.2}$$

The negation of condition (3.2) leads to the conclusion that the locality condition should indeed be given by

$$f(x)=0, \quad \text{for } \tilde{x}^2 - (x_1^2 + x_2^2 - l^2) \equiv x_0^2 - x_3^2 - (x_1^2 + x_2^2 - l^2) < 0,$$

or, equivalently,

$$f(x)=0, \quad \text{for } x_0^2 - x_3^2 - (x_1^2 + x_2^2) < -l^2, \tag{3.3}$$

where l^2 is a constant proportional to the NC parameter θ. When $l^2 \to 0$ (3.3) becomes the usual locality condition.

When $x_1^2 + x_2^2 > l^2$, for the propagation of a signal only the difference $x_1^2 + x_2^2 - l^2$ is time-consuming and thus in the locality condition it is the quantity $x_0^2 - x_3^2 - (x_1^2 + x_2^2 - l^2)$ which will occur. Therefore, we shall have again the locality condition of the form (3.3).

Since there is no noncommutativity in the momentum space, the spectral condition will read now as

$$p_0^2 - p_1^2 - p_2^2 - p_3^2 \geqslant 0, \quad p_0 > 0. \tag{3.4}$$

At this point we recall that the maximal symmetry of a NC QFT with $\theta_{\mu\nu}$ a constant matrix is not the classical $O(1,1) \times SO(2)$ symmetry, but a quantum symmetry, namely the twisted Poincaré symmetry,[26] whose representation content is identical to the usual Poincaré symmetry. Moreover, the usual space–time interval $x^2 = x_0^2 - x_1^2 - x_2^2 - x_3^2$ is invariant under the twisted Poincaré algebra, as well as the scale of nonlocality l, since the latter is expressed in terms of the twisted Poincaré-invariant θ. Consequently (3.3) and (3.4) are compatible with the twisted Poincaré algebra.

In fact, the consideration of nonlocal theories of the type (3.3) and (3.4) was initiated by Wightman.[30] It was proven later[31–33] (see also Ref. 34) that, indeed, in a quantum field theory which satisfies the translational invariance and the spectral axiom (3.4), the nonlocal commutativity

$$\left[j_1\left(\frac{x}{2}\right), j_2\left(-\frac{x}{2}\right)\right] = 0, \quad \text{for } x_0^2 - x_1^2 - x_2^2 - x_3^2 < -l^2$$

implies the local commutativity

$$\left[j_1\left(\frac{x}{2}\right), j_2\left(-\frac{x}{2}\right)\right] = 0, \quad \text{for } x_0^2 - x_1^2 - x_2^2 - x_3^2 < 0. \tag{3.5}$$

This powerful theorem (stating the "global nature of local commutativity"), which does not require standard Lorentz invariance, but only translational invariance, can be applied in the noncommutative case with postulated finite nonlocality, with the conclusion that the causality properties of a QFT with space–space noncommutativity are physically identical to those of the corresponding commutative QFT.

It is then obvious that the Jost-Lehmann-Dyson representation (2.28) obtained in the commutative case holds also on the NC space for any orientation of the vector $\vec{\beta}$. Consequently, the NC two-particle→two-particle scattering amplitude will have the same form as in the commutative case,

$$M(E, \cos\Theta) = i \int d^4u d\kappa^2 \frac{\phi(u, \kappa^2, k+p)}{\left[\frac{1}{2}(k'-p') + u\right]^2 - \kappa^2}. \tag{3.6}$$

This leads to the analyticity of the NC scattering amplitude in $\cos\Theta$ in the analog of the Lehmann ellipse, which behaves at high energies E the same way as in the commutative case, i.e., with the semimajor axis as

$$y_L = (\cos\Theta)_{\max} = 1 + \frac{\text{const}}{E^4}. \tag{3.7}$$

1. Enlargement of the domain of analyticity in $\cos\Theta$ *and use of unitarity. Martin's ellipse*

Two more ingredients are needed in order to enlarge the domain of analyticity in $\cos\Theta$ to the Martin's ellipse and to obtain the Froissart-Martin bound: the dispersion relations and the unitarity constraint on the partial-wave amplitudes.[22]

When using the causality condition (2.3), the forward dispersion relation cannot be obtained in NC theory with general direction of the $\vec{\beta}$-vector.[2] However, the conclusion at which we arrived by imposing the nonlocal commutativity condition (3.3) and reducing it to the local commutativity (3.5) leads straightforwardly to the usual forward dispersion relation also in the NC case with a general $\vec{\beta}$ direction.

As for the unitarity constraint on the partial wave amplitudes, the problem has been investigated in Ref. 29, for a general case of noncommutativity $\theta_{\mu\nu}$, $\theta_{0i} \neq 0$. For space–space noncommutativity ($\theta_{0i}=0$), the scattering amplitude depends, besides the center-of-mass energy, E, on three angular variables. In a system where we take the incoming momentum $\vec{p}$ in the z-direction, these variables are the polar angles of the outgoing particle momentum, Θ and ϕ, and the angle α between the vector $\vec{\beta}$ and the incoming momentum. The partial-wave expansion in this case reads

$$A(E, \Theta, \phi, \alpha) = \sum_{l,l',m} (2l'+1) a_{ll'm}(E) Y_{lm}(\Theta, \phi) P_{l'}(\cos\alpha), \tag{3.8}$$

where Y_{lm} are the spherical harmonics and $P_{l'}$ are the Legendre polynomials.

Imposing the unitarity condition directly on (3.8) or using the general formulas given in Ref. 29, it can be shown that a simple unitarity constraint which involves single partial-wave amplitudes one at a time can be obtained only in a setting where the incoming momentum is orthogonal

to the NC plane (equivalently, it is parallel to the vector $\vec{\beta}$). In this case the amplitude depends only on one angle, Θ, and the unitarity constraint is reduced to the well-known one of the commutative case, i.e.,

$$\mathrm{Im}\, a_l(E) \geqslant |a_l(E)|^2. \tag{3.9}$$

For this particular setting, $\vec{p} \| \vec{\beta}$, it is then straightforward, following the prescription developed for commutative QFT, to enlarge the analyticity domain of scattering amplitude to Martin's ellipse with the semimajor axis at high energies as

$$y_M = 1 + \frac{\mathrm{const}}{E^2}, \tag{3.10}$$

and subsequently obtain the NC analog of the Froissart-Martin bound on the total cross section, in the CMS and for $\vec{p} \| \vec{\beta}$,

$$\sigma_{\mathrm{tot}}(E) \leqslant c \ln^2 \frac{E}{E_0}. \tag{3.11}$$

Thus, the unitarity constraint on the partial-wave amplitudes distinguishes a particular setting ($\vec{p} \| \vec{\beta}$) in which the Lehmann's ellipse can be enlarged to the Martin's ellipse and the Froissart-Martin bound can be obtained, with the assumption of finite nonlocality. Nevertheless, this does not necessarily exclude the possibility of obtaining a rigorous high-energy bound on the cross section for $\vec{p}$ not parallel to $\vec{\beta}$, and the issue deserves further investigation.

B. Causality and nonlocality in NC QFT

It was shown in the previous subsection that the violation of Lorentz invariance in itself does not forbid the existence of an analyticity domain of the scattering amplitude in $\cos\Theta$ and the derivation of a high-energy bound, compatible with the twisted Poincaré symmetry.

However, for the derivation of the analog of the Froissart-Martin bound the key ingredient was the assumption of finite nonlocality. This issue deserves a more thorough investigation, in the light of the Lagrangian models studied so far. We have to point out from the very beginning that the Lagrangian models have been studied up to at most two loops, and that no definite statement about the renormalizability of NC quantum field theories in general has been made so far.

It is well known that in NC QFT treated with the Weyl-Moyal correspondence (i.e., with the usual product of fields replaced by Moyal $\star$-product in the Lagrangian) the short distance (UV) effects are related to the long-distance (topological) features of the space–time. This fact was first noticed in Ref. 35, where it was shown that noncommutativity leads to UV-regular theories when at most one dimension of the space–time is noncompact. For the NC flat space–time UV-regularity is not achieved, but instead the exotic phenomenon of UV/IR mixing appears.[36] The physical meaning of this mixing is that at quantum level, even very low-energy processes receive contributions from high-energy virtual particles. The nonlocality is energy dependent, and for virtual particles of arbitrarily high energy, the nonlocality is arbitrarily large.

Another investigation leading to the same conclusion was performed in the first paper dealing with the causality in NC QFT in the Lagrangian approach.[15] There it was shown, through the study of a scattering process, that space–space NC ϕ^4 in $2+1$ dimensions is causal at macroscopical level. However the incident particles should be viewed as extended rigid rods, of the size θp, perpendicular to their momentum. In other words, the noncommutativity introduces an energy-dependent scale of spatial nonlocality θp.

Judging by the above-mentioned results obtained in specific NC models up to one-loop level, the previous analysis of analyticity and high-energy bounds in axiomatic NC QFT becomes inconclusive. It appears that the finite nonlocality condition (3.3) is solely a conjecture, but only based on this conjecture one can derive rigorously the analyticity properties and high-energy

bounds on the scattering amplitude (see Sec. III). We should recall, however, that the infinite nonlocality in NC QFT has been found up to one-loop level and there is no indication that the infinite nonlocality is not an artifact of perturbation theory.

Nevertheless, in the case of a *compact* noncommutative space–time, the NC QFT is finite, i.e., there are no UV divergences,[35] consequently no UV/IR mixing, and the range of nonlocality is finite. For such NC QFT the finite nonlocality is no longer a conjecture and one may reconsider the rigorous axiomatic derivation of the analyticity and high-energy bounds along the lines of Sec. III A.

IV. CONCLUSION AND DISCUSSIONS

In this paper we have tackled the problem of high-energy bounds on the two-particle $\rightarrow$two-particle scattering amplitude in NC QFT. The key issue in the analysis proved to be the scale of nonlocality of the quantum field theory on NC space–time.

We have found that, assuming infinite nonlocality and using the causal and spectral conditions (2.3) and (2.4) proposed in Ref. 28 for NC theories with $O(1,1)\times SO(2)$ symmetry, a new form of the Jost-Lehmann-Dyson representation (2.27) is obtained, which does not permit us to draw any conclusion about the analyticity of the scattering amplitude (2.29) in $\cos\Theta$. Therefore, the derivation of high-energy bounds on the scattering amplitude is impossible.

However, by postulating that the nonlocality in the noncommuting coordinates is finite, we were led to impose a new causality condition (3.3), which accounts for the finitness of the range of nonlocality and prevents the *instantaneous propagation of signals* in the *entire* noncommutative plane (x_1,x_2). We proved that the new causality condition, compatible also with the twisted Poincaré symmetry, is formally identical to the one corresponding to the commutative case (3.5), using the Wightman-Vladimirov-Petrina theorem.

Thus, with the assumption of finite nonlocality, the scattering amplitude in NC QFT is proved to be analytical in $\cos\Theta$ in the Lehmann ellipse, just as in the commutative case; moreover, dispersion relations can be written on the same basis as in commutative QFT. Finally, based on the unitarity constraint on the partial-wave amplitudes in NC QFT, we can conclude that, for theories with space–space noncommutativity ($\theta_{0i}=0$), the total cross section is subject to an upper bound (3.11) identical to the Froissart-Martin bound in its high-energy behavior, when the incoming particle momentum $\vec{p}$ is orthogonal to the NC plane.

Though the perturbative studies performed so far (up to one loop) indicate an infinite range of nonlocality as more plausible, it is not yet clear whether this is a mere artifact of the perturbation theory or not. Therefore, a clear-cut conclusion about the existence of high-energy bounds in NC QFT cannot be drawn, unless the question of the scale of nonlocality is elucidated. In perturbative terms, this is equivalent to the standing problem of UV/IR mixing. However, for compact noncommutative spaces, where the range of nonlocality is finite and the NC QFT models do not exhibit UV divergences, we trust that an analog of the Froissart-Martin bound holds.

Note added: Recently, the validity of the Froissart-Martin bound in NC QFT has been studied based on the AdS/CFT correspondence.[37] The original idea appeared in Ref. 38, where the AdS/CFT correspondence was used to infer the Froissart-Martin bound in high-energy QCD scattering. According to Ref. 37, the Froissart-Martin bound holds as well in NC QFT. This might appear to contradict the results of the present paper. However, in Ref. 37 the Froissart-Martin bound was derived in a specific scalar field model, perturbatively and essentially by using an IR cutoff brane. It turns out that in the considered toy model the Froissart-Martin bound is saturated in both the commutative and noncommutative directions; however, the size of the cross section is smaller in the commutative directions than in the noncommutative ones, with a ratio which depends only on the noncommutative parameter and the IR cutoff. This strongly suggests that the IR cutoff actually acts as a restriction on the range of nonlocality to a finite region in the noncommutative plane.

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Higher-dimensional knotlike topological defects in local non-Abelian topological tensor currents

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We present the novel topological tensor currents to describe the infinitesimal thin higher-dimensional topological defects in the local $SO(n)$ gauge theory. The topological quantization of defects and the inner structure of the currents are obtained. As the generalization of Nielsen-Olesen local $U(1)$ field theory for Nambu string, the local $SO(n)$ gauge-invariant Lagrangian and the motion equation of the higher-dimensional topological defects are derived. Moreover, for closed defects, we study their important topological configuration, i.e., the higher-dimensional knotlike structures. Using the topological tensor currents and their preimages, we construct a series of metric independent integrals and prove their gauge independence. Similar to the helicity integral characterizing one-dimensional knotlike vortex filament, these topological invariants are evaluated to the generalized linking numbers of higher-dimensional knotlike defects. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Topological defects play an important role in many areas of physics. Generally speaking, in condensed matter systems they determine such phenomena as response to external stresses,[1,2] the nature of phase transitions,[3,4] or the approach to equilibrium after a quench into an ordered phase.[5] In particle physics, defects, sometimes called as solitons, act as either stable or long-lived elementary particles.[6,7] In quantum field theory, their existence means that the full nonperturbative theory may have a much richer structure than is apparent in perturbation theory.[8,9] As evidence of cosmological phase transitions in the early universe, topological defects remain somewhere in our universe, and can help to resolve the origin of large-scale structure formation and the anisotropies of the cosmic microwave background, as well as in various high-energy phenomena.[10–13] Various defects can be classified by their topological property and independent of concrete physical models. A systematic topological theory of defects has been extensively summarized by Mermin,[14] Anderson,[15] and Vilenkin.[11] Roughly speaking, topological defects represent regions in space–time where the order parameter (order parameter in condensed matter physics or Higgs field in particle physics) is frustrated. It cannot relax into the vacuum state by topological obstructions. The order parameter space may be identical with coset space G/H if the system has undergone a symmetry breaking $G \to H$. Correspondingly, the homotopy groups of coset space detect and classify the topological defects that can arise in this theory. A more detailed inner structure of defects and their evolution and correlation, which play a special role in certain cosmological[13] and phase ordering

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problems,[5] needs to study the topological density of defects. This has been carried out by Halperin[16] and exploited by Liu and Mazenko[17] in the case of point defects. Duan *et al.* have obtained the complete expression of the topological current of point defects (its time component is the density)[18] and generalized the case to line defects,[19] then to arbitrary dimensional defects.[20] The corresponding generalized topological tensor currents are defined in terms of direction field of the n-component order parameter $n^a=\phi^a/|\phi|(a=1,\ldots,n)$

$$J_0 = *\,(c_0\epsilon_{a_1a_2\cdots a_n}dn^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n}), \tag{1}$$

where * denote the Hodge star on $D+1$-dimensional (dim) Euclidean space–time R^{D+1} and c_0 is the normalized coefficient. These currents J_0 are natural conversed $*d*J_0=0$, whose Hodge star carry integer topological charges

$$\int_{R^{D+1}} *J_0 = \text{winding number } W,$$

where the coefficient c_0 is normalized as $1/[A(S^{n-1})(n-1)!]$ up to the sign **. Using ϕ-mapping theory,[21] the inner structure of topological currents can be demonstrated

$$J_0^{\mu_1\cdots\mu_{D+1-n}}(x)=\sum_{i=1}^{l}\beta_i\eta_i\int_{N_i}\delta^{D+1}(x-z_i(u))dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_{D+1-n}}, W=\sum_{i=1}^{l}\beta_i\eta_i, \tag{2}$$

where the Hopf index β_i and Brower degree η_i of zero points of order parameter ϕ^a characterize the topological charges of l $D-n$-dim defects which localized on their $D+1-n$-dim world volume N_i. The topological evolution of defects involving generating, annihilating, colliding, splitting, and merging can be described explicitly.[20] Obviously, these topological currents provide a unified framework for various defects in 3+1-dim space–time and the higher-dim extended objects, e.g., p–branes[22,23] which originate from M–theory[24,25] and the brane worlds[26–28] which have been the focus of a lot of attention recently, which may actually just represent topological defects in a higher-dimensional space.[29–34]

However, the topological currents made of order parameter ϕ have not obvious local gauge symmetry. This is a deficiency in this framework which seems to exclude the extensive local defects. Moreover, for the closed defects with dimension $\geqslant 1$, their nontrivial geometric configuration, namely, the (one-dim) knot and higher-dim knotlike structures should be demonstrated in a sound framework. Especially, the knotlike structure recently has attracted intense interest in disparate fields[35–38] since Faddev and Niemi[39] in a realistic 3+1-dim model found the knotlike structure appears as stable, finite energy solitons.

In this paper, we will present novel topological tensor currents with local SO(n) gauge symmetry in arbitrary $D+1$ dimensional Euclidean space–time. The desired local defects in these currents are explored as the higher-dim generalization of classical Abrikosov–Nielsen-Olesen (ANO) vortex[40,41] or instantons[42] for even-n case and of the 't Hooft–Polyakov magnetic monopole[43] for odd-n case. The quantized topological charges of these currents can be obtained under corresponding lower energy boundary conditions. For the topological defects with infinitesimal core size, these boundary conditions are naively extended to whole space except the locations of the defects. We hence obtain an essential result that the local topological currents act as above global topological currents. In other words, the local topological currents may actually describe the infinitesimal thin higher-dimensional local defects in terms of the inner structure of the global topological currents. As the generalization of Nielson-Olesien local $U(1)$ field theory[44] for Nambu string,[45] the local $SO(n)$ fields theory for higher-dimensional infinitesimal thin defects are also obtained. Moreover, using the local topological currents and their preimages, we construct a series of metric independent integrals and prove their gauge independence. Similar to the helicity integral characterizing one-dimensional knotlike vortex filament,[46] these topological invariants are

evaluated to the generalized linking numbers of higher-dimensional knotlike, infinitesimal thin defects. Thus, we perfect the unified framework for higher-dim topological defects in the context of topological currents.

II. TOPOLOGICAL TENSOR CURRENTS OF LOCAL HIGHER-DIM DEFECTS

In this paper, the desired local defects are restricted in $SO(n)$ gauge theory. We select this group because it is enough to accommodate various defects and it makes the framework compact and simple. Also, due to the latter reason, we express the $SO(n)$ group and Higgs fields configuration in the notation of Clifford algebra valued differential form.[47] Consider an $SO(n)$ group, and define connection $\omega=\frac{1}{2}\omega_{\mu}^{ab}I_{ab}dx^{\mu}$, where $I_{ab}=\frac{1}{4}[\gamma_a,\gamma_b]$ is the generator of $SO(n)$ group, γ_a $(a=1,\ldots,n)$ and $\gamma=\gamma_1\gamma_2\cdots\gamma_n$ are the bases of Clifford algebra satisfied $\gamma_a\gamma_b+\gamma_b\gamma_a=2\delta_{ab}I$.[48] The curvature $F=d\omega-\omega\wedge\omega$. The n vector multiplet Higgs field $\phi=\phi^a\gamma_a$ with covariant derivative $D\phi=d\phi-[\omega,\phi]$.

On $D+1$-dim Euclidean space–time R^{D+1} we present two kinds of topological tensor currents with local $SO(n)$ gauge symmetry for even-$n=2r$ and odd-$n=2r+1$ cases, respectively,

$$J=\begin{cases} *a\ \mathrm{Tr}(\gamma F^r)=\ *a\ \mathrm{Tr}(\gamma F\wedge F\cdots\wedge F) & \text{for } n=2r \\ *b\ \mathrm{Tr}(\gamma D\phi F^r)=\ *b\ \mathrm{Tr}(\gamma D\phi F\wedge F\cdots\wedge F) & \text{for } n=2r+1, \end{cases}$$

where a,b are the normalized coefficients which will be given later. These currents J are natural conversed $*d*J=0$, i.e., $*J$ are the closed differential forms due to their invariant symmetries and the Bianchi identity $DF=0$. The topological charges of currents are defined as the integrals of the Hodge star of currents on a subspace R^n of total space–time R^{D+1},

$$Q=\int_{R^n} *J. \tag{3}$$

In $3+1$-dim space-time, they are proportional to the topological charges of ANO vortex for $n=2$ and 't Hooft–Polyakov magnetic monopole for $n=3$, respectively. The similar topological charge of general n cases has been discussed by Tchrakian[49] for generalized monopole on $n+1$-dim space-time $(D-n=0)$ and instantons on n-dim space-time $(D-n=-1)$. But we focus on imbedding the topological charge, exactly, the $*J$ to higher-dim $D+1$-dim space-time $(D-n>0)$. In other words, we explore the desired local defects as the higher-dim generalization (i.e., the extended objects, string, membrane, 3-brane,…) of classical ANO vortex for even-n case and of the 't Hooft–Polyakov magnetic monopole for odd-n case. It is well known that the finite energy conditions for these two classical defects need a converged field configuration at space infinity,[41,43] which may be generalized to higher-dim space R^D (Ref. 50)

$$F\to 0,\ \text{i.e.},\ \omega\to\text{pure gauge}; \tag{4}$$

$$D\phi\to 0,\quad \text{and}\quad |\phi|\to\text{vacuum value}. \tag{5}$$

Under these finite energy conditions, we can quantize topological charges of the topological tensor currents.

For even-$n=2r$ case we have

$$
\begin{aligned}
Q = a\int_{R^n} \mathrm{Tr}(\gamma F^r) &= ar\int_{R^n} d\int_0^1 dt\ \mathrm{Tr}(\gamma\omega F_t^{r-1}) \\
&= ar\int_{\partial R^n = S^{n-1}} \int_0^1 dt\ \mathrm{Tr}(\gamma\omega F_t^{r-1}) \\
&= \sum_{k=0}^{r-1}\left[(-1)^{r-k}\binom{r-1}{k}\frac{ar}{r+k}\right]\int_{S^{n-1}} \mathrm{Tr}[\gamma n(dn)^{n-1}] \\
&= \int_{S^{n-1}} \frac{1}{A(S^{n-1})(n-1)!}\epsilon_{a_1 a_2,\ldots,a_n} n^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n} = W. \qquad (6)
\end{aligned}
$$

In the above first equation, sign ** has been absorbed in normalized coefficient a; in the second equation, the Chern-Weil homomorphism[51] is used as $\omega_t = t\omega, F_t = td\omega - t^2\omega^2$; in the third equation, the Stokes theorem is used and the boundary of R^n at infinity is compact as $n-1$-dim sphere; in the fourth equation, we use the boundary condition (4) and set the pure gauge as dnn without losing the generalization, where unit vector n is well defined as the direction of Higgs field ϕ at infinity if the singularity of n, i.e., zero of ϕ has been localized inside the sphere. Noticing the trace formula about even-dim Clifford base $\mathrm{Tr}(\gamma\gamma_{a_1}\gamma_{a_2,\ldots,}\gamma_{a_n}) = \epsilon_{a_1 a_2\cdots a_n}(-1)^{n/2}2^{n/2}$, the normalized coefficient can be obtained in the fifth equation $a = 1/[A(S^{n-1})(n-1)!]/\Sigma_{k=0}^{r-1}\left[(-1)^k\binom{r-1}{k}\right][(r2^r)/(r+k)]$; the last equation is just the definition of winding number W.

For odd-$n = 2r+1$ case we have

$$
\begin{aligned}
Q = b\int_{R^n} \mathrm{Tr}(\gamma D\phi F^r) &= b\int_{R^n} d\ \mathrm{Tr}(\gamma\phi F^r) \\
&= b\int_{\partial R^n = S^{n-1}} \mathrm{Tr}(\gamma\phi F^r) \\
&= b(-4)^{-r}|\phi|_{\mathrm{vacuum}}\int_{S^{n-1}} \mathrm{Tr}[\gamma n(dn)^{n-1}] \\
&= \int_{S^{n-1}} \frac{1}{A(S^{n-1})(n-1)!}\epsilon_{a_1 a_2,\ldots,a_n} n^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n} = W. \qquad (7)
\end{aligned}
$$

The first, third, and last equations have similar derivation of the even-dim case. In the second equation, the invariant symmetries $\mathrm{Tr}(\gamma[\omega, n]F^r) + r\ \mathrm{Tr}(\gamma n[\omega, F]F^{r-1}) = 0$[51] and Bianchi identity $DF = 0$ have been used; in the fourth equation, we use the boundary condition (5), which may solve the connection as $\frac{1}{2}dnn$ without losing the generalization and replace the Higgs field as $\phi = |\phi|_{\mathrm{vacuum}} n$ at infinity. The unit vector n is well defined as even-dim cases. By another trace formula about odd-dim Clifford base $\mathrm{Tr}(\gamma\gamma_{a_1}\gamma_{a_2},\ldots,\gamma_{a_n}) = \epsilon_{a_1 a_2,\ldots,a_n}(-1)^{(n-1)/2}2^{(n-1)/2}$, the normalized coefficient can be obtained $b = 1/[A(S^{n-1})(n-1)!]/2^{-r}|\phi|_{\mathrm{vacuum}}$.

Hereto, the topological charges of tensor currents have been topologically quantized as $Q = W$. In $n = 2$ and 3, the topological charges degenerate as quantized magnetic flux of ANO vortex and quantized magnetic charge of 't Hooft–Polyakov magnetic monopole, respectively.

In the following, we progress to explore the inner structure of topological tensor currents and expect that they indeed describe the desired higher-dim defects. It is known that the framework for higher-dim defects in terms of topological tensor currents must be independent of concrete dynamic models, so we need to find the defects only involving topological information. It sounds difficult but in fact Nielsen and Olesen have pointed out[41] that the Ginzburg-Landau Lagrangian may only leave the δ-function-like vortex contribution if the vortex core is infinitesimally thin. And, this kind of vortex may be described by a Nielsen-Olesen Lagrangian[44] as the Nambu string which only carries the topological information of the world sheet of free string.[45] This argument

does not even rely on the detail of the Ginzburg-Landau Lagrangian. Here, we will generalize this idea to higher-dim defects. We notice an important result that the infinitesimal thin defects indeed mean that the boundary conditions (4) and (5) should be naively extended to whole space except for the location of defects.[52] Thus, without solving the concrete dynamic soliton solution, we still can discuss the behavior of topological currents. One can find F, $D\phi$, then both currents J are nonzero only on the location of infinitesimal thin defects. Since the extended boundary conditions are well defined except on the singularity of n, the infinitesimal thin defects should be localized on the zero points of Higgs fields ϕ for consistency. Moreover, observing the formulas (3), (6), and (7)

$$Q=\int_{R^n} {}^*J=\int_{S^{n-1}} \frac{1}{A(S^{n-1})(n-1)!}\epsilon_{a_1a_2,\ldots,a_n}n^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n},$$

and using the Stokes theorem, we have

$$\int_{R^n} {}^*J=\int_{R^n} \frac{1}{A(S^{n-1})(n-1)!}\epsilon_{a_1a_2,\ldots,a_n}dn^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n}=\int_{R^n} {}^*J_0,$$

where J_0 are just the global currents (1). Using the known ϕ-mapping theory,[21] we can prove the ${}^*J_0$ have the following structure:

$$\frac{1}{A(S^{n-1})(n-1)!}\epsilon_{a_1a_2,\ldots,a_n}dn^{a_1}\wedge dn^{a_2}\wedge\cdots\wedge dn^{a_n}=\delta(\vec{\phi})J\left(\frac{\phi}{x}\right), \tag{8}$$

where $J(\phi/x)$ is the Jacobian determinant $J(\phi/x)=1/n!\,\epsilon_{a_1,\ldots,a_n}\epsilon^{\mu_1\mu_2,\ldots,\mu_n}\partial_{\mu_1}\phi^{a_1}\cdots\partial_{\mu_n}\phi^{a_n}$. One can find that J_0 is nonzero only when $\vec{\phi}=0$, which is identical to the behavior of local currents J under extended boundary conditions. Hereto, we obtain an important result under extended boundary conditions

$$J=J_0.$$

This means the local currents J have the identical inner structure (2)

$$J^{\mu_1\cdots\mu_{D+1-n}}(x)=\sum_{i=1}^{l}\beta_i\eta_i\int_{N_i}\delta^{D+1}(x-z_i(u))dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_{D+1-n}}. \tag{9}$$

From this expression, we conclude that the constructed topological tensor currents J with local gauge symmetry may actually describe the l infinitesimal thin $D-n$-dim defects spanning the $D+1-n$-dim world volume N_i, which carry the quantized topological charges $\beta_i\eta_i$. It is one of the essential results of this paper. Moreover, as the generalization of Nielsen-Olesen $U(1)$ local field theory for Nambu string, we construct local $SO(n)$ gauge-invariant Lagrangian in $D+1$-dim Euclidean space–time,

$$L=\frac{1}{(D+1-n)!}\sqrt{J^{\mu_1\cdots\mu_{D+1-n}}J_{\mu_1\cdots\mu_{D+1-n}}}.$$

Substituting the inner structure of J (9) into the action of L, we obtain

$$S=\int_{R^{D+1}}Ld^{D+1}x=\sum_{i=1}^{l}\beta_i\eta_i\int_{N_i}\sqrt{g_u}d^{(D+1-n)}u=\sum_{i=1}^{l}\beta_i\eta_iS_i,$$

where S_i is the area of singular world volume N_i. This action is just the generalized Nambu action for multi $D-n$-dim local defects, which is the straightforward generalization of Nambu action for the string of $D-n=1$. From the principle of least action, we obtain the evolution equation of these higher-dim topological defects,

$$\frac{1}{\sqrt{g_u}}\frac{\partial}{\partial u^A}\left(\sqrt{g_u}g^{AB}\frac{\partial x^\mu}{\partial u^B}\right)=0,$$

where $A,B=1,\ldots,D+1-n$, $\mu=1,\ldots,D+1$ and g_u is the determinant of induced metric g^{AB} of world volume N_i. As a matter of fact, this is just the equation of harmonic map.[53]

III. HIGHER-DIM KNOTLIKE LOCAL DEFECTS

The knotlike structures should be characterized by knot or link invariants. At the classical level, a knot is characterized by helicity[46] or Hopf invariants.[54,55] The generalization of helicity based on the so-called Novikov invariants[56] recently have been proposed.[57] But they maintain Abelian gauge symmetry and describe the linking of the higher-dim knots with only codimension two. There are no non-Abelian higher-dim link invariants, at least to our knowledge. At the quantum level, the knot invariants include the linking number and its generalization have been rigorously considered in the known topological quantum field theory[58] as the vacuum expectation values of constructed Wilson line or surface operators. There are various methods[59–61] to evaluate the quantum operators. The simplest[59] is to compute their Gaussian integral directly, where an integral expression of the generalized linking number of p-dim knot N^p and $D-p-1$-dim knot N^{D-p-1} in D-dim spacelike manifold X is obtained,

$$Lk(N^p,N^{D-p-1})=\int_X d^{-1}j_{p+1}\wedge j_{D-p}, \tag{10}$$

where $j_{n=p+1,D-p}$ are the n-rank closed differential-form deRham currents satisfying

$$\int_X f_{D-n}(x)\wedge j_n(x)=\int_{N^{D-n}} f_{D-n}(y)$$

for any $D-n$-form f on the $D-n$-dim closed submanifold N^{D-n} of X.

Based on this expression of the generalized linking number, in this section we will construct the classical-level non-Abelian higher-dim link invariants to describe the infinitesimal thin local higher-dim knotlike defects in the topological tensor currents.

Observing the time component of topological currents in R^{D+1} space–time, one can easily find their Hodge star in D-dim space R^D

$$*J=*J_0=\left[\sum_{i=1}^{l}\beta_i\eta_i\int_{N_i}\delta^D(x-z_i(u))d^Dx\right],$$

where N_i represent infinitesimal thin $D-n$-dim defects (not world volume hereafter). If these defects N_i are *closed*, this Hodge star is just proportional to the deRham current, which can be formulated as

$$*J=\sum_{i=1}^{l}\beta_i\eta_i j_{D-n,i}, \tag{11}$$

where $j_{D-n,i}$ represents the ith $D-n$-rank deRham current in R^D. We have known that $*J$ have well-defined preimages on flat space R^D up to coefficients

$$(d^{-1} * J_n) = \begin{cases} \int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{r-1}) & \text{for } n = 2r \\ \mathrm{Tr}(\gamma\phi F^r) & \text{for } n = 2r+1, \end{cases} \tag{12}$$

where the subscript n on J denotes the rank of differential form $*J$. Using two kinds of $*J$ and their two kinds of preimages, we may construct the following four kinds of metric-independent integrals in a D-dim space R^D:

$$H = c\int_{R^D} (d^{-1} * J_{p+1}) \wedge * J_{D-p}, \tag{13}$$

where c are the normalized coefficients. Obviously, when $p+1$ is odd, these integrals H have local non-Abelian product gauge symmetry $SO(p+1)\times SO(D-p)$. Below, we will discuss the cases of even $p+1$. Consider the infinitesimal gauge transformation $\delta_v\omega = Dv$, $\delta_v F = [v, F]$. We know that $*J_{p+1}$ is gauge invariant and use its preimage (12)

$$\delta_v(*J_{p+1}) = \delta_v\left[d\int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{(p+1)/2-1}) \right] = d\,\delta_v\left[\int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{(p+1)/2-1}) \right] = 0.$$

According to Poincare's lemma,[51] the last equation implies $\delta_v[\int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{(p+1)/2-1})]$ can be written as an exact form on flat R^D

$$\delta_v\left[\int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{(p+1)/2-1}) \right] = dA.$$

We do not need to know the explicit expression of A, which can be determined similar to the well-known work of Zumino *et al.* for generalized chiral anomaly.[62] Now, we consider the infinitesimal gauge transformation of the integral for the even $p+1$ cases (13)

$$\delta_v H = c\int_{R^D} \delta_v\left[\int_0^1 dt\, \mathrm{Tr}(\gamma\omega F_t^{(p+1)/2-1}) \right] \wedge * J_{D-p} = c\int_{R^D} dA \wedge * J_{D-p} = c\int_{\partial R^D = S^{D-1}} A \wedge * J_{D-p} = 0,$$

where the third equation has used Stokes theorem and the last equation has used the boundary conditions (4) and (5). Hereto we have proved the gauge independence of the metric independent integrals, namely, which also have local non-Abelian product gauge symmetry $SO(p+1)\times SO(D-p)$. Thus, we indeed obtain four kinds of classical local non-Abelian topological invariants. Furthermore, substitute the relation between the topological currents and deRham currents (11) into the topological invariants (13) with respect to the integral expression of the generalized linking number (10), then we have

$$\begin{aligned} H = c\int_{R^D} (d^{-1} * J_{p+1}) \wedge * J_{D-p} &= \sum_{i=1}^{l} \beta_i\eta_i \sum_{j=1}^{k} \beta_j\eta_j \int_{R^D} (d^{-1} j_{p+1,i}) \wedge j_{D-p,j} \\ &= \sum_{i=1}^{l} \beta_i\eta_i \sum_{j=1}^{k} \beta_j\eta_j Lk(N_i^p, N_j^{D-p-1}). \end{aligned}$$

The topological invariants are evaluated as generalized linking numbers of l p-dim knots N_i^p and k $D-p-1$-dim knots N_j^{D-p-1} with quantized topological charges $\beta_i\eta_i$ and $\beta_j\eta_j$. In a given D-dim space, one can find that four kinds of topological invariants exactly describe the four types of generalized linking numbers of two odd-dim knots; two even-dim knots; one odd p-dim knot and one even $D-p-1$-dim knot; and one even p-dim knot and one odd $D-p-1$-dim knot. Correspondingly, the normalized coefficients are $-1, 1, 1, -1$, respectively. Especially, when $D=3$, the topological invariant degenerates as the helicity integral $H=\int_{R^3} A\wedge F$, which normally characterizes the linking number of one-dim knotlike vortex filament.[46]

IV. CONCLUSION

This paper describes a unified framework for higher-dim knotlike and local topological defects in terms of topological currents. We propose the novel topological tensor currents with local SO(n) gauge symmetry in arbitrary-dim Euclidean space–time. These topological currents have quantized topological charges and may actually describe the infinitesimal thin multi-higher-dim defects. As the generalization of Nielsen-Olesen local $U(1)$ field theory for Nambu string, the local $SO(n)$ gauge-invariant Lagrangian and the motion equation of the higher-dim topological defects are derived. In the theory of extra dimensions,[63] it is best to think of the brane world as the topological defect of almost-zero width, so we suggest that our theory for $D-N=4$ case can be applied to describe its topological structure. Moreover, we construct the classical-level non-Abelian higher-dim link invariants to characterize the higher-dim knotlike infinitesimal thin defects in the topological currents. This theory can be treated as the higher-dim generalization of well-known helicity theory.

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D-brane charges in Gepner models

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We construct Gepner models in terms of coset conformal field theories and compute their twisted equivariant K-theories. These classify the *D*-brane charges on the associated geometric backgrounds and therefore agree with the topological K-theories. We show this agreement for various cases, in particular, the Fermat quintic.
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I. INTRODUCTION

It is by now firmly established[1,2] that the K-theory groups of space-time are the *D*-brane charge groups. More precisely, the claim is that the isomorphism classes of *D*-brane boundary states modulo boundary renormalization group (RG) flow are in one to one correspondence[3] with suitable K-theory classes of the string theory background in question. For geometrical backgrounds such as Calabi-Yau manifolds, one can construct a variety of *D*-branes by applying methods from boundary CFT, matrix factorizations, and geometry.[4–11] However, determining the endpoint of the RG flow[12] is unfortunately not easy.

Most well understood in this context are purely geometrical backgrounds of string theory, such as tori, orbifolds, and Calabi-Yau manifolds. In these instances, the K-theories were either already available in the mathematics literature or are easily computed by standard techniques and the complementary string theory computation of D-brane charges is relatively straightforward.

Less trivial is the situation of string theory backgrounds with nontrivial NSNS three-form flux H, where it is believed that twisted K-theory is the correct structure to classify D-brane charges.[2,13,14] Explicit checks of this claim have so far been restricted to backgrounds with large symmetries, namely supersymmetric WZW and coset conformal field theories (CFT)s.[15–26] The computation of twisted K-theories for compact Lie groups and coset models thereof were greatly simplified by the theorem of Freed, Hopkins, and Teleman.[27–29]

Our objective in this paper is to test the twisted K-theory proposal beyond standard CFT backgrounds by extending it to Gepner models. These are essentially orbifolds of tensor products of $\mathcal{N}=2$ minimal models, realized for our purposes in terms of $SU(2)/U(1)$ supersymmetric coset models. They are known to describe certain tori and Calabi-Yau spaces at particular points in their moduli space. Because the K-groups are a topological quantity, the *D*-brane charge group should be independent of the moduli. Therefore the twisted equivariant K-theory of the Gepner models has to agree with the topological K-theory of the corresponding Calabi-Yau manifold. This provides a non-trivial check of the brane charge classification.

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Technically, we are going to make use of the twisted equivariant Chern character. Consequently, we are going to compute the complexified K-groups,

$$K^*(X;\mathbb{C}) := K^*(X)\otimes_{\mathbb{Z}}\mathbb{C} \tag{1}$$

only. The downside is that one looses interesting torsion[30–32] information, since

$$K^*(X) = \mathbb{Z}^r \oplus \mathbb{Z}_{n_1} \oplus \cdots \oplus \mathbb{Z}_{n_k} \Rightarrow K^*(X;\mathbb{C}) = \mathbb{C}^r. \tag{2}$$

However, since none of the Calabi-Yau threefolds with Gepner points actually have torsion in their K group, we do not expect to find any in the Gepner models either.

During the final stage of this work, we received a preprint[11] that constructs a basis of *D*-branes for the *D*-brane charge group. We will discuss a few details of their approach in Sec. VI.

II. THE QUINTIC

As an hors d'œuvre to our work, let us discuss[4,33] the $(k=3)^5$ Gepner model. It is known to correspond to the Fermat quintic

$$Q = \left\{ [x_0{:}x_1{:}x_2{:}x_3{:}x_4] \,\middle|\, \sum_{i=0}^{4} x_i^5 = 0 \,\right\} \subset \mathbb{P}^4 \Bigg\}. \tag{3}$$

The Hodge diamond of the quintic is by now quite familiar to all string theorists, and reads

$$h^{pq}(Q) = \begin{array}{ccccccccc} & & & & 1 & & & & \\ & & & 0 & & 0 & & & \\ & & 0 & & 1 & & 0 & & \\ & 1 & & 101 & & 101 & & 1 & \\ & & 0 & & 1 & & 0 & & \\ & & & 0 & & 0 & & & \\ & & & & 1 & & & & \end{array} . \tag{4}$$

We also know that there is no torsion in its cohomology, which then determines its K-theory to be

$$K^0(Q) = H^{\text{even}}(Q;\mathbb{C}) = \mathbb{Z}^4 \Rightarrow K^0(Q;\mathbb{C}) = \mathbb{C}^4,$$

$$K^1(Q) = H^{\text{odd}}(Q;\mathbb{Z}) = \mathbb{Z}^{204} \Rightarrow K^1(Q;\mathbb{C}) = \mathbb{C}^{204}. \tag{5}$$

We are going to arrive at the same answer for the complexified K-groups directly from the Gepner model, without making any reference to the quintic hypersurface.

The Gepner model corresponding to the quintic is a $\mathbb{Z}_5$ orbifold of 5 copies of the level $k=3$ minimal model; see Secs. III B and III F for more details. Moreover, the minimal model can be realized as an $\mathfrak{su}(2)_k/\mathfrak{u}(1)$ coset CFT. The coset CFT has a nice sigma model interpretation; it is an $SU(2)$ WZW model with a gauged $U(1)$ action. More precisely, the $U(1)$ acts as

$$U(1)\times SU(2) \to SU(2), \quad \left[e^{i\theta}, \begin{pmatrix} a & b \\ c & d \end{pmatrix} \right] \mapsto \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}^{-1} . \tag{6}$$

[The cognoscente of course realize that our choice of maximal torus $U(1)\subset SU(2)$ is random. Since all maximal tori are conjugate, we just picked this one for explicitness.] Also see Fig. 1 for a picture of the orbits. The fixed point set of the $U(1)$ action is a circle inside $SU(2)\simeq S^3$, which we denote by

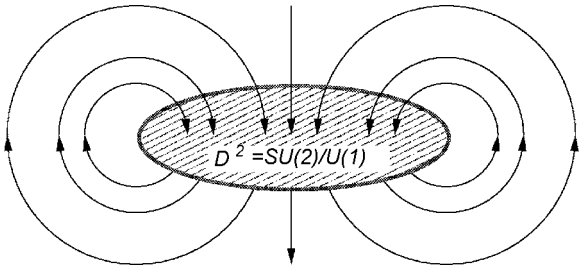

FIG. 1. $U(1)$ action on $SU(2)$.

$$S_A^1 \overset{\text{def}}{=} [SU(2)]^{U(1)} = \left\{ \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \middle| \varphi \in [0, \ldots, 2\pi) \right\}. \tag{7}$$

(For any space X with action of a group G, we write X^G for the G-fixed points. If $g \in G$, then we write X^g for the points fixed by the subgroup $\langle g \rangle \subset G$.) The space of orbits $SU(2)/U(1)$ is a disk, bounded by the fixed points S_A^1. Rotating this disk is another symmetry of the geometry, but arbitrary rotations are not a symmetry of the theory. The reason is that the H field is not symmetric under arbitrary rotations of the disk. Rather, the rotation group is broken to rotations by $2\pi/5$. This $\mathbb{Z}_5$ group action lifts to an action on the $SU(2)$ with fixed point set S_B^1; see Fig. 2. The fixed point sets S_A^1 and S_B^1 form a Hopf link inside $SU(2) \simeq S^3$.

By now it is firmly established that the charge group is given by the K-theory of space-time. More precisely, one has to pick the right "flavor" of K-theory depending on which $\mathcal{N}=1$ supersymmetric theory one formulates on the background.[19,22,26,34] For the coset model, the background is $SU(2)$ with an H flux. The latter implies that the correct K-theory is the so-called twisted K-theory, which we denote by ${}^tK$. Moreover, we want to gauge a $U(1)$ symmetry. As is familiar to all string theorists, this does *not* mean that we work on the set theoretic quotient $SU(2)/U(1)$. Instead, we have to correctly incorporate the twisted sectors, which on the level of cohomology means that we have to compute the $U(1)$ equivariant cohomology groups. Therefore, the correct K-theory for the minimal model is

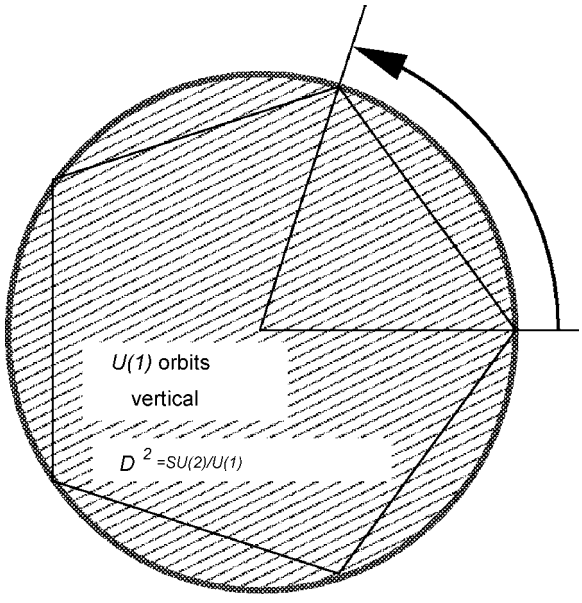

FIG. 2. $\mathbb{Z}_5$ action on $SU(2)$.

$$D\text{-brane charges in } \mathfrak{su}(2)_k/\mathrm{u}(1) \text{ coset} = {}^tK_{U(1)}(SU(2)), \tag{8}$$

with the twist class

$$t = k+2 \in \mathbb{Z} = H^3_{U(1)}(SU(2);\mathbb{Z}). \tag{9}$$

Hence, the D-brane charges in the tensor product of five minimal models are

$${}^tK_{U(1)\times U(1)\times U(1)\times U(1)\times U(1)}(SU(2)\times SU(2)\times SU(2)\times SU(2)\times SU(2)), \tag{10}$$

where each $U(1)$ acts on just one of the $SU(2)$ factors. Finally, the Gepner model is the $\mathbb{Z}_5$ orbifold by the diagonal $\mathbb{Z}_5$ action. Therefore

$$D\text{-brane charges in the } (k=3)^5 \text{ Gepner model} = {}^tK_{U(1)^5\times\mathbb{Z}_5}(SU(2)^5) \tag{11}$$

To compute these K-groups, we are using a twisted version of the equivariant Chern isomorphism,

$$\mathrm{ch}: K^{0,1}_G(X;\mathbb{C}) \xrightarrow{\sim} \bigoplus_{g\in G} H^{\mathrm{even,odd}}_G(X^g;\mathbb{C}). \tag{12}$$

(In this paper, we are only concerned with Abelian groups G. In general the sum is over conjugacy classes.) Adding an additional twist to the equivariant Chern character has two consequences. First, one is lead to twisted cohomology, which is roughly the cohomology of $d+[H]$ instead of d on differential forms. Second, the cohomology is with local coefficients, that is, with coefficients in a flat line bundle ${}^t\mathcal{L}$ instead of the trivial flat line bundle $\mathbb{C}$. The ensuing twisted equivariant Chern character (see Sec. III C)

$$\mathrm{ch}: {}^tK^*_G(X;\mathbb{C}) \to \bigoplus_{g\in G} {}^tH^*_G(X^g;{}^t\mathcal{L}(g)) \tag{13}$$

is an isomorphism, provided that only finitely many summands on the right are nonvanishing. This turns out to be the case here, and

$$\begin{aligned} {}^tK^*_{U(1)^5\times\mathbb{Z}_5}(SU(2)^5;\mathbb{C}) &\simeq \bigoplus_{g\in U(1)^5\times\mathbb{Z}_5} {}^tH^*_{U(1)^5\times\mathbb{Z}_5}([SU(2)^5]^g;{}^t\mathcal{L}(g)) \\ &= \bigoplus_{g\in U(1)^5\times\mathbb{Z}_5} [{}^tH^*_{U(1)^5}([SU(2)^5]^g;{}^t\mathcal{L}(g))]^{\mathbb{Z}_5} \end{aligned} \tag{14}$$

is indeed an isomorphism. More specifically, as we are going to show in Sec. III C the only contributions are from the 4^5+4 group elements

$$g = (\omega^{m_1},\omega^{m_2},\omega^{m_3},\omega^{m_4},\omega^{m_5},1), \quad m_i \in \{1,\ldots,4\}, \tag{15a}$$

$$g = (1,1,1,1,1,n), \quad n \in \{1,\ldots,4\}, \tag{15b}$$

in $U(1)^5\times\mathbb{Z}_5$, where we write $\omega \overset{\text{def}}{=} \exp(2\pi i/5)$. The corresponding fixed point sets are of the form

$$g = (\omega^{m_1},\omega^{m_2},\omega^{m_3},\omega^{m_4},\omega^{m_5},1) \Rightarrow [SU(2)^5]^g = (S^1_A)^5, \tag{16a}$$

$$g = (1,1,1,1,1,n) \Rightarrow [SU(2)^5]g = (S^1_B)^5. \tag{16b}$$

As we are going to discuss in more detail in the next section, the twisted equivariant cohomology for a single factor ${}^tH_{U(1)}(SU(2)^g;{}^t\mathcal{L}(g))$ for $g\in U(1)\times\mathbb{Z}_5$ is

$$g = (\omega^m,1) \Rightarrow {}^tH^0_{U(1)}(S^1_A;{}^t\mathcal{L}(g)) = 0, \quad {}^tH^1_{U(1)}(S^1_A;{}^t\mathcal{L}(g)) = \omega^m, \tag{17a}$$

$$g=(1,n)\Rightarrow {}^tH^0_{U(1)}(S^1_B;{}^t\mathcal{L}(g))=1,\quad {}^tH^1_{U(1)}(S^1_B;{}^t\mathcal{L}(g))=0, \tag{17b}$$

where we write the cohomology groups as $\mathbb{Z}_5$ characters. [By abuse of notation, we denote the generator for the character ring again ω. In other words, $m\in\mathbb{Z}_5=\{0,\ldots,4\}$ acts by multiplication with $\omega^m=\exp(2\pi im/5)$.] The cohomology groups for the tensor product of 5 such factors is readily determined from the Künneth formula, and one obtains

$$\bigoplus_{g=(\omega^{m_1},\ldots,\omega^{m_5},1)} {}^tH^*_{U(1)^5}((S^1_A)^5;{}^t\mathcal{L}(g))=\begin{cases}0, & *=0;\\ (\omega+\omega^2+\omega^3+\omega^4)^5, & *=5\equiv 1 \bmod 2;\end{cases} \tag{18a}$$

$$\bigoplus_{g=(1,\ldots,1,\omega^n)} {}^tH^*_{U(1)^5}((S^1_B)^5;{}^t\mathcal{L}(g))=\begin{cases}4, & *=0;\\ 0, & *=1.\end{cases} \tag{18b}$$

It is now easy to determine the $\mathbb{Z}_5$-invariant part. Using the twisted equivariant Chern character, Eq. (14), we obtain

$${}^tK^*_{U(1)^5\times\mathbb{Z}_5}(SU(2)^5;\mathbb{C})=\begin{cases}\mathbb{C}^4, & *=0;\\ [(\omega+\omega^2+\omega^3+\omega^4)^5]^{\mathbb{Z}_5}=\mathbb{C}^{204}, & *=1\end{cases} \tag{19}$$

which precisely equals the K-theory of the quintic hypersurface. (Perhaps not surprisingly, formally the same computation arises when one tries[35] to construct Gepner models using matrix factorizations. However, the authors of Ref. 35 fail to address the twisted sector branes that arise when the Gepner model contains minimal models of different levels.)

III. K-theory OF GEPNER MODELS

A. Group theory

As we saw in the quintic example discussed in Sec. II, one has to determine cohomology groups that form representations under a discrete group G_{GSO} ($=\mathbb{Z}_5$ for the quintic) that implements the GSO (After Gliozzi, Scherk, and Olive[36]) projection. Now we could always work with polynomials of characters as in Eq. (19), but this becomes cumbersome if one has to deal with tensor products of different minimal models.

For cyclic groups $\mathbb{Z}_\kappa$, the following representations will appear again and again. (In this paper, we are only going to consider complex representations.)

- The trivial representation $\mathbb{C}$.
- The regular representation $R\mathbb{Z}_\kappa$, which is defined as follows: Take the vector space $\mathbb{C}^\kappa$. The group acts by cyclically permuting the κ basis vectors. The regular representation can be diagonalized to the sum of all one-dimensional representations. Explicitly, if $\chi:\mathbb{Z}_\kappa\to\mathbb{C}$, $\chi(1)=\exp(2\pi i/\kappa)$ is the generating character, then

$$R\mathbb{Z}_\kappa=\bigoplus_{i=0}^{\kappa-1}\chi^i. \tag{20}$$

- The representation $\widetilde{R\mathbb{Z}_\kappa}$, which is the regular representation without its trivial subrepresentation,

$$\widetilde{R\mathbb{Z}_\kappa}=\bigoplus_{i=1}^{\kappa-1}\chi^i. \tag{21}$$

More formally, it is the cokernel

$$0 \to \mathbb{C} \to R\mathbb{Z}_\kappa \to \widetilde{R\mathbb{Z}}_\kappa \to 0. \tag{22}$$

Moreover, since we are actually computing cohomology groups, everything has a cohomological $\mathbb{Z}_2$ grade. By definition, we assign

$$\deg(\mathbb{C}) = 0, \tag{23a}$$

$$\deg(R\mathbb{Z}_\kappa) = \deg(\widetilde{R\mathbb{Z}}_\kappa) = 1. \tag{23b}$$

Of course, we have the usual operations of restriction and induction (transfer) to relate G_{GSO} representations and representations of subgroups of G_{GSO}. However, G_{GSO} is always a cyclic group and we have yet another operation that will occur frequently. This works as follows. Given any subgroup $\mathbb{Z}_\kappa \subset G_{\mathrm{GSO}}$, we have in addition to the inclusion i also a projection π,

$$\mathbb{Z}_\kappa \underset{\pi:\, n \mapsto n \bmod \kappa}{\overset{i:\, n \mapsto \frac{|G_{\mathrm{GSO}}|}{\kappa} n}{\rightleftarrows}} G_{\mathrm{GSO}} \simeq \mathbb{Z}_{|G_{\mathrm{GSO}}|} \tag{24}$$

by modding out by κ. Given a representation $\rho: \mathbb{Z}_\kappa \to \mathbb{C}^n$, we can then define a representation $p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_\kappa}(\rho)$ of G_{GSO} on the same vector space $\mathbb{C}^n$ by composing

$$p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_\kappa}(\rho) \overset{\mathrm{def}}{=} \rho \circ \pi : G_{\mathrm{GSO}} \to \mathbb{C}^n, (n,v) \mapsto \rho(n \bmod \kappa, v). \tag{25}$$

Now, in general, the projection π depends on which generators you chose for G_{GSO}, a random choice. However, for the identity, the regular, and the reduced regular representation of $\mathbb{Z}_\kappa$ the resulting G_{GSO} representation does *not* depend on that choice. We are only going to use the $p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_\kappa}$ operation in these cases.

For example, consider the group $\mathbb{Z}_{12} = \{0, 1, \ldots, 11\}$ with the character $\chi(1) = e^{2\pi i/12}$. Then the representation

$$p^{\mathbb{Z}_{12}}_{\mathbb{Z}_3}(\widetilde{R\mathbb{Z}_3}) \otimes_{\mathbb{C}} p^{\mathbb{Z}_{12}}_{\mathbb{Z}_4}(\widetilde{R\mathbb{Z}_4}) = (\chi^4 + \chi^8)(\chi^3 + \chi^6 + \chi^9) = \chi + \chi^2 + \chi^5 + \chi^7 + \chi^{10} + \chi^{11}, \tag{26}$$

is the six-dimensional representation of $\mathbb{Z}_{12}$ of cohomology degree $2 \equiv 0 \bmod 2$ generated by

$$\mathrm{diag}(e^{2\pi i/12}, e^{4\pi i/12}, e^{10\pi i/12}, e^{14\pi i/12}, e^{20\pi i/12}, e^{22\pi i/12}). \tag{27}$$

In the future, we are just going to write $\otimes$, and it will be understood that we are tensoring over $\mathbb{C}$.

B. Minimal model as coset

The minimal models for the $\mathcal{N}=2$ superconformal algebra have equivalent realizations in terms of super-GKO coset models,

$$\frac{\mathfrak{su}(2)_k \oplus \mathfrak{u}(1)_2}{\mathfrak{u}(1)_{k+2}}, \tag{28}$$

as well as Landau-Ginzburg models. The modular invariant partition functions fall into an ADE classification.[37–39] From the coset CFT point of view these are obtained from the ADE modular invariants of the $\mathfrak{su}(2)_k$ WZW model. We shall focus on the A series minimal models. There are various subtleties concerning that modular invariant corresponds to the A-type superpotential, and it will turn out that there are essentially four distinct models that will be of interest. The fields of the coset CFT are labeled by (j,n,s), where $j = 0, \ldots, k/2$ is the $\mathfrak{su}(2)_k$ highest weight, $n \in \mathbb{Z}_{2(k+2)}$ labels the representations of the denominator $\mathfrak{u}(1)_{k+2}$ and $s \in \mathbb{Z}_4$ labels the free fermion representations in $\mathfrak{u}(1)_2$. There is a $\mathbb{Z}_{k+2} \times \mathbb{Z}_2$ discrete group acting on the fields in the following fashion:

$$\alpha:\Phi_{(j,n,s)} \mapsto (-1)^{2n/k+2}\Phi_{(j,n,s)},$$

$$\beta:\Phi_{(j,n,s)} \mapsto (-1)^{s}\Phi_{(j,n,s)}. \tag{29}$$

The $\mathbb{Z}_{k+2}$ action is realized geometrically in the gauged WZW model by the rotation of the disk target space. Orbifolding the A-type theory with respect to these symmetries yields new modular invariants, as was first observed in Ref. 15. Note that a related issue arose in the context of WZW models for nonsimply laced groups in Ref. 22, where nontrivial automorphisms acting on the fermions gave rise to new modular invariants for the supersymmetric WZW models.

Since $s=1,3$ corresponds to the Ramond sector, the orbifold by $\mathbb{Z}_2=\langle\beta\rangle$ is from a space-time point of view the same as modding out $(-1)^F$. The state space of the (charge conjugate) diagonal modular invariant is

$$\mathcal{H}_{MM_k} = \bigoplus_{(j,n,s)} \mathcal{H}_{(j,n,s)} \otimes \overline{\mathcal{H}}_{(j,n,s)}, \tag{30}$$

where the direct sum is over the standard range of super-parafermion representations, including the selection and identification rules

$$(j,n,s) \equiv (k/2-j,n+k+2,s+2), \quad 2j+n+s \in 2\mathbb{Z}. \tag{31}$$

The state space of the $\mathbb{Z}_2$ orbifold is then obtained as

$$\mathcal{H}_{MM_k/\mathbb{Z}_2} = \bigoplus_{(j,n,s)} \mathcal{H}_{(j,n,s)} \otimes \overline{\mathcal{H}}_{(j,n,-s)}. \tag{32}$$

Orbifolding MM_k by $\mathbb{Z}_{k+2}\times\mathbb{Z}_2$, it was observed in Ref. 15 that the partition function is the same as in MM_k, and that this model is, in fact, dual to MM_k. Likewise, $MM_k/\mathbb{Z}_{k+2}$ is T-dual to $MM_k/\mathbb{Z}_2$.

Gepner models are orbifolds of tensor products of minimal models with not necessarily equal level, which give rise to consistent GSO-projected string theory backgrounds. Consider a tensor product of r minimal models, of level $(k_1,\ldots,k_r)$, and define

$$\lambda = (j_1,\ldots,j_r), \quad \mu = (n_1,\ldots,n_r;s_1\ldots,s_r), \tag{33}$$

and $\beta_j=(0,\ldots,0,2,0,\ldots,0)$, with the nonzero entry at slot s_j and $\beta_0=(1,\ldots,1)$. Further define $K=lcm(2,k_j+2)$. Then the partition function for the Gepner model is given by

$$Z_{(k_1,\ldots,k_r)} = \sum_{\lambda,\mu}\sum_{b_0=0}^{2K-1}\sum_{b_j=0,1}\delta_\beta(-1)^{b_0}\chi_{\lambda,\mu}\overline{\chi}_{\lambda,\mu+b_0\beta_0+\Sigma b_j\beta_j}. \tag{34}$$

The characters of the tensor product of the minimal models are denoted by χ. In principle, one can define the conserved *D*-brane charges using RG flow,[3,40] but in practice this is not feasible.

C. Chern character of the minimal model

Now that we have defined all the ingredients, we can start to compute the relevant *K*-groups. Our main tool is going to be the twisted equivariant Chern character.[28,41] For explicitness, let us consider a single minimal model whose complexified *D*-brane charge group is

$${}^{\kappa}K_{U(1)}(SU(2))\otimes_{\mathbb{Z}}\mathbb{C} \overset{\text{def}}{=} {}^{\kappa}K_{U(1)}(SU(2);\mathbb{C}), \tag{35}$$

where $\kappa=k+2$ is going to be the twist class for the remainder of this section. [That is, the twist class is κ times the generator of $H^3_{U(1)}(SU(2);\mathbb{Z})$.] Now, given a twisted equivariant vector bundle, we can tensor it with any group representation, and get another equivariant vector bundle with the same twist. In other words, there is an action of $K_{U(1)}(\{\text{pt.}\};\mathbb{C})=RU(1)=\mathbb{C}[z,z^{-1}]$ on the twisted equivariant K-theory.

In geometrical terms, $\mathbb{C}[z,z^{-1}]$ is the ring of functions on $\mathbb{C}^\times \overset{\text{def}}{=} \mathbb{C}\backslash\{0\}$. And the twisted equivariant K-theory ${}^\kappa K_{U(1)}(SU(2);\mathbb{C})$ is a module over this function algebra, that is a sheaf over the base space $\mathbb{C}^\times$. The twisted equivariant Chern character identifies the stalks (fibers) of this sheaf over a point in $\mathbb{C}^\times$ with a certain cohomology group. More precisely, Freed-Hopkins-Teleman[28] identify the stalk over $\zeta \in \mathbb{C}^\times$ with

$$ {}^\kappa K^*_{U(1)}(SU(2);\mathbb{C})\big|_\zeta \simeq {}^\kappa H^*_{U(1)}(SU(2)^\zeta; {}^\kappa\mathcal{L}(\zeta)), \tag{36}$$

where ${}^\kappa\mathcal{L}(\zeta)$ is a certain flat line bundle. Note that when we say that ζ acts on $SU(2)$, we really mean that $\zeta/|\zeta| \in U(1)$ acts on $SU(2)$.

In general, the knowledge of the stalks is not enough to reconstruct the sheaf, for example, every fiber of a line bundle is just isomorphic to $\mathbb{C}$. However, in the case of a single minimal model, the sheaf turns out to be a skyscraper sheaf, and can indeed be reconstructed.

D. Twisted equivariant cohomology of the minimal model

In this section, we are going to determine the twisted equivariant cohomology groups that appear in the Chern character formula, Eq. (36). We advise the reader who is not interested in all the details to note the result, Eqs. (45a) and (45b), and then proceed with the next section.

In fact, the problem is very similar to ${}^\kappa K_{SU(2)}(SU(2);\mathbb{C})$ that is explicitly worked out as an example in Ref. 28. Depending on ζ, there are two different fixed point sets. One possibility is $\zeta \in \mathbb{R}_{>0}$, which acts trivially on the whole $SU(2)$. It turns out[28] that the line bundle ${}^\kappa\mathcal{L}(\zeta)$ is trivial in that case. Therefore, the *untwisted* equivariant cohomology is

$$ H^*_{U(1)}(SU(2)^\zeta; {}^\kappa\mathcal{L}(\zeta)) = H^*_{U(1)}(SU(2);\mathbb{C}) = \mathbb{C}[u,t]/u^2, \tag{37}$$

where we used the Leray spectral sequence

$$ H^p(BU(1); H^q(SU(2);\mathbb{C})) \Rightarrow H^{p+q}_{U(1)}(SU(2);\mathbb{C}) \tag{38}$$

with $t \in H^2(BU(1);\mathbb{C})$ of degree 2 and $u \in H^3(SU(2);\mathbb{C})$ of degree 3. To determine the twisted equivariant cohomology ${}^\kappa H^*_{U(1)}(SU(2);\mathbb{C})$ from the untwisted one, we have to mode out by the additional differential $d_3 = \kappa u$. (More formally, we are using the untwisted to twisted cohomology spectral sequence. Note that $(d_3)^2 \sim u^2 = 0$ in $\mathbb{C}[u,t]/u^2$.) An easy computation shows that

$$ {}^\kappa H^*_{U(1)}(SU(2)^\zeta; {}^\kappa\mathcal{L}(\zeta)) = {}^\kappa H^*_{U(1)}(SU(2);\mathbb{C}) = \frac{\ker(d_3)}{\mathrm{img}(d_3)} = 0. \tag{39}$$

This settles the case where the whole $SU(2)$ is fixed under the ζ action. The other possibility is the generic case where $SU(2)^\zeta = S^1_A$. In that case, the flat line bundle ${}^\kappa\mathcal{L}(\zeta)$ over S^1_A has[28] holonomy ζ^κ, so all cohomology groups vanish unless $\zeta^\kappa = 1$. In that case, that is over the $\kappa - 1$ points,

$$ \zeta_m \overset{\text{def}}{=} e^{2\pi i m/\kappa}, \quad m = 1, \ldots, \kappa - 1, \tag{40}$$

the untwisted cohomology is

$$ H^*_{U(1)}(S^1_A; {}^\kappa\mathcal{L}(\zeta_m)) = H^*(BU(1);\mathbb{C}) \otimes H^*(S^1_A; {}^\kappa\mathcal{L}(\zeta_m)) = \mathbb{C}[t] \otimes \mathbb{C}[v]/v^2 = \mathbb{C}[v,t]/v^2, \tag{41}$$

where $\deg(v) = 1$ and $\deg(t) = 2$. The twist class is in $H^3_{U(1)}(S^1_A; {}^\kappa\mathcal{L}(\zeta_m)) = \mathbb{C}\cdot tv$. Hence, if one normalizes the tv properly, then $d_3 = \kappa tv$. The d_3 cohomology is

$$ {}^{\kappa}H^{*}_{U(1)}(S^1_A;{}^{\kappa}\mathcal{L}(\zeta_m)) = \frac{\ker(d_3)}{\mathrm{img}(d_3)} = \mathbb{C}v = \begin{cases} \mathbb{C}, & *=1; \\ 0, & \text{otherwise}. \end{cases} \tag{42} $$

In addition to the $U(1)$ action on $SU(2)$, we can also act with $\mathbb{Z}_\kappa$. We find two more cases: the fixed point set can be either S^1_B or empty. The cohomology of the empty set, of course, vanishes. In the former case, note that $U(1)$ acts simply transitive on S^1_B, so the equivariant cohomology is just the cohomology of a point. To summarize, there are four different cases corresponding to different $g \in U(1)\times\mathbb{Z}_\kappa$. The twisted cohomology groups are (ignoring the $\mathbb{Z}_\kappa$ action on the cohomology and the precise degrees for now)

$$ g=(1,0) \Rightarrow {}^{\kappa}H^{*}_{U(1)}(SU(2)^g;{}^{\kappa}\mathcal{L}(g)) = {}^{\kappa}H^{*}_{U(1)}(SU(2);\mathbb{C}) = 0, \tag{43a} $$

$$ g=(\zeta,0) \Rightarrow {}^{\kappa}H^{*}_{U(1)}(SU(2)^g;{}^{\kappa}\mathcal{L}(g)) = {}^{\kappa}H^{*}_{U(1)}(S^1_A;{}^{\kappa}\mathcal{L}(g)) = \delta_{\zeta^\kappa,1}\mathbb{C}, \tag{43b} $$

$$ g=(1,n) \Rightarrow {}^{\kappa}H^{*}_{U(1)}(SU(2)^g;{}^{\kappa}\mathcal{L}(g)) = H^{*}_{U(1)}(S^1_B;\mathbb{C}) = H^{*}(\{\mathrm{pt}\,.\,\}) = \mathbb{C}, \tag{43c} $$

$$ g=(\zeta,n) \Rightarrow {}^{\kappa}H^{*}_{U(1)}(SU(2)^g;{}^{\kappa}\mathcal{L}(g)) = H^{*}_{U(1)}(\varnothing;\mathbb{C}) = 0, \tag{43d} $$

where we took $n \in \mathbb{Z}_\kappa\backslash\{0\}$ and $\zeta \in \mathbb{C}^\times\backslash\{1\}$.

All that remains is to determine the precise action of $\mathbb{Z}_\kappa$ on the cohomology group, Eq. (43b). For that, note that even though the line bundle ${}^{\kappa}\mathcal{L}(\zeta_m)$ in Eq. (41) is trivial, the trivializing section winds m times around the S^1_A relative to *the* trivial line bundle. Therefore rotating S^1_A by $2\pi/\kappa$ multiplies v with the phase $\exp(2\pi i m/\kappa)$. In terms of the character $\chi:\mathbb{Z}_\kappa\to U(1)$, $m\mapsto\exp(2\pi i m/\kappa)$, this means that

$$ \bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)}(SU(2)^\zeta;{}^{\kappa}\mathcal{L}(\zeta)) = \begin{Bmatrix} 0, & *=0 \\ \chi+\chi^2+\cdots+\chi^{\kappa-1}, & *=1 \end{Bmatrix} = \widetilde{R\mathbb{Z}}_\kappa, \tag{44} $$

as the $\mathbb{Z}_\kappa$ representation. In other words, we can write the twisted equivariant cohomology groups as

$$ n=0\in\mathbb{Z}_\kappa \Rightarrow \bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)}(SU(2)^{(\zeta,n)};{}^{\kappa}\mathcal{L}(\zeta,n)) = \widetilde{R\mathbb{Z}}_\kappa, \tag{45a} $$

$$ n\neq 0\in\mathbb{Z}_\kappa \Rightarrow \bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)}(SU(2)^{(\zeta,n)};{}^{\kappa}\mathcal{L}(\zeta,n)) = \mathbb{C}, \tag{45b} $$

using the conventions for cohomology degrees in Eqs. (23a), (23b).

E. Mirror symmetry for minimal models

As a quick application, let us compute the K-groups of the minimal model and its $\mathbb{Z}_\kappa$ orbifold. According to the twisted equivariant Chern character, the K-groups of the minimal model are

$$ {}^{\kappa}K^{*}_{U(1)}(SU(2);\mathbb{C}) = \bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)}(SU(2)^\zeta;{}^{\kappa}\mathcal{L}(\zeta)) = \widetilde{R\mathbb{Z}}_\kappa \simeq \begin{cases} 0, & *=0; \\ \mathbb{C}^{\kappa-1}, & *=1, \end{cases} \tag{46} $$

using the cohomology groups computed in Eq. (45a). We recover the known[19] *D*-brane charge groups for the coset minimal model.

Similarly, we can compute the *D*-brane charge group in the $\mathbb{Z}_\kappa$ orbifold, which is known to be the mirror of the minimal model. One obtains

$$\begin{aligned}
{}^{\kappa}K^{*}_{U(1)\times\mathbb{Z}_\kappa}\left(SU(2);\mathbb{C}\right) &= \bigoplus_{(\zeta,n)\in\mathbb{C}^\times\times\mathbb{Z}_\kappa} {}^{\kappa}H^{*}_{U(1)\times\mathbb{Z}_\kappa}\left(SU(2)^{(\zeta,n)};{}^{\kappa}\mathcal{L}(\zeta,n)\right)\\
&= \bigoplus_{n\in\mathbb{Z}_\kappa}\bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)\times\mathbb{Z}_\kappa}\left(SU(2)^{(\zeta,n)};{}^{\kappa}\mathcal{L}(\zeta,n)\right)\\
&= \bigoplus_{n\in\mathbb{Z}_\kappa}\left[\bigoplus_{\zeta\in\mathbb{C}^\times} {}^{\kappa}H^{*}_{U(1)}\left(SU(2)^{(\zeta,n)};{}^{\kappa}\mathcal{L}(\zeta,n)\right)\right]^{\mathbb{Z}_\kappa}\\
&= \left[\underbrace{\widetilde{R\mathbb{Z}}_\kappa}_{n=0}\oplus\underbrace{\mathbb{C}}_{n=1}\ominus\cdots\oplus\underbrace{\mathbb{C}}_{n=\kappa-1}\right]^{\mathbb{Z}_\kappa}\\
&= \mathbb{C}^{\kappa-1}\simeq\begin{cases}\mathbb{C}^{\kappa-1}, & *=0;\\ 0, & *=1.\end{cases}
\end{aligned}\tag{47}$$

Note that the $\mathbb{Z}_\kappa$ equivariant cohomology is simply the $\mathbb{Z}_\kappa$ invariant subspace of the cohomology group. For that, it is important to work with complex coefficients, because it would generate torsion contributions over the integers. Also note that the $\mathbb{Z}_\kappa$ equivariant K-theory is in general *not* the same as the $\mathbb{Z}_\kappa$ invariant K-groups.

To summarize, we observe that the $\mathbb{Z}_\kappa$ orbifold indeed exchanges $K^0\leftrightarrow K^1$, as we expect from the mirror involution. Furthermore, recall the distinction between *A*- and *B*-type branes.[15] The *A*-branes carry the charges in Eq. (45a), contributing to K^1 of the minimal model. On the other hand, the *B*-branes Eq. (45b), are only stable in the $\mathbb{Z}_\kappa$ orbifold of the minimal model where they contribute to K^0.

F. K-groups for Gepner models

Having tackled a single minimal model, we now proceed to Gepner models.[4,37–39] For that we take *d* copies of the $SU(2)$ with the action of *d* copies of $U(1)$ factor by factor. That is,

$$U(1)^d\times SU(2)^d\to SU(2)^d,\tag{48}$$

with a choice of twist

$$\overline{\kappa}=(\kappa_1,\kappa_2,\ldots,\kappa_d),\tag{49}$$

where $k_i=\kappa_i-2$ is the level in the CFT of the *i*th factor. The overall central charge is

$$c=\sum_{i=1}^{d}\frac{3k_i}{k_i+2}=\sum_{i=1}^{d}\frac{3(\kappa_i-2)}{\kappa_i}.\tag{50}$$

Whenever $c/3$ is integer, this could be the central charge of a geometric compactification of that dimension. However, a mere tensor product of minimal models is never geometric because of noninteger charges. In other words, it does not have space-times supersymmetry. The solution to this problem[37] is to orbifold by a certain discrete symmetry group G_{GSO}.

As we have seen, each of the minimal models has a discrete symmetry group $\mathbb{Z}_{\kappa_i}=\{0,1,\ldots,\kappa_i-1\}$. The GSO projection is the group generated by

$$(1,1,\ldots,1)\in\prod_{i=1}^{d}\mathbb{Z}_{\kappa_i}.\tag{51}$$

It follows that

$$G_{\mathrm{GSO}} = \mathbb{Z}_{\mathrm{lcm}(\kappa_1,\kappa_2,\ldots,\kappa_d)}. \tag{52}$$

According to the general dictionary between *D*-brane charge groups and K-theory group, the *D*-brane charges in the Gepner model are

$$\overline{{}^{\kappa}K}_{U(1)^d\times G_{\mathrm{GSO}}}(SU(2)^d). \tag{53}$$

We can again compute (the complexification) through the twisted equivariant Chern character. Once we translate the K-groups into cohomology, we can use the following:

- the G_{GSO} equivariant cohomology is the G_{GSO} invariant cohomology and
- the Künneth theorem for cohomology,

neither of which hold in general for twisted equivariant K-theory. Again, we have to complexify

$$U(1)^d \times G_{\mathrm{GSO}} \rightsquigarrow (\mathbb{C}^\times)^d \times G_{\mathrm{GSO}} \tag{54}$$

and think of the cohomology and K-groups as sheaves over this space. According to Sec. III D, the only potentially nonvanishing cohomology groups for the ith minimal model sit over the κ_ith roots of unity,

$$\mathcal{Z}_i \overset{\mathrm{def}}{=} \{e^{2\pi i m/\kappa_i} | m \in \mathbb{Z}_{\kappa_i} = \{0,\ldots,\kappa_i - 1\}\} \subset \mathbb{C}^\times, \tag{55}$$

therefore the only nonvanishing cohomology groups of the product are over the points

$$\mathcal{Z} \overset{\mathrm{def}}{=} \prod_{i=1}^{d} \mathcal{Z}_i = \{(e^{2\pi i m_1/\kappa_1},\ldots,e^{2\pi i m_d/\kappa_d} | m_i \in \mathbb{Z}_{\kappa_i}\} \subset (\mathbb{C}^\times)^d. \tag{56}$$

Using all that, we obtain

$$\begin{aligned}
\overline{{}^{\kappa}K}^{*}_{U(1)^d}(SU(2)^d;\mathbb{C}) &= \bigoplus_{g\in G_{\mathrm{GSO}}}\left[\bigoplus_{\overline{z}\in(\mathbb{C}^\times)^d} \overline{{}^{\kappa}H}^{*}_{U(1)^d}\left(\bigtimes_{i=1}^{d} SU(2)^{(z_i,g)}; \bigotimes_{i=1}^{d} {}^{\kappa_i}\mathcal{L}(z_i,g)\right)\right]^{G_{\mathrm{GSO}}} \\
&= \bigoplus_{g\in G_{\mathrm{GSO}}}\left[\bigoplus_{\overline{z}\in\mathcal{Z}} \overline{{}^{\kappa}H}^{*}_{U(1)^d}\left(\bigtimes_{i=1}^{d} SU(2)^{(z_i,g)}; \bigotimes_{i=1}^{d} {}^{\kappa_i}\mathcal{L}(z_i,g)\right)\right]^{G_{\mathrm{GSO}}} \\
&= \bigoplus_{g\in G_{\mathrm{GSO}}}\left[\bigotimes_{i=1}^{d}\left\{\bigoplus_{z_i\in\mathcal{Z}_i} {}^{\kappa_i}H^{*}_{U(1)}(SU(2)^{(z_i,g)}; {}^{\kappa_i}\mathcal{L}(z_i,g))\right\}\right]^{G_{\mathrm{GSO}}}.
\end{aligned} \tag{57}$$

Note that according to Eqs. (45a) and (45b),

$$\bigoplus_{z_i\in\mathcal{Z}_i} {}^{\kappa_i}H^{*}_{U(1)}(SU(2)^{(z_i,g)}; {}^{\kappa_i}\mathcal{L}(z_i,g)) = \begin{cases} \widetilde{R\mathbb{Z}}_{\kappa_i}, & g \equiv 0 \bmod \kappa_i \Leftrightarrow \kappa_i | g; \\ \mathbb{C}, & \kappa_i \nmid g. \end{cases} \tag{58}$$

Moreover, G_{GSO} obviously acts on $\widetilde{R\mathbb{Z}}_{\kappa_i}$ as $p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_{\kappa_i}}(\widetilde{R\mathbb{Z}}_{\kappa_i})$, see Eq. (25). Therefore, we can simplify Eq. (57) to

TABLE I. Elliptic curves with enhanced automorphism groups.

Complex structure	Symmetry	Gepner model	Hypersurface
$\tau=i$	$\mathbb{Z}_4$	$k=(0,2,2)$	$\{x_0^2+x_1^4+x_2^4=0\}\subset \mathbb{WP}_{2,1,1}$
$\tau=e^{2\pi i/3}$	$\mathbb{Z}_6$	$k=(1,1,1)$	$\{x_0^3+x_1^3+x_2^3=0\}\subset \mathbb{WP}_{1,1,1}$
$\tau=e^{2\pi i/3}$	$\mathbb{Z}_6$	$k=(0,1,4)$	$\{x_0^2+x_1^3+x_2^6=0\}\subset \mathbb{WP}_{3,2,1}$

$$ {}^{\bar{\kappa}}K^*_{U(1)^d}(SU(2)^d;\mathbb{C}) = \bigoplus_{g\in G_{\mathrm{GSO}}}\left[\bigotimes_{\kappa_i|g} p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_{\kappa_i}}(\widetilde{R\mathbb{Z}}_{\kappa_i})\right]^{G_{\mathrm{GSO}}}, \tag{59}$$

where we would like to remind the reader that $n|0$ for all n, that $\otimes_{i\in\emptyset}=\mathbb{C}$, and that we defined $\widetilde{R\mathbb{Z}}_{\kappa_i}$ to have cohomological degree 1.

IV. EXAMPLES

A. Toroidal theories

There are three Gepner models[42] that describe an elliptic curve. Two of them, $k=(1,1,1)$ and $k=(0,1,4)$, turn out to be the same CFT (for example, have identical partition functions). Hence, we obtain two different CFTs corresponding to the two orbifold singularities in the complex structure moduli space of the torus; see Table I. Recall that each elliptic curve $\mathbb{C}/(\mathbb{Z}\oplus\tau\mathbb{Z})$ has a $\mathbb{Z}_2$ symmetry, but at $\tau=i$ and $\tau=\exp(2\pi i/3)$ the symmetry is enhanced to $\mathbb{Z}_4$ and $\mathbb{Z}_6$, respectively. We easily compute using Eq. (59) that in all three cases,

$$ {}^{\bar{\kappa}}K^*_{U(1)^3\times G_{\mathrm{GSO}}}(SU(2)^3;\mathbb{C}) = \left\{\begin{matrix}\mathbb{C}^2, & *=0\\ \mathbb{C}^2, & *=1\end{matrix}\right\} = K^*(T^2;\mathbb{C}), \tag{60}$$

as expected, since we are dealing with a topological invariant of the torus. Note that the toroidal Gepner models always have three factors, even if that forces one of the levels to be zero. It is important to realize[43,44] that adding one factor with $c=0$ in the Gepner model does indeed have a physical effect. For example, we can easily compute the D-brane charges in the $k=(2,2)\Leftrightarrow\kappa=(4,4)$ model and obtain

$$ {}^{(4,4)}K^*_{U(1)^2\times G_{\mathrm{GSO}}}(SU(2)^2;\mathbb{C}) = \begin{cases}\mathbb{C}^6, & *=0;\\ 0, & *=1.\end{cases} \tag{61}$$

This is not the D-brane charge group of any geometric $c=3$ CFT. Note that the usual argument why $k=0$ factors do not matter is wrong: in the corresponding Landau-Ginzburg model, the $k=0$ factor corresponds to a field Φ that appears in the superpotential as

$$W_{\mathrm{LG}} = \cdots + \Phi^2. \tag{62}$$

Folklore says that one can integrate out Φ at no cost. But that is only true if one restricts to the closed string sector, if one considers D-branes and open strings,[43] then one must include a boundary action that will contain Φ as well.

B. Twisted sectors

Let us have a closer look at the formula for the K-groups of a Gepner model, Eq. (59). First, let us rewrite it as

$$ {}^{\bar{\kappa}}K^*_{U(1)^d}(SU(2)^d;\mathbb{C}) = \bigoplus_{g\in G_{\mathrm{GSO}}}(\mathcal{K}_g)^{G_{\mathrm{GSO}}}, \tag{63}$$

with

$$\mathcal{K}_g \overset{\text{def}}{=} \bigotimes_{\kappa_i | g} p_{\mathbb{Z}_{\kappa_i}}^{G_{\text{GSO}}}(\widetilde{R\mathbb{Z}}_{\kappa_i}). \tag{64}$$

Obviously, this has an interpretation of $\mathcal{K}_g^{G_{\text{GSO}}}$ being the contribution of the g-twisted sector in the G_{GSO} orbifold. Note that a single tensor factor $p_{\mathbb{Z}_{\kappa_i}}^{G_{\text{GSO}}}(\widetilde{R\mathbb{Z}}_{\kappa_i})$ does not have any G_{GSO}-invariant subspace, so the only way to obtain something invariant is to either have zero factors (which yields a *B*-type brane), or ≥ 2 factors. This is very familiar from the geometric interpretation as hypersurfaces in weighted projective spaces. If two or more weights $|G_{\text{GSO}}|/\kappa_i$ have a common factor, then the Calabi-Yau hypersurface inherits an orbifold singularity from the ambient space. The exceptional divisor from the resolution of the singularity increases the rank of the K-groups.

Specifically, in complex dimension ≥ 2 one can have genuine singularities that require resolutions and contribute twisted sector *D*-brane charges. To see that explicitly within the Gepner model context, let us consider the following two *K*3 Gepner models. First consider the $(k=2)^4$ Gepner model, corresponding to the Fermat quartic,

$$\{x_0^4 + x_1^4 + x_2^4 + x_3^4 = 0\} \subset \mathbb{P}^3. \tag{65}$$

In this case, the ambient space and the hypersurface are nonsingular. The contribution of the untwisted and the three g-twisted sectors is

$$\begin{array}{l|cccc} g \in G_{\text{GSO}} & 0 & 1 & 2 & 3 \\ \mathcal{K}_g & (\widetilde{R\mathbb{Z}}_4)^4 & \mathbb{C} & \mathbb{C} & \mathbb{C} \\ \dim_{\mathbb{C}} \mathcal{K}_g^{G_{\text{GSO}}} & 21 & 1 & 1 & 1 \\ \text{Type: Even/Odd} & O^4 & E^4 & E^4 & E^4 \end{array} \Rightarrow {}^{(4,4,4,4)}K^*_{U(1)^4}\left(SU(2)^4;\mathbb{C}\right) = \begin{cases} \mathbb{C}^{24}, & *=0; \\ 0, & *=1. \end{cases} \tag{66}$$

We can do the same for the $k=(1,2,2,4) \Leftrightarrow \kappa=(3,4,4,6)$ Gepner model. It corresponds to the singular *K*3 hypersurface,

$$X \overset{\text{def}}{=} \{x_0^3 + x_1^4 + x_2^4 + x_3^6 = 0\} \subset \mathbb{WP}_{4,3,3,2}. \tag{67}$$

The weighted projective space has a rational curve C_2 of $\mathbb{C}^2/\mathbb{Z}_2$ singularities and another rational curve C_3 of $\mathbb{C}^2/\mathbb{Z}_3$ singularities embedded as

$$C_2 \hookrightarrow \mathbb{WP}_{4,3,3,2}, \quad [s_0,s_1] \mapsto [s_0,0,0,s_1],$$

$$C_3 \hookrightarrow \mathbb{WP}_{4,3,3,2}, \quad [s_0,s_1] \mapsto [0,s_0,s_1,0]. \tag{68}$$

The surface inherits $4A_1$ and $6A_2$ orbifold singularities from

$$C_2 \cap X = 4, \quad C_3 \cap X = 6. \tag{69}$$

The resolution $\widetilde{X}$ is then a smooth *K*3 surface. This concludes the geometric point of view, now let us analyze the K-theory computation from the Gepner model side. Using Eq. (63), we find

$$\begin{array}{l|cccccccccccc} g \in G_{\text{GSO}} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 \\ \mathcal{K}_g & \widetilde{R\mathbb{Z}}_{3,4,4,6} & \mathbb{C} & \mathbb{C} & \widetilde{R\mathbb{Z}}_3 & \widetilde{R\mathbb{Z}}_{4,4} & \mathbb{C} & \widetilde{R\mathbb{Z}}_{3,6} & \mathbb{C} & \widetilde{R\mathbb{Z}}_{4,4} & \widetilde{R\mathbb{Z}}_3 & \mathbb{C} & \mathbb{C} \\ \dim_{\mathbb{C}} \mathcal{K}_g^{G_{\text{GSO}}} & 10 & 1 & 1 & 0 & 3 & 1 & 2 & 1 & 3 & 0 & 1 & 1 \\ \text{Type: Even/Odd} & O^4 & E^4 & E^4 & - & EO^2E & E^4 & OE^2O & E^4 & EO^2E & - & E^4 & E^4 \end{array} \tag{70}$$

where we abbreviated

$$\widetilde{R\mathbb{Z}}_{\kappa_1,\kappa_2,\ldots} \overset{\text{def}}{=} \bigotimes_{i=1,2,\ldots} p^{G_{\text{GSO}}}_{\mathbb{Z}_{\kappa_i}}(\widetilde{R\mathbb{Z}}_{\kappa_i}). \tag{71}$$

Of course, in the end we obtain again the K-groups of the $K3$ manifold. However, this times some of the charge groups involve mixtures of even- and odd-dimensional branes. In the same way one can analyze all $K3$ Gepner models; see Appendix A.

V. KNÖRRER PERIODICITY

If one adds two variables with a quadratic superpotential to the Landau-Ginzburg theory[45–47] with fields $\Phi=(\phi_1,\ldots)$,

$$W_{\text{LG}}(\Phi) \to \widehat{W}_{\text{LG}} = W_{\text{LG}}(\Phi) + x^2 + y^2, \tag{72}$$

then one obtains the same theory again. This is quite nontrivial, because adding a single variable with a quadratic superpotential certainly does yield an inequivalent theory as discussed in Sec. IV A.

The evidence for periodicity is that the topological B-branes, that is the category of matrix factorizations, are equivalent. This fact is known as Knörrer periodicity,[48]

$$\mathbf{MF}(\mathbb{C}[\Phi]/W_{\text{LG}}(\Phi)) \simeq \mathbf{MF}(\mathbb{C}[\Phi,x,y]/\widehat{W}_{\text{LG}}(\Phi,x,y)). \tag{73}$$

This periodicity manifests itself in our formula Eq. (59), as follows. Adding two factors with $k=0 \Leftrightarrow \kappa=2$ amounts to inserting

$$p^{G_{\text{GSO}}}_{\mathbb{Z}_2}(\widetilde{R\mathbb{Z}}_2) \otimes p^{G_{\text{GSO}}}_{\mathbb{Z}_2}(\widetilde{R\mathbb{Z}}_2) = \mathbb{C} \tag{74}$$

whenever $2|g$. But

$$(\cdots) \otimes \mathbb{C} = (\cdots) \tag{75}$$

is the identity, so we obtain again the same K-groups.

Note that the above argument is flawed since adding the $\kappa=2$ factors might change the G_{GSO} group Eq. (52). If the initial order $|G_{\text{GSO}}|$ was odd, that is,

$$\text{lcm}(\kappa_1,\ldots,\kappa_d) \in 2\mathbb{Z}+1, \tag{76}$$

then

$$\text{lcm}(\kappa_1,\ldots,\kappa_d,2,2) = 2\text{lcm}(\kappa_1,\ldots,\kappa_d). \tag{77}$$

Therefore, periodicity only holds if one had already an even κ_i. In general, Knörrer periodicity need not hold for the first time one adds two $k=0$ factors, but it always holds from the second time onward,

$${}^{(\kappa_1,\ldots,\kappa_d,2)}K_{U(1)^{d+1}\times G_{\text{GSO}}}(SU(2)^{d+1};\mathbb{C}) = {}^{(\kappa_1,\ldots,\kappa_d,2,2,2)}K_{U(1)^{d+3}\times G_{\text{GSO}}}(SU(2)^{d+3};\mathbb{C}). \tag{78}$$

This is somewhat reminiscent of stabilization in K-theory.

VI. GENERALIZED PERMUTATION BRANES

In this section, we are going to focus on the Calabi-Yau ($c=9$) Gepner models. It is clear from Sec. III E that all D-brane charges can be found as suitable combinations of the D-branes in the coset or its mirror ($\mathbb{Z}_\kappa$ orbifold). In particular, the usual tensor product and permutation branes give

TABLE II. Gepner models associated to $K3$.

$\overline{k}=(1,1,1,1,1,1)$,	$\overline{k}=(0,1,1,1,1,4)$,	$\overline{k}=(2,2,2,2)$,	$\overline{k}=(1,2,2,4)$
$\overline{k}=(1,1,4,4)$,	$\overline{k}=(1,1,2,10)$,	$\overline{k}=(0,4,4,4)$,	$\overline{k}=(0,3,3,8)$
$\overline{k}=(0,2,6,6)$,	$\overline{k}=(0,2,4,10)$,	$\overline{k}=(0,2,3,18)$,	$\overline{k}=(0,1,10,10)$
$\overline{k}=(0,1,8,13)$,	$\overline{k}=(0,1,7,16)$,	$\overline{k}=(0,1,6,22)$,	$\overline{k}=(0,1,5,40)$

all the *D*-brane charges in the untwisted sector, corresponding to $g=0$ in Eq. (59). Similarly, one obtains zero or one brane in the twisted ($g=1,\ldots,|G_{\mathrm{GSO}}|$) sectors. But the latter is not enough to fill out the *D*-brane charge lattice, in general, since sometimes there are two or more independent charges coming from a twisted sector. Of course, all that means is that the boundary state construction is incomplete. Using Landau-Ginzburg models and matrix factorizations one obtains[11,49] all brane charges.

Inspection of the formula for the K-groups, Eq. (59), shows that two or more brane charges can only come from a $g\in G_{\mathrm{GSO}}$ sector where some κ_i divides g. Moreover, if only a single κ_i divides g, then there is no contribution because

$$[p^{G_{\mathrm{GSO}}}_{\mathbb{Z}_{\kappa_i}}(\widetilde{R\mathbb{Z}}_{\kappa_i})]^{G_{\mathrm{GSO}}}=0 \tag{79}$$

has no invariant subspace. Hence, the interesting case is if two or more κ_i have a common factor. Following Ref. 11, let us consider the case where r of the shifted levels $\overline{\kappa}=(\kappa_1,\ldots)$ have the same divisor $d>2$. (If the common divisor $d=2$, then there is again only a one-dimensional contribution to the K group in the $g\in d\mathbb{Z}$ twisted sectors, which is not so interesting. Of course, our arguments hold in that case as well).

First, note that r odd contributes to K^1 only, as is evident from our degree convention, Eqs. (23a) and (23b). Not so surprisingly, if one[11] restricts oneself to K^0 then there are no *D*-brane charges for $r=1,3,5$. This leaves the cases $r=2$ and $r=4$. Looking at the list of Gepner models, $r=4$ can only occur if the Gepner model has more than five minimal model factors. There is nothing wrong with that, and our formula, Eq. (59), gives the correct answer for the K-groups. However, if one[11] were to restrict oneself to 5 minimal model factors, then $r=4$ cannot occur either.

VII. CONCLUSIONS

There is a very simple formula, Eq. (59), for the rank of the K-groups of Gepner models. The summands in the formula have a natural interpretation as the contributions from twisted sectors. We checked the computation in $c=3,6,9$ Gepner models and find agreement with the topology of the associated Calabi-Yau manifolds.

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APPENDIX A: K3 GEPNER MODELS

There are 16 Gepner models that are associated to $K3$ surfaces[50–52] listed in Table II. We checked that we obtain

$$\overline{\kappa}K^*_{U(1)^d\times G_{\mathrm{GSO}}}(SU(2)^d;\mathbb{C}) = \left\{\begin{matrix}\mathbb{C}^{24}, & *=0\\ 0, & *=1\end{matrix}\right\} = K^*(K3;\mathbb{C}) \tag{A1}$$

in all 16 cases. It is important that the right number of $k=0$ factors appears so that there are four minimal models altogether (exceptionally, six in the first two Gepner models).

In addition to the 16 known $K3$ Gepner models, we found that

$$^{(2,3,3,3,3,3,3)}K^*_{U(1)^7\times G_{\mathrm{GSO}}}(SU(2)^7;\mathbb{C}) = K^*(K3;\mathbb{C}), \tag{A2}$$

as well. Although it has not the conventional number of factors, this $\overline{k}=(0,1,1,1,1,1,1)$ Gepner model seems to yield yet another $K3$ CFT.

There is yet another combination of levels such that the total central charge $c=6$, which is $\overline{k}=(0,1,1,1,2,2)$. One can easily compute that

$$^{(2,3,3,3,4,4)}K^*_{U(1)^6\times G_{\mathrm{GSO}}}(SU(2)^6;\mathbb{C}) = \left\{\begin{matrix}\mathbb{C}^8, & *=0\\ \mathbb{C}^8, & *=1\end{matrix}\right\} = K^*(T^4;\mathbb{C}).$$

Clearly, this Gepner model describes a T^4 compactification with (accidentally) enhanced $\mathcal{N}=8$ space-time supersymmetry.

APPENDIX B: CALABI-YAU THREEFOLD GEPNER MODELS

First, note that a proper Calabi-Yau threefold X, that is a compact Kähler manifold of holonomy $SU(3)$ satisfies

$$\operatorname{rank} K^0(X) = 2h^{11}(X)+2, \quad \operatorname{rank} K^1(X) = 2h^{21}(X)+2. \tag{B1}$$

We can check this formula against the known list[53] of 168 Gepner models with central charge $c=9$, which are associated to Calabi-Yau threefolds. The list of all Gepner models is reproduced in Table III. If one uses these $N=(2,2)$ SCFTs as the compactification of the $E_8\times E_8$ heterotic string, then their low-energy spectrum consists of a number $n_{\overline{\mathbf{27}}}=h^{11}(X)$ of matter fields transforming in the $\overline{\mathbf{27}}$ and $n_{\overline{\mathbf{27}}}=h^{21}(X)$ of field in the $\mathbf{27}$ representation of E_6.

One can check that the formula, Eq. (B1), is obeyed for each Gepner model except for the seven cases with $n_{\overline{\mathbf{27}}}=n_{\mathbf{27}}=21$. The obvious explanation is that this misfit is associated $K3\times T^2$, which has Hodge numbers

$$h^{pq}(K3\times T^2) = \begin{array}{ccccccc} & & & 1 & & & \\ & & 1 & & 1 & & \\ & 1 & & 21 & & 1 & \\ 1 & & 21 & & 21 & & 1 \\ & 1 & & 21 & & 1 & \\ & & 1 & & 1 & & \\ & & & 1 & & & \end{array}. \tag{B2}$$

Since $K3\times T^2$ has only $SU(2)$ holonomy, that is, it is not a proper Calabi-Yau manifold, it does not have to obey Eq. (B1). Adding up the even and odd cohomology groups, we find that

$$K^0(K3\times T^2) = \mathbb{Z}^{48}, \quad K^1(K3\times T^2) = \mathbb{Z}^{48}. \tag{B3}$$

These topological K-groups are in precise agreement with what we computed using the coset, Eq. (59).

TABLE III. $c=9$ Gepner models.

$\overline{k}=(k_1,k_2,\ldots)$	n_{27}^{-}	n_{27}	$\mathrm{rk}K^1$	$\mathrm{rk}K^0$
(1, 1, 1, 1, 1, 1, 1, 1, 1)	0	84	2	170
(1, 1, 1, 1, 1, 1, 1, 4, 0)	0	84	2	170
(1, 1, 1, 1, 1, 1, 2, 2, 0)	21	21	48	48
(1, 1, 1, 1, 1, 2, 10),	2	62	6	126
(1, 1, 1, 1, 1, 4, 4)	1	73	4	148
(1, 1, 1, 1, 2, 2, 4)	11	35	24	72
(1, 1, 1, 2, 2, 2, 2)	21	21	48	48
(1, 1, 1, 1, 5, 40, 0)	23	47	48	96
(1, 1, 1, 1, 6, 22, 0)	16	52	34	106
(1, 1, 1, 1, 7, 16, 0)	8	68	18	138
(1, 1, 1, 1, 8, 13, 0)	17	41	36	84
(1, 1, 1, 1, 10, 10, 0)	7	79	16	160
(1, 1, 1, 2, 3, 18, 0)	21	21	48	48
(1, 1, 1, 2, 4, 10, 0)	2	62	6	126
(1, 1, 1, 2, 6, 6, 0)	21	21	48	48
(1, 1, 1, 3, 3, 8, 0)	21	21	48	48
(1, 1, 1, 4, 4, 4, 0)	0	84	2	170
(1, 1, 2, 2, 2, 10, 0)	10	46	22	94
(1, 1, 2, 2, 4, 4, 0)	3	51	8	104
(1, 2, 2, 2, 2, 4, 0)	1	61	4	124
(2, 2, 2, 2, 2, 2, 0)	0	90	2	182
(1, 1, 2, 11, 154)	71	71	144	144
(1, 1, 2, 12, 82)	40	76	82	154
(1, 1, 2, 13, 58)	26	86	54	174
(1, 1, 2, 14, 46)	26	86	54	174
(1, 1, 2, 16, 34)	16	100	34	202
(1, 1, 2, 18, 28)	31	55	64	112
(1, 1, 2, 19, 26)	41	41	84	84
(1, 1, 2, 22, 22)	11	131	24	264
(1, 1, 3, 6, 118)	55	55	112	112
(1, 1, 3, 7, 43)	19	67	40	136
(1, 1, 3, 8, 28)	19	69	40	140
(1, 1, 3, 10, 18)	31	31	64	64
(1, 1, 3, 13, 13)	7	103	16	208
(1, 1, 4, 5, 40)	17	65	36	132
(1, 1, 4, 6, 22)	10	70	22	142
(1, 1, 4, 7, 16)	7	79	16	160
(1, 1, 4, 8, 13)	12	48	26	98
(1, 1, 4, 10, 10)	5	101	12	204
(1, 1, 5, 5, 19)	17	65	36	132
(1, 1, 6, 6, 10)	19	43	40	88
(1, 1, 7, 7, 7)	4	112	10	226
(1, 2, 2, 5, 40)	35	35	72	72
(1, 2, 2, 6, 22)	8	68	18	138
(1, 2, 2, 7, 16)	19	43	40	88
(1, 2, 2, 8, 13)	27	27	56	56
(1, 2, 2, 10, 10)	5	89	12	180
(1, 2, 3, 3, 58)	23	47	48	96
(1, 2, 3, 4, 18)	15	39	32	80
(1, 2, 4, 4, 10)	2	74	6	150
(1, 2, 4, 6, 6)	7	55	16	112
(1, 3, 3, 3, 13)	3	75	8	152
(1, 3, 3, 4, 8)	15	39	32	80
(1, 4, 4, 4, 4)	1	103	4	208

TABLE III. (*Continued.*)

$\overline{k}=(k_1,k_2,\ldots)$	n_{27}^{-}	n_{27}	$\mathrm{rk}K^1$	$\mathrm{rk}K^0$
(2, 2, 2, 3, 18)	5	65	12	132
(2, 2, 2, 4, 10)	3	69	8	140
(2, 2, 2, 6, 6)	2	86	6	174
(2, 2, 3, 3, 8)	15	39	32	80
(2, 2, 4, 4, 4)	6	60	14	122
(3, 3, 3, 3, 3)	1	101	4	204
(0, 1, 5, 41, 1804)	251	251	504	504
(0, 1, 5, 42, 922)	137	257	276	516
(0, 1, 5, 43, 628)	95	263	192	528
(0, 1, 5, 44, 481)	143	143	288	288
(0, 1, 5, 46, 334)	47	287	96	576
(0, 1, 5, 47, 292)	47	287	96	576
(0, 1, 5, 49, 236)	107	107	216	216
(0, 1, 5, 52, 187)	53	173	108	348
(0, 1, 5, 54, 166)	23	335	48	672
(0, 1, 5, 58, 138)	59	131	120	264
(0, 1, 5, 61, 124)	17	377	36	756
(0, 1, 5, 68, 103)	29	221	60	444
(0, 1, 5, 76, 89)	83	83	168	168
(0, 1, 5, 82, 82)	11	491	24	984
(0, 1, 6, 23, 598)	119	167	240	336
(0, 1, 6, 24, 310)	66	174	134	350
(0, 1, 6, 25, 214)	48	180	98	362
(0, 1, 6, 26, 166)	34	190	70	382
(0, 1, 6, 28, 118)	24	204	50	410
(0, 1, 6, 30, 94)	18	222	38	446
(0, 1, 6, 31, 86)	57	81	116	164
(0, 1, 6, 34, 70)	14	242	30	486
(0, 1, 6, 38, 58)	23	143	48	288
(0, 1, 6, 40, 54)	33	105	68	212
(0, 1, 6, 46, 46)	9	321	20	644
(0, 1, 7, 17, 340)	71	143	144	288
(0, 1, 7, 18, 178)	42	150	86	302
(0, 1, 7, 19, 124)	28	160	58	322
(0, 1, 7, 20, 97)	45	93	92	188
(0, 1, 7, 22, 70)	15	183	32	368
(0, 1, 7, 25, 52)	10	214	22	430
(0, 1, 7, 28, 43)	18	126	38	254
(0, 1, 7, 34, 34)	7	271	16	544
(0, 1, 8, 14, 238)	50	134	102	270
(0, 1, 8, 16, 88)	17	155	36	312
(0, 1, 8, 18, 58)	10	178	22	358
(0, 1, 8, 22, 38)	22	82	46	166
(0, 1, 8, 28, 28)	5	251	12	504
(0, 1, 9, 12, 229)	79	79	160	160
(0, 1, 9, 13, 108)	59	59	120	120
(0, 1, 9, 20, 31)	9	129	20	260
(0, 1, 10, 11, 154)	23	143	48	288
(0, 1, 10, 12, 82)	15	147	32	296
(0, 1, 10, 13, 58)	11	155	24	312
(0, 1, 10, 14, 46)	8	164	18	330
(0, 1, 10, 16, 34)	5	185	12	372
(0, 1, 10, 18, 28)	10	106	22	214
(0, 1, 10, 19, 26)	16	76	34	154

TABLE III. (*Continued.*)

$\bar{k}=(k_1,k_2,\ldots)$	n_{27}^{-}	n_{27}	$\mathrm{rk}K^1$	$\mathrm{rk}K^0$
(0, 1, 10, 22, 22)	3	243	8	488
(0, 1, 11, 11, 76)	23	143	48	288
(0, 1, 12, 12, 40)	6	180	14	362
(0, 1, 12, 13, 33)	43	43	88	88
(0, 1, 12, 19, 19)	7	151	16	304
(0, 1, 13, 13, 28)	4	208	10	418
(0, 1, 13, 18, 18)	11	107	24	216
(0, 1, 14, 14, 22)	7	127	16	256
(0, 1, 16, 16, 16)	2	272	6	546
(0, 2, 3, 19, 418)	119	119	240	240
(0, 2, 3, 20, 218)	65	125	132	252
(0, 2, 3, 22, 118)	33	141	68	284
(0, 2, 3, 23, 98)	33	141	68	284
(0, 2, 3, 26, 68)	39	87	80	176
(0, 2, 3, 28, 58)	17	173	36	348
(0, 2, 3, 34, 43)	55	55	112	112
(0, 2, 3, 38, 38)	11	227	24	456
(0, 2, 4, 11, 154)	53	89	108	180
(0, 2, 4, 12, 82)	30	96	62	194
(0, 2, 4, 13, 58)	20	104	42	210
(0, 2, 4, 14, 46)	16	112	34	226
(0, 2, 4, 16, 34)	12	126	26	254
(0, 2, 4, 18, 28)	20	74	42	150
(0, 2, 4, 19, 26)	28	52	58	106
(0, 2, 4, 22, 22)	8	164	18	330
(0, 2, 5, 8, 138)	44	80	90	162
(0, 2, 5, 10, 40)	23	59	48	120
(0, 2, 5, 12, 26)	8	116	18	234
(0, 2, 6, 7, 70)	19	91	40	184
(0, 2, 6, 8, 38)	12	96	26	194
(0, 2, 6, 10, 22)	6	114	14	230
(0, 2, 6, 14, 14)	4	148	10	298
(0, 2, 7, 7, 34)	19	91	40	184
(0, 2, 7, 10, 16)	10	70	22	142
(0, 2, 8, 8, 18)	6	120	14	242
(0, 2, 8, 10, 13)	18	42	38	86
(0, 2, 10, 10, 10)	3	165	8	332
(0, 3, 3, 9, 108)	39	79	80	160
(0, 3, 3, 10, 58)	25	85	52	172
(0, 3, 3, 12, 33)	27	59	56	120
(0, 3, 3, 13, 28)	9	117	20	236
(0, 3, 3, 18, 18)	7	143	16	288
(0, 3, 4, 6, 118)	33	69	68	140
(0, 3, 4, 7, 43)	19	67	40	136
(0, 3, 4, 8, 28)	7	91	16	184
(0, 3, 4, 10, 18)	13	49	28	100
(0, 3, 4, 13, 13)	7	103	16	208
(0, 3, 5, 5, 68)	23	71	48	144
(0, 3, 6, 6, 18)	7	63	16	128
(0, 3, 8, 8, 8)	1	145	4	292
(0, 4, 4, 5, 40)	8	86	18	174
(0, 4, 4, 6, 22)	6	90	14	182
(0, 4, 4, 7, 16)	3	99	8	200
(0, 4, 4, 8, 13)	7	61	16	124

TABLE III. (*Continued.*)

$\overline{k}=(k_1,k_2,\ldots)$	n_{27}^{-}	n_{27}	$\mathrm{rk}K^1$	$\mathrm{rk}K^0$
(0, 4, 4, 10, 10)	2	128	6	258
(0, 4, 5, 5, 19)	17	65	36	132
(0, 4, 6, 6, 10)	6	66	14	134
(0, 4, 7, 7, 7)	4	112	10	226
(0, 5, 5, 5, 12)	2	122	6	246
(0, 6, 6, 6, 6)	1	149	4	300

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Electromagnetic and gravitational interactions of the spinning particle

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We consider the invariance of the spinning free particle Lagrangian under the global coordinate transformations for the classical model of the electron with internal degrees of freedom and obtain the conservation of the energy-momentum, total angular momentum, and electric charge. The local gauge transformations give the electromagnetic and gravitational interactions of the spinning particle in the Riemann-Cartan space from the generalized spin connections. We show that the covariant constancy of the Dirac matrices gives; (i) the form invariance of the classical equations of motion, except the gravitational force terms in nongeodesic equation, (ii) the conservation of the electromagnetic current, (iii) the quantum Hamiltonian and equations of motion from the classical ones without the quantum ordering corrections, and (iv) the minimal coupling of the gravitation with the spinning particle in the Hamiltonian and in wave equations in the Riemann-Cartan space–time. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2337847]

I. INTRODUCTION

Soon after Einstein proposed his gravitational theory, Weyl extended it to include electromagnetism and later revitalized his gauge idea, U(1) gauge invariance. In 1954, Yang and Mills generalized U(1) into SU(2). In 1956, Utiyama gauged the Lorentz group, SO(1,3),[1] and later Kibble extended it into Poincare group, **P**.[2]

In the field theory, the matter fields are the definite eigenstates of the mass, the electric (intrinsic) charge and the spin. In this connection, the minimal couplings of the matter field with the gravitation and the electromagnetism are discussed separately. The space–time symmetries are built by the requirement that the Lagrangian density for the free matter fields be invariant under the action of the corresponding symmetry group. Here, **P**, consisting of translations and the Lorentz rotations, is an important example. On the other hand, the inner symmetries require the invariance of the Lagrangian density for the matter fields under the action of some Lie group which is only represented in the space of fields and does not act on space–time. Here the example is the invariance under U(1) for electromagnetism.

In most of the gauge theories of gravitation, **P** is considered partly as a space–time symmetry group and partly as an inner symmetry group. They generate the translations and Lorentz rotations, and SO(1, 3) frame rotations of matter fields, respectively.[3–9] The global covariance of the matter field under the translation and rotation subgroups of **P** yields the conservation of the energy-momentum and the total angular momentum, respectively. In the local extension of the gauge group **P**, its space–time part becomes the diffeomorphism group, the gauged theory is invariant under the general coordinate transformations and the local SO(1, 3) frame rotations. In another approach, **P** is considered as the internal symmetry group of matter fields in Minkowski space–time to obtain a complementary gauge formulation of gravitation and to discuss the renormalization procedure.[10]

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From the matter fields, the Klein-Gordon equation is generalized into a curved space–time without SO(1, 3) frame rotations. However, the Dirac equation is generalized into the curved space–time by introducing the Fock-Ivananko two-vector or the spin connection as the contribution of SO(1, 3) frame rotations.[11] The Dirac algebra relates the metric tensor of the space–time to the anti-commutator of the space–time dependent Dirac matrices. In this generalization, the electromagnetic potential and spin connection appear together. In their pioneering investigations, Schrödinger[12] and Bargmann[13] discussed the generalization of the spin connection and showed that it gives the space–time curvature, the spin-2 gravitational field, and an Abelian spin-1 curvature. Since the spin-1 part of the connection is coupled to all spinors with the identical charge, this part is not identified with the electromagnetism. Recently, Crawford also discussed the generalization of the spin connection.[14] He investigated the coupling of the torsion with the spinning particle by evaluating the commutators of the covariant derivatives for the Dirac matrices, $[\nabla_\mu, \nabla_\nu]\gamma^\alpha$, and showed that it is possible only by relaxing the constraint about the covariant constancy of the Dirac matrices. He obtained the same conclusion for the spin-1 curvature as in Ref. 12.

Kibble and later Barducci *et al.* investigated the coupling of the spinning particle directly to the torsion[2,15] and obtained that there is no coupling between the spinning particle and the torsion. However, Hehl derived the equations of motion for a spinning object with independent velocity and momentum, and obtained the coupling of the spinning particle directly to the torsion.[16]

In the classical and quantum field theories, the scalar product is defined by the local **P** invariant determinant of the tetrads, $\det e^{-1}$, for the Riemann-Cartan space–time, but there is an ambiguity about the covariant constancy of $\det e^{-1}$ and the minimal coupling of the fields to the gravitation in the Riemann-Cartan space–time.[17] If $\det e^{-1}$ is not covariantly constant then, there is not the minimal coupling of the gravitation in the Lagrangian density.

The aim of this study is to derive the minimal coupling of the electromagnetism and the gravitation for the spinning particle in the Riemann-Cartan space–time by deriving a unified spin connection in a complementary approach. For this aim, our motivation is the spinning particle model presented as the classical model of the zitterbewegung.[18] In this model, the spinning particle does not correspond to definite mass, charge, and the spin eigenstates contrary to the field theories. The quantities, the mass and spin, are identified by using the conserved dynamical variables of the particle without discussing the corresponding global gauge transformations, but the electric charge is introduced manually into the interaction Lagrangian,[19] where the coupling of the gravitation and electromagnetism are discussed separately in the Riemann space–time without any discussion on the generalization of the spin connection.

In the spinning particle model, the phase space of the particle consists of two sets of coordinates and momenta: The space–time coordinates and the complex, four internal coordinates and conjugate external and internal momenta, respectively. In usual approaches, the gauge transformations are performed in fields, which have infinite degrees of freedom. In this approach, the space–time and internal Lorentz transformations of the fields are considered together and the electromagnetic phase transformations are considered separately. Thus the spin connection and electromagnetic field are considered as separate gauge fields. In this study, we perform the space–time and internal gauge transformations in a unified way in the particle system with finite degrees of freedom. Since the phase space of the particle is divided into two separate parts, we perform the space–time transformations as the gauge transformations of the **P** and the internal coordinate transformations as the gauge transformations of the group U(2,2), which leaves the bilinear of the complex four internal coordinates and momenta. It includes the gauge transformations corresponding to the internal Lorentz transformations and the electromagnetic phase transformations. Due to the gauge group U(2,2), we realize the non-Abelian phase transformations represented by the generalized spin connection which corresponds to the gauge fields of $\mathrm{U}(1) \times \mathrm{SU}(2,\mathrm{C})$ subgroup of U(2,2).

First, we formulate the global Poincare transformations for the external space–time coordinates, and the rotations and phase transformations between the holomorphic, internal coordinates

of the spinning particle. The gauge groups of these transformations are **P** and U(2,2), respectively. The invariance of the free particle Lagrangian under the following subgroups of **P** and U(2,2) gives the conservation of the following physical quantities:

(1) The translation subgroup of **P** gives the conservation of the energy-momentum one-vector.
(2) The space–time rotation subgroup of **P** with the internal rotation group SU(2, C) together gives the conservation of the angular momentum two-vector.
(3) The internal U(1) phase transformation subgroup of U(2,2) gives the conservation of a scalar and real quantity, which will be identified as the electric charge of the particle.
The free particle Lagrangian is also invariant under the global proper time translations and another real, non-negative scalar quantity is conserved, and this quantity will be identified as the mass of the particle.

Second, we derive the gravitational and electromagnetic interactions of the spinning particle as the local gauge transformations for the gauge groups, **P**, and $\mathrm{SU}(2,\mathrm{C})\times\mathrm{U}(1)$ subgroup of U(2,2).

In Sec. I, we review the classical model of the zitterbewegung, in Sec. II, we discuss the invariance of the free particle Lagrangian under the global gauge transformations and derive the interaction Lagrangian by applying the local gauge transformations to the free particle Lagrangian. In Sec. III, we derive the classical equations of motion and compare them with the flat space–time equations except for the electromagnetic and gravitational force terms in nongeodesic equations. In Sec. IV we show that covariant constancy of the Dirac matrices gives the conservation of the electromagnetic current. Section V presents conclusions.

Classical spinning particle model. We use the classical spinning particle model developed to represent the classical analogue of the zitterbewegung motion of the electron. In this model, the particle has both usual space–time degrees of freedom and four additional internal degrees of freedom. These additional degrees of freedom correspond to the zitterbewegung oscillations and the spin of the particle. They are represented by the four complex internal holomorphic coordinates. In this model, the conjugate momenta of the space–time coordinates and velocity are linearly independent. Then, the Lagrangian of the free particle is defined by a constraint between the space–time four velocity and one-vector part of the Dirac algebra denoted by the bilinear of the complex four internal coordinates and momenta. Since external and internal coordinates are dynamically independent, the gauge transformations are Poincare transformations of the space–time coordinates of the particle with gauge group **P** and the internal coordinate transformations between the holomorphic coordinates of the four harmonic oscillators with the gauge group U(2,2). The generators of U(2,2) are the elements of the Dirac algebra. The gauge group $\mathrm{U}(1)\times\mathrm{SU}(2,\mathrm{C})$ includes the electromagnetism and gravitational interactions of the particle with the gauge potential represented by the generalized spin connection in Refs. 12–14.

To discuss the classical analogous of the zitterbewegung it is assumed that the internal configuration space of the particle consists from the four complex coordinates, z^i with $i=1,..,4$. We denote z^i by the complex four component spinor, z. In the Minkowski space–time, M_4 the Hermitian conjugate of z is $\bar{z}=(z_1^*,z_2^*,-z_3^*,-z_4^*)$ and we denote internal momenta of the particle as the complex spinors $\bar{z}$. Then, the Lagrangian for the free spinning particle, L is

$$L=\frac{1}{2i}\left(\frac{\mathrm{d}\bar{z}}{\mathrm{d}s}z-\bar{z}\frac{\mathrm{d}z}{\mathrm{d}s}\right)+p_a\left(\frac{\mathrm{d}x^a}{\mathrm{d}s}-\bar{z}\gamma^a z\right), \tag{1}$$

where x^a and p_a are the space–time coordinates and the momenta of the particle in the Minkowski space–time, M_4, with the metric $\eta_{ab}=(1,-1,-1,-1)$, s is the proper time of the particle and γ^a are constant Dirac matrices. The dynamical variables z_i are four complex coordinates and configuration space is C^4. The signatures of the bilinear in the quadratic form $\bar{z}z$ are $(+,+,-,-)$ and the transformations between the holomorphic coordinates conserve these signatures. We use the Latin indices for local Lorentz frames and the Greek indices for noncoordinate frames..

The classical spinning particle, represented by Eq. (1), has continuous values for spin. The quantization of this system corresponds to the coherent eigenstates of the internal, four complex

operators $\hat{z}$. In general, the harmonic oscillator coherent states are the continuous eigenstates with complex eigenvalues of the lowering operator $\hat{a}$. In this model the lowering operators of the internal oscillators are $\hat{z}^i$. The expectation values of the spin operators, $\hat{S}^{ab}$ between these coherent states also have continuous values. In quantum mechanics the physical particles correspond to the eigenstates of the spin operator, $\hat{S}^{ab}$, with discrete eigenvalues and they correspond to definite and discrete energy or internal angular momentum eigenstates of the four harmonic oscillators. The coherent spinning particle states represent the unphysical particle states, which are the coherent superposition of the physical spinning particle states. Thus, the dynamical variables of the classical zitterbewegung system correspond to the expectation of the corresponding operators between the minimum uncertain quantum spinning particle system.

In Eq. (1), p_a may be considered as the four Lagrange multipliers with the constraints

$$\dot{x}^a - \bar{z}\gamma^a z = 0, \tag{2}$$

where the overdot means the derivative with respect to s. This constraint relates the external and internal dynamics of the particle. Since the Lagrangian in Eq. (1) is defined in the phase space, the Hamiltonian structure of the system is known or chosen at the beginning.

II. GAUGE TRANSFORMATIONS

A. Global coordinate and phase transformations

In M_4, there are two kinds of coordinate transformations. These are the space–time translations and external Lorentz rotations:

$$x^a \to x'^a = x^a - i\xi^c P_c x^a - \frac{i}{2}\epsilon^{cd} L_{cd} x^a, \tag{3}$$

where P_c and L_{cd} are the generators of the translations and rotations, respectively. The Lagrangian in Eq. (1) is invariant under the translations. The Noether current is the energy momentum current

$$T^{ab}(u) = \int ds \bar{z}\gamma^a z p^b \delta^4[u - x(s)]$$

and the conserved charge of the translations is

$$p^a = \int T^{ab}(u) \mathrm{d}\sigma_b = p^a \int \mathrm{d}s \mathrm{d}\sigma_b \frac{du^b}{\mathrm{d}s} \delta^4[u - x(s)], \tag{4}$$

where σ_b is the three-dimensional hypersurface along the direction n_b.

In C^4, there are two kinds of internal transformations. These are the phase transformations generated by the SU(2, C) and U(1) subgroups of U(2,2) and they conserve the signatures of the frequencies of the zitterbewegung oscillations $(+,+,-,-)$:

$$z_i \to z_i' = \exp\left(-i\phi 1 - \frac{i}{2}\epsilon^{cd}\Sigma_{cd}\right)_i^j z_j, \tag{5}$$

$$\bar{z}^i \to \bar{z}'^i = \bar{z}^j \exp\left(+i\phi 1 + \frac{i}{2}\epsilon^{cd}\Sigma_{cd}\right)_j^i, \tag{6}$$

where Σ_{cd} is

$$\Sigma_{cd} = \frac{1}{2i}[\gamma_c, \gamma_d].$$

In Eqs. (5) and (6), there are two kinds of phase transformations: The first part, U(1) transformations, corresponds to the multiplication of all the complex spinor, z_i with $\exp(-i\phi 1_i^j)$ and the second part, SU(2, C) transformations, corresponds to the multiplication of the complex spinors, z_i with $\exp[(-(i/2)\epsilon^{cd}(\Sigma_{cd})_i^j)]$ term. The second part corresponds to the internal Lorentz rotations between the complex spinor, z_i.

The Lagrangian (1) is invariant under the external and internal Lorentz rotations and phase transformations and the Noether currents are

$$J^a(u) = \int \bar{z}\gamma^a z\bar{z}z\delta^4[u - x(s)]\mathrm{d}s, \tag{7}$$

and

$$M^{abc}(u) = \int \mathrm{d}s\left(x^a p^b - x^b p^a + \frac{1}{2}\bar{z}\Sigma^{ab}z\right)\bar{z}\gamma^c z\delta^4[u - x(s)].$$

The corresponding conserved charges are defined as

$$Q = \int \mathrm{d}\sigma_b J^b(u) = \bar{z}z \int \mathrm{d}s\mathrm{d}\sigma_b \frac{\mathrm{d}u^b}{\mathrm{d}s}\delta^4[u - x(s)] = \bar{z}z, \tag{8}$$

and

$$J^{ab} = \int M^{abc}(u)\mathrm{d}\sigma_c = (x^a p^b - x^b p^a + S^{ab}), \tag{9}$$

where the spin tensor, S^{ab} is

$$S^{ab} = \frac{1}{2}\bar{z}\Sigma^{ab}z. \tag{10}$$

There are no translation terms like $\exp(-i\zeta^c\gamma_c)$ in U(2,2) because they do not conserve the constraint in the Lagrangian. The generators of the $\mathrm{U}(1)\times\mathrm{SU}(2,\mathrm{C})$ are 1 and Σ_{cd} and correspond to the zero-vector and two-vectors of the four-dimensional Clifford or Dirac algebra.

The Lagrangian (1) is also invariant under the translation of the proper time s:

$$s \to s' = s - i\tau H s,$$

where H is the generator of the proper time translations, the Hamiltonian and the conserved quantity is the energy of the particle in proper time:

$$H = p_a\bar{z}\gamma^a z. \tag{11}$$

B. Local coordinate and phase transformations

Here, we consider the local coordinate and phase transformations as gauge transformations. The external translations and Lorentz rotations are expressed by the nonholonomic transformations

$$\mathrm{d}x^a \to \mathrm{d}x^\mu = (\delta^\mu{}_b + \zeta^\mu{}_{,b} + \epsilon^\mu{}_{c,b}x^c)\mathrm{d}x^b. \tag{12}$$

The internal transformations are

$$z_i \to z_i' = U_i^j z_j, \tag{13}$$

$$\bar{z}^i \to \bar{z}'^i = \bar{z}^j (U^{-1})_j^{\ i}, \tag{14}$$

where U is

$$U[x(s)] = \exp\left[- i\phi(x) 1 - \frac{i}{4} \epsilon^{cd}(x) \Sigma_{cd} \right]. \tag{15}$$

Under these transformations

$$\dot{x}^a \to \dot{x}^\mu = (\delta^\mu_{\ b} + \zeta^\mu_{\ ,b} + \epsilon^\mu_{\ c,b} x^c) \dot{x}^b, \tag{16}$$

and

$$\bar{z} \gamma^a z \to (\bar{z} \gamma^a z)' = \bar{z} \gamma^a z. \tag{17}$$

Then the Lagrange multiplier term in the Lagrangian becomes

$$p_a (\dot{x}^a - \bar{z} \gamma^a z) \to p_a e^a_{\ \mu} (\dot{x}^\mu - \bar{z} e^\mu_{\ b} \gamma^b z),$$

where the tetrads $e^\mu_{\ b}$ are defined as

$$e^\mu_{\ b}(x) = (\delta^\mu_{\ b'} + \zeta^\mu_{\ ,b'} + \epsilon^\mu_{\ c,b'} x^c),$$

and $e^a_{\ \mu}$ are the inverse of the tetrads, $e^\mu_{\ a}$. In the same way, space dependent Dirac matrices $\gamma^\mu(x)$ are defined as

$$\gamma^\mu(x) = e^\mu_{\ a}(x) \gamma^a. \tag{18}$$

These coordinates define the metric, $g_{\mu\nu}$:

$$g_{\mu\nu}(x) = e^a_{\ \mu}(x) e^b_{\ \nu}(x) \eta_{ab}.$$

The momentum, p_μ, is defined in global coordinates as

$$p_\mu = e^a_{\ \mu}(x) p_a.$$

Then the Lagrange multiplier term is rewritten as

$$p_\mu (\dot{x}^\mu - \bar{z} \gamma^\mu z), \tag{19}$$

and it is form invariant under the transformations (12).

The kinetic part of the Lagrangian is transformed as

$$\frac{1}{2i}(\dot{\bar{z}} z - \bar{z} \dot{z}) \to \frac{1}{2i}(\dot{\bar{z}} z - \bar{z} \dot{z})' = \frac{1}{2i}(\dot{\bar{z}} z - \bar{z} \dot{z}) + \frac{1}{2i}\left(\bar{z} \frac{\mathrm{d}U^{-1}}{\mathrm{d}s} U z - \bar{z} U^{-1} \frac{\mathrm{d}U}{\mathrm{d}s} z \right). \tag{20}$$

By evaluating the derivatives and considering the Lagrange multiplier, Eq. (20) gives

$$\frac{1}{2i}\left(\bar{z} \frac{\mathrm{d}U^{-1}}{\mathrm{d}s} U z - \bar{z} U^{-1} \frac{\mathrm{d}U}{\mathrm{d}s} z \right) = \bar{z} B_\mu(x) z \bar{z} \gamma^\mu z.$$

The $\bar{z} B_\mu(x) z \bar{z} \gamma^\mu z$ is the additional gauge interaction term and B_μ is

$$B_\mu(x) = e^a_{\ \mu}(x) \left[\phi_{,a}(x) + \tfrac{1}{4} \epsilon^{cd}_{\ \ ,a}(x) \Sigma_{cd} \right], \tag{21}$$

where $\frac{1}{4} e^a_{\ \mu}(x) \epsilon^{cd}_{\ \ ,a}(x)$ is the nonholonomic connection, $\Gamma_\mu^{\ cd}(x)$. To compensate for the effects of the local transformations, we introduce $B_\mu(x)$ as the gauge potentials that $e^a_{\ \mu}(x) \phi_{,a}(x)$ and $\frac{1}{4} \Gamma_\mu^{\ cd}(x) \Sigma_{cd}$ are introduced as the gauge potential of the U(1) and SU(2, C) phase transformations, respectively. They are the electromagnetic potential, $A_\mu(x)$, and the Fock-Ivanenko two-vectors, Γ_μ:

$$A_\mu(x) = e^a{}_\mu(x)\phi_{,a}(x),$$

$$\Gamma_\mu(x) = \tfrac{1}{4}\Gamma_\mu{}^{cd}(x)\Sigma_{cd}.$$

We rewrite the additional interaction terms as

$$\bar{z}B_\mu(x)z = \bar{z}[A_\mu(x) + \Gamma_\mu(x)]z. \tag{22}$$

Then, Lagrangian of the spinning particle, interacting with electromagnetic and gravitational fields, is

$$L = \frac{1}{2i}(\dot{\bar{z}}z - \bar{z}\dot{z}) + p_\mu\dot{x}^\mu - H, \tag{23}$$

where H is the Hamiltonian:

$$H = (p_\mu - \bar{z}B_\mu z)\bar{z}\gamma^\mu z = \Pi_\mu\bar{z}\gamma^\mu z. \tag{24}$$

The H in Eq. (24) looks like the Dirac or spin-1/2 particle Hamiltonian, but it, in fact, corresponds to the classical Hamiltonian of the zitterbewegung system with internal degrees of freedom and so the dynamical variables of the system have continuous values.

III. EQUATIONS OF MOTION

In this section, we derive the classical equations of motion. They are

$$\frac{\mathrm{d}}{\mathrm{d}s}x^\mu = \dot{x}^\mu = e^\mu{}_b\bar{z}\gamma^b z, \tag{25}$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\bar{z} = -i\bar{z}B_\mu\dot{x}^\mu + i\bar{z}\gamma^\alpha\Pi_\alpha, \tag{26}$$

$$\frac{\mathrm{d}}{\mathrm{d}s}z = iB_\mu z\dot{x}^\mu - i\gamma^\alpha z\Pi_\alpha. \tag{27}$$

We define the covariant time derivatives of the spinors $\bar{z}$ and z and rewrite Eqs. (26) and (27) as

$$\frac{D\bar{z}}{Ds} = \frac{\mathrm{d}}{\mathrm{d}s}\bar{z} + i\bar{z}\Gamma_\alpha\dot{x}^\alpha = i\bar{z}\gamma^\alpha\Pi_\alpha - i\bar{z}A_\alpha\dot{x}^\alpha, \tag{28}$$

$$\frac{Dz}{Ds} = \frac{\mathrm{d}}{\mathrm{d}s}z - i\Gamma_\alpha z\dot{x}^\alpha = -i\gamma^\alpha z\Pi_\alpha + i\bar{z}\Gamma_\alpha\dot{x}^\alpha. \tag{29}$$

To define the covariant derivatives we evaluate the derivatives of $\dot{x}^\mu$:

$$\frac{D\dot{x}^\mu}{Ds} = \bar{z}\frac{D\gamma^\mu}{Ds}z + \frac{D\bar{z}}{Ds}\gamma^\mu z + \bar{z}\gamma^\mu\frac{Dz}{Ds} = \bar{z}\gamma^\mu{}_{;\alpha}z\dot{x}^\alpha + i\bar{z}[\gamma^\alpha, \gamma^\mu]z\Pi_\alpha.$$

The covariant derivative of γ^μ is

$$\gamma^\mu{}_{;\alpha} = \nabla_\alpha\gamma^\mu + \gamma^\lambda\Gamma_{\alpha\lambda}{}^\mu.$$

Since

$$\nabla_\alpha \gamma^\mu = -\gamma^\lambda \Gamma_{\alpha\lambda}{}^{\mu},$$

the covariant derivative of γ^μ vanishes. Then

$$\frac{D\dot{x}^\mu}{Ds} = 4S^{\mu\nu}\Pi_\nu. \tag{30}$$

In a similar way, the covariant derivative of $S^{\mu\nu}$ is

$$\frac{DS^{\mu\nu}}{Ds} = \frac{1}{4i}\frac{D\bar{z}}{Ds}[\gamma^\mu,\gamma^\nu]z + \frac{1}{4i}\bar{z}[\gamma^\mu,\gamma^\nu]\frac{Dz}{Ds} + \frac{1}{4i}\bar{z}[\gamma^\mu{}_{;\alpha},\gamma^\nu]z\dot{x}^\alpha + \frac{1}{4i}\bar{z}[\gamma^\mu,\gamma^\nu{}_{;\alpha},]z\dot{x}^\alpha,$$

or

$$\frac{DS^{\mu\nu}}{Ds} = \dot{x}^\nu\Pi^\mu - \dot{x}^\mu\Pi^\nu. \tag{31}$$

Here the equations of motion for $\dot{x}^\mu$ and $S^{\mu\nu}$ are derived for completeness and they are equivalent to Eqs. (28) and (29).

To derive $D\Pi_\mu/Ds$ we first evaluate $\mathrm{d}p_\mu/\mathrm{d}s$:

$$\frac{\mathrm{d}p_\mu}{\mathrm{d}s} = \frac{\mathrm{d}(e^a_\mu p_a)}{\mathrm{d}s} = p_a\frac{\mathrm{d}e^a_\mu}{\mathrm{d}s} + e^a_\mu\frac{\mathrm{d}p_a}{\mathrm{d}s} = p_a\frac{\mathrm{d}e^a_\mu}{\mathrm{d}s} + e^a_\mu\frac{\partial L}{\partial x^a} = p_c\frac{\mathrm{d}e^c_\mu}{\mathrm{d}s} - e^c_\mu\frac{\partial H}{\partial x^c}.$$

Then

$$\frac{\mathrm{d}\Pi_\mu}{\mathrm{d}s} = \frac{\mathrm{d}p_\mu}{\mathrm{d}s} - \frac{\mathrm{d}(\bar{z}B_\mu z)}{\mathrm{d}s} = \dot{x}^\alpha e^c_\alpha\frac{\partial e^b_\mu}{\partial x^c}p_b - e^c_\mu\frac{\partial H}{\partial x^c} - \frac{d(\bar{z}B_\mu z)}{ds}.$$

We evaluate the second and third terms by using Eqs. (24)–(26):

$$e^c_\mu\frac{\partial H}{\partial x^c} = \bar{z}\gamma^\alpha z\left[\frac{\partial p_\alpha}{\partial x^\mu} - \frac{\partial(\bar{z}B_\alpha z)}{\partial x^\mu}\right] + \bar{z}\frac{\partial\gamma^\alpha}{\partial x^\mu}z\Pi_\alpha = \dot{x}^\alpha(p_b e^b_{\alpha,\mu} - \bar{z}B_{\alpha,\mu}z) + \bar{z}\gamma^\alpha{}_{,\mu}z\Pi_\alpha,$$

$$\frac{\mathrm{d}(\bar{z}B_\mu z)}{\mathrm{d}s} = \dot{x}^\alpha\bar{z}\frac{\partial B_\mu}{\partial x^\alpha}z + \frac{\mathrm{d}\bar{z}}{\mathrm{d}s}B_\mu z + \bar{z}B_\mu\frac{\mathrm{d}z}{\mathrm{d}s} = \dot{x}^\alpha\bar{z}B_{\mu,\alpha}z - i\bar{z}[B_\alpha,B_\mu]z\dot{x}^\alpha + i\bar{z}[\gamma^\alpha,B_\mu]z\Pi_\alpha.$$

Then $\mathrm{d}\Pi_\mu/\mathrm{d}s$ becomes

$$\frac{\mathrm{d}\Pi_\mu}{\mathrm{d}s} = \dot{x}^\alpha c_{\alpha\mu}{}^c p_c - \bar{z}e^c_\mu(\gamma^\alpha{}_{,c} + i[\gamma^\alpha,B_c])z\Pi_\alpha + \dot{x}^b e^c_\mu\bar{z}(B_{b,c} - B_{c,b} + i[B_b,B_c])z, \tag{32}$$

where the commutator coefficients, $c_{\mu\nu}{}^c$ are

$$\frac{\partial p_\mu}{\partial x^\nu} - \frac{\partial p_\nu}{\partial x^\mu} = \left(e^c_\nu\frac{\partial e^b_\mu}{\partial x^c} - e^c_\mu\frac{\partial e^b_\nu}{\partial x^c}\right)p_b = c_{\mu\nu}{}^c p_c = (\Gamma_{\mu\nu}{}^c - \Gamma_{\nu\mu}{}^c - T_{\mu\nu}{}^c)p_c.$$

We define the covariant derivative of Π_μ by considering its covariant vector character:

$$\frac{D\Pi_\mu}{Ds} = \frac{d\Pi_\mu}{ds} - \Gamma_{\mu\nu}{}^c\dot{x}^\nu e^\beta_c\Pi_\beta = -\dot{x}^\nu[(\Gamma_{\mu\nu}{}^c - \Gamma_{\nu\mu}{}^c - c_{\mu\nu}{}^c)e^\beta_c\Pi_\beta - \bar{z}(B_{\nu,\mu} - B_{\mu,\nu} + i[B_\nu,B_\mu] - c_{\mu\nu}{}^c e^\beta_c B_\beta)z].$$

The first term in square brackets is proportional to the energy-momentum tensor, $\dot{x}^\alpha\Pi_\beta$, and the proportionality factor is the gauge field of the translations, the torsion tensor, $T_{\mu\nu}{}^c$:

$$T_{\mu\nu}{}^{c} = (\Gamma_{\mu\nu}{}^{c} - \Gamma_{\nu\mu}{}^{c} - c_{\mu\nu}{}^{c}).$$

We define the curvature two-form for the generalized spin connection $B_{\mu\nu}$ as

$$B_{\mu\nu} = \bar{z}(B_{\nu,\mu} - B_{\mu,\nu} + i[B_{\nu}, B_{\mu}] - c_{\mu\nu}{}^{c} B_{c})z.$$

The second term is the product of the velocity of the particle and the curvature two-form, $B_{\mu\nu}$, and it can be decomposed as

$$B_{\mu\nu} = e_{\mu}^{m} e_{\nu}^{n} \left[\bar{z} z F_{mn} + \frac{1}{2} R_{mnab} \frac{1}{2} \bar{z} \Sigma^{ab} z \right],$$

where F_{mn} is the field strength tensor of the electromagnetic interactions, R_{mnab} is the generalized Riemann tensor for the noncoordinate frames. These are the gauge fields of the U(1) phase transformations and SO(3,1) Lorentz rotations and SU(2, C) subgroup of U(2,2). Then the expression of the Lorentz force for the spinning particle in the electromagnetic and gravitational interactions becomes

$$\frac{D\Pi_{\mu}}{Ds} = -\dot{x}^{\alpha} \Pi^{\beta} T_{\mu\alpha\beta} + \bar{z} z F_{\mu\nu} \dot{x}^{\nu} + \frac{1}{2} R_{\alpha\beta\mu\nu} \frac{1}{2} \bar{z} \Sigma^{\alpha\beta} z \dot{x}^{\nu}. \tag{33}$$

The equations of motion can also be derived by using the Hamiltonion, H and the following generalized Poisson parentheses:

$$\{f, g\} = \left(\frac{\partial f}{\partial x^{\alpha}} \frac{\partial g}{\partial p_{\alpha}} - \frac{\partial g}{\partial x^{\alpha}} \frac{\partial f}{\partial p_{\alpha}} \right) + \frac{1}{i} \left(\frac{\partial f}{\partial z} \frac{\partial g}{\partial \bar{z}} - \frac{\partial g}{\partial z} \frac{\partial f}{\partial \bar{z}} \right).$$

Then the equations of motion become

$$\frac{\mathrm{d}}{\mathrm{d}s} x^{a} = \{x^{a}, H\}, \quad \frac{\mathrm{d}p_{a}}{\mathrm{d}s} = \{p_{a}, H\},$$

$$\frac{\mathrm{d}}{\mathrm{d}s} \bar{z} = \{\bar{z}, H\}, \quad \frac{\mathrm{d}}{\mathrm{d}s} z = \{z, H\}.$$

IV. CONSERVATION OF THE CURRENTS

To derive the form of the energy-momentum current, $T^{\mu\nu}$, we rewrite the Hamiltonian as

$$H = g_{\mu\nu} T^{\mu\nu},$$

where $T^{\mu\nu}$ is

$$T^{\mu\nu} = \Pi^{\mu} \bar{z} \gamma^{\nu} z.$$

In Eq. (33), the Lorentz force can be written as the covariant derivative of $T^{\mu\nu}$:

$$T^{\mu\nu}{}_{;\nu} = \bar{z} \gamma^{\nu} z \Pi^{\mu}{}_{;\nu} = \frac{D}{Ds} \Pi^{\mu}. \tag{34}$$

Equation (34) shows that the energy-momentum current is not conserved for the spinning particle in the presence of the electromagnetic gauge field, $F_{\mu\nu}$, the torsion gauge field $T_{\mu\alpha}{}^{\beta}$, and the gauge field of the Lorentz rotations $R_{\alpha\beta\mu\nu}$.

The electromagnetic current, j^{μ} is defined as

$$j^{\mu} = \bar{z} z \bar{z} \gamma^{\mu} z. \tag{35}$$

The covariant derivative of j^{μ} is

$$j^{\mu}{}_{;\mu} = \bar{z} z \bar{z} \gamma^{\mu}{}_{;\mu} z = 0. \tag{36}$$

V. CONCLUSION

In Sec. III we show that Eqs. (30) and (31) are in the *same form* with the corresponding equations of motion in flat space–time. Equation (33) is the nongeodesic generalization of the corresponding flat space–time equation of motion. In Sec. IV we show that the covariant constancy of the Dirac matrices gives the conservation of the electric current.

To derive the quantum equations of motion we choose x^a and $\bar{z}_i$ as the variables in the configuration space of the particle and represent them by c-number variables. Then we represent the canonical conjugate variables p_a, and $\bar{z}_i$ as derivatives with $\hbar = 1$:

$$\hat{p}_a = i \frac{\partial}{\partial x^a},$$

$$\hat{z} = - \frac{\partial}{\partial \bar{z}}.$$

Since γ^{μ} is covariant constant then the quantum Hamiltonian is obtained from the classical one in Eq. (24) by replacing the classical dynamical variables with the corresponding quantum operators for $\hat{x}^a$, $\hat{z}^i$, $\hat{p}_a$, and $\hat{\bar{z}}_i$ without any ordering corrections:

$$\hat{H} = (\hat{p}_{\mu} - \hat{\bar{z}} \hat{B}_{\mu} \hat{z}) \hat{\bar{z}} \gamma^{\mu} \hat{z}.$$

The quantum equations of motion are derived by evaluating the following commutators:

$$\frac{\mathrm{d}}{\mathrm{d}s} x^a = i[x^a, \hat{H}], \quad \frac{\mathrm{d}p_a}{\mathrm{d}s} = i[p_a, \hat{H}],$$

$$\frac{\mathrm{d}}{\mathrm{d}s} \bar{z} = i[\bar{z}, \hat{H}], \quad \frac{\mathrm{d}}{\mathrm{d}s} z = i[z, \hat{H}].$$

Since there is no ordering corrections in the quantum Hamiltonian, the quantum equations of motion will be in the same form with the classical equations of motion in the Riemann-Cartan space–time.

The Hamiltonian in Eq. (24) corresponds to the classical Hamiltonian of the zitterbewegung system with the continuous, complex internal degrees of freedom and the continuous spin values. The corresponding quantum Hamiltonian, $\hat{H}$, gives the evolution of the continuous coherent eigenstates of $\hat{z}$, in proper time. To derive the Hamiltonians for the discrete spin eigenstates we evaluate the evolution operators for each spin eigenstate separately and this gives the Dirac Hamiltonian $\hat{H}_{\mathrm{D}} = \hat{\Pi}_{\mu} \gamma^{\mu}$ for spin $1/2$ eigenstates.[23]

In this space–time the scalar product is defined as

$$(\chi, \varphi) = \int \mathrm{d}^4 x \det e^{-1} \bar{\chi} \varphi,$$

and the minimal coupling of the Dirac field with gravitation is described by

$$(\Psi,\hat{H}_{\mathrm{D}}\Psi)=i\int \mathrm{d}^4x\ \det e^{-1}\bar{\Psi}\gamma^{\mu}\nabla_{\mu}\Psi.$$

Since γ^{μ} is covariant constant, then $(\det e^{-1})$ is also covariant constant and the scalar product and the interaction Hamiltonian is Hermitian:

$$(\Psi,\hat{H}_{\mathrm{D}}\Psi)=\frac{1}{2}\int \mathrm{d}^4x\ \det e^{-1}[\bar{\Psi}\gamma^{\mu}i\nabla_{\mu}\Psi+\overline{(i\nabla_{\mu}\Psi)}\gamma^{\mu}\Psi].$$

Thus we see that the ambiguity about the minimal coupling of matter with gravitation is solved by the covariant constancy of the Dirac matrices.

We see from Eqs. (26) and (27) that $\bar{z}z$ term is a constant of motion. Since it may be negative, zero, or positive we identify it as the charge of the particle, e.

In Eq. (33) the electromagnetic field is coupled with the electric current, $\bar{z}z\dot{x}^{\nu}$ and it is the source of the electromagnetic interactions. In a similar way, the Riemann tensor and the torsion tensor are coupled with the spin angular momentum current and the energy-momentum (current) tensor of the spinning particle, respectively, and they are the sources of the internal and the space–time rotations and space–time translations.

In Eq. (31), $DS_{\mu\nu}/Ds$ is proportional to the normal components of Π^{μ} with respect to velocity, $\dot{x}^{\nu}$. To derive the other form of the equation of motions for Π_{μ}, we decompose it into the parallel and normal components with respect to the velocity, $\dot{x}^{\nu}$:

$$\Pi_{\mu}=\frac{1}{(\dot{x})^2}\left(Hg_{\mu\nu}\dot{x}^{\nu}+\dot{x}^{\nu}\frac{DS_{\mu\nu}}{Ds}\right). \tag{37}$$

In Eq. (37), the first term of Π_{μ} is proportional to $\dot{x}_{\mu}$ and the proportionality constant is the Hamiltonian, H and we identify it as the mass of the particle, m. Then Eqs. (31), (30), and (33) become

$$\frac{DS^{\mu\nu}}{Ds}=\frac{1}{(\dot{x})^2}\left[\dot{x}^{\mu}\dot{x}_{\alpha}\frac{DS^{\nu\alpha}}{Ds}-\dot{x}^{\nu}\dot{x}_{\alpha}\frac{DS^{\mu\alpha}}{Ds}\right], \tag{38}$$

$$\frac{D\dot{x}^{\mu}}{Ds}=4S^{\mu\nu}\frac{1}{\sqrt{(\dot{x})^2}}\left(Hg_{\nu\alpha}\frac{\dot{x}^{\alpha}}{\sqrt{(\dot{x})^2}}+\frac{\dot{x}^{\alpha}}{\sqrt{(\dot{x})^2}}\frac{DS_{\nu\alpha}}{Ds}\right), \tag{39}$$

$$\frac{D}{Ds}\left[\left(mg_{\mu\nu}\dot{x}^{\nu}+\dot{x}^{\nu}\frac{DS_{\mu\nu}}{Ds}\right)\right]=-\dot{x}^{\alpha}T_{\mu\alpha}{}^{\beta}\left(mg_{\beta\nu}\dot{x}^{\nu}+\dot{x}^{\nu}\frac{DS_{\beta\nu}}{Ds}\right)+eF_{\mu\nu}\dot{x}^{\nu}+\frac{1}{2}R_{\alpha\beta\mu\nu}\frac{1}{2}\bar{z}\Sigma^{\alpha\beta}z\dot{x}^{\nu}. \tag{40}$$

Since the existence of the zitterbewegung oscillations, Eq. (39) shows that $(\dot{x})^2$ is not constant:

$$\dot{x}_{\mu}\frac{D\dot{x}^{\mu}}{Ds}=\frac{4\dot{x}_{\mu}S^{\mu\nu}}{\sqrt{(\dot{x})^2}}\frac{\dot{x}^{\alpha}}{\sqrt{(\dot{x})^2}}\frac{DS_{\nu\alpha}}{Ds}\neq 0.$$

In the phenomenological spin models, $(\dot{x})^2$ is taken as a constant and then $p_{\mu}S^{\mu\nu}/\sqrt{(\dot{x})^2}=0$.

Audretsch showed the vanishing of the covariant derivative of the spin polarization pseudovector, $S^{5\mu}$, by using only the positive energy solutions of the Dirac equation.[20] In our case the corresponding spin polarization pseudovector is

$$S^{5\mu}=\frac{1}{4i}\bar{z}[i\gamma^5,\gamma^{\mu}]z, \tag{41}$$

and the covariant proper time dependence is given as

$$\frac{DS^{5\mu}}{Ds} = \dot{x}^5 \Pi^\mu, \tag{42}$$

where $\dot{x}^5$ is $\bar{z} i\gamma^5 z$. In a separate study we will show that the correct spin polarization pseudovector is defined as

$$S_\perp^{5\mu} = \frac{1}{4i}\bar{z}[i\gamma^5, \gamma^\mu - \gamma\cdot\pi\pi^\mu/\pi^2]z.$$

In the Minkowski space–time, $S_\perp^{5\mu}$ is a constant of motion. In the presence of the electromagnetic interactions it satisfies the Bargmann-Michel-Teledgi equation with zitterbewegung corrections.[21] In the Riemann-Cartan space–time, the covariant derivative of spin polarization pseudovector is also proportional to the generalized Lorentz force in Eq. (33).

The right-hand side of Eq. (33) is the generalization of the electromagnetic Lorentz force to the Riemann-Cartan space, U_4. Except for the electromagnetic force the other terms are derived also by Hehl[16] in the nongeodesic equation for p_μ. For the Riemann space, V_4, the torsion tensor is zero and we obtain the classical Papapetrou equation.[19] For the Weitzenbock space, W_4, the curvature is zero and we obtain the nongeodesic equation for spinning particle with the Cartan connection.

For the spinless particle $S^{\alpha\beta}$ vanishes, $(\dot{x})^2$ becomes 1, and $\Pi_\mu = m g_{\mu\nu}\dot{x}^\nu$. Then the Lorentz force becomes

$$\frac{D}{Ds}(g_{\mu\nu}\dot{x}^\nu) = -T_{\mu\alpha\beta}\dot{x}^\alpha\dot{x}^\beta + \frac{e}{m}F_{\mu\nu}\dot{x}^\nu$$

for the Riemann-Cartan space, U_4. For the Riemann space, V_4, the torsion tensor is zero and we obtain the geodesic equation with the electromagnetic force. For the Weitzenbock space, W_4, the curvature is zero and we obtain the nongeodesic equation with Cartan connection and it coincides with the previous expression,[22] and is also equivalent to the geodesic equation.

We show in Eq. (33) that the spin-1 part of the generalized spin connection can be identified as the electromagnetism and the torsion is coupled with the spinning particle in the presence of the condition about the covariant constancy of the Dirac matrices.[12–14]

The other interactions can be formulated in a similar way by considering the groups larger than U(2,2). The invariant properties of the spinning particles under the conformal transformations can be discussed also by using the group U(2,2). The quantization of the spinning particle in the Riemann-Cartan Maxwell space will be studied later. The Lagrangian in Eq. (4) gives the Dirac equation for spin-1/2 case, spin-1 (symmetric) part of the DKP equation, and the higher spin wave equations.[23,24]

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On the essential constants in Riemannian geometries

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In the present work the problem of distinguishing between essential and spurious (i.e., absorbable) constants contained in a metric tensor field in a Riemannian geometry is considered. The contribution of the study is the presentation of a sufficient and necessary criterion, in terms of a covariant statement, which enables one to determine whether a constant is essential or not. It turns out that the problem of characterization is reduced to that of solving a system of partial differential equations of the first order. In any case, the metric tensor field is assumed to be smooth with respect to the constant to be tested. It should be stressed that the entire analysis is purely of local character. © *2006 American Institute of Physics.*
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I. INTRODUCTION

When dealing with Riemannian spaces, especially in a local description and in a coordinate approach, one frequently encounters the problem of attributing a character to a constant (or a parameter) which may appear in the metric tensor field. Generally, there are two possibilities: this constant is either essential (i.e., a true degree of freedom) or spurious (i.e., absorbable with the help of a change in the coordinates).

The issue is of great interest in the context of general relativity, where the metric tensor field is the solution to the Einstein equations, and the constants emerge from the integration procedure. But, this observation will not limit the spirit of the present work.

There is a variety of ways to attack the problem under discussion. In the relevant literature, one can find two main approaches:

A_1 The first main approach consists simply of trying to find that particular change in the coordinates which can serve to eliminate the "suspect" constant. When this is possible, the constant is incorporated in the very definition of the new coordinate system, being thus absorbed. The difficulty here is that, in general, there is no systematic way to find the desired transformation. Obviously, failure to find such a transformation does not necessarily imply the essentiality of the constant.

A_1 The second main approach, which is more elaborate and sophisticated, can be divided into two subcategories: one can either use the invariant classification methods for a single Riemannian space, or implement the methods of the *equivalence problem* (Ref. 1). The second way (which may be more laborious than the first) consists of the following steps: one considers twice the metric tensor field, once for a given value of the constant and once for another value of it. The final step is to compare these two metrics and to check whether they are equivalent or not. A positive answer dictates that the constant is spurious (and a negative, that it is essential) (see also Ref. 2 for a connection between limits of space–time and the problem of essentiality).

The nonequivalence between two given Riemannian spaces can easily be checked using the

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notion of *curvature invariant relations*, functionally independent relations among scalars. These scalars are constructed either from the Riemann tensor and its covariant derivatives up to a given order by contracting all the indices, or as "ratios" between two tensors (obtained from the Riemann tensor) which differ only by a factor. The first case gives scalars entering *syzygies, polynomial invariants, mixed invariants*, and the *Cartan invariants*—see Ref. 1 and the references therein for details. The second case is described in Ref. 3 (especially the last two references therein). It is sufficient for the two given spaces to differ in only one such relation in order to be inequivalent.

Curvature-invariant relations have one very important property: they do not depend on points of the Riemannian space; thus, their functional forms are invariant statements (i.e., they retain the same functional form in all coordinate systems). Consequently, if these functional forms depend on some constants, that means these constants, which clearly are some from those in the metric tensor field, are not affected by a change in the coordinates. If a constant of the metric tensor field could be eliminated by such a change, then the metric tensor field in the new coordinate system as well as all the curvature invariant relations based on it, would lack this particular constant, an invariant statement, since the curvature invariant relations are invariant in form. Therefore, only essential constants will appear in the curvature-invariant relations.

An example will elucidate the above arguments: consider the well-known Schwarzschild metric in the usual local coordinate system $\{t,r,\theta,\phi\}$ and e.g., the two curvature scalars,

$$S_1 \equiv R_{\alpha\beta\mu\nu}R^{\alpha\beta\mu\nu} = 48M^2/r^6, \tag{1.1}$$

$$S_2 \equiv S_{1;\mu}^{;\mu} = -3456M^3/r^9 + 1440M^2/r^8, \tag{1.2}$$

which are, of course, r-dependent. However, if r is eliminated between them, one arrives at the relation

$$R(S_1,S_2,M) \equiv S_2 + 6\sqrt{3}S_1^{3/2} - 5M^{-2/3}\sqrt[3]{9/2}S_1^{4/3} = 0. \tag{1.3}$$

This relation is not only independent of the space–time points, i.e., it can be evaluated everywhere in the Schwarzschild space–time (except, of course, the true singularity at $r=0$), but also invariant under any change in the local coordinate system; although the functional form (in terms of the coordinates) of the two curvature scalars S_1, S_2 will change, the relation $R(S_1,S_2,M)$ will retain its form (as a function of its arguments S_1, S_2, and M) and thus constitutes a curvature invariant relation. Indeed, consider for example the change $r\to\tilde{r}: r=M^{1/3}\tilde{r}$, which eliminates the parameter M from S_1 and alters the form of S_2, yet keeps the relation $R(S_1,S_2,M)$ unchanged. To use the above considerations in order to deduce equivalence between two Riemannian spaces is problematic, since it would require the existence of a countable basis for an arbitrary functional space.

The following section presents a sufficient and necessary criterion, in a covariant language which offers one the ability to check whether a constant, appearing in a metric tensor field, is essential or not. In the second case, the criterion also provides a way to find the desired local finite transformation of the change in the coordinates.

II. CRITERION

Before presenting the criterion, a word must be said for the existence of yet another kind of constant, namely the global (topological) constants: indeed, there are cases where a constant can be removed from local coordinate patches but it does appear in the transforms between them (e.g., in the appropriate range of the coordinates).

From the previous section, it is clear that *essential* and *spurious* are mutually complementary notions. It will turn out more practical, though equivalent, to deal with spurious. Indeed, if the constant is spurious one can, in the coordinates in which the constant is removed, take a product metric tensor field on $\mathcal{S}\times I$ (where $\mathcal{S}$ is the initial n-dimensional manifold and I the domain of definition of the spurious constant), and then deduce that the only nonzero components of curvature in $n+1$ dimensions are those which correspond to the curvature tensor of the n-dimensional metric tensor field. In these coordinates the normals to $\mathcal{S}$ form a symmetry. Alternatively, one can

also consider the $(n+1)$-dimensional manifold using the original coordinates, with the spurious constant as the extra coordinate, and use the constant to label the n-dimensional slices.

The above arguments can be made more precise as follows: Let $\mathcal{S}$ be a Riemannian space which is described by the pair $(\mathcal{M},g)$ (this definition is influenced by the definition of space–time, but C^∞-instead of simply C^r, connectedness as well as the Hausdorff condition seem to be minimal extensions), where $\mathcal{M}$ is an n-dimensional, connected, Hausdorff, and (C^∞) manifold and g is a (C^r) metric tensor field on it; (the value of r depends on the applications. In the context e.g., of general relativity, it is assumed that $r\geq 2$—see Ref. 4, pp. 55–59 for a relevant discussion) a nondegenerate, covariant tensor field of order 2, with the property that at each point of $\mathcal{M}$ one can choose a frame of n vectors $\{z_0,\ldots,z_{n-1}\}$, such that: $g(z_\alpha,z_\beta)=\eta_{\alpha\beta}$, where η is a diagonal matrix with entries $\{\varepsilon_0,\ldots,\varepsilon_{n-1}\}$, and $\varepsilon_\alpha=\pm 1$. [Small Greek indices take the values $\{0,\ldots,n-1\}$.]

Let also this metric tensor field depend on a constant λ; so, in a local coordinate system $\{x^\mu\}$, it is

$$g_{\alpha\beta}=g_{\alpha\beta}(x^\gamma;\lambda). \tag{2.1}$$

It is also supposed that the metric tensor field g is a (C^∞) function (i.e., smooth) with respect to λ—a basic assumption which is also encountered in Ref. 2, where limits of space–time are considered [which of course have to be defined in terms of essential constant(s)].

Let $I\subseteq\mathbb{R}$ be the domain of definition (i.e., the range of possible values) of the constant λ. Another Riemannian space $\widetilde{\mathcal{S}}$ can, naturally, emerge; the product: $\widetilde{\mathcal{S}}=\mathcal{S}\times I$. By this it is meant that the initial Riemannian space is nothing but the hypersurface $\lambda=$const. in $\widetilde{\mathcal{S}}$; a local isometric embedding. If $p\in\widetilde{\mathcal{S}}$, then the tangent space $T_p\mathcal{S}$ of $\mathcal{S}$ is a subspace of $T_p\widetilde{\mathcal{S}}$. Since $\mathcal{S}$ is a regular submanifold of $\widetilde{\mathcal{S}}$, there exists a basis $\{\mathbf{e}_0,\mathbf{e}_\mu\}\equiv\mathbf{e}_N$ of $T_p\widetilde{\mathcal{S}}$ such that its "spatial" part $\{\mathbf{e}_\mu\}$ is the basis of $T_p\mathcal{S}$. [Capital Latin indices take the values $\{0,\ldots,n\}$.] Since the difference of dimensions is 1, the subspace has no torsion. Consequently there is only one normal to it, vector $\mathbf{n}$. Without loss of generality it is taken to be of unit length. Then, one assigns

$$\mathbf{n}=n^A\mathbf{e}_A=\frac{1}{N}\mathbf{e}_0-\frac{N^\alpha}{N}\mathbf{e}_\alpha\Rightarrow n^A=\frac{1}{N}\{1,-N^\alpha\}, \tag{2.2}$$

with

$$\widetilde{g}(\mathbf{n},\mathbf{n})=\varepsilon=\pm 1 \tag{2.3}$$

(the sign is rather irrelevant), so

$$\mathbf{e}_0=N\mathbf{n}+N^\alpha\mathbf{e}_\alpha. \tag{2.4}$$

The quantity N is the *lapse function* and the object N^α is the *shift vector*. By definition,

$$\widetilde{g}_{00}=\widetilde{g}(\mathbf{e}_0,\mathbf{e}_0)=N^2\widetilde{g}(\mathbf{n},\mathbf{n})+N^\alpha N^\beta\widetilde{g}(\mathbf{e}_\alpha,\mathbf{e}_\beta), \tag{2.5}$$

$$\widetilde{g}_{0\alpha}=\widetilde{g}(\mathbf{e}_0,\mathbf{e}_\alpha)=N_\alpha\equiv N^\beta g_{\alpha\beta}, \tag{2.6}$$

$$\widetilde{g}_{\alpha\beta}=\widetilde{g}(\mathbf{e}_\alpha,\mathbf{e}_\beta)=g_{\alpha\beta}. \tag{2.7}$$

Thus, the Greek indices change position with the initial metric $g_{\alpha\beta}$, while the capital Latin indices change position with the new metric $\widetilde{g}_{AB}$. Finally,

$$\widetilde{g}_{AB}=\begin{pmatrix} N_\rho N^\rho+\varepsilon N^2 & N_\beta \\ N_\alpha & g_{\alpha\beta}\end{pmatrix}. \tag{2.8}$$

A straightforward calculation results in

$$\widetilde{\Gamma}^0_{00} = \frac{\dot{N}}{N} + \varepsilon \frac{N^\mu N^\nu}{N} K_{\mu\nu} + \frac{N^\mu}{N} N_{|\mu}, \tag{2.9a}$$

$$\widetilde{\Gamma}^0_{0\nu} = \varepsilon \frac{N^\mu}{N} K_{\mu\nu} + \frac{N_{|\nu}}{N}, \tag{2.9b}$$

$$\widetilde{\Gamma}^0_{\mu\nu} = \varepsilon \frac{K_{\mu\nu}}{N}, \tag{2.9c}$$

$$\widetilde{\Gamma}^\kappa_{00} = -\frac{\dot{N}}{N} N^\kappa - \varepsilon \frac{N^\mu N^\nu N^\kappa}{N} K_{\mu\nu} - \frac{N^\mu N_{|\mu}}{N} N^\kappa + \dot{N}^\kappa - \varepsilon N N^{|\kappa} + N^\kappa_{|\nu} N^\nu - 2N K^\kappa_\nu N^\nu, \tag{2.9d}$$

$$\widetilde{\Gamma}^\kappa_{0\nu} = -\frac{N^\kappa}{N} N_{|\nu} - \varepsilon \frac{N^\kappa N^\mu}{N} K_{\mu\nu} + N^\kappa_{|\nu} - N K^\kappa_\nu, \tag{2.9e}$$

$$\widetilde{\Gamma}^\kappa_{\mu\nu} = \Gamma^\kappa_{\mu\nu} - \varepsilon \frac{N^\kappa}{N} K_{\mu\nu}, \tag{2.9f}$$

where

$$K_{\mu\nu} = \frac{1}{2N}(N_{\mu|\nu} + N_{\nu|\mu} - \dot{g}_{\mu\nu}) \tag{2.10}$$

is the *extrinsic curvature* (in the literature of the theory of surfaces, it is also known as *second fundamental form*, of *shape tensor*) and describes the embedding curvature.

The bar (|) denotes covariant derivative with respect to the initial metric g of the subspace, while the dot $(\cdot)$ denotes differentiation with respect to the extra coordinate, i.e., λ.

The general theory of embedding can be found in any book on differential geometry, e.g., Ref. 5 are some classical references. There, one can see that the present case, where the difference in the dimensions is 1 (resulting in zero torsion for the subspace) is very simple. In fact, the Mainardi-Codazzi conditions are identically satisfied, while the Weingarten-Gauss conditions assume the form

$$\widetilde{R}_{\alpha\beta\mu\nu} = R_{\alpha\beta\mu\nu} - \varepsilon(K_{\alpha\mu}K_{\beta\nu} - K_{\alpha\nu}K_{\beta\mu}), \tag{2.11a}$$

$$\widetilde{R}_{\perp\beta\mu\nu} = K_{\beta\nu|\mu} - K_{\beta\mu|\nu}, \tag{2.11b}$$

of course, after the use of the projections

$$T^{A\ldots}_{B\ldots} n^B \equiv T^{A\ldots}_{\perp\ldots}, \quad T^{A\ldots}_{B\ldots} n_A \equiv T^{\perp\ldots}_{B\ldots}, \quad T^{A\ldots}_{B\ldots} y^B_{,\alpha} \equiv T^{A\ldots}_{\alpha\ldots}, \tag{2.12}$$

$y^B_{,\alpha}$ being the Jacobian $\partial y^A / \partial x^\alpha$ between a set of local coordinates in $\widetilde{\mathcal{S}}$, say $\{y^A\}$, and the set of the corresponding local coordinates in $\mathcal{S}$, say $\{x^\alpha\}$.

For the chosen embedding it is $\{y^A\}=\{\lambda, x^\alpha\}$

If one defines the tensor on $\widetilde{\mathcal{S}}$

$$C_{AB} \doteq -\frac{1}{2}\mathcal{L}_{\mathbf{n}} \widetilde{g}_{AB} \equiv -\frac{1}{2}(\mathbf{n}_{A;B} + \mathbf{n}_{B;A}), \tag{2.13}$$

where the semicolon (;) denotes covariant differentiation with respect to the new metric $\widetilde{g}$, one will have

$$C_{AB} = \begin{pmatrix} N^\mu N^\nu K_{\mu\nu} + \varepsilon N^\mu N_{|\mu} & \varepsilon \frac{1}{2} N_{|\beta} + K_{\beta\mu} N^\mu \\ \varepsilon \frac{1}{2} N_{|\alpha} + K_{\alpha\mu} N^\mu & K_{\alpha\beta} \end{pmatrix}. \tag{2.14}$$

In order for the two spaces, i.e., the embedding and the embedded, to have exactly the same geometrical information (in other words, exactly the same curvature properties), something which happens when and only when the constant (i.e., the extra coordinate) λ is absorbable, the Weingarten-Gauss conditions (2.11) suggest that the extrinsic curvature must vanish—for any embedding

$$K_{\alpha\beta} = 0. \tag{2.15}$$

Condition (2.15) as well as the demand for its validity for any embedding, and thus for the particular embedding in a Gaussian system of coordinates $N=1$ or $N=N(\lambda)$ and $N^\alpha=0$, result in the vanishing of the tensor C_{AB}; an invariant statement. Hence, follows the:

Criterion. The constant λ contained in the metric tensor field g of the Riemannian space $\mathcal{S}$ is spurious, if and only if the Lie derivative of the metric tensor field $\tilde{g}$ of the embedding space $\tilde{\mathcal{S}}$ with respect to the normal (to the subspace) vector $\mathbf{n}$, $\mathcal{L}_{\mathbf{n}}\tilde{g}$, vanishes.

Proof. First, one observes that the vanishing of the tensor field C_{AB} results in the following set of partial differential equations (PDEs):

$$C_{00} = 0 \Rightarrow N^\mu N_{|\mu} = 0, \tag{2.16a}$$

$$C_{0\alpha} = 0 \Rightarrow N_{|\alpha} = 0, \tag{2.16b}$$

$$C_{\alpha\beta} = 0 \Rightarrow K_{\alpha\beta} = 0, \tag{2.16c}$$

or

$$N = N(\lambda) \quad \text{(though an arbitrary function)}, \tag{2.17a}$$

$$N_{\alpha|\beta} + N_{\beta|\alpha} = \dot{g}_{\alpha\beta}. \tag{2.17b}$$

The lines preceding the criterion prove its necessity. In order to prove its sufficiency, let $n^A = 1/[N(\lambda)]\{1, -N^\alpha(\lambda, x^\beta)\}$ a normal vector whose components satisfy (2.17b). The set of its integral curves, parametrized by a parameter s, has the form

$$\frac{dy^A}{ds} = n^A(y^B(s)), \tag{2.18}$$

and, from the theory of ordinary differential equations, it is known that this problem is well posed and it always has a solution. Written out in detail,

$$\frac{dy^0}{ds} = \frac{1}{N(y^0)}, \tag{2.19a}$$

$$\frac{dy^\alpha}{ds} = -\frac{N^\alpha(y^0, y^\beta)}{N(y^0)}, \tag{2.19b}$$

As usual, this set defines a one-parametric (s being the parameter) family of transformations from the set $\{y^A\}$ to the set $\{\overline{y}^A\}$, the latter being the constants of integration of the flow lines of the vector $\mathbf{n}$. It is very easy to see that the emerging transformation has the general functional form

$$y^0 \to \overline{y}^0 : \overline{y}^0 = f(y^0), \tag{2.20a}$$

$$y^\alpha \to \overline{y}^\alpha : \overline{y}^\alpha = f^\alpha(y^0, y^\gamma), \tag{2.20b}$$

while the vector **n** undergoes a change,

$$\mathbf{n} \to \overline{\mathbf{n}} : \overline{n}^A = \frac{\partial \overline{y}^A}{\partial y^B} n^B, \tag{2.21}$$

with the help of the transformation (2.20),

$$\overline{n}^A = \frac{1}{N(y^0)} \left\{ \frac{\partial f(y^0)}{\partial y^0}, \frac{\partial f^\alpha(y^0, y^\gamma)}{\partial y^0} - \frac{\partial f^\alpha(y^0, y^\gamma)}{\partial y^\beta} N^\beta(y^E) \right\}. \tag{2.22}$$

But,

$$\frac{d\overline{y}^\alpha}{ds} = 0 \Rightarrow \frac{\partial f^\alpha(y^0, y^\gamma)}{\partial y^0} - \frac{\partial f^\alpha(y^0, y^\gamma)}{\partial y^\beta} N^\beta(y^E) = 0 \tag{2.23}$$

by virtue of the flow lines equations (2.19). Thus,

$$\mathbf{n} \to \overline{\mathbf{n}} : \overline{n}^A = \frac{1}{N(y^0)} \left\{ \frac{\partial f(y^0)}{\partial y^0}, 0 \right\}, \tag{2.24}$$

i.e., a Gaussian system of coordinates. Hence, in the new coordinate system, the vanishing of the tensor $\overline{C}_{AB}$, obviously, is tantamount to

$$\frac{\partial \overline{g}_{\alpha\beta}}{\partial \overline{y}^0} = 0, \tag{2.25}$$

i.e., the transformed metric tensor field of the subspace does not contain the corresponding extra coordinate $\overline{y}^0$, which is a function of the constant under discussion. Q.E.D.

III. AN APPLICATION AND A PEDAGOGICAL EXAMPLE

One immediate and simple application of the criterion is achieved when the latter is applied to the case where the "suspect" constant is an overall factor; i.e., in a local system of coordinates $\{x^\mu\}$,

$$g_{\alpha\beta} = g_{\alpha\beta}(x^\gamma; \lambda) \equiv \lambda G_{\alpha\beta}(x^\gamma). \tag{3.1}$$

Then, the criterion, in its "solved form" (2.17b), results in

$$N_{\alpha|\beta} + N_{\beta|\alpha} = \dot{g}_{\alpha\beta} = G_{\alpha\beta} \Rightarrow N_{\alpha|\beta} + N_{\beta|\alpha} = \frac{1}{\lambda} g_{\alpha\beta}, \tag{3.2}$$

which is nothing but the homothety equations for the subspace—a well-known result.

For the sake of simplicity and brevity, the paper concludes with a pedagogical example.

Let a two-dimensional metric tensor field, which in a local coordinate system $\{x^\mu\} \equiv \{u, v\}$, has the form

$$g_{\alpha\beta}(u, v; \lambda) = (1 + \lambda^2) \begin{pmatrix} 0 & 1 + u^2 + (1 + \lambda^2)^2 v^2 \\ 1 + u^2 + (1 + \lambda^2)^2 v^2 & 0 \end{pmatrix}. \tag{3.3}$$

Solution to

$$N_{\alpha|\beta} + N_{\beta|\alpha} = \dot{g}_{\alpha\beta} \tag{3.4}$$

results in

$$N^{\alpha} = \left\{0, \frac{2\lambda v}{1+\lambda^2}\right\} \equiv \left\{0, \frac{2y^0 y^2}{1+(y^0)^2}\right\}, \tag{3.5}$$

and hence

$$n^A = \frac{1}{N(y^0)}\left\{1,0,-\frac{2y^0 y^2}{1+(y^0)^2}\right\}. \tag{3.6}$$

The corresponding flow lines are described by

$$\frac{dy^0}{ds} = \frac{1}{N(y^0)}, \tag{3.7a}$$

$$\frac{dy^1}{ds} = 0, \tag{3.7b}$$

$$\frac{dy^2}{ds} = -\frac{1}{N(y^0)}\frac{2y^0 y^2}{(1+(y^0)^2)}, \tag{3.7c}$$

and the integral curves

$$\int N(y^0)dy^0 = s + \bar{y}^0, \tag{3.8a}$$

$$y^1 = \bar{y}^1, \tag{3.8b}$$

$$y^2 = \bar{y}^2(1+(y^0)^2)^{-1}. \tag{3.8c}$$

Then, as expected, it is

$$\bar{n}^A = \{1,0,0\}, \tag{3.9}$$

leading to the transformed embedding metric,

$$\bar{\bar{g}}_{AB} = \begin{pmatrix} \varepsilon & 0 \\ 0 & \bar{g}_{\alpha\beta} \end{pmatrix}, \tag{3.10}$$

with

$$\bar{g}_{\alpha\beta} = \begin{pmatrix} 0 & 1+\bar{u}^2+\bar{v}^2 \\ 1+\bar{u}^2+\bar{v}^2 & 0 \end{pmatrix}. \tag{3.11}$$

Though the example may seem simple and trivial, its purpose is to exhibit not only the implementation of the criterion but also all the details connected to it.

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Intersecting hypersurfaces in anti-de Sitter and Lovelock gravity

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Colliding and intersecting hypersurfaces filled with matter (membranes) are studied in the Lovelock higher order curvature theory of gravity. Lovelock terms couple hypersurfaces of different dimensionalities, extending the range of possible intersection configurations. We restrict the study to constant curvature membranes in constant curvature anti-de Sitter (AdS) and dS background and consider their general intersections. This illustrates some key features which make the theory different from the Einstein gravity. Higher co-dimension membranes may lie at the intersection of co-dimension one hypersurfaces in Lovelock gravity; the hypersurfaces are located at the discontinuities of the first derivative of the metric, and they need not carry matter. The example of colliding membranes shows that general solutions can only be supported by (spacelike) matter at the collision surface, thus naturally conflicting with the dominant energy condition (DEC). The imposition of the DEC gives selection rules on the types of collision allowed. When the hypersurfaces do not carry matter, one gets a solitonlike configuration. Then, at the intersection one has a co-dimension two or higher membrane standing alone in AdS-vacuum space–time *without conical singularities*. Another result is that if the number of intersecting hypersurfaces goes to infinity the limiting space–time is free of curvature singularities if the intersection is put at the boundary of each AdS bulk. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2338143]

I. INTRODUCTION

Lately, a strange idea has become popular in cosmology. It has been suggested[1] that we live on a $(3+1)$-dimensional membrane, called a brane world, living in a higher dimensional space–time. Many general relativity models have been invented to describe the gravitational behavior of such a brane world. Although there is a clear conceptual link with string theory, i.e., the extra dimensions and the existence of membranes with matter and gauge fields confined to their world-sheets, it is also clear that this is a highly speculative idea.

This idea motivates a general study of hypersurfaces in d-dimensional curved space–time. Co-dimension one hypersurfaces are understood as co-dimension one submanifolds which are the locus of the discontinuities of the first derivative of the metric. To draw specific conclusions we need a theory of gravity, determining the metric of the d-dimensional space–time locally. Lovelock gravity is a natural choice in d dimensions in place of Einstein gravity in four dimensions; it is the only theory (action functional) for the metric which gives second-order field equations when torsion is zero, that is, when the covariant derivative is given by the usual formula.[2,3] One can get

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a relation between the discontinuity of the first derivative of the metric to the energy tensor of matter on the hypersurface. Hypersurfaces of any co-dimensionality which (potentially) carry matter will be called membranes.

The more complicated, compared to Einstein's theory, structure of derivatives in Lovelock gravity makes it possible to have membranes of co-dimensionality higher than one, via intersections of co-dimension one hypersurfaces, without any space–time singularities. Put slightly differently, high co-dimension membranes can be embedded in space–time without causing conical or more pathological curvature singularities if they are embedded at the intersection of co-dimension one hypersurfaces. In fact, in d dimensions there exist membranes of co-dimensionality up to the integer part of $(d-1)/2$, such that the metric is everywhere continuous, its first derivative has (bounded) discontinuities at the hypersurfaces and space–time is everywhere, and especially at the membranes, a manifold.[4,5]

The higher dimensional gravity theory of Lovelock[3] is an interesting generalization of general relativity. In $d \geqslant 5$ the Einstein–Hilbert is not the most general Lagrangian that produces second-order field equations and it was extended by Lovelock to a more general theory with this property. The latter gives the theory familiar features, in accordance with our experience from classical mechanics and field theory. It allows for a Hamiltonian formulation[6] and the possibility of a well-posed initial value problem.[7] The Lagrangian which possesses this property was found by Lovelock[3] and it is a linear combination of terms corresponding to the Euler densities in all lower even dimensions,[2]

$$\mathcal{L} = \sum_{n=0}^{[(d-1)/2]} \frac{1}{2^n} \beta_n \delta^{\mu_1 \cdots \mu_{2n}}_{\nu_1 \cdots \nu_{2n}} R^{\nu_1 \nu_2}_{\mu_1 \mu_2} \cdots R^{\nu_{2n-1} \nu_{2n}}_{\mu_{2n-1} \mu_{2n}} \sqrt{g} d^d x, \tag{1}$$

where $[x]$ is the integer part x. The generalization of the Einstein tensor is the Lovelock tensor:

$$H^{\mu}_{\nu} = - \sum_{n=0}^{[(d-1)/2]} \frac{1}{2^{n+1}} \beta_n \delta^{\mu \mu_1 \cdots \mu_{2n}}_{\nu \nu_1 \cdots \nu_{2n}} R^{\nu_1 \nu_2}_{\mu_1 \mu_2} \cdots R^{\nu_{2n-1} \nu_{2n}}_{\mu_{2n-1} \mu_{2n}}. \tag{2}$$

The delta is the generalized totally antisymmetrized Kronecker delta. It is the determinant of a matrix with elements δ^M_N,

$$\delta^{\mu_1 \cdots \mu_p}_{\nu_1 \cdots \nu_p} = \det \begin{pmatrix} \delta^{\mu_1}_{\nu_1} & \delta^{\mu_2}_{\nu_1} & \cdots & \delta^{\mu_p}_{\nu_1} \\ \delta^{\mu_1}_{\nu_2} & \delta^{\mu_2}_{\nu_2} & \cdots & \delta^{\mu_p}_{\nu_2} \\ \vdots & \vdots & \ddots & \vdots \\ \delta^{\mu_1}_{\nu_p} & \delta^{\mu_2}_{\nu_p} & \cdots & \delta^{\mu_p}_{\nu_p} \end{pmatrix} = p! \delta^{\mu_1}_{[\nu_1} \cdots \delta^{\mu_p}_{\nu_p]}. \tag{3}$$

The Lovelock theories have been studied extensively. Higher dimensional black hole solutions have been found.[8–10] This has shed some interesting light on questions of black hole entropy. Some cosmological metrics have been studied.[11]

The $n_{\max}=2$ Lovelock theory, which we call the Gauss–Bonnet theory, has a special physical significance. This is because the $n=2$ term is the only quadratic term which has a ghost free perturbation theory about flat space–time. It has been conjectured that the Gauss–Bonnet term is the leading order, purely geometric, correction to the effective action of an underlying unitary fundamental theory.[12] In particular, the Lovelock contributions, motivated by string theory, have played a role in brane-world cosmology.[13,14]

It was Zumino[2] who formulated the theory in the way we prefer, as an elegant way to prove suggestions by Zwiebach related to low energy string theory.[12] We use the vielbein formulation: E^a is the vielbein frame, ω^{ab} the spin connection, and Ω^{ab} is the curvature two-form,

$$\Omega^{ab} = \tfrac{1}{2} R^{cd}{}_{ab} E^c \wedge E^d,$$

$$R^{cd}{}_{ab} = E^a_\mu E^b_\nu R^{\mu\nu}_{\kappa\lambda} E^\kappa_c E^\lambda_d.$$

In this language, the Lovelock Lagrangian is

$$\mathcal{L} = \sum_{n=0}^{[(d-1)/2]} \beta_n \Omega^{a_1 a_2} \wedge \cdots \Omega^{a_{2n-1} a_{2n}} \wedge e_{a_1 \cdots a_{2n}}, \tag{4}$$

where

$$e_{a_1 \cdots a_p} = \frac{1}{(d-p)!} \epsilon_{a_1 \ldots a_d} E^{a_{p+1}} \wedge \cdots \wedge E^{a_d} \tag{5}$$

and we have defined the totally antisymmetric tensor such that $\epsilon_{(1)\ldots(d)} = 1$. The Latin letters from the beginning of the alphabet are used for the local Lorentz indices (d-dimensional). Greek letters from the middle of the alphabet are used for space–time coordinate indices (d-dimensional).

In the Lovelock theory, singular hypersurfaces of co-dimension one can be meaningfully defined in terms of distributions,[14,15] due to the property of quasilinearity in second derivatives.[16] Brane worlds of co-dimension one have thus been the most well studied and understood. They can also be formulated by means of boundary terms in the action. The correct boundary term is most elegantly derived by a dimensional continuation of the Gauss–Bonnet theorem for a manifold with boundary.[17] The latter approach is the one we have adopted.

The possibility of colliding shells or branes of matter has been studied in the context of GR.[18] In Lovelock gravity, there has been some study of intersecting brane worlds, see, e.g., Ref. 19 and more recently, Refs. 20 and 21, but so far there has been no study of collisions in this context except for our comments in our recent work.[4,5] In that work, we restricted the smoothness of the metric so that there were well-defined orthonormal vectors at the intersection/collision. The most striking fact, physically, about intersections or collisions is that they could carry their own singular stress-energy tensor. This is a phenomenon that does not occur in the Einstein theory. That difference and related properties of the Gauss–Bonnet term were used in Ref. 19 to address the cosmological constant problem and formulate higher co-dimension brane worlds via intersections, continuing on previous work in GR context, see, e.g., Ref. 22. Our aim here will be to discuss general properties of the intersections and collisions of hypersurfaces in Lovelock gravity, mostly via the example of anti-de Sitter (AdS) and dS background, which may be useful also outside the brane-world context.

In the Einstein theory, singular matter can only be accommodated at an intersection of co-dimension two if there is a conical singularity, with a deficit angle. Then, it is impossible to define two orthonormal vectors normal to the intersection. Although Lovelock gravity with a conical singularity can be described in terms of distributions,[23–25] there is a certain ambiguity about the solutions—in general, we would not expect the thin brane to be the unique limit of a thick brane solution.[26,27] We shall not consider this kind of singularity in the present work.

There is, however, an interesting possibility. We consider intersections of hypersurfaces, non-null as well as null, which carry zero energy tensor. At their intersections there appear higher co-dimension membranes. For non-null co-dimension one hypersurfaces we have an intersection of solitonlike configurations, pure (cosmological constant-) vacuum gravitational field self-supported and with a nonzero jump in the extrinsic curvature; for null hypersurfaces we have intersection/collision of gravitational shock waves. In both cases one has at their intersections membranes of co-dimension $\geqslant 2$ surrounded by pure AdS background on a nonsingular space–time. This is a phenomenon not possible in Einstein gravity.[26]

Previous works on related problems in the brane world were in the context of: Einstein gravity, e.g., Ref. 22; in supergravity, where intersection rules for branes carrying form field charges were derived in Refs. 28–30; and in various formulations when Gauss–Bonnet or higher Euler densities are included, e.g., Refs. 31 and 19, 20, 21, and 24. An important difference in this work and our previous ones[4,5] is that one may have a high co-dimension membrane without the

cost of making space–time singular.[31,24,21] Our primary intention really is to point out properties of Lovelock gravity which are interesting on their own, but our results may be useful to other endeavors.

In Secs. II–IV we present the example of intersecting hypersurfaces in an AdS background. In Sec. V we discuss colliding hypersurfaces in dS background and point out the spontaneous dominant energy condition violation in collisions. In Sec. VI, we discuss the dimensionalities of the intersection in relation to a four-dimensional universe. In Sec. VII we discuss higher co-dimension membranes using intersections of solitonic configurations and shock waves.

The intersection junction conditions. For our purposes, hypersurfaces are $(d-1)$-dimensional surfaces which divide the space–time up into d-dimensional bulk regions. We shall assume that they are space–time like (i.e., with space-like normal vector). If there is a nonzero singular component to the stress-energy tensor with its support on the hypersurface, we shall also call it a brane.

The mathematics of the intersections becomes simple if we consider a kind of minimal intersection, which involves the minimum number of hypersurfaces needed to build the intersection of a given co-dimensionality (dimensionality of its normal space). Put differently, in such an intersection any bulk region has (a co-dimension one) common boundary with *any other* bulk region. Not without a reason we call them simplicial intersections: if abstractly we assign a point to every bulk region in which the connection is continuous, then a co-dimension p intersection corresponds to a p-dimensional simplex, that is, the p-dimensional polyhedron with the minimum number of vertices. This abstraction turns into a practical method of calculating the Lagrangian densities integrated over the intersections.[4,5]

One of the simplifications related to the simplicial intersection is that if we label the bulk regions with i (and designate $\{i\}$) then the co-dimension p intersection can be labeled by an antisymmetric symbol involving the labels of the $p+1$ bulk regions meeting there; the simplest example are the co-dimension one hypersurfaces designated in general as $\{i_0 i_1\}=-\{i_1 i_0\}$. So we introduce the following.[4,5]

Definition 1.1: (simplicial intersection) Let $\{i\}$ be a bulk region. $\{i_0 \ldots i_p\}$ is a simplicial intersection where bulk regions $i_0, \ldots, i_p$ meet, if it is a $(d-p)$-dimensional submanifold. The connections in the bulk regions are $\omega_0, \ldots, \omega_p$, respectively. $\{i_0 \ldots i_p\}$ is a part of the boundary of the $(p-1)$-intersection $\{i_0 \ldots i_{p-1}\}$. The orientation is $\partial\{i_0 \ldots i_{p-1}\}=+\{i_0 \ldots i_p\}+\cdots$. Swapping any pair of indices reverses the orientation.

Note that intersections may be spacelike, timelike, or null (or vary between them).

There are junction conditions relating the singular stress-energy to the geometry.[4,5] Let ω_i be the connection in region $\{i\}$. At a hypersurface $\{ij\}$ there can be a discontinuity $\omega_i \neq \omega_j$. The junction conditions at a p-intersection are obtained from the intersection Lagrangian:

$$\sum_{n=1}^{[(d-1)/2]} \beta_n \mathcal{L}^n_{(p)},$$

$$\mathcal{L}^n_{(p)}(E, \omega_0, \ldots, \omega_p) = A_p \int_{s_{0\ldots p}} d^p t (\omega_1 - \omega_0)^{a_1 b_1} \cdots (\omega_p - \omega_0)^{a_p b_p} \Omega(t)^{a_{p+1} b_{p+1} \ldots a_n b_n} e_{a_1 \ldots b_n}, \qquad (6)$$

$$A_p = (-1)^{p(p-1)/2} \frac{n!}{(n-p)!}.$$

$\Omega(t)$ is the curvature of the interpolating connection $\omega(t)$:

$$\omega(t) := \sum_{i=0}^{p} t^i \omega_i, \quad \Omega(t) = d\omega(t) + \omega(t) \wedge \omega(t). \tag{7}$$

The $\Omega(t)^{a_{p+1}\ldots b_n}$ is short for the $(n-p)$-fold product: $\Omega(t)\wedge\cdots\wedge\Omega(t)$. The integral is over the p-dimensional simplex

$$s_{0\ldots p} = \left\{ t \in \mathbf{R}^{p+1} \,\middle|\, \sum_{i=0}^{p} t_i = 1, \text{ all } t_i \geqslant 0 \right\}. \tag{8}$$

The junction conditions come from explicit Euler variation with respect to the vielbein: $\delta_{E^c}\mathcal{L}_{(p)} = -2(T_{(d,d-p)})^b_c \tilde{e}_b$, where $T_{(d,d-p)}$ is the part of the singular stress-energy tensor with support on the intersection. The factor of -2 is explained in the Appendix. So the junction conditions can be written as

$$(T_{(d,d-p)})^b_c \tilde{e}_b = \frac{1}{2}(-1)^{(p-1)(p-2)/2} \sum_{n=p}^{[(d-1)/2]} \frac{n!}{(n-p)!} (\mathcal{E}^n_{(p)})_c, \tag{9}$$

$$(\mathcal{E}^n_{(p)})_c \equiv \int_{s_{1\ldots p+1}} d^p t (\omega_2 - \omega_1)^{a_1 b_1} \cdots (\omega_{p+1} - \omega_1)^{a_p b_p} \Omega(t)^{a_{p+1} b_{p+1} \ldots a_n b_n} e_{a_1 \ldots b_n c}. \tag{10}$$

$\tilde{e}$ is the natural volume element on the intersection. We note that $\mathcal{E}^n_{(p)}$ is zero if $p > n$. (In Einstein theory the only junction condition is that of the hypersurface, where if the energy tensor carried by it vanishes then so does the discontinuity of the connection, in the non-null case. For a general intersection in Lovelock gravity the energy tensor may vanish without implying vanishing of the connection discontinuities. Even for the single hypersurface case, $\mathcal{E}_{(1)} = \Sigma_n \beta_n \mathcal{E}^n_{(1)} = 0$ does not imply that the connection becomes continuous. Simple solutions where this happens can easily be found and such space–times have been called solitons.[31] If such a hypersurface is spacelike, there is a breakdown of causality. Another important case of vanishing energy tensor is that of the null hypersurface, that is, of the shock wave. Shock waves exist in GR[32] as well as in higher order Lovelock theory.)

Also there is another implicit junction condition: there is a well-defined (pseudo-) orthonormal frame everywhere. If this condition is not obeyed, then the above-presented formula is not valid. In the case of a hypersurface junction condition, it is equivalent to a well-defined induced geometry on the hypersurface. For higher co-dimension intersections it is a quite stringent condition. For example, for a co-dimension two intersection, there can be no deficit angle.

II. INTERSECTIONS IN AdS AND GAUSS-BONNET TERM

We have seen that there is a possibility to localize matter on an intersection in the Gauss–Bonnet theory. We now proceed to a specific example.

A. The bulk vacuum solution

We shall take the simplest kind of bulk solution. Each bulk region is a constant curvature region of space–time. Such a space–time satisfies $R_{\mu\nu\rho\sigma} = 1/[d(d-1)]R(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho})$, R being a constant.[33] There are three possibilities:

(i) de Sitter space ($R > 0$),
(ii) anti-de Sitter space ($R < 0$),
(iii) flat space ($R = 0$).

In the Einstein theory, constant curvature empty space will be one of the above three, depending on whether the cosmological constant is positive, negative, or zero. In the higher order Lovelock theory, it is possible that more than one type of constant curvature space–time will

satisfy the vacuum field equations. The different possibilities arise because the field equations are polynomial in the curvature. For a constant curvature, this just reduces to a polynomial equation in the curvature scalar.

A more general space–time would be made up of regions of less symmetric vacuum space–time. We will not attempt this here, but leave it as a project for the future.

We take the example of AdS bulk space–time, motivated by: (1) the Randall–Sundrum idea of the nonfactorizable metric[1] which allows gravitons to be approximately localized in a large extra dimension; (2) the special role of AdS space in recent advances;[35] (3) the simplicity of the problem from a mathematical point of view. AdS space has constant negative curvature:

$$\Omega^{ab} = -\frac{1}{l^2} E^a \wedge E^b. \tag{11}$$

The constant l has dimensions of length. It is easy to check that if we write

$$\omega^{ab} = \frac{1}{l}(u^a E^b - u^b E^a), \tag{12}$$

where u^a is a constant vector, we have, assuming zero torsion $dE^a = -\omega^a{}_b \wedge E^b$,

$$\Omega^{ab} = -\frac{u^2}{l^2} E^a \wedge E^b. \tag{13}$$

Above $u^2 = \eta_{ab} u^a u^b$. For an AdS solution, we take u to be space-like $u^2 = +1$. The opposite sign choice gives dS space–time. AdS, dS, or flat space is a vacuum solution of the general Lovelock theory (4) provided that the following relation is satisfied:

$$\sum_{n=0}^{[(d-1)/2]} \frac{(-u^2)^n (d-1)!}{(d-1-2n)!} \frac{\beta_n}{l^{2n}} = 0. \tag{14}$$

Now let us write the solution in terms of coordinates. We will write the AdS metric in conformally flat form. Define $u \cdot x \equiv \eta_{\mu\nu} u^{(\mu)} x^\nu$,

$$ds^2 = \frac{1}{((u \cdot x)/l + C)^2} \eta_{\mu\nu} dx^\mu dx^\nu, \quad (u \cdot x)/l + C > 0, \tag{15}$$

with C an arbitrary constant. Contact between (15) and (12) is made by the choice for the vielbein:

$$E^a = \frac{1}{(u \cdot x)/l + C} \delta^a_{(\mu)} dx^\mu.$$

We will only be interested in the vicinity of the intersection and will not worry here about the global details of joining together regions of AdS.

B. Three-way intersection

We will consider the simplest three-way vertex. There is a plane covered by coordinates $(x, y) \equiv (x^{d-2}, x^{d-1})$. It will also be convenient to use cylindrical coordinates: $x = \rho \cos\theta$, $y = \rho \sin\theta$. There are three bulk regions, $i = 1, 2, 3$, broken up by three hypersurfaces, $\{ij\}$, at $\theta = \text{const}$. The hypersurfaces meet at the intersection, $\{123\}$, at $\rho = 0$. The space–time is divided into regions:

region 1: $0 < \theta < \theta_1$,

region 2: $\theta_1 < \theta < \theta_2$,

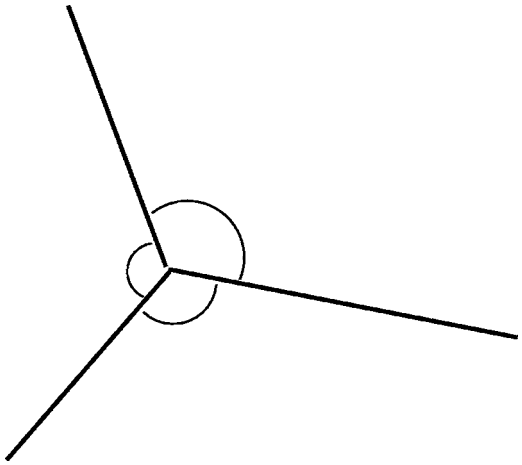

FIG. 1. The intersection of three hypersurfaces. Each bulk region, denoted by $\{i\}$, is a piece of constant curvature space–time. If there is no deficit angle we have $\theta_3=2\pi$. The three angles shown are θ_1, $\theta_2-\theta_1$, and $\theta_3-\theta_2$.

region 3: $\theta_2<\theta<\theta_3$, with the identification $\theta_3\equiv 0$. One can have a conical singularity at the intersection with deficit angle $2\pi-\theta_3$ but we will not do so for reasons we will mention. So we take $\theta_3=2\pi$ (Fig. 1). In each region i let $u_i=(0,\ldots,0,\cos\phi_i,\sin\phi_i)$ such that $u_i\cdot x=\rho\cos(\theta-\phi_i)$. The metric in each region takes the following form:

$$ds_i^2=\frac{1}{(\rho\cos(\theta-\phi_i)/l+1)^2}\eta_{\mu\nu}dx^\mu dx^\nu. \tag{16}$$

We have chosen $C=1$ here for convenience. We insist that the metric is continuous, so the factor $(u\cdot x)/l+1$ should be continuous across the walls:

$$\cos(\theta_1-\phi_1)=\cos(\theta_1-\phi_2), \tag{17}$$

$$\cos(\theta_2-\phi_2)=\cos(\theta_2-\phi_3), \tag{18}$$

$$\cos(\phi_3)=\cos(\phi_1). \tag{19}$$

There is the trivial solution $\phi_i=\phi_{i+1}$, which is smooth across the hypersurface. If we are to have any matter on the hypersurfaces (a brane) we must choose the nonsmooth solutions:

$$\begin{aligned}\phi_1&=-\phi_3=\theta_1-\theta_2,\\ \phi_2&=\theta_1+\theta_2.\end{aligned} \tag{20}$$

This allows for u to be different in each region. The spin-connection (12) is not single-valued at the walls.

At the intersection, we need more than just continuity of the metric. We must have a well-defined orthonormal basis

$$E_\mu^a E_\nu^b g^{\mu\nu}=\eta^{ab}$$

everywhere, including at $\rho=0$. Now, since the metric is conformally flat, the angle between two vectors is

$$v \angle w = \frac{v^\mu w^\nu g_{\mu\nu}}{(v^\mu v^\nu g_{\mu\nu})^{1/2}(w^\mu w^\nu g_{\mu\nu})^{1/2}} = \frac{v^\mu w^\nu \eta_{\mu\nu}}{(v^\mu v^\nu \eta_{\mu\nu})^{1/2}(w^\mu w^\nu \eta_{\mu\nu})^{1/2}}.$$

This is well known—a conformal transformation preserves angle. So theta is indeed a measure of the angle between vectors. At $\rho=0$, we have $E^a=(\ldots,\cos\theta_a,\sin\theta_a)$, but with the identification $\theta\equiv\theta+\theta_3$. Since $\eta^{ab}=E^a\angle E^b=\cos(\theta_b-\theta_a)$, for a well-defined orthonormal frame we require $\cos(\theta_b-\theta_a+r\theta_3)=1$ *or* 0 for arbitrary integer r, so we should set $\theta_3=2\pi$. Thus we insist upon having no deficit angle at the intersection.

C. The junction conditions

Recall that the junction condition at each p-intersection is (9). In the next section we shall evaluate the general form of $\mathcal{E}^n$ for the intersections in AdS. Here we shall stick to the codimension two intersection in the Einstein–Gauss–Bonnet theory. Furthermore, we shall not calculate the energy-momentum tensor on the branes but proceed to find what is at the intersection.

There is no contribution from the Einstein term: $\mathcal{E}^1_{(2)}=0$. Only the Gauss–Bonnet contributes. $\mathcal{E}^2_{(2)}$ is

$$(\mathcal{E}^2_{(2)})_f = (\omega_2-\omega_1)^{ab}\wedge(\omega_3-\omega_1)^{cd}\wedge e_{abcdf}\int_{s_{123}} d^2t.$$

The volume of the two-simplex is 1/2,

$$\begin{aligned}(\mathcal{E}^2_{(2)})_f &= \tfrac{1}{2}(\omega_2-\omega_1)^{ab}\wedge(\omega_3-\omega_1)^{cd}\wedge e_{fabcd}\\ &= -2(u_2-u_1)^a(u_3-u_1)^b E^c\wedge E^d\wedge e_{fabcd}\\ &= -2(d-4)(d-3)[(u_2-u_1)^{(1)}(u_3-u_1)^{(2)}-(u_2-u_1)^{(2)}(u_3-u_1)^{(1)}]e_{f(1)(2)}.\end{aligned}$$

The factor in square brackets is

$$\begin{aligned}&(\cos\phi_2-\cos\phi_1)(\sin\phi_3-\sin\phi_1)-(\cos\phi_3-\cos\phi_1)(\sin\phi_2-\sin\phi_1)\\ &\quad=\sin(\phi_3-\phi_2)+\sin(\phi_2-\phi_1)+\sin(\phi_1-\phi_3)\\ &\quad=\sin(2\theta_2)+\sin(2\theta_1-2\theta_2)-\sin(2\theta_1).\end{aligned}$$

Note $e_{(1)(2)}=\tilde{e}$ is the natural volume element on the intersection. Putting this into (9), we get the following result:

Proposition 2.1: The junction condition for the intersection is

$$(T_{123})^a_b = -2(d-4)(d-3)\beta_2[\sin(2\theta_2)+\sin(2\theta_1-2\theta_2)-\sin(2\theta_1)]\delta^a_b. \tag{21}$$

The singular matter on the intersection is a $(d-2)$-dimensional cosmological constant or tension. (If the energy tensor T^a_b on a hypersurface takes the form $-V\delta^a_b$, we will call the constant V the cosmological constant or tension of the membrane, which in some cases might be negative where it amounts to pressure. In this paper we are mainly interested in whether the value of the energy tensor is zero or not and we will be writing the tensor as $T^a_b=\Lambda\delta^a_b$ so one should bear in mind that $V=-\Lambda$.)

Using the double angle formulas, we can prove that this tension vanishes in $d\geqslant 5$ if and only if: either $\cos(2\theta_1)=1$, $\cos(2\theta_2)=1$, or $\cos(2\theta_1)=\cos(2\theta_2)$ and $\sin(2\theta_1)=\sin(2\theta_2)$. These solutions are not really intersections at all:

(i) $\theta_1=\theta_2\Rightarrow\phi_1=\phi_3=0$, region 2 is shrunk to zero; $\theta_1=0\Rightarrow\phi_2=\phi_3$, region 1 is shrunk to zero; or $\theta_2=2\pi\Rightarrow\phi_2=\phi_1$, region 3 is shrunk to zero. In these cases there is just a smooth AdS bulk.

(ii) $\theta_1=\pi\Rightarrow\phi_2=\phi_3$, $\theta_2=\pi\Rightarrow\phi_2=\phi_1$ or $\theta_1-\theta_2=\pi\Rightarrow\phi_3=\phi_1=\pi$ In these cases there is just a single hypersurface.

III. HIGHER CO-DIMENSION INTERSECTIONS IN AdS

So far we have dealt with co-dimension two intersections. We now proceed to look at the higher co-dimension simplicial intersection in AdS background. There are $p+1$ bulk regions, $\{i\}$, separated by $p+1$ hypersurfaces, $\{ij\}$, intersecting at the simplicial intersection $\{i_0 \ldots i_p\}$. The metric in each bulk region is, cf. (15):

$$ds^2 = \frac{1}{(u_i \cdot x + 1)^2}(\delta_{\alpha\beta} dx^\alpha dx^\beta + dx^2_{(d-p)}). \tag{22}$$

The branes intersect at $x^\alpha = (0, \ldots, 0)$. Each brane is paramterized generally by $f(x^\alpha) = 0$, and is assumed to be maximally symmetric in the other $d-p$ dimensions.

The continuity of the metric at each hypersurface $\{ij\}$: $(u_i - u_j) \cdot x = 0$, implies that $(u_i - u_j)$ is proportional to the normal vector to $\{ij\}$. Each AdS region is characterized by a unit spacelike vector $u_i^a, i = 0, \ldots, p$ and the same AdS scale l which we set to 1. Define

$$u_{ij} = u_i - u_j \tag{23}$$

and

$$u(t) = \sum_{i=0}^{p} t^i u_i \tag{24}$$

with $\Sigma_{i=0}^p t^i = 1$, and

$$R(t)^a_b = u(t)^2 \delta^a_b + N^a_b, \quad N^{ab} = \sum_{i=0}^{p} \sum_{j=0}^{p} t^i t^j u^a_{ij} u^b_{ij}. \tag{25}$$

Proposition 3.1: The curvature of the interpolating connection is

$$\Omega^{ab}(t) = - R(t)^{c[a} E_c \wedge E^{b]}, \tag{26}$$

where the symmetric matrix $R(t)$ is defined in (25).

Note: We will *not* need to take the u_i all of the same causal nature in this proof; each u_i may be time- or spacelike, or null.

Proof: By (12) the connection on each region i is assumed to be given by

$$\omega_i^{ab} = u_i^a E_i^b - u_i^b E_i^a. \tag{27}$$

The curvature of the interpolating connection $\omega(t) = \Sigma_{i=0}^p t^i \omega_i$ then is

$$\Omega(t)^{ab} = d\omega(t)^{ab} + \omega(t)^a_c \wedge \omega(t)^{cb} = - u(t)^2 E^a \wedge E^b + \sum_{i=0}^{p} t^i u_i^a u_{ic} E^b \wedge E_c + \sum_{ij} u_i^a u_{jc} E^c \wedge E^b - (a \leftrightarrow b) \tag{28}$$

where we have used zero torsion and metric continuity to calculate

$$d\omega(t)^{ab} = \sum_i t^i d\omega_i^{ab} = \sum_i t^i (u_i^a dE_i^b - u_i^b dE_i^a) = \sum_i t^i (- u_i^a \omega_{ic}^b \wedge E^c + u_i^b \omega_{ic}^a \wedge E^c), \tag{29}$$

where we drop the region index from the frame E after the derivative is taken as the metric itself is continuous, all E_i agree at the hypersurface, only its derivative jumps.

Now, by using $\Sigma_{i=0}^p t^i = 1$, we have

$$\sum_{ij} t^i t^j (u_i - u_j)^a (u_i - u_j)_c = 2\sum_i t^i u_i^a u_{ic} - 2\sum_{ij} t^i t^j u_i^a u_{jc} \tag{30}$$

so by (25) and (23) we get (26). □

The intersection junction conditions are (9) with

$$\mathcal{E}^n_{(p)} = 2^p(-1)^{n-p}\int_{s_{01\ldots p}} d^p t u^{a_1}_{10}\ldots u^{a_p}_{p0} E^{b_1\ldots b_p} R(t)^{a_{p+1}}_{c_{p+1}}\ldots R(t)^{a_n}_{c_n} E^{c_{p+1}b_{p+1}\ldots c_n b_n} e_{a_1\ldots b_n c}. \tag{31}$$

Note first that by $u_{ij}=u_{i0}-u_{j0}$ all terms involving N^a_b defined by (25) and (23) drop out in the previous equation by the presence of the factors $u_{10}\ldots u_{p0}$ (involving all vectors which span the normal space) and the antisymmetry of the volume form $e_{a1\ldots b_n c}$. Note that this also true if some u_{i0}'s are null. Now applying the identity

$$E^{c_1\ldots c_n}\wedge e_{d_1\ldots d_m} = \frac{m!}{(m-n)!}\delta^{c_1}_{[d_{m-n+1}}\ldots\delta^{c_n}_{d_m} e_{\ d_1\ldots d_{m-n}]}, \tag{32}$$

we can then write

$$\mathcal{E}^n_{(p)} = (-1)^{n-p}(-1)^{p(p-1)/2}2^p\int_{s_{01\ldots p}} d^p t u^{a_1}_{10}\ldots u^{a_p}_{p0}(u(t)^2)^{n-p}$$
$$\times\frac{(2n+1)!}{(p+1)!}\delta^{b_1}_{[b_1}\ldots\delta^{b_p}_{b_p}\delta^{a_{p+1}}_{a_{p+1}}\delta^{b_{p+1}}_{b_{p+1}}\ldots\delta^{a_n}_{a_n}\delta^{b_n}_{b_n} e_{\ ca_1\ldots a_p]}. \tag{33}$$

The factor of $(-1)^{p(p-1)/2}$ comes from the rearrangement of the indices. The quantity after the symbol $\times$ equals

$$\frac{(d-p-1)!}{(d-2n-1)!} e_{ca_1\ldots a_p} \tag{34}$$

and is calculated in the Appendix.

Let $n^1,\ldots,n^p$ be orthonormal vectors that span the normal space. The one free index intersection volume form is defined by

$$\tilde{e}_c = \prod_{i=1}^{p}(n^i\cdot n^i)(n^1)^{a_1}\ldots(n^p)^{a_p} e_{a_1\ldots a_p c}. \tag{35}$$

Note the difference in the position of the free index c from the previous formula.

If we define the matrix of components

$$u^j_i := u^a_{i0} n^j_a, \tag{36}$$

expanding the vectors u_{i0} in (33) in the orthonormal basis we have

$$u^{a_1}_{10}\ldots u^{a_p}_{p0} e_{a_1\ldots a_p c} = \det(u^j_i)\tilde{e}_c, \tag{37}$$

so finally

$$(\mathcal{E}^n_{(p)})_c = \frac{n!}{(n-p)!}\frac{(d-p-1)!}{(d-2n-1)!}(-1)^{n-p}(-1)^{p(p-1)/2}2^p\det(u^j_i)\int_{s_{01\ldots p}} d^p t(u(t)^2)^{n-p}\tilde{e}_c. \tag{38}$$

Substituting this in (9) and reinstating l, we get:

Proposition3.2: The junction condition for the simplicial p-intersection is

$$(T_{d,01\ldots p})^a_b = \Lambda_{d,01\ldots p}\delta^a_b,$$
$$\Lambda_{d,01\ldots p} = \sum_{n=p}^{[(d-1)/2]} \frac{\beta_n}{l^{2n-p}}(-1)^{n-p+1}\frac{n!}{(n-p)!}\frac{(d-p-1)!}{(d-2n-1)!}2^{p-1}\det(u_i^j)\int_{s_{01\ldots p}} d^p t(u(t)^2)^{n-p}, \tag{39}$$

where $T_{d,01\ldots p}$ is the energy-momentum tensor on the intersection.

Before proceeding let us first look at the Einstein case where only β_1 is nonzero. AdS and dS space–times correspond to the vector u being spacelike and timelike, respectively, so we find that the bulk cosmological constant is

$$V_d = -\Lambda_d = \mp \beta_1 \frac{(d-1)(d-2)}{2l^2}, \tag{40}$$

which is the standard formula with beta related to the Newton's constant G by $\beta_1 = (8\pi G)^{-1}$. The tension of a hypersurface in Einstein gravity reads

$$V_{d,10} = -\Lambda_{d,10} = (d-2)\frac{\beta_1}{l}(u_1 - u_0)^a n_a, \tag{41}$$

where n^a is the normal vector on the hypersurface $\{10\}$. Applying this to the geometry of the three-way intersection discussed in Sec. II B we find

$$V_{d,10} = (d-2)\frac{\beta_1}{l}(\sin(\phi_1 - \theta_0) - \sin(\phi_0 - \theta_0)) = (d-2)\frac{\beta_1}{l}2\sin(\phi_1 - \theta_0), \tag{42}$$

where $u_i = (\cos\phi_i, \sin\phi_i)$ and $n_i = (-\sin\theta_i, \cos\theta_i)$, and the positions of the hypersurfaces $\{10\}$,$\{21\}$,$\{02\}$ are $\theta_0, \theta_1, \theta_2$, respectively. We have labeled the regions by 0,1,2 instead of 1,2,3 as in Sec. II B. We have applied the continuity conditions (17) to get the left-hand side of (42). Then the tension is positive if $\phi_1 - \theta_0$ is greater than zero and smaller than π. In a similar fashion it is possible for all three to have positive tensions. In particular, the tensions become equal (and positive) in the symmetric case where the vectors u are symmetrically arranged and so are the hypersurfaces, with the directions of the u's lying in between the hypersurfaces at $\pi/3$ angle from them.[37] This setup on AdS background has been studied in the past, see, e.g., Ref. 39. In the following we will use the symmetrically arranged vectors u in the case of general co-dimension to show that $\det(u_i^j)$ in (39) is always positive. For special Lovelock gravities we will see that the tensions of the intersections are all positive.

Something interesting about the contributions of the individual Euler terms, that is, about the value of $\Lambda_{d,01\ldots p}$ when a single such term is considered or contributes, is that it never vanishes.

Proposition 3.3: Each term in (39) cannot vanish unless β_n is zero. (The terms can possibly cancel among themselves).

Proof: First recall:

$$u_i^j = \begin{pmatrix} u_{10}^{(1)} & \cdots & u_{10}^{(p)} \\ \vdots & \ddots & \vdots \\ u_{p0}^{(p)} & \cdots & u_{p0}^{(p)} \end{pmatrix}$$

and each vector u_{i0} is proportional to the normal vector of the hypersurface $\{0i\}$. If the determinant of u_i^j is zero then the vectors u_{i0} are not linearly independent. That is, they cannot span the p-dimensional normal space of the codimension p simplicial intersection so the configuration degenerates to a lower co-dimension intersection.

Also since

$$u(t) = \sum_{i=0}^{p} t^i u_i = u_0 + \sum_{i=1}^{p} t^i u_{i0}$$

and u_i's are spacelike vectors then $u(t)^2 \geqslant 0$. But u_{i0} are linearly independent space-like vectors which span the normal space and u_0 a spacelike vector on it, that is, $u(t)$ cannot be zero everywhere on the p-simplex. So the integral in (39) does not vanish. □

Now define

$$P_{d,p}(x) := 2^{p-1} \sum_{n=p}^{[(d-1)/2]} \frac{\beta_n}{l^{2n-p}} (-1)^{n-p+1} \frac{n!}{(n-p)!} \frac{(d-p-1)!}{(d-2n-1)!} x^{n-p}, \tag{43}$$

where the dependence of $P_{d,p}$ on β's and l is suppressed. $\Lambda_{d,01\ldots p}$ then reads

$$\Lambda_{d,01\ldots p} = \det(u_i^j) \int_{s_{01\ldots p}} d^p t P_{d,p}(u(t)^2). \tag{44}$$

We have the following

Proposition 3.4: A sufficient condition for $\Lambda_{d,01\ldots p} \neq 0$ is $P_{d,p}(x) > 0$ (or <0) for $0 < x < 1$.

Proof: Since, $|u(t)| \leqslant \Sigma_{i=0}^{p} t^i |u_i| = \Sigma_{i=0}^{p} t^i = 1$, by $|u_i| = 1$ with $|u| = \sqrt{u^2}$, the proposition is clear for $x = u(t)^2$ and $0 \leqslant x \leqslant 1$. Also if $u(t)^2 = 0$ then $0 = u(t) = \Sigma_{i=0}^{p} t^i u_i$, so by linear independence of the t^i we get that all $u_i = 0$; this happens only at one point on the simplex. On a similar basis, if $u(t)^2 = 1$ then all vectors u_i must be equal; $u(t)^2 = 1$ happens only at the $p+1$ points, the zero-dimensional faces of the simplex. So for the integral (44) one may take $0 < x < 1$ and if $P_{d,p} > 0$ (or <0) in this region the integral does not vanish. □

An interesting case we can study is Chamseddine's Chern–Simons theory with AdS gauge group, in d=odd.[40,9] It is a Chern-Simons theory from an Euler density in $d+1$=even dimensions with tangent space being AdS instead of Minkowski. This Chern-Simons theory is classically equivalent to a Lovelock gravity, existing in d=odd, with coefficients

$$\beta_n^C = \kappa (d-2n)! \frac{(\pm 1)^{n+1} \lambda^{2n-d}}{d-2n} \binom{k}{n} = \kappa (\pm 1)^{n+1} \lambda^{2n-d} (d-2n-1)! \binom{k}{n}, \tag{45}$$

where $n = 0, \ldots, k$ with $k = (d-1)/2 = [(d-1)/2]$ and the minus (plus) sign corresponds to the dS (AdS) group case and λ is the dS (AdS) gauge group length parameter and κ a dimensionless constant. [By considering intersections in Chamseddine's theory we go through a curious kind of cycle- Chern–Simons (gauge theory) → Lovelock Gravity → Chern–Simons (intersection terms). Whether there is anything deep behind this or just coincidence, we do not know.] The factor $(d-2n)!$ comes from our definition of the Euler terms in (4) compared to the definition in the references.

It is easy to see that the bulk equations of motion for our AdS background (11) implies $l^2 = \lambda^2$. This is the vacuum solution of the theory. As both variables are assumed positive we have $\lambda = l$. Using the formula for β_n^C above in (43) and redefining the summed index as $n-p=m$ we see that

$$\begin{aligned} P_{d,p}(x) &= -\kappa 2^{p-1} l^{p-d} \frac{k!(2k-p)!}{(k-p)!} \sum_{m=0}^{k-p} (\pm x)^m \frac{(k-p)!}{m!(k-p-m)!} \\ &= -\kappa 2^{p-1} l^{p-d} \frac{k!(2k-p)!}{(k-p)!} (1-x)^{k-p}, \quad k := \frac{d-1}{2}. \end{aligned} \tag{46}$$

So we obtain the following formula for the co-dimension p membrane embedded at the intersection of the regions labeled by $0, 1, \ldots, p$ in Chamseddine's theory

$$\Lambda_{d,01\ldots p} = -\kappa 2^{p-1} l^{p-d} \frac{k!(2k-p)!}{(k-p)!} \det(u_i^j) \int_{s_{01\ldots p}} d^p t (1-u(t)^2)^{k-p}. \tag{47}$$

All these Λ's are nonzero: as the polynomial does not change sign for $0<x<1$ so we see from Proposition 3.4 that (for Chamseddine's theory with AdS group) $\Lambda_{d,01\ldots p} \neq 0$.

Let the vectors $u_0, \ldots, u_p$ be symmetrically arranged in the normal space forming a symmetric hedgehog. This is discussed in Appendix D where formulas for $\det(u_i^j)$ and $u(t)^2$ are obtained. One finds

$$\Lambda_{d,p} = -\kappa l^{p-d} \sqrt{2} (2\sqrt{6})^{p-1} \frac{k!(2k-p)!}{(k-p)!} \left(1+\frac{1}{k}\right)^{k-p/2} \int_{s_p} d^p t \left\{1 - \sum_{i=0}^{p} t_i^2\right\}^{k-p}, \tag{48}$$

where s_p is any p-simplex, as by symmetry the tensions of all $(d-p)$-dimensional membranes in the configuration are the same. One could say that $V_{d,p} = -\Lambda_{d,p}$ is the tension of *the* (maximally symmetric) co-dimension p membrane in the vacuum of Chamseddine's gravity; it has been emphasized at the introduction that these membranes are embedded in space–time without causing singularities or changing its topology, for $p=1, \ldots, k$. The tensions in this formula depend only on the dimensionless κ, the length l, and the dimensions d and p and they are all positive.

Let us now turn to d=even. Consider the following Lagrangian in $d=2k+2$ dimensions defined as

$$\kappa f\left(\left(\Omega \pm \frac{1}{\lambda^2} E \wedge E\right)^{k+1}\right) = \kappa \sum_{n=0}^{k} \frac{(k+1)!}{n!(k+1-n)!} (\pm 1)^{k+1-n} \lambda^{2n-2k-2} f(\Omega^n E^{2k+2-2n}) + \kappa f(\Omega^{k+1}). \tag{49}$$

For the $+$ $(-)$ sign choice the constant curvature vacuum solution is an AdS (dS) space–time with curvature proportional to λ^{-2} where λ is a length parameter; we will call (49) the AdS and dS Born–Infeld theories, respectively.[41,9] κ is again a dimensionless parameter.

The last term is topological (exact form locally) and drops out of the equations of motion. So using (5) and the general definition of the Lovelock Lagrangian (4) we find

$$\beta_n^{\mathrm{BI}} = \kappa (\pm 1)^{k+1-n} \lambda^{2n-d} d(d-2n-1)! \binom{k}{n}, \tag{50}$$

where again $k=d/2-1=[(d-1)/2]$, $n=0, \ldots, k$. These coefficients are similar to β_n^C's so one may say that Born–Infeld theory is the analogue to Chamseddine theory in d=even.

Again the bulk equations of motion for our AdS background (11) give that $\lambda^2 = l^2$ for the AdS Born–Infeld theory. Putting the AdS β_n^{BI}'s into (43) we have

$$P_{d,p}(x) = -\kappa 2^{p-1} d \frac{k!(d-p-1)!}{(k-p)!} l^{p-d} (1-x)^{k-p}. \tag{51}$$

From this we obtain formulas similar to (47) and (48), and from Proposition 4 we have that for (AdS Born–Infeld theory) all $\Lambda_{d,01\ldots p}$ are nonzero.

Note that the results for nonvanishing simplicial intersection's energy tensors are due to the high symmetry of the system: the bulk regions are portions of the same, highly symmetric space–time, AdS, and the gravity theories have an AdS with a given radius as the single vacuum solution. In general, vanishing (simplicial) intersection's tensor does *not* imply degeneration of the intersection, that is, the connection can be discontinuous at the hypersurfaces. On the other hand, it is an interesting fact that the high symmetry of the background and of the theory makes all these intersection energy tensors (tensions of the embedded membranes) strictly nonzero.

In d=even it is easy to see why the polynomials get these summed expressions (49) and in turn by the similarity of the coefficients, to see why in Chamseddine's Lagrangian expressions get

simplified too. In fact the simplicity has nothing to do with the AdS background we mainly use in this work: according to our discussion in Ref. 5 the simplicial intersection Lagrangians are generated by expanding the polynomial

$$\eta_{\mathrm{BI}} = \kappa f((\Omega_F \pm \lambda^{-2} E(t) \wedge E(t))^{k+1}) = \kappa f((d_t \omega + \Omega(t) \pm \lambda^{-2} E(t) \wedge E(t))^{k+1}). \tag{52}$$

The intersection Lagrangians read[5]

$$\int_{s_{01\ldots p}} \eta_{\mathrm{BI}} = \kappa(-1)^{p(p-1)/2} \frac{(k+1)!}{(k+1-p)!} \int_{s_{01\ldots p}} d^p t f((\omega_1 - \omega_0) \ldots (\omega_p - \omega_0)[\Omega(t) \pm \lambda^{-2} E \wedge E]^{k+1-p}) \tag{53}$$

from which the equations of motion (junction conditions) are obtained by merely varying with respect to the frame E, as the variation with respect to the connection vanishes under the zero torsion condition for the frame on each bulk region.[5] For AdS backgrounds and going through the steps that lead to (39) we can show that (53) leads to (51). (53) can be applied to more general backgrounds such as the asymptotically AdS black holes of these theories, see, e.g., Refs. 41, 9, and 10 which will support less trivial energy tensors and time evolution at the intersection hypersurfaces.

IV. NONSIMPLICIAL INTERSECTIONS AND AdS BOUNDARY

We now return to a co-dimension two intersection. Let us now see what happens if there are four or more hypersurfaces intersecting. We have bulk regions $i=1,\ldots,m$ with hypersurfaces given by the configuration of angles: $\theta_1,\ldots,\theta_m$. We label the intersection as I.

The metric continuity condition $(u_i - u_{i+1}) \cdot x_i = 0$ for the ith hypersurface gives

$$\cos(\theta_i - \phi_i) = \cos(\theta_i - \phi_{i+1}) \tag{54}$$

writing $x_i = \rho_i(\cos\theta_i, \sin\theta_i)$ where (ρ_i, θ_i) is the position of the ith hypersurface on plane. One solution of this equation says that $\phi_i - \phi_{i+1}$ is integer multiple of 2π which is rejected as implying that $u_i = u_{i+1}$ which would make the connection continuous there by (12). The other is $\theta_i - \phi_{i+1} = -(\theta_i - \phi_i) + 2\pi\nu_i$ or

$$\theta_i = \tfrac{1}{2}(\phi_i + \phi_{i+1}) + \nu_i \pi. \tag{55}$$

$i=1,\ldots,m$ with the convention $\phi_{m+1} = \phi_1$. ν_i's are integers. There is a discontinuity $u_i \neq u_{i+1}$ which implies also the discontinuity $\omega_i \neq \omega_{i+1}$ of the connection, from the formula (12).

Now one finds

$$\sum_{j=1}^{i-1} (-1)^j \theta_j + \sum_{j=i}^{m} (-1)^{m-j} \theta_j = (-1)^i \frac{(-1)^m - 1}{2} \phi_i + \bar{\nu}_i \pi, \tag{56}$$

where $\bar{\nu}_i = \Sigma_{j=1}^{i-1}(-1)^j \nu_j + \Sigma_{j=i}^{m}(-1)^{m-j}\nu_j$.

For $m=$even one finds for all i the single expression

$$\theta_1 - \theta_2 + \theta_3 - \theta_4 + \cdots + \theta_{m-1} - \theta_m = -\bar{\nu}\pi, \tag{57}$$

where all $\bar{\nu}_i$'s are equal and denoted $\bar{\nu}$. The angles ϕ_i drop out. We have chosen $0 \leqslant \theta_1 < \theta_2 < \ldots < \theta_m < 2\pi$. It is not hard to see that the above-presented equation makes sense only for $\bar{\nu} = 1$. So in this case we cannot put the discontinuity hypersurfaces anywhere we like, without making the metric discontinuous. So ϕ_i's cannot be expressed in terms of the positions of the hypersurfaces. The tension in I is only a function of the bulk regions data ϕ_i. The intersection behaves rather as part of the background. The same happens to the analogous situation when we study collisions.

For an $m=$odd number of hypersurfaces we have from the above-presented formula

$$\sum_{j=1}^{i-1}(-1)^j\theta_j-\sum_{j=i}^{m}(-1)^j\theta_j=(-1)^{i-1}\phi_i+\bar{\nu}_i\pi. \tag{58}$$

We then derive:

$$(-1)^i(\phi_{i+1}-\phi_i)=2\sum_{j=1}^{i-1}(-1)^j\theta_j-2\sum_{j=i+1}^{m}(-1)^j\theta_j-(\bar{\nu}_{i+1}+\bar{\nu}_i)\pi. \tag{59}$$

We need the junction conditions for a nonsimplicial intersection. It is worthwhile digressing to explain a bit the abstract approach of Ref. 5, which allows us at once to write down the answer. In the following we give only a sketch of the method. For a full account the reader should consult Ref. 5.

The intersection Lagrangians are obtained by expanding a polynomial

$$\eta=(d_t\omega(t)+\Omega(t))^{a_1\ldots a_{2n}}\wedge e_{a_1\ldots a_{2n}}. \tag{60}$$

The structure of the Lagrangian at the intersection {123} of the hypersurfaces {12}, {23}, {31}, separating three bulk regions, given by

$$\mathcal{L}_{123}=\int_{s_{123}}\eta \tag{61}$$

is a result of the simplex boundary rule

$$\partial s_{123}=s_{23}-s_{13}+s_{12}. \tag{62}$$

See Appendix C for the general definition of the simplex and the associated boundary operator. The form η is a generalized Lagrangian, an example of which we used in (52). η generates the intersection Lagrangians according to a rule like (61) by integrating over t. Here t is the coordinate on the simplex. More generally t is the coordinate on a chain which is dual to the intersection in the following sense.

Consider a nonsimplicial intersection, for example of four hypersurfaces {12}, {23}, {34}, {41}, separating four bulk regions. We consider a three-dimensional simplex with vertices labeled by 1,…,4. The Lagrangian at the intersection is constructed by finding a chain (a chain or p-chain is, for our purposes, a linear combination of p-dimensional simplices with integer or rational coefficients.) c on that simplex such that

$$\partial c=s_{12}+s_{23}+s_{34}+s_{41}, \tag{63}$$

where the right-hand side reflects the arrangement of the hypersurfaces on the normal plane of their intersection.

By (62) it is easy to see that such a chain is

$$c=s_{123}+s_{134}, \tag{64}$$

where the boundary operator acts linearly; c is not unique, different c's obeying (63) differ by a chain which is itself a boundary. Then the Lagrangian, given by

$$\int_c\eta \tag{65}$$

is

$$\mathcal{L}_{123}+\mathcal{L}_{134}. \tag{66}$$

As c is not unique, this Lagrangian is not unique either. If c' is another chain satisfying (63) then $c'=c+\partial\sigma$ for some chain σ, so by Stokes theorem the Lagrangians corresponding to them are

related by $\int_{c'}\eta=\int_c\eta+\int_\sigma d_t\eta$. It is a special property of the polynomials (60) that the pull back of $d_t\eta+d_x\eta$ onto the $d+1$ dimensional space $\sigma\times$ (intersection) vanishes. So Lagrangians constructed by different chains c differ only by exact forms

$$\int_c \eta=\int_{c'} \eta+d\int_\sigma \eta.$$

It easy to construct now the Lagrangian for the nonsimplicial intersection of m hypersurfaces which reads $\mathcal{L}_I=\mathcal{L}_{123}+\mathcal{L}_{134}+\cdots+\mathcal{L}_{1,m-1,m}$. This gives

$$\begin{aligned}(T_I)^a_b&=-2(d-4)(d-3)\beta_2\Delta\,\delta^a_b,\\ \Delta&=\sum_{i=1}^{m}\sin(\phi_{i+1}-\phi_i)\end{aligned}\tag{67}$$

with $\phi_{m+1}\equiv\phi_1$. Using (59), we can express Δ purely in terms of the configuration:

$$\Delta=\sum_i \sin\left(2\sum_{j=1}^{i-1}(-1)^{i-j}\theta_j-2\sum_{j=i+1}^{m}(-1)^{i-j}\theta_j-(-1)^i(\bar{\nu}_{i+1}+\bar{\nu}_i)\pi\right).\tag{68}$$

The solution $\phi_i=\phi_{i+1}$ is trivial so the terms in brackets cannot vanish individually. However, there are more degrees of freedom than for the three-way intersection. There should be nontrivial zeroes of Δ. The simplest three-way planar intersection (Sec. II) in AdS background will have singular matter at the intersection. The intersection of a higher odd number of branes may or may not, depending on the geometry.

We now point out an interesting relation between the limit $m\to\infty$ of the number of intersecting hypersurfaces and the boundary of AdS. In the example of a nonsimplicial co-dimension two intersection of m hypersurfaces let the vectors u_i be arranged symmetrically by

$$\phi_i=(i-1)\frac{2\pi}{m},\quad i=1,2,\ldots,m.\tag{69}$$

From (55) and taking $\nu_1=\ldots\nu_{m-1}=0$ and $\nu_m=1$, which is also consistent with the constraint $\bar{\nu}=1$ in (57) for $m=$even, we find

$$\begin{aligned}\theta_{i|i\neq m}&=\left(i-\frac{1}{2}\right)\frac{2\pi}{m},\\ \theta_m&=\frac{(m-1)}{m}\pi+\pi=\left(m-\frac{1}{2}\right)\frac{2\pi}{m}.\end{aligned}\tag{70}$$

So the direction of the u vector of every bulk region is in between the directions of the hypersurfaces bounding that region.

From the ϕ_i's and θ_i's we find that the metric is given by $g_{\mu\nu}=\eta_{\mu\nu}(C+(1/l)\rho g_m(\theta))^{-2}$ where ρ is the radial variable on the normal plane, $C>0$ is a constant we usually set to 1, and

$$g_m(\theta)=\left\{\cos\left(\theta-i\frac{2\pi}{m}\right)\quad,\quad -\frac{\pi}{m}+i\frac{2\pi}{m}\leqslant\theta\leqslant\frac{\pi}{m}+i\frac{2\pi}{m},\quad i=0,1,\ldots,m-1.\right.\tag{71}$$

It is continuous and 2π-periodic in the 2π-periodic variable θ. In fact the function repeats the same values in every region: at all hypersurfaces it has the value $\cos(\pi/m)$ and approaches the value 1 in the middle of the interval; it is a copy of

$$\cos\theta, \quad \theta \in \left[-\frac{\pi}{m}, \frac{\pi}{m}\right] \tag{72}$$

for m times. So the interior of the bulk regions is a copy of that piece of the AdS space–time with radius l, a $1/m$ of the whole. In particular we have that

$$\cos\left(\frac{\pi}{m}\right) \leqslant g_m(\theta) \leqslant 1, \quad \forall\ \theta \in [0, 2\pi]. \tag{73}$$

If we take the limit $m \to \infty$ the function $g_m(\theta)$ approaches the constant value 1. In this limit the metric of the space–time becomes

$$ds^2_{m\to\infty} = \left(C + \frac{1}{l}\rho\right)^{-2} (d\rho^2 + \rho^2 d\theta^2 + \eta_{\alpha\beta} dx^\alpha dx^\beta), \tag{74}$$

where x^α are the coordinates parallel to the co-dimension two intersection. The curvature two-form is calculated to be

$$\Omega^{ab} = \delta^a_i \frac{1}{l^2}\left(1 + C\frac{l}{\rho}\right) Q^i_j E^j \wedge E^b - \delta^b_i \frac{1}{l^2}\left(1 + C\frac{l}{\rho}\right) Q^i_j E^j \wedge E^a - \frac{1}{l^2} E^a \wedge E^b, \tag{75}$$

where $i, j = 1, 2$ are indices of the Cartesian coordinates on (ρ, θ) plane and $Q^i_j = \delta^{ij} - x^i x^j/\rho^2$ projection operator on it, and the Ricci scalar is

$$R = 2(d-1)\frac{1}{l^2}\left(1 + C\frac{l}{\rho}\right) - d(d-1)\frac{1}{l^2}. \tag{76}$$

For $C \neq 0$ the space develops a curvature singularity.

The curvature singularity can actually be removed if the intersection is located within the boundary of each AdS bulk region. The constant C, taken to be the same for all regions, restricts the coordinates via $C + u_i \cdot x/l > 0$ for the ith region. Call A_i the space defined by this inequality. If we set $(C=0)$ we have that the metric in A_i is

$$ds^2_i = \frac{l^2}{(u_i \cdot x)^2} \eta_{\mu\nu} dx^\mu dx^\nu \tag{77}$$

with $u_i \cdot x > 0$. We want to include the space $u_i \cdot x = 0$ in A_i i.e., to consider the closure $\bar{A}_i$ of the open A_i. The metric (77) does not extend over the boundary of this space and it is given a meaning along the lines of Penrose's conformal compactification. One may multiply this metric with a function f with a first-order zero at the points x with $u_i \cdot x = 0$, to get a metric $d\tilde{s}^2_i = f^2 ds^2_i$ which extends to the boundary $u_i \cdot x = 0$ of A_i and defines a metric $d\tilde{s}^2_{ib}$ in it; the function f is arbitrarily chosen in $\bar{A}_i$, as long as it has a first-order zero at the boundary. As there is no natural choice of f, the coefficient of the zero is arbitrary and the metric $d\tilde{s}^2_{ib}$ is only well-defined up to conformal transformations. A_i is a part of the AdS space–time, the patch covered in Poincare coordinates which we have used to write the AdS metric in (77) and $u_i \cdot x = 0$ is a part of the AdS boundary. The boundary has the topology of sphere times the real line: $\mathbf{S}^{d-1} \times \mathbf{R}$.[33,34]

So let $C=0$ in the bulk regions so that the ith region is a subspace of A_i. The intersection is located at a common co-dimension two subset of the boundary of all A_i's; it is given by $\rho = 0$ in each one of them. When this is the case the infinite m metric reads

$$ds^2_{m\to\infty} = \frac{l^2}{\rho^2}(d\rho^2 + \rho^2 d\theta^2 + \eta_{\alpha\beta} dx^\alpha dx^\beta) = \frac{l^2}{\rho^2}(d\rho^2 + \eta_{\alpha\beta} dx^\alpha dx^\beta) + l^2 d\theta^2, \tag{78}$$

which is nothing but a $(d-1)$-dimensional AdS times a circle with radius l: $\mathrm{AdS}_{d-1} \times \mathbf{S}^1$. That is, a dimension gets compactified and $\rho = 0$ becomes the boundary of an AdS (a single Poincare patch of an AdS_{d-1}). The AdS_{d-1} metric is conformal (with a constant factor) to that of the $\mathrm{AdS}_{d|\theta=\mathrm{const.}}$

and it is the AdS living at each hypersurface, ending at $\rho=0$. The boundary of the limiting space–time has topology $\mathbf{S}^{d-2}\times\mathbf{S}^1\times\mathbf{R}$.

We have mentioned that because the metric at the boundary of the AdS is defined up to conformal transformations the energy tensor there has to be traceless. In our case it is diagonal so it should vanish identically. Now for finite m the tension at the intersection (67) via (69) reads

$$2(d-3)(d-4)\beta_2 l^{-2}\cdot m\sin\frac{2\pi}{m}. \tag{79}$$

Absence of a curvature singularity in the limit $m\to\infty$ is consistent only with $\beta_2=0$ (or $d\leqslant 4$) i.e., only Einstein gravity. This is for the symmetric configuration (69). On the other hand take m =even and consider the configuration

$$\phi_i=(i-1)\frac{2\pi}{m}+(-1)^i\epsilon,\quad i=1,\ldots,m=\text{even}, \tag{80}$$

where ϵ is a constant so that by the metric continuity condition (55) the positions (70) remain unchanged, employing the fact that for m=even the positions θ_i do not fix completely the ϕ_i's. The limiting metric in this case is

$$ds^2_{m\to\infty}=\frac{l^2}{\cos^2\epsilon}\frac{1}{\rho^2}(d\rho^2+\eta_{\alpha\beta}dx^\alpha dx^\beta)+\frac{l^2}{\cos^2\epsilon}d\theta^2, \tag{81}$$

namely just the radii l of (78) are rescaled. From (67) and finite m one finds for the tension on the intersection

$$2(d-3)(d-4)\beta_2 l^{-2}\cdot m\sin\frac{2\pi}{m}\cdot\cos(2\epsilon). \tag{82}$$

For conformal matter on the intersection this should vanish, which happens in Einstein–Gauss–Bonnet theory if and only if

$$\cos^2\epsilon=\tfrac{1}{2} \tag{83}$$

determining completely the limiting metric (81).

Conversely, note that in $d\geqslant 5$ Einstein gravity alone could not completely fix the metric (81). It is the higher Lovelock term which can reach the co-dimension two submanifold $\rho=0$ and fix the metric. In fact one can prove the following

Proposition 4.1: Any configuration converges in the limit $m\to\infty$ to the family of metrics (81). In Einstein gravity the whole family is allowed and the limit is ambiguous. When the Gauss–Bonnet term is included a single element is picked by (83).

Proof: From (55) we have

$$\theta_{i+1}-\theta_i=\tfrac{1}{2}(\phi_{i+2}-\phi_i)+(\nu_{i+1}-\nu_i)\pi. \tag{84}$$

In the $i+1$th region the argument of the cosine in the intersections metric (77) ranges according to

$$\tfrac{1}{2}(\phi_i-\phi_{i+1})+\nu_i\pi\leqslant\theta-\phi_{i+1}\leqslant\tfrac{1}{2}(\phi_{i+2}-\phi_{i+1})+\nu_{i+1}\pi. \tag{85}$$

In the limit $m\to\infty$, $(\theta_{i+1}-\theta_i)\to 0$ (or to 2π when $i=m$ with $\theta_{m+1}\equiv\theta_1+2\pi$.) From the first formula we see that the argument of the cosine goes to the fixed value

$$\tfrac{1}{2}(\phi_i-\phi_{i+1})+\nu_i\pi=\tfrac{1}{2}(\phi_{i+2}-\phi_{i+1})+\nu_{i+1}\pi \tag{86}$$

up to a possible 2π. From this equality we see that in the limit $m\to\infty$,

$$\tfrac{1}{2}(\phi_{i+1}-\phi_i)=(-1)^i\epsilon+\nu\pi \tag{87}$$

for some constant ϵ for an integer ν. (Comparing with (55), this implies $\phi_i\to\theta_i+(-1)^{i-1}\epsilon$ plus integer multiples of $\pi/2$.) That is, the limiting metric is given by the one-parameter family of metrics (81).

Now the quantity Δ in (67) reads for large m,

$$\Delta=\frac{1}{2}\sum_{i=1}^{m}\cos(\phi_{i+1}-\phi_i)\sin 2(\theta_i-\theta_{i-1}), \tag{88}$$

neglecting terms of order $(\theta_i-\theta_{i+1})^2\sim 1/m^2$ in the sum. As the sines in (88) are of order $1/m$ only the order one part of the cosine's argument matters for large m. This has been identified as $(-1)^i 2\epsilon$. Δ converges to $2\pi\cos(2\epsilon)$ and the tension on the intersection vanishes under (83). Put differently, one sets this tension to zero for any m obtaining relations among ϕ whose limit constrained by (84) is given by (83) with (87). □

Summarizing, if the number m of intersecting hypersurfaces separated by AdS backgrounds goes to infinity, the limiting space–time does not have $1/\rho$ curvature singularities if the intersection is put at the boundary of each AdS region. The constraint for a traceless energy tensor at the intersection can be satisfied, as described in Proposition (4.1).

V. COLLIDING SHELLS AND DOMINANT ENERGY CONDITION

A collision is described by an intersection with the timelike coordinate being on the plane of intersection. We take the vectors u to be timelike, that is, we consider dS space–time. The three normal vectors u_i-u_j are spacelike; let $u_i=(\cosh\zeta_i,\sinh\zeta_i)$ so $(u_i-u_j)^2=2(\cosh(\zeta_i-\zeta_j)-1)>0$, so the hypersurfaces are actually timelike. Let the positions of the hypersurfaces be given by the configuration of rapidities: ψ_1, ψ_2 ψ_3. A general point on a hypersurface is labeled $\tau(\cosh\psi_i,\sinh\psi_i)$, suppressing the other dimensions. (It is clear that the description of collisions in dS is an analytic continuation of that of intersections in AdS, so some aspects of intersections can be translated to the collisions. Consider then a nonsimplicial collision, of m hypersurfaces. When $m=\text{even}>4$ without much thought we get the constraint

$$\psi_1-\psi_2+\cdots+\psi_{m-1}-\psi_m=0 \tag{89}$$

with the right-hand side being zero as there is no 2π periodicity here. An explicit calculation confirms this. In this case the pressure p at the intersection is not completely determined by the rapidities ψ_i. One of the ζ_i must also be specified.)

From the calculation of Sec. IV we have that the pressure p in the spacelike collision surface is

$$\mathsf{p}=2\sum_{n=2}(-1)^n\frac{\beta_n}{l^{2n-2}}n(n-1)\frac{(d-3)!}{(d-2n-1)!}\det(u_j^i)\int_{s_{012}}d^2t(u(t)^2)^{n-2}. \tag{90}$$

[Calculating the energy tensor on a spacelike hypersurface one should keep in mind that we define the volume element (35) to be negative for such hypersurfaces so the energy tensor is minus the value given at (39).] One can prove an analogous situation to Proposition 3.3. The reasoning is similar, only now $u(t)^2\leqslant 0$, or more specifically $u(t)^2\leqslant -1$. None of the terms in the sum vanishes alone. So in general, and in particular for the special Lovelock gravities described by the above-discussed Chamseddine and Born-Infeld Lagrangians, the pressure p does not vanish. That is in general intersecting inflationary space–times with different timelike coordinate lead to matter with pressure at their spacelike intersection in Lovelock gravity.

This explicit example gives us the chance to point out the following, already clear from the general formulas: in a collision, i.e., intersection of *timelike* hypersurfaces, there is in general matter appearing at the spacelike collision surface. Viewed on the normal space, this looks like a collision of particles such that an instanton may appear at the collision event. Now, the dominant

energy condition[33] is that for all timelike ξ^a, $T_{ab}\xi^a\xi^b \geqslant 0$ and $T^{ab}\xi_a$ is a nonspacelike vector, where T^{ab} is the energy tensor. This is clearly violated by the above-noted energy tensor. Thus the dominant energy condition (DEC) can be violated at collisions in Lovelock gravity.

In Einstein's theory, the gravitational field equations themselves cannot impose the dominant energy condition. One must also specify the matter equations of motion or, equivalently, the stress-energy tensor. For example, the junction conditions allow a spacelike hypersurface with spacelike matter.

However as we discussed in Ref. 4, for colliding shells, the dominant energy condition at the collision is obeyed if and only if there is no conical defect. So the dominant energy condition arises naturally *at the collision* from a condition on the regularity of the metric. Suppose that we have some matter action to describe the free shells which respects the dominant energy condition. When the shells collide, perhaps there could also be some contact interaction at the collision surface, so in principle, we could add an interaction term to the matter action. The regularity of the metric imposes that this interaction term must vanish.

For the higher order Lovelock theories, this condition does not arise naturally. The junction conditions for the collision surface are nontrivial. They allow for pressure and momentum localized at the collision. This pressure and momentum is purely tangential to the surface. So the collision process will involve something flowing along the space-like collision surface in violation of the dominant energy condition. So the higher order Lovelock theories impose no energy condition on the type of interaction allowed. In general, we could have a collision where all of the shells are ingoing and annihilate each other, with the energy flowing away to spatial infinity along the collision surface. These novelties arise from the peculiar fact that in the energy exchange relations[4] for the collision of shells the purely stress tensor at the spacelike collision surface contributes with components normal on the surface.

On the other hand, when we consider the matter component of the theory it is very natural to impose the DEC, which is interpreted as that the energy cannot flow faster than the speed of light. If the matter part of the theory is such that the DEC is respected, then this places a strong restriction on the kinds of geometry which are allowed. For example, if two maximally symmetric shells collide in dS, it is impossible to have a single outgoing maximally symmetric brane in dS bulk. There must be more than one outgoing brane and/or some disturbance of the bulk. So we have a constraint which is a kind of selection rule for the allowed collisions due to the higher order Lovelock terms.

As a last comment, we should note that the other energy conditions are also violated in general. The dominant condition for a perfect fluid with energy density ϱ and pressure p reads $\varrho \geqslant |\mathsf{p}|$. As discussed this is not satisfied in an arbitrary collision of shells in Lovelock gravity because $\varrho = 0$ and p is in general nonzero. The weak energy condition reads $\varrho \geqslant 0$ and $\varrho + \mathsf{p} \geqslant 0$. This is satisfied in the above-discussed examples if $\mathsf{p} \geqslant 0$. [Note that (regarding the bulk cosmological constant as matter) the dS background itself satisfies the dominant and weak energy conditions, and also the null energy condition which simply reads $\varrho + \mathsf{p} \geqslant 0$. It does not satisfy the strong energy condition: $\varrho + \mathsf{p} \geqslant 0$ and $\varrho + 3\mathsf{p} \geqslant 0$ as $\mathsf{p} = -\varrho \leqslant 0$. The AdS background satisfies the null and strong energy condition but it does not agree with the weak and the dominant energy conditions.] This is certainly not the case in general: for example if we calculate (90) for the case of Chamseddine gravity we get

$$\mathsf{p} = (-1)^{k+1} \cdot \frac{1}{2}\kappa l^{2-d}(d-1)(d-3)(d-3)!\det(u^i_j)\int_{s_{012}} d^2t(-1-u(t)^2)^{k-2}, \tag{91}$$

where $k=(d-1)/2$. This is positive if $d=4m-1$, for some integer m, and violates the weak energy condition by being negative in $d=4m+1$ dimensions.

VI. DIMENSIONALITIES OF INTERSECTIONS AND FOUR-DIMENSIONAL BRANE UNIVERSE

In d bulk dimensions Lovelock Lagrangian contains terms of nth power of the curvature, with $d>2n$, or $n_{\max}=[(d-1)/2]$, [] the integer part. The lowest dimensional intersection is $d-n_{\max}$ or

$$d-\left[\frac{d-1}{2}\right]. \tag{92}$$

That is, one cannot have an intersection of dimension lower than roughly half the bulk dimensionality, or, for a given intersection dimensionality the maximum possible bulk dimensions are roughly twice that. In particular if we are interested in four-dimensional submanifolds it is easy to see that the available bulk dimensionalities are $d=5,6,7$.

Consider a space–time without boundary or with boundary that is smooth, i.e., the normal direction changes continuously along it. Let us also insist that space–time is a (differentiable) manifold. The metric is assumed nonsingular in the sense of being C^{1-},[33] which in particular means that the first derivative of the metric may have only finite discontinuities and remains bounded in general. This excludes conical singularities. Also, it excludes the general case of orbifolds.

We want to restrict matter in submanifolds under these conditions. Consider a manifold and let finite discontinuities of the first derivative of the metric occur at hypersurfaces, which in general intersect. This respects the above-presented conditions. Also, in Lovelock gravity matter does get localized at (restricted on) the discontinuities and their intersections. One may say that this is the only way to get matter restricted in submanifolds under the conditions set in the previous paragraph as an alternative is not known.

So intersections provide the means to restrict matter in submanifolds of co-dimension two or higher in a nonsingular space–time. Lovelock gravity is in a certain sense a natural generalization of Einstein theory in $d\geqslant 5$ dimensions: (1) it is the most general action for the metric field which produces at most second-order field equations under the condition of zero torsion.[3,2] Under these conditions and the above-discussed conditions, one may say that the four-dimensional intersections in $d\leqslant 7$ dimensions exhaust the list of possibilities in the spirit of the idea to think of our universe as a subspace of higher dimensional space–time; one of course may consider theories of fourth or higher order field equations, hypersurfaces of arbitrary thickness, conical or other singularities in the bulk geometry, etc., but all these add a very large number of model-dependent possibilities in the already not entirely economical RS-scenario. Another possibility is to assume that subspaces have their own intrinsic gravity terms, apart from the ones induced by the bulk. Then one has to invent mechanisms of how they arise.

Let now the boundary of the space–time be not smooth, the direction of its normal vector changes discontinuously crossing hypersurfaces embedded in the boundary. Then new surface terms should be added in action involving various angles. In Einstein gravity this has been analyzed in the past,[42] and has also been used in the intersecting brane world literature.[43] This kind of action could also be constructed for the general Lovelock gravity.

VII. VACUUM SOLUTIONS AND HIGHER CO-DIMENSION MEMBRANES

The higher order derivative structure of Lovelock gravity allows for vacuum solutions when the connection is discontinuous at non-null as well as null hypersurfaces. As in general there are nontrivial junction conditions at the intersections, higher co-dimension membranes are allowed to exist in vacuum without deficit angle or more pathological curvature singularities.

A. Solitonic configurations

Consider a single hypersurface between the regions labeled by 0 and 1 and a case where

$$\Lambda_{d,01} = 0. \tag{93}$$

This is to be satisfied for β_n's, l, and the u's, along with the bulk equation of motion (14). Solving (93) for l, when it is possible, we obtain an $l=l(\beta_{n\geqslant 1}, u_i)$. This put in (14) gives the bulk cosmological constant $\Lambda_{\text{bulk}}=-\frac{1}{2}\beta_0=-\frac{1}{2}\beta_0(\beta_{n\geqslant 1}, u_i)$.

This is a solitonic configuration in the sense that via a discontinuity in the connection at a hypersurface there exists in space–time a self-supported vacuum gravitational field (modulo the bulk cosmological constant). For Einstein–Gauss–Bonnet theory such a space–time was considered, in relation to brane-world problems, in Ref. 31.

These kinds of solutions (stable or not) existing for some Lovelock gravities are not related to topological numbers and one obvious statement is that they are due to the appearance of more than one delta function (or, to delta function $\times$ zero) in the field equations in Lovelock gravity in the presence of a hypersurface. A different way to put it is that they are possible because Lovelock gravity is on the verge of not having a well-defined initial value problem:[7] as a spacelike hypersurface evolves it is possible to pass through a stage where its extrinsic curvature jumps without matter being responsible for that. This is of course not a problem in the solitonic configurations, as they *are* solutions over the whole of time.

Now, when hypersurfaces intersect, in general matter will be localized at the intersection and so the same can happen when solitons intersect. Consider first a co-dimension two intersection. When the energy tensor at the co-dimension two hypersurface does not vanish we have a case where a co-dimension two matter is standing alone in space–time without the appearance of a conical singularity. By (39), define coefficients $c^n_{01\ldots p}$ via

$$\Lambda_{d,01\ldots p} = \sum_{n=p}^{k} c^n_{01\ldots p}\beta_n \tag{94}$$

with $k=[(d-1)/2]$. The dependence of the c's on d is understood. Let $d\geqslant 5$ and consider Einstein–Gauss–Bonnet theory. Three intersecting solitonic configurations of the above-discussed kind means that $\Lambda_{d,01}=\Lambda_{d,12}=\Lambda_{d,20}=0$ so

$$\begin{aligned} c^1_{01}\beta_1 + c^2_{01}\beta_2 &= 0, \\ c^1_{12}\beta_1 + c^2_{12}\beta_2 &= 0, \\ c^1_{20}\beta_1 + c^2_{20}\beta_2 &= 0. \end{aligned} \tag{95}$$

For β's not to be zero the relations have to be linearly dependent. This is possible: it is adequate to take all three angles between u_0, u_1, u_2 equal, as then $u(t)^2$ will give the same integral over all one-simplices. One then obtains a relation for the couplings constants, that is, is specified a class of the Lovelock gravities that accommodates such a configuration. Let $u_0=(1,0)$, $u_1=(-1/2,\sqrt{3}/2)$, $u_2=(-1/2,-\sqrt{3}/2)$. We find

$$-l^{-1}(d-2)\det(u)\beta_1 + l^{-3}(d-2)(d-3)(d-4)\det(u)\beta_2 = 0. \tag{96}$$

So for $d\geqslant 5$ solving for β_2 we have by (94)

$$\Lambda_{d,012} = c^2_{012}\beta_2 = -3\sqrt{3}\beta_1, \tag{97}$$

where we used also the volume of the two-simplex $\int_{s_{012}} d^2t=\frac{1}{2}$. As the geometry does not contain a deficit angle (which is not hard to see employing the metric continuity conditions) we have a co-dimension two surface filled with matter in space–time without conical singularities. Moreover the energy density is positive, the tension on the co-dimension two intersection is $V_{d,012}=-\Lambda_{d,012}=3\sqrt{3}\beta_1>0$. We discuss higher than two co-dimension membranes in AdS and the associated Lovelock gravities in Appendix D. In general backgrounds, solitonic solutions are possible

with no relations among the beta couplings. This interesting implication of Lovelock gravity is discussed in future work.

B. Shock waves

We turn now to the case of shock waves.[32] Let a hypersurface separating a dS region with vector u_0, $u_0^2=-1$, and an AdS region with vector u_1, $u_1^2=1$. The hypersurface is given by the continuity condition $(u_0-u_1)\cdot x=0$. Let the vector u_0-u_1 be null. Then also $u_0\cdot u_1=0$.

Proposition 7.1: Consider pure Gauss–Bonnet gravity with cosmological constant. Then a null hypersurface separating a dS and an AdS with the same length scale l is a shock wave.

Proof: First, by the bulk equations (14) we see that if β_n is not zero for $n=0,2=$even, the same l can be a solution for both dS and AdS. Now, let us repeat Eq. (33),

$$\mathcal{E}^n_{(p)}=(-1)^{n-p}(-1)^{p(p-1)/2}2^p\int_{s_{01\ldots p}} d^p t u^{a_1}_{10}\ldots u^{a_p}_{p0}(u(t)^2)^{n-p}\frac{(d-p-1)!}{(d-2n-1)!}e_{ca_1\ldots a_p}. \tag{98}$$

This is still valid even if one (or more) of the u_{i0}'s is null. It is important that we nowhere refer to the intrinsic geometry of the null hypersurface. If this quantity vanishes there cannot be a nonzero energy tensor in the null hypersurface.

For Gauss–Bonnet gravity and a null hypersurface discontinuity the single contribution is β_2 times (putting the common length l back)

$$-2l^{-3}(d-3)(d-4)\int_0^1 dtu(t)^2u^a_{10}e_{ca}. \tag{99}$$

But

$$u(t)^2=-t_0^2+t_1^2=-(1-t)^2+t^2 \tag{100}$$

taking $t_1=t$, that is

$$\int_0^1 dtu(t)^2=0 \tag{101}$$

so the energy tensor at the null discontinuity vanishes identically. □

Also we have

Proposition 7.2: Let Lovelock gravity be given by a sum of even order Euler terms. Then a null hypersurface separating a dS and an AdS with the same length scale l is a shock wave.

Proof: By the bulk equations (14) we see that if β_n is not zero for $n=$even, the same l can be a solution for both dS and AdS. For the null hypersurface between dS and AdS with the same scale we have from before that $u(t)^2=-(1-t)^2+t^2=2t-1$ so

$$\int_0^1 dt(u(t)^2)^{n-1}=\int_0^1 dt(2t-1)^{n-1}=\frac{(-1)^{n-1}+1}{2}\frac{1}{n} \tag{102}$$

so from (98) for $p=1$ we have that the energy tensor at the null hypersurface vanishes for all $n=$even. □

Consider now the nonsimplicial intersection such that four dS and AdS regions are put alternatively: $u_0=(1,0)$, $u_1=(0,1)$, $u_2=(-1,0)$, $u_3=(0,-1)$. Let the gravity be pure Gauss–Bonnet. Then all four hypersurfaces are null and shocks.

The co-dimension two hypersurface is spacelike. Its Lagrangian is

$$\mathcal{L}_{012}+\mathcal{L}_{023}. \tag{103}$$

The intersection is non-null so by (39) we get the energy tensor on it is pure pressure equal to

$$8\beta_2 l^{-2}(d-3)(d-4). \tag{104}$$

This is calculated via the determinants of $\binom{u_{10}}{u_{20}}$ and $\binom{u_{20}}{u_{30}}$ which both equal to 2.

In general, consider the same configuration for a Lovelock gravity involving all possible even order Euler terms. The Lagrangian is still given by (103). Over the simplex s_{012} we have

$$u(t)^2 = -t_0^2 + t_1^2 - t_2^2 + 2t_0t_2 = t_1^2 - (t_0 - t_2)^2 = (1-2t_0)(1-2t_2) \tag{105}$$

using the u's above and that $t_0+t_1+t_2=1$ over this simplex. There is a similar expression over s_{023}. So we have

$$\int_{s_{012}} d^2t(u(t)^2)^{n-2} = \int_0^1 dt_0 \int_0^{1-t_0} dt_2((1-2t_0)(1-2t_2))^{n-2} = \frac{1}{2(n-1)^2}, \tag{106}$$

where we used formula (102) and that n=even. The same quantity is obtained from the simplex s_{023}. Having calculated the above-noted determinants (equal to 2) we use these results in formula (39) to get for the pressure at the intersection

$$\sum_{n=\text{even}\geqslant 2} \frac{4n}{n-1}\frac{\beta_n}{l^{2n-2}}\frac{(d-3)!}{(d-2n-1)!}. \tag{107}$$

We see then that in a collision of shocks a co-dimension two matter is required to exist at the collision event surface. As noted earlier this spacelike matter violates the dominant energy condition, as a general feature of collisions in Lovelock gravity, here seen in the case of shock waves.

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APPENDIX A: SOME MANIPULATIONS WITH KRONECKER DELTA

In this appendix, we derive the quantity given in Eq. (34). We would like to determine the constants $A(d)_{mn}$ in

$$\frac{(m+n+1)!}{(n+1)!}\delta^{a_1}_{[a_1}\ \dots\ \delta^{a_m}_{a_m}e_{\ cb_1\dots b_m]} = A(d)_{mn}e_{cb_1\dots b_m}. \tag{A1}$$

In components this means

$$\frac{(m+n+1)!}{(n+1)!}\delta^{a_1}_{[a_1}\ \dots\ \delta^{a_m}_{a_m}\epsilon_{\ cb_1\dots b_m]c_{n+2}\dots c_d} = A(d)_{mn}\epsilon_{cb_1\dots b_mc_{n+2}\dots c_d}. \tag{A2}$$

Contracting with the same epsilon symbol with indices upstairs we have, using standard formulas (see, e.g., the Appendix of Ref. 36),

$$-d!A(d)_{mn} = -(d-n-1)!(m+n+1)!\delta^{a_1}_{[a_1}\ \dots\ \delta^{a_m}_{a_m}\delta^c_c\delta^{b_1}_{b_1}\dots\ \delta^{b_n}_{b_n]}. \tag{A3}$$

It is easy to show that the contracted delta's times $(m+n+1)!$ give

$$\frac{d!}{(d-m-n-1)!} \tag{A4}$$

so

$$A(d)_{mn} = \frac{(d-n-1)!}{(d-m-n-1)!}. \tag{A5}$$

APPENDIX B: VARIATIONAL PRINCIPLE FOR METRIC AND VIELBEIN

The action for Lovelock theory with matter is

$$\mathcal{S} = \int_M \mathcal{L}_{\text{Lovelock}} + \int_M \mathcal{L}_{\text{mat}}.$$

The Euler variation with respect to $g^{\mu\nu}$ (neglecting boundary terms) leads to

$$\delta S = \int_M (H_{\mu\nu} - T_{\mu\nu})\delta g^{\mu\nu} e,$$

where $H_{\mu\nu}$ is the Lovelock tensor, $T^{\mu\nu}$ the stress-energy tensor. The volume element e is

$$e = \sqrt{-g}dx^1 \wedge \cdots \wedge dx^d.$$

These more familiar expressions for the gravitational action principle are in terms of variation with respect to the metric. Since we have used the vielbein language,[37] it is useful to be able to translate between the two. The volume element is, in terms of vielbeins:

$$e = \frac{1}{d!}\epsilon_{a_1\ldots a_d}E^{a_1} \wedge \cdots \wedge E^{a_d} = E^{(1)} \wedge \cdots \wedge E^{(d)}. \tag{B1}$$

We also define

$$e_{a_1\ldots a_p} := \frac{1}{(d-p)!}\epsilon_{a_1\ldots a_d}E^{a_{p+1}} \wedge \cdots \wedge E^{a_d} \tag{B2}$$

We shall need these identities:

$$E^{c_1\ldots c_n} \wedge e_{d_1\ldots d_m} = \frac{m!}{(m-n)!}\delta^{c_1}_{[d_{m-n+1}} \ldots \delta^{c_n}_{d_m} e_{\ d_1\ldots d_{m-n}]}, \tag{B3}$$

$$\delta E^b = \delta E^b_\mu E^\mu_c E^c, \tag{B4}$$

$$\delta E^b_\mu E^\mu_a = -E^b_\mu \delta E^\mu_a, \tag{B5}$$

$$\delta g^{\mu\nu} = 2\eta^{ab}\delta E^\mu_a E^\nu_b. \tag{B6}$$

The point is that because the ω equation of motion vanishes identically, we can use (B6) to replace metric variations directly for vielbein variations, $\delta_g\mathcal{L} = \delta_{g(E)}\mathcal{L}$. First, we define

$$T_{ab} := E^\mu_a T_{\mu\nu}E^\nu_b, \tag{B7}$$

Using (B3)–(B6) and noting that

$$\delta E^b \wedge E_a = -E^b_\mu \delta E^\mu_a e,$$

we find that

$$T_{\mu\nu}\delta g^{\mu\nu} e = -2T^c_b \delta E^b \wedge e_c.$$

The field equations in terms of the vielbeins are

$$\delta_{E^c}\mathcal{L}_{\text{Lovelock}} = -2T^b_c e_b. \tag{B8}$$

If there is singular matter with support on some intersection I, we have a term in the action:

$$\int_I \tilde{\mathcal{L}}_{\text{mat}}. \tag{B9}$$

The variation gives the stress-energy tensor on I:

$$\delta\tilde{\mathcal{L}}_{\text{mat}} \equiv -\tilde{T}_{\mu\nu}\delta h^{\mu\nu}\tilde{e} \tag{B10}$$

is the energy-momentum tensor on I. On the intersection we have an induced metric h and the corresponding volume element

$$\tilde{e} = \sqrt{|h|}d^{d-p}x. \tag{B11}$$

The stress-energy tensor will be related to the variation of the appropriate boundary term in the Lovelock action:

$$\sum_n \beta_n \int_I \mathcal{L}^n_{(p)}.$$

Let $n^1,\ldots,n^p$ be an ordered set of orthonormal vectors which spans the space of vectors normal to I. In terms of the vielbeins, the volume element is

$$\tilde{e} = \prod_{i=1}^{p} (n^i \cdot n^i)(n^1)^{a_1}\cdots(n^p)^{a_p} e_{a_1\ldots a_p}. \tag{B12}$$

The order of the normal vectors gives the orientation on I. The factor $\Pi(n^i\cdot n^i)$ is ± 1 depending on whether I is timelike or spacelike.

If we vary the frames tangential to I such that they remain tangent to I, there is a simple relation:

$$\delta E^a \wedge \tilde{e}_b = E^\mu_b \delta E^a_\mu \tilde{e} \quad (\delta E^a \text{ tangential}). \tag{B13}$$

(This is sufficient if we vary $\tilde{\mathcal{L}}_{\text{mat}}$ only with respect to the induced metric h and not the position of the intersection. In this paper, we consider only dS/AdS bulk solutions, where the terms involving δE^0 not tangential always vanish anyway.) Following the same procedure as above, we then derive

$$\sum_n \beta_n \delta_{E^c}\mathcal{L}^n_{(p)} = -2\tilde{T}^b_c e_b. \tag{B14}$$

It is important to remember this factor of $-1/2$ when relating the stress-energy tensor to the Euler variation with respect to the vielbein. This has been used in Eq. (9).

APPENDIX C: A WORD ON THE SIMPLEX

A (Euclidean) p-dimensional simplex or p-simplex s_p is defined as $\{t \in \mathbf{R}^{p+1} \,|\, \Sigma_{i=0}^p t^i = 1, \text{ all } t^i \geqslant 0\}$. A bit more generally is defined as the set of points $\Sigma_{i=0}^p t^i a_i$ with the same conditions for the t_i's as above, for $a_0,\ldots,a_p$ points in the Euclidean space $\mathbf{R}^{p+1}$ such that $a_1-a_0,\ldots,a_p-a_0$ are linearly independent.[38] This reflects nicely the properties of the vector $u(t)$ encountered in this paper.

A zero-simplex is a point, a one-simplex is an interval, a two-simplex is a triangle, a three-simplex is a tetrahedron, etc. A k-dimensional face of the simplex, designated $s_{i_0}\ldots i_k$, is the subset of s_p such that

$$s_{i_0\ldots i_k} = \{t \in s_p | t^j = 0,\ \forall\, j \neq i_0, \ldots, i_k\}. \tag{C1}$$

Of course by definition a k-dimensional face is itself a k-simplex. It is easy to see that there are $\binom{p+1}{k+1}$ k-dimensional faces on the p-simplex.

Clearly $(k-1)$-simplices are parts of the boundary of the k-simplices. The rule which takes into account orientations is

$$\partial s_{i_0\ldots i_k} = \sum_{r=0}^{k} (-1)^r s_{i_0\ldots \hat{i_r}\ldots i_k}, \tag{C2}$$

where the caret means that this is index is absent. The symbols $s_{i_0}\ldots i_k$ are completely antisymmetric.

APPENDIX D: MEMBRANES OF CO-DIMENSION HIGHER THAN TWO IN AdS BULK

1. The symmetric hedgehog

Let the vectors u be symmetrically arranged in the k-dimensional normal space, forming a symmetric hedgehog. In particular the average position defined by their ends (the barycenter) coincides with the origin

$$u_0 + \cdots + u_k = 0. \tag{D1}$$

Also by symmetry all inner products are equal. Call this cosine $\cos\phi_k$. Taking the square of the above we have

$$(1 + k\cos\phi_k)(k+1) = 0. \tag{D2}$$

So

$$\cos\phi_k = -\frac{1}{k}. \tag{D3}$$

Then

$$u(t)^2 = \left(\sum_{i=0}^{p} u_i t_i\right)^2 = \sum_{i=0}^{p} t_i^2 + \cos\phi_k \sum_{i\neq j} t_i t_j = \left(1 + \frac{1}{k}\right)\sum_{i=0}^{p} t_i^2 - \frac{1}{k}, \tag{D4}$$

where in the last equality we used (D3) and that $(\Sigma_i t_i)^2 = 1$.

The other bit we need is the determinants made out of the vectors u_{i0}. It equals the volume of a p dimensional parallelepiped made out of vectors with length

$$|u_i - u_0| = \sqrt{2 - 2\cos\phi_k} = \sqrt{2 + \frac{2}{k}} \tag{D5}$$

and angle between any two vectors u_{i0} and u_{j0} given by the cosine

$$\frac{(u_i - u_0)\cdot(u_j - u_0)}{|u_i - u_0||u_j - u_0|} = \frac{1 - \cos\phi_k}{2(1 - \cos\phi_k)} = \frac{1}{2} = \cos 60^\circ. \tag{D6}$$

So all "heights" of the parallelepiped are given by the length in (D5) times $\sin 60^\circ = \sqrt{3}/2$. The determinant related to a p-simplex face of the k-simplex is

$$\det(u_i^j) = \left(\frac{\sqrt{3}}{2}\right)^{p-1}\left(2 + \frac{2}{k}\right)^{p/2}. \tag{D7}$$

2. Gravity

In the case of Chamseddine and Born-Infeld type of Lovelock gravity we considered (AdS) vacuum and intersections such that the u vectors are symmetrically arranged. Here we find the Lovelock gravity such that the tension of all membranes with co-dimension $p \neq k=[(d-1)/2]$ is zero.

So $\Lambda_{d,01\ldots p}=\Lambda_{d,p}$ here and for each p we consider one expression and call the coefficients in (94) simply c_p^n. If all except the co-dimension k intersection Λ's vanish, we have

$$\begin{aligned} c_1^1\beta_1 + c_1^2\beta_2 + \cdots + c_1^{k-1}\beta_{k-1} &= -c_1^k\beta_k, \\ c_2^2\beta_2 + \cdots + c_2^{k-1}\beta_{k-1} &= -c_2^k\beta_k, \\ &\vdots \\ c_{k-1}^{k-1}\beta_{k-1} &= -c_{k-1}^k\beta_k, \end{aligned} \tag{D8}$$

where we put the last term in the sums on the right-hand side to give it the form of an upper triangular $(k-1)\times(k-1)$ linear system.

The inverse of the matrix $\mu=(c_p^n)$ of the coefficients is rather easily calculated by the method of forming a $(k-1)\times 2(k-1)$ matrix by putting a unit matrix on the side of μ and adding appropriate multiples of lines to other lines of this big matrix until in the place of μ the unit matrix appears; then in place the unit matrix μ^{-1} appears. Then we find that the inverse μ^{-1} is an upper triangular matrix. The diagonal terms are $1/c_p^p$ and the upper triangular part is

$$(\mu^{-1})_p^n = -\frac{c_p^n}{c_n^n c_p^p} \tag{D9}$$

$n=p+1,\ldots,k-1$. So

$$\beta_p = -\frac{c_p^k}{c_p^p}\beta_k + \sum_{n=p+1}^{k-1}\frac{c_p^n}{c_n^n c_p^p}c_n^k\beta_k = \left(-\tilde{c}_p^k + \sum_{n=p+1}^{k-1}\tilde{c}_p^n\tilde{c}_n^k\right)\beta_k, \tag{D10}$$

$p=1,\ldots,k-1$, where

$$\tilde{c}_p^n := \frac{c_p^n}{c_p^p} = l^{2p-2n}(-1)^{n-p}\frac{n!}{(n-p)!}\frac{(d-2p-1)!}{(d-2n-1)!}\int_{s_p} d^p t(u(t)^2)^{n-p} \tag{D11}$$

These coefficients depend on d and the AdS radius l but also on a coupling beta which is left arbitrary. In detail, β_0 is fixed in terms of a given bulk cosmological constant $\Lambda_{\text{bulk}}=-\frac{1}{2}\beta_0$, and by the bulk equations of motion (14) the coupling β_k is fixed in terms of l and Λ_{bulk}. Einstein gravity with arbitrary cosmological constant is the trivial case of these.

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Meromorphic Lax representations of (1+1)-dimensional multi-Hamiltonian dispersionless systems

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Rational Lax hierarchies introduced by Krichever are generalized. A systematic construction of infinite multi-Hamiltonian hierarchies and related conserved quantities is presented. The method is based on the classical R-matrix approach applied to Poisson algebras. A proof that Poisson operators constructed near different points of Laurent expansion of Lax functions are equal is given. All results are illustrated by several examples. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In Refs. 1 and 2 I. M. Krichever introduced the so-called universal Whitham hierarchies by means of moduli spaces of Riemann surfaces of all genera. There is an important class of finite-field reductions of the zero-genus case, being the so-called algebraic orbits, given by rational Lax functions on $\mathbb{C}P^1$ of the form

$$L = p^N + \sum_{k=0}^{N-1} a_k p^k + \sum_{l=1}^{\alpha} \sum_{i=1}^{i_l} \frac{a_{l,i}}{(p-p_l)^i}, \quad n \geqslant 0, \quad i_l \geqslant 0, \tag{1.1}$$

where a's and the poles p_l are smooth dynamical fields. These reductions permit the construction of integrable (1+1)-dimensional dispersionless system. Around all poles of (1.1), i.e., ∞ and p_l, the powers of Laurent expansions of L generate infinite Lax hierarchies of commuting vector fields with Lie bracket being the canonical Poisson bracket (3.1) with $r=0$. Moreover, near these poles one can construct infinite hierarchies of constants of motion. Rational Lax functions (1.1) with related Lax hierarchies have been introduced in Ref. 2 in the context of topological field theories. From this point of view they have been considered also in Refs. 3 and 4. The bi-Hamiltonian structures of Benney and Toda like Lax hierarchies, but with Poisson bracket (3.1) with $r=1$, and rational Lax functions was developed in Ref. 5. Their various reductions were also studied. They also have been investigated in the context of degenerate Frobenius manifolds.[6] In Ref. 7, it was shown how to construct recursion operators for some classes of such rational Lax representations.

(1+1)-dimensional dispersionless (or hydrodynamic) systems are first-order PDEs of the form

$$(u_i)_t = \sum_j A_i^j(u)(u_j)_x, \quad i,j = 1, \ldots, n.$$

An important subclass of such systems are these which have multi-Hamiltonian structure, infinite hierarchy of symmetries, and conservation laws. Differential Poisson structures for hydrodynamic systems were introduced for the first time by Dubrovin and Novikov[8] in the form (1.2) with $c=0$, where g^{ij} is a contravariant nondegenerate flat metric and Γ_k^{ij} are related coefficients of the

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contravariant Levi-Civita connection. Then, they were generalized by Mokhov and Ferapontov[9] to the nonlocal form

$$\pi_{ij} = g^{ij}(u)\partial_x - \sum_k \Gamma^{ij}_k(u)(u_k)_x + c\ (u_i)_x \partial_x^{-1} (u_j)_x \tag{1.2}$$

in the case when g^{ij} is of constant curvature c. The natural geometric setting of related bi-Hamiltonian structures (Poisson pencils) is the theory of Frobenious manifolds based on the geometry of pencils of contravariant metrics.[10] Nevertheless, the condition of nondegeneracy of g^{ij} for the above-mentioned Poisson tensors is not necessary. The degenerate hydrodynamic Poisson tensors were considered by Grinberg[11] and Dorfmann.[12]

In the theory of nonlinear evolutionary PDEs (dynamical systems) one of the most important problems is a systematic construction of integrable systems. By integrable systems we understand those which have infinite hierarchy of commuting symmetries. It is well known that a very powerful tool, called the classical R-matrix formalism, can be used for systematic construction of $(1+1)$-dimensional field and lattice integrable dispersive systems (soliton systems)[13–17] as well as dispersionless integrable field systems.[18–20] Moreover, the R-matrix approach allows a construction of Hamiltonian structures and conserved quantities.

In this paper the systematic approach of classical R-matrices to $(1+1)$-integrable dispersionless multi-Hamiltonian systems with meromorphic Lax hierarchies is presented. In the frames of that formalism we generalize the rational Lax functions defined by Krichever onto a wider class of Lax hierarchies considered in Refs. 19 and 20. However, these articles only presented theory of polynomial Lax functions with Lax hierarchies generated only by powers constructed at ∞. In the following article it is shown that, in applicable cases, for a given appropriate meromorphic Lax function one can construct Lax hierarchies not only related to poles of Lax function, as in the case considered by Krichever, but also to its roots. These Lax hierarchies mutually commute. As well, it is shown how to construct Poisson tensors and infinite hierarchies of constants of motion. It is proved that Poisson tensors, from the original function space, reconstructed for different poles and roots are equal. Also, we have examined systematically the forms of appropriate meromorphic Lax functions, with finite number of dynamical fields, allowing construction of consistent dispersionless systems. We illustrate results by a large number of examples. Let us notice that symmetries generated by logarithmic functions are not considered in this article, see the related comment in Sec. V.

II. CLASSICAL *R*-MATRIX THEORY ON POISSON ALGEBRAS

Let $\mathcal{A}$ be a commutative associative algebra with unit. If there is a Lie bracket on $\mathcal{A}$ such that for each element $a \in \mathcal{A}$, the operator $\mathrm{ad}_a : b \mapsto \{a,b\}$ is a derivation of the multiplication, i.e., $\{a,bc\}=\{a,b\}c+b\{a,c\}$, then $(\mathcal{A},\{\cdot,\cdot\})$ is called a Poisson algebra and bracket $\{\cdot,\cdot\}$ is a Poisson bracket. Thus, the Poisson algebras are Lie algebras with an additional structure. We assume the existence of a nondegenerate ad-invariant scalar product $(\cdot,\cdot)$ on $\mathcal{A}$ with respect to which the operation of multiplication is symmetric, i.e., $(ab,c)=(a,bc)$, $\forall a,b,c \in \mathcal{A}$.

A linear map $R:\mathcal{A}\to\mathcal{A}$ being an R-matrix defines a second Lie product on $\mathcal{A}$ given by

$$\{a,b\}_R := \{Ra,b\} + \{a,Rb\}. \tag{2.1}$$

We will additionally assume that R commutes with derivatives with respect to evolution parameters, i.e.,

$$(RL)_t = RL_t. \tag{2.2}$$

This property is equivalent to the assumption that R commutes with differentials of smooth maps from $\mathcal{A}$ to $\mathcal{A}$. This property is used in the proof of Theorem 4.2 in Ref. 18, although not explicitly stressed there. The equality (2.2) will be used in Sec. III E to show a commutation between particular Lax hierarchies. Then, for each integer $n \geqslant 0$, the formula

$$\{H,F\}_n = (L,\{R(L^n dF),dH\} + \{dF,R(L^n dH)\}) \tag{2.3}$$

defines a Poisson structure on algebra of smooth functions $\mathcal{C}^\infty\mathcal{A}$, where differentials $dF, dH \in \mathcal{A}$.[18] Moreover, all $\{\cdot,\cdot\}_n$ are compatible. The related Poisson bivectors π_n, such that $\{H,F\}_n = (dF, \pi_n dH)$, are given by the following Poisson maps:

$$\pi_n: dH \mapsto \{R(L^n dH),L\} + L^n R^*(\{dH,L\}), \quad n \geqslant 0, \tag{2.4}$$

where the adjoint of R is defined by the relation $(R^*a,b)=(a,Rb)$. Notice that the bracket (2.3) with $n=0$ is just a Lie-Poisson bracket with respect to the Lie bracket (2.1). Referring to the dependence on L, Poisson maps (2.4) are called linear for $n=0$, quadratic for $n=1$, and cubic for $n=2$, respectively.

We will look for a natural set of functions in involution with respect to the Poisson brackets (2.3). Such functions are Casimirs of the natural Lie-Poisson bracket $\{H,F\}=(L,\{dF,dH\})$. A sufficient condition for smooth function $C(L)$ to be a Casimir function is that its differential $dC \in \ker \mathrm{ad}_L$, i.e. $[dC,L]=0$. Let us assume that an appropriate scalar product on Poisson algebra $\mathcal{A}$ is given by the trace form $\mathrm{Tr}: \mathcal{A} \to \mathbb{R}$ or $\mathbb{C}$, such that $(a,b)=\mathrm{Tr}(ab)$. Then, the most natural Casimirs are functionals given by the trace of powers of L, i.e.,

$$dC_q(L) = L^q \Leftrightarrow \begin{cases} C_q(L) = \dfrac{1}{q+1}\,\mathrm{Tr}(L^{q+1}) & \text{for } q \neq -1 \\ C_{-1}(L) = \mathrm{Tr}(\ln L) & \text{for } q = -1. \end{cases} \tag{2.5}$$

Hence, taking these $C_q(L)$ as Hamiltonian functionals, one finds a Lax hierarchy of evolution equations which are multi-Hamiltonian dynamical systems

$$L_{t_q} = \{R(dC_q),L\} = \pi_0(dC_q) = \pi_1(dC_{q-1}) = \ldots = \pi_l(dC_{q-l}) = \ldots . \tag{2.6}$$

For any R-matrix each two evolution equations in the hierarchy (2.6) commute due to the involutivity of the Casimirs C_q. Each equation admits all the Casimir functionals as a set of conserved quantities in involution. In this sense we will regard (2.6) as a hierarchy of integrable evolution equations.

One can construct the simplest R-structures decomposing the Poisson algebra $\mathcal{A}$ into a direct sum of Lie subalgebras $\mathcal{A}_+$ and $\mathcal{A}_-$, i.e., $\mathcal{A}=\mathcal{A}_+ \oplus \mathcal{A}_-$, $[\mathcal{A}_\pm,\mathcal{A}_\pm] \subset \mathcal{A}_\pm$. Denoting the projections onto these subalgebras by $P_\pm$, the classical R-matrix is well defined as

$$R = \tfrac{1}{2}(P_+ - P_-) = P_+ - \tfrac{1}{2} = \tfrac{1}{2} - P_-. \tag{2.7}$$

Following the above-mentioned scheme, we are able to construct in a systematic way integrable multi-Hamiltonian dispersionless systems, with infinite hierarchy of involutive constants of motion and infinite hierarchy of related commuting symmetries, on appropriate Poisson algebras. Finally, in the last step, we reconstruct our multi-Hamiltonian hierarchies in the original function space of related dispersionless systems.

III. LAX HIERARCHIES FOR DISPERSIONLESS SYSTEMS

A. Poisson algebras of meromorphic functions

Let $\mathcal{F}$ be the algebra of meromorphic functions with a finite number of poles, i.e., these analytic functions which have no essential singularities, on a Riemann sphere $\mathbb{C}P^1$ (i.e., complex plane with point at ∞). Let p be a point in $\mathbb{C}P^1$. Assume now that this algebra depends effectively on an additional spatial variable $x \in \Omega$. Denote by $\mathcal{A}$ the algebra of all smooth functions: $f: \Omega \to \mathcal{F}$, i.e., $\mathcal{A}=\mathcal{C}^\infty(\Omega,\mathcal{F})$. Let $\Omega=\mathbb{S}^1$ if we assume these functions to be periodic in x or $\Omega=\mathbb{R}$ if these functions are supposed to belong to the Schwartz space for a fixed parameter p. The Poisson bracket on $\mathcal{A}$ can be introduced in infinitely many ways as

$$\{f,g\}_r := p^r(\partial_p f \partial_x g - \partial_x f \partial_p g), \quad r \in \mathbb{Z}, \quad f,g \in \mathcal{A}. \tag{3.1}$$

Then, fixing r, $\mathcal{A}$ is the Poisson algebra with an appropriate bracket (3.1). Poisson brackets (3.1) are generalizations of canonical Poisson bracket ($r=0$) through the addition of p^r factor.

To construct classical R-matrices we have to decompose $\mathcal{A}$ into a direct sum of Lie subalgebras. It can be done by expanding functions belonging to $\mathcal{A}$ in an appropriate annulus near a given point λ. Three kinds of points on $\mathbb{C}P^1$, parameterized by p, will be important. Two fixed points: ∞ and 0, as well as points being smooth fields $v(x)$ from Ω to $\mathbb{C}P^1$.

B. Classical *R*-matrices

Once we fixed Poisson algebra we are able to construct R-matrices and related Lax vector fields for which the algebra $\mathcal{A}$ constitutes the phase space.

Expanding meromorphic functions from $\mathcal{A}$ into Laurent series at λ we decompose the algebra $\mathcal{A}$ in the following way:

$$\mathcal{A} = \mathcal{A}^{\infty}_{\geqslant k-r} \oplus \mathcal{A}^{\infty}_{<k-r} := \left\{ \sum_{i=k-r}^{N} a_i(x)p^i \right\} \oplus \left\{ \sum_{i<k-r} a_i(x)p^i \right\}, \quad \lambda = \infty, \tag{3.2}$$

$$\mathcal{A} = \mathcal{A}^{\lambda}_{\geqslant k-r} \oplus \mathcal{A}^{\lambda}_{<k-r} := \left\{ \sum_{i\geqslant k-r} a_i(p-\lambda)^i \right\} \oplus \left\{ \sum_{i=-m_\lambda}^{k-r-1} a_i(p-\lambda)^i \right\}, \quad \lambda = 0 \text{ or } v(x), \tag{3.3}$$

where $a_i(x)$ and $v(x)$ are dynamical fields. Let ap^m and bp^n be elements from (3.2) or (3.3) for $\lambda=0$ of order m and n, respectively. Poisson bracket (3.1) between these elements has the order $m+n+r-1$ as

$$\{ap^m, bp^n\}_r = (mab_x - na_x b)p^{m+n+r-1}.$$

For $\lambda=v(x)$ the situation is a bit more complicated as one has to expand p^r in (3.1) at $v(x)$, i.e.,

$$p^r = \sum_{s=0}^{\infty} \binom{r}{s} v(x)^{r-s}(p-v(x))^s,$$

where $\binom{r}{s} = (-1)^s \binom{-r+s-1}{s}$ for $r<0$. Hence, p^r as the element of $\mathcal{A}$ has the lowest order equal zero, the highest order equal r for $r\geqslant 0$, and infinity for $r<0$. Therefore

$$\{a(p-v)^m, b(p-v)^n\}_r = ((p-v)^{\alpha} + \cdots + v^r) \times (mab_x - na_x b)(p-v)^{m+n-1},$$

where $\alpha=r$ for $r\geqslant 0$ and α goes to ∞ for $r<0$. Now, simple inspection shows that $\mathcal{A}^{\lambda}_{\geqslant k-r}, \mathcal{A}^{\lambda}_{<k-r}$ are Lie subalgebras of $\mathcal{A}$ in the following cases:

$$\text{for } \lambda = \infty, 0 \text{ if } \begin{cases} r=0,\ k=0 \\ r\in\mathbb{Z},\ k=1,2 \\ r=2,\ k=3 \end{cases}$$

$$\text{for } \lambda = v(x) \text{ if } \begin{cases} r=0,\ k=0,1,2 \\ r=1,\ k=1,2 \\ r=2,\ k=2,3. \end{cases}$$

So, fixing r we fix the Lie algebra structure with k numbering the R-matrices given in the following form:

$$R = P^{\lambda}_{\geqslant k-r} - \tfrac{1}{2} = \tfrac{1}{2} - P^{\lambda}_{<k-r}, \tag{3.4}$$

where $P^{\lambda}_{\cdot}$ are appropriate projections onto respective Lie subalgebras. All R-matrices for $\lambda = \infty, 0$ commute with derivatives with respect to evolution parameters. Let $L=\Sigma_i a_i(p-v)^i$, then

$$(RL)_t - RL_t = P^{v}_{<k-r}L_t - (P^{v}_{<k-r}L)_t = (k-r)a_{k-r-1}v_t(p-v)^{k-r-1}$$

and equality (2.2) holds for $\lambda=v(x)$ when $k-r=0$. Hence, in the case $\lambda=v(x)$ further on we will consider only R-matrices (3.4) for $k=r=0,1,2$. Henceforth, calling for appropriate r and k we will refer to these for which R-matrices (3.4), with respect to λ, are well defined and satisfy (2.2).

Let $L \in \mathcal{A}$ be a meromorphic function with pole or root at λ. Then, the Lax hierarchy assigned by (3.4) has the form

$$\frac{\partial L}{\partial t_{\lambda,q}} = \{\Omega^{\lambda}_q, L\}_r, \quad q \in \mathbb{Z}_+, \tag{3.5}$$

for appropriate r and k. The functions $\Omega_{\lambda,q}$ coupled with evolution parameters $t_{\lambda,q}$ are defined by

$$\Omega^{\infty}_q := \left(L^{q/N}\right)^{\infty}_{\geqslant k-r} \quad \text{for } \lambda = \infty, \quad \Omega^{\lambda}_q := -\left(L^{q/m_\lambda}\right)^{\lambda}_{<k-r} \quad \text{for } \lambda = 0 \text{ or } v(x), \tag{3.6}$$

where $(A)^{\lambda}_{\geqslant k-r} \equiv P^{\lambda}_{\geqslant k-r}(A)$. If L has pole at λ the powers in (3.6) are positive as $N, m_\lambda > 0$ for $\lambda = \infty$ or $\lambda = 0, v(x)$, respectively. In this case N, m_λ are orders of respective poles. If L has root at λ the powers in (3.6) are negative as $N, m_\lambda < 0$ and $-N, -m_\lambda$ are orders of respective roots.

Now, we will show that schemes for Lax hierarchies defined for ∞ and 0 are interrelated.

Proposition 3.1: Under the transformation: $x'=x$, $p'=p^{-1}$, $t'=t$; *the Lax hierarchy* (3.5) *for* $\lambda=\infty$ *and appropriate* r,k *with Lax function* L *transforms into* (3.5) *for* $\lambda=0$ *and* $k'=3-k, r'=2-r$ *where Lax function is given by* $L'(p')=L(p)$.

Proof: It follows from the observation that $\{\cdot,\cdot\}_r = p^r\partial_p \wedge \partial_x = -p'^{2-r}\partial_{p'} \wedge \partial_{x'} = -\{\cdot,\cdot\}'_{r'}$ and $(L^n)^{\infty}_{\geqslant k-r} = (L'^n)^{0}_{\leqslant r-k} = (L'^n)^{0}_{<k'-r'}$. □

C. Scalar products

To construct Poisson structures one has to define an appropriate scalar product on $\mathcal{A}$. We will define it near a given point λ by means of the trace form in the algebra $\mathcal{A}$ with the Poisson structure (3.1) for fixed r by

$$\mathrm{Tr}_\infty f := -\int_\Omega \mathrm{res}_\infty(p^{-r}f)\mathrm{d}x \quad \text{for } \lambda = \infty, \quad \mathrm{Tr}_\lambda f := \int_\Omega \mathrm{res}_\lambda(p^{-r}f)\mathrm{d}x \quad \text{for } \lambda = 0, v(x),$$

where $f \in \mathcal{A}$ and res is the standard residue. In further considerations the residue theorem will be very useful. Let Γ be a set of all finite poles of f. Then, according to the residue theorem

$$\sum_{\lambda\in\Gamma,\ \lambda\neq\infty} \mathrm{res}_\lambda f = \frac{1}{2\pi i}\oint_{\gamma_\Gamma} f\,\mathrm{d}p \equiv -\mathrm{res}_\infty f, \tag{3.7}$$

where γ_Γ is a closed curve encircling all finite poles of f. So, residue at ∞ may be different than zero even if f does not have singularity at this point.

Lemma 3.2: For two arbitrary functions $f,g \in \mathcal{A}$ *the scalar product:*

$$(f,g)_\lambda := \mathrm{Tr}_\lambda(fg), \quad \lambda = \infty, 0, v(x) \tag{3.8}$$

is symmetric, *nondegenerate*, *and* ad-*invariant*.

Proof: The nondegeneracy and symmetry of (3.8) are obvious. Let γ_λ be a closed curve circling once a finite pole λ, then

$$\mathrm{Tr}_\lambda\{f,g\}_r = \int_\Omega \mathrm{res}_\lambda(\partial_p f \partial_x g)\,\mathrm{d}x - \int_\Omega \mathrm{res}_\lambda(\partial_x f \partial_p g)\,\mathrm{d}x = \frac{1}{2\pi i}\int_\Omega \oint_{\gamma_\lambda} (\partial_p f \partial_x g)\,\mathrm{d}p\,\mathrm{d}x$$
$$- \frac{1}{2\pi i}\int_\Omega \oint_{\gamma_\lambda} (\partial_x f \partial_p g)\,\mathrm{d}p\,\mathrm{d}x = 0,$$

where the last equality follows by integrating by parts with respect to p and x. Similar proof is for $\lambda=\infty$. Therefore

$$(\{f,g\}_r,h)_\lambda - (\{g,h\}_r,f)_\lambda = \mathrm{Tr}_\lambda(\{f,g\}_r h) - \mathrm{Tr}_\lambda(\{g,h\}_r f) = \mathrm{Tr}_\lambda(\{fh,g\}_r - f\{h,g\}_r) + \mathrm{Tr}_\lambda(f\{h,g\}_r)$$
$$= \mathrm{Tr}_\lambda\{fh,g\}_r = 0,$$

i.e., ad-invariance is proved. □

For functional $H=\int_\Omega h(u_i)\,\mathrm{d}x$, where u_i are dynamical coefficients of $L\in\mathcal{A}$, we have to show how to construct its differential near a given point λ denoted by $d_\lambda H\in\mathcal{A}$. Coefficients of $d_\lambda H$ depend on dynamical fields and usual variational derivatives $\delta H/\delta u_i$ in such a way that the trace duality assumes the usual Euclidean form, i.e.,

$$(d_\lambda H, L_t)_\lambda = \mathrm{Tr}_\lambda(d_\lambda H L_t) = \sum_i \int_\Omega \frac{\delta H}{\delta u_i}(u_i)_t\,\mathrm{d}x. \tag{3.9}$$

Notice that from (3.9) it follows that at different points λ and μ the following equality holds:

$$(d_\lambda H, K)_\lambda = (d_\mu H, K)_\mu, \tag{3.10}$$

where K is vector field on $\mathcal{A}$ such that it spans exactly the same subspace of $\mathcal{A}$ as L_t.

To find R^* needed in (2.4), i.e., the adjoints of R-matrices (3.4), one has to determine the adjoint projections related to given point λ from the following relation $((P^\lambda)^* f,g)_\lambda=(f,P^\lambda g)_\lambda$, where $f,g\in\mathcal{A}$. So, for 0 and ∞ we have that

$$(P^0_{<k-r})^* = 1 - P^0_{<2r-k}, \quad (P^\infty_{\geqslant k-r})^* = 1 - P^\infty_{\geqslant 2r-k}.$$

The case of $\lambda=v(x)$ is more delicate. Let $A=\Sigma_m a_m(p-v)^m$ and $B=\Sigma_n b_n(p-v)^n$, then for $r\geqslant 0$:

$$(A,P^v_{<0}B)_v = \int_\Omega \mathrm{res}_v\left(\sum_{s\geqslant 0}\sum_m\sum_{n<0}\binom{-r}{s} v^{-r-s} a_m b_n (p-v)^{m+n+s}\right)\mathrm{d}x$$

$$= \int_\Omega \sum_{s\geqslant 0}\sum_{n<0}\binom{-r}{s} v^{-r-s} a_{-n-s-1} b_n\,\mathrm{d}x = \int_\Omega \sum_{s\geqslant 0}\sum_{m\geqslant -s}\binom{-r}{s} v^{-r-s} a_m b_{-m-s-1}\,\mathrm{d}x$$

$$= \int_\Omega \mathrm{res}_v\left(\sum_{s\geqslant 0}\sum_{m\geqslant -s}\sum_n \binom{-r}{s} v^{-r-s} a_m b_n (p-v)^{m+n+s}\right)\mathrm{d}x$$

$$= \left(p^r \sum_{s\geqslant 0}\binom{-r}{s} v^{-r-s}(p-v)^s P^v_{\geqslant -s} A, B\right)_v,$$

where we used an appropriate expansion of p^{-r} at v. Hence

$$(P^v_{<0})^* = 1 - p^r \sum_{s=0}^{\infty}\binom{-r}{s} v^{-r-s}(p-v)^s P^v_{<-s}, \quad r\geqslant 0,$$

when $r=0$ it reduces to $(P^v_{<0})^*=1-P^v_{<0}$. We will use simplified notation

$$P'_v = \sum_{s=0}^{\infty} \binom{-r}{s} v^{-r-s}(p-v)^s P^v_{<-s}$$

as then $(P^v_{<0})^* = 1 - p^r P'_v$.

D. Poisson structures

The Poisson structures (2.3) at respective points, related to respective R-matrices, are

$$\{H,F\}^n_\lambda = (d_\lambda F, \pi^\lambda_n d_\lambda H)_\lambda, \quad \lambda = \infty, 0, v(x), \quad n \geqslant 0 \tag{3.11}$$

for which Poisson operators (2.4) are given by the following forms:

$$\pi^\infty_n d_\infty H = \{(L^n d_\infty H)^\infty_{\geqslant k-r}, L\}_r - L^n(\{d_\infty H, L\}_r)^\infty_{\geqslant 2r-k},$$

$$\pi^0_n d_0 H = \{L, (L^n d_0 H)^0_{<k-r}\}_r - L^n(\{L, d_0 H\}_r)^0_{<2r-k}, \tag{3.12}$$

$$\pi^v_n d_v H = \{L, (L^n d_v H)^v_{<0}\}_r - L^n p^r P'_v(\{L, d_v H\}_r).$$

It is important here to mention that for a given Lax operator L it may happen that L_t does not span a proper subspace of the full Poisson algebra $\mathcal{A}$, i.e., the image of the Poisson operator $\pi_n dH$ does not coincide with this subspace. Then, in general, the Dirac reduction can be invoked for restriction of a given Poisson tensor to a suitable subspace.

Lemma 3.3: The following relations will be needed to prove the forthcoming theorem:

$$(d_\infty F, \{L, (L^n d_0 H)^0_{<k-r}\}_r)_\infty = (d_0 H, L^n(\{d_\infty F, L\}_r)^\infty_{\geqslant 2r-k})_0,$$

$$(d_\infty F, L^n(\{L, d_0 H\}_r)^0_{<2r-k})_\infty = (d_0 H, \{(L^n d_\infty F)^\infty_{\geqslant k-r}, L\}_r)_0,$$

for arbitrary k and r, and

$$(d_\infty F, \{L, (L^n d_v H)^v_{<0}\}_r)_\infty = (d_v H, L^n(\{d_\infty F, L\}_r)^\infty_{\geqslant r})_v, \tag{3.13}$$

$$(d_\infty F, L^n p^r P'_v(\{L, d_v H\}_r))_\infty = (d_v H, \{(L^n d_\infty F)^\infty_{\geqslant 0}, L\}_r)_v, \tag{3.14}$$

where $r \geqslant 0$.

Proof: We will prove only the first and last relations as for the two remaining ones the proof is similar. We use property of ad-invariance and we omit (or add) these elements which do not contribute in calculations of residues:

$$(d_\infty F, \{L, (L^n d_0 H)^0_{<k-r}\}_r)_\infty = ((L^n d_0 H)^0_{<k-r}, \{d_\infty F, L\}_r)_\infty$$

$$= \int_\Omega \operatorname{res}_\infty (p^{-r}(L^n d_0 H)^0_{<k-r}\{L, d_\infty F\}_r)\, \mathrm{d}x = \int_\Omega \operatorname{res}_\infty (p^{-r}(L^n d_0 H)^0_{<k-r}(\{L, d_\infty F\}_r)^\infty_{\geqslant 2r-k})\, \mathrm{d}x$$

$$\overset{\text{by (3.7)}}{=} \int_\Omega \operatorname{res}_0 (p^{-r}(L^n d_0 H)^0_{<k-r}(\{d_\infty F, L\}_r)^\infty_{\geqslant 2r-k})\, \mathrm{d}x$$

$$= \int_\Omega \operatorname{res}_0 (p^{-r} L^n d_0 H(\{d_\infty F, L\}_r)^\infty_{\geqslant 2r-k})\, \mathrm{d}x = (d_0 H, L^n(\{d_\infty F, L\}_r)^\infty_{\geqslant 2r-k})_0.$$

Let $r \geqslant 0$. Using proper expansion of p^{-r} at v we have

$$(d_\infty F, L^n p^r P_v'(\{L, d_v H\}_r))_\infty = -\int_\Omega \operatorname{res}_\infty (d_\infty F L^n P_v'(\{L, d_v H\}_r))\, \mathrm{d}x$$

$$= \int_\Omega \operatorname{res}_\infty ((L^n d_\infty F)^\infty_{\geqslant 0} P_v'(\{d_v H, L\}_r))\, \mathrm{d}x \overset{\text{by (3.7)}}{=} \int_\Omega \operatorname{res}_v ((L^n d_\infty F)^\infty_{\geqslant 0} P_v'(\{L, d_v H\}_r))\, \mathrm{d}x$$

$$= \int_\Omega \operatorname{res}_v ((L^n d_\infty F)^\infty_{\geqslant 0} \{L, d_v H\}_r)\, \mathrm{d}x = ((L^n d_\infty F)^\infty_{\geqslant 0}, \{L, d_v H\}_r)_v$$

$$= (d_v H, \{(L^n d_\infty F)^\infty_{\geqslant 0}, L\}_r)_v.$$

Thus all relations are valid. □

Theorem 3.4: *Let $H(L)$ and $F(L)$ be smooth functions of $L \in \mathcal{A}$. Then for all appropriate k and r*

$$\forall_\lambda \{H, F\}^n_\lambda = \{H, F\}^n_\infty \quad \textit{and} \quad \pi^\lambda_n d_\lambda H = \pi^\infty_n d_\infty H.$$

Therefore, Poisson structures, from the original function space of related dispersionless systems, calculated for appropriate fixed r and k at different points are equal.

Proof: We will prove only the case for $\lambda = v(x)$ as for other cases the proof is similar. Thus,

$$\{H, F\}^n_v = (d_v F, \pi^v_n d_v H)_v \overset{\text{by (3.10)}}{=} (d_\infty F, \pi^v_n d_v H)_\infty$$

$$= (d_\infty F, \{L, (L^n d_v H)^v_{<0}\}_r - L^n p^r P_v'(\{L, d_v H\}_r))_\infty$$

$$\overset{\text{by (3.13-3.14)}}{=} (d_v H, L^n (\{d_\infty F, L\}_r)^\infty_{\geqslant r} - \{(L^n d_\infty F)^\infty_{\geqslant 0}, L\}_r)_v$$

$$= -(d_v H, \pi^\infty_n d_\infty F)_{v,r} \overset{\text{by (3.10)}}{=} -(d_\infty H, \pi^\infty_n d_\infty F)_\infty = \{H, F\}^n_\infty.$$

Now, from the equality of the above-noted Poisson brackets it follows that

$$(d_\infty F, \pi^\infty_n d_\infty H)_\infty = (d_\lambda F, \pi^\lambda_n d_\lambda H)_\lambda \overset{\text{by (3.10)}}{=} (d_\infty F, \pi^\lambda_n d_\lambda H)_\infty \Leftrightarrow \pi^\lambda_n d_\lambda H = \pi^\infty_n d_\infty H.$$

Hence the theorem is proved. □

E. Commuting multi-Hamiltonian Lax hierarchies

Let $L \in \mathcal{A}$ be a Lax function and Γ be a set of all poles and roots of L. Then, one can construct the following multi-Hamiltonian Lax hierarchies (2.6) for appropriate r and k,

$$\frac{\partial L}{\partial t_{\lambda,q}} = \{\Omega^\lambda_q, L\}_r = \pi^\lambda_0 d_\lambda H^\lambda_{q/n} = \pi^\lambda_1 d_\lambda H^\lambda_{q/n-1} = \cdots \quad \lambda \in \Gamma,\ q > 0, \tag{3.15}$$

where $n = N$ for $\lambda = \infty$ and $n = m_\lambda$ for $\lambda \neq \infty$. The Hamiltonians are then defined through trace forms near these poles and are given by (2.5) for $q \geqslant 0$ as

$$H^\lambda_{q/n}(L) = \frac{\epsilon}{\dfrac{q}{n} + 1} \int_\Omega \operatorname{res}_\lambda (p^{-r} L^{q/n+1})\, \mathrm{d}x \quad \text{for } q \neq -n \tag{3.16}$$

$$H^{\lambda}_{-1}(L) = \epsilon \int_{\Omega} \mathrm{res}_{\lambda}(p^{-r} \ln L)\, \mathrm{d}x \quad \text{for } q = -n,$$

where $\epsilon = -1$ for $\lambda = \infty$ and $\epsilon = 1$ for $\lambda \neq \infty$. Calculations of H^{λ}_{-n} from (3.16) for λ being the root of L may cause difficulties as then $\ln L$ has at λ logarithmic singularity. However, due to Poincare lemma, as $\mathcal{A}$ is convex, all one-forms $d_{\lambda} H^{\lambda}_{-1}$ are exact and we are able to find H^{λ}_{-1} in an alternative approach. For example, we first look for coefficients of dH^{λ}_{-1} which can be simply obtained from

$$\mathrm{Tr}_{\lambda}(L^{-1} L_t) = \sum\nolimits_i \int_{\Omega} \frac{\delta H^{\lambda}_{-1}}{\delta u_i} (u_i)_t \, \mathrm{d}x,$$

since $d_{\lambda} H^{\lambda}_{-1} = L^{-1}$. Then, we calculate the functional H^{λ}_{-1} integrating a respective system of equations.

Let us show that Lax hierarchies (3.15) related to different $\lambda \in \Gamma$ for fixed r and k mutually commute. Hamiltonians (3.16), as Casimirs of the natural Lie-Poisson bracket, are in involution with respect to Poisson brackets (3.11) related to all applicable $\lambda \in \Gamma$. From Theorem 3.4 it follows that $\pi^{\lambda}_n d_{\lambda} = \pi^{\mu}_n d_{\mu}$ for $\lambda, \mu \in \Gamma$. Now, hence πd is the Lie algebra homomorphism, from the algebra of smooth functions to the Lie algebra of vector fields, the commutation between Lax hierarchies (3.15) is immediate. Hence, the following corollary is valid.

Corollary 3.5: Let L be a Lax function from algebra $\mathcal{A}$ with fixed Poisson bracket given by r and let us fix an appropriate k. Then, around each applicable point being pole or root of L one finds infinite hierarchy of commuting multi-Hamiltonian symmetries and infinite hierarchy of constants of motion. Moreover, vector fields from these different hierarchies mutually commute.

In further considerations we are interested in extracting closed systems with finite number of dynamical functions. Therefore, we will look for meromorphic Lax functions, with finite number of dynamical coefficients, which allow a construction of consistent evolution Lax hierarchies. So, in the following section we will select appropriate meromorphic Lax functions.

IV. MEROMORPHIC LAX FUNCTIONS

We would like to investigate the general form of meromorphic Lax functions being appropriate ones, i.e., such which allow a construction of integrable dispersionless equations. The meromorphic Lax function L is an appropriate one if the right-hand sides of Lax hierarchies (3.15) can be written in the form of evolutions L_t, i.e., left-hand sides. We will distinguish among three cases: the first one when L is a finite formal Laurent series at 0, the second one when L is a finite formal Laurent series at pole $v(x)$, and finally more general case of meromorphic functions.

A. Polynomial Lax functions in p and p^{-1}

Let us consider Lax functions of the form

$$L = u_N p^N + u_{N-1} p^{N-1} + \cdots + u_{1-m} p^{1-m} + u_{-m} p^{-m}, \tag{4.1}$$

i.e., formal finite Laurent series at 0. The coefficients u_i are dynamical fields. For Lax functions (4.1), in general, we can construct powers near ∞ and 0 which will generate related Lax hierarchies (3.15). If $k = r$ negative powers calculated around roots of L generate additional Lax hierarchies.

From now on, without loss of generality, we will choose all appearing constants in the form that will simplify all formulas.

Proposition 4.1: Lax function of the form (4.1) *is an appropriate one in the following cases:*

1. $k=0$, $r=0$: $N \geqslant 2$, $u_N = 1$, $u_{N-1} = 0$, $m = 0$;
2. $k=1$, $r \in \mathbb{Z}$: $N \neq 0$, $u_N = 1$, $m \neq 0$ *for* $r=1$;
3. $k=2$, $r \in \mathbb{Z}$: $N \neq 0$ for $r=1$, $m \neq 0$, $u_{-m} = 1$;

4. $k=3$, $r=2$: $N=0$, $m\geqslant 2$, $u_{1-m}=0$, $u_{-m}=1$.

We will not prove this proposition as it is the standard case considered in Ref. 20.

Proposition 4.2: Under the transformation $p'=p^{-1}$ Lax hierarchies, from Proposition 4.1, *generated by powers calculated at ∞ and* 0 *for appropriate r and k transforms into Lax hierarchies for* 0 *and ∞ with $r'=2-r$ and $k'=3-k$, respectively.*

The proof immediately follows from Proposition 3.1. Notice that by transformation $p'=p^{-1}$ for $r=k=0,1,2$ Lax hierarchies (3.15) defined at roots of L being dynamical fields fall out from the scheme presented in this article. On the other hand, for: $k=1,r=0$; $k=2,r=1$; $k=3,r=2$; according to Proposition 4.1 one can construct Lax hierarchies only at ∞ and 0. However, by $p'=p^{-1}$ they transform into cases: $k=2,r=2$; $k=1,r=1$; $k=0,r=0$; respectively, for which one is able to construct Lax hierarchies related to all poles (including poles being dynamical fields) of L' and L'^{-1}. Hence, the relevant cases from Proposition 4.1 are:

- $k=0$, $r=0$;
- $k=1$, $r\in\mathbb{Z}\backslash\{0\}$;
- $k=2$, $r=2$.

The remaining cases can be obtained by transformation $p'=p^{-1}$ according to Proposition 4.2.

To construct Poisson operators we have to choose a point near which we will perform the calculations. Nevertheless, as follows from Theorem 3.4, the explicit form of Poisson operators in the original function space is the same for all points. Thus, we choose the ∞ as it is the standard case. Then, as we assumed the usual Euclidean form (3.9), differentials of functional H are given by

$$dH \equiv d_\infty H = \sum_{i=-m}^{N+k-2} \frac{\delta H}{\delta u_i} p^{r-1-i},$$

where $m=0$ for $k=0$. Still we have to check whether the above-mentioned Lax functions span proper subspaces, with respect to Poisson operators (3.12), of the full Poisson algebras. We will limit ourselves to linear ($n=0$) and quadratic ($n=1$) Poisson tensors, as obviously it is enough to define bi-Hamiltonian structures. Besides, in the all nontrivial cases Lax functions do not span proper subspaces with respect to Poisson tensors for $n\geqslant 2$.

Poisson tensors restricted to finite number of fields are properly defined if the highest and lowest orders of $\pi_n^\infty dH$ and L_t will coincide. Simple inspection shows that the highest order of $\pi_n^\infty dH$ is equal to $\max\{N+k-2, nN+2r-k-1\}$ and the lowest is 0 for $k=0$ and $\min\{k-1-m, -nm+2r-k\}$ for $k=1,2$. Hence, in the case $k=0$ the Lax function always span the proper subspace with respect to the linear Poisson tensor, but for $k=1,2$ only in case when $N\geqslant 2r-2k+1\geqslant -m$, otherwise the Dirac reduction is required. The linear Poisson tensor is of the form

$$\pi_0^\infty dH = \{(dH)_{\geqslant k-r}^\infty, L\}_r - (\{dH, L\}_r)_{\geqslant 2r-k}^\infty. \tag{4.2}$$

The reduced linear tensor for $N=-1$ and $k=r=1,2$ is given by (4.12). For the quadratic Poisson tensors the Dirac reduction is always necessary. The calculation procedure of Dirac reduction is explained in Ref. 20 (in a bit different notation). The reduced quadratic Poisson tensor for $k=r=0,1,2$ is given by

$$(\pi_1^\infty)^{\mathrm{red}} dH = \{(LdH)_{\geqslant 0}^\infty, L\}_r - L(\{dH, L\}_r)_{\geqslant r}^\infty + \frac{1}{N}\{L, \partial_x^{-1}\mathrm{res}_\infty\{dH, L\}_0\}_r, \tag{4.3}$$

and for $k=1,r=0$ and $k=2,r=1$ takes the form

$$(\pi_1^\infty)^{\mathrm{red}} dH = \{(LdH)_{\geqslant 1}^\infty, L\}_r - L(\{dH, L\}_r)_{\geqslant r-1}^\infty + \frac{1}{m}\{L, \partial_x^{-1}\mathrm{res}_\infty\{dH, L\}_0\}_r. \tag{4.4}$$

Both reduced Poisson tensors are always local as $\mathrm{res}_\infty\{\cdot,\cdot\}_0=(\cdots)_x$.

In the article, in general, we present examples for the simplest Lax functions, where calculations are not very complicated. From the Lax hierarchies considered we exhibit only the first nontrivial systems.

Example 4.3: Two field system: $k=1$, $r\in\mathbb{Z}$.

Let us consider the Lax function of the form

$$L=p+u+vp^{-1}. \tag{4.5}$$

It has poles at ∞ *and* 0. *Then, for* ∞ *we have*

$$L_{t_{2-r}}=\{\Omega^{\infty}_{2-r},L\}_r\Leftrightarrow\begin{pmatrix}u\\v\end{pmatrix}_{t_{2-r}}=(2-r)\begin{pmatrix}(1-r)uu_x-v_x\\-u_xv-(1-r)uv_x\end{pmatrix}=\pi_0 dH^{\infty}_{2-r}=\pi_1^{\mathrm{red}}dH^{\infty}_{1-r}, \tag{4.6}$$

where $\Omega^{\infty}_{2-r}=(L^{2-r})^{\infty}_{\geqslant 1-r}=p^{2-r}+(2-r)up^{1-r}$. *When* $r=2$ *the next equation from the hierarchy is the first nontrivial one. For* $r=1$ *this is the well-known dispersionless Toda system. The hierarchy for* 0 *is the same as L has only two poles of the same order and* $(L^q)^{\infty}_{\geqslant 1-r}=L-(L^q)^{0}_{<1-r}$. *The roots of L are* $\lambda_{\pm}=\frac{1}{2}(-u\pm\sqrt{u^2-4v})$. *Thus, for* $r=1$,

$$\Omega_1^{\lambda_{\pm}}=-(L^{-1})^{\lambda_{\pm}}_{<0}=-\frac{1}{1-\dfrac{4v}{\lambda_{\pm}}}(p-\lambda_{\pm})^{-1}$$

and one finds the following:

$$L_{\tau_1^{\pm}}=\{\Omega^{\lambda_{\pm}}_{-1},L\}_1\Leftrightarrow\begin{pmatrix}u\\v\end{pmatrix}_{\tau_1^{\pm}}=\frac{\pm 1}{(u^2-4v)^{\frac{3}{2}}}\begin{pmatrix}2u_xv-uv_x\\v(2v_x-uu_x)\end{pmatrix}=\pi_0 dH^{\lambda_{\pm}}_{-1}=\pi_1^{\mathrm{red}}dH^{\lambda_{\pm}}_{-2}.$$

Of course, for $k=r=1$ *all equations mutually commute.*

The Lax function (4.5) *defines proper subspace with respect to the linear Poisson tensor* (4.2) *only for* $r=0,1$. *In the cases, the reduced quadratic Poisson tensors are given by* (4.4) and (4.3), *respectively. Hence, for* $r=0$,

$$\pi_0=\begin{pmatrix}0&\partial\\\partial&0\end{pmatrix},\quad \pi_1^{\mathrm{red}}=\begin{pmatrix}2\partial&\partial u\\u\partial&\partial v+v\partial\end{pmatrix}, \tag{4.7}$$

and related Hamiltonians are $H_1^{\infty}=\int_{\Omega}uv\ \mathrm{d}x$, $H_2^{\infty}=\int_{\Omega}(u^2v+v^2)\ \mathrm{d}x$. *For* $r=1$,

$$\pi_0=\begin{pmatrix}0&\partial v\\v\partial&0\end{pmatrix},\quad \pi_1^{\mathrm{red}}=\begin{pmatrix}\partial v+v\partial&u\,\partial v\\v\,\partial u&2v\,\partial v\end{pmatrix}$$

and

$$H_0^{\infty}=\int_{\Omega}uv\ \mathrm{d}x,\quad H_1^{\infty}=\int_{\Omega}(u^2v+v^2)\ \mathrm{d}x,$$

$$H^{\lambda_{\pm}}_{-2}=\int_{\Omega}\frac{\mp 1}{\sqrt{u^2-4v}}\ \mathrm{d}x,\quad H^{\lambda_{\pm}}_{-1}=\pm\int_{\Omega}\ln\frac{u+\sqrt{u^2-4v}}{v}\ \mathrm{d}x.$$

Example 4.4: Two field system: $k=2$, $r=2$.

We will consider Lax function of the form

$$L=vp+u+p^{-1}$$

i.e., function (4.5) *transformed by* $p\mapsto p^{-1}$. *By Proposition 4.2 the hierarchy for* ∞ *is given by hierarchy* (4.6) *for* $k=1$, $r=0$ *from the above-presented example. The roots of L are* $\alpha_{\pm}$

$=(-u\pm\sqrt{u^2-4v})/2v$. *Thus, for*

$$\Omega_1^{\alpha_\pm}=-(L^{-1})_{<0}^{\alpha_\pm}=-\frac{1}{v-\frac{4v^2}{\alpha_\pm^2}}(p-\alpha_\pm)^{-1}$$

one finds

$$L_{\xi_1^\pm}=\{\Omega_{-1}^{\alpha_\pm},L\}_2\Leftrightarrow\begin{pmatrix}u\\v\end{pmatrix}_{\xi_1^\pm}=\frac{\pm1}{(u^2-4v)^{3/2}}\begin{pmatrix}-uu_x+2v_x\\2u_xv-uv_x\end{pmatrix}=\pi_0 dH_{-1}^{\alpha_\pm}=\pi_1^{\mathrm{red}}dH_{-2}^{\alpha_\pm}.$$

This system by Proposition 4.2 commutes with (4.6) *for* $r=0$. *Thus, the Poisson tensors are given by* (4.7) *with Hamiltonians*

$$H_{-2}^{\alpha_\pm}=\int_\Omega\frac{\pm u}{2\sqrt{u^2-4v}}\mathrm{d}x,\quad H_{-1}^{\alpha_\pm}=\mp\int_\Omega\frac{1}{2}(u+\sqrt{u^2-4v})\mathrm{d}x.$$

B. Polynomial Lax functions in $(p-v)$ and $(p-v)^{-1}$

Let us consider Lax functions which are formal Laurent series around v, with a finite number of dynamical coefficients, of the form

$$L=u_N(p-v)^N+u_{N-1}(p-v)^{N-1}+\cdots+u_{1-m}(p-v)^{1-m}+u_{-m}(p-v)^{-m},\quad m\neq0.\tag{4.8}$$

Lax functions (4.8) have poles at ∞ and v, near which calculated powers generate, if allowed by k and r, respective Lax hierarchies. Additional powers with related hierarchies can be constructed around the roots of L.

Proposition 4.5: Lax function of the form (4.8) *is an appropriate one in the following cases:*

1. $k=r=0$: $u_N=1$, $u_{N-1}=Nv$;
2. $k=1$, $r\in\mathbb{Z}$: $N\neq0$, $u_N=1$, $L|_{p=0}=0$ *for* $r=1$;
3. $k=2$, $r\in\mathbb{Z}$: $N\neq0$ *when* $r=1$, $L|_{p=0}=0$, $\frac{d}{dp}L|_{p=0}=1$;
4. $k=3$, $r=2$: $N=0$, $L|_{p=0}=0$, $\frac{d}{dp}L|_{p=0}=1$, $\frac{d^2}{dp^2}L|_{p=0}=0$.

Moreover, for fixed r and k, the respective Lax hierarchies commute.

Proof: It is enough to consider the Lax hierarchy related to ∞. Function (4.8) will be appropriate Lax function if the left- and right-hand sides of Lax hierarchy (3.15) for $\lambda=\infty$ will coincide and the number of independent equations will be the same as the number of dynamical coefficients in L. This Lax hierarchy can be written in two equivalent representations

$$L_t=\{A_{\geqslant k-r}^\infty,L\}_r=-\{A_{<k-r}^\infty,L\}_r.$$

So, we have to examine expansions of this hierarchy near ∞ and v as well as at 0, since the factor p^r occurs in Poisson bracket. It turns out that the first representation yields direct access to terms with lowest orders, whereas the second representation yields information about terms with highest orders. Near ∞ we have

$$L_t=(u_N)_tp^N+(u_{N-1}-Nv)_tp^{N-1}+\textit{lower terms},$$

$$L_t=-\{A_{<k-r}^\infty,L\}_r=-\{\alpha p^{k-r-1}+l.t.,u_Np^N+l.t.\}_r=(\ldots)p^\alpha+l.t.,$$

where $\alpha=N+k-2$ for $N\neq0$ or $r\neq k-1$; and $\alpha=0$ for $N=0$ and $r=k-1$. This imposes the constraints on fields u_N and u_{N-1} given in the Proposition. The expansion of $A_{\geqslant k-r}^\infty$ near v is of the form $A_{\geqslant k-r}^\infty=$*higher terms*$+\gamma_1(p-v)+\gamma_0$ as $A_{\geqslant k-r}^\infty$ does not have singularity at v. So, near v we have

$$L_t = higher\ terms + (u_{-m} + (m-1)v)_t (p-v)^{-m} + mv_t (p-v)^{-m-1},$$

$$L_t = \{A^{\infty}_{\geqslant k-r}, L\}_r = \{h\,.\,t\,.\, + \gamma_0, h\,.\,t\,.\, + u_{-m}(p-v)^{-m}\}_r = h\,.\,t\,.\, + (\ldots)(p-v)^{-m-1}$$

and the lowest order of the left- and right-hand side are always the same. The expansion of $A^{\infty}_{\geqslant k-r}$ near 0 is of the form $A^{\infty}_{\geqslant k-r} = higher\ terms + \gamma p^{k-r}$. So we have

$$L_t = higher\ terms + \tfrac{1}{2}\left(\tfrac{d^2}{dp^2}L\big|_{p=0}\right)_t p^2 + \left(\tfrac{d}{dp}L\big|_{p=0}\right)_t p + (L|_{p=0})_t,$$

$$L_t = \{A^{\infty}_{\geqslant k-r}, L\}_r = \left\{h\,.\,t\,.\, + \gamma p^{k-r}, h\,.\,t\,.\, + \tfrac{d}{dp}L\big|_{p=0} p + L|_{p=0}\right\}_r = h\,.\,t\,.\, + (\ldots)p^{\alpha}.$$

For $k=r=0$ we have $\alpha=0$ and there is no need for additional constraints. For $k=1$ if $r\neq 1$: $\alpha=0$ and both sides have the same order in expansion at 0. But for $k=r=1$ we have $\alpha=1$. Hence, $(L|_{p=0})_t=0$ and we have to impose the constraint $L|_{p=0}=0$. Then, both sides have the same form. For $k=2$ and arbitrary r: $\alpha>0$ and the first constraint of the form $L|_{p=0}=0$ is needed. Taking into consideration this constraint: $\alpha=2$ and it follows that $((d/dp)L|_{p=0})_t=0$. Hence, both sides will agree if we impose an additional constraint $(d/dp)L|_{p=0}=1$. For $k=3$ the reasoning is similar to the case $k=2$, but there will be one more constraint of the form $(d^2/dp^2)L|_{p=0}=0$ needed. Commutation of Lax hierarchies follows from Corollary 3.5. □

Proposition 4.6: Lax hierarchies defined at ∞ and v for the case k=r=0 of Proposition 4.5 by the transformation p↦p−v turns to Lax hierarchies related to ∞ and 0, *respectively, for the case k=1, r=0 of Proposition 4.1.*

Proof: Consider the transformation $p'=p-v$, $x'=x$, $t'=t$. Then, $\partial_p=\partial_{p'}$, $\partial_x=\partial_{x'}-v_x\partial_{p'}$ and $\partial_t=\partial_{t'}-v_t\partial_{p'}$. The points at ∞ and v transform into points at ∞ and 0, respectively, and the Poisson bracket (3.1) for $r=0$ is preserved:

$$\{\cdot,\cdot\}_0 = \partial_p \wedge \partial_x = \partial_{p'} \wedge (\partial_{x'} + v_{x'}\partial_{p'}) = \partial_{p'} \wedge \partial_{x'} = \{\cdot,\cdot\}'_0.$$

Let L be the Lax function of the form (4.8) from Proposition 4.5 for $r=k=0$. Then, by the above-noted transformation $L'=L$ is a Lax function of the form (4.1) from Proposition 4.5 for $r=0$, $k=1$. For meromorphic function $A\in\mathcal{A}$, let $[A]_\lambda$ mean the zero-order term of Laurent series at λ. From (3.15) for $\lambda=\infty$ and v it follows that $v_{t_{\infty,q}}=([L^{q/N}]_\infty)_x$ and $v_{t_{v,q}}=([L^{q/m}]_v)_x$, respectively. Thus the left- and right-hand sides of (3.15) for $\lambda=v$ are equal

$$L_\tau = L'_{\tau'} - v_\tau L'_{p'} = L'_{\tau'} - ([L'^{\frac{q}{m}}]^v)_x L'_{p'} = L'_{\tau'} + \{[L'^{\frac{q}{m}}]^0, L'\}'_0,$$

$$L_\tau = -\{(L'^{\frac{q}{m}})^v_{<0}, L\}_0 = -\{(L'^{\frac{q}{m}})^0_{<0}, L'\}'_0,$$

where $\tau=t_{v,q}$ and $\tau'=t'_{v,q}$. Hence,

$$L'_{\tau'} = -\{(L'^{\frac{q}{m}})^0_{<1}, L'\}'_0.$$

Similar calculations are valid at ∞. □

A similar observation as in the above-noted Proposition has been made earlier in Ref. 4.

Notice that for the case $k=r=0$ of Proposition 4.5 one is able to construct Lax hierarchies related to the roots of L, which is not possible for the case $k=1, r=0$ of Proposition 4.1. In this sense, the first case is more general.

Proposition 4.7: Under the transformation $p'=p^{-1}$, the following equalities between some cases from Proposition 4.5 hold:

- *the Lax hierarchy related to* 0 *for $k=3, r=2$ is equivalent to the Lax hierarchy related to ∞ for $k=r=0$ with $N=-1$;*
- *the Lax hierarchy related to* 0 *for $k=2, r\neq 1$ with $N=0$ is equivalent to the Lax hierarchy related to ∞ for $k=1, r\neq 1$ with $N=-1$;*

- *Lax hierarchies related to* ∞ *and* 0 *for* $k=2, r=1$ *with* $N=-1$ *are equivalent to Lax hierarchies related to* 0 *and* ∞ *for* $k=1, r=1$ *with* $N=-1$, $L|_{p=0}=0$, *respectively*.

Proof: The appropriate Lax function from Proposition 4.5 for $k=3$, $r=2$ has the form

$$L = u_0 + u_{-1}(p-v)^{-1} + \cdots + u_{-m}(p-v)^{-m},$$

where $L|_{p=0}=0$, $(d/dp)L|_{p=0}=1$ and $(d^2/dp^2)L|_{p=0}=0$. Taking into consideration the above-noted constraints, expansion of L around 0 is $L=\cdots+(\cdots)p^2+p$. By transformation $p'=p^{-1}$ we have that

$$(p-v)^{-1} = (p'^{-1}-v)^{-1} = -v' - v'^2(p'-v')^{-1}$$

where $v'=v^{-1}$. Thus L transforms into

$$L' = u'_0 + u'_{-1}(p'-v')^{-1} + \cdots + u'_{-m}(p'-v')^{-m}.$$

From the expansion around 0 of L it follows that expansion of L' near ∞ is $L'=p'^{-1}+(\cdots)p'^{-2}+\cdots$. Hence, $u'_0=0$, $u'_{-1}=1$ and the Lax function L' is an appropriate one for $k=r=0$. An analogues approach must be taken for the next two relations. The rest holds by Proposition 3.1. □

Now, let us pass to the Hamiltonian formulation of Lax hierarchies related to the appropriate Lax functions from Proposition 4.5. In general, the relevant cases are for $k=0,1,2$. Further we will consider only them. The differential at ∞ of functional H for the Lax function of the general form (4.8) is given by

$$dH \equiv d_\infty H = p^r\left(\frac{1}{mu_{-m}}\left(\frac{\delta H}{\delta v} + \sum_{i=1-m}^{N} iu_i\frac{\delta H}{\delta u_{i-1}}\right)(p-v)^m + \sum_{i=1-m}^{N+1}\frac{\delta H}{\delta u_{i-1}}(p-v)^{-i}\right) \tag{4.9}$$

as

$$\mathrm{Tr}_\infty(L_t dH) = -\int_\Omega \mathrm{res}_\infty(p^{-r}L_t dH)\,\mathrm{d}x \overset{\text{by (3.7)}}{=} \int_\Omega \mathrm{res}_v(p^{-r}L_t dH)\,\mathrm{d}x = \int_\Omega\left(\sum_{i=-m}^{N}(u_i)_t\frac{\delta H}{\delta u_i} + v_t\frac{\delta H}{\delta v}\right)\mathrm{d}x.$$

For the Lax functions with constraints from Proposition 4.5 one has to modify differentials (4.9) in an appropriate way or construct them by (4.11), i.e., in the same way as in the next section. One has to examine when a given Lax function from Proposition spans the proper subspace with respect to Poisson tensors. The procedure is rather technical and similar to the proof of this proposition. Thus, we omit it and we will present only the final results. The Lax functions from Proposition 4.5 for $k=0,1,2$ span proper subspace with respect to linear Poisson tensor $n=0$ if $N\geqslant 2r-2k+1$, $m\geqslant -1$ and $r\geqslant k$. Then, it is given by (4.2). If it is not the case, Dirac reduction is required. The reduced linear Poisson tensor for $N=-1$, $m\geqslant 1$ and $k=r=0,1,2$ is given by (4.12). These Lax functions do not form a proper subspace with respect to quadratic Poisson tensor $n=1$ and always the Dirac reduction procedure is needed. For $k=r=0,1,2$ reduced quadratic Poisson tensors have the form (4.3).

Example 4.8: Two-field system: $k=r=1$.

The Lax function, taking into consideration appropriate constraints, is given by the form

$$L = (p-v) + u + v(u-v)(p-v)^{-1} = \frac{p(p+u-2v)}{p-v}.$$

For ∞ *one finds* $\Omega_1^\infty=(L)^\infty_{\geqslant 0}=p+u-v$ *and*

$$L_{t_1} = \{\Omega_1^\infty, L\}_1 \Leftrightarrow \begin{pmatrix} u \\ v \end{pmatrix}_{t_1} = \begin{pmatrix} 2u_x v + uv_x - 2vv_x \\ u_x v \end{pmatrix} = \pi_0 dH_1^\infty = \pi_1^{\mathrm{red}} dH_0^\infty.$$

The Lax hierarchy related to v *is the same as* $L=(L)^\infty_{\geqslant 0}+(L)^v_{<0}$. *The Lax function has two roots* 0 *and* $2v-u$. *Then, for* $\Omega_1^0=-(L^{-1})^0_{<0}=-[v/(2v-u)]p^{-1}$ *we have*

$$L_{\tau_1} = \{\Omega_1^0, L\}_1 \Leftrightarrow \begin{pmatrix} u \\ v \end{pmatrix}_{\tau_1} = \begin{pmatrix} \dfrac{v_x}{2v-u} \\ \dfrac{2vv_x - u_x v}{(u-2v)^2} \end{pmatrix} = \pi_0 dH_{-1}^0 = \pi_1^{\mathrm{red}} dH_{-2}^0.$$

The Lax hierarchy related to the root $2v-u$ *is up to the sign the same as above since* $L^{-1} = (L^{-1})_{\geqslant 0}^0 + (L^{-1})_{<0}^{2v-u}$.

The general form for a differential of a given functional H according to (4.9) *is*

$$dH = \frac{(2-u)\dfrac{\delta H}{\delta u} + v\dfrac{\delta H}{\delta v}}{(u-v)v^2} p(p-v) + \frac{1}{v}\frac{\delta H}{\delta v} p.$$

The Lax function defines the proper subspace with respect to the linear Poisson tensor (4.2). *The reduced quadratic Poisson tensors are given by* (4.4). *Then*,

$$\pi_0 = \begin{pmatrix} \partial v + v\,\partial & \partial v \\ v\,\partial & 0 \end{pmatrix} \quad \pi_1^{\mathrm{red}} = \begin{pmatrix} 2\,\partial uv + 2uv\,\partial & u\,\partial v + 2v\,\partial v \\ v\,\partial u + 2v\,\partial v & 2v\,\partial v \end{pmatrix}.$$

The respective Hamiltonians are

$$H_0^\infty = \int_\Omega (u-v)\,\mathrm{d}x, \quad H_1^\infty = \frac{1}{2}\int_\Omega (u^2 - v^2)\,\mathrm{d}x,$$

$$H_{-2}^0 = \int_\Omega \frac{v-u}{(u-2v)^2}\,\mathrm{d}x, \quad H_{-1}^0 = \int_\Omega \ln\left(\frac{u}{v} - 2\right)\mathrm{d}x.$$

C. Rational Lax functions

Let us consider the general form of meromorphic Lax function given by

$$L = \sum_{k=-m_0}^{N} u_k p^k + \sum_{i=1}^{\alpha} \sum_{k_i=1}^{m_i} a_{i,k_i} (p - v_i)^{-k_i}, \tag{4.10}$$

where u_k, a_{i,k_i}, and v_i are dynamical fields. From this class of functions considered in the following section we exclude those which have been examined earlier, i.e., (4.1) and (4.8). Any function (4.10) in general has a pole at ∞ of order N, at 0 of order m_0 and α evolution poles at v_j of order m_j. Then, one can construct positive powers of Laurent series at poles of L. Additional Lax hierarchies are generated by negative powers constructed near to the roots of L.

Proposition 4.9: Function of the form (4.10) *is an appropriate one in the following cases:*

1. $k=r=0$:
   - $N \geqslant 1$, $u_N=1$, $u_{N-1}=0$, $m_0=0$,
   - $\forall_k\ u_k=0$, $\Sigma_{i=1}^{\alpha} a_{i,1}=1$, $\Sigma_{i=1}^{\alpha}(a_{i,1}v_i + a_{i,2})=0$;
2. $k=1$, $r \in \mathbb{Z}$:
   - $N \geqslant 1$, $u_N=1$, $m_0 \geqslant 1$,
   - $N=-1$, $u_{-1} + \Sigma_{i=1}^{\alpha} a_{i,1}=1$, $m_0 \geqslant 1$,
   - $N \geqslant 1$, $u_N=1$, $m_0=0$, $L|_{p=0}=0$ *for* $r=1$,
   - $\forall_k\ u_k=0$, $\Sigma_{i=1}^{\alpha} a_{i,1}=1$, $L|_{p=0}=0$ *for* $r=1$;
3. $k=2$, $r \in \mathbb{Z}$:

- $N \geqslant 1$, $m_0 \geqslant 1$, $u_{-m_0}=1$,
- $N \geqslant 1$, $m_0=0$, $L|_{p=0}=0$, $\frac{d}{dp}L|_{p=0}=1$,
- $N=0$, $u_0=0$ for $r=1$, $m_0 \geqslant 1$, $u_{-m_0}=1$,
- $\forall_{k\neq 0}\ u_k=0$, $u_0=0$ *for* $r=1$, $L|_{p=0}=0$, $\frac{d}{dp}L|_{p=0}=1$;

4. $k=3$ and $r=2$

- $N=0$, $m_0 \geqslant 1$, $u_{1-m_0}=0$, $u_{-m_0}=1$,
- $\forall_{k\neq 0}\ u_k=0$, $L|_{p=0}=0$, $\frac{d}{dp}L|_{p=0}=1$, $\frac{d^2}{dp^2}L|_{p=0}=0$.

Moreover Lax hierarchies calculated at different points for fixed r and k mutually commute. We excluded here the Lax functions of the form (4.1) and (4.8).

The proof is similar to the one of Proposition 4.5. So, the meromorphic function of the form (4.10) will be an appropriate Lax function with respect to Lax hierarchies (3.15) defined at poles and roots of L if:

- the right-hand sides of the Lax hierarchy considered and the time derivatives L_t will have the same order at all above poles,
- the number of independent equations, resulting from Lax hierarchies, will be the same as that of dynamical coefficients included in L.

The first condition implies all constraints considered in Proposition 4.9. To see that, an analysis like that in the proof of Proposition 4.5 is needed. So, by the first condition the right-hand sides of considered Lax hierarchies for appropriate r and k can be uniquely presented in the form of L_t, i.e., the left-hand sides. So, the second condition immediately follows from the first one.

The simplest way of deriving dispersionless systems related to given meromorphic Lax functions is to transform Lax hierarchies into purely polynomial form in p through removal of finite singularities. It can be done by multiplication of both sides of Lax hierarchies by a proper factor.

Proposition 4.10: Under transformation $p'=p^{-1}$ *Lax hierarchies*, *from Proposition* 4.9, *defined at* ∞ *and* 0 *for appropriate r and k transforms into Lax hierarchies defined at* 0 *and* ∞ *for* $r'=2-r$ *and* $k'=3-k$, *respectively*.

See proof of Proposition 4.7 and the comment after Proposition 4.2. Hence, the relevant cases from Proposition 4.9 are exactly the same as in Sec. IV A for Proposition 4.1.

Once again we will consider Poisson tensors defined at ∞. This time we are not going to present the explicit form of differentials $d_\infty H$ for the general meromorphic Lax function, but we will explain how to construct them. We postulate that

$$dH \equiv d_\infty H = \sum_{i=N_\infty-\beta+1}^{N_\infty} \gamma_i p^{r-i-1}, \tag{4.11}$$

where β is a number of dynamical coefficients in L and N_∞ is the highest order of Laurent series of L_t at ∞. The form (4.11) allows us to solve (3.9) ($\lambda=\infty$) to obtain functions γ_i in terms of dynamical coefficients of L and its variational derivatives such that we obtain the required Euclidean form. We will consider only relevant cases of meromorphic Lax functions from Proposition 4.9. Verification that they span the proper subspace with respect to Poisson tensors is similar to the proof of this proposition. These Lax functions span the proper subspace with respect to the linear Poisson tensor (4.2) for $k=0$ if $N \geqslant 1$ and for $k=1,2$ if $N \geqslant 2r-2k+1 \geqslant -m_0$. If not the case, the Dirac reduction is required. The reduced linear tensors for $k=r=0,1,2$ and $N=-1$ (N is the highest order of Laurent series of$L$ at ∞) are given by

$$\pi_0^\infty dH = \{(dH)_{\geqslant 0}^\infty, L\}_r - (\{dH, L)_r\}_{\geqslant r}^\infty + \{\gamma_1 p + \gamma_0, L\}_r,$$

$$\gamma_1 = \partial_x^{-1}\mathrm{res}_\infty\{dH, L\}_0, \tag{4.12}$$

$$\gamma_0 = \partial_x^{-1}\mathrm{res}_\infty\{dH,L\}_1 - \partial_x^{-1}(\gamma_1((L)_{-2}^\infty)_x + 2(\gamma_1)_x(L)_{-2}^\infty),$$

where $(L)_{-2}^\infty$ is the coefficient staying at the term of order -2 in Laurent series at ∞. For $k=r=0$ we have $(L)_{-2}^\infty=0$ and (4.12) simplified. Notice that for $k=r=0$ the reduced Poisson tensor (4.12) is always local, but for the remaining cases it is in general not. In the case of quadratic Poisson tensors, considered Lax functions do not span proper subspaces and the Dirac reduction is needed. The reduced quadratic Poisson tensor for $k=r=0,1,2$ are given by (4.3), and for $k=1,r=0$ and $k=2,r=1$ by (4.4) where $m=m_0$.

Example 4.11: The two-field system: $k=r=0$.

The Lax function has the form

$$L = u(p-v)^{-1} + (1-u)\left(p - \frac{uv}{u-1}\right)^{-1},$$

where constraints from Proposition 4.9 *are properly taken into consideration. The roots of L are* ∞ *and* $\alpha=(2uv-v)/(u-1)$. *Then, for* ∞ *we have*

$$L_{t_2} = \{\Omega_2^\infty, L\}_0 \Leftrightarrow \begin{pmatrix} u \\ v \end{pmatrix}_{t_2} = \begin{pmatrix} 2uv \\ \dfrac{(3u-1)v^2}{u-1} \end{pmatrix}_x = \pi_0^{\mathrm{red}} dH_{-2}^\infty = \pi_1^{\mathrm{red}} dH_{-3}^\infty,$$

where $\Omega_2^\infty=(L^{-2})_{\geqslant 0}^\infty=p^2+2uv^2/(u-1)$. *The hierarchy for* α *is the same as* $(L^q)_{\geqslant 0}^\infty=L-(L^q)_{<0}^\alpha$. *The function L has poles at v and* $\lambda=uv/(u-1)$. *At the point v one finds the following system:*

$$L_{\tau_1} = \{\Omega_1^v, L\}_0 \Leftrightarrow \begin{pmatrix} u \\ v \end{pmatrix}_{\tau_1} = \begin{pmatrix} \dfrac{u(u-1)^3}{v^2} \\ \dfrac{(u-1)^2}{v} \end{pmatrix}_x = \pi_0^{\mathrm{red}} dH_1^v = \pi_1^{\mathrm{red}} dH_0^v,$$

where $\Omega_1^v=-(L)_{<0}^v=-u(p-v)^{-1}$. *The Lax function is invariant with respect to the transformation* $u\mapsto 1-u$, $v\mapsto uv/(u-1)$. *Therefore, the Lax hierarchy related to* λ *can be obtained through this transformation.*

In this case the differential of a given functional calculated by (4.11) *is*

$$dH = \left(\frac{2(u-1)^3}{v^3}\frac{\delta H}{\delta u} + \frac{(u-1)^2}{uv^2}\frac{\delta H}{\delta v}\right)p^3 + \left(\frac{3(u-1)^2(2u-1)}{v^2}\frac{\delta H}{\delta u} + \frac{(u-1)(3u-1)}{uv}\frac{\delta H}{\delta v}\right)p^2.$$

Then, from (4.12) and (4.3) *we find the following Poisson tensors:*

$$\pi_0^{\mathrm{red}} = \begin{pmatrix} 0 & \partial(1-u) \\ (1-u)\partial & -\partial v - v\partial \end{pmatrix}, \quad \pi_1^{\mathrm{red}} = \begin{pmatrix} \partial\dfrac{u}{v^2}(u-1)^3 + \dfrac{u}{v^2}(u-1)^3\partial & \dfrac{(u-1)^2}{v}\partial \\ \partial\dfrac{(u-1)^2}{v} & 0 \end{pmatrix},$$

respectively. The Hamiltonians are

$$H_{-3}^\infty = \int_\Omega \frac{uv}{1-u}\,\mathrm{d}x, \quad H_{-2}^\infty = \int_\Omega \frac{uv^2}{1-u}\,\mathrm{d}x, \quad H_0^v = \int_\Omega v\,\mathrm{d}x, \quad H_1^v = \int_\Omega \frac{u(u-1)^2}{v}\,\mathrm{d}x.$$

Example 4.12: The four-field dispersionless system: $k=r=0$.

For the Lax function of the form

$$L = p + a(p-v)^{-1} + b(p-w)^{-1} \tag{4.13}$$

near ∞ *one finds*

$$L_{t_2}=\{\Omega_2^\infty,L\}_0\Leftrightarrow\begin{pmatrix}a\\b\\v\\w\end{pmatrix}_{t_2}=\begin{pmatrix}2av\\2bw\\2a+2b+v^2\\2a+2b+w^2\end{pmatrix}_x=\pi_0 dH_2^\infty=\pi_1^{\mathrm{red}}dH_1^\infty,$$

where $\Omega_2^\infty=(L^2)_{\geqslant 0}^\infty=p^2+2a+2b$. *Near the* v *we have*

$$L_{\tau_1}=\{\Omega_1^v,L\}_0\Leftrightarrow\begin{pmatrix}a\\b\\v\\w\end{pmatrix}_{\tau_1}=\begin{pmatrix}a-\dfrac{ab}{(v-w)^2}\\[2mm]\dfrac{ab}{(v-w)^2}\\[2mm]v+\dfrac{b}{v-w}\\[2mm]\dfrac{a}{v-w}\end{pmatrix}_x=\pi_0 dH_1^v=\pi_1^{\mathrm{red}}dH_0^v,$$

where $\Omega_1^v=-(L)_{<0}^v=-a(p-v)^{-1}$. *There are three, very complicated, roots of L. Thus, we are not going to calculate the respective equations.*

The differential of a functional H is

$$dH=\left(\frac{2}{v-w}\frac{\delta H}{\delta b}+\frac{1}{b}\frac{\delta H}{\delta w}\right)\frac{(p-v)^2(p-w)}{(v-w)^2}+\left(\frac{2}{w-v}\frac{\delta H}{\delta a}+\frac{1}{a}\frac{\delta H}{\delta v}\right)\frac{(p-v)(p-w)^2}{(w-v)^2}$$
$$+\frac{1}{(v-w)^2}\frac{\delta H}{\delta b}(p-v)^2+\frac{1}{(w-v)^2}\frac{\delta H}{\delta a}(p-w)^2.$$

Then, from (4.2) and (4.3) *one finds the linear*

$$\pi_0=\begin{pmatrix}0&0&\partial&0\\0&0&0&\partial\\\partial&0&0&0\\0&\partial&0&0\end{pmatrix}$$

and quadratic Poisson tensors

$$\pi_1^{\mathrm{red}}=\begin{pmatrix}\partial a+a\,\partial-\partial\dfrac{ab}{(v-w)^2}-\dfrac{ab}{(v-w)^2}\partial & \partial\dfrac{ab}{(v-w)^2}+\dfrac{ab}{(v-w)^2}\partial & \left(v+\dfrac{b}{v-w}\right)\partial & \dfrac{a}{v-w}\partial\\[2mm]\partial\dfrac{ab}{(v-w)^2}+\dfrac{ab}{(v-w)^2}\partial & \partial b+b\,\partial-\partial\dfrac{ab}{(v-w)^2}-\dfrac{ab}{(v-w)^2}\partial & -\dfrac{b}{v-w}\partial & \left(w-\dfrac{a}{v-w}\right)\partial\\[2mm]\partial\left(v+\dfrac{b}{v-w}\right) & -\partial\dfrac{b}{v-w} & 2\partial & \partial\\[2mm]\partial\dfrac{a}{v-w} & \partial\left(w-\dfrac{a}{v-w}\right) & \partial & 2\partial\end{pmatrix},$$

respectively. The Hamiltonians are

$$H_1^\infty=\int_\Omega(av+bw)\,\mathrm{d}x,\quad H_2^\infty=\int_\Omega((a+b)^2+av^2+bw^2)\,\mathrm{d}x,$$

$$H_0^v=\int_\Omega a\,\mathrm{d}x,\quad H_1^v=\int_\Omega\left(av+\frac{ab}{v-w}\right)\mathrm{d}x.$$

Example 4.13: Four-field system: $k=1$, $r\in\mathbb{Z}$.

Let us consider a Lax function of the form

$$L = p + u + vp^{-1} + w(p-s)^{-1}. \tag{4.14}$$

It has poles at ∞, 0, *and* w. *Related equations to* ∞ *for* $\Omega^{\infty}_{2-r}=(L^{2-r})^{\infty}_{\geqslant 1-r}=p^{2-r}+(2-r)up^{1-r}$ *are*

$$L_{t_{2-r}} = \{\Omega^{\infty}_{2-r}, L\}_r \Leftrightarrow \begin{pmatrix} u \\ v \\ w \\ s \end{pmatrix}_{t_{2-r}} = (2-r)\begin{pmatrix} (1-r)uu_x + v_x + w_x \\ u_x v + (1-r)uv_x \\ u_x w + (1-r)uw_x + (ws)_x \\ u_x s + (1-r)us_x + ss_x \end{pmatrix} = \pi_0 dH^{\infty}_{2-r} = \pi_1^{\mathrm{red}} dH^{\infty}_{1-r}.$$

The first equations from Lax hierarchies related to 0 *for* $r\neq 0$ *are*

$$L_{\tau_r} = \{\Omega^0_r, L\}_r \Leftrightarrow \begin{pmatrix} u \\ v \\ w \\ s \end{pmatrix}_{\tau_r} = rv^r \begin{pmatrix} \ln v \\ u - \dfrac{w}{s} \\ \dfrac{w}{s} \\ \ln \dfrac{s}{v} \end{pmatrix}_x = \pi_0 dH^0_r = \pi_1^{\mathrm{red}} dH^0_{r-1},$$

where $\Omega^0_r=-(L^r)^0_{<1-r}=-v^r p^{-r}$. *But for* $r=0$ *we have*

$$L_{\tau_1'} = \{\Omega^0_1, L\}_0 \Leftrightarrow \begin{pmatrix} u \\ v \\ w \\ s \end{pmatrix}_{\tau_1'} = \begin{pmatrix} u - \dfrac{w}{s} \\ v - \dfrac{vw}{s^2} \\ \dfrac{vw}{s^2} \\ \dfrac{w-v}{s} - u \end{pmatrix}_x = \pi_0 dH^0_1 = \pi_1^{\mathrm{red}} dH^0_0,$$

where $\Omega^0_1=-(L)^0_{<1}=w/s-u-vp^{-1}$. *For* $r=1$ *and* $\Omega^s_1=-(L)^s_{<0}=-w(p-s)^{-1}$ *one finds*

$$L_{\xi_1} = \{\Omega^s_1, L\}_1 \Leftrightarrow \begin{pmatrix} u \\ v \\ w \\ s \end{pmatrix}_{\xi_1} = \begin{pmatrix} w_x \\ v\left(\dfrac{w}{s}\right)_x \\ u_x w + (ws)_x - v\left(\dfrac{w}{s}\right)_x \\ u_x s + ss_x + s\left(\dfrac{v}{s}\right)_x \end{pmatrix} = \pi_0 dH^s_1 = \pi_1^{\mathrm{red}} dH^s_0.$$

Once again we are not going to consider Lax hierarchies related to roots of L.

The differential of a functional H *is*

$$dH = \left(\frac{\delta H}{\delta s} + \frac{1}{s^2}\left(\frac{\delta H}{\delta v} - \frac{\delta H}{\delta w}\right)\right)p^{r+2} - \left(\frac{2}{s}\left(\frac{\delta H}{\delta v} - \frac{\delta H}{\delta w}\right) + \frac{1}{w}\frac{\delta H}{\delta s}\right)p^{r+1} + \frac{\delta H}{\delta v}p^r + \frac{\delta H}{\delta u}p^{r-1}.$$

The Lax function (4.14) *span the proper subspace with respect to linear Poisson tensor* (4.2) *only for* $r=0,1$. *The reduced quadratic tensors are for* $r=0,1$ *given by* (4.4) and (4.3), *respectively*. *Thus, for* $r=0$:

$$\pi_0 = \begin{pmatrix} 0 & \partial & 0 & 0 \\ \partial & 0 & 0 & -\partial \\ 0 & 0 & 0 & \partial \\ 0 & -\partial & \partial & 0 \end{pmatrix} \tag{4.15}$$

and

$$\pi_1^{red} = \begin{pmatrix} 2\partial & \partial\left(u - \frac{w}{s}\right) & \partial\frac{w}{s} & -\partial \\ \left(u - \frac{w}{s}\right)\partial & \partial v\left(1 - \frac{w}{s^2}\right) - v\left(1 - \frac{w}{s^2}\right)\partial & \partial\frac{vw}{s^2} + \frac{vw}{s^2}\partial & \left(\frac{w-v}{s} - u\right)\partial \\ \frac{w}{s}\partial & \partial\frac{vw}{s^2} + \frac{vw}{s^2}\partial & \partial w\left(1 - \frac{v}{s^2}\right) - w\left(1 - \frac{v}{s^2}\right)\partial & \left(u + s + \frac{v-w}{s}\right)\partial \\ -\partial & \partial\left(\frac{w-v}{s} - u\right) & \partial\left(u + s + \frac{v-w}{s}\right) & 2\partial \end{pmatrix}. \tag{4.16}$$

The related Hamiltonians are

$$H_1^\infty = \int_\Omega \left(uv + uw + ws\right)\,\mathrm{d}x, \quad H_2^\infty = \int_\Omega \left(u^2v + v^2 + ws^2 + 2uws + u^2w + 2vw + w^2\right)\,\mathrm{d}x,$$

$$H_0^0 = \int_\Omega v\mathrm{d}x, \quad H_1^0 = \int_\Omega v\left(u - \frac{w}{s}\right)\,\mathrm{d}x.$$

For $r=1$ *we have*

$$\pi_0 = \begin{pmatrix} 0 & \partial v & \partial w & \partial s \\ v\partial & 0 & 0 & 0 \\ w\partial & 0 & s\,\partial w + w\,\partial s & s\,\partial s \\ s\partial & 0 & s\,\partial s & 0 \end{pmatrix}$$

and

$$\pi_1^{\mathrm{red}} = \begin{pmatrix} \partial(v+w) + (v+w)\partial & u\,\partial v & 2\,\partial ws + ws\,\partial + u\,\partial w & (u+s)\,\partial s \\ v\,\partial u & 2v\,\partial v & 2v\,\partial w & v\,\partial s \\ \partial ws + 2ws\,\partial + w\,\partial u & 2w\,\partial v & \pi_{ww} & (s^2 + us + v + 2w)\,\partial s \\ s\,\partial(u+s) & s\,\partial v & s\,\partial(s^2 + us + v + 2w) & 2s\,\partial s \end{pmatrix},$$

where $\pi_{ww} = \partial uws + uws\,\partial + w\,\partial(2s^2+w) + (2s^2+w)\,\partial w$. *The related Hamiltonians are*

$$H_0^\infty = \int_\Omega u\mathrm{d}x, \quad H_1^\infty = \int_\Omega \left(\frac{1}{2}u^2 + v + w\right)\mathrm{d}x,$$

$$H_0^0 = \int_\Omega \left(u - \frac{w}{s}\right)\mathrm{d}x, \quad H_1^0 = \int_\Omega \left(\frac{1}{2}u^2 + v - \frac{uw}{s} - \frac{vw}{s^2} + \frac{w^2}{2s^2}\right)\mathrm{d}x,$$

$$H_0^s = \int_\Omega \frac{w}{s}\mathrm{d}x, \quad H_1^s = \int_\Omega \left(w + \frac{uw}{s} + \frac{vw}{s^2} - \frac{w^2}{2s^2}\right)\mathrm{d}x.$$

Example 4.14: Four-field system: $k=r=2$.
Lax function (4.14) *transformed by* $p\mapsto p^{-1}$ *has the form*

$$L=vp+u-\frac{w}{s}+p^{-1}-\frac{w}{s^2}(p-s^{-1})^{-1}.$$

For $\Omega_1^{s^{-1}}=-(L)_{<0}^{s^{-1}}=-(w/s^2)(p-s^{-1})^{-1}$ *one finds the system*

$$L_{\xi_1'}=\{\Omega_1^{s^{-1}},L\}_1\Leftrightarrow\begin{pmatrix}u\\v\\w\\s\end{pmatrix}_{\xi_1'}=\begin{pmatrix}-\frac{w}{s}\\-\frac{vw}{s^2}\\w\left(\frac{v}{s^2}-1\right)\\-u-s+\frac{v-w}{s}\end{pmatrix}_x=\pi_0 dH_1^{s^{-1}}=\pi_1^{\mathrm{red}}dH_0^{s^{-1}}$$

commuting, *by Proposition* (4.10), *with equations from Example* 4.13 *for* $r=0$. *The linear and quadratic Poisson tensors are given by* (4.15) and (4.16), *respectively*. *Hamiltonian functionals are given by*

$$H_0^{s^{-1}}=-\int_\Omega w\,\mathrm{d}x,\quad H_1^{s^{-1}}=\int_\Omega w\left(u+\frac{v-1}{s}\right)\mathrm{d}x.$$

V. COMMENTS

The case $r=k=0$ of meromorphic Lax hierarchies considered in this article are finite-field reductions to zero-genus Whitham hierarchy.[2]. Originally in Ref. 2 each Lax hierarchy defined at pole v of Lax function, being dynamical field, is extended over additional symmetry related to the generating function $\Omega_0^v=\ln(p-v)$. For example, for Lax function (4.13) the additional symmetry at v is

$$L_s=\{\Omega_0^v,L\}_0\Leftrightarrow\begin{pmatrix}a\\b\\v\\w\end{pmatrix}_s=\begin{pmatrix}v+\frac{b}{v-w}\\-\frac{b}{v-w}\\\ln a\\\ln(v-w)\end{pmatrix}_x.$$

The calculus including ln-terms is discussed in Ref. 4. In Ref. 22 it is shown how the Toda hierarchy from Example 4.3 can be extended over a whole family of symmetries generated by functions containing beside powers logarithms of Lax function $\ln L$. However, $\ln L$ at poles and roots of L has singularities of logarithmic type. So, such additional symmetries fall out from the scheme of meromorphic functions considered in this article. In Ref. 22 they manage with this problem representing $\ln L$ as a sum of two infinite series convergent near ∞ and 0, respectively. Following this idea, one is able to directly generalize this result from Ref. 22 only onto Lax functions from Secs. IV A and IV B. However, the general theory of such symmetries seems to be problematic. This problem is under investigation.

All the Poisson tensors constructed in the following article are nondegenerate. References 5 and 6 deal with rational Lax functions from the algebra with fixed Poisson bracket for $r=1$. However, only the Lax hierarchies generated by powers constructed near ∞ have been considered there. For the class of rational Lax functions used in these papers the bi-Hamiltonian structures are

degenerate, i.e., the determinants of the related metrics vanish. The reason is that the constraint of the form $L|_{p=0}=0$ is not taken into consideration. So, one dynamical field always can be represented as a function of all others. This fact entails the degeneracy of Poisson tensors.

There is a different approach to meromorphic Lax functions. From the complex analysis it is well known that meromorphic function can be uniquely presented in the factorized form. Because of such a factorization there is no problem in finding poles and roots of L near which one constructs powers and related Lax hierarchies. Another advantage is that the dispersionless systems obtained have very symmetrical form. However, the disadvantage is that Poisson tensors are significantly more complicated. Such factorized form of Lax functions as well allows for finding new reductions which are not obvious when we have Lax function in the standard form, see Refs. 5 and 6.

In this paper we have considered dispersionless systems with a finite number of dynamical fields. However, Lax function being infinite formal Laurent series leads to the construction of dispersionless infinite-field Benney moment like equations. Such systems for Laurent series at ∞ have been considered earlier in Ref. 19. The original Benney moment equation can be obtained for $k=r=0$. If we consider formal Laurent series at a pole being a dynamical field $v(x)$ we will construct new classes of infinite-field dispersionless systems. They, together with bi-Hamiltonian structures, will be studied in a forthcoming article. Furthermore, all finite-field dispersionless systems, with meromorphic Lax functions, considered in this paper may be considered as reductions of these infinite-field systems.

All Lax functions used in the article belong to the algebras of meromorphic functions. However, there are known the so-called waterbag hydrodynamic type systems with Lax functions, containing logarithmic terms, that are not meromorphic functions.[23,24] Similar systems are also considered in Ref. 25, but by means of the Riemann surfaces rather than Lax functions.

Another issue is the extension of the theory of meromorphic Lax representations presented for dispersionless systems in order to construct integrable dispersive soliton systems for rational Lax operators. The first approach toward this was made in Ref. 21. However, the authors constructed soliton systems related only to the case $k=r=0$ from our article. A more general theory of dispersive deformations of formal Lax functions being polynomials in p and p^{-1} is presented in Ref. 17. This approach is based on the Weyl-Moyal-like quantization procedure. The idea relies on the deformation of the usual multiplication in the algebra $\mathcal{A}$ to the new associative but noncommutative $\star$-product. However, this theory works only for $r=0,1,2$. Deformations of Poisson algebras for $r=0,2$ are equivalent and lead to the construction of field soliton systems, but for $r=1$ they lead to the construction of lattice soliton systems. So, in a forthcoming article we are going to study the field and lattice soliton systems for rational Lax operators.

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Map of discrete system into continuous

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Continuous limits of discrete systems with long-range interactions are considered. The map of discrete models into continuous medium models is defined. A wide class of long-range interactions that give the fractional equations in the continuous limit is discussed. The one-dimensional systems of coupled oscillators for this type of long-range interactions are considered. The discrete equations of motion are mapped into the continuum equation with the Riesz fractional derivative. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2337852]

I. INTRODUCTION

Equations which involve derivatives or integrals of noninteger order[1–5] have found many applications in recent studies in mechanics and physics.[6–11] Usually the fractional equations for dynamics or kinetics appear as some phenomenological models. Recently, the method to obtain fractional analogues of equations of motion was considered for sets of coupled particles with a long-range interaction.[12–14] Examples of systems with interacting oscillators, spins, or waves are used for numerous applications in physics, chemistry, biology.[15–26] Transfer from the equations of motion for discrete systems to the continuous media equation with fractional derivatives is an approximate procedure. Different applications of the procedure have already been used to derive fractional sine-Gordon and fractional wave Hilbert equation,[12,14] to study synchronization of coupled oscillators,[13] and for fractional Ginzburg-Landau equation.[13]

Long-range interaction has been the subject of great interest for a long time. Thermodynamics of the model of classical spins with long-range interactions has been studied in Refs. 15–17 and 19. An infinite one-dimensional Ising model with long-range interactions was considered by Dyson.[15] The d-dimensional classical Heisenberg model with long-range interaction is described in Refs. 16 and 19, and their quantum generalization can be found in Ref. 17. The long-range interactions have been widely studied in discrete systems on lattices as well as in their continuous analogues. Solitons in a one-dimensional lattice with the long-range Lennard-Jones-type interaction were considered in Ref 27. Kinks in the Frenkel-Kontorova model with long-range interparticle interactions were studied in Ref. 28. The properties of time periodic spatially localized solutions (breathers) on discrete chains in the presence of algebraically decaying interactions were considered in Refs. 24 and 25. Energy and decay properties of discrete breathers in systems with long-range interactions have also been studied in the framework of the Klein-Gordon,[22] and discrete nonlinear Schrödinger equations.[29] A remarkable property of the dynamics described by the equation with fractional space derivatives is that the solutions have power-like tails. Similar features were observed in the lattice models with power-like long-range interactions.[23–25,30–32,14] As it was shown in Refs. 13 and 14, analysis of the equations with fractional derivatives can provide results for the space asymptotics of their solutions.

The goal of this paper is to study a connection between the dynamics of system of particles with long-range interactions and the fractional continuous medium equations by using the transform operation. Here, we consider the one-dimensional lattice of coupled nonlinear oscillators. We make the transform to the continuous limit and derive the fractional equation which describes the

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dynamics of the oscillatory medium. We show how the continuous limit for the systems of oscillators with long-range interaction can be described by the corresponding fractional equation.

In Sec. II, the equations of motion for the system of oscillators with long-range interaction are considered. In Sec. III, the transform operation that maps the discrete equations into continuous medium equation is defined. In Sec. IV, the Fourier series transform of the equations of a system with long-range interaction is realized. In Sec. V, we consider a wide class of long-range interactions that can give the fractional equations in the continuous limit. In Sec. VI, the simple example of nearest-neighbor interaction is considered to demonstrate the application of the transform operation to the well-known case. In Sec. VII, the power-law long-range interactions with positive integer powers are considered. In Sec. VIII, the power-law long-range interactions with noninteger powers and the correspondent continuous medium equations are discussed. In Sec. IX, the nonlinear long-range interactions for the discrete systems are used to derive the Burgers, Korteweg-de Vries, and Boussinesq equations and their fractional generalizations in the continuous limit. In Sec. X, the fractional equations are obtained from the dispersion law for three-dimensional discrete system. The conclusion is given in Sec. XI.

II. EQUATIONS OF MOTION FOR INTERACTING OSCILLATORS

Consider a one-dimensional system of interacting oscillators that are described by the equations of motion,

$$\frac{\partial^2 u_n}{\partial t^2} = g\hat{\mathcal{I}}_n(u) + F(u_n), \tag{1}$$

where u_n are displacements from the equilibrium. The terms $F(u_n)$ characterize an interaction of the oscillators with the external on-site force. The term $\hat{\mathcal{I}}_n(u)$ is defined by

$$\hat{\mathcal{I}}_n(u) \equiv \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)E(u_n,u_m), \tag{2}$$

and it takes into account the interaction of the oscillators in the system.

Examples:

1) If $J(n,m)=\delta_{n+1,m}-\delta_{n,m}$, and $E(u_n,u_m)=u_m$, then $\hat{\mathcal{I}}_n(u)=u_{n+1}-u_n=\Delta u_n$.

2) For $J(n,m)=\delta_{n+1,m}-2\delta_{n,m}+\delta_{n-1,m}$, and $E(u_n,u_m)=u_m$, we get

$$\hat{\mathcal{I}}_n(u) = u_{n+1} - 2u_n + u_{n-1} = \Delta^2 u_n.$$

3) We can consider the long-range interaction that is given by $J(n)=|n|^{-(1+\alpha)}$, where α is a positive real number. In this case, we have nonlocal coupling given by the power-law function. Constant α is a physical relevant parameter. Some integer values of α correspond to the well-known physical situations: Coulomb potential corresponds to $\alpha=0$, dipole-dipole interaction corresponds to $\alpha=2$, and the limit $\alpha\to\infty$ is for the case of nearest-neighbor interaction.

For the term (2) with $E(u_n,u_m)=u_m$, the translation invariance condition is

$$\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m) = 0 \tag{3}$$

for all n. If (3) cannot be satisfied, we must define $E(u_n,u_m)=u_n-u_m$, and the interaction term (2) is

$$\hat{\mathcal{I}}_n(u) \equiv \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)[u_n - u_m]. \tag{4}$$

This interaction term is translation invariant. Note that the noninvariant terms lead to the divergences in the continuous limit (see the Appendix).

In this paper, we consider the wide class of interactions (4) that create a possibility to present the continuous medium equations with fractional derivatives. We also discuss the term (2) with $E(u_n,u_m)=f(u_n)-f(u_m)$ as nonlinear long-range interaction. As the examples, we consider $f(u)=u^2$ and $f(u)=u-gu^2$ that gives the Burgers, Korteweg-de Vries, and Boussinesq equations and their fractional generalizations in the continuous limit.

III. TRANSFORM OPERATION

In this section, we define the operation that transforms the system of equations for $u_n(t)$ into continuous medium equation for $u(x,t)$.

To derive a continuous medium equation, we suppose that $u_n(t)$ are Fourier coefficients of some function $\hat{u}(k,t)$. We define the field $\hat{u}(k,t)$ on $[-K/2,K/2]$ as

$$\hat{u}(k,t) = \sum_{n=-\infty}^{+\infty} u_n(t)e^{-ikx_n} = \mathcal{F}_\Delta\{u_n(t)\}, \tag{5}$$

where $x_n=n\Delta x$, $\Delta x=2\pi/K$ is distance between oscillators, and

$$u_n(t) = \frac{1}{K}\int_{-K/2}^{+K/2} \mathrm{d}k\hat{u}(k,t)e^{ikx_n} = \mathcal{F}_\Delta^{-1}\{\hat{u}(k,t)\}. \tag{6}$$

These equations are the basis for the Fourier transform, which is obtained by transforming $u_n(t)$ from discrete variable to a continuous one in the limit $\Delta x\to 0$ $(K\to\infty)$. The Fourier transform can be derived from (5), (6) in the limit as $\Delta x\to 0$. Replace the discrete $u_n(t)$ with continuous $u(x,t)$ while letting $x_n=n\Delta x=2\pi n/K\to x$. Then change the sum to an integral, and Eqs. (5) and (6) become

$$\tilde{u}(k,t) = \int_{-\infty}^{+\infty} \mathrm{d}x e^{-ikx}u(x,t) = \mathcal{F}\{u(x,t)\}, \tag{7}$$

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k e^{ikx}\tilde{u}(k,t) = \mathcal{F}^{-1}\{\tilde{u}(k,t)\}, \tag{8}$$

where

$$\tilde{u}(k,t) = \mathcal{L}\hat{u}(k,t), \tag{9}$$

and $\mathcal{L}$ denotes the passage to the limit $\Delta x\to 0$ $(K\to\infty)$. Note that $\tilde{u}(k,t)$ is a Fourier transform of the field $u(x,t)$, and $\hat{u}(k,t)$ is a Fourier series transform of $u_n(t)$. The function $\tilde{u}(k,t)$ can be derived from $\hat{u}(k,t)$ in the limit $\Delta x\to 0$.

The procedure of the replacement of a discrete model by the continuous one is defined by the transform operation.

Definition 1: Transform operation $\hat{T}$ is a combination $\hat{T}=\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_\Delta$ of the operations:

1) The Fourier series transform:

$$\mathcal{F}_\Delta: \quad u_n(t) \to \mathcal{F}_\Delta\{u_n(t)\} = \hat{u}(k,t). \tag{10}$$

2) The passage to the limit $\Delta x\to 0$:

$$\mathcal{L}: \quad \hat{u}(k,t) \to \mathcal{L}\{\hat{u}(k,t)\} = \tilde{u}(k,t). \tag{11}$$

3) The inverse Fourier transform:

$$\mathcal{F}^{-1}: \quad \tilde{u}(k,t) \to \mathcal{F}^{-1}\{\tilde{u}(k,t)\} = u(x,t). \tag{12}$$

The operation $\hat{T}=\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_{\Delta}$ is called a transform operation, since it performs a transform of a discrete model of coupled oscillators into the continuous medium model.

Proposition 1: The transform operation $\hat{T}$ maps the function $F(u_n)$ into the function $F(u(x,t))$, i.e.,

$$\hat{T}F(u_n(t)) = F(u(x,t)), \tag{13}$$

where $u(x,t)=\hat{T}u_n(t)$, if the function F satisfies $\mathcal{L}F(u_n)=F(\mathcal{L}u_n)$.

Proof: The Fourier series transform leads to

$$\mathcal{F}_{\Delta}: \quad F(u_n) \to \mathcal{F}_{\Delta}F(u_n). \tag{14}$$

Note that $\mathcal{F}_{\Delta}F(u_n) \neq F(\mathcal{F}_{\Delta}u_n)=F(\hat{u}(k,t))$. The passage to the limit $\Delta x \to 0$ gives

$$\mathcal{L}: \quad \mathcal{F}_{\Delta}F(u_n) \to \mathcal{L}\mathcal{F}_{\Delta}F(u_n). \tag{15}$$

Then

$$\mathcal{L}\mathcal{F}_{\Delta}\{F(u_n)\} = \mathcal{F}\{\mathcal{L}F(u_n)\} = \mathcal{F}\{F(\mathcal{L}u_n)\} = \mathcal{F}\{F(u(x,t))\}, \tag{16}$$

where we use $\mathcal{L}\mathcal{F}_{\Delta}=\mathcal{F}\mathcal{L}$. The inverse Fourier transform get

$$\mathcal{F}^{-1}: \quad \mathcal{F}\{F(u(x,t))\} \to \mathcal{F}^{-1}\{\mathcal{F}\{F(u(x,t))\}\} = F(u(x,t)). \tag{17}$$

As the result, we prove (13).

IV. EQUATIONS FOR MOMENTUM SPACE

Let us consider a system of infinite numbers of oscillators with interparticle interaction that is described by (4). We suppose that $J(n,m)$ satisfies the condition

$$J(n,m) = J(n-m), \quad \sum_{n=1}^{\infty} |J(n)|^2 < \infty, \tag{18}$$

where $J(-n)=J(n)$.

Proposition 2: The Fourier series transform $\mathcal{F}_{\Delta}$ maps the equations of motion

$$\frac{\partial^2 u_n(t)}{\partial t^2} = g \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)[u_n - u_m] + F(u_n), \tag{19}$$

where u_n is the position of the nth oscillator, and F is an external on-site force, into

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} = g[\hat{J}_{\alpha}(0) - \hat{J}_{\alpha}(k\Delta x)]\hat{u}(k,t) + \mathcal{F}_{\Delta}\{F(u_n)\}, \tag{20}$$

where

$$\hat{u}(k,t) = \mathcal{F}_{\Delta}\{u_n(t)\}, \quad \hat{J}_{\alpha}(k\Delta x) = \mathcal{F}_{\Delta}\{J(n)\},$$

and $\mathcal{F}_{\Delta}\{F(u_n)\}$ is an operator notation for the Fourier series transform of $F(u_n)$.

Proof: To derive the equation for the field $\hat{u}(k,t)$, we multiply Eq. (19) by $\exp(-ikn\Delta x)$, and summing over n from $-\infty$ to $+\infty$. Then

$$\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}\frac{\partial^2}{\partial t^2}u_n(t) = g\sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x}J(n,m)[u_n - u_m] + \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}F(u_n). \tag{21}$$

From

$$\hat{u}(k,t) = \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_n(t), \tag{22}$$

the left-hand side of (21) gives

$$\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}\frac{\partial^2 u_n(t)}{\partial t^2} = \frac{\partial^2}{\partial t^2}\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_n(t) = \frac{\partial^2\hat{u}(k,t)}{\partial t^2}. \tag{23}$$

The second term of the right-hand side of (21) is

$$\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}F(u_n) = \mathcal{F}_\Delta\{F(u_n)\}. \tag{24}$$

The first term of the right-hand side (r.h.s) of (21) is defined by the function $J(n,m)$. Let us introduce the notation

$$\hat{J}_\alpha(k\Delta x) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikn\Delta x}J(n). \tag{25}$$

Using $J(-n)=J(n)$, the function (25) can be presented by

$$\hat{J}_\alpha(k\Delta x) = \sum_{n=1}^{+\infty} J(n)(e^{-ikn\Delta x} + e^{ikn\Delta x}) = 2\sum_{n=1}^{+\infty} J(n)\cos(k\Delta x). \tag{26}$$

From (26) it follows that

$$\hat{J}_\alpha(k\Delta x + 2\pi m) = \hat{J}_\alpha(k\Delta x), \tag{27}$$

where m is an integer.

The interaction term in (21) is

$$\sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x}J(n,m)[u_n - u_m] = \sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x}J(n,m)u_n - \sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x}J(n,m)u_m. \tag{28}$$

Using (22) and (25), the first term on the r.h.s. of (28) gives

$$\sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x}J(n,m)u_n = \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_n\sum_{\substack{m'=-\infty \\ m'\neq 0}}^{+\infty} J(m') = \hat{u}(k,t)\hat{J}_\alpha(0), \tag{29}$$

where we use (18) and $J(m'+n,n)=J(m')$, and

$$\hat{J}_\alpha(0) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} J(n) = 2\sum_{n=1}^{\infty} J(n). \tag{30}$$

For the second term on the r.h.s. of (28):

$$\sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m) u_m = \sum_{m=-\infty}^{+\infty} u_m \sum_{\substack{n=-\infty \\ n\neq m}}^{+\infty} e^{-ikn\Delta x} J(n,m)$$

$$= \sum_{m=-\infty}^{+\infty} u_m e^{-ikm\Delta x} \sum_{\substack{n'=-\infty \\ n'\neq 0}}^{+\infty} e^{-ikn'\Delta x} J(n') = \hat{u}(k,t)\hat{J}_\alpha(k\Delta x), \tag{31}$$

where we use $J(m,n'+m)=J(n')$.

As a result, Eq. (21) has the form

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} = g[\hat{J}_\alpha(0) - \hat{J}_\alpha(k\Delta x)]\hat{u}(k,t) + \mathcal{F}_\Delta\{F(u_n)\}, \tag{32}$$

where $\mathcal{F}_\Delta\{F(u_n)\}$ is an operator notation for the Fourier series transform of $F(u_n)$.

V. ALPHA-INTERACTION

Let us consider the interaction term

$$\hat{\mathcal{I}}_n(u) \equiv \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)[u_n - u_m], \tag{33}$$

where

$$J(n,m) = J(n-m) = J(m-n), \quad \sum_{n=1}^{\infty} |J(n)|^2 < \infty. \tag{34}$$

In Sec. IV, we prove that the Fourier series transform $\mathcal{F}_\Delta$ of (33) gives

$$\mathcal{F}_\Delta\{\hat{\mathcal{I}}_n(u)\} = g[\hat{J}_\alpha(0) - \hat{J}_\alpha(k\Delta x)]\hat{u}(k,t), \tag{35}$$

where $\hat{u}(k,t)=\mathcal{F}_\Delta\{u_n(t)\}$, and

$$\hat{J}_\alpha(k) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikn} J(n) = 2\sum_{n=1}^{\infty} J(n)\cos(kn). \tag{36}$$

Definition 2: The interaction term (33) in the equation of motion (1) is called α-interaction if the function (36) satisfies the condition

$$\lim_{k\to 0} \frac{[\hat{J}_\alpha(k) - \hat{J}_\alpha(0)]}{|k|^\alpha} = A_\alpha, \tag{37}$$

where $\alpha>0$ *and* $0<|A_\alpha|<\infty$.

If the function $\hat{J}_\alpha(k)$ is given, then $J(n)$ can be defined by

$$J(n) = \frac{1}{\pi}\int_0^{\pi} \hat{J}_\alpha(k)\cos(nk)\mathrm{d}k. \tag{38}$$

The condition (37) means that $\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = O(|k|^\alpha)$, i.e.,

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = A_\alpha|k|^\alpha + R_\alpha(k), \tag{39}$$

for $k \to 0$, where

$$\lim_{k\to 0} R_\alpha(k)/|k|^\alpha = 0. \tag{40}$$

Examples:

1) The first example of the α-interaction is

$$\hat{J}_\alpha(k) = A_\alpha|k|^\alpha.$$

Using (38), we obtain

$$J(n) = A_\alpha\left(\frac{(-1)^n\pi^{\alpha+1}}{\alpha+1} - \frac{(-1)^n\pi^{1/2}}{(\alpha+1)|n|^{\alpha+1/2}}L_1(\alpha+3/2,1/2,\pi n)\right), \tag{41}$$

where $L_1(\mu,\nu,z)$ is the Lommel function.[33]

2) The second example of the α-interaction is

$$J(n) = \frac{(-1)^n}{n^2}. \tag{42}$$

Using (Ref. 34, Sec. 5.4.2.12)

$$\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\cos(nk) = \frac{1}{4}\left(k^2 - \frac{\pi^2}{3}\right), \quad |k| \leqslant \pi,$$

we get

$$\hat{J}_\alpha(k) = 2\sum_{n=1}^{+\infty}\frac{(-1)^n}{n^2}\cos(kn) = \frac{1}{2}k^2 - \frac{\pi^2}{6}, \quad |k| \leqslant \pi. \tag{43}$$

Then we have $\alpha=2$, and

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = (1/2)k^2. \tag{44}$$

The inverse Fourier transform of this expression gives the coordinate derivatives of second order

$$\mathcal{F}^{-1}\{\hat{J}_\alpha(k) - \hat{J}_\alpha(0)\} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}.$$

3) For the interaction (42), we have $\alpha=2$ and the inverse Fourier transform of (44) gives the second-order derivative. At the same time, the interaction

$$J(n) = \frac{1}{n^2}$$

gives $\alpha=1$ and then the first-order coordinate derivative. It can be proved by using (Ref. 34, Sec. 5.4.2.12)

$$\hat{J}_\alpha(k) = 2\sum_{n=1}^{+\infty} \frac{\cos(kn)}{n^2} = \frac{1}{6}[3k^2 - 6\pi k + 2\pi^2], \quad (0 \leqslant k \leqslant 2\pi), \tag{45}$$

and $\hat{J}_\alpha(k) - \hat{J}_\alpha(0) \approx -\pi k$ for $k \to 0$. Therefore, the inverse Fourier transform leads to the derivative of first order.

4) For noninteger and odd numbers s,

$$J(n) = |n|^{-(s+1)}, \quad s > 0 \tag{46}$$

is an α-interaction.

For $0 < s < 2 (s \neq 1)$, we get

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = 2\Gamma(-s)\cos(\pi s/2)|k|^s. \tag{47}$$

For $s = 1$,

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = -(\pi/2)k. \tag{48}$$

For noninteger $s > 2$,

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = -\zeta(\alpha - 1)k^2, \tag{49}$$

where $\zeta(z)$ is the Riemann zeta-function, The interaction (46) is considered in Sec. VII.

5) The other example is

$$J(n) = \frac{(-1)^n}{\Gamma(1 + \alpha/2 + n)\Gamma(1 + \alpha/2 - n)}. \tag{50}$$

Using the series (Ref. 34, Sec. 5.4.8.12)

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{\Gamma(\beta + 1 + n)\Gamma(\beta + 1 - n)} \cos(nk) = \frac{2^{2\beta-1}}{\Gamma(2\beta + 1)} \sin^{2\beta}\left(\frac{k}{2}\right) - \frac{1}{2\Gamma^2(\beta + 1)}, \tag{51}$$

where $\beta > -1/2$ and $0 < k < 2\pi$, we get

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = \frac{2^\alpha}{\Gamma(\alpha + 1)} \sin^\alpha\left(\frac{k}{2}\right). \tag{52}$$

In the limit $k \to 0$, we obtain

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) \approx \frac{1}{\Gamma(\alpha + 1)}|k|^\alpha. \tag{53}$$

For noninteger α, the inverse Fourier transform of (53) gives the fractional Riesz derivative[1] of order α.

6) The α-interaction

$$J(n) = \frac{(-1)^n}{a^2 - n^2},$$

gives

$$\hat{J}(k) = \frac{\pi}{a \sin(\pi a)} \cos(ak) - \frac{1}{a^2}. \tag{54}$$

For $k \to 0$, we obtain

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) \approx \frac{a\pi}{2\sin(a\pi)} k^2. \tag{55}$$

The inverse Fourier transform of (55) leads to the coordinate derivative of second order.

7) For $J(n)=1/n!$, we use

$$\sum_{n=1}^{\infty} \frac{\cos(kn)}{n!} = e^{\cos k} \cos(\sin k), \quad |k| < \infty. \tag{56}$$

The passage to the limit $k \to 0$ gives

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) \approx -4ek. \tag{57}$$

Then $\alpha=1$, and we get the derivative of first order.

Proposition 3: The transform operation $\hat{T}$ maps the discrete equations of motion

$$\frac{\partial^2 u_n}{\partial t^2} = g \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)[u_n - u_m] + F(u_n) \tag{58}$$

with noninteger α-interaction into the fractional continuous medium equations:

$$\frac{\partial^2}{\partial t^2} u(x,t) - G_\alpha A_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) - F(u(x,t)) = 0, \tag{59}$$

where $\partial^\alpha / \partial |x|^\alpha$ is the Riesz fractional derivative, and

$$G_\alpha = g|\Delta x|^\alpha \tag{60}$$

is a finite parameter.

Proof: The Fourier series transform $\mathcal{F}_\Delta$ of (58) gives (20). We will be interested in the limit $\Delta x \to 0$. Then Eq. (20) can be written as

$$\frac{\partial^2}{\partial t^2} \hat{u}(k,t) - G_\alpha \hat{\mathcal{T}}_{\alpha,\Delta}(k) \hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{61}$$

where we use finite parameter (60), and

$$\hat{\mathcal{T}}_{\alpha,\Delta}(k) = -A_\alpha |k|^\alpha - R_\alpha(k\Delta x)|\Delta x|^{-\alpha}. \tag{62}$$

Note that R_α satisfies the condition

$$\lim_{\Delta x \to 0} \frac{R_\alpha(k\Delta x)}{|\Delta x|^\alpha} = 0.$$

The expression for $\hat{\mathcal{T}}_{\alpha,\Delta}(k)$ can be considered as a Fourier transform of the operator (4). Note that $g \to \infty$ for the limit $\Delta x \to 0$, if G_α is a finite parameter.

In the limit $\Delta x \to 0$, Eq. (61) gets

$$\frac{\partial^2}{\partial t^2} \tilde{u}(k,t) - G_\alpha \hat{\mathcal{T}}_\alpha(k) \tilde{u}(k,t) - \mathcal{F}^{-1}\{F(u(x,t))\} = 0, \tag{63}$$

where

$$\tilde{u}(k,t) = \mathcal{L}\hat{u}(k,t), \quad \hat{\mathcal{T}}_\alpha(k) = \mathcal{L}\hat{\mathcal{T}}_{\alpha,\Delta}(k) = -A_\alpha |k|^\alpha.$$

The inverse Fourier transform of (63) gives

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_\alpha \mathcal{T}_\alpha(x)u(x,t) - F(u(x,t)) = 0, \tag{64}$$

where $\mathcal{T}_\alpha(x)$ is an operator

$$\mathcal{T}_\alpha(x) = \mathcal{F}^{-1}\{\hat{\mathcal{T}}_\alpha(k)\} = A_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha}. \tag{65}$$

Here, we have used the connection between the Riesz fractional derivative and its Fourier transform:[1]

$$|k|^\alpha \leftrightarrow -\frac{\partial^\alpha}{\partial |x|^\alpha}. \tag{66}$$

The properties of the Riesz derivative can be found in Refs. 1–4. Note that the Riesz derivative could be represented as

$$\frac{\partial^\alpha}{\partial |x|^\alpha}u(x,t) = -\frac{1}{2\cos(\pi\alpha/2)}(\mathcal{D}^\alpha_+ u(x,t) + \mathcal{D}^\alpha_- u(x,t)), \tag{67}$$

where $\alpha \neq 0,1,3,5,\ldots$, and $\mathcal{D}^\alpha_\pm$ are Riemann-Liouville left and right fractional derivatives defined by[1–4]

$$\begin{aligned} \mathcal{D}^\alpha_+ u(x,t) &= \frac{1}{\Gamma(m-\alpha)}\frac{\partial^m}{\partial x^m}\int_{-\infty}^{x}\frac{u(\xi,t)\mathrm{d}\xi}{(x-\xi)^{\alpha-m+1}}, \\ \mathcal{D}^\alpha_- u(x,t) &= \frac{(-1)^m}{\Gamma(m-\alpha)}\frac{\partial^m}{\partial x^m}\int_{x}^{\infty}\frac{u(\xi,t)\mathrm{d}\xi}{(\xi-x)^{\alpha-m+1}}, \end{aligned} \tag{68}$$

where $m-1<\alpha<m$.

As the result, we obtain continuous medium equations (59) from (64) and (65).

VI. SIMPLE EXAMPLE OF NEAREST-NEIGHBOR INTERACTION

In this section, we demonstrate the application of transform operation to the well-known case:

$$J(n,m) = \delta_{n+1,m} - 2\delta_{n,m} + \delta_{n-1,m}, \tag{69}$$

where $\delta_{n,m}$ is the Kronecker symbol. Then the interaction term (2) has the form

$$\hat{\mathcal{I}}_n(u) = (u_{n+1} - u_n) - (u_n - u_{n-1}), \tag{70}$$

and describes the nearest-neighbor interaction. As the result, equations of motion (19) have the form

$$\frac{\partial^2 u_n}{\partial t^2} = g[u_{n+1} - 2u_n + u_{n-1}] + F(u_n). \tag{71}$$

The well-known result is the following.

Proposition 4: The transform operation $\hat{T}$ maps the equation of motion (71) into the continuous medium equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = G_2\frac{\partial^2}{\partial x^2}u(x,t) + F(u), \tag{72}$$

where

$$G_2 = g(\Delta x)^2 \tag{73}$$

is a finite parameter.

Proof: To derive the equation for the field $\hat{u}(k,t)$, we multiply Eq. (71) by $\exp(-ikn\Delta x)$, and summing over n from $-\infty$ to $+\infty$. Then

$$\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}\frac{\partial^2}{\partial t^2}u_n(t) = g\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}[u_{n+1} - 2u_n + u_{n-1}] + \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}F(u_n). \tag{74}$$

The first term on the r.h.s. of (74) is

$$\begin{aligned}
\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}J(n,m)u_m &= \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}[u_{n+1} - 2u_n + u_{n-1}] \\
&= \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_{n+1} - 2\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_n + \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}u_{n-1} \\
&= \sum_{m'=-\infty}^{+\infty} e^{-ik(m-1)\Delta x}u_m - 2\hat{u}(k,t) + \sum_{s=-\infty}^{+\infty} e^{-ik(s+1)\Delta x}u_s \\
&= e^{ik\Delta x}\sum_{m'=-\infty}^{+\infty} e^{-ikm\Delta x}u_m - 2\hat{u}(k,t) + e^{-ik\Delta x}\sum_{s=-\infty}^{+\infty} e^{-iks\Delta x}u_s \\
&= e^{ik\Delta x}\hat{u}(k,t) - 2\hat{u}(k,t) + e^{-ik\Delta x}\hat{u}(k,t) = [e^{ik\Delta x} + e^{-ik\Delta x} - 2]\hat{u}(k,t) \\
&= 2[\cos(k\Delta x) - 1]\hat{u}(k,t) = -4\sin^2(k\Delta x)\hat{u}(k,t).
\end{aligned} \tag{75}$$

As the result, we obtain

$$\frac{\partial^2\hat{u}(k,t)}{\partial t^2} = g\hat{J}_\alpha(k\Delta x)\hat{u}(k,t) + \mathcal{F}_\Delta\{F(u_n(t))\}, \tag{76}$$

where

$$\hat{J}_\alpha(k\Delta x) = -4\sin^2(k\Delta x). \tag{77}$$

For $\Delta x \to 0$, the asymptotics of the sine is

$$\sin(z) = \sum_{m=0}^{\infty}\frac{(-1)^{m+1}}{(2m+1)!}z^{2m+1} \approx z - \frac{1}{6}z^3,$$

and (77) can be presented by

$$\hat{J}_\alpha(k\Delta x) \approx -(k\Delta x)^2 + \tfrac{1}{12}(k\Delta x)^4. \tag{78}$$

Using the finite parameter (73), the transition to the limit $\Delta x \to 0$ in Eq. (76) gives

$$\frac{\partial^2\tilde{u}(k,t)}{\partial t^2} = -G_2k^2\tilde{u}(k,t) + \mathcal{F}^{-1}\{F(u)\}, \tag{79}$$

where we use $0 < |G_2| < \infty$. As the result, the inverse Fourier transform of (79) leads to the continuous medium equation (72).

VII. INTEGER POWER-LAW INTERACTION

Let us consider the power-law interaction (4) with

$$J(n) = |n|^{-(s+1)} \tag{80}$$

with positive integer number s.

Proposition 5: The power-law interaction (80) for the odd number s is α-interaction with α =1 for s=1, and α=2 for s=3,5,7,…. For even numbers s, (80) is not α-interaction. For odd number s, the transform operation $\hat{T}$ maps the equations of motion with the interaction (80) into the continuous medium equation with derivatives of first order for s=1, and the second order for other odd s.

Proof: From (20), we get the equation for $\hat{u}(k,t)$ in the form

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} + g[\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0)]\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{81}$$

where

$$\hat{J}_\alpha(k\Delta x) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikn\Delta x}|n|^{-(1+s)}. \tag{82}$$

The function (82) can be presented by

$$\hat{J}_\alpha(k\Delta x) = \sum_{n=1}^{+\infty} \frac{1}{n^{1+s}}(e^{-ikn\Delta x} + e^{ikn\Delta x}) = 2\sum_{n=1}^{+\infty} \frac{1}{n^{1+s}} \cos(kn\Delta x). \tag{83}$$

Then we can use (Ref. 46, Sec. 5.4.2.12 and 5.4.2.7) the relations

$$\sum_{n=1}^{\infty} \frac{\cos(nk)}{n^2} = \frac{1}{12}(3k^2 - 6\pi k + 2\pi^2), \quad (0 \leqslant k \leqslant 2\pi), \tag{84}$$

$$\sum_{n=1}^{\infty} \frac{\cos(nk)}{n^{2m}} = \frac{(-1)^{m-1}(2\pi)^{2m}}{2(2m)!} B_{2m}\left(\frac{k}{2\pi}\right), \quad (0 \leqslant k \leqslant 2\pi), \tag{85}$$

where $m=1,2,3,\ldots$, and $B_{2m}(z)$ are the Bernulli polynomials.[35] These polynomials are defined by

$$B_n(k) = \sum_{s=0}^{n} C_n^s B_s k^{n-s}, \tag{86}$$

where B_s are the Bernoulli numbers from

$$\frac{z}{e^z - 1} = \sum_{s=0}^{\infty} B_s \frac{z^s}{s!}, \quad (|z| < 2\pi). \tag{87}$$

For example,

$$B_2(k) = k^2 - k + 1/6, \quad B_4(k) = k^4 - 2k^3 + k^2 - 1/30. \tag{88}$$

Note $B_{2m-1}=0$ for $m=2,3,4,\ldots$.[35]

For $s=1$, we have

$$\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0) = \tfrac{1}{2}(k\Delta x)^2 - \pi k\Delta x \approx -\pi k\Delta x. \tag{89}$$

For $s=2m-1$ $(m=2,3,\ldots)$, we have

$$\hat{J}_\alpha(k) = \frac{(-1)^{m-1}}{(2m)!}(2\pi)^{2m}B_{2m}\left(\frac{k}{2\pi}\right) \quad (0 \leqslant k \leqslant 2\pi). \tag{90}$$

Then

$$\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0) \approx \frac{(-1)^{m-1}(2\pi)^{2m-2}}{4(2m-2)!}B_{2m-2}(k\Delta x)^2. \tag{91}$$

For example, the interaction (80) with $s=3$ gives

$$\hat{J}_\alpha(k) - \hat{J}_\alpha(0) = -\frac{1}{48}[k^4 - 4\pi k^3 + 4\pi^2 k^2] \approx -\frac{\pi^2}{12}k^2. \tag{92}$$

For $s=0$, we have (Ref. 34, Sec. 5.4.2.9) the relation

$$\sum_{n=1}^{\infty}\frac{\cos(nk)}{n} = -\ln[2\sin(k/2)]. \tag{93}$$

Then, the limit $\Delta x \to 0$ gives

$$\hat{J}_\alpha(k\Delta x) \approx -\ln(k\Delta x) \to \infty. \tag{94}$$

For even numbers s,

$$|\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0)|/|k\Delta x|^s \to \infty \tag{95}$$

since the expression has the logarithmic poles.

The transition to the limit $\Delta x \to 0$ in Eq. (81) with $s=1$ gives

$$\frac{\partial^2 \tilde{u}(k,t)}{\partial t^2} - G_1 k\tilde{u}(k,t) - \mathcal{F}^{-1}\{F(u(x,t))\} = 0, \tag{96}$$

where $G_1 = \pi g\Delta x$ is a finite parameter. The inverse Fourier transform of (96) leads to the continuous medium equation with coordinate derivative of first order:

$$\frac{\partial^2}{\partial t^2}u(x,t) - iG_1\frac{\partial}{\partial x}u(x,t) - F(u(x,t)) = 0. \tag{97}$$

This equation can be considered as the nonlinear Schrödinger equation.

The limit $\Delta x \to 0$ in Eq. (81) with $s=2m-1$ $(m=2,3,\ldots)$ gives

$$\frac{\partial^2 \tilde{u}(k,t)}{\partial t^2} + G_2 k^2\tilde{u}(k,t) - \mathcal{F}^{-1}\{F(u(x,t))\} = 0, \tag{98}$$

where

$$G_2 = \frac{(-1)^{m-1}(2\pi)^{2m-2}}{4(2m-2)!}B_{2m-2}g(\Delta x)^2$$

is a finite parameter. The inverse Fourier transform of (98) leads to the partial differential equation of second order:

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_2\frac{\partial^2}{\partial x^2}u(x,t) - F(u(x,t)) = 0. \tag{99}$$

This equation can be considered as a nonlinear wave equation.

VIII. NONINTEGER POWER-LAW INTERACTION

Let us consider the power-law interaction with

$$J(n) = |n|^{-(s+1)}, \tag{100}$$

where s is a positive noninteger number.

Proposition 6: The power-law interaction (100) with noninteger s is α-interaction with $\alpha=s$ for $0<s<2$, and $\alpha=2$ for $s>2$. For $0<s<2$ $(s\neq 1)$, the transform operation $\hat{T}$ maps the discrete equations with the interaction (100) into the continuous medium equation with fractional Riesz derivatives of order α. For $\alpha>2$ $(\alpha\neq 3,4,5,\ldots)$, the continuous medium equation has the coordinate derivatives of second order.

Proof: From (20), we obtain the equation for $\hat{u}(k,t)$ in the form

$$\frac{\partial^2\hat{u}(k,t)}{\partial t^2} + g[\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0)]\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{101}$$

where

$$\hat{J}_\alpha(k\Delta x) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikn\Delta x}\frac{1}{|n|^{1+\alpha}}. \tag{102}$$

For fractional positive α, the function (102) can be presented by

$$\hat{J}_\alpha(k\Delta x) = \sum_{n=1}^{+\infty}\frac{1}{n^{1+\alpha}}(e^{-ikn\Delta x} + e^{ikn\Delta x}) = Li_{1+\alpha}(e^{ik\Delta x}) + Li_{1+\alpha}(e^{-ik\Delta x}), \tag{103}$$

where $Li_\beta(z)$ is a polylogarithm function. Using the series representation of the polylogarithm:[36]

$$Li_\beta(e^z) = \Gamma(1-\beta)(-z)^{\beta-1} + \sum_{n=0}^{\infty}\frac{\zeta(\beta-n)}{n!}z^n, \quad |z|<2\pi, \quad \beta\neq 1,2,3,\ldots, \tag{104}$$

we obtain

$$\hat{J}_\alpha(k\Delta x) = A_\alpha|\Delta x|^\alpha|k|^\alpha + 2\sum_{n=0}^{\infty}\frac{\zeta(1+\alpha-2n)}{(2n)!}(\Delta x)^{2n}(-k^2)^n, \quad \alpha\neq 0,1,2,3,\ldots, \tag{105}$$

where $\zeta(z)$ is the Riemann zeta-function, $|k\Delta x|<2\pi$, and

$$A_\alpha = 2\Gamma(-\alpha)\cos\left(\frac{\pi\alpha}{2}\right). \tag{106}$$

From (105), we have

$$J_\alpha(0) = 2\zeta(1+\alpha).$$

Then

$$\hat{J}_\alpha(k\Delta x) - \hat{J}_\alpha(0) = A_\alpha|\Delta x|^\alpha|k|^\alpha + 2\sum_{n=1}^{\infty} \frac{\zeta(1+\alpha-2n)}{(2n)!}(\Delta x)^{2n}(-k^2)^n, \tag{107}$$

where $\alpha \neq 0,1,2,3,\ldots$, and $|k\Delta x| < 2\pi$.

Substitution of (107) into Eq. (101) gives

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} + gA_\alpha|\Delta x|^\alpha|k|^\alpha\hat{u}(k,t) + 2g\sum_{n=1}^{\infty} \frac{\zeta(\alpha+1-2n)}{(2n)!}(\Delta x)^{2n}(-k^2)^n\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0. \tag{108}$$

We will be interested in the limit $\Delta x \to 0$. Then Eq. (108) can be written in a simple form

$$\frac{\partial^2}{\partial t^2}\hat{u}(k,t) + G_\alpha\hat{\mathcal{T}}_{\alpha,\Delta}(k)\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \quad \alpha \neq 0,1,2,\ldots, \tag{109}$$

where we use the finite parameter

$$G_\alpha = g|\Delta x|^{\min\{\alpha;2\}}, \tag{110}$$

and

$$\hat{\mathcal{T}}_{\alpha,\Delta}(k) = \begin{cases} A_\alpha|k|^\alpha - |\Delta x|^{2-\alpha}\zeta(\alpha-1)k^2, & 0 < \alpha < 2 \quad (\alpha \neq 1) \\ |\Delta x|^{\alpha-2}A_\alpha|k|^\alpha - \zeta(\alpha-1)k^2, & \alpha > 2 \quad (\alpha \neq 3,4,\ldots). \end{cases} \tag{111}$$

The expression for $\hat{\mathcal{T}}_{\alpha,\Delta}(k)$ can be considered as a Fourier transform of the interaction operator (2). From (110), we see that $g \to \infty$ for the limit $\Delta x \to 0$, and finite value of G_α.

Note that (111) has a scale k_0:

$$k_0 = |A_\alpha/\zeta(\alpha-1)|^{1/(2-\alpha)}|\Delta x|^{-1} \tag{112}$$

such that the nontrivial expression $\hat{\mathcal{T}}_{\alpha,\Delta}(k) \sim |k|^\alpha$ appears only for $0 < \alpha < 2$, $(\alpha \neq 1)$, $k \ll k_0$.

The transition to the limit $\Delta x \to 0$ in Eq. (109) gives

$$\frac{\partial^2}{\partial t^2}\tilde{u}(k,t) + G_\alpha\hat{\mathcal{T}}_\alpha(k)\tilde{u}(k,t) - \mathcal{F}^{-1}\{F(u(x,t))\} = 0 \quad (\alpha \neq 0,1,2,\ldots), \tag{113}$$

where

$$\hat{\mathcal{T}}_\alpha(k) = \begin{cases} A_\alpha|k|^\alpha, & 0 < \alpha < 2, \quad \alpha \neq 1 \\ -\zeta(\alpha-1)k^2, & 2 < \alpha, \quad \alpha \neq 3,4,\ldots. \end{cases} \tag{114}$$

The inverse Fourier transform to (113) is

$$\frac{\partial^2}{\partial t^2}u(x,t) + G_\alpha\mathcal{T}_\alpha(x)u(x,t) - F(u(x,t)) = 0 \quad \alpha \neq 0,1,2,\ldots, \tag{115}$$

where

$$\mathcal{T}_\alpha(x) = \mathcal{F}^{-1}\{\hat{\mathcal{T}}_\alpha(k)\} = \begin{cases} -A_\alpha\partial^\alpha/\partial|x|^\alpha & (0 < \alpha < 2, \quad \alpha \neq 1) \\ \zeta(\alpha-1)\partial^2/\partial|x|^2 & (\alpha > 2, \quad \alpha \neq 3,4,\ldots). \end{cases}$$

Here, we have used the connection between the Riesz fractional derivative and its Fourier transform:[1]

$$|k|^{\alpha} \leftrightarrow -\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}, \quad k^2 \leftrightarrow -\frac{\partial^2}{\partial|x|^2}. \tag{116}$$

The properties of the Riesz derivative can be found in Refs. 1–4.

As the result, we obtain the continuous medium equations

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_{\alpha}A_{\alpha}\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x,t) = F(u(x,t)), \quad 0 < \alpha < 2 \quad (\alpha \neq 1), \tag{117}$$

and

$$\frac{\partial^2}{\partial t^2}u(x,t) + G_{\alpha}\zeta(\alpha-1)\frac{\partial^2}{\partial|x|^2}u(x,t) = F(u(x,t)), \quad \alpha > 2 \quad (\alpha \neq 3,4,\ldots). \tag{118}$$

Analogously, the continuous limit for the system

$$\frac{\partial u_n}{\partial t} = g\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} |n-m|^{-\alpha-1}[u_n - u_m] + F(u_n) \tag{119}$$

gives the partial differential equations

$$\frac{\partial}{\partial t}u(x,t) - G_{\alpha}A_{\alpha}\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x,t) = F(u(x,t)), \quad 0 < \alpha < 2 \quad (\alpha \neq 1), \tag{120}$$

and

$$\frac{\partial}{\partial t}u(x,t) + G_{\alpha}\zeta(\alpha-1)\frac{\partial^2}{\partial|x|^2}u(x,t) = F(u(x,t)), \quad \alpha > 2 \quad (\alpha \neq 3,4,\ldots). \tag{121}$$

For $F(u)=0$, Eq. (120) is the fractional kinetic equation that describes the fractional superdiffusion.[37–39] If $F(u)$ is a sum of linear and cubic terms, then Eq. (120) has the form of the fractional Ginzburg-Landau equation.[40–44] A remarkable property of the dynamics described by the equation with fractional space derivatives is that the solutions have power-like tails.

IX. NONLINEAR LONG-RANGE INTERACTION

In this section, we consider the discrete equations with nonlinear long-range interaction:

$$\hat{\mathcal{I}}_n(u) = \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_{\alpha}(n,m)[f(u_n) - f(u_m)], \tag{122}$$

where $f(u)$ is a nonlinear function of $u_n(t)$, and $J_{\alpha}(n,m)$ defines the α-interaction. As the example of $J_{\alpha}(n,m)=J_{\alpha}(n-m)$, we can use the functions

$$J_{\alpha}(n) = \frac{(-1)^n}{\Gamma(1+\alpha/2+n)\Gamma(1+\alpha/2-n)}. \tag{123}$$

We consider the interaction with $f(u)=u^2$ and $f(u)=u-gu^2$ that gives the Burgers, Korteweg-de Vries, and Boussinesq equations in the continuous limit for $\alpha=1,2,3,4$. If we use the fractional α in Eq. (123), we can obtain the fractional generalization of these equations.

Proposition 7: The Fourier series transform $\mathcal{F}_{\Delta}$ maps the equations of motion

$$\frac{\partial^2 u_n(t)}{\partial t^2} = g \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_\alpha(n-m)[f(u_n) - f(u_m)] + F(u_n), \tag{124}$$

where F is an external on-site force, into

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} = g[\hat{J}_\alpha(0) - \hat{J}_\alpha(k\Delta x)]\mathcal{F}_\Delta\{f(u_n)\} + \mathcal{F}_\Delta\{F(u_n)\}, \tag{125}$$

where $\hat{u}(k,t) = \mathcal{F}_\Delta\{u_n(t)\}$, *and* $\hat{J}_\alpha(k\Delta x) = \mathcal{F}_\Delta\{J(n)\}$.

If $J_\alpha(n)$ *defines the* α*-interaction, then the continuous limit* $\Delta x \to 0$ *and the inverse Fourier transform give*

$$\frac{\partial^2 u(x,t)}{\partial t^2} = G_\alpha A_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} f(u(x,t)) + F(u(x,t)), \tag{126}$$

where $G_\alpha = g|\Delta x|^\alpha$ *is a finite parameter.*

Proof: The Fourier series transform of the interaction term (122) can be presented as

$$\begin{aligned}\sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x}\hat{\mathcal{I}}_n(u) &= \sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m)[f(u_n) - f(u_m)] \\ &= \sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m) f(u_n) - \sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m) f(u_m). \end{aligned} \tag{127}$$

For the first term on the r.h.s. of (127):

$$\sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m) f(u_n) = \sum_{n=-\infty}^{+\infty} e^{-ikn\Delta x} f(u_n) \sum_{\substack{m'=-\infty \\ m'\neq 0}}^{+\infty} J(m') = \mathcal{F}_\Delta\{f(u_n)\}\hat{J}_\alpha(0), \tag{128}$$

where we use $J(m'+n,n) = J(m')$. For the second term on the r.h.s. of (127):

$$\begin{aligned}\sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikn\Delta x} J(n,m) f(u_m) &= \sum_{m=-\infty}^{+\infty} f(u_m) \sum_{\substack{n=-\infty \\ n\neq m}}^{+\infty} e^{-ikn\Delta x} J(n,m) \\ &= \sum_{m=-\infty}^{+\infty} f(u_m) e^{-ikm\Delta x} \sum_{\substack{n'=-\infty \\ n'\neq 0}}^{+\infty} e^{-ikn'\Delta x} J(n') = \mathcal{F}_\Delta\{f(u_n)\}\hat{J}_\alpha(k\Delta x), \end{aligned} \tag{129}$$

where we use $J(m,n'+m) = J(n')$.

As the result, we obtain Eq. (125).

For the limit $\Delta x \to 0$, Eq. (125) can be written as

$$\frac{\partial^2}{\partial t^2}\hat{u}(k,t) - G_\alpha \hat{\mathcal{I}}_{\alpha,\Delta}(k)\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{130}$$

where we use finite parameter $G_\alpha = g|\Delta x|^\alpha$, and

$$\hat{\mathcal{T}}_{\alpha,\Delta}(k) = -A_\alpha |k|^\alpha - R_\alpha(k\Delta x)|\Delta x|^{-\alpha}. \tag{131}$$

Here, the function R_α satisfies the condition

$$\lim_{\Delta x \to 0} \frac{R_\alpha(k\Delta x)}{|\Delta x|^\alpha} = 0.$$

In the limit $\Delta x \to 0$, we get

$$\frac{\partial^2}{\partial t^2}\tilde{u}(k,t) - G_\alpha \hat{\mathcal{T}}_\alpha(k)\mathcal{F}^{-1}\{f(u(x,t))\} - \mathcal{F}^{-1}\{F(u(x,t))\} = 0, \tag{132}$$

where

$$\tilde{u}(k,t) = \mathcal{L}\hat{u}(k,t), \quad \hat{\mathcal{T}}_\alpha(k) = \mathcal{L}\hat{\mathcal{T}}_{\alpha,\Delta}(k) = -A_\alpha |k|^\alpha.$$

The inverse Fourier transform of (132) gives

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_\alpha \mathcal{T}_\alpha(x) f(u(x,t)) - F(u(x,t)) = 0, \tag{133}$$

where $\mathcal{T}_\alpha(x)$ is an operator

$$\mathcal{T}_\alpha(x) = \mathcal{F}^{-1}\{\hat{\mathcal{T}}_\alpha(k)\} = A_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha}. \tag{134}$$

As the result, we obtain the continuous medium equation (126).

Let us consider examples of quadratic-nonlinear long-range interactions.

1) The continuous limit of the lattice equations

$$\frac{\partial u_n(t)}{\partial t} = g_1 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_1(n,m)[u_n^2 - u_m^2] + g_2 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_2(n,m)[u_n - u_m], \tag{135}$$

where $J_i(n)$ $(i=1,2)$ define the α_i-interactions with $\alpha_1=1$ and $\alpha_2=2$, gives the Burgers equation[45] that is a nonlinear partial differential equation of second order:

$$\frac{\partial}{\partial t}u(x,t) + G_1 u(x,t)\frac{\partial}{\partial x}u(x,t) - G_2 \frac{\partial^2}{\partial x^2}u(x,t) = 0. \tag{136}$$

It is used in fluid dynamics as a simplified model for turbulence, boundary layer behavior, shock wave formation, and mass transport. If we consider $J_2(n,m)$ with fractional $\alpha_2=\alpha$, then we get the fractional Burgers equation that is suggested in Ref. 46.

2) The continuous limit of the system of equations

$$\frac{\partial u_n(t)}{\partial t} = g_1 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_1(n,m)[u_n^2 - u_m^2] + g_3 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_3(n,m)[u_n - u_m], \tag{137}$$

where $J_i(n)$ $(i=1,3)$ define the α_i-interactions with $\alpha_1=1$ and $\alpha_3=3$, gives Korteweg-de Vries (KdV) equation

$$\frac{\partial}{\partial t}u(x,t) - G_1 u(x,t)\frac{\partial}{\partial x}u(x,t) + G_3 \frac{\partial^3}{\partial x^3}u(x,t) = 0. \tag{138}$$

First formulated as part of an analysis of shallow-water waves in canals, it has subsequently been found to be involved in a wide range of physics phenomena, especially those exhibiting shock

waves, traveling waves, and solitons. Certain theoretical physics phenomena in the quantum mechanics domain are explained by means of a KdV model. It is used in fluid dynamics, aerodynamics, and continuum mechanics as a model for shock wave formation, solitons, turbulence, boundary layer behavior, and mass transport.

If we use noninteger α_i-interactions for $J_i(n)$, then we get the fractional generalization of the KdV equation.[47,48]

3) The continuous limit of

$$\frac{\partial^2 u_n(t)}{\partial t^2} = g_2 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_2(n,m)[f(u_n) - f(u_m)] + g_4 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J_4(n,m)[u_n - u_m], \tag{139}$$

where

$$f(u) = u - gu^2,$$

and $J_i(n)$ define the α_i-interactions with $\alpha_2=2$ and $\alpha_4=4$, gives the Boussinesq equation that is a nonlinear partial differential equation of fourth order

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_2\frac{\partial^2}{\partial x^2}u(x,t) + gG_2\frac{\partial^2}{\partial x^2}u^2(x,t) + G_4\frac{\partial^4}{\partial x^4}u(x,t) = 0. \tag{140}$$

This equation was formulated as part of an analysis of long waves in shallow water. It was subsequently applied to problems in the percolation of water in porous subsurface strata. It also crops up in the analysis of many other physical processes.

X. FRACTIONAL DERIVATIVES FROM DISPERSION LAW

Let us consider the three-dimensional lattice that is described by the equations of motion

$$\frac{\partial u_{\mathbf{n}}}{\partial t} = g \sum_{\substack{\mathbf{m}=-\infty \\ \mathbf{m}\neq \mathbf{n}}}^{+\infty} J(\mathbf{n},\mathbf{m})[u_{\mathbf{n}} - u_{\mathbf{m}}] + F(u_{\mathbf{n}}), \tag{141}$$

where $\mathbf{n}=(n_1,n_2,n_3)$, and $J(\mathbf{n},\mathbf{m})=J(\mathbf{n}-\mathbf{m})=J(\mathbf{m}-\mathbf{n})$. We suppose that $u_{\mathbf{n}}(t)$ are Fourier coefficients of the function $\hat{u}(\mathbf{k},t)$:

$$\hat{u}(\mathbf{k},t) = \sum_{\mathbf{n}=-\infty}^{+\infty} u_{\mathbf{n}}(t)e^{-i\mathbf{k}\mathbf{r}_{\mathbf{n}}} = \mathcal{F}_\Delta\{u_{\mathbf{n}}(t)\}, \tag{142}$$

where $\mathbf{k}=(k_1,k_2,k_3)$, and

$$\mathbf{r}_{\mathbf{n}} = \sum_{i=1}^{3} n_i \mathbf{a}_i.$$

Here, $\mathbf{a}_i$ are translational vectors of the lattice. The continuous medium model can be derived in the limit $|\mathbf{a}_i| \to 0$.

To derive the equation for $\hat{u}(\mathbf{k},t)$, we multiply (141) by $\exp(-i\mathbf{k}\mathbf{r}_{\mathbf{n}})$, and summing over $\mathbf{n}$. Then, we obtain

$$\frac{\partial \hat{u}(\mathbf{k},t)}{\partial t} = g[\hat{J}_\alpha(0) - \hat{J}_\alpha(\mathbf{k}\mathbf{a})]\hat{u}(\mathbf{k},t) + \mathcal{F}_\Delta\{F(u_{\mathbf{n}})\}, \tag{143}$$

where $\mathcal{F}_\Delta\{F(u_{\mathbf{n}})\}$ is an operator notation for the Fourier series transform of $F(u_{\mathbf{n}})$, and

$$\hat{J}_\alpha(\mathbf{ka}) = \sum_{\mathbf{n}=-\infty}^{+\infty} e^{-i\mathbf{k}\mathbf{r}_\mathbf{n}} J(\mathbf{n}). \tag{144}$$

For the three-dimensional lattice, we define the α-interaction with $\alpha=(\alpha_1,\alpha_2,\alpha_3)$, as an interaction that satisfies the conditions:

$$\lim_{k\to 0} \frac{[\hat{J}_\alpha(\mathbf{k}) - \hat{J}_\alpha(0)]}{|k_i|^{\alpha_i}} = A_{\alpha_i} \quad (i=1,2,3), \tag{145}$$

where $0<|A_{\alpha_i}|<\infty$. The conditions (145) mean that

$$\hat{J}_\alpha(0) - \hat{J}_\alpha(\mathbf{k}) = \sum_{i=1}^{3} A_{\alpha_1} |k_i|^{\alpha_i} + \sum_{i=1}^{3} R_{\alpha_i}(\mathbf{k}), \tag{146}$$

where

$$\lim_{k_i\to 0} R_{\alpha_i}(\mathbf{k})/|k_i|^{\alpha_i} = 0. \tag{147}$$

In the continuous limit ($|\mathbf{a}_i|\to 0$), the α-interaction in the three-dimensional lattice gives the continuous medium equations with the derivatives $\partial^{\alpha_1}/\partial x^{\alpha_1}$, $\partial^{\alpha_2}/\partial y^{\alpha_2}$, and $\partial^{\alpha_3}/\partial z^{\alpha_3}$.

Let us recall the appearance of the nonlinear parabolic equation.[49–52] Consider wave propagation in some media and present the wave vector $\mathbf{k}$ in the form

$$\mathbf{k} = \mathbf{k}_0 + \boldsymbol{\kappa} = \mathbf{k}_0 + \boldsymbol{\kappa}_\parallel + \boldsymbol{\kappa}_\perp, \tag{148}$$

where $\mathbf{k}_0$ is the unperturbed wave vector and subscripts ($\parallel$, $\perp$) are taken, respectively, to the direction of $\mathbf{k}_0$. A symmetric dispersion law

$$\omega(k) = \omega(\mathbf{k}) = \hat{J}_\alpha(\mathbf{ka}) - \hat{J}_\alpha(0) \tag{149}$$

for $\kappa=|\mathbf{k}-\mathbf{k}_0| \ll k_0=|\mathbf{k}_0|$ can be written as

$$\omega(k) = \omega(|\mathbf{k}|) = \omega(k_0 + [|\mathbf{k}| - k_0]) \approx \omega(k_0) + v_g(|\mathbf{k}| - k_0) + \tfrac{1}{2} v_g'(|\mathbf{k}| - k_0)^2, \tag{150}$$

where

$$v_g = \left(\frac{\partial\omega}{\partial k}\right)_{k=k_0}, \quad v_g' = \left(\frac{\partial^2\omega}{\partial k^2}\right)_{k=k_0}, \tag{151}$$

and

$$|\mathbf{k}| = |\mathbf{k}_0 + \boldsymbol{\kappa}| = \sqrt{(\mathbf{k}_0 + \kappa_\parallel)^2 + \kappa_\perp^2} \approx k_0 + \kappa_\parallel + \frac{1}{2k_0}\kappa_\perp^2. \tag{152}$$

Substitution of (152) into (150) gives

$$\omega(k) \approx \omega_0 + v_g\kappa_\parallel + \frac{v_g}{2k_0}\kappa_\perp^2 + \frac{v_g'}{2}\kappa_\parallel^2, \tag{153}$$

where $\omega_0=\omega(k_0)$. Expressions (143) and (153) in the dual space ("momentum representation") correspond to the following equation for $u=u(\mathbf{r},t)$ in the coordinate space:

$$i\frac{\partial u}{\partial t} = \omega_0 u - iv_g\frac{\partial u}{\partial x} - \frac{v_g}{2k_0}\Delta_\perp u - \frac{v_g'}{2}\Delta_\parallel u + F(u) \tag{154}$$

with respect to the field $u=u(t,x,y,z)$, where x is along $\mathbf{k}_0$, and we use the operator correspondence between the dual space and usual space-time:

$$\omega(k) \leftrightarrow i\frac{\partial}{\partial t}, \quad \boldsymbol{\kappa}_\parallel \leftrightarrow -i\frac{\partial}{\partial x},$$
$$(\boldsymbol{\kappa}_\perp)^2 \leftrightarrow -\Delta_\perp = -\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}, \quad (\boldsymbol{\kappa}_\parallel)^2 \leftrightarrow -\Delta_\parallel = -\frac{\partial^2}{\partial x^2}. \tag{155}$$

Equation (154) is known as the nonlinear parabolic equation.[49–52] The change of variables from (t,x,y,z) to $(t,x-v_g t,y,z)$ gives

$$-i\frac{\partial u}{\partial t} = \frac{v_g}{2k_0}\Delta_\perp u + \frac{v_g'}{2}\Delta_\parallel u - \omega_0 u - F(u), \tag{156}$$

which is also known as the nonlinear Schrödinger equation.

Wave propagation in oscillatory medium with long-range interaction of oscillators can be easily generalized by rewriting the dispersion law (153), in the following way:

$$\omega(k) = \omega_0 + v_g\kappa_\parallel + G_\alpha(\boldsymbol{\kappa}_\perp^2)^{\alpha/2} + G_\beta(\boldsymbol{\kappa}_\parallel^2)^{\beta/2} \quad (1<\alpha,\beta<2) \tag{157}$$

with new finite constants G_α and G_β.

Using the connection between Riesz fractional derivative and its Fourier transform[1]

$$(-\Delta_\perp)^{\alpha/2} \leftrightarrow (\boldsymbol{\kappa}_\perp^2)^{\alpha/2} \quad (-\Delta_\parallel)^{\beta/2} \leftrightarrow (\boldsymbol{\kappa}_\parallel^2)^{\beta/2}, \tag{158}$$

we obtain from (157)

$$i\frac{\partial u}{\partial t} = -iv_g\frac{\partial u}{\partial x} + G_\alpha(-\Delta_\perp)^{\alpha/2}u + G_\beta(-\Delta_\parallel)^{\beta/2}u + \omega_0 u + F(u), \tag{159}$$

where $u=u(t,x,y,z)$. By changing the variables from (t,x,y,z) to (t,ξ,y,z), $\xi=x-v_g t$, and using

$$(-\Delta_\parallel)^{\beta/2} = \frac{\partial^\beta}{\partial|x|^\beta} = \frac{\partial^\beta}{\partial|\xi|^\beta}, \tag{160}$$

we obtain from (159)

$$i\frac{\partial u}{\partial t} = G_\alpha(-\Delta_\perp)^{\alpha/2}u + G_\beta(-\Delta_\parallel)^{\beta/2}u + \omega_0 u + F(u), \tag{161}$$

which can be called the fractional nonlinear parabolic equation. For $G_\beta=0$ and $F(u)=b|u|^2u$, we get the fractional Ginzburg-Landau equation.[40–44]

We may consider one-dimensional simplifications of Eq. (161), i.e.,

$$i\frac{\partial u}{\partial t} = G_\beta\frac{\partial^\beta u}{\partial|\xi|^\beta} + \omega_0 u + F(u), \tag{162}$$

where $u=u(t,\xi)$, $\xi=x-v_g t$, or

$$i\frac{\partial u}{\partial t} = G_\alpha\frac{\partial^\alpha u}{\partial|z|^\alpha} + \omega_0 u + F(u), \tag{163}$$

where $u=u(t,z)$.

Let us comment on the physical structure of (161). The first and second terms on the right-hand side are related to wave propagation in oscillatory medium with long-range interaction of oscillators. The term with $F(u)$ on the right-hand side of Eqs. (159) and (161) correspond to wave interaction due to the nonlinear properties of the media. Thus, Eq. (161) can describe fractal processes of self-focusing and related issues.

XI. CONCLUSION

One-dimensional system of long-range interacting oscillators serves as a model for numerous applications in physics, chemistry, biology, etc. Long-range interactions are important types of interactions for complex media. An interesting situation arises when we consider the wide class of α-interactions, where α is noninteger. A remarkable feature of these interactions is the existence of a transform operation that replaces the set of coupled individual oscillator equations by the continuous medium equation with the space derivative of noninteger order α. Such transform operation is an approximation that appears in the continuous limit. This limit allows us to consider different models in a unified way by applying tools of fractional calculus.[53,54]

Periodic space-localized oscillations, which arise in discrete systems, have been widely studied for short-range interactions. In the paper, the systems with long-range interactions were considered. The method to map the discrete equations of motion into the continuous fractional order differential equation is developed by the transform operation. It is known that the properties of a system with long-range interaction are very different from short-range one. The method of fractional calculus can be a new tool for the analysis of different lattice systems.

APPENDIX: DIVERGENCE OF NONINVARIANT INTERACTION TERM

Noninvariant interaction term leads to the infinity in the continuous medium equation. To demonstrate this property, we prove the following proposition.

Proposition 8. The α-interaction term

$$g \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)u_m, \tag{A1}$$

where $J(n,m)=|n-m|^{-(\alpha+1)}$ is not translation-invariant. The transform operation $\hat{T}$ of the term (A1) leads to the divergence of order $|\Delta x|^{-\alpha}$ in the continuous medium equations.

Let us prove this proposition for $0<\alpha<2$ ($\alpha\neq 1$), and the following equations of motion

$$\frac{\partial^2 u_n}{\partial t^2} + g \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m)u_m - F(u_n) = 0. \tag{A2}$$

Since

$$\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} J(n,m) = \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} |n-m|^{-(\alpha+1)} \neq 0,$$

then the interparticle interaction term in (A2) is noninvariant with respect to translations. To derive the equation for $\hat{u}(k,t)$, we multiply Eq. (A2) by $\exp(-ikn\Delta x)$, and summing over n. Then, we obtain

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} + g\hat{J}_\alpha(k\Delta x)\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{A3}$$

where $\hat{J}_\alpha(k)$ is defined by (102). Using (105), we present Eq. (A3) in the form

$$\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} + gA_\alpha |\Delta x|^\alpha |k|^\alpha \hat{u}(k,t) + 2g\zeta(\alpha+1)\hat{u}(k,t) + 2g\sum_{n=1}^{\infty} \frac{\zeta(\alpha+1-2n)}{(2n)!}(\Delta x)^{2n}(-k^2)^n \hat{u}(k,t)$$
$$- \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{A4}$$

where ζ is the Riemann zeta-function and A_α is defined by (106). For the limit $\Delta x \to 0$ and $0 < \alpha < 2$ $(\alpha \neq 1)$, Eq. (A4) can be written as

$$\frac{\partial^2}{\partial t^2}\hat{u}(k,t) + G_\alpha A_\alpha |k|^\alpha \hat{u}(k,t) + 2g\zeta(\alpha+1)\hat{u}(k,t) - \mathcal{F}_\Delta\{F(u_n(t))\} = 0, \tag{A5}$$

where $0 < \alpha < 2$, $\alpha \neq 1$, and $G_\alpha = g|\Delta x|^\alpha$ is a finite parameter. Note that $g \to \infty$ for $\Delta x \to 0$, if G_α is a finite. Therefore, the transition to the limit $\Delta x \to 0$ in Eq. (A5) gives the divergence term

$$\lim_{\Delta x \to 0} g\zeta(\alpha+1)\hat{u}(k,t) = \zeta(\alpha+1)G_\alpha \tilde{u}(k,t) \lim_{\Delta x \to 0} |\Delta x|^{-\alpha} \to \infty. \tag{A6}$$

To have the continuous model equations without divergences, we must consider $[u_m(t) - u_n(t)]$ instead of $u_m(t)$ in the interaction terms (A1).

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Domain wall and periodic solutions of coupled ϕ^4 models in an external field

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Coupled double well (ϕ^4) one-dimensional potentials abound in both condensed matter physics and field theory. Here we provide an exhaustive set of exact periodic solutions of a coupled ϕ^4 model in an external field in terms of elliptic functions (domain wall arrays) and obtain single domain wall solutions in specific limits. We also calculate the energy and interaction between solitons for various solutions. Both topological and nontopological (e.g., some pulse-like solutions in the presence of a conjugate field) domain walls are obtained. We relate some of these solutions to the recently observed magnetic domain walls in certain multiferroic materials and also in the field theory context wherever possible. Discrete analogs of these coupled models, relevant for structural transitions on a lattice, are also considered. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2345110]

I. INTRODUCTION

There are many physical situations, both in condensed matter and field theory, where two double well potentials model the phenomena of interest with a specific coupling between the two fields. One such phenomenon of current intense interest is the coexistence of magnetism and ferroelectricity (i.e., magnetoelectricity) in a given material. This is a highly desired functionality in technological applications involving cross-field response, switching, and actuation. In general, this phenomenon is referred to as multiferroic behavior.[1] Recently, two different classes of (single phase) multiferroics, namely the orthorhombically distorted perovskites[2] and rare earth hexagonal structures,[3] have emerged. The latter show magnetic domain walls in the basal planes which can be modeled by a coupled ϕ^4 model[4] in the presence of a magnetic field. Coupled ϕ^4 models[5–7] also arise in the context of many ferroelectric and other second-order phase transitions. The coupled ϕ^4 model for multiferroics[4] has a biquadratic coupling whereas the coupled ϕ^4 model for a surface phase transition with hydration forces,[7] relevant in biophysics context, has a bilinear coupling. Other types of couplings are also known for structural phase transitions with strain.[8]

Similarly, there are analogous coupled models in field theory.[9,10] Several related models have been discussed in the literature and their soliton solutions have been found[11–18] including periodic ones.[19–21] Here our motivation is to obtain various possible domain wall solutions of these models with either a bilinear or a biquadratic coupling and then connect to experimental observations wherever possible.

The paper is organized as follows. In Sec. II we provide the solutions for the coupled ϕ^4 model with an explicit biquadratic coupling in the presence of an external field (with an additional linear-quadratic coupling) and calculate their energy as well as interaction between the solitons. We also obtain solutions in the limit of no field. In Sec. III we consider a coupled ϕ^4 model with

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a bilinear coupling. In Sec. IV we obtain several solutions of a coupled discrete ϕ^4 model with biquadratic coupling (but without an external field). In Sec. V we obtain a solution of the coupled discrete ϕ^4 model with bilinear coupling. To the best of our knowledge, no solution of the coupled ϕ^4 model in an external field is known. Similarly, no solutions of either the coupled continuum ϕ^4 model with a bilinear coupling or the discrete case are known. Even for the continuum coupled case with a biquadratic coupling and zero external field, out of the six possible solutions only three were known previously[20] but the other three are new. Finally, we conclude in Sec. VI with remarks on related models.

II. COUPLED ϕ^4 SOLUTIONS IN AN EXTERNAL FIELD

We consider several exact solutions of the coupled ϕ^4 system in a magnetic field (H_z) as given in Ref. 4 for hexagonal multiferroics. In particular, there are nine periodic solutions (valid for arbitrary m, the modulus of elliptic functions), which at $m=1$ reduce to just four solutions. In particular, there is one "bright-bright," one "dark-dark," and one each of bright-dark and dark-bright solutions. Notice that the equations of motion are asymmetric in the two scalar fields (ϕ and ψ) due to different coupling of the scalar fields to the magnetic field. Thus, the dark-bright and the bright-dark solutions are distinct.

The potential, with a *biquadratic* coupling between the two fields and in an external magnetic field (H_z), is given by

$$V = \alpha_1\phi^2 + \beta_1\phi^4 + \alpha_2\psi^2 + \beta_2\psi^4 + \gamma\phi^2\psi^2 - H_z[\rho_1\phi + \rho_2\phi^3 + \rho_3\phi\psi^2], \tag{1}$$

where α_i, β_i, γ, and ρ_i are material (or system) dependent parameters. Hence the (static) equations of motion are

$$\frac{d^2\phi}{dx^2} = 2\alpha_1\phi + 4\beta_1\phi^3 + 2\gamma\phi\psi^2 - H_z[\rho_1 + 3\rho_2\phi^2 + \rho_3\psi^2], \tag{2}$$

$$\frac{d^2\psi}{dx^2} = 2\alpha_2\psi + 4\beta_2\psi^3 + 2\gamma\phi^2\psi - 2H_z\rho_3\phi\psi. \tag{3}$$

These coupled set of equations admit several periodic solutions which we now discuss one by one systematically.

For static solutions the energy is given by

$$E = \int \left[\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 + \frac{1}{2}\left(\frac{d\psi}{dx}\right)^2 + V(\phi,\psi)\right]dx, \tag{4}$$

where the limits of integration are from $-\infty$ to ∞ in the case of hyperbolic solutions (i.e., single solitons) on the full line. On the other hand, in the case of periodic solutions (i.e., soliton lattices), the limits are from $-K(m)$ to $+K(m)$. Here $K(m)$ [and $E(m)$ below] denote the complete elliptic integral of the first (and second) kind.[22] Using equations of motion, one can show that for all of our solutions

$$V(\phi,\psi) = \left[\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 + \frac{1}{2}\left(\frac{d\psi}{dx}\right)^2\right] + C, \tag{5}$$

where the constant C in general varies from solution to solution. Hence the energy $\hat{E}=E-\int C dx$ is given by

$$\hat{E} \equiv E - \int C\mathrm{d}x = \int \left[\left(\frac{\mathrm{d}\phi}{\mathrm{d}x} \right)^2 + \left(\frac{\mathrm{d}\psi}{\mathrm{d}x} \right)^2 \right] \mathrm{d}x. \tag{6}$$

In the following we will give explicit expressions for energy in the case of all nine periodic solutions (and hence the corresponding four hyperbolic solutions). In each case we also provide an expression for the constant C.

A. Solution I

We look for the most general periodic solutions in terms of the Jacobi elliptic functions $\mathrm{sn}(x,m)$, $\mathrm{cn}(x,m)$, and $\mathrm{dn}(x,m)$.[22] It is not difficult to show that

$$\phi = F + A\mathrm{sn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{sn}[D(x+x_0),m], \tag{7}$$

is an exact solution provided the following eight coupled equations are satisfied:

$$2\alpha_1 F + 4\beta_1 F^3 + 2\gamma FG^2 - H_z\rho_1 - 3H_z\rho_2 F^2 - H_z\rho_3 G^2 = 0, \tag{8}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + 4\gamma BFG + 2\gamma AG^2 - 6H_z\rho_2 AF - 2H_z\rho_3 BG = -(1+m)AD^2, \tag{9}$$

$$12\beta_1 FA^2 + 2\gamma FB^2 + 4\gamma ABG - 3H_z\rho_2 A^2 - H_z\rho_3 B^2 = 0, \tag{10}$$

$$2\beta_1 A^2 + \gamma B^2 = mD^2, \tag{11}$$

$$2\alpha_2 G + 4\beta_2 G^3 + 2\gamma GF^2 - 2H_z\rho_3 GF = 0, \tag{12}$$

$$2\alpha_2 B + 12\beta_2 G^2 B + 4\gamma AFG + 2\gamma BF^2 - 2H_z\rho_3(BF+AG) = -(1+m)BD^2, \tag{13}$$

$$12\beta_2 GB^2 + 2\gamma GA^2 + 4\gamma ABF - 2H_z\rho_3 AB = 0, \tag{14}$$

$$2\beta_2 B^2 + \gamma A^2 = mD^2. \tag{15}$$

Here A and B denote the amplitudes of the "kink lattice," F and G are constants, D is an inverse characteristic length, and x_0 is the (arbitrary) location of the kink. Five of these equations determine the five unknowns A,B,D,F,G while the other three equations give three constraints between the nine parameters $\alpha_{1,2},\beta_{1,2},\gamma,H_z,\rho_1,\rho_2,\rho_3$. In particular, A and B are given by

$$A^2 = \frac{mD^2[2\beta_2 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \quad B^2 = \frac{mD^2[2\beta_1 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}. \tag{16}$$

Thus this solution exists provided $2\beta_1 > \gamma$ and $2\beta_2 > \gamma$.

It may be noted here that in case both $F,G=0$ then no solution exists so long as $H_z \neq 0$. In fact this is true for all nine solutions that we discuss in the following. There are two special cases (i.e., when either $F=0$ or $G=0$) when the analysis becomes somewhat simpler.

$G=0$, $F\neq 0$: In this case A,B are again given by Eq. (16) while

$$(1+m)D^2 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} - \frac{2\rho_1\gamma}{\rho_3}, \quad F = \frac{\rho_3 H_z}{2\gamma}. \tag{17}$$

The three (and not four, since one of the equations is identically satisfied) constraints are

$$\beta_1 = \frac{\rho_2\gamma}{2\rho_3}, \quad \alpha_1 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3}, \quad \alpha_2 = \frac{\rho_3^2 H_z^2}{4\gamma} - \frac{\rho_2\rho_3 H_z^2}{4\gamma} + \frac{\rho_1\gamma}{\rho_3}. \tag{18}$$

m=1: In this limiting case we have a bright-bright soliton solution given by

$$\phi = F + A\tanh[D(x+x_0)], \quad \psi = B\tanh[D(x+x_0)], \tag{19}$$

with A, B, and D determined by

$$A^2 = \frac{D^2[2\beta_2 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \quad B^2 = \frac{D^2[2\beta_1 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \quad 2D^2 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} - \frac{2\rho_1\gamma}{\rho_3}, \tag{20}$$

while the other relations remain unchanged and are again given by Eqs. (17) and (18).

F=0, *G≠0*: In this case A, B are again given by Eq. (16) with

$$(1+m)D^2 = 4\alpha_2 + \frac{2\rho_3 H_z AG}{B}, \quad G^2 = -\frac{\alpha_2}{2\beta_2}, \tag{21}$$

and the corresponding four constraints are

$$\beta_2 = \frac{\rho_3\alpha_2}{2\rho_1}, \quad (1+m)D^2 = -2\alpha_1 - 2\gamma G^2 + \frac{2\rho_3 H_z BG}{A},$$
$$4\gamma ABG = 3H_z\rho_2 A^2 + H_z\rho_3 B^2, \quad \rho_3 H_z AB = \gamma GA^2 + 6\beta_2 GB^2. \tag{22}$$

The solution at $m=1$ can be easily written down as above.

Special case of $H_z=0$: In this case the field equations are completely symmetric in the two fields ϕ, ψ and solution exists even if both $F, G=0$. In particular, with $H_z=0$, the solution is as given by Eq. (7) but with $F=0=G$[20] where A, B are again as given by Eq. (16) and further both α_1, α_2 turn out to be negative, i.e.,

$$\alpha_1 = \alpha_2 = -\frac{(1+m)D^2}{2}. \tag{23}$$

Special case of $\gamma^2=4\beta_1\beta_2$: One can show that the solution (7) exists even in case $\gamma^2 = 4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{24}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$A^2 + B^2 = \frac{mD^2}{\gamma}. \tag{25}$$

Other relations can be easily worked out depending on if F or G (or neither) is zero. For example, in case $G=0$, $F\neq 0$, one has

$$\rho_2 = \rho_3, \quad \alpha_2 = \frac{\rho_1\gamma}{\rho_3}, \quad \alpha_1 - \alpha_2 = \frac{\rho_3^2 H_z^2}{2\gamma}. \tag{26}$$

Energy: Corresponding to the periodic solution [Eq. (7) with $G=0$] the energy $\hat{E}$ and the constant C are given by

$$\hat{E} = \frac{2(A^2+B^2)D}{3m}[(1+m)E(m) - (1-m)K(m)],$$
$$C = -\tfrac{1}{2}(A^2+B^2)D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F]. \tag{27}$$

It is worth pointing out that even in the case of the solution (7) with either $F=0$, $G\neq 0$ or both F,G nonzero, the energy $\hat{E}$ is the same. Only the value of C is different. For example, in the case of $F=0$, $G\neq 0$, C is given by

$$C=-\frac{1}{2}(A^2+B^2)D^2-\frac{\alpha_2^2}{4\beta_2}, \tag{28}$$

while in the case of both F, G being nonzero, C is

$$C=-\tfrac{1}{2}(A^2+B^2)D^2-F^2[\alpha_1+3\beta_1F^2-2H_z\rho_2F]-G^2[\alpha_2+3\beta_2G^2+3\gamma F^2-2H_z\rho_3F]. \tag{29}$$

On using the expansion formulas for $E(m)$ and $K(m)$ around $m=1$ as given in[22]

$$K(m)=\ln\left(\frac{4}{\sqrt{1-m}}\right)+\frac{(1-m)}{4}\left[\ln\left(\frac{4}{\sqrt{1-m}}\right)-1\right]+\cdots, \tag{30}$$

$$E(m)=1+\frac{(1-m)}{2}\left[\ln\left(\frac{4}{\sqrt{1-m}}\right)-\frac{1}{2}\right]+\cdots, \tag{31}$$

for m near one, the energy of the periodic solution can be rewritten as the energy of the corresponding hyperbolic (bright-bright) soliton solution [Eq. (19)] plus the interaction energy. We find

$$\hat{E}=E_{\text{kink}}+E_{\text{int}}=(A^2+B^2)D\left[\frac{4}{3}+\frac{(1-m)}{3}\right]. \tag{32}$$

Note that this solution exists only when $2\beta_1\geqslant\gamma$, $2\beta_2\geqslant\gamma$ and $4\beta_1\beta_2\geqslant\gamma^2$. The interaction energy vanishes at exactly $m=1$, as it should.

B. Solution II

A different type of solution ("pulse lattice") is given by

$$\phi=F+A\,\text{cn}[D(x+x_0),m],\quad \psi=G+B\,\text{cn}[D(x+x_0),m], \tag{33}$$

provided the following eight coupled equations are satisfied:

$$2\alpha_1F+4\beta_1F^3+2\gamma FG^2-H_z\rho_1-3H_z\rho_2F^2-H_z\rho_3G^2=0, \tag{34}$$

$$2\alpha_1A+12\beta_1F^2A+4\gamma BFG+2\gamma AG^2-6H_z\rho_2AF-2H_z\rho_3BG=(2m-1)AD^2, \tag{35}$$

$$12\beta_1FA^2+2\gamma FB^2+4\gamma ABG-3H_z\rho_2A^2-H_z\rho_3B^2=0, \tag{36}$$

$$2\beta_1A^2+\gamma B^2=-mD^2, \tag{37}$$

$$2\alpha_2G+4\beta_2G^3+2\gamma GF^2-2H_z\rho_3GF=0, \tag{38}$$

$$2\alpha_2B+12\beta_2G^2B+4\gamma AFG+2\gamma BF^2-2H_z\rho_3(BF+AG)=(2m-1)BD^2, \tag{39}$$

$$12\beta_2GB^2+2\gamma GA^2+4\gamma ABF-2H_z\rho_3AB=0, \tag{40}$$

$$2\beta_2B^2+\gamma A^2=-mD^2. \tag{41}$$

Notice that two of these equations are meaningful only if $\gamma<0$ since $\beta_1,\beta_2>0$ from stability considerations. Thus, we write $\gamma=-|\gamma|$. Five of these equations determine the five unknowns

A,B,D,F,G while the other three equations give three constraints between the nine parameters $\alpha_{1,2},\beta_{1,2},\gamma,H_z,\rho_1,\rho_2,\rho_3$. In particular, A and B are given by

$$A^2=\frac{mD^2[2\beta_2+|\gamma|]}{[\gamma^2-4\beta_1\beta_2]},\quad B^2=\frac{mD^2[2\beta_1+|\gamma|]}{[\gamma^2-4\beta_1\beta_2]}. \tag{42}$$

Thus this solution exists provided $\gamma^2>4\beta_1\beta_2$.

There are two special cases when the analysis becomes somewhat simpler and we consider both cases one by one.

$G=0$, $F\neq 0$: In this case A,B are again given by Eq. (42) while

$$(2m-1)D^2=\frac{\rho_2\rho_3H_z^2}{2|\gamma|}-\frac{2\rho_1|\gamma|}{\rho_3},\quad F=-\frac{\rho_3H_z}{2|\gamma|}, \tag{43}$$

and the corresponding three constraints are

$$\beta_1=-\frac{\rho_2|\gamma|}{2\rho_3},\quad \alpha_1=-\frac{\rho_2\rho_3H_z^2}{2|\gamma|}-\frac{\rho_1|\gamma|}{\rho_3},\quad \alpha_2=-\frac{\rho_3^2H_z^2}{4|\gamma|}+\frac{\rho_2\rho_3H_z^2}{4|\gamma|}-\frac{\rho_1|\gamma|}{\rho_3}. \tag{44}$$

$F=0$, $G\neq 0$: In this case A,B are again given by Eq. (42) with

$$(2m-1)D^2=2\alpha_1-\frac{2\rho_3H_zBG}{A}-2|\gamma|G^2,\quad G^2=-\frac{\alpha_2}{2\beta_2}, \tag{45}$$

and the corresponding four constraints are

$$\begin{gathered}\beta_2=\frac{\rho_3\alpha_2}{2\rho_1},\quad (2m-1)D^2=-4\alpha_2-\frac{2\rho_3H_zAG}{B},\\ -4|\gamma|ABG=3H_z\rho_2A^2+H_z\rho_3B^2,\quad \rho_3H_zAB=-|\gamma|GA^2+6\beta_2GB^2.\end{gathered} \tag{46}$$

Special case of $H_z=0$: In this case the field equations are completely symmetric in the two fields ϕ,ψ and a solution exists even when both $F,G=0$. In particular, with $H_z=0$, the solution is as given by Eq. (33) but with $F=0=G$[20] where A,B are again as given by Eq. (42) and furthermore, α_1,α_2 are positive (negative) so long as $m>(<)1/2$, i.e.,

$$\alpha_1=\alpha_2=\frac{(2m-1)D^2}{2}. \tag{47}$$

Energy: Corresponding to the "pulse lattice" solution [Eq. (33) with $G=0$] the energy is given by

$$\begin{gathered}\hat{E}=\frac{2(A^2+B^2)D}{3m}[(2m-1)E(m)+(1-m)K(m)],\\ C=-\tfrac{1}{2}(1-m)(A^2+B^2)D^2-F^2[\alpha_1+3\beta_1F^2-2H_z\rho_2F].\end{gathered} \tag{48}$$

It is worth pointing out that even in the case of the solution (33) with either $F=0$, $G\neq 0$ or both F, G nonzero, the energy $\hat{E}$ is the same. Only the value of C is different. For example, in the case of $F=0$, $G\neq 0$, C is given by

$$C=-\frac{1}{2}(1-m)(A^2+B^2)D^2-\frac{\alpha_2^2}{4\beta_2}, \tag{49}$$

while in the case of both F, G being nonzero, C is

$$C = -\tfrac{1}{2}(1-m)(A^2+B^2)D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F] - G^2[\alpha_2 + 3\beta_2 G^2 + 3\gamma F^2 - 2H_z\rho_3 F]. \tag{50}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-dark) soliton solution

$$\phi = F + A\,\mathrm{sech}[D(x+x_0)], \quad \psi = B\,\mathrm{sech}[D(x+x_0)], \tag{51}$$

plus the interaction energy. We find

$$\hat{E} = E_{\mathrm{pulse}} + E_{\mathrm{int}} = (A^2+B^2)D\left[\frac{2}{3} - \frac{5(1-m)}{6} + (1-m)\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{52}$$

Note that this solution exists only when $\gamma<0$, $4\beta_1\beta_2<\gamma^2$. Again, the interaction energy vanishes at $m=1$.

C. Solution III

In this case, there is another "pulse lattice" solution which is given by

$$\phi = F + A\,\mathrm{dn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{dn}[D(x+x_0),m], \tag{53}$$

provided the following eight coupled equations are satisfied

$$2\alpha_1 F + 4\beta_1 F^3 + 2\gamma F G^2 - H_z\rho_1 - 3H_z\rho_2 F^2 - H_z\rho_3 G^2 = 0, \tag{54}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + 4\gamma BFG + 2\gamma AG^2 - 6H_z\rho_2 AF - 2H_z\rho_3 BG = (2-m)AD^2, \tag{55}$$

$$12\beta_1 FA^2 + 2\gamma FB^2 + 4\gamma ABG - 3H_z\rho_2 A^2 - H_z\rho_3 B^2 = 0, \tag{56}$$

$$2\beta_1 A^2 + \gamma B^2 = -D^2, \tag{57}$$

$$2\alpha_2 G + 4\beta_2 G^3 + 2\gamma GF^2 - 2H_z\rho_3 GF = 0, \tag{58}$$

$$2\alpha_2 B + 12\beta_2 G^2 B + 4\gamma AFG + 2\gamma BF^2 - 2H_z\rho_3(BF+AG) = (2-m)BD^2, \tag{59}$$

$$12\beta_2 GB^2 + 2\gamma GA^2 + 4\gamma ABF - 2H_z\rho_3 AB = 0, \tag{60}$$

$$2\beta_2 B^2 + \gamma A^2 = -D^2. \tag{61}$$

Notice that (as in the cn–cn case) two of these equations are meaningful only if $\gamma<0$ since $\beta_1,\beta_2>0$ from stability considerations. We therefore write $\gamma=-|\gamma|$. Five of these equations determine the five unknowns A,B,D,F,G while the other three equations give three constraints between the nine parameters $\alpha_{1,2},\beta_{1,2},|\gamma|,H_z,\rho_1,\rho_2,\rho_3$. In particular, A and B are given by

$$A^2 = \frac{D^2[2\beta_2+|\gamma|]}{[\gamma^2-4\beta_1\beta_2]}, \quad B^2 = \frac{D^2[2\beta_1+|\gamma|]}{[\gamma^2-4\beta_1\beta_2]}. \tag{62}$$

There are two special cases when the analysis becomes somewhat simpler and we consider both the cases one by one.

$G=0$, $F\neq 0$: In this case A,B are again given by Eq. (62) while

$$(2-m)D^2 = \frac{\rho_2\rho_3 H_z^2}{2|\gamma|} - \frac{2\rho_1|\gamma|}{\rho_3}, \quad F = -\frac{\rho_3 H_z}{2|\gamma|}, \tag{63}$$

and the three constraints are

$$\beta_1 = -\frac{\rho_2|\gamma|}{2\rho_3}, \quad \alpha_1 = -\frac{\rho_2\rho_3 H_z^2}{2|\gamma|} - \frac{\rho_1|\gamma|}{\rho_3}, \quad \alpha_2 = -\frac{\rho_3^2 H_z^2}{4|\gamma|} + \frac{\rho_2\rho_3 H_z^2}{4|\gamma|} - \frac{\rho_1|\gamma|}{\rho_3}. \tag{64}$$

$F=0$, $G\neq 0$: In this case A, B are again given by Eq. (62) with

$$(2-m)D^2 = 2\alpha_1 - \frac{2\rho_3 H_z BG}{A} - 2|\gamma|G^2, \quad G^2 = -\frac{\alpha_2}{2\beta_2}, \tag{65}$$

and the corresponding four constraints are

$$\begin{gathered}\beta_2 = \frac{\rho_3\alpha_2}{2\rho_1}, \quad (2-m)D^2 = -4\alpha_2 - \frac{2\rho_3 H_z AG}{B}, \\ -4|\gamma|ABG = 3H_z\rho_2 A^2 + H_z\rho_3 B^2, \quad \rho_3 H_z AB = -|\gamma|GA^2 + 6\beta_2 GB^2.\end{gathered} \tag{66}$$

Special case of $H_z=0$: With $H_z=0$, the solution is as given by Eq. (53) but with $F=0=G$[20] where A, B are again as given by Eq. (62) and furthermore, both α_1, α_2 are positive definite:

$$\alpha_1 = \alpha_2 = \frac{(2-m)D^2}{2}. \tag{67}$$

Energy: Corresponding to the "pulse lattice" solution [Eq. (53) with $G=0$] the energy is given by

$$\begin{gathered}\hat{E} = \frac{2(A^2+B^2)D}{3}[(2-m)E(m) - (1-m)K(m)], \\ C = \tfrac{1}{2}(1-m)(A^2+B^2)D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F].\end{gathered} \tag{68}$$

It is worth pointing out that even in the case of the solution (53) with either $F=0$, $G\neq 0$ or both F, G nonzero, the energy $\hat{E}$ is the same. Only the value of C is different. For example, in the case of $F=0$, $G\neq 0$, C is given by

$$C = \frac{1}{2}(1-m)(A^2+B^2)D^2 - \frac{\alpha_2^2}{4\beta_2}, \tag{69}$$

while in the case of both F, G being nonzero, C is

$$C = \tfrac{1}{2}(1-m)(A^2+B^2)D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F] - G^2[\alpha_2 + 3\beta_2 G^2 + 3\gamma F^2 - 2H_z\rho_3 F]. \tag{70}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-dark) soliton solution as given by Eq. (51) plus the interaction energy. We find

$$\hat{E} = E_{\text{pulse}} + E_{\text{int}} = (A^2+B^2)D\left[\frac{2}{3} - \frac{(1-m)}{2} - (1-m)\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{71}$$

Note that this solution also exists only when $\gamma<0$, $4\beta_1\beta_2<\gamma^2$. Again, the interaction energy vanishes at $m=1$.

D. Solution IV

In addition to the cn–cn and dn–dn solutions discussed earlier, there are two novel (mixed) soliton solutions of dn–cn and cn–dn type. Let us discuss them one by one. We shall see that for these two solutions (in fact it is true for all six solutions that we discuss in the following) G is necessarily zero while F is necessarily nonzero (unless $H_z=0$), otherwise the solution does not exist. In particular, it is easily shown that

$$\phi = F + A\,\mathrm{dn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{cn}[D(x+x_0),m], \tag{72}$$

is a solution provided $G=0$ and further, the following seven coupled equations are satisfied:

$$2\alpha_1 F + 4\beta_1 F^3 + (2/m)\gamma(m-1)FB^2 - H_z\rho_1 - 3H_z\rho_2 F^2 + (1/m)(1-m)H_z\rho_3 B^2 = 0, \tag{73}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + (2/m)(m-1)\gamma AB^2 - 6H_z\rho_2 AF = (2-m)AD^2, \tag{74}$$

$$12\beta_1 FA^2 + (2/m)\gamma FB^2 - 3H_z\rho_2 A^2 - (1/m)H_z\rho_3 B^2 = 0, \tag{75}$$

$$\gamma B^2 + 2m\beta_1 A^2 = -mD^2, \tag{76}$$

$$2\alpha_2 B + 2(1-m)\gamma A^2 B + 2\gamma BF^2 - 2H_z\rho_3 BF = (2m-1)BD^2, \tag{77}$$

$$2\beta_2 B^2 + m\gamma A^2 = -mD^2, \tag{78}$$

$$4\gamma FAB - 2H_z\rho_3 AB = 0. \tag{79}$$

Again a solution exists only if $\gamma<0$ and thus we write $\gamma=-|\gamma|$. The solution (72) exists provided

$$A^2 = \frac{D^2[|\gamma| + 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{mD^2[2\beta_1 + |\gamma|]}{[\gamma^2 - 4\beta_1\beta_2]}, \tag{80}$$

where

$$(2-m)D^2 = \frac{2}{m}(1-m)|\gamma|B^2 - \frac{2\rho_1|\gamma|}{\rho_3} + \frac{\rho_2\rho_3 H_z^2}{2|\gamma|}, \quad F = -\frac{\rho_3 H_z}{2|\gamma|}, \tag{81}$$

and the three constraints are

$$\begin{aligned} \beta_1 &= -\frac{\rho_2|\gamma|}{2\rho_3}, \quad \alpha_2 = -\frac{\rho_2\rho_3 H_z^2}{2|\gamma|} - \frac{\rho_1|\gamma|}{\rho_3}, \\ (2m-1)D^2 &= 2\alpha_2 - 2(1-m)|\gamma|A^2 + \frac{H_z^2\rho_3^2}{2|\gamma|}. \end{aligned} \tag{82}$$

Special case of $H_z=0$: With $H_z=0$, the solution is as given by Eq. (72) but with $F=0=G$ where A and B are again as given by Eq. (80) and furthermore, α_2 is positive, i.e.,

$$\alpha_1 = \frac{mD^2}{2} - 2(1-m)\beta_1 A^2, \quad m\alpha_2 = m\frac{D^2}{2} + 2(1-m)\beta_2 B^2 > 0. \tag{83}$$

Energy: Corresponding to the "pulse lattice" solution [Eq. (72) with $G=0$] the energy $\hat{E}$ and C are given by

$$\hat{E} = \frac{2D}{3m}\left([(2-m)mA^2 + (2m-1)B^2]E(m) + (1-m)(B^2 - 2mA^2)K(m)\right),$$

$$C = \frac{1}{2}A^2D^2(1-m) - F^2[\alpha_1 + 3\beta_1F^2 - 2H_z\rho_2F] + \frac{(1-m)}{m^2}[m\gamma F^2 - \alpha_2 m + \beta_2(1-m)B^2]B^2. \tag{84}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-dark) soliton solution (51) plus the interaction energy. We find

$$\hat{E} = E_{\text{pulse}} + E_{\text{int}} = D\left[\frac{2}{3}(A^2+B^2) + \frac{(1-m)}{6}(3A^2 - 5B^2) + (1-m)(B^2 - A^2)\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{85}$$

Note that this solution also exists only when $\gamma < 0$, $4\beta_1\beta_2 < \gamma^2$. The interaction energy vanishes for $m=1$, as it should.

E. Solution V

It is easily shown that there is also a cn–dn solution which is distinct from the above-noted dn–cn solution. This solution is given by

$$\phi = F + A\,\text{cn}[D(x+x_0), m], \quad \psi = G + B\,\text{dn}[D(x+x_0), m], \tag{86}$$

provided $G=0$ and the following seven coupled equations are satisfied:

$$2\alpha_1F + 4\beta_1F^3 + 2\gamma(1-m)FB^2 - H_z\rho_1 - 3H_z\rho_2F^2 - (1-m)H_z\rho_3B^2 = 0, \tag{87}$$

$$2\alpha_1A + 12\beta_1F^2A + 2(1-m)\gamma AB^2 - 6H_z\rho_2AF = -(1-2m)AD^2, \tag{88}$$

$$12\beta_1FA^2 + 2m\gamma FB^2 - 3H_z\rho_2A^2 - mH_z\rho_3B^2 = 0, \tag{89}$$

$$m\gamma B^2 + 2\beta_1A^2 = -mD^2, \tag{90}$$

$$2\alpha_2B - (2/m)(1-m)\gamma A^2B + 2\gamma BF^2 - 2H_z\rho_3BF = (2-m)BD^2, \tag{91}$$

$$2m\beta_2B^2 + \gamma A^2 = -mD^2, \tag{92}$$

$$4\gamma FAB - 2H_z\rho_3AB = 0. \tag{93}$$

Again a solution exists only if $\gamma < 0$ and hence we put $\gamma = -|\gamma|$. The solution turns out to be

$$A^2 = \frac{mD^2[|\gamma| + 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{D^2[2\beta_1 + |\gamma|]}{[\gamma^2 - 4\beta_1\beta_2]}, \tag{94}$$

where

$$(2m-1)D^2 = -2(1-m)|\gamma|B^2 - \frac{2\rho_1|\gamma|}{\rho_3} + \frac{\rho_2\rho_3H_z^2}{2|\gamma|}, \quad F = -\frac{\rho_3H_z}{2|\gamma|}, \tag{95}$$

and the three constraints are

$$\beta_1 = -\frac{\rho_2|\gamma|}{2\rho_3}, \quad \alpha_1 = -\frac{\rho_2\rho_3 H_z^2}{2|\gamma|} - \frac{\rho_1|\gamma|}{\rho_3},$$
$$(2-m)D^2 = 2\alpha_2 + (2/m)(1-m)|\gamma|A^2 + \frac{H_z^2\rho_3^2}{2|\gamma|}. \tag{96}$$

Special case of $H_z=0$: With $H_z=0$, the solution is as given by Eq. (86) but with $F=0=G$ where A and B are again as given by Eq. (94) and furthermore, α_1 is positive, i.e.,

$$m\alpha_1 = m\frac{D^2}{2} + 2(1-m)\beta_1 A^2 > 0, \quad \alpha_2 = \frac{mD^2}{2} - 2(1-m)\beta_2 B^2. \tag{97}$$

It is worth pointing out that with $H_z=0$, the field equations are completely symmetric between the two fields ϕ and ψ and hence solutions IV and V are identical in the limit $H_z=0$.

$m=1$: In the special case of $m=1$ and $G=0$, $F\neq 0$, all four solutions II to V reduce to a dark-dark type soliton solution (51), i.e.,

$$\phi = F + A\,\mathrm{sech}[D(x+x_0)], \quad \psi = B\,\mathrm{sech}[D(x+x_0)], \tag{98}$$

with A, B, and D given by

$$A^2 = \frac{D^2[|\gamma| + 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{D^2[2\beta_1 + |\gamma|]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad D^2 = -\frac{2\rho_1|\gamma|}{\rho_3} + \frac{\rho_2\rho_3 H_z^2}{2|\gamma|}, \tag{99}$$

while the other relations remain unchanged and are again given by Eqs. (43) and (44).

Similarly, in the special case of $m=1$ and $F=0$, $G\neq 0$, both solutions II and III reduce to a dark-dark type soliton solution

$$\phi = A\,\mathrm{sech}[D(x+x_0)], \quad \psi = G + B\,\mathrm{sech}[D(x+x_0)], \tag{100}$$

with A and B again given by Eq. (99) while

$$D^2 = 2\alpha_1 - \frac{2\rho_3 H_z BG}{A} - 2|\gamma|G^2, \quad D^2 = -4\alpha_2 - \frac{2\rho_3 H_z AG}{B}. \tag{101}$$

Other relations remain unchanged and are again given by Eqs. (45) and (46).

Energy: Corresponding to the "pulse lattice" solution [Eq. (86) with $G=0$] the energy is given by

$$\hat{E} = \frac{2D}{3m}\big([(2-m)mB^2 + (2m-1)A^2]E(m) + (1-m)(A^2 - 2mB^2)K(m)\big),$$
$$C = -\tfrac{1}{2}A^2D^2(1-m) - F^2[\alpha_1 + 3\beta_1F^2 - 2H_z\rho_2F] + [-\gamma F^2 + \alpha_2 + \beta_2(1-m)B^2]B^2. \tag{102}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-dark) soliton solution [Eq. (51)] plus the interaction energy. We find

$$\hat{E} = E_{\mathrm{pulse}} + E_{\mathrm{int}} = D\left[\frac{2}{3}(A^2+B^2) + \frac{(1-m)}{6}(3B^2 - 5A^2) + (1-m)(A^2-B^2)\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{103}$$

Note that this solution also exists only when $\gamma<0$, $4\beta_1\beta_2<\gamma^2$. Again, the interaction energy vanishes at $m=1$. It is amusing to note that the energy of solution V is easily obtained from that of solution IV by simply interchanging A and B.

F. Solution VI

Apart from the solutions which at $m=1$ reduce to the bright-bright and dark-dark solutions, there are four solutions which at $m=1$ go over to either bright-dark or dark-bright solutions, which we now discuss one by one.

One such solution, kink-like in ϕ and pulse-like in ψ, is

$$\phi = F + A\,\mathrm{sn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{cn}[D(x+x_0),m], \tag{104}$$

provided $G=0$ and the following seven coupled equations are satisfied:

$$2\alpha_1 F + 4\beta_1 F^3 + 2\gamma F B^2 - H_z\rho_1 - 3H_z\rho_2 F^2 - H_z\rho_3 B^2 = 0, \tag{105}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + 2\gamma A B^2 - 6H_z\rho_2 AF = -(1+m)AD^2, \tag{106}$$

$$12\beta_1 F A^2 - 2\gamma F B^2 - 3H_z\rho_2 A^2 + H_z\rho_3 B^2 = 0, \tag{107}$$

$$2\beta_1 A^2 - \gamma B^2 = mD^2, \tag{108}$$

$$2\alpha_2 B + 2\gamma A^2 B + 2\gamma B F^2 - 2H_z\rho_3 BF = (2m-1)BD^2, \tag{109}$$

$$2\beta_2 B^2 - \gamma A^2 = -mD^2, \tag{110}$$

$$(4\gamma F - 2H_z\rho_3)AB = 0. \tag{111}$$

In this case it turns out that the solution exists only if either $2\beta_1 > \gamma > 2\beta_2$, $\gamma^2 > 4\beta_1\beta_2$ or $2\beta_2 > \gamma > 2\beta_1$, $\gamma^2 < 4\beta_1\beta_2$. We find that

$$A^2 = \frac{mD^2[\gamma - 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{mD^2[2\beta_1 - \gamma]}{[\gamma^2 - 4\beta_1\beta_2]}, \tag{112}$$

where

$$-(1+m)D^2 = 2\gamma B^2 + \frac{2\rho_1\gamma}{\rho_3} - \frac{\rho_2\rho_3 H_z^2}{2\gamma}, \quad F = \frac{\rho_3 H_z}{2\gamma}, \tag{113}$$

and the three constraints are

$$\beta_1 = \frac{\rho_2\gamma}{2\rho_3}, \quad \alpha_1 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3},$$
$$(2m-1)D^2 = 2\alpha_2 + 2\gamma A^2 - \frac{H_z^2\rho_3^2}{2\gamma}. \tag{114}$$

Special case of $H_z=0$*:* With $H_z=0$, the solution is again given by Eq. (104) but with $F=0=G$ where A and B are again as given by Eq. (112) and furthermore, α_1, α_2 turn out to be negative, i.e.,

$$\alpha_1 = -\frac{(1+m)D^2}{2} - \gamma B^2, \quad \alpha_2 = -\frac{D^2}{2} - 2\beta_2 B^2. \tag{115}$$

Special case of $\gamma^2=4\beta_1\beta_2$*:* One can show that the solution (104) exists even in case $\gamma^2=4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{116}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$A^2 - B^2 = \frac{mD^2}{\gamma}. \tag{117}$$

Further, one has

$$\rho_2 = \rho_3, \quad \alpha_1 = \frac{\rho_3^2 H_z^2}{2\gamma} + \frac{\rho_1 \gamma}{\rho_3}, \quad \alpha_2 - \alpha_1 = \frac{mD^2}{2} - \frac{\rho_3^2 H_z^2}{2\gamma}. \tag{118}$$

Energy: Corresponding to the mixed "kink-pulse lattice" solution [Eq. (104)] the energy is given by

$$\hat{E} = \frac{2D}{3m}\big([(2-m)mB^2 + (1+m)A^2]E(m) - (1-m)(A^2+2B^2)K(m)\big),$$
$$C = -\tfrac{1}{2}A^2D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F] + [-\gamma F^2 + \alpha_2 + \beta_2 B^2]B^2. \tag{119}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (bright-dark) soliton solution

$$\phi = F + A\tanh[D(x+x_0)], \quad \psi = B\,\mathrm{sech}[D(x+x_0)], \tag{120}$$

plus the interaction energy. We find

$$\hat{E} = E_{\mathrm{soliton}} + E_{\mathrm{int}} = D\left[\frac{2}{3}(2A^2+B^2) + \frac{(1-m)}{6}(2A^2+3B^2) - (1-m)B^2\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{121}$$

Note that this solution also exists only when either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \geqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \leqslant 4\beta_1\beta_2$. The interaction energy vanishes at $m=1$.

G. Solution VII

It is easy to show that another such (kink- and pulse-like) solution is

$$\phi = F + A\,\mathrm{sn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{dn}[D(x+x_0),m], \tag{122}$$

provided $G=0$ and the following seven coupled equations are satisfied:

$$2\alpha_1 F + 4\beta_1 F^3 + 2\gamma F B^2 - H_z\rho_1 - 3H_z\rho_2 F^2 - H_z\rho_3 B^2 = 0, \tag{123}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + 2\gamma A B^2 - 6H_z\rho_2 AF = -(1+m)AD^2, \tag{124}$$

$$12\beta_1 FA^2 - 2m\gamma FB^2 - 3H_z\rho_2 A^2 + mH_z\rho_3 B^2 = 0, \tag{125}$$

$$2\beta_1 A^2 - m\gamma B^2 = mD^2, \tag{126}$$

$$2\alpha_2 B + (2/m)\gamma A^2 B + 2\gamma BF^2 - 2H_z\rho_3 BF = (2-m)BD^2, \tag{127}$$

$$2m\beta_2 B^2 - \gamma A^2 = -mD^2, \tag{128}$$

$$4\gamma FAB - 2H_z\rho_3 AB = 0. \tag{129}$$

In this case also it turns out that the solution exists only if either $2\beta_1 > \gamma > 2\beta_2$ and $\gamma^2 > 4\beta_1\beta_2$ or $2\beta_2 > \gamma > 2\beta_1$ and $\gamma^2 < 4\beta_1\beta_2$. We find that

$$A^2 = \frac{mD^2[\gamma - 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{D^2[2\beta_1 - \gamma]}{[\gamma^2 - 4\beta_1\beta_2]}, \tag{130}$$

where

$$-(1+m)D^2 = 2\gamma B^2 + \frac{2\rho_1\gamma}{\rho_3} - \frac{\rho_2\rho_3 H_z^2}{2\gamma}, \quad F = \frac{\rho_3 H_z}{2\gamma}, \tag{131}$$

and the three constraints are

$$\beta_1 = \frac{\rho_2\gamma}{2\rho_3}, \quad \alpha_1 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3},$$
$$(2-m)D^2 = 2\alpha_2 + (2/m)\gamma A^2 - \frac{H_z^2\rho_3^2}{2\gamma}. \tag{132}$$

Special case of $H_z=0$: With $H_z=0$, the solution is again given by Eq. (122) but with $F=0=G$ where A and B are again as given by Eq. (130) and furthermore, α_1, α_2 turn out to be negative, i.e.,

$$\alpha_1 = -\frac{(1+m)D^2}{2} - \gamma B^2, \quad \alpha_2 = -\frac{mD^2}{2} - 2\beta_2 B^2. \tag{133}$$

$m=1$: In the special case of $m=1$ and $G=0$, $F\neq 0$, both solutions VI and VII reduce to a bright-dark type of solution as given by Eq. (120), i.e.,

$$\phi = F + A\tanh[D(x+x_0)], \quad \psi = B\,\mathrm{sech}[D(x+x_0)], \tag{134}$$

with A, B, and D given by

$$A^2 = \frac{D^2[\gamma - 2\beta_2]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad B^2 = \frac{D^2[2\beta_1 - \gamma]}{[\gamma^2 - 4\beta_1\beta_2]}, \quad D^2 = -\gamma B^2 - \frac{\rho_1\gamma}{\rho_3} + \frac{\rho_2\rho_3 H_z^2}{4\gamma}, \tag{135}$$

while the other relations remain unchanged and are again given by Eqs. (131) and (132).

Special case of $\gamma^2=4\beta_1\beta_2$: One can show that the solution (122) exists even in case $\gamma^2=4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{136}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$A^2 - mB^2 = \frac{mD^2}{\gamma}. \tag{137}$$

Further, one has

$$\rho_2 = \rho_3, \quad \alpha_1 = \frac{\rho_3^2 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3}, \quad \alpha_2 - \alpha_1 = \frac{D^2}{2} - \frac{\rho_3^2 H_z^2}{2\gamma}. \tag{138}$$

Energy: Corresponding to the mixed "kink-pulse lattice" solution [Eq. (122)] the energy and the constant C are given by

$$\hat{E} = \frac{2D}{3m}\big([(2m-1)B^2 + (1+m)A^2]E(m) - (1-m)(A^2 - B^2)K(m)\big), \tag{139}$$

$$C = -\tfrac{1}{2}A^2D^2 - F^2[\alpha_1 + 3\beta_1F^2 - 2H_z\rho_2F] + [-\gamma F^2 + \alpha_2 + \beta_2B^2]B^2. \tag{140}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (bright-dark) soliton solution [Eq. (120)] plus the interaction energy. We find

$$\hat{E} = E_{\text{soliton}} + E_{\text{int}} = D\left[\frac{2}{3}(2A^2 + B^2) + \frac{(1-m)}{6}(2A^2 - 5B^2) + (1-m)B^2\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{141}$$

Note that this solution also exists only when either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \geqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \leqslant 4\beta_1\beta_2$. The interaction energy vanishes for $m=1$.

H. Solution VIII

Finally, we discuss two periodic solutions both of which at $m=1$ reduce to a dark-bright type of solution. The first such (pulse-like in ϕ and kink-like in ψ) solution is given by

$$\phi = F + A\,\mathrm{cn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{sn}[D(x+x_0),m], \tag{142}$$

provided $G=0$ and the following seven coupled equations are satisfied:

$$2\alpha_1F + 4\beta_1F^3 + 2\gamma FB^2 - H_z\rho_1 - 3H_z\rho_2F^2 - H_z\rho_3B^2 = 0, \tag{143}$$

$$2\alpha_1A + 12\beta_1F^2A + 2\gamma AB^2 - 6H_z\rho_2AF = (2m-1)AD^2, \tag{144}$$

$$12\beta_1FA^2 - 2\gamma FB^2 - 3H_z\rho_2A^2 + H_z\rho_3B^2 = 0, \tag{145}$$

$$2\beta_1A^2 - \gamma B^2 = -mD^2, \tag{146}$$

$$2\alpha_2B + 2\gamma A^2B + 2\gamma BF^2 - 2H_z\rho_3BF = -(1+m)BD^2, \tag{147}$$

$$2\beta_2B^2 - \gamma A^2 = mD^2, \tag{148}$$

$$4\gamma FAB - 2H_z\rho_3AB = 0. \tag{149}$$

In this case it turns out that the solution exists only if either $2\beta_1 > \gamma > 2\beta_2$ and $\gamma^2 < 4\beta_1\beta_2$ or $2\beta_2 > \gamma > 2\beta_1$ and $\gamma^2 > 4\beta_1\beta_2$. We find that

$$A^2 = \frac{mD^2[\gamma - 2\beta_2]}{[4\beta_1\beta_2 - \gamma^2]}, \quad B^2 = \frac{mD^2[2\beta_1 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \tag{150}$$

where

$$(2m-1)D^2 = 2\gamma B^2 + \frac{2\rho_1\gamma}{\rho_3} - \frac{\rho_2\rho_3H_z^2}{2\gamma}, \quad F = \frac{\rho_3H_z}{2\gamma}, \tag{151}$$

and the three constraints are

$$\beta_1 = \frac{\rho_2\gamma}{2\rho_3}, \quad \alpha_1 = \frac{\rho_2\rho_3H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3},$$
$$-(1+m)D^2 = 2\alpha_2 + 2\gamma A^2 - \frac{H_z^2\rho_3^2}{2\gamma}. \tag{152}$$

Special case of $H_z=0$: When $H_z=0$, the solution is again given by Eq. (142) but with $F=0=G$ where A and B are again as given by Eq. (150) and furthermore, α_1, α_2 turn out to be negative, i.e.,

$$\alpha_1 = -\frac{D^2}{2} - 2\beta_1 A^2, \quad \alpha_2 = -\frac{(1+m)D^2}{2} - \gamma A^2. \tag{153}$$

It is worth pointing out that with $H_z=0$, the field equations are completely symmetric between the two fields ϕ and ψ and hence the solutions VI and VIII are identical in the limit $H_z=0$.

Special case of $\gamma^2=4\beta_1\beta_2$: One can show that the solution (142) exists even in case $\gamma^2=4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{154}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$B^2 - A^2 = \frac{mD^2}{\gamma}. \tag{155}$$

Further, one has

$$\rho_2 = \rho_3, \quad \alpha_1 = \frac{\rho_3^2 H_z^2}{2\gamma} + \frac{\rho_1 \gamma}{\rho_3}, \quad \alpha_1 - \alpha_2 = \frac{mD^2}{2} + \frac{\rho_3^2 H_z^2}{2\gamma}. \tag{156}$$

Energy: Corresponding to the mixed "kink-pulse lattice" solution [Eq. (142)] the energy and the constant C are given by

$$\hat{E} = \frac{2D}{3m}\big([(2m-1)A^2 + (1+m)B^2]E(m) - (1-m)(B^2-A^2)K(m)\big), \tag{157}$$

$$C = -\tfrac{1}{2}(1-m)A^2D^2 - F^2[\alpha_1 + 3\beta_1 F^2 - 2H_z\rho_2 F] + [-\gamma F^2 + \alpha_2 + \beta_2 B^2]B^2. \tag{158}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-bright) soliton solution

$$\phi = F + A\,\mathrm{sech}[D(x+x_0)], \quad \psi = B\tanh[D(x+x_0)], \tag{159}$$

plus the interaction energy. We find

$$\hat{E} = E_{\mathrm{soliton}} + E_{\mathrm{int}} = D\left[\frac{2}{3}(2B^2+A^2) + \frac{(1-m)}{6}(2B^2-5A^2) + (1-m)A^2\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{160}$$

Note that this solution also exists only when either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \leqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \geqslant 4\beta_1\beta_2$. Again, the interaction energy vanishes at $m=1$. It is amusing to note that the energy of the solution VIII is easily obtained from that of solution VI by simply interchanging A and B.

I. Solution IX

Another solution which at $m=1$ reduces to a dark-bright type of soliton solution is given by

$$\phi = F + A\,\mathrm{dn}[D(x+x_0),m], \quad \psi = G + B\,\mathrm{sn}[D(x+x_0),m], \tag{161}$$

provided $G=0$ and the following seven coupled equations are satisfied:

$$2\alpha_1 F + 4\beta_1 F^3 + (2/m)\gamma F B^2 - H_z\rho_1 - 3H_z\rho_2 F^2 - \frac{H_z\rho_3 B^2}{m} = 0, \tag{162}$$

$$2\alpha_1 A + 12\beta_1 F^2 A + (2/m)\gamma A B^2 - 6H_z\rho_2 AF = (2-m)AD^2, \tag{163}$$

$$12\beta_1 F A^2 - (2/m)\gamma F B^2 - 3H_z\rho_2 A^2 + \frac{H_z\rho_3 B^2}{m} = 0, \tag{164}$$

$$2m\beta_1 A^2 - \gamma B^2 = -mD^2, \tag{165}$$

$$2\alpha_2 B + 2\gamma A^2 B + 2\gamma B F^2 - 2H_z\rho_3 BF = -(1+m)BD^2, \tag{166}$$

$$2\beta_2 B^2 - m\gamma A^2 = mD^2, \tag{167}$$

$$4\gamma FAB - 2H_z\rho_3 AB = 0. \tag{168}$$

In this case it turns out that the solution exists only if either $2\beta_1 > \gamma > 2\beta_2$ and $\gamma^2 < 4\beta_1\beta_2$ or $2\beta_2 > \gamma > 2\beta_1$ and $\gamma^2 > 4\beta_1\beta_2$. We find that

$$A^2 = \frac{D^2[\gamma - 2\beta_2]}{[4\beta_1\beta_2 - \gamma^2]}, \quad B^2 = \frac{mD^2[2\beta_1 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \tag{169}$$

where

$$(2-m)D^2 = (2/m)\gamma B^2 + \frac{2\rho_1\gamma}{\rho_3} - \frac{\rho_2\rho_3 H_z^2}{2\gamma}, \quad F = \frac{\rho_3 H_z}{2\gamma}, \tag{170}$$

and the three constraints are

$$\begin{aligned} \beta_1 &= \frac{\rho_2\gamma}{2\rho_3}, \quad \alpha_1 = \frac{\rho_2\rho_3 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3}, \\ -(1+m)D^2 &= 2\alpha_2 + 2\gamma A^2 - \frac{H_z^2\rho_3^2}{2\gamma}. \end{aligned} \tag{171}$$

Special case of $H_z=0$: When $H_z=0$, the solution is again given by Eq. (161) but with $F=0=G$ where A and B are again as given by Eq. (169) and furthermore, α_1, α_2 turn out to be negative, i.e.,

$$\alpha_1 = -\frac{mD^2}{2} - 2\beta_1 A^2, \quad \alpha_2 = -\frac{(1+m)D^2}{2} - \gamma A^2. \tag{172}$$

It is worth pointing out that with $H_z=0$, the field equations are completely symmetric between the two fields ϕ and ψ and hence the solutions VII and IX are identical in the limit $H_z=0$.

$m=1$: In the special case of $m=1$ and $G=0$, $F\neq 0$, both solutions VIII and IX reduce to a dark-bright type of solution (159), i.e.,

$$\phi = F + A\,\mathrm{sech}[D(x+x_0)], \quad \psi = B\tanh[D(x+x_0)], \tag{173}$$

with A, B, and D given by

$$A^2 = \frac{D^2[\gamma - 2\beta_2]}{[4\beta_1\beta_2 - \gamma^2]}, \quad B^2 = \frac{D^2[2\beta_1 - \gamma]}{[4\beta_1\beta_2 - \gamma^2]}, \quad D^2 = 2\gamma B^2 + \frac{2\rho_1\gamma}{\rho_3} - \frac{\rho_2\rho_3 H_z^2}{2\gamma}, \tag{174}$$

while the other relations remain unchanged and are given by Eqs. (151) and (152).

Special case of $\gamma^2 = 4\beta_1\beta_2$*:* One can show that the solution (161) exists even in case $\gamma^2 = 4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{175}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$B^2 - mA^2 = \frac{mD^2}{\gamma}. \tag{176}$$

Further, one has

$$\rho_2 = \rho_3, \quad \alpha_1 = \frac{\rho_3^2 H_z^2}{2\gamma} + \frac{\rho_1\gamma}{\rho_3}, \quad \alpha_1 - \alpha_2 = \frac{D^2}{2} + \frac{\rho_3^2 H_z^2}{2\gamma}. \tag{177}$$

Energy: Corresponding to the mixed "pulse-kink lattice" solution [Eq. (161)] the energy and the constant C are given by

$$\hat{E} = \frac{2D}{3m}\big([(2-m)mA^2 + (1+m)B^2]E(m) - (1-m)(B^2 + 2A^2)K(m)\big), \tag{178}$$

$$C = \tfrac{1}{2}(1-m)A^2D^2 - F^2[\alpha_1 + 3\beta_1F^2 - 2H_z\rho_2F] + [-m\gamma F^2 + m\alpha_2 + \beta_2B^2]\frac{B^2}{m^2}. \tag{179}$$

For m near one, the energy of this periodic solution can be rewritten as the energy of the corresponding hyperbolic (dark-bright) soliton solution [Eq. (159)] plus the interaction energy. We find

$$\hat{E} = E_{\text{soliton}} + E_{\text{int}} = D\left[\frac{2}{3}(2B^2 + A^2) + \frac{(1-m)}{6}(2B^2 + 3A^2) - (1-m)A^2\ln\left(\frac{4}{\sqrt{1-m}}\right)\right]. \tag{180}$$

Note that this solution also exists only when either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \leqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \geqslant 4\beta_1\beta_2$. The interaction energy vanishes at $m=1$. It is amusing to note that the energy of solution IX is easily obtained from that of solution VII by simply interchanging A and B.

Summarizing, we have obtained nine periodic solutions in terms of Jacobi elliptic functions, in the case of a coupled ϕ^4 field theory with biquadratic coupling and an external magnetic field. This was possible because the magnetic field interaction is not symmetric between the two fields ϕ and ψ. In the special case when the modulus parameter m of the Jacobi elliptic function is one, these nine solutions reduce to four different soliton solutions valid on the full line and expressed in terms of hyperbolic functions. Note, however, that in case the external field $H_z=0$, instead of nine, we only obtain six distinct periodic solutions (of which three are previously known[20]), which in the limit $m=1$ give three distinct soliton solutions.

It is worth emphasizing the restrictions on the various parameters in the case of the nine solutions. For example, in the case of sn–sn solution (with $G=0$), $2\beta_1 \geqslant \gamma$, $2\beta_2 \geqslant \gamma$. Further, in the special case of $H_z=0=F=G$, one can show that $\alpha_1 < 0$, $\alpha_2 < 0$. On the other hand, in the case of cn–cn, dn–dn, cn–dn, and dn–cn solutions (with $G=0$), $\gamma < 0$ and further $\gamma^2 > 4\beta_1\beta_2$. In the special case of $H_z=0=F=G$, in addition one finds that (i) for the cn–cn case α_1, $\alpha_2 > (<) 0$ provided $m > (<) 1/2$, (ii) $\alpha_1 > 0$, $\alpha_2 > 0$ for the dn–dn solution, (iii) for the dn–cn solution, $\alpha_2 > 0$, (iv) $\alpha_1 < 0$ for the cn–dn solution. Instead, for the sn–cn as well as sn–dn solutions, either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \geqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \leqslant 4\beta_2\beta_4$. Finally, in the cn–sn and dn–sn

cases, either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \leqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $\gamma^2 \geqslant 4\beta_1\beta_2$. If in addition $H_z = 0 = F = G$, then for all four solutions (i.e., sn–cn, cn–sn, sn–dn, dn–sn), $\alpha_1 < 0$ and $\alpha_2 < 0$.

III. SOLUTIONS WITH BILINEAR COUPLING

Several years ago, a coupled ϕ^4 model was considered in the context of a surface phase transition with hydration forces[7] which is similar to the one considered in the last section except that there was no external magnetic field H_z and instead of a biquadratic coupling there was a bilinear coupling between the two fields. The purpose of this section is to obtain a bright-bright soliton solution of that model.

The potential (i.e., free energy) is given by

$$V = \alpha_1\phi^2 + \beta_1\phi^4 + \alpha_2\psi^2 + \beta_2\psi^4 + \delta_1(\phi - \psi)^2 + \delta_2(\phi + \psi)^2, \tag{181}$$

with δ_1, δ_2 being the coupling parameters between the two fields. The (static) equations of motion which follow from here are

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = 2\alpha_1\phi + 4\beta_1\phi^3 + 2\delta_1(\phi - \psi) + 2\delta_2(\phi + \psi), \tag{182}$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = 2\alpha_2\psi + 4\beta_2\psi^3 - 2\delta_1(\phi - \psi) + 2\delta_2(\phi + \psi). \tag{183}$$

It is not difficult to show that this pair of coupled field equations admits the "kink-kink" type periodic solution

$$\phi = A\,\mathrm{sn}[D(x + x_0), m], \quad \psi = B\,\mathrm{sn}[D(x + x_0), m], \tag{184}$$

provided

$$\begin{gathered} mD^2 = 2\beta_1A^2 = 2\beta_2B^2, \\ A^2 = \frac{-m}{(1+m)\beta_1}\left[\alpha_1 + \delta_1 + \delta_2 + (\delta_2 - \delta_1)\sqrt{\frac{\beta_1}{\beta_2}}\right], \end{gathered} \tag{185}$$

and furthermore the parameters $\alpha_1, \alpha_2, \beta_1, \beta_2, \delta_1, \delta_2$ satisfy the constraint

$$\alpha_2 - \alpha_1 = (\delta_1 - \delta_2)\left[\sqrt{\frac{\beta_2}{\beta_1}} - \sqrt{\frac{\beta_1}{\beta_2}}\right]. \tag{186}$$

Since $A^2 > 0$, the relation (185) gives us a strong constraint on some of the parameters. The energy $\hat{E}$ and the constant C corresponding to the periodic solution [Eq. (184)] are

$$\begin{gathered} \hat{E} = \frac{2(A^2 + B^2)D}{3m}[(1+m)E(m) - (1-m)K(m)], \\ C = -\tfrac{1}{2}(A^2 + B^2)D^2. \end{gathered} \tag{187}$$

In the limit $m = 1$, this solution reduces to the bright-bright soliton solution

$$\phi = A\tanh[D(x + x_0)], \quad \psi = B\tanh[D(x + x_0)], \tag{188}$$

provided

$$D^2 = 2\beta_1 A^2 = 2\beta_2 B^2,$$
$$A^2 = \frac{-1}{2\beta_1}\left[\alpha_1 + \delta_1 + \delta_2 + (\delta_2 - \delta_1)\sqrt{\frac{\beta_1}{\beta_2}}\right], \tag{189}$$

while relation (186) remains unchanged. For m near one, the energy of the periodic solution can be rewritten as the energy of the corresponding hyperbolic (bright-bright) soliton solution [Eq. (188)] plus the interaction energy. We find

$$\hat{E} = E_{\text{kink}} + E_{\text{int}} = (A^2 + B^2)D\left[\frac{4}{3} + \frac{(1-m)}{3}\right]. \tag{190}$$

The interaction energy vanishes at $m=1$. In view of the requirement $\beta_1, \beta_2 > 0$ arising from stability, we are unable to find any other solution to this coupled set of equations with a bilinear coupling.

IV. SOLUTIONS OF DISCRETE COUPLED ϕ^4-TYPE EQUATIONS WITH BIQUADRATIC COUPLING

Discrete coupled ϕ^4 models arise in the context of structural transitions on a lattice, collective proton dynamics in ice,[23] etc. The purpose of this section is to give an exhaustive list of solutions to the discrete coupled ϕ^4-type equations with biquadratic coupling (but in the absence of an external magnetic field H_z). In the next section, we shall obtain a solution of the discrete coupled ϕ^4-type equations with bilinear coupling.

We start from the coupled static field equations (2) and (3). The discrete analog of these field equations, for $H_z=0$, has the form

$$\frac{1}{h^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - 2\alpha_1\phi_n - 2[2\beta_1\phi_n^2 + \gamma\psi_n^2]\phi_n = 0, \tag{191}$$

$$\frac{1}{h^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - 2\alpha_2\psi_n - 2[2\beta_2\psi_n^2 + \gamma\phi_n^2]\psi_n = 0, \tag{192}$$

where h is the lattice spacing. We are unable to find any solution to this coupled set of field equations. However, as in the Ablowitz-Ladik discretization of the discrete nonlinear Schrödinger equation,[24] if we replace ϕ_n and ψ_n in the last term in Eqs. (191) and (192) by their average, then we can find exact solutions to this coupled system. In particular, instead of Eqs. (191) and (192), we consider the discretized equations

$$\frac{1}{h^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - 2\alpha_1\phi_n - [2\beta_1\phi_n^2 + \gamma\psi_n^2][\phi_{n+1} + \phi_{n-1}] = 0, \tag{193}$$

$$\frac{1}{h^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - 2\alpha_2\psi_n - [2\beta_2\psi_n^2 + \gamma\phi_n^2][\psi_{n+1} + \psi_{n-1}] = 0. \tag{194}$$

Note that single solitons and their stability in coupled Ablowitz-Ladik chains have been studied previously.[25] We now show that this modified set of coupled discrete equations has six different periodic solutions which in the limit $m=1$ reduce to the bright-bright, bright-dark, and dark-dark soliton solutions. In all the solutions, we shall see that the static kink can be placed anywhere with respect to the lattice. Hence we suspect that in all these cases, there may be an absence of the Peierls-Nabarro barrier,[26–28] which is the energy cost associated with moving a localized solution such as a soliton by a half lattice constant on a discrete lattice. It would be nice if one can demonstrate this explicitly.

A. Solution I

It is easy to show that the field Eqs. (193) and (194) admit the kink-kink type solution

$$\phi_n = A\,\mathrm{sn}[hD(n+x_0),m], \quad \psi_n = B\,\mathrm{sn}[hD(n+x_0),m], \tag{195}$$

provided

$$A^2 = \frac{m(2\beta_2-\gamma)\mathrm{sn}^2(hD,m)}{h^2(4\beta_1\beta_2-\gamma^2)}, \quad B^2 = \frac{m(2\beta_1-\gamma)\mathrm{sn}^2(hD,m)}{h^2(4\beta_1\beta_2-\gamma^2)},$$
$$\alpha_1 = \alpha_2 = -\frac{1}{h^2}[1-\mathrm{cn}(hD,m)\mathrm{dn}(hD,m)], \tag{196}$$

where h is the lattice spacing. Thus, note that as in the continuum case, this solution exists provided $2\beta_1>\gamma$, $2\beta_2>\gamma$, $\alpha_1<0$, $\alpha_2<0$. It is interesting to note that the solutions to both the discrete and the continuum model exist under the same set of conditions.

Continuum limit: It is instructive to consider the continuum limit $h\to 0$ and show that the above-noted solution smoothly goes over to the corresponding continuum solution. In particular, on using the fact that as $h\to 0$,

$$\mathrm{sn}(hD,m)\to hD, \quad \mathrm{cn}^2(hD,m)\to 1-h^2D^2, \quad \mathrm{dn}^2(hD,m)\to 1-mh^2D^2, \tag{197}$$

it readily follows that the above-noted solution indeed reduces to the corresponding continuum solution [Eq. (7)] obtained in Sec. II (when $H_z=F=G=0$), i.e.,

$$A^2 = \frac{m(2\beta_2-\gamma)D^2}{(4\beta_1\beta_2-\gamma^2)}, \quad B^2 = \frac{m(2\beta_1-\gamma)D^2}{(4\beta_1\beta_2-\gamma^2)}, \quad \alpha_1=\alpha_2=-\frac{(1+m)D^2}{2}. \tag{198}$$

In fact we shall see that all six solutions of this coupled discrete model smoothly go over to the corresponding continuum solutions obtained in Sec. II in the limit $h\to 0$.

In the limit $m=1$, the periodic solution (195) reduces to the bright-bright soliton solution

$$\phi_n = A\tanh[hD(n+x_0)], \quad \psi_n = B\tanh[hD(n+x_0)]. \tag{199}$$

Special case of $\gamma^2=4\beta_1\beta_2$: One can show that the solution (195) exists even in case $\gamma^2=4\beta_1\beta_2$. It turns out that such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{200}$$

and that in this case one cannot determine A,B. However, they must satisfy the constraint

$$A^2+B^2 = \frac{m\,\mathrm{sn}^2(hD,m)}{h^2\gamma}. \tag{201}$$

In the continuum limit $h\to 0$, as expected, this reduces to the constraint equation (25) obtained in Sec. II.

B. Solution II

It is easily shown that a kink-pulse type solution

$$\phi_n = A\,\mathrm{sn}[hD(n+x_0),m], \quad \psi_n = B\,\mathrm{cn}[hD(n+x_0),m], \tag{202}$$

is an exact solution to the field Eqs. (193) and (194) provided

$$A^2 = \frac{m(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2 - 4\beta_1\beta_2)}, \quad B^2 = \frac{m(2\beta_1 - \gamma)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2 - 4\beta_1\beta_2)}. \tag{203}$$

Furthermore,

$$-\alpha_1 = \frac{1}{h^2} + \frac{\mathrm{cn}(hD,m)[2m\beta_1(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m) - (\gamma^2 - 4\beta_1\beta_2)]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{dn}(hD,m)}, \tag{204}$$

$$-\alpha_2 = \frac{1}{h^2} + \frac{\mathrm{cn}(hD,m)[m\gamma(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m) - (\gamma^2 - 4\beta_1\beta_2)]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{dn}^2(hD,m)}. \tag{205}$$

Again, as in the continuum case either $2\beta_1 > \gamma > 2\beta_2$ and $\gamma^2 > 4\beta_1\beta_2$ or $2\beta_2 > \gamma > 2\beta_1$ and $4\beta_1\beta_2 > \gamma^2$. It is, however, not clear here if α_1 and α_2 have a definite sign. However, in the limit $m=1$, as in the continuum case, one finds that $\alpha_1 < 0$, $\alpha_2 < 0$.

It is readily checked that in the continuum limit this solution smoothly goes over to the corresponding continuum solution, Eqs. (104) and (112). Furthermore, the corresponding bright-dark solution is easily obtained in the limit $m=1$.

Special case of $\gamma^2 = 4\beta_1\beta_2$*:* One can show that the solution (202) exists even in case $\gamma^2 = 4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{206}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$A^2 - B^2\mathrm{dn}^2(hD,m) = \frac{m\,\mathrm{sn}^2(hD,m)}{h^2\gamma}. \tag{207}$$

In the continuum limit $h \to 0$, as expected, this reduces to the constraint equation (117) obtained in Sec. II.

C. Solution III

Yet another kink-pulse type solution is given by

$$\phi_n = A\,\mathrm{sn}[hD(n + x_0), m], \quad \psi_n = B\,\mathrm{dn}[hD(n + x_0), m], \tag{208}$$

provided

$$A^2 = \frac{m(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2 - 4\beta_1\beta_2)}, \quad B^2 = \frac{(2\beta_1 - \gamma)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2 - 4\beta_1\beta_2)}. \tag{209}$$

Furthermore,

$$-\alpha_1 = \frac{1}{h^2} + \frac{\mathrm{dn}(hD,m)[2\beta_1(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m) - (\gamma^2 - 4\beta_1\beta_2)]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{cn}(hD,m)}, \tag{210}$$

$$-\alpha_2 = \frac{1}{h^2} + \frac{\mathrm{dn}(hD,m)[\gamma(\gamma - 2\beta_2)\mathrm{sn}^2(hD,m) - (\gamma^2 - 4\beta_1\beta_2)]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{cn}^2(hD,m)}. \tag{211}$$

Special case of $\gamma^2 = 4\beta_1\beta_2$*:* One can show that the solution (208) exists even in case $\gamma^2 = 4\beta_1\beta_2$. It turns out such a solution exists only if

$$2\beta_1 = 2\beta_2 = \gamma, \tag{212}$$

and that in this case one cannot determine A, B. However, they must satisfy the constraint

$$A^2 - mB^2\,\mathrm{cn}^2(hD,m) = \frac{m\,\mathrm{sn}^2(hD,m)}{h^2\gamma}. \tag{213}$$

In the continuum limit $h\to 0$, as expected, this reduces to the constraint equation (137) obtained in Sec. II.

Note that in the $m=1$ limit the solutions II and III reduce to the same bright-dark soliton solution. In addition, as in the continuum case, this solution exists if either $2\beta_1 \geqslant \gamma \geqslant 2\beta_2$ and $\gamma^2 \geqslant 4\beta_1\beta_2$ or $2\beta_2 \geqslant \gamma \geqslant 2\beta_1$ and $4\beta_1\beta_2 \geqslant \gamma^2$. It is, however, not clear here if α_1 and α_2 have a definite sign. However, in the limit $m=1$, as in the continuum case, one finds that $\alpha_1<0$ and $\alpha_2<0$.

D. Solution IV

Finally, we present three periodic solutions, all of which in the limit $m=1$ reduce to the dark-dark soliton solution. One of the pulse-pulse type periodic solutions is given by

$$\phi_n = A\,\mathrm{cn}[hD(n+x_0),m], \quad \psi_n = B\,\mathrm{cn}[hD(n+x_0),m], \tag{214}$$

provided as in the continuum case, $\gamma<0$ and $\gamma^2>4\beta_1\beta_2$. We find

$$A^2 = \frac{2m(\beta_2+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-4\beta_1 4\beta_2)\mathrm{dn}^2(hD,m)}, \quad B^2 = \frac{2m(\beta_1+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-4\beta_1 4\beta_2)\mathrm{dn}^2(hD,m)},$$
$$\alpha_1 = \alpha_2 = -\frac{1}{h^2}\left[1-\frac{\mathrm{cn}(hD,m)}{\mathrm{dn}^2(hD,m)}\right]. \tag{215}$$

Using Eq. (197) it is easily shown that as in the continuum case, α_1, $\alpha_2>(<)\ 0$ provided $m>(<)\ 1/2$. This solution is equivalent to the continuum solution, Eqs. (33) and (42).

E. Solution V

Another pulse-pulse type solution is given by

$$\phi_n = A\,\mathrm{dn}[hD(n+x_0),m], \quad \psi_n = B\,\mathrm{dn}[hD(n+x_0),m], \tag{216}$$

provided as in the continuum case, $\gamma<0$ and $\gamma^2>4\beta_1\beta_2$. We find

$$A^2 = \frac{2(\beta_2+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-4\beta_1\beta_2)\mathrm{cn}^2(hD,m)}, \quad B^2 = \frac{2(\beta_1+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-\beta_1 4\beta_2)\mathrm{cn}^2(hD,m)},$$
$$\alpha_1 = \alpha_2 = -\frac{1}{h^2}\left[1-\frac{\mathrm{dn}(hD,m)}{\mathrm{cn}^2(hD,m)}\right]. \tag{217}$$

Using Eq. (197) it is easily shown that as in the continuum case, α_1, $\alpha_2>0$. This solution is equivalent to the continuum solution, Eqs. (53) and (62).

F. Solution VI

Yet another pulse-pulse type solution is

$$\phi_n = A\,\mathrm{dn}[hD(n+x_0),m], \quad \psi_n = B\,\mathrm{cn}[hD(n+x_0),m], \tag{218}$$

provided as in the continuum case, $\gamma<0$ and $\gamma^2>4\beta_1\beta_2$. We find

$$A^2 = \frac{(2\beta_2+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-4\beta_1\beta_2)\mathrm{cn}^2(hD,m)}, \quad B^2 = \frac{m(2\beta_1+|\gamma|)\mathrm{sn}^2(hD,m)}{h^2(\gamma^2-4\beta_1\beta_2)\mathrm{dn}^2(hD,m)}. \tag{219}$$

Furthermore,

$$-\alpha_1 = \frac{1}{h^2} + \frac{[2\beta_1(2\beta_2 + |\gamma|)\mathrm{dn}^2(hD,m) - \gamma(2\beta_1 + |\gamma|)\ \mathrm{cn}^2(hD,m))]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{dn}(hD,m)\mathrm{cn}^2(hD,m)}, \tag{220}$$

$$-\alpha_2 = \frac{1}{h^2} + \frac{[2\beta_2(2\beta_1 + |\gamma|)\mathrm{cn}^2(hD,m) - |\gamma|(|\gamma| + 2\beta_2)\mathrm{dn}^2(hD,m)]}{h^2(\gamma^2 - 4\beta_1\beta_2)\mathrm{dn}^2(hD,m)\mathrm{cn}(hD,m)}. \tag{221}$$

It is not clear if in general α_1 and α_2 have a definite sign. However, it is easily checked that at $m=1$, α_1, $\alpha_2 > 0$. This solution is equivalent to the continuum solution, Eqs. (72) and (80).

Note that the last three (i.e., IV, V, VI) solutions reduce to the (same) dark-dark soliton solution in the limit $m=1$. Since we do not know the Hamiltonian corresponding to Eqs. (193) and (194), we are unable to find the energy and soliton interaction explicitly for any of the above-noted discrete solutions. Similarly, for $H_z \neq 0$ we have not succeeded in finding exact solutions.

V. SOLUTIONS OF DISCRETE COUPLED ϕ^4-TYPE EQUATIONS WITH BILINEAR COUPLING

Coupled lattice chains, with a bilinear coupling, undergoing a second-order structural phase transition can represent this case. We start from the coupled static field Eqs. (182) and (183). The discrete analog of these field equations has the form

$$\frac{1}{h^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - 2[\alpha_1 + \delta_1 + \delta_2]\phi_n + 2[\delta_1 - \delta_2]\psi_n - 4\beta_1\phi_n^3 = 0, \tag{222}$$

$$\frac{1}{h^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - 2[\alpha_2 + \delta_1 + \delta_2]\psi_n + 2[\delta_1 - \delta_2]\phi_n - 4\beta_2\psi_n^3 = 0. \tag{223}$$

We are unable to find any solution to this coupled set of field equations. However, as in the Ablowitz-Ladik discretization of the discrete nonlinear Schrödinger equation,[24] if we replace ϕ_n and ψ_n in the last term in Eqs. (222) and (223) by their average, then we can find exact solutions to this coupled system. In particular, instead of Eqs. (222) and (223) we consider the discretized equations

$$\frac{1}{h^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - 2[\alpha_1 + \delta_1 + \delta_2]\phi_n + 2[\delta_1 - \delta_2]\psi_n - 2\beta_1\phi_n^2[\phi_{n+1} + \phi_{n-1}] = 0, \tag{224}$$

$$\frac{1}{h^2}(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - 2[\alpha_2 + \delta_1 + \delta_2]\psi_n + 2[\delta_1 - \delta_2]\phi_n - 2\beta_2\psi_n^2[\psi_{n+1} + \psi_{n-1}] = 0. \tag{225}$$

It is easy to show that the field Eqs. (224) and (225) admit the kink-kink type solution

$$\phi_n = A\ \mathrm{sn}[hD(n + x_0), m], \quad \psi_n = B\ \mathrm{sn}[hD(n + x_0), m], \tag{226}$$

provided

$$\frac{m\ \mathrm{sn}^2(hD,m)}{h^2} = 2\beta_1 A^2 = 2\beta_2 B^2,$$
$$A^2 = \frac{-m\ \mathrm{sn}^2(hD,m)}{2\beta_1[1 - \mathrm{cn}(hD,m)\mathrm{dn}(hD,m)]}\left[\alpha_1 + \delta_1 + \delta_2 + (\delta_2 - \delta_1)\sqrt{\frac{\beta_1}{\beta_2}}\right], \tag{227}$$

and furthermore the parameters α_1, α_2, β_1, β_2, δ_1, δ_2 satisfy the constraint

$$\alpha_2 - \alpha_1 = (\delta_1 - \delta_2)\left[\sqrt{\frac{\beta_2}{\beta_1}} - \sqrt{\frac{\beta_1}{\beta_2}}\right]. \tag{228}$$

As expected, in the continuum limit of $h \to 0$, this solution smoothly goes over to the corresponding continuum solution, Eqs. (184)–(186), obtained in Sec. III. Since we do not know the Hamiltonian corresponding to Eqs. (224) and (225), we are unable to find the energy and soliton interaction explicitly for this discrete solution. Similarly, for $H_z \neq 0$ we have not succeeded in finding an exact solution.

VI. CONCLUSION

We have systematically provided an exhaustive set of exact periodic domain wall solutions for a coupled ϕ^4 model with and without an external field, and for both bilinear and biquadratic couplings. Only a bright-bright solution could be obtained for the bilinear case. For both the biquadratic and bilinear couplings the corresponding discrete case was also considered—with an Ablowitz-Ladik like modification of the coupled discrete equations—and we obtained several exact solutions. For the solutions of the discrete model, the calculation of the Peierls-Nabarro barrier[26–28] and soliton scattering[29,30] remain topics of further study. Similarly, scattering of solitons in the coupled ϕ^4 continuum and discrete models with either the biquadratic or bilinear coupling is an interesting open issue. To this end, the static solutions presented here need to be boosted with a certain velocity.

It would be instructive to explore whether the nine different solutions reported in Sec. II (or the six solutions in Sec. IV) are completely disjoint or if there are any possible bifurcations linking them via, for instance, analytical continuation. We have not tried to carry out an explicit stability analysis of various periodic solutions. However, the energy calculations and interaction energy between solitons (for $m \sim 1$) in the case of both the biquadratic and bilinear couplings could provide useful insight in this direction.

Our results are relevant for spin configurations, domain walls, and magnetic phase transitions in multiferroic materials;[3,4] periodic domain walls are yet to be observed in the hexagonal multiferroics.[3] Similarly, our solutions are important for understanding structural phase transitions in ferroelectrics[5,6] and elastic materials,[8] biophysics problems such as multilamellar lipid systems,[7] as well as field theoretic contexts.[9,10] These ideas and exact solutions can be generalized to other coupled models such as ϕ^6 (for first-order phase transitions) and are discussed elsewhere.[31]

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Steady states of self-gravitating incompressible fluid in two dimensions

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In this paper we develop a simple model for the steady state of two-dimensional self-gravitating incompressible gas which is based on the hydrodynamic equations for stratified fluid. These equations are then reduced to a system of two equations for the mass density and the gravitational field. Analytical analysis and numerical solutions of these equations under different modeling assumptions (with special attention to the isothermal case) are then used to study the structure of the resulting steady state of the fluid. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The steady states of self-gravitating fluid in three dimensions have been studied by a long list of illustrious mathematical physicists. (For an extensive list of references see Refs. 1–3). The motivation for this research was due to the interest in the shape and stability of celestial bodies. We now know however that many celestial objects such as galaxies exhibit (effectively) "two dimensional structure."[4–7] Similarly, recent discoveries are leading us to believe that systems similar to our solar system are "abundant" in the galaxy and their existence might be due to the collapse of a two-dimensional primordial gas cloud under gravitation.[8–11] This background motivates us to investigate in this paper the steady states of self-gravitating fluid in two dimensions. This problem has been explored by a large number of investigators using analytic methods and computer simulations (see Refs. 8–10 for a complete list of references). What is missing however is a simple analytic model that is able to capture the basic physics of this process and leads to some insights about the "parameters" that govern its outcome.

In this paper we attempt to develop such a model using the basic hydrodynamic equations that govern the steady state flow of an incompressible, stratified (i.e., nonconstant density) fluid in two dimensions under gravity but with no magnetic field.[1–3] Under these assumptions we show that the number of basic equations can be reduced to a system of two coupled equations. One for the mass density and the second for the gravitational field. The only "parameter" in this these equations is a function that encodes the information about the momentum distribution in the interstellar cloud. We then consider radial solutions to these equations with special attention to the steady state of a gas cloud with isothermal equation of state.[10] We find that under proper choices of the parameter function there will exist out-of-core regions where the mass density peaks out locally. These regions might therefore represent the formation of out-of-core structures in the primordial gas cloud. (The region close to the "center" of the cloud where the density and velocities are expected to be large is usually referred to as the core region. Other regions in the cloud are referred to as out-of-core regions.)

We emphasize, however, that the model we develop here is a steady state one. Accordingly, it cannot address questions about the stability of the mass distribution pattern that is predicted by the model equations. It might be argued also that the assumptions of steady state and incompressibility

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are not realistic from an astrophysical point of view. However, our main goal in this paper is to capture analytically (as far as possible) the nonlinear aspects of the processes under consideration. Accordingly, our results might be useful to provide some analytic insights for more realistic work on this topic. Moreover, they provide a natural extension to the results on the equilibrium states of three-dimensional bodies under gravity.

The plan of the paper is as follows: In Sec. II we present the basic hydrodynamic equations and show how one can reduce them to a coupled system of two equations. We also discuss the conditions under which the two-dimensional approximation is justified. In Sec. III we derive the pressure equation for the fluid under consideration with particular emphasis on isothermal conditions. In Sec. IV we discuss radial solutions to these equations and present the results of some simulations under these assumptions. We end up in Sec. V with a summary and conclusions.

II. DERIVATION OF THE MODEL EQUATIONS

Following the standard convention,[1,12–14] we model the steady state flow of an incompressible fluid in two dimensions (x,y) by the hydrodynamic equations of inviscid and incompressible stratified fluid

$$u_x + v_y = 0, \tag{2.1}$$

$$u\rho_x + v\rho_y = 0, \tag{2.2}$$

$$\rho(uu_x + vu_y) = -p_x - \rho\phi_x, \tag{2.3}$$

$$\rho(uv_x + vv_y) = -p_y - \rho\phi_y, \tag{2.4}$$

$$\nabla^2\phi = 4\pi G\rho, \tag{2.5}$$

where subscripts indicate differentiation with respect to the indicated variable, $\mathbf{u}=(u,v)$ is the fluid velocity, ρ is its density, p is the pressure, ϕ is the gravitational field, and G is the gravitational constant.

We can nondimensionalize these equations by introducing the following scalings:

$$x = L\tilde{x}, \quad y = L\tilde{y}, \quad u = U_0\tilde{u}, \quad v = U_0\tilde{u}, \quad \rho = \rho_0\tilde{\rho}, \quad p = \rho_0 U_0^2\tilde{p}, \quad \phi = U_0^2\tilde{\phi}, \tag{2.6}$$

where L, U_0, ρ_0 are some characteristic length, velocity, and mass density, respectively, that characterize the problem at hand. Substituting these scalings in Eqs. (2.1)–(2.5) and dropping the tildes, these equations remain unchanged (but the quantities that appear in these equations become nondimensional) while G is replaced by $\tilde{G}=G\rho_0 L^2/U_0^2$. (Once again we drop the tilde.)

At this point, we observe that in relativistic physics there is a natural velocity (viz. c-the speed of light) by which one scales the velocities. In the nonrelativistic approach (which we are adopting here) there is no such speed and accordingly U_0 is a "charateristic speed" which one chooses to nondimensionalize the velocities. From a practical (astrophysical) point of view $1 \leqslant U_0 \leqslant 100$ m/s in most typical cases.[3,8] In any case, all quantities (including velocities) in this paper are nondimensional.

Equations (2.1)–(2.5) form a two-dimensional approximation to the three-dimensional analog of these equations (which requires an additional equation for the flow in the z-direction which is similar to Eq. (2.3)). To justify this approximation in our context we assume in the following that we are considering matter distribution whose spatial extension (with characteristic length L) in the x,y directions is much larger than that in z direction (with characteristic "height" H). That is $H/L=O(\epsilon)$ where $0 \leqslant \epsilon \ll 1$. Furthermore we assume that

$$\frac{\partial \rho}{\partial x} = O(1), \quad \frac{\partial \rho}{\partial y} = O(1), \quad \frac{\partial \rho}{\partial z} = O(\epsilon). \tag{2.7}$$

Under these assumptions, the three-dimensional analog of Eq. (2.5) can be approximated by

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = 4\pi G\left[\rho(x,y,0) + z\frac{\partial \rho(x,y,0)}{\partial z}\right]. \tag{2.8}$$

Under the scaling introduced by Eq. (2.6) (with $z=L\bar{z}$) we then have

$$\bar{z}\frac{\partial \rho(x,y,0)}{\partial \bar{z}} = O(\epsilon^2) \tag{2.9}$$

while the other terms in Eq. (2.8) are of order $O(1)$. It follows then that we can approximate this equation by its two-dimensional analog

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 4\pi G\rho(x,y,0). \tag{2.10}$$

The justification for the two-dimensional approximation to the other equations follows along similar lines and has been discussed by many authors. (A lucid treatment is given in Ref. 12, pp. 1–12).

In view of Eq. (2.1), we can introduce a stream function ψ so that

$$u = \psi_y, \quad v = -\psi_x. \tag{2.11}$$

Using this stream function we can rewrite Eq. (2.2) as[13,15]

$$J\{\rho, \psi\} = 0, \tag{2.12}$$

where for any two (smooth) functions f, g,

$$J\{f,g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial y} - \frac{\partial f}{\partial y}\frac{\partial g}{\partial x}. \tag{2.13}$$

Equation (2.12) implies that the functions ρ, ψ are dependent on each other and we can express each of them in terms of the other. Thus we can write ψ as $\psi(\rho)$ or ρ as $\rho(\psi)$.

Using ψ the momentum equations (2.3) and (2.4) become

$$\rho(\psi_y\psi_{yx} - \psi_x\psi_{yy}) = -p_x - \rho\phi_x, \tag{2.14}$$

$$\rho(-\psi_y\psi_{xx} + \psi_x\psi_{xy}) = -p_y - \rho\phi_y. \tag{2.15}$$

To eliminate p from these equations we differentiate Eqs. (2.14) and (2.15) with respect to y, x, respectively, and subtract. This leads to

$$\rho_y(\psi_y\psi_{yx} - \psi_x\psi_{yy}) + \rho(\psi_y\psi_{yx} - \psi_x\psi_{yy})_y - \rho_x(-\psi_y\psi_{xx} + \psi_x\psi_{xy}) - \rho(-\psi_y\psi_{xx} + \psi_x\psi_{xy})_x = -J\{\phi,\rho\}. \tag{2.16}$$

Using Eq. (2.12), we can rewrite this equation (after some algebra) as

$$\rho J\{\nabla^2\psi, \psi\} + J\left\{\tfrac{1}{2}(\psi_x^2 + \psi_y^2), \rho\right\} = -J\{\phi,\rho\}. \tag{2.17}$$

However, in view of Eq. (2.12) $\psi=\psi(\rho)$ and this fact can be used to eliminate ψ from Eq. (2.17). To this end we observe that

$$\psi_x = \psi_\rho \rho_x, \quad \psi_y = \psi_\rho \rho_y, \quad \nabla^2 \psi = \psi_{\rho\rho}[\rho_x^2 + \rho_y^2] + \psi_\rho \nabla^2 \rho \tag{2.18}$$

and note that for any function of $F(\rho)$ we have $J\{F(\rho), \rho\} = 0$. This leads after long algebra to the following relation:

$$J\left\{(\rho\psi_\rho^2)\nabla^2\rho + \tfrac{1}{2}(\rho\psi_\rho^2)_\rho[\rho_x^2 + \rho_y^2] + \phi, \rho\right\} = 0. \tag{2.19}$$

Hence, we infer that

$$h(\rho)\nabla^2\rho + \frac{1}{2}h'(\rho)[\rho_x^2 + \rho_y^2] + \phi = S(\rho), \quad h' = \frac{\mathrm{d}h(\rho)}{\mathrm{d}\rho}, \tag{2.20}$$

where

$$h(\rho) = \rho\psi_\rho^2 \tag{2.21}$$

and $S(\rho)$ is some function of ρ.

The function $h(\rho)$ can be considered as a parameter function which is determined by the momentum (and angular momentum) distribution in the fluid. From a practical point of view the choice of this function determines the structure of the steady state density distribution. The corresponding flow field can be computed then *a posteriori* (that is after solving for ρ) from the following relations:

$$u = \sqrt{\frac{h(\rho)}{\rho}}\frac{\partial\rho}{\partial y}, \quad v = -\sqrt{\frac{h(\rho)}{\rho}}\frac{\partial\rho}{\partial x}. \tag{2.22}$$

The function $S(\rho)$ that appears in Eq. (2.20) can be determined from the asymptotic values of ρ and ϕ on the boundaries of the domain on which Eqs. (2.5) and (2.20) are solved. When these asymptotic values are imposed or known one can evaluate the left-hand side of Eq. (2.20) on the domain boundaries and re-express it in terms of ρ only to determine $S(\rho)$ (on the boundary of the domain). However, the resulting functional relationship of S on ρ must then hold also within the domain itself since S does not depend on x, y directly. For example assume that on an infinite domain we let $h(\rho) = 1$ and

$$\lim_{r\to\infty} \rho(x,y) = e^{-r}, \quad \lim_{r\to\infty} \phi(x,y) = 1/r \tag{2.23}$$

(where $r^2 = x^2 + y^2$). Under these assumptions, the left-hand side of Eq. (2.20) evaluates asymptotically to $e^{-r}(1 - 1/r) + 1/r$. Rewriting this expression in terms of ρ, we obtain

$$S(\rho) = \rho + \frac{(\rho - 1)}{\ln\rho}. \tag{2.24}$$

When such asymptotic relations are not given, $S(\rho)$ can be viewed as a "gauge." In the following, we let $S(\rho) = 0$ under these circumstances.

We observe that Eq. (2.20) can be rewritten in the form

$$h(\rho)^{1/2}\,\nabla\cdot(h(\rho)^{1/2}\,\nabla\rho) + \phi = S(\rho). \tag{2.25}$$

Using this equation, we can eliminate ϕ from Eqs. (2.25) and (2.5) to obtain one fourth-order equation for ρ,

$$\nabla^2(h(\rho)^{1/2}\,\nabla\cdot(h(\rho)^{1/2}\,\nabla\rho)) + 4\pi G\rho = \nabla^2 S(\rho). \tag{2.26}$$

Equation (2.20) can be simplified considerably by introducing a new dependent variable

$$\eta(\rho) = \int^{\rho} h^{1/2}(s)\mathrm{d}s. \tag{2.27}$$

With this new variable, Eq. (2.20) transforms into

$$\nabla^2\eta + h^{-1/2}(\rho)(\phi - S(\rho)\ = 0, \tag{2.28}$$

where $h(\rho)$ and $S(\rho)$ have to be expressed in terms of η. (We assume implicitly that the transformation given by Eq. (2.27) is invertible).

Thus, we reduced the original nonlinear system of partial differential equations (2.1)–(2.5) to a coupled system of two equations consisting of Eqs. (2.5) and (2.28).

III. EQUATION FOR THE PRESSURE

In order to derive Eq. (2.20) we eliminated the pressure from Eqs. (2.14) and (2.15). However, in some practical astrophysical applications it is important to know the equation of state of the fluid under consideration. For this reason, we derive here an equation analogous to Eq. (2.20) for the pressure. To this end, we divide Eqs. (2.14) and (2.15) by ρ, differentiate the first with respect to y, the second with respect to x, and subtract. This leads to

$$\rho^2 J\{\nabla^2\psi, \psi\} = J\{p, \rho\}. \tag{3.1}$$

Eliminating ψ from this equation (using Eq. (2.18)) yields

$$J\{\rho^2\psi_\rho^2\nabla^2\rho + \rho^2\psi_\rho\psi_{\rho\rho}(\rho_x^2 + \rho_y^2) - p, \rho\} = 0. \tag{3.2}$$

Hence,

$$\rho\psi_\rho^2\nabla^2\rho + \rho\psi_\rho\psi_{\rho\rho}(\rho_x^2 + \rho_y^2) - \frac{p}{\rho} = R(\rho), \tag{3.3}$$

where $R(\rho)$ is some function of ρ. Re-expressing this equation using $h(\rho)$ we have

$$h(\rho)\nabla^2\rho + \frac{1}{2}[h'(\rho) - \psi_\rho^2](\rho_x^2 + \rho_y^2) - \frac{p}{\rho} = R(\rho). \tag{3.4}$$

Subtracting this equation from Eq. (2.20) we then have

$$\frac{p}{\rho} = S(\rho) - R(\rho) - \frac{1}{2}\psi_\rho^2(\rho_x^2 + \rho_y^2) - \phi. \tag{3.5}$$

Therefore, the solution of Eqs. (2.20) and (2.5) determines the pressure distribution in the fluid (assuming that the functions R, S have been determined from the boundary conditions).

Conversely, if the pressure distribution is known *a priori*, e.g., if we assume that the fluid is an isothermal gas where $p = c^2\rho$ (c is the isothermal sound speed which is a constant for this medium) then Eq. (3.5) can be used to eliminate ϕ from Eq. (2.5),

$$\nabla^2(R) = \nabla^2\left[S - \tfrac{1}{2}\psi_\rho^2(\rho_x^2 + \rho_y^2)\right] - 4\pi G\rho. \tag{3.6}$$

It follows then that for an isothermal gas Eqs. (3.3) and (3.6) form a closed system of coupled equations for ρ and R with a parameter function ψ_ρ^2. However, if we eliminate R from these two equations we recover Eq. (2.26).

IV. SOLUTIONS OF Eq. (2.26)

Equation (2.26) is, in general, a nonlinear equation which (to our best knowledge) cannot be solved analytically. The only exception is the case where $h=1$ under which the resulting equation is linear. (In the following we let $S(\rho)=0$.) For this choice of h, $\nabla\psi = (1/\sqrt{\rho})\nabla\rho$. That is with the

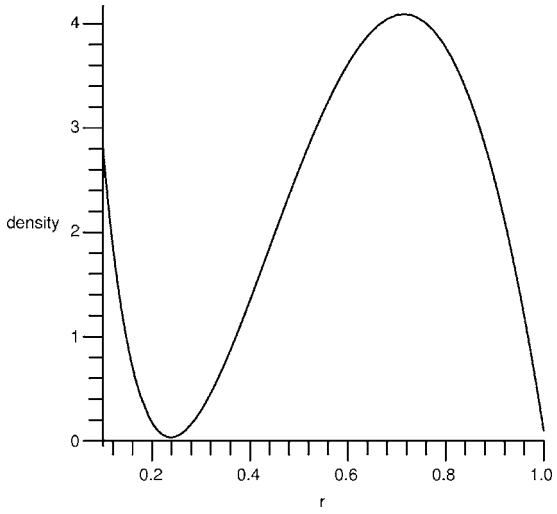

FIG. 1. Radial (analytic) solution of Eq. (2.26) with $h(\rho)=1$ subject to the conditions given by Eq. (4.3).

same gradient of ρ the gradient of ψ will increase as ρ decreases. We conclude then that, in general, matter in regions with low density might have higher momentum than in regions of higher density.

Under the constraint $h=1$ the general solution of Eq. (2.26) can be written in the form

$$\rho = f_0(r) + \sum_{m=1}^{\infty} f_m(r)(E_m \cos m\theta + F_m \sin m\theta), \tag{4.1}$$

where the real form of the solution for $f_m(r)$ is given by

$$f_m(r) = A_m[I_m(\beta R) + I_m(\bar{\beta} R)] + iB_m[I_m(\beta R) - I_m(\bar{\beta} R)] + C_m[K_m(\beta R) + K_m(\bar{\beta} R)] + iD_m[K_m(\beta R) - K_m(\bar{\beta} R)],$$

$$m = 0, 1, 2, \ldots . \tag{4.2}$$

Here $\beta=(\sqrt{2}/2)(-1+i)$, I_m, K_m are the modified Bessel functions of the first and second kinds, overbars denote complex conjugation and $R=(4\pi G)^{1/4}r$. (A_m, B_m, C_m, D_m are arbitrary real constants). However, since K_m have a singularity at the origin we must let $C_m=D_m=0$ if the origin is included in the domain. The remaining arbitary constants that appear in the solution must be adjusted to the boundary conditions one wishes to impose on ρ, ϕ (and subject to the physical requirement that $\rho \geqslant 0$ in the domain under consideration). Obviously various patterns can be obtained for ρ by a proper combination of these functions.

Figure 1 represents the solution given by Eq. (4.2) for $\rho=\rho(r)$, with $h(\rho)=1$ for $r\epsilon[0.1, 1]$ subject to the conditions

$$\rho(0.1) = 2.8, \quad \rho(0.5) = 2.6, \quad \rho(0.9) = 2.5, \quad \rho(1) = 0.1. \tag{4.3}$$

This solution exhibits clearly out-of-core region where the density is larger than its surroundings. It demonstrates also the existence of a region in which matter density is almost zero. This is in line with recent findings from simulations about planet formation in rings.[11] We observe that the parameters for this solution were chosen to accentuate the existence of a region in which the density is almost zero thus creating a "gap" between the core and the out-of-core region.

In polar coordinates the flow field is related to the stream function by the relations

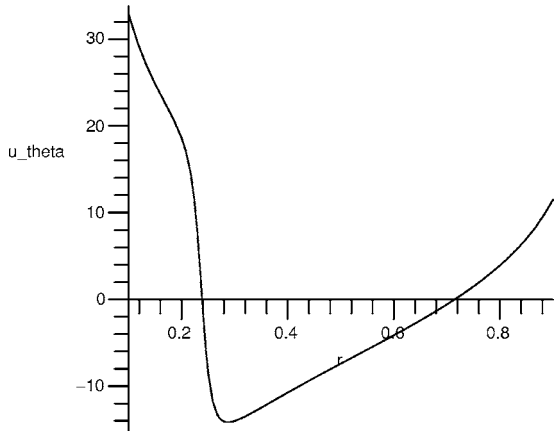

FIG. 2. u_θ as a function of r for solution presented in Fig. 1.

$$u_r = \frac{1}{r}\frac{\partial \psi}{\partial \theta}, \quad u_\theta = -\frac{\partial \psi}{\partial r}. \tag{4.4}$$

Since $\rho = \rho(r)$ it follows that $u_r = 0$ and

$$u_\theta = -\sqrt{\frac{h(\rho)}{\rho}}\frac{\partial \rho}{\partial r}. \tag{4.5}$$

Observe that u_θ is a nondimensional number. To obtain the actual "dimensional" velocities one has to multiply u_θ by U_0.

Figure 2 presents a plot of u_θ vs r for this case. From this figure we see that matter in the 2-d disk can be divided into three "rings." In the first ring where $0.1 \leqslant r \leqslant 0.24$ matter circulates counterclockwise. This is followed by a very narrow region where the u_θ is changing rapidly. (Observe that the density in this region is almost zero.) In the second ring where $0.24 \leqslant r \leqslant 0.72$ the circulation is clockwise. Finally for $0.72 \leqslant r \leqslant 1$ the circulation is counterclockwise again. (However, we have here a "smooth" transition between the second and third rings.)

For other choices of the function $h(\rho)$ one has to resort to numerical integration of Eq. (2.26). This was carried out in two cases for which $\rho = \rho(r)$. In the first case we let $h(\rho) = \rho^\alpha$ with $\alpha = -1, -0.5, 0, 0.5, 1$. In the second case, we choose $h(\rho) = \rho[1 + A \sin(n\pi\rho)]$ with $n = 2$ and $A = \pm 0.5, 0$.

The solutions to Eq. (2.26) for these two cases on the interval $r \epsilon [0.1, 1]$ with the boundary conditions

$$\rho(0.1) = 1, \quad \rho'(0) = 0, \quad \rho(1) = 0.1(0.2), \quad \rho'(1) = 0 \tag{4.6}$$

are presented in Figs. 3 and 4, respectively. The corresponding flow fields for these density profiles are presented in Figs. 5 and 6. These profiles and flow fields are physically "reasonable" in the sense that they contain no singularities and the circulation is unidirectional.

V. SUMMARY AND CONCLUSIONS

As a first task in this paper, we showed how to reduce the governing equations for the steady state of an incompressible stratified (two-dimensional) fluid under gravity (which comprise a set of five coupled nonlinear partial differential equations) to two equations. The resulting equations contain only one parameter function $h(\rho)$. We also derived a separate equation for the pressure in order to investigate the equation of state of the fluid under consideration. We then explored both analytically and numerically radial solutions to these equations with different choices of $h(\rho)$.

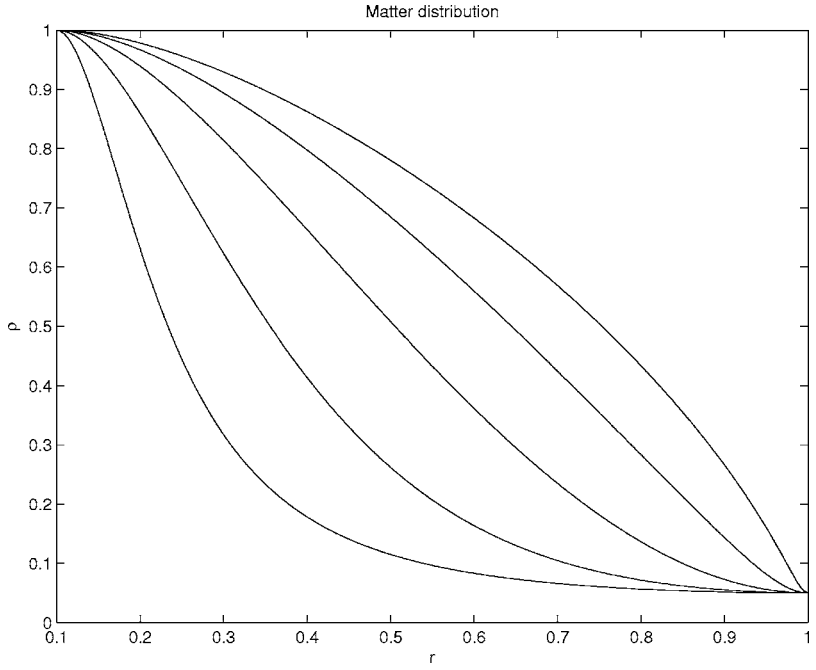

FIG. 3. Numerical solution of Eq. (2.26) with $h(\rho)=\rho^{\alpha}$ and $\alpha=-1,-0.5,0,0.5,1$. The lowest curve corresponds to $\alpha=-1$. The other curves correspond in progression to the other values of α.

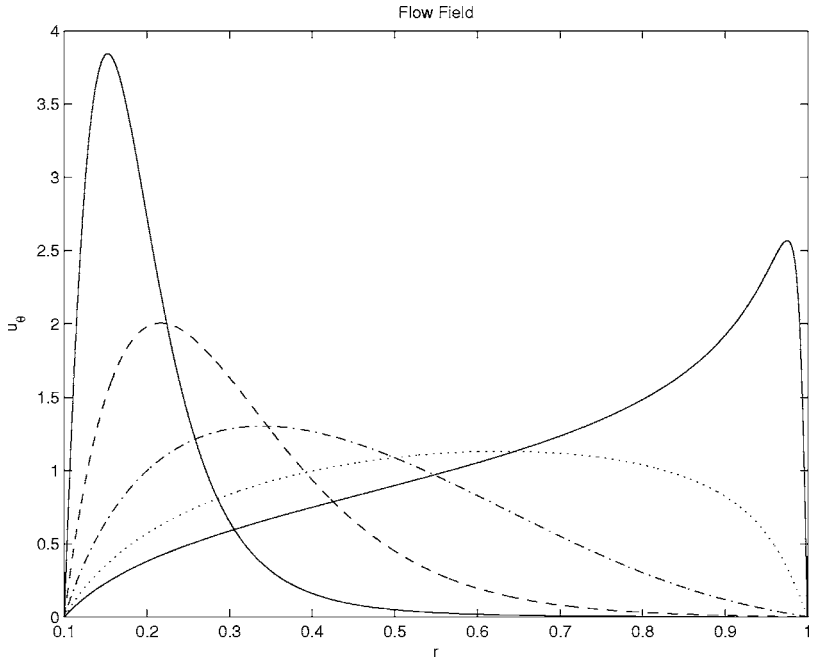

FIG. 4. u_θ as a function of r for the solutions presented in Fig. 3. The dashed, dash-dot and the dot-dot curves represent respectively u_θ for $\alpha=-0.5,0,0.5$. The solid line with a peak near the origin corresponds to $\alpha=-1$ while the other solid line corresponds to $\alpha=1$.

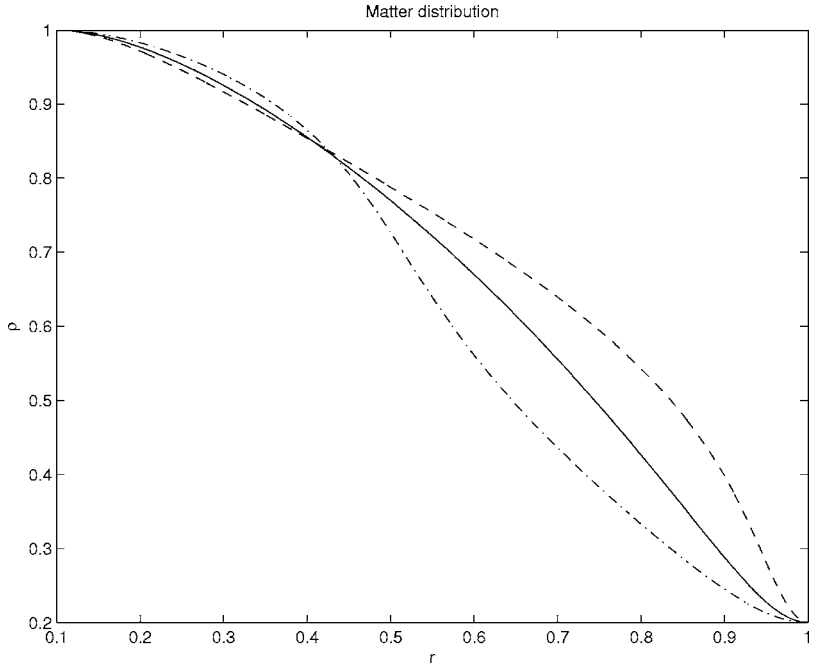

FIG. 5. Numerical solution of Eq. (2.26) with $h(\rho)=\rho(1+A\sin(n\pi\rho))$ with $n=2$. The dashed curve corresponds to $A=0.5$. The dash-dot curve corresponds to $A=-0.5$ and the solid one to $A=0$.

These solutions show that different choices of the parameter function $h(\rho)$ can lead to density profiles which contain out-of-core bands of matter whose density is higher than that of their surroundings. This is suggestive of the early stages of structure formation in these gas clouds. However this result might be sensitive to the choice of the function $h(\rho)$.

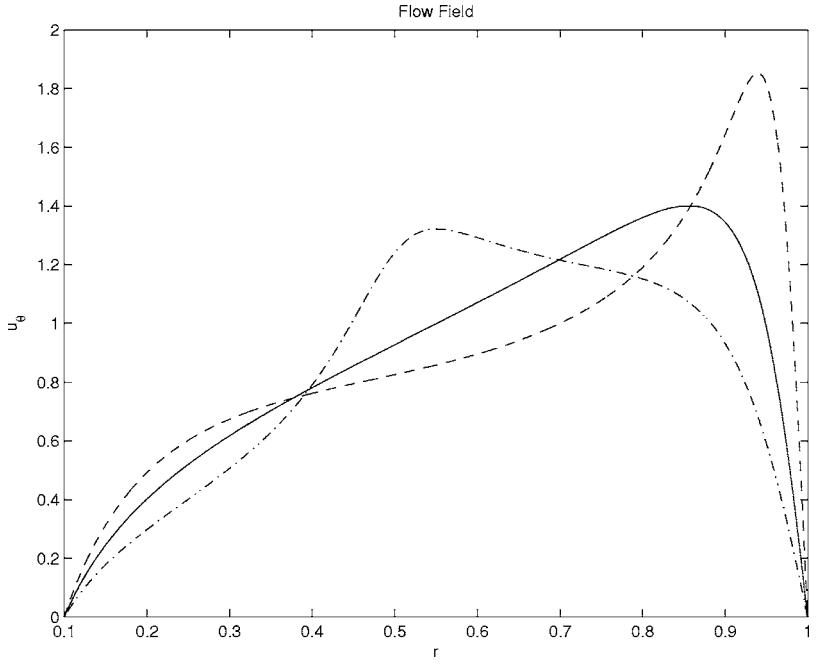

FIG. 6. u_θ as a function of r for the solutions presented in Fig. 5. The lines legend is the same as in Fig. 5.

A problem that our results raise but leave open is the determination of the general conditions on $h(\rho)$ which lead to a solution for ρ which is non-negative and oscillatory.

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Stokes flow in ellipsoidal geometry

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Particle-in-cell models for Stokes flow through a relatively homogeneous swarm of particles are of substantial practical interest, because they provide a relatively simple platform for the analytical or semianalytical solution of heat and mass transport problems. Despite the fact that many practical applications involve relatively small particles (inorganic, organic, biological) with axisymmetric shapes, the general consideration consists of rigid particles of arbitrary shape. The present work is concerned with some interesting aspects of the theoretical analysis of creeping flow in ellipsoidal, hence nonaxisymmetric domains. More specifically, the low Reynolds number flow of a swarm of ellipsoidal particles in an otherwise quiescent Newtonian fluid, that move with constant uniform velocity in an arbitrary direction and rotate with an arbitrary constant angular velocity, is analyzed with an ellipsoid-in-cell model. The solid internal ellipsoid represents a particle of the swarm. The external ellipsoid contains the ellipsoidal particle and the amount of fluid required to match the fluid volume fraction of the swarm. The nonslip flow condition on the surface of the solid ellipsoid is supplemented by the boundary conditions on the external ellipsoidal surface which are similar to those of the sphere-in-cell model of Happel (self-sufficient in mechanical energy). This model requires zero normal velocity component and shear stress. The boundary value problem is solved with the aim of the potential representation theory. In particular, the Papkovich–Neuber complete differential representation of Stokes flow, valid for nonaxisymmetric geometries, is considered here, which provides the velocity and total pressure fields in terms of harmonic ellipsoidal eigenfunctions. The flexibility of the particular representation is demonstrated by imposing some conditions, which made the calculations possible. It turns out that the velocity of first degree, which represents the leading term of the series, is sufficient for most engineering applications, so long as the aspect ratios of the ellipsoids remains within moderate bounds. Analytical expressions for the leading terms of the velocity, the total pressure, the angular velocity, and the stress tensor fields are obtained. Corresponding results for the prolate and the oblate spheroid, the needle and the disk, as well as for the sphere are recovered as degenerate cases. Novel relations concerning the ellipsoidal harmonics are included in the Appendix. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2345474]

I. INTRODUCTION

The behavior of systems involving the motion of aggregates of small particles relative to viscous fluids, in which they are immersed, covers a wide range of heat and mass transfer phe-

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nomena of great importance in practical applications. In order to construct tractable mathematical models of the flow systems involving particles, it is necessary to resort to a number of simplifications. A dimensionless criterion, which determines the relative importance of inertial and viscous effects, is the Reynolds number.[1] The steady and creeping flow (low Reynolds number) of an incompressible, viscous fluid is described by the well-known Stokes equations which have been known for over one and a half centuries (1851) and connect the biharmonic vector velocity with the harmonic scalar pressure field.[1] For many interior and exterior flow problems involving small particles, spherical and spheroidal (either prolate or oblate) geometry[2] provides a very good approximation for many important applications where the flow is considered to be axisymmetric. Nevertheless, more realistic models include particles of arbitrary shape where it is impossible to take advantage of the symmetry and the orientation of the particle must be taken into account. Ellipsoidal geometry[2] provides the most widely used framework for representing small particles of arbitrary shape embedded within a fluid that flows according to Stokes law. This nonaxisymmetric flow is governed by the genuine three-dimensional (3D) ellipsoidal geometry.

The introduction of a stream function[1] serves to unify the method on all two-dimensional incompressible fluid motions, as we shall see in the historical comments that follow. For these situations, the solutions of the equations of motion are reduced to the search for a single scalar function. Unfortunately, in the general case of three-dimensional motions this unified method of approach is not possible. Of course, it should be noted here that fully 3D flow could also be represented by a *pair* of stream functions, in which case the streamlines are the intersections of the two families that correspond to the two stream functions. However, this causes a number of difficulties and the appearance of certain indeterminacies in the solution of physical problems forces us to look for more general approaches. In order to avoid such problems the introduction of three-dimensional representations[3] of the flow fields is necessary. This is probably due to the fact that these representations use more than one potential to represent the physical fields, allowing for more flexibility. Papkovich (1932) and Neuber (1934) proposed a differential representation of the flow fields in terms of harmonic functions.[3,4] Their representation holds true also for nonaxisymmetric problems and is derivable from the well-known Naghdi–Hsu solution.[5] Since the last one is proved to be complete,[3] the Papkovich–Neuber differential representation also forms a complete solution of Stokes equations.

One of the important areas of applications concern the construction of particle-in-cell models which are useful in the development of simple but reliable analytical expressions for heat and mass transfer in swarms of particles in the case of concentrated suspensions. In applied type analysis it is not usually necessary to have detailed solution of the flow field over the entire swarm of particles taking into account the exact positions of the particles, since such solutions are cumbersome to use. Thus, the technique of cell models is adopted where the mathematical treatment of each problem is based on the assumption that a three-dimensional assemblage may be considered to consist of a number of identical unit cells. Each of these cells contains a particle surrounded by a fluid envelope, containing a volume of fluid sufficient to make the fractional void volume in the cell identical to that in the entire assemblage.

Of course, a good approximation of the solution of flow through a swarm of particles is also possible with the help of powerful numerical methods, notably Stokesian dynamics[6] or lattice—Boltzmann simulation.[7] In addition, Refs. 8 and 9 provide an excellent exposure of numerical approaches for the solution of physical problems concerning ellipsoidal particles. However, these methods involve the use of elaborate computer codes for each case. There is always room and need for analytical methods, which capture the essential features of the transport process under consideration in an analytic formula. It is to this end that particle-in-cell flow models serve as platforms both for theoretical investigation and for checking the reliability of complicated numerical codes.

Uchida[10] proposed a cell model where a spherical particle is surrounded by a fluid envelope with cubic outer boundary. The cubic shape offers the advantage that it is space filling but the nature of the boundaries leads to a three-dimensional flow problem.

Happel[11] and Kuwabara[12] proposed cell models in which both the particle and the outer

envelope are spherical, having the significant advantage of preserving the axial symmetry of the flow and of providing a simple analytical solution in closed form. On the other hand, their models have the disadvantage that the outer envelope is not space filling, a difficulty that must be dealt with, when one tries to pass from the single unit cell to the assemblage of particles. The Happel and the Kuwabara formulations are slightly different in the sense that the Happel model assumes that the inner sphere moves with a constant velocity along the axis within a quiescent fluid, while the Kuwabara model assumes that the inner sphere is stationary and that the fluid passes through the unit cell with a constant velocity. Under the assumption of pseudosteady state, this difference effects the boundary conditions of each formulation. Hence, for the Happel model a nonslip flow condition in the inner sphere is imposed, and zero radial velocity and shear stress on the outer envelope. On the other hand, for the Kuwabara formulation the radial and the tangential velocity are assumed to be equal to zero on the inner sphere, while there exists a velocity with axial component equal to a constant approach velocity on the outer envelope. In addition, zero vorticity on the outer envelope is assumed. Despite the fact that both formulations give essentially the same velocity fields, with the appropriate change of frame of reference, it is the Happel model that is slightly superior. This is due to the fact that it does not require an exchange of mechanical energy between the cell and the environment. On the contrary, the Kuwabara model permits a small but significant exchange of mechanical energy with the environment.

Neale and Nader[13] improved the formulation of Happel and Kuwabara by considering that the unit cell under consideration is embedded in an unbounded, continuous, homogeneous, and isotropic permeable medium, which has the same permeability with that of the swarm of spheres. The Happel and the Kuwabara models also provide good agreement, but somewhat inferior to the Neale and Nader model.

Epstein and Masliyah[14] proposed a useful generalization by considering a spheroid-in-cell, instead of a sphere-in-cell, model for swarms of spheroidal particles. However, they had to solve the creeping flow problem numerically since the well-known equation of motion $E^4\psi=0$ (ψ: Stokes stream function) in spheroidal coordinates is not separable. This difficulty of nonseparation was resolved recently by Dassios *et al.*[15] with the use of semiseparation of solutions, which is based on an appropriate finite dimensional spectral decomposition of the operator E^4. This way an analytical solution for the Kuwabara model was obtained. Using this method, Dassios *et al.*[16] solved the Happel model in spheroidal coordinates analytically and the results were compared with those obtained by using the Kuwabara-type boundary conditions. Moreover, the problem of space filling, when we refer to the assemblage of particles as well as to the relation between the approach velocity and the mean interstitial velocity through the swarm, was discussed in detail in Ref. 16.

An indeterminacy appears when the Happel-type or the Kuwabara-type spheroidal models are solved in terms of the Stokes stream function. This indeterminacy does *not* appear in the case of a perfect sphere. The indeterminacy can be overcome through the imposition of an additional geometrical condition that secures the correct reduction to the perturbed-sphere case.[15,16] However, the introduction of the Papkovich–Neuber differential representation,[3,4] as we already mentioned, seems to offer certain advantages in solving such problems. More specific, despite the fact that a similar indeterminacy appears when the Papkovich–Neuber differential representation is used and it is handled in the same way, the degrees of freedom, which this representation offers,[17] make the Papkovich–Neuber solution a powerful tool. This representation was demonstrated recently by Dassios and Vafeas,[18] where the Kuwabara model is solved analytically in spheroidal domains and a comparison with the already solved flow problem with Kuwabara-type boundary conditions was made. The major advantage of the utilization of the Papkovich–Neuber differential representation is that it can be used to obtain solutions of creeping flow in cell models where the shape of the particles is genuine three-dimensional. Dassios and Vafeas[19] have demonstrated the practical efficiency of the above 3D representation by solving the three-dimensional Stokes flow problem in an assemblage of spherical particles, which translate and rotate, using Happel-type boundary conditions. The loss of symmetry is caused by the imposed rotation of the particles. The full solution is obtained in a closed form. The present work concerns the next step of our inves-

tigation where the sphere, that represents the isotropy, is replaced by a triaxial ellipsoid, which carries the complete anisotropy of the three-dimensional space.

The solution to the Stokes flow problem in an ellipsoid-in-cell with Happel-type boundary conditions is obtained here with the aim of the Papkovich–Neuber representation. The incentive for this is that the Happel-type boundary conditions are more compatible with the physics of the flow in a swarm, since they ensure that each unit cell is self-sufficient in mechanical energy. Under the assumption of very small Reynolds number and pseudosteady state, a three-dimensional Stokes flow in an ellipsoidal envelope of appropriate shape and dimensions is adopted as a fair approximation to the flow around a typical particle of the swarm, in accordance with the concept introduced by Happel.[11] The inner ellipsoid, which represents a particle in the assemblage, is solid, moves with a constant arbitrary velocity, and rotates arbitrarily with a constant angular velocity, whereas the outer ellipsoid represents a fictitious fluid envelope identifying the surface of a unit cell (ellipsoid-in-cell). The volume of the fluid cell is chosen so that the solid volume fraction in the cell coincides with the volume fraction of the swarm. The appropriate boundary conditions, resulting from these assumptions, are: nonslip flow on the inner ellipsoid, no normal flow, and zero tangential stresses on the outer ellipsoidal envelope.

In order to produce ready-to-use basic functions for Stokes flow in ellispoidal coordinates,[2] we calculate the Papkovich–Neuber eigensolutions, generated by the appropriate ellipsoidal eigenfunctions.[20,21] This way, we determine the flow fields as a full series expansion via the Papkovich–Neuber representation, which represents the velocity and the total pressure fields in terms of harmonic functions. The velocity, to the first degree, which represents the leading term of the series, is sufficient for most engineering applications and provides us, also, with the corresponding full 3D solution for the sphere given in Ref. 19 after a proper reduction. Besides, the first-order velocity field suits properly with the first-order nonslip flow condition on the surface of the ellipsoidal particle. Thus, this program offers us the opportunity to restrict to this appropriate degree of approximation. The application of the boundary conditions is accompanied by a set of extra conditions, which form the key to our work. They are based on the flexibility of the Papkovich–Neuber differential representation.[17] The imposition of these conditions is necessary in order to overcome certain difficulties caused by the geometry. Specifically, since we have two boundary surfaces to satisfy our conditions, we use twice the convenience that our representation offers[17] on each boundary. Hence, we adopt the so-called *techniques* mentioned during our analysis, as the result of the above-noted flexibility.

The whole analysis is based on the Lamé functions and the theory of ellipsoidal harmonics.[20,21] In fact, only harmonics of degree less than or equal to two are needed to obtain the velocity field of the first degree. Besides the velocity field, analytical expressions for the leading terms of the total pressure, the angular velocity, and the stress tensor fields are provided. Since the purely ellipsoidal expressions are not easy to handle, the results are given in the more tractable form where Cartesian coordinates are used for the interior harmonics plus the standard elliptic integrals that appear in the exterior Lamé products. Many relations involving the constants of the ellipsoidal harmonics as well as relations among the elliptic integrals had to be worked out in order to bring the result into its final form. The particular way the elliptic integrals are interconnected is provided in the Appendix, where one can also find useful relations that are used extensively and are necessary in order to transform from the Cartesian to the ellipsoidal system and vice versa. We must point out that our analytical method has been followed by the introduction of a new set of elliptic integrals, which do not differ from the aforementioned ones and which helped us to derive certain coefficients in a simple way as well as to overcome the difficulty of the corresponding boundary condition. Finally, the laborious task of reducing the results to the spheroidal and spherical geometry is included. The reduction of general results from the ellipsoidal to the spheroidal or spherical geometry is not a straightforward task because of the complicated indeterminacies that occur as the three semifocal distances of the ellipsoidal system approach zero. The only way to deal with these indeterminacies is to group appropriately the terms of the solution and to perform the algebraic manipulations, which eliminate the indeterminacies before the limiting process is applied.

Section II provides the mathematical formulation of the problem and Sec. III discusses the fundamentals of the ellipsoidal system and the eigenfunctions for the Papkovich–Neuber potentials in ellipsoidal coordinates. The Stokes flow fields are also provided as full series expansions and the boundary conditions are presented in the appropriate ellipsoidal shape. The Happel-type problem for an ellipsoid-in-cell model is solved explicitly in Sec. IV where the results are presented in a manageable Cartesian-ellipsoidal form. Section V is dedicated to the reduction of our expressions to the corresponding prolate–oblate spheroidal (including their limiting cases) and spherical ones. Section VI is devoted to a discussion of the obtained results. The necessary material from the theory of ellipsoidal harmonics as well as some useful formulas associated with ellipsoidal functions is collected in the Appendix. These formulas are the key identities of the present work.

II. MATHEMATICAL DEVELOPMENT

Under the assumption of pseudosteady, nonaxisymmetric, creeping flow (Reynolds number $\mathrm{Re} \ll 1$) which characterizes Stokes flow,[1] the governing equations of motion for an incompressible, viscous fluid in smooth, bounded domain $\Omega(\mathbb{R}^3)$, with dynamic viscosity μ_0 and mass density ρ_0, are a pair of partial differential equations connecting the biharmonic velocity field $\mathbf{v}$ with the harmonic total pressure field P,

$$\mu_0 \Delta \mathbf{v}(\mathbf{r}) = \nabla P(\mathbf{r}), \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{1}$$

$$\nabla \cdot \mathbf{v}(\mathbf{r}) = 0, \quad \mathbf{r} \in \Omega(\mathbb{R}^3). \tag{2}$$

Equation (1) states that, in creeping flow, the viscous force compensates for the force caused by the pressure gradient on any material point of the fluid, while Eq. (2) secures the incompressibility of the fluid. Once the velocity field is obtained, the harmonic vorticity field $\boldsymbol{\omega}$ is defined as

$$\boldsymbol{\omega}(\mathbf{r}) = \tfrac{1}{2} \nabla \times \mathbf{v}(\mathbf{r}), \quad \mathbf{r} \in \Omega(\mathbb{R}^3). \tag{3}$$

Papkovich–Neuber[3,4] proposed the following differential representation of the solution for Stokes flow, in terms of the harmonic potentials $\boldsymbol{\Phi}$ and Φ_0,

$$\mathbf{v}(\mathbf{r}) = \boldsymbol{\Phi}(\mathbf{r}) - \tfrac{1}{2} \nabla (\mathbf{r} \cdot \boldsymbol{\Phi}(\mathbf{r}) + \Phi_0(\mathbf{r})), \quad \mathbf{r} \in \Omega(\mathbb{R}^3) \tag{4}$$

and

$$P(\mathbf{r}) = P_0 - \mu_0 \nabla \cdot \boldsymbol{\Phi}(\mathbf{r}), \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{5}$$

whereas P_0 is a constant pressure of reference usually assigned at a convenient point. The potential functions $\boldsymbol{\Phi}$ and Φ_0 solve the equations

$$\Delta \boldsymbol{\Phi}(\mathbf{r}) = \mathbf{0}, \quad \Delta \Phi_0 = 0, \quad \mathbf{r} \in \Omega(\mathbb{R}^3). \tag{6}$$

If we define the thermodynamic pressure p, then the following relation gives the total pressure as a function of the thermodynamic pressure

$$P(\mathbf{r}) = p(\mathbf{r}) + \rho_0 g h, \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{7}$$

where the contribution of the term $\rho_0 g h$ (g is the acceleration of the gravity) refers to the gravitational pressure force, corresponding to a height of reference h.

The stress dyadic $\tilde{\boldsymbol{\Pi}}$ is defined as follows:

$$\tilde{\boldsymbol{\Pi}}(\mathbf{r}) = -p(\mathbf{r}) \tilde{\mathbf{I}} + \mu_0 [\nabla \otimes \mathbf{v}(\mathbf{r}) + (\nabla \otimes \mathbf{v}(\mathbf{r}))^{\mathsf{T}}], \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{8}$$

where $\tilde{\mathbf{I}}$ stands for the unit dyadic and the symbol "T" denotes transposition.

The Happel-type boundary conditions for a general 3D particle-in-cell model. By means of

Ref. 1, we consider a fluid–particle system consisting of any finite number of rigid particles of arbitrary shape. Introducing the particle-in-cell model, we examine the Stokes flow of one of the assemblage of particles neglecting the interaction with other particles or with the bounded walls of a container. Let S_i denote the surface of the particle of the swarm, which is solid, is moving with a constant translational velocity $\mathbf{U}$ in an arbitrary direction (the relation between the velocity $\mathbf{U}$ and the mean interstitial velocity through a swarm of spheroidal particles was discussed in Ref. 16 and is rotating, also arbitrarily, with a constant angular velocity $\mathbf{\Omega}$. It lives within an otherwise quiescent fluid layer, which is confined by the outer surface denoted by S_o. Following the formulation of Happel,[11] the velocity component normal to S_o and the tangential stresses are assumed to vanish on S_o. These boundary conditions are supplemented by the necessary nonslip flow conditions on the surface of the particle. Thus, the general BCs for a three-dimensional consideration of the Happel-type boundary value problem are:

$$\text{BC(1)}: \quad \mathbf{v}(\mathbf{r}) = \mathbf{U} + \mathbf{\Omega} \times \mathbf{r} \quad \text{for } \mathbf{r} \in S_i, \tag{9}$$

$$\text{BC(2)}: \quad \hat{\mathbf{n}} \cdot \mathbf{v}(\mathbf{r}) = 0 \quad \text{for } \mathbf{r} \in S_o, \tag{10}$$

$$\text{BC(3)}: \quad \hat{\mathbf{n}} \cdot \tilde{\mathbf{\Pi}}(\mathbf{r}) \cdot (\tilde{\mathbf{I}} - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) = \mathbf{0} \quad \text{for } \mathbf{r} \in S_o, \tag{11}$$

where $\hat{\mathbf{n}}$ is the outer unit normal vector. Equations (1)–(11) define a well-posed Happel-type boundary value problem for 3D domains, $\mathbf{r} \in \Omega(\mathbb{R}^3)$, bounded by two arbitrary surfaces S_i and S_o.

Our goal is to solve the above-noted Happel problem with the appropriate boundary conditions given by Eqs. (9)–(11), with the aim of the Papkovich–Neuber differential representation using the ellipsoidal system, which represents the most general geometrical system, which is orthogonal and embodies the complete anisotropy of the three-dimensional space.

III. ELLIPSOIDAL GEOMETRY: FLOW FIELDS AND BOUNDARY CONDITIONS

The basic triaxial ellipsoid is defined by

$$\frac{x_1^2}{\alpha_1^2} + \frac{x_2^2}{\alpha_2^2} + \frac{x_3^2}{\alpha_3^2} = 1, \tag{12}$$

where $0 < \alpha_3 < \alpha_2 < \alpha_1 < +\infty$ are its semiaxes. The three positive numbers h_1, h_2, and h_3, which denote the semifocal distances of the system, are given by

$$h_1^2 = \alpha_2^2 - \alpha_3^2, \quad h_2^2 = \alpha_1^2 - \alpha_3^2, \quad h_3^2 = \alpha_1^2 - \alpha_2^2 = h_2^2 - h_1^2. \tag{13}$$

Define the system of ellipsoidal coordinates (ρ, μ, ν),[2,20] which are connected to the Cartesian ones (x_1, x_2, x_3), via

$$x_1 = \frac{\rho\mu\nu}{h_2 h_3}, \tag{14}$$

$$x_2 = \frac{\sqrt{\rho^2 - h_3^2}\sqrt{\mu^2 - h_3^2}\sqrt{h_3^2 - \nu^2}}{h_1 h_3}, \tag{15}$$

$$x_3 = \frac{\sqrt{\rho^2 - h_2^2}\sqrt{h_2^2 - \mu^2}\sqrt{h_2^2 - \nu^2}}{h_1 h_2}. \tag{16}$$

The three families of second-degree surfaces, which are shown in Fig. 1, share the same set of foci at the points $\pm h_1$, $\pm h_2$, and $\pm h_3$.

In terms of the position vector $\mathbf{r} = x_1\hat{\mathbf{x}}_1 + x_2\hat{\mathbf{x}}_2 + x_3\hat{\mathbf{x}}_3$ expressed via the Cartesian basis $\hat{\mathbf{x}}_\kappa$, $\kappa = 1, 2, 3$, the variable ρ, $h_2 \leqslant \rho < +\infty$ specifies the ellipsoid

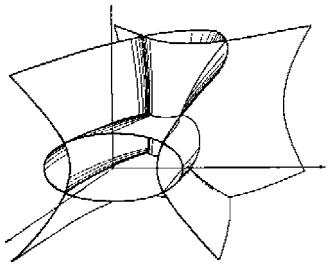

FIG. 1. Ellipsoidal geometry and coordinate surfaces.

$$\frac{x_1^2}{\rho^2}+\frac{x_2^2}{\rho^2-h_3^2}+\frac{x_3^2}{\rho^2-h_2^2}=\sum_{i=1}^{3}\frac{x_i^2}{\rho^2-\alpha_1^2+\alpha_i^2}=\mathbf{r}\cdot\sum_{i=1}^{3}\frac{\hat{\mathbf{x}}_i\otimes\hat{\mathbf{x}}_i}{\rho^2-\alpha_1^2+\alpha_i^2}\cdot\mathbf{r}=1, \tag{17}$$

the variable μ, $h_3\leqslant\mu\leqslant h_2$ specifies the hyperboloid of one sheet

$$\frac{x_1^2}{\mu^2}+\frac{x_2^2}{\mu^2-h_3^2}-\frac{x_3^2}{h_2^2-\mu^2}=\sum_{i=1}^{3}\frac{x_i^2}{\mu^2-\alpha_1^2+\alpha_i^2}=1 \tag{18}$$

and the variable ν, $-h_3\leqslant\nu\leqslant h_3$ specifies the hyperboloid of two sheets

$$\frac{x_1^2}{\nu^2}-\frac{x_2^2}{h_3^2-\nu^2}-\frac{x_3^2}{h_2^2-\nu^2}=\sum_{i=1}^{3}\frac{x_i^2}{\nu^2-\alpha_1^2+\alpha_i^2}=1. \tag{19}$$

In the limit as the semifocal distances tend to zero ($h_1=h_2=h_3\to 0$), our system degenerates to the corresponding spherical one with radial component r given by

$$\|\mathbf{r}\|=\sqrt{\rho^2+\mu^2+\nu^2-(h_2^2+h_3^2)}\to r,\quad 0\leqslant r<+\infty. \tag{20}$$

In terms of the metric coefficients of the system

$$h_\rho=\frac{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}},\quad h_\mu=\frac{\sqrt{\rho^2-\mu^2}\sqrt{\mu^2-\nu^2}}{\sqrt{\mu^2-h_3^2}\sqrt{h_2^2-\mu^2}},\quad h_\nu=\frac{\sqrt{\rho^2-\nu^2}\sqrt{\mu^2-\nu^2}}{\sqrt{h_3^2-\nu^2}\sqrt{h_2^2-\nu^2}}, \tag{21}$$

the Jacobian determinant is $J=h_\rho h_\mu h_\nu$ and the differential operators ∇, Δ, assume the forms

$$\nabla=\sum_{i=1}^{3}\hat{\mathbf{x}}_i\frac{\partial}{\partial x_i}=\frac{\hat{\boldsymbol{\rho}}}{h_\rho}\frac{\partial}{\partial\rho}+\frac{\hat{\boldsymbol{\mu}}}{h_\mu}\frac{\partial}{\partial\mu}+\frac{\hat{\boldsymbol{\nu}}}{h_\nu}\frac{\partial}{\partial\nu} \tag{22}$$

and

$$\Delta=\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2}=\frac{1}{J}\left\{\frac{\partial}{\partial\rho}\left[\frac{J}{h_\rho^2}\frac{\partial}{\partial\rho}\right]+\frac{\partial}{\partial\mu}\left[\frac{J}{h_\mu^2}\frac{\partial}{\partial\mu}\right]+\frac{\partial}{\partial\nu}\left[\frac{J}{h_\nu^2}\frac{\partial}{\partial\nu}\right]\right\}, \tag{23}$$

where $\hat{\boldsymbol{\rho}},\hat{\boldsymbol{\mu}},\hat{\boldsymbol{\nu}}$ denote the orthonormal coordinate vectors of the system, i.e.,

$$\hat{\boldsymbol{\rho}}=\frac{\rho}{h_\rho}\sum_{i=1}^{3}\frac{x_i\hat{\mathbf{x}}_i}{\rho^2-\alpha_1^2+\alpha_i^2},\quad \hat{\boldsymbol{\mu}}=\frac{\mu}{h_\mu}\sum_{i=1}^{3}\frac{x_i\hat{\mathbf{x}}_i}{\mu^2-\alpha_1^2+\alpha_i^2},\quad \hat{\boldsymbol{\nu}}=\frac{\nu}{h_\nu}\sum_{i=1}^{3}\frac{x_i\hat{\mathbf{x}}_i}{\nu^2-\alpha_1^2+\alpha_i^2}. \tag{24}$$

The outward unit normal vector on the surface of the ellipsoid $\rho=$const coincides with the unit normal vector $\hat{\boldsymbol{\rho}}$, thus

$$\hat{\mathbf{n}}(\mathbf{r}) = \frac{\rho}{h_\rho}\left[\frac{x_1\hat{\mathbf{x}}_1}{\rho^2} + \frac{x_2\hat{\mathbf{x}}_2}{\rho^2 - h_3^2} + \frac{x_3\hat{\mathbf{x}}_3}{\rho^2 - h_2^2}\right] = \frac{\rho}{h_\rho}\sum_{i=1}^{3}\frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{\rho^2 - \alpha_1^2 + \alpha_i^2}\cdot\mathbf{r} \equiv \hat{\boldsymbol{\rho}}, \tag{25}$$

while the unit dyadic assumes the ellipsoidal form

$$\tilde{\mathbf{I}} = \sum_{i=1}^{3}\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i = \hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\rho}} + \hat{\boldsymbol{\mu}} \otimes \hat{\boldsymbol{\mu}} + \hat{\boldsymbol{\nu}} \otimes \hat{\boldsymbol{\nu}}. \tag{26}$$

From now on we shall refer to ellipsoidal domains, in terms of which

$$\Omega(\mathbb{R}^3) \equiv \mathbb{R}^3 = \{(\rho,\mu,\nu):\rho \in [h_2, +\infty), \mu \in [h_3,h_2], \nu \in [-h_3,h_3]\}. \tag{27}$$

In order to construct the flow fields (3)–(5) and (8) in an appropriate form for the application of the boundary conditions (9)–(11), we need to represent the harmonic potentials $\mathbf{\Phi}$ and Φ_0 in this system by solving the corresponding Laplace's equations (6) in spectral form. This procedure leads to the Lamé equation[20]

$$(x^2 - h_3^2)(x^2 - h_2^2)E''(x) + x(2x^2 - h_3^2 - h_2^2)E'(x) + (Ax^2 + B)E(x) = 0, \tag{28}$$

for each one of the factors $E(\rho)$, $E(\mu)$, and $E(\nu)$ within the corresponding intervals $\rho \in [h_2, +\infty)$, $\mu \in [h_3,h_2]$, and $\nu \in [-h_3,h_3]$, where $A,B \in \mathbb{R}$ are constants. For each $n=0,1,\ldots$, which corresponds to the degree of the Lamé equation, and for each $m=1,2,\ldots,2n+1$, which stands for its order, Eq. (28) has two linearly independent solutions. The first one, E_n^m, is regular at the origin and it is known as the Lamé function of the first kind (interior solution), while the second one, F_n^m, is regular at infinity and gives the Lamé function of the second kind (exterior solution). In particular, the interior solution $E_n^m(\rho)$ is related to the exterior solution $F_n^m(\rho)$ via

$$F_n^m(\rho) = (2n+1)E_n^m(\rho)I_n^m(\rho), \quad \rho \in [h_2, +\infty), \tag{29}$$

where the elliptic integrals I_n^m are given by

$$I_n^m(\rho) = \int_\rho^{+\infty}\frac{\mathrm{d}u}{[E_n^m(u)]^2\sqrt{u^2 - h_2^2}\sqrt{u^2 - h_3^2}}, \quad \rho \in [h_2, +\infty) \tag{30}$$

for every value of $n=0,1,\ldots$ and $m=1,2,\ldots,2n+1$. In terms of the Lamé functions of the first and of the second kind, the Lamé products

$$\mathbb{E}_n^m(\mathbf{r}) = E_n^m(\rho)E_n^m(\mu)E_n^m(\nu), \quad n = 0,1,\ldots, \quad m = 1,2,\ldots,2n+1, \quad \mathbf{r} \in \Omega(\mathbb{R}^3) \tag{31}$$

define the interior solid ellipsoidal harmonics, while the products

$$\mathbb{F}_n^m(\mathbf{r}) = F_n^m(\rho)E_n^m(\mu)E_n^m(\nu), \quad n = 0,1,\ldots, \quad m = 1,2,\ldots,2n+1, \quad \mathbf{r} \in \Omega(\mathbb{R}^3) \tag{32}$$

define the exterior solid ellipsoidal harmonics. On the other hand, the complete orthogonal set $E_n^m(\mu)E_n^m(\nu)$ form the surface ellipsoidal harmonics on the surface of any ellipsoid $\rho=\rho_s$, which, with respect to the weighting function

$$l_{\rho_s}(\mu,\nu) = \frac{1}{\sqrt{(\rho_s^2 - \mu^2)(\rho_s^2 - \nu^2)}}, \quad \mu \in [h_3,h_2], \quad \nu \in [-h_3,h_3], \tag{33}$$

satisfy the orthogonality relation

$$\int\int_{\rho=\rho_s} E_n^m(\mu)E_n^m(\nu)E_{n'}^{m'}(\mu)E_{n'}^{m'}(\nu)l_{\rho_s}(\mu,\nu)\mathrm{d}S = \gamma_n^m\delta_{nn'}\delta_{mm'}, \tag{34}$$

for every $n,n'=0,1,\ldots$ and $m,m'=1,2,\ldots,2n+1$. Here, $\delta_{nn'}$ denotes the Kronecker delta function, whilst γ_n^m are the ellipsoidal normalization constants given by

$$\gamma_n^m = \int\int_{\rho=\rho_s} (E_n^m(\mu)E_n^m(\nu))^2 l_{\rho_s}(\mu,\nu)\mathrm{d}S, \quad n=0,1,\ldots, \quad m=1,2,\ldots,2n+1. \tag{35}$$

According to the aforementioned analysis of ellipsoidal harmonic functions, the complete representation of the Papkovich–Neuber potentials $\mathbf{\Phi}$ and Φ_0, which belong to the kernel space of Δ, assume the expressions

$$\mathbf{\Phi}(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=1}^{2n+1} [\mathbf{e}_n^{(i)m}\mathbb{E}_n^m(\mathbf{r}) + \mathbf{e}_n^{(e)m}\mathbb{F}_n^m(\mathbf{r})], \quad \mathbf{r}\in\Omega(\mathbb{R}^3) \tag{36}$$

and

$$\Phi_0(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=1}^{2n+1} [d_n^{(i)m}\mathbb{E}_n^m(\mathbf{r}) + d_n^{(e)m}\mathbb{F}_n^m(\mathbf{r})], \quad \mathbf{r}\in\Omega(\mathbb{R}^3). \tag{37}$$

Note that, for $n\geqslant 0$, the coefficients

$$\mathbf{e}_n^{(i/e)m} = a_n^{(i/e)m}\hat{\mathbf{x}}_1 + b_n^{(i/e)m}\hat{\mathbf{x}}_2 + c_n^{(i/e)m}\hat{\mathbf{x}}_3, \quad d_n^{(i/e)m}, \quad m=1,2,\ldots,2n+1 \tag{38}$$

denote the vector and the scalar coefficients of the harmonic potentials $\mathbf{\Phi}$ and Φ_0, respectively.

Let u, v and $\mathbf{f}$, $\mathbf{g}$ denote two scalar and two vector fields, respectively. Then, if we define by $\widetilde{\mathbb{S}}$ a dyadic, the basic identities that we are using in the sequel concern the action of the gradient operator on the following expressions, i.e.,

$$\nabla\otimes(u\mathbf{f}) = u\nabla\otimes\mathbf{f} + \nabla u\otimes\mathbf{f}, \tag{39}$$

$$\nabla\cdot(u\mathbf{f}) = u\nabla\cdot\mathbf{f} + \nabla u\cdot\mathbf{f}, \tag{40}$$

$$\nabla\times(u\mathbf{f}) = u\nabla\times\mathbf{f} + \nabla u\times\mathbf{f}, \tag{41}$$

$$\nabla(\mathbf{f}\cdot\mathbf{g}) = (\nabla\otimes\mathbf{f})\cdot\mathbf{g} + (\nabla\otimes\mathbf{g})\cdot\mathbf{f}, \tag{42}$$

$$\nabla(uv) = u\nabla v + v\nabla u, \tag{43}$$

$$\nabla\otimes(\widetilde{\mathbb{S}}\cdot\mathbf{f}) = (\nabla\otimes\widetilde{\mathbb{S}})\cdot\mathbf{f} + (\nabla\otimes\mathbf{f})\cdot\widetilde{\mathbb{S}}^{\mathrm{T}}, \tag{44}$$

$$\nabla\otimes(\mathbf{f}\otimes\mathbf{g}) = (\nabla\otimes\mathbf{f})\otimes\mathbf{g} + [\mathbf{f}\otimes(\nabla\otimes\mathbf{g})]^{213}, \tag{45}$$

whereas $\widetilde{\mathbb{S}}^{\mathrm{T}}$ is the inverted dyadic and the symbol $(\,)^{213}$ denotes left transposition for a triadic. Inserting the potentials (36) and (37) in the flow fields (4), (5), (3), (8) and making use of the above identities (39)–(45), we derive the relation

$$\begin{aligned}\mathbf{v}(\mathbf{r}) = \frac{1}{2}\sum_{n=0}^{\infty}\sum_{m=1}^{2n+1} \{&\mathbf{e}_n^{(i)m}\mathbb{E}_n^m(\mathbf{r}) \\ &- [(\mathbf{e}_n^{(i)m}\cdot\mathbf{r}) + d_n^{(i)m}]\nabla\mathbb{E}_n^m(\mathbf{r}) + \mathbf{e}_n^{(e)m}\mathbb{F}_n^m(\mathbf{r}) - [(\mathbf{e}_n^{(e)m}\cdot\mathbf{r}) + d_n^{(e)m}]\nabla\mathbb{F}_n^m(\mathbf{r})\}, \quad \mathbf{r}\in\Omega(\mathbb{R}^3)\end{aligned} \tag{46}$$

for the velocity field, while for the total pressure field, taking into account relation (7), we obtain

$$P(\mathbf{r}) = P_0 - \mu_0 \sum_{n=0}^{\infty} \sum_{m=1}^{2n+1} \{\mathbf{e}_n^{(i)m} \cdot \nabla \mathbb{E}_n^m(\mathbf{r}) + \mathbf{e}_n^{(e)m} \cdot \nabla \mathbb{F}_n^m(\mathbf{r})\} = p(\mathbf{r}) + \rho_0 g h, \tag{47}$$

for every $\mathbf{r} \in \Omega(\mathbb{R}^3)$. The vorticity field is then written as

$$\boldsymbol{\omega}(\mathbf{r}) = \frac{1}{2} \sum_{n=0}^{\infty} \sum_{m=1}^{2n+1} \{\nabla \mathbb{E}_n^m(\mathbf{r}) \times \mathbf{e}_n^{(i)m} + \nabla \mathbb{F}_n^m(\mathbf{r}) \times \mathbf{e}_n^{(e)m}\}, \quad \mathbf{r} \in \Omega(\mathbb{R}^3) \tag{48}$$

and the stress tensor field is expressed as

$$\widetilde{\mathbf{\Pi}}(\mathbf{r}) = -p(\mathbf{r})\widetilde{\mathbf{I}} - \mu_0 \sum_{n=0}^{\infty} \sum_{m=1}^{2n+1} \{[(\mathbf{e}_n^{(i)m} \cdot \mathbf{r}) + d_n^{(i)m}] \nabla \otimes \nabla \mathbb{E}_n^m(\mathbf{r}) + [(\mathbf{e}_n^{(e)m} \cdot \mathbf{r}) + d_n^{(e)m}] \nabla \otimes \nabla \mathbb{F}_n^m(\mathbf{r})\},$$
$$\mathbf{r} \in \Omega(\mathbb{R}^3). \tag{49}$$

The coefficients $\mathbf{e}_n^{(i)m}$, $\mathbf{e}_n^{(e)m}$, $d_n^{(i)m}$, and $d_n^{(e)m}$ for $n=0,1,\ldots$ and $m=1,2,\ldots,2n+1$ are to be determined from the boundary conditions (9)–(11), which also have to be expressed in ellipsoidal form. In accordance with the Happel formulation,[11] two confocal ellipsoids are considered. The inner one, indicated by S_a, at $\rho=\rho_a$ with semiaxes ρ_a, $\sqrt{\rho_a^2-h_3^2}$ and $\sqrt{\rho_a^2-h_2^2}$ is solid, it is moving with a constant translational velocity $\mathbf{U}$ in an arbitrary direction and is rotating arbitrarily with a constant angular velocity $\mathbf{\Omega}$, given by

$$\mathbf{U} = \sum_{i=1}^{3} U_i \hat{\mathbf{x}}_i, \quad \mathbf{\Omega} = \sum_{i=1}^{3} \Omega_i \hat{\mathbf{x}}_i, \tag{50}$$

where U_i and Ω_i, $i=1,2,3$ are the components at the Cartesian orthogonal basis. The outer ellipsoid indicated by S_b at $\rho=\rho_b$ with semiaxes ρ_b, $\sqrt{\rho_b^2-h_3^2}$ and $\sqrt{\rho_b^2-h_2^2}$ defines the quiescent fluid layer. Thus, the boundary conditions (9)–(11) are rewritten as follows:

$$\text{BC(1):} \quad \mathbf{v}(\mathbf{r}) = \mathbf{U} + \mathbf{\Omega} \times \mathbf{r} \quad \text{for } \mathbf{r} \in S_a, \tag{51}$$

$$\text{BC(2):} \quad \hat{\boldsymbol{\rho}} \cdot \mathbf{v}(\mathbf{r}) = 0 \quad \text{for } \mathbf{r} \in S_b, \tag{52}$$

$$\text{BC(3):} \quad \hat{\boldsymbol{\rho}} \cdot \widetilde{\mathbf{\Pi}}(\mathbf{r}) \cdot (\widetilde{\mathbf{I}} - \hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\rho}}) = \mathbf{0} \quad \text{for } \mathbf{r} \in S_b, \tag{53}$$

where $\hat{\boldsymbol{\rho}}$ is the unit curvilinear vector relative to the variable ρ. These BCs must be applied to Eqs. (46) and (49) in order to calculate the coefficients and obtain the flow fields (46)–(49). Note that the domain $\Omega(\mathbb{R}^3)$ (27) is specified by the variable ρ that varies in the interval $[\rho_a, \rho_b]$.

IV. SOLUTION OF THE 3D HAPPEL-TYPE ELLIPSOID-IN-CELL MODEL

The purpose of this section is to solve the 3D Stokes ellipsoid-in-cell model with the Happel-type BCs (51)–(53). In our related work, for the corresponding complete isotropic Stokes flow,[19] the solution was obtained by using the full series representation for the velocity, the total pressure, the vorticity, and the stress tensor. Unfortunately, this is not possible when the present complex ellipsoidal geometry is used. The reason is that, although the form of ellipsoidal harmonics is known, the analytical expressions of those harmonics in terms of the semiaxes $\alpha_1, \alpha_2, \alpha_3$ are manageable only for degree $n \leqslant 3$. This difficulty restricts the analytical solutions of related physical problems to the 16th-dimensional harmonic subspace spanned by the harmonics of degree less than or equal to three for $m=1,2,\ldots,2n+1$.[20] The interior Lamé functions of degree less than or equal to 3 are given by

$$E_0^1(x) = 1, \tag{54}$$

$$E_1^{\kappa}(x) = \sqrt{|x^2 - \alpha_1^2 + \alpha_{\kappa}^2|}, \quad \kappa = 1,2,3, \tag{55}$$

$$E_2^1(x) = x^2 - \alpha_1^2 + \Lambda, \tag{56}$$

$$E_2^2(x) = x^2 - \alpha_1^2 + \Lambda', \tag{57}$$

$$E_2^{6-\kappa}(x) = \frac{x\sqrt{|x^2 - h_3^2|}\sqrt{|x^2 - h_2^2|}}{\sqrt{|x^2 - \alpha_1^2 + \alpha_{\kappa}^2|}}, \quad \kappa = 1,2,3 \tag{58}$$

or in terms of the semiaxes,

$$E_2^{\kappa+l}(x) = \sqrt{|x^2 - \alpha_1^2 + \alpha_{\kappa}^2|}\sqrt{|x^2 - \alpha_1^2 + \alpha_l^2|}, \quad \kappa,l = 1,2,3, \quad \kappa \neq l \tag{59}$$

and

$$E_3^{2\kappa-1}(x) = \sqrt{|x^2 - \alpha_1^2 + \alpha_{\kappa}^2|}(x^2 - \alpha_1^2 + \Lambda_{\kappa}), \quad \kappa = 1,2,3, \tag{60}$$

$$E_3^{2\kappa}(x) = \sqrt{|x^2 - \alpha_1^2 + \alpha_{\kappa}^2|}(x^2 - \alpha_1^2 + \Lambda'_{\kappa}), \quad \kappa = 1,2,3, \tag{61}$$

$$E_3^7(x) = x\sqrt{|x^2 - h_3^2|}\sqrt{|x^2 - h_2^2|}, \tag{62}$$

where the variable x represents the values of $\rho \in [h_2, +\infty)$, $\mu \in [h_3, h_2]$, $\nu \in [-h_3, h_3]$, the constants

$$\left.\begin{matrix}\Lambda \\ \Lambda'\end{matrix}\right\} = \frac{1}{3}\sum_{i=1}^{3} \alpha_i^2 \pm \frac{1}{3}\left[\sum_{i=1}^{3}\left(\alpha_i^4 - \frac{\alpha_1^2\alpha_2^2\alpha_3^2}{\alpha_i^2}\right)\right]^{1/2} \tag{63}$$

satisfy the quadratic equation

$$\sum_{i=1}^{3} \frac{1}{\Lambda - \alpha_i^2} = 0, \tag{64}$$

and the constants

$$\left.\begin{matrix}\Lambda_{\kappa} \\ \Lambda'_{\kappa}\end{matrix}\right\} = \frac{2}{5}\sum_{i=1}^{3} \alpha_i^2 - \frac{1}{5}\alpha_{\kappa}^2 \pm \frac{1}{5}\left\{4\sum_{i=1}^{3} \alpha_i^4 - 3\alpha_{\kappa}^4 - \alpha_1^2\alpha_2^2\alpha_3^2\left(\sum_{i=1}^{3} \frac{1}{\alpha_i^2} + \frac{6}{\alpha_{\kappa}^2}\right)\right\}^{1/2} \tag{65}$$

for $\kappa = 1,2,3$ satisfy the relations

$$\sum_{i=1}^{3} \frac{1 + 2\delta_{i\kappa}}{(\Lambda_{\kappa} - \alpha_i^2)} = 0, \quad \kappa = 1,2,3. \tag{66}$$

The Cartesian representation of the ellipsoidal harmonics are given by

$$\mathbb{E}_0^1(\mathbf{r}) = 1, \tag{67}$$

$$\mathbb{E}_1^{\kappa}(\mathbf{r}) = \frac{h_1h_2h_3}{h_{\kappa}}x_{\kappa}, \quad \kappa = 1,2,3, \tag{68}$$

$$\mathbb{E}_2^1(\mathbf{r}) = (\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2)\left[\sum_{i=1}^{3} \frac{x_i^2}{\Lambda - \alpha_i^2} + 1\right] \equiv \mathbb{E}_2^1(\Lambda), \tag{69}$$

$$\mathbb{E}_2^2(\mathbf{r}) = \mathbb{E}_2^1(\Lambda'), \tag{70}$$

$$\mathbb{E}_2^{6-\kappa}(\mathbf{r}) = h_1 h_2 h_3 h_\kappa \frac{x_1 x_2 x_3}{x_\kappa}, \quad \kappa = 1,2,3 \tag{71}$$

or equivalently,

$$\mathbb{E}_2^{\kappa+l}(\mathbf{r}) = \frac{h_1^2 h_2^2 h_3^2}{h_\kappa h_l} x_\kappa x_l, \quad \kappa,l = 1,2,3, \quad \kappa \neq l \tag{72}$$

and

$$\mathbb{E}_3^{2\kappa-1}(\mathbf{r}) = h_1 h_2 h_3 (\Lambda_\kappa - \alpha_1^2)(\Lambda_\kappa - \alpha_2^2)(\Lambda_\kappa - \alpha_3^2) \frac{x_\kappa}{h_\kappa} \left[\sum_{i=1}^{3} \frac{x_i^2}{\Lambda_\kappa - \alpha_i^2} + 1 \right] \equiv \mathbb{E}_3^{2\kappa-1}(\Lambda_\kappa), \quad \kappa = 1,2,3, \tag{73}$$

$$\mathbb{E}_3^{2\kappa}(\mathbf{r}) = \mathbb{E}_3^{2\kappa-1}(\Lambda'_\kappa), \quad \kappa = 1,2,3, \tag{74}$$

$$\mathbb{E}_3^7(\mathbf{r}) = h_1^2 h_2^2 h_3^2 x_1 x_2 x_3, \tag{75}$$

where $\mathbf{r} \in \Omega(\mathbb{R}^3)$. On the other hand, the Cartesian monomials of degree less than or equal to three are expressed via the ellipsoidal harmonic functions as

$$1 = \mathbb{E}_0^1(\mathbf{r}) = E_0^1(\rho) E_0^1(\mu) E_0^1(\nu), \tag{76}$$

$$x_\kappa = \frac{h_\kappa}{h_1 h_2 h_3} \mathbb{E}_1^\kappa(\mathbf{r}) = \frac{h_\kappa}{h_1 h_2 h_3} E_1^\kappa(\rho) E_1^\kappa(\mu) E_1^\kappa(\nu), \quad \kappa = 1,2,3, \tag{77}$$

$$x_\kappa^2 = \frac{\rho^2 - \alpha_1^2 + \alpha_\kappa^2}{3} \left[1 - \frac{E_2^1(\mu) E_2^1(\nu)}{(\Lambda - \Lambda')(\Lambda - \alpha_\kappa^2)} + \frac{E_2^2(\mu) E_2^2(\nu)}{(\Lambda - \Lambda')(\Lambda' - \alpha_\kappa^2)} \right], \tag{78}$$

$$\frac{x_1 x_2 x_3}{x_\kappa} = \frac{1}{h_1 h_2 h_3 h_\kappa} \mathbb{E}_2^{6-\kappa}(\mathbf{r}) = \frac{1}{h_1 h_2 h_3 h_\kappa} E_2^{6-\kappa}(\rho) E_2^{6-\kappa}(\mu) E_2^{6-\kappa}(\nu), \quad \kappa = 1,2,3 \tag{79}$$

or

$$x_\kappa x_l = \frac{h_\kappa h_l}{h_1^2 h_2^2 h_3^2} \mathbb{E}_2^{\kappa+l}(\mathbf{r}) = \frac{h_\kappa h_l}{h_1^2 h_2^2 h_3^2} E_2^{\kappa+l}(\rho) E_2^{\kappa+l}(\mu) E_2^{\kappa+l}(\nu), \quad \kappa,l = 1,2,3, \quad \kappa \neq l, \tag{80}$$

$$x_\kappa x_l^2 = \frac{\sqrt{\rho^2 - \alpha_1^2 + \alpha_\kappa^2}(\rho^2 - \alpha_1^2 + \alpha_l^2) h_\kappa}{5 h_1 h_2 h_3} \{ (1 + 2\delta_{\kappa l}) E_1^\kappa(\mu) E_1^\kappa(\nu) \tag{81}$$

$$+ \frac{5(-1)^l h_l^2}{h_1^2 h_2^2 h_3^2 (\Lambda_\kappa - \Lambda'_\kappa)} [(\Lambda'_\kappa - \alpha_l^2) E_3^{2\kappa-1}(\mu) E_3^{2\kappa-1}(\nu) - (\Lambda_\kappa - \alpha_l^2) E_3^{2\kappa}(\mu) E_3^{2\kappa}(\nu)] \Big\}, \quad \kappa,l = 1,2,3, \tag{82}$$

$$x_1 x_2 x_3 = \frac{1}{h_1^2 h_2^2 h_3^2} \mathbb{E}_3^7(\mathbf{r}) = \frac{1}{h_1^2 h_2^2 h_3^2} E_3^7(\rho) E_3^7(\mu) E_3^7(\nu). \tag{83}$$

Relations (67)–(83) form the basis for moving from the Cartesian coordinates to the ellipsoidal ones and vice versa. Relations (76)–(83) are necessary for the application of the orthogonality relation (34). Note that

$$\mathbb{F}_n^m(\mathbf{r}) = (2n+1) I_n^m(\rho) \mathbb{E}_n^m(\mathbf{r}), \quad n = 0,1,2,3, \quad m = 1,2,\ldots,2n+1, \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{84}$$

while the set of

$$x_l^2 - x_\kappa^2 = \frac{\alpha_l^2 - \alpha_\kappa^2}{3} - \frac{\mathbb{E}_2^1(\mathbf{r})}{3(\Lambda - \Lambda')}\left[\frac{1}{\Lambda - \alpha_l^2} - \frac{1}{\Lambda - \alpha_\kappa^2}\right] + \frac{\mathbb{E}_2^2(\mathbf{r})}{3(\Lambda - \Lambda')}\left[\frac{1}{\Lambda' - \alpha_l^2} - \frac{1}{\Lambda' - \alpha_\kappa^2}\right], \quad \mathbf{r} \in \Omega(\mathbb{R}^3) \tag{85}$$

for every $\kappa, l = 1,2,3$, are harmonic functions.

Before we proceed to the full solution of our physical problem, it is necessary to write down the Cartesian-ellipsoidal representations for the single and the double action of the gradient operator (22) on the interior and on the exterior ellipsoidal harmonic eigenfunctions of degree $n \leqslant 3$. Consequently, some long but straightforward calculations lead to

$$\nabla \mathbb{E}_0^1(\mathbf{r}) = \mathbf{0}, \tag{86}$$

$$\nabla \mathbb{E}_1^\kappa(\mathbf{r}) = \frac{h_1 h_2 h_3}{h_\kappa} \hat{\mathbf{x}}_\kappa = \frac{h_1 h_2 h_3}{h_\kappa} \mathbb{E}_0^1(\mathbf{r}) \hat{\mathbf{x}}_\kappa, \quad \kappa = 1,2,3, \tag{87}$$

$$\begin{aligned} \nabla \mathbb{E}_2^1(\mathbf{r}) &= 2(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2) \sum_{i=1}^3 \frac{x_i \hat{\mathbf{x}}_i}{\Lambda - \alpha_i^2} \\ &= 2 \frac{(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2)}{h_1 h_2 h_3} \sum_{i=1}^3 \frac{h_i}{\Lambda - \alpha_i^2} \mathbb{E}_1^i(\mathbf{r}) \hat{\mathbf{x}}_i \equiv \nabla \mathbb{E}_2^1(\Lambda), \end{aligned} \tag{88}$$

$$\nabla \mathbb{E}_2^2(\mathbf{r}) = \nabla \mathbb{E}_2^1(\Lambda'), \tag{89}$$

$$\nabla \mathbb{E}_2^{6-\kappa}(\mathbf{r}) = h_1 h_2 h_3 h_\kappa \sum_{i=1}^3 (1 - \delta_{\kappa i}) \frac{x_1 x_2 x_3}{x_\kappa x_i} \hat{\mathbf{x}}_i = h_1 h_2 h_3 \sum_{i=1}^3 \frac{(1 - \delta_{\kappa i})}{h_i} \mathbb{E}_1^{6-(\kappa+i)}(\mathbf{r}) \hat{\mathbf{x}}_i, \quad \kappa = 1,2,3 \tag{90}$$

or with equivalent notation,

$$\nabla \mathbb{E}_2^{\kappa+l}(\mathbf{r}) = \frac{h_1^2 h_2^2 h_3^2}{h_\kappa h_l} (x_\kappa \hat{\mathbf{x}}_l + x_l \hat{\mathbf{x}}_\kappa) = h_1 h_2 h_3 \left(\frac{1}{h_l} \mathbb{E}_1^\kappa(\mathbf{r}) \hat{\mathbf{x}}_l + \frac{1}{h_\kappa} \mathbb{E}_1^l(\mathbf{r}) \hat{\mathbf{x}}_\kappa \right), \quad \kappa, l = 1,2,3, \quad \kappa \neq l, \tag{91}$$

and

$$\begin{aligned} \nabla \mathbb{E}_3^{2\kappa-1}(\mathbf{r}) &= \frac{h_1 h_2 h_3}{h_\kappa} (\Lambda_\kappa - \alpha_1^2)(\Lambda_\kappa - \alpha_2^2)(\Lambda_\kappa - \alpha_3^2) \left[\hat{\mathbf{x}}_\kappa \left(\sum_{i=1}^3 \frac{x_i^2}{\Lambda_\kappa - \alpha_i^2} + 1 \right) + 2 x_\kappa \sum_{i=1}^3 \frac{x_i \hat{\mathbf{x}}_i}{\Lambda_\kappa - \alpha_i^2} \right] \\ &\equiv \nabla \mathbb{E}_3^{2\kappa-1}(\Lambda_\kappa), \quad \kappa = 1,2,3, \end{aligned} \tag{92}$$

$$\nabla \mathbb{E}_3^{2\kappa}(\mathbf{r}) = \nabla \mathbb{E}_3^{2\kappa-1}(\Lambda_\kappa'), \quad \kappa = 1,2,3, \tag{93}$$

$$\nabla \mathbb{E}_3^7(\mathbf{r}) = h_1^2 h_2^2 h_3^2 \sum_{i=1}^{3} \frac{x_1 x_2 x_3}{x_i} \hat{\mathbf{x}}_i = h_1 h_2 h_3 \sum_{i=1}^{3} \frac{1}{h_i} \mathbb{E}_2^{6-i}(\mathbf{r}) \hat{\mathbf{x}}_i. \tag{94}$$

The form of the stress tensor (49) requires the double action of the gradient operator on the following ellipsoidal harmonics:

$$\nabla \otimes \nabla \mathbb{E}_0^1(\mathbf{r}) = \tilde{\mathbf{0}}, \tag{95}$$

$$\nabla \otimes \nabla \mathbb{E}_1^\kappa(\mathbf{r}) = \tilde{\mathbf{0}}, \quad \kappa = 1,2,3, \tag{96}$$

$$\begin{aligned} \nabla \otimes \nabla \mathbb{E}_2^1(\mathbf{r}) &= 2(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2) \sum_{i=1}^{3} \frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{\Lambda - \alpha_i^2} \\ &= 2(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2) \mathbb{E}_0^1(\mathbf{r}) \sum_{i=1}^{3} \frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{\Lambda - \alpha_i^2} \equiv \nabla \otimes \nabla \mathbb{E}_2^1(\Lambda), \end{aligned} \tag{97}$$

$$\nabla \otimes \nabla \mathbb{E}_2^2(\mathbf{r}) = \nabla \otimes \nabla \mathbb{E}_2^1(\Lambda'), \tag{98}$$

$$\begin{aligned} \nabla \otimes \nabla \mathbb{E}_2^{6-\kappa}(\mathbf{r}) &= h_1 h_2 h_3 h_\kappa \sum_{i=1}^{3} (1 - \delta_{\kappa i})(\hat{\mathbf{x}}_{6-(\kappa+i)} \otimes \hat{\mathbf{x}}_i) \\ &= h_1 h_2 h_3 h_\kappa \mathbb{E}_0^1(\mathbf{r}) \sum_{i=1}^{3} (1 - \delta_{\kappa i})(\hat{\mathbf{x}}_{6-(\kappa+i)} \otimes \hat{\mathbf{x}}_i), \quad \kappa = 1,2,3 \end{aligned} \tag{99}$$

and with equivalent notation for every $\kappa, l = 1,2,3$ and $\kappa \neq l$,

$$\nabla \otimes \nabla \mathbb{E}_2^{\kappa+l}(\mathbf{r}) = \frac{h_1^2 h_2^2 h_3^2}{h_\kappa h_l} (\hat{\mathbf{x}}_\kappa \otimes \hat{\mathbf{x}}_l + \hat{\mathbf{x}}_l \otimes \hat{\mathbf{x}}_\kappa) = \frac{h_1^2 h_2^2 h_3^2}{h_\kappa h_l} \mathbb{E}_0^1(\mathbf{r})(\hat{\mathbf{x}}_\kappa \otimes \hat{\mathbf{x}}_l + \hat{\mathbf{x}}_l \otimes \hat{\mathbf{x}}_\kappa) \tag{100}$$

and

$$\begin{aligned} \nabla \otimes \nabla \mathbb{E}_3^{2\kappa-1}(\mathbf{r}) &= \frac{2 h_1 h_2 h_3}{h_\kappa} (\Lambda_\kappa - \alpha_1^2)(\Lambda_\kappa - \alpha_2^2)(\Lambda_\kappa - \alpha_3^2) \\ &\quad \times \left[\sum_{i=1}^{3} \frac{x_\kappa}{\Lambda_\kappa - \alpha_i^2} (\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i) + \sum_{i=1}^{3} \frac{x_i}{\Lambda_\kappa - \alpha_i^2} (\hat{\mathbf{x}}_\kappa \otimes \hat{\mathbf{x}}_i + \hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_\kappa) \right] \\ &= \frac{2}{h_\kappa} (\Lambda_\kappa - \alpha_1^2)(\Lambda_\kappa - \alpha_2^2)(\Lambda_\kappa - \alpha_3^2) \\ &\quad \times \left[h_\kappa \mathbb{E}_1^\kappa(\mathbf{r}) \sum_{i=1}^{3} \frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{\Lambda_\kappa - \alpha_i^2} + \sum_{i=1}^{3} \frac{h_i \mathbb{E}_1^i(\mathbf{r})}{\Lambda_\kappa - \alpha_i^2} (\hat{\mathbf{x}}_\kappa \otimes \hat{\mathbf{x}}_i + \hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_\kappa) \right] \\ &\equiv \nabla \otimes \nabla \mathbb{E}_3^{2\kappa-1}(\Lambda_\kappa), \quad \kappa = 1,2,3, \end{aligned} \tag{101}$$

$$\nabla \otimes \nabla \mathbb{E}_3^{2\kappa}(\mathbf{r}) = \nabla \otimes \nabla \mathbb{E}_3^{2\kappa-1}(\Lambda_\kappa'), \quad \kappa = 1,2,3, \tag{102}$$

$$\nabla \otimes \nabla \mathbb{E}_3^7(\mathbf{r}) = h_1^2 h_2^2 h_3^2 \sum_{i,j=1}^{3} (1 - \delta_{ij}) \frac{x_1 x_2 x_3}{x_i x_j} (\hat{\mathbf{x}}_j \otimes \hat{\mathbf{x}}_i) = h_1^2 h_2^2 h_3^2 \sum_{i,j=1}^{3} (1 - \delta_{ij}) \frac{\hat{\mathbf{x}}_j \otimes \hat{\mathbf{x}}_i}{h_i h_j} \mathbb{E}_1^{6-(i+j)}(\mathbf{r}). \tag{103}$$

Unfortunately, it is not possible to write similar Cartesian expressions for the gradient of the external harmonic eigenmodes, because of the existence of the elliptic integrals (30) in relation (84). As we shall see later, this is the reason for the appearance of a number of difficulties in the application of the boundary conditions. Thus, we keep a mixed ellipsoidal-Cartesian formula of the above-mentioned expressions. In view of Eq. (30), we obtain

$$I_n^{m\prime}(\rho) = -\frac{1}{[E_n^m(\rho)]^2\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}, \quad \rho \in [h_2, +\infty) \tag{104}$$

and according to relations (21) and (22)

$$\nabla \mathbb{F}_n^m(\mathbf{r}) = (2n+1)\left[I_n^m(\rho)(\nabla \mathbb{E}_n^m(\mathbf{r})) - \frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\frac{\mathbb{E}_n^m(\mathbf{r})}{[E_n^m(\rho)]^2}\right]. \tag{105}$$

Although expression (105) is the simplest one possible it is still problematic because of the appearance of the vectorial factor

$$\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = \frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}, \quad \rho \in [h_2, +\infty), \quad \mu \in [h_3, h_2], \quad \nu \in [-h_3, h_3]. \tag{106}$$

This problem becomes even more complicated in the case of the double action of the gradient operator on the external harmonics, where

$$\begin{aligned}\nabla \otimes \nabla \mathbb{F}_n^m(\mathbf{r}) = (2n+1)[&I_n^m(\rho)(\nabla \otimes \nabla \mathbb{E}_n^m(\mathbf{r})) + \nabla I_n^m(\rho) \otimes \nabla \mathbb{E}_n^m(\mathbf{r}) + \nabla \mathbb{E}_n^m(\mathbf{r}) \otimes \nabla I_n^m(\rho) \\ &+ \mathbb{E}_n^m(\mathbf{r})(\nabla \otimes \nabla I_n^m(\rho))]\end{aligned} \tag{107}$$

for $n=0,1,2,\ldots$ and $m=1,2,\ldots,2n+1$. The dyadic $\nabla \otimes \nabla \mathbb{E}_n^m$ has been introduced earlier, and we can easily obtain the following relation:

$$\nabla I_n^m(\rho) = -\frac{\hat{\boldsymbol{\rho}}}{[E_n^m(\rho)]^2\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} = -\frac{1}{[E_n^m(\rho)]^2}\mathbf{R}^{\mathrm{el}}(\mathbf{r}), \quad \mathbf{r} \in \Omega(\mathbb{R}^3). \tag{108}$$

As far as the factor $\nabla \otimes \nabla I_n^m$ is concerned that appears in (107), we actually need the formula

$$\nabla \otimes \hat{\boldsymbol{\rho}} = \frac{\rho}{h_\rho}\left[\frac{\hat{\boldsymbol{\mu}} \otimes \hat{\boldsymbol{\mu}}}{\rho^2-\mu^2} + \frac{\hat{\boldsymbol{\nu}} \otimes \hat{\boldsymbol{\nu}}}{\rho^2-\nu^2}\right] + \frac{\mu}{h_\mu}\frac{\hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\mu}}}{\rho^2-\mu^2} + \frac{\nu}{h_\nu}\frac{\hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\nu}}}{\rho^2-\nu^2} \tag{109}$$

with the metric coefficients given by Eq. (21) and

$$\frac{\partial}{\partial \rho}\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = \frac{\partial}{\partial \rho}\left(\frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\right), \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{110}$$

which is also written as

$$\begin{aligned}\frac{\partial}{\partial \rho}\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = \frac{1}{(\rho^2-\mu^2)(\rho^2-\nu^2)}\Bigg\{&-\frac{2\rho(2\rho^2-\mu^2-\nu^2)}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\hat{\boldsymbol{\rho}} + \frac{1}{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}[(2\rho^2-h_3^2-h_2^2)x_1\hat{\mathbf{x}}_1 \\ &+ (2\rho^2-h_2^2)x_2\hat{\mathbf{x}}_2 + (2\rho^2-h_3^2)x_3\hat{\mathbf{x}}_3]\Bigg\}\end{aligned} \tag{111}$$

or in ellipsoidal coordinates alone

$$\frac{\partial}{\partial\rho}\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = \frac{1}{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\rho^2-\mu^2)(\rho^2-\nu^2)} \times\left[-2\rho(2\rho^2-\mu^2-\nu^2)\frac{\rho}{h_\rho}\hat{\boldsymbol{\rho}}+(\rho^2-\nu^2)\frac{\mu}{h_\mu}\hat{\boldsymbol{\mu}}+(\rho^2-\mu^2)\frac{\nu}{h_\nu}\hat{\boldsymbol{\nu}}\right],\quad \mathbf{r}\in\Omega(\mathbb{R}^3). \tag{112}$$

These formulas seem to be complicated, but they are given in the appropriate form for the application of the boundary condition (53).

The nature of condition (51), restricts the degree of the velocity field (46) to one. Hence, we use ellipsoidal harmonics of degree $n\leqslant 2$, which provide the appropriate flow fields that are adequate for most applications. Besides, these terms are enough to calculate the most important term of the velocity. Consequently, we observe that the potential $\mathbf{\Phi}$ in (36) must be of degree one and the potential Φ_0 in (37) must be of degree two in the surface variables μ and ν. This implies that all the coefficients $\mathbf{e}_n^{(i)m}$, $\mathbf{e}_n^{(e)m}$ for $n>2$ and $d_n^{(i)m}$, $d_n^{(e)m}$ for $n>3$, vanish, i.e.,

$$\mathbf{e}_n^{(i)m}=\mathbf{e}_n^{(e)m}=\mathbf{0},\quad n=2,3,\ldots,\quad m=1,2,\ldots,2n+1 \tag{113}$$

and

$$d_n^{(i)m}=d_n^{(e)m}=0,\quad n=3,4,\ldots,\quad m=1,2,\ldots,2n+1. \tag{114}$$

Hence, the expansions (46)–(49) degenerate to the following finite sums, where for particles of a particular size, the first term of the series is enough for most real applications. Our aim is to calculate the terms of the flow fields, which correspond to ellipsoidal harmonics of degree less or equal than two. Inserting the restrictions (113) and (114) into the flow fields, we conclude the finite dimensional projections that correspond to the first term of the velocity field, denoted by $\mathbf{v}^{(0)}$, $P^{(0)}$, $\boldsymbol{\omega}^{(0)}$, and $\widetilde{\mathbf{\Pi}}^{(0)}$. Thus,

$$\mathbf{v}^{(0)}(\mathbf{r})=\frac{1}{2}\Bigg\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\left[\mathbf{e}_n^{(i)m}\cdot(\widetilde{\mathbf{I}}\mathbb{E}_n^m(\mathbf{r})-\mathbf{r}\otimes\nabla\mathbb{E}_n^m(\mathbf{r}))+\mathbf{e}_n^{(e)m}\cdot(\widetilde{\mathbf{I}}\mathbb{F}_n^m(\mathbf{r})-\mathbf{r}\otimes\nabla\mathbb{F}_n^m(\mathbf{r}))\right] -\sum_{n=0}^{2}\sum_{m=1}^{2n+1}\left[d_n^{(i)m}\nabla\,\mathbb{E}_n^m(\mathbf{r})+d_n^{(e)m}\nabla\,\mathbb{F}_n^m(\mathbf{r})\right]\Bigg\},\quad \mathbf{r}\in\Omega(\mathbb{R}^3) \tag{115}$$

defines the *first term* of the velocity field,

$$P^{(0)}(\mathbf{r})=P_0-\mu_0\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\{\mathbf{e}_n^{(i)m}\cdot\nabla\mathbb{E}_n^m(\mathbf{r})+\mathbf{e}_n^{(e)m}\cdot\nabla\mathbb{F}_n^m(\mathbf{r})\}=p^{(0)}(\mathbf{r})+\rho_0 gh,\quad \mathbf{r}\in\Omega(\mathbb{R}^3) \tag{116}$$

defines the *first term* of the total pressure field,

$$\boldsymbol{\omega}^{(0)}(\mathbf{r})=\frac{1}{2}\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\{\nabla\mathbb{E}_n^m(\mathbf{r})\times\mathbf{e}_n^{(i)m}+\nabla\mathbb{F}_n^m(\mathbf{r})\times\mathbf{e}_n^{(e)m}\},\quad \mathbf{r}\in\Omega(\mathbb{R}^3) \tag{117}$$

defines the *first term* of the vorticity field, and

$$\widetilde{\mathbf{\Pi}}^{(0)}(\mathbf{r})=-p^{(0)}(\mathbf{r})\widetilde{\mathbf{I}}-\mu_0\Bigg\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\left[(\mathbf{e}_n^{(i)m}\cdot\mathbf{r})\,\nabla\otimes\nabla\mathbb{E}_n^m(\mathbf{r})+(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})\,\nabla\otimes\nabla\mathbb{F}_n^m(\mathbf{r})\right] +\sum_{n=0}^{2}\sum_{m=1}^{2n+1}\left[d_n^{(i)m}\nabla\otimes\nabla\mathbb{E}_n^m(\mathbf{r})+d_n^{(e)m}\nabla\otimes\nabla\mathbb{F}_n^m(\mathbf{r})\right]\Bigg\},\quad \mathbf{r}\in\Omega(\mathbb{R}^3) \tag{118}$$

defines the *first term* of the stress tensor field. Of course, the remaining coefficients $\mathbf{e}_0^{(i)1}$, $\mathbf{e}_0^{(e)1}$ for $n=0$ and $\mathbf{e}_1^{(i)\kappa}$, $\mathbf{e}_1^{(e)\kappa}$, $\kappa=1,2,3$ for $n=1$, as well as the coefficients $d_0^{(i)1}$, $d_0^{(e)1}$ for $n=0$, $d_1^{(i)\kappa}$, $d_1^{(e)\kappa}$, $\kappa=1,2,3$ for $n=1$ and $d_2^{(i)1}$, $d_2^{(e)1}$, $d_2^{(i)2}$, $d_2^{(e)2}$, $d_2^{(i)6-\kappa}$, $d_2^{(e)6-\kappa}$, $\kappa=1,2,3$ or $d_2^{(i)\kappa+l}$, $d_2^{(e)\kappa+l}$, $\kappa,l=1,2,3$, $\kappa\neq l$ for $n=2$ have to be determined from the boundary conditions (51)–(53).

Application of the BCs (51)–(53) to the velocity (115) and to the stress tensor (118). By virtue of the initial definitions (50), we insert the velocity field (115) to the boundary condition (51) on the surface S_a of the solid ellipsoid and we conclude that

$$2(\mathbf{U}+\boldsymbol{\Omega}\times\mathbf{r})=\left\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}[(\mathbf{e}_n^{(i)m}+(2n+1)I_n^m(\rho)\mathbf{e}_n^{(e)m})\cdot(\tilde{\mathbf{I}}\mathbb{E}_n^m(\mathbf{r})-\mathbf{r}\otimes\nabla\mathbb{E}_n^m(\mathbf{r}))]-\sum_{n=0}^{2}\sum_{m=1}^{2n+1}[(d_n^{(i)m}+(2n+1)I_n^m(\rho)d_n^{(e)m})\nabla\mathbb{E}_n^m(\mathbf{r})]\right\}+\mathbf{R}^{\mathrm{el}}(\mathbf{r})\left\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}[(2n+1)(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})\times[E_n^m(\rho)]^{-2}\mathbb{E}_n^m(\mathbf{r})]+\sum_{n=0}^{2}\sum_{m=1}^{2n+1}[(2n+1)d_n^{(e)m}[E_n^m(\rho)]^{-2}\mathbb{E}_n^m(\mathbf{r})]\right\},\quad \rho=\rho_a, \tag{119}$$

where we have used Eqs. (84) and (105) as well as the complicated ellipsoidal factor (106) for every $\mu\in[h_3,h_2]$ and $\nu\in[-h_3,h_3]$. The three sums in the first curly brace on the right-hand side of (119) are of the first degree in the variables μ, ν. The two sums inside the second curly brace are of the second degree. We observe that due to the factor $\mathbf{R}^{\mathrm{el}}$ it is not possible to express the second curly brace in terms of a finite expression of surface ellipsoidal harmonics. Therefore, in practice, it is impossible to evaluate the coefficients from BC (119) explicitly. Nevertheless, since the harmonic potentials $\boldsymbol{\Phi}$ and Φ_0 of the general solution (4) and (5) are not independent,[17] the corresponding d's and $\mathbf{e}$'s coefficients are also not independent as well. Thus, based on the flexibility of the Papkovich–Neuber differential representation, we *choose* to express the $d_n^{(e)m}$ in terms of the $\mathbf{e}_n^{(e)m}$ in such a way that the two sums on the right-hand side of (119), which are multiplied by $\mathbf{R}^{\mathrm{el}}$, vanish for $\mathbf{r}\in S_a$. When this is done the "bad term" of the BC (119) will disappear and we can apply orthogonality to obtain relations between the rest unknown coefficients $d_n^{(i)m}$, $e_n^{(i)m}$, and $e_n^{(e)m}$. In that sense, the use of the aforementioned *technique* on $\rho=\rho_a$ forms the key to our method. For $\rho=\rho_a$ the vanishing of the ellipsoidal part of the boundary condition (119) implies that

$$\left\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}[(2n+1)(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})[E_n^m(\rho)]^{-2}\mathbb{E}_n^m(\mathbf{r})]+\sum_{n=0}^{2}\sum_{m=1}^{2n+1}[(2n+1)d_n^{(e)m}[E_n^m(\rho)]^{-2}\mathbb{E}_n^m(\mathbf{r})]\right\}=0,\quad \mathbf{r}\in S_a. \tag{120}$$

Representing now the factor $\mathbf{r}\mathbb{E}_n^m$ via surface ellipsoidal harmonics at $\rho=\rho_a$ with the aim of the formulas (67), (68), and (76)–(80), as well as relations (A20), (A32), and (A33) from the Appendix and using orthogonality arguments, the assumption (120) provides the following relations between the coefficients, i.e.,

$$d_0^{(e)1}=-h_1h_2h_3\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i}, \tag{121}$$

$$d_1^{(e)\kappa}=-\frac{h_\kappa(E_1^\kappa(\rho_a))^2}{3h_1h_2h_3}(\mathbf{e}_0^{(e)1}\cdot\hat{\mathbf{x}}_\kappa),\quad \kappa=1,2,3, \tag{122}$$

$$d_2^{(e)1}=\frac{h_1h_2h_3}{5(\Lambda-\Lambda')}E_2^1(\rho_a)\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda-\alpha_i^2)}, \tag{123}$$

$$d_2^{(e)2} = -\frac{h_1 h_2 h_3}{5(\Lambda - \Lambda')} E_2^2(\rho_a) \sum_{i=1}^{3} \frac{(\mathbf{e}_1^{(e)i} \cdot \hat{\mathbf{x}}_i)}{h_i(\Lambda' - \alpha_i^2)}, \tag{124}$$

$$d_2^{(e)\kappa+l} = -\frac{3}{5h_1 h_2 h_3}[h_\kappa (E_1^\kappa(\rho_a))^2 (\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa) + h_l (E_1^l(\rho_a))^2 (\mathbf{e}_1^{(e)\kappa} \cdot \hat{\mathbf{x}}_l)] \tag{125}$$

for $\kappa, l = 1,2,3$, $\kappa \neq l$. Having expressed the external d-coefficients as a function of the external $\mathbf{e}$-coefficients and according to the *technique* (120), the ellipsoidal part of the boundary condition (119) is not present any more and eventually it becomes

$$2(\mathbf{U} + \boldsymbol{\Omega} \times \mathbf{r}) = \left\{ \sum_{n=0}^{1} \sum_{m=1}^{2n+1} [(\mathbf{e}_n^{(i)m} + (2n+1) I_n^m(\rho) \mathbf{e}_n^{(e)m}) \cdot (\tilde{\mathbf{I}} \mathbb{E}_n^m(\mathbf{r}) - \mathbf{r} \otimes \nabla \mathbb{E}_n^m(\mathbf{r}))] \right.$$
$$\left. - \sum_{n=0}^{2} \sum_{m=1}^{2n+1} [(d_n^{(i)m} + (2n+1) I_n^m(\rho) d_n^{(e)m}) \nabla \mathbb{E}_n^m(\mathbf{r})] \right\}, \quad \mathbf{r} \in S_a. \tag{126}$$

In order to handle the condition (126) properly, we perform the following actions. First we use the Cartesian form of the solid ellipsoidal harmonics $\mathbb{E}_n^m$ and of the gradient acting on it $\nabla \mathbb{E}_n^m$ from (67), (68), and (86)–(91), respectively. Next we calculate the factor $\mathbf{r} \otimes \nabla \mathbb{E}_n^m$ in Cartesian form and finally, by virtue of the definitions (38), of Eqs. (76) and (77), of the connection formulas (121)–(124) and of the orthogonality relation (34), the condition (126), after long and tedious calculations, results

$$\frac{h_1 h_2 h_3}{h_\kappa} d_1^{(i)\kappa} = -2(\mathbf{U} \cdot \hat{\mathbf{x}}_\kappa) + (\mathbf{e}_0^{(i)1} \cdot \hat{\mathbf{x}}_\kappa) + [I_0^1(\rho_a) + (E_1^\kappa(\rho_a))^2 I_1^\kappa(\rho_a)](\mathbf{e}_0^{(e)1} \cdot \hat{\mathbf{x}}_\kappa), \quad \kappa = 1,2,3, \tag{127}$$

as well as

$$-\left[\frac{(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2)}{(\Lambda - \alpha_\kappa^2)} \frac{d_2^{(i)1}}{h_1 h_2 h_3} + \frac{(\Lambda' - \alpha_1^2)(\Lambda' - \alpha_2^2)(\Lambda' - \alpha_3^2)}{(\Lambda' - \alpha_\kappa^2)} \frac{d_2^{(i)2}}{h_1 h_2 h_3} \right]$$
$$= \frac{(\Lambda - \alpha_1^2)(\Lambda - \alpha_2^2)(\Lambda - \alpha_3^2)}{(\Lambda - \alpha_\kappa^2)} \frac{E_2^1(\rho_a) I_2^1(\rho_a)}{(\Lambda - \Lambda')} \sum_{i=1}^{3} \frac{(\mathbf{e}_1^{(e)i} \cdot \hat{\mathbf{x}}_i)}{h_i(\Lambda - \alpha_i^2)}$$
$$- \frac{(\Lambda' - \alpha_1^2)(\Lambda' - \alpha_2^2)(\Lambda' - \alpha_3^2)}{(\Lambda' - \alpha_\kappa^2)} \frac{E_2^2(\rho_a) I_2^2(\rho_a)}{(\Lambda - \Lambda')} \sum_{i=1}^{3} \frac{(\mathbf{e}_1^{(e)i} \cdot \hat{\mathbf{x}}_i)}{h_i(\Lambda' - \alpha_i^2)} \tag{128}$$

and

$$h_\kappa[(\mathbf{e}_1^{(i)l} \cdot \hat{\mathbf{x}}_\kappa) + 3I_1^l(\rho_a)(\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa)] - h_l[(\mathbf{e}_1^{(i)\kappa} \cdot \hat{\mathbf{x}}_l) + 3I_1^\kappa(\rho_a)(\mathbf{e}_1^{(e)\kappa} \cdot \hat{\mathbf{x}}_l)] - h_1 h_2 h_3$$
$$\times [d_2^{(i)\kappa+l} + 5I_2^{\kappa+l}(\rho_a) d_2^{(e)\kappa+l}] = \frac{2\lambda_{\kappa l}}{h_{6-(\kappa+l)}} (\boldsymbol{\Omega} \cdot \hat{\mathbf{x}}_{6-(\kappa+l)}), \quad \kappa, l = 1,2,3, \quad \kappa \neq l, \tag{129}$$

where

$$\lambda_{\kappa l} = \begin{cases} +1, & (\kappa, l) = (1,3),(2,1),(3,2) \\ -1, & (\kappa, l) = (1,2),(2,3),(3,1) \end{cases}, \quad \kappa, l = 1,2,3, \quad \kappa \neq l. \tag{130}$$

The next step now will be the investigation of the second condition on the boundary $\rho = \rho_b$ of the fictitious ellipsoidal surface S_b. In view of the boundary condition (52) we obtain

$$\left\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}[(\hat{\boldsymbol{\rho}}\cdot\mathbf{e}_n^{(i)m})\mathbb{E}_n^m(\mathbf{r})-(\mathbf{e}_n^{(i)m}\cdot\mathbf{r})(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{E}_n^m(\mathbf{r}))+(\hat{\boldsymbol{\rho}}\cdot\mathbf{e}_n^{(e)m})\mathbb{F}_n^m(\mathbf{r})-(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{F}_n^m(\mathbf{r}))]\right.$$
$$\left.-\sum_{n=0}^{2}\sum_{m=1}^{2n+1}[d_n^{(i)m}(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{E}_n^m(\mathbf{r}))+d_n^{(e)m}(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{F}_n^m(\mathbf{r}))]\right\}=0,\quad \mathbf{r}\in S_b, \tag{131}$$

where we utilized the assumption for the velocity field (115). It is obvious that the appearance of the unit normal vector $\hat{\boldsymbol{\rho}}$, provided by expression (25), increases the degree of the harmonic eigenmodes in Eq. (131) up to $n=2$. More specifically using the Cartesian-ellipsoidal formulas (67)–(72), (76)–(80), and (86)–(91), as well as

$$\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{F}_n^m(\mathbf{r})=(2n+1)\left[I_n^m(\rho)(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{E}_n^m(\mathbf{r}))-\frac{1}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\frac{\mathbb{E}_n^m(\mathbf{r})}{[E_n^m(\rho)]^2}\right] \tag{132}$$

for $\rho=\rho_b$ and $n=0,1,2$, $m=1,2,\ldots,2n+1$, we convert, after long calculations, condition (131) to a suitable form, which is appropriate for applying orthogonality via (34). Thus, after having produced the ellipsoidal form of the factors $(\hat{\boldsymbol{\rho}}\cdot\nabla\mathbb{E}_n^m)$ for $n=0,1,2$, $m=1,2,\ldots,2n+1$ and $(\hat{\boldsymbol{\rho}}\cdot\mathbf{e}_n^{(i/e)m})$, $(\mathbf{r}\cdot\mathbf{e}_n^{(i/e)m})$ for $n=0,1$, $m=1,2,\ldots,2n+1$, we apply orthogonality and obtain nine more relations involving the still unknown coefficients. The number of equations we obtain is a result of the scalar character of the boundary condition (131) and, of course, of the number of the surface ellipsoidal harmonics for $n\leqslant 2$. We mention that no indeterminacy appeared in our program and all the calculations were easily performed. Actually, orthogonality of the surface ellipsoidal harmonic $E_0^1(\mu)E_0^1(\nu)$ provides the already known relation (121), which is independent of the boundary. On the other hand, by orthogonality arguments of $E_1^\kappa(\mu)E_1^\kappa(\nu)$, $\kappa=1,2,3$ and relation (127) we evaluate the coefficient $\mathbf{e}_0^{(e)1}$ in the form

$$(\mathbf{e}_0^{(e)1}\cdot\hat{\mathbf{x}}_\kappa)=-\frac{2E_3^7(\rho_b)}{N_\kappa}(\mathbf{U}\cdot\hat{\mathbf{x}}_\kappa),\quad \kappa=1,2,3, \tag{133}$$

where

$$N_\kappa=E_3^7(\rho_b)[(I_0^1(\rho_b)-I_0^1(\rho_a))+(E_1^\kappa(\rho_a))^2(I_1^\kappa(\rho_b)-I_1^\kappa(\rho_a))]+(E_1^\kappa(\rho_b))^2-(E_1^\kappa(\rho_a))^2,\quad \kappa=1,2,3. \tag{134}$$

Until now, four of the nine equations, which came up from boundary condition (131), have been used. The five remaining equations correspond to orthogonality on the surface ellipsoidal harmonics of degree $n=2$ for every $m=1,2,\ldots,5$. Hence, the surface ellipsoidal harmonics $E_2^1(\mu)E_2^1(\nu)$ and $E_2^2(\mu)E_2^2(\nu)$ lead to

$$-5d_2^{(e)1}+2E_2^1(\rho_b)E_3^7(\rho_b)(d_2^{(i)1}+5I_2^1(\rho_b)d_2^{(e)1})+\frac{h_1h_2h_3E_2^1(\rho_b)}{(\Lambda-\Lambda')}\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda-\alpha_i^2)}=0 \tag{135}$$

and

$$-5d_2^{(e)2}+2E_2^2(\rho_b)E_3^7(\rho_b)(d_2^{(i)2}+5I_2^2(\rho_b)d_2^{(e)2})-\frac{h_1h_2h_3E_2^2(\rho_b)}{(\Lambda-\Lambda')}\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda'-\alpha_i^2)}=0, \tag{136}$$

respectively, where the identity (A20) has been used. Inserting Eqs. (123) and (124) to relation (128), we obtain the following 2×2 homogeneous system of linear equations, in the variables $(d_2^{(i)1}+5I_2^1(\rho_a)d_2^{(e)1})$ and $(d_2^{(i)2}+5I_2^2(\rho_a)d_2^{(e)2})$. For example, for $\kappa=1,2$ we have

$$(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)(d_2^{(i)1}+5I_2^1(\rho_a)d_2^{(e)1})+(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)(d_2^{(i)2}+5I_2^2(\rho_a)d_2^{(e)2})=0 \tag{137}$$

and

$$(\Lambda-\alpha_1^2)(\Lambda-\alpha_3^2)(d_2^{(i)1}+5I_2^1(\rho_a)d_2^{(e)1})+(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_3^2)(d_2^{(i)2}+5I_2^2(\rho_a)d_2^{(e)2})=0. \quad (138)$$

Since the determinant is not zero, it follows that

$$d_2^{(i)1}+5I_2^1(\rho_a)d_2^{(e)1}=d_2^{(i)2}+5I_2^2(\rho_a)d_2^{(e)2}=0 \quad (139)$$

or

$$d_2^{(i)1}=-5I_2^1(\rho_a)d_2^{(e)1}, \quad d_2^{(i)2}=-5I_2^2(\rho_a)d_2^{(e)2}. \quad (140)$$

We could come up with the same result if we had used expression (128) for $\kappa=1,3$ or for $\kappa=2,3$.

Our next step involves the substitution of the results (140) to (135) and (136), to obtain

$$\frac{h_1h_2h_3E_2^1(\rho_b)}{(\Lambda-\Lambda')}\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda-\alpha_i^2)}\left[1-\frac{E_2^1(\rho_a)}{E_2^1(\rho_b)}+2E_3^7(\rho_b)E_2^1(\rho_a)(I_2^1(\rho_b)-I_2^1(\rho_a))\right]=0 \quad (141)$$

and

$$\frac{h_1h_2h_3E_2^2(\rho_b)}{(\Lambda-\Lambda')}\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda'-\alpha_i^2)}\left[1-\frac{E_2^2(\rho_a)}{E_2^2(\rho_b)}+2E_3^7(\rho_b)E_2^2(\rho_a)(I_2^2(\rho_b)-I_2^2(\rho_a))\right]=0, \quad (142)$$

where the nonvanishing of the two square brackets implies

$$\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda-\alpha_i^2)}=\sum_{i=1}^{3}\frac{(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i)}{h_i(\Lambda'-\alpha_i^2)}=0. \quad (143)$$

As a consequence relations (123) and (124) force the coefficients $d_2^{(e)1}$ and $d_2^{(e)2}$ to vanish and then from (140) we obtain

$$d_2^{(i)1}=d_2^{(e)1}=0 \quad (144)$$

and

$$d_2^{(i)2}=d_2^{(e)2}=0. \quad (145)$$

In addition, working on the two summations (143) and with proper use of identities (A22) and (A23) we conclude that

$$(\mathbf{e}_1^{(e)3}\cdot\hat{\mathbf{x}}_3)=\frac{h_3}{h_1}(\mathbf{e}_1^{(e)1}\cdot\hat{\mathbf{x}}_1)=\frac{h_3}{h_2}(\mathbf{e}_1^{(e)2}\cdot\hat{\mathbf{x}}_2), \quad (146)$$

where two of the three diagonal scalar coefficients of $\mathbf{e}_1^{(e)\kappa}$, $\kappa=1,2,3$ have been evaluated via the third one. Finally, by means of orthogonality on the BC (131) of $E_2^{6-\kappa}(\mu)E_2^{6-\kappa}(\nu)$, $\kappa=1,2,3$, we derive the following elaborate relation, valid on the ellipsoidal surface S_b:

$$\begin{aligned}&E_3^7(\rho_b)h_{6-(\kappa+l)}^2\{h_\kappa[(\mathbf{e}_1^{(i)l}\cdot\hat{\mathbf{x}}_\kappa)+3I_1^l(\rho_b)(\mathbf{e}_1^{(e)l}\cdot\hat{\mathbf{x}}_\kappa)]-h_l[(\mathbf{e}_1^{(i)\kappa}\cdot\hat{\mathbf{x}}_l)+3I_1^\kappa(\rho_b)(e_1^{(\mathbf{e})\kappa}\cdot\hat{\mathbf{x}}_l)]\}\\&\quad+h_1h_2h_3[5d_2^{(e)\kappa+l}-E_3^7(\rho_b)((E_1^\kappa(\rho_b))^2+(E_1^l(\rho_b))^2)(d_2^{(i)\kappa+l}+5I_2^{\kappa+l}(\rho_b)d_2^{(e)\kappa+l})]\\&\quad+3[h_\kappa(E_1^\kappa(\rho_b))^2(\mathbf{e}_1^{(e)l}\cdot\hat{\mathbf{x}}_\kappa)+h_l(E_1^l(\rho_b))^2(\mathbf{e}_1^{(e)\kappa}\cdot\hat{\mathbf{x}}_l)]=0, \quad \kappa,l=1,2,3, \quad \kappa>l, \end{aligned} \quad (147)$$

where by $\kappa>l$ we mean all the possible combinations such as $(\kappa,l)=(2,1),(3,1),(3,2)$. At this point, we take advantage of the particular form of the three pairs of equations in relation (129) by substracting one relation from the other of each pair that contains the same components of the applied vorticity $\mathbf{\Omega}$, to obtain the three equations

$$d_2^{(i)\kappa+l}+5I_2^{\kappa+l}(\rho_a)d_2^{(e)\kappa+l}=0\Rightarrow d_2^{(i)\kappa+l}=-5I_2^{\kappa+l}(\rho_a)d_2^{(e)\kappa+l}, \quad \kappa,l=1,2,3, \quad \kappa\neq l. \quad (148)$$

If we return to condition (147), we observe that we have to deal with three different relations for every value of $(\kappa,l)=(2,1),(3,1),(3,2)$. Therefore, by virtue of (148) and inserting (125) and (129) to (147), we conclude the symmetric expression

$$P_\kappa^l h_\kappa(\mathbf{e}_1^{(e)l}\cdot\hat{\mathbf{x}}_\kappa)+P_l^\kappa h_l(\mathbf{e}_1^{(e)\kappa}\cdot\hat{\mathbf{x}}_l)=R^{\kappa+l},\quad \kappa,l=1,2,3,\quad \kappa\neq l \tag{149}$$

with

$$P_\kappa^l=\frac{\rho_b^2-\rho_a^2}{(E_2^{\kappa+l}(\rho_b))^2}+E_3^7(\rho_b)\frac{\alpha_l^2-\alpha_\kappa^2}{(E_2^{\kappa+l}(\rho_b))^2}(I_1^l(\rho_b)-I_1^l(\rho_a))+E_3^7(\rho_b)(E_1^\kappa(\rho_a))^2\left(\frac{1}{(E_1^\kappa(\rho_b))^2}+\frac{1}{(E_1^l(\rho_b))^2}\right)$$
$$\times(I_2^{\kappa+l}(\rho_b)-I_2^{\kappa+l}(\rho_a)) \tag{150}$$

for every $\kappa,l=1,2,3$ and $\kappa\neq l$, and

$$R^{\kappa+l}=\frac{2h_{6-(\kappa+l)}\Omega_{6-(\kappa+l)}}{3}(-1)^{\kappa+l}\frac{E_1^{6-(\kappa+l)}(\rho_b)}{E_2^{\kappa+l}(\rho_b)}$$
$$=\frac{2h_1h_2h_3\Omega_{6-(\kappa+l)}}{3}(-1)^{\kappa+l}\frac{E_3^7(\rho_b)}{(E_2^{\kappa+l}(\rho_b))^2},\quad \kappa,l=1,2,3,\quad \kappa\neq l. \tag{151}$$

Recapitulating, we see that the effect of the two first boundary conditions (51) and (52) to the evaluation of the unknown coefficients, in the flow fields (115)–(118), is to obtain nine unknown coefficients $\mathbf{e}_1^{(e)\kappa}$, $\kappa=1,2,3$ from five relations, two from (146) and three from (149). Thus, there remain four coefficients that must be calculated explicitly from the final condition (53) on the ellipsoid $\rho=\rho_b$. However, the diagonal components of $\mathbf{e}_1^{(e)\kappa}$, $\kappa=1,2,3$, appearing in Eq. (146), will not enter the flow fields, as we shall see later on. This means that in practice we need to calculate three instead of four coefficients.

The application of the boundary condition (53), where in view of the stress tensor field (118), and according to the form of the unit dyadic (26) gives

$$\hat{\boldsymbol{\rho}}\cdot\tilde{\mathbf{I}}\cdot(\tilde{\mathbf{I}}-\hat{\boldsymbol{\rho}}\otimes\hat{\boldsymbol{\rho}})=\hat{\boldsymbol{\rho}}\cdot\tilde{\mathbf{I}}\cdot(\hat{\boldsymbol{\mu}}\otimes\hat{\boldsymbol{\mu}}+\hat{\boldsymbol{\nu}}\otimes\hat{\boldsymbol{\nu}})=\mathbf{0}, \tag{152}$$

provides the following expression in terms of the unit normal vector $\hat{\boldsymbol{\rho}}$,

$$(\tilde{\mathbf{I}}-\hat{\boldsymbol{\rho}}\otimes\hat{\boldsymbol{\rho}})\cdot\left\{\sum_{n=0}^{1}\sum_{m=1}^{2n+1}[(\mathbf{e}_n^{(i)m}\cdot\mathbf{r})(\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{E}_n^m(\mathbf{r}))+(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})(\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{F}_n^m(\mathbf{r}))]\right.$$
$$\left.+\sum_{n=0}^{2}\sum_{m=1}^{2n+1}[d_n^{(i)m}(\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{E}_n^m(\mathbf{r}))+d_n^{(e)m}(\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{F}_n^m(\mathbf{r}))]\right\}=\mathbf{0},\quad \mathbf{r}\in S_b. \tag{153}$$

In order to deal with condition (153) we perform the following operations. First, we use the double action of the gradient operator on the interior solid ellipsoidal harmonics provided by relations (95)–(100) for the evaluation of the $\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{E}_n^m$, $n=0,1,2$, $m=1,2,\ldots,2n+1$. Then, using the expression

$$\hat{\boldsymbol{\rho}}=\frac{E_3^7(\rho)}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\sum_{i=1}^{3}\frac{x_i\hat{\mathbf{x}}_i}{(E_1^i(\rho))^2},\quad \rho=\rho_b \tag{154}$$

for the unit outward normal on S_b, we obtain

$$\hat{\boldsymbol{\rho}}\cdot\nabla I_n^m(\rho)=-\frac{1}{[E_n^m(\rho)]^2\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}},\quad \rho=\rho_b, \tag{155}$$

because

$$\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = \frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}, \quad \rho=\rho_b. \tag{156}$$

Also, according to the definition (22), and with the help of relation (108), we reach at

$$\begin{aligned}\hat{\boldsymbol{\rho}}\cdot\nabla\nabla I_n^m(\rho) &= \frac{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\frac{\partial}{\partial\rho}\nabla I_n^m(\rho)\\ &= -\frac{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\left[\frac{\partial}{\partial\rho}[E_n^m(\rho)]^{-2}\mathbf{R}^{\mathrm{el}}(\mathbf{r})+[E_n^m(\rho)]^{-2}\frac{\partial}{\partial\rho}\mathbf{R}^{\mathrm{el}}(\mathbf{r})\right]\end{aligned} \tag{157}$$

for $\rho=\rho_b$. Some easy algebra on Eq. (157) furnishes

$$\hat{\boldsymbol{\rho}}\cdot\nabla\nabla I_n^m(\rho) = \frac{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}{[E_n^m(\rho)]^3\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}}\left[2E_n^{m\prime}(\rho)\mathbf{R}^{\mathrm{el}}(\mathbf{r})-E_n^m(\rho)\frac{\partial\mathbf{R}^{\mathrm{el}}(\mathbf{r})}{\partial\rho}\right], \tag{158}$$

where $\rho=\rho_b$, whilst the ρ-derivative of the factor $\mathbf{R}^{\mathrm{el}}$ has been calculated through its Cartesian (111) and its ellipsoidal (112) representation. Substituting expressions (155) and (158) into the double gradient of the exterior solid ellipsoidal harmonics (107), inserting relations (86)–(91) and (95)–(100) at (107) and using

$$\hat{\boldsymbol{\rho}}\otimes\hat{\boldsymbol{\rho}} = E_3^7(\rho)\sum_{i=1}^{3}\frac{x_i}{(E_1^i(\rho))^2}\hat{\mathbf{x}}_i\otimes\mathbf{R}^{\mathrm{el}}(\mathbf{r}) = E_3^7(\rho)\sum_{i=1}^{3}\frac{x_i}{(E_1^i(\rho))^2}\mathbf{R}^{\mathrm{el}}(\mathbf{r})\otimes\hat{\mathbf{x}}_i, \quad \rho=\rho_b, \tag{159}$$

the boundary condition (153), on $\rho=\rho_b$, is written as

$$\begin{aligned}&(-\widetilde{\mathbf{I}}+\hat{\boldsymbol{\rho}}\otimes\hat{\boldsymbol{\rho}})\cdot\left\{\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}\frac{\partial\mathbf{R}^{\mathrm{el}}(\mathbf{r})}{\partial\rho}\left[\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\frac{(2n+1)}{[E_n^m(\rho)]^2}\mathbb{E}_n^m(\mathbf{r})(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})\right.\right.\\ &\left.+\sum_{n=0}^{2}\sum_{m=1}^{2n+1}\frac{(2n+1)}{[E_n^m(\rho)]^2}\mathbb{E}_n^m(\mathbf{r})d_n^{(e)m}\right]-\sum_{m=1}^{5}[(d_2^{(i)m}+5I_2^m(\rho)d_2^{(e)m})\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}(\hat{\boldsymbol{\rho}}\cdot\nabla\otimes\nabla\mathbb{E}_n^m(\mathbf{r}))]\\ &\left.+\left[\sum_{n=0}^{1}\sum_{m=1}^{2n+1}\frac{(2n+1)}{[E_n^m(\rho)]^2}\nabla\mathbb{E}_n^m(\mathbf{r})(\mathbf{e}_n^{(e)m}\cdot\mathbf{r})+\sum_{n=0}^{2}\sum_{m=1}^{2n+1}\frac{(2n+1)}{[E_n^m(\rho)]^2}\nabla\mathbb{E}_n^m(\mathbf{r})d_n^{(e)m}\right]\right\}=\mathbf{0}, \quad \rho=\rho_b.\end{aligned} \tag{160}$$

A careful observation of condition (160) reveals the difficulty to manipulate it in Cartesian coordinates and the impossibility of direct application of orthogonality arguments. Nevertheless, the use of purely ellipsoidal terms simplifies Eq. (160). In particular, we perform all the necessary calculations, use (67)–(72), (76)–(80), and (86)–(91), insert the already known coefficients, and use the fact that

$$\begin{aligned}(\hat{\boldsymbol{\mu}}\otimes\hat{\boldsymbol{\mu}}+\hat{\boldsymbol{\nu}}\otimes\hat{\boldsymbol{\nu}})\cdot\sum_{i=1}^{3}x_i\hat{\mathbf{x}}_i\frac{3h_1h_2h_3}{h_i(E_1^i(\rho_b))^2}(\mathbf{e}_1^{(e)i}\cdot\hat{\mathbf{x}}_i) &= 3h_1h_2(\mathbf{e}_1^{(e)3}\cdot\hat{\mathbf{x}}_3)(\hat{\boldsymbol{\mu}}\otimes\hat{\boldsymbol{\mu}}+\hat{\boldsymbol{\nu}}\otimes\hat{\boldsymbol{\nu}})\cdot\sum_{i=1}^{3}\frac{x_i\hat{\mathbf{x}}_i}{(E_1^i(\rho_b))^2}\\ &= 3h_1h_2(\mathbf{e}_1^{(e)3}\cdot\hat{\mathbf{x}}_3)(\hat{\boldsymbol{\mu}}\otimes\hat{\boldsymbol{\mu}}+\hat{\boldsymbol{\nu}}\otimes\hat{\boldsymbol{\nu}})\cdot\left(\frac{h_\rho}{\rho_b}\hat{\boldsymbol{\rho}}\right)=\mathbf{0},\\ \rho&=\rho_b,\end{aligned} \tag{161}$$

to rewrite the boundary condition (160) in the simple form

$$\mathrm{A}(\rho_b,\mu,\nu)\hat{\boldsymbol{\mu}}+\mathrm{B}(\rho_b,\mu,\nu)\hat{\boldsymbol{\nu}}=\mathbf{0}, \tag{162}$$

where the quantities A and B contain surface ellipsoidal harmonics, the coefficients under evaluation, and some known constants. The orthogonality of the unit normal vectors $\hat{\boldsymbol{\mu}}$ and $\hat{\boldsymbol{\nu}}$ implies that A and B are equal to zero, i.e.,

$$\sum_{i=1}^{3} B_i\left(\frac{(E_1^i(\rho_a))^2}{x^2-\alpha_1^2+\alpha_i^2}-1\right)E_1^i(\mu)E_1^i(\nu)+\sum_{\substack{i,j=1\\ i\neq j}}^{3}\left(\frac{A_i^j+(E_1^i(\rho_b))^2C_i^j}{x^2-\alpha_1^2+\alpha_i^2}-C_i^j\right)E_2^{i+j}(\mu)E_2^{i+j}(\nu)=0, \tag{163}$$

where x assumes the values μ and ν, and

$$A_\kappa^l=\frac{3(E_1^\kappa(\rho_b))^2(\rho_b^2-\rho_a^2)h_l}{E_2^{\kappa+l}(\rho_b)}(\mathbf{e}_1^{(e)\kappa}\cdot\hat{\mathbf{x}}_l),\quad \kappa,l=1,2,3,\quad \kappa\neq l, \tag{164}$$

$$B_\kappa=\frac{2E_3^7(\rho_b)E_1^\kappa(\rho_b)h_\kappa U_\kappa}{N_\kappa},\quad \kappa=1,2,3, \tag{165}$$

with N_κ, $\kappa=1,2,3$ given in (134), while

$$C_\kappa^l=\frac{3}{E_2^{\kappa+l}(\rho_b)}[-h_\kappa(E_1^\kappa(\rho_a))^2(\mathbf{e}_1^{(e)l}\cdot\hat{\mathbf{x}}_\kappa)+E_3^7(\rho_b)(E_1^\kappa(\rho_b))^2(I_2^{\kappa+l}(\rho_b)-I_2^{\kappa+l}(\rho_a))(h_\kappa(E_1^\kappa(\rho_a))^2(\mathbf{e}_1^{(e)l}\cdot\hat{\mathbf{x}}_\kappa)$$
$$+h_l(E_1^l(\rho_a))^2(\mathbf{e}_1^{(e)\kappa}\cdot\hat{\mathbf{x}}_l))],\quad \kappa,l=1,2,3,\quad \kappa\neq l. \tag{166}$$

On the other hand, $(\mathbf{e}_1^{(e)\kappa}\cdot\hat{\mathbf{x}}_l)$ for $\kappa,l=1,2,3$ and $\kappa\neq l$ provide the six unknown coefficients, which must be evaluated with the aid of (149).

At this stage we have to deal with two major problems. The first one reflects the difficulty of applying orthogonality of the surface ellipsoidal harmonics $E_n^m(\mu)E_n^m(\nu)$ in (163), and the second concerns the number of the equations that we have to satisfy. In fact, we are left with five relations (three from (149) and two from (163)) to evaluate the six coefficients mentioned earlier. As far as the first difficulty is concerned, we introduce the new set of elliptic integrals on the surface of the ellipsoid $\rho=\rho_s$,

$$J_{n,\kappa}^m(\rho_s)=\int\int_{\rho=\rho_s}\frac{E_n^m(\mu)E_n^m(\nu)}{(x^2-\alpha_1^2+\alpha_\kappa^2)\sqrt{\rho_s^2-\mu^2}\sqrt{\rho_s^2-\nu^2}}\mathrm{d}S,\quad \kappa=1,2,3 \tag{167}$$

for $\mu\in[h_3,h_2]$, $\nu\in[-h_3,h_3]$, where we define the following values of x:

$$\text{for } x=\mu\Rightarrow J_{n,\kappa}^m\equiv M_{n,\kappa}^m \quad\text{and for } x=\nu\Rightarrow J_{n,\kappa}^m\equiv N_{n,\kappa}^m. \tag{168}$$

Therefore, we multiply (163) by the weighting function (33) and use the orthogonality relation (34) and the zeroth degree eigenfunction $E_0^1(\mu)E_0^1(\nu)\equiv 1$ to obtain

$$\sum_{\substack{i,j=1\\ i\neq j}}^{3} X_i^j h_i(\mathbf{e}_1^{(e)j}\cdot\hat{\mathbf{x}}_i)=Q_x,\quad x=\mu,\nu,\quad \mu\in[h_3,h_2],\quad \nu\in[-h_3,h_3], \tag{169}$$

with

$$X_\kappa^l = \frac{3}{E_2^{\kappa+l}(\rho_b)}\{(E_1^l(\rho_b))^4 J_{2,l}^{\kappa+l}(\rho_b) - (E_1^\kappa(\rho_a))^2[J_{2,l}^{\kappa+l}(\rho_b)(E_1^l(\rho_b))^2(1 - E_3^7(\rho_b)(E_1^l(\rho_b))^2(I_2^{\kappa+l}(\rho_b) - I_2^{\kappa+l}(\rho_a))) + J_{2,\kappa}^{\kappa+l}(\rho_b)(E_1^\kappa(\rho_b))^2(1 - E_3^7(\rho_b)(E_1^\kappa(\rho_b))^2(I_2^{\kappa+l}(\rho_b) - I_2^{\kappa+l}(\rho_a)))]\} \tag{170}$$

for every $\kappa, l = 1,2,3$ and $\kappa \neq l$, and

$$Q_x = -\sum_{i=1}^{3} \frac{2E_3^7(\rho_b)E_1^i(\rho_b)(E_1^i(\rho_a))^2 h_i U_i}{N_i} J_{1,i}^i(\rho_b) \tag{171}$$

for $x = \mu, \nu$. The constants N_κ, $\kappa = 1,2,3$ are given in (134). Relation (169) refers to two different equations for the values of $x = \mu, \nu$ containing the two different types of elliptic integrals appearing in (168). Despite the simplification of the final boundary condition by the introduction of a new set of elliptic integrals, our already reduced potential problem remains undetermined as far as one coefficient is concerned. Indeed, combining (149) with relation (169) we see that we are missing one more condition. Hence, we adopt, once more, our previous analysis, which springs from the flexibility of the Papkovich–Neuber differential representation.[17] In fact, since we have two boundary surfaces to satisfy our conditions, we use our technique twice, one for each boundary. Therefore, in terms of the elliptic integrals

$$L_{n,\kappa}^m(\rho_s) = N_{n,\kappa}^m(\rho_s) - M_{n,\kappa}^m(\rho_s) = \int\int_{\rho=\rho_s} \frac{(\mu^2 - \nu^2)E_n^m(\mu)E_n^m(\nu)}{(\mu^2 - \alpha_1^2 + \alpha_\kappa^2)(\nu^2 - \alpha_1^2 + \alpha_\kappa^2)} \frac{\mathrm{d}S}{\sqrt{\rho_s^2 - \mu^2}\sqrt{\rho_s^2 - \nu^2}}, \quad \kappa = 1,2,3, \tag{172}$$

we substract by parts Eq. (169) for the different values of $x = \mu, \nu$ and we *choose* the following condition for the unknown coefficients, i.e.,

$$Q_\kappa^l h_\kappa(\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa) + Q_l^\kappa h_l(\mathbf{e}_1^{(e)\kappa} \cdot \hat{\mathbf{x}}_l) \equiv \tfrac{1}{3}(Q_\nu - Q_\mu) = Q, \quad \kappa, l = 1,2,3, \quad \kappa \neq l, \tag{173}$$

where

$$Q_\kappa^l = \frac{3}{E_2^{\kappa+l}(\rho_b)}\{(E_1^l(\rho_b))^4 L_{2,l}^{\kappa+l}(\rho_b) - (E_1^\kappa(\rho_a))^2[L_{2,l}^{\kappa+l}(\rho_b)(E_1^l(\rho_b))^2(1 - E_3^7(\rho_b)(E_1^l(\rho_b))^2(I_2^{\kappa+l}(\rho_b) - I_2^{\kappa+l}(\rho_a))) + L_{2,\kappa}^{\kappa+l}(\rho_b)(E_1^\kappa(\rho_b))^2(1 - E_3^7(\rho_b)(E_1^\kappa(\rho_b))^2(I_2^{\kappa+l}(\rho_b) - I_2^{\kappa+l}(\rho_a)))]\} \tag{174}$$

and

$$Q = -\frac{2E_3^7(\rho_b)}{3}\sum_{i=1}^{3} \frac{E_1^i(\rho_b)(E_1^i(\rho_a))^2 h_i U_i}{N_i} L_{1,i}^i(\rho_b), \tag{175}$$

with the constants N_κ, $\kappa = 1,2,3$ given by (134). This way we generate an additional relation for the evaluation of the coefficients through condition (173). This is the second and final restriction to our problem, which provided the three explicit equations (173).

We solve a system of six equations for the last six unknown coefficients $(\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa)$, $\kappa, l = 1,2,3$, $\kappa \neq l$, taking into account relations (149) and (173). Defining $(\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa) \equiv e_\kappa^l$, we rewrite the solution as

$$(\mathbf{e}_1^{(e)l} \cdot \hat{\mathbf{x}}_\kappa) \equiv \mathbf{e}_\kappa^l = \frac{P_l^\kappa Q - Q_l^\kappa R^{\kappa+l}}{h_\kappa(P_l^\kappa Q_\kappa^l - P_\kappa^l Q_l^\kappa)}, \quad \kappa, l = 1,2,3, \quad \kappa \neq l, \tag{176}$$

where the constants P_κ^l, Q_κ^l, $R^{\kappa+l}$ for $\kappa, l = 1,2,3$, $\kappa \neq l$, and Q are given by (150), (174), (151), and (175), respectively. It is easily proved that $P_l^\kappa Q_\kappa^l - P_\kappa^l Q_l^\kappa \neq 0$. Hence, having used all the boundary conditions (51)–(53) we evaluated all the coefficients.

The final step contains the presentation of a mixed Cartesian-ellipsoidal form of the *first terms*

of the flow fields formulated by expressions (115)–(118), using the information (67)–(112). Introducing all the evaluated coefficients from the previous steps and using the Cartesian-ellipsoidal formulation of the interior and exterior ellipsoidal harmonics, as well as their gradients, some extended algebra on the velocity field (115) leads to

$$\mathbf{v}^{(0)}(\mathbf{r}) = \mathbf{U} + \mathbf{\Omega} \times \mathbf{r} + \mathbf{Z}(\rho) + \sum_{j=1}^{3} \mathbf{H}_j(\rho)\mathbb{E}_1^j(\mathbf{r}) + \frac{\hat{\boldsymbol{\rho}}}{2\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} \times \left[\sum_{j=1}^{3} \Theta_j(\rho)\mathbb{E}_1^j(\mathbf{r}) + \sum_{\substack{i,j=1 \\ i\neq j}}^{3} \Phi_i^j(\rho)\mathbb{E}_2^{i+j}(\mathbf{r}) \right], \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{177}$$

where for every $\rho_a \leqslant \rho \leqslant \rho_b$ we define the vector quantities

$$\mathbf{Z}(\rho) = -E_3^7(\rho_b)\mathbf{U} \cdot \sum_{i=1}^{3} [(I_0^1(\rho) - I_0^1(\rho_a)) + (E_1^i(\rho_a))^2(I_1^i(\rho) - I_1^i(\rho_a))] \frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{N_i} \tag{178}$$

and

$$\mathbf{H}_\kappa(\rho) = \frac{3}{2} \sum_{\substack{i=1 \\ i\neq\kappa}}^{3} \{h_i e_i^\kappa (I_1^\kappa(\rho) - I_1^\kappa(\rho_a)) - h_\kappa e_\kappa^i (I_1^i(\rho) - I_1^i(\rho_a)) + [h_i e_i^\kappa (E_1^i(\rho_a))^2 + h_\kappa e_\kappa^i (E_1^\kappa(\rho_a))^2](I_2^{i+\kappa}(\rho) - I_2^{i+\kappa}(\rho_a))\} \frac{\hat{\mathbf{x}}_i}{h_i}, \quad \kappa = 1,2,3. \tag{179}$$

Furthermore, the scalar products for the same interval $\rho_a \leqslant \rho \leqslant \rho_b$ are

$$\Theta_\kappa(\rho) = -\frac{2h_\kappa E_3^7(\rho_b)}{h_1h_2h_3} \frac{(\mathbf{U} \cdot \hat{\mathbf{x}}_\kappa)}{N_\kappa} \left[1 - \left(\frac{E_1^\kappa(\rho_a)}{E_1^\kappa(\rho)} \right)^2 \right], \quad \kappa = 1,2,3 \tag{180}$$

and

$$\Phi_\kappa^l(\rho) = \frac{3h_\kappa}{h_1h_2h_3} e_\kappa^l \left[1 - \left(\frac{E_1^\kappa(\rho_a)}{E_1^\kappa(\rho)} \right)^2 \right] \frac{1}{(E_1^l(\rho))^2}, \quad \kappa,l = 1,2,3, \quad \kappa \neq l. \tag{181}$$

Once the constants N_κ for $\kappa=1,2,3$ in (134) and e_κ^l for $\kappa,l=1,2,3$, $\kappa \neq l$ in (176) are calculated, the velocity field is obtained in terms of the applied fields $\mathbf{U}$ and $\mathbf{\Omega}$ via Eq. (50). The total pressure field (116) assumes the expression

$$P^{(0)}(\mathbf{r}) = P_0 + \mu_0 \frac{E_3^7(\rho)}{(\rho^2-\mu^2)(\rho^2-\nu^2)} \left[\sum_{j=1}^{3} \frac{\Theta_j(\rho)}{\rho^2-\rho_a^2} \mathbb{E}_1^j(\mathbf{r}) + \frac{3}{h_1h_2h_3} \sum_{\substack{i,j=1 \\ i\neq j}}^{3} \frac{h_i e_i^j}{(E_2^{i+j}(\rho))^2} \mathbb{E}_2^{i+j}(\mathbf{r}) \right]$$
$$= p^{(0)}(\mathbf{r}) + \rho_0 g h, \quad \mathbf{r} \in \Omega(\mathbb{R}^3), \tag{182}$$

where the coefficients e_κ^l for $\kappa,l=1,2,3$, $\kappa \neq l$ are given by (176), where the identity (A4) and formula

$$\sum_{i=1}^{3} \frac{x_i^2}{(E_1^i(\rho))^2} = \frac{h_\rho^2}{\rho^2}, \quad \rho_a \leqslant \rho \leqslant \rho_b \tag{183}$$

have been used. The reference constant h is appropriately chosen depending upon the physical requirements. Here, we must mention that the constant pressure of reference P_0 is written as

$$P_0 = -\mu_0 h_1 h_2 h_3 \sum_{j=1}^{3} \frac{1}{h_j}(\mathbf{e}_1^{(i)j} \cdot \hat{\mathbf{x}}_j), \tag{184}$$

which actually contains the coefficients $(\mathbf{e}_1^{(i)\kappa} \cdot \hat{\mathbf{x}}_\kappa)$, $\kappa = 1,2,3$ that were not evaluated by the boundary conditions. Nevertheless, P_0 enter Stokes equations (1) and (2) under the action of the gradient operator, providing that way $\nabla P_0 = \mathbf{0}$. Thus, we can use the very same physical arguments to specify this constant pressure. As far as the vorticity field is concerned we can expand relation (117) in view of (67)–(112), and substitute the obtained coefficients. Nevertheless, an easier root is followed with respect to the definition (3), by taking the rotation of the velocity field (177). After the application of certain identities we obtain

$$\nabla \times \mathbf{U} = \mathbf{0}, \quad \nabla \times (\mathbf{\Omega} \times \mathbf{r}) = 2\mathbf{\Omega} \tag{185}$$

and some extensive algebra leads to

$$\nabla \times \frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2 - \mu^2}\sqrt{\rho^2 - \nu^2}} = \mathbf{0}, \quad \mathbf{r} \in \Omega(\mathbb{R}^3). \tag{186}$$

Matching (185) and (186) and utilizing definitions (178)–(181), we arrive at

$$\begin{aligned}\boldsymbol{\omega}^{(0)}(\mathbf{r}) = \mathbf{\Omega} + \frac{h_1 h_2 h_3}{2} \sum_{j=1}^{3} \frac{1}{h_j}(\hat{\mathbf{x}}_j \times \mathbf{H}_j(\rho)) + \frac{\sqrt{\rho^2 - h_3^2}\sqrt{\rho^2 - h_2^2}\hat{\boldsymbol{\rho}}}{2\sqrt{\rho^2 - \mu^2}\sqrt{\rho^2 - \nu^2}} \times \left[\mathbf{Z}'(\rho) + \sum_{j=1}^{3} \mathbf{H}_j'(\rho)\mathbb{E}_1^j(\mathbf{r}) \right] \\ - \frac{h_1 h_2 h_3 \hat{\boldsymbol{\rho}}}{4\sqrt{\rho^2 - \mu^2}\sqrt{\rho^2 - \nu^2}} \times \left[\sum_{j=1}^{3} \frac{\Theta_j(\rho)}{h_j}\hat{\mathbf{x}}_j + \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \Phi_i^j(\rho)\left(\frac{\mathbb{E}_1^i(\mathbf{r})}{h_j}\hat{\mathbf{x}}_j + \frac{\mathbb{E}_1^j(\mathbf{r})}{h_i}\hat{\mathbf{x}}_i \right) \right]\end{aligned} \tag{187}$$

for every $\mathbf{r} \in \Omega(\mathbb{R}^3)$, where $\mathbf{\Omega}$ stands for the constant vorticity (50), with

$$\mathbf{Z}'(\rho) = \frac{E_3^7(\rho_b)\mathbf{U}}{\sqrt{\rho^2 - h_3^2}\sqrt{\rho^2 - h_2^2}} \cdot \sum_{i=1}^{3} \frac{\hat{\mathbf{x}}_i \otimes \hat{\mathbf{x}}_i}{N_i}\left[1 + \left(\frac{E_1^i(\rho_a)}{E_1^i(\rho)} \right)^2 \right], \quad \rho_a \leqslant \rho \leqslant \rho_b \tag{188}$$

and

$$\begin{aligned}\mathbf{H}_\kappa'(\rho) = \frac{3}{2\sqrt{\rho^2 - h_3^2}\sqrt{\rho^2 - h_2^2}} \sum_{\substack{i=1 \\ i \neq \kappa}}^{3} \frac{\hat{\mathbf{x}}_i}{h_i}\Bigg\{ - \frac{h_i e_i^\kappa}{(E_1^\kappa(\rho))^2}\left[1 + \left(\frac{E_1^i(\rho_a)}{E_1^i(\rho)} \right)^2 \right] \\ + \frac{h_\kappa e_\kappa^i}{(E_1^i(\rho))^2}\left[1 - \left(\frac{E_1^\kappa(\rho_a)}{E_1^\kappa(\rho)} \right)^2 \right] \Bigg\}, \quad \kappa = 1,2,3\end{aligned} \tag{189}$$

for $\rho_a \leqslant \rho \leqslant \rho_b$. The constants N_κ for $\kappa = 1,2,3$ are given by (134) and the coefficients e_κ^l for $\kappa, l = 1,2,3$, $\kappa \neq l$ are provided by (176). Next, in order to obtain the expression for the stress tensor field, we use identities (39)–(45) so that

$$\nabla \otimes \mathbf{U} = (\nabla \otimes \mathbf{U})^{\mathsf{T}} = \widetilde{\mathbf{0}}, \quad \nabla \otimes (\mathbf{\Omega} \times \mathbf{r}) = \mathbf{\Omega} \times \widetilde{\mathbf{I}} \tag{190}$$

and we use relations (22) and (109) to obtain the dyadic $\widetilde{\mathbf{S}}$ in the form

$$\widetilde{\mathbf{S}}(\mathbf{r}) \equiv \nabla \otimes \left(\frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} \right) + \left[\nabla \otimes \left(\frac{\hat{\boldsymbol{\rho}}}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} \right) \right]^{\mathsf{T}}$$
$$= \frac{2}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} \left\{ \frac{\rho}{h_\rho} \left[-\left(\frac{1}{\rho^2-\mu^2} + \frac{1}{\rho^2-\nu^2} \right) \hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\rho}} + \frac{\hat{\boldsymbol{\mu}} \otimes \hat{\boldsymbol{\mu}}}{\rho^2-\mu^2} + \frac{\hat{\boldsymbol{\nu}} \otimes \hat{\boldsymbol{\nu}}}{\rho^2-\nu^2} \right] \right.$$
$$\left. + \frac{\mu}{h_\mu(\rho^2-\mu^2)} (\hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\mu}} + \hat{\boldsymbol{\mu}} \otimes \hat{\boldsymbol{\rho}}) + \frac{\nu}{h_\nu(\rho^2-\nu^2)} (\hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\nu}} + \hat{\boldsymbol{\nu}} \otimes \hat{\boldsymbol{\rho}}) \right\}. \tag{191}$$

Further calculations lead to

$$\widetilde{\mathbf{\Pi}}^{(0)}(\mathbf{r}) = (\rho_0 g h - P^{(0)}(\mathbf{r}))\widetilde{\mathbf{I}} - \mu_0 \left\{ \frac{1}{h_\rho} (\hat{\boldsymbol{\rho}} \otimes \mathbf{Z}'(\rho) + \mathbf{Z}'(\rho) \otimes \hat{\boldsymbol{\rho}}) + \sum_{j=1}^{3} \left[\frac{\mathbb{E}_1^j(\mathbf{r})}{h_\rho} (\hat{\boldsymbol{\rho}} \otimes \mathbf{H}_j'(\rho) + \mathbf{H}_j'(\rho) \right.\right.$$
$$\left.\left. \otimes \hat{\boldsymbol{\rho}}) + \frac{h_1 h_2 h_3}{h_j} (\hat{\mathbf{x}}_j \otimes \mathbf{H}_j(\rho) + \mathbf{H}_j(\rho) \otimes \hat{\mathbf{x}}_j) \right] \right\} - \frac{\mu_0}{2} \widetilde{\mathbf{S}}(\mathbf{r}) \left[\sum_{j=1}^{3} \Theta_j(\rho) \mathbb{E}_1^j(\mathbf{r}) \right.$$
$$\left. + \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \Phi_i^j(\rho) \mathbb{E}_2^{i+j}(\mathbf{r}) \right] - \frac{\mu_0}{\sqrt{\rho^2-\mu^2}\sqrt{\rho^2-\nu^2}} \left\{ \frac{\hat{\boldsymbol{\rho}} \otimes \hat{\boldsymbol{\rho}}}{h_\rho} \left[\sum_{j=1}^{3} \Theta_j'(\rho) \mathbb{E}_1^j(\mathbf{r}) + \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \Phi_i^{j'}(\rho) \mathbb{E}_2^{i+j}(\mathbf{r}) \right] \right.$$
$$+ \frac{h_1 h_2 h_3}{2} \left[\sum_{j=1}^{3} \frac{\Theta_j(\rho)}{h_j} (\hat{\boldsymbol{\rho}} \otimes \hat{\mathbf{x}}_j + \hat{\mathbf{x}}_j \otimes \hat{\boldsymbol{\rho}}) + \sum_{\substack{i,j=1 \\ i \neq j}}^{3} \Phi_i^j(\rho) \left(\frac{\mathbb{E}_1^i(\mathbf{r})}{h_j} (\hat{\boldsymbol{\rho}} \otimes \hat{\mathbf{x}}_j + \hat{\mathbf{x}}_j \otimes \hat{\boldsymbol{\rho}}) \right.\right.$$
$$\left.\left.\left.\left. + \frac{\mathbb{E}_1^j(\mathbf{r})}{h_i} (\hat{\boldsymbol{\rho}} \otimes \hat{\mathbf{x}}_i + \hat{\mathbf{x}}_i \otimes \hat{\boldsymbol{\rho}}) \right) \right] \right\} \tag{192}$$

for $\mathbf{r} \in \Omega(\mathbb{R}^3)$, where $P^{(0)}$ is the total pressure (182), while in view of the applied field $\mathbf{U}$ (50)

$$\Theta_\kappa'(\rho) = -\frac{4 h_\kappa E_3^7(\rho_b)}{h_1 h_2 h_3} \frac{(\mathbf{U} \cdot \hat{\mathbf{x}}_\kappa)}{N_\kappa} \frac{(E_1^\kappa(\rho_a))^2}{(E_1^\kappa(\rho))^4} \rho, \quad \kappa = 1,2,3 \tag{193}$$

and

$$\Phi_\kappa^{l'}(\rho) = -\frac{6 h_\kappa}{h_1 h_2 h_3} \frac{\rho e_\kappa^l}{(E_1^l(\rho))^4} \left\{ 1 - \left(\frac{E_1^\kappa(\rho_a)}{E_1^\kappa(\rho)} \right)^2 \left[1 + \left(\frac{E_1^l(\rho)}{E_1^\kappa(\rho)} \right)^2 \right] \right\}, \quad \kappa,l = 1,2,3, \quad \kappa \neq l \tag{194}$$

for every $\rho_a \leqslant \rho \leqslant \rho_b$. We remind that the coefficients e_κ^l for $\kappa,l=1,2,3$, $\kappa \neq l$ are satisfied by (176), the metric coefficient h_ρ is given by Eq. (21), N_κ for $\kappa=1,2,3$ are provided by (134) and expressions (178)–(181), (188), and (189) have been used. Recapitulating, the *first terms*, of the velocity field (177), of the total pressure field (182), of the vorticity field (187), and of the stress tensor field (192) have been analytically calculated on the basis of the Happel-type boundary conditions.

V. GEOMETRICALLY DEGENERATE CASES

The strict inequalities

$$0 < \alpha_3 < \alpha_2 < \alpha_1 < +\infty \tag{195}$$

form the basic reason why the triaxial ellipsoid reflects the general anisotropy of the three-dimensional space. As it is well known,[20] the reduction of general results from the ellipsoidal to the spheroidal, or to the spherical geometry is not straightforward, since certain indeterminacies appear during the limiting process. This is due to the fact that the spherical system springs from a zero-dimensional manifold (i.e., the center), while the ellipsoidal system springs from a two-dimensional manifold (i.e., the focal ellipse). Nevertheless, formulas (A42)–(A51) ensure the appropriate reductions. In particular, we consider every case separately.

The geometrically degenerate cases of spheroids: The equality of the two of the axis (195) of an ellipsoid degenerates it to a spheroid, whose axial symmetry coincides with the third axis. More specific, *a prolate spheroid* is obtained whenever

$$0 < \alpha_3 = \alpha_2 < \alpha_1 < +\infty, \tag{196}$$

while the case of an *oblate spheroid* corresponds to

$$0 < \alpha_3 < \alpha_2 = \alpha_1 < +\infty. \tag{197}$$

The axis of symmetry is the x_1 axis for the prolate spheroid and the x_3 axis for the oblate spheroid. The asymptotic case of the *needle* can be reached by a prolate spheroid where

$$0 < \alpha_3 = \alpha_2 \ll \alpha_1 < +\infty, \tag{198}$$

while in the case where

$$0 < \alpha_3 \ll \alpha_2 = \alpha_1 < +\infty, \tag{199}$$

the oblate spheroid takes the shape of a circular *disk*. As far as the semifocal distances are concerned, we have that

$$h_1 = 0, \quad h_2 = h_3 = c, \quad c > 0 \tag{200}$$

for the case of a prolate spheroid with semifocal distance c, and

$$h_3 = 0, \quad h_1 = h_2 = \bar{c}, \quad \bar{c} > 0 \tag{201}$$

for the case of an oblate spheroid with semifocal distance $\bar{c}$. The simple transformation

$$c \to -i\bar{c}, \quad c, \bar{c} > 0 \tag{202}$$

allows the transition from the prolate to the oblate spheroid, while the replacement

$$\bar{c} \to ic, \quad c, \bar{c} > 0 \tag{203}$$

secures the converse. In terms of the notation $\tau \equiv \cosh \eta$, $\zeta \equiv \cos \theta$, and φ for $1 \leqslant \tau < +\infty$, $-1 \leqslant \zeta \leqslant 1$ and $\varphi \in [0, 2\pi)$, respectively, for the prolate spheroid, the corresponding results for the oblate spheroid can be obtained through the transformation

$$\tau \to i\lambda, \quad 1 \leqslant \tau < +\infty, \tag{204}$$

where $0 \leqslant \lambda \equiv \sinh \eta < +\infty$ is the characteristic variable of the oblate system λ, ζ, and φ. Obviously the inverse transformation

$$\lambda \to -i\tau, \quad 0 \leqslant \lambda < +\infty \tag{205}$$

leads to the converse. Consequently, from this point on we shall refer to the prolate spheroidal geometry, since the oblate spheroidal geometry is recovered via

$$\tau \to i\lambda, \quad c \to -i\bar{c}. \tag{206}$$

In terms of the unit normal vector $\hat{\boldsymbol{\tau}}$ for the prolate spheroidal coordinates, the ellipsoidal variables are connected with the τ, ζ, and φ by

$$\rho = c\tau, \quad \hat{\boldsymbol{\rho}} \to \hat{\boldsymbol{\tau}}, \quad \rho \in [h_2, +\infty), \quad 1 \leqslant \tau < +\infty \tag{207}$$

and

$$\frac{\mu\nu}{h_2 h_3} = \zeta, \tag{208}$$

$$\frac{\sqrt{\mu^2 - h_3^2}\sqrt{h_3^2 - \nu^2}}{h_1 h_3} = \sqrt{1-\zeta^2}\cos\varphi, \tag{209}$$

$$\frac{\sqrt{h_2^2 - \mu^2}\sqrt{h_2^2 - \nu^2}}{h_1 h_2} = \sqrt{1-\zeta^2}\sin\varphi, \tag{210}$$

whereas $\mu \in [h_3, h_2]$, $\nu \in [-h_3, h_3]$ and $1 \leqslant \tau < +\infty$, $\varphi \in [0, 2\pi)$. For $\alpha_2 = \alpha_3$ (prolate spheroid) the constants (63) provide

$$\lim_{\alpha_2 \to \alpha_3} \Lambda = \frac{2\alpha_1^2 + \alpha_2^2}{3}, \quad \lim_{\alpha_2 \to \alpha_3} \Lambda' = \alpha_2^2, \tag{211}$$

while as a consequence of the limits (211) for $\alpha_2 = \alpha_3$,

$$\lim_{\alpha_2 \to \alpha_3} (\Lambda - \Lambda') = \lim_{\alpha_2 \to \alpha_3} (\Lambda - \alpha_2^2) = \lim_{\alpha_2 \to \alpha_3} (\Lambda - \alpha_3^2) = \frac{2c^2}{3}, \tag{212}$$

$$\lim_{\alpha_2 \to \alpha_3} (\Lambda - \alpha_1^2) = -\frac{c^2}{3}, \tag{213}$$

$$\lim_{\alpha_2 \to \alpha_3} (\Lambda' - \alpha_1^2) = -c^2, \tag{214}$$

$$\lim_{\alpha_2 \to \alpha_3} (\Lambda' - \alpha_2^2) = \lim_{\alpha_2 \to \alpha_3} (\Lambda' - \alpha_3^2) = 0. \tag{215}$$

Moreover, the constants (65) for $\alpha_2 = \alpha_3$ ($\Lambda_2 = \Lambda_3$, $\Lambda_2' = \Lambda_3'$, prolate spheroid) become

$$\lim_{\alpha_2 \to \alpha_3} \left.\begin{matrix} \Lambda_\kappa \\ \Lambda_\kappa' \end{matrix}\right\} = \frac{2}{5}(\alpha_1^2 + 2\alpha_2^2) - \frac{1}{5}\alpha_\kappa^2 \pm \frac{1}{5}\left\{ 4(\alpha_1^4 + 2\alpha_2^4) - 3\alpha_\kappa^4 - \alpha_1^2\alpha_2^4\left[\left(\frac{1}{\alpha_1^2} + \frac{2}{\alpha_2^2}\right) + \frac{6}{\alpha_\kappa^2}\right]\right\}^{1/2}, \quad \kappa = 1,2, \tag{216}$$

where one can calculate the $(\Lambda_\kappa - \alpha_l^2)$ and $(\Lambda_\kappa' - \alpha_l^2)$ for $\kappa, l = 1,2,3$. On the other hand, the integrals I_n^m in prolate spheroidal geometry ($\alpha_2 = \alpha_3$)

$$\lim_{\alpha_2\to\alpha_3} I_n^m(\rho)=\int_\rho^{+\infty}\frac{\mathrm{d}u}{[\lim_{\alpha_2\to\alpha_3} E_n^m(u)]^2|u^2-\alpha_1^2+\alpha_2^2|},\quad \rho\in[h_2,+\infty) \tag{217}$$

for $n=0,1,\ldots$ and $m=1,2,\ldots,2n+1$ are no more elliptic and they can be evaluated with analytic manipulations. Specifically, the determination of I_0^1 demands the calculation of the corresponding integral (217) for $n=0$ and $m=1$ in terms of the variable τ, that is

$$\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)=\frac{1}{2c}\ln\frac{\tau+1}{\tau-1},\quad \rho\in[h_2,+\infty),\quad 1\leqslant\tau<+\infty. \tag{218}$$

The other elliptic integrals, which concern the already known exterior ellipsoidal harmonic eigenfunctions for degree $n=1,2,3$ and order $m=1,2,\ldots,2n+1$, are given explicitly in terms of the $\lim_{\alpha_2\to\alpha_3} I_0^1$ and their prolate spheroidal expressions ($\alpha_2=\alpha_3$) give

$$\lim_{\alpha_2\to\alpha_3} I_1^1(\rho)=\frac{1}{c^2}\left(\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{1}{c\tau}\right),\quad c>0, \tag{219}$$

$$\lim_{\alpha_2\to\alpha_3} I_1^2(\rho)=\lim_{\alpha_2\to\alpha_3} I_1^3(\rho)=-\frac{1}{2c^2}\left(\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{\tau}{c(\tau^2-1)}\right),\quad c>0, \tag{220}$$

$$\lim_{\alpha_2\to\alpha_3} I_2^1(\rho)=\frac{9}{4c^4}\left(\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{\tau}{c(3\tau^2-1)}\right),\quad c>0, \tag{221}$$

$$\lim_{\alpha_2\to\alpha_3} I_2^2(\rho)=\lim_{\alpha_2\to\alpha_3} I_2^5(\rho)=\frac{3}{8c^4}\left(\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{\tau(3\tau^2-5)}{3c(\tau^2-1)^2}\right),\quad c>0, \tag{222}$$

$$\lim_{\alpha_2\to\alpha_3} I_2^3(\rho)=\lim_{\alpha_2\to\alpha_3} I_2^4(\rho)=-\frac{3}{2c^4}\left(\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{3\tau^2-2}{3c\tau(\tau^2-1)}\right),\quad c>0. \tag{223}$$

Much more complicated calculations leads us to

$$\lim_{\alpha_2\to\alpha_3} I_3^1(\rho)=\frac{25}{c^6}\left(\frac{1}{4}\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{25\tau}{36c(5\tau^2-3)}-\frac{1}{9c\tau}\right), \tag{224}$$

$$\lim_{\alpha_2\to\alpha_3} I_3^2(\rho)=\lim_{\alpha_2\to\alpha_3} I_3^7(\rho)=\frac{1}{c^6}\left(\frac{15}{8}\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)+\frac{\tau}{4c(\tau^2-1)^2}-\frac{7\tau}{8c(\tau^2-1)}-\frac{1}{c\tau}\right), \tag{225}$$

$$\lim_{\alpha_2\to\alpha_3} I_3^3(\rho)=\lim_{\alpha_2\to\alpha_3} I_3^5(\rho)=-\frac{25}{c^6}\left(\frac{3}{16}\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{\tau}{32c(\tau^2-1)}-\frac{25\tau}{32c(5\tau^2-1)}\right), \tag{226}$$

$$\lim_{\alpha_2\to\alpha_3} I_3^4(\rho)=\lim_{\alpha_2\to\alpha_3} I_3^6(\rho)=-\frac{1}{c^6}\left(\frac{5}{16}\lim_{\alpha_2\to\alpha_3} I_0^1(\rho)-\frac{\tau}{6c(\tau^2-1)^3}+\frac{5\tau}{24c(\tau^2-1)^2}-\frac{5\tau}{16c(\tau^2-1)}\right) \tag{227}$$

for $c>0$. As far as the interior solid ellipsoidal harmonics as well as their gradients are concerned, their Cartesian representation easily implies the relative reductions. Finally, the limiting cases of the needle and of the disk are asymptotic reductions of the prolate and the oblate spheroidal geometry, respectively. For the *needle* we obtain

$$\alpha_1/\alpha_2 = \tau/\sqrt{\tau^2 - 1} \to +\infty, \quad 1 \leqslant \tau < +\infty, \tag{228}$$

and for the *disk* we obtain

$$\alpha_3/\alpha_2 = \lambda/\sqrt{\lambda^2 + 1} \to 0^+, \quad 0 \leqslant \lambda < +\infty. \tag{229}$$

The geometrically degenerate case of sphere: The sphere corresponds to

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha, \tag{230}$$

where α is the radius. In this case,

$$h_\kappa = 0, \quad \kappa = 1,2,3, \tag{231}$$

which means that all the semifocal distances of the ellipsoid coincide at the origin. Defining the limit from the ellipsoid to the sphere as "$\lim_{e\to s}$", the constants (63) give

$$\lim_{e\to s} \Lambda = \lim_{e\to s} \Lambda' = \alpha^2, \tag{232}$$

while from Eq. (65) we derive

$$\lim_{e\to s} \Lambda_\kappa = \lim_{e\to s} \Lambda'_\kappa = \alpha^2, \quad \kappa = 1,2,3 \tag{233}$$

so that

$$\lim_{e\to s}(\Lambda - \Lambda') = \lim_{e\to s}(\Lambda_\kappa - \Lambda'_\kappa) = 0, \quad \kappa = 1,2,3, \tag{234}$$

$$\lim_{e\to s}(\Lambda - \alpha_\kappa^2) = \lim_{e\to s}(\Lambda' - \alpha_\kappa^2) = 0, \quad \kappa = 1,2,3, \tag{235}$$

$$\lim_{e\to s}(\Lambda_\kappa - \alpha_l^2) = \lim_{e\to s}(\Lambda'_\kappa - \alpha_l^2) = 0, \quad \kappa,l = 1,2,3. \tag{236}$$

The intervals of variation of the variables μ and ν imply that

$$\lim_{e\to s} \mu = \lim_{e\to s} \nu = 0, \quad \kappa = 1,2,3. \tag{237}$$

In terms of the unit normal vector $\hat{\mathbf{r}}$ of the spherical system, the connection between the ellipsoidal variables and the corresponding spherical variables r, $\zeta \equiv \cos\theta$, and φ for $0 \leqslant r < +\infty$, $-1 \leqslant \zeta \leqslant 1$ and $\varphi \in [0, 2\pi)$ is

$$\lim_{e\to s} \rho = \lim_{e\to s}(\sqrt{\rho^2 - h_2^2}) = \lim_{e\to s}(\sqrt{\rho^2 - h_3^2}) = r, \quad \hat{\boldsymbol{\rho}} \to \hat{\mathbf{r}}, \quad \rho \in [h_2, +\infty), \quad r \geqslant 0 \tag{238}$$

for the radial component and

$$\frac{\mu\nu}{h_2 h_3} = \zeta, \tag{239}$$

$$\frac{\sqrt{\mu^2 - h_3^2}\sqrt{h_3^2 - \nu^2}}{h_1 h_3} = \sqrt{1 - \zeta^2}\cos\varphi, \tag{240}$$

$$\frac{\sqrt{h_2^2-\mu^2}\sqrt{h_2^2-\nu^2}}{h_1 h_2}=\sqrt{1-\zeta^2}\sin\varphi \tag{241}$$

for the angular dependence. The integrals I_n^m assume the values,

$$\lim_{e\to s} I_n^m(\rho)=\frac{1}{(2n+1)r^{2n+1}},\quad n\geqslant 0,\quad m=1,2,\ldots,2n+1,\quad \kappa=1,2,3 \tag{242}$$

for every $\rho\in[h_2,+\infty)$ and $r\geqslant 0$.

We mention that a proper reduction of our results for the velocity field (177) gives the *first term* of the series. The full solution of the above-mentioned Happel-type boundary value problem in spherical coordinates is given in Ref. 19, where the three-dimensional complete solution is obtained. For the sake of completeness, we provide the solution from Ref. 19 in the following.

If we define the sphere

$$B_r=\{\mathbf{r}\in\mathbb{R}^3 | x_1^2+x_2^2+x_3^2\leqslant r^2\}, \tag{243}$$

where

$$\mathbf{r}=\sum_{i=1}^{3} x_i\hat{\mathbf{x}}_i=r\zeta\hat{\mathbf{x}}_1+r\sqrt{1-\zeta^2}\cos\varphi\hat{\mathbf{x}}_2+r\sqrt{1-\zeta^2}\sin\varphi\hat{\mathbf{x}}_3, \tag{244}$$

then the *total* velocity assumes the form

$$\mathbf{v}^{(\text{sphere})}(\mathbf{r})=\mathbf{U}+\boldsymbol{\Omega}\times\mathbf{r}+\mathbf{Z}(r)+f(r)(x_1\mathbf{r}),\quad \mathbf{r}\in\Omega(\mathbb{R}^3). \tag{245}$$

We introduce the expression

$$\mathbf{Z}(r)=\frac{\mathbf{U}\cdot(\hat{\mathbf{x}}_1\otimes\hat{\mathbf{x}}_1)}{K}\left[-2(3\gamma^5+2)+4\gamma^5\left(\frac{r}{a}\right)^2+\left(\frac{a}{r}\right)^3+(2\gamma^5+3)\left(\frac{a}{r}\right)\right] \tag{246}$$

and

$$f(r)=\frac{1}{a^2}\left[(2\gamma^5+3)\left(\frac{a}{r}\right)^3-3\left(\frac{a}{r}\right)^5-2\gamma^5\right], \tag{247}$$

whereas

$$\gamma=\frac{a}{b}<1,\quad K=2-3\gamma+3\gamma^5-2\gamma^6,\quad \mathbf{U}=U_1\hat{\mathbf{x}}_1. \tag{248}$$

Note that, a,b are the radii of the concentric spheres of the corresponding Happel boundary value problem for Stokes flow around spherical particles.

VI. DISCUSSION

The physical interpretation of the mathematical problem analyzed in this work involves a method for solving three-dimensional Stokes flow problems with Happel-type boundary conditions. Based on this method we examine the flow in an ellipsoidal cell as a means of modeling flow through a swarm of ellipsoidal particles with the aim of the Papkovich–Neuber differential representation, which offers solutions for such problems in several orthogonal curvilinear geometries. The terms of major significance of the important physical flow fields such as the velocity, the total pressure, the vorticity, and the stress tensor are evaluated in closed form. The difficulty of this problem is focused on the determination of the coefficients, which characterize the nature of the corresponding potentials. This is caused by the appearance of certain indeterminacies, which reflect the complexity of the ellipsoidal geometry. The present work invoked a useful tool for dealing with nonaxisymmetric problems, which is the differential representation theory. The free-

dom that 3D representations offer, makes the solution of creeping flow problems within such domains feasible, a fact which is justified by the freedom, which this kind of representation offers. Consequently, a convenient handling of those extra conditions in order to cancel the singular behavior of the calculated expressions makes the calculations possible and leads to the explicit evaluation of the coefficients. It turns out that the velocity, to the first degree, which represents the leading term of the series, is sufficient for most real life applications, so long as the aspect ratios of the ellipsoids remains within moderate bounds. This is feasible, since the Stokes flow approximation requires a strict consideration of small particles and, then, our method stays valid. We conclude by showing the means for obtaining the corresponding results for the prolate and the oblate spheroid, the needle and the disk, and the sphere as degenerate ellipsoids.

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APPENDIX: RELATIONS ON ELLIPSOIDAL HARMONICS

For a detailed analysis of the ellipsoidal harmonics and related useful properties, one can refer to Ref. 20. However, in the interest of making this work complete and independent, we provide some useful material on ellipsoids and ellipsoidal harmonics, which were used in this work and most of them cannot be found in literature. They appear here for the first time.

We begin with the following connection formulas:

$$\rho^2+\mu^2+\nu^2=\sum_{i=1}^{3}x_i^2+h_2^2+h_3^2, \tag{A1}$$

$$\rho^2\mu^2+\rho^2\nu^2+\mu^2\nu^2=\sum_{i=1}^{3}h_i^2x_i^2+2x_1^2h_3^2+h_2^2h_3^2, \tag{A2}$$

$$\rho^2\mu^2\nu^2=x_1^2h_2^2h_3^2 \tag{A3}$$

for every $\rho\in[h_2,+\infty)$, $\mu\in[h_3,h_2]$, and $\nu\in[-h_3,h_3]$.

The elliptic integrals that enter the exterior ellipsoidal harmonics $\mathbb{F}_n^m$ are interconnected via the following relations:

$$\sum_{i=1}^{3}I_1^i(\rho)=\frac{1}{\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}=\frac{1}{E_3^7(\rho)}, \tag{A4}$$

$$\sum_{i=1}^{3}\alpha_i^2I_1^i(\rho)=I_0^1(\rho)-\frac{\rho^2-\alpha_1^2}{\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}, \tag{A5}$$

$$I_2^1(\rho)=\frac{1}{2(\Lambda-\alpha_1^2+\rho^2)\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}-\frac{1}{2}\sum_{i=1}^{3}\frac{I_1^i(\rho)}{\Lambda-\alpha_i^2}, \tag{A6}$$

$$I_2^2(\rho)=\frac{1}{2(\Lambda'-\alpha_1^2+\rho^2)\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}}-\frac{1}{2}\sum_{i=1}^{3}\frac{I_1^i(\rho)}{\Lambda'-\alpha_i^2}, \tag{A7}$$

$$I_2^{\kappa+l}(\rho)=\frac{I_1^l(\rho)-I_1^\kappa(\rho)}{\alpha_\kappa^2-\alpha_l^2},\quad \kappa,l=1,2,3,\quad \kappa\neq l, \tag{A8}$$

$$I_3^7(\rho)=\frac{1}{h_1^2h_2^2h_3^2}\sum_{i=1}^{3}(-1)^{i+1}h_i^2I_1^i(\rho)=\frac{1}{h_1^2h_2^2h_3^2}\sum_{i=1}^{3}(-1)^{i+1}\alpha_i^2h_i^2I_2^{6-i}(\rho), \tag{A9}$$

$$\sum_{i=1}^{3}\frac{I_1^i(\rho)}{(\Lambda-\alpha_i^2)(\Lambda'-\alpha_i^2)}=3I_3^7(\rho), \tag{A10}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^2I_1^i(\rho)}{(\Lambda-\alpha_i^2)(\Lambda'-\alpha_i^2)}=\frac{3}{h_1^2}[I_1^2(\rho)-I_1^3(\rho)]+3\alpha_1^2I_3^7(\rho)=-3I_2^5(\rho)+3\alpha_1^2I_3^7(\rho), \tag{A11}$$

$$[\alpha_l^2I_1^\kappa(\rho)+\alpha_\kappa^2I_1^l(\rho)]=[\alpha_l^2I_1^l(\rho)+\alpha_\kappa^2I_1^\kappa(\rho)]+(\alpha_l^2-\alpha_\kappa^2)^2I_2^{\kappa+l}(\rho),\quad \kappa,l=1,2,3,\quad \kappa\neq l, \tag{A12}$$

$$\sum_{i=1}^{3}(-1)^ih_i^2I_2^{6-i}(\rho)=0. \tag{A13}$$

The essence of relations (A4)–(A13) is that between the ten integrals I_n^m, $n\leqslant 2$, and I_3^7 only two are linearly independent. For example, if I_0^1 and I_3^7 are known, then the other eight integrals can be written via these two.

The constants Λ and Λ', from Eq. (63), the semifocal distances h_κ, $\kappa=1,2,3$ and the semiaxes α_κ, $\kappa=1,2,3$ satisfy the following useful expressions:

$$\Lambda+\Lambda'=\frac{2}{3}\sum_{i=1}^{3}\alpha_i^2, \tag{A14}$$

$$\Lambda-\Lambda'=\frac{2}{3}\sqrt{h_1^4+h_2^2h_3^2}, \tag{A15}$$

$$\Lambda\Lambda'=\frac{\alpha_1^2\alpha_2^2\alpha_3^2}{3}\sum_{i=1}^{3}\frac{1}{\alpha_i^2} \tag{A16}$$

and

$$\sum_{i=1}^{3}(-1)^i(\Lambda-\alpha_i^2)h_i^2=\sum_{i=1}^{3}(-1)^i(\Lambda'-\alpha_i^2)h_i^2=0, \tag{A17}$$

$$\sum_{i=1}^{3}(-1)^i(\Lambda-\alpha_i^2)h_i^2\alpha_i^2=\sum_{i=1}^{3}(-1)^i(\Lambda'-\alpha_i^2)h_i^2\alpha_i^2=h_1^2h_2^2h_3^2, \tag{A18}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^2}{\Lambda-\alpha_i^2}=\sum_{i=1}^{3}\frac{\alpha_i^2}{\Lambda'-\alpha_i^2}=-3. \tag{A19}$$

Furthermore,

$$(\Lambda-\alpha_\kappa^2)(\Lambda'-\alpha_\kappa^2)=\frac{(-1)^{\kappa+1}h_1^2h_2^2h_3^2}{3h_\kappa^2},\quad \kappa=1,2,3, \tag{A20}$$

which implies that

$$\tfrac{3}{2}(\Lambda-\Lambda')-3(\Lambda-\alpha_1^2)=-\tfrac{3}{2}(\Lambda-\Lambda')-3(\Lambda'-\alpha_1^2)=h_2^2+h_3^2, \tag{A21}$$

$$(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)+(\Lambda-\alpha_1^2)(\Lambda-\alpha_3^2)+(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)=0, \tag{A22}$$

$$(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)+(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_3^2)+(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)=0 \tag{A23}$$

and

$$\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{(\Lambda-\alpha_\kappa^2)}=(-1)^{\kappa+1}\frac{h_1^2h_2^2h_3^2}{3h_\kappa^2}-\frac{(\Lambda-\alpha_\kappa^2)(\Lambda-\Lambda')}{2}, \tag{A24}$$

$$\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{(\Lambda'-\alpha_\kappa^2)}=(-1)^{\kappa+1}\frac{h_1^2h_2^2h_3^2}{3h_\kappa^2}+\frac{(\Lambda'-\alpha_\kappa^2)(\Lambda-\Lambda')}{2} \tag{A25}$$

for every $\kappa=1,2,3$. It is also easy to show that

$$\frac{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}{(\Lambda-\alpha_\kappa^2)(\Lambda-\alpha_l^2)}=\alpha_\kappa^2+\alpha_l^2-\frac{\Lambda+3\Lambda'}{2}+3(\Lambda'-\alpha_l^2)\delta_{\kappa l}, \tag{A26}$$

$$\frac{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}{(\Lambda'-\alpha_\kappa^2)(\Lambda'-\alpha_l^2)}=\alpha_\kappa^2+\alpha_l^2-\frac{3\Lambda+\Lambda'}{2}+3(\Lambda-\alpha_l^2)\delta_{\kappa l}. \tag{A27}$$

An important group of relations is given by

$$\sum_{i=1}^{3}\frac{\alpha_i^4}{\Lambda-\alpha_i^2}=-\frac{3}{2}(3\Lambda+\Lambda'), \tag{A28}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^4}{\Lambda'-\alpha_i^2}=-\frac{3}{2}(3\Lambda'+\Lambda), \tag{A29}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^4}{(\Lambda-\alpha_i^2)^2}=3-3\frac{\Lambda^2(\Lambda-\Lambda')}{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}, \tag{A30}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^4}{(\Lambda'-\alpha_i^2)^2}=3+3\frac{\Lambda'^2(\Lambda-\Lambda')}{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}, \tag{A31}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^2}{(\Lambda-\alpha_i^2)^2}=\Lambda\sum_{i=1}^{3}\frac{1}{(\Lambda-\alpha_i^2)^2}=-\frac{3\Lambda(\Lambda-\Lambda')}{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}, \tag{A32}$$

$$\sum_{i=1}^{3}\frac{\alpha_i^2}{(\Lambda'-\alpha_i^2)^2}=\Lambda'\sum_{i=1}^{3}\frac{1}{(\Lambda'-\alpha_i^2)^2}=\frac{3\Lambda'(\Lambda-\Lambda')}{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)} \tag{A33}$$

and

$$\sum_{i=1}^{3}\frac{(-1)^{i+1}h_i^2}{\Lambda-\alpha_i^2}=\frac{h_1^2h_2^2h_3^2}{(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)}, \tag{A34}$$

$$\sum_{i=1}^{3}\frac{(-1)^{i+1}h_i^2}{\Lambda'-\alpha_i^2}=\frac{h_1^2h_2^2h_3^2}{(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)}. \tag{A35}$$

The following relations connect the semifocal distances and the semiaxes of an ellipsoid:

$$\alpha_1^2h_1^2-\alpha_2^2h_2^2+\alpha_3^2h_3^2=0, \tag{A36}$$

$$\alpha_1^2h_1^2(h_2^2+h_3^2)-\alpha_2^2h_2^4+\alpha_3^2h_3^4=h_1^2h_2^2h_3^2, \tag{A37}$$

$$\alpha_1^4h_1^2-\alpha_2^4h_2^2+\alpha_3^4h_3^2=h_1^2h_2^2h_3^2, \tag{A38}$$

$$h_1^2\alpha_2^2\alpha_3^2-\alpha_1^2h_2^2\alpha_3^2+\alpha_1^2\alpha_2^2h_3^2=h_1^2h_2^2h_3^2, \tag{A39}$$

$$(\alpha_1^4\alpha_2^2-\alpha_1^2\alpha_2^4)+(\alpha_2^4\alpha_3^2-\alpha_2^2\alpha_3^4)+(\alpha_3^4\alpha_1^2-\alpha_3^2\alpha_1^4)=h_1^2h_2^2h_3^2, \tag{A40}$$

$$h_lh_\kappa h_{6-(\kappa+l)}=h_1h_2h_3,\quad \kappa,l=1,2,3,\quad \kappa\neq l. \tag{A41}$$

The tricky task of reducing the results from the ellipsoidal to the spheroidal and to the spherical geometry requires gathering terms containing ellipsoidal and Cartesian factors so as to eliminate the generated indeterminacies. We shall give some formulas, where these indeterminacies are suitably grouped. These are

$$(\alpha_\kappa^2-\alpha_l^2)(\Lambda-\alpha_s^2)\sum_{i=1}^{3}\frac{x_i^2}{\Lambda-\alpha_i^2}=3(\Lambda'-\alpha_\kappa^2)x_\kappa^2-3(\Lambda'-\alpha_l^2)x_l^2+(\alpha_\kappa^2-\alpha_l^2)\|\mathbf{r}\|^2, \tag{A42}$$

$$(\alpha_\kappa^2-\alpha_l^2)(\Lambda'-\alpha_s^2)\sum_{i=1}^{3}\frac{x_i^2}{\Lambda'-\alpha_i^2}=3(\Lambda-\alpha_\kappa^2)x_\kappa^2-3(\Lambda-\alpha_l^2)x_l^2+(\alpha_\kappa^2-\alpha_l^2)\|\mathbf{r}\|^2, \tag{A43}$$

where $\kappa,l,s=1,2,3$ and $\kappa\neq l$, $\kappa\neq s$, $l\neq s$, while

$$\frac{\mathbb{E}_2^1(\mathbf{r})}{(\Lambda-\Lambda')(\Lambda-\alpha_\kappa^2)}-\frac{\mathbb{E}_2^2(\mathbf{r})}{(\Lambda-\Lambda')(\Lambda'-\alpha_\kappa^2)}=\|\mathbf{r}\|^2-3x_\kappa^2+\alpha_\kappa^2-\frac{1}{3}\sum_{i=1}^{3}\alpha_i^2 \tag{A44}$$

for every $\kappa=1,2,3$. This is a useful relation, which with the aim of the identity

$$\frac{I_2^1(\rho)-I_2^2(\rho)}{\Lambda-\Lambda'}=\frac{3}{2}I_3^7(\rho)-\frac{1}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)} \tag{A45}$$

implies that

$$\frac{\mathbb{E}_2^1(\mathbf{r})I_2^1(\rho)}{(\Lambda-\Lambda')(\Lambda-\alpha_\kappa^2)}-\frac{\mathbb{E}_2^2(\mathbf{r})I_2^2(\rho)}{(\Lambda-\Lambda')(\Lambda'-\alpha_\kappa^2)}=\left(\|\mathbf{r}\|^2-3x_\kappa^2+\alpha_\kappa^2-\frac{1}{3}\sum_{i=1}^{3}\alpha_i^2\right)\times I_2^1(\rho)+\frac{\mathbb{E}_2^2(\mathbf{r})}{\Lambda'-\alpha_\kappa^2}\left[\frac{3}{2}I_3^7(\rho)-\frac{1}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)}\right] \tag{A46}$$

for $\kappa=1,2,3$. The factor that multiplies the square brackets on the second part of the right-hand side of Eq. (A46) has no indeterminacy, since

$$\frac{\mathbb{E}_2^1(\mathbf{r})}{\Lambda-\alpha_\kappa^2}=(\Lambda-\alpha_1^2)(\Lambda-\alpha_2^2)(\Lambda-\alpha_3^2)\left[\sum_{i=1}^{3}\frac{x_i^2-x_\kappa^2}{\Lambda-\alpha_i^2}+1\right]\frac{1}{\Lambda-\alpha_\kappa^2} \tag{A47}$$

and

$$\frac{\mathbb{E}_2^2(\mathbf{r})}{\Lambda'-\alpha_\kappa^2}=(\Lambda'-\alpha_1^2)(\Lambda'-\alpha_2^2)(\Lambda'-\alpha_3^2)\left[\sum_{i=1}^{3}\frac{x_i^2-x_\kappa^2}{\Lambda'-\alpha_i^2}+1\right]\frac{1}{\Lambda'-\alpha_\kappa^2}, \tag{A48}$$

where $\kappa=1,2,3$. Two important expressions are

$$\frac{\Lambda'\mathbb{E}_2^1(\mathbf{r})}{(\Lambda-\Lambda')(\Lambda-\alpha_\kappa^2)}-\frac{\Lambda\mathbb{E}_2^2(\mathbf{r})}{(\Lambda-\Lambda')(\Lambda'-\alpha_\kappa^2)}=\sum_{i=1}^{3}x_i^2\left[\frac{3}{2}(\Lambda+\Lambda')-\alpha_i^2-\alpha_\kappa^2+3\delta_{i\kappa}(\alpha_i^2-\Lambda-\Lambda')\right]+\Lambda\Lambda'-\frac{\alpha_1^2\alpha_2^2\alpha_3^2}{\alpha_\kappa^2},\quad \kappa=1,2,3 \tag{A49}$$

and

$$\begin{aligned}&\frac{(\alpha_\kappa^2-\alpha_l^2)\Lambda\mathbb{E}_2^1(\mathbf{r})I_2^1(\rho)}{(\Lambda-\Lambda')(\Lambda-\alpha_\kappa^2)(\Lambda-\alpha_l^2)}-\frac{(\alpha_\kappa^2-\alpha_l^2)\Lambda'\mathbb{E}_2^2(\mathbf{r})I_2^2(\rho)}{(\Lambda-\Lambda')(\Lambda'-\alpha_\kappa^2)(\Lambda'-\alpha_l^2)}\\&=\alpha_\kappa^2\left(\|\mathbf{r}\|^2-3x_\kappa^2+\alpha_\kappa^2-\frac{1}{3}\sum_{i=1}^{3}\alpha_i^2\right)I_2^1(\rho)-\alpha_l^2\left(\|\mathbf{r}\|^2-3x_l^2+\alpha_l^2-\frac{1}{3}\sum_{i=1}^{3}\alpha_i^2\right)I_2^1(\rho)+\left(\frac{\alpha_\kappa^2\mathbb{E}_2^2(\mathbf{r})}{\Lambda'-\alpha_\kappa^2}\right.\\&\left.-\frac{\alpha_l^2\mathbb{E}_2^2(\mathbf{r})}{\Lambda'-\alpha_l^2}\right)\left[\frac{3}{2}I_3^7(\rho)-\frac{1}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)}\right]\end{aligned} \tag{A50}$$

for every $\kappa,l=1,2,3$, $\kappa\neq l$. Finally, we provide the relation

$$\frac{\Lambda I_2^1(\rho)-\Lambda' I_2^2(\rho)}{\Lambda-\Lambda'}=\frac{3}{2}[\alpha_1^2 I_3^7(\rho)-I_2^5(\rho)]+\frac{(\rho^2-\alpha_1^2)}{2\rho\sqrt{\rho^2-h_3^2}\sqrt{\rho^2-h_2^2}(\Lambda-\alpha_1^2+\rho^2)(\Lambda'-\alpha_1^2+\rho^2)},\quad \rho\in[h_2,+\infty), \tag{A51}$$

which also eliminates the indeterminacies in an appropriate way. We observe that relations (A42)–(A51) contain ellipsoidal functions of the second degree ($n=2$) and of order $m=1,2$. This is due to the fact that these ellipsoidal harmonics carry the indeterminacies, which enter the expressions, via the factors $\Lambda-\Lambda'$, $\Lambda-\alpha_\kappa^2$ and $\Lambda'-\alpha_\kappa^2$, $\kappa=1,2,3$ in the dominators. Similar expressions containing the factors $\Lambda_\kappa-\Lambda'_\kappa$, $\Lambda_\kappa-\alpha_l^2$ and $\Lambda'_\kappa-\alpha_l^2$ for $\kappa,l=1,2,3$ are much more complicated but they do not concern the present work.

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Second-order superintegrable systems in conformally flat spaces. V. Two- and three-dimensional quantum systems

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This paper is the conclusion of a series that lays the groundwork for a structure and classification theory of second-order superintegrable systems, both classical and quantum, in conformally flat spaces. For two-dimensional and for conformally flat three-dimensional spaces with nondegenerate potentials we have worked out the structure of the classical systems and shown that the quadratic algebra always closes at order 6. Here we describe the quantum analogs of these results. We show that, for nondegenerate potentials, each classical system has a unique quantum extension. We also correct an error in an earlier paper in the series (that does not alter the structure results) and we elucidate the distinction between superintegrable systems with bases of functionally linearly independent and functionally linearly dependent symmetries. © *2006 American Institute of Physics.*
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I. INTRODUCTION

This is the conclusion of a series[1–4] whose purpose is to lay the groundwork for a structure and classification theory of second-order superintegrable systems, both classical and quantum, in complex conformally flat spaces. Real spaces are considered as restrictions of these to the various real forms. In Refs. 1 and 3 we have given examples in two and three dimensions (2D and 3D), described the background as well as the interest and importance of these systems in mathematical physics, and given dozens of relevant references. Observed features of the systems are multiseparability, closure of the quadratic algebra of second-order symmetries at order 6, use of representation theory of the quadratic algebra to derive spectral properties of the quantum Schrödinger operator, and a close relationship with exactly solvable and quasi-exactly solvable problems.[5] Our approach is, rather than focus on particular spaces and systems, to use a general theoretical method based on integrability conditions to derive structure common to all systems.

We recall some basic facts and results about conformally flat superintegrable systems. An n-dimensional complex Riemannian space is conformally flat if and only if it admits a set of local coordinates $x_1,\ldots,x_n$ such that the contravariant metric tensor takes the form $g^{ij}=\delta^{ij}/\lambda(\mathbf{x})$. A classical superintegrable system $\mathcal{H}=\Sigma_{ij}g^{ij}p_ip_j+V(\mathbf{x})$ on the phase space of this manifold is one that admits $2n-1$ functionally independent generalized symmetries (or constants of the motion) $\mathcal{S}_k$, $k=1,\ldots,2n-1$ with $\mathcal{S}_1=\mathcal{H}$ where the $\mathcal{S}_k$ are polynomials in the momenta p_j.[6–11] It is easy to

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see that $2n-1$ is the maximum possible number of functionally independent symmetries and, locally, such (in general nonpolynomial) symmetries always exist. The system is second-order superintegrable if the $2n-1$ functionally independent symmetries can be chosen to be quadratic in the momenta. Second-order superintegrable systems, though complicated, are tractable because standard orthogonal separation of variables techniques are associated with second-order symmetries, e.g., Refs. 12–17, and these techniques can be brought to bear. Thus we concentrate on second-order superintegrable systems in which the symmetries take the form $\mathcal{S}=\Sigma a^{ij}(\mathbf{x})p_ip_j+W(\mathbf{x})$, quadratic in the momenta.

There is an analogous definition for second-order quantum superintegrable systems with Schrödinger operator

$$H=\Delta+V(\mathbf{x}),\quad \Delta=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}g^{ij})\partial_{x_j},$$

the Laplace-Beltrami operator plus a potential function.[12] Here there are $2n-1$ second-order symmetry operators

$$S_k=\frac{1}{\sqrt{g}}\sum_{ij}\partial_{x_i}(\sqrt{g}a^{ij}_{(k)})\partial_{x_j}+W^{(k)}(\mathbf{x}),\quad k=1,\ldots,2n-1$$

with $S_1=H$ and $[H,S_k]\equiv HS_k-S_kH=0$. Again multiseparable systems yield many examples of superintegrability.

The structure theory for classical second-order superintegrable systems with nondegenerate potential for 2D spaces and for 3D conformally flat spaces has been worked out recently.[1–4,18] (This paper depends heavily on the results and methods of those papers and we shall refer to them repeatedly.) Each such system has quadratic algebra structure. Let $\{\mathcal{S}_j\}$ be a basis for the second-order constants of the motion for the Hamiltonian $\mathcal{H}$. By the superintegrability assumption, the Poisson brackets $\{\mathcal{S}_i,\mathcal{S}_j\}$ must be functionally dependent on the basis symmetries $\mathcal{S}_k$, as are $\{\{\mathcal{S}_i,\mathcal{S}_j\},\mathcal{S}_h\}$ and $\{\{\mathcal{S}_i,\mathcal{S}_j\},\{\mathcal{S}_h,\mathcal{S}_s\}\}$. For these systems it is always true that the squares $\{\mathcal{S}_i,\mathcal{S}_j\}^2$ and products $\{\mathcal{S}_i,\mathcal{S}_j\}\{\mathcal{S}_k,\mathcal{S}_\ell\}$ as well as $\{\{\mathcal{S}_i,\mathcal{S}_j\},\mathcal{S}_h\}$ and $\{\{\mathcal{S}_i,\mathcal{S}_j\},\{\mathcal{S}_h,\mathcal{S}_s\}\}$ are always uniquely expressible as *polynomials* in the $\{\mathcal{S}_k\}$. This remarkable closure of the algebra generated by the second-order symmetries leads to the very special properties enjoyed by the classical superintegrable systems.

Observed common features of the quantum analogs of these systems are that they are usually multiseparable and that the eigenfunctions of one separable system can be expanded in terms of the eigenfunctions of another. This is the source of nontrivial special function expansion theorems in the quantum case.[19] The quantum symmetry operators are in formal self-adjoint form and suitable for spectral analysis. Also, the quadratic algebra identities allow us to relate eigenbases and eigenvalues of one symmetry operator to those of another. The representation theory of the abstract quadratic algebra can be used to derive spectral properties of the second-order generators in a manner analogous to the use of Lie algebra representation theory to derive spectral properties of quantum systems that admit Lie symmetry algebras.[19–22]

The structure theory of classical superintegrable systems is simpler than for the quantum case, and we studied it first. However, we now show that each of the classical superintegrable systems with nondegenerate potential has a unique extension to a quantum superintegrable system.

We review, briefly, some basic definitions and notation in the classical 3D case; the corresponding 2D definitions can be obtained by obvious restriction. For a classical 3D system on a conformally flat space (note that all 2D spaces are conformally flat) we can always choose local coordinates x,y,z, not unique, such that the Hamiltonian takes the form $\mathcal{H}=(p_1^2+p_2^2+p_3^2)/\lambda(x,y,z)+V(x,y,z)$. This system is *second-order superintegrable* with *nondegenerate* potential $V=V(x,y,z,\alpha,\beta,\gamma,\delta)$ if it admits five functionally independent quadratic constants of the motion (i.e., generalized symmetries)

$$\mathcal{S}_k = \sum_{ij} a^{ij}_{(k)} p_i p_j + W_{(k)}(x,y,\alpha,\beta,\gamma). \tag{1}$$

As described in Ref. 3, the potential V is *nondegenerate* if it satisfies a system of coupled PDEs of the form

$$V_{22} = V_{11} + A^{22}(x,y,z)V_1 + B^{22}(x,y,z)V_2 + C^{22}(x,y,z)V_3,$$

$$V_{33} = V_{11} + A^{33}(x,y,z)V_1 + B^{33}(x,y,z)V_2 + C^{33}(x,y,z)V_3,$$

$$V_{12} = A^{12}(x,y,z)V_1 + B^{12}(x,y,z)V_2 + C^{12}(x,y,z)V_3,$$

$$V_{13} = A^{13}(x,y,z)V_1 + B^{13}(x,y,z)V_2 + C^{13}(x,y,z)V_3,$$

$$V_{23} = A^{23}(x,y,z)V_1 + B^{23}(x,y,z)V_2 + C^{23}(x,y,z)V_3, \tag{2}$$

whose integrability conditions are satisfied identically. Here, $V_1 = \partial V/\partial x$, $V_2 = \partial V/\partial y$, etc. The analytic functions A^{ij}, B^{ij}, C^{ij} are determined uniquely from the Bertrand-Darboux equations for the five constants of the motion (under the assumption that the quadratic constants of the motion are functionally linearly independent) and are analytic except for a finite number of poles. At any regular point $\mathbf{x}_0 = (x_0, y_0, z_0)$, i.e., a point where the A^{ij}, B^{ij}, C^{ij} are defined and analytic and the constants of the motion are functionally independent, we can prescribe the values of $V(\mathbf{x}_0)$, $V_1(\mathbf{x}_0)$, $V_2(\mathbf{x}_0)$, $V_3(\mathbf{x}_0)$, $V_{11}(\mathbf{x}_0)$ arbitrarily and obtain a unique solution of (2). The significance of the four parameters for a nondegenerate potential (in addition to the usual additive constant) is that it is the maximum dimension of the space of solutions to the Bertrand-Darboux equations that can appear in a superintegrable system with functionally linearly independent symmetries. If the number of parameters is fewer than four, we say that the superintegrable potential is *degenerate*.

We clarify our definition of nondegenerate potential and our parameter count by considering the generalized Calogero potential

$$V^{(1)} = \frac{a}{(x-y)^2} + \frac{b}{(y-z)^2} + \frac{c}{(z-x)^2}, \tag{3}$$

and its further generalization

$$V^{(2)} = \frac{a}{(m_1 x - m_2 y)^2} + \frac{b}{(m_2 y - m_3 z)^2} + \frac{c}{(m_3 z - m_1 x)^2}, \tag{4}$$

where $m_i \neq 0$, see Refs. 11 and 23–25. These potentials are superintegrable on Euclidean space and the second contains six parameters, which exceeds the count of four for nondegenerate superintegrable systems. How can this be?

Our definition of the number of parameters in a superintegrable system is that it is the dimension of the space of solutions of the set of Bertrand-Darboux equations for this system (ignoring the trivial added constant). Let us consider the system of symmetries defining the system with potential $V^{(1)}$. A basis for the space of symmetries is (using $P_x = p_1, P_y = p_2, P_z = p_3, J_1 = yp_3 - zp_2, J_2 = zp_1 - xp_3, J_3 = xp_2 - yp_1$),

$$\mathcal{S}_1 = \mathcal{H} = P_x^2 + P_y^2 + P_z^2 + V_1, \quad \mathcal{S}_2 = (P_x + P_y + P_z)^2, \quad \mathcal{S}_3 = J_1^2 + J_2^2 + J_3^2 + W_3,$$

$$\mathcal{S}_4 = P_x(J_2 - J_3) + P_y(J_3 - J_1) + P_z(J_1 - J_2) + W_4, \quad \mathcal{S}_5 = J_3 J_2 + J_1 J_3 + J_2 J_1 + W_5,$$

where the potential terms W_i contain the parameters.

We can write the Bertrand-Darboux equations for each symmetry $\mathcal{S} = \Sigma a^{jk} p_j p_k + W$ of $\mathcal{H} = (p_1^2 + p_2^2 + p_3^3)/\lambda(\mathbf{x}) + V$ in the matrix form

$$0=\begin{pmatrix} 0 & a^{12} & a^{11}-a^{22} & a^{31} & -a^{32} \\ a^{13} & 0 & -a^{23} & a^{21} & a^{11}-a^{33} \\ a^{32} & -a^{32} & -a^{13} & a^{22}-a^{33} & a^{12} \end{pmatrix}\begin{pmatrix} V_{33}-V_{11} \\ V_{22}-V_{11} \\ V_{12} \\ V_{32} \\ V_{31} \end{pmatrix}-\frac{1}{\lambda}\begin{pmatrix} (\lambda a^{12})_1-(\lambda a^{11})_2 \\ (\lambda a^{31})_1-(\lambda a^{11})_3 \\ (\lambda a^{31})_2-(\lambda a^{21})_3 \end{pmatrix}V_1$$
$$-\frac{1}{\lambda}\begin{pmatrix} (\lambda a^{22})_1-(\lambda a^{21})_2 \\ (\lambda a^{32})_1-(\lambda a^{12})_3 \\ (\lambda a^{32})_2-(\lambda a^{22})_3 \end{pmatrix}V_2-\frac{1}{\lambda}\begin{pmatrix} (\lambda a^{32})_1-(\lambda a^{31})_2 \\ (\lambda a^{33})_1-(\lambda a^{13})_3 \\ (\lambda a^{33})_2-(\lambda a^{23})_3 \end{pmatrix}V_3. \tag{5}$$

In the Euclidean case, $\lambda=1$. Evaluating these equations for potential $V^{(1)}$ we find that they are

$$V_1+V_2+V_3=0,\quad (x-y)V_{12}+(z-y)V_{23}-V_1+2V_2-V_3=0,$$
$$(x-z)V_{13}+(y-z)V_{23}-V_1-V_2+2V_3=0, \tag{6}$$

and their differential consequences. The complete system of equations is in involution and a particular solution is determined unquely by choosing V_2, V_3, V_{23} at a regular point. Thus we have a three parameter potential. The apparent six parameter potential $V^{(2)}$ is actually three parameter by our count, because the m_i are parametrizing a family of defining symmetries $\mathcal{S}(m_1,m_2,m_3)$, i.e., the Bertrand-Darboux equations themselves are functions of the m_1. For example, the symmetry $\mathcal{S}_2$ is replaced by $\mathcal{S}_2(m_1,m_2,m_3)=(P_x/m_1+P_y/m_2+P_z/m_3)^2$. Another way to see this is to note that the potentials $V^{(2)}$ do not form a vector space. For each fixed value of the m_i, i.e., for each fixed choice of the space of defining quadratic symmetries, we have a three parameter potential.

What is important to notice here is the occurrence of the first-order condition $V_1+V_2+V_3=0$ for the potential as a consequence of the Bertrand-Darboux equations. Thus the potential is a function of only two variables, impossible for nondegenerate potentials. To understand this, observe the relation

$$(x+y+z)^2\hat{\mathcal{S}}_1-(x^2+y^2+x^2)\hat{\mathcal{S}}_2+2\hat{\mathcal{S}}_3-2(x+y+z)\hat{\mathcal{S}}_4-2\hat{\mathcal{S}}_5=0$$

obeyed by the purely quadratic terms in the symmetries, i.e., where we have set $\mathcal{S}_i=\hat{\mathcal{S}}_i+W_i$. This means that the five functionally independent symmetries $\mathcal{S}_i$ are functionally linearly dependent. This dependence reduces the rank of second derivative terms in the system of 12 Bertrand-Darboux equations so that we do not obtain the canonical form (2) which is required for nondegeneracy. As shown in Ref. 3, if we have a 3D superintegrable system with a basis of functionally linear independent symmetries, then we always obtain the canonical system (2) and its differential consequences.

Functional linear dependence of a functionally independent maximal set of symmetries is hard to achieve. In 2D it is well known that essentially, there is only one example, corresponding to Lie form. In 3D Theorem 1 of Ref. 3 stated, incorrectly, that all functionally independent superintegrable systems were functionally linearly independent. The Calogero potential is a counterexample. Thus the results of papers Refs. 3 and 4 hold under the explicit assumption that the functionally independent basis of symmetries is also functionally linearly independent. This is exactly the same situation as in the 2D case.[1]

For the following result the system need not be superintegrable.

Theorem 1: *Let the functionally independent set* $\{\mathcal{H}=\mathcal{S}_1,\mathcal{S}_2,\ldots,\mathcal{S}_t\}$, $(t>2)$ *be a functionally linearly dependent basis of second-order symmetries for the system* $\mathcal{H}=(p_1^2+p_2^2+p_3^3)/\lambda(\mathbf{x})+V$ *with nontrivial potential* V, *i.e., there is a relation* $\Sigma_h c^{(h)}(x)\hat{\mathcal{S}}_h\equiv 0$ *in an open set, where not all* $c^{(h)}\times(x)$ *are constants, and no such relation holds for the* $c^{(h)}$ *all constant, except if the constants are all zero. (Here* $\mathcal{S}_i=\hat{\mathcal{S}}+W_i$ *where the* W_i *are the potential terms.) Then the potential must satisfy a first-order relation* $AV_1+BV_2+CV_3=0$ *where not all of the functions* A,B,C *are zero.*

Proof: By relabeling, we can express one of the quadratic parts of the constants of the motion

$\hat{\mathcal{S}}_0$ as a linear combination of a functionally independent subset $\{\hat{\mathcal{S}}_1,\ldots,\hat{\mathcal{S}}_r, 1\leqslant r\leqslant 4\}$: $\hat{\mathcal{S}}_0 = \Sigma_{\ell=1}^r c^{(\ell)}(x)\hat{\mathcal{S}}_\ell$. Taking the Poisson bracket of both sides of this equation with $(p_1^2+p_2^2+p_3^3)/\lambda$ and using the fact that each of the $\mathcal{S}_h$ is a constant of the motion, we obtain the identity

$$\sum_{\ell=1}^{r}\sum_{i,j=1}^{3}(\partial_{x_k}c^{(\ell)})a_{(\ell)}^{ij}p_ip_jp_k=0, \tag{7}$$

where $(x,y,z)\equiv(x_1,x_2,x_3)$. It is straightforward to check that this identity can be satisfied if and only if the functions

$$c_k^{ij}=\sum_{\ell=1}^{r}(\partial_{x_k}c^{(\ell)})a_{(\ell)}^{ij},\quad 1\leqslant i,j,k\leqslant 3$$

satisfy

$$c_i^{ii}=0,\quad c_j^{ii}+2c_i^{ij}=0,\quad (i\neq j),\quad c_3^{12}+c_1^{23}+c_2^{31}=0. \tag{8}$$

Note that $c_k^{ij}=c_k^{ji}$. Corresponding to each of the basis symmetries $\mathcal{S}_h$ there is a linear set $C_h=0$ of Bertrand-Darboux equations (5). A straightforward substitution into the identity $C_0-\Sigma_{\ell=1}^r c^{(\ell)}\times(x)C_\ell=0$ yields the relation

$$\begin{pmatrix}c_1^{12}-c_2^{11}\\ c_1^{31}-c_3^{11}\\ c_2^{31}-c_3^{21}\end{pmatrix}V_1+\begin{pmatrix}c_1^{22}-c_2^{21}\\ c_1^{32}-c_3^{12}\\ c_2^{32}-c_3^{22}\end{pmatrix}V_2+\begin{pmatrix}c_1^{32}-c_2^{31}\\ c_1^{33}-c_3^{13}\\ c_2^{33}-c_3^{23}\end{pmatrix}V_3=0.$$

These first-order differential equations for the potential cannot all vanish identically. Indeed if they did all vanish then we would have the conditions

$$c_1^{12}=c_2^{11},\quad c_1^{31}=c_3^{11},\quad c_2^{31}=c_3^{21},\quad c_1^{22}=c_2^{21},\quad c_1^{32}=c_3^{12},$$

$$c_2^{32}=c_3^{22},\quad c_1^{32}=c_2^{31},\quad c_1^{33}=c_3^{13},\quad c_2^{33}=c_3^{23}.$$

These conditions, together with conditions (8), show that $c_i^{jk}=0$ for all i,j,k. Thus we have $\Sigma_{\ell=1}^r(\partial_{x_k}c^{(\ell)})a_{(\ell)}^{ij}=0$, $1\leqslant i,j,k\leqslant 3$. Since the set $\{\hat{\mathcal{S}}_1,\ldots,\hat{\mathcal{S}}_r\}$, is functionally linearly independent, we have $\partial_{x_k}c^{(\ell)}\equiv 0$ for $1\leqslant k\leqslant 3, 1\leqslant \ell\leqslant r$. Hence the $c^{(\ell)}$ are constants, which means that $\hat{\mathcal{S}}_0-\Sigma_{\ell=1}^r c^{(\ell)}\hat{\mathcal{S}}_\ell=0$. Thus the set $\{\mathcal{S}_0,\ldots,\mathcal{S}_4\}$ is functionally dependent. This is a contradiction.

Q.E.D.

This shows that the potential function for any system, superintegrable or not, with a basis of symmetries that is functionally linearly dependent must satisfy at least one nontrivial first-order partial differential equation $AV_1+BV_2+CV_3=0$ where the functions A,B,C are parameter free. The method of proof of the Theorem shows how to find such equations. This means that all such potentials depend on either one or two coordinates. The 3D nondegenerate potentials that are the primary subject of this series depend essentially on all three coordinates.

II. NONDEGENERATE 2D QUANTUM SYSTEMS

Here we discuss how the analysis of classical 2D superintegrable systems with nondegenerate potentials carries over to the quantum case. The quantization is much simpler in the 2D case than for dimensions greater than two. For a manifold with metric $ds^2=\lambda(x,y)(dx^2+dy^2)$ the Hamiltonian system $\mathcal{H}=(p_1^2+p_2^2)/\lambda(x,y)+V(x,y)$ is replaced by the Hamiltonian (Schrödinger) operator with potential

$$H = \frac{1}{\lambda(x,y)}(\partial_{11} + \partial_{22}) + V(x,y) \tag{9}$$

in local orthogonal coordinates. A second-order symmetry of the Hamiltonian system $\mathcal{S} = \Sigma_{k,j=1}^{2} a^{kj}(x,y)p_k p_j + W(x,y)$, with $a^{kj} = a^{jk}$, corresponds to the operator

$$S = \frac{1}{\lambda(x,y)} \sum_{k,j=1}^{2} \partial_k (a^{kj}(x,y)\lambda(x,y)\partial_j) + W(x,y), \quad a^{kj} = a^{jk}.$$

These operators are formally self-adjoint with respect to the bilinear product

$$\langle f,g \rangle = \int f(x,y)g(x,y)\lambda(x,y)\mathrm{d}x\mathrm{d}y$$

on the manifold, i.e.,

$$\langle f,Hg \rangle = \langle Hf,g \rangle, \quad \langle f,Sg \rangle = \langle Sf,g \rangle$$

for all local C^∞ functions f,g with compact support on the manifold, where we set all boundary terms equal to 0.

A first-order symmetry of the Hamiltonian system $\mathcal{L} = \Sigma_{k=1}^{2} a^k(x,y)p_k$ corresponds to the operator

$$L = \sum_{k=1}^{2} a^k(x,y)\partial_k.$$

It is easy to show that L_1 is formally skew-adjoint, i.e.,

$$\langle f,Lg \rangle = -\langle Lf,g \rangle.$$

The following results that relate the operator commutator $[A,B] = AB - BA$ and the Poisson bracket are straightforward to verify.

Lemma 1:

$$\{\mathcal{H},\mathcal{S}\} = 0 \Leftrightarrow [H,S] = 0.$$

This result is not generally true for higher dimensional manifolds.

Lemma 2:

$$\{\mathcal{H},\mathcal{L}\} = 0 \Leftrightarrow [H,L] = 0.$$

The definition of a nondegenerate potential $V(x,y)$ is identical with that for the classical case, i.e., it obeys

$$V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2,$$

$$V_{12} = A^{12}V_1 + B^{12}V_2 \tag{10}$$

Again, V_1, V_2, V_{11} can be prescribed arbitrarily at a fixed regular point. Note that if V is a nondegenerate potential then there will be *no* first-order symmetries.

It follows from Lemma 1 that the classical results for the space of second-order symmetries corresponding to a nondegenerate potential can be taken over without change. The space is three dimensional and at any regular point $\mathbf{x}_0$ there exists exactly one symmetry, up to an additive constant, such that $a^{jk}(\mathbf{x}_0) = \alpha^{jk}$ for any constant symmetric matrix α.

Now we investigate the space of third-order symmetries, i.e., third-order differential operators K that commute with the Hamiltonian: $[H,K] = 0$. In general, determination of the possible operators K is very difficult, but in this case, simplifications make the problem tractable:

1. We are interested, principally, in the space of third-order symmetries that is spanned by the commutators of second-order symmetries S. Since the second-order symmetries are formally self-adjoint, the commutators will be skew-adjoint. Thus we can limit ourselves to K that are skew adjoint.

2. A second reason for considering only skew adjoint K follows from the well-known unique decomposition of a symmetry into a formally skew-adjoint part and a formally self-adjoint part, each of which must itself be a symmetry. Clearly the self-adjoint part of a third-order symmetry must be at most a second-order symmetry, i.e., the third-order terms vanish. For a nondegenerate superintegrable system we already know the three-dimensional space of these second-order symmetries.

3. Since H encodes a three-parameter family of potentials, the symmetry K must also be a function of the parameters. The highest order terms $a^{kji}\partial_{kji}$ in K (symmetric in k,j,i) will be independent of the parameters but lower order terms may have linear parameter dependence.

4. The skew-adjoint requirement uniquely determines the coefficients of the second-order terms in K. They are

$$\frac{3}{2\lambda}(a^{kji}\lambda)_i\partial_{kj}.$$

5. Further, the skew-adjoint requirement means that there exist functions $a^{kji},\tilde{b}^i$ such that K has the unique representation

$$K=\sum_{k,j,i=1}^{2}\left(a^{kji}\partial_{kji}+\frac{3}{2\lambda}(a^{kji}\lambda)_i\partial_{kj}+\frac{1}{2\lambda}(a^{kji}\lambda)_{kj}\partial_i\right)+\sum_{i=1}^{2}\left(\tilde{b}^i\partial_i+\frac{1}{2\lambda}(\tilde{b}^i\lambda)_i\right), \tag{11}$$

where the functions $\tilde{b}^i(x,y,z)$ contain the parameter dependence.

6. Equating coefficients of the fourth-order terms in the operator condition $[H,K]=0$ where K is given by (11) we obtain the relations

$$2\frac{\partial a^{iii}}{\partial x_i}=-3\left(\frac{\partial \ln\lambda}{\partial_{x_i}}a^{iii}+\frac{\partial \ln\lambda}{\partial_{xj}}a^{jii}\right),\quad i\neq j,$$

$$3\frac{\partial a^{jii}}{\partial x_i}+\frac{\partial a^{iii}}{\partial x_j}=3\left(-\frac{\partial \ln\lambda}{\partial_{x_i}}a^{iij}-\frac{\partial \ln\lambda}{\partial_{x_j}}a^{ijj}\right),\quad i\neq j,$$

$$2\left(\frac{\partial a^{122}}{\partial x_1}+\frac{\partial a^{112}}{\partial x_2}\right)=-\frac{\partial \ln\lambda}{\partial_{x_1}}a^{122}-\frac{\partial \ln\lambda}{\partial_{x_1}}a^{111}-\frac{\partial \ln\lambda}{\partial_{x_2}}a^{222}-\frac{\partial \ln\lambda}{\partial_{x_2}}a^{112}, \tag{12}$$

which are just the requirements that the a^{kji} be the components of a third-order Killing tensor.

7. Equating coefficients of the third-order terms in the condition $[H,K]=0$ we obtain relations that are consequences of the Killing tensor relations (12).

8. The remaining conditions on K intertwine λ, a^{kji}, $\tilde{b}^i$, and V, and are complicated. Rather than solve them directly, we note that we can make the unique decomposition

$$\tilde{b}^i(x_1,x_2,V_{x_1},V_{x_2})=c^i(x_1,x_2)+b^i(x_1,x_2,V_{x_1},V_{x_2}),$$

where

$$b^i = \sum_{j=1}^{2} f^{\ell,j}(x_1,x_2)\frac{\partial V}{\partial x_j}(x_1,x_2), \tag{13}$$

i.e., we can split off the parameter-dependent terms of $\tilde{b}^i$ from the rest. Then, equating the linear parameter-dependent coefficients of the second-order terms in the symmetry operator condition, we obtain the requirements

$$\frac{\partial b^1}{\partial x_2} + \frac{\partial b^2}{\partial x_1} = 3\sum_{s=1}^{2} \lambda a^{s21}\frac{\partial V}{\partial x_s},$$

$$\frac{\partial b^j}{\partial x_j} = \frac{3}{2}\sum_{s=1}^{2} a^{sjj}\frac{\partial V}{\partial x_s} - \frac{1}{2}\sum_{s=1}^{2}\frac{\partial \ln \lambda}{\partial x_s}b^s, \quad j=1,2, \tag{14}$$

identical to the corresponding classical equations in Ref. 1. Equating the quadratic parameter-dependent coefficients of the zeroth-order terms in the symmetry operator condition, we obtain the requirement

$$\sum_{s=1}^{2} b^s\frac{\partial V}{\partial x_s} = 0, \tag{15}$$

again identical to the corresponding classical equation in Ref. 1.

9. Conditions (14) and (15), and third-order Killing tensor conditions are clearly necessary for K to be a skew-adjoint symmetry. To see that they are sufficient will take several steps.

10. Uniqueness: Suppose K,K' are two third-order skew-adjoint symmetries with the same functions a^{kji},b^i (but possibly different c^i). Note that $K-K'$ is a skew-adjoint, parameter-independent symmetry that is first order (since the third- and second-order terms in K and K' are the same). However, there can be no nonzero parameter-independent symmetry for a nondegenerate superintegrable system. Therefore $K=K'$. Though we have not given an explicit expression for the c^i we see that they are uniquely determined by the functions a^{kji},b^i.

11. Existence: This also involves several steps. We first employ the results of our construction of third-order symmetries for the classical case. There we used (13) to show

$$f^{\ell,j} + f^{j,\ell} = 0, \quad 1 \leqslant \ell,j \leqslant 2,$$

and (14) to show that

$$b_1^1 = f_1^{1,2}V_2 + f^{1,2}V_{12}, \quad b_2^1 = f_2^{1,2}V_2 + f^{1,2}V_{22},$$

$$b_1^2 = f_1^{2,1}V_1 + f^{2,1}V_{11}, \quad b_2^2 = f_2^{2,1}V_1 + f^{2,1}V_{12},$$

and

$$\lambda a^{111} = \tfrac{1}{3}f^{1,2}(2A^{12} - (\ln\lambda)_2), \quad \lambda a^{222} = \tfrac{1}{3}f^{1,2}(-2B^{12} + (\ln\lambda)_1),$$

$$\lambda a^{112} = \tfrac{1}{9}f^{1,2}(2A^{22} + 2B^{12} + (\ln\lambda)_1),$$

$$\lambda a^{122} = \tfrac{1}{9}f^{1,2}(-2A^{12} + 2B^{22} - (\ln\lambda)_2),$$

$$f_1^{1,2} = \tfrac{1}{3}f^{1,2}(A^{22} - 2B^{12} - (\ln\lambda)_1), \quad f_2^{1,2} = \tfrac{1}{3}f^{1,2}(-2A^{12} - B^{22} + (\ln\lambda)_2).$$

Thus the a^{ijk} can be expressed in terms of $f^{1,2}$ and the $A^{k\ell},B^{k\ell}$ functions, and we have an involutive system for $f^{1,2}$. Thus any third symmetry is uniquely determined by the constant

$f^{1,2}(x_0,y_0)$ at some regular point (x_0,y_0). This means that the space of third-order skew-adjoint symmetries is at most one dimensional.

12. Consider the case where all $a^{ijk}\equiv 0$. Then $2A^{12}=B^{22}=(\ln\lambda)_2$, $2B^{12}=-A^{22}=(\ln\lambda)_1$. The integrability conditions require $(\ln\lambda)_{11}+(\ln\lambda)_{22}=0$, which is the condition for flat space, Thus by an appropriate orthogonal change of coordinates we can assume that $\lambda\equiv 1$. In these new coordinates we see that $A^{ij}=B^{ij}\equiv 0$ for all i,j. The general solution is

$$f^{1,2}=c_1,$$

where c_1, is a constant. This is the *homogeneous isotropic oscillator:*

$$V(x,y)=\alpha x+\beta y+\gamma(x^2+y^2).$$

One can easily check that for this very special case a nonzero commutator of two second-order symmetries is first order, parameter-dependent.

13. The second case is that not all a^{ijk} vanish. We show that the space of symmetries is exactly one dimensional. Let

$$S_1=\frac{1}{\lambda}\sum \partial_k(\,a^{kj}_{(1)}\lambda)\partial_j)+W_{(1)},\quad S_2=\sum \partial_k(a^{kj}_{(2)}\lambda\partial_j)+W_{(2)}$$

be second-order symmetries and let $\mathcal{A}_{(i)}(x_1,x_2)=\{a^{kj}_{(i)}(x_1,x_2)\}$, $i=1,2$ be 2×2 matrix functions. Then the commutator $[S_1,S_2]$ of these symmetries is a third-order symmetry K with a^{kji} and $f^{k,\ell}$ such that

$$f^{k,\ell}=2\lambda\sum_j (a^{kj}_{(2)}a^{j\ell}_{(1)}-a^{kj}_{(1)}a^{j\ell}_{(2)}).$$

Thus $K=[S_1,S_2]$ is uniquely determined by the skew-symmetric matrix

$$[\mathcal{A}_{(2)},\mathcal{A}_{(1)}]\equiv\mathcal{A}_{(2)}\mathcal{A}_{(1)}-\mathcal{A}_{(1)}\mathcal{A}_{(2)},$$

hence by the constant matrix $[\mathcal{A}_{(2)}(x_0,y_0),\mathcal{A}_{(1)}(x_0,y_0)]$ evaluated at a regular point.

Theorem 2: *Let K be a third-order skew-adjoint symmetry (11) for a superintegrable system with nondegenerate potential V and* $\tilde{b}^i=c^i(x,y)+b^i(x,y,V_1,V_2)$ *where*

$$b^i=\sum_{j=1}^{2} f^{i,j}(x,y)\frac{\partial V}{\partial x_j}(x,y).$$

Then

$$f^{\ell,j}+f^{j,\ell}=0,\quad 1\leqslant \ell,j\leqslant 2$$

and K is uniquely determined by the number

$$f^{1,2}(x_0,y_0)$$

at some regular point (x_0,y_0) *of V.*

Corollary 1: Let V be a superintegrable nondegenerate potential, Then the space of third-order skew-adjoint symmetries is one dimensional and is spanned by commutators of the second-order self-adjoint symmetries.

Corollary 2: Let V be a superintegrable nondegenerate potential and S_1,S_2 *be second-order formally self-adjoint symmetries with matrices* $\mathcal{A}_{(1)},\mathcal{A}_{(2)}$, *respectively. Then*

$$[S_1,S_2]\equiv 0\Leftrightarrow[\mathcal{A}_{(1)},\mathcal{A}_{(2)}]\equiv 0\Leftrightarrow[\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]=0$$

at a regular point $\mathbf{x}_0$.

III. A STANDARD FORM FOR 2D QUANTUM SYSTEMS

In analogy with the classical case, there is a standard structure for 2D quantum nondegenerate superintegrable systems allowing the identification of the space of second-order symmetry operators with the space of 2×2 symmetric matrices, and identification of the space of third-order symmetry operators with the space of 2×2 skew-symmetric matrices. Indeed, if $\mathbf{x}_0$ is a regular point then there is a 1-1 linear correspondence between second-order operators S and their associated symmetric matrices $\mathcal{A}(\mathbf{x}_0)$. Let $[S_1,L_2]'=[S_2,S_1]$ be the reversed operator commutator. Then the map

$$[S_1,S_2]' \leftrightarrow [\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$$

is an algebraic isomorphism. Here, S_1,S_2 are in involution if and only if matrices $\mathcal{A}_{(1)}(\mathbf{x}_0),\mathcal{A}_{(2)}\times(\mathbf{x}_0)$ commute. If $[S_1,S_2]\neq 0$ then it is a truly third-order symmetry operator (except in the isotropic oscillator case) and can be uniquely associated with the skew-symmetric matrix $[\mathcal{A}_{(1)}\times(\mathbf{x}_0),\mathcal{A}_{(2)}(\mathbf{x}_0)]$. Since commutators of second-order symmetries span the space of third-order symmetries, we can identify these 1-1 with 2×2 skew-symmetric matrices. Let $\mathcal{E}^{ij}$ be the 2×2 matrix with a 1 in row i, column j and 0 for every other matrix element. Then the symmetric matrices

$$\mathcal{A}^{(ij)}=\tfrac{1}{2}(\mathcal{E}^{ij}+\mathcal{E}^{ji})=\mathcal{A}^{(ji)},\quad i,j=1,2 \tag{16}$$

form a basis for the three-dimensional space of symmetric matrices. Moreover,

$$[\mathcal{A}^{(ij)},\mathcal{A}^{(k\ell)}]=\tfrac{1}{2}(\delta_{jk}\mathcal{B}^{(i\ell)}+\delta_{j\ell}\mathcal{B}^{(ik)}+\delta_{ik}\mathcal{B}^{(j\ell)}+\delta_{i\ell}\mathcal{B}^{(jk)}), \tag{17}$$

where

$$\mathcal{B}^{(ij)}=\tfrac{1}{2}(\mathcal{E}^{ij}-\mathcal{E}^{ji})=-\mathcal{B}^{(ji)},\quad i,j=1,2.$$

Here $\mathcal{B}^{(ii)}=0$ and $\mathcal{B}^{(12)}$ forms a basis for the space of skew-symmetric matrices. Thus (17) gives the commutation relations for the second-order symmetry operators. If V is the isotropic oscillator then there is no truly third-order symmetry. For any other nondegenerate potential, the space of symmetries is exactly one dimensional.

We reformulate the problem of determining the second-order symmetry operators of (9) by setting

$$W(x)=f^1V_1+f^2V_2+f^{11}V_{11}$$

and substituting this expression into $W_i=\lambda\Sigma_{j=1}^2a^{ij}V_j$. Additionally we must impose the Killing tensor conditions. We obtain the equations for the a^{ij}:

$$\lambda a^{11}=f^1_1+f^2A^{12}+f^{11}A^{13},$$

$$\lambda a^{12}=f^1_2+f^1A^{12}+f^2A^{22},$$

$$\lambda a^{22}=f^2_2+f^1B^{12}+f^2B^{22}, \tag{18}$$

and the condition on the first derivatives of the f^i:

$$f^1_2-f^2_1=-f^1A^{12}+f^2(A^{22}-B^{12})-f^{11}B^{13}. \tag{19}$$

Note the expressions for f^{11}_1 and f^{11}_2 in terms of f^1,f^2,f^{11}:

$$f^{11}_1+f^1+f^{11}(B^{12}-A^{22})=0,\quad f^{11}_2+f^2+f^{11}A^{12}=0.$$

It follows that we can express each of the second derivatives of f^1,f^2 in terms of lower order derivatives of f^1,f^2,f^{11}. Thus the system is in involution at the second derivative level, but not at

the first derivative level because we have only one condition for the four derivatives $f_1^1, f_2^1, f_1^2, f_2^2$. We can uniquely determine a symmetry operator at a regular point by choosing the six parameters $(f^1, f^2, f^{11}, f_1^1, f_2^1, f_2^2)$. The values of f^1, f^2, f^{11} at the regular point are analogous to the three parameters that we can add to the potentials in the three parameter family. For our standard basis, we fix $(f^1, f^2, f^{11})_{\mathbf{x}_0} = (0,0,0)$. Then from (18) and (19), we have

$$\begin{pmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{pmatrix} = \lambda \begin{pmatrix} a^{11} & a^{12} \\ a^{21} & a^{22} \end{pmatrix}.$$

Thus we can define a standard set of basis symmetry operators $S^{(jk)} = \lambda^{-1}(\mathbf{x})(\Sigma \partial_i (a^{ij}(\mathbf{x})\lambda(\mathbf{x})\partial_j) + W^{(ij)}(\mathbf{x})$ corresponding to a regular point $\mathbf{x}_0$ by

$$\begin{pmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{pmatrix}_{\mathbf{x}_0} = \lambda(\mathbf{x}_0) \begin{pmatrix} a^{11} & a^{12} \\ a^{21} & a^{22} \end{pmatrix}_{\mathbf{x}_0} = \lambda(\mathbf{x}_0)\mathcal{A}^{(jk)}, \quad W^{(jk)}(\mathbf{x}_0) = 0.$$

The condition on $W^{(jk)}$ is actually three conditions since $W^{(jk)}$ depends on three parameters. Note that the derivative terms a_i^{ij} in the expression for the basis symmetries can be computed explicitly from the conditions for classical second order symmetries in Ref. 1.

In exact analogy with the classical case, we can use the standard form to prove multiseparabilty for quantum systems.

Theorem 3. *Let V be a quantum superintegrable nondegenerate potential and S be a second-order symmetry operator with matrix function $\mathcal{A}(\mathbf{x})$. If at some regular point $\mathbf{x}_0$ the matrix $\mathcal{A}(\mathbf{x}_0)$ has two distinct eigenvalues, then H, S characterize an orthogonal separable coordinate system.*

Since a generic 2×2 symmetric matrix has distinct roots, it follows that any such superintegrable nondegenerate potential is multiseparable.

IV. THE QUANTUM QUADRATIC ALGEBRA

We investigate the space of fourth-order differential operators F that commute with the Hamiltonian: $[H,F]=0$. Determination of all possible operators F is very difficult but, again, there are simplifications that make the problem tractable:

1. We are interested, principally, in the space of fourth-order symmetries that is spanned by the double commutators $[[S^{(1)}, S^{(2)}], S^{(3)}]$ of second-order formally self-adjoint symmetries $S^{(j)}$ of the superintegrable system. The double commutators will be formally self-adjoint, so we can limit ourselves to F that are self-adjoint.

2. Since H encodes a three-parameter family of potentials, the symmetry F must also be a function of the parameters. The highest order terms $a^{\ell kji}\partial_{kji}$ in F (symmetric in ℓ, k, j, i) will be independent of the parameters but lower order terms may have linear or quadratic parameter dependence.

3. The self-adjoint requirement uniquely determines the third-order terms in F. They are

$$\sum_{\ell,k,j,i} \frac{2}{\lambda}(a^{\ell kji}\lambda)_i \partial_{\ell kj}.$$

4. Further, the self-adjoint requirement means that there exist functions $a^{\ell kji}, \tilde{b}^{ij}, \tilde{W}$ such that F has the unique representation

$$F = \sum_{\ell,k,j,i=1}^{2} \frac{1}{\lambda}\partial_{ij}(a^{\ell kji}\lambda\partial_{k\ell}) + \sum_{i,j=1}^{2} \frac{1}{\lambda}\partial_i(\tilde{b}^{ij}\lambda\partial_j) + \tilde{W}, \tag{20}$$

where the functions $\tilde{b}^{ij}(x_1,x_2), \tilde{W}(x_1,x_2)$ contain the parameter dependence.

5. Equating coefficients of the fifth-order terms in the operator condition $[H,F]=0$ where F is given by (20) we obtain the relations

$$\frac{\partial a^{iiii}}{\partial x_i} = -2\sum_{s=1}^{2} a^{siii}\frac{\partial \ln \lambda}{\partial x_s},$$

$$4\frac{\partial a^{jiii}}{\partial x_i} + \frac{\partial a^{iiii}}{\partial x_j} = -6\sum_{s=1}^{2} a^{siij}\frac{\partial \ln \lambda}{\partial x_s}, \quad i \neq j,$$

$$3\frac{\partial a^{jjii}}{\partial x_i} + 2\frac{\partial a^{iiij}}{\partial x_j} = -\sum_{s=1}^{2} a^{siii}\frac{\partial \ln \lambda}{\partial x_s} - 3\sum_{s=1}^{2} a^{sijj}\frac{\partial \ln \lambda}{\partial x_s}, \quad i \neq j, \tag{21}$$

which are the conditions for $a^{\ell kji}$ to be a fourth-order Killing tensor.

6. The remaining conditions on F intertwine λ, $a^{\ell kji}$, $\tilde{b}^{ji}$, $\tilde{W}$, and V, and are complicated. Rather than solve them directly, we make the unique decomposition

$$\tilde{b}^{ji}(x_1,x_2,V_{x_1},V_{x_2},V_{x_1x_1}) = c^{ji}(x_1,x_2) + b^{ji}(x_1,x_2,V_{x_1},V_{x_2},V_{x_1x_1}),$$

where

$$b^{ji} = \sum_{\alpha=1}^{3} f^{ji,\alpha}W^{(\alpha)}, \quad f^{ji,\alpha} = f^{ij,\alpha},$$

and $W^{(\alpha)}$ is defined by

$$\begin{pmatrix} W^{(1)} \\ W^{(2)} \\ W^{(3)} \end{pmatrix} = \begin{pmatrix} V_{x_1} \\ V_{x_2} \\ V_{x_1x_1} \end{pmatrix}.$$

Then, equating the linear parameter-dependent terms of third order in the derivatives we obtain the conditions

$$\frac{\partial}{\partial x_h}f^{jk,\alpha} + \frac{\partial}{\partial x_k}f^{hj,\alpha} + \frac{\partial}{\partial x_j}f^{kh,\alpha} - 2\lambda a^{\alpha hjk} = -\sum_{\gamma=1}^{3}(f^{jk,\gamma}A^{(h)}_{\gamma\alpha} + f^{hj,\gamma}A^{(k)}_{\gamma\alpha} + f^{kh,\gamma}A^{(j)}_{\gamma\alpha}) - \sum_{s=1}^{2}(f^{sk,\alpha}\delta_{hk} + f^{sj,\alpha}\delta_{kh} + f^{sh,\alpha}\delta_{jk})\frac{\partial}{\partial x_s}\ln\lambda, \tag{22}$$

where $1 \leqslant j,k,h \leqslant 2$ and we set $a^{3hjk} \equiv 0$. These conditions are identical to the corresponding classical conditions in Ref. 1. Similarly, we set

$$\tilde{W} = U^{(0)}(x_1,x_2) + U^{(1)}(x_1,x_2,W^{(\alpha)}) + W(x_1,x_2,W^{(\alpha)}),$$

where $U^{(1)}$ depends linearly and W depends quadratically on the $W^{(\alpha)}$ and equate the quadratic parameter-dependent terms of first order in the derivatives. We obtain the conditions

$$\lambda\sum_{s=1}^{3} b^{si}\frac{\partial V}{\partial x_s} = \frac{\partial W}{\partial x_i}. \tag{23}$$

Equating the quadratic parameter-dependent coefficients of the zeroth-order terms in the symmetry operator condition, we obtain the requirement

$$\sum_{s=1}^{2} b^s \frac{\partial V}{\partial x_s} = 0, \tag{24}$$

identical to (13). From the integrabilty conditions $(\partial/\partial x_j)(\partial W/\partial x_i) = (\partial/\partial x_i)(\partial W/\partial x_j), i \neq j$ for Eq. (23) we obtain the conditions

$$\begin{aligned}\partial_{x_j} f^{\beta k,\alpha} + \partial_{x_j} f^{\alpha k,\beta} - \partial_{x_k} f^{\beta j,\alpha} - \partial_{x_k} f^{\alpha j,\beta} = \sum_{s=1}^{2} (A^{(k)}_{\beta s} f^{sj,\alpha} + A^{(k)}_{\alpha s} f^{sj,\beta} - A^{(j)}_{\beta s} f^{sk,\alpha} - A^{(j)}_{\alpha s} f^{sk,\beta}) + \sum_{\gamma=1}^{3} (f^{\beta j,\gamma} A^{(k)}_{\gamma\alpha} \\ + f^{\alpha j,\gamma} A^{(k)}_{\gamma\beta} - f^{\beta k,\gamma} A^{(j)}_{\gamma\alpha} - f^{\alpha k,\gamma} A^{(j)}_{\gamma\beta}) - (f^{\beta k,\alpha} + f^{\alpha k,\beta}) \frac{\partial}{\partial x_j} \ln \lambda \\ + (f^{\beta j,\alpha} + f^{\alpha j,\beta}) \frac{\partial}{\partial x_k} \ln \lambda,\end{aligned} \tag{25}$$

where $j \neq k, 1 \leqslant \alpha, \beta \leqslant 3$, and we set $f^{3j,\alpha} \equiv 0$.

7. There are eight independent equations (22) with $\alpha \neq 3$ and we use five of these to define the five components a^{ihjk} as linear combinations of $(\partial/\partial x_h) f^{jk,\alpha}$ and $f^{jk,\alpha}$. We can then eliminate the a^{ihjk} from the remaining three equations to obtain three conditions relating $(\partial/\partial x_h) f^{jk,\alpha}$ and $f^{jk,\alpha}$. There are six terms of the form $(\partial/\partial x_h) f^{jk,3}$. Equation (25) with $\alpha = \beta = 3$ is satisfied identically. There are two equations (25) with $\beta = 3$, $1 \leqslant \alpha \leqslant 2$ and four equations (22) with $\alpha = 3$. Thus all six terms of the form $(\partial/\partial x_h) f^{jk,3}$ can be expressed as linear combinations of $f^{jk,\alpha}$. There are a total of twelve distinct terms of the form $(\partial/\partial x_h) f^{jk,m}, 1 \leqslant h, j, k, m \leqslant 2$. We have seen that there are three conditions on these terms remaining from (22); there are an additional three such conditions from (25) with $\alpha, \beta \neq 3$. Thus there is a shortfall of six conditions on the first derivatives $(\partial/\partial x_h) f^{jk,m}$.

8. There are a total of eighteen distinct terms of the form $(\partial^2/\partial x_h \partial x_\ell) f^{jk,m}$ with $1 \leqslant h, j, k, \ell, m \leqslant 2$. Differentiating with respect to x_1, x_2 the three first-order conditions of (22), from which the a^{ihjk} have been eliminated, we obtain six independent conditions on these second derivatives. Differentiating each of our expressions for the a^{ihjk} and substituting into Eq. (21) we find six additional conditions on the second derivatives. Also, we can differentiate the three equations from (23) with $\alpha, \beta \neq 3$ to obtain six additional conditions on the second derivatives. This allows us to express each second-order derivative as a linear combination of lower order derivatives. Thus the system is in involution.

9. Conditions (22) and (23), and the fourth-order Killing tensor conditions are clearly necessary for F to be a skew-adjoint symmetry. To see that they are sufficient will take several steps.

10. Suppose F, F' are two fourth-order self-adjoint symmetries with the same functions $a^{\ell kji}, b^{ij}, W$ (but possibly different $c^{ij}, U^{(j)}$). Then $F - F'$ is a self-adjoint, symmetry that is second order and at most linear in the parameters in the zeroth-order term. Thus the only ambiguity is a second-order symmetry operator and we already know these.

11. We conclude that any (truly) fourth-order symmetry operator is uniquely determined, up to an additive second-order symmetry operator, by the values $f^{jk,\alpha}(\mathbf{x}_0)$ and a subset of six of the values $(\partial/\partial_{x_h}) f^{jk,m}(\mathbf{x}_0)$ at a regular point $\mathbf{x}_0$. Note that by adding an appropriate linear combination of purely second-order symmetry operators to the fourth-order symmetry we can achieve $f^{jk,\alpha}(\mathbf{x}_0) = 0$ for all j, k, α, so the maximum possible dimension of the space of purely fourth-order symmetries is six.

Now any symmetric second-order polynomial in the second-order symmetry operators is a fourth-order symmetry operator, and the subspace of polynomial symmetries is at least five and at most six. We show that it is exactly six. If A, B are linear operators, we define their symmetrized product by

$$\{A, B\} \equiv \tfrac{1}{2}(AB + BA).$$

Theorem 4: *The six distinct monomials*

$$\{S^{(11)},S^{(11)}\},\quad \{S^{(22)},S^{(22)}\},\quad \{S^{(12)},S^{(12)}\},\quad \{S^{(11)},S^{(22)}\},\quad \{S^{(11)},S^{(12)}\},\quad \{S^{(12)},S^{(22)}\},$$

form a basis for the space of fourth-order symmetry operators.

Proof: Since the second-order parts of the three symmetry operators $S^{(11)},S^{(22)},S^{(12)}$ are functionally independent, the six monomials listed above are linearly independent. Hence they form a basis. Q.E.D.

We can use this result to expand explicitly a general fourth-order self-adjoint symmetry

$$F=\sum_{\ell,k,j,i=1}^{2}\frac{1}{\lambda}\partial_{ij}(a^{\ell kji}\lambda\partial_{k\ell})+\sum_{i,j=1}^{2}\frac{1}{\lambda}\partial_{i}(\tilde{b}^{ij}\lambda\partial_{j})+\tilde{W}$$

in terms of the standard basis. Without loss of generality we can assume that $(0,0)=\mathbf{0}$ is a regular point. Then F is uniquely determined (up to an additive second-order self-adjoint symmetry) by the data $a^{\ell kji}(\mathbf{0}),\partial_m a^{\ell kji}(\mathbf{0}),b^{mq}(\mathbf{0}),W(\mathbf{0})$. We can uniquely match the data $a^{\ell kji}(\mathbf{0})$ by taking a linear combination of the basis symmetries

$$\{S^{(11)},S^{(11)}\},\quad \{S^{(22)},S^{(22)}\},\quad \{S^{(12)},S^{(12)}\},\quad \{S^{(11)},S^{(12)}\},\quad \{S^{(12)},S^{(22)}\},\quad \{S^{(11)},S^{(11)}\}.$$

This leaves the symmetry $\{S^{(11)},S^{(22)}\}-\{S^{(12)},S^{(12)}\}$ whose leading order terms vanish at the regular point. The expansion coefficient for this term is obtained uniquely from the derivative data $\partial_m a^{\ell kji}(\mathbf{0})$. Now we have matched all of the fourth-order terms in F with an expansion of the self-adjoint form $F'=\Sigma\xi_{ijk\ell}\{S^{(ij)},S^{(k\ell)}\}$. The difference $F-F'$ is a second-order self-adjoint symmetry. The second derivative terms are uniquely determined by the data $b^{mq}(\mathbf{0})$, $W(\mathbf{0})$, which has not changed since $W^{(ij)}(\mathbf{0})=0$ for all terms in the standard basis, by the data $\partial_m a^{\ell kji}(\mathbf{0})$, $\partial_{ms}a^{\ell kji}(\mathbf{0})$, and by the coefficients $\xi_{ijk\ell}$ which have changed. Thus we can expand the original symmetry in terms of second-order polynomials in the standard basis, and finally add any constant parameter-dependent terms. In contrast to the classical case, however, this expansion is more complicated because the expansion coefficients at the fourth-order level effect the expansion coefficients at the second-order level

Using an approach very similar to the above we can easily show that the space of truly sixth-order formally self-adjoint operator symmetries of H cannot exceed the classical maximal dimension of ten. The difference between any two such sixth-order symmetries with the same classical data will be a formally self-adjoint fourth-order symmetry. It remains to show that the maximum possible dimension is actually achieved. If A, B, C are linear operators, we define their symmetrized product by

$$\{A,B,C\}\equiv\tfrac{1}{6}(ABC+BAC+CAB+ACB+BCA+CBA).$$

Theorem 5: *The ten distinct monomials*

$$\{S^{(ii)},S^{(ii)},\quad S^{(ii)}\},\quad \{S^{(ij)},S^{(ij)},S^{(ij)}\},\quad \{S^{(ii)},S^{(ii)},S^{(ij)}\},$$

$$\{S^{(ij)},S^{(ij)},S^{(ii)}\},\quad \{S^{(11)},S^{(12)},S^{(22)}\},$$

for $i,j=1,2$, $i\neq j$ form a basis for the space of sixth-order symmetries.

Proof: Since the three symmetries $S^{(11)}$, $S^{(22)}$, $S^{(12)}$ have functionally independent second-order terms, the ten monomials listed above are linearly independent. Hence they form a basis. Q.E.D.

These theorems establish the closure of the quadratic algebra for 2D quantum superintegrable potentials: All fourth-order and sixth-order symmetry operators can be expressed as symmetric polynomials in the second-order symmetry operators.

Again, we can use these results to expand explicitly a general sixth-order formally self-adjoint symmetry operator

$$G=\sum_{n,m,\ell,k,j,i=1}^{2}\frac{1}{\lambda}\partial_{nm\ell}(a^{nm\ell kji}\lambda\partial_{kji})+\sum_{\ell,k,j,i=1}^{2}\frac{1}{\lambda}\partial_{ij}(\tilde{b}^{\ell kji}\lambda\partial_{k\ell})+\sum_{i,j=1}^{2}\frac{1}{\lambda}\partial_{i}(\tilde{c}^{ij}\lambda\partial_{j})+\tilde{W}$$

in terms of the standard symmetrized basis. Here $\tilde{b}^{\ell kji},\tilde{c}^{ij},\tilde{W}$ are at most linear, quadratic, and cubic in the parameters of the potential, respectively. Without loss of generality we can assume that $(0,0)=\mathbf{0}$ is a regular point. We can uniquely match the data $a^{ijklmn}(\mathbf{0})$ by taking a linear combination of the seven symmetries

$$\{S^{(ii)},S^{(ii)},S^{(ii)}\},\quad \{S^{(ij)},S^{(ij)},S^{(ij)}\},\quad \{S^{(ii)},S^{(ii)},S^{(jj)}\},\quad \{S^{(ii)},S^{(ii)},S^{(ij)}\},$$

for $i,j=1,2$, $i\neq j$. This leaves the three symmetries

$$\{S^{(11)},S^{(11)},S^{(22)}\}-\{S^{(11)},S^{(12)},S^{(12)}\},\quad \{S^{(12)},S^{(11)},S^{(22)}\}-\{S^{(12)},S^{(12)},S^{(12)}\},$$

$$\{S^{(22)},S^{(22)},S^{(11)}\}-\{S^{(22)},S^{(12)},S^{(12)}\},$$

whose leading order terms vanish at the regular point. The expansion coefficients for these three terms are obtained uniquely from the derivative data $\partial_q a^{ijklmn}$. Now we have matched all of the sixth-order terms in G with a self-adjoint expansion of the form $G'=\Sigma\xi_{ijklmn}\{S^{(ij)},S^{(kl)},S^{(mn)}\}$. The difference $G-G'$ is a fourth-order self-adjoint symmetry. It is uniquely determined by the data for the even order terms of G and by the new data for the even order terms of G'. Now we can use the above-presented argument to expand this fourth-order symmetry in terms of polynomials in the standard basis. The expansion coefficients ξ_{ijklmn} will be the same as for the classical case, but the lower order expansion coefficients will differ.

V. THE STÄCKEL TRANSFORM FOR 2D QUANTUM SYSTEMS

The quantum analog of the Stäckel transform[26] or coupling constant metamorphosis[27] for classical systems is straightforward in the 2D case. Suppose we have a superintegrable system

$$H=\frac{1}{\lambda(x,y)}(\partial_{11}+\partial_{22})+V(x,y)=H_0+V \tag{26}$$

in local orthogonal coordinates, with nondegenerate potential $V(x,y)$:

$$V_{22}=V_{11}+A^{22}V_1+B^{22}V_2,$$

$$V_{12}=A^{12}V_1+B^{12}V_2 \tag{27}$$

and suppose $U(x,y)$ is a particular solution of Eq. (27), nonzero in an open set. Then the transformed system

$$\tilde{H}=\frac{1}{\tilde{\lambda}(x,y)}(\partial_{11}+\partial_{22})+\tilde{V}(x,y) \tag{28}$$

with nondegenerate potential $\tilde{V}(x,y)$:

$$\tilde{V}_{22}=\tilde{V}_{11}+\tilde{A}^{22}\tilde{V}_1+\tilde{B}^{22}\tilde{V}_2,$$

$$\tilde{V}_{12}=\tilde{A}^{12}\tilde{V}_1+\tilde{B}^{12}\tilde{V}_2 \tag{29}$$

is also superintegrable, where

$$\tilde{\lambda}=\lambda U,\quad \tilde{V}=\frac{V}{U},$$

$$\tilde{A}^{12} = A^{12} - \frac{U_2}{U}, \quad \tilde{A}^{22} = A^{22} + 2\frac{U_1}{U}, \quad \tilde{B}^{12} = B^{12} - \frac{U_1}{U}, \quad \tilde{B}^{22} = B^{22} - 2\frac{U_2}{U}.$$

Indeed, let $S=\Sigma 1/\lambda\partial_i(a^{ij}\lambda\partial_j)+W=S_0+W$ be a second-order formally self-adjoint symmetry operator of H and $S_U=\Sigma 1/\lambda\partial_i(a^{ij}\lambda\partial_j)+W_U=S_0+W_U$ be the special case of this that is in involution with $(1/\lambda)(\partial_{11}+\partial_{22})+U$. Then

$$\tilde{S} = S_0 - \frac{W_U}{U}H + \frac{1}{U}H$$

is the corresponding formally self-adjoint symmetry operator of $\tilde{H}$, with respect to the metric $d\tilde{s}^2=\lambda U(dx^2+dy^2)$.

Theorem 6:

1.

$$[\tilde{H},\tilde{S}] = 0 \Leftrightarrow [H,S] = 0.$$

2.

$$\tilde{S} = \sum_{ij} \frac{1}{\lambda U}\partial_i\left(\left(a^{ij} + \delta^{ij}\frac{1-W_U}{\lambda U}\right)\lambda U\right)\partial_j + \left(W - \frac{W_U V}{U} + \frac{V}{U}\right).$$

Proof:

1. This is a straightforward verification, using the identities

$$[H_0,S_0] = 0, \quad [H_0+V,S_0+W] = 0, \quad [H_0+U,S_0+W_U] = 0$$

and

$$[A,BC] = B[A,C] + [A,B]C, \quad \left[A,\frac{1}{U}\right] = -\frac{1}{U}[A,U]\frac{1}{U}$$

for linear operators A, B, C and nonzero function U.

2. This follows from the fact that $\partial_i W_U = \lambda\Sigma_j a^{ij}U_j$.

Q.E.D.

Corollary 3: If $S^{(1)}, S^{(2)}$ are second-order symmetry operators for H, then

$$[\tilde{S}^{(1)},\tilde{S}^{(2)}] = 0 \Leftrightarrow [S^{(1)},S^{(2)}] = 0.$$

Since one can always add a constant to a nondegenerate potential, it follows that $1/U$ defines an inverse Stäckel transform of $\tilde{H}$ to H. We say that two quantum superintegrable systems are *Stäckel equivalent* if one can be obtained from the other by a Stäckel transform. We can now use Theorem 6 to carry over immediately the basic result for 2D Stäckel transforms of classical superintegrable systems to 2D quantum superintegrable systems.[2]

Theorem 7: *Every nondegenerate second-order quantum superintegrable system in two variables is Stäckel equivalent to a superintegrable system on a constant curvature space.*

VI. NONDEGENERATE 3D QUANTUM SYSTEMS

Here we extend our analysis of classical 3D superintegrable systems with nondegenerate potentials to the quantum case. (This is less straightforward than in the 2D case.) As mentioned earlier, these systems arise only for functionally linearly independent bases of symmetries. For a manifold with metric $ds^2=\lambda(x,y,z)(dx^2+dy^2+dz^2)$ we replace the Hamiltonian $\mathcal{H}=(p_1^2+p_2^2+p_3^2)/\lambda(x,y,z)+V(x,y,z)$ by a formally self-adjoint operator

$$\hat{H} = \frac{1}{\mu(x,y,z)} \sum_{k,j=1}^{3} \partial_k \left(\frac{\delta^{kj}}{\lambda(x,y,z)} \mu(x,y,z) \partial_j \right) + V(x,y,z) \tag{30}$$

in local orthogonal coordinates. Here δ^{kj} is the Kronecker delta and the weight function μ is to be determined. Similarly, we replace a second-order symmetry of the Hamiltonian system $\mathcal{S} = \Sigma_{k,j=1}^{3} a^{kj}(x,y,z) p_k p_j + W(x,y,z)$, with $a^{kj} = a^{jk}$, by the formally self-adjoint operator

$$\hat{S} = \frac{1}{\mu} \sum_{k,j=1}^{3} \partial_k (a^{kj} \mu \partial_j) + W + \hat{W}, \quad a^{kj} = a^{jk}, \tag{31}$$

where the function $\hat{W}(x,y,z)$ is to be determined. These operators are formally self-adjoint with respect to the bilinear product

$$\langle f,g \rangle = \int f(x,y,z) g(x,y,z) \mu(x,y,z) \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z \tag{32}$$

on the manifold, i.e.,

$$\langle f, \hat{H} g \rangle = \langle \hat{H} f, g \rangle, \quad \langle f, \hat{S} g \rangle = \langle \hat{S} f, g \rangle$$

for all local C^∞ functions f,g with compact support on the manifold, where we set all boundary terms equal to 0.

Now we assume that $\{\mathcal{H},\mathcal{S}\}=0$ and require $[\hat{H},\hat{S}]=0$. Since $\hat{H},\hat{S}$ are formally self-adjoint, $[\hat{H},\hat{S}]$ must be formally skew-adjoint. From our assumption $\{\mathcal{H},\mathcal{S}\}=\mathbf{0}$ it is clear that the coefficients of the third-derivative terms ∂_{ijk} in the commutator must vanish, hence also the coefficients of the second-order terms vanish. Thus there are functions b_i such that

$$[\hat{H},\hat{S}] = \frac{1}{\mu} \sum_{i=1}^{3} \partial_i (b^i \mu) = \sum_{i=1}^{3} \left(b^i \partial_i + \frac{(b^i \mu)_i}{\mu} \right).$$

Using $\{\mathcal{H},\mathcal{S}\}=0$, we see that

$$b^j = \sum_{i=1}^{3} \left(\frac{1}{\lambda} \partial_{ii} + \frac{1}{\mu} \left(\frac{\mu}{\lambda} \right)_i \partial_i \right) \left(\frac{1}{\mu} \sum_{k=1}^{3} (a^{kj} \mu)_k \right) - \sum_{i,\ell=1}^{3} \left(a^{i\ell} \partial_{i\ell} + \frac{1}{\mu} (a^{i\ell} \mu)_i \partial_\ell \right) \left(\frac{1}{\mu} \left(\frac{\mu}{\lambda} \right)_j \right) + \frac{2}{\lambda} \hat{W}_j.$$

This formula simplifies greatly if we choose $\mu=\lambda$. Indeed, we find

$$b^j = -\frac{1}{\lambda} \partial_{jik} a^{ik} + \frac{2}{\lambda} \hat{W}_j.$$

Here i,j, and k are pairwise distinct. We can choose $\hat{W}_j = \frac{1}{2} \partial_{jik} a^{ik}$, so that $b^j \equiv 0$ provided the integrability conditions

$$\partial_{iijk} a^{ik} = \partial_{ijjk} a^{jk}$$

hold for i,j,k pairwise distinct. These conditions are satisfied, as we can verify from the explicit expressions for second-order conformal Killing tensors contained in Ref. 3

Theorem 8:

$$\{\mathcal{H},\mathcal{S}\} = 0 \Leftrightarrow [\hat{H},\hat{S}] = 0,$$

where $\hat{H},\hat{S}$ are given by (30) and (31) with $\mu=\lambda$ and $\hat{W}_j = \frac{1}{2} \partial_{jik} a^{ik}$ (for i,j,k pairwise distinct).

We can follow a similar approach to find the quantum analogies of first-order symmetries $\mathcal{L}=\Sigma_{j=1}^{2}a^{j}(x,y,z)p_j$, by the formally skew-adjoint first-order operator (with respect to the bilinear product (32))

$$\hat{L}=\frac{1}{\lambda}\sum_{j=1}^{3}\partial_j(a^{kj}\lambda). \tag{33}$$

It is straightforward to prove the following result.

Theorem 9:

$$\{\mathcal{H},\mathcal{L}\}=0\Leftrightarrow[\hat{H},\hat{L}]=0,$$

where $\hat{H},\hat{L}$ *are given by* (30) and (33) *with* $\mu=\lambda$.

VII. THE SPACE OF THIRD-ORDER SYMMETRIES

Now we investigate the third-order differential operators K that commute with the Hamiltonian: $[H,K]=0$. The treatment for the conformally flat 3D case proceeds in almost exact analogy to the 2D case, so we just sketch the results.

1. Since the second-order symmetries are formally self-adjoint, the commutators will be skew-adjoint. Thus we can limit ourselves to K that are skew adjoint.

2. Since H encodes a four-parameter family of potentials, the symmetry K must also be a function of the parameters. The highest order terms $a^{kji}\partial_{kji}$ in K (symmetric in k,j,i) will be independent of the parameters but lower order terms may have linear parameter dependence.

3. The skew-adjoint requirement uniquely determines the coefficients of the second-order terms in K. They are

$$\frac{3}{2\lambda}(a^{kji}\lambda)_i\partial_{kj}.$$

4. The skew-adjoint requirement means that there exist functions $a^{kji},\tilde{b}^i$ such that K has the unique representation

$$K=\sum_{k,j,i=1}^{3}\left(a^{kji}\partial_{kji}+\frac{3}{2\lambda}(a^{kji}\lambda)_i\partial_{kj}+\frac{1}{2\lambda}(a^{kji}\lambda)_{kj}\partial_i\right)+\sum_{i=1}^{3}\left(\tilde{b}^i\partial_i+\frac{1}{2\lambda}(\tilde{b}^i\lambda)_i\right), \tag{34}$$

where the functions $\tilde{b}^i(x,y,z)$ contain the parameter dependence.

5. Equating coefficients of the fourth-order terms in the operator condition $[H,K]=0$ where K is given by (34) we obtain the classical requirements that the a^{kji} be the components of a third-order Killing tensor.

6. Equating coefficients of the third-order terms in the condition $[H,K]=0$ we obtain relations that are consequences of the Killing tensor requirements.

7. The remaining conditions on K intertwine $\lambda,a^{kji},\tilde{b}^i$, and V, and are complicated. Rather than solve them directly, we make the unique decomposition

$$\tilde{b}^i(x_1,x_2,x_3,V_{x_1},V_{x_2},V_{x_3})=c^i(x_1,x_2,x_3)+b^i(x_1,x_2,x_3,V_{x_1},V_{x_2},V_{x_3}),$$

where

$$b^i = \sum_{j=1}^{3} f^{\ell,j}(x_1,x_2,x_3)\frac{\partial V}{\partial x_j}(x_1,x_2,x_3),$$

i.e., we can split off the parameter-dependent terms of $\tilde{b}^i$ from the rest. Then, equating the linear parameter-dependent coefficients of the second-order terms in the symmetry operator condition, we obtain the conditions

$$b_k^j + b_j^k = 3\lambda \sum_s a^{skj} V_s, \quad j \neq k, \quad j,k = 1,2,3,$$

$$b_j^j = \frac{3}{2}\lambda \sum_s a^{sjj} V_s - \frac{1}{2}\sum_s b^s (\ln \lambda)_s, \quad j = 1,2,3, \tag{35}$$

identical to the classical requirement.

8. Equating the quadratic parameter-dependent coefficients of the zeroth-order terms in the symmetry operator condition, we obtain the requirement

$$\sum_s b^s V_s = 0, \tag{36}$$

identical to the classical equation. There can be at most one skew adjoint K with given a^{ijk}, b^ℓ.

Theorem 10: *Let K be a third-order skew-adjoint symmetry* (11) *for a superintegrable system with nondegenerate potential V and $\tilde{b}^i = c^i(x,y,z) + b^i(x,y,z,V_1,V_2,V_3)$ where*

$$b^i = \sum_{j=1}^{3} f^{i,j}(x,y)\frac{\partial V}{\partial x_j}(x,y,z).$$

Then

$$f^{\ell,j} + f^{j,\ell} = 0, \quad 1 \leqslant \ell, j \leqslant 3$$

and K is uniquely determined by the four numbers

$$f^{1,2}(x_0,y_0,z_0), \quad f^{1,3}(x_0,y_0,z_0), \quad f^{2,3}(x_0,y_0,z_0), \quad f_3^{1,2}(x_0,y_0,z_0)$$

at any regular point (x_0,y_0,z_0) of V.

Corollary 4: Let V be a superintegrable nondegenerate potential. Then the space of third-order skew-adjoint symmetries is four-dimensional and is spanned by commutators of the second-order self-adjoint symmetries.

In exact analogy with the classical case, we can use the standard form to prove multiseparabilty for conformally flat 3D quantum systems.[4]

Theorem 11: *Let V be a quantum superintegrable nondegenerate potential. Then the associated system is multiseparable.*

VIII. THE QUANTUM 3D QUADRATIC ALGEBRA

We investigate the space of fourth-order differential operators F that commute with the Hamiltonian: $[H,F]=0$. The treatment for the conformally flat 3D case proceeds in almost exact analogy to the 2D case, so we sketch the results.

1. We are interested in the space of fourth-order symmetries that is spanned by the double commutators $[[S^{(1)},S^{(2)}],S^{(3)}]$ of second-order formally self-adjoint symmetries $S^{(j)}$ of the superintegrable system. The double commutators will be formally self-adjoint, so we can limit ourselves to F that are self-adjoint.

2. Since H encodes a three-parameter family of potentials, the symmetry F must also be a function of the parameters. The highest order terms $a^{\ell kji}\partial_{kji}$ in F (symmetric in ℓ,k,j,i) will be independent of the parameters but lower order terms may have linear or quadratic parameter dependence.

3. The self-adjoint requirement uniquely determines the third-order terms in F. They are

$$\sum_{\ell,k,j,i}\frac{2}{\lambda}(a^{\ell kji}\lambda)_i\partial_{\ell kj}.$$

4. The self-adjoint requirement means that there exist functions $a^{\ell kji},\tilde{b}^{ij},\tilde{W}$ such that F has the unique representation

$$F=\sum_{\ell,k,j,i=1}^{3}\frac{1}{\lambda}\partial_{ij}(a^{\ell kji}\lambda\partial_{k\ell})+\sum_{i,j=1}^{3}\frac{1}{\lambda}\partial_i(\tilde{b}^{ij}\lambda\partial_j)+\tilde{W}, \tag{37}$$

where the functions $\tilde{b}^{ij}(x_1,x_2,x_3),\tilde{W}(x_1,x_2,x_3)$ contain the parameter dependence.

5. Equating coefficients of the fifth-order terms in the operator condition $[H,F]=0$ we obtain the conditions for $a^{\ell kji}$ to be a fourth-order Killing tensor.

6. The remaining conditions on F intertwine $\lambda,a^{\ell kji},\tilde{b}^{ji},\tilde{W}$, and V, and are complicated. However, we can make the unique decomposition

$$\tilde{b}^{ji}(x_1,x_2,x_3,V_{x_1},V_{x_2},V_{x_3})=c^{ji}(x_1,x_2,x_3)+b^{ji}(x_1,x_2,x_3,V_{x_1},V_{x_2},V_{x_3})$$

where

$$b^{ji}=\sum_{\alpha=1}^{4}f^{ji,\alpha}W^{(\alpha)},\quad f^{ji,\alpha}=f^{ij,\alpha},$$

and $W^{(j)}=V_{x_j}$, $W^{(4)}=V_{x_1x_1}$.

Then, equating the linear parameter-dependent terms of third order in the derivatives, and the quadratic parameter-dependent terms of first order in the derivatives, we obtain exactly the classical conditions on the $f^{ji,\alpha}$.

Since at most one self-adjoint F can have data $a^{\ell kji},b^{kj}$, we find[3]

Theorem 12: *The subspace of truly fourth-order self-adjoint symmetry operators is of dimension at most twenty-one.*

If A,B are linear operators, we define their symmetrized product by

$$\{A,B\}\equiv\tfrac{1}{2}(AB+BA).$$

Theorem 13: *The twenty-one distinct monomials* $\{S^{(ij)},S^{(jk)}\}$ *form a basis for the space of fourth-order self-adjoint symmetry operators.*

Using an approach very similar to the above we can easily show that the space of truly sixth-order formally self-adjoint operator symmetries of H cannot exceed the classical maximal dimension of fifty-six. If A,B,C are linear operators, we define their symmetrized product by

$$\{A,B,C\}\equiv\tfrac{1}{6}(ABC+BAC+CAB+ACB+BCA+CBA).$$

Theorem 14: *The fifty-six distinct standard monomials* $\{S^{(hi)},S^{(jk)},S^{(\ell m)}\}$ *form a basis for the space of sixth-order self-adjoint symmetry operators.*

These theorems establish the closure of the quadratic algebra for 3D quantum superintegrable potentials: All fourth-order and sixth-order symmetry operators can be expressed as symmetric polynomials in the second-order symmetry operators.

IX. COVARIANT FORMULATION FOR THE 3D QUANTUM CASE

Theorem 8 yields an operator realization of the classical commutator brackets for second-order symmetries but the differential operator part of $\hat{H}$, though formally self-adjoint with respect to the weight function λ, is not the Laplace-Beltrami operator on the manifold. We can obtain the Laplace-Beltrami operator, at the expense of altering the potential V, by means of an appropriate gauge transformation. We now turn to this construction.

Set

$$H = e^{-\mathcal{R}}\hat{H}e^{\mathcal{R}}, \quad S = e^{-\mathcal{R}}\hat{S}e^{\mathcal{R}},$$

where $\mathcal{R}(x,y,z)$ is a function to be determined. Then $[H,S]=0$ if and only if $[\hat{H},\hat{S}]=0$. We will choose $\mathcal{R}$ such that the differential operator part of H is the Laplace-Beltrami operator on the manifold with metric $ds^2=\lambda(dx^2+dy^2+dz^2)$.

It is straightforward to show that

$$H = e^{-\mathcal{R}}\hat{H}e^{\mathcal{R}} = \frac{1}{\lambda}\sum_{i=1}^{3}(\partial_{ii} + 2\mathcal{R}_i\partial_i + \mathcal{R}_{ii} + \mathcal{R}_i^2) + V$$

so, if we set $\mathcal{R}=1/4\ln\lambda$, we have

$$H = \sum_{i=1}^{3}\left(\frac{1}{\lambda^{3/2}}\partial_i(\lambda^{1/2}\partial_i) + \frac{\mathcal{R}_{ii}+\mathcal{R}_i^2}{\lambda}\right) + V.$$

Similarly

$$S = \sum_{i,j=1}^{3}\left(\frac{1}{\lambda^{3/2}}\partial_i(a^{ij}\lambda^{3/2}\partial_j) + a^{ij}(\mathcal{R}_{ij} + 5\mathcal{R}_i\mathcal{R}_j) + a_i^{ij}\mathcal{R}_j\right) + W + \hat{W}.$$

The eigenvalue equation for $\hat{H}$ on the space with weight function $\mu=\lambda$ is $\hat{H}\Psi=E\Psi$. Setting $\Psi=e^{\mathcal{R}}\Phi=\lambda^{1/4}\Phi$ we see that the eigenvalue equation for Φ is $H\Phi=E\Phi$ and the eigenfunctions Φ lie in the space with weight function $\lambda^{3/2}$. Note that

$$\sum_{i=1}^{3}(\mathcal{R}_{ii}+\mathcal{R}_i^2)/\lambda = -\frac{1}{8}R,$$

where R is the Riemannian scalar curvature. The quantum potential is

$$\tilde{V} = -\tfrac{1}{8}R + V. \tag{38}$$

If we supplement the classical symmetries with quantum adjustments the corresponding operators are

$$H = \frac{1}{\sqrt{g}}\partial_i(g^{ij}\sqrt{g}\partial_j) + \frac{1}{8}R,$$

$$S = \frac{1}{\sqrt{g}}\partial_i(a^{ij}\sqrt{g}\partial_j) + \frac{1}{16}a_i^iR - \frac{5}{16}a^{ij}R_{ij} - \frac{1}{16}\nabla_i\nabla_j a^{ij}.$$

Here ∇_j is the usual covariant derivative on the Riemannian space. This formula always works, though a^{ij} must be a Killing tensor for a conformally flat space, Indeed for a Hamiltonian $\mathcal{H}=\lambda(x,y,z)(p_x^2+p_y^2+p_z^2)$ with symmetry $\mathcal{S}=a^{ij}p_ip_j$ the following conditions must be satisfied. If a_{ij} is a Killing tensor for a conformally flat space with infinitesimal distance

$$ds^2 = e^{-J(x,y,z)}(dx^2 + dy^2 + dz^2)$$

then it must satisfy the equations

$$\partial_{(i}a_{jk)} = g_{(ij}a_{k)}, \tag{39}$$

where

$$a_1 = e^{2J(x,y,z)}(a_{11}J_x - a_{12}J_y - a_{13}J_z), \quad a_2 = e^{2J(x,y,z)}(-a_{12}J_x + a_{22}J_y - a_{23}J_z),$$

$$a_3 = e^{2J(x,y,z)}(-a_{13}J_x - a_{23}J_y + a_{33}J_z).$$

Here (39) are the necessary and sufficient conditions that a_{ij} is a conformal Killing tensor in flat space. We know all solutions for this set of equations. The only constraint is that there exist a function $J(x,y,z)$ such that the a_l have the form indicated. Indeed, if we found the a_l from the considerations of flat space it is clear that

$$a_k = \frac{1}{5}\sum_j (\partial_j a_{jk} + \partial_k a_{jj}).$$

These results carry over in a very satisfactory manner for superintegrable systems with nondegenerate potential. In this case the parameters occurring in the potential appear only in the V and W terms, exactly as before. The quantum corrections are independent of these parameters.

Theorem 15: *Let $\mathcal{H}$, $\hat{H}$, and H be defined as above where $\mathcal{H}$ defines a classical superintegrable system with nondegenerate potential V. Let $\mathcal{S}^{(1)}, \mathcal{S}^{(2)}$ be second-order symmetries of $\mathcal{H}$, with corresponding symmetry operators $\hat{S}^{(j)}, S^{(j)}$. Then*

$$\{\mathcal{S}^{(1)}, \mathcal{S}^{(2)}\} = 0 \Leftrightarrow [\hat{S}^{(1)}, \hat{S}^{(2)}] = 0 \Leftrightarrow [S^{(1)}, S^{(2)}] = 0.$$

Corollary 5: Every conformally flat 3D classical superintegrable system with nondegenerate potential extends to a unique covariant quantum superintergrable system. The symmetries of the quantum system admit a quadratic algebra structure.

X. THE STÄCKEL TRANSFORM FOR 3D QUANTUM SYSTEMS

We work out the quantum analog of the Stäckel transform[26,27] for classical systems. Suppose we have a superintegrable system with Schrödinger operator

$$H = \frac{1}{\lambda^{3/2}(x,y,z)}\sum_{i=1}^{3} \partial_i(\lambda^{1/2}(x,y,z)\partial_i) - \frac{1}{8}R_\lambda(x,y,z) + V(x,y,z) \tag{40}$$

in local orthogonal coordinates, with scalar curvature R_λ and nondegenerate potential $V(x,y,z)$:

$$V_{33} = V_{11} + A^{33}V_1 + B^{33}V_2 + C^{33}V_3,$$

$$V_{22} = V_{11} + A^{22}V_1 + B^{22}V_2 + C^{22}V_3,$$

$$V_{23} = A^{23}V_1 + B^{23}V_2 + C^{23}V_3,$$

$$V_{13} = A^{13}V_1 + B^{13}V_2 + C^{13}V_3,$$

$$V_{12} = A^{12}V_1 + B^{12}V_2 + C^{12}V_3 \tag{41}$$

and suppose $U(x,y,z)$ is a particular solution of Eq. (41), nonzero in an open set. Then the transformed system

$$\tilde{H} = H = \frac{1}{\tilde{\lambda}^{3/2}(x,y,z)} \sum_{i=1}^{3} \partial_i (\tilde{\lambda}^{1/2}(x,y,z)\partial_i) - \frac{1}{8} R_{\tilde{\lambda}}(x,y,z) + \tilde{V}(x,y,z) \tag{42}$$

with nondegenerate potential $\tilde{V}(x,y,z)$:

$$\tilde{V}_{33} = \tilde{V}_{11} + \tilde{A}^{33}\tilde{V}_1 + \tilde{B}^{33}\tilde{V}_2 + \tilde{C}^{33}\tilde{V}_3,$$

$$\tilde{V}_{22} = \tilde{V}_{11} + \tilde{A}^{22}\tilde{V}_1 + \tilde{B}^{22}\tilde{V}_2 + \tilde{C}^{22}\tilde{V}_3,$$

$$\tilde{V}_{23} = \tilde{A}^{23}\tilde{V}_1 + \tilde{B}^{23}\tilde{V}_2 + \tilde{C}^{23}\tilde{V}_3,$$

$$\tilde{V}_{13} = \tilde{A}^{13}\tilde{V}_1 + \tilde{B}^{13}\tilde{V}_2 + \tilde{C}^{13}\tilde{V}_3,$$

$$\tilde{V}_{12} = \tilde{A}^{12}\tilde{V}_1 + \tilde{B}^{12}\tilde{V}_2 + \tilde{C}^{12}\tilde{V}_3, \tag{43}$$

is also superintegrable, where

$$\tilde{\lambda} = \lambda U, \quad \tilde{V} = \frac{V}{U},$$

$$\tilde{A}^{33} = A^{33} + 2\frac{U_1}{U}, \quad \tilde{B}^{33} = B^{33}, \quad \tilde{C}^{33} = C^{33} - 2\frac{U_3}{U},$$

$$\tilde{A}^{22} = A^{22} + 2\frac{U_1}{U}, \quad \tilde{B}^{22} = B^{22} - 2\frac{U_2}{U}, \quad \tilde{C}^{22} = C^{22},$$

$$\tilde{A}^{23} = A^{23}, \quad \tilde{B}^{23} = B^{23} - \frac{U_3}{U}, \quad \tilde{C}^{23} = C^{23} - \frac{U_2}{U},$$

$$\tilde{A}^{13} = A^{13} - \frac{U_3}{U}, \quad \tilde{B}^{13} = B^{13}, \quad \tilde{C}^{13} = C^{13} - \frac{U_1}{U},$$

$$\tilde{A}^{12} = A^{12} - \frac{U_2}{U}, \quad \tilde{B}^{12} = B^{12} - \frac{U_1}{U}, \quad \tilde{C}^{12} = C^{12}.$$

Indeed, let $S = \Sigma(1/\lambda^{3/2})\partial_i(a^{ij}\lambda^{3/2}\partial_j) + \mathcal{W}_R + W = S_0 + \mathcal{W}_R + W$ be a second-order formally self-adjoint symmetry operator of H, where $\mathcal{W}_R$ is the potential term that depends on the curvature R and W is the part that depends on V. Let $S_U = \Sigma(1/\lambda^{3/2})\partial_i(a^{ij}\lambda^{3/2}\partial_j) + \mathcal{W}_R + W_U = S_0 + \mathcal{W}_R + W_U$ be the special case of this that is in involution with

$$\frac{1}{\lambda^{3/2}} \sum_{i=1}^{3} \partial_i(\lambda^{1/2}\partial_i) - \frac{1}{8} R_\lambda + U.$$

Then

$$\tilde{S} = S_0 - \frac{W_U}{U}H + \frac{1}{U}H$$

is the corresponding formally self-adjoint symmetry operator of $\tilde{H}$, with respect to the metric $d\tilde{s}^2 = \lambda U(dx^2 + dy^2 + dz^2)$.

Theorem 16:

1.

$$[\tilde{H}, \tilde{S}] = 0 \Leftrightarrow [H, S] = 0.$$

2.

$$\tilde{S} = \sum_{ij} \frac{1}{(\lambda U)^{3/2}} \partial_i \left(\left(a^{ij} + \delta^{ij} \frac{1 - W_U}{\lambda U} \right) (\lambda U)^{3/2} \right) \partial_j + \left(\mathcal{W}_R + \left(\frac{W_U}{U} - \frac{1}{U} \right) \frac{R_\lambda}{8} + \left(W - \frac{W_U V}{U} + \frac{V}{U} \right) \right).$$

Proof:

1. We perform an inverse gauge transformation on H, S to return them to the forms $\hat{H}, \hat{S}$, (30) and (31), with $\mu = \lambda$ and $\hat{W}_j = \frac{1}{2}\partial_{jik} a^{ik}$ (for i, j, k pairwise distinct). Similarly we perform an inverse gauge transformation on $\tilde{H}, \tilde{S}$ to return them to the forms $\hat{\tilde{H}}, \hat{\tilde{S}}$, (30) and (31), with $\mu = U\lambda$. These commuting operators are formally self-adjoint with respect to the weight function $U\lambda$. Then it is a straightforward computation to verify that $[\hat{\tilde{H}}, \hat{\tilde{S}}] = 0 \Leftrightarrow [\hat{H}, \hat{S}] = 0$. Indeed, just as in the 2D case, one needs only the identities

$$[\hat{H}_0, \hat{S}_0] = 0, \quad [\hat{H}_0 + V, \hat{S}_0 + W] = 0, \quad [\hat{H}_0 + U, \hat{S}_0 + W_U] = 0$$

and

$$[A, BC] = B[A, C] + [A, B]C, \quad \left[A, \frac{1}{U} \right] = -\frac{1}{U}[A, U]\frac{1}{U}$$

for linear operators A, B, C and nonzero function U. Then the first part of the theorem follows from applying the original gauge transformations to take $\hat{H}, \hat{S}$ to H, S and $\hat{\tilde{H}}, \hat{\tilde{S}}$ to $\tilde{H}, \tilde{S}$.

2. This follows from the fact that $\partial_i W_U = \lambda \Sigma_j a^{ij} U_j$.

Q.E.D.

Corollary 6: If $S^{(1)}, S^{(2)}$ are second-order symmetry operators for H, then

$$[\tilde{S}^{(1)}, \tilde{S}^{(2)}] = 0 \Leftrightarrow [S^{(1)}, S^{(2)}] = 0.$$

At this point it is clear that the basic classical result for 3D Stäckel transforms of conformally flat classical superintegrable systems contained in Ref. 4 can be carried over to 3D quantum superintegrable systems.

Theorem 17: *Every nondegenerate second-order quantum superintegrable system on a 3D conformally flat space is Stäckel equivalent to a superintegrable system on a constant curvature space.*

XI. CONCLUSIONS AND OUTLOOK

We showed that 2D classical second-order superintegrable systems with nondegenerate potential and the corresponding 3D conformally flat systems each have a unique quantum superintegrable extension, and that the closure of the quadratic algebra and basic structure theory is unchanged at the quantum level. A critical feature of the proofs is use of the formal self-adjoint and skew-adjoint properties of the higher order symmetry operators. For the 2D case the extension is completely straightforward and the quantum extension has the same nondegenerate potential as the classical system. For the 3D systems a two-step procedure is required. First the classical

system is extended to a quantum system with appropriate formal self and skew adjoint symmetries and such that the potential remains unchanged. This quantum system, however, is not covariant, i.e., the Schrödinger operator does not correspond to a Laplace-Beltrami operator on a curved manifold. The second step in the procedure is to perform a gauge transformation to obtain covariantly correct Schrödinger operators. This alters the potential by adding a term that depends on the scalar curvature. We also showed that the Stäckel transform has a unique quantum extension and it remains true that all of our quantum superintegrable systems are Stäckel transforms of constant curvature superintegrable systems.

All 2D systems have been classified and we are making considerable progress on the 3D classification theory for systems with functionally linearly independent bases of symmetries,[4] though the problem is complicated. The next steps in our program are (1) to study 3D superintegrable systems with degenerate potentials and (2) to study nondegenerate superintegrable systems in higher dimensions.

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A referee's suggestion that we show how our structure theory relates to the generalized Calogero potential enabled us to clarify this relation and to point out the importance of the concept of functional linear independence for functionally independent symmetries. In the process we found and corrected an error in a paper (Ref. 3) of the series.

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On $su_q(1,1)$-models of quantum oscillator

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Models of the quantum oscillator, based on the discrete series representations of the quantum algebra $su_q(1,1)$, are constructed. The position and momentum operators in these models are twisted generators J_2 and J_1 for such $su_q(1,1)$-representations, respectively. As in the case of the standard harmonic oscillator in quantum mechanics, the position and momentum operators here have continuous simple spectra. These spectra cover a finite interval on the real line, which depends on a value of q. Eigenfunctions of these operators are explicitly found. It is shown that the Macfarlane–Biedenharn q-oscillator is a limit case of the oscillators under discussion. The $q=1$ limit case, in which spectra of the position and momentum operators cover the whole real line, is also considered in detail. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2338141]

I. INTRODUCTION

A $su_q(1,1)$-model of the quantum oscillator is a model that obeys the dynamics of the harmonic oscillator, with the position and momentum operators and Hamiltonian being functions of elements of the quantum algebra $su_q(1,1)$. The aim of this paper is to develop the theory of such oscillators by using the discrete series representations of the quantum algebra $su_q(1,1)$.

There exist many algebraic constructions which can be used for building up different models of quantum oscillators. For most of them it is difficult to construct a complete theory of such an oscillator: spectra of observables, explicit form of eigenfunctions of observables, the description of time evolution, etc. Only for some such models is it possible to develop a corresponding theory. In Refs. 1 and 2 the so-called q-oscillator was constructed, which is a q-deformed analogue of the standard linear harmonic oscillator in quantum mechanics. A theory of this oscillator was elaborated in detail. There are physical problems for which the q-oscillator is more adequate than the quantum harmonic oscillator (see, for example, Refs. 3 and 4). Unlike the quantum field theory, constructed on the base of the standard quantum harmonic oscillator, the quantum field theory, built on the base of the q-oscillator, is free of some divergences. The q-oscillator has many useful properties, which are absent in the common quantum harmonic oscillator (see, for example, Refs. 5 and 6).

However, in the case of the q-oscillator the basic commutator relations

$$[H,Q] = -\mathrm{i}P, \quad [H,P] = \mathrm{i}Q, \tag{1}$$

are broken. That is why the q-oscillator is not so attractive for many physicists.

For this reason, many efforts have been made to construct those models of the quantum oscillator that preserve the relations (1). Postulates, which have to be satisfied for constructing such models of the quantum oscillator, were formulated in Ref. 7. These postulates are:

1. There exists an essentially self-adjoint (Hermitian) *position* operator, denoted as Q, whose spectrum Spec Q is the set of positions of the system.

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2. There exists a self-adjoint *Hamiltonian* operator, H, which generates time evolution through the Newton–Lie, or equivalent Hamilton–Lie, equations:

$$[H,[H,Q]] = Q \Leftrightarrow \begin{cases} [H,Q] =: -\mathrm{i}P \\ [H,P] = \mathrm{i}Q, \end{cases} \tag{2}$$

where $[\cdot,\cdot]$ is the commutator. The first Hamilton equation in (2) defines the *momentum* operator P, while the second one contains the harmonic oscillator dynamics. The set of momentum values of the system is the spectrum Spec P of P.

3. The three operators, Q, P, and H, closed into an *associative algebra*, satisfy the Jacobi identity,

$$[P,[H,Q]] + [Q,[P,H]] + [H,[Q,P]] = 0. \tag{3}$$

The second and third postulates determine that $[Q,P]$ must commute with H, which implies that it can only be of the form $[Q,P]=\mathrm{i}f(H)$, where f is some function of H (including constants) and the i is placed to make $f(H)$ self-adjoint, but do not otherwise specify this basic commutator further. For a constant $f(H)=\hbar\hat{1}$, one recovers the standard oscillator algebra $H_4 = \mathrm{span}\{H,Q,P,\hat{1}\}$, which contains the basic Heisenberg-Weyl subalgebra $W_1=\mathrm{span}\{Q,P,\hat{1}\}$ of quantum mechanics. In Ref. 8 the authors examined the cases which, in the unitary irreducible representations of spin $j=\frac{1}{2}N$ ($N\in\{0,1,\ldots\}$ is fixed), correspond to the linear function $f(H)=H-\left(j+\frac{1}{2}\right)\hat{1}=:J_3$, and so the operators close into the Lie algebra $\mathrm{so}(3)\equiv\mathrm{su}(2)=\mathrm{span}\{Q,P,J_3\}$. In Ref. 9 the above-noted postulates are used to construct the so-called finite q-oscillator, for which (contrary to the Macfarlane–Biedenharn q-oscillator, mentioned earlier) the relations $[H,Q] = -\mathrm{i}P$ and $[H,P]=\mathrm{i}Q$ take place.

The quantum oscillators, constructed in Refs. 8 and 9, are characterized by the property that the position and momentum operators have finite *discrete spectra*. In the present paper we use the quantum algebra $\mathrm{su}_q(1,1)$ in order to construct, by means of the above-presented postulates, models of the quantum oscillator, which have *continuous bounded spectra* of the position and momentum operators.

For deriving properties of oscillators under discussion, we essentially employ the theory of special functions and orthogonal polynomials. Namely, using the interrelation between self-adjoint operators (in our case they are the position and momentum operators) and orthogonal polynomials, we find spectra of the position and momentum operators and derive an explicit form of their eigenfunctions. We define an explicit form of the evolution operator in the coordinate space. An analogue of the Fourier integral transform, which connects the coordinate and momentum spaces, is also constructed.

We show that oscillators under study, parametrized by a positive number l, in the limit as $l \to \infty$ coincide with the Macfarlane–Biedenharn q-oscillator.

At the end of the paper we study the limit case when $q=1$. In this case we obtain models of the quantum oscillator, also parametrized by a positive number l. In the limit $l\to\infty$ these models give the standard quantum harmonic oscillator, that is, these models give us new deformations of the standard model, for which (contrary to the case of the Macfarlane–Biedenharn q-oscillator) the relations (1) are fulfilled.

We employ the standard notations of the theory of basic hypergeometric functions and q-orthogonal polynomials (see, for example, Ref. 10). We shall use q-numbers, defined as

$$[a]_q := \frac{q^{a/2} - q^{-a/2}}{q^{1/2} - q^{-1/2}}$$

for any complex number a. Everywhere in the following it is assumed that $0<q<1$.

II. DISCRETE SERIES REPRESENTATIONS OF $su_q(1,1)$

The quantum algebra $su_q(1,1)$ is defined as the associative algebra, generated by the elements J_+, J_-, J_3, satisfying the commutation relations

$$[J_3,J_\pm] = \pm J_\pm, \quad [J_-,J_+] = \frac{q^{J_3} - q^{-J_3}}{q^{1/2} - q^{-1/2}} \equiv [2J_3]_q, \tag{4}$$

and the conjugation relations

$$J_3^* = J_3, \quad J_+^* = J_-. \tag{5}$$

(Observe that here we have replaced J_- by $-J_-$ in the usual definition of the algebra $sl_q(2)$.)

Introducing the elements $J_1 = \frac{1}{2}(J_+ + J_-)$ and $J_2 = (1/2i)(J_+ - J_-)$, we characterize the algebra $su_q(1,1)$ by the relations

$$[J_3,J_1] = iJ_2, \quad [J_2,J_3] = iJ_1, \quad [J_1,J_2] = -\frac{i}{2}[2J_3]_q. \tag{6}$$

The Casimir element of the algebra $su_q(1,1)$ is given by the formula

$$C_q := [J_3 - 1/2]_q^2 + \tfrac{1}{2}[2J_3]_q - J_1^2 - J_2^2 - 1/4 = [J_3 - 1/2]_q^2 - J_+J_- - 1/4.$$

We are interested in the discrete series representations of $su_q(1,1)$ with lowest weights. These irreducible representations will be denoted by T_l, where l is a lowest weight, which may be any positive number (see, for example, Ref. 11).

In order to realize these representations, we consider the space $\mathcal{P}$ of all polynomials in one variable y. We fix l and introduce the monomials

$$e_n^l \equiv e_n^l(y) := c_n^l y^n, \quad n = 0,1,2,3, \ldots, \tag{7}$$

where

$$c_0^l = 1, \quad c_n^l = \prod_{k=1}^{n} \frac{[2l+k-1]_q^{1/2}}{[k]_q^{1/2}} = q^{(1-2l)n/4} \frac{(q^{2l};q)_n^{1/2}}{(q;q)_n^{1/2}}, \quad n = 1,2,3, \ldots,$$

and $(a;q)_n := (1-a)(1-aq)\ldots(1-aq^{n-1})$. They form a basis in $\mathcal{P}$. The representation T_l is then realized by the operators (see Ref. 12)

$$J_3 = y\frac{d}{dy} + l, \quad J_\pm = y^{\pm 1}[J_3 \pm l]_q.$$

In this explicit realization one has

$$J_+e_n^l = \sqrt{[2l+n]_q[n+1]_q}\,e_{n+1}^l, \quad J_-e_n^l = \sqrt{[2l+n-1]_q[n]_q}\,e_{n-1}^l,$$

$$J_3e_n^l = (l+n)e_n^l.$$

Obviously, these operators satisfy the commutation relations (4). The basis functions $e_n^l(y)$ are eigenfunctions of the operators J_3 and C_q: $C_qe_n^l = \left([l-1/2]_q^2 - \frac{1}{4}\right)e_n^l$.

It is known that the discrete series representations T_l can be realized on a Hilbert space, on which the conjugation relations (5) hold. In order to obtain such a Hilbert space, we assume that the monomials $e_n^l(y)$, $n=0,1,2,\ldots$, constitute an orthonormal basis in this Hilbert space. This introduces a scalar product into the space $\mathcal{P}$. Then one closes this space with respect to this scalar product and obtains the Hilbert space, which will be denoted by $\mathcal{H}_l$. The Hilbert space $\mathcal{H}_l$ consists of functions (series)

$$f(y)=\sum_{n=0}^{\infty} b_n e_n^l(y)=\sum_{n=0}^{\infty} b_n c_n^l y^n=\sum_{n=0}^{\infty} a_n y^n,$$

where $a_n=b_n c_n^l$. Since $\langle e_n^l, e_m^l\rangle=\delta_{nm}$ by definition, for $f(y)=\Sigma_{n=0}^{\infty} a_n y^n$ and $f'(y)=\Sigma_{n=0}^{\infty} a_n' y^n$ we have

$$\langle f,f'\rangle=\sum_{n=0}^{\infty} a_n a_n'/|c_n^l|^2.$$

This means that the Hilbert space $\mathcal{H}_l$ consists of functions $f(y)=\Sigma_{n=0}^{\infty} a_n y^n$, such that

$$\|f\|^2\equiv\sum_{n=0}^{\infty}|a_n/c_n^l|^2<\infty.$$

III. DESCRIPTION OF $su_q(1,1)$-MODELS

In order to describe models of the quantum oscillator, which are based on irreducible representations of the algebra $su_q(1,1)$, we fix a positive number l and consider the discrete series representation T_l from Sec. II. We define Hamiltonian H and position and momentum operators Q and P in terms of the generators J_3, J_2, J_1 of this representation as

$$H=J_3-l+1/2,\quad Q=q^{J_3/4}J_2q^{J_3/4},\quad P=q^{J_3/4}J_1q^{J_3/4}. \tag{8}$$

Then, due to (6), for Q, P, and H we have the commutation relations

$$[H,Q]=-\mathrm{i}P,\quad [H,P]=\mathrm{i}Q, \tag{9}$$

$$\begin{aligned}[Q,P]&=\frac{\mathrm{i}}{2}q^{(1/2)J_3}(q^{-(1/2)}J_+J_--q^{(1/2)}J_-J_+)q^{(1/2)J_3}=:\mathrm{i}F_q(C_q,J_3)\\&=\mathrm{i}\left(e^{-\kappa J_3}\left[\left(C_q+\frac{1}{4}\right)\sinh\frac{\kappa}{2}+\frac{1}{2}\operatorname{csch}\frac{\kappa}{2}\right]-\frac{1}{2}e^{-2\kappa J_3}\coth\frac{\kappa}{2}\right),\end{aligned} \tag{10}$$

where $q:=e^{-\kappa}$. The operator $F_q(C_q,J_3)$, defined in (10), commutes with J_3 and therefore is also diagonal in the standard basis $\{e_n^l\}$; in the irreducible representation T_l we have

$$F_q e_m^j=\frac{e^{-2m\kappa}\cosh\frac{\kappa}{2}-e^{-m\kappa}\cosh\left(j+\frac{1}{2}\right)\kappa}{2\sinh\frac{\kappa}{2}}e_m^j,$$

but its spectrum is *not* a good candidate for an oscillator Hamiltonian, because it is not equally spaced, and so the corresponding time evolution would be dispersive rather than harmonic.

The basis e_n^l, $n=0,1,2,\ldots$, in the Hilbert space $\mathcal{H}_l$ consists of eigenfunctions of the Hamiltonian H:

$$He_n^l=(n+1/2)e_n^l,\quad n=0,1,2,\ldots, \tag{11}$$

that is, the spectrum of H coincides with the spectrum of the Hamiltonian of the standard quantum harmonic oscillator.

The operators (8) satisfy the postulates 1–3 of Sec. I. The time evolution of our system is the harmonic motion with

$$e^{i\tau H}\begin{pmatrix} Q \\ P \end{pmatrix} e^{-i\tau H} =: \begin{pmatrix} Q(\tau) \\ P(\tau) \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix}\begin{pmatrix} Q \\ P \end{pmatrix}.$$

This is a group U(1) of inner automorphisms of the algebra $su_q(1,1)$ and of rotations of the phase-space surface. We have

$$\exp(i\tau H) = \exp[i\tau(J_3 - l + 1/2)] = e^{-i(l-1/2)\tau}\exp(i\tau J_3). \tag{12}$$

Explicit form of the time evolution in the coordinate space will be derived in the following.

Thus, to each positive number l there corresponds a model of the quantum oscillator: distinct values of l give rise to mutually nonequivalent models.

IV. SPECTRUM AND EIGENFUNCTIONS OF THE MOMENTUM OPERATOR

Since $P = q^{J_3/4} J_1 q^{J_3/4}$, the momentum operator P in the basis of the Hamiltonian eigenfunctions e_n^l, $n = 0,1,2,\ldots$, has the form

$$Pe_n^l = \frac{q^{(l+n)/2}}{2}\left(q^{1/4}\sqrt{[2l+n]_q[n+1]_q}e_{n+1}^l + q^{-1/4}\sqrt{[2l+n-1]_q[n]_q}e_{n-1}^l\right)$$

$$= \frac{1}{2(q^{-1/2}-q^{1/2})}\left(\sqrt{(1-q^{n+1})(1-q^{2l+n})}e_{n+1}^l + \sqrt{(1-q^n)(1-q^{2l+n-1})}e_{n-1}^l\right).$$

We wish to find the spectrum and eigenfunctions of this operator. Let $\psi_p(y)$ be an eigenfunction of P, corresponding to the eigenvalue p, $P\psi_p(y) = p\psi_p(y)$. Then

$$\psi_p(y) = \sum_{n=0}^{\infty} h_n(p)e_n^l(y), \tag{13}$$

where $h_n(p)$ are coefficients, which may depend on the eigenvalues p.

In order to find an explicit form of eigenfunctions $\psi_p(y)$, we substitute expression (13) for $\psi_p(y)$ into equation $P\psi_p(y) = p\psi_p(y)$:

$$\frac{1}{2}\sum_{n=0}^{\infty} h_n(p)\left(\frac{\sqrt{(1-q^{n+1})(1-q^{2l+n})}}{q^{-1/2}-q^{1/2}}e_{n+1}^l + \frac{\sqrt{(1-q^n)(1-q^{2l+n-1})}}{q^{-1/2}-q^{1/2}}e_{n-1}^l\right) = p\sum_{n=0}^{\infty} h_n(p)e_n^l.$$

Equating coefficients of a fixed basis element e_n^l, we obtain a three-term recurrence relation for the coefficients $h_n(p)$:

$$2ph_n(p) = \frac{\sqrt{(1-q^{n+1})(1-q^{2l+n})}}{q^{-1/2}-q^{1/2}}h_{n+1}(p) + \frac{\sqrt{(1-q^n)(1-q^{2l+n-1})}}{q^{-1/2}-q^{1/2}}h_{n-1}(p). \tag{14}$$

It is clear from (14) that the coefficients $h_n(p)$ are uniquely determined up to a common constant factor. We have $h_{-1}(p) = 0$ and setting $h_0(p) = 1$, we see that $h_n(p)$, $n = 1,2,\ldots$, are evaluated uniquely. Moreover, relation (14) shows that the $h_n(p)$ are polynomials in p of degree n.

To solve the recurrence relation (14), make the substitution

$$h_n(p) = \left(\frac{(q;q)_n}{(q^{2l};q)_n}\right)^{1/2} h_n'(p).$$

Then (14) turns into the equality

$$2(q^{-1/2}-q^{1/2})ph_n'(p) = (1-q^{n+1})h_{n+1}'(p) + (1-q^{2l+n-1})h_{n-1}'(p). \tag{15}$$

Comparing this relation with the recurrence relation

$$(1-q^{n+1})P_{n+1}(z;a|q)-2[z-2aq^n\cos\varphi]P_n(z;a|q)+(1-a^2q^{n-1})P_{n-1}(z;a|q)=0$$

[see formula (3.9.3) in Ref. 13] for the q-Meixner–Pollaczek polynomials

$$P_n(z;a|q)=\frac{(a^2;q)_n}{(q;q)_n}a^{-n}e^{-in\varphi}{}_3\phi_2(q^{-n},ae^{i(\theta+2\varphi)},ae^{-i\theta};a^2,0;q,q),$$

$$z=\cos(\theta+\varphi),$$

with $a=q^l$ and $\varphi=\pi/2$, one finds that

$$h_n'(p)=P_n((q^{-1/2}-q^{1/2})p;q^l|q)=i^{-n}q^{-ln}\frac{(q^{2l};q)_n}{(q;q)_n}{}_3\phi_2(q^{-n},-q^le^{i\theta},q^le^{-i\theta};q^{2l},0;q,q),$$

where $\sin\theta=(q^{-1/2}-q^{1/2})p$ and ${}_3\phi_2\ (q^{-n},\dots)$ is the basic hypergeometric polynomial. Consequently, for the coefficients in (13) one obtains that

$$h_n(p)=\left(\frac{(q;q)_n}{(q^{2l};q)_n}\right)^{1/2}P_n((q^{-1/2}-q^{1/2})p;q^l|q). \tag{16}$$

Thus, the eigenfunctions of the momentum operator P are of the form

$$\psi_p(y)=\sum_{n=0}^{\infty}\left(\frac{(q;q)_n}{(q^{2l};q)_n}\right)^{1/2}P_n(\sin\theta;q^l|q)e_n^l(y)=\sum_{n=0}^{\infty}q^{(1-2l)n/4}P_n(p(q^{-1/2}-q^{1/2});q^l|q)y^n, \tag{17}$$

where expression (7) for the basis elements has been taken into account. This result agrees with those derived in Refs. 12 and 14.

Expression (17) for the eigenfunctions $\psi_p(y)$ can be summed up by employing generating function (3.9.11) in Ref. 13 and we finally conclude that *the eigenfunctions of the momentum operator are of the form*

$$\psi_p(y)=\frac{(ciy;q)_\infty(-ciy;q)_\infty}{(-c'ie^{i\theta}y;q)_\infty(c'ie^{-i\theta}y;q)_\infty}, \tag{18}$$

where $c=q^{(2l+1)n/4}$, $c'=q^{(1-2l)n/4}$ and, as before, $p=(\sin\theta)/(q^{-1/2}-q^{1/2})$.

The spectrum of the momentum operator P can be found with the aid of formula (17). Indeed, it is easy to verify that the operator P, coinciding with the operator $q^{J_3/4}J_1q^{J_3/4}$ of the discrete series representation T_l, is bounded and self-adjoint. Moreover, P is representable in the basis $\{e_n^l\}$ by a Jacobi matrix, that is, by a tridiagonal matrix of the form

$$M=\begin{pmatrix} b_0 & a_0 & 0 & 0 & 0 & \cdots \\ a_0 & b_1 & a_1 & 0 & 0 & \cdots \\ 0 & a_1 & b_2 & a_2 & 0 & \cdots \\ 0 & 0 & a_2 & b_3 & a_3 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \quad a_i\neq 0.$$

There exists a theory (see Ref. 15, Chap. VII; a short description of this theory can be found in Ref. 6), which allows one to connect spectra of operators of such type with orthogonality measures for appropriate orthogonal polynomials. To employ this theory, we note that the eigenfunctions $\psi_p(y)$ are expressed in terms of the basis elements e_n^l by formula (13) with the *polynomial* coefficients (16). According to the results of Chap. VII in Ref. 15, these polynomials are orthogonal with respect to some measure $d\mu(p)$. (This measure is unique, up to a constant factor, since the operator P is self-adjoint; see Ref. 6.) A set (a subset of $\mathbb{R}$), on which the polynomials are orthogonal, coincides with the spectrum of the operator P and $d\mu(p)$ determines the spectral measure of this operator. Moreover, the spectrum of P is simple.

Thus, to find the spectrum of the momentum operator P, we recall that the q-Meixner–Pollaczek polynomials $P_n(z) \equiv P_n(z;a|q)$ are orthogonal and the orthogonality relation is of the form

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} P_m(\sin\theta)P_n(\sin\theta)w(\sin\theta)\mathrm{d}\theta = \frac{(q^{2l};q)_n}{(q;q)_n}\delta_{mn},$$

where [see formula (3.9.2) in Ref. 13]

$$w(\sin\theta) = (q;q)_\infty(q^{2l};q)_\infty\left|\frac{(-e^{2i\theta};q)_\infty}{(-q^l e^{i\theta};q)_\infty(q^l e^{i\theta};q)_\infty}\right|^2.$$

This orthogonality relation can be written as

$$\frac{(q;q)_n}{(q^{2l};q)_n}\int_{-b}^{b} P_m(p/b)P_n(p/b)\tilde{w}(p)\mathrm{d}p = \delta_{mn}, \tag{19}$$

where $b := (q^{-1/2}-q^{1/2})^{-1}$ and $\tilde{w}(p) = w(p/b)/b\cos\theta$. This means that the spectrum of P coincides with the finite interval,

$$\mathrm{Spec}\ P = [-b,b], \quad b = (q^{-1/2}-q^{1/2})^{-1}.$$

Thus, the spectrum is continuous and simple. Continuity of the spectrum means that the eigenfunctions $\psi_p(y)$ are not elements of the Hilbert space $\mathcal{H}_l$. These functions of y for $p \in [-b,b]$ form a continuous basis in $\mathcal{H}_l$ (similar to the basis $\{e^{ipx}\}$ in the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions on $\mathbb{R}$).

We see that the spectrum of P covers the infinite interval $(-\infty,\infty)$ in the limit as $q\to 1$. When $q\to 0$, the spectrum accumulates into the zero point.

Eigenfunctions of P are determined up to constant factors. In order to normalize the eigenfunctions $\psi_p(y)$, we take into account the orthogonality relation (19) for q-Meixner–Pollaczek polynomials. Since these polynomials are associated with the determinate moment problem (see, for example, Ref. 6 for the description of this correspondence), the set $P_n(p/b)$, $n=0,1,2,\ldots$, is complete in the Hilbert space $L^2([-b,b],\tilde{w})$ with the scalar product

$$\langle f_1,f_2\rangle = \int_{-b}^{b} f_1(p)\overline{f_2(p)}\tilde{w}(p)\mathrm{d}p, \tag{20}$$

where b and $\tilde{w}(p)$ are the same as in (19). This means that

$$\sum_{n=0}^{\infty}\frac{(q;q)_n}{(q^{2l};q)_n}\tilde{w}(p)P_n(p/b;q^{2l}|q)P_n(p'/b;q^{2l}|q) = \delta(p-p').$$

Then, on account of (17), one gets

$$\langle\psi_p(y),\psi_{p'}(y)\rangle = \sum_{n=0}^{\infty}\frac{(q;q)_n}{(q^{2l};q)_n}P_n(p/b;q^{2l}|q)P_n(p'/b;q^{2l}|q) = \frac{\delta(p-p')}{\tilde{w}(p)}.$$

Therefore, the normalized functions are

$$\tilde{\psi}_p(y) = \tilde{w}(p)^{1/2}\psi_p(y), \quad p\in[-b,b],$$

that is, $\langle\tilde{\psi}_p(y),\tilde{\psi}_{p'}(y)\rangle = \delta(p-p')$.

V. SPECTRUM AND EIGENFUNCTIONS OF THE POSITION OPERATOR

The position operator Q in the basis e_n^l, $n=0,1,2,\ldots$, has the form

$$Qe_n^l = \frac{q^{(l+n)/2}}{2\mathrm{i}}[q^{1/4}\sqrt{[2l+n]_q[n+1]_q}e_{n+1}^l - q^{-1/4}\sqrt{[2l+n-1]_q[n]_q}e_{n-1}^l].$$

By changing the basis $\{e_n^l\}$ to the basis $\{\tilde{e}_n^l\}$, where $\tilde{e}_n^l = \mathrm{i}^{-n}e_n^l$, we see that the position operator Q is given in the latter basis by the same formula as the momentum operator is given in the former basis $\{e_n^l\}$ (see Sec. IV). This means that the spectrum of the operator Q coincides with the spectrum of P, that is,

$$\mathrm{Spec}\ Q = [-b,b], \quad b = (q^{-1/2} - q^{1/2})^{-1}.$$

Eigenfunctions of the position operator can be found (by using the basis $\{\tilde{e}_n^l\}$) in the same way as in the case of the momentum operator. For this reason, we exhibit here only the result.

Let $\phi_x(y)$ be an eigenfunction of Q, corresponding to the eigenvalue x, $Q\phi_x(y) = x\phi_x(y)$. Then

$$\phi_x(y) = \sum_{n=0}^{\infty} \tilde{h}_n(x)e_n^l(y), \tag{21}$$

where, as before, the $e_n^l(y)$ are given by (7) and the $\tilde{h}_n(x)$ are coefficients, which may depend on the eigenvalues x.

Repeating the reasoning of Sec. IV, one derives a three-term recurrence relation for the polynomials $\tilde{h}_n(x)$ and concludes that

$$\tilde{h}_n(x) = \mathrm{i}^{-n}h_n(x) = \mathrm{i}^{-n}\left(\frac{(q;q)_n}{(q^{2l};q)_n}\right)^{1/2} P_n(x/b;q^l|q), \quad b := (q^{-1/2} - q^{1/2})^{-1}, \tag{22}$$

where $P_n(z;q^l|q)$ is the q-Meixner–Pollaczek polynomial as in Sec. IV. One thus deduces that eigenfunctions of the position operator Q are of the form

$$\phi_x(y) = \sum_{n=0}^{\infty} \mathrm{i}^{-n}\left(\frac{(q;q)_n}{(q^{2l};q)_n}\right)^{1/2} P_n(x/b;q^l|q)e_n^l(y) = \sum_{n=0}^{\infty} \mathrm{i}^{-n}q^{(1-2l)n/4}P_n(x/b;q^l|q)y^n. \tag{23}$$

One can sum up expression (23) for the eigenfunctions $\phi_x(y)$ by employing formula (3.9.11) in Ref. 13. Thus *the eigenfunctions of the position operator Q are of the form*

$$\phi_x(y) = \frac{(-cy;q)_\infty (cy;q)_\infty}{(c'e^{\mathrm{i}\theta}y;q)_\infty (-c'e^{-\mathrm{i}\theta}y;q)_\infty},$$

where $c = q^{(2l+1)n/4}$, $c' = q^{(1-2l)n/4}$, and $x = b\sin\theta$ with $b = (q^{-1/2} - q^{1/2})^{-1}$.

Eigenfunctions of Q are determined up to constant factors. To normalize the eigenfunctions $\phi_x(y)$, we employ the orthogonality relation (19) for q-Meixner–Pollaczek polynomials. The set $P_n(x/b)$, $n = 0,1,2,\ldots$, is complete in the Hilbert space $L^2([-b,b],\tilde{w}(x))$, $b = (q^{-1/2} - q^{1/2})^{-1}$, with the scalar product

$$\langle f_1, f_2\rangle = \int_{-b}^{b} f_1(x)\overline{f_2(x)}\tilde{w}(x)\mathrm{d}x,$$

where $\tilde{w}$ is the same as in (19). Consequently, the normalized functions are

$$\tilde{\phi}_x(y) = \tilde{w}(x)^{1/2}\phi_x(y), \quad x \in [-b,b],$$

that is, $\langle \tilde{\phi}_x(y), \tilde{\phi}_{x'}(y)\rangle = \delta(x-x')$.

VI. MOMENTUM REALIZATION OF THE OSCILLATOR

We have constructed in Sec. III a realization of the oscillator (depending on a value of l) on the space of functions in the supplementary variable y. It is natural to look for its realization on the space of functions in the coordinate x and on the space of functions in the momentum p.

Let $L^2([-b,b],\tilde{w})$, $b=(q^{-1/2}-q^{1/2})^{-1}$, be the space of square-integrable functions $f(p)$ (where p is the momentum of the oscillator) with respect to the scalar product (20). From (19) it is clear that the polynomials (16) constitute an orthonormal basis in $L^2([-b,b],\tilde{w})$.

We construct first a one-to-one linear isometry Ω from the Hilbert space $\mathcal{H}_l$, considered in Sec. II, onto the Hilbert space $L^2([-b,b],\tilde{w})$, given by the formula

$$\Omega\colon \mathcal{H}_l \ni e(y) \to f(p) := \langle e(y), \psi_p(y)\rangle_{\mathcal{H}_l} \in L^2([-b,b],\tilde{w}), \tag{24}$$

where $\psi_p(y)$ are the eigenfunctions (18) of P. It follows from (17) that

$$\mathcal{H}_l \ni e_n^l(y) \to \langle e_n^l(y), \psi_p(y)\rangle_{\mathcal{H}_l} = h_n(p), \tag{25}$$

that is, Ω maps the orthonormal basis $\{e_n^l(y)\}$ of $\mathcal{H}_l$ onto the orthonormal basis $\{h_n(p)\}$ in $L^2([-b,b],\tilde{w})$. This means that Ω indeed is a one-to-one isometry.

The operator P acts on $L^2([-b,b],\tilde{w})$ as the multiplication operator,

$$Pf(p) = pf(p).$$

Indeed, according to (25) if $\Omega e(y)=f(p)=\langle e(y), \psi_p(y)\rangle_{\mathcal{H}_l}$, then

$$Pe(y) \to Pf(p) = \langle Pe(y), \psi_p(y)\rangle_{\mathcal{H}_l} = \langle e(y), P\psi_p(y)\rangle_{\mathcal{H}_l} = \langle e(y), p\psi_p(y)\rangle_{\mathcal{H}_l} = pf(p).$$

We can find how P acts upon the basis elements $h_n(p)$, $n=0,1,2,\ldots$, of the Hilbert space $L^2([-b,b],\tilde{w})$. According to the recurrence relation for the polynomials (16) (which follows from the recurrence relation for the polynomials $P_n(z;q^l|q)$), we have

$$Ph_n(p) = ph_n(p) = \frac{1}{2(q^{-1/2}-q^{1/2})}\left(\sqrt{(1-q^{n+1})(1-q^{2l+n})}h_{n+1}(p) + \sqrt{(1-q^n)(1-q^{2l+n-1})}h_{n-1}(p)\right).$$

The Hamiltonian H acts upon the polynomials $h_n(p)$ in the Hilbert space $L^2([-b,b],\tilde{w})$ as

$$Hh_n(p) = (n+1/2)h_n(p).$$

Indeed, since $He_n^l(y)=(n+1/2)e_n^l(y)$, then according to (25) one has

$$Hh_n(p) = \langle He_n^l(y), \psi_p(y)\rangle_{\mathcal{H}_l} = (n+1/2)\langle e_n^l(y), \psi_p(y)\rangle_{\mathcal{H}_l} = (n+1/2)h_n(p).$$

Let us find how the operator Q acts on the Hilbert space $L^2([-b,b],\tilde{w})$. To achieve this we use the results of Ref. 16.

The polynomials $h_n(p)$ from (16) can be expressed in terms of the Askey–Wilson polynomials, defined as

$$p_n\left(\frac{1}{2}(z+z^{-1});a,b,c,d|q\right) \equiv p_n[z] = \frac{(ab,ac,ad;q)_n}{a^n}\,{}_4\phi_3\left(\begin{matrix}q^{-n},q^{n-1}abcd,az,az^{-1}\\ ab,ac,ad\end{matrix}\Big|q,q\right),$$

where $(\alpha,\beta,\gamma;q)_n := (\alpha;q)_n(\beta;q)_n(\gamma;q)_n$. We have

$$h_n(p) = [(q^{2l};q)_n(q;q)_n]^{-1/2}p_n\left(\frac{1}{2}(z+z^{-1});iq^l,-iq^l,0,0|q\right), \tag{26}$$

where $z=e^{i(\theta+\pi/2)}$. For convenience we denote the polynomials $h_n(p)$ by $h_n[z]$, where z is the same as in (26). It follows from (26) and from formula (4.5) in Ref. 16 that the polynomials $h_n[z]$ satisfy the difference equation

$$Dh_n[z] = \frac{2(q^{-n}-1)}{1-q^{-1}} h_n[z],$$

where the difference operator D acts as

$$Df(z) = \frac{1-q^{2l}z}{(1-z^2)(1-qz^2)} f(qz) - \left(\frac{1-q^{2l}z}{(1-z^2)(1-qz^2)} + \frac{1-q^{2l}z^{-1}}{(1-z^{-2})(1-qz^{-2})} \right) f(z) + \frac{1-q^{2l}z^{-1}}{(1-z^{-2})(1-qz^{-2})} f(q^{-1}z).$$

We shall also need an operator of the form

$$D' := \tfrac{1}{2}(1-q^{-1})D + 1,$$

whose action on the polynomials $h_n[z]$ is

$$D'h_n[z] = q^{-n}h_n[z].$$

This means that the operator D' acts on the polynomials $h_n[z]$ as q^{-N}, where N is the number operator,

$$Nh_n[z] = nh_n[z].$$

In order to find a difference form for the momentum operator, we need the operator L, which is defined as

$$Lf(z) = (z-z^{-1})^{-1}[(1-q^{2l}z^2)z^{-2}f(qz) - (1-q^{2l}z^{-2})z^2 f(q^{-1}z)].$$

This is the operator (4.7) in Ref. 16 for our case. Then from formulas (4.11) and (4.12) from Ref. 16 one derives that

$$(L - q^{1-n}(z+z^{-1}))h_n[z] = -\frac{1+q}{q^n}\sqrt{(1-q^{n+1})(1-q^{2l+n})}h_{n+1}[z] = -(1+q)q^{(n+l+1/2)/2}\sqrt{[2l+n]_q[n+1]_q}h_{n+1}[z],$$

and

$$(L + q^{-n}(z+z^{-1}))h_n[z] = \frac{1+q}{q^n}\sqrt{(1-q^n)(1-q^{2l+n-1})}h_{n-1}[z] = (1+q)q^{(n+l-1/2)/2}\sqrt{[2l+n-1]_q[n]_q}h_{n-1}[z].$$

Note that the operators

$$J_+ := -\frac{q^{-(l+1/2)/2}}{(1+q)}(L - q(z+z^{-1})q^{-N})q^{-N/2}, \tag{27}$$

$$J_- := \frac{q^{-(l-1/2)/2}}{(1+q)}(L + (z+z^{-1})q^{-N})q^{-N/2}, \tag{28}$$

act upon the polynomials $h_n[z]$ as

$$J_+h_n[z] = \sqrt{[2l+n]_q[n+1]_q}h_{n+1}[z], \quad J_-h_n[z] = \sqrt{[2l+n-1]_q[n]_q}h_{n-1}[z].$$

One may express the position operator $Q = q^{J_3/4}J_2q^{J_3/4}$ in terms of the difference operators (27) and (28) as

$$Q = \mathrm{i}\frac{q^{1/2}}{2(1-q^2)}[L - q(z+z^{-1})q^{-N} + L + (z+z^{-1})q^{-N}]q^N = \mathrm{i}\frac{q^{1/2}}{2(1-q^2)}[2L + (1-q)(z+z^{-1})q^{-N}]q^N,$$

which can be represented in the form

$$Q = \mathrm{i}\frac{q^{1/2}}{2(1-q^2)}[2Lq^N + (1-q)(z+z^{-1})]. \tag{29}$$

It is easy to find that Q acts upon the polynomials $h_n[z]$ as

$$Qh_n(p) = \frac{1}{2\mathrm{i}(q^{-1/2}-q^{1/2})}[\sqrt{(1-q^{n+1})(1-q^{2l+n})}h_{n+1}(p) - \sqrt{(1-q^n)(1-q^{2l+n-1})}h_{n-1}(p)],$$

that is, this is the position operator. Thus, formula (29) gives us the difference form of the position operator.

VII. COORDINATE REALIZATION OF THE OSCILLATOR

Let $\widetilde{L}^2([-b,b],\widetilde{w})$, $b=(q^{-1/2}-q^{1/2})^{-1}$, be the space of square-integrable functions $f(x)$ (where x is the coordinate of the oscillator) with respect to the same scalar product as in (20). It follows from (19) that the polynomials $\widetilde{h}_n(x)$ from (22) constitute an orthonormal basis in $\widetilde{L}^2([-b,b],\widetilde{w})$.

We construct a one-to-one linear isometry $\widetilde{\Omega}$ from the Hilbert space $\mathcal{H}_l$, considered in Sec. II, onto the Hilbert space $\widetilde{L}^2([-b,b],\widetilde{w})$ given by the formula

$$\widetilde{\Omega}\colon \mathcal{H}_l \ni e(y) \to f(x) := \langle e(y), \phi_x(y)\rangle_{\mathcal{H}_l} \in \widetilde{L}^2([-b,b],\widetilde{w}), \tag{30}$$

where $\phi_x(y)$ are the eigenfunctions (23) of Q. From (23) it is then evident that

$$\mathcal{H}_l \ni e_n^l(y) \to \langle e_n^l(y), \phi_x(y)\rangle_{\mathcal{H}_l} = \widetilde{h}_n(x),$$

that is, $\widetilde{\Omega}$ maps the orthonormal basis $\{e_n^l(y)\}$ from $\mathcal{H}_l$ onto the orthonormal basis $\{\widetilde{h}_n(x)\}$ in $\widetilde{L}^2([-b,b],\widetilde{w})$. This means that $\widetilde{\Omega}$ indeed is a one-to-one isometry.

The operator Q acts on $\widetilde{L}^2([-b,b],\widetilde{w})$ as the multiplication operator,

$$Qf(x) = xf(x).$$

We can find how Q acts upon the basis elements $\widetilde{h}_n(x)$, $n=0,1,2,\ldots$, in the Hilbert space $\widetilde{L}^2([-b,b],\widetilde{w})$. According to the recurrence relation for the polynomials (22), one has

$$Q\widetilde{h}_n(x) = x\widetilde{h}_n(x) = \frac{\mathrm{i}}{2(q^{-1/2}-q^{1/2})}[\sqrt{(1-q^{n+1})(1-q^{2l+n})}\widetilde{h}_{n+1}(x) - \sqrt{(1-q^n)(1-q^{2l+n-1})}\widetilde{h}_{n-1}(x)].$$

Clearly, $H\widetilde{h}_n(x) = (n+1/2)\widetilde{h}_n(x)$.

One can also find a difference form for the momentum operator P in the coordinate space. To this end, one has to repeat the reasoning of Sec. VI.

VIII. THE EVOLUTION OPERATOR IN THE COORDINATE SPACE

According to (12), the time evolution operator $\exp(\mathrm{i}\tau H)$ acts upon the basis elements e_n^l, $n=0,1,2,\cdots$, of the Hilbert space $\mathcal{H}_l$ as

$$\exp(\mathrm{i}\tau H)e_n^l = e^{-\mathrm{i}(l-1/2)\tau}e^{\mathrm{i}(l+n)\tau}e_n^l = e^{\mathrm{i}(n+1/2)\tau}e_n^l.$$

We wish to find how this operator acts in the coordinate space, that is, on the Hilbert space $\widetilde{L}^2([-b,b],\widetilde{w})$ from Sec. VII. If the isometry $\widetilde{\Omega}$ maps a function $e(y)\in\mathcal{H}_l$ to a function $f(x)$

$\in \widetilde{L}^2([-b,b],\tilde{w})$, then to $\exp(\mathrm{i}\tau H)e(y) \in \mathcal{H}_l$ there corresponds the function

$$\begin{aligned}
\exp(\mathrm{i}\tau H)f(x) &= \langle \exp(\mathrm{i}\tau H)e(y), \phi_x(y)\rangle_{\mathcal{H}_l} = \langle e(y), \exp(-\mathrm{i}\tau H)\phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \langle e(y), e_n^l\rangle_{\mathcal{H}_l}\langle e_n^l, \exp(-\mathrm{i}\tau H)\phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \langle e(y), e_n^l\rangle_{\mathcal{H}_l}\langle \exp(\mathrm{i}\tau H)e_n^l, \phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \int_{-b}^{b} \langle e(y), \widetilde{\phi}_{x'}(y)\rangle_{\mathcal{H}_l}\langle \widetilde{\phi}_{x'}(y), e_n^l\rangle_{\mathcal{H}_l} \mathrm{d}x' \cdot \exp(\mathrm{i}\tau(n+1/2))\langle e_n^l, \phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \int_{-b}^{b} f(x')K^{\tau}(x,x')\tilde{w}(x')\mathrm{d}x',
\end{aligned}$$

where the kernel $K^{\tau}(x,x')$ is given by

$$K^{\tau}(x,x') = \sum_{n=0}^{\infty} \langle \phi_{x'}(y), e_n^l\rangle_{\mathcal{H}_l}\langle e_n^l, \phi_x(y)\rangle_{\mathcal{H}_l} \exp(\mathrm{i}\tau(n+1/2)).$$

Taking into account the expression for $\widetilde{h}_n(x) = \langle e_n^l, \phi_x(y)\rangle_{\mathcal{H}_l}$ with $x = b\sin\theta$, one finds that

$$\begin{aligned}
K^{\tau}(x,x') &= \sum_{n=0}^{\infty} \exp(\mathrm{i}\tau(n+1/2))\widetilde{h}_n(x)\overline{\widetilde{h}_n(x')} \\
&= e^{\mathrm{i}\pi/2}\sum_{n=0}^{\infty} e^{\mathrm{i}n\tau}q^{-2ln}\frac{(q^{2l};q)_n}{(q;q)_n}\,{}_3\phi_2(q^{-n},-q^l e^{\mathrm{i}\theta},q^l e^{-\mathrm{i}\theta};q^{2l},0;q,q) \\
&\quad \times {}_3\phi_2(q^{-n},-q^l e^{\mathrm{i}\theta'},q^l e^{-\mathrm{i}\theta'};q^{2l},0;q,q),
\end{aligned}$$

upon employing the explicit expression for the q-Meixner-Pollaczek–polynomials from Sec. IV. Due to formula (8.15) in Ref. 17, one finally obtains that

$$\begin{aligned}
K^{\tau}(x,x') = e^{\mathrm{i}\pi/2}&\frac{(q^l e^{\mathrm{i}\theta'}e^{\mathrm{i}\tau},-q^l e^{-\mathrm{i}\theta'}e^{\mathrm{i}\tau},q^l e^{\mathrm{i}\theta}e^{\mathrm{i}\tau},-q^l e^{-\mathrm{i}\theta}e^{\mathrm{i}\tau},e^{\mathrm{i}\tau};q)_{\infty}}{(e^{\mathrm{i}(\theta+\theta')}e^{\mathrm{i}\tau},-e^{\mathrm{i}(\theta'-\theta)}e^{\mathrm{i}\tau},-e^{\mathrm{i}(\theta-\theta')}e^{\mathrm{i}\tau},e^{-\mathrm{i}(\theta+\theta')}e^{\mathrm{i}\tau},q^{2l}e^{\mathrm{i}\tau};q)_{\infty}} \\
&\times {}_8W_7(q^{2l-1}e^{\mathrm{i}\tau};-q^l e^{\mathrm{i}\theta},q^l e^{-\mathrm{i}\theta},-q^l e^{\mathrm{i}\theta'},q^l e^{-\mathrm{i}\theta'},e^{\mathrm{i}\tau};q,e^{\mathrm{i}\tau}),
\end{aligned} \tag{31}$$

where $(a_1,a_2,\ldots,a_r;q)_{\infty} \equiv (a_1;q)_{\infty}(a_2,q)_{\infty}\cdots(a_r;q)_{\infty}$ and ${}_8W_7$ is the basic hypergeometric function (2.1.11) from Ref. 10. Expressing the function ${}_8W_7$ in (31) in terms of the basic hypergeometric function ${}_8\phi_7$ (see Ref. 10, Sec. 2.1) and using relation (III.17) from Appendix III in Ref. 10, one can reduce the ${}_8W_7$ in (31) to the basic hypergeometric function ${}_4\phi_3$:

$$\begin{aligned}
&{}_8W_7(q^{2l-1}e^{\mathrm{i}\tau};-q^l e^{\mathrm{i}\theta},q^l e^{-\mathrm{i}\theta},-q^l e^{\mathrm{i}\theta'},q^l e^{\mathrm{i}\theta'},e^{\mathrm{i}\tau};q,e^{\mathrm{i}\tau}) \\
&\quad = \frac{(q^{2l}e^{\mathrm{i}\tau},-e^{\mathrm{i}\tau},-q^l e^{-\mathrm{i}\theta'},q^l e^{\mathrm{i}\theta'};q)_{\infty}}{(-q^l e^{-\mathrm{i}\theta'}e^{\mathrm{i}\tau},q^l e^{\mathrm{i}\theta'}e^{\mathrm{i}\tau},q^{2l},-1;q)_{\infty}}\,{}_4\phi_3\left(\begin{matrix}-e^{\mathrm{i}\tau},e^{\mathrm{i}\tau},-q^l e^{\mathrm{i}\theta'},q^l e^{-\mathrm{i}\theta'} \\ -q^l e^{-\mathrm{i}\theta}e^{\mathrm{i}\tau},q^l e^{\mathrm{i}\theta}e^{\mathrm{i}\tau},-q\end{matrix}\,\middle|\,q,q\right).
\end{aligned}$$

As a result, one arrives at the following expression for the kernel $K^{\tau}(x,x')$:

$$K^{\tau}(x,x') = \frac{(q^l e^{i\theta} e^{i\tau}, -q^l e^{-i\theta} e^{i\tau}, e^{i\tau}, -e^{i\tau}, -q^l e^{-i\theta'}, q^l e^{i\theta'}; q)_\infty}{(e^{i(\theta+\theta')} e^{i\tau}, -e^{i(\theta'-\theta)} e^{i\tau}, -e^{i(\theta-\theta')} e^{i\tau}, e^{-i(\theta+\theta')} e^{i\tau}, q^{2l} e^{i\tau}, q^{2l}, -1; q)_\infty}$$
$$\times e^{i\pi/2} {}_4\phi_3\left(\begin{matrix} -e^{i\tau}, e^{i\tau}, -q^l e^{i\theta'}, q^l e^{-i\theta'} \\ -q^l e^{-i\theta} e^{i\tau}, q^l e^{i\theta} e^{i\tau}, -q \end{matrix} \middle| q, q \right). \tag{32}$$

Thus, *the evolution operator* $\exp(i\tau H)$ *is given by the formula*

$$\exp(i\tau H) f(x) = \int_{-b}^{b} K^{\tau}(x,x') f(x') \tilde{w}(x') dx',$$

where the kernel $K^{\tau}(x,x')$ *is given by* (32). Since $e^{i\tau H} e^{i\tau' H} = e^{i(\tau+\tau')H}$, this kernel satisfies the relation

$$\int_{-b}^{b} K^{\tau}(x,x') \overline{K^{\tau}(x',x'')} \tilde{w}(x') dx' = K^{\tau+\tau'}(x,x'').$$

Observe that the above-presented relation leads to the corresponding integral relation for the basic hypergeometric function ${}_4\phi_3$ in (32).

IX. AN ANALOGUE OF THE FOURIER TRANSFORM

Let us first recall the case of the standard linear harmonic oscillator in quantum mechanics, determined by the commutator

$$aa^+ - a^+ a = 1.$$

For the position and momentum operators $\mathcal{Q}$ and $\mathcal{P}$ we have

$$\mathcal{Q} = \frac{1}{\sqrt{2}}(a^+ + a), \quad \mathcal{P} = \frac{i}{\sqrt{2}}(a^+ - a).$$

The Hilbert space of states $\mathcal{H}$ is spanned by the orthonormal vectors $|n\rangle$, $n=0,1,2,\ldots$. For eigenvectors of $\mathcal{Q}$ and $\mathcal{P}$, we have

$$\mathcal{Q}|x\rangle = x|x\rangle, \quad \mathcal{P}|p\rangle = p|p\rangle,$$

and Spec $\mathcal{Q}$=Spec $\mathcal{P}$=$\mathbb{R}$.

For $h \in \mathcal{H}$, one gets

$$\langle h,x\rangle_{\mathcal{H}} = h(x), \quad \langle h,p\rangle_{\mathcal{H}} = \tilde{h}(p). \tag{33}$$

In this way one obtains a realization of $\mathcal{H}$ as a space of functions either in the coordinate or in the momentum. Then the functions $h(x)$ and $\tilde{h}(p)$ from (33) are related with each other by the well-known integral Fourier transform:

$$h(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{h}(p) e^{ipx} dp.$$

Our aim in this section is to find an analogue of the Fourier transform for the model of the oscillator under discussion. Let $e(y)$ be a function on the Hilbert space $\mathcal{H}_l$. Then

$$\Omega: e(y) \to f(p) \in L^2([-b,b],\tilde{w}), \quad \tilde{\Omega}: e(y) \to \tilde{f}(x) \in \tilde{L}^2([-b,b],\tilde{w}).$$

We need to find out how the functions $f(p)$ and $\tilde{f}(x)$ are connected with each other. One has

$$\widetilde{f}(x)=\langle e(y),\phi_x(y)\rangle_{\mathcal{H}_l}=\int_{-b}^{b}\langle e(y),\widetilde{\psi}_p(y)\rangle_{\mathcal{H}_l}\langle\widetilde{\psi}_p(y),\phi_x(y)\rangle_{\mathcal{H}_l}\mathrm{d}p=\int_{-b}^{b}f(p)\langle\psi_p(y),\phi_x(y)\rangle_{\mathcal{H}_l}\widetilde{w}(p)\mathrm{d}p$$

$$=\int_{-b}^{b}f(p)F(x,p)\widetilde{w}(p)\mathrm{d}p,$$

where the kernel $F(x,p)$ is given as

$$F(x,p)=\langle\psi_p(y),\phi_x(y)\rangle_{\mathcal{H}_l}=\sum_{n=0}^{\infty}\langle\psi_p(y),e_n^l\rangle_{\mathcal{H}_l}\langle e_n^l,\phi_x(y)\rangle_{\mathcal{H}_l}=\sum_{n=0}^{\infty}\mathrm{i}^{-n}h_n(x)\overline{h_n(p)}$$

$$=\sum_{n=0}^{\infty}\mathrm{i}^{-n}q^{-2ln}\frac{(q^{2l};q)_n}{(q;q)_n}{}_3\phi_2(q^{-n},-q^le^{\mathrm{i}\theta},q^le^{-\mathrm{i}\theta};q^{2l},0;q,q){}_3\phi_2(q^{-n},-q^le^{\mathrm{i}\theta'},q^le^{-\mathrm{i}\theta'};q^{2l},0;q,q),$$

with $x=b\sin\theta$ and $p=b\sin\theta'$. Taking into account formula (8.15) in Ref. 17 and repeating the reasoning of Sec. VIII, one obtains that

$$F(x,p)=\frac{(\mathrm{i}q^le^{-\mathrm{i}\theta},-\mathrm{i}q^le^{\mathrm{i}\theta},\mathrm{i},-\mathrm{i},-q^le^{-\mathrm{i}\theta'},q^le^{\mathrm{i}\theta'};q)_\infty}{(\mathrm{i}e^{\mathrm{i}(\theta-\theta')},-\mathrm{i}e^{\mathrm{i}(\theta+\theta')},\mathrm{i}e^{\mathrm{i}(\theta'-\theta)},-\mathrm{i}e^{-\mathrm{i}(\theta+\theta')},-\mathrm{i}q^{2l},q^{2l},-1;q)_\infty}$$
$$\times{}_4\phi_3\left(\begin{matrix}\mathrm{i},-\mathrm{i},-q^le^{\mathrm{i}\theta'},q^le^{-\mathrm{i}\theta'}\\ \mathrm{i}q^le^{-\mathrm{i}\theta},-\mathrm{i}q^le^{\mathrm{i}\theta},-q\end{matrix}\middle|q,q\right).\tag{34}$$

Thus, *an analogue of the Fourier transform* $\mathcal{F}:f(p)\to\widetilde{f}(x)$ *for our oscillator is given by the formula*

$$\mathcal{F}f(p)=\widetilde{f}(x)=\int_{-b}^{b}f(p)F(x,p)\widetilde{w}(p)\mathrm{d}p,$$

where the kernel $F(x,p)$ *is defined by formula* (34). The integral transform $\mathcal{F}$ is linear and isometric, that is, it preserves the scalar product. Therefore, the inverse transform $\mathcal{F}^{-1}$ is given by

$$\mathcal{F}^{-1}\widetilde{f}(x)=f(p)=\int_{-b}^{b}\widetilde{f}(x)\overline{F(x,p)}\widetilde{w}(x)\mathrm{d}x,\tag{35}$$

where $\overline{F(x,p)}$ means the complex conjugate of $F(x,p)$. Obviously, the Plancherel formula

$$\int_{-b}^{b}|f(p)|^2|\widetilde{w}(p)\mathrm{d}p=\int_{-b}^{b}|\widetilde{f}(x)|^2\widetilde{w}(x)\mathrm{d}x$$

holds.

X. A LIMIT TO THE MACFARLANE–BIEDENHARN *q*-OSCILLATOR

We have constructed an infinite number of models of quantum oscillator, characterized by the number l. The corresponding models will be denoted by osc_l. We prove in the following that

$$\lim_{l\to\infty}\sqrt{2}(q^{-1/2}-q^{1/2})\mathrm{osc}_l=\mathrm{osc}_q,$$

where osc_q denotes the Macfarlane–Biedenharn q-oscillator. This formula means that

$$\lim_{l\to\infty}\sqrt{2}(q^{-1/2}-q^{1/2})Q_l=\mathcal{Q},\quad \lim_{l\to\infty}\sqrt{2}(q^{-1/2}-q^{1/2})P_l=\mathcal{P}, \tag{36}$$

where $Q\equiv Q_l$, $P\equiv P_l$ are the position and momentum operators for osc_l, and $\mathcal{Q}$, $\mathcal{P}$ are the position and momentum operators for osc_q. The validity of the relations (36) follows from the fact that in this limit the operators Q_l and P_l turn into

$$\mathcal{Q}\tilde{e}_n=\frac{1}{\sqrt{2}}\left[\left(\frac{1-q^{n+1}}{1-q}\right)^{1/2}e_{n+1}+\left(\frac{1-q^n}{1-q}\right)^{1/2}e_{n-1}\right],$$

$$\mathcal{P}\tilde{e}_n=\frac{\mathrm{i}}{\sqrt{2}}\left[\left(\frac{1-q^{n+1}}{1-q}\right)^{1/2}e_{n+1}-\left(\frac{1-q^n}{1-q}\right)^{1/2}e_{n-1}\right].$$

Considering that

$$\mathcal{Q}=\frac{1}{\sqrt{2}}(a^+ + a),\quad \mathcal{P}=\frac{\mathrm{i}}{\sqrt{2}}(a^+ - a),$$

one readily derives that

$$a^+e_n=\left(\frac{1-q^{n+1}}{1-q}\right)^{1/2}e_{n+1},\quad ae_n=\left(\frac{1-q^n}{1-q}\right)^{1/2}e_{n-1}.$$

These operators together with the operator q^N, given as $q^Ne_n=q^ne_n$, satisfy the relations

$$aa^+-qa^+a=1,\quad q^Na^+=qa^+q^N,\quad q^Na=q^{-1}aq^N,$$

that is, they generate the q-oscillator algebra of Macfarlane–Biedenharn.

XI. THE CASE $q=1$: DESCRIPTION OF THE MODELS

The models, which correspond to the case $q=1$, can be considered either by setting $q=1$ into the previous results or by repeating the foregoing reasoning, based now on the Lie algebra su(1,1) instead of the quantum algebra $su_q(1,1)$. The latter case is simpler and we prefer to adopt it.

The Lie algebra su(1,1) has the generators I_0,I_1,I_2, which satisfy the commutation relations

$$[I_0,I_1]=\mathrm{i}I_2,\quad [I_1,I_2]=-\mathrm{i}I_0,\quad [I_2,I_0]=\mathrm{i}I_1.$$

The generators $I_\pm$ and I_0 are also used, where $I_\pm=I_1\pm\mathrm{i}I_2$; they obey the commutation relations $[I_0,I_\pm]=\pm I_\pm$ and $[I_-,I_+]=2I_0$.

For constructing the su(1,1)-models of the quantum oscillator the positive discrete series of irreducible representations of su(1,1) are employed. They are given by a positive number l and are denoted by R_l. The representation R_l acts on the Hilbert space $\tilde{\mathcal{H}}_1$ of functions in the variable y, such that the monomials

$$\tilde{e}_n^l(y)=\tilde{a}_n^l y^n,\quad \tilde{a}_n^l=\left(\frac{\Gamma(2l+n)}{n!}\right)^{1/2},\quad n=0,1,2,3,\ldots, \tag{37}$$

are orthonormal, that is, $\langle\tilde{e}_m^l,\tilde{e}_n^l\rangle=\delta_{mn}$ (see Ref. 18, Chap. 7). An explicit realization of the generators I_i, $i=0,1,2$, in the representation R_l is given in terms of the first-order differential operators as

$$I_0=y\frac{\mathrm{d}}{\mathrm{d}y}+l,\quad I_1=\frac{1}{2}(1+y^2)\frac{\mathrm{d}}{\mathrm{d}y}+ly,\quad I_2=\frac{\mathrm{i}}{2}(1-y^2)\frac{\mathrm{d}}{\mathrm{d}y}-\mathrm{i}ly.$$

Acting by these operators upon the basis elements $\tilde{e}_n^l\equiv\tilde{e}_n^l(y)$, $n=0,1,2\ldots$, one readily verifies that

$$I_0\tilde{e}_n^l = (l+n)\tilde{e}_n^l, \quad I_+\tilde{e}_n^l = \sqrt{(2l+n)(n+1)}\tilde{e}_{n+1}^l, \quad I_-\tilde{e}_n^l = \sqrt{(2l+n-1)n}\tilde{e}_{n-1}^l.$$

If one defines the Hamiltonian H and position and momentum operators Q and P as

$$H = I_0 - l + 1/2, \quad Q = I_2, \quad P = I_1,$$

then Q, P, and H obey the commutation relations

$$[H,Q] = -\mathrm{i}P, \quad [H,P] = \mathrm{i}Q, \quad [Q,P] = \mathrm{i}(H + l - 1/2). \tag{38}$$

These operators satisfy the postulates 1–3 of Sec. I. The time evolution of this system is the harmonic motion with

$$e^{\mathrm{i}\tau H}\begin{pmatrix} Q \\ P \end{pmatrix} e^{-\mathrm{i}\tau H} = \begin{pmatrix} Q(\tau) \\ P(\tau) \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix}\begin{pmatrix} Q \\ P \end{pmatrix}.$$

This is a group U(1) of inner automorphisms of the Lie algebra su(1,1) and of rotations of the phase-space surface. Explicit form of the time evolution in the coordinate space will be given in the following.

The basis $\tilde{e}_n^l$, $n=0,1,2,\ldots$, in the Hilbert space $\tilde{\mathcal{H}}_l$ consists of eigenfunctions of the Hamiltonian H:

$$H\tilde{e}_n^l = (n + 1/2)\tilde{e}_n^l, \quad n = 0,1,2, \ldots,$$

that is, the spectrum of H coincides with the spectrum of the Hamiltonian for the standard harmonic oscillator in quantum mechanics.

Let us show that in the limit as $l \to \infty$ the oscillators (38) reduce to the standard linear harmonic oscillator in quantum mechanics. We denote the model (38), which corresponds to l, by osc_l. Then we state that

$$\lim_{l\to\infty} (2l)^{-1/2}\mathrm{osc}_l = \mathrm{osc},$$

where osc denotes the standard quantum harmonic oscillator, that is,

$$\lim_{l\to\infty} (2l)^{-1/2}Q_l = \mathsf{Q}, \quad \lim_{l\to\infty} (2l)^{-1/2}P_l = \mathsf{P},$$

$Q \equiv Q_l$ and $P \equiv P_l$ are the position and momentum operators for osc_l, whereas Q, P are the position and momentum operators for osc. The validity of these limit relations follows from the fact that the relations (38) in this limit turn into

$$[H,\mathsf{Q}] = -\mathrm{i}\mathsf{P}, \quad [H,\mathsf{P}] = \mathrm{i}\mathsf{Q}, \quad [\mathsf{Q}, \quad \mathsf{P}] = \mathrm{i}.$$

These are the standard formulas for $\mathsf{Q} = (1/\sqrt{2})(a^+ + a)$ and $\mathsf{P} = (\mathrm{i}/\sqrt{2})(a^+ - a)$. Thus, *the oscillators* (38) *can be considered as deformations of the standard quantum harmonic oscillator*. Contrary to the q-oscillators of Macfarlane and Biedenharn, for these deformations the relations (1) remain valid.

XII. COORDINATE AND MOMENTUM SPACES FOR $q=1$

Using the explicit differential form of the operators $P=I_1$, one finds that *the eigenfunctions of the momentum operators P are of the form*

$$\psi_p(y) = (1 + \mathrm{i}y)^{-l-\mathrm{i}p}(1 - \mathrm{i}y)^{-l+\mathrm{i}p}. \tag{39}$$

Expanding the expressions $(1+\mathrm{i}y)^{-l-\mathrm{i}p}$ and $(1-\mathrm{i}y)^{-l+\mathrm{i}p}$ into power series in y and multiplying then these two series, one can obtain an expansion for the eigenfunctions $\psi_p(y)$ in terms of the basis functions $\tilde{e}_n^l(y)$ of the Hilbert space $\tilde{\mathcal{H}}_l$,

$$\psi_p(y)=\sum_{n=0}^{\infty}\left(\frac{n!}{\Gamma(2l+n)}\right)^{1/2}P_n^{(l)}(p;\pi/2)\tilde{e}_n^l(y)=\sum_{n=0}^{\infty}P_n^{(l)}(p;\pi/2)y^n \tag{40}$$

with the coefficients $P_n^{(l)}(p,\pi/2)$, which are the Meixner–Pollaczek polynomials

$$P_n^{(\lambda)}(z;\varphi)=\frac{(2\lambda)_n}{n!}e^{in\varphi}{}_2F_1(-n,\lambda+iz;2\lambda;1-e^{-2i\varphi})$$

(see Ref. 13, formula (1.7.3)) with $\varphi=\pi/2$ and $\lambda=l$.

To find the spectrum of the momentum operator P, we recall that the Meixner–Pollaczek polynomials $P_n^{(l)}(p;\pi/2)$ are orthogonal and this orthogonality relation is of the form

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}|\Gamma(l+ip)|^2P_m^{(l)}(p;\pi/2)P_n^{(l)}(p;\pi/2)dp=\frac{\Gamma(n+2l)}{2^{2l}n!}\delta_{mn}$$

(see formula (1.7.2) in Ref. 13). Repeating the same reasoning as in Sec. IV, one concludes that the spectrum of P coincides with the whole real line:

$$\text{Spec } P=\mathbb{R}.$$

The spectrum is continuous and simple. The continuity of the spectrum means that the eigenfunctions $\psi_p(y)$ are not elements of the Hilbert space $\mathcal{H}_l$. They form a continuous basis in $\mathcal{H}_l$ (similar to the basis $\{e^{ipx}\}$ in the Hilbert space $L^2(\mathbb{R})$).

Eigenfunctions of P are determined up to constants. One may normalize the eigenfunctions $\psi_p(y)$ with the aid of the orthogonality relation for Meixner–Pollaczek polynomials. Since these polynomials correspond to determinate moment problem, the set $P_n^{(l)}(p,\pi/2)$, $n=0,1,2,\ldots$, is complete in the Hilbert space $L^2(\mathbb{R},\mu(p))$ with respect to the orthogonality measure $\mu(p):=|\Gamma(l+ip)|^2$ for these polynomials. This means that

$$\sum_{n=0}^{\infty}\frac{2^{2l}n!}{2\pi\Gamma(n+2l)}|\Gamma(l+ip)|^2P_n^{(l)}(p,\pi/2)P_n^{(l)}(p',\pi/2)=\delta(p-p').$$

Then, by (40),

$$\langle\psi_p(y),\psi_{p'}(y)\rangle=\sum_{n=0}^{\infty}\frac{n!}{\Gamma(2l+n)}P_n^{(l)}(p,\pi/2)P_n^{(l)}(p',\pi/2)=\frac{2\pi\delta(p-p')}{2^{2l}|\Gamma(l+ip)|^2}.$$

Therefore, the normalized functions are

$$\tilde{\psi}_p(y)=(2\pi)^{-1/2}2^l|\Gamma(l+ip)|\psi_p(y),\quad p\in\mathbb{R},$$

that is, $\langle\tilde{\psi}_p(y),\tilde{\psi}_{p'}(y)\rangle=\delta(p-p')$.

Similarly, *the eigenfunctions of the position operator Q are of the form*

$$\phi_x(y)=(1+y)^{-l-ix}(1-y)^{-l+ix}. \tag{41}$$

We have

$$\phi_x(y)=\sum_{n=0}^{\infty}i^{-n}\left(\frac{n!}{\Gamma(2l+n)}\right)^{1/2}P_n^{(l)}(x;\pi/2)\tilde{e}_n^l(y)=\sum_{n=0}^{\infty}i^{-n}P_n^{(l)}(x;\pi/2)y^n. \tag{42}$$

Consequently, the normalized functions are

$$\tilde{\phi}_x(y) = \frac{2^l|\Gamma(l+\mathrm{i}x)|}{\sqrt{2\pi}}\phi_x(y),$$

that is, they satisfy the normalization condition $\langle\tilde{\phi}_x(y), \tilde{\phi}_{x'}(y)\rangle_{\mathcal{H}_l} = \delta(x-x')$.

The spectrum of the position operator coincides with the whole real line:

$$\mathrm{Spec}\ Q = \mathbf{R}.$$

This spectrum is simple.

Let us consider now the coordinate realization of the oscillator. Let $L^2(\mathbb{R};\mu(x))$ be the space of square-integrable functions $f(x)$ (where x is the coordinate of the oscillator and $\mu(x) := |\Gamma(l+\mathrm{i}x)|^2$) with the scalar product

$$\langle f(x), g(x)\rangle = \frac{2^{2l}}{2\pi}\int_{-\infty}^{\infty} f(x)\overline{g(x)}|\Gamma(l+\mathrm{i}x)|^2\mathrm{d}x.$$

From the orthogonality relation for the Meixner–Pollaczek polynomials it follows that the polynomials

$$\tilde{h}_n(x) = \mathrm{i}^{-n}\left(\frac{n!}{\Gamma(2l+n)}\right)^{1/2} P_n^{(l)}(x;\pi/2),$$

which are coefficients in the expansion (42) with respect to $\tilde{e}_n^l$, constitute an orthonormal basis in $L^2(\mathbb{R};\mu(x))$.

The next step is to construct a one-to-one linear isometry Ω from the Hilbert space $\mathcal{H}_l$ onto the Hilbert space $L^2(\mathbb{R};\mu(x))$ given by the formula

$$\Omega{:}\mathcal{H}_l \ni g(y) \to f(x) = \langle g(y), \phi_x(y)\rangle_{\mathcal{H}_l} \in L^2(\mathbb{R};\mu(x)),$$

where $\phi_x(y)$ are the eigenfunctions (42) of Q. Then

$$\mathcal{H}_l \ni \tilde{e}_n^l(y) \to \langle\tilde{e}_n^l(y), \phi_x(y)\rangle_{\mathcal{H}_l} = \tilde{h}_n(x),$$

that is, Ω maps the orthonormal basis $\{\tilde{e}_n^l(y)\}$ in $\mathcal{H}_l$ onto the orthonormal basis $\{\tilde{h}_n(x)\}$ in $L^2(\mathbb{R};\mu(x))$.

The operator Q acts on $L^2(\mathbb{R};\mu(x))$ as the multiplication operator,

$$Qf(x) = xf(x).$$

Indeed, if $\Omega g(y) = f(x) = \langle g(y), \phi_x(y)\rangle_{\mathcal{H}_l}$, then one has

$$Qg(y) \to Qf(x) = \langle Qg(y), \phi_x(y)\rangle_{\mathcal{H}_l} = \langle g(y), Q\phi_x(y)\rangle_{\mathcal{H}_l} = \langle g(y), x\phi_x(y)\rangle_{\mathcal{H}_l} = xf(x).$$

Clearly, $H\tilde{h}_n(x) = (n+1/2)\tilde{h}_n(x)$.

We note that in Ref. 19 it was shown that one can construct a relativistic model of the linear harmonic oscillator in the configuration x-representation, which is governed by a difference Hamiltonian with the square-integrable eigenfunctions of the form

$$\psi_n(x) := \frac{\mathrm{i}^n 2^l}{\sqrt{2\pi}}[l(l-1)]^{-\mathrm{i}x/2}\tilde{h}_n(x)\Gamma(l+\mathrm{i}x).$$

Let $\tilde{L}^2(\mathbb{R};\mu(p))$ be the Hilbert space of square-integrable functions $f(p)$ (where p is the momentum of the oscillator) with respect to the scalar product

$$\langle f(p), g(p)\rangle = \frac{2^{2l}}{2\pi}\int_{-\infty}^{\infty} f(p)\overline{g(p)}|\Gamma(l+\mathrm{i}p)|^2\mathrm{d}p.$$

The polynomials

$$h_n(x) = \left(\frac{n!}{\Gamma(2l+n)}\right)^{1/2} P_n^{(l)}(x;\pi/2),$$

which are coefficients of $\tilde{e}_n^l$ in expansion (40), constitute an orthonormal basis in $\tilde{L}^2(\mathbb{R};\mu(x))$.

One can construct a one-to-one isometry $\tilde{\Omega}$ from the Hilbert space $\mathcal{H}_l$ onto the Hilbert space $\tilde{L}^2(\mathbb{R};\mu(p))$, given by the formula

$$\tilde{\Omega}\colon \mathcal{H}_l \ni g(y) \to \tilde{f}(p) := \langle g(y), \psi_p(y)\rangle_{\mathcal{H}_l} \in \tilde{L}^2(\mathbb{R};\mu(p)),$$

where $\psi_p(y)$ are the eigenfunctions of the momentum operator P. Then

$$\mathcal{H}_l \ni \tilde{e}_n^l(y) \to \langle \tilde{e}_n^l(y), \psi_p(y)\rangle_{\mathcal{H}_l} = h_n(p),$$

that is, $\tilde{\Omega}$ maps the orthonormal basis $\{\tilde{e}_n^l(y)\}$ in $\mathcal{H}_l$ onto the orthonormal basis $\{h_n(p)\}$ in $\tilde{L}^2(\mathbb{R};\mu(p))$.

The operator P acts on $\tilde{L}^2(\mathbb{R};\mu(p))$ as the multiplication operator, $Pf(p)=pf(p)$.

It is noteworthy that in the limit as the representation label l tends to infinity, one returns to the standard linear harmonic oscillator wave functions on account of the limit relation

$$\lim_{l\to\infty} l^{-n/2} P_n^{(l)}(\sqrt{l}x;\pi/2) = \frac{H_n(x)}{n!}$$

between the Meixner–Pollaczek and Hermite polynomials (see Ref. 13, formula (2.7.2)).

XIII. THE EVOLUTION OPERATOR FOR THE CASE $q=1$

We wish to find how the evolution operator $\exp(\mathrm{i}\tau H)$ acts on the coordinate space, that is, on the Hilbert space $L^2(\mathbb{R};\mu(x))$. If the isometry Ω maps a function $g(y)\in\mathcal{H}_l$ to a function $f(x)\in L^2(\mathbb{R};\mu(x))$, then to the function $\exp(\mathrm{i}\tau H)g(y)\in\mathcal{H}_l$ there corresponds the function

$$\begin{aligned}
\exp(\mathrm{i}\tau H)f(x) &= \langle \exp(\mathrm{i}\tau H)g(y), \phi_x(y)\rangle_{\mathcal{H}_l} = \langle g(y), \exp(-\mathrm{i}\tau H)\phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \langle g(y), \tilde{e}_n^l\rangle_{\mathcal{H}_l}\langle \tilde{e}_n^l, \exp(-\mathrm{i}\tau H)\phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \langle g(y), \tilde{e}_n^l\rangle_{\mathcal{H}_l}\langle \exp(\mathrm{i}\tau H)\tilde{e}_n^l, \phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \langle g(y), \tilde{\phi}_{x'}(y)\rangle_{\mathcal{H}_l}\langle \tilde{\phi}_{x'}(y), \tilde{e}_n^l\rangle_{\mathcal{H}_l}\mathrm{d}x' \exp(\mathrm{i}\tau(n+1/2))\langle \tilde{e}_n^l, \phi_x(y)\rangle_{\mathcal{H}_l} \\
&= \frac{2^{2l}}{2\pi}\int_{-\infty}^{\infty} f(x')K^{\tau}(x,x')|\Gamma(l+ix')|^2\mathrm{d}x',
\end{aligned}$$

where the kernel $K^{\tau}(x,x')$ is defined as

$$K^{\tau}(x,x') = \sum_{n=0}^{\infty} \langle \phi_{x'}(y), \tilde{e}_n^l \rangle_{\mathcal{H}_l} \langle \tilde{e}_n^l, \phi_x(y) \rangle_{\mathcal{H}_l} \exp(\mathrm{i}\tau(n+1/2)).$$

Taking into account the explicit expression for $\langle \tilde{e}_n^l, \phi_x(y) \rangle_{\mathcal{H}_l}$, one finds that

$$K^{\tau}(x,x') = \sum_{n=0}^{\infty} \exp(\mathrm{i}\tau(n+1/2)) \tilde{h}_n(x) \overline{\tilde{h}_n(x')}$$

$$= \frac{e^{\mathrm{i}\pi/2}}{\Gamma(2l)} \sum_{n=0}^{\infty} e^{\mathrm{i}n\tau} \frac{(2l)_n}{n!} {}_2F_1(-n, l+\mathrm{i}x; 2l; 2)\, {}_2F_1(-n, l-\mathrm{i}x'; 2l; 2),$$

upon taking into account the fact that $\tilde{h}_n(x) = (1/\Gamma(2l))\sqrt{\Gamma(2l+n)/n!}\, {}_2F_1(-n, l+\mathrm{i}x; 2l; 2)$. Due to formula (12) from Sec. 2.5.2 in Ref. 20, one finally concludes that

$$K^{\tau}(x,x') = \frac{e^{\mathrm{i}\pi/2}}{\Gamma(2l)} (1+e^{\mathrm{i}\tau})^{-2l} \left[\frac{1-e^{\mathrm{i}\tau}}{1+e^{\mathrm{i}\tau}} \right]^{\mathrm{i}(x+x')} {}_2F_1\left(l+\mathrm{i}x, l-\mathrm{i}x'; 2l; \frac{1}{\cos^2 \pi/2} \right). \tag{43}$$

Thus, *the evolution operator* $\exp(\mathrm{i}\tau H)$ *acts by the formula*

$$\exp(\mathrm{i}\tau H) f(x) = \frac{2^{2l}}{2\pi} \int_{-\infty}^{\infty} K^{\tau}(x,x') f(x') |\Gamma(l+ix')|^2 \mathrm{d}x',$$

where the kernel $K^{\tau}(x,x')$ *is given by* (43).

XIV. AN ANALOGUE OF THE FOURIER TRANSFORM AT $q=1$

Let us briefly discuss here an analogue of the Fourier integral transform for our oscillators. If $g(y)$ is a function on the Hilbert space $\mathcal{H}_l$ from Sec. XI, then

$$\Omega: g(y) \to f(x) \in L^2(\mathbb{R}, \mu(x)), \quad \tilde{\Omega}: g(y) \to \tilde{f}(p) \in \tilde{L}^2(\mathbb{R}, \mu(p)).$$

We have to find how the functions $f(x)$ and $\tilde{f}(p)$ are connected with each other. One has

$$\tilde{f}(p) = \langle g(y), \psi_p(y) \rangle_{\mathcal{H}_l} = \int_{-\infty}^{\infty} \langle g(y), \tilde{\phi}_x(y) \rangle_{\mathcal{H}_l} \langle \tilde{\phi}_x(y), \psi_p(y) \rangle_{\mathcal{H}_l} \mathrm{d}x$$

$$= \frac{2^{2l}}{2\pi} \int_{-\infty}^{\infty} |\Gamma(l+\mathrm{i}x)|^2 f(x) \langle \phi_x(y), \psi_p(y) \rangle_{\mathcal{H}_l} \mathrm{d}x$$

$$= \frac{2^{2l}}{2\pi} \int_{-\infty}^{\infty} f(x) K(x,p) |\Gamma(l+\mathrm{i}x)|^2 \mathrm{d}x,$$

where the kernel $K(x,p)$ is given by

$$K(x,p) = \langle \phi_x(y), \psi_p(y) \rangle_{\mathcal{H}_l} = \sum_{n=0}^{\infty} \frac{\mathrm{i}^{-n} n!}{\Gamma(2l+n)} P_n^{(l)}(x, \pi/2) \overline{P_n^{(l)}(p, \pi/2)}$$

$$= \frac{1}{\Gamma(2l)} \sum_{n=0}^{\infty} i^{-n} \frac{(2l)_n}{n!} {}_2F_1(-n, l+\mathrm{i}x; 2l; 2)\, {}_2F_1(-n, l-\mathrm{i}p; 2l; 2).$$

Taking into account formula (12) of Sec. 2.5.2 in Ref. 20, one finally obtains that

$$K(x,p) = \frac{1}{\Gamma(2l)(1-\mathrm{i})^{2l}} \left[\frac{1+\mathrm{i}}{1-\mathrm{i}} \right]^{\mathrm{i}(x+p)} {}_2F_1(l+\mathrm{i}x, l-\mathrm{i}p; 2l; 2). \tag{44}$$

Thus, *an analogue* $\mathsf{F}: f(x) \to \tilde{f}(p)$ *of the Fourier transform for our oscillator is given by the formula*

$$\mathsf{F}f(x) = \tilde{f}(p) = \frac{2^{2l}}{2\pi} \int_{-\infty}^{\infty} f(x) K(x,p) |\Gamma(l + \mathrm{i}x)|^2 \mathrm{d}x,$$

where the kernel $K(x,p)$ *is defined by formula* (44). The integral transform F is linear and isometric, that is, it preserves the scalar product. Therefore, the inverse transform F^{-1} is given by

$$\mathsf{F}^{-1}\tilde{f}(p) = f(x) = \frac{2^{2l}}{2\pi} \int_{-\infty}^{\infty} \tilde{f}(p) \overline{K(x,p)} |\Gamma(l + \mathrm{i}p)|^2 \mathrm{d}p,$$

where $\overline{K(x,p)}$ means the complex conjugate of $K(x,p)$. The Plancherel formula

$$\int_{-\infty}^{\infty} |f(x)|^2 |\Gamma(l + \mathrm{i}x)|^2 \mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}(p)|^2 |\Gamma(l + \mathrm{i}p)|^2 \mathrm{d}p$$

holds.

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On Fay identity[a)]

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In the first part of this paper we consider the transformation of the cubic identities for general Korteweg–de Vries (KdV) tau functions from [Mishev, J. Math. Phys. **40**, 2419–2428 (1999)] to the specific identities for trigonometric KdV tau functions. Afterwards, we consider the Fay identity as a functional equation and provide a wide set of solutions of this equation. The main result of this paper is Theorem 3.4, where we generalize the identities from Mishev. An open problem is the transformation of the cubic identities from Mishev to the specific identities for elliptic KdV tau functions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We consider the relation (functional Fay identity)

$$f(z_0-z_1)f(z_2-z_3)g(t+[z_0]+[z_1])g(t+[z_2]+[z_3])+f(z_0-z_2)f(z_3-z_1)g(t+[z_0]+[z_2])g(t+[z_3]+[z_1])+f(z_0-z_3)f(z_1-z_2)g(t+[z_0]+[z_3])g(t+[z_1]+[z_2])=0$$

as an equation for the functions $f(z)$ and $g(t)$, $t\equiv(t_1,t_2,t_3,\ldots)\in\mathbb{C}^\infty$, $z\in\mathbb{C}$. We know that $f(z)=z$ and $g(t)=\tau(t)$ (KP tau function) are solutions of this equation (i.e., we have the Fay identity for Kadomtzev–Petviashvili (KP) tau functions.) Studying the relation as a functional equation will give us unification of the results from Ref. 3.

In our previous publication (Ref. 3) we have obtained some cubic (and more generally (2^n-1) – order, $n=2,3,\ldots$) identities, specific for Korteweg–de Vries (KdV) tau functions only. These tau functions are related to the KdV hierarchy of completely integrable equations; the first of them is the famous KdV equation $u_t=6uu_x-u_{xxx}$, $u=u(x,t)$. The KdV tau functions satisfy the conditions $\partial_{t_{2n}}\tau(t)=0$, $n=1,2,\ldots$, and these conditions are equivalent to $\tau(t-[z])=\tau(t+[-z])$ (for the notations see Sec. I).

It is well known that examples of KdV tau functions are some polynomials, and some modifications of trigonometric and hyperelliptic theta functions. In Ref. 3 it was pointed out that we cannot easily translate the Fay identity for KdV tau functions to the trigonometric and hyperelliptic cases. The problem in the hyperelliptic case is that in the original Fay identity for theta functions[2] the prime form is used (e.g., in the $g=1$ case $\theta_{11}(z_0-z_1)\theta_{11}'^{-1}(0)$) instead of the difference (z_0-z_1). Shiota showed that after suitable change of the variables it is possible to obtain the trigonometric form of the Fay identity starting from the Fay identity for KdV tau functions.[7]

In Sec. II we give some preliminary results and the transition from the cubic identity for KdV tau functions to its trigonometric form. In Sec. III we introduce the functional Fay identity and prove the main result in this article—Theorem 3.4. In Sec. IV we relate the functional Fay identity to the Fay identity for tau functions.

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II. PRELIMINARY RESULTS

Let $\tau(t)$, $t \equiv (t_1, t_2, t_3, \ldots) \in \mathbb{C}^\infty$, $t_1 \equiv x$ is an arbitrary tau function, related to the KP hierarchy.[1] Let us denote ($z \in \mathbb{C}$):

$$[z] := (z, z^2/2, z^3/3, \ldots) \in \mathbb{C}^\infty,$$

$$\tau(t + [z]) := \tau(t_1 + z, t_2 + z^2/2, t_3 + z^3/3, \ldots).$$

The following identity ($z_0, z_1, z_2, z_3 \in \mathbb{C}$):

$$\begin{aligned}(z_0 - z_1)(z_2 - z_3)\tau(t + [z_0] + [z_1])\tau(t + [z_2] + [z_3]) + (z_0 - z_2)(z_3 - z_1)\tau(t + [z_0] + [z_2]) \\ \times \tau(t + [z_3] + [z_1]) + (z_0 - z_3)(z_1 - z_2)\tau(t + [z_0] + [z_3])\tau(t + [z_1] + [z_2]) = 0\end{aligned} \tag{2.1}$$

is called Fay identity[6] for the KP tau function $\tau(t)$. It was first obtained[2] for theta functions related to Jacobians. In genus $g = 1$ case its form is

$$\begin{aligned}\theta_{11}(z_0 - z_1)\theta_{11}(z_2 - z_3)\theta_{11}(x + z_0 + z_1)\theta_{11}(x + z_2 + z_3) + \theta_{11}(z_0 - z_2)\theta_{11}(z_3 - z_1)\theta_{11}(x + z_0 + z_2) \\ \times \theta_{11}(x + z_3 + z_1) + \theta_{11}(z_0 - z_3)\theta_{11}(z_1 - z_2)\theta_{11}(x + z_0 + z_3)\theta_{11}(x + z_1 + z_2) = 0\end{aligned} \tag{2.2}$$

(we use the notations for thetas from Ref. 4). It was used[4] in geometric treatment of soliton equations. Later it was generalized for tau functions.[6]

Let $\tau(t)$ be a KdV tau function, i.e., $\tau(t - [z]) = \tau(t + [-z])$. In Ref. 3 the following cubic identity was obtained:

$$\begin{aligned}(z_2 - z_1)[\tau(t + [z_1] + [z_2])\tau(t - [z_1])\tau(t - [z_2]) - \tau(t - [z_1] - [z_2])\tau(t + [z_1])\tau(t + [z_2])] \\ = (z_2 + z_1)[\tau(t + [z_1] - [z_2])\tau(t - [z_1])\tau(t + [z_2]) - \tau(t - [z_1] + [z_2])\tau(t + [z_1])\tau(t - [z_2])]\end{aligned} \tag{2.3}$$

and its trigonometric and elliptic versions were considered:

$$\begin{aligned}\sin(z_2 - z_1)[\sin(x + z_1 + z_2)\sin(x - z_1)\sin(x - z_2) - \sin(x - z_1 - z_2)\sin(x + z_1)\sin(x + z_2)] \\ = \sin(z_1 + z_2)[\sin(x + z_1 - z_2)\sin(x - z_1)\sin(x + z_2) - \sin(x - z_1 + z_2)\sin(x + z_1)\sin(x - z_2)],\end{aligned} \tag{2.4}$$

$$\begin{aligned}\theta_{11}(z_2 - z_1)[\theta_{11}(x + z_1 + z_2)\theta_{11}(x - z_1)\theta_{11}(x - z_2) - \theta_{11}(x - z_1 - z_2)\theta_{11}(x + z_1)\theta_{11}(x + z_2)] \\ = \theta_{11}(z_1 + z_2)[\theta_{11}(x + z_1 - z_2)\theta_{11}(x - z_1)\theta_{11}(x + z_2) - \theta_{11}(x - z_1 + z_2)\theta_{11}(x + z_1)\theta_{11}(x - z_2)].\end{aligned} \tag{2.5}$$

In this section we will explain how starting from (2.3) we can obtain (2.4). The possibility for this is based on the correct choice of trigonometric KdV tau function.

Lemma 2.1: (T. Shiota) The function:

$$\tau(t) = \sin\left(\sum_{k=0}^{\infty} (-1)^k t_{2k+1}\right) \tag{2.6}$$

is a trigonometric KdV tau function. The Fay identity (2.1) *for it has the form:*

$$\begin{aligned}\sin(z_0 - z_1)\sin(z_2 - z_3)\sin(x + z_0 + z_1)\sin(x + z_2 + z_3) + \sin(z_0 - z_2)\sin(z_3 - z_1)\sin(x + z_0 + z_2) \\ \times \sin(x + z_3 + z_1) + \sin(z_0 - z_3)\sin(z_1 - z_2)\sin(x + z_0 + z_3)\sin(x + z_1 + z_2) = 0,\end{aligned} \tag{2.7}$$

where $x \equiv \Sigma_{k=0}^{\infty}(-1)^k t_{2k+1}$.

Proof: If we find a trigonometric Baker–Akhiezer function in the form: $w(t, z)$

$=\exp(\Sigma_{k=0}^{\infty} t_{2k+1} z^{2k+1})(z+c(t))$ with restriction $w(t,i)=w(t,-i)$, $i=\sqrt{-1}$, and compare the result with the well-known expression:

$$w(t,z)=\exp\left(\sum_{k=0}^{\infty} t_{2k+1} z^{2k+1}\right)\frac{\tau(t-[z^{-1}])}{\tau(t)}$$

we obtain (2.6).

For given shifts: $s_j, j=0,1,2,3$ let us introduce the new shifts: $z_j, j=0,1,2,3$ by the relations: $z_j=\tan(s_j)$. Then for the tau function (2.6) we have

$$\tau(t+[z_j])=\sin\left(\sum_{k=0}^{\infty}(-1)^k t_{2k+1}+\sum_{k=0}^{\infty}\frac{(-1)^k}{2k+1}z_j^{2k+1}\right)=\sin\left(\sum_{k=0}^{\infty}(-1)^k t_{2k+1}+s_j\right),$$

where we have used: $\Sigma_{k=0}^{\infty}[(-1)^k/2k+1]z_j^{2k+1}=\arctan(z_j)=s_j$. So, we have

$$\tau(t+[z_0]+[z_1])=\sin\left(\sum_{k=0}^{\infty}(-1)^k t_{2k+1}+s_0+s_1\right),\quad \text{etc.}$$

We have also

$$(z_0-z_1)=(\tan(s_0)-\tan(s_1))=\frac{\sin(s_0-s_1)}{\cos(s_0)\cos(s_1)},\quad \text{etc.}$$

So, from the Fay identity (2.1) we obtain the form (2.7) ($x\equiv\Sigma_{k=0}^{\infty}(-1)^k t_{2k+1}$) for the tau function given by (2.6). □

Theorem 2.2: *From the cubic identity for KdV tau functions* (2.3) *follows its trigonometric version* (2.4).

Proof: Let us substitute in the identity (2.1) the form (2.6) of trigonometric KdV tau function, with the new shifts: $z_j=\tan(s_j), j=0,1,2,3$. The same way as in the proof of Lemma 1.1 we obtain (2.4) (with $x\equiv\Sigma_{k=0}^{\infty}(-1)^k t_{2k+1}$). □

III. FUNCTIONAL FAY IDENTITY

Let us consider the Fay identity as our starting point. Let $f(z)$ and $g(t)$ be arbitrary functions (we use the notations from Sec. II: $t\equiv(t_1,t_2,t_3,\ldots)\in\mathbb{C}^{\infty}$, $z\in\mathbb{C}$).

Definition 3.1: The following relation we will call the *functional Fay identity*:

$$f(z_0-z_1)f(z_2-z_3)g(t+[z_0]+[z_1])g(t+[z_2]+[z_3])+f(z_0-z_2)f(z_3-z_1)g(t+[z_0]+[z_2])g(t+[z_3]+[z_1])+f(z_0-z_3)f(z_1-z_2)g(t+[z_0]+[z_3])g(t+[z_1]+[z_2])=0 \tag{3.1}$$

Lemma 3.2: Let functions $f(z)$ and $g(t)$ be once differentiable and $f(z)$ is odd. Let them satisfy the functional Fay identity. Then $f(z)$ and $g(t)$ satisfy the differential functional Fay identity:

$$W(g(t+[z_1]),g(t+[z_2]))=\left(\frac{f'(0)f(z_2-z_1)}{f(z_1)f(z_2)}\right)g(t)g(t+[z_1]+[z_2])+\left(\frac{f(z_1)f'(z_2)-f'(z_1)f(z_2)}{f(z_1)f(z_2)}\right)\times g(t+[z_1])g(t+[z_2]),$$

where the Wronskian is: $W(g_1(t),g_2(t)):=g_1(t)\partial_{t_1}g_2(t)-g_2(t)\partial_{t_1}g_1(t)$, and $'\equiv\partial_z$.

Proof: The proof is the same as for obtaining the differential Fay identity for KP taus, starting from the Fay identity for them:[1] differentiate (3.1) with respect to z_0, put $z_0=z_3=0$, and divide by $f(z_1)f(z_2)$. □

Shifting the argument t to $(t-[z_1]-[z_2])$ we could obtain an expression for the Wronskian: $W(g(t-[z_1]),g(t-[z_2]))$. But, shifting t we cannot obtain an expression, e.g., for the Wronskian: $W(g(t+[z_1]),g(t-[z_2]))$. This is possible only if we pose an additional condition on $g(t)$, namely

that $g(t)$ is of *KdV type*, i.e.,

$$\partial_{t_{2n}} g(t) = 0, n = 1,2,\ldots, \quad \text{or equivalently} \quad g(t-[z]) = g(t+[-z]).$$

As a corollary of Lemma 3.2 we obtain:

Lemma 3.3: Let functions $f(z)$ and $g(t)$ satisfy the functional Fay identity (3.2), *as well as the following conditions:*

(i) *$f(z)$ and $g(t)$ are once differentiable;*
(ii) *$f(-z)=-f(z)$;*
(iii) *$g(t)$ is of KdV type.*

Then we have the following forms of the differential functional Fay identity:

$$W(g(t\pm[z_1]),g(t\pm[z_2])) = \left(\frac{f'(0)f(z_2-z_1)}{f(z_1)f(z_2)}\right) g(t)g(t\pm[z_1]\pm[z_2]) \pm \left(\frac{f(z_1)f'(z_2)-f'(z_1)f(z_2)}{f(z_1)f(z_2)}\right) \times g(t\pm[z_1])g(t\pm[z_2]),$$

$$W(g(t\pm[z_1]),g(t\mp[z_2])) = \pm\left(\frac{f'(0)f(z_1+z_2)}{f(z_1)f(z_2)}\right) g(t)g(t\pm[z_1]\mp[z_2]) \mp \left(\frac{f(z_1)f'(z_2)+f'(z_1)f(z_2)}{f(z_1)f(z_2)}\right) \times g(t\pm[z_1])g(t\mp[z_2]).$$

Now it is easy to obtain the analog of the cubic identity for KdV taus (2.3).

Theorem 3.4: *Let functions $f(z)$ and $g(t)$ satisfy the functional Fay identity and conditions* (*i*), (*ii*), (*iii*) *from Lemma* 3.3. *Then $f(z)$ and $g(t)$ satisfy the cubic functional identity*:

$$\begin{aligned} &f(z_2-z_1)[g(t+[z_1]+[z_2])g(t-[z_1])g(t-[z_2]) - g(t-[z_1]-[z_2])g(t+[z_1])g(t+[z_2])] \\ &\quad = f(z_2+z_1)[g(t+[z_1]-[z_2])g(t-[z_1])g(t+[z_2]) - g(t-[z_1]+[z_2])g(t+[z_1])g(t-[z_2])], \end{aligned} \tag{3.2}$$

as well as

$$\begin{aligned} &f'(0)[g(t+2[z])g^2(t-[z]) - g(t-2[z])g^2(t+[z])] \\ &\quad = f(2z)\sum_{k=0}^{\infty} z^{2k}[g(t-[z])W_{2k+1}(g(t),g(t+[z])) + g(t+[z])W_{2k+1}(g(t),g(t-[z]))], \end{aligned} \tag{3.3}$$

where $W_{2k+1}(f,g) := f(\partial_{t_{2k+1}}g) - (\partial_{t_{2k+1}}f)g, k=0,1,2,\ldots$.

Proof: The proof is the same as for obtaining the cubic identity for KdV tau functions:[3] we evaluate the Wronskian:

$$W(g(t+[z_1])g(t-[z_1]),g(t+[z_2])g(t-[z_2])),$$

using the results from Lemma 3.3 and the obvious identity for Wronskians:

$$W(f_1f_2,g_1g_2) = f_1g_1W(f_2,g_2) + f_2g_2W(f_1,g_1) = f_1g_2W(f_2,g_1) + f_2g_1W(f_1,g_2).$$

The identity (3.3) follows from (3.2) after letting $z_2 \to z_1$ (cf. Ref. 3). □

Corollary 3.5: If, the same way, we evaluate the Wronskian:

$$W\left(\prod_{k=1}^{2^n} g(t+[z_{2k-1}])g(t-[z_{2k-1}]), \prod_{k=1}^{2^n} g(t+[z_{2k}])g(t-[z_{2k}])\right)$$

we will obtain (2^n-1)*-order in g identity* (cf. Ref. 3).

Corollary 3.6: We know some solutions of the functional equation (3.1), *which satisfy the conditions from Lemma 3.3:*

(i) $f(z)=z$ *and* $g(t)=\tau(t)$, *where* $\tau(t)$ *is an arbitrary KdV tau function*;
(ii) $f(z)=\sin(z)$ *and* $g(t)=\sin(t_1)$, $t_1\equiv x$;
(iii) $f(z)=\theta_{11}(z)$ *and* $g(t)=\theta_{11}(t_1)$, $t_1\equiv x$.

They correspond, respectively, to the (known) identities (2.1), (2.7), and (2.2). *This way the relations* (2.3)–(2.5) *are particular cases of the cubic functional identity* (3.2).

In order to clarify the range of the cubic identity (3.2), it is necessary to solve the functional equation (3.1) in the class of functions f and g satisfying conditions (i), (ii), (iii) from Lemma 3.3. As a first step in this direction, let us find a class of solutions of Eq. (3.1), for which the differential functional Fay identity has the form of the differential Fay identity for KP taus. Let us pose an additional condition on the function $f(z)$:

Condition **F**: *For every* $z_1,z_2\in\mathbb{C}$, $f(z)$ *satisfies the relation*:

$$f(z_1+z_2)=f(z_1)f'(z_2)+f'(z_1)f(z_2). \tag{3.4}$$

Then, the differential functional Fay identity has the form:

$$W(g(t+[z_1]),g(t+[z_2]))=\frac{f(z_2-z_1)}{f(z_1)f(z_2)}[f'(0)g(t)g(t+[z_1]+[z_2])-g(t+[z_1])g(t+[z_2])]$$

(moreover, we will see that $f'(0)=1$).

First, let us show that condition **F** gives us a solution of (3.1).

Lemma 3.7: Let $f(z)$ *be a twice differentiable*, *odd function that satisfies the condition* **F**. *Then the functions* $f(z)$ *and* $g(t)=f(t_1)$ *satisfy the identity* (3.1).

Proof: From

$$f(z_1+z_2)=f(z_1)f'(z_2)+f'(z_1)f(z_2),$$

$$f(z_1-z_2)=f(z_1)f'(z_2)-f'(z_1)f(z_2)$$

it follows that for every z_0 we have

$$f'(z)=\frac{f(z+z_0)-f(z-z_0)}{2f(z_0)}.$$

Letting $z_0\to 0$ we obtain $f'(0)=1$. Moreover, expanding $f'(z_1+z_2)$ in two ways:

$$\frac{f((z_1+z_0)+z_2)-f((z_1-z_0)+z_2)}{2f(z_0)},$$

$$\frac{f((z_2+z_0)+z_1)-f((z_2-z_0)+z_1)}{2f(z_0)}$$

and letting $z_0\to 0$, we obtain: $f''(z_1)f(z_2)=f(z_1)f''(z_2)$, i.e., $f''(z_1)/f(z_1)=f''(z_2)/f(z_2)=c=\text{const}$. So, we have

$$f'(z_1+z_2)=f'(z_1)f'(z_2)+cf(z_1)f(z_2).$$

From here and from (3.4) it follows that

$$f(z_1+z_2+z_3)=f(z_1)f'(z_2)f'(z_3)+f'(z_1)f(z_2)f'(z_3)+f'(z_1)f'(z_2)f(z_3)+cf(z_1)f(z_2)f(z_3).$$

From here and from (3.4) it follows that the identity (3.1) for the functions $f(z)$ and $g(t)=f(t_1)$ is equivalent to a trivial identity, which can be checked directly. □

Now we can generalize the construction from Lemma 2.1 to all functions $f(z)$, which satisfy the condition **F**. We will explain such a change of variables that $f(z)$ will be replaced by z. Let us define the function $s=h(z)$ by its inverse function:

$$z = h^{-1}(s) := \frac{f(s)}{f'(s)}. \tag{3.5}$$

Then, as a corollary of (3.4) we have ($s_j := h(z_j)$, $j=1,2$):

$$(z_1 - z_2) = \frac{f(s_1 - s_2)}{f'(s_1)f'(s_2)}. \tag{3.6}$$

From (3.5) it follows that the function $h^{-1}(s)$ is odd, and so $h(z)$ is also odd function. Let us write its power series expansion: $h(z)=\Sigma_{k=0}^{\infty}[h^{(2k+1)}(0)/(2k+1)!]z^{2k+1}$, where $h^{(n)}$ is the nth derivative of h. Following the idea of the proof of Lemma 2.1, let us pose additional restriction on the function $g(t)$:

Condition **G***: Function* $g(t)$ *has the form*:

$$g(t) := f\left(\sum_{k=0}^{\infty} \frac{h^{(2k+1)}(0)}{(2k)!} t_{2k+1}\right), \tag{3.7}$$

where $h(z)$ *is given by* (3.5).

Then we have

$$g(t+[z]) = f\left(\sum_{k=0}^{\infty} \frac{h^{(2k+1)}(0)}{(2k)!}\left(t_{2k+1} + \frac{z^{2k+1}}{2k+1}\right)\right) = f\left(\sum_{k=0}^{\infty} \frac{h^{(2k+1)}(0)}{(2k)!} t_{2k+1} + \sum_{k=0}^{\infty} \frac{h^{(2k+1)}(0)}{(2k+1)!} z^{2k+1}\right)$$
$$= f\left(\sum_{k=0}^{\infty} \frac{h^{(2k+1)}(0)}{(2k)!} t_{2k+1} + h(z)\right). \tag{3.8}$$

In this way we are in a position to prove the following

Lemma 3.8: Let $f(z)$ *be an odd function and* $f(z)$, $g(t)$ *satisfy the conditions* **F** *and* **G**. *Than* $f(z)$ *and* $g(t)$ *satisfy the functional Fay identity* (3.1).

Proof: Let the shifts z_j, $j=0,1,2,3$ be given and let us define new shifts by: $s_j=h(z_j)$, $j=0,1,2,3$, where $h(z)$ is given by (3.5). Then from (3.8) and the condition **G** it follows that:

$$g(t+[z_0]+[z_1]) = f(x+s_0+s_1), \quad \text{etc.}$$

($x=\Sigma_{k=0}^{\infty}[h^{(2k+1)}(0)/(2k)!]t_{2k+1}$). From here and relation (3.6) it is clear that the statement of this Lemma follows from Lemma 3.7. □

This construction does not give us some new solutions of (3.1), because Eq. (3.4) and the condition that $f(z)$ is odd function are too strong restrictions.

Lemma 3.9: The odd solutions of Eq. (3.4) *are the functions*: $f(z)=z$, $\sin(z)$, $\sinh(z)$, *up to the obvious symmetry*: *if* $f(z)$ *is a solution of* (3.4), *than for every* $0 \neq a \in \mathbb{C}$ *the functions* $f_a(z) := (1/a)f(az)$ *are also solutions of* (3.4).

Proof: In the proof of Lemma 3.7 we came to the equality: $f''(z_1)/f(z_1)=f''(z_2)/f(z_2)=c=\text{const}$. It is equivalent to the differential equation: $f''=cf$. Now using the conditions that $f(z)$ is an odd function and $f'(0)=1$ we obtain the statement of this Lemma. □

Corollary 3.10: The functions: $f(z)=\sinh(z)$ *and* $g(t)=\sinh(t_1)$ *give a solution of Eq.* (3.1). *For them the cubic identity* (3.2) *is fulfilled.*

Remark 2.11: The condition **G** is too restrictive. If we take the solution $f(z)=z$ of (3.4), we know solutions of (3.1) for which the functions $g(t)$ do not satisfy the condition **G**. These are all KP tau functions.

Remark 3.12: The condition **F** is also too restrictive. The Fay identity (2.2) for the elliptic

theta function θ_{11} shows that $f(z)=\theta_{11}(z)$ is a possible choice for the function $f(z)$, but for it the condition **F** is not fulfilled.

IV. THE RANGE OF THE FUNCTIONAL FAY IDENTITY

Let us mention that from the result of Ref. 8 (Proposition B.3) follows that under some conditions on $f(z)$, for general functions $g(t)$ (i.e., non KdV type), the functional Fay identity (3.1) is equivalent to the Fay identity for KP tau functions. We have the following

Lemma 4.1: Let $f(z)$ be an odd function, for which: $f'(0)\neq 0$, and the following expansion holds: $\ln[f(z)/z]=\Sigma_{n=0}^{\infty}a_n z^n$. *Then for every KP tau function $\tau(t)$, there exists set of numbers b_{ij}, $i,j=1,2,\ldots$ (depending on $f(z)$), such that the pair:*

$$f(z),\quad g(t) := \tau(t)\exp\left[-\frac{1}{2}\sum_{i,j=1}^{\infty} b_{ij}t_i t_j\right]$$

is a solution of the functional Fay identity (3.1). *Every solution of* (3.1) (*with the posed restrictions on $f(z)$, and $g(t)$ - of general type*) *can be obtained this way.*

Proof: Let us take:

$$\ln\left[\frac{f(z_1-z_2)}{z_1-z_2}\right]=\sum_{n=0}^{\infty}a_n(z_1-z_2)^n=\sum_{i,j=0}^{\infty}c_{ij}z_1^i z_2^j,\quad \text{where } c_{ij}=c_{ji}.$$

But $\Sigma_{i=0}^{\infty}c_{i0}z_1^i=\ln[f(z1)/z_1]$ and $\Sigma_{i=0}^{\infty}c_{0j}z_2^j=\ln[f(z_2)/z_2]$. So, we can rewrite:

$$\ln\left[\frac{f(z_1-z_2)}{z_1-z_2}\right]=\ln\left[\frac{f(z_2)}{z_2}\right]+\ln\left[\frac{f(z_1)}{z_1}\right]+\sum_{i,j=1}^{\infty}c_{ij}z_1^i z_2^j=\ln\left[\frac{f(z_2)}{z_2}\right]+\ln\left[\frac{f(z_1)}{z_1}\right]$$
$$+\sum_{i,j=1}^{\infty}b_{ij}\frac{z_1^i}{i}\frac{z_2^j}{j},\quad \text{where } b_{ij}=b_{ji}.$$

We state that the numbers b_{ij}, $i,j=1,2,\ldots$ are suitable for our aim. We have:

$$g(t+[z_0]+[z_1])=\tau(t+[z_0]+[z_1])\exp\left[-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}\left(t_i+\frac{z_0^i}{i}+\frac{z_1^i}{i}\right)\left(t_j+\frac{z_0^j}{j}+\frac{z_1^j}{j}\right)\right]$$
$$=\tau(t+[z_0]+[z_1])\exp\left[-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}\left[t_i t_j+2t_i\left(\frac{z_0^j+z_1^j}{j}\right)+\left(\frac{z_0^{i+j}+z_1^{i+j}}{ij}\right)+2\left(\frac{z_0^i z_1^j}{ij}\right)\right]\right],$$

and from here:

$$g(t+[z_0]+[z_1])g(t+[z_2]+[z_3])=\tau(t+[z_0]+[z_1])\tau(t+[z_2]+[z_3])$$
$$\times\exp\left[-\sum_{i,j=1}^{\infty}b_{ij}\left(\frac{z_0^i z_1^j+z_2^i z_3^j}{ij}\right)\right]\psi(t,z_0,z_1,z_2,z_3),$$

where

$$\psi(t,z_0,z_1,z_2,z_3)=\exp\left[-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}\left[2t_i t_j+2t_i\left(\frac{z_0^j+z_1^j+z_2^j+z_3^j}{j}\right)+\left(\frac{z_0^{i+j}+z_1^{i+j}+z_2^{i+j}+z_3^{i+j}}{ij}\right)\right]\right].$$

But, we have also

$$f(z_0-z_1)f(z_2-z_3)=(z_0-z_1)(z_2-z_3)\exp\left[\sum_{i,j=1}^{\infty}b_{ij}\left(\frac{z_0^i z_1^j+z_2^i z_3^j}{ij}\right)\right]\frac{f(z_0)}{z_0}\frac{f(z_1)}{z_1}\frac{f(z_2)}{z_2}\frac{f(z_3)}{z_3}.$$

So, it is clear that we have

$$(z_0-z_1)(z_2-z_3)\tau(t+[z_0]+[z_1])\tau(t+[z_2]+[z_3])=f(z_0-z_1)f(z_2-z_3)g(t+[z_0]+[z_1])g(t+[z_2]+[z_3])\Psi(t,z_0,z_1,z_2,z_3),$$

and analogous expressions for the second and the third terms in (2.1), where $\Psi(t,z_0,z_1,z_2,z_3)$ is a common factor for the three expressions. So, if $\tau(t)$ is a KP tau function, then the Fay identity for $\tau(t)$ is fulfilled, and hence (3.1) is fulfilled. The statement, that all solutions of (3.1) (with the posed restrictions on $f(z)$ and $g(t)$ - of general type) can be obtained this way, follows from Ref. 8. □

Remark 4.2: The construction from Lemma 4.1 is not applicable to the functions $g(t)$ of KdV type, because in the expression $\exp\left[-1/2\Sigma_{i,j=1}^{\infty}b_{ij}t_it_j\right]$ there are even t-variables t_{2k}. As an example, for $f(z)=\sin(z)$ we have

$$\ln\left[\frac{\sin(z_1-z_2)}{z_1-z_2}\right]=-\frac{z_1^2}{6}-\frac{z_2^2}{6}+\frac{z_1z_2}{3}-\frac{z_1^4}{180}-\frac{z_2^4}{180}+\frac{z_1^3z_2}{45}+\frac{z_1z_2^3}{45}-\frac{z_1^2z_2^2}{30}+\cdots$$

and hence

$$\exp\left[-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}t_it_j\right]=\exp\left[-\frac{1}{6}t_1^2-\frac{1}{15}t_1t_3+\frac{1}{15}t_2^2+\cdots\right].$$

The critical observation here is that it is possible to overcome the dependence from even variables of the form: $e^{Q(t)}$, ($Q(t)$ - quadratic in t_n), by linear change of the variables t_n. This kind of dependence is irrelevant for us, because roughly speaking we have a lot of freedom with tau functions. As an example, it is well known that the KP theory is not sensitive to the following transformation of tau functions: $\tau(t)\to\tau(t)e^{\Sigma c_nt_n}$, where c_n are constants.

It is known that the expressions of the coefficients of the Lax operator $L(t)$ in terms of tau functions[1] are differential polynomials of $\partial_{t_it_j}^2\log\tau(t)$:[5]

$$L(t)=\partial_x+[\partial_{t_1t_1}^2\log\tau(t)]\partial_x^{-1}+\left[\tfrac{1}{2}(-\partial_{t_1t_1t_1}^3+\partial_{t_2t_1}^2)\log\tau(t)\right]\partial_x^{-2}+\left[\tfrac{1}{6}(\partial_{t_1t_1t_1t_1}^4-3\partial_{t_2t_1t_1}^3+2\partial_{t_3t_1}^2)\log\tau(t)-(\partial_{t_1t_1}^2\log\tau(t))^2\right]\partial_x^{-3}+\cdots.$$

But we have

$$\partial_{t_it_j}^2\log\left[\tau(t)\exp\left(-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}t_it_j\right)\right]=[\partial_{t_it_j}^2\log\tau(t)]-b_{ij},$$

so the effect of the multiplier $\exp\left(-1/2\Sigma_{i,j=1}^{\infty}b_{ij}t_it_j\right)$ is simply additional constants in the coefficients of L-operator, not some of t-variables which appear in exp(…).

Lemma 4.3: Let $\tau_0(t)$ be an arbitrary kdV tau function. Let for arbitrary $b_{i,j}\in\mathbb{C}$, $i,j=1,2,\ldots$ define the function:

$$\tau(t):=\tau_0(t)\exp\left(-\frac{1}{2}\sum_{i,j=1}^{\infty}b_{ij}t_it_j\right)$$

and $L(t)$ is the Lax operator, related to $\tau(t)$. Then, there exists a change of variables $t_n\to t_n'$, another KdV tau function $\tau_1(t')$ and Lax operator $L_1(t')$ related to $\tau_1(t')$, such that the KP flows for $\tau(t)$ and $\tau_1(t')$ coincide, i.e., operators $L(t)$ and $L_1(t')$ are equivalent (cf. Ref. 6, p. 339).

Proof: Let $L(t)$ be the Lax operator related to the function $\tau(t)$:

$$L(t)=\sum_{i,j=0}^{\infty}\frac{p_i(-\tilde{\partial})\tau(t)}{\tau(t)}\partial_x^{1-i-j}\frac{p_j(\tilde{\partial})\tau(t)}{\tau(t)}.$$

Because of: $\partial^2_{t_it_j}\log\left[\tau(t)\exp\left(-1/2\Sigma_{i,j=1}^{\infty}b_{ij}t_it_j\right)\right]=[\partial^2_{t_it_j}\log\tau(t)]-b_{ij}$, we have $\partial_{t_{2n}}L(t)=0$ and hence $[(L^{2n})_+,L]=0$. In this case we have ($a_k,k=1,2,\ldots$ are some constants):

$$(L^2)_+=L^2+\sum_{k=1}^{\infty}a_kL^{-k}.$$

Let us define the operator L' ($b_k,k=1,2,\ldots$ are another constants):

$$L':=\sqrt{(L^2)_+}=\sqrt{L^2+\sum_{k=1}^{\infty}a_kL^{-k}}=L\left[\sum_{m=0}^{\infty}\binom{\frac{1}{2}}{m}\left(\sum_{k=1}^{\infty}a_kL^{-2-k}\right)^m\right]=L+\sum_{k=2}^{\infty}b_kL^{-k}.$$

Then $(L')^2$ is a differential operator, i.e., $\partial_{2n}(L')^2=0$.

From $L'=L+\Sigma_{k=2}^{\infty}b_kL^{-k}$ follows $((L')^n)_+=\Sigma_{k=1}^{n}c_{n,k}(L^k)_+$ ($c_{n,k}$, $n=1,2,\ldots$, $k=1,2,\ldots,n$ are constants). We have $\partial_{t_n}L=[(L^n)_+,L]$, so let us define new t'_n-derivatives by the following connection with the old t_n-derivatives: $\partial_{t'_n}:=\Sigma_{k=1}^{n}c_{n,k}\partial_{t_n}$. Then the new variables t'_n could be expressed linearly by t_n and this is the change of variables we were searching for. If we denote $L_1(t')=L'(t_n\rightarrow t'_n)$ and $\tau_1(t')$—a tau function related to $L_1(t')$, we obtain the statement of this Lemma. □

Remark 4.4: The proof of Lemma 4.3 is not constructive and hence it is difficult to apply the result for translating, for example, the original Fay identity for genus $g=1$-case 2.2 (where $f(z)=\theta_{11}(z)$) to the Fay identity for tau functions (2.1).

Combining the results of Lemmas 4.1 and 4.3 we obtain the following

Theorem 4.5: Modulo the restrictions on the function $f(z)$ from Lemma 4.1 *the functional Fay identity* (3.1) *for functions $g(t)$ of KdV type is equivalent to the Fay identity* (2.1) *for KdV tau functions*.

Remark 4.6: An open problem remains to clarify the *geometrical interpretation* of the cubic identity (3.2) from the viewpoint of the theory of theta functions.

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Clifford-Finsler algebroids and nonholonomic Einstein–Dirac structures

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We propose a new framework for constructing geometric and physical models on nonholonomic manifold provided both with Clifford-Lie algebroid symmetry and nonlinear connection structure. Explicit parametrizations of generic off-diagonal metrics and linear and nonlinear connections define different types of Finsler, Lagrange, and/or Riemann–Cartan spaces. A generalization to spinor fields and Dirac operators on nonholonomic manifolds motivates the theory of Clifford algebroids defined as Clifford bundles, in general, enabled with nonintegrable distributions defining the nonlinear connection. In this work, we elaborate the algebroid spinor differential geometry and formulate the (scalar, Proca, graviton, spinor, and gauge) field equations on Lie algebroids. The paper communicates new developments in geometrical formulation of physical theories and this approach is grounded on a number of previous examples when exact solutions with generic off-diagonal metrics and generalized symmetries in modern gravity define nonholonomic spacetime manifolds with uncompactified extra dimensions. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2339016]

I. INTRODUCTION

A class of spacetimes possessing noncommutative and/or Lie algebroid symmetries can be defined as exact solutions in string and Einstein gravity.[1,2] This leads to new developments in formulation of classical and quantum field theories following the geometry of nonholonomic manifolds[3] possessing Lie algebroid symmetry.[4] Lie algebroid structures in gravity are modeled by generic off-diagonal metrics and nonholonomic frames (vielbeins) with associated nontrivial nonlinear connection (*N*-connection). The spacetimes provided with compatible metric, linear connection, and *N*-connection structures and possessing Lie algebroid symmetry are called Einstein–Cartan algebroids, or (in a more general context, for various extensions of the Riemann–Cartan geometry) Lie *N*-algebroids. Usually, the Lie algebroids can be defined for a vector, or tangent, bundle but, in general, they can be considered for any nonholonomic manifold provided with a nonintegrable (nonholonomic) distribution. [In our works we use distributions defining *N*-connection structures with the coefficients induced by the metric's off-diagonal terms and corresponding vielbein's coefficients. The geometric constructions are performed for nonholonomic manifolds, i.e., spaces provided with nonintegrable distributions. In a particular case, when such distributions are related to the exact sequences of subspaces defining an *N*–connection, the spaces are called *N* anholonomic]. In brief, such spaces are called Lie *N*-algebroids. Similar constructions elaborated for the Einstein–Dirac spaces give rise to the geometry of Clifford algebroids. If the curved spinor spaces are also enabled with Finsler, or Lagrange, structures, we deal with Clifford–Finsler, or Clifford–Lagrange, algebroids.

We note that the methods of Finsler and Lagrange geometry[5,6] were recently reconsidered in a new way in order to solve physical problems related to standard theories of gravity and field

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interactions.[1,7,6,8,9] If the former physical applications of Finsler geometry were elaborated on tangent/vector bundles, with less straightforward connections to standard physical theories (see reviews and references in Refs. 1, 7, and 6), in our approach we tried to define Finsler-type structures as exact solutions in Einstein and extra dimension gravity[8,9] when certain dimensions are not compactified. Such constructions are related to the geometry of nonholonomic manifolds possessing generalized symmetries (Lie algebroid and/or Clifford symmetries, noncommutative structures induced by anholonomic frames, etc.) and a number of ideas and methods from Finsler geometry seem to be of general interest and significant importance for physical applications. Here we note that this paper is not just on Clifford–Finsler geometry and related Lie algebroid structures but rather on (pseudo) Riemann geometry and gravitational and field interactions (and extensions to nontrivial torsion induced, for instance, from string theory and/or by nonholonomic frame effects) when the spinor and Lie algebroid structures are defined in nonholonomic form and certain methods from Finsler geometry became very important and efficient in order to solve nonlinear physical problems.[10]

This work develops the geometry of Clifford *N*-algebroids and generalized Finsler–spinor spaces elaborated in Refs. 11–13 and 7. If the first applications of algebroid methods were in geometric mechanics,[14–17] the recent works suggest a very promising route toward the theory of gauge fields, gravity and strings and noncommutative geometry.[7,18,1] We cite Ref. 4 for details on algebroid theory and related bibliography.

In the present paper, we address essentially the following two purposes: The *first one* is to define and study the geometry of Clifford algebroids and their *N*-anholonomic deformations, Clifford *N*-algebroids, and analysis of their main properties in relation to spinors in gravity theories and on nonholonomic manifolds. The *second* aim is the formulation of the field equations on Lie algebroids.

The structure of the paper is the following: The theory of Clifford algebroids is formulated in Sec. II: we remember the main definitions of nonholonomic manifolds provided with *N*-connection structure, define Clifford *N*-algebroids, and study the related spinor differential geometry. Section III is devoted to the field equations on *N*-anholonomic manifolds and their redefinition on Clifford *N*-anholonomic algebroids. We start with a study of the Dirac operator and spin connections on nonholonomic manifolds. Then the constructions are completed with spinor formulations of the basic equations for scalar, Proca, graviton, Dirac, and gauge fields interactions and related Lie/Clifford *N*-algebroid structures. In Sec. IV, we present conclusions and outlook.

II. CLIFFORD ALGEBROIDS AND *N*-CONNECTIONS

The geometry of spinor spaces enabled with nonlinear connection (*N*-connection) structure was elaborated in a series of works[11–13] (see also Refs. 19–21 for general references on Clifford and spinor differential geometry and applications to physics). Here we note that the concept of *N*-connection was originally proposed in the framework of Finsler geometry and geometric mechanics but such nonholonomic structures [defined by exact sequences of subspaces of the tangent space to the spacetime manifold and related nonintegrable distributions] may be also considered on (pseudo) Riemannian and Einstein–Cartan–Weyl spaces, see the discussion and historical remarks in Ref. 7. A class of nonholonomic spinor configurations can be defined by exact solutions of the Einstein–Dirac equations parametrized by generic off-diagonal metric ansatz, nonholonomic vielbeins associated to nontrivial *N*-connections, and arbitrary linear connections with nontrivial torsion.

The aim of this section is to formulate the theory of Clifford algebroids provided with nonlinear connection (*N*-connection) structures, i.e., the theory of Clifford *N*-algebroids. For holonomic configurations, the Clifford algebroids can be defined as usual Lie algebroids[4] but associated to a Clifford bundle instead of a vector or tangent bundle.

A. Nonholonomic manifolds and nonlinear connections

We outline some basic definitions and formulas from the geometry of manifolds provided with N-connection structure, see details in Refs. 6 and 7.

Let us consider a Riemann–Cartan manifold V of dimension $n+m$ and necessary smooth class and provided with general metric (of arbitrary signature) and linear connection structures. The local coordinates are denoted $u=(x,y)$, or $u^{\alpha}=(x^i,y^a)$, where the abstract, or coordinate, indices take, respectively, the values $i,j,k,\ldots=1,2,\ldots,n$ and $a,b,c,\ldots=n+1,n+2,\ldots,n+m$. Such a splitting of dimension and coordinates will be adapted below to the nonlinear connection structure. We denote by M a subspace of V, $\dim M=n$, provided with local coordinates x^i. The metric on V is parametrized in the form

$$\mathbf{g}=g_{\alpha\beta}\mathbf{e}^{\alpha}\otimes\mathbf{e}^{\beta}=g_{ij}(u)\mathbf{e}^{i}\otimes\mathbf{e}^{j}+h_{ab}(u)\mathbf{e}^{a}\otimes\mathbf{e}^{b}, \tag{1}$$

where

$$\mathbf{e}^{\mu}=[e^i=\mathrm{d}x^i,\mathbf{e}^a=\mathrm{d}y^a+N_i^a(u)\mathrm{d}x^i] \tag{2}$$

is the dual frame to

$$\mathbf{e}_{\nu}=\left[e_i=\frac{\partial}{\partial x^i}-N_i^a(u)\frac{\partial}{\partial y^a},e_a=\frac{\partial}{\partial y^a}\right]. \tag{3}$$

Such vielbeins are called N-adapted frames. [In order to preserve a relation with the previous denotations,[7,11–13] we note that $\mathbf{e}_{\nu}=(e_i,e_a)$ and $\mathbf{e}^{\mu}=(e^i,e^a)$ are, respectively, the former $\delta_{\nu}=\delta/\partial u^{\nu}=(\delta_i,\partial_a)$ and $\delta^{\mu}=\delta u^{\mu}=(d^i,\delta^a)$ which emphasize that operators (3) and (2) define, correspondingly, certain "N-elongated" partial derivatives and differentials which are more convenient for calculations on such nonholonomic manifolds].

We denote by $\pi^{\intercal}:TV\to TM$ the differential of a map $\pi:TV\to hV$, where hV is locally isomorphic to M, defined by fiber preserving morphisms of the tangent bundles TV and TM. The kernel of $\pi^{\intercal}$ is just the vertical subspace vV, $\dim(vV)=m$, with a related inclusion mapping $i:vV\to TV$ and hV is a horizontal subspace. It should be emphasized that such maps and local decompositions exist when $V\to M$ is a surjective submersion. A particular case is that of a fiber bundle but we can obtain the results in the general case [see the discussions and references in Refs. 3 and 7 related to almost sympletic manifolds, (pseudo) Riemannian spaces, and vector bundles and generalizations]. A *nonlinear connection* (*N-connection*) N on a manifold V is defined by the splitting on the left of an exact sequence

$$0\to vV\to TV\to TV/vV\to 0,$$

i.e., by a morphism of submanifolds $\mathbf{N}:TV\to vV$ such that $\mathbf{N}\circ\mathbf{i}$ is the unity in vV.

Equivalently, a N-connection is defined by a Whitney sum of horizontal (h) subspace, $hV\simeq M$ (we shall use the symbol "$\simeq$" in order to emphasize some isomorphisms of spaces) and vertical (v) subspace, vV,

$$T\mathbf{V}=hV\oplus vV. \tag{4}$$

The spaces provided with N-connection structure are denoted by boldface symbols. For instance, we write $\mathbf{V}$ for a manifold V provided with a distribution (4) (being, in general, nonintegrable, i.e., nonholonomic—in the literature an equivalent term it is also used: anholonomic). Such manifolds are called N-anholonomic with the nonholonomy defined by a N-connection structure. In a similar manner, we can define nonholonomic manifolds enabled with certain more general nonintegrable (nonholonomic) distributions of subspaces in TV, or in TTV, and so on, but in this paper we shall restrict our considerations only to N-anholonomic manifolds with N-connection splitting on TV. We shall use boldfaced indices for the geometric objects adapted to the N-connection.

Locally, a N-connection is defined by its coefficients $N_i^a(u)$,

$$\mathbf{N} = N_i^a(u)\mathrm{d}x^i \otimes \frac{\partial}{\partial y^a}.$$

The well-known class of linear connections consists on a particular subclass with the coefficients being linear on y^a, i.e., $N_i^a(u)=\Gamma_{bj}^a(x)y^b$. Any N-connection is characterized by its N-connection curvature

$$\mathbf{\Omega} = \frac{1}{2}\Omega_{ij}^a \mathrm{d}x^i \wedge \mathrm{d}x^j \otimes \frac{\partial}{\partial y^a},$$

with N-connection curvature coefficients

$$\Omega_{ij}^a = \delta_{[j}N_{i]}^a = \delta_j N_i^a - \delta_i N_j^a = \frac{\partial N_i^a}{\partial x^j} - \frac{\partial N_j^a}{\partial x^i} + N_i^b \frac{\partial N_j^a}{\partial y^b} - N_j^b \frac{\partial N_i^a}{\partial y^b},$$

and states the condition that the vielbeins (2) satisfy the nonholonomy (equivalently, anholonomy) relations

$$[\mathbf{e}_\alpha, \mathbf{e}_\beta] = \mathbf{e}_\alpha \mathbf{e}_\beta - \mathbf{e}_\beta \mathbf{e}_\alpha = W_{\alpha\beta}^\gamma \mathbf{e}_\gamma$$

with (antisymmetric) nontrivial anholonomy coefficients $W_{ia}^b = \partial_a N_i^b$ and $W_{ji}^a = \Omega_{ij}^a$.

All our further geometric constructions will be for spaces with nonholonomic splitting (4) and performed in "N-adapted" form with respect to local frames of type (2) and (3).

B. Clifford *N*-algebroids

Let us state the notations for abstract (coordinate) d-tensor indices of geometrical objects defined with respect to an arbitrary (coordinate) local basis, i.e., system of reference. For a local basis on $\mathbf{V}$, we write $e_\alpha=(e_i,v_a)$. The small Greek indices $\alpha,\beta,\gamma,\ldots$ are considered to be general ones, running values $1,2,\ldots,n+m$ and $i,j,k,\ldots$ and $a,b,c,\ldots$, respectively, label the geometrical objects on the base and typical "fiber" and run, correspondingly, the values $1,2,\ldots,n$ and $1,2,\ldots,m$. The dual base is denoted by $e^\alpha=(e^i,v^a)$. The local coordinates of a point $u\in\mathbf{V}$ are written $\mathbf{u}=(x,y)$, or $u^\alpha=(x^i,y^a)$, where y^a is the ath coordinate with respect to the basis (v_a) and (x^i) are local coordinates on $h\mathbf{V}$ with respect to e_i. We shall use "boldface" symbols in order to emphasize that the objects are defined on spaces provided with N-connection structure.

We suppose that the N-anholonomic manifold $\mathbf{V}$ admits a d-spinor structure which allows us to introduce spinor coordinates and parametrizations of geometrical objects. Let

$$\mathbf{e}_{\acute{\alpha}}{}^{\acute{\boldsymbol{\alpha}}} = (e_{\acute{i}}{}^{\acute{\mathbf{1}}}, e_{\acute{i}}{}^{\acute{\mathbf{2}}}, \ldots, e_{\acute{i}}{}^{\tilde{\mathbf{k}}_{(n)}}, e_{\acute{a}}{}^{\acute{\mathbf{1}}}, e_{\acute{a}}{}^{\acute{\mathbf{2}}}, \ldots, e_{\acute{a}}{}^{\tilde{\mathbf{k}}_{(m)}}),$$

with boldfaced indices running coordinate values on dimensions of d-spinor spaces, $\tilde{\mathbf{k}}_{(n)}$ and $\tilde{\mathbf{k}}_{(m)}$, being the coefficients of a d-spinor basis

$$\mathbf{e}_{\acute{\alpha}} = (e_{\acute{i}}, e_{\acute{a}}). \tag{5}$$

The dual basis (co-basis)

$$\mathbf{e}^{\acute{\alpha}} = (e^{\acute{i}}, e^{\acute{a}}) \tag{6}$$

has the coefficients

$$\mathbf{e}_{\acute{\boldsymbol{\alpha}}}{}^{\acute{\alpha}} = (e_{\acute{\mathbf{1}}}{}^{\acute{i}}, e_{\acute{\mathbf{2}}}{}^{\acute{i}}, \ldots, e_{\tilde{\mathbf{k}}_{(n)}}{}^{\acute{i}}, e_{\acute{\mathbf{1}}}{}^{\acute{a}}, e_{\acute{\mathbf{2}}}{}^{\acute{a}}, \ldots, e_{\tilde{\mathbf{k}}_{(m)}}{}^{\acute{a}}).$$

Similar formulas hold for the associated d-spinor spaces provided with local bases $\mathbf{e}_{\grave{\boldsymbol{\alpha}}}{}^{\grave{\alpha}}$ and $\mathbf{e}_{\grave{\alpha}}{}^{\grave{\alpha}}$. Such spinor bases are stated to be compatible to the N-connection splitting, i.e. to the vielbeins (3) and (2). For a given d-metric structure on $\mathbf{V}$ and its spinor decomposition, with associated spinor

bases $\mathbf{e}_{\grave{\alpha}}=(e_{\grave{i}},e_{\grave{a}})$, which allows us to introduce the γ objects, we can define, for instance, a N-adapted basis

$$\mathbf{e}_{\alpha}=(\gamma_{\alpha})^{\acute{\alpha}\grave{\alpha}}\mathbf{e}_{\acute{\alpha}}\mathbf{e}_{\grave{\alpha}}=[e_i=(\gamma_i)^{\hat{i}\acute{i}}e_{\acute{i}}e_{\grave{i}},e_a=(\gamma_a)^{\acute{a}\grave{a}}e_{\acute{a}}e_{\grave{a}}].$$

As a result, we can alternatively consider spinor coordinates, for instance,

$$u^{\alpha}=(x^i,y^a)\to u^{\acute{\alpha}\grave{\alpha}}=(x^{\hat{i}\hat{i}},y^{\acute{a}\grave{a}}).$$

For even dimensions of n, or m, further reductions are possible, when $x^{\hat{i}\hat{i}}\to x^{II'}$, or $y^{\acute{a}\grave{a}}\to y^{AA'}$. This way, the d-tensor indices can be transformed into the d-spinor ones and inversely.

The standard definition of a Lie algebroid $\mathcal{A}\doteq(E,[\cdot,\cdot],\rho)$ is associated to a vector bundle $\mathcal{E}=(E,\pi,M)$, with a surjective map $\pi:E\to M$ of the total spaces E to the base manifold M, of respective dimensions dim $E=n+m$ and dim $M=n$. The algebroid structure is stated by the anchor map $\rho:E\to TM$ (TM is the tangent bundle to M) and a Lie bracket on the $C^{\infty}(M)$-module of sections of E, denoted Sec(E), such that

$$[X,fY]=f[X,Y]+\rho(X)(f)Y$$

for any $X,Y\in\mathrm{Sec}(E)$ and $f\in C^{\infty}(M)$. The anchor also induces a homomorphism of $C^{\infty}(M)$-modules $\rho:\mathrm{Sec}(A)\to\mathcal{X}^1(M)$ where $\wedge^r(M)$ and $\mathcal{X}^r(M)$ will denote, respectively, the spaces of differential r-forms and r-multivector fields on M.

In local form, the Lie algebroid structure on the manifold $\mathbf{V}$ is defined by its structure functions $\rho^i_a(x)$ and $C^f_{ab}(x)$ defining the relations

$$\rho(e_a)=\rho^i_a(x)e_i=\rho^{\underline{i}}_a(x)\partial_{\underline{i}}, \tag{7}$$

$$[e_a,e_b]=C^c_{ab}(x)e_c \tag{8}$$

and subjected to the structure equations

$$\rho^j_a\frac{\partial\rho^i_b}{\partial x^j}-\rho^j_b\frac{\partial\rho^i_a}{\partial x^j}=\rho^j_cC^c_{ab},\qquad\sum_{\mathrm{cyclic}(a,b,c)}\left(\rho^j_a\frac{\partial C^d_{bc}}{\partial x^j}+C^d_{af}C^f_{bc}\right)=0; \tag{9}$$

for simplicity, we shall omit underlying coordinate indices if it will not result in ambiguities. Such equations are standard ones for the Lie algebroids but defined on N-anholonomic manifolds. In brief, we call them Lie N-algebroids.

Definition 2.1: *A Clifford algebroid* $\mathcal{C}(E)\doteq(\mathbb{C}l(E),{}^s[\cdot,\cdot],{}^s\rho)$ *is associated to a Clifford bundle* $\mathbb{C}l(E)\doteq\mathbb{C}l(T^*E)$ *defined by the vector bundle* $\mathcal{E}=(E,\pi,M)$ *and provided with* "*spin*" *anchor* ${}^s\rho$ and (*Lie type*) *commutator structure* ${}^s[\cdot,\cdot]$ *defined on the Clifford module* Sec($\mathbb{C}l(M)$).

The Clifford algebroid structure on a manifold M is defined $\mathcal{C}(TM)\doteq(\mathbb{C}l(TM),{}^s[\cdot,\cdot],{}^s\rho)$.

In local form, the spinor structure functions are written

$$\rho(e_{\acute{a}\grave{a}})=\rho^i_{\acute{a}\grave{a}}(x)e_i=\rho^{\underline{i}}_{\acute{a}\grave{a}}(x)\partial_{\underline{i}}, \tag{10}$$

$$[e_{\acute{a}\grave{a}},e_{\acute{b}\grave{b}}]=C^{\acute{c}\grave{c}}_{\acute{a}\grave{a}\acute{b}\grave{b}}(x)e_{\acute{c}\grave{c}}, \tag{11}$$

where we can consider a spinor decomposition on M with redefinition of indices like $i\to\acute{i},\grave{i}$. Such structure functions can be induced by pure spinor ones,

$$\hat{\rho}(e_{\acute{a}})=\rho^i_{\acute{a}}(x)e_i \tag{12}$$

and

$$[e_{\acute{a}}, e_{\acute{b}}] = C^{\acute{c}}_{\acute{a}\acute{b}}(x) e_{\acute{c}},$$

where, for instance, we can consider $\rho^i_{\acute{a}\grave{a}}(x) = \rho^i_{\acute{a}}(x)\rho^i_{\grave{a}}(x)$ for any fixed value of i. The structure equations (9) can be written in spinor form by introducing spinor variables (see examples of calculus with spinors in the next section).

We can write down the Lie algebroid and N-connection structures in a compatible form by introducing the "N-adapted" anchor

$$\hat{\rho}^j_a(x,u) \doteq \mathbf{e}^j{}_{\underline{j}}(x,u)\mathbf{e}_a{}^{\underline{a}}(x,u)\rho^{\underline{j}}_{\underline{a}}(x) \tag{13}$$

and "N-adapted" (boldfaced) structure functions

$$\mathbf{C}^f_{ag}(x,u) = \mathbf{e}^f{}_{\underline{f}}(x,u)\mathbf{e}_a{}^{\underline{a}}(x,u)\mathbf{e}_g{}^{\underline{g}}(x,u)C^{\underline{f}}_{\underline{a}\underline{g}}(x), \tag{14}$$

respectively, into formulas (7)–(9). In general, the RC-algebroids are defined by the corresponding sets of functions $\hat{\rho}^i_a(x,y)$ and $\mathbf{C}^f_{ag}(x,y)$ with additional dependencies on v-variables y^b for the N-adapted structure functions. For such Lie N-algebroids, the structure relations became

$$\hat{\rho}(e_b) = \hat{\rho}^i_b(x,y)e_i, \tag{15}$$

$$[e_d, e_b] = \mathbf{C}^f_{db}(x,y)e_f \tag{16}$$

and the structure equations of the Lie N-algebroid are written

$$\begin{gathered}\hat{\rho}^j_a e_j(\hat{\rho}^i_b) - \hat{\rho}^j_b e_j(\hat{\rho}^i_a) = \hat{\rho}^j_e \mathbf{C}^e_{ab}, \\ \sum_{\text{cyclic}(a,b,e)} (\hat{\rho}^j_a e_j(\mathbf{C}^f_{be}) + \mathbf{C}^f_{ag}\mathbf{C}^g_{be} - \mathbf{C}^{f'}_{b'e'}\hat{\rho}^j_a \mathbf{Q}^{fb'e'}_{f'bej}) = 0,\end{gathered} \tag{17}$$

for $\mathbf{Q}^{fb'e'}_{f'bej} = \mathbf{e}^{b'}{}_{\underline{b}}\mathbf{e}^{e'}{}_{\underline{e}}\mathbf{e}_{f'}{}^{\underline{f}}e_j(\mathbf{e}_b{}^{\underline{b}}\mathbf{e}_{e'}{}^{\underline{e}}\mathbf{e}^f{}_{\underline{f}})$ with the values $\mathbf{e}^{b'}{}_{\underline{b}}$ and $\mathbf{e}_{f'}{}^{\underline{f}}$ defined by the N-connection. The Lie N-algebroid structure will be characterized by the data $\hat{\rho}^i_b(x,y)$ and $\mathbf{C}^f_{db}(x,y)$ stated with respect to the N-adapted frames (3) and (2).

A Riemann–Cartan algebroid (in brief, RC–algebroid) is a Lie algebroid $\mathcal{A} \doteq (\mathbf{V}, [\cdot,\cdot], \rho)$ associated to a N-anholonomic manifold $\mathbf{V}$ provided with a N-connection $\mathbf{N}$, symmetric metric $\mathbf{g}(\mathbf{u})$ and linear connection $\mathbf{\Gamma}(\mathbf{u})$ structures resulting in a metric compatible and N-adapted covariant derivative $\mathbf{D}$, when $\mathbf{Dg}=\mathbf{0}$, but, in general, with nonvanishing torsion. In spinor variables, the RC-algebroids transform into Clifford N-algebroids associated to corresponding N-anholonomic manifolds instead of vector bundles. They are characterized by the same set of relations (13)–(17) rewritten in d-spinor variables.

C. *N*-algebroid spinor differential geometry

The goal of the section is to outline the main results from the differential geometry of d-spinors for the Clifford N-algebroids and related N-anholonomic manifolds. The d-tensor and d-connection formulas and basic equations are investigated in details in Ref. 2. Such Lie N-algebroid relations can be obtained by "anchoring" the formulas for d-connections, d-torsions and d-curvatures stated. In result, one obtains certain differential geometric objects on the set of sections like $\mathrm{Sec}(v\mathbf{V})$ or $\mathrm{Sec}(\mathbf{E})$, when the "fiber" derivatives are changed into horizontal ones, $\partial/\partial y^a \to \rho^i_a \partial/\partial x^a$, or in N-adapted form, $e_a \to \hat{\rho}^j_a e_j$. In spinor/ d-spinor variables, such formulas transform into certain analogous on Clifford N-algebroids provided with arbitrary but N-adapted and compatible d-metric and d-connection structure.

We use denotations

$$e^{\alpha}=(e^{i},e^{a})\in\gamma^{\alpha}=(\gamma^{i},\gamma^{a}),\quad \zeta^{\acute{\alpha}}=(\zeta^{\acute{i}},\zeta^{\acute{a}})\in\gamma^{\acute{\alpha}}=(\gamma^{\acute{i}},\gamma^{\acute{a}})$$

for, respectively, elements of modules of d-vector and irreduced d-spinor fields (see details in Ref. 11). D-tensors and d-spinor tensors (irreduced or reduced) will be interpreted as elements of corresponding γ–modules, for instance,

$$q^{\alpha}{}_{\beta\ldots}\in\gamma^{\alpha}{}_{\beta},\psi^{\acute{\alpha}\ \acute{\gamma}}{}_{\acute{\beta}\ \ldots}\in\gamma^{\acute{\alpha}\ \acute{\gamma}}{}_{\acute{\beta}\ \ldots},\xi^{II'}{}_{JK'N'}\in\gamma^{II'}{}_{JK'N'},\ldots\ .$$

We can establish a correspondence between the d-metric $g_{\alpha\beta}$ (1) and d-spinor metric $\epsilon_{\acute{\alpha}\acute{\beta}}$ for both h- and v-subspaces of $\mathbf{V}$ by using the relation

$$g_{\alpha\beta}=\frac{1}{\widetilde{k}_{(n)}+\widetilde{k}_{(m)}}((\gamma_{(\alpha}(u))^{\acute{\alpha}\grave{\alpha}}(\gamma_{\beta)}(u))^{\acute{\beta}\grave{\beta}}\epsilon_{\acute{\alpha}\grave{\beta}}\epsilon_{\acute{\beta}\grave{\alpha}},\tag{18}$$

where $(\alpha\beta)$ denotes symmetrization on such indices and

$$(\gamma_{\alpha}(u))^{\acute{\alpha}\grave{\alpha}}=l_{\alpha}^{\hat{\alpha}}(u)(\gamma_{\hat{\alpha}})^{\acute{\alpha}\grave{\alpha}}.\tag{19}$$

In brief, we can write (18) in the form

$$g_{\alpha\beta}=\epsilon_{\acute{\alpha}\grave{\beta}}\epsilon_{\acute{\beta}\grave{\alpha}}\tag{20}$$

if the γ-objects are considered as a fixed structure, whereas ϵ-objects are treated as caring for the metric "dynamics". This variant is used, for instance, in the so-called two-spinor geometry[19,20] and should be preferred if we have to make explicit the algebraic symmetry properties of d-spinor objects. An alternative way is to consider as fixed the algebraic structure of ϵ-objects and to use variable components of γ-objects of type (19) for developing a variational d-spinor approach to gravitational and matter field interactions (the spinor Ashtekar variables[26] are introduced in this manner). In this paper we shall follow in the bulk the first approach but we note that the second type of spinor calculus is more convenient for finding exact solutions with nonholonomic variables.

We note that a d-spinor metric

$$\epsilon_{\acute{\alpha}\grave{\beta}}=\begin{pmatrix}\epsilon_{\hat{i}\hat{j}} & 0\\ 0 & \epsilon_{\acute{a}\grave{b}}\end{pmatrix}$$

on the d-spinor space $\mathbf{S}=(S_{(h)},S_{(v)})$ may have symmetric or antisymmetric $h(v)$ -components $\epsilon_{\hat{i}\hat{j}}$ $(\epsilon_{\acute{a}\grave{b}})$. For simplicity, in this section (in order to avoid cumbersome calculations connected with eight fold periodicity on dimensions n and m on a N-anholonomic manifold) we shall develop a general d-spinor formalism only by using irreduced spinor spaces $\mathbf{S}_{(h)}$ and $\mathbf{S}'_{(h)}$.

1. D-covariant derivation

For a d-covariant operator

$$\mathbf{D}_{\alpha}=(D_{i},D_{a})=(\gamma_{\alpha})^{\acute{\alpha}\grave{\alpha}}\mathbf{D}_{\acute{\alpha}\grave{\alpha}}=((\gamma_{i})^{\hat{i}\hat{i}}D_{\hat{i}\hat{i}},(\gamma_{a})^{\acute{a}\grave{a}}D_{\acute{a}\grave{a}}),$$

in brief, we shall write

$$\mathbf{D}_{\alpha}=\mathbf{D}_{\acute{\alpha}\grave{\alpha}}=(D_{\hat{i}\hat{i}},D_{\acute{a}\grave{a}}),$$

being constructed by using the coefficients of a d-connection, we define the action on a d-spinor $\gamma^{\acute{\beta}}$ as a map

$$\mathbf{D}_{\acute{\alpha}\grave{\alpha}}:\ \gamma^{\acute{\beta}} \to \gamma^{\acute{\beta}}_{\alpha} = \gamma^{\acute{\beta}}_{\acute{\alpha}\grave{\alpha}}$$

satisfying conditions

$$\mathbf{D}_{\alpha}(\xi^{\acute{\beta}} + \eta^{\acute{\beta}}) = \mathbf{D}_{\alpha}\xi^{\acute{\beta}} + \mathbf{D}_{\alpha}\eta^{\acute{\beta}}, \quad \mathbf{D}_{\alpha}(f\xi^{\acute{\beta}}) = f\mathbf{D}_{\alpha}\xi^{\acute{\beta}} + \xi^{\acute{\beta}}\mathbf{D}_{\alpha}f,$$

for every $\xi^{\acute{\beta}}, \eta^{\acute{\beta}} \in \gamma^{\acute{\beta}}$ and f being a scalar field on $\mathbf{V}$. It is also required that one holds the Leibnitz rule

$$(\mathbf{D}_{\alpha}\zeta_{\acute{\beta}})\,\eta^{\acute{\beta}} = \mathbf{D}_{\alpha}(\zeta_{\acute{\beta}}\eta^{\acute{\beta}}) - \zeta_{\acute{\beta}}\mathbf{D}_{\alpha}\eta^{\acute{\beta}}$$

and that $\mathbf{D}_{\alpha}$ is a real operator, i.e., it commuters with the operation of complex conjugation:

$$\overline{\mathbf{D}_{\alpha}\psi_{\underline{\alpha\beta\gamma}\ldots}} = \mathbf{D}_{\alpha}(\overline{\psi}_{\underline{\alpha\beta\gamma}\ldots}).$$

Let us now analyze the question on uniqueness of action on d-spinors of an operator $\mathbf{D}_{\alpha}$ satisfying some necessary conditions. Denoting by $\mathbf{D}^{(1)}_{\alpha}$ and $\mathbf{D}_{\alpha}$ two such d-covariant operators, we consider the map

$$(\mathbf{D}^{(1)}_{\alpha} - \mathbf{D}_{\alpha}):\ \gamma^{\acute{\beta}} \to \gamma^{\acute{\beta}}_{\acute{\alpha}\grave{\alpha}}. \tag{21}$$

Because the action on a scalar f of both operators $\mathbf{D}^{(1)}_{\alpha}$ and $\mathbf{D}_{\alpha}$ must be identical, i.e.

$$\mathbf{D}^{(1)}_{\alpha}f = \mathbf{D}_{\alpha}f, \tag{22}$$

the action (21) on $f = \omega_{\acute{\beta}}\xi^{\acute{\beta}}$ must be written as

$$(\mathbf{D}^{(1)}_{\alpha} - \mathbf{D}_{\alpha})(\omega_{\acute{\beta}}\xi^{\acute{\beta}}) = 0.$$

We conclude that there is an element $\Theta_{\acute{\alpha}\grave{\alpha}\acute{\beta}}{}^{\acute{\gamma}} \in \gamma_{\acute{\alpha}\grave{\alpha}\acute{\beta}}{}^{\acute{\gamma}}$ for which

$$\mathbf{D}^{(1)}_{\acute{\alpha}\grave{\alpha}}\xi^{\acute{\gamma}} = \mathbf{D}_{\acute{\alpha}\grave{\alpha}}\xi^{\acute{\gamma}} + \Theta_{\acute{\alpha}\grave{\alpha}\acute{\beta}}{}^{\acute{\gamma}}\xi^{\acute{\beta}} \tag{23}$$

and

$$\mathbf{D}^{(1)}_{\acute{\alpha}\grave{\alpha}}\omega_{\acute{\beta}} = \mathbf{D}_{\acute{\alpha}\grave{\alpha}}\omega_{\acute{\beta}} - \Theta_{\acute{\alpha}\grave{\alpha}\acute{\beta}}{}^{\acute{\gamma}}\omega_{\acute{\gamma}}.$$

The action of the operator (21) on a d-vector $v^{\beta} = v^{\acute{\beta}\grave{\beta}}$ can be written by using formula (23) for both indices $\acute{\beta}$ and $\grave{\beta}$:

$$(\mathbf{D}^{(1)}_{\alpha} - \mathbf{D}_{\alpha})v^{\acute{\beta}\grave{\beta}} = \Theta_{\alpha\acute{\gamma}}{}^{\acute{\beta}}v^{\acute{\gamma}\grave{\beta}} + \Theta_{\alpha\grave{\gamma}}{}^{\grave{\beta}}v^{\acute{\beta}\grave{\gamma}} = (\Theta_{\alpha\acute{\gamma}}{}^{\acute{\beta}}e^{\grave{\beta}}_{\grave{\gamma}} + \Theta_{\alpha\grave{\gamma}}{}^{\grave{\beta}}e^{\acute{\beta}}_{\acute{\gamma}})v^{\acute{\gamma}\grave{\gamma}} = Q^{\beta}_{\alpha\gamma}v^{\gamma},$$

where

$$Q^{\beta}{}_{\alpha\gamma} = Q^{\acute{\beta}\grave{\beta}}{}_{\acute{\alpha}\grave{\alpha}\acute{\gamma}\grave{\gamma}} = \Theta_{\alpha\acute{\gamma}}{}^{\acute{\beta}}e^{\grave{\beta}}_{\grave{\gamma}} + \Theta_{\alpha\grave{\gamma}}{}^{\grave{\beta}}e^{\acute{\beta}}_{\acute{\gamma}}. \tag{24}$$

The commutator $\mathbf{D}_{[\alpha}\mathbf{D}_{\beta]}$ defines the d-torsion. Applying operators $\mathbf{D}^{(1)}_{[\alpha}\mathbf{D}^{(1)}_{\beta]}$ and $\mathbf{D}_{[\alpha}\mathbf{D}_{\beta]}$ on $f = \omega_{\acute{\beta}}\xi^{\acute{\beta}}$, we can write

$$T^{(1)\gamma}{}_{\alpha\beta} - T^{\gamma}{}_{\alpha\beta} = Q^{\gamma}{}_{\beta\alpha} - Q^{\gamma}{}_{\alpha\beta}$$

with $Q^{\gamma}{}_{\alpha\beta}$ from (24).

The action of operator $\mathbf{D}^{(1)}_{\alpha}$ on d-spinor tensors must be constructed by using formula (23) for every upper indices and formula (24) for every lower indices.

2. N-adapted Infeld–van der Waerden coefficients

A d-spinor $\kappa^{\acute{\alpha}} \in \gamma^{\acute{\alpha}}$ has the components $\kappa^{\acute{\alpha}}=\kappa^{\acute{\alpha}}\mathbf{e}^{\acute{\alpha}}_{\acute{\alpha}}=(\kappa^{\acute{i}}, \kappa^{\acute{\mathbf{a}}})$ defined with respect to the N-adapted spinor basis (5). Taking into account that

$$\mathbf{e}_{\acute{\alpha}}{}^{\acute{\alpha}}\mathbf{e}_{\grave{\beta}}{}^{\grave{\beta}}\mathbf{D}_{\acute{\alpha}\grave{\beta}}=\mathbf{D}_{\acute{\alpha}\grave{\beta}},$$

we compute the components $\mathbf{D}_{\acute{\alpha}\grave{\beta}}\kappa^{\acute{\gamma}}$,

$$\mathbf{e}_{\acute{\alpha}}{}^{\acute{\alpha}}\mathbf{e}_{\grave{\beta}}{}^{\grave{\beta}}\mathbf{e}^{\acute{\gamma}}_{\acute{\gamma}}\mathbf{D}_{\acute{\alpha}\grave{\beta}}\kappa^{\acute{\gamma}}=\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\tau}}\mathbf{e}_{\acute{\tau}}{}^{\acute{\gamma}}\mathbf{D}_{\acute{\alpha}\grave{\underline{\beta}}}\kappa^{\acute{\epsilon}}+\kappa^{\acute{\epsilon}}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\gamma}}\mathbf{D}_{\acute{\alpha}\grave{\beta}}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}=\mathbf{D}_{\acute{\alpha}\grave{\beta}}\kappa^{\acute{\gamma}}+\kappa^{\acute{\epsilon}}\varpi^{\acute{\gamma}}{}_{\acute{\alpha}\grave{\beta}\acute{\epsilon}}, \tag{25}$$

where the coordinate components of the d-spinor connection are defined

$$\varpi^{\acute{\gamma}}{}_{\acute{\alpha}\grave{\beta}\acute{\epsilon}} \doteq \mathbf{e}_{\acute{\tau}}{}^{\acute{\gamma}}\mathbf{D}_{\acute{\alpha}\grave{\beta}}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\tau}}. \tag{26}$$

We call the Infeld–van der Waerden d-symbols a set of objects $\varpi^{\acute{\gamma}}{}_{\acute{\alpha}\grave{\beta}\acute{\epsilon}}$ parametrized with respect to a coordinate d-spinor basis. Defining $\mathbf{D}_{\alpha}=(\gamma_{\alpha})^{\acute{\alpha}\grave{\beta}}\mathbf{D}_{\acute{\alpha}\grave{\beta}}$, introducing denotations $\varpi^{\gamma}{}_{\alpha\acute{\tau}} \doteq \varpi^{\acute{\gamma}}{}_{\acute{\alpha}\grave{\beta}\acute{\tau}}(\gamma_{\alpha})^{\acute{\alpha}\grave{\beta}}$and using properties (25), we write the relations

$$l^{\alpha}_{\alpha}\mathbf{e}^{\acute{\beta}}_{\acute{\beta}}\mathbf{D}_{\alpha}\kappa^{\acute{\beta}}=\mathbf{D}_{\alpha}\kappa^{\acute{\beta}}+\kappa^{\acute{\delta}}\varpi^{\acute{\beta}}{}_{\alpha\acute{\delta}} \tag{27}$$

and

$$l^{\alpha}_{\alpha}\mathbf{e}^{\acute{\beta}}_{\acute{\beta}}\mathbf{D}_{\alpha}\mu_{\acute{\beta}}=\mathbf{D}_{\alpha}\mu_{\acute{\beta}}-\mu_{\acute{\delta}}\varpi^{\acute{\delta}}{}_{\alpha\acute{\beta}} \tag{28}$$

for d-covariant derivations $\mathbf{D}_{\alpha}\kappa^{\acute{\beta}}$ and $\mathbf{D}_{\alpha}\mu_{\acute{\beta}}$.

We can consider expressions similar to (27) and (28) for values having both types of d-spinor and d-tensor indices, for instance,

$$l^{\alpha}_{\alpha}l^{\gamma}_{\gamma}\mathbf{e}^{\acute{\delta}}_{\acute{\delta}}\mathbf{D}_{\alpha}\theta^{\gamma}_{\acute{\delta}}=\mathbf{D}_{\alpha}\theta^{\gamma}_{\acute{\delta}}-\theta^{\gamma}_{\acute{\epsilon}}\varpi^{\acute{\epsilon}}{}_{\alpha\acute{\delta}}+\theta^{\tau}_{\acute{\delta}}\Gamma^{\gamma}{}_{\alpha\tau}$$

(we can prove this by a straightforward calculation of the derivation $\mathbf{D}_{\alpha}(\theta^{\tau}_{\acute{\delta}}\,\mathbf{e}^{\acute{\delta}}_{\acute{\delta}}l^{\gamma}_{\tau})$).

Now we shall consider some possible relations between components of d-connections $\varpi^{\acute{\epsilon}}_{\alpha\acute{\delta}}$ and $\Gamma^{\gamma}_{\alpha\tau}$ and derivations of $(\gamma_{\alpha})^{\acute{\alpha}\grave{\beta}}$. We can write

$$\begin{aligned}\Gamma^{\alpha}_{\beta\tau}&=l^{\alpha}_{\alpha}\mathbf{D}_{\tau}l^{\alpha}_{\beta}=l^{\alpha}_{\alpha}\mathbf{D}_{\tau}(\gamma_{\beta})^{\acute{\epsilon}\grave{\tau}}=l^{\alpha}_{\alpha}\mathbf{D}_{\tau}((\gamma_{\beta})^{\acute{\epsilon}\grave{\tau}}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}\mathbf{e}_{\grave{\tau}}{}^{\grave{\tau}})=l^{\alpha}_{\alpha}\mathbf{e}_{\acute{\alpha}}{}^{\acute{\alpha}}\mathbf{e}_{\acute{\epsilon}}{}^{\grave{\epsilon}}\mathbf{D}_{\tau}(\gamma_{\beta})^{\acute{\alpha}\grave{\epsilon}}+l^{\alpha}_{\alpha}(\gamma_{\beta})^{\acute{\epsilon}\grave{\tau}}(\mathbf{e}_{\grave{\tau}}{}^{\grave{\tau}}\mathbf{D}_{\tau}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}+\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}\mathbf{D}_{\tau}\mathbf{e}_{\grave{\tau}}{}^{\grave{\tau}})\\&=l^{\boldsymbol{\alpha}}_{\acute{\alpha}\acute{\epsilon}}\mathbf{D}_{\tau}(\gamma_{\beta})^{\acute{\alpha}\grave{\epsilon}}+l^{\alpha}_{\acute{\alpha}\grave{\epsilon}}\mathbf{e}_{\acute{\alpha}}{}^{\acute{\alpha}}\mathbf{e}_{\acute{\epsilon}}{}^{\grave{\epsilon}}(\gamma_{\beta})^{\acute{\epsilon}\grave{\tau}}(\mathbf{e}_{\grave{\tau}}{}^{\grave{\tau}}\mathbf{D}_{\tau}\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}+\mathbf{e}_{\acute{\epsilon}}{}^{\acute{\epsilon}}\mathbf{D}_{\tau}\mathbf{e}_{\grave{\tau}}{}^{\grave{\tau}}),\end{aligned}$$

where $l^{\alpha}_{\alpha}=(\gamma_{\acute{\alpha}\grave{\alpha}})^{\alpha}$, from which one follows

$$(\gamma_{\alpha})^{\acute{\mu}\grave{\nu}}(\gamma^{\beta})_{\acute{\alpha}\grave{\beta}}\Gamma^{\alpha}_{\gamma\beta}=(\gamma^{\beta})_{\acute{\alpha}\grave{\beta}}\mathbf{D}_{\gamma}(\gamma_{\beta})^{\acute{\mu}\grave{\nu}}+\mathbf{e}_{\grave{\beta}}{}^{\grave{\nu}}\varpi^{\acute{\mu}}{}_{\gamma\acute{\alpha}}+\mathbf{e}_{\acute{\alpha}}{}^{\acute{\mu}}\varpi^{\grave{\nu}}{}_{\gamma\grave{\beta}}.$$

Contracting the last expression on $\grave{\nu}$ and $\grave{\beta}$ and using an orthonormalized d-spinor basis when $\varpi^{\boldsymbol{\beta}}{}_{\gamma\acute{\beta}}=0$ (a consequence from (26)), we have

$$\varpi^{\acute{\mu}}{}_{\gamma\acute{\alpha}}=\frac{1}{\widetilde{k}_{(n)}+\widetilde{k}_{(m)}}(\Gamma^{\acute{\mu}\grave{\beta}}{}_{\boldsymbol{\gamma}\,\acute{\alpha}\grave{\beta}}-(\gamma^{\beta})_{\acute{\alpha}\grave{\beta}}\mathbf{D}_{\gamma}(\gamma_{\beta})^{\acute{\mu}\grave{\beta}}), \tag{29}$$

where

$$\Gamma^{\acute{\mu}\grave{\beta}}_{\boldsymbol{\gamma}\,\acute{\alpha}\grave{\beta}}=(\gamma_\alpha)^{\acute{\mu}\grave{\beta}}(\gamma^\beta)_{\acute{\alpha}\grave{\beta}}\Gamma^\alpha_{\gamma\beta}. \tag{30}$$

The *d*-spinor connection (30) can be defined by various type of *d*-connections, inclusively, by the canonical one, see Ref. 1. Such formulas can be applied on Clifford algebroid $\mathcal{C}(E)\doteq(\mathbb{C}l(E),{}^s[\cdot,\cdot],{}^s\rho)$ or on a Clifford *N*-algebroid $\mathcal{C}(v\mathbf{V})\doteq(\mathbb{C}l(v\mathbf{V}),{}^s[\cdot,\cdot],{}^s\rho)$. We have to change the *v*-derivatives into anchored ones, $\partial/\partial y^a\rightarrow\rho^i_a\partial/\partial x^a$, or in *N*-adapted form, $e_a\rightarrow\hat{\rho}^j_a e_j$, and put the results in formulas (29) and (30). As a result, one defines a canonical covariant spinor differential calculus, adapted to the *N*-connection structure, acting on the set of sections Sec(**E**) or Sec($v\mathbf{V}$).

3. D-spinors of curvature and torsion on N-anholonomic manifolds

The *d*-tensor indices of the commutator $\Delta_{\alpha\beta}$ can be transformed into *d*-spinor ones:

$$\Box_{\acute{\alpha}\grave{\beta}}=(\gamma^{\alpha\beta})_{\acute{\alpha}\grave{\beta}}\Delta_{\alpha\beta}=(\Box_{\hat{\imath}\hat{\imath}},\Box_{\acute{a}\grave{a}}), \tag{31}$$

with *h*- and *v*-components,

$$\Box_{\hat{\imath}\hat{\imath}}=(\gamma^{\alpha\beta})_{\hat{\imath}\hat{\imath}}\Delta_{\alpha\beta},\quad\text{and}\quad\Box_{\acute{a}\grave{a}}=(\gamma^{\alpha\beta})_{\acute{a}\grave{a}}\Delta_{\alpha\beta},$$

being symmetric or antisymmetric in dependence of corresponding values of dimensions *n* and *m*. Considering the actions of operator (31) on *d*-spinors $\pi^{\acute{\gamma}}$ and $\mu_{\acute{\gamma}}$ we introduce the *d*-spinor curvature $X^{\acute{\gamma}}_{\acute{\tau}\acute{\alpha}\grave{\beta}}$ satisfying

$$\Box_{\acute{\alpha}\grave{\beta}}\pi^{\acute{\gamma}}=X^{\acute{\gamma}}_{\acute{\tau}\acute{\alpha}\grave{\beta}}\pi^{\acute{\tau}} \tag{32}$$

and

$$\Box_{\acute{\alpha}\grave{\beta}}\mu_{\acute{\gamma}}=X^{\acute{\tau}}_{\acute{\gamma}\acute{\alpha}\grave{\beta}}\mu_{\acute{\tau}}.$$

The gravitational *d*-spinor $\Psi_{\acute{\tau}\acute{\gamma}\acute{\alpha}\grave{\beta}}$ is defined by a corresponding symmetrization of *d*-spinor indices:

$$\Psi_{\acute{\tau}\acute{\gamma}\acute{\alpha}\grave{\beta}}=X_{(\acute{\tau}\acute{\gamma}\acute{\alpha})\grave{\beta}}. \tag{33}$$

We note that *d*-spinor tensors $X^{\acute{\tau}}_{\acute{\gamma}\acute{\alpha}\grave{\beta}}$ and $\Psi_{\acute{\tau}\acute{\gamma}\acute{\alpha}\grave{\beta}}$ are transformed into similar two-spinor objects if the *N*-connection vanishes and the spinor constructions are defined in global form on $\mathbf{V}$.[19,20]

Putting $\mathbf{e}_{\acute{\gamma}}{}^{\acute{\gamma}}$ instead of $\mu_{\acute{\gamma}}$ in (32) and using (33), we can express, respectively, the curvature and gravitational *d*-spinors as

$$X_{\acute{\gamma}\acute{\delta}\acute{\alpha}\grave{\beta}}=\mathbf{e}_{\acute{\gamma}\acute{\tau}}\Box_{\acute{\alpha}\grave{\beta}}\mathbf{e}_{\acute{\delta}}{}^{\acute{\tau}}$$

and

$$\Psi_{\acute{\delta}\acute{\gamma}\acute{\alpha}\grave{\beta}}=\mathbf{e}_{\acute{\delta}(\acute{\tau}}\Box_{\acute{\alpha}|\grave{\beta}|}\mathbf{e}_{\acute{\gamma})}{}^{\acute{\tau}}$$

where we omit symmetrization on $\grave{\beta}$.

The *d*-spinor torsion $T^{\acute{\gamma}\grave{\gamma}}_{\acute{\alpha}\grave{\beta}}$ is defined by using the *d*-spinor commutator (31) and

$$\Box_{\acute{\alpha}\grave{\beta}}f=T^{\acute{\gamma}\grave{\gamma}}_{\acute{\alpha}\grave{\beta}}\nabla_{\acute{\gamma}\grave{\gamma}}f.$$

The *d*-spinor components $R^{\acute{\delta}\grave{\delta}}{}_{\acute{\gamma}\grave{\gamma}\acute{\alpha}\grave{\beta}}$ of the curvature *d*-tensor $R^\delta{}_{\gamma\alpha\beta}$ can be computed by using relations (30), (31), and (33) and

$$(\Box_{\acute{\alpha}\grave{\beta}} - T^{\acute{\gamma}\grave{\gamma}}{}_{\acute{\alpha}\grave{\beta}}\nabla_{\acute{\gamma}\grave{\gamma}})V^{\acute{\delta}\grave{\delta}} = R^{\acute{\delta}\grave{\delta}}{}_{\acute{\gamma}\grave{\gamma}\acute{\alpha}\grave{\beta}}V^{\acute{\gamma}\grave{\gamma}}, \tag{34}$$

here d-vector $V^{\acute{\gamma}\grave{\gamma}}$ is considered as a product of d-spinors, i.e., $V^{\acute{\gamma}\grave{\gamma}}=\nu^{\acute{\gamma}}\mu^{\grave{\gamma}}$. We find

$$R^{\acute{\delta}\grave{\delta}}{}_{\acute{\gamma}\grave{\gamma}\acute{\alpha}\grave{\beta}} = (X^{\acute{\delta}}{}_{\acute{\gamma}\acute{\alpha}\grave{\beta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}}\boldsymbol{\varpi}^{\acute{\delta}}{}_{\hat{\tau}\hat{\tau}\acute{\gamma}})\mathbf{e}_{\grave{\gamma}}{}^{\grave{\delta}} + (X^{\grave{\delta}}{}_{\grave{\gamma}\acute{\alpha}\grave{\beta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}}\boldsymbol{\varpi}^{\grave{\delta}}{}_{\hat{\tau}\hat{\tau}\grave{\gamma}})\mathbf{e}_{\acute{\gamma}}{}^{\acute{\delta}}.$$

It is convenient to use this d-spinor expression for the curvature d-tensor in order to get the d-spinor components of the Ricci d-tensor,

$$R_{\acute{\gamma}\grave{\gamma}\acute{\alpha}\grave{\beta}} = R^{\acute{\delta}\grave{\delta}}{}_{\acute{\gamma}\grave{\gamma}\acute{\alpha}\grave{\beta}\acute{\delta}\grave{\delta}} = X^{\acute{\delta}}{}_{\acute{\gamma}\acute{\alpha}\grave{\beta}\acute{\delta}\acute{\gamma}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}\acute{\gamma}}\boldsymbol{\varpi}^{\acute{\delta}}{}_{\hat{\tau}\hat{\tau}\acute{\gamma}} + X^{\grave{\delta}}{}_{\grave{\gamma}\acute{\alpha}\grave{\beta}\grave{\gamma}\grave{\delta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}\acute{\gamma}\grave{\delta}}\boldsymbol{\varpi}^{\grave{\delta}\hat{\tau}\hat{\tau}\grave{\gamma}}{}_{\hat{\tau}\hat{\tau}\grave{\gamma}} \tag{35}$$

and this d-spinor decomposition of the scalar curvature $\overleftarrow{R}=R^{\acute{\alpha}\grave{\beta}}{}_{\acute{\alpha}\grave{\beta}}$,

$$\overleftarrow{R} = R^{\acute{\delta}\grave{\delta}\acute{\alpha}\grave{\beta}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}\grave{\delta}} = X^{\acute{\delta}\acute{\alpha}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}}{}^{\grave{\beta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}}{}^{\grave{\beta}}\boldsymbol{\varpi}^{\acute{\delta}\hat{\tau}\hat{\tau}\acute{\alpha}} + X^{\grave{\delta}\grave{\beta}\acute{\alpha}}{}_{\acute{\alpha}\grave{\beta}\grave{\delta}} + T^{\hat{\tau}\hat{\tau}\acute{\alpha}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}}\boldsymbol{\varpi}^{\grave{\delta}\grave{\beta}}{}_{\hat{\tau}\hat{\tau}}.$$

Finally, we write down the d-spinor components of the Einstein d-tensor $\mathbf{G}_{\gamma\beta}$,

$$\begin{aligned}\mathbf{G}_{\acute{\gamma}\grave{\gamma}\acute{\beta}\grave{\beta}} &= X^{\acute{\delta}}{}_{\acute{\gamma}\acute{\beta}\grave{\beta}\acute{\delta}\grave{\gamma}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\beta}\grave{\beta}\acute{\delta}\grave{\gamma}}\boldsymbol{\varpi}^{\acute{\delta}}{}_{\hat{\tau}\hat{\tau}\acute{\gamma}} + X^{\grave{\delta}}{}_{\grave{\gamma}\acute{\beta}\grave{\beta}\grave{\gamma}\grave{\delta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\beta}\grave{\beta}\acute{\gamma}\grave{\delta}}\boldsymbol{\varpi}^{\grave{\delta}}{}_{\hat{\tau}\hat{\tau}\grave{\gamma}} \\ &\quad - \frac{1}{2}\boldsymbol{\epsilon}_{\acute{\gamma}\grave{\beta}}\boldsymbol{\epsilon}_{\acute{\beta}\grave{\gamma}}[X^{\acute{\delta}\acute{\alpha}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}}{}^{\grave{\beta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}\acute{\delta}}{}^{\grave{\beta}}\boldsymbol{\varpi}^{\acute{\delta}}{}_{\hat{\tau}\hat{\tau}}{}^{\acute{\alpha}} + X^{\grave{\delta}\grave{\beta}}{}_{\acute{\alpha}\grave{\beta}}{}^{\acute{\alpha}}{}_{\grave{\delta}} + T^{\hat{\tau}\hat{\tau}}{}_{\acute{\alpha}\grave{\beta}}{}^{\acute{\alpha}}{}_{\grave{\delta}}\boldsymbol{\varpi}^{\grave{\delta}}{}_{\hat{\tau}\hat{\tau}}{}^{\grave{\beta}}].\end{aligned} \tag{36}$$

It should be noted that further reductions of (35) and (36) depend on dimensions n and m of the, respectively, h- and v-subspaces, and that the symmetry properties are defined by the $\boldsymbol{\epsilon}$-objects. On Clifford N-algebroids, such formulas have to be considered for anchored v-derivatives (15) and (7) (for d-spinor considerations, we have to apply spinor anchors (10) and (12)), for instance, in the case of canonical d-connections and their spinor variants (29).

III. FIELD EQUATIONS AND LIE ALGEBROIDS

Lie algebroid structures can be modeled as spacetime geometries with generalized symmetries (defined by anchors and Lie algebra commutators and nontrivial N-connection structure).[2] It is possible to extend the constructions on Clifford N-algebroids by introducing spinor variables. In this section we shall analyze the basic field equations for gravitational and matter field interactions modeled on N-anholonomic manifolds and Clifford N-algebroids.

A. The Dirac operator on *N*-anholonomic spaces

The aim of this section is to elucidate the possibility of definition of Dirac operators for general N-anholonomic manifolds. It should be noted that such geometric constructions depend on the type of linear connections which are used for the complete definition of the Dirac operator. They are metric compatible and N-adapted if the canonical d-connection is used (we can similarly use any of its deformations resulting in a metric compatible d-connection).

1. Noholonomic vielbeins and spin d-connections

For a local dual coordinate basis $e^{\underline{i}}\doteq \mathrm{d}x^{\underline{i}}$ on a manifold M, $\dim M=n$, we may respectively, introduce certain classes of orthonormalized vielbeins and the N-adapted vielbeins (depending both on the base coordinates $x\doteq x^i$ and some "fiber" coordinates $y\doteq y^a$)

$$e^{\hat{i}} \doteq e^{\hat{i}}_{\underline{i}}(x,y)e^{\underline{i}}, \quad e^{i} \doteq e^{i}_{\underline{i}}(x,y)e^{\underline{i}}, \tag{37}$$

where

$$g^{\underline{ij}}(x,y)e^{\hat{i}}_{\underline{i}}(x,y)e^{\hat{j}}_{\underline{j}}(x,y)=\delta^{\hat{i}\hat{j}},\quad g^{\underline{ij}}(x,y)e^{i}_{\underline{i}}(x,y)e^{j}_{\underline{j}}(x,y)=g^{ij}(x,y).$$

We define the algebra of Dirac's gamma matrices (in brief, h-gamma matrices defined by self-adjoint matrices $M_k(\mathbb{C})$ where $k=2^{n/2}$ is the dimension of the irreducible representation of $\mathbb{C}l(M)$ for even dimensions, or of $\mathbb{C}l(M)^+$ for odd dimensions) from the relation

$$\gamma^{\hat{j}}\gamma^{\hat{j}}+\gamma^{\hat{j}}\gamma^{\hat{j}}=2\delta^{\hat{i}\hat{j}}\mathbb{I}. \tag{38}$$

We can consider the action of $\mathrm{d}x^i\in\mathbb{C}l(M)$ on a spinor $\psi\in S$ via representations

$$^{-}c(\mathrm{d}x^{\hat{i}})\doteq\gamma^{\hat{j}},\quad {}^{-}c(\mathrm{d}x^{i})\psi\doteq\gamma^{j}\psi\equiv e^{i}_{\ \hat{i}}\gamma^{\hat{j}}\psi. \tag{39}$$

For any type of spaces T_xM, TM or $\mathbf{V}$ possessing a local (in any point) or global fibered structure and enabled with a N-connection structure, we can introduce similar definitions of the gamma matrices following algebraic relations and metric structures on fiber subspaces,

$$e^{\hat{a}}\doteq e^{\hat{a}}_{\underline{a}}(x,y)e^{\underline{a}},\quad e^{a}\doteq e^{a}_{\underline{a}}(x,y)e^{\underline{a}}, \tag{40}$$

where

$$g^{\underline{ab}}(x,y)e^{\hat{a}}_{\underline{a}}(x,y)e^{\hat{b}}_{\underline{b}}(x,y)=\delta^{\hat{a}\hat{b}},\quad g^{\underline{ab}}(x,y)e^{a}_{\underline{a}}(x,y)e^{b}_{\underline{b}}(x,y)=h^{ab}(x,y).$$

Similarly, we define the algebra of Dirac's matrices related to typical fibers (in brief, v-gamma matrices described by self-adjoint matrices $M'_k(\mathbb{C})$ where $k'=2^{m/2}$ is the dimension of the irreducible representation of $\mathbb{C}l(F)$ for even dimensions, or of $\mathbb{C}l(F)^+$ for odd dimensions, of the typical fiber F) from the relation

$$\gamma^{\hat{a}}\gamma^{\hat{b}}+\gamma^{\hat{b}}\gamma^{\hat{a}}=2\delta^{\hat{a}\hat{b}}\mathbb{I}. \tag{41}$$

The formulas (38) and (41) are respectively, the h- and v-components of relation (18) (with redefined coefficients which is more convenient for further constructions). The action of $\mathrm{d}y^a\in\mathbb{C}l(F)$ on a spinor ${}^{\star}\psi\in{}^{\star}S$ is considered via representations

$$^{\star}c(\mathrm{d}y^{\hat{a}})\doteq\gamma^{\hat{a}},\quad {}^{\star}c(\mathrm{d}y^{a})^{\star}\psi\doteq\gamma^{a\star}\psi\equiv e^{a}_{\ \hat{a}}\gamma^{\hat{a}\star}\psi. \tag{42}$$

We note that in additionally to formulas (39) and (42) we may write, respectively,

$$c(\mathrm{d}x^{\underline{i}})\psi\doteq\gamma^{\underline{i}}\psi\equiv e^{\underline{i}}_{\ i}\gamma^{\hat{j}}\psi,\quad c(\mathrm{d}y^{\underline{a}})^{\star}\psi\doteq\gamma^{\underline{a}\star}\psi\equiv e^{\underline{a}}_{e^{a}\ \hat{a}}\gamma^{\hat{a}\star}\psi$$

but such operators are not adapted to the N-connection structure.

A more general gamma matrix calculus with distinguished gamma matrices (in brief, d-gamma matrices) can be elaborated for any N-anholonomic manifold $\mathbf{V}$ provided with d-metric structure $\mathbf{g}=[g,{}^{\star}g]$ and for d-spinors $\breve{\psi}\doteq(\psi,{}^{\star}\psi)\in\mathbf{S}\doteq(S,{}^{\star}S)$. First, we should write in a unified form, related to a d-metric (1), formulas (37) and (40),

$$e^{\ \hat{\alpha}}\doteq e^{\hat{\alpha}}_{\underline{a}}(u)e^{\underline{\alpha}},\quad e^{\alpha}\doteq e^{\alpha}_{\ \underline{a}}(u)e^{\underline{\alpha}}, \tag{43}$$

where

$$g^{\underline{\alpha\beta}}(u)e^{\hat{\alpha}}_{\ \underline{\alpha}}(u)e^{\hat{\beta}}_{\ \underline{\beta}}(u)=\delta^{\hat{\alpha}\hat{\beta}},\quad g^{\underline{\alpha\beta}}(u)e^{\alpha}_{\ \underline{\alpha}}(u)e^{\beta}_{\ \underline{\beta}}(u)=g^{\alpha\beta}(u).$$

The second step is to consider gamma d-matrix relations (unifying (38) and (41))

$$\gamma^{\hat{\alpha}}\gamma^{\hat{\beta}}+\gamma^{\hat{\beta}}\gamma^{\hat{\alpha}}=2\delta^{\hat{\alpha}\hat{\beta}}\mathbb{I}, \tag{44}$$

with the action of $\mathrm{d}u^{\alpha}\in\mathbb{C}l(\mathbf{V})$ on a d-spinor $\breve{\psi}\in\mathbf{S}$ resulting in distinguished irreducible representations (unifying (39) and (42))

$$\mathbf{c}(\mathrm{d}u^{\hat{\alpha}})\doteq\gamma^{\hat{\alpha}},\quad \mathbf{c}=(\mathrm{d}u^{\alpha})\breve{\psi}\doteq\gamma^{\alpha}\breve{\psi}\equiv e^{\alpha}_{\ \hat{\alpha}}\gamma^{\hat{\alpha}}\breve{\psi}, \tag{45}$$

which allows one to write

$$\gamma^{\alpha}(u)\gamma^{\beta}(u)+\gamma^{\beta}(u)\gamma^{\alpha}(u)=2g^{\alpha\beta}(u)\mathbb{I}. \tag{46}$$

In the canonical representation, we can write in irreducible form $\breve{\gamma}\doteq\gamma\oplus{}^{\star}\gamma$ and $\breve{\psi}\doteq\psi\oplus{}^{\star}\psi$, for instance, by using block type of h- and v-matrices, or, writing alternatively as couples of gamma and/or h- and v-spinor objects written in N-adapted form,

$$\gamma^{\alpha}\doteq(\gamma^{i},\gamma^{a}),\quad \breve{\psi}\doteq(\psi,{}^{\star}\psi). \tag{47}$$

The decomposition (46) holds with respect to a N-adapted vielbein (3). We also note that for a spinor calculus, the indices of spinor objects should be treated as abstract spinorial ones possessing certain reducible, or irreducible, properties depending on the space dimension. For simplicity, we shall consider that spinors like $\breve{\psi},\psi,{}^{\star}\psi$ and all types of gamma objects can be enabled with corresponding spinor indices running certain values which are different from the usual coordinate space indices.

The spin connection ∇^{S} for the Riemannian manifolds is induced by the Levi-Civita connection ${}^{\nabla}\Gamma$,

$$\nabla^{S}\doteq d-\frac{1}{4}{}^{\nabla}\Gamma^{i}_{jk}\gamma_{i}\gamma^{j}\mathrm{d}x^{k}. \tag{48}$$

On N-anholonomic spaces, it is possible to define spin connections which are N-adapted by replacing the Levi-Civita connection by any d-connection.

The canonical spin d-connection is defined by the canonical d-connection,

$$\hat{\nabla}^{\mathbf{S}}\doteq\delta-\frac{1}{4}\hat{\mathbf{\Gamma}}^{\alpha}_{\ \beta\mu}\gamma_{\alpha}\gamma^{\beta}\delta u^{\mu}, \tag{49}$$

where the absolute differential δ acts in N-adapted form resulting in one-forms decomposed with respect to N-elongated differentials $\delta u^{\mu}=(\mathrm{d}x^{i},\delta y^{a})$ (2).

We note that the canonical spin d-connection $\hat{\nabla}^{\mathbf{S}}$ is metric compatible and contains nontrivial d-torsion coefficients induced by the N-anholonomy relations. It is possible to introduce more general spin d-connections $\mathbf{D}^{\mathbf{S}}$ by using the same formula (49) but for arbitrary metric compatible d-connection $\mathbf{\Gamma}^{\alpha}_{\beta\mu}$. For the spaces provided with generic off-diagonal metric structure (1) on a N-anholonomic manifold, there is a canonical spin d-connection (49) induced by the off-diagonal metric coefficients with nontrivial N^{a}_{i} and associated nonholonomic frames in gravity theories.

In a particular case of N-anholonomic manifolds of even dimensions, we can define, for instance, the canonical spin d-connections for a local modeling of a tangent bundle space with the canonical d-connection $\hat{\mathbf{\Gamma}}^{\gamma}_{\alpha\beta}=(\hat{L}^{i}_{jk},\hat{B}^{i}_{jk})$. The N-connection structure N^{j}_{i} states a global h- and v-splitting of the spin d-connection operators, for instance,

$$\hat{\nabla}\doteq\delta-\frac{1}{4}\hat{L}^{i}_{\ jk}\gamma_{i}\gamma^{j}\mathrm{d}x^{k}-\frac{1}{4}\hat{B}^{a}_{\ bc}\gamma_{a}\gamma^{b}\delta y^{c}. \tag{50}$$

So, any spin d-connection is a d-operator with conventional splitting of action like $\nabla^{(\mathbf{S})}\equiv({}^{-}\nabla^{(\mathbf{S})},{}^{\star}\nabla^{(\mathbf{S})})$, or $\nabla\equiv({}^{-}\nabla,{}^{\star}\nabla)$. For instance, for $\hat{\nabla}\equiv({}^{-}\hat{\nabla},{}^{\star}\hat{\nabla})$, the operators ${}^{-}\hat{\nabla}$ and ${}^{\star}\hat{\nabla}$ act, respectively, on a h-spinor ψ as

$$^{-}\hat{\nabla}\psi \doteq \mathrm{d}x^i \frac{\delta\psi}{\partial x^i} - \mathrm{d}x^k \frac{1}{4}\hat{L}^i_{jk}\gamma_i\gamma^j\psi \tag{51}$$

and

$$^{\star}\hat{\nabla}\psi \doteq \delta y^a \frac{\partial\psi}{\partial y^a} - \delta y^c \frac{1}{4}\hat{B}^a_{bc}\gamma_a\gamma^b\psi$$

being defined by the canonical d-connection, which (in its turn) is completely defined by $N^j_i(x,y)$ and $g_{ij}(x,y)$.

The operators (51) can be adapted to the Lie algebroid structure by anchoring the partial v-derivatives. For instance,

$$\frac{\delta\psi}{\partial x^i}(x^k,y^b(x^j)) = \frac{\partial\psi}{\partial x^i} - N^a_i\frac{\partial\psi}{\partial y^a} = \left(\frac{\partial\psi}{\partial x^i} - N^a_i\rho^k_a(x^j)\frac{\partial\psi}{\partial x^k}\right) = \left(\frac{\partial\psi}{\partial x^i} - {}^{\rho}N^k_i\frac{\partial\psi}{\partial x^k}\right)(x^k,y^b(x^j))$$

where the anchor ρ^k_a (7) induces a N-connection ${}^{\rho}N^k_i \doteq N^a_i\rho^k_a$. We can also perform a N-adapted Clifford algebroid calculus by using the "boldface" algebroid $\hat{\rho}^j_a$ (15) with explicit dependence on variables y^b,

$$\frac{\delta\psi}{\partial x^i}(x^k,y^b) = \frac{\partial\psi}{\partial x^i} - N^a_i e_a\psi = \left(\frac{\partial\psi}{\partial x^i} - N^a_i\hat{\rho}^k_a\frac{\partial\psi}{\partial x^k}\right) = \left(\frac{\partial\psi}{\partial x^i} - {}^{\rho}\hat{N}^k_i\frac{\partial\psi}{\partial x^k}\right)$$

for ${}^{\rho}\hat{N}^k_i = N^a_i\hat{\rho}^k_a$. Such anchoring of partial/N-elongated derivatives has to be considered for the canonical d-connection $\hat{L}^i_{jk}$ and $\hat{B}^a_{bc}$.

2. Dirac d-operators

We consider a vector bundle $\mathbf{E}$ on an N-anholonomic manifold M (with two compatible N-connections defined as h- and v-splittings of $T\mathbf{E}$ and TM)). A d-connection

$$\mathcal{D}:\mathrm{Sec}^{\infty}(\mathbf{E}) \to \mathrm{Sec}^{\infty}(\mathbf{E}) \otimes \Omega^1(M)$$

preserves by parallelism splitting of the tangent total and base spaces and satisfy the Leibniz condition

$$\mathcal{D}(f\sigma) = f(\mathcal{D}\sigma) + \delta f \otimes \sigma$$

for any $f \in C^{\infty}(M)$, and $\sigma \in \mathrm{Sec}^{\infty}(\mathbf{E})$ and δ defining an N-adapted exterior calculus by using N-elongated operators (3) and (2) which emphasize d-forms instead of usual forms on M, with the coefficients taking values in $\mathbf{E}$.

The metricity and Leibniz conditions for $\mathcal{D}$ are written, respectively,

$$\mathbf{g}(\mathcal{D}\mathbf{X},\mathbf{Y}) + \mathbf{g}(\mathbf{X},\mathcal{D}\mathbf{Y}) = \delta[\mathbf{g}(\mathbf{X},\mathbf{Y})], \tag{52}$$

for any $\mathbf{X},\mathbf{Y} \in \chi(M)$, and

$$\mathcal{D}(\sigma\beta) \doteq \mathcal{D}(\sigma)\beta + \sigma\mathcal{D}(\beta), \tag{53}$$

for any $\sigma,\beta \in \mathrm{Sec}^{\infty}(\mathbf{E})$.

For local computations, we may define the corresponding coefficients of the geometric d-objects and write

$$\mathcal{D}\sigma_{\check{\beta}} \doteq \mathbf{\Gamma}^{\check{\alpha}}_{\check{\beta}\mu}\sigma_{\check{\alpha}} \otimes \delta u^{\mu} = \mathbf{\Gamma}^{\check{\alpha}}_{\check{\beta}i}\sigma_{\check{\alpha}} \otimes \mathrm{d}x^i + \mathbf{\Gamma}^{\check{\alpha}}_{\check{\beta}a}\sigma_{\check{\alpha}} \otimes \delta y^a,$$

where fiber "inverse-caret" indices, in their turn, may split $\check{\alpha} \doteq (\check{i},\check{a})$ if any N-connection structure is defined on $T\mathbf{E}$. For some constructions of particular interest, we can take $\mathbf{E} = T^*\mathbf{V}$, $= T^*V_{(g)}$

and/or any Clifford d-algebra $\mathbf{E}=\mathbb{C}l(\mathbf{V}),\mathbb{C}l(V_{(g)}),\ldots$ with a corresponding treating of "acute" indices to d-tensor and/or d-spinor type as well when the d-operator $\mathcal{D}$ transforms into respective d-connection $\mathbf{D}$ and spin d-connections $\hat{\nabla}^{\mathbf{S}}$ (49), $\hat{\nabla}^{(g)}\ldots$. All such, adapted to the N-connections, computations are similar for both N-anholonomic (co) vector and spinor bundles.

The respective actions of the Clifford d-algebra and the Clifford-Lagrange algebra can be transformed into maps $\mathrm{Sec}^{\infty}(\mathbf{S})\otimes\mathrm{Sec}(\mathbb{C}l(\mathbf{V}))$ and $\mathrm{Sec}^{\infty}(S_{(g)})\otimes\mathrm{Sec}(\mathbb{C}l(V_{(g)}))$ to $\mathrm{Sec}^{\infty}(\mathbf{S})$ and, respectively, $\mathrm{Sec}^{\infty}(S_{(g)})$ by considering maps of type (39) and (45)

$$\hat{\mathbf{c}}(\breve{\psi}\otimes\mathbf{a})\doteqdot\mathbf{c}(\mathbf{a})\breve{\psi},\quad \hat{c}(\psi\otimes a)\doteqdot c(a)\psi.$$

Definition 3.1: *The Dirac d-operator* (*or Dirac N-anholonomic operator*) *on a spin N-anholonomic manifold* $(\mathbf{V},\mathbf{S},J)$ (*or on a spin manifold* $(M_{(g)},S_{(g)},J)$) *is defined*

$$\mathbb{D}\doteqdot -i(\hat{\mathbf{c}}\circ\nabla^{\mathbf{S}})$$

$$=({}^{-}\mathbb{D}=-i({}^{-}\hat{c}\circ{}^{-}\nabla^{\mathbf{S}}),{}^{\star}\mathbb{D}=-\mathbf{i}({}^{\star}\hat{c}\circ{}^{\star}\nabla^{\mathbf{S}})) \tag{54}$$

$$({}_{(g)}\mathbb{D}\doteqdot -i(\hat{c}\circ\nabla^{(g)}))$$

$$=({}_{(g)}{}^{-}\mathbb{D}=-i({}^{-}\hat{c}\circ{}^{-}\nabla^{(g)}),{}^{\star}_{(g)}\mathbb{D}=-i({}^{\star}\hat{c}\circ{}^{\star}\nabla^{(g)})). \tag{55}$$

Such N-adapted Dirac d-operators are called canonical and denoted $\hat{\mathbb{D}}=({}^{-}\hat{\mathbb{D}},{}^{-\star}\hat{\mathbb{D}})$ $({}_{(g)(g)}\hat{\mathbb{D}}=({}_{(g)}{}^{-}\hat{\mathbb{D}},{}^{\star}_{(g)}\hat{\mathbb{D}}))$ *if they are defined for the canonical d-connection and respective spin d-connection* (49).

Now we can formulate the

Theorem 3.1: *Let* $(\mathbf{V},\mathbf{S},J)$ $((M_{(g)},S_{(g)},J)$ *be a spin N-anholonomic manifold. There is the canonical Dirac d-operator* (*Dirac N-anholonomic operator*) *defined by the almost Hermitian spin d-operator*

$$\hat{\nabla}^{\mathbf{S}}:\mathrm{Sec}^{\infty}(\mathbf{S})\to\mathrm{Sec}^{\infty}(\mathbf{S})\otimes\Omega^{1}(\mathbf{V})$$

(*N-anholonomic spin operator*

$$\hat{\nabla}^{(g)}:\mathrm{Sec}^{\infty}(S_{(g)})\to\mathrm{Sec}^{\infty}(S_{(g)})\otimes\Omega^{1}(M_{(g)})$$

commuting with J and satisfying the conditions

$$(\hat{\nabla}^{\mathbf{S}}\breve{\psi}|\breve{\phi})+(\breve{\psi}|\hat{\nabla}^{\mathbf{S}}\breve{\phi})=\delta(\breve{\psi}|\breve{\phi}) \tag{56}$$

and

$$\hat{\nabla}^{\mathbf{S}}(\mathbf{c}(\mathbf{a})\breve{\psi})=\mathbf{c}(\hat{\mathbf{D}}\mathbf{a})\breve{\psi}+\mathbf{c}(\mathbf{a})\hat{\nabla}^{\mathbf{S}}\breve{\psi}$$

for $\mathbf{a}\in\mathbb{C}l(\mathbf{V})$ *and* $\breve{\psi}\in\mathrm{Sec}^{\infty}(\mathbf{S})$,

$$((\hat{\nabla}^{(g)}\breve{\psi}|\breve{\phi})+(\breve{\psi}|\hat{\nabla}^{(g)}\breve{\phi})=\delta(\breve{\psi}|\breve{\phi}) \tag{57}$$

and

$$\hat{\nabla}^{(g)}(\mathbf{c}(\mathbf{a})\breve{\psi})=\mathbf{c}(\hat{\mathbf{D}}\mathbf{a})\breve{\psi}+\mathbf{c}(\mathbf{a})\hat{\nabla}^{(g)}\breve{\psi}$$

for $\mathbf{a}\in\mathbb{C}l(M_{(g)})$ *and* $\breve{\psi}\in\mathrm{Sec}^{\infty}(S_{(g)})$ *determined by the metricity* (52) *and Leibnitz* (53) *conditions.*[22,23]

Proof: We sketch the main idea of such a proof being similar to that given in Ref. 24, Theorem 9.8, for the Levi-Civita connection, see also Ref. 25. In our case, we have to extend the constructions for d-metrics and canonical d-connections by applying N-elongated operators for differentials and partial derivatives and distinguishing the formulas into h- and v-irreducible components. □

The canonical Dirac d-operator has very similar properties for spin N-anholonomic manifolds and spin Lagrange, or Finsler spaces.[11–13,7]

B. Field equations on *N*-anholonomic manifolds

The general idea is to formulate such equations with respect to a nonholonomic frame on (pseudo) Riemann–Cartan space. Then the constructions are N-adapted by considering N-elongated frames. For Lie/Clifford N-algebroid structures, we have to anchor the formulas.

1. Scalar field on N-anholonomic manifolds

Let $\varphi(u)=(\varphi_1(u),\varphi_2(u);\ldots,\varphi_k(u))$ be a complex k-component scalar field of mass μ on a N-anholonomic manifold $\mathbf{V}$. The d-covariant generalization of the conformally invariant (in the massless case) scalar field equation[19,20] can be defined by using the d'Alambert operator $\Box=\mathbf{D}^{\alpha}\mathbf{D}_{\alpha}$, where $\mathbf{D}_{\alpha}$ is a metric compatible d-connection,

$$\left(\Box+\frac{n+m-2}{4(n+m-1)}\overleftarrow{R}+\mu^2\right)\varphi(u)=0. \tag{58}$$

We have to elongate the covariant d-operator, $\check{D}_{\alpha}=\mathbf{D}_{\alpha}+ieA_{\alpha}$, and take into account the d-vector current

$$J^{(0)}_{\alpha}(u)=i((\overline{\varphi}(u)\mathbf{D}_{\alpha}\varphi(u)-\mathbf{D}_{\alpha}\overline{\varphi}(u))\varphi(u))$$

if there are considered interactions with the electromagnetic field (d-vector potential A_{α}), where e is the electromagnetic constant, and a charged scalar field φ. Equation (58) is just the Euler equations for the Lagrangian

$$\mathcal{L}^{(0)}(u)=\sqrt{|g|}\left[\mathbf{g}^{\alpha\beta}e_{\alpha}\overline{\varphi}(u)e_{\beta}\varphi(u)-\left(\mu^2+\frac{n+m-2}{4(n+m-1)}\right)\overline{\varphi}(u)\varphi(u)\right], \tag{59}$$

where $|g|=\det|\mathbf{g}_{\alpha\beta}|$ and $\mathbf{e}_{\alpha}$ is defined by (3), and must be anchored for Lie algebroid structures.

The N-adapted variations of the action with Lagrangian (59) on variables $\varphi(u)$ and $\overline{\varphi}(u)$ lead to the energy-momentum d-tensor,

$$E^{(0,c)}_{\alpha\beta}(u)=\mathbf{e}_{\alpha}\overline{\varphi}(u)\mathbf{e}_{\beta}\varphi(u)+\mathbf{e}_{\beta}\overline{\varphi}(u)\mathbf{e}_{\alpha}\varphi(u)-\frac{1}{\sqrt{|g|}}\mathbf{g}_{\alpha\beta}\mathcal{L}^{(0)}(u), \tag{60}$$

and a similar variation on the components of a d-metric (1) leads to a symmetric energy-momentum d-tensor,

$$E^{(0)}_{\alpha\beta}(u)=E^{(0,c)}_{(\alpha\beta)}(u)-\frac{n+m-2}{2(n+m-1)}[\mathbf{R}_{(\alpha\beta)}+\mathbf{D}_{(\alpha\mathbf{D}_{\beta)}}-\mathbf{g}_{\alpha\beta}\Box]\overline{\varphi}(u)\varphi(u). \tag{61}$$

We also conclude that the N-connection results in a nonequivalence of energy–momentum d-tensors (60) and (61), nonsymmetry of the Ricci tensor, non-vanishing of the d-covariant derivation of the Einstein d-tensor, $\mathbf{D}_{\alpha}\overleftarrow{\mathbf{G}}^{\alpha\beta}\neq 0$ and, in consequence, a corresponding modification of conservation laws on N-anholonomic manifolds.[27]

2. Proca equations

Let us consider a d-vector field $\varphi_\alpha(u)$ with mass μ^2 (Proca field) interacting with exterior gravitational field. From the Lagrangian

$$\mathcal{L}^{(1)}(u) = \sqrt{|\mathbf{g}|}\left[-\tfrac{1}{2}\overline{f}_{\alpha\beta}(u)f^{\alpha\beta}(u) + \mu^2\overline{\varphi}_\alpha(u)\varphi^\alpha(u)\right], \tag{62}$$

where

$$f_{\alpha\beta} = \mathbf{D}_\alpha\varphi_\beta - \mathbf{D}_\beta\varphi_\alpha,$$

one follows the Proca equations on N-anholonomic manifolds

$$\mathbf{D}_\alpha f^{\alpha\beta}(u) + \mu^2\varphi^\beta(u) = 0. \tag{63}$$

Equation (63) transforms into a first type constraints for $\beta=0$. Acting with $\mathbf{D}_\alpha$ on (63), for $\mu \neq 0$ we obtain second type constraints

$$\mathbf{D}_\alpha\varphi^\alpha(u) = 0. \tag{64}$$

Putting (64) into (63) we obtain second-order field equations with respect to φ_α:

$$\Box\varphi_\alpha(u) + \mathbf{R}_{\alpha\beta}\varphi^\beta(u) + \mu^2\varphi_\alpha(u) = 0. \tag{65}$$

Anchoring of derivatives has to be considered for the operators $\mathbf{D}_\alpha$ and (as a consequence) for $\Box$ and $\mathbf{R}_{\alpha\beta}$. The energy-momentum d-tensor and d-vector current following from the (65) can be written

$$E^{(1)}_{\alpha\beta}(u) = -\mathbf{g}^{\varepsilon\tau}(\overline{f}_{\beta\tau}f_{\alpha\varepsilon} + \overline{f}_{\alpha\varepsilon}f_{\beta\tau}) + \mu^2(\overline{\varphi}_\alpha\varphi_\beta + \overline{\varphi}_\beta\varphi_\alpha) - \frac{\mathbf{g}_{\alpha\beta}}{\sqrt{|\mathbf{g}|}}\mathcal{L}^{(1)}(u).$$

and

$$J^{(1)}_\alpha(u) = i(\overline{f}_{\alpha\beta}(u)\varphi^\beta(u) - \overline{\varphi}^\beta(u)f_{\alpha\beta}(u)).$$

For $\mu=0$ the d-tensor $f_{\alpha\beta}$ and the Lagrangian (62) are invariant with respect to gauge transforms of type

$$\varphi_\alpha(u) \to \varphi_\alpha(u) + \delta_\alpha\Lambda(u),$$

where $\Lambda(u)$ is a d-differentiable scalar function, and we obtain a variant of Maxwell theory on N-anholonomic manifolds.

3. Gravitons N-anholonomic backgrounds

Let us consider a massless d-tensor field $\mathbf{q}_{\alpha\beta}(u)$ as a small perturbation of the d-metric $\mathbf{g}_{\alpha\beta}(u)$. Considering, for simplicity, a torsionless background we have the Fierz–Pauli equations

$$\Box\mathbf{q}_{\alpha\beta}(u) + 2\mathbf{R}_{\tau\alpha\beta\nu}(u)\mathbf{q}^{\tau\nu}(u) = 0 \tag{66}$$

and d-gauge conditions

$$D_\alpha\mathbf{q}^\alpha_\beta(u) = 0, \quad \mathbf{q}(u) \equiv \mathbf{q}^\alpha_\beta(u) = 0, \tag{67}$$

where $\mathbf{R}_{\tau\alpha\beta\nu}(u)$ is curvature d-tensor (these formulas can be obtained by using a perturbation formalism with respect to $\mathbf{q}_{\alpha\beta}(u)$; in our case we must take into account the distinguishing of geometrical objects.

We note that we can rewrite d-tensor formulas (58)–(67) into similar d-spinor ones by considering spinor variables.

4. N-anholonomic Dirac equation

Let us denote the Dirac d-spinor field by $\psi(u)=(\psi^{\acute{\alpha}}(u))$ and consider as the generalized Lorentz transforms the group of automorphysm of the metric $g_{\hat{\alpha}\hat{\beta}}$ (for a N-adapted frame decomposition of d-metric). The d-covariant derivation of field $\psi(u)$ is written as

$$\overrightarrow{\nabla}_{\alpha}\psi=\left[\mathbf{e}_{\alpha}+\tfrac{1}{4}C_{\hat{\alpha}\hat{\beta}\hat{\gamma}}(u)l^{\hat{\alpha}}_{\alpha}(u)\gamma^{\hat{\beta}}\gamma^{\hat{\gamma}}\right]\psi, \tag{68}$$

where coefficients $C_{\hat{\alpha}\hat{\beta}\hat{\gamma}}=(\mathbf{D}_{\gamma}l^{\alpha}_{\hat{\alpha}})l_{\hat{\beta}\alpha}l^{\gamma}_{\hat{\gamma}}$ generalize for N-anholonomic spaces the corresponding Ricci coefficients on Riemannian spaces. Using γ-objects $\gamma^{\alpha}(u)$ (see (19)), we define the Dirac equations on N-anholonomic manifolds:

$$(i\gamma^{\alpha}(u)\overrightarrow{\nabla}_{\alpha}-\mu)\psi=0, \tag{69}$$

which are the Euler equations for the Lagrangian

$$\mathcal{L}^{(1/2)}(u)=\sqrt{|g|}\{[\psi^{+}(u)\gamma^{\alpha}(u)\overrightarrow{\nabla}_{\alpha}\psi(u)-(\overrightarrow{\nabla}_{\alpha}\psi^{+}(u))\gamma^{\alpha}(u)\psi(u)]-\mu\psi^{+}(u)\psi(u)\}, \tag{70}$$

where $\psi^{+}(u)$ is the complex conjugation and transposition of the column $\psi(u)$. We have to consider anchoring of the operator $\overrightarrow{\nabla}_{\alpha}$ on the N-anholonomic manifolds.

From (70), we obtain the d-metric energy-momentum d-tensor

$$E^{(1/2)}_{\alpha\beta}(u)=\frac{i}{4}[\psi^{+}(u)\gamma_{\alpha}(u)\overrightarrow{\nabla}_{\beta}\psi(u)+\psi^{+}(u)\gamma_{\beta}(u)\overrightarrow{\nabla}_{\alpha}\psi(u)-(\overrightarrow{\nabla}_{\alpha}\psi^{+}(u))\gamma_{\beta}(u)\psi(u)$$
$$-(\overrightarrow{\nabla}_{\beta}\psi^{+}(u))\gamma_{\alpha}(u)\psi(u)]$$

and the d-vector source

$$J^{(1/2)}_{\alpha}(u)=\psi^{+}(u)\gamma_{\alpha}(u)\psi(u).$$

We emphasize that interactions with exterior gauge fields can be introduced by changing the locally anisotropic partial derivation from (68) in this manner:

$$e_{\alpha}\rightarrow e_{\alpha}+ie^{\star}B_{\alpha}, \tag{71}$$

where $e^{\star}$ and B_{α} are, respectively, the constant and the d-vector potential of gauge fields.

5. Yang–Mills equations in d-spinor form

We consider a vector bundle $\mathcal{B}_E,\pi_B:\mathcal{B}\rightarrow\mathbf{V}$ on $\mathbf{V}$. Additionally to the d-tensor and d-spinor indices, we use capital Greek letters, $\Phi,\Upsilon,\Xi,\Psi,\ldots$ for fiber (of this bundle) indices (see details in Refs. 19 and 20). Let $\underline{\nabla}_{\alpha}$ be, for simplicity, a torsionless, linear connection in $\mathcal{B}_E$ satisfying conditions:

$$\underline{\nabla}_{\alpha}:\Upsilon^{\Theta}\rightarrow\Upsilon^{\Theta}_{\alpha}[\text{or}\Xi^{\Theta}\rightarrow\Xi^{\Theta}_{\alpha}],$$

$$\underline{\nabla}_{\alpha}(\lambda^{\Theta}+\nu^{\Theta})=\underline{\nabla}_{\alpha}\lambda^{\Theta}+\underline{\nabla}_{\alpha}\nu^{\Theta},$$

$$\underline{\nabla}_{\alpha}(f\lambda^{\Theta})=\lambda^{\Theta}\underline{\nabla}_{\alpha}f+f\underline{\nabla}_{\alpha}\lambda^{\Theta},\quad f\in\Upsilon^{\Theta}[\text{or}\Xi^{\Theta}],$$

where by $\Upsilon^{\Theta}(\Xi^{\Theta})$ we denote the module of sections of the real (complex) v-bundle $\mathcal{B}_E$ provided with the abstract index Θ. The curvature of connection $\underline{\nabla}_{\alpha}$ is defined as

$$K_{\alpha\beta\Omega}{}^{\Theta}\lambda^{\Omega}=(\underline{\nabla}_{\alpha}\underline{\nabla}_{\beta}-\underline{\nabla}_{\beta}\underline{\nabla}_{\alpha})\lambda^{\Theta}.$$

For Yang–Mills fields, as a rule, one considers that $\mathcal{B}_E$ is enabled with a unitary (complex) structure (complex conjugation changes mutually the upper and lower Greek indices). It is useful to introduce instead of $K_{\alpha\beta\Omega}{}^{\Theta}$ a Hermitian matrix $F_{\alpha\beta\Omega}{}^{\Theta}=i\,K_{\alpha\beta\Omega}{}^{\Theta}$ connected with components of the Yang–Mills d-vector potential $B_{\alpha\Xi}{}^{\Phi}$ according the formula:

$$\frac{1}{2}F_{\alpha\beta\Xi}{}^{\Phi}=\underline{\nabla}_{[\alpha}B_{\beta]\Xi}{}^{\Phi}-iB^{\Phi}_{[\alpha|\Lambda|}B_{\beta]\Xi}{}^{\Lambda}, \tag{72}$$

where the spacetime indices commute with capital Greek indices. The gauge transforms are written in the form:

$$B_{\alpha\Theta}{}^{\Phi}\mapsto B_{\alpha\hat{\Theta}}{}^{\hat{\Phi}}=B^{\Phi}_{\alpha\Theta}s^{\hat{\Phi}}_{\Phi}q^{\Theta}_{\hat{\Theta}}+is^{\hat{\Phi}}_{\Theta}\underline{\nabla}_{\alpha}q_{\hat{\Theta}}{}^{\Theta},$$

$$F_{\alpha\beta\Xi}{}^{\Phi}\mapsto F_{\alpha\beta\hat{\Xi}}{}^{\hat{\Phi}}=F_{\alpha\beta\Xi}{}^{\Phi}s^{\hat{\Phi}}_{\Phi}q_{\hat{\Xi}}{}^{\Xi},$$

where matrices $s^{\hat{\Phi}}_{\Phi}$ and $q^{\Xi}_{\hat{\Xi}}$ are mutually inverse (Hermitian conjugated in the unitary case). The Yang–Mills d-equations are written

$$\underline{\nabla}^{\alpha}F_{\alpha\beta\Theta}{}^{\Psi}=J_{\beta\Theta}{}^{\Psi}, \tag{73}$$

$$\underline{\nabla}_{[\alpha}F_{\beta\gamma]\Theta}{}^{\Xi}=0. \tag{74}$$

We must introduce deformations of connection of type, $\nabla^{\star}_{\alpha}-\rightarrow\underline{\nabla}_{\alpha}+P_{\alpha}$, (the deformation d-tensor P_{α} is induced by the torsion in the vector bundle $\mathcal{B}_E$) into the definition of the curvature of gauge fields (72) and motion equations (73) and (74) if the interactions are considered for nontrivial torsions.

IV. CONCLUSIONS AND OUTLOOK

In this work we formulated a spinor approach to the geometry of nonholonomic spacetimes and classical field interactions with constraints possessing Lie algebroid symmetry. Such geometric constructions are performed for a special case of nonholonomic distributions defining nonlinear connection (N-connection) structures resulting in preferred classes of vielbein (frame) systems of reference. The main goals we have achieved are the following:

(1) We gave an intrinsic formulation of the geometry of Clifford N-anholonomic structures. In addition, we investigated the N-anholonomic spin structures (i.e., spinor nonholonomic spaces with associated N-connection).
(2) We defined and analyzed the main properties of the Dirac operator on N-anholonomic manifolds. We showed how the formulas may be "anchored" in order to be considered on spacetimes with Lie/ Clifford algebroid symmetries.
(3) We formulated a geometric approach to field equations on N-anholonomic manifolds. There were considered the examples of scalar, Proca, graviton, spinor and gauge filed interactions when the formulas have a straightforward redefinition on Lie/Clifford N-algebroids (i.e., spacetimes with algebroid symmetries and nonholonomic distributions).

Among the subjects we will study in forthcoming papers, we note the following points:

- To construct exact solutions of the gravitational field equations in string gravity with nontrivial limits to general relativity, parametrized by generic off-diagonal metrics and nonholonomic frames and possessing Lie algebroid symmetries (the first examples of "gravitational" algebroids were analyzed in Ref. 2).

- Certain extension of the metrics to configurations defining solutions of the Einstein–Dirac equations will be considered. We shall analyze the symmetries of such spacetimes and possible physical applications in modern gravity.
- In explicit form, we shall construct nonholonomically deformed metrics, with algebroid symmetries, describing locally anisotropic cosmological models, black holes, anholonomic wormholes, solitons, and gravitational monopoles and instantons.
- To make a detailed investigation of classical field theories and their quantum deformations possessing nontrivial noncommutative symmetries and possible Lie/ Clifford algebroid structure.

Finally, we note that the method of anholonomic frames with associated *N*-connection structure elaborated in Finsler geometry and further, in our works, applied to constructing exact solutions in gravity was applied in this paper for a study of Dirac operators on nonholonomic manifolds possessing Lie algebroid symmetry. The constructions can be extended for spacetimes with uncompactified extra dimensions and such investigations are regarded as interesting research in modern physics and noncommutative geometry.

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A class of superintegrable systems of Calogero type

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We show that the three-body Calogero model with inverse square potentials can be interpreted as a maximally superintegrable and multiseparable system in Euclidean three-space. As such it is a special case of a family of systems involving one arbitrary function of one variable. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The purpose of this article is to investigate the relation between the rational three-body Calogero model in one dimension[3] and superintegrable systems in two and three dimensions.[5,7,16]

The original (quantum) Calogero model was written in the form

$$\left\{-\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)+\frac{1}{8}\omega^2[(x_1-x_2)^2+(x_2-x_3)^2+(x_3-x_1)^2]+\frac{g_1}{(x_2-x_3)^2}+\frac{g_2}{(x_1-x_3)^2}+\frac{g_3}{(x_1-x_2)^2}\right\}\Psi=E\Psi. \tag{1}$$

Upon introducing the center-of-mass coordinate R and the Jacobi relative coordinates ρ and λ,[13]

$$R=\frac{1}{3}(x_1+x_2+x_3),\quad \rho=\frac{1}{\sqrt{2}}(x_1-x_2),\quad \lambda=\frac{1}{\sqrt{6}}(x_1-x_2-2x_3) \tag{2}$$

Eq. (1) was rewritten[3] as follows:

$$\left\{-\left(\frac{\partial^2}{\partial\rho^2}+\frac{\partial^2}{\partial\lambda^2}\right)+\frac{3}{8}\omega^2(\rho^2+\lambda^2)+\frac{1}{2}\frac{g_1}{(\sqrt{3}\lambda-\rho)^2}+\frac{1}{2}\frac{g_2}{(\sqrt{3}\lambda+\rho)^2}+\frac{1}{2}\frac{g_3}{\rho^2}\right\}\Psi=E\Psi, \tag{3}$$

where the motion of the center-of-mass has been factored out.

A superintegrable system is one that admits more integrals of motion than it has degrees of freedom. Systematic searches for superintegrable systems of the form

$$H(\boldsymbol{x},\boldsymbol{p})=\tfrac{1}{2}\boldsymbol{p}^2+V(\boldsymbol{x}) \tag{4}$$

have been conducted in Euclidean spaces $\mathbb{E}^n$ for $n=2$ and 3.[5,7,16] The classical or quantum Hamiltonian (4) is said to be *superintegrable* if it admits $n+k$, $1\leqslant k\leqslant n-1$ integrals of motion, n of them in involution. It is *minimally superintegrable* for $k=1$ and *maximally superintegrable* for

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$k=n-1$. For $n=2$ the two cases coincide and superintegrability simply means the existence of three functionally independent integrals of motion (including the Hamiltonian). For $n=3$ a superintegrable system can have either four or five functionally independent integrals of motion.

The N-body Calogero model[4] (and, in particular, the three-body one[3]) is known to be superintegrable.[1,2,12,20,21,26] An extensive literature exists on superintegrability in classical and quantum systems of the form (4) (see Refs. 14, 22, and 24, and references therein) devoted mainly, though not exclusively[9,8] to systems with integrals of motion of at most second order in the momenta. Superintegrable systems with complete sets of commuting quadratic integrals of motion are *multiseparable*. This means that the corresponding Hamilton-Jacobi, or Schrödinger equation allows the separation of variables in more than one system of (orthogonal) coordinates. Alternatively, multiseparability can be described in terms of the geometric properties of the Killing two-tensors determined by the first integrals of motion that are quadratic in the momenta (see Ref. 12 as well as the relevant references therein).

In what follows, we shall deal with the quantum mechanical problem, but all conclusions are the same (mutatis mutandis) for the classical ones. For the systems admitting integrals of motion of order three or higher, this is not necessarily the case.[9,8,11]

II. THE CALOGERO MODEL IN THE CLASSIFICATION OF SUPERINTEGRABLE SYSTEMS

In a recent article[12] the *invariant theory of Killing tensors* (see also Refs. 17, 18, and 25, and relevant references therein) was used to classify orthogonally separable Hamiltonian systems in the Euclidean space $\mathbb{E}^3$. In particular, it was shown that the inverse square Calogero model with the potential

$$V=\frac{1}{(x_1-x_2)^2}+\frac{1}{(x_2-x_3)^2}+\frac{1}{(x_3-x_1)^2} \tag{5}$$

allows the (orthogonal) separation of variables in five different coordinate systems, namely spherical, circular cylindrical, rotational parabolic, prolate spheroidal, and oblate spheroidal (see also Refs. 2 and 21).

In this study[12] the potential (5) was viewed as a potential in the Hamiltonian (4), corresponding to a single particle in a potential field in $\mathbb{E}^3$. The potential (5) was shown to allow five functionally independent first integrals (including the Hamiltonian). From them it is possible to construct five inequivalent pairs of integrals in involution (in addition to the Hamiltonian). Each such pair is determined by two Killing tensors that share the same orthogonal eigenvectors, thus generating an orthogonal separable system of coordinates. For example, the spherical coordinate system is generated by the following pencil of Killing tensors (including the metric) whose components given in terms of the Cartesian coordinates (x_1,x_2,x_3) are as follows:[12]

$$\begin{bmatrix} a_1+c_2x_3^2+c_3x_2^2 & -c_3x_1x_2 & -c_2x_1x_3 \\ -c_3x_1x_2 & a_1+c_3x_1^2+c_2x_3^2 & -c_2x_2x_3 \\ -c_2x_1x_3 & -c_2x_2x_3 & a_1+c_2x_1^2+c_2x_2^2 \end{bmatrix}. \tag{6}$$

The formula (6) can be rewritten as

$$a_1g^{ij}+c_2K_1^{ij}+c_3K_2^{ij}, \quad i,j=1,2,3, \tag{7}$$

where K_1^{ij} and K_2^{ij} are the components of two *canonical* Killing tensors $\boldsymbol{K}_1$, $\boldsymbol{K}_2$ that share the same orthogonally integrable (i.e., surface forming) eigenvectors and g^{ij} are the components of the metric $\boldsymbol{g}$ of $\mathbb{E}^3$ (see Ref. 12 for more details).

That notwithstanding, the Calogero potential (5) does not appear (at least explicitly) in the list of superintegrable systems in $\mathbb{E}^3$, established earlier[5,16] under the assumption that the first integrals that afford maximal or minimal superintegrability were to be quadratic in the momenta. To unravel this mystery we first observe that the Killing tensors that determine the corresponding integrals of

motion obtained for the potential (5) in Ref. 12 are not in a *canonical* form (as in (6), for example), but are rotated with respect to this form. As an example, let us consider again spherical coordinates (r,θ,ϕ) in $\mathbb{E}^3$ generated by the hypersurfaces of the orthogonally integrable eigenvectors of the Killing tensor (6) given by the following coordinate transformations to the Cartesian coordinates (x_1,x_2,x_3):

$$x_1 = r\sin\theta\cos\phi, \quad x_2 = r\sin\theta\sin\phi, \quad x_3 = r\cos\theta. \tag{8}$$

A potential that allows separation in these coordinates must have the form

$$V(r,\theta,\phi) = f(r) + \frac{1}{r^2}g(\theta) + \frac{1}{r^2\sin^2\theta}k(\phi) \tag{9}$$

and the corresponding additional integrals of motion quadratic in the momenta will be in their standard form, namely

$$F_1 = L_1^2 + L_2^2 + L_3^2 + 2\left[g(\theta) + \frac{1}{\sin^2\theta}k(\phi)\right],$$

$$F_2 = L_3^2 + 2k(\phi), \tag{10}$$

where $L_i, i=1,2,3$ are the infinitesimal generators of SO(3), that can be determined in terms of the Cartesian coordinates x_i, $i=1,2,3$ as follows: $L_1=x_2p_3-x_3p_2$, $L_2=x_3p_1-x_1p_3$, $L_3=x_1p_2-x_2p_1$. Note that the first integrals (10) in terms of the Cartesian coordinates can be rewritten as

$$\begin{aligned} F_1 &= K_1^{ij}p_ip_j + U_1(x_1,x_2,x_3), \\ F_2 &= K_2^{ij}p_ip_j + U_2(x_1,x_2,x_3), \end{aligned} \tag{11}$$

where $i,j=1,2,3$, K_1^{ij}, K_2^{ij} are the components of the "spherical" Killing tensors (7) and (p_1,p_2,p_3) are the operators $(\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$, respectively (quantum mechanics case) or the momenta components corresponding to the Cartesian coordinates (x_1,x_2,x_3) (classical mechanics case).

If we rotate the x_1, x_2, and x_3 axes in (8), the form of the potential (9) changes, so do the integrals (10), but separation of variables will still occur (in spherical coordinates with different axes).

In the case of the potential (5) the rotation taking the Killing tensors into their standard form is a nontrivial one, given by12 (compare with (2))

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 & 0 & \sqrt{2} \\ -1 & \sqrt{3} & \sqrt{2} \\ -1 & -\sqrt{3} & \sqrt{2} \end{pmatrix}\begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \end{pmatrix}. \tag{12}$$

Accordingly, for the Calogero potential (5) we obtain

$$V = 2\left[\frac{1}{(\sqrt{3}\tilde{x}_1 - \tilde{x}_2)^2} + \frac{1}{(\sqrt{3}\tilde{x}_1 + \tilde{x}_2)^2} + \frac{1}{\tilde{x}_2^2}\right] \tag{13}$$

and we see that the variable $\tilde{x}_3$ is absent from (13). Expressing $\tilde{x}_1$ and $\tilde{x}_2$ in terms of spherical coordinates (8), we get

$$V = \frac{2}{r^2\sin^2\theta}\left[\frac{1}{(\sqrt{3}\cos\phi - \sin\phi)^2} + \frac{1}{(\sqrt{3}\cos\phi + \sin\phi)^2} + \frac{1}{\sin^2\phi}\right], \tag{14}$$

i.e., a potential in the form (9) with $f(r)=0$, $g(\theta)=0$ and $k(\phi)$ specified.

In what follows we show that after the rotation (12) it is possible to see that the Calogero potential (13) is a member of an infinite family of potentials, depending on one arbitrary function and sharing a number of important properties, such as superintegrability. Indeed, recall that all superintegrable potentials that separate in spherical coordinates plus at least one other system were derived in Ref. 16. The potential

$$V = \frac{k(\phi)}{r^2 \sin^2 \theta} \tag{15}$$

occurs several times. In what follows we list five *functionally independent* first integrals (including the Hamiltonian H) that afford multiseparability for the potential (15):

$$\begin{aligned} H &= \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + \frac{k(\phi)}{r^2 \sin^2 \theta}, \\ F_1 &= L_1^2 + L_2^2 + L_3^2 + \frac{2k(\phi)}{\sin^2 \theta}, \\ F_2 &= L_3^2 + 2k(\phi), \\ F_3 &= \tfrac{1}{2}p_3^2, \\ F_4 &= L_1 p_2 + p_2 L_1 - p_1 L_2 - L_2 p_1 - 4\frac{\cos \theta}{r \sin^2 \theta} k(\phi), \end{aligned} \tag{16}$$

where $k(\phi)$ is an arbitrary function. The functional independence of the first integrals (16) has been verified with the aid of a computer algebra package (i.e., the Jacobian $\partial(H, F_1, F_2, F_3, F_4)/\partial(x_1, x_2, x_3, p_1, p_2, p_3)$ is of rank 5 at a generic point). It is important to note that the functionally independent first integrals (16) are *linearly connected*, which means that they are subject to an additional constraint specified by the following expression in terms of the coordinates $\boldsymbol{x} = (x_1, x_2, x_3)$:

$$f_0(\boldsymbol{x})H + f_1(\boldsymbol{x})F_1 + f_2(\boldsymbol{x})F_2 + f_3(\boldsymbol{x})F_3 + f_4(\boldsymbol{x})F_4 = 0, \tag{17}$$

where $f_0(\boldsymbol{x}) = 2x_3^2$, $f_1(\boldsymbol{x}) = 1$, $f_2(\boldsymbol{x}) = -1$, $f_3(\boldsymbol{x}) = -2(x_1^2 + x_2^2 + x_3^2)$, $f_4 = x_3$. This formula is a consequence of the following "rotational" symmetry, that can be defined in a coordinate-free way. We can write all of the expressions in formula (16) as $F_k = K_k^{ij} p_i p_j + U_k$, where $i, j = 1, 2, 3$. Then the Killing tensor $\boldsymbol{K}_k$ with the components K_k^{ij} (including the metric) is subject to the following formula:

$$\mathcal{L}_{L_3} \boldsymbol{K}_k = 0, \tag{18}$$

where $\mathcal{L}$ denotes the Lie derivative. We also note that the vector space spanned by the quadratic parts of the first integrals (16) are invariant with respect to translations along the x_3 axis.

It is easy to show now that the potential (15) is orthogonally separable with respect to other systems of coordinates as well. Indeed, the pairs of involutive first integrals leading to the orthogonal separation of variables in the Schrödinger equation are $\{F_1, F_2\}$ (spherical), $\{F_2, F_3\}$ (circular cylindrical), $\{F_2, F_4\}$ (rotational parabolic), and $\{F_2, F_1 \mp a^2 2F_3\}$ (oblate, and prolate spheroidal). Another way to see this is by looking at the separable potentials derived in Ref. 16. In terms of Cartesian coordinates the potential (15) is given by

$$V = \frac{k(x_2/x_1)}{x_1^2 + x_2^2}. \tag{19}$$

Recall[16] that the separable potentials corresponding to "rotational" coordinates, namely spherical, circular cylindrical, rotational parabolic, oblate and prolate spheroidal in the Cartesian coordinates (x_1, x_2, x_3) all have the form

$$V = f + g + \frac{k(x_2/x_1)}{x_1^2 + x_2^2}, \tag{20}$$

where k are arbitrary functions, while f and g are specified differently in each case. The common part of the five separable potentials is exactly the potential (19).

These observations put in evidence that the potential (19) defines a family of maximally superintegrable potentials separable with respect to the five "rotational" orthogonal coordinate systems, namely spherical, circular cylindrical, rotational parabolic, oblate, and prolate spheroidal whose Killing tensors are constrained by the rotational symmetry condition (18). As for the Calogero potential (13), in the coordinates $(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$ determined by the transformation (14), it assumes the form (19) for

$$k(t) = 2(1 + t^2)\left[\frac{3 + t^2}{(3 - t^2)^2} + 1\right], \tag{21}$$

where $t = \tilde{x}_2/\tilde{x}_1$.

The potential (15) can be imbedded into more general families of potentials in $\mathbb{E}^3$ that are *minimally* superintegrable. In contrast to maximally superintegrable potentials they admit three additional integrals rather than four. They are

$$V_1 = \alpha(x_1^2 + x_2^2 + x_3^2) + \frac{\beta}{x_3^2} + \frac{1}{x_1^2 + x_2^2} h(\phi),$$

$$V_2 = \frac{\alpha}{r} + \beta \frac{\cos\theta}{r^2 \sin^2\theta} + \frac{1}{r^2 \sin^2\theta} h(\phi), \tag{22}$$

$$V_3 = k(x_1^2 + x_2^2) + 4k x_3^2 + \frac{1}{x_1^2 + x_2^2} h(\phi).$$

The potential V_1 with $(\alpha, \beta) \neq (0, 0)$ separates in all of the five "rotational" coordinate systems considered above except rotational parabolic ones. V_2 separates only in spherical and rotational parabolic, while V_3 in cylindrical and rotational parabolic. We mention that a special case of V_2 with $\beta = 0$ and $h(\phi) = \text{const}$ is the Hartmann potential used in molecular physics to describe ring-shaped molecules.[10,15]

The rotation (12) in $\mathbb{E}^3$ has a simple meaning for three particles on a line with inverse square potentials. Comparing (3) with (14), we see that the rotation corresponds to introducing center-of-mass coordinates (2). If we factor out the center-of-mass motion (i.e., drop the term $1/2p_3^2$ in the kinetic energy), we reobtain the Hamiltonian (3) with $\omega = 0$.

The system (3) can be viewed as one particle in a potential in the Euclidean plane $\mathbb{E}^2$. Interestingly, it is not multiseparable. For both $\omega = 0$ and $\omega \neq 0$ it separates only in polar coordinates, so it allows only one second-order integral of motion (in addition to the Hamiltonian), namely

$$F = L_3^2 - \left[\frac{g_1}{(\sqrt{3}\sin\phi - \cos\phi)^2} + \frac{g_2}{(\sqrt{3}\sin\phi + \cos\phi)^2} + \frac{g_3}{\cos^2\phi} \right]. \tag{23}$$

If the system (3) is superintegrable in $\mathbb{E}^2$, the second integral of motion must be of higher order in the momenta, not commuting with F given by (23). Multiseparability of a physical system, in particular the Calogero model, may also be of interest from the point of view of different possible quantizations. In a recent article Féher *et al.*[6] have used separation of variables in circular cylindrical coordinates in the three-body Calogero model to investigate all possible self-adjoint extensions of the corresponding angular and radial Hamiltonians. The question arises whether separation of variables in other coordinates might not lead to different quantizations.

III. CONCLUSIONS

The beauty of the Calogero model is lost when its potential is written in the form (13). The formula (13) does however show that this system is a member of a family of maximally superintegrable systems determined by the general formula (15), involving an arbitrary function of one variable, the azimuthal angle ϕ. All of them allow the orthogonal separation of variables in the five different "rotational" coordinate systems. The complete set of commuting operators (first integrals) in each case consists of the Hamiltonian H and F_2 of (16) and one more operator (F_1, F_3, F_4 and $F_1 \mp a^2 p_3^2$, respectively). The operator F_2 that is thus singled out corresponds, in the case of the free motion, to a one-dimensional subgroup of the (orientation-preserving) isometry group $I(\mathbb{E}^3)$, which is the symmetry group of the Schrödinger equation without a potential. This subgroup generates the angle ϕ, common to all five "rotational" orthogonally separable coordinate systems.

This raises the question whether other maximally superintegrable systems involving arbitrary functions exist. All superintegrable systems in $\mathbb{E}^3$ separating in spherical coordinates and in one further system were found in Ref. 16. All further systems separable in (at least) two coordinate systems were found in Ref. 5. In the lists provided by Evans[5] five systems are maximally superintegrable and each one depends on artibrary constants. In addition, eight systems are listed as minimally superintegrable, each depending on one arbitrary function and up to three constants. One of the minimally superintegrable systems has the potential

$$V_1 = F(r) + \frac{c_1}{x_1^2} + \frac{c_2}{x_2^2} + \frac{c_3}{x_3^2}, \tag{24}$$

where c_1, c_2, and c_3 are arbitrary constants. Here and in the following, r, θ, and ϕ are spherical coordinates as specified by (8). Its superintegrability is due to the fact that the corresponding Hamiltonian commutes with the operators

$$F_1 = L_1^2 + \frac{2c_2\cos^2\theta}{\sin^2\theta\sin^2\phi} + \frac{2c_3\sin^2\theta\sin^2\phi}{\cos^2\theta},$$

$$F_2 = L_2^2 + \frac{2c_1\cos^2\theta}{\sin^2\theta\cos^2\phi} + \frac{2c_3\sin^2\theta\cos^2\phi}{\cos^2\theta}, \tag{25}$$

$$F_3 = L_3^2 + \frac{2c_1}{\cos^2\phi} + \frac{2c_2}{\sin^2\phi}.$$

This potential becomes maximally superintegrable for $F=\omega(x_1^2+x_2^2+x_3^2)$. For $c_1=c_2=c_3=0$ it simply becomes rotationally invariant (but not maximally superintegrable). Four of the minimally superintegrable potentials have the form

$$V_i(x_1,x_2,x_3) = \tilde{V}_i(x_1,x_2) + f(x_3), \quad i = 2,3,4,5, \tag{26}$$

where $\tilde{V}_i(x,y)$ is one of the four multiseparable potentials in $\mathbb{E}^2$.[7] In each case the set of integrals of motion consists of

$$F_1 = \tfrac{1}{2}p_3^2 + f(x_3) \tag{27}$$

and three further operators, the principal parts of which lie in the enveloping algebra of the Lie algebra of the isometry group $I(\mathbb{E}^2)$. In particular, for $\tilde{V}_i(x_1,x_2)=0$ the Hamiltonian and F_1 of (27) commutes with the Lie algebra $\{L_3,p_1,p_2\}$, i.e., H and F_1 are invariant under the orientation-preserving isometry group $I(\mathbb{E}^2)$. This provides a total of four integrals of motion, never five. Out of these four functionally independent integrals of motion we can form four inequivalent triplets of integrals of motion in involution, namely (H,F_1,X_i), $i=1,2,3,4$ with

$$X_1 = p_1^2, \quad X_2 = L_3^2, \quad X_3 = L_3p_1 + p_1L_3, \quad X_4 = L_3^2 + a^2(p_1^2 - p_2^2),$$

where $a \neq 0$.These triplets correspond to the separation of variables in the Cartesian, polar, parabolic translational, and elliptic translational, coordinates, respectively. Within the x_1x_2 plane the origin and the orientation of axes can be chosen arbitrarily.

Finally, three of the minimally superintegrable systems depend on an arbitrary function of the azimuthal angle ϕ. They all have the form

$$V_i(r,\theta,\phi) = \tilde{V}_i(r,\theta) + \frac{k(\phi)}{r^2\sin^2\theta}, \quad i = 4,7,8. \tag{28}$$

The integral F_2 of (16) is present in each case, together with H and one of F_1, F_3, or F_4. In particular, for $\tilde{V}_i(r,\theta)=0$ all of the operators (16) are integrals of motion.

We conclude that in $\mathbb{E}^3$ the potential (15) is the only potential that is maximally superintegrable and depends on an arbitrary function (of one variable). The three-body Calogero model corresponds to one particular choice of this function, namely that given in (15) and (21).

An important question arises in this context. Namely, what are the physical consequences in classical and quantum mechanics, of the existence of a maximally superintegrable system, depending on an arbitrary function? In classical mechanics maximally superintegrable sysetms have the property that their finite trajectories are closed.[19] In quantum mechanics they have degenerate energy levels and it has been conjectured[23,22] that they are exactly solvable. We cannot expect these properties to hold for the potential (15) with $k(\phi)$ arbitrary. We suspect that the reason for this paradox is that the five integrals (16) are functionally independent, but linearly connected.

One of the messages that we arrive at is that results considered to be "canonical" in one approach to a problem may be quite nonobvious in another. Thus, the Killing tensors obtained in Ref. 12 were not in canonical (standard) form for the Calogero model viewed as an $\mathbb{E}^3$ problem. The advantage of the invariant approach used in Refs. 12, 17, 18, and 25 is the following. For a given isometry group action in a vector space of Killing tensors one can employ the approach developed in Refs. 12, 17, 18, and 25 to determine which orbit a Killing tensor belongs to and then find the corresponding isometry group action mapping the Killing tensor in question to its canonical form (i.e., the corresponding *moving frames map*).

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Nonintegrability of the three-body problems for the classical helium atom

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We give a proof of the nonintegrability of an important three-body problem in atomic physics. We consider the classical model for the helium atom in full dimension, thus completing our previous proof for the frozen planetary approximation. To our knowledge there is not any such a proof in the literature. We apply a theorem due to Morales-Ruiz and Ramis: if a Hamiltonian system, derived from a homogeneous potential is integrable, then all integrability factors, related to the Hessian of the homogeneous potentials, satisfy certain conditions related to the degree of homogeneity. In the helium atom case, these coefficients should *all* be discrete. We exhibit a set of nondiscrete values determined analytically. This implies the nonintegrability of the helium atom without any computer aid. We also extend this theorem to various two-electron atoms. In the case of strange helium atoms we provide a computer aided proof of nonintegrability. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2339013]

I. INTRODUCTION

The three-body problem, either Coulombian or gravitational, is one the most important problems in Physics. The two-electron atoms, e.g., the helium atom, is a subclass of that problem. The helium atom is a model to study the classical, semiclassical, and quantum mechanics of a generic nonintegrable system,[1] although so far there has not appeared in the literature an analytical proof of its nonintegrability, as opposed to studies with the gravitational three-body problem that goes back to Euler, Lagrange, and Poincaré. For example, the two fixed center problem, largely used in many areas of Physics, was integrated by Euler, in two and three dimension. Numerical studies on the classical helium atom can be found for example in Yamamoto and Kaneko[2] and Carati.[3]

The quest for criteria of integrability in Hamiltonian systems has been a very active field. The results of Morales-Ruiz and Ramis[4] is on the connection between two different concepts of integrability: the integrability of a Hamiltonian system of equations and the integrability of the variational equations along a particular solution of these equations. The main theorems on integrability[4] from Poincaré, Kowalevski, Arnold and Krylov, Ziglin to Morales-Ruiz and Ramis, can all be cast in this context. The version of Ziglin's theorem, due to Yoshida[5] for homogeneous two degrees of freedom, has been applied to many important problems, including Calogero-Moser

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collinear three-body problem for some values of the degree, say k, of the potential. The study of Calogero-Moser integrability problem was completed in Ref. 4, using the more general theorem due to Morales-Ruiz and Ramis. This theorem is used in this work.

In Almeida *et al.*[10] we have found that the "frozen planetary approximation" (FPA) is nonintegrable, since the algebraic equations to be solved are easily solvable due to the restriction to the x axis. The extension to the full helium problem is not trivial. The main difficulty in applying the above-noted theorem to the helium atom stems from the three dimension nature of the model. To solve the correspondent full coupled algebraic set of equations is not feasible even using software like MAPLE and MATHEMATICA. However, we avoid this difficulty by considering a particular symmetric configuration; then we evaluate the integrability coefficients using the full 6×6 Hessian matrix, thus extending our previous result on the FPA case.

We consider here classical heliumlike atoms only. Of course, the corresponding microscopic systems are governed by quantum mechanics or at least described by semiclassical techniques. The classical integrability does not guarantee quantum integrability (see Refs. 6–9 and reference therein). However, we remark that if a problem is not classically integrable there are no action-angle variables that can become the corresponding quantum operators. We hope that our contribution on the classical case may shed some light on the discussion of the quantum counterparts.

II. THEORY AND METHOD

The Hamiltonian for the three-dimensional (3D) heliumlike atom in infinite nuclear mass approximation is shown as follows:

$$H=\frac{1}{2}(\mathbf{p}_1^2+\mathbf{p}_2^2)-\frac{Z}{|\mathbf{r}_1|}-\frac{Z}{|\mathbf{r}_2|}+\frac{1}{|\mathbf{r}_{12}|}, \tag{1}$$

where $\mathbf{r}_i$ is the position of the ith electron, $\mathbf{r}_{12}$ the distance between the electrons, and $\mathbf{p}_i$ are the corresponding momentum of the electrons. This six degree of freedom system is usually reduced to four degrees by energy and momentum conservation. In this case, even if the three particles are constrained to move in the plane the number of degrees of freedom is three.

In Almeida *et al.*[10] we have found that the "frozen planetary approximation" of this problem (two electrons on the same side of the atom with two degrees of freedom) and its modifications (heliumlike atoms) are not integrable. The motivation was the apparently integrable Poincaré section of this approximation in the case of the one-dimensional helium atom ($Z=2$). In this paper, we extend our previous result on nonintegrability to the full 3D problem (as well as for the 2D case) since we devised a way of overcoming the difficulty in solving the full set of equations. The result is also extended to the case of finite values of the alpha-particle mass. We also consider the case where the place of one of the electrons is taken by heavier particles with the same charge: muon, pion, kaon, and antiproton.

To prove the nonintegrability we use a theorem by Morales and Ramis for homogeneous potentials,[4,10] which is a generalization of Yoshida's[5] theorem for more than two degrees of freedom, and without its limitations at resonances. Briefly, consider a Hamiltonian system with n-degree of freedom with the Hamiltonian $H(\mathbf{p},\mathbf{q})=\mathbf{p}^2/2+V(\mathbf{q})$, where $\mathbf{q}=(q_1,\ldots,q_n)$ and $\mathbf{p}=(p_1,\ldots,p_n)$. If $V(\mathbf{q})$ is a homogeneous potential of degree k, $V(a\mathbf{q})=a^kV(\mathbf{q})$, there exists in general straight-line solutions of the corresponding Hamilton's equations as follows:

$$q_i=c_if(t),\quad p_i=c_i\dot{f}(t),\quad i=1,\ldots,n. \tag{2}$$

The f's are solution of the differential equation

$$\dot{f}^2=\frac{2}{k}(1-f^k),\quad k\neq 0.$$

Then, it is possible to show that c_i's are solutions of the n equations given by

$$c_j = \frac{\partial V}{\partial q_j}(c_1, \ldots, c_n), \quad j = 1, \ldots, n. \tag{3}$$

Orbits that are described by this condition are known as homographic solutions in the literature of Celestial Mechanics. The linear variational equations (VE) of the system around the above particular solution are given by ($\delta\mathbf{q} = \xi$ and $\delta\mathbf{p} = \eta$):

$$\dot{\xi} = \eta \quad and \quad \dot{\eta} = -f^{k-2}\frac{\partial^2 V}{\partial q_i \partial q_j}(\mathbf{c})\xi,$$

or

$$\ddot{\xi} = -f^{k-2}\frac{\partial^2 V}{\partial q_i \partial q_j}(\mathbf{c})\xi, \quad i = 1, \ldots, n.$$

In terms of the eigenvalues of the Hessian matrix the VE can be expressed as the n second-order differential equations:

$$\ddot{\xi} = -f^{k-2}(\lambda_i)\xi, \quad i = 1, \ldots, n,$$

the λ_i are still called Yoshida's integrability coefficients, although the theorem of Morales-Ruiz and Ramis applies to n degrees of freedom. The equation with $i=n$, corresponding to the eigenvalue $\lambda_n = k-1$, is the tangential variational equation which is trivially solvable. The NVE (normal variational equation) are the $n-1$ remaining equations. By the symmetries of this problem the NVE is a system of independent hypergeometric differential equations in the independent variable $x=f^k$,

$$x(1-x)\frac{\mathrm{d}^2\xi}{\mathrm{d}x^2} + \left(\frac{k-1}{k} - \frac{3k-2}{2k}x\right)\frac{\mathrm{d}\xi}{\mathrm{d}x} + \frac{\lambda_i}{2k}\xi = 0, \quad i = 1,2, \ldots, n-1.$$

This system of equations is called the algebraic normal variational equation (ANVE). The identity component of the Galois Group of the NVE is the same as the identity component of the Galois Group of the ANVE. The ANVE_i for the scalar second-order equation corresponding to the integrability coefficient λ_i, can be written as

$$\mathrm{ANVE}_i = \mathrm{ANVE}_1 + \mathrm{ANVE}_2 + \cdots + \mathrm{ANVE}_{n-1}.$$

The ANVE is integrable if, and only if, each ANVE_i is integrable, that is, if each one of the identities of the Galois Group is solvable. This leads to the following result.[4]

Morales-Ruiz and Ramis theorem: A Hamiltonian system, with a homogeneous potential of degree k, to be completely integrable (with the holomorphic or meromorphic first integrals), is that each pair (k, λ_i) belongs to one of the following list (with the exception of the trivial case $k=0$):

(1) $(k, p+p(p-1)k/2)$

(2) (2, arbitrary complex number)

(3) (−2, arbitrary complex number)

(4) $\left(-5, \frac{49}{40} - \frac{1}{40}\left(\frac{10}{3}+10p\right)^2\right)$

(5) $\left(-5, \frac{49}{40} - \frac{1}{40}(4+10p)^2\right)$

(6) $\left(-4, \frac{9}{8} - \frac{1}{8}\left(\frac{4}{3}+4p\right)^2\right)$

(7) $\left(-3, \frac{25}{24} - \frac{1}{24}(2+6p)^2\right)$,

(8) $\left(-3, \frac{25}{24} - \frac{1}{24}\left(\frac{3}{2}+6p\right)^2\right)$

(9) $\left(-3, \frac{25}{24} - \frac{1}{24}\left(\frac{6}{5}+6p\right)^2\right)$

(10) $\left(-3, \frac{25}{24} - \frac{1}{24}\left(\frac{12}{5}+6p\right)^2\right)$

(11) $\left(3, -\frac{1}{24} + \frac{1}{24}(2+6p)^2\right)$,

(12) $\left(3, -\frac{1}{24} + \frac{1}{24}\left(\frac{3}{2}+6p\right)^2\right)$

(13) $\left(3, -\frac{1}{24} + \frac{1}{24}\left(\frac{6}{5}+6p\right)^2\right)$

(14) $\left(3, -\frac{1}{24} + \frac{1}{24}\left(\frac{12}{5}+6p\right)^2\right)$

(15) $\left(4,-\frac{1}{8}+\frac{1}{8}\left(\frac{4}{3}+4p\right)^2\right)$ (16) $\left(5,-\frac{9}{40}+\frac{1}{40}\left(\frac{10}{3}+10p\right)^2\right)$

(17) $\left(5,-\frac{9}{40}+\frac{1}{40}(4+10p)^2\right)$ (18) $\left(k,\frac{1}{2}\left(\frac{k-1}{k}+p(p+1)k\right)\right)$,

where p is an arbitrary integer.

III. RESULTS

A. Helium and heliumlike atoms in infinite mass approximation

The potential of the two-electron atoms is homogeneous of degree $k=-1$ in Cartesian coordinates (x_i,y_i,z_i), $i=1,2$. In the infinite nuclear mass approximation, it takes the form ($Z=2$ for He):

$$V=-\frac{Z}{(x_1^2+y_1^2+z_1^2)^{1/2}}-\frac{Z}{(x_2^2+y_2^2+z_2^2)^{1/2}}+\frac{1}{((x_2-x_1)^2+(y_2-y_1)^2+(z_1-z_2)^2)^{1/2}}.$$

Note that in order to apply the above-mentioned theorem we have considered six degrees of freedom without reduction to four, a price we pay to have the homogeneity of the potential. Therefore, system (3) corresponds to six scalar coupled equations in the variables $(x_1,y_1,z_1,x_2,y_2,z_2)$, whose whole set of solutions is very hard to find. However, if we consider a subset of particular solutions of the type $(c_1,0,0,c_2,0,0)$ in (3) of the six scalar equations there remain only two:

$$\begin{aligned}\frac{Zx_1}{|x_1|^3}+\frac{x_2-x_1}{|x_2-x_1|^3}-x_1=0,\\ \frac{Zx_2}{|x_2|^3}-\frac{x_2-x_1}{|x_2-x_1|^3}-x_2=0.\end{aligned} \tag{4}$$

This simple idea allows us to solve what looked to be at first sight an unsurmountable difficulty. With this particular set of solutions of Eq. (4) [or full Eq. (3)] we proceed to the next step, the calculation of the eigenvalues of the (full) Hessian matrix of the potential at these solutions. Our strategy makes the problem easier to handle and the Hess$[V(c_1,0,0,c_2,0,0)]$ matrix is still a 6×6 blocked matrix.

We first have to discuss the allowed values of λ according to the Morales-Ruiz and Ramis theorem. As the degree of homogeneity is $k=-1$, the eigenvalue in the tangential direction is $\lambda=k-1=-2$, and only cases (1) and (18) of the above-mentioned theorem apply:

$$\begin{aligned}(i)\ p-p(p-1)/2=\lambda,\\ (ii)\ 1-p(p+1)/2=\lambda.\end{aligned} \tag{5}$$

We note that in the case of $k=-1$ the above two expressions are equivalent by making $p=q\pm 2$. Therefore the solution given by one of these equations for integer p is the presumed values of the λ's for which the system could be integrable. If we look at the set generated in Almeida *et al.*,[10] for $-8<p<8$:

$$\{\ldots-44,-35,-27,-20,-14,-9,-5,-2,0,1\}. \tag{6}$$

These values of λ form open sets in which we can be sure that the system is nonintegrable. If just one value of λ is sufficiently far from these presumed integer values or complex, then the nonintegrability for the helium atom can be guaranteed. We note that the converse is not true since the Morales-Ruiz and Ramis theorem is a necessary condition only.

Therefore, in order to prove nonintegrability the first step is to find *any* solution of Eq. (3),

like Eq. (4), substitute them in the Hessian matrix and find the corresponding eigenvalues λ_i. If just one of these eigenvalues does not satisfy Eq. (5) for any integer p (one obvious case being complex λ) then we can assure that the system is not integrable. Therefore, our strategy has been to exhaust the possibilities starting with a subset of particular solutions of Eq. (3) with higher symmetry to facilitate the calculation. We stress that our strategy permits us to find feasible solution in contrast with the near nonsolvable full Eq. (3).

We observed that if Eq. (4) were to have two real solutions then it should have the symmetry $R_1=(r,-r)$ and $R_2=(-r,r)$. Thus, substituting R_1 or R_2 in Eq. (4) (or $R_1=(r,0,0,-r,0,0)$ or $R_2=(-r,0,0,r,0,0)$ in Eq. (3)) we obtain analytically that

$$r=(Z-1/4)^{1/3}$$

and the analytical eigenvalues of the Hessian matrix for these real roots are

$$\{-2,1,1,-2/(1-1/4Z),1/(1-1/4Z),1/(1-1/4Z)\}. \tag{7}$$

For $Z=2$ the value of $\lambda_4=-2/(1-1/4Z)=-16/7\approx-2.285\,714\,3$. Note that it does not coincide with any of the presumed *integer* values in (6). Therefore, the system He atom cannot be integrable since the theorem requires that all values of λ should satisfy (5). Note that the eigenvalue in the tangential direction, which is known to be $k-1=-2$, has been obtained independently of this assumption. Therefore, the helium atom is not integrable in the approximation of infinite nuclear mass and the result has been established analytically. We note that according to MAPLE and MATHEMATICA software there are ten solutions for Eq. (4): a pair of real solutions and an octet of complex values, of course the real values are the same as the ones found analytically. The above-found values allow one to examine the integrability of a series of heliumlike atoms, i.e., for any value of Z. In fact, taking one of the real eigenvalues of the set above, say

$$\lambda_4=\frac{-2}{\left(1-\frac{1}{4Z}\right)}$$

we find that $-5<-2/(1-1/4Z)<-2$ for $Z>5/12\approx0.417$. Therefore, all the heliumlike atoms with $Z>(5/12)$ are not integrable. Note that for $Z=1/4$ the values of the $\lambda_i's$, $i=4,5,6$ diverge and for $Z\to\infty$, e.g., $\lambda_4=-2$ (independent particle approximation).

B. Helium, heliumlike, and strange helium atoms

The helium atom ($Z=2$) can be modified by substituting one of its electrons by a heavier particle. In this case we need a Hamiltonian which takes into account the relative masses of the particles:[11]

$$H(r_1,r_2,p_1,p_2)=\frac{\mathbf{p}_1^2}{2\mu_{12}}+\frac{\mathbf{p}_2^2}{2\mu_3}-\frac{Z}{|\mathbf{r}_1|}-\frac{Z}{\left|\mathbf{r}_2+\frac{m_2}{m_1+m_2}\mathbf{r}_1\right|}+\frac{1}{\left|\mathbf{r}_2-\frac{m_1}{m_1+m_2}\mathbf{r}_1\right|}, \tag{8}$$

where the reduced masses are: $\mu_{12}=m_1m_2/(m_1+m_2)$ and $\mu_3=m_3(m_1+m_2)/(m_1+m_2+m_3)$, being $m_1=m_\alpha$ and m_i, $i=2,3$ are either the electron or a heavier particle. Before proceeding to calculations we make a canonical change of variables in the Hamiltonian (8). We take $r_i'=r_i/u_i$ and $p_i'=p_iu_i$, where $u_1=1/\sqrt{\mu_{12}}$ and $u_2=1/\sqrt{\mu_3}$. Now the problem is isotropic in the masses and we use Eq. (3) obtaining for the particular solution $(c_1,0,0,c_2,0,0)$ the following system:

$$\frac{Z\sqrt{\mu_{12}}\chi_1}{|\chi_1|^3}+\frac{Z\sqrt{\mu_{12}}\left(\frac{\chi_2}{\sqrt{\mu_3}}+\frac{\sqrt{\mu_{12}}\chi_1}{m_1}\right)}{\left|\frac{\chi_2}{\sqrt{\mu_3}}+\frac{\sqrt{\mu_{12}}\chi_1}{m_1}\right|^3m_1}-\frac{\sqrt{\mu_{12}}\left(\frac{\chi_2}{\sqrt{\mu_3}}-\frac{\sqrt{\mu_{12}}\chi_1}{m_2}\right)}{\left|\frac{\chi_2}{\sqrt{\mu_3}}-\frac{\sqrt{\mu_{12}}\chi_1}{m_2}\right|^3m_2}-\chi_1=0,$$

$$\frac{Z\left(\frac{\chi_2}{\sqrt{\mu_3}}+\frac{\sqrt{\mu_{12}}\chi_1}{m_1}\right)}{\left|\frac{\chi_2}{\sqrt{\mu_3}}+\frac{\sqrt{\mu_{12}}\chi_1}{m_1}\right|^3\sqrt{\mu_3}}+\frac{\left(\frac{\chi_2}{\sqrt{\mu_3}}-\frac{\sqrt{\mu_{12}}\chi_1}{m_2}\right)}{\left|\frac{\chi_2}{\sqrt{\mu_3}}-\frac{\sqrt{\mu_{12}}\chi_1}{m_2}\right|^3\sqrt{\mu_3}}-\chi_2=0. \tag{9}$$

In particular, we have been able to find an analytic solution for the case of the helium atom ($Z=2$) and all heliumlike atoms (any Z), that is, when $m_2=m_3=m_e$. We find that the potential of (8) is reduced to that of the infinite α-particle mass by means of the linear transformation:

$$\chi_1=\sqrt{\mu_{12}}x_1, \quad \chi_2=\sqrt{\mu_3}\left(x_2-\frac{m_2}{m_1+m_2}x_1\right), \tag{10}$$

where χ_i and x_i denote the coordinates for finite and infinite mass systems, respectively.

Then using the symmetry discussed in the previous section we find the solutions $R_1=(-r,r)$ and $R_2=(r,-r)$ for the Jacobi variables; recall that $r=(Z-1/4)^{1/3}$. Using this guess (10) with $x_1=-x_2$ in (9) we find that

$$R_{1,2}=\left[\pm\sqrt{\mu_{12}}\left(\frac{Z-1/4}{m_e}\right)^{1/3}, \mp\sqrt{\mu_3}\left(\frac{Z-1/4}{m_e}\right)^{1/3}\left(1+\frac{m_e}{m_\alpha+m_e}\right)\right] \tag{11}$$

solves the system of equations if $m_2=m_3=m_e$.

The corresponding eigenvalues for the Hessian matrix are

$$\lambda=\left\{-2,1,1,\frac{-2\left(\frac{2m_e}{m_\alpha}+1\right)}{1-\frac{1}{4Z}},\frac{\left(\frac{2m_e}{m_\alpha}+1\right)}{1-\frac{1}{4Z}},\frac{\left(\frac{2m_e}{m_\alpha}+1\right)}{1-\frac{1}{4Z}}\right\},$$

where m_e is the electron mass. Taking $Z=2$ we find

$$\lambda=\{-2,1,1,-2.286\,340,1.143\,170,1.143\,170\}$$

to be compared with the first value evaluated numerically in the table to follow. Note that it is not in the end of the intervals generated by the set (6) required for integrability. This completes the study of the nonintegrability for the helium atom.

Solving Eq. (3) numerically (MAPLE or MATHEMATICA) using the strategy used so far, we find the following set of eigenvalues for Hess$[V(\mathbf{c})]$:

particle	λ
Electron	$\{-2,1,1,-2.286\,340,1.143\,170,1.143\,170\}$
Muon	$\{-2,1,1,-2.212\,536,1.106\,268,1.106\,268\}$,
Pion	$\{-2,1,1,-2.207\,143,1.103\,571,1.103\,571\}$,
Kaon	$\{-2,1,1,-2.190\,079,1.095\,040,1.095\,040\}$,
Antiproton	$\{-2,1,1,-2.188\,614,1.094\,307,1.094\,307\}$,

for the masses $5.485\,799\times10^{-4}\mu$, $0.113\,428\,92\mu$, $0.149\,837\,65\mu$, $0.529\,994\,32\mu$, and $1.007\,295\,93\mu$, respectively. For the mass of the α particle (He nucleus) we have used $4.002\,602\mu$, $\mu=931.494\,32$ MeV/c^2. We have not been able to find an analytical solution for the strange helium case.

It is easy to see that there are eigenvalues which are not the end of the intervals shown in set (6), as required for possible integrability. So none of these heliumlike problems are integrable.

C. CONCLUSION

We apply the theorem of Morales-Ramis, one of the latest theorems on integrability of Hamiltonian systems, and prove mainly that the helium atom as well as several heliumlike atoms are not integrable in any physical dimension. We thus have extended our previous result on the frozen planetary approximation to the full helium system. We remark that in this paper the proof is completely analytic. The proof is also extended to several strange helium atoms. In the case of the strange helium atoms we have not been able to solve the equations by radicals but our proof is a rigorous computer aided proof because the integrability coefficients are a set of integers, and the actual numerical values are sufficiently far from these integers.

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Explicit solutions for *N*-dimensional Schrödinger equations with position-dependent mass

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With the consideration of spherical symmetry for the potential and mass function, one-dimensional solutions of nonrelativistic Schrödinger equations with spatially varying effective mass are successfully extended to arbitrary dimensions within the frame of recently developed elegant nonperturbative technique, where the BenDaniel-Duke effective Hamiltonian in one dimension is assumed like the unperturbed piece, leading to well-known solutions, whereas the modification term due to possible use of other effective Hamiltonians in one dimension and, together with the corrections coming from the treatments in higher dimensions, are considered as an additional term like the perturbation. Application of the model and its generalization for the completeness are discussed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2354333]

I. INTRODUCTION

Gaining confidence from the successful applications[1] of the recently developed simple model[2] in different fields of physics, we have investigated[3] the relation between the solutions of physically acceptable effective mass Hamiltonians proposed in the literature for the treatment of one-dimensional problems. Using the spirit of the prescription suggested in Ref. 3, we aim here to tackle the more difficult problem of generating exact solutions for position-dependent mass Schrödinger equations (PDMSE) in N dimension, as most of the related works in the literature have been devoted to one-dimensional systems except the ones in Ref. 4.

The concept of PDMSE is known to play an important role in different branch of physics. This formalism has been extensively used in nuclei, quantum liquids, ^{3}He, and metal clusters. Another area wherein such concepts provide a very useful tool is the study of electronic properties of many condensed-matter systems, such as semiconductors and quantum dots. In particular, recent progress in crystal-growth techniques for producing nonuniform semiconductor specimens, wherein the carrier effective mass depends on position, has considerably enhanced the interest in the theoretical description of semiconductor heterostructures. It has also recently been signaled in the rapidly growing field of PT-symmetric or more generally pseudo-Hermitian quantum mechanics. For an excellent recent review, leading to the related references, the reader is referred to Ref. 4.

In Sec. II, the systematic treatment of N-dimensional PDMSE is presented and closed expressions corresponding to the full wave function and energy spectrum for exactly solvable potentials are given. Section III contains the application of the model while the generalization of the formalism is discussed in Sec. IV. Concluding remarks are given in the last section.

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II. THEORETICAL CONSIDERATION

Tracking down solvable potentials in PDMSE has always aroused interest. Apart from being useful in understanding of many physical phenomena, the importance of searching for them also stems from the fact that they very often provide a good starting point for undertaking perturbative calculations of more complex systems.

As is well known (see, e.g., Refs. 3 and 5), the general form of radial PDMSE with Hermitian Hamiltonians in one dimension gives rise to

$$-\frac{\mathrm{d}}{\mathrm{dz}}\left[\frac{1}{M(z)}\frac{\mathrm{d}\Phi(z)}{\mathrm{dz}}\right]+V^{\mathrm{eff}}(z)\Phi(z)=\lambda\Phi(z), \tag{1}$$

where the effective potential

$$V^{\mathrm{eff}}(z)=V_0(z)+U_{\alpha\gamma}(z)=V_0(z)-\frac{(\alpha+\gamma)}{2}\frac{M''}{M^2}+(\alpha\gamma+\alpha+\gamma)\frac{M'^2}{M^3}, \tag{2}$$

depends on the mass term and ambiguity parameters. Here a prime denotes derivative with respect to the variable, $M(z)$ is the dimensionless form of the mass function $m(z)=m_0M(z)$ and we have set $\hbar=2m_0=1$. The effective potential is the sum of the real potential profile $V_0(z)$ and the modification $U_{\alpha\gamma}(z)$ emerged from the location dependence of the effective mass. A different Hamiltonian leads to a different modification term. Some of them are the ones proposed by[6] BenDaniel-Duke ($\alpha=\gamma=0$), Bastard ($\alpha=-1$), Zhu-Kroemer ($\alpha=\gamma=-1/2$), and Li-Kuhn ($\gamma=-1/2,\alpha=0$).

Considering the works in Refs. 3 and 7, the radial piece of PDMSE in arbitrary dimensions for spherically symmetric potentials and mass functions reads

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{M'}{M}\left(\frac{N-1}{2r}-\frac{\mathrm{d}}{\mathrm{d}r}\right)-\frac{L(L+N+2)+(N-1)(N-3)/4}{r^2}+M[E-V_{\mathrm{eff}}(r)]\right\}\Psi(r)=0, \tag{3}$$

where we assume that $\Psi(r)=F(r)G(r)$, which leads to

$$\frac{1}{M}\left(\frac{F''}{F}+\frac{G''}{G}+2\frac{F'}{F}\frac{G'}{G}\right)-\frac{M'}{M^2}\left(\frac{F'}{F}+\frac{G'}{G}\right)=U_{\mathrm{eff}}-E. \tag{4}$$

The effective potential in higher dimensions ($N>1$) now is transformed to the form

$$U_{\mathrm{eff}}(r)=V_0(r)+U_{\alpha\gamma}(r)-\frac{M'}{M^2}\frac{(N-1)}{2r}+\frac{L(L+N-2)+(N-1)(N-3)/4}{Mr^2}, \tag{5}$$

in which L is the angular momentum. As the one-dimensional calculations require $N=1$ and $L=0$, Eq. (5) reduces in this case to $U_{\mathrm{eff}}=V_{\mathrm{eff}}=V_0+U_{\alpha\gamma}$ as in Ref. 3, which provides a safe testing ground.

Keeping in mind the spirit of the technique used simply in Ref. 3, we split Eq. (4) in two parts deviating from the treatments in[4]

$$W^2(r)-\left[\frac{W(r)}{\sqrt{M}}\right]'=V_0(r)-\varepsilon, \quad W=-\frac{F'}{\sqrt{M}F}, \tag{6}$$

where ε is the corresponding energy of the required quantum state F_n ($n=0,1,2,\ldots$) for V_0 which is assumed in this model as an exactly solvable mass-dependent potential, and

$$\Delta W^2(r) - \left[\frac{\Delta W(r)}{\sqrt{M}}\right]' + 2W(r)\Delta W(r) = \Delta V(r) - \Delta E, \quad \Delta W = -\frac{G'}{\sqrt{M}G}, \tag{7}$$

where

$$\Delta V(r) = U_{\alpha\gamma}(r) - \frac{M'}{M^2}\frac{(N-1)}{2r} + \frac{L(L+N-2)+(N-1)(N-3)/4}{Mr^2}. \tag{8}$$

Note that the total energy appearing in (4) is $E=\varepsilon+\Delta E$ and, in one dimension the modification term ΔV becomes $U_{\alpha\gamma}$ as in Ref. 3. This clarifies that the corrections due to the higher dimensions arise because of the second and third terms on the right-hand side of Eq. (8).

From the present theoretical consideration, Eq. (6) has an algebraic solution leading to closed analytical expressions for the wave functions and energy eigenvalues, hence one needs to solve Eq. (7) exactly. To proceed further, with the consideration of relativistic Dirac equations having no ambiquity parameters, we confidently choose

$$\Delta W(r) = \frac{(\alpha+\gamma)}{2}\frac{M'}{M^{3/2}} - \frac{(N+2L-1)}{2\sqrt{M}r}, \tag{9}$$

in which the second term disappears for $N=1$ as in Ref. 3. Within the frame of Eq. (7), this choice leads us to

$$W(r)\Delta W(r) = \frac{M'}{2rM^2}\left[\frac{(\alpha+\gamma)(N-1)}{2} + (\alpha+\gamma+1)L\right] - \frac{\Delta E}{2}, \tag{10}$$

which is the main result of the present work.

From the definition of the effective potential in Eq. (2), we also note that the use of Eqs. (7) and (8) naturally restricts the choice of some ambiguity parameters yielding different physically acceptable effective mass Hamiltonians, allowing only $\alpha=\gamma=0$ (Ben-Daniel Duke Hamiltonian) and $\alpha=\gamma=-1/2$ (Zhu-Kroemer Hamiltonian) cases. This observation clarifies that the unperturbed part (V_0) of the effective potential in (6) should correspond to the case $\alpha=\gamma=0$, having well-known solutions in one dimension, while $\alpha=\gamma=-1/2$ is used to calculate $U_{\alpha\gamma}$ in (8). Obviously, all the corrections coming from the higher dimensions to the energy and well-behaved wave function terms can be systematically calculated for a given M with the consideration of Eqs. (7)–(10) in light of the corresponding W in (6).

III. APPLICATION

Recently, some research has been devoted to the analysis of the classification of quantum systems with position-dependent mass regarding their exact solvability (Refs. 3–5, and references therein). On a similar basis, Plastino and his co-workers[8] applied an approach within the supersymmetric quantum mechanical framework, for the case $\alpha=\gamma=0$, to such systems and succeed to show that some one-dimensional systems with nonconstant mass have a supersymmetric partner with the same effective mass. They were also able to solve exactly some particular cases by constructing the superpotential $[W(r)]$ from the form of the effective mass $[M(r)]$ and generalize the concept of the shape invariance for these systems.

For illustration, the superpotential expressions given by Ref. 8 for the systems having harmonic oscillator and Morse-like spectra can be easily used in Eq. (6) to serve explicit expressions for the corrections to the one-dimensional solutions obtained by considering the Ben-Daniel-Duke effective Hamiltonian in their[8] calculations. This simple investigation enables us to test our results, because all the corrections should disappear in case $N=1$ and $\alpha=\gamma=0$ leading to the expressions in Ref. 8. For clarity, this section involves only the application on the harmonic oscillator system. However, the generalization of the present model yielding self-consistent calculations, reproducing $W(r)$ term within the model for any system of interest, will be discussed in the next section.

According to Ref. 8, $W(r)$ term in Eqs. (6) and (10) is

$$W(r)=\frac{\omega}{2}\int^{r}\sqrt{M(z)}\mathrm{d}z+\frac{1}{2}\left(\frac{1}{\sqrt{M}}\right)', \quad \omega=2\varepsilon_{n=0}, \tag{11}$$

for the systems having harmonic oscillator spectra. Hence, use of Eqs. (7)–(10) gives

$$\Delta E=\frac{M'}{rM^{2}}\left[\frac{(\alpha+\gamma)(N-1)}{2}+L(\alpha+\gamma+1)\right]+\frac{(N+2L-1)\omega}{2r\sqrt{M}}\int^{r}\sqrt{M(z)}\mathrm{d}z$$
$$+\left(\frac{1}{\sqrt{M}}\right)'\left\{(\alpha+\gamma)\left[\omega\int^{r}\sqrt{M(z)}\mathrm{d}z+\left(\frac{1}{\sqrt{M}}\right)'\right]+\frac{(N+2L-1)}{2r\sqrt{M}}\right\}, \tag{12}$$

which is the explicit form of the energy corrections for a given smooth mass. Clearly, it can be seen that for a constant mass $M\rightarrow 1$, Eq. (12) reduces to $(N+2L-1)w/2$ for arbitrary dimensions[7] while in one dimension it goes to zero for a nonconstant mass in case $\alpha=\gamma=0$.[8] Furthermore, from Eqs. (7) and (9), the modification term for the corresponding wave function is

$$G(r)=\exp\left(-\int^{r}\sqrt{M(z)}\Delta W(z)\mathrm{d}z\right)=r^{(N+2L-1)/2}M^{-(\alpha+\gamma)/2}. \tag{13}$$

As Eq. (6) is analytically solvable having a closed expression for $W(r)$ given by (11) reproducing explicit expressions for ε and F, the corresponding total energy and wave function can easily be calculated through $E=\varepsilon+\Delta E$ and $\Psi=FG$ for the system of interest with a location dependent mass. At this stage it is also noted that the formalism suggested here seems superior to the usual treatment in supersymmetric quantum theory that in principle starts with the ground state and builds up excited state wave functions by the use of some linear operators ($A^{\pm}$) whereas there is no such restriction in the present theory providing flexible investigations.

IV. DISCUSSION

Although the procedure used in the formalism seems reasonable, the use of other works as in the previous section for an appropriate $W(r)$term to solve Eq. (6) may be seen as a drawback of the model. To remove this seeming deficiency, we propose here a unified treatment within the model considering the recent work in Ref. 9.

Many of the special functions $H(g)$ of mathematics represent solutions to differential equations of the form

$$\frac{\mathrm{d}^{2}H(g)}{\mathrm{d}g^{2}}+Q(g)\frac{\mathrm{d}H(g)}{\mathrm{d}g}+R(g)H(g)=0, \tag{14}$$

where the functions $Q(g)$and $R(g)$ are well defined for any particular function.[10] Since in this article we are interested in bound state wave functions, we should restrict ourselves to polynomial solutions of Eq. (14). Bearing in mind Eq. (14), the substitution of $\Phi(z)=H[g(z)]f(z)$ in Eq. (1) leads to the second-order differential equation

$$\frac{1}{M}\left(\frac{f''}{f}+\frac{H''g'^{2}}{H}+\frac{g''H'}{H}+2\frac{H'g'f'}{Hf}\right)-\frac{M'}{M^{2}}\left(\frac{f'}{f}+\frac{H'g'}{H}\right)=V_{\mathrm{eff}}-\lambda, \tag{15}$$

in which primes denote derivatives with respect to g and z for the functions $H(g)$, $g(z)$, and $f(z)$, respectively. With the confidence gained by the similarity between Eqs. (15) and (4), one can safely use the present treatment splitting Eq. (15) in two pieces

$$W^{2}(z)-\left[\frac{W(z)}{\sqrt{M}}\right]'=V_{0}(z)-\varepsilon, \quad W=-\frac{f'}{\sqrt{M}f}, \tag{16}$$

and

$$\Delta W^2(z) - \left[\frac{\Delta W(z)}{\sqrt{M}}\right]' + 2W(z)\Delta W(z) = \Delta V(z) - \Delta E, \quad \Delta W = -\frac{H'g'}{\sqrt{MH}}, \tag{17}$$

which are similar to Eqs. (6) and (7), where $\lambda = \varepsilon + \Delta E$ and $V_{\text{eff}} = V_0 + \Delta V$.

After all, it can be clearly seen that Eq. (16) is the one required for obtaining an explicit expression for W term used in Eq. (6) corresponding to an exactly solvable system considered in one dimension ($\alpha = \gamma = 0$). However, to proceed further, the functions f and g should be solved as H, Q, and R are known in principle. Now, equating like terms between the resulting expression in (15) and (14) gives

$$Q[g(z)] = \frac{1}{g'}\left(\frac{g''}{g'} + \frac{2f'}{f} - \frac{M'}{M}\right), \quad R[g(z)] = \frac{1}{g'^2}\left[\frac{f''}{f} - \frac{M'}{M}\frac{f'}{f} + M(E - V)\right], \tag{18}$$

where, from the definition of Q,

$$f(z) \approx \left(\frac{M}{g'}\right)^{1/2} \exp\left[\frac{1}{2}\int^{g(z)} Q(g)\mathrm{d}g\right]. \tag{19}$$

Consideration of Eqs. (15)–(18) suggests a novel prescription

$$\Delta V(z) - \Delta E = -\frac{g'^2}{M} R[g(z)], \tag{20}$$

which, for plausible M and R functions, provides a reliable expression for $g(z)$. It is remarked that in the constant mass case $M \to 1$ this procedure reduces to the well-known formalism which has been thoroughly investigated[11] that, together with Ref. 9, justify our new proposal in solving PDMSE. The more detailed investigation of this treatment will be discussed elsewhere.

V. CONCLUDING REMARKS

In this article, a general method has been presented to address the question of corrections to the solution in one dimension for a large class of N-dimensional and exactly solvable PDMSE. We have also described how to extend the method to the case where the necessary function $W(r)$ in (6) generating algebraically solvable potentials in one dimension are present, which initiates calculations in the model leading to explicit expressions for the modifications due to both the use of physically plausible Zho-Kroemer effective Hamiltonian ($\alpha = \gamma = -1/2$) and higher dimensional treatments. The main results are consistent with the other related works in the literature, which allow a nonperturbative treatment of these issues.

Although, for clarity, we have illustrated an application of the method for an easily accessible case of interest, it can be readily employed in various typical situations. In view of the importance in calculating such corrections in physics, we believe that the present model would serve as a useful toolbox to treat even more realistic situations which now occur in experimental observations with the advent of the quantum technology.

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Unified theory of annihilation-creation operators for solvable ("discrete") quantum mechanics

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The annihilation-creation operators $a^{(\pm)}$ are defined as the positive/negative frequency parts of the exact Heisenberg operator solution for the "sinusoidal coordinate". Thus $a^{(\pm)}$ are hermitian conjugate to each other and the relative weights of various terms in them are solely determined by the energy spectrum. This unified method applies to most of the solvable quantum mechanics of single degree of freedom including those belonging to the "discrete" quantum mechanics. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2349485]

I. INTRODUCTION

The annihilation and creation operators are probably the most basic and important tools in quantum mechanics. Modern quantum physics is almost unthinkable without them. Approximately 80 years after its birth, the list of exactly solvable systems in quantum mechanics[1] is quite long now, including those of the so-called "discrete" quantum mechanics.[2,3] One natural question is that if these exactly solvable quantum mechanical systems also possess the algebraic solution method embodied in the annihilation-creation operators. We will answer the question in the affirmative and give a *unified dynamical* derivation of the annihilation-creation operators for most of the solvable quantum mechanics of single degree of freedom including those belonging to the discrete quantum mechanics.

The method is quite simple and elementary. One identifies a special function $\eta(x)$ of the space-coordinate x, which undergoes "sinusoidal motion" at the classical and quantum levels (2.10) and (2.14). The latter is simply the exact Heisenberg operator solution for $\eta(x)$. The function η is the argument of the orthogonal polynomial (2.3) constituting the eigenfunctions of the system. The positive/negative frequency parts of the exact Heisenberg operator solution of the "sinusoidal coordinate" $\eta(x)$ [(2.28) and (2.29)] give the annihilation-creation operators. This is essentially the same recipe as used by Heisenberg for solving the harmonic oscillator in matrix mechanics. To the best of our knowledge, the sinusoidal coordinate was first introduced in a rather broad sense for general (not necessarily solvable) potentials as a useful means for coherent state research by Nieto and Simmons.[4]

By similarity transformation in terms of the ground state wave function, the results of the present article will be translated to those of the corresponding orthogonal polynomials. In particular, the exact Heisenberg operator solution of the sinusoidal coordinate corresponds to the so-called *structure relation*[5] for the orthogonal polynomials. Our method provides the unified derivation of the structure relations for the Askey-Wilson, Wilson, continuous dual Hahn, continuous Hahn and Meixner-Pollaczek polynomials[6] based on the Hamiltonian principle. These polynomials are the eigenfunctions of the various discrete quantum mechanical systems[2,3] and they are the deformations of the Jacobi, Laguerre, and Hermite polynomials.[7]

This article is organized as follows. The general theory of the annihilation-creation operators is explained with typical examples; one from the ordinary quantum mechanics and two from the discrete version in Sec. II. Further explicit results are presented in Sec. III. They include the

(symmetric) Pöshl-Teller, symmetric Rosen-Morse, Morse and x^2+1/x^2 potentials on top of the five examples belonging to the discrete quantum mechanics mentioned previously. Section IV is for a summary and comments. In Appendix A, the necessary and sufficient condition for the existence of the sinusoidal coordinate is analyzed within the context of ordinary quantum mechanics. It turns out that those potentials having the sinusoidal coordinate are all *shape invariant*.[8] In Appendix B, interpretation of the annihilation-creation operators within the framework of shape invariance is given. It is the mechanism underlying the solvability of all systems considered in this article. Appendix C gives various definitions of the orthogonal polynomials, hypergeometric functions and their q analog.[7,6]

II. GENERAL THEORY WITH TYPICAL EXAMPLES

The purpose of the present paper is to present a *unified dynamical* theory of **annihilation-creation** operators. It is applicable to most of the *exactly solvable* quantum mechanical systems of one degree of freedom, including the so-called discrete quantum mechanics which are certain deformation of the solvable quantum mechanics.[2,3] They satisfy certain *difference equations* instead of the second order differential equations. Generalization to the systems of many degrees of freedom will be discussed elsewhere. The restriction to the solvable quantum systems is rather trivial and inevitable, since a system is obviously solvable if it possesses explicitly defined annihilation and creation operators and any one single eigenstate to work on. Then the entire set of exact eigenstates are easily and concretely generated.

Except for the simple harmonic oscillator, which gives probably the only so far universally accepted example of the annihilation-creation operators, there are quite a wide variety of proposed annihilation and creation operators in the literature.[9] Historically most of these annihilation-creation operators are connected to the so-called *algebraic theory of coherent states*, which are usually defined as eigenstates of *annihilation operators*. Therefore, for a given potential or a quantum Hamiltonian, there could be as many coherent states as the definitions of the annihilation operators.

Our new unified definition of the annihilation-creation operators is, on the contrary, based on the dynamical properties of a special coordinate, the sinusoidal coordinate shared by a class of solvable dynamical systems discussed in this article. A quantum mechanical system with a self-adjoint Hamiltonian $\mathcal{H}$ is solvable (or solved) if the entire set of its energy eigenvalues $\{\mathcal{E}_n\}$ and the corresponding eigenvectors $\{\phi_n\}$, $n=0,1,\ldots$ are known:

$$\mathcal{H}\phi_n = \mathcal{E}_n\phi_n, \quad n=0,1,\ldots. \tag{2.1}$$

As is well-known a quantum Hamiltonian (together with its discrete analog) has in general discrete as well as continuous spectrum. In this article we will concentrate on the discrete energy levels only, either finite or infinite in number. Then, because of the one dimensionality, the eigenvalues are not degenerate

$$\mathcal{E}_0 < \mathcal{E}_1 < \cdots, \tag{2.2}$$

and the eigenvectors have finite norms $\|\phi_n\|^2=N_n^2<\infty$. (When normalized vectors are needed we denote them by adding a hat, $\{\hat{\phi}_n \overset{\text{def}}{=} \phi_n/N_n\}$, $\|\hat{\phi}_n\|=1$.) This is the solution in the Schrödinger picture and the eigenvectors $\{\phi_n\}$ are usually expressed as functions $\{\phi_n(x)\}$ of the space-coordinate x. For the majority of the solvable quantum systems, the nth eigenfunction has the following general structure[1]:

$$\phi_n(x) = \phi_0(x)P_n(\eta(x)) \tag{2.3}$$

in which $\phi_0(x)$ is the *ground state* wave function. It has no nodes and we may choose it to be always real and positive. The second factor $P_n(\eta(x))$ is a polynomial of degree n in a real variable η. We also take $P_n(\eta)$ as real and use a convention $P_{-1}(\eta)=0$. Reflecting the orthogonality

theorem of the eigenvectors of a self-adjoint Hamiltonian, $\{P_n(\eta)\}$ form *orthogonal polynomials* with respect to a weight function (measure)

$$\phi_0(x)^2 dx \propto w(\eta) d\eta. \tag{2.4}$$

Throughout this article we follow the definition and notation of Szegö's book[7] for the classical orthogonal polynomials and the review by Koekoek and Swarttouw[6] for the Askey scheme of hypergeometric orthogonal polynomials and its q analog, which are deformations of the classical orthogonal polynomials.

There are certain exactly solvable quantum systems, for example, the one-dimensional Kepler problem, etc., for which the general form of eigenfunction (2.3) does not hold. For them, the present unified theory does not apply. See Appendix A.

Our main claim is that this $\eta(x)$ undergoes a *sinusoidal motion* under the given Hamiltonian $\mathcal{H}$, at the classical as well as quantum level, by mimicking the simple harmonic oscillator. This fact is the basis of our dynamical and unified definition of the annihilation-creation operators. To be more specific, at the classical level we have

$$\{\mathcal{H},\{\mathcal{H},\eta\}\} = -\eta R_0(\mathcal{H}) - R_{-1}(\mathcal{H}) \tag{2.5}$$

in which the canonical Poisson bracket relations are defined for the canonical coordinate x, its conjugate momentum p and for any functions $A(x,p)$ and $B(x,p)$ as

$$\{x,p\} = 1, \quad \{x,x\} = \{p,p\} = 0, \quad \{A,B\} = \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}. \tag{2.6}$$

The two coefficients R_0 and R_{-1} are, in general, polynomials in the Hamiltonian $\mathcal{H}$. The effect of R_{-1} is to shift the origin of $\eta(x)$ by a quantity (possibly) depending on $\mathcal{H}$. It is convenient to introduce a shifted sinusoidal coordinate $\tilde{\eta}(x)$

$$\tilde{\eta}(x) \overset{\text{def}}{=} \eta(x) + R_{-1}(\mathcal{H})/R_0(\mathcal{H}) \quad (\Rightarrow \{\mathcal{H},\{\mathcal{H},\tilde{\eta}\}\} = -\tilde{\eta}R_0(\mathcal{H})). \tag{2.7}$$

Relation (2.5) would allow to evaluate the multiple Poisson brackets of η with $\mathcal{H}$ easily:

$$\text{ad}\,\mathcal{H}\,\eta \overset{\text{def}}{=} \{\mathcal{H},\eta\}, \quad (\text{ad}\,\mathcal{H})^2\eta = \{\mathcal{H},\{\mathcal{H},\eta\}\}, \quad (\text{ad}\,\mathcal{H})^n\eta = \{\mathcal{H},(\text{ad}\,\mathcal{H})^{n-1}\eta\}, \tag{2.8}$$

which leads to a simple sinusoidal time evolution:

$$\tilde{\eta}(x;t) = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!}(\text{ad}\,\mathcal{H})^n\tilde{\eta}, = -\{\mathcal{H},\tilde{\eta}\}_0 \frac{\sin[t\sqrt{R_0(\mathcal{H}_0)}]}{\sqrt{R_0(\mathcal{H}_0)}} + \tilde{\eta}(x)_0 \cos[t\sqrt{R_0(\mathcal{H}_0)}]. \tag{2.9}$$

In the original variable it reads

$$\eta(x;t) = -\{\mathcal{H},\eta\}_0 \frac{\sin[t\sqrt{R_0(\mathcal{H}_0)}]}{\sqrt{R_0(\mathcal{H}_0)}} - R_{-1}(\mathcal{H}_0)/R_0(\mathcal{H}_0) + (\eta(x)_0 + R_{-1}(\mathcal{H}_0)/R_0(\mathcal{H}_0))\cos[t\sqrt{R_0(\mathcal{H}_0)}], \tag{2.10}$$

in which $\eta(x)_0$ ($\tilde{\eta}(x)_0$), and $\{\mathcal{H},\eta\}_0$ are the initial values (at $t=0$) of these variables and $\mathcal{H}_0$ denotes the value of the Hamiltonian (the energy) for these initial data. In general, the frequency of the simple oscillation $\sqrt{R_0(\mathcal{H}_0)}$ can depend on the initial data. This is the reason why we call $\eta(x)$ the sinusoidal coordinate avoiding the more appealing but misleading "harmonic coordinate."

At the quantum level with the canonical commutation relations

$$[x,p] = i, \quad [x,x] = [p,p] = 0, \quad \hbar \equiv 1, \tag{2.11}$$

the formula corresponding to (2.5) reads

$$[\mathcal{H},[\mathcal{H},\eta]] = \eta R_0(\mathcal{H}) + [\mathcal{H},\eta]R_1(\mathcal{H}) + R_{-1}(\mathcal{H}). \tag{2.12}$$

In other words, the multiple commutators of $\mathcal{H}$ with η form a closed algebra at level two. Here, the quantum coefficients R_0 and R_{-1} could differ from the classical ones by quantum corrections. But we use the same symbols as there is no risk of confusion. Obviously $R_1(\mathcal{H})$ is the quantum effect. As in the classical case, the multiple commutators of η with $\mathcal{H}$

$$\text{ad}\,\mathcal{H}\,\eta \overset{\text{def}}{=} [\mathcal{H},\eta], \quad (\text{ad}\,\mathcal{H})^2\eta = [\mathcal{H},[\mathcal{H},\eta]], \quad (\text{ad}\,\mathcal{H})^n\eta = [\mathcal{H},(\text{ad}\,\mathcal{H})^{n-1}\eta], \tag{2.13}$$

can be easily evaluated from (2.12). This leads to the *exact operator solution* in the Heisenberg picture:

$$e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}} = \sum_{n=0}^{\infty}\frac{(it)^n}{n!}(\text{ad}\,\mathcal{H})^n\eta, = [\mathcal{H},\eta(x)]\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})} - R_{-1}(\mathcal{H})/R_0(\mathcal{H})$$
$$+ (\eta(x) + R_{-1}(\mathcal{H})/R_0(\mathcal{H}))\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t} + \alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})}, \tag{2.14}$$

in which the two "frequencies" $\alpha_\pm(\mathcal{H})$ are

$$\alpha_\pm(\mathcal{H}) = (R_1(\mathcal{H}) \pm \sqrt{R_1(\mathcal{H})^2 + 4R_0(\mathcal{H})})/2, \tag{2.15}$$

$$\alpha_+(\mathcal{H}) + \alpha_-(\mathcal{H}) = R_1(\mathcal{H}), \quad \alpha_+(\mathcal{H})\alpha_-(\mathcal{H}) = -R_0(\mathcal{H}). \tag{2.16}$$

If the quantum effects are neglected, i.e., $R_1 \equiv 0$ and $\mathcal{H} \to \mathcal{H}_0$ [on the right-hand side (r.h.s.)], we have $\alpha_+ = -\alpha_- = \sqrt{R_0(\mathcal{H}_0)}$, the previous Heisenberg operator solution reduces to the classical one (2.10) in terms of the quantum-classical correspondence:

$$[A,B]/i\hbar \to \{A,B\}, \quad (\hbar \to 0). \tag{2.17}$$

The above-mentioned exact operator solution looks slightly simpler if the shifted sinusoidal coordinate is used

$$e^{it\mathcal{H}}\tilde{\eta}(x)e^{-it\mathcal{H}} = [\mathcal{H},\tilde{\eta}(x)]\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})} + \tilde{\eta}(x)\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t} + \alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})}. \tag{2.18}$$

Like the exact classical solution (2.10), the exact quantum solution (2.14) contains all the dynamical information of the quantum system. One can, for example, determine the entire discrete spectrum $\{\mathcal{E}_n\}$ by following Heisenberg and Pauli's arguments for the harmonic oscillator and the hydrogen atom. Let us first note that the ground state energy $\mathcal{E}_0 = 0$ is known explicitly, because of our choice of the factorised form of the exactly solvable Hamiltonian (see the following examples):

$$\mathcal{H} = \mathcal{A}^\dagger\mathcal{A}/2, \quad \mathcal{A}\phi_0 = 0 \Rightarrow \mathcal{H}\phi_0 = 0, \quad \mathcal{E}_0 = 0. \tag{2.19}$$

Let us apply (2.14) to the nth eigenvector ϕ_n:

$$e^{it(\mathcal{H}-\mathcal{E}_n)}\eta(x)\phi_n = ([\mathcal{H},\eta(x)]\phi_n + (-\eta(x)\alpha_-(\mathcal{E}_n) + R_{-1}(\mathcal{E}_n)/\alpha_+(\mathcal{E}_n))\phi_n)e^{i\alpha_+(\mathcal{E}_n)t}/(\alpha_+(\mathcal{E}_n) - \alpha_-(\mathcal{E}_n))$$
$$+ (-[\mathcal{H},\eta(x)]\phi_n + (\eta(x)\alpha_+(\mathcal{E}_n) - R_{-1}(\mathcal{E}_n)/\alpha_-(\mathcal{E}_n))\phi_n)e^{i\alpha_-(\mathcal{E}_n)t}/(\alpha_+(\mathcal{E}_n) - \alpha_-(\mathcal{E}_n))$$
$$- (R_{-1}(\mathcal{E}_n)/R_0(\mathcal{E}_n))\phi_n. \tag{2.20}$$

As the r.h.s. has only two different time dependences except for the constant term, the left-hand-side (l.h.s.) can only have two nonvanishing matrix elements when sandwiched by ϕ_m, except for the obvious ϕ_n corresponding to the constant term. In accordance with the general structure of the eigenfunctions (2.3), they are $\phi_{n\pm1}$:

$$\langle \phi_m | \eta(x) | \phi_n \rangle = 0 \quad \text{for } m \neq n \pm 1, n. \tag{2.21}$$

This imposes the following conditions on the energy eigenvalues:

$$\mathcal{E}_{n+1} - \mathcal{E}_n = \alpha_+(\mathcal{E}_n), \quad \mathcal{E}_{n-1} - \mathcal{E}_n = \alpha_-(\mathcal{E}_n). \tag{2.22}$$

Likewise we obtain the "hermitian conjugate" conditions

$$\mathcal{E}_n - \mathcal{E}_{n-1} = \alpha_+(\mathcal{E}_{n-1}), \quad \mathcal{E}_n - \mathcal{E}_{n+1} = \alpha_-(\mathcal{E}_{n+1}) \tag{2.23}$$

relating these three neighboring eigenvalues. These overdetermined conditions (2.22), (2.23), and $\mathcal{E}_0 = 0$ determine the entire energy spectrum $\{\mathcal{E}_n\}$ completely for each Hamiltonian. The consistency of the procedure requires that the second term on r.h.s. of (2.20) should vanish when applied to the ground state ϕ_0:

$$-[\mathcal{H}, \eta(x)]\phi_0 + (\eta(x)\alpha_+(0) - R_{-1}(0)/\alpha_-(0))\phi_0 = 0, \tag{2.24}$$

which could be interpreted as the equation determining the ground state eigenvector ϕ_0 in the Heisenberg picture. If the number of the discrete levels is finite $(M+1)$ a corresponding condition must be met that the first term on r.h.s. of (2.20) should not belong to the Hilbert space of normalizable vectors when applied to the highest discrete level eigenvector ϕ_M:

$$\|[\mathcal{H}, \eta(x)]\phi_M + (-\eta(x)\alpha_-(\mathcal{E}_M) + R_{-1}(\mathcal{E}_M)/\alpha_+(\mathcal{E}_M))\phi_M\| = \infty. \tag{2.25}$$

As is clear by now, (2.14) and (2.21) are the physical embodiment of the **three term recursion relations** satisfied by any orthogonal polynomial of single variable:

$$\eta P_n(\eta) = A_n P_{n+1}(\eta) + B_n P_n(\eta) + C_n P_{n-1}(\eta). \tag{2.26}$$

The coefficients A_n, B_n, and C_n are also real for a real polynomial $P_n(\eta)$. For the systems treated in this article, that is those having the general structure of the eigenvectors (2.3), this implies the three term recurrence relations of the eigenfunctions

$$\eta(x)\phi_n(x) = A_n\phi_{n+1}(x) + B_n\phi_n(x) + C_n\phi_{n-1}(x). \tag{2.27}$$

At the same time the above-mentioned arguments and the treatment of the harmonic oscillator by Heisenberg clearly show that the operator coefficient of $e^{it\alpha_-(\mathcal{H})}$ on the r.h.s. of the Heisenberg operator solution (2.14) is the annihilation operator, that is, acting on ϕ_n it produces a state ϕ_{n-1}. Likewise, the operator coefficient of $e^{it\alpha_+(\mathcal{H})}$ of the Heisenberg operator solution (2.14) is the creation operator. Thus we arrive at a *dynamical and unified definition* of the **annihilation-creation operators**:

$$e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}} = a^{(+)}(\mathcal{H}, \eta)e^{i\alpha_+(\mathcal{H})t} + a^{(-)}(\mathcal{H}, \eta)e^{i\alpha_-(\mathcal{H})t} - R_{-1}(\mathcal{H})/R_0(\mathcal{H}), \tag{2.28}$$

$$a^{(\pm)} = a^{(\pm)}(\mathcal{H}, \eta) \overset{\text{def}}{=} (\pm[\mathcal{H}, \eta(x)] \mp (\eta(x) + R_{-1}(\mathcal{H})/R_0(\mathcal{H}))\alpha_\mp(\mathcal{H}))/(\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})). \tag{2.29}$$

When acting on the eigenvector ϕ_n, they read

$$a^{(\pm)}\phi_n(x) = \frac{\pm 1}{\mathcal{E}_{n+1} - \mathcal{E}_{n-1}}\left([\mathcal{H}, \eta(x)] + (\mathcal{E}_n - \mathcal{E}_{n\mp 1})\eta(x) + \frac{R_{-1}(\mathcal{E}_n)}{\mathcal{E}_{n\pm 1} - \mathcal{E}_n}\right)\phi_n(x). \tag{2.30}$$

Before going to the detailed discussion of the annihilation-creation operators for various Hamiltonians in Secs. II A and III, let us analyze annihilation-creation operators in a more general context. A minimal requirement for annihilation-creation operators is the following: (0) Annihilation-creation operators map ϕ_n to ϕ_{n-1} and ϕ_{n+1} (up to an overall constant), respectively. It should be stressed that there is no *a priori* principle for fixing the normalization of the operators.

Sometimes it is convenient to introduce the annihilation-creation operators with a different normalization

$$a'^{(\pm)} \overset{\text{def}}{=} a^{(\pm)}(\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})) = \pm[\mathcal{H}, \eta(x)] \mp (\eta(x) + R_{-1}(\mathcal{H})/R_0(\mathcal{H}))\alpha_\mp(\mathcal{H}), \tag{2.31}$$

which gives

$$a'^{(\pm)}\phi_n(x) = \pm\left([\mathcal{H}, \eta(x)] + (\mathcal{E}_n - \mathcal{E}_{n\mp1})\eta(x) + \frac{R_{-1}(\mathcal{E}_n)}{\mathcal{E}_{n\pm1} - \mathcal{E}_n}\right)\phi_n(x). \tag{2.32}$$

On the r.h.s. the coefficients of the operator $\eta(x)$ and the identity operator depend on n in general.

The annihilation-creation operators of the **harmonic oscillator** have several remarkable properties:

(i) Annihilation/creation operator is the positive/negative frequency part of the Heisenberg operator of the sinusoidal coordinate;
(ii) (annihilation operator)†=(creation operator);
(iii) $\mathcal{H}$=const. (creation operator)(annihilation operator).

The first property (i) is the principle leading to our unified definition of the annihilation-creation operators as in (2.28) and (2.29). Next we show that they are hermitian conjugate to each other. That is, they satisfy the property (ii), too. By using the three-term recursion relation, we obtain

$$e^{it\mathcal{H}}\eta e^{-it\mathcal{H}}\phi_n = e^{it(\mathcal{E}_{n+1}-\mathcal{E}_n)}A_n\phi_{n+1} + B_n\phi_n + e^{it(\mathcal{E}_{n-1}-\mathcal{E}_n)}C_n\phi_{n-1}. \tag{2.33}$$

Comparing this with (2.28) and (2.29), we arrive at

$$a^{(+)}\phi_n = A_n\phi_{n+1}, \quad a^{(-)}\phi_n = C_n\phi_{n-1}, \quad R_{-1}(\mathcal{E}_n)/R_0(\mathcal{E}_n) = -B_n. \tag{2.34}$$

Here use is made of the facts

$$\alpha_+(\mathcal{E}_n) = \mathcal{E}_{n+1} - \mathcal{E}_n, \quad \alpha_-(\mathcal{E}_n) = \mathcal{E}_{n-1} - \mathcal{E}_n,$$

$$R_1(\mathcal{E}_n) = \mathcal{E}_{n+1} + \mathcal{E}_{n-1} - 2\mathcal{E}_n, \quad R_0(\mathcal{E}_n) = -(\mathcal{E}_{n+1} - \mathcal{E}_n)(\mathcal{E}_{n-1} - \mathcal{E}_n), \tag{2.35}$$

and that $\alpha_\pm(\mathcal{H})$ and $R_i(\mathcal{H})$ $(i=1,0,-1)$ are hermitian. Hermitian conjugate of $a^{(-)}$ is

$$a^{(-)\dagger} = (\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H}))^{-1}([\mathcal{H}, \eta(x)] + \alpha_+(\mathcal{H})(\eta(x) + R_{-1}(\mathcal{H})/R_0(\mathcal{H}))), \tag{2.36}$$

and its action on ϕ_n is

$$\begin{aligned} a^{(-)\dagger}\phi_n &= (\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H}))^{-1}(\mathcal{H}\eta\phi_n - \eta\mathcal{E}_n\phi_n + \alpha_+(\mathcal{H})(\eta\phi_n + R_{-1}(\mathcal{E}_n)/R_0(\mathcal{E}_n)\phi_n)) \\ &= (\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H}))^{-1}((\mathcal{E}_{n+1} - \mathcal{E}_n)A_n\phi_{n+1} + (\mathcal{E}_{n-1} - \mathcal{E}_n)C_n\phi_{n-1} + \alpha_+(\mathcal{H})(A_n\phi_{n+1} + C_n\phi_{n-1})) \\ &= (\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H}))^{-1}(\mathcal{E}_{n+2} - \mathcal{E}_n)A_n\phi_{n+1} = A_n\phi_{n+1} = a^{(+)}\phi_n. \end{aligned} \tag{2.37}$$

Therefore $a^{(\pm)}$ are hermitian conjugate to each other, $a^{(-)\dagger}=a^{(+)}$. This also means that

$$e^{-it\alpha_-(\mathcal{H})}a^{(+)} = a^{(+)}e^{it\alpha_+(\mathcal{H})}, \quad e^{-it\alpha_+(\mathcal{H})}a^{(-)} = a^{(-)}e^{it\alpha_-(\mathcal{H})}, \tag{2.38}$$

reflecting the obvious hermiticity of the l.h.s. of (2.28). Note that $a'^{(\pm)}$ are not hermitian conjugate to each other, $a'^{(-)\dagger} \neq a'^{(+)}$, in general.

In the special case of the equi-spaced spectrum $\mathcal{E}_n=an$ (a: constant), to which many interesting examples belong including the harmonic oscillator and its deformation, we have $\alpha_\pm(\mathcal{H})=\pm a$, $R_1(\mathcal{H})=0$, $R_0(\mathcal{H})=a^2$ and

$$2aa^{(\pm)} = a'^{(\pm)} = \pm[\mathcal{H}, \eta(x)] + a\eta(x) + R_{-1}(\mathcal{H})/a. \tag{2.39}$$

For the simplest harmonic oscillator $\mathcal{H}=(p+ix)(p-ix)/2$, we have $\eta(x)=x$, $R_0=1$, $R_1=R_{-1}=0$ and $[\mathcal{H},x]=-ip$ and $2a^{(+)}=x-ip$, $2a^{(-)}=x+ip$, which differ from the conventional ones by a factor $\sqrt{2}$.

In contrast to the above two properties, the third the property (iii) of the annihilation-creation operators is achieved by a very specific modification of the definition as follows:

$$a''^{(-)} \overset{\text{def}}{=} a^{(-)} f(\mathcal{H}), \quad a''^{(+)} \overset{\text{def}}{=} a''^{(-)\dagger} = f(\mathcal{H}) a^{(+)}, \tag{2.40}$$

where $f(\mathcal{H})=f(\mathcal{H})^\dagger$ is an as yet unspecified function of $\mathcal{H}$. Then we have

$$a''^{(+)} a''^{(-)} \phi_n = f(\mathcal{E}_n)^2 A_{n-1} C_n \phi_n. \tag{2.41}$$

If $f(\mathcal{H})$ is chosen to satisfy

$$f(\mathcal{E}_n)^2 = \mathcal{E}_n/(A_{n-1}C_n) \overset{\text{def}}{(=g(n))}, \tag{2.42}$$

then we obtain

$$\mathcal{H} = a''^{(+)} a''^{(-)}. \tag{2.43}$$

Such an operator $f(\mathcal{H})$ function can be constructed as $f(\mathcal{H})=\sqrt{g(\mathcal{N})}$, where the number (or level) operator $\mathcal{N}$ is defined by

$$\mathcal{N}\phi_n = n\phi_n. \tag{2.44}$$

This operator $\mathcal{N}$ can be expressed in terms of the Hamiltonian, for example,

$$\mathcal{E}_n = an \Rightarrow \mathcal{N} = \mathcal{H}/a, \tag{2.45}$$

$$\mathcal{E}_n = an^2 + bn \Rightarrow \mathcal{N} = (\sqrt{4a\mathcal{H} + b^2} - b)/(2a), \tag{2.46}$$

$$\mathcal{E}_n = a(q^{-n} - 1)(1 - bq^n) \Rightarrow q^{\mathcal{N}} = (\mathcal{H}/a + b + 1 - \sqrt{(\mathcal{H}/a + b + 1)^2 - 4b})/(2b), \tag{2.47}$$

where a, b, and q are constant ($b>0$ in the second equation, $b<1$ in the third equation). This $a''^{(\pm)}$ satisfies the property (ii) by definition, but the property (i) becomes ugly or unnatural in general.

Let us close the general theory by a brief discussion of the coherent states. One definition of the coherent state ψ is the eigenvector of the annihilation operator [annihilation operator coherent state (AOCS)]:

$$a^{(-)}\psi = \lambda\psi, \quad \lambda \in \mathbb{C}. \tag{2.48}$$

In terms of the simple parametrization $\psi=\Sigma_{n=0}^{\infty} c_n \phi_n(x)$ (with $c_0=1$ as normalization) and the formula (2.34), we arrive at

$$\psi = \psi(\lambda, x) = \phi_0(x) \sum_{n=0}^{\infty} \frac{\lambda^n}{\prod_{k=1}^{n} C_n} \cdot P_n(\eta(x)). \tag{2.49}$$

For the equispaced spectrum $\mathcal{E}_n=an$ (a: constant), the coherent state has the property of temporal stability

$$e^{it\mathcal{H}}\psi(\lambda, x) = \psi(e^{iat}\lambda, x). \tag{2.50}$$

It should be remarked that the concrete form of the AOCS depends on the specific normalization of the annihilation operator. For the annihilation operators $a'^{(-)}$, $a''^{(-)}$ and others, we denote the

corresponding coherent states as ψ', ψ'', etc. Which coherent state is useful depends on the physics of the system.

A. Some typical examples

Now let us look at typical examples[1–3] to show the actual content of our new unified theory of annihilation-creation operators. In their pioneering work, Nieto and Simmons[4] treated four solvable cases, those discussed in Secs. II A 1, III A 1, III A 3, and III A 4. Some of our results were reported in Ref. 4. Here and throughout this article we put the dimensionfull quantities as unity, including the Planck's constant.

1. $1/\sin^2 x$ *potential, or symmetric Pöschl-Teller potential*

The first example has the $1/\sin^2 x$ potential, which is the one-body case of the well-known Sutherland model.[10,11] This provides the simplest example of the annihilation-creation operators depending on n. The corresponding coherent state (2.72) or (2.75) had not yet been known, to the best of our knowledge. The system is confined in a finite interval, say $(0,\pi)$ and it has an infinite number of discrete eigenstates. Although this potential is a special $(g=h)$ case of the Pöschl-Teller potential discussed in Sec. III A 2, it merits separate analysis. The Hamiltonian, the eigenvalues and the eigenfunctions are as follows:

$$\mathcal{H} \overset{\text{def}}{=} (p - ig\cot x)(p + ig\cot x)/2, \quad (\overset{\text{Q.M.}}{\Rightarrow} 2\mathcal{H} + g^2 = p^2 + g(g-1)/\sin^2 x), \tag{2.51}$$

$$\mathcal{E}_n = n(n/2+g), \quad n = 0,1,2,\ldots, \quad g > 0, \quad 0 < x < \pi, \quad \eta(x) = \cos x, \tag{2.52}$$

$$\phi_n(x) = (\sin x)^g P_n^{(\beta,\beta)}(\cos x), \quad \beta \overset{\text{def}}{=} g - 1/2, \tag{2.53}$$

in which $P_n^{(\alpha,\beta)}(\eta)$ is the Jacobi polynomial (C8) and $P_n^{(\beta,\beta)}(\eta)$ is proportional to the Gegenbauer polynomial $C_n^{(\beta+1/2)}(\eta)$ (C9)

$$\frac{P_n^{(\beta,\beta)}(\eta)}{(\beta+1)_n} = \frac{C_n^{(\beta+1/2)}(\eta)}{(2\beta+1)_n}. \tag{2.54}$$

Hereafter we often use the Pochhammer symbol $(a)_n$, see (C1).

It is straightforward to evaluate the Poisson brackets

$$\{\mathcal{H},\cos x\} = p\sin x, \quad \{\mathcal{H},\{\mathcal{H},\cos x\}\} = -\cos x\, 2\mathcal{H}', \quad \mathcal{H}' \overset{\text{def}}{=} \mathcal{H} + g^2/2, \tag{2.55}$$

leading to the solution of the initial value problem:

$$\cos x(t) = \cos x(0)\cos[t\sqrt{2\mathcal{H}_0'}] - p(0)\sin x(0)\frac{\sin[t\sqrt{2\mathcal{H}_0'}]}{\sqrt{2\mathcal{H}_0'}}. \tag{2.56}$$

It is straightforward to verify $|\cos x(t)| < 1$. The corresponding quantum expressions are

$$[\mathcal{H},\cos x] = i\sin x\, p + \cos x/2, \tag{2.57}$$

$$[\mathcal{H},[\mathcal{H},\cos x]] = \cos x(2\mathcal{H}' - 1/4) + [\mathcal{H},\cos x], \tag{2.58}$$

$$\alpha_\pm(\mathcal{H}) = 1/2 \pm \sqrt{2\mathcal{H}'}. \tag{2.59}$$

The exact operator solution reads

$$e^{it\mathcal{H}}\cos x\, e^{-it\mathcal{H}} = (i\sin x\, p + \cos x/2)\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}} + \cos x\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t} + \alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}}. \tag{2.60}$$

The annihilation and creation operators are

$$a'^{(\pm)} = a^{(\pm)}2\sqrt{2\mathcal{H}'} = \pm i\sin x\, p + \cos x\,\sqrt{2\mathcal{H}'} = \pm\sin x\frac{\mathrm{d}}{\mathrm{d}x} + \cos x\,\sqrt{2\mathcal{H}'}. \tag{2.61}$$

It is now obvious that they ($a'^{(\pm)}$) are not hermitian conjugate to each other. The square root sign is neatly removed when applied to the eigenvector ϕ_n as $2\mathcal{E}_n+g^2=(n+g)^2$:

$$a'^{(-)}\phi_n = -\sin x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (n+g)\cos x\,\phi_n = (n+\beta)\phi_{n-1}, \tag{2.62}$$

$$a'^{(+)}\phi_n = \sin x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (n+g)\cos x\,\phi_n = \frac{2(n+1)(n+2g)}{2n+2g+1}\phi_{n+1}. \tag{2.63}$$

This is a rule rather than exception as expected from the relations between the neighboring energy levels, (2.22) and (2.23). The right-hand sides are the results of the application. In particular, when acting on the ground state ϕ_0, the annihilation ($a'^{(-)}$) and creation ($a'^{(+)}$) operators are proportional to the factorization operators $\mathcal{A}$ and $\mathcal{A}^\dagger$ of the Hamiltonian $\mathcal{H}=\mathcal{A}^\dagger\mathcal{A}/2$, respectively:

$$a'^{(-)}\phi_0 = \left(-\sin x\frac{\mathrm{d}}{\mathrm{d}x} + g\cos x\right)\phi_0 = -\sin x\left(\frac{\mathrm{d}}{\mathrm{d}x} - g\cot x\right)\phi_0 = \eta'(x)\mathcal{A}\phi_0 = 0,$$

$$a'^{(+)}\phi_0 = \left(\sin x\frac{\mathrm{d}}{\mathrm{d}x} + g\cos x\right)\phi_0 = -\sin x\left(-\frac{\mathrm{d}}{\mathrm{d}x} - g\cot x\right)\phi_0 = \eta'(x)\mathcal{A}^\dagger\phi_0. \tag{2.64}$$

In a rough sense, the factor $\eta'(x)=-\sin x$, in the creation operator, compensates the downward shift of the parameter (g) caused by $\mathcal{A}^\dagger$. Similar situations are encountered in all the other quantum systems. In particular, for the systems with equispaced spectrum $\mathcal{E}_n=an$ (a: constant), the factorization of $a'^{(-)}$ and $a'^{(+)}$ into $\mathcal{A}$ and $\mathcal{A}^\dagger$ is n independent, (2.94), (3.14), (3.15), and (3.92). Their significance will be discussed in some detail for the "discrete" quantum mechanics cases in Appendix B.

The following interesting commutation relations ensue from (2.62) and (2.63):

$$[\mathcal{H},a'^{(\pm)}] = \pm(\sqrt{2\mathcal{H}'}a'^{(\pm)} + a'^{(\pm)}\sqrt{2\mathcal{H}'})/2, \tag{2.65}$$

$$[a'^{(-)},a'^{(+)}] = 2\sqrt{2\mathcal{H}'}, \tag{2.66}$$

$$a'^{(-)}a'^{(+)} + a'^{(+)}a'^{(-)} = 4\mathcal{H} + 2g. \tag{2.67}$$

The relation (2.67) could be accepted as a substitute of the property (iii) of the annihilation-creation operators discussed previously.

By the similarity transformation in terms of the ground state wave function $\phi_0(x)=(\sin x)^g$, we obtain the so-called shift down and up operators for the Jacobi (Gegenbauer) polynomial ($\beta=g-1/2$):

$$\text{down:}\quad (1-\eta^2)\frac{\mathrm{d}}{\mathrm{d}\eta}P_n^{(\beta,\beta)}(\eta) + n\eta P_n^{(\beta,\beta)}(\eta) = (n+\beta)P_{n-1}^{(\beta,\beta)}(\eta), \tag{2.68}$$

$$\text{up:}\quad -(1-\eta^2)\frac{\mathrm{d}}{\mathrm{d}\eta}P_n^{(\beta,\beta)}(\eta)+(n+2g)\,\eta P_n^{(\beta,\beta)}(\eta)=\frac{2(n+1)(n+2g)}{2n+2g+1}P_{n+1}^{(\beta,\beta)}(\eta). \tag{2.69}$$

As expected they are the same Jacobi polynomials of degree $n-1$ and $n+1$. It should be stressed that these shift down-up operators are naturally derived from our annihilation-creation operators without assuming the explicit form of the three term recursion relation.

The coherent state ψ (2.48) is

$$\psi(x)=\phi_0(x)\sum_{n=0}^{\infty}(2\lambda)^n\frac{(\beta+3/2)_n}{(\beta+1)_n}P_n^{(\beta,\beta)}(\cos x)=\phi_0(x)\sum_{n=0}^{\infty}(2\lambda)^n\frac{(g+1)_n}{(2g)_n}C_n^{(g)}(\cos x), \tag{2.70}$$

where we have used $a^{(-)}\phi_n=a'^{(-)}\phi_n/(2(n+g))$, (2.62) and (2.54). A generating function of the Gegenbauer polynomials (γ: arbitrary),[6]

$$\sum_{n=0}^{\infty}t^n\frac{(\gamma)_n}{(2g)_n}C_n^{(g)}(\eta)=(1-\eta t)^{-\gamma}{}_2F_1\left(\begin{matrix}\gamma/2,(\gamma+1)/2\\ g+1/2\end{matrix}\middle|\frac{(\eta^2-1)t}{(1-\eta t)^2}\right), \tag{2.71}$$

gives a concise expression of the coherent state ψ:

$$\psi(x)=(1-2\lambda\cos x)^{-g-1}\,{}_2F_1\left(\begin{matrix}(g+1)/2,g/2+1\\ g+1/2\end{matrix}\middle|\frac{-2\lambda\sin^2 x}{(1-2\lambda\cos x)^2}\right). \tag{2.72}$$

Here ${}_2F_1$ is the hypergeometric function (C3). For the annihilation operator $a'^{(-)}$, the corresponding coherent state ψ' is

$$\psi'(x)=\phi_0(x)\sum_{n=0}^{\infty}\frac{\lambda^n}{(\beta+1)_n}P_n^{(\beta,\beta)}(\cos x)=\phi_0(x)\sum_{n=0}^{\infty}\frac{\lambda^n}{(2g)_n}C_n^{(g)}(\cos x). \tag{2.73}$$

A generating function of the Gegenbauer polynomials,[6]

$$\sum_{n=0}^{\infty}\frac{t^n}{(2g)_n}C_n^{(g)}(\eta)=e^{\eta t}{}_0F_1\left(\begin{matrix}-\\ g+1/2\end{matrix}\middle|\frac{(\eta^2-1)t^2}{4}\right), \tag{2.74}$$

gives a concise expression of the coherent state ψ':

$$\psi'(x)=\Gamma(g+1/2)e^{\lambda\cos x}(\lambda/2)^{1/2-g}\sqrt{\sin x}J_{g-1/2}(\lambda\sin x), \tag{2.75}$$

in which $J_a(x)$ is the Bessel function (C5).

2. Deformed harmonic oscillator ⇒ Meixner-Pollaczek polynomial

The deformed harmonic oscillator is a simplest example of shape invariant discrete quantum mechanics. The Hamiltonian of discrete quantum mechanics studied in this article has the following form[2] (with some modification for the Askey-Wilson case in Sec. II A 3):

$$\mathcal{H}\overset{\text{def}}{=}(\sqrt{V(x)}e^p\sqrt{V(x)}^*+\sqrt{V(x)}^*e^{-p}\sqrt{V(x)}-V(x)-V(x)^*)/2. \tag{2.76}$$

The eigenvalue problem for $\mathcal{H}$, $\mathcal{H}\phi=\mathcal{E}\phi$ is a difference equation, instead of a second order differential equation. Let us define $S_\pm$, $T_\pm$, and $\mathcal{A}$ by

$$S_+\overset{\text{def}}{=}e^{p/2}\sqrt{V(x)}^*,\quad S_-\overset{\text{def}}{=}e^{-p/2}\sqrt{V(x)},\quad S_+^\dagger=\sqrt{V(x)}e^{p/2},\quad S_-^\dagger=\sqrt{V(x)}^*e^{-p/2}, \tag{2.77}$$

$$T_+\overset{\text{def}}{=}S_+^\dagger S_+=\sqrt{V(x)}e^p\sqrt{V(x)}^*,\quad T_-\overset{\text{def}}{=}S_-^\dagger S_-=\sqrt{V(x)}^*e^{-p}\sqrt{V(x)}, \tag{2.78}$$

$$\overset{\text{def}}{\mathcal{A}} = i(S_+ - S_-), \quad \mathcal{A}^\dagger = -i(S_+^\dagger - S_-^\dagger). \tag{2.79}$$

Then the Hamiltonian is factorized

$$\mathcal{H} = (T_+ + T_- - V(x) - V(x)^*)/2 = (S_+^\dagger - S_-^\dagger)(S_+ - S_-)/2 = \mathcal{A}^\dagger \mathcal{A}/2. \tag{2.80}$$

The potential function $V(x)$ of the deformed harmonic oscillator is

$$V(x) = a + ix, \quad -\infty < x < \infty, \quad a > 0. \tag{2.81}$$

As shown in some detail in our previous paper,[2] it has an equispaced spectrum and the corresponding eigenfunctions are a special case of the Meixner-Pollaczek polynomial $P_n^{(a)}(x;\pi/2)$ (C10),

$$\mathcal{E}_n = n, \quad n = 0,1,2,\ldots, \tag{2.82}$$

$$\phi_0(x) = \sqrt{\Gamma(a+ix)\Gamma(a-ix)}, \quad \eta(x) = x, \tag{2.83}$$

$$\phi_n(x) = \phi_0(x)P_n(x), \quad \overset{\text{def}}{P_n(x)} = P_n^{(a)}\left(x;\tfrac{\pi}{2}\right), \tag{2.84}$$

which could be considered as a deformation of the Hermite polynomial.

The Poisson bracket relations are

$$\{\mathcal{H},x\} = -\sqrt{a^2+x^2}\sinh p, \quad \{\mathcal{H},\{\mathcal{H},x\}\} = -x, \tag{2.85}$$

leading to the harmonic oscillation,

$$x(t) = x(0)\cos t + \sqrt{a^2+x^2(0)}\sinh p(0)\sin t, \tag{2.86}$$

which endorses the naming of the deformed harmonic oscillator. The corresponding quantum expressions are also simple:

$$[\mathcal{H},x] = -i(T_+ - T_-)/2, \quad [\mathcal{H},[\mathcal{H},x]] = x, \tag{2.87}$$

$$e^{it\mathcal{H}}xe^{-it\mathcal{H}} = x\cos t + i[\mathcal{H},x]\sin t = x\cos t + (T_+ - T_-)/2\sin t. \tag{2.88}$$

The annihilation and creation operators are

$$a'^{(\pm)} = 2a^{(\pm)} = x \pm [\mathcal{H},x] = x \mp i(T_+ - T_-)/2, \tag{2.89}$$

which are hermitian conjugate to each other. These operators were also introduced by Degasperis and Ruijsenaars[12] by a different reasoning from ours. By similarity transformation in terms of the ground state wave function $\phi_0(x) = \sqrt{\Gamma(a+ix)\Gamma(a-ix)}$, we obtain

$$\phi_0(x)^{-1}a'^{(\pm)}\phi_0(x) = x \mp i(V(x)e^p - V(x)^*e^{-p})/2. \tag{2.90}$$

The action of the annihilation creation operators on the eigenvectors

$$a'^{(-)}\phi_n = (n+2a-1)\phi_{n-1}, \quad a'^{(+)}\phi_n = (n+1)\phi_{n+1} \tag{2.91}$$

is consistent with the three term recurrence relation of the Meixner-Pollaczek polynomial:

$$(n+1)P_{n+1}^{(a)}\left(x;\tfrac{\pi}{2}\right) - 2xP_n^{(a)}\left(x;\tfrac{\pi}{2}\right) + (n+2a-1)P_{n-1}^{(a)}\left(x;\tfrac{\pi}{2}\right) = 0. \tag{2.92}$$

From these it is easy to verify the su(1,1) commutation relations including the Hamiltonian $\mathcal{H}$:

$$[\mathcal{H},a'^{(\pm)}]=\pm a'^{(\pm)},\quad [a'^{(-)},a'^{(+)}]=2(\mathcal{H}+a). \tag{2.93}$$

It is interesting to note that $a^{(\pm)}$ are factorized by the factors of the Hamiltonian $\mathcal{H}=\mathcal{A}^\dagger\mathcal{A}/2$,

$$4a^{(-)}=X^\dagger\mathcal{A},\quad 4a^{(+)}=\mathcal{A}^\dagger X, \tag{2.94}$$

$$\overset{\text{def}}{X}=S_+ +S_-,\quad X^\dagger=S_+^\dagger+S_-^\dagger. \tag{2.95}$$

These X and $X^\dagger$ compensate the shift of the parameter a caused by $\mathcal{A}^\dagger$ and $\mathcal{A}$. See Appendix B for more details.

The coherent state (2.48), (2.49), is simply obtained from formula (2.91) and $a'^{(-)}=2a^{(-)}$:

$$\psi(x)=\phi_0(x)\sum_{n=0}^{\infty}\frac{(2\lambda)^n}{(2a)_n}P_n^{(a)}\left(x;\tfrac{\pi}{2}\right). \tag{2.96}$$

A generating function of the Meixner-Pollaczek polynomial,[6]

$$\sum_{n=0}^{\infty}\frac{t^n}{(2a)_n}P_n^{(a)}\left(x;\tfrac{\pi}{2}\right)=e^{it}{}_1F_1\left(\begin{matrix}a+ix\\2a\end{matrix}\middle|-2it\right), \tag{2.97}$$

gives a concise expression of the coherent state ψ:

$$\psi(x)=\phi_0(x)e^{2i\lambda}{}_1F_1\left(\begin{matrix}a+ix\\2a\end{matrix}\middle|-4i\lambda\right), \tag{2.98}$$

in which ${}_1F_1$ is the hypergeometric function (C3).

3. Askey-Wilson polynomial

The Askey-Wilson polynomial belongs to the so-called q-scheme of hypergeometric polynomials.[6] It has four parameters a_1,a_2,a_3, and a_4 on top of q $(0<q<1)$, and is considered as a three-parameter deformation of the Jacobi polynomial. As shown in previous articles,[3,2] it also describes the equilibrium positions of the trigonometric Ruijsenaars-Schneider systems based on the BC root system.[13] Thus, as a dynamical system, it could be called a deformed Pöschl-Teller potential or one body case of the trigonometric BC Ruijsenaars-Schneider systems. The quantum-classical correspondence has some more subtlety than the other discrete quantum mechanical systems treated in Sec. III B because of another "classical" limit $q\to 1$.

The factorized Hamiltonian of the Askey-Wilson polynomial has a bit different form from that of the Meixner-Pollaczek polynomial (2.76):

$$\overset{\text{def}}{\mathcal{H}}=(\sqrt{V(z)}q^D\sqrt{V(z)}^*+\sqrt{V(z)}^*q^{-D}\sqrt{V(z)}-V(z)-V(z)^*)/2, \tag{2.99}$$

with a potential function $V(z)$:

$$V(z)=\frac{\prod_{j=1}^4(1-a_jz)}{(1-z^2)(1-qz^2)},\quad z=e^{ix},\quad 0<x<\pi,\quad \overset{\text{def}}{D}=z\frac{d}{dz}=-i\frac{\mathrm{d}}{\mathrm{d}x}=p. \tag{2.100}$$

We assume $-1<a_1,a_2,a_3,a_4<1$ and $a_1a_2a_3a_4<q$. This Hamiltonian is also factorized $\mathcal{H}=\mathcal{A}^\dagger\mathcal{A}/2$, where $\mathcal{A}$ and $\mathcal{A}^\dagger$ are given in (2.77)–(2.79) with the replacement $V(x)\Rightarrow V(z)$, $e^{\pm p/2}\Rightarrow q^{\pm D/2}$, etc. The eigenvalues and eigenfunctions are:[2,3]

$$\mathcal{E}_n=(q^{-n}-1)(1-a_1a_2a_3a_4q^{n-1})/2,\quad n=0,1,2,\dots, \tag{2.101}$$

$$\phi_0(x) = \sqrt{\frac{(z^2;q)_\infty}{\prod_{j=1}^4 (a_j z;q)_\infty}\frac{(z^{-2};q)_\infty}{\prod_{j=1}^4 (a_j z^{-1};q)_\infty}}, \quad \eta(x) = \frac{z+z^{-1}}{2} = \cos x, \tag{2.102}$$

$$\phi_n(x) = \phi_0(x) P_n(\cos x), \quad P_n(\eta) \overset{\text{def}}{=} p_n(\eta;a_1,a_2,a_3,a_4|q), \tag{2.103}$$

in which $p_n(\eta;a_1,a_2,a_3,a_4|q)$ is the Askey-Wilson polynomial (C14).

The presence of the q factor has only superficial effects at the classical level with the Hamiltonian ($\gamma = \log q$):

$$\mathcal{H}_c = \sqrt{V_c(z)V_c(z)^*}\cosh\gamma p - (V_c(z) + V_c(z)^*)/2, \quad V_c(z) = \frac{\prod_{j=1}^4 (1-a_j z)}{(1-z^2)^2}, \tag{2.104}$$

$$\{\mathcal{H}_c, \cos x\} = \gamma\sqrt{\prod_{j=1}^4 (1-a_j z)\prod_{j=1}^4 (1-a_j/z)}/(4\sin x)\sinh\gamma p, \tag{2.105}$$

$$\{\mathcal{H}_c, \{\mathcal{H}_c, \cos x\}\} = -\cos x\, R_0(\mathcal{H}_c) - R_{-1}(\mathcal{H}_c), \tag{2.106}$$

$$R_0(\mathcal{H}_c) = \gamma^2(\mathcal{H}_c^2 + c_1\mathcal{H}_c + c_2), \quad R_{-1}(\mathcal{H}_c) = -\gamma^2(c_3\mathcal{H}_c + c_4), \tag{2.107}$$

with coefficients $c_1, \ldots, c_4$:

$$c_1 = 1 + b_4, \quad c_2 = (1-b_4)^2/4, \quad c_3 = (b_1+b_3)/4, \quad c_4 = (1-b_4)(b_1-b_3)/8. \tag{2.108}$$

Here we use the abbreviation

$$b_1 \overset{\text{def}}{=} \sum_{1\le j\le 4} a_j, \quad b_3 \overset{\text{def}}{=} \sum_{1\le j<k<l\le 4} a_j a_k a_l, \quad b_4 \overset{\text{def}}{=} \prod_{j=1}^4 a_j. \tag{2.109}$$

The corresponding quantum expressions are

$$[\mathcal{H}, \cos x] = (q^{-1}-1)(z^{-1}(1-qz^2)T_+ + z(1-qz^{-2})T_-)/4, \tag{2.110}$$

$$[\mathcal{H}, [\mathcal{H}, \cos x]] = \cos x R_0(\mathcal{H}) + [\mathcal{H}, \cos x]R_1(\mathcal{H}) + R_{-1}(\mathcal{H}), \tag{2.111}$$

$$R_0(\mathcal{H}) = q(q^{-1}-1)^2((\mathcal{H}')^2 - (1+q^{-1})^2 b_4/4), \tag{2.112}$$

$$R_1(\mathcal{H}) = q(q^{-1}-1)^2\mathcal{H}', \quad \mathcal{H}' \overset{\text{def}}{=} \mathcal{H} + (1+q^{-1}b_4)/2, \tag{2.113}$$

$$R_{-1}(\mathcal{H}) = -q(q^{-1}-1)^2((b_1+q^{-1}b_3)\mathcal{H}/4 + (1-q^{-2}b_4)(b_1-b_3)/8). \tag{2.114}$$

The two frequencies are:

$$\alpha_\pm(\mathcal{H}) = (q^{-1}-1)((1-q)\mathcal{H}' \pm (1+q)\sqrt{(\mathcal{H}')^2 - q^{-1}b_4})/2, \tag{2.115}$$

in which

$$\mathcal{H}'\phi_n = (q^{-n} + b_4 q^{n-1})/2\phi_n, \quad ((\mathcal{H}')^2 - q^{-1}b_4)\phi_n = (q^{-n} - b_4 q^{n-1})^2/4\phi_n. \tag{2.116}$$

The annihilation-creation operators are

$$a^{(\pm)} = (\pm(q^{-1}-1)(z^{-1}(1-qz^2)T_+ + z(1-qz^{-2})T_-)/4 \mp \cos x\ \alpha_{\mp}(\mathcal{H}) \pm R_{-1}(\mathcal{H})\alpha_{\pm}(\mathcal{H})^{-1})/(\alpha_+(\mathcal{H})-\alpha_-(\mathcal{H})). \tag{2.117}$$

Their effects on the eigenvectors are

$$a^{(-)}\phi_n = \frac{(1-q^n)\prod_{1\le j<k\le 4}(1-a_ja_kq^{n-1})}{2(1-b_4q^{2n-2})(1-b_4q^{2n-1})}\phi_{n-1}, \tag{2.118}$$

$$a^{(+)}\phi_n = \frac{1-b_4q^{n-1}}{2(1-b_4q^{2n-1})(1-b_4q^{2n})}\phi_{n+1}, \tag{2.119}$$

which are consistent with the three-term recurrence relation of the Askey-Wilson polynomial. The "annihilation-creation" operators on the polynomial $P_n(\cos x)$ read

$$\phi_0(x)^{-1}a^{(\pm)}\phi_0(x)\cdot P_n(\cos x) = \frac{1}{\mathcal{E}_{n+1}-\mathcal{E}_{n-1}}\left(\pm(q^{-1}-1)(z^{-1}(1-qz^2)V(z)q^D + z(1-qz^{-2})V(z)^*q^{-D})/4 \pm (\mathcal{E}_n-\mathcal{E}_{n\mp 1})\cos x \pm \frac{R_{-1}(\mathcal{E}_n)}{\mathcal{E}_{n\pm 1}-\mathcal{E}_n}\right)P_n(\cos x). \tag{2.120}$$

The coherent state is

$$\psi(x) = \phi_0(x)\sum_{n=0}^{\infty}\frac{(2\lambda)^n}{(q;q)_n}\frac{(a_1a_2a_3a_4;q)_{2n}}{\prod_{1\le j<k\le 4}(a_ja_k;q)_n}P_n(\cos x). \tag{2.121}$$

We are not aware if a concise summation formula exists or not.

III. VARIOUS RESULTS

In this section we will briefly present many interesting results on the annihilation-creation operators, their algebraic properties and coherent states, etc., for various exactly solvable quantum mechanical systems, including the discrete quantum mechanical systems. All these solvable systems share *shape invariance*[8,1,2] which is a purely quantum mechanical notion that guarantees quantum solvability. But that property plays no active role in the present theory. On the other hand, the sinusoidal motion exists at the classical and quantum levels. In Appendix A we will show that a system realizing the exact sinusoidal motion is quite limited and that all of them belong to the known shape invariant systems. In other words there are shape invariant systems that do not have sinusoidal motion.

A. Ordinary quantum mechanical systems

1. x^2+1/x^2 potential

When a centrifugal barrier (a $1/x^2$ potential) is added, the harmonic oscillator keeps its exact solvability, but the particle is restricted to a half line, either $x>0$ or $x<0$. This is the one-body case of the well-known Calogero model.[10,11] The eigenfunctions are described by the Laguerre polynomial and the annihilation-creation operators within the su(1,1) scheme are well-known.[4,14] Our unified theory predicts these operators naturally. The coherent and squeezed states in the su(1,1) were already known.[14] Its Hamiltonian, the eigenvalues and the eigenfunctions are:

$$\mathcal{H} \overset{\text{def}}{=} (p+ix-ig/x)(p-ix+ig/x)/2, \quad 0<x<\infty, \quad g>0, \tag{3.1}$$

$$\mathcal{E}_n = 2n, \quad n = 0,1,2,\ldots, \quad \eta(x) = x^2, \tag{3.2}$$

$$\phi_n(x) = \phi_n(x;g) = e^{-x^2/2}x^g L_n^{(\beta)}(x^2), \quad \beta \overset{\text{def}}{=} g - 1/2, \tag{3.3}$$

in which $L_n^{(\beta)}(\eta)$ is the Laguerre polynomial (C7).

The Poisson bracket relations are simple

$$\{\mathcal{H},x^2\} = -2px, \quad \{\mathcal{H},\{\mathcal{H},x^2\}\} = -4(x^2 - \mathcal{H} - g), \tag{3.4}$$

leading to the simple sinusoidal motion

$$x^2(t) = x^2(0)\cos 2t + (1 - \cos 2t)(\mathcal{H}_0 + g) + p(0)x(0)\sin 2t. \tag{3.5}$$

It is straightforward to verify $x^2(t) > 0$. The quantum theory is almost the same as the classical one:

$$[\mathcal{H},x^2] = -i(xp + px), \quad [\mathcal{H},[\mathcal{H},x^2]] = 4(x^2 - \mathcal{H}'), \quad \mathcal{H}' \overset{\text{def}}{=} \mathcal{H} + g + 1/2, \tag{3.6}$$

$$e^{it\mathcal{H}}x^2e^{-it\mathcal{H}} = x^2\cos 2t + (1 - \cos 2t)\mathcal{H}' + (xp + px)/2\sin 2t, \tag{3.7}$$

which leads to the following annihilation and creation operators:

$$a^{(\pm)} = (x^2 - \mathcal{H}')/2 \mp i(xp + px)/4 = \left(\left(\frac{\mathrm{d}}{\mathrm{d}x} \mp x\right)^2 - \frac{g(g-1)}{x^2}\right) \Big/ 4. \tag{3.8}$$

The action of these operators are ($\beta = g - 1/2$)

$$a^{(-)}\phi_n = -(n + \beta)\phi_{n-1}, \quad a^{(+)}\phi_n = -(n + 1)\phi_{n+1}, \tag{3.9}$$

which are consistent with the three term recurrence relation of the Laguerre polynomial

$$(n + 1)L_{n+1}^{(\beta)}(\eta) + (\eta - 2n - \beta - 1)L_n^{(\beta)}(\eta) + (n + \beta)L_{n-1}^{(\beta)}(\eta) = 0. \tag{3.10}$$

From these follow the su(1,1) relations

$$[\mathcal{H},a^{(\pm)}] = \pm 2a^{(\pm)}, \quad [a^{(-)},a^{(+)}] = \mathcal{H}' = \mathcal{H} + g + 1/2. \tag{3.11}$$

The coherent state (AOCS) (2.49) is obtained simply as

$$\psi(x) = \sum_{n=0}^{\infty} \frac{(-\lambda)^n}{(\beta + 1)_n}\phi_n(x) = \phi_0(x)\frac{e^{-\lambda}\Gamma(\beta + 1)}{(-x^2\lambda)^{\beta/2}}J_\beta(2x\sqrt{-\lambda}), \tag{3.12}$$

in which a generating function of the Laguerre polynomial.[6]

$$\sum_{n=0}^{\infty} \frac{t^n}{(\alpha + 1)_n}L_n^{(\alpha)}(x) = e^t{}_0F_1\left(\begin{array}{c|} - \\ \alpha + 1 \end{array} -xt\right) \tag{3.13}$$

and (C5) are used.

The annihilation and creation operators (3.8) are factorised by the factors of the Hamiltonian $\mathcal{H} = \mathcal{A}^\dagger\mathcal{A}/2$:

$$4a^{(-)} = \left(\frac{\mathrm{d}}{\mathrm{d}x} + x + \frac{g}{x}\right)\cdot\mathcal{A}, \quad \mathcal{A} = i(p - ix + ig/x), \tag{3.14}$$

$$4a^{(+)} = \mathcal{A}^\dagger \cdot \left(-\frac{\mathrm{d}}{\mathrm{d}x} + x + \frac{g}{x} \right), \quad \mathcal{A}^\dagger = -i(p + ix - ig/x). \tag{3.15}$$

This is a degenerate case of (3.92) and the action of the other factors is to compensate the parameter shifts caused by the operators $\mathcal{A}^\dagger$ and $\mathcal{A}$:

$$\left(-\frac{\mathrm{d}}{\mathrm{d}x} + x + \frac{g}{x} \right) \phi_n(x;g) = 2\phi_n(x;g+1), \tag{3.16}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}x} + x + \frac{g}{x} \right) \phi_n(x;g+1) = (2n + 2g + 1)\phi_n(x;g). \tag{3.17}$$

2. Pöschl-Teller potential

The Pöschl-Teller potential has two parameters g and h and its eigenfunctions are related to the Jacobi polynomial. It is the one body case of the BC type Sutherland systems.[10,11] Its Hamiltonian, the eigenvalues and the eigenfunctions are:

$$\overset{\text{def}}{\mathcal{H}} = (p - ig\cot x + ih\tan x)(p + ig\cot x - ih\tan x)/2, \quad 0 < x < \pi/2, \tag{3.18}$$

$$\mathcal{E}_n = 2n(n + g + h), \quad n = 0,1,2,\ldots, \quad g,h > 0, \quad \eta(x) = \cos 2x, \tag{3.19}$$

$$\phi_n(x) = (\sin x)^g (\cos x)^h P_n^{(\alpha,\beta)}(\cos 2x), \quad \overset{\text{def}}{\alpha} = g - 1/2, \quad \overset{\text{def}}{\beta} = h - 1/2, \tag{3.20}$$

in which $P_n^{(\alpha,\beta)}(\eta)$ is the Jacobi polynomial (C8). It is straightforward to evaluate the Poisson brackets

$$\{\mathcal{H}, \cos 2x\} = 2p \sin 2x, \tag{3.21}$$

$$\{\mathcal{H}, \{\mathcal{H}, \cos 2x\}\} = -\cos 2x\, 8\mathcal{H}' - 4(g^2 - h^2), \quad \overset{\text{def}}{\mathcal{H}'} = \mathcal{H} + (g+h)^2/2, \tag{3.22}$$

leading to the solution of the initial value problem:

$$\cos 2x(t) = \left(\cos 2x(0) + \frac{g^2 - h^2}{2\mathcal{H}_0'} \right) \cos[2t\sqrt{2\mathcal{H}_0'}] - p(0)\sin 2x(0) \frac{\sin[2t\sqrt{2\mathcal{H}_0'}]}{\sqrt{2\mathcal{H}_0'}} - \frac{g^2 - h^2}{2\mathcal{H}_0'}. \tag{3.23}$$

Note that $|\cos 2x(t)| < 1$ is satisfied. The corresponding quantum expressions are

$$[\mathcal{H}, \cos 2x] = 2(i \sin 2x p + \cos 2x), \tag{3.24}$$

$$[\mathcal{H}, [\mathcal{H}, \cos 2x]] = \cos 2x(8\mathcal{H}' - 4) + 4[\mathcal{H}, \cos 2x] + 4(\alpha^2 - \beta^2), \tag{3.25}$$

$$\alpha_\pm(\mathcal{H}) = 2 \pm 2\sqrt{2\mathcal{H}'}. \tag{3.26}$$

The exact operator solution reads

$$e^{it\mathcal{H}}\cos 2x\, e^{-it\mathcal{H}} = (i\sin 2x\, p + \cos 2x)\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}} - \frac{\alpha^2-\beta^2}{2\mathcal{H}'-1}$$
$$+ (\cos 2x(2\mathcal{H}'-1) + \alpha^2 - \beta^2)\frac{1}{\sqrt{2\mathcal{H}'}}\left(\frac{e^{i\alpha_+(\mathcal{H})t}}{\alpha_+(\mathcal{H})} - \frac{e^{i\alpha_-(\mathcal{H})t}}{\alpha_-(\mathcal{H})}\right). \tag{3.27}$$

The annihilation and creation operators are

$$a'^{(\pm)}/2 = a^{(\pm)}2\sqrt{2\mathcal{H}'} = \pm\sin 2x\frac{\mathrm{d}}{\mathrm{d}x} + \cos 2x\sqrt{2\mathcal{H}'} + \frac{\alpha^2-\beta^2}{\sqrt{2\mathcal{H}'}\pm 1}. \tag{3.28}$$

It is now obvious that they ($a'^{(\pm)}$) are not hermitian conjugate to each other. When applied to the eigenvector ϕ_n as $2\mathcal{E}_n+(g+h)^2=(2n+g+h)^2$, we obtain:

$$a'^{(-)}/2\phi_n = -\sin 2x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (2n+g+h)\cos 2x\phi_n + \frac{\alpha^2-\beta^2}{2n+\alpha+\beta}\phi_n = \frac{4(n+\alpha)(n+\beta)}{2n+\alpha+\beta}\phi_{n-1}, \tag{3.29}$$

$$a'^{(+)}/2\phi_n = \sin 2x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (2n+g+h)\cos 2x\ \phi_n + \frac{\alpha^2-\beta^2}{2n+\alpha+\beta+2}\phi_n = \frac{4(n+1)(n+\alpha+\beta+1)}{2n+\alpha+\beta+2}\phi_{n+1}. \tag{3.30}$$

The right-hand sides are the results of the application. From (3.29) and $a'^{(-)}\phi_n=4(2n+g+h)a^{(-)}\phi_n$, the coherent state ψ and ψ' are

$$\psi(x) = \phi_0(x)\sum_{n=0}^{\infty}(\lambda/2)^n\frac{(\alpha+\beta+2)_{2n}}{(\alpha+1)_n(\beta+1)_n}P_n^{(\alpha,\beta)}(\cos 2x), \tag{3.31}$$

$$\psi'(x) = \phi_0(x)\sum_{n=0}^{\infty}(\lambda/4)^n\frac{\left(\frac{\alpha+\beta}{2}+1\right)_n}{(\alpha+1)_n(\beta+1)_n}P_n^{(\alpha,\beta)}(\cos 2x). \tag{3.32}$$

We are not aware if concise summation formulas exist or not.

3. Soliton potential, or the symmetric Rosen-Morse potential

As is well-known $-g(g+1)/\cosh^2 x$ potential is *reflectionless* for integer coupling constant g, corresponding to the Korteweg de Vries (KdV) soliton. It has a finite number $1+[g]'$ (the greatest integer not equal or exceeding g) of bound states:

$$\mathcal{H} \overset{\text{def}}{=} (p+ig\tanh x)(p-ig\tanh x)/2, \quad -\infty < x < \infty, \quad g>0, \tag{3.33}$$

$$\mathcal{E}_n = n(-n/2+g), \quad n=0,1,\ldots,[g]', \quad \eta(x)=\sinh x, \tag{3.34}$$

$$\phi_n(x) = i^{-n}(\cosh x)^{-g}P_n^{(\beta,\beta)}(i\sinh x), \quad \beta \overset{\text{def}}{=} -g-1/2. \tag{3.35}$$

These eigenfunctions are real due to the parity $P_n^{(\alpha,\beta)}(-x)=(-1)^nP_n^{(\beta,\alpha)}(x)$. The Poisson brackets are

$$\{\mathcal{H},\sinh x\} = -p\cosh x, \quad \{\mathcal{H},\{\mathcal{H},\sinh x\}\} = \sinh x\, 2\mathcal{H}', \quad \mathcal{H}' \overset{\text{def}}{=} \mathcal{H} - g^2/2, \tag{3.36}$$

leading to the solution of the initial value problem:

$$\sinh x(t) = \sinh x(0)\cos[t\sqrt{-2\mathcal{H}_0'}] + p(0)\cosh x(0)\frac{\sin[t\sqrt{-2\mathcal{H}_0'}]}{\sqrt{-2\mathcal{H}_0'}}. \tag{3.37}$$

It describes sinusoidal motion for bound states $\mathcal{H}_0' < 0$ only. But the previous expression is valid for the unbound motion $\mathcal{H}_0' > 0$, too.

The corresponding quantum expressions are

$$[\mathcal{H}, \sinh x] = -i\cosh x\, p - \sinh x/2, \tag{3.38}$$

$$[\mathcal{H}, [\mathcal{H}, \sinh x]] = -\sinh x(2\mathcal{H}' + 1/4) - [\mathcal{H}, \sinh x], \tag{3.39}$$

$$\alpha_\pm(\mathcal{H}) = -1/2 \pm \sqrt{-2\mathcal{H}'}. \tag{3.40}$$

The exact operator solution reads

$$e^{it\mathcal{H}}\sinh x\, e^{-it\mathcal{H}} = (-i\cosh xp - \sinh x/2)\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{-2\mathcal{H}'}} - \sinh x\frac{2\mathcal{H}' + 1/4}{2\sqrt{-2\mathcal{H}'}}\left(\frac{e^{i\alpha_+(\mathcal{H})t}}{\alpha_+(\mathcal{H})} - \frac{e^{i\alpha_-(\mathcal{H})t}}{\alpha_-(\mathcal{H})}\right). \tag{3.41}$$

The annihilation and creation operators are

$$a'^{(\pm)} = a^{(\pm)}2\sqrt{-2\mathcal{H}'} = \mp\cosh x\frac{\mathrm{d}}{\mathrm{d}x} + \sinh x\sqrt{-2\mathcal{H}'}. \tag{3.42}$$

When applied to the eigenvector ϕ_n, we obtain as $2\mathcal{E}_n - g^2 = -(g-n)^2$:

$$a'^{(-)}\phi_n = \cosh x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (g-n)\sinh x\,\phi_n = (n+\beta)\phi_{n-1}, \tag{3.43}$$

$$a'^{(+)}\phi_n = -\cosh x\frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (g-n)\sinh x\,\phi_n = -\frac{(n+1)(n+2\beta+1)}{n+\beta+1}\phi_{n+1}. \tag{3.44}$$

We obtain the following interesting commutation relations:

$$[\mathcal{H}, a'^{(\pm)}] = \pm(\sqrt{-2\mathcal{H}'}a'^{(\pm)} + a'^{(\pm)}\sqrt{-2\mathcal{H}'})/2, \tag{3.45}$$

$$[a'^{(-)}, a'^{(+)}] = 2\sqrt{-2\mathcal{H}'}, \quad a'^{(-)}a'^{(+)} + a'^{(+)}a'^{(-)} = 4\mathcal{H} + 2g, \tag{3.46}$$

which look very similar to those for the $1/\sin^2 x$ potential (2.65)–(2.67). In contrast to the $1/\sin^2 x$ case, the present case has only finite dimensional representation, $n = 0, 1, \ldots, [g]'$, that is from the ground state to the highest level. There is no coherent state as the eigenvector of the annihilation operator (3.42).

4. Morse potential

This is another well-known example of exactly solvable potential with a finite number of bound states:[1]

$$\mathcal{H} \overset{\text{def}}{=} (p + i\mu e^x - ig)(p - i\mu e^x + ig)/2, \quad -\infty < x < \infty, \quad \mu, g > 0, \tag{3.47}$$

$$\mathcal{E}_n = n(-n/2 + g), \quad n = 0, 1, \ldots, [g]', \quad \eta(x) = e^{-x}, \tag{3.48}$$

$$\phi_n(x) = e^{-\mu e^x + gx} e^{-nx} L_n^{(2g-2n)}(2\mu e^x). \tag{3.49}$$

The Poisson brackets are

$$\{\mathcal{H}, e^{-x}\} = pe^{-x}, \quad \{\mathcal{H}, \{\mathcal{H}, e^{-x}\}\} = e^{-x} 2\mathcal{H}' + \mu g, \quad \mathcal{H}' \overset{\text{def}}{=} \mathcal{H} - g^2/2, \tag{3.50}$$

leading to the solution of the initial value problem:

$$e^{-x(t)} = \left(e^{-x(0)} + \frac{\mu g}{2\mathcal{H}_0'} \right) \cos[t\sqrt{-2\mathcal{H}_0'}] - p(0) e^{-x(0)} \frac{\sin[t\sqrt{-2\mathcal{H}_0'}]}{\sqrt{-2\mathcal{H}_0'}} - \frac{\mu g}{2\mathcal{H}_0'}. \tag{3.51}$$

It describes sinusoidal motion for bound states $\mathcal{H}_0' < 0$ only. But the previous expression is valid for the unbound motion $\mathcal{H}_0' > 0$, too. It is easy to verify $e^{-x(t)} > 0$.

The corresponding quantum expressions are

$$[\mathcal{H}, e^{-x}] = ie^{-x} p - e^{-x}/2, \tag{3.52}$$

$$[\mathcal{H}, [\mathcal{H}, e^{-x}]] = -e^{-x}(2\mathcal{H}' + 1/4) - [\mathcal{H}, e^{-x}] - \mu(g + 1/2), \tag{3.53}$$

$$\alpha_\pm(\mathcal{H}) = -1/2 \pm \sqrt{-2\mathcal{H}'}. \tag{3.54}$$

The exact operator solution reads

$$\begin{aligned} e^{it\mathcal{H}} e^{-x} e^{-it\mathcal{H}} = (ie^{-x} p - e^{-x}/2) \frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{-2\mathcal{H}'}} - \frac{\mu(g + 1/2)}{2\mathcal{H}' + 1/4} - (e^{-x}(2\mathcal{H}' + 1/4) \\ + \mu(g + 1/2)) \frac{1}{2\sqrt{-2\mathcal{H}'}} \left(\frac{e^{i\alpha_+(\mathcal{H})t}}{\alpha_+(\mathcal{H})} - \frac{e^{i\alpha_-(\mathcal{H})t}}{\alpha_-(\mathcal{H})} \right). \end{aligned} \tag{3.55}$$

The annihilation and creation operators are

$$a'^{(\pm)} = a^{(\pm)} 2\sqrt{-2\mathcal{H}'} = \pm e^{-x} \frac{\mathrm{d}}{\mathrm{d}x} + e^{-x}\sqrt{-2\mathcal{H}'} - \frac{\mu(2g + 1)}{2\sqrt{-2\mathcal{H}'} \mp 1}. \tag{3.56}$$

When applied to the eigenvector ϕ_n, we obtain as $2\mathcal{E}_n - g^2 = -(g-n)^2$:

$$a'^{(-)}\phi_n = -e^{-x} \frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (g - n) e^{-x} \phi_n - \frac{\mu(2g + 1)}{2(g - n) + 1} \phi_n = \frac{4\mu^2}{2(g - n) + 1} \phi_{n-1}, \tag{3.57}$$

$$a'^{(+)}\phi_n = e^{-x} \frac{\mathrm{d}\phi_n}{\mathrm{d}x} + (g - n) e^{-x} \phi_n - \frac{\mu(2g + 1)}{2(g - n) - 1} \phi_n = \frac{(n + 1)(2g - n)}{2(g - n) - 1} \phi_{n+1}. \tag{3.58}$$

B. Discrete quantum mechanical systems

For specifying the dynamical systems belonging to the discrete quantum mechanics,[2,3] we use the name of the polynomial eigenfunctions for want of universally accepted naming. The factorized Hamiltonian is given by (2.76).

1. Continuous Hahn polynomial (special case)

The factorized Hamiltonian of the continuous Hahn polynomial (special case) has a potential function V depending on two parameters:

$$V(x)=(a_1+ix)(a_2+ix),\quad -\infty<x<\infty,\quad a_1,a_2>0. \tag{3.59}$$

The eigenvalues and eigenfunctions are

$$\mathcal{E}_n=n(n+2a_1+2a_2-1)/2,\quad n=0,1,2,\dots, \tag{3.60}$$

$$\phi_0(x)=\sqrt{\prod_{j=1}^{2}\Gamma(a_j+ix)\Gamma(a_j-ix)},\quad \eta(x)=x, \tag{3.61}$$

$$\phi_n(x)=\phi_0(x)P_n(x),\quad P_n(x)\overset{\text{def}}{=}p_n(x;a_1,a_2,a_1,a_2), \tag{3.62}$$

in which $p_n(x;a_1,a_2,a_1,a_2)$ is a special case of the continuous Hahn polynomial (C11). This is a two parameter deformation of the Hermite polynomial. Thus this dynamical system is a deformed oscillator. The classical solution shows this fact clearly:

$$\{\mathcal{H},x\}=-\sqrt{(a_1^2+x^2)(a_2^2+x^2)}\sinh p,\quad \{\mathcal{H},\{\mathcal{H},x\}\}=-x(2\mathcal{H}+(a_1+a_2)^2), \tag{3.63}$$

$$x(t)=x(0)\cos[t\sqrt{2\mathcal{H}_0+(a_1+a_2)^2}]+\sqrt{(a_1^2+x(0)^2)(a_2^2+x(0)^2)}\sinh p(0)\frac{\sin[t\sqrt{2\mathcal{H}_0+(a_1+a_2)^2}]}{\sqrt{2\mathcal{H}_0+(a_1+a_2)^2}}. \tag{3.64}$$

The corresponding quantum solution is also simple:

$$[\mathcal{H},x]=-i(T_+-T_-)/2, \tag{3.65}$$

$$[\mathcal{H},[\mathcal{H},x]]=x(2\mathcal{H}'-1/4)+[\mathcal{H},x],\quad 2\mathcal{H}'\overset{\text{def}}{=}2\mathcal{H}+(a_1+a_2-1/2)^2, \tag{3.66}$$

$$e^{it\mathcal{H}}xe^{-it\mathcal{H}}=[\mathcal{H},x]\frac{e^{i\alpha_+(\mathcal{H})t}-e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}}+x\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t}+\alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}}, \tag{3.67}$$

$$\alpha_\pm(\mathcal{H})=1/2\pm\sqrt{2\mathcal{H}'}. \tag{3.68}$$

The annihilation and creation operators are:

$$a'^{(\pm)}=a^{(\pm)}2\sqrt{2\mathcal{H}'}=\pm[\mathcal{H},x]\mp x\alpha_\mp(\mathcal{H})=\mp i(T_+-T_-)/2+x(\sqrt{2\mathcal{H}'}\mp 1/2). \tag{3.69}$$

When applied to the eigenvector ϕ_n, we obtain as $2\mathcal{E}_n+(a_1+a_2-1/2)^2=(n+a_1+a_2-1/2)^2$:

$$2a'^{(-)}\phi_n=i(T_+-T_-)\phi_n+2x(n+a_1+a_2)\phi_n=(n+a_1+a_2-1)(n+2a_1-1)(n+2a_2-1)\phi_{n-1}, \tag{3.70}$$

$$2a'^{(+)}\phi_n=-i(T_+-T_-)\phi_n+2x(n+a_1+a_2-1)\phi_n=\frac{(n+1)(n+2a_1+2a_2-1)}{n+a_1+a_2}\phi_{n+1}. \tag{3.71}$$

The similarity transformed operators act as

$$\phi_0(x)^{-1}a'^{(\pm)}\phi_0(x)\cdot P_n(x)=\left(x\left(n+a_1+a_2-\tfrac{1}{2}\mp\tfrac{1}{2}\right)\mp\tfrac{i}{2}(V(x)e^p-V(x)^*e^{-p})\right)P_n(x). \tag{3.72}$$

The coherent state ψ and ψ' are

$$\psi(x) = \phi_0(x)\sum_{n=0}^{\infty} \frac{\lambda^n (2a_1 + 2a_2)_{2n}}{(2a_1)_n (2a_2)_n (a_1 + a_2)_n^2} P_n(x), \tag{3.73}$$

$$\psi'(x) = \phi_0(x)\sum_{n=0}^{\infty} \frac{(2\lambda)^n}{(2a_1)_n (2a_2)_n (a_1 + a_2)_n} P_n(x). \tag{3.74}$$

We do not know if these sums have concise expressions or not.

2. Continuous dual Hahn polynomial

The continuous dual Hahn polynomial has three parameters (a_1, a_2, a_3) and is considered as a two parameter deformation of the Laguerre polynomial $L_n^{(\alpha)}$. The factorized Hamiltonian of the continuous dual Hahn polynomial has a potential function V:

$$V(x) = \frac{\prod_{j=1}^{3} (a_j + ix)}{2ix(2ix + 1)}, \quad 0 < x < \infty, \quad a_1, a_2, a_3 > 0. \tag{3.75}$$

As a dynamical system this is a deformed Calogero model, or a deformed $x^2 + 1/x^2$ potential. Like the Calogero model it has a linear spectrum and the eigenfunctions are:

$$\mathcal{E}_n = n/2, \quad n = 0, 1, 2, \ldots, \tag{3.76}$$

$$\phi_0(x) = \sqrt{\frac{\prod_{j=1}^{3} \Gamma(a_j + ix)}{\Gamma(2ix)} \frac{\prod_{j=1}^{3} \Gamma(a_j - ix)}{\Gamma(-2ix)}}, \quad \eta(x) = x^2, \tag{3.77}$$

$$\phi_n(x) = \phi_0(x) P_n(x^2), \quad P_n(\eta) \overset{\text{def}}{=} S_n(\eta; a_1, a_2, a_3), \tag{3.78}$$

in which $S_n(\eta; a_1, a_2, a_3)$ is the continuous dual Hahn polynomial (C12). For deriving the classical solution, let us note that the quantum potential (3.75) has acquired quantum corrections from the classical one:

$$V_c(x) = \frac{\prod_{j=1}^{3} (a_j + ix)}{(2ix)^2}. \tag{3.79}$$

The classical motion is simple:

$$\{\mathcal{H}_c, x^2\} = -\frac{\sqrt{\prod_{j=1}^{3} (a_j^2 + x^2)}}{2x} \sinh p, \tag{3.80}$$

$$\{\mathcal{H}_c, \{\mathcal{H}_c, x^2\}\} = -x^2/4 + 2\mathcal{H}_c^2 + b_1 \mathcal{H}_c + b_2/4, \quad b_1 \overset{\text{def}}{=} \sum_{1 \le j \le 3} a_j, \quad b_2 \overset{\text{def}}{=} \sum_{1 \le j < k \le 3} a_j a_k, \tag{3.81}$$

$$\begin{aligned} x^2(t) = {} & (x^2(0) - 8\mathcal{H}_{c0}^2 - 4b_1 \mathcal{H}_{c0} - b_2)\cos[t/2] + 8\mathcal{H}_{c0}^2 + 4b_1 \mathcal{H}_{c0} + b_2 \\ & + \frac{\sqrt{\prod_{j=1}^{3} (a_j^2 + x^2(0))}}{x(0)} \sinh p(0) \sin[t/2]. \end{aligned} \tag{3.82}$$

The quantum version is almost the same:

$$[\mathcal{H}, x^2] = -ix(T_+ - T_-) - (T_+ + T_-)/2, \tag{3.83}$$

$$[\mathcal{H},[\mathcal{H},x^2]]=x^2/4+R_{-1}(\mathcal{H}),\quad R_{-1}(\mathcal{H})=-(2\mathcal{H}^2+(b_1-1/2)\mathcal{H}+b_2/4), \tag{3.84}$$

$$e^{it\mathcal{H}}x^2e^{-it\mathcal{H}}=2i[\mathcal{H},x^2]\sin[t/2]+(x^2+4R_{-1}(\mathcal{H}))\cos[t/2]-4R_{-1}(\mathcal{H}). \tag{3.85}$$

The annihilation and creation operators are:

$$a^{(\pm)}=\pm[\mathcal{H},x^2]+x^2/2+2R_{-1}(\mathcal{H})=\mp ix(T_+-T_-)\mp(T_++T_-)/2+x^2/2+2R_{-1}(\mathcal{H}). \tag{3.86}$$

When applied to the eigenvector ϕ_n, we obtain:

$$a^{(-)}\phi_n=-n\prod_{1\le j<k\le 3}(n+a_j+a_k-1)\cdot\phi_{n-1}, \tag{3.87}$$

$$a^{(+)}\phi_n=-\phi_{n+1}. \tag{3.88}$$

The similarity transformed operators are:

$$\phi_0(x)^{-1}a^{(\pm)}\phi_0(x)=x^2/2-4\tilde{\mathcal{H}}^2-2(b_1-1/2)\tilde{\mathcal{H}}-b_2/2\mp((1/2+ix)V(x)e^p+(1/2-ix)V(x)^*e^{-p}), \tag{3.89}$$

in which $\tilde{\mathcal{H}}=\phi_0(x)^{-1}\mathcal{H}\phi_0(x)=(V(x)e^p+V(x)^*e^{-p}-V(x)-V(x)^*)/2$ is the Hamiltonian counterpart at the polynomial level satisfying $\tilde{\mathcal{H}}P_n(x^2)=n/2P_n(x^2)$, see Appendix C. The coherent state is

$$\psi(x)=\phi_0(x)\sum_{n=0}^{\infty}\frac{(-\lambda)^n}{n!\prod_{1\le j<k\le 3}(a_j+a_k)_n}P_n(x^2). \tag{3.90}$$

We do not know if this sum has a concise expression or not. The commutation relations among $\mathcal{H}$, and $a^{(\pm)}$ are more complicated than su(1,1):

$$[\mathcal{H},a^{(\pm)}]=\pm a^{(\pm)}/2,$$

$$[a^{(-)},a^{(+)}]=32\mathcal{H}^3+24(b_1-1/2)\mathcal{H}^2+(4(b_1-1/2)^2+4b_2+1)\mathcal{H}+b_1b_2-a_1a_2a_3. \tag{3.91}$$

As in the Meixner-Pollaczek case (2.94), the annihilation and creation operators for the continuous dual Hahn polynomial factorise into the operators $\mathcal{A}$ and $\mathcal{A}^\dagger$ appearing in the Hamiltonian $\mathcal{H}=\mathcal{A}^\dagger\mathcal{A}/2$:

$$a^{(-)}=X^\dagger\mathcal{A},\quad a^{(+)}=\mathcal{A}^\dagger X. \tag{3.92}$$

The operator X in this case reads

$$\begin{aligned}X=&-iS_+T_+ +\left(x-iV\left(x-\tfrac{i}{2}\right)^*-i\frac{\prod_{j=1}^3(2a_j-1)}{8(1+x^2)}\right)S_+ +iS_-T_-\\&+\left(x+iV\left(x-\tfrac{i}{2}\right)+i\frac{\prod_{j=1}^3(2a_j-1)}{8(1+x^2)}\right)S_-.\end{aligned} \tag{3.93}$$

These X and $X^\dagger$ compensate the shift of the parameters (a_1,a_2,a_3) caused by $\mathcal{A}^\dagger$ and $\mathcal{A}$, respectively. See Appendix B for more details.

3. Wilson polynomial

The Wilson polynomial has four parameters (a_1,a_2,a_3,a_4) and is considered as a three parameter deformation of the Laguerre polynomial $L_n^{(\alpha)}$. The factorized Hamiltonian (2.76) of the Wilson polynomial has a potential function V:

$$V(x)=\frac{\prod_{j=1}^{4}(a_j+ix)}{2ix(2ix+1)},\quad 0<x<\infty,\quad a_1,a_2,a_3,a_4>0. \tag{3.94}$$

As a dynamical system this is another deformation of the Calogero model, or a deformed x^2+1/x^2 potential. The spectrum is now quadratic in n and the eigenfunctions are:

$$\mathcal{E}_n=n\left(n+\sum_{j=1}^{4}a_j-1\right)/2,\quad n=0,1,2,\ldots, \tag{3.95}$$

$$\phi_0(x)=\sqrt{\frac{\prod_{j=1}^{4}\Gamma(a_j+ix)}{\Gamma(2ix)}\frac{\prod_{j=1}^{4}\Gamma(a_j-ix)}{\Gamma(-2ix)}},\quad \eta(x)=x^2, \tag{3.96}$$

$$\phi_n(x)=\phi_0(x)P_n(x^2),\quad P_n(\eta)\overset{\text{def}}{=}W_n(\eta;a_1,a_2,a_3,a_4), \tag{3.97}$$

in which $W_n(\eta;a_1,a_2,a_3,a_4)$ is the Wilson polynomial (C13). The classical motion looks like a cross between those of the continuous Hahn and the continuous dual Hahn potentials with the classical potential V_c:

$$\{\mathcal{H}_c,x^2\}=-\frac{\sqrt{\prod_{j=1}^{4}(a_j^2+x^2)}}{2x}\sinh p,\quad V_c(x)=\frac{\prod_{j=1}^{4}(a_j+ix)}{(2ix)^2} \tag{3.98}$$

$$\{\mathcal{H}_c,\{\mathcal{H}_c,x^2\}\}=-2x^2(\mathcal{H}_c+c_1)-R_{-1}(\mathcal{H}_c), \tag{3.99}$$

$$R_{-1}(\mathcal{H}_c)=-2(\mathcal{H}_c^2+c_2\mathcal{H}_c+c_3),\quad c_1=b_1^2/8,\quad c_2=b_2,\quad c_3=b_1b_3/4, \tag{3.100}$$

$$\begin{aligned}x^2(t)=&\left(x^2(0)+\frac{R_{-1}(\mathcal{H}_{c0})}{2(\mathcal{H}_{c0}+c_1)}\right)\cos\left[t\sqrt{2(\mathcal{H}_{c0}+c_1)}\right]-\frac{R_{-1}(\mathcal{H}_{c0})}{2(\mathcal{H}_{c0}+c_1)}\\&+\frac{\sqrt{\prod_{j=1}^{4}(a_j^2+x^2(0))}}{2x(0)}\sinh p(0)\frac{\sin[t\sqrt{2(\mathcal{H}_{c0}+c_1)}]}{\sqrt{2(\mathcal{H}_{c0}+c_1)}},\end{aligned} \tag{3.101}$$

where we use the abbreviation

$$b_1\overset{\text{def}}{=}\sum_{1\le j\le 4}a_j,\quad b_2\overset{\text{def}}{=}\sum_{1\le j<k\le 4}a_ja_k,\quad b_3\overset{\text{def}}{=}\sum_{1\le j<k<l\le 4}a_ja_ka_l. \tag{3.102}$$

The quantum version has almost the same form with quantum corrections in the coefficients c_1, c_2, and c_3:

$$[\mathcal{H},x^2]=-ix(T_+-T_-)-(T_++T_-)/2, \tag{3.103}$$

$$[\mathcal{H},[\mathcal{H},x^2]]=[\mathcal{H},x^2]+2x^2(\mathcal{H}+c_1)+R_{-1}(\mathcal{H}), \tag{3.104}$$

$$R_{-1}(\mathcal{H}) = -2(\mathcal{H}^2 + c_2\mathcal{H} + c_3), \tag{3.105}$$

$$c_1 = b_1(b_1-2)/8, \quad c_2 = b_2 - b_1/2, \quad c_3 = (b_1-2)b_3/4, \tag{3.106}$$

$$e^{it\mathcal{H}}x^2e^{-it\mathcal{H}} = [\mathcal{H},x^2]\frac{e^{i\alpha_+(\mathcal{H})t} - e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}} - \frac{R_{-1}(\mathcal{H})}{2(\mathcal{H}+c_1)} + \left(x^2 + \frac{R_{-1}(\mathcal{H})}{2(\mathcal{H}+c_1)}\right)\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t} + \alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{2\sqrt{2\mathcal{H}'}}. \tag{3.107}$$

$$\alpha_\pm(\mathcal{H}) = 1/2 \pm \sqrt{2\mathcal{H}'}, \quad 2\mathcal{H}' \overset{\text{def}}{=} 2\mathcal{H} + 2c_1 + 1/4. \tag{3.108}$$

The annihilation and creation operators are

$$a'^{(\pm)} = a^{(\pm)}2\sqrt{2\mathcal{H}'} = \pm[\mathcal{H},x^2] \mp x^2\alpha_\mp(\mathcal{H}) + \frac{R_{-1}(\mathcal{H})}{\sqrt{2\mathcal{H}'} \pm 1/2}$$
$$= \mp ix(T_+ - T_-) \mp (T_+ + T_-)/2 \mp x^2\alpha_\mp(\mathcal{H}) + \frac{R_{-1}(\mathcal{H})}{\sqrt{2\mathcal{H}'} \pm 1/2}. \tag{3.109}$$

When applied to the eigenvector ϕ_n, we obtain as $2\mathcal{E}_n + 2c_1 + 1/4 = (2n+b_1-1)^2/4$:

$$a'^{(-)}\phi_n = -\frac{n\prod_{1\le j<k\le 4}(n+a_j+a_k-1)}{(2n+b_1-2)(2n+b_1-1)}\phi_{n-1}, \tag{3.110}$$

$$a'^{(+)}\phi_n = -\frac{n+b_1-1}{(2n+b_1-1)(2n+b_1)}\phi_{n+1}. \tag{3.111}$$

The similarity transformed operators act as

$$\phi_0(x)^{-1}a'^{(\pm)}\phi_0(x)\cdot P_n(x^2) = \left(\pm(\mathcal{E}_n - \mathcal{E}_{n\mp1})x^2 \pm \frac{R_{-1}(\mathcal{E}_n)}{\mathcal{E}_{n\pm1} - \mathcal{E}_n} \mp ((1/2+ix)V(x)e^p + (1/2-ix)V(x)^*e^{-p})\right)P_n(x^2). \tag{3.112}$$

The coherent state ψ and ψ' are

$$\psi(x) = \phi_0(x)\sum_{n=0}^{\infty}\frac{(-\lambda)^n}{n!}\frac{(a_1+a_2+a_3+a_4)_{2n}}{\prod_{1\le j<k\le 4}(a_j+a_k)_n}P_n(x^2), \tag{3.113}$$

$$\psi'(x) = \phi_0(x)\sum_{n=0}^{\infty}\frac{(-2\lambda)^n}{n!}\frac{((a_1+a_2+a_3+a_4)/2)_n}{\prod_{1\le j<k\le 4}(a_j+a_k)_n}P_n(x^2). \tag{3.114}$$

IV. SUMMARY AND COMMENTS

Unified theory of annihilation-creation operators $a^{(\pm)}$ is developed for various exactly solvable quantum mechanical systems possessing the sinusoidal coordinate. It applies to most of the degree one solvable quantum mechanical systems as well as the solvable discrete quantum mechanical

systems, which are also shape invariant.[2] The eigenfunctions of the latter are described by the Askey-scheme of hypergeometric orthogonal polynomials.[6] The method provides an independent *algebraic solution* of these quantum systems. The energy spectrum is obtained à la Heisenberg and Pauli from the Heisenberg operator solution for the 'sinusoidal coordinate' η, $e^{it\mathcal{H}}\eta e^{-it\mathcal{H}}$ and the entire eigenfunctions are explicitly obtained as $\{(a^{(+)})^n\phi_0\}$, $n=0,1,\ldots$, in which ϕ_0 is determined by $a^{(-)}\phi_0=0$. Various examples are worked out in Secs. II and III. It also applies to theories with a finite number of bound states. It should be stressed that these annihilation-creation operators are *natural* ones containing the differential (difference) operators, in contradistinction to those annihilation-creation operators introduced in the algebraic theory of coherent states.[9] By a similarity transformation in terms of the ground state wavefunction ϕ_0, the Heisenberg operator solution gives the structure relation for the corresponding orthogonal polynomials[5] and the annihilation-creation operators provide their shift down-up operators. Another characteristic feature is the uniqueness. Except for the overall factor, which is intrinsically undetermined, the action $a^{(\pm)}\phi_n$ is completely determined by the Hamiltonian of the system. This means that the relative weights of the terms in $a^{(\pm)}\phi_n$ are governed by the energy spectrum. We have shown in some detail that this type of algebraic exact solvability is valid at both classical and quantum levels. This is in good contrast with shape-invariance, which is a strictly quantum notion. The necessary and sufficient condition for the existence of the sinusoidal coordinate is worked out for the ordinary quantum mechanical systems in Appendix A. It is a good challenge to derive a corresponding result for the 'discrete' quantum mechanical systems.

Generalization of the present formalism to multiparticle systems is highly desirable. Simplest multiparticle systems possessing the sinusoidal coordinate and the corresponding Heisenberg operator solution is the Calogero systems based on any root system.[11] In fact a more general Hamiltonian

$$\mathcal{H}=\frac{1}{2}\sum_{j=1}^{n}(p_j^2+x_j^2)+V(x),\quad \sum_{j=1}^{n}x_j\frac{\partial}{\partial x_j}V(x)=-2V(x), \tag{4.1}$$

$$[\mathcal{H},[\mathcal{H},\eta]]=4(\eta-\mathcal{H}),\quad \eta=\sum_{j=1}^{n}x_j^2, \tag{4.2}$$

of harmonic oscillators modified by a generic homogeneous degree minus two potential has the same property. The corresponding eigenfunctions are the Laguerre polynomials again.[15,11] As is well known the annihilation-creation operators of the harmonic oscillator have a quite wide applicability in many branches of physics. We wonder if the newly found annihilation-creation operators for the other solvable quantum mechanical systems might find an equally wide range of applications.

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APPENDIX A: DETERMINATION OF THE POTENTIALS HAVING THE SINUSOIDAL COORDINATE

We have seen that the existence of the sinusoidal coordinate or the exact Heisenberg operator solution (2.14) leads to the unified definition of the annihilation-creation operators. All the examples discussed in the text share the common property of "shape-invariance," thanks to which the corresponding quantum systems are exactly solvable. Here in Appendix A we analyse, within the context of ordinary quantum mechanics, the necessary and sufficient condition for the existence of the sinusoidal coordinate and show that such systems constitute a sub-group of known

shape-invariant quantum mechanics. For the discrete quantum mechanical systems, writing down corresponding conditions is easy. It would be a good challenge to provide a complete list of discrete quantum mechanical systems admitting the sinusoidal coordinate or the exact Heisenberg operator solution.

For a given pair $(\eta(x),\mathcal{H})$ of a coordinate function $\eta(x)$ and a Hamiltonian $\mathcal{H}$ to satisfy the exact Heisenberg operator solution (2.14) is equivalent to the condition (2.12) that the multiple commutators of $\mathcal{H}$ with η form a closed algebra at level two

$$(\mathrm{ad}\mathcal{H})^2\eta(x) \equiv [\mathcal{H},[\mathcal{H},\eta(x)]] = \eta R_0(\mathcal{H}) + [\mathcal{H},\eta(x)]R_1(\mathcal{H}) + R_{-1}(\mathcal{H}). \tag{A1}$$

Here the coefficients $R_0(\mathcal{H})$, $R_1(\mathcal{H})$, and $R_{-1}(\mathcal{H})$ are polynomials in the Hamiltonian $\mathcal{H}$. It should be stressed that this condition is purely algebraic and the knowledge that the eigenfunctions have the general structure (2.3) is irrelevant. The latter (2.3) is a consequence of the condition (A1). For the ordinary quantum mechanical system with potential $V(x)$

$$\mathcal{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{A2}$$

the commutator between $\mathcal{H}$ and η reads

$$[\mathcal{H},\eta] = -\eta'\frac{\mathrm{d}}{\mathrm{d}x} - \frac{1}{2}\eta'', \tag{A3}$$

$$(\mathrm{ad}\,\mathcal{H})^2\eta = \eta''\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \eta'''\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{4}\eta'''' + \eta' V', \tag{A4}$$

in which primes denote differentiation with respect to x. From (A4) we see that the l.h.s. of (A1) contains the derivative operator (the momentum operator) at most quadratic degree. So must be the r.h.s. since the momentum operator can come in as a part of $\mathcal{H}$ (as $p^2/2$) or as $[\mathcal{H},\eta]$, see (A3). Then we can parametrize

$$R_0(\mathcal{H}) = r_0^{(1)}\mathcal{H} + r_0^{(0)}, \quad R_1(\mathcal{H}) = r_1, \quad R_{-1}(\mathcal{H}) = r_{-1}^{(1)}\mathcal{H} + r_{-1}^{(0)}, \tag{A5}$$

in which $r_j^{(k)}$ are all constants. Then the coefficients of the operators $\mathrm{d}^2/\mathrm{d}x^2$, $\mathrm{d}/\mathrm{d}x$, and the function part of (A1) give the conditions:

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}x^2} = -\frac{1}{2}(r_0^{(1)}\eta + r_{-1}^{(1)}), \tag{A6}$$

$$\frac{\mathrm{d}^3\eta}{\mathrm{d}x^3} = -r_1\frac{\mathrm{d}\eta}{\mathrm{d}x}, \tag{A7}$$

$$\frac{1}{4}\frac{\mathrm{d}^4\eta}{\mathrm{d}x^4} + \frac{\mathrm{d}\eta}{\mathrm{d}x}\frac{\mathrm{d}V}{\mathrm{d}x} = -\frac{1}{2}r_1\frac{\mathrm{d}^2\eta}{\mathrm{d}x^2} + (r_0^{(1)}\eta + r_{-1}^{(1)})V + r_0^{(0)}\eta + r_{-1}^{(0)}. \tag{A8}$$

The first condition (A6) simply means that $\eta(x)$ is either a *trigonometric* or a *hyperbolic* function of x which gives an *exponential* function or a *quadratic* and *linear polynomial* in x in the degenerate limits. By comparing (A6) and (A7) we obtain

$$r_0^{(1)} = 2r_1. \tag{A9}$$

Then (A8) reduces to

$$\frac{\mathrm{d}\eta}{\mathrm{d}x}\frac{\mathrm{d}V}{\mathrm{d}x}+\frac{\mathrm{d}^2\eta}{\mathrm{d}x^2}\left(2V+\frac{1}{4}r_1\right)=r_0^{(0)}\eta+r_{-1}^{(0)},$$

which integrates easily when multiplied by $d\eta/dx$:

$$\left(\frac{\mathrm{d}\eta}{\mathrm{d}x}\right)^2\left(V+\frac{r_1}{8}\right)=\frac{r_0^{(0)}}{2}\eta^2+r_{-1}^{(0)}\eta+c. \tag{A10}$$

Here c is the constant of integration. Thus we have determined the possible form of the potential V in terms of the 'sinusoidal coordinate' $\eta(x)$ and its first derivative $d\eta/dx$, with five parameters r_1, $r_0^{(0)}$, $r_{-1}^{(1)}$, $r_{-1}^{(0)}$ and c in (A10) and two more possible constants of integration of (A6):

$$V(x)=\frac{1}{\left(\frac{\mathrm{d}\eta}{\mathrm{d}x}\right)^2}\left(\frac{r_0^{(0)}}{2}\eta^2+r_{-1}^{(0)}\eta+c\right)-\frac{r_1}{8}. \tag{A11}$$

The actual number of essentially free parameters is much less, as the origin of the quadratic potential, or the location of the singularity, etc, could be freely adjusted by introducing new variable $x_{\mathrm{new}}=\alpha x+\beta$ ($\mathcal{H}_{\mathrm{new}}=\mathcal{H}/\alpha^2$). The condition that the Hamiltonian must be bounded from below imposes some constraints on the parameters. The overall additive constant is fixed uniquely when the ground state energy is required to be vanishing $\mathcal{E}_0=0$.

It is rather straightforward to determine all the potentials possessing the 'sinusoidal coordinate' and thus algebraically exactly solvable. They all belong to the known group of shape-invariant potentials. Except for the trivial case $V=0$, we have

1. Rational case, $r_1=0$. The generic solution of (A6) is

$$\eta(x)=-\frac{1}{4}r_{-1}^{(1)}x^2+c_1x+c_2, \tag{A12}$$

with c_1 and c_2 being the constant of integration. Two special cases are of interest: $\eta(x)=x$ gives the harmonic oscillator and $\eta(x)=x^2$ leads to the x^2+1/x^2 potential discussed in Sec. III A 1.

2. Trigonometric case, $r_1>0$. The generic solution of (A6) is

$$\eta(x)=-\frac{r_{-1}^{(1)}}{2r_1}+c_1\cos\sqrt{r_1}x+c_2\sin\sqrt{r_1}x, \tag{A13}$$

with c_1 and c_2 being real constants of integration due to the reality (hermiticity) of η. By rescaling and shift of the coordinate x, it reduces to the Pöschl-Teller potential discussed in Sec. III A 2. The $1/\sin^2 x$ potential in Sec. II A 1 and the symmetric top are obtained as degenerate cases.

3. Hyperbolic and exponential cases, $r_1<0$. The generic solution of (A6) is

$$\eta(x)=-\frac{r_{-1}^{(1)}}{2r_1}+c_1\cosh\sqrt{-r_1}x+c_2\sinh\sqrt{-r_1}x, \tag{A14}$$

in which the constants of integration c_1 and c_2 could be vanishing or equal $c_1=\pm c_2$. The generic case leads to the hyperbolic Pöschl-Teller potential and the degenerate cases contain the soliton potential in Sec. III A 3 and hyperbolic symmetric tops and the Morse potential in Sec. III A 4, etc. We could not discuss all due to space limitation.

In all these examples, the prepotential W has also a simple expression in terms of η and $\mathrm{d}\eta/\mathrm{d}x$:

$$\frac{\mathrm{d}W}{\mathrm{d}x}=\frac{a\eta+b}{\frac{\mathrm{d}\eta}{\mathrm{d}x}},\quad a=-\sqrt{r_0^{(0)}+r_1^2/4},\quad b=\frac{2r_{-1}^{(0)}}{2a+r_1}+\frac{r_{-1}^{(1)}}{4}. \tag{A15}$$

Here the prepotential W is related to the ground state wave function ϕ_0 and thus to the potential V as

$$\phi_0(x)=e^{W(x)},\quad V=\frac{1}{2}\left(\left(\frac{\mathrm{d}W}{\mathrm{d}x}\right)^2+\frac{\mathrm{d}^2W}{\mathrm{d}x^2}\right),$$

and it plays an important role in supersymmetric (shape-invariant) quantum mechanics.[1,16]

It should be stressed that not all shape-invariant and exactly solvable potentials admit the sinusoidal coordinate. Such examples are the Kepler problems in rational, spherical and hyperbolic coordinates and the Rosen-Morse potential, respectively:

$$V(x)=\frac{1}{2}\left(-\frac{2}{x}+\frac{g(g-1)}{x^2}+\frac{1}{g^2}\right), \tag{A16}$$

$$V(x)=\frac{1}{2}\left(-2\mu\cot x+\frac{g(g-1)}{\sin^2 x}+\frac{\mu^2}{g^2}-g^2\right), \tag{A17}$$

$$V(x)=\frac{1}{2}\left(-2\mu\coth x+\frac{g(g-1)}{\sinh^2 x}+\frac{\mu^2}{g^2}+g^2\right), \tag{A18}$$

$$V(x)=\frac{1}{2}\left(2\mu\tanh x-\frac{g(g+1)}{\cosh^2 x}+\frac{\mu^2}{g^2}+g^2\right). \tag{A19}$$

Their wave functions do not have the general structure (2.3), either.

APPENDIX B: INTERPRETATION IN TERMS OF SHAPE INVARIANCE

As shown in Sec. II, the annihilation-creation operators are completely determined once the closed relationship (2.12) among η, $[\mathcal{H},\eta]$ and $[\mathcal{H},[\mathcal{H},\eta]]$ is obtained. Although it plays no active role in the determination of the annihilation-creation operators, *shape invariance* is the common property underlying all these exactly solvable Hamiltonians discussed in this paper. Therefore it is interesting as well as illuminating to understand the mechanism of the annihilation-creation operators within the framework of shape invariance. For this purpose we concentrate on the annihilation-creation operators of the Meixner-Pollaczek polynomials (2.94) and of the continuous dual Hahn polynomials (3.92), which factorize into the operators $\mathcal{A}$ and $\mathcal{A}^\dagger$ constituting the shape invariant Hamiltonian $\mathcal{H}=\mathcal{A}^\dagger\mathcal{A}/2$. Another motivation of this appendix is to provide a bridge between the physics of discrete quantum mechanics[2] and the analysis of Askey-scheme of hypergeometric polynomials.[6] The latter focuses on the polynomial part of the eigenfunctions, whose orthogonal measure is provided by the ground state wave function (2.4).

Let us start with recapitulating the rudimentary facts of the shape-invariant discrete quantum mechanics as developed in Ref. 2. Knowledgeable readers may jump to the main results (B26)–(B29), but some intermediate results (B7) and (B13)–(B17) would also be interesting in connection with the sinusoidal coordinate $\eta(x)$.

A shape invariant quantum mechanical system consists of a series of isospectral Hamiltonians $\{\mathcal{H}(\boldsymbol{\lambda})\}$ parametrised by (a set of) parameters $\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\ldots)$:

$$\mathcal{H}(\boldsymbol{\lambda})=\mathcal{A}(\boldsymbol{\lambda})^\dagger\mathcal{A}(\boldsymbol{\lambda})/2,\quad \phi_n(x;\boldsymbol{\lambda})=\phi_0(x;\boldsymbol{\lambda})P_n(\eta(x);\boldsymbol{\lambda}),\quad \mathcal{E}_n(\boldsymbol{\lambda}),\ \text{etc}.$$

Shape invariance is tersely expressed as

$$\mathcal{A}(\boldsymbol{\lambda})\mathcal{A}(\boldsymbol{\lambda})^{\dagger} = \mathcal{A}(\boldsymbol{\lambda}+\boldsymbol{\delta})^{\dagger}\mathcal{A}(\boldsymbol{\lambda}+\boldsymbol{\delta}) + 2\mathcal{E}_1(\boldsymbol{\lambda}), \tag{B1}$$

where $\boldsymbol{\delta}$ is a shift of the parameter. [In the case of the Askey-Wilson polynomials, this is modified to $\mathcal{A}(\boldsymbol{\lambda})\mathcal{A}(\boldsymbol{\lambda})^{\dagger} = q^{2\delta'}\mathcal{A}(\boldsymbol{\lambda} * q^{\boldsymbol{\delta}})^{\dagger}\mathcal{A}(\boldsymbol{\lambda} * q^{\boldsymbol{\delta}}) + 2\mathcal{E}_1(\boldsymbol{\lambda})$, where δ' is a constant and $\boldsymbol{\lambda} * q^{\boldsymbol{\delta}} = (\lambda_1 q^{\delta_1}, \lambda_2 q^{\delta_2}, \cdots)$]. The operator $\mathcal{A}(\boldsymbol{\lambda})$ maps the eigenvectors of $\mathcal{H}(\boldsymbol{\lambda})$ to those of $\mathcal{H}(\boldsymbol{\lambda}+\boldsymbol{\delta})$ and the other operator $\mathcal{A}(\boldsymbol{\lambda})^{\dagger}$ acts in the opposite direction. In each case studied in this article, the parameter $\boldsymbol{\lambda}$ and the shift $\boldsymbol{\delta}$ are

$$\text{Meixner-Pollaczek:} \quad \boldsymbol{\lambda} = a, \quad \boldsymbol{\delta} = 1/2, \tag{B2}$$

$$\text{continuous Hahn:} \quad \boldsymbol{\lambda} = (a_1, a_2), \quad \boldsymbol{\delta} = (1/2, 1/2), \tag{B3}$$

$$\text{continuous dual Hahn:} \quad \boldsymbol{\lambda} = (a_1, a_2, a_3), \quad \boldsymbol{\delta} = (1/2, 1/2, 1/2), \tag{B4}$$

$$\text{Wilson:} \quad \boldsymbol{\lambda} = (a_1, a_2, a_3, a_4), \quad \boldsymbol{\delta} = (1/2, 1/2, 1/2, 1/2), \tag{B5}$$

$$\text{Askey} - \text{Wilson:} \quad \boldsymbol{\lambda} = (a_1, a_2, a_3, a_4), \quad \boldsymbol{\delta} = (1/2, 1/2, 1/2, 1/2), \quad \delta' = -1/2. \tag{B6}$$

The ground state $\phi_0(x)$ and the orthogonal polynomial $P_n(\eta(x))$ are given in (2.83) and (2.84), (3.61) and (3.62), (3.77) and (3.78), (3.96) and (3.97), and (2.102) and (2.103). These ground states satisfy [for the Askey-Wilson polynomials, this relation reads $\phi_0(x - i\gamma/2; \boldsymbol{\lambda} * q^{\boldsymbol{\delta}}) = \sqrt{V(z;\boldsymbol{\lambda})}\varphi(x - i\gamma/2)\phi_0(x;\boldsymbol{\lambda})$, where $\gamma = \log q$]

$$\phi_0(x - i/2; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \sqrt{V(x;\boldsymbol{\lambda})}\varphi(x - i/2)\phi_0(x;\boldsymbol{\lambda}), \tag{B7}$$

where $\varphi(x) \propto \eta'(x)$ is given by

$$\text{Meixner-Pollaczek:} \quad \varphi(x) = 1, \tag{B8}$$

$$\text{continuous Hahn:} \quad \varphi(x) = 1, \tag{B9}$$

$$\text{continuous dual Hahn:} \quad \varphi(x) = 2x, \tag{B10}$$

$$\text{Wilson:} \quad \varphi(x) = 2x, \tag{B11}$$

$$\text{Askey-Wilson:} \quad \varphi(x) = -2\sin x = i(z - z^{-1}). \tag{B12}$$

Let us consider $S_{\pm}(\boldsymbol{\lambda})$, $T_{\pm}(\boldsymbol{\lambda})$, $\mathcal{A}(\boldsymbol{\lambda})$ given in (2.77)–(2.79). By using the property (B7), we have

$$\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}\, S_{\pm}(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) = \varphi(x)^{-1}e^{\pm p/2}, \tag{B13}$$

$$\phi_0(x;\boldsymbol{\lambda})^{-1}\, S_{\pm}(\boldsymbol{\lambda})^{\dagger}\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) = \begin{cases} V(x;\boldsymbol{\lambda})e^{p/2}\varphi(x) \\ V(x;\boldsymbol{\lambda})^{*}e^{-p/2}\varphi(x). \end{cases} \tag{B14}$$

(In the case of the Askey-Wilson polynomials, the following replacement is needed: $\boldsymbol{\lambda} + \boldsymbol{\delta} \Rightarrow \boldsymbol{\lambda} * q^{\boldsymbol{\delta}}$, $e^{\pm p/2} \Rightarrow q^{\pm D/2}$, $V(x;\boldsymbol{\lambda}) \Rightarrow V(z;\boldsymbol{\lambda})$. Hereafter we will omit similar remarks.) From this, we obtain

$$F(\boldsymbol{\lambda}) \overset{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}\mathcal{A}(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) = i\varphi(x)^{-1}(e^{p/2} - e^{-p/2}), \tag{B15}$$

$$B(\boldsymbol{\lambda}) \overset{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda})^{-1}\mathcal{A}(\boldsymbol{\lambda})^{\dagger}\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) = -i(V(x;\boldsymbol{\lambda})e^{p/2} - V(x;\boldsymbol{\lambda})^{*}e^{-p/2})\varphi(x), \tag{B16}$$

$$\widetilde{T}_{\pm}(\boldsymbol{\lambda}) \overset{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda})^{-1}T_{\pm}(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) = \begin{cases} V(x;\boldsymbol{\lambda})e^{p} \\ V(x;\boldsymbol{\lambda})^{*}e^{-p}. \end{cases} \tag{B17}$$

Therefore the similarity transformed Hamiltonian is

$$\widetilde{\mathcal{H}}(\boldsymbol{\lambda}) \overset{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda})^{-1}\mathcal{H}(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) = B(\boldsymbol{\lambda})F(\boldsymbol{\lambda})/2 = (\widetilde{T}_{+}(\boldsymbol{\lambda}) + \widetilde{T}_{-}(\boldsymbol{\lambda}) - V(x;\boldsymbol{\lambda}) - V(x;\boldsymbol{\lambda})^{*})/2. \tag{B18}$$

which acts on $P_n(\eta(x);\boldsymbol{\lambda})$ as $\widetilde{H}(\boldsymbol{\lambda})P_n(\eta(x);\boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda})P_n(\eta(x);\boldsymbol{\lambda})$.

The forward shift operator $F(\boldsymbol{\lambda})$ and backward shift operator $B(\boldsymbol{\lambda})$ act on $P_n(\eta;\boldsymbol{\lambda})$ as

$$F(\boldsymbol{\lambda})P_n(\eta;\boldsymbol{\lambda}) = f_n(\boldsymbol{\lambda})P_{n-1}(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}), \tag{B19}$$

$$B(\boldsymbol{\lambda})P_n(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}) = b_n(\boldsymbol{\lambda})P_{n+1}(\eta;\boldsymbol{\lambda}), \tag{B20}$$

where $f_n(\boldsymbol{\lambda})$ and $b_n(\boldsymbol{\lambda})$ are constants satisfying the relation $f_n(\boldsymbol{\lambda})b_{n-1}(\boldsymbol{\lambda})/2 = \mathcal{E}_n(\boldsymbol{\lambda})$:

$$\text{Meixner-Pollaczek:} \quad f_n(\boldsymbol{\lambda}) = 2, \quad b_n(\boldsymbol{\lambda}) = n+1, \tag{B21}$$

$$\text{continuous Hahn:} \quad f_n(\boldsymbol{\lambda}) = n + 2a_1 + 2a_2 - 1, \quad b_n(\boldsymbol{\lambda}) = n+1, \tag{B22}$$

$$\text{continuous dual Hahn:} \quad f_n(\boldsymbol{\lambda}) = -n, \quad b_n(\boldsymbol{\lambda}) = -1, \tag{B23}$$

$$\text{Wilson:} \quad f_n(\boldsymbol{\lambda}) = -n\Big(n + \textstyle\sum_{j=1}^{4} a_j - 1\Big), \quad b_n(\boldsymbol{\lambda}) = -1, \tag{B24}$$

$$\text{Askey-Wilson:} \quad f_n(\boldsymbol{\lambda}) = -q^{n/2}(q^{-n}-1)(1-a_1a_2a_3a_4q^{n-1}), \quad b_n(\boldsymbol{\lambda}) = -q^{-(n+1)/2}. \tag{B25}$$

For the Meixner-Pollaczek and the continuous dual Hahn cases, we have seen that the annihilation-creation operators are factorized $a^{(-)} \propto X^{\dagger}\mathcal{A}$ and $a^{(+)} \propto \mathcal{A}^{\dagger}X$, (2.94), (3.92). By using (B13), (B14), and (B17), $\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}X(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda})$ and $\phi_0(x;\boldsymbol{\lambda})^{-1}\,X(\boldsymbol{\lambda})^{\dagger}\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})$ can be written down explicitly. They act on $P_n(\eta;\boldsymbol{\lambda})$ as for the Meixner-Pollaczek case:

$$\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}X(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) \cdot P_n(\eta;\boldsymbol{\lambda}) = 2P_n(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}), \tag{B26}$$

$$\phi_0(x;\boldsymbol{\lambda})^{-1}X(\boldsymbol{\lambda})^{\dagger}\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) \cdot P_n(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}) = (n+2a)P_n(\eta;\boldsymbol{\lambda}), \tag{B27}$$

and for the continuous dual Hahn case:

$$\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}X(\boldsymbol{\lambda})\phi_0(x;\boldsymbol{\lambda}) \cdot P_n(\eta;\boldsymbol{\lambda}) = P_n(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}), \tag{B28}$$

$$\phi_0(x;\boldsymbol{\lambda})^{-1}X(\boldsymbol{\lambda})^{\dagger}\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) \cdot P_n(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}) = \prod_{1\le j<k\le 3}(n+a_j+a_k) \cdot P_n(\eta;\boldsymbol{\lambda}). \tag{B29}$$

Therefore $X^{\dagger}$ (X) compensates the parameter shift caused by $\mathcal{A}$ ($\mathcal{A}^{\dagger}$), so that the effect of $a^{(-)}$ ($a^{(+)}$) is to give the polynomial with the same parameter $\boldsymbol{\lambda}$ of degree one lower (higher). This result is new.

Let us close this appendix with a remark on the formal definition of the annihilation-creation operators used within the framework of shape-invariant quantum mechanics.[9,2] A unitary operator $\mathcal{U}$ ($\mathcal{U}^{\dagger}$) is defined as a map between two orthonormal bases with neighbouring parameters, $\{\hat{\phi}_n(x;\boldsymbol{\lambda})\}$ and $\{\hat{\phi}_n(x;\boldsymbol{\lambda}+\boldsymbol{\delta})\}$:

$$\mathcal{U}\hat{\phi}_n(x;\boldsymbol{\lambda}) \overset{\text{def}}{=} \hat{\phi}_n(x;\boldsymbol{\lambda}+\boldsymbol{\delta}), \quad \mathcal{U}^\dagger\hat{\phi}_n(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) = \hat{\phi}_n(x;\boldsymbol{\lambda}). \tag{B30}$$

This allows to introduce new annihilation-creation operators in a factorized form

$$\hat{a} \overset{\text{def}}{=} \mathcal{U}^\dagger\mathcal{A}(\boldsymbol{\lambda}), \quad \hat{a}^\dagger = \mathcal{A}(\boldsymbol{\lambda})^\dagger\mathcal{U}, \tag{B31}$$

which satisfy $\mathcal{H}=\hat{a}^\dagger\hat{a}/2=\mathcal{A}(\boldsymbol{\lambda})^\dagger\mathcal{A}(\boldsymbol{\lambda})/2$. The operator $\mathcal{U}$ is rather formal and it cannot be expressed as a differential or a difference operator. This operator $\mathcal{U}$ can be considered as unitarisation of the natural factorization operator X discussed above.

APPENDIX C: SOME DEFINITIONS RELATED TO THE HYPERGEOMETRIC AND *q*-HYPERGEOMETRIC FUNCTIONS

For reader's convenience we collect several definitions related to the (q-)hypergeometric functions.[6]

- Pochhammer symbol $(a)_n$:

$$(a)_n \overset{\text{def}}{=} \prod_{k=1}^{n}(a+k-1) = a(a+1)\cdots(a+n-1) = \Gamma(a+n)/\Gamma(a). \tag{C1}$$

- q-Pochhammer symbol $(a;q)_n$:

$$(a;q)_n \overset{\text{def}}{=} \prod_{k=1}^{n}(1-aq^{k-1}) = (1-a)(1-aq)\cdots(1-aq^{n-1}). \tag{C2}$$

- hypergeometric series ${}_rF_s$:

$${}_rF_s\left(\begin{matrix}a_1,\ldots,a_r\\ b_1,\ldots,b_s\end{matrix}\middle| z\right) \overset{\text{def}}{=} \sum_{n=0}^{\infty}\frac{(a_1,\ldots,a_r)_n}{(b_1,\ldots,b_s)_n}\frac{z^n}{n!}, \tag{C3}$$

  where $(a_1,\ldots,a_r)_n \overset{\text{def}}{=} \prod_{j=1}^{r}(a_j)_n = (a_1)_n\cdots(a_r)_n$.
- q-hypergeometric series (the basic hypergeometric series) ${}_r\phi_s$:

$${}_r\phi_s\left(\begin{matrix}a_1,\ldots,a_r\\ b_1,\ldots,b_s\end{matrix}\middle| q;z\right) \overset{\text{def}}{=} \sum_{n=0}^{\infty}\frac{(a_1,\ldots,a_r;q)_n}{(b_1,\ldots,b_s;q)_n}(-1)^{(1+s-r)n}q^{(1+s-r)n(n-1)/2}\frac{z^n}{(q;q)_n}, \tag{C4}$$

  where $(a_1,\ldots,a_r;q)_n \overset{\text{def}}{=} \prod_{j=1}^{r}(a_j;q)_n = (a_1;q)_n\cdots(a_r;q)_n$.
- Bessel function $J_a(z)$:

$$J_a(z) \overset{\text{def}}{=} \frac{(z/2)^a}{\Gamma(a+1)}{}_0F_1\left(\begin{matrix}-\\ a+1\end{matrix}\middle| -\frac{z^2}{4}\right). \tag{C5}$$

- Hermite polynomial $H_n(x)$:

$$H_n(x) \overset{\text{def}}{=} (2x)^n{}_2F_0\left(\begin{matrix}-n/2,-(n-1)/2\\ -\end{matrix}\middle| -\frac{1}{x^2}\right). \tag{C6}$$

- Laguerre polynomial $L_n^{(\alpha)}(x)$:

$$L_n^{(\alpha)}(x) \overset{\text{def}}{=} \frac{(\alpha+1)_n}{n!}{}_1F_1\left(\begin{matrix}-n\\ \alpha+1\end{matrix}\middle| x\right). \tag{C7}$$

- Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$:

$$P_n^{(\alpha,\beta)}(x)\overset{\text{def}}{=}\frac{(\alpha+1)_n}{n!}{}_2F_1\left(\begin{matrix}-n,n+\alpha+\beta+1\\ \alpha+1\end{matrix}\middle|\frac{1-x}{2}\right), \tag{C8}$$

which satisfies $P_n^{(\beta,\alpha)}(x)=(-1)^nP_n^{(\alpha,\beta)}(-x)$.

- Gegenbauer polynomial $C_n^{(\lambda)}(x)$:

$$C_n^{(\lambda)}(x)\overset{\text{def}}{=}\frac{(2\lambda)_n}{(\lambda+1/2)_n}P_n^{(\lambda-1/2,\lambda-1/2)}(x). \tag{C9}$$

- Meixner-Pollaczek polynomial $P_n^{(a)}(x;\phi)$:

$$P_n^{(a)}(x;\phi)\overset{\text{def}}{=}\frac{(2a)_n}{n!}e^{in\phi}{}_2F_1\left(\begin{matrix}-n,,a+ix\\ 2a\end{matrix}\middle|1-e^{-2i\phi}\right). \tag{C10}$$

- Continuous Hahn polynomial $p_n(x;a_1,a_2,a_1',a_2')$:

$$p_n(x;a_1,a_2,a_1',a_2')\overset{\text{def}}{=}i^n\frac{(a_1+a_1')_n(a_1+a_2')_n}{n!}{}_3F_2\left(\begin{matrix}-n,n+a_1+a_2+a_1'+a_2'-1,a_1+ix\\ a_1+a_1',a_1+a_2'\end{matrix}\middle|1\right), \tag{C11}$$

which is symmetric under $a_1\leftrightarrow a_2$ and $a_1'\leftrightarrow a_2'$ separately.

- Continuous dual Hahn polynomial $S_n(x^2;a_1,a_2,a_3)$:

$$S_n(x^2;a_1,a_2,a_3)\overset{\text{def}}{=}(a_1+a_2)_n(a_1+a_3)_n{}_3F_2\left(\begin{matrix}-n,a_1+ix,a_1-ix\\ a_1+a_2,a_1+a_3\end{matrix}\middle|1\right), \tag{C12}$$

which is symmetric under the permutations of (a_1,a_2,a_3).

- Wilson polynomial $W_n(x^2;a_1,a_2,a_3,a_4)$:

$$\begin{aligned}W_n(x^2;a_1,a_2,a_3,a_4)\overset{\text{def}}{=}&(a_1+a_2)_n(a_1+a_3)_n(a_1+a_4)_n\\ &\times{}_4F_3\left(\begin{matrix}-n,n+\sum_{j=1}^4a_j-1,a_1+ix,a_1-ix\\ a_1+a_2,a_1+a_3,a_1+a_4\end{matrix}\middle|1\right),\end{aligned} \tag{C13}$$

which is symmetric under the permutations of (a_1,a_2,a_3,a_4).

- Askey-Wilson Hahn polynomial $p_n(\cos x;a_1,a_2,a_3,a_4|q)$:

$$\begin{aligned}p_n(\cos x;a_1,a_2,a_3,a_4|q)\overset{\text{def}}{=}&a_1^{-n}(a_1a_2,a_1a_3,a_1a_4;q)_n\\ &\times{}_4\phi_3\left(\begin{matrix}q^{-n},a_1a_2a_3a_4q^{n-1},a_1e^{ix},a_1e^{-ix}\\ a_1a_2,a_1a_3,a_1a_4\end{matrix}\middle|q;q\right),\end{aligned} \tag{C14}$$

which is symmetric under the permutations of (a_1,a_2,a_3,a_4).

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A note on the infimum problem of Hilbert space effects

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The quantum effects for a physical system can be described by the set $\mathcal{E}(\mathcal{H})$ of positive operators on a complex Hilbert space $\mathcal{H}$ that are bounded above by the identity operator I. The infimum problem of Hilbert space effects is to find under what condition the infimum $A\wedge B$ exists for two quantum effects A and $B\in\mathcal{E}(\mathcal{H})$. The problem has been studied in different contexts by Kadison, Gudder, Moreland, and Ando. In this Note, using the method of the spectral theory of operators, we give a affirmative answer of a conjecture of [S. Gudder, J. Math. Phys. **37**, 2637–2642 (1996)]. In addition, some properties of generalized infimum $A\sqcap B$ were considered. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2358392]

I. INTRODUCTION

Let $\mathcal{H}$ be a Hilbert space and $\mathcal{B}(\mathcal{H})$ the set of all bounded linear operators on $\mathcal{H}$. We use the notation

$$\mathcal{B}(\mathcal{H})^+=\{A\in\mathcal{B}(\mathcal{H}):0\leqslant A\},\quad \mathcal{E}(\mathcal{H})=\{A\in\mathcal{B}(\mathcal{H}):0\leqslant A\leqslant I\},$$

that is, $\mathcal{E}(\mathcal{H})$ is the set of quantum effects.[1–7,11] For operators $A,B\in\mathcal{B}(\mathcal{H})^+$ we denote by $A\wedge B$, the infimum, equivalently, the greatest lower bound, of A and B over the partially ordered set $(\mathcal{B}(\mathcal{H})^+,\geqslant)$, if it exists. To be more precise, $A\wedge B$ is an operator in $\mathcal{B}(\mathcal{H})^+$ uniquely determined by the following properties: $A\wedge B\leqslant A$, $A\wedge B\leqslant B$, and an operator $D\in\mathcal{B}^+(\mathcal{H})$ satisfies both $D\leqslant A$ and $D\leqslant B$ if and only if $D\leqslant A\wedge B$. As it is well known, in general, the infimum of two effects A and B may not exist. However, the infimum $A\wedge B$ always exists if A and B are comparable. Two positive operator A and B are said to be comparable if $A\geqslant B$ or $A\leqslant B$. The Hilbert space infimum question refers to the characterization of pairs of positive bounded operators that admit infimum over the cone of positive operators in a Hilbert space. The problem was earlier studied in different contexts by Kadison,[9] Ando,[1] Gudder[6,7] Moreland,[12] and Gheondea.[4] For example, Moreland and Gudder in Ref. 11 have proved that if A and $B\in\mathcal{E}(C^n)$ are injective positive definite matrices, then the infimum $A\wedge B$ exists if and only if A and B are comparable. If $A\in\mathcal{E}(\mathcal{H})$ and P is an orthogonal projection, then $P\wedge A$ exists. In Ref. 6, Gudder proposes the following conjecture: If $A,B\in\mathcal{E}(\mathcal{H})$ are invertible operators, then $A\wedge B$ exists if and only if A and B are comparable.

Before proving the main results in this paper, let us introduce some notations and terminology which are used later. For an operator $A\in\mathcal{B}(\mathcal{H})$, we shall denote by $N(A)$, $R(A)$, and $\sigma(A)$ the null space, the range, and the spectrum of A, respectively. An operator $A\in\mathcal{B}(\mathcal{H})$ is said to be injective if $N(A)=\{0\}$. The identity onto a Hilbert space $\mathcal{K}$ is denoted by $I_{\mathcal{K}}$ or I if there does not exist confusion. An operator $A\in\mathcal{B}(\mathcal{H})$ is said to be positive if $(Ax,x)\geqslant 0$ for all $x\in\mathcal{H}$. An operator $D\in\mathcal{B}(\mathcal{H})$ is said to be a contraction if $\|D\|\leqslant 1$. For self-adjoint operators $A$and B, $A\leqslant B$ means that $(Ax,x)\leqslant(Bx,x)$ for all $x\in\mathcal{H}$. For a self-adjoint operator $A\in\mathcal{B}(\mathcal{H})$, we define $|A|=(A^2)^{1/2}$, where $(A^2)^{1/2}$ is the unique positive square root of A^2. For self-adjoint operators A, $B\in\mathcal{B}(\mathcal{H})$, the generalized infimum $A\sqcap B$ is defined by

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$$A \sqcap B = \frac{1}{2}(A + B - |A - B|).$$

The generalized infimum has been studied in many works. It is easy to see that $A \sqcap B$ always exists. However, for $A, B \in \mathcal{E}(\mathcal{H})$, it is not necessarily true that $A \sqcap B \in \mathcal{E}(\mathcal{H})$, because $A \sqcap B$ may not be positive. Nevertheless, if A and B are comparable or if A and B commute, then $A \sqcap B \in \mathcal{E}(\mathcal{H})$.

In this Note, we first obtained that if $B \in \mathcal{B}(\mathcal{H})^+$, then $I \wedge B$ exists if and only if $\sigma(B) \subseteq \{0\} \cup [1, \|B\|]$ or $\sigma(B) \subseteq [0,1]$. As a corollary, we give a affirmative answer of Conjecture 4.2 of Ref. 6. In addition, we consider some properties of generalized infimum $A \sqcap B$.

II. $A \wedge B$

We begin with some lemmas.

First, we recall Douglas factorization theorem:

Lemma 2.1: Let $B, C \in \mathcal{B}(\mathcal{H})$. Then the following conditions are equivalent:

(1) $R(B) \subseteq R(C)$.
(2) There exists a positive number λ such that $BB^* \leqslant \lambda CC^*$.
(3) There exists $D \in \mathcal{B}(\mathcal{H})$ such that $B = CD$.

Lemma 2.2: Let $A \in \mathcal{B}(\mathcal{H})$ have the following operator matrix form:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{1}$$

according to the space decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$. Then, $A \geqslant 0$ if and only if

(1) $A_{ii} \in \mathcal{B}(\mathcal{H}_i)$ and $A_{ii} \geqslant 0$, $i = 1, 2$;
(2) $A_{21} = A_{12}^*$;
(3) There exists a contraction D from $\mathcal{H}_2$ into $\mathcal{H}_1$ such that $A_{12} = A_{11}^{1/2} D A_{22}^{1/2}$, where $A_{ii}^{1/2}$ is the positive square root of A_{ii}, $i = 1, 2$.

Lemma 2.3: If $A \in \mathcal{B}(\mathcal{H})$ has the form

$$A = \begin{pmatrix} A_{11} & BA_{22}^{1/2} \\ A_{22}^{1/2} B^* & A_{22} \end{pmatrix}$$

with respect to the space decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where $A_{22} \geqslant 0$ is a positive invertible operator on $\mathcal{H}_2$ and B is an operator from $\mathcal{H}_2$ into $\mathcal{H}_1$, then $A \geqslant 0$ if and only if $A_{11} - BB^* \geqslant 0$.

Proof: Since $A_{22} \geqslant 0$ is a positive invertible operator, then $A_{22}^{-1/2} \in \mathcal{B}(\mathcal{H})$. Let

$$C = \begin{pmatrix} I & -BA_{22}^{-1/2} \\ 0 & I \end{pmatrix}.$$

Since $CAC^* \geqslant 0$ if and only if $A \geqslant 0$, but

$$CAC^* = \begin{pmatrix} I & -BA_{22}^{-1/2} \\ 0 & I \end{pmatrix} \begin{pmatrix} A_{11} & BA_{22}^{1/2} \\ A_{22}^{1/2} B^* & A_{22} \end{pmatrix} \begin{pmatrix} I & 0 \\ -A_{22}^{-1/2} B^* & I \end{pmatrix} = \begin{pmatrix} A_{11} - BB^* & 0 \\ 0 & A_{22} \end{pmatrix}$$

and $A_{22} \geqslant 0$, these imply that $A \geqslant 0$ if and only if $A_{11} - BB^* \geqslant 0$.

Using Lemma 2.2, we can easily get the following result.

Lemma 2.4: Let $A \in \mathcal{B}(\mathcal{H})$ be a positive operator. If A has the operator matrix representation $A = (A_{ij})_{n \times n}$ with respect to the space decomposition $\mathcal{H} = \oplus_{i=1}^n \mathcal{H}_i$, then the following statements hold:

(1) A_{ii} as an operator on $\mathcal{H}_i$ is positive, $1 \leqslant i \leqslant n$.

(2) $A_{ij}=A_{ii}^{1/2}D_{ij}A_{jj}^{1/2}$ for some contraction $D_{ij}\in\mathcal{B}(\mathcal{H}_j,\mathcal{H}_i)$, $1\leqslant i,j\leqslant n$.

Lemma 2.5: Let $B\in\mathcal{B}(\mathcal{H})^+$ be injective. Then, $C=I\wedge B$ exists if and only if I and B are comparable.

Proof: Suppose that $I\wedge B$ exists. We show that I and B are comparable. It is clear that we need only to show that $\sigma(B)\subseteq[0,1]$ or $\sigma(B)\subseteq[1,\infty)$.

On the contrary, if $\sigma(B)\cap[0,1)\neq\emptyset$ and $\sigma(B)\cap(1,\infty)\neq\emptyset$, we will prove that $I\wedge B$ does not exist.

Since B is injective, 0 is an accumulation of $\sigma(B)$ or B is invertible. Thus, there exist $0<\mu<1$ and $1<\nu<\infty$ such that $[\frac{1}{2}\mu,\mu]\cap\sigma(B)\neq\emptyset$ and $[\nu,2\nu]\cap\sigma(B)\neq\emptyset$. Let $B=\int_0^{\|B\|}\lambda dE_\lambda$ be the spectral representation of B, we denote $\sigma_1=[0,1/2\mu)\cap\sigma(B)$, $\sigma_2=[\frac{1}{2}\mu,\mu]\cap\sigma(B)$, $\sigma_3=(\mu,1)\cap\sigma(B)$,$\sigma_4=[1,\nu)\cap\sigma(B)$, $\sigma_5=[\nu,2\nu]\cap\sigma(B)$, and $\sigma_6=(2\nu,\|B\|]\cap\sigma(B)$. Thus, B has the operator matrix form

$$B=\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{B}_4,\mathrm{B}_5,\mathrm{B}_6)$$

with respect to the space decomposition $\mathcal{H}=\oplus_{i=1}^6\mathcal{H}_i$, where $\mathcal{H}_1=E([0,\frac{1}{2}\mu))\mathcal{H}$, $\mathcal{H}_2=E([\frac{1}{2}\mu,\mu])\mathcal{H}$, $\mathcal{H}_3=E((\mu,1))\mathcal{H}$, $\mathcal{H}_4=E([1,\nu))\mathcal{H}$, $\mathcal{H}_5=E([\nu,2\nu])\mathcal{H}$, and $\mathcal{H}_6=E((2\nu,\|B\|])\mathcal{H}$. It is clear that $B_2(\leqslant I_{\mathcal{H}_2})$ and $B_5(\geqslant I_{\mathcal{H}_3})$ are invertible positive operators onto $\mathcal{H}_2$ and $\mathcal{H}_5$, respectively, and $\|B_2\|\leqslant\mu$ and $\|B_5^{-1}\|^{-1}\geqslant\nu$.

If $C=I\wedge B$ exists, then $C\leqslant I$ and C has the operator matrix form

$$C=(C_{ij})_{1\leqslant i,j\leqslant 6},$$

with respect to the space decomposition $\mathcal{H}=\oplus_{i=1}^6\mathcal{H}_i$. Note that

$$I\geqslant\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{I},\mathrm{I},\mathrm{I})$$

and

$$B=\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{B}_4,\mathrm{B}_5,\mathrm{B}_6)\geqslant\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{I},\mathrm{I},\mathrm{I});$$

then

$$\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{I},\mathrm{I},\mathrm{I})\leqslant(\mathrm{C}_{ij})_{1\leqslant i,j\leqslant 6}\leqslant\mathrm{I}$$

and

$$\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{I},\mathrm{I},\mathrm{I})\leqslant(\mathrm{C}_{ij})_{1\leqslant i,j\leqslant 6}\leqslant\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{B}_4,\mathrm{B}_5,\mathrm{B}_6).$$

Hence, by Lemma 2.4, $C_{11}=B_1$, $C_{22}=B_2$, $C_{33}=B_3$, $C_{44}=I_{\mathcal{H}_4}$, $C_{55}=I_{\mathcal{H}_5}$, $C_{66}=I_{\mathcal{H}_6}$, $C_{ij}=0$, $1\leqslant i,j\leqslant 6$, and $i\neq j$. This shows that

$$C=\mathrm{diag}(\mathrm{B}_1,\mathrm{B}_2,\mathrm{B}_3,\mathrm{I},\mathrm{I},\mathrm{I}).$$

Now take $\alpha=\frac{3}{4}$, $\beta=\frac{3}{4}$. Then, there exists a small positive number $1>\delta>0$ such that $\min\{(1-\alpha)(\nu-\beta),(\mu^{-1}-\alpha)(1-\beta)\}>(1+\delta)/16>(1-\alpha)(1-\beta)$. Set $\gamma^2=(1+\delta)/16$.

Define an operator $C_{\alpha\beta\gamma}$ by

$$C_{\alpha\beta\gamma}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \alpha B_2 & 0 & 0 & \gamma B_2^{\frac{1}{2}} D & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \gamma D^* B_2^{\frac{1}{2}} & 0 & 0 & \beta I_{\mathcal{H}_5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where D is a partial isometry from $\mathcal{H}_5$ into $\mathcal{H}_2$ with $D\neq 0$ and $I_{\mathcal{H}_2}-DD^*\neq 0$.

Note that $\alpha\beta=9/16>(1+\delta)/16=\gamma^2$. Since $\alpha\beta>\gamma^2$ implies that $\alpha\beta I_{\mathcal{H}_2}-\gamma^2 DD^*\geqslant 0$, then $\alpha\beta B_2-\gamma^2 B_2^{1/2}DD^*B_2^{1/2}=B_2^{1/2}(\alpha\beta I_{\mathcal{H}_2}-\gamma^2 DD^*)B_2^{1/2}\geqslant 0$, by Lemma 2.3, $C_{\alpha\beta\gamma}\geqslant 0$.

It follows from $B_5\geqslant \nu I_{\mathcal{H}_5}$ that $B_5-\beta I_{\mathcal{H}_5}\geqslant(\nu-\beta)I_{\mathcal{H}_5}$, then $(B_5-\beta I_{\mathcal{H}_5})^{-1}\leqslant[1/(\nu-\beta)]I_{\mathcal{H}_5}$. Thus,

$$\begin{aligned}(1-\alpha)B_2-\gamma^2 B_2^{1/2}D(B_5-\beta I_{\mathcal{H}_5})^{-1}D^*B_2^{1/2} &\geqslant B_2^{1/2}\left[(1-\alpha)I_{\mathcal{H}_2}-\gamma^2 D\frac{1}{\nu-\beta}I_{\mathcal{H}_5}D^*\right]B_2^{1/2}\geqslant B_2^{1/2}\Bigg\{(1-\alpha)\\ &\quad\times(I_{\mathcal{H}_2}-DD^*)+\frac{DD^*}{\nu-\beta}[(1-\alpha)(\nu-\beta)-\gamma^2]I_{\mathcal{H}_2}\Bigg\}B_2^{1/2}\\ &\geqslant 0,\end{aligned}$$

since $(1-\alpha)(\nu-\beta)-\gamma^2\geqslant 0$. By Lemma 2.3, $B-C_{\alpha\beta\gamma}\geqslant 0$.

Similarly, $B_2\leqslant\mu I_{\mathcal{H}_2}$ implies that

$$\begin{aligned}(1-\beta)(I_{\mathcal{H}_2}-\alpha B_2)-\gamma^2 B_2^{1/2}DD^*B_2^{1/2} &= (1-\beta)I_{\mathcal{H}_2}-B_2^{1/2}[(1-\beta)\alpha I_{\mathcal{H}_2}+\gamma^2 DD^*]B_2^{1/2}\\ &= B_2^{1/2}[(1-\beta)B_2^{-1}-(1-\beta)\alpha I_{\mathcal{H}_2}-\gamma^2 DD^*]B_2^{1/2}\\ &\geqslant B_2^{1/2}[(1-\beta)(\mu^{-1}-\alpha)I_{\mathcal{H}_2}-\gamma^2 DD^*]B_2^{12}\\ &= B_2^{1/2}[(1-\beta)(\mu^{-1}-\alpha)(I_{\mathcal{H}_2}-DD^*)]B_2^{1/2}\\ &\quad+B_2^{1/2}[(1-\beta)(\mu^{-1}-\alpha)-\gamma^2]DD^*B_2^{1/2}\geqslant 0,\end{aligned}$$

since $(1-\beta)(\mu^{-1}-\alpha)-\gamma^2\geqslant 0$. By Lemma 2.3, $I-C_{\alpha\beta\gamma}\geqslant 0$.

In a similar way, we obtain that $\gamma^2=(1+\delta)/16>1/16=(1-\alpha)(1-\beta)$ implies $C-C_{\alpha\beta\gamma}\not\geqslant 0$. It is a contradiction.

This shows that $I\wedge B$ does not exist when $\sigma(B)\cap(0,1)\neq\emptyset$ and $\sigma(B)\cap(1,\|B\|)\neq\emptyset$.

Conversely, it is clear that $I\wedge B$ exists if I and B are comparable.

Theorem 2.6: *Let* $B\in\mathcal{B}(\mathcal{H})^+$. *Then*, $I\wedge B$ *exists if and only if* $\sigma(B)\subseteq\{0\}\cup[1,\|B\|]$ *or* $\sigma(B)\subseteq[0,1]$.

Proof: Necessity. *Case 1*: B is injective, then by Lemma 2.5, I and B are comparable. Thus, $B\geqslant I$ or $B\leqslant I$, so $\sigma(B)\subseteq[1,\|B\|]$ or $\sigma(B)\subseteq[0,1]$.

Case 2: B is not injective, then

$$B=\begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix}: N(B)^\perp\oplus N(B)\to N(B)^\perp\oplus N(B),$$

where B_1 is injective from $N(B)^\perp$ into $N(B)^\perp$. It is clear that $\sigma(B)=\sigma(B_1)\cup\{0\}$. It follows from Case 1 that $\sigma(B)\subseteq\{0\}\cup[1,\|B\|]$ or $\sigma(B)\subseteq[0,1]$.

Sufficiency: If $\sigma(B)\subseteq[0,1]$, then $B\in\mathcal{B}(\mathcal{H})^+$ implies $B\leqslant I$, so $I\wedge B$ exists. Similarly, If $\sigma(B)\subseteq[1,\|B\|]$, then $B\in\mathcal{B}(\mathcal{H})^+$ implies $B\geqslant I$, so $I\wedge B$ exists. If $0\in\sigma(B)\subseteq\{0\}\cup[1,\|B\|]$, then 0 is an isolated point of $\sigma(B)$, so we have the Riesz idempotent

$$E_0 := \frac{1}{2\pi i}\int_{\partial D}(z-B)^{-1}\mathrm{d}z,$$

where $\{0\}\in D$ is an open disk which is far from the rest of $\sigma(B)$. Since $B\in\mathcal{B}(\mathcal{H})^+$, then it follows from Ref. 8, Theorem 2.5 that E_0 is a projection and $E_0\mathcal{H}=N(B)$. Thus, B can be decomposed as the form of

$$B=\begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix}: E_0^{\perp}\oplus E_0 \to E_0^{\perp}\oplus E_0,$$

where $\sigma(B_1)\subseteq[1,\|B\|]$ is an invertible operator. Similarly,

$$I=\begin{pmatrix} I_1 & 0 \\ 0 & I_2 \end{pmatrix}: E_0^{\perp}\oplus E_0 \to E_0^{\perp}\oplus E_0,$$

where I_1 and I_2 are identity operators on $E_0^{\perp}$ and E_0, respectively. Thus, $I_1\wedge B_1=I_1$, so

$$\begin{pmatrix} I_1 & 0 \\ 0 & 0 \end{pmatrix}\leqslant\begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix},\quad \begin{pmatrix} I_1 & 0 \\ 0 & I_2 \end{pmatrix}.$$

If

$$0\leqslant C=\begin{pmatrix} C_1 & C_2 \\ C_3 & C_4 \end{pmatrix}\leqslant\begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix},\quad \begin{pmatrix} I_1 & 0 \\ 0 & I_2 \end{pmatrix},$$

then it follows from Lemma 2.2 that $C_4=0$, so $C_2=0$ and $C_3=0$. Thus, $C\leqslant\begin{pmatrix} I_1 & 0 \\ 0 & 0 \end{pmatrix}$, we get $I\wedge B=\begin{pmatrix} I_1 & 0 \\ 0 & 0 \end{pmatrix}$.

Lemma 2.7: Suppose A, B, $C\in\mathcal{B}(\mathcal{H})^+$. If A is injective, then $B\wedge C$ exists if and only if $A^{1/2}BA^{1/2}\wedge A^{1/2}CA^{1/2}$ exists. In this case, $A^{1/2}(B\wedge C)A^{1/2}=A^{1/2}BA^{1/2}\wedge A^{1/2}CA^{1/2}$.

Proof: If $B\wedge C$ exists then it is clear that $A^{1/2}(B\wedge C)A^{1/2}\leqslant A^{1/2}BA^{1/2}$, $A^{1/2}CA^{1/2}$. Let $0\leqslant E\leqslant A^{1/2}CA^{1/2}$, $A^{1/2}BA^{1/2}$. By Lemma 2.1, $R(E^{1/2})\subseteq R(A^{1/2}C^{1/2})$, that is $E^{1/2}=A^{1/2}C^{1/2}D$, for some $D\in\mathcal{B}(\mathcal{H})$. Thus, $A^{1/2}C^{1/2}DD^*C^{1/2}A^{1/2}\leqslant A^{1/2}CA^{1/2}$. It follows from $\overline{R(A^{1/2})}=\mathcal{H}$ that $C^{1/2}DD^*C^{1/2}\leqslant C$. Similarly, $A^{1/2}C^{1/2}DD^*C^{1/2}A^{1/2}\leqslant A^{1/2}BA^{1/2}$implies $C^{1/2}DD^*C^{1/2}\leqslant B$, so $C^{1/2}DD^*C^{1/2}\leqslant B\wedge C$. Then, it easy to see that $E=A^{1/2}C^{1/2}DD^*C^{1/2}A^{1/2}\leqslant A^{1/2}(B\wedge C)A^{1/2}$, so $A^{1/2}(B\wedge C)A^{1/2}=A^{1/2}BA^{1/2}\wedge A^{1/2}CA^{1/2}$.

Conversely, assume that $F=A^{1/2}BA^{1/2}\wedge A^{1/2}CA^{1/2}$. By Lemma 2.1, $F\leqslant A^{1/2}BA^{1/2}$ implies $F^{1/2}=A^{1/2}F_1$, for some $F_1\in\mathcal{B}(\mathcal{H})$. Hence, $F=A^{1/2}F_1F_1^*A^{1/2}$. It follows from $\overline{R(A^{1/2})}=\mathcal{H}$ that $F_1F_1^*\leqslant C,B$. Let $0\leqslant G\leqslant B,C$. Then, $A^{1/2}GA^{1/2}\leqslant A^{1/2}BA^{1/2},A^{1/2}CA^{1/2}$, so $A^{1/2}GA^{1/2}\leqslant F=A^{1/2}F_1F_1^*A^{1/2}$. Hence, $G\leqslant F_1F_1^*$, since $\overline{R(A^{1/2})}=\mathcal{H}$. It follows $F_1F_1^*=B\wedge C$, so $A^{1/2}(B\wedge C)A^{1/2}=A^{1/2}BA^{1/2}\wedge A^{1/2}CA^{1/2}$.

The following is a extension of Conjecture 4.2 in Ref. 6.

Theorem 2.8: *Let $A\in\mathcal{B}(\mathcal{H})^+$ be an injective operator and $B\in\mathcal{B}(\mathcal{H})^+$ be an invertible operator. Then, there exists $A\wedge B$ if and only if A and B are comparable.*

Proof: Since $B\in\mathcal{B}(\mathcal{H})^+$ is an invertible operator, then $B^{-1/2}\in\mathcal{B}(\mathcal{H})^+$. It follows from Lemma 2.7 that $A\wedge B$ exists if and only if $B^{-1/2}AB^{-1/2}\wedge B^{-1/2}BB^{-1/2}$ exists if and only if $B^{-1/2}AB^{-1/2}\wedge I$ exists. Since $B^{-1/2}AB^{-1/2}\in\mathcal{B}(\mathcal{H})^+$ is an injective operator, by Lemma 2.5, $A\wedge B$ exists if and only if I and $B^{-1/2}AB^{-1/2}$ are comparable. Hence, $I\geqslant B^{-1/2}AB^{-1/2}$ or $I\geqq B^{-1/2}AB^{-1/2}$, so $A\geqslant B$ or $A\leqslant B$.

Corollary 2.9: (see Theorem 3.6 in Ref. 10) If A, $B\in\mathcal{E}(C^n)$ are incomparable and A, $B>0$, then $A\wedge B$ does not exist.

In general, for A, B, $C\in\mathcal{E}(\mathcal{H})$, the assertion that if $A\wedge B$ exists, then $(A+C)\wedge(B+C)$ exists is not true. we give a example as follows.

Example 2.10: Let A, B, $C\in\mathcal{E}(C^3)$,

$$A=\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{2} \end{pmatrix}, \quad B=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{8} \end{pmatrix}.$$

Then

$$A+C=\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{5}{8} \end{pmatrix}, \quad B+C=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{8} \end{pmatrix}.$$

It is clear that $A+C$ and $B+C$ are invertible and that $A+C \geqslant B+C$ and $A+C \leqslant B+C$. By Corollary 2.9, $(A+C)\wedge(B+C)$ does not exist. But $A\wedge B$ exists, since B is a projection.

Proposition 2.11: Let $A \in \mathcal{E}(\mathcal{H})$. (1) If $2A\wedge I$ exists, then $A\wedge(I-A)$ exists.

(2) If $A\wedge(I-A)$ exists and $I-A$ is invertible, then $2A\wedge I$ exists.

Proof: (1) If $2A\wedge I=B$, then $A\leqslant B$, so $B-A\geqslant 0$. Clearly, $B-A\leqslant A$ and $B-A\leqslant I-A$. Let $0\leqslant C\leqslant A$ and $C\leqslant I-A$. Then it is clear that $C+A\leqslant B$, so $C\leqslant B-A$. Thus, $A\wedge(I-A)=B-A$.

(2) *Case 1*: $N(A)=\{0\}$. Since $A\wedge(I-A)$ exists and $I-A$ is invertible, by Theorem 2.8, $A\geqslant(I-A)$ or $A\leqslant(I-A)$, so $2A\wedge I$ exists.

Case 2: $N(A)\neq\{0\}$. It is clear that

$$A=\begin{pmatrix} A_1 & 0 \\ 0 & 0 \end{pmatrix}: N(A)^{\perp}\oplus N(A)\to N(A)^{\perp}\oplus N(A),$$

where A_1 is injective from $N(A)^{\perp}$ into $N(A)^{\perp}$. Then,

$$I=\begin{pmatrix} I_1 & 0 \\ 0 & I_2 \end{pmatrix}: N(A)^{\perp}\oplus N(A)\to N(A)^{\perp}\oplus N(A), \quad I-A=\begin{pmatrix} I_1-A_1 & 0 \\ 0 & I_2 \end{pmatrix}.$$

It is easy to show that $A\wedge(I-A)$ exists if and only if $A_1\wedge(I_1-A_1)$ exists and also that $2A\wedge I$ exists if and only if $2A_1\wedge I_1$ exists. It follows from Case 1 that $A_1\wedge(I_1-A_1)$ exists implies that $2A_1\wedge I_1$ exists.

Consequently, we obtain

Corollary 2.12: (see Ref. 4) Let $A\in\mathcal{E}(\mathcal{H})$. Then, the following assertions are equivalent:

(1) $A\wedge(I-A)$ exists;
(2) $\sigma(A)$ is contained either in $\{0\}\cup[\frac{1}{2},1]$ or in $[0,\frac{1}{2}]\cup\{1\}$;
(3) $A\wedge P_{A,I-A}$ and $(I-A)\wedge P_{A,I-A}$ are comparable, where $P_{A,B}$ is the orthogonal projection on the closure of $R(A^{1/2})\cap R(B^{1/2})$.

Proof: (1)⇒(2). Suppose that $A\wedge(I-A)$ exists. We assume that $I-A$ is invertible. By Proposition 2.11 (2), $2A\wedge I$ exists. It follows from Theorem 2.6 that $\sigma(2A)\subseteq\{0\}\cup[1,2]$ or $\sigma(2A)\subseteq[0,1]$. Thus, $\sigma(A)\backslash\{1\}\subseteq\{0\}\cup[\frac{1}{2},1]$ or $\sigma(A)\backslash\{1\}\subseteq[0,\frac{1}{2}]$. This shows that (2) holds.

(2)⇒(3). Denote $\mathcal{H}_0=(N(A)\oplus N(I-A))^{\perp}$. According to the space decomposition $\mathcal{H}=\mathcal{H}_0\oplus N(A)\oplus N(I-A)$, A and $I-A$ have the following operator matrix representations:

$$A=\begin{pmatrix} A_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I \end{pmatrix} \quad \text{and } I-A=\begin{pmatrix} I-A_0 & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

respectively, where A_0 and $I-A_0$ are injective on $\mathcal{H}_0$. It is clear that

$$P_{A,I-A}=\begin{pmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad A\wedge P_{A,I-A}=\begin{pmatrix} A_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and

$$(I-A)\wedge P_{A,I-A}=\begin{pmatrix} I-A_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

If (2) holds, then $\sigma(A_0)\subseteq\sigma(A)\subseteq\{0\}\cup\left[\frac{1}{2},1\right]$ or $\sigma(A_0)\subseteq\left[0,\frac{1}{2}\right]\cup\{1\}$. Thus, $\sigma(A_0)\subseteq\left[\frac{1}{2},1\right]$ or $\sigma(I-A_0)\subseteq\left[\frac{1}{2},1\right]$, since A_0 and $I-A_0$ are injective. Thus, A_0 and $I-A_0$ are comparable, that is, $A\wedge P_{A,I-A}$ and $(I-A)\wedge P_{A,I-A}$ are comparable.

(3)⇒(1). If A has the operator matrix representation as above, then $A\wedge P_{A,I-A}$ and $(I-A)\wedge P_{A,I-A}$ are comparable, which implies that A_0 and $I-A_0$ are comparable. Thus, $A_0\wedge(I-A_0)$ exists. It is easily seen that

$$A\wedge(I-A)=\begin{pmatrix} A_0\wedge(I-A_0) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Corollary 2.13: Let $A\in\mathcal{B}(\mathcal{H})^+$ and $B\in\mathcal{B}(\mathcal{H})^+$ be an invertible operator. Then, $A\wedge B=0$ if and only if $A=0$.

Proof: By Lemma 2.7, $A\wedge B=0$ if and only if $B^{-1/2}AB^{-1/2}\wedge I=0$. By the proof of Theorem 2.6, we have $B^{-1/2}AB^{-1/2}=0$, so $A=0$. See Refs. 11 and 12.

III. $A\sqcap B$

Gudder[7] has obtained the following result: For A, $B\in\mathcal{E}(\mathcal{H})$, If $A\sqcap B\in\mathcal{E}(\mathcal{H})$, then

(a) $A\sqcap B$ is a maximal lower bound for A and B in $\mathcal{E}(\mathcal{H})$.
(b) If $A\wedge B$ exists, then $A\wedge B=A\sqcap B$.

In Theorem 4.4 of Ref. 12, it is proved that the infimum $A\wedge P$ exists for any $A\in\mathcal{E}(\mathcal{H})$ and any projection $P\in\mathcal{E}(\mathcal{H})$. As a consequence, we may conjecture that $A\sqcap P\in\mathcal{E}(\mathcal{H})$. However this is not true.

Example 3.1: Let A, $P\in\mathcal{E}(C^3)$,

$$A=\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{2} \end{pmatrix}, \quad P=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Then

$$|A-P| = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{\sqrt{5}}{4} & 0 \\ 0 & 0 & \frac{\sqrt{5}}{4} \end{pmatrix}, \quad A+P = \begin{pmatrix} \frac{3}{2} & 0 & 0 \\ 0 & \frac{3}{2} & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{2} \end{pmatrix}.$$

It follows from $1/2-\sqrt{5}/4<0$ that $A+P \not\geqslant |A-P|$. Thus, $A \sqcap P \notin \mathcal{E}(\mathcal{H})$.

In Lemma 3.7 of Ref. 12, authors have obtained that $A \wedge B$ exists if and only if $(A \wedge P_{A,B}) \wedge (B \wedge P_{A,B})$ exists. For the generalized infimum $A \sqcap B$, we also get a similar result. we need following lemmas.

Lemma 3.2: (Ref. 7, Theorem 2.3 and Lemma 2.5) (a) If $A, B \in \mathcal{E}(\mathcal{H})$, then $(A-A \sqcap B)(B-A \sqcap B)=0$.

(b) For A, $B \in \mathcal{E}(\mathcal{H})$, $A \sqcap B=0$ if and only if $AB=0$.

Lemma 3.3: If $0 \leqslant A \leqslant B$, $0 \leqslant C \leqslant D$ and $BD=0$, then $AC=0$.

Proof: Since $BD=0=DB$, then $BD^{1/2}=D^{1/2}B$, so $D^{1/2}BD^{1/2}=DB=0$. It follows from $0 \leqslant D^{1/2}AD^{1/2} \leqslant D^{1/2}BD^{1/2}=0$ that $D^{1/2}AD^{1/2}=0$. Hence, $A^{1/2}D^{1/2}=0$. Similarly, $0 \leqslant A^{1/2}CA^{1/2} \leqslant A^{1/2}DA^{1/2}=0$, then $A^{1/2}C^{1/2}=0$. Thus $AC=0$.

Theorem 3.4: Let $A, B \in \mathcal{E}(\mathcal{H})$. If $A \sqcap B \in \mathcal{E}(\mathcal{H})$ then $(A \wedge P_{A,B}) \sqcap (B \wedge P_{A,B}) \in \mathcal{E}(\mathcal{H})$. In this case, $(A \wedge P_{A,B}) \sqcap (B \wedge P_{A,B})=A \sqcap B$.

Proof. Since $A \sqcap B \leqslant A$ and $A \sqcap B \leqslant B$, then $R(A \sqcap B) \subseteq R(A \sqcap B)^{1/2} \subseteq R(A^{1/2})$ and $R(A \sqcap B) \subseteq R(B^{1/2})$, by Lemma 2.1. Thus, $R(A \sqcap B) \subseteq R(A^{1/2}) \cap R(B^{1/2})$, so $A \sqcap B \leqslant P_{A,B}$. It follows that $A \sqcap B \leqslant A \wedge P_{A,B}$ and $A \sqcap B \leqslant B \wedge P_{A,B}$. By Lemma 3.2, $(A-A \sqcap B)(B-A \sqcap B)=0$. Since $A \wedge P_{A,B} \leqslant A$ and $B \wedge P_{A,B} \leqslant B$, by Lemma 3.3, we have $(A \wedge P_{A,B}-A \sqcap B)(B \wedge P_{A,B}-A \sqcap B)=0$. It follows from Lemma 3.2 again that

$$(A \wedge P_{A,B}-A \sqcap B) \sqcap (B \wedge P_{A,B}-A \sqcap B)=0,$$

so

$$(A \wedge P_{A,B}-A \sqcap B)+(B \wedge P_{A,B}-A \sqcap B)-|(A \wedge P_{A,B}-A \sqcap B)-(B \wedge P_{A,B}-A \sqcap B)|=0.$$

Thus

$$\tfrac{1}{2}[A \wedge P_{A,B}+B \wedge P_{A,B}-|A \wedge P_{A,B}-B \wedge P_{A,B}|]=A \sqcap B \geqslant 0.$$

Remark: The converse assertion of Theorem 3.4 does not hold, that is, there is $A, B \in \mathcal{E}(\mathcal{H})$ such that $A \sqcap B \notin \mathcal{E}(\mathcal{H})$ and $(A \wedge P_{A,B}) \sqcap (B \wedge P_{A,B}) \in \mathcal{E}(\mathcal{H})$.

Example 3.4: Let A, $B \in \mathcal{E}(C^3)$ and let $B=\frac{1}{2}P$, with A and P as above in Example 3.1. It is clear that

$$B \wedge P_{A,B} = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

From a direct calculation, we have

$$|A-B|=\begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{4\sqrt{2}} & \frac{1}{4\sqrt{2}} \\ 0 & \frac{1}{4\sqrt{2}} & \frac{3}{4\sqrt{2}} \end{pmatrix}, \quad A+B=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{2} \end{pmatrix}.$$

It follows from $(3/4\sqrt{2})-1/2>0$ that $A+B\not\geqslant|A-B|$, then $A\sqcap B\notin\mathcal{E}(\mathcal{H})$. It is easy to calculate that

$$A\wedge P_{A,B}=\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{3}{8} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

In fact, $\mathrm{diag}(\frac{1}{2},\frac{3}{8},0)\leqslant A$, $P_{A,B}$ is clear. Then, $A\wedge P_{A,B}\geqslant\mathrm{diag}(\frac{1}{2},\frac{3}{8},0)$. Therefore, by Lemma 2.3, $A\wedge P_{A,B}=\mathrm{diag}(\frac{1}{2},\frac{3}{8},0)$. Clearly, $(A\wedge P_{A,B})\sqcap(B\wedge P_{A,B})\in\mathcal{E}(\mathcal{H})$.

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Quaternionic diffusion by a potential step

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In looking for *qualitative* differences between quaternionic and complex formulations of quantum physical theories, we provide a detailed discussion of the behavior of a wave packet in the presence of a quaternionic time-independent potential step. In this paper, we restrict our attention to diffusion phenomena. For the group velocity of the wave packet moving in the potential region and for the reflection and transmission times, the study shows a striking difference between the complex and quaternionic formulations which could be matter of further theoretical discussions and could represent the starting point for a possible experimental investigation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2359577]

I. INTRODUCTION

Despite much research on quaternionic quantum mechanics, reviewed in its mathematical and physical aspects in the excellent book of Adler,[1] there have been few breakthroughs on the most natural question about the effect that quaternionic potentials play in the dynamics of elementary particles[2–5] and, as a consequence of it, about the possibility to look for an experimental proposal.[6–9] In this paper, by using the new mathematical tools developed in the analytic resolution of eigenvalue problems[10,11] and differential equations,[6,12–14] we analyze in detail the diffusion of a wave packet by a quaternionic potential step.

For the convenience of the reader and to facilitate access to the individual topics, this work is rendered as self-contained as possible. In Sec. II, we set up notation and terminology and proceed with the study of diffusion by quaternionic potentials. This section contains the (analytic) plane wave solution of the quaternionic Schrödinger equation in the presence of a potential step. This represents a fundamental mathematical tool in the discussion of the quaternionic stationary phase method (see Sec. III). We will touch only a few aspects of the theory of quaternionic integral transforms and restrict our attention to the diffusion of quaternionic wave packets with a peaked convolution function. The advantage of using the stationary phase method lies in the fact that, in the presence of a potential step, the motion of the wave packet can be correctly estimated by analyzing the phase derivative calculated at the maximum of the convolution function.[15–17] For a different shape of potentials, see, for example, the barrier, the stationary phase method, depending on the width of the potential and on the group velocity of the incoming particle, could break down. There is a rich number of articles leading with this problem in standard quantum mechanics.[18–23]

The results of this paper (a conclusion and outlooks are drawn in Sec. IV) shed some new light on the properties of quaternionic potentials. In particular, it is explicitly shown how the presence of a quaternionic perturbation modifies the momentum of the nonrelativistic incoming particle and its reflection (transmission) time. The study presented in this paper represents a starting point in view of a complete understanding of the behavior of wave packets impinging on quaternionic potentials. A detailed analysis of this topic could be fundamental in looking for experiments in which deviations from the complex quantum theory could be really seen. It is

worth pointing out that the question of finding the best experimental proposal to prove the existence of quaternionic potentials is, at present, far from being solved and in this paper we aim to contribute to this debate.

II. REFLECTION AND TRANSMISSION COEFFICIENTS

The quaternionic Schrödinger equation in the presence of a constant potential is given by

$$i\frac{\hbar}{2m}\Psi_{xx}(x,t)-\frac{iV_1+jV_2+kV_3}{\hbar}\Psi(x,t)=\Psi_t(x,t), \tag{1}$$

where $iV_1+jV_2+kV_3$ represents the quaternionic generalization of the anti-Hermitian complex potential iV_1. For a complete discussion, see Ref. 1. This partial differential equation, by the substitution

$$\Psi(x,t)=\Phi(x)\exp[-iEt/\hbar], \tag{2}$$

can be reduced to the following ordinary second order differential equation with constant quaternionic coefficients,

$$i\frac{\hbar^2}{2m}\Phi''(x)-\left(iV_1+jV_2+kV_3\right)\Phi(x)=-\Phi(x)Ei. \tag{3}$$

The solution of the Schrödinger equation in the presence of constant quaternionic potential has been matter of study in recent years.[4–6] New mathematical techniques, essentially based on the right eigenvalue problem for quaternionic operators,[10,12] allow us to obtain the solution without the need to translate the quaternionic problem in its complex counterpart.[2,3] In particular, in the presence of a potential step and for the diffusion case,

$$E>\sqrt{V_1^2+V_2^2+V_3^2},$$

the quaternionic plane wave solutions (for a detailed derivation, see Ref. 6) are as follows:

$$\text{(I) Free region } (x<0): \quad \Phi_I(x)=\exp[i\epsilon x]+r\exp[-i\epsilon x]+j\tilde{r}\exp[\epsilon x];$$

$$\text{(II) Potential region } (x>0): \quad \Phi_{II}(x)=(1+jw)t\exp[i\rho_- x]+(\overline{w}+j)\tilde{t}\exp[-\rho_+ x], \tag{4}$$

where

$$\epsilon=\sqrt{\frac{2m}{\hbar^2}E}, \quad \rho_\pm=\sqrt{\frac{2m}{\hbar^2}\left(\sqrt{E^2-V_2^2-V_3^2}\pm V_1\right)}, \quad w=-i\frac{V_2-iV_3}{E+\sqrt{E^2-V_2^2-V_3^2}},$$

and

$$t=\frac{2\epsilon}{\epsilon+\rho_-}\left[1-|w|^2\frac{\epsilon-i\rho_-}{\epsilon+\rho_-}\frac{\epsilon+i\rho_+}{\epsilon+\rho_+}\right]^{-1}, \quad \tilde{t}=\frac{i\rho_--\epsilon}{\epsilon+\rho_+}wt,$$

$$r=\frac{\epsilon-\rho_-}{2\epsilon}\left[1-|w|^2\frac{\epsilon-i\rho_-}{\epsilon-\rho_-}\frac{\epsilon-i\rho_+}{\epsilon+\rho_+}\right]t, \quad \tilde{r}=\frac{i\rho_-+\rho_+}{\epsilon+\rho_+}wt.$$

From the current conservation,

$$[\overline{\Psi}(x,t)\Psi(x,t)]_t=\frac{\hbar}{2m}[\overline{\Psi}(x,t)i\Psi_{xx}(x,t)+\text{h.c.}], \tag{5}$$

by recalling that we are considering stationary solutions of the Schrödinger equation, we obtain

$$\overline{\Phi}(x)i\Phi''(x) + \text{h.c.} = 0.$$

This implies that the current density,

$$J(x) = \overline{\Phi}(x)i\Phi'(x) + \text{h.c.}, \tag{6}$$

is a quantity independent of x. Due to the continuity of the wave function and its derivative, the current density has to satisfy the following constraint:

$$J_{\text{I}}(0) = J_{\text{II}}(0). \tag{7}$$

By using the explicit form of the plane wave solutions given in Eqs. (4), and the condition (7), a straightforward calculation conduces to

$$R + T = 1, \tag{8}$$

where

$$R = |r|^2 \quad \text{and} \quad T = \frac{\rho_-}{\epsilon}(1 - |w|^2)|t|^2.$$

Similar to the predictions of complex quantum mechanics, the incident particle has a nonzero probability of turning back. Nevertheless, we know that in standard quantum mechanics no phase is created by such reflection.[17] The situation drastically changes in the presence of a quaternionic perturbation. We shall come back to this point in Sec. III.

A. Reflection and transmission phases

From the stationary wave functions given in Eqs. (4), we shall construct, by linear superposition, wave packets and we shall study their time evolution (see Sec. III). In this spirit, it is convenient to rewrite the reflection and transmission coefficients in terms of their modulus and phases. By simple algebraic manipulations, we find

$$r = \sqrt{\frac{[(\epsilon-\rho_-)(\epsilon+\rho_+) - |w|^2(\epsilon^2-\rho_-\rho_+)]^2 + |w|^4\epsilon^2(\rho_-+\rho_+)^2}{[(\epsilon+\rho_-)(\epsilon+\rho_+) - |w|^2(\epsilon^2+\rho_-\rho_+)]^2 + |w|^4\epsilon^2(\rho_--\rho_+)^2}}\exp[i\theta_r],$$

$$t = \frac{2\epsilon(\epsilon+\rho_+)}{\sqrt{[(\epsilon+\rho_-)(\epsilon+\rho_+) - |w|^2(\epsilon^2+\rho_-\rho_+)]^2 + |w|^4\epsilon^2(\rho_--\rho_+)^2}}\exp[i\theta_t], \tag{9}$$

where

$$\theta_r = \arctan\left(\frac{\epsilon(\rho_++\rho_-)|w|^2}{(\epsilon-\rho_-)(\epsilon+\rho_+) - |w|^2(\epsilon^2-\rho_-\rho_+)}\right) + \theta_t,$$

$$\theta_t = \arctan\left(\frac{\epsilon(\rho_+-\rho_-)|w|^2}{(\epsilon+\rho_-)(\epsilon+\rho_+) - |w|^2(\epsilon^2+\rho_-\rho_+)}\right). \tag{10}$$

The important point to be noted here is the dependence on the energy, E, and the complex imaginary part of the potential, V_1, as expected from the standard quantum case, and the *new* dependence on the modulus of the pure quaternionic part of the potential, $|V_2+iV_3|$. This last result means that once fixed the modulus of the quaternionic perturbation any rotation in the plane (V_2, V_3) does not modify the reflection and transmission coefficients. The quaternionic rotation invariance is due to the choice of i as the imaginary unit in the anti-Hermitian momentum operator, $i\hbar\,\partial_{xx}/2m$, which appears in the quaternionic Scrhödinger equation (1).

B. The complex limit

The standard (complex) quantum results can be obtained by taking a simple limit case, i.e., $V_{2,3}\to 0$. In fact, by observing that

$$V_{2,3}\to 0 \Rightarrow \begin{cases} w \to 0, \\ \rho_- \to \sigma = \sqrt{\dfrac{2m}{\hbar^2}(E-V_1)}, \end{cases}$$

we find

$$R=|r|^2 \quad \text{and} \quad T=\frac{\sigma}{\epsilon}|t|^2,$$

where

$$r=\frac{\epsilon-\sigma}{\epsilon+\sigma} \quad \text{and} \quad t=\frac{2\epsilon}{\epsilon+\sigma}. \tag{11}$$

As expected, the reflection and transmission coefficients (r and t) are real ($\theta_r=\theta_t=0$), and this implies that there is no phase created by reflection or transmission.[17]

C. The pure quaternionic limit

It is interesting to consider a second limit, i.e., $V_1\to 0$. This represents the case of a *pure* quaternionic potential. Noting that

$$V_1\to 0 \Rightarrow \begin{cases} \rho_\pm \to \rho = \sqrt{\dfrac{2m}{\hbar^2}\sqrt{E^2-V_2^2-V_3^2}}, \\ |w|^2 \to \dfrac{\epsilon^2-\rho^2}{\epsilon^2+\rho^2}, \end{cases}$$

we obtain

$$R=|r|^2 \quad \text{and} \quad T=\frac{2\rho^3}{\epsilon(\epsilon^2+\rho^2)}|t|^2,$$

where

$$r=\frac{\epsilon-\rho}{\sqrt{\epsilon^2+\rho^2}}\exp\left[i\arctan\left(\frac{\epsilon}{\rho}\right)\right] \quad \text{and} \quad t=\frac{\epsilon}{\rho}. \tag{12}$$

In this limit, the symmetry between reflection and transmission times is broken down. For a pure quaternionic potential step, we find an instantaneous transmission but *not* an instantaneous reflection (we shall discuss in detail this point in Sec. III).

III. STATIONARY PHASE METHOD

Until now, we have been concerned only with plane waves. In this Section, we are going to study the time evolution of quaternionic wave packets and deducing from them several important properties. The principle of superposition guarantees that every *real* linear combination of the plane waves $\Phi_{\mathrm{I}}(x)\exp[-iEt/\hbar]$ and $\Phi_{\mathrm{II}}(x)\exp[-iEt/\hbar]$ will satisfy the Schrödinger equation in the presence of a quaternionic potential step.

Let $g(\epsilon)$ be a real convolution function with a maximum in ϵ_0. In the free region ($x<0$), the superposition can be written as follows:

$$\Omega_{\mathrm{I}}(x,t)=\int_{\epsilon_{\min}}^{\infty}\mathrm{d}\epsilon\, g(\epsilon)\{\exp[i\epsilon x]+r\exp[-i\epsilon x]+j\tilde{r}\exp[\epsilon x]\}\exp[-i\epsilon^2\hbar\, t/2m], \tag{13}$$

where

$$\epsilon_{\min}=\sqrt{\frac{2m}{\hbar^2}\sqrt{V_1^2+V_2^2+V_3^2}}.$$

The first term in Eq. (13) represents the incident wave, the second term the reflected wave and the third term an evanescent wave. The phases for the incoming and reflected waves are

$$\theta_{\mathrm{inc}}[\epsilon;x,t]=\epsilon x-\epsilon^2\frac{\hbar t}{2m},$$

$$\theta_{\mathrm{ref}}[\epsilon;x,t]=-\epsilon x-\epsilon^2\frac{\hbar t}{2m}+\theta_r. \tag{14}$$

The stationary phase condition (the derivative with respect to ϵ of the argument calculated in ϵ_0 equal to zero) enables us to calculate the position of the maximum of the incident and reflected wave packets:

$$x_{\mathrm{inc}}^{\max}(t)=\frac{\hbar\epsilon_0}{m}t,$$

$$x_{\mathrm{ref}}^{\max}(t)=-\frac{\hbar\epsilon_0}{m}t+\left[\frac{\mathrm{d}\theta_r}{\mathrm{d}\epsilon}\right]_0. \tag{15}$$

The maximum of the incident wave packet arrives at the step discontinuity at time $t=0$ (as it occurs in the complex case). During a certain interval of time, the wave packet is localized in the region $x\sim 0$. For large times the incident wave packet has practically disappeared and we only find the reflected wave packet. It is important to observe that contrary to the predictions of complex quantum mechanics ($\theta_r=0$), the maximum of the reflected wave packets is found at $x=0$ at time $t=(m/\hbar\epsilon_0)[\mathrm{d}\theta_r/\mathrm{d}\epsilon]_0$. This means that in the presence of a quaternionic perturbation we do *not* have an instantaneous reflection: for large times the maximum of the reflected wave packet is *not* at $-\hbar\epsilon_0 t/m$ but is shifted with respect to this value by a quantity equal to $[\mathrm{d}\theta_r/\mathrm{d}\epsilon]_0$.

An analogous discussion for the transmitted wave packet ($x>0$),

$$\Omega_{\mathrm{II}}(x,t)=\int\mathrm{d}\epsilon\, g(\epsilon)\{t\exp[i\rho_- x]+\tilde{wt}\exp[-\rho_+ x]\}\exp[-i\epsilon^2\hbar\, t/2m]+j\int\mathrm{d}\epsilon\, g(\epsilon)\{wt\exp[i\rho_- x]$$
$$+\tilde{t}\exp[-\rho_+ x]\}\exp[-i\epsilon^2\hbar\, t/2m], \tag{16}$$

where the phases to be considered are

$$\theta_{\mathrm{tra}}^{(1,i)}[\epsilon;x,t]=\rho_- x-\epsilon^2\frac{\hbar t}{2m}+\theta_t$$

$$\theta_{\mathrm{tra}}^{(j,k)}[\epsilon;x,t]=\rho_- x-\epsilon^2\frac{\hbar t}{2m}+\theta_t+\arctan\left[\frac{V_2}{V_3}\right], \tag{17}$$

leads to a similar conclusion for the transmitted time. Contrary to what happens in the standard (complex) quantum mechanics, where there is an instantaneous transmission, in the presence of a quaternionic potential step, the maximum of the transmitted wave packet,

$$x_{\mathrm{tra}}^{\max}(t)=\left\{\frac{\hbar\epsilon_0}{m}t-\left[\frac{\mathrm{d}\theta_t}{\mathrm{d}\epsilon}\right]_0\right\}\Bigg/\left[\frac{\mathrm{d}\rho_-}{\mathrm{d}\epsilon}\right]_0, \tag{18}$$

is found at $x=0$ at time $t=(m/\hbar\epsilon_0)[\mathrm{d}\theta_t/\mathrm{d}\epsilon]_0$. At first glance, it could appear a logical consequence of the result obtained for the reflection time. Nevertheless, it is important to note that $\theta_r\neq\theta_t$ and, consequently, the symmetry between reflection and transmission times is always broken down. For example, as it was explicitly shown in the previous section, instantaneous transmission does not necessarily imply instantaneous reflection.

In order to simplify the discussion about the results obtained in our study, let us introduce the following notation:

$$V_0=\sqrt{V_1^2+V_2^2+V_3^2},$$

and rewrite the maximum of the incident, reflected and transmitted wave packets in terms of E_0 (the maximum value of the energy spectrum of the incoming particles)

$$x_{\mathrm{inc}}^{\max}(t)=\sqrt{\frac{2E_0}{m}}t,$$

$$x_{\mathrm{ref}}^{\max}(t)=-\sqrt{\frac{2E_0}{m}}t+\frac{\hbar}{\sqrt{2mV_0}}\left[\frac{\mathrm{d}\theta_r}{\mathrm{d}\sqrt{\frac{E}{V_0}}}\right]_0,$$

$$x_{\mathrm{tra}}^{\max}(t)=\left\{\sqrt{\frac{2E_0}{m}}t-\frac{\hbar}{\sqrt{2mV_0}}\left[\frac{\mathrm{d}\theta_t}{\mathrm{d}\sqrt{\frac{E}{V_0}}}\right]_0\right\}\Bigg/\left[\frac{\mathrm{d}\rho_-}{\mathrm{d}\epsilon}\right]_0. \tag{19}$$

The incident and reflected wave packets propagate, respectively, with velocities of v_0 and $-v_0$,

$$v_0=\sqrt{2E_0/m}. \tag{20}$$

This is the standard result obtained in complex quantum mechanics. For the transmitted wave packet, the velocity is given by

$$v_{\mathrm{tra}}=v_0\Bigg/\left[\frac{\mathrm{d}\rho_-}{\mathrm{d}\epsilon}\right]_0. \tag{21}$$

Due to the fact that the quantity ρ_- has an additional dependence on $|V_2+iV_3|$ with respect to the standard dependence on V_1, the complex and quaternionic formulations give different predictions. For example, of particular interest, it is the comparison between the group velocity of the transmitted wave packet for the complex case, $V_0=V_1$,

$$v_{\mathrm{tra}}^{(i)}=v_0\Bigg/\left(\sqrt{\epsilon^2-\frac{2m}{\hbar^2}V_0}\right)_\epsilon=v_0\sqrt{1-\frac{V_0}{E_0}}, \tag{22}$$

and that one for the *pure* quaternionic case, $V_0=|V_2+iV_3|$,

$$v_{\mathrm{tra}}^{(j,k)}=v_0\Bigg/\left\{\left[\epsilon^4-\left(\frac{2m}{\hbar^2}V_0\right)^2\right]^{1/4}\right\}_\epsilon=v_0\left[1-\left(\frac{V_0}{E_0}\right)^2\right]^{3/4}. \tag{23}$$

A first *important* observation is that whereas $v_{\mathrm{tra}}^{(i)}$ is greater or smaller than v_0 depending on the sign of V_1, $v_{\mathrm{tra}}^{(j,k)}$ is always smaller than the group velocity in the fre region. For incident particles with an energy spectrum peaked in E_0, with $E_0\gg V_0$, the group velocities of the wave packet

traveling in the potential region, (22) and (23), can be approximated by taking the first terms in their Taylor expansions,

$$v_{\mathrm{tra}}^{(i)} = v_0\left[1 - \frac{1}{2}\frac{V_0}{E_0} - \frac{1}{8}\left(\frac{V_0}{E_0}\right)^2\right] + \mathcal{O}\left[\left(\frac{V_0}{E_0}\right)^3\right],$$

$$v_{\mathrm{tra}}^{(j,k)} = v_0\left[1 - \frac{3}{4}\left(\frac{V_0}{E_0}\right)^2\right] + \mathcal{O}\left[\left(\frac{V_0}{E_0}\right)^4\right].$$

This means that a clear difference between the complex and the (pure) quaternionic case is expected for the group velocity of a wave packet traveling in a region in which a small perturbation is turned on. In this spirit, it is also interesting to compare the reflection and transmission times,

$$\frac{\sqrt{2mV_0}}{\hbar}x_{\mathrm{ref}}^{\max}(0) = \left[\frac{\mathrm{d}\theta_r}{\mathrm{d}\sqrt{\frac{E}{V_0}}}\right]_0,$$

$$\frac{\sqrt{2mV_0}}{\hbar}x_{\mathrm{tra}}^{\max}(0) = -\left[\frac{\mathrm{d}\theta_t}{\mathrm{d}\sqrt{\frac{E}{V_0}}}\right]_0 \Bigg/ \left[\frac{\mathrm{d}\rho_-}{\mathrm{d}\epsilon}\right]_0. \tag{24}$$

Standard quantum mechanics predicts instantaneous reflection and transmission, i.e.,

$$x_{\mathrm{ref}}^{(i)\max}(0) = x_{\mathrm{tra}}^{(i)\max}(0) = 0.$$

For a pure quaternionic potential, the transmission, in analogy to the complex case, is instantaneous,

$$x_{\mathrm{tra}}^{(j,k)\max}(0) = 0,$$

but the reflection time is different from zero (breaking down the instantaneity),

$$\frac{\sqrt{2mV_0}}{\hbar}x_{\mathrm{ref}}^{(j,k)\max}(0) = -\left\{2\sqrt{\frac{E_0}{V_0}}\left[\frac{E_0}{V_0} + \sqrt{\left(\frac{E_0}{V_0}\right)^2 - 1}\right]\left[\left(\frac{E_0}{V_0}\right)^2 - 1\right]^{3/4}\right\}^{-1}.$$

This predicts, for large times, that the maximum of the reflected wave packet should be found at the left of the position predicted by standard quantum mechanics, i.e., $-\hbar\,\epsilon_0 t/m$. For $E_0 \gg V_0$, the difference between the complex and (pure) quaternionic case is *only* manifest at the third order in V_0/E_0,

$$\frac{\sqrt{2mV_0}}{\hbar}x_{\mathrm{ref}}^{\max}(0) = -\frac{1}{4}\left(\frac{V_0}{E_0}\right)^3 + \mathcal{O}\left[\left(\frac{V_0}{E_0}\right)^4\right],$$

and, consequently, for small perturbations, we practically find an instantaneous reflection. It is important to note that the shift in the position of the maximum of the reflected wave packet becomes important when E_0 approaches V_0, this implies $x_{\mathrm{ref}}^{(j,k)\max}(0) \to \infty$. Nevertheless, for incident wave packets peaked in $E_0 \sim V_0$, a more careful analysis is needed. In fact, in this limit new effects have to be considered and these effects cannot be obtained by simply using the stationary phase method.[19–21]

IV. CONCLUSIONS AND OUTLOOKS

The study presented in this paper, and based on the use of wave packets, represents, from our point of view, a first important attempt to discuss deviations from the standard (complex) quantum

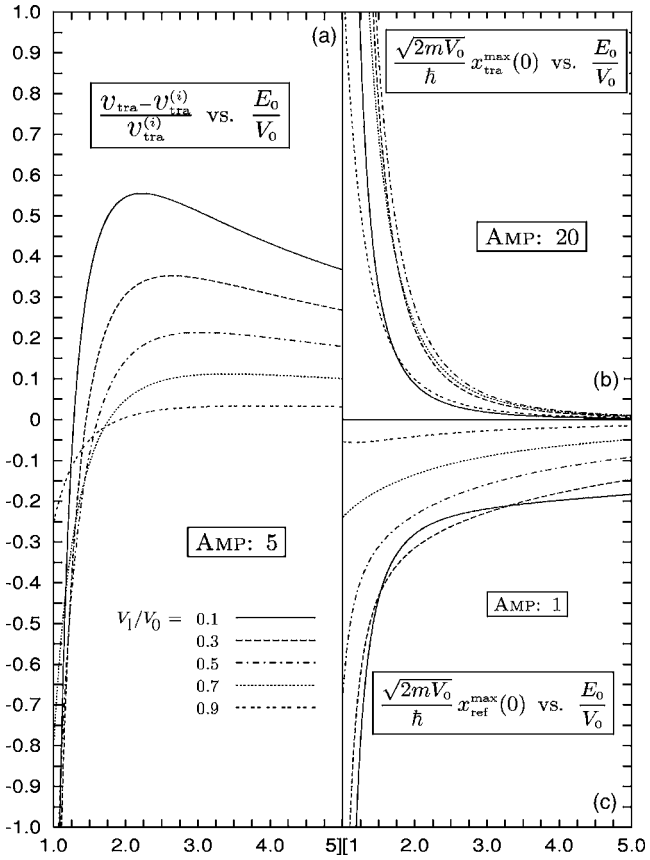

FIG. 1. Fixing the value of $V_0=|iV_1+jV_2+kV_3|$ and varying its complex component V_1, the group velocity of the transmitted wave packet (a) and the transmission/reflection times, (b) and (c) are plotted as a function of E_0/V_0, where E_0 is the maximum of the energy spectrum of the incident wave packet. The analysis is done for diffusion phenomena ($E_0>V_0$).

mechanics in the presence of quaternionic potentials. The wave packet formalism, with respect to the previous analysis, essentially based on the plane wave solutions, surely gives a more "physical" focus. For example, this formalism allows us to explicitly show the effect that quaternionic perturbations play in the momentum distribution of elementary particles and, in the particular case of a potential step, to calculate the new reflection and transmission times due to quaternionic interference phenomena. To emphasize the main differences between the complex and the quaternionic formulation of quantum mechanics for diffusion phenomena by a potential step, we have given, in the previous section, a detailed discussion based on the *analytic* study of the group velocities in the potential region and of the reflection time for complex and (pure) quaternionic potentials.

Now, let us return to the discussion for the general case, i.e., a complex potential in the presence of a quaternionic perturbation. In Fig. 1(a), fixing the value of V_0 and varying its complex component V_1, we draw

$$\frac{v_{\mathrm{tra}}-v_{\mathrm{tra}}^{(i)}}{v_{\mathrm{tra}}^{(i)}}, \tag{25}$$

as a function of E_0/V_0. The continuous line represents the case of a small complex component in the quaternionic potential, consequently such a curve approximates the case of a pure quaternionic potential,

$$\frac{v_{\mathrm{tra}}^{(j,k)}-v_{\mathrm{tra}}^{(i)}}{v_{\mathrm{tra}}^{(i)}}=\left(1-\frac{V_0}{E_0}\right)^{1/4}\left(1+\frac{V_0}{E_0}\right)^{3/4}-1\underset{E_0\gg V_0}{\longrightarrow}\frac{1}{2}\frac{V_0}{E_0}-\frac{3}{8}\left(\frac{V_0}{E_0}\right)^2+\mathcal{O}\left[\left(\frac{V_0}{E_0}\right)^3\right].$$

It is also interesting to observe that the maximum of $(v_{\mathrm{tra}}^{(j,k)}-v_{\mathrm{tra}}^{(i)})/v_{\mathrm{tra}}^{(i)}$ is found at $E_0=2V_0$.

The plots in Fig. 1(b) and Fig. 1(c), respectively, show the behavior of the transmission and reflection times as a function of E_0/V_0. Let us list some results coming out from our analysis. The quaternionic interefernce phenomena at the step discontinuity produce an new interesting effect in the reflected and transmitted wave packets: the maxima of such packets are found at $x=0$ before that the incident wave packet reaches the potential step discontinuity. The symmetry between reflection and transmission time is broken down [see the amplification if Fig. 1(b) and Fig. 1(c)].

Evidently, all the physical consequences of our analysis, regardless of whether we use a complex or a quaternionic potential in the Schrödinger equation deserve further investigation. Nevertheless, we think that the discussion presented in this paper and based on the use of the wave packet formalism represents the starting point for further theoretical studies and a fundamental tool in looking for possible experimental deviations from standard (complex) quantum mechanics.

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Resonance counting function in black box scattering

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Sjostrand and Zworski [J. Am. Math. Soc. **4**, 729–769 (1991)] proved a universal upper bound for the resonance counting function in black box scattering. Examples are presented which show that there is no corresponding general lower bound.
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I. INTRODUCTION

Consider the Schrödinger operator $-\Delta+V$ defined on R^n, where n is odd. We assume that V is bounded and compactly supported. The resolvent $(-\Delta+V-\lambda^2)^{-1}$ continues from $\mathrm{Im}\ \lambda>0$ to a meromorphic function on the complex λ plane. Its poles are known as resonances. Let $N(r)$ denote the number of resonances in a ball of radius r, i.e., $|\lambda|\leqslant r$. Zworski showed that $N(r)\leqslant c(r+1)^n$. In fact, Sjöstrand and Zworski showed that the same type of upper bound occurs much more generally as formalized in their theory of black box scattering.[1] The formalism of black box scattering allows a simultaneous treatment of potential, metric, and obstacle scattering, without entering into their particular features. It also allows completely abstract perturbations, some of which have geometric meaning, for instance scattering on manifolds with cusps. The situation for lower bounds is less well understood. For potential scattering, Sá Barreto[2] proved that $\limsup N(r)/r\geqslant c$, as $r\to\infty$. The lecture notes of Melrose[3] and the survey article of Zworski[4] contain more extensive references and foundational material. The lectures on resonances, available on the home page of Sjostrand, provide another source for background material. Christiansen and Hilsop[5] showed that for generic compactly supported potentials one has $\limsup \log N(r)/\log r = n$. Stefanov[6] discusses the optimality of constants appearing in the upper bounds for $N(r)$.

The purpose of this note is to provided some examples of compactly supported perturbations of $-\Delta$ where $N(r)\leqslant cr^{\beta}$, for any $1\leqslant\beta\leqslant n$. These examples satisfy the axioms of black box scattering. They are obtained by amalgamating collections of rotationally symmetric potentials. One applies estimates of Zworski[7] to verify that our examples satisfy the upper bound. Study of Zworski's paper about rotationally symmetric potentials lead to some ideas for simplifying his work. These ideas are outlined in the final section of this paper. The author thanks the referee for providing additional references and for suggestions concerning the exposition.

II. EXAMPLES OF BLACK BOX SCATTERING

Suppose that $V\in L^{\infty}(R^n)$ is compactly supported and rotationally symmetric. By separation of variables and renormalization of measures $-\Delta+V$ decomposes into a sum of one dimensional operators

$$\mathcal{D}_{\ell}\psi=-\psi''+\frac{\ell(\ell+1)}{s^2}\psi+V(s)\psi,\quad s\in R^{+}.$$

The parameter ℓ represents the order of the spherical harmonic using separation of variables (Ref. 7, p. 372).

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The study of rotationally symmetric potentials suggests the definition of more general perturbations of $-\Delta$. In particular, for a real and non-negative, we set

$$\mathcal{D}_{\ell,\alpha}\psi = -\psi'' + \frac{\ell(\ell+1)}{s^2}\psi + \ell^{2\alpha}V(\ell^{\alpha}s)\psi.$$

The direct sum $\overline{\mathcal{D}}_{\alpha}=\Sigma_{\ell}\mathcal{D}_{\ell,\alpha}$ satisfies the axioms of black box scattering, as formulated in Ref. 1. If $N_{\alpha}(r)$ denotes the number of resonances, for the meromorphic continuation of the resolvent $(\overline{\mathcal{D}}_{\alpha}-\lambda^2)^{-1}$, in a ball of radius r, then the general result[1] for black box scattering yields $N_{\alpha}(r) \leqslant cr^n$.

To obtain a more precise upper bound, observe that by change of variables $x=\ell^{\alpha}s$, one has $N_{\alpha,\ell}(r)=N_{0,\ell}(r/\ell^{\alpha})$. Extending the argument of (Ref. 7, p. 385) gives, for large r,

$$N_{\alpha}(r) \leqslant c_1 \sum_{\ell} \ell^{n-2} N_{\alpha,\ell}(r) = c_1 \sum_{\ell} \ell^{n-2} N_{0,\ell}\left(\frac{r}{\ell^{\alpha}}\right).$$

If $\ell \geqslant c_2 r$, then $N_{0,\ell}(r)=0$, so that

$$N_{\alpha}(r) \leqslant c_1 \sum_{\ell \leqslant c_2 r \ell^{-\alpha}} \ell^{n-2} N_{0,\ell}\left(\frac{r}{\ell^{\alpha}}\right) \leqslant c_3 r \sum_{\ell \leqslant c_2 r \ell^{-\alpha}} \ell^{n-2-\alpha}.$$

When $\alpha > n-1$, this gives $N_{\alpha}(r) \leqslant c_4 r$. If $0 \leqslant \alpha < n-1, N_{\alpha}(r) \leqslant c_5 r^{n/(1+\alpha)}$. In particular, by suitable choice of α, we obtain $N_{\alpha}(r) \leqslant c_6 r^{\beta}$, for any given $1 \leqslant \beta \leqslant n$. These examples show that lower bounds in black box scattering do not have the same universality as upper bounds. To some extent this is already clear from consideration of the trivial case when V is identically zero.

For V satisfying a jump condition, i.e., $V \in C^2[0,a], V(a) \neq 0$, the method of (Ref. 7, p. 400) extends to give $N_{\alpha}(r) \sim cr^{\beta}$, for $1 \leqslant \beta \leqslant n$. Note that the linear case $N(r) \sim cr$ is easily obtained by taking the direct sum of $\widetilde{\mathcal{D}}_{\ell}$ where $\widetilde{\mathcal{D}}_{\ell} = -\psi'' + [\ell(\ell+1)/s^2]\psi$, except for finitely many values of ℓ, where $\widetilde{\mathcal{D}}_{\ell} = -\psi'' + [\ell(\ell+1)/s^2]\psi + V(s)\psi$.

Any axiomatic approach to lower bounds must exclude the $\overline{\mathcal{D}}_{\alpha}$, if one desires the conclusion $N(r) \geqslant cr^n$, i.e., the lower bound comparable to the upper bound. However, the $\overline{\mathcal{D}}_{\alpha}$ seem quite similar to potentials from the mathematical point of view. The author does not know whether or not they are physically reasonable.

III. ROTATIONALLY SYMMETRIC POTENTIALS

The purpose of this section is to outline some simplifications of Zworski's work[7] concerning the resonance counting function for rotationally symmetric potentials. The proofs presented in Ref. 7 are long and require intricate calculations. It is possible to handle some of the technical problems in a more elementary way.

Let $V(r)$ be bounded and compactly supported. The letter ℓ denotes the separation parameter corresponding to the order of the spherical harmonic on S^{n-1} and the letter λ corresponds to the resonance. After separation of variables the resolvent $-\Delta+V$ decomposes into a direct sum of one dimensional operators $R_V^{\ell}(\lambda)=\{(-d^2/dr^2)+[\ell(\ell+1)/r^2]+V(r)-\lambda^2\}^{-1}$. For each fixed choice of ℓ, the resonance counting function $N_{\ell}(|\lambda|) \sim c|\lambda|$ by standard results [Ref. 8, pp. 328–329], provided that $V(r)$ satisfies a jump condition. The problem is to obtain upper bounds and asymptotics for $N(|\lambda|)=\Sigma_{\ell}N_{\ell}(|\lambda|)$.

Clearly, for fixed $|\lambda|$ and ℓ sufficiently large, we have $N_{\ell}(|\lambda|)=0$. It is crucial to establish the more precise statement that $N_{\ell}(|\lambda|)=0$ for $\ell > c|\lambda|$. To see this observe that $R_V^{\ell}(\lambda)$ has no pole at λ if $I+R_0^{\ell}(\lambda)V$ is invertible, by the resolvent equation. Fredholm theory guarantees that $I+R_0^{\ell}(\lambda)V$ is invertible if $R_0^{\ell}(\lambda)V$ has no eigenvalue -1. If $\ell > c|\lambda|$, then $\|R_0^{\ell}(\lambda)\| \leqslant d\ell^{-2}$on the support of V. So if λ is sufficiently large, then $\||V|^{1/2}\mathrm{sgn}(V)R_0^{\ell}(\lambda)|V|^{1/2}\| < \epsilon$, and consequently neither this operator nor $R_0^{\ell}(\lambda)V$ has eigenvalue -1. Suppose that V is supported on $[0,b]$. Then

$R_V^\ell(\lambda)$ is holomorphic for $\ell > c|\lambda|$, where c can be made arbitrarily small by choosing a sufficiently small b. Scaling in the space variables reduces one to sufficiently small b.

Having quantified the existence of pole free regions, we need only consider $N_\ell(r)$ for $\ell < cr$. Let $\tilde{f}_0^\ell(x,\lambda)$ be the Bessel function satisfying the unperturbed equation $(-d^2\phi/dx^2)+[\ell(\ell+1)/(x^2)]\phi=\lambda^2\phi$ and having the asymptotics $\tilde{f}_0^\ell(x,\lambda)\sim e^{ix\lambda}$ as $x\to\infty$. Set $\phi(x)=\psi(\lambda x)=\psi(y)$, so that $(-d^2\psi/dy^2)+[\ell(\ell+1)/(y^2)]\psi=\psi$. If $|y|>c\ell$, elementary asymptotic formulas for Bessel functions[9] give $\tilde{f}_0^\ell(x,\lambda)\sim e^{ix\lambda}$ uniformly for $x>b/2$ and $|\lambda|>c\ell$, where c is sufficiently large. Consequently, the Bessel transform stabilizes uniformly to the Fourier transform when $|\lambda|>c\ell$. This means that the asymptotics of $N_\ell(r)$, for V satisfying a jump condition on its derivatives,[8] are uniformly $N_\ell(r)\sim cr$, for $r>c\ell$. Summing over $\ell<cr$ gives the asymptotics $N(r)=\Sigma_{\ell<cr}\ell^{n-2}N_\ell(r)=cr\Sigma_{\ell<cr}\ell^{n-2}+o(r^n)$. In the absence of the jump condition, the uniform stabilization of the Bessel transform suffices to give the upper bound $N_\ell(r)<cr$ and thus $N(r)<cr^n$. In particular, the entire function $\mathcal{M}^{(\ell)}(\lambda)$ defined by Zworski[7] is uniformly of order one, i.e., $\log|\mathcal{M}^\ell(\lambda)|\leqslant c_1|\lambda|+c_2$. The upper bound for $N(r)$ then follows from Jensen's formula.

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Quantum invariants, modular forms, and lattice points II

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We study the SU(2) Witten-Reshetikhin-Turaev (WRT) invariant for the Seifert fibered homology spheres with M-exceptional fibers. We show that the WRT invariant can be written in terms of (differential of) the Eichler integrals of modular forms with weight $1/2$ and $3/2$. By use of nearly modular property of the Eichler integrals we shall obtain asymptotic expansions of the WRT invariant in the large-N limit. We further reveal that the number of the gauge equivalent classes of flat connections, which dominate the asymptotics of the WRT invariant in $N\to\infty$, is related to the number of integral lattice points inside the M-dimensional tetrahedron. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2349484]

I. INTRODUCTION

The Witten invariant for the three-manifold $\mathcal{M}$ is defined by the Chern-Simons path integral as[1] (see also Ref. 2)

$$Z_k(\mathcal{M}) = \int \exp(2\pi i k \mathrm{CS}(A))\mathcal{D}A, \tag{1.1}$$

where $k \in \mathbb{Z}$, and $\mathrm{CS}(A)$ is the Chern-Simons functional

$$\mathrm{CS}(A) = \frac{1}{8\pi^2}\int_{\mathcal{M}} \mathrm{Tr}\left(A\wedge \mathrm{d}A + \frac{2}{3}A\wedge A\wedge A\right). \tag{1.2}$$

In a limit $k\to\infty$ of the Witten invariant $Z_k(\mathcal{M})$, we may apply the saddle point method. As the saddle point of the Chern-Simons functional (1.2) denotes the flat connection

$$\mathrm{d}A + A\wedge A = 0 \tag{1.3}$$

the asymptotics of the partition function becomes a sum of the Chern-Simons invariants, and it is expected to be[1–3]

$$Z_k(\mathcal{M}) \sim \frac{1}{2}e^{-(3/4)\pi \mathrm{i}(1+b^1)}\sum_{\alpha}(k+2)^{(\dim H^1 - \dim H^0)/2}\times \sqrt{T_\alpha}\mathrm{e}^{-2\pi \mathrm{i}(I_\alpha/4+\dim H^0/8)}\mathrm{e}^{2\pi \mathrm{i}(k+2)\mathrm{CS}(A_\alpha)}. \tag{1.4}$$

Here the sum of α denotes a gauge equivalent class of flat connections, and T_α and I_α, respectively, denote the Reidemeister torsion and the spectral flow. The first Betti number is b^1, and H^i is the cohomology space.

To study the asymptotic behavior of the Witten invariant rigorously, we need explicit expression of the invariant. Alternative and combinatorial definition of this quantum invariant was given by Reshetikhin and Turaev[4] (see also Ref. 5). We denote $\tau_N(\mathcal{M})$ as the Witten-Reshetikhin-Turaev (WRT) invariant, which is related to the Witten invariant $Z_k(\mathcal{M})$ by

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$$Z_k(\mathcal{M}) = \frac{\tau_{k+2}(\mathcal{M})}{\tau_{k+2}(S^2 \times S^1)} \tag{1.5}$$

and we have

$$\tau_N(S^3) = 1,$$

$$\tau_N(S^2 \times S^1) = \sqrt{\frac{N}{2}} \frac{1}{\sin(\pi/N)}.$$

Using this definition of the WRT invariant, asymptotic behavior of the WRT invariants for certain three-manifolds has been extensively studied.[6–13]

Several years ago, Lawrence and Zagier found a connection between the WRT invariant and modular form.[14] They showed that the WRT invariant $\tau_N(\mathcal{M})$ for the Poincaré homology sphere $\mathcal{M}=\Sigma(2,3,5)$ can be regarded as a limiting value of the Eichler integral of vector modular form with weight 3/2. Thanks to this correspondence, the exact asymptotic expansion of the WRT invariant in the large-N limit can be computed, and topological invariants such as the Chern-Simons invariant and the Reidemeister torsion can be interpreted from the viewpoint of modular forms. Meanwhile it has been established that this remarkable structure of the quantum invariants holds for the WRT invariants for three-manifolds such as the Brieskorn homology spheres,[15] four exceptional fibered Seifert homology spheres,[16] and the spherical Seifert manifolds.[17] Also established is a connection between the Eichler integrals of vector modular forms with weight 1/2 and the special values of the colored Jones polynomial for the torus knot $\mathcal{T}_{s,t}$ (Ref. 18 and see also Refs. 19–22) and the torus link $\mathcal{T}_{2,2m}$.[23]

One of the benefits of the quantum invariant/modular form correspondence is an observation that a limiting value of the Ramanujan mock theta functions[24] in $q \to e^{2\pi i/N}$ from outside a unit circle coincides with the WRT invariants for the spherical Seifert manifolds.[25] This fact opens up a new insight to modular forms and the Ramanujan mock theta functions, and we can expect that further studies on the quantum invariant/modular form correspondence should be fruitful.

In this article, as a continuation of Refs. 15 and 16, we study an exact asymptotic expansion of the WRT invariant $\tau_N(\mathcal{M})$ for the M-exceptional fibered Seifert integral homology sphere $\mathcal{M}=\Sigma(p_1,p_2,\ldots,p_M)$, where p_j are pairwise coprime positive integers. By use of modular forms with half-integral weight, we derive an asymptotic expansion in $N \to \infty$ number theoretically.

This article is organized as follows. In Sec. II we review the construction of the WRT invariant for the Seifert fibered homology spheres following Ref. 8. An explicit form of the WRT invariant is given. Also discussed is an integral expression of the invariant. In Sec. III we introduce a family of vector modular forms with half-integral weight. We define the Eichler integrals thereof, and study the nearly modular property of a limiting value of the Eichler integrals. By use of this quasimodular transformation property, we compute the asymptotic expansion of the WRT invariant in the large-N limit in Sec. IV. We shall see that the invariant is a limiting value of the holomorphic function.[26] We study a contribution of dominating terms in the large-N limit in detail, and reveal a relationship with the number of the integral lattice points inside the higher dimensional tetrahedron. Also given is an explicit relationship between the Casson invariant and the first nontrivial coefficient of the Ehrhart polynomial. In Sec. V we give some results based on numerical computations. We compare the exact value of the WRT invariant with our asymptotic formula. The last section is devoted to conclusion and discussions.

II. WRT INVARIANT FOR SEIFERT INTEGRAL HOMOLOGY SPHERE

Following Ref. 8, we compute the WRT invariant $\tau_N(\mathcal{M})$ for the Seifert fibered integral homology sphere with M-exceptional fibers $\mathcal{M}=\Sigma(\vec{p})=\Sigma(p_1,p_2,\ldots,p_M)$ where p_j are pairwise coprime positive integers. Hereafter we use $\vec{p}$ as M-tuple

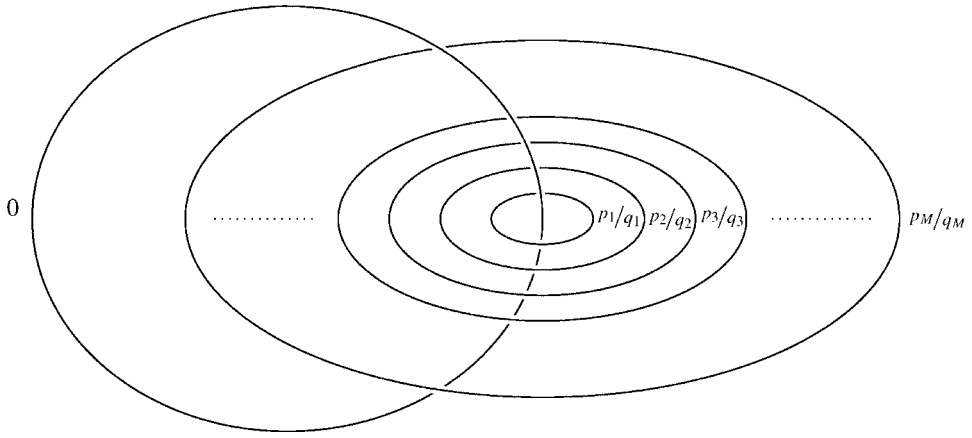

FIG. 1. Surgery description of the Seifert homology sphere $\Sigma(p_1,\ldots,p_M)$

$$\vec{p}=(p_1,p_2,\ldots,p_M).$$

The Seifert fibered integral homology sphere $\Sigma(\vec{p})$ has a rational surgery description as Fig. 1 (see, e.g., Refs. 27–29), and the fundamental group has a presentation

$$\pi_1(\Sigma(\vec{p}))=\left\langle x_1,x_2,\ldots,x_M,h \,\middle|\, \begin{array}{c} h \text{ is center} \\ x_j^{p_j}=h^{-q_j} \text{ for } 1\leqslant j\leqslant M \\ x_1x_2\cdots x_M=1 \end{array} \right\rangle. \tag{2.1}$$

Here $q_j\in\mathbb{Z}$ is coprime to p_j, and we have a constraint so that the fundamental group (2.1) gives the homology sphere;

$$P\sum_{j=1}^{M}\frac{q_j}{p_j}=1. \tag{2.2}$$

Here and hereafter we use

$$P=P(\vec{p})=\prod_{j=1}^{M}p_j. \tag{2.3}$$

When the three-manifold $\mathcal{M}$ is constructed by the rational surgeries p_j/q_j on the jth component of n-component link $\mathcal{L}$, it was shown[4,30] that the SU(2) WRT invariant $\tau_N(\mathcal{M})$ is given by

$$\tau_N(\mathcal{M})=e^{(\pi\mathrm{i}/4)[(N-2)/N](\Sigma_{j=1}^{n}\Phi(U^{(p_j,q_j)})-3\ \mathrm{sign}(\mathbf{L}))}\sum_{k_1,\ldots,k_n=1}^{N-1}J_{k_1,\ldots,k_n}(\mathcal{L})\prod_{j=1}^{n}\rho(U^{(p_j,q_j)})_{k_j,1}. \tag{2.4}$$

Here the surgery data p_j/q_j is encoded by an $\mathrm{SL}(2;\mathbb{Z})$ matrix

$$U^{(p_j,q_j)}=\begin{pmatrix} p_j & r_j \\ q_j & s_j \end{pmatrix}.$$

The Rademacher Φ function $\Phi(U)$ is defined by[31]

$$\Phi\left(\begin{pmatrix} p & r \\ q & s \end{pmatrix}\right) = \begin{cases} \dfrac{p+s}{q} - 12s(p,q) & \text{for } q \neq 0 \\ \dfrac{r}{s} & \text{for } q = 0 \end{cases} \tag{2.5}$$

where $s(b,a)$ denotes the Dedekind sum (A1). An $n \times n$ matrix $\mathbf{L}$ is a linking matrix

$$\mathbf{L}_{j,k} = \mathrm{lk}(j,k) + \frac{p_j}{q_j} \cdot \delta_{j,k} \tag{2.6}$$

where $1\mathrm{k}(j,k)$ denotes the linking number of the j- and kth components of link $\mathcal{L}$, and $\mathrm{sign}(\mathbf{L})$ denotes a signature of $\mathbf{L}$, i.e., the difference between the number of positive and negative eigenvalues of $\mathbf{L}$. The polynomial $J_{k_1,\ldots,k_n}(\mathcal{L})$ denotes the colored Jone polynomial for link $\mathcal{L}$ with color k_j for the jth component link, and $\rho(U^{(p,q)})$ is a representation ρ of $\mathrm{PSL}(2;\mathbb{Z})$ defined by

$$\rho(U^{(p,q)})_{a,b} = -\mathrm{i}\frac{\mathrm{sign}(q)}{\sqrt{2N|q|}} \mathrm{e}^{-(\pi\mathrm{i}/4)\Phi(U^{(p,q)})} \mathrm{e}^{(\pi\mathrm{i}/2Nq)sb^2} \sum_{\substack{\gamma \bmod 2Nq \\ \gamma = a \bmod 2N}} \mathrm{e}^{(\pi\mathrm{i}/2Nq)p\gamma^2} (\mathrm{e}^{(\pi\mathrm{i}/Nq)\gamma b} - \mathrm{e}^{-(\pi\mathrm{i}/Nq)\gamma b}) \tag{2.7}$$

for $1 \leqslant a,b \leqslant N-1$.[30] This representation is constructed from

$$\rho(S)_{a,b} = \sqrt{\frac{2}{N}} \sin\left(\frac{ab}{N}\pi\right),$$
$$\rho(T)_{a,b} = \mathrm{e}^{(\pi\mathrm{i}/2N)a^2 - (\pi\mathrm{i}/4)} \delta_{a,b} \tag{2.8}$$

with

$$S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \tag{2.9}$$

satisfying

$$S^2 = (ST)^3 = 1.$$

Based on the fact that the Seifert fibered manifold $\Sigma(\vec{p})$ has a surgery description as in Fig. 1, we have the following result.

Proposition 1 (Ref. 8): For the Seifert fibered integral homology sphere with M-exceptional fibers $\mathcal{M} = \Sigma(\vec{p})$, the WRT invariant is given by

$$\mathrm{e}^{(2\pi\mathrm{i}/N)(\phi(\vec{p})/4 - 1/2)} (\mathrm{e}^{2\pi\mathrm{i}/N} - 1) \tau_N(\mathcal{M}) = \frac{\mathrm{e}^{\pi\mathrm{i}/4}}{2\sqrt{2PN}} \sum_{\substack{n=0 \\ N \nmid n}}^{2PN-1} \mathrm{e}^{-(1/2PN)n^2\pi\mathrm{i}} \frac{\prod_{j=1}^{M} (\mathrm{e}^{(n/Np_j)\pi\mathrm{i}} - \mathrm{e}^{-(n/Np_j)\pi\mathrm{i}})}{(\mathrm{e}^{(n/N)\pi\mathrm{i}} - \mathrm{e}^{-(n/N)\pi\mathrm{i}})^{M-2}}. \tag{2.10}$$

Here $\phi(\vec{p})$ is defined by

$$\phi(\vec{p}) = 3 - \frac{1}{P} + 12\sum_{j=1}^{M} s\left(\frac{P}{p_j}, p_j\right), \tag{2.11}$$

where $s(b,a)$ denotes the Dedekind sum (A1).

Outline of Proof: We use the surgery formula (2.4), in which the colored Jones polynomial for a variant of Hopf link $\mathcal{L}$ depicted in Fig. 1 is given by

$$J_{k_0,k_1,\ldots,k_M}(\mathcal{L}) = \frac{1}{\sin(\pi/N)} \frac{\prod_{j=1}^{M} \sin\left(\frac{k_0 k_j}{N}\pi\right)}{\left[\sin\left(\frac{k_0}{N}\pi\right)\right]^{M-1}}.$$

Here k_0 is a color of component which has a linking number 1 with any other components of $\mathcal{L}$. After some computations using the Gauss sum reciprocity formula (A7), we get

$$\begin{aligned} e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M}) = {} & \frac{e^{\pi i/4}}{2\sqrt{2PN}} \sum_{k_0=1}^{N-1} \sum_{n_j \bmod p_j} \frac{1}{(e^{(k_0/N)\pi i} - e^{-(k_0/N)\pi i})^{M-2}} \\ & \times \prod_{j=1}^{M} e^{-(q_j/p_j)(k_0+2Nn_j)^2/2N} (e^{[(k_0+2Nn_j)/Np_j]\pi i} - e^{-[(k_0+2Nn_j)/Np_j]\pi i}). \end{aligned} \tag{2.12}$$

We see that the summand in (2.12) is invariant under

- $k_0 \to k_0+2N$ and $n_j \to n_j-1$ for all j,
- $n_j \to n_j+p_j$.

Using that p_j are pairwise coprime, we can then rewrite the multisum of (2.12) into a single sum of (2.10). □

The WRT invariant can be rewritten in the integral form as follows.

Proposition 2 (Ref. 8):

$$e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M}) = \frac{e^{\pi i/4}}{2\sqrt{2PN}} \left(-2\pi i \sum_{m=0}^{2P-1} \operatorname*{Res}_{z=mN} \frac{g(z)}{1-e^{-2\pi i z}} + \int_{\mathcal{C}} g(z)dz \right), \tag{2.13}$$

where

$$g(z) = e^{-(z^2/2PN)\pi i} \frac{\prod_{j=1}^{M} (e^{(z/Np_j)\pi i} - e^{-(z/Np_j)\pi i})}{(e^{(z/N)\pi i} - e^{-(z/N)\pi i})^{M-2}} \tag{2.14}$$

and the integration path $\mathcal{C}$ passes the origin from $(-1+i)\infty$ to $(1-i)\infty$.

Outline of proof: Key identity is

$$\Theta_M(x) = \Theta_M(x-N)e^{4\pi i P x} + 2\pi i \sum_{m=0}^{2P-1} \operatorname*{Res}_{z=mN} h_M(z,x) + \sum_{\substack{n=0 \\ N \nmid n}}^{2PN-1} f_M(n,x). \tag{2.15}$$

Here the function $\Theta_M(x)$ is defined by

$$\Theta_M(x) = \int_{\mathcal{C}} h_M(z,x)dz,$$

where

$$h_M(z,x) = e^{-(z^2/2PN)\pi i + 2x(z/N)\pi i} \frac{1}{(e^{(z/N)\pi i} - e^{-(z/N)\pi i})^{M-2}} \cdot \frac{1}{1-e^{-2\pi i z}} \equiv \frac{f_M(z,x)}{1-e^{-2\pi i z}}.$$

As the function $g(z)$ is a linear combination of $f_M(x,z)$, we obtain the expression (2.13). □

In view of (2.13), we can decompose the invariant as

$$\tau_N(\mathcal{M}) = \tau_N^{\rm res}(\mathcal{M}) + \tau_N^{\rm int}(\mathcal{M}) \tag{2.16}$$

where $\tau_N^{\rm res}(\mathcal{M})$ and $\tau_N^{\rm int}(\mathcal{M})$ respectively denote contributions from the residue terms and the integral term in (2.13). It was identified in Ref. 8 that the residue part $\tau_N^{\rm res}(\mathcal{M})$ is the contribution from irreducible flat connections while the integral term $\tau_N^{\rm int}(\mathcal{M})$ is the trivial connection contribution. The trivial connection contribution is related to the Ohtsuki series,[32] and we have as follows.

Proposition 3: In the limit $N\to\infty$, the trivial connection contribution has the asymptotic expansion as

$$e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{(2\pi i/N)}-1)\tau_N^{\rm int}(\mathcal{M}) \simeq \sum_{k=0}^{\infty} \frac{T_{\vec{p}}(k)}{k!}\left(\frac{\pi i}{2PN}\right)^k, \tag{2.17}$$

where the T series is given by

$$\frac{\prod_{j=1}^{M} \sinh\left(\frac{P}{p_j}x\right)}{[\sinh(Px)]^{M-2}} = \frac{1}{2}\sum_{k=0}^{\infty} \frac{T_{\vec{p}}(k)}{(2k)!}x^{2k}. \tag{2.18}$$

We will discuss later the relationship with the Ohtsuki series.

Similar integral with $\tau_N^{\rm int}(\mathcal{M})$ in the case of the three exceptional fibers $M=3$ appeared in studies[33,34] of the Ramanujan mock theta functions, which still remain to be mysterious and fascinating topics. This suggests the remarkable fact that the Ramanujan mock theta functions[24] are related to the WRT invariant for the Seifert fibered manifolds. See Refs. 17, 25, and 35 for detail.

The dominating term of the WRT invariant in a limit $N\to\infty$ follows from the irreducible flat connection contributions $\tau_N^{\rm res}(\mathcal{M})$ as was expected from the saddle point approximation (1.4). In terms of the Witten partition function $Z_k(\mathcal{M})$, the asymptotic expansion of the invariant is given by

$$Z_{k-2}(\mathcal{M}) \simeq \sum_{a=0}^{M-3} N^{M-3-a} Z_{N-2}^{(a)}(\mathcal{M}) + \text{trivial connection contribution}$$

and the dominating term $Z_{N-2}^{(0)}(\mathcal{M})$ in $N\to\infty$ can be computed as follows when we use an identity

$$\sin(\pi z) = \pi z \prod_{n=1}^{\infty}\left(1-\frac{z^2}{n^2}\right)$$

Proposition 4: In the large N limit, the Witten partition function $Z_N(\mathcal{M})$ for the M-exceptional fibered Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ is dominated by

$$Z_{N-2}(\mathcal{M}) \sim N^{M-3}\frac{2^{M-2}}{(M-2)!\sqrt{P}} e^{-(\phi(\vec{p})/2N)\pi i} e^{-[(2M-3)/4]\pi i} \times \sum_{m=0}^{2P-1} (-1)^{mM} B_{M-2}\left(\frac{m}{2P}\right) e^{-(m^2/2P)\pi i N}\left[\prod_{j=1}^{M} \sin\left(\frac{m}{p_j}\pi\right)\right], \tag{2.19}$$

*where $B_k(x)$ is the k*th *Bernoulli polynomial* (A8).

Among a sum of $2P$ terms on the right-hand side (r.h.s.) of (2.19), we can classify the summation by the Chern-Simons invariant, which corresponds to an exponential factor $-(m^2/4P)$ mod 1 as will be discussed later.

III. MODULAR FORMS AND EICHLER INTEGRAL

We introduce the vector modular forms with half-integral weight which play a crucial role in analysis of the WRT invariants for the Seifert fibered homology spheres.

A. Vector modular forms with half-integral weight

We set M-tuple

$$\vec{\ell} = (\ell_1, \ldots, \ell_M), \tag{3.1}$$

where ℓ_j are integers satisfying $0 < \ell_j < p_j$. As before we assume that p_j are pairwise coprime positive integers. For M-tuple $\vec{\ell}$, we define the periodic function $\chi_{2P}^{\vec{\ell}}(n)$ with modulus $2P$ by

$$\chi_{2P}^{\vec{\ell}}(n) = \begin{cases} -\prod_{j=1}^{M} \varepsilon_j & \text{if } n = P\left(1 + \sum_{j=1}^{M} \varepsilon_j \frac{\ell_j}{p_j}\right) \bmod 2P, \\ 0 & \text{otherwise} \end{cases} \tag{3.2}$$

where $\varepsilon_j = \pm 1$ for $\forall j$. We see that $\chi_{2P}^{\vec{\ell}}(n)$ is even (respectively odd) when M is even (respectively odd),

$$\chi_{2P}^{\vec{\ell}}(-n) = (-1)^M \chi_{2P}^{\vec{\ell}}(n) \tag{3.3}$$

and that it has a mean value zero,

$$\sum_{n=0}^{2P-1} \chi_{2P}^{\vec{\ell}}(n) = 0. \tag{3.4}$$

We define an involution σ_j on M-tuple $\vec{\ell}$ by

$$\sigma_j(\vec{\ell}) = (\ell_1, \ldots, \ell_{j-1}, p_j - \ell_j, \ell_{j+1}, \ldots, \ell_M) \tag{3.5}$$

for $1 \leqslant j \leqslant M$. As we have

$$\chi_{2P}^{\sigma_i \sigma_j(\vec{\ell})}(n) = \chi_{2P}^{\vec{\ell}}(n) \tag{3.6}$$

for $1 \leqslant i, j \leqslant M$, the number of the independent periodic functions $\chi_{2P}^{\vec{\ell}}(n)$ for given $\vec{p}$ is

$$D = D(\vec{p}) = \frac{1}{2^{M-1}} \prod_{j=1}^{M} (p_j - 1). \tag{3.7}$$

We note that

$$\chi_{2P}^{\vec{\ell}}(n+P) = -\chi_{2P}^{\sigma_j(\vec{\ell})}(n) \tag{3.8}$$

for $1 \leqslant j \leqslant M$.

We set

$$q = \exp(2\pi \mathrm{i} \tau), \tag{3.9}$$

where τ is in the upper half plane, $\tau \in \mathbb{H}$. By use of the periodic functions (3.2) we define the q series by

$$\Phi_{\vec{p}}^{\vec{\ell}}(\tau)=\frac{1}{2}\sum_{n\in\mathbb{Z}} n^{\mathrm{m}_2(M)}\chi_{2P}^{\vec{\ell}}(n)q^{n^2/4P}, \tag{3.10}$$

where we mean

$$\mathrm{m}_2(M)=\frac{1-(-1)^M}{2}=M \bmod 2=\begin{cases}0 & \text{when } M \text{ is even}\\ 1 & \text{when } M \text{ is odd.}\end{cases} \tag{3.11}$$

The q-series $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ is proved to be a vector modular form with half-integral weight. The T transformation is trivial, and by use of the Poisson summation formula,

$$\sum_{n\in\mathbb{Z}} f(n)=\sum_{n\in\mathbb{Z}}\int_{-\infty}^{\infty} \mathrm{e}^{-2\pi \mathrm{i}tn}f(t)\mathrm{d}t \tag{3.12}$$

we obtain the transformation formula under the S transformation as follows.

Proposition 5: The q-series $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ *is a vector modular form with weight* $3/2$ (*respectively* $1/2$) *when* M *is even (respectively odd). Under the* S *and* T *transformations* (2.9) *we have*

$$\Phi_{\vec{p}}^{\vec{\ell}}(\tau)=\left(\frac{\mathrm{i}}{\tau}\right)^{3/2-\mathrm{m}_2(M)}\sum_{\vec{\ell}'}\mathbf{S}_{\vec{\ell}'}^{\vec{\ell}}\Phi_{\vec{p}}^{\vec{\ell}'}(-1/\tau), \tag{3.13}$$

$$\Phi_{\vec{p}}^{\vec{\ell}}(\tau+1)=\mathbf{T}^{\vec{\ell}}\Phi_{\vec{p}}^{\vec{\ell}}(\tau). \tag{3.14}$$

Here a sum of $\vec{\ell}'$ *runs over D-dimensional space* (3.7), *and matrix elements of* $D\times D$ *matrices* $\mathbf{S}$ *and* $\mathbf{T}$ *are respectively given by*

$$\mathbf{S}_{\vec{\ell}'}^{\vec{\ell}}=\frac{2^M\mathrm{i}^{M-\mathrm{m}_2(M)}}{\sqrt{2P}}(-1)^{P(1+\Sigma_{j=1}^M(\ell_j+\ell_j')/p_j)+P\Sigma_j\Sigma_{k\neq j}\ell_j\ell_k'/p_jp_k}\prod_{j=1}^M \sin\left(P\frac{\ell_j\ell_j'}{p_j^2}\pi\right), \tag{3.15}$$

$$\mathbf{T}^{\vec{\ell}}=\exp\left(\frac{P}{2}\left(1+\sum_{j=1}^M\frac{\ell_j}{p_j}\right)^2\pi\mathrm{i}\right). \tag{3.16}$$

Our vector modular form $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ may be a generalization of modular forms which appear as the character of the affine Lie algebra $\widehat{\mathrm{su}(2)}$ (a case of $M=1$, and $\Psi_P^{(a)}(\tau)$ defined below) and as the minimal Virasoro model (a case of $M=2$) up to the power of the Dedekind η function.

For our later use, we introduce other families of vector modular forms. We define the even periodic functions by

$$\theta_{2P}^{(a)}(n)=\begin{cases}1 & \text{for } n=\pm a \bmod 2P\\ 0 & \text{otherwise}\end{cases} \tag{3.17}$$

for $0\leqslant a\leqslant P$, and the odd periodic function by

$$\psi_{2P}^{(a)}(n)=\begin{cases}\pm 1 & \text{for } n\equiv \pm a \bmod 2P\\ 0 & \text{otherwise}\end{cases} \tag{3.18}$$

for $0<a<P$. We then define two families of q-series by

$$\Theta_P^{(a)}(\tau)=\frac{1}{2}\sum_{n\in\mathbb{Z}}\theta_{2P}^{(a)}(n)q^{n^2/4P}, \tag{3.19}$$

$$\Psi_P^{(a)}(\tau)=\frac{1}{2}\sum_{n\in\mathbb{Z}} n\psi_{2P}^{(a)}(n)q^{n^2/4P}. \tag{3.20}$$

These families are also vector modular forms with half-integral weight. Namely we see that $\Theta_P^{(a)}(\tau)$ is a vector modular form with weight $1/2$ satisfying

$$\Theta_P^{(a)}(\tau)=\sqrt{\frac{\mathrm{i}}{\tau}}\sum_{b=0}^{P}\mathbf{N}_b^a\Theta_P^{(b)}(-1/\tau), \tag{3.21}$$

$$\Theta_P^{(a)}(\tau+1)=\exp\left(\frac{a^2}{2P}\pi\mathrm{i}\right)\Theta_P^{(a)}(\tau), \tag{3.22}$$

where $\mathbf{N}$ is $(P+1)\times(P+1)$ matrix defined by

$$\mathbf{N}_b^a=\begin{cases}\dfrac{1}{\sqrt{2P}} & \text{for } a=0\\ \sqrt{\dfrac{2}{P}}\cos\left(\dfrac{ab}{P}\pi\right) & \text{for } a\neq 0,P\\ \dfrac{1}{\sqrt{2P}}\cos(b\pi) & \text{for } a=P.\end{cases} \tag{3.23}$$

The vector modular form $\Psi_P^{(a)}(\tau)$ with weight $3/2$ fulfills the following transformation formulae;

$$\Psi_P^{(a)}(\tau)=\left(\frac{\mathrm{i}}{\tau}\right)^{3/2}\sum_{b=1}^{P-1}\mathbf{M}_b^a\Psi_P^{(b)}(-1/\tau), \tag{3.24}$$

$$\Psi_P^{(a)}(\tau+1)=\exp\left(\frac{a^2}{2P}\pi\mathrm{i}\right)\Psi_P^{(a)}(\tau), \tag{3.25}$$

where $\mathbf{M}$ is a $(P-1)\times(P-1)$ matrix defined by

$$\mathbf{M}_b^a=\sqrt{\frac{2}{P}}\sin\left(\frac{ab}{P}\pi\right). \tag{3.26}$$

B. Eichler integrals

The Eichler integral is originally defined for modular forms with integral weight $\geqslant 2$ (see, e.g., Ref. 36). In our cases, the vector modular forms $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ have a half-integral weight, so we follow a method of Refs. 14 and 22 to define a variant of the Eichler integrals.

We define the Eichler integrals $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$ of the vector modular form $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ by

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)=\sum_{n=0}^{\infty} n^{1-\mathrm{m}_2(M)}\chi_{2P}^{\vec{\ell}}(n)q^{n^2/4P}. \tag{3.27}$$

This can be regarded as a "half-derivative" (respectively "half-integral") of the modular form $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ with respect to τ when M is even (respectively odd). When M is odd, the q-series $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$ might be called the false theta function à la Rogers.[37]

Proposition 6: We assume N_1 and N_2 are coprime integers, and $N_1>0$. Limiting values of the Eichler integrals $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$ in $\tau\to N_2/N_1$ are given as follows;

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(N_2/N_1) = -(PN_1)^{1-\mathrm{m}_2(M)} \sum_{k=0}^{2PN_1} \chi_{2P}^{\vec{\ell}}(k) \mathrm{e}^{(N_2/N_1)(k^2/2P)\pi \mathrm{i}} B_{2-\mathrm{m}_2(M)}\left(\frac{k}{2PN_1}\right), \tag{3.28}$$

where $B_k(x)$ is the kth Bernoulli polynomial.

We note that

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau+1) = \mathbf{T}^{\vec{\ell}} \widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$$

from which we have for $N \in \mathbb{Z}$

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(N) = (\mathbf{T}^{\vec{\ell}})^N \widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(0) = -(\mathbf{T}^{\vec{\ell}})^N P^{1-\mathrm{m}_2(M)} \sum_{k=0}^{2P} \chi_{2P}^{\vec{\ell}}(k) B_{2-\mathrm{m}_2(M)}\left(\frac{k}{2P}\right).$$

A proof follows straightforwardly when we use the following lemma[14] (see also Ref. 38).

Lemma 7: Let $C_f(n)$ is a periodic function with modulus f and mean value zero. Then we have as $t \searrow 0$

$$\sum_{n=1}^{\infty} C_f(n) \mathrm{e}^{-n^2 t} \simeq \sum_{n=0}^{\infty} L(-2n, C_f) \frac{(-t)^n}{n!}, \tag{3.29}$$

$$\sum_{n=1}^{\infty} n C_f(n) \mathrm{e}^{-n^2 t} \simeq \sum_{n=0}^{\infty} L(-2n-1, C_f) \frac{(-t)^n}{n!}, \tag{3.30}$$

where the L function is

$$L(s, C_f) = \sum_{n=1}^{\infty} \frac{C_f(n)}{n^s} = f^{-s} \sum_{k=1}^{f} C_f(k) \zeta\left(s, \frac{k}{f}\right). \tag{3.31}$$

Note that the Hurwitz zeta function $\zeta(s,z)$, defined by

$$\zeta(s,z) = \sum_{n=0}^{\infty} \frac{1}{(n+z)^s}, \tag{3.32}$$

has an analytic continuation for $k \in \mathbb{Z}_{>0}$ as

$$\zeta(1-k, s) = -\frac{B_k(z)}{k}. \tag{3.33}$$

Proposition 8: The limiting values $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\alpha)$ of the Eichler integrals with $\alpha \in \mathbb{Q}$ satisfy a nearly modular property. In a limit $N \to \infty$, we have the transformation formula as an asymptotic expansion as follows;

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(1/N) + \left(\frac{N}{\mathrm{i}}\right)^{3/2-\mathrm{m}_2(M)} \sum_{\vec{\ell}'} \mathbf{S}_{\vec{\ell}'}^{\vec{\ell}} \widetilde{\Phi}_{\vec{p}}^{\vec{\ell}'}(-N) \simeq \sum_{k=0}^{\infty} \frac{L(-2k-1+\mathrm{m}_2(M), \chi_{2P}^{\vec{\ell}})}{k!} \left(\frac{\pi \mathrm{i}}{2PN}\right)^k. \tag{3.34}$$

Here $N \in \mathbb{Z}$, and a sum of M-tuples $\vec{\ell}'$ runs over D-dimensional space.

Proof: We introduce another variant of the Eichler integral by

$$\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(z)=\begin{cases}-\sqrt{\dfrac{P\mathrm{i}}{2\pi^2}}\displaystyle\int_{\bar{z}}^{\infty}\frac{\Phi_{\vec{p}}^{\vec{\ell}}(\tau)}{(\tau-z)^{3/2}}\mathrm{d}\tau & \text{when } M \text{ is even}\\ \dfrac{1}{\sqrt{2P\mathrm{i}}}\displaystyle\int_{\bar{z}}^{\infty}\frac{\Phi_{\vec{p}}^{\vec{\ell}}(\tau)}{\sqrt{\tau-z}}\mathrm{d}\tau & \text{when } M \text{ is odd,}\end{cases}\tag{3.35}$$

where we assume that z is in the lower half-plane, $z\in\mathbb{H}^-$, and $\bar{z}$ denotes a complex conjugate of z. By use of the S-transformation (3.13), we have

$$\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(z)+\left(\frac{1}{\mathrm{i}z}\right)^{3/2-\mathrm{m}_2(M)}\sum_{\vec{\ell}'}\mathbf{S}_{\vec{\ell}'}^{\vec{\ell}}\hat{\Phi}_{\vec{p}}^{\vec{\ell}'}(-1/z)=r_{\Phi_{\vec{p}}^{\vec{\ell}}}(z;0).\tag{3.36}$$

Here $r_{\Phi_{\vec{p}}^{\vec{\ell}}}(z;\alpha)$ is an analogue of the period function defined by

$$r_{\Phi_{\vec{p}}^{\vec{\ell}}}(z;\alpha)=\begin{cases}-\sqrt{\dfrac{P\mathrm{i}}{2\pi^2}}\displaystyle\int_{\alpha}^{\infty}\frac{\Phi_{\vec{p}}^{\vec{\ell}}(\tau)}{(\tau-z)^{3/2}}\mathrm{d}\tau & \text{when } M \text{ is even}\\ \dfrac{1}{\sqrt{2P\mathrm{i}}}\displaystyle\int_{\alpha}^{\infty}\frac{\Phi_{\vec{p}}^{\vec{\ell}}(\tau)}{\sqrt{\tau-z}}\mathrm{d}\tau & \text{when } M \text{ is odd,}\end{cases}\tag{3.37}$$

where $\alpha\in\mathbb{Q}$. We find that $\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(z)$ takes the same limiting value with that of $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$ in a limit z, $\tau\to\alpha\in\mathbb{Q}$;

$$\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)\big|_{\tau\to\alpha}=\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(z)\big|_{z\to\alpha}.\tag{3.38}$$

The r.h.s. of (3.34) arises from an asymptotic expansion of $r_{\Phi_{\vec{p}}^{\vec{\ell}}}(z;0)$, and we obtain (3.34). □

For our later use, we study differentials of the Eichler integral $\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)$, i.e., "fractional derivatives" of the vector modular form $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$. From the definition (3.27) of the Eichler integral, we have for $b\in\mathbb{Z}_{\geqslant 0}$

$$\left(\frac{2P}{\pi\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)^b\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)=\sum_{n=0}^{\infty}n^{2b+1-\mathrm{m}_2(M)}\chi_{2P}^{\vec{\ell}}(n)q^{n^2/4P}.\tag{3.39}$$

By the same computation with (3.28), we have the following.

Proposition 9: The limiting values of fractional derivative of the vector modular forms $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ *are given by*

$$\left(\frac{2P}{\pi\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)^b\widetilde{\Phi}_{\vec{p}}^{\vec{\ell}}(\tau)\bigg|_{\tau\to N_2/N_1}=-\frac{(2PN_1)^{2b+1-\mathrm{m}_2(M)}}{2b+2-\mathrm{m}_2(M)}\sum_{n=1}^{2PN_1}\chi_{2P}^{\vec{\ell}}(n)\mathrm{e}^{(N_2/N_1)(n^2/2P)\pi\mathrm{i}}B_{2b+2-\mathrm{m}_2(M)}\left(\frac{n}{2PN_1}\right),\tag{3.40}$$

where $N_1>0$ *and* N_2 *are coprime integers.*

The nearly modular property (3.34) of the Eichler integral gives the following asymptotic expansion of (3.40).

Proposition 10: In the limit $N\to\infty$, *we have the following asymptotic expansion*;

$$N^{2b+1-\mathrm{m}_2(M)}\sum_{n=1}^{2PN}\chi_{2P}^{\vec{\ell}}(n)\mathrm{e}^{(n^2/2PN)\pi\mathrm{i}}B_{2b+2-\mathrm{m}_2(M)}\left(\frac{n}{2PN}\right)$$

$$\simeq\frac{-1}{\mathrm{i}^{3/2-\mathrm{m}_2(M)}}\sum_{j=0}^{b}N^{b+j+3/2-\mathrm{m}_2(M)}\left(\frac{\mathrm{i}}{2P\pi}\right)^{b-j}K_{b,\mathrm{m}_2(M)}^{(j)}$$

$$\times\frac{2b+2-\mathrm{m}_2(M)}{2j+2-\mathrm{m}_2(M)}\sum_{\vec{\ell}'}\mathrm{S}_{\vec{\ell}'}^{\vec{\ell}}\left[\sum_{n=1}^{2P}\chi_{2P}^{\vec{\ell}'}(n)B_{2j+2-\mathrm{m}_2(M)}\left(\frac{n}{2P}\right)\right]\mathrm{e}^{-(P/2)(1+\sum_j(\ell_j'/p_j))^2\pi\mathrm{i}N}$$

$$-\frac{2b+2-\mathrm{m}_2(M)}{(2P)^{2b+1-\mathrm{m}_2(M)}}\sum_{k=0}^{\infty}\frac{L(-2k-2b-1+\mathrm{m}_2(M),\chi_{2P}^{\vec{\ell}})}{k!}\left(\frac{\pi\mathrm{i}}{2PN}\right)^k, \tag{3.41}$$

where the sum of M-tuples $\vec{\ell}'$ *runs over D-dimensional space, and we have*

$$K_{b,x}^{(j)}=\binom{b}{j}\prod_{k=0}^{b-j-1}\left(\frac{1}{2}+b-x-k\right). \tag{3.42}$$

Proof: We differentiate (3.36) with respect to z, and then take a limit $z\to 1/N$. We get

$$\frac{\mathrm{d}^b}{\mathrm{d}z^b}\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(z)\Big|_{z\to 1/N}+\frac{1}{\mathrm{i}^{1/2+\mathrm{m}_2(M)}}\sum_{\vec{\ell}'}\mathrm{S}_{\vec{\ell}'}^{\vec{\ell}}\left(w^2\frac{\mathrm{d}}{\mathrm{d}w}\right)^b w^{3/2-\mathrm{m}_2(M)}\hat{\Phi}_{\vec{p}}^{\vec{\ell}'}(w)\Big|_{w\to -N}$$

$$\simeq\left(\frac{\pi\mathrm{i}}{2P}\right)^b\sum_{k=0}^{\infty}\frac{L(-2k-2b-1+\mathrm{m}_2(M),\chi_{2P}^{\vec{\ell}})}{k!}\left(\frac{\pi\mathrm{i}}{2PN}\right)^k. \tag{3.43}$$

On the left-hand side, we use

$$\left(w^2\frac{\mathrm{d}}{\mathrm{d}w}\right)^n=\sum_{m=1}^{n}A_n^{(m)}w^{n+m}\frac{\mathrm{d}^m}{\mathrm{d}w^m},$$

where $A_n^{(m)}$ is the Lah number defined by

$$A_n^{(m)}=\frac{n!}{m!}\binom{n-1}{m-1}.$$

This denotes the number of partitions of $\{1,2,\ldots,n\}$ into m *lists* (a "list" denotes an ordered subset),[39,40] and satisfies the recursion relation

$$A_{n+1}^{(m)}=A_n^{(m-1)}+(n+m)A_n^{(m)}.$$

Thus we have

$$\left(w^2\frac{\mathrm{d}}{\mathrm{d}w}\right)^b w^{3/2-\mathrm{m}_2(M)}\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(w)=\sum_{j=0}^{b}w^{3/2-\mathrm{m}_2(M)+b+j}K_{b,\mathrm{m}_2(M)}^{(j)}\frac{\mathrm{d}^j\hat{\Phi}_{\vec{p}}^{\vec{\ell}}(w)}{\mathrm{d}w^j}.$$

Here the K number is computed as

$$K_{b,x}^{(j)}=\sum_{k=j}^{b}A_b^{(k)}\binom{k}{j}\frac{\Gamma\left(\frac{5}{2}-x\right)}{\Gamma\left(\frac{5}{2}-x-k+j\right)}$$

which reduces to (3.42) applying (A14) and (A17).

As we have (3.38), we get (3.41) with a help of (3.40).

In the same method, we have formulas of the asymptotic expansions concerning to the periodic functions with mean value zero.

Corollary 11: We assume that $C_{2P}(n)$ is an odd or even periodic function with modulus $2P$, and that it satisfies

- *a mean value zero condition*,

$$\sum_{n=0}^{2P-1} C_{2P}(n) = 0,$$

- $C_{2P}(0)=0$.

In the limit $N\to\infty$, we have the following asymptotic expansions;

- $C_{2P}(n)$ *is odd*;

$$N^{2b}\sum_{n=1}^{2PN} C_{2P}(n)\mathrm{e}^{(n^2/2PN)\pi\mathrm{i}}B_{2b+1}\left(\frac{n}{2PN}\right) \simeq \frac{-2}{\mathrm{i}^{1/2}}\sum_{j=0}^{b} N^{b+j+1/2}\left(\frac{\mathrm{i}}{2P\pi}\right)^{b-j} K_{b,1}^{(j)}\frac{2b+1}{2j+1} \times\sum_{a=1}^{P-1} C_{2P}(a)\sum_{c=1}^{P-1}\mathbf{M}_c^a B_{2j+1}\left(\frac{c}{2P}\right)\mathrm{e}^{-N(c^2/2P)\pi\mathrm{i}} - \frac{2b+1}{(2P)^{2b}}\sum_{k=0}^{\infty}\frac{L(-2k-2b,C_{2P})}{k!}\left(\frac{\pi\mathrm{i}}{2PN}\right)^k, \tag{3.44}$$

- $C_{2P}(n)$ *is even*;

$$N^{2b+1}\sum_{n=1}^{2PN} C_{2P}(n)\mathrm{e}^{(n^2/2PN)\pi\mathrm{i}}B_{2b+2}\left(\frac{n}{2PN}\right) \simeq \frac{-1}{\mathrm{i}^{3/2}}\sum_{j=0}^{b} N^{b+j+3/2}\left(\frac{\mathrm{i}}{2P\pi}\right)^{b-j} K_{b,0}^{(j)}\frac{b+1}{j+1}\sum_{a=1}^{P} C_{2P}(a) \times\sum_{c=0}^{P}\mathbf{N}_c^a(2-\delta_{c,0}-\delta_{c,P})B_{2j+2}\left(\frac{c}{2P}\right)\mathrm{e}^{-N(c^2/2P)\pi\mathrm{i}} - \frac{2b+2}{(2P)^{2b+1}}\sum_{k=0}^{\infty}\frac{L(-2k-2b-1,C_{2P})}{k!}\left(\frac{\pi\mathrm{i}}{2PN}\right)^k. \tag{3.45}$$

Proof: We use that

$$C_{2P}(n) = \begin{cases} \displaystyle\sum_{a=1}^{P-1} C_{2P}(a)\psi_{2P}^{(a)}(n) & \text{when } C_{2P}(n) \text{ is odd} \\ \displaystyle\sum_{a=1}^{P} C_{2P}(a)\theta_{2P}^{(a)}(n) & \text{when } C_{2P}(n) \text{ is even.} \end{cases}$$

In both cases, due to a condition $C_{2P}(0)=0$, we see that periodic functions which appear in the modular transformation formula such as (3.43) have a mean value zero. Applying Lemma 7, we obtain asymptotic expansions. □

IV. EXACT ASYMPTOTIC EXPANSION OF THE WRT INVARIANTS

A. Exact asymptotic expansion

As a preparation to obtain the exact asymptotic expansion of the WRT invariant $\tau_N(\mathcal{M})$ for the M-exceptional fibered Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ by use of the vector modular form $\Phi_{\vec{p}}^{\vec{\ell}}(\tau)$ defined in previous section, we give q-series identities at the root of unity related to the Bernoulli polynomials.

Lemma 12: We set ω_N as the Nth primitive root of unity;

$$\omega_N = \exp\left(\frac{2\pi \mathrm{i}}{N}\right)$$

and assume that a and k are positive integers satisfying $0 \leqslant a \leqslant N-1$. We have

$$\sum_{c=1}^{N-1} \frac{\omega_N^{(a+1)c}}{(1-\omega_N^c)^k} = \frac{(-1)^k}{(k-1)!} \sum_{j=1}^{k} \frac{S_k^{(j)}}{j} \left(B_j(1) - N^j B_j\left(\frac{a+1}{N}\right)\right), \tag{4.1}$$

where $S_k^{(j)}$ is the Stirling number of the first kind (A14).

Proof: We follow a method in Ref. 41.

We define the function $P(t;k,a)$ by

$$P(t;k,a) = \sum_{c=1}^{N-1} \frac{\omega_N^{(a+1)c}}{(1-\omega_N^c \mathrm{e}^t)^k}, \tag{4.2}$$

where a and k are positive integers. The function $P(t;k=1,a)$ is computed as follows;

$$\begin{aligned} P(t;k=1,a) &= \sum_{n=0}^{\infty} \sum_{c=1}^{N-1} \omega_N^{(a+1)c+nc} \mathrm{e}^{nt} = -\frac{1}{1-\mathrm{e}^t} + N\mathrm{e}^{-(a+1)t} \frac{\mathrm{e}^{Nt}}{1-\mathrm{e}^{Nt}} \\ &= \sum_{m=0}^{\infty} \frac{1}{(m+1)!} \left(B_{m+1}(0) - N^{m+1} B_{m+1}\left(1-\frac{a+1}{N}\right)\right) t^m. \end{aligned} \tag{4.3}$$

Here we have used

$$\sum_{c=1}^{N-1} \omega_N^{nc} = \begin{cases} N-1 & \text{if } N|n \\ -1 & \text{otherwise.} \end{cases}$$

We further introduce the function $Q(t;k,c)$ by

$$Q(t;k,c) = \frac{1}{(1-\omega_N^c \mathrm{e}^t)^k}, \tag{4.4}$$

where k and c are positive integers. By definitions we have

$$P(t;k,a) = \sum_{c=1}^{N-1} \omega_N^{(a+1)c} Q(t;k,c). \tag{4.5}$$

Definition (4.4) indicates that the function $Q(t;k,c)$ satisfies a differential-difference equation,

$$\frac{\mathrm{d}}{\mathrm{d}t} Q(t;k,c) = k(Q(t;k+1,c) - Q(t;k,c)).$$

We can check by induction that the function $Q(t;k,c)$ can be written in terms of $Q(t;k=1,c)$ as

$$Q(t;k,c)=\frac{(-1)^{k+1}}{(k-1)!}\sum_{m=0}^{k-1}(-1)^m S_k^{(m+1)}\frac{\mathrm{d}^m}{\mathrm{d}t^m}Q(t;1,c) \tag{4.6}$$

From (4.5) we find that $P(t;k,a)$ is solved as

$$P(t;k,a)=\frac{(-1)^{k+1}}{(k-1)!}\sum_{m=0}^{k-1}(-1)^m S_k^{(m+1)}\frac{\mathrm{d}^m}{\mathrm{d}t^m}P(t;1,a) \tag{4.7}$$

Substituting (4.3) for the previous solution, we complete the proof. □

Using the arithmetic identity (4.1), we can rewrite the WRT invariant (2.10) in terms of the Bernoulli polynomials.

Proposition 13: The WRT invariant for the M-exceptional fibered Seifert integral homology sphere $\mathcal{M}=\Sigma(\vec{p})$, *which was computed as in* (2.10), *is written in terms of the Bernoulli polynomials as*

$$\begin{aligned}
&\mathrm{e}^{(2\pi\mathrm{i}/N)(\phi(\vec{p})/4-1/2)}(\mathrm{e}^{(2\pi\mathrm{i}/N)}-1)\tau_N(\mathcal{M})\\
&=-\frac{1}{2}\frac{1}{(M-3)!}\sum_{j=0}^{M-3}(-N)^j\frac{S_{M-2}^{(j+1)}}{j+1}\times\sum_{n=0}^{2PN-1}\chi_{2P}^{\vec{E}}(n)\mathrm{e}^{(1/2PN)(n+P(M-3))^2\pi\mathrm{i}}B_{j+1}\left(\frac{1}{N}\left\lfloor\frac{n}{2P}\right\rfloor\right)\\
&\quad+\frac{(-1)^M}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}\sum_{\vec{\eta}(a)}{}'\sum_{n=0}^{N-1}\sum_{j=1}^{M-3}\frac{S_{M-3}^{(j)}}{j}\mathrm{e}^{\pi\mathrm{i}(2P/N)(n-b-(M-4)/2+(1/2)\sum_{i=1}^{M}\eta_i/p_i)^2}\\
&\quad\times\left(N^{j-1}B_j\left(\frac{n+1}{N}\right)-\frac{1}{N}B_j(1)\right),
\end{aligned} \tag{4.8}$$

where for our brevity we have used M-tuple

$$\vec{E}=\underbrace{(1,1,\ldots,1)}_{M} \tag{4.9}$$

and $\Sigma'_{\vec{\eta}(a)}$ *is a signed sum*

$$\sum_{\vec{\eta}(a)}{}'\cdots=\sum_{\substack{\vec{\eta}\in\{\pm1\}^M s.t.\\ 2a-1<\sum_{j=1}^{M}\eta_j/p_j<2a+1}}\left[\prod_{j=1}^{M}\eta_j\right]\cdots.$$

We remark that the second term including a sum of a in (4.8) vanishes when

$$\sum_{j=1}^{M}\frac{1}{p_j}<1$$

Even when $\Sigma_{j=1}^{M}1/p_j>1$, the second term is a finite sum. It is well known that the sum of inverse of prime numbers, $\Sigma_{p:\mathrm{prime}}1/p$ diverges, although the sum up to the 10 000th prime numbers is still 2.709 258 ….

Proof of Prop. 13: We first study a case of $\Sigma_j 1/p_j<1$. In this case, we have

$$-z^P\prod_{j=1}^{M}(z^{P/p_j}-z^{-P/p_j})=\sum_{m=0}^{2P-1}\chi_{2P}^{\vec{E}}(m)z^m, \tag{4.10}$$

where the periodic function $\chi_{2P}^{\vec{E}}(m)$ is defined in (3.2). Using this identity in (2.10), we have

$$
\begin{aligned}
&e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M})\\
&=-\frac{e^{\pi i/4}}{2\sqrt{2PN}}\sum_{m=0}^{2P-1}\sum_{k=1}^{N-1}\chi_{2P}^{\vec{E}}(m)\frac{e^{(\pi i/2PN)(m+(M-3)P)^2}}{(e^{(2\pi i/N)k}-1)^{M-2}}\sum_{j=0}^{2P-1}e^{-\pi i(N/2P)(j+(k-m-(M-3)P)/N)^2}\\
&=\frac{-1}{2N}\sum_{m=0}^{2P-1}\sum_{n=0}^{N-1}\chi_{2P}^{\vec{E}}(m)e^{(\pi i/2PN)(2Pn-m-(M-3)P)^2}\sum_{k=1}^{N-1}\frac{e^{(2\pi i/N)kn}}{(e^{2\pi ik/N}-1)^{M-2}}\\
&=\frac{-1}{2}\frac{1}{(M-3)!}\sum_{m=0}^{2P-1}\sum_{n=0}^{N-1}\chi_{2P}^{\vec{E}}(m)e^{(\pi i/2PN)(2Pn+m+(M-3)P)^2}\\
&\quad\times\sum_{j=0}^{M-3}\frac{S_{M-2}^{(j+1)}}{j+1}\left(\frac{1}{N}B_{j+1}(1)-N^jB_{j+1}\left(1-\frac{n}{N}\right)\right).
\end{aligned}
$$

Here in the first equality we have used (4.10), and decomposed a sum of n by setting $n=Nj+k$. We have then applied the Gauss sum reciprocity formula (A7) in the second equality, and then used our formula (4.1) in the last equality. As we have

$$
\sum_{n=0}^{2PN-1}\chi_{2P}^{\vec{\ell}}(n)e^{(\pi i/2PN)n^2}=0 \tag{4.11}
$$

due to (3.4), we obtain the first term of (4.8).

For other cases $\Sigma_j 1/p_j>1$, the generating function (4.10) of the periodic function $\chi_{2P}^{\vec{E}}(n)$ is replaced with

$$
\begin{aligned}
&-z^P\prod_{j=1}^{M}(z^{P/p_j}-z^{-P/p_j})+\sum_{a=1}^{\infty}{\sum_{\vec{\eta}(a)}}'z^P(z^{aP}-z^{-aP})\times(z^{P(\Sigma_j n_j/p_j-a)}+(-1)^{M+1}z^{-P(\Sigma_j\eta_j/p_j-a)})\\
&=\sum_{n=0}^{2P-1}\chi_{2P}^{\vec{E}}(n)z^n.
\end{aligned}
\tag{4.12}
$$

Thus comparing with a case of $\Sigma_j 1/p_j<1$, we need additional term τ_{add} defined by

$$
\begin{aligned}
\tau_{\mathrm{add}}=&\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\sum_{\substack{n=0\\ N\nmid n}}^{2PN-1}\frac{e^{\pi i/4}}{2\sqrt{2PN}}\frac{e^{-(n^2/2PN)\pi i}}{(e^{(n/N)\pi i}-e^{-(n/N)\pi i})^{M-3}}\\
&\times(e^{\pi i(n/N)(\Sigma_j\eta_j/p_j-2b-1)}+(-1)^{M+1}e^{-\pi i(n/N)(\Sigma_j\eta_j/p_j-2b-1)}).
\end{aligned}
\tag{4.13}
$$

We decompose a sum of n by setting $n=Nj+k$, and apply the Gauss sum reciprocity formula (A7). After some computations, we obtain

$$
\begin{aligned}
\tau_{\mathrm{add}}=&\frac{1}{2N}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\sum_{k=1}^{N-1}\sum_{n=0}^{N-1}\frac{e^{\pi i(2P/N)(n-(M-2)/2+(1/2))\sum_j\eta_j/p_j)^2}}{(e^{(k/N)\pi i}-e^{-(k/N)\pi i})^{M-3}}\\
&\times(e^{\pi i(k/N)(M-3-2b-2n)}+(-1)^{M+1}e^{\pi i(k/N)(2b+2n-M+3)})\\
=&\frac{1}{N}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\sum_{n=0}^{N-1}e^{\pi i(2P/N)(n-(M-2)/2+(1/2))\sum_j\eta_j/p_j)^2}\sum_{k=1}^{N-1}\frac{e^{2\pi i(k/N)(b+n)}}{(1-e^{2\pi i(k/N)})^{M-3}},
\end{aligned}
$$

where we have used the fact that the sum (4.1) is real. Substituting (4.1) for the previous equation, we find that τ_{add} gives the second term of r.h.s. of (4.8), and thus we complete the proof. □

We now aim to relate this expression with limiting values of the Eichler integrals (3.28) and differentials (3.40) thereof. For our convention, we introduce an analog of the Bernoulli polynomial defined by

$$f_m^M(x) = \sum_{k=m}^{M} \frac{1}{k} S_M^{(k)} \binom{k}{m} \left(x + \frac{M}{2}\right)^{k-m}, \tag{4.14}$$

where $M, m \in \mathbb{Z}$ satisfying $M \geqslant m > 0$. For a case of $m=0$, we set

$$f_0^M(x) = \sum_{k=1}^{M} \frac{S_M^{(k)}}{k} \left(x + \frac{M}{2}\right)^k. \tag{4.15}$$

Some of explicit forms of the polynomials $f_m^M(x)$ are given as follows:

$$f_M^M(x) = \frac{1}{M},$$

$$f_{M-1}^M(x) = x,$$

$$f_{M-2}^M(x) = \frac{1}{M}\binom{M}{2}\left(x^2 - \frac{M}{12}\right),$$

$$f_{M-3}^M(x) = \frac{1}{M}\binom{M}{3}\left(x^3 - \frac{M}{4}x\right),$$

$$f_{M-4}^M(x) = \frac{1}{M}\binom{M}{4}\left(x^4 - \frac{M}{2}x^2 + \frac{1}{240}M(5M+2)\right).$$

Lemma 14: Let the polynomial $f_m^M(x)$ be defined by (4.14). Then the polynomial $f_{M-k\neq 0}^M(x)$ is even (respectively odd) when k is even (respectively odd).

Proof: We introduce the generating function of the polynomials $f_M^m(x)$ by

$$F_M(x,y) = \sum_{m=0}^{M} m f_m^M(x) y^{m-1}. \tag{4.16}$$

Recalling the generating function (A14) of the Stirling number of the first kind, we get

$$F_M(x,y) = \prod_{j=1}^{M-1} \left(y + x + \frac{M}{2} - j\right) \tag{4.17}$$

which shows that $F_M(x,y)$ is a polynomial of $x+y$. Further $F_M(x,y)$ becomes an odd (respectively even) polynomial of $x+y$ when M is even (respectively odd). Then we can conclude that the polynomial $f_{M-k}^M(x)$ is even (respectively odd) if k is even (respectively odd). □

By use of the generating function (4.17), we obtain the following differential equation and recursion relation of $f_m^M(x)$:

$$\frac{\mathrm{d}}{\mathrm{d}x} f_m^M(x) = (m+1) f_{m+1}^M(x), \tag{4.18}$$

$$f_j^{M+1}\left(x-\frac{1}{2}\right)=\left(x-\frac{M}{2}\right)f_j^M(x)+\frac{j-1}{j}f_{j-1}^M(x). \tag{4.19}$$

We can rewrite the WRT invariant in Proposition 13 in terms of these polynomials as follows.

Proposition 15: The WRT invariant $\tau_N(\mathcal{M})$ for the M-exceptional fibered Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ is written as

$$\begin{aligned}
e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M})=&-\frac{1}{2}\frac{1}{(M-3)!}\sum_{k=1}^{M-2}(-N)^{k-1}\sum_{n=0}^{2PN-1}\chi_{2P}^{\vec{E}}(n)f_k^{M-2}\left(\frac{n}{2P}-\left\lfloor\frac{n}{2P}\right\rfloor-\frac{1}{2}\right)\\
&\times e^{(1/2PN)(n+P(M-3))^2\pi i}B_k\left(\frac{n+P(M-3)}{2PN}\right)\\
&+\frac{(-1)^M}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}\sum_{\vec{\eta}(a)}{}'\sum_{n=0}^{N-1}e^{\pi i(2P/N)(n-b-(M-4)/2+(1/2)\sum_j \eta_j/p_j)^2}\\
&\times\sum_{k=0}^{M-3}\left(N^{k-1}f_k^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_j\frac{\eta_j}{p_j}\right)\right.\\
&\left.\times B_k\left(\frac{2n-2b-M+4+\sum_j\frac{\eta_j}{p_j}}{2N}\right)-\frac{1}{N}f_k^{M-3}\left(\frac{5-M}{2}\right)B_k(0)\right).
\end{aligned} \tag{4.20}$$

Proof: To prove for a case of $\Sigma_j 1/p_j<1$, in which the second term in (4.20) vanishes, we only need to apply (A13) to $B_{j+1}((1/N)\lfloor n/2P\rfloor)$ in the first term of (4.8). As we have an identity

$$\sum_{j=1}^{M}\frac{S_M^{(j)}}{j}B_j(x+y)z^j=\sum_{k=0}^{M}f_k^M\left(yz-\frac{M}{2}\right)B_k(x)z^k \tag{4.21}$$

we obtain the required expression.

In the case of $\Sigma_j 1/p_j>1$, we need to evaluate the second term in (4.8), which we have set τ_{add} in the proof of Proposition 13. This term τ_{add} can be transformed into expression (4.20) when we apply (4.21). □

Theorem 16: The exact asymptotic expansion of the WRT invariant $\tau_N(\mathcal{M})$ for the Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ withM-singular fibers in $N\to\infty$ is given as follows;

$$\begin{aligned}
&e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M})\\
&\simeq\frac{1}{2}\frac{1}{(M-3)!}\frac{1}{i^{3/2-m_2(M)}}\sum_{j=0}^{\lfloor(M-3)/2\rfloor}N^{j+\lfloor M/2\rfloor-1/2}\left(\frac{i}{2P\pi}\right)^{\lfloor(M-3)/2\rfloor-j}K^{(j)}_{\lfloor(M-3)/2\rfloor,m_2(M)}\\
&\times\frac{1}{2j+2-m_2(M)}\sum_{\vec{\ell}'}\mathbf{S}_{\vec{\ell}'}^{\sigma_1^{M-1}(\vec{E})}\left[\sum_{n=1}^{2P}\chi_{2P}^{\vec{\ell}'}(n)B_{2j+2-m_2(M)}\left(\frac{n}{2P}\right)\right]e^{-N(P/2)(1+\sum_j\ell_j'/p_j)^2\pi i}\\
&+\frac{1}{(M-3)!}\frac{(-1)^{M\lfloor(M-3)/2\rfloor}}{i^{3/2}}\sum_{m=1}^{\lfloor(M-3)/2\rfloor}\sum_{a=0}^{P}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(a)f_{2m}^{M-2}\left(\frac{a}{2P}-\frac{m_2(M)}{2}\right)\\
&\times\sum_{j=1}^{m}N^{m+j-1/2}\left(\frac{i}{2P\pi}\right)^{m-j}K^{(j-1)}_{m-1,0}\frac{m}{j}\sum_{c=0}^{P}\mathbf{N}_c^a\frac{2-\delta_{c,0}-\delta_{c,P}}{2}B_{2j}\left(\frac{c}{2P}\right)e^{-N(c^2/2P)\pi i}
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{(M-3)!}\frac{(-1)^{M-1}}{\mathrm{i}^{1/2}}\sum_{m=0}^{\lfloor (M-4)/2\rfloor}\sum_{a=1}^{P}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(a)f_{2m+1}^{M-2}\left(\frac{a}{2P}-\frac{\mathrm{m}_2(M)}{2}\right)\\
&\times\sum_{j=0}^{m}N^{m+j+1/2}\left(\frac{\mathrm{i}}{2P\pi}\right)^{m-j}K_{m,1}^{(j)}\frac{2m+1}{2j+1}\sum_{c=1}^{P-1}\mathbf{M}_c^a B_{2j+1}\left(\frac{c}{2P}\right)\mathrm{e}^{-N(c^2/2P)\pi\mathrm{i}}\\
&+\frac{(-1)^M}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\left\{\sum_{m=1}^{\lfloor (M-3)/2\rfloor}f_{2m}^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}\right)\frac{-1}{\mathrm{i}^{3/2}}\sum_{j=1}^{m}N^{m+j-1/2}\left(\frac{\mathrm{i}}{2P\pi}\right)^{m-j}\right.\\
&\times K_{m-1,0}^{(j-1)}\frac{m}{j}\sum_{c=0}^{P}\mathbf{N}_c^{\sigma^{M-1}(P\Sigma_i\eta_i/p_i-P(2a-1))}\frac{2-\delta_{c,0}-\delta_{c,P}}{2}B_{2j}\left(\frac{c}{2P}\right)\mathrm{e}^{-N(c^2/2P)\pi\mathrm{i}}\\
&+(-1)^{M-1}\sum_{m=0}^{\lfloor (M-4)/2\rfloor}f_{2m+1}^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}\right)\frac{-1}{\mathrm{i}^{1/2}}\sum_{j=0}^{m}N^{m+j+1/2}\left(\frac{\mathrm{i}}{2P\pi}\right)^{m-j}\\
&\left.\times K_{m,1}^{(j)}\frac{2m+1}{2j+1}\sum_{c=1}^{P-1}\mathbf{M}_c^{\sigma^{M-1}(P\Sigma_i\eta_i/p_i-P(2a-1))}B_{2j+1}\left(\frac{c}{2P}\right)\mathrm{e}^{-N(c^2/2P)\pi\mathrm{i}}\right\}+\sum_{k=0}^{\infty}\frac{T_{\vec{p}}(k)}{k!}\left(\frac{\pi\mathrm{i}}{2PN}\right)^k,
\end{aligned}
\tag{4.22}
$$

where we have used an involution σ *on* $x\in\mathbb{Z}_{2P}$ *defined by*

$$
\sigma(x)=P-x \bmod 2P. \tag{4.23}
$$

The coefficients $T_{\vec{p}}(k)$ *in a tail part are defined by*

$$
\begin{aligned}
T_{\vec{p}}(k)=&\frac{(-1)^{M+1}}{2}\frac{(2P)^{2k}}{(M-3)!}\sum_{n=1}^{2P}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(n)\sum_{j=1}^{M-2}(-1)^j\frac{j}{2k+j}B_{2k+j}\left(\frac{n}{2P}\right)\\
&\times f_j^{M-2}\left(\frac{n+(M-1)P}{2P}-\left\lfloor\frac{n+(M-1)P}{2P}\right\rfloor-\frac{1}{2}\right)-\frac{(2P)^{2k}}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\sum_{j=1}^{M-3}(-1)^{(M+1)(j+1)}\\
&\times\frac{j}{2k+j}f_j^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}\right)B_{2k+j}\left(\frac{1}{2P}\sigma^{M-1}\left(P\sum_i\frac{\eta_i}{p_i}-(2a-1)P\right)\right).
\end{aligned}
\tag{4.24}
$$

Proof. We first study the case $\Sigma_j 1/p_j<1$, in which we only have the first term in (4.20). We shift the parameter n by $P(3-M)$, and we have

$$
\chi_{2P}^{\vec{E}}(n-P(M-3))=(-1)^{1-m_2(M)}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(n)
$$

As we see that

$$
\chi_{2P}^{\vec{\ell}}(n)f_k^{M-2}\left(\frac{n+(M-1)P}{2P}-\left\lfloor\frac{n+(M-1)P}{2P}\right\rfloor-\frac{1}{2}\right)
$$

is an even (respectively odd) periodic function when k is even (respectively odd), we can write by use of $f_M^M(x)=1/M$ that

$$
\begin{aligned}
&e^{(2\pi i/N)(\phi(\vec{p})/4-1/2)}(e^{2\pi i/N}-1)\tau_N(\mathcal{M})\\
&=-\frac{1}{2}\frac{N^{M-3}}{(M-2)!}\sum_{n=0}^{2PN-1}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(n)e^{(n^2/2PN)\pi i}B_{M-2}\left(\frac{n}{2PN}\right)-\frac{(-1)^M}{2}\frac{1}{(M-3)!}\sum_{c=1}^{\lfloor (M-3)/2\rfloor}N^{2c-1}\\
&\times\left[\sum_{n=0}^{2PN-1}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(n)f_{2c}^{M-2}\left(\frac{n}{2P}-\frac{m_2(M)}{2}\right)e^{(n^2/2PN)\pi i}B_{2c}\left(\frac{n}{2PN}\right)\right]\\
&+\frac{(-1)^M}{2}\frac{1}{(M-3)!}\sum_{c=0}^{\lfloor (M-4)/2\rfloor}N^{2c}\\
&\times\left[\sum_{n=0}^{2PN-1}\chi_{2P}^{\sigma_1^{M-1}(\vec{E})}(n)f_{2c+1}^{M-2}\left(\frac{n}{2P}-\frac{m_2(M)}{2}\right)e^{(n^2/2PN)\pi i}B_{2c+1}\left(\frac{n}{2PN}\right)\right].
\end{aligned}
$$

Generating function (4.10) proves

$$
\sum_{n=0}^{2P-1}\chi_{2P}^{\vec{E}}(n)g(n)=0,
$$

where $g(n)$ is an arbitrary polynomial of n of order at most $M-1$. So we find that $\chi_{2P}^{\vec{E}}(n)f_k^{M-2}(n/2P-\lfloor n/2P\rfloor-1/2)$ is a periodic function of n with mean value zero, and that the expression (4.20) can be identified with a limiting value of the Eichler integrals and their derivatives studied in the previous section. This proves that the WRT invariant is a limiting value of the holomorphic function of q in $q\to e^{2\pi i/N}$.[26] Substituting both (3.44) and (3.45) for the previous expression, we get (4.22).

For the second term τ_{add} in (4.20), recalling the periodic functions $\psi_{2P}^{(a)}(n)$ and $\theta_{2P}^{(a)}(n)$ we can rewrite it into

$$
\begin{aligned}
\tau_{\mathrm{add}}=&\frac{1}{2}\frac{(-1)^M}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}{\sum_{\vec{\eta}(a)}}'\left\{\sum_{m=0}^{\lfloor (M-3)/2\rfloor}N^{2m-1}f_{2m}^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}\right)\right.\\
&\times\sum_{n=0}^{2PN-1}\theta_{2P}^{(\sigma^{M-1}(P\sum_i \eta_i/p_i-(2a-1)P))}(n)e^{\pi i(n^2/2PN)}B_{2m}\left(\frac{n}{2PN}\right)\\
&+(-1)^{M-1}\sum_{m=0}^{\lfloor (M-4)/2\rfloor}N^{2m}f_{2m+1}^{M-3}\left(b+\frac{1}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}\right)\\
&\left.\times\sum_{n=0}^{2PN-1}\psi_{2P}^{(\sigma^{M-1}(P\sum_i \eta_i/p_i-(2a-1)P))}(n)e^{\pi i(n^2/2PN)}B_{2m+1}\left(\frac{n}{2PN}\right)\right\}.
\end{aligned}
$$

With this term, the mean value zero condition is satisfied even in this case, and we can apply the result of Corollary 11 to obtain the exact asymptotic expansion as required. □

We have thus obtained that the WRT invariant $Z_{N-2}(\mathcal{M})$ for the M-exceptional fibered Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ is written in a limit $N\to\infty$ as a sum of exponentially divergent terms and a *tail* part;

$$
Z_{N-2}(\mathcal{M})\simeq\sum_{k=0}^{M-3}N^{M-3-k}Z_{N-2}^{(k)}(\mathcal{M})+\text{a tail part}\tag{4.25}
$$

Here a *tail part* means an infinite power series of $1/N$, and it corresponds to a contribution from the trivial connection. Among the divergent terms in (4.25), the dominating term in the limit $N\to\infty$ is $Z_{N-2}^{(0)}(\mathcal{M})$, which is read as follows.

Corollary 17: In a limit $N\to\infty$, the asymptotics of the WRT invariant $\tau_N(\mathcal{M})$ for the

M-exceptional fibered Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ *is dominated by* N^{M-3}. $Z^{(0)}_{N-2}(\mathcal{M})$, *namely*

$$Z_{N-2}(\mathcal{M}) \sim N^{M-3}\cdot \mathrm{e}^{-[\phi(\vec{p})/2N]\pi \mathrm{i}}\frac{\mathrm{i}^{\mathrm{m}_2(M)-1}\mathrm{e}^{-(3/4)\pi \mathrm{i}}}{2\sqrt{2}(M-2)!}\times \sum_{\vec{\ell}} \mathbf{S}_{\vec{\ell}}^{\sigma_1^{M-1}(\vec{E})} C_{\vec{p}}(\vec{\ell})\mathrm{e}^{-(P/2)\left(1+\sum_{j=1}^{M}\ell_j/p_j\right)^2\pi \mathrm{i}N}, \tag{4.26}$$

i.e.,

$$Z_{N-2}(\mathcal{M}) \sim N^{M-3}\frac{2^{M-2}}{(M-2)!\sqrt{P}}\mathrm{e}^{-[\phi(\vec{p})/2N]\pi \mathrm{i}}\mathrm{e}^{-[(2M+1)/4]\pi \mathrm{i}}\sum_{\vec{\ell}} C_{\vec{p}}(\vec{\ell})\mathrm{e}^{-(P/2)\left(1+\sum_{j=1}^{M}\ell_j/p_j\right)^2\pi \mathrm{i}N}$$
$$\times (-1)^{MP\left(1+\sum_j \ell_j/p_j\right)+P\sum_j 1/p_j+P\sum_j\sum_{k\neq j}\ell_k/p_jp_k}\left[\prod_{j=1}^{M}\sin\left(P\frac{\ell_j}{p_j^2}\pi\right)\right], \tag{4.27}$$

where the sum of M-tuples $\vec{\ell}$ *runs over D-dimensional space* (3.7), *and the function* $C_{\vec{p}}(\vec{\ell})$ *is defined by*

$$C_{\vec{p}}(\vec{\ell})=\sum_{n=1}^{2P}\chi^{\vec{\ell}}_{2P}(n)B_{M-2}\left(\frac{n}{2P}\right). \tag{4.28}$$

We note that the invariance (3.6) of the periodic function $\chi^{\vec{\ell}}_{2P}(n)$ indicates that

$$C_{\vec{p}}(\sigma_i\sigma_j(\vec{\ell}))=C_{\vec{p}}(\vec{\ell}). \tag{4.29}$$

By construction, the asymptotics (4.26) should coincide with (2.19) which follows from residue part of (2.16). We do not have a direct proof, and we have checked the equivalence numerically for several $\vec{p}$'s. Recalling the path integral approach, the sum of M-tuple $\vec{\ell}$ can be regarded as a label of the gauge equivalent class of flat connections α in (1.4), and we can identify the Chern-Simons invariant with

$$\mathrm{CS}(A_{\alpha(\vec{\ell})})=-\frac{P}{4}\left(1+\sum_{j=1}^{M}\frac{\ell_j}{p_j}\right)^2 \mod 1. \tag{4.30}$$

See Refs. 42 and 43 for computations of the Chern-Simons invariant for the Seifert homology spheres. Note that this value originates from the T matrix (3.16) of the vector modular form. Correspondingly, the Reidemeister torsion is given by

$$\sqrt{T_{\alpha(\ell)}}=\left|\prod_{j=1}^{M}\sin\left(P\frac{\ell_j}{p_j^2}\pi\right)\right|\cdot C_{\vec{p}}(\vec{\ell}). \tag{4.31}$$

Here the product of sin functions originates from the S matrix of the vector modular form.

B. Ohtsuki series

A tail part in the asymptotic formula (4.22) has a simple generating function as was studied in (2.17).

Theorem 18: *Let the T series be defined by* (4.24). *Then the generating function of the T series is*

$$\frac{\prod_{j=1}^{M}\sinh\left(\frac{P}{p_j}x\right)}{[\sinh(Px)]^{M-2}}=\frac{1}{2}\sum_{k=0}^{\infty}\frac{T_{\vec{p}}(k)}{(2k)!}x^{2k}. \tag{4.32}$$

Proof: We first study a case of $\Sigma_j 1/p_j < 1$. Using (4.10), we have

$$\frac{\prod_{j=1}^{M} \sinh\left(\frac{P}{p_j}x\right)}{[\sinh(Px)]^{M-2}} = \frac{(-1)^{M-1}}{2}\sum_{k=0}^{\infty}\sum_{n=0}^{2P-1}\binom{k+M-3}{k}\vec{\chi}_{2P}^{E}(n)\mathrm{e}^{-(n+2P(k+(M-3)/2))x}.$$

We equate this expression with $\Sigma_{k=0}^{\infty}[T_k/(2k)!]x^{2k}$. Applying the Mellin transformation, we get

$$T_k = \frac{(-1)^M}{2}\frac{(2P)^{2k}}{(M-3)!}\sum_{n=0}^{2P-1}\vec{\chi}_{2P}^{E}(n)\sum_{j=0}^{M-3}\frac{1}{1+j+2k}B_{1+j+2k}\left(\frac{n+P(M-3)}{2P}\right)$$
$$\times\sum_{k=j}^{M-3}S_{M-3}^{(k)}\binom{k}{j}\left(\frac{P(M-3)-n}{2P}\right)^{k-j}.$$

Here we have used (3.33). Identities (4.14) and (4.19) give

$$\sum_{k=j}^{M-3}S_{M-3}^{(k)}\binom{k}{j}\left(\frac{P(M-3)-n}{2P}\right)^{k-j} = (-1)^{M+1+j}(j+1)f_{j+1}^{M-2}\left(\frac{n}{2P}-\frac{1}{2}\right),$$

then we have

$$T_k = \frac{1}{2}\frac{(2P)^{2k}}{(M-3)!}\sum_{n=0}^{2P-1}\vec{\chi}_{2P}^{E}(n)\times\sum_{j=1}^{M-2}(-1)^j\frac{j}{j+2k}f_j^{M-2}\left(\frac{n}{2P}-\frac{1}{2}\right)B_{2k+j}\left(\frac{n+P(M-3)}{2P}\right). \tag{4.33}$$

For this expression, we substitute an identity

$$B_{2k+j}\left(\frac{n+P(M-3)}{2P}\right) = B_{2k+j}\left(\frac{n}{2P}+\frac{\mathrm{m}_2(M)-1}{2}\right)+(2k+j)\sum_{m=0}^{\lfloor (M-4)/2\rfloor}\left(\frac{n}{2P}+m+\frac{\mathrm{m}_2(M)-1}{2}\right)^{2k+j-1}$$

which follows from (A10). As we have

$$\sum_{j=1}^{M-2}jf_j^{M-2}\left(\frac{n}{2P}-\frac{1}{2}\right)\left(-\frac{n}{2P}-m-\frac{\mathrm{m}_2(M)-1}{2}\right)^{j-1} = F_{M-2}\left(\frac{n}{2P}-\frac{1}{2},-\frac{n}{2P}-m-\frac{\mathrm{m}_2(M)-1}{2}\right)=0$$

from (4.17), we obtain (4.32).

When $\Sigma_j(1/p_j)>1$, we have another term coming from the second term in (4.12). This gives an additional term to (4.33);

$$T_k^{\mathrm{add}} = \frac{(-1)^M}{2}\frac{(2P)^{2k}}{(M-4)!}\sum_{a=1}^{\infty}\sum_{b=0}^{a-1}\sum_{\vec{\eta}(a)}{}'\sum_{j=1}^{M-3}(-1)^j\frac{j}{2k+j}f_j^{M-3}\left(\frac{1}{2}\sum_i\frac{\eta_i}{p_i}-b-\frac{1}{2}\right)$$
$$\times\left(B_{2k+j}\left(\frac{M-4}{2}+\frac{1}{2}\sum_i\frac{\eta_i}{p_i}-b\right)+(-1)^jB_{2k+j}\left(\frac{M-2}{2}-\frac{1}{2}\sum_i\frac{\eta_i}{p_i}+b\right)\right).$$

Recalling Lemma 14 and applying the same method with the previous, we recover (4.24). □

We give explicit forms of some T series as follows;

$$T_{\vec{p}}(0) = 0, \tag{4.34}$$

$$T_{\vec{p}}(1) = 4P, \tag{4.35}$$

$$T_{\vec{p}}(2) = 8P^3\left(2 - M + \sum_{j=1}^{M} \frac{1}{p_j^2}\right), \tag{4.36}$$

$$T_{\vec{p}}(3) = 4P^5\left(5\left(\sum_{j=1}^{M} \frac{1}{p_j^2} + 2 - M\right)^2 - 2\left(\sum_{j=1}^{M} \frac{1}{p_j^4} + 2 - M\right)\right), \tag{4.37}$$

Based on the exact asymptotic expansion (4.22) of the WRT invariant, we extract the *tail* part and define the formal q-series $\tau_\infty(\mathcal{M})$ as a quantum invariant of the Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$ by identifying $\exp(2\pi\mathrm{i}/N)$ with q;

$$q^{\phi(\vec{p})/4-1/2}(q-1)\cdot\tau_\infty(\mathcal{M}) = \sum_{k=0}^{\infty} \frac{T_{\vec{p}}(k)}{k!}\left(\frac{\log q}{4P}\right)^k. \tag{4.38}$$

This invariant $\tau_\infty(\mathcal{M})$ of the formal q series coincides with the invariant $\tau_N^{\mathrm{int}}(\mathcal{M})$ defined in (2.16). Namely we have an integral expression for $\tau_\infty(\mathcal{M})$.

The Ohtsuki series[32] $\lambda_n(\mathcal{M})$ is defined from the formal q series $\tau_\infty(\mathcal{M})$ by

$$\tau_\infty(\mathcal{M}) = \sum_{n=0}^{\infty} \lambda_n(\mathcal{M})(q-1)^n \tag{4.39}$$

Then the Ohtsuki series $\lambda_n(\mathcal{M})$ for $\mathcal{M}=\Sigma(\vec{p})$ is computed as follows.

Theorem 19: *The Ohtsuki series* $\lambda_n(\mathcal{M})$ *for the Seifert homology sphere* $\mathcal{M}=\Sigma(\vec{p})$ *is written in terms of* $\vec{p}$ *and* $\phi(\vec{p})$ *defined in* (2.11) *as*

$$\lambda_n(\mathcal{M}) = \frac{2}{(n+1)!}\left[\prod_{j=0}^{n}\left(\frac{P}{4}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2} - \frac{\phi(\vec{p})}{4} - j\right)\right]G(x)\Bigg|_{x=0}, \tag{4.40}$$

where the function $G(x)$ *is*

$$G(x) = \frac{\prod_{j=1}^{M}\sinh\left(\frac{x}{p_j}\right)}{[\sinh(x)]^{M-2}}. \tag{4.41}$$

Proof: From (4.38) and (A15), we have

$$(q-1)\tau_\infty(\mathcal{M}) = \sum_{m=0}^{\infty}\binom{\frac{1}{2} - \frac{\phi(\vec{p})}{4}}{m}(q-1)^m \sum_{j=0}^{\infty}\sum_{k=0}^{j}\frac{S_j^{(k)}}{j!}\frac{T_{\vec{p}}(k)}{(4P)^k}(q-1)^j.$$

We then have

$$\begin{aligned}\lambda_n(\mathcal{M}) &= \sum_{j=0}^{n}\frac{1}{(j+1)!}\binom{\frac{1}{2} - \frac{\phi(\vec{p})}{4}}{n-j}\sum_{k=1}^{j+1} S_{j+1}^{(k)}\frac{T_{\vec{p}}(k)}{(4P)^k} \\ &= \frac{1}{(n+1)!}\sum_{m=0}^{n}\sum_{k=1}^{n+1-m}\binom{m+k}{m}S_{n+1}^{(m+k)}\left(\frac{1}{2} - \frac{\phi(\vec{p})}{4}\right)^m\frac{T_{\vec{p}}(k)}{(4P)^k},\end{aligned}$$

where in the second equality we have expanded the binomial coefficient in terms of the Stirling number of the first kind using (A14), then we have applied (A17). Theorem 18 shows that the function $G(x)$ (4.41) gives

$$\left(P\frac{\mathrm{d}}{\mathrm{d}x}\right)^{2k} G(x)\Big|_{x=0} = \frac{1}{2}T_{\vec{p}}(k).$$

Substituting this expression and recalling (A14), we obtain the required formula. □

Explicit forms of the lowest three Ohtsuki series $\lambda_n(\mathcal{M})$ for $\mathcal{M}=\Sigma(\vec{p})$ are

$$\lambda_0(\mathcal{M}) = 1, \tag{4.42}$$

$$\lambda_1(\mathcal{M}) = 6\lambda_C(\mathcal{M}), \tag{4.43}$$

$$\lambda_2(\mathcal{M}) = \frac{3(\phi(\vec{p}))^2 + 12\phi(\vec{p}) - 4}{96} - \frac{P}{16}\left(2 - M + \sum_{j=1}^{M}\frac{1}{p_j^2}\right)(\phi(\vec{p}) + 2) + \frac{P^2}{96}\left(5\left(2 - M + \sum_{j=1}^{M}\frac{1}{p_j^2}\right)^2 - 2\left(2 - M + \sum_{j=1}^{M}\frac{1}{p_j^4}\right)\right), \tag{4.44}$$

where $\lambda_C(\mathcal{M})$ is the Casson invariant of the Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$[44,45]

$$\lambda_C(\mathcal{M}) = -\frac{1}{8} + \frac{1}{24P}\left(1 + \sum_{k=1}^{M}\left(\frac{P}{p_k}\right)^2 - (M-2)P^2\right) - \frac{1}{2}\sum_{k=1}^{M} s\left(\frac{P}{p_k}, p_k\right). \tag{4.45}$$

The relationship between the Casson invariant $\lambda_C(\mathcal{M})$ and the Ohtsuki series $\lambda_1(\mathcal{M})$ was first proved in Ref. 46. See Ref. 47 for a computation of $\lambda_2(\mathcal{M})$.

C. Lattice points

We have seen that the asymptotics of the WRT invariant is dominated by the term (4.26), which shows that the number of terms in the sum of $\vec{\ell}$ are at most D defined in (3.7). Though, as was studied in Refs. 15 and 16 for cases of $M=3$ and $M=4$, the function $C_{\vec{p}}(\vec{\ell})$ may vanish for some $\vec{\ell}$'s.

Theorem 20: *We fix M-tuple $\vec{p}$ with pairwise coprime positive integers p_j, and let the function $C_{\vec{p}}(\vec{\ell})$ be defined by (4.28) for $\vec{\ell}\in\mathbb{Z}^M$ satisfying $1\leqslant \ell_j \leqslant p_j - 1$. Due to (4.29), we have D independent functions. We set $\gamma(\vec{p})$ as the number of M-tuples $\vec{\ell}$ satisfying*

$$C_{\vec{p}}(\vec{\ell}) \neq 0,$$

and $L(\vec{p})$ as the integral lattice points $\vec{\ell}\in\mathbb{Z}^M_{>0}$ inside the M-dimensional tetrahedron,

$$0 < \sum_{j=1}^{M}\frac{\ell_j}{p_j} < 1.$$

Then we have

$$D - \gamma(\vec{p}) \geqslant L(\vec{p}). \tag{4.46}$$

Proof: As a generalization of the function $C_{\vec{p}}(\vec{\ell})$ defined in (4.28), we define $C^k_{\vec{p}}(\vec{\ell})$ for $k\geqslant 0$ by

$$C^k_{\vec{p}}(\vec{\ell}) = \sum_{n=1}^{2P}\chi^{\vec{\ell}}_{2P}(n)B_k\left(\frac{n}{2P}\right) \tag{4.47}$$

in terms of the Bernoulli polynomials. We have $C_{\vec{p}}(\vec{\ell})=C^{M-2}_{\vec{p}}(\vec{\ell})$. As a generating function $Z^{\vec{\ell}}_{\vec{p}}(t)$ of these polynomials, we define

$$Z_{\vec{p}}^{\vec{\ell}}(t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} C_{\vec{p}}^{k}(\vec{\ell}). \tag{4.48}$$

Using (A8), we have

$$Z_{\vec{p}}^{\vec{\ell}}(t) = \frac{t}{e^t - 1} \sum_{n=1}^{2P} \chi_{2P}^{\vec{\ell}}(n) e^{(t/2P)n}. \tag{4.49}$$

In the case of $0 < \Sigma_j (\ell_j / p_j) < 1$, we have

$$\sum_{n=0}^{2P} \chi_{2P}^{\vec{\ell}}(n) z^n = -z^P \prod_{j=1}^{M} (z^{P\ell_j/p_j} - z^{-P\ell_j/p_j}) \tag{4.50}$$

which gives

$$Z_{\vec{p}}^{\vec{\ell}}(t) = -\frac{t}{e^{t/2} - e^{-t/2}} \prod_{j=1}^{M} (e^{(\ell_j/2p_j)t} - e^{-(\ell_j/2p_j)t}).$$

This shows that

$$Z_{\vec{p}}^{\vec{\ell}}(t) = -\left(\prod_{j=1}^{M} \frac{\ell_j}{p_j} \right) t^M + O(t^{M+2})$$

and that $C_{\vec{p}}^{k}(\vec{\ell}) = 0$ for $0 \leqslant k \leqslant M-1$. So we have $C_{\vec{p}}(\vec{\ell}) = 0$ when $0 < \Sigma_j \ell_j / p_j < 1$.

The invariance (3.6) of the periodic functions $\chi_{2P}^{\vec{\ell}}(n)$ proves the statement of the theorem. □

In the case of $\Sigma_j \ell_j / p_j > 1$, the generating function (4.50) should be replaced with a formula like (4.12), and we do not know whether the function $C_{\vec{p}}(\vec{\ell})$ vanishes. We conjecture that, when $\Sigma_j \ell_j / p_j > 1$, we have $C_{\vec{p}}(\ell) = 0$ iff $\chi_{2P}^{\vec{\ell}}(n)$ coincides with $\chi_{2P}^{\vec{\ell}'}(n)$ such that $\Sigma_j \ell_j' / p_j < 1$.

Conjecture 1: Under the conditions of Theorem 20, we have

$$D - \gamma(\vec{p}) = L(\vec{p}). \tag{4.51}$$

This conjecture was proved for $M \leqslant 4$ in Refs. 15 and 16. It states that the number of the flat connections which contribute as (4.26) coincides with the number of integral lattice points inside the M-dimensional tetrahedron.

D. Ehrhart polynomial

Explicit form of the number $L(\vec{p})$ of the lattice points inside the M-dimensional tetrahedron was first computed by Mordell[48] for cases of $M=3$ and $M=4$;

- $M=3$;

$$L(p_1,p_2,p_3) = \frac{1}{4}(p_1-1)(p_2-1)(p_3-1) + \frac{1}{12P} - \frac{1}{4} - \frac{P}{12}\left(1 - \frac{1}{p_1^2} - \frac{1}{p_2^2} - \frac{1}{p_3^2}\right) - s(p_1p_2,p_3) - s(p_2p_3,p_1) - s(p_1p_3,p_2), \tag{4.52}$$

- $M=4$,

$$L(p_1,p_2,p_3,p_4)=\frac{1}{8}\prod_{j=1}^{4}(p_j-1)+\frac{3}{8}-\frac{P}{12}+\frac{P}{24}\sum_{j=1}^{4}\frac{1+p_j}{p_j^2}+\frac{1}{24P}\left(1-\sum_{j=1}^{4}p_j\right)-\frac{P}{24}\sum_{j\neq k}^{4}\frac{1}{p_j^2p_k}$$
$$-\frac{1}{2}\sum_{j=1}^{4}s\left(\frac{P}{p_j},p_j\right)+\frac{1}{2}\sum_{j\neq k}^{4}s\left(\frac{P}{p_jp_k},p_j\right). \tag{4.53}$$

Here $s(b,a)$ is the Dedekind sum (A1). For higher dimension M, the lattice points $L(\vec{p})$ might be written in terms of Zagier's higher-dimensional Dedekind sum,[60] but there seems to exist no applicable expressions.

Although, there is a useful tool to count the lattice points (see, *e.g.*, Ref. 49). Let $\mathcal{P}$ be the M-dimensional open tetrahedron with integer vertices, $(p_1,0,\ldots,0)$, $(0,p_2,0,\ldots,0),\ldots,(0,\ldots,0,p_M)$, and (0,...,0);

$$\mathcal{P}=\left\{(\ell_1,\ldots,\ell_M)\in\mathbb{Z}^M\,\middle|\,\sum_{j=1}^{M}\frac{\ell_j}{p_j}<1,\ell_k>0\right\}. \tag{4.54}$$

Let $E_{\mathcal{P}}(t)$ denote the number of lattice points in the dilated tetrahedron $t\mathcal{P}$. So we have

$$L(\vec{p})=E_{\mathcal{P}}(t=1).$$

In the same manner, we suppose that $E_{\bar{\mathcal{P}}}(t)$ denotes the number of lattice points of the closure of $t\mathcal{P}$,

$$E_{\bar{\mathcal{P}}}(t)=\#\left\{(m_1,\ldots,m_M)\in\mathbb{Z}^M\,\middle|\,\sum_{j=1}^{M}\frac{m_j}{p_j}\leqslant t,m_k\geqslant 0\right\}.$$

These functions, $E_{\mathcal{P}}(t)$ and $E_{\bar{\mathcal{P}}}(t)$, become polynomials of t,[50] which are called the Ehrhart polynomial. Moreover we have the Ehrhart-Macdonald reciprocity formula,[50,51]

$$E_{\mathcal{P}}(-t)=(-1)^ME_{\bar{\mathcal{P}}}(t). \tag{4.55}$$

In general, the number of lattice points $E_{\bar{\mathcal{P}}}(t)$ becomes polynomial of t for arbitrary polytope $\bar{\mathcal{P}}$.[50] We set the coefficients of the Ehrhart polynomial as

$$E_{\bar{\mathcal{P}}}(t)=c_M(\mathcal{P})t^M+c_{M-1}(\mathcal{P})t^{M-1}+\cdots+c_0(\mathcal{P}). \tag{4.56}$$

It is well known that $c_M(\mathcal{P})$ is the volume of $\mathcal{P}$, $c_M(\mathcal{P})=\mathrm{Vol}(\mathcal{P})$, $c_{M-1}(\mathcal{P})$ is a half of the boundary surface area, $c_{M-1}(\mathcal{P})=\frac{1}{2}\,\mathrm{Vol}(\partial\mathcal{P})$. The coefficient $c_0(\mathcal{P})$ is the Euler characteristic $\chi(\mathcal{P})$, and $c_0(\mathcal{P})=1$ when $\mathcal{P}$ is the convex polytope.

The first nontrivial coefficient of the Ehrhart polynomial for the M-dimensional tetrahedron is thus $c_{M-2}(\mathcal{P})$. In our case of the M-dimensional tetrahedron with pairwise coprime integers p_j, we have[52,53]

$$(M-2)!\cdot c_{M-2}(\mathcal{P})=\frac{M}{4}+\frac{1}{24P}\left(2-\sum_{k=1}^{M}\left(\frac{P}{p_k}\right)^2+3\left(\sum_{k=1}^{M}\frac{P}{p_k}\right)^2\right)-\sum_{k=1}^{M}s\left(\frac{P}{p_k},p_k\right). \tag{4.57}$$

Recalling the Casson invariant $\lambda_C(\mathcal{M})$ (4.45) for the Seifert homology sphere $\mathcal{M}=\Sigma(\vec{p})$, which is proportional to the first Ohtsuki series (4.43), we have the following.

Proposition 21: The Casson invariant $\lambda_C(\mathcal{M})$ for $\mathcal{M}=\Sigma(\vec{p})$ is related to the first nontrivial coefficient of the Ehrhart polynomial for the M-dimensional tetrahedron $\mathcal{P}$ (4.54);

$$\lambda_C(\mathcal{M})-\frac{(M-2)!}{2}c_{M-2}(\mathcal{P})=-\frac{M+1}{8}+\frac{M-2}{24}P-\frac{P}{8}\sum_{1\leqslant j<k\leqslant M}\frac{1}{p_jp_k}. \tag{4.58}$$

TABLE I. The WRT invariant $Z_N(\mathcal{M})$ for $\mathcal{M}=\Sigma(2,3,5,7,11)$. Asymptotic formula for $Z_N^{(0)}(\mathcal{M})$ is from (4.26).

N	Exact result for Z_N	Asymptotics $Z_N^{(0)}$
22	−13.346 013+17.397 906i	−12.2403+16.7013i
23	−0.576 825 56−0.511 081 47i	0.020 572+0.004 140i
98	0.932 635 90−0.496 554 57i	0.323 366+0.005 702 3i
99	22.826 764−367.893 60i	22.8460−365.870i
100	464.334 37−287.595 56i	475.688−287.973i
998	9.229 211 0−9.332 412 9i	10.7013−1.605 81i
999	−52 995.123−87 204.076i	−53 072.7−87 187.8i
1000	694.743 44+9 181.2935i	683.369+9 183.49i
2398	−64.891 808+46.620 794i	−62.4971+47.927 5i
2399	320 910.08+27 551.395i	321 128+27 510.1i
2400	142 206.21−1871.8080i	142 145−1869.06i
2401	214 250.48−80 025.187i	214 270−79 907.4i

It is remarked that the residue formula for $c_{M-2}(\mathcal{P})$ given in Ref. 52 looks like an expression (2.10) of the WRT invariant $\tau_N(\mathcal{M})$ for $\mathcal{M}=\Sigma(\vec{p})$.

V. SOME EXAMPLES OF NUMERICAL EXPERIMENTS

We give some numerical experiments on the asymptotic behavior of the WRT invariants for the Seifert homology spheres.

A. $\Sigma(2,3,5,7,11)$

For $\vec{p}=(2,3,5,7,11)$, we have $P=2310$, $D=30$, and $\phi(\vec{p})=34\,189/2310$. The bases for 30-dimensional space is given by $\vec{\ell}=(1,1,\ell_3,\ell_4,\ell_5)$ with $1\leqslant\ell_3\leqslant 2$, $1\leqslant\ell_4\leqslant 3$, $1\leqslant\ell_5\leqslant 5$. For all these 5-tuples $\vec{\ell}$, we can check that $C_{\vec{p}}(\vec{\ell})\neq 0$, which supports Conjecture 1 as we have $\Sigma_j 1/p_j = 2927/2310>1$.

In Table I we give numerical results on the Witten invariant $Z_N(\mathcal{M})$ for $\mathcal{M}=\Sigma(2,3,5,7,11)$, which is performed with a help of PARI/GP. We give both the exact value $Z_N(\mathcal{M})$ and asymptotic value $Z_N^{(0)}(\mathcal{M})$ for several N's. They vary much with N, and comparing these data we see an agreement.

B. $\Sigma(3,7,8,11,13,17)$

For $\vec{p}=(3,7,8,11,13,17)$, we have $\phi(\vec{p})=338\,099/408\,408$ and $D=5040$. This $D=5040$-dimensional vector space is spanned by $\vec{\ell}=(1,1\leqslant\ell_2\leqslant 3,1\leqslant\ell_3\leqslant 7,1\leqslant\ell_4\leqslant 5,1\leqslant\ell_5\leqslant 6,1\leqslant\ell_6\leqslant 8)$. Among these $D=5040$ bases, we check that $C_{\vec{p}}(\vec{\ell})=0$ when $\vec{\ell}=(1,1,1,1,1,1)$, (1, 1, 1, 1, 1, 2), (1, 1, 1, 1, 1, 3) (1, 1, 1, 1, 2, 1), (1, 1, 1, 1, 2, 2), (1, 1, 1, 1, 3, 1), (1, 1, 1, 2, 1, 1), (1, 1, 1, 2, 1, 2), (1, 1, 1, 2, 2, 1), (1, 1, 2, 1, 1, 1), (1, 2, 1, 1, 1, 1), which supports Conjecture 1.

Numerical results on the exact value and the asymptotics of the Witten invariant for $\Sigma(\vec{p})$ are summarized in Table II. We see an agreement.

VI. CONCLUSION AND DISCUSSION

We have studied the asymptotic expansion of the SU(2) WRT invariant $\tau_N(\mathcal{M})$ for the M-exceptional fibered Seifert homology spheres $\mathcal{M}=\Sigma(\vec{p})$ in $N\to\infty$ number theoretically. We have found that the invariant can be written in terms of a limiting value of *fractional* derivative, i.e., derivative of the Eichler integral, of the vector modular forms with weight 3/2 and 1/2. This supports a result[26] that the WRT invariant is a *limiting* value of the holomorphic function in a limit that q tends to the Nth root of unity. By use of the nearly modular property of the Eichler integral,

TABLE II. The WRT invariant $Z_N(\mathcal{M})$ for $\mathcal{M}=\Sigma(3,7,8,11,13,17)$. Asymptotic formula for $Z_N^{(0)}(\mathcal{M})$ is from (4.26).

N	Exact value $Z_N(\mathcal{M})$	Asymptotics $Z_N^{(0)}(\mathcal{M})$
58	365.328 95+679.070 06i	351.149+691.982i
59	1331.846 0−433.950 47i	1 358.51−437.953i
60	−944.994 93+765.344 51i	−915.949+742.606i
61	130.910 99+2 814.574 4i	62.848 9+2 763.93i
118	−0.820 601 7+61.590 246i	0.782 372+60.124 8i
119	8.185 778 1+13.369 868i	0.019 566 2+0.006 267 5i
120	5 259.285 3+4 064.402 9i	5 232.38+4 043.94i
121	8733.014 0+5 274.827 3i	8 659.21+5 338.15i
238	−219.367 38−1.608 943i	−216.499+1.534 62i
239	−6 151.056 2−5617.755 86i	−6 220.64−5 620.95i
240	−11.492 746+6.119 235 8i	1.674 54+2.349 20i
241	−26 057.019−52 201.108i	−25 950.5−52 634.8i
242	49 736.853−46 390.033i	49 818.0−46 337.0i
243	189 895.62+265 408.04i	189 029. +265 225. i
244	3 782.8814−12 474.142i	3 814.35−12 433.5i
998	21 039.448+18 091.568i	21 107.1+18 191.2i
999	−12.505 553+49.861 847i	−0.033 154 9+0.033 885 2i
1000	78 229.306−164 203.36i	7 8333.1−164 618. i

we have obtained an asymptotic expansion of $\tau_N(\mathcal{M})$ in the large N limit.

Although an asymptotic behavior of the WRT invariant was previously studied in, e.g., Ref. 8, the correspondence between modular forms and the quantum invariants enables us to relate topological invariants such as the Chern-Simons invariants, the Reidemeister torsion, and the Casson invariant, with geometries of modular forms. For example, we have found that the number of the gauge equivalent classes of flat connections, which dominate the WRT invariant in the large-N limit, is related to the number of integral lattice points inside the M-dimensional tetrahedron. From this view, we have established that the Casson invariant for the Seifert homology sphere has a relationship with the first non-trivial coefficient of the Ehrhart polynomial.

In our previous papers[17,25] we have shown that the WRT invariants for the Seifert manifolds with three-exceptional fibers coincides with a limiting value of the Ramanujan mock theta functions. Investigated[35] is a modular transformation formula of the newly proposed mock theta functions based on explicit form of the WRT invariants. This intriguing correspondence seems to originate from a result that the integral expression (2.16) of the WRT invariant has a connection with the Mordell integral.[34] Our results presented here will shed a new light on geometric and topological aspects of modular forms.

Though we have studied only the SU(2) invariant, the Witten partition function (1.1) can be defined for arbitrary gauge group, and an explicit form of the invariant for the Seifert manifold is given.[54] Extending the method of Lawrence and Rozansky, it is shown[55] that the partition function can be written in the integral form which can be interpreted as the matrix model, and that it becomes a sum of local contributions from the flat connections. This fact is recently reinterpreted from the viewpoint of the path integral by use of non-abelian localization.[56] As it is well known that the Chern-Simons perturbation theory of the SU(N) Witten invariant as a $1/N$ expansion can be interpreted from the string theory (see, e.g., Ref. 57), it will be interesting to investigate the quantum invariants/modular forms correspondence for the WRT invariant associated with SU(N) gauge group as a generalization of the present work.

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APPENDIX: SPECIAL FUNCTIONS AND IDENTITIES

1. Dedekind sum

The Dedekind sum is defined by (see, e.g., Ref. 58)

$$s(b,a)=\sum_{k=1}^{a-1}\left(\left(\frac{k}{a}\right)\right)\left(\left(\frac{kb}{a}\right)\right), \tag{A1}$$

where $((x))$ is the sawtooth function

$$((x))=\begin{cases} x-\lfloor x\rfloor-\dfrac{1}{2} & \text{when } x\notin\mathbb{Z} \\ 0 & \text{when } x\in\mathbb{Z}. \end{cases}$$

The Dedekind sum can also be written as

$$s(b,a)=\frac{1}{4a}\sum_{k=1}^{a-1}\cot\left(\frac{k}{a}\pi\right)\cot\left(\frac{kb}{a}\pi\right). \tag{A2}$$

The Dedekind sum is known to satisfy the reciprocity formula

$$s(b,a)+s(a,b)=-\frac{1}{4}+\frac{1}{12}\left(\frac{a}{b}+\frac{b}{a}+\frac{1}{ab}\right). \tag{A3}$$

We note

$$s(-b,a)=-s(b,a), \tag{A4}$$

$$s(b,a)=s(c,a)\quad \text{for } bc=1 \bmod a. \tag{A5}$$

2. Gauss sum

As a discrete analogue of the Gaussian integral, we have a formula of the Gauss sum as

$$\sum_{n=0}^{2N-1}\mathrm{e}^{-(1/2N)n^2\pi\mathrm{i}}=\sqrt{2N}\mathrm{e}^{-(1/4)\pi\mathrm{i}}. \tag{A6}$$

The reciprocity formula of the Gauss sum follows from the Gauss integral as (see, e.g., Refs. 30 and 59)

$$\sum_{n \bmod N}\mathrm{e}^{\pi\mathrm{i}(M/N)n^2+2\pi\mathrm{i}kn}=\sqrt{\left|\frac{N}{M}\right|}\mathrm{e}^{(\pi\mathrm{i}/4)\mathrm{sign}(NM)}\sum_{n \bmod M}\mathrm{e}^{-\pi\mathrm{i}(N/M)(n+k)^2}, \tag{A7}$$

where N, $M\in\mathbb{Z}$ and $N\,k\in\mathbb{Z}$, and $N\,M$ is even.

3. Bernoulli polynomial

The nth Bernoulli polynomial $B_n(x)$ is defined from the generating function as

$$\frac{t\mathrm{e}^{xt}}{\mathrm{e}^t-1}=\sum_{k=0}^{\infty}B_k(x)\frac{t^k}{k!}. \tag{A8}$$

Some of them are written as follows;

$$B_0(x)=1,$$

$$B_1(x) = x - \frac{1}{2},$$

$$B_2(x) = x^2 - x + \frac{1}{6},$$

$$B_3(x) = x^3 - \frac{3}{2}x^2 + \frac{1}{2}x.$$

These polynomials satisfy the following relations;

$$B_k(1-x) = (-1)^k B_k(x), \tag{A9}$$

$$B_k(x+1) - B_k(x) = kx^{k-1}, \tag{A10}$$

$$\frac{\mathrm{d}}{\mathrm{d}x} B_n(x) = nB_{n-1}(x). \tag{A11}$$

Note that the Bernoulli function has the Fourier expansion as

$$B_k(x - \lfloor x \rfloor) = k! \sum_{\substack{n \in \mathbb{Z} \\ n \neq 0}} \frac{\mathrm{e}^{2\pi \mathrm{i} n x}}{(2\pi \mathrm{i} n)^k} \tag{A12}$$

and that

$$B_n(x+y) = \sum_{k=0}^{n} \binom{n}{k} B_k(x) y^{n-k}. \tag{A13}$$

4. Stirling number

The Stirling number of the first kind $S_n^{(m)}$ denotes the (signed) number of permutations of n elements which contain m permutation cycles (see, e.g., Ref. 40). The generating function of $S_n^{(m)}$ is written as

$$\prod_{j=0}^{n-1} (x-j) = \sum_{m=0}^{n} S_n^{(m)} x^m \tag{A14}$$

and $S_n^{(m)} \neq 0$ when $n \geqslant m \geqslant 0$. Another form of the generating function is given by[41]

$$\frac{(\log q)^m}{m!} = \sum_{n=m}^{\infty} S_n^{(m)} \frac{(q-1)^n}{n!} \tag{A15}$$

Based on these generating functions, we have the recursion relations of $S_n^{(m)}$ as follows;

$$S_{n+1}^{(m)} = S_n^{(m-1)} - nS_n^{(m)}, \tag{A16}$$

$$\binom{m}{r} S_n^{(m)} = \sum_{k=m-r}^{n-r} \binom{n}{k} S_{n-k}^{(r)} S_k^{(m-r)}. \tag{A17}$$

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Canonical quantization of lattice Higgs-Maxwell-Chern-Simons fields: Krein Self-adjointness

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It is shown how techniques from constructive quantum field theory may be applied to indefinite metric gauge theories in Hilbert space for the case of a Higgs-Maxwell-Chern-Simons theory on a lattice. The Hamiltonian operator is shown to be Krein essentially self-adjoint by means of unbounded but Krein unitary transformations relating the Hamiltonian to an essentially maximal accretive operator.
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I. INTRODUCTION

The mathematical study of Higgs gauge theories has been focused mainly on gauge-invariant quantities undertaken using Euclidean functional integrals.[1–3] However, in the theoretical physics literature, it is mostly the Higgs and gauge fields that are used directly.[4–7] In this direction we consider a $(2+1)$ dimensional space-time Maxwell-Chern-Simons field minimally coupled to a charged scalar field in the indefinite metric framework proposed by Wightman and Gårding.[8] By using a representation of the canonically quantized Chern-Simons field in a Hilbert space with a Krein indefinite metric, we show the Chern-Simons field to be a Hilbert normal and Krein self-adjoint operator. Regularizing field operators with a finite periodic lattice allows construction of the Hamiltonian operator. Initially this operator is densely defined and closable but exhibits no immediate spectral properties which would suggest direct implementation of techniques from constructive quantum field theory in obtaining a Euclidean path-space representation for a semigroup generated by this Hamiltonian. In this paper, we show the underlying structure of the Hamiltonian to be that of an accretive operator masked by unbounded Krein unitary "gauge" transformations. This leads to an unbounded semigroup which, unlike Fröhlich's theory of unbounded symmetric semigroups, is not Hilbert self-adjoint.[9] In a second paper,[10] we will obtain the corresponding Euclidean theory and examine the relation between the physical states in the Wightman-Gårding framework and Osterwalder-Schrader positivity provided by this unbounded semigroup.

In Sec. II, we describe our representation for the Maxwell-Chern-Simons field which differs from those in Refs. 11 and 12 and establish regularity of the field that we use. It is convenient to represent these fields in terms of harmonic oscillator variables in Sec. III and the Appendix since the Krein gauge transformations then become transparent as well as their properties as unbounded operators. In Sec. IV, it is shown that the real part of the transformed Hamiltonian defines an essentially self-adjoint operator which is bounded below. The gauge-transformed Hamiltonian is then shown to be an accretive operator in Sec. V. The bounds from Sec. IV allow us to prove a quadratic estimate for the transformed Hamiltonian by which it becomes a maximal accretive operator after closure, and thus Krein essentially self-adjoint.

II. MAXWELL-CHERN-SIMONS FIELDS

We work in $d=s+1$ dimensional space-time, where the number of spatial dimensions is $s=2$. The metric is given by $g_{00}=+1$ and $g_{ij}=-\delta_{ij}$, with the remaining components vanishing. As usual, Latin indices are spatial, ranging from 1 to s, while Greek indices include the time component, 0. We write the inner product of d-vectors k and x alternately as

$$kx = k_\mu x^\mu = k^\mu x_\mu = k_0 x_0 - k \cdot x = k_0 x_0 - k_i x_i,$$

where indices are raised or lowered by contraction with g and repeated indices are summed over their range. It should always be clear from context whether k and x refer to d-vectors or s-vectors. We use analogous notation for d-divergences, e.g., $\partial A \equiv \partial_\mu A^\mu$. Our units are such that $\hbar=c=1$. Finally, we make use of the notation $\omega=\omega(k)=\sqrt{k\cdot k}$ and $\mu=\mu(k)=\sqrt{k\cdot k+m^2}=\sqrt{\omega^2+m^2}$. Hopefully, our conventions are now clear.

The Maxwell-Chern-Simons (MCS) Lagrangian density is given by

$$\mathcal{L} = -\frac{1}{2}\partial_\mu A_\nu \partial^\mu A^\mu + \frac{\lambda}{2}(\partial A)^2 + \frac{m}{2}\epsilon^{\mu\nu\rho}\partial_\mu A_\nu A_\rho. \tag{1}$$

The term $(\partial A)^2$ fixes the gauge with the parameter λ

$$\lambda = \frac{2\xi}{2\xi - 1} = -\frac{\gamma}{1-\gamma} \tag{2}$$

interpolating between the various covariant gauges. Here, $\gamma=\lambda=\xi=0$ corresponds to the Feynman gauge while $\gamma=1$, $\lambda\to\infty$, $\xi=1/2$ all correspond to Landau gauge. The parameters ξ and γ are more convenient than λ for our representation below. The parameter γ is introduced for comparison with other works that start with a different Lagrangian such as Ref. 11, while ξ is introduced for comparison with works such as Refs. 12 and 13.

The Euler-Lagrange equations corresponding to Eq. (1) are

$$\Box A^\mu - \lambda \partial^\mu(\partial A) + m\epsilon^{\mu\alpha\beta}\partial_\alpha A_\beta = 0. \tag{3}$$

The homogeneous Green's function for (3) can be written

$$\begin{aligned}\langle A_\mu(x)A_\nu(y)\rangle = {} & \frac{1}{(2\pi)^2}\int d\Omega_m(k)e^{-ik(x-y)}\left[\frac{k_\mu k_\nu}{m^2} - g_{\mu\nu} - \frac{i}{m}\epsilon_{\mu\nu\rho}k^\rho\right] + \frac{1}{(2\pi)^2}\int d\Omega_0(k)e^{-ik(x-y)} \\ & \times\left[-\frac{k_\mu k_\nu}{m^2} + \frac{i}{m}\epsilon_{\mu\nu\rho}k^\rho\right] - \frac{1-2\xi}{(2\pi)^2}\int d\Omega_0(k)e^{-ik(x-y)} \\ & \times\frac{1}{2\omega}\left[\delta_{\mu 0}k_\nu + \delta_{\nu 0}k_\mu - i(x_0-y_0)k_\mu k_\nu - \frac{k_\mu k_\nu}{\omega}\right],\end{aligned} \tag{4}$$

which has support both on the light cone and the mass m hyperboloid. The canonical momenta associated with (1) are

$$\pi^0 \equiv \frac{\delta\mathcal{L}}{\delta(\partial_0 A_0)} = -\partial_0 A^0 + \lambda\,\partial A \tag{5}$$

$$\pi^j \equiv \frac{\delta\mathcal{L}}{\delta(\partial_0 A_j)} = -\partial_0 A^j + \frac{m}{2}\epsilon^{0jn}A_n. \tag{6}$$

It is convenient to express (3) in terms of differential forms. For this, we define a 1-form $A \equiv A_\mu dx^\mu$. We let $*$ denote the Hodge duality operator associated with our metric g and the orientation given by the volume form $dx^0\wedge dx^1\wedge dx^2$, so that $**=+1$. Furthermore, we define the codifferential δ in the usual way on k-forms by

$$\delta = -\det(g)(-1)^{d(k+1)} * d * = -(-1)^{3(k+1)} * d * = (-1)^k * d* \tag{7}$$

so that, for a k-form β, we have

$$\delta\beta = \delta\left(\frac{1}{k!}\beta_{\mu_1\cdots\mu_k}dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_k}\right) = -\frac{1}{(k-1)!}\partial^{\mu_1}\beta_{\mu_1\cdots\mu_k}dx^{\mu_2}\wedge\cdots\wedge dx^{\mu_k}.$$

Then, we find that $\Box \equiv \partial^\mu\partial_\mu$ is given by

$$\Box = -(\delta d + \mathrm{d}\delta), \tag{8}$$

in analogy with the Laplace-Beltrami operator in the Riemannian case. With this notation, we may write (3) as

$$\delta dA - m * dA = (\lambda - 1)d\delta A. \tag{9}$$

From this standpoint, it becomes easy to prove the following decomposition theorems, which we shall utilize in the process of canonical quantization.

Theorem II.1 (MCS Decomposition). *Let A be a 1-form satisfying (9). Then, there exist 1-forms V and S satisfying the equations*

$$dV = m * V, \quad * dS = -\frac{(\lambda-1)}{m}d\delta S \tag{10}$$

such that $A = V + S$.

Conversely, given 1-forms V and S satisfying (10), the 1-form $A = V + S$ satisfies (9).

Proof:

For the first statement, define

$$V \equiv \frac{1}{m} * dA + \frac{1}{m^2}(\lambda-1)d\delta A$$

so that

$$*dV = \frac{1}{m} * d * dA = \frac{1}{m}\delta dA = \frac{1}{m}(m * dA + (\lambda-1)d\delta A) = mV,$$

where we have used (9). Now, define the 1-form $S \equiv A - V$. This satisfies

$$*dS = *dA - *dV = *dA - mV = *dA - \left(*dA + \frac{\lambda-1}{m}d\delta A\right) = -\frac{\lambda-1}{m}d\delta A.$$

Then, the result (10) follows by noting that

$$\delta A = \delta S + \delta V = \delta S + \delta\left(\frac{*dV}{m}\right) = \delta S.$$

For the converse, we note that Eqs. (10) imply

$$\delta dV = (-1)^2 * d * dV = + * d(mV) = m^2 V,$$

$$\delta V = (-1)^1 * d * V = - * d * \left(\frac{*dV}{m}\right) = 0,$$

$$\delta dS = (-1)^2 * d * dS = + * d\left(-\frac{\lambda - 1}{m} d\delta S\right) = 0.$$

Then, we simply substitute $A = V + S$ into Eq. (9) to find

$$\text{LHS} = \delta d(V+S) - m * d(V+S) = m^2 V - m * dV - m * dS = -m\left(-\frac{\lambda - 1}{m} d\delta S\right) = (\lambda - 1) d\delta S,$$

$$\text{RHS} = (\lambda - 1) d\delta(V+S) = (\lambda - 1) d\delta S,$$

and note that RHS=LHS. Q.E.D.

Notice that the gauge dependence, as parametrized by λ, has been separated into the field S in Eqs. (10). For this reason, we often refer to V as the physical MCS field. We can say more about V and S. It has long been known that there are certain necessary conditions that a valid decomposition of a solution of (3) into the sum of a massive and a massless vector field must satisfy Refs. 14 and 15. These conditions follow easily from our theorem, so we state them as a corollary.

Corollary II.2: *The vector field* V_μ *corresponding to the* 1*-form* V *satisfies*

$$(\Box + m^2) V_\mu = 0$$

$$\partial V = 0,$$

which are the Proca field equations. The vector field S_μ *corresponding to the* 1*-form* S *satisfies*

$$\Box S_\mu = \partial_\mu (\partial S)$$

$$\Box (\partial S) = 0,$$

provided $\lambda \neq 1$.

One should note that, although V_μ satisfies the Proca field equations, it is not a true Proca field since it also satisfies the additional constraint (10). Thus, one expects the quantized version of V_μ to propagate one less physical mode than a 2+1- dimensional Proca field. We shall see that this is indeed the case. In fact, even at the classical level, we have the following result.

Proposition II.3 (*Proca Decomposition*): *Let* U *be a* 1*-form satisfying the Klein-Gordon equation*

$$(\Box + m^2) U = 0$$

for $m > 0$. *Then, it is both necessary and sufficient that* U *satisfy the decomposition*

$$U = V^+ + V^- + d\phi, \tag{11}$$

where $V^\pm$ *satisfy* $*dV^\pm = \pm m V^\pm$ *and* ϕ *is a scalar solution to the Klein-Gordon equation. If* U *is additionally a Proca field* (*i.e.*, $\delta U = 0$), *then we may choose* $\phi \equiv 0$.

Proof:

For necessity, define

$$V^\pm \equiv -\frac{1}{2}\left(\frac{1}{m^2} d\delta U \mp \frac{1}{m} * dU - U\right) \quad \text{and} \quad \phi \equiv \frac{1}{m^2}\delta U \tag{12}$$

The remainder then follows by straightforward calculations. Q.E.D.

The well-known bosonization of the MCS field exhibiting its single, massive, physical degree of freedom (see, e.g., Ref. 4) also follows easily from Theorem II.1. Thus, we state it as a corollary as well.

Corollary II.4: *A vector field satisfying*

$$\epsilon_{\mu\nu\rho}\partial^{\nu}V^{\rho} = mV_{\mu} \tag{13}$$

[*i.e.*, $*dV=mV$ *as per* (10)] *must necessarily be of the form*

$$V_0 = \frac{\sqrt{-\triangle}}{m}\phi$$

$$V_j = -\left[\frac{\partial_0\partial_j}{m\sqrt{-\triangle}} - \frac{\epsilon_{jn}\partial_n}{\sqrt{-\triangle}}\right]\phi$$

for some scalar field ϕ.

Proof:

Taking the time derivative of (13) for $\mu=j$, we find

$$m\partial_0 V_j = -\epsilon_{jn}\partial_n\partial_0 V_0 + \epsilon_{jn}\partial_0\partial_0 V_n = -\epsilon_{jn}\partial_n\partial_0 V_0 + \epsilon_{jn}(\triangle - m^2)V_n,$$

and noting that

$$m^2 V_n = m\epsilon_{nk}(\partial_0 V_k - \partial_k V_0)$$

we obtain the necessary condition

$$\triangle V_j = m\epsilon_{jn}\partial_n V_0 - \partial_0\partial_j V_0,$$

from which the result follows by defining

$$\phi \equiv \frac{m}{\sqrt{-\triangle}}V_0.$$

Q.E.D.

We proceed now to the quantization. Using the intuition gained from Theorem II.1, we seek a massive vector field $V_\mu(x)$ satisfying

$$(\Omega_R, V_\mu(x)V_\nu(y)\Omega_R)_R = \frac{1}{(2\pi)^2}\int d\Omega_m(k)\left[\frac{k_\mu k_\nu}{m^2} - g_{\mu\nu} - i\frac{\epsilon_{\mu\nu\lambda}k^\lambda}{m}\right]e^{-ik(x-y)}, \tag{14}$$

and a commuting massless vector field $S_\mu(x)$ satisfying

$$\begin{aligned}(\Omega_R, S_\mu(x)S_\nu(y)\Omega_R)_R = {} & \frac{1}{(2\pi)^2}\int d\Omega_0(k)e^{-ik(x-y)}\left[-\frac{k_\mu k_\nu}{m^2} + \frac{i}{m}\epsilon_{\mu\nu\rho}k^\rho\right] \\ & - \frac{1-2\xi}{(2\pi)^2}\int d\Omega_0(k)e^{-ik(x-y)}\frac{1}{2\omega}\left[\delta_{\mu 0}k_\nu + \delta_{\nu 0}k_\mu - i(x_0-y_0)k_\mu k_\nu - \frac{k_\mu k_\nu}{\omega}\right]\end{aligned} \tag{15}$$

so that

$$(\Omega_R, V_\mu(x)V_\nu(y)\Omega_R)_R + (\Omega_R, S_\mu(x)S_\nu(y)\Omega_R)_R = \langle A_\mu(x)A_\nu(y)\rangle \tag{16}$$

given in Eq. (4). First, we consider the massive field $V_\mu(x)$.

Guided by Proposition II.3, we define

$$V_\mu(x) = \frac{1}{\sqrt{2}}\left(-\frac{\partial_\mu\partial_\alpha}{m^2} - g_{\mu\alpha} + \frac{1}{m}\epsilon_{\mu\alpha\beta}\partial^\beta\right)U^\alpha(x) \tag{17}$$

$$= \frac{1}{2\pi\sqrt{2}} \int d\Omega_m(k) \left[b^{\alpha}(k) \left(\frac{k_\alpha k_\mu}{m^2} - g_{\mu\alpha} - \frac{i}{m} \epsilon_{\alpha\mu\beta} k^{\beta} \right) e^{-ikx} \right.$$
$$\left. + b^{\dagger\alpha}(k) \left(\frac{k_\alpha k_\mu}{m^2} - g_{\mu\alpha} + \frac{i}{m} \epsilon_{\alpha\mu\beta} k^{\beta} \right) e^{ikx} \right], \tag{18}$$

where U is a massive vector field given by

$$U_\mu(x) = \frac{1}{2\pi} \int d\Omega_m(k) [e^{-ikx} b_\mu(k) + e^{ikx} b_\mu^\dagger(k)], \tag{19}$$

with $d\Omega_m(k)$ denoting the invariant measure on the positive mass m hyperboloid and b, $b^\dagger$ satisfying the commutation relations

$$[b_\mu(k), b_\nu^\dagger(k')] = -g_{\mu\nu} 2\mu(k) \delta(k-k'). \tag{20}$$

This is clearly a covariant field that, by construction, satisfies the field equations $\epsilon_{\mu\nu\rho}\partial^\nu V^\rho(x) = mV_\mu(x)$. Furthermore, one checks that (14) is satisfied under the usual assumption $b_\mu(k)\Omega_R = 0$.

In fact, all is made rigorous by realizing the expressions as bilinear forms on the Proca Fock space $\mathcal{H}_R^P$ given by

$$\mathcal{H}_R^P \equiv \Gamma_{\text{sym}}(L^2(R^d, d\Omega_m(k)) \otimes C^d),$$

i.e., the symmetric Fock space over $\mathcal{H}_R^{P(1)} \equiv L^2(R^d, d\Omega_m(k)) \otimes C^d$. Given $\Phi \in \mathcal{H}_R^P$, we denote its projection onto the n-particle subspace $\mathcal{H}_R^{P(n)}$ by $\Phi^{(n)}$. With this notation, the inner product on $\mathcal{H}_R^P$ is given by

$$(\Phi, \Psi)_R = \sum_{n=0}^{\infty} (\Phi^{(n)}, \Psi^{(n)})_R^{(n)},$$

with

$$(f,g)_R^{(n)} = \prod_{j=1}^{n} \left[\int d\Omega_m(k_j) \right] \overline{f_{\mu_1 \cdots \mu_n}(k_1, \ldots, k_n)} g_{\mu_1 \cdots \mu_n}(k_1, \ldots, k_n) \tag{21}$$

for $f, g \in \mathcal{H}_R^{P(n)}$ with $n > 0$ and $(f,g)_R^{(0)} = \bar{f}g$ for $f, g \in \mathcal{H}_R^{P(0)}$. We denote adjoints with respect to $(\cdot,\cdot)_R$ by a superscript $*$ and refer to them as Hilbert adjoints.

We introduce the usual Fock creation and annihilation bilinear forms on $\mathcal{H}_R^P$ by

$$[c_\mu^*(k)\Phi]_{\mu_1 \cdots \mu_n}^{(n)}(k_1, \ldots, k_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \delta_{\mu\mu_j} \delta(k-k_j) 2\mu(k_j) \Phi_{\mu_1 \cdots \widehat{\mu_j} \cdots \mu_n}^{(n-1)}(k_1, \ldots, \widehat{k_j}, \ldots, k_n) \tag{22}$$

$$[c_\mu(k)\Phi]_{\mu_1 \cdots \mu_n}^{(n)}(k_1, \ldots, k_n) = \sqrt{n+1}\, \Phi_{\mu\mu_1 \cdots \mu_n}^{(n+1)}(k, k_1, \ldots, k_n), \tag{23}$$

where a hat over a variable or an index means to omit it. These are well-defined (as bilinear forms) on vectors $\Phi \in D(N^{1/2}) \subset \mathcal{H}_R$, where N is the self-adjoint number operator. In fact, $c_\mu(k)$ defines an operator on this domain.[16] These formally satisfy the canonical commutation relations

$$[c_\mu(k), c_\nu^*(k')] = \delta_{\mu\nu} 2\mu(k) \delta(k-k'). \tag{24}$$

We also need to introduce the indefinite metric on $\mathcal{H}_R^P$ which is given by $\{\Phi, \Psi\}_R = (\Phi, \eta\Psi)_R$. The action of η on the n-particle subspace is given by

$$(f,\eta g)_R^{(n)} = \prod_{j=1}^{n}\left[\int d\Omega_m(k_j)(-g)_{\mu_j\nu_j}\right]\overline{f_{\mu_1\cdots\mu_n}(k_1,\ldots,k_n)}\,g_{\nu_1\cdots\nu_n}(k_1,\ldots,k_n), \tag{25}$$

which in turn determines its action on $\mathcal{H}_R^P$. In short, η is the second quantization of the operator

$$f_\mu(k) \mapsto (-g_{\mu\nu}f_\nu)(k)$$

on $\mathcal{H}_R^{P(1)}$.[16,17] With respect to the indefinite inner product $\{\cdot,\cdot\}_R$, $\mathcal{H}_R^P$ is a Krein space.[18] This follows from the observations that $\eta=\eta^*$ and $\eta^2=1$. We denote adjoints with respect to the Krein metric by a superscript †. Clearly, it is also true that $\eta=\eta^\dagger$.

Finally, we can define b, $b^\dagger$ as Krein creation and annihilation forms,

$$b_\mu^\dagger(k) = g_{\mu\nu}c_\nu^*(k), \quad b_\mu(k) = -c_\mu(k). \tag{26}$$

These, then, formally satisfy Eq. (20). Furthermore, as bilinear forms, we have the relations

$$N = \int d\Omega_m(k)c_\mu^*(k)c_\mu(k) = \int d\Omega_m(k)b_\mu^\dagger(k)(-g_{\mu\nu})b_\nu(k).$$

Calculating the commutator, we obtain

$$[V_\mu(x),V_\nu(y)] = -i\left(\partial_\mu\partial_\nu + g_{\mu\nu} - \frac{\epsilon_{\mu\nu\lambda}\partial^\lambda}{m}\right)\Delta_m(x-y). \tag{27}$$

Note that this is not a local expression, despite the facts that the Pauli-Jordan function $\Delta_m(x)$ given by

$$\Delta_m(x) = \frac{-i}{(2\pi)^s}\int d^dk\ \mathrm{sgn}(k_0)\,\delta(k^2-m^2)e^{-ikx}. \tag{28}$$

vanishes for spacelike separations and differential operators are, in general, local. This subtlety arises from the fact that a time derivative of $\Delta_m(x)$ evaluated at time zero yields a delta function (see, e.g., Appendix I of Ref. 19). Thus, we have the following nonvanishing equal-time commutators:

$$\left[V_0(t,x),V_n(t,y)\right] = \frac{i\partial_n}{m^2}\delta(x-y) \tag{29}$$

$$\left[V_j(t,x),V_n(t,y)\right] = -i\epsilon_{jn}\delta(x-y). \tag{30}$$

This is analogous to the situation that arises in canonical quantization of the Proca field without use of an indefinite metric.[19]

In order to exhibit the bosonization (and, hence, the single physical mode of Refs. 4 and 12) within this framework, we note that (18) can be written

$$V_\mu(x) = \frac{1}{2\pi\sqrt{2}}\int d\Omega_m(k)\left[(Lgb)_\mu(k)e^{-ikx} + (\bar{L}gb^\dagger)_\mu(k)e^{ikx}\right], \tag{31}$$

where

$$L_{\mu\nu} \equiv \frac{k_\mu k_\nu}{m^2} - g_{\mu\nu} - \frac{i}{m}\epsilon_{\mu\nu\lambda}k^\lambda \tag{32}$$

$$= \left(\frac{\sqrt{\mu^2+\omega^2}}{m}\hat{w}_3 - \hat{w}_2 \right) \otimes \left(\frac{\sqrt{\mu^2+\omega^2}}{m}\hat{w}_3 - \hat{w}_2 \right)^* \tag{33}$$

using the basis

$$\hat{w}_1 = \frac{1}{\sqrt{\mu^2+\omega^2}} \begin{pmatrix} \mu \\ -k_1 \\ -k_2 \end{pmatrix}$$

$$\hat{w}_2 = \frac{i}{\omega} \begin{pmatrix} 0 \\ k_2 \\ -k_1 \end{pmatrix} \tag{34}$$

$$\hat{w}_3 = \frac{1}{\omega\sqrt{\mu^2+\omega^2}} \begin{pmatrix} \omega^2 \\ \mu k_1 \\ \mu k_2 \end{pmatrix},$$

which is orthonormal in the C^3 Euclidean inner product.

Then, we can define

$$a(k) = \frac{1}{\sqrt{2}} \left(\frac{\sqrt{\mu^2+\omega^2}}{m}\hat{w}_3 - \hat{w}_2 \right)^*_\alpha g_{\alpha\beta} b_\beta(k) \tag{35}$$

$$a^\dagger(k) = \frac{1}{\sqrt{2}} \left(\frac{\sqrt{\mu^2+\omega^2}}{m}\hat{w}_3 + \hat{w}_2 \right)^*_\alpha g_{\alpha\beta} b^\dagger_\beta(k), \tag{36}$$

where we've used $\bar{\hat{w}}_2 = -\hat{w}_2$. Hence,

$$[a(k), a^\dagger(k')] = 2\mu\delta(k-k'), \tag{37}$$

and suppressing the vector index we have the representation

$$V(x) = \frac{1}{2\pi} \int d\Omega_m(k) \left[\left(\frac{\sqrt{\omega^2+\mu^2}}{m}\hat{w}_3 - \hat{w}_2 \right) a(k) e^{-ikx} + \left(\frac{\sqrt{\omega^2+\mu^2}}{m}\hat{w}_3 + \hat{w}_2 \right) a^\dagger(k) e^{ikx} \right], \tag{38}$$

for which the time evolution is implemented by

$$H_0^V = \int d\Omega_m(k) \mu(k) a^\dagger(k) a(k). \tag{39}$$

From this expression for V_μ, it is clear that the physical field is both Krein and Hilbert symmetric. It also has a dense set of analytic vectors, thereby making its closure self-adjoint.

Next, we turn to the ghost field S_μ. We wish to realize S_μ on the Maxwell Fock space $\mathcal{H}_R^M$ given as the symmetric Fock space over the single particle space

$$\mathcal{H}_R^{M(1)} \equiv L^2(R^d, d\Omega_0) \otimes C^d, \tag{40}$$

where $d\Omega_0$ is the invariant measure on the forward light cone. As before, we equip $\mathcal{H}_R^M$ with an indefinite metric $\{\cdot,\cdot\}_R \equiv (\cdot, \eta\cdot)_R$, where $\eta = -g$ on $\mathcal{H}_R^{M(1)}$. Then, we will have a realization of the Maxwell-Chern-Simons field $A_\mu \equiv V_\mu \otimes 1 + 1 \otimes S_\mu \equiv V_\mu + S_\mu$ on $\mathcal{H}_R = \mathcal{H}_R^P \otimes \mathcal{H}_R^M$. For this, we first choose the following C^3-orthonormal vectors:

$$\hat{v}_1 = \frac{1}{\omega\sqrt{2}}\begin{pmatrix} \omega \\ k_1 \\ k_2 \end{pmatrix}, \tag{41}$$

$$\hat{v}_2 = \frac{i}{\omega}\begin{pmatrix} 0 \\ k_2 \\ -k_1 \end{pmatrix}, \tag{42}$$

$$\hat{v}_3 = \frac{1}{\omega\sqrt{2}}\begin{pmatrix} \omega \\ -k_1 \\ -k_2 \end{pmatrix}. \tag{43}$$

Next, we define bilinear forms

$$a_R(k) = (\hat{v}_3)_\alpha g^{\alpha\beta} a_\beta(k), \tag{44}$$

$$a_Q(k) = (\hat{v}_1)_\alpha g^{\alpha\beta} a_\beta(k), \tag{45}$$

$$a_Q^\dagger(k) = (\hat{v}_1)_\alpha g^{\alpha\beta} a_\beta^\dagger(k), \tag{46}$$

$$a_R^\dagger(k) = (\hat{v}_3)_\alpha g^{\alpha\beta} a_\beta^\dagger(k), \tag{47}$$

in terms of the Maxwell Krein forms a, $a^\dagger$ satisfying

$$[a_\mu(k), a_\nu^\dagger(k')] = -g_{\mu\nu} 2\omega(k)\delta(k-k'). \tag{48}$$

These differ slightly from analogous forms given in Refs. 11 and 12, but are more convenient for our purposes. They satisfy the algebra

$$[a_Q(k), a_R^\dagger(k')] = -2\omega\delta(k-k') = [a_R(k), a_Q^\dagger(k')] \tag{49}$$

with the remaining commutators vanishing.

Then, we can define the field

$$S(x;\gamma) = \frac{1}{2\pi}\int d\Omega_0(k)\left\{ e^{-ikx}\left[\frac{\omega}{m}\hat{v}_1 a_R(k) + \left(\frac{\omega}{m}\hat{v}_1 - \sqrt{2}\hat{v}_2 + (1-\gamma)\left(\frac{m}{2\omega}\hat{v}_3 - ix_0 m\hat{v}_1\right)\right)a_Q(k)\right]\right.$$
$$\left. + e^{ikx}\left[\frac{\omega}{m}\hat{v}_1^* a_R^\dagger(k) + \left(\frac{\omega}{m}\hat{v}_1^* - \sqrt{2}\hat{v}_2^* + (1-\gamma)\left(\frac{m}{2\omega}\hat{v}_3^* + ix_0 m\hat{v}_1^*\right)\right)a_Q^\dagger(k)\right]\right\}, \tag{50}$$

where we have again suppressed the vector index. Clearly, this expression simplifies considerably in Landau gauge $\gamma=1$. One can check that (50) yields the correct two-point expression (15) on $\mathcal{H}_R^M$.

The time evolution of S_μ is implemented by the Hamiltonian

$$H_0^S(\gamma) = \int d\Omega_0(k)\omega\left[-a_Q^\dagger(k)a_R(k) - a_Q^\dagger(k)a_R(k) - (1-\gamma)\frac{m^2}{\omega^2}a_Q^\dagger(k)a_Q(k)\right]$$
$$= \int d\Omega_0(k)\omega a_\mu^\dagger(k)\left(-g^{\mu\nu} - (1-\gamma)\frac{m^2 k^\mu k^\nu}{2\omega^4}\right)a_\nu(k)$$
$$= \int d\Omega_0(k)\omega c_\mu^*(k)\left(\delta_\mu^\nu + (1-\gamma)\frac{m^2 k_\mu k^\nu}{2\omega^4}\right)c_\nu(k). \tag{51}$$

It is Krein symmetric, but not Hilbert symmetric unless one chooses Landau gauge $\gamma=1$. However, standard arguments show its closure to be Hilbert normal and Krein self-adjoint. By techniques similar to the Maxwell case,[13] we find

Theorem II.5:

1. $[0,\infty)\subset\sigma(H_0^S)$

2. H_0^S *is accretive*

We note that the field S_μ is also nonlocal. We have, in fact, the nonvanishing equal-time commutation relations

$$[S_0(t,x),S_n(t,y)]=\frac{-i}{m^2}\partial_n\delta(x-y) \tag{52}$$

$$[S_j(t,x),S_n(t,y)]=\frac{i}{m}\epsilon_{jn}\delta(x-y). \tag{53}$$

However, the full MCS field $A_\mu=V_\mu+S_\mu$ is local since

$$[A_0(t,x),A_n(t,y)]=[V_0(t,x),V_n(t,y)]+[S_0(t,x),S_n(t,y)]=0 \tag{54}$$

$$[A_j(t,x),A_n(t,y)]=[V_j(t,x),V_n(t,y)]+[S_j(t,x),S_n(t,y)]=0, \tag{55}$$

where we have used Eqs. (29) and (30).

We regularize the above fields by restricting them to a finite spatial volume $V\subset(\delta Z)^s$ with periodic boundary conditions (thus, V is a product of finite cyclic groups). We denote the volume of V by $|V|$. We denote the dual group of V by Γ. The measure on V is taken to be

$$\frac{1}{\sqrt{|V|}}\sum_{x\in V}\delta^s, \tag{56}$$

while that on Γ is

$$\frac{1}{\sqrt{|V|}}\sum_{k\in\Gamma}, \tag{57}$$

with Fourier transform

$$\tilde{f}(k)=\frac{1}{\sqrt{|V|}}\sum_{x\in V}\delta^s e^{-ik\cdot x}f(x). \tag{58}$$

We choose to use midpoint derivatives on the lattice so that

$$k_n=\frac{2}{\delta}\sin\left(\frac{k_n\delta}{2}\right) \tag{59}$$

and

$$\omega^2=k_nk_n=\sum_{n=1}^{s}\frac{4}{\delta^2}\sin^2\left(\frac{k_n\delta}{2}\right). \tag{60}$$

With these conventions, the regularized MCS field becomes

$$A(x) = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma_0} \frac{1}{2\mu} \left[\left(\frac{\sqrt{\omega^2+\mu^2}}{m} \hat{w}_3 - \hat{w}_2 \right) a(k) e^{-ikx} + \left(\frac{\sqrt{\omega^2+\mu^2}}{m} \hat{w}_3 + \hat{w}_2 \right) a^\dagger(k) e^{ikx} \right]_{k_0=\mu}$$
$$+ \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma_0} \frac{1}{2\omega} \left\{ e^{-ikx} \left[\frac{\omega}{m} \hat{v}_1 a_R(k) + \left(\frac{\omega}{m} \hat{v}_1 - \sqrt{2}\hat{v}_2 + (1-\gamma) \left(\frac{m}{2\omega} \hat{v}_3 - i x_0 m \hat{v}_1 \right) \right) a_Q(k) \right] \right.$$
$$\left. + e^{ikx} \left[\frac{\omega}{m} \hat{v}_1^* a_R^\dagger(k) + \left(\frac{\omega}{m} \hat{v}_1^* - \sqrt{2}\hat{v}_2^* + (1-\gamma) \left(\frac{m}{2\omega} \hat{v}_3^* + i x_0 m \hat{v}_1^* \right) \right) a_Q^\dagger(k) \right]_{k_0=\omega} \right\}, \tag{61}$$

in which our infrared regularization is to sum over $\Gamma_0 \equiv \Gamma \backslash \{0\}$. This field is defined as a distribution-valued unbounded operator on the lattice Fock space $\mathcal{H}_R = \mathcal{H}_R^P \otimes \mathcal{H}_R^M$. Here, $\mathcal{H}_R^P$ is the symmetric Fock space over $L^2(\Gamma_0) \otimes C^d$ with measure

$$\frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma_0} \frac{1}{2\mu}, \tag{62}$$

while $\mathcal{H}_R^M$ is the symmetric Fock space over $L^2(\Gamma_0) \otimes C^d$ with measure

$$\frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma_0} \frac{1}{2\omega}. \tag{63}$$

In the following sections, we shall loosely use Γ to indicate whichever momentum sums are appropriate.

III. KREIN GAUGE TRANSFORMATIONS

The formal Lagrangian density for the MCS-Higgs model will be

$$\mathcal{L} = \mathcal{L}^{\text{cs}} + \mathcal{L}^{\text{boson}}, \tag{64}$$

where $\mathcal{L}^{\text{cs}}$ is given by Eq. (1) and the boson term is

$$\mathcal{L}^{\text{boson}} = \sum_{j=1}^{2} [D_\mu(\phi_j) D^\mu(\phi_j) - m_0^2 (\phi_j)^2] - V(\phi_1(x), \phi_2(x)) \tag{65}$$

for two neutral scalar fields $\phi_j, j=1,2$ with a potential $V(\phi_1(x), \phi_2(x)) = \lambda_4(\phi_1^2(x) + \phi_2^2(x))^2 + \lambda_2(\phi_1^2(x) + \phi_2^2(x))$ with $m_0 \geq 0, \lambda_4 > 0$ and covariant derivative $D_\mu(\phi) = (\partial_\mu + ieA_\mu)(\phi)$. The usual canonical construction produces a Hamiltonian operator on the lattice of the form

$$H(V, \delta) = H_0^{\text{cs}} + H_0^{\text{boson}} + H_{int} + V(\phi_1, \phi_2), \tag{66}$$

with the free MCS-Hamiltonian in Eqs. (39) and (51) and a free boson-Hamiltonian with mass m_0. The interaction terms contain the MCS field as

$$H_{\text{int}} = H_{\text{el}} + H_{\text{mag}},$$

$$H_{\text{el}} = \sum_{x\in V} \delta^s [e\{\pi_1(x)\phi_2(x) - \pi_2(x)\phi_1(x)\} A_0(x)],$$

$$H_{\text{mag}} = \sum_{x\in V} \delta^s \left[e\{\partial_\ell \phi_2(x)\phi_1(x) - \partial_\ell \phi_1(x)\phi_2(x)\} A_\ell(x) + \frac{e^2}{2} \{(\phi_1^2(x) + \phi_2^2(x)\} A_\ell^2(x) \right],$$

$$V(\phi_1,\phi_2)=\sum_{x\in V}\delta^s V(\phi_1(x),\phi_2(x)). \tag{67}$$

Since in our representation the MCS-field is a normal operator, the "magnetic" part of the Hamiltonian has lost the positivity which would normally arise from the spatial covariant derivatives, while the "electric" part has both real and imaginary terms in its numerical range. Usually, to maintain positivity of the Hamiltonian operator for a gauge theory of this type, quantization would be carried out in either the Coulomb or axial gauges. However, such gauges are not particularly amenable for renormalization issues arising when taking the continuum limit of the lattice theory. In order to understand the structure of $H(V,\delta)$ above and make transparent the Krein transformations that we use below, we resort to transforming the annihilation and creation operators into harmonic oscillator coordinates and momenta. Our particular conventions are standard for the boson terms and which we shall say little about them, while those for the MCS-field are given in more detail. Both are described in the Appendix.

From Eq. (A13) in the Appendix, the Fourier components of $A_0(x)$ contain both skew-symmetric and symmetric terms. The first Krein transformation removes the symmetric terms in $A_0(x)$ by means of

$$T_1=\sum_{p\in\Gamma'}(-i)\sqrt{\frac{\omega}{\mu}}q^{\mathrm{cs}}_{\ell,2}(p)p^{\mathrm{cs}}_{\ell,0}(p), \tag{68}$$

while the second Krein transformation

$$T_2=\sum_{p\in\Gamma'}(-i)q^{\mathrm{cs}}_{\ell,0}(p)p^{\mathrm{cs}}_{\ell,1}(p) \tag{69}$$

removes the skew-symmetric terms from $A'_\ell(x)$ after a Krein unitary transformation using T_1. Each of the expressions above is realized as a sum of commuting essentially self-adjoint operators for which the finite particle vectors D_F are analytic vectors. Each is also skew-symmetric with respect to the Krein metric and so will be the infinitesimal generator of a Krein unitary but unbounded operator. The number of particle estimate for each T_j on a k-particle vector increases as $O((n+k+1)^n)$ in the analytic vector calculation, which leads to geometric convergence in t as below.

Lemma III.1: The operators $\widetilde{T}_j, j=1,2$ are self-adjoint and †-skew-symmetric. Further, each $\exp[t\widetilde{T}_j]$ is self-adjoint and †-unitary for real t and satisfies

$$e^{t\widetilde{T}_2}e^{t\widetilde{T}_1}\widetilde{A_0(x)}e^{-t\widetilde{T}_1}e^{-t\widetilde{T}_2}\Phi=(A_0(x)+t[T_1,A_0(x)])=A'_0(x;t)\Phi \tag{70}$$

$$e^{t\widetilde{T}_2}e^{t\widetilde{T}_1}\widetilde{A_\ell(x)}e^{-t\widetilde{T}_1}e^{-t\widetilde{T}_2}\Phi=\big(A_\ell(x)+t[T_1,A_\ell(x)]+t[T_2,A_\ell(x)]\big)\Phi=A'_\ell(x;t)\Phi \tag{71}$$

for all $\Phi\in D_F$ and complex t with $|t|<t_0$.

To begin the proof, notice that $\eta T_j\eta=T_j$ on vectors in D_F so by closure this relation is valid for $\widetilde{T}_j$. Nelson's theorem on analytic vectors shows $\eta e^{tT_j}\eta=e^{tT_j}$, proving the first statement.

For their Krein unitary property, consider $\Phi,\Psi\in D(e^{z\widetilde{T}_j})$ for suitable complex z and sequences of vectors Φ_n,Ψ_n which have compact support with respect to the spectrum of $\widetilde{T}_j$ and converge strongly to Φ,Ψ. Then, notice $T_j^\dagger=-T_j=\eta T_j^*\eta=\eta T_j\eta$ as bounded operators on Φ_n,Ψ_n, so

$$\begin{aligned}\{e^{z\widetilde{T}_j}\Phi,e^{z'\widetilde{T}_j}\Psi\}&=\lim_{n\to\infty}\{e^{z\widetilde{T}_j}\Phi_n,e^{z'\widetilde{T}_j}\Psi_n\}=\lim_{n\to\infty}(\Phi_n,e^{z\widetilde{T}_j}\eta e^{z'\widetilde{T}_j}\Psi_n)\\&=\lim_{n\to\infty}(\Phi_n,\eta e^{(z'-z)\widetilde{T}_j}\Psi_n)=\lim_{n\to\infty}\{\Phi_n,e^{(z'-z)\widetilde{T}_j}\Psi_n\}=\{\Phi,e^{(z'-z)\widetilde{T}_j}\Psi\}.\end{aligned}$$

For the commutator identities, set $\Phi_N=\Sigma_{n=0}^N(z^nT_1^n/n!)\Phi$, which converges strongly to $e^{z\widetilde{T}_1}\Phi$ for

$\Phi \in D_F$ and $|z| < z_0$. Each Φ_N is a finite particle vector belonging to the domain of $A_\mu(x)^k$ for any positive integer k and $\mu=0,1,2$, so we may calculate the expression

$$A_0(x)\Phi_N = \sum_{n=0}^{N} \frac{z^n A_0(x) T_1^n}{n!}\Phi = \sum_{n=0}^{N} \frac{z^n T_1^n}{n!} A_0(x)\Phi + z\sum_{n=0}^{N-1} \frac{z^n T_1^n}{n!}[T_1, A_0(x)]\Phi.$$

Taking the limit in N shows the right-hand side converges for $|z| < z_0$ with $e^{\widetilde{zT_1}}\Phi$ in the domain of the closure of $A_0(x)$ and $\widetilde{A_0(x)}e^{\widetilde{zT_1}}\Phi$ in the range of $e^{\widetilde{zT_1}}$ leading to Eq. (70) since T_2 commutes with $A_0'(x)$. A similar calculation results in Eq. (71)). A short calculation produces expressions for the gauge-transformed fields which for $t=1$ are

$$A_0'(x) = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma} \frac{\sqrt{2\omega}}{m} \{q_{1,0}^{\mathrm{cs}}(k)\cos(k\cdot x) + q_{2,0}^{\mathrm{cs}}(k)\sin(k\cdot x)\} \tag{72}$$

$$\begin{aligned} A_\ell'(x) = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma} \Bigg\{ & \left(\frac{2\epsilon_{\ell n} k_n}{\omega\sqrt{2\omega}} q_{2,1}^{\mathrm{cs}}(k) - \frac{2\mu k_\ell}{m\omega\sqrt{2\mu}} p_{2,2}^{\mathrm{cs}}(k) \right) \cos(k\cdot x) \\ & + \left(-\frac{2\epsilon_{\ell n} k_n}{\omega\sqrt{2\omega}} q_{1,1}^{\mathrm{cs}}(k) + \frac{2\mu k_\ell}{m\omega\sqrt{2\mu}} p_{1,2}^{\mathrm{cs}}(k) \right) \sin(k\cdot x) \Bigg\}, \end{aligned} \tag{73}$$

which are, respectively, skew-symmetric and symmetric.

Turning our attention to the Hamiltonian, we find a completely analogous result in

Lemma III.2: *For all* $\Phi \in D_F$ *and complex* t *with* $|t| < t_0$

$$e^{\widetilde{tT_2}} e^{\widetilde{tT_1}} \widetilde{H} e^{-\widetilde{tT_1}} e^{-\widetilde{tT_2}} \Phi = H'(V,\delta;t)\Phi$$

$$H'(V,\delta;t) = H_0^{\mathrm{boson}} + H_0^{\mathrm{cs}\prime}(t) + H_{\mathrm{int}}'(t), \tag{74}$$

where $H_{\mathrm{int}}'(t)$ *is* $H_{\mathrm{int}}(t)$ *with* $A_\mu(x)$ *replaced by* $A_\mu'(x;t)$ *and the gauge-transformed Chern-Simons part of the free Hamiltonian given by*

$$\begin{aligned} H_0^{\mathrm{cs}\prime}(t) = \sum_{k\in\Gamma} \Bigg\{ & \frac{(\mu^2 - t^2\omega^2)}{2} q_{\ell,2}^{\mathrm{cs}}(k)^2 - \mu + \frac{\omega}{2}(q_{\ell,1}^{\mathrm{cs}}(k)^2 - 4) + \frac{\left(\sqrt{\mu} p_{\ell,2}^{\mathrm{cs}}(k) - t\sqrt{\omega} p_{\ell,1}^{\mathrm{cs}}(k)\right)_2}{2} \\ & + t\omega q_{\ell,0}^{\mathrm{cs}}(k)\left(q_{\ell,1}^{\mathrm{cs}}(k) + \sqrt{\omega/\mu} q_{\ell,2}^{\mathrm{cs}}(k)\right) - t\sqrt{\omega\mu} p_{\ell,2}^{\mathrm{cs}}(k) p_{\ell,0}^{\mathrm{cs}}(k) + \omega(1-t) p_{\ell,0}^{\mathrm{cs}}(k) p_{\ell,1}^{\mathrm{cs}}(k) \\ & + (1-t^2)\frac{\omega}{2}(p_{\ell,0}^{\mathrm{cs}}(k)^2 - q_{\ell,0}^{\mathrm{cs}}(k)^2) + \frac{\omega}{2}(1-t^2) p_{\ell,1}^{\mathrm{cs}}(k)^2 \Bigg\} \end{aligned} \tag{75}$$

The statements for the domains of the unbounded operators are the same as for Lemma III.1 while calculations use the relation $e^{tT_2}e^{tT_1} S^2 e^{-tT_1}e^{-tT_2}\Phi = \{e^{tT_2}e^{tT_1} S e^{-tT_1}e^{-tT_2}\}^2\Phi$ for $|t| < t_0$, which is valid on D_F after taking closures. In each of Lemmas III.1 and III.2 the left-hand side is analytic in a disk $|t| < t_0$ while the right-hand side is an entire function of t and provides a unique analytic continuation of the operator on the left-hand side to the entire complex plane. However, it is straightforward to find a dense domain D_0 which is a common core for all these operators and their powers on which both sides of Eqs. (70), (71), and (74) are valid as entire functions in t. Consider a k-finite particle vector Φ_k realized as a normalized Hermite function $\Phi_k(\{q_{\ell,2}^{\mathrm{cs}}\},\{q_{\ell,1}^{\mathrm{cs}}\},q')$ in the q-harmonic oscillator variables with the coordinates appearing in $\{T_j | j=1,2\}$ denoted explicitly. Let $\chi \in C_0^\infty(R_+)$ be positive, 1 for $0 \le t \le 1/2$, and 0 for $t \ge 1$ say. Form the cutoff functions $\chi_{j,N}(q) = \chi(\Sigma_{k\in\Gamma,j} q_{\ell,j}^{cs}(k)^2/N^2)$ for $N=1,2,\ldots$ which have support inside a ball of radius N. Then, by taking products and convolutions in different variables, we find

Lemma III.3: *Let* D_0 *denote the linear span of vectors formed by*

$$\Phi_{k,N}(q) = \chi_{2,N}(q)(\chi_{1,N} * \Phi_k)(q) \tag{76}$$

as k and N vary over the positive integers. For each of the operators and their powers appearing in Lemmas III.1 and III.2, D_0 forms a common dense core. Moreover, each of the relations in Eqs. (70), (71), and (74) *is valid as entire analytic functions of t. In particular, the corresponding operator relations are densely defined on D_0 for $t=1$.*

That D_0 is dense and a common core is clear as is also the analyticity. Upon re-examining convergence of the exponential series in Eqs. (70), (71), and (74), the $q^{\mathrm{cs}}_{\ell,2}(k)$ and $p^{\mathrm{cs}}_{\ell,1}(k)$ operators are bounded by N when acting on vectors in D_0 while the N-particle estimates applied to the operators $q^{\mathrm{cs}}_{\ell,0}(k)$ and $p^{\mathrm{cs}}_{\ell,0}(k)$ acting on Φ_k provide a bound $O((n+k+1)^{n/2})$. Vectors in D_0 are now entire vectors for each of the Krein gauge transformations.

The gauge transformations in Lemma III.2 are "natural" for the Hamiltonian $H(V,\delta)$, as may be seen from

$$\tilde{H}e^{itT_j}\Phi_{k,N} = e^{itT_j}\{H + it[H,T_j] + (it)^2/2[[H,T_j],T_j]\}\Phi_{k,N}, \tag{77}$$

with $\Phi_{k,N} \in D_0$ and $-\infty < t < \infty$. By using a Riemann approximation and then taking strong limits, the right-hand side converges and defines convergence of the left-hand side to the relation

$$\begin{aligned}\tilde{H}\int_{-\infty}^{\infty} F(\lambda)dE_j(\lambda)\Phi_{k,N} &= \int_{-\infty}^{\infty} \widetilde{F(t)}\tilde{H}e^{itT_j}\Phi_{k,N}dt \\ &= \int_{-\infty}^{\infty} F(\lambda)dE_j(\lambda)H\Phi_{k,N} + \int_{-\infty}^{\infty} F'(\lambda)dE_j(\lambda)[H,T_j]\Phi_{k,N} \\ &\quad + \int_{-\infty}^{\infty} F''(\lambda)/2dE_j(\lambda)[[H,T_j],T_j]\Phi_{k,N},\end{aligned} \tag{78}$$

where $\{E_j(\lambda)\}$ is the spectral measure associated with the essentially self-adjoint operator T_j. Choosing $F \in C_0^2(R)$ shows that a large class of the bounded functions of $\widetilde{T_j}$ belongs to the domain of $\tilde{H}$. As we shall show in Sec. V, the Hamiltonians $H(V,\delta)$ and $H'(V,\delta;1)$ give Krein equivalent dynamics.

IV. REAL PART OF THE HAMILTONIAN

Following the Krein gauge transformations in the previous section, all operators in the remainder of this article will take their physical values at $t=1$. The transformed Hamiltonian is thereby split into two parts. One part defines a symmetric operator while the other part defines a skew-symmetric operator. We now show that the symmetric part is bounded below and in fact is essentially self-adjoint; hence the transformed Hamiltonian is accretive. The transformed lattice Hamiltonian operator may be recast as

$$H'(V,\delta) = H_0^{\mathrm{cs}\prime} + H_0^{\mathrm{boson}} + V(\phi_1,\phi_2) + H'_{\mathrm{int}}. \tag{79}$$

To exploit positivity in the real part of the Hamiltonian, it is convenient to remove the gradient terms from H_0^{boson} and rewrite this as

$$H_0^{\mathrm{boson}} = H_0^{\mathrm{boson}\prime} + \sum_{x\in V}\frac{\delta^s}{2}[\nabla\phi_j(x)]^2, \tag{80}$$

in which

$$H_0^{\text{boson}'} = \sum_{k\in\Gamma} \frac{1}{2}[p_{j,\ell}^2(k) + m_0^2 q_{j,\ell}^2(k) - 4\mu(k)] \tag{81}$$

is again a free massive harmonic oscillator which on the lattice acts in the same way as a number operator for determining domains. By reincorporating the gradient terms into the covariant derivative, the real part of $H'(V,\delta)$ takes the form

$$\text{Re}\, H'(V,\delta) + c_1 I = X + Y, \tag{82}$$

where c_1 is a positive constant to be chosen later and

$$X = H_0^{\text{cs}\prime\prime} + H_0^{\text{boson}\prime} + c_1 I, \quad Y = Y_{\text{deg}} + Y_+, \tag{83}$$

with

$$Y_{\text{deg}} = \sum_{k\in\Gamma} [-\sqrt{\mu\omega} p_{\ell,1}^{\text{cs}}(k) p_{\ell,2}^{\text{cs}}(k)] \tag{84}$$

and

$$Y_+ = \sum_{x\in V} \frac{\delta^s}{2}[\{\partial_\ell \phi_1(x) - e\phi_2(x)A_\ell(x)\}^2 + \{\partial_\ell \phi_2(x) + e\phi_1(x)A_\ell(x)\}^2] + V(\phi_1,\phi_2). \tag{85}$$

The operator $H_0^{\text{cs}\prime\prime}$ denotes the real part of $H_0^{\text{cs}\prime}$ with the degeneracy producing term Y_{deg} removed. As a sum of squares of symmetric operators which have dense analytic vectors, Y_+ clearly defines a symmetric operator which is bounded below since the Higgs potential is taken to be bounded below. The degenerate quadratic term Y_{deg} will be treated as a perturbation which is of the same size as the Chern-Simons number operator. Following the notation used in Reed and Simon (Ref. 16, p. 174–176 and Theorem X.14, p. 164), it is a straightforward matter to use the Konrady trick for Y_+ with $Z = c_2 X^2$ to obtain the quadratic estimate

$$Z^2 \le (X + Y + Z)^2 + c_3 I \tag{86}$$

for some positive constant c_3. The degenerate quadratic piece changes none of the estimates for the commutator $[X,[X,Y]]$ and is easily bounded in the term $XY_{\text{deg}}X$ by completing the square as

$$Y_{\text{deg}} = \sum_{k\in\Gamma} \frac{1}{2}[-\mu p_{\ell,2}^{\text{cs}\,2}(k) - \omega p_{\ell,1}^{\text{cs}\,2}(k) + (\sqrt{\mu} p_{\ell,2}^{\text{cs}}(k) - \sqrt{\omega} p_{\ell,1}^{\text{cs}}(k))^2] = -Y_{\text{deg},1} + Y_{\text{deg},+}, \tag{87}$$

whereupon $XY_{\text{deg},+}X \ge 0$ and may be discarded with the other positive terms in obtaining the quadratic estimate above. The terms in $Y_{\text{deg},1}$ are canceled by terms that appear in $H_0^{\text{cs}\prime\prime}$ with the result $H_0^{\text{cs}\prime\prime} - Y_{\text{deg},1} \ge 0$. Now we find

$$2c_2X^3 + 2c_2XYX \ge 2c_2X[X + Y_+ + Y_{\text{deg},+} - Y_{\text{deg},1}]X \ge 2c_2X[H_0^{\text{boson},\prime} + c_1 I]X,$$

so

$$2c_2X^3 + 2c_2XYX + c_2[X,[X,Y]] \ge c_2(2c_1 - c_3)X^2 \ge 0 \tag{88}$$

provided we choose $c_1 \ge c_3/2$. The quadratic estimate and Wüst's theorem allow us to conclude that $\text{Re}\, H'(V,\delta) + c_1 I = X + Y$ is essentially self-adjoint and bounded below. It is important to notice that the term $2c_2XH_0^{\text{boson},\prime}X$ is a large positive operator and only its positivity is needed for the estimate (86). In fact, we have the sharper estimate

$$(X + Y + Z)^2 \ge Z^2 + c_2(2c_1 - c_3)X^2 + 2c_2XH_0^{\text{boson},\prime}X \ge Z^2 \tag{89}$$

on $D_F \times D_F$, which is used in the next section.

V. SKEW-SYMMETRIC PART OF THE HAMILTONIAN

The Krein transformations in Sec. III were chosen to obtain a Hamiltonian of the form

$$H'(V,\delta) = \mathrm{Re}\, H'(V,\delta) + S, \tag{90}$$

in which S is a densely defined skew-symmetric operator given by

$$S = S_1 + S_2,$$

where

$$S_1 = \sum_{x\in V} \delta^s e[\pi_1\phi_2 - \pi_2\phi_1](x)A_0'(x), \tag{91}$$

$$S_2 = \sum_{k\in\Gamma}\left[\omega(k)q^{\mathrm{cs}}_{\ell,0}(k)\left\{q^{\mathrm{cs}}_{\ell,1}(k) + \sqrt{\frac{\omega}{\mu}}q^{\mathrm{cs}}_{\ell,2}(k)\right\} - \sqrt{\omega\mu}p^{\mathrm{cs}}_{\ell,0}(k)p^{\mathrm{cs}}_{\ell,2}(k)\right]. \tag{92}$$

As $\mathrm{Re}\, H'(V,\delta)$ is essentially self-adjoint and bounded below, Chernoff's extension of Wüst's theorem[20] will show that $H'(V,\delta)$ is essentially maximal accretive given the estimate

$$\|Zu\| \le \|(X+Y+Z+S)u\| + c_5 I\|u\|$$

for vectors u in the core domain D_F, or equivalently

$$(Z)^2 \le (X+Y+Z)^2 + [X+Y+Z,S] + S^*S + c_5 I \tag{93}$$

as a quadratic form on $D_F \times D_F$. Using the estimate of the last section, it will then be sufficient to verify

$$c_2(2c_1 - c_3)X^2 + 2c_2 X H_0^{\mathrm{boson}\prime} X + [X+Y+Z,S] + S^*S + c_5 I \ge 0, \tag{94}$$

which follows from

Lemma V.1: *On the domain* D_F, *the commutator* $[X+Y+Z,S]$ *is Kato-tiny relative to* $XH_0^{\mathrm{boson}\prime}X$.

To prove the lemma we calculate individual terms in the commutator. From $[Z,S] = c_2[X^2,S] = c_2(X[X,S]+[X,S]X)$ since X acts as a free Hamiltonian, $[X,S]$ is bounded by $H_0^{\mathrm{boson}\prime}X^{1/2}$, while [Z,S] is bounded by $H_0^{\mathrm{boson}\prime}X^{3/2}$. Both of these are Kato-tiny relative to $2c_2XH_0^{\mathrm{boson}\prime}X$. In $X+Y$ let us recombine the gradient boson terms in Y with the boson terms in X to replace $H_0^{\mathrm{boson}\prime}$ by H_0^{boson} leading to $X+Y = H_0^{\mathrm{cs}\prime} + H_0^{\mathrm{boson}} + c_1 I + Y_{\mathrm{deg}} + Y_0$, where the "magnetic part" of the Chern-Simons interaction now appears with the boson potential in

$$\begin{aligned} Y_0 &= \sum_{x\in V}\frac{\delta^s}{2}\left[-e\{\partial_\ell\phi_1(x)\phi_2(x) - \partial_\ell\phi_2(x)\phi_1(x)\}A'_\ell(x) + \frac{e^2}{2}\{\phi_1^2(x)+\phi_2^2(x)\}A'_\ell(x)^2\right] + V(\phi_1,\phi_2) \\ &= Y_{\mathrm{mag}} + V(\phi_1,\phi_2). \end{aligned} \tag{95}$$

Clearly $[Y_{\mathrm{deg}},S_1]=0$, with the remaining terms for this part of the commutator given by

$$[Y_{\mathrm{deg}},S_2] = \sum_{k\in\Gamma}[-i\sqrt{\mu}\omega^{3/2}q^{\mathrm{cs}}_{\ell,0}(k)p^{\mathrm{cs}}_{\ell,2}(k) - i\omega^2 q^{\mathrm{cs}}_{\ell,0}(k)p^{\mathrm{cs}}_{\ell,1}(k)]. \tag{96}$$

on the core domain, $-[Y_{\mathrm{deg}},S] \le c_6 X$ for c_1 large enough as the commutator is quadratic in Chern-Simons harmonic oscillators. It is useful to look at the commutators in $[Y_{\mathrm{mag}},S]$ separately. For $[Y_{\mathrm{mag}},S_1]$ the fields A_0' and A_ℓ' commute so it is only necessary to calculate the boson field commutators. Lattice quantization preserves enough locality for the boson fields that for terms quadratic in the individual boson fields, the relation $[\phi_j^2(x),\pi_j(y)] = 2i\delta_{P,V}(x-y)\phi_j(x)$ with the periodic lattice $\delta_{P,V}$ shows their contribution to $[Y_{\mathrm{mag}},S_1]$ vanishes. As we use a symmetric $k\leftrightarrow$

$-k$ summation range, it is possible to effect an integration by parts of sorts; nevertheless, the remaining terms in this commutator are not zero and we arrive at

$$[Y_{\mathrm{mag}},S_1]=\sum_{x\in V}\delta^s ie^2[\partial_\ell\phi_1(x)\phi_1(x)+\partial_\ell\phi_2(x)\phi_2(x)]A'_\ell(x)A'_0(x)$$
$$+\sum_{x\in V}\delta^{2s}(-ie^2)[\partial_{x,\ell}\delta_{P,V}(x-y)\phi_1(x)\phi_1(y)]A'_\ell(x)A'_0(x)$$
$$+\sum_{x\in V}\delta^{2s}(-ie^2)[\partial_{x,\ell}\delta_{P,V}(x-y)\phi_2(x)\phi_2(y)]A'_\ell(x)A'_0(x). \tag{97}$$

Using $H_0^{\mathrm{boson}\prime}$ to bound $\phi_j(x)\phi_j(y)$ and X to bound $A'_\ell(x)A'_0(x)$, the commutator $-[Y_{\mathrm{mag}},S_1]\leq c_7H_0^{\mathrm{boson}\prime}X$, which is also Kato-tiny compared to $H_0^{\mathrm{boson}\prime}X^2$. Up to multiplicative terms quadratic in the boson fields, the size of the commutator $[Y_{\mathrm{mag}},S_2]$ is determined by $[A'_\ell,S_2]$. From the Landau gauge expression for $A'_\ell(x)$ in Sec. III, it is straightforward to arrive at the expression

$$[A'_\ell(x),S_2]=\frac{1}{\sqrt{|V|}}\sum_{k\in\Gamma}\left[\left\{-i\frac{\sqrt{2\omega}}{m}k_\ell q^{\mathrm{cs}}_{2,0}(k)\right\}\cos(k\cdot x)+\left\{i\frac{\sqrt{2\omega}}{m}k_\ell q^{\mathrm{cs}}_{1,0}(k)\right\}\sin(k\cdot x)\right], \tag{98}$$

which is dominated by $H_0^{\mathrm{boson}\prime}X^{1/2}$. Hence, the quadratic term $[A'^2_\ell(x),S_2]$ requires an additional factor $X^{1/2}$ to produce the estimate $-[Y_{\mathrm{mag}},S_2]\leq c_8H_0^{\mathrm{boson}\prime}X$, which is also Kato-tiny relative to $H_0^{\mathrm{boson}\prime}X^2$.

Finally $[V(\phi_1,\phi_2),S]=0$. This is immediate for $[V(\phi_1,\phi_2),S_2]=0$, while the commutator identities

$$[\phi_j(x)^4,\pi_j(y)]=4i\delta_{P,V}(x-y)\phi_j(x)^3$$

$$[\phi_1^2(x)\phi_2^2(x),\pi_1(y)]=2i\delta_{P,V}(x-y)\phi_1(x)\phi_2^2(x)$$

readily show that $[V(\phi_1,\phi_2),S_1]=0$ as well. Collecting together these estimates for the various commutators leads to the inequality

$$(X+Y+Z)^2+[X+Y+Z,S]\geq Z^2-c_5I \tag{99}$$

for some constant $c_5>0$ provided c_2 is large enough and $c_1>c_3/2$. As $(X+Y+Z)^*$ and Z^* are densely defined on the finite particle vectors, Chernoff's theorem applied to $X+Y+S=X+Y+Z+S-Z$ produces:

Theorem V.2: *After Krein gauge transformations, the transformed Hamiltonian* $H'(V,\delta)=\mathrm{Re}\,H'(V,\delta)+S$ *is maximal accretive after closure on the finite particle domain* D_F *and hence Krein essentially self-adjoint.*

Krein self-adjointness follows by a simple argument which can be found in Ref. 21, Lemma 2.2, p. 5.

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APPENDIX: HARMONIC OSCILLATOR COORDINATES

We choose standard harmonic oscillator coordinates for the time-zero boson field and its conjugate momentum, yielding (see, e.g., Ref. 22, Chap. II, Sec. B])

$$\phi_j(x) = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma} \frac{1}{2\mu}[e^{ik\cdot x} a_j(k) + e^{-ik\cdot x} a_j^*(k)] = \frac{1}{\sqrt{2|V|}} \sum_{k\in\Gamma} \frac{1}{2\mu}[q_{1,j}(k)\cos(k\cdot x) + q_{2,j}(k)\sin(k\cdot x)], \tag{A1}$$

$$\pi_j(x) = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma} \frac{-i}{2}[e^{ik\cdot x} a_j(k) - e^{-ik\cdot x} a_j^*(k)] = \frac{1}{\sqrt{2|V|}} \sum_{k\in\Gamma} \frac{1}{2\mu}[p_{1,j}(k)\cos(k\cdot x) + p_{2,j}(k)\sin(k\cdot x)], \tag{A2}$$

for $j=1,2$. The free boson Hamiltonian with Wick ordering then becomes

$$H_0^{\text{boson}} = \sum_{k\in\Gamma} \frac{1}{2} a_j^*(k) a_j(k) = \sum_{k\in\Gamma} \frac{1}{2}[p_{\ell,j}^2 + \mu^2 q_{\ell,j}^2]. \tag{A3}$$

In order to define harmonic oscillator coordinates for the MCS field $A_\mu = V_\mu + S_\mu$ in Landau gauge ($\gamma=1$), we first express the MCS field in terms of Fock operators b_μ defined by

$$b_0(k) = \frac{c_0(k)}{\sqrt{2\omega}}, \quad b_1(k) = \frac{k_n c_n(k)}{\omega\sqrt{2\omega}}, \quad b_2(k) = \frac{a(k)}{\sqrt{2\mu}}, \tag{A4}$$

so that b_0, b_1 represent the ghost degrees of freedom while b_2 corresponds to the single physical mode. In terms of these, we have for the time-zero MCS field

$$A_\mu = \frac{1}{\sqrt{|V|}} \sum_{k\in\Gamma} [M_{\mu\nu} b_\nu(k) e^{ik\cdot x} + \bar{M}_{\mu\alpha}(-g)_{\alpha\beta} b_\beta^*(k) e^{-ik\cdot x}], \tag{A5}$$

with

$$M = \begin{pmatrix} -\dfrac{\omega}{m\sqrt{2\omega}} & 0 & -\dfrac{\omega}{m\sqrt{2\mu}} \\ -\dfrac{1}{\sqrt{2\omega}}\left(\dfrac{k_1}{m} - \dfrac{ik_2}{\omega}\right) & \dfrac{-ik_2}{\omega\sqrt{2\omega}} & -\dfrac{1}{\sqrt{2\mu}}\left(\dfrac{\mu k_1}{m\omega} - \dfrac{ik_2}{\omega}\right) \\ -\dfrac{1}{\sqrt{2\omega}}\left(\dfrac{k_2}{m} + \dfrac{ik_1}{\omega}\right) & \dfrac{ik_1}{\omega\sqrt{2\omega}} & -\dfrac{1}{\sqrt{2\mu}}\left(\dfrac{\mu k_2}{m\omega} + \dfrac{ik_1}{\omega}\right) \end{pmatrix}. \tag{A6}$$

Note the appearance of the indefinite metric in the second term of (A5). We define Krein operators $a_\mu = -b_\mu$ and $a_\mu^\dagger = g_{\mu\beta} b_\beta^*$. It is in terms of these that we define our harmonic oscillator coordinates for the MCS field,

$$q_{1,\mu}^{\text{cs}}(k) = \frac{1}{2}[a_\mu(k) + a_\mu^\dagger(k) + a_\mu(-k) + a_\mu^\dagger(-k)], \tag{A7}$$

$$q_{2,\mu}^{\text{cs}}(k) = \frac{i}{2}[a_\mu(k) - a_\mu^\dagger(k) - a_\mu(-k) + a_\mu^\dagger(-k)], \tag{A8}$$

$$p_{1,\mu}^{\text{cs}}(k) = \frac{i}{2}[a_\mu(k) - a_\mu^\dagger(k) + a_\mu(-k) - a_\mu^\dagger(-k)], \tag{A9}$$

$$p_{2,\mu}^{\text{cs}}(k) = \frac{1}{2}[-a_\mu(k) - a_\mu^\dagger(k) + a_\mu(-k) + a_\mu^\dagger(-k)]. \tag{A10}$$

These satisfy the relations

$$q^{\mathrm{cs}}_{\ell,\mu}(-k) = (-1)^{\ell+1} q^{\mathrm{cs}}_{\ell,\mu}(k) \quad \text{and} \quad p^{\mathrm{cs}}_{\ell,\mu}(-k) = (-1)^{\ell+1} p^{\mathrm{cs}}_{\ell,\mu}(k). \tag{A11}$$

Thus, upon restriction to "allowed" momenta $k, k' \in \Gamma'$, we have the commutation relations

$$[q^{\mathrm{cs}}_{\ell,\mu}(k), p^{\mathrm{cs}}_{n,\nu}(k')] = i g_{\mu\nu} \delta_{\ell n} \delta_{k,k'}. \tag{A12}$$

This leads to the following expressions for the time-zero MCS field in Landau gauge:

$$A_0(x) = \frac{1}{\sqrt{|V|}} \sum_{k \in \Gamma'} \left\{ \cos(k \cdot x) \left[\frac{2\omega}{m\sqrt{2\omega}} q^{\mathrm{cs}}_{1,0}(k) + \frac{2\omega}{m\sqrt{2\mu}} q^{\mathrm{cs}}_{1,2}(k) \right] + \sin(k \cdot x) \left[\frac{2\omega}{m\sqrt{2\omega}} q^{\mathrm{cs}}_{2,0}(k) + \frac{2\omega}{m\sqrt{2\mu}} q^{\mathrm{cs}}_{2,2}(k) \right] \right\},$$

$$\begin{aligned} A_\ell(x) = \frac{1}{\sqrt{|V|}} \sum_{k \in \Gamma'} \Bigg\{ & \cos(k \cdot x) \left[-\frac{2k_\ell}{m\sqrt{2\omega}} p^{\mathrm{cs}}_{2,0}(k) - \frac{2\mu k_\ell}{m\omega\sqrt{2\mu}} p^{\mathrm{cs}}_{2,2}(k) \right. \\ & \left. - \frac{2\epsilon_{\ell n} k_n}{\omega} \left(\frac{q^{\mathrm{cs}}_{2,0}(k)}{\sqrt{2\omega}} - \frac{q^{\mathrm{cs}}_{2,1}(k)}{\sqrt{2\omega}} + \frac{q^{\mathrm{cs}}_{2,2}(k)}{\sqrt{2\mu}} \right) \right] \\ & + \sin(k \cdot x) \left[\frac{2k_\ell}{m\sqrt{2\omega}} p^{\mathrm{cs}}_{1,0}(k) + \frac{2\mu k_\ell}{m\omega\sqrt{2\mu}} p^{\mathrm{cs}}_{1,2}(k) \right. \\ & \left. + \frac{2\epsilon_{\ell n} k_n}{\omega} \left(\frac{q^{\mathrm{cs}}_{1,0}(k)}{\sqrt{2\omega}} - \frac{q^{\mathrm{cs}}_{1,1}(k)}{\sqrt{2\omega}} + \frac{q^{\mathrm{cs}}_{1,2}(k)}{\sqrt{2\mu}} \right) \right] \Bigg\}. \end{aligned} \tag{A13}$$

For the free MCS Hamiltonian in Landau gauge with Wick ordering, this leads to

$$\begin{aligned} H^{\mathrm{cs}}_0 = \sum_{k \in \Gamma'} \Bigg\{ & -\frac{\omega}{2} (p^{\mathrm{cs}}_{\ell,0}(k) p^{\mathrm{cs}}_{\ell,0}(k) + q^{\mathrm{cs}}_{\ell,0}(k) q^{\mathrm{cs}}_{\ell,0}(k)) + \frac{\omega}{2} (p^{\mathrm{cs}}_{\ell,1}(k) p^{\mathrm{cs}}_{\ell,1}(k) + q^{\mathrm{cs}}_{\ell,1}(k) q^{\mathrm{cs}}_{\ell,1}(k)) \\ & + \frac{\mu}{2} (p^{\mathrm{cs}}_{\ell,2}(k) p^{\mathrm{cs}}_{\ell,2}(k) + q^{\mathrm{cs}}_{\ell,2}(k) q^{\mathrm{cs}}_{\ell,2}(k)) \Bigg\}. \end{aligned} \tag{A14}$$

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Large chiral diffeomorphisms on Riemann surfaces and $\mathcal{W}$-algebras

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The diffeomorphism action lifted on truncated (chiral) Taylor expansion of a complex scalar field over a Riemann surface is presented in the paper under the name of large diffeomorphisms. After an heuristic approach, we show how a linear truncation in the Taylor expansion can generate an algebra of symmetry characterized by some structure functions. Such a linear truncation is explicitly realized by introducing the notion of Forsyth frame over the Riemann surface with the help of a conformally covariant algebraic differential equation. The large chiral diffeomorphism action is then implemented through a Becchi-Rouet-Stora (BRS) formulation (for a given order of truncation) leading to a more algebraic setup. In this context the ghost fields behave as holomorphically covariant jets. Subsequently, the link with the so-called $\mathcal{W}$-algebras is made explicit once the ghost parameters are turned from jets into tensorial ghost ones. We give a general solution with the help of the structure functions pertaining to all the possible truncations lower or equal to the given order. This provides another contribution to the relationship between Korteweg-de Vries (KdV) flows and $\mathcal{W}$-diffeomorphims. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The notion of symmetry gives a structure to spacetime (or configuration space) and/or internal spaces of the model under consideration, in the sense that the former is closely related to a geometrical setup.

At the infinitesimal level, the concept of algebra turns out to be very useful. It generally gives rise to a solution when the linearity is fulfilled. In the nonlinear situation, however, we sometimes have to explore further behind the first infinitesimal transformation step.

The development of nonlinear sciences has supported these needs,[1] and many basic physical systems were described by nonlinear extensions of algebras. This is the case for integrable systems, two-dimensional conformal models (with application to strings, gravity, or solid state physics, see e.g., Ref. 2).

Particular interest has been devoted to the so-called $\mathcal{W}$-algebras,[3] which come out from different principles,[4–6] and the question of their geometric origin still remains unclear or unsatisfactory despite various attempts given in Refs. 5 and 7–11.

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In particular, the relationship between a conformally covariant sth-order differential equation

$$(\partial_{(s)} + a^{(s)}_{(2)}(z,\bar{z})\partial_{(s-2)} + \cdots + a^{(s)}_{(s)}(z,\bar{z}))f(z,\bar{z}) = 0,$$

over a generic Riemann surface and some of the so-called $\mathcal{W}$-algebra has been well established for 15 years.[6] The differential equations can be thought of as equations of motion for some matter fields. The former can also be derived as vanishing covariant derivative condition,[12] and to some extent, more general $\mathcal{W}$-algebra such as the Bershadsky one[13] can be related to a system of conformally covariant coupled differential equations.

Focusing here only on one sth-order differential equation, one may either work directly with the solutions or with uniformizing coordinates considered as ratios of linear independent solutions.[14,8] It turns out to be a matter of taste of working either with homogeneous coordinates or inhomogeneous ones on $\mathbb{C}P^{s-1}$. However, in his textbook,[14] Forsyth uses rather inhomogeneous coordinates in order to get some differential invariants. The inhomogeneous coordinates have to satisfy $s+1$th-order equations. Accordingly, our point of view proposed in Ref. 15 traced back in the literature, found an unexpected origin in the past[14] related to some algebraic type differential equations, once covariantly formulated over a generic Riemann surface. Indeed the definition of general well-defined differential operators over a (two-dimensional) Riemann surface requires some care,[16] and puts forward a deep insight into the links between covariance required by physical considerations and projective geometry. Related studies of projectively invariant differential operators as well differential invariants can be found in Ref. 17.

In Ref. 15 the notion of Laguerre-Forsyth frames was promoted. In order to avoid possible confusion with the named Laguerre-Forsyth form of a conformally covariant differential equation,[8] in the present paper, we adopt the name Forsyth frames. We simply have in mind the ideas of, first, pursuing further the method given by Forsyth in Ref. 14, and second, dealing with scalar coordinates considered as solutions of generalized Beltrami equations (see, e.g., Ref. 8 or 18 Appendix C2) just about the approach given in Refs. 8 and 10. Our motivation for using the inhomogeneous coordinates rests on the fact that they seem to be more natural for constructing projective invariants—projective action of $\mathrm{SL}(s,\mathbb{C})$ on $\mathbb{C}P^{s-1}$. In general,[19] the smooth coefficients in the above-noted sth-order covariant differential equation have been proven to be projectively invariant. Inhomogeneous coordinates are the local coordinates for projective curves in $\mathbb{C}P^{s-1}$ on which there is a symplectic structure related to the Gelfand-Dickey brackets.[20,19] Moreover, inhomogeneous coordinates offer the possibility to work with scalar fields instead of densities.

In Ref. 15, these Forsyth frames were thus made of coordinate scalar fields on some finite dimensional target space and constructed from solutions of a finite order holomorphically covariant linear differential equation over a Riemann surface of the above-mentioned type. At the quantum level, these scalar fields surprisingly have already gained at the one-loop level a noncommutative character. This phenomenon gives a quantum origin to a noncommutative structure on the target space. The noncommutativity came out by anomaly cancellation as a nonlocal effect.

The basic novelties of these Forsyth frames lie in their nontrivial properties under differentiations, which allow one to expand beyond first order the holomorphic reparametrization process still maintaining the algebra closure property. Thus investigating this type of extended algebra appears as a necessity, since this "new" structure encapsulates the (general) covariance laws.

In this paper, the construction of Forsyth frames is proposed in great detail and it strongly relies on a symmetry principle. The latter will be systematically studied in the algebraic Becchi-Rouet-Stora (BRS) language more suitable for a possible field theoretical treatment of the model.

The paper is organized as follows. Section II goes over some motivations for this extended notion of symmetry, beyond linearity. It requires the use of higher order derivatives and the closure of the algebra obliges one to introduce new fields which will play the role of structure functions for the (nonlinear) reduced symmetry algebra. Section III is devoted to the definition of the Forsyth frames and to a deep study of their properties. In Sec. IV, a convenient BRS approach is presented for the algebra of symmetry. It will be useful for improving in particular the covariance laws which come out from these properties. Section V treats the covariance under holomorphic change charts of the algebra elements. Nontensorial structures (jet) come out, in particular

under the form of jet-BRS ghosts which are harmful for physical considerations since covariant quantities are required. A rather tricky link with tensorial ghosts is presented as a change of basis of generators. Section VI gives a way (using all the differential properties of the Forsyth frames, including the ones of the subframes encapsulated into the maximal one) to decompose into tensors the jet-BRS ghosts. The process is obviously defined up to a tensorial rescaling. Some detailed examples are given and illustrate the striking property of canceling out the effects of all the subframes, in favor of a standard presentation of the $\mathcal{W}$-algebra structure. Exploiting some known results in the literature[10] allows one to clarify the algorithm. We conclude in Sec. VII.

II. MOTIVATIONS

The issue of finding the most general expression of a spacetime symmetry can find an answer in the concept of generalized frames, perhaps rather than that of prolongated frames whose local expression is obtained by successive derivations.[21] In order to consider such objects, let us first think of the Fock space of some smooth complex scalar field Z defined over a given Riemann surface Σ, endowed with a complex analytic (holomorphic) structure; this requires the use of local complex coordinates $(z,\bar{z})$. Smoothness of the complex scalar field $Z=Z(z,\bar{z})$ is understood with respect to the differential structure on Σ with which the complex structure is subordinated to. From the locality principle, recall that the Fock space for Z is generated by all the z and $\bar{z}$ derivatives of any order considered as independent monomials.

Consider now the infinitesimal action of smooth diffeomorphisms on Σ which is usually expressed by means of the Lie derivative $L_\xi Z=(\xi(z,\bar{z})\partial+\bar{\xi}(z,\bar{z})\bar{\partial})Z$.

With respect to the complex structure we shall be concerned with the so-called "chiral" diffeomorphisms acting on the complex scalar field Z which consist in separating the Lie derivative according to z-derivative, so that $Z\to Z+\xi\partial Z$; there is the complex conjugate expression as well. Denoting in the Fock space the various z-derivatives of order ℓ by $\partial_{(\ell)}Z$, $\ell=1,2,\ldots$ one wants to consider a fully chiral local variation for the complex scalar field Z (going thus beyond the first order) of the following type:

$$(\delta Z)(z,\bar{z})=\sum_{\ell\geqslant 1}\gamma^{(\ell)}(z,\bar{z})\partial_{(\ell)}Z(z,\bar{z}), \tag{2.1}$$

together with the complex conjugate expression, and into which all the z-derivatives appear.

Hence, constructing a local field theory over $\mathbb{C}$ amounts to working *a priori* on local functionals in the various z-derivatives of Z. So to speak, the physical model is built over the infinite z-frames which is locally represented by $(Z(z,\bar{z}),\partial Z(z,\bar{z}),\partial_{(2)}Z(z,\bar{z}),\ldots)$, which reproduces the "chiral" Taylor expansion of the field Z (i.e., only with respect to the z-coordinate) at the point $(z,\bar{z})$ of Σ, in other words, the infinite jet of Z.

What is called large chiral diffeomorphisms in the paper is the lifted action of usual local chiral diffeomorphisms on $\mathbb{C}$ to the infinite jet space $J^\infty(\mathbb{C},\mathbb{C})$, i.e., on the z-Taylor expansion. The former are viewed as transformations acting on the complex scalar field Z itself and they require, on the one hand, infinitely many local parameters $\gamma^{(\ell)}$ of conformal type $(-\ell,0)$ which generalize vector fields of type $(-1,0)$, and, on the other hand, any higher order derivatives of Z.

Accordingly, it is called a large chiral diffeomorphism symmetry the invariance of some observables or functional on $J^\infty(\mathbb{C},\mathbb{C})$ under the transformation (2.1). Translating this problem of symmetry on the space of local functionals in the infinite jet of the scalar field Z,

$$\delta Z(z,\bar{z})=\left(\sum_{\ell\geqslant 1}\int_{\mathbb{C}}d\bar{w}\wedge dw\,\gamma^{(\ell)}(w,\bar{w})\mathcal{W}_{(\ell)}(w,\bar{w})\right)Z(z,\bar{z}), \tag{2.2}$$

amounts to introducing local Ward operators associated to the local parameters $\gamma^{(\ell)}$,

$$\mathcal{W}_{(\ell)}(z,\bar{z}) = \partial_{(\ell)} Z(z,\bar{z}) \frac{\delta}{\delta Z(z,\bar{z})} \quad \text{for } \ell \geqslant 1, \tag{2.3}$$

which generate an infinite dimensional Lie algebra. But note that the only Lie subalgebra is for $\ell=1$ of which the bracket (as tensorial product of distributions) writes

$$\begin{aligned}\left[\mathcal{W}_{(1)}(z,\bar{z}),\mathcal{W}_{(1)}(w,\bar{w})\right] &= \mathcal{W}_{(1)}(z,\bar{z})\partial_w\delta(w-z) - \mathcal{W}_{(1)}(w,\bar{w})\partial_z\delta(z-w)\\ &= \mathcal{W}_{(1)}(w,\bar{w})\partial_w\delta(w-z) - \mathcal{W}_{(1)}(z,\bar{z})\partial_z\delta(z-w)\end{aligned} \tag{2.4}$$

and translates by duality the Lie algebra structure of vector fields to the functional level, namely, if $W_1(\xi)=\langle \mathcal{W}_1 | \xi\rangle$ then

$$\begin{aligned}[W_1(\xi),W_1(\eta)] &= \langle [\mathcal{W}_{(1)}(z,\bar{z}),\mathcal{W}_{(1)}(w,\bar{w})] | \xi(z,\bar{z})\,\eta(w,\bar{w})\rangle\\ &= \langle \mathcal{W}_1 | \eta\,\partial\,\xi - \xi\,\partial\,\eta\rangle = \langle \mathcal{W}_1 | [\eta,\xi]\rangle = W_1([\eta,\xi])\end{aligned} \tag{2.5}$$

and thus reproduces the bracket between the parameters of usual conformal transformations. (The pairing $\langle|\rangle$ stands for the functional evaluation of distributions.) In full generality, the brackets for $k,\ell \geqslant 1$ read

$$[\mathcal{W}_{(k)}(z,\bar{z}),\mathcal{W}_{(\ell)}(w,\bar{w})] = \sum_{m=1}^{\ell} \binom{\ell}{m} \partial_w^m \delta(w-z)\mathcal{W}_{(k+\ell-m)}(w,\bar{w}) - \sum_{m=1}^{k} \binom{k}{m} \partial_z^m \delta(z-w)\mathcal{W}_{(k+\ell-m)}(z,\bar{z}) \tag{2.6}$$

and close onto subspaces generated by $\{\mathcal{W}_{(u)}\}_{u=\min(k,\ell)}^{k+\ell-1}$ and leads to introducing higher order generators at each step. Note that the bracket (2.6) fulfills the Jacobi identity. Moreover for arbitrary k and $\ell=1$ one obtains by duality

$$\begin{aligned}\langle [\mathcal{W}_{(k)}(z,\bar{z}),\mathcal{W}_{(1)}(w,\bar{w})] | \xi^{(k)}(z,\bar{z})\,\eta^{(1)}(w,\bar{w})\rangle &= \langle \mathcal{W}_{(k)} | \eta^{(1)}\,\partial\,\xi^{(k)} - k\,\partial\,\eta^{(1)}\xi^{(k)}\rangle - \sum_{m=2}^{k\geqslant 2} \binom{k}{m}\\ &\quad \times \langle \mathcal{W}_{(k-m+1)} | \xi^{(k)}\partial^m\eta^{(1)}\rangle,\end{aligned} \tag{2.7}$$

where the first smearing bracket on the right-hand side shows that the conformal transformations $\mathcal{W}_{(1)}$ preserve the $\mathcal{W}_{(k)}$ transformations up to lower orders. It also defines a covariant bracket $[\eta^{(1)},\xi^{(k)}]^{(k)} = \eta^{(1)}\partial\xi^{(k)} - k\partial\eta^{(1)}\xi^{(k)}$ showing that the parameter $\xi^{(k)}$ carries a conformal weight $(-k,0)$.

The closure onto a finite dimensional Lie sub-algebra for $\ell>1$ can be obtained by a truncation in the z-derivatives of $Z(z,\bar{z})$ at the some finite order, say $s-1$, $(s\geqslant 2)$. Setting for z-derivatives of order greater than $s-1$, namely for $m\geqslant s$, the following linear combinations

$$\partial_{(m)} Z(z,\bar{z}) = \sum_{\ell=1}^{s-1} \mathcal{R}^{(\ell)}_{(m)}(z,\bar{z})\partial_{(\ell)} Z(z,\bar{z}) = \Rightarrow \mathcal{W}_{(m)}(z,\bar{z}) = \sum_{\ell=1}^{s-1} \mathcal{R}^{(\ell)}_{(m)}(z,\bar{z})\mathcal{W}_{(\ell)}(z,\bar{z}) \tag{2.8}$$

where the finite summation runs over $\ell=1,\ldots,s-1$, thus the immediate consequence is that the bracket (2.6) reduces to

$$\begin{aligned}[\mathcal{W}_{(k)}(z,\bar{z}),\mathcal{W}_{(\ell)}(w,\bar{w})] = \sum_{u=1}^{s-1} \Bigg\{ &\sum_{m=1}^{\ell} \binom{\ell}{m} \partial_w^m \delta(w-z)\mathcal{R}^{(u)}_{(k+\ell-m)}(w,\bar{w})\mathcal{W}_{(u)}(w,\bar{w})\\ &- \sum_{m=1}^{k} \binom{k}{m} \partial_z^m \delta(z-w)\mathcal{R}^{(u)}_{(k+\ell-m)}(z,\bar{z})\mathcal{W}_{(u)}(z,\bar{z})\Bigg\},\end{aligned} \tag{2.9}$$

and closes onto the generators $\{\mathcal{W}_{(u)}\}_{u=1}^{s-1}$. However, the truncation spoils the Jacobi identity due to

the restriction of the order to the range $\ell=1,\ldots,s-1$. The Jacobi identity (which guarantees the associativity of the Lie algebra) will be restored by modifying the generators $\{\mathcal{W}_{(u)}\}_{u=1}^{s-1}$ in such a way to take into account the reduction coefficients $\mathcal{R}_{(v)}^{(u)}(z,\bar{z})$ introduced in (2.8). These coefficients will play the role of "structure functions" for the finite dimensional Lie algebra generated by the modified generators $\{\tilde{\mathcal{W}}_{(u)}\}_{u=1}^{s-1}$. Owing to (2.8), this is achieved by computing, for $k\geqslant s$ and for $\ell=1,\ldots,s-1$, the difference

$$[\mathcal{W}_{(k)}(z,\bar{z}),\mathcal{W}_{(\ell)}(w,\bar{w})]-\sum_{p=1}^{s-1}\mathcal{R}_{(k)}^{(p)}(z,\bar{z})[\mathcal{W}_{(p)}(z,\bar{z}),\mathcal{W}_{(\ell)}(w,\bar{w})]$$
$$=:\sum_{u=1}^{s-1}\left[\mathcal{R}_{(k)}^{(u)}(z,\bar{z}),\mathcal{F}_{(\ell)}\left(\mathcal{R}(w,\bar{w}),\frac{\delta}{\delta\mathcal{R}(w,\bar{w})}\right)\right]\mathcal{W}_{(u)}(z,\bar{z}), \tag{2.10}$$

where $\mathcal{F}_{(\ell)}(\mathcal{R}(w,\bar{w}),\delta/\delta\mathcal{R}(w,\bar{w}))$ is a functional differential polynomial in the $\mathcal{R}$'s and ensures the modification of the generator, for each $\ell=1,\ldots,s-1$, according to

$$\mathcal{W}_{(\ell)}(w,\bar{w})\to\tilde{\mathcal{W}}_{(\ell)}(w,\bar{w})=\partial_{(\ell)}Z(w,\bar{w})\frac{\delta}{\delta Z(w,\bar{w})}+\mathcal{F}_{(\ell)}\left(\mathcal{R}(w,\bar{w}),\frac{\delta}{\delta\mathcal{R}(w,\bar{w})}\right) \tag{2.11}$$

in view to fulfill the Jacobi identity. Furthermore, of course one has for $\ell=1,\ldots,s-1$,

$$\mathcal{R}_{(k)}^{(\ell)}(z,\bar{z})=\begin{cases}\delta_k^\ell & \text{if } 1\leqslant k\leqslant s-1\\ \mathcal{R}_{(k)}^{(\ell)}(z,\bar{z}) & \text{if } k\geqslant s,\end{cases} \tag{2.12}$$

and therefore the functional operator $\mathcal{F}_{(\ell)}$ must contain functional derivatives with respect to the structure functions $\mathcal{R}_{(k)}^{(p)}$ for $k\geqslant s$ only. Thus inserting twice the brackets (2.9) into the right-hand side of (2.10), a direct comparison with the left-hand side of (2.10) amounts, on the one hand, to the vanishing of the coefficient terms of the $\mathcal{W}_{(u)}(w,\bar{w})$'s. This gives rise to some compatibility conditions that must be fulfilled by the structure functions, namely,

$$\mathcal{R}_{(k+n)}^{(u)}(w,\bar{w})=\sum_{p=1}^{s-1}\sum_{j=0}^{n}\binom{n}{j}\partial_{(j)}\mathcal{R}_{(k)}^{(p)}(w,\bar{w})\mathcal{R}_{(p+n-j)}^{(u)}(w,\bar{w})\quad\text{for } n=0,\ldots,\ell\quad\text{and } k\geqslant s. \tag{2.13}$$

If k is taken to be lower or equal to $s-1$ then (2.13) restricts to $\mathcal{R}_{(k+n)}^{(u)}=\mathcal{R}_{(k+n)}^{(u)}$, since $\mathcal{R}_{(k)}^{(p)}=\delta_k^p$.

On the other hand, the coefficient term of $\mathcal{W}_{(u)}(z,\bar{z})$ provides the functional differential operator

$$\mathcal{F}_{(\ell)}\left(\mathcal{R}(w,\bar{w}),\frac{\delta}{\delta\mathcal{R}(w,\bar{w})}\right)=\sum_{i\geqslant s}\sum_{j=1}^{s-1}\left\{\sum_{m=0}^{i}\binom{i}{m}(-1)^m\partial_{(m)}\left(\mathcal{R}_{(i+\ell-m)}^{(j)}(w,\bar{w})\frac{\delta}{\delta\mathcal{R}_{(i)}^{(j)}(w,\bar{w})}\right)-\sum_{p=1}^{s-1}\sum_{q=0}^{p}\binom{p}{q}\right.$$
$$\left.\times(-1)^q\partial_{(q)}\left(\mathcal{R}_{(i)}^{(p)}(w,\bar{w})\mathcal{R}_{(p+\ell-q)}^{(j)}(w,\bar{w})\frac{\delta}{\delta\mathcal{R}_{(i)}^{(j)}(w,\bar{w})}\right)\right\}. \tag{2.14}$$

Therefore, in addition to the scalar field Z, the structure functions $\mathcal{R}$'s come as new fields to be taken into account in the theory. Their variation is obtained to be

$$\delta\mathcal{R}^{(p)}_{(n)}(z,\bar z)=\left(\int_{\mathbb{C}}\mathrm{d}\bar w\wedge\mathrm{d}w\left[\sum_{\ell=1}^{s-1}\gamma^{(\ell)}(w,\bar w)+\sum_{u\geqslant s}\gamma^{(u)}(w,\bar w)\mathcal{R}^{(\ell)}_{(u)}(w,\bar w)\right]\tilde{\mathcal{W}}_{(\ell)}(w,\bar w)\right)\mathcal{R}^{(p)}_{(n)}(z,\bar z)$$
$$=\sum_{\ell=1}^{s-1}\left[\sum_{m=0}^{n}\binom{n}{m}\partial_{(m)}\left(\gamma^{(\ell)}+\sum_{u\geqslant s}\gamma^{(u)}\mathcal{R}^{(\ell)}_{(u)}\right)\mathcal{R}^{(p)}_{(n+\ell-m)}\right.$$
$$\left.-\sum_{j=1}^{s-1}\mathcal{R}^{(j)}_{(n)}\sum_{q=0}^{j}\binom{j}{q}\partial_{(q)}\left(\gamma^{(\ell)}+\sum_{u\geqslant s}\gamma^{(u)}\mathcal{R}^{(\ell)}_{(u)}\right)\mathcal{R}^{(p)}_{(j+\ell-q)}\right](z,\bar z),\tag{2.15}$$

while the variation (2.2) for Z rewrites

$$\delta Z(z,\bar z)=\left(\int_{\mathbb{C}}\mathrm{d}\bar w\wedge\mathrm{d}w\left[\sum_{\ell=1}^{s-1}\gamma^{(\ell)}(w,\bar w)+\sum_{u\geqslant s}\gamma^{(u)}(w,\bar w)\mathcal{R}^{(\ell)}_{(u)}(w,\bar w)\right]\tilde{\mathcal{W}}_{(\ell)}(w,\bar w)\right)Z(z,\bar z).\tag{2.16}$$

To this change $\mathcal{W}_{(\ell)}\to\tilde{\mathcal{W}}_{(\ell)}$ (for $\ell=1,\ldots,s-1$) of generators there corresponds a reduction from an infinite number to a finite number of local parameters

$$\gamma^{(m)}\to\Gamma^{(\ell)}=\sum_{m\geqslant 1}\gamma^{(m)}\mathcal{R}^{(\ell)}_{(m)},\qquad \ell=1,\ldots,s-1\tag{2.17}$$

as suggested by both the variations (2.15) and (2.16). The $s-1$ local parameters $\Gamma^{(\ell)}$ secure the fact that the $s-1$ generators $\tilde{\mathcal{W}}_{(\ell)}$ fulfill indeed the algebra (2.9). In short, this leads to a reduction of the symmetry algebra, and (2.1) reduces to the variation

$$(\delta Z)(z,\bar z)=\sum_{\ell=1}^{s-1}\Gamma^{(\ell)}(z,\bar z)\partial_{(\ell)}Z(z,\bar z).\tag{2.18}$$

By duality the following brackets $[,]^{(u)}$ corresponding to the generators $\tilde{\mathcal{W}}_{(u)}$ are found to be

$$[\eta^{(\ell)},\xi^{(k)}]^{(u)}=\sum_{m=0}^{\ell-1}\binom{\ell}{m}\mathcal{R}^{(u)}_{(k+m)}\eta^{(\ell)}\partial_{(\ell-m)}\xi^{(k)}-\sum_{m=0}^{k-1}\binom{k}{m}\mathcal{R}^{(u)}_{(\ell+m)}\xi^{(k)}\partial_{(k-m)}\eta^{(\ell)}.\tag{2.19}$$

These brackets are involved in the defining Poisson brackets for $\mathcal{W}$-algebras.[3,22,23] This leads to the

Conclusion 2.1: *The realization of large diffeomorphism algebra* (2.6) *requires the definition of frames which verify the truncation property* (2.8) *which realizes a derivative order reduction (D.O.R). So the structure functions* $\mathcal{R}^{(u)}_{(v)}(z,\bar z)$ *uniquely define the properties of the algebra.*

The problem we are after is twofold. First, due to the presence of higher order derivatives which carry a nontensorial nature (jets), one wants to perform the construction in a well-defined way, in the sense that this local symmetry has indeed a global meaning over the Riemann surface Σ. That is, constructing a field theory over the coframes $J^\infty(\Sigma,\mathbb{C})$. Second, find the appropriate generators for the symmetry algebra, (jets or tensors), which give rise to covariant quantities over the Riemann surface, these quantities being constructed from covariant differential operators, covariant in the sense to be holomorphically well defined on Σ. This would correspond to a change of generators $\{\tilde{\mathcal{W}}_{(u)}\}_{u=1}^{s-1}$ in order to get a presentation of the Poisson $\mathcal{W}$-algebras which are no longer Lie algebras. This means in particular that the lower orders in the brackets (2.7) should not be present any more.[23]

This second goal requires one in fact to work with a finite number of $s-1$ complex scalar fields Z instead of one only. Therefore, one is led to consider the jet space $J^\infty(\Sigma,\mathbb{C}^{s-1})$ on which local diffeomorphisms of $\mathbb{C}^{s-1}$ stabilizing the target point $(Z^{(1)},\ldots,Z^{(s-1)})$ are lifted by jet composition and act linearly. Presently, a truncation in the order of the jet can be implemented by means

of relations given by some PDEs. The simplest ones are given by a linear PDE which yields an algebraic relation between jet coordinates. This is what will be developed in the next section.

III. THE FORSYTH FRAMES

Over a Riemann surface Σ, let us introduce the algebraic PDE of fixed order s with smooth coefficients and defined by

$$L_s f(z,\bar{z}) = 0 \quad \text{with } L_s = \sum_{j=0}^{s} a^{(s)}_{(s-j)}(z,\bar{z})\partial_{(j)}, \quad \text{where } a^{(s)}_{(0)}(z,\bar{z}) = 1, \quad \text{and } a^{(s)}_{(1)}(z,\bar{z}) = 0. \tag{3.1}$$

When $\bar{z}$ is viewed to play the role of a parameter the PDE is considered as an ODE in the independent variable z and the function f is the unknown. It thus introduces a chiral splitting between the complex coordinates. Around any point of Σ this ODE admits s linearly independent *local* solutions $f^{(R)}$, $R=1,\ldots,s$ on a small enough neighborhood of any point. Actually, any solution turns out to be a scalar density under holomorphic changes of charts $(U,z)\to(\hat{U},w(z))$ with conformal weight $(1-s)/2$ in order to have a well-defined covariance on the Riemann surface Σ which yields

$$L_s(w,\bar{w}) = (w')^{-(1+s)/2} L_s(z,\bar{z})(w')^{(1-s)/2} \quad \text{on } U\cap\hat{U}\neq\varnothing\,. \tag{3.2}$$

Recall that $L_s f$ has conformal weight $(1+s)/2$. For an overview see, e.g., Ref. 24, and references therein. Equation (3.1) can be recast as a first-order differential operator if the jet of order $s-1$ of any solution f is considered as the variable. One has

$$(\partial + A^{(s)}(z,\bar{z}))\begin{pmatrix} f(z,\bar{z}) \\ \partial f(z,\bar{z}) \\ \vdots \\ \partial_{(r-1)} f(z,\bar{z}) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ L_s f(z,\bar{z}) \end{pmatrix} = 0 \tag{3.3}$$

where the $s\times s$ matrix

$$A^{(s)}(z,\bar{z}) = \begin{pmatrix} 0 & -1 & 0 & \ldots & 0 \\ 0 & 0 & -1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \ldots & 0 & -1 \\ a^{(s)}_{(s)}(z,\bar{z}) & a^{(s)}_{(s-1)}(z,\bar{z}) & \ldots & a^{(s)}_{(2)}(z,\bar{z}) & a^{(s)}_{(1)}(z,\bar{z}) \end{pmatrix} \tag{3.4}$$

has entries

$$[A^{(s)}(z,\bar{z})]_{lm} = \begin{cases} -1 & \text{for } m = l+1 \\ a^{(s)}_{(s-m+1)}(z,\bar{z}) & \text{for } l = s, \quad \text{with } a^{(s)}_{(1)}(z,\bar{z}) \equiv 0 \\ 0 & \text{otherwise}. \end{cases} \tag{3.5}$$

Moreover, each of them in the last row carries a z lower index content of covariant order $s-m+1$. But on account of (3.3), $A^{(s)}$ is expected to carry a covariant index z as the derivative ∂_z.

This allows one to associate to the ODE a system of s identical equations by introducing s unknowns $f^{(R)}$, $R=1,\ldots,s$. So it is a system of the same ODE over $\Sigma\times\mathbb{C}^s$. Note that any linear change in the local linearly independent solutions $\tilde{f}^{(R)}(z,\bar{z}) = A^{(R)}_{(S)} f^{(S)}(z,\bar{z})$ over $U\subset\Sigma$ preserves (3.1), $A\in GL(s,\mathbb{C})$. For the time being, the matrix A does not depend on the local complex coordinates $(z,\bar{z})$ on Σ, but this issue should be tackled as the gauging of the largest symmetry group of the ODE (3.1).

However, adapting Gunning[25] for a well-defined ODE over Σ according to (3.2) if one selects s linearly independent local solutions of (3.1), on the one hand, $f^{(R)}(z,\bar{z})$ on the coordinate neighborhood $U\subset\Sigma$, and on the other hand, $\hat{f}^{(R)}(w,\bar{w})$ on the coordinate neighborhood $\hat{U}\subset\Sigma$, then on the overlapping of these coordinate neighborhoods one has, in full generality, the following gluing rule for solutions:

$$\text{on } U\cap\hat{U}\neq\varnothing\,,\quad \hat{f}^{(R)}(w,\bar{w})=(w')^{-(1-s)/2}T^{(R)}_{(S)}f^{(S)}(z,\bar{z}), \tag{3.6}$$

where the unique constant matrix T turns out to be a one-cocycle of the chosen coordinate covering on Σ with values in $GL(s,\mathbb{C})$. To prove (3.6), for the given linearly independent s solutions $\hat{f}^{(R)}(w,\bar{w})$ in the open set $\hat{U}\subset\Sigma$, let us introduce the functions $g^{(R)}(z,\bar{z})$ on $U\cap\hat{U}\subset U$ defined by

$$g^{(R)}(z,\bar{z})=(w')^{(1-s)/2}\hat{f}^{(R)}(w,\bar{w})\quad\text{on } U\cap\hat{U}\neq\varnothing\,. \tag{3.7}$$

Upon using the covariance law (3.2) it is readily seen that the s functions $g^{(R)}(z,\bar{z})$ are linearly independent solutions of (3.1) over $U\cap\hat{U}\subset U$. Accordingly, for any other s linearly independent $f^{(R)}(z,\bar{z})$ of (3.1) in the open set U, the functions $g^{(R)}(z,\bar{z})$ are unique linear combinations of the functions $f^{(R)}(z,\bar{z})$, that is $g^{(R)}(z,\bar{z})=T^{(R)}_{(S)}f^{(S)}(z,\bar{z})$ a fact which demonstrates (3.6).

According to Ref. 14, (see also Ref. 8) one may define *locally* $s-1$ smooth scalar fields over a neighborhood of any point of Σ as quotients of $s-1$ local solutions by a preferred one which does not vanish on a neighborhood of a given point, say on U,

$$Z^{(R)}(z,\bar{z})=\frac{f^{(R+1)}(z,\bar{z})}{f^{(1)}(z,\bar{z})},\quad R=1,\ldots,s-1, \tag{3.8}$$

where the functions $f^{(R+1)}$ and $f^{(1)}$ belong to the same set of linearly independent solutions over U. By virtue of (3.6) one checks that

$$\text{on } U\cap\hat{U}\neq\varnothing\,,\quad \hat{Z}^{(R)}(w,\bar{w})=\frac{T^{(R+1)}_{(S+1)}Z^{(S)}(z,\bar{z})+T^{(R+1)}_{(1)}}{T^{(1)}_{(S+1)}Z^{(S)}(z,\bar{z})+T^{(1)}_{(1)}}, \tag{3.9}$$

a transformation law which shows that the local scalar fields Z have to be transformed in a homographic way in accordance with the Zucchini's point of view[7] on $\mathcal{W}$-algebras.

Moreover, note that any linear change in the linearly independent solutions $f^{(R)}$ on U induces a homographic transformation in the $Z^{(R)}$ on U as

$$\tilde{Z}^{(R)}(z,\bar{z})=\frac{A^{(R+1)}_{(S+1)}Z^{(S)}(z,\bar{z})+A^{(R+1)}_{(1)}}{A^{(1)}_{(S+1)}Z^{(S)}(z,\bar{z})+A^{(1)}_{(1)}}. \tag{3.10}$$

The question of gauging whether or not the matrix $A\in GL(s,\mathbb{C})$ into $A(z,\bar{z})$, in other words, render local the above-presented transformation law should also be tackled in the sequel.

This is the point where now one has to decide if $Z^{(R)}$ is a genuine scalar field on Σ or not, namely keeping T as general as possible or reduce it to the identity. If one chooses the latter what would be the meaning of $T=I$ for the space of solutions of the ODE (3.1)? A possible answer would be that there exists basis of solutions which is globally defined on Σ according to (3.6) with $T=I$. But there is a more precise statement which is the following. Consider

$$\text{on } \hat{U},\quad \hat{Z}^{(R)}(w,\bar{w})=\frac{\hat{f}^{(R+1)}(w,\bar{w})}{\hat{f}^{(1)}(w,\bar{w})},\quad R=1,\ldots,s-1 \tag{3.11}$$

and thus with (3.7) one can define on the overlapping the scalar functions

$$\text{on } U\cap\hat{U}\neq\emptyset,\quad \zeta^{(R)}(z,\bar{z})=\frac{g^{(R+1)}(z,\bar{z})}{g^{(1)}(z,\bar{z})}=\hat{Z}^{(R)}(w,\bar{w}),\quad R=1,\ldots,s-1, \tag{3.12}$$

which thus coincide with the scalar functions $\hat{Z}^{(R)}$ on the intersection $U\cap\hat{U}\neq\emptyset$. Since in the glueing rule given by (3.6) the matrix T only depends on the two coordinate neighborhoods U and $\hat{U}$, let us perform the following linear change $\tilde{f}=aTf$ of linearly independent solutions on the open set U, with given $a:U\to\mathbb{C}^*$. This yields a gauge transformation over U of the type (3.10) with $A=T$ so that

$$\text{on } U\cap\hat{U}\neq\emptyset,\quad \zeta^{(R)}(z,\bar{z})=\hat{Z}^{(R)}(w,\bar{w})=\tilde{Z}^{(R)}(z,\bar{z}),\quad R=1,\ldots,s-1. \tag{3.13}$$

Hence by these redefinitions through gauge transformations, one can construct $s-1$ scalar fields on Σ, still denoted by $Z^{(R)}$, each of those being a collection of scalar maps defined on the various coordinate neighborhoods satisfying (3.13) as matching rule.

Suppose now that a family of linear differential equations of the type (3.1) is indexed by the order $r\geqslant 2$. Accordingly, solutions must be labeled by the order r, and the above-presented construction holds for each of the orders r. One may state the

Conjecture 3.1: *Around each point of the Riemann surface* Σ *and for each integer* $r\geqslant 2$, *there is a map*, $\Sigma\to\mathbb{C}P^{r-1}$ *which defines local inhomogeneous coordinates on* $\mathbb{C}P^{r-1}$, *collectively denoted by the vector valued in* $\mathbb{C}^{r-1}$ *smooth function on* Σ,

$$\vec{Z}(z,\bar{z}|r)=(Z^{(1)}(z,\bar{z}|r),\ldots,Z^{(r-1)}(z,\bar{z}|r)), \tag{3.14}$$

where the $r-1$ *components are given by*

$$Z^{(R)}(z,\bar{z}|r)=\frac{f^{(R+1)}(z,\bar{z}|r)}{f^{(1)}(z,\bar{z}|r)},\quad R=1,\ldots,r-1. \tag{3.15}$$

$\vec{Z}(z,\bar{z}|r)$ *will be called a Forsyth frame. For a given a point on* Σ, *all the frames must be equivalent for all the physical points of view.*

Returning to the general discussion with a given equation (3.1) of order s which introduces the truncation in the jet order, the following theorem comes as a by-product.

Theorem 3.1: *For any* $m\geqslant 1$, *given an order* s *of truncation dictated by a differential equation of the type* (3.1), *one has*

$$\partial_{(m)}\vec{Z}(z,\bar{z})=\sum_{l=1}^{s-1}\mathcal{R}^{(l)}_{(m)}(z,\bar{z})\partial_{(l)}\vec{Z}(z,\bar{z})\quad\text{and}\quad\mathcal{R}^{(l)}_{(m)}(z,\bar{z})=\delta^{(l)}_{(m)}\quad\text{if } 1\leqslant m\leqslant s-1. \tag{3.16}$$

The decomposition is universal for all the inhomogeneous coordinates, $Z^{(R)}(z,\bar{z})$ *in the sense that each* $\mathcal{R}^{(l)}_{(m)}$ *does not depend on the index* (R) *of the former. The* $\mathcal{R}$*'s correspond exactly to those heuristically introduced in* (2.8) *and are specific to the order* s *of truncation imposed by* (3.1). *However the vectorial character of* $\vec{Z}$ *gives rise to some additional compatibility conditions between themselves.*

Proof 1: *The proof of Theorem 3.1 is trivial by direct computation. Indeed we can compute* $\partial_s f^{(P+1)}(z,\bar{z})$ *for all* $P=1,\ldots,s-1$ *in two different ways. The first one comes from the very definition Eq.* (3.8) *and the Leibniz rule*

$$\partial_{(s)}f^{(P+1)}=\partial_{(s)}(Z^{(P)}f^{(1)})=\partial_{(s)}Z^{(P)}f^{(1)}+Z^{(P)}\partial_{(s)}f^{(1)}+\sum_{j=1}^{s-1}\binom{s}{j}\partial_{(j)}Z^{(P)}\partial_{(s-j)}f^{(1)}. \tag{3.17}$$

The second one comes from the very definition Eq. (3.8) *and the fact that both* $f^{(P+1)}$ *and* $f^{(1)}$ *are solutions of Eq.* (3.1):

$$\partial_{(s)}f^{(P+1)} = -\sum_{j=0}^{s-1} a^{(s)}_{(s-j)}\partial_{(j)}(Z^{(P)}f^{(1)}) = -\sum_{j=0}^{s-1} a^{(s)}_{(s-j)}\sum_{m=0}^{j}\binom{j}{m}\partial_{(m)}Z^{(P)}\partial_{(j-m)}f^{(1)} = -Z^{(P)}\sum_{j=0}^{s-1} a^{(s)}_{(s-j)}\partial_{(j)}f^{(1)}(z,\bar{z})$$
$$-\sum_{j=1}^{s-1} a^{(s)}_{(s-j)}\sum_{m=1}^{j}\binom{j}{m}\partial_{(m)}Z^{(P)}\partial_{(j-m)}f^{(1)} = Z^{(P)}\partial_{(s)}f^{(1)} - \sum_{m=1}^{s-1}\partial_{(m)}Z^{(P)}\sum_{j=m}^{s-1} a^{(s)}_{(s-j)}\binom{j}{m}\partial_{(j-m)}f^{(1)}. \tag{3.18}$$

A direct comparison between Eqs. (3.17) and (3.18) *entails*

$$\partial_{(s)}Z^{(P)} = \frac{-1}{f^{(1)}}\sum_{m=1}^{s-1}\left(\binom{s}{m}\partial_{(s-m)}f^{(1)} + \sum_{j=m}^{s-1} a^{(s)}_{(s-j)}\binom{j}{m}\partial_{(j-m)}f^{(1)}\right)\partial_{(m)}Z^{(P)}. \tag{3.19}$$

The decomposition (3.16) *combined with the nonvanishing of the Wronskian determinant* (3.21) *yields*

$$\mathcal{R}^{(m)}_{(s)}(z,\bar{z}) \equiv \frac{-1}{f^{(1)}(z,\bar{z})}\left(\binom{s}{m}\partial_{(s-m)}f^{(1)}(z,\bar{z}) + \sum_{j=m}^{s-2} a^{(s)}_{(s-j)}(z,\bar{z})\binom{j}{m}\partial_{(j-m)}f^{(1)}(z,\bar{z})\right), \tag{3.20}$$

where $\mathcal{R}^{(m)}_{(s)}$ *for* $m=1,\ldots,s-1$ *depend on the coefficients* $a^{(s)}_{(s-j)}$ *and* $f^{(1)}$ *and its* z *derivatives up to order* $s-2$ *since* $a^{(s)}_{(1)}=0$. *It is readily seen that the decomposition does not depend on the index of the solution* $f^{(P+1)}$. *One can extend* (3.20) *to the case* $m=0$ *since* $f^{(1)}$ *is solution of* (3.1) *by setting* $\mathcal{R}^{(0)}_{(s)}\equiv 0$.

Let us introduce the Wronskian as a $(s-1)\times(s-1)$-matrix

$$\varpi(z,\bar{z}) = (\varpi^{(R)}_{(\ell)}(z,\bar{z})) = \begin{pmatrix} \partial Z^{(1)}(z,\bar{z}) & \cdots & \partial Z^{(s-1)}(z,\bar{z}) \\ \vdots & \ddots & \vdots \\ \partial_{(s-1)}Z^{(1)}(z,\bar{z}) & \cdots & \partial_{(s-1)}Z^{(s-1)}(z,\bar{z}) \end{pmatrix}. \tag{3.21}$$

Hence in the algebra of squared matrices of order $s-1$ the relationships (3.16) state that any z-derivative of the Wronskian ϖ can be decomposed as a product of a rectangular matrix with the functions $\mathcal{R}$ as entries by ϖ, in detail,

$$\partial_{(m)}\varpi^{(R)}_{(\ell)} = \sum_{k=1}^{s-1}\mathcal{R}^{(k)}_{(m+\ell)}\varpi^{(R)}_{(k)}. \tag{3.22}$$

In order to be the most general as possible, the Wronskian may be extended to an $m\times(s-1)$ rectangular matrix when higher derivatives $m\geqslant s$ of the $Z^{(R)}$'s are considered. In account of (3.16), the rectangular matrix of derivatives of Z up to order m can always be expressed in terms of the Wronskian matrix (3.21). We shall call this mechanism connected to the truncation heuristically introduced in (2.9) as a derivative order reduction, or in shorthand DOR. Note also that thanks to (3.16) a straightforward computation gives

$$\mathcal{R}^{(s-1)}_{(s)}(z,\bar{z}) = \partial \ln\det\varpi(z,\bar{z}). \tag{3.23}$$

The preferred solution $f^{(1)}$ which crucially takes place in the computation of the $\mathcal{R}$'s plays a distinguished role in the construction as it has already been seen. In particular it infers a linear relationship for $f^{(1)}$ with $j=s-1$ in Eq. (3.20)

$$\mathcal{R}^{(s-1)}_{(s)}(z,\bar{z}) = -s\,\partial\,\ln f^{(1)}(z,\bar{z}), \tag{3.24}$$

which yields, on the one hand, together with (3.23)

$$f^{(1)}(z,\bar{z}) = (\det \varpi(z,\bar{z}))^{-1/s}, \tag{3.25}$$

and on the other hand,

$$= \Rightarrow \partial f^{(1)} = \mathcal{Q}_{(1)} f^{(1)}, \quad \text{where } \mathcal{Q}_{(1)} = -\tfrac{1}{s}\mathcal{R}^{(s-1)}_{(s)} \tag{3.26}$$

and by successive z derivatives one gets a recursive formula

$$\partial_{(n)} f^{(1)}(z,\bar{z}) = \mathcal{Q}_{(n)}(z,\bar{z}) f^{(1)}(z,\bar{z}) \quad \text{with } \mathcal{Q}_{(n)} = \partial \mathcal{Q}_{(n-1)} + \mathcal{Q}_{(n-1)}\mathcal{Q}_{(1)} \quad \text{and } \mathcal{Q}_{(0)} = 1, \tag{3.27}$$

so that $\mathcal{Q}_{(n)}$ turns to be a differential polynomial in $\mathcal{Q}_{(1)}$ (i.e., in $\mathcal{R}^{(s-1)}_{(s)}$), namely $\mathcal{Q}_{(n)} = (\partial + \mathcal{Q}_{(1)})^{n-1}\mathcal{Q}_{(1)}$. Using (3.27) into (3.20) and eliminating $f^{(1)}$ allows one to write a linear system in a Gauss form with respect to the a's coefficients

$$\mathcal{R}^{(j)}_{(s)} + \binom{s}{j}\mathcal{Q}_{(s-j)} + \sum_{l=j}^{s-1}\binom{\ell}{j} a^{(s)}_{(s-\ell)}\mathcal{Q}_{(\ell-j)} = 0 \quad \text{for } j = 0, \ldots, s-1, \tag{3.28}$$

which expresses the relationship between the $a^{(s)}$'s and the $\mathcal{R}_{(s)}$'s. This step is independent of $f^{(1)}$ provided that the $\mathcal{R}_{(s)}$'s are given (together with some compatibility conditions) and we will consider from now on and throughout all the paper that the degrees of freedom will be the $\mathcal{R}_{(s)}$'s. Hence, solving iteratively the system (3.28) with respect to the $a^{(s)}$'s one gets

$$\begin{aligned}
&a^{(s)}_{(1)} = 0 && \text{for } j = s-1,\\
&a^{(s)}_{(2)} = -\mathcal{R}^{(s-2)}_{(s)} - \binom{s}{s-2}\mathcal{Q}_{(2)} && \text{for } j = s-2,\\
&a^{(s)}_{(3)} = -\mathcal{R}^{(s-3)}_{(s)} - \binom{s}{s-3}\mathcal{Q}_{(3)} - \binom{s-2}{s-3}a^{(s)}_{(2)}\mathcal{Q}_{(1)} && \text{for } j = s-3,\\
&\quad\vdots && \text{and so on up to } j = 0.
\end{aligned} \tag{3.29}$$

This shows that to a given a DOR (3.16) there corresponds a holomorphically covariant differential equation of the type (3.1) whose smooth coefficients are expressed as differential polynomials in the structure function $\mathcal{R}^{(s-1)}_{(s)}$ and linearly with respect to the others.

Moreover one has the following property which is exactly the compatibility condition (2.13).

Properties 1: *For* $p = 1, \ldots, s-1$ *and* $n \geqslant s$,

$$\mathcal{R}^{(p)}_{(m+n)}(z,\bar{z}) = \sum_{j=0}^{m}\binom{m}{j}\sum_{\ell=1}^{s-1}\partial_{(j)}\mathcal{R}^{(\ell)}_{(n)}(z,\bar{z})\mathcal{R}^{(p)}_{(m+\ell-j)}(z,\bar{z}), \tag{3.30}$$

where $1 \leqslant l \leqslant s-1$; *so, recursively all the* $\mathcal{R}^{(l)}_{(s+m)}(z,\bar{z})$ $m > 0$ *coefficients can be derived from the basic* $\mathcal{R}^{(l)}_{(s)}(z,\bar{z})$ *ones*.

In particular, for the case $m = 1$, one has

$$\mathcal{R}^{(p)}_{(n+1)}(z,\bar{z}) = \partial\mathcal{R}^{(p)}_{(n)}(z,\bar{z}) + \sum_{\ell=1}^{s-1}\mathcal{R}^{(\ell)}_{(n)}(z,\bar{z})\mathcal{R}^{(p)}_{(\ell+1)}(z,\bar{z}), \tag{3.31}$$

an equation which will be useful for future applications.

The basic $\mathcal{R}^{(l)}_{(s)}$'s, namely the structure functions given in the introductory section, play a central role and it would be worthwhile to have some hints about their geometric nature. In order to be closer as possible to a differential geometric setting for our approach, let us proceed as follows. For the z-jet of a fixed order, one has the following holomorphic gluing rules under the change $z \mapsto w = w(z)$:

$$\partial_z^{k+1} Z(z,\bar{z}) = \begin{cases} w'(z)\partial_w Z(w,\bar{w}) & \text{if } k=0 \\ w^{(k+1)}(z)\partial_w Z(w,\bar{w}) + \sum_{\ell=1}^{k} \partial_w^{\ell+1} Z(w,\bar{w})(z) & \\ \quad \times \sum_{r=\ell}^{k} \frac{k!}{(k-r)!} w^{(k-r+1)}(z) \left(\sum_{\substack{a_1+\cdots+ra_r=r \\ a_1+\cdots+a_r=\ell}} \left(\prod_{n=1}^{r} \frac{1}{a_n!} \left(\frac{w^{(n)}(z)}{n!} \right)^{a_n} \right) \right) & \text{if } k \geqslant 1, \end{cases} \tag{3.32}$$

where the last expression comes from the use of the Faà di Bruno formula for higher order chain rule of derivatives. For further calculations, one has more explicitly and under a more elegant form, for $k \geqslant 3$

$$\begin{aligned} (\partial_{(k+1)} Z)(z,\bar{z}) = (w')^{k+1} (\partial_{(k+1)} Z)(w,\bar{w}) &+ \binom{k+1}{2} (w')^k \partial_z \ln w' (\partial_{(k)} Z)(w,\bar{w}) \\ &+ \binom{k+1}{3} (w')^{k-1} \left(\{w,z\} + \tfrac{3}{4} k (\partial_z \ln w')^2 \right) (\partial_{(k-1)} Z)(w,\bar{w}) \\ &+ \binom{k+1}{4} (w')^{k-2} \Big(\partial_z \{w,z\} + 2(k-1)\{w,z\} \partial_z \ln w' \\ &+ \binom{k}{2} (\partial_z \ln w')^3 \Big) (\partial_{(k-2)} Z)(w,\bar{w}) + \text{lower order derivatives}, \end{aligned} \tag{3.33}$$

where $\{w,z\} = \partial_z^2 \ln w' - \frac{1}{2}(\partial_z \ln w')^2 = w'''/w' - \frac{3}{2}(w''/w')^2$ denotes the Schwarzian derivative.

Now for fixed s, one can obtain the geometric properties of the $s-1$ structure functions $\mathcal{R}$'s by solving the linear system (3.16) with respect to the $\mathcal{R}$'s by Cramer method, one gets the following Lie form associated to the PDEs (3.16) (see, e.g., Ref. 26) for $m=1,\ldots,s-1$,

$$\Phi^{(m)}(\vec{Z}_s) := (-1)^{s-1-m} \frac{\det(\partial\vec{Z}, \partial_{(2)}\vec{Z}, \ldots, \widehat{\partial_{(m)}\vec{Z}}, \ldots, \partial_{(s-1)}\vec{Z}, \partial_{(s)}\vec{Z})}{\det \varpi} = \mathcal{R}_{(s)}^{(m)}(z,\bar{z}), \tag{3.34}$$

where the caret (^) means omission. This expression can simply be rewritten as

$$\mathcal{R}_{(s)}^{(m)} = \partial_{(s)} Z^{(R)} [\varpi^{-1}]_{(R)}^{(m)}. \tag{3.35}$$

For $s=2$, one has the obvious relations $\mathcal{R}_{(m)}^{(1)} = \partial_{(m)} Z / \partial_{(1)} Z$. According to an approach advocated by Vessiot to the Picard-Vessiot theory (Ref. 26, and references therein) one can construct, regarding the present case and by a repeated use of (3.33), a natural holomorphic bundle with a $(s-1)$-dimensional fiber with fiber coordinates $(u^{(1)},\ldots,u^{(s-1)})$. It is defined by the following holomorphic transition functions induced by the holomorphic change of chart $w=\varphi(z)$ on Σ

$$w = \varphi(z),$$

$$U^{(s-1)} = \frac{1}{w'} \left(u^{(s-1)} - \binom{s}{2} \partial \ln w' \right) \text{ affine bundle } !,$$

$$U^{(s-2)} = \frac{1}{w'^2} \left(u^{(s-2)} + \binom{s-1}{2} u^{(s-1)} \partial \ln w' - \binom{s}{3} \left(\{w,z\} + \tfrac{3}{4} \binom{s-1}{1} (\partial \ln w')^2 \right) \right),$$

$$U^{(s-3)}=\frac{1}{w'^3}\left(u^{(s-3)}+\binom{s-2}{2}u^{(s-2)}\,\partial\,\ln w'+u^{(s-1)}\binom{s-1}{3}\left(\{w,z\}+\tfrac{3}{4}\binom{s-2}{1}(\partial\ln w')^2\right)-\binom{s}{4}\right.$$
$$\left.\times\left(\partial\{w,z\}+2\binom{s-2}{1}\{w,z\}\,\partial\,\ln w'+\binom{s-1}{2}(\partial\ln w')^3\right)\right),$$

$$\vdots$$

$$U^{(1)}=\text{a very intricate expression depending on all the } u^{(i)\prime}\text{s}, \tag{3.36}$$

where the transition laws become more and more involved. This bundle can be recast into a holomorphic natural bundle of geometric objects (but however with smooth sections $\mathcal{R}$ in accordance with locality) as fibered product over the Riemann surface Σ,

$$\mathcal{F}_{\text{affine}}\times_{\Sigma}\mathcal{F},$$

where $\mathcal{F}_{\text{affine}}$ is the affine bundle and $\mathcal{F}$ is the bundle with very intricate remaining but important patching rules for the sequel. Having at our disposal some of the main gluing rules of the fundamental $\mathcal{R}$'s, it is possible to obtain the geometrical nature of some of the coefficients of (3.1). Indeed, in terms of the Wronskian $\mathcal{R}^{(s-1)}_{(s)}=\partial\ln\det\varpi$, one finds for the coefficient

$$a^{(s)}_{(2)}=\tfrac{s-1}{2}\left(\partial\mathcal{R}^{(s-1)}_{(s)}-\tfrac{1}{s}(\mathcal{R}^{(s-1)}_{(s)})^2\right)-\mathcal{R}^{(s-2)}_{(s)}, \tag{3.37}$$

while both $\mathcal{R}^{(s-1)}_{(s)}$ and $\mathcal{R}^{(s-2)}_{(s)}$ glue as smooth sections of the bundle defined by (3.36). After a direct computation

$$a^{(s)}_{(2)}(z,\bar{z})=(w')^2a^{(s)}_{(2)}(w,\bar{w})+\tfrac{s(s^2-1)}{12}\left(\partial^2\ln w'-\tfrac{1}{2}(\partial\ln w')^2\right), \tag{3.38}$$

which shows that $a^{(s)}_{(2)}$ is proportional to a projective connection as is well known, since the inhomogeneous term in the gluing rule is nothing but the Schwarzian derivative $\{w,z\}=\partial^2\ln w'-\frac{1}{2}(\partial\ln w')^2$. The projective connection is constructed over the frame $\vec{Z}$ according to (3.37).

Remark 3.1: *For the case* $s=3$, *one has* $\mathcal{R}^{(2)}_{(3)}=\partial\ln\det\varpi$, *and* $\mathcal{R}^{(1)}_{(3)}=\det(\partial^3\vec{Z},\partial^2\vec{Z})/\det\varpi$. *With* $\mathcal{Q}_{(1)}=\frac{-1}{3}\mathcal{R}^{(2)}_{(3)}$, *one readily gets*

$$a^{(3)}_{(2)}=-\mathcal{R}^{(1)}_{(3)}-3\mathcal{Q}_{(2)}=-\mathcal{R}^{(1)}_{(3)}-3(\partial\mathcal{Q}_{(1)}+(\mathcal{Q}_{(1)})^2),$$
$$a^{(3)}_{(3)}=\mathcal{R}^{(1)}_{(3)}\mathcal{Q}_{(1)}+2(\mathcal{Q}_{(1)})^3-\partial^2\mathcal{Q}_{(1)}=\tfrac{1}{3}\left(\partial a^{(3)}_{(2)}+\partial\mathcal{R}^{(1)}_{(3)}+\tfrac{2}{3}\mathcal{R}^{(2)}_{(3)}a^{(3)}_{(2)}-\tfrac{1}{3}\mathcal{R}^{(1)}_{(3)}\mathcal{R}^{(2)}_{(3)}\right), \tag{3.39}$$

which are exactly those coefficients obtained for the so-called $\mathcal{W}_3$*-algebra.*[14,27] *The last expression is given in terms of the projective connection and the structure functions only.*

Remark 3.2: *The factorization property of the differential operator* L_s *of order* s *in terms of first-order differential operators with nowhere vanishing coefficients can be obtained if and only if* L_s *is a nonoscillating operator, see Ref.* 20 *for some details. For more concreteness, let us illustrate this factorization property for* $s=2,3$.

1. *The* $s=2$ *case. Take* $f^{(1)}=(\partial Z)^{-1/2}=:\lambda^{-1/2}$ *as a nowhere vanishing particular solution of* $L_2f=0$. *One can write*

$$L_2=\partial^2+a^{(2)}_{(2)}=(\partial-b)(\partial+b)\quad \textit{with } a^{(2)}_{(2)}=\partial b-b^2,\quad \textit{and } b=-\partial\ln f^{(1)}=:-\mathcal{Q}_{(1)}. \tag{3.40}$$

One finds the expected factorization

$$L_2=\left(\partial-\tfrac{1}{2}\,\partial\,\ln\,\partial\lambda\right)\left(\partial+\tfrac{1}{2}\,\partial\,\ln\,\partial\lambda\right),\quad \textit{and } a^{(2)}_{(2)}=\tfrac{1}{2}\partial^2\ln\,\partial\lambda-\tfrac{1}{4}(\partial\ln\,\partial\lambda)^2. \tag{3.41}$$

2. *The* $s=3$ *case amounts to writing*

$$L_3 = (\partial - b_1 - b_2)(\partial + b_2)(\partial + b_1) \tag{3.42}$$

with $b_1 = -\partial \ln f^{(1)} = -\mathcal{Q}_{(1)}$ *and a possible choice for* b_2 *is given by* $b_2 = b_1 - \partial \ln \partial Z^{(1)}$*—it could be possible to choose* $b_2 = b_1 - \partial \ln \partial Z^{(2)}$ *since* b_1 *never vanishes. Then substituting into*

$$a^{(3)}_{(2)} = \partial(b_1 + b_2) - (b_1 + b_2)^2 + \partial b_1 + b_1 b_2,$$

$$a^{(3)}_{(3)} = \partial^2 b_1 + \partial(b_1 b_2) - (b_1 + b_2)(\partial b_1 + b_1 b_2),$$

one exactly recovers the above-given expressions in (3.39) *for the coefficients of* L_3.

Still with a fixed given order s, it is possible to construct a connection-like object. With the Dolbeault decomposition of the de Rham differential $d = \boldsymbol{\partial} + \bar{\boldsymbol{\partial}} z$ let us define the flat connection (pure gauge)

$$\mathcal{J} = \mathrm{d}\varpi\, \varpi^{-1} = \boldsymbol{\partial}\varpi\varpi^{-1} + \bar{\boldsymbol{\partial}}\varpi\varpi^{-1} = \mathrm{d}z\mathcal{J}_z + \mathrm{d}\bar{z}\mathcal{J}_{\bar{z}}. \tag{3.43}$$

Obviously its curvature vanishes

$$\mathcal{F} = \mathrm{d}\mathcal{J} - \mathcal{J}^2 = 0 \Rightarrow \bar{\partial}_{\bar{z}}\mathcal{J}_z - \partial_z \mathcal{J}_{\bar{z}} + [\mathcal{J}_z, \mathcal{J}_{\bar{z}}] = 0. \tag{3.44}$$

The $(1,0)$-component of the $(s-1)\times(s-1)$-matrix connection of $\mathcal{J}$ is by construction

$$\mathcal{J}^{(n)}_{(z)_{(m)}}(z,\bar{z}) \equiv \sum_{R=1}^{s-1} \partial\, \varpi^{(R)}_{(m)}(z,\bar{z})[\varpi^{-1}]^{(n)}_{(R)}(z,\bar{z}) = \mathcal{R}^{(n)}_{(m+1)}(z,\bar{z}), \quad m,n = 1,\ldots,s-1 \tag{3.45}$$

or more explicitly in matrix form

$$\mathcal{J}_{(z)}(z,\bar{z}) = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ \mathcal{R}^{(1)}_{(s)}(z,\bar{z}) & \mathcal{R}^{(2)}_{(s)}(z,\bar{z}) & \cdots & \cdots & \cdots & \mathcal{R}^{(s-1)}_{(s)}(z,\bar{z}) \end{pmatrix}. \tag{3.46}$$

This matrix turns out to be of Frobenius type (similar to the matrix (3.4)) and therefore $\mathcal{J}_z$ is not a Lie algebra-valued covariant component of an usual connection. Note that the form of the matrix is close to the Drinfeld-Sokolov one,[4] but differs by the nonvanishing term $\mathcal{R}^{(s-1)}_{(s)}$. Furthermore, it is useful to notice that

$$\mathcal{R}^{(s-1)}_{(s)}(z,\bar{z}) = \mathrm{Tr}\mathcal{J}_{(z)}(z,\bar{z}) = \mathrm{Tr}(\partial\varpi(z,\bar{z})\varpi^{-1}(z,\bar{z})), \tag{3.47}$$

in accordance with (3.23).

IV. BRS APPROACH

In this section, the heuristic presentation of the truncation procedure and its consequences on the formulation of the algebra of Ward operators given in Sec. II is translated into the BRS language. As is well known, this allows are to reformulate in more algebraic terms the presentation of a symmetry, and in particular, will give a more universal character of the possible variations on truncated Taylor expansions of the scalar fields Z.

Having still in mind that we are at a fixed given order s for the truncation (2.8) or (3.16), and by recalling Theorem 3.1, we can turn the $s-1$ local parameters $\Gamma^{(\ell)}$ to Faddeev-Popov ($\Phi\Pi$) ghosts $\mathcal{K}^{(l)}$. The variation (2.16) can be recast in a BRS algebraic language as

$$\delta_{\mathcal{W}_s} Z^{(R)}(z,\bar{z}|s) = \sum_{\ell=1}^{s-1} \mathcal{K}^{(\ell)}(z,\bar{z}|s)\partial_{(\ell)} Z^{(R)}(z,\bar{z}|s), \quad 1 \leqslant R \leqslant s-1, \tag{4.1}$$

where the variation is given by a summand over the independent derivatives up to order $s-1$ due to the DOR of order s. The ghost fields $\mathcal{K}^{(l)}$, of which number is restricted to the range $\ell = 1, \ldots, s-1$, serve to define the $\mathcal{W}_s$-algebra relative to the truncation at the level s. We emphasize that the operation $\delta_{\mathcal{W}_s}$ which is required to be nilpotent, depends on the level s of truncation. Accordingly, the ghost parameters $\mathcal{K}^{(l)}$ depend on the truncation process by their number, see (4.1), and generate a $\mathcal{W}$-algebra once the level is fixed. By an argument based on the nilpotency, for $l = 1, \ldots, s-1$,

$$\begin{aligned}\delta_{\mathcal{W}_s} \mathcal{K}^{(l)}(z,\bar{z}|s) =: \sum_{m=1}^{s-1} \mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{B}^{(l)}_{(m)}(z,\bar{z}|s) \\ = \sum_{m,n=1}^{s-1} \mathcal{K}^{(m)}(z,\bar{z}|s) \sum_{j=1}^{m} \binom{m}{j} \partial_{(j)}\mathcal{K}^{(n)}(z,\bar{z}|s)\mathcal{R}^{(l)}_{(n+m-j)}(z,\bar{z}|s),\end{aligned} \tag{4.2}$$

where on the right-hand side the dependence on the level s of truncation has been explicitly written. Note also that the products of two underived ghosts drop out by $\Phi\Pi$ charge argument. This variation defines a $(s-1)\times(s-1)$-matrix $\mathcal{B}$ carrying ghost number one, and thus depending on the level s of truncation through the structure functions $\mathcal{R}$ pertaining to that level s. In more detail,

$$\mathcal{B}^{(l)}_{(m)}(z,\bar{z}|s) := \sum_{n=1}^{s-1} \sum_{j=0}^{m} \binom{m}{j} \partial_{(m-j)}\mathcal{K}^{(n)}(z,\bar{z}|s)\mathcal{R}^{(l)}_{(n+j)}(z,\bar{z}|s), \tag{4.3}$$

a remarkable combination over the ghosts $\mathcal{K}^{(\ell)}$, $\ell = 1, \ldots, s-1$ which could have been readily read from the variation (2.15). For the Wronskian (3.21) the $\mathcal{W}_s$-algebra extended to

$$\delta_{\mathcal{W}_s} \varpi^{(R)}_{(\ell)}(z,\bar{z}|s) = \sum_{n=1}^{s-1} \mathcal{B}^{(n)}_{(\ell)}(z,\bar{z}|s)\varpi^{(R)}_{(n)}(z,\bar{z}|s), \quad \ell, R = 1, \ldots, s-1 \tag{4.4}$$

where the matrix product is understood for $(s-1)\times(s-1)$-matrices. One also has

$$\delta_{\mathcal{W}_s} \varpi^{-1} = -\varpi^{-1}\mathcal{B}, \tag{4.5}$$

and accordingly, using $\delta_{\mathcal{W}}\mathrm{d} + \mathrm{d}\delta_{\mathcal{W}} = 0$,

$$\delta_{\mathcal{W}_s} \mathcal{J} = -\mathrm{d}\mathcal{B} + [\mathcal{B}, \mathcal{J}], \tag{4.6}$$

where the bracket is graded on forms with $(s-1)\times(s-1)$-matrix values. The nilpotency property provides first,

$$\delta_{\mathcal{W}_s} \mathcal{B}(z,\bar{z}|s) = \mathcal{B}(z,\bar{z}|s)\mathcal{B}(z,\bar{z}|s) = \mathcal{B}^2(z,\bar{z}|s) \tag{4.7}$$

and second, by $\Phi\Pi$ argument

$$\delta_{\mathcal{W}_s} \mathrm{Tr}(\mathcal{B}(z,\bar{z}|s)^{(2n+1)}) = 0, \quad n = 0, 1, \ldots, \tag{4.8}$$

where Tr is the usual trace on matrices. The BRS variation of all the structure functions $\mathcal{R}^{(p)}_{(n)}(z,\bar{z}|s)$ ($p = 1, \ldots, s-1$ and even for $n \geqslant s$) can be directly found from the variation (2.15) to write

$$\delta_{\mathcal{W}_s}\mathcal{R}^{(p)}_{(n)}(z,\bar{z}|s)=\mathcal{B}^{(p)}_{(n)}(z,\bar{z}|s)-\sum_{q=1}^{s-1}\mathcal{R}^{(q)}_{(n)}(z,\bar{z}|s)\mathcal{B}^{(p)}_{(q)}(z,\bar{z}|s), \tag{4.9}$$

where $\mathcal{B}$ defined earlier, in (4.3) may be extended to a rectangular matrix for lower indices greater than $s-1$, while the upper ones are still lower than this value imposed by the level of truncation, since all the $\mathcal{R}$'s can be gathered into a rectangular matrix. One checks that it is compatible with the case $\mathcal{R}^{(k)}_{(\ell)}=\delta^k_\ell$, which is kept invariant. We stress that while the first $\mathcal{B}$ term of the right-hand side of the variation (4.9) is a rectangular matrix, the $\mathcal{B}$ under the summand is a squared one. As noted before the matrix $\varpi^R_{(m)}$ can be taken to be a rectangular as well, when $m\geqslant s$, and the variation (4.4) relative to the algebra $\mathcal{W}_s$ is accordingly modified by

$$\delta_{\mathcal{W}_s}\varpi^{(R)}_{(m)}(z,\bar{z}|s)=\sum_{\ell=1}^{s-1}\mathcal{B}^{(\ell)}_{(m)}(z,\bar{z}|s)\varpi^{(R)}_{(\ell)}(z,\bar{z}|s),\quad R=1,\ldots,s-1 \text{ and } m\geqslant 1, \tag{4.10}$$

where the matrix $(\mathcal{B}^{(\ell)}_{(m)})$ can be rectangular. Supported by the fact that the ghosts $\mathcal{K}^{(\ell)}$ are subordinated to the given level of truncation s, one may now define,[28] for $\ell=1,\ldots,s-1$, the ℓth derivatives $\partial_{(\ell)}=\{\partial/\partial\mathcal{K}^{(\ell)},\delta_{\mathcal{W}_s}\}$ as an anticommutator, thus the DOR equation (3.22) is recovered,

$$\partial_{(\ell)}\varpi^{(R)}_{(m)}(z,\bar{z}|s)=\sum_{u=1}^{s-1}\mathcal{R}^{(u)}_{(\ell+m)}(z,\bar{z}|s)\varpi^{(R)}_{(u)}(z,\bar{z}|s),\quad R,\ \ell\ =1,\ldots,s-1,\ \text{and}\ m\geqslant 1. \tag{4.11}$$

This shows that the BRS algebra encapsulates the DOR mechanism just by construction and provides a consistency of the present approach.

Furthermore, from Eq. (4.4) one has

$$\delta_{\mathcal{W}_s}\ln\det\varpi(z,\bar{z}|s)=\mathrm{Tr}\,\mathcal{B}(z,\bar{z}|s), \tag{4.12}$$

which gives for the variation of $\mathcal{R}^{(s-1)}_{(s)}$,

$$\delta_{\mathcal{W}_s}\mathcal{R}^{(s-1)}_{(s)}(z,\bar{z}|s)=\partial\,\mathrm{Tr}\,\mathcal{B}(z,\bar{z}|s)=\mathrm{Tr}\ \partial\mathcal{B}(z,\bar{z}|s).$$

V. COVARIANCE UNDER HOLOMORPHIC REPARAMETRIZATION

The covariance property under holomorphic change of local coordinates on the Riemann surface is analyzed for the so far obtained quantities. As will be shown, this analysis will amount to switching to new ghost fields of a tensorial nature in contrast to that of the $\mathcal{K}$'s.

In view of the patching rules (3.32) under finite holomorphic reparametrizations, it possibly renders more explicit some of the covariance properties of the theory relative to a fixed order s. As will be shown, the study of covariance will appear as a key step in the construction of $\mathcal{W}$-algebras.

Under finite holomorphic change of charts $z\to w(z)$ the covariance property of the $s-1$ scalar fields (emerging from the truncation at level s) writes

$$Z^{(R)}(z,\bar{z}|s)=Z^{(R)}(w,\bar{w}|s),\quad R=1,\ldots,s-1 \tag{5.1}$$

and implies that the Wronskian matrix ϖ behaves as a nontensorial covariant quantity

$$\varpi^{(R)}_{(n)}(w,\bar{w}|s)=\sum_{m=1}^{s-1}\Phi^{(m)}_{(n)}(z)\varpi^{(R)}_{(m)}(z,\bar{z}|s), \tag{5.2}$$

and while for its inverse

$$[\varpi^{-1}]^{(n)}_{(R)}(w,\bar{w}|s)=\sum_{m=1}^{s-1}[\varpi^{-1}]^{(m)}_{(R)}(z,\bar{z}|s)\Phi^{-1\,(n)}_{(m)}(z), \tag{5.3}$$

where the patching rules are governed by the $(s-1)\times(s-1)$ lower triangular holomorphic matrix $\Phi^{(\ell)}_{(k)}(z)$ for $k,\ell=1,\ldots,s-1$, depending on the Jacobian w' and its derivatives. Its inverse matrix is more easily computable and given by (see (3.32))

$$[\Phi^{-1}]^{(\ell)}_{(k)}(z)=\begin{cases} w^{(k)}(z) & \text{if } \ell=1 \\ \displaystyle\sum_{r=\ell-1}^{k-1}\frac{(k-1)!\,w^{(k-r)}(z)}{(k-r-1)!}\sum_{\substack{a_1+\cdots+ra_r=r\\ a_1+\cdots+a_r=\ell-1}}\left(\prod_{n=1}^{r}\frac{1}{a_n!}\left(\frac{w^{(n)}(z)}{n!}\right)^{a_n}\right), & k\geqslant\ell\geqslant 2 \\ 0, & k<\ell \end{cases} \tag{5.4}$$

with nonvanishing determinant, $\det\Phi^{-1}(z)=(w'(z))^{s(s-1)/2}$, since the diagonal entries are given by $[\Phi^{-1}]^{(\ell)}_{(\ell)}(z)=(w'(z))^{\ell}$. Note also that the order of the matrix $\Phi^{(\ell)}_{(k)}(z)$ (or that of its inverse as well) is subject to the order s of truncation. Accordingly, since the variation (4.1) relative to the order s has to behave as a scalar, the $s-1$ ghosts of the level s of truncation turn out to be contravariant quantities

$$\mathcal{K}^{(l)}(w,\bar{w}|s)=\mathcal{K}^{(m)}(z,\bar{z}|s)[\Phi^{-1}]^{(l)}_{(m)}(z). \tag{5.5}$$

Taking into account (5.4), the ghosts $\mathcal{K}^{(m)}(z,\bar{z})$ behave as jets, except for the top one of order $s-1$ which turns out to be a contravariant tensor of order $s-1$. For the sake of completeness, the behaviors of the rectangular matrices $\mathcal{B}^{(l)}_{(p)}(z,\bar{z}|s)$ and $\mathcal{R}^{(l)}_{(p)}(z,\bar{z}|s)$, respectively, come from (5.2), (4.4), and (3.16) or (4.9). They are respectively found to be

$$\mathcal{B}(w,\bar{w}|s)=\Phi(z)\mathcal{B}(z,\bar{z}|s)\Phi^{-1}(z), \tag{5.6}$$

and for $\ell\leqslant s-1$,

$$\mathcal{R}^{(\ell)}_{(k)}(w,\bar{w}|s)=\sum_{m=1}^{k}\sum_{p=\ell}^{s-1}\Phi^{(m)}_{(k)}(z)\mathcal{R}^{(p)}_{(m)}(z,\bar{z}|s)[\Phi^{-1}]^{(\ell)}_{(p)}(z). \tag{5.7}$$

Thanks to the their definition (2.12), one obtains the following identities for $k\leqslant s-1$:

$$[\Phi^{-1}]^{(k)}_{(k)}(z)\Phi^{(k)}_{(k)}(z)=1 \quad \text{(no summation)}, \quad \sum_{u=\ell}^{k}[\Phi^{-1}]^{(u)}_{(k)}(z)\Phi^{(\ell)}_{(u)}(z)=0 \quad \text{if } \ell<k\leqslant s-1. \tag{5.8}$$

VI. JETS VERSUS TENSORS, OR HOW TO RECOVER $\mathcal{W}$-ALGEBRAS

The algebra of transformations (4.1) and (4.2) are written in terms of ghosts which under holomorphic change of charts (see Eq. (5.5)) behave as jets, and thus do not carry any tensorial nature.

We want to show that these transformations encode a structure of $\mathcal{W}_s$-algebra if the DOR mechanism is provided by a truncation at the sth level. The latter may be implemented by means of a given differential equation (3.1) which serves to generate what it is called in the paper, the Forsyth frames. Since objects of jet nature are heavy to handle, and that (physical) fields are usually considered to be of tensorial nature in some representation space of a symmetry, it is first necessary for the BRS algebra presentation of $\mathcal{W}$-symmetry to switch from the jet-ghosts to tensor ones. This will make some contact with the results on the subject disseminated through the

literature.[1,6,5,8,10] This kind of problem is often encountered in the treatment of a local field theory, and even in the BRST quantization scheme, see, e.g., Refs. 29 and 30. The solution to this problem is obviously not unique since a tensor is defined up to a change of basis among tensors. This is why it must be solved for the moment with the tools at hand.

Let us consider the hypothesis where the $\mathcal{K}$'s are *not* universal, except the top one. Given a level s of truncation, consider the hierarchy of all lower orders of truncation $j+1 \leqslant s$ which come into the game with their own structure functions. At the level s, if $\vec{Z}$ denotes a vector in $\mathbb{C}P^{s-1}$, one has, respectively, for the DOR and the variation

$$\partial_{(s)}\vec{Z}(z,\bar{z}|s) = \sum_{\ell=1}^{s-1} \mathcal{R}^{(\ell)}_{(s)}(z,\bar{z}|s)\partial_{(\ell)}\vec{Z}(z,\bar{z}|s), \quad \delta_{\mathcal{W}_s}\vec{Z}(z,\bar{z}|s) = \sum_{\ell=1}^{s-1} \mathcal{K}^{(\ell)}(z,\bar{z}|s)\partial_{(\ell)}\vec{Z}(z,\bar{z}|s). \tag{6.1}$$

Suppose now that the DOR is rather implemented at the sublevel $s-1$ on the $s-1$ scalar fields, with

$$\partial_{(s-1)}\vec{Z}(z,\bar{z}|s) = \sum_{\ell=1}^{s-2} \mathcal{R}^{(\ell)}_{(s-1)}(z,\bar{z}|s-1)\partial_{(\ell)}\vec{Z}(z,\bar{z}|s), \tag{6.2}$$

then the above-mentioned variation can be projected onto that of the level $s-1$,

$$\begin{aligned}\delta_{\mathcal{W}_s}\vec{Z}(z,\bar{z}|s) &= \sum_{\ell=1}^{s-2} (\mathcal{K}^{(\ell)}(z,\bar{z}|s) + \mathcal{K}^{(s-1)}(z,\bar{z}|s)\mathcal{R}^{(\ell)}_{(s-1)}(z,\bar{z}|s-1))\partial_{(\ell)}\vec{Z}(z,\bar{z}|s) \stackrel{!}{=} \delta_{\mathcal{W}_{s-1}}\vec{Z}(z,\bar{z}|s) \\ &= \sum_{\ell=1}^{s-2} \mathcal{K}^{(\ell)}(z,\bar{z}|s-1)\partial_{(\ell)}\vec{Z}(z,\bar{z}|s).\end{aligned} \tag{6.3}$$

Upon requiring that $\delta_{\mathcal{W}_s}\vec{Z}(z,\bar{z}|s) = \delta_{\mathcal{W}_{s-1}}\vec{Z}(z,\bar{z}|s)$, one can identify the top tensorial ghost of the level $s-1$ in terms of those of the upper level s through the structure functions of the level $s-1$, by

$$\mathcal{K}^{(s-2)}(z,\bar{z}|s-1) = \mathcal{K}^{(s-2)}(z,\bar{z}|s) + \mathcal{K}^{(s-1)}(z,\bar{z}|s)\mathcal{R}^{(s-2)}_{(s-1)}(z,\bar{z}|s-1). \tag{6.4}$$

Repeating the DOR from the level s to an arbitrary sublevel j, with $2 \leqslant j \leqslant s-1$, the requirement that $\delta_{\mathcal{W}_s}\vec{Z}(z,\bar{z}|s) = \delta_{\mathcal{W}_j}\vec{Z}(z,\bar{z}|s)$ yields for each top tensorial ghost

$$\mathcal{K}^{(j-1)}(z,\bar{z}|j) = \mathcal{K}^{(j-1)}(z,\bar{z}|s) + \sum_{m=j}^{s-1} \mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(j-1)}_{(m)}(z,\bar{z}|j) = \sum_{m=j-1}^{s-1} \mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(j-1)}_{(m)}(z,\bar{z}|j). \tag{6.5}$$

Next, taking the ghost of highest conformal weight in each of the subalgebras, one generates a hierarchy of j-contravariant conformal tensors as

$$\mathcal{C}^{(j)}(z,\bar{z}) := \mathcal{K}^{(j)}(z,\bar{z}|j+1). \tag{6.6}$$

All the above-noted considerations suggest to take as an ansatz for the j-contravariant ghost conformal tensors the following pretty tricky linear combination:

$$\mathcal{C}^{(j)}(z,\bar{z}) = \sum_{m=j}^{s-1} \mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(j)}_{(m)}(z,\bar{z}|j+1) \quad \text{for } 1 \leqslant j \leqslant s-1, \tag{6.7}$$

where the lower orders of truncation (implemented by the $\mathrm{DOR}_{s-1\to j}$) crucially enter the construction. Due to the requirement that $\delta_{\mathcal{W}}\vec{Z}(z,\bar{z}|s) = \delta_{\mathcal{W}_k}\vec{Z}(z,\bar{z}|s)$, for $k=2,\ldots,s$, it is worthwhile to emphasize that the tensorial ghosts $\mathcal{C}^{(j)}$ carry an universal nature (regarding all the hierarchy of

$\mathcal{W}_j$-algebras), in the sense that for $j=1,\ldots,k-1$, $k\geqslant j+1$ one has the identity

$$\mathcal{C}^{(j)}(z,\bar{z})=\sum_{m=j}^{s-1}\mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(j)}_{(m)}(z,\bar{z}|j+1)=\sum_{m=j}^{k-1}\mathcal{K}^{(m)}(z,\bar{z}|k)\mathcal{R}^{(j)}_{(m)}(z,\bar{z}|j+1). \tag{6.8}$$

The latter (which generalizes (6.7)) shows that the $\mathcal{C}^{(j)}$'s do not depend on the level k of truncation for $k\geqslant j$. This strongly suggests that the tensorial ghosts $\mathcal{C}^{(j)}$'s are of universal nature. Moreover, one gets for the $\mathrm{DOR}_{s-1\to k-1}$ and with $\ell=1,\ldots,k-1$,

$$\mathcal{K}^{(\ell)}(z,\bar{z}|k)=\mathcal{K}^{(\ell)}(z,\bar{z}|s)+\sum_{m=k}^{s-1}\mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(\ell)}_{(m)}(z,\bar{z}|k)=\sum_{m=1}^{s-1}\mathcal{K}^{(m)}(z,\bar{z}|s)\mathcal{R}^{(\ell)}_{(m)}(z,\bar{z}|k). \tag{6.9}$$

Next, by comparing in order to guarantee the transitivity property, $\mathrm{DOR}_{s-1\to j}$ with $\mathrm{DOR}_{s-1\to k-1}$ followed by $\mathrm{DOR}_{k-1\to j}$, the structure functions must verify for any $m\geqslant k$ with $j+1\leqslant k\leqslant s-1$,

$$\mathcal{R}^{(j)}_{(m)}(z,\bar{z}|j+1)=\sum_{\ell=j}^{k-1}\mathcal{R}^{(\ell)}_{(m)}(z,\bar{z}|k)\mathcal{R}^{(j)}_{(\ell)}(z,\bar{z}|j+1), \tag{6.10}$$

an identity which has to be checked with the help of (3.34) and both the choices of j and of $k-1$ coordinates among the $s-1$ coordinates given by $\vec{Z}\in\mathbb{C}P^{s-1}$ (identity between determinants). These two choices of subcoordinates define submanifolds in $\mathbb{C}P^{s-1}$. This phenomenon is the signature of the presence of flag manifolds denoted by $F_{j\cdots s-2}\mathbb{C}^{s-1}$ over $\mathbb{C}P^{s-1}$, a geometric concept already mentioned as related to $\mathcal{W}$-algebras in Ref. 5. In particular the choice $j=1$ and $k=s$ in (6.10) corresponds to the whole hierarchy (6.7) of the $\mathcal{C}$ ghosts and is associated to the flag manifold $F_{12\cdots s-2}\mathbb{C}^{s-1}$.

Owing to the above considerations, let us define now, for a fixed level s, the following nilpotent operator $\delta_{\mathcal{W}_s}=\overset{s-1}{\underset{\ell=2}{\oplus}}\delta_{\mathcal{W}_\ell}$, with $\delta^2_{\mathcal{W}_\ell}=0$ and $\{\delta_{\mathcal{W}_k},\delta_{\mathcal{W}_\ell}\}=0$, which is in some sense filtrated by the various sub-DORs relative to the flag submanifold $F_{12\cdots s-2}\mathbb{C}^{s-1}$. Then the task is to figure out the variations $\delta_{\mathcal{W}_s}\mathcal{C}^{(j)}$ for $j=1,\ldots,s-1$ in terms of the tensorial $\mathcal{C}$'s themselves.

Note that the tensorial ansatz (6.7) gives an universal character to each of the tensorial top ghosts $C^{(\ell-1)}(z,\bar{z})\coloneqq\mathcal{K}^{(\ell-1)}(z,\bar{z}|\,\ell)$ of each sublevels. By virtue of (6.9), the latter linearly depend on both the jet ghosts $\mathcal{K}(z,\bar{z}|\,\ell)$'s of the top order s of truncation and the structure functions relative to the various truncations up to order $s-1$.

In the course of checking that the $\mathcal{C}^{(j)}$'s are indeed j-contravariant conformal tensors, (5.5), (5.7) and the identities (5.8) were repeatedly used. The tensor character of $\mathcal{C}^{(j)}$ is secured by the choice of $\mathcal{R}^{(j)}_{(n)}(z,\bar{z}|j+1)$ with maximum upper index j relative to the truncation of level $j+1$. This is possible if one picks up these objects from the whole underlying DOR decompositions with a truncation mechanism at each level lower than s. So the price to pay is the introduction of all the $\mathcal{R}^{(j)}_{(n)}(z,\bar{z}|j+1)$ coefficients relative to all the (sub-)truncations from $j=1$ to $j=s-1$. The latter could have been implemented by a hierarchy of differential equations of the type (3.1). The ansatz (6.7) is a linear system in a Gauss form which is easily inverted as

$$\begin{gathered}\mathcal{K}^{(\ell)}(z,\bar{z}|s)=\sum_{m=\ell}^{s-1}\mathcal{C}^{(m)}(z,\bar{z})\mathcal{U}^{(\ell)}_{(m)}(z,\bar{z}|\,\ell+1,\ldots,s-1),\quad \ell=1,\ldots,s-2,\\ \mathcal{K}^{(s-1)}(z,\bar{z}|s)=\mathcal{C}^{(s-1)}(z,\bar{z}),\end{gathered} \tag{6.11}$$

where $\mathcal{U}^{(\ell)}_{(m)}(z,\bar{z}|\,\ell+1,\ldots,s-1)$ is the coefficient of the inverse upper triangular matrix which depends polynomially on structure functions pertaining to the sublevels from $\ell+1$ to $s-1$. More explicitly, for $k,\ell=1,\ldots,s-1$,

$$\mathcal{U}^{(\ell)}_{(k)}(z,\bar{z}|\,\ell\,+1,\ldots,s-1)=\begin{cases}1 & \text{if } k=\ell\\ 0 & \text{if } k<\ell\\ \displaystyle\sum_{j=1}^{k-\ell}(-1)^j\left[\prod_{i=1}^{j}\mathcal{R}^{(\ell_i)}_{(k_i)}(z,\bar{z}|\ell_i+1)\right]\Big|_{\substack{\ell_1=\ell,k_j=k\\ k_i>\ell_i\\ k_i=\ell_{i+1}\ \text{for}\ k-\ell\geqslant 2}} & \text{if } k>\ \ell\ .\end{cases} \tag{6.12}$$

The variation of the $\mathcal{C}^{(j)}$'s given by (6.7) is computed upon using the variation (4.2) for the level s and the variation (4.9) for all the sublevels up to $s-1$ owing to the DOR filtrations. It writes

$$\delta_{\mathcal{W}_s}\mathcal{C}^{(j)}(z,\bar{z})=\sum_{\ell=j}^{s-1}\left(\delta_{\mathcal{W}_s}\mathcal{K}^{(\ell)}(z,\bar{z}|s)\mathcal{R}^{(j)}_{(\ell)}(z,\bar{z}|j+1)-\mathcal{K}^{(\ell)}(z,\bar{z}|s)\delta_{\mathcal{W}_{j+1}}\mathcal{R}^{(j)}_{(\ell)}(z,\bar{z}|j+1)\right) \tag{6.13}$$

and after some algebra we get the following variation:

$$\begin{aligned}\delta_{\mathcal{W}_s}\mathcal{C}^{(j)}(z,\bar{z})=&\sum_{n=1}^{s-1}\sum_{a=n}^{s-1}\sum_{b=1}^{s-1}\sum_{r=0}^{n}\mathcal{C}^{(a)}(z,\bar{z})\partial_{(r)}\mathcal{C}^{(b)}(z,\bar{z})\mathcal{U}^{(n)}_{(a)}(z,\bar{z}|a+1,\ldots,s-1)\sum_{\ell=1}^{b}\sum_{k=r}^{n}\binom{k}{r}\binom{n}{k}\\
&\times\partial_{(k-r)}\mathcal{U}^{(\ell)}_{(b)}(z,\bar{z}|b+1,\ldots,s-1)\left(\sum_{p=j}^{s-1}\mathcal{R}^{(p)}_{(n+\ell-k)}(z,\bar{z}|s)\mathcal{R}^{(j)}_{(p)}(z,\bar{z}|j+1)\right)\\
&+\sum_{n=j}^{s-1}\sum_{a=n}^{s-1}\sum_{b=1}^{j}\left[\sum_{u=1}^{j}\sum_{r=0}^{u}\mathcal{C}^{(a)}(z,\bar{z})\partial_{(r)}\mathcal{C}^{(b)}(z,\bar{z})\mathcal{U}^{(n)}_{(a)}(z,\bar{z}|a+1,\ldots,s-1)\sum_{\ell=1}^{b}\sum_{k=r}^{u}\binom{k}{r}\binom{u}{k}\right.\\
&\times\partial_{(k-r)}\mathcal{U}^{(\ell)}_{(b)}(z,\bar{z}|b+1,\ldots,j)\mathcal{R}^{(u)}_{(n)}(z,\bar{z}|j+1)\mathcal{R}^{(j)}_{(u+\ell-k)}(z,\bar{z}|j+1)\\
&-\sum_{r=0}^{n}\mathcal{C}^{(a)}(z,\bar{z})\partial_{(r)}\mathcal{C}^{(b)}(z,\bar{z})\mathcal{U}^{(n)}_{(a)}(z,\bar{z}|a+1,\ldots,s-1)\sum_{\ell=1}^{b}\sum_{k=r}^{n}\binom{k}{r}\\
&\left.\times\partial_{(k-r)}\mathcal{U}^{(\ell)}_{(b)}(z,\bar{z}|b+1,\ldots,j)\mathcal{R}^{(j)}_{(n+\ell-k)}(z,\bar{z}|j+1)\right].\end{aligned} \tag{6.14}$$

Equation (6.14) can be disassembled into

$$\delta_{\mathcal{W}_s}\mathcal{C}^{(j)}(z,\bar{z})\equiv\sum_{n=1}^{j}n\mathcal{C}^{(n)}(z,\bar{z})\,\partial\,\mathcal{C}^{(j-n+1)}(z,\bar{z})+\chi^{(j)}(z,\bar{z}|j+1,\ldots,s), \tag{6.15}$$

where the first summand looks like the variation coming from a symplectic approach[11] to $\mathcal{W}$-algebra.

It is clear that the last term χ is related to the whole symmetry in the sense that it is a tensorial differential expression of ghost grading two in the various structure functions $\mathcal{R}$'s of the sublevel. Due to the nilpotency of the $\delta_{\mathcal{W}_s}$ BRS operation, the $\chi^{(j)}$'s defined in (6.15) do transform according to

$$\begin{aligned}\delta_{\mathcal{W}_s}\chi^{(j)}(z,\bar{z}|j+1,\ldots,s)=&\sum_{n=1}^{j}n(\mathcal{C}^{(n)}(z,\bar{z})\,\partial\,\chi^{(j-n+1)}(z,\bar{z}|j+1,\ldots,s)\\
&-\chi^{(n)}(z,\bar{z}|j+1,\ldots,s)\,\partial\,\mathcal{C}^{(j-n+1)}(z,\bar{z})).\end{aligned} \tag{6.16}$$

The full completion of the last equation (6.16) amounts to introducing (together with their $\mathcal{W}_s$-variations) all sets of primary fields ($\mathcal{W}$-currents) which belong to the tower of all the nested subalgebras according to the DOR filtration and the respective variations for each sublevels. This

provides a general solution for any j, and is, according to our opinion, the most general explicit expression given, up to now, for *any* $\mathcal{W}$-algebra in a BRS setting. Of course, the generic expression (6.14) contains the $\mathcal{R}$ reduction coefficients of *all* the Forsyth subframes. However, the variations given by Eq. (6.14) do not generally coincide with the ones found in the literature: this fact will be illustrated in the next two examples. In order to recover the familiar expressions[12,23] nontrivial redefinitions of the tensorial ghosts involving derivative terms must be performed. The ansatz (6.11) relating the jet ghosts to the tensorial ones is recast into the form:[15]

$$\text{for } \ell = 1, \ldots, s-2, \quad \mathcal{K}^{(\ell)}(z,\bar{z}|s) = \mathcal{C}^{(\ell)}(z,\bar{z}) + \sum_{p=\ell+1}^{s-1} \sum_{r=0}^{p-\ell} \partial_{(r)} \mathcal{C}^{(p)}(z,\bar{z}) \mathcal{T}_{(p)}^{(r,\ell)}(z,\bar{z}|s), \tag{6.17}$$

where derivatives in the tensorial ghosts explicitly enter and where $\mathcal{T}_{(p)}^{(b,m)}(z,\bar{z}|s)$ depends only on the structure functions $\mathcal{R}_{(s)}^{(\ell)}(z,\bar{z}|s)$, $\ell=1,\ldots,s-1$ with $\mathcal{T}_{(p)}^{(r,m)}(z,\bar{z}|s)=0$ for $p<m$ and $\mathcal{T}_{(p)}^{(r,m)}(z,\bar{z}|s)=\delta_{(0)}^{(r)}$ for $p=m$.

In this case, the new $\chi^{(j)}$'s will depend only on the structure functions of the level s. So, we stress, that this is a consequence of the technical difficulties coming from the jets to tensor reduction, and it is not a problem of the $\mathcal{W}$-symmetry itself.

In fact this is deduced by searching the algebraic conditions (in terms of ghosts and their derivatives, considered as independent fields), which put to zero, in all the equations (6.14) all the terms containing the structure functions of the sublevels $\mathcal{R}(z,\bar{z}|j)$, for $j<s$. For s of reasonable order, we find that the number of vanishing conditions allows one to get an unique solution, and numerically provides the $\mathcal{W}$ examples found in the literature.

The present upshot greatly improves some previous work[27,31] in the sense that it is now possible to construct explicitly the χ-term which breaks by truncation the $\mathcal{W}_\infty$-symmetry governed by an underlying symplectomorphism symmetry[11,32] to a finite $\mathcal{W}_s$-algebra.

To distinguish in a clear way a realization of such a $\mathcal{W}_s$-structure, the $\mathcal{W}_3$ and $\mathcal{W}_4$ cases will be next computed in great detail. Then, despite the lack of well-settled examples in the literature for (even if some examples exist[33,34]) $\mathcal{W}_s$ ($s\geqslant 5$), remarkable results in Ref. 10 will allow one to find out a general setting.

A. The $\mathcal{W}_3$ example

According to the general construction, one has with $s=3$ as top level, the two tensorial ghosts

$$\begin{aligned} \mathcal{C}^{(1)}(z,\bar{z}) &= \mathcal{K}^{(1)}(z,\bar{z}|2) = \mathcal{K}^{(1)}(z,\bar{z}|3) + \mathcal{K}^{(2)}(z,\bar{z}|3)\mathcal{R}_{(2)}^{(1)}(z,\bar{z}|2), \\ \mathcal{C}^{(2)}(z,\bar{z}) &= \mathcal{K}^{(2)}(z,\bar{z}|3), \end{aligned} \tag{6.18}$$

and their holomorphically covariant variations according to the DOR filtration read

$$\begin{aligned} \delta_{\mathcal{W}_3}\mathcal{C}^{(2)}(z,\bar{z}) &= \mathcal{C}^{(1)}(z,\bar{z})\,\partial\mathcal{C}^{(2)}(z,\bar{z}) + 2\mathcal{C}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(1)}(z,\bar{z}) + \mathcal{C}^{(2)}(z,\bar{z})\partial_{(2)}\mathcal{C}^{(2)}(z,\bar{z}) \\ &\quad + \mathcal{C}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(2)}(z,\bar{z})[2\mathcal{R}_{(3)}^{(2)}(z,\bar{z}|3) - 3\mathcal{R}_{(2)}^{(1)}(z,\bar{z}|2)], \end{aligned} \tag{6.19}$$

$$\begin{aligned} \delta_{\mathcal{W}_3}\mathcal{C}^{(1)}(z,\bar{z}) &= \mathcal{C}^{(1)}(z,\bar{z})\,\partial\mathcal{C}^{(1)}(z,\bar{z}) + 2\mathcal{C}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(2)}(z,\bar{z})[\mathcal{R}_{(3)}^{(1)}(z,\bar{z}|3) - \partial\mathcal{R}_{(2)}^{(1)}(z,\bar{z}|2) \\ &\quad + \mathcal{R}_{(3)}^{(2)}(z,\bar{z}|3)\mathcal{R}_{(2)}^{(1)}(z,\bar{z}|2) - (\mathcal{R}_{(2)}^{(1)}(z,\bar{z}|2))^2], \end{aligned} \tag{6.20}$$

where in the course of the calculation Eq. (3.31) has been used. Performing the holomorphically covariant change of generators

$$\mathcal{C}^{(1)}(z,\bar{z}) \to \widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) := \mathcal{C}^{(1)}(z,\bar{z}) + \tfrac{1}{2}\,\partial\mathcal{C}^{(2)}(z,\bar{z}) + \mathcal{C}^{(2)}(z,\bar{z})\Big[\tfrac{2}{3}\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3) - \mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)\Big], \tag{6.21}$$

allows one to remove the $\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)$ dependence and (6.11) rewrites

$$\begin{aligned}\mathcal{K}^{(1)}(z,\bar{z}|3) &= \widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) - \tfrac{1}{2}\,\partial\mathcal{C}^{(2)}(z,\bar{z}) - \tfrac{2}{3}\mathcal{C}^{(2)}(z,\bar{z})\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3),\\ \mathcal{K}^{(2)}(z,\bar{z}|3) &= \mathcal{C}^{(2)}(z,\bar{z}),\end{aligned} \tag{6.22}$$

and depends only on the level $s=3$. Next, we get the well-known transformations[12,27] upon redefining $\widetilde{\mathcal{C}}^{(2)}=\frac{1}{2}\mathcal{C}^{(2)}$ by a numerical rescaling

$$\begin{aligned}\delta_{\mathcal{W}_3}\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) &= \widetilde{\mathcal{C}}^{(1)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) - \tfrac{4}{3}\mathcal{T}_{(2)}(z,\bar{z}|3)\mathcal{C}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(2)}(z,\bar{z})\\ &\quad + \tfrac{1}{4}\big(\partial\mathcal{C}^{(2)}(z,\bar{z})\partial^2\mathcal{C}^{(2)}(z,\bar{z}) - \tfrac{2}{3}\mathcal{C}^{(2)}(z,\bar{z})\partial^3\mathcal{C}^{(2)}(z,\bar{z})\big)\delta_{\mathcal{W}_3}\\ \delta_{\mathcal{W}_3}\mathcal{C}^{(2)}(z,\bar{z}) &= \widetilde{\mathcal{C}}^{(1)}(z,\bar{z})\,\partial\mathcal{C}^{(2)}(z,\bar{z}) + 2\mathcal{C}^{(2)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}),\end{aligned} \tag{6.23}$$

where the expected combination (3.37) which introduces into the game a projective connection, is recovered for the case $s=3$,

$$\mathcal{T}_{(2)}(z,\bar{z}|3) = \tfrac{1}{2}\Big(\partial\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3) - \tfrac{1}{3}(\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3))^2 - \mathcal{R}^{(1)}_{(3)}(z,\bar{z}|3)\Big) = \tfrac{1}{2}a^{(3)}_{(2)}(z,\bar{z}), \tag{6.24}$$

an expression which depends on the level $s=3$ only. The remarkable fact in the course of the computation of (6.23) is that all the quantities pertaining to the suborder 2 of truncation have disappeared thanks to the change of generators (6.21) in the tensorial sector.

Comforted into this approach, one can compute also the variation of $\mathcal{T}_{(2)}(z,\bar{z}|3)$. After a straightforward but rather tedious calculation one successively obtains

$$\begin{aligned}\delta_{\mathcal{W}_3}\mathcal{T}_{(2)}(z,\bar{z}|3) &= (\partial_{(3)}\mathcal{K}^{(1)} + 2\mathcal{T}_{(2)}\,\partial\mathcal{K}^{(1)} + \mathcal{K}^{(1)}\mathcal{T}_{(2)})(z,\bar{z}|3) + \Big(\mathcal{K}^{(2)}\Big[\partial_{(3)}\mathcal{R}^{(2)}_{(3)} + \partial_{(2)}\mathcal{R}^{(1)}_{(3)} + \partial_{(2)}(\mathcal{R}^{(2)}_{(3)})^2\\ &\quad - \tfrac{2}{3}\mathcal{R}^{(2)}_{(3)}\partial_{(2)}\mathcal{R}^{(2)}_{(3)} - \tfrac{2}{3}\mathcal{R}^{(2)}_{(3)}\,\partial(\mathcal{R}^{(2)}_{(3)})^2 - 2\mathcal{R}^{(1)}_{(3)}\,\partial\mathcal{R}^{(2)}_{(3)} - \tfrac{4}{3}\mathcal{R}^{(2)}_{(3)}\,\partial\mathcal{R}^{(1)}_{(3)}\Big] + \partial\mathcal{K}^{(2)}\Big[4\partial_{(2)}\mathcal{R}^{(2)}_{(3)}\\ &\quad + \partial\mathcal{R}^{(1)}_{(3)} + \partial(\mathcal{R}^{(2)}_{(3)})^2 - \tfrac{2}{3}(\mathcal{R}^{(2)}_{(3)})^3 - \tfrac{7}{3}\mathcal{R}^{(2)}_{(3)}\mathcal{R}^{(1)}_{(3)}\Big] + \partial_{(2)}\mathcal{K}^{(2)}\Big[5\,\partial\mathcal{R}^{(2)}_{(3)} - \mathcal{R}^{(1)}_{(3)} - \tfrac{1}{3}(\mathcal{R}^{(2)}_{(3)})^2\Big]\\ &\quad + \tfrac{4}{3}\mathcal{R}^{(2)}_{(3)}\partial_{(3)}\mathcal{K}^{(2)} + \partial_{(4)}\mathcal{K}^{(2)}\Big)(z,\bar{z}|3),\end{aligned} \tag{6.25}$$

in terms of the two $\mathcal{K}$ ghosts and the structure functions relative to the level $s=3$. According to (6.22), this variation can be reexpressed in terms of the two tensorial $\widetilde{\mathcal{C}}$ ghosts as

$$\begin{aligned}\delta_{\mathcal{W}_3}\mathcal{T}_{(2)}(z,\bar{z}|3) &= \partial_{(3)}\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) + 2\mathcal{T}_{(2)}(z,\bar{z}|3)\,\partial\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) + \widetilde{\mathcal{C}}^{(1)}(z,\bar{z})\mathcal{T}_{(2)}(z,\bar{z}|3) - 2\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\,\partial\Big[\tfrac{1}{6}\partial_{(2)}\mathcal{R}^{(2)}_{(3)}\\ &\quad - \tfrac{1}{6}\,\partial(\mathcal{R}^{(2)}_{(3)})^2 + \tfrac{1}{3}\mathcal{R}^{(2)}_{(3)}\mathcal{R}^{(1)}_{(3)} + \tfrac{2}{27}(\mathcal{R}^{(2)}_{(3)})^3 - \tfrac{1}{2}\,\partial\mathcal{R}^{(1)}_{(3)}\Big](z,\bar{z}|3) - 3\,\partial\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\Big[\tfrac{1}{6}\partial_{(2)}\mathcal{R}^{(2)}_{(3)}\\ &\quad - \tfrac{1}{6}\,\partial(\mathcal{R}^{(2)}_{(3)})^2 + \tfrac{1}{3}\mathcal{R}^{(2)}_{(3)}\mathcal{R}^{(1)}_{(3)} + \tfrac{2}{27}(\mathcal{R}^{(2)}_{(3)})^3 - \tfrac{1}{2}\,\partial\mathcal{R}^{(1)}_{(3)}\Big](z,\bar{z}|3).\end{aligned} \tag{6.26}$$

The expression between the brackets corresponds to the associated W_3-current as a cubic differential relative to the level $s=3$ (up to a factor),

$$\begin{aligned}8W_{(3)}(z,\bar{z}|3) &= \Big(\tfrac{1}{6}\partial_{(2)}\mathcal{R}^{(2)}_{(3)} - \tfrac{1}{6}\,\partial(\mathcal{R}^{(2)}_{(3)})^2 + \tfrac{1}{3}\mathcal{R}^{(2)}_{(3)}\mathcal{R}^{(1)}_{(3)} + \tfrac{2}{27}(\mathcal{R}^{(2)}_{(3)})^3 - \tfrac{1}{2}\,\partial\mathcal{R}^{(1)}_{(3)}\Big)(z,\bar{z}|3)\\ &= \Big(\tfrac{1}{2}\,\partial a^{(3)}_{(2)} - a^{(3)}_{(3)}\Big)(z,\bar{z}),\end{aligned} \tag{6.27}$$

where the $a^{(3)}$'s were given in (3.39).

To sump up, the general conformally covariant differential operator (3.1) for $s=3$ can be recast in terms of the two $\mathcal{W}$-currents

$$L_3(z,\bar{z}) = \partial_{(3)} + 2\mathcal{T}_{(2)}(z,\bar{z}|3)\,\partial + \partial\mathcal{T}_{(2)}(z,\bar{z}|3) - 8W_{(3)}(z,\bar{z}|3), \tag{6.28}$$

where the last type $(3,0)$-term indicates the difference with the so-called Bol operator of order 3, see e.g., Ref. 24.

At the level of the BRS differential algebra, dropping the tilde $(\tilde{\ })$ for the tensorial ghosts, one has an explicit realization of the so-called principal $\mathcal{W}_3$-algebra, related to what it is called the pure $\mathcal{W}_3$-gravity.[35] The nilpotent BRS algebra for $\mathcal{W}_3$ writes in terms of an $\mathcal{S}$-operation acting on $\mathcal{T}$ and $W_{(3)}$ which are of spin 2 and spin 3 $\mathcal{W}$-currents, respectively, and of two conformal ghost fields $\mathcal{C}^{(1)},\mathcal{C}^{(2)}$,

$$\begin{aligned}
\mathcal{S}\mathcal{C}^{(1)} &= \mathcal{C}^{(1)}\,\partial\mathcal{C}^{(1)} + \partial\mathcal{C}^{(2)}\partial^2\mathcal{C}^{(2)} - \tfrac{2}{3}\mathcal{C}^{(2)}\partial^3\mathcal{C}^{(2)} - \tfrac{16}{3}\mathcal{T}\mathcal{C}^{(2)}\,\partial\mathcal{C}^{(2)},\\
\mathcal{S}\mathcal{C}^{(2)} &= \mathcal{C}^{(1)}\,\partial\mathcal{C}^{(2)} + 2\mathcal{C}^{(2)}\,\partial\mathcal{C}^{(1)},\\
\mathcal{S}\mathcal{T} &= \partial^3\mathcal{C}^{(1)} + 2\mathcal{T}\partial\mathcal{C}^{(1)} + \mathcal{C}^{(1)}\,\partial\mathcal{T} - 8(2\mathcal{C}^{(2)}\,\partial W_{(3)} + 3W_{(3)}\,\partial\mathcal{C}^{(2)}),
\end{aligned} \tag{6.29}$$

$$\begin{aligned}
\mathcal{S}W_{(3)} = {}& \tfrac{1}{24}(\partial^5\mathcal{C}^{(2)} + 2\mathcal{C}^{(2)}\partial^3\mathcal{T} + 10\mathcal{T}\partial^3\mathcal{C}^{(2)} + 15\,\partial\mathcal{T}\partial^2\mathcal{C}^{(2)} + 9\partial^2\mathcal{T}\partial\mathcal{C}^{(2)} + 16\mathcal{T}\partial\mathcal{T}\mathcal{C}^{(2)} + 16\mathcal{T}^2\,\partial\mathcal{C}^{(2)})\\
&+ \mathcal{C}^{(1)}\,\partial W_{(3)} + 3W_{(3)}\,\partial\mathcal{C}^{(1)}.
\end{aligned}$$

However, at the practical level, the $\mathcal{W}_3$ case stands as a particular example in the sense that the change of generators emerges by itself. But for the instance of $\mathcal{W}_4$, it is not evident at first sight, to figure out which change of generators for $C^{(1)}$ and $C^{(2)}$ must be performed. For the moment, there is no general criterion at our disposal giving any guidance on that step. Nevertheless, an explicit realization of the so-called principal $\mathcal{W}_4$-algebra can be constructed along both the ideas of respecting the covariance and the dependence of the top level $s=4$ only. These two main ideas are the crux of all the construction and must be explained in a more geometric setup.

B. The $\mathcal{W}_4$ case

According to the general construction, this time one has with $s=4$ as top level the three tensorial ghosts

$$\begin{aligned}
\mathcal{C}^{(1)}(z,\bar{z}) &= \mathcal{K}^{(1)}(z,\bar{z}|2) = \mathcal{K}^{(1)}(z,\bar{z}|4) + \mathcal{K}^{(2)}(z,\bar{z}|4)\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2) + \mathcal{K}^{(3)}(z,\bar{z}|4)\mathcal{R}^{(1)}_{(3)}(z,\bar{z}|2),\\
\mathcal{C}^{(2)}(z,\bar{z}) &= \mathcal{K}^{(2)}(z,\bar{z}|3) = \mathcal{K}^{(2)}(z,\bar{z}|4) + \mathcal{K}^{(3)}(z,\bar{z}|4)\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3),\\
\mathcal{C}^{(3)}(z,\bar{z}) &= \mathcal{K}^{(3)}(z,\bar{z}|4).
\end{aligned} \tag{6.30}$$

The holomorphically covariant variation according to the DOR filtration of the top ghost is found to be

$$\begin{aligned}
\delta_{\mathcal{W}_4}\mathcal{C}^{(3)}(z,\bar{z}) = {}& (\mathcal{C}^{(1)}\,\partial\mathcal{C}^{(3)} + 3\mathcal{C}^{(3)}\,\partial\mathcal{C}^{(1)} + 2\mathcal{C}^{(2)}\,\partial\mathcal{C}^{(2)} + \mathcal{C}^{(3)}\partial_{(3)}\mathcal{C}^{(3)} + 3\mathcal{C}^{(3)}\partial_{(2)}\mathcal{C}^{(2)} + \mathcal{C}^{(2)}\partial_{(2)}\mathcal{C}^{(3)})(z,\bar{z})\\
&+ (\mathcal{C}^{(3)}\,\partial\mathcal{C}^{(3)})(z,\bar{z})[3\,\partial\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) + 3\mathcal{R}^{(2)}_{(4)}(z,\bar{z}|4) + 3(\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4))^2 - 6\,\partial\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3)\\
&- 4\,\partial\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2) - 5\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3)\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - 4(\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2))^2 + 4\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)\mathcal{R}^{(2)}_{(3)}\\
&\times(z,\bar{z}|3) + 2(\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3))^2] + (\mathcal{C}^{(3)}\partial_{(2)}\mathcal{C}^{(3)})(z,\bar{z})[3\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - 4\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3)]\\
&+ (\mathcal{C}^{(3)}\mathcal{C}^{(2)})(z,\bar{z})[2\,\partial\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3) - 3\,\partial\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)] + (\mathcal{C}^{(2)}\,\partial\mathcal{C}^{(3)})(z,\bar{z})[2\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)
\end{aligned}$$

$$- 2\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3) - \mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)] + (\mathcal{C}^{(3)}\,\partial\,\mathcal{C}^{(2)})(z,\bar{z})[3\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - 2\mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3)$$
$$- 3\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)]. \tag{6.31}$$

The general ansatz for the conformally covariant change of ghosts which does lead to the cancellation of the structure functions of the sublevels ($s=2,3$) in the above variation (6.31) is given by

$$\begin{aligned}\mathcal{C}^{(2)}(z,\bar{z}) &= \tilde{\mathcal{C}}^{(2)}(z,\bar{z}) + H_{(0)}(z,\bar{z})\,\partial\,\mathcal{C}^{(3)}(z,\bar{z}) + H_{(1)}(z,\bar{z})\mathcal{C}^{(3)}(z,\bar{z}),\\ \mathcal{C}^{(1)}(z,\bar{z}) &= \tilde{\mathcal{C}}^{(1)}(z,\bar{z}) + F_{(0)}(z,\bar{z})\,\partial\,\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) + F_{(1)}(z,\bar{z})\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) + L_{(0)}(z,\bar{z})\partial_{(2)}\mathcal{C}^{(3)}(z,\bar{z})\\ &\quad + L_{(1)}(z,\bar{z})\,\partial\,\mathcal{C}^{(3)}(z,\bar{z}) + L_{(2)}(z,\bar{z})\mathcal{C}^{(3)}(z,\bar{z}).\end{aligned} \tag{6.32}$$

Cancellation of the sublevels in (6.31) gives

$$H_{(0)}(z,\bar{z}) = -\tfrac{1}{2}, \quad F_{(0)}(z,\bar{z}) = -1, \quad H_{(1)}(z,\bar{z}) = \mathcal{R}^{(2)}_{(3)}(z,\bar{z}|3) - \tfrac{3}{4}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)$$

$$F_{(1)}(z,\bar{z}) = \mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2) - \tfrac{1}{2}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4), \quad L_{(1)}(z,\bar{z}) = \tfrac{1}{4}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - \tfrac{1}{2}\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2) - \partial L_{(0)}(z,\bar{z}),$$

and the gluing rules for $\mathcal{C}^{(1)}$ infers $L_{(0)}(z,\bar{z})=\frac{1}{5}$. Plugging these results into (6.32) and inverting (6.30) the three $\mathcal{K}$ ghosts of the level $s=4$ are reexpressed as

$$\mathcal{K}^{(3)}(z,\bar{z}|4) = \mathcal{C}^{(3)}(z,\bar{z}),$$

$$\begin{aligned}\mathcal{K}^{(2)}(z,\bar{z}|4) &= \tilde{\mathcal{C}}^{(2)}(z,\bar{z}) - \tfrac{1}{2}\,\partial\,\mathcal{C}^{(3)}(z,\bar{z}) - \tfrac{3}{4}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)\mathcal{C}^{(3)}(z,\bar{z}),\\ \mathcal{K}^{(1)}(z,\bar{z}|4) &= \tilde{\mathcal{C}}^{(1)}(z,\bar{z}) - \partial\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) - \tfrac{1}{2}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) + \tfrac{1}{5}\partial_{(2)}\mathcal{C}^{(3)}(z,\bar{z})\\ &\quad + \tfrac{1}{4}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)\,\partial\,\mathcal{C}^{(3)}(z,\bar{z}) + \mathcal{C}^{(3)}(z,\bar{z})\Big(L_{(2)}(z,\bar{z}) + \tfrac{3}{4}\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - \mathcal{R}^{(1)}_{(3)}(z,\bar{z}|2)\Big).\end{aligned} \tag{6.33}$$

Since there are various possibilities to cancel the sublevels, the remaining function coefficient $L_{(2)}(z,\bar{z})$ must be determined with the help of $\delta_{\mathcal{W}_4}\tilde{\mathcal{C}}^{(2)}$ computed from the second equation of (6.33) and the known variations at the level $s=4$ for $\mathcal{K}^{(3)}(z,\bar{z}|4)$, $\mathcal{K}^{(2)}(z,\bar{z}|4)$, and $\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)$ according to the general theory. This step will secure the nilpotency $\delta^2_{\mathcal{W}_4}=0$. After lengthy computations performed with the help of MATHEMATICA, one ends with

$$L_{(2)}(z,\bar{z}) = \tfrac{12}{25}\,\partial\,\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - \tfrac{3}{25}(\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4))^2 - \tfrac{41}{50}\mathcal{R}^{(2)}_{(4)}(z,\bar{z}|4) - \tfrac{3}{4}\mathcal{R}^{(1)}_{(2)}(z,\bar{z}|2)\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) + \mathcal{R}^{(1)}_{(3)}(z,\bar{z}|2),$$

which once substituted yields

$$\begin{aligned}\mathcal{K}^{(1)}(z,\bar{z}|4) &= \tilde{\mathcal{C}}^{(1)}(z,\bar{z}) - \partial\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) - \tfrac{1}{2}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)\tilde{\mathcal{C}}^{(2)}(z,\bar{z}) + \tfrac{1}{5}\partial_{(2)}\mathcal{C}^{(3)}(z,\bar{z}) + \tfrac{1}{4}\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)\,\partial\,\mathcal{C}^{(3)}(z,\bar{z})\\ &\quad + \mathcal{C}^{(3)}(z,\bar{z})\Big(\tfrac{12}{25}\Big(\partial\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4) - \tfrac{1}{4}(\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4))^2\Big) - \tfrac{41}{50}\mathcal{R}^{(2)}_{(4)}(z,\bar{z}|4)\Big).\end{aligned} \tag{6.34}$$

This shows that the system (6.11) can be rewritten in terms of the structure functions of the level $s=4$ only thanks to the redefinition (6.32) of the tensorial ghosts coming from the sublevels. Recall that these redefinitions are required for reabsorbing the structure functions of the sublevels. The change of generators (6.33) also confirms the general ansatz (6.17) given in Ref. 15. The variation (6.31) then reduces to

$$\delta_{\mathcal{W}_4}\mathcal{C}^{(3)}(z,\bar{z}) = \widetilde{\mathcal{C}}^{(1)}(z,\bar{z})\,\partial\mathcal{C}^{(3)}(z,\bar{z}) + 3\mathcal{C}^{(3)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) + 2\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(2)}(z,\bar{z}) + \tfrac{1}{10}(\mathcal{C}^{(3)}(z,\bar{z})\partial_{(3)}\mathcal{C}^{(3)} \times(z,\bar{z}) - 2\,\partial\mathcal{C}^{(3)}(z,\bar{z})\partial_{(2)}\mathcal{C}^{(3)}(z,\bar{z}) + 14\mathcal{T}_{(2)}(z,\bar{z}|4)\mathcal{C}^{(3)}(z,\bar{z})\,\partial\mathcal{C}^{(3)}(z,\bar{z})) \tag{6.35}$$

from which emerges the projective connection $\mathcal{T}_{(2)}(z,\bar{z}|4)$ associated to the level $s=4$,

$$\mathcal{T}_{(2)}(z,\bar{z}|4) := \left(\tfrac{3}{10}\,\partial\mathcal{R}^{(3)}_{(4)} - \tfrac{3}{40}(\mathcal{R}^{(3)}_{(4)})^2 - \tfrac{1}{5}\mathcal{R}^{(2)}_{(4)}\right)(z,\bar{z}|4) = \tfrac{1}{5}a^{(4)}_{(2)}(z,\bar{z}), \tag{6.36}$$

where $a^{(4)}_{(2)}$ given by (3.37) carries the projective connection property as was already checked by using the general gluing rules (3.36). The variation $\delta_{\mathcal{W}_4}\widetilde{\mathcal{C}}^{(2)}$ is then computed to be

$$\begin{aligned}\delta_{\mathcal{W}_4}\widetilde{\mathcal{C}}^{(2)}(z,\bar{z}) = {}& \widetilde{\mathcal{C}}^{(1)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(2)}(z,\bar{z}) + 2\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\,\partial\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) - \tfrac{3}{32}\mathcal{C}^{(3)}(z,\bar{z})\,\partial\mathcal{C}^{(3)}(z,\bar{z})W_{(3)}(z,\bar{z}|4)\\ & - \tfrac{1}{10}(\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\partial_{(3)}\mathcal{C}^{(3)}(z,\bar{z}) - 3\,\partial\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\partial_{(2)}\mathcal{C}^{(3)}(z,\bar{z}) + 5\partial_{(2)}\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(3)}(z,\bar{z})\\ & - 5\partial_{(3)}\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\mathcal{C}^{(3)}(z,\bar{z}) + (18\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\,\partial\mathcal{C}^{(3)}(z,\bar{z}) - 34\,\partial\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\mathcal{C}^{(3)}(z,\bar{z}))\mathcal{T}_{(2)}(z,\bar{z}|4)\\ & - 7\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\mathcal{C}^{(3)}(z,\bar{z})\,\partial\mathcal{T}_{(2)}(z,\bar{z}|4)),\end{aligned} \tag{6.37}$$

where one also gets the conformally covariant spin three $\mathcal{W}$-current associated to the top level $s=4$,

$$W_{(3)}(z,\bar{z}|4) := (8\,\partial\mathcal{R}^{(2)}_{(4)} - 4\partial_{(2)}\mathcal{R}^{(3)}_{(4)} + 3\,\partial(\mathcal{R}^{(3)}_{(4)})^2 - 4\mathcal{R}^{(2)}_{(4)}\mathcal{R}^{(3)}_{(4)} - 8\mathcal{R}^{(1)}_{(4)})(z,\bar{z}|4). \tag{6.38}$$

Going on through the computation of the variation with the help of the third equation in (6.33) and the known variations at the level $s=4$ for $\mathcal{C}^{(3)}$, $\widetilde{\mathcal{C}}^{(2)}$, $\mathcal{R}^{(3)}_{(4)}(z,\bar{z}|4)$ and $\mathcal{R}^{(2)}_{(4)}(z,\bar{z}|4)$, and after redefining $\mathcal{C}^{(3)} := -320\widetilde{\mathcal{C}}^{(3)}$ by a numerical factor for later convenience, one gets

$$\begin{aligned}\delta_{\mathcal{W}_4}\widetilde{\mathcal{C}}^{(1)}(z,\bar{z}) = {}& (\widetilde{\mathcal{C}}^{(1)}\,\partial\widetilde{\mathcal{C}}^{(1)})(z,\bar{z}) + \tfrac{3}{5}\left(\partial\widetilde{\mathcal{C}}^{(2)}\partial_{(2)}\widetilde{\mathcal{C}}^{(2)} - \tfrac{2}{3}\widetilde{\mathcal{C}}^{(2)}\partial_{(3)}\widetilde{\mathcal{C}}^{(2)} - \tfrac{16}{3}\widetilde{\mathcal{C}}^{(2)}\,\partial\widetilde{\mathcal{C}}^{(2)}\mathcal{T}_{(2)}(z,\bar{z}|4)\right)(z,\bar{z})\\ & + \left(20\widetilde{\mathcal{C}}^{(2)}\,\partial\widetilde{\mathcal{C}}^{(3)} - \tfrac{108}{5}\,\partial\widetilde{\mathcal{C}}^{(2)}\widetilde{\mathcal{C}}^{(3)}\right)(z,\bar{z})W_{(3)}(z,\bar{z}|4) + \tfrac{28}{5}\widetilde{\mathcal{C}}^{(2)}(z,\bar{z})\widetilde{\mathcal{C}}^{(3)}(z,\bar{z})\,\partial W_{(3)}(z,\bar{z}|4)\\ & + 1024[3\widetilde{\mathcal{C}}^{(3)}\partial_{(5)}\widetilde{\mathcal{C}}^{(3)} - 5\,\partial\widetilde{\mathcal{C}}^{(3)}\partial_{(4)}\widetilde{\mathcal{C}}^{(3)} + 6\partial_{(2)}\widetilde{\mathcal{C}}^{(3)}\partial_{(3)}\widetilde{\mathcal{C}}^{(3)} + 57\widetilde{\mathcal{C}}^{(3)}\partial_{(2)}\widetilde{\mathcal{C}}^{(3)}\,\partial\mathcal{T}_{(2)}(z,\bar{z}|4)\\ & + (78\widetilde{\mathcal{C}}^{(3)}\partial_{(3)}\widetilde{\mathcal{C}}^{(3)} - 118\,\partial\widetilde{\mathcal{C}}^{(3)}\partial_{(2)}\widetilde{\mathcal{C}}^{(3)})\mathcal{T}_{(2)}(z,\bar{z}|4) + \widetilde{\mathcal{C}}^{(3)}\,\partial\widetilde{\mathcal{C}}^{(3)}(57\partial_{(2)}\mathcal{T}_{(2)}(z,\bar{z}|4)\\ & + 432(\mathcal{T}_{(2)}(z,\bar{z}|4))^2 - 14W_{(4)}(z,\bar{z}|4))](z,\bar{z}),\end{aligned} \tag{6.39}$$

from where emerges a $\mathcal{W}$-current of spin 4 (a $(4,0)$-type conformally covariant differential) associated to the level $s=4$, as can be checked by using (3.36),

$$\begin{aligned}800W_{(4)}(z,\bar{z}|4) = {}& (144(\mathcal{R}^{(2)}_{(4)})^2 + 400\mathcal{R}^{(1)}_{(4)}\mathcal{R}^{(3)}_{(4)} + 208\mathcal{R}^{(2)}_{(4)}(\mathcal{R}^{(3)}_{(4)})^2 + 39(\mathcal{R}^{(3)}_{(4)})^4 - 800\,\partial\mathcal{R}^{(1)}_{(4)}\\ & - 400\mathcal{R}^{(3)}_{(4)}\,\partial\mathcal{R}^{(2)}_{(4)} - 432\mathcal{R}^{(2)}_{(4)}\,\partial\mathcal{R}^{(3)}_{(4)} - 104\,\partial(\mathcal{R}^{(3)}_{(4)})^3 + 264(\partial\mathcal{R}^{(3)}_{(4)})^2 + 320\partial_{(2)}\mathcal{R}^{(2)}_{(4)}\\ & + 240\mathcal{R}^{(3)}_{(4)}\partial_{(2)}\mathcal{R}^{(3)}_{(4)} - 80\partial_{(3)}\mathcal{R}^{(3)}_{(4)})(z,\bar{z}|4).\end{aligned} \tag{6.40}$$

Hence, the general conformally covariant differential operator (3.1) for $s=4$ expressed in terms of the three $\mathcal{W}_4$-currents is

$$\begin{aligned}L_4(z,\bar{z}) = {}& \partial_{(4)} + 5\mathcal{T}_{(2)}(z,\bar{z}|4)\partial_{(2)} + 5\,\partial\mathcal{T}_{(2)}(z,\bar{z}|4)\,\partial + \tfrac{3}{2}\left(\partial_{(2)}\mathcal{T}_{(2)}(z,\bar{z}|4) + \tfrac{3}{2}(\mathcal{T}_{(2)}(z,\bar{z}|4))^2\right)\\ & + \tfrac{1}{8}W_{(3)}(z,\bar{z}|4)\,\partial + \tfrac{1}{16}\,\partial W_{(3)}(z,\bar{z}|4) - \tfrac{1}{2}W_{(4)}(z,\bar{z}|4),\end{aligned} \tag{6.41}$$

where the first line is the Bol operator of order 4, see, e.g., Ref. 24, depending only on the projective connection $\mathcal{T}_{(2)}$.

All this BRS algebra is an explicit realization of the so-called principal $\mathcal{W}_4$-algebra for pure $\mathcal{W}_4$-gravity.[23,36] Performing the rescaling

$$\tilde{\mathcal{C}}^{(2)} \to -8i\sqrt{5}\tilde{\mathcal{C}}^{(2)}, \quad W_{(3)}(z,\bar{z}|4) \to \tfrac{i}{8\sqrt{5}} W_{(3)}(z,\bar{z}|4),$$

and dropping out both the tilde (~) for the tensorial ghosts and the explicit reference to the level $s=4$, one gets the presentation as a full nilpotent BRS algebra for $\mathcal{W}_4$-algebra,

$$\begin{aligned}
\mathcal{S}\mathcal{C}^{(1)} &= \mathcal{C}^{(1)}\partial\mathcal{C}^{(1)} - 192\Big(\partial\mathcal{C}^{(2)}\partial_{(2)}\mathcal{C}^{(2)} - \tfrac{2}{3}\mathcal{C}^{(2)}\partial_{(3)}\mathcal{C}^{(2)} - \tfrac{16}{3}\mathcal{T}\mathcal{C}^{(2)}\partial\mathcal{C}^{(2)}\Big) + 256(27\,\partial\mathcal{C}^{(2)}\mathcal{C}^{(3)}W_{(3)} \\
&\quad - 25\mathcal{C}^{(2)}\partial\mathcal{C}^{(3)}W_{(3)} - 7\mathcal{C}^{(2)}\mathcal{C}^{(3)}\partial W_{(3)}) + 1024(3\mathcal{C}^{(3)}\partial_{(5)}\mathcal{C}^{(3)} - 5\,\partial\mathcal{C}^{(3)}\partial_{(4)}\mathcal{C}^{(3)} + 6\partial_{(2)}\mathcal{C}^{(3)}\partial_{(3)}\mathcal{C}^{(3)} \\
&\quad + 57\partial_{(2)}\mathcal{T}\mathcal{C}^{(3)}\partial\mathcal{C}^{(3)} + 57\,\partial\mathcal{T}\mathcal{C}^{(3)}\partial_{(2)}\mathcal{C}^{(3)} + (78\mathcal{C}^{(3)}\partial_{(3)}\mathcal{C}^{(3)} - 118\,\partial\mathcal{C}^{(3)}\partial_{(2)}\mathcal{C}^{(3)})\mathcal{T} \\
&\quad - 14\mathcal{C}^{(3)}\partial\mathcal{C}^{(3)}W_{(4)} + 432\mathcal{C}^{(3)}\partial\mathcal{C}^{(3)}\mathcal{T}^2),
\end{aligned}$$

$$\begin{aligned}
\mathcal{S}\mathcal{C}^{(2)} &= \mathcal{C}^{(1)}\partial\mathcal{C}^{(2)} + 2\mathcal{C}^{(2)}\partial\mathcal{C}^{(1)} + 32(\mathcal{C}^{(2)}\partial_{(3)}\mathcal{C}^{(3)} - 3\,\partial\mathcal{C}^{(2)}\partial_{(2)}\mathcal{C}^{(3)} + 5\partial_{(2)}\mathcal{C}^{(2)}\partial\mathcal{C}^{(3)} - 5\partial_{(3)}\mathcal{C}^{(2)}\mathcal{C}^{(3)} \\
&\quad + 18\mathcal{C}^{(2)}\partial\mathcal{C}^{(3)}\mathcal{T} - 34\,\partial\mathcal{C}^{(2)}\mathcal{C}^{(3)}\mathcal{T} - 7\mathcal{C}^{(2)}\mathcal{C}^{(3)}\partial\mathcal{T}) - 9600\mathcal{C}^{(3)}\partial\mathcal{C}^{(3)}W_{(3)},
\end{aligned}$$

$$\mathcal{S}\mathcal{C}^{(3)} = \mathcal{C}^{(1)}\partial\mathcal{C}^{(3)} + 3\mathcal{C}^{(3)}\partial\mathcal{C}^{(1)} + 2\mathcal{C}^{(2)}\partial\mathcal{C}^{(2)} - 32(\mathcal{C}^{(3)}\partial_{(3)}\mathcal{C}^{(3)} - 2\,\partial\mathcal{C}^{(3)}\partial_{(2)}\mathcal{C}^{(3)} + 14\mathcal{T}\mathcal{C}^{(3)}\partial\mathcal{C}^{(3)}),$$

$$\mathcal{S}\mathcal{T} = \partial_{(3)}\mathcal{C}^{(1)} + 2\mathcal{T}\partial\mathcal{C}^{(1)} + \mathcal{C}^{(1)}\partial\mathcal{T} - 8(2\mathcal{C}^{(2)}\partial W_{(3)} + 3W_{(3)}\partial\mathcal{C}^{(2)}) + 32(3\mathcal{C}^{(3)}\partial W_{(4)} + 4W_{(4)}\partial\mathcal{C}^{(3)}), \tag{6.42}$$

$$\begin{aligned}
\mathcal{S}W_{(3)} &= \mathcal{C}^{(1)}\partial W_{(3)} + 3W_{(3)}\partial\mathcal{C}^{(1)} - 8(\partial_{(5)}\mathcal{C}^{(2)} + 2\mathcal{C}^{(2)}\partial_{(3)}\mathcal{T} + 10\mathcal{T}\partial_{(3)}\mathcal{C}^{(2)} + 15\,\partial\mathcal{T}\partial_{(2)}\mathcal{C}^{(2)} + 9\partial_{(2)}\mathcal{T}\partial\mathcal{C}^{(2)} \\
&\quad + 16\mathcal{T}\partial\mathcal{T}\mathcal{C}^{(2)} + 16\mathcal{T}^2\partial\mathcal{C}^{(2)} + \mathcal{C}^{(2)}\partial W_{(4)} + 2W_{(4)}\partial\mathcal{C}^{(2)}) + 32(5\mathcal{C}^{(3)}\partial_{(3)}W_{(3)} + 10\,\partial\mathcal{C}^{(3)}\partial_{(2)}W_{(3)} \\
&\quad + 28\partial_{(2)}\mathcal{C}^{(3)}\partial W_{(3)} + 14\partial_{(3)}\mathcal{C}^{(3)}W_{(3)} + 34\mathcal{C}^{(3)}\mathcal{T}\partial W_{(3)} + 27\mathcal{C}^{(3)}W_{(3)}\partial\mathcal{T} + 52\,\partial\mathcal{C}^{(3)}\mathcal{T}W_{(3)}),
\end{aligned}$$

$$\begin{aligned}
\mathcal{S}\mathcal{W}_{(4)} &= \mathcal{C}^{(1)}\partial W_{(4)} + 4W_{(4)}\partial\mathcal{C}^{(1)} - 8(\mathcal{C}^{(2)}\partial_{(3)}W_{(3)} + 6\,\partial\mathcal{C}^{(2)}\partial_{(2)}W_{(3)} + 14\partial_{(2)}\mathcal{C}^{(2)}\partial W_{(3)} \\
&\quad + 14\partial_{(3)}\mathcal{C}^{(2)}W_{(3)} + 18\mathcal{C}^{(2)}\mathcal{T}\partial W_{(3)} + 25\mathcal{C}^{(2)}\partial\mathcal{T}W_{(3)} + 52\,\partial\mathcal{C}^{(2)}\mathcal{T}W_{(3)}) + 32(\partial_{(7)}\mathcal{C}^{(3)} \\
&\quad + 3\mathcal{C}^{(3)}\partial_{(5)}\mathcal{T} + 20\,\partial\mathcal{C}^{(3)}\partial_{(4)}\mathcal{T} + 56\partial_{(2)}\mathcal{C}^{(3)}\partial_{(3)}\mathcal{T} + 84\partial_{(3)}\mathcal{C}^{(3)}\partial_{(2)}\mathcal{T} + 70\partial_{(4)}\mathcal{C}^{(3)}\partial\mathcal{T} + 28\partial_{(5)}\mathcal{C}^{(3)}\mathcal{T} \\
&\quad + \mathcal{C}^{(3)}(177\,\partial\mathcal{T}\partial_{(2)}\mathcal{T} + 78\mathcal{T}\partial_{(3)}\mathcal{T}) + \partial\mathcal{C}^{(3)}(352\mathcal{T}\partial_{(2)}\mathcal{T} + 295(\partial\mathcal{T})^2) + 588\partial_{(2)}\mathcal{C}^{(3)}\mathcal{T}\partial\mathcal{T} \\
&\quad + 196\partial_{(3)}\mathcal{C}^{(3)}\mathcal{T}^2 + 432\mathcal{C}^{(3)}\mathcal{T}^2\partial\mathcal{T} + 288\,\partial\mathcal{C}^{(3)}\mathcal{T}^3 + 75\mathcal{C}^{(3)}W_{(3)}\partial W_{(3)} + 75\,\partial\mathcal{C}^{(3)}(W_{(3)})^2 \\
&\quad - \mathcal{C}^{(3)}\partial_{(3)}W_{(4)} - 5\,\partial\mathcal{C}^{(3)}\partial_{(2)}W_{(4)} - 9\partial_{(2)}\mathcal{C}^{(3)}\partial W_{(4)} - 6\partial_{(3)}\mathcal{C}^{(3)}W_{(4)} - 14\mathcal{C}^{(3)}\partial(\mathcal{T}W_{(4)}) \\
&\quad - 28\,\partial\mathcal{C}^{(3)}\mathcal{T}W_{(4)}).
\end{aligned}$$

Recall once more that there is a breaking term in the top ghost variation $\mathcal{S}C^{(3)}$ with respect to the symplectic variation, so that the mechanisms using the so-called θ-trick described in previous papers[11,31] for the $\mathcal{W}_3$ case do not work in the $\mathcal{W}_4$ case. Let us remark that if one sets $\mathcal{C}^{(3)}=0$ and $W_{(4)}=0$ and performs the rescalings of the generators $\mathcal{C}^{(2)} \to (i\sqrt{3}/24)\mathcal{C}^{(2)}$ and $W_{(3)} \to -8i\sqrt{3}W_{(3)}$ in (6.42) then the $\mathcal{W}_3$-algebra (6.29) is recovered. This confirms the universal definition (6.6) of the tensorial ghosts as $\mathcal{C}^{(s-1)}(z,\bar{z}) = \mathcal{K}^{(s-1)}(z,\bar{z}|s)$ as the top ghost of each level s and also the interweaving of the algebras dictated by the successive DORs.

C. Comparison with some previous work

The general ansatz (6.17) given in Ref. 15 and exemplified in (6.22), (6.33), and (6.34) for $s=3,4$, respectively, can be put into relation with some previous pioneer work.[6,5,8,10] Indeed, Ref. 10 will be of particular interest. There "Beltrami differentials" emerging from a multi-time ap-

proach for Korteweg-de Vries (KdV) flows were related to "Bilal-Fock-Kogan" generalized tensorial Beltrami coefficients[5] appearing in $\mathcal{W}$-gravity along the ideas of Ref. 6. According to their contravariant behavior these various type of Beltrami deformation parameters can be used in order to recover our ansatz (6.17).

As said in Sec. I, working with either homogeneous or inhomogeneous coordinates seems to be a matter of taste. In our construction, the latter were preferred because they strengthen the role of the symmetry algebra.

If one considers the homogeneous solutions f of the sth order conformally covariant linear equation (3.1), these solutions as $((1-s)/2)$-conformal fields are equivalently subject to a DOR since the sth order derivative can be expressed in terms of the lower order ones and the smooth coefficient of the operator L_s. Their variation under large chiral diffeomorphisms were computed in Ref. 18 to be

$$\delta_{\mathcal{W}_s} f(z,\bar{z}) = \sum_{\ell=0}^{s-1} \mathcal{M}^{(\ell)}(z,\bar{z}|s)\partial_{(\ell)} f(z,\bar{z}). \tag{6.43}$$

This variation for homogeneous coordinates must be related to the variation (4.1) for the inhomogeneous coordinates. Indeed Eqs. (3.8), (3.27) allow one to find a complete link between the ghosts $\mathcal{K}^{(m)}(z,\bar{z}|s)$ and $\mathcal{M}^{(\ell)}(z,\bar{z}|s)$,

$$\mathcal{K}^{(m)}(z,\bar{z}|s) = \sum_{\ell=m}^{s-1} \binom{\ell}{m} \mathcal{M}^{(\ell)}(z,\bar{z}|s)\mathcal{Q}_{(\ell-m)}(z,\bar{z}|s), \quad m=1,\ldots,s-1 \tag{6.44}$$

and gives a direct answer to a problem raised in Ref. 6 about the $\mathcal{W}$ deformations of the f functions via the KdV "multi-time" approach, providing a direct expression of the KdV hierarchy.

Inspired by Ref. 10, one can mimic the construction used for relating KdV flows and $\mathcal{W}$-diffeomorphisms according to the following dictionary:

$$\delta \leftrightarrow \bar{\partial}, \quad \mathcal{M}^{(\ell)} \leftrightarrow \mu_\ell, \quad \text{and} \quad \widetilde{\mathcal{C}}^{(k)} \leftrightarrow \rho_k, \tag{6.45}$$

where the $\mathcal{M}$ play the role of the ghost parameters for KdV flows and $\widetilde{\mathcal{C}}$ (for the sake of consistency with the treated examples one uses the $\widetilde{\mathcal{C}}$ ghosts) those for the infinitesimal $\mathcal{W}$-diffeomorphisms.

One can conformally covariantize the variation (6.43) by introducing tensorial ghosts $\widetilde{\mathcal{C}}$ which serve to filtrate the variation by their conformal weight according to

$$\delta_{\mathcal{W}_s} f = \sum_{k=1}^{s-1} \mathfrak{B}_{(k)}(\widetilde{\mathcal{C}}^{(k)}, a_{(2)}^{(s)}) f, \tag{6.46}$$

where the $\mathfrak{B}_{(k)}$ are the conformally covariant differential operators constructed in Ref. 10 mapping $((1-s)/2)$ conformal fields into themselves. The coefficient function $a_{(2)}^{(s)}$ has a prominent role since it is related to a projective connection (see (3.37)) and controls the Möbius transformations. For $a_{(2)}^{(s)} \equiv 0$ (owing to (3.37) this implies a nontrivial differential constraint on the structure functions and then a kind of group contraction) one recalls that[10]

$$\mathfrak{B}_{(k)}(\widetilde{\mathcal{C}}^{(k)}, a_{(2)}^{(s)} \equiv 0) = \sum_{j=k}^{s-1} \gamma_{(k)}^{(k-j)}[s](\partial_{(mkj)}\widetilde{\mathcal{C}}^{(k)})\partial_{(j)} \tag{6.47}$$

with $\gamma_{(k)}^{(0)}[s]=1$ fixing the normalization between $\mathcal{M}$ and $\widetilde{\mathcal{C}}$. Comparison between the variations (6.43) and (6.46) yields

$$\mathcal{M}^{(0)}(z,\bar{z}|s)=\sum_{k=1}^{s-1}\gamma_{(k)}^{(k)}[s]\partial_{(k)}\widetilde{\mathcal{C}}^{(k)}(z,\bar{z}),$$

$$\mathcal{M}^{(\ell)}(z,\bar{z}|s)=\sum_{k=\ell}^{s-1}\gamma_{(k)}^{(k-\ell)}[s]\partial_{(k-\ell)}\widetilde{\mathcal{C}}^{(k)}(z,\bar{z}),\qquad \ell=1,\ldots,s-1, \tag{6.48}$$

where the numerical coefficients were given in[10]

$$\gamma_{(k)}^{(j)}[s]=(-1)^j\frac{\binom{s+j-k-1}{j}\binom{k}{j}}{\binom{2k}{j}}\quad\text{with}\ \gamma_{(k)}^{(0)}[s]=1 \tag{6.49}$$

as solutions of the recursive equation

$$(j+1)(2k-j)\gamma_{(k)}^{(j+1)}[s]+(k-j)(s+j-k)\gamma_{(k)}^{(j)}[s]=0$$

coming from the study of the covariance of (6.46) under projective holomorphic transformations.

Inserting (6.48) into (6.44) one gets at $a_{(2)}^{(s)}\equiv 0$,

$$\mathcal{K}^{(m)}(z,\bar{z}|s)=\sum_{\ell=m}^{s-1}\binom{\ell}{m}\mathcal{Q}_{(\ell-m)}(z,\bar{z}|s)\sum_{k=\ell}^{s-1}\gamma_{(k)}^{(k-\ell)}[s]\partial_{(k-\ell)}\widetilde{\mathcal{C}}^{(k)}(z,\bar{z}),\qquad m=1,\ldots,s-1 \tag{6.50}$$

The dependence in $a_{(2)}^{(s)}$ can be restored by studying the conformal covariance of (6.46) under an arbitrary holomorphic transformation. The change (6.50) corresponds to

$$\delta_{\mathcal{W}_s}Z(z,\bar{z}|s)=\sum_{k=1}^{s-1}\mathfrak{D}_{(k)}(\widetilde{\mathcal{C}}^{(k)},a_{(2)}^{(s)})Z(z,\bar{z}|s). \tag{6.51}$$

an equivalent to (6.46). Thanks to filtration by the tensorial ghosts $\mathcal{C}^{(k)}$, for each k, the operator $\mathfrak{D}_{(k)}(\widetilde{\mathcal{C}}^{(k)},a_{(2)}^{(s)})$ acting on scalar fields has no constant term (by (4.1)) and must be a scalar under holomorphic transformations. They can be obtained by using the $\mathcal{B}$ operators computed in Ref. 10 without taking into account their constant terms since the inhomogeneous coordinates Z are used in the present paper. For the sake of completeness, one rewrites the first few of them

$$\mathfrak{D}_{(1)}(\widetilde{\mathcal{C}}^{(1)},a_{(2)}^{(s)})=\widetilde{\mathcal{C}}^{(1)}\,\partial\,,$$

$$\mathfrak{D}_{(2)}(\widetilde{\mathcal{C}}^{(2)},a_{(2)}^{(s)})=\widetilde{\mathcal{C}}^{(2)}\partial_{(2)}-\tfrac{s-2}{2}\,\partial\,\widetilde{\mathcal{C}}^{(2)}\,\partial\,, \tag{6.52}$$

$$\mathfrak{D}_{(3)}(\widetilde{\mathcal{C}}^{(3)},a_{(2)}^{(s)})=\widetilde{\mathcal{C}}^{(3)}\partial_{(3)}-\tfrac{s-3}{2}\,\partial\,\widetilde{\mathcal{C}}^{(2)}\partial_{(2)}+\left(\tfrac{(s-2)(s-3)}{10}\partial_{(2)}\widetilde{\mathcal{C}}^{(3)}+\tfrac{6(3s^2-7)}{5(s^3-s)}\widetilde{\mathcal{C}}^{(3)}a_{(2)}^{(s)}\right)\partial\,.$$

A direct confrontation of (6.50) (in which the $a_{(2)}^{(s)}$-dependence has been made explicit) with (6.22), (6.33), and (6.34) for, respectively, $s=3,4$ gives a perfect accord upon using the recursion (3.27) and the definition (3.37).

The general ansatz (6.17) can thus be recovered with the help of existing results in the literature. But the linear decomposition (6.11) depending on the structure functions of all the possible sublevels shows the origin of the tensorial ghosts as the highest conformal weighted parameter in each of the nested subalgebras governed by the DOR filtration. According to the treated examples $\mathcal{W}_3$ and $\mathcal{W}_4$-algebras, the appropriate ghost parameters for the linear $\mathcal{W}$-diffeomorphisms are those constructed by redefining $\mathcal{C}^{(\ell)}\to\widetilde{\mathcal{C}}^{(\ell)}$, for the intermediate DOR

decompositions in order to reabsorb all the structure functions of the sublevels. It is worthwhile to notice that the algorithm is performed in a conformally covariant manner and in the respect of the nilpotency of the $\mathcal{W}$-algebra.

VII. CONCLUSION AND PERSPECTIVE

Throughout the paper, we have considered conformal differential operators defined on a Riemann surface whose solutions are homogeneous coordinates of some complex projective space. The latter lead to the notion of Forsyth frames as projective coordinates. In this context, our main results are as follows

(i) Linear differential order reductions (DOR), see Theorem 3.1, determine the structure functions of the large chiral symmetry algebra. These structure functions are the central objects of all our construction;

(ii) Conformal differential operators can be explicitly constructed from the given structure functions entering the linear DOR.

(iii) The extension to the chiral truncated Taylor expansion of complex scalar fields of the usual infinitesimal chiral diffeomorphisms induces an algebraic framework, which, embedded into a BRS setting, leads to another presentation of $\mathcal{W}$-algebras (Eq. (4.2)) written in terms of jet-ghosts.

(iv) Physical considerations require one to transform these ghosts from jets into tensors. Obviously, this change of generators is not unique.
In doing so, we have given a general solution (for any order s of the algebra), which put into the game all the truncation mechanisms of the Forsyth frames up to order s via a differential order reduction (DOR). The price to pay in keeping the entire generality of the solution is to carry the weight of the whole hierarchy of differential equations (with orders lower than s) which rule all the linear truncations. However, if one considers, for a given level, the general solution (6.14) as (physically) uncompleted, removing the role of the intermediate levels to the benefit of the standard $\mathcal{W}$-algebra presentation comes as a satisfying surprise. It has been shown that the cancellation holds in a rather tractable way for the lowest orders and can be related with some known computation.[10] However, the existence of nontrivial redefinitions of the $\mathcal{C}\to\widetilde{\mathcal{C}}$ ghosts leading to the reabsorption of the intermediate DOR decompositions could be a very interesting problem. This gives a sharper indication on the nature of the tensorial ghosts $\widetilde{\mathcal{C}}$ associated to infinitesimal $\mathcal{W}$-diffeomorphisms. It is a close issue to the one concerning the relationship between the parameters of the KdV flows and those of infinitesimal $\mathcal{W}$-diffeomorphisms.[10] In particular, how the nested variations pertaining to the various sublevels are finally disentangled to the benefit of the top level only, deserve to be better studied. All come from both the conformal covariance (geometry and global meaning) and the nilpotency of the BRS operation (associative algebra of symmetry). This gives an algorithm similar to one obtained in Ref. 10, in which conformal covariance governs the calculation as well.

(v) $\mathcal{W}$-currents are differential polynomials in the structure functions $\mathcal{R}(z,\bar{z}|s)$ only.

Further, a window on the so-called $\mathcal{W}$-gravity is open, once the BRS algebra is given, with the use of the algebraic trick given in Refs. 28, 11, and 32 in order to incorporate the sources of the $\mathcal{W}$-currents. The relationship between the $\mathcal{W}$-diffeomorphism symmetry and the Beltrami deformation parameters for the complex geometry is given by

$$\bar{\partial}=\left\{\delta_{\mathcal{W}_s},\frac{\partial}{\partial\bar{c}}\right\},\quad \rho^{(\ell)}=\frac{\partial\widetilde{\mathcal{C}}^{(\ell)}}{\partial\bar{c}},$$

where $\bar{c}$ is the true diffeomorphism ghost along the direction $\bar{\partial}$ and the $\rho^{(\ell)}$ are expected to be the sources for the $\mathcal{W}$-currents. This justifies (6.45) and allows one to get the whole BRS algebra for $\mathcal{W}$-gravity directly from the BRS algebra for $\mathcal{W}$-algebra (e.g., (6.29) or (6.42)). In particular, this will be useful for a systematic study of $\mathcal{W}$-anomalies possibly arising at the quantum level.

As a final conclusion, we emphasize once more that, due to the nonlinearity of this type of symmetry algebra of large (chiral) diffeomorphisms, the technical intricacy is just a consequence of the reduction from jets to tensors for which nontrivial explicit solutions have been obtained. The latter can be considered as a starting point for a more pleasant treatment, and a more suitable physical formulation for general $\mathcal{W}$-algebras and their relationship not only with linear algebraic differential equations,[14,6] but also with some kind of differential systems. For instance, one ought to expect that the Bershadsky $\mathcal{W}_3^{(2)}$-algebra be rather related to a conformally covariant system of coupled differential equations (with as unknowns f and g) of the form[12]

$$(\partial_{(2)} + a_{(1)}(z,\bar{z})\,\partial + a_{(2)}(z,\bar{z}))f(z,\bar{z}) + b(z,\bar{z})g(z,\bar{z}) = 0,$$

$$\left(\partial - \tfrac{1}{2}a_{(1)}(z,\bar{z})\right)g(z,\bar{z}) + B(z,\bar{z})f(z,\bar{z}) = 0,$$

over a generic Riemann surface.

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Three-dimensional loop quantum gravity: Particles and the quantum double

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It is well known that the quantum double structure plays an important role in three-dimensional quantum gravity coupled to matter field. In this paper, we show how this algebraic structure emerges in the context of three-dimensional Riemannian loop quantum gravity (LQG) coupled to a finite number of massive spinless point particles. In LQG, physical states are usually constructed from the notion of SU(2) cylindrical functions on a Riemann surfaced Σ and the Hilbert structure is defined by the Ashtekar-Lewandowski measure. In the case where Σ is the sphere S^2, we show that the physical Hilbert space is in fact isomorphic to a tensor product of simple unitary representations of the Drinfeld double DSU(2): the masses of the particles label the simple representations, the physical states are tensor products of vectors of simple representations, and the physical scalar product is given by intertwining coefficients between simple representations. This result is generalized to the case of any Riemann surface Σ. © *2006 American Institute of Physics.*
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I. MOTIVATIONS

Most of the articles dealing with any aspect of three-dimensional (3D) gravity are introduced and motivated by the well-known fact that 3D gravity would provide a nice framework to answer some questions that are too cumbersome to solve in the four-dimensional (4D) context. It is true that 3D (pure) gravity is a topological theory which admits only a finite number of degrees of freedom: this makes the classical theory exactly solvable and different quantization schemes have been deeply studied in the literature.[8] The theory is nevertheless far from being trivial and exhibits very rich mathematical structures that are still extensively studied: topological invariants, knots invariants, quantum groups, moduli spaces, teichmuller spaces, and so on. The main objection is that it is not true that all these techniques will shed light on the problem of quantizing four-dimensional general relativity. The interest of 3D gravity is widely limited by the fact that there is no local degrees of freedom in the theory and therefore there are many aspects of 4D gravity that will never be clarified thanks to this toy-model. In order to make 3D gravity a richer tool, one should try to introduce local degrees of freedom in the theory.

Coupling 3D gravity to an external (nontrivial) field is a natural extension of the model that contains local degrees of freedom. Furthermore, it makes the model physically more interesting. But, the problem of defining a consistent (full) quantization of a self-gravitating field theory is very difficult and impossible to solve by making use of standard perturbative quantum field theory techniques, which are so successful for describing the physics of elementary particles. Recently, Freidel and Livine[11] proposed a solution of the problem in the context of 3D spin-foam models: they have shown that (under certain hypothesis) a quantum self-gravitating field theory is equivalent to a non-self-gravitating but noncommutative quantum field theory. The authors claim that the

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noncommutativity encodes the quantum gravity effects on the field. Even if 3D gravity is physically irrelevant, it is rather interesting to have a model at hand where one has complete control of the quantum gravity effects. For these reasons, Ref. 11 certainly deserves attention for it is a first step in the understanding of a theory of quantum gravity with local degrees of freedom. Since, then other interesting articles dealing with different aspects of this problem have been proposed.[15,19,26]

This paper is a first step in the understanding and the analysis of Ref. 11 in the Hamiltonian context. The Hamiltonian quantization is a very interesting quantization scheme because the notions of quantum states and quantum operators are very well understood in that framework. Therefore, one can compute explicit transition amplitudes whereas spin-foam models give *a priori* only the partition function of the theory. The main problems with the Hamiltonian quantization of gravity is that it breaks the covariance of general relativity: there is an explicit choice of time slicing. Topology changings are not allowed because the topology of the spacelike surface is *a priori* fixed once and for all. On the contrary, spin-foam models propose a covariant, quantization of general relativity; this makes this approach so attractive. In this article, we reformulate the loop quantum gravity (LQG) description of 3D gravity coupled to massive point particles where we make clear the crucial role of quantum groups in the quantization. Therefore, we end up with a clear description of the n-particle states evolving in a quantum background which is an essential step toward the Hamiltonian description of a self-gravitating quantum scalar field theory. The last point is presented in a companion paper.[22]

The paper is organized as follows. After the introduction, we start by recalling the techniques used in Refs. 23 and 24 to perform the Hamiltonian quantization a la LQG of three-dimensional gravity (pure or coupled to particles). In particular, we clarified the link between the canonical quantization and the covariant spin-foam quantization. However, in previous works, we have never underlined the role of the quantum double DSU(2) in our construction whereas it is clear that it should play a central role.[13,18,19] We fill this gap within the present paper. To that aim, we first define in Sec. II the notions of partial kinematical and physical Hilbert space. These spaces are constructed from a particular observer: this observer is a given particle which defines a reference frame where the momenta of the other particles and the energy of the global system are defined. This description will appear very important above all in the construction of the Fock space.[22] In Sec. III, we show how the quantum double DSU(2) is naturally present in the (partial) physical Hilbert space: (partial) physical states are defined as vectors of a tensor product of simple representations of DSU(2) and the (partial) physical scalar product is nothing but an intertwining coefficient between simple representations of DSU(2). In this section, we also discuss some aspects concerning the observables: definition, computation of expectation values etc. We present the construction first in the case of the sphere then we generalize to the case of any Riemann surface. We conclude with same perspectives and we postpone the construction of the Fock space to the companion paper.[22]

In this paper, we will work with dimensionless quantities, in particular for the masses of the particles. But, the natural mass unit is the Planck mass m_P defined from the Newton constant G by $m_P=1/(4\pi G)$. Then, any mass value has to be understood in terms of the Plank unit.

II. SPACE OF PHYSICAL STATES

Loop quantum gravity is presented as a two step quantization of general relativity: the construction of the kinematical Hilbert space and the construction of the physical Hilbert space. The first point is completely under control, and gave rise to what is commonly called quantum geometry (for a review see Refs. 2, 28, and 30, or 32): the kinematical states (or states of quantum geometry) are described in term of spin-networks and their set is endowed with a Hilbert structure defined by the Ashtekar-Lewandowski measure. But the construction of the physical Hilbert space is one of the biggest difficulties and one of the most interesting problems of LQG. Different ways have been explored to attack the problem: construction of the extractor P by using a regularization of the Hamiltonian constraint,[16,31] the master constraint program,[33] spin-foam models,[25,27] etc.

Very recently, Thiemann[34] and Han and Ma[17] proved the existence of the physical Hilbert space in the context of the master program using spectral techniques. Nevertheless, no consistent solution has been found so far!

In a couple of papers[23,24] we have successfully studied 3D general relativity (pure gravity and gravity coupled to particles) as a toy-model for LQG. In particular, we have constructed the extractor P and have shown that the physical scalar product between states has a spin-foam representation. Thus, we made the explicit relation between LQG and spin-foam models.

This section is devoted to recalling the construction in the pure gravity case and in the case where gravity is coupled to massive spinless point particles. Then, we propose an alternative description for the physical Hilbert space from where the quantum double structure emerges naturally.

A. Pure gravity: Review and notations

Let $\mathcal{M}$ be a three-dimensional manifold. In the first-order formalism, the degrees of freedom of the gravitational field in $\mathcal{M}$ are encoded in a triad $e(x)=e^i_\mu(x)J_i\mathrm{d}x^\mu$ and in a spin-connection $\omega(x)=\omega^i_\mu(x)J_i\mathrm{d}x^\mu$ where J_1,J_2,J_3 are the generators of the Lie algebra $\mathfrak{g}=\mathfrak{su}(2)$ satisfying the Lie-algebra relation $[J_i,J_k]=\epsilon^l_{ij}J_l$. Indices are lowered and raised by the Kronecker symbols $\delta_{ij}=\delta^{ij}$. The dynamics is governed by the BF-action for the group $G=\mathrm{SU}(2)$.

When the manifold has the topology $\mathcal{M}=\Sigma\times I$, Σ being a Riemann surface of genus g and I a compact part of the real line $\mathbb{R}$, then gravity admits a Hamiltonian formulation. The nonreduced phase space is (schematically) defined by

$$\mathcal{E}\equiv\{(A,E)|A \text{ a } G \text{ connection on } \Sigma \text{ and } E \text{ an electric field on } \Sigma\}. \tag{1}$$

The variables A and E form a canonical variables pair and are, respectively, defined by the pullbacks of the spin-connection and of the triad on the surface Σ. The theory admits first class constraints that generate infinitesimal symmetries in the nonreduced phase space $\mathcal{E}$. An element $X\in\mathcal{E}$ is called $\mathcal{G}$-invariant when it Poisson-commutes with the constraints. The symmetry group is given by $\mathcal{G}=\mathcal{C}^\infty(\Sigma;\mathrm{ISU}(2))$ where ISU(2) is the (universal cover of the) group of Euclidean transformations. It is a semidirect group:

$$\mathrm{ISU}(2)=\mathrm{SU}(2)\ltimes\mathbb{R}^3 \quad \text{where } G \text{ acts on } \mathbb{R}^3 \text{ by the vectorial representation}. \tag{2}$$

Note that the symmetry group $\mathcal{G}$ contains (on-shell) the diffeomorphisms group on Σ but is not the diffeomorphism group. Important discrepencies between gravity and BF theory appears because of this fact.[20]

The physical phase space $\mathcal{P}$ is obtained by applying an infinite dimensional version of the Dirac reduction to the space $\mathcal{E}$ and schematically reads:

$$\mathcal{P}\equiv\{X\in\mathcal{E}|X \text{ is } \mathcal{G}\text{-invariant}\}/\mathcal{G}. \tag{3}$$

The space $\mathcal{P}$ is a finite dimensional symplectic manifold and it is isomorphic to the moduli space of flat ISU(2)-connections on the surface Σ. Functions on $\mathcal{P}$ are called observables and, by definition, are invariant under the (induced) action of the symmetry group $\mathcal{G}$.

Different strategies have been developed in the last 15 years to quantize the theory (see Ref. 8, and references therein). Most of them (combinatorial quantization,[1,7,6] functional quantization,[36] Nelson-Regge quantization,[21] etc.) are proper to 3D gravity and cannot be generalized to higher dimensions. What makes the loop and the spin-foam quantizations very attractive is precisely that these schemes can, in principle, be applied in 4D, even if neither LQG nor spin-foam models provide so far a complete and consistent quantization of 4D gravity.

The loop quantization program consists in first quantizing the nonphysical phase space $\mathcal{E}$, then promoting the first class constraints into quantum operators, and then finding the kernel of these quantum operators. In 4D gravity, all the constraints but one can be solved in the quantum theory.

The remaining and problematic constraint is known as the Hamiltonian constraint. In the context of 3D pure gravity, this program can be completely achieved and one can find solutions of all the constraints.[23] We proceed as follows.

1. Space of cylindrical functions on Σ: Cyl(Σ, G)

We start by choosing the connection A to be the configuration variable (choice of polarization) and we denote $\mathcal{A}$ the space of G-connections on Σ. We introduce the space of discrete connections associated to a graph γ (with E edges and V vertices), denoted $\mathcal{A}_\gamma$ by, roughly speaking, replacing local connections A with holonomies U_e of the connection along the edges e of the graph. A cylindrical function on the graph γ is an element $\psi \in \mathrm{Fun}(\mathcal{A}_\gamma) \subset \mathrm{Fun}(\mathcal{A})$ such that there exists a function $f \in \mathrm{Fun}(G^{\otimes E})$ and $\psi(A) = f(\otimes_{e=1}^{E} U_e)$. The space of cylindrical functions is denoted $\mathrm{Cyl}(\gamma; G)$ and is naturally endowed with a measure $\mathrm{d}\mu_\gamma = \otimes_{e=1}^{E} \mathrm{d}\mu_e$ where $\mathrm{d}\mu_e$ is the normalized G Haar measure associated to the edge e. Finally, we define the space of cylindrical functions on the surface Σ as the following union:

$$\mathrm{Cyl}(\Sigma; G) = \bigcup_{\gamma} \mathrm{Cyl}(\gamma; G). \tag{4}$$

This space inherits a natural measure, known as the Ashtekar-Lewandowski measure, and the completion of $\mathrm{Cyl}(\Sigma; G)$ with respect to this measure is the Hilbert space of non-physical states, denoted $\mathcal{H}(\Sigma; G)$. The action of the symmetry group $\mathcal{G}$ on the connections induces a (co-) action on $\mathrm{Cyl}(\Sigma; G)$ and on $\mathcal{H}(\Sigma; G)$ and we will use the same notation $\mathcal{G}$ to denote the symmetry group acting on $\mathrm{Cyl}(\Sigma; G)$. Physical states are those functions which are left invariant under this symmetry.

2. Invariance under the symmetry group G

The action of the symmetry subgroup $C^\infty(\Sigma; G)$ reduces to an action on the vertices of any element of $\mathcal{A}_\gamma$ for any graph γ. Invariant states under this action are called kinematical states. The set of kinematical states is a vector subspace of $\mathrm{Cyl}(\Sigma; G)$ and, due to left and right invariance of the G Haar measure, inherits the pre-Hilbert structure of $\mathrm{Cyl}(\Sigma; G)$. After completion, we obtain the kinematical Hilbert space, denoted $\mathcal{H}_{\mathrm{kin}}(\Sigma; G)$. Spin-network states provide an orthonormal basis of $\mathcal{H}_{\mathrm{kin}}(\Sigma; G)$.

3. Invariance under the translations $\mathbb{R}^3$

Physical states are *a priori* kinematical states that are invariant under the action of the residual symmetry subgroup. However, there are no physical states in the kinematical Hilbert space. This is a well-known fact that is a consequence of the noncompactness of the subgroup $\mathbb{R}^3$. Physical states are in fact "distributional," in the sense that they are elements of $\mathrm{Cyl}(\Sigma; G)^*$, the topological dual of $\mathrm{Cyl}(\Sigma; G)$. Finding physical states is equivalent to finding a physical extractor (abusively called a projector), i.e., an operator:

$$P: \mathrm{Cyl}(\Sigma; G) \to \mathrm{Cyl}(\Sigma; G)^*, \tag{5}$$

which satisfies the property $P(\psi_1)(\psi_2) = P(\psi_1)(\xi \cdot \psi_2)$ for any cylindrical functions ψ_1 and ψ_2 and any element $\xi \in \mathcal{G}$. We have denoted by $\cdot$ the action of $\mathcal{G}$ on $\mathrm{Cyl}(\Sigma; G)$. Thus the physical Hilbert space $H_{\mathrm{phys}}(\Sigma; G)$ is defined as the image of $\mathrm{Cyl}(\Sigma; G)$ by P. Given two physical states ϕ_1 and ϕ_2, there exists $\psi_1, \psi_2 \in \mathrm{Cyl}(\Sigma; G)$ such that $\phi_1 = P(\psi_1)$ and $\phi_2 = P(\psi_2)$, and the physical scalar product is defined by

$$\langle \phi_1, \phi_2 \rangle_{\mathrm{phys}} \equiv \langle \psi_1, \psi_2 \rangle_{\mathrm{phys}} \equiv P(\psi_1)(\psi_2). \tag{6}$$

The physical scalar product does not depend on the choice of the functions φ_1 and φ_2. Generally, we omit to mention the elements ϕ_1 and ϕ_2, and we write the physical scalar product between cylindrical functions. The operator P "extracts" the physical component of any cylindrical function.

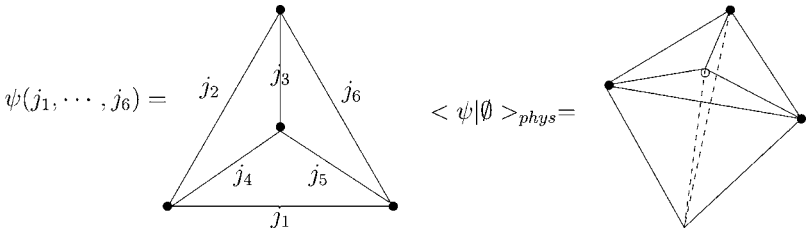

FIG. 1. The picture on the left is a spin-network state whose edges are labeled with irreps of SU(2) and vertices with normalized SU(2) intertwiners. On the right side, we have drawn the spin-foam picture illustrating the transition amplitude between the no-state and the state on the left. The amplitude associated to this spin-foam is a $(6j)$ symbol

The explicit construction of P has been done in Ref. 23. In fact, the extractor has been constructed by imposing locally the flatness condition $F(A)=0$ after a choice of regularization. The physical scalar product so obtained is well-defined (i.e., convergent), is positive, and satisfies Hermiticity condition. Moreover, the relation to the spin-foam model has been established and is briefly recalled in the following. Given two spin-network states ψ_1 and ψ_2 respectively associated to the colored graphs $\gamma_1,\gamma_2\subset\Sigma$, one associates a cellular decomposition Δ of the three-dimensional manifold $\Sigma\times I$ which interpolates the graphs γ_1 and γ_2 at the boundaries. Moreover, Δ is colored in the usual way: faces are associated with irreps of SU(2), edges with intertwiners and the colors are compatible with the boundaries' colors. At this point, one introduces the dual graph Γ whose edges are now colored with SU(2) irreps. The spin-foam amplitude associated to the graph Δ (or in an equivalent way to the dual graph Γ) gives the physical scalar product between the two spin-network states if and only ifΔ is free of bubles, i.e., Δ has a tree structure. The last condition makes the amplitude convergent and appears naturally in the Hamiltonian framework as a consequence of the regularization of the constraint $F(A)=0$. Therefore, in the case where Γ is a triangulation of $\Sigma\times I$ we have

$$\langle\psi_1,\psi_2\rangle_{\text{phys}}=\sum_{j_e}\prod_{e\in\Gamma}W_e(\{j_e\})\prod_{t\in\Gamma}W_t(\{j_e\}),\tag{7}$$

where the sum runs over SU(2) irreps coloring the edges e of Γ, the weight W_e is generically given by $d_{j_e}=2j_e+1$ and is $d_{j_e}\delta_{je,j\ell}$ if the edge e is dual to a face whose boundary contains an edge of γ_1 or γ_2 colored by $j\ell$; $W_t=(6j)$ is the normalized symmetric $(6j)$ symbols defined by the six representations coloring the edges of the tetrahedron t. This property is illustrated by the following example:

$$\langle\emptyset|\psi(j_1,\ldots,j_6)\rangle_{\text{phys}}=N(j_1,j_2,j_4)N(j_2,j_3,j_6)N(j_1,j_5,j_3)\begin{Bmatrix}j_1 & j_2 & j_6\\ j_4 & j_5 & j_3\end{Bmatrix},\tag{8}$$

where $N(j_1,j_2,j_3)$ is the norm of three-valent intertwiners (evaluation of Θ spin-network) taken to be 1. The state $\psi(j_1,\ldots,j_6)$ is the spin-network state defined on the sphere and represented in Fig. 1.

Let us finish with a remark. We consider two cylindrical functions ψ_1 and ψ_2 which differ only by the fact that their associated graphs are different but related by a diffeomorphism. Therefore, the state $P(\psi_1)-P(\psi_2)$ is a null-vector in the physical Hilbert space and we can identify the spaces $P(\text{Cyl}(\gamma;G))$ and $P(\text{Cyl}(\gamma';G))$. This is a consequence of the invariance of the theory under the diffeomorphisms group. Furthermore, the identification of the spaces still holds when the graphs γ and γ' are homotopic and not necessarily related by a diffeormorphism. Thus, we identify states that are not related by a diffeomorphism when we impose the flatness condition. We have to be aware of this fact, which is a consequence of the fact that we are working with first order gravity and then we include degenerate metrics in the model. How to avoid degenerate metrics in the quantum theory is still an open question.

B. Coupling to a finite number of particles

In order to couple particles to the gravitational field, we now consider a surface Σ with boundary: the genus of Σ is still denoted g and we assume the boundary is a disjoint union of n boundaries whose topology is a circle, i.e., $\partial\Sigma=\cup_{i=0}^{n-1}\mathcal{B}_i$. Each boundary $\mathcal{B}_i$ is associated to one particle $\mathcal{P}_i$ whose degrees of freedom are encoded in an element $X_i=(\Lambda_i,q_i)\in \mathrm{ISU}(2):q_i\in\mathbb{R}^3$ is the position of the particle and $\Lambda_i\in G$ is related to the momemtum by $\vec{p}_i=m_i\Lambda_i\vec{n}$ where $\vec{n}\in S^2$. The mass m_i of each particle$\mathcal{P}_i$ is fixed by appropriate boundary conditions of the gravitational field on $\mathcal{B}_i$.[5,9] The action of the coupled system is obtained via a minimal coupling and takes the form:

$$S=S_{BF}[e,\omega]+\sum_{i=0}^{n-1}S_{P_i}[q_i,\Lambda_i]-S_C[e,\omega;(q_i,\Lambda_i)_i]. \tag{9}$$

The explicit expression of the action is given in Ref. 24: S_{BF} is the usual SU(2) BF-action, S_P is the (first order) action of free relativistic particles and S_C represents the minimal coupling term. Note that S_C enforces the appropriate boundary conditions which fixes the masses of the particles.

The loop quantization of the action (9) is conceptually similar to the pure gravity case and has been performed in Ref. 24 Let us recall the main results.

1. Particles-cylindrical functions

Particles-cylindrical functions are a direct generalization of the usual notion of cylindrical functions. A particles-cylindrical function ψ is now a function of the connection A and of the momenta Λ_i. Such a function is defined by a graph $\gamma\subset\Sigma$ which can admit open ends at the boundaries and by a function $f\in\mathrm{Fun}(G^{\otimes(E+O)})$ where E is the number of edges and O the number of open ends such that

$$\psi(A,\Lambda_i)=f(\otimes_{e=1}^{E}U_e\otimes_{o=1}^{O}\Lambda_o). \tag{10}$$

Recall that U_e is the holonomy of the connection along the edge e and $\Lambda_o=\Lambda_i$ if the open end $o\in\mathcal{B}_i$. Therefore, the vector space of particles-cylindrical functions $\mathrm{Cyl}(\Sigma,\mathcal{P};G)$ is given by

$$\mathrm{Cyl}(\Sigma,\mathcal{P};G)\equiv\mathrm{Cyl}(\Sigma;G)\otimes\ \mathrm{Fun}(SU(2))^{\otimes n}. \tag{11}$$

$\mathcal{P}$ labels the set of the particles. This space is naturally endowed with a measure (constructed from the AL measure and the SU(2) normalized Haar measure) which makes it a pre-Hilbert space. Its completion is denoted $\mathcal{H}(\Sigma,\mathcal{P};G)$.

2. Symmetries of the system

The system admits first class constraints that generate infinitesimal symmetries. The symmetry group of the Hamiltonian theory is a Cartesian product $\mathcal{G}\times\mathcal{C}$. Any element of $\mathcal{G}$ is an element of $C^\infty(\Sigma,\mathrm{ISU}(2))$ which is constant at each boundary $\mathcal{B}_i$. As in the pure gravity case, we distinguish the "compact" subgroup $C^\infty(\Sigma,\mathrm{SU}(2))$ from the noncompact one $C^\infty(\Sigma,\mathbb{R}^3)$. The compact part generates usual gauge transformations which read on the variables A and Λ_i:

$$\forall g\in\mathcal{G}\ \text{s.t.}\ g\big|_{\mathcal{B}_i}=g(i)(A,\Lambda_i)\mapsto(g^{-1}Ag+g^{-1}\mathrm{d}g,g(i)^{-1}\Lambda_i). \tag{12}$$

The noncompact part is related to the diffeomorphisms group of the manifold $\Sigma\times I$ and acts nortrivially on the momenta canonically conjugated to the connection A.

The group $\mathcal{C}=\mathrm{Cst}(\partial\Sigma,\Gamma)$ is the set of functions on $\partial\Sigma$ which are constant on each component $\mathcal{B}_i$ and takes value in the Cartan torus Γ of ISU(2) (Note that Γ is the two-dimensional group $\mathbb{R}\times S^1$). Therefore $\mathcal{C}\simeq\Gamma^{\times n}$. It acts trivially on the connection A and by right multiplication on the momenta as shown in the following:

$$\forall(\lambda(i),\pi(i))_{i\in[0,n-1]}\in\mathcal{C}\ \text{s.t.}\ \lambda(i)\in \mathrm{SU}(2),\quad \pi(i)\in\mathbb{R}^3,\quad \Lambda_i\mapsto\Lambda_i h(i). \tag{13}$$

One can show that $\mathbb{R}\subset\Gamma$ is the subgroup of time reparatrizations of the world line of each particle whereas $S^1\subset\Gamma$ is the subgroup of internal frame rotations which preserves the momentum of each particle. It is then natural that only the SU(2) Cartan subgroup has a nontrivial action on the momenta.

The action of $\mathcal{G}$ induces a co-action on $\mathrm{Cyl}(\Sigma,\mathcal{P};G)$ and particles-physical states are the elements of $\mathrm{Cyl}(\Sigma,\mathcal{P};G)$ which are co-invariant under $\mathcal{G}$.

3. Imposing the constraints and the particles-physical Hilbert space

Invariance under reparametrization is trivial because we work in the momentum representation and invariance under internal frame rotations imposes that states are functions on the sphere $S^2=\mathrm{SU}(2)/\mathrm{U}(1)$ instead of a function on the whole group SU(2) (see Ref. 24 for more details). Therefore, the set of particles-cylindrical functions satisfying these invariances reads:

$$\mathrm{Cyl}_{\mathcal{C}}(\Sigma,\mathcal{P};G)\equiv\mathrm{Cyl}(\Sigma,\mathcal{P};G)/\mathcal{C}=\mathrm{Cyl}(\Sigma;G)\otimes\mathrm{Fun}(S^2)^{\otimes n}. \tag{14}$$

Due to the left and right invariance of the G Haar measure, the space $\mathrm{Cyl}_{\mathcal{C}}(\Sigma,\mathcal{P};G)$ inherits the measure of $\mathrm{Cyl}(\Sigma,\mathcal{P};G)$. To find particles-physical states, we have to impose the invariance under $\mathcal{G}$. As in the pure gravity case, this is a two-step procedure. First, we impose the invariance under the subgroup of gauge transformations: this is immediate to do and we obtain the particles-kinematical Hilbert space $\mathcal{H}_{\mathrm{kin}}(\Sigma,\mathcal{P};G)$. Particles-spin-network states provide an orthonormal basis of $\mathcal{H}_{\mathrm{kin}}(\Sigma,\mathcal{P};G)$ Note that particles-spin-network states are associated to graphs with (eventually) open ends at the location of the particles.

Imposing the remaining constraint (which generates the noncompact symmetry group) is done in the same way as in the pure gravity case. This means finding an extractor P:

$$P{:}\mathrm{Cyl}_{\mathcal{C}}(\Sigma,P;G)\to\mathrm{Cyl}_{\mathcal{C}}(\Sigma,P;G)^{*} \tag{15}$$

such that $P(\psi_1)(\psi_2)=P(\psi_1)(\xi\cdot\psi_2)$ for any particles-cylindrical functions ψ_1 and ψ_2 and any $\xi\in\mathcal{G}$. The image of $\mathrm{Cyl}_{\mathcal{C}}(\Sigma,\mathcal{P};G)$ by the extractor is a vector space. We endow this space with a (Ashtekar-Lewandowski) measure and after completion we end up with the particles-physical Hilbert space $\mathcal{H}_{\mathrm{phys}}(\Sigma,\mathcal{P};G)$.

The explicit construction of P has been done in Ref. 24. The relation to spin-foam models has been unraveled: the particles-physical scalar product reproduces spin-foam amplitudes of Ref. 13 as shown in the following section. It would be very interesting to ask the question of the unicity of the extractor P in the context of three-dimensional gravity because it seems that the same kinematical space is the starting point of the construction of different physical states depending on whether we are dealing with pure gravity, gravity coupled to particles or in the presence of a cosmological constant.

C. The physical states

As presented before, any physical state can be viewed as an equivalent class of a particles-cylindrical function (two states are equivalent if their difference has a nonzero physical norm) or equivalently as the image of a particles-cylindrical function by the extractor P defined above (15). A particles-physical state ψ is said to be explicitly dependent of the particles degrees of freedom if any of its representative is a particles-cylindrical function defined on a graph which has at least one open vertex (at a boundary). Otherwise, the state does not depend explicitly on the particles-degrees of freedom.

States which do not depend explicitly on the particles degrees of freedom characterize the three-dimensional space-time geometry with conical singularities but do not contain any information (apart from the masses) concerning the particles. The physical scalar product between two such (spin-network) states ψ_1 and ψ_2 has a regularized well-defined spin-foam representation of the type of Ref. 13. Indeed, one fixes a tridimensional graph $\tilde{\Gamma}\subset\Sigma\times I$ with no-buble interpolating

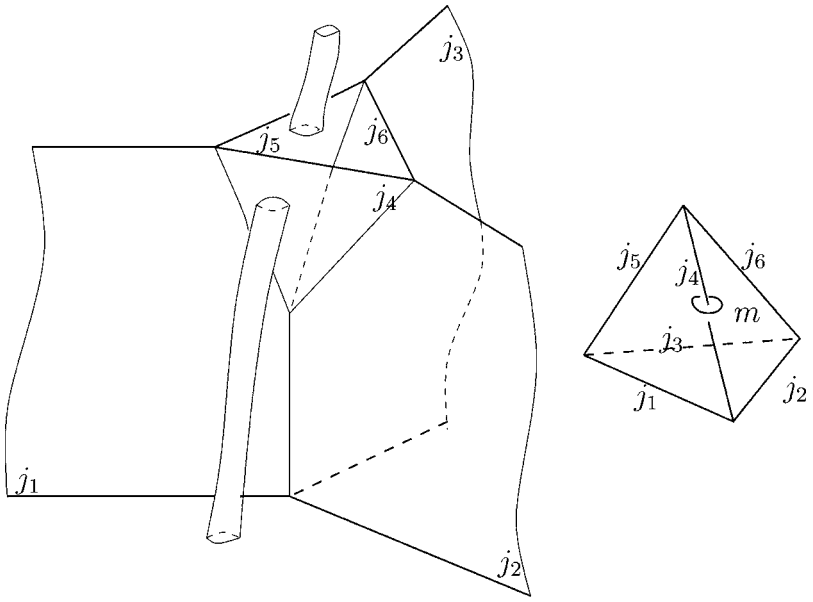

FIG. 2. Left panel: chunk of spin-foam amplitude between two spin-network states represented in thick lines: the boundary crosses the face labeled with the irrep j_4. Right panel: the dual picture the circle around the edge j_4 reminds one of the presence of the boundary.

the flat graphs γ_1 and γ_2 associated to the cylindrical functions ψ_1 and ψ_2 and the dual graph Γ, and we still have the identity (7). In that case, edges e of Γ are still colored with a representation j_e. The weight associated to each tetrahedron is still given by $W_t(\{j_e\})=(6j)_t$ but the weight W_e associated to eachedge is slightly modified: $W_e=\chi_{je}(m_i)$ where $\chi_j(m)\equiv \sin(2j+1)m/\sin m$ if the boundary associated to the particle of mass m_i crosses the dual face f of the edge e; $W_e=2j_\ell+1$ where j_ℓ is the representation coloring one edge ℓ of the graphs γ_φ or γ_ψ if the boundary of the dual face of e contains the edge ℓ; $W_e=2j_e+1$ otherwise. Note that, in the construction of Ref. 13 one has to fix a maximal tree T of Γ and to impose the condition $W_e=\delta_{j_e,0}$ to each edge $e$of T in order to make the sum (7) convergent. In our construction, we do not have such a condition because the graph $\tilde{\Gamma}$ is chosen to be free of bubbles. The two conditions are in fact equivalent.

Relation (7) is illustrated in the example of Fig. 2.

The spin-foam amplitude associated to the spin-foam on the left-hand side is given by

$$\frac{\chi_{j_4}(m)}{d_{j_4}}\begin{Bmatrix} j_1 & j_2 & j_6 \\ j_4 & j_5 & j_3 \end{Bmatrix}. \tag{16}$$

Reciprocally, the amplitude of any spin-foam of the type of Ref. 13 can be interpreted as the physical scalar product between two states which do not depend explicitly on the particles degrees of freedom.

Of particular interest is the physical scalar product between states which depend explicitly on the particles degrees of freedom. This kind of physical scalar product does not admit a spin-foam representation of the previous type.[13] In that case, the cellular decomposition of the manifold $\Sigma \times I$, defining the eventual spin-foam model, involves faces whose edges belong to, the boundaries (see Fig. 3 as an example) whereas the faces were crossed by the boundaries in the previous case.

It would be very interesting to generalize the spin-foam model developed in Ref. 13 in order to include transitions of the type of Fig. 3. We leave this issue for future investigations. In the sequel, we concentrate on the physical scalar product between particles-physical states and we do not ask for the moment the question of its spin-foam representation. Then, we want to choose a basis of physical states and we are going to compute the physical scalar product between the

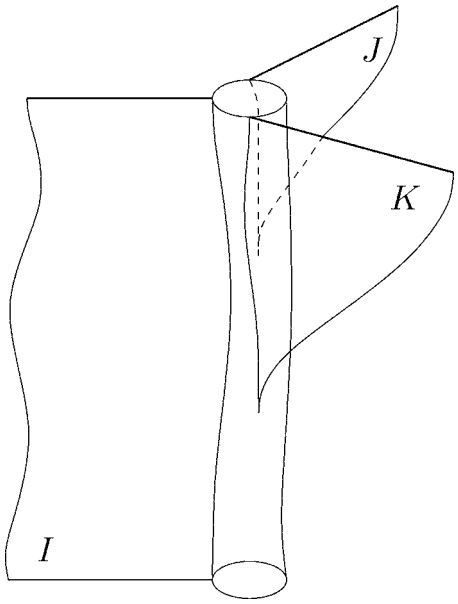

FIG. 3. Example of transition between spin-network states explicitly involving boundaries degrees of freedom. New faces can emerge from the boundaries.

elements of the basis. In other words we are going to compute explicitly the matrix elements of the extractor P whose definition and properties were briefly recalled above (15).

For that purpose, we start by choosing a minimal graph γ on the Riemann surface with boundaries $\Sigma:g$ and n denote, respectively, the genus of Σ and the number of connected components of $\partial\Sigma$. A minimal graph (Fig. 4) consists in a choice of a base point $x\in\Sigma$, a choice of n oriented edges linking x and a point on each boundary $\mathcal{B}_i$ (let E be the set of these edges), and a choice of $2g$ oriented noncontractible loops around each handle of the surface (let $H=A\cup B$ be the set of these loops that we separate as usual into two sets A and B).

The space of discrete connections on the minimal graph is denoted $\mathcal{A}_\gamma$: any discrete connection is a family $A=(U_a,U_b;U_e,\Lambda_i)_{a,b,e,i}\in G^{2(g+n)}$ where $e\in[0,n-1]$ labels the elements of E, $a,b\in[1,g]$ the elements of $H=A\cup B$, and $i\in[1,n]$ the particles. The infinite dimensional symmetry group $\mathcal{G}\times\mathcal{C}(12,13)$ acting on the space of connections reduces to a finite dimensional group when acting on $\mathcal{A}_\gamma$. The compact part of this group is trivially isomorphic to $G\times(G\times S^1)^{\times n}$. Its action on $\mathcal{A}_\gamma$ is given by

$$(G\times(G\times S^1)^{\times n})\times\mathcal{A}_\gamma\to\mathcal{A}_\gamma,$$

$$(y,(g(i),\lambda(i))_i)\times(U_a,U_b;U_e,\Lambda_i)\mapsto(y^{-1}U_a y,y^{-1}U_b y;y^1U_e g(i),g(i)^{-1}\Lambda_i\lambda(i)). \tag{17}$$

The noncompact subgroup acts trivially on the variables A and Λ_i and has a nontrivial action on the variables canonically conjugated. Imposing invariance under the noncompact subgroup is done by finding the appropriate extractor P.

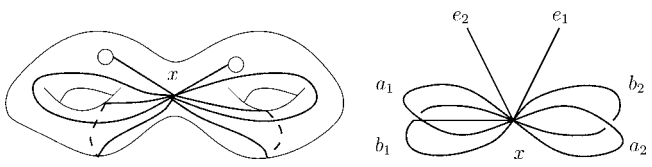

FIG. 4. A minimal graph on a genus 2 surface with two particles. On the right-hand side, the "flat projection" of the minimal graph with the labelings of each edge or loop.

The functions on discrete connections form the set $\mathrm{Cyl}(\gamma;G)$ of cylindrical functions on the minimal graph γ. Recall that $\psi\in\mathrm{Cyl}(\gamma;G)$ if there exists a function $f\in\mathrm{Fun}(G^{2(g+n)})$ such that given $\mathcal{A}\in\mathcal{A}_\gamma$ we have

$$\psi(A)=f\left(\bigotimes_{a,b=1}^{g} U_a\otimes U_b\otimes\bigotimes_{e,i=0}^{n-1} U_e\otimes\Lambda_i\right). \tag{18}$$

Due to the compactness of the gauge group $G=\mathrm{SU}(2)$, it is clear that $\mathrm{Cyl}(\gamma;G)$ is isomorphic to the space $\mathrm{Fun}(G)^{2(g+n)}$. Then, the space of cylindrical functions is naturally endowed with a pre-Hilbert structure defined by the Haar measure on the group G and its completion, denoted $\mathcal{H}(\gamma;G)$, is called the space of nonphysical states. This space is essential in the constructions of the kinematical Hilbert space and the physical Hilbert space. Obviously, these constructions do not depend on the choice of the base point x on the surface: indeed, the base point has no physical meaning and it is natural that "physical" quantities do not depend on it. Technically, it is the adjoint action of the gauge group G which makes the physical Hilbert space independent of the base point. Even the kinematical Hilbert space does not depend on that choice.

Therefore, one can choose x to be a point of a given boundary, let us say $\mathcal{B}_0$. Yet, there now exist two types of symmetries acting on the variables denned on $\mathcal{B}_0$: the action of G and the action of S^1. The former is the usual action of the gauge group SU(2) whereas S^1 is the group of internal frame symmetries (associated to the particle $\mathcal{P}_0$). To construct kinematical states, one has to consider both symmetries and find invariant functions under these two symmetries. However, it is interesting to forget the S^1 invariance. This is equivalent to choosing in particular internal frame for the particle $\mathcal{P}_0$. Thus, one can capture interesting information concerning the particles: in particular one can define the momenta of each particle in the internal frame of the particle $\mathcal{P}_0$. This is obviously impossible if we do not choose a particular frame. Thus, one can interpret the particle $\mathcal{P}_0$ as an observer sitting somewhere in the surface Σ. This observer is measuring the physical characteristics of each particle and also the properties of the spacelike geometries in its reference frame. G-invariant states defined in this reference frame are not kinematical states in the sense of LQG; in the sequel they arecalled partial kinematical states. The set of partial kinematical states is naturally endowed with a pre-Hilbert structure. Its completion is called the partial kinematical Hilbert space and is denoted $\mathcal{H}_{\mathrm{Pkin}}$. Note that one can extend the space $\mathcal{H}_{\mathrm{Pkin}}$ to distributions in the sense that one can choose the element ψ defining the spin-network to be a distribution rather than a function. In that case, one can define pure momenta states for instance as "delta" functions. As the manifold under consideration (G or S^2) is compact, we will identify the space of function with the space of distributions on this manifold. We keep this remark in mind for the following.

Proposition 1 (partial kinematical Hilbert space): *The Hilbert space of partial kinematical states* $\mathcal{H}_{\mathrm{Pkin}}$ *is isomorphic to the space* $\mathrm{Fun}(G^{2g}\otimes(S^2)^{n-1})$ *endowed with the measure* $\mathrm{d}\mu_G^{\otimes 2g}\otimes\mathrm{d}\mu_{S^2}^{\otimes(n-1)}$. *Indeed, a function* $\psi\in\mathcal{H}(\gamma;G)$ *is a partial kinematical state if and only if there exists a function* $f\in\mathrm{Fun}(G^{2g}\otimes(S^2)^{n-1})$ *such that*

$$\psi(A)=f\left(\bigotimes_{a,b}\Lambda_0^{-1}U_a\Lambda_0\otimes\Lambda_0^{-1}U_b\Lambda_0\bigotimes_{e=1}^{n-1}\Lambda_0^{-1}U_c\tilde{\Lambda}_e\right), \tag{19}$$

where $\tilde{\Lambda}_e=f\mathrm{d}h\Lambda_e h\in S^2$ *and* $\mathrm{d}h$ *is the measure on the Carton torus of G. We have used the notation* $g\tilde{\Lambda}=f\mathrm{d}hg\Lambda h$ *for the action of the group element* $g\in\mathrm{SU}(2)$ *on a point* $\tilde{\Lambda}\in\mathrm{S}^2$.

Proof: First, let us impose the invariance under the action of G on the boundary $\mathcal{B}_e$ associated to any particle $\mathcal{P}_e$ but the observer $\mathcal{P}_0$. The group G acts nontrivially on the degrees of freedom Λ_e and U_e according to the following maps (12):

$$\forall g\in G\Lambda_e\mapsto g\Lambda_e,\quad U_e\mapsto U_e g^{-1}. \tag{20}$$

This action induces a co-action on $\mathrm{Cyl}(\gamma;G)$ and it is obvious that any function $\psi\in\mathrm{Cyl}(\gamma;G)$ is co-invariant if and only if it is a function of $U_e\lambda_e$. This results holds for any particle $e\neq 0$. The action of G at the boundary $\mathcal{P}_0$ is more involved because there are many edges ending and starting

at $\mathcal{P}_0$. But the conclusion is similar because any function ψ which is G invariant at $\mathcal{P}_0$ can be written as a sum of functions of the variables $\Lambda_0^{-1}U_e$, $\Lambda_0^{-1}U_a\Lambda_0$ and $\Lambda_0^{-1}U_b\Lambda_0$. To prove this point, we decompose the function ψ into (tensor product of) irreducible unitary finite dimensional representations (irreps) of Gusing the Plancherel formula and we obtain

$$\psi(A) = \sum_{[I],[j],[k]} \overset{[I]}{f}{}^{[k]}_{[j]}(\Lambda_e) \prod_{\ell} \overset{I_\ell}{\pi}{}^{j_\ell}_{k_\ell}(U_\ell) \times \overset{I_0}{\pi}{}^{j_0}_{k_0}(\Lambda_0). \tag{21}$$

$[I] \in (\frac{1}{2}\mathbb{N})^{2g+n}$ are SU(2) irreps labeling the edges ℓ (for the links e and the noncontractible loops a,b) and the reference particle $\mathcal{P}_0$;$[j]$ and $[k]$ are families of magnetic numbers. We have denoted $\overset{I}{\pi}{}^{j}_{k} = \langle \overset{I}{e}{}^{j} | \overset{I}{\pi} | \overset{I}{e}_{k} \rangle$, the matrix elements of irreps of SU(2). $\overset{I}{V}$ is the vector space associated to the spin I representation and $\overset{I}{e}_i$, (respectively, $\overset{I}{e}{}^i$) the (respectively dual) basis of $\overset{I}{V}$ (respectively, $\overset{I}{V}{}^*$)The dependence in the variables $\Lambda_e, e \neq 0$, is contained in the definitions of the Fourier components $\overset{[I]}{f}{}^{[k]}_{[j]}(\Lambda_e)$. The decomposition (21) is nothing else but the spin-network decomposition of the state.

The G invariance at $\mathcal{P}_0$ implies that there exists a G intertwiner ι defined by

$$\iota \in \mathrm{Hom}\left(\overset{I_0}{V} \otimes \bigotimes_{\ell=1}^{2g+n-1} \overset{I_\ell}{V}; \bigotimes_{a,b=1}^{g} \overset{I_a}{V} \otimes \overset{I_b}{V} \right) \otimes \left(\overset{I_0}{V} \otimes \bigotimes_{\ell=1}^{n-1} \overset{I_e}{V} \right)^* \quad \text{such that}$$

$$\overset{[I]}{f}{}^{[k]}_{[j]} = \left\langle \bigotimes_{a,b=1}^{g} \overset{I_a}{e}{}^{k_a} \otimes \overset{I_b}{e}{}^{k_b} \middle| \iota \left(\overset{I_0}{e}{}^{k_0} \otimes \bigotimes_{e=1}^{n-1} \overset{I_e}{e}{}^{k_e} \right) \middle| \overset{I_0}{e}_{i_0} \otimes \bigotimes_{\ell=1}^{2g+n-1} \overset{I_\ell}{e}_{j_\ell} \right\rangle. \tag{22}$$

In the language of LQG, we color the vertex $\mathcal{P}_0$ with the intertwiner ι. Due to the invariance of the intertwiner ι, we have

$$\psi(A) = \sum_{[I],[j],[k]} \overset{[I]}{f}{}^{[k]}_{[j]}(\Lambda_e) \delta^{j_0}_{k_0} \prod_a \overset{I_a}{\pi}{}^{j_a}_{k_a}(\Lambda_0^{-1}U_a\Lambda_0) \prod_b \overset{I_b}{\pi}{}^{j_b}_{k_b}(\Lambda_0^{-1}U_b\Lambda_0) \prod_e \overset{I_e}{\pi}{}^{j_e}_{k_e}(\Lambda_0^{-1}U_e). \tag{23}$$

Then, we impose the G invariance at the location of each particle and we obtain in the same way that

$$\psi(A) = \sum_{[I],[j],[k]} \overset{[I]}{f}{}^{[k]}_{[j]}(1) \delta^{j_0}_{k_0} \prod_a \overset{I_a}{\pi}{}^{j_a}_{k_a}(\Lambda_0^{-1}U_a\Lambda_0) \prod_b \overset{I_b}{\pi}{}^{j_b}_{k_b}(\Lambda_0^{-1}U_b\Lambda_0) \prod_e \overset{I_e}{\pi}{}^{j_e}_{k_e}(\Lambda_0^{-1}U_e). \tag{24}$$

Finally, the invariance under the action of $\mathcal{C}$ on each (spinless) particle but the observer implies directly that $k_e=0$ for all $e=1,\ldots,n-1$. Yet $\overset{I}{\pi}{}^{j}_{0}$ are functions on the sphere $G/(U)(1)$ (spherical harmonic functions) and we can write them as follows:

$$\forall g \in \mathrm{SU}(2), \quad \overset{I}{\pi}(g)^j_0 = \int \mathrm{d}h \overset{I}{\pi}(gh)^j_0 \quad \text{where } h \in \mathrm{U}(1). \tag{25}$$

The space of such invariant functions will be denoted $\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma;G)$. It inherits the measure from $\mathrm{Cyl}(\gamma;G)$ due to left and right invariance of the Haar measure and then it possesses a natural pre-Hilbert structure. Its completion is the partial kinematical Hilbert space $H_{\mathrm{pkin}}(\gamma;G)$ and it is a sub-Hilbert space of $\mathcal{H}(\gamma;G)$.

Moreover, it is straightforward to show that any element of $\mathrm{Fun}(G^{2g} \otimes (S^2)n-1)$ is a kinematical partial Hilbert space. Finally, the proposition (1) follows immediately. □

Let us propose several remarks concerning the partial kinematical Hilbert space.

1. Note that one can precisely state the proposition in the sense that the isomorphism holds when the partial kinematical Hilbert space is defined with elements ψ which are distributional for

the observer variable and functional for the others. To clarify this claim, let us illustrate it in the case of the sphere with particles. Indeed, the fact that the observer is colored with an intertwiner means that any spin-network states can be written as

$$\psi(A) = \int \mathrm{d}g f(\Lambda_0 g, \Lambda_1 g, \ldots, \Lambda_{n-1} g). \tag{26}$$

It is then clear that to make $\psi(A)$ a function on $(S^2)^{n-1}$, it is enough to require that f is a distribution on the first argument and a function for the others. We implicitly made this asumption in the proof of the proposition.

2. We underline the fact that the proposition (1) is valid whatever the choice of observer among the different particles. Indeed, each partial kinematical Hilbert space is isomorphic one to the other. In fact, the previous proposition is still valid when the base point x is not a point of $\partial\Sigma$. To understand this point, we recall that $\mathcal{H}_{\mathrm{pkin}}(\gamma, G)$ is a sub-Hilbert space of $\mathcal{H}(\gamma; G)$ and there exists a projector $P_{\mathrm{Pkin}}: \mathcal{H}(\gamma; G) \to \mathcal{H}_{\mathrm{Pkin}}(\gamma; G)$ given by a product $P_{\mathrm{Pkin}} = P_C \cdot P_{\mathcal{C}}$ defined by

$$(P_G \psi)(A) = \int \mathrm{d}y \prod_{j=0}^{n-1} \mathrm{d}y_j f\left(\bigotimes_{a,b=1}^{g} y^{-1} U^{-1} U_a y \otimes y^{-1} U_b y \otimes \bigotimes_{i,e=0}^{n-1} y^{-1} U_e y_e \otimes y_i^{-1} \Lambda_i \right), \tag{27}$$

$$(P_{\mathcal{C}} \psi)(A) = f \prod_{j=0}^{n-1} \mathrm{d}h_j f\left(\bigotimes_{a,b-1}^{g} U_a \otimes U_b \otimes \bigotimes_{i,e=0}^{n-1} U_e \otimes \Lambda_i h_i \right), \tag{28}$$

for any $\psi \in \mathcal{H}(\gamma; G)$ associated to a function $f \in \mathrm{Fun}(G^{2(g+n)})$. Note that $\mathrm{d}y$ or $\mathrm{d}y_i$ is the Haar measure on the group G and $\mathrm{d}h_i$ the Haar measure on the group S^1. Thus, any state $\tilde{\psi} \in \mathcal{H}(\gamma; G)$ is a partial kinematical state if there exists a state $\psi \in \mathcal{H}(\gamma; G)$ associated to a function $f \in \mathrm{Fun}(G^{2(g+n)})$ such that

$$\tilde{\psi}(A) = (P\psi)(A) = (P_G \cdot P_C \psi)(A). \tag{29}$$

Therefore, after some calculations it is direct to see that there exists $j \in [0, n-1]$ such that

$$\tilde{\psi}(A) = \tilde{f}\left(\bigotimes_{a,b=1}^{g} \Lambda_j^{-1} U_j^{-1} U_a U_j \Lambda_j \otimes \Lambda_j^{-1} U_j^{-1} U_b U_j \Lambda_j \otimes \bigotimes_{e \neq j} \Lambda_j^{-1} U_j^{-1} U_e \tilde{\Lambda}_e \right) \tag{30}$$

where the function $\tilde{f} \in \mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$ is related to the function f by

$$\tilde{f}\left(\bigotimes_{a,b=1}^{g} U_a \otimes U_b \otimes \bigotimes_{e \neq j} U_e \right) \equiv \int \mathrm{d}y \prod_{j=0}^{n-1} \mathrm{d}y_j \mathrm{d}h_j,$$

$$f\left(\bigotimes_{a,b=1}^{g} y^{-1} (U_j \Lambda_j)^{-1} U_a U_j \Lambda_j y \otimes y^{-1} (U_j \Lambda_j)^{-1} U_b U_j \Lambda_j y \otimes \bigotimes_{e,i=0}^{n} y^{-1} (U_j \Lambda_j)^{-1} U_e \Lambda_e h_e \otimes 1 \right).$$

The choice of j corresponds to the choice of the observer. Therefore, the proposition (1) is valid for any choice of the base point. In the sequel, we will assume that the observer is the particle $\mathcal{P}_0$.

3. The final remark is that one can recover the kinematical Hilbert space from the partial kinematical Hilbert space as follows:

$$\mathcal{H}_{\mathrm{kin}}(\gamma; G) = \mathcal{H}_{\mathrm{Pkin}}(\gamma; G)/S^1, \tag{31}$$

where S^1 is the symmetry group which acts by right multiplication on the variable Λ_0 (13).

The next step is the construction of the partial physical Hilbert space $\mathcal{H}_{\mathrm{Pphys}}(\gamma; G)$. For that purpose, we start by defining the extractor $P: \mathrm{Cyl}(\gamma; G) \to \mathrm{Cyl}^*(\gamma; G)$ formally defined by

$$\forall \varphi, \psi \in \mathrm{Cyl}(\gamma; G), \quad P(\psi)(\varphi) \equiv \int \mathrm{d}\mu[A] \overline{\psi(A)} \mathcal{K}(A) \varphi(A). \tag{32}$$

The measure on the space of discrete connections $\mathcal{A}_\gamma$ is constructed from the SU(2) Haar measure $\mathrm{d}\mu$ via the relation $\mathrm{d}\mu[A] = \mathrm{d}\mu^{\otimes 2(g+n)}$ for $\mathcal{A}_\gamma$ is isomorphic to $2(g+n)$ copies of SU(2). The Kernel $\mathcal{K}$ is a distribution defined by

$$\mathcal{K}[A] \equiv \delta\left(\Lambda_0 h(m_0) \Lambda_0^{-1} \prod_{e=1}^{n-1} U_e \Lambda_e h(m_e) \Lambda_e^{-1} U_e^{-1} \prod_{(a,b)} [U_a, U_b] \right). \tag{33}$$

We have introduced the usual notation $[U_a, U_b] = U_a U_b U_a^{-1} U_b^{-1}$; (a,b) denotes the set of the pairs of noncontractible loops; and the elements $h(m_e)$ are in the Cartan (diagonal) torus of SU(2) fixed by the mass m_e by $h(me) = \mathrm{diag}(e^{+ime}, e^{-ime})$ in the SU(2) fundamental representation.

The extractor P defines a bilinear form on the space $P(\mathrm{Cyl}(\gamma; G)) \subset \mathrm{Cyl}(\gamma; G)^*$; it is denoted $\langle ; \rangle$ and is given by

$$\forall \psi, \varphi \in \mathrm{Cyl}(\gamma; G), \quad \langle P(\psi); P(\varphi) \rangle \equiv P(\psi)(\varphi). \tag{34}$$

In fact, this bilinear form defines a scalar product for it satisfies the following properties:

1. It is definite positive: the kernel $\mathcal{K}$ is a delta distribution on the group and therefore can be obtained as a limit of positive functions on G.

2. It is convergent as soon as the stability condition $2g+n-1>0$ is satisfied; we have the following bound:

$$\langle P(\varphi), P(\psi) \rangle \leq \|\varphi\| \cdot \|\psi\| \frac{1}{\prod_{e=0}^{n-1} \sin(m_e)} \sum_{k=1}^{\infty} \frac{\prod_{e=0}^{n-1} \sin(k m_e)}{k^{2g+n-2}}. \tag{35}$$

We have introduced the notation $\|\cdot\|$ for the L^2 norm on the group SU(2). The bound (35) is a direct consequence of the Plancherel theorem for SU(2) and of the expression of the SU(2) character in any $I \in \frac{1}{2}\mathbb{N}$ irrep, i.e., $X_I(H(m_e)) = \sin((2I+I)m_e)/\sin(m_e)$.

The vector space of partial physical states is defined by $P(\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma; G))$. It is clear that the kernel $\mathcal{K}$ is in fact a distribution on the space $\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma; G)$ and therefore $P(\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma; G)) \subset \mathrm{Cyl}_{\mathrm{Pinv}}(\gamma; G)^*$. In particular, the kernel $\mathcal{K}$ is co-invariant under the transformations $\Lambda_e \mapsto \Lambda_e h_e$ for any e and $h_e \in U(1) \subset (\mathrm{SU})(2)$. Thus, $\mathcal{K}$ depends only on the equivalent classes $\tilde{\Lambda}_e \equiv \int \mathrm{d}h_e \Lambda_e h_e \in S^2$ where $\mathrm{d}h_e$ is the U(1) Haar measure. For convenience, it will be useful to introduce the notation $\mathrm{d}\tilde{\Lambda}$ for the normalized measure on the two-sphere.

The bilinear form (34) defines a pre-Hilbert structure on $P(\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma; G))$ whose completion (up to null-vectors) is the partial physical Hilbert space $\mathcal{H}_{\mathrm{Pphys}}(\gamma; G)$. When restricted on $\mathcal{H}_{\mathrm{Pphys}}(\gamma; G)$, the scalar product (34) is called the partial physical scalar product and is denoted $\langle ; \rangle$Pphys.

Proposition 2 (partial physical Hilbert space): *Let* $f \in \mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$. *One defines a partial physical state* $P(\psi)$ *where* $\psi \in Cyl_{Pinv}(\gamma; G)$ *was introduced in Proposition* 1. *Therefore*, *there is a map*

$$\mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1}) \to \mathcal{H}_{\mathrm{Pphys}}(\gamma; G).$$

When $\mathrm{Fun}(G^{2g} \times (S^2)^{n-1})$ *is endowed with the following Hilbert structure*:

$$\forall f, g \in \mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1}),$$

$$(f, G) \equiv \int \mathrm{d}a \mathrm{d}b \mathrm{d}\tilde{z} \overline{f(a,b,\tilde{z})} \delta\left(h(m_0) \prod_{e=1}^{n-1} z_e h(m_e) z_e^{-1} \prod_{i=1}^{g} [a_i, b_i] \right) g(a,b,\tilde{z}),$$

the previous map is an isometry. Note that we have introduced the notation $a=(a_i)_i,(b_i)_i,z=(z_e)_e$, *and* $\mathrm{d}a=\Pi_a a_i, \mathrm{d}_b=\Pi_i \mathrm{d}b_i$ *for the measures.*

Proof: The proof of Proposition 1 tells us that any invariant cylindrical function ψ is completely characterized by a function $f \in \mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$ (to be more precise, the vector space $\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma;G)$ corresponds to the set of polynomial functions on $G^{2g} \otimes (S^2)^{n-1}$ and after completion with respect to the kinematical measure one sees $\mathrm{Cyl}_{\mathrm{Pinv}}(\gamma;G)$ as the set of functions on $G^{2g} \otimes (S^2)^{n-1}$).

Yet, by definition, the partial physical Hilbert space $\mathcal{H}_{\mathrm{pphys}}(\gamma;G)$ is the image of $\mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$ by the operator P and then any elemental of $\mathcal{H}_{\mathrm{Pphys}}(\gamma;G)$ can be written as $\mathcal{K}[A]\psi(A) \in \mathrm{Cyl}_{\mathrm{Pinv}}(\gamma;G)^*$. It is then natural to identify $\mathcal{H}_{\mathrm{Pphys}}(\gamma;G)$ with the space $\mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$.

The last point of the proposition is a direct consequence of the right/left invariances of the SU(2) Haar measure. □

Let us finish this section with some remarks.

Remark 1: The isometry given in the previous proposition holds for any choice of minimal graph γ and any choice of observer. Partial physical Hilbert spaces $\mathcal{H}_{\mathrm{Pphys}}(\gamma;G)$ where γ is any minimal graph are isomorphic one to the other and therefore are equivalent. For that reason, we will use the notation $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ to denote the partial physical Hilbert space where $[m]=(m_0,\ldots,m_{n-1})$. We have emphasized the explicit characteristics of the partial physical Hilbert space: the topological structure of Σ, the colors of the boundaries, i.e., the masses of the particles and the gauge group G of course.

Remark 2: The order of the particles matters in the definition of $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$. The space $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ is completely and uniquely characterized by a given flat graph of the type of Fig. 4 where there is an order between the links. If one modifies the order between the links, then the definition of the structure of the partial physical Hilbert space is slightly modified. However, two different orders define isomorphic partial physical Hilbert space. For instance, if we consider a sphere $\Sigma=S^2$ with three particles associated to the masses (m_0,m_1,m_2), then the following map is an isometry:

$$\mathcal{H}^{0.3}_{\mathrm{Pphys}}(m_0,m_1,m_2;G) \to \mathcal{H}^{0.3}_{\mathrm{Pphys}}(m_0,m_1,m_2;G),$$

$$f \mapsto g:(\tilde{z}_1,\tilde{z}_2) \mapsto g(\tilde{z}_1,\tilde{z}_2)=f(\tilde{z}_1,z_1 h(m_1)^{-1} z_1^{-1}\tilde{z}_2). \tag{36}$$

It is indeed easy to verify that $\|f\|_{\mathrm{Pphys}}=\|g\|_{\mathrm{Pphys}}$. One can establish a more general property that we will discuss in the next section.

Remark 3: The physical Hilbert space $\mathcal{H}^{g,n}_{\mathrm{phys}}([m];G)$ is easily obtained as the coset:

$$\mathcal{H}^{g,n}_{\mathrm{phys}}([m];G) \equiv \mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)/S^1.$$

The action of S^1 on $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ is naturally defined by

$$S^1 \times \mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G) \to \mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G), \tag{37}$$

$$(h,f) \mapsto f^h:y,\tilde{z} \mapsto f^h(a,b,\tilde{z})=f(h^{-1}ah,h^{-1}bh,h^{-1}\tilde{z}). \tag{38}$$

We have used the notations of Proposition 2 with $h^{-1}ah-(h^{-1}a_i h)_i$ and so on. Therefore, the physical Hilbert space is obviously a sub-Hilbert space $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ and can be obtained as the image of the following projector:

$$\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G) \to \mathcal{H}^{g,n}_{\mathrm{phys}}([m];G), \quad f \to \tilde{f}(a,b,\vec{z}) = \int \mathrm{d}h f(h^{-1}ah, h^{-1}bh, h^{-1}\vec{z}). \tag{39}$$

This is in fact a trivial application of refined algebra techniques in the compact S^1 case. The Hilbert structure of $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ is defined from this map as the kernel $\mathcal{K}$ is invariant by the action (37).

Remark 4: From the very definition of the partial physical Hilbert space as a subset of $\mathrm{Cyl}(\gamma;G)^*$, $\mathcal{H}^{g,n}_{\mathrm{Pphys}}(\gamma;G)$ is in fact a subset of $\mathbb{C}[G]^{2g} \otimes \mathbb{C}[S^2]^{n-1}$ where $\mathbb{C}[G]$ is the group algebra and $\mathbb{C}[S^2] = \mathbb{C}[G]/\mathrm{U}(1)$ is called the two-sphere algebra. The group algebra is defined as the algebra of formal sum of group elements. As G is compact there is a trivial isomorphism which identifies the spaces $\mathbb{C}[G]^{2g} \otimes \mathbb{C}[S^2]^{n-1}$ and $\mathrm{Fun}(G^{2g} \otimes (S^2)^{n-1})$.

Remark 5: Let us recall that any particle $e \in [0, n-1]$ is classically completely characterized by its mass m_e and the direction of its momentum given by Λ_e. The particle $\mathcal{P}_0$ plays the role of the observer and the variable Λ_0 does not appear anymore in the definition of partial physical states. One can interpret this observation by the fact that we work in the rest-frame of the observer and then Λ_0 is set to the identity: the momenta of the other particles are defined in that frame.

Besides, one can characterize the particle e by an element $k_e \in G$ such that $k_e = \Lambda_e h(m_e) \Lambda_e^{-1}$, i.e., k_e is an element of the conjugacy class of the element $h(m_e)$, denoted $C(m_e)$:

$$C(m_e) \equiv \{k \in \mathrm{SU}(2) \,|\, \exists\, y \in \mathrm{SU}(2), \text{ such that } k = y h(m_e) y^{-1}\}. \tag{40}$$

Thus, any element of $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ can be viewed as an element of $\mathrm{Fun}(G^{2g} \otimes \otimes_{e=1}^{n=1} C(m_e))$. Using the Kirillov formula for the Su(2) Haar measure,

$$\mathrm{d}k_e = \frac{1}{\pi} \sin^2(m_e) \mathrm{d}m_e \mathrm{d}\tilde{\Lambda}_e, \tag{41}$$

the partial physical scalar product between two states ψ and φ respectively associated to the functions f and g is then given by

$$\langle \psi; \varphi \rangle_{\mathrm{Pphys}} = (f,g) = \frac{\pi^{n-1}}{\prod_{e=1}^{n-1} \sin^2(m_e)} \int \mathrm{d}u \mathrm{d}k \overline{f(a,b,k)} \delta\left(h(m_0) \prod_{i=1}^{n-1} k_e \prod_{i=1}^{g} [a_i, b_i] \right) g(a,b,k). \tag{42}$$

We recall that the functions f and g are non-null if $g_e \in C(m_e)$. This reformulation of the partial physical Hilbert space will be convenient in the next section.

Remark 6: The last remark concerns the normalization of the partial physical scalar product, defined only up to a constant $\lambda(g,n,[m]) > 0$. The constant depends *a priori* on the genus g of Σ, the number of particles n, and the masses of the particles. By a direct calculation, one shows that the squared norm of the identity function $e^{g,n}[m] \in \mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ is given by the volume of the space of flat SU(2) connections on the punctured surface Σ, i.e.,

$$\| e^{g,n}[m] \|^2_{\mathrm{Pphys}} = \lambda(g,n,[m]) \sum_{k=1}^{+\infty} k^{2-2g-n} \prod_{e=0}^{n-1} \frac{\sin(k m_e)}{\sin(m_e)}. \tag{43}$$

At this point, there is no physical reason to impose the value of λ. But, we can show that the value of $\lambda(g,n,[m])$ is completely determined by the coefficients $\lambda(0,3,[m])$ and the problem to fix it reduces to the fixation of the normalization factor in the (minimal) case of the sphere with three punctures. The method is similar to the one proposed in Ref. 1 and is given in Appendix B: if we assume that $\lambda(0,3,[m]) = \lambda$ is a constant independent of the masses, then we show that $\lambda(g,n,[m]) = \lambda^{n+2g-2}$.

III. TRANSITION AMPLITUDES AND THE QUANTUM DOUBLE

In the following, we are going to show how the Drinfeld double DSU(2) structure appears in the context of three-dimensional Riemannian gravity coupled to massive point particles: the partial physical Hubert space is in fact isomorphic as a Hilbert space to a tensor product of simple representations of DSU(2). In that picture, the partial physical scalar product between two states is an intertwining coefficient between simple representations. Thus, the so-called Barrett-Crane (BC) intertwiner[4] plays a crucial role in three-dimensional quantum gravity whereas it was introduced as a model of four-dimensional gravity.

The following is organized as follows. First, we recall basic facts concerning the Drinfeld double DSU(2): definition, representation theory. We also introduce the notion of simple representation and symmetric (or BC) intertwiner. Then, we show the role of DSU(2) in the case of a sphere with n particles: DSU(2) appears as the symmetry group of the quantum theory and the nontrivial braiding is interpreted in the language of LQG. Finally, we generalize the previous results in the case of any Riemann surface Σ.

A. The quantum double DSU(2): Definition and properties

The general definition of the quantum double (or the Drinfeld double) of a Hopf algebra A is briefly recalled in Appendix A. The general definition is then illustrated in the generic case of a finite group.[10] Here, we consider the case of the compact group SU(2), i.e., the case where $A = \mathbb{C}[\mathrm{SU}(2)]$.[18]

The Drinfeld double $\mathrm{DSU}(2) = \mathbb{C}[\mathrm{SU}(2)] \otimes F(\mathrm{SU}(2))^{\mathrm{op}}$ is a Hopf algebra whose definition is precisely given in the appendix. In particular, it is quasitriangular and admits the group algebra $\mathbb{C}[\mathrm{SU}(2)]$ and the algebra of functions $F(\mathrm{SU}(2))^{\mathrm{op}}$ (with opposite co-product) as sub-Hopf algebra.

1. Hopf algebra structure

The Hopf algebra structure of $\mathbb{C}[\mathrm{SU}(2)]$ is defined by the group law and the following co-algebra relations:

$$\forall x \in \mathrm{SU}(2), \quad \Delta(x) = x \otimes x, \quad S(x) = x^{-1}, \quad \epsilon(x) = \delta(x). \tag{44}$$

Note that there exists a right and left invariant Haar measure on $\mathbb{C}[\mathrm{SU}(2)]$ given by

$$h : \mathbb{C}[\mathrm{SU}(2)] \longrightarrow \mathbb{C}, \quad h(x) = \delta(x). \tag{45}$$

The algebra of functions $F(\mathrm{SU}(2))$ is commutative and its coalgebra structure is given by

$$\Delta(f)(x,y) = f(xy), \quad S(f)(x) = f(x^{-1}), \quad \epsilon(f) = f(1), \tag{46}$$

where f is a function and $x, y \in G$. We know that $F(\mathrm{SU}(2))$ admits a Haar measure that we have denoted $\int \mathrm{d}x$ as usual.

Finally, the Drinfeld double is defined by the previous formulas and the following ones (which are a direct application of the definition given in the appendix):

$$(x \otimes f)(y \otimes g) = xy \otimes (f \circ Ad_y)g, \tag{47}$$

$$\Delta(x \otimes f)(a,b) = f(ba)x \otimes x, \tag{48}$$

where $f, g \in F(\mathrm{SU}(2))$, $x, y, a, b \in \mathrm{SU}(2)$. The action of the antipode reads

$$S(x \otimes f)(a) = x^{-1} \otimes f(x^{-1}a^{-1}x) \tag{49}$$

for any $a \in G$ and the co-unit is simply given by $\epsilon(x \otimes f) = f(1)$.

2. Representation theory

Unitary irreducible representations of DSU(2) have been studied in Ref. 18 and are classified by a couple $(m,s):m\in[0,2\pi]$ labels a conjugacy class of SU(2), denoted $C(m)$, whose representative is still chosen to be $h(m);s\in\mathbb{Z}$ is an integer which labels irreducible representations of the centralizer $Z(m)$ of the element $h(m)$. Note that $Z(m)\simeq \mathrm{U}(1)$ for $m\neq 0,2\pi$; otherwise $Z(m)$ is obviously the group $G=\mathrm{SU}(2)$ itself. In the generic case $m\neq 0,2\pi$, the vector space of a representation (m,s) consists in the subspace of functions on SU(2) defined by

$$\mathcal{V}_{m,s}\equiv\{\varphi:SU(2)\to\mathbb{C}|\ \forall\ a\in SU(2),\varphi(ah_m)=e^{\mathrm{ism}}\varphi(a)\}. \tag{50}$$

The representation of any element $(x\times f)\in\mathrm{DSU}(2)$ on the above-noted vector space is defined by

$$(\pi_{m,s}(x\otimes f)\varphi)(a)=f(ah_ma^{-1})\varphi(x^{-1}a). \tag{51}$$

The vector space $\mathcal{V}_{m,s}$ inherits a natural Hilbert space structure. The particular case $m\in\{0,2\pi\}$ has been considered in Ref. 18. In the sequel, we use the notation $\bar{m}=2\pi-m$.

3. Simple representations and symmetric intertwiners

Representations of the form $(m,0)$ are called simple representations[14] and are the building blocks of the Barrett-Crane model.[4] The vector space of a simple representation is isomorphic to the space of functions on the sphere $S^2=\mathrm{SU}(2)/\mathrm{U}(1)$. Any simple representation admits a normalized SU(2)-invariant vector denoted $\omega=1$. The vector space associated to a simple representation m will be denoted $\mathcal{V}_m$ (we omit the subscript 0 for the spin). It is obvious that $\mathcal{V}_m\simeq\mathrm{Fun}(S^2)$ and we will identify in the following the spaces $\mathcal{V}_m$ and the conjugacy class $C(m)$ which contains the information on the mass. We will use the same notation $\psi(\tilde{x})$ or $\psi(xh(m)x^{-1})$ for the state ψ when viewed as an element of $\mathrm{Fun}(S^2)$ or an element of $C(m)$.

The notion of symmetric intertwiner (or the Barrett-Crane intertwiner) was introduced a long time ago[4,14] and is defined as an intertwiner between simple representations whose decomposition into three-valent intertwiners introduces only simple representations in the intermediate channel. Up to a normalization, the simple intertwiner is unique.[29]

There exists an integral formulation of the symmetric intertwiner. To present this formulation, we need to recall the definition ofthe symmetric propagator.[14]

Given a simple representation labeled by m, the symmetric kernel K_m is an element of $F(\mathrm{SU}(2))^*\subset\mathrm{DSU}(2)^*$ defined by

$$K_m:F(\mathrm{SU}(2))\to\mathbb{C},\quad f\mapsto K_m(f)=\int \mathrm{d}x f(xh(m)x^{-1}). \tag{52}$$

It is convenient and equivalent to view (by duality) the symmetric kernel as an element of $\mathbb{C}[\mathrm{SU}(2)]$ as follows:

$$K_m=\int \mathrm{d}x\mathbb{I}_m(x)x\quad\text{with}\quad \mathbb{I}_m(x)=\int \mathrm{d}y\,\delta(xyh(\bar{m})y^{-1}). \tag{53}$$

Note that $\mathbb{I}_m$ is the characteristic function of the conjugacy class $C(m)$ and can be decomposed into Fourier modes as follows:

$$\mathbb{I}_m(x)=\sum_{I\in(1/2)\mathbb{N}}\chi_I(m)\chi_I(x)\quad\text{with}\quad \chi_I(m)\equiv\chi_I(h(m)). \tag{54}$$

If K_m had been a function on a "classical" group G, we would have defined the "classical" propagator as the function $K(x,y)\equiv K(xy^{-1})\in F(G)^{\otimes 2}$. In our case, the propagator, denoted $K_m(x,y)$, is an element of $\mathbb{C}[\mathrm{SU}(2)]^{\otimes 2}$ defined by

$$K_m(x,y) \equiv (1 \otimes S)\Delta(K_m) = \int \mathrm{d}x \mathbb{I}_m(x) x \otimes x^{-1}. \tag{55}$$

This propagator is the building block of the symmetric intertwiner whose construction is given next.[14] Let $[p]=(p_1,\ldots,p_a)$ and $[q]=(q_1,\ldots,q_b)$ be two ordered families of simple representations. One defines the symmetric intertwiner between the representations $[p]$ and $[q]$,

$$\iota_s([p];[q]): \overset{a}{\underset{i=1}{\otimes}} \mathcal{V}_{p_i} \to \overset{b}{\underset{j=1}{\otimes}} \mathcal{V}_{q_j},$$

by its matrix elements given by

$$\left\langle \overset{b}{\underset{\ell=1}{\otimes}} \varphi_i | \iota_s([p];[q]) \overset{a}{\underset{k=1}{\otimes}} \psi_k \right\rangle = h\left(\prod_{j=1}^{b} (\bar{\varphi}_j \otimes 1) K_{qj}(x_j,g) \prod_{i=a}^{1} (\psi_i \otimes 1) K_{pi}(y_i,g) \right), \tag{56}$$

where $\psi_i \in \mathcal{V}_{p_i}$ and $\varphi_j \in \mathcal{V}_{q_j}$ for any i or j. Note that h is the Haar measure on the group algebra $\mathbb{C}[\mathrm{SU}(2)]$ and the products in the formula (56) are ordered such that when one develops the expression, one obtains

$$\left\langle \overset{b}{\underset{\ell=1}{\otimes}} \varphi_\ell | \iota_s([p];[q]) \overset{a}{\underset{k=1}{\otimes}} \psi_k \right\rangle = \int \prod_{i,j} \mathrm{d}x_j \mathrm{d}y_i \mathbb{I}_{qj}(x_j) \overline{\varphi_j(x_j)} \delta\left(\prod_{\ell=1}^{b} x_\ell^{-1} \prod_{k=a}^{1} y_k \right) \mathbb{I}_{p_i}(y_i) \psi_i(y_i). \tag{57}$$

Let us propose several remarks concerning the symmetric intertwiner.

Remark 1: If one views the states ψ_i and φ_j as functions on the two-sphere, the previous formula reduce to the following one:

$$\left\langle \overset{b}{\underset{\ell=1}{\otimes}} \varphi_\ell | \iota_s([p];[q]) \overset{a}{\underset{k=1}{\otimes}} \psi_k \right\rangle = \int \prod_{j=1}^{b} \overline{\varphi_j(\tilde{x}_j)} \mathrm{d}\tilde{x}_j \prod_{i=1}^{a} \psi_i(\tilde{y}_i) \mathrm{d}\tilde{y}_i \delta\left(\prod_{l=1}^{b} x_l h(\bar{q}_l) x_l^{-1} \prod_{k=a}^{1} y_k h(p_k) y_k^{-1} \right).$$

In the particular (and singular) case where φ_ℓ and ψ_k are picked at the values $\tilde{x}_\ell$ and $\tilde{y}_k$ on the sphere, the symmetric intertwiner is a distribution given by

$$\left\langle \overset{b}{\underset{\ell=1}{\otimes}} \tilde{x}_\ell | \iota_s([p];[q]) \overset{a}{\underset{k=1}{\otimes}} \tilde{y}_k \right\rangle = \delta\left(\prod_{\ell=1}^{b} x_\ell h(\bar{q}_l) x_\ell^{-1} \prod_{k=a}^{1} y_k h(p_k) y_k^{-1} \right). \tag{58}$$

Remark 2: We easily show that the decomposition of the symmetric intertwiner introduces only simple representations in the intermediate channel. Using the previous notations, we have for instance:

$$\iota_s([p];[q]) = \frac{1}{\pi} \int \mathrm{d}r P(r) \iota_s(p_1,p_2;r) \circ \iota_s(\bar{r},p_3,\ldots,p_a;[q]), \tag{59}$$

where $\circ$ denotes the usual composition between intertwiners and $P(r)=\sin^2 r/\pi$ is the Plancherel measure.

Remark 3: Therefore, we concentrate for the moment on the three valent intertwiner $\iota_s(p;q_1,q_2): \mathcal{V}_p \to \mathcal{V}_{q_1} \otimes \mathcal{V}_{q_2}$. We start by saying that it is indeed an intertwiner, i.e., it satisfies the following identity:

$$\iota_s(p;q_1,q_2)(\pi_p(z \otimes f)) = (\pi_{q1} \otimes \pi_{q2}) \Delta(z \otimes f) \iota_s(p;q_1,q_2) \tag{60}$$

for any $z \otimes f \in \mathrm{DSU}(2)$. The symmetric intertwiner is not normalized and we define the coefficient $\Theta(p,q_1,q_2)$ such that the intertwiner $\Theta(p,q_1,q_2)^{-1/2} \iota_s(p;q_1,q_2)$ is normalized, i.e.,

$$\frac{1}{\sqrt{\Theta(p,q_1,q_2)\Theta(q_1,q_2,p')}}\iota_s(p;q_1,q_2)\circ\iota_s(q_1,q_2;p')=\frac{\delta(p-p')}{P(p)}i\mathrm{d}_{\mathcal{V}_p}. \tag{61}$$

A straightforward calculation shows that

$$\Theta(p,q_1,q_2)=\langle 1\otimes 1|\iota_s([p];[q])|1\rangle=\frac{\pi}{4}\frac{Y(p,q_1,q_2)}{4\sin p\sin q_1\sin q_2}, \tag{62}$$

where Y is the characteristic function of the set $\{(a,b,c)\,|\,a\leq b+c,b\leq c+a,c\leq a+b\}$.

Remark 4: From the previous remarks, it is easy to show that $\iota_s([p];[q])$ is an intertwiner, i.e., it satisfies

$$\iota_s([p];[q])\left(\otimes_{i=1}^{a}\pi_{p_i}\right)\Delta^{(a)}(z\otimes f)=\left(\otimes_{i=1}^{b}\pi_{q_i}\right)\Delta^{(b)}(z\otimes f)\iota_s([p];[q]). \tag{63}$$

We used the notation $\Delta^{(n)}$ defined by $\Delta^{(1)}=\Delta$ and $\Delta^{(n)}=(id\otimes\cdots\otimes id\otimes\Delta)\Delta^{(n-1)}$.

Remark 5: It is straightforward to extend the action of the symmetric intertwiner $\iota_s([p];[q])$ to the space $\mathrm{Fun}((S^2)^{\times a})$.

4. R-matrix and braiding

Another important property of the quantum double is its quasitriangularity. Indeed, the quantum double is, by construction, a quasitriangular Hopf-algebra and therefore admits an R-matrix. The universal expression of R is given by

$$R=\int \mathrm{d}g(g\otimes 1)\otimes(1\otimes\delta_g). \tag{64}$$

Then, we can evaluate the R-matrix on any pair of representations. We are particularly interested in the case of simple representations. Let (p,q) be a pair of simple representations, the evaluation of R in these representations is given by

$$R_{p,q}\equiv\pi_p\otimes\pi_q(R):\mathcal{V}_p\otimes\mathcal{V}_q-\to\mathcal{V}_q\otimes\mathcal{V}_p \tag{65}$$

such that, for any $\psi,\varphi\in\mathrm{Fun}(S^2)$, then:

$$R_{p,q}(\psi\otimes\varphi)(\tilde{x},\tilde{y})=\varphi(xh(\bar{p})x^{-1}\tilde{y})\psi(\tilde{x}), \tag{66}$$

where $g\tilde{x}$ means the action of $g\in\mathrm{SU}(2)$ on the point $\tilde{x}\in S^2$. The evaluation of the inverse R-matrix on simple representations is given by

$$R_{p,q}^{-1}(\psi\otimes\varphi)(\tilde{x},\tilde{y})=\varphi(\tilde{y})\psi(yh(q)y^{-1}\tilde{x}). \tag{67}$$

It is convenient to write the action of the R-matrix and of its inverse on the states viewed as functions on the conjugacy class. In that context, we do not need to specify the evaluation representation of the R-matrix (and its inverse R^{-1}) and we have

$$R(\psi\otimes\varphi)(x,y)=\varphi(x^{-1}yx)\psi(x),\quad R^{-1}(\psi\otimes\varphi)(x,y)=\varphi(y)\psi(yxy^{-1}). \tag{68}$$

It is then straightforward to extend the action of the R-matrix (and its inverse) to any function on $\mathrm{SU}(2)^{\otimes 2}$.

Note the important property that the symmetric intertwiner is invariant under braidings, i.e.,

$$\iota_s([p];[q])R^{\epsilon}_{p_i,p_{i+1}}=R^{\epsilon}_{q_j,q_{j+1}}\iota_s([p];[q])=\iota_s([p];[q]), \tag{69}$$

for any $i\in[1,a-1],j\in[1,b-1]$ (using the notations of the previous sections) and $\epsilon\in\{+1,-1\}$. This is known as the pivotal symmetry of the BC intertwiner.

B. Particles on the sphere S^2

We are going to show how the Drinfeld double appears in the context of 3D LQG coupled to point particles. This is in fact immediate and we have the following theorem:

Theorem 1 (the Drinfeld double in LQG): *Let* $[m]=(m_0,\dots,m_{n,\dots,1})$ *be the masses of n particles*; $[m]$ *also labels a family of simple representations of* DSU(2). *Let us define the trivial map between the partial physical Hilbert space* $\mathcal{H}^{0,n}_{\mathrm{Pphys}}([m];G)$ *and the tensor product* $\otimes_{i=0}^{n-1}\mathcal{V}_{\overline{m_i}} \simeq \mathrm{Fun}((S^2)^{\times n})$ *of simple representations as follows*:

$$\mathcal{F}:\mathcal{H}^{0,n}_{\mathrm{Pphys}}([m];G) \longrightarrow \bigotimes_{i=0}^{n-1}\mathcal{V}_{\overline{m_i}}, \quad \varphi\mapsto\mathcal{F}(\varphi):(\tilde{x}_0,\dots,\tilde{x}_{n-1})\mapsto\mathbb{I}(\tilde{x}_0)\varphi(\tilde{x}_1,\dots,\tilde{x}_{n-1}). \tag{70}$$

This map is obviously linear and is trivially extended to the algebra of functions. Moreover, the partial physical Hilbert space between two states φ *and* ψ *is given by*

$$\langle\varphi:\psi\rangle_{\mathrm{Pphys}} = \iota_s([\overline{m}];0)\big|\mathcal{F}(\overline{\varphi}\psi)\rangle. \tag{71}$$

Proof: This theorem is an immediate consequence of the results of the previous section. □

As a consequence, a (partial) physical state is a tensor product of vectors of simple representations of the quantum double DSU(2): each particle is represented by a vector of a simple representation. Therefore, the quantum double is the symmetry group of the quantum theory: given an element $x\otimes f\in\mathrm{DSU}(2)$, x is a rotation and f is a translation acting on a one-particle state. It is immediate to understand that the SU(2) part of the double generates rotations; to see that the $F(\mathrm{SU}(2))$ part generates translations, we take $\vec{a}\in\mathbb{R}^3$ and we consider the element $f_{\vec{a}}$ defined by $f_{\vec{a}}(x)=e^{i\vec{p}(x)\cdot\vec{a}}$ where $\vec{p}(x)=m\Lambda\vec{n}$ with $x=\Lambda h(m)\Lambda^{-1}$ ($\vec{n}$a unitary vector). It is clear that $f_{\vec{a}}$ acts on a state by translation.

Let us discuss some consequences of this theorem.

First of all, we note that physical processes conserve the momenta of each particle: a pure momenta state has a nontrivial physical amplitude with the same pure momenta state.

Next, we say some words concerning computation of expectation value of operators. An operator can be viewed as (a product of) the evaluation (on simple representations) of elements of DSU(2): such elements act naturally on $\mathcal{H}^{0,p}_{\mathrm{Pphys}}([m];G)$. Particular examples of operators are the multiplicative $m_i(f)$ and the derivative operator $\mathrm{d}_i(g)$, respectively, associated to a function f and a group element x acting on a given particle $i\in[1,n-1]$ as follows:

$$m_i(f)|\varphi> = f(\Lambda_i)\varphi(\Lambda_1,\dots,\Lambda_{n-1}), \quad \mathrm{d}_i(x)|\varphi> = \varphi(\Lambda_1,\dots,x\Lambda_i,\dots,\Lambda_{n-1}). \tag{72}$$

Note that the multiplicative operator can be naturally extended to the case where f is a distribution. In fact, any operator (in our sense) on the partial physical Hilbert space can be decomposed into a sum of products of these basic operators. We introduce a star (antilinear involutive) operator in the algebra of operator generated by $m_i(f)$ and $\mathrm{d}_i(x)$ as follows: $\mathrm{d}_i(x)^*=\mathrm{d}_i(x^{-1})$ and $m_i(f)^*=m_i(\overline{f})$.

An operator $\mathcal{O}$ is unitary in the partial physical Hilbert space if it satisfies the identity

$$\langle\varphi|\mathcal{O}\psi\rangle = \langle\mathcal{O}^*\varphi|\psi\rangle \tag{73}$$

for any state φ and ψ. Note that m_i is trivially an unitary operator in the partial physical Hilbert space whereas d_i is not in general. Both operators are unitary in the partial kinematical Hilbert space. To construct (nontrivial) unitary operator in the partial physical Hilbert space, one needs to consider braiding operators that are a particular combination of multiplicative and derivative operators. We will see their definition in the sequel.

There is a natural adjoint action DSU(2) on the set of operators defined by

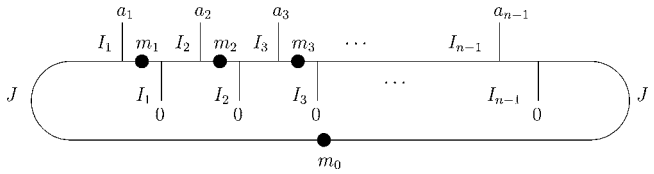

FIG. 5. Pictorial illustration of expression (78). The dot colored with the mass m denotes insertion of the element $h(m)$; any trivalent vertex denotes $(3j)$ coefficients of SU(2); each edge is colored with an irrep of SU(2) and can end up with a magnetic number like a_i or 0.

$$X \in \mathrm{DSU}(2), \quad X \triangleright \mathcal{O} = S(X_{(1)})\mathcal{O}X_{(2)}, \tag{74}$$

where we have used the Sweedler notation and $\mathcal{O}$ is an operator. This action is well-defined. Among the operators, one distinguishes particularly the so-called observables, i.e., the operators that are invariant under the action of the quantum double (74).

Given a physical process involving in and out states denoted φ_{in} and φ_{out}, the expectation value of any operator $\mathcal{O}$ during this process is given by

$$\langle \varphi_{\mathrm{out}}|\mathcal{O}|\varphi_{\mathrm{in}}\rangle_{\mathrm{Pphys}} = \iota([\bar{m}];0)|\mathcal{F}(\overline{\varphi_{\mathrm{out}}}\mathcal{O}\varphi_{\mathrm{in}})\rangle. \tag{75}$$

The mean value of any operator $\mathcal{O}$ is trivially given by

$$\langle \mathcal{O} \rangle \equiv \frac{\mathrm{Tr}(\mathcal{O})}{\mathrm{Tr}(1)} = \frac{\iota_s([\overline{m}];0)|\mathcal{F}(\mathcal{O})\rangle}{\mathrm{Tr}(1)}. \tag{76}$$

Mean values of any operator are therefore given by coefficients of simple intertwining coefficients.

Interesting operators are the monodromy around the particles and their trace are quite easy to compute. Given a finite dimensional representation K of SU(2) and a loop ℓ around p particles among the $n-1$ particles (let us denote by α_ℓ the set of particles), a monodromy $M_K(\ell)$ is defined by $M_K(\ell)=\chi_K(H_\ell)$ where the expression of the holonomy H_ℓ depends on the choice of the loop ℓ. If ℓ_i is a loop around the particle i, then $M_K(\ell_i)$ is obviously a diagonal operator whose mean value is given by the character $\langle M_K(\ell_i)\rangle=\chi_K(m_i)$. In the case where ℓ is any loop, the computation of the mean value is more involved but the result does not depend on the homotopy class of the loop $\ell$and is given by

$$\mathrm{Tr}(M_K(\ell)) = \sum_{I,J} Y(I,J,K)\mathrm{d}_I\mathrm{d}_J \prod_{i\notin\alpha_\ell} \frac{\chi_I(h(m_i))}{d_I} \prod_{j\in\alpha_\ell} \frac{\chi_J(h(m_j))}{\mathrm{d}_J} \tag{77}$$

where $Y(I,J,K)=1$ if I,J,K satisfy triangular inequalities and $Y(I,J,K)=0$ if not.

One can compute the mean value of more general operators if one knows explicitly simple intertwining coefficients. The expression of a simple intertwining coefficient in the basis of functions $\overset{I}{\pi}{}^i_j$ is explicitly given by

$$\langle \overset{n-1}{\underset{i=1}{\otimes}} \overset{I_i}{\pi}{}^{a_i}_0 \rangle_{\mathrm{Pphys}} = \sum_J \mathrm{d}_J \sum_{j_i,k_i} \prod_{i=0}^{n} C^{I_i J a_i j_i}_{k_i} \tag{78}$$

in term of the following coefficients:

$$\overset{I_i J}{C}{}^{a_i j_i}_{k_i} J \equiv \sum_k \overset{J}{\pi}{}^k_k(h(m_i)) \int \mathrm{d}\Lambda \overset{I_i}{\pi}{}^a_0(\Lambda) \overset{J}{\pi}{}^{j_i}_k(\Lambda) \overline{\overset{J}{\pi}{}^{k_i}_k(\Lambda)}, \tag{79}$$

which can easily be expressed in term of the coefficients of $(3j)$ symbols of Su(2) (see Fig. 5 for an illustration).

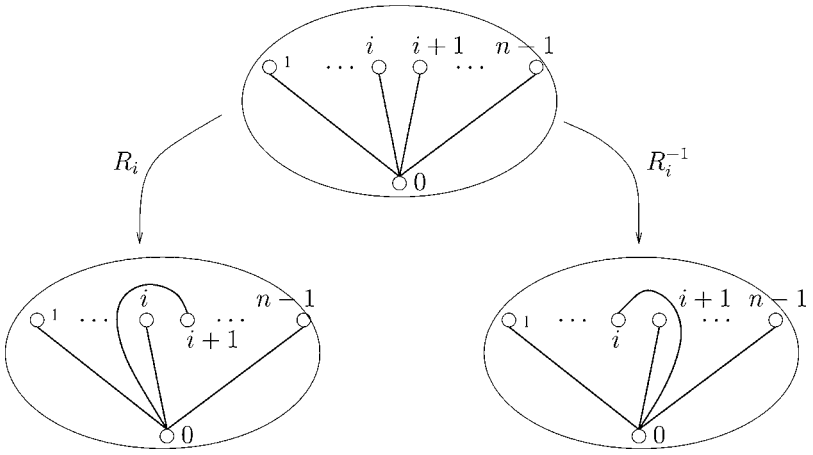

FIG. 6. Illustration of the braiding between two particles i and $i+1$. On the left, the braiding is associated to the R-matrix whereas it is associated to its inverse R^{-1} on the right.

Now, let us discuss some aspects concerning the braiding. First of all, we remark that the R matrix, as introduced in the previous section (66), defines an isomorphism of (partial physical) Hilbert spaces. Indeed, if one considers the particle labeled by $i \in [1,n-2]$, we define the following map:

$$R_{i,i+1}:\mathcal{H}^{0,n}_{\text{Pphys}}([m];G) \to \mathcal{H}^{0,n}_{\text{Pphys}}(P_i[m];G), \tag{80}$$

where $P_i[m]=(m_0,\ldots,m_{i+1},m_i,\ldots,m_{n-1})$ permutes the particles i and $i+1$. The fact that the previous map is an isometry is a consequence of the invariance of the simple intertwiner under braidings. Let us remark that the operator (80) can be written in term of multiplicative and derivative basic operators as follows:

$$R_{i,i+1} = \int \mathrm{d}x m_i(\delta_x)\mathrm{d}_{i+1}(xh(m_i)x^{-1}).$$

Then, it is easy to compute the action of the star operator on R and we show that it is an unitary operator.

Physically, the braiding operator (80) corresponds to a braiding between the two spin-network edges that link the observer with the particles i and $i+1$. In fact, there are two ways to braid the edges: one is associated to the R-matrix and the other to its inverse. This point is illustrated in Fig. 6.

This braiding property means that the partial physical Hilbert space does not depend on the order on the particles.

One can generalize the braiding operator to any pair of particles (i,j) (let us assume that $i<j$). There are many ways to do so and a simple example of such an operator is given by

$$R_{i,j} \equiv \prod_{k=i}^{j-1} R_{k,k+1} \prod_{\ell=j-2}^{i} R_{\ell,\ell+1}. \tag{81}$$

One can as well define an operator which involves not only R-matrices but also its inverse. The operator (81) defines an isometry between the Hilbert spaces $\mathcal{H}^{0,n}_{\text{Pphys}}([m],G)$ and $\mathcal{H}^{0,n}_{\text{Pphys}}(P_{ij}[m];G)$ where P_{ij} permutes the particles i and j.

C. Particles on any Riemann surface

The generalization of Theorem 1 to the case where Σ is any Riemann surface (of genus g) is quite simple. To do so, we first need the following proposition:

Proposition 3 (reduction of the genus): *Let p be a simple representation. We define the map* Υ_p *as follows*:

$$\Upsilon_p : \mathcal{H}^{g,n}_{\text{Pphys}}([m];G) \to \mathcal{H}^{g-1,n+2}_{\text{Pphys}}([m],p,\bar{p};G),$$

$$\psi \to \Upsilon_p(\psi)(A^{g-1,n},\tilde{x},\tilde{y}) = \int \mathrm{d}a_1 \mathrm{d}b_1 \delta(b_1 y h(p) y^{-1}) \delta(a y x^{-1}) \psi(A^{g,n}), \tag{82}$$

where we have used the notations of Proposition 4.

This map satisfies the following property:

$$\langle \psi, \varphi \rangle_{\text{Pphys}} = \int \mathrm{d}\mu(p) \langle \Upsilon_p(\psi), \Upsilon_p(\varphi) \rangle_{\text{Pphys}}, \tag{83}$$

where the partial physical scalar products are, respectively, those of $\mathcal{H}^{g,n}_{\text{Pphys}}([m];G)$ *and* $\mathcal{H}^{g-1,n+2}_{\text{Pphys}}([m],p,\bar{p};G)$.

Proof: Given two states ψ and φ in $\mathcal{H}^{g,n}_{\text{Pphys}}([m];G)$, we start by computing the partial physical scalar product in $\mathcal{H}^{g-1,n+2}_{\text{Pphys}}([m],p,\bar{p};G)$ and a direct calculation shows that

$$\begin{aligned}\langle \Upsilon_p(\psi), \Upsilon_p(\varphi) \rangle_{\text{Pphys}} = \int \prod_{i=1}^{n} \mathrm{d}\bar{z}_i \prod_{j=2}^{g} \mathrm{d}a_j \mathrm{d}b_j \mathrm{d}x \mathrm{d}y \overline{\psi(A^{g-1,n},x,yh(\bar{p})y^{-1})} \varphi(A^{g-1,n},x,yh(\bar{p})y^{-1}) \\ \times \delta\left(h_0 \prod_{i=1}^{n} z_i h(m_i) z_i^{-1} x y h(p) y^{-1} x^{-1} y h(\bar{p}) y^{-1} \prod_{j=2}^{g} [a_j,b_j] \right).\end{aligned} \tag{84}$$

A straightforward application of the Kirillov formula, $\int \mathrm{d}x = \int \mathrm{d}\mu(p) \mathrm{d}\tilde{\Lambda}$ where $x = \Lambda h(p) \Lambda^{-1}$, leads to (83). □

An immediate consequence of this proposition is that one can reduce the case of a Riemann surface to the case of the sphere (regarding the computation of the partial physical scalar product) and we have the following theorem:

Theorem 2 (Reduction to the case of the sphere): *Let* $[p]=(p_1,\ldots,p_g)$ *be a family of g simple representations. We define the map* $\Upsilon_{[p]} = \Upsilon_{p_g} \circ \cdots \circ \Upsilon_{p1}$ *and the partial physical scalar product between two states* $\varphi, \psi \in \mathcal{H}^{g,n}_{\text{Pphys}}([m];G)$ *is expressed in term of symmetric intertwiner as follows*:

$$\langle \varphi, \psi \rangle_{\text{Pphys}} = \int \prod_{i=1}^{g} \mathrm{d}\mu(p_i) \iota_s([m],[p,\bar{p}];0) | \mathcal{F} \circ \Upsilon_{[p]}(\bar{\varphi}\psi), \tag{85}$$

where $[p,\bar{p}]=(p_1,\bar{p}_1,\ldots,p_g,\bar{p}_g)$ *and* $\mathcal{F}$ *has been introduced in Theorem* 1.

Proof: Let $\varphi, \psi \in \mathcal{H}^{g,n}_{\text{Pphys}}([m];G)$. By a recursive use of the proposition (83), we immediately show that

$$\langle \varphi, \psi \rangle_{\text{Pphys}} = \int \prod_{i=1}^{g} \mathrm{d}\mu(p_i) \langle \Upsilon_{[p]}(\varphi), \Upsilon_{[p]}(\psi) \rangle, \tag{86}$$

where the scalar product on the right-hand side is the partial physical scalar product in the case of the sphere. Then, we conclude immediately thanks to Theorem 1. □

Let us discuss some consequences of this theorem.

1. The quantum group structure still holds when Σ is any Riemann surface. However, to make the contact between the Hilbert structure and the simple intertwiner is more involved than the case of the sphere. Anyway, the quantum double is manisfestly the symmetry group of the quantum theory.

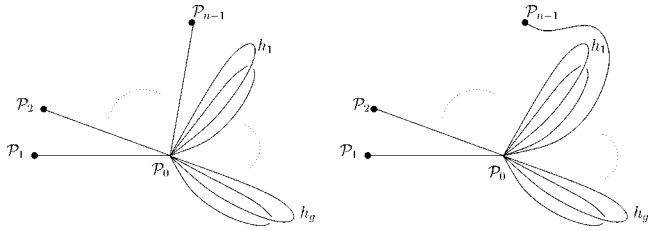

FIG. 7. Pictorial illustration of the braiding: the partial kinematical Hilbert spaces associated to the minimal graphs on the left and on the right are isometric and the isometry is defined by a "general" braiding operator. Note that $\mathcal{P}_i$ denotes the particles and h_i the handles.

2. What about the braiding? We have chosen an order to define the partial physical Hilbert space: this order is illustrated in Fig. 7 and consists in putting the particles variables first and the handledodies variables next.

We have shown previously that permuting two particles variables corresponds to acting with an R-matrix. In fact the same thing happens when one permutes particles with handles or handles with handles. Indeed, in Theorem 2, we see that one handle is decomposed into a pair of particles whose masses are m and $\bar{m}$; therefore permuting one particle with one handle corresponds to permuting this particle with the two particles associated to the handle, as a consequence this operation corresponds to acting twice with an R-matrix. To be more concrete, let us consider the example of Fig. 7. The Hilbert spaces $\mathcal{H}^{g,n}_{\text{Pphys}}([m],\gamma_1;G)$ and $\mathcal{H}^{g,n}_{\text{Pphys}}([m],\gamma_2;G)$ where γ_1 and γ_2 are the minimal graphs associated, are related by the following isometry:

$$R_{\gamma_1,\gamma_2} \equiv \int \mathrm{d}\mu(p_1) \overset{m_{n-1},\bar{p}_1}{R}{}_{n,n+1} \circ \overset{m_{n-1,n},p_1}{R}{}_{n,n-1} \circ \Upsilon_{p_1}, \tag{87}$$

where the R-matrix $R_{i,i+1}$ acts on the particles variables i and $i+1$. We have explicitly shown the representation for the evaluation of the R-matrices in order to be clear. On can easily show that this map is an isometry. It is easy to generalize this map to the case where γ_2 is any minimal graph.

3. The next remark concerns some factorization properties of the partial physical scalar product. To clarify what we mean by that we use the notation $\langle ;\rangle^{g,n}_{\text{Pphys}}[m]$ for the partial physical scalar product within this remark and we have

$$\langle ;\rangle^{g,n}_{\text{Pphysc}}([m]) = \int \mathrm{d}\mu(p) \langle ;\rangle^{g-1,n+1}_{\text{Pphys}}([m],p) \otimes \langle ;\rangle^{1,1}_{\text{Pphysc}}(\bar{p}). \tag{88}$$

Therefore, the physical scalar product can be factorized into scalar product on the torus. This property is well-known and is illustrated in the picture of Fig. 8.

The last remark concerns the evaluation of geometric observables. Indeed, in the case of a nontrivial topology, there exists nontrivial "geometric" operators which corresponds to monodromies around handles. For instance, the trace of $M_K(a_i)$ where a_i is a loop around one handle is given by

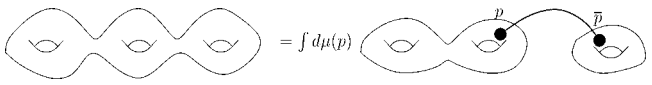

FIG. 8. Illustration of the factorization property of the partial physical scalar product: the physical scalar product on any Riemann surface can be factorized into partial physical scalar product on the torus.

$$\mathrm{Tr}(M_K(a_i)) = \sum_J (J,J,K) \frac{\Pi_{i=0}^{n-1} \chi_J(h(m_i))}{d_J^{2g+n-2}} = \sum_{j \geq [K/2]} \frac{\Pi_{i=0}^{n-1} \chi_J(h(m_i))}{d_J^{2g+n-2}}. \tag{89}$$

in the case of a genus g surface with n particles. $[x]$ denotes the entire part of x. There are at least two different ways to prove this identity: one can use the last Theorem 2 to come back to the case of the sphere or one can make a direct calculation.

As a consequence, we have now a complete description à la LQG of three-dimensional gravity coupled to massive particles.

IV. CONCLUSION AND PERSPECTIVES

In this paper, we have performed the Hamiltonian quantization of three-dimensional Riemannian gravity (with no cosmological constant) coupled with a finite number of massive spinless point particles using loop quantum gravity techniques. The work we have proposed contains: a complete description of the (partial) physical Hilbert space in the general case of any Riemann surface (i.e., states and scalar product) and a discussion concerning the question of the observables (i.e., their definition and the computation of their expectation values in some examples).

We have emphasized the crucial role of the Drinfeld double, which is clearly the symmetry group of the quantum theory, as expected. In the LQG approach, the Drinfeld double appears as a result of the dynamics in the sense that its role becomes obvious when one imposes the three-dimensional analog of the "Hamiltonian" constraint. This point of view is quite interesting because it is a nontrivial example where one sees the emergence of a noncompact quantum group (at the level of the physical Hibert space) starting from a classical compact group (at the level of the kinematical Hilbert space). Our construction is in that sense very different, at the conceptual level, from the combinatorial quantization, the group field theory quantization or the spin-foam quantization where the quantum group is put by hand as the basic starting block of these methods. From the point of view of a particles physicist, our approach might seem more satisfying for we describe particles as simple representations of the "Poincare" (in Riemannian space) group and we notice that, using LQG techniques, scattering amplitudes of these particles in a quantum background are described in terms of intertwiners of a quantum group. In fact, in three dimensions, we see that the Hamiltonian constraint (in the presence of particles) is in fact simple intertwiners!

Thus, physical states are constructed from simple representations of the Drinfeld double and the physical scalar product is in fact given by a symmetric (or Barrett-Crane—BC) intertwiner between the simple representations defining the states. The ressemblance with the usual BC model is obvious and asks the question whether the BC model is really a model of four-dimensional quantum gravity or a model of three-dimensional gravity coupled to particles.

This paper opens new insights into LQG techniques. The first one would be to see the emergence of the quantum group $\mathrm{SU}_q(2)$ when one imposes the Hamiltonian constraint with a cosmological constant (the quantum parameter q is related to Λ in the usual way). We are currently working in that direction. It also seems possible to generalize our construction to the Lorentzian case because we finally do not need to make sense of the whole space of cylindrical functions but only of the space of cylindrical functions on one graph, the minimal graph. Therefore, the obstruction raised in Refs. 12 and 35 should not be problematic in our context. Going from one minimal graph to another reduces to a nontrivial braiding which is still well defined in the Lorentzian regime. Moreover, one could introduce new types of particles: lightlike, spacelike, or timelike particles. We could also think of introducing particles that would describe a black hole in the presence of a negative cosmological constant.

Another issue to be solved is to extend this construction to the case of spinning particles. This case has been considered briefly in the spin-foam approach in Ref. 11. In the LQG point of view, the description of the kinematical Hilbert space has been performed completely in Ref. 24 but the way that the physical scalar product is related to the quantum double remains to be understood. We expect that this link works in the same way as the nonspinning case with the difference being that the physical scalar product (or spinning particles scattering amplitudes in a quantum background)

is no longer given by a simple intertwiner but a more general DSU(2) intertwiner. In our point of view, the case of spinning particles is not a conceptual issue but only a technical issue.

In fact, the original motivation for this work is the construction of a self-gravitating quantum field theory in the Hamiltonian framework. This means a precise description of the Fock space associated to its creation and annihilation operators. We are finishing a work in that direction[22] and we have shown in particular that the quantum field theory so obtained is closely related to the one constructed in Ref. 11 in the context of spin-foam models.

Finally, the last but not the least is to make use of this construction to describe a coupling of quantum gravity to matter field in four dimensions. It seems quite obvious how to generalize, at the level of the kinematical Hilbert space, the coupling of spin-networks to some matter fields. The more interesting question would be to understand what kind of matter that represents and what is the dynamics of such a coupling (see Ref. 3 for ideas in that direction).

ACKNOWLEDGMENTS

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APPENDIX A: THE DRINFELD DOUBLE

We recall the general definition of the quantum double that we illustrate in the case of a finite group.

Let A be a Hopf algebra, the quantum double of A is denoted $D(A)$ (or DA), is a quasitriangular Hopf algebra containing A as a sub-Hopf algebra and has different equivalent definitions.

If A is a Hopf algebra, we denote m the multiplication and Δ the coproduct; it will be useful to introduce a permutation operator σ. From A, we can construct different Hopf algebra: A_{op} is the Hopf algebra with multiplication $m_{\mathrm{op}}=m\circ\sigma$ and coproduct Δ; A^{op} the Hopf algebra with multiplication m and coproduct $\sigma\circ\Delta$; the dual Hopf algebra A^* construted from the duality bracket $\langle,\rangle$ between A and $A*$.

The quantum double (or Drinfeld double) $D(A)$ is the Hopf algebra defined by the following:

1. $D(A)=A\otimes A^{*\mathrm{op}}$ as a coalgebra.
2. The algebra law is given by

$$(x\otimes\xi)(y\otimes\eta)=\sum_{(y),(\xi)} xy_{(2)}\otimes\xi_{(2)}\eta\langle\xi_{(1)},S^{-1}y_{(1)}\rangle\langle\xi_{(3)},y_{(3)}\rangle, \tag{A1}$$

where $\Delta(x)=\Sigma_{(x)}x_{(1)}\otimes x_{(2)}$ and $\Delta_{A^{*\mathrm{op}}}(\xi)=\Sigma_{xi}\xi_{(1)}\otimes\xi_{(2)}$ is the usual Sweedler notation. $D(A)$ is quasitriangular and the R-matrix is given by $R=\Sigma_i e_i\otimes 1\otimes 1\otimes e^i$ where $(e_i)_i$ (respectively, $(e^i)_i$) is a basis of A (respectively, A^*).

Let us illustrate this construction in the case of a finite group to be more concrete. Let G be a finite group and we assume that A is the group algebra of G, i.e., $A=\mathbb{C}[G]$. As a result $A^*=F(G)$, the algebra of functions on G, and the quantum double $D(\mathbb{C}[G])=\mathbb{C}[G]\otimes F(G)^{\mathrm{op}}$ is usually denoted $D(G)$. A basis of $D(G)$ is $(x\otimes\delta_g)_{x,g\in G}$ and the Hopf algebra and coalgebra structures are, respectively, given by

$$(x\otimes\delta_g)\cdot(y\otimes\delta_h)=xy\otimes\delta_h(y^{-1}gy)\delta_h\Delta(x\otimes\delta_g)=\sum_{g_1,g_2|g_1g_2=H}(x\otimes g_2)\otimes(x\otimes g_1). \tag{A2}$$

The action of the antipode on the previous basis is given by $S(x\otimes\delta_g)=x^{-1}\otimes\delta_{x^{-1}g^{-1}x}$ and the co-unit is defined by $\epsilon(x\otimes\delta_g)=\delta(g)$. The R-matrix is given by $R=\Sigma_{x,g}(x\otimes 1)\otimes(1\otimes\delta_g)$. This construction can be directly generalized to the case where G is locally compact.[18]

Representation theory of $D(G)$ has been done in Ref. 10 and generalized to the compact group case ($G=\mathrm{Su}(2)$) in Ref. 18. The main results are recalled in the core of the paper.

APPENDIX B: NORMALIZATION OF THE PHYSICAL SCALAR PRODUCT

We introduce the group $\mathcal{B}^{g,n} \simeq G^{4g+1-1}$ which acts on $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$: it acts by right G-action of each variable $\tilde{z}_e$ and by right and left G-action on each variable a_i or b_i. Given a partial physical state s and an element $y \in \mathcal{B}^{g,n}$, we will use the notation $B_y(s)$ for the action of y on s. There exist many couples (g,n) such that the state s can be viewed as an element of $\mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ and we denote $(g_{\min},n_{\min})$ the minimal couple. Then, we define the invariance group transformations of $s$by $\mathcal{B}[s] \equiv \mathcal{B}^{g_{\min},n_{\min}}$. To be more concrete, $\mathcal{B}[s]$ transforms only the variables which appear explicitly in the state s. There is a natural action of $\mathcal{B}[s]$ on $\mathcal{H}^{n,g}[m]$ and we define the sub-Hilbert space $C^{g,n}[s] \subset \mathcal{H}^{n,g}[m]$ as follows:

$$C^{g,n}[s] \equiv \{f \in \mathcal{H}^{g,n}[m] |\ \forall\, y \in \mathcal{B}[s],\ B_y(f) = f\}. \tag{B1}$$

Proposition 4 (inclusions): Let $v,u \in \mathcal{H}^{g,n}_{\mathrm{Pphys}}([m];G)$ *defined by* $u=\mathrm{tr}([a_1,b_1])$ *and* $v=\mathrm{tr}(z_{n-2}h(m_{n-2})z_{n-2}^{-1}z_{n-1}h(m_{n-1})z_{n-1}^{-1})$ *where* tr *denotes the trace in the fundamental representation of* SU(2). *We have the following inclusions of Hilbert spaces*:

$$C^{g,n}[u] \hookrightarrow \int^{\oplus} \mathrm{d}\mu(p)\mathcal{H}^{g-1,n+2}_{\mathrm{Pphys}}([m],p;\bar{p};G), \tag{B2}$$

$$C^{g,n}[v] \hookrightarrow \int^{\oplus} \mathrm{d}\mu(q)\mathcal{H}^{g,n-1}_{\mathrm{Pphys}}(m_0,\ldots,m_{n-3},\bar{q};G) \otimes \mathcal{H}^{0,3}_{\mathrm{Pphys}}(q,m_{n-2},m_{n-1};G). \tag{B3}$$

The measures are given by $\mathrm{d}\mu(p)=(1/\pi)\sin^2 p\mathrm{d}p$ *where* $\mathrm{d}p$ *is the measure on the circle* S^1 *such that* $\int \mathrm{d}p = 2\pi$. *We have introduced the notation* $\bar{p}=2\pi-p$.

Proof: We concentrate on the first map (B2) and we show that an explicit map is given as follows:

$$f \mapsto \phi(A^{g-1,n},\tilde{x}_1,\tilde{y}_1) \equiv \int \mathrm{d}a_1\mathrm{d}b_1\,\delta(a_1x_1h(\bar{p})x_1^{-1})\,\delta(b_1a_1b_1^{-1}y_1h(p)y_1^{-1})f(A^{g,n}), \tag{B4}$$

where the family $A^{g,n}=(a_1,b_1;\ldots;a_g,b_g;\tilde{z}_1,\ldots,\tilde{z}_{n-1})$ contains the $n+2g$ arguments of the function f and $A^{g-1,n}=(a_2,b_2;\ldots;a_g,b_g;\tilde{z}_1,\ldots,\tilde{z}_{n-1})$ contains $n+2g-2$ arguments. The norm of the function ϕ viewed as an element of the space $\mathcal{H}^{n+2,9-1}([m],p,\bar{p};G)$ is given by

$$\|\phi\|^2_{\mathrm{Pphys}} = \int \prod_{e=1}^{n-1} \mathrm{d}\tilde{z}_e\mathrm{d}\tilde{x}_1\mathrm{d}\tilde{y}_1 \prod_{i=2}^{g} \mathrm{d}a_i\mathrm{d}b_i |\phi(A^{g-1,n},\tilde{x}_1,\tilde{y}_1)|^2 \times \delta\left(h(m_0)\prod_{e=1}^{n-1} z_e h(m_e) z_e^{-1} x_1 h(p) x_1^{-1} y_1 h(\bar{p}) y_1^{-1} \prod_{i=2}^{g} [a_i,b_i]\right).$$

It is then straightforward to verify that

$$\int \mathrm{d}\mu(p)\|\phi\|^2_{\mathrm{Pphys}} = \int \prod_{e=1}^{n-1} \mathrm{d}\tilde{z}_e \prod_{i=1}^{g} \mathrm{d}a_i\mathrm{d}b_i\,\delta\left(h(m_0)\prod_{e=1}^{n-1} z_e h(m_e) z_e^{-1} \prod_{i=1}^{g} [a_i,b_i]\right) \times \int \mathrm{d}x\,\delta([x,a_1])\overline{f(a_1,b_1;\ldots)}f(a_1,b_1x;\ldots).$$

As $f \in C^{g,n}[u]$ and $B_x(u)=u$ if $[x,a_1]=1$ then we conclude immediately that

$$\int \mathrm{d}\mu(p)\|\phi\|^2_{\mathrm{Pphys}} = \|f\|^2_{\mathrm{Pphys}}. \tag{B5}$$

Therefore, the first inclusion (B2) proven.

To prove the second one (B3), we proceed in the same way. We start by claiming that the following map trivially realizes the injection (B3):

$$f \mapsto \psi((A^{g,n-2},\tilde{x}) \otimes (\tilde{z}_{n-2},\tilde{z}_{n-1})) = f(A^{g,n})e^{g,n-2}(m_0,\ldots,m_{n-3},q) \otimes e^{0,3}(\bar{q},m_{n-2},m_{n-1}) \tag{B6}$$

Note that ψ is viewed as an element of $\mathcal{H}^{g,n-1}_{\text{Pphys}}(m_0,\ldots,m_{n-3},\bar{q};G) \otimes \mathcal{H}^{0,3}_{\text{Pphys}}(q,m_{n-2},m_{n-1};G)$ and we have introduced the notation $(A^{g,n-2,x}) = (a_1,b_1;\ldots,a_g,b_g;\tilde{z}_1,\ldots,\tilde{z}_{n-3},\tilde{x})$. The norm of ψ is trivially given by

$$\|\phi\|^2_{Pphys} = \int \prod_{i=1}^{n-1} \mathrm{d}\tilde{z}_e \mathrm{d}\tilde{x} \prod_{i=1}^{g} \mathrm{d}a_i \mathrm{d}b_i |f(A^{g,n})|^2 \delta\left(h(m_0)\prod_{e=1}^{n-3} z_e h(m_e) z_e^{-1} x h(q) x^{-1} \prod_{i=1}^{g} [a_i,b_i]\right) \times \delta(h(\bar{q}) z_{n-2} h(m_{n-2}) z_{n-2}^{-1} z_{n-1} h(m_{n-1}) z_{n-1}^{-1}).$$

Therefore, we verify easily that

$$\int \mathrm{d}\mu(q)\|\phi\|^2_{\text{Pphys}} = \int \prod_{i=1}^{n-1} \mathrm{d}\tilde{z}_e \mathrm{d}\tilde{x} \prod_{i=1}^{g} \mathrm{d}a_i \mathrm{d}b_i |f(a_1,b_1;\ldots,a_g,b_g;\tilde{z}_1,\ldots,\tilde{z}_{n-3},x\tilde{z}_{n-2},x\tilde{z}_{n-1})|^2 \times \delta\left(h(m_0)\prod_{i=1}^{n-1} z_e h(m_e) z_e^{-1} \prod_{i=1}^{g} [a_i,b_i]\right).$$

Finally, as $f \in C^{g,n}[v]$, then we conclude that

$$\int \mathrm{d}\mu(q)\|\phi\|^2_{\text{Pphys}} = \|f\|^2_{\text{Pphys}},$$

and the Hilbert spaces inclusion (B3) is proven. □

It is clear that the unit element $e^{g,n}[m] \in C^{n,g}[u]$ for any function u. Therefore, we can decompose the unit as a tensor product of unit elements of partial Hilbert spaces associated to the sphere with three particles. This is a direct consequence of the previous proposition and the explicit decomposition of $e^{g,n}[m]$ is given by

$$e^{g,n}[m] = \int \prod_{i=0}^{g-1} \mathrm{d}\mu(p_i) \prod_{j=0}^{g-1} \mathrm{d}\mu(m_{n+i}) \prod_{k=1}^{n+g-2} \mathrm{d}\mu(q_k) \bigotimes_{a=0}^{g-1} e^{0,3}(p_a,\overline{p_a},m_{n+a}) \bigotimes_{b=1}^{n+g-2} e^{0,3}(\overline{r_{b-1}},m_b,r_b) \tag{B7}$$

with the conventions $r_0 = \overline{m_0}$ and $r_{n+g-2} = m_{n+g-1}$. As a consequence, one can compute the norm of the identity in two ways and therefore one can relate the coefficients $\lambda(g,n,[m])$ to the coefficients $\lambda(0,3,[m])$. Let us assume that the coefficients $\lambda(0,3,[m]) = \lambda$ do not depend on the values of the masses, then the relation (B7) implies that

$$\|e^{g,n}[m]\|^2_{\text{Pphys}} = \lambda^{n+2g-2} \int \prod_{i=0}^{g-1} \mathrm{d}\mu(p_i) \prod_{j=0}^{g-1} \mathrm{d}\mu(m_{n+i}) \prod_{k+1}^{n+g-2} \mathrm{d}\mu(q_k) \times \prod_{a=0}^{g-1} \|e^{0,3}(p_a,\overline{p_a},m_{n+a})\|^2_{\text{Pphys}} \prod_{b=1}^{n+g-2} \|e^{0,3}(\overline{r_{b-1}},m_b,r_b)\|^2_{\text{Pphys}}. \tag{B8}$$

After some direct calculations, we show that

$$\|e^{g,n}[m]\|^2_{\text{Pphys}} = \lambda^{n+2g-2}\sum_{k=1}^{+\infty} k^{1-2g-n}\prod_{e=0}^{n-1}\frac{\sin(km_e)}{\sin(m_e)}. \tag{B9}$$

Then, by comparison with expression (43) we conclude that $\lambda(g,n.[m])$ is also independent of the values of the masses and we have

$$\lambda(g,n,[m]) \equiv \lambda(g,n) = \lambda^{n+2g-2}. \tag{B10}$$

This fixes the normalization of the partial physical scalar product.

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Automorphisms and a cartography of the solution space for vacuum Bianchi cosmologies: The Type III case

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The theory of symmetries of systems of coupled, ordinary differential equations (ODEs) is used to develop a concise algorithm for cartographing the space of solutions to vacuum Bianchi Einstein's Field Equations (EFE). The symmetries used are the well known automorphisms of the Lie algebra for the corresponding isometry group of each Bianchi Type, as well as the scaling and the time reparametrization symmetry. The application of the method to Type III results in (a) the recovery of all known solutions without a prior assumption of any extra symmetry; (b) the enclosure of the entire unknown part of the solution space into a single, second order ODE in terms of one dependent variable; and (c) a partial solution to this ODE. It is also worth mentioning that the solution space is seen to be naturally partitioned into three distinct, disconnected pieces: one consisting of the known Siklos (pp-wave) solution, another occupied by the Type III member of the known Ellis-MacCallum family and the third described by the aforementioned ODE in which a one parameter subfamily of the known Kinnersley geometries resides. Lastly, preliminary results reported show that the unknown part of the solution space for other Bianchi Types is described by a strikingly similar ODE, pointing to a natural operational unification as far as the problem of solving the cosmological EFE's is concerned. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Since the early times of cosmology, automorphisms have been identified as possible key elements for a unified treatment of spatially homogeneous Bianchi Geometries.[1] Harvey has found the automorphisms of all three-dimensional Lie Algebras,[2] while the corresponding results for the four-dimensional Lie Algebras have been reported in Ref. 3. Jantzen's tangent space approach sees the automorphic matrices as the means for achieving a convenient parametrization of a full scale-factor matrix in terms of a desired, diagonal matrix.[4] Samuel and Ashtekar were the first to look upon automorphisms from a space viewpoint.[5] The notion of *Time-Dependent Automorphism Inducing Diffeomorphisms* (A.I.D.'s), i.e., coordinate transformations mixing space and time in the new spatial coordinates and inducing automorphic motions on the scale-factor matrix, the lapse, and the shift has been developed in Ref. 6.

In this paper we revisit the problem of solving the EFE's for vacuum Bianchi Geometries. We begin with a full metric, i.e., we make no assumption for the lapse function N^2, the shift vector N^α and the spatial metric $\gamma_{\alpha\beta}$. Then we use the time-dependent A.I.D.'s to put the shift vector to zero. At this point the idea is to exploit, in a systematic way, the remaining symmetries of the field equations—sometimes called "rigid"[7]—to transform them to the most simple form possible, without loss of generality. These are the well known symmetries following from the constant auto-

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morphism group within each Bianchi Type, as well as the scaling of the metric by a constant and the time reparametrization symmetry (see, e.g., Ref. 8). Applying this analysis to Bianchi Type III Vacuum Cosmology, we produce an exhaustive cartography of the entire space of its solutions.

The paper is organized as follows: in Sec. II, we present our method. In Sec. III, after a brief description of Bianchi Type III Cosmology, we apply the method. We thus recover all known solutions, describe the unknown part of the solution space with a single, second order ODE in terms of one dependent variable, and present a new solution. A brief preview of the corresponding results obtained for other Bianchi Types is also included. Finally, some discussion and concluding remarks are given in Sec. IV.

II. THE METHOD

As is well known, for spatially homogeneous space-times with a simply transitive action of the corresponding isometry group,[10,8] the line element, assumes the form

$$ds^2 = (N^\alpha N_\alpha - N^2)dt^2 + 2N_\alpha \sigma_i^\alpha \, dx^i \, dt + \gamma_{\alpha\beta}\sigma_i^\alpha \sigma_j^\beta \, dx^i \, dx^j, \tag{2.1}$$

where the 1-forms σ_i^α are defined from

$$d\sigma^\alpha = C_{\beta\gamma}^\alpha \sigma^\beta \wedge \sigma^\gamma \Leftrightarrow \sigma_{i,j}^\alpha - \sigma_{j,i}^\alpha = 2C_{\beta\gamma}^\alpha \sigma_i^\gamma \sigma_j^\beta. \tag{2.2}$$

Then the field equations are (e.g., Ref. 6):

$$E_o \doteq K^{\alpha\beta}K_{\alpha\beta} - K^2 - \mathbf{R} = 0, \tag{2.3}$$

$$E_\alpha \doteq K_\alpha^\mu C_{\mu\epsilon}^\epsilon - K_\epsilon^\mu C_{\alpha\mu}^\epsilon = 0, \tag{2.4}$$

$$E_{\alpha\beta} \doteq \dot{K}_{\alpha\beta} + N(2K_\alpha^\tau K_{\tau\beta} - KK_{\alpha\beta}) + 2N^\rho(K_{\alpha\nu}C_{\beta\rho}^\nu + K_{\beta\nu}C_{\alpha\rho}^\nu) - N\mathbf{R}_{\alpha\beta} = 0, \tag{2.5}$$

where

$$K_{\alpha\beta} = -\frac{1}{2N}(\dot{\gamma}_{\alpha\beta} + 2\gamma_{\alpha\nu}C_{\beta\rho}^\nu N^\rho + 2\gamma_{\beta\nu}C_{\alpha\rho}^\nu N^\rho) \tag{2.6}$$

is the extrinsic curvature and

$$\mathbf{R}_{\alpha\beta} = C_{\sigma\tau}^\kappa C_{\mu\nu}^\lambda \gamma_{\alpha\kappa}\gamma_{\beta\lambda}\gamma^{\sigma\nu}\gamma^{\tau\mu} + 2C_{\beta\lambda}^\kappa C_{\alpha\kappa}^\lambda + 2C_{\alpha\kappa}^\mu C_{\beta\lambda}^\nu \gamma_{\mu\nu}\gamma^{\kappa\lambda} + 2C_{\beta\kappa}^\lambda C_{\mu\nu}^\mu \gamma_{\alpha\lambda}\gamma^{\kappa\nu} + 2C_{\alpha\kappa}^\lambda C_{\mu\nu}^\mu \gamma_{\beta\lambda}\gamma^{\kappa\nu}, \tag{2.7}$$

the Ricci tensor of the hypersurface.

In Ref. 6, particular spacetime coordinate transformations have been found, which reveal as symmetries of (2.3), (2.4), (2.5) the following transformations of the dependent variables $N, N_\alpha, \gamma_{\alpha\beta}$:

$$\tilde{N} = N, \quad \tilde{N}_\alpha = \Lambda_\alpha^\rho(N_\rho + \gamma_{\rho\sigma}P^\sigma), \quad \tilde{\gamma}_{\mu\nu} = \Lambda_\mu^\alpha \Lambda_\nu^\beta \gamma_{\alpha\beta}, \tag{2.8}$$

where the matrix Λ and the triplet P^α must satisfy

$$\Lambda_\rho^\alpha C_{\beta\gamma}^\rho = C_{\mu\nu}^\alpha \Lambda_\beta^\mu \Lambda_\gamma^\nu, \tag{2.9}$$

$$2P^\mu C_{\mu\nu}^\alpha \Lambda_\beta^\nu = \dot{\Lambda}_\beta^\alpha. \tag{2.10}$$

For all Bianchi Types, this system of equations admits solutions that contain three arbitrary functions of time plus several constants depending on the automorphism group of each type. The three functions of time are distributed among Λ and P (which also contains derivatives of these

functions). So one can use this freedom either to simplify the form of the scale factor matrix or to set the shift vector to zero. The second action can always be taken, since, for every Bianchi type, all three functions appear in P^α.

In this work we adopt the latter point of view. When the shift has been set to zero, there is still a remaining "gauge" freedom consisting of all constant Λ^α_β (automorphism group matrices). Indeed, the system (2.9), (2.10) accepts the solution Λ^α_β=const, $P^\alpha=\mathbf{0}$. The generators of the corresponding motions, induced in the space of dependent variables spanned by $\gamma'_{\alpha\beta}$s (the lapse is given in terms of $\gamma_{\alpha\beta}$, $\dot{\gamma}_{\alpha\beta}$ by algebraically solving the quadratic constraint equation) $\tilde{\gamma}_{\mu\nu}=\Lambda^\alpha_\mu\Lambda^\beta_\nu\gamma_{\alpha\beta}$ are[11]

$$X_{(I)}=\lambda^\rho_{(I)\alpha}\gamma_{\rho\beta}\frac{\partial}{\partial\gamma_{\alpha\beta}}, \tag{2.11}$$

with λ satisfying

$$\lambda^\alpha_{(I)\rho}C^\rho_{\beta\gamma}=\lambda^\rho_{(I)\beta}C^\alpha_{\rho\gamma}+\lambda^\rho_{(I)\gamma}C^\alpha_{\beta\rho}. \tag{2.12}$$

Now, these generators define a Lie algebra and each one of them induces, through its integral curves, a transformation on the configuration space spanned by the $\gamma_{\alpha\beta}$'s. If a generator is brought to its normal form (e.g., $\partial/\partial z_i$), then the Einstein equations, written in terms of the new dependent variables, will not explicitly involve z_i. They thus become a *first order* system in the function $\dot{z}_i$.[12] If the above Lie algebra happens to be Abelian, then all generators can be brought to their normal form simultaneously. If this is not the case, we can diagonalize in one step the generators corresponding to any eventual Abelian subgroup. The rest of the generators (not brought in their normal form) continue to define a symmetry of the reduced system of EFE's if the algebra of the $X_{(I)}$'s is solvable.[13] One can thus repeat the previous step by choosing one of these remaining generators. This choice will, of course, depend upon the simplifications brought to the system at the previous level. Finally, if the algebra does not contain any Abelian subgroup, one can always choose one of the generators, bring it to its normal form, reduce the system, and search for its symmetries (if there are any). Lastly, two further symmetries of (2.3), (2.4), (2.5) are also present and can be used in conjunction with the constant automorphisms: The time reparametrization $t\rightarrow f(t)+\alpha$, owing to the nonexplicit appearance of time in these equations, and the scaling by a constant $\gamma_{\alpha\beta}\rightarrow\mu\gamma_{\alpha\beta}$, as can be straightforwardly verified. Their corresponding generators are

$$Y_1=\frac{1}{\dot{f}}\frac{\partial}{\partial t}, \tag{2.13}$$

$$Y_2=\gamma_{\alpha\beta}\frac{\partial}{\partial\gamma_{\alpha\beta}}. \tag{2.14}$$

These generators commute among themselves, as well as with the $X_{(I)}$'s, as can be easily checked.

III. APPLICATION TO BIANCHI TYPE III

We are now going to apply the method, previously discussed, to the case of Bianchi Type III. For this type the structures constants are[14]

$$C^1_{13}=-C^1_{31}=1,$$
$$C^\alpha_{\beta\gamma}=0, \quad \textit{for all other values of } \alpha\beta\gamma. \tag{3.1}$$

Using these values in the defining relation (2.2) of the 1-forms σ^α_i, we obtain

$$\sigma_i^\alpha = \begin{pmatrix} 0 & e^{-x} & 0 \\ 0 & 0 & 1 \\ \frac{1}{2} & 0 & 0 \end{pmatrix}. \tag{3.2}$$

The corresponding vector fields ξ_α^i (satisfying $[\xi_\alpha, \xi_\beta] = c_{\alpha\beta}^\gamma \xi_\gamma$) with respect to which the Lie Derivative of the above 1-forms is zero are

$$\xi_1 = \partial_y, \quad \xi_2 = \partial_z, \quad \xi_3 = \partial_x + y\partial_y. \tag{3.3}$$

The Time Dependent A.I.D.'s are described by

$$\Lambda_\beta^\alpha = \begin{pmatrix} e^{-2P(t)} & 0 & x(t) \\ 0 & c_{22} & c_{23} \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.4}$$

$$P^\alpha = \left(x(t)\dot{P}(t) + \frac{1}{2}\dot{x}(t), P^2(t), \dot{P}(t) \right), \tag{3.5}$$

where $P(t)$, $x(t)$, and $P^2(t)$ are arbitrary functions of time. As we have already remarked, the three arbitrary functions appear in P^α, and thus can be used to set the shift vector to zero.

The remaining symmetry of the EFEs is, consequently, described by the constant matrix:

$$M = \begin{pmatrix} e^{s_1} & 0 & s_4 \\ 0 & e^{s_2} & s_3 \\ 0 & 0 & 1 \end{pmatrix}, \tag{3.6}$$

where the parametrization has been chosen so that the matrix becomes identity for the zero value of all parameters.

Thus, the induced transformation on the scale factor matrix is $\tilde{\gamma}_{\alpha\beta} = M_\alpha^\mu M_\beta^\nu \gamma_{\mu\nu}$, which explicitly reads as

$$\begin{aligned} \tilde{\gamma}_{11} &= e^{2s_1}\gamma_{11}, \\ \tilde{\gamma}_{12} &= e^{s_1+s_2}\gamma_{12}, \\ \tilde{\gamma}_{13} &= e^{s_1}(s_3\gamma_{11} + s_4\gamma_{12} + \gamma_{13}), \\ \tilde{\gamma}_{22} &= e^{2s_2}\gamma_{22}, \\ \tilde{\gamma}_{23} &= e^{s_2}(s_3\gamma_{12} + s_4\gamma_{22} + \gamma_{23}), \\ \tilde{\gamma}_{33} &= s_3^2\gamma_{11} + 2s_3(s_4\gamma_{12} + \gamma_{13}) + s_4^2\gamma_{22} + 2s_4\gamma_{23} + \gamma_{33}. \end{aligned} \tag{3.7}$$

The previous equations define a group of transformations G_r of dimension $r = \dim(\mathrm{Aut}(III)) = 4$. The four generators of the group can be evaluated from the relation

$$X_A = \left(\frac{\partial \tilde{\gamma}_{\alpha\beta}}{\partial s_A} \right)_{s=0} \frac{\partial}{\partial \gamma_{\alpha\beta}}, \tag{3.8}$$

where $A = \{1,2,3,4\}$. Applying this definition to (3.7), we have the generators

$$X_1 = 2\gamma_{11}\frac{\partial}{\partial\gamma_{11}} + \gamma_{12}\frac{\partial}{\partial\gamma_{12}} + \gamma_{13}\frac{\partial}{\partial\gamma_{13}}, \tag{3.9}$$

$$X_2 = \gamma_{12}\frac{\partial}{\partial\gamma_{12}} + 2\gamma_{22}\frac{\partial}{\partial\gamma_{22}} + \gamma_{23}\frac{\partial}{\partial\gamma_{23}}, \tag{3.10}$$

$$X_3 = \gamma_{12}\frac{\partial}{\partial\gamma_{13}} + \gamma_{22}\frac{\partial}{\partial\gamma_{23}} + 2\gamma_{23}\frac{\partial}{\partial\gamma_{33}}, \tag{3.11}$$

$$X_4 = \gamma_{11}\frac{\partial}{\partial\gamma_{13}} + \gamma_{12}\frac{\partial}{\partial\gamma_{23}} + 2\gamma_{13}\frac{\partial}{\partial\gamma_{33}}. \tag{3.12}$$

The algebra g_r that corresponds to the group G_r has the following table of commutators:

$$\begin{aligned} &[X_1,X_2]=0, \quad [X_1,X_3]=0, \quad [X_1,X_4]=X_4, \\ &[X_2,X_3]=X_3, \quad [X_2,X_4]=0, \quad [X_3,X_4]=0. \end{aligned} \tag{3.13}$$

As is evident from the above commutators (3.13), the group is non-Abelian, so we cannot diagonalize at the same time all the generators. However, if we calculate the derived algebra of g_r, we have

$$g_{r'} = \{[X_A,X_B]:X_A,X_B \in g_r\} \Rightarrow g_{r'} = \{X_3,X_4\}, \tag{3.14}$$

and, furthermore, its second derived algebra reads as

$$g_{r''} = \{[X_A,X_B]:X_A,X_B \in g_{r'}\} \Rightarrow g_{r''} = \{0\}. \tag{3.15}$$

Thus, the group G_r is solvable since the $g_{r''}$ is zero. As is evident, X_3, X_4, Y_2 generate an Abelian subgroup, and we can, therefore, bring them to their normal form simultaneously. The appropriate transformation of the dependent variables is

$$\begin{aligned} \gamma_{11} &= e^{u_1+2u_6}, \\ \gamma_{12} &= e^{u_1+u_2+u_4+u_6}, \\ \gamma_{13} &= e^{u_1+u_6}(e^{u_6}u_3 + e^{u_2+u_4}u_5), \\ \gamma_{22} &= e^{u_1+2u_4}, \\ \gamma_{23} &= e^{u_1+u_4}(e^{u_2+u_6}u_3 + e^{u_4}u_5), \\ \gamma_{33} &= e^{u_1}(1 + e^{2u_6}u_3^2 + 2e^{u_2+u_4+u_6}u_3u_5 + e^{2u_4}u_5^2). \end{aligned} \tag{3.16}$$

In these coordinates the generators Y_2, X_A assume the form

$$Y_2 = \frac{\partial}{\partial u_1}, \quad X_3 = \frac{\partial}{\partial u_3}, \quad X_4 = \frac{\partial}{\partial u_5},$$
$$X_2 = \frac{\partial}{\partial u_4} - u_5 \frac{\partial}{\partial u_5}, \quad X_1 = \frac{\partial}{\partial u_6} - u_3 \frac{\partial}{\partial u_3}. \tag{3.17}$$

Except for the parametrization (3.16) there is also another one achieving the same result (3.17), which simply attributes a - sign to γ_{12}, and therefore any solution later described will remain valid under this change.

Evidently, a first look at (3.16) gives the feeling that it would be hopeless even to write down the Einstein equation. However, the simple form of the generators (3.17) ensures us that these equations will be of first order in the functions $\dot{u}_1$, $\dot{u}_3$, and $\dot{u}_5$.

A. Description of the solution space

Before we begin solving Einstein equations, a few comments for the possible values of the functions u_i, $i=1,\ldots,6$ will prove very useful.

The determinant of $\gamma_{\alpha\beta}$ is

$$\det[\gamma_{\alpha\beta}] = e^{3u_1+2(u_4+u_6)}(1-e^{2u_2}), \tag{3.18}$$

so we must have $u_2<0$.

The transformation from the γ' s to the u' s becomes singular when $\gamma_{12}=0$, since the function u_2 equals

$$u_2 = \ln(|\gamma_{12}|) - \frac{\ln(\gamma_{11}\gamma_{22})}{2}. \tag{3.19}$$

So two cases are naturally arising, according to whether γ_{12} is different or equal to zero. If $\gamma_{12} \neq 0$ the two linear constraint equations, written in the new variables (3.16), give

$$E_1 = 0 \Rightarrow -e^{u_6}(e^{u_6}\dot{u}_3 + e^{u_2+u_4}\dot{u}_5) = 0, \tag{3.20}$$

$$E_2 = 0 \Rightarrow -\frac{1}{2}e^{u_4}(e^{u_2+u_6}\dot{u}_3 + e^{u_4}\dot{u}_5) = 0. \tag{3.21}$$

This system admits only the trivial solution, since the determinant of the 2×2 matrix formed by the coefficients of $\dot{u}_3$, $\dot{u}_5$ becomes zero only for the forbidden value $u_2=0$. We thus have

$$u_3 = k_3, \quad u_5 = k_5. \tag{3.22}$$

Now, these values of u_3, u_5 make γ_{13}, γ_{23} functionally dependent upon γ_{11}, γ_{12}, γ_{22} [see (3.16)]. It is thus possible to set these two components to zero by means of an appropriate constant automorphism.

In the case $\gamma_{12}=0$, we can again bring simultaneously into normal form the corresponding X_3, X_4, Y_2. The appropriate change of dependent variables is given by

$$\gamma_{\alpha\beta} = \begin{pmatrix} e^{u_1+2u_6} & 0 & e^{u_1+2u_6}u_3 \\ 0 & e^{u_1+2u_5} & e^{u_1-u_4+u_5} \\ e^{u_1+2u_6}u_3 & e^{u_1-u_4+u_5} & e^{u_1}(1+e^{-2u_4}+e^{2u_6}u_3^2) \end{pmatrix}. \tag{3.23}$$

In these variables all three linear constraint equations can be integrated, yielding

$$E_1 = 0 \Rightarrow -e^{2u_6}\dot{u}_3 = 0 \Rightarrow u_3 = k_3, \tag{3.24}$$

$$E_2 = 0 \Rightarrow -\frac{1}{2}e^{-u_4+u_5}(\dot{u}_4 + \dot{u}_5) = 0 \Rightarrow u_5 = k_5 - u_4, \tag{3.25}$$

$$E_3 = 0 \Rightarrow -2e^{2u_4+2u_6}u_3\dot{u}_3 + \dot{u}_4 + \dot{u}_5 + 2e^{2u_4}\dot{u}_6 = 0 \Rightarrow u_6 = k_6. \tag{3.26}$$

Again, these values imply that a constant automorphism suffices to set the (13) and (23) components of the scale-factor matrix to zero, i.e., to put it into diagonal form. We have thus reached a first important conclusion, that is the following.

Without loss of generality, we can start our investigation of the solution space for Type III vacuum Bianchi Cosmology from a block-diagonal form of the scale-factor matrix (and, of course, zero shift),

$$\gamma_{\alpha\beta} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & 0 \\ \gamma_{12} & \gamma_{22} & 0 \\ 0 & 0 & \gamma_{33} \end{pmatrix}. \tag{3.27}$$

Note that this conclusion could have not been reached off mass shell, due to the fact that the time-dependent automorphism (3.4) does not contain the necessary two arbitrary functions of time in the (13) and (23) components (besides the fact that all the freedom in arbitrary functions of time has been used to set the shift to zero). As we have earlier remarked, since the algebra (3.13) is solvable, the remaining (reduced) generators X_1, X_2 (corresponding to diagonal constant automorphisms) as well as Y_2 continue to define a Lie-Point symmetry of the reduced EFEs and can thus be used for further integration of this system of equations.

1. Case I: $\gamma_{12}=0$

The remaining (reduced) automorphism generators are

$$X_1 = 2\gamma_{11}\frac{\partial}{\partial\gamma_{11}}, \quad X_2 = 2\gamma_{22}\frac{\partial}{\partial\gamma_{22}}.$$

The appropriate change of dependent variables that brings these generators—along with Y_2 into normal form, is described by the following scale-factor matrix:

$$\gamma_{\alpha\beta} = \begin{pmatrix} e^{u_1+u_3} & 0 & 0 \\ 0 & e^{u_2+u_3} & 0 \\ 0 & 0 & e^{u_3} \end{pmatrix}. \tag{3.28}$$

In these variables the first two linear constraint equations are identically satisfied, while the third reads as $E_3=0\Rightarrow -2\dot{u}_1=0\Rightarrow u_1=k_1$. Substituting this value of u_1 into the quadratic constraint equation E_0, we obtain the lapse function

$$N^2 = \frac{1}{16}e^{u_3}\dot{u}_3(2\dot{u}_2 + 3\dot{u}_3). \tag{3.29}$$

Now, the substitution of $u_1=k_1$ and the above value for the lapse N^2 into the spatial EFE's results in the single, independent equation:

$$(\dot{u}_2 + \dot{u}_3)(2\dot{u}_3\ddot{u}_2 - 2\dot{u}_2\ddot{u}_3 + 2\dot{u}_2^2\dot{u}_3 + 3\dot{u}_3^2 + 5\dot{u}_2\dot{u}_3^2). \tag{3.30}$$

This equation is, as expected from the theory, of the first order in $\dot{u}_2$, $\dot{u}_3$. Notice that this result could have not been reached had we chosen any particular time gauge, such as $N^2=F(u_2,u_3,t)$: Not only u_2, u_3, t would appear in the Spatial EFE's, but also the number of independent such equations would have been increased to 2. This remark should not be taken as a negative view for complete gauge fixing, but rather as pointing to the fact that keeping the gauge freedom into the game helps manifesting the symmetries of the system and eventually solving the equations.

Equation (3.30) is readily integrated, leading to two different space-times according to which the parenthesis is set to zero. If the first is made to vanish, i.e., $u_2=k_2-u_3$, the ensuing line element is the known (Type III) cosmological disguise of Minkowski space-time (Ref. 15):

$$ds^2=-\frac{1}{16}e^{u_3}\dot{u}_3^2\,dt^2+\frac{1}{4}e^{u_3}\,dx^2+e^{k_1+u_3-2x}\,dy^2+e^{k_2}\,dz^2 \tag{3.31}$$

the constants being, of course, absorbable by the constant automorphisms and a shift in u_3.

If the second parenthesis of (3.30) is set to zero, i.e., $u_2=k_3-3u_3/2+\ln(1+k_2e^{u_3/2})$, we obtain an equivalent form of the Type III member of the known Ellis-MacCallum family of solutions (Refs. 8 and 15):

$$ds^2=\kappa^2\left(-\frac{e^{3u_3/2}\dot{u}_3^2}{4(e^{u_3/2}-1)}dt^2+e^{u_3}\,dx^2+e^{u_3-2x}\,dy^2+e^{-u_3/2}(e^{u_3/2}-1)dz^2\right), \tag{3.32}$$

where again we have used constant automorphisms and a shift of u_3 to take outside of the metric an overall constant. We can be assured that the constant is essential either by checking that indeed the metric inside the parenthesis does not admit a homothetic Killing vector field or, more primarily, by finding an invariant relation between curvature and higher derivative curvature scalars that explicitly involves κ. For metric (3.32), one such invariant relation is

$$\frac{18Q_1^4}{\left(Q_2-\frac{g^{AB}Q_{1;A}Q_{1;B}}{Q_1}\right)^3}=\kappa^2,\quad Q_1=R^{KLMN}R_{KLMN},\quad Q_2=\Box R^{KLMN}R_{KLMN}, \tag{3.33}$$

where capital Latin letters denote space-time indices ranging in the interval (0–3), the semicolon stands for covariant differentiation, and the $\Box$ for the covariant D'Alebertian.

This relation, being a constant scalar constructed out of the intrinsic geometry (the Riemmann tensor and its covariant derivatives), characterizes, along with many others that can be found, this metric: It will be valid for any equivalent, under general coordinate transformations, form of (3.32). It is also noteworthy to observe that in both the above line elements, the arbitrary function of time u_3 appears; This is because the number of symmetry generators matches the number of scale factors (both are 3), so that the system of spatial EFEs is reduced to first order without any choice of time. In the case of a block-diagonal scale-factor matrix, one of the four scale factors will have to play the role of time before the corresponding system can be reduced. Lastly, metric (3.32) admits, except for (3.3), a fourth Killing vector field acting on the surfaces of simultaneity, namely

$$\xi_4=-2y\partial_x+(e^{2x}-y^2)\partial_y. \tag{3.34}$$

There is thus a G_4 symmetry group acting (of course, multiply transitively) on each V_3 of this metric, with an algebra having the following table of (nonvanishing) commutators:

$$[\xi_1,\xi_3]=\xi_1,\quad [\xi_1,\xi_4]=-2\xi_3,\quad [\xi_3,\xi_4]\xi_4. \tag{3.35}$$

However, it is interesting to note that we have not imposed the extra symmetry from the beginning, but rather it emerged as a result of the investigation process.

2. Case II: $\gamma_{12}\neq 0$

The remaining (reduced) automorphism generators are

$$X_1=2\gamma_{11}\frac{\partial}{\partial\gamma_{11}}+\gamma_{12}\frac{\partial}{\partial\gamma_{12}},\quad X_2=\gamma_{12}\frac{\partial}{\partial\gamma_{12}}+2\gamma_{22}\frac{\partial}{\partial\gamma_{22}}.$$

The appropriate change of dependent variables that brings these generators—along with Y_2—into normal form, is now given by

$$\gamma_{\alpha\beta}=\begin{pmatrix} e^{u_1+2u_4} & e^{u_1+u_2+u_4} & 0 \\ e^{u_1+u_2+u_4} & e^{u_1+2u_2}u_3 & 0 \\ 0 & 0 & e^{u_1} \end{pmatrix}. \tag{3.36}$$

The generators are now reduced to

$$Y_2=\frac{\partial}{\partial u_1},\quad X_2=\frac{\partial}{\partial u_2},\quad X_1=\frac{\partial}{\partial u_4}, \tag{3.37}$$

indicating that the system will be of first order in the derivatives of these variables. The remaining variable u_3 will enter (along with $\dot{u}_3$, $\ddot{u}_3$) explicitly in the system and is therefore advisable (if not mandatory) to be used as the time parameter, i.e., to effect the change of time coordinate

$$t\to u_3(t)=s,\quad u_1(t)\to u_1(t(s)),\quad u_2(t)\to u_2(t(s)),\quad u_4(t)\to u_4(t(s)). \tag{3.38}$$

This choice of time will, of course, be valid only if u_3 is not a constant. We are thus led to consider two cases according to the constancy or nonconstancy of this variable.

a. The case $u_3=k_3$

The determinant of the scale-factor matrix becomes $\det[\gamma_{\alpha\beta}]=e^{3u_1+2(u_2+u_4)}(-1+k_3)$. We thus have $k_3>1$. The two linear constraint equations are identically satisfied, while the third yields

$$E_3=0\Rightarrow\frac{\dot{u}_2+(1-2k_3)\dot{u}_4}{2(1-k_3)}=0\Rightarrow u_4=k_4+\frac{u_2}{2k_3-1}.$$

Inserting these values of u_3, u_4 into the quadratic constraint equation we obtain the following lapse:

$$(N)^2=\frac{e^{u_1}(-1+k_3)(3(1-2k_3)^2\dot{u}_1^2+8k_3(-1+2k_3)\dot{u}_1\dot{u}_2+4k_3\dot{u}_2^2)}{4(1-2k_3)^2(-3+4k_3)}. \tag{3.39}$$

The use of these values of u_3, u_4, $(N)^2$ in the spatial EFE's results, as expected, in a system that is of the first order in the unknown variables $\dot{u}_1$, $\dot{u}_2$. The coefficient of $\ddot{u}_2$ in $E_{33}=0$ is

$$\frac{2e^{u_1}k_3\dot{u}_1((-1+2k_3)\dot{u}_1+\dot{u}_2)}{3(1-2k_3)^2\dot{u}_1^2+8k_3(-1+2k_3)\dot{u}_1\dot{u}_2+4k_3\dot{u}_2^2},$$

and can be safely regarded different from zero, since the possibilities $\dot{u}_1=0$, $\dot{u}_2=(1-2k_3)\,\dot{u}_1$ easily lead (through $E_{33}=0$ itself) to zero and negative lapse, respectively. We can thus solve $E_{33}=0$ for $\ddot{u}_2$ and substitute into $E_{12}=0$, which becomes

$$\frac{e^{k_4+u_1+2k_3u_2/(-1+2k_3)}k_3(\dot{u}_1+2\dot{u}_2)((-3+6k_3)\dot{u}_1+2(3-2k_3)\dot{u}_2)}{6-20k_3+16k_3^2}=0.$$

Again, the second parenthesis in the numerator leads to zero lapse, leaving us with the only alternative $\dot{u}_1=-2\dot{u}_2\Rightarrow u_1=2k_1-2u_2$, which indeed satisfies all spatial EFEs. Finally, inserting these values of u_3, u_4, u_1 in the lapse (3.39) and the scale-factor matrix (3.36), we obtain the following line element (after using the constant automorphisms and a shift in u_2 to purify the metric from the absorbable constants):

$$ds^2=-\lambda^2\,d\xi^2+\frac{\xi^2}{4}\,dx^2+e^{-2x}\xi^{4\lambda}\,dy^2+\frac{\lambda-1}{2\lambda-1}\,dz^2+2e^{-x}\xi^{2\lambda}\,dy\,dz, \tag{3.40}$$

where the constant λ is related to k_3 by $k_3=(\lambda-1)/(2\lambda-1)\Rightarrow 0<\lambda<\frac{1}{2}$, and we have adopted the

time gauge $e^{-u_2}=\xi$ for simplicity.

This metric is an equivalent form of a solution originally given by Siklos[16] and reproduced in.[15] An overall multiplicative constant has been omitted from (3.40) since it admits the following Homothetic Killing vector field ($\mathcal{L}_H g_{AB}=\mu g_{AB}$),

$$H^A=\xi\frac{\partial}{\partial\xi}+(1-2\lambda)y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}.$$

It also admits three more Killing vector fields [except (3.3)] acting on space-time, namely

$$\xi_4=e^{-x/2\lambda}\partial_\xi+\frac{2\lambda}{\xi}e^{-x/2\lambda}\partial_x$$

$$\xi_5=e^{-x/2\lambda}y\partial_\xi+\frac{2\lambda y}{\xi}e^{-x/2\lambda}\partial_x+\frac{\lambda(\lambda-1)}{4\lambda-1}e^{[(4\lambda-1)/2\lambda x]}\xi^{-4\lambda+1}\partial_y-\lambda e^{[(2\lambda-1)/2\lambda]x}\xi^{-2\lambda+1}\partial_z$$

$$\xi_6=e^{-x/2\lambda}z\partial_\xi+\frac{2\lambda z}{\xi}e^{-x/2\lambda}\partial_x-\lambda e^{[(2\lambda-1)/2\lambda]x}\xi^{-2\lambda+1}\partial_y-\lambda(2\lambda-1)e^{-x/2\lambda}\xi\partial_z.$$

The ξ_5 field breaks down for $\lambda=\frac{1}{4}$, in which case the valid expression is

$$\xi_5'=\left\{\frac{y}{e^{2x}},\frac{y}{2e^{2x}\xi},\frac{3(-2x+\log(\xi))}{16},\frac{-\sqrt{\xi}}{4e^x}\right\}. \tag{3.41}$$

The first of these is null $\xi_4^A\xi_4^B g_{AB}=0$ and covariantly constant $\xi^A_{4;B}=0$, signaling that the metric is a pp wave. Consequently, all scalar curvatures, constructed by forming scalar contractions of the tensor product of the Riemmann tensor and its covariant derivatives of any order [such as Q_1, Q_2 in (3.33)], vanish identically (see, e.g., Ref. 17). This raises the interesting question of how can we be certain that the constant λ is essential. An answer can be found in terms of equalities between tensors—constructed out of the Riemmann tensor and its covariant derivatives—that hold true in these space-times.[18,19] For metric (3.40) such a relation is

$$R^A{}_B{}^C{}_D R_{AECF;G;H}=\frac{4\lambda^2-2\lambda+3}{-4\lambda^2+2\lambda+2}R^A{}_B{}^C{}_{D;E}R_{AFCG;H}. \tag{3.42}$$

By the quotient law, the expression of λ on the right-hand side of this relation is a scalar function, and being a constant it cannot change value under any coordinate transformation; thus λ cannot be altered by such a transformation and is, therefore, essential.

The algebra of the six killing fields, (3.3), (3.41) has the following table of nonvanishing commutators:

$$[\xi_1,\xi_3]=\xi_1,\quad [\xi_1,\xi_5]=\xi_4,\quad [\xi_3,\xi_4]=-\frac{\xi_4}{2\lambda},\quad [\xi_3,\xi_5]=\frac{2\lambda-1}{2\lambda}\xi_5,\quad [\xi_3,\xi_6]=\frac{-1}{2\lambda}\xi_6. \tag{3.43}$$

There is an isotropy group G_2 of null rotations emanating from this algebra, which is easily seen by taking a linear combination of these fields:

$$Y_1=\xi_1-2\lambda\xi_3,\quad Y_2=\xi_4,\quad Y_3=-\xi_6,$$
$$Y_4=\xi_2,\quad Y_5=\xi_3,\quad Y_6=\xi_5, \tag{3.44}$$

e.g., $[Y_1, Y_2] = Y_2$ and $[Y_1, Y_3] = Y_3$.

The space (being a pp wave) does not obviously have curvature singularities; it thus seems to be geodesically complete and is of Petrov Type *N*.

b. The case $u_3 \neq k_3$

The function u_3 is now a valid choice of time and $\det[\gamma_{\alpha\beta}] = e^{3u_1+2(u_2+u_6)}(-1+s)$ implies the range $(1, +\infty)$ for the new time s. The only nonvanishing linear constraint equation $E_3 = 0$ yields

$$u_4 = \int \frac{\dot{u}_2}{2s-1} ds + k_4 \tag{3.45}$$

while the quadratic constraint equation $E_0 = 0$ gives the lapse

$$(N)^2 = \frac{e^{u_1}}{4(1-2s)^2(-3+4s)}\left[2(2s-1)^2\dot{u}_1 + 3(2s-1)^2(s-1)\dot{u}_1^2 + (4s-2)\dot{u}_2 + 8s(s-1)(2s-1)\dot{u}_1\dot{u}_2 + 4s(s-1)\dot{u}_2^2\right]. \tag{3.46}$$

If we insert these values $(N)^2$, u_4 into the spatial EFEs, they become the following polynomial system of first order in $\dot{u}_1$, $\dot{u}_2$,

$$\ddot{u}_1 = (1\dot{u}_1\dot{u}_1^2\dot{u}_1^3)A_1\begin{pmatrix} 1 \\ \dot{u}_2 \\ \dot{u}_2^2 \\ \dot{u}_2^3 \end{pmatrix}, \quad \ddot{u}_2 = (1\dot{u}_1\dot{u}_1^2\dot{u}_1^3)A_2\begin{pmatrix} 1 \\ \dot{u}_2 \\ \dot{u}_2^2 \\ \dot{u}_2^3 \end{pmatrix}, \tag{3.47}$$

$$A_1 = \begin{pmatrix} 0 & \frac{2}{4s^2-7s+3} & \frac{4s}{8s^2-10s+3} & 0 \\ \frac{1}{4s^2-7s+3} & 4 & \frac{8s(2s-3)(s-1)}{8s^2+10s-3} & 0 \\ \frac{2s-3}{4s-3} & -\frac{16s^2(s-1)}{8s^2-10s+3} & 0 & 0 \\ -\frac{6s(s-1)}{4s-3} & 0 & 0 & 0 \end{pmatrix}, \tag{3.48}$$

$$A_2 = \begin{pmatrix} 0 & \frac{-8s+5}{8s^3-18s^2+13s-3} & \frac{24s^2-50s+18}{8s^2-10s+3} & \frac{8s(2s-3)(s-1)}{8s^2-10s+3} \\ \frac{-4s+2}{4s^2-7s+3} & \frac{12s}{-2s+3} & -\frac{16s^2(s-1)}{8s^2+10s-3} & 0 \\ \frac{-6s+3}{4s-3} & -\frac{6s(s-1)}{4s-3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.49}$$

Due to the form of A_1, A_2 (their components are rational functions of the time s), system (3.47) can be partially integrated with the help of the following Lie-Bäklund transformation:

$$\dot{u}_1(s) = \frac{(2s-3)\tan r(s) - 2s(8s^2-10s+3)\dot{r}(s)}{4s\sqrt{s-1}(4s-3)},$$
$$\dot{u}_2(s) = \frac{2s-1}{8s(4s-3)\sqrt{(s-1)^3}}(2(-4s+3)\sqrt{s-1} + 3(s-1)\tan r(s) + 2s(s-1)(4s-3)\dot{r}(s)), \tag{3.50}$$

resulting in the single, second order ODE for the variable $r(s)$,

$$\ddot{r}=\left(\tan r-\frac{\sqrt{s-1}}{2}\right)\dot{r}^2+\frac{(-16s+6)\sqrt{s-1}+(5s-3)\tan r}{2s(4s-3)\sqrt{(s-1)}}\dot{r}$$
$$+\frac{-9(s-1)^2\tan^2 r+18(s-1)^{3/2}\tan r+4s(4s-3)}{8s^2(4s-3)^2(s-1)^{3/2}}. \tag{3.51}$$

This equation contains all the information concerning the unknown part of the solution space of the Type III vacuum Cosmology. Unfortunately, it does not posses any Lie-point symmetries that can be used to reduce its order and ultimately solve it. However, its form can be substantially simplified through the use of a new dependent and independent variable $(\rho, u(\rho))$ according to $r(s)=\pm\arcsin u(\rho)/\sqrt{\rho^2-1}$, $s=3(\rho-1)/3\rho-5$, $\rho>\frac{5}{3}$ thereby obtaining the equation

$$\ddot{u}=\pm\frac{1-\dot{u}^2}{\sqrt{(6\rho-10)(\rho^2-u^2-1)}}\Rightarrow\ddot{u}^2=\frac{(1-\dot{u}^2)^2}{(6\rho-10)(\rho^2-u^2-1)}, \tag{3.52}$$

with the corresponding lapse

$$(N)^2=\frac{\dot{u}^2-1}{8(3\rho-5)(\rho^2-u^2-1)}e^{u_1} \tag{3.53}$$

($\dot{u}=du/d\rho$) and the scale-factor matrix is given by (3.36) after insertion of (3.45), $u_3=s=3(\rho-1)/3\rho-5$ and the transformations of u_1, u_2 that led to u. Independently of the way we have reached this result, one can check (through an algebraic computing facility such as MATHEMATICA) that the line element thus described is indeed a solution of all the EFEs, provided, of course, that (3.52) is satisfied. One can also check that it does not admit any homothetic or null, covariantly constant vector field. Therefore, the two independent constants of the general solution to (3.52) along with a multiplicative constant will comprise the expected three essential constants of the general Type III vacuum Cosmology: The general algorithm for calculating this number when a space-time gauge has been chosen (usually zero shift and unit lapse), in which case the constraints must be viewed as restrictions on the initial data, reads as follows[15]: 12 (for the six components of $\gamma_{\alpha\beta}$)-1 (for the time reparametrization covariance)-number of independent constraints-dimension of Automorphism Group.

When a space-time gauge has not been fixed, i.e., when constraints are being viewed as symmetry generators, the relevant counting is given by[20]

$$D=2\times(\text{number of }\gamma_{\alpha\beta})-2\times(\text{number of linear constraints})-2\times(\text{quadratic constraint})$$
$$-(\text{number of parameters of outer}-\text{aut})-(n),$$

where $n\equiv$ dim(inner-aut)-number of independent linear constraints.

In our case the number of independent linear constraints is 3, and the dimension of the inner-aut is 2, so $n=-1$. The constants that appear at the outer-aut are 2, and obviously the number of $\gamma_{\alpha\beta}$ is 6. Thus, the expected maximal number of essential constants is indeed **3**, by both ways of counting.

Despite the relatively simple form of (3.52), its general solution is, to the best of our knowledge, not known. However, we have managed to obtain a partial solution in the parametric form,

$$u(\xi)=\frac{4(1+2e^{2\xi})^{3/2}}{3(1+e^{2\xi})^2}\quad\rho=\tfrac{1}{3}(5+\operatorname{sech}^2\xi),$$

which makes the functions u_1, u_2, u_4 read as

$$u_1(\xi) = k_1 + \xi + \ln\cosh\xi,$$

$$u_2(\xi) = k_2 + \ln\operatorname{sech}\xi - \frac{1}{2}\ln(\cosh 2\xi + 2),$$

$$u_4(\xi) = k_4 - \ln\cosh\xi + \frac{1}{2}\ln(\cosh 2\xi + 2),$$

and the lapse $(N)^2 = e^{k_1+2\xi}(e^{2\xi}+1)/4(2e^{2\xi}+1)$. The ensuing metric, after the usual purification with the constant automorphisms and a shift in ξ, is given by

$$ds^2 = \kappa^2\left(-\frac{e^{2\xi}(e^{2\xi}+1)}{4(2e^{2\xi}+1)}d\xi^2 + \frac{e^{\xi}}{4}\cosh\xi\, dx^2 + e^{-2x+\xi}(\cosh 2\xi + 2)\operatorname{sech}\xi\, dy^2 + e^{\xi}\operatorname{sech}\xi\, dz^2 + 2e^{-x+\xi}\operatorname{sech}\xi\, dy\, dz\right). \tag{3.54}$$

As we have already remarked, this metric does not admit a homothety and therefore the constant κ is essential. It does not satisfy the invariant relation (3.33), and it is not a pp wave. Therefore we conclude that it is inequivalent to (3.32) or (3.40). This mono-parametric family belongs to the Kinnersley vacuum solutions.[9] It is quite interesting that it also admits a fourth killing vector field,

$$\xi_4 = -16y\partial_x + (e^{2x} - 8y^2)\partial_y - 2e^x\partial_z, \tag{3.55}$$

which produces with (3.3) the following table of (nonvanishing) commutators:

$$[\xi_1, \xi_3] = \xi_1, \quad [\xi_1, \xi_4] = -16\xi_3, \quad [\xi_3, \xi_4] = \xi_4. \tag{3.56}$$

The isotropy group inferred from the above algebra (see the last commutator) is a G_1 spatial rotation.

Curiously enough, this algebra is equivalent to (3.35), as a simple scaling of ξ_1, ξ_4 by $2\sqrt{2}$ shows. Of course, the multiply transitive character of the action of the underlying group on the corresponding V_3's allows for these, and thus for the space-times in which they are embedded, to be inequivalent.

Again, the extra symmetry emerged in the course of the investigation of the solution space. Of course, it must have something to do with the particular nature of the solution, but it was not set as a starting point.

B. Preview for other Bianchi Types

The method described in the previous sections can be applied to other Types as well. The general pattern is s similar to that of Type III: The pp-wave solutions (for types admitting such geometries) occupy one part of the solution space, the other known solutions reside on another part, and the unknown part of the solution space is always described by an ODE strikingly similar to (3.52), namely,

$$\ddot{u}^2 = \frac{(-1+\dot{u}^2)^2}{(\kappa+\lambda\rho)(\rho^2 - u^2 - 1)}. \tag{3.57}$$

Details will be included in a forthcoming work. As indicative examples we give the form of the ODE for Types IV and VII_h:

Type IV:

$$\ddot{u}^2 = \frac{(-1+\dot{u}^2)^2}{(\kappa+\lambda\rho)(\rho^2-u^2-1)}, \quad \kappa=-6, \quad \lambda=6. \tag{3.58}$$

Type VII$_h$:

$$\ddot{u}^2 = \frac{(-1+\dot{u}^2)^2}{(\kappa+\lambda\rho)(\rho^2-u^2-1)}, \quad \kappa=-6+\frac{4}{h^2}, \quad \lambda=-6, \tag{3.59}$$

and of course the following.

Type III:

$$\ddot{u}^2 = \frac{(-1+\dot{u}^2)^2}{(\kappa+\lambda\rho)(\rho^2-u^2-1)}, \quad \kappa=-10, \quad \lambda=6. \tag{3.60}$$

IV. DISCUSSION

When one is trying to solve Einstein's Equations in cosmology, one has to deal with a nonlinear system of coupled, *ordinary differential* equations. The strategy that is frequently used is to simplify the system by choosing, a convincing form for the scale factor matrix, usually obtained by an *a priori* assumption of extra symmetry [e.g., $\gamma_{\alpha\beta}=\mathrm{diag}(a(t),b(t),c(t))$], and then try to solve it, hoping to find *some* solution. Clearly, this procedure can by no means guarantee access to the full space of solutions for the problem at hand. In this work we have presented a method for solving Einstein's Field Equations in the case of vacuum Bianchi Geometries. The main idea is to consider the Group of constant automorphisms, which emerges as the residual freedom left after the time dependent A.I.D.'s (2.8), (2.9) have been used to set the shift N^α to zero, as a Lie point symmetry of the EFEs. In a step-by-step procedure, one can bring some of the generators of this group in normal form and simplify the rest, thereby reducing the order of the system of equations. Which of the generators, and how, can be utilized in each step depends upon the characteristics of their Lie Algebra (Abelian, solvable etc.). It is also important that the information gained at a particular level must be used and, in fact, may be vital for the implementation of the next step. The method is, by construction, sweeping out all possible solutions, since no ad-hoc assumption has been made. Therefore, *if successfully applied to a given Bianchi Cosmology*, it will result in the cartography of the entire space of solutions.

The successful application of the procedure to Bianchi Type III resulted in the recovery of all known solutions without the prior assumption of any extra symmetry [(3.32), (3.40)], the enclosure of the entire unknown part of the solution space into a single, second order ODE in terms of one dependent variable (3.52), and a partial solution to this ODE. It is of interest that the solution space is naturally partitioned into three distinct disconnected pieces. Of great importance may be considered the fact that a strikingly similar ODE describes the unknown part of the solution space for other lower Bianchi Types. For Types VIII, IX there remain no rigid automorphisms after the shift has been set to zero and the constant rotations have been used to diagonalize the scale-factor matrix. However, there is the scaling symmetry Y_2 that can serve as a starting point. This issue, along with the presentation of the detailed cartography for the lower types is in our immediate scopes. Finally, the method can be extended toward either the inclusion of matter content, or in 4+1 spatially homogeneous cosmologies.

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Spectral analysis of radial Dirac operators in the Kerr-Newman metric and its applications to time-periodic solutions

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We investigate the existence of time-periodic solutions of the Dirac equation in the Kerr-Newman background metric. To this end, the solutions are expanded in a Fourier series with respect to the time variable t, and the Chandrasekhar separation ansatz is applied so that the question of existence of a time-periodic solution is reduced to the solvability of a certain coupled system of ordinary differential equations. First, we prove the already known result that there are no time-periodic solutions in the nonextreme case. Then, it is shown that in the extreme case for fixed black hole data there is a sequence of particle masses $(m_N)_{N\in\mathbb{N}}$ for which a time-periodic solution of the Dirac equation does exist. The period of the solution depends only on the data of the black hole described by the Kerr-Newman metric. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2358394]

I. INTRODUCTION

In this paper we consider the system consisting of a Kerr-Newman black hole and an electron. The Kerr-Newman metric describing the black hole is the most general electrovac solution of Einstein's field equations. It describes a rotating, electrically charged, massive black hole; see, e.g., Refs. 15 and 9. We are interested in the stability of a system consisting of such a black hole and an electron. To this end, we have to consider the Dirac equation for the electron in the Kerr-Newman metric; see Eqs. (1) and (2)–(6). The Dirac equation is a complicated system of partial differential equations in all four space-time variables. We call the system consisting of the black hole and the electron *stable* if there exists a nontrivial time-periodic solution of the Dirac equation which can be interpreted as the wave function of the electron.

Since the black hole is rotating, the background metric is only axisymmetric, whereas in the nonrotating cases (the Schwarzschild and the Reissner-Nordstrøm geometries) the background metric is spherically symmetric. This loss of symmetry leads to a complicated coupling of the angular and the radial coordinates in the Dirac equation. Chandrasekhar[4] showed that, in spite of this complicated coupling, the Dirac equation can be separated into a system of ordinary differential equations, the so-called angular equation (13) and the radial equation (14). These differential equations have realizations as eigenvalue equations in appropriate Hilbert spaces. For the radial equation, $\omega=\nu\omega_0$ plays the role of the eigenvalue parameter. The eigenvalue ω has the physical interpretation as the energy of the electron. It should be emphasized that, due to the lack of spherical symmetry of the space-time, the eigenvalues of the radial and the angular equation are

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intertwined in a highly complex way. Hence, to show the stability of the system under consideration, it does not suffice to find eigenvalues of the radial and the angular equation separately; we need to show that the eigenvalues are compatible with each other.

In Sec. II we present the separation ansatz for time-periodic solutions of the Dirac equation in the Kerr-Newman background metric due to Chandrasekhar with mathematical rigor, and we derive the radial and angular equation. In the next section we consider the radial equation. It has been shown by Belgiorno and Martellini[2] that the essential spectrum of the radial operator covers the real axis. Finster *et al.*,[7,8] show the nonexistence of time-periodic solutions of the Dirac equation in the nonextreme Kerr-Newman geometry. Schmid[12] investigates the Dirac equations in the extreme Kerr-Newman geometry with the help of special functions, and shows the existence of bounded states in the extreme Kerr case, which implies the existence theorem of time-periodic solutions. Our aim is to study the difference between the extreme and nonextreme case from the viewpoint of spectral analysis of the radial Dirac operators. We give also the existence theorem of time-periodic solutions in the extreme Kerr-Newman case. In Theorem IV. 5 we show that in the nonextreme Kerr-Newman metric the Dirac equation has no time-periodic solution that has an interpretation as a particle wave function. The case of the extreme Kerr-Newman metric is investigated in Sec. V. It turns out that in this case there may be an eigenvalue of the radial equation. Schmid[12] proved a sufficient condition for the existence of a time-periodic solution of the Dirac equation. However, it is not easy to verify that for given particle data there are black hole parameters such that this condition can be satisfied. This problem is discussed in Sec. VI. We show that for fixed data of an extreme Kerr-Newman black hole there is a sequence of particle masses such that the system consisting of the quantum particle and the black hole permits time-periodic solutions.

II. SEPARATION OF THE DIRAC EQUATION IN THE KERR-NEWMAN BACKGROUND METRIC

We consider the Dirac equation (see, e.g., Page,[11] Chandrasekhar[4])

$$(\widehat{\mathcal{R}} + \widehat{\mathcal{A}})\hat{\Psi} = 0 \tag{1}$$

for a spin-$\frac{1}{2}$ particle with the mass $m \geq 0$ and the charge e in the Kerr-Newman geometry, where

$$\widehat{\mathcal{R}} := \begin{pmatrix} imr & 0 & \sqrt{\Delta}\mathcal{D}_+ & 0 \\ 0 & -imr & 0 & \sqrt{\Delta}\mathcal{D}_- \\ \sqrt{\Delta}\mathcal{D}_- & 0 & -imr & 0 \\ 0 & \sqrt{\Delta}\mathcal{D}_+ & 0 & imr \end{pmatrix}, \tag{2}$$

$$\widehat{\mathcal{A}} := \begin{pmatrix} -am\cos\theta & 0 & 0 & \mathcal{L}_+ \\ 0 & am\cos\theta & -\mathcal{L}_- & 0 \\ 0 & \mathcal{L}_+ & -am\cos\theta & 0 \\ -\mathcal{L}_- & 0 & 0 & am\cos\theta \end{pmatrix}, \tag{3}$$

$$\mathcal{D}_\pm := \frac{\partial}{\partial r} \mp \frac{1}{\Delta}\left[(r^2 + a^2)\frac{\partial}{\partial t} + a\frac{\partial}{\partial \varphi} - ieQr\right], \tag{4}$$

$$\mathcal{L}_\pm := \frac{\partial}{\partial \theta} + \frac{\cot\theta}{2} \mp i\left[a\sin\theta\frac{\partial}{\partial t} + \frac{1}{\sin\theta}\frac{\partial}{\partial \varphi}\right], \tag{5}$$

$$\Delta(r) := r^2 - 2Mr + a^2 + Q^2 \tag{6}$$

and $\hat{\Psi}$ is the wave function of the spin-$\frac{1}{2}$ particle under consideration. If the so-called black hole condition

$$M^2 - a^2 - Q^2 \geq 0 \tag{7}$$

holds, then the Kerr-Newman geometry is interpreted as the space-time geometry generated by a black hole with the mass $M \geq 0$, the electric charge Q, and the angular moment J; if $M \neq 0$, then the so-called Kerr parameter $a = J/M$ is the angular momentum of the black hole per unit mass. The black hole condition (7) ensures that the function Δ can be written as the product

$$\Delta(r) = (r - r_+)(r - r_-), \tag{6'}$$

with

$$r_\pm = M \pm \sqrt{M^2 - a^2 - Q^2}. \tag{8}$$

The special case $M^2 - a^2 - Q^2 = 0$, that is the case where $r_+ = r_- = M$, is referred to as the extreme Kerr-Newman metric.

Let us recall that the Kerr-Newman metric is the most general electrovac solution of Einstein's field equations.[9] Special cases contained in the Kerr-Newman geometry are the Kerr geometry (if $Q=0$), the Reissner-Nordstrøm geometry (if $a=0$), and the Schwarzschild geometry (if $Q=0$ and $a=0$).

A solution $\hat{\Psi}$ of (1) for $(r,\theta,\varphi,t) \in \hat{\Omega} := (r_+,\infty) \times (0,\pi) \times (-\pi,\pi) \times (-\infty,\infty)$ such that for every fixed time t the function $\hat{\Psi}(\cdot,\cdot,\cdot,t)$ lies in a suitable L^2-space $\mathcal{H}_{r,\theta,\varphi}$ [see (9)] can be interpreted as the wave function of the electron. Hence, the existence of such a $\hat{\Psi}$ would imply that the system consisting of the black hole and the spin-$\frac{1}{2}$ particle in its exterior is stable.

Remark II.1 (Dirac equation in flat space time): In the case of flat space-time, i.e., for $a=0$, $M=0$, $Q=0$, the Dirac equation given in (1) is unitarily equivalent to the familiar Dirac equation

$$\left(-i\frac{\partial}{\partial t} - i\vec{\alpha}\cdot\vec{\nabla} + \beta m\right)\Psi = 0$$

as given, for instance, in Davydov.[5] For the proof we refer to Winklmeier.[18]

A. Time-periodic solutions

In this paper we consider time-periodic solutions $\hat{\Psi}$, that is, solutions such that

$$\hat{\Psi}(r,\theta,\varphi,t) = \hat{\Psi}\left(r,\theta,\varphi,t + \frac{2\pi}{\omega_0}\right) \quad ((r,\theta,\varphi,t) \in \hat{\Omega})$$

for some $\omega_0 > 0$. In this case, the solutions can be expanded in a Fourier series

$$\hat{\Psi}(r,\theta,\varphi,t) = \sum_{\nu\in\mathbb{Z}} \exp(-i\nu\omega_0 t)\Psi^\nu(r,\theta,\varphi).$$

For physical reasons, each wave function Ψ^ν must be an element of the Hilbert space

$$\mathcal{H}_{r,\theta,\varphi} := L^2\left((r_+,\infty) \times (0,\pi) \times (-\pi,\pi); \frac{r^2+a^2}{\Delta(r)} \sin\theta \, dr \, d\theta \, d\varphi\right)^4 \tag{9}$$

with the inner product according to Finster *et al.*[7,8]

$$(\Psi,\Phi)=\int_{r_+}^{\infty}\int_0^{\pi}\int_{-\pi}^{\pi}\langle\Psi(r,\theta,\varphi),\Phi(r,\theta,\varphi)\rangle_{\mathbb{C}^4}\frac{r^2+a^2}{\Delta(r)}\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi. \tag{10}$$

Here $\langle\cdot,\cdot\rangle_{\mathbb{C}^4}$ is the usual scalar product on $\mathbb{C}^4$. In order to separate also the φ-dependence of the solution Ψ^ν we use the complete system $\{\exp(i\kappa\varphi):\kappa\in\mathbb{Z}+\frac{1}{2}\}$ in $L^2((-\pi,\pi);d\varphi)$ to employ the ansatz

$$\Psi^\nu(r,\theta,\varphi)=\sum_{\kappa\in\mathbb{Z}+(1/2)}\exp(-i\kappa\varphi)\Psi^{\nu,\kappa}(r,\theta).$$

Thus, if

$$\hat{\Psi}(r,\theta,\varphi,t)=\sum_{\nu\in\mathbb{Z}}\sum_{\kappa\in\mathbb{Z}+(1/2)}\exp(-i\omega_0\nu t)\exp(-i\kappa\varphi)\Psi^{\nu,\kappa}(r,\theta)$$

satisfies (1), then each $\Psi^{\nu,\kappa}$ is a solution of

$$(\mathcal{R}_{\nu,\kappa}+\mathcal{A}_{\nu,\kappa})\Psi^{\nu,\kappa}=0\quad\text{on}\quad(r_0,\infty)\times(0,\pi), \tag{11}$$

where $\mathcal{R}_{\nu,\kappa}$ and $\mathcal{A}_{\nu,\kappa}$ are obtained from (2) and (3) by replacing $\mathcal{D}_\pm$ and $\mathcal{L}_\pm$ by

$$\mathcal{D}_{\pm,\nu,\kappa}:=\frac{\partial}{\partial r}\pm\frac{i}{\Delta}[\omega_0\nu(r^2+a^2)+\kappa a+eQr],$$

$$\mathcal{L}_{\pm,\nu,\kappa}:=\frac{\partial}{\partial\theta}+\frac{\cot\theta}{2}\mp\left[a\omega_0\nu\sin\theta+\frac{\kappa}{\sin\theta}\right],$$

respectively (see the proof of Theorem IV.5).

B. Separation of the radial and the angular coordinate

To study Eq. (11) we consider the formal differential expression

$$\mathfrak{A}_{\nu,\kappa}:=\begin{pmatrix}-am\cos\theta & \mathcal{L}_{-,\nu,\kappa}\\ -\mathcal{L}_{+,\nu,\kappa} & am\cos\theta\end{pmatrix}$$

for $\theta\in(0,\pi)$. For any half integer κ the differential expression $\mathfrak{A}_{\nu,\kappa}$ has a unique self-adjoint realization $A_{\nu,\kappa}$ in the Hilbert space $L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)^2$ which has purely discrete spectrum $\sigma(A_{\nu,\kappa})=\{\lambda_{\nu,\kappa,n}:n\in\mathbb{Z}\setminus\{0\}\}\subseteq\mathbb{R}$, where each eigenvalue is simple (see, e.g., Batic *et al.*,[1] Winklmeier[18]). Hence, there is a complete set of orthonormal eigenfunctions of $A_{\nu,\kappa}$

$$g^{\nu,\kappa,n}:=\begin{pmatrix}g_1^{\nu,\kappa,n}\\ g_2^{\nu,\kappa,n}\end{pmatrix}\in L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)^2\quad(n\in\mathbb{Z}\setminus\{0\}) \tag{12}$$

with eigenvalues $\lambda_{\nu,\kappa,n}$. The family (12) allows us to make the ansatz

$$\Psi^{\nu,\kappa}=\sum_{n\in\mathbb{Z}\setminus\{0\}}\Psi^{\nu,\kappa,n}$$

with

$$\Psi^{\nu,\kappa,n}(r,\theta)=\begin{pmatrix} X_-^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta) \\ X_+^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta) \\ X_+^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta) \\ X_-^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta) \end{pmatrix} \quad (r\in(r_+,\infty),\theta\in(0,\pi)),$$

which leads to a separation of the angular coordinate θ and the radial coordinate r (cf. Chandrasekhar[4]): the angular function $g^{\nu,\kappa,n}$ satisfies the angular equation

$$A_{\nu,n}g^{\nu,\kappa,n}=\lambda_{\nu,\kappa,n}g^{\nu,\kappa,n}, \tag{13}$$

with the integrability condition $g^{\nu,\kappa,n}\in L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)$ and the radial function $X^{\nu,\kappa,n}={}^t(X_+^{\nu,\kappa,n},X_-^{\nu,\kappa,n})$ satisfies the radial equation

$$\begin{pmatrix} -imr-\lambda_{\nu,\kappa,n} & \sqrt{\Delta}\mathcal{D}_{-,\nu,\kappa} \\ \sqrt{\Delta}\mathcal{D}_{+,\nu,\kappa} & imr-\lambda_{\nu,\kappa,n} \end{pmatrix}\begin{pmatrix} X_+^{\nu,\kappa,n}(r) \\ X_-^{\nu,\kappa,n}(r) \end{pmatrix}=0, \tag{14}$$

with the integrability condition arising from the inner product on $\mathcal{H}_{r,\theta,\varphi}$

$$\int_{r_+}^{\infty}(|X_+^{\nu,\kappa,n}(r)|^2+|X_-^{\nu,\kappa,n}(r)|^2)\frac{r^2+a^2}{\Delta(r)}\mathrm{d}r<\infty. \tag{15}$$

C. The radial equation

Let

$$W:=\frac{1}{\sqrt{2}}\begin{pmatrix} -i & i \\ -1 & -1 \end{pmatrix},\quad V:=\begin{pmatrix} 0 & -1/\sqrt{\Delta} \\ 1/\sqrt{\Delta} & 0 \end{pmatrix},$$

$$\tilde{f}^{\nu,\kappa,n}(r):=\begin{pmatrix} \tilde{f}_1^{\nu,\kappa,n}(r) \\ \tilde{f}_2^{\nu,\kappa,n}(r) \end{pmatrix}:=W\begin{pmatrix} X_+^{\nu,\kappa,n}(r) \\ X_-^{\nu,\kappa,n}(r) \end{pmatrix}. \tag{16}$$

Then, we obtain from (14)

$$\begin{aligned} 0&=VW\begin{pmatrix} -imr-\lambda_{\nu,\kappa,n} & \sqrt{\Delta}\mathcal{D}_{-,\nu,\kappa} \\ \sqrt{\Delta}\mathcal{D}_{+,\nu,\kappa} & imr-\lambda_{\nu,\kappa,n} \end{pmatrix}W^{-1}\tilde{f}^{\nu,\kappa,n}(r) \\ &=\begin{pmatrix} \dfrac{mr}{\sqrt{\Delta}}-\dfrac{a\kappa+eQr+\omega_0\nu(r^2+a^2)}{\Delta} & -\dfrac{d}{dr}+\dfrac{\lambda_{\nu,\kappa,n}}{\sqrt{\Delta}} \\ \dfrac{d}{dr}+\dfrac{\lambda_{\nu,\kappa,n}}{\sqrt{\Delta}} & -\dfrac{mr}{\sqrt{\Delta}}-\dfrac{a\kappa+eQr+\omega_0\nu(r^2+a^2)}{\Delta} \end{pmatrix}\tilde{f}^{\nu,\kappa,n}(r) \end{aligned} \tag{17}$$

for $r\in(r_+,\infty)$ (see Winklmeier[18]).

Remark II.2: If we take into account only terms of first order in $1/r$ for large r, then the radial equation becomes

$$\begin{pmatrix} m-\dfrac{eQ}{r}+\omega_0\nu & -\dfrac{d}{dr}+\dfrac{\lambda_{\nu,n,\kappa}}{r} \\ \dfrac{d}{dr}+\dfrac{\lambda_{\nu,n,\kappa}}{r} & -m-\dfrac{eQ}{r}+\omega_0\nu \end{pmatrix}\tilde{f}(r)=0,$$

which is exactly the radial equation for the relativistic hydrogen atom see; e.g., Bjorken and Drell.[3]

Remark II.3: It is important to note that in the case $a \neq 0$ the eigenvalue λ for the angular equation does depend on $\omega_0 \nu$. In the case $a=0$, the eigenvalues can be calculated explicitly; they are given by

$$\sigma(A_{\nu,\kappa}) = \left\{ \lambda_{\nu,\kappa,n} = \operatorname{sign}(n)\left(|\kappa| - \frac{1}{2} + |n| \right) : n \in \mathbb{Z} \setminus \{0\} \right\} \subseteq \mathbb{R}. \tag{18}$$

In particular, the eigenvalues $\lambda_{\nu,\kappa,n}$ of the radial equation do not depend on the eigenvalues of the radial equation. Hence, in the case $a=0$, for a solution of the complete problem (14)–(13) first the angular problem $(A_{\nu,\kappa}-\lambda_{\nu,\kappa})g=0$ is solved for the eigenvalues $\lambda_{\nu,\kappa,n}$, and then the radial equation (14) can be attacked for fixed $\lambda_{\nu,\kappa,n}$.

We introduce a new coordinate x such that

$$\frac{dx}{dr} = \frac{r^2+a^2}{\Delta(r)} \quad (r > r_+), \tag{19}$$

that is,

$$x(r) = \begin{cases} r + \dfrac{r_+^2+a^2}{r_+-r_-}\log(r-r_+) - \dfrac{r_+^2+a^2}{r_+-r_-}\log(r-r_-) + x_0 & (r_+ \neq r_-), \\ r + 2r_+\log(r-r_+) - \dfrac{r_+^2+a^2}{r-r_+} + x_0 & (r_+ = r_-), \end{cases} \tag{20}$$

where x_0 is a constant of integration that can be set $x_0=0$. The correspondence between $r>r_+$ and $x \in (-\infty, \infty)$ is a bijection. With the new coordinate x Eq. (17) becomes

$$H_{\nu,\kappa,n} f^{\nu,\kappa,n} := \begin{pmatrix} \dfrac{mr\sqrt{\Delta}}{r^2+a^2} - \dfrac{a\kappa+eQr}{r^2+a^2} & -\dfrac{d}{dx} + \dfrac{\lambda_{\nu,\kappa,n}\sqrt{\Delta}}{r^2+a^2} \\ \dfrac{d}{dx} + \dfrac{\lambda_{\nu,\kappa,n}\sqrt{\Delta}}{r^2+a^2} & -\dfrac{mr\sqrt{\Delta}}{r^2+a^2} - \dfrac{a\kappa+eQr}{r^2+a^2} \end{pmatrix} f^{\nu,\kappa,n} = \omega_0 \nu f^{\nu,\kappa,n}, \tag{21}$$

where r has to be understood as $r(x)$ and $f^{\nu,\kappa,n}(x) = \tilde{f}^{\nu,\kappa,n}(r(x))$, $f_j^{\nu,\kappa,n}(x) = \tilde{f}_j^{\nu,\kappa,n}(r(x))$ for all $x \in (-\infty, \infty)$ and $j \in \{1,2\}$. In view of (16) and (19) the integrability condition (15) becomes

$$\int_{-\infty}^{\infty} \|f^{\nu,\kappa,n}(x)\|_{\mathbb{C}^2}^2 dx = \int_{-\infty}^{\infty} [|f_1^{\nu,\kappa,n}(x)|^2 + |f_2^{\nu,\kappa,n}(x)|^2] \, dx < \infty. \tag{22}$$

The operator $H_{\nu,\kappa,n}$ is formally symmetric in the Hilbert space $\mathcal{H}_x := L^2((-\infty,\infty);dx)^2$, so it is natural to look for an operator theoretical realization of $H_{\nu,\kappa,n}$ in the Hilbert space $\mathcal{H}_x$. The purpose of this article is to investigate the spectral properties of the self-adjoint operator $H_{\nu,\kappa,n}$ in $\mathcal{H}_x = L^2((-\infty,\infty);dx)^2$ and to study the nonexistence of nontrivial solutions satisfying (11). In Sec. VI we will investigate the existence of so-called energy eigenvalues of $H_{\nu,\kappa,n}$ (cf. Schmid[12]).

Definition II. 4: We call $\omega \in \mathbb{R}$ an *energy eigenvalue* of $H_{\nu,\kappa,n}$ if there are $\lambda_{\nu,\kappa,n}$ such that ω is an eigenvalue of $H_{\nu,\kappa,n}$ and $\lambda_{\nu,\kappa,n}$ is an eigenvalue of $A_{\nu,\kappa}$, that is, if Eqs. (13) and (14) can be solved simultaneously with functions satisfying the corresponding integrability conditions.

III. THE OPERATOR *H*

In this and the following sections we consider the eigenvalue equation $(H_{\nu,\kappa,n}-\omega\nu_0)f^{\nu,\kappa,n}=0$ from (21) on the Hilbert space $\mathcal{H}_x = L^2((-\infty,\infty);dx)^2$.

If there is no ambiguity, we omit the indices ν, n, and κ in the following for the sake of clarity; for instance, we write simply H instead of $H_{\nu,\kappa,n}$, λ instead of $\lambda_{\nu,\kappa,n}$, and ω instead of $\omega_0\nu$. We decompose the operator H into the sum

$$H = H_0 + V,$$

where

$$H_0 = \begin{pmatrix} 0 & -\frac{d}{dx} \\ \frac{d}{dx} & 0 \end{pmatrix}, \quad \mathcal{D}(H_0) = \mathcal{C}_0^\infty(-\infty, \infty)^2,$$

$$V(x) = \begin{pmatrix} A(x) & B(x) \\ B(x) & C(x) \end{pmatrix},$$

$$A(x) = \frac{mr(x)\sqrt{\Delta(r(x))}}{r(x)^2 + a^2} - \frac{a\kappa + eQr(x)}{r(x)^2 + a^2},$$

$$B(x) = \lambda \frac{\sqrt{\Delta(r(x))}}{r(x)^2 + a^2},$$

$$C(x) = -\frac{mr(x)\sqrt{\Delta(r(x))}}{r(x)^2 + a^2} - \frac{a\kappa + eQr(x)}{r(x)^2 + a^2},$$

$$\Delta(x) = (r(x) - r_+)(r(x) - r_-).$$

The operator H_0 is symmetric and has a unique self-adjoint extension on the space $L^2((-\infty, \infty); dx)^2$, see, e.g., Weidmann (Ref. 17, Theorem 6.8). Since $x \to -\infty$ is equivalent to $r(x) \to r_+$ and $x \to \infty$ is equivalent to $r(x) \to \infty$, we have

$$\lim_{x \to -\infty} A(x) = -\frac{a\kappa + eQr_+}{r_+^2 + a^2} =: A_0, \quad \lim_{x \to +\infty} A(x) = m,$$

$$\lim_{x \to -\infty} C(x) = A_0, \quad \lim_{x \to +\infty} C(x) = -m,$$

$$\lim_{x \to \pm\infty} B(x) = 0$$

which implies that the functions $A(\cdot)$, $B(\cdot)$, and $C(\cdot)$ are bounded. Since we assume that the black hole condition (7) holds, the multiplication operator V is symmetric. Therefore, $H = H_0 + V$ has a unique self-adjoint extension which we again denote by H.

In what follows, a prime $'$ always denotes differentiation with respect to x.

Lemma III.1 (*Asymptotic behavior of V for* $x \to -\infty$):

(i) *For* $x \to -\infty$ *the functions*

$$A(x) - A_0, \quad B(x), \quad C(x) - A_0$$

decay exponentially in the case $r_+ \neq r_-$, *and they are of order* $O(x^{-1})$ *in the case* $r_+ = r_-$. *More precisely, in the latter case we have*

$$A(x) - A_0 = \frac{mM - \mu}{-x} + O\left(\frac{1}{x^2}\right) \quad \text{as } x \to -\infty,$$

$$A_0 - C(x) = \frac{mM+\mu}{-x} + O\left(\frac{1}{x^2}\right) \quad \text{as } x \to -\infty,$$

$$B(x) = \frac{\lambda}{x} + O\left(\frac{1}{x^2}\right) \quad \text{as } x \to -\infty,$$

where

$$\mu := -\frac{2a\kappa M}{M^2+a^2} - eQ\frac{M^2-a^2}{M^2+a^2}.$$

(ii) *The derivatives* A', B', *and* C' *are integrable with respect to* x *on* $(-\infty, 0]$.
(iii) $A'(x) = O(x^{-2})$, $B'(x) = O(x^{-2})$, *and* $C'(x) = O(x^{-2})$ *hold as* $x \to +\infty$.

Proof. We prove the assertions for the functions B and A only. The corresponding assertions for C can be obtained from those for A by substituting m by $-m$. We remark that (20) shows

$$r(x) - r_+ = O(\exp(\alpha x)) \quad \text{as } x \to -\infty \quad (r_+ \neq r_-), \tag{23}$$

$$r(x) - r_+ = O(x^{-1}) \quad \text{as } x \to -\infty \quad (r_+ = r_-) \tag{24}$$

for a positive constant α. To keep notation simple, let us write r instead of $r(x)$ in this proof.

(i) Note that

$$\frac{1}{r^2+a^2} = \frac{1}{r_+^2+a^2} - \frac{(r-r_+)(r+r_+)}{(r_+^2+a^2)(r^2+a^2)} = \frac{1}{r_+^2+a^2} + O(r-r_+). \tag{25}$$

Hence, it follows immediately that

$$B(x) = \lambda\frac{\sqrt{\Delta(r)}}{r^2+a^2} = \lambda\sqrt{\Delta(r)}\left(\frac{1}{r_+^2+a^2} + O(r-r_+)\right).$$

If we recall that $\Delta(r(x)) = (r(x)-r_+)(r(x)-r_-)$ and use the relations (23) and (24), we see that the assertion for B holds.

Now we prove the assertions for A. Simple calculations show

$$\begin{aligned} A(x) - A_0 &= \frac{mr\sqrt{\Delta(r)}}{r^2+a^2} + \frac{(r^2+a^2)(a\kappa+eQr_+) - (r_+^2+a^2)(a\kappa+eQr)}{(r^2+a^2)(r_+^2+a^2)} \\ &= \frac{mr\sqrt{\Delta(r)}}{r^2+a^2} + \frac{(r-r_+)[(r-r_+)(a\kappa+eQr_+) + 2a\kappa r_+ + eQ(r_+^2-a^2)]}{(r^2+a^2)(r_+^2+a^2)} \\ &= \frac{mr_+\sqrt{\Delta(r)}}{r^2+a^2} + \frac{r-r_+}{r^2+a^2}\left[m\sqrt{\Delta(r)} + \frac{(r-r_+)(a\kappa+eQr_+) + 2a\kappa r_+ + eQ(r_+^2-a^2)}{r_+^2+a^2}\right]. \end{aligned}$$

Using the relations (25) and (23), we see that the assertion holds for the case $r_+ \neq r_-$. In the case $r_+ = r_-$ we have $\Delta(r) = (r-r_+)^2 = (r-M)^2$; hence, we can continue the calculation above as follows:

$$A(x)-A_0=\frac{r-r_+}{r^2+a^2}\left[mr_+ +\frac{2a\kappa r_+ +eQ(r_+^2-a^2)}{r_+^2+a^2}+(r-r_+)\left(m+\frac{a\kappa+eQr_+}{r_+^2+a^2}\right)\right]$$
$$=\frac{r-r_+}{r^2+a^2}\left[mr_+ -\mu+(r-r_+)\left(m+\frac{a\kappa+eQr_+}{r_+^2+a^2}\right)\right].$$

The assertion follows now from (25) and (24).

(ii) A simple calculation gives

$$\frac{d}{dx}A(x)=\frac{dr}{dx}\frac{d}{dr}A(x(r))=\frac{\Delta(r)}{r^2+a^2}\frac{d}{dr}A(x(r))$$
$$=\frac{\sqrt{\Delta(r)}}{r^2+a^2}\left\{m\left(\frac{\Delta(r)}{r^2+a^2}+\frac{r\Delta'(r)}{2(r^2+a^2)}-\frac{2r^2\Delta(r)}{(r^2+a^2)^2}\right)\right.$$
$$\left.+\frac{2(a\kappa+eQr)r\sqrt{\Delta(r)}}{(r^2+a^2)^2}-\frac{eQ\sqrt{\Delta(r)}}{r^2+a^2}\right\}$$
$$=\begin{cases}O((r-r_+)^{1/2})=O(\exp[(1/2)\alpha x]), & (r_+\neq r_-),\\ O((r-r+)^2)=O(x^{-2}), & (r_+=r_-),\end{cases}\tag{26}$$

as $x\to-\infty$.

$$\frac{d}{dx}B(x)=\frac{dr}{dx}\frac{d}{dr}B(x(r))=\frac{\Delta(r)}{r^2+a^2}\frac{d}{dr}B(x(r))=\lambda\frac{\sqrt{\Delta(r)}}{r^2+a^2}\left\{\frac{\Delta'(r)}{2(r^2+a^2)}-\frac{2r\Delta(r)}{(r^2+a^2)^2}\right\}$$
$$=\begin{cases}O((r-r_+)^{1/2})=O(\exp[(1/2)\alpha x]), & (r_+\neq r_-),\\ O((r-r+)^2)=O(x^{-2}), & (r_+=r_-),\end{cases}\tag{27}$$

as $x\to-\infty$.

(iii) Since

$$\frac{dr}{dx}=\frac{\Delta(r)}{r^2+a^2}\sim 1,\quad x\sim r\quad \text{as } x\to+\infty,$$

and

$$2(r^2+a^2)\Delta(r)+r(r^2+a^2)\Delta'(r)-4r^2\Delta(r)=2Mr^3+2r^2(a^2-Q^2)$$
$$-6a^2Mr+2a^2(a^2+Q^2)\sim r^3\quad \text{as } r\to\infty,$$

the assertion follows from (26). The proof of the assertion concerning $B'(x)$ follows directly from (27). □

IV. ABSOLUTELY CONTINUOUS SPECTRUM

The following proposition has been shown by Belgiorno and Martellini.[2]

Proposition IV.1: $\sigma_{\mathrm{ess}}(H)=\mathbb{R}$. □

We point out that the proof of the proposition relies on the fact that

$$\lim_{x\to-\infty}[V(x)-A_0I_2]=0,\tag{28}$$

where I_2 is the 2×2 unit matrix. Lemma III.1 yields the following theorem.

Theorem IV.2:

(i) *H has purely absolutely continuous spectrum in $\mathbb{R}\backslash\{A_0\}$.*

(ii) *H has purely absolutely continuous spectrum in $(-\infty,-m)$ and $(m,+\infty)$, that is, H is absolutely continuous in the complement of $[-m,m]\cap\{A_0\}$.*

Proof.

(i) *Lemma III.1 gives (28) and any component of V' is integrable at $-\infty$. Therefore, we can prove the theorem in view of Weidmann,[16] Schmidt,[13] and also Thaller (Ref. 14, Theorem 4.18).*

(ii) The proof is the same as in (i) by using Lemma III.1 (iii). □

Remark IV.3: The above theorem has already been proven by Schmid by different means [see Schmid (Ref. 12, Corollary 3.4)]; in addition, he has shown that neither $\omega=m$ nor $\omega=-m$ is an eigenvalue of H (Ref. 12, Lemma 3.5).

Theorem IV.4: *If $r_+\neq r_-$, then A_0 is not an eigenvalue of H.*

Proof. Let us assume that $U={}^t(u_1,u_2)\in\mathcal{H}_x$ satisfies

$$\begin{pmatrix} A & B-\dfrac{d}{dx} \\ B+\dfrac{d}{dx} & C \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}=A_0\begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

that is,

$$U'=\begin{pmatrix} u_1' \\ u_2' \end{pmatrix}=\begin{pmatrix} -B & A_0-C \\ A-A_0 & B \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{29}$$

As seen in Sec. III, $A(x)-A_0$, $B(x)$ and $C(x)-A_0$ decay exponentially as $x\to-\infty$. Therefore, the Levinson theorem (e.g., Eastham[6]) gives that there are two linearly independent solutions U^1, U^2 of (29) such that

$$U^1(x)=\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix}+o(1)\right\}\quad \text{as } x\to-\infty,$$

$$U^2(x)=\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}+o(1)\right\}\quad \text{as } x\to-\infty.$$

Hence there are constants c_1 and c_2 such that $U(x)=c_1U^1(x)+c_2U^2(x)$, which is square integrable on $(-\infty,0)$ only if $c_1=c_2=0$. □

As an important corollary we obtain the following theorem.

Theorem IV.5 (Nonexistence of time-periodic solutions for $r_+\neq r_-$): *Let $\hat{\Psi}\in C^1((r_0,\infty)\times(0,\pi)\times[-\pi,\pi]\times\mathbb{R},\mathbb{C}^4)$ be a solution of (1) satisfying the periodicity conditions*

$$\begin{aligned}&\hat{\Psi}(r,\theta,\varphi,t)=\hat{\Psi}\left(r,\theta,\varphi,t+\frac{2\pi}{\omega_0}\right), \quad (r,\theta,\varphi,t)\in\hat{\Omega}\\ &\hat{\Psi}(r,\theta,\pi,t)=\hat{\Psi}(r,\theta,-\pi,t),\end{aligned} \tag{30}$$

for some $\omega_0>0$. Furthermore, assume that for all $(\varphi,t)\in[-\pi,\pi]\times\mathbb{R}$ we have $\hat{\Psi}(\cdot,\cdot,\varphi,t)\in C^0((r_0,\infty)\times(0,\pi);\mathcal{H}_{r,\theta})$, where

$$\mathcal{H}_{r,\theta}:=L^2\left((r_+,\infty)\times(0,\pi);\ \frac{r^2+a^2}{\Delta(r)}\sin\theta\,dr\,d\theta\right)^4$$

with the norm denoted by $\|\cdot\|_{\mathcal{H}_{r,\theta}}$ and the inner product denoted by $\langle\cdot,\cdot\rangle_{\mathcal{H}_{r,\theta}}$.

If $r_- \neq r_+$, *then* $\hat{\Psi} \equiv 0$.

Proof. Let $\hat{\Psi}$ be a time-periodic solution satisfying the conditions of the theorem. Then, $\hat{\Psi}(\cdot,\cdot,\cdot,t)$ is an $\mathcal{H}_{r,\theta,\varphi}$-valued strongly continuous function with respect to t since $\hat{\Psi}(\cdot,\cdot,\varphi,t)$ is uniformly continuous in $\mathcal{H}_{r,\theta}$ with respect to $(\varphi,t) \in [-\pi,\pi]\times\mathbb{R}$. Therefore, we can expand $\hat{\Psi}(r,\theta,\varphi,t)$ as the Fourier series with respect to t

$$\hat{\Psi}(r,\theta,\varphi,t) = \sum_{\nu\in\mathbb{Z}} \exp(-i\omega_0\nu t)\Psi^{\nu}(r,\theta,\varphi)$$

strongly in $L^2([0,2\pi/\omega_0];\mathcal{H}_{r,\theta,\varphi};dt)$, where

$$\Psi^{\nu}(r,\theta,\varphi) = \frac{\omega_0}{2\pi}\int_0^{2\pi/\omega_0} \exp(i\omega_0\nu t)\hat{\Psi}(r,\theta,\varphi,t)dt, \quad \sum_{\nu} \|\Psi^{\nu}\|^2_{\mathcal{H}_{r,\theta,\varphi}} < \infty .$$

Moreover, each $\Psi^{\nu}(r,\theta,\varphi)$ can be expanded as

$$\Psi^{\nu}(r,\theta,\varphi) = \sum_{\kappa\in\mathbb{Z}+(1/2)} \exp(-i\kappa\varphi)\Psi^{\nu,\kappa}(r,\theta)$$

strongly in $L^2([-\pi,\pi];\mathcal{H}_{r,\theta};d\varphi)$ with

$$\Psi^{\nu}(\theta,\varphi) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \exp(i\kappa\varphi)\Psi^{\nu}(r,\theta,\varphi)d\varphi, \quad \sum_{\kappa} \|\Psi^{\nu,\kappa}\|^2_{\mathcal{H}_{r,\theta}} < \infty .$$

For every $\Phi \in \mathcal{C}_0^{\infty}((r_0,\infty)\times(0,\pi))^4$ of the form

$$\Phi(r,\theta) = \begin{pmatrix} \rho_-(r)\,\eta_2(\theta) \\ \rho_+(r)\,\eta_1(\theta) \\ \rho_+(r)\,\eta_2(\theta) \\ \rho_-(r)\,\eta_1(\theta) \end{pmatrix}$$

with $\rho_{\pm}(r) \in \mathcal{C}_0^{\infty}((r_+,\infty))$, $\eta_1(\theta)$, $\eta_2(\theta) \in \mathcal{C}_0^{\infty}((0,\pi))$ we obtain, by using (30),

$$\begin{aligned}
0 &= \int_0^{2\pi/\omega_0} \mathrm{d}t \int_{-\pi}^{\pi} \mathrm{d}\varphi\, \langle (\hat{\mathcal{R}}+\hat{\mathcal{A}})\hat{\Psi}, \exp(-i\omega_0\nu t)\exp(-i\kappa\varphi)\Phi\rangle_{\mathcal{H}_{r,\theta}} \\
&= \int_0^{2\pi/\omega_0} \mathrm{d}t \int_{-\pi}^{\pi} \mathrm{d}\varphi\, \langle \hat{\Psi}, (\hat{\mathcal{R}}+\hat{\mathcal{A}})^* \exp(-i\omega_0\nu t)\exp(-i\kappa\varphi)\Phi\rangle_{\mathcal{H}_{r,\theta}} \\
&= \int_0^{2\pi/\omega_0} \mathrm{d}t \int_{-\pi}^{\pi} \mathrm{d}\varphi\, \langle \hat{\Psi}, \exp(-i\omega_0\nu t)\exp(-i\kappa\varphi)(\mathcal{R}_{\nu,\kappa}+\mathcal{A}_{\nu,\kappa})^*\Phi\rangle_{\mathcal{H}_{r,\theta}} \\
&= \int_0^{2\pi/\omega_0} \langle \hat{\Psi}, \exp(-i\omega_0\nu t)\exp(-i\kappa\varphi)(\mathcal{R}_{\nu,\kappa}+\mathcal{A}_{\nu,\kappa})^*\Phi\rangle_{\mathcal{H}_{r,\theta,\varphi}} \mathrm{d}t \\
&= \frac{2\pi}{\omega_0}\int_{-\pi}^{\pi} \langle \Psi^{\nu}, \exp(-i\kappa\varphi)(\mathcal{R}^*_{\nu,\kappa}+\mathcal{A}^*_{\nu,\kappa})\Phi\rangle_{\mathcal{H}_{r,\theta}} \mathrm{d}\varphi = \frac{4\pi^2}{\omega_0}\langle \Psi^{\nu,\kappa}, (\mathcal{R}^*_{\nu,\kappa}+A^*_{\nu,\kappa})\Phi\rangle_{\mathcal{H}_{r,\theta}}. \qquad (31)
\end{aligned}$$

In the above calculation, the superscript * denotes the formal adjoint operator. As in (12), for fixed ν and κ let

$$g^{\nu,\kappa,n}(\theta)=\begin{pmatrix} g_1^{\nu,\kappa,n}(\theta)\\ g_2^{\nu,\kappa,n}(\theta)\end{pmatrix}\quad (n\in\mathbb{Z}\setminus\{0\})$$

be a complete family of orthonormal eigenfunctions of $A_{\nu,\kappa}$ with eigenvalues $\lambda_{\nu,\kappa,n}$, respectively. Then, $\Psi^{\nu,\kappa}(r,\theta)$ can be expanded in terms of $g^{\nu,\kappa,n}$ $(n\in\mathbb{Z}\setminus\{0\})$ as follows:

$$\Psi^{\nu,\kappa}(r,\theta)=\sum_{n\in\mathbb{Z}\setminus\{0\}}\begin{pmatrix} X_-^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta)\\ X_+^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta)\\ X_+^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta)\\ X_-^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta)\end{pmatrix},$$

where the series converges in the strong sense in $L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)^4$ and $X_\pm^{\nu,\kappa,n}(r)$ satisfies

$$\sum_{n\in\mathbb{Z}\setminus\{0\}}\int_{r_+}^{\infty}(|X_+^{\nu,\kappa,n}(r)|^2+|X_-^{\nu,\kappa,n}(r)|^2)\frac{r^2+a^2}{\Delta(r)}\mathrm{d}r<\infty.$$

Since $\mathfrak{A}_{\nu,\kappa}$ on $C_0^\infty((0,\pi))^2$ is essentially self-adjoint in $L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)^2$, for any $g^{\nu,\kappa,n}(\theta)$ there exists a convergent sequence $\eta^\ell\in C_0^\infty((0,\pi))^2$ $(\ell=1,2,\dots)$ such that

$$A_{\nu,\kappa}\eta^\ell=A_{\nu,\kappa}\begin{pmatrix}\eta_1^\ell\\ \eta_2^\ell\end{pmatrix}\longrightarrow A_{\nu,\kappa}g^{\nu,\kappa,n}=\lambda_{\nu,\kappa,n}g^{\nu,\kappa,n}$$

in $L^2((0,\pi);\sin\theta\,\mathrm{d}\theta)^2$. Substituting Φ in (31) by

$$\Phi^\ell(r,\theta)=\begin{pmatrix}\rho_-(r)\eta_2^\ell(\theta)\\ \rho_+(r)\eta_1^\ell(\theta)\\ \rho_+(r)\eta_2^\ell(\theta)\\ \rho_-(r)\eta_1^\ell(\theta)\end{pmatrix}$$

and taking the limit $\ell\to\infty$, we have

$$\left\langle\sum_{m\in\mathbb{Z}\setminus\{0\}}\begin{pmatrix} X_-^{\nu,\kappa,m}(r)g_2^{\nu,\kappa,m}(\theta)\\ X_+^{\nu,\kappa,m}(r)g_1^{\nu,\kappa,m}(\theta)\\ X_+^{\nu,\kappa,m}(r)g_2^{\nu,\kappa,m}(\theta)\\ X_-^{\nu,\kappa,m}(r)g_1^{\nu,\kappa,m}(\theta)\end{pmatrix},\quad (R_{\nu,\kappa}^*-\lambda_{\nu,\kappa,n})\begin{pmatrix}\rho_-(r)g_2^{\nu,\kappa,n}(\theta)\\ \rho_+(r)g_1^{\nu,\kappa,n}(\theta)\\ \rho_+(r)g_2^{\nu,\kappa,n}(\theta)\\ \rho_-(r)g_2^{\nu,\kappa,n}(\theta)\end{pmatrix}\right\rangle_{\mathcal{H}_{r,\theta}}=0,$$

which gives

$$0=\int_{r_+}^{\infty}\mathrm{d}r\frac{r^2+a^2}{\Delta(r)}\left\langle\begin{pmatrix}X_+^{\nu,\kappa,n}\\ X_-^{\nu,\kappa,n}\end{pmatrix},\quad\begin{pmatrix} imr-\lambda_{\nu,\kappa,n} & \mathcal{D}_{+,\nu,\kappa}^*\sqrt{\Delta}\\ \mathcal{D}_{-,\nu,\kappa}^*\sqrt{\Delta} & -imr-\lambda_{\nu,\kappa,n}\end{pmatrix}\begin{pmatrix}\rho_+\\ \rho_-\end{pmatrix}\right\rangle_{\mathbb{C}^2},$$

which implies

$$\begin{pmatrix} -imr-\lambda_{\nu,\kappa,n} & \sqrt{\Delta}\mathcal{D}_{-,\nu,\kappa}\\ \sqrt{\Delta}\,\mathcal{D}_{+,\nu,\kappa} & imr-\lambda_{\nu,\kappa,n}\end{pmatrix}\begin{pmatrix}X_+^{\nu,\kappa,n}(r)\\ X_-^{\nu,\kappa,n}(r)\end{pmatrix}=0.$$

If we set [cf. (16) and (22)]

$$f^{\nu,\kappa,n}(x)=\begin{pmatrix}f_1^{\nu,\kappa,n}(r(x))\\ f_2^{\nu,\kappa,n}(r(x))\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}-i & i\\ -1 & -1\end{pmatrix}\begin{pmatrix}X_+^{\nu,\kappa,n}(r(x))\\ X_-^{\nu,\kappa,n}(r(x))\end{pmatrix},$$

we have

$$H_{\nu,\kappa,n} f^{\nu,\kappa,n} = \omega_0 \nu f^{\nu,\kappa,n}$$

[see (21)]. Then, Theorem IV.2 and Theorem IV.4 give $f^{\nu,\kappa,n}=0$ for any $n \in \mathbb{Z}\backslash\{0\}$ and $\kappa \in \mathbb{Z}+(1/2)$, which yields $\Psi^{\nu,\kappa}(r,\theta)=0$.

The nonexistence of time-periodic solutions is shown by Finster *et al.*[7,8] by different means.

V. THE CASE $r_+=r_-$

In the previous section we have seen that there are no eigenvalues of (1) in the case $r_+ \neq r_-$. In this section we discuss whether A_0 is an eigenvalue of H in the case $r_+=r_-$. Recall that in this case the function Δ has only one zero and that $r_+=r_-=M$.

Theorem V.1: *If*

$$\lambda^2 + m^2M^2 - \mu^2 \leq \frac{1}{4},$$

then A_0 is not an eigenvalue of H.

Proof. Let us assume that $U={}^t(u_1,u_2) \in \mathcal{H}_x$ satisfies (29), that is,

$$U' = \begin{pmatrix} u_1' \\ u_2' \end{pmatrix} = \begin{pmatrix} -B & A_0 - C \\ A - A_0 & B \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

Lemma III.1 yields for $x \to -\infty$

$$U'(x) = -\frac{1}{x} \begin{pmatrix} \lambda & mM+\mu \\ mM-\mu & -\lambda \end{pmatrix} U(x) + O(x^{-2})U(x).$$

If we introduce $s=\log(-x)$, we have

$$\frac{d}{ds}U(x(s)) = \begin{pmatrix} \lambda & mM+\mu \\ mM-\mu & -\lambda \end{pmatrix} U(x(s)) + O(\exp(-s))U(x(s)) \quad \text{as } s \to +\infty. \tag{32}$$

The matrix

$$S := \begin{pmatrix} \lambda & mM+\mu \\ mM-\mu & -\lambda \end{pmatrix}$$

can be diagonalized by a nonsingular matrix T as

$$T^{-1}ST = \begin{pmatrix} \sqrt{\lambda^2 + m^2M^2 - \mu^2} & 0 \\ 0 & -\sqrt{\lambda^2 + m^2M^2 - \mu^2} \end{pmatrix}$$

if $\lambda^2+m^2M^2-\mu^2 \neq 0$. If $\lambda^2+m^2M^2-\mu^2=0$, its Jordan canonical form is

$$T^{-1}ST = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

According to Theorem 1.8.1 and Theorem 1.10.1 in Eastham,[6] we have two linearly independent solutions $U^1(s)$, $U^2(s)$ of (32) such that if $\lambda^2+m^2M^2-\mu^2 \neq 0$,

$$U^1(s) = \{v_1 + o(1)\}\exp(\sqrt{\lambda^2 + m^2M^2 - \mu^2}s) = \{v_1 + o(1)\}(-x)^{\sqrt{\lambda^2+m^2M^2-\mu^2}},$$

$$U^2(s) = \{v_2 + o(1)\}\exp(-\sqrt{\lambda^2 + m^2M^2 - \mu^2}s) = \{v_2 + o(1)\}(-x)^{-\sqrt{\lambda^2+m^2M^2-\mu^2}}$$

as $x \to -\infty$ and, if $\lambda^2+m^2M^2-\mu^2=0$,

$$U^1(s) = v_1 + o(1),$$

$$U^2(s) = sv_1 + v_2 + o(s) = v_1 \log(-x) + v_2 + o(\log(-x))$$

as $x \to -\infty$, where $T=(v_1, v_2)$.

Therefore, a necessary condition for the existence of an $\mathcal{L}^2(-\infty, 0)$-eigenfunction is

$$\sqrt{\lambda^2 + m^2M^2 - \mu^2} \in (1/2, \infty), \quad \text{i.e.}, \ \lambda^2 + m^2M^2 - \mu^2 > 1/4.$$

□

Remark V.2: The above discussions show that for ω to be an eigenvalue of H the following conditions are necessary:

$$r_+ = r_- = M \quad \text{(Theorem IV.4)}, \tag{33}$$

$$\omega = A_0 = -\frac{a\kappa + eQr_+}{r_+^2 + a^2} \quad \text{(Theorem IV.2(i))}, \tag{34}$$

$$\omega^2 < m^2 \quad \text{(Theorem IV.2(ii), Remark IV.3)}, \tag{35}$$

$$\lambda^2 + m^2M^2 - \mu^2 > \frac{1}{4} \quad \text{(Theorem V.1)}. \tag{36}$$

However, the solvability of the above system is not yet sufficient for the existence of an energy eigenvalue.

Schmid[12] showed that if in addition either

$$\beta - \sigma\lambda = 0, \quad \alpha + \eta = 0 \tag{37a}$$

or

$$N + \alpha + \eta = 0 \quad \text{for some positive integer } N, \tag{37b}$$

holds, then the solvability of the system (33)–(36) with (37a) or (37b) is sufficient for the existence of an eigenvalue ω of H.

In the above formulas, we used

$$\sigma := \operatorname{sign} \omega, \quad \eta := \sqrt{\lambda^2 + M^2m^2 - \mu^2}, \quad \mu = 2M\omega + eQ = -\frac{2a\kappa M}{M^2 + a^2} - eQ\frac{M^2 - a^2}{M^2 + a^2},$$

$$\alpha := \frac{Mm^2 - \omega\mu}{\sqrt{m^2 - \omega^2}}, \quad \beta := \frac{(M|\omega| - \sigma\mu)m}{\sqrt{m^2 - \omega^2}}.$$

Note that the variable η is denoted by κ in Ref. 12.

VI. ENERGY EIGENVALUES IN THE CASE $r_+ = r_-$

If ω is an energy eigenvalue of (1), then there must be an $N \in \mathbb{N}_0$ such that ω satisfies the complicated system of conditions (33)–(36) with (37a) or (37b). It is not clear that for given data of the black hole and the particle there are tuples $(\nu\omega_0, \kappa, \lambda_{\nu,\kappa,n})$ that solve the system (33)–(36) with (37a) or (37b). Schmid[12] has shown that in the so-called Kerr case (i.e., if $Q=0$) for fixed data of the spin-$\frac{1}{2}$ particle there exist two sequences $(a_N^{\pm})_{N\in\mathbb{N}}$ such that for $a = a_N^{\pm}$ the value $\omega_N = -\eta/2a_N^{\pm}$ is an energy eigenvalue.

Here, we fix the black hole data M, Q, and a and vary the mass of the fermion to obtain the existence of energy eigenvalues in the case $r_- = r_+$.

Theorem VI.1: *Fix $M>0$, $a, Q, e \in \mathbb{R}$, $\nu \in \mathbb{Z}$ and $\kappa \in \mathbb{Z} + \frac{1}{2}$. Let $\omega := -(\kappa a + eQM)/(a^2 + M^2)$. Take $\lambda = \lambda_{\nu,\kappa,n}$ for any sufficiently large $|n|$. If $\omega(eQ + M\omega) > 0$ then there are no energy eigenval-*

ues of $H_{\nu,\kappa,n}$. *If* $\omega(eQ+M\omega)>0$ *then there is a sequence* $(m_N)_{N\in\mathbb{N}}\subseteq(|\omega|,\infty)$ *such that if* $m\in\{m_N:N\in\mathbb{N}\}$, *then* ω *is an energy eigenvalue of* $H_{\nu,\kappa,n}$. *For* N_0 *large enough, the sequence* $(m_N)_{N\geq N_0}$ *is monotonously decreasing and converges to* $|\omega|$.

Before we prove the theorem, let us emphasize that $\lambda=\lambda_{\nu,\kappa,n}$ does depend also on m. Therefore, we denote it by $\lambda=\lambda_{\nu,\kappa,n}(m)$. In order to check the condition (36) we prepare the following lemma.

Lemma VI.2. Fix $\nu\in\mathbb{Z}$ *and* $\kappa\in\mathbb{Z}+1/2$. *If* $|n|$ *is sufficiently large, then the inequality* (36) *holds for any* $m>0$, $M>0$ *and* $\mu\in\mathbb{R}$, *that is*,

$$\lambda_{\nu,\kappa,n}^2+m^2M^2-\mu^2>\frac{1}{4}.$$

Proof. It follows from standard perturbation theory (applied to the angular operator with m as perturbation parameter, see Winklmeier,[18] Kato[10]) that

$$\left|\frac{d}{dm}\lambda_{\nu,\kappa,n}(m)\right|\leq\left\|\begin{matrix}-a\cos\theta & 0\\ 0 & a\cos\theta\end{matrix}\right\|=|a|,$$

hence, for $m>|\omega|$,

$$|\lambda_{\nu,\kappa,n}(|\omega|)|-|a|(m-|\omega|)\leq|\lambda_{\nu,\kappa,n}(m)|\leq|\lambda_{\nu,\kappa,n}(|\omega|)|+|a|(m-|\omega|). \tag{38}$$

Let $\tilde{m}=M^{-1}\sqrt{\mu^2+1/4}$. Since the sequence $(\lambda_{\nu,\kappa,n})_n$ is monotonously increasing and unbounded from below and from above, there is an integer n_0 such that

$$|\lambda_{\nu,\kappa,n}(|\omega|)|>|a|(\tilde{m}-|\omega|)+\sqrt{\mu^2+1/4}$$

for all $|n|\geq n_0$. If $m\in(|\omega|,\tilde{m}]$, we have

$$|\lambda_{\nu,\kappa,n}(m)|\geq|\lambda_{\nu,\kappa,n}(|\omega|)|-|a|(m-|\omega|)\geq|\lambda_{\nu,\kappa,n}(|\omega|)|-|a|(\tilde{m}-|\omega|)>\sqrt{\mu^2+1/4},$$

which implies

$$\sqrt{\lambda_{\nu,\kappa,n}(m)^2+M^2m^2-\mu^2}\geq\sqrt{\mu^2+1/4+m^2M^2-\mu^2}>1/2.$$

If $m>\tilde{m}=M^{-1}\sqrt{\mu^2+1/4}$, then we have

$$\sqrt{\lambda_{\nu,\kappa,n}(m)^2+M^2m^2-\mu^2}>\sqrt{M^2\tilde{m}^2-\mu^2}=1/2.$$

□

Now we shall prove Theorem VI.1.

Proof of Theorem VI.1: By definition, ω satisfies condition (34). As seen in Lemma VI.2, there is an $n_0\in\mathbb{N}$ such that condition (36) is satisfied for all $|n|\geq n_0$. From now on, let us assume that condition (36) holds. Next we consider the conditions (37a) and (37b). To this end we compute

$$\alpha+\eta=\frac{Mm^2-\omega\mu}{\sqrt{m^2-\omega^2}}+\sqrt{\lambda_{\kappa,n}^2+M^2m^2-\mu^2}=-\frac{\omega(eQ+M\omega)}{\sqrt{m^2-\omega^2}}+M\sqrt{m^2-\omega^2}+\sqrt{\lambda_{\kappa,n}^2+M^2m^2-\mu^2}.$$

If $\omega(eQ+M\omega)\leq0$, then $\alpha+\eta>\frac{1}{2}$ and condition (37a) nor (37b) cannot be satisfied for any $N\in\mathbb{N}_0$. Assume now that $\omega(eQ+M\omega)>0$. Then, the function

$$A:(|\omega|,\infty)\longrightarrow\mathbb{R},$$

$$m \mapsto -\frac{\omega(eQ+M\omega)}{\sqrt{m^2-\omega^2}} + M\sqrt{m^2-\omega^2} + \sqrt{\lambda_{\nu,\kappa,n}(m)^2 + M^2m^2 - \mu^2}$$

is continuous, satisfies $\lim_{m\searrow|\omega|}A(m)=-\infty$, $\lim_{m\to\infty}A(m)=\infty$ in view of (38). Hence, for every $N \in \mathbb{N}$ there is at least one $m_N \in (|\omega|,\infty)$ such that $A(m_N)=-N$ and therefore satisfies condition (37b). Since the function A is monotonously increasing in an interval $(|\omega|,|\omega|+\delta)$ for a sufficiently small $\delta>0$, it follows that for N large enough there is only one m_N satisfying $A(m_N)=-N$ and that the sequence $(m_N)_N$ is decreasing. □

Remark VI.3: The proof shows that for fixed m only a finite number of $\lambda_{\nu,\kappa,n}$ is allowed in order to satisfy condition (37b). The closer m is to $|\omega|$, the more (and the larger) values for $\lambda_{\nu,\kappa,n}$ are allowed.

Remark VI.4: The condition $\omega(eQ+M\omega)>0$ is satisfied if the ratio eQ/κ is sufficiently small since

$$\begin{aligned}
\omega(eQ+M\omega) &= -\frac{a}{(a^2+M^2)^2}(\kappa a + eQM)(eQa-\kappa M)\\
&= \frac{a}{(a^2+M^2)^2}[aM\kappa^2 + eQ(M^2-a^2)\kappa - aMe^2Q^2]\\
&= \frac{a^2M}{(a^2+M^2)^2}\left[\left(\kappa - \frac{eQa}{2M} + \frac{eQM}{2a}\right)^2 - \frac{e^2Q^2}{4}\left(\left(\frac{a}{M}-\frac{M}{a}\right)^2+4\right)\right]\\
&= -\frac{a^2\kappa^2M}{4(a^2+M^2)^2}\left[\left(\frac{2eQ}{\kappa} + \left(\frac{a}{M}-\frac{M}{a}\right)\right)^2 - \left(4+\left(\frac{a}{M}-\frac{M}{a}\right)^2\right)\right].
\end{aligned}$$

Remark VI.5: Let ω be an energy eigenvalue, $m \in \{m_N : N \in \mathbb{N}\}$ (see Theorem VI.1), and $f^{\nu,\kappa,n}$ the eigenfunctions of $H_{\nu,\kappa,n}$. If we set

$$\begin{pmatrix} X_+^{\nu,\kappa,n}(r) \\ X_-^{\nu,\kappa,n}(r) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} i & -1 \\ -i & -1 \end{pmatrix}\begin{pmatrix} f_1^{\nu,\kappa,n}(x) \\ f_2^{\nu,\kappa,n}(x), \end{pmatrix},$$

then

$$\hat{\Psi}(r,\theta,\phi,t) = \exp(-i\omega t)\exp(-i\kappa\varphi)\begin{pmatrix} X_-^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta) \\ X_+^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta) \\ X_+^{\nu,\kappa,n}(r)g_2^{\nu,\kappa,n}(\theta) \\ X_-^{\nu,\kappa,n}(r)g_1^{\nu,\kappa,n}(\theta) \end{pmatrix}$$

is a time-periodic solution of (1).

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Symmetries of the Robinson-Trautman equation

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We study point symmetries of the Robinson-Trautman equation. The cases of one- and two-dimensional algebras of infinitesimal symmetries are discussed in detail. The corresponding symmetry reductions of the equation are given. Higher dimensional symmetries are shortly discussed. It turns out that all known exact solutions of the Robinson-Trautman equation are symmetric. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2359139]

I. INTRODUCTION

In 1960, Robinson and Trautman introduced[1] a class of space-times admitting a diverging shear- and twist-free congruence of null geodesics. Such space-times, if asymptotically Minkowskian, are believed to describe gravitational radiation outgoing from spatially bounded sources. Recent numerical results suggest that the Robinson-Trautman metrics can be used to estimate the mass loss during the final phase of the collision of two black holes.[2] There are also suggestions that the subclass of the so called C-metrics[3] (and their twisting generalizations[4]) can describe space-times containing accelerating black holes.[5–8]

In terms of standard coordinates $u, r, \xi, \overline{\xi}$, where u and r are real and ξ is complex, the Robinson-Trautman metrics are given by[9]

$$g = 2\,\mathrm{d}u(H\,\mathrm{d}u + \mathrm{d}r) - 2r^2P^{-2}\,\mathrm{d}\xi\,\mathrm{d}\overline{\xi}. \tag{1}$$

The function P is independent of r. Vacuum Einstein equations imply

$$H = -r\partial_u \ln P - m(u)/r + P^2\partial_\xi\partial_{\overline{\xi}}\ln P \tag{2}$$

and a fourth order equation for P, referred to as the Robinson-Trautman equation:

$$P^2\partial_\xi\partial_{\overline{\xi}}(P^2\partial_\xi\partial_{\overline{\xi}}\ln P) + 3m\partial_u(\ln P) - \partial_u m = 0. \tag{3}$$

Using coordinate freedom m can be transformed to the value ± 1 or 0. The Gaussian curvature K of surfaces of constant u and r is given by

$$K = 2P^2\partial_\xi\partial_{\overline{\xi}}\ln P. \tag{4}$$

The existence of asymptotically flat Robinson-Trautman metrics has been recently examined.[10–12] Also, their large u asymptotic behavior is known.[13,14] These results, however, do not give any hint of how to look for explicit solutions. Only a few of them are known since 1960, none of them being asymptotically flat except for the cases of the Minkowski and the Schwarzschild metrics.

Assuming asymptotic flatness of metrics (1), the Bondi energy,[15,16] the Bondi mass aspect, and the news function were found in terms of P.[11,17–19] The asymptotic flatness of (1) with positive m follows from the assumption that in the gauge $m=1$ the function $\hat{P}=P(1+1/2\xi\overline{\xi})^{-1}$ is positive and regular on $R\times S_2$, ξ being interpreted as a complex stereographic coordinate on S_2.

The subclass of metrics with $m=0$ is characterized by the fact that K is a solution of the Laplace equation, so K must be either constant or singular. No nontrivial asymptotically flat metric exists in this subclass.

In the present paper we consider symmetries of the Robinson-Trautman equation and classify the conjugacy classes of one- and two-dimensional symmetry algebras. We find symmetry reductions of Eq. (3) for solutions preserved by these algebras. Some of these solutions might correspond to asymptotically flat metrics with a simple dependence on the time u. This research may also be of help for studying the numerical solutions of the Robinson-Trautman equation, providing natural ansatzes with smaller number of variables than in generic situations.

II. SYMMETRY TRANSFORMATIONS FOR $m \neq 0$

Suppose $m \neq 0$ and consider Eq. (3) in the gauge $m=1$,

$$P^2 \partial_\xi \partial_{\bar{\xi}} (P^2 \partial_\xi \partial_{\bar{\xi}} \ln P) + 3 \partial_u \ln P = 0. \tag{5}$$

It is easy to prove that (5) is invariant with respect to the following point transformations:

$$\begin{aligned} u &\mapsto u' = a^4 u + b, \\ \xi &\mapsto \xi' = f(\xi), \\ P &\mapsto P' = a^{-1} |f_{,\xi}| P, \end{aligned} \tag{6}$$

where $a \neq 0$ and b are real constants and f is a holomorphic function of ξ and $f_{,\xi} \neq 0$. If (6) is supplemented by

$$r' = a^2 r, \tag{7}$$

the corresponding metric transforms as $g \mapsto a^6 g$. Thus, (6) together with (7) induces a homothety of the metric. It is an isometry when $a=1$.

Infinitesimal transformations corresponding to (6) are given by the vector field

$$k = (4Au + B)\partial_u + F(\xi)\partial_\xi + \overline{F}(\bar{\xi})\partial_{\bar{\xi}} + (\operatorname{Re} F_{,\xi} - A) P \partial_P, \tag{8}$$

where A and B are real constants and F is a holomorphic function of ξ. These fields form the symmetry algebra $\mathfrak{g}$.

Solutions of (3) invariant with respect to (8) have to satisfy the following linear equation:

$$(4Au + B) P_{,u} + F P_{,\xi} + \overline{F} P_{,\bar{\xi}} + (A - \operatorname{Re} F_{,\xi}) P = 0. \tag{9}$$

We will perform the symmetry reduction of (5), assuming that its solution is preserved by vector fields (8) forming a one- or two-dimensional subalgebra of $\mathfrak{g}$ (higher-dimensional subalgebras will also be discussed shortly.) First, we will classify these subalgebras under the action of the pseudogroup of transformations (6). This way we will obtain the conjugacy classes (CC) of one- and two-dimensional subalgebras of $\mathfrak{g}$.

III. SOLUTIONS WITH ONE OR TWO SYMMETRIES

Consider a one-dimensional algebra generated by a vector field (8). Applying an appropriate transformation (6), we can simplify the coefficients A and B and the function F, obtaining one representative of each conjugacy class. For instance, if $A=0$, $B \neq 0$, and $F \neq 0$, we can scale u and ξ so that $B=1$ and $F=\xi$. This leads to

$$k = \partial_u + \xi \partial_\xi + \bar{\xi} \partial_{\bar{\xi}} + P \partial_P. \tag{10}$$

In the same way we can distinguish five conjugacy classes that are listed in Table I, together with corresponding vector k, the form of the invariant solution P, and the reduced Robinson-Trautman equation. Whenever it is needed, we explicitly write the definition of the new variable $z(u, \xi)$

TABLE I. Invariant solutions with single symmetry.

CC	k	P	RT equation
1	∂_u	$p(\xi,\overline{\xi})$	$p^2\partial_\xi\partial_{\overline{\xi}}\ln p=\mathrm{Re}\,\xi$
2	$4u\partial_u-P\partial_P$	$u^{-1/4}p(\xi,\overline{\xi})$	$p^2\partial_\xi\partial_{\overline{\xi}}(p^2\partial_\xi\partial_{\overline{\xi}}\ln p)=\frac{3}{4}$
3	$\partial_u-\xi\partial_\xi-\overline{\xi}\partial_{\overline{\xi}}-P\partial_P$	$e^u p(z,\overline{z})$	$p^2\partial_z\partial_{\overline{z}}(p^2\partial_z\partial_{\overline{z}}\ln p)-3(z\partial_z+\overline{z}\partial_{\overline{z}})\ln p+3=0,\ z=e^{-u}\xi$
4	∂_y	$p(u,x)$	$p^2\partial_x^2(p^2\partial_x^2\ln p)+3\partial_u\ln p=0$
5	$4Au\partial_u+\xi\partial_\xi+\overline{\xi}\partial_{\overline{\xi}}+P(1-A)\partial_P$	$u^{(1-A)/4A}p(z,\overline{z})$	$4Ap^2\partial_z\partial_{\overline{z}}(p^2\partial_z\partial_{\overline{z}}\ln p)+3(A-1)+3(z\partial_z+\overline{z}\partial_{\overline{z}})\ln p=0,$ $z=u^{-(4A)^{-1}}\xi$

appearing in the invariant solution. Throughout the text, we use x and y to denote, respectively, the real and imaginary parts of ξ.

Consider now the case of two-dimensional subalgebra $\mathfrak{g}_2$ of $\mathfrak{g}$. We denote the basis vectors of $\mathfrak{g}_2$ by k_1 and k_2. There are two nonisomorphic two-dimensional Lie algebras such that either

$$[k_1,k_2]=0 \tag{11}$$

or

$$[k_1,k_2]=k_2. \tag{12}$$

The Lie bracket of two fields given by (8) reads as

$$[k_1,k_2]=4(B_1A_2-B_2A_1)\partial_u+(F_1F_{2,\xi}-F_2F_{1,\xi})\partial_\xi+(\overline{F}_1\overline{F}_{2,\overline{\xi}}-\overline{F}_2\overline{F}_{1,\overline{\xi}})\partial_{\overline{\xi}}+P\,\mathrm{Re}(F_1F_{2,\xi\xi}-F_2F_{1,\xi\xi})\partial_P \tag{13}$$

where the indices 1,2 refer to vectors k_1, k_2, respectively.

In the Abelian case, Eq. (11) implies

$$A_1B_2=A_2B_1, \tag{14a}$$

$$F_1F_{2,\xi}=F_2F_{1,\xi}, \tag{14b}$$

$$\mathrm{Re}(F_1F_{2,\xi\xi}-F_2F_{1,\xi\xi})=0. \tag{14c}$$

It follows from (14b) that F_1 is proportional to F_2 and (14c) is satisfied.

Due to (14a) we can assume without loss of generality that $A_2=B_2=0$. Then $F_2\neq 0$, and using the gauge freedom in ξ we can set $F_2=i$. Then $F_1=C=\mathrm{const}\in R$ follows from (14b) and the remaining freedom in the choice of k_1. Therefore, the symmetry generators are

$$k_1=(4Au+B)\partial_u+C\partial_x-AP\partial_P,\quad k_2=\partial_y. \tag{15}$$

The invariance of a solution P of (5) with respect to k_2 implies

$$P=p(u,x). \tag{16}$$

Invariance with respect to k_1 gives

$$(4Au+B)P_{,u}+CP_{,x}=-AP. \tag{17}$$

Depending on values of A, B, and C, we can distinguish five conjugacy classes of two-dimensional Abelian subalgebras of $\mathfrak{g}$. They are listed in Table II. (Here, as well as in Tables III and IV, the symbol p' denotes a derivative of p with respect to its argument.)

In the non-Abelian case, Eq. (12) gives

TABLE II. Invariant solutions with two Abelian symmetries.

CC	k_1	k_2	P	RT equation
A.1	∂_u	∂_y	$p(x)$	$p^2(\ln p)''=x$
A.2	∂_x	∂_y	$p(u)$	$p'=0$
A.3	$\partial_u+\partial_x$	∂_y	$p(u-x)$	$p^2(p^2(\ln p)'')''+3(\ln p)'=0$
A.4	$4u\partial_u-P\partial_P$	∂_y	$u^{-1/4}p(x)$	$p^2(p^2(\ln p)'')''=\frac{3}{4}$
A.5	$4Au\partial_u+\partial_x-AP\partial_P$	∂_y	$u^{-1/4}p((4A)^{-1}\ln u-x)$	$p^2(p^2(\ln p)'')''+\frac{3}{4A}(\ln p)'=\frac{3}{4}$

$$4(A_2B_1-A_1B_2)=4A_2u+B_2, \tag{18a}$$

$$F_1F_{2,\xi}-F_2F_{1,\xi}=F_2, \tag{18b}$$

$$P\,\mathrm{Re}(F_1F_{2,\xi\xi}-F_2F_{1,\xi\bar{\xi}})=P(\mathrm{Re}\,F_{2,\xi}-A_2). \tag{18c}$$

It follows from (18a) that

$$A_2=0,\quad B_2(1+4A_1)=0. \tag{19}$$

Differentiating (18b) and its complex conjugate, we conclude that (18c) follows from (18b). Proceeding as in the Abelian case, we obtain results summarized in Table III.

IV. SOLUTIONS WITH MORE SYMMETRIES

All Lie algebras of dimension greater than three contain a three-dimensional subalgebra. Let k_i, $i=1,2,3$ be its generators. In the case of Bianchi type *VIII* or *IX*, it follows from (13) that $A_i=B_i=0$. Then the fields k_1, k_2, and k_3 are tangent to a two-dimensional surface and invariant solutions are excluded. For all other Bianchi types, the algebra contains a two-dimensional Abelian subalgebra. One can construct invariant solutions as special cases of those described in Table II. After lengthy calculations one obtains only the trivial solution $P=\mathrm{const}$ or $P=\mathrm{const}\cdot x^{3/2}$ given by Robinson and Trautman.[20] These are also solutions of the Robinson-Trautman equation for $m=0$. Thus, the assumption of three or more symmetries does not lead to any new interesting solutions.

V. SYMMETRY TRANSFORMATIONS FOR $m=0$

Suppose now that $m=0$. In this case Eq. (3) can be integrated to a second order equation,

$$P^2\partial_\xi\partial_{\bar{\xi}}\ln P=\mathrm{Re}\,\phi(u,\xi), \tag{20}$$

where ϕ is holomorphic with respect to ξ. If $\phi_{,\xi}\neq 0$, one can transform (20) to the equation[9]

TABLE III. Invariant solutions with two non-Abelian symmetries.

CC	k_1	k_2	P	RT equation
NA.1	$\epsilon\partial_u-x\partial_x-y\partial_y-P\partial_P$, $\epsilon=0$ or $\epsilon=1$	∂_y	$xp(u+\epsilon\ln x)$	$\epsilon[p^3(p'''-2p'''-p''+2p')$ $-p^2(p''^2+2p'p''+p'^2)]+3(\ln p)'=0$
NA.2	$4Au\partial_u-x\partial_x-y\partial_y-(1+A)P\partial_P$	∂_y	$u^{-\frac{1+A}{4A}}p(\underbrace{u^{\frac{1}{4A}}x}_{X})$	$p^2(p^2(\ln p)'')''+3X(\ln p)'=3(1+A)$
NA.3	$-u\partial_u+\partial_x+\frac{1}{4}P\partial_P$	∂_u	$p(x)$	$p^2(\ln p)''=x$
NA.4	$-u\partial_u+\partial_x+\frac{1}{4}P\partial_P$	$\partial_u+e^{\xi}\partial_\xi+e^{\bar{\xi}}\partial_{\bar{\xi}}$ $+P\,\mathrm{Re}\,e^{\xi}\partial_P$	$u^{-1/4}\lvert 1+u^{-1}e^{-\xi}\rvert^{3/4}p(z)$, $z=\frac{1+u^{-1}e^{-\xi}}{1+u^{-1}e^{-\bar{\xi}}}$.	$p^2(p^2(\ln p)'')''+\frac{1}{4}p^4(\ln p)''$ $-36\cos z+48(\ln p)'\sin z=0$

TABLE IV. Invariant solutions for $m=0$.

CC	k	P	RT equation
0.1	$i(\xi^2-1)\partial_\xi - i(\bar{\xi}^2-1)\partial_{\bar{\xi}}$	$p(r)$, $r=\lvert\frac{\xi+1}{\xi-1}\rvert$	$\frac{1}{4}(1-r^2)^2\frac{1}{r}(r(\ln p)')' - \frac{3}{8}+p^{-2}=0$
0.2	$\xi\partial_\xi + \bar{\xi}\partial_{\bar{\xi}}$	$p(\phi)$, $\xi=re^{i\phi}$	$\frac{1}{4}\cos^2\phi(\ln p)'' - \frac{3}{8}+p^{-2}=0$
0.3	$i(\partial_\xi - \partial_{\bar{\xi}})$	$p(x)$	$\frac{1}{4}x^2(\ln p)'' - \frac{3}{8}+p^{-2}=0$

$$P^2\partial_\xi\partial_{\bar{\xi}}\ln P = -\operatorname{Re}\xi. \tag{21}$$

Substituting

$$P = x^{3/2}p(\xi,\bar{\xi}) \tag{22}$$

into (21), we get

$$p^2(\Delta \ln p - 3/8) = -1. \tag{23}$$

Here $\Delta = x^2\partial_\xi\partial_{\bar{\xi}}$ is the Laplace operator on a pseudosphere with the metric

$$g = \frac{d\xi\, d\bar{\xi}}{x^2}, \tag{24}$$

which can be put into the standard form

$$g = \frac{4\, d\zeta\, d\bar{\zeta}}{(1-\zeta\bar{\zeta})^2}, \tag{25}$$

by means of the transformation $\zeta=(\xi+1)/(\xi-1)$. The operator Δ is preserved by the transformations

$$\xi \mapsto \xi' = \frac{a\xi+ib}{ic\xi+d}, \quad a,b,c,d \in R, \tag{26}$$

corresponding to an action of $\mathrm{SL}(2,R)$ on the pseudosphere.

It follows from (26) that infinitesimal transformations are generated by vector fields of the form

$$k = (iA\xi^2 + B\xi + iC)\partial_\xi + \text{c.c.}, \tag{27}$$

where A, B, and C are real constants. Using symmetry transformations, we can distinguish three conjugacy classes of one-dimensional subalgebras of the symmetry algebra for $m=0$ (Table IV).

Given a solution of (21), we can apply the transformation $\xi'=f(u,\xi)$ to obtain a class of solutions of (20).

Note that the only solution of (23) invariant with respect to two independent fields of the form (27) is $p=\sqrt{8/3}$, which gives the well known solution $P=\text{const}\cdot x^{3/2}$ found by Robinson and Trautman.[20]

VI. DISCUSSION

We have examined point symmetries of the Robinson-Trautman equation (3). Forms of solutions in the case of one or two symmetries were given, as well as the corresponding reduced equations. Note that all known[9] exact solutions of (3) have two or three symmetries and belong to one of the cases considered here.

The assumption of symmetry does not seem to exclude regular solutions corresponding to asymptotically flat metrics. The coordinates $\xi,\bar{\xi}$ used in Tables I–III can differ from the hypotheti-

cal Bondi-Sachs coordinates. For instance, in case 4 of Table I, the function P depends on x, which becomes $\ln|\xi'|$ under the transformation $\xi \mapsto \xi' = \exp(\xi)$. To achieve regularity of $\hat{P}$, one should demand that P is everywhere finite, positive, and

$$\lim_{|\xi'|\to\infty} |\xi'|^{-1} P = a(u), \quad \lim_{|\xi'|\to 0} |\xi'| P = b(u), \tag{28}$$

for some positive functions a and b. Rewriting (28) in terms of ξ, we get

$$\lim_{x\to-\infty} e^{x} P = a(u), \quad \lim_{x\to\infty} e^{-x} P = b(u), \tag{29}$$

which means that P behaves like $e^{|x|} f(u)$ for large $|x|$.

In the case A.3 (see Table II), the Robinson-Trautman equation can be solved analytically. This way one obtains the so-called C-metrics. A possible physical interpretation of these metrics as well as their twisting generalizations (the spinning C-metrics) was given recently.[5–8]

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Goldfishing: A new solvable many-body problem

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A recent technique allows one to identify and investigate *solvable* dynamical systems naturally interpretable as classical many-body problems, being characterized by equations of motion of Newtonian type (generally in two-dimensional space). In this paper we tersely review results previously obtained in this manner and present novel findings of this kind: mainly *solvable* variants of the *goldfish* many-body model, including models that feature *isochronous* classes of *completely periodic* solutions. Different formulations of these models are presented. The behavior of one of these *isochronous* dynamical systems in the neighborhood of its equilibrium configuration is investigated, and in this manner some remarkable *Diophantine* findings are obtained. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Over a quarter century ago a class of *solvable* dynamical systems was introduced, naturally interpretable as classical many-body problems characterized by Newtonian equations of motion ("accelerations proportional to forces:" with appropriate velocity-dependent one- and two-body forces).[2]

Terminology: A dynamical system is called *solvable* whenever the solution of its initial-value problem can be reduced to purely algebraic operations, typically to finding the zeros of a polynomial the coefficients of which are explicitly known in terms of the initial data and of time, or equivalently to finding the eigenvalues of a matrix the time evolution of which is explicitly known.

The simplest example of this kind is characterized by the equations of motion

$$\ddot{z}_n = i\omega\dot{z}_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m}{z_n - z_m}. \tag{1}$$

Notation: Here and hereafter superimposed dots denote differentiations with respect to the (*real*) independent variable t ("time"), i is the imaginary unit ($i^2=-1$), the dependent variables $z_n \equiv z_n(t)$ are generally *complex*, N is a positive integer ($N \geqslant 2$), indices such as n, m generally range from 1 to N (unless otherwise stated), and ω is a *real* constant (for definiteness, *nonnegative*) to which (whenever this constant does not vanish) is associated the basic period

$$T = \frac{2\pi}{\omega}. \tag{2}$$

The model with $\omega=0$ might be considered the simplest one; but the model with $\omega>0$ has the remarkable property to be *isochronous* and is in any case related by a simple transformation to the same model with $\omega=0$, see the following

Remark 1.1: The model characterized by the equations of motion (1) with $\omega=0$, i.e.,

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$$\zeta_n'' = 2 \sum_{m=1, m\neq n}^{N} \frac{\zeta_n' \zeta_m'}{\zeta_n - \zeta_m} \tag{3}$$

(where we conveniently changed notation, denoting the dependent variables as $\zeta_n(\tau)$ and differentiations with respect to the independent variable τ by appended primes), is related to the model characterized by the equations of motion

$$\ddot{z}_n = (2\lambda+1) i\omega \dot{z}_n + \lambda(\lambda+1)\omega^2 z_n + 2 \sum_{m=1, m\neq n}^{N} \frac{(\dot{z}_n - i\lambda\omega z_n)(\dot{z}_m - i\lambda\omega z_m)}{z_n - z_m} \tag{4}$$

(which reduce to (1) for $\lambda = 0$) via the following change of dependent and independent variables:

$$z_n(t) = \exp(i\lambda\omega t)\zeta_n(\tau), \quad \tau = \frac{\exp(i\omega t) - 1}{i\omega}. \tag{5}$$

This transformation, introduced in Ref. 3 and often referred to as "the trick," has been subsequently largely exploited to create "ω-modified" dynamical systems that generally feature (provided λ is *real* and *rational*) the remarkable property to be *isochronous*, with the period T, see (2), or an integer multiple of it: see for instance Refs. 5, 6, 13, 7, 8, 17, 1, 15, 11, 12, 9, 10, and 21 (and additional references quoted in these papers). This can in particular be seen as the cause underlying the *isochronous* character of the *goldfish* model (1) with $\omega > 0$, as indeed shown by its solution, see the following. ■

Terminology: A dynamical system is called *isochronous* if it features in its phase space an *open* region (having therefore *full dimensionality*) where *all* its solutions are *completely periodic* (i.e., periodic in *all* degrees of freedom) with the *same* period (independent of the initial data, provided they are inside the *isochronicity* region). And let us moreover emphasize that dynamical systems obtained via the trick, see (5), from *completely integrable*, or *solvable*, systems, often feature the even more remarkable property that *all* their *nonsingular* solutions (namely, not only those in some appropriate subregion of their natural phase space) are *completely periodic* with periods that are *integer multiples* of T, see (2), besides being independent of the initial data for sufficiently small variations of these data (why this is so is explained in the literature, see for instance Ref. 6). It is therefore justified to consider them as instances of "nonlinear harmonic oscillators."[16]

Remark 1.2: The Newtonian equations of motion (1) are yielded in the standard manner by the *Hamiltonian*

$$H(\underline{p},\underline{z}) = \sum_{n=1}^{N} \left[\frac{i\omega z_n}{c} + \exp(cp_n) \prod_{m=1, m\neq n}^{N} \frac{1}{z_n - z_m} \right], \tag{6}$$

where c is an *arbitrary* (nonvanishing) constant. Some, but not all, of the Newtonian equations of motion written in the following are as well *Hamiltonian*, namely they can be obtained in the standard manner from an appropriate *Hamiltonian*. But in this paper we do not elaborate any further on this aspect of the results presented herein.[19] ■

Remark 1.3: Clearly (see (1) and (4) with $\lambda \neq -\frac{1}{2}$) if ω does *not* vanish the time evolutions of the dependent variables $z_n(t)$ *necessarily* take place in the *complex* z-plane. Only in the special case when $\omega = 0$ (or $\lambda = -\frac{1}{2}$) the motion of the N coordinates $z_n(t)$ could be limited to the *real* axis. In the following (as already mentioned earlier) we assume that the coordinates $z_n(t)$ are *complex:* motions taking place in the (*complex*) plane are in any case more interesting (see also the following *Remark 1.4*) than those limited to the *real* axis. ■

Remark 1.4: By identifying the *complex* z-plane with the *real* ("physical") horizontal plane via the correspondence $z \leftrightarrow \vec{r}$ with the assignment

$$z = x + iy, \quad \vec{r} = (x, y, 0), \tag{7}$$

the Newtonian equations of motion (4) take the following *rotation-invariant* form:

$$\ddot{\vec{r}}_n = (2\lambda+1)\omega\hat{k}\wedge\dot{\vec{r}}_n + \lambda(\lambda+1)\omega^2\vec{r}_n + 2\sum_{m=1,m\neq n}^{N} r_{nm}^{-2}\{(\dot{\vec{r}}-i\lambda\omega\vec{r}_n)[(\dot{\vec{r}}_m-i\lambda\omega\vec{r}_m)\cdot\vec{r}_{nm}] + (\dot{\vec{r}}_m-i\lambda\omega\vec{r}_m)$$

$$\times[(\dot{\vec{r}}_n-i\lambda\omega\vec{r}_n)\cdot\vec{r}_{nm}] - \vec{r}_{nm}[(\dot{\vec{r}}_n-i\lambda\omega\vec{r}_n)\cdot(\dot{\vec{r}}_m-i\lambda\omega\vec{r}_m)]\}, \tag{8}$$

where $\hat{k}=(0,0,1)$ is the unit vector orthogonal to the horizontal plane, the symbols $\wedge$ respectively $\cdot$ sandwiched between two vectors denote the standard vector, respectively, scalar products, and we use the short-hand notation $\vec{r}_{nm}\equiv\vec{r}_n-\vec{r}_m$ entailing $r_{nm}^2=r_n^2+r_m^2-2\vec{r}_n\cdot\vec{r}_m$. The models considered in the following could be similarly reformulated in terms of motions in the physical horizontal plane; we will refrain from doing so, leaving this task to the interested reader, who will find guidance to perform this transition, for instance, in Ref. 4 or in Chapter 4 ("Solvable and/or integrable many-body problems in the plane, obtained by complexification") of Ref. 6 or in Ref. 13. But we will hereafter feel free to refer to the coordinates $z_n(t)$ as describing the positions of point *particles* moving in the (*complex*) z-plane, in the context of a many-body dynamics characterized by Newtonian equations of motion. ■

The *solvable* character of the model (1) is demonstrated by the following result:[2,6] *the solution of the initial-value problem for the Newtonian equations of motion (1) is given by the N roots* $z_n(t)$ *of the following algebraic equation in the variable* z:

$$\sum_{n=1}^{N}\frac{\dot{z}_n(0)}{z-z_n(0)} = \frac{i\omega}{\exp(i\omega t)-1}. \tag{9}$$

Note that, by multiplying this algebraic equation by $\Pi_{n=1}^{N}[z-z_n(0)]$, one transforms it into a polynomial equation of degree N in the variable z, evidencing thereby that it indeed has generally N roots. Also note that, provided $\omega>0$, the time evolutions of *all* the coefficients of this polynomial are *periodic* with period T, see (2), entailing that the time evolution of each particle coordinate $z_n(t)$ is as well *periodic* with such a period (in an *open* region of phase space), or possibly (in every other region of phase space) with an *integer multiple* of this period (not exceeding N, indeed generally much smaller[21]) due to the possibility that the zeros of the polynomial get exchanged among each other through the motion.

The neat character of the Newtonian equations of motion (1), as well as their Hamiltonian character, see (6), and their physical version, see (8) with $\lambda=0$, suggested attributing (in the context of a conference devoted to the celebration of the 60th birthday of V. E. Zakharov[5]) to this many-body problem the honorary name of "goldfish" (this name was originally attributed to model (1) with $\omega=0$, but is as well used for this model with *nonvanishing real* ω, having the additional remarkable property to be *isochronous*; anyway these two models are related by the simple transformation (5) with $\lambda=0$). This terminology originated from the following description of the search for integrable systems given by V. E. Zakharov: "A mathematician, using the dressing method to find a new integrable system, could be compared with a fisherman, plunging his net into the sea. He does not know what a fish he will pull out. He hopes to catch a goldfish, of course. But too often his catch is something that could not be used for any known to him purpose. He invents more and more sophisticated nets and equipments and plunges all that deeper and deeper. As a result he pulls on the shore after a hard work more and more strange creatures. He should not despair, nevertheless. The strange creatures may be interesting enough if you are not too pragmatic. And who knows how deep in the sea do goldfishes live?"[28] Subsequently the name "goldfish" has been, more generally, used to refer to various variants (generally *isochronous*, but possibly *not* integrable) of the original model (1): see, for instance, Refs. 14, 13, 7, 8, 17, and 1. The title of the present paper reflects as well this language and refers to a current development—as detailed in the following—that calls to mind the research pattern poetically described by V. E. Zakharov, as quoted earlier.

Indeed recently a direct technique to manufacture *solvable* dynamical systems has been

used[13,7,8,17,1] to identify many-body problems, many of which can be considered variants of the basic *goldfish* model (1). This technique is tersely reviewed in Sec. II, where we also list the main *solvable* many-body problems obtained in this manner and we report the additional, novel results of this kind obtained in the present paper. As explained in the following, a natural first outcome of this technique is to yield *solvable* many-body problems characterized by Newtonian equations of motion with one- and two-body forces, the latter of which however feature generally multiplicative coefficients, playing the role of "coupling constants" but being instead time-dependent, their time evolution being characterized by a system of coupled ODEs that also contain the independent variables $z_n(t)$ identifying the particle positions in the many-body context. Only in exceptional cases—each of which seems to require a "miracle" to occur—it is possible to get rid of these time-dependent coefficients via an appropriate *ansatz* and to thereby identify a proper *solvable* many-body problem involving *only* the particle coordinates $z_n(t)$ and no additional "auxiliary variables." Hence this research strategy has so far proceeded via a sequence of contributions[13,7,8,17,1] each of which has essentially identified (and investigated) some new *solvable* many-body problem obtained in this manner; and the present paper is one more step in this sequence, its very title echoing this characteristic. And let us mention immediately—for the hasty browser—that the (in our opinion) most interesting *novel* finding reported in the following is the *isochronous N*-body model problem characterized by the Newtonian equations of motion (52) and its solution as given by **Proposition 2.7**, as well as its alternative formulation ((66a)–(66c)) the solution of which is provided by **Proposition 2.11**. Likewise, the hasty browser only interested in the *Diophantine* findings may go immediately to the end of Sec. II.

The developments that yield the main novel results reported in Sec. II are detailed in Sec. III. At the end of Sec. II we also exhibit alternative versions—obtained, and more fully presented, in Sec. IV—of the main *solvable* models identified in this paper, as well as some *Diophantine* findings obtained in Sec. V by investigating the behavior in the neighborhood of its equilibrium configuration of the (alternative version of the) main new *solvable isochronous* system identified in this paper. Hints regarding future developments are proffered in Sec. VI, and a list of useful relations is provided in the Appendix.

II. RESULTS

The starting point of this approach is a *solvable* matrix evolution equation, say

$$\ddot{U} = F(U, \dot{U}). \tag{10}$$

Here and hereafter $U = U(t)$ is a time-dependent $N \times N$ matrix, and the assumed *solvability* of this matrix ODE entails the possibility to write in *explicit* form the solution of the corresponding initial-value problem.

The function $F(U, \dot{U})$ is assumed not to depend on any other matrix besides U and $\dot{U}$ (the ordering of which in its definition is of course relevant, since these two matrices generally do not commute), so that there hold the relation

$$RF(U, \dot{U})R^{-1} = F(RUR^{-1}, R\dot{U}R^{-1}), \tag{11}$$

for any (invertible) $N \times N$ matrix R.

The main idea is then quite simple: *to investigate the time evolution of the eigenvalues* $z_n(t)$ *of the matrix* $U(t)$. And let us immediately emphasize, before proceeding to exhibit the form taken by the equations that describe this time evolution, that whenever the time evolution of the $N \times N$ matrix $U(t)$ is *periodic* with a period T, the corresponding evolution of each of its eigenvalues—unless it runs into a singularity (this may happen, but only for special, *nongeneric*, initial data)—is obviously as well *periodic* with the same period T or with a period $\widetilde{T} = pT$ with p a *positive integer* (again, due to the possibility that through the time evolution some eigenvalues get exchanged: this entails that the largest possible value of p is N, although generally it is much less, see for instance Ref. 21).

To investigate the time evolution of the eigenvalues $z_n(t)$ of $U(t)$ we set

$$U(t) = R(t)Z(t)[R(t)]^{-1}, \quad Z(t) = \mathrm{diag}[z_n(t)], \tag{12}$$

and we take note of the consequential identities

$$\dot{U} = R\{\dot{Z} + [M,Z]\}R^{-1}, \tag{13a}$$

$$\ddot{U} = R\{\ddot{Z} + [\dot{M},Z] + 2[M,\dot{Z}] + [M,[M,Z]]\}R^{-1}, \tag{13b}$$

where we set

$$M = R^{-1}\dot{R}. \tag{14}$$

Notation: Here and hereafter $[A,B]$ denotes the commutator of the two matrices A and B,

$$[A,B] \equiv AB - BA. \tag{15}$$

Remark 2.1: The diagonalizing matrix R, see (12), is clearly defined up to multiplication from the right by an *arbitrary diagonal* $N \times N$ matrix D, hence the matrix M is defined up to the "gauge transformation"

$$M \mapsto D^{-1}MD + D^{-1}\dot{D}, \tag{16}$$

which, thanks to the *arbitrariness* of the *diagonal* matrix D, entails that the *diagonal* part of the matrix M can be assigned *arbitrarily* (of course modifying correspondingly its *off-diagonal* part). ■

Via (12) and (13) the *solvable* matrix ODE (10) becomes

$$\ddot{Z} + [\dot{M},Z] + 2[M,\dot{Z}] + [M,[M,Z]] = F(Z,\dot{Z} + [M,Z]), \tag{17}$$

hence by separating the diagonal and off-diagonal parts of this matrix ODE one immediately arrives at the following systems of (altogether N^2 coupled scalar) ODEs:

$$\ddot{z}_n = -2\sum_{m=1,m\neq n}^{N}(z_n - z_m)M_{nm}M_{mn} + [F(Z,\dot{Z} + [M,Z])]_{nn}, \tag{18a}$$

$$\dot{M}_{nm} = -2\frac{\dot{z}_n - \dot{z}_m}{z_n - z_m}M_{nm} - (\mu_n - \mu_m)M_{nm} + \sum_{\ell=1,\ell\neq m,n}^{N}\frac{z_n + z_m - 2z_\ell}{z_n - z_m}M_{n\ell}M_{\ell m} - \frac{[F(Z,\dot{Z} + [M,Z])]_{nm}}{z_n - z_m}, \quad n \neq m. \tag{18b}$$

Note that we denote the *diagonal* elements of the $N \times N$ matrix M as μ_n, $M_{nn}(t) \equiv \mu_n(t)$ (we never use the convention according to which repeated indices are summed upon), and recall that, as explained earlier (see *Remark 2.1*), their values can be chosen at our convenience; the rest of the notation is, we trust, self-evident. Note that (10) (a matrix evolution equation amounting to N^2 coupled ODEs), characterizing the time evolution of the N^2 matrix elements of the $N \times N$ matrix $U(t)$, has now been replaced by the system (18), amounting again altogether to $N + N(N-1) = N^2$ coupled ODEs, and characterizing the time evolution of the N eigenvalues $z_n(t)$ and of the $N(N-1)$ off-diagonal matrix elements $M_{nm}(t)$, $n \neq m$.

Because of the way these systems of ODEs have been derived they are, as it were by definition, *solvable*. And it is clear that the first system of N coupled ODEs, (18a), has indeed the structure of a Newtonian N-body problem characterizing the motion of the N particle coordinates $z_n(t)$, while the second system of $N(N-1)$ ODEs, (18b), characterizes the evolution of the $N(N$

-1) "auxiliary variables" $M_{nm}(t)$ (with $n \neq m$). It might be possible to attribute as well to these auxiliary variables $M_{nm}(t)$ a physical meaning in terms of internal ("spin") degrees of freedom: pioneering steps in this direction were made long ago, simultaneously and independently, by Gibbons and Hermsen[20] and by Stefan Wojciechowski.[26,27] As already mentioned, in the series of papers[13,7,8,17,1] of which the present one is a natural continuation a different goal has instead been sought: to identify cases in which, via an appropriate *ansatz* (expressing the auxiliary variables in terms of the particle coordinates, and possibly also of their derivatives: see the following), thanks to some "miraculous" identities, it is possible to satisfy *identically* the second system, (18b), namely to get rid altogether of the auxiliary variables, obtaining thereby from (18a) a genuine N-body problem characterized by Newtonian equations of motion involving *only* the particle coordinates $z_n(t)$. The possibility to do so depends on the specific choice of the original *solvable* matrix ODE (see (10); actually in some cases, see the following, it might be preferable to take as starting point a first-order matrix ODE or two coupled first-order matrix ODEs rather than a second-order matrix ODE), and moreover on the identification of an appropriate *ansatz:* general rules to identify a suitable combination of these two elements are not known, so the approach followed so far has been a trial and error one, which has yielded over time a few successes, as reported in previous papers[13,7,8,17,1] and in the present one. We now review tersely these previous results, and then report the novel ones.

In Ref. 13 the starting point of the treatment is the *linear* (and obviously *solvable*) second-order matrix ODE

$$\ddot{U} + a\dot{U} + bU = 0, \tag{19}$$

where a and b are two *arbitrary* constants, and the *solvable* many-body problems manufactured are well-known classical models[6] the *solvability* of which was already known thanks to the technique invented by M. A. Olshanetsky and A. M. Perelomov, which indeed has a close relationship to that described herein: see their original papers,[22,24,25] as well as Section 2.1.3.2 ("The technique of solution of Olshanetsky and Perelomov (OP)") of Ref. 6.

In Ref. 7 the starting point of the treatment is the *solvable* second-order matrix ODE

$$\ddot{U} = a\dot{U}U^{-1}\dot{U}, \tag{20}$$

and the *solvable* many-body problems manufactured are again well-known classical models the *solvability* of which was already known thanks to the technique invented by M. A. Olshanetsky and A. M. Perelomov, but they include in addition the following *generalized goldfish* model:

$$\ddot{z}_n = i\omega\dot{z}_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m}{z_n - z_m} + a\sum_{n=1}^{N} \frac{\dot{z}_n\dot{z}_m}{z_m}. \tag{21}$$

Here and in (20) a is an *arbitrary* (of course scalar) constant; it is plain that for $a=0$ the Newtonian equations of motion (21) coincide with those, (1), of the basic *goldfish* model. It has moreover been shown[7] that the *solvability* of this *generalized goldfish* model, (21), could be directly inferred from the *solvability* of the *goldfish* many-body model (1). The treatment can be easily extended to a more general (and *isochronous* if λ is *rational*) model bearing to (21) the same relation that (4) bears to (1).

In Ref. 8 the starting point of the treatment is the *solvable* second-order matrix ODE

$$\ddot{U} = a(\dot{U}U + U\dot{U}), \tag{22}$$

and the *solvable* many-body problem manufactured is characterized by the Newtonian equations of motion

$$\ddot{z}_n = 2a\dot{z}_n z_n + 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n\dot{z}_m}{z_n - z_m}. \tag{23}$$

Here a is again an *arbitrary* (of course scalar) constant, and these equations of motion constitute again a generalization of those of the (*nonisochronous goldfish*) model with $\omega=0$, to which they clearly reduce for $a=0$. An *isochronous* variant of these Newtonian equations of motion obtains via the trick (see (5) with $\lambda=1$):

$$\ddot{z}_n = 3i\omega\dot{z}_n + 2\omega^2 z_n + 2a(\dot{z}_n - i\omega z_n)z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - i\omega z_n)(\dot{z}_m - i\omega z_m)}{z_n - z_m}. \tag{24}$$

In Ref. 17 the starting point of the treatment is the *solvable* first-order matrix ODE,

$$\dot{U} = aU^2 + C, \tag{25}$$

where a is again an *arbitrary* scalar constant and C is an *arbitrary* constant matrix. Note that time-differentiation of this first-order matrix ODE reproduces the second-order matrix ODE (22); indeed the novelty of the results of Ref. 17 relative to those of Ref. 8 is *not* due to the selection of a different solvable matrix ODE as starting point of the treatment, but rather to the identification of a *different ansatz* to get rid of the auxiliary variables, yielding the *solvable* many-body problem characterized by the Newtonian equations of motion

$$\ddot{z}_n = 2a\dot{z}_n z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - az_n^2)(\dot{z}_m - az_m^2)}{z_n - z_m}. \tag{26}$$

These Newtonian equations of motion differ from (23), but they provide again a generalization of those of the (*nonisochronous*) *goldfish* model with $\omega=0$, to which they clearly reduce for $a=0$. And an *isochronous* variant of these Newtonian equations of motion obtains again via the trick (see (5) with $\lambda=1$):

$$\ddot{z}_n = 3i\omega\dot{z}_n + 2\omega^2 z_n + 2a(\dot{z}_n - i\omega z_n)z_n + 2\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n - i\omega z_n - az_n^2)(\dot{z}_m - i\omega z_m - az_m^2)}{z_n - z_m}. \tag{27}$$

In Ref. 1 the starting point of the treatment is the *solvable* system of two coupled first-order matrix ODEs,

$$\dot{U} = aU^2 + V, \quad \dot{V} = bV, \tag{28}$$

where a is again an *arbitrary* scalar constant and the scalar b might be an *arbitrarily* given function of time. Note that for $b=0$ this matrix ODE reduces to (25) (with $V=C$). The main contribution of Ref. 1 is to identify (and investigate) two *solvable* many-body problems. The first is characterized by the following (*autonomous*) Newtonian equations of motion:

$$\ddot{z}_n = 2a\dot{z}_n z_n + b[\dot{z}_n - az_n^2] + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n - az_n^2][\dot{z}_m - az_m^2]}{z_n - z_m}. \tag{29}$$

Here b is an *arbitrary* constant; clearly for $b=0$ this model reduces to (26). The second is characterized by the following (*autonomous*) Newtonian equations of motion (which obtains[1] via the trick from an appropriate time-dependent choice of the function $b(t)$ in (28)):

$$\ddot{z}_n = (3+k)i\omega\dot{z}_n + (2+k)\omega^2 z_n + a[2\dot{z}_n - (2+k)i\omega z_n]z_n + 2\sum_{m=1,m\neq n}^{N} \frac{[\dot{z}_n - i\omega z_n - az_n^2][\dot{z}_m - i\omega z_m - az_m^2]}{z_n - z_m}. \tag{30}$$

Here k is also an *arbitrary* constant, but the case with k a (*positive* or *negative*) *integer* is particularly interesting, since this model is then *isochronous* (with the single exception of the case

$k=-2$, when the solutions are instead *multiply periodic*). And note that this model reduces to (27) for $k=0$.

Let us now turn to the presentation of the *new* results that constitute the main contribution of the present paper.

The starting point is the following *solvable* system of two coupled first-order matrix ODEs:

$$\dot{U} = \alpha + \beta VU, \tag{31a}$$

$$\dot{V} = aV^2 + bV + c. \tag{31b}$$

Here α, β, a, b, c are five *scalar* quantities, and it is clear that this system is *solvable* (at least in the sense that its solution is achievable by quadratures) if the three parameters a, b, c, are all *constant* or if either a or c vanishes, while α, β can be two (*arbitrarily* assigned) functions of time: indeed the solution can then be obtained by first solving the second, (31b), of these two matrix ODEs, determining thereby explicitly $V(t)$, and by then solving the first, (31a), of these two matrix ODEs, which is linear in $U(t)$ and hence *solvable* (at least in the sense of being reducible to quadratures) once $V(t)$ is known. But in fact we shall need to consider this system of matrix ODEs only in some special cases, see the following.

Remark 2.2: It is clear that adding linear terms (namely, *arbitrary* constants times U or V) to the right-hand side of (31a) entails no significant generalization, since it corresponds to adding a scalar term to V in (31a) (which merely amounts to redefining the three constants a, b, c, in (31b)) or a scalar term to U in (31a) (which merely shifts all the eigenvalues of U by a constant). Likewise, as long as we restrict consideration to a constant β (as we will hereafter do), it is clear that no generality is lost by setting this constant to unity, as we will indeed hereafter do,

$$\beta = 1, \tag{31c}$$

since this merely amounts to a redefinition of V that can be compensated by appropriate modifications of the three constants a, b, c in (31b). And adding a term γVU to the right-hand side of (31a) entails no significant generalization, since it amounts to a change of the constant β and moreover to adding the term $\gamma[V,U]$, the presence of which on the right-hand side of (31a) has no effect on the eigenvalues of $U(t)$. Finally let us note that some of the constants we keep (such as α) or introduce in the following (such as ω) could be rescaled away: we prefer not to do so, because one forsakes in this manner the possibility to make quick dimensional checks of the equations one writes, and also to consider special cases in which some of these constants vanish. However at the end of this section, and in some of the following sections—when we obtain results the interest of which is presumably rather "mathematical" than "physical"—we get rid of all unessential constants and deal only with dimensionless quantities. ■

The system (31) can clearly be reformulated as a single second-order (and of course as well *solvable*) ODE for the matrix $U(t)$:

$$\ddot{U} = cU + (\dot{U} - \alpha)\{b - U^{-1}[a\alpha - (a+1)\dot{U}]\} \tag{32}$$

(to obtain this matrix ODE note first that (31a) with (31c) entails

$$V = (\dot{U} - \alpha)U^{-1}, \tag{33}$$

then time differentiate (31a), use (31b) to eliminate $\dot{V}$, and finally use (33) to eliminate V; note that to make these steps we assumed α to be time-independent, but we made no assumption on the time-dependence of a, b, c).

It can then be shown (see Sec. III) that via two (quite different) appropriate *ansatzen* two (quite different) *solvable* many-body problems can be manufactured.

The first (and less interesting) one of these two many-body systems obtains provided

$$b=0, \quad a=-\tfrac{1}{2}, \tag{34}$$

and is characterized by the following Newtonian equations of motion:

$$\ddot{z}_n = cz_n + \frac{\dot{z}_n^2-\alpha^2}{2z_n} - \frac{g^2}{2}\sum_{m=1,m\neq n}^{N}\frac{z_n(z_n+3z_m)}{(z_n-z_m)^3}, \tag{35}$$

where g is an *arbitrary* constant. Via the following redefinition of the dependent variables,

$$z_n(t) = w_n^2(t), \tag{36}$$

this system of ODEs gets reformulated as follows:

$$\ddot{w}_n = \frac{c}{2}w_n - \frac{\alpha^2}{4w_n^3} - \frac{g^2}{8}\sum_{m=1,m\neq n}^{N}\left[\frac{1}{(w_n-w_m)^3}+\frac{1}{(w_n+w_m)^3}\right], \tag{37}$$

and it is thereby recognized as a known system the *solvability* of which was established long ago.[23] Hence this case is not pursued in the following.

The second of these two *solvable* systems of ODEs obtains when c vanishes,

$$c=0, \tag{38}$$

and it reads as follows:

$$\ddot{z}_n = (\dot{z}_n-\alpha)\left[b+\frac{\alpha}{z_n}+(1+a)\sum_{m=1}^{N}\frac{\dot{z}_m-\alpha}{z_m}+2\sum_{m=1,m\neq n}^{N}\frac{\dot{z}_m-\alpha}{z_n-z_m}\right], \tag{39}$$

where b might also be time-dependent (see the following). In the *autonomous* case with constant $b=i\omega$, when this equation reads

$$\ddot{z}_n = (\dot{z}_n-\alpha)\left[i\omega+\frac{\alpha}{z_n}+(1+a)\sum_{m=1}^{N}\frac{\dot{z}_m-\alpha}{z_m}+2\sum_{m=1,m\neq n}^{N}\frac{\dot{z}_m-\alpha}{z_n-z_m}\right], \tag{40}$$

it can be clearly considered a generalized *goldfish* model: indeed for $\alpha=0$ and $a=-1$ this system reduces to (1). And more generally, whenever α vanishes, in which case this system reads

$$\ddot{z}_n = [i\omega+(1+a)S]\dot{z}_n + 2\sum_{m=1,m\neq n}^{N}\frac{\dot{z}_n\dot{z}_m}{z_n-z_m}, \tag{41a}$$

$$S = \sum_{n=1}^{N}\frac{\dot{z}_n}{z_n}, \tag{41b}$$

it can again be reduced (albeit less trivially so) to the standard *goldfish* model. Indeed it is easily seen (by dividing (41a) by z_n and summing over n from 1 to N) that the system of ODEs (41) entails

$$\dot{S}(t) = i\omega S + aS^2, \tag{42a}$$

hence

$$S(t) = S(0)\exp(i\omega t)\left[1-aS(0)\frac{\exp(i\omega t)-1}{i\omega}\right]^{-1}, \tag{42b}$$

hence (as the diligent reader will readily verify) via the change of dependent variable

$$z_n(t) = \zeta_n(\tau), \quad \tau = \frac{1}{S(0)}\left\{\left[1 - aS(0)\frac{\exp(i\omega t) - 1}{i\omega}\right]^{-1/a} - 1\right\} \tag{43}$$

the system of ODEs (41) gets transformed into the *goldfish* system (3).

But when α does *not* vanish (as we hereafter assume, $\alpha \neq 0$, unless otherwise explicitly indicated), the many-body problem of *goldfish* type characterized by the Newtonian equations of motion (40) cannot be reduced to any previously known system: it is a *solvable* model the *novelty* of which is demonstrated by the fact that its solution involves special functions not featured in the solution of any previously known *solvable* model. Indeed, as shown in the following Sec. III, the solution $z_n(t)$ of the initial-value problem for the Newtonian equations of motion (40) is given by the following **Proposition 2.3** that is now formulated for the case with ω *real* (for a more general formulation see Sec. III).

Proposition 2.3: *The particle coordinates $z_n(t)$ that provide the solution to the initial-value problem for the many-body system characterized by the Newtonian equations of motion (40) with ω real are the N eigenvalues of the $N \times N$ matrix $U(t)$ defined in terms of the initial data $z_n(0)$, $\dot{z}_n(0)$ as follows:*

$$U(t) = (1 - P)[U(0) + \alpha t] + P\{1 + a\eta[\exp(i\omega t) - 1]\}^{-1/a}[U(0) + \alpha u(t)], \tag{44a}$$

where the $N \times N$ matrix $U(0)$, the $N \times N$ projection matrix P, and the scalar constant η are defined as follows:

$$U(0) = \mathrm{diag}[z_n(0)], \tag{44b}$$

$$P_{nm} = -\frac{\{[\dot{z}_n(0) - \alpha][\dot{z}_m(0) - \alpha]\}^{1/2}}{\eta i\omega z_m(0)}, \quad P^2 = P, \tag{44c}$$

$$\eta = -\sum_{n=1}^{N} \frac{\dot{z}_n(0) - \alpha}{i\omega z_n(0)}, \tag{44d}$$

and the scalar function $u(t)$ is defined as follows: if

$$|1 - a\eta| < |a\eta|, \quad \text{i.e., } \mathrm{Re}(a\eta) > \tfrac{1}{2}, \tag{44e}$$

then

$$u(t) = \eta^{1/a}\sum_{s=0}^{\infty}\binom{1/a}{s}\left(\frac{1 - a\eta}{a\eta}\right)^s \frac{1 - \exp\left[\left(s - \frac{1}{a}\right)i\omega t\right]}{\left(s - \frac{1}{a}\right)i\omega}, \tag{44f}$$

if instead

$$|1 - a\eta| > |a\eta|, \quad \text{i.e., } \mathrm{Re}(a\eta) < \tfrac{1}{2}, \tag{44g}$$

then

$$u(t) = (1 - a\eta)^{1/a}\left[t + \sum_{s=1}^{\infty}\binom{1/a}{s}\left(\frac{a\eta}{1 - a\eta}\right)^s \frac{\exp(si\omega t) - 1}{si\omega}\right]. \tag{44h}$$

These formulas are applicable as written provided $a \neq 0$ (and note that the sums in (44f) and (44h) terminate, yielding of course the same result, if a is the inverse of a positive integer); if $a = 0$ the expression $\{1 + a\eta[\exp(i\omega t) - 1]\}^{-1/a}$ in (44a) becomes $\exp\{-\eta[\exp(i\omega t) - 1]\}$, and expression (44h) becomes

$$u(t) = \exp(-\eta)\left[t + \sum_{s=1}^{\infty} \frac{\eta^s}{s!} \frac{\exp(si\omega t) - 1}{si\omega} \right]. \tag{44i}$$

Finally, let us note that the above-written formulas assume that $\eta \neq 0$ *(see in particular (44c)). For the special case in which* η *vanishes the expression of* $U(t)$ *is somewhat simpler:*

$$U(t) = U(0) + \alpha t + V(0)\left\{ \frac{\exp(i\omega t) - 1}{i\omega} \left[U(0) - \frac{\alpha}{i\omega} \right] + \alpha t \exp(i\omega t) \right\} \tag{45a}$$

with

$$[V(0)]_{nm} = \frac{\{[\dot{z}_n(0) - \alpha][\dot{z}_m(0) - \alpha]\}^{1/2}}{z_m(0)} . \quad \blacksquare \tag{45b}$$

Notation: Here and throughout the symbol $\binom{x}{y}$ denotes the generalized binomial coefficient:

$$\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}. \tag{46}$$

This of course implies that $\binom{x}{y}$ vanishes whenever y or $x-y$ are *negative integers*, unless x is also a *negative integer*.

Remark 2.4: If α vanishes and the inequality (44e) holds and $a \neq 1/p$ with p an arbitrary *positive* integer, then the $N \times N$ matrix $U(t)$ is *periodic with period* T, see (2):

$$U(t+T) = U(t) . \blacksquare \tag{47}$$

Remark 2.5: As entailed by the preceding *Remark 2.4* and by **Proposition 2.3**, the many-body problem characterized by the Newtonian equations of motion of *goldfish* type (40) is *isochronous* provided $\alpha = 0$ and $a \neq 1/p$ with p an arbitrary *positive* integer: a condition on the initial data sufficient to guarantee that its solution be *completely periodic* with a period which is an *integer multiple* of T, see (2), is validity of the inequality (44e) with

$$\eta = -\frac{S(0)}{i\omega} \tag{48}$$

(see (41b) and (44d) with $\alpha = 0$). But, as noted earlier, this model with $\alpha = 0$ is not new, indeed its time evolution is rather trivial, see (44), hence the study of this case is not pursued in the following.

Remark 2.6: If $a \neq 1/p$ with p an arbitrary *positive* integer and the inequality (44e) holds, the $N \times N$ matrix $PU(t)$ is *periodic* with period T, see (2):

$$PU(t+T) = PU(t) . \blacksquare \tag{49}$$

It is moreover possible to manufacture another *isochronous* many-body problem of *goldfish* type, by starting from the following version of the system of ODEs (39),

$$\zeta_n'' = (\zeta_n' - \alpha)\left[b(\tau) + \frac{\alpha}{\zeta_n} + (1+a) \sum_{m=1}^{N} \frac{\zeta_m' - \alpha}{\zeta_m} + 2 \sum_{m=1, m \neq n}^{N} \frac{\zeta_m' - \alpha}{\zeta_n - \zeta_m} \right]. \tag{50a}$$

Note that this system coincides with (39), except for a merely notational change (the dependent variables are here denoted as $\zeta_n \equiv \zeta_n(\tau)$, appended primes indicating differentiations with respect to the independent variable τ).

It is now easy to verify that, provided

$$b(\tau) = \frac{ki\omega}{1 + i\omega\tau}, \tag{50b}$$

via the change of dependent and independent variables (as it were, just the version of the trick (5) with $\lambda = -1$)

$$\tilde{z}_n(t) = \exp(-i\omega t)\zeta_n(\tau), \tag{51a}$$

$$\tau = \frac{\exp(i\omega t) - 1}{i\omega}, \quad \exp(i\omega t) = 1 + i\omega\tau, \tag{51b}$$

the (*nonautonomous*) system of ODEs ((50a) and (50b)) yields the *solvable* many-body problem characterized by the following *autonomous* Newtonian equations of motion:

$$\ddot{\tilde{z}}_n = -i\omega\dot{\tilde{z}}_n + (\dot{\tilde{z}}_n + i\omega\tilde{z}_n - \alpha)\cdot\left[ki\omega + \frac{\alpha}{\tilde{z}_n} + (1+a)\sum_{m=1}^{N}\frac{\dot{\tilde{z}}_m + i\omega\tilde{z}_m - \alpha}{\tilde{z}_m} + 2\sum_{m=1,m\neq n}^{N}\frac{\dot{\tilde{z}}_m + i\omega\tilde{z}_m - \alpha}{\tilde{z}_n - \tilde{z}_m}\right]. \tag{52}$$

Clearly the "particle coordinates" $\tilde{z}_n(t)$ are the eigenvalues of the $N\times N$ matrix $\tilde{U}(t)$ that is related to the matrix U by the analog of (51),

$$\tilde{U}(t) = \exp(-i\omega t)U(\tau), \tag{53}$$

of course with τ related to t by (51b). It is easily seen that this implies that this matrix $\tilde{U}(t)$ evolves according to

$$\ddot{\tilde{U}} = -i\omega\dot{\tilde{U}} + (\dot{\tilde{U}} + i\omega\tilde{U} - \alpha)\{(k+1+a)i\omega - \tilde{U}^{-1}[a\alpha - (a+1)\dot{\tilde{U}}]\}, \tag{54}$$

as clearly implied (via (53)) by the basic matrix evolution equation (32) (with (38) and (50b)) satisfied by the matrix U, namely

$$U'' = (U' - \alpha)\left\{\frac{ki\omega}{1 + i\omega\tau} - U^{-1}[a\alpha - (a+1)U']\right\}, \tag{55}$$

where clearly $U \equiv U(\tau)$ and appended primes denote differentiations with respect to τ. And the solution of the Newtonian equations of motion (52) is provided, as demonstrated in Sec. III, by the following

Proposition 2.7: *The particle coordinates $\tilde{z}_n(t)$ that provide the solution to the initial-value problem for the many-body problem characterized by these Newtonian equations of motion, (52), are the N eigenvalues of the $N\times N$ matrix $\tilde{U}(t)$ defined in terms of the initial data $z_n(0)$, $\dot{z}_n(0)$ as follows:*

$$\tilde{U}(t) = \exp(-i\omega t)\{1 + [\tilde{\phi}(t) - 1]\tilde{P}\}\tilde{U}(0) + (1 - \tilde{P})\alpha\frac{1 - \exp(-i\omega t)}{i\omega} + \alpha\tilde{P}\tilde{u}(t)\tilde{\phi}(t), \tag{56a}$$

where the $N\times N$ matrix $\tilde{U}(0)$, the $N\times N$ projection matrix $\tilde{P}$, the scalar constant $\tilde{\eta}$, and the scalar function $\tilde{\phi}(t)$ are defined as follows:

$$\tilde{U}(0) = \mathrm{diag}[z_n(0)], \tag{56b}$$

$$\tilde{P}_{nm} = -\frac{\{[\dot{\tilde{z}}_n(0) + i\omega\tilde{z}_n(0) - \alpha][\dot{\tilde{z}}_m(0) + i\omega\tilde{z}_m(0) - \alpha]\}^{1/2}}{\tilde{\eta}i\omega\tilde{z}_m(0)}, \quad P^2 = P, \tag{56c}$$

$$\tilde{\eta} = -\sum_{n=1}^{N} \frac{\dot{\tilde{z}}_n(0) + i\omega\tilde{z}_n(0) - \alpha}{i\omega\tilde{z}_n(0)}, \tag{56d}$$

$$\tilde{\phi}(t) = \{1 + a\tilde{\eta}[\exp(\tilde{k}i\omega t) - 1]\}^{-1/a}, \tag{56e}$$

and the function $\tilde{u}(t)$ *is defined as follows: if*

$$|1 - a\tilde{\eta}| < |a\tilde{\eta}|, \quad \text{i.e., } \mathrm{Re}(a\tilde{\eta}) > \tfrac{1}{2}, \tag{56f}$$

then

$$\tilde{u}(t) = (a\tilde{\eta})^{1/a} \sum_{s=0}^{\infty} \binom{1/a}{s} \left(\frac{1 - a\tilde{\eta}}{a\tilde{\eta}}\right)^s \frac{\exp(-i\omega t) - \exp\left\{\left[-\tilde{k}\left(s - \frac{1}{a}\right)\right] i\omega t\right\}}{\left[\tilde{k}\left(s - \frac{1}{a}\right) - 1\right] i\omega}, \tag{56g}$$

if instead

$$|1 - a\tilde{\eta}| > |a\tilde{\eta}|, \quad \text{i.e., } \mathrm{Re}(a\tilde{\eta}) < \tfrac{1}{2}, \tag{56h}$$

then

$$\tilde{u}(t) = (1 - a\tilde{\eta})^{1/a} \left[\sum_{s=0}^{\infty} \binom{1/a}{s} \left(\frac{a\tilde{\eta}}{1 - a\tilde{\eta}}\right)^s \frac{\exp(\tilde{k}si\omega t) - \exp(-i\omega t)}{(\tilde{k}s + 1)i\omega}\right]. \tag{56i}$$

Note that we use throughout the short-hand notation

$$\tilde{k} = k + 1. \tag{56j}$$

These formulas are applicable as written provided $a \neq 0$ *(and note that the sums in (56g) and (56i) terminate, yielding of course the same result, if a is the inverse of a positive integer); if a* $= 0$ *the definition (56e) must be modified to read*

$$\tilde{\phi}(t) = \exp\{\tilde{\eta}[1 - \exp(\tilde{k}i\omega t)]\}, \tag{56k}$$

and the definition (56i) of $\tilde{u}(t)$ *must be modified to read*

$$\tilde{u}(t) = \exp(-\tilde{\eta}) \sum_{s=0}^{\infty} \frac{\tilde{\eta}^s}{s!} \frac{\exp[\tilde{k}si\omega t] - \exp(-i\omega t)}{(\tilde{k}s + 1)i\omega}. \tag{56l}$$

In the special case with $k = 0$, $\tilde{k} = 1$, *the sums in the definition of the function* $\tilde{u}(t)$ *can be performed in closed form, and one gets*

$$\tilde{u}(t) = (a\tilde{\eta})^{1/a} \frac{\exp(i\omega t/a) - \exp(-i\omega t)}{i\omega} \quad \text{for } a \neq 0, \tag{56m}$$

$$\tilde{u}(t) = \exp(-i\omega t) \frac{\exp\{\tilde{\eta}[\exp(i\omega t) - 1]\} - 1}{i\omega\tilde{\eta}} \quad \text{for } a = 0. \tag{56n}$$

Finally, let us note that the formulas written above assume that $\tilde{\eta} \neq 0$ *(see in particular (56c)). For the special case in which* $\tilde{\eta}$ *vanishes the expression of* $\tilde{U}(t)$ *is somewhat simpler:*

$$\tilde{U}(t) = \exp(-i\omega t)\tilde{U}(0) + \alpha \frac{1 - \exp(-i\omega t)}{i\omega} \tilde{V}(0) \tag{57a}$$

with

$$\widetilde{V}_{nm}(0) = \frac{[\dot{\widetilde{z}}_n(0) + i\omega\widetilde{z}_n(0) - \alpha]^{1/2}[\dot{\widetilde{z}}_m(0) + i\omega\widetilde{z}_m(0) - \alpha]^{1/2}}{i\omega\widetilde{z}_m(0)} . \quad \blacksquare \tag{57b}$$

Remark 2.8: The formulas, as written earlier, are valid for *arbitrary* values of the two constants a and $\widetilde{k}$, provided $\widetilde{k}\omega$ hence $\widetilde{k}$ itself are *real* ($\mathrm{Im}(\widetilde{k})=0$; this condition is required to guarantee the convergence for all *real* values of t of the infinite series on the right-hand sides of (56g), (56i), and (56l)). But the most interesting case is when $\widetilde{k}$ hence k (see (56j)) are *rational* numbers,

$$\widetilde{k} = \frac{\widetilde{p}}{\widetilde{q}}, \quad k = \frac{\widetilde{p} - \widetilde{q}}{\widetilde{q}}, \tag{58}$$

of course with $\widetilde{p}$ and $\widetilde{q}$ *integers* (and $\widetilde{q}>0$). Then whenever the initial data entail, via (56d), that there holds the inequality (56h), and provided moreover $\widetilde{k}s \neq -1$ for every *positive integer* s hence $\widetilde{p} \neq -1$ (see (58)), clearly (see (56a), (56e), and (56i)) the matrix $\widetilde{U}(t)$ is *periodic* with period $\widetilde{T}$, see (2),

$$\widetilde{T} = \widetilde{q}T, \quad \widetilde{U}(t + \widetilde{T}) = \widetilde{U}(t). \tag{59}$$

If the initial data entail instead that the inequality (56f) prevails (rather than (56h)) and moreover a is also *rational*, hence $\widetilde{k}/a$ is as well *rational*,

$$\frac{\widetilde{k}}{a} = \frac{k+1}{a} = \frac{\check{p}}{\check{q}}, \tag{60}$$

of course again with $\check{p}$ and $\check{q}$ *integers* (and $\check{q}>0$), then provided $\widetilde{k}(s-1/a) \neq 1$ hence $\widetilde{q}(\check{q}+\check{p}) \neq s\check{q}\widetilde{p}$ for any *nonnegative integer* s (see (58) and (60)), clearly (see (56a), (56e), and (56g)) $\widetilde{U}(t)$ is again *periodic*, but now with a period $\check{T}$ (generally) larger than $\widetilde{T}$,

$$\check{T} = \max(\widetilde{q},\check{q})T, \quad \widetilde{U}(t + \check{T}) = U(t) . \quad \blacksquare \tag{61}$$

Remark 2.9: As entailed by the preceding *Remark 2.8* and by **Proposition 2.7**, the novel many-body problem characterized by the Newtonian equations of motion of *goldfish* type (52) with k *rational* is *isochronous:* if a is *real* but otherwise *arbitrary*, a condition on the initial data sufficient to guarantee that its solution be *completely periodic* with a period which is an *integer multiple* of T, see (2), is validity of the inequality (56h) (provided moreover $\widetilde{p} \neq -1$, see (58)); if a is moreover *rational*, then *all* its solutions are *completely periodic* with a period which is an *integer multiple* of T (provided moreover $\widetilde{k}(s-1/a) \neq 1$ hence $\widetilde{q}(\check{q}+\check{p}) \neq s\check{q}\widetilde{p}$ for any *non-negative integer* s, see (58) and (60)). ■

In the rest of this section, and in Secs. IV and V (but not in Sec. III) we get rid of the unessential constants ω and α. This can be done by appropriate rescaling, or equivalently by setting (as we hereafter do, except in Sec. III)

$$\omega = 1, \quad \alpha = i. \tag{62}$$

Let us emphasize that hereafter (except in Sec. III) whenever we refer to previous formulas we understand that such assignments have been made in them.

As explained in Sec. IV, an alternative version of the system (40) is characterized by the following system of N ODEs satisfied by the N dependent variables $c_m(t)$:

$$\ddot{c}_m - [1 + (1+a)\gamma]i\dot{c}_m + (2N+1-2m)i\dot{c}_{m-1} + [(N-m)\gamma + (N-m+1)(1+a\gamma)]c_{m-1} - (N-m)(N-m+2)c_{m-2} = 0, \quad m = 1, \ldots, N, \quad c_0 = 1, \quad c_{-1} = 0, \tag{63a}$$

where

$$\gamma \equiv \gamma(t) = \frac{c_{N-1}(t) - i\dot{c}_{N-1}(t)}{c_N(t)}. \tag{63b}$$

This system of N coupled ODEs is *no less solvable* than (40), indeed, as shown by the developments reported in Sec. IV, its solution is provided by the following

Proposition 2.10: *The dependent variables $c_m(t)$ that solve the system ((63a) and (63b)) are the N coefficients of the (monic) polynomial $\psi(z,t)$ of degree N in z having the N coordinates $z_n(t)$ solutions of (40) as its zeros*,

$$\psi(z,t) = \prod_{n=1}^{N} [z - z_n(t)] = z^N + \sum_{m=1}^{N} c_m(t) z^{N-m}, \tag{64}$$

so that, as implied by ***Proposition 2.3****, this polynomial is given by the formula*

$$\psi(z,t) = \det[z - U(t)] \tag{65}$$

where $U(t)$ is the $N \times N$ matrix the time-dependence of which is given by the explicit formula (44) [with (62)]. ■

Note that this system, ((63a) and (63b)), is identically satisfied also for $m=N+1$ and for $m=N+2$, provided one sets $c_{N+1}=c_{N+2}=0$ (consistent with (64)). And also note that this new *solvable* system of N ODEs, (63a), looks superficially linear, but is in fact *nonlinear* due to the presence in it of the quantity γ, see (63b). Indeed, the highly nonlinear (and nontrivial) character of this system will be evident to the diligent reader who will take the trouble to write it out in the simpler cases with $N=2$ and with $N=1$ (in the latter case the single equation of motion ((63a) and (63b)) can be directly compared with (32), since for $N=1$ $U(t)=-c_1(t)$, see (65) and (64)).

Likewise, an alternative formulation of the system (52) is characterized by the following system of N ODEs satisfied by the N dependent variables $\tilde{c}_m(t)$:

$$\ddot{\tilde{c}}_m - (K-2m)i\dot{\tilde{c}}_m + (2N+1-2m)i\dot{\tilde{c}}_{m-1} + m(K-m)\tilde{c}_m + [(N+1-m)(K-2m) - \tilde{\gamma}]\tilde{c}_{m-1} - (N-m)(N+2-m)\tilde{c}_{m-2} = 0,$$

$$m = 1, \ldots, N, \quad \tilde{c}_0 = 1, \quad \tilde{c}_{-1} = 0, \tag{66a}$$

where

$$K \equiv K(t) = \tilde{k} + (a+1)[N + \tilde{\gamma}(t)] \tag{66b}$$

and

$$\tilde{\gamma} \equiv \tilde{\gamma}(t) = \frac{\tilde{c}_{N-1}(t) - i\dot{\tilde{c}}_N(t)}{\tilde{c}_N(t)}. \tag{66c}$$

Here of course superimposed dots denote differentiations with respect to the independent variable t.

Again, this system of N coupled ODEs is *no less solvable* than (52), indeed, as shown by the developments reported in Sec. IV, its solution is provided by the following.

Proposition 2.11:*The dependent variables $\tilde{c}_m(t)$ that solve the system ((66a)–(66c)) are the N coefficients $\tilde{c}_m(t)$ of the (monic) polynomial $\tilde{\psi}(z,t)$ of degree N in z having the N coordinates $\tilde{z}_n(t)$ solutions of (52) as its zeros*,

$$\widetilde{\psi}(z,t) = \prod_{n=1}^{N} [z - \widetilde{z}_n(t)] = z^N + \sum_{m=1}^{N} \widetilde{c}_m(t) z^{N-m}, \tag{67}$$

so that, as implied by ***Proposition 2.7****, this polynomial is given by the formula*

$$\widetilde{\psi}(z,t) = \det[z - \widetilde{U}(t)], \tag{68}$$

where $\widetilde{U}(t)$ *is the* $N \times N$ *matrix the time-dependence of which is given by (56a)–(56j) [with (62)].*■

We do not repeat the remarks proffered above (after **Proposition 2.10**), but merely note that they are as well relevant now (up to obvious modifications).

Remark 2.12: Provided $\widetilde{k}$ is a *rational number*, $\widetilde{k} = \widetilde{p}/\widetilde{q}$ (with $\widetilde{p}$ and $\widetilde{q}$ *integers* and $\widetilde{q} > 0$, see (58), and moreover $\widetilde{p} \neq -1$), the **Proposition 2.11** and the *Remark 2.9* entail that the solution of the nonlinear system of ODEs ((66a)–(66c)) is *completely periodic* with a period which is an *integer multiple* Q of 2π,

$$\widetilde{c}_m(t + 2\pi Q) = \widetilde{c}_m(t), \tag{69}$$

in the following cases. (i) If a is an arbitrary (possibly even *complex*) number and the initial data entail the inequality

$$\mathrm{Re}[-a\{N + \gamma(0)\}] < \tfrac{1}{2} \tag{70}$$

(see (66c)), then (69) holds with $Q = \widetilde{q}$. (ii) If a is an arbitrary *real* and *rational* number so that the number $\widetilde{k}/a$ is itself *rational*, $\widetilde{k}/a = \check{p}/\check{q}$ (with $\check{p}$ and $\check{q}$ *integers* and $\check{q} > 0$, see (60) and moreover $\widetilde{q}(\check{q} + \check{p}) \neq s\check{q}\widetilde{p}$ for any *non-negative integer* s), then *all* solutions of the nonlinear system of ODEs ((66a)–(66c)) are *completely periodic*, see (69) with $Q = \max(\widetilde{q}, \check{q})$.

We end this section by formulating certain conjectures (having a *Diophantine* connotation, which becomes particularly evident if one assigns *integer* values to all the numbers that are left *arbitrary*, see the following) arrived at (up to trivial notational changes) from the results of the preceding *Remark 2.12* via the treatment of Sec. V, and by reporting some examples illustrating them.

Conjecture 5.13: *Let the two* $N \times N$ *matrices* A *and* B *be defined componentwise as follows:*

$$A_{nm} = (2n - \nu)\delta_{n,m} + (2N + 1 - 2n)\delta_{n-1,m} + C_n \delta_{N,m}, \tag{71a}$$

$$\begin{aligned} B_{nm} = {} & n(n - \nu)\delta_{n,m} - [N + (N + 1 - n)(\nu - 2n)]\delta_{n-1,m} \\ & + (N - n)(N + 2 - n)\delta_{n-2,m} + C_n(\delta_{N-1,m} + N\delta_{N,m}), \end{aligned} \tag{71b}$$

where

$$C_n = -(-)^{N-n} \frac{1}{1+f} \left[\binom{N}{n-1} + f \frac{N + (N-n)\nu}{(N-\nu)} \binom{N-\nu}{n-\nu-1} + g \binom{N-\nu-1}{n-\nu} \right], \tag{71c}$$

with ν, f, *and* g arbitrary *numbers; then*

$$\det[p^2 + pA + B] = \prod_{n=1}^{N} [(p + n)(p - \nu - 1 + n)]\,. \quad \blacksquare \tag{71d}$$

Conjecture 5.14: *Let the two* $N \times N$ *matrices* A *and* B *be defined componentwise as follows:*

$$A_{nm} = (2n - \nu - 1)\delta_{n,m} + (2N + 1 - 2n)\delta_{n-1,m} + C_n \delta_{N,m}, \tag{72a}$$

$$\begin{aligned} B_{nm} = {} & n(n - \nu - 1)\delta_{n,m} + [(N - n)(2n - \nu - 3) + N]\delta_{n-1,m} + (N - m)(N + 2 - n)\delta_{n-2,m} \\ & + C_n[\delta_{N-1,m} + (N - \nu - 1)\delta_{N,m}], \end{aligned} \tag{72b}$$

where

$$C_n = (-)^{N-n}\frac{1}{1+f}\left\{\frac{g(N+1-n)-N}{N}\binom{N}{n-1}+f\left[(g-\nu-1)\binom{N-\nu-1}{n-\nu-1}-\binom{N-\nu-1}{n-\nu-2}\right]\right\}, \tag{72c}$$

with ν, f, *and* g arbitrary *numbers; then*

$$\det[p^2+pA+B] = (p+g)\left[\prod_{n=1}^{N-1}(p+n)\right]\left[\prod_{n=1}^{N}(p-\nu-1+n)\right]. \quad \blacksquare \tag{72d}$$

Examples: For $N=5$ the **Conjecture 5.13** states that

$$\begin{vmatrix} p^2+p(2-\nu)1-\nu & 0 & 0 & C_1 & (p+5)C_1 \\ 7p+11-4\nu & p^2+p(4-\nu)+2(2-\nu) & 0 & C_2 & (p+5)C_2 \\ 8 & 5p+13-3\nu & p^2+p(6-\nu)+3(3-\nu) & C_3 & (p+5)C_3 \\ 0 & 3 & 3p+11-2\nu & p^2+p(8-\nu)+4(4-\nu)+C_4 & (p+5)C_4 \\ 0 & 0 & 0 & p+5-\nu+C_5 & p^2+p(10-\nu+C_5)+5(5-\nu+C_5) \end{vmatrix}$$
$$= (p+1)(p+2)(p+3)(p+4)(p+5)\cdot(p-\nu)(p-\nu+1)(p-\nu+2)(p-\nu+3)(p-\nu+4) \tag{73a}$$

provided

$$C_1 = -\frac{1}{1+f}\left\{1+\frac{(4-\nu)(3-\nu)(2-\nu)}{6}\left[\frac{(5+4\nu)(1-\nu)f}{20}+g\right]\right\}, \tag{73b}$$

$$C_2 = \frac{1}{1+f}\left\{5+\frac{(4-\nu)(3-\nu)}{2}\left[\frac{(5+3\nu)(2-\nu)f}{12}+g\right]\right\}, \tag{73c}$$

$$C_3 = -\frac{1}{1+f}\left\{10+(4-\nu)\left[\frac{(5+2\nu)(3-\nu)f}{6}+g\right]\right\}, \tag{73d}$$

$$C_4 = \frac{1}{1+f}\left[10+\frac{(5+\nu)(4-\nu)f}{2}+g\right], \tag{73e}$$

$$C_5 = -5. \tag{73f}$$

Likewise, for $N=5$ the **Conjecture 5.14** states that

$$\begin{vmatrix} p^2p(1-\nu)-\nu & 0 & 0 & C_1 & (p+4-\nu)C_1 \\ 7p+8-3\nu & p^2+p(3-\nu)+2(1-\nu) & 0 & C_2 & (p+4-\nu)C_2 \\ 8 & 5p+11-2\nu & p^2+p(5-\nu)+3(2-\nu) & C_3 & (p+4-\nu)C_3 \\ 0 & 3 & 3p+10-\nu & p^2+p(7-\nu)+4(3-\nu)+C_4 & (p+4-\nu)C_4 \\ 0 & 0 & 0 & p+5+C_5 & p^2+p(9-\nu+C_5)+(4-\nu)(5+C_5) \end{vmatrix}$$
$$= (p+1)(p+2)(p+3)(p+4)(p+5)\cdot(p-\nu)(p-\nu+1)(p-\nu+2)(p-\nu+3)(p-\nu+4) \tag{74a}$$

provided

$$C_1 = \frac{1}{1+f}\left[g-1+\frac{(4-\nu)(3-\nu)(2-\nu)(1-\nu)f(5g-4\nu-5)}{120}\right], \tag{74b}$$

$$C_2 = -\frac{1}{1+f}\left[4g-5+\frac{(4-\nu)(3-\nu)(2-\nu)f(4g-3\nu-5)}{24}\right], \tag{74c}$$

$$C_3 = \frac{1}{1+f}\left[2(3g-5) + \frac{(4-\nu)(3-\nu)(2-\nu)f(3g-2\nu-5)}{6}\right], \tag{74d}$$

$$C_4 = -\frac{1}{1+f}\left[2(2g-5) + \frac{(4-\nu)(3-\nu)f(2g-\nu-5)}{2}\right], \tag{74e}$$

$$C_5 = g-5. \tag{74f}$$

Remark 5.15: These two examples could be verified by hand computation, although only a masochist would try to do so. They, as well as several others, have been verified by computer assisted computations, so that we are reasonably certain of the validity of the above-noted conjectures; but we have not yet managed to prove them for all values of N. ■

III. PROOFS

First, let us obtain the systems of ODEs (35) and (40) from the *solvable* matrix evolution equation (32).

Remark 3.1: Here we take the second-order matrix ODE (32) as a starting point for our treatment, but one could as well take as a starting point the system of two coupled first-order matrix ODEs (31a) and (31b). ■

Via (18) we get

$$\ddot{z}_n = cz_n + (\dot{z}_n - \alpha)\left(b + \frac{\dot{z}_n}{z_n} + a\frac{\dot{z}_n - \alpha}{z_n}\right) - \sum_{m=1, m\neq n}^{N} \frac{(z_n - z_m)[z_n + z_m + a(z_n - z_m)]}{z_m} M_{nm}M_{mn}, \tag{75a}$$

$$\frac{\dot{M}_{nm}}{M_{nm}} = -2\frac{\dot{z}_n - \dot{z}_m}{z_n - z_m} + b + (1+a)\left(\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m}\right) - \alpha\left(\frac{1+a}{z_n} + \frac{a}{z_m}\right) - (\mu_n - \mu_m)$$
$$+ \sum_{\ell=1, \ell\neq m,n}^{N} \left\{\frac{(z_n - z_\ell) + (z_m - z_\ell)}{(z_n - z_m)} + \frac{(1+a)(z_n - z_\ell)(z_m - z_\ell)}{(z_n - z_m)z_\ell}\right\}\frac{M_{n\ell}M_{\ell m}}{M_{nm}},$$
$$n \neq m. \tag{75b}$$

As a first educated guess we now make the *ansatz*

$$M_{nm} = \frac{(\dot{z}_n\dot{z}_m)^{1/2}g}{(z_n - z_m)^2}, \quad n \neq m. \tag{76}$$

Remark 3.2: This *ansatz* (as well as analogous ones made in the following) is only applicable provided $z_n \neq z_m$ whenever $n \neq m$. Indeed the models obtained in this paper, when interpreted as N-body problems in which the N quantities z_n identify the positions of the particles (generally in the complex z-plane), feature two-body forces that are *singular* at zero separation, so that the equations of motion become *singular* whenever two particles *collide*. This constitutes no difficulty, because the initial data leading to collisions are *exceptional*, the set of such data having generally *zero* measure in the space of initial data $z_n(0)$, $\dot{z}_n(0)$ (assigned in the complex z-plane). But this entails that one cannot assign initial data in which the coordinates of two or more particles coincide, and moreover that the study of the motion in the neighborhood of such data requires caution to avoid wrong inferences (as will be illustrated in the following in the context of the investigation of motions in the neighborhood of equilibria for some of the systems discussed herein). ■

Insertion of the *ansatz* (76) in (75b) yields

$$\frac{\dot{g}}{g} = b + \left(\frac{1}{2} + a\right)\left(\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m}\right) - \alpha\left(\frac{1+a}{z_n} + \frac{a}{z_m}\right) - (\mu_n - \mu_m) + g \sum_{\ell=1,\ell\neq m,n}^{N} \frac{(z_n - z_m)}{(z_n - z_\ell)(z_m - z_\ell)} \left\{\frac{z_\ell}{z_n - z_\ell} + \frac{z_\ell}{z_m - z_\ell} + (1+a)\right\}, \quad n \neq m. \tag{77}$$

Using the identity

$$\frac{(z_n - z_m)}{(z_n - z_\ell)(z_m - z_\ell)} = -\left(\frac{1}{z_n - z_\ell} - \frac{1}{z_m - z_\ell}\right) \tag{78}$$

we now rewrite this equation as follows:

$$\frac{\dot{g}}{g} = b + \left(\frac{1}{2} + a\right)\left[\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m} - \alpha\left(\frac{1}{z_n} + \frac{1}{z_m}\right)\right] - (\tilde{\mu}_n - \tilde{\mu}_m) - g \sum_{\ell=1,\ell\neq m,n}^{N} \left[\frac{z_\ell}{(z_n - z_\ell)^2} - \frac{z_\ell}{(z_m - z_\ell)^2} + \frac{1+a}{z_n - z_\ell} - \frac{1+a}{z_m - z_\ell}\right], \quad n \neq m, \tag{79}$$

having conveniently set

$$\mu_n = \tilde{\mu}_n - \frac{\alpha}{2z_n}. \tag{80}$$

Recalling the freedom to assign the diagonal elements μ_n we moreover conveniently set

$$\tilde{\mu}_n = -g \sum_{\ell=1,\ell\neq n}^{N} \left\{\frac{z_\ell}{(z_n - z_\ell)^2} - \frac{1+a}{z_n - z_\ell}\right\}, \tag{81}$$

and we thereby see that (79) now reads

$$\frac{\dot{g}}{g} = b + \left(\frac{1}{2} + a\right)\left[\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m} - \alpha\left(\frac{1}{z_n} + \frac{1}{z_m}\right) - \frac{2g}{z_n - z_m}\right], \quad n \neq m. \tag{82}$$

This equation is therefore consistent provided the two conditions $b=0$ and $a=-\frac{1}{2}$ hold (see (34)), and it implies that g is an (*arbitrary*) *constant*. It is then easy to verify that the insertion of (76) and (34) in (75a) yields (35). The first part of our first task is thus completed.

To prove the second part we use the following, different, *ansatz* for the *off-diagonal* elements of the matrix $M(t)$:

$$M_{nm} = \frac{[(\dot{z}_n - \alpha)(\dot{z}_m - \alpha)]^{1/2} g}{z_n - z_m}, \quad n \neq m. \tag{83}$$

Its insertion in (75) yields

$$\frac{\ddot{z}_n}{\dot{z}_n - \alpha} = \frac{cz_n}{\dot{z}_n - \alpha} + b + \frac{(1+a)\dot{z}_n}{z_n} - \frac{\alpha a}{z_n} + g^2 \sum_{m=1,m\neq n}^{N} (\dot{z}_m - \alpha)\left(\frac{2}{z_n - z_m} + \frac{1+a}{z_m}\right), \tag{84a}$$

$$\frac{\dot{g}}{g} + \frac{1}{2}\left(\frac{\ddot{z}_n}{\dot{z}_n - \alpha} + \frac{\ddot{z}_m}{\dot{z}_m - \alpha}\right) = -\frac{\dot{z}_n - \dot{z}_m}{z_n - z_m} + b + (1+a)\left(\frac{\dot{z}_n}{z_n} + \frac{\dot{z}_m}{z_m}\right) - \alpha\left(\frac{1+a}{z_n} + \frac{a}{z_m}\right) - (\mu_n - \mu_m) - g \sum_{\ell=1,\ell\neq m,n}^{N} (\dot{z}_\ell - \alpha)\left(\frac{1}{z_n - z_\ell} + \frac{1}{z_m - z_\ell} + \frac{1+a}{z_\ell}\right), \quad n \neq m. \tag{84b}$$

Insertion of the first of these two equations in the second yields (using again the assignment (80))

$$\frac{\dot{g}}{g}+\frac{c}{2}\left(\frac{z_n}{\dot{z}_n-\alpha}+\frac{z_m}{\dot{z}_m-\alpha}\right)+(g^2-1)\left[-\frac{\dot{z}_n-\dot{z}_m}{z_n-z_m}+\frac{1+a}{2}\left(\frac{\dot{z}_n}{z_n}+\frac{\dot{z}_m}{z_m}-\frac{\alpha}{z_n}-\frac{\alpha}{z_m}\right)\right]+\tilde{\mu}_n-\tilde{\mu}_m$$
$$=-g(1+g)\sum_{\ell=1,\ell\neq m,n}^{N}(\dot{z}_\ell-\alpha)\left(\frac{1}{z_n-z_\ell}+\frac{1}{z_m-z_\ell}+\frac{1+a}{z_\ell}\right),\quad n\neq m. \tag{84c}$$

If we now set (using our privilege to assign this quantity as we wish) $\tilde{\mu}_n=0$ (or equivalently $\tilde{\mu}_n=\tilde{\mu}$) we see that, provided there holds the condition $c=0$, see (38), the assignment

$$g=-1 \tag{85}$$

is consistent with this system of ODEs, and clearly its insertion in (84a) yields (39).

Remark 3.3: This derivation of (40) does not require that the quantity b be time-independent. ■

Having completed our first task, let us now compute the solution $U(t)$ of the system of two matrix ODEs ((31a) and (31b)) in the cases of interest to us, with *vanishing* c (see (38)), *constant* a, and b either *constant* or time-dependent as specified by (50b).

Consider first the case with a and $b=i\omega$ both *constant*. Then from (31b) with $c=0$ we get

$$V(t)=V(0)\exp(i\omega t)\left[1-aV(0)\frac{\exp(i\omega t)-1}{i\omega}\right]^{-1}. \tag{86a}$$

As we will see in the following, in the case of interest to us the $N\times N$ matrix $V(0)$ turns out to be *dyadic*, hence this formula can be simplified to read

$$V(t)=V(0)\exp(i\omega t)\{1+a\eta[\exp(i\omega t)-1]\}^{-1}, \tag{86b}$$

with

$$\eta=-\frac{\mathrm{trace}[V(0)]}{i\omega}. \tag{86c}$$

(To obtain this simplification, and analogous ones to follow, we take advantage of the following property: *if* Δ *is a dyadic matrix*,

$$\Delta_{nm}=\breve{\delta}_n\hat{\delta}_m, \tag{87a}$$

there holds the identity

$$f(\Delta)=f(0)+\frac{f(\mathrm{trace}[\Delta])-f(0)}{\mathrm{trace}[\Delta]}\Delta \tag{87b}$$

for any (scalar) function f for which the above-noted formula makes good sense.)

Then from (31a) with (31c) we get

$$U(t)=(1+[\{1+a\eta[\exp(i\omega t)-1]\}^{-1/a}-1]P)U(0)$$
$$+\alpha\int_0^t dt'\left(1+\left[\left\{\frac{1+a\eta[\exp(i\omega t)-1]}{1+a\eta[\exp(i\omega t')-1]}\right\}^{-1/a}-1\right]P\right), \tag{88a}$$

$$U(t)=(1-P)[U(0)+\alpha t]+P\{1+a\eta[\exp(i\omega t)-1]\}^{-1/a}[U(0)+\alpha u(t)], \tag{88b}$$

where η is of course defined by (86c) and P is the following "projector" $N\times N$ matrix,

$$P = \frac{V(0)}{\text{trace}[V(0)]}, \quad P^2 = P, \tag{88c}$$

where (see (33) and the following)

$$V(0) = [\dot{U}(0) - \alpha][U(0)]^{-1}, \tag{88d}$$

and

$$u(t) = \int_0^t \mathrm{d}t' \{1 + a\eta[\exp(i\omega t') - 1]\}^{1/a}. \tag{88e}$$

The integration on the right-hand side of this formula could be performed in terms of hypergeometric functions, but this is not particularly enlightening. More useful, in view of the results of interest to us is to consider the case with ω *real* and *nonvanishing* (for definiteness, $\omega > 0$), and to note that, by appropriately expanding as a (generally infinite) series the power under the integral on the right-hand side of (88e) and then integrating term by term, $u(t)$ can be rewritten as an infinite series, see the explicit expressions provided in the formulation of **Proposition 2.3.** (Of course if a is the inverse of a *positive integer*, the integration in (88e) can be performed in terms of elementary functions; in this case the infinite sums in the explicit expressions provided in **Proposition 2.3** become finite sums)

Likewise, if a is *constant* but b has the time-dependence (50b), from the version of (31b) with $c=0$ (see (38)) and the variable t formally replaced by τ,

$$V' = aV^2 + \frac{ki\omega V}{1 + i\omega\tau}, \tag{89a}$$

we get

$$V(\tau) = V(0)(1 + i\omega\tau)^k \left\{ 1 - \frac{aV(0)}{(k+1)i\omega}[(1 + i\omega\tau)^{k+1} - 1] \right\}^{-1}. \tag{89b}$$

By taking again advantage of the *dyadic* character of $V(0)$ (see the following) this formula can be simplified to read

$$V(\tau) = V(0)(1 + i\omega\tau)^k [1 - a\tilde{\eta} + a\tilde{\eta}(1 + i\omega\tau)^{k+1}]^{-1} \tag{89c}$$

with

$$\tilde{\eta} = -\frac{\text{trace}[V(0)]}{i\tilde{k}\omega}. \tag{89d}$$

In the last formula and hereafter we use whenever convenient the short-hand notation $k+1=\tilde{k}$ (see (56j)). Then from (31a) with (31c) (of course with the variable t replaced by τ)

$$U'(\tau) = \alpha + V(\tau)U(\tau), \tag{90}$$

we get

$$U(\tau) = (1 - P)[U(0) + \alpha\tau] + P\phi(\tau)\left[U(0) + \alpha \int_0^\tau \frac{\mathrm{d}\tau'}{\phi(\tau')} \right], \tag{91a}$$

$$\phi(\tau) = [1 - a\tilde{\eta} + a\tilde{\eta}(1 + i\omega\tau)^{\tilde{k}}]^{-1/a}, \tag{91b}$$

where we took again advantage of the *dyadic* character of $V(0)$ and we use again the definition (88c) of the projection matrix P.

We now use the transformation (53), of course with τ related to t by (51b), and thereby obtain (from the preceding formulas):

$$\widetilde{U}(t) = \exp(-i\omega t)\{1 + [\widetilde{\phi}(t) - 1]\widetilde{P}\}\widetilde{U}(0) + (1 - \widetilde{P})\alpha\frac{1 - \exp(-i\omega t)}{i\omega} + \alpha\widetilde{P}\widetilde{u}(t)\widetilde{\phi}(t), \tag{92a}$$

$$\widetilde{\phi}(t) = \{1 + a\widetilde{\eta}[\exp(\widetilde{k}i\omega t) - 1]\}^{-1/a}, \tag{92b}$$

$$\widetilde{u}(t) = \int_0^t \mathrm{d}t' \exp[i\omega(t' - t)][\widetilde{\phi}(t')]^{-1} \tag{92c}$$

$$= \int_0^t \mathrm{d}t' \exp[i\omega(t' - t)][1 - a\widetilde{\eta} + a\widetilde{\eta}\exp(\widetilde{k}i\omega t')]^{1/a}. \tag{92d}$$

Note that we use again the short-hand notation $k+1=\widetilde{k}$, see (56j), and we also introduced the notation $\widetilde{P}$, to avoid any confusion with the projection operator P defined previously: both P and $\widetilde{P}$ are related to $V(0)$ by the formula (88c), and in both cases $V(\tau)$ is related to $U(\tau)$ and $U'(\tau)$ by (90), but now (53) with (51b) implies

$$V(0) = [\dot{\widetilde{U}}(0) + i\omega\widetilde{U}(0) - \alpha][\widetilde{U}(0)]^{-1} = [\dot{\widetilde{U}}(0) - \alpha][\widetilde{U}(0)]^{-1} + i\omega. \tag{93}$$

The integral on the right-hand side of the formula (92d) could be expressed in terms of hypergeometric functions, but this would not be particularly enlightening. We rather perform it explicitly by series, under the assumption that the quantity $\widetilde{k}\omega$ is *real* (to guarantee the convergence of the sums), and we thereby get the results displayed in the formulation of **Proposition 2.7.** (Of course if a is the inverse of a *positive integer*, the integration in (92d) can be performed in terms of elementary functions; in this case the infinite sums in the explicit expressions provided in **Proposition 2.7** become finite sums).

The final step to prove the results (reported in the preceding section as **Propositions 2.3**) is to observe that one can set $R(0)=1$, entailing (see (12))

$$U(0) = \mathrm{diag}[z_n(0)], \tag{94}$$

and (see (13a), (83), and (85))

$$[\dot{U}(0)]_{nm} = \delta_{nm}\dot{z}_n(0) + (1 - \delta_{nm})\{[\dot{z}_n(0) - \alpha][\dot{z}_m(0) - \alpha]\}^{1/2}, \tag{95}$$

implying via (88d)

$$[V(0)]_{nm} = \frac{\{[\dot{z}_n(0) - \alpha][\dot{z}_m(0) - \alpha]\}^{1/2}}{z_m(0)}, \tag{96a}$$

which evidences the *dyadic* character of this $N\times N$ matrix and entails

$$\mathrm{trace}[V(0)] = \sum_{n=1}^{N} \frac{\dot{z}_n(0) - \alpha}{z_n(0)}, \tag{96b}$$

as well as the definitions (44c) and (44d). To complete the proof of **Proposition 2.3** one must treat the special case in which the initial data cause the quantity η, see (44d), to vanish. It is easily seen, via (96a), that this causes the square of the (dyadic) matrix $V(0)$ to vanish. This property holds as well for the matrix $V(t)$ (see (97)):

$$[V(t)]^2 = 0, \tag{97}$$

and it drastically simplifies the remaining calculations, which are analogous to those reported above and hence need not be reported.

And the analogous completion of the proof of **Proposition 2.7** is now sufficiently straightforward that we can leave it as a task for the diligent reader.

IV. ALTERNATIVE FORMULATIONS OF THE SOLVABLE MODELS

In this section we provide an alternative formulation of the *solvable* many-body models obtained in this paper, characterized by equations of motions of Newtonian type. We do not elaborate on the technique to obtain these results, since it can be considered by now rather standard (see for instance Sec. 2.3 of Ref. 6). We merely note that key to such reformulations are the relations among the *zeros* of a polynomial and its *coefficients*, hence the formulas reported in the Appendix, as applied to the *monic* polynomial $\psi(z,t)$ (respectively, $\tilde{\psi}(z,t)$), of degree N in z, having the N "particle coordinates" $z_n(t)$ (respectively, $\tilde{z}_n(t)$) as its *zeros* and the N coefficients $c_m(t)$ (respectively, $\tilde{c}_m(t)$) (see below (99), respectively, (101), and recall (62)).

Using those formulas it is indeed seen that, if the coordinates $z_n(t)$ evolve according to the equations of motion (40), that can be conveniently rewritten as follows (recall (62)),

$$\ddot{z}_n - 2\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n \dot{z}_m}{z_n - z_m} = -2i \sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n + \dot{z}_m}{z_n - z_m} - 2\sum_{m=1,m\neq n}^{N} \frac{1}{z_n - z_m} + (i\dot{z}_n + 1)\left[1 + \frac{1}{z_n} - (1+a)\sum_{m=1}^{N} \frac{i\dot{z}_m + 1}{z_m}\right], \tag{98}$$

then the polynomial $\psi(z,t)$ of degree N in z characterized by the N zeros $z_n(t)$,

$$\psi(z,t) = \prod_{n=1}^{N} [z - z_n(t)] = z^N + \sum_{m=1}^{N} c_m(t) z^{N-m} = \sum_{m=0}^{N} c_m(t) z^{N-m}, \quad c_0 = 1 \tag{99}$$

satisfies the evolution equation

$$\psi_{tt} + 2i\psi_{zt} - \psi_{zz} - i\psi_t + \psi_z - \frac{i}{z}\left[\psi_t - \frac{\dot{c}_N}{c_N}\psi\right] + \frac{1}{z}\left[\psi_z - \frac{c_{N-1}}{c_N}\psi\right] - (1+a)\left(\frac{\dot{c}_N}{c_N} + \frac{ic_{N-1}}{c_N}\right)(\psi_t + i\psi_z) = 0. \tag{100a}$$

Notation: Here and hereafter subscripted variables denote partial differentiations.

Clearly this result is a direct consequence of the (relevant) formulas ((A4)) and ((A6)), and it can be conveniently rewritten in the following two ways:

$$\psi_{tt} + 2i\psi_{zt} - i\psi_t - \psi_{zz} + \psi_z - i\left[\frac{1}{z} + (1+a)\gamma\right][\psi_t + i\psi_z] - \frac{1}{z}\gamma\psi = 0, \tag{100b}$$

$$\psi_{tt} + 2i\psi_{tz} - i\psi_t - \psi_{zz} + \psi_z - i\frac{\psi_t - \dot{c}_N}{z} + \frac{\psi_z - c_{N-1}}{z} - \frac{\psi - c_N}{z} + (1+a)(-i\psi_t + \psi_z) = 0, \tag{100c}$$

where (see (63b))

$$\gamma \equiv \gamma(t) = \frac{c_{N-1}(t) - i\dot{c}_N(t)}{c_N(t)} = \frac{\psi_z(0,t) - i\psi_t(0,t)}{\psi(0,t)}. \tag{100d}$$

And now, via the (relevant) formulas (A8), one easily obtains that the N coefficients $c_m(t)$ of the polynomial $\psi(z,t)$, see (A1), evolve according to the system of ODEs ((63a) and (63b)).

Likewise—as the diligent reader will check—analogous results can be obtained starting from the system (52) rather than (40). Then the analog of the evolution equation (100c), satisfied now by the monic polynomial $\tilde{\psi}(z,t)$ of degree N in z that has the N zeros $\tilde{z}_n(t)$,

$$\tilde{\psi}(z,t) = \prod_{n=1}^{N} [z - \tilde{z}_n(t)] = z^N + \sum_{m=1}^{N} \tilde{c}_m(t) z^{N-m} = \sum_{m=0}^{N} \tilde{c}_m(t) z^{N-m}, \quad \tilde{c}_0 = 1, \tag{101}$$

reads

$$\tilde{\psi}_{tt} + 2(1-z)i\tilde{\psi}_{tt} - \left(\frac{1}{z} - 2N + K\right) i\tilde{\psi}_t - (1-z)^2 \tilde{\psi}_{zz} + \left[\frac{1}{z} + 1 - 2N + K\right]$$
$$\times (1-z)\tilde{\psi}_z + \left[\frac{\tilde{\gamma}}{z} + N(K-N)\right]\tilde{\psi} = 0, \tag{102a}$$

where (see (66b) and (66c))

$$K \equiv K(t) = \tilde{k} + (a+1)[N + \tilde{\gamma}(t)], \tag{102b}$$

$$\tilde{\gamma} \equiv \tilde{\gamma}(t) = \frac{\tilde{c}_{N-1}(t) - i\tilde{c}_N(t)}{\tilde{c}_N(t)} = \frac{\tilde{\psi}_z(0,t) - i\tilde{\psi}_t(0,t)}{\tilde{\psi}(0,t)}. \tag{102c}$$

And the analog of the system of N ODEs ((63a) and (63b)), satisfied now by the N coefficients $\tilde{c}_m(t)$ of the polynomial $\tilde{\psi}(z,t)$, is then easily seen to be just the system ((66a)–(66c)).

Remark 4.1: The evolution equations (100c) and ((102a)–(102c)) are themselves *solvable:* note that in spite of their superficial appearance they are not (*linear*) PDEs but rather *nonlinear functional* equations, see (63b) and (102c).

V. EQUILIBRIUM CONFIGURATIONS OF THE ISOCHRONOUS SYSTEM, BEHAVIOR IN THEIR NEIGHBORHOODS, *DIOPHANTINE* FINDINGS

In this section we investigate the behavior of the system ((66a)–(66c)) in the neighborhood of its "equilibrium configurations,"

$$\tilde{c}_m(t) = \bar{c}_m, \quad \ddot{\tilde{c}}_m(t) = \dot{\tilde{c}}_m(t) = 0. \tag{103}$$

Analogous results could be investigated for the other solvable models considered in this paper, but we leave this task to the interested reader. Our motivation for focusing on the system ((66a)–(66c)) comes from its property of *isochronicity*, see *Remark 2.12:* indeed by taking advantage of it we obtain in the following the *Diophantine* findings reported at the end of Sec. II. Moreover, as we will see, there exist interesting equilibrium configurations of the system ((66a)–(66c)) that do not yield (for $N>1$)*genuine* equilibrium configurations $\bar{z}_n$ of the corresponding N-body problem (52) (namely, configurations characterized by the condition that $\bar{z}_n \neq \bar{z}_m$ whenever $n \neq m$; see the denominator in the second sum on the right-hand side of (52)), but nevertheless allow an interesting treatment.

First of all let us find these equilibrium configurations. The quantities $\bar{c}_m$ are clearly the solutions of the following system of algebraic equations (see ((66a)–(66c))):

$$m(\bar{K} - m)\bar{c}_m + \{(N+1-m)(\bar{K} - 2m) - \bar{\gamma}\}\bar{c}_{m-1} - (N-m)(N+2-m)\bar{c}_{m-2} = 0,$$

$$m = 1, \ldots, N, \quad \bar{c}_0 = 1, \quad \bar{c}_{-1} = 0, \tag{104a}$$

$$\bar{K} = \tilde{k} + (1+a)(N+\bar{\gamma}), \tag{104b}$$

$$\bar{\gamma} = \frac{\bar{c}_{N-1}}{\bar{c}_N}. \tag{104c}$$

Note that these equations are also identically satisfied for $m=N+1$ and for $m=N+2$, provided of course one sets $\bar{c}_{N+1}=\bar{c}_{N+2}=0$. While for $m=N$ via (104c) one finds that the quantity $\bar{\gamma}$ must satisfy the second-order equation

$$a\bar{\gamma}^2 + (\tilde{k}+2aN)\bar{\gamma} + N(\tilde{k}+aN) = 0 \tag{105}$$

entailing either ("*case 1*")

$$\bar{\gamma} = -N \tag{106}$$

or ("*case 2*")

$$\bar{\gamma} = -\frac{aN+\tilde{k}}{a} = -N - \frac{\tilde{k}}{a}. \tag{107}$$

To obtain the solution of the system of algebraic equations (104) we proceed as follows. Let $\bar{\psi}(z)$ be the (*monic*) polynomial of degree N in z that has the N numbers $\bar{c}_m$ as its N coefficients,

$$\bar{\psi}(z) = \sum_{m=0}^{N} \bar{c}_m z^{N-m}, \tag{108a}$$

$$\bar{c}_0 = 1. \tag{108b}$$

Then clearly (see (101)) $\bar{\psi}(z)$ is the "equilibrium" (i.e., time-independent) solution of (102a). Hence $\bar{\psi}(z)$ satisfies the ODE

$$(z-1)^2\bar{\psi}'' + \left(\frac{1}{z} + 1 - 2N + \bar{K}\right)(z-1)\bar{\psi}' + \left[\frac{\bar{\gamma}}{z} + N(N-\bar{K})\right]\bar{\psi} = 0, \tag{109}$$

with $\bar{K}$ defined by (104b) and $\bar{\gamma}$ by (104c). Here of course the appended primes indicate differentiations with respect to the independent variable z.

It is clearly convenient to set

$$\bar{\psi}(z) = \Phi(v), \quad v = z-1, \tag{110}$$

so that the ODE satisfied by $\Phi(v)$ then reads

$$(1+v)v^2\Phi'' + (1+H+Hv)v\Phi' + [\bar{\gamma} - N(H+N-1) - N(H+N-1)v]\Phi = 0, \tag{111a}$$

where we temporarily introduced the notation

$$H = 1 - 2N + \bar{K} = (1+a)\bar{\gamma} + \tilde{k} + 1 + N(a-1) \tag{111b}$$

(see also (104b)). Here of course the appended primes indicate differentiations with respect to the independent variable v.

We are seeking a solution of this ODE that is a (*monic*) polynomial of degree N in the independent variable v. Hence we set

$$\Phi(v) = \sum_{m=0}^{N} \varphi_m v^{N-m}, \tag{112a}$$

$$\varphi_0 = 1, \tag{112b}$$

which via (108a) and (112a) entails

$$\bar{c}_m = \sum_{j=0}^{m} (-)^j \binom{N+j-m}{j} \varphi_{m-j}. \tag{113}$$

It is then easily seen that the polynomial $\Phi(v)$ is a solution of (111a) provided the coefficients φ_m satisfy the recursion relation

$$(m+1)[m+1-\tilde{k}-(1+a)(N+\bar{\gamma})]\varphi_{m+1} = -[m(m-1-\tilde{k})-(m-1)(N+\bar{\gamma})]\varphi_m, \tag{114a}$$

with the "boundary conditions"

$$\varphi_{-1} = \varphi_{N+1} = 0. \tag{114b}$$

Let us consider first *case 1* (see (106)). Then the recursion (114a) takes the neat form

$$(m+1)(m+1-\tilde{k})\varphi_{m+1} = -m(m-1-\tilde{k})\varphi_m. \tag{115}$$

Remarkably, the constant a has completely dropped out of this formula.

Clearly this recursion relation, for a *generic* value of the parameter $\tilde{k}$, has the solution (clearly consistent with the boundary conditions (114b) and with (112b))

$$\varphi_m = \delta_{0,m}. \tag{116}$$

But it is moreover easily seen that, if the parameter $\tilde{k}$ is a *positive integer* less that N,

$$\tilde{k} = \nu, \tag{117a}$$

$$\nu = 1, 2, \ldots, N-1, \tag{117b}$$

then the recursion relations ((114a) and (114b)) admit the more general solution (also clearly consistent with the boundary conditions (114b) and with (112b))

$$\varphi_m = \delta_{0,m} + \left(\delta_{\nu,m} + \frac{\nu}{\nu+1}\delta_{\nu+1,m}\right)h, \tag{118}$$

with h an *arbitrary* number. Hereafter we treat this more general solution, of course on the understanding that the constant h must be set to *zero* if the parameter $\tilde{k}$ does *not* satisfy the condition (117). The corresponding equilibrium solution of the system ((66a)–(66c)) is (see (113))

$$\bar{c}_m = (-)^m \left[\binom{N}{m} + (-)^\nu \frac{N(\nu+1)-\nu(m+1)}{(\nu+1)(N-\nu)} \binom{N-\nu}{m-\nu} h\right]. \tag{119}$$

Note the consistency (via (104c)) of this expression of the coefficients $\bar{c}_m$ with the condition (106).

Hence in this *case 1* (see (108))

$$\bar{\psi}(z) = (z-1)^N + (z-1)^{N-1-\nu}\left(z - \frac{1}{\nu+1}\right)h. \tag{120}$$

Remark 5.1: Clearly the N zeros $\bar{z}_n$ of this polynomial $\bar{\psi}(z)$ can *all* be *distinct* (entailing that

the corresponding equilibrium configuration of the N-body problem (52) is *genuine*) only if $\nu = N-1$ and $h \neq 0$, so that

$$\bar{\psi}(z) = (z-1)^N + \left(z - \frac{1}{N}\right)h\,. \quad \blacksquare \tag{121}$$

Next, let us ascertain the equilibrium configuration corresponding to *case 2* (see (107)). Then the recursion (114a) takes the neat form

$$(m+1)(m-\mu)\varphi_{m+1} = -(m-1)(m-\mu-1)\varphi_m, \tag{122}$$

where we now introduce the convenient parameter μ via the assignment

$$\mu = -\frac{\tilde{k}+a}{a}, \quad \tilde{k} = -(\mu+1)a. \tag{123}$$

Now it is easily seen that, for *generic* values of this parameter μ, this recursion has the solution (clearly consistent with the boundary conditions (114b) and with (112b))

$$\varphi_m = \delta_{0,m} + \delta_{1,m}\frac{\mu+1}{\mu}, \tag{124}$$

while if μ is a *positive* integer less than N,

$$\mu = 1,2,\ldots,N-1, \tag{125}$$

then the more general solution

$$\varphi_m = \delta_{0,m} + \delta_{1,m}\frac{\mu+1}{\mu} + \delta_{\mu+1,m}h, \tag{126}$$

with h an *arbitrary* number, also solves the recursion relation (122) and is compatible with the boundary conditions (114b) and with (112b). Hereafter we treat this more general solution, of course on the understanding that the constant h must be set to *zero* if the parameters a and $\tilde{k}$ do not satisfy via (123) the condition (125). The corresponding equilibrium solution of the system ((66a)–(66c)) is (see (113))

$$\bar{c}_m = (-)^m\left[\binom{N}{m}\frac{N\mu - m(\mu+1)}{N\mu} + (-)^{\mu+1}\binom{N-\mu-1}{m-\mu-1}h\right]. \tag{127}$$

Note the consistency (via (104c) and (123)) of this expression of the coefficients $\bar{c}_m$ with the condition (107).

Hence in this *case 2* (see (108))

$$\bar{\psi}(z) = (z-1)^{N-1}\left(z + \frac{1}{\mu}\right) + (z-1)^{N-\mu-1}h. \tag{128}$$

Remark 5.2: Clearly for $N>2$ the N zeros $\bar{z}_n$ of this polynomial $\bar{\psi}(z)$ can *all* be *distinct* (entailing that the corresponding equilibrium configuration of the N-body problem (52) is *genuine*) only if $\mu = N-1$ or $\mu = N-2$ and if moreover $h \neq 0$. ■

Next, let us investigate the behavior of the system of ODEs ((66a)–(66c)) in the neighborhood of these equilibrium configurations, (119) (entailing (106)) and (127) (entailing (107)). To this end we set

$$\tilde{c}_m(t) = \tilde{c}_m + \varepsilon\rho_m(t) + \mathcal{O}(\varepsilon^2), \tag{129}$$

treating in the standard manner ε as a small parameter. We thus obtain the linearized system of ODEs

$$\ddot{\rho}_m + (2m - \bar{K})i\dot{\rho}_m + (2N + 1 - 2m)i\dot{\rho}_{m-1} + m(\bar{K} - m)\rho_m + [(N + 1 - m)(\bar{K} - 2m) - \bar{\gamma}]\rho_{m-1} - (N - m)$$
$$\times(N + 2 - m)\rho_{m-2} + \frac{m(1 + a)\bar{c}_m + [(N + 1 - m)(1 + a) - 1]\bar{c}_{m-1}}{\bar{c}_N}(\rho_{N-1} - i\dot{\rho}_N - \bar{\gamma}\rho_N) = 0,$$

$$m = 1, \ldots, N, \quad \rho_0 = 0, \quad \rho_{-1} = 0, \tag{130}$$

with $\bar{K}$ defined by (104b). To obtain this system of ODEs from ((66a)–(66c)) we used the relation

$$\tilde{\gamma}(t) = \bar{\gamma} + \varepsilon\frac{\rho_{N-1}(t) - i\dot{\rho}_N(t) - \bar{\gamma}\rho_N(t)}{\bar{c}_N} + O(\varepsilon^2) \tag{131}$$

implied by (66c) and (129)

The general solution of this linear system of ODEs, (130), reads

$$\rho_m(t) = \sum_{n=1}^{N} [a_n^{(+)} r_m^{(+)(n)} \exp(ip_n^{(+)}t) + a_n^{(-)} r_m^{(-)(n)} \exp(ip_n^{(-)}t)], \tag{132}$$

where the $2N$ numbers $a_n^{(\pm)}$ are *arbitrary* (to be fixed by the initial data) while the $2N$ numbers $p_n^{(\pm)}$, respectively, the $2N$ corresponding (t-independent) N-vectors $\underline{r}^{(\pm)(n)} \equiv (r_1^{(\pm)(n)}, \ldots, r_N^{(\pm)(n)})$, are the eigenvalues, respectively, the eigenvectors, of the (N-vector) generalized eigenvalue equation

$$(p^2 + Ap + B)\underline{r} = 0, \tag{133}$$

with the two $N \times N$ matrices A and B defined (componentwise) as follows:

$$A_{nm} = (2n - \bar{K})\delta_{n,m} + (2N + 1 - 2n)\delta_{n-1,m} + C_n\delta_{Nm}, \tag{134a}$$

$$B_{nm} = n(n - \bar{K})\delta_{n,m} + [(N + 1 - n)(2n - \bar{K}) + \bar{\gamma}]\delta_{n-1,m} + (N - n)(N + 2 - n)\delta_{n-2,m}$$
$$+ C_n(\delta_{N-1,m} - \bar{\gamma}\delta_{N,m}), \tag{134b}$$

where

$$C_n = -\frac{n(1 + a)\bar{c}_n + [(N + 1 - n)(1 + a) - 1]\bar{c}_{n-1}}{\bar{c}_N}. \tag{134c}$$

These formulas imply of course that the $2N$ numbers $p_n^{(\pm)}$ are the roots of the polynomial equation (of degree $2N$ in p)

$$\det[p^2 + Ap + B] = 0, \tag{135a}$$

namely

$$\det[p^2 + Ap + B] = \prod_{n=1}^{N} [(p - p_n^{(+)})(p - p_n^{(-)})]. \tag{135b}$$

Let us now consider the two cases, as discussed earlier.

In *case 1*, via (104b) with (106) (implying $\bar{K} = \tilde{k} = \nu$), (117) and (119), and setting for notational convenience

$$(-)^{\nu}(\nu+1)h=f, \quad (-)^{\nu}\nu(1+a)h=g \tag{136}$$

one finds for the matrices A and B the expression ((71a)–(71d)).

Likewise, in *case 2*, via (104b) with (107) (implying $\bar{K}=-\tilde{k}/a=\mu+1$, $\bar{\gamma}=-N+\mu+1$), (123), (125), and (127), and setting for notational convenience

$$(-)^{\mu}\mu h=f, \quad \mu=\nu, \quad \tilde{k}=g, \tag{137}$$

one finds for the matrices A and B the expression ((72a)–(72d)).

Remark 5.3: A shortcut to arrive at the solution (116) entailing

$$\bar{\psi}(z)=(z-1)^N \tag{138}$$

goes as follows. Let the $N\times N$ matrix $\bar{U}$ be an "equilibrium," i.e., time-independent, solution of the matrix equation (54), so that it satisfies (recall (62) and (56j))

$$(\bar{U}-1)\left(\bar{U}-\frac{a}{a+\tilde{k}}\right)=0, \tag{139}$$

and notice that

$$\bar{U}=\mathbf{1} \tag{140}$$

is clearly a solution of this equation. Then the determinantal expression (65) (recall (62)) of $\bar{\psi}(z)$, with this assignment of $\bar{U}$, yields immediately (138).

But this approach is quite misleading, because one is dealing here with the singular case in which some eigenvalues of the matrix U coincide—indeed all of them.

A hint of the misleading character of this result is provided by the following observation. The solution we just mentioned, which is clearly characterized by the "equilibrium configuration" (recall (62))

$$\bar{z}_n=1 \tag{141}$$

(for *all* values of n), might be considered to satisfy the equations of motions (52) (recall (62)), although of course only by assigning an appropriate value to an ambiguous expression ("zero divided by zero"). And of course, as entailed by the above-mentioned analysis, and implied by

$$\bar{\gamma}=-\sum_{n}^{N}\frac{1}{z_n} \tag{142}$$

(see (104c) and the first equation of Eq. (A6)), this equilibrium configuration is consistent with the value of $\bar{\gamma}$ corresponding to *case 1* (see (119)). One might then guess that the other analogous solution of (139),

$$\bar{U}=\frac{a}{a+\tilde{k}}\mathbf{1}, \tag{143}$$

yields an equilibrium configuration corresponding to *case 2*. But this does *not* happen. Indeed this solution entails (by the same argument as given earlier; again, for *all* values of n)

$$\bar{z}_n=\frac{a+\tilde{k}}{a}, \tag{144}$$

and via the same argument as given earlier this yields

$$\overline{\gamma} = -\frac{a+\widetilde{k}}{a}N = -N - N\frac{\widetilde{k}}{a}, \tag{145}$$

which does *not* agree with (107) (except for $N=1$, when indeed there is no trouble with coinciding values of z_n). And it is moreover clear that this "equilibrium configuration," (144), is inconsistent with the equations of motion (52) (recall (62)).

The singular character of the "equilibrium positions" of the N-body problems considered herein is also manifested by the following phenomenon. In order to try and study the motion of the system (52) in the neighborhood of the "equilibrium configuration" (141) (a quite legitimate enterprise), set

$$z_n(t) = 1 + \varepsilon w_n(t), \tag{146}$$

assign some arbitrary (of course, not all vanishing) values $w_n(0)$, $\dot{w}_n(0)$ and try to extract the time evolution of the coordinate $w_n(t)$ via **Proposition 2.7**, treating ε as a small parameter. One thereby discovers that such a procedure is *inconsistent:* as soon as the evolution starts (namely as soon as $t>0$), the coordinates $z_n(t)$ differ from unity by amounts of order unity rather than of order ε, in contrast to what the assignment (146) assumed to begin with.

This situation makes it impossible—or at least quite difficult—to follow such a route in order to prove the *Diophantine* findings obtained above and formulated at the end of Sec. II. ■

But as we saw earlier, no inconsistency arises when one investigates the behavior of solutions of the system of evolution equation ((66a)–(66c)) in the neighborhood of their equilibrium configurations—even when the analogous treatment of the evolution equations (52) in the neighborhood of the corresponding equilibrium configurations causes trouble, as indicated in *Remark 5.3*. Hence the periodicity properties discussed in *Remark 2.12* must hold as well for the solutions $\rho_m(t)$, and this implies that the numbers $p_m^{(\pm)}$ yielded by the generalized eigenvalue problem discussed earlier must satisfy certain *Diophantine* restrictions, in all the cases identified in *Remark 2.12*, and for the appropriate choices of the parameters $\widetilde{k}$, ν, μ, and h as discussed earlier. For the sake of brevity we leave to the interested reader the formulation of the corresponding results. Motivated by these findings we investigated numerically the solutions of the determinantal equations ((135a) and (135b)) with ((71a)–(71d)) and ((72a)–(72d)), and we were thereby led to formulate the conjectures reported at the end of Sec. II—the validity of which extends, remarkably, beyond the restricted values of the parameters ν, f, and g that are implied by the above-mentioned treatment.

VI. OUTLOOK

As mentioned in Sec. I, there is a simple procedure to manufacture *solvable* systems of equations of motion describing (according to the Newtonian paradigm: "the acceleration of each particle equals a force assigned in terms of the position, and possibly also of the velocities, of all the N particles") the evolution of N coordinates $z_n(t)$ in the (*complex*) z-plane: (i) start from a *solvable* matrix ODE describing the time evolution (within an appropriate class) of an $N\times N$ matrix $U(t)$, (ii) identify the coordinates $z_n(t)$ as the N *eigenvalues* of the matrix $U(t)$ and identify the equations of motion that then describe their evolution, (iii) find a suitable *ansatz*, compatible with the time evolution of (all the N^2 matrix elements of) $U(t)$, expressing in terms of the N eigenvalues $z_n(t)$ (and possibly of their time-derivatives) the other $N(N-1)$ variables that are generally needed, in addition to the N eigenvalues, in order to identify completely the $N\times N$ matrix $U(t)$, and whose time-evolution is therefore generally entangled with that of the N eigenvalues $z_n(t)$. Thereby the system of evolution ODEs satisfied by the coordinates $z_n(t)$ becomes self-contained, and it is likely to be interpretable as a (possibly interesting—but this is a value judgment) N-body problem characterized by Newtonian equations of motions. And this N-body model is then, by construction, *solvable:* indeed its solution consists now in the (merely algebraic) task of finding the N eigenvalues of the matrix $U(t)$, whose time evolution is supposed to be known inasmuch as we started to begin with from a *solvable* matrix evolution equation.

Of the three steps just outlined, the first one is to some extent (but not quite) amenable to systematic analysis, the second works according to a well-understood machinery, the third requires that a *miracle* occur, and some *guess-work* to identify it. So far this approach has yielded several (new) *solvable* models, but finding each one of them constituted a nontrivial challenge. In this paper we have tersely surveyed (some of) the results obtained in this manner, and we have described and analyzed some *new* N-body models obtained in this manner. Can this approach be further exploited to manufacture/discover additional *solvable* models? Presumably yes: indeed one more *integrable/solvable* model of goldfish type has just been discovered, as will be reported in a forthcoming paper.[18] Does it make sense to continue this fishing expedition? Presumably yes, as long as the catch is interesting; but this, let us repeat, entails a value judgment.

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APPENDIX: SOME USEFUL IDENTITIES

In this Appendix we list certain useful relations; several of them reproduce (but in a more convenient notation) results already reported in Appendix B of Ref. 1, while the derivation of the new ones is sufficiently straightforward not to required any explicit elaboration here. Note that not all the formulas reported here are used in this paper, but we thought it useful to collect a rather complete compilation here as a convenient tool for future utilizations.

Let $\psi(z,t)$ be a *monic* polynomial of degree N in z, and let us indicate as $z_n \equiv z_n(t)$ its N zeros and as $c_m \equiv c_m(t)$ its N coefficients (see (99)):

$$\psi(z,t) = \prod_{n=1}^{N} [z - z_n(t)] = z^N + \sum_{m=1}^{N} c_m(t) z^{N-m} = \sum_{m=0}^{N} c_m(t) z^{N-m}, \quad c_0 = 1. \tag{A1}$$

Then clearly

$$\psi_z(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1}, \tag{A2a}$$

$$\psi_t(z,t) = \psi(z,t) \sum_{n=1}^{N} [z - z_n(t)]^{-1} [-\dot{z}_n(t)]. \tag{A2b}$$

Here (and throughout) subscripted variables denote partial differentiations, $\psi_z \equiv \partial\psi/\partial z$, $\psi_t \equiv \partial\psi/\partial t$. To conveniently streamline the look of these, and of the following, formulas, we rewrite these two relations via the self-evident notation

$$\psi_z \Leftrightarrow 1, \tag{A3a}$$

$$\psi_t \Leftrightarrow -\dot{z}_n, \tag{A3b}$$

and we write accordingly the following relations:

$$z\psi_z - N\psi \Leftrightarrow z_n, \tag{A3c}$$

$$z^2\psi_z + (c_1 - Nz)\psi \Leftrightarrow z_n^2, \tag{A3d}$$

$$z^3\psi_z - (Nz^2 - c_1 z + c_1^2 - 2c_2)\psi \Leftrightarrow z_n^3, \tag{A3e}$$

$$\frac{1}{z}\left[\psi_z - \frac{c_{N-1}}{c_N}\psi\right] \Leftrightarrow \frac{1}{z_n}, \tag{A3f}$$

$$z\psi_t - \dot{c}_1\psi \Leftrightarrow -\dot{z}_n z_n, \tag{A3g}$$

$$\frac{1}{z}\left[\psi_t - \frac{\dot{c}_N}{c_N}\psi\right] \Leftrightarrow -\frac{\dot{z}_n}{z_n}, \tag{A3h}$$

$$\psi_{zz} \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2}{z_n - z_m}, \tag{A3i}$$

$$z\psi_{zz} - 2(N-1)\psi_z \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_m}{z_n - z_m}, \tag{A3j}$$

$$z\psi_{zz} \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n}{z_n - z_m}, \tag{A3k}$$

$$z\psi_{zz} - (N-1)\psi_z \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{z_n + z_m}{z_n - z_m}, \tag{A4}$$

$$z^2\psi_{zz} - N(N-1)\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n^2}{z_n - z_m}, \tag{A5a}$$

$$z^2\psi_{zz} - 2[(N-2)z - c_1]\psi_z + N(N-3)\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_m^2}{z_n - z_m}, \tag{A5b}$$

$$z^2\psi_{zz} - [(N-2)z - c_1]\psi_z - N\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{z_n^2 + z_m^2}{z_n - z_m}, \tag{A5c}$$

$$z^2\psi_{zz} - 2(N-1)z\psi_z + N(N-1)\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n z_m}{z_n - z_m}, \tag{A5d}$$

$$z^3\psi_{zz} - N(N-1)z\psi + 2(N-1)c_1\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n^3}{z_n - z_m}, \tag{A5e}$$

$$z[z^2\psi_{zz} - 2(N-1)z\psi_z + N(N-1)\psi] \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n^2 z_m}{z_n - z_m}, \tag{A5f}$$

$$z^3\psi_{zz} - 2(N-2)z^2\psi_z + 2c_1 z\psi_z + [N(N+1)z - 2(N-1)c_1]\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n z_m^2}{z_n - z_m}, \tag{A5g}$$

$$z^3\psi_{zz} - (2N-3)z^2\psi_z + c_1 z\psi_z + [N^2 z - (N-1)c_1]\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{z_n z_m^2 + z_n^2 z_m}{z_n - z_m}, \tag{A5h}$$

$$z^4\psi_{zz} - [N(N-1)z^2 - 2(N-1)c_1 z + 2(N-1){c_1}^2 - 2(2N-3)c_2]\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n^4}{z_n - z_m}, \tag{A5i}$$

$$z^4\psi_{zz} - 2z^2[(N-2)z - c_1]\psi_z + [N(N-3)z^2 - 2(N-1)c_1 z + 2c_2]\psi \Leftrightarrow \sum_{m=1,m\neq n}^{N} \frac{2z_n^2 z_m^2}{z_n - z_m}, \tag{A5j}$$

$$\psi_{zt} \Leftrightarrow -\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n + \dot{z}_m}{z_n - z_m}, \tag{A5k}$$

$$z\psi_{zt} \Leftrightarrow -\sum_{m=1,m\neq n}^{N} \frac{(\dot{z}_n + \dot{z}_m)z_n}{z_n - z_m}, \tag{A5l}$$

$$z\psi_{zt} - (N-1)\psi_t \Leftrightarrow -\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n z_m + \dot{z}_m z_n}{z_n - z_m}, \tag{A5m}$$

$$z^2\psi_{zt} + [c_1 - (N-2)z]\psi_t - \dot{c}_1\psi \Leftrightarrow -\sum_{m=1,m\neq n}^{N} \frac{\dot{z}_n z_m^2 + \dot{z}_m z_n^2}{z_n - z_m}, \tag{A5n}$$

$$\psi_{tt} \Leftrightarrow = -\ddot{z}_n(t) + \sum_{m=1,m\neq n}^{N} \frac{2\dot{z}_n \dot{z}_m}{z_n - z_m}. \tag{A5o}$$

To obtain those of the formulas written above which are not just streamlined versions of equations already reported in Appendix B of Ref. 1, we used the relations

$$\frac{c_{N-1}}{c_N} = -\sum_{n=1}^{N} \frac{1}{z_n}, \quad \frac{\dot{c}_N}{c_N} = \sum_{n=1}^{N} \frac{\dot{z}_n}{z_n}, \tag{A6}$$

which are obvious consequences of the formulas

$$c_N(t) = \prod_{n=1}^{N} [-z_n(t)] = \psi(0,t), \quad c_{N-1}(t) = \sum_{n=1}^{N} \prod_{m=1,m\neq n}^{N} [-z_m(t)] = \psi_z(0,t), \tag{A7}$$

themselves direct consequences of (A1).

Likewise, we introduce the following notation whereby in the formulas written in the following (which are also straightforward consequences of (A1)) the expression on the right-hand side identifies the coefficient of z^{N-m} in the polynomial (of degree N or less) appearing on the left-hand side:

$$\psi \leftrightarrow c_m, \tag{A8a}$$

$$\frac{\psi - c_N}{z} \leftrightarrow c_{m-1}, \tag{A8b}$$

$$\psi_z \leftrightarrow (N-m+1)c_{m-1}, \tag{A8c}$$

$$z\psi_z \leftrightarrow (N-m)c_m, \tag{A8d}$$

$$\frac{\psi_z - c_{N-1}}{z} \leftrightarrow (N-m+2)c_{m-2}, \tag{A8e}$$

$$\psi_{zz} \leftrightarrow (N-m+2)(N-m+1)c_{m-2}, \tag{A8f}$$

$$z\psi_{zz} \leftrightarrow (N-m+1)(N-m)c_{m-1}, \tag{A8g}$$

$$z^2\psi_{zz} \leftrightarrow (N-m)(N-m-1)c_m, \tag{A8h}$$

$$\psi_t \leftrightarrow \dot{c}_m, \tag{A8i}$$

$$z\psi_t \leftrightarrow \dot{c}_{m+1}, \tag{A8j}$$

$$\frac{\psi_t - \dot{c}_N}{z} \leftrightarrow \dot{c}_{m-1}, \tag{A8k}$$

$$\psi_{zt} \leftrightarrow (N-m+1)\dot{c}_{m-1}, \tag{A8l}$$

$$z\psi_{zt} \leftrightarrow (N-m)\dot{c}_m, \tag{A8m}$$

$$\psi_{tt} \leftrightarrow \ddot{c}_m, \tag{A8n}$$

$$N\psi - z\psi_z \leftrightarrow mc_m, \tag{A8o}$$

$$N^2\psi - (2N-1)z\psi_z + z^2\psi_{zz} \leftrightarrow m^2c_m, \tag{A8p}$$

$$(N+1)\frac{\psi - c_N}{z} - \psi_z \leftrightarrow mc_{m-1}, \tag{A8q}$$

$$(N+1)^2\frac{\psi - c_N}{z} - (2N+1)\psi_z + z\psi_{zz} \leftrightarrow m^2c_{m-1}, \tag{A8r}$$

$$\frac{\psi - c_N - c_{N-1}z}{z^2} \leftrightarrow c_{m-2}, \tag{A8s}$$

$$\frac{(N+2)\psi - z\psi_z - (N+2)c_N - (N+1)zc_{N-1}}{z^2} \leftrightarrow mc_{m-2}, \tag{A8t}$$

$$\frac{(N+2)^2(\psi - c_N) - z[(2N+3)\psi_z + (N+1)^2 c_{N-1}] + z^2\psi_{zz}}{z^2} \leftrightarrow m^2 c_{m-2}, \tag{A8u}$$

$$(N+1)\frac{\psi_t - \dot{c}_N}{z} - \psi_{zt} \leftrightarrow m\dot{c}_{m-1}. \tag{A8v}$$

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On kernel formulas and dispersionless Hirota equations of the extended dispersionless BKP hierarchy

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We derive dispersionless Hirota equations of the extended dispersionless BKP(EdBKP) hierarchy proposed by Takasaki from the method of kernel formula provided by Carroll and Kodama. Moreover, we verify associativity equations (WDVV equations) in the EdBKP hierarchy from dispersionless Hirota equations and give a realization of associative algebra with structure constants expressed in terms of the residue formula. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2358002]

I. INTRODUCTION

Dispersionless integrable systems (DIS) are integrable hierarchies in dispersionless limit (or quasiclassical limit). Among them the dispersionless Kadomtsev-Petviashvili (dKP) and dispersionless Toda (dToda) hierarchies are special since they have been recognized as universal DIS in several fields of theoretical physics and mathematics (see, e.g., Refs. 1, 4, 9, 11, 13–15, 18, 19, 27, and 29 and references therein). The solutions of the dKP and dToda hierarchies can be characterized by a single function called τ functions, the logarithm of them; namely, $\mathcal{F}=\log\tau$ describe free energy of some two-dimensional topological field theories in genus zero and satisfy the Witten-Dijkgraaf-Verlinde-Verlinde (WDVV) equations.[10,11,32] In particular, the finite-dimensional reductions of dKP and dToda systems are realized as special solutions of topological Landau-Ginzburg models of A-type and topological CP^1 models, respectively.[1,10,12,18] In terms of free energy $\mathcal{F}$, the hierarchy flows of dKP and dToda can be written as a set of second derivatives of $\mathcal{F}$ called dispersionless Hirota (dHirota) equations. There are a lot of works devoted to derive dHirota equations. In Ref. 29, Takasaki and Takebe derived dHirota equations of the dKP hierarchy from dispersionless limit of differential Fay identity. Carroll and Kodama[5] studied the same dHirota equation from the method of kernel formula. On the other hand, Wiegmann, Zabrodin *et al.*[17,31] investigated dHirota equations of the dToda hierarchy in the context of conformal mapping. More recently, Teo[30] derived dHirota equations of the dKP and dToda hierarchies from complex analysis using the notions of Grunsky coefficients and Faber polynomials.

Our main purpose in this work is to demonstrate the applicability of the kernel formula to other dispersionless integrable hierarchies. In particular, we would like to derive dHirota equations of a universal integrable hierarchy underlying topological Landau-Ginzburg models of a D-type proposed by Takasaki.[24] Since this integrable hierarchy is an extension of the dispersionless BKP (dBKP) hierarchy[2,8,16,23] with two sets of time variables, we refer it to the extended dispersionless BKP (EdBKP) hierarchy.[6] The EdBKP hierarchy resembles the dToda hierarchy in many formulations such as dressing operators, Orlov functions, the Riemann-Hilbert problem, additional symmetries, w algebras, hodograph solutions, etc.[6,24] Motivated by the work for dKP,[5] we shall show that the method of a kernel formula can be applied to the EdBKP hierarchy without difficulty. As a byproduct, associativity equations (WDVV equations) in the EdBKP hierarchy can be verified

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directly from dHirota equations. Therefore our results indeed provide another point of view to understand the integrability of the dBKP hierarchy in connection with topological field theories.

Let us briefly recall the method of the kernel formula[5] for the derivation of dHirota equations of the dKP hierarchy. The dKP hierarchy is defined by the Lax equations,

$$\partial_{t_n}\lambda = \{\mathcal{B}_n, \lambda\}, \quad \mathcal{B}_n = (\lambda^n)_{\geq 0}, \quad n = 1,2, \ldots,$$

where the Lax operator λ is a Laurent series of the form

$$\lambda = p + \sum_{n=1}^{\infty} u_{n+1} p^{-n},$$

where u_j are functions of the time variables $t=(x=t_1,t_2,\ldots)$, $(A(p))_{\geq 0}$ denotes the projection on the polynomial part of $A(p)$, and $\{A,B\}$ stands for the Poisson bracket,

$$\{A,B\} = \frac{\partial A}{\partial p}\frac{\partial B}{\partial x} - \frac{\partial A}{\partial x}\frac{\partial B}{\partial p}.$$

It can be shown[27,29] that there exists a function $\mathcal{F}(t)$ called free energy such that

$$\mathcal{B}_n(\lambda) = \lambda^n - \sum_{m=1}^{\infty} \frac{\mathcal{F}_{n,m}}{m}\lambda^{-m},$$

where $\mathcal{F}_{n,m}=\partial_{t_n}\partial_{t_m}\mathcal{F}$ and thus $\mathcal{F}_{n,m}=\mathcal{F}_{m,n}$. Particularly, for $\mathcal{B}_1=p$ we have

$$p(\lambda) = \lambda - \sum_{m=1}^{\infty} \frac{\mathcal{F}_{1,m}}{m}\lambda^{-m}, \tag{1}$$

which can be viewed as the inverse map of $\lambda(p)$. Multiplying $\lambda^{n-1}\partial_p\lambda$ with $n\geq 1$ to (1) and taking the projection $()_{\geq 0}$, we obtain

$$\partial_p Q_{n+1}(\lambda) - p(\lambda)\partial_p Q_n(\lambda) - \sum_{m=1}^{n-1} \frac{\mathcal{F}_{1,m}}{m}\partial_p Q_{n-m}(\lambda), \quad n \geq 1,$$

where $Q_n=\mathcal{B}_n/n$. Multiplying μ^{-n} and summing over $n\geq 0$, we have

$$1 = \left(\mu - p(\lambda) - \sum_{m=1} \frac{\mathcal{F}_{1,m}}{m}\mu^{-m}\right)\sum_{j=1} \partial_p Q_j(\lambda)\mu^{-j},$$

$$= (p(\mu) - p(\lambda))\sum_{j=1} \partial_p Q_j(\lambda)\mu^{-j},$$

or

$$\frac{1}{p(\mu)-p(\lambda)} = \sum_{j=1}^{\infty} \partial_p Q_j(\lambda)\mu^{-j},$$

which is the kernel formula for the generating function of $\partial_p Q_j(\lambda)$. Integrating above with respect to $p(\lambda)$ and fixing the normalization at $\mu=\infty$, then

$$\frac{\mu}{p(\mu)-p(\lambda)} = e^{\sum_{j=1}^{\infty} Q_j(\lambda)\mu^{-j}},$$

which together with the expressions of the second derivatives of $\mathcal{F}$ for $\mathcal{B}_j(\lambda)$ and $p(\lambda)$ yields dHirota equations of the dKP hierarchy:[5,29]

$$D(\mu)\partial_{t_1}\mathcal{F} - D(\lambda)\partial_{t_1}\mathcal{F} = (\mu-\lambda)(1-e^{D(\mu)D(\lambda)\mathcal{F}}), \tag{2}$$

where $D(z)=\Sigma_{m=1}^{\infty} z^{-m}\partial_{t_m}/m$. A convenient way to obtain a set of relations defined by $\mathcal{F}_{m,n}$ is to consider (2) under the limit $\mu\to\lambda$. Then one gets

$$\partial_\lambda D(\lambda)\partial_{t_1}\mathcal{F} = 1 - e^{D(\lambda)D(\lambda)\mathcal{F}}.$$

By comparing the coefficients of λ^{-n} on both sides, one obtains[5]

$$\mathcal{F}_{1j} = P_{j+1}(Z_1=0, Z_2, \ldots, Z_{j+1}), \quad j\geq 1,$$

where P_j are elementary Schur polynomials and $Z_j=\Sigma_{n+m=j}(\mathcal{F}_{nm}/nm)$. A few equations from such an expansion have been given in Ref. 5. Here we just mention the simplest nontrivial equation,

$$\frac{1}{2}\mathcal{F}_{11}^2 - \frac{1}{3}\mathcal{F}_{13} + \frac{1}{4}\mathcal{F}_{22} = 0,$$

which, after noticing $u=u_2=\mathcal{F}_{11}$ and setting $t_2=y$, $t_3=t$, is just the (2+1)-dimensional dKP equation,[14]

$$u_t = 3uu_x + \frac{3}{4}\partial_x^{-1}u_{yy}.$$

Therefore, the kernel formula provides an elementary and convenient way to derive dHirota equations of dKP from the Lax formulation without referring to its dispersive counterparts, such as the (differential) Fay identity. For the dToda hierarchy,[26,28,29] its associated dHirota equations (see, e.g., Refs. 17, 30, 31, and 33) can also be derived from the method of kernel formula. We omit the derivation here and refer to our preprint[7] for details. The rest of the paper is organized as follows. In Sec. II we turn to the EdBKP hierarchy to investigate its dHirota equations. In Sec. III we verify associativity equations (or WDVV equations) in the EdBKP hierarchy from dHirota equations. The realization of associative algebra and the residue formula for structure constants of the associative algebra are also given. Section IV is devoted to the concluding remarks.

II. EXTENDED DISPERSIONLESS BKP HIERARCHY

A. Lax formalism

Having illustrated the derivation of dHirota equations of the dKP hierarchy, now we like to apply the method of kernel formula to the EdBKP hierarchy, which is the integrable hierarchy underlying topological Landau-Ginzburg models of a D type proposed by Takasaki[24] (see also Ref. 6). The EdBKP hierarchy is described by

$$\begin{gathered}\partial_{t_{2n+1}}\lambda = \{\mathcal{B}_{2n+1},\lambda\}, \quad \partial_{\bar{t}_{2n+1}}\lambda = \{\bar{\mathcal{B}}_{2n+1},\lambda\},\\ \partial_{t_{2n+1}}\bar{\lambda} = \{\mathcal{B}_{2n+1},\bar{\lambda}\}, \quad \partial_{\bar{t}_{2n+1}}\bar{\lambda} = \{\bar{\mathcal{B}}_{2n+1},\bar{\lambda}\}, \quad n=0,1,2,\ldots,\end{gathered} \tag{3}$$

with

$$\lambda = p + \sum_{n=1}^{\infty} u_{2n}p^{-2n+1}, \quad \bar{\lambda} = \sum_{n=0}^{\infty}\bar{u}_{2n}p^{2n+1}, \quad \bar{u}_0 \neq 0$$

and

$$\mathcal{B}_{2n+1} = (\lambda^{2n+1})_{\geq 0}, \quad \bar{\mathcal{B}}_{2n+1} = (\bar{\lambda}^{-2n-1})_{\leq -1},$$

where the coefficient functions u_{2n} and $\bar{u}_{2n}$ depend on the time variables $t=(t_1=x,t_3,\ldots)$ and $\bar{t}=(\bar{t}_1,\bar{t}_3,\ldots)$, the Poisson bracket $\{,\}$ here is defined as before and $(A)_{\leq -1}=A-(A)_{\geq 0}$. One can view

λ as a map defined in domain D_∞ containing $p=\infty$, while $\overline{\lambda}$ in D_0 containing $p=0$. Noting that $\lambda(-p)=-\lambda(p)$ and $\overline{\lambda}(-p)=-\overline{\lambda}(p)$ and thus $(\mathcal{B}_{2n+1})_{[0]}=(\overline{\mathcal{B}}_{2n+1})_{[0]}=0$.

The Lax equations (3) are equivalent to the zero curvature equations,

$$\partial_{t_{2n+1}}\mathcal{B}_{2m+1}-\partial_{t_{2m+1}}\mathcal{B}_{2n+1}+\{\mathcal{B}_{2m+1},\mathcal{B}_{2n+1}\}=0,$$

$$\partial_{\overline{t}_{2n+1}}\overline{\mathcal{B}}_{2m+1}-\partial_{\overline{t}_{2m+1}}\overline{\mathcal{B}}_{2n+1}+\{\overline{\mathcal{B}}_{2m+1},\overline{\mathcal{B}}_{2n+1}\}=0,$$

$$\partial_{\overline{t}_{2n+1}}\mathcal{B}_{2m+1}-\partial_{t_{2m+1}}\overline{\mathcal{B}}_{2n+1}+\{\mathcal{B}_{2m+1},\overline{\mathcal{B}}_{2n+1}\}=0,$$

which guarantees that the Lax equations (3) commute between themselves. Since the first member involving t_{2n+1} flows only is just the dBKP hierarchy and that is the reason why we call this integrable hierarchy the EdBKP hierarchy. It can be shown[24] that there exists a single function $\mathcal{F}(t,\overline{t})$ (free energy) from which one can define the functions

$$S(\lambda)=\sum_{n=0}^{\infty}t_{2n+1}\lambda^{2n+1}-\sum_{n=0}^{\infty}\frac{1}{2n+1}\partial_{t_{2n+1}}\mathcal{F}\lambda^{-2n-1},$$

$$\overline{S}(\overline{\lambda})=\sum_{n=0}^{\infty}\overline{t}_{2n+1}\overline{\lambda}^{-2n-1}-\sum_{n=0}^{\infty}\frac{1}{2n+1}\partial_{\overline{t}_{2n+1}}\mathcal{F}\overline{\lambda}^{2n+1},$$

such that

$$\mathcal{B}_{2n+1}(\lambda)=\partial_{t_{2n+1}}S\Big|_{\lambda\ \text{fixed}}=\lambda^{2n+1}-\sum_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{2n+1,2m+1}\lambda^{-2m-1},\tag{4}$$

$$\mathcal{B}_{2n+1}(\overline{\lambda})=\partial_{t_{2n+1}}\overline{S}\Big|_{\overline{\lambda}\ \text{fixed}}=-\sum_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{2n+1,\overline{2m+1}}\overline{\lambda}^{2m+1},\tag{5}$$

$$\overline{\mathcal{B}}_{2n+1}(\lambda)=\partial_{\overline{t}_{2n+1}}S\Big|_{\lambda\ \text{fixed}}=-\sum_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{\overline{2n+1},2m+1}\lambda^{-2m-1},\tag{6}$$

$$\overline{\mathcal{B}}_{2n+1}(\overline{\lambda})=\partial_{\overline{t}_{2n+1}}\overline{S}\Big|_{\overline{\lambda}\ \text{fixed}}=\overline{\lambda}^{-2n-1}-\sum_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{\overline{2n+1},\overline{2m+1}}\overline{\lambda}^{2m+1},\tag{7}$$

where $\mathcal{F}_{n,\overline{m}}=\partial_{t_n}\partial_{\overline{t}_m}\mathcal{F}$ and $\mathcal{F}_{\overline{n},\overline{m}}=\partial_{\overline{t}_n}\partial_{\overline{t}_m}\mathcal{F}$. Noticing that (4) and (6) are defined in D_∞, while (5) and (7) are in D_0. From (4)–(7), we have, for $n=0$,

$$p(\lambda)=\partial_{t_1}S(\lambda)=\lambda-\sum_{m=1}^{\infty}f_{2m}\lambda^{-2m+1},\quad f_{2m}=\frac{1}{2m-1}\mathcal{F}_{1,2m-1},\tag{8}$$

$$p(\overline{\lambda})=\partial_{t_1}\overline{S}(\overline{\lambda})=\sum_{m=0}^{\infty}\overline{f}_{2m}\overline{\lambda}^{2m+1},\quad \overline{f}_{2m}=-\frac{1}{2m+1}\mathcal{F}_{1,\overline{2m+1}},\tag{9}$$

$$\overline{u}_0^{-1}p^{-1}(\lambda)=\partial_{\overline{t}_1}S(\lambda)=\sum_{m=0}^{\infty}g_{2m}\lambda^{-2m-1},\quad g_{2m}=-\frac{1}{2m+1}\mathcal{F}_{\overline{1},2m+1},\tag{10}$$

$$\overline{u_0}^{-1}p^{-1}(\overline{\lambda}) = \partial_{\overline{t}_1}\overline{S}(\overline{\lambda}) = \overline{\lambda}^{-1} - \sum_{m=1}^{\infty} \overline{g}_{2m}\overline{\lambda}^{2m-1}, \quad \overline{g}_{2m} = \frac{1}{2m-1}\mathcal{F}_{\overline{1},\overline{2m-1}}, \tag{11}$$

where we use the notations $\partial_{t_1}S(\lambda) \equiv \partial_{t_1}S|_{\lambda \text{ fixed}}$, etc. for brevity. Therefore the dynamical variables u_{2j} and $\overline{u}_{2j}$ of the system are characterized by the second derivatives of the free energy $\mathcal{F}$. In particular, from (8) and (9), we have $u_2 = \mathcal{F}_{11}$ and $\overline{u}_0^{-1} = -\mathcal{F}_{1,\overline{1}}$, respectively. Note that $p(\overline{\lambda})$ is the inverse map of $\overline{\lambda}(p)$ and cannot be viewed as the same function as $p(\lambda)$ with λ replaced by $\overline{\lambda}$.

B. Kernel formulas

In contrast to the dKP hierarchy, where only one Lax operator is defined in D_∞, the EdBKP hierarchy contains two Lax operators, λ and $\overline{\lambda}$, that are defined in domains D_∞ and D_0, respectively. To derive dHirota equations for the EdBKP hierarchy, we shall generalize the method of kernel formula to the domains D_∞, D_0, and $D_\infty \cap D_0$.

In D_∞ multiplying (8) by $\lambda^{2n-1}\,\partial_p\lambda$ for $n \geq 1$, we have

$$\lambda^{2n}\,\partial_p\lambda = p\lambda^{2n-1}\,\partial_p\lambda + \sum_{j=1}^{\infty} f_{2j}\lambda^{2n-2j}\,\partial_p\lambda,$$

which, after taking the polynomial part, leads to the recurrence relation

$$\partial_p Q_{2n+1}(\lambda) = p(\lambda)\partial_p Q_{2n}(\lambda) + \sum_{j=1}^{n} f_{2j}\,\partial_p Q_{2n-2j+1}(\lambda), \tag{12}$$

where $Q_{2n+1} \equiv \mathcal{B}_{2n+1}/(2n+1)$ and $Q_{2n} \equiv (\lambda^{2n})_{\geq 0}/(2n)$. Multiplying (12) by μ^{-2n} $(n \geq 0)$ and summing over n we obtain

$$p(\mu)\sum_{n=0}^{\infty} \partial_p Q_{2n+1}(\lambda)\mu^{-2n-1} - p(\lambda)\sum_{n=0}^{\infty} \partial_p Q_{2n+2}(\lambda)\mu^{-2n-2} = 1. \tag{13}$$

On the other hand, multiplying both sides on (8) by $\lambda^{2n}\,\partial_p\lambda$ for $n \geq 1$, it follows that

$$\lambda^{2n+1}\,\partial_p\lambda = p\lambda^{2n}\,\partial_p\lambda + \sum_{j=1}^{\infty} f_{2j}\lambda^{2n-2j+1}\,\partial_p\lambda.$$

After taking the polynomial part we get another recurrence relation

$$\partial_p Q_{2n+2}(\lambda) = p(\lambda)\partial_p Q_{2n+1}(\lambda) + \sum_{j=1}^{n} f_{2j}\,\partial_p Q_{2n-2j+2}(\lambda). \tag{14}$$

Multiplying (14) by μ^{-2n-1} $(n \geq 0)$ and summing over n, we obtain

$$p(\mu)\sum_{n=0}^{\infty} \partial_p Q_{2n+2}(\lambda)\mu^{-2n-2} = p(\lambda)\sum_{n=0}^{\infty} \partial_p Q_{2n+1}(\lambda)\mu^{-2n-1}. \tag{15}$$

Plugging (15) into (13) to eliminate $\Sigma_{n=0}^{\infty}\partial_p Q_{2n+2}(\lambda)\mu^{-2n-2}$, we obtain the generating function of $\partial_p Q_{2n+1}(\lambda)$ as

$$\frac{p(\mu)}{p^2(\mu) - p^2(\lambda)} = \sum_{n=0}^{\infty} \partial_p Q_{2n+1}(\lambda)\mu^{-2n-1}. \tag{16}$$

Now we integrate the kernel (16) with respect to $p(\lambda)$, and normalize at $\mu = \infty$ to obtain

$$\frac{p(\mu)-p(\lambda)}{p(\mu)+p(\lambda)}=\exp\left(-2\sum_{n=0}^{\infty}Q_{2n+1}(\lambda)\mu^{-2n-1}\right). \tag{17}$$

If we denote $D(z)$ the differential operator,

$$D(z)=\sum_{n=0}^{\infty}\frac{z^{-2n-1}}{2n+1}\partial_{t_{2n+1}},$$

then (17) can be rewritten as

$$\frac{p(\mu)-p(\lambda)}{p(\mu)+p(\lambda)}=\exp(-2D(\mu)S(\lambda))=\frac{\mu-\lambda}{\mu+\lambda}e^{2D(\lambda)D(\mu)\mathcal{F}}, \tag{18}$$

which is the same result derived by Bogdanov and Konopelchenko,[2] where they obtained dHirota equations of the dBKP hierarchy from that of the dKP hierarchy by taking into account the symmetry condition $S(-\lambda)=-S(\lambda)$.

In D_0 to obtain the generating function of $\partial_p\overline{Q}_{2n+1}(\overline{\lambda})$ we multiplying (11) by $\overline{\lambda}^{-2n-1}\,\partial_p\overline{\lambda}$ for $n\geq 1$; then

$$\overline{\lambda}^{-2n-2}\,\partial_p\overline{\lambda}=\overline{u}_0^{-1}p^{-1}(\overline{\lambda})\overline{\lambda}^{-2n-1}\,\partial_p\overline{\lambda}+\sum_{j=1}^{\infty}\overline{g}_{2j}\overline{\lambda}^{-2n+2j-2}\,\partial_p\overline{\lambda}.$$

Taking the negative part leads to the recurrence relation

$$\partial_p\overline{Q}_{2n+1}(\overline{\lambda})=\overline{u}_0^{-1}p^{-1}(\overline{\lambda})\partial_p\overline{Q}_{2n}(\overline{\lambda})+\sum_{j=1}^{n}\overline{g}_{2j}\partial_p\overline{Q}_{2n-2j+1}(\overline{\lambda}), \tag{19}$$

where $\overline{Q}_{2n+1}\equiv\overline{\mathcal{B}}_{2n+1}/(2n+1)$ and $\overline{Q}_{2n}\equiv(\overline{\lambda}^{-2n})_{\leq -1}/(2n)$. Multiplying (19) by $\overline{\mu}^{2n}$ $(n\geq 0)$ and summing over n, we obtain

$$p^{-1}(\overline{\mu})\sum_{n=0}^{\infty}\partial_p\overline{Q}_{2n+1}(\overline{\lambda})\overline{\mu}^{2n+1}-p^{-1}(\overline{\lambda})\sum_{n=1}^{\infty}\partial_p\overline{Q}_{2n}(\overline{\lambda})\overline{\mu}^{2n}=-p^{-2}(\overline{\lambda}). \tag{20}$$

On the other hand, multiplying (11) by $\overline{\lambda}^{-2n}\partial_p\overline{\lambda}$ for $n\geq 1$, it follows that

$$\overline{\lambda}^{-2n-1}\,\partial_p\overline{\lambda}=\overline{u}_0^{-1}p^{-1}(\overline{\lambda})\overline{\lambda}^{-2n}\,\partial_p\overline{\lambda}+\sum_{j=1}^{\infty}\overline{g}_{2j}\overline{\lambda}^{-2n+2j-1}\,\partial_p\overline{\lambda}.$$

After taking the negative part, we get another recurrence relation,

$$\partial_p\overline{Q}_{2n}(\overline{\lambda})=\overline{u}_0^{-1}p^{-1}(\overline{\lambda})\partial_p\overline{Q}_{2n-1}(\overline{\lambda})+\sum_{j=1}^{n-1}\overline{g}_{2j}\,\partial_p\overline{Q}_{2n-2j}(\overline{\lambda}). \tag{21}$$

Multiplying (21) by $\overline{\mu}^{2n-1}$ $(n\geq 1)$ and summing over n, we obtain

$$p^{-1}(\overline{\mu})\sum_{n=1}^{\infty}\partial_p\overline{Q}_{2n}(\overline{\lambda})\overline{\mu}^{2n}=p^{-1}(\overline{\lambda})\sum_{n=0}^{\infty}\partial_p\overline{Q}_{2n+1}(\overline{\lambda})\overline{\mu}^{2n+1}. \tag{22}$$

Plugging (22) into (20) to eliminate $\Sigma_{n=1}\,\partial_p\overline{Q}_{2n}(\overline{\lambda})\overline{\mu}^{2n}$, which yields the generating function of $\partial_p\overline{Q}_{2n+1}(\overline{\lambda})$ as

$$\frac{p(\bar{\mu})}{p^2(\bar{\mu})-p^2(\bar{\lambda})}=\sum_{n=0}^{\infty}\partial_p\bar{Q}_{2n+1}(\bar{\lambda})\bar{\mu}^{2n+1}. \tag{23}$$

Now we integrate the kernel (23) with respect to $p(\bar{\lambda})$, and normalize at $\bar{\mu}=0$ to obtain

$$\frac{p(\bar{\lambda})-p(\bar{\mu})}{p(\bar{\lambda})+p(\bar{\mu})}=\exp\left(-2\sum_{n=0}^{\infty}\bar{Q}_{2n+1}(\bar{\lambda})\bar{\mu}^{2n+1}\right), \tag{24}$$

which can be expressed as

$$\frac{p(\bar{\lambda})-p(\bar{\mu})}{p(\bar{\lambda})+p(\bar{\mu})}=\frac{\bar{\lambda}-\bar{\mu}}{\bar{\lambda}+\bar{\mu}}e^{2\bar{D}(\bar{\lambda}^{-1})\bar{D}(\bar{\mu}^{-1})\mathcal{F}}, \tag{25}$$

where

$$\bar{D}(z)=\sum_{n=0}^{\infty}\frac{z^{-2n-1}}{2n+1}\partial_{\bar{t}_{2n+1}}.$$

In $D_\infty\cap D_0$ in view of (4) and (5), the functional $Q_{2n+1}(\lambda)$ and $p(\lambda)$ can be replaced by $\partial_{t_{2n+1}}\bar{S}(\bar{\lambda})/(2n+1)$ and $\partial_{t_1}\bar{S}(\bar{\lambda})$, respectively. Then (17) becomes

$$\frac{p(\mu)-\partial_{t_1}\bar{S}(\bar{\lambda})}{p(\mu)+\partial_{t_1}\bar{S}(\bar{\lambda})}=e^{2D(\mu)\bar{D}(\bar{\lambda}^{-1})\mathcal{F}}. \tag{26}$$

Similarly, in view of (6) and (7), the functional $\bar{Q}_{2n+1}(\bar{\lambda})$ and $\bar{u}_0^{-1}p^{-1}(\bar{\lambda})$ can be replaced by $\partial_{\bar{t}_{2n+1}}S(\lambda)/(2n+1)$ and $\partial_{\bar{t}_1}S(\lambda)$, respectively. Then (24) becomes

$$\frac{\bar{u}_0^{-1}p^{-1}(\bar{\mu})-\partial_{\bar{t}_1}S(\lambda)}{\bar{u}_0^{-1}p^{-1}(\bar{\mu})+\partial_{\bar{t}_1}S(\lambda)}=e^{2D(\lambda)\bar{D}(\bar{\mu}^{-1})\mathcal{F}}. \tag{27}$$

Note that, after making the replacements $\lambda\to\mu$ and $\bar{\mu}\to\bar{\lambda}$, the right-hand side of (27) coincides with that of (26). Hence,

$$p(\mu)\partial_{\bar{t}_1}S(\mu)=\bar{u}_0^{-1}p^{-1}(\bar{\lambda})\partial_{t_1}\bar{S}(\bar{\lambda})=\bar{u}_0^{-1}, \tag{28}$$

where the last equality is determined by setting $\mu\to\infty$ and $\bar{\lambda}\to 0$:

$$\lim_{\mu\to\infty}p(\mu)\partial_{\bar{t}_1}S(\mu)=\lim_{\bar{\lambda}\to 0}\bar{u}_0^{-1}p^{-1}(\bar{\lambda})\partial_{t_1}\bar{S}(\bar{\lambda})=-\bar{\mathcal{F}}_{11}=\bar{u}_0^{-1}.$$

Equation (28) contains the definitions (9) and (10) and can be regarded as an extra condition, besides the dHirota equations (18), (25), and (26).

In summary, the EdBKP hierarchy can be characterized by a single function $\mathcal{F}$ satisfying (18) and (25)–(27) [or (18), (25), (26), and (28)].

C. Dispersionless Hirota equations

Let us rewrite (18) and (25)–(27) as a set of equations satisfied by the second derivatives of $\mathcal{F}$.

(1) We first rewrite the equation (18) in the form

$$\log\left(\frac{p(\lambda)-p(\mu)}{\lambda-\mu}\frac{\lambda+\mu}{p(\lambda)+p(\mu)}\right)=2D(\lambda)D(\mu)\mathcal{F},$$

where $p(\lambda)$ is defined by (8), and for $\lambda\to\mu$ we have

$$\log(\mu\partial_\mu \log p(\mu))=2D^2(\mu)\mathcal{F},$$

$$=\sum_{j=1}^{\infty}\left(\sum_{\substack{m+n=j-1\\ m,n\geq 0}}\frac{2\mathcal{F}_{2m+1,2n+1}}{(2m+1)(2n+1)}\right)\mu^{-2j}.$$

Then, using the elementary Schur polynomials and (8), we obtain

$$\frac{1+\Sigma_{m=0}^{\infty}\mathcal{F}_{1,2m+1}\mu^{-2m-2}}{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{1,2m+1}\mu^{-2m-2}}=\sum_{k=0}^{\infty}P_k(\theta_1,\theta_2,\ldots,\theta_k)\mu^{-2k},$$

where θ_i, $i\geq 1$ are defined by

$$\theta_i=\sum_{\substack{m+n=i-1\\ m,n\geq 0}}\frac{2\mathcal{F}_{2m+1,2n+1}}{(2m+1)(2n+1)}.$$

By comparing the coefficients of μ^{-2k} on both sides, we obtain a set of relations satisfied by $\mathcal{F}_{2i+1,2j+1}$:

$$\frac{2m+2}{2m+1}\mathcal{F}_{1,2m+1}-P_{m+1}(\theta)+\sum_{\substack{j+k=m-1\\ j,k\geq 0}}\frac{1}{2j+1}\mathcal{F}_{1,2j+1}P_{k+1}(\theta)=0. \tag{29}$$

(2) Similarly, we consider (25) by taking the limit $\bar{\lambda}\to\bar{\mu}$. Then

$$\log(\bar{\mu}\partial_{\bar{\mu}}\log p(\bar{\mu}))=2D^2(\bar{\mu})\mathcal{F},$$

$$=\sum_{j=1}^{\infty}\left(\sum_{\substack{m+n=j-1\\ m,n\geq 0}}\frac{2\mathcal{F}_{\overline{2m+1},\overline{2n+1}}}{(2m+1)(2n+1)}\right)\bar{\mu}^{2j}.$$

Also, using the elementary Schur polynomials and (11), we obtain

$$\frac{1+\Sigma_{m=0}^{\infty}\mathcal{F}_{\overline{1,2m+1}}\bar{\mu}^{2m+2}}{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}\mathcal{F}_{\overline{1,2m+1}}\bar{\mu}^{2m+2}}=\sum_{k=0}^{\infty}P_k(\bar{\theta}_1,\bar{\theta}_2,\ldots,\bar{\theta}_k)\bar{\mu}^{2k},$$

where $\bar{\theta}_i$, $i\geq 1$ are defined by

$$\bar{\theta}_i=\sum_{\substack{m+n=i-1\\ m,n\geq 0}}\frac{2\mathcal{F}_{\overline{2m+1},\overline{2n+1}}}{(2m+1)(2n+1)}.$$

By comparing the coefficients of $\bar{\mu}^{2k}$ on both sides, we obtain a set of relations satisfied by $\mathcal{F}_{\overline{2i+1},\overline{2j+1}}$:

$$\frac{2m+2}{2m+1}\mathcal{F}_{\overline{1,2m+1}}-P_{m+1}(\bar{\theta})+\sum_{\substack{j+k=m-1\\ j,k\geq 0}}\frac{1}{2j+1}\mathcal{F}_{\overline{1,2j+1}}P_{k+1}(\bar{\theta})=0. \tag{30}$$

(3) From (26), by taking $\overline{\lambda}\to 1/\mu$ and using (8) and (9), it is straightforward to obtain

$$\frac{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}(\mathcal{F}_{1,2m+1}-\mathcal{F}_{1,\overline{2m+1}})\mu^{-2m-2}}{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}(\mathcal{F}_{1,2m+1}+\mathcal{F}_{1,\overline{2m+1}})\mu^{-2m-2}}=\sum_{k=0}^{\infty}P_k(\tilde{\theta}_1,\tilde{\theta}_2,\ldots,\tilde{\theta}_k)\mu^{-2k},$$

where $P_k(\tilde{\theta})$ are elementary Schur polynomials and $\tilde{\theta}_i$, $i\geq 1$ are defined by

$$\tilde{\theta}_i=\sum_{\substack{m+n=i-1\\ m,n\geq 0}}\frac{2\mathcal{F}_{2n+1,\overline{2m+1}}}{(2m+1)(2n+1)}.$$

By comparing the coefficients of μ^{-2k} on both sides, we obtain a set of relations satisfied by $\mathcal{F}_{2i+1,\overline{2j+1}}$:

$$\frac{2}{2m+1}\mathcal{F}_{1,\overline{2m+1}}-P_{m+1}(\tilde{\theta})+\sum_{\substack{j+k=m-1\\ j,k\geq 0}}\frac{1}{2j+1}(\mathcal{F}_{1,2j+1}+\mathcal{F}_{1,\overline{2j+1}})P_{k+1}(\tilde{\theta})=0. \tag{31}$$

(4) From (27), it is straightforward to taking $\overline{\mu}\to 1/\lambda$ and by (11) and (10) we have

$$\frac{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}(\mathcal{F}_{\overline{1,2m+1}}-\mathcal{F}_{\overline{1,2m+1}})\lambda^{-2m-2}}{1-\Sigma_{m=0}^{\infty}\frac{1}{2m+1}(\mathcal{F}_{\overline{1,2m+1}}+\mathcal{F}_{\overline{1,2m+1}})\lambda^{-2m-2}}=\sum_{k=0}^{\infty}P_k(\tilde{\theta}_1,\tilde{\theta}_2,\ldots,\tilde{\theta}_k)\lambda^{-2k},$$

where $P_k(\tilde{\theta})$ is defined as before and the above equation can be simplified as

$$\frac{2}{2m+1}\mathcal{F}_{\overline{1,2m+1}}-P_{m+1}(\tilde{\theta})+\sum_{\substack{j+k=m-1\\ j,k\geq 0}}\frac{1}{2j+1}(\mathcal{F}_{\overline{1,2j+1}}+\mathcal{F}_{\overline{1,2j+1}})P_{k+1}(\tilde{\theta})=0. \tag{32}$$

Note that for $u_2=\mathcal{F}_{11}$, the first equation in (29) is nothing but the 2+1-dimensional dBKP equation,[8]

$$3u_t+15u^2u_x-5uu_y-5u_x\partial_x^{-1}u_y-\frac{5}{3}\partial_x^{-1}u_{yy}=0,$$

where $t_1=x$, $t_3=y$, $t_5=t$ and $u\equiv u_2$, while the first equation in (31) is the simplest nontrivial 2+1-dimensional equation of EdBKP hierarchy involving $t_1=x$, $t_3=y$, and $\overline{t_1}$:

$$uu_{\overline{t_1}}+u_x\partial_x^{-1}u_{\overline{t_1}}-\frac{1}{3}\partial_x^{-1}u_{y\overline{t_1}}=0.$$

For convenience, we list other higher flows of (29)–(32) in Appendix .

III. ASSOCIATIVITY EQUATIONS IN EdBKP HIERARCHY

A. WDVV equations and generating functions

Following Ref. 3, let us briefly recall the basic notions of associativity equations. Let $\mathcal{F}$ be a differentiable functions of a set of time variables $t=(t_1,t_2,\ldots)$; namely, $\mathcal{F}=\mathcal{F}(t_1,t_2,t_3,\ldots)$ and define $\mathcal{F}_{ij}=\partial_{t_i}\partial_{t_j}\mathcal{F}$, $\mathcal{F}_{ijk}=\partial_{t_i}\partial_{t_j}\partial_{t_k}\mathcal{F}$. One can choose one of the time variables, say t_1, and assume the nondegenerate metric $\eta_{ij}=\mathcal{F}_{ij1}$, which can be regarded as a transform from $\{t_i\}$ to $\{\mathcal{F}_{j1}\}$. Define the matrix $C_{ij}^{l}=\partial\mathcal{F}_{ij}/\partial\mathcal{F}_{l1}$; then

$$\mathcal{F}_{ijk} = \sum_l C_{ij}^l \eta_{lk} = \sum_l C_{ij}^l \mathcal{F}_{lk1} \tag{33}$$

connects $\mathcal{F}_{ijk}$ and η_{ij}. It can also be treated as a definition of C_{ij}^l.

If C_{ij}^l is the structure constant of an associativity algebra generated by $\{\phi_i\}$; namely, $\phi_i \cdot \phi_j = \Sigma_l C_{ij}^l \phi_l$, then we have the constraints $\Sigma_l C_{ij}^l C_{lk}^n = \Sigma_l C_{jk}^l C_{il}^n$, or, equivalently,

$$\sum_l C_{ij}^l \mathcal{F}_{lkm} = \sum_l C_{jk}^l \mathcal{F}_{ilm},$$

which is the so-called WDVV equations arising from topological field theories.[10,32] Thus

$$X_{ijkn} \equiv \sum_l C_{ij}^l \mathcal{F}_{lkn} \tag{34}$$

is symmetric with respect to permutations of any indices. In general, one may choose any t_a to define the metric $\eta(a)_{ij} = \mathcal{F}_{ija}$, and the structure constants $C_{ij}^l(a) = \partial \mathcal{F}_{ij} / \partial \mathcal{F}_{la}$; then they obey the same associativity relations,

$$\sum_l C_{ij}^l(a) \mathcal{F}_{lkm} = \sum_l C_{jk}^l(a) \mathcal{F}_{ilm}. \tag{35}$$

Introducing matrices $\mathbf{F}_a$ with matrix elements $(\mathbf{F}_a)_{ij} = \mathcal{F}_{ija}$, one can rewrite the WDVV equations as

$$\mathbf{F}_j \mathbf{F}_a^{-1} \mathbf{F}_m = \mathbf{F}_m \mathbf{F}_a^{-1} \mathbf{F}_j.$$

In the case of infinitely many variables, it is convenient to define generating functions for $\mathcal{F}_{ij}$, $\mathcal{F}_{ijk}$, C_{ij}^l, and X_{ijkl} as follows:[3]

$$D_1 D_2 \mathcal{F} = \sum_{i,j=1}^{\infty} \frac{z_1^{-i}}{i} \frac{z_2^{-j}}{j} \mathcal{F}_{ij},$$

$$D_1 D_2 D_3 \mathcal{F} = \sum_{i,j,k=1}^{\infty} \frac{z_1^{-i}}{i} \frac{z_2^{-j}}{j} \frac{z_3^{-k}}{k} \mathcal{F}_{ijk},$$

$$C^l(z_1, z_2) = \sum_{i,j=1}^{\infty} \frac{z_1^{-i}}{i} \frac{z_2^{-j}}{j} C_{ij}^l,$$

$$X(z_1, z_2, z_3, z_4) = \sum_{i,j,k,n=1}^{\infty} \frac{z_1^{-i}}{i} \frac{z_2^{-j}}{j} \frac{z_3^{-k}}{k} \frac{z_4^{-n}}{n} X_{ijkn},$$

where $D_i \equiv D(z_i) = \Sigma_{j=1}^{\infty} z_i^{-j} \partial_{t_j} / j$. From the definition (34), it is easy to see that X_{ijkn} is symmetric in (ij) and (kn), while the associativity equations (35) implies that $X_{ijkn} = X_{ikjn}$ or, in terms of the generating function,

$$X(z_1, z_2, z_3, z_4) = X(z_1, z_3, z_2, z_4). \tag{36}$$

In Ref. 3, the associativity equations in the dKP and dToda hierarchies were verified from the corresponding dHirota equations by investigating the symmetric property (36).

B. From dHirota to WDVV

To derive WDVV equations from dHirota equations for EdBKP we set $\bar{t}_{-2k-1}=t_{2k+1}$ $(k\leq -1)$ for convenience and rewrite the operator $\bar{D}(z)$ as

$$\bar{D}(z)=\sum_{k\leq -1}\frac{-z^{2k+1}}{2k+1}\partial_{t_{2k+1}}.$$

We will use the notation $D(z_i)=D_i$ and $\bar{D}(z_i)=\bar{D}_i$ for brevity. The functions

$$D_1D_2\mathcal{F}=\sum_{k,m\geq 0}\frac{z_1^{-2k-1}z_2^{-2m-1}}{(2k+1)(2m+1)}\mathcal{F}_{2k+1,2m+1},$$

and $D_1D_2D_3\mathcal{F}$ generate separately the sets of $\mathcal{F}_{2k+1,2m+1}$ and $\mathcal{F}_{2k+1,2m+1,2n+1}$ for all $k,m,n\geq 0$. On the other hand, the functions

$$D_1\bar{D}_2\mathcal{F}=\sum_{k\geq 0,m\leq -1}\frac{-z_1^{-2k-1}z_2^{2m+1}}{(2k+1)(2m+1)}\mathcal{F}_{2k+1,2m+1}$$

generate the set of $\mathcal{F}_{2k+1,2m+1}$ for all $k\geq 0$, and $m\leq -1$, etc. We also introduce generating functions for the structure constants $C^{2l+1}_{2i+1,2j+1}$:

$$C^l(z_1^+,z_2^+)=\sum_{i,j\geq 0}C^{2l+1}_{2i+1,2j+1}\frac{z_1^{-2i-1}z_2^{-2j-1}}{(2i+1)(2j+1)},$$

$$C^l(z_1^-,z_2^-)=\sum_{i,j\leq -1}C^{2l+1}_{2i+1,2j+1}\frac{z_1^{2i+1}z_2^{2j+1}}{(2i+1)(2j+1)}, \tag{37}$$

$$C^l(z_1^+,z_2^-)=\sum_{i\geq 0,j\leq -1}C^{2l+1}_{2i+1,2j+1}\frac{-z_1^{-2i-1}z_2^{2j+1}}{(2i+1)(2j+1)},$$

and the X_{ijkn}:

$$X(z_1,z_2,z_3,z_4)\equiv\sum_{i,j,k,n=-\infty}^{\infty}\frac{z_1^{-|i|}}{|i|}\frac{z_2^{-|j|}}{|j|}\frac{z_3^{-|k|}}{|k|}\frac{z_4^{-|n|}}{|n|}X_{ijkn},\quad i,j,k,n\in\mathbf{Z_{odd}}. \tag{38}$$

Notice that from (37) the property holds: $C^l(z_1^+,z_2^-)=C^l(z_2^-,z_1^+)$. The infinite WDVV equations are thus equivalent to the symmetry of the $X(z_1,z_2,z_3,z_4)$ under permutations of z_1, z_2, z_3, and z_4. In the following, we shall show that the associativity equations in the EdBKP hierarchy can be verified in a similar way as the dToda case.[3]

Let us rewrite the dHirota equations (18), (25), and (26) as

$$\frac{p_1-p_2}{p_1+p_2}=\frac{z_1-z_2}{z_1+z_2}e^{2D_1D_2\mathcal{F}}, \tag{39}$$

$$\frac{\bar{p}_1-\bar{p}_2}{\bar{p}_1+\bar{p}_2}=\frac{z_1-z_2}{z_1+z_2}e^{2\bar{D}_1\bar{D}_2\mathcal{F}}, \tag{40}$$

$$\frac{p_1+\overline{D}_2\partial_{t_1}\mathcal{F}}{p_1-\overline{D}_2\partial_{t_1}\mathcal{F}}=e^{2D_1\overline{D}_2\mathcal{F}}, \tag{41}$$

where $p_i\equiv p(z_i)=z_i-D_i\,\partial_{t_1}\mathcal{F}$ and $\overline{p_i}\equiv\overline{u_0}^{-1}p^{-1}(z_i^{-1})=z_i-\overline{D_i}\,\partial_{t_{-1}}\mathcal{F}$. The symmetric form of Eqs. (39) and (40) are[2]

$$f_{12}f_{23}f_{31}+f_{12}+f_{23}+f_{31}=0, \tag{42}$$

$$\overline{f}_{12}\overline{f}_{23}\overline{f}_{31}+\overline{f}_{12}+\overline{f}_{23}+\overline{f}_{31}=0, \tag{43}$$

where

$$f_{ij}=\frac{p_i-p_j}{p_i+p_j}=\frac{z_i-z_j}{z_i+z_j}e^{2D_iD_j\mathcal{F}},\quad 1\le i,j\le 3,$$

$$\overline{f}_{ij}=\frac{\overline{p_i}-\overline{p_j}}{\overline{p_i}+\overline{p_j}}=\frac{z_i-z_j}{z_i+z_j}e^{2\overline{D}_i\overline{D}_j\mathcal{F}},\quad 1\le i,j\le 3.$$

By taking the D_4 and $\overline{D}_4$ derivatives of (42), we get the following useful identities:

$$p_1^2(p_3D_2-p_2D_3)D_1D_4\mathcal{F}+p_2^2(p_1D_3-p_3D_1)D_2D_4\mathcal{F}+p_3^2(p_2D_1-p_1D_2)D_3D_4\mathcal{F}=0, \tag{44}$$

$$p_1^2(p_3D_2-p_2D_3)D_1\overline{D}_4\mathcal{F}+p_2^2(p_1D_3-p_3D_1)D_2\overline{D}_4\mathcal{F}+p_3^2(p_2D_1-p_1D_2)D_3\overline{D}_4\mathcal{F}=0. \tag{45}$$

Similarly, we have another two identities if we apply D_4 and $\overline{D}_4$ to (43). We define a nondegenerate metric to be $\eta_{2i+1,2j+1}=\mathcal{F}_{2i+1,2j+1,1}$, and the structure constants as

$$\mathcal{F}_{2i+1,2j+1,2k+1}=\sum_{l=-\infty}^{\infty}C_{2i+1,2j+1}^{2l+1}\mathcal{F}_{2l+1,2k+1,1},$$

where the indices take integer values. From the definition of the metric, we have $C_{1,2j+1}^{2l+1}=\delta_j^l$ for all l,j. To find other structure constants, apply $\partial_{t_{2k+1}}$ to the dHirota equations (39)–(41):

$$D_1D_2\,\partial_{2k+1}\mathcal{F}=\frac{p_1D_2-p_2D_1}{p_1^2-p_2^2}\mathcal{F}_{2k+1,1}, \tag{46}$$

$$\overline{D}_1\overline{D}_2\,\partial_{2k+1}\mathcal{F}=\frac{\overline{p}_1\overline{D}_2-\overline{p}_2\overline{D}_1}{\overline{p}_1^2-\overline{p}_2^2}\mathcal{F}_{2k+1,-1}, \tag{47}$$

$$D_1\overline{D}_2\,\partial_{2k+1}\mathcal{F}=\frac{p_1\overline{D}_2+(\overline{D}_2\partial_{t_1}\mathcal{F})D_1}{p_1^2-(\overline{D}_2\partial_{t_1}\mathcal{F})^2}\mathcal{F}_{2k+1,1}. \tag{48}$$

Comparing with (33), the generating functions of structure constants (37) can be read out from the right-hand side of these equations, except that the rhs of Eq. (47) is related to the partial derivative of $\mathcal{F}$ with respect to t_{-1} (not t_1), which forbids us to extract structure constants from (47) directly. Fortunately, this problem can be removed by considering (28) in the form

$$D_1\partial_{t_{-1}}\mathcal{F}=\frac{\overline{p_2}}{p_1}\overline{D_2}\,\partial_{t_1}\mathcal{F}. \tag{49}$$

Differentiating above with respect to t_{2k+1} yields

$$D_1\mathcal{F}_{2k+1,-1}=\frac{\partial_{2k+1}\overline{p_2}}{p_1}\overline{D_2}\,\partial_{t_1}\mathcal{F}+\frac{\overline{p_2}}{p_1}\overline{D_2}\mathcal{F}_{2k+1,1}-\frac{\overline{p_2}\partial_{2k+1}p_1}{p_1^2}\overline{D_2}\,\partial_{t_1}\mathcal{F},$$

which, together with $\partial_{2k+1}p_1=-D_1\mathcal{F}_{2k+1,1}$ and $\partial_{2k+1}\overline{p_2}=-\overline{D_2}\mathcal{F}_{2k+1,-1}$, implies that

$$D_1\mathcal{F}_{2k+1,-1}=-\frac{\overline{D_2}\,\partial_{t_1}\mathcal{F}}{p_1}\overline{D_2}\mathcal{F}_{2k+1,-1}+\frac{\overline{p_2}}{p_1}\overline{D_2}\mathcal{F}_{2k+1,1}+\frac{\overline{p_2}}{p_1^2}(\overline{D_2}\,\partial_{t_1}\mathcal{F})D_1\mathcal{F}_{2k+1,1}. \tag{50}$$

Taking the limit $z_1\to\infty$ in (50), we obtain

$$\overline{D_2}\mathcal{F}_{2k+1,-1}=\frac{\overline{p_2}}{\overline{D_2}\mathcal{F}_1}\overline{D_2}\mathcal{F}_{2k+1,1}, \tag{51}$$

which, after substituting back into (50), yields

$$D_1\mathcal{F}_{2k+1,-1}=\frac{\overline{p_2}}{p_1^2}(\overline{D_2}\,\partial_{t_1}\mathcal{F})D_1\mathcal{F}_{2k+1,1}.$$

On the other hand, exchanging the variables $z_1\leftrightarrow z_2$, we have

$$\overline{D_1}\mathcal{F}_{2k+1,-1}=\frac{\overline{p_1}}{\overline{D_1}\mathcal{F}_1}\overline{D_1}\mathcal{F}_{2k+1,1}, \tag{52}$$

$$D_2\mathcal{F}_{2k+1,-1}=\frac{\overline{p_1}}{p_2^2}(\overline{D_1}\mathcal{F}_1)D_2\mathcal{F}_{2k+1,1}.$$

Substituting (51) and (52) into the numerator of (47) and taking into account (49), then (47) becomes

$$\overline{D_1}\overline{D_2}\partial_{2k+1}\mathcal{F}=\frac{(\overline{D_2}\partial_{t_1}\mathcal{F})\overline{D_1}-(\overline{D_1}\partial_{t_1}\mathcal{F})\overline{D_2}}{(\overline{D_1}\partial_{t_1}\mathcal{F})^2-(\overline{D_2}\partial_{t_1}\mathcal{F})^2}\mathcal{F}_{2k+1,1}. \tag{53}$$

Now we can find all structure constants by using Eqs. (46), (48), and (53). First, we conclude from (46) and (53) that $C^{2l+1}_{2i+1,2j+1}=0$ for $i,j\geq 0$ and $l\leq -1$, or $i,j\leq -1$ and $l\geq 0$. Next, if all the indices are positive, we have

$$C^l(z_1^+,z_2^+)=\frac{p_1z_2^{-2l-1}-p_2z_1^{-2l-1}}{(2l+1)(p_1^2-p_2^2)},\quad l\geq 0, \tag{54}$$

while all the indices are negative, it gives

$$C^l(z_1^-,z_2^-)=\frac{(\overline{D_1}\partial_{t_1}\mathcal{F})z_2^{2l+1}-(\overline{D_2}\partial_{t_1}\mathcal{F})z_1^{2l+1}}{(2l+1)((\overline{D_1}\,\partial_{t_1}\mathcal{F})^2-(\overline{D_2}\,\partial_{t_1}\mathcal{F})^2)},\quad l\leq -1. \tag{55}$$

When i and j have different signs, we use (48) to obtain

$$C^l(z_1^+,z_2^-)=\begin{cases}\dfrac{(\overline{D}_2\,\partial_{t_1}\mathcal{F})z_1^{-2l-1}}{(2l+1)(p_1^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2)}, & l\geq 0,\\ \dfrac{-p_1 z_2^{2l+1}}{(2l+1)(p_1^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2)}, & l\leq -1.\end{cases} \tag{56}$$

Making use of the structure constants, we show that any solution $\mathcal{F}$ of the EdBKP hierarchy obeys the WDVV equations:

$$\sum_{l=-\infty}^{\infty} C_{2i+1,2j+1}^{2l+1}\mathcal{F}_{2l+1,2k+1,2n+1}=\sum_{l=-\infty}^{\infty} C_{2i+1,2k+1}^{2l+1}\mathcal{F}_{2l+1,2j+1,2n+1},\quad i,j,k,n\in\mathbf{Z}. \tag{57}$$

To show that the generating functions (38) is totally symmetric w.r.t. permutations of $z_1,\ldots,z_4$, however, it is enough to prove the symmetry w.r.t. the permutations of z_2 and z_3 in (38), i.e., $X(z_1,z_2,z_3,z_4)=X(z_1,z_3,z_2,z_4)$.

For all positive indices in (57), we use (54) to obtain the generating function

$$X(z_1,z_2,z_3,z_4)=\frac{1}{p_1^2-p_2^2}(p_1D_2-p_2D_1)D_3D_4\mathcal{F}.$$

Hence we have to prove

$$(p_1^2-p_3^2)(p_1D_2-p_2D_1)D_3D_4\mathcal{F}=(p_1^2-p_2^2)(p_1D_3-p_3D_1)D_2D_4\mathcal{F}. \tag{58}$$

It is straightforward to bring (58) into the identity (44) by eliminating $p_1^3D_2D_3D_4\mathcal{F}$ to both sides of (58), which concludes the proof for this case. If the index n in (57) is negative, then with the help of (45) the same arguments go through.

Let all the indices in (57) be negative; then by (55) we have the following equation to be verified:

$$\begin{aligned}0=&(\overline{D}_1\,\partial_{t_1}\mathcal{F})^2((\overline{D}_3\,\partial_{t_1}\mathcal{F})\overline{D}_2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})\overline{D}_3)\overline{D}_1\overline{D}_4\mathcal{F}+(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2((\overline{D}_1\,\partial_{t_1}\mathcal{F})\overline{D}_3\\&-(\overline{D}_3\,\partial_{t_1}\mathcal{F})\overline{D}_1)\overline{D}_2\overline{D}_4\mathcal{F}+(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2((\overline{D}_2\,\partial_{t_1}\mathcal{F})\overline{D}_1-(\overline{D}_1\,\partial_{t_1}\mathcal{F})\overline{D}_2)\overline{D}_3\overline{D}_4\mathcal{F},\end{aligned}$$

which, after consulting (53), is indeed an identity. This completes the proof for this case.

Let j in (57) be negative; and all others be positive. In terms of the generating functions the WDVV equations now reads as

$$\frac{(p_1\overline{D}_2+(\overline{D}_2\,\partial_{t_1}\mathcal{F})D_1)D_3D_4\mathcal{F}}{p_1^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2}=\frac{(p_1D_3-p_3D_1)\overline{D}_2D_4\mathcal{F}}{p_1^2-p_3^2}. \tag{59}$$

We express $D_3\overline{D}_2D_4$ and $D_1\overline{D}_2D_4$ from (48) [multiplying it by $z_4^{-2k-1}/(2k+1)$, and summing over k] and substitute them back into (59). It follows that

$$D_1D_3D_4\mathcal{F}=\frac{(p_1D_3-p_3D_1)D_4\,\partial_{t_1}\mathcal{F}}{p_1^2-p_3^2},$$

which is provided by (46). We conclude the proof of this case.

Finally, let j,k be negative and i,n be positive. In this case we have the following WDVV equations to prove:

$$\frac{(p_1\overline{D}_2+(\overline{D}_2\,\partial_{t_1}\mathcal{F})D_1)\overline{D}_3D_4\mathcal{F}}{p_1^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2}=\frac{(p_1\overline{D}_3+(\overline{D}_3\,\partial_{t_1}\mathcal{F})D_1)\overline{D}_2D_4\mathcal{F}}{p_1^2-(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2}, \tag{60}$$

where we have used $C^l(z_2^-,z_1^+)$ and $C^l(z_3^-,z_1^+)$ defined in (56) to the lhs and rhs of (60), respectively. Expressing $D_1\overline{D}_3D_4$ and $D_1\overline{D}_2D_4$ from (48) and substituting them back into (60), then

$$\overline{D}_2\overline{D}_3D_4\mathcal{F}=\frac{((\overline{D}_3\,\partial_{t_1}\mathcal{F})\overline{D}_2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})\overline{D}_3)D_4\,\partial_{t_1}\mathcal{F}}{(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2-(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2},$$

which is provided by (53). This completes the proof of WDVV equations for the EdBKP hierarchy.

C. Associative algebra and residue formula

The realization of the associative algebra with the structure constants (54)–(56) is obtained with the help of the kernel formulas (16) and (23) by introducing the generators

$$\phi_{2k+1}(p)=\frac{d\mathcal{B}_{2k+1}(p)}{dp},\quad k\in\mathbf{Z},$$

where $\mathcal{B}_{2k+1}\equiv\overline{\mathcal{B}}_{-2k-1}$ for $k\leq -1$. Then the kernel formulas (16) and (23) give us the following relations:

$$\frac{p(z)}{p^2-p^2(z)}=-\sum_{k\geq 0}\frac{z^{-2k-1}}{2k+1}\phi_{2k+1}(p), \tag{61}$$

$$\frac{\overline{D}(z)\partial_{t_1}\mathcal{F}}{p^2-(\overline{D}(z)\partial_{t_1}\mathcal{F})^2}=-\sum_{k\leq -1}\frac{z^{2k+1}}{2k+1}\phi_{2k+1}(p). \tag{62}$$

For example, we start by writing the identity

$$\frac{p_1p_2}{(p^2-p_1^2)(p^2-p_2^2)}=\frac{p_1p_2}{p_1^2-p_2^2}\left(\frac{1}{p^2-p_1^2}-\frac{1}{p^2-p_2^2}\right), \tag{63}$$

and expanding both sides in z_1^{-1},z_2^{-1}. Then, using (61) and (63), and comparing with (54), we obtain the algebra

$$\phi_{2i+1}(p)\phi_{2j+1}(p)=\sum_{l\geq 0}C_{2i+1,2j+1}^{2l+1}\phi_{2l+1}(p),\quad i,j\geq 0.$$

Next, we can expand both sides of the identity,

$$\frac{p_1\overline{D}_2\,\partial_{t_1}\mathcal{F}}{(p^2-p_1^2)(p^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2)}=\frac{p_1\overline{D}_2\,\partial_{t_1}\mathcal{F}}{p_1^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2}\left(\frac{1}{p^2-p_1^2}-\frac{1}{p^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2}\right), \tag{64}$$

in z_1^{-1},z_2. Using (61), (62), and (64), and comparing with (56), we have the algebra

$$\phi_{2i+1}(p)\phi_{2j+1}(p)=\sum_{l=-\infty}^{\infty}C_{2i+1,2j+1}^{2l+1}\phi_{2l+1}(p),\quad i\geq 0,\ j\leq -1.$$

The other algebra for $i,j,l\leq -1$ can be verified in a similar way and the structure constants are given by (55).

Now let us derive the residue formulas for third order derivatives of $\mathcal{F}$ (i.e., $\mathcal{F}_{2j+1,2k+1,2m+1}$) directly from dHirota equations. For the case of all positive indices, using (46) for $k=0$,

$$D_1D_2\,\partial_{t_1}\mathcal{F}=\frac{p_1D_2-p_2D_1}{p_1^2-p_2^2}\partial_{t_1}^2\mathcal{F},$$

we can express $D_1D_2D_3\mathcal{F}$ in terms of $D_i\partial_{t_1}^2\mathcal{F}$ only:

$$D_1D_2D_3\mathcal{F}=2\sum_{i=1}^{3}\operatorname{res}_{p_i}\left(\frac{p_1p_2p_3D(z(p))\partial_{t_1}^2\mathcal{F}}{(p^2-p_1^2)(p^2-p_2^2)(p^2-p_3^2)}dp\right). \tag{65}$$

Expanding both sides of (65) in the series in z_1,z_2,z_3 and using (61), we obtain

$$\mathcal{F}_{2j+1,2k+1,2m+1}=\frac{-1}{\pi i}\oint_{C_\infty}\frac{\partial_{t_1}z(p)}{z'(p)}\phi_{2j+1}(p)\phi_{2k+1}(p)\phi_{2m+1}(p)dp,\quad j,k,m\geq 0,$$

where, due to the fact that $0=\partial_{t_1}p(p)=\partial_{t_1}p(z)+\partial_zp(z)\partial_{t_1}z$, we have rewritten $D(z(p))\partial_{t_1}^2\mathcal{F}=-\partial_{t_1}p(z)=\partial_{t_1}z/z'(p)$ in the numerator of (65).

Similarly, for those cases containing nonpositive indices, we have

$$D_1D_2\overline{D}_3\mathcal{F}=2\sum_{i=1}^{3}\operatorname{res}_{p_i}\left(\frac{p_1p_2(\overline{D}_3\,\partial_{t_1}\mathcal{F})\partial_{t_1}p}{(p^2-p_1^2)(p^2-p_2^2)(p^2-(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2)}dp\right),$$

$$D_1\overline{D}_2\overline{D}_3\mathcal{F}=2\sum_{i=1}^{3}\operatorname{res}_{p_i}\left(\frac{-p_1(\overline{D}_2\,\partial_{t_1}\mathcal{F})(\overline{D}_3\,\partial_{t_1}\mathcal{F})\partial_{t_1}p}{(p^2-p_1^2)(p^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2)(p^2-(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2)}dp\right),$$

$$\overline{D}_1\overline{D}_2\overline{D}_3\mathcal{F}=2\sum_{i=1}^{3}\operatorname{res}_{p_i}\left(\frac{(\overline{D}_1\partial_{t_1}\mathcal{F})(\overline{D}_2\,\partial_{t_1}\mathcal{F})(\overline{D}_3\,\partial_{t_1}\mathcal{F})\partial_{t_1}p}{(p^2-(\overline{D}_1\,\partial_{t_1}\mathcal{F})^2)(p^2-(\overline{D}_2\,\partial_{t_1}\mathcal{F})^2)(p^2-(\overline{D}_3\,\partial_{t_1}\mathcal{F})^2)}dp\right),$$

where $\partial_{t_1}p_i=-D_i\,\partial_{t_1}^2\mathcal{F}$ when we evaluate the residue at $p=p_i$, while $\partial_{t_1}p_i=\overline{D}_i\,\partial_{t_1}^2\mathcal{F}$ at $p=\overline{D}_i\,\partial_{t_1}\mathcal{F}$. Using (61) and (62), similar residue formulas can be written down.

IV. CONCLUDING REMARKS

We have demonstrated the method of kernel formula to derive dHirota equations for dispersionless integrable hierarchies. After recalling the original approach to the dKP hierarchy, we apply the method to the EdBKP hierarchy. The results enables us to investigate the associativity equations in the EdBKP hierarchy.

Three remarks are in order. First, we like to mention that Takasaki[25] recently obtained dHirota equations of two-component BKP hierarchy by taking the quasi-classical limit of the corresponding(differential) Fay identities. Both approaches (that in Ref. 25 and ours) basically reach the same dHirota equations, except that the free energy differs by a factor 2. However in Ref. 25 the dispersionless Lax equations for a two-component BKP hierarchy can be formulated in two different ways, which reveals that the system has two spatial dimensions (t_1 and $\overline{t_1}$). It would be interesting to investigate this peculiar property from the viewpoint of WDVV equations. Second, the associativity equations discussed in Sec. III is an infinite-dimensional version of WDVV equations in which the number of variables t_k is infinite. However, in Ref. 6, some finite-dimensional reductions of the EdBKP hierarchy have been obtained via Riemann-Hilbert construction. Therefore, it is quite natural to ask whether these solutions satisfy the finite-dimensional version of WDVV equations. Third, in Refs. 20–22 Pavlov discussed dHirota equations of dBKP

system from the point of view of Egorov hydrodynamic chains and constructed associated solutions of WDVV equations. His approach in some sense gave a Hamiltonian approach to the dBKP system. Therefore it is also interesting to investigate the Hamiltonian formulation to the EdBKP hierarchy, which has the advantage of studying solutions of WDVV equations. Works in these directions are now in progress.

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APPENDIX: dHirota for EdBKP

Equation (29):

$$\mu^{-6}: \quad \frac{1}{5}\mathcal{F}_{15}+\frac{1}{3}\mathcal{F}_{11}^{3}-\frac{1}{3}\mathcal{F}_{11}\mathcal{F}_{13}-\frac{1}{9}\mathcal{F}_{33}=0,$$

$$\mu^{-8}: \quad \frac{2}{7}\mathcal{F}_{17}+\frac{1}{3}\mathcal{F}_{11}^{4}+\frac{1}{3}\mathcal{F}_{11}^{2}\mathcal{F}_{13}-\frac{1}{5}\mathcal{F}_{11}\mathcal{F}_{15}-\frac{1}{9}\mathcal{F}_{11}\mathcal{F}_{33}-\frac{2}{9}\mathcal{F}_{13}^{2}-\frac{2}{15}\mathcal{F}_{35}=0,$$

$$\mu^{-10}: \quad \frac{1}{3}\mathcal{F}_{19}+\frac{1}{5}\mathcal{F}_{11}^{5}+\frac{2}{3}\mathcal{F}_{11}^{3}\mathcal{F}_{13}+\frac{1}{5}\mathcal{F}_{11}^{2}\mathcal{F}_{15}-\frac{1}{7}\mathcal{F}_{11}\mathcal{F}_{17}-\frac{2}{15}\mathcal{F}_{11}\mathcal{F}_{35}$$

$$-\frac{4}{15}\mathcal{F}_{13}\mathcal{F}_{15}-\frac{1}{9}\mathcal{F}_{13}\mathcal{F}_{33}-\frac{2}{21}\mathcal{F}_{37}-\frac{1}{25}\mathcal{F}_{55}=0.$$

Equation (30):

$$\bar{\mu}^{6}: \quad \frac{1}{5}\mathcal{F}_{\bar{15}}+\frac{1}{3}\mathcal{F}_{11}^{\bar{3}}-\frac{1}{3}\mathcal{F}_{\bar{11}\bar{13}}-\frac{1}{9}\mathcal{F}_{\bar{33}}=0,$$

$$\bar{\mu}^{8}: \quad \frac{2}{7}\mathcal{F}_{\bar{17}}+\frac{1}{3}\mathcal{F}_{11}^{\bar{4}}+\frac{1}{3}\mathcal{F}_{11}^{\bar{2}}\mathcal{F}_{\bar{13}}-\frac{1}{5}\mathcal{F}_{\bar{11}\bar{15}}-\frac{1}{9}\mathcal{F}_{\bar{11}\bar{33}}-\frac{2}{9}\mathcal{F}_{13}^{\bar{2}}-\frac{2}{15}\mathcal{F}_{\bar{35}}=0,$$

$$\bar{\mu}^{10}: \quad \frac{1}{3}\mathcal{F}_{\bar{19}}+\frac{1}{5}\mathcal{F}_{11}^{\bar{5}}+\frac{2}{3}\mathcal{F}_{11}^{\bar{3}}\mathcal{F}_{\bar{13}}+\frac{1}{5}\mathcal{F}_{11}^{\bar{2}}\mathcal{F}_{\bar{15}}-\frac{1}{7}\mathcal{F}_{\bar{11}\bar{17}}-\frac{2}{15}\mathcal{F}_{\bar{11}\bar{35}}$$

$$-\frac{4}{15}\mathcal{F}_{\bar{13}\bar{15}}-\frac{1}{9}\mathcal{F}_{\bar{13}\bar{33}}-\frac{2}{21}\mathcal{F}_{\bar{37}}-\frac{1}{25}\mathcal{F}_{\bar{55}}=0.$$

Equation (31):

$$\mu^{-4}: \quad \mathcal{F}_{11}\mathcal{F}_{\bar{1}\bar{1}}-\frac{1}{3}\mathcal{F}_{\bar{3}\bar{1}}=0,$$

$$\mu^{-6}: \quad \mathcal{F}_{11}\mathcal{F}_{\bar{1}\bar{1}}^{2}+\frac{1}{3}\mathcal{F}_{11}\mathcal{F}_{\bar{1}\bar{3}}+\frac{1}{3}\mathcal{F}_{11}\mathcal{F}_{\bar{3}\bar{1}}+\frac{1}{3}\mathcal{F}_{\bar{1}\bar{1}}^{3}+\frac{1}{3}\mathcal{F}_{\bar{1}\bar{1}}\mathcal{F}_{13}-\frac{1}{3}\mathcal{F}_{\bar{1}\bar{1}}\mathcal{F}_{\bar{3}\bar{1}}$$

$$-\frac{1}{9}\mathcal{F}_{33}^{-}-\frac{1}{5}\mathcal{F}_{51}^{-}=0,$$

$$\mu^{-8}:\quad \frac{2}{3}\mathcal{F}_{11}\mathcal{F}_{11}^{-}\mathcal{F}_{31}^{-}+\frac{2}{3}\mathcal{F}_{11}\mathcal{F}_{11}^{3-}+\frac{1}{5}\mathcal{F}_{11}\mathcal{F}_{15}^{-}+\frac{1}{9}\mathcal{F}_{11}\mathcal{F}_{33}^{-}+\frac{1}{5}\mathcal{F}_{11}\mathcal{F}_{51}^{-}$$

$$+\frac{2}{3}\mathcal{F}_{11}\mathcal{F}_{11}^{-}\mathcal{F}_{13}^{-}+\frac{1}{3}\mathcal{F}_{13}\mathcal{F}_{11}^{2-}+\frac{1}{9}\mathcal{F}_{13}\mathcal{F}_{13}^{-}+\frac{1}{9}\mathcal{F}_{13}\mathcal{F}_{31}^{-}+\frac{1}{3}\mathcal{F}_{11}^{4-}$$

$$+\frac{1}{3}\mathcal{F}_{11}^{2-}\mathcal{F}_{13}^{-}-\frac{1}{9}\mathcal{F}_{11}^{-}\mathcal{F}_{33}^{-}-\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{51}^{-}+\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{15}-\frac{1}{9}\mathcal{F}_{13}^{-}\mathcal{F}_{31}^{-}$$

$$-\frac{1}{9}\mathcal{F}_{31}^{2-}-\frac{1}{15}\mathcal{F}_{35}^{-}-\frac{1}{15}\mathcal{F}_{53}^{-}-\frac{1}{7}\mathcal{F}_{71}^{-}=0.$$

Equation (32):

$$\lambda^{-4}:\quad \mathcal{F}_{11}^{-}\mathcal{F}_{11}^{-}-\frac{1}{3}\mathcal{F}_{13}^{-}=0,$$

$$\lambda^{-6}:\quad \mathcal{F}_{11}^{-}\mathcal{F}_{11}^{2-}+\frac{1}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{13}^{-}+\frac{1}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{31}^{-}+\frac{1}{3}\mathcal{F}_{11}^{3-}+\frac{1}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{13}^{-}-\frac{1}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{31}^{-}$$

$$-\frac{1}{9}\mathcal{F}_{33}^{-}-\frac{1}{5}\mathcal{F}_{51}^{-}=0,$$

$$\lambda^{-8}:\quad \frac{2}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{11}^{-}\mathcal{F}_{31}^{-}+\frac{2}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{11}^{3-}+\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{15}^{-}+\frac{1}{9}\mathcal{F}_{11}^{-}\mathcal{F}_{33}^{-}+\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{51}^{-}$$

$$+\frac{2}{3}\mathcal{F}_{11}^{-}\mathcal{F}_{11}^{-}\mathcal{F}_{13}^{-}+\frac{1}{3}\mathcal{F}_{13}^{-}\mathcal{F}_{11}^{2-}+\frac{1}{9}\mathcal{F}_{13}^{-}\mathcal{F}_{13}^{-}+\frac{1}{9}\mathcal{F}_{13}^{-}\mathcal{F}_{31}^{-}+\frac{1}{3}\mathcal{F}_{11}^{4}$$

$$+\frac{1}{3}\mathcal{F}_{11}^{2-}\mathcal{F}_{13}^{-}-\frac{1}{9}\mathcal{F}_{11}^{-}\mathcal{F}_{33}^{-}-\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{51}^{-}+\frac{1}{5}\mathcal{F}_{11}^{-}\mathcal{F}_{15}^{-}-\frac{1}{9}\mathcal{F}_{13}^{-}\mathcal{F}_{31}^{-}$$

$$-\frac{1}{9}\mathcal{F}_{31}^{2}-\frac{1}{15}\mathcal{F}_{35}^{-}-\frac{1}{15}\mathcal{F}_{53}^{-}-\frac{1}{7}\mathcal{F}_{71}^{-}=0.$$

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Polarizability of the dielectric double-sphere

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An explicit solution for the longitudinal and transverse polarizability of the symmetric dielectric intersecting double sphere is obtained as a rapidly converging series of integral operators, which is fast enough for real time calculation in Java Applet. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2359140]

I. INTRODUCTION

The problem of polarizability of an intersecting metallic double sphere was solved in 1949 by Schiffer and Szego. Fifty years later it was reinvented by Felderhof and Palaniappan in their article.[1] Their solution is given in terms of a one-dimensional integral and applies also to the asymmetric double spheres. The problem of a symmetric intersecting dielectric double sphere has not yet been solved in explicit form. In the year 1994, Radchik, Paley, and Smith gave a nice try in their article,[2] but they did not show enough respect to the normal boundary conditions, and eventually their results were proven to be false by Felderhof and Palaniappan.

Polarizability is a property of an object that measures its ability to interact with an electromagnetic force field. It depends on the electric properties of the matter and the shape of the object. When studying heterogeneous mixtures of dielectric objects, the polarizability of a single object provides crucial information.[3]

II. TOROIDAL COORDINATE SYSTEM

We define a coordinate transformation Λ from toroidal coordinates (u,v,φ) to Cartesian coordinates (x,y,z) by formulas

$$x=\frac{\sinh u\cos\varphi}{R^2},\quad y=\frac{\sinh u\sin\varphi}{R^2},\quad z=\frac{\sin v}{R^2},$$

where $R=\sqrt{\cosh u-\cos v}$. Coordinates (u,v,ϕ) have ranges $0\leq u<\infty$, $-\pi\leq v<\pi$, and $-\pi\leq\varphi<\pi$. The parametric surface $(v,\varphi)\mapsto\Lambda(u_1,v,\varphi)$ defines a family of toroidal surfaces parametrized by the coordinate u_1 and $(u,\varphi)\mapsto\Lambda(u,v_1,\varphi)$ defines a family of surfaces of intersecting double spheres parametrized by the coordinate v_1. In other words, the set

$$\mathcal{B}(v_1)=\{\Lambda(u,v,\varphi)\in\mathbb{R}^3|0\leq u<\infty,|v|=v_1,-\pi<\varphi<\pi\}$$

defines the surface of a symmetric intersecting double sphere. We can see that the surface $\mathcal{B}(\pi/2)$ is a sphere with unit radius, the surface $\mathcal{B}(\pi)$ is a disk with unit radius, and the surface $\mathcal{B}(0)$ is touching spheres having an infinite radius. All the other surfaces are between these extreme cases.

In the following, we shall be considering a domain:

$$\mathcal{D}(v_1)=\{\Lambda(u,v,\varphi)\in\mathbb{R}^3|0\leq u<\infty,v_1\leq|v|\leq\pi,-\pi<\varphi<\pi\},$$

which describes a symmetric double sphere with permittivity ε with a separation parameter v_1 that is connected to the relative distance d between the centers of the spheres by $d=2\cos v_1$. In

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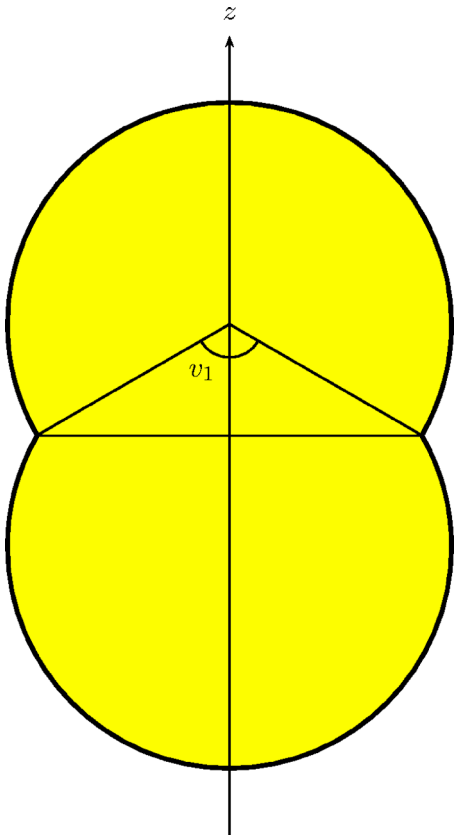

FIG. 1. A symmetric intersecting double sphere when separation parameter $v_1=\pi/3$.

particular, when $0\leq d<2$, we have an intersecting double sphere, and when $-2\leq d<0$ we have a lens. (See Fig. 1)

III. LONGITUDINAL POLARIZABILITY

Let ϕ be the scattered potential when the incident field $\mathbf{E}(\mathbf{r})=\mathbf{u}_z$, having potential $\phi_0=-z$, is applied. We can see that the Laplacian of the incident potential ϕ_0 vanishes meaning that for the scattered potential ϕ, we have $(\nabla^2\phi)(\mathbf{r})=0$ when $\mathbf{r}\notin\mathcal{B}(v_1)$. Therefore, it is a good idea to split the solution ϕ into two pieces:

$$\phi(u,v)=\begin{cases}\phi_1(u,v), & v<v_1,\\ \phi_2(u,v), & v\geq v_1,\end{cases}$$

because they both satisfy the Laplace's equation separately and are connected through the continuity and normal boundary conditions,

$$\phi_1(u,v_1)=\phi_2(u,v_1), \tag{1}$$

$$\partial\phi_1(u,v_1)-\varepsilon\ \partial\phi_2(u,v_1)=(1-\varepsilon)\,\partial\phi_0(u,v_1), \tag{2}$$

where we have used the notation $\partial\Phi(u,v)=(\partial/\partial v)\Phi(u,v)$. In addition, the symmetry of the scatterer and incident potential require that the potential ϕ is independent of the coordinate φ. The scattered potential must also vanish when $z=0$; thus we need to demand that $\phi_1(u,0)=0$ and $\phi_2(u,\pi)=0$ for all $0\leq u<\infty$.

Having now all the necessary integredients to solve the Laplace's equations, we shall proceed by introducing our main mathematical tool: the Mehler-Fock transform.

The Mehler-Fock Transform $\mathcal{F}$ is a mapping $f \mapsto F$, where f and F are mappings $\mathbb{R}^+ \to \mathbb{R}$ such that

$$F(\lambda) = \lambda \tanh(\pi\lambda) \int_0^\infty P_{-1/2+i\lambda}(\cosh u) \sinh u f(u) \mathrm{d}u.$$

According to Ref. 4, the inverse transform $\mathcal{F}^{-1}$ is the mapping $F \mapsto f$, where

$$f(u) = \int_0^\infty P_{-1/2+i\lambda}(\cosh u) F(\lambda) \mathrm{d}\lambda.$$

We shall use a more convenient notation $\overline{\Phi} = \mathcal{F}(\Phi)$ in the following. The Legendre function of the first kind P_ν in the core of the Mehler-Fock transform satisfies the well-known Legendre's differential equation,

$$(1 - x^2) P_\nu''(x) - 2x P_\nu'(x) + \nu(\nu + 1) P_\nu(x) = 0, \tag{3}$$

where the degree $\nu = -1/2 + i\lambda$ is a complex number, making it crucially different from the familiar Legendre's polynomials P_n.

It can be shown that Laplace's equation in the toroidal coordinate system is separable when we define a new function Φ_i by $\phi_i = R\Phi_i$, where the index $i \in \{1, 2\}$. Now, we may try to find solutions of the form

$$\Phi_i(u, v) = U(u) V_i(v),$$

and it turns out that we get two ordinary differential equations: the equation for the function U is the Legendre's equation (3) and for the functions V_i we have the equations

$$V_i'' = \lambda^2 V_i,$$

where λ is an arbitrary non-negative number, meaning that we have a continuous spectrum of solutions. Solutions satisfying the conditions $V_1(0) = 0$ and $V_2(\pi) = 0$ and the antisymmetry of the potential ϕ are given by

$$V_1(v) = c_1(\lambda) \sinh(v\lambda),$$

$$V_2(v) = c_2(\lambda) \begin{cases} \sinh((\pi - v)\lambda), & 0 \le v < \pi, \\ -\sinh((\pi + v)\lambda), & -\pi \le v < 0. \end{cases}$$

In the following, we may assume that $0 \le v < \pi$ because the boundary conditions (1) and (2) remain unchanged if we change the sign of the separation parameter v_1.

Now, the superposition principle suggests that the solutions could be of the form

$$\Phi_1(u, v) = \int_0^\infty c_1(\lambda) P_{-1/2+i\lambda}(\cosh u) \sinh(v\lambda) \mathrm{d}\lambda,$$

$$\Phi_2(u, v) = \int_0^\infty c_2(\lambda) P_{-1/2+i\lambda}(\cosh u) \sinh((\pi - v)\lambda) \mathrm{d}\lambda,$$

which indeed look like an inverse Mehler-Fock transform when the corresponding transforms are

$$\bar{\Phi}_1(\lambda,v) = c_1(\lambda)\sinh(v\lambda),$$

$$\bar{\Phi}_2(\lambda,v) = c_2(\lambda)\sinh((\pi - v)\lambda).$$

We shall begin our hunt for the unknown amplitude functions c_1 and c_2 by transforming the continuity equation (1) to obtain an equation,

$$c_1(\lambda)\sinh(v_1\lambda) = c_2(\lambda)\sinh((\pi - v_1)\lambda),$$

that we use to choose a new coefficient function c, which gives us the transforms

$$\bar{\Phi}_1(\lambda,v) = c(\lambda)\frac{\sinh(v\lambda)}{\sinh(v_1\lambda)},$$

$$\bar{\Phi}_2(\lambda,v) = c(\lambda)\frac{\sinh((\pi - v)\lambda)}{\sinh((\pi - v_1)\lambda)}.$$

Now, the solutions read as

$$\phi_i(u,v) = R(u,v)\int_0^\infty P_{-1/2+i\lambda}(\cosh u)\bar{\Phi}_i(\lambda,v)\mathrm{d}\lambda,$$

when $0 < v < \pi$.

There seems to be only one condition left to be fulfilled and one degree of freedom, namely the function c, to play with. We immediately see that the boundary condition (2) is an integral equation for the function c. It could be solved by means of the method of moments, however, due to the oscillatory kernel, it is not a good idea. Instead, we shall use the Mehler-Fock transform to obtain a much more nicely behaving integral equation.

A. Conducting double sphere

Next, we analyze briefly the case $\varepsilon \to \infty$. The boundary condition for a symmetric metallic double sphere is

$$\phi(u,v_1) = \phi_0(u,v_1) = \frac{\sin v}{R(u,v_1)^2},$$

which can be written in the form

$$\Phi(u,v_1) = \frac{\sin v_1}{R(u,v_1)^3}.$$

The Mehler-Fock transform of this equation yields

$$c_\infty = \bar{\Phi}(\lambda,v_1) = \sin v_1 \mathcal{F}\left(\frac{1}{R^3}\right). \tag{4}$$

Fortunately, the transform $\mathcal{F}(1/R^3)$ has a simple analytical expression, which we shall soon derive from the solution obtained by Felderhof and Palaniappan.

B. Dielectric double sphere

Using the definition $\phi_i = R\Phi_i$, the normal boundary condition (2) at $v = v_1$ can be written in the form

$$\frac{1}{2}\sin v_1 \frac{\Phi_{12}}{R^2} + \partial\Phi_{12} = (\varepsilon - 1)\left(\frac{\cos v_1}{R^3} - \frac{\sin^2 v_1}{R^5}\right),$$

where $\partial\Phi(u,v) = (\partial/\partial v)\Phi(u,v)$ and $\Phi_{12} = \Phi_1 - \varepsilon\Phi_2$. Now, we apply the Mehler-Fock transform with respect to coordinate u and obtain the equation

$$\partial\overline{\Phi}_{12} + \frac{1}{2}\sin v_1 \mathcal{F}\left(\frac{\Phi_{12}}{R^2}\right) = (\varepsilon - 1)\left(\cos v_1 \mathcal{F}\left(\frac{1}{R^3}\right) - \sin^2 v_1 \mathcal{F}\left(\frac{1}{R^5}\right)\right),$$

which, as it turns out, can be transformed to a Fredholm integral equation of the second kind.

In the article of Ref. 1, the case $\varepsilon \to \infty$ has been solved analytically. From that solution, we can extract the unknown function,

$$c_\infty = 2\sqrt{2}\lambda\left(\frac{\sinh((\pi - v_1)\lambda)}{\cosh(\pi\lambda)}\right).$$

Now, comparing this equation to Eq. (4), we conclude that

$$\mathcal{F}\left(\frac{1}{R^3}\right) = \frac{c_\infty}{\sin v_1},$$

and differentiating this with respect to parameter v_1 yields the transform

$$\mathcal{F}\left(\frac{1}{R^5}\right) = -\frac{2}{3\sin v_1}\partial\mathcal{F}\left(\frac{1}{R^3}\right) = \frac{4}{3}\sqrt{2}\lambda\left(\frac{\lambda\cosh((\pi - v_1)\lambda) + \cot v_1 \sinh((\pi - v_1)\lambda)}{\sin^2 v_1 \cosh(\pi\lambda)}\right).$$

A simple differentiation gives us the derivative

$$\partial\overline{\Phi}_{12} = (\coth(v_1\lambda) + \varepsilon\coth((\pi - v_1)\lambda))\lambda c(\lambda),$$

evaluated at $v = v_1$. Finally, we make a substitution $p = \cosh u$ and change the order of integration, giving us the term

$$\mathcal{F}\left(\frac{\Phi_{12}}{R^2}\right) = (1 - \varepsilon)\lambda\tanh(\pi\lambda)\int_1^\infty \frac{P_{-1/2+i\lambda}(p)}{p - \cos v_1}\int_0^\infty P_{-1/2+i\tau}(p)c(\tau)\mathrm{d}\tau\mathrm{d}p$$

$$= (1 - \varepsilon)\lambda\tanh(\pi\lambda)\int_0^\infty c(\tau)\underbrace{\int_1^\infty \frac{P_{-1/2+i\lambda}(p)P_{-1/2+i\tau}(p)}{p - \cos v_1}\mathrm{d}p}_{\mathcal{K}(\lambda,\tau)}\mathrm{d}\tau$$

So, our normal boundary condition has taken the form of a Fredholm's integral equation of the second kind:

$$c(\lambda) - \int_0^\infty k(\lambda,\tau)c(\tau)\mathrm{d}\tau = f(\lambda), \tag{5}$$

where the kernel k and the function f are given by expressions

$$k(\lambda,\tau) = \frac{(1 - \varepsilon)\sin v_1 \tanh(\pi\lambda)\mathcal{K}(\lambda,\tau)}{2(\coth(v_1\lambda) + \varepsilon\coth((\pi - v_1)\lambda))},$$

$$f(\lambda) = \frac{(\varepsilon - 1)\left(\cos v_1 \mathcal{F}\left(\frac{1}{R^3}\right) - \sin^2 v_1 \mathcal{F}\left(\frac{1}{R^5}\right)\right)}{\lambda(\coth(v_1\lambda) + \varepsilon\coth((\pi - v_1)\lambda))}.$$

It turns out that the integral operator K, defined by

$$(Kg)(\lambda) = \int_0^\infty k(\lambda,\tau)g(\tau)\mathrm{d}\tau,$$

is small (meaning that $\|K\| < 1$), so that the solution function c can be written in terms of the Neumann series,

$$c = \sum_{n=0}^{\infty} K^n f,$$

which converges for all $\varepsilon \geq 0$ and $0 < v_1 < \pi$. The convergence is quite fast: For instance, when $\varepsilon = 2$ and $v_1 = \pi/2$ only 5 terms was needed to get 4 digit precision. However, it seems that $\|K\| \to 1$ when $\varepsilon \to \infty$ and $v_1 \to 0$.

A highly recommended way to evaluate the Neumann series is to use a so-called nested form, which means that $c_n \to c$, where $c_{n+1} = Kc_n + f$ and $c_0 = f$.

C. Polarizability

The polarizability of the double sphere is obtained by looking the behavior of the potential ϕ on the z axis, where the coordinate $u = 0$. Using the Taylor expansions $\sin v \approx v$ and $\cos v \approx 1 - v^2/2$ we have $v \approx 2/z$ and $R \approx \sqrt{2}/z$ when z is large. We also need the expansion $\sinh(v\lambda) \approx v\lambda \approx 2\lambda/z$. Now we have the farfield expression for the potential on the z axis,

$$\phi(z) = \frac{2\sqrt{2}}{z^2}\int_0^\infty \frac{\lambda c(\lambda)}{\sinh(v_1\lambda)}\mathrm{d}\lambda,$$

where we have used the property $P_{-1/2+i\lambda}(1) = 1$ for all $\lambda \geq 0$. Now, we can compare this and the potential of the $\mathbf{u}_z$ directed dipole to get the normalized longitudinal polarizability,

$$\alpha_z = \frac{8\sqrt{2}\pi}{\mathcal{V}}\int_0^\infty \frac{\lambda c(\lambda)}{\sinh(v_1\lambda)}\mathrm{d}\lambda,$$

where $\mathcal{V}$ is the volume of the double sphere.

To calculate the volume of the double sphere, we need the Jacobian determinant

$$J = \frac{\sinh u}{R^3}$$

in the toroidal coordinate system. Now, the volume can be integrated analytically:

$$\mathcal{V} = 2\int_{-\pi}^{\pi}\int_0^\infty\int_{\pi}^{v_1} J\,\mathrm{d}v\,\mathrm{d}u\,\mathrm{d}\phi$$

$$= \frac{\pi}{6}\left(\frac{\cos\left(\frac{3v_1}{2}\right) - 3\cos\left(\frac{v_1}{2}\right)}{\sin^3\left(\frac{v_1}{2}\right)}\right).$$

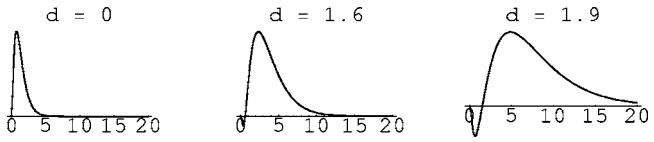

FIG. 2. Function f when $\varepsilon=2$ with different separation values.

IV. IMPLEMENTATION

To solve the integral equation (5), we approximate the functions c_n by vectors $c_n(\lambda_i)$, where the numbers λ_i are the integration points determined by the numerical integration method. The integrand of the integral operator K is a very smooth function, hence, the Gaussian quadrature is the best choice for the numerical integration. The iteration proceeds as

$$c_{n+1}(\lambda_i) = \sum_{j=1}^{j} w_j k(\lambda_i, \lambda_j)\, c_n(\lambda_j) + f(\lambda_i).$$

In each iteration, the kernel k has to be evaluated j^2 times. Therefore, we need a fast implementation for the subkernel $\mathcal{K}(\lambda, \tau)$, which we shall consider briefly, but first, we need to determine a proper choice for the integration points λ_i.

As we can see from Fig. 2, the initial guess function $f(\lambda)$ spreads when the separation parameter v_1 gets smaller. In addition, the integrand of the subkernel $\mathcal{K}$ becomes very oscillatory for large values of λ. Therefore, we need to exclude those values of v_1 that are close to 0, which correspond the touching case. When we choose 192 Gaussian points on the interval $[0,100]$, it is possible to analyze the cases $d \in [-1.99, 1.99]$.

A. Calculation of the subkernel

First, it is a good idea to do the integration with respect to variable u (meaning that $p = \cosh u$), which leads to integrand that decays as e^{-u} as $u \to \infty$ and oscillates with constant frequency.

The easiest way to calculate the subkernel $\mathcal{K}$ is to use the software package MATHEMATICA 5.2, which provides an implementation for the Legendre function P_ν and sophisticated numerical integration methods. When the Gaussian points λ_i are chosen, one can pick some separation parameter v_1 of interest and calculate the table $\mathcal{K}(\lambda_i, \lambda_j)$, which will be used in the iteration process.

In order to do real-time calculations, for example, in Java Applet, we need to choose another set of integration points u_i. Once again, the Gaussian quadrature outperforms the other methods, but now, due to the oscillatory behavior of the integrand of the subkernel, we need a lot of integration points. Using 1024 Gaussian points on the interval $[0, 20]$ provides a precision such that the polarizability can be calculated to precision that is 5 significant digits at worse. (See Fig. 3)

B. Speeding things up

We have to do about 20 000 evaluations of the subkernel $\mathcal{K}$ to calculate the table $\mathcal{K}(\lambda_i, \lambda_j)$. Every evaluation of the subkernel requires 2048 Legendre function evaluations. How to calculate a Legendre function 40 million times in one second?

Evaluating it by definition, as a hypergeometric series, is far too slow. A better idea is to save the values of the Legendre function $P_{-1/2+i\lambda_n}(\cosh u_m)$ in a table to 16-digit precision using MATHEMATICA. Such a high precision is a good idea because there occurs loss of precision in the integration. Constructing 1024 Gaussian points is not easy, but can be done with MATHEMATICA's command `Findroot` with initial guesses given by the formula $\cos(\pi(j-1/4)/(n+1/2))$. These Gaussian points (abscissas) should be calculated with 600-digit precision to get the desired

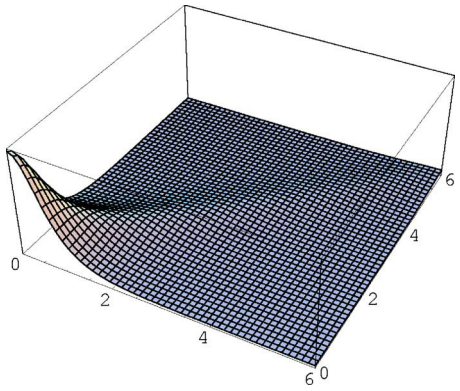

FIG. 3. The subkernel $\mathcal{K}(\lambda,\tau)$ when $v_1=\pi/2$.

16-digit precision for the weights. More details can be found, for example, in the paper of Ref. 5.

Evaluating the Legendre function $P^{\mu}_{-1/2+i\lambda}(\cosh u)$ as MATHEMATICA's function `LegendreP` is very time consuming for large values of λ. A faster way is to use a Formula 8.11.1 of the book[6] for small values of u and Formula 8.11.1 with the hypergeometric part replaced by the formula 15.3.6 for large values of u. The condition for which one to use is the number $u=0.1371+0.202e^{-0.0312\lambda}$, which we found in Appendix C of the article in Ref. 7.

V. TRANSVERSE POLARIZABILITY

To obtain the transverse polarizability, we need to apply the incident field $\mathbf{E}_0=\mathbf{u}_x$ corresponding to the potential $\phi_0=\cos\varphi$, which now depends on the coordinate φ. Fortunately, the solution is quite similar to the solution of the longitudinal case, in fact, the solutions are

$$\Phi_1(u,v,\varphi)=\cos\varphi\int_0^{\infty}c(\lambda)P^1_{-1/2+i\lambda}(\cosh u)\left(\frac{\cosh(v\lambda)}{\cosh(v_1\lambda)}\right)\mathrm{d}\lambda,$$

$$\Phi_2(u,v,\varphi)=\cos\varphi\int_0^{\infty}c(\lambda)P^1_{-1/2+i\lambda}(\cosh u)\left(\frac{\cosh((\pi-v)\lambda)}{\cosh((\pi-v_1)\lambda)}\right)\mathrm{d}\lambda.$$

The dependence of the coordinate φ causes no additional difficulties because it cancels out in the boundary conditions.

The function c should satisfy the integral equation

$$c(\lambda)-\int_0^{\infty}k(\lambda,\tau)c(\tau)\mathrm{d}\tau=f(\lambda), \tag{6}$$

where the kernel k and the function f are in this case given by expressions

$$k(\lambda,\tau)=-\frac{(1-\varepsilon)\sin v_1\tanh(\pi\lambda)\mathcal{K}(\lambda,\tau)}{2(\tanh(v_1\lambda)+\varepsilon\tanh((\pi-v_1)\lambda))},$$

$$f(\lambda)=\frac{(\varepsilon-1)\left(\sin v_1\mathcal{F}_{-1}\left(\frac{\cosh u}{R^5}\right)\right)}{\lambda(\tanh(v_1\lambda)+\varepsilon\tanh((\pi-v_1)\lambda))},$$

and the subkernel $\mathcal{K}$ is defined by the integral

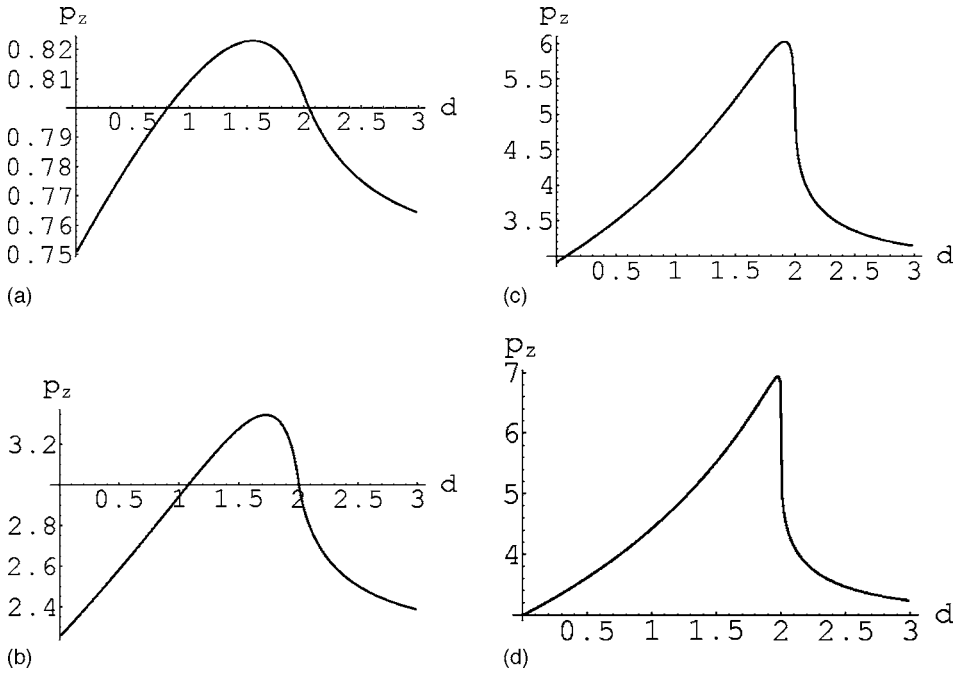

FIG. 4. Longitudinal polarizability as a function of d with different permittivities.

$$\mathcal{K}(\lambda,\tau)=\int_1^\infty \frac{P^{-1}_{-1/2+i\lambda}(p)P^{1}_{-1/2+i\tau}(p)}{p-\cos v_1}\mathrm{d}p.$$

The required Mehler-Fock transforms of order -1 can be derived from order 0 by differentiating the expressions with respect to coordinate u. Felderhof and Palaniappan[1] provide us with the metal limit

$$c_\infty=\frac{1}{2\sqrt{2}}\left(\frac{\cosh((\pi-v_1)\lambda)}{\cosh(\pi\lambda)}\right),$$

which, by taking the Mehler-Fock transform of order -1 of the incident potential, can be stated such that

$$c_\infty=-\mathcal{F}_{-1}\left(\frac{\cosh u}{R^3}\right).$$

Now, the differentiate this respect to the coordinate v_1 to obtain the missing term for the function f.

The transverse polarizability of the double sphere is obtained by looking the behavior of the potential ϕ on the neighborhood of the z axis, where the coordinate $u\approx 0$ and potential decays as x/z^3 for large z. Using the Taylor expansions $\sin v\approx v$ and $\cos v\approx 1-v^2/2$, we have $v\approx 2/z$ and $R\approx\sqrt{2}/z$ when z is large. This time we need also the expansion $\cosh(v\lambda)\approx 1$, which, together with the identity $P^1_{-1/2+i\lambda}(\cosh u)=\sinh u P'_{-1/2+i\lambda}(\cosh u)$, gives a farfield expression for the potential

$$\phi(z)=-2\sqrt{2}\frac{x}{z^3}\int_0^\infty \frac{(1+4\lambda^2)c(\lambda)}{\cosh(v_1\lambda)}\mathrm{d}\lambda,$$

where we have used the property $P'_{-1/2+i\lambda}(1)=-(1+4\lambda^2)/8$. Next, we can compare this and the potential of the $\mathbf{u}_z$ directed dipole to get the normalized longitudinal polarizability,

$$\alpha_x = -\frac{8\sqrt{2}\pi}{\mathcal{V}} \int_0^\infty \frac{(1+4\lambda^2)c(\lambda)}{\cosh(v_1\lambda)} d\lambda,$$

where $\mathcal{V}$ is the volume of the double sphere.

VI. CONCLUSION

The old electrostatic problem of a symmetric intersecting dielectric double sphere is solved explicitly for the first time. The solution is given in terms of an integral of a function c, which is given by a Neumann series. Using the high precision capabilities of the MATHEMATICA software package and efficient numerical integration techniques, the polarizabilities are implemented to real time calculations in the Java Applet:

`users.tkk.fi/~mpitkone/Kaksoispallo/Kaksoispallo.html`

where five-digit precision is achieved for the longitudinal polarizability and six-digit precision for the transversal polarizability. The results were verified at the metal limit $\varepsilon \to \infty$ using the solutions provided by Felderhof and Palaniappan.

Figure 4 represents the behavior of the longitudinal polarizability as a function of the separation d with different permittivity values. For values $d > 2$, the polarizability is calculated from the difference equation (3.9) of Ymeri's article[8] simply by solving that difference equation as an ordinary linear system. The same difference equation approach analysis was presented also in the article in Ref. 9 in 1976. It should be mentioned that Ymeri's article has a misprint in the formula (4.8), which should read as $\alpha_n = (n-1)(e^{-\eta_0} + \Delta_1 e^{-2n\eta_0})$. These results were verified at the metal limit using very accurate results from article in Ref. 10.

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On characterization of reversible Markov processes by monotonicity of the fluctuation spectral density

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For the system driven by a stationary Markov process $\{\xi_t: t \in \mathbb{R}^+\}$, if it is in nonequilibrium steady state (i.e., irreversible), then there exists a function φ such that the fluctuation spectrum (or say: power spectrum density) of $\{\varphi(\xi_t)\}$ is nonmonotonic in $[0, +\infty)$ under mild conditions, which means that there exist nonzero spectrum peaks of the fluctuation spectrum. For the system driven by a Markov chain with discrete time $\{\xi_t: t \in \mathbb{Z}^+\}$, even if it is in equilibrium state (i.e., reversible), one cannot distinguish the equilibrium and nonequilibrium steady state in terms of the monotonicity of the fluctuation spectrum any more. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2338763]

I. INTRODUCTION

We explain the main terminology used, hoping that this paper can be interested by both the probability kingdom and the statistical physics kingdom readers. In the present paper, unlike the classical probability theory, equilibrium means not just a stationary distribution but a stationary distribution of the reversible Markov process, and the term "nonequilibrium steady state" means a stationary distribution of the irreversible Markov process.

It is significant to consider the fluctuation spectrums (or say: power spectrum, power spectrum density, spectrum density of fluctuation) in the study of nonequilibrium steady states and especially of stochastic resonance since they have immediate intuitive meaning and are readily measurable.[1,2] In Refs. 3–5, the authors proved that when a stationary Markov process $\{\xi_t: t \in \mathbb{R}^+\}$ is in an equilibrium state, the fluctuation spectrum of any stationary process $\{\varphi(\xi_t)\}$ (where φ is a complex-valued function) decreases monotonically on $[0, +\infty)$ as a function of the frequency.

The question naturally arises if there is some nonmonotonic fluctuation spectrum for a stationary Markov process $\{\xi_t: t \in \mathbb{R}^+\}$ in nonequilibrium steady state; in other words, whether monotonicity of all fluctuation spectrums characterizes equilibrium.

Reference 6 gives a positive answer to the above-presented question in the situation of continuous-time finite states Markov chains. It proves that if the process $\{\xi_t\}$ is in nonequilibrium steady state, then one can always find a complex function φ such that the fluctuation spectrum of $\{\varphi(\xi_t)\}$ is nonmonotonic on $[0, +\infty)$.

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In the present paper, we extend the above-presented result to more general stationary Markov processes, including n-dimensional diffusions and denumerable Markov chains with continuous time. Under several mild technical conditions, we prove that the conclusion for the fluctuation spectrum in Ref. 6 remains true (see Theorem 2.1).

That is to say, for continuous-time Markov processes, equilibrium can be characterized by the monotonicity of all fluctuation spectrum under some technical conditions. For the nonequilibrium steady state Markov processes, the nonmonotonic fluctuation spectrums on $[0,\infty)$ mean that there exist off-zero peaks in the fluctuation spectrums. Reference 7 gave some criteria to show the stochastic resonance maximum in terms of the center frequency of the spectrum peak, spectrum peak height, and quality factor or signal-to-noise ratio. All the criteria are relevant to the off-zero peak in the fluctuation spectrums. The difference between Ref. 7 and this paper is that various values of the noise strength are not considered here.

But for a discrete-time irreducible aperiodic Markov chain $\{\xi_t: t\in\mathbb{Z}^+\}$ in equilibrium, if there exist two real eigenvalues λ_i and λ_j of the transient matrix P with $\lambda_i\cdot\lambda_j<0$ and $|\lambda_i|<1, |\lambda_j|<1$, then there exists a real function φ such that the fluctuation spectrum of $\{\varphi(\xi_t)\}$ is nonmonotonic on $[0,\pi]$, so one cannot distinguish the equilibrium and nonequilibrium steady state in terms of the monotonicity of the fluctuation spectrum any more. (see Sec. III). This gives an useful insight about continuous time Markov processes and explains why we treat only continuous time Markov processes on characterization of Markov processes in equilibrium by monotonicity of the fluctuation spectral density.

II. NONMONOTONIC FLUCTUATION SPECTRUM OF GENERAL STATIONARY MARKOV PROCESSES

In this section $\xi=\{\xi_t: t\geqslant 0\}$ always denotes a stationary Markov process, with its steady distribution written μ and infinitesimal generator written $\mathcal{A}$. The state space of the process is denoted by E, which is an abstract Polish space. The transition semigroup of the process is written $\{\mathsf{P}_t: t\geqslant 0\}$.

We shall need the following notations. Denote the real Hilbert space as $L^2(E,\mu)$. Denote the complex Hilbert space $\{h_1+\mathrm{i}h_2: h_1,h_2\in L^2(\mathrm{E},\mu)\}$ by $L^2_{\mathbb{C}}(E,\mu)$, where $\mathrm{i}=\sqrt{-1}$. The inner product on this complex Hilbert space is naturally defined by

$$\langle f,g\rangle=\int_E f(x)g^*(x)\mu(\mathrm{d}x),\quad \forall\, f,g\in L^2_{\mathbb{C}}(E,\mu),$$

where $g^*(x)$ stands for the conjugate complex number of $g(x)$, and the norm on $L^2_{\mathbb{C}}(E,\mu)$ as $\|\cdot\|$. For any $h\in L^2_{\mathbb{C}}(E,\mu)$, we write

$$\mu(h)=\int_E h(x)\mu(\mathrm{d}x),$$

$$\mathsf{P}_t h(x)=\int_E h(y)\mathsf{P}(t,x,\mathrm{d}y),$$

$$(\mathsf{P}_t-\mu)h(x)=\mathsf{P}_t h(x)-\mu(h).$$

Assume that $\{\mathsf{P}_t: t\geqslant 0\}$ is strongly continuous, i.e.,

$$\lim_{t\downarrow 0}\|\mathsf{P}_t f-f\|=0,\quad \forall\, f\in L^2_{\mathbb{C}}(E,\mu). \tag{1}$$

It is $L^2_{\mathbb{C}}(E,\mu)$ on which we consider the semigroup and the generator in the present paper. So if we suppose that $f\in\mathcal{D}(\mathcal{A})$ where $\mathcal{D}(\mathcal{A})$ is the domain of the operator $\mathcal{A}$, we mean that $f,\mathcal{A}f$

$\in L^2_{\mathbb{C}}(E,\mu)$ at the same time. Similarly, if we suppose $f \in \mathcal{D}(\mathcal{A}^2)$, we mean that $f, \mathcal{A}f, \mathcal{A}^2 f \in L^2_{\mathbb{C}}(E,\mu)$ at the same time.

A. Statement of the main results

Theorem 2.1: *For a continuous-time Markov process* $\{\xi_t\}$ *in nonequilibrium steady state, if there exist real functions* $f, g \in \mathcal{D}(\mathcal{A}^2) \cap L^2(E,\mu)$ *such that*

$$\langle \mathcal{A}^2 f, g\rangle - \langle f, \mathcal{A}^2 g\rangle \neq 0, \tag{2}$$

$$\begin{aligned} &\lim_{t\to+\infty} \langle \mathsf{P}_t f, \mathcal{A}^2 g\rangle = 0, \quad \lim_{t\to+\infty} \langle \mathsf{P}_t g, \mathcal{A}^2 f\rangle = 0, \\ &\lim_{t\to+\infty} t\langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle = 0, \quad \lim_{t\to+\infty} t\langle \mathsf{P}_t \mathcal{A} g, \mathcal{A}^2 f\rangle = 0, \end{aligned} \tag{3}$$

and

$$\begin{aligned} &t\langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 f\rangle, \quad t\langle \mathsf{P}_t \mathcal{A}^2 g, \mathcal{A}^2 g\rangle \in L^1([0,\infty)), \\ &t\langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle, \quad t\langle \mathsf{P}_t \mathcal{A}^2 g, \mathcal{A}^2 f\rangle \in L^1([0,\infty)), \end{aligned} \tag{4}$$

then the fluctuation spectrum of either $\{\mathcal{A}^2 f(\xi_t) + \mathrm{i}\mathcal{A}^2 g(\xi_t)\}$ *or* $\{\mathcal{A}^2 f(\xi_t) - \mathrm{i}\mathcal{A}^2 g(\xi_t)\}$ *is nonmonotonic on* $[0,+\infty)$.

When we have some information on the point spectrum and the eigenfunctions of the generator $\mathcal{A}$ of the irreversible stationary Markov process, we can yield the following

Corollary 2.2: For a continuous-time Markov process $\{\xi_t\}$ *in nonequilibrium steady state, if any one of the following conditions is satisfied:*

1) *There exists a complex eigenvalue* $-a+\mathrm{i}\omega$ *of* $\mathcal{A}$ *corresponding to an eigenfunction* $f(x) + \mathrm{i}g(x)$ *such that* $a>0, \omega \neq 0$.
2) *There exist two distinct real eigenvalues* $\lambda_1<0, \lambda_2<0$ *of* $\mathcal{A}$ *corresponding to eigenfunctions* $f(x), g(x)$, *respectively, such that* $\langle f, g\rangle \neq 0$.
3) *There exists a real eigenvalue* $\lambda<0$ *of* $\mathcal{A}$ *and there exist general eigenfunctions* $f(x), g(x)$ *with the following property*

$$\mathcal{A}f(x) = \lambda f(x), \quad \mathcal{A}g(x) = f(x) + \lambda g(x),$$

then one can find a complex function φ *such that the fluctuation spectrum of* $\{\varphi(\xi_t)\}$ *is nonmonotonic on* $[0,+\infty)$.

B. Proof of the main results

In order to prove the main theorem, we need some propositions and lemmas.

Let $f_1, f_2 \in L^2(E,\mu)$ and $\varphi = f_1 + \mathrm{i}f_2$. Denote the autocorrelation function and the fluctuation spectrum of $\{\varphi(\xi_t)\}$ as $B_\varphi(t), S_\varphi(\omega)$, respectively, which are defined as

$$B_\varphi(t) = \mathbb{E}[(\varphi(\xi_t) - \mu(\varphi))((\varphi^*(\xi_0) - \mu(\varphi)^*))] \quad \text{if } t \geqslant 0,$$

$$B_\varphi(t) = \mathbb{E}[(\varphi(\xi_0) - \mu(\varphi))((\varphi^*(\xi_{-t}) - \mu(\varphi)^*))] \quad \text{if } t < 0,$$

$$S_\varphi(\omega) = \frac{1}{2\pi}\int e^{-\mathrm{i}\omega t} B_\varphi(t)\mathrm{d}t,$$

where $\mathbb{E}$ is the expectation operator with respect to the process ξ.

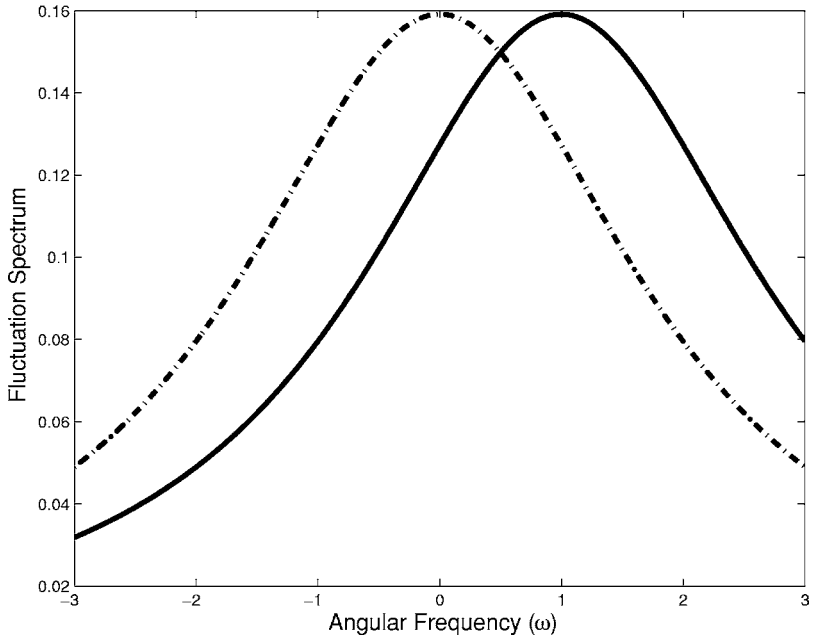

FIG. 1. Two fluctuation spectrums with the frequency limited on $[-3,3]$.

Lemma 2.3: If $B_\varphi(t) \in L^1(\mathbb{R})$, $S'_\varphi(\omega)$ *exists and* $[\mathrm{d}S_\varphi(\omega)]/\mathrm{d}\omega|_{\omega=0} > 0$, *then* $S_\varphi(\omega)$ *is nonmonotonic on* $[0,+\infty)$.

Proof: Since $B_\varphi(t) \in L^1(\mathbb{R})$, $\lim_{\omega\to+\infty} S_\varphi(\omega)=0$ by Riemann-Lebesgue's lemma. It is well known that $S_\varphi(\omega) \geqslant 0$, and since $S'_\varphi(0) > 0$, there exists some $\delta > 0$ such that $S_\varphi(\delta) > 0$.

Now suppose on the contrary that $S_\varphi(\omega)$ is monotonic in $[0,+\infty)$, then it must increase monotonically since $S'_\varphi(0) > 0$. Then $S_\varphi(\omega) \geqslant S_\varphi(\delta) > 0$ for all $\omega > \delta$. Therefore $\underline{\lim}_{\omega\to+\infty} S_\varphi(\omega) > 0$, a contradiction. □

Remark 1: Lemma 2.3 is the start point of the proof of the main theorem. The following sketch map gives two fluctuation spectrums with the frequency limited on $[-3,3]$. One is nonmonotonic on $[0,\infty)$ with $S'_\varphi(0) > 0$, the other is monotonic on $[0,\infty)$ with $S'_\varphi(0)=0$ (Fig. 1).

It is clear that

$$B_\varphi(t) = \langle \mathsf{P}_t\varphi,\varphi\rangle - |\mu(\varphi)|^2 = \langle (\mathsf{P}_t - \mu)\varphi,\varphi\rangle \quad \text{if } t \geqslant 0,$$

$$B_\varphi(t) = \langle \varphi,\mathsf{P}_{-t}\varphi\rangle - |\mu(\varphi)|^2 = \langle \varphi,(\mathsf{P}_{-t} - \mu)\varphi\rangle \quad \text{if } t < 0.$$

For $t \geqslant 0$, let us write

$$F(t) = \langle \mathsf{P}_t f_1, f_1\rangle - |\mu(f_1)|^2 + \langle \mathsf{P}_t f_2, f_2\rangle - |\mu(f_2)|^2,$$

$$G(t) = \langle f_1, \mathsf{P}_t f_2\rangle - \langle \mathsf{P}_t f_1, f_2\rangle.$$

Since the transition semigroup $\{\mathsf{P}_t : t \geqslant 0\}$ is strongly continuous, then one can get that $F(t)$ is a continuous function of t on $[0,\infty)$ by Proposition 4.3.1 of Ref. 5 (p. 112). And similarly that $G(t)$ is a continuous function of t on $[0,\infty)$.

Lemma 2.4: For the above complex-valued function φ, *we have*

$$B_\varphi(t) = F(|t|) + \mathrm{i}\cdot \mathrm{sgn}(t) G(|t|), \tag{5}$$

where $\mathrm{sgn}(t) := 1$ *for* $t \geqslant 0$ *and* $\mathrm{sgn}(t) := -1$ *for* $t < 0$. *And if* $F(t), G(t) \in L^1([0,\infty))$, *then* $S_\varphi(\omega)$ *exists and*

$$S_\varphi(\omega)=\frac{1}{\pi}\int_0^{+\infty}[F(t)\cos(\omega t)+G(t)\sin(\omega t)]\mathrm{d}t. \tag{6}$$

Proof: When $t\geqslant 0$, the correlation function of $\{\varphi(\xi_t)\}$ is

$$B_\varphi(t)=\langle \mathsf{P}_t\varphi,\varphi\rangle-|\mu(\varphi)|^2$$

$$=\langle \mathsf{P}_t f_1+\mathrm{i}\mathsf{P}_t f_2, f_1+\mathrm{i}f_2\rangle-|\mu(f_1)+\mathrm{i}\mu(f_2)|^2$$

$$=\langle \mathsf{P}_t f_1,f_1\rangle-|\mu(f_1)|^2+\langle \mathsf{P}_t f_2,f_2\rangle-|\mu(f_2)|^2$$

$$+\mathrm{i}(\langle f_1,\mathsf{P}_t f_2\rangle-\langle \mathsf{P}_t f_1,f_2\rangle)$$

$$=F(t)+\mathrm{i}G(t).$$

And when $t<0$,

$$B_\varphi(t)=B_\varphi^*(-t)=F(-t)-\mathrm{i}G(-t).$$

This means

$$B_\varphi(t)=F(|t|)+\mathrm{i}\cdot\mathrm{sgn}(t)G(|t|),\quad t\in\mathbb{R},$$

where $\mathrm{sgn}(\cdot)$ is the sign function. If $F(t),G(t)\in L^1([0,\infty))$, then it is clear that $B_\varphi(t)\in L^1(\mathbb{R})$. So the fluctuation spectrum exists and

$$S_\varphi(\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}B_\varphi(t)\exp(-\mathrm{i}\omega t)\mathrm{d}t=\frac{1}{\pi}\int_0^{+\infty}F(t)\cos(\omega t)\mathrm{d}t+\frac{1}{\pi}\int_0^{+\infty}G(t)\sin(\omega t)\mathrm{d}t.$$

□

Lemma 2.5: If $tF(t),tG(t)\in L^1([0,\infty))$, *then* $S'_\varphi(\omega)$ *exists, and*

$$\frac{\mathrm{d}S_\varphi(\omega)}{\mathrm{d}\omega}=-\frac{1}{\pi}\int_0^{+\infty}t[F(t)\sin(\omega t)-G(t)\cos(\omega t)]\mathrm{d}t. \tag{7}$$

Especially,

$$S'_\varphi(0)=\frac{1}{\pi}\int_0^{+\infty}tG(t)\mathrm{d}t. \tag{8}$$

And if

$$\int_0^{+\infty}tG(t)\mathrm{d}t>0, \tag{9}$$

then the fluctuation spectrum of $\{\varphi(\xi_t)\}$ *is nonmonotonic on* $[0,+\infty)$.

Proof: Since $tF(t),tG(t)\in L^1([0,\infty))$, it is clear that $tB_\varphi(t)\in L^1(\mathbb{R})$. So $S'_\varphi(\omega)$ exists and by Lemma 2.4, we have

$$\frac{\mathrm{d}S_\varphi(\omega)}{\mathrm{d}\omega}=-\frac{1}{\pi}\int_0^{+\infty}t[F(t)\sin(\omega t)-G(t)\cos(\omega t)]\mathrm{d}t,$$

$$S'_{\varphi}(0) = \frac{1}{\pi}\int_0^{+\infty} tG(t)\mathrm{d}t.$$

If condition (9) is satisfied, then $S'_{\varphi}(0) > 0$. This ends the proof by Lemma 2.3. □

By Lemma 2.5, now the last key point is to find two real functions $f_1, f_2 \in L^2(\mathrm{E}, \mu)$ such that Eq. (9) is satisfied. The following lemma is needed.

Lemma 2.6: *For any Markov process* $\{\xi_t\}$ *in steady state, if* $f, g \in \mathcal{D}(\mathcal{A}^2) \cap L^2(E, \mu)$ *and*

$$\lim_{t\to+\infty} \langle \mathsf{P}_t f, \mathcal{A}^2 g\rangle = 0, \tag{10}$$

$$\lim_{t\to+\infty} t\langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle = 0, \tag{11}$$

then

$$\langle f, \mathcal{A}^2 g\rangle = \int_0^{+\infty} t\langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle \mathrm{d}t. \tag{12}$$

Proof: When $t \geqslant 0$, by Kolmogorov equations,

$$\mathrm{d}\mathsf{P}_t f = \mathsf{P}_t \mathcal{A} f \mathrm{d}t,$$

$$\text{and} \quad \mathrm{d}\langle \mathsf{P}_t f, g\rangle = \langle \mathsf{P}_t \mathcal{A} f, g\rangle \mathrm{d}t.$$

Hence we have

$$\int_0^{+\infty} t\langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle \mathrm{d}t = \int_0^{+\infty} t\mathrm{d}\langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle$$

$$= t\langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle|_{t=0}^{+\infty} - \int_0^{+\infty} \langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle \mathrm{d}t$$

$$= \lim_{t\to+\infty} t\langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle - \int_0^{+\infty} \langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle \mathrm{d}t$$

$$= -\int_0^{+\infty} \langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle \mathrm{d}t.$$

And by Kolmogorov equations again,

$$\int_0^{+\infty} \langle \mathsf{P}_t \mathcal{A} f, \mathcal{A}^2 g\rangle \mathrm{d}t = \int_0^{+\infty} \mathrm{d}\langle \mathsf{P}_t f, \mathcal{A}^2 g\rangle = \lim_{t\to+\infty} \langle \mathsf{P}_t f, \mathcal{A}^2 g\rangle - \langle f, \mathcal{A}^2 g\rangle = -\langle f, \mathcal{A}^2 g\rangle.$$

□

Now we start the proof of the main theorem and Corollary.

Proof of Theorem 2.1: Without loss of generality, let us assume $\langle \mathcal{A}^2 f, g\rangle - \langle f, \mathcal{A}^2 g\rangle > 0$. Let $f_1 = \mathcal{A}^2 f, f_2 = \mathcal{A}^2 g$. Since $\mu(\mathcal{A}^2 f) = \mu(\mathcal{A}^2 g) = 0$,

$$F(t) = \langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 f\rangle + \langle \mathsf{P}_t \mathcal{A}^2 g, \mathcal{A}^2 g\rangle,$$

$$G(t) = \langle \mathcal{A}^2 f, \mathsf{P}_t \mathcal{A}^2 g\rangle - \langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle.$$

By condition (4), $tF(t), tG(t) \in L^1([0,\infty))$. Then $S'_\varphi(\omega)$ exists by Lemma 2.5.

By condition (3), the following equations

$$\int_0^{+\infty} t\langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle \mathrm{d}t = \langle f, \mathcal{A}^2 g\rangle,$$

$$\int_0^{+\infty} t\langle \mathcal{A}^2 f, \mathsf{P}_t \mathcal{A}^2 g\rangle \mathrm{d}t = \langle \mathcal{A}^2 f, g\rangle$$

hold by Lemma 2.6.

By Eq. (8) of Lemma 2.5

$$S'_\varphi(0) = \frac{1}{\pi}\int_0^{+\infty} tG(t)\mathrm{d}t = \frac{1}{\pi}\int_0^{+\infty} t[\langle \mathcal{A}^2 f, \mathsf{P}_t \mathcal{A}^2 g\rangle - \langle \mathsf{P}_t \mathcal{A}^2 f, \mathcal{A}^2 g\rangle]\mathrm{d}t = \langle \mathcal{A}^2 f, g\rangle - \langle f, \mathcal{A}^2 g\rangle > 0.$$

Thus the fluctuation spectrum of $\{\varphi(\xi_t)\}$ is nonmonotonic by Lemma 2.5. □

Proof of Corollary 2.2: Conditions (2)–(4) of Theorem 2.1 are satisfied when applied with the functions $f(x)$ and $g(x)$ appearing in conditions 1), 2) or 3) of Corollary 2.2. This ends the proof.□

C. Applications

Example 1: If $\{\xi_t : t \in \mathbb{R}\}$ is a stationary continuous-time finite states Markov chain, if it is in nonequilibrium steady state, then by the Lemma 2.4 of Ref. 6, one of the conditions in Corollary 2.2 is satisfied at least. Thus one can always find a nonmonotonic fluctuation spectrum by Corollary 2.2.

Example 2: For Ornstein-Uhlenbeck equation (or Langevin equation)

$$\begin{bmatrix} \mathrm{d}X_1(t) \\ \mathrm{d}X_2(t) \end{bmatrix} = \begin{bmatrix} -r & \Omega \\ -\Omega & -r \end{bmatrix} \begin{bmatrix} X_1(t) \\ X_2(t) \end{bmatrix} \mathrm{d}t + \sigma \begin{bmatrix} \mathrm{d}B_1(t) \\ \mathrm{d}B_2(t) \end{bmatrix}, \tag{13}$$

where $r > 0, \Omega > 0$ (Ref. 8, pp. 181–186), the generator is

$$\mathcal{A} = (-rx + \Omega y)\frac{\partial}{\partial x} + (-\Omega x - ry)\frac{\partial}{\partial y} + \frac{1}{2}\sigma^2 \cdot \triangle, \tag{14}$$

with the stationary distribution

$$\mu(\mathrm{d}x, \mathrm{d}y) = \frac{r}{\pi\sigma^2} \exp\left\{-\frac{r(x^2+y^2)}{\sigma^2}\right\} \mathrm{d}x\mathrm{d}y. \tag{15}$$

Since $-r+\mathrm{i}\Omega$ is the complex eigenvalue of the generator $\mathcal{A}$ corresponding to the eigenfunction $x-\mathrm{i}y$, the generator $\mathcal{A}$ is a nonsymmetric operator with respect to μ. So the existence of a nonmonotonic fluctuation spectrum is solved by Corollary 2.2.

Example 3: Let $\{\xi_t : t \in \mathbb{R}^1\}$ be a continuous-time Markov chain, with the state space $E = \{-2,-1,0,1,2,\ldots\}$ and the transition rate matrix

$$\mathsf{Q} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 0 & -2 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & -4 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 4 & -7 & 3 & \cdots \\ 0 & 0 & 0 & 0 & 6 & -10 & \cdots \\ \vdots & \ddots & \ddots & & & & \end{bmatrix}.$$

That is $q_{-2,-1}=q_{-1,0}=q_{0,-2}=1$, and when $n\geqslant 0$, $q_{n,n+1}=n+1$ and $q_{n,n-1}=2n$. Clearly the steady distribution μ is defined by $\mu(-2)=\mu(-1)=1/4$, and $\mu(n)=1/4(1/2)^n$ for $n\geqslant 0$. Let $f(x)=\delta_{-2,x}$ and $g(x)=\delta_{-1,x}$, where the Kronecker delta $\delta_{-2,x}$ is 1 when x is equal to -2, and is 0 otherwise. One can check that condition (2) is satisfied. By Ref. 9, Theorem 3, Ref. 10, Theorem 6.5 and Example 4.57 in Ref. 11, pp. 162, it is clear that this Markov chain is exponentially ergodic. And since $\mathcal{A}f(x), \mathcal{A}g(x), \mathcal{A}^2 f(x), \mathcal{A}^2 g(x)$ are all compact supported, conditions (3) and (4) are valid. Therefore a nonmonotonic fluctuation spectrum is found by Theorem 2.1.

III. FLUCTUATION SPECTRUM FOR DISCRETE-TIME MARKOV CHAINS IN EQUILIBRIUM

Let $\{\xi_t : t\in\mathbb{Z}^+\}$ be a discrete-time finite states Markov chain, and let P be its $k\times k$ irreducible probability transition matrix, where k is the number of states. If $\{\xi_t\}$ is in equilibrium state, then all the eigenfunctions of P can be chosen to be orthonormal with respect to the steady distribution μ, and denote them by $\{f_1, f_2, \ldots, f_k\}$, and let λ_i be the eigenvalue of the matrix P corresponding to the eigenfunction f_i. We might as well let $\lambda_1=1$ with the eigenvector $f_1=(1,1,\ldots,1)$. For any complex function $\varphi\in\mathbb{C}^k$, let $\varphi=\Sigma_{j=1}^k a_j f_j$. Denote the autocorrelation function and the fluctuation spectrum of $\{\varphi(\xi_t)\}$ as $B_\varphi(t), S_\varphi(\omega)$, respectively, which are defined as

$$B_\varphi(t) = \mathbb{E}[(\varphi(\xi_t)-\mu(\varphi))((\varphi^*(\xi_0)-\mu(\varphi)^*))] \quad \text{if } t\in\mathbb{Z}^+,$$

$$B_\varphi(t) = \mathbb{E}[(\varphi(\xi_0)-\mu(\varphi))((\varphi^*(\xi_{-t})-\mu(\varphi)^*))] \quad \text{if } t\in\mathbb{Z}^-,$$

$$S_\varphi(\omega) = \frac{1}{2\pi}\sum_{t=-\infty}^{\infty} B_\varphi(t)e^{-\mathrm{i}t\omega}, \quad -\pi\leqslant\omega\leqslant\pi,$$

where $\mathbb{E}$ is the expectation operator with respect to the process ξ.

And similar to Refs. 6 and 12, based on elementary facts of self-adjoint operators in finite dimensional spaces and obvious elementary calculus, one can obtain that

Proposition 3.1: If $\{\xi_t : t\in\mathbb{Z}^+\}$ *is in equilibrium state, and its probability transition matrix* P *is irreducible, then*

$$B_\varphi(t) = \sum_{i=2}^{k} |a_i|^2 \lambda_i^{|t|}, \quad t\in\mathbb{Z}. \tag{16}$$

If P *is aperiodic in addition, then the fluctuation spectrum of* $\{\varphi(\xi_t)\}$ *exists and*

$$S_\varphi(\omega) = \frac{1}{2\pi}\sum_{i=2}^{k} |a_i|^2 \frac{1-\lambda_i^2}{1+\lambda_i^2-2\lambda_i\cos\omega}. \tag{17}$$

In particular, the fluctuation spectrum is monotonic if and only if all eigenvalues of the irreducible, aperiodic transient matrix P *which are not equal to 1 have same signs.*

Example 4:

$$P = \begin{bmatrix} 0 & \frac{1}{4} & \frac{3}{4} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{3}{4} & \frac{1}{4} & 0 \end{bmatrix}.$$

The above transition matrix is obviously symmetrical with an equilibrium state $\mu = (1/3, 1/3, 1/3)$. Clearly $-3/4, 1/4$ are two eigenvalues with different signs. This example shows the existence of the nonmonotonic fluctuation spectrum for the discrete-time Markov chains in equilibrium.

IV. CONCLUSION

For continuous-time Markov processes, equilibriums can be characterized by the monotonicity of all fluctuation spectrum under some good conditions. For discrete-time irreducible aperiodic Markov chains, one cannot distinguish the equilibrium and nonequilibrium steady state in terms of the monotonicity of the fluctuation spectrum any more.

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Nonlinear diffusion equation and nonlinear external force: Exact solution

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The solutions of the nonlinear diffusion equation $\partial_t\rho=r^{1-\mathcal{N}}\mathcal{D}\partial_r\{r^{\mathcal{N}-1-\theta}\rho^\gamma\partial_r[r^{-\eta}\rho^\nu]\}-r^{1-\mathcal{N}}\partial_r[r^{\mathcal{N}-1}\mathcal{F}\rho]$ are investigated by considering the presence of an external force $\mathcal{F}$ which exhibits an explicit dependence on the distribution. First, the stationary case is considered; after that the dynamical case, i.e., the case dependent on time. The stationary solution is obtained by considering the external force $\mathcal{F}(r;\rho)=\mathcal{F}_1(r)+\mathcal{F}_2(r)[\rho(r)]^{\nu+\gamma-1}$ and the result found is related to the distributions which emerge from the Tsallis statistics or the Boltzmann-Gibbs statistics. The dynamical solution is investigated by considering the external force $\mathcal{F}(r,t;\rho)=-k(t)r+\mathcal{K}/r^{1+\theta+\eta}[\rho(r,t)]^{\gamma+\nu-1}$ and related to the Levy distributions in the asymptotic limit. In both cases, the solutions are expressed in terms of the q-exponentials and the q-logarithmics functions which emerge from the Tsallis formalism. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2354334]

I. INTRODUCTION

The broadness of the anomalous diffusion processes covering many physical contexts has motivated the study of several approaches.[1–8] One of them is based on the nonlinear diffusion equations[4] which has been used to investigate many situations such as percolation of gases through porous media,[9] thin saturated regions in porous media,[10] a standard solid-on-solid model for surface growth, thin liquid films spreading under gravity,[11] the axisymmetric flow of a very viscous fluid,[12] turbulent diffusion,[13] and the nonlinear diffusion in hard and soft superconductors.[14] A representative nonlinear diffusion equation is the *porous medium equation* ($\partial_t\rho=\mathcal{D}\nabla^2\rho^\nu$) which has been intensively investigated. In fact, it has been analyzed by considering several situations such as the presence of external forces,[15] a spatial time dependent diffusion coefficient,[16–18] and reaction diffusion terms.[19] In this direction, in Refs. 20 and 21 was obtained a Langevin equation related to the porous medium equation and in Refs. 22 and 23 the connection between the solutions and distribution of probability that emerges from the Tsallis formalism was investigated. The escape time, or mean first passage time, has also been studied leading eventually to a generalization of the Arrhenius law.[24] However, the presence of nonlinear drift in the porous medium equation and its connection with the Tsallis formalism[25] or the usual thermostatistics (Boltzmann-Gibbs statistics)[26] have not been properly investigated. Thus, we dedicate the present work to establish some classes of solutions of a general nonlinear diffusion equation and investi-

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gate the connections with the Tsallis formalism and the usual thermostatistics. We focus our attention on the following generalized equation:

$$\frac{\partial}{\partial t}\rho(r,t)=\frac{\mathcal{D}}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left\{r^{\mathcal{N}-1-\theta}[\rho(r,t)]^{\gamma}\frac{\partial}{\partial r}[r^{-\eta}(\rho(r,t))^{\nu}]\right\}-\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\{r^{\mathcal{N}-1}\mathcal{F}(r,t;\rho)\rho(r,t)\},\tag{1}$$

where $\mathcal{D}$ is a (dimensionless) diffusion coefficient, r is non-negative, $\mathcal{N}$ represents the dimension of the system, $\mathcal{F}(r,t;\rho)$ is a (dimensionless) nonlinear convection or transport term (external force). For $\alpha(t)=0$, it can be verified that $\int_0^\infty dr r^{\mathcal{N}-1}\rho(r,t)$ is time independent (hence, if ρ is normalized at $t=0$, it will remain so forever). Indeed, if we write the equation in the $\partial_t\rho=r^{1-\mathcal{N}}\partial_r\mathcal{J}$ form and assume the boundary condition $\mathcal{J}(\infty,t)\to 0$, it can be shown that $\int_0^\infty dr r^{\mathcal{N}-1}\rho(r,t)$ is a constant of motion. Note that Eq. (1) has as particular case several situations such as mentioned above and also recovers, for $(\eta,\gamma,\theta,\nu)=(0,0,0,1)$ and $\mathcal{F}(r,t;\rho)=0$ the standard Fokker-Planck equation[27] in the absence of drift and to $(\eta,\gamma,\theta,\nu,\mathcal{N})=(0,0,0,1,1)$ with $\mathcal{F}(r,t;\rho)=\mathcal{K}[\rho(r,t)]^2/2$ the Burgers equation[28] in the one-dimensional case. Thus, our present discussion involves extensions of these cases taking a wide variety of situations into account by employing a nonlinear diffusion equation with a nonlinear convection or transport term. In particular, in Sec. II, we consider several situations for Eq. (1) by starting to the stationary case and after we analyze the dynamical, i.e., the time dependent solutions. For the stationary case, we consider the external force $\mathcal{F}(r;\rho)=\mathcal{F}_1(r)+\mathcal{F}_2(r)[\rho(r)]^{\nu+\gamma-1}$ ($\mathcal{F}_1(r)$ and $\mathcal{F}_2(r)$ are arbitrary functions) and for the time dependent case we employ $\mathcal{F}(r,t;\rho)=-k(t)r+\mathcal{K}/r^{1+\theta+\eta}[\rho(r,t)]^{\nu+\gamma-1}$ ($k(t)$ is a time dependent function and $\mathcal{K}$ is a constant). In Sec. III, we present our conclusions.

II. NONLINEAR DIFFUSION EQUATION

Let us start our study by investigating the stationary solutions for Eq. (1). For this case, by taking into account the external force $\mathcal{F}(r;\rho)=\mathcal{F}_1(r)+\mathcal{F}_2(r)[\rho(r)]^{\nu+\gamma-1}$ and employing the stationary condition,[27,29] we can reduce Eq. (1) to

$$\mathcal{D}r^{-\theta}[\rho(r)]^{\gamma}\frac{d}{dr}[r^{-\eta}(\rho(r))^{\nu}]-\mathcal{F}_1(r)\rho(r)-\mathcal{F}_2(r)[\rho(r)]^{\nu+\gamma}=0\tag{2}$$

for an arbitrary $\mathcal{N}$. Note that this equation has a nonlinear diffusive term and also a nonlinear convection or transport term. This nonlinear term incorporated in the external force may produce in the solution a new behavior to the stationary solution which was not present in the results found in Refs. 15–17. In fact, the solution which emerges from this equation may present two behaviors, one of them is a power-law (Tsallis formalism) and the other is an exponential (Boltzmann-Gibbs statistics). In order to show this feature and obtain the solution of this equation, we may use the procedure employed by Plastino and Plastino in Ref. 22 which is based on the Tsallis formalism.[25] Following Ref. 22, we consider the solution given by

$$\rho(r)=r^{\eta/\nu}\exp_q[-\mathcal{G}(r)]/\mathcal{Z},\tag{3}$$

where $\mathcal{G}(r)$ is determined by the equation which emerges by substituting Eq. (3) in Eq. (2), $\mathcal{Z}$ is obtained from the normalization condition, and $\exp_q$ is the q-exponential present in the Tsallis formalism. The $\exp_q$ is given by $\exp_q[x]=(1+(1-q)x)^{1/(1-q)}$ if $1+(1-q)x\geqslant 0$ and $\exp_q[x]=0$ if $1+(1-q)x<0$ and it emerges from the Tsallis formalism by maximizing the Tsallis entropy $S_q=(1-\int dx(\rho(x))^q)/(q-1)$ with suitable constraints. Substituting Eq. (3) in Eq. (2) and taking $q=2-\nu-\gamma$ into account, the equation satisfied by $\mathcal{G}(r)$ is

$$\frac{d}{dr}\mathcal{G}(r)-(1-q)r^{\eta+\theta}\frac{\mathcal{F}_2(r)}{\mathcal{D}\nu}\mathcal{G}(r)=-\frac{r^{\theta+\eta}}{\mathcal{D}\nu}\left[\mathcal{F}_2(r)+\left(\frac{\mathcal{Z}}{r^{\frac{\eta}{\nu}}}\right)^{\gamma+\nu-1}\mathcal{F}_1(r)\right].\tag{4}$$

The solution for this equation is given by

$$\mathcal{G}(r) = -\frac{\mathcal{Z}^{\nu+\gamma-1}}{\mathcal{D}\nu}\int_0^r d\bar{r}\bar{r}^{(\eta/\nu)(1-\gamma)+\theta}\mathcal{F}_1(\bar{r})\exp\left(-\frac{1-q}{\mathcal{D}\nu}\left[\int_0^{\bar{r}} d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\eta+\theta} - \int_0^r d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\eta+\theta}\right]\right) - \ln_q\left[\exp\left(\frac{1}{\mathcal{D}\nu}\int_0^r d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\theta+\eta}\right)\right], \tag{5}$$

where $\ln_q[x]=(x^{1-q}-1)/(1-q)$ is the q-logarithmic function which is the inverse function of the above-defined q-exponential. By applying Eq. (5) in Eq. (3) we found the stationary solution

$$\rho(r) = r^{\eta/\nu}\exp_q\left[\frac{\mathcal{Z}^{\nu+\gamma-1}}{\mathcal{D}\nu}\int_0^r d\bar{r}\bar{r}^{(\eta/\nu)(1-\gamma)+\theta}\mathcal{F}_1(\bar{r})\exp\left(-\frac{1-q}{\mathcal{D}\nu}\left(\int_0^{\bar{r}} d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\eta+\theta} - \int_0^r d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\eta+\theta}\right)\right) + \ln_q\left[\exp\left(\frac{1}{\mathcal{D}\nu}\int_0^r d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\theta+\eta}\right)\right]\right] \Big/ \mathcal{Z}. \tag{6}$$

From Eq. (6), we note that the stationary solution may behave, as we mentioned before, as a Boltzmann-Gibbs distribution or as a Tsallis distribution depending on the choice of $\mathcal{F}_1(r)$ and $\mathcal{F}_2(r)$. In fact, by taking $\mathcal{F}_1(r)=0$ in Eq. (6) we obtain $\rho(r)=r^{\eta/\nu}\exp((1/\mathcal{D}\nu)\int_0^r d\tilde{r}\mathcal{F}_2(\tilde{r})\tilde{r}^{\theta+\eta})/\mathcal{Z}$ which essentially behaves like a Boltzmann-Gibbs distribution and for $\mathcal{F}_2(r)=0$ we obtain the Tsallis distribution $\rho(r)=r^{\eta/\nu}\exp_q[\mathcal{Z}^{\nu+\gamma-1}\int_0^r d\bar{r}\bar{r}^{(\eta/\nu)(1-\gamma)+\theta}\mathcal{F}_1(\bar{r})/\mathcal{D}\nu]/\mathcal{Z}$. The presence of a stationary solution with an exponential behavior like the Boltzmann-Gibbs distribution indicates that the solution may have an anomalous relaxation to a usual stationary solution. A similar effect is verified in the fractional diffusion equations which employ a time fractional derivative.[3] In Fig. 1, we illustrate by using numerical calculation based on the method of finite difference[30] how a solution of Eq. (1) for a typical choice of $\mathcal{F}_1(r)$ and $\mathcal{F}_2(r)$, for simplicity, in the one-dimensional case, evolves in time and has Eq. (6) as stationary solution.

Now, we consider the dynamical case by taking into account the external force $\mathcal{F}(r,t;\rho)=-k(t)r+\mathcal{K}/r^{1+\theta+\eta}[\rho(r,t)]^{\gamma+\nu-1}$ which depends on the distribution of the system. For this case, after substituting this external force in Eq. (1) we obtain

$$\frac{\partial}{\partial t}\rho(r,t) = \frac{\mathcal{D}}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left\{r^{\mathcal{N}-1-\theta}[\rho(r,t)]^{\gamma}\frac{\partial}{\partial r}[r^{-\eta}(\rho(r,t))^{\nu}]\right\} + \frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left\{r^{\mathcal{N}-1}\left[k(t)r - \frac{\mathcal{K}}{r^{1+\theta+\eta}}[\rho(r,t)]^{\gamma+\nu-1}\right]\rho(r,t)\right\}. \tag{7}$$

In order to obtain the solution for this case, we use, for simplicity, the similarity method to reduce this partial differential equation to ordinary differential equations. The explicit form for these ordinary differential equations depends on the boundary conditions or on restrictions in the form of conservation laws. Thus, we restrict our analysis to the solutions of the type

$$\rho(r,t) = \left[\frac{1}{\Phi(t)}\right]^{\mathcal{N}}\mathcal{P}\left(\frac{r}{\Phi(t)}\right), \tag{8}$$

which need to satisfy the initial, the boundary conditions, and the normalization condition. By substituting Eq. (8) in Eq. (7) we obtain

$$-\frac{\dot{\Phi}(t)}{(\Phi(t))^2}\frac{d}{dz}[z^{\mathcal{N}}\mathcal{P}(z)] = \frac{\mathcal{D}}{(\Phi(t))^{\xi}}\frac{d}{dz}\left\{z^{\mathcal{N}-1-\theta}[\mathcal{P}(z)]^{\gamma}\frac{d}{dz}[z^{-\eta}(\mathcal{P}(z))^{\nu}]\right\} + \frac{k(t)}{\Phi(t)}\frac{d}{dz}[z^{\mathcal{N}}\mathcal{P}(z)] - \frac{1}{(\Phi(t))^{\xi}}\frac{d}{dz}\left\{z^{\mathcal{N}-1}\left[\frac{\mathcal{K}}{z^{1+\theta+\eta}}(\mathcal{P}(z))^{\gamma+\nu}\right]\right\}, \tag{9}$$

where $\xi=3+\theta+\eta+\mathcal{N}(\gamma+\nu-1)$ and $z=r/\Phi(t)$. From Eq. (9) we can obtain

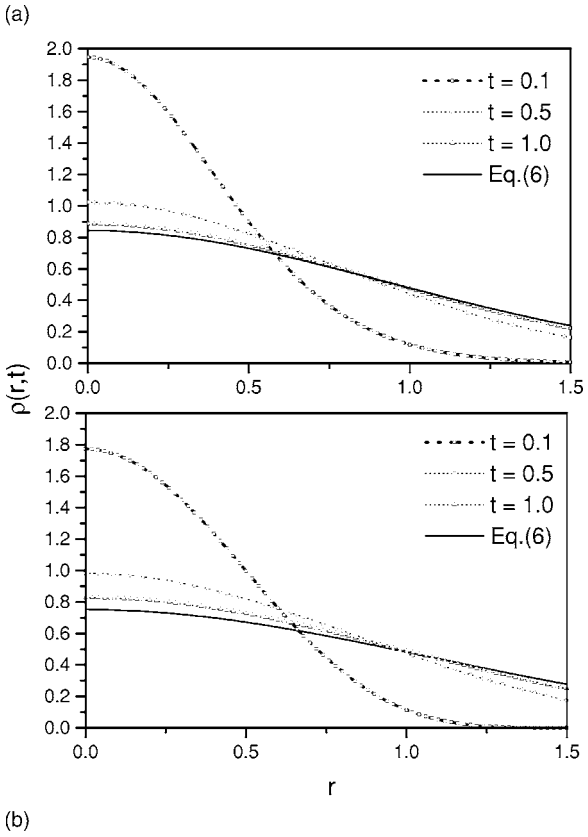

FIG. 1. Behavior of $\rho(r,t)$ vs r, which illustrates Eq. (1) for typical values of ν and t by considering, for simplicity, $\mathcal{D}=1$, $\gamma=0$, $\theta=0$, $\eta=0$, $\mathcal{N}=1$, $\mathcal{F}_1(r)=0$, and $\mathcal{F}_2(r)=-kr$ with $k=1$. In (a), we illustrated the case characterized by $\nu=0.9$ and in (b) the case $\nu=1.2$. Note that in both cases the solutions for long time have the stationary case given by Eq. (6).

$$\frac{\dot{\Phi}(t)}{(\Phi(t))^2}+\frac{k(t)}{\Phi(t)}=\frac{k'}{(\Phi(t))^{\xi}} \tag{10}$$

and

$$-k'\frac{\mathrm{d}}{\mathrm{d}z}[z^{\mathcal{N}}\mathcal{P}(z)]=\mathcal{D}\frac{\mathrm{d}}{\mathrm{d}z}\left\{z^{\mathcal{N}-1-\theta}[\mathcal{P}(z)]^{\gamma}\frac{\mathrm{d}}{\mathrm{d}z}[z^{-\eta}(\mathcal{P}(z))^{\nu}]\right\}-\frac{\mathrm{d}}{\mathrm{d}z}\left\{z^{\mathcal{N}-1}\left[\frac{\mathcal{K}}{z^{1+\theta+\eta}}(\mathcal{P}(z))^{\gamma+\nu}\right]\right\} \tag{11}$$

by introducing the constant of separation k' which can be determined by the normalization condition. After some calculations, we obtain that the solution to Eq. (10) is given by

$$\Phi(t)=\left[(\Phi(0))^{\xi-1}+(\xi-1)k'\int_0^t \mathrm{d}\tilde{t}e^{(\xi-1)\int_0^{\tilde{t}}\mathrm{d}t'k(t')}\right]^{1/(\xi-1)}e^{-\int_0^t \mathrm{d}t'k(t')}. \tag{12}$$

Note that similar solutions for the time dependent function have been found for different nonlinear fractional diffusion equations.[31–35] This fact indicates that different diffusion equations have a similar anomalous spreading for the probability distribution and the difference is on the parameters present in the diffusion equation. From this solution it is also possible to obtain the behavior of spreading of Eq. (7) by using $\rho(0,t)$, since for this case $\langle r^2\rangle \propto 1/[\rho(0,t)]^2 \propto [\Phi(t)]^2$. Thus, depending on the parameters ν,γ,θ, and η, we may have an anomalous or usual behavior for the spreading and consequently to the second moment. In particular, for the case characterized by the

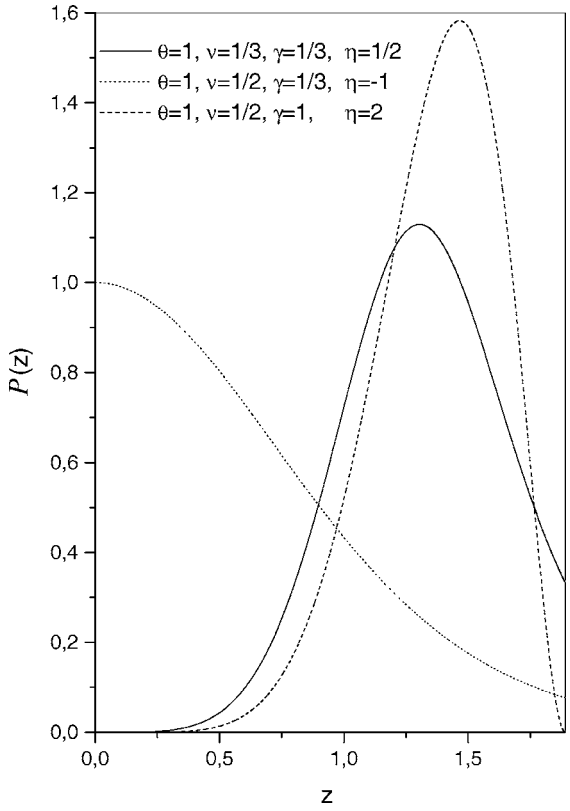

FIG. 2. Behavior of $\mathcal{P}(z)$ vs z, which illustrates Eq. (14) for typical values for θ, ν, η, and γ, for simplicity, by taking into account $\mathcal{K}=1$, $\mathcal{N}=1$, and $\mathcal{D}=1$. Notice that depending on the choice of these parameters the distribution may have a compact or a long tail behavior.

absence of external forces the second moment is $\langle r^2\rangle \sim t^{2/(\xi-1)}$, where $\xi>3, \xi=3$ or $\xi<3$ lead us to a subdiffusive, normal or superdiffusive behavior, respectively. Now let us address our discussion to the solution of Eq. (11). Performing an integration in Eq. (11) results in

$$-k' z^{\mathcal{N}}\mathcal{P}(z) = \mathcal{D} z^{\mathcal{N}-1-\theta}[\mathcal{P}(z)]^{\gamma}\frac{\mathrm{d}}{\mathrm{d}z}[z^{-\eta}(\mathcal{P}(z))^{\nu}] - \mathcal{K} z^{\mathcal{N}-(2+\theta+\eta)}[\mathcal{P}(z)]^{\gamma+\nu} + \mathcal{C}. \tag{13}$$

We take $\mathcal{C}=0$ in order to simplify our analysis about the solutions which satisfy the boundary condition $\mathcal{P}(z\to\infty)\to 0$. By applying the last consideration in Eq. (13), after some calculation we obtain that

$$\mathcal{P}(z) = z^{\eta/\nu+\mathcal{K}/\mathcal{D}\nu}\exp_q\left[-\frac{k' z^{\bar{\xi}}}{\mathcal{D}\nu\bar{\xi}}\right], \tag{14}$$

where $q=2-\nu-\gamma$ and $\bar{\xi}=2+\theta+\eta(1-\gamma)/\nu-\mathcal{K}(\nu+\gamma-1)/(\mathcal{D}\nu)$ (see Fig. 2). Note that the behavior of Eq. (14) can be compact or characterized by long tail depending on the parameters η, ν, γ, and θ. For the last case, we may relate the solution obtained to the Levy distributions in the asymptotic limit. In fact, by taking the asymptotic limit of the above equation for large z ($\mathcal{P}(z) \sim 1/z^{(2+\theta+\eta)/(q-1)}$) and comparing to the asymptotic limit of the Levy distributions ($\mathcal{P}(z) \sim 1/z^{1+\mu}$)[8] we obtain $q=(3+\theta+\eta+\mu)/(1+\mu)$. Now, in order to show the explicit form of the time dependent solution for this case, we substitute Eq. (14) in Eq. (8) to obtain

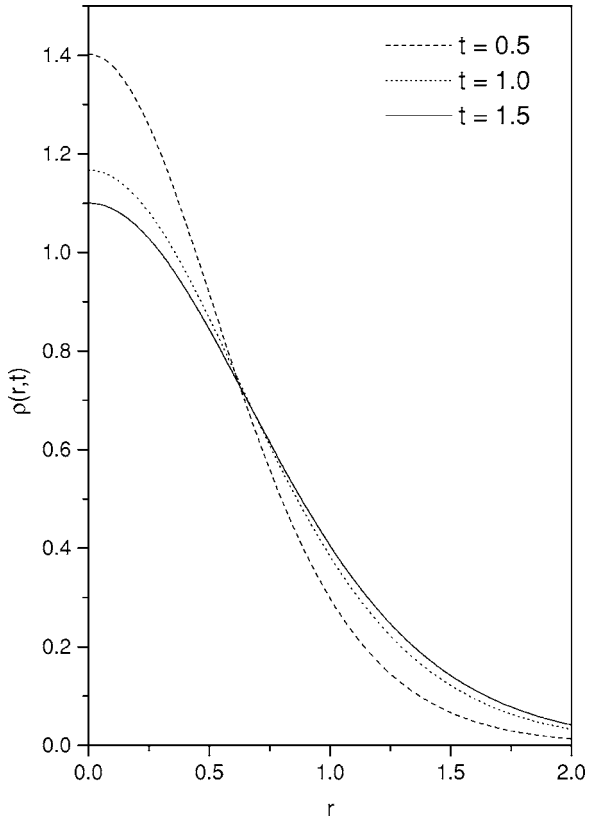

FIG. 3. Behavior of $\rho(r,t)$ vs r, which illustrates how Eq. (15) evolves on the time for $\theta=1$, $\nu=1/2$, $\eta=-1$, and $\gamma=1/3$, for simplicity, by taking into account $\mathcal{K}=1$, $\mathcal{N}=1$, $\Phi(0)=0$, $k(t)=1$, and $\mathcal{D}=1$.

$$\rho(r,t)=\left(\frac{1}{\Phi(t)}\right)^{\mathcal{N}}\left(\frac{r}{\Phi(t)}\right)^{\eta/\nu+\mathcal{K}/\mathcal{D}\nu}\exp_q\left[-\frac{k'}{\mathcal{D}\nu\bar{\xi}}\left(\frac{r}{\Phi(t)}\right)^{\bar{\xi}}\right] \tag{15}$$

with $\Phi(t)$ defined by Eq. (12) (see Fig. 3).

III. SUMMARY AND CONCLUSION

In summary, we have worked out an $\mathcal{N}$-dimensional nonlinear diffusion equation by considering a nonlinear convective or transport term. We have analyzed a stationary solution and a time dependent case which emerge from this equation. For the stationary case it was verified that the solution obtained may present a power-law or an exponential behavior. Thus for the first case, it was possible to relate the solution found here with the Tsallis formalism and in the second case may be established a connection to the Boltzmann-Gibbs formalism. The last behavior is very interesting since it indicates that the solution may have an anomalous relaxation to the usual stationary solution. Similar behavior is found in the fractional diffusion equations which employ a time fractional time derivative. For the time dependent case, we have shown that it admits exact solutions where space scales with a function of time and lead us to a power-law distribution with a compact or a long tailed behavior depending on the parameters values $\nu,\theta,\eta,\gamma,\mathcal{K}$, and $\mathcal{D}$. In particular, for the case characterized by a long tailed behavior, the distribution was connected to the Levy distribution in the asymptotic limit. However, it is interesting to note that the time dependent solution has a power-law behavior due to the choice of the convective term. Other choices to this term may lead us to obtain different solutions. Finally, we hope that the results obtained here may be useful to study physical systems exhibiting anomalous diffusion.

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Limiting laws of linear eigenvalue statistics for Hermitian matrix models

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We study the variance and the Laplace transform of the probability law of linear eigenvalue statistics of unitary invariant Matrix Models of $n \times n$ Hermitian matrices as $n \to \infty$. Assuming that the test function of statistics is smooth enough and using the asymptotic formulas by Deift *et al.* [Commun. Pure Appl. Math. **52**, 1325–1425 (1999)] for orthogonal polynomials with varying weights, we show first that if the support of the Density of States of the model consists of $q \geq 2$ intervals, then in the global regime the variance of statistics is a quasiperiodic function of n as $n \to \infty$ generically in the potential, determining the model. We show next that the exponent of the Laplace transform of the probability law is not, in general, $1/2 \times$ variance, as it should be if the Central Limit Theorem would be valid, and we find the asymptotic form of the Laplace transform of the probability law in certain cases. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Random matrix theory deals mostly with eigenvalue distributions of various ensembles of $n \times n$ random matrices as $n \to \infty$. Many questions of this branch of the theory can be formulated in terms of the Eigenvalue Counting Measure $\mathcal{N}_n$, $\mathcal{N}_n(\Delta_n)$ is the number of eigenvalues in a given part Δ_n of the spectrum of a matrix M_n. In a particular case of $n \times n$ Hermitian matrices, eigenvalues are real, and we can write for $\Delta_n \subset \mathbb{R}$,

$$\mathcal{N}_n(\Delta_n) := \#\{\lambda_l^{(n)} \in \Delta_n, l = 1, \ldots, n\} = \sum_{l=1}^{n} \chi_{\Delta_n}(\lambda_l^{(n)}), \tag{1.1}$$

where χ_Δ is the indicator of Δ. A more general object is a linear eigenvalue statistic, defined as

$$\mathcal{N}_n[\varphi_n] := \sum_{l=1}^{n} \varphi_n(\lambda_l^{(n)}) = \mathrm{Tr}\, \varphi_n(M_n) = \int_{\mathbb{R}} \varphi_n(\lambda) \mathcal{N}_n(d\lambda), \tag{1.2}$$

for a certain test function,

$$\varphi_n : \mathbb{R} \to \mathbb{C}. \tag{1.3}$$

It is known that in many cases there exists a scaling of matrix entries (i.e., a choice of the scale of the spectral axis), such that for a sufficiently big class of n-independent intervals in (1.1) [test functions in (1.2)] the Normalized Counting Measure of eigenvalues,

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$$N_n = \mathcal{N}_n/n, \tag{1.4}$$

converges weakly to a non-random measure N, known as the Integrated Density of States measure (IDS) of the ensemble,

$$N_n \to N. \tag{1.5}$$

The corresponding scale (asymptotic regime) is called the *global* (or *macroscopic*). The convergence is either in probability or even with probability 1. We refer the reader to the works in Refs. 19, 9, and 30, where this fact is proved and discussed for two most widely studied classes of random matrix ensembles: the Wigner Ensembles (independent or weakly dependent entries) and the Matrix Models (invariant matrix probability laws). Analogous facts are also known for many other ensembles.

Besides, in many cases the measure N possesses a bounded and continuous density:[16,29]

$$N(d\lambda) = \rho(\lambda)d\lambda. \tag{1.6}$$

We call ρ the Density of States (DOS) of the ensemble.

These results can be viewed as analogs of the Law of Large Numbers of probability theory. Hence, a natural next question, important also for applications, concerns the limiting probability law of fluctuation of the Normalized Counting Measures of eigenvalues or their linear statistics, i.e., an analog of the Central Limit Theorem of probability theory. The question is not going to be completely trivial, because eigenvalues of random matrices are strongly dependent, and, as a result, the variance of the linear statistics (1.2) with a C^1 test function does not grow with n [see, e.g., formulas (2.36) and (2.37) later]. Nevertheless, it was found that in a variety of cases, the fluctuations of various spectral characteristics of eigenvalues of random matrix ensembles are asymptotically Gaussian (see, e.g., Refs. 5, 6, 13, 15, 18, 19, 21, 23–25, and 35–39). In particular, for the global scale and a C^1 test function in (1.2), this requires, roughly speaking, the same order of magnitude of the entries for the Wigner Ensembles (see Refs. 19 and 25 for exact conditions, similar to the Lindeberg condition of the probability theory), and for the Matrix Models one needs to assume that the support of the IDS (1.5) is a connected interval of the spectral axis:[23] $\operatorname{supp} N = [a,b]$. The last result was obtained by using variational techniques, introduced in the random matrix theory in the paper in Ref. 9 in order to prove (1.5).

Being applicable to Matrix Models of all three symmetry classes of the random matrix theory (real symmetric, Hermitian, and quaternion real matrices), the variational techniques were efficient so far in the study of fluctuations of eigenvalue statistics only in the case where $\operatorname{supp} N = [a,b]$. In this paper we consider only the Matrix Models of Hermitian matrices, but for a general case of a multi-interval support of N:

$$\sigma := \operatorname{supp} N = \bigcup_{l=1}^{q} [a_l, b_l], \quad q \geq 1. \tag{1.7}$$

In this case we can use the recent powerful results by Deift *et al.*[17] on the asymptotics of a special class of orthogonal polynomials. We find that if φ is smooth enough, then the traditional Central Limit Theorem is not always valid for the case $q \geq 2$. In particular, the variance and the probability law oscillate in n as $n \to \infty$, hence their limiting form depends on a sequence $n_j \to \infty$. Moreover, the limiting probability laws are not always Gaussian.

The paper is organized as follows. In Sec. II we study the variance of linear eigenvalue statistics in the global regime, i.e., for n-independent φ in (1.2), confining ourselves mostly to the case of C^1 test functions φ. We find that the variance is quasiperiodic in n, in general, and its frequency module is determined by the charges

$$\beta_l = N([a_{l+1}, \infty)), \quad l = 1, \ldots, q-1, \tag{1.8}$$

determined by the IDS of (1.5) and its support (1.7). Hence, the variance has no limit as $n \to \infty$ for $q \geq 2$ and its asymptotic forms are indexed by points of the subset $\mathbb{H}^{q-1} \subset \mathbb{T}^{q-1}$, which is the closure of limit points of the vectors,

$$(\{\beta_1 n\}, \ldots, \{\beta_{q-1} n\}) \in \mathbb{T}^{q-1}, \tag{1.9}$$

where $\{\beta_l n\}, l = 1, \ldots, q-1$ are the fractional parts of $\beta_l n, l = 1, \ldots, q-1$. This phenomenon has been already found in certain cases,[3,8] but we give its general description.

In Sec. III we study the Laplace transform of the probability law of linear eigenvalue statistics (1.2) in the global regime, passing to the limit along a subsequence,

$$(\{\beta_1 n_j(x)\}, \ldots, \{\beta_{q-1} n_j(x)\}) \to x \in \mathbb{H}^{q-1}, \tag{1.10}$$

and confining ourselves to real analytic test functions. We give first a general formula for the corresponding limit. Since the formula is rather complex, we consider several particular cases, where we show that the exponent of the limiting [in the sense (1.10)] Laplace transform is not quadratic in φ, hence the limiting law is not Gaussian [see formulas (3.1), (3.13), (3.19), and (3.20)]. This has to be compared with results of the paper in Ref. 14, according to which the limits of variance and the probability law are the same for all sequences $n_j \to \infty$ (i.e., exist), and the limiting probability law is Gaussian.

The random matrix theory deals also with two more asymptotic regimes in addition to the global one. Namely, if, having fixed the global spectral scale allowing us to prove (1.5), we set in (1.2),

$$\varphi_n(\lambda) = \varphi((\lambda - \lambda_0) n^{\alpha}), \quad 0 < \alpha < 1, \quad \lambda_0 \in \operatorname{supp} N, \tag{1.11}$$

where φ is n independent, we obtain the *intermediate* regime, and if

$$\varphi_n(\lambda) = \varphi((\lambda - \lambda_0) n), \quad \lambda_0 \in \operatorname{supp} N, \tag{1.12}$$

then we have the *local* (or *microscopic*) regime. In Sec. IV we discuss the form of variance and the validity of the CLT in these regimes.

In the Appendix we compute the variational derivative of β_1 in the case $q=2$, which is used in Sec. III, and discuss related topics.

We note that a completely rigorous derivation of the results of this paper, especially those of Sec. III, requires rather technical and tedious arguments. They will not be presented in this paper. Rather, we confine ourselves to the presentation of results, their discussion, and outline of corresponding proofs.

II. VARIANCE OF LINEAR EIGENVALUE STATISTICS

A. Generalities

Recall that unitary invariant Matrix Models are $n \times n$ Hermitian random matrices, defined by the probability law

$$\mathbf{P}_n(dM_n) = Z_n^{-1} \exp\{-n \operatorname{Tr} V(M_n)\} dM_n, \tag{2.1}$$

where $M_n = \{M_{jk}\}_{j,k=1}^n, M_{jk} = \overline{M_{kj}}$,

$$dM_n = \prod_{j=1}^n dM_{jj} \prod_{1 \leq j < k \leq n} d\Re M_{jk}\, d\Im, M_{jk},$$

and $V: \mathbb{R} \to \mathbb{R}_+$ is a continuous function, called the potential, and such that

$$V:\mathbb{R}\to\mathbb{R}_+,\quad V(\lambda)\geq(2+\delta)\log|\lambda|,\quad |\lambda|>L, \tag{2.2}$$

for some positive δ and L.

The limit (1.5) can be described as follows.[9,23] Consider the functional:

$$\mathcal{E}_V[m]=-\int_{\mathbb{R}}\int_{\mathbb{R}}\log|\lambda-\mu|m(d\lambda)m(d\mu)+\int_{\mathbb{R}}V(\lambda)m(d\lambda), \tag{2.3}$$

where m is a non-negative unit measure.

The variational problem, defined by (2.3), goes back to Gauss and is called the minimum energy problem in the external field V. The unit measure N minimizing (2.3) is called the equilibrium measure in the external field V because of its evident electrostatic interpretation as the equilibrium distribution of linear charges on the ideal conductor occupying the axis $\mathbb{R}$ and confined by the external electric field of potential V. We stress that the respective minimizing procedure determines both the support σ of the measure and the form of the measure. This should be compared with the variational problem of the theory of logarithmic potential, where the external field is absent but the support σ is given [see (2.50)]. The minimum energy problem in the external field (2.3) arises in various domains of analysis and its applications (see a recent book[34] for a rather complete account of results and references concerning the problem).

The measure N and its support σ are uniquely determined by the Euler-Lagrange equation of the variational problem:[9,34]

$$V_{\mathrm{eff}}(\lambda)=F,\quad \lambda\in\sigma, \tag{2.4}$$

$$V_{\mathrm{eff}}(\lambda)\geq F,\quad \lambda\notin\sigma, \tag{2.5}$$

where

$$V_{\mathrm{eff}}(\lambda)=V(\lambda)-2\int_\sigma\log|\lambda-\mu|N(d\mu), \tag{2.6}$$

and F is a constant [the Lagrange multiplier of the normalization condition $N(\mathbb{R})=1$].

According to Ref. 9 (see also Ref. 23), if the potential V in (2.1) and (2.2) satisfies the local Lipshitz condition,

$$|V(\lambda_1)-V(\lambda_2)|\leq C|\lambda_1-\lambda_2|^\gamma,\quad |\lambda_1|,|\lambda_2|\leq L, \tag{2.7}$$

valid for any $L>0$ and some positive C and γ; then (1.5) holds with probability 1, and N is the minimizer of (2.3). Moreover, if V' is continuously differentiable, and the support (1.7) is a finite union of disjoint finite intervals, then (1.6) is valid[16,29] and the Density of States can be written as

$$\rho(\lambda)=P(\lambda)\sqrt{R_q(\lambda)},\quad \lambda\in\sigma, \tag{2.8}$$

where $P(\lambda)$ is a continuous function,

$$\sqrt{R_q(\lambda)}=\sqrt{R_q(z)}\big|_{z=\lambda+i0},\quad R_q(z)=\prod_{l=1}^{q}(z-a_l)(z-b_l), \tag{2.9}$$

and $\sqrt{R_q(z)}$ is the branch, determined by the condition $\sqrt{R_q(z)}=z^q+O(z^{q-1}), z\to\infty$. To obtain these formulas, provided that the support (1.7) is given, we differentiate (2.4) and (2.6) and obtain the singular integral equation,

$$\text{v.p.}\int_\sigma\frac{\rho(\mu)d\mu}{\mu-\lambda}=-\frac{V'(\lambda)}{2},\quad \lambda\in\sigma. \tag{2.10}$$

Then the bounded solution of the equation has the form (2.8) (see, e.g., Ref. 28) in which

$$P(\lambda) = \frac{1}{2\pi^2} \int_\sigma \frac{V'(\mu) - V'(\lambda)}{\mu - \lambda} \frac{d\mu}{\sqrt{R_q(\mu)}}. \tag{2.11}$$

The endpoints of the support are rather complex functionals of the potential, in general. Thus, it is of interest to mention a simple case.[11]

Let $v : \mathbb{R} \to \mathbb{R}$ be a monic polynomial of degree q with real coefficients. Assume that for some $g > 0$ all zeros of $v^2 - 4g$ are real and simple and set

$$V(\lambda) = \frac{v^2(\lambda)}{2gq}. \tag{2.12}$$

Then the DOS of the matrix model (2.1) with this potential is

$$\rho(\lambda) = \frac{|v'(\lambda)|}{2\pi g q} |v^2(\lambda) - 4g|^{1/2}, \quad \lambda \in \sigma, \tag{2.13}$$

where

$$\sigma = \{\lambda \in \mathbb{R} : v^2(\lambda) \leq 4g\}. \tag{2.14}$$

Besides, in this case we have for the charges (1.8),

$$\beta_l = \frac{q-l}{q}, \quad l = 1, \ldots, q-1, \tag{2.15}$$

hence the set $\mathbb{H}^{q-1}$ is $\{0, 1/q, \ldots, (q-1)/q\}$.

The case $q = 1$ corresponds to the Gaussian Unitary Ensemble and (2.13) yields the semicircle law by Wigner:

$$V = \frac{\lambda^2}{2g}, \quad \sigma = [-2g, 2g], \quad \rho(\lambda) = \frac{1}{2\pi g} \begin{cases} \sqrt{4g - \lambda^2}, & \lambda \in \sigma, \\ 0, & \lambda \notin \sigma. \end{cases} \tag{2.16}$$

In the case $q = 2$ and

$$v(\lambda) = \lambda^2 - m^2, \quad m^2 > 2\sqrt{g}, \tag{2.17}$$

we have

$$\sigma = [-b, -a] \cup [a, b], \quad a = \sqrt{m^2 - 2\sqrt{g}}, \quad b = \sqrt{m^2 + 2\sqrt{g}}, \tag{2.18}$$

and

$$\rho(\lambda) = \frac{|\lambda|}{2\pi g} \begin{cases} \sqrt{(b^2 - \lambda^2)(\lambda^2 - a^2)}, & \lambda \in \sigma, \\ 0, & \lambda \notin \sigma. \end{cases} \tag{2.19}$$

We will use in this paper the expressions for the variance of linear statistics (1.2) and for the Laplace transform of their probability law via special orthogonal polynomials. The technique dates back to works by Dyson, Gaudin, Mehta, and Wigner of the 1960s (see, e.g., Ref. 27). Namely, we have for the joint probability density of eigenvalues of ensemble (2.1):

$$p_n(\lambda_1, \ldots, \lambda_n) = (\det\{\psi_{j-1}^{(n)}(\lambda_k)\}_{j,k=1}^n)^2 / n!, \tag{2.20}$$

where

$$\psi_l^{(n)} = e^{-nV/2} P_l^{(n)}, \tag{2.21}$$

and

$$\{P_l^{(n)}\}_{l\geq 0} \tag{2.22}$$

is the system of orthonormal polynomials with respect to the weight

$$w_n = e^{-nV}, \tag{2.23}$$

so that

$$\int_{\mathbb{R}} e^{-nV(\lambda)} P_l^{(n)}(\lambda) P_m^{(n)}(\lambda) d\lambda = \delta_{l,m}, \quad l,m = 0,1,\ldots . \tag{2.24}$$

The polynomials satisfy the three-term recurrence relation for $l=0,1,\ldots$:

$$r_l^{(n)}\psi_{l+1}^{(n)}(\lambda) + s_l^{(n)}\psi_l^{(n)}(\lambda) + r_{l-1}^{(n)}\psi_{l-1}^{(n)}(\lambda) = \lambda\psi_l^{(n)}(\lambda), \quad r_{-1}^{(n)} = 0, \tag{2.25}$$

thereby determining a semi-infinite Jacobi matrix:

$$J_{j,k}^{(n)} = r_j^{(n)}\delta_{j+1,k} + s_k^{(n)}\delta_{j,k} + r_{j-1}^{(n)}\delta_{j-1,k}, \quad j,k = 0,1,\ldots . \tag{2.26}$$

By using (2.20) it can be shown that[28]

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} = \frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} |\varphi(\lambda_1) - \varphi(\lambda_2)|^2 K_n^2(\lambda_1,\lambda_2)\, d\lambda_1 d\lambda_2, \tag{2.27}$$

$$= \int_{\mathbb{R}}\int_{\mathbb{R}} \left|\frac{\Delta\varphi}{\Delta\lambda}\right|^2 \mathcal{V}_n(\lambda_1,\lambda_2) d\lambda_1\, d\lambda_2, \tag{2.28}$$

where

$$K_n(\lambda_1,\lambda_2) = \sum_{l=0}^{n-1} \psi_l^{(n)}(\lambda_1)\psi_l^{(n)}(\lambda_2) \tag{2.29}$$

is known as the reproducing kernel of the system (2.21),

$$\frac{\Delta\varphi}{\Delta\lambda} = \frac{\varphi(\lambda_1) - \varphi(\lambda_2)}{\lambda_1 - \lambda_2}, \tag{2.30}$$

and

$$\mathcal{V}_n(\lambda_1,\lambda_2) = \{r_{n-1}^{(n)}[\psi_n^{(n)}(\lambda_1)\psi_{n-1}^{(n)}(\lambda_2) - \psi_{n-1}^{(n)}(\lambda_1)\psi_n^{(n)}(\lambda_2)]\}^2/2. \tag{2.31}$$

Note that in passing from (2.27) and (2.28), we used the Christoffel-Darboux formula,[40]

$$K_n(\lambda_1,\lambda_2) = r_{n-1}^{(n)}\frac{\psi_n^{(n)}(\lambda_1)\psi_{n-1}^{(n)}(\lambda_2) - \psi_{n-1}^{(n)}(\lambda_1)\psi_n^{(n)}(\lambda_2)}{\lambda_1 - \lambda_2}. \tag{2.32}$$

It is of interest to have a spectral-theoretic interpretation of the above formulas. Notice that the $J^{(n)}$ of (2.26) determines a self-adjoint operator, that we denote again as $J^{(n)}$. It acts in $l^2(\mathbb{Z}_+)$, and the matrix

$$\mathcal{E}^{(n)}(d\lambda) = e^{(n)}(\lambda)d\lambda, \quad e^{(n)}(\lambda) = \{e_{lm}^{(n)}(\lambda)\}_{l,m=0}^{\infty}, \quad e_{lm}^{(n)}(\lambda) = \psi_l^{(n)}(\lambda)\psi_m^{(n)}(\lambda) \tag{2.33}$$

is its resolution of identity.[1] This allows us to write (2.31) in the form

$$\mathcal{V}_n(\lambda_1,\lambda_2) = (r_{n-1}^{(n)})^2(e_{n,n}^{(n)}(\lambda_1)e_{n-1,n-1}^{(n)}(\lambda_2) + e_{n,n}^{(n)}(\lambda_2)e_{n-1,n-1}^{(n)}(\lambda_1) - 2e_{n-1,n}^{(n)}(\lambda_1)e_{n,n-1}^{(n)}(\lambda_2))/2. \tag{2.34}$$

Assume now that φ satisfies the Hölder condition:

$$|\varphi(\lambda_1) - \varphi(\lambda_2)| \le C|\lambda_1 - \lambda_2|, \tag{2.35}$$

for some positive C. It follows then from (2.24) and (2.28)–(2.31) that

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} \le C^2(r_{n-1}^{(n)})^2. \tag{2.36}$$

It can be shown[33] that if the potential satisfies the local Lipshitz condition (2.7), then the coefficients $r_{n-1}^{(n)}$ are bounded in n. We conclude that the variance of a linear statistic (1.2) is bounded in n if the test function satisfies (2.35):

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} \le \mathrm{Const}. \tag{2.37}$$

This has to be compared with the well known fact of probability theory, according to which the variance of a linear statistics of i.i.d. random variables is $O(n)$ for any test function.

B. Asymptotic behavior of $\psi_l^{(n)}(\lambda)$

We present now powerful asymptotic formulas for orthonormal functions $\psi_l^{(n)}$ of (2.21)–(2.24) of Deift *et al.*,[17] valid in the case of a real analytic potential V in (2.1). We give a bit different form that will be more convenient later. Our form is reminiscent of standard semiclassical formulas and is similar to that, given in Refs. 7 and 8. Notice that Ref. 8 contains another, although heuristic, derivation of the asymptotic formulas as well as an interesting heuristic explanation of the quasiperiodicity of formulas for $q \ge 2$, based on ideas of statistical mechanics and quantum field theory.

Assume that V is real analytic. Then the support (1.7) of N is a union of $q < \infty$ finite disjoint intervals.[17] The function P in (2.8), (2.11) is also real analytic. Following Ref. 17, we say that V is regular if the inequality (2.5) is strict and P is strictly positive on σ. Hence, the DOS ρ of (1.6) is strictly positive inside σ and vanishes precisely like a square root at the endpoints. Denote

$$N(\lambda) = N([\lambda, \infty)). \tag{2.38}$$

According to Ref. 17, in the regular case there exist functions $d_n(\lambda)$, and $\gamma_n(\lambda)$ such that if λ belongs to the interior of the support (1.7), then

$$\psi_n^{(n)}(\lambda) = (2d_n(\lambda))^{1/2}\cos(\pi n N(\lambda) + \gamma_n(\lambda)) + O(n^{-1}), \quad n \to \infty. \tag{2.39}$$

Moreover, $d_n(\lambda)$ and $\gamma_n(\lambda)$ depend on n via the vector $n\beta$, where $\beta = (\beta_1, \ldots, \beta_{q-1})$ is given by (1.8). This means that there exist n-independent continuous functions $\mathcal{D}: \sigma \times \mathbb{T}^{q-1} \to \mathbb{R}_+$, and $\mathcal{G}: \sigma \times \mathbb{T}^{q-1} \to \mathbb{R}$, such that

$$d_n(\lambda) = \mathcal{D}(\lambda, n\beta), \quad \gamma(\lambda) = \mathcal{G}(\lambda, n\beta). \tag{2.40}$$

If λ belongs to the exterior of σ, then $\psi_n^{(n)}(\lambda)$ decays exponentially in n as $n \to \infty$.

Similar asymptotic formulas are valid for coefficients of the Jacobi matrix $J^{(n)}$ of (2.26), i.e., there exist n-independent continuous functions $\mathcal{R}: \mathbb{T}^{q-1} \to \mathbb{R}_+$ and $\mathcal{S}: \mathbb{T}^{q-1} \to \mathbb{R}$ such that

$$r_{n-1}^{(n)} = \mathcal{R}(n\beta) + O(n^{-1}), \quad s_n^{(n)} = \mathcal{S}(n\beta) + O(n^{-1}), \quad n \to \infty. \tag{2.41}$$

The functions $\mathcal{D}, \mathcal{G}, \mathcal{R}$, and $\mathcal{S}$ can be expressed via the Riemann theta function, associated in the standard way with a two-sheeted Riemann surface obtained by gluing together two copies of the complex plane slit along the gaps $(b_1, a_2), \ldots, (b_{q-1}, a_q), (b_q, a_1)$ of the support of the measure N, the last gap goes through infinity.

The components of the vector $\beta = \{\beta_l\}_{l=1}^{q-1}$ are rationally independent generically in V; thus the functions $\mathcal{D}(\lambda, n\beta), \mathcal{G}(\lambda, n\beta), \mathcal{R}(n\beta)$, and $\mathcal{S}(n\beta)$ are quasiperiodic in n, in general.

We will also need asymptotic formulas for $\psi_{n+k}^{(n)}$ as $n\to\infty$ and $k=O(1)$ [in particular, we need the case $k=-1$ in (2.31)]. They can be extracted from Ref. 17 (see also Ref. 8), but it will be convenient to present a different derivation, because the corresponding argument will be used in our analysis of limiting laws for linear eigenvalue statistics. To this end we replace a regular potential V in (2.20) by $V/g, g>0$, introducing explicitly the amplitude of the potential. Then the quantities of asymptotic formulas (2.38)–(2.41) will depend on g, and it follows from the results of Ref. 17 and 26 that these quantities will be differentiable functions of g in a certain neighborhood of $g=1$, provided that the support (1.7) for $g=1$ consists of q disjoint intervals. Consider now $r_{n+k-1}^{(n)}(g)$. Taking into account that the origin of the super-index n in the above formulas is the factor n in front of V in (2.23), we can write

$$n\frac{V}{g}=(n+k)\frac{V}{g(1+k/n)}. \tag{2.42}$$

In other words, to obtain $r_{n+k-1}^{(n)}(g)$ and $\psi_{n+k}^{(n)}(\lambda,g)$, we have to make the change

$$g\to g+\frac{k}{n}g \tag{2.43}$$

in the inverse amplitude of the potential. We obtain, in view of (2.41), for $k=o(n)$:

$$r_{n+k-1}^{(n)}(g)=r_{n+k-1}^{(n+k)}((1+k/n)g)\simeq\mathcal{R}((1+k/n)g,(n+k)\beta((1+k/n)g))\simeq\mathcal{R}(g,n\beta(g)+k\alpha(g)), \tag{2.44}$$

where

$$\alpha(g)=(g\beta(g))', \tag{2.45}$$

and the symbol "$\simeq$" denotes here and below the leading term(s) of the corresponding lhs as $n\to\infty$.

We have an analogous formula for (2.38):

$$(n+k)N(\lambda,(1+k/n)g)\simeq nN(\lambda,g)+k\nu(\lambda,g),$$

where

$$\nu(\lambda,g)=\frac{\partial}{\partial g}(gN(\lambda,g)). \tag{2.46}$$

By using these formulas, we can write for any fixed k [in fact $k=o(n)$]:

$$\psi_{n+k}^{(n)}(\lambda,g)\simeq(2\mathcal{D}(\lambda,g,n\beta+k\alpha))^{1/2}\cos(\pi nN(\lambda,g)+\pi k\nu(\lambda,g)+\mathcal{G}(\lambda,g,n\beta+k\alpha)). \tag{2.47}$$

Applying to (2.44) and its analog for $s_{n+k}^{(n)}$ the limiting procedure (1.10), we obtain the coefficients

$$r_{k-1}(x)=\mathcal{R}(x+k\alpha),\quad s_k(x)=\mathcal{S}(x+k\alpha),\quad x\in\mathbb{T}^{q-1},\ k\in\mathbb{Z}. \tag{2.48}$$

They determine a family of the double infinite Jacobi matrices $J(x), x\in\mathbb{T}^{q-1}$:

$$(J(x)\psi)_k=r_k(x)\psi_{k+1}+s_k(x)\psi_k+r_{k-1}(x)\psi_{k-1},\quad k\in\mathbb{Z}, \tag{2.49}$$

that can be viewed as a quasiperiodic operator, acting in $l^2(\mathbb{Z})$.

Consider now the functional

$$\mathcal{E}[m] = -\int_{\sigma} \log|\lambda - \mu| m(d\lambda) m(d\mu), \tag{2.50}$$

defined on unit non-negative measures, whose support is contained in σ. This is the standard variational problem of the potential theory.[34] Denote ν the unique minimizer of (2.50). Then, according to Ref. 12 (see also Refs. 11 and 29), the nonincreasing function $\nu(\lambda) = \nu([\lambda, \infty))$ [cf. (2.38)] coincides with the function, defined in (2.46). Moreover, according to Ref. 31 the measure ν is the Integrated Density of States (IDS) measure of $J(x)$ (see Ref. 32 for a definition of the IDS measure in a general setting of ergodic operators), the support (1.7) is a spectrum of $J(x)$, and [cf. (1.8)]

$$\alpha_l = \nu([a_l, \infty)), \quad l = 1, \ldots, q-1 \tag{2.51}$$

are the frequencies of quasiperiodic coefficients (2.48) of $J(x)$. In other words, $J(x)$ is a "finite band" Jacobi matrix, well known in spectral theory and integrable systems.[41]

By using these facts and also taking into account that $\psi_n^{(n)}(\lambda)$ decays exponentially in n outside the support,[17] we can prove that for any continuous $\Phi: \mathbb{R} \to \mathbb{C}$ of a compact support we have, in the limit (1.10) of (2.33),

$$\lim_{n_j(x)\to\infty} \int_{\mathbb{R}} \Phi(\lambda) e^{(n)}_{n_j(x)+l, n_j(x)+m}(\lambda) d\lambda = \int_{\sigma} \Phi(\lambda) e_{lm}(\lambda, x) d\lambda, \tag{2.52}$$

where we have for $\lambda \in \sigma$:

$$e_{lm}(\lambda, x) = \psi_l^+(\lambda, x)\overline{\psi_m^+(\lambda, x)} + \psi_l^-(\lambda, x)\overline{\psi_m^-(\lambda, x)}, \tag{2.53}$$

$$\psi_l^+(\lambda, x) = e^{i\pi l \nu(\lambda)} \mathcal{U}(\lambda, x + l\alpha), \quad \mathcal{U}(\lambda, x) = (\mathcal{D}(\lambda, x)/2)^{1/2} e^{i\mathcal{G}(\lambda, x)}, \tag{2.54}$$

and $\psi_l^- = \overline{\psi_l^+}$. The above formula can also be written as

$$\psi_l^{\pm}(\lambda, x) = \psi_0^{\pm}(\lambda, x + T^l \alpha), \tag{2.55}$$

where $T: \mathbb{T}^{q-1} \to \mathbb{T}^{q-1}$ is defined as $Tx = x + \alpha$. This shows that $\Psi^{\pm}(\lambda, x) = \{\psi_l^{\pm}(\lambda, x)\}_{l \in \mathbb{Z}}$ is a generalized (quasi-Bloch) eigenfunction of $J(x)$:

$$J(x)\Psi^{\pm}(\lambda, x) = \lambda \Psi^{\pm}(\lambda, x).$$

In fact, $\{\Psi^{\pm}(\lambda, x)\}_{\lambda \in \sigma}$ form a complete system in $l^2(\mathbb{Z})$.

We refer the reader to Ref. 31 for more details of this aspect of asymptotic formulas of Ref. 17.

C. Asymptotic behavior of variance

We assume in this section that the test function φ in (1.2) is of the class C^1 and does not depend on n. Hence, function (2.30) is continuous in (λ_1, λ_2). As a result, fast oscillating in n functions, entering (2.47), do not contribute to the limit, as was already in obtaining (2.52)–(2.54). We have then, from (2.28), (2.34), and (2.52)–(2.54),

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} \simeq \mathcal{V}(n\beta), \tag{2.56}$$

where

$$\mathcal{V}(x) = \int_{\sigma}\int_{\sigma} \left|\frac{\Delta\varphi}{\Delta\lambda}\right|^2 \mathcal{V}(\lambda_1, \lambda_2, x) d\lambda_1\, d\lambda_2, \tag{2.57}$$

$$\mathcal{V}(\lambda_1,\lambda_2,x)=\mathcal{R}^2(x)(e_{0,0}(\lambda_1,x)e_{-1,-1}(\lambda_2,x)-e_{-1,0}(\lambda_1,x)e_{-1,0}(\lambda_2,x)), \tag{2.58}$$

and $e_{lm}(\lambda,x)$ are given by (2.53) and (2.54), in particular,

$$\int_\sigma e_{lm}(\lambda,x)d\lambda=\delta_{lm}. \tag{2.59}$$

Since the charges $\beta_l, l=1,\dots,q-1$ of (1.8) are continuous and nonconstant functionals of the potential (see Refs. 17 and 26), the leading term of variance is a quasiperiodic function generically in the potential. In particular, it has no limit as $n\to\infty$. Its limiting points are indexed by the subset $\mathbb{H}^{q-1}\subset\mathbb{T}^{q-1}$, the closure of limiting points of the $q-1$ dimensional vectors (1.9). $\mathbb{H}^{q-1}$ is $\mathbb{T}^{q-1}$ generically in V, but it can also be a proper subset of $\mathbb{T}^{q-1}$ [see, e.g. (2.15)].

The simplest case is $q=1$ of a single interval support. Here $\mathbb{H}^0$ is a point, there exist the limits[2,16]

$$\lim_{n\to\infty} r_{n+k-1}^{(n)}=r,\quad \lim_{n\to\infty} s_{n+k}^{(n)}=s,\quad \forall\, k\in\mathbb{Z}, \tag{2.60}$$

and the "limiting" Jacobi matrix $J(x)$ of (2.49) has constant coefficients:

$$J_{jk}=r\delta_{j+1,k}+s\delta_{j,k}+r\delta_{j-1,k}.$$

Placing the origin of the spectral axis at s, we obtain that $\lambda=2r\cos\pi\nu$, $\psi^\pm$ are just the plane waves,

$$\sigma=[-2r,2r],$$

and

$$\mathcal{D}(\lambda)=-\nu'(\lambda)=\frac{1}{\pi\sqrt{4r^2-\lambda^2}},\quad \lambda\in\sigma. \tag{2.61}$$

This and general formula (2.58) yield a version of (2.56) and (2.57), in which the role of $\mathcal{V}(x,\lambda_1,\lambda_2)$ plays

$$\mathcal{V}^{(1)}(\lambda_1,\lambda_2)=\frac{1}{4\pi^2}\frac{4r^2-\lambda_1\lambda_2}{\sqrt{4r^2-\lambda_1^2}\sqrt{4r^2-\lambda_2^2}},\quad \lambda_1,\lambda_2\in\sigma. \tag{2.62}$$

This form of the variance was first found in physical papers[4,10] and proved rigorously in Ref. 23. We see that in the single interval case the variance is universal, i.e., its functional form does not depend explicitly on the potential, the information on the potential being encoded in the unique parameter r of (2.60). In particular, we have (2.62) for the Gaussian Unitary Ensemble (2.16).[13]

In the case (2.12)–(2.15), $\mathbb{H}^{q-1}$ consists of q points [see (2.15)], and the variance is a q-periodic function of n. Example (2.17)–(2.19) corresponds to the simplest nontrivial case $q=2$, where $\beta_1=1/2, \mathbb{H}^1=\{0,1/2\}$, the matrix $J(x)$ is 2-periodic, its coefficients are

$$r_k=\frac{b-(-1)^k a}{2},\quad s_k=0, \tag{2.63}$$

and the variance is asymptotically a 2-periodic function in n:[8,3]

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\}\simeq\mathcal{V}^{(2)}(n/2),$$

where $\mathcal{V}^{(2)}(x)$ is given by (2.57), in which $\mathcal{V}(\lambda_1,\lambda_2,x), x\in\mathbb{H}^1=\{0,1/2\}$ is

$$\mathcal{V}^{(2)}(\lambda_1,\lambda_2,x)=\frac{1}{2\pi^2}\frac{\varepsilon_{\lambda_1}\varepsilon_{\lambda_2}}{\sqrt{|R_2(\lambda_1)|}\sqrt{|R_2(\lambda_2)|}}((a^2-\lambda_1\lambda_2)(b^2-\lambda_1\lambda_2)-(-1)^{2x}ab(\lambda_1-\lambda_2)^2),$$

$$\lambda_1,\lambda_2\in\sigma, \tag{2.64}$$

with

$$R_2(\lambda)=(\lambda^2-a^2)(\lambda^2-b^2), \tag{2.65}$$

and $\varepsilon_\lambda=1$ if $\lambda\in(-b,-a)$ and $\varepsilon_\lambda=-1$ if $\lambda\in(a,b)$. In fact, these formulas are valid for any real analytic and even potential, producing a symmetric two-interval support,

$$\sigma=[-b,-a]\cup[a,b],\quad 0<a<b<\infty, \tag{2.66}$$

(see Refs. 3 and 8). The general case of a two-interval and not necessarily symmetric support was analyzed in Ref. 8, where it was found that the variance can be expressed via the classical elliptic functions of Jacobi and Weierstrass.

We conclude that a minimum modification of the limiting law of linear eigenvalue statistics in the case of a multi-interval support of the IDS, comparing with the case of i.i.d. random variables, could be a family of normal laws, indexed by the points of $\mathbb{H}^{q-1}$. We shall see below that this modification is not sufficient in certain cases.

We remark in the conclusion of this section that formulas (2.56)–(2.58) allow us to characterize the universality classes of ensembles (2.1) with respect to the variance in the global regime, i.e., the sets of ensembles (potentials), leading to the same asymptotic form of the variance of linear statistics in the regime. Namely, since the potential is present in (2.56)–(2.58) only via the endpoints $(a_1,\ldots,b_q)$ of support and via the charges $(\beta_1,\ldots,\beta_{q-1})$ of all but one intervals of the support, these parameters determine a universality class. Notice that the parameters are not necessarily independent.

III. LIMITING LAWS

A. Laplace transform of the probability law of linear eigenvalue statistics

In this section we obtain an expression for the Laplace transform of the probability law of linear eigenvalue statistics (1.2) via orthogonal polynomials. We consider here real-valued test functions $\varphi:\mathbb{R}\to\mathbb{R}$. The Laplace transform is evidently

$$Z_n[\varphi]=\mathbf{E}_V\{e^{\overset{\circ}{\mathcal{N}}_n[\varphi]}\}, \tag{3.1}$$

where $\mathbf{E}_V\{\cdots\}$ denotes the expectation with respect to (2.1) [or (2.20)], determined by a given potential V, and

$$\overset{\circ}{\mathcal{N}}_n[\varphi]=\mathcal{N}_n[\varphi]-\mathbf{E}_V\{\mathcal{N}_n[\varphi]\}.$$

It is convenient to introduce the parameter $s\in[0,1]$ and to consider the function

$$F_n(s)=\log Z_n[s\varphi],\quad s\in[0,1].$$

It is easy to see that

$$F_n(0)=0,F_n'(0)=-\mathbf{E}_V\{\overset{\circ}{\mathcal{N}}_n[\varphi]\}=0,$$

and

$$F_n''(s)=\mathbf{E}_{V+s\varphi/n}\{\mathcal{N}_n^2[\varphi]\}-\mathbf{E}_{V+s\varphi/n}^2\{\mathcal{N}_n[\varphi]\}:=\mathbf{Var}_{V+s\varphi/n}\{\mathcal{N}_n[\varphi]\}.$$

This yields the following expression for the logarithm of (3.1):

$$\log Z_n[\varphi] = F_n(1) := F_n[\varphi] = \int_0^1 (1-s)\mathbf{Var}_{V+s\varphi/n}\{\mathcal{N}_n[\varphi]\}ds. \tag{3.2}$$

We mention that there exists another expression for the Laplace transform (3.1). It dates back to the Heine formulas in the theory of orthogonal polynomials (see, e.g., Ref. 40, Theorem 2.1.1) and can be easily obtained from the Gram theorem:

$$Z_n[\varphi] = \det\left\{\int_{\mathbb{R}} e^{-\overset{\circ}{\varphi}(\lambda)}\psi_j^{(n)}(\lambda)\psi_k^{(n)}(\lambda)d\lambda\right\}_{j,k=1}^n = e^{\mathbf{E}\{\mathcal{N}_n[\varphi]\}}\det(1-K_{n,\varphi}),$$

where

$$\overset{\circ}{\varphi}(\lambda) = \varphi(\lambda) - \mathbf{E}_V\{\mathcal{N}_n[\varphi]\}, \quad \mathbf{E}_V\{\mathcal{N}_n[\varphi]\} = n\int_{\mathbb{R}} \varphi(\lambda)\mathbf{E}_V\{N_n(d\lambda)\},$$

and $K_{n,\varphi}$ is the integral operator, defined as

$$(K_{n,\varphi}f)(\lambda) = \int_{\mathbb{R}} K_n(\lambda,\mu)(1-e^{-\varphi(\mu)})f(\mu)d\mu, \quad \lambda\in\mathbb{R}.$$

These formulas and their analogs for unitary matrices were used to prove various versions of the Central Limit Theorem (see, e.g., Refs. 6, 23, 24, 37–39, and 42).

B. Asymptotic behavior of the Laplace transform

We will assume in this section that φ is real analytic. According to (3.2), (2.28), and (2.31), we have to find the asymptotic form of $\psi_n^{(n)}$ and $\psi_{n-1}^{(n)}$ for the potential $V+s\varphi/n$. We have already seen in the previous section that adding terms of the order $O(n^{-1})$ to the potential, we obtain nontrivial contributions to the asymptotic formulas because of fast oscillating in n functions on the rhs of (2.39)–(2.41), etc. The $O(n^{-1})$ terms appeared there because of the passage $n\to n+k$, leading to (2.45)–(2.48). In this case the terms are proportional to the potential, since we just change its amplitude: $V\to V(1-k/n)$ [see (2.42) and (2.43)]. This required derivatives (2.45) and (2.46) of "frequencies" β_l, $l=1,\ldots,q-1$, and $N(\lambda)$ of fast oscillating functions in (2.39)–(2.41) with respect to the inverse amplitude g of the potential.

On the other hand, to find the asymptotic behavior of the Laplace transform, we have to add to the potential the term $s\varphi/n$ [see (3.2)]. Since $\varphi\neq V$, in general, this requires variational derivatives of frequencies with respect to potential, i.e., we have to add the term $\varepsilon\varphi$ to the potential, and find the derivative of $\beta_l, l=1,\ldots,q-1$, and $N(\lambda)$ with respect to ε at $\varepsilon=0$.

Consider first the case $q=1$, where the support of the IDS is a single interval. Here the dependence on x of functions $\mathcal{D},\mathcal{G},\mathcal{R}$, and $\mathcal{S}$ of (2.39)–(2.41) is absent [see (2.60)–(2.62)]. Hence the term $s\varphi/n$ is negligible in the limit $n\to\infty$, because there are no fast oscillating in n functions in the asymptotics of $\psi_{n+k}^{(n)}$, $k=0,-1$, $r_{n-1}^{(n)}$, and $s_n^{(n)}$, and we obtain from (3.2) and (2.62),

$$\lim_{n\to\infty} F_n[\varphi] = \lim_{n\to\infty} \mathbf{Var}\{\mathcal{N}_n[\varphi]\}/2. \tag{3.3}$$

Notice also that we have here the "genuine" limit as $n\to\infty$, but not a sublimit (1.10) along a subsequence. We conclude that the Central Limit Theorem is valid in this case. This was proved in Ref. 23 by the variational method and for a rather broad class of potentials and test functions (not necessarily real analytic).

As it was shown in the previous section, the variance of a linear statistics with a C^1 test function has no limit as $n\to\infty$ if $q\geq 2$. Its sublimits are indexed by points of the "hull" $\mathbb{H}^{q-1}\subset\mathbb{T}^{q-1}$. Hence we cannot expect the traditional CLT (3.3), as in the case of $q=1$. Rather this should be a collection of the CLT, indexed by $\mathbb{H}^{q-1}$:

$$\lim_{n_j(x)\to\infty} F_{n_j(x)}[\varphi] = \lim_{n_j(x)\to\infty} \mathbf{Var}\{\mathcal{N}_{n_j(x)}[\varphi]\}/2 = \mathcal{V}(x)/2,\ x \in \mathbb{H}^{q-1}, \tag{3.4}$$

where $\{n_j(x)\}$ and $\mathcal{V}(x)$ are defined in (1.10), (2.57), and (2.58). We will call this the generalized CLT.

We will show now that the generalized CLT is not always the case for $q \geq 2$. Recall that $N(\lambda)$ and β_l are functionals of V and denote

$$\dot{\beta}_l[\varphi] = \frac{\partial}{\partial\varepsilon}\beta_l\bigg|_{\varepsilon=0}, \quad l = 1, \ldots, q-1, \quad \dot{N}[\varphi] = \frac{\partial}{\partial\varepsilon}N(\lambda)\bigg|_{\varepsilon=0} \tag{3.5}$$

the variational derivatives of β_l and $N(\lambda)$ with respect to V. $\dot{\beta}_l[\varphi]$ and $\dot{N}[\varphi]$ are linear functionals of φ and nonlinear functionals of V. It follows from Ref. 26 that they are well defined if V is real analytic and regular and φ is real analytic and such that $\max_{\lambda\in\mathbb{R}}|V(\lambda)/\varphi(\lambda)| < \infty$.

Arguing as in Sec. II B, we obtain that in this case $\psi_{n+k}^{(n)}$ is given by (2.47) and (2.48) with the replacement

$$k\alpha_l \to k\alpha_l + s\dot{\beta}_l[\varphi], \quad \pi k\nu \to \pi k\nu + \pi s\dot{N}[\varphi].$$

Now, assuming (1.10) and taking into account (3.2), (2.28), and (2.34), we obtain from (3.2),

$$F[\varphi] := \lim_{n_j(x)\to\infty} \log Z_{n_j(x)}[\varphi] = \int_0^1 (1-s)\mathcal{V}(x + s\dot{\beta}[\varphi])ds, \tag{3.6}$$

where $\mathcal{V}$ is given by (2.57). According to (2.57), $\mathcal{V}$ is a quadratic functional of φ. Hence, the functional $F[\varphi]$ is not quadratic in general, because of the presence of the term $s\dot{\beta}[\varphi]$ in the argument of the integrand in (3.6). In other words, we have here a limiting law in the sense of (1.10), but the law is not necessarily Gaussian.

It seems that a general classification of possible cases is rather complex. We thus will give several examples showing different cases of asymptotic behavior of the Laplace transform of the probability law of linear eigenvalue statistics.

Consider first the case where the test function is a multiple of the potential:

$$\varphi(\lambda) = tV(\lambda), \quad t \in \mathbb{R}. \tag{3.7}$$

Then (2.45) and the relation $\dot{\beta}_l[V] = -\beta'(g)|_{g=1}$ yield

$$\dot{\beta}_l[\varphi] = \dot{\beta}_l[tV] = -t(\beta_l(1) - \alpha_l(1)), \quad l = 1, \ldots, q-1,$$

where $\alpha_l, l = 1, \ldots, q-1$ are defined in (2.51). Hence, if

$$\beta_l(1) = \alpha_l(1), \quad l = 1, \ldots, q-1, \tag{3.8}$$

then the integrand in (3.6) does not depend on s, and we obtain in view of (2.56) and (2.57) the generalized Central Limit Theorem (3.4).

The equality (3.8) is valid for any potential of the form (2.12) with $g=1$ and v^2-4 having only simple and real zeros, because, according to Ref. 26,

$$\beta_l(1) = \alpha_l(1) = \frac{q-l}{q}, \quad l = 1, \ldots, q-1.$$

It is also valid for any even potential, having two equal local minima and one local maximum, which is high enough to produce a two-interval support (2.66). In this case (3.8) results from the symmetry, implying

$$\beta_1 = \alpha_1 = 1/2 \tag{3.9}$$

[recall that in this case the vectors β of (1.8) and α of (2.45) are one-dimensional: $\beta_1 = N(a), \alpha_1 = \nu(a)$].

In all these cases the limiting Jacobi matrix J of (2.49) is q periodic [$q=2$ in the case of (2.66); see (2.63)].

It can also be shown that we have the generalized Central Limit Theorem for potentials (2.12) and $\varphi = tv$ (here the limiting matrix J is also q periodic).

To demonstrate a possibility to have a non-Gaussian limiting law, we consider a simplest nontrivial case of even potential with the two-interval support (2.66) and of the test function

$$\varphi(\lambda) = t\lambda, \quad t \in \mathbb{R}, \tag{3.10}$$

i.e., the case of "linear" linear statistic

$$t\sum_{l=1}^{n} \lambda_l^{(n)} = t \operatorname{Tr} M_n. \tag{3.11}$$

Since in this case $\Delta\varphi/\Delta\lambda$ of (2.30) is equal to t, it follows from (2.58) and (2.59) that

$$\mathcal{V}(x) = t^2\mathcal{R}^2(x), \tag{3.12}$$

and then (3.6) implies that in the case (3.10) (and for any support) we have for the exponent of the limiting Laplace transform:

$$F[\varphi]\big|_{\varphi(\lambda)=t\lambda} = \lim_{n_j(x)\to\infty} \log Z_{n_j(x)}[\varphi]\big|_{\varphi(\lambda)=t\lambda} = t^2\int_0^1 (1-s)\mathcal{R}^2\Big(x + s\dot{\beta}[\varphi]\Big|_{\varphi(\lambda)=t\lambda}\Big)ds. \tag{3.13}$$

According to Ref. 8, it is possible to express the coefficient $\mathcal{R}(x)$, corresponding to the two-interval support, via the Jacobi elliptic function:

$$\mathcal{R}^2(x) = \frac{(b-a)^2}{4} + \frac{ab}{2}\operatorname{cn}^2(x+1/2), \tag{3.14}$$

where $\operatorname{cn}(x) = \operatorname{cn}(2K(k)x|k), k^2 = 4ab/(a+b)^2, K(k)$ is the elliptic integral of the first kind. In view of (3.9), the coefficient r_k of (2.48) is given by (2.63):

$$r_{k-1} = \mathcal{R}\left(\frac{k}{2}\right) = \frac{b-(-1)^k a}{2},$$

and is 2-periodic (see also Ref. 2). In view of (3.12) this implies that the variance of (3.11) is asymptotically 2-periodic in n:

$$\mathcal{R}^2\left(\frac{n}{2}\right) = \frac{b^2+a^2}{4} - (-1)^n\frac{ab}{2}. \tag{3.15}$$

Furthermore, it is shown in the Appendix that

$$\dot{\beta}_1[\varphi]\big|_{\varphi(\lambda)=t\lambda} = t\omega, \quad \omega = \frac{a}{4K(a/b)}, \tag{3.16}$$

Hence we obtain from (3.14),

$$F[\varphi]|_{\varphi(\lambda)=t\lambda} = \int_0^t (t-s)\mathcal{R}^2(x+s\omega)ds. \tag{3.17}$$

It follows from (3.16) that ω is irrational generically in a, and b; hence $\mathcal{R}^2(x+s\omega)$ is quasiperiodic in s in these cases. Since $\mathcal{R}^2$ is 1-periodic and real analytic, we can write its Fourier series,

$$\mathcal{R}^2(x) = \sum_{m\in\mathbb{Z}} c_m e^{2\pi imx}, \tag{3.18}$$

with fast decaying coefficients. Plugging (3.16) and (3.18) in (3.13), we obtain

$$F[\varphi]|_{\varphi(\lambda)=t\lambda} = \frac{c_0 t^2}{2} - tA'(x) - A(x) + A(x+\omega t), \tag{3.19}$$

where

$$A(x) = \sum_{m\in\mathbb{Z}\setminus\{0\}} \frac{c_m}{(2\pi im\omega)^2} e^{2\pi imx}. \tag{3.20}$$

We see that the logarithm of the limiting Laplace transform of the probability law of statistics (3.11) contains not only a multiple of $t^2/2$, that would correspond to the CLT, but also a linear in t term, a constant in t term, and either quasiperiodic (generically in a,b, when ω is irrational) or periodic (in special cases, where ω is rational) function of t. Besides, while the variance of statistics (3.11) is (3.15) in the limit (1.10), the coefficient in front of $t^2/2$ is

$$c_0 = \int_{\mathbb{T}} \mathcal{R}^2(x)dx = \frac{b^2+a^2}{4},$$

hence is not the variance (3.15).

Notice also that in the case $q\geq 3$ we would have in (3.20) the sum over $\mathbb{Z}^{q-1}\setminus\{0\}$, and the expression

$$\dot\beta\cdot m := \dot\beta_1 m_1 + \ldots \dot\beta_{q-1} m_{q-1},$$

in the denominator, that can be arbitrary small for certain collections of $(m_1,\ldots,m_{q-1})\in\mathbb{Z}^{q-1}$ and $\dot\beta := (\dot\beta_1,\ldots,\dot\beta_{q-1})\in\mathbb{R}^{q-1}$ in the case, where the components of $\dot\beta$ are irrational. Hence, to make the series in (3.20) convergent, we have to assume that the components of $\dot\beta$ are sufficiently bad approximated by rationals (e.g., a Diophantine condition).

According to the Appendix , in a general case of a real analytic φ and a two-interval support,

$$\sigma = [a_1,b_1]\cup[a_2,b_2], \quad -\infty < a_1 < b_1 < a_2 < b_2 < \infty, \tag{3.21}$$

we have

$$\dot\beta_1[\varphi] = -\frac{1}{2\pi i I}\int_\sigma \frac{\varphi(\mu)}{\sqrt{R_2(\mu)}}d\mu, \tag{3.22}$$

where $\sqrt{R_2(\mu)}$ is defined in (2.9),

$$I = \int_{b_1}^{a_2} \frac{d\mu}{\sqrt{(b_2-\mu)(a_2-\mu)(\mu-b_1)(\mu-a_1)}} = \frac{2}{((b_2-b_1)(a_2-a_1))^{1/2}}K(\kappa), \tag{3.23}$$

and

$$\kappa^2 = \frac{(a_2 - b_1)(b_2 - a_1)}{(b_2 - b_1)(a_2 - a_1)}$$

[see Ref. 20, formula (3.149.4)]. In the symmetric case (2.66), we have

$$I = \frac{2}{b+a} K\left(\frac{2\sqrt{ab}}{b+a}\right) = \frac{2}{a} K\left(\frac{b}{a}\right),$$

where the second equality results from the formula $(1+k)^{-1}K[2\sqrt{k}/(1+k)]=K(k)$,[41] formula (8.126.3). It follows then that in this case and for $\varphi=t\lambda$, (3.22) coincides with (3.16).

Formula (3.22) allows us to characterize the class of potentials and test functions for which the (generalized) Central Limit Theorem (3.4) is valid in the case of a general two-interval support (3.21). Indeed, for any pair (V,φ) for which the rhs of (3.22) is zero, the integrand of (3.6) does not depend on s and we have the generalized CLT (3.4). In particular, in the symmetric case (2.66) it follows from (3.22) that $\dot{\beta}_1[\varphi]$ is zero if and only if

$$\int_a^b \frac{\varphi(\mu) - \varphi(-\mu)}{\sqrt{(b^2 - \mu^2)(\mu^2 - a^2)}} d\mu = 0.$$

In particular, for an even potential of support (2.66) and an even test function φ, the generalized CLT is valid.

One can view φ as an analog of external field in statistical mechanics. Hence, we can say that in this case an even external field "does not break the symmetry." On the other hand, a "generic" φ or an odd φ, such that

$$\int_a^b \frac{\varphi(\mu) d\mu}{\sqrt{(b^2 - \mu^2)(\mu^2 - a^2)}} \neq 0,$$

is a "breaking symmetry field" and leads to a non-Gaussian limiting law. Its simplest case $\varphi(\lambda)=t\lambda$ (3.10) is given by (3.19).

IV. INTERMEDIATE AND LOCAL REGIMES

In this section we consider limiting laws of linear eigenvalue statistics for the test functions, given by (1.11) and (1.12) with a C^1 function φ and λ_0 belonging to the interior of σ.

We begin again by calculating the asymptotic form of the variance in these cases. Changing variables to

$$\lambda_{1,2} = \lambda_0 + t_{1,2}/n^\alpha, \quad 0 < \alpha \leq 1, \tag{4.1}$$

we obtain from (2.28),

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} = \int_{\mathbb{R}} \int_{\mathbb{R}} \left(\frac{\Delta\varphi}{\Delta t}\right)^2 \mathcal{V}_n(\lambda_0 + t_1/n^\alpha, \lambda_0 + t_2/n^\alpha) dt_1\, dt_2. \tag{4.2}$$

To find the asymptotic form of the rhs we will use again (2.34) and (2.33) in which $\psi_{n+k}^{(n)}(\lambda)$, $k=0.-1$ is given by (2.47) with $\lambda=\lambda_0+t/n^\alpha$. Taking into account that $\mathcal{D}, N$, and $\mathcal{G}$ are smooth functions of λ in a sufficiently small neighborhood of λ_0, we can write

$$\psi_{n+k}^{(n)}(\lambda) \simeq (2\mathcal{D}(\lambda_0, n\beta + k\alpha))^{1/2} \cos(\pi n N(\lambda_0) + \pi k \nu(\lambda_0) - \pi\rho(\lambda_0) n^{1-\alpha} + \mathcal{G}(\lambda_0, n\beta + k\nu)),$$

where $\rho(\lambda)=-N'(\lambda)$, and we do not indicate the dependence on g (in fact, it suffices to consider the case $g=1$). Plugging this into (2.33) and (2.34), and omitting in the resulting integrand of the rhs of (4.2) the fast oscillating terms, we obtain

$$\mathbf{Var}\{\mathcal{N}_n[\varphi]\} \simeq B(\lambda_0, n\beta)\int_{\mathbb{R}}\int_{\mathbb{R}}(\varphi(t_1)-\varphi(t_2))^2\frac{\sin^2(\pi\rho(\lambda_0)(t_1-t_2)n^{1-\alpha})}{2\pi^2(t_1-t_2)^2}dt_1\,dt_2, \tag{4.3}$$

where

$$B(\lambda,x) = 2\pi^2\mathcal{R}^2(x)\mathcal{D}(\lambda,x)\mathcal{D}(\lambda,x-\alpha)\sin^2(\pi\nu(\lambda)+\mathcal{G}(\lambda,x)-\mathcal{G}(\lambda,x-\alpha)). \tag{4.4}$$

This leads to the following result in the local regime $\alpha=1$, and for the limit (1.10),

$$\lim_{n_j(x)\to\infty}\mathbf{Var}\{\mathcal{N}_{n_j(x)}[\varphi_{n_j(x)}]\} = B(\lambda_0,x)\int_{\mathbb{R}}\int_{\mathbb{R}}(\varphi(t_1)-\varphi(t_2))^2\frac{\sin^2(\pi\rho(\lambda_0)(t_1-t_2))}{2\pi^2(t_1-t_2)^2}dt_1\,dt_2. \tag{4.5}$$

It is known that in the local regime the variance of linear eigenvalue statistics has a universal limiting form[17,33]

$$\lim_{n\to\infty}\mathbf{Var}\{N_n[\varphi_n]\} = \int_{\mathbb{R}}\int_{\mathbb{R}}(\varphi(t_1)-\varphi(t_2))^2\frac{\sin^2(\pi\rho(\lambda_0)(t_1-t_2))}{2\pi^2(t_1-t_2)^2}dt_1\,dt_2, \tag{4.6}$$

in which all the information on the potential is encoded in $\rho(\lambda_0)$. This and (4.5) imply the identity

$$B(\lambda,x) = 1, \tag{4.7}$$

valid for all $x\in\mathbb{T}^{q-1}$ and λ, belonging to the interior of the σ (a direct proof of the identity can be extracted from the proof of Lemma 6.1 of Ref. 20).

In the intermediate regime $0<\alpha<1$, we still have a fast oscillating factor,

$$\sin^2(n^{1-\alpha}\pi\rho(\lambda_0)(t_1-t_2))$$

in the integrand of (4.3). Replacing the factor by its average 1/2, and using (4.7), we obtain in this regime

$$\lim_{n\to\infty}\mathbf{Var}\{N_n[\varphi_n]\} = \int_{\mathbb{R}}\int_{\mathbb{R}}\frac{(\varphi(t_1)-\varphi(t_2))^2}{4\pi^2(t_1-t_2)^2}dt_1\,dt_2. \tag{4.8}$$

As in the case of the local regime, the limit here is the same for any subsequence (1.10); hence we do not need to assume (1.10). We conclude that the variance of linear statistics has a well defined limit in the intermediate regime as well. Moreover, (4.8) is the "smoothed" version of variance (4.6) in the local regime, since (4.8) is (4.6), in which the "oscillating" factor $\sin^2(\pi\rho(\lambda_0)(t_1-t_2))$ is replaced by its average 1/2.

Passing to the Fourier transform,

$$\widehat{\varphi}(k) = \frac{1}{2\pi}\int_{\mathbb{R}}e^{ikt}\varphi(t)dt,$$

we can rewrite the rhs of (4.8) in the form

$$\int_{\mathbb{R}}|k|\widehat{\varphi}(k)\widehat{\varphi}(-k)dk,$$

appearing in the continuous analog of the strong Szegö theorem (see Refs. 6, 18, and 37 and references therein).

The universality property of unitary invariant Matrix Models[17,33] implies that the Laplace transform of the probability law of linear eigenvalue statistics has the following limiting form in the local regime:

$$\lim_{n\to\infty} Z_n[\varphi_n]\Big|_{\varphi_n(\lambda)=\varphi((\lambda-\lambda_0)n)} = e^{2\pi\rho(\lambda_0)\widehat{\varphi}(0)} \det(1-S_\varphi), \tag{4.9}$$

where S_φ is the integral operator, defined as

$$(S_\varphi f)(t) = \int_{\mathbb{R}} \frac{\sin \pi\rho(\lambda_0)(t-u)}{\pi\rho(\lambda_0)(t-u)}(1-e^{-\varphi(u)})f(u)du, \tag{4.10}$$

and we assume that φ in (1.12) is continuous and integrable on $\mathbb{R}$. It is obvious that the logarithm of the rhs of (4.9) is not quadratic in φ; hence the CLT is not valid in the local regime (see, e.g., Ref. 22 for related results).

If, however, we take in the above formulas,

$$\varphi(t) = \Phi((t-t_0)\delta),$$

where Φ does not depend on $\delta\to 0$, and $t_0 \in \mathbb{R}$, i.e., we assume that the test function in (4.9) and (4.10) is "slow varying," then it can be shown (see, e.g., Refs. 6, 15, and 39) that the limit of the rhs of (4.9) as $\delta\to 0$ is the rhs of (4.8), divided by 2.

On the other hand, take as a test function in (3.6),

$$\varphi(\lambda) = \Phi((\lambda-\lambda_0)/\delta), \tag{4.11}$$

where Φ does not depend on $\delta\to 0$, and λ_0 belongs to the interior of the support of N, i.e., assume that φ is "fast varying." Since the variational derivatives (linear functionals of φ) $\dot{\beta}_l[\varphi]$, $l=1,\ldots,q-1$ of (3.5) can be written as

$$\dot{\beta}_l[\varphi] = \int_{\mathbb{R}} b_l(\lambda)\varphi(\lambda)d\lambda,$$

we have

$$\dot{\beta}_l[\varphi] = \delta\int_{\mathbb{R}} b_l(\lambda_0+\delta t)\Phi(t)dt \to 0, \quad \delta\to 0.$$

Hence, the term $s\dot{\beta}$ in the argument of the integrand of (3.6) vanishes in the limit $\delta\to 0$ and we obtain from (2.57), changing variables to $\lambda_{1,2}=\lambda_0+\delta t_{1,2}$:

$$\lim_{\delta\to\infty} F[\varphi]\Big|_{\varphi(\lambda)=\Phi(\lambda-\lambda_0)/\delta} = \frac{1}{2}\mathcal{V}(x), \tag{4.12}$$

where

$$\mathcal{V}(x) = \mathcal{V}(\lambda_0,\lambda_0,x)\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{(\Phi(t_1)-\Phi(t_2))^2}{2\pi^2(t_1-t_2)^2}dt_1\,dt_2.$$

Now it can be shown, by using (2.58), (2.54), (2.55), and (4.4), that the rhs of the last formula coincides with (4.8). Hence, the limit (4.12) coincides again with the rhs of (4.8), divided by 2.

The above suggests that the CLT is valid in the intermediate regime. This was indeed proved in several cases (see Ref. 37 and references therein).

APPENDIX: VARIATIONAL DERIVATIVE OF FREQUENCY IN THE TWO-INTERVAL CASE

Here we derive formula (3.16). We will use the variational approach, based on the functional (2.3).

Write the minimum condition (2.4) and (2.6) for $V+\varepsilon\varphi$, and compute its derivative at $\varepsilon=0$. This yields

$$\varphi(\lambda) - 2\int_\sigma \log|\lambda-\mu|\dot\rho(\mu)d\mu = \text{const}, \quad \lambda\in\sigma, \tag{A1}$$

where

$$\dot\rho = \left.\frac{\partial}{\partial\varepsilon}\rho\right|_{\varepsilon=0},$$

and ρ is the density of the measure N of (1.5). Notice that the differentiation of the limits of integration in (2.6) does not contribute to (A1), because ρ vanishes at each endpoint of the support according to (2.8).

The derivative of (A1) in λ is the singular integral equation [cf. (2.10)],

$$\text{v.p.}\int_\sigma \frac{\rho(\mu)d\mu}{\mu-\lambda} = -\frac{\varphi'(\lambda)}{2}, \quad \lambda\in\sigma.$$

The general solution of the equation in the case (2.66) is[25]

$$\frac{C_1\lambda + C}{X_2(\lambda)} + \frac{1}{2\pi^2 X_2(\lambda)}\text{v.p.}\int_\sigma \frac{\varphi'(\mu)X_2(\mu)d\mu}{\mu-\lambda},$$

where

$$X_2(\lambda) = -i\sqrt{R_2(\lambda)}, \quad \sqrt{R_2(\lambda)} = \sqrt{R_2(z)}|_{z=\lambda+i0},$$

$R_2(z)=(z^2-a^2)(z^2-b^2)$ [see (2.9) for $q=2$] and $\sqrt{R_2(z)}$ is the branch of the square root, fixed by the condition $\sqrt{R(z)}=z^2+O(z), z\to\infty$. The branch assumes pure imaginary values of opposite sides on the edges of σ, seen as a cut of $\mathbb{C}$.

Taking into account the equalities

$$\int_\sigma \dot\rho(\mu)d\mu = 0,$$

and

$$\int_\sigma \frac{d\mu}{\sqrt{R_2(\mu)}} = 0, \int_\sigma \frac{\mu d\mu}{\sqrt{R_2(\mu)}} = -\pi i,$$

we find that

$$\dot\rho(\lambda) = \frac{iC}{\sqrt{R_2(\lambda)}} + \frac{1}{2\pi^2\sqrt{R_2(\lambda)}}\text{v.p.}\int_\sigma \frac{\varphi'(\mu)\sqrt{R_2(\mu)}d\mu}{\mu-\lambda}. \tag{A2}$$

The constant C can be found as follows. Denote $f(z)$ the Stieltjes transform of ρ:

$$f(z) = \int_\sigma \frac{\rho(\mu)d\mu}{\mu-z}, \quad z\notin\sigma. \tag{A3}$$

Recalling that V is real analytic, using (2.8), (2.11), and arguing as above, we find that

$$f(z) = -\frac{V'(z)}{2} - \frac{\sqrt{R_2(z)}}{2\pi i}\int_\sigma \frac{V'(\mu)-V'(z)}{\mu-z}\frac{d\mu}{\sqrt{R_2(\mu)}} \tag{A4}$$

[the analog of the formula with R_q instead of R_2 is valid for any finite number q of intervals in (1.7)].

Write now the minimum condition (2.4) as

$$V_{\text{eff}}(b) - V_{\text{eff}}(a) = 0,$$

or, in view of (2.6) and (A3), as

$$\int_{-a}^{a} \left(f(\lambda) + \frac{V'(\lambda)}{2} \right) d\lambda = 0. \tag{A5}$$

The condition is valid for any potential, in particular, for $V+\varepsilon\varphi$. According to (A4) for any sufficiently small ε, the integrand here is proportional to $\sqrt{R_2(\lambda)}$, in which a and b are now functions of ε. Hence, the integrand vanishes at the edges of the support and the derivative of (A5) with V replaced by $V+\varepsilon\varphi$ with respect to ε at $\varepsilon=0$ is

$$\int_{-a}^{a} \left(\dot{f}(\lambda) + \frac{\varphi'(\lambda)}{2} \right) d\lambda = 0. \tag{A6}$$

This and the formula

$$\dot{f}(z) = \int_{\sigma} \frac{\dot{\rho}(\mu) d\mu}{\mu - z} = -\frac{\pi C}{\sqrt{R_2(z)}} - \frac{1}{2\pi i \sqrt{R_2(z)}} \int_{\sigma} \frac{\varphi'(\mu)\sqrt{R_2(\mu)}}{\mu - z} d\mu, \tag{A7}$$

following from (A2), yield in the case $\varphi(\lambda)=t\lambda$:

$$\dot{\rho}(\lambda) = \frac{C}{\sqrt{(b^2-\lambda^2)(\lambda^2-a^2)}} + \frac{P_2(\lambda)}{2\pi\sqrt{(b^2-\lambda^2)(\lambda^2-a^2)}}, \quad \lambda \in \sigma,$$

where $P_2(\lambda)=\lambda^2-(a^2+b^2)/2$,

$$C = \frac{tI_2}{2\pi I_1}, \tag{A8}$$

and

$$I_1 = \int_{-a}^{a} \frac{d\lambda}{\sqrt{(b^2-\lambda^2)(a^2-\lambda^2)}}, \quad I_2 = 2\int_{-a}^{a} \frac{P_2(\lambda) d\lambda}{\sqrt{(b^2-\lambda^2)(a^2-\lambda^2)}}. \tag{A9}$$

Now we can find $\dot{\beta}_1[\varphi]$ for $\varphi(\lambda)=t\lambda$. We have by (A8) and (A9),

$$\dot{\beta}_1 := \int_{a}^{b} \dot{\rho}(\lambda) d\lambda = \frac{t}{2\pi I_1}(I_2 J_1 - I_1 J_2), \tag{A10}$$

where

$$J_1 = \int_{a}^{b} \frac{d\lambda}{\sqrt{(b^2-\lambda^2)(\lambda^2-a^2)}}, \quad J_2 = \int_{a}^{b} \frac{P_2(\lambda) d\lambda}{\sqrt{(b^2-\lambda^2)(\lambda^2-a^2)}}.$$

By using standard formulas (see, e.g., Ref. 20, formulas (3.159)], we find

$$I_1 = 2K(k)/a, \quad I_2 = 2a\left(\frac{1-k^2}{2} K(k) - E(k) \right), \tag{A11}$$

$$J_1 = K(k')/a, \quad J_2 = a\left(E(k') - \frac{1+k^2}{2}K(k')\right), \tag{A12}$$

where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kind, $k=b/a, k'=\sqrt{1-k^2}$. These formulas and the identity $EK'+E'K-KK'=\pi/2$, where $K'=K(k'), E'=E(k')$ [Ref. 20, formula (8.122)] imply (3.16).

A more involved version of the above argument leads to (3.22). We note first that to prove the formula for a real analytic φ, it suffices to consider

$$\varphi_{z_0}(\lambda) = \frac{1}{\lambda - z_0}, \quad z_0 \notin \sigma.$$

We have in this case (see below)

$$\dot{\beta}_1[\varphi_{z_0}] = -\frac{1}{2I\sqrt{R_2(z_0)}}, \tag{A13}$$

where I is defined in (3.23).

Assuming that this formula is valid and using the Cauchy theorem to write

$$\varphi(\lambda) = \frac{1}{2\pi i}\int_{C_\sigma} \frac{\varphi(z_0)dz_0}{\lambda - z_0}, \quad \lambda \in \sigma,$$

where C_σ is the contour encircling σ in the clockwise direction; we obtain in view of the linearity of $\dot{\beta}_1[\varphi]$ in φ,

$$\dot{\beta}_1[\varphi] = \frac{1}{2\pi i}\int_{C_\sigma} \dot{\beta}_1[\varphi_{z_0}]\varphi(z_0)dz_0 = -\frac{1}{2I}\frac{1}{2\pi i}\int_{C_\sigma} \frac{\varphi(z_0)}{\sqrt{R_2(z_0)}}dz_0.$$

Now the relation $\sqrt{R_2(\lambda - i0)} = -\sqrt{R_2(\lambda + i0)}$ yields (3.22).

To prove (A13) we use the general formulas (A2), (A7), and (A6) with

$$\varphi'_{z_0}(\lambda) = -\frac{1}{(\lambda - z_0)^2} = -\frac{\partial}{\partial z_0}\frac{1}{\lambda - z_0}.$$

Arguing as in the case $\varphi(\lambda)=t\lambda$ above, we obtain an analog of (A10) whose denominator contains I of (3.23) instead of I_1 of (A9), and whose numerator is a bilinear combination of integrals of $|R_2(\mu)|^{-1/2}$ over $[a_2,b_2]$ and of derivatives with respect to z_0 of the integrals over $[b_1,a_2]$ and $[a_2,b_2]$ of $[(\mu - z_0)|R_2(\mu)|^{1/2}]^{-1}$ and $P_2(\mu)[(\mu - z_0)|R_2(\mu)|^{1/2}]^{-1}$, where P_2 is defined now by the relation $\sqrt{R_2(z)} = P_2(z) + O(1/z), z \to \infty$. These integrals can be expressed via the complete elliptic integrals of the first, second, and third kinds. Furthermore, the complete elliptic integrals of the third kind can be expressed via the incomplete elliptic integrals of the first and the second kinds, whose arguments depend on z_0. This allows us to obtain a formula for $\dot{\beta}_1[\varphi_{z_0}]$, whose numerator is expressed via the complete elliptic integrals of the first and the second kind and derivatives with respect to z_0 of the incomplete elliptic integrals of the first and the second kind. The derivatives are proportional to $(R_2(z_0))^{-1/2}$ [see Ref. 41, formulas (8.123)] This and a bit tedious algebra lead eventually to (A13).

Another derivation of (A13) is given in Ref. 8 (see formula (3.14) of the paper). The derivation is based on a two step procedure of the minimization of (2.3): the first step is the minimization over all unit measures with a given charge $\beta_1 \in (0,1)$ of the "band" $[a_2,b_2]$ of the support, and the second is the minimization of this minimum over β_1.

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Energy correlations for a random matrix model of disordered bosons

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Linearizing the Heisenberg equations of motion around the ground state of an interacting quantum many-body system, one gets a time-evolution generator in the positive cone of a real symplectic Lie algebra. The presence of disorder in the physical system determines a probability measure with support on this cone. The present paper analyzes a discrete family of such measures of exponential type, and does so in an attempt to capture, by a simple random matrix model, some generic statistical features of the characteristic frequencies of disordered bosonic quasiparticle systems. The level correlation functions of the said measures are shown to be those of a determinantal process, and the kernel of the process is expressed as a sum of biorthogonal polynomials. While the correlations in the bulk scaling limit are in accord with sine-kernel or Gaussian Unitary Ensemble universality, at the low-frequency end of the spectrum an unusual type of scaling behavior is found. [DOI: 10.1063/1.2356798]

I. INTRODUCTION

Perturbing the ground state of an interacting quantum many-body system and linearizing the Heisenberg equations of motion for the boson Fock operators, one faces the standard problem of small oscillations. Concrete examples are furnished by the vibrational modes of a solid, the spin waves in a magnet, the electromagnetic modes in an optical medium, and the oscillations of the superfluid density of a Bose–Einstein condensate. Common to these excitations is that they second-quantize as bosons or bosonic quasiparticles.

Adding some amount of disorder to the system, one may ask: what are the statistical features of the excitation spectrum and, in particular, which of these features (if any) reflect the bosonic nature of the quasiparticle excitations? Is there some kind of universality akin to the Wigner–Dyson universality known from other disordered systems? If so, what are the universal laws, and what is the role of symmetry in determining these laws?

In the parallel case of fermionic quasiparticles the situation is now fairly well understood. If the system is of metallic type and in the ergodic limit, the statistical behavior at high energies is in accord with the universal laws of Wigner–Dyson statistics. For low excitation energies, however, the canonical anticommutation relations obeyed by the fermion operators make themselves felt: they constrain the form of the Hamiltonian matrix and thus give rise to several new universality classes beyond Dyson's threefold way.[1] Some of these are realized by chiral Dirac fermions in a random gauge field,[2] others by quasiparticles in disordered gapless superconductors.[3,4] A

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complete symmetry classification of quadratic fermion Hamiltonians has been carried out,[5] and the role of Riemannian symmetric spaces and superspaces in providing an effective description has been emphasized.[6,7]

Progress has been slower for bosonic systems, and so for good reason, as these are set apart by several distinctive features from other random problems studied and solved in the past. For one thing, in the case of bosons it makes little sense to choose—as one often does for fermions—the matrix elements of the quasiparticle Hamiltonian as independent and identically distributed random variables. In fact, most of the boson Hamiltonians produced in such a manner would generate runaway dynamics rather than oscillatory motion around a stable ground state. In the case of bosons one therefore has to pay attention to the fact that the matrix elements depend in a complicated way on the ground state of the many-boson system and, hence, on the disorder of the microscopic parent problem.[8,9] As a technical consequence, a direct analog of the so-called Gaussian Ensembles, which were pivotal in initiating the Wigner–Dyson theory and establishing its universal statistics, is unavailable in the context of bosons.

For another complication, low-frequency bosons are usually insensitive to weak disorder. Many of the excitations listed above are Goldstone bosons associated with a spontaneously broken symmetry, and for such excitations low frequency is tantamount to low wave number, or large wavelength, which causes the scattering by disorder to be suppressed, as the disorder is effectively seen only on average over regions of size given by the large wavelength. Thus the disorder averages out and becomes less effective, and hence, the behavior of weakly disordered Goldstone bosons tends to be system specific. (Of course this still leaves it possible for weakly disordered bosons of *non*-Goldstone type to exhibit universal statistics.[8,9]) In order for any universality to set in, the disorder strength often has to be so large that standard calculational tools such as the impurity diagram technique fail to apply.

In the present paper we are going to introduce and completely solve a simple random matrix model of disordered bosonic quasiparticles, which we believe to be most closely analogous to the Wigner–Dyson Gaussian Ensembles while retaining the crucial features of bosonic statistics and stability of the motion. In a follow-up paper we will investigate the question whether this simple model might be representative of a whole universality class of related problems.

To formulate the model, let q_j, p_j $(j=1,\ldots,N)$ be a canonical set of position and momentum operators, and consider their linearized Heisenberg equations of motion in the most general form

$$\dot{q}_j = \sum_{i=1}^{N} (q_i A_{ij} + p_i C_{ij}), \qquad -\dot{p}_j = \sum_{i=1}^{N} (q_i B_{ij} + p_i A_{ji}),$$

where $B_{ij}=B_{ji}$, $C_{ij}=C_{ji}$, and A_{ij} are real numbers. If the system was invariant under time reversal $(q_j \mapsto q_j, p_j \mapsto -p_j)$, the coefficients A_{ij} would have to be zero, but we here consider the generic case without symmetries. The criterion for stability of the dynamics is that the stability matrix be positive

$$h := \begin{pmatrix} B & A \\ A^t & C \end{pmatrix} > 0.$$

Assuming $h^t=h>0$, the generator of the Heisenberg time evolution

$$X := \begin{pmatrix} A & -B \\ C & -A^t \end{pmatrix},$$

has eigenvalues that come as imaginary pairs $\pm i\omega_j$ where $\omega_j>0$ $(j=1,\ldots,N)$ are the characteristic frequencies (or single-boson energies) of the small-amplitude motion. In a classical setting one would introduce the generator X as the symplectic gradient of the Hamiltonian function linearized at a stable equilibrium point of the classical flow.

The natural transformation group of the problem at hand is the real symplectic group in $2N$ dimensions, $\mathrm{Sp}_{2N}(\mathbb{R})$, acting by linear canonical transformations on the operators q_j, p_j and by

conjugation on the generator X. We can now explain one of the distinctive features of the present problem: when formulating the Gaussian Ensembles of the Wigner–Dyson theory one makes the postulate that the transformation group of the problem (O_N, U_N, or USp_{2N}, as the case may be) also be the symmetry group of the chosen probability measure, whereas in our case no such simplification is possible. Indeed, $Sp_{2N}(\mathbb{R})$ is noncompact, and a probability measure $d\mu$ cannot be invariant under a noncompact group action and at the same time have total mass $\int d\mu = 1$.

One is therefore looking for some construction principle other than symmetry. Our key here is the positivity of the real symmetric stability matrix h: a natural way of building positive real symmetric matrices h is by adding a sufficient number of rank-one projectors with positive weights. Equivalently, we may put

$$h_{ij} = \sum_{\alpha=1}^{M} v_{i\alpha} v_{j\alpha} \quad (i,j = 1, \ldots, 2N) \tag{1.1}$$

for some set of real numbers $v_{i\alpha}$. We now consider the $v_{i\alpha}$ as the fundamental variables, and choose them to be independent and normal (or Gaussian) distributed random variables with zero mean and variance τ^{-1}. Then we use Eq. (1.1) to push forward the normal distribution for the $v_{i\alpha}$ to a probability distribution $d\mu(h)$ for h (and, hence, for X). If $M \geqslant 2N$, the result is

$$d\mu(h) \propto e^{-(1/2)\tau \mathrm{Tr} h} \mathrm{Det}(h)^{(1/2)(l-1)} \prod_{i \leqslant j} dh_{ij}, \quad l = M - 2N \geqslant 0, \tag{1.2}$$

with the domain for h still defined by $h > 0$. The probability distribution (1.2) is the object of study of this paper.

We now give a summary of the contents and the results of the paper. After collecting some basic facts from symplectic linear algebra in Sec. II, we reduce $d\mu(h)$ in Sec. III to a probability distribution on the space of characteristic frequencies $\omega_1, \ldots, \omega_N$ (the positive eigenvalues of $-iX$), and find this to be

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = c_{N,l}(\tau) \prod_{i<j} (\omega_i - \omega_j)(\omega_i^2 - \omega_j^2) \prod_{k=1}^{N} \omega_k^l e^{-r\omega_k} d\omega_k. \tag{1.3}$$

Using the method of biorthogonal polynomials we show in Sec. V C that the n-level correlation functions of this probability distribution are of determinant type and are completely determined in the usual way—see Eq. (5.19)—by a certain kernel $K_N(\omega, \tilde{\omega})$ given as a sum over biorthogonal polynomials. We compute the large-N asymptotics of this kernel in the bulk of the spectrum (in Sec. V D) and at the "hard" edge $\omega = 0$ (Sec. V E), using a contour integral representation of the biorthogonal polynomials (Sec. V C). In the former case we establish the scaling limit

$$\tau \lim_{N\to\infty} K_N(Nx/\tau + \omega, Nx/\tau + \tilde{\omega}) = \frac{\sin[\pi\rho_\infty(x)(\omega - \tilde{\omega})]}{\pi(\omega - \tilde{\omega})} e^{-r(x)(\omega - \tilde{\omega})}, \tag{1.4}$$

which is independent of l. The function $\rho_\infty(x)$ of the scaling variable $x = \omega\tau/N$ is the large-N limit of the level density. Viewing $\pi\rho_\infty(x)$ as the imaginary part of a Green's function $\lim_{\epsilon\to 0+} g(x + i\epsilon)$, the function $r(x)$ is the real part. We compute $\rho_\infty(x)$ by two independent methods (from a variational calculation in Sec. IV, and from biorthogonal polynomials in Sec. V D), with the result being

$$\rho_\infty(x) = \frac{\tau}{2\pi} (x/b)^{-1/3} [(1 + \sqrt{1 - x^2/b^2})^{1/3} - (1 - \sqrt{1 - x^2/b^2})^{1/3}] \quad (0 < x \leqslant b = 3\sqrt{3}). \tag{1.5}$$

Apart from the last factor, which is irrelevant since it cancels on passing to the level correlation functions, the right-hand side of Eq. (1.4) is the famous sine kernel known from systems with unitary symmetry. Thus we recover Wigner–Dyson universality of the class of the Gaussian Unitary Ensemble (GUE) at bulk frequencies.

At low frequencies $\omega \sim N^{-1/2}$ we find convergence to an unusual kind of scaling limit

$$\lim_{N\to\infty} N^{-1/2} K_N(N^{-1/2}y_1/\tau, N^{-1/2}y_2/\tau) = \frac{\tau^2}{2\pi^2}\int_{i\mathbb{R}+\epsilon} du \oint_{\mathrm{U}_1} \frac{dv}{v} e^{-y_1/u+y_2/v}(v/u)^l \frac{e^{u^2-v^2}-1}{u^2-v^2}, \tag{1.6}$$

where U_1 denotes the unit circle in $\mathbb{C}$, and $i\mathbb{R}+\epsilon$ is any axis in the right half plane parallel to the imaginary axis. The result (1.6) is reminiscent of formulas obtained by Efetov's supersymmetry method, with u and v playing the role of radial polar coordinates of a Riemannian symmetric superspace. We intend to elucidate this connection in a future publication.

II. THE HAMILTONIANS OF STABLE MOTIONS

Let there be some position variables $q_1, \ldots, q_N$ and canonical momenta $p_1, \ldots, p_N$, and consider Hamiltonians H of the quadratic form

$$H = \frac{1}{2}\sum_{i,j=1}^{N} [C_{ij}p_ip_j + B_{ij}q_iq_j + A_{ij}(q_ip_j + p_jq_i)], \tag{2.1}$$

where A, B, and C are real matrices satisfying $B=B^t$ and $C=C^t$. Rewriting H as

$$H = \frac{1}{2}(q\ p)\begin{pmatrix} A & -B \\ C & -A^t \end{pmatrix}\begin{pmatrix} p \\ -q \end{pmatrix},$$

we see that the matrix, X, of H satisfies the linear condition

$$X^tJ + JX = 0, \quad J = \begin{pmatrix} 0 & -1_N \\ 1_N & 0 \end{pmatrix}, \quad X = \begin{pmatrix} A & -B \\ C & -A^t \end{pmatrix}. \tag{2.2}$$

This is saying that X lies in $\mathfrak{sp}_{2N}(\mathbb{R})$, the Lie algebra of the real symplectic group defined by

$$\mathrm{Sp}_{2N}(\mathbb{R}) = \{g \in \mathrm{GL}_{2N}(\mathbb{R}) | g^tJg = J\}.$$

A matrix $X \in \mathfrak{sp}_{2N}(\mathbb{R})$ need not be diagonalizable (e.g., the generator of free motion, $A=B=0$ and $C=1_N$, is not); and even if it is, the eigenvalues will in general be complex.

We now impose the condition

$$h := \begin{pmatrix} B & A \\ A^t & C \end{pmatrix} > 0, \tag{2.3}$$

i.e., we require all eigenvalues of the real symmetric matrix h to be positive. The corresponding domain in $\mathfrak{sp}_{2N}(\mathbb{R})$ will be denoted by $\mathfrak{E}^0$:

$$\mathfrak{E}^0 := \{X \in \mathfrak{sp}_{2N}(\mathbb{R}) | X = hJ, h = h^t > 0\}. \tag{2.4}$$

Although the eigenvalues of h have no direct relation to the dynamics of the system, positivity of h ensures that the motion generated by the Hamiltonian H is stable, or "elliptic." As a consequence of ellipticity, there exists some linear canonical transformation $(\mathbf{q},\mathbf{p}) \to (\mathbf{Q},\mathbf{P})$ which takes the Hamiltonian to a sum of harmonic oscillators

$$H = \frac{1}{2}\sum_{i=1}^{N} (P_i^2 + \omega_i^2 Q_i^2),$$

with $\omega_i^2 > 0$. Put differently, for $X \in \mathfrak{E}^0$ one can always find a symplectic transformation $g \in \mathrm{Sp}_{2N}(\mathbb{R})$ that conjugates X to quasidiagonal form

$$X = g\Omega g^{-1}, \quad \Omega = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}, \quad \omega = \mathrm{diag}(\omega_1, \omega_2, \ldots, \omega_N), \tag{2.5}$$

with real and positive ω_i $(i=1,\ldots,N)$.

All of the discussion below will be based on the elliptic domain $\mathfrak{E}^0$. Let us therefore collect some of its mathematical properties. First of all, if X is in $\mathfrak{E}^0$, then so is its conjugate gXg^{-1} by any element $g \in \mathrm{Sp}_{2N}(\mathbb{R})$. Thus $\mathfrak{E}^0$ is invariant under the action of $\mathrm{Sp}_{2N}(\mathbb{R})$ on $\mathfrak{E}^0$ by conjugation. Second, let $\mathfrak{t}$ denote the Abelian algebra of block-diagonal matrices of the form of Ω in Eq. (2.5) but with diagonal elements ω_i that are any real numbers (not necessarily positive). Let $\mathfrak{t}_+ \subset \mathfrak{t}$ be the subset of block-diagonal Ω with positive ω_i. Then, as we said earlier, every $X \in \mathfrak{E}^0$ is conjugate to a unique $\Omega \in \mathfrak{t}_+$ by some $g \in \mathrm{Sp}_{2N}(\mathbb{R})$. Third, introducing $T := \exp(\mathfrak{t})$, which is an N-dimensional compact torus, $T \cong (S^1)^N$, let G/T be the quotient of $G \equiv \mathrm{Sp}_{2N}(\mathbb{R})$ by the right action of T. Then the mapping

$$(G/T) \times \mathfrak{t}_+ \to \mathfrak{E}^0, \quad (gT, \Omega) \mapsto g\Omega g^{-1} \tag{2.6}$$

(the reverse of the process of quasidiagonalization), is a smooth bijection.

We are stating these facts without proof, as they are standard facts of symplectic linear algebra.

III. PROBABILITY MEASURE

By placing a probability distribution on the elliptic domain $\mathfrak{E}^0$, one gets a random matrix model for disordered bosonic quasiparticles. We are then interested in the statistics of the characteristic frequencies or levels ω_i.

It is well known that in the Wigner–Dyson situation of random Hermitian or random real symmetric matrices, where the symmetry group is compact, the level correlation functions exhibit universal behavior in a suitable scaling limit. One may therefore ask whether a similar scenario—leading to universal laws, possibly of a new kind—might be at work in the case being considered.

To answer this question we need to investigate a class of probability distributions on $\mathfrak{E}^0$ as wide as possible. As a first step, the present paper deals with a family of well motivated distributions which are easy to analyze.

A. Choice of measure

Coming from the standard Wigner–Dyson situation with a compact symmetry group, one might be inclined to try and consider a Gaussian distribution

$$P(X)dX \overset{?}{\propto} e^{-\mathrm{Tr}X^2} dX,$$

where dX is a Lebesgue measure for $\mathfrak{E}^0$:

$$dX := \prod_{i,j} dA_{ij} \prod_{i \leqslant j} dB_{ij} dC_{ij}. \tag{3.1}$$

However, such a distribution has infinite mass, since it is invariant under the action $X \mapsto gXg^{-1}$ by the *noncompact* group $\mathrm{Sp}_{2N}(\mathbb{R})$, and it therefore cannot be normalized to be a probability measure.

Staying within the class of Gaussian distributions, a better choice of distribution function is

$$P(X = Jh) \propto e^{-\tau \mathrm{Tr}h/2 - \sigma \mathrm{Tr}h^2} = e^{-\tau \mathrm{Tr}(J^{-1}X)/2 - \sigma \mathrm{Tr}(J^{-1}X)^2} \tag{3.2}$$

for some positive parameters σ, τ. Because of the presence of J^{-1} under the trace, this distribution function is invariant under conjugation $X \mapsto gXg^{-1}$ only if $g \in \mathrm{Sp}_{2N}(\mathbb{R})$ satisfies the additional condition $g^{-1}Jg = J$. Combining the two conditions, $g^t Jg = J = g^{-1}Jg$, one sees that the invariance group of the function $P(X)$ in Eq. (3.2) is the intersection of the real symplectic and orthogonal groups in $2N$ dimensions

$$K = \mathrm{Sp}_{2N}(\mathbb{R}) \cap \mathrm{SO}_{2N}(\mathbb{R}). \tag{3.3}$$

This group K is isomorphic to U_N, the group of unitary transformations in N complex dimensions. Indeed, changing from the symplectic basis $\{q_1, \ldots, q_N, p_1, \ldots, p_N\}$ to the oscillator basis

$$\{a_1, \ldots, a_N, a_1^\dagger, \ldots, a_N^\dagger\}, \quad a_j = \frac{1}{\sqrt{2}}(q_j + ip_j), \quad a_j^\dagger = \frac{1}{\sqrt{2}}(q_j - ip_j),$$

one finds that K is the subgroup of canonical transformations that do not mix the lowering operators $\{a_j\}$ with the raising operators $\{a_j^\dagger\}$. Moreover, $\mathrm{U}_N \cong K \subset \mathrm{Sp}_{2N}(\mathbb{R})$ is known to be a maximal compact subgroup. It therefore is the biggest symmetry group possible in our problem.

In the sequel we will consider Eq. (3.2) with $\sigma = 0$. Thus we take our probability distribution to be

$$P(X)dX := c_N(\tau) e^{-\tau \mathrm{Tr}(J^{-1}X)/2} dX, \tag{3.4}$$

with the normalization constant $c_N(\tau)$ chosen in such a way that $\int_{\mathfrak{E}^0} P(X)dX = 1$. Further motivation for this choice of distribution was put forth in the introduction (Sec. I).

B. Polar decomposition and reduction

Let now $F(X) = F(gXg^{-1})$ be some function on $\mathfrak{E}^0$ which is *radial*, i.e., invariant under conjugation by every element $g \in \mathrm{Sp}_{2N}(\mathbb{R})$. Given such a function F, which depends only on the eigenfrequencies $\omega_1, \ldots, \omega_N$ of X, we wish to take the expectation of F with respect to the probability measure $P(X)dX$:

$$\langle F \rangle := \int_{\mathfrak{E}^0} F(X)P(X)dX. \tag{3.5}$$

The problem of computing such expectations is best tackled by using the polar decomposition $\mathfrak{E}^0 \cong \mathfrak{t}_+ \times (G/T)$ which is given by quasidiagonalization of X; see Eq. (2.6). Inserting that decomposition into Eq. (3.5) one has

$$\langle F \rangle = \int_{\mathfrak{t}_+} \left[\int_{G/T} P(g\Omega g^{-1}) dg_T \right] F(\Omega) j(\Omega) d\Omega, \quad d\Omega = d\omega_1 d\omega_2 \cdots d\omega_N, \tag{3.6}$$

where g_T is a G-invariant measure for G/T, and $j(\Omega)$ is the Jacobian of the change of variables $X = g\Omega g^{-1}$.

Let us calculate this Jacobian. Differentiating the polar coordinate mapping Eq. (2.6) we get

$$\delta(g\Omega g^{-1}) = g(\delta\Omega + [g^{-1}\delta g, \Omega])g^{-1}.$$

The Jacobian we are seeking is the product of all nonzero eigenvalues of the linear operator $X \mapsto [X, \Omega]$. These eigenvalues are called the roots of the pair $[\mathfrak{sp}_{2N}(\mathbb{R}), \mathfrak{t}]$. They are

$$\pm(\omega_i + \omega_j) \quad (i \leqslant j), \qquad \pm(\omega_i - \omega_j) \quad (i < j),$$

each with multiplicity one. Thus, by taking the product of all nonvanishing roots

$$j(\Omega)d\Omega = \prod_{i<j} (\omega_i^2 - \omega_j^2)^2 \prod_{k=1}^{N} (2\omega_k)^2 d\omega_k. \tag{3.7}$$

To complete the polar integration formula (3.6) we need $\int_{G/T} P(g\Omega g^{-1}) dg_T$. In the next subsection we are going to show that this integral can be calculated in closed form and depends on $\omega_1, \ldots, \omega_N$ as

$$\int_{G/T} P(g\Omega g^{-1})dg_T \propto \prod_{i<j}(\omega_i+\omega_j)^{-1}\prod_{k=1}^{N}\omega_k^{-1}e^{-\tau\omega_k}. \tag{3.8}$$

Thus, in total, the expectation of a radial observable $F(X)=F(\Omega)\equiv F(\omega_1,\ldots,\omega_N)$ becomes

$$\langle F\rangle = \tilde{c}_N(\tau)\int_{\mathbb{R}_+^N} F(\omega_1,\ldots,\omega_N)\prod_{i<j}(\omega_i-\omega_j)(\omega_i^2-\omega_j^2)\prod_{k=1}^{N}e^{-\tau\omega_k}\omega_k d\omega_k, \tag{3.9}$$

where $\tilde{c}_N(\tau)$ is another normalization constant. This expectation, for the special choices of F that give the level correlation functions, will be calculated in Sec. V of the paper.

C. Computation of the integral (3.8)

We now establish Eq. (3.8). Omitting a normalization constant, we denote the integral on the left-hand side of Eq. (3.8) by

$$I(\Omega) := \int_{G/T} e^{-\tau \mathrm{Tr}(J^{-1}g\Omega g^{-1})/2}dg_T. \tag{3.10}$$

What makes this integral computable in closed form is that J lies in $\mathfrak{sp}_{2N}(\mathbb{R})$ and $\Omega\mapsto g\Omega g^{-1}$ is the adjoint action of $G=\mathrm{Sp}_{2N}(\mathbb{R})$ on its Lie algebra. These circumstances place the integral in the class of integrals of Harish–Chandra–Itzykson–Zuber type, which are covered by the Duistermaat–Heckman theorem and its generalizations. In the present case, the integral can be computed in a particularly simple manner, as follows.

Let dg and dt be Haar measures for G and T, respectively, with $dg=dg_T dt$ and $\int_T dt=\mathrm{vol}(T)$. Our first step is to switch from G/T to integrating over the full symplectic group G:

$$I(\Omega)=\frac{1}{\mathrm{vol}(T)}\int_G e^{-\tau \mathrm{Tr}(J^{-1}g\Omega g^{-1})/2}dg.$$

Next we use that dg is invariant under inversion, $g\mapsto g^{-1}$. After this transformation the integrand is expressed in terms of the combination $gJ^{-1}g^{-1}=-gJg^{-1}$. Since $kJk^{-1}=J$ for $k\in K\cong \mathrm{U}_N$, we can push down the resulting integral over G to an integral over the quotient space G/K. Let dg_K and dk be invariant resp. Haar measures for G/K and K so that $dg=dg_K dk$. Then

$$I(\Omega)=\frac{\mathrm{vol}(K)}{\mathrm{vol}(T)}\int_{G/K} e^{\tau \mathrm{Tr}(\Omega gJg^{-1})/2}dg_K, \quad \mathrm{vol}(K)=\int_K dk. \tag{3.11}$$

The homogeneous space $G/K\cong \mathrm{Sp}_{2N}(\mathbb{R})/\mathrm{U}_N$ has the salient feature of being a noncompact symmetric space of Hermitian type. Such spaces carry the structure of a Kähler manifold, which means that G/K comes with a non-degenerate, closed, and G-invariant two-form (the Kähler form of G/K). Writing $gJg^{-1}=:Q$ this is the form

$$\beta=\mathrm{Tr}(Q\mathrm{d}Q\wedge \mathrm{d}Q). \tag{3.12}$$

Notice that $\dim_{\mathbb{R}} G/K=N(2N+1)-N^2=N(N+1)$. Raising β to its $(1/2)N(N+1)$th exterior power one obtains a top-dimensional form, $\beta^{(1/2)N(N+1)}$, which is still G-invariant and nonzero. Since G/K is homogeneous, there can be at most one such form up to multiplication by scalars. Therefore, there exists some (nonzero) constant such that

$$dg_K=\mathrm{const}\,\beta^{(1/2)N(N+1)}. \tag{3.13}$$

By Darboux's theorem one can find local symplectic coordinates for G/K that bring β into canonical form. While this fact by itself would not be of much practical help, in the present case such coordinates exist *globally* and, moreover, they can be chosen in such a way that $\mathrm{Tr}(\Omega gJg^{-1})$

depends on them *quadratically*.

To describe these perfect coordinates, consider the space of complex symmetric $N\times N$ matrices, $\mathrm{Sym}(\mathbb{C}^N)$, which has dimension $(1/2)N(N+1)$ over $\mathbb{C}$ and thus shares with G/K the dimension $N(N+1)$ over $\mathbb{R}$. With every $Z\in\mathrm{Sym}(\mathbb{C}^N)$ associate a positive Hermitian $2N\times 2N$ matrix $\tilde{g}$ by

$$\tilde{g}=\tilde{g}(Z,Z^\dagger)=\begin{pmatrix}(1+ZZ^\dagger)^{1/2} & Z\\ Z^\dagger & (1+Z^\dagger Z)^{1/2}\end{pmatrix}. \tag{3.14}$$

Now if S is the matrix of the unitary transformation from the real symplectic basis $\{p_j,q_j\}$ of $\mathbb{R}^{2N}$ to the oscillator basis $\{a_j,a_j^\dagger\}$:

$$S:=\frac{1}{\sqrt{2}}\begin{pmatrix}1_N & i1_N\\ -1_N & i1_N\end{pmatrix},$$

then $g:=S^{-1}\tilde{g}S$ is immediately seen to be a real matrix and, using the relation

$$SJS^{-1}=i\Sigma_3,\quad \Sigma_3=\begin{pmatrix}1_N & 0\\ 0 & -1_N\end{pmatrix},$$

one finds that $g=S^{-1}\tilde{g}S$ satisfies $g^\dagger Jg=g^tJg=J$ and hence lies in $\mathrm{Sp}_{2N}(\mathbb{R})$. Moreover, the reverse correspondence $k\mapsto\tilde{k}=SkS^{-1}$ is the isomorphism between K and U_N discussed in the paragraph after Eq. (3.3); it takes $k\in K$ to the block-diagonal form

$$\tilde{k}=\begin{pmatrix}U & 0\\ 0 & \bar{U}\end{pmatrix},\quad U\in\mathrm{U}_N.$$

It is now clear that the mapping $\mathrm{Sym}(\mathbb{C}^N)\to G/K$ by $Z\mapsto S^{-1}\tilde{g}(Z,Z^\dagger)SK\equiv gK$ is a bijection. Using it to express the Kähler form β in terms of the complex symmetric matrix Z, one obtains

$$\beta=\mathrm{Tr}(Q\mathrm{d}Q\wedge\mathrm{d}Q)=-4i\mathrm{Tr}(\Sigma_3\mathrm{d}\tilde{g}^{-1}\wedge\mathrm{d}\tilde{g})=8i\mathrm{Tr}(\mathrm{d}Z\wedge\mathrm{d}Z^\dagger). \tag{3.15}$$

Thus, the top-dimensional form $\beta^{(1/2)N(N+1)}$ is constant in Z:

$$\frac{\beta^{(1/2)N(N+1)}}{\left[\frac{1}{2}N(N+1)\right]!}=(8i)^{(1/2)N(N+1)}2^{(1/2)N(N-1)}\prod_{i\leqslant j}dZ_{ij}\wedge d\bar{Z}_{ij}, \tag{3.16}$$

and from Eq. (3.13) the invariant measure dg_K is a constant multiple of the Lebesgue measure for $\mathrm{Sym}(\mathbb{C}^N)$.

Finally, from $g=S^{-1}\tilde{g}S$, $SJS^{-1}=\mathrm{i}\Sigma_3$, and Eq. (3.14) one has

$$-\mathrm{Tr}(\Omega gJg^{-1})=\mathrm{Tr}\omega(1+2ZZ^\dagger)+\mathrm{Tr}\omega(1+2Z^\dagger Z),\quad \omega=\mathrm{diag}(\omega_1,\ldots,\omega_N).$$

Our integral (3.11) now becomes a Gaussian integral

$$I(\Omega)=\mathrm{const}\,e^{-\tau\Sigma_k\omega_k}\int e^{-2\tau\mathrm{Tr}Z^\dagger(Z\omega+\omega Z)}\prod_{i\leqslant j}dZ_{ij}d\bar{Z}_{ij}.$$

Doing this integral one immediately obtains the result for $I(\Omega)$ stated in Eq. (3.8).

D. Generalization

A slight generalization of Eq. (3.4) is afforded by the observation that the determinant of X in Eq. (2.2) is always positive:

$$\mathrm{Det}(X) = \mathrm{Det}(\Omega) = \prod_{k=1}^{N} \omega_k^2.$$

Thus, by multiplying the probability measure $P(X)dX$ by some power $l-1>-1$ of the positive square root $\mathrm{Det}(X)^{1/2}$ and adjusting the normalization constant, we get another probability measure

$$P_l(X)dX = \text{const}\ \mathrm{Det}(X)^{(1/2)(l-1)} e^{-(1/2)\tau \mathrm{Tr}(J^{-1}X)} dX. \tag{3.17}$$

This measure is still U_N invariant. By the process of quasidiagonalization and drawing on our results above, we push it forward to a measure for the eigenfrequencies. The result is

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = c_{N,l}(\tau) \prod_{i<j} (\omega_i - \omega_j)^2 (\omega_i + \omega_j) \prod_{k=1}^{N} \omega_k^l e^{-\tau\omega_k} d\omega_k. \tag{3.18}$$

This, for any non-negative power $l \in \mathbb{Z}$, is the family of probability distributions to be studied in the present paper.

IV. LARGE-*N* LIMIT OF THE ONE-POINT DENSITY IN THE BULK

The one-point density $\rho(\omega)d\omega$ is defined as the probability density for any one of the eigenfrequencies ω_i to have the value of ω, irrespective of what the values of the other eigenfrequencies are; thus $\rho(\omega)$ is the function

$$\rho(\omega) := \int \sum_{i=1}^{N} \delta(\omega - \omega_i) d\mu_{N,l}(\omega_1, \ldots, \omega_N), \tag{4.1}$$

which has the properties $\rho(\omega) \geqslant 0$ and

$$\int_0^\infty \rho(\omega) d\omega = N. \tag{4.2}$$

We are now interested in the behavior of the density function $\rho(\omega)$ in the limit of $N \to \infty$. From the expression (3.18) and experience with similar problems (see, e.g., Ref. 11), we expect that this limit can be obtained by maximizing the functional

$$F = \frac{1}{2} \int_0^\infty \int_0^\infty \ln[(\omega - \omega')^2(\omega + \omega')] \rho(\omega)\rho(\omega') d\omega' d\omega + \int_0^\infty \ln(\omega^l e^{-\omega\tau}) \rho(\omega) d\omega \tag{4.3}$$

subject to the constraint (4.2) and the condition $\rho(\omega) \geqslant 0$. More precisely, the limit is expected to exist in the scaled variable $x := \omega\tau/N$; i.e., there should exist a certain non-negative function $\rho_\infty(x)$ with $\int \rho_\infty(x)dx = 1$ such that $\rho(\omega)$ is asymptotic to $\tau\rho_\infty(\omega\tau/N)$.

Varying F with respect to $\rho(\omega)$ we get

$$\frac{\delta F}{\delta \rho(\omega)} = \int_0^\infty [2 \ln|\omega - \omega'| + \ln(\omega + \omega')] \rho(\omega') d\omega' + l \ln \omega - \omega\tau.$$

We now insert the asymptotic equality $\rho(Nx/\tau) \approx \tau\rho_\infty(x)$ and pass to the limit $N \to \infty$ in the scaling variable x. Let $\mathrm{supp}(\rho_\infty) = [0, b]$ be the region of support of ρ_∞. Then the condition $\delta F / \delta \rho(\omega) = N\lambda$, where λ is a Lagrange multiplier for the constraint (4.2), yields the equation

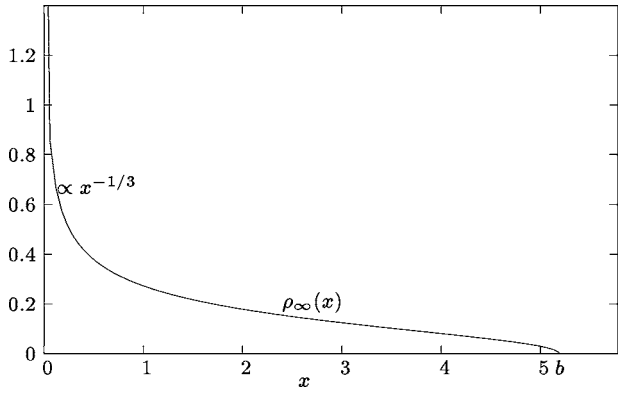

FIG. 1. The graph of the function ρ_∞.

$$\int_0^b [2\ln|x-x'|+\ln(x+x')]\rho_\infty(x')dx' - x = \lambda \quad (0<x<b), \tag{4.4}$$

which no longer depends on the parameter l. It can be shown that our functional F is convex; as a result, the solution ρ_∞ of Eq. (4.4) exists and is unique when supplemented by the normalization condition

$$\int_0^b \rho_\infty(x)dx = 1. \tag{4.5}$$

In the following subsections, we are going to construct the solution to the mathematical problem posed by Eqs. (4.4) and (4.5). It will turn out to be

$$\rho_\infty(x) = \frac{1}{2\pi}(x/b)^{-1/3}[(1+\sqrt{1-x^2/b^2})^{1/3} - (1-\sqrt{1-x^2/b^2})^{1/3}] \quad (0<x\leqslant b=3\sqrt{3}). \tag{4.6}$$

The graph of this function is plotted in Fig. 1. From the expression (4.6) the behavior near the lower edge $x=0$ is

$$\rho_\infty(x) \simeq \frac{1}{2\pi}(2b/x)^{1/3} \quad (0<x\ll b),$$

while close to the upper edge $x=b$ one gets

$$\rho_\infty(x) \simeq \frac{1}{3\pi}(1-x^2/b^2)^{1/2} \quad (x<b,\ x\to b).$$

In the vicinity of the upper and lower edges there exists crossover to a fine-scale behavior that cannot be found by the present method of maximization of the functional F. The crossover at the upper edge involves Airy functions on a scale $N^{1/3}$, which is small compared to the bulk scale N. At the lower edge, the crossover occurs on a very fine scale, $N^{-1/2}$, which is small even in comparison with the bulk mean level spacing (which is of order N^0).

A. Method of solution (idea)

We do not know how to solve Eq. (4.4) for the unknown function $\rho_\infty(x)$ directly. Therefore, to simplify the problem we differentiate once with respect to x to obtain the equation

$$2\mathcal{P}\int_0^b \frac{\rho_\infty(x')dx'}{x-x'} + \int_0^b \frac{\rho_\infty(x')dx'}{x+x'} = 1, \tag{4.7}$$

where $\mathcal{P}$ means the principal value of the integral. At this stage, the value of b is unknown but assumed to be finite.

Introducing the Green's function (or Stieltjes transform)

$$g(z) := \int_0^b \frac{\rho(x)dx}{x-z}, \quad z \in \mathbb{C}\backslash[0,b], \tag{4.8}$$

and the related functions

$$g_\pm(x) := \lim_{\varepsilon\to 0+} g(x \pm i\varepsilon), \quad g_0(x) := -g(-x), \tag{4.9}$$

we bring Eq. (4.7) into the form

$$g_+(x) + g_-(x) + g_0(x) = -1 \quad (0 < x < b). \tag{4.10}$$

To solve this equation, we are led to do an exercise in complex analysis which is motivated as follows.

Let $w \mapsto f(w)$ be some meromorphic function of a complex variable w, and let the equation $z=f(w)$ have r simple roots $w_1(z), w_2(z), \ldots, w_r(z)$, i.e., $z=f[w_1(z)]=\ldots=f[w_r(z)]$. If the function f is analytic in $1/w$ at $w=\infty$, these roots add up to a constant

$$\sum_{i=1}^{r} w_i(z) = \text{const} =: c \quad (\text{independent of } z). \tag{4.11}$$

Indeed, if γ is a closed contour encircling all of the roots in the counterclockwise sense, then

$$\sum w_i'(z) = \sum \frac{1}{f'[w_i(z)]} = \frac{1}{2\pi i}\oint_\gamma \frac{dw}{f(w)-z} = 0,$$

where the second equality is by the residue theorem, and the last equality follows by contracting γ to the point at infinity. Thus $\Sigma w_i'(z)=0$ and, hence, $\Sigma w_i(z)=$const.

Equation (4.11) for $r=3$ looks similar to Eq. (4.10) and can, in fact, be made to look identical to it by the following observation. Notice that the function $z \mapsto g(z)$ defined by Eq. (4.8) is holomorphic in the interior of the left half of the complex plane. Suppose, therefore, that we have found a root $g(z)$ of $z=f[g(z)]$ which is holomorphic in the left half plane, and that $g_\pm(x) = \lim_{\varepsilon\to 0+} g(x\pm i\varepsilon)$ are its two analytic continuations to positive real $x \in (0,b)$. Moreover, suppose that the function f has a reflection symmetry

$$f(w) = -f(2a-w) \quad (a \in \mathbb{C}). \tag{4.12}$$

Then $z \mapsto 2a-g(-z)$ is a root of $z=f(w)$ holomorphic in the right half plane, and from Eq. (4.11) we infer that

$$g_+(x) + g_-(x) + [2a - g(-x)] = c.$$

Setting $g_0(x) \equiv -g(-x)$ this becomes the same as Eq. (4.10) if

$$c - 2a = -1. \tag{4.13}$$

Thus we are inspired to interpret g_+, g_-, and $2a+g_0$ as the three roots of an equation $z=f(w)$. Given this interpretation, solving Eq. (4.10) amounts to finding the function f.

B. The good function *f* to consider

We are looking for a certain meromorphic function f on $\mathbb{C}$. By adding a point at infinity we can view such a function f as a mapping of the Riemann sphere $S^2=\mathbb{C}\cup\{\infty\}$ to itself. We want this mapping to have degree $r=3$; i.e., every regular point z of f is to have three distinct preimages

$$f^{-1}(z)=\{w_1(z),w_2(z),w_3(z)\}.$$

Such a mapping can be presented in the general form

$$f(\omega)=f_\infty+\sum_{i=1}^{3}\frac{b_i}{w-a_i} \tag{4.14}$$

with some complex numbers a_i, b_i, and f_∞.

Let us narrow down the choice of parameters. From the normalization condition (4.5) and the definition of $g(z)$ in Eq. (4.8), we have the limit $zg(z)\to -1$ for $z\to\infty$. Therefore, since $f[g(z)]=z$ by construction, we need $f(w)$ to have a pole at $w=g(\infty)=0$ with residue -1. So we choose $a_1=0$ and $b_1=-1$. The reflection symmetry (4.12) is then implemented by setting $f_\infty=0$, $b_3=b_1$, and $a_i=(i-1)\ a$ for $i=1,2,3$ and some $a\in\mathbb{C}$. Thus

$$f(w)=-\frac{1}{w}+\frac{b_2}{w-a}-\frac{1}{w-2a},$$

where the parameters a and b_2 are still unknown.

Next observe that for a degree-r holomorphic mapping f: $S^2\to S^2$, the number of singular points, where $f'(w)=0$, is $2r-2$. Indeed, writing f as $f(w)=p(w)/q(w)$ where p and q are polynomials of degree r, one has

$$f'(w)=\frac{p'(w)q(w)-p(w)q'(w)}{q(w)^2},$$

the numerator of which is a polynomial of degree $2r-2$ and so has $2r-2$ zeros.

Thus we should expect our function (4.14) to have $2\times 3-2=4$ singular points. The reflection symmetry (4.12) makes for their images $\{f(w)\in\mathbb{C}\,|\,f'(w)=0\}$ to be arranged symmetrically around $z=0$. Now notice that our Green's function $g(z)$, being the Stieltjes transform of $\rho_\infty(x)$ with support $[0,b]$, must have singularities at $z=0$ and $z=b$. The image of the singular set had better contain these values, and thus is determined to be $\{-b,0,+b\}$ by reflection symmetry. Actually, since our situation calls for f to have four singular points, the singularity at $z=0$ (corresponding to $w=\infty$) must have multiplicity two. This is achieved by choosing $b_2=-b_1-b_3=+2$, so that

$$f(w)=-\frac{1}{w}+\frac{2}{w-a}-\frac{1}{w-2a}=\frac{-2a^2}{w(w-a)(w-2a)},$$

resulting in the behavior $f(w)\sim w^{-3}$ for $w\to\infty$. The singular points of f now are $w=a\pm a/\sqrt{3}$, and ∞. These correspond to $z=f(w)=\pm 3\sqrt{3}/a$, and 0, respectively, so we infer

$$b=3\sqrt{3}/|a|. \tag{4.15}$$

It remains to pin down the last unknown parameter a. For that purpose, recall that the sum of the roots $f^{-1}(z)=\{w_1(z),w_2(z),w_3(z)\}$ is a constant, c, independent of z. To determine this constant, look at $\Sigma w_i(\infty)$ and use that the poles of f are at $w=0$, a, $2a$ to obtain

$$c=\Sigma w_i(z)=\Sigma w_i(\infty)=3a. \tag{4.16}$$

We then conclude $a=-1$ from Eq. (4.13), and $b=3\sqrt{3}$ from Eq. (4.15). In summary, the good meromorphic function f for us to consider is

$$w \mapsto f(w) = \frac{-2}{w(w+1)(w+2)}. \tag{4.17}$$

Let us mention in passing that the idea to consider the equation $z=f(w)$ or, equivalently

$$w(w+1)(w+2) + 2/z = 0,$$

first came to one of us (H.-J.S.) from previous work[10] on the Green's function of the Bures measure, whose large-N limit leads to a similar equation.

C. Solution of the problem

The situation can now be succinctly described like this: thinking of

$$W := \mathbb{C}\setminus\{-1+1/\sqrt{3}, -1-1/\sqrt{3}\}, \quad Z := (\mathbb{C}\setminus\{b,0,-b\}) \cup \{\infty\} \quad (b = 3\sqrt{3}),$$

as two Riemann surfaces W and Z, the function f of Eq. (4.17) gives us a holomorphic cover

$$f: W \to Z, \quad f^{-1}(z) = \{w_1(z), w_2(z), w_3(z)\}.$$

What is the monodromy of this cover, i.e., what happens when the locally defined functions $z \mapsto w_i(z)$ are analytically continued around one of the singular points $z=b,0,-b$? At the point $z=0$ (or $w=\infty$) we have a cubic singularity $z \sim w^{-3}$. Consequently, the monodromy at $z=0$ cyclically permutes the roots $w_i(z)$. Turning to $z=\pm b$, we see that linearization $z=\pm b+\delta z$ and $w=f^{-1}(\pm b)+\delta w$ gives

$$\delta z \sim (\delta w)^2.$$

In the latter two cases the monodromy must exchange two of the $w_i(z)$ while leaving the third one invariant.

Now focus on the situation near the singular point $z=-b$ and denote by $w(z) \equiv g(z)$ the root which, there, is trivial under monodromy and, hence, exists as a holomorphic function in some neighborhood of $z=-b$. With the remaining two singularities being at $z=0$ and $z=b$, the function $g(z)$ actually extends to a holomorphic function on the Riemann sphere $\mathbb{C}\cup\{\infty\}$ cut along, say, $[0,b] \subset \mathbb{R}$. Let us verify that this holomorphic function $g: (\mathbb{C}\setminus[0,b]) \cup \{\infty\} \to W$ coincides with the Green's function (4.8) solving our problem (4.10).

By the holomorphic nature of g and Cauchy's theorem, we have that

$$g(z) = \frac{1}{2\pi i} \oint_{\gamma} \frac{g(z')dz'}{z'-z},$$

where γ is a small loop running around z in the counterclockwise sense. Since g is holomorphic at infinity, the loop γ can be deformed (through infinity) to a loop encircling the cut $[0,b]$, but now with the orientation reversed. Collapse the deformed loop to the two line segments connecting 0 with b. Then, setting $g_{\pm}(x) = \lim_{\varepsilon \to 0+} g(x \pm i\varepsilon)$ and

$$\rho_{\infty}(x) := \frac{g_+(x) - g_-(x)}{2\pi i} \quad (0 < x < b), \tag{4.18}$$

$g(z)$ is obviously given by the integral in Eq. (4.8).

Because $g_+(x)$ and $g_-(x)$ arise by analytic continuation from $g(z) \in f^{-1}(z)$, these are two of the three elements in the set $f^{-1}(x)$. How is the third element of $f^{-1}(x)$ related to $g(z)$? To see that, recall $a=-1$ and from Eq. (4.12) the invariance of the equation $z=f(w)$ under $(z,w) \mapsto (-z, 2a-w)$. Thus, if $g(-z)$ is a root over $-z$, then $-2-g(-z)$ is a root over z, and it follows that $g_0(x)-2$ with $g_0(x) := -g(-x)$ (for $0<x<b$) is a root over x. The roots $g_+(x)$, $g_-(x)$, and $g_0(x)-2$ all are different as functions. In fact, $\Im\mathrm{m}\, g_+(x) > 0 = \Im\mathrm{m}\, g_0(x) > \Im\mathrm{m}\, g_-(x)$ for $0<x<b$. So,

$$f^{-1}(x) = \{g_+(x), g_-(x), g_0(x) - 2\},$$

and from Eq. (4.16) we deduce that

$$g_+(x) + g_-(x) + g_0(x) - 2 = \sum_{w \in f^{-1}(x)} w = c = 3a = -3 \quad (0 < x < b),$$

which agrees with Eq. (4.10). Recall that in order for our analysis to work out we must choose

$$b = 3\sqrt{3}. \tag{4.19}$$

With a full understanding of the situation in hand, it is now an easy exercise to obtain $\rho_\infty(x)$ in explicit form. Solving the equation $z=f(w)$ one finds the holomorphic function $g(z)$ in the interval $-b<x<0$ to be

$$g(x) = (-x)^{-1/3}(1 + \sqrt{1 - x^2/b^2})^{1/3} + (-x)^{-1/3}(1 - \sqrt{1 - x^2/b^2})^{1/3} - 1,$$

where all square roots and cubic roots are understood to be positive. This function indeed extends holomorphically to a neighborhood of $x=-b$, as the Taylor expansion at $x=-b$ contains only even powers of $\sqrt{1-x^2/b^2}$. Analytic continuation around the singularity at $z=0$ gives

$$g_\pm(x) = x^{-1/3}e^{\pm \pi i/3}(1 + \sqrt{1 - x^2/b^2})^{1/3} + x^{-1/3}e^{\mp \pi i/3}(1 - \sqrt{1 - x^2/b^2})^{1/3} - 1 \quad (0 < x \leqslant b).$$

Computing the difference (4.18) we then get the result for $\rho_\infty(x)$ claimed in Eq. (4.6), with the value for b given by Eq. (4.19).

As a final remark, let us note that the good form of $g(z)$ to use near infinity is

$$g(z) = -1 + e^{i\pi/6}\left(\sqrt{\frac{1}{b^2} - \frac{1}{z^2}} + \frac{i}{z}\right)^{1/3} + e^{-i\pi/6}\left(\sqrt{\frac{1}{b^2} - \frac{1}{z^2}} - \frac{i}{z}\right)^{1/3}. \tag{4.20}$$

From this, all moments of $\rho_\infty(x)dx$ can be found by expanding $g(z)$ in powers of $1/z$.

V. EXACT SOLUTION USING BIORTHOGONAL POLYNOMIALS

We now express the probability measure (3.18) as

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = c_{N,l}(\tau)\prod_{i<j}(\omega_i - \omega_j)(\omega_i^2 - \omega_j^2)\prod_{k=1}^{N} e^{-\tau\omega_k}\omega_k^l d\omega_k, \tag{5.1}$$

and embark on another approach to handling it.

To get started, recall the formula for the Vandermonde determinant

$$\prod_{i>j}(\omega_i - \omega_j) = \mathrm{Det}(\omega_j^{i-1})_{i,j=1,\ldots,N} = \begin{vmatrix} 1 & 1 & \cdots & 1 \\ \omega_1 & \omega_2 & \cdots & \omega_N \\ \vdots & \vdots & \ddots & \vdots \\ \omega_1^{N-1} & \omega_2^{N-1} & \cdots & \omega_N^{N-1} \end{vmatrix}.$$

Using it we reorganize the probability measure (5.1) as

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = c_{N,l}(\tau)\mathrm{Det}(\omega_j^{i-1})\mathrm{Det}(\omega_j^{2i-2})\prod_{k=1}^{N} e^{-\tau\omega_k}\omega_k^l d\omega_k. \tag{5.2}$$

We also simplify our notation by setting $\tau=1$.

By standard properties of the determinant, $\mathrm{Det}(\omega_j^{i-1})$ changes only by a multiplicative constant when the monomials ω_j^{i-1} are replaced by any polynomials in ω_j of degree $i-1$. We have two

Vandermonde determinants, $\Pi_{i<j}(\omega_i-\omega_j)$ and $\Pi_{i<j}(\omega_i^2-\omega_j^2)$, so we introduce two sets of polynomials, denoting those of the first set by $P_{i-1}(\omega_j)$ and those of the second one by $Q_{i-1}(\omega_j^2)$. Our measure then becomes

$$d\mu_{N,l}(\omega_1,\ldots,\omega_N)=\tilde{c}_{N,l}\mathrm{Det}[P_{i-1}(\omega_j)]\mathrm{Det}[Q_{i-1}(\omega_j^2)]\prod_{k=1}^{N}e^{-\omega_k}\omega_k^l d\omega_k. \tag{5.3}$$

In order for the introduction of the polynomials $P_n(\omega)$ and $Q_n(\omega^2)$ to be useful we require them to be orthogonal with respect to the integration measure $e^{-\omega}\omega^l d\omega$:

$$I_{m,n}\equiv\int_0^\infty P_m(\omega)Q_n(\omega^2)e^{-\omega}\omega^l d\omega=h_n\delta_{m,n}, \tag{5.4}$$

where the numbers $h_n=I_{n,n}$ depend on the choice of normalization for $P_n(\omega)$ and $Q_n(\omega^2)$. Such polynomials are constructed by a variant of the Gram–Schmidt algorithm, as follows.

A. Biorthogonal polynomials

We review the construction in the general setting of two real vector spaces V, W with a pairing (or nondegenerate bilinear form)

$$\gamma: V\times W\to\mathbb{R}.$$

Given some basis $v_0,v_1,v_2,\ldots$ of V, and a basis $w_0,w_1,w_2,\ldots$ of W, let the entries of the corresponding pairing matrix be denoted by

$$\gamma_{m,n}:=\gamma(v_m,w_n)\quad(m,n=0,1,2,\ldots).$$

The goal now is to construct a new basis $e_0,e_1,e_2,\ldots$ of V, and a new basis $f_0,f_1,f_2,\ldots$ of W such that

$$e_n=v_n+\sum_{n'=0}^{n-1}A_{nn'}v_{n'},\quad f_n=w_n+\sum_{n'=0}^{n-1}B_{nn'}w_{n'},$$

(with real coefficients $A_{nn'}$ and $B_{nn'}$), and the transformed basis vectors form a biorthogonal system

$$\gamma(e_m,f_n)=0\quad m\neq n.$$

This problem has a unique solution by the process of Gram–Schmidt orthogonalization. A nice way of presenting the solution is by means of the following determinants (where, by a slight abuse of notation, the matrix entries in the last column resp. last row are vectors, whereas all of the other matrix entries are numbers)

$$e_n=D_{n-1}^{-1}\begin{vmatrix}\gamma_{0,0}&\cdots&\gamma_{0,n-1}&v_0\\ \gamma_{1,0}&\cdots&\gamma_{1,n-1}&v_1\\ \vdots&\ddots&\vdots&\vdots\\ \gamma_{n,0}&\cdots&\gamma_{n,n-1}&v_n\end{vmatrix},\quad f_n=D_{n-1}^{-1}\begin{vmatrix}\gamma_{0,0}&\gamma_{0,1}&\cdots&\gamma_{0,n}\\ \vdots&\vdots&\ddots&\vdots\\ \gamma_{n-1,0}&\gamma_{n-1,1}&\cdots&\gamma_{n-1,n}\\ w_0&w_1&\cdots&w_n\end{vmatrix}\quad(n=1,2,\ldots), \tag{5.5}$$

with normalization factor

$$D_n=\begin{vmatrix}\gamma_{0,0}&\cdots&\gamma_{0,n}\\ \vdots&\ddots&\vdots\\ \gamma_{n,0}&\cdots&\gamma_{n,n}\end{vmatrix}.$$

These formulas are easily verified. Indeed, pairing e_m with w_n for $m>n$ one gets

$$\gamma(e_m,w_n)=D_{m-1}^{-1}\begin{vmatrix}\gamma_{0,0} & \cdots & \gamma_{0,m-1} & \gamma_{0,n}\\ \gamma_{1,0} & \cdots & \gamma_{1,m-1} & \gamma_{1,n}\\ \vdots & \ddots & \vdots & \vdots\\ \gamma_{m,0} & \cdots & \gamma_{m,m-1} & \gamma_{m,n}\end{vmatrix}=0,$$

which vanishes because the last column coincides with one of the other columns. Since f_n is a linear combination of the vectors $w_{n'}$ with $n'\leqslant n$, it follows that $\gamma(e_m,f_n)=0$ for $m>n$. The same conclusion for $m<n$ follows by reversing the roles of V and W. Notice that $e_n=1v_n+\ldots$ and $f_n=1w_n+\ldots$ by insertion of the factor D_{n-1}^{-1}. The nonvanishing pairing matrix elements for $n\geqslant 1$ are $\gamma_{n,n}=\gamma(e_n,f_n)=\gamma(e_n,w_n)=D_n/D_{n-1}$.

To apply these general formulas to the case under consideration, we choose the vectors v_m and w_n to be the functions $\omega\mapsto\omega^m$ resp. $\omega\mapsto\omega^{2n}$, and take the pairing to be given by integration with our measure $e^{-\omega}\omega^l d\omega$:

$$\gamma_{m,n}=\int_0^\infty \omega^{m+2n}e^{-\omega}\omega^l d\omega=\Gamma(m+2n+l+1). \tag{5.6}$$

Making the identification $e_n\equiv P_n(\omega)$, the general formula for e_n in Eq. (5.5) then gives $P_0(\omega)=1$ and

$$P_n(\omega)=D_{n-1}^{-1}\begin{vmatrix}\Gamma(l+1) & \cdots & \Gamma(l+2n-1) & \omega^0\\ \Gamma(l+2) & \cdots & \Gamma(l+2n) & \omega^1\\ \vdots & \ddots & \vdots & \vdots\\ \Gamma(l+n+1) & \cdots & \Gamma(l+3n-1) & \omega^n\end{vmatrix}\quad (n\geqslant 1). \tag{5.7}$$

Similarly, identifying $f_n\equiv Q_n(\omega^2)$ we obtain $Q_0(\omega^2)=1$ and

$$Q_n(\omega^2)=D_{n-1}^{-1}\begin{vmatrix}\Gamma(l+1) & \Gamma(l+3) & \cdots & \Gamma(l+2n+1)\\ \vdots & \vdots & \ddots & \vdots\\ \Gamma(l+n) & \Gamma(l+n+2) & \cdots & \Gamma(l+3n)\\ \omega^0 & \omega^2 & \cdots & \omega^{2n}\end{vmatrix}\quad (n\geqslant 1). \tag{5.8}$$

Using the relation $\Gamma(z+1)=z\Gamma(z)$ an easy Gauss elimination process gives the normalization constant as

$$D_n=\begin{vmatrix}\Gamma(l+1) & \cdots & \Gamma(l+2n+1)\\ \vdots & \ddots & \vdots\\ \Gamma(l+n+1) & \cdots & \Gamma(l+3n+1)\end{vmatrix}=\prod_{k=0}^{n}2^k k!(2k+1)!. \tag{5.9}$$

From this, note the diagonal pairing matrix elements $h_0=l!$ and

$$\int_0^\infty P_n(\omega)Q_n(\omega^2)e^{-\omega}\omega^l d\omega=h_n=D_n/D_{n-1}=2^n n!(2n+l)!\quad (n\geqslant 1). \tag{5.10}$$

B. *n*-level correlation functions

The n-level correlation function $R_n(\omega_1, \ldots, \omega_n)$ in the present context is defined as

$$R_n(\omega_1, \omega_2, \ldots, \omega_n) = n! \int_{\mathbb{R}_+^N} \sum_{i_1<i_2<\cdots<i_n} \delta(\omega_1 - \tilde{\omega}_{i_1}) \delta(\omega_2 - \tilde{\omega}_{i_2}) \cdots \delta(\omega_n - \tilde{\omega}_{i_n}) d\mu_{N,l}(\tilde{\omega}_1, \ldots, \tilde{\omega}_N). \tag{5.11}$$

A closed-form expression for it can be given from the biorthogonal polynomials $P_{n'}(\omega)$ and $Q_{n'}(\omega^2)$ for $0 \leqslant n' \leqslant N$. The result will take its most succinct form when expressed in terms of the modified functions

$$\tilde{P}_n(\omega) := (-2)^{-n} n!^{-1} e^{-\omega} P_n(\omega), \tag{5.12}$$

$$\tilde{Q}_n(\omega) := (-1)^n (2n+l)!^{-1} \omega^l Q_n(\omega^2), \tag{5.13}$$

[the motivation for the sign $(-1)^n$ will become clear later], which from Eqs. (5.4) and (5.10) obey the orthogonality relations

$$\int_0^\infty \tilde{P}_m(\omega) \tilde{Q}_n(\omega) d\omega = \delta_{m,n}. \tag{5.14}$$

The probability measure (5.3) expressed by these functions takes the form

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = \frac{1}{N!} \mathrm{Det}[\tilde{P}_{i-1}(\omega_j)] \mathrm{Det}[\tilde{Q}_{i-1}(\omega_j)] \prod_k d\omega_k.$$

Now, by using the multiplicative property of the determinant, we can also write

$$d\mu_{N,l}(\omega_1, \ldots, \omega_N) = \frac{1}{N!} \mathrm{Det}[K_N(\omega_i, \omega_j)]_{i,j=1,\ldots,N} \prod_k d\omega_k, \tag{5.15}$$

where the kernel $K(\omega_i, \omega_j)$ is defined by

$$K_N(\omega_i, \omega_j) = \sum_{n=0}^{N-1} \tilde{P}_n(\omega_i) \tilde{Q}_n(\omega_j). \tag{5.16}$$

From the orthogonality relations (5.14) this kernel has the reproducing property

$$\int_0^\infty K_N(\omega_i, \omega) K_N(\omega, \omega_j) d\omega = K_N(\omega_i, \omega_j), \tag{5.17}$$

and the trace

$$\int_0^\infty K_N(\omega, \omega) d\omega = N. \tag{5.18}$$

To proceed further, take notice of the relation

$$\int_0^\infty \begin{vmatrix} K_N(\omega_1, \omega_1) & \cdots & K_N(\omega_1, \omega_n) \\ \vdots & \ddots & \vdots \\ K_N(\omega_n, \omega_1) & \cdots & K_N(\omega_n, \omega_n) \end{vmatrix} d\omega_n = (N-n+1) \begin{vmatrix} K_N(\omega_1, \omega_1) & \cdots & K_N(\omega_1, \omega_{n-1}) \\ \vdots & \ddots & \vdots \\ K_N(\omega_{n-1}, \omega_1) & \cdots & K_N(\omega_{n-1}, \omega_{n-1}) \end{vmatrix},$$

which is proved by expanding the determinant with respect to the last row or column and exploiting the properties (5.17) and (5.18). Using it, an inductive procedure starting from

$R_N(\omega_1, \ldots, \omega_N) = \mathrm{Det}[K_N(\omega_i, \omega_j)]_{i,j=1,\ldots,N}$ gives the n-level correlation functions as

$$R_n(\omega_1, \ldots, \omega_n) = \mathrm{Det}[K_N(\omega_i, \omega_j)]_{i,j=1,\ldots,n}. \tag{5.19}$$

Thus the correlations are those of a determinantal process and are completely determined by the kernel $K_N(\omega_i, \omega_j)$. The remaining discussion therefore focuses on this kernel, but first we make another preparatory step.

C. Contour integral representation

We are now going to show that the functions $\widetilde{P}_n(\omega)$ and $\widetilde{Q}_n(\omega)$ have expressions as complex contour integrals

$$\widetilde{P}_n(\omega) = \oint_{S_\epsilon(1)} e^{-\omega u}(1-u^{-2})^{-n-1}u^{l-2}du/\pi i, \tag{5.20}$$

$$\widetilde{Q}_n(\omega) = \oint_{S_\epsilon(0)} e^{\omega v}(1-v^{-2})^{n}u^{-l-1}dv/2\pi i. \tag{5.21}$$

Both integrals are over circles in the complex plane with radius ϵ and counterclockwise orientation; the first circle is centered at $u=1$ and has radius $\epsilon<2$ (to avoid the singularity at $u=-1$), the second one is centered at $v=0$.

Our proof of these expressions for $\widetilde{P}_n(\omega)$ and $\widetilde{Q}_n(\omega)$ will be indirect and in two steps. First, we establish some information on power series. In the case of $\widetilde{Q}_n(\omega)$ we insert the power series of the exponential function $e^{\omega v}$, use the binomial expansion of $(1-v^{-2})^n$, and compute a residue to obtain

$$\widetilde{Q}_n(\omega) = \sum_{k=0}^{n} \binom{n}{k} \frac{(-1)^k \omega^{2k+l}}{(2k+l)!}. \tag{5.22}$$

In the case of $\widetilde{P}_n(\omega)$, calculating the residue at $u=1$ we have that

$$\widetilde{P}_n(\omega) = \frac{2}{n!}\frac{d^n}{du^n}\left[\frac{e^{-\omega u}u^{n+l-1}}{(1+u^{-1})^{n+1}}\right]\Bigg|_{u=1}. \tag{5.23}$$

In both cases, defining $P_n(\omega)$ and $Q_n(\omega^2)$ by the reverse of the relations (5.12) and (5.13), we see from Eqs. (5.22) and (5.23) that these are polynomials of degree n in ω resp. ω^2 and that the highest-degree term (ω^n resp. ω^{2n}) has coefficient one.

Recall now from Sec. V A that, given these properties, the polynomials $P_n(\omega)$ and $Q_n(\omega^2)$ are completely determined by the orthogonality relations (5.4) for $m \neq n$. Via Eqs. (5.12) and (5.13) the latter are in one-to-one correspondence with the orthogonality relations (5.14) (still for $m \neq n$). Therefore, defining

$$\widetilde{I}_{m,n} = \int_0^\infty \widetilde{P}_m(\omega)\widetilde{Q}_n(\omega)d\omega, \tag{5.24}$$

the second and final step of our proof is to show that $\widetilde{I}_{m,n}=0$ for $m \neq n$.

To that end, we insert the expressions (5.20) and (5.21) into Eq. (5.24). The ω dependence then is $e^{-\omega(u-v)}$ with $u \in S_\epsilon(1)$ and $v \in S_\epsilon(0)$. Taking the radius ϵ to be very small ($\epsilon \ll 1$), we have that $e^{-\omega(u-v)}$ decreases rapidly as ω goes to $+\infty$. Therefore, the integral over ω exists, and we may interchange the order of integrations. Doing first the ω integral

$$\int_0^\infty e^{-\omega(u-v)}d\omega = \frac{1}{u-v},$$

the remaining contour integrals for $\tilde{I}_{m,n}$ defined by Eq. (5.24) are

$$\tilde{I}_{m,n} = \oint_{S_\epsilon(1)} \frac{u^{l-2}}{(1-u^{-2})^{m+1}} \left[\oint_{S_\epsilon(0)} \frac{(1-v^{-2})^n dv}{v^{l+1}(v-u)} \right] \frac{du}{2\pi^2}.$$

To simplify the inner integral over v we use the identity

$$\left(\frac{1-v^{-2}}{1-u^{-2}}\right)^n = 1 - \frac{v^2-u^2}{v^2(1-u^2)} \sum_{k=0}^{n-1} \left(\frac{1-v^{-2}}{1-u^{-2}}\right)^k.$$

Inserting this into the expression for $\tilde{I}_{m,n}$ we see that the terms in the k sum do not contribute as the residue at $v=0$ vanishes for all of those terms. Doing the v integral for the first term on the right-hand side, we get

$$\oint_{S_\epsilon(0)} v^{-l-1}(v-u)^{-1}dv = -2\pi i u^{-l-1},$$

so the remaining u integral is

$$\tilde{I}_{m,n} = (\pi i)^{-1} \oint_{S_\epsilon(1)} (1-u^{-2})^{n-m-1} u^{-3} du.$$

This integrand is holomorphic near $u=1$ for $m<n$, and the integral therefore vanishes in that case. For $m>n$ we use the invariance of the integration form under $u \to -u$ to write $I_{m,n}$ as an integral over a sum of two circles

$$\tilde{I}_{m,n} = \frac{1}{2\pi i} \oint_\gamma \frac{u^{2m-2n-1}du}{(u^2-1)^{m-n+1}}, \quad \gamma = S_\epsilon(1) + S_\epsilon(-1).$$

The integrand in this case is holomorphic near $u=0$. In the punctured plane $\mathbb{C}\backslash\{1,-1\}$ the chain $S_\epsilon(1)+S_\epsilon(-1)$ is homologous to the circle at infinity, where the integrand vanishes. Therefore the integral again is zero. This proves that $\tilde{I}_{m,n}=0$ for $m \neq n$, which in turn completes our proof that the contour integrals (5.20) and (5.21) are the same as the functions $\tilde{P}_n(\omega)$, $\tilde{Q}_n(\omega)$ defined from Eqs. (5.7) and (5.8) by Eqs. (5.12) and (5.13). As a final check, note that

$$\tilde{I}_{n,n} = (\pi i)^{-1} \oint_{S_\epsilon(1)} \frac{du}{u(u^2-1)} = 1,$$

which is what it ought to be in view of Eq. (5.14).

Now we harvest a major benefit from the contour integral representations (5.20) and (5.21): using these, we can carry out the sum in the definition (5.16) of the kernel K_N as a geometric sum. The result is a double contour integral

$$K_N(\omega_1,\omega_2) = \oint_{S_\epsilon(1)} du \oint_{S_\epsilon(0)} dv F_N(u,v;\omega_1,\omega_2), \tag{5.25}$$

$$F_N(u,v;\omega_1,\omega_2)=\frac{1}{2\pi^2}e^{-\omega_1 u+\omega_2 v}\frac{u^l v^{-l+1}}{u^2-v^2}\left[\left(\frac{1-v^{-2}}{1-u^{-2}}\right)^N-1\right]. \tag{5.26}$$

This exact expression represents the complete solution of our problem. We will now use it to determine the large-N asymptotics in the bulk and at the hard edge $\omega=0$.

D. Asymptotics in the bulk

The kernel on the diagonal $\omega_1=\omega_2$ is the same as the one-level function, $R_1(\omega)=K_N(\omega,\omega)$; see Eq. (5.19). We already know from Sec. IV the asymptotics of $R_1(\omega)\equiv\rho(\omega)$ in the bulk: introducing the scaling variable $x=\omega/N$ (formerly $x=\omega\tau/N$), this is

$$\lim_{N\to\infty} K_N(Nx,Nx)=\rho_\infty(x),$$

with $\rho_\infty(x)$ given by Eq. (4.6). In the present subsection we are going to demonstrate that the scaling limit of the kernel $K_N(\omega_1,\omega_2)$ off the diagonal leads to sine-kernel universality for all level correlation functions:

$$\lim_{N\to\infty} R_n(Nx+\omega_1,\ldots,Nx+\omega_n)=\mathrm{Det}\left\{\frac{\sin[\pi\rho_\infty(x)(\omega_i-\omega_j)]}{\pi(\omega_i-\omega_j)}\right\}_{i,j=1,\ldots,n}, \tag{5.27}$$

as is expected for systems in the universality class of the Gaussian Unitary Ensemble. As a corollary, we will obtain an independent confirmation of the result (4.6).

Looking at the integral representation (5.25) one might think that the large-N limit could be taken by applying the saddle-point method to that integral. However, as we shall see, the dominant saddle points lie on the line $u=v$ where the integrand has a singularity of type 0/0 which, albeit removable, complicates the saddle-point evaluation.

Therefore, rather than calculating $K_N(\omega_1,\omega_2)$ directly, we look at the product $(\omega_1-\omega_2)K_N(\omega_1,\omega_2)$. Using the relation $(\omega_2-\omega_1)\mathrm{e}^{\omega_2 v-\omega_1 u}=(\partial_v+\partial_u)\mathrm{e}^{\omega_2 v-\omega_1 u}$ and partially integrating, we rewrite Eq. (5.25) as

$$(\omega_1-\omega_2)K_N(\omega_1,\omega_2)=\oint_{S_\epsilon(1)}du\oint_{S_\epsilon(0)}dv\,\widetilde{F}_N(u,v;\omega_1,\omega_2), \tag{5.28}$$

$$\widetilde{F}_N(u,v;\omega_1,\omega_2)=\frac{1}{2\pi^2}e^{-\omega_1 u+\omega_2 v}\left(\frac{\partial}{\partial u}+\frac{\partial}{\partial u}\right)\frac{u^l v^{-l+1}}{u^2-v^2}\left[\left(\frac{1-v^{-2}}{1-u^{-2}}\right)^N-1\right], \tag{5.29}$$

which constitutes the starting point for the following analysis.

In preparation for taking the limit $N\to\infty$, we set $\omega_1=Nx+\omega$ and $\omega_2=Nx+\tilde{\omega}$. The deciding factor in the integrand of $(\omega_1-\omega_2)K_N(\omega_1,\omega_2)$ in the large-N limit will then be

$$\exp[-Nx(u-v)+N\log(1-v^{-2})-N\log(1-u^{-2})],$$

leading to the saddle-point equation

$$\varphi(u)=x=\varphi(v),\quad \varphi(w)=-\partial_w\log(1-w^{-2})=\frac{-2}{w(w^2-1)}. \tag{5.30}$$

Notice that φ is related to our function (4.17) by $f(w-1)=\varphi(w)$. A comprehensive study of the equation $f(w)=z$ and its solutions for w was made in Sec. IV. From there we know that the saddle-point equation $\varphi(w)=x$ has three solutions in general, and for $0<x\leqslant b=3\sqrt{3}$ these are

$$w_\alpha(x) = -x^{-1/3}e^{-2\pi i\alpha/3}(1+\sqrt{1-x^2/b^2})^{1/3} - x^{-1/3}e^{2\pi i\alpha/3}(1-\sqrt{1-x^2/b^2})^{1/3} \quad (\alpha = 1,-1,0). \tag{5.31}$$

In the range of interest $(0<x<b)$ the first two solutions, $w_{\pm 1}(x)$, are complex conjugates of each other while the third one, $w_0(x)$, is negative. Expanding the logarithm of $(1-v^{-2})^N/(1-u^{-2})^N$ to second order around a pair of saddle points w_α, w_β we encounter the Gaussian

$$\exp\left\{\frac{1}{2}N\varphi'[w_\alpha(x)](\delta u)^2 - \frac{1}{2}N\varphi'[w_\beta(x)](\delta v)^2\right\}, \quad \varphi'(x) = \frac{6w^2-2}{w^2(w^2-1)^2}.$$

For the negative saddle point one has $\varphi'[w_0(x)]>0$, so its path of steepest descent would be perpendicular to the real axis in the case of u and along the real axis in the case of v. The latter is inconsistent with the original integration contour for v being $S_\epsilon(0)$. In the former case, $w_0(x)<-1$ is inaccessible because of the singularity of $(1-u^{-2})^{-N}$ intervening at $u=-1$. Thus this saddle point is irrelevant for present purposes and may be discarded.

We now make another preparation of the saddle-point evaluation of the integral, by investigating the behavior of the integrand near the two remaining saddle points. We set

$$u = w_\alpha(x) + N^{-1/2}\delta u, \quad v = w_\beta(x) + N^{-1/2}\delta v \quad (\alpha,\beta = \pm 1),$$

and first look at the diagonal case, $\alpha=\beta$. Using the identity

$$\frac{1}{u-v}\left(\frac{\partial}{\partial u}+\frac{\partial}{\partial v}\right)\left(\frac{1-u^{-2}}{1-u^{-2}}\right)^N = 2N\frac{u^2+uv+v^2-1}{u(u^2-1)v(v^2-1)}\left(\frac{1-v^{-2}}{1-u^{-2}}\right)^N, \tag{5.32}$$

we find the scaling limit of the integrand $\tilde{F}_N$ to be

$$\lim_{N\to\infty} N^{-1}\tilde{F}_N[w_\alpha(x)+N^{-1/2}\delta u, w_\alpha(x)+N^{-1/2}\delta v; Nx+\omega, Nx+\tilde{\omega}]$$
$$= (2\pi)^{-2}e^{-w_\alpha(x)(\omega-\tilde{\omega})}\varphi'[w_\alpha(x)]e^{(1/2)\varphi'[w_\alpha(x)](\delta u^2-\delta v^2)}.$$

The same limit in the off-diagonal case $(\alpha\neq\beta)$ vanishes. Indeed,

$$w_\alpha^2 + w_\alpha w_\beta + w_\beta^2 - 1 = \frac{w_\alpha(w_\alpha^2-1) - w_\beta(w_\beta^2-1)}{w_\alpha - w_\beta} = \frac{-2}{w_\alpha - w_\beta}(x^{-1}-x^{-1}) = 0 \quad (\alpha\neq\beta),$$

and therefore the factor in the numerator on the right-hand side of Eq. (5.32) gives zero.

We now deform the contours of integration as indicated in Fig. 2. The deformed contours pass through the saddle points $w_{\pm 1}$ but miss the saddle point w_0. At $w_{\pm 1}$ the paths of steepest descent for u and v cross at right angles, valleys in one case being mountains in the other case and vice versa.

Next we do the Gaussian integrals. Given the counterclockwise orientations of the original contours $S_\epsilon(1)$ resp. $S_\epsilon(0)$, and taking into account the directions of the paths of steepest descent, we get

$$\int e^{(1/2)\varphi'(w_{+1})\delta u^2}d(\delta u) = \sqrt{2\pi}|\varphi'(w_{+1})|^{-1/2}e^{(1/2)[-\pi i - i\arg\varphi'(w_{+1})]},$$

$$\int e^{-(1/2)\varphi'(w_{+1})\delta v^2}d(\delta v) = \sqrt{2\pi}|\varphi'(w_{+1})|^{-1/2}e^{(1/2)[2\pi i - i\arg\varphi'(w_{+1})]}.$$

The product of these two integrals is $2\pi i/\varphi'(w_{+1})$. The same calculation for the other saddle w_{-1} gives $-2\pi i/\varphi'(w_{-1})$. Thus, putting the factors together and summing over the contributions from diagonal pairs of saddle points $(\alpha=\beta)$ we obtain

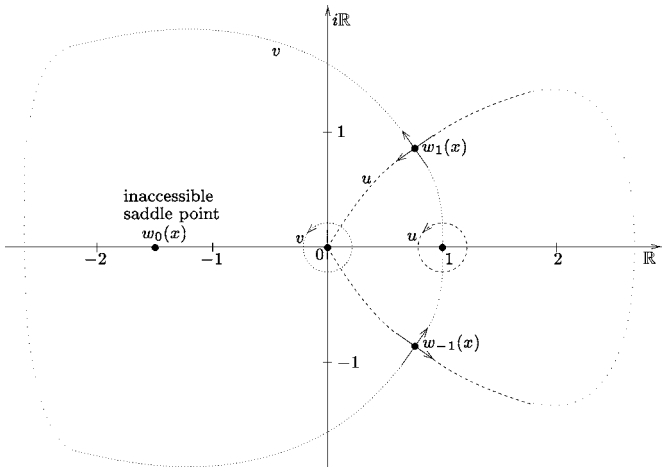

FIG. 2. Sketch of the saddle points for the case of $x=1$. By deforming the original contours, which are small circles around the singular points $u=1$ and $v=0$, one arranges for the contours of integration to pass through the saddle points $w_{\pm 1}(x)$ in the direction of steepest descent. Away from the saddle points the deformed contours are drawn as paths of constant phase, which interpolate between different zeroes of the integrand: they run between 0 and $+\infty$ for u, and between 1 and $-\infty$ for v.

$$(\omega-\tilde{\omega})\lim_{N\to\infty} K_N(Nx+\omega,Nx+\tilde{\omega})=\frac{1}{2\pi i}(e^{-w_{-1}(x)(\omega-\tilde{\omega})}-e^{-w_{+1}(x)(\omega-\tilde{\omega})}).$$

Since $\Re e w_{+1}=\Re e w_{-1}$ and $\Im m w_{+1}=-\Im m w_{-1}$ this means that, with $\Im m w_{+1}(x)=:\pi\rho_\infty(x)$, we have

$$\lim_{N\to\infty} K_N(Nx+\omega,Nx+\tilde{\omega})=e^{-\Re e w_{\pm 1}(x)(\omega-\tilde{\omega})}\frac{\sin[\pi\rho_\infty(x)(\omega-\tilde{\omega})]}{\pi(\omega-\tilde{\omega})}.$$

The exponential factor $e^{-\Re e w_{\pm 1}(x)(\omega-\tilde{\omega})}$ drops out when forming the determinant on the right-hand side of Eq. (5.19). Thus we arrive at the universal sine-kernel (or GUE) correlation functions (5.27).

Setting $\omega=\tilde{\omega}$ notice the special result $\lim_{N\to\infty}K_N(Nx,Nx)=\rho_\infty(x)$. Since the kernel on the diagonal is none other than the one-level function, $K_N(\omega,\omega)=\rho(\omega)$, this gives another determination of the large-N level density ρ_∞. From Eq. (5.31) one sees that $\rho_\infty(x)=\pi^{-1}\Im m w_{+1}(x)$ agrees with our earlier result Eq. (4.6).

E. Asymptotics near $\omega=0$

At the lower edge ($\omega=0$) of the spectrum, a new type of behavior is expected to emerge. This behavior, as we shall see presently, occurs on a scale $\omega\sim N^{-1/2}$.

To exhibit the scaling limit near $\omega=0$, it is best to send the integration variables u, v to their reciprocals, $u\to u^{-1}$ and $v\to v^{-1}$. Then $du\to -u^{-2}du$, $dv\to -v^{-2}dv$, and the integration contour for v has its radius inverted and orientation reversed, $S_\epsilon(0)\to -S_{1/\epsilon}(0)$. However, since the integrand is holomorphic in v on $\mathbb{C}\backslash\{0\}$ we may return to the original radius ϵ (or any other radius, for that matter). In the case of u we take the radius ϵ of $S_\epsilon(1)$ to be very small. Then inversion $u\to u^{-1}$ sends $S_\epsilon(1)$ to itself (or, in any case, to the same homology class on $\mathbb{C}\backslash\{1\}$), with no change of orientation. Altogether, then, carrying out the transformation $(u,v)\to(u^{-1},v^{-1})$ the integral representation (5.25) continues to hold true if we make the replacement

$$F_N(u,v;\omega_1,\omega_2)\to -u^{-2}v^{-2}F_N(u^{-1},v^{-1};\omega_1,\omega_2)=\frac{1}{2\pi^2}e^{-\omega_1/u+\omega_2/v}\frac{u^{-l}v^{l-1}}{u^2-v^2}\left[\left(\frac{1-v^2}{1-u^2}\right)^N-1\right].$$

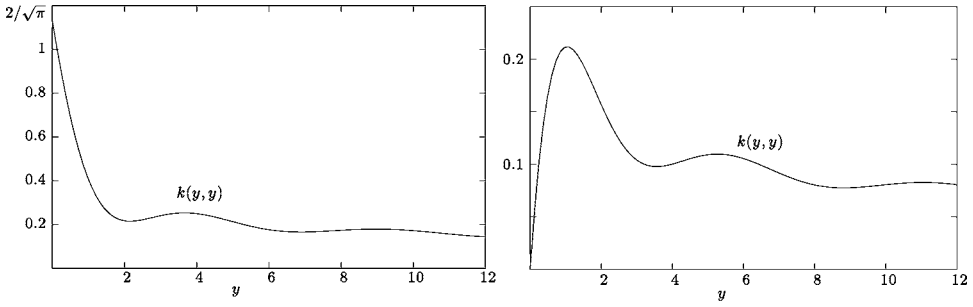

FIG. 3. The graph of the scaling function $k(y,y)$ for the case of $l=0$ (left) and $l=1$ (right).

Next, as another preparation for taking the limit $N\to\infty$, we deform the u-contour $S_\epsilon(1)$ to some axis parallel to the imaginary axis. The deformed contour crosses the real axis between $u=0$ and $u=1$ and is directed from $u=+i\infty$ to $u=-i\infty$. We also reverse the direction of integration for u and change the overall sign of the integral.

Then we set $\omega_j=N^{-1/2}y_j$ and rescale $u\to N^{-1/2}u$ and $v\to N^{-1/2}v$ accordingly. Again, in view of the analytic properties of the integrand we can keep the integration contours fixed while rescaling. Because the u integral converges at infinity we have a good limit

$$\lim_{N\to\infty}(1-u^2/N)^{-N}=\exp(u^2).$$

In total, we thus obtain the following scaling limit for our kernel K_N:

$$k(y_1,y_2):=\lim_{N\to\infty}N^{-1/2}K_N(N^{-1/2}y_1,N^{-1/2}y_2)=\frac{1}{2\pi^2}\int_{i\mathbb{R}+\epsilon}du\int_{\mathrm{U}_1}\frac{dv}{v}e^{-y_1/u+y_2/v}(v/u)^l\frac{e^{u^2-v^2}-1}{u^2-v^2},\tag{5.33}$$

where $\mathrm{U}_1\equiv S_1(0)$ means the unitary numbers, and $i\mathbb{R}+\epsilon$ is the imaginary axis translated by $\epsilon>0$ into the right half of the complex plane. Plots of the scaling function $k(y,y)$ for $l=0,1$ are shown in Fig. 3. Using the method of saddle-point evaluation as in Sec. V C one can show that this function behaves as $k(y,y)\sim y^{-1/3}$ for large y.

Taking the same scaling limit for the functions $\tilde{P}_N(\omega)$ and $\tilde{Q}_N(\omega)$ in Eqs. (5.20) and (5.21) one gets

$$p(y)=\lim_{N\to\infty}N^{-(l-1)/2}\tilde{P}_N(N^{-1/2}y)=\frac{1}{\pi i}\int_{i\mathbb{R}+\epsilon}e^{u^2-y/u}u^{-l}du,\tag{5.34}$$

$$q(y)=\lim_{N\to\infty}N^{l/2}\tilde{Q}_N(N^{-1/2}y)=\frac{1}{2\pi i}\int_{\mathrm{U}_1}e^{-v^2+y/v}v^{l-1}dv.\tag{5.35}$$

Both functions have convergent series expansions

$$p(y)=\sum_{n=0}^{\infty}\frac{(-y)^n}{n!\Gamma[(l+n+1)/2]},\quad q(y)=y^l\sum_{n=0}^{\infty}\frac{(-y^2)^n}{n!(2n+l)!}.\tag{5.36}$$

The expansion for $q(y)$ can be obtained either directly from Eq. (5.35), or by taking the limit $N\to\infty$ in Eq. (5.22). In the case of $p(y)$, the earlier formula (5.23) is not suitable; rather, in order to verify Eq.(5.36) for $p(y)$ one expands the integrand of Eq. (5.34) in powers of y, makes use of $\mathfrak{Re}u=\epsilon>0$ to write

$$u^{-n-l} = (n+l-1)!^{-1} \int_0^\infty e^{-tu} t^{n+l-1} dt \quad (n+l>0),$$

does the Gaussian u integral by completing the square, and uses the duplication formula for the Gamma function.

Note added in proof. After submission of this manuscript, P. Forrester pointed out to us that the joint eigenvalue distribution derived and analyzed here falls in a broad class of models solved by Borodin.[12] Borodin's expression for the kernel $K_N(x,y)$ is equivalent to ours by old work of Konhauser.[13] The mathematical results of Konhauser were first introduced into random matrix physics by Muttalib,[14] who suggested to use them for an approximate treatment of the statistics of transmission eigenvalues of disordered conductors.

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Overlap fluctuations from the Boltzmann random overlap structure

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We investigate overlap fluctuations of the Sherrington-Kirkpatrick mean field spin glass model in the framework of the Random Overlap Structure (ROSt). The concept of ROSt has been introduced recently by Aizenman and co-workers, who developed a variational approach to the Sherrington-Kirkpatrick model. Here we propose an iterative procedure to show that, in the so-called Boltzmann ROSt, Aizenman-Contucci polynomials naturally arise for almost all values of the inverse temperature (not in average over some interval only). These polynomials impose restrictions on the overlap fluctuations in agreement with Parisi theory. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2357995]

I. INTRODUCTION

The study of mean field spin glasses has been very challenging from both a physical and a mathematical point of view. It took several years after the main model (the Sherrington-Kirkpatrick, or simply SK) was introduced before Giorgio Parisi was able to compute the free energy so ingeniously (Ref. 12 and references therein), and it took much longer still until a fully rigorous proof of Parisi's formula was found.[11,14] Parisi went beyond the solution for the free energy and gave an Ansatz about the pure states of the model as well, prescribing the so-called ultrametric or hierarchical organization of the phases (Ref. 12 and references therein). From a rigorous point of view, the closest the community could get so far to ultrametricity are identities constraining the probability distribution of the *overlaps*, namely, the Aizenman-Contucci (AC) and the Ghirlanda-Guerra identities (see Refs. 1 and 9, respectively). For further reading, we refer to Refs. 6, 7, and 13, but also to the general references.[5,15] Most of the few important rigorous results about mean field spin glasses can be elegantly summarized within a powerful and physically profound approach introduced recently by Aizenman *et al.* in Ref. 2. We want to show here that in this framework the AC identities can be deduced too. This is achieved by studying a stochastic stability of some kind, similarly to what is discussed in Ref. 6, inside the environment (the *Random Overlap Structure*) suggested in Ref. 2, and taking into account also the intensive nature of the internal energy density. A central point of the treatment is a power series expansion similar to the one performed in Ref. 3.

The paper is organized as follows. In Sec. II we introduce the concept of Random Overlap Structure (henceforth ROSt), and use it to state the related Extended Variational Principle. In Sec. III we present the main results regarding the ac identities and similar families of relations. Section IV is left for a few concluding remarks.

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II. MODEL, NOTATIONS, PREVIOUS BASIC RESULTS

The Hamiltonian of the SK model is defined on Ising spin configurations $\sigma: i \to \sigma_i = \pm 1$ of N spins, labeled by $i = 1, \ldots, N$, as

$$H_N(\sigma; J) = -\frac{1}{\sqrt{N}} \sum_{i<j}^{1,N} J_{ij} \sigma_i \sigma_j$$

where J_{ij} are i.i.d. centered unit Gaussian random variables. We will assume there is no external field. Being a centered Gaussian variable, the Hamiltonian is determined by its covariance,

$$\mathbb{E}[H_N(\sigma) H_N(\sigma')] = \frac{1}{2} N q_{\sigma\sigma'}^2$$

where

$$q_{\sigma\sigma'} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \sigma_i'$$

is the overlap, and here $\mathbb{E}$ denotes the expectation with respect to all the (quenched) Gaussian variables.

The partition function $Z_N(\beta)$, the quenched free energy density $f_N(\beta)$, and pressure $\alpha_N(\beta)$ are defined as

$$Z_N(\beta) = \sum_{\sigma} \exp(-\beta H_N(\sigma)),$$

$$-\beta f_N(\beta) = \frac{1}{N} \mathbb{E} \ln Z_N(\beta) = \alpha_N(\beta).$$

The Boltzmann-Gibbs average of an observable $\mathcal{O}(\sigma)$ is denoted by ω and defined as

$$\omega(\mathcal{O}) = Z_N(\beta)^{-1} \sum_{\sigma} \mathcal{O}(\sigma) \exp(-\beta H_N(\sigma)),$$

but we will use the same ω to indicate, in general (weighted) sums over spins or nonquenched variables, to be specified when needed, and with Ω we will mean the product (*replica*) measure of the needed number of copies of ω.

Let us now introduce an auxiliary system.

Definition 1: A Random Overlap Structure $\mathcal{R}$ *is a triple* $(\Sigma, \tilde{q}, \xi)$, *where*

- $\Sigma \ni \gamma$ *is a discrete space* (*set of abstract spin configurations*);
- $\tilde{q}: \Sigma^2 \to [0,1]$ *is a positive definite kernel* (*overlap kernel*), *with* $|\tilde{q}| \leq 1$ (*and* $\tilde{q} = 1$ *on the diagonal of* Σ^2);
- $\xi: \Sigma \to \mathbb{R}_+$ *is a normalized discrete positive random measure, i.e., a system of random weights such that there is a probability measure* μ *on* $[0,1]^{\Sigma}$ *so that* $\Sigma_{\gamma \in \Sigma} \xi_\gamma < \infty$ *almost surely in the* μ *sense*.

The randomness in the weights ξ is independent of the randomness of the quenched variables from the original system with spins σ. We equip a ROSt with two families of independent and centered Gaussians $\tilde{h}_i$ and $\hat{H}$ with covariances

$$\mathbb{E}[\tilde{h}_i(\gamma) \tilde{h}_j(\gamma')] = \delta_{ij} \tilde{q}_{\gamma\gamma'}, \tag{1}$$

$$\mathbb{E}[\hat{H}(\gamma)\hat{H}(\gamma')] = \tilde{q}^2_{\gamma\gamma'}. \tag{2}$$

Given a ROSt $\mathcal{R}$, we define the trial pressure as

$$G_N(\mathcal{R}) = \frac{1}{N}\mathbb{E}\ln\frac{\sum_{\sigma,\gamma}\xi_\gamma \exp\left(-\beta\sum_{i=1}^N \tilde{h}_i(\gamma)\sigma_i\right)}{\sum_\gamma \xi_\gamma \exp(-\beta\sqrt{N/2}\hat{H}(\gamma))}, \tag{3}$$

where $\mathbb{E}$ denotes hereafter the expectation with respect to all the (quenched) random variables (including the randomness in the random weights ξ) but spins σ and the abstract spins γ, the sum over which is, in fact, written explicitly.

The following theorem (Ref. 2) can be easily proven by interpolation.

Theorem 1 (Extended Variational Principle): *Infimizing for each N separately the trial function* $G_N(\mathcal{R})$ *defined in* (3) *over the whole ROSt space, the resulting sequence tends to the limiting pressure* $-\beta f(\beta)$ *of the SK model as N tends to infinity*,

$$\alpha(\beta) \equiv \lim_{N\to\infty} \alpha_N(\beta) = \lim_{N\to\infty} \inf_{\mathcal{R}} G_N(\mathcal{R}).$$

For a given ROSt and a given inverse temperature β, the trial pressures $\{G_N\}$ are a well defined sequence of real numbers indexed by N; a ROSt $\mathcal{R}$ is said to be optimal if $\alpha \equiv \lim_{N\to\infty}\alpha_N(\beta) = \lim_{N\to\infty} G_N(\mathcal{R})$ for all β.

An optimal ROSt is the Parisi one (Refs. 12 and 14), another optimal one is the so-called Boltzmann ROSt $\mathcal{R}_B$, defined as follows. Take $\Sigma = \{-1,1\}^M$, and denote by τ the points of Σ. We clearly have in mind an auxiliary spin system (and that is why we use τ as opposed to the previous γ to denote its points). In fact, we also choose

$$\tilde{h}_i = -\frac{1}{\sqrt{M}}\sum_{k=1}^M \tilde{J}_{ik}\tau_k, \quad \hat{H} = -\frac{1}{M}\sum_{k,l}^{1,M} \hat{J}_{kl}\tau_k\tau_l,$$

which satisfy (1) and (2) with $\tilde{q}_{\tau\tau'} = (1/M)\Sigma_k \tau_k\tau'_k$, and $\tilde{J}$ and $\hat{J}$ are families of i.i.d. random variables independent of the original couplings J, with whom they share the same distribution (i.e., all the $\tilde{J}$ and $\hat{J}$ are centered unit Gaussian random variables). The variables $\tilde{h}_\cdot$ are called *cavity fields*. Let us also choose

$$\xi_\tau = \exp(-\beta H_M(\tau;\hat{J})) = \exp\left(\beta\frac{1}{\sqrt{M}}\sum_{k,l}^{1,M}\hat{J}_{kl}\tau_k\tau_l\right).$$

If we call $\mathcal{R}_{\mathrm{B}}(M)$ the structure defined above, we will formally write $\mathcal{R}_{\mathrm{B}}(M)\to\mathcal{R}_{\mathrm{B}}$ as $M\to\infty$, and we call $\mathcal{R}_{\mathrm{B}}$ the Boltzmann ROSt. The reason why such a ROSt is optimal is purely thermodynamic, and equivalent to the existence of the thermodynamic limit of the free energy per spin. A detailed proof of this fact can be found in Ref. 2; here we just mention the main point:

$$\alpha(\beta) = \mathbf{C}\lim_M \frac{1}{N}\mathbb{E}\ln\frac{Z_{N+M}}{Z_M} = \lim_{N\to\infty}\mathbf{C}\lim_M G_N(\mathcal{R}_{\mathrm{B}}(M)) = G_N(\mathcal{R}_{\mathrm{B}}) = G(\mathcal{R}_{\mathrm{B}}),$$

where **C** lim is the limit in the Cesàro sense. Notice that the Boltzmann ROSt does not depend on N, after the M limit.

III. ANALYSIS OF THE BOLTZMANN ROSt

In this section we show that in the optimal Boltzmann ROSt's the overlap fluctuations obey some restrictions, namely, those found by Aizenman and Contucci in Ref. 1. In other words, we exhibit a recipe to generate the ac polynomials within the ROSt approach.

A. The internal energy term

Let us focus on the denominator of the trial pressure $G(\mathcal{R}_B)$, defined in (3), computed at the Boltzmann ROSt $\mathcal{R}_B$, defined in the previous section. Let us normalize this quantity by dividing by Z_N and weight $\hat{H}$ with an independent variable β' as opposed to β, which appears in the *Boltzmannfaktor* ξ_τ. As in the Boltzmann structure we have actual spins (τ) and we do not use the spins σ here; we will still use ω (or Ω) to denote the Boltzmann-Gibbs (replica) measure (at inverse temperature β) in the space $\Sigma=\{-1,1\}^M$. Moreover, we will use the notation $\langle\cdot\rangle=\mathbb{E}\Omega(\cdot)$ and, if present, a subscript β recalls that the *Boltzmannfaktor* in Ω has inverse temperature β. More precisely, we are computing the left hand side of the next equality to get this.

Lemma 1:

$$\frac{1}{N}\mathbb{E}\ln\Omega\exp\left(-\beta'\sqrt{\frac{N}{2}}\hat{H}(\tau)\right)=\frac{\beta'^2}{4}(1-\langle\tilde{q}^2\rangle_\beta). \tag{4}$$

Similar calculations have been performed already, but in this specific context the result has been only stated without proof in Ref. 10, while a detailed proof is given only in the dilute case in Ref. 8. So let us prove the lemma. Let us take M finite. Thanks to the property of the addition of independent Gaussian variables, the left hand side of (4) is the same as

$$\frac{1}{N}\mathbb{E}\ln\frac{Z_M(\beta^*)}{Z_M(\beta)}=\frac{M}{N}(\alpha_M(\beta^*)-\alpha_M(\beta)),\quad \beta^*=\sqrt{\beta^2+\frac{\beta'^2N}{M}},$$

which, in turn, thanks to the convexity of α, can be estimated as follows:

$$\frac{M}{N}(\beta^*-\beta)\alpha'_M(\beta)\le\frac{M}{N}(\alpha_M(\beta^*)-\alpha_M(\beta))\le\frac{M}{N}(\beta^*-\beta)\alpha'_M(\beta^*).$$

Now

$$\frac{M}{N}(\beta^*-\beta)=\frac{\beta'^2}{2\beta}+o\left(\frac{1}{M}\right),\quad \alpha'(\beta)=\frac{\beta}{2}(1-\langle\tilde{q}^2\rangle_\beta).$$

Therefore, when $M\to\infty$, we get (4) for almost all β, i.e., whenever $\alpha'(\beta^*)\to\alpha'(\beta)$, or, equivalently, whenever $\langle\cdot\rangle_{\beta^*}\to\langle\cdot\rangle_\beta$. Notice that the quantity in (4) does not depend on N.[8,10]

Theorem 2: *The following statements hold:*

- *The left hand side of (4) is intensive (does not depend on N);*
- *The left hand side of (4) is a monomial of order two in β';*
- *The Aizenman-Contucci identities hold.*

Proof: Recall that $\hat{H}$ is a centered Gaussian, and so is therefore $-\hat{H}$, and the Gibbs measure is such that the substitution $\hat{H}\to\hat{H}-\hat{H}'$ implies

$$\frac{1}{N}\mathbb{E}\ln\Omega\exp\left(-\beta'\sqrt{\frac{N}{2}}\hat{H}\right)=\frac{1}{2N}\mathbb{E}\ln\Omega\exp\left(-\beta'\sqrt{\frac{N}{2}}(\hat{H}-\hat{H}')\right).$$

Expand now in powers of β' the exponential first and then the logarithm:

$$\frac{1}{N}\mathbb{E}\ln\Omega\exp\left(-\beta'\sqrt{\frac{N}{2}}\hat{H}\right)=\frac{\beta'^2}{4}(1-\langle\tilde{q}^2\rangle)$$

$$=\frac{1}{2N}\mathbb{E}\ln\Omega\left(1+\frac{\beta'^2}{2}\frac{N}{2}(\hat{H}-\hat{H}')^2+\frac{\beta'^4}{4!}\frac{N^2}{4}(\hat{H}-\hat{H}')^4+\cdots\right)$$

$$=\frac{1}{2N}\mathbb{E}\left[\left(\frac{N\beta'^2}{4}(2\Omega(\hat{H}^2)-2\Omega^2(\hat{H}))\right)\right.$$

$$+\frac{N^2}{4}\frac{\beta'^4}{4!}[2\Omega(\hat{H}^4)-8\Omega(\hat{H})\Omega(\hat{H}^3)+6\Omega^2(\hat{H}^2)]$$

$$\left.-\frac{N^2}{2}\frac{\beta'^4}{4}[\Omega^2(\hat{H}^2)+\Omega^4(\hat{H})-2\Omega(\hat{H}^2)\Omega^2(\hat{H})]+\cdots\right].$$

A straightforward calculation yields

$$\mathbb{E}\Omega(\hat{H}^4)=3,\quad \mathbb{E}[\Omega(\hat{H}^3)\Omega(\hat{H})]=3\langle\tilde{q}_{12}^2\rangle,\quad \mathbb{E}\Omega^2(\hat{H}^2)=1+2\langle\tilde{q}_{12}^4\rangle,$$

$$\mathbb{E}[\Omega(\hat{H}^2)\Omega^2(\hat{H})]=\langle\tilde{q}_{12}^2\rangle+2\langle\tilde{q}_{12}^2\tilde{q}_{13}^2\rangle,\quad \mathbb{E}\Omega^4(\hat{H})=3\langle\tilde{q}_{12}^2\tilde{q}_{34}^2\rangle,$$

and so on. All quantities of this sort can be computed in the same way. As an example, let us calculate $\mathbb{E}[\Omega(\hat{H}^2)\Omega^2(\hat{H})]=\mathbb{E}[\omega(\hat{H}_1^2)\omega(\hat{H}_2)\omega(\hat{H}_3)]$. Like, for overlaps, subscripts denote replicas. In order to evaluate the expectation of products of Gaussian variables, we can use Wick's theorem: we just count all the possible ways to contract the four Gaussian terms $\hat{H}_1$, $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and sum over every nonvanishing contribution,

$$\langle\overbrace{\hat{H}_1\hat{H}_2}\overbrace{\hat{H}_1\hat{H}_3}\rangle = \langle\tilde{q}_{12}^2\tilde{q}_{23}^2\rangle\ ,$$

$$\langle\overbrace{\hat{H}_1\hat{H}_1}\overbrace{\hat{H}_2\hat{H}_3}\rangle = \langle 1\cdot\tilde{q}_{12}^2\rangle\ ,$$

$$\langle\overbrace{\hat{H}_1\hat{H}_3}\overbrace{\hat{H}_1\hat{H}_2}\rangle = \langle\tilde{q}_{12}^2\tilde{q}_{23}^2\rangle\ .$$

The sum of all the terms gives the exactly $\langle\tilde{q}_{12}^2\rangle+2\langle\tilde{q}_{12}^2\tilde{q}_{23}^2\rangle$. Now Eq. (4) is therefore expressed in terms of an identity for all β' of two polynomials in β': one is of order two; the other is a whole power series. We can then equate the coefficient of the same order, or equivalently put to zero all the terms of order higher than two in β'. The consequent equalities are exactly the Aizenman-Contucci ones (Ref. 1); an example of these is

$$\langle\tilde{q}_{12}^4\rangle-4\langle\tilde{q}_{12}^2\tilde{q}_{13}^2\rangle+3\langle\tilde{q}_{12}^2\tilde{q}_{34}^2\rangle=0,$$

which arises from the lowest order in the expansion above. □

B. The entropy term

In the same spirit as in the previous section, let us move on to the normalized numerator of the trial pressure $G(\mathcal{R}_B)$, defined in (3), computed at the Boltzmann ROSt $\mathcal{R}_B$, defined in the previous section. If we define

$$c_i=2\cosh(-\beta\tilde{h}_i)=\sum_{\sigma_i}\exp(-\beta\tilde{h}_i\sigma_i);$$

then

$$\frac{1}{N}\mathbb{E}\ln\Omega\sum_{\sigma}\exp\left(-\beta\sum_{i=1}^{N}\tilde{h}_i\sigma_i\right)=\frac{1}{N}\mathbb{E}\ln\Omega(c_1\cdots c_N) \tag{5}$$

does not depend on N,[8,10] if we consider the infinite Boltzmann ROSt, where $M\to\infty$.

Again, assume we replace the β in front of the cavity fields $\tilde{h}$ (but not in the state Ω) with a parameter $\sqrt{t}$, and define, upon rescaling,

$$\Psi(t)=\mathbb{E}\ln\Omega\sum_{\sigma}\exp\frac{\sqrt{t}}{\sqrt{N}}\sum_{i=1}^{N}\tilde{h}_i\sigma_i. \tag{6}$$

We want to study the flux (in t) of Eq. (6) to obtain an integrable expansion. The t flux of the cavity function Ψ is given by

$$\partial_t\Psi(t)=\frac{1}{2}(1-\langle q_{12}\tilde{q}_{12}\rangle_t), \tag{7}$$

which is easily seen by means of a standard use of Gaussian integration by parts. The subscript in $\langle\cdot\rangle_t=\mathbb{E}\Omega_t$ means that such an average includes the t-dependent exponential appearing in (6), beyond the sum over σ.

Theorem 3: *Let F_s be measurable with respect to the σ algebra generated by the overlaps of s replicas of $\{\sigma\}$ and $\{\tau\}$. Then the cavity streaming equation is*

$$\partial_t\langle F_s\rangle_t=\left\langle F_s\left(\sum_{\gamma,\delta}^{1,s}q_{\gamma,\delta}\tilde{q}_{\gamma,\delta}-s\sum_{\gamma=1}^{s}q_{\gamma,s+1}\tilde{q}_{\gamma,s+1}+\frac{s(s+1)}{2}q_{s+1,s+2}\tilde{q}_{s+1,s+2}\right)\right\rangle_t. \tag{8}$$

Proof: We consider the Boltzmann ROSt $\mathcal{R}_{\mathrm{B}}(M)$ with any value of M. The proof relies on the repeated application of the usual integration by parts formula for Gaussian variables:

$$\partial_t\langle F_s\rangle_t=\partial_t\mathbb{E}\frac{\sum_{\sigma\tau}F_s\exp(-\beta H_M(\tau))\exp\left(\sqrt{\frac{t}{MN}}\sum_{ij}\sum_{\gamma}\tilde{J}_{ij}\tau_i^{\gamma}\sigma_j^{\gamma}\right)}{\sum_{\sigma\tau}\exp(-\beta H_M(\tau))\exp\left(\sqrt{\frac{t}{MN}}\sum_{ij}\sum_{\gamma}\tilde{J}_{ij}\tau_i^{\gamma}\sigma_j^{\gamma}\right)}$$

$$=\frac{1}{2\sqrt{tMN}}\mathbb{E}\sum_{ij}J_{ij}\sum_{\gamma}^{s}(\Omega_t[F_s\tau_i^{\gamma}\sigma_j^{\gamma}]-\Omega_t[F_s]\Omega_t[\tau_i^{\gamma}\sigma_j^{\gamma}])$$

$$=\frac{1}{2\sqrt{tMN}}\sum_{ij}\mathbb{E}J_{ij}\left(\sum_{\gamma}\Omega_t[F_s\tau_i^{\gamma}\sigma_j^{\gamma}]-s\Omega_t[F_s]\omega[\tau_i\sigma_j]\right)$$

$$=\frac{1}{2MN}\sum_{ij}\mathbb{E}\left(\sum_{\gamma,\delta}\Omega_t[F_s\sigma_j^{\gamma}\tau_i^{\gamma}\sigma_j^{\delta}\tau_i^{\delta}]-\sum_{\gamma,\delta}\Omega_t[F_s\tau_i^{\gamma}\sigma_j^{\gamma}]\Omega_t[\tau_i^{\delta}\sigma_j^{\delta}]-s\omega_t[\tau_i\sigma_j]\sum_{\delta}(\Omega_t[F_s\tau_i^{\delta}\sigma_j^{\delta}]\right.$$

$$\left.-\Omega_t[F_s]\Omega_t[\tau_i^{\delta}\sigma_j^{\delta}]-s\Omega_t[F_s](1-\omega_t^2[\tau_i\sigma_j]))\right)$$

$$=\frac{1}{2}\mathbb{E}\left(\sum_{\gamma,\delta}\Omega_t[F_sq_{\gamma,\delta}\tilde{q}_{\gamma,\delta}]-s\sum_{\gamma}\Omega_t[F_sq_{\gamma,s+1}\tilde{q}_{\gamma,s+1}]\right.$$

$$\left.+ss\Omega_t[F_sq_{s+1,s+2}\tilde{q}_{s+1,s+2}]-s\Omega_t[F_s]\Omega_t[F_sq_{s+1,s+2}\tilde{q}_{s+1,s+2}]\right),$$

where in Ω_t we have included the sum over σ and τ, the *Boltzmannfaktor* in τ, and the t-dependent exponential. At this point, remembering that $\tilde{q}_{\gamma\gamma}=1$, we can write

$$\sum_{\gamma,\delta} \Omega_t[F_s q_{\gamma\delta} \tilde{q}_{\gamma\delta}] = 2 \sum_{\gamma,\delta} \Omega_t[F_s q_{\gamma\delta} \tilde{q}_{\gamma\delta}] + s\Omega_t[F_s]$$

which completes the proof. □

Now the way to proceed is simple: we have to expand the t derivative of $\Psi(t)$ [the right hand side of (7)] using the cavity streaming equation (8), and we will stop the iteration at the first nontrivial order (that is expected to be at least four, being the first ac relation of that order). Once a closed-form expression is in our hands, we can write down an order by order expansion of the (modified) denominator of the Boltzmann ROSt (that is, the function $N^{-1}\psi(t)$ evaluated for $t = N\beta^2$).

We have

$$\partial_t \langle q_{12}\tilde{q}_{12}\rangle_t = \langle q_{12}^2\tilde{q}_{12}^2 - 4q_{12}\tilde{q}_{12}q_{23}\tilde{q}_{23} + 3q_{12}\tilde{q}_{12}q_{34}\tilde{q}_{34}\rangle_t.$$

After the first iteration:

$$\partial_t \langle q_{12}^2\tilde{q}_{12}^2\rangle_t = \langle q_{12}^3\tilde{q}_{12}^3 - 4q_{12}^2\tilde{q}_{12}^2\tilde{q}_{23}p_{23} + 3q_{12}^2\tilde{q}_{12}^2\tilde{q}_{34}\rangle_t,$$

$$\partial_t \langle \tilde{q}_{12}q_{12}\tilde{q}_{23}q_{23}\rangle_t = \langle \tilde{q}_{12}q_{12}\tilde{q}_{23}q_{23}\tilde{q}_{13}q_{13} + 2\tilde{q}_{12}^2q_{12}^2\tilde{q}_{23}q_{23} - 6\tilde{q}_{12}q_{12}\tilde{q}_{23}q_{23}\tilde{q}_{34}q_{34} - 3\tilde{q}_{12}q_{12}\tilde{q}_{13}q_{13}\tilde{q}_{14}q_{14} + 6\tilde{q}_{12}q_{12}\tilde{q}_{34}q_{34}\tilde{q}_{45}q_{45}\rangle_t,$$

$$\partial_t \langle \tilde{q}_{12}q_{12}\tilde{q}_{34}q_{34}\rangle_t = \langle 4\tilde{q}_{12}q_{12}\tilde{q}_{23}q_{23}\tilde{q}_{34}q_{34} + 2\tilde{q}_{12}^2q_{12}^2\tilde{q}_{34}q_{34} - 16\tilde{q}_{12}q_{12}\tilde{q}_{34}q_{34}\tilde{q}_{45}q_{45} + 10\tilde{q}_{12}q_{12}\tilde{q}_{34}q_{34}\tilde{q}_{56}q_{56}\rangle_t.$$

The higher orders can be obtained exactly in the same way, so we can write down right away the expression for $\langle q_{12}\tilde{q}_{12}\rangle$, referring to Refs. 1 and 3 for a detailed explanation of this iterative method:

$$\langle q_{12}\tilde{q}_{12}\rangle_t = \langle q_{12}^2\tilde{q}_{12}^2\rangle t - 2\langle q_{12}\tilde{q}_{12}q_{23}\tilde{q}_{23}q_{13}\tilde{q}_{13}\rangle t^2 - \frac{1}{6}\langle q_{12}^4\tilde{q}_{12}^4\rangle t^3 - 2\langle q_{12}^2\tilde{q}_{12}^2q_{23}^2\tilde{q}_{23}^2\rangle t^3 + \frac{3}{2}\langle q_{12}^2\tilde{q}_{12}^2q_{34}^2\tilde{q}_{34}^2\rangle t^3 + 6\langle q_{12}\tilde{q}_{12}q_{23}\tilde{q}_{23}q_{34}\tilde{q}_{34}q_{14}\tilde{q}_{14}\rangle t^3. \tag{9}$$

Notice that the averages no longer depend on t. In this expansion we considered both q overlaps and $\tilde{q}$ overlaps, but as the sum over the spins σ can be performed explicitly, we can obtain an explicit expression at least for the q overlaps, and get

$$\langle q_{12}^2\rangle = \frac{1}{N^2}\mathbb{E}\sum_{ij} \omega^2(\sigma_i\sigma_j) = \frac{1}{N},$$

$$\langle q_{12}q_{23}q_{31}\rangle = \frac{1}{N^3}\mathbb{E}\sum_{ijk} \omega(\sigma_i\sigma_j)\omega(\sigma_j\sigma_k)\omega(\sigma_k\sigma_i) = \frac{1}{N^2},$$

$$\langle q_{12}^2q_{34}^2\rangle = \frac{1}{N^4}\mathbb{E}\sum_{ijkl} \omega^2(\sigma_i\sigma_j)\omega^2(\sigma_k\sigma_l) = \frac{1}{N^2},$$

$$\langle q_{12}q_{23}q_{34}q_{14}\rangle = \frac{1}{N^4}\mathbb{E}\sum_{ijkl} \omega(\sigma_i\sigma_j)\omega(\sigma_j\sigma_k)\omega(\sigma_k\sigma_l)\omega(\sigma_l\sigma_i) = \frac{1}{N^3},$$

$$\langle q_{12}^4\rangle = \frac{1}{N^4}\mathbb{E}\sum_{ijkl} \omega(\sigma_i\sigma_j\sigma_k\sigma_l)\omega(\sigma_i\sigma_j\sigma_k\sigma_l) = \frac{3(N-1)}{N^3} + \frac{1}{N^3},$$

$$\langle q_{12}^2 q_{23}^2 \rangle = \frac{1}{N^4} \mathbb{E} \sum_{ijkl} \omega(\sigma_i \sigma_j) \omega(\sigma_i \sigma_j \sigma_k \sigma_l) \omega(\sigma_i \sigma_j) = \frac{1}{N^2}.$$

Moreover, as the q overlaps have been calculated explicitly, we can use a graphical formalism.[1,3] In such a formalism we use points to identify replicas and lines for the overlaps between them. So, for example,

$$\langle \bullet\!\!-\!\!\bullet \rangle = \langle \tilde{q}_{12} \rangle, \qquad \langle \text{O} \rangle = \langle \tilde{q}_{12}^2 \rangle, \qquad \langle \triangle \rangle = \langle \tilde{q}_{12} \tilde{q}_{23} \tilde{q}_{13} \rangle$$

and so on. Now we can integrate (7) thanks to the polynomial expansion based on (9) and to the expressions for the q fluctuations. We obtain

$$\Psi(t) = \frac{1}{2} \int_0^t [1 - \langle q_{12} \tilde{q}_{12} \rangle_{t'}] dt',$$

$$\frac{1}{N} \Psi(t = N\beta^2) = \frac{\beta^2}{2} - \langle \text{O} \rangle \frac{\beta^4}{4} + \langle \triangle \rangle \frac{\beta^6}{3} - \langle \text{θ} \rangle \frac{\beta^8}{24} - \langle \square \rangle \frac{3\beta^8}{4} + N\beta^8 \left[\frac{1}{16} \langle \text{θ} \rangle - \frac{1}{4} \langle \infty \rangle + \frac{3}{16} \langle \text{8} \rangle \right]. \tag{10}$$

This expression, though truncated at this low order, already looks pretty much alike the expansion found using the internal energy part of the Boltzmann pressure.

We stress, however, two important features of expression (10). The first is that within this approach we do not have problems concerning the Replica Symmetry Anzatz (RS),[12] and this can be seen by the proliferating of the overalaps fluctuations, via which we expand the entropy (a RS theory does not allow such fluctuations). Second, we note that not all the terms inside the equations (10) are intensive: the last three graphs are all multiplied by a factor N. Recalling that this expansion does not depend on N, and physically a density is intensive by definition, we put to zero all the terms in the squared bracket, so to have

$$\langle \text{θ} - 4 \infty + 3 \text{8} \rangle = 0.$$

Again we can find the AC identities.

IV. CONCLUSIONS AND OUTLOOK

We have shown how some constraints on the distribution of the overlap naturally arise within the Random Overlap Structure approach. As our analysis of the Boltzmann ROSt is similar to the study of stochastic stability, it is not surprising that the constraints coincide with the Aizenman-Contucci identities. In the ROSt context, such identities are easily connected with the existence of the thermodynamic limit of the free energy density (which is equivalent to the optimality of the Boltzmann ROSt) and with the physical fact that the internal energy is intensive. We also showed that, as expected, the entropy part of the free energy yields the same constraints as the other part (i.e., the internal energy).

The hope for the near future is that the ROSt approach will lead eventually to a good understanding of the pure states and the phase transitions of the model. A first step has been taken in Ref. 10, and our present results can be considered as a second step in this direction. (Other more interesting results regarding the phase transition at $\beta=1$ can also be obtained with the same techniques employed here, including the graphical representation.[4]) A further step should bring the Ghirlanda-Guerra identities, and then hopefully a proof of ultrametricity.

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Geometric prequantization of the moduli space of the vortex equations on a Riemann surface

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The moduli space of solutions to the vortex equations on a Riemann surface are well known to have a symplectic (in fact, Kähler) structure. We show this symplectic structure explictly and proceed to show a family of symplectic (in fact, Kähler) structures Ω_{Ψ_0} on the moduli space, parametrized by Ψ_0, a section of a line bundle on the Riemann surface. Next, we show that corresponding to these, there is a family of prequantum line bundles $\mathcal{P}_{\Psi_0}$ on the moduli space whose curvature is proportional to the symplectic forms Ω_{Ψ_0}. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2352858]

I. INTRODUCTION

Geometric prequantization is a construction, if possible, of a prequantum line bundle $\mathcal{L}$ on a symplectic manifold, $(\mathcal{M},\Omega)$ whose curvature is proportional to the symplectic form. The Hilbert space of the quantization is the space of the square integrable sections of $\mathcal{L}$. To every $f \in C^\infty(\mathcal{M})$, we associate an operator acting on the Hilbert space, namely, $\hat{f}=-i\hbar[X_f - (i/\hbar)\theta(X_f)]+f$, where X_f is the vector field defined by $\Omega(X_f,\cdot)=-df$ and θ is a symplectic potential corresponding to Ω. Then if $f_1, f_2 \in C^\infty(\mathcal{M})$ and $f_3=\{f_1,f_2\}$, the Poisson bracket of the two induced by the symplectic form, then $[\hat{f}_1,\hat{f}_2]=-i\hbar\hat{f}_3$.[1]

The motivating example in our context would be the geometric quantization of the moduli space of flat connections on a principal G bundle P on a compact Riemann surface Σ.[2,3] Let $\mathcal{A}$ be the space of Lie-algebra valued connections on the principal bundle P. Let $\mathcal{N}$ be the moduli space of flat connections (i.e., the space of flat connections modulo the gauge group). One can construct the determinant line bundle of the Cauchy-Riemann operator, namely, $\mathcal{L}=\wedge^{\text{top}}(\text{Ker}\ \bar{\partial}_A)^* \otimes \wedge^{\text{top}}(\text{Coker}\ \bar{\partial}_A)$ on $\mathcal{A}$.[4] The curvature induced by the Quillen metric on this bundle coincides with the natural Kähler form $\mathcal{A}$, namely, $-\text{Tr}\int_\Sigma \alpha\wedge\beta$, where $\alpha,\beta \in T_A\mathcal{A}=\Omega^1(M,\text{ad}\ P)$. It can be shown, using a moment map construction, that this symplectic form descends to the moduli space of flat connections $\mathcal{N}$. The determinant line bundle is also well defined on $\mathcal{N}$ and is the candidate for the prequantum line bundle of the geometric quantization.

Inspired by this construction, we constructed three prequantum line bundles on the moduli space of solutions to the self-duality equations over a Riemann surface[5,6] corresponding to the three symplectic forms that give rise to the hyper-Kähler structure of the moduli space.

In this paper we geometrically quantize the moduli space of vortex equations. Geometric quantization of the vortex moduli space has been done before in Refs. 7 and 8. In the first paper the authors use algebraic geometry and in the second paper the author uses the special form of the moduli space when the Riemann surface is a sphere. It would be interesting to see what the relation is of the present quantization to the ones in Refs. 7 and 8. The relation may not be straightforward, since in the present quantization we find a whole family of (topologically equivalent, but perhaps holomorphically nonequivalent) prequantum line bundles $\mathcal{P}_{\Psi_0}$ whose curvatures correspond to a family of symplectic forms Ω_{Ψ_0} parametrized by Ψ_0 a section of a line bundle on the Riemann surface, as explained later. This symplectic form Ω_{Ψ_0} is a variant of the standard symplectic form Ω on the vortex moduli space.

The vortex equations are as follows. Let M be a compact Riemann surface and let $\omega = h^2\, dz\wedge d\bar{z}$ be the purely imaginary volume form on it (i.e., h is real.) Let A be a unitary connection on a principal $U(1)$ bundle P, i.e., A is a purely imaginary valued one form, i.e., $A=A^{(1,0)}+A^{(0,1)}$ such that $A^{(1,0)}=-\overline{A^{(0,1)}}$. Let L be a complex line bundle associated to P by the defining representation. Let Ψ be a section of L, i.e., $\Psi\in\Gamma(M,L)$ and $\bar{\Psi}$ be a section of its dual, $\bar{L}$. There is a Hermitian metric H on L, i.e., the inner product $\langle\Psi_1,\Psi_2\rangle_H=\Psi_1 H\bar{\Psi}_2$ is a smooth function on M. (Here H is real).

The pair (A,Ψ) will be said to satisfy the vortex equations if

$$F(A)=(1-|\Psi|_H^2)\omega, \tag{1}$$

$$\bar{\partial}_A\Psi=0, \tag{2}$$

where $F(A)$ is the curvature of the connection A and $d_A=\partial_A+\bar{\partial}_A$ is the decomposition of the covariant derivative operator into (1,0) and (0,1) pieces. Let $\mathcal{S}$ be the space of solutions to (1) and (2). There is a gauge group G acting on the space of (A,Ψ) that leaves the equations invariant. We take the group G to be Abelian and locally it looks like Maps $(M,U(1))$. If g is an $U(1)$ gauge transformation, then (A_1,Ψ_1) and (A_2,Ψ_2) are gauge equivalent if $A_2=g^{-1}\,dg+A_1$ and $\Psi_2=g^{-1}\Psi_1$. Taking the quotient by the gauge group of $\mathcal{S}$ gives the moduli space of solutions to these equations and is denoted by $\mathcal{M}$. It is well known that there is a natural metric on the moduli space $\mathcal{M}$ and, in fact, the metric is Kähler; see Refs. 9–11, 8, and 12–14, and the references there.

In this paper, we show the metric explicitly and write down the symplectic (in fact, the Kähler form) Ω arising from this metric and the complex structure. This is because some modification of this symplectic form gives us a whole family of symplectic forms Ω_{Ψ_0} parametrized by a fixed section Ψ_0 of the line bundle L that vanishes on a set of measure zero. Ω_{Ψ_0} coincides with Ω when L is a trivial bundle with $|\Psi_0|_H=1$. In fact, Ω_{Ψ_0} is a Kähler form on the moduli space. We show that there exists a holomorphic prequantum line bundle, namely, a determinant line bundle, whose Quillen curvature is proportional to the symplectic form Ω_{Ψ_0}. Thus, as Ψ_0 varies, we get a whole family of prequantum line bundles that are topologically equivalent, but perhaps not holomorphically equivalent.

II. METRIC AND SYMPLECTC FORMS

Let $\mathcal{A}$ be the space of all unitary connections on P and $\Gamma(M,L)$ be sections of L. Let $\mathcal{C}=\mathcal{A}\times\Gamma(M,L)$ be the configuration space on which Eqs. (1) and (2) are imposed. Let $p=(A,\Psi)\in\mathcal{C}$, $X=(\alpha_1,\beta)$, $Y=(\alpha_2,\eta)\in T_p\mathcal{C}\equiv\Omega^1(M,i\mathbb{R})\times\Gamma(M,L)$, i.e., $\alpha_i=\alpha_i^{(0,1)}+\alpha_i^{(1,0)}$, such that $\alpha_i^{(0,1)}=-\alpha_i^{(1,0)}, i=1,2$. On $\mathcal{C}$ one can define a metric,

$$\mathcal{G}(X,Y)=\int_M *_1\alpha_1\wedge\alpha_2+2i\int_M \mathrm{Re}\langle\beta,\eta\rangle_H\omega$$

and an almost complex structure

$$\mathcal{I}=\begin{bmatrix} *_1 & 0\\ 0 & i\end{bmatrix}:T_p\mathcal{C}\to T_p\mathcal{C},$$

where $*_1:\Omega^1\to\Omega^1$ is the Hodge star operator on M such that $*_1(\eta\,dz)=-i\eta\,dz$ and $*_1(\bar{\eta}\,d\bar{z})=i\bar{\eta}\,d\bar{z}$.

It is easy to check that $\mathcal{G}$ is positive definite. In fact, if $\alpha_1=\alpha^{(1,0)}+\alpha^{(0,1)}=a\,dz-\bar{a}\,d\bar{z}$ is an imaginary valued 1-form, $*_1\alpha_1=-i(a\,dz+\bar{a}\,d\bar{z})$ and $\mathcal{G}(X,X)=4\int_M|a|^2\,dx\wedge dy+4\int_M|\beta|_H^2h^2\,dx\wedge dy$, where $\omega=h^2\,dz\wedge d\bar{z}=-2ih^2\,dx\wedge dy$.

The symplectic form Ω: We define

$$\Omega(X,Y) = -\int_M \alpha_1 \wedge \alpha_2 + 2i\int_M \mathrm{Re}\langle i\beta, \eta\rangle_H \omega = -\int_M \alpha_1 \wedge \alpha_2 - \int_M (\beta H\bar{\eta} - \bar{\beta}H\eta)\omega,$$

such that $\mathcal{G}(\mathcal{I}X,Y)=\Omega(X,Y)$. Moreover, we have the following.

Proposition 2.1: The metrics $\mathcal{G}$, the symplectic form Ω, and the almost complex structure $\mathcal{I}$ are invariant under the gauge group action on $\mathcal{C}$.

Proof: Let $p=(A,\Psi)\in\mathcal{C}$ and $g\in G$, the gauge group, where $g\cdot p=(A+g^{-1}\,dg, g^{-1}\Psi)$.

Then $g_*: T_p\mathcal{C}\to T_{g\cdot p}\mathcal{C}$ is given by the mapping (Id, g^{-1}) and it is now easy to check that g and Ω are invariant and $\mathcal{I}$ commutes with g_*. □

Proposition 2.2: The equation (1) *can be realized as a moment map $\mu=0$ with respect to the action of the gauge group and the symplectic form Ω.*

Proof: Let $\zeta\in\Omega(M,i\mathbb{R})$ be the Lie algebra of the gauge group (the gauge group element being $g=e^{\zeta}$); note that ζ is purely imaginary. It generates a vector field X_ζ on $\mathcal{C}$ as follows:

$$X_\zeta(A,\Psi) = (d\zeta, -\zeta\Psi) \in T_p\mathcal{C},$$

where $p=(A,\Psi)\in\mathcal{C}$.

We show next that X_ζ is Hamiltonian. Namely, define $H_\zeta:\mathcal{C}\to\mathbb{C}$ as follows:

$$H_\zeta(p) = \int_M \zeta\cdot(F_A - (1-|\Psi|_H^2)\omega).$$

Then, for $X=(\alpha,\beta)\in T_p\mathcal{C}$,

$$dH_\zeta(X) = \int_M \zeta\, d\alpha + \int_M \zeta(\Psi H\bar{\beta} + \bar{\Psi}H\beta)\omega = -\int_M (d\zeta)\wedge\alpha + 2i\int_M \mathrm{Re}\big(i(-\zeta\Psi)H\bar{\beta}\big)\omega = \Omega(X_\zeta, X),$$

where we use that $\bar{\zeta}=-\zeta$.

Thus we can define the moment map $\mu:\mathcal{C}\to\Omega^2(M,i\mathbb{R})=\mathcal{G}^*$ (the dual of the Lie algebra of the gauge group) to be

$$\mu(A,\Psi) = \big(F(A) - (1-|\Psi|_H^2)\omega\big).$$

Thus, Eq. (1) is $\mu=0$. □

Lemma 2.3: *Let $\mathcal{S}$ be the solution spaces to Eqs. (1) and (2), $X\in T_p\mathcal{S}$. Then $\mathcal{I}X\in T_p\mathcal{S}$ if and only if X is $\mathcal{G}$ orthogonal to the gauge orbit $O_p=G\cdot p$.*

Proof: Let $X_\zeta\in T_pO_p$, where $\zeta\in\Omega^0(M,i\mathbb{R})$, $\mathcal{G}(X,X_\zeta)=-\Omega(\mathcal{I}X,X_\zeta)=-\int_M\zeta\cdot d\mu(\mathcal{I}X)$, and therefore $\mathcal{I}X$ satisfies the linearization of Eq. (1) iff $d\mu(\mathcal{I}X)=0$, i.e., iff $\mathcal{G}(X,X_\zeta)=0$ for all ζ. Second, it is easy to check that $\mathcal{I}X$ satisfies the linearization of Eq. (2) whenever X does. □

Theorem 2.4: *$\mathcal{M}$ has a natural symplectic structure and an almost complex structure compatible with the symplectic form Ω and the metric $\mathcal{G}$.*

Proof: First we show that the almost complex structure descends to $\mathcal{M}$. Then using this and the symplectic quotient construction, we will show that Ω gives a symplectic structure on $\mathcal{M}$.

(a) To show that $\mathcal{I}$ descends as an almost complex structure, we let $\mathrm{pr}:\mathcal{S}\to\mathcal{S}/G=\mathcal{M}$ be the projection map and set $[p]=pr(p)$. Then we can naturally identify $T_{[p]}\mathcal{M}$ with the quotient space $T_p\mathcal{S}/T_pO_p$, where $O_p=G\cdot p$ is the gauge orbit. Using the metric $\mathcal{G}$ on $\mathcal{S}$ we can realize $T_{[p]}\mathcal{M}$ as a subspace in $T_p\mathcal{S}$, $\mathcal{G}$ orthogonal to T_pO_p. Then by Lemma 2.3, this subspace is invariant under $\mathcal{I}$. Thus $I_{[p]}=\mathcal{I}|_{T_p(O_p)^\perp}$, gives the desired almost complex structure. This construction does not depend on the choice of p since $\mathcal{I}$ is G invariant.

(b) The symplectic structure Ω descends to $\mu^{-1}(0)/G$, (by Proposition 2.2 and by the Marsden-Weinstein symplectic quotient construction,[15,16] since the leaves of the characteristic foliation are the gauge orbits). Now, as a 2-form Ω descends to $\mathcal{M}$, due to Proposition 2.1 so does the metric $\mathcal{G}$. The closure of Ω is easy. We check that Eq. (2) does not give rise to new degeneracy

of Ω [i.e., the only degeneracy of Ω is due to (1) but along gauge orbits]. Thus, Ω is symplectic on $\mathcal{M}$. Since $\mathcal{G}$ and $\mathcal{I}$ descend to $\mathcal{M}$, the latter is symplectic and almost complex. □

The family of symplectic forms Ω_{Ψ_0}. Choose a fixed $\Psi_0 \in \Gamma(M,L)$ such that $|\Psi_0|_H=0$ only on a set of measure zero on M. (This Ψ_0 has nothing to do with Ψ.)

Define a symplectic form on $\mathcal{C}$ as

$$\Omega_{\Psi_0}(X,Y) = -\int_M \alpha_1 \wedge \alpha_2 + 2i\int_M \mathrm{Re}\langle i\beta,\eta\rangle_H |\Psi_0|_H^2 \omega = -\int_M \alpha_1 \wedge \alpha_2 - \int_M (\beta H\bar{\eta} - \bar{\beta} H\eta)|\Psi_0|_H^2\omega.$$

$|\Psi_0|_H^2$ plays the role of a conformal rescaling of the volume form ω on M that appears in Ω, where we allow the conformal factor to have zeros on sets of measure zero.

Theorem 2.5: *Ω_{Ψ_0} descends to $\mathcal{M}$ as a symplectic form.*

Proof: Let $p=(A,\Psi)$.

It is easy to show that Ω_{Ψ_0} is closed [this follows from the fact that on $\mathcal{C}$ it is a constant form—does not depend on (A,Ψ)]. We have to show it is nondegenerate.

Suppose there exists $(\alpha_1,\beta) \in T_{[p]}(\mathcal{M})$, s.t.,

$$\Omega_{\Psi_0}((\alpha_2,\eta),(\alpha_1,\beta)) = 0,$$

$\forall (\alpha_2,\eta) \in T_{[p]}(\mathcal{M})$. Using the metric $\mathcal{G}$, we identify $T_{[p]}\mathcal{M}$ with the subspace in $T_p\mathcal{S},\mathcal{G}$ orthogonal to T_pO_p (i.e., the tangent space to the moduli space is identified to the tangent space to solutions that are orthogonal to the gauge orbits, the orthogonality is with respect to the metric $\mathcal{G}$). Thus $(\alpha_1,\beta),(\alpha_2,\eta)$ satisfy the linearization of Eqs. (1) and (2) and $\mathcal{G}((\alpha_1,\beta),X_\zeta)=0$ and $\mathcal{G}((\alpha_2,\eta),X_\zeta)=0$ for all ζ.

Now, by 2.3, $\mathcal{I}(\alpha_2,\eta) \in T_pS$. Also,

$$\mathcal{G}(\mathcal{I}(\alpha_1,\beta),X_\zeta) = \Omega((\alpha_1,\beta),X_\zeta) = -\int_M \zeta\, d\mu((\alpha_1,\beta)) = 0,$$

since $d\mu((\alpha_1,\beta))=0$ is precisely one of the equations saying that $(\alpha_1,\beta) \in T_pS$. Thus $\mathcal{I}(\alpha_1,\beta) \in T_{[p]}\mathcal{M}$, (since it is in T_pS and $\mathcal{G}$ orthogonal to gauge orbits).

Take $(\alpha_2,\eta)=\mathcal{I}(\alpha_1,\beta)=(*_1\alpha_1, i\beta)$. Then

$$\begin{aligned} 0 = \Omega_{\Psi_0}(\mathcal{I}(\alpha_1,\beta),(\alpha_1,\beta)) &= -\int_M (*_1\alpha_1 \wedge \alpha_1) + 2i\int_M \mathrm{Re}\langle i(i\beta),\beta\rangle_H |\Psi_0|_H^2\omega \\ &= -4\int_M |\alpha|^2\, dx\wedge dy - 4\int_M |\beta|_H^2 |\Psi_0|_H^2 h^2\, dx\wedge dy, \end{aligned}$$

where $\omega=-2ih^2\, dx\wedge dy$ and $\alpha_1=a\, dz-\bar{a}\, d\bar{z} \in \Omega^1(M,i\mathbb{R})$ and $*_1\alpha_1=-i(a\, dz+\bar{a}\, d\bar{z})$. By negativity of both the terms and the fact that Ψ_0 has zero on a set of measure zero on M, $(\alpha_1,\beta)=0$, a.e. Thus Ω_{Ψ_0} is symplectic. □

III. PREQUANTUM LINE BUNDLE

In this section we briefly review the Quillen construction of the determinant line bundle of the Cauchy Riemann operator $\bar{\partial}_A=\bar{\partial}+A^{(0,1)}$,[4] which enables us to construct a prequantum line bundle on the vortex moduli space.

First let us note that a connection A on a $U(1)$-principal bundle induces a connection on any associated line bundle L. We will denote this connection also by A since the same "Lie-algebra valued 1-form" A (modulo representations) gives a covariant derivative operator enabling you to take derivatives of sections of L,[17] p. 348. A very clear description of the determinant line bundle can be found in Refs. 4 and 18. Here we mention the formula for the Quillen curvature of the determinant line bundle $\wedge^{\mathrm{top}}(\mathrm{Ker}\,\bar{\partial}_A)^* \otimes \wedge^{\mathrm{top}}(\mathrm{Coker}\,\bar{\partial}_A)=\det(\bar{\partial}_A)$, given the canonical unitary con-

nection ∇_Q, induced by the Quillen metric.[4] Recall that the affine space $\mathcal{A}$ (the notation as in Ref. 4) is an infinite-dimensional Kähler manifold. Here each connection is identified with its (0,1) part that is the holomorphic part. Since the connection A is unitary (i.e., $A=A^{(1,0)}+A^{(0,1)}$, s.t., $\overline{A^{(1,0)}}=-A^{(0,1)}$) this identification is easy. In fact, for every $A\in\mathcal{A}$, $T'_A(\mathcal{A})=\Omega^{0,1}(M,i\mathbb{R})$ and the corresponding Kähler form is given by

$$F(\alpha_1^{(0,1)},\alpha_2^{(0,1)})=\mathrm{Re}\int_M(\alpha_1^{(0,1)}\wedge *_2\alpha_2^{(0,1)}),=-\frac{1}{2}\int_M\alpha_1\wedge\alpha_2,$$

where $\alpha^{(0-1)}$, $\beta^{(0,1)}\in\Omega^{0,1}(M,i\mathbb{R})$ and $*_2$ is the Hodge-star operator such that $*_2(\eta\,dz)=-\bar{\eta}\,d\bar{z}$ and $*_2(\bar{\eta}\,d\bar{z})=\eta\,dz$, and we have used $\overline{\alpha_i^{(0,1)}}=-\alpha_i^{(1,0)}$, $i=1,2$. Let ∇_Q be the connection induced from the Quillen metric. Then the Quillen curvature of $\det(\bar{\partial}_A)$ is

$$\mathcal{F}(\nabla_Q)=\frac{i}{\pi}F.$$

IV. PREQUANTUM BUNDLE ON $\mathcal{M}$

First we note that to the connection A we can add any one form and still obtain a derivative operator.

Let $\omega=h^2\,dz\wedge d\bar{z}$ where recall h is real. Let $\theta=h\,dz$, $\bar{\theta}=h\,d\bar{z}$ be 1-forms (Ref. 19, p. 28), such that $\omega=\theta\wedge\bar{\theta}=h^2\,dz\wedge d\bar{z}$. Let Ψ_0 be the same *fixed* section used to define Ω_{Ψ_0}. Recall that Ψ_0 has zero on a set of measure zero on M. Note, that $\Psi H\bar{\Psi}_0$ is a smooth function on M. Thus $B^{(0,1)}=\Psi H\bar{\Psi}_0\bar{\theta}$ is a (0,1) form we would like to add to the connection $A^{(0,1)}$ to make another connection form. Note that $B^{(0,1)}$ is gauge invariant, since Ψ and Ψ_0 gauge transform in the same way. Note that $A^{(0,1)}\pm B^{(0,1)}$ are the (0,1) parts of a connection defined by $A\pm B=A^{(0,1)}\pm B^{(0,1)}+A^{(1,0)}+\pm B^{(1,0)}$, where $B^{(1,0)}$ is defined to be $\overline{B^{(1,0)}}=-B^{(0,1)}$.

Definitions: Let us denote by $\mathcal{L}_\pm=\det(\bar{\partial}+A^{(0,1)}\pm B^{(0,1)})$ a determinant bundle on $\mathcal{T}_\pm=\{A^{(0,1)}\pm\Psi H\bar{\Psi}_0\bar{\theta}|A\in A,\Psi\in\Gamma(M,L)\}$ that is isomorphic to $\mathcal{C}=\mathcal{A}\times\Gamma(M,L)$.

Thus $\mathcal{P}_{\Psi_0}=\mathcal{L}_+\otimes\mathcal{L}_-$ well-defined line bundle on $\mathcal{C}$.

Lemma 4.1: *$\mathcal{P}_{\Psi_0}$ is a well-defined line bundle over $\mathcal{M}\subset\mathcal{C}/G$, where G is the gauge group.*

Proof: First consider the Cauchy-Riemann operator $D=\bar{\partial}+A^{(0,1)}+B^{(0,1)}$. Under the gauge transformation, $D=\bar{\partial}+A^{(0,1)}+B^{(0,1)}\to D_g=g(\bar{\partial}+A^{(0,1)}+B^{(0,1)})g^{-1}$. We can show that the operators D and D_g have an isomorphic kernel and cokernel and their corresponding Laplacians have the same spectrum and the eigenspaces are of the same dimension. Let Δ denote the Laplacian corresponding to D and Δ_g that correspond to D_g. The Laplacian is $\Delta=\tilde{D}D$, where $\tilde{D}=\partial+A^{(1,0)}+B^{(1,0)}$, where we recall that $\overline{A^{(1,0)}}=-A^{(0,1)}$ and $\overline{B^{(1,0)}}=-B^{(0,1)}$. Note that $\tilde{D}\to\tilde{D}_g=g\tilde{D}g^{-1}$ under a gauge transformation. Then $\Delta_g=g\,\Delta g^{-1}$. Thus, the isomorphism of eigenspaces is $s\to gs$. We describe here how to define the line bundle on the moduli space. Let $K^a(\Delta)$ be the direct sum of eigenspaces of the operator Δ of eigenvalues $<a$, over the open subset $U^a=\{A^{(0,1)}+B^{(0,1)}|a\notin\mathrm{Spec}\,\Delta\}$ of the affine space $\mathcal{T}_+$. The determinant line bundle is defined using the exact sequence,

$$0\to\mathrm{Ker}\,D\to K^a(\Delta)\to D(K^a(\Delta))\to\mathrm{Coker}\,D\to 0.$$

Thus one identifies the following.

$\wedge^{\mathrm{top}}(\mathrm{Ker}\,D)^*\otimes\wedge^{\mathrm{top}}(\mathrm{Coker}\,D)$ with $\wedge^{\mathrm{top}}(K^a(\Delta))^*\otimes\wedge^{\mathrm{top}}(D(K^a(\Delta)))$ (see Ref. 18, for more details) and there is an isomorphism of the fibers as $D\to D_g$. Thus one can identify

$$\wedge^{\mathrm{top}}(K^a(\Delta))^*\otimes\wedge^{\mathrm{top}}(D(K^a(\Delta)))\equiv\wedge^{\mathrm{top}}(K^a(\Delta_g))^*\otimes\wedge^{\mathrm{top}}(D(K^a(\Delta_g))).$$

By extending this definition from U^a to $V^a=\{(A,\Psi)|a\notin\mathrm{Spec}\,\Delta\}$, an open subset of $\mathcal{C}$, we can define the fiber over the quotient space V^a/G to be the equivalence class of this fiber. Covering $\mathcal{C}$ with open sets of the type V^a, we can define it on $\mathcal{C}/G$. Then we can restrict it to $\mathcal{M}\subset\mathcal{C}/G$.

Similarly, one can deal with the other case of $\bar{\partial}+A^{(0,1)}-B^{(0,1)}$. Let $([A],[\Psi]) \in \mathcal{C}/G$ where $[A],[\Psi]$ are gauge equivalence classes of A, Ψ, respectively. Then associated to the equivalence class $([A],[\Psi])$ in the base space, there is an equivalence class of fibers coming from the identifications of $\det(\bar{\partial}+A^{(0,1)}-B^{(0,1)})$ with $\det\mathbf{(}g(\bar{\partial}+A^{(0,1)}-B^{(0,1)})g^{-1}\mathbf{)}$, as mentioned in the previous case.

This way one can prove that P_{Ψ_0} is well defined on $\mathcal{C}/G$. Then we restrict it to $\mathcal{M} \subset \mathcal{C}/G$.

A. Curvature and symplectic form

Let $p=(A,\Psi) \in \mathcal{S}$. Let X, $Y \in T_{[p]}\mathcal{M}$. Since $T_{[p]}\mathcal{M}$ can be identified with a subspace in T_pS orthogonal to T_pO_p, if we write $X=(\alpha_1,\beta)$ and $Y=(\alpha_2,\eta)$, $\alpha_1,\alpha_2 \in T_A\mathcal{A}=\Omega^1(M,i\mathbb{R})$, and β, $\eta \in T_\Psi\Gamma(M,L)=\Gamma(M,L)$, then X, Y can be said to satisfy (a) X, $Y \in T_pS$ and (b) X,Y are $\mathcal{G}$ orthogonal to T_pO_p, the tangent space to the gauge orbit.

Let $\mathcal{F}_{\mathcal{L}_\pm}$ denote the Quillen curvatures of the determinant line bundles $\mathcal{L}_\pm$, respectively. $\mathcal{L}_\pm$ are determinants of Cauchy-Riemann operators of the connections $A^{(0,1)} \pm \Psi H \bar{\Psi}_0 \bar{\theta}$. Thus, in the curvature, we will have $\alpha_1^{(0,1)} \pm \beta H \bar{\Psi}_0 \bar{\theta}$ and $\alpha_2^{(0,1)} \pm \eta H \bar{\Psi}_0 \bar{\theta}$ (see Quillen's formula in the section above),

$$\mathcal{F}_{\mathcal{L}_\pm}(X,Y) = \frac{i}{\pi}\mathrm{Re}\int_M (\alpha_1^{(0,1)} \pm \beta H \bar{\Psi}_0 \bar{\theta}) \wedge *_2(\alpha_2^{(0,1)} \pm \eta H \bar{\Psi}_0 \bar{\theta})$$

$$= \frac{i}{\pi}\mathrm{Re}\int_M (\alpha_1^{(0,1)} \pm \beta H \bar{\Psi}_0 \bar{\theta}) \wedge (-\alpha_2^{(1,0)} \pm \bar{\eta} H \Psi_0 \theta).$$

Note that $\mathrm{Re}\int_M \alpha_1^{(0,1)} \wedge \alpha_2^{(1,0)} = (1/2)\int_M \alpha_1 \wedge \alpha_2$, where we have used the fact that $\alpha_i = \alpha^{(0,1)} + \alpha_i^{(1,0)}$, s.t., $\overline{\alpha_i^{(0,1)}} = -\alpha_i^{(1,0)}$, $i=1,2$. We have also used that $\bar{\theta} \wedge \theta = -\omega = 2ih^2\, dx \wedge dy$, is purely imaginary. One can easily compute that

$$(\mathcal{F}_{\mathcal{L}+} + \mathcal{F}_{\mathcal{L}-})(X,Y) = \frac{i}{\pi}\left[-\int_M \alpha_1 \wedge \alpha_2 - \int_M (\beta H \bar{\eta} - \bar{\beta} H \eta)|\Psi_0|_H^2 \omega \right] = \frac{i}{\pi}\Omega_{\Psi_0}(X,Y).$$

Now $A^{(0,1)}$ is holomorphic w.r.t. the complex structure $*_1$ and Ψ is holomorphic w.r.t. multiplying by i, $A^{(0,1)} \pm B^{(0,1)}$ is holomorphic w.r.t. the complex structure $\mathcal{I}$. Thus $\mathcal{L}_+$, $\mathcal{L}_-$, and $\mathcal{P}_{\Psi_0}$ are holomorphic (the same argument as in Ref. 4).

Thus, we have proven the following theorem.

Theorem 4.2: *$\mathcal{P}_{\Psi_0} = \mathcal{L}_+ \otimes \mathcal{L}_-$ is a well-defined holomorphic line bundle on $\mathcal{M}$ whose Quillen curvature is $\mathcal{F}_{\mathcal{L}+} + \mathcal{F}_{\mathcal{L}-}$, which is $(i/\pi)\Omega_{\Psi_0}$. Thus $\mathcal{P}_{\Psi_0}$ is a prequantum bundle on $\mathcal{M}$.*

B. Polarization

In passing from prequantization to quantization, one needs a polarization. It can be shown that the almost complex structure $\mathcal{I}$ is integrable on $\mathcal{M}$ (see, for example, Ruback's argument mentioned in Ref. 9 or matscinet review of Refs. 11 and 10). In fact, Ω_{Ψ_0} is a Kähler form and $\mathcal{G}_{\Psi_0}(X,Y) = \Omega_{\Psi_0}(X,\mathcal{I}Y)$ is a Kähler metric on the moduli space (since it is positive definite). $\mathcal{P}_{\Psi_0}$ is a holomorphic line bundle on $\mathcal{M}$. Thus we can take holomorphic square integrable sections of $\mathcal{P}_{\Psi_0}$ as our Hilbert space. The dimension of the Hilbert space is not easy to compute. [For instance, the holomorphic sections of the determinant line bundle on the moduli space of flat connections for $SU(2)$ gauge group is the Verlinde dimension of the space of conformal blocks in a certain conformal field theory.] This would be a topic for future work.

C. Remark

As Ψ_0 varies, the corresponding line bundles are all topologically equivalent since the curvature forms have to be of integral cohomology, and that would be constant. Thus, they have the same Chern class. However, they may not be holomorphically equivalent.

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Removable singularities for solutions of coupled Yang-Mills-Dirac equations

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We prove a removable singularity theorem for solutions of coupled Yang-Mills-Dirac equations on compact four-dimensional manifolds. We show that a field satisfying the coupled equations with a point singularity is gauge equivalent to a smooth field if the energy functional is finite. The hypotheses are very natural. Only conformally invariant conditions are placed on force field and particle field interacting with the force field. It is noticeable that there is no assumption on the derivative of the particle field. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We consider the problem of removable isolated singularities of coupled Yang-Mills-Dirac fields in four dimensions.

In the case of non-coupled fields, i.e., pure Yang-Mills fields, Uhlenbeck's theorem[1] states that apparent point singularities in finite action solutions may be removed by a continuous gauge transformation.

Parker[2] generalized the result to coupled systems in four dimensions: solutions of coupled Yang-Mills-Dirac equations cannot have point singularities if the total energy of the coupled field is finite.

As noted by Uhlenbeck, the coupled equations (2.1) becomes elliptic in A (connection 1-form) only when $d^*A=0$. This constraint is always satisfied in a specific local trivialization, which is called the broken Hodge gauge.[1] By making a gauge transformation to Hodge gauge, one can obtain a co-closed connection satisfying a system of equations whose principal part is the Laplacian. However, because of the borderline assumptions made on curvature, i.e. the Yang-Mills field F is required to be an element of the space L^2, the gauge transformation which gives the elliptic system need not be continuous[3] and, hence, the topology in the original bundle with which we began may be altered. Therefore, the heart of the proof is to show that $F \in L^p$ for some $p>2$. Then the gauge transformation to Hodge gauge can be continuous. At this point, standard elliptic theory applies.[3]

Distinguishing from Parker's method of estimating the total field, we estimate the curvature F and the particle field ϕ, respectively. This results in a meticulous analytic proof. First, small energy regularity is proved, then a broken Hodge gauge could be applied to prove that finite energy solutions of coupled field equations cannot have isolated singularities. It is noticeable that we place no condition on the derivative of ϕ.

For convenience, we concentrate on bundles over flat manifolds. For the regularity theory, the curvature of the base manifold itself is not particularly important. The restriction to a flat base manifold does not crucially affect our results.

In Sec. I we give a brief description of the problem. The basic geometric framework is well documented in the literatures.[2,1] In Sec. III we prove the small energy regularity, which allows us

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to apply the broken Hodge gauge. In Sec. IV, we make use of the broken Hodge gauge to prove that the finite energy solutions of the coupled field equations cannot have isolated singularities.

II. YANG-MILLS-DIRAC FIELDS

We assume (M,g) is a compact oriented four-dimensional Riemannian manifold with usual Riemannian connection ∇ and Riemannian curvature R.

Fix a principal bundle $\pi: P \to M$ with compact structure group G whose Lie algebra is denoted by $\mathfrak{g}$. If $\rho: G \to \mathrm{Aut}(\tilde{E})$ is a unitary representation of G, define vector bundle $E = P \times_\rho \tilde{E}$. We define a connection ∇^E on E, which is required to be compatible with the Riemannian structure. Locally, we represent ∇^E as a Lie-algebra valued 1-form $A \in \Gamma(\Lambda \otimes \mathrm{ad}\, E)$ and its curvature $F \in \Gamma(\Lambda^2 \otimes \mathrm{End}\, E)$ as the Lie-algebra valued 2-form $dA + \frac{1}{2}[A,A]$, where $[,]$ is the Lie bracket on $\mathfrak{g}$.

We also need to assume M admits spin structures. Let V be the spin bundle over M. Then we can form a product $V \otimes E$ of two complex vector bundles that are both four-dimensional, such that End $V = C(E)$, where $C(E)$ is the Clifford algebra associated with E. If $\{e_i\}$ is an orthonormal basis for E, $C(E)$ is the graded algebra generated by the relation $e_i e_j + e_j e_i = -2\delta_{ij}$.

Sections $\phi \in \Gamma(V \otimes E)$ are called *E-valued spinors*.

Define $\tilde{\nabla} = \nabla \otimes 1 + 1 \otimes \nabla^E$ to be the total covariant derivative on $V \otimes E$. Let $\{e^i\}$ be an orthonormal local frame around a point $x \in M$. Then the *Dirac operator*

$$\not{D}: \Gamma(V \otimes E) \to \Gamma(V \otimes E)$$

is defined for E-valued spinors by

$$\not{D} = e^i \tilde{\nabla}_i.$$

As we noted, the essential geometry occurs in the bundle, thus in the sequel we expediently ignore the curvature of the base manifold.

The following *Weitzenböck formula* gives an important algebraic decomposition for the square of Dirac operator into Laplacian and curvature terms,[2]

$$\not{D}^2 = \tilde{\nabla}^* \tilde{\nabla} + \frac{1}{2} e^i e^j F_{ij}.$$

The coupled Yang-Mills-Dirac equations are the following nonlinear system of partial differential equations:[2]

$$\begin{aligned} D^* F = J(\phi) :&= -\frac{1}{2} \langle \phi, e^i \varrho(\sigma^\alpha) \phi \rangle e_i \otimes \sigma_\alpha, \\ \not{D}\phi &= m\phi, \end{aligned} \tag{2.1}$$

where D is the exterior covariant derivative, $*: \Lambda^p \to \Lambda^{4-p}$ is the Hodge star operator, $\{\sigma_\alpha\}$ is a local orthogonal basis in $\Gamma(\mathrm{Ad}\, \mathfrak{g})$, $\varrho: \mathfrak{g} \to \mathrm{End}(\tilde{E})$ is the Lie algebra representation induced by the Lie group representation $\rho: G \to \mathrm{Aut}(\tilde{E})$, and $\langle , \rangle$ is the inner product on $V \otimes E$. The eigenvalue m of $\not{D}$ is a real constant since $\not{D}$ is self-adjoint.

Conformal invariance is crucial for our results. Let ω be a positive number, if u takes values in a vector bundle E, by setting $u_r(x) = r^\omega u(y)$ under the local scale transformation $y = rx (r > 0)$ the L^p norm of u will satisfy

$$\|u(y)\|_{L^p(\Omega(y))} = r^{4/p - \omega} \|u_r(x)\|_{L^p(\Omega(x))}.$$

If $\omega p = 4$, we say u has *conformal weight* ω under the L^p norm, i.e.,

$$\|u(y)\|_{L^p(\Omega(y))} = \|u_r(x)\|_{L^p(\Omega(x))}.$$

The curvature form F, the particle mass m, and the spinor ϕ have conformal weight $2,1$, and $3/2$, respectively.[2]

III. SMALL ENERGY REGULARITY

Now we consider the local behavior of the coupled equations (2.1). Since the removable singularity theorem is a fact about arbitrarily small domains, in the sequel we may assume M to be a domain on $\mathbb{R}^4$ with trivial spin structure. The ball of radius r on M will be denoted by B_r.

Definition 3.1: Let U be a domain on M, the energy of (F,ϕ) on U is defined by

$$E(F,\phi,U):=\int_U |F|^2\,dV_g+\left(\int_U |\phi|^{8/3}\,dV_g\right)^{3/4}=\|F\|^2_{L^2(U)}+\|\phi\|^2_{L^{8/3}(U)}.$$

Note that the energy is conformally invariant. It is crucial for our results.

The main result of this section is small energy regularity as the following, which will be proved at the end of this section.

Theorem 3.2: *There exists a constant $\varepsilon>0$ such that if (F,ϕ) is a smooth solution of the coupled Yang-Mills-Dirac equations* (2.1) on B_2, *satisfying $E(F,\phi,B_2)<\varepsilon$, then there holds*

$$\|F\|_{C^0(B_1)}+\|\phi\|_{C^0(B_1)}\le C(\|F\|_{L^2(B_2)}+\|\phi\|_{L^{8/3}(B_2)}),$$

where C is a positive constant depending only on ε.

A. Three subelliptic inequalities

Our starting point is the following three subelliptic inequalities, where $\{k_i\}$ are non-negative constants. Let Δ be the ordinary Laplacian on functions.

Proposition 3.3: There holds the following subelliptic inequalities for the solutions (F,ϕ) of the coupled Yang-Mills-Dirac equations (2.1):

$$\Delta|\phi|+k_1|F||\phi|\ge 0, \tag{3.1}$$

$$\Delta|\tilde{\nabla}\phi|+k_2(|F||\tilde{\nabla}\phi|+|\phi|^2)\ge 0, \tag{3.2}$$

$$\Delta|F|+k_3(|F|^2+|\phi||\tilde{\nabla}\phi|)\ge 0. \tag{3.3}$$

Proof: (i) Using Kato's inequality $|d|\phi||\le|\tilde{\nabla}\phi|$, we have

$$|\phi|\Delta|\phi|=\langle\phi,\tilde{\nabla}^*\tilde{\nabla}\phi\rangle+\langle\tilde{\nabla}\phi,\tilde{\nabla}\phi\rangle-|d|\phi||^2\ge\langle\phi,\tilde{\nabla}^*\tilde{\nabla}\phi\rangle.$$

Applying the Weitzenböck formula and noting $\not{D}^2\phi=m^2\phi$ gives

$$|\phi|\Delta|\phi|\ge\langle\phi,m^2\phi\rangle-\frac{1}{2}\langle\phi,e^ie^jF_{ij}(\phi)\rangle\ge-\frac{1}{2}\langle\phi,e^ie^jF_{ij}(\phi)\rangle\ge-|\phi||e^ie^jF_{ij}(\phi)|.$$

Dividing by $|\phi|$ then gives (3.1).

(ii) Set $\psi=\tilde{\nabla}\phi$. The Weitzenböck formula gives

$$\tilde{\nabla}^*\tilde{\nabla}\psi=\not{D}^2\psi-\frac{1}{2}e^ie^jF_{ij}\psi=\not{D}^2(\tilde{\nabla}\phi)-\frac{1}{2}e^ie^jF_{ij}\psi.$$

Combining the identity $\not{D}^2\tilde{\nabla}=\tilde{\nabla}\not{D}^2+J+2e^ie^jF_{ij}\tilde{\nabla}$ (Ref. 3) and $\not{D}^2\phi=m^2\phi$, we get

$$\tilde{\nabla}^*\tilde{\nabla}\psi = \tilde{\nabla}(\not{D}^2\phi) + J(\phi) + 2e^i e^j F_{ij}(\tilde{\nabla}\phi) - \tfrac{1}{2}e^i e^j F_{ij}\psi = \tilde{\nabla}(m^2\phi) + J(\phi) + \tfrac{3}{2}e^i e^j F_{ij}\psi$$
$$= m^2\psi + J(\phi) + \tfrac{3}{2}e^i e^j F_{ij}\psi.$$

Using Kato's inequality, we have

$$|\psi|\Delta|\psi| \geq \langle\psi, \tilde{\nabla}^*\tilde{\nabla}\psi\rangle = m^2|\psi|^2 + \langle\psi, J(\phi)\rangle + \left\langle\psi, \tfrac{3}{2}e^i e^j F_{ij}\psi\right\rangle \geq \langle\psi, J(\phi)\rangle + \left\langle\psi, \tfrac{3}{2}e^i e^j F_{ij}\psi\right\rangle$$
$$\geq -k_2|\psi|(|\phi|^2 + |F||\psi|).$$

Dividing by $|\psi|$ gives (3.2).

(iii) Differentiating the field equation $D^*F = J(\phi)$ and using Bianchi identity $DF = 0$, we have

$$(D^*D + DD^*)F = DJ.$$

The Laplacians $D^*D + DD^*$ and $\tilde{\nabla}^*\tilde{\nabla}$ differ by a curvature term:[1]

$$\tilde{\nabla}^*\tilde{\nabla}F - (D^*D + DD^*)F = [F, F].$$

Hence

$$\tilde{\nabla}^*\tilde{\nabla}F = [F, F] + DJ.$$

By Kato's inequality again,

$$|F|\Delta|F| \geq \langle F, \tilde{\nabla}^*\tilde{\nabla}F\rangle = \langle F, [F, F]\rangle + \langle F, DJ\rangle \geq -k_3|F|(|F|^2 + |DJ|).$$

Hence

$$\Delta|F| + k_3(|F|^2 + |DJ|) \geq 0.$$

By the definition of $J(\phi)$, a direct computation shows that

$$|DJ| \leq k_3'|\phi||\tilde{\nabla}\phi|,$$

which gives (3.3). ■

B. Some *a priori* estimates in PDE

Before proving Theorem 3.2, we state some standard *a priori* estimates in PDE that will be used repeatedly.

Theorem 3.4:[4] *Assume $n \geq 3$; B_1 is the unit ball in $\mathbb{R}^n$. Suppose $a^{ij} \in L^\infty(B_1)$ satisfies*

$$\lambda|\xi|^2 \leq a^{ij}(x)\xi_i\xi_j \leq \Lambda|\xi|^2, \quad \text{for any } x \in B_1,\ \xi \in R^n,$$

for some positive constants λ and Λ.

Assume $c \in L^{n/2}(B_1)$ and $f \in L^q(B_1)$ for some $q \in [2n/(n+2), n/2)$. Suppose that $u \in H^1(B_1)$ is a subsolution in the following sense:

$$\int_{B_1} a^{ij} D_i u\, D_j\varphi + cu\varphi \leq \int_{B_1} f\varphi,$$

for any $\varphi \in H_0^1(B_1)$ and $\varphi \geq 0$ in B_1, then $u^+ \in L^{q^*}_{\mathrm{loc}}(B_1)$ for $1/q^* = 1/q - 2/n$.

Moreover, there exists a small constant $\varepsilon > 0$ such that if $\|c\|_{L^{n/2}(B_1)} < \varepsilon$ there holds

$$\|u^+\|_{L^{q^*}(B_{1/2})} \leq C\{\|u^+\|_{L^2(B_1)} + \|f\|_{L^q(B_1)}\},$$

where $C = C(n, \lambda, \Lambda, q, \varepsilon)$ is a positive constant. ■

Theorem 3.5:[5] *Assume* $b \in L^q(U)$, $q > n/2$, $u^\lambda \in W^{1,2}_{\mathrm{loc}}(U)$ *with* $1/2 < \lambda \leq 1$, $u \geq 0$ *satisfy the following subelliptic inequality in a weak sense:*

$$\Delta u + bu \geq 0,$$

then u is bounded on compact subdomains of U. Moreover, if $B(x,a) \subset B(x_0,a_0) \subset U$, *there holds that*

$$|u^\lambda(x)|^2 \leq Ca^{-n} \int_{B(x_0,a_0)} |u^\lambda|^2,$$

where constant C depends on n, q, λ *and* $a_0^{2/n-1/q}\|b\|_{L^q(B(x_0,a_0))}$. ■

C. Small energy regularity

Now we start to prove Theorem 3.2 by the approach of applying the above *a priori* estimates to the coupled equations (2.1) in the case of four dimensions. In the proof, C is a constant varying from line to line and $B_1 \subset B_{R_1} \subset B_{R_2} \subset B_2$ are fixed balls with the same center.

Lemma 3.6: For any given $p \geq 4$, *there exists a positive constant* ε_p *such that if* $\|F\|^2_{L^2(B_2)} < \varepsilon_p$, *there holds that*

$$\|\phi\|_{L^p(B_{R_2})} \leq C_p \|\phi\|_{L^{8/3}(B_2)},$$

where C_p *is a positive constant depending on p and* ε_p.

Proof: By (3.1), ϕ *satisfies*

$$\Delta|\phi| + k_1|F||\phi| \geq 0.$$

Let $u = |\phi|$, $c = -k_1|F|$, $f = 0$ and $n = 4$. Note that $f \in L^q$ for any arbitrarily fixed $q \in [2n/(n+2), n/2) = [\frac{4}{3}, 2)$. Applying Theorem 3.4, there exists constant $\delta > 0$ such that if $\|c\|_{L^2(B_2)} < \delta$, i.e., $\|F\|_{L^2(B_2)} < \delta/k_1$, there holds that

$$\|\phi\|_{L^{q^*}(B_{R_2})} \leq C_q \|\phi\|_{L^2(B_2)},$$

where $q^* \in [4, +\infty)$. Noting that $\|\phi\|_{L^2(B_2)} \leq C\|\phi\|_{L^{8/3}(B_2)}$ and q^* runs over $[4, +\infty)$ while q runs over $[\frac{4}{3}, 2)$, we prove the lemma by choosing $\varepsilon = (\delta/k_1)^2$. ■

Next, we estimate the derivative of ϕ. Since F is smooth, Uhlenbeck's theorem[3] ensures that, by rescaling to get $\|F\|_{L^2}$ sufficiently small, there exists a continuous gauge transformation such that

$$\|A\|_{W^{1,2}(B_2)} \leq C(n)\|F\|_{L^2(B_2)},$$

where n is the dimension of the base manifold.

Then the Sobolev embedding theorem for four dimensions implies

$$\|A\|_{L^4(B_2)} \leq C\|F\|_{L^2(B_2)}.$$

Lemma 3.7: For any given $p < 4$ *there holds that*

$$\|\tilde{\nabla}\phi\|_{L^p(B_{R_2})} \leq C_p(1 + \|F\|_{L^2(B_2)})\|\phi\|_{L^{4p/(4-p)}(B_2)},$$

where constant C_p *depends on p.*

Proof: We write the Dirac operator in the form $\not{D} = e^i(\nabla_i + A_i)$; then the eigenvalue equation $\not{D}\phi = m\phi$ can be rewritten as

$$e^i \nabla_i \phi = m\phi - e^i A_i \phi.$$

Applying the interior estimate for first-order elliptic operator and noting m is locally constant, we get

$$\begin{aligned}\|\phi\|_{W^{1,p}(B_{R_2})} &\le C\|\phi\|_{L^p(B_2)} + C\|m\phi\|_{L^p(B_2)} + C\|A\phi\|_{L^p(B_2)}\\ &\le C\|\phi\|_{L^p(B_2)} + C\|m\|_{L^4(B_2)}\|\phi\|_{L^{4p/(4-p)}(B_2)} + C\|A\|_{L^4(B_2)}\|\phi\|_{L^{4p/(4-p)}(B_2)}\\ &\le C\|\phi\|_{L^{4p/(4-p)}(B_2)} + C\|\phi\|_{L^{4p/(4-p)}(B_2)} + C\|F\|_{L^2(B_2)}\|\phi\|_{L^{4p/(4-p)}(B_2)}\\ &\le C(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{4p/(4-p)}(B_2)}.\end{aligned}$$

Hence,

$$\begin{aligned}\|\tilde{\nabla}\phi\|_{L^p(B_{R_2})} &\le \|\nabla\phi\|_{L^p(B_{R_2})} + \|A\phi\|_{L^p(B_{R_2})} \le \|\phi\|_{W^{1,p}(B_{R_2})} + \|A\phi\|_{L^p(B_{R_2})}\\ &\le C(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{4p/(4-p)}(B_2)} + C\|F\|_{L^2(B_2)}\|\phi\|_{L^{4p/(4-p)}(B_2)}\\ &\le C(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{4p/(4-p)}(B_2)}.\end{aligned}$$

■

Since $4p/(4-p) \ge 4 \Leftrightarrow 2 \le p < 4$, the arguments of Lemma 3.6 and Lemma 3.7 can be used to obtain the following corollary.

Corollary 3.8: Assume $2 \le p < 4$. *There exists a positive constant* ε_p *such that if* $\|F\|^2_{L^2(B_2)} < \varepsilon_p$ *there holds that*

$$\|\tilde{\nabla}\phi\|_{L^p(B_{R_2})} \le C_p(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{8/3}(B_2)},$$

where C_p *is a positive constant depending on* p *and* ε_p.

Proof: By an argument similar to the one used in Lemma 3.7, we have

$$\|\tilde{\nabla}\phi\|_{L^p(B_{R_2})} \le C_p(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{4p/(4-p)}(B_{R_3})}$$

with some ball B_{R_3} satisfying $B_{R_2} \subset B_{R_3} \subset B_2$.

Then by an argument similar to the one used in Lemma 3.6, there exists a positive constant ε_p such that if $\|F\|^2_{L^2(B_2)} < \varepsilon_p$ there holds that

$$\|\phi\|_{L^{4p/(4-p)}(B_{R_3})} \le C_p\|\phi\|_{L^{8/3}(B_2)}.$$

This proves the corollary. ■

Corollary 3.9: There exists a small constant $\varepsilon_1 > 0$ *such that if* $\|F\|^2_{L^2(B_2)} < \varepsilon_1$ *there holds that*

$$\||\phi||\tilde{\nabla}\phi|\|_{L^{4/3}(B_{R_2})} \le C(1+\|F\|_{L^2(B_2)})\|\phi\|^2_{L^{8/3}(B_2)},$$

where C_p *is a positive constant depending on* p *and* ε_1.

Proof: Hölder's inequality gives

$$\||\phi||\tilde{\nabla}\phi|\|_{L^{4/3}(B_{R_2})} \le \|\phi\|_{L^4(B_{R_2})}\|\tilde{\nabla}\phi\|_{L^2(B_{R_2})},$$

where $\|\phi\|_{L^4(B_{R_2})}$ and $\|\tilde{\nabla}\phi\|_{L^2(B_{R_2})}$ can be estimated by Lemma 3.6 and Corollary 3.8, respectively. ■

Now we can get the L^4 norm estimates for $\tilde{\nabla}\phi$ and F as the following Lemma 3.10 Lemma 3.11, respectively, which are combinations of Theorem 3.4 with Corollary 3.8 and Corollary 3.9, respectively.

Lemma 3.10: There exists a small constant $\varepsilon_2 > 0$ *such that if* $\|F\|^2_{L^2(B_2)} < \varepsilon_2$ *there holds that*

$$\left\|\tilde{\nabla}\phi\right\|_{L^4(B_{R_1})} \le C(\|\phi\|_{L^{8/3}(B_2)} + \|\phi\|^2_{L^{8/3}(B_2)} + \|F\|_{L^2(B_2)}\|\phi\|_{L^{8/3}(B_2)}),$$

where constant C depends on ε_2.

Proof: Recall in Proposition 3.3 that $\tilde{\nabla}\phi$ satisfies the subelliptic inequality

$$\Delta|\tilde{\nabla}\phi| + k_2(|F||\tilde{\nabla}\phi| + |\phi|^2) \ge 0.$$

Applying Theorem 3.4 with $u=|\tilde{\nabla}\phi|$, $c=-k_2|F|$, $f=k_2|\phi|^2$, $n=4$, and $q=2n/(n+2)=\frac{4}{3}$ (consequently $q^*=4$), there exists small constant $\delta>0$ such that if $\|c\|_{L^2(B_{R_2})}<\delta$, i.e., $\|F\|^2_{L^2(B_{R_2})} < (\delta/k_2)^2$, there holds that

$$\|\tilde{\nabla}\phi\|_{L^4(B_{R_1})} \le C_\delta(\|\tilde{\nabla}\phi\|_{L^2(B_{R_2})} + \||\phi|^2\|_{L^{4/3}(B_{R_2})}) \le C_\delta(\|\tilde{\nabla}\phi\|_{L^2(B_{R_2})} + \|\phi\|^2_{L^{8/3}(B_2)}).$$

Applying Corollary 3.8 with $p=2$, there exists small constant $\delta'>0$ such that if $\|F\|^2_{L^2(B_2)} < \delta'$ there holds that

$$\|\tilde{\nabla}\phi\|_{L^2(B_{R_2})} \le C_{\delta'}(1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{8/3}(B_2)}.$$

Choose $\varepsilon_2 \le \min\{(\delta/k_2)^2, \delta'\}$, then if $\|F\|^2_{L^2(B_2)} < \varepsilon_2$ there holds that

$$\begin{aligned}\|\tilde{\nabla}\phi\|_{L^4(B_{R_1})} &\le C_{\varepsilon_2}((1+\|F\|_{L^2(B_2)})\|\phi\|_{L^{8/3}(B_2)} + \|\phi\|^2_{L^{8/3}(B_2)}) \\ &\le C_{\varepsilon_2}(\|\phi\|_{L^{8/3}(B_2)} + \|\phi\|^2_{L^{8/3}(B_2)} + \|F\|_{L^2(B_2)}\|\phi\|_{L^{8/3}(B_2)}).\end{aligned}$$

■

Lemma 3.11: There exists small constant $\varepsilon_3>0$ *such that if* $\|F\|^2_{L^2(B_2)}<\varepsilon_3$ *there holds that*

$$\|F\|_{L^4(B_{R_1})} \le C(\|F\|_{L^2(B_2)} + \|\phi\|^2_{L^{8/3}(B_2)} + \|F\|_{L^2(B_2)}\|\phi\|^2_{L^{8/3}(B_2)}),$$

where constant C depends on ε_3.

Proof: Recall in Proposition 3.3 F satisfies the subelliptic inequality:

$$\Delta|F| + k_3|F||F| + k_3|\phi||\tilde{\nabla}\phi| \ge 0.$$

Applying Theorem 3.4 with $u=|F|$, $c=-k_3|F|$, $f=k_3|\phi||\tilde{\nabla}\phi|$, $n=4$, and $q=2n/(n+2)=\frac{4}{3}$ (consequently $q^*=4$), there exists small constant $\delta>0$ such that if $\|c\|_{L^2(B_{R_2})}<\delta$, i.e., $\|F\|^2_{L^2(B_{R_2})} < (\delta/k_3)^2$, there holds that

$$\|F\|_{L^4(B_{R_1})} \le C_\delta(\|F\|_{L^2(B_{R_2})} + \||\phi||\tilde{\nabla}\phi|\|_{L^{4/3}(B_{R_2})}) \le C_\delta(\|F\|_{L^2(B_2)} + \||\phi||\tilde{\nabla}\phi|\|_{L^{4/3}(B_{R_2})}).$$

Choose $\varepsilon_3 \le \min\{\varepsilon_1, (\delta/k_3)^2\}$; then if $\|F\|^2_{L^2(B_2)}<\varepsilon_3$ we can substitute the estimate for $\||\phi||\tilde{\nabla}\phi|\|_{L^{4/3}(B_{R_2})}$ in Corollary 3.9 onto the right-hand side of the inequality above, so we get

$$\begin{aligned}\|F\|_{L^4(B_{R_1})} &\le C_{\varepsilon_3}(\|F\|_{L^2(B_2)} + C_{\varepsilon_3}(1+\|F\|_{L^2(B_2)})\|\phi\|^2_{L^{8/3}(B_2)}) \\ &\le C_{\varepsilon_3}(\|F\|_{L^2(B_2)} + \|\phi\|^2_{L^{8/3}(B_2)} + \|F\|_{L^2(B_2)}\|\phi\|^2_{L^{8/3}(B_2)}).\end{aligned}$$

■

Now we can prove the main result of this section.

Proof of Theorem 3.2: Set $u=|F|+|\phi|$ and $b=k_4(|F|+|\tilde{\nabla}\phi|)$. Adding (3.1) and (3.3) gives

$$\Delta u + bu \ge 0.$$

Choose $\varepsilon=\min\{\varepsilon_2,\varepsilon_3\}$. If $\|F\|^2_{L^2(B_2)}<\varepsilon$ we can apply Lemma 3.10 and Lemma 3.11 to get a bound on $\|b\|_{L^4(B_{R_1})}$ as the following:

$$\begin{aligned}\|b\|_{L^4(B_{R_1})} &\le k_4\|F\|_{L^4(B_{R_1})}+k_4\|\tilde{\nabla}\phi\|_{L^4(B_{R_1})}\\ &\le C(\|F\|_{L^2(B_2)}+\|\phi\|_{L^{8/3}(B_2)}+\|\phi\|^2_{L^{8/3}(B_2)}+\|F\|_{L^2(B_2)}\|\phi\|_{L^{8/3}(B_2)}+\|F\|_{L^2(B_2)}\|\phi\|^2_{L^{8/3}(B_2)}),\end{aligned}$$

where constant C depends on ε.

Now Theorem 3.5 applies with $u=|F|+|\phi|$, $b=k_4(|F|+|\tilde{\nabla}\phi|)$, $\lambda=1$, and $q=4$. For any $x\in B_1$ there holds that

$$(|F(x)|+|\phi(x)|)^2\le C\int_{B_{R_1}}(|F|+|\phi|)^2\le C\int_{B_2}(|F|+|\phi|)^2.$$

Hence

$$\|F\|_{C^0(B_1)}+\|\phi\|_{C^0(B_1)}\le C(\|F\|_{L^2(B_2)}+\|\phi\|_{L^2(B_2)})\le C(\|F\|_{L^2(B_2)}+\|\phi\|_{L^{8/3}(B_2)}).$$

Since $\|F\|_{L^2(B_2)}$ and $\|\phi\|_{L^{8/3}(B_2)}$ are both invariant under dilation, the size of the ball does not affect the constant C of Theorem 3.5. ■

Theorem 3.2 is immediately applicable to the problem of the behavior of fields around a singularity.

Corollary 3.12: There exists a constant $\varepsilon>0$ such that if (F,ϕ) is a smooth solution of the coupled Yang-Mills-Dirac equations (2.1) *on $B_2\backslash\{0\}$ satisfying $E(F,\phi,B_2)<\varepsilon$; then for any $x\in B_1\backslash\{0\}$ there holds that*

$$|F(x)||x|^2+|\phi(x)||x|^{3/2}\le C(\|F\|_{L^2(B_2)}+\|\phi\|_{L^{8/3}(B_2)}),$$

where constant C depends on ε.

Proof: Choose ε as in Theorem 3.2. For any fixed $x_0\in B_1\backslash\{0\}$ we define

$$\tilde{F}(x):=\left(\frac{|x_0|}{2}\right)^2F\left(x_0+\frac{|x_0|}{2}x\right),\quad \tilde{\phi}(x):=\left(\frac{|x_0|}{2}\right)^{3/2}\phi\left(x_0+\frac{|x_0|}{2}x\right).$$

It is clear that $(\tilde{F},\tilde{\phi})$ is a smooth solution of the coupled Yang-Mills-Dirac equations on B_2 and $E(\tilde{F},\tilde{\phi},B_2)<\varepsilon$ by conformal invariance. Applying Theorem 3.2, we have

$$\|\tilde{F}\|_{C^0(B_1)}+\|\tilde{\phi}\|_{C^0(B_1)}\le C(\|\tilde{F}\|_{L^2(B_2)}+\|\tilde{\phi}\|_{L^{8/3}(B_2)}).$$

Scaling back, we prove the corollary. ■

IV. REMOVABLE SINGULARITY THEOREM

Now we state the main result of this paper, which will be proved at the end.

Theorem 4.1 (removable singularity): *Let (F,ϕ) be a smooth solution of the coupled Yang-Mills-Dirac equations with finite energy on $B_2\backslash\{0\}$. Then (F,ϕ) is gauge equivalent by a continuous gauge transformation to a smooth solution on B_2.*

By rescaling, we can assume that the energy $E(F,\phi,B_2)$ is sufficiently small, i.e., $E(F,\phi,B_2)<\varepsilon$ with ε is chosen as in Corollary 3.12. Then for any $x\in B_1\backslash\{0\}$ there holds that

$$|F(x)||x|^2\le CE(F,\phi,B_2)\le C\varepsilon.$$

The above inequality guarantees the existence of a specific choice of gauge that is the so called *broken Hodge gauge*. The existence of this gauge is crucial for removing singularities, since in such a gauge the powerful regularity argument of elliptic theory can be applied to the coupled

equations (2.1). An important theorem of Uhlenbeck[1] provides such a gauge around the singularity and includes rather specific information about the connection and curvature forms in this gauge.

Theorem 4.2:[2,1] *Let A be a smooth connection form on $B_2\backslash\{0\}$ with curvature F. Then there is a constant $\kappa>0$ such that if $|F(x)||x|^2\leq\varepsilon<\kappa$ on $B_1\backslash\{0\}$ then there exists a broken Hodge gauge on $B_1\backslash\{0\}$ whose properties we now describe. Set*

$$U_i=\{x:2^{-i}\leq|x|\leq 2^{-i+1}\},\quad i=1,2,3,\ldots,$$

$$S_i=\{x:|x|=2^{-i}\},\quad i=1,2,3,\ldots\ .$$

The broken Hodge gauge is smooth on each U_i and the gauges from U_i and U_{i+1} agree on S_i. Write

$$A^i=A\big|_{U_i},\quad F^i=F\big|_{U_i}.$$

Then $\{A^i\}$ and $\{F^i\}$ satisfy

(a) $d^*A^i=0$,

(b) $A^i_\theta\big|_{S_i}=A^{i+1}_\theta\big|_{S_i}$, $\quad A_\theta=$ *tangential components of* A,

(c) $d^*A^i_\theta\big|_{S_i}=0=d^*A^i_\theta\big|_{S_{i-1}}$,

(d) $\displaystyle\int_{S_i}A^i_r=0=\int_{S_{i-1}}A^i_r$, $\quad A_r=$ *radial component of* A,

$$(e)\quad \int_{S_0}|A^1|^2\leq b\int_{S_0}|F^1|^2, \tag{4.1}$$

$$(f)\quad \int_{U_i}|A^i|^4\leq c_0\varepsilon^2\int_{U_i}|F^i|^2,\quad \int_{B_1}|A|^4\leq c_0\varepsilon^2\int_{B_1}|F|^2\leq c_0\varepsilon^4, \tag{4.2}$$

for some positive constants b and c_0 whenever ε is sufficiently small. ■

Since we are assuming that the energy of the fields is small enough, we can apply Corollary 3.12 to obtain a field on $B_2\backslash\{0\}$ satisfying the hypotheses of Theorem 4.2. Hence ***there exists a broken Hodge gauge***. In the sequel the broken Hodge gauge is used as a "reference frame" in which to observe the particle field and to obtain our gauge dependent estimates.

Proof of Theorem 4.1: The proof consists of three parts. We will give the estimates with boundary data for F, ϕ, and $\nabla\phi$, respectively. In the sequel $\{c_k\}$ are nonnegative constants.

(i) **Part 1: estimate for F with boundary data.** Integrating by parts on U_i gives

$$\int_{U_i}|F^i|^2=\int_{U_i}\langle D^*F^i,A^i\rangle-\frac{1}{2}\int_{U_i}\langle F^i,[A^i,A^i]\rangle+\left(\int_{S_{i-1}}-\int_{S_i}\right)A^i_\theta\wedge(*F^i)_\theta:=I_1+I_2+\text{boundary term}.$$

Using the field equation $D^*F=J(\phi)$ and the properties of broken Hodge gauge, we get

$$\begin{aligned}I_1&=\int_{U_i}\langle J(\phi),A^i\rangle\leq c_1\int_{U_i}|\phi|^2|A^i|=c_1\int_{U_i}(\varepsilon^{1/4}|\phi|^2)(\varepsilon^{-1/4}|A^i|)\\&\leq c_2\left(\varepsilon^{1/3}\int_{U_i}|\phi|^{8/3}+\varepsilon^{-1}\int_{U_i}|A^i|^4\right)\leq c_2\left(\varepsilon^{1/3}\int_{U_i}|\phi|^{8/3}+c_0\varepsilon\int_{U_i}|F^i|^2\right),\end{aligned}$$

$$I_2 \le \frac{1}{2}\int_{U_i} |F^i||A^i|^2$$
$$\le \frac{1}{2}\left(\int_{U_i}|F^i|^2\right)^{1/2}\left(\int_{U_i}|A^i|^4\right)^{1/2} \le \frac{1}{2}\left(\int_{U_i}|F^i|^2\right)^{1/2}\left(c_0\varepsilon^2\int_{U_i}|F^i|^2\right)^{1/2} \le c_3\varepsilon\int_{U_i}|F^i|^2.$$

Since the energy bound ε appearing in I_1 and I_2 could be sufficiently small, we have

$$(1-\varepsilon')\int_{U_i}|F^i|^2 \le c_4\varepsilon^{1/3}\int_{U_i}|\phi|^{8/3} + \left(\int_{S_{i-1}} - \int_{S_i}\right)A^i_\theta \wedge (*F^i)_\theta.$$

Summing on i, noting that $|A^1_\theta \wedge (*F^1)_\theta| \le |A^1||F^1|$, and using Hölder's inequality gives

$$(1-\varepsilon')\int_{B_1}|F|^2 \le c_4\varepsilon^{1/3}\int_{B_1}|\phi|^{8/3} + \left(\int_{\partial B_1}|A^1|^2\right)^{1/2}\left(\int_{\partial B_1}|F^1|^2\right)^{1/2}.$$

Noting the property (4.1) of the broken Hodge gauge, we get

$$\int_{B_1}|F|^2 \le C\varepsilon^{1/3}\int_{B_1}|\phi|^{8/3} + C\int_{\partial B_1}|F|^2.$$

By a scaling argument, we have, for $0 \le r \le 1$;

$$\int_{B_r}|F|^2 \le C\varepsilon^{1/3}\int_{B_r}|\phi|^{8/3} + Cr\int_{\partial B_r}|F|^2. \tag{4.3}$$

(ii) **Part 2: estimate for ϕ with boundary data.** In the sequel, we denote $\|\ \|_{W^{k,p}(B)}$ by $\|\ \|_{B,k,p}$, where B is the unit ball B_1.

Write the eigenvalue equation $\not{D}\phi = m\phi$ in the form $e^i\,\boldsymbol{\nabla}_i\phi = m\phi - e^iA_i\phi$. Choose a cutoff function $\eta_\rho \in C_0^\infty(B_{2\rho})$ with $2\rho < 1$ such that $\eta_\rho|_{B_\rho} \equiv 1$ and $|\boldsymbol{\nabla}\eta_\rho| \le C/\rho$. Then we have

$$e^i\nabla_i((1-\eta_\rho)\phi) = (1-\eta_\rho)e^i\,\boldsymbol{\nabla}_i\phi + e^i\boldsymbol{\nabla}_i(1-\eta_\rho)\phi = (1-\eta_\rho)(m\phi - e^iA_i\phi) + e^i\boldsymbol{\nabla}_i(1-\eta_\rho)\phi.$$

The estimate with boundary data for a first-order elliptic operator gives

$$\|(1-\eta_\rho)\phi\|_{B,1,8/5} \le C\|m\phi - e^iA_i\phi\|_{B,0,8/5} + C\|\boldsymbol{\nabla}\eta_\rho\,\phi\|_{B,0,8/5} + C\|\phi\|_{\partial B,1,8/5}.$$

Letting $\rho \to 0$, using

$$\lim_{\rho\to 0}\|\boldsymbol{\nabla}\eta_\rho\phi\|_{B,0,8/5} \le \lim_{\rho\to 0}\frac{C}{\rho}\|\phi\|_{B_{2\rho},0,8/5} = 0,$$

the Sobolev embedding theorem and (4.2), we get

$$\|\phi\|_{B,0,8/3} \le C\|m\phi - e^iA_i\phi\|_{B,0,8/5} + C\|\phi\|_{\partial B,1,8/5} \le C(\|m\|_{B,0,4} + \|A\|_{B,0,4})\|\phi\|_{B,0,8/3} + C\|\phi\|_{\partial B,1,8/5}$$
$$\le C(\|m\|_{B,0,4} + \sqrt[4]{c_0}\varepsilon)\|\phi\|_{B,0,8/3} + C\|\phi\|_{\partial B,1,8/5}.$$

We can assume $\|m\|_{B,0,4}$ is sufficiently small by a scaling argument. Noting ε is also sufficiently small, we transfer the term that contains $\|\phi\|_{B,0,8/3}$ on the right-hand side of the above inequality to the left-hand side. This gives

$$\|\phi\|_{B,0,8/3} \le C\|\phi\|_{\partial B,1,8/5} \le C\|\phi\|_{\partial B,0,8/3} + C\|\nabla\phi\|_{\partial B,0,8/5}.$$

By rescaling, we have for any $0 \le r \le 1$,

$$\left(\int_{B_r}|\phi|^{8/3}\right)^{3/8} \le C\left(r\int_{\partial B_r}|\phi|^{8/3}\right)^{3/8} + C\left(r\int_{\partial B_r}|\nabla\phi|^{8/5}\right)^{5/8}$$
$$\le C\left(r\int_{\partial B_r}|\phi|^{8/3}\right)^{3/8} + C\left(r\int_{\partial B_r}|\nabla\phi|^{8/5}\right)^{3/8}.$$

Thus

$$\int_{B_r}|\phi|^{8/3} \le Cr\int_{\partial B_r}|\phi|^{8/3} + Cr\int_{\partial B_r}|\nabla\phi|^{8/5}. \tag{4.4}$$

(iii) **Part 3: estimate for $\nabla\phi$ with boundary data.** Set $\bar{\phi}=(1/|\partial B|)\int_{\partial B}\phi$, $\psi=\phi-\bar{\phi}$. Choosing the same cut-off function η_ρ as in Part 2, we have

$$e^i\nabla_i((1-\eta_\rho)\psi) = (1-\eta_\rho)e^i\,\nabla_i\psi + e^i\nabla_i(1-\eta_\rho)\psi.$$

Again, the estimate with boundary data for the first-order elliptic operator gives

$$\|(1-\eta_\rho)\psi\|_{B,1,8/5} \le C\|e^i\,\nabla_i\psi\|_{B,0,8/5} + C\|\nabla\eta_\rho\psi\|_{B,0,8/5} + C\|\psi\|_{\partial B,1,8/5}.$$

Letting $\rho\to 0$, using

$$\lim_{\rho\to 0}\|\nabla\eta_\rho\psi\|_{B,0,8/5} = 0,$$

we get

$$\|\psi\|_{B,1,8/5} \le C\|e^i\nabla_i\psi\|_{B,0,8/5} + C\|\psi\|_{\partial B,1,8/5} := CI_3 + CI_4.$$

Since

$$e^i\,\nabla_i\psi = e^i\,\nabla_i\phi = m\phi - e^iA_i\phi = (m\psi - e^iA_i\psi) + (m\bar{\phi} - e^iA_i\bar{\phi}),$$

there holds that

$$I_3 \le \|m\psi - e^iA_i\psi\|_{B,0,8/5} + \|m\bar{\phi} - e^iA_i\bar{\phi}\|_{B,0,8/5}$$
$$\le (\|m\|_{B,0,4} + \|A\|_{B,0,4})\|\psi\|_{B,0,8/3} + (\|m\|_{B,0,8/5} + \|A\|_{B,0,8/5})|\bar{\phi}|$$
$$\le (\|m\|_{B,0,4} + \sqrt[4]{c_0}\varepsilon)\|\psi\|_{B,1,8/5} + (\|m\|_{B,0,8/5} + \|A\|_{B,0,8/5})|\bar{\phi}|.$$

Applying Poincaré's inequality gives an estimate for I_4:

$$I_4 = \|\psi\|_{\partial B,1,8/5} \le C\|\nabla\phi\|_{\partial B,0,8/5}.$$

Hence

$$\|\psi\|_{B,1,8/5} \le C(\|m\|_{B,0,4} + \sqrt[4]{c_0}\varepsilon)\|\psi\|_{B,1,8/5} + C(\|m\|_{B,0,8/5} + \|A\|_{B,0,8/5})|\bar{\phi}| + C\|\nabla\phi\|_{\partial B,0,8/5}.$$

Again, by the smallness of $\|m\|_{B,0,4}$ and ε, we get

$$\|\nabla\phi\|_{B,0,8/5} \le C(\|m\|_{B,0,8/5} + \|A\|_{B,0,8/5})|\bar{\phi}| + C\|\nabla\phi\|_{\partial B,0,8/5}$$
$$\le C(\|m\|_{B,0,4} + \|A\|_{B,0,4})\|\phi\|_{\partial B,0,8/3} + C\|\nabla\phi\|_{\partial B,0,8/5}.$$

Hence,

$$\int_B |\nabla\phi|^{8/5} \le C\left(\int_B |m|^4\right)^{2/5}\left(\int_{\partial B} |\phi|^{8/3}\right)^{3/5} + C\left(\int_B |A|^4\right)^{2/5}\left(\int_{\partial B} |\phi|^{8/3}\right)^{3/5} + C\int_{\partial B} |\nabla\phi|^{8/5}.$$

Applying Young's inequality to the first two terms on the right-hand side of the above inequality with conjugate indices $\frac{5}{2}$ and $\frac{5}{3}$, we have

$$\begin{aligned}\int_B |\nabla\phi|^{8/5} &\le C\delta\int_B |m|^4 + C\delta\int_B |A|^4 + \frac{C}{\sqrt[3]{\delta^2}}\int_{\partial B} |\phi|^{8/3} + C\int_{\partial B} |\nabla\phi|^{8/5} \\ &\le C\delta\int_B |m|^4 + C\ \delta c_0\varepsilon^2\int_B |F|^2 + \frac{C}{\sqrt[3]{\delta^2}}\int_{\partial B} |\phi|^{8/3} + C\int_{\partial B} |\nabla\phi|^{8/5},\end{aligned}$$

where $\delta>0$ is a sufficiently small constant. Hence, for $0\le r\le 1$,

$$\int_{B_r} |\nabla\phi|^{8/5} \le C\delta\int_{B_r} |m|^4 + Cc_0\ \delta\varepsilon^2\int_{B_r} |F|^2 + \frac{C}{\sqrt[3]{\delta^2}}r\int_{\partial B_r} |\phi|^{8/3} + Cr\int_{\partial B_r} |\nabla\phi|^{8/5}. \tag{4.5}$$

Finally, putting (4.3)–(4.5) together, we have for any $0\le r\le 1$ and some constant $C>0$, that

$$\int_{B_r} (|F|^2 + |\phi|^{8/3} + |\nabla\phi|^{8/5}) \le Cr\int_{\partial B_r} (|F|^2 + |\phi|^{8/3} + |\nabla\phi|^{8/5}) + Cr^4, \tag{4.6}$$

where the last term r^4 comes from the term $\int_{B_r}|m|^4$ in (4.5) by noting m is a constant locally.

Denote $f(r) := \int_{B_r}(|F|^2+|\phi|^{8/3}+|\nabla\phi|^{8/5})$; then (4.6) implies that

$$f(r) \le Crf'(r) + Cr^4. \tag{4.7}$$

Since $f'(r)\ge 0$, we can choose $C>\frac{1}{3}$. Then we write (4.7) in the form

$$\frac{d}{dr}\left(\frac{f(r)}{r^\alpha}\right) + r^{3-\alpha} \ge 0,$$

where $\alpha := 1/C$. Integrating this inequality between r and 1 gives

$$f(r) \le \widetilde{C}r^\alpha.$$

From this it is easy to conclude that there exist some $2>\beta>1$ and $2>p>\frac{8}{5}$ such that

$$F \in L^{2\beta}(B), \quad \phi \in W^{1,p}(B).$$

Furthermore, since $d^*A=0$ in the broken Hodge gauge,

$$|\nabla A| = |dA| = \left|F - \frac{1}{2}[A,A]\right| \le |F| + |A|^2,$$

and hence $A \in W^{1,2\beta}(B)$ [using (4.2)].

Then Sobolev embedding theorem implies

$$A \in L^{4\beta/(2-\beta)}(B), \quad \phi \in L^{p^*}(B),$$

where $p^*=4p/(4-p)$.

Choose positive constants p_1, p', and q' as follows:

$$p_1 = \frac{2\beta p}{2\beta-(\beta-1)p}, \quad p' = \frac{4\beta}{(2-\beta)p_1}, \quad q' = \frac{p^*}{p_1}.$$

One can check that $1/p'+1/q'=1$ and $p<p_1<p^*$ (since $1<\beta<2$).

Using the eigenvalue equation $\not{D}\phi = m\phi$, we have

$$\begin{aligned}\int_B |\nabla\phi|^{p_1} &\le C\int_B (|m||\phi| + |A||\phi|)^{p_1} \\ &\le C\left(\int_B |m|^{p_1 p'}\right)^{1/p'}\left(\int_B |\phi|^{p_1 q'}\right)^{1/q'} + C\left(\int_B |A|^{p_1 p'}\right)^{1/p'}\left(\int_B |\phi|^{p_1 q'}\right)^{1/q'} \\ &= C\left(\int_B |m|^{p_1 p'}\right)^{1/p'}\left(\int_B |\phi|^{p^*}\right)^{1/q'} + C\left(\int_B |A|^{4\beta/(2-\beta)}\right)^{1/p'}\left(\int_B |\phi|^{p^*}\right)^{1/q'} < \infty .\end{aligned}$$

Hence, $\nabla\phi \in L^{p_1}(B)$. Noting $\phi \in L^{p_1}(B)$ since $p_1 < p^*$, we have

$$\phi \in W^{1,p_1}(B), \quad \text{with } p_1 = \frac{2\beta p}{2\beta - (\beta - 1)p} > p.$$

From above, we see that $F \in L^{2\beta}(B)$ and $\phi \in W^{1,p}(B)$ imply $F \in L^{2\beta}(B)$ and $\phi \in W^{1,p_1}(B)$. By iteration, $F \in L^{2\beta}(B)$ and $\phi \in W^{1,p_k}(B)$ imply $F \in L^{2\beta}(B)$ and $\phi \in W^{1,p_{k+1}}(B)$ with

$$p_0 = p, \quad p_{k+1} = \frac{2\beta p_k}{2\beta - (\beta - 1)p_k}, \quad k = 0, 1, \ldots .$$

Since

$$\frac{p_{k+1}}{p_k} = \frac{2\beta}{2\beta - (\beta - 1)p_k} > 1,$$

there exists some k such that $p_k > 2$. Therefore, we have that $F \in L^{\beta_0}(B)$ and $\phi \in W^{1,p}(B)$ for some $\beta_0 > 2$ and $p > 2$. We can then conclude that (F, ϕ) is smooth on B_1 through the standard bootstrap method. This completes the proof of Theorem 4.1. ■

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Fractional Hamiltonian analysis of higher order derivatives systems

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The fractional Hamiltonian analysis of $1+1$ dimensional field theory is investigated and the fractional Ostrogradski's formulation is obtained. The fractional path integral of both simple harmonic oscillator with an acceleration-squares part and a damped oscillator are analyzed. The classical results are obtained when fractional derivatives are replaced with the integer order derivatives. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2356797]

I. INTRODUCTION

Fractional calculus deals with the generalization of differentiation and integration to noninteger orders. Fractional calculus has gained importance, especially during the last three decades.[1–5] A large body of mathematical knowledge on fractional integrals and derivatives has been constructed. Fractional calculus, as a natural generalization of classical calculus, has played a significant role in engineering, science, and pure and applied mathematics in recent years. The fractional derivatives are the infinitesimal generators of a class of translation invariant convolution semigroups that appear universally as attractors.

Various applications of fractional calculus are based on replacing the time derivative in an evolution equation with a derivative of fractional order. The results of several recent researchers confirm that fractional derivatives seem to arise for important mathematical reasons.[5–21]

The fractional variational principles represents an important part of fractional calculus and it is deeply related to the fractional quantization procedure. There are several proposed methods to obtain the fractional Euler-Lagrange equations and the corresponding fractional Hamiltonians. However, this issue is not yet complectly clarified and it requires a more further detailed analysis.

The quantization of systems with fractional derivatives is a novel area in the theory of application of fractional differential and integral calculus. *Schrödinger* equation was considered with the first order time derivative modified to Caputo fractional ones in Ref. 22. In this case the obtained Hamiltonian was found to be non-Hermitian and nonlocal in time. In addition, the obtained wave functions are not invariant under the time reversal. The quantization of fractional Klein-Gordon field and fractional electromagnetic potential in the Coulomb gauge and the temporal gauge were investigated very recently in Ref. 23.

Recently, the fractional variational principles and the fractional Euler-Lagrange were obtained.[24,25]

Even more recently, the fractional constrained Lagrangian and Hamiltonian were analyzed.[26,27] The notion of the fractional Hessian[27] was introduced and the Euler-Lagrange equations were obtained for a Lagrangian linear in velocities.[26] Besides, the Hamiltonian equations

have been obtained for systems with linear velocities.[28] The classical fields with fractional derivatives were investigated by using the fractional Lagrangian formulation and the fractional Euler-Lagrange equations were obtained in Ref. 29.

Nonlocal theories have been investigated in several physical problems.[30] During the last decade, the nonlocal theories were subjected to an intense debate.[31–35] A Hamilton formalism for nonlocal Lagrangians was developed in Refs. 34 and 35, an equivalent singular first order Lagrangian was obtained and the corresponding Hamiltonian was pulled back on the phase space by using the corresponding constraints.[34] It was shown the space-time noncommutative field theories are acausal and the unitarity is lost.[36,37] The fractional Lagrangians and Hamiltonians are typical examples of nonlocal theories.

For these reasons the fractional quantization of field theory is an interesting issue to be investigated.

In this paper we analyze the fractional Hamiltonian quantization of nonsingular systems possessing higher order derivatives.

The plan of the paper is as follows.

In Sec. II the $1+1$ classical dimensional field theory analysis of nonlocal theories is briefly reviewed and the fractional generalization of Ostrogradski's formulation is presented. In Sec. III the path integral quantization of the simple harmonic oscillator with an acceleration-squares part is analyzed. Section IV is dedicated to the fractional path integral formulation of the damped oscillator. Finally, Sec. V is dedicated to our conclusions.

II. FRACTIONAL FIELD THEORY

A. Classical nonlocal theory

Let us start with an ordinary local Lagrangian depending on a finite number of derivatives at a given time, namely,

$$L(q(t),\dot{q}(t),\ldots,q^{(n)}(t)). \tag{1}$$

The next step is to consider a Lagrangian depending on a piece of the trajectory $q(t,\lambda)$ for $\forall\lambda$ belonging to an interval $[a,b]$,

$$L^{\mathrm{non}}(t)=L(q(t+\lambda)), \tag{2}$$

where a,b are real numbers. Therefore a nonlocal Lagrangian was introduced. In this case the action function corresponding to (2) is given by

$$S(q)=\int dt\, L^{\mathrm{non}}(t) \tag{3}$$

and the Euler-Lagrange equation corresponding to (3) are given by

$$\int dt\frac{\delta L^{\mathrm{non}}(t)}{\delta(q(t))}=0. \tag{4}$$

Equations (4) should be understood as a functional relation to be satisfied by physical trajectories, i.e., a Lagrangian constraint. These functional relations define a subspace J_R of physical trajectories $J_R\subset J$, in the space of all possible trajectories.[32,34] The crucial point is that there is no dynamics except the displacement inside the trajectory, namely,

$$q(t)\rightarrow q(t+\lambda). \tag{5}$$

Let us introduce now the dynamical variable $Q(t,\lambda)$ as follows:

$$Q(t,\lambda)=q(t+\lambda). \tag{6}$$

If we consider a field $Q(t,\lambda)$ instead of a trajectory $q(t)$, such that

$$\dot{Q}(t,\lambda) = Q'(t,\lambda), \tag{7}$$

where $\dot{Q} = \partial Q(t,\lambda)/\partial t$ and $Q'(t,\lambda) = \partial Q(t,\lambda)/\partial \lambda$ we obtain a field theory in one spatial and one time dimension, namely a $1+1$ dimensional formulation of nonlocal Lagrangians.[32,34]

The coordinates and momenta are suppose to have the following forms:

$$Q(t,\lambda) = \sum_{m=0}^{\infty} e_m(\lambda) q^{(m)}(t), \quad P(t,\lambda) = \sum_{m=0}^{\infty} e^m(\lambda) p_{(m)}(t), \tag{8}$$

where

$$\{q^{(n)}(t), p_{(m)}(t)\} = \delta_m^n \tag{9}$$

and

$$e_m(\lambda) = \frac{\lambda^m}{m!}, \quad e^m(\lambda) = (-\partial_\lambda)^m \delta(\lambda). \tag{10}$$

Therefore, the Hamiltonian for the $1+1$ dimensional field becomes

$$H(t,[Q,P]) = \int d\lambda\, P(t,\lambda) Q'(t,\lambda) - \tilde{L}(t,[Q]), \tag{11}$$

where P denotes the canonical momentum of Q. The phase space is T^*J together with the fundamental Poisson brackets,

$$\{Q(t,\lambda), P(t,\lambda')\} = \delta(\lambda - \lambda'). \tag{12}$$

The functional $\tilde{L}(t,[Q])$ is defined as follows:

$$\tilde{L}(t,[Q]) = \int d\lambda\, \delta(\lambda) \mathcal{L}(t,\lambda). \tag{13}$$

By using (13), the primary constraint arises as given below:

$$\phi(t,\lambda,[q,P]) = P(t,\lambda) - \int d\sigma\, \chi(\lambda,-\sigma) \varepsilon(t;\sigma,\lambda) \approx 0. \tag{14}$$

Here $\varepsilon(t;\sigma,\lambda)$ and $\chi(\lambda,-\sigma)$ have the following definition:

$$\varepsilon(t;\sigma,\lambda) = \frac{\partial \mathcal{L}(t,\sigma)}{\partial Q(t,\lambda)}, \quad \chi(\lambda,-\sigma) = \frac{\varepsilon(\lambda) - \varepsilon(\sigma)}{2}, \tag{15}$$

where $\varepsilon(\lambda)$ is the sigma distribution. The Euler-Lagrange equation is guaranteed by itself,

$$\dot{\phi} \sim \psi = \int d\sigma\, \xi(t;\sigma,\lambda). \tag{16}$$

B. Fractional Ostrogradski's construction

Higher-derivatives theories[38,39] appear naturally as corrections to general relativity and cosmic strings.[40] Unconstrained higher order derivatives possess specific features, namely they have more degrees of freedom than lower-derivative theories and they lack a lower-energy bound. A method how to remove all these problems was presented in Ref. 41. It was observed that the nonlocal formulation translates into infinite order Ostrogradski's formulation.[34,35]

In this section, we would like to derive both the Lagrangian and the Hamiltonian formalisms for nonsingular Lagrangians with fractional order derivatives starting from the Hamiltonian formalism of nonlocal theories.[32] Let us consider the following Lagrangian to start with:

$$L(q,t) = L(t, q^{\alpha_m}), \tag{17}$$

where the generalized coordinates are defined as

$$q^{\alpha_m} = {}_a\mathbf{D}_t^{\alpha_m} x(t), \tag{18}$$

where m is a natural number.

To obtain the reduced phase space quantization, we start with the infinite dimensional phase space $T^*J(t)=\{Q(t,\lambda), P(t,\lambda)\}$.

The key issue is to find an appropriate generalization of (10) for the fractional case. As it was pointed out in Refs. 32 and 34, the coordinates and the momenta are considered as a Taylor series. Therefore, the first step is to generalize the classical series to the fractional case. A natural extension is to use instead of the factorial the Gamma function. In this way we introduce naturally the generalized functions[42] instead of $e_m(\lambda)$ and $e^m(\lambda)$ given by (10).

As it is already known, several fractional Taylor's series expansions were developed,[3,43] therefore we have to decide which one is appropriate for our generalization. Since we are dealing with fractional Riemann-Liouville derivatives we choose the generalization proposed in Ref. 44, namely,

$$Q(t,\lambda) = \sum_{m=-\infty}^{\infty} e_{\alpha_m}(\lambda) q^{(\alpha_m)}(t),$$

$$P(t,\lambda) = \sum_{m=-\infty}^{\infty} e^{\alpha_m}(\lambda) p_{(\alpha_m)}(t), \tag{19}$$

where

$$e_{\alpha_m}(\lambda) = \frac{(\lambda-\lambda_0)^{\alpha_m}}{\Gamma(\alpha_m+1)}, \quad e^{\alpha_m}(\lambda) = \mathbf{D}_\lambda^{\alpha_m}\delta(\lambda-\lambda_0), \tag{20}$$

and $\alpha_m = m+\alpha$, with $0 \le \alpha < 1$. Here λ_0 is a constant. The coefficients in (19) are new canonical variables,

$$\{q^{(\alpha_m)}, p_{(\alpha_{m'})}\} = \delta_{\alpha_m}^{\alpha_{m'}}. \tag{21}$$

By using (21), we obtain that

$$\sum_{m=-\infty}^{\infty} e^{\alpha_m}(\lambda) e_{\alpha_m}(\lambda') = \delta(\lambda-\lambda'), \tag{22}$$

and

$$\int_{-\infty}^{+\infty} d\lambda\, e^{\alpha_m}(\lambda) e_{\alpha_{m'}}(\lambda) = \delta_{\alpha'_m}^{\alpha_m}. \tag{23}$$

Therefore, $e^{\alpha_m}(\lambda)$ and $e_{\alpha_m}(\lambda)$ form an orthonormal basis.

We stress the fact that (22) and (23) involve the generalized functions and the relations have the meaning in the sense of generalized functions approach.[42,44]

The fractional Hamiltonian is now given by

$$H = \sum_{m=-\infty}^{\infty} p^{\alpha_m} q^{\alpha_{m+1}} - L(q^0, q^{\alpha_m}). \tag{24}$$

The momenta constraints become an infinite set of constraints,

$$\phi_n = p_{\alpha_n}(t) - \sum_{m=n}^{\infty} {}_t\mathbf{D}_b^{\alpha_{m-n}} \frac{\partial L}{\partial q^{(\alpha_{m+1})}(t)} = 0. \tag{25}$$

The fractional Euler-Lagrange equations are as follows;

$$\sum_{l=-\infty}^{\infty} {}_t\mathbf{D}_b^{\alpha_l} \frac{\partial L(t)}{\partial q^{\alpha_l}(t)} = 0. \tag{26}$$

An interesting property of the fractional series proposed by Riemann and discussed by Hardy in Ref. 44 is that when α_m become integers, the usual form of Taylor series is obtained. Therefore one should notice that for integer values of α_m, we have

$$p_{\alpha_m}(t) - \sum_{l=0}^{n-m-1} \left(-\frac{d}{dt}\right)^l \frac{\partial L(t)}{\partial(\partial_t^{l+m+1} q(t))} = 0, \tag{27}$$

which is the definition of Ostrogradski's momenta.[38]

In this case the Euler-Lagrange equation for the original fractional derivative Lagrangian[26–30] is given below,

$$\sum_{l=0}^{n} {}_t\mathbf{D}_b^{\alpha_l} \frac{\partial L(t)}{\partial q^{\alpha_l}(t)} = 0. \tag{28}$$

Now, from this equation, for integer values of α_m we obtain the Euler-Lagrange equation for a higher derivative Lagrangian,[32,34,38] namely

$$\sum_{l=0}^{n} \left(-\frac{d}{dt}\right)^l \frac{\partial L(t)}{\partial(\partial_t^l q(t))} = 0. \tag{29}$$

The constraints (27) and (29) lead us to eliminate canonical pairs $\{q^{\alpha_l}, p_{\alpha_l}\}(l \geq n)$.

In this case the infinite dimensional phase space is reduced to a finite dimensional one. The reduced space is coordinated by $T^*J^n = \{q^{\alpha_l}, p_{\alpha_l}\}$ with $l = 0, 1, \ldots, n-1$. The Hamiltonian in the reduced space is given by

$$H = \sum_{m=0}^{n-1} p^{\alpha_m} q^{\alpha_{m+1}} - L(q^0, q^{\alpha_m}). \tag{30}$$

One should notice that the canonical reduced phase space Hamiltonian (30) is obtained in terms of the reduce canonical phase space coordinates $\{q^{\alpha_l}, p_{\alpha_l}\}$ with $l = 0, 1, \ldots, n-1$. In this case the path integral quantization of a field system is given by

$$K = \int \prod_{m=0}^{n-1} dq^{\alpha_m}\, dp^{\alpha_m}\, e^{i\{\int dt(\Sigma_{m=0}^{n-1} p^{\alpha_m} q^{\alpha_{m+1}} - H)\}}. \tag{31}$$

We observe that when α are integers, we obtain the path integral for systems with higher order Lagrangians.[32,45,46]

III. FRACTIONAL PATH INTEGRAL QUANTIZATION OF A SIMPLE HARMONIC OSCILLATOR POSSESSING AN ACCELERATION-SQUARES PART

The classical Lagrangian to start with is given by[41]

$$L_c = \frac{1}{2}(1+\epsilon^2\omega^2)\dot{x}^2 - \frac{1}{2}\omega^2 x^2 - \frac{1}{2}\epsilon^2\ddot{x}^2. \tag{32}$$

The fractional generalization of (32) has the following form:

$$L = \frac{1}{2}(1+\epsilon^2\omega^2)({}_t\mathbf{D}_a^{\alpha}x(t))^2 - \frac{1}{2}\omega^2 x^2 - \frac{1}{2}\epsilon^2[{}_t\mathbf{D}_a^{\alpha}({}_t\mathbf{D}_a^{\alpha}x(t))]^2. \tag{33}$$

The independent coordinates are $x(t)$ and ${}_t\mathbf{D}_a^{\alpha}x(t)$, respectively. Let us denote their corresponding momenta as $p_1^{\alpha}=p_x$ and $p_2^{\alpha}=p_{({}_t\mathbf{D}_a^{\alpha}x(t))}$. The fractional canonical momenta are[38]

$$p_1^{\alpha} = \frac{\partial L}{\partial {}_t\mathbf{D}_a^{\alpha}x(t)} - {}_t\mathbf{D}_a^{\alpha}\left(\frac{\partial L}{\partial {}_t\mathbf{D}_a^{2\alpha}x(t)}\right), \quad p_2^{\alpha} = \frac{\partial L}{\partial {}_t\mathbf{D}_a^{2\alpha}x(t)}. \tag{34}$$

By making use of (33), we obtain the forms of the fractional canonical momenta, as given below:

$$p_1^{\alpha} = (1+\epsilon^2\omega^2){}_t\mathbf{D}_a^{\alpha}x(t) + \epsilon^2{}_t\mathbf{D}_a^{3\alpha}x(t), \tag{35}$$

$$p_2^{\alpha} = -\epsilon^2{}_t\mathbf{D}_a^{2\alpha}x(t). \tag{36}$$

The fractional canonical Hamiltonian becomes

$$H = p_1^{\alpha}{}_t\mathbf{D}_a^{\alpha}x(t) + p_2^{\alpha}{}_t\mathbf{D}_a^{2\alpha}x(t) - L. \tag{37}$$

Taking into account (33), (35), and (36) the form of (37) is given by

$$H = \frac{1}{2}\left[2p_1^{\alpha}{}_t\mathbf{D}_a^{\alpha}x(t) - \frac{(p_2^{\alpha})^2}{\epsilon^2} + \omega^2x^2(t) - (1+\epsilon^2\omega^2)({}_t\mathbf{D}_a^{\alpha}x(t))^2\right]. \tag{38}$$

By making use of (38), the fractional path integral is written as

$$K = \int dx\, d({}_t\mathbf{D}_a^{\alpha}x(t))dp_1^{\alpha}\, dp_2^{\alpha}\, e^{i\{\int dt(p_1^{\alpha}x(t)+p_2^{\alpha}{}_t\mathbf{D}_a^{\alpha}x(t)-H)\}}. \tag{39}$$

IV. FRACTIONAL PATH INTEGRAL QUANTIZATION OF DAMPED HARMONIC OSCILLATOR

The Lagrangian for this system in Ostrogradski's notations[38] takes the form[9]

$$L = \frac{1}{2}mq_1^2 + i\frac{\gamma}{2}q_{1/2}^2 - V(q_0), \tag{40}$$

where

$$q^{\alpha_n} = {}_t\mathbf{D}_b^{\alpha_n}x, \quad n=0,1,2. \tag{41}$$

Here $\alpha_0=0, \alpha_1=1/2$, $\alpha_2=1$, and $q_0=x$, $q_1=\dot{x}$, $q_{1/2}={}_t\mathbf{D}_b^{1/2}x$, $q_2=\ddot{x}$.

The expressions for canonical momenta are

$$p_0 = i\gamma x_{(1/2)} + imx_{(3/2)}, \tag{42}$$

$$p_{1/2} = m\dot{x}. \tag{43}$$

By using (40) the classical Euler-Lagrange equation of motion read as[9]

$$m\ddot{x} + \gamma\dot{x} + \frac{\partial V}{\partial x} = 0. \tag{44}$$

The canonical reduced Hamiltonian has the following expression:

$$H = \frac{p_{1/2}^2}{2m} + q_{1/2}p_0 - i\frac{\gamma}{2}q_{1/2}^2 + V(q_0). \tag{45}$$

As a result the corresponding fractional path integral representation is given by

$$K = \int d\mu \exp i\left[\int \left(q_1 p_{1/2} - \frac{p_{1/2}^2}{2m} + i\frac{\gamma}{2}q_{1/2}^2 - V(q_0)\right)dt\right], \tag{46}$$

where $d\mu = dq_0\, dp_0\, dq_{1/2}\, dp_{1/2}$.

The path integral representation for (46) is an integration over the canonical phase space coordinates (q_0, p_0) and $(q_{1/2}, p_{1/2})$. Integrating over $p_{1/2}$ and p_0, we obtain

$$K = \int dq_0\, dq_{1/2} \exp i \int \left(\frac{1}{2}mq_1^2 - V(q_0) + i\frac{\gamma}{2}q_{1/2}^2\right)dt. \tag{47}$$

Equation (47) can be put in a compact form as follows:

$$K = \int dq_0\, e^{i\int((1/2)mq_1^2 - V(q_0))dt}\, dq_{1/2}\, e^{i\int(i(\gamma/2)q_{1/2}^2)dt}. \tag{48}$$

After performing an integration over $q_{1/2}$, (48) becomes

$$K = C\int dq_0\, e^{i\int((1/2)mq_1^2 - V(q_0))dt}\, dt,$$

where C represents a constant.

V. CONCLUSIONS

The interest in fractional quantization appears because it describes both conservative systems and nonconservative systems as well. The fractional quantization of field theory is not an easy task, especially when the fractional Hamiltonian is involved. The fractional derivatives represent the generalization of the classical ones, and therefore some of the classical properties are lost, e.g., the fractional Leibniz rule or the chain rule that becomes more complicated than the classical counterparts. The fractional path integral formulation deserves further investigations, mainly because the fractional generalization of the classical case is not yet complectly understood. Namely, for a system possessing second class constraints in Dirac's classification it is difficult to find the corresponding fractional generalization. In addition, there are no fractional formulations of the classical secondary or tertiary constraints due to the fact that the fractional Hamiltonian is not a constant of motion.

In this paper we generalize to the fractional case the nonlocal theories in one space and one time dimension via the infinite Ostrogradski's formalism. The classical Taylor series involved in this problem are convergent because of the properties of the Dirac's delta function. Namely, the coordinates and the corresponding momenta are defined as Taylor series and the Ostrogradski's canonical pairs fulfill the classical Poisson's brackets commutation relations. The generalization to the fractional case of all the above mentioned results is not straightforward because there exist many formulations for the fractional Taylor series. However, a powerful tool in fractional field theory is to work to the Riemann-Liouville derivatives because of their important property of integration by parts. Therefore, in this paper we focus on the fractional Taylor series involving the Riemann-Liouville derivatives. We assumed that the fractional Lagrangian density has a compact

support in the x directions. In this work we have obtained the path integral quantization for fractional generalization of a $1+1$ dimensional nonlocal field theory. The path integral formulation for the simple harmonic oscillator with an acceleration-squares part as well as for the damped oscillator are obtained. It is worthwhile to mention that the general expression for the path integral leads to the path integral representation for systems with higher order Lagrangians.

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Uncertainty relation for Fisher information of *D*-dimensional single-particle systems with central potentials

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An uncertainty Fisher information relation in quantum mechanics is derived for multidimensional single-particle systems with central potentials. It is based on the concept of Fisher information in the two complementary position and momentum spaces, which is a gradient functional of the corresponding probability distributions. The lower bound of the product of position and momentum Fisher informations is shown to depend on the orbital and magnetic quantum numbers of the physical state and the space dimensionality. Applications to various elementary systems is discussed. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Quantum-mechanical uncertainty relations state that probability distributions of canonically conjugate variables of a physical system cannot be simultaneously sharply localized. The standard uncertainty relation is the variance-based Heisenberg principle[1,2] given by the expression

$$V_\rho V_\gamma \geqslant \frac{1}{4}, \tag{1}$$

where $V_\rho(V_\gamma)$ denotes the variance of the probability density in the position $\rho(\boldsymbol{r})$ [momentum $\gamma(\boldsymbol{p})$] space, assumed to be normalized to unity. This inequality is so relevant in quantum mechanics, not because of its accuracy (generally, very small), but because it indicates that refined single-particle position measurements require large indeterminations for the single-particle momenta. This principle and its moment-based generalizations[3] reflect the essential inadequacy of the classical concepts of one-particle position and momentum to describe real systems.

The use of information-theoretic quantities as uncertainty measures has led to derive uncertainty relations that provide a strict improvement upon the standard uncertainty relation. This is the case of the celebrated entropic uncertainty relation,[4–6]

$$S_\rho + S_\gamma \geqslant D(1 + \ln \pi),$$

where $S_\rho = -\langle \ln \rho \rangle = -\int_{\mathbb{R}^D} \rho(\boldsymbol{r}) \ln \rho(\boldsymbol{r}) d^D r$ describes the Shannon information entropy of the position probability density in the D-dimensional space $\mathbb{R}^D$,[7,8] and S_γ denotes the corresponding momentum Shannon entropy of the system. This relation was conjectured by Hirschman[4] in 1957 and proved by Beckner[5] and Bialynicki-Birula and Mycielski.[6] For probabilistic and dimensional reasons, it is more convenient to reformulate it as

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$$N_\rho N_\gamma \geqslant \frac{1}{4}, \tag{2}$$

where $N_\rho(N_\gamma)$ denotes the Shannon entropy power[9] of the position (momentum) density, defined by $N_\rho=(2\pi e)^{-1}\exp(2S_\rho/D)$.

A most important information-theoretic alternative to the Shannon entropy as uncertainty measure is the Fisher information,[10,11] given by

$$I_\rho = \int_{\mathbb{R}^D} \frac{|\nabla_D \rho(\mathbf{r})|^2}{\rho(\mathbf{r})} d^D r = 4\int_{\mathbb{R}^D} |\nabla_D \sqrt{\rho(\mathbf{r})}|^2 d^D r. \tag{3}$$

Contrary to the Shannon entropy, which is a global measure of the spreading of the density because it is a logarithmic functional, the Fisher information has a property of locality as it is a gradient functional of the density. The higher is this quantity, the more localized is the density, the smaller is the uncertainty, and the higher is the accuracy in predicting the localization of the particle.[12,13]

On the other hand, the Fisher information is the basic variable of the principle of extreme physical information[12] in the same manner as the Shannon entropy is the cornerstone of the maximum entropy method.[14–16] The former principle has allowed us to derive various fundamental equations of quantum physics.[12,17] Moreover, it has been used (a) to describe some macroscopic quantities such as the kinetic[18] and the Weiszäcker[19,20] energies, (b) to characterize correlation properties in atomic systems[21] and (c) to identify the most distinctive nonlinear phenomena (the avoided crossings) of the energy spectra of atomic and molecular systems in strong external fields.[22] For other quantum-mechanical uses of the Fisher information, see Refs. 12, 23, and 24.

Moreover, the Fisher information is involved in the so-called Stam uncertainty relations,[13,24–26]

$$\langle r^2\rangle I_\gamma^{-1} \geqslant \frac{1}{4}; \quad \langle p^2\rangle I_\rho^{-1} \geqslant \frac{1}{4}.$$

However, we do not know yet an uncertainty relation based on the position and momentum Fisher information, of the same type as the variance-based Heisenberg principle (1) and the entropic uncertainty relation (2). To find such a relation for multidimensional central potentials is the main purpose of this paper; that is, to derive a lower bound for the product of the Fisher informations in position and momentum spaces of arbitrary dimensions. This is done in Sec. II. We have used a two-step methodology. First, we express the position (momentum) Fisher information in terms of the radial expectation values $\langle p^2\rangle$ and $\langle r^{-2}\rangle$ ($\langle r^2\rangle$ and $\langle p^{-2}\rangle$); this is proved in Sec. II A. Second, we obtain some radial uncertainty-like inequalities that involve these expectation values, which is proved in Sec. II B. Then, the Fisher informations of some elementary D-dimensional systems (hydrogen atom, isotropic harmonic oscillator) are calculated in a closed form in Sec. III, and some concluding remarks and open problems are given.

II. THE FISHER UNCERTAINTY RELATION FOR CENTRAL POTENTIALS

Here we prove that the Fisher information of single-particle systems with a central potential $V_D(r)$ in D-dimensional ($D\geqslant 3$) position and momentum spaces satisfy the uncertainty relation

$$I_\rho I_\gamma \geqslant 4D^2\left(1-\frac{(2l+D-2)|m|}{2l(l+D-2)}\right)^2 \quad (l>0), \tag{4}$$

where the hyperangular quantum numbers l and m have the values given below. When $l=0$ the inequality reduces to $I_\rho I_\gamma \geqslant 4D^2$, and when $D=2$ it gives the trivial inequality $I_\rho I_\gamma \geqslant 0$.

The position probability density $\rho(\mathbf{r})=|\Psi(\mathbf{r})|^2$, where the wave function $\Psi(\mathbf{r})$ is the physical solution of the Schrödinger equation,

$$\left(-\frac{1}{2}\nabla_D^2 + V_D(r)\right)\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}), \tag{5}$$

where atomic units are used.

Due to the spherical symmetry of the problem, it is most convenient to work it out by use of the polar hyperspherical coordinates $(r,\theta_1,\theta_2,\ldots,\theta_{D-1}\equiv\phi)=(r,\Omega_{D-1})$ $(0\leqslant\theta_k\leqslant\pi,\ k=1,\ldots,D-2$, and $0\leqslant\theta_{D-1}\leqslant 2\pi)$, instead of Cartesian coordinates $(x_1,\ldots,x_D)$, defined by

$$x_1 = r\cos\theta_1,$$

$$x_2 = r\sin\theta_1\cos\theta_2,$$

$$\vdots$$

$$x_k = r\sin\theta_1\ldots\sin\theta_{k-1}\cos\theta_k,$$

$$\vdots$$

$$x_{D-1} = r\sin\theta_1\ldots\sin\theta_{D-2}\cos\theta_{D-1},$$

$$x_D = r\sin\theta_1\ldots\sin\theta_{D-2}\sin\theta_{D-1},$$

$$\sum_{i=1}^{D} x_i^2 = r^2,$$

in which case the D-dimensional gradient is

$$\begin{aligned}\nabla_D &= \left(\frac{\partial}{\partial r},\frac{1}{r}\frac{\partial}{\partial\theta_1},\frac{1}{r\sin\theta_1}\frac{\partial}{\partial\theta_2},\ldots,\frac{1}{r\prod_{j=1}^{k-1}\sin\theta_j}\frac{\partial}{\partial\theta_k},\ldots,\frac{1}{r\prod_{j=1}^{D-2}\sin\theta_j}\frac{\partial}{\partial\theta_{D-1}}\right)\\ &= \hat{r}\frac{\partial}{\partial r} + \sum_{k=1}^{D-1}\hat{\theta}_k\frac{1}{r\prod_{j=1}^{k-1}\sin\theta_j}\frac{\partial}{\partial\theta_k},\end{aligned} \tag{6}$$

so that the Laplacian operator ∇_D^2 has the expression

$$\nabla_D^2 = \frac{1}{r^{D-1}}\frac{\partial}{\partial r}r^{D-1}\frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2}. \tag{7}$$

The operator Λ is the D-dimensional generalization of the square of the angular momentum operator,[27–29] which only depends on the $D-1$ angular coordinates Ω_{D-1} of the D-dimensional sphere in the form

$$\Lambda^2 = -\sum_{i=1}^{D-1}\frac{(\sin\theta_i)^{i+1-D}}{(\prod_{j=1}^{i-1}\sin\theta_j)^2}\frac{\partial}{\partial\theta_i}\left((\sin\theta_i)^{D-i-1}\frac{\partial}{\partial\theta_i}\right). \tag{8}$$

This operator is known to fulfill

$$\Lambda^2\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = l(l+D-2)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \tag{9}$$

where the $\mathcal{Y}$ symbol denotes the hyperspherical harmonics described by the $D-1$ hyperangular quantum numbers $(l\equiv\mu_1,\mu_2,\ldots,\mu_{D-1}\equiv m)\equiv(l,\{\mu\})$, which are natural numbers with values l

$=0,1,2,\ldots$, and $l\equiv\mu_1\geqslant\mu_2\geqslant\cdots\geqslant\mu_{D-2}\geqslant|\mu_{D-1}|\equiv|m|$. These hyperfunctions are known to have the form[27–31]

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})=\mathcal{N}_{l,\{\mu\}}e^{im\theta_{D-1}}\prod_{j=1}^{D-2}C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}=\frac{e^{im\theta_{D-1}}}{\sqrt{2\pi}}\prod_{j=1}^{D-2}Y_{\mu_j,\mu_{j+1}}^{(j)}(\theta_j), \tag{10}$$

where the normalization constant is given by

$$|\mathcal{N}_{l,\{\mu\}}|^2=\frac{1}{2\pi}\prod_{j=1}^{D-2}\frac{(\alpha_j+\mu_j)(\mu_j-\mu_{j+1})!\,\Gamma^2(\alpha_j+\mu_{j+1})}{\pi 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j+\mu_j+\mu_{j+1})}=\frac{1}{2\pi}\prod_{j=1}^{D-2}N_{\mu_j,\mu_{j+1}}^{(j)}, \tag{11}$$

$\alpha_j=(D-j-1)/2$, and $C_k^{\lambda}(t)$ denotes the Gegenbauer polynomial of degree k and parameter λ. In addition we have used the notation

$$Y_{\mu_j,\mu_{j+1}}^{(j)}(\theta_j)=N_{\mu_j,\mu_{j+1}}^{(j)}C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}. \tag{12}$$

[Remark that for $D=2$ there are no products in Eqs. (10) and (11) so that the corresponding spherical harmonics for this case is just $e^{im\phi}/\sqrt{2\pi}$.]

The hyperspherical harmonics $\mathcal{Y}(\Omega_{D-1})$ satisfy the orthonormalization conditions

$$\int_{S_{D-1}}d\Omega_{D-1}\,\mathcal{Y}_{l',\{\mu'\}}(\Omega_{D-1})\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})=\delta_{ll'}\delta_{\{\mu\},\{\mu'\}}, \tag{13}$$

and the harmonics $Y_{\mu_j,\mu_{j+1}}^{(j)}(\theta_i)$ have the two following integral properties:[23,28]

$$\int_0^{\pi}[Y_{\mu_j,\mu_{j+1}}^{j}(\theta_j)]^2(\sin\theta_j)^{D-j-1}\,d\theta_j=1 \tag{14}$$

and

$$\int_0^{\pi}[Y_{\mu_j,\mu_{j+1}}^{j}(\theta_j)]^2(\sin\theta_j)^{D-j-3}\,d\theta_j=\frac{2\mu_j+D-j-1}{2\mu_{j+1}+D-j-2}. \tag{15}$$

Notice that, when $j=D-2$, $\int_0^{\pi}[Y_{\mu_{D-2},\mu_{D-1}}^{j}(\theta_{D-2})]^2(\sin\theta_{D-2})^{-1}\,d\theta_{D-2}=(2\mu_{D-2}+1)/2|\mu_{D-1}|$.

Then, the wave functions $\Psi(\boldsymbol{r})$ of the problem (5)–(7) can be separated out as

$$\Psi_{E,l,\{\mu\}}(\boldsymbol{r})=R_{E,l}(r)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}).$$

To prove the inequality (4), we first find that the position and momentum Fisher information are related to the radial expectation values $\langle r^k\rangle$ and $\langle p^k\rangle$, $k=-2$ and 2, by means of the expressions

$$I_\rho=4\langle p^2\rangle-2|m|(2l+D-2)\langle r^{-2}\rangle, \tag{16}$$

$$I_\gamma=4\langle r^2\rangle-2|m|(2l+D-2)\langle p^{-2}\rangle, \tag{17}$$

respectively. This is done in Sec. II A. Then, we use the radial uncertainty-like relations,

$$\langle p^2\rangle\geqslant l(l+D-2)\langle r^{-2}\rangle, \tag{18}$$

$$\langle r^2\rangle\geqslant l(l+D-2)\langle p^{-2}\rangle, \tag{19}$$

which are proved in Sec. II B.

Combining the expressions (16)–(19), one has that

$$I_\rho I_\gamma \geqslant 16\left(1-\frac{(2l+D-2)|m|}{2l(l+D-2)}\right)^2\langle r^2\rangle\langle p^2\rangle, \tag{20}$$

which emphasizes the uncertainty character of the inequality. Now, it remains to use the modified Heisenberg uncertainty inequality,

$$\langle r^2\rangle\langle p^2\rangle \geqslant \frac{D^2}{4}, \tag{21}$$

to finally obtain the new uncertainty relation (4). In the case that $l=0$, expressions (16)–(19) lead to $I_\rho I_\gamma \geqslant 4D^2$.

The use of the grand orbital quantum number $L=l+(D-3)/2$ leads to write $2l+D-2=2L+1$ and $l(l+D-2)=\frac{1}{4}(2L-D+3)(2L+D-1)=L(L+1)-\frac{1}{4}(D-1)(D-3)$, so that the new uncertainty relation can be expressed as

$$I_\rho I_\gamma \geqslant 4D^2\left(1-\frac{(2L+1)|m|}{2L(L+1)-\frac{1}{2}(D-1)(D-3)}\right)^2,$$

which reduces to

$$I_\rho I_\gamma \geqslant 36\left(1-\frac{(2l+1)|m|}{2l(l+1)}\right)^2,$$

for tridimensional systems, as recently found by the authors[32] in a semiheuristic way. Moreover, let us highlight that for states with $m=0$ the new uncertainty relation gets simplified as

$$I_\rho I_\gamma \geqslant 4D^2, \tag{22}$$

which saturates for the isotropic harmonic oscillator case (see Sec. III B). Finally, it is also known[33] that for arbitrary monodimensional systems with even wave functions the uncertainty inequality $I_\rho I_\gamma \geqslant 4$ is fulfilled.

Let us finally point out that when D goes to infinity and $m=0$, expression (4) reaches the equality for the particular cases of the D-dimensional hydrogen atom and isotropic harmonic potential [see Eqs. (37), (38), (42), and (43) in Sec. III].

A. Position and momentum Fisher's informations for central potentials

Here we derive the expressions (16) and (17), which gives the position (momentum) Fisher information of a single-particle system with a D-dimensional central potential in terms of the radial expectation values $\langle p^2\rangle$ and $\langle r^{-2}\rangle$ ($\langle r^2\rangle$ and $\langle p^{-2}\rangle$). To begin with, we realize that the position density $\rho(\boldsymbol{r})$ is equal to

$$\rho(\boldsymbol{r}) = |\Psi_{El\{\mu\}}(\boldsymbol{r})|^2 = |\Psi_{El\{\mu\}}(r,\theta_1,\theta_2,\ldots,\theta_{D-2},0)|^2.$$

Then, the position Fisher information $I_\rho(D)\equiv I_\rho$ defined by Eq. (3) gets reduced as

$$I_\rho(D) = 4\int_{\mathbb{R}^D} |\boldsymbol{\nabla}_D \Psi_{El\{\mu\}}(r,\theta_1,\theta_2,\ldots,\theta_{D-2},0)|^2\, d^D r, \tag{23}$$

where the D-dimensional volume element $d^D r$ is

$$d^D r = r^{D-1}\, dr\, d\Omega_{D-1};$$
$$d\Omega_{D-1} = \left(\prod_{j=1}^{D-2} (\sin\theta_j)^{2\alpha_j}\, d\theta_j \right) d\theta_{D-1}. \tag{24}$$

On the other hand, we know that the momentum expectation value $\langle p^2 \rangle$ given by

$$\langle p^2 \rangle = \int_{\mathbb{R}^D} |\nabla_D \Psi_{El\{\mu\}}(r, \theta_1, \theta_2, \ldots, \theta_{D-1})|^2\, d^D r, \tag{25}$$

can be decomposed, according to polar coordinate form (6) of the gradient, as

$$\langle p^2 \rangle = \int_{\mathbb{R}^D} |\nabla_D \Psi_{El\{\mu\}}(r, \theta_1, \theta_2, \ldots, \theta_{D-2}, 0)|^2\, d^D r + K_{lm}(D). \tag{26}$$

The K symbol denotes the integral

$$\begin{aligned} K_{lm}(D) &= \int_{\mathbb{R}^D} \left| \frac{1}{r} \prod_{i=1}^{D-2} (\sin\theta_i)^{-1} \frac{\partial}{\partial \theta_{D-1}} \Psi_{El\{\mu\}}(\mathbf{r}) \right|^2 d^D r \\ &= \langle r^{-2} \rangle \prod_{i=1}^{D-2} \int_0^{\pi} |Y^{(i)}_{\mu_i,\mu_{i+1}}(\theta_i)|^2 (\sin\theta_i)^{D-i-3}\, d\theta_i \frac{1}{2\pi} \int_0^{2\pi} \left| \frac{\partial}{\partial \theta_{D-1}} (e^{im\theta_{D-1}}) \right|^2 d\theta_{D-1} \\ &= \langle r^{-2} \rangle m^2 \prod_{i=1}^{D-2} \frac{2\mu_i + D - i - 1}{2\mu_{i+1} + D - i - 2} \\ &= \frac{1}{2} \langle r^{-2} \rangle |m| (2l + D - 2), \end{aligned} \tag{27}$$

where we have taken into account the integral properties (14) and (15) for the harmonics $Y(\theta_i)$, $i = 1, 2, \ldots, D-2$, in the second equality, and the expression

$$\prod_{i=1}^{D-2} \frac{2\mu_i + D - i - 1}{2\mu_{i+1} + D - i - 2} = \frac{2l + D - 2}{2|m|}$$

in the third equality. Moreover, the radial expectation value,

$$\langle r^{-2} \rangle = \int_{\mathbb{R}^D} r^{-2} \rho(\mathbf{r}) d^D r = \int_0^{\infty} r^{-2} R^2_{El}(r) r^{D-1}\, dr,$$

has been used. The combination of Eqs. (23), (26), and (27) leads to the following relation between the position Fisher information $I_\rho(D)$ and the radial expectation values $\langle p^2 \rangle$ and $\langle r^{-2} \rangle$:

$$\langle p^2 \rangle = \frac{1}{4} I_\rho(D) + \frac{1}{2} |m| (2l + D - 2) \langle r^{-2} \rangle,$$

which gives the searched expression (16) for the position Fisher information.

The application of the same procedure in momentum space has allowed us to obtain that

$$\langle r^2\rangle = \frac{1}{4}I_\gamma(D) + \frac{1}{2}|m|(2l+D-2)\langle p^{-2}\rangle,$$

which provides the searched expression (17) for the momentum Fisher information in terms of the radial expectation values $\langle r^2\rangle$ and $\langle p^{-2}\rangle$. These expressions have been previously found for the tridimensional case.[32]

Let us mention that when $D=2$, having only one angular quantum number l, these expressions reduce to $\langle p^2\rangle = I_\rho/4 - l^2\langle r^{-2}\rangle$ and $\langle r^2\rangle = I_\gamma/4 - l^2\langle p^{-2}\rangle$.

B. Radial uncertainty-like relations

Let us here derive the dual uncertainty-like relations (18) and (19) between the radial expectation values $\langle p^2\rangle$ and $\langle r^{-2}\rangle$, and $\langle r^2\rangle$ and $\langle p^{-2}\rangle$, respectively. To find Eq. (18), we start from the expressions (6) and (25), which provide

$$\langle p^2\rangle = J_R(D) + \langle r^{-2}\rangle J_A(D), \tag{28}$$

where the radial integral

$$J_R(D) = \int_{\mathbb{R}^D} \left|\frac{\partial}{\partial r}\Psi(\boldsymbol{r})\right|^2 d^D r = \int_0^\infty \left(\frac{dR_{El}}{dr}\right)^2 r^{D-1}\, dr,$$

and the angular integral

$$\begin{aligned} J_A(D) &= \int_{S_{D-1}} \sum_{i=1}^{D-1} \left| \frac{1}{\prod_{j=1}^{i-1}\sin\theta_j}\frac{\partial}{\partial\theta_i}\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})\right|^2 d\Omega_{D-1} \\ &= \sum_{i=1}^{D-1}\int_{S_{D-1}} \frac{1}{\left(\prod_{j=1}^{i-1}\sin\theta_j\right)^2}\frac{\partial}{\partial\theta_i}\mathcal{Y}^*_{l,\{\mu\}}(\Omega_{D-1})\frac{\partial}{\partial\theta_i}\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})\prod_{j=1}^{D-2}[(\sin\theta_j)^{D-j-1}\, d\theta_j]d\theta_{D-1}, \end{aligned} \tag{29}$$

where we have used the expression (24) of the volume element $d\Omega_{D-1}$. Remark that, for convention, the products $\Pi_{j=1}^{i-1}$ and $\Pi_{j=1}^{D-2}$ are empty when $i=1$ and $D=2$, respectively. Then, taken into account the non-negativity of the radial integral $J_R(D)$, one has that

$$\langle p^2\rangle \geqslant \langle r^{-2}\rangle J_A(D). \tag{30}$$

In momentum space, a similar procedure has allowed us to obtain that

$$\langle r^2\rangle \geqslant \langle p^{-2}\rangle J_A(D). \tag{31}$$

To calculate $J_A(D)$, we perform an integration by parts in the integral of Eq. (29). Then, one obtains that

$$\begin{aligned} J_A(D) = &-\sum_{i=1}^{D-1}\int_{S_{D-1}} \mathcal{Y}^*_{l,\{\mu\}}(\Omega_{D-1})\frac{1}{(\prod_{j=1}^{i-1}\sin\theta_j)^2}\frac{\partial}{\partial\theta_i}\left((\sin\theta_i)^{D-i-1}\frac{\partial}{\partial\theta_i}\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})\right) \\ &\times \prod_{j=1,j\neq i}^{D-2}[(\sin\theta_j)^{D-j-1}\, d\theta_j]d\theta_{D-1} \\ = &-\sum_{i=1}^{D-1}\int_{S_{D-1}} \mathcal{Y}^*_{l,\{\mu\}}(\Omega_{D-1})\frac{(\sin\theta_i)^{1+i-D}}{(\prod_{j=1}^{i-1}\sin\theta_j)^2}\frac{\partial}{\partial\theta_i}\left((\sin\theta_i)^{D-i-1}\frac{\partial}{\partial\theta_i}\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})\right) \end{aligned}$$

$$\times \prod_{j=1}^{D-2} [(\sin\theta_j)^{D-j-1}\, d\theta_j] d\theta_{D-1}$$

$$= \int_{S_{D-1}} \mathcal{Y}^*_{l,\{\mu\}}(\Omega_{D-1}) \Lambda^2 \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) d\Omega_{D-1} = l(l+D-2), \tag{32}$$

where we have used the expression (8) in the third equality and the expressions (9) and (13) in the last equality.

Finally, the substitution of the value (32) for the angular integral $J_A(D)$ into the inequalities (30) and (31) produces the radial uncertainty-like inequalities (18) and (19),

$$\langle p^2 \rangle \geqslant l(l+D-2)\langle r^{-2}\rangle,$$

$$\langle r^2 \rangle \geqslant l(l+D-2)\langle p^{-2}\rangle,$$

respectively, which we were looking for.

For the case $D=3$ the former inequality has been recently and rigorously found by completely different means, while the latter one was only suggested.[32]

Finally, let us point out that up until now the only existing inequality of this type, to the best of our information, has been shown by one of us[26] to be

$$\langle p^2 \rangle \geqslant \left(\frac{D-2}{2}\right)^2 \langle r^{-2}\rangle, \tag{33}$$

for general systems. The comparison of Eqs. (18) and (33) shows that (i) the former one is stronger than the latter one when $l > (\sqrt{2}-1)(D-2)/2$, indicating its greater accuracy when $D \leqslant 6$ for states with $l>0$; and (ii) the latter one is stronger for $l=0$ regardless of the value of the space dimensionality.

III. THE FISHER INFORMATIONS FOR SOME *D*-DIMENSIONAL ELEMENTARY SYSTEMS

Here we find the position and momentum Fisher informations for the most prominent prototypes of D-dimensional systems: the hydrogen atom and the isotropic harmonic oscillator.

A. Hydrogen atom

In this case, $V(r)=1/r$. The energies of the bound states are given by

$$E = -\frac{1}{2\eta^2}, \tag{34}$$

where η denotes the grand principal quantum number,

$$\eta = n + \frac{D-3}{2}; \quad n = 1,2,3,\ldots .$$

The radial expectation values $\langle r^{-2}\rangle$ and $\langle r^2\rangle$ are known[34] to have the expressions

$$\langle r^{-2}\rangle = \frac{2}{\eta^3}\frac{1}{2L+1}; \quad \langle r^2\rangle = \frac{1}{2}\eta^2[5\eta^2 - 3L(L+1)+1], \tag{35}$$

and the momentum expectation values $\langle p^{-2}\rangle$ and $\langle p^2\rangle$ are given[35] by

$$\langle p^{-2}\rangle = \frac{8\eta - 3(2L+1)}{2L+1}\eta^2; \quad \langle p^2\rangle = \frac{1}{\eta^2}. \tag{36}$$

Then, according to Eqs. (16), (35), and (36), the Fisher information of the D-dimensional hydrogen atom in position space has the value

$$I_\rho = 4\langle p^2\rangle - 2|m|(2L+1)\langle r^{-2}\rangle = \frac{4}{\eta^3}(\eta - |m|), \tag{37}$$

which has been recently found by different means.[23] Moreover, let us notice that for the real ($D=3$) hydrogen atom one has I_ρ (hydrogen)$=4(n-|m|)/n^3$, as recently derived.[32,36]

On the other hand, according to Eqs. (17), (35), and (36), the Fisher information of the D-dimensional hydrogen atom in momentum space has the value

$$I_\gamma = 4\langle r^2\rangle - 2|m|(2L+1)\langle p^{-2}\rangle = 2\eta^2\{5\eta^2 - 3L(L+1) - [8\eta - 3(2L+1)]|m| + 1\}, \tag{38}$$

which has also been recently shown.[23] It is worthy to point out that for the tridimensional hydrogen atom one straightforwardly has the known value[32]

$$I_\gamma(\text{hydrogen}) = 2n^2\{5n^2 - 3l(l+1) - [8n - 3(2l+1)]|m| + 1\},$$

since the grand quantum numbers η, L, and m for $D=3$ reduces to the familiar tridimensional quantum numbers (n,l,m).

Finally, it is worthy to point out that for $l=n-1$ the accuracy of inequalities (18) and (19) for this system improves when n is increasing; moreover, they get saturated when $n\to\infty$.

B. Isotropic harmonic oscillator

Here, $V(r)=\frac{1}{2}\omega^2 r^2$ (mass$=1$). The energies of the physical states are given by

$$E = \left(\eta + \frac{3}{2}\right)\omega, \tag{39}$$

with

$$\eta = n + \frac{D-3}{2} = 2n_r + l + \frac{D-3}{2} \equiv 2n_r + L; \quad n_r = 0,1,2,\ldots, \quad l = 0,1,2,\ldots .$$

For this system the radial expectation values $\langle r^{-2}\rangle$ and $\langle r^2\rangle$ have the form[34,37,38]

$$\langle r^{-2}\rangle = \frac{2\omega}{2L+1}; \quad \langle r^2\rangle = \left(\eta + \frac{3}{2}\right)\omega^{-1}, \tag{40}$$

and the momentum expectation values $\langle p^\alpha\rangle = \omega^\alpha\langle r^\alpha\rangle$, so that

$$\langle p^{-2}\rangle = \frac{2}{2L+1}\omega^{-1}; \quad \langle p^2\rangle = \left(\eta + \frac{3}{2}\right)\omega. \tag{41}$$

Then the Fisher information of the D-dimensional isotropic harmonic oscillator in position space has, according to Eqs. (16), (40), and (41), the value

$$I_\rho = 4\left(\eta - |m| + \frac{3}{2}\right)\omega = 4\left(2n_r + l - |m| + \frac{D}{2}\right)\omega. \tag{42}$$

Similarly, according to Eqs. (17), (40), and (41), we have found the following value for the Fisher information of the D-dimensional isotropic harmonic oscillator in momentum space,

$$I_\gamma = 4\left(\eta - |m| + \frac{3}{2}\right)\omega^{-1} = 4\left(2n_r + l - |m| + \frac{D}{2}\right)\omega^{-1}. \tag{43}$$

Let us point out that these expressions for the position and momentum D-dimensional Fisher informations reduces to the corresponding known three-dimensional quantities for $D=3$.[32]

It is most interesting to realize that for the ground state ($n_r=l=m=0$), one has that $I_\rho = 2D\omega$ and $I_\gamma = 2D\omega^{-1}$, so that the Fisher uncertainty product $I_\rho I_\gamma = 4D^2$. Therefore, the D-dimensional Fisher uncertainty relation (22) for $m=0$ states of arbitrary central potential gets saturated at the harmonic oscillator ground state.

Furthermore, it is nice to remark from Eqs. (34) and (37), and Eqs. (39) and (42), that the position Fisher information for the two multidimensional central potentials of the r^α type considered in this section, has the following behavior:

$$I_\rho = aE_{\eta L} + b|m|\eta^{\alpha-2},$$

where real parameters a and b are controlled by the strength of the potential, being aware that $E_{\eta L}$ goes as $\eta^{\alpha-1}$.

For completeness, let us also point out that the equality in inequalities (18) and (19) is obtained for this system when l goes to infinity.

IV. CONCLUSIONS

The spreading of the quantum-mechanical wave functions of physical systems in a D-dimensional space can be measured by moments of different orders of the corresponding probability density (particularly, the second moment or variance) and, more recently, by some information-theoretic measures, the Shannon entropy and the Fisher information. These spreading measures grasp differently the distribution of the quantum-mechanical probability cloud of the system. The development of uncertainty relations associated to the probability distributions of canonically conjugate spreading measures is at the heart of the quantum physics from its early days. The variance-based Heisenberg-Kennard relation[1,2] and its generalizations[3] based on moments with orders bigger than 2, have played a fundamental role in understanding the quantum behavior of the physical systems in a deeper way. The advent of the entropic uncertainty relation based on the Shannon information entropy[4–6] has strictly improved the standard relation, mainly because of the true information-theoretic character of the involved spreading measure.

The uncertainty relation based on the Fisher information is not yet known. This is a serious lack because this quantity has a local character, contrary to both the moments and the Shannon entropy that are global spreading measures. Here we have derived this Fisher uncertainty relation, not for general systems but "only" for D-dimensional single-particle systems with central potentials. The lower bound of the Fisher informations in the two complementary spaces has been found to depend on the orbital and magnetic quantum numbers and the space dimensionality. To do that, we have first calculated the explicit expressions for the position and momentum Fisher informations [see Eqs. (16) and (17)] in terms of the radial expectation values $(\langle p^2\rangle, \langle r^{-2}\rangle)$ and $(\langle r^2\rangle, \langle p^{-2}\rangle)$, respectively. Second, we have derived uncertainty relations for these two pairs of radial expectation values as given by Eqs. (18) and (19). Then, the Fisher product $I_\rho I_\gamma$ is bounded from below in terms of the Heisenberg uncertainty product $\langle p^2\rangle\langle r^2\rangle$ [see Eq. (20)]. Finally, the $D^2/4$ lower bound for the latter product has allowed us to find the new Fisher uncertainty inequality (4). The application to some quantum prototypes of physical systems is also shown not only for checking reasons but also because of their intrinsic and fundamental interests.

Two open problems come naturally. First, to improve the new uncertainty relation given by Eq. (4) mainly by means of increasing the accuracy of the Heisenberg principle (21); and second, to find the Fisher uncertainty relation for general systems; that is, systems with quantum potentials of any character.

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The Lyapunov stability of the *N*-soliton solutions in the Lax hierarchy of the Benjamin-Ono equation

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The Lyapunov stability is established for the *N*-soliton solutions in the Lax hierarchy of the Benjamin-Ono (BO) equation. We characterize the *N*-soliton profiles as critical points of certain Lyapunov functional. By using several results derived by the inverse scattering transform of the BO equation, we demonstrate the convexity of the Lyapunov functional when evaluated at the *N*-soliton profiles. From this fact, we deduce that the *N*-soliton solutions are energetically stable. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2344854]

I. INTRODUCTION

The Benjamin-Ono (BO) equation describes the unidirectional propagation of long internal waves in stratified fluids of great depth. It may be written in an appropriate dimensionless form as

$$u_t + 2uu_x + Hu_{xx} = 0. \tag{1.1a}$$

Here, $u=u(x,t)$ represents the amplitude of wave, H is the Hilbert transform given by

$$Hu(x,t) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{u(y,t)}{y-x} \mathrm{d}y, \tag{1.1b}$$

and the subscripts t and x appended to u denote partial differentiation. The BO equation can be written as an infinite-dimensional completely integrable Hamiltonian dynamical system.[1,2] A common feature of integrable evolution equations is the existence of an infinite sequence of conservation laws. The Lax hierarchy of the BO equation is generated by the conservation laws, which we shall denote by $I_n (n=2,3,4,\ldots)$. The first three of I_n read

$$I_2 = \frac{1}{2} \int_{-\infty}^{\infty} u^2 \mathrm{d}x, \tag{1.2a}$$

$$I_3 = -\int_{-\infty}^{\infty} \left(\frac{1}{3} u^3 + \frac{1}{2} uHu_x \right) \mathrm{d}x, \tag{1.2b}$$

$$I_4 = \int_{-\infty}^{\infty} \left(\frac{1}{4} u^4 + \frac{3}{4} u^2 Hu_x + \frac{1}{2} u_x^2 \right) \mathrm{d}x. \tag{1.2c}$$

In (1.2), the mass conservation has been excluded since it is irrelevant in the present analysis. The BO hierarchy is defined by the following nonlinear evolution equations:

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$$\frac{\partial u}{\partial t_n} = \frac{\partial}{\partial x}\frac{\delta I_{n+2}}{\delta u}, \quad (n = 0,1,2,\ldots), \tag{1.3}$$

where $\delta/\delta u$ is the variational derivative defined by

$$\frac{\partial}{\partial \epsilon} I_{n+2}(u+\epsilon v)\bigg|_{\epsilon=0} = \int_{-\infty}^{\infty} \frac{\delta I_{n+2}}{\delta u(x)} v(x)\mathrm{d}x. \tag{1.4}$$

When $n=1$, (1.3) becomes the BO equation (1.1) with the identification $t_1=t$ while when $n=2$, it yields the first higher-order BO equation[3]

$$u_{t_2} = \left(u^3 + \tfrac{3}{2}uHu_x + \tfrac{3}{2}H(uu_x) - u_{xx}\right)_x. \tag{1.5}$$

Note that the first member of (1.3) reduces simply to a linear equation $u_{t_o}=u_x$. As will be shown in the following, all the members of the BO hierarchy exhibit the N-soliton solution characterized by the $2N$ parameters a_j and $x_{j0}(j=1,2,\ldots,N)$ where N is an arbitrary positive integer:

$$u = u_N(x-x_1, x-x_2, \ldots, x-X_N). \tag{1.6a}$$

Here

$$x_j = \sum_{s=0}^{\infty} (-1)^{s+1}\frac{s+1}{2^s}a_j^s t_s + x_{j0}, \quad (j=1,2,\ldots,N), \tag{1.6b}$$

a_j are amplitude parameters satisfying the conditions $a_j>0, a_j\neq a_k$ for $j\neq k(j,k=1,2,\ldots,N)$ and x_{j0} are arbitrary phase parameters. Explicitly, u_N has a simple expression in terms of a tau function f,

$$u_N = i\frac{\partial}{\partial x}\ln\frac{f}{f^*}, \quad f = \det F, \tag{1.7a}$$

where $F=(f_{jk})_{i\leq j,k\leq N}$ is an $N\times N$ matrix with elements

$$f_{jk} = \left(x - x_j + \frac{i}{a_j}\right)\delta_{jk} - \frac{2i}{a_j - a_k}(1-\delta_{jk}). \tag{1.7b}$$

Here, f^* is a complex conjugate of f and δ_{jk} is Kronecker's delta. In particular, for $N=1$, (1.7) represents the one-soliton solution with a Lorenzian profile

$$u_1 = \frac{2a_1}{a_1^2(x-x_1)^2+1}. \tag{1.8}$$

A direct proof of (1.7) using an elementary theory of determinants will be presented in Appendix A.

The definition of the stability of solitons may be classified according to the following three categories: i) linear (or spectral) stability, ii) energetic stability, iii) nonlinear stability. The energetic stability implies that the second variation of certain Lyapunov functional becomes strictly positive when evaluated at the soliton solutions. It would also lead to the linear stability since the second variation is preserved for the linearized equation. In order to extend the energetic stability to the nonlinear stability which deals with small but finite amplitude perturbations, one must take into account higher-order nonlinear terms neglected in evaluating the Lyapunov functional and this makes the analysis more difficult. In accordance with the above classification of the stability, we shall briefly review some known results associated with the stability characteristics of the BO solitons. The linear stability of the BO one-soliton solution has been proved by solving the eigenvalue problem associated with the linearized BO equation.[4] A subsequent nonlinear analysis shows that the soliton is also stable against small but finite perturbations.[5] As for the general

N-soliton solution, its linear stability characteristic has been established by solving explicitly the initial value problem of the linearlized BO equation and investigating the large-time asymptotic of the solution.[6,7] In the process, the completeness relation for the eigenfunctions of the BO equation linearized around the N-soliton solution has played a central role. The recent study demonstrates the orbital stability of the two-soliton solution in which the stability problem has been settled based on the Lyapunov method combined with the spectral analysis of the operators associated with the linearized BO equation.[8] The approach used in this paper originates from the stability analysis of the multisoliton solutions of the Korteweg-de Vries (KdV) equation by means of the constrained variational principle.[9] See also an analogous work dealing with the spectral stability of the multisoliton solutions in the KdV hierarchy.[10] All the above-mentioned works are concerned with the stability of solitons for the BO equation. The stability characteristics of solitons in the BO hierarchy have not been considered as yet.

The purpose of this paper is to establish the Lyapunov stability of the general N-soliton solution (1.6). To be more specific, let us consider the following higher-order BO equation which consists of the commuting flows of the BO hierarchy

$$u_t = \frac{\partial}{\partial x}\frac{\delta H_N}{\delta u}, \tag{1.9a}$$

where the Lyapunov functional H_N is given by

$$H_N(u) = I_{N+2} + \sum_{n=1}^{N} \mu_n I_{n+1}, \tag{1.9b}$$

and μ_n are Lagrange multipliers which will be expressed in terms of the elementary symmetric functions of $a_1, a_2, \ldots, a_N$. See Sec. III for details. We define the profile (or shape) of the N-soliton solution by $U_N = U_N(x) \equiv u_N|_{t_0=t_1=\cdots=0}$. We observe from (1.7) that the N-soliton profile has the same functional form for all the members of the hierarchy, the only difference being the velocities of the solitons. We show that U_N is a stationary solution of (1.9) decaying at infinity. Namely, U_N is realized as a critical point of the functional H_N. Using (1.9b), this condition can be written as the Euler-Lagrange equation

$$\frac{\delta I_{N+2}}{\delta u} + \sum_{n=1}^{N} \mu_n \frac{\delta I_{n+1}}{\delta u} = 0 \quad \text{at } u = U_N. \tag{1.10}$$

The Lyapunov stability of U_N may characterize U_N as a minimal point of the functional I_{N+2} subjected to N constraints

$$I_{n+1}(u) = d_n, \quad (n = 1,2, \ldots, N), \tag{1.11}$$

where d_n are real constants and consequently the second variation of H_N is strictly positive at U_N. This means that H_N is convex at U_N, so that the following inequality holds:

$$H_N(U_N + \epsilon v) - H_N(U_N) > 0, \tag{1.12}$$

where ϵv is a perturbation imposed on U_N which belongs to certain function space specified by the $2N$ integral conditions. We assume that the L^2 norm of v is finite. The small parameter ϵ has been introduced to measure the magnitude of the perturbation. The inequality (1.12) shows that the N-soliton solutions are energetically stable. We give a direct proof of (1.12) with the aid of the results obtained by the inverse scattering transform (IST) for the BO equation.[1,2,11,12] In Sec. II, we summarize the background results arising from the perturbation theory and the Hamiltonian formulation of the BO equation which provide the necessary machinery in carrying out the stability analysis. In Sec. III, we prove the inequality and hence establish the Lyapunov stability of the N-soliton solutions in the Lax hierarchy of the BO equation. In Appendix A, we present a direct

proof of the N-soliton solution (1.7). In Appendix B, we evaluate the number of positive eigenvalues of the Hessian matrix associated with H_N.

II. BACKGROUND RESULTS OF IST

The IST has been applied successfully to solve the initial value problem of the BO equation.[11,12] Furthermore, for real generic potentials it has been used to prove the complete integrability of the BO equation.[1,2] Here, we summarize some background results of the IST necessary for the stability analysis.

A. Eigenvalue problem

The eigenvalue problem associated with the IST of the BO equation may take the form

$$i\phi_x^+ + \lambda(\phi^+ - \phi^-) = -u\phi^+, \tag{2.1}$$

where $\phi^+(\phi^-)$ is the boundary value of the analytic function in the upper(lower)-half complex x plane, u is a real potential rapidly decreasing at infinity, and λ is the eigenvalue (or the spectral parameter). We define the two Jost solutions of (2.1) specified by the boundary condition as $x \to +\infty$,

$$N(x,\lambda) \to e^{i\lambda x}, \quad \overline{N}(x,\lambda) \to 1, \tag{2.2}$$

and the analogous ones as $x \to -\infty$,

$$\overline{M}(x,\lambda) \to 1, \quad M(x,\lambda) \to e^{i\lambda x}. \tag{2.3}$$

These solutions satisfy the linear integral equations

$$N_x - i\lambda N = iP_+(uN), \tag{2.4a}$$

$$\overline{N}_x - i\lambda \overline{N} = iP_+(u\overline{N}) - i\lambda, \tag{2.4b}$$

$$M_x - i\lambda M = iP_+(uM) - i\lambda, \tag{2.4c}$$

$$\overline{M}_x - i\lambda \overline{M} = iP_+(u\overline{M}), \tag{2.4d}$$

where P_+ is the projection operator defined by $P_+ = \frac{1}{2}(1 - iH)$. The solutions of (2.4) subjected to the boundary conditions (2.2) and (2.3) exist for $\lambda > 0$. The Jost functions M, N, and $\overline{N}$ are then related by

$$M = \overline{N} + \beta N, \tag{2.5}$$

where β is a reflection coefficient. For pure soliton potentials, this reflection coefficient vanishes identically.

There exists a set of solutions $\Phi_j(x)$ for negative $\lambda = \lambda_j (j = 1, 2, \ldots, N)$ which satisfy

$$\Phi_{j,x} - i\lambda_j \Phi_j = iP_+(u\Phi_j), \quad (j = 1,2, \ldots, N), \tag{2.6a}$$

with the boundary conditions

$$\Phi_j \to \frac{1}{x}, \quad x \to +\infty, \quad (j = 1,2, \ldots, N). \tag{2.6b}$$

B. Conservation laws

It follows from (1.1), (2.4b), and the time evolution equation for $\overline{N}$,

$$\overline{N}_t - 2\lambda\overline{N}_x - i\overline{N}_{xx} - 2(P_+u_x)\overline{N} = 0, \tag{2.7}$$

that the quantity $\int_{-\infty}^{\infty} u(x,t)\overline{N}(x,t)\mathrm{d}x$ is conserved in time. Expanding $\overline{N}$ in inverse powers of λ,

$$\overline{N} = \sum_{n=0}^{\infty} \frac{(-1)^n \overline{N}_{n+1}}{\lambda^n}, \quad \overline{N}_1 = 1, \tag{2.8a}$$

and substituting (2.8a) into (2.4b), we obtain the following recursion relation that determines $\overline{N}_n$:

$$\overline{N}_{n+1} = i\overline{N}_{n,x} + P_+(u\overline{N}_n), \quad n \geq 1. \tag{2.8b}$$

The nth conservation law may be taken as

$$I_n = (-1)^n \int_{-\infty}^{\infty} u\overline{N}_n \,\mathrm{d}x, \tag{2.9}$$

where a factor $(-1)^n$ is multiplied for convenience. The first three of I_n except I_1 are already given by (1.2). In terms of the scattering data β and λ_j, I_n can be evaluated as

$$I_n = (-1)^n \left\{ 2\pi \sum_{j=1}^{N} (-\lambda_j)^{n-1} + \frac{(-1)^n}{2\pi} \int_0^{\infty} \lambda^{n-2} \beta^*(\lambda)\beta(\lambda)\,\mathrm{d}\lambda \right\}, \quad (n = 1,2,\ldots). \tag{2.10}$$

The first term on the right-hand side of (2.10) is the contribution from solitons and the second term comes from radiations. It is important that both contributions are additive. A remarkable feature of the conservation laws is that they are in involution, namely $I_n (n=1,2,\ldots)$ commute each other in an appropriate Poisson bracket. In particular,

$$\int_{-\infty}^{\infty} \left(\frac{\delta I_n}{\delta u(x)} \right)_{u=U_N} \frac{\partial}{\partial x} \left(\frac{\delta I_m}{\delta u(x)} \right)_{u=U_N} \mathrm{d}x = 0, \quad (n,m = 1,2,\ldots). \tag{2.11}$$

C. Variational derivatives

The variational derivatives of the scattering date with respect to the potential are calculated explicitly. In developing the Lyapunov stability, we need the formulas of the variational derivatives evaluated for the N-soliton potential $u=U_N$. In particular, the following formula plays an important role in our analysis:

$$\left(\frac{\delta \lambda_j}{\delta u(x)} \right)_{u=U_N} = \frac{1}{2\pi\lambda_j} \Phi_j^*(x)\Phi_j(x), \quad (j = 1,2,\ldots,N). \tag{2.12}$$

Here, the eigenfunction Φ_j corresponding to the discrete spectrum λ_j satisfies the system of linear algebraic equations

$$(x - \gamma_j)\Phi_j + i \sum_{\substack{k=1 \\ (k\neq j)}}^{N} \frac{1}{\lambda_j - \lambda_k} \Phi_k = 1, \quad (j = 1,2,\ldots,N), \tag{2.13}$$

where $\gamma_j = x_{j0} + i/(2\lambda_j)$ and x_{j0} are real constants. Recall that λ_j are related to the amplitude parameters a_j introduced in (1.7) by the relations $\lambda_j = -a_j/2 (j=1,2,\ldots,N)$. Taking account of the fact that the reflection coefficient β becomes zero for $u=U_N$, we can derive from (2.10) and (2.12) the formula

$$\left(\frac{\delta I_n}{\delta u(x)}\right)_{u=U_N} = (-1)^n(n-1)\sum_{j=1}^{N}(-\lambda_j)^{n-3}\Phi_j^*(x)\Phi_j(x), \quad (n=2,3,\ldots,N). \tag{2.14}$$

In terms of Φ_j, U_N has the following two alternative expressions:

$$U_N = i\sum_{j=1}^{N}(\Phi_j - \Phi_j^*), \tag{2.15}$$

$$U_N = -\sum_{j=1}^{N}\frac{1}{\lambda_j}\Phi_j^*\Phi_j. \tag{2.16}$$

The positive definiteness of U_N is obvious from (2.16) since all λ_j are negative quantities. One can derive (2.16) by using (2.13) and (2.15). The formula (2.16) also follows from (1.2a), (2.10) and (2.14). In Appendix A, we show that U_N can be rewritten in a compact form in terms of a determinant.

The following relation concerning the variational derivative of β with respect to u is useful in evaluating the contribution of the continuous part to the functional H_N:

$$\frac{\delta\beta(\lambda)}{\delta u(x)} = iM(x,\lambda)N^*(x,\lambda). \tag{2.17}$$

For the N-soliton potential $u=U_N$, M reduces to $\overline{N}$ by (2.5) and $\beta\equiv 0$. The function MN^* satisfies the orthogonality conditions

$$\int_{-\infty}^{\infty} M(x,\lambda)N^*(x,\lambda)\frac{\partial}{\partial x}(\Phi_j^*(x)\Phi_j(x))\,dx = 0, \quad (j=1,2,\ldots,N). \tag{2.18}$$

Finally, we emphasize that all the results presented here are obtained through the analysis of the spatial part (2.1) of the Lax pair for the BO equation.

III. LYAPUNOV STABILITY

A. Variational characterization of the *N*-soliton profile

We first show that the stationary solution U_N of the higher-order BO equation (1.9) satisfies (1.10) if one prescribes the Lagrange multipliers μ_n appropriately. This provides a variational characterization of U_N. Let $\Psi_j=\Phi_j^*\Phi_j$ and $b_j=-\lambda_j=a_j/2$. With this notation, (1.10) and (2.14) give a linear relation among Ψ_j,

$$(N+1)\sum_{j=1}^{N} b_j^{N-1}\Psi_j + \sum_{n=1}^{N}(-1)^{N-n+1}n\mu_n\sum_{j=1}^{N} b_j^{n-2}\Psi_j = 0. \tag{3.1}$$

In view of the fact that Ψ_j are functionally independent squared eigenfunctions,[1,2] μ_n must satisfy the following system of linear algebraic equations:

$$\sum_{n=1}^{N}(-1)^{N-n}nb_j^{n-1}\mu_n = (N+1)b_j^N, \quad (j=1,2,\ldots,N). \tag{3.2}$$

To solve (3.2), we introduce an $N\times N$ matrix V

$$V=(v_{jk})_{1\le j,k\le N}, \quad v_{jk}=b_j^{k-1}, \tag{3.3}$$

and the cofactor of v_{jk} by

$$V_{jk} = \frac{\partial |V|}{\partial v_{jk}}, \quad |V| = \det V, \tag{3.4}$$

where $|V|$ is the Vandermonde determinant. Notably, since $|V| = \Pi_{1 \le j < k \le N}(b_k - b_j)$ and $b_j \neq b_k$ for $j \neq k$, $|V|$ never vanishes. This fact will be used essentially in the following calculation. It is also convenient to define the polynomials $g(x)$ and $g_k(x)$ by

$$g(x) = \prod_{j=1}^{N} (x - b_j) = \sum_{s=1}^{N} (-1)^s \sigma_s x^{N-s}, \tag{3.5}$$

$$g_k(x) = \prod_{\substack{j=1 \\ (j \neq k)}}^{N} (x - b_j) = \sum_{s=1}^{N-1} (-1)^s \sigma_{k,s} x^{N-s}, \tag{3.6}$$

where $\sigma_0 = 1$ and $\sigma_s (1 \le s \le N)$ are elementary symmetric functions of $b_1, b_2, \ldots, b_N$,

$$\sigma_1 = \sum_{j=1}^{N} b_j, \quad \sigma_2 = \sum_{\substack{j,k=1 \\ (j<k)}}^{N} b_j b_k, \ldots, \sigma_N = \prod_{j=1}^{N} b_j, \tag{3.7a}$$

and $\sigma_{k,s}$ are given by the relation

$$\sigma_{k,s} = \sum_{j=0}^{s} \sigma_j (-b_k)^{s-j}. \tag{3.7b}$$

Obviously, all σ_j are positive quantities since $b_j > 0 (j = 1, 2, \ldots, N)$. Now, applying Cramer's rule to (3.2) with use of the fact $|V| \neq 0$, we find that μ_n are determined uniquely as

$$\mu_n = (-1)^{N-n} \frac{N+1}{n} \frac{\Sigma_{k=1}^{N} V_{kn} b_k^N}{|V|}, \quad (n = 1, 2, \ldots, N). \tag{3.8}$$

Substituting the formulas[13]

$$V_{kn} = \frac{(-1)^{N-n} \sigma_{k,N-n|V|}}{g_k(b_k)}, \quad (k, n = 1, 2, \ldots, N), \tag{3.9}$$

$$\sum_{k=1}^{N} \frac{\sigma_{k,N-n} b_k^N}{g_k(b_k)} = \sigma_{N-n+1}, \quad (n = 1, 2, \ldots, N), \tag{3.10}$$

into (3.8), we arrive at a simple expression of μ_n

$$\mu_n = \frac{N+1}{n} \sigma_{N-n+1}, \quad (n = 1, 2, \ldots, N). \tag{3.11}$$

If we use the relations $b_j = a_j/2 (j = 1, 2, \ldots, N)$, we can see that μ_n are expressed in terms of elementary symmetric functions of $a_1, a_2, \ldots, a_N$.

B. Stability

Let us now prove the inequality (1.12) which assures that the functional H_N is convex at the N-soliton profile U_N. The method used here is based on the ideas developed in a recent work[10] on the spectral stability of the N-soliton solution of the KdV hierarchy as well as an earlier work[14] on the algebraic structure of the BO N-soliton solution. We first rewrite (2.10) as

$$I_{n+1}(u) = (-1)^{n+1}\left\{ 2\pi \sum_{j=1}^{N} b_j^n + (-1)^{n+1} r_n \right\}, \tag{3.12a}$$

where we have put $b_j = -\lambda_j$ and

$$r_n = \frac{1}{2\pi}\int_{\infty}^{0} \lambda^{n-1}\beta^*(\lambda)\beta(\lambda)\, d\lambda. \tag{3.12b}$$

Let ΔQ be the increment of any functional $Q(u)$ around $u=U_N$, i.e.,

$$\Delta Q = Q(U_N + \epsilon v) - Q(U_N). \tag{3.13}$$

It then follows from the constraints (1.11) that

$$\Delta I_{n+1} = 0, \quad (n = 1,2,\ldots,N). \tag{3.14}$$

We then use (3.12) to rewrite (3.14) in the form

$$2\pi n \sum_{j=1}^{N} b_j^{n-1}\Delta b_j + (-1)^{n+1}\Delta r_n = 0, \quad (n = 1,2,\ldots,N), \tag{3.15}$$

where we have neglected the higher-order terms $(\Delta b_j)^s (s=2,3,\ldots,N)$. These relations indicate that the increments of soliton amplitudes are balanced with the increments of radiations. We recall that $\beta \equiv 0$ for $u=U_N$ and consequently $\Delta(\beta^*\beta) = \Delta\beta^*\Delta\beta$. This leads to the estimates $\Delta r_n \sim O(\epsilon^2)$ and $\Delta r_n > 0$ for all n. The case $\Delta r_n = 0$ calls a special attention and it will be considered in detail later. Hence, (3.15) can be solved consistently in Δb_j only if $\Delta b_j \sim O(\epsilon^2)$. Since by the definition (1.4)

$$\Delta b_j = \epsilon \int_{-\infty}^{\infty} \left(\frac{\delta b_j}{\delta u} \right)_{u=U_N} v(x)dx + O(\epsilon^2), \tag{3.16}$$

one must impose the integral conditions on the perturbation $v(x)$,

$$\int_{-\infty}^{\infty} \left(\frac{\delta b_j}{\delta u} \right)_{u=U_N} v(x)dx = 0, \quad (j = 1,2,\ldots,N), \tag{3.17}$$

in accordance with the above-presented estimate for Δb_j. We can see from (2.12), (2.14) together with the relations $b_j = -\lambda_j (j=1,2,\ldots,N)$ and $|V| \neq 0$ that (3.17) are equivalent to

$$\int_{-\infty}^{\infty} \left(\frac{\delta I_{n+1}}{\delta u} \right)_{u=U_N} v(x)dx = 0, \quad (n = 1,2,\ldots,N). \tag{3.18}$$

Owing to (3.14), however, these conditions are satisfied automatically. The above-noted observations allow us to solve (3.15). Indeed, the solutions are written, with use of Cramer's rule, as

$$\Delta b_j = \frac{1}{2\pi} \frac{\Sigma_{n=1}^{N} \dfrac{(-1)^n}{n} V_{jn}\Delta r_n}{|V|}, \quad (j = 1,2,\ldots,N). \tag{3.19}$$

It now follows from (1.9b), (3.12), and (3.14) that

$$\Delta H_N = (-1)^N \left\{ 2\pi(N+1) \sum_{j=1}^{N} b_j^N \Delta b_j + (-1)^{N+2}\Delta r_{N+1} \right\}. \tag{3.20}$$

If we substitute (3.19) into (3.20) and use the formulas (3.9) and (3.10), ΔH_N simplifies to

$$\Delta H_N = (N+1)\sum_{n=1}^{N} \frac{\sigma_{N-n+1}}{n}\Delta r_n + \Delta r_{N+1}. \tag{3.21}$$

Since $\sigma_{N-n+1} > 0$ for $n=1,2,\ldots,N$ by the definition (3.7), we find that if at least one of Δr_n is not zero, then $\Delta H_N > 0$. On the other hand, if all Δr_n become zero, then $\Delta H_N = 0$. In the latter case, we see from (3.15) that $\Delta b_j = 0$ for all j. This situation will happen when the perturbation ϵv represents the small variation of U_N with respect to the phase parameters x_{j0}. Specifically

$$\epsilon v(x) = \sum_{j=1}^{N} \frac{\partial U_N}{\partial x_{j0}}\delta x_{j0}, \tag{3.22}$$

where δx_{j0} are small perturbations of order ϵ. If we impose the following N integral conditions on $v(x)$ in addition to (3.28)

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left(\frac{\delta I_{n+1}}{\delta u}\right)_{u=U_N} v(x)\mathrm{d}x = 0, \quad (n=1,2,\ldots,N), \tag{3.23}$$

then the perturbation of the form (3.22) ceases to be admissible, as we shall now demonstrate. We first notice that the right-hand side of (3.22) can be expressed in terms of the x derivative of $(\delta I_{n+1}/\delta u)_{u=U_N}$. Indeed, we take $u=u_N$ in (1.3) and then put $t_0=t_1=\cdots=0$ to obtain

$$(-1)^n n\sum_{j=1}^{N} b_j^{n-1}\frac{\partial U_N}{\partial x_{j0}} = \frac{\partial}{\partial x}\left(\frac{\delta I_{n+1}}{\delta u}\right)_{u=U_N}, \quad (n=1,2,\ldots,N), \tag{3.24}$$

where we have used (1.6), the definition of U_N and $b_j = a_j/2$. Thanks to the fact $|V| \neq 0$, the relations (3.24) can be inverted to give

$$\frac{\partial U_N}{\partial x_{j0}} = \sum_{n=1}^{N} \frac{(-1)^n}{n}\frac{V_{jn}}{|V|}\frac{\partial}{\partial x}\left(\frac{\delta I_{n+1}}{\delta u}\right)_{u=U_N}, \quad (j=1,2,\ldots,N). \tag{3.25}$$

An alternative expression of (3.22) follows immediately upon introducing (3.25) into (3.22), which reads

$$\epsilon v(x) = \sum_{j=1}^{N}\sum_{n=1}^{N} \frac{(-1)^n}{n}\frac{V_{jn}}{|V|}\frac{\partial}{\partial x}\left(\frac{\delta I_{n+1}}{\delta u}\right)_{u=U_N}\delta x_{j0}. \tag{3.26}$$

We observe that this perturbation satisfies the conditions (3.18) by virtue of (2.11). It is important that the $N\times N$ matrix $C=(c_{jk})_{1\le j,k\le N}$ with elements

$$c_{jk} = \int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left(\frac{\delta I_{j+1}}{\delta u}\right)_{u=U_N}\frac{\partial}{\partial x}\left(\frac{\delta I_{k+1}}{\delta u}\right)_{u=U_N}\mathrm{d}x \tag{3.27}$$

is positive definite and hence $|C| \neq 0$. In view of this fact, we deduce from (3.23) and (3.26) that $\delta x_{j0} = 0 (j=1,2,\ldots,N)$ and consequently $v=0$, which implies the above-mentioned assertion. An additional relation which deserves remark is

$$\int_{-\infty}^{\infty} \left(\frac{\delta\beta}{\delta u}\right)_{u=U_N} v(x)\mathrm{d}x = 0, \tag{3.28}$$

which follows from (2.14), (2.17), (2.18), and (3.26). This leads to the estimates $\Delta\beta \sim O(\epsilon^2)$ and $\Delta r_n \sim O(\epsilon^4)$. As a result, the pertubation (3.26) gives rise to higher-order contributions to (3.21) which also means that the second variation of H_N turns out to be zero. In conclusion, the inequality $\Delta H_N > 0$ holds under the simultaneous conditions (3.18) and (3.25) imposed on $v(x)$, which completes the proof of (1.12). The convexity of H_N implies that the second variation of H_N is

strictly positive and consequently the N-soliton solutions are energetically stable.

C. Remark

In this paper, the convexity of H_N has been proved by invoking some results obtained by the IST of the BO equation. There exists, however, another method to establish the same convex property without recourse to the IST. To illustrate this, we put $u(x,t)=U_N(x)+\epsilon v(x)e^{\lambda t}$ and linearize (1.9) around U_N. The resulting eigenvalue equation can be written as

$$\frac{\partial}{\partial x}\mathcal{L}_N v = \lambda v, \tag{3.29}$$

where $\mathcal{L}_N$ is a self-adjoint operator. This operator may be defined through the relation

$$\delta^2 H_N = \frac{\epsilon^2}{2}\int_{-\infty}^{\infty} v(x)\mathcal{L}_N v(x)\mathrm{d}x, \tag{3.30}$$

where $\delta^2 H_N$ denotes the second variation of H_N. Let $n(\mathcal{L}_N)$ be the number of negative eigenvalues of $\mathcal{L}_N$ and $p(\mathcal{H}_N)$ be the number of positive eigenvalues of the Hessian matrix defined by

$$\mathcal{H}_N = (h_{jk})_{1\le j,k\le N}, \quad h_{jk} = \frac{\partial^2 H_N}{\partial \mu_j\, \partial \mu_k}. \tag{3.31}$$

Then, under the conditions (3.18) and (3.23) the positivity of $\delta^2 H_N$ is satisfied if and only if $n(\mathcal{L}_N)=p(\mathcal{H}_N)$. The above-noted criterion of the positivity property has been proved in Ref. 15 and has been applied to the Lyapunov stability of the N-soliton solution of the KdV equation.[9] In particular, the spectral property of the $2N$th-order differential operator associated with the linearized KdV equation has been investigated by extending the classical Sturmian theory. See also a related work dealing with the stability of the N-soliton solutions in the KdV hierarchy.[10] In the case of the BO equation, however, the eigenvalue equation (3.29) is not purely differential equation but actually integrodifferential equation since it includes the Hilbert transform. This makes the spectral analysis more difficult. Quite recently, a new method was developed to characterize the spectral property of $\mathcal{L}_N$ for $N=2$.[8] The extension to the general N-soliton solutions of the BO equation and its hierarchy is still to be resolved. It is noteworthy that $P(\mathcal{H}_N)$ can be evaluated explicitly for the N-soliton profile U_N. This calculation is presented in Appendix B. The stability analysis developed in this paper would suggest that $n(\mathcal{L}_N)$ is equal to $P(\mathcal{H}_N)$. This interesting issue will be pursued in a future study.

APPENDIX A: PROOF OF THE *N*-SOLITON SOLUTION

In this Appendix, we provide a direct proof of the N-soliton solution (1.7) of the nth higher-order BO equation (1.3) by means of an elementary theory of determinants. For convenience, we write down some basic formulas for determinants upon which our proof relies. Let F be an $N\times N$ matrix with elements f_{jk} given by (1.7b) and F_{jk} be the cofactor of f_{jk}. The expansion of $|F|$ by elements and their cofactors is given in two ways:

$$\sum_{k=1}^{N} f_{jk}F_{lk} = \delta_{jl}|F|, \tag{A1a}$$

$$\sum_{j=1}^{N} f_{jk}F_{jl} = \delta_{kl}|F|. \tag{A1b}$$

The following formula is a consequence of (A1):

$$\sum_{j,k=1}^{N}(f_j+g_k)f_{jk}F_{jk}=\sum_{j=1}^{N}(f_j+g_j)|F|. \tag{A2}$$

The differential rule applied to the determinant $|F|$ gives

$$|F|_x=\sum_{j=1}^{N}F_{jj}, \tag{A3a}$$

$$|F|_{t_n}=(-1)^n\sum_{j=1}^{N}c_jF_{jj}, \tag{A3b}$$

where $c_j=(n+1)a_j^n/2^n$. To carry out the proof, it is necessary to assign the time dependence of the eigenfunction Φ_j for the discrete spectrum λ_j. This can be accomplished simply by replacing the phase factor γ_j introduced in (2.13) by x_j which is defined in (1.6). We first show that (2.15) can be rewritten in an alternative determinantal form (1.7). The solution to (2.13) is found by using Cramer's rule as

$$\Phi_j=i\sum_{k=1}^{N}\frac{F_{kj}}{|F|}. \tag{A4}$$

We put $f_j=a_j$ and $g_j=-a_j$ in (A2) to derive the relation

$$\sum_{j,k=1}^{N}F_{jk}=\sum_{j=1}^{N}F_{jj}. \tag{A5}$$

It follows from (A3) to (A5) that

$$\sum_{j=1}^{N}\Phi_j=i(\ln|F|)_x. \tag{A6}$$

Substituting (A6) and its complex conjugate expression into (2.15), we find that (2.15) coincides with (1.7).

Let us now proceed to the proof of the N-soliton solution. We substitute (1.7) and (2.14) into (1.3) and integrate it once with respect to x to recast (1.3) into the form

$$i(|F|^*|F|_{t_n}-|F||F|^*_{t_n})/|F|^*|F|=(-1)^n(n+1)\sum_{j=1}^{N}\left(\frac{a_j}{2}\right)^{n-1}\Phi_j^*\Phi_j, \tag{A7}$$

where we have used the relation $\lambda_j=-a_j/2$. The following identity has been established by using Jacobi's formula for determinants:

$$i\left(\frac{|F|^*F_{jk}}{a_k}-\frac{|F|F^*_{kj}}{a_j}\right)=2\frac{(|F|\Phi_j)^*(|F|\Phi_k)}{a_ja_k},\quad (j,k=1,2,\ldots,n). \tag{A8}$$

Indeed, (A8) coincides with (A20) in Ref. 7 with the identification $f=|F|^*, \Delta_{jk}=F^*_{jk}, \psi_j=\Phi_j^*$. If we multiply (A8) with $j=k$ by c_j and sum up with respect to j, we obtain

$$\frac{i}{2}\sum_{j=1}^{N}c_j(|F|^*F_{jj}-|F|F^*_{jj})=\frac{n+1}{2^n}\sum_{j=1}^{N}a_j^{n-1}\Phi_j^*\Phi_j|F|^*|F|. \tag{A9}$$

The left-hand side of (A9) is modified further by introducing the formula (A3b) and its complex conjugate expression. It leads, after dividing the resultant expression by $|F|^*|F|$, to (A7) and thus completing the proof.

APPENDIX B: POSITIVE EIGENVALUES OF THE HESSIAN MATRIX $\mathcal{H}_N$

The Hessian matrix $\mathcal{H}_N$ is defined by (3.31). It is a real symmetric matrix whose elements are calculated explicitly for the N-soliton solution. Indeed, by taking $\beta=0$ in (2.10), the nth conservation law corresponding to $u=u_N$ reduces to

$$I_n = 2\pi(-1)^n \sum_{l=1}^{N} b_l^{n-1}, \quad (b_l = -\lambda_l). \tag{B1}$$

If we regard H_N as a function of $\mu_j (j=1,2,\ldots,N)$, we obtain from (1.9b) and (1.10)

$$\frac{\partial H_N}{\partial \mu_j} = I_{j+1}, \quad (j = 1,2,\ldots,N). \tag{B2}$$

Hence

$$h_{jk} = \frac{\partial I_{j+1}}{\partial \mu_k} = 2\pi(-1)^{j+1} j \sum_{l=1}^{N} b_l^{j-1} \frac{\partial b_l}{\partial \mu_k}. \tag{B3}$$

Let $P=(p_{jk})_{1\le j,k\le N}$ and $Q=(q_{jk})_{i\le j,k\le N}$ be $N\times N$ matrices with elements

$$p_{jk} = 2\pi(-1)^{j+1} j b_k^{j-1}, \tag{B4a}$$

$$q_{jk} = \frac{\partial \mu_j}{\partial b_k} = \frac{N+1}{j} \frac{\partial \sigma_{N-j+1}}{\partial b_k}, \tag{B4b}$$

respectively. Note that the right-hand side of (B4b) follows from (3.11). Using the above-presented definition, we can rewrite (B3) in the form

$$\mathcal{H}_N = PQ^{-1}, \tag{B5}$$

if Q^{-1} exists. To show the nonsingular nature of Q, we use the definition (3.7a) of σ_{N-j+1} and (B4b) to evaluate the determinant of Q. A simple calculation immediately leads to

$$|Q| = \frac{(N+1)^N}{N!} \prod_{1\le j<k\le N} (b_k - b_j). \tag{B6}$$

Since $b_j \neq b_k$ for $j \neq k$, we confirm that $|Q| \neq 0$, implying that Q is invertible.

It now follows from (B5) that

$$Q^T \mathcal{H}_N Q = Q^T P. \tag{B7}$$

In accordance with Sylvester's law of inertia, one can see from (B7) that the number of positive eigenvalues of $\mathcal{H}_N$ coincides.with that of Q^TP. The latter can be counted easily, as we shall now demonstrate. Using (B4), the (j,k) element of Q^TP becomes

$$(Q^T P)_{jk} = 2\pi(N+1) \sum_{l=1}^{N} (-1)^{l+1} \frac{\partial \sigma_{N-l+1}}{\partial b_j} b_k^{l-1}. \tag{B8}$$

We differentiate (3.5) by b_j and then put $x=b_k$ to derive the relation

$$\sum_{l=1}^{N}(-1)^{l+1}\frac{\partial\sigma_{N-l+1}}{\partial b_j}b_k^{l-1}=\delta_{jk}\prod_{\substack{l=1\\(l\neq j)}}(b_l-b_k). \tag{B9}$$

Introducing (B9) into (B8), we find that Q^TP is a diagonal matrix. We can order the magnitude of b_j as $b_1>b_2>\cdots>b_N>0$ without loss of generality. Then, (B8) and (B9) indicate that the number of positive eigenvalues of Q^TP is equal to $[(N+1)/2]$ where $[x]$ denotes the integer part of x. If we take account of (B7) and Sylvester's law of inertia, we conclude that $p[\mathcal{H}_N]=[(N+1)/2]$.

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Variational principles for eigenvalues of the Klein–Gordon equation

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In this paper variational principles for eigenvalues of an abstract model of the Klein–Gordon equation with electromagnetic potential are established. They are used to characterize and estimate eigenvalues in cases where the essential spectrum has a gap around 0, even in the presence of complex eigenvalues. As a consequence, a comparison between eigenvalues of the Klein–Gordon equation in $\mathbb{R}^d$ and eigenvalues of certain Schrödinger operators is obtained. The results are illustrated on examples including the Klein–Gordon equation with Coulomb and square-well potential. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2345108]

I. INTRODUCTION

The motion of a relativistic spinless particle of mass m and charge e in an electromagnetic field with scalar potential φ and vector potential $\vec{A}$ is described by the Klein–Gordon equation

$$\left(-\left(-\mathrm{i}\hbar\frac{\partial}{\partial t}-e\varphi\right)^2+c^2\left(-\mathrm{i}\hbar\,\nabla-\frac{e}{c}\vec{A}\right)^2+m^2c^4\right)U=0; \tag{1.1}$$

here c is the speed of light and $\hbar$ is the Planck constant. If we set

$$U(x,t)=:e^{(i\lambda/\hbar)t}u(x),\quad x\in\mathbb{R}^d,\quad t\in\mathbb{R},$$

denote the multiplication operator by $e\varphi$ in $L^2(\mathbb{R}^d)$ by V, the positive symmetric operator $c^2(-\mathrm{i}\hbar\nabla-(e/c)\vec{A})^2$ in $L^2(\mathbb{R}^d)$ by A_0 and set $\gamma:=mc^2$, then (1.1) becomes a quadratic eigenvalue problem of the form

$$(-(\lambda-V)^2+A_0+\gamma^2)u=0,\quad \lambda\in\mathbb{C}. \tag{1.2}$$

As a consequence, the spectral properties of (1.2) determine the solvability of the time-dependent Klein–Gordon equation (1.1) subject to certain initial conditions. The abstract spectral problem (1.2) has been studied by a number of authors under various conditions on V and on A_0, using different techniques (see Ref. 6 for a list of references).

In recent papers[6,7] the abstract Klein–Gordon equation (1.2) was investigated by means of associated block operator matrices and suitable indefinite inner products, imposing rather general conditions on the unbounded operator V. These conditions, which will also be used in the present paper, ensure that the essential spectrum of problem (1.2) has a gap around 0, but they do not exclude the occurrence of complex eigenvalues.

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It is the aim of this paper to establish variational principles for eigenvalues of the spectral problem (1.2) in the spectral gap around 0 and to derive eigenvalue estimates and comparisons with eigenvalues of certain Schrödinger operators. As in the case of Dirac operators, standard variational principles do not apply to eigenvalues in gaps of the essential spectrum; to overcome this difficulty, other functionals than the classical Rayleigh functional have been used, see, e.g., Refs. 2 and 4, and references therein.

In general the assumptions on V do not guarantee that the sum of operators on the left-hand side of (1.2) is densely defined, and hence the corresponding operator $T(\lambda)$ has to be introduced by means of quadratic forms. The variational principles are proved for abstract quadratic eigenvalue problems of the form (1.2) in a Hilbert space $\mathcal{H}$ with an arbitrary self-adjoint operator $A_0 \geqslant 0$ in $\mathcal{H}$ and a symmetric operator V in $\mathcal{H}$; the proof uses variational principles for eigenvalues of operator functions defined on an arbitrary interval, recently proved in Ref. 2. As a result of the possible presence of complex eigenvalues, an index shift occurs, which is characterized by means of a linearization of the operator polynomial T.

The paper is organized as follows. In Sec. II we associate an operator polynomial T formally given by

$$T(\lambda) = A_0 + \gamma^2 - (\lambda - V)^2, \quad \lambda \in \mathbb{C},$$

with (1.2). Assuming that $\mathcal{D}(A_0^{1/2}) \subset \mathcal{D}(V)$ and $S := V(A_0 + \gamma^2)^{-1/2} = S_0 + S_1$ with $\|S_0\| < 1$ and S_1 compact (cf. Ref. 6), we obtain the operators $T(\lambda)$ via the forms

$$\mathbf{t}(\lambda)[x,y] = (A_0^{1/2}x, A_0^{1/2}y) + \gamma^2(x,y) - ((V-\lambda)x, (V-\bar{\lambda})y),$$

which are defined for all $x, y \in \mathcal{D}(A_0^{1/2})$. The spectrum, eigenvalues, etc., of the abstract Klein–Gordon equation (1.2) are given by the spectrum, eigenvalues, etc., of the operator polynomial T.

In order to investigate the spectral properties of T, we use two different auxiliary objects. First we employ the operator polynomial L given by

$$L(\lambda) = I - (S^* - \lambda H_0^{-1/2})(S - \lambda H_0^{-1/2}), \quad \lambda \in \mathbb{C},$$

whose values are bounded operators in $\mathcal{H}$. We show that $T(\lambda) = H_0^{1/2} L(\lambda) H_0^{1/2}$ and that the essential spectrum of T on the real axis has a gap around 0 and for every point λ in this gap the number of negative eigenvalues of T is finite. Second, we introduce a family

$$\mathcal{A}_{\lambda_0} = \begin{pmatrix} \lambda_0 & I \\ T(\lambda_0) & 2V - \lambda_0 \end{pmatrix}, \quad \lambda_0 \in \mathbb{C},$$

of operators in the space $\mathcal{H}_{1/2} \oplus \mathcal{H}$, where $\mathcal{H}_{1/2} = (\mathcal{D}(H_0^{1/2}), (H_0^{1/2}\cdot, H_0^{1/2}\cdot))$. For every fixed $\lambda_0 \in \rho(T)$, $\mathcal{A}_{\lambda_0}$ can be considered as a linearization of T. We prove that the spectra, eigenvalues, and essential spectra of T and $\mathcal{A}_{\lambda_0}$, respectively, coincide. Note that the particular operator $\mathcal{A}_0$ coincides with the block operator matrix used in Ref. 6 to study the spectral problem (1.2). We use the more flexible choice of λ_0, e.g., to maximize the range of applicability of our variational principle in the spectral gap. Using an indefinite product on $\mathcal{H}_{1/2} \oplus \mathcal{H}$ induced by the form $\mathbf{t}(\lambda_0)$ in the first component, we show that the essential spectrum of $\mathcal{A}_{\lambda_0}$, and hence of T, is real and has a gap around 0, and that the nonreal spectrum consists of at most finitely many pairs of complex conjugate eigenvalues of finite algebraic multiplicity.

In Sec. III we establish variational principles for real eigenvalues of T in the spectral gap around 0; for the result of Ref. 2 that is applied here it is convenient that the domain of the form $\mathbf{t}(\lambda)$ is independent of λ. The functionals $p_\pm$ used in this characterization, which replace the Rayleigh functionals used for linear spectral problems, are defined as the roots $p_\pm(x)$ of the quadratic equation $\mathbf{t}(\lambda)[x] = 0$ (if the latter are real). In certain circumstances including the presence of complex eigenvalues an index shift may occur in the variational principle.

In Sec. IV we use the variational principles derived in Sec. III to establish various bounds for the eigenvalues of the abstract Klein–Gordon equation (1.2). These bounds are obtained by esti-

mating the functionals $p_\pm$ in the particular cases that V is semibounded, bounded, or has a definite sign. Further refined estimates for eigenvalues of the Klein–Gordon equation in the spectral gap are obtained by comparing them with eigenvalues of Schrödinger operators of the form

$$H_\pm = \pm \frac{1}{2\gamma} A_0 + V = \pm \frac{1}{2m} \left(-i\hbar \nabla - \frac{e}{c} \vec{A} \right)^2 + e\varphi.$$

It turns out that for the Klein–Gordon equation in $\mathbb{R}^d$ these estimates are sharp in the sense that for $c \to \infty$ the eigenvalues of the Klein–Gordon equation converge to the respective eigenvalues of the Schrödinger operators above.

Finally, in Sec. V we illustrate our results by applying them to the Klein–Gordon equation in $\mathbb{R}^d$ with Coulomb and square-well potential. In the Coulomb case we compare our results with the explicitly known eigenvalues. In the square-well case we choose the depth of the potential so that complex eigenvalues occur (cf. Ref. 11) and illustrate how our results apply in this situation.

In the following we introduce some notation, which is used throughout the paper.

For a closed linear operator A in a Hilbert space we denote by $\mathcal{D}(A)$ the domain of A and, if applicable, by $\mathcal{Q}(A)$ its form domain. We also use $\mathcal{D}(\cdot)$ for domains of quadratic forms.

Let T be an operator function on $\mathbb{C}$ such that $T(\lambda)$ is a closed linear operator in a Hilbert space for every $\lambda \in \mathbb{C}$. The *spectrum*, the *resolvent set*, the *point spectrum*, and the *essential spectrum* of T are defined by

$$\sigma(T) := \{\lambda \in \mathbb{C}: 0 \in \sigma(T(\lambda))\}, \quad \rho(T) := \mathbb{C} \setminus \sigma(T),$$

$$\sigma_p(T) := \{\lambda \in \mathbb{C}: 0 \in \sigma_p(T(\lambda))\},$$

$$\sigma_{\mathrm{ess}}(T) := \{\lambda \in \mathbb{C}: T(\lambda) \text{ is not Fredholm}\},$$

respectively; here a closed operator is called *Fredholm* if its kernel is finite dimensional and its range has finite (algebraic) co-dimension (which implies that the range is closed). Note that $\lambda \in \sigma_{\mathrm{ess}}(T) \Leftrightarrow 0 \in \sigma_{\mathrm{ess}}(T(\lambda))$; thus the above-presented definition of the essential spectrum corresponds to the essential spectrum $\sigma_{e3}(\cdot)$ of linear operators defined in Ref. 1, Chap IX.

For a self-adjoint operator A in a Hilbert space and an interval $I \subset \mathbb{R}$ let $\mathcal{L}_I(A)$ denote the spectral subspace of A corresponding to I. Further, we define

$$\kappa_-(A) := \dim \mathcal{L}_{(-\infty,0)}(A).$$

If $\kappa_-(A)$ is finite, then the negative spectrum of A consists only of finitely many eigenvalues of finite multiplicity and $\kappa_-(A)$ is equal to the number of these eigenvalues counted with multiplicities.

II. THE QUADRATIC OPERATOR POLYNOMIAL *T*

Let $(\mathcal{H}, (\cdot,\cdot))$ be a Hilbert space with corresponding norm $\|\cdot\|$, $A_0 \geqslant 0$ a self-adjoint operator in $\mathcal{H}$, $\gamma > 0$ a real constant, and V a symmetric operator in $\mathcal{H}$ and set

$$H_0 := A_0 + \gamma^2.$$

Note that $H_0 \geqslant \gamma^2$ and $\mathcal{D}(H_0^{1/2}) = \mathcal{D}(A_0^{1/2})$.

The following assumptions play a crucial role throughout the paper:

(A1) $\mathcal{D}(A_0^{1/2}) \subset \mathcal{D}(V)$,

(A2) $S := VH_0^{-1/2} = S_0 + S_1$ such that $\|S_0\| < 1$ and S_1 is compact.

Note that in order to satisfy assumption (A2) an arbitrary constant may be added to the operator V, which induces a shift in the spectral parameter in (1.2).

Assumption (A1) implies that V is both $A_0^{1/2}$-bounded and $H_0^{1/2}$-bounded, i.e., there exist a_1, b_1, a_2, $b_2 \geqslant 0$ such that

$$\|Vx\| \leqslant a_1\|x\| + b_1\|A_0^{1/2}x\|, \tag{2.1}$$

$$\|Vx\| \leqslant a_2\|x\| + b_2\|H_0^{1/2}x\| \tag{2.2}$$

for $x \in \mathcal{D}(A_0^{1/2}) = \mathcal{D}(H_0^{1/2})$. This shows that the operator S in assumption (A2) is bounded in $\mathcal{H}$; assumption (A2) then implies that (2.1) and (2.2) hold with $b_1 < 1$ and $b_2 < 1$, respectively.

Remark 2.1: Note that (2.1) is equivalent to

$$\|Vx\|^2 \leqslant a_3\|x\|^2 + b_3\|A_0^{1/2}x\|^2, \quad x \in \mathcal{D}(A_0^{1/2}), \tag{2.3}$$

with constants a_3, $b_3 \geqslant 0$; moreover, (2.1) holds with $b_1 < 1$ if and only if (2.3) holds with $b_3 < 1$ (cf. Ref. 3, Sec. V.4.1).

Under the above-noted assumptions we introduce the family $\mathfrak{t}(\lambda)$, $\lambda \in \mathbb{C}$, of sesquilinear forms by

$$\mathfrak{t}(\lambda)[x,y] := (A_0^{1/2}x, A_0^{1/2}y) + \gamma^2(x,y) - ((V-\lambda)x, (V-\bar\lambda)y) = (H_0^{1/2}x, H_0^{1/2}y) - ((V-\lambda)x, (V-\bar\lambda)y) \tag{2.4}$$

for all $x, y \in \mathcal{D}(\mathfrak{t}(\lambda)) := \mathcal{D}(A_0^{1/2})$. As usual, the corresponding quadratic form is defined by the relation $\mathfrak{t}(\lambda)[x] := \mathfrak{t}(\lambda)[x,x]$ for $x \in \mathcal{D}(\mathfrak{t}(\lambda))$.

Proposition 2.2: The form $\mathfrak{t}(\lambda)$ *is closed and sectorial for all* $\lambda \in \mathbb{C}$. *Moreover*, $\mathfrak{t}(\cdot)[x]$ *is holomorphic on* $\mathbb{C}$ *for* $x \in \mathcal{D}(A_0^{1/2})$.

Proof: The holomorphy of the function $t(\cdot)[x]$ is clear. From (2.1) and Remark 2.1 it follows that there exist a_4, $b_4 \geqslant 0$, $b_4 < 1$, such that for all $x \in \mathcal{D}(A_0^{1/2})$,

$$\|(V-\lambda)x\|^2 \leqslant a_4\|x\|^2 + b_4\|A_0^{1/2}x\|^2.$$

This together with

$$|((V-\lambda)x, (V-\bar\lambda)x)| \leqslant \|(V-\lambda)x\| \cdot \|(V-\bar\lambda)x\| = \|(V-\lambda)x\|^2$$

implies that the quadratic form $((V-\lambda)\cdot, (V-\bar\lambda)\cdot)$ is relatively bounded with respect to the form $(A_0^{1/2}\cdot, A_0^{1/2}\cdot)$ with relative bound less than 1. Hence, by Ref. 3, Theorem VI.1.33, the quadratic form $\mathfrak{t}(\lambda)$ is closed and sectorial for $\lambda \in \mathbb{C}$. □

Proposition 2.2 and the first representation theorem (see Ref. 3, Theorem VI.2.1 or Ref. 10, Theorem VIII.16) show that there exist m-sectorial operators $T(\lambda)$, $\lambda \in \mathbb{C}$, in $\mathcal{H}$ such that

$$\mathfrak{t}(\lambda)[x,y] = (T(\lambda)x, y), \quad x \in \mathcal{D}(T(\lambda)), \quad y \in \mathcal{D}(\mathfrak{t}(\lambda)). \tag{2.5}$$

Since the domain of $\mathfrak{t}(\lambda)$ is independent of λ, the family T is a holomorphic family of operators of type (B) (cf. Ref. 3, Sec. VII.4). Formally, $T(\lambda)$ is given by

$$T(\lambda) = A_0 + \gamma^2 - (V-\lambda)^2;$$

this is a correct identity, e.g., if V is bounded, but in general the right-hand side of the latter equality may have a very small domain.

In the following we show that there exists a real point λ_0 in the resolvent set of T such that the negative spectral subspace of $T(\lambda_0)$ is finite dimensional. For this purpose we consider the operator polynomial

$$L(\lambda) := I - (S^* - \lambda H_0^{-1/2})(S - \lambda H_0^{-1/2}), \quad \lambda \in \mathbb{C},$$

which was introduced in Ref. 6. Assumption (A1) guarantees that the coefficients of L are bounded operators.

Proposition 2.3: Suppose that assumption (A1) *holds*.

(i) *For every* $\lambda \in \mathbb{C}$ *the operator identity*

$$T(\lambda) = H_0^{1/2} L(\lambda) H_0^{1/2} \tag{2.6}$$

holds; hence,

$$\begin{aligned}\mathcal{D}(T(\lambda)) &= \{x \in \mathcal{D}(H_0^{1/2}) : L(\lambda) H_0^{1/2} x \in \mathcal{D}(H_0^{1/2})\} \\ &= \{x \in \mathcal{D}(H_0^{1/2}) : (I - S^* S) H_0^{1/2} x \in \mathcal{D}(H_0^{1/2})\} = \mathcal{D}(T(0)),\end{aligned} \tag{2.7}$$

which is independent of λ.

(ii) $\sigma(T) \cap \mathbb{R} = \sigma(L) \cap \mathbb{R}$, $\sigma_p(T) = \sigma_p(L)$, $\sigma_{\mathrm{ess}}(T) \cap \mathbb{R} = \sigma_{\mathrm{ess}}(L) \cap \mathbb{R}$.

(iii) *For* $\lambda, \lambda_0 \in \mathbb{C}$ *the following relation holds:*

$$T(\lambda) = T(\lambda_0) + (\lambda - \lambda_0)(2V - \lambda - \lambda_0). \tag{2.8}$$

Proof: (i) For $x, y \in \mathcal{D}(\mathfrak{t}(\lambda))$ we have

$$\begin{aligned}(L(\lambda) H_0^{1/2} x, H_0^{1/2} y) &= ((I - (S^* - \lambda H_0^{-1/2})(S - \lambda H_0^{-1/2})) H_0^{1/2} x, H_0^{1/2} y) \\ &= (H_0^{1/2} x, H_0^{1/2} y) - ((S - \lambda H_0^{1/2}) H_0^{1/2} x, (S - \bar{\lambda} H_0^{-1/2}) H_0^{1/2} y) \\ &= (H_0^{1/2} x, H_0^{1/2} y) - ((V - \lambda) x, (V - \bar{\lambda}) y) = \mathfrak{t}(\lambda)[x, y].\end{aligned} \tag{2.9}$$

For the inclusion $H_0^{1/2} L(\lambda) H_0^{1/2} \subset T(\lambda)$, let $x \in \mathcal{D}(H_0^{1/2} L(\lambda) H_0^{1/2}) \subset \mathcal{D}(H_0^{1/2}) = \mathcal{D}(\mathfrak{t}(\lambda))$. Then for all $y \in \mathcal{D}(H_0^{1/2})$ we have

$$(H_0^{1/2} L(\lambda) H_0^{1/2} x, y) = (L(\lambda) H_0^{1/2} x, H_0^{1/2} y) = \mathfrak{t}(\lambda)[x, y].$$

Now Ref. 3 (Theorem VI.2.1.iii) implies that $x \in \mathcal{D}(T(\lambda))$ and $H_0^{1/2} L(\lambda) H_0^{1/2} x = T(\lambda) x$.

For the converse inclusion we observe that (2.9) together with (2.5) implies that

$$(T(\lambda) x, y) = (L(\lambda) H_0^{1/2} x, H_0^{1/2} y), \quad x \in \mathcal{D}(T(\lambda)), \quad y \in (\mathfrak{t}(\lambda)) = \mathcal{D}(H_0^{1/2}).$$

Since the left-hand side is continuous in y, this shows that for $x \in \mathcal{D}(T(\lambda))$ we have $L(\lambda) H_0^{1/2} x \in \mathcal{D}((H_0^{1/2})^*) = \mathcal{D}(H_0^{1/2})$.

The first equality in (2.7) is obvious. For the second equality we note that $H_0^{-1/2} V \subset \overline{H_0^{-1/2} V} = S^*$ and hence for $y \in \mathcal{D}(H_0^{1/2}) \subset \mathcal{D}(V)$ we have $S^* y = H_0^{-1/2} V y \in \mathcal{D}(H_0^{1/2})$. Thus

$$\begin{aligned}\mathcal{D}(T(\lambda)) &= \{x \in \mathcal{D}(H_0^{1/2}) : (I - (S^* - \lambda H_0^{-1/2})(S - \lambda H_0^{-1/2})) H_0^{1/2} x \in \mathcal{D}(H_0^{1/2})\} \\ &= \{x \in \mathcal{D}(H_0^{1/2}) : (I - S^* S) H_0^{1/2} x + \lambda (H_0^{-1/2} S H_0^{1/2} + S^*) x - \lambda^2 H_0^{-1/2} x \in \mathcal{D}(H_0^{1/2})\} \\ &= \{x \in \mathcal{D}(H_0^{1/2}) : (I - S^* S) H_0^{1/2} x \in \mathcal{D}(H_0^{1/2})\} = \mathcal{D}(T(0)).\end{aligned}$$

(ii) Since $H_0^{1/2}$ is bijective, it is clear from (1) that $\sigma_p(T) = \sigma_p(L)$. If $L(\lambda)$ is boundedly invertible, then obviously $T(\lambda)^{-1} = H_0^{-1/2} L(\lambda)^{-1} H_0^{-1/2}$ is bounded, which shows that $\sigma(T) \subset \sigma(L)$. Conversely, let $\lambda \in \mathbb{R}$ be such that $T(\lambda)$ is boundedly invertible. Then $T(\lambda)$ is self-adjoint and we can write

$$H_0^{1/2} T(\lambda)^{-1} H_0^{1/2} = H_0^{1/2} |T(\lambda)|^{-1/2} \operatorname{sgn}(T(\lambda)) |T(\lambda)|^{-1/2} H_0^{1/2}.$$

The operator $H_0^{1/2} |T(\lambda)|^{-1/2}$ is closed and everywhere defined since $\mathcal{D}(H_0^{1/2}) = \mathcal{D}(\mathfrak{t}(\lambda)) = \mathcal{D}(|T(\lambda)|^{1/2})$. Thus $H_0^{1/2} |T(\lambda)|^{-1/2}$ is bounded and so is the operator $|T(\lambda)|^{-1/2} H_0^{1/2} \subset (H_0^{1/2} |T(\lambda)|^{-1/2})^*$. Altogether this shows that $L(\lambda)^{-1} = \overline{H_0^{1/2} T(\lambda)^{-1} H_0^{1/2}}$ is bounded and hence $\sigma(L) \cap \mathbb{R} \subset \sigma(T) \cap \mathbb{R}$.

Next we prove that $\sigma_{\mathrm{ess}}(L) \cap \mathbb{R} \subset \sigma_{\mathrm{ess}}(T) \cap \mathbb{R}$. Let $\lambda \in \mathbb{R}$ be such that $T(\lambda)$ is a Fredholm operator. Then $T(\lambda)$ is self-adjoint, and we can write

$$L(\lambda) = (|T(\lambda)|^{1/2}H_0^{-1/2})^* \operatorname{sgn}(T(\lambda))|T(\lambda)|^{1/2}H_0^{-1/2}.$$

Since $T(\lambda)$ is Fredholm, so are $|T(\lambda)|^{1/2}$ and $\operatorname{sgn}(T(\lambda))$ by the spectral theorem. As $H_0^{-1/2}$ is a bijection from $\mathcal{H}$ onto $\mathcal{D}(H_0^{1/2}) = \mathcal{D}(\mathfrak{t}(\lambda)) = \mathcal{D}(|T(\lambda)|^{1/2})$, the operator $|T(\lambda)|^{1/2}H_0^{-1/2}$ is a bounded Fredholm operator. Hence also $(|T(\lambda)|^{1/2}H_0^{-1/2})^*$ is a bounded Fredholm operator (cf. Ref. 1, Theorem IX.1.1). Altogether this implies that $L(\lambda)$ is Fredholm.

Conversely, assume that $\lambda \in \sigma_{\mathrm{ess}}(T) \cap \mathbb{R}$; then (cf. Ref. 1, Theorem IX.1.3 and Theorem IX.1.6) there exists a singular sequence (x_n) for $T(\lambda)$, i.e., $x_n \in \mathcal{D}(T(\lambda))$ such that $\|x_n\| = 1$, $\lim_{n\to\infty} T(\lambda)x_n = 0$ and (x_n) has no convergent subsequence. Set $y_n := H_0^{1/2}x_n / \|H_0^{1/2}x_n\|$. We prove that (y_n) is a singular sequence for $L(\lambda)$. First it is clear that $\|y_n\| = 1$. Then

$$L(\lambda)y_n = \frac{1}{\|H_0^{1/2}x_n\|} L(\lambda)H_0^{1/2}x_n = \frac{1}{\|H_0^{1/2}x_n\|} H_0^{-1/2}T(\lambda)x_n \to 0$$

for $n \to \infty$ since $H_0^{-1/2}$ is bounded and $\|H_0^{1/2}x_n\| \geqslant \gamma$. Assume now that (y_n) has a convergent subsequence (y_{n_k}) with limit y. Then $y \neq 0$ as $\|y_n\| = 1$ and

$$x_{n_k} = \frac{1}{\|H_0^{-1/2}y_{n_k}\|} H_0^{-1/2}y_{n_k} \to \frac{1}{\|H_0^{-1/2}y\|} H_0^{-1/2}y,$$

a contradiction. So (y_n) is a singular sequence for $L(\lambda)$ and $\lambda \in \sigma_{\mathrm{ess}}(L)$.

(iii) Note that by (i), $\mathcal{D}(T(\lambda)) = \mathcal{D}(T(0)) = \mathcal{D}(T(\lambda_0)) \subset \mathcal{D}(H_0^{1/2}) \subset \mathcal{D}(V)$. Hence, the left- and right-hand sides of (2.8) have the same domain. So it suffices to prove this equality for the corresponding forms. For $x, y \in \mathcal{D}(H_0^{1/2})$ we have

$$\begin{aligned}\mathfrak{t}(\lambda)[x,y] - \mathfrak{t}(\lambda_0)[x,y] &= -((V-\lambda)x,(V-\overline{\lambda})y) + ((V-\lambda_0)x,(V-\overline{\lambda_0})y)\\ &= 2\lambda(Vx,y) - 2\lambda_0(Vx,y) - (\lambda^2 - \lambda_0^2)(x,y) = (\lambda-\lambda_0)((2V-(\lambda+\lambda_0))x,y),\end{aligned}$$

which proves the assertion. □

Lemma 2.4: Suppose that assumptions (A1) *and* (A2) *hold. Let* $\alpha := \gamma(1 - \|S_0\|)$ *and set* $\lambda_e^- := \sup \sigma_{\mathrm{ess}}(T) \cap (-\infty, 0)$, $\lambda_e^+ := \inf \sigma_{\mathrm{ess}}(T) \cap (0, +\infty)$. *Then*

$$\sigma_{\mathrm{ess}}(T) \cap (-\alpha, \alpha) = \emptyset,$$

that is, $\lambda_e^- \leqslant -\alpha < 0 < \alpha \leqslant \lambda_e^+$, *and for all* $\lambda \in (\lambda_e^-, \lambda_e^+)$,

$$\kappa_-(T(\lambda)) < \infty.$$

Proof: According to assumption (A2) we have the decomposition

$$L(\lambda) = L_0(\lambda) + K(\lambda), \quad \lambda \in \mathbb{C},$$

where $K(\lambda)$ is compact and

$$L_0(\lambda) := I - (S_0^* - \lambda H_0^{-1/2})(S_0 - \lambda H_0^{-1/2}).$$

Now let $\lambda \in (-\alpha, \alpha)$. Then

$$c_\lambda := \|S_0\| + |\lambda|\|H_0^{-1/2}\| < \|S_0\| + \gamma(1 - \|S_0\|)\frac{1}{\gamma} = 1$$

and hence

$$L_0(\lambda) \geqslant I - \|S_0 - \lambda H_0^{-1/2}\|^2 \geqslant 1 - c_\lambda^2 > 0.$$

In particular, $\sigma(L_0) \cap (-\alpha, \alpha) = \emptyset$ and $\kappa_-(L_0(\lambda)) = 0$ for $\lambda \in (-\alpha, \alpha)$. Since $K(\lambda)$ is compact, we have

$$\sigma_{\mathrm{ess}}(L) = \sigma_{\mathrm{ess}}(L_0). \tag{2.10}$$

Now Proposition 2.3 (ii) shows that

$$\sigma_{\mathrm{ess}}(T) \cap \mathbb{R} = \sigma_{\mathrm{ess}}(L) \cap \mathbb{R} = \sigma_{\mathrm{ess}}(L_0) \cap \mathbb{R}, \tag{2.11}$$

which implies the first assertion.

For the second assertion we first observe that $\lambda_e^- = \max \sigma_{\mathrm{ess}}(L_0) \cap (-\infty, 0)$, and $\lambda_e^+ = \min \sigma_{\mathrm{ess}}(L_0) \cap (0, +\infty)$ by (2.11). Using the fact that the operator $L_0(0) = I - S_0^* S_0$ is strictly positive and, e.g., Ref. 2, Theorem 2.1 and Lemma 2.9, we obtain that $\kappa_-(L_0(\lambda)) < \infty$ for $\lambda \in (\lambda_e^-, \lambda_e^+)$. Since $K(\lambda)$ is compact, it follows that $\kappa_-(L(\lambda)) < \infty$ for $\lambda \in (\lambda_e^-, \lambda_e^+)$. Finally, (2.6) implies that $\kappa_-(T(\lambda)) = \kappa_-(L(\lambda)) < \infty$ for $\lambda \in (\lambda_e^-, \lambda_e^+)$. □

Remark 2.5: If $S_1 = 0$, then the proof of the previous lemma and Proposition 2.3(ii) show that $\sigma(T) \cap (-\alpha, \alpha) = \emptyset$.

Next we construct a family of linearizations of T in order to investigate the spectral properties of T.

To this end we introduce the Hilbert spaces $\mathcal{H}_{1/2} := (\mathcal{D}(H_0^{1/2}), (H_0^{1/2} \cdot, H_0^{1/2} \cdot))$ and $\mathcal{G} := \mathcal{H}_{1/2} \oplus \mathcal{H}$. Then according to assumption (A1), for $\lambda_0 \in \mathbb{C}$, the operator $\mathcal{A}_{\lambda_0}$ in $\mathcal{G}$ given by

$$\mathcal{A}_{\lambda_0} := \begin{pmatrix} \lambda_0 & I \\ T(\lambda_0) & 2V - \lambda_0 \end{pmatrix}, \quad \mathcal{D}(\mathcal{A}_{\lambda_0}) = \mathcal{D}(T(\lambda_0)) \oplus \mathcal{H}_{1/2}, \tag{2.12}$$

is well defined. The operator $\mathcal{A}_0$ was investigated in Ref. 6. In certain cases, however, e.g., if $0 \in \sigma(T)$, the operator $\mathcal{A}_0$ is not suitable for our purpose.

Lemma 2.6: Suppose that assumption (A1) *holds. If* $\lambda_0 \in \rho(T)$, *then* $\mathcal{A}_{\lambda_0} - \lambda_0$ *is boundedly invertible in* $\mathcal{G}$ *and hence closed.*

Proof: The equation $(\mathcal{A}_{\lambda_0} - \lambda_0)(x\ y)^{\mathsf{T}} = (f\ g)^{\mathsf{T}}$ is equivalent to the relations $y = f$ and $T(\lambda_0)x + 2(V - \lambda_0)y = g$. The latter equation can be solved for x, namely $x = T(\lambda_0)^{-1}(-2(V - \lambda_0)f + g)$. Hence the inverse of $\mathcal{A}_{\lambda_0} - \lambda_0$ is given by

$$(\mathcal{A}_{\lambda_0} - \lambda_0)^{-1} = \begin{pmatrix} -2T(\lambda_0)^{-1}(V - \lambda_0) & T(\lambda_0)^{-1} \\ I & 0 \end{pmatrix}. \tag{2.13}$$

We have to show that this operator is bounded in $\mathcal{G}$. The operator $T(\lambda_0)^{-1}$ is closed in $\mathcal{H}$ with $\mathcal{D}(T(\lambda_0)) \subset \mathcal{H}_{1/2}$ and hence also closed from $\mathcal{H}$ to $\mathcal{H}_{1/2}$; therefore it is bounded from $\mathcal{H}$ to $\mathcal{H}_{1/2}$. As V is bounded from $\mathcal{H}_{1/2}$ to $\mathcal{H}$ by assumption (A1), the left upper entry in (2.13) is bounded in $\mathcal{H}_{1/2}$. Since the embedding from $\mathcal{H}_{1/2}$ into $\mathcal{H}$ is bounded, also the left lower entry is bounded. □

For fixed $\lambda_0 \in \mathbb{R}$ an inner product

$$\left[\begin{pmatrix} x \\ y \end{pmatrix}, \begin{pmatrix} x' \\ y' \end{pmatrix} \right]_{\lambda_0} := \mathfrak{t}(\lambda_0)[x, x'] + (y, y'), \quad \begin{pmatrix} x \\ y \end{pmatrix}, \begin{pmatrix} x' \\ y' \end{pmatrix} \in \mathcal{G},$$

is defined on $\mathcal{G}$, which may be indefinite. If $\lambda_0 \in \rho(T) \cap \mathbb{R}$ and $\kappa_-(T(\lambda_0)) < \infty$, then $(\mathcal{G}, [\cdot, \cdot]_{\lambda_0})$ becomes a Pontryagin space with negative index $\kappa_-(T(\lambda_0))$, i.e., $\mathcal{G}$ is the direct sum of a Hilbert space and a $\kappa_-(T(\lambda_0))$-dimensional anti-Hilbert space.

Due to Lemma 2.4 the assumptions (A1) and (A2) ensure the existence of a point λ_0 with the above-mentioned properties.

Proposition 2.7: Suppose that assumptions (A1) *and* (A2) *hold and let* $\lambda_0 \in \rho(T) \cap \mathbb{R}$ *be such that* $\kappa_-(T(\lambda_0)) < \infty$. *Then the following assertions are true.*

(i) *The operator* $\mathcal{A}_{\lambda_0}$ *is self-adjoint in the Pontryagin space* $(\mathcal{G}, [\cdot, \cdot]_{\lambda_0})$.
(ii) *The various parts of the spectra of* T *and* $\mathcal{A}_{\lambda_0}$ *coincide:*

$$\sigma(T) = \sigma(\mathcal{A}_{\lambda_0}), \quad \sigma_p(T) = \sigma_p(\mathcal{A}_{\lambda_0}), \quad \sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{ess}}(\mathcal{A}_{\lambda_0}).$$

Proof: (i) For $(x\ y)^{\mathsf{T}} \in \mathcal{D}(\mathcal{A}_{\lambda_0})$ we have

$$\left[\mathcal{A}_{\lambda_0}\begin{pmatrix}x\\y\end{pmatrix},\begin{pmatrix}x\\y\end{pmatrix}\right]_{\lambda_0} = \mathfrak{t}(\lambda_0)[\lambda_0 x + y, x] + (T(\lambda_0)x + (2V - \lambda_0)y, y)$$
$$= \lambda_0 \mathfrak{t}(\lambda_0)[x,x] + \mathfrak{t}(\lambda_0)[y,x] + \mathfrak{t}(\lambda_0)[x,y] + ((2V - \lambda_0)y, y),$$

which is real; hence $\mathcal{A}_{\lambda_0}$ is symmetric in $(\mathcal{G}, [\cdot,\cdot]_{\lambda_0})$. Since $\mathcal{A}_{\lambda_0} - \lambda_0$ is boundedly invertible by Lemma 2.6, $\mathcal{A}_{\lambda_0}$ is self-adjoint.

(ii) Using relation (2.8) in Proposition 2.3(iii) one can easily show that the following equality holds:

$$\begin{pmatrix}T(\lambda) & 0\\ 0 & I\end{pmatrix} = \begin{pmatrix}-2V + \lambda + \lambda_0 & I\\ I & 0\end{pmatrix}(\mathcal{A}_{\lambda_0} - \lambda)\begin{pmatrix}I & 0\\ \lambda - \lambda_0 & I\end{pmatrix}, \quad \lambda \in \mathbb{C}. \tag{2.14}$$

Since the operators $T(\lambda)$ and $\mathcal{A}_{\lambda_0} - \lambda$ are closed in $\mathcal{H}$ and $\mathcal{G}$, respectively, it is sufficient to show that the dimensions of the kernels and the algebraic co-dimensions of the ranges of $T(\lambda)$ and $\mathcal{A}_{\lambda_0} - \lambda$ coincide.

To see this we consider the operator on the left-hand side as an operator from the space $\mathcal{D}(T(\lambda)) \oplus \mathcal{H}_{1/2}$ into $\mathcal{H} \oplus \mathcal{H}_{1/2}$ and $\mathcal{A}_{\lambda_0} - \lambda$ as an operator from $\mathcal{D}(T(\lambda_0)) \oplus \mathcal{H}_{1/2}$ into $\mathcal{H}_{1/2} \oplus \mathcal{H}$; note that according to Eq. (2.7), $\mathcal{D}(T(\lambda_0)) = \mathcal{D}(T(\lambda))$. Next we observe that the last operator on the right-hand side of (2.14) is bijective from $\mathcal{D}(T(\lambda_0)) \oplus \mathcal{H}_{1/2}$ onto $\mathcal{D}(T(\lambda_0)) \oplus \mathcal{H}_{1/2}$ since $\mathcal{D}(T(\lambda_0)) \subset \mathcal{H}_{1/2}$, and that the first operator is bijective from $\mathcal{H}_{1/2} \oplus \mathcal{H}$ onto $\mathcal{H} \oplus \mathcal{H}_{1/2}$ since $\mathcal{H}_{1/2} \subset \mathcal{D}(V)$.

Therefore the factorization (2.14) implies that

$$\dim \ker T(\lambda) = \dim \ker(\mathcal{A}_{\lambda_0} - \lambda), \tag{2.15}$$

$$\dim(\mathcal{H}/\operatorname{ran} T(\lambda)) = \dim((\mathcal{H}_{1/2} \oplus \mathcal{H})/\operatorname{ran}(\mathcal{A}_{\lambda_0} - \lambda)), \tag{2.16}$$

where in the latter equation the factor spaces are purely algebraic. Now the claim follows from the facts that $\lambda \notin \sigma(T)$ if and only if both numbers on the left-hand sides of (2.15) and (2.16) are 0, $\lambda \in \sigma_p(T)$ if and only if $\dim \ker(T(\lambda)) \neq 0$, and $\lambda \notin \sigma_{\mathrm{ess}}(T)$ if and only if both numbers on the left-hand sides of (2.15) and (2.16) are finite, and analogously for $\mathcal{A}_{\lambda_0} - \lambda$. □

Theorem 2.8: *Suppose that assumptions* (A1) *and* (A2) *hold.*

(i) *The essential spectrum* $\sigma_{\mathrm{ess}}(T)$ *is real and has a gap around* 0; *more exactly*,

$$\sigma_{\mathrm{ess}}(T) \cap (-\alpha, \alpha) = \emptyset,$$

where $\alpha := (1 - \|S_0\|)\gamma$.

(ii) *The nonreal spectrum of T is symmetric with respect to the real axis and consists of at most finitely many complex conjugate pairs of eigenvalues of finite algebraic multiplicity.*

(iii) *If* $S_1 = 0$, *then the spectrum of T is real and*

$$\sigma(T) \cap (-\alpha, \alpha) = \emptyset.$$

If $S_0 = 0$, *then*

$$\sigma_{\mathrm{ess}}(T) = \{\lambda \in \mathbb{R} : \lambda^2 \in \sigma_{\mathrm{ess}}(H_0)\}.$$

Proof: Claim (ii) and the first assertion in (i) follow from Proposition 2.7 and general properties of self-adjoint operators in Pontryagin spaces (cf. Ref. 5 and also Ref. 6, Sec. II). The remaining assertions in (i) are immediate from Lemma 2.4. The first claim in (iii) follows from Remark 2.5. Since by (i) $\sigma_{\mathrm{ess}}(T) \subset \mathbb{R}$, Proposition 2.3 (ii) shows that $\sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{ess}}(L)$. According to (2.10) we have $\sigma_{\mathrm{ess}}(L) = \sigma_{\mathrm{ess}}(L_0)$, where $L_0(\lambda) = I - \lambda^2 H_0^{-1}$ since $S_0 = 0$. Now the claim follows from the spectral mapping theorem. □

III. VARIATIONAL PRINCIPLE

In this section we characterize the eigenvalues of T in certain parts of the gap of the essential spectrum around 0. To this end we introduce functionals p_+ and p_- on the set $\mathcal{D}(H_0^{1/2})\backslash\{0\}$ as follows. For $x\in\mathcal{D}(H_0^{1/2})$, $x\neq 0$, we define $p_+(x)$ and $p_-(x)$, with $p_-(x)\leqslant p_+(x)$, to be the roots of the quadratic equation

$$\mathbf{t}(\lambda)[x]=-\lambda^2\|x\|^2+2(Vx,x)\lambda-(Vx,Vx)+(H_0^{1/2}x,H_0^{1/2}x)=0$$

if the latter are real; otherwise we set $p_+(x):=-\infty$ and $p_-(x):=+\infty$. If $p_\pm(x)$ are finite and $\|x\|=1$, then $p_\pm(x)$ are given by the formula

$$p_\pm(x)=(Vx,x)\pm\sqrt{(Vx,x)^2-(Vx,Vx)+(H_0^{1/2}x,H_0^{1/2}x)}; \tag{3.1}$$

for $\|x\|\neq 1$ we observe that $p_\pm(cx)=p_\pm(x)$ for $c\in\mathbb{C}\backslash\{0\}$. Moreover, set

$$\nu_-:=\sup\{p_-(x):\ x\in\mathcal{D}(H_0^{1/2}),p_-(x)\neq\ +\infty\},$$

$$\nu_+:=\inf\{p_+(x):\ x\in\mathcal{D}(H_0^{1/2}),p_+(x)\neq -\infty\}.$$

The functionals $p_\pm$ are related to the numerical range of the form polynomial $\mathbf{t}$,

$$W(\mathbf{t})=\{\lambda\in\mathbb{C}:\ \mathbf{t}(\lambda)[x]=0 \text{ for some } x\in\mathcal{D}(H_0^{1/2}),x\neq 0\}.$$

In fact, $W(\mathbf{t})\cap\mathbb{R}$ is equal to the union of all finite values of $p_+(x)$ and $p_-(x)$ with $x\in\mathcal{D}(H_0^{1/2})$, $x\neq 0$. Obviously, $\sigma_p(T)\subset W(\mathbf{t})$, and for every $\lambda\in\sigma_p(T)\cap\mathbb{R}$ with eigenvector x, we have $\lambda=p_+(x)$ or $\lambda=p_-(x)$.

The following theorem contains a variational characterization of the eigenvalues of T in the spectral gap around 0 to the right of ν_- in terms of the functionals p_+.

Theorem 3.1: *Suppose that assumptions* (A1) *and* (A2) *are satisfied and assume that* $\nu_-<\lambda_e^+:=\min(\sigma_{\mathrm{ess}}(T)\cap(0,\infty))$.

(i) $(\nu_-,\lambda_e^+)\cap\sigma_{\mathrm{ess}}(T)=\emptyset$ *and there exists an* $\varepsilon>0$ *with* $(\nu_-,\nu_-+\varepsilon)\subset\rho(T)$.

(ii) *Let* $\lambda_0\in(\nu_-,\lambda_e^+)\cap\rho(T)$ *and denote by* $\lambda_1^+\leqslant\lambda_2^+\leqslant\cdots\leqslant\lambda_{N_+}^+$, $N_+\in\mathbb{N}_0\cup\{\infty\}$, *the finite or infinite sequence of the eigenvalues of* T *in the interval* (λ_0,λ_e^+), *counted with multiplicities. Then* $\kappa_+:=\kappa_-(T(\lambda_0))<\infty$ *and*

$$\lambda_n^+=\min_{\substack{\mathcal{L}\subset\mathcal{D}(H_0^{1/2})\\ \dim\mathcal{L}=n+\kappa_+}}\ \max_{\substack{x\in\mathcal{L}\\ x\neq 0}} p_+(x),\quad n=1,2,\ldots,N_+. \tag{3.2}$$

If $N_+=\infty$, *then* $\lim_{n\to\infty}\lambda_n^+=\lambda_e^+$; *otherwise*,

$$\inf_{\substack{\mathcal{L}\subset\mathcal{D}(H_0^{1/2})\\ \dim\mathcal{L}=n+\kappa_+}}\ \max_{\substack{x\in\mathcal{L}\\ x\neq 0}} p_+(x)=\lambda_e^+,\quad n>N_+.$$

Remark 3.2: The condition $x\neq 0$ in the second variations above can be replaced by $\|x\|=1$.

Proof: We want to apply Ref. 2, Theorem 2.1 to $\mathbf{t}$ defined on the intervals (ν_-,λ_e^+) and $[\lambda_0,\lambda_e^+)$, respectively. Assumptions (i) and (ii) of this theorem are satisfied because T is a holomorphic family of operators of type (B). For assumption (iii) of this theorem we have to show that if $\mathbf{t}(\mu_0)[x]=0$ for $\mu_0>\nu_-$ and $x\in\mathcal{D}(H_0^{1/2})$, $x\neq 0$, then

$$\mathbf{t}(\lambda)[x]>0\quad\text{for } \lambda\in(\nu_-,\mu_0),$$

$$\mathbf{t}(\lambda)[x] < 0 \quad \text{for } \lambda > \mu_0. \tag{3.3}$$

In fact, if $\mathbf{t}(\mu_0)[x]=0$ and $\mu_0 > \nu_-$, then $\mathbf{t}(\cdot)[x]$ has two zeros, μ_0 is the larger one of these and the smaller one is $\leqslant \nu_-$. Since $\mathbf{t}(\cdot)[x]$ is concave, (3.3) follows.

Lemma 2.4 shows that there exists a $\nu_0 \in (\nu_-, \lambda_e^+)$ such that $\kappa_-(T(\nu_0)) < \infty$, which is exactly assumption (iv) of Ref. 2, Theorem 2.1.

Finally, assumption (v) of Ref. 2, Theorem 2.1 requires that for every $\mu_0 > \nu_-$ and $\varepsilon > 0$ there exists a positive number $\delta(\mu_0, \varepsilon)$ such that $0 < \mathbf{t}(\mu_0)[x] < \delta(\mu_0, \varepsilon)$ for $x \in \mathcal{D}(H_0^{1/2})$, $\|x\|=1$, implies $\mathbf{t}(\mu_0+\varepsilon)[x] \leqslant 0$. We show that we can choose $\delta(\mu_0, \varepsilon) = \varepsilon(\mu_0 - \nu_-)$. In fact, it follows from $\mathbf{t}(\mu_0)[x] > 0$ that $p_\pm(x) \neq \mp\infty$, and hence we can write $\mathbf{t}(\mu_0)[x] = (\mu_0 - p_-(x))(p_+(x) - \mu_0)$. Therefore if $0 < \mathbf{t}(\mu_0)[x] < \delta(\mu_0, \varepsilon)$, then

$$p_+(x) = \frac{\mathbf{t}(\mu_0)[x]}{\mu_0 - p_-(x)} + \mu_0 < \frac{\delta(\mu_0, \varepsilon)}{\mu_0 - \nu_-} + \mu_0 = \varepsilon + \mu_0,$$

which implies that $\mathbf{t}(\mu_0+\varepsilon)[x] < 0$.

Now all assumptions of Ref. 2, Theorem 2.1 are satisfied on the interval (ν_-, λ_e^+) and hence also for every subinterval. The second claim in (i) follows directly from Ref. 2, Theorem 2.1 applied on the interval (ν_-, λ_e^+). The first part of (i) is obvious if $\nu_- \geqslant 0$; if $\nu_- < 0$, then $(\nu_-, 0) \cap \sigma_{\text{ess}}(T) = \emptyset$ follows from Ref. 2, Lemma 2.9 and the fact that $\kappa_-(T(0)) < \infty$ by Lemma 2.4.

All assertions in (ii) follow from Ref. 2, Theorem 2.1 applied on the interval $[\lambda_0, \lambda_e^+)$. Note that the functional p_+ defined here differs slightly from the definition in Ref. 2, where $p_+(x) = -\infty$ if both zeros of $\mathbf{t}(\cdot)[x]$ are $\leqslant \nu_-$; however, this modification does not affect the maximum in (3.2) since in every subspace of dimension greater than κ_+ there exists an x such that $p_+(x) > \nu_-$. □

The following theorem is the analogue of Theorem 3.1 for the eigenvalues in the spectral gap of T around 0 to the left of ν_+. In this case the functionals p_- are used for the variational principle.

Theorem 3.3: *Suppose that assumptions* (A1) *and* (A2) *are satisfied and assume that* $\nu_+ > \lambda_e^- := \max(\sigma_{\text{ess}}(T) \cap (-\infty, 0))$.

(i) $(\lambda_e^-, \nu_+) \cap \sigma_{\text{ess}}(T) = \emptyset$ *and there exists an* $\varepsilon > 0$ *with* $(\nu_+ - \varepsilon, \nu_+) \subset \rho(T)$.

(ii) *Let* $\lambda_0 \in (\lambda_e^-, \nu_+) \cap \rho(T)$ *and denote by* $\lambda_1^- \geqslant \lambda_2^- \geqslant \cdots \geqslant \lambda_{N_-}^-$, $N_- \in \mathbb{N}_0 \cup \{\infty\}$, *the finite or infinite sequence of the eigenvalues of* T *in the interval* (λ_e^-, λ_0), *counted with multiplicities. Then* $\kappa_- := \kappa_-(T(\lambda_0)) < \infty$ *and*

$$\lambda_n^- = \max_{\substack{\mathcal{L} \subset \mathcal{D}(H_0^{1/2}) \\ \dim \mathcal{L} = n + \kappa_-}} \min_{\substack{x \in \mathcal{L} \\ x \neq 0}} p_-(x), \quad n = 1, 2, \ldots, N_-.$$

If $N_- = \infty$, *then* $\lim_{n\to\infty} \lambda_n^- = \lambda_e^-$; *otherwise*,

$$\sup_{\substack{\mathcal{L} \subset \mathcal{D}(H_0^{1/2}) \\ \dim \mathcal{L} = n + \kappa_-}} \min_{\substack{x \in \mathcal{L} \\ x \neq 0}} p_-(x) = \lambda_e^-, \quad n > N_-.$$

In the following we characterize the index shift in the variational principles above by means of the types of eigenvalues of T with respect to the indefinite inner product $[\cdot, \cdot]_{\lambda_0}$. As a consequence we obtain an estimate of the number of nonreal eigenvalues of T in terms of the index shift.

Proposition 3.4: Suppose that assumptions (A1) *and* (A2) *hold. Let* $\lambda_0 \in \rho(T) \cap \mathbb{R}$ *be such that* $\kappa_-(T(\lambda_0)) < \infty$. *Further, let* $\lambda \in \mathbb{R}$ *be an eigenvalue of* T *and* $x \in \mathcal{D}(T(\lambda_0))$, $x \neq 0$, *a corresponding eigenvector, i.e.,* $T(\lambda_0)x = 0$. *Then* $\mathbf{x} = \begin{pmatrix} x \\ (\lambda - \lambda_0)x \end{pmatrix}$ *is an eigenvector of* $\mathcal{A}_{\lambda_0}$ *corresponding to* λ. *Moreover, the following equivalences are true:*

$$[\mathbf{x},\mathbf{x}]_{\lambda_0} > 0 \Leftrightarrow \begin{cases} \lambda > \lambda_0 \text{ and } \lambda \neq p_-(x) \\ \text{or} \\ \lambda < \lambda_0 \text{ and } \lambda \neq p_+(x) \end{cases}$$

$$[\mathbf{x},\mathbf{x}]_{\lambda_0} < 0 \Leftrightarrow \begin{cases} \lambda > \lambda_0 \text{ and } \lambda \neq p_+(x) \\ \text{or} \\ \lambda < \lambda_0 \text{ and } \lambda \neq p_-(x) \end{cases}$$

$$[\mathbf{x},\mathbf{x}]_{\lambda_0} = 0 \Leftrightarrow \lambda = p_+(x) = p_-(x).$$

Proof: From the definition of $\mathcal{A}_{\lambda_0}$ in (2.12) and Proposition 2.3(iii) it follows that

$$(\mathcal{A}_{\lambda_0} - \lambda)\begin{pmatrix} x \\ (\lambda - \lambda_0)x \end{pmatrix} = \begin{pmatrix} 0 \\ T(\lambda_0)x + (\lambda - \lambda_0)(2V - \lambda_0 - \lambda)x \end{pmatrix} = \begin{pmatrix} 0 \\ T(\lambda)x \end{pmatrix} = 0.$$

Without loss of generality we can assume that $\|x\|=1$. Using (2.8) we obtain

$$\begin{aligned} \left[\begin{pmatrix} x \\ (\lambda - \lambda_0)x \end{pmatrix}, \begin{pmatrix} x \\ (\lambda - \lambda_0)x \end{pmatrix}\right]_{\lambda_0} &= \mathfrak{t}(\lambda_0)[x,x] + ((\lambda - \lambda_0)x, (\lambda - \lambda_0)x) = (T(\lambda_0)x,x) + (\lambda - \lambda_0)^2 \\ &= (T(\lambda)x,x) - (\lambda - \lambda_0)((2V - \lambda - \lambda_0)x,x) + (\lambda - \lambda_0)^2 \\ &= (\lambda - \lambda_0)(-(2Vx,x) + \lambda + \lambda_0 + \lambda - \lambda_0) = 2(\lambda - \lambda_0)(\lambda - (Vx,x)). \end{aligned} \tag{3.4}$$

Formula (3.1) shows that $(Vx,x)=\frac{1}{2}(p_+(x)+p_-(x))$. Since $\lambda=p_+(x)$ or $\lambda=p_-(x)$, this implies that

$$\lambda > (Vx,x) \Leftrightarrow \lambda \neq p_-(x),$$

$$\lambda < (Vx,x) \Leftrightarrow \lambda \neq p_+(x),$$

$$\lambda = (Vx,x) \Leftrightarrow \lambda = p_+(x) = p_-(x).$$

Now the claim is immediate from (3.4) □

Proposition 3.5: Suppose that the assumptions of Theorem 3.1 hold and choose λ_0 as in Theorem 3.1. Then every eigenvalue $\lambda > \lambda_0$ of T is of positive type with respect to the inner product $[\cdot,\cdot]_{\lambda_0}$, i.e., $[\mathbf{x},\mathbf{x}]_{\lambda_0} > 0$ for every eigenvector x and $\mathbf{x}=\binom{x}{(\lambda-\lambda_0)x}$. Moreover, the index shift κ_+ in Theorem 3.1 satisfies

$$\kappa_+ = \sum_{\lambda \in \sigma(T) \cap \mathbb{C}^+} \dim \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}) + \sum_{\lambda \in \sigma(T) \cap (-\infty, \lambda_0)} \dim_- \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}), \tag{3.5}$$

where $\mathcal{L}_\lambda(\mathcal{A}_{\lambda_0})$ denotes the algebraic eigenspace of $\mathcal{A}_{\lambda_0}$ at λ and $\dim_- \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0})$ denotes the maximal dimension of a nonpositive subspace of $\mathcal{L}_\lambda(\mathcal{A}_{\lambda_0})$.

Proof: Since $\lambda_0 > \nu_-$, it is clear that for every eigenvalue $\lambda > \lambda_0$ with eigenvector x we have $\lambda \neq p_-(x)$. Hence by the previous theorem it follows that $[\mathbf{x},\mathbf{x}]_{\lambda_0} > 0$. According to Theorem 3.1, the index shift κ_+ is the negative index of the Pontryagin space $(\mathcal{G}, [\cdot,\cdot]_{\lambda_0})$. By Ref. 5 it is hence equal to

$$\sum_{\lambda \in \sigma(T) \cap \mathbb{C}^+} \dim \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}) + \sum_{\lambda \in \sigma(T) \cap \mathbb{R}} \dim_- \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}).$$

By the first claim we have $\dim_- \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}) = 0$ for $\lambda > \lambda_0$. □

Since $\dim \mathcal{L}_\lambda(\mathcal{A}_{\lambda_0}) = \dim \mathcal{L}_{\bar\lambda}(\mathcal{A}_{\lambda_0})$, the following corollary is an immediate consequence of (3.5).

Corollary 3.6: The number of nonreal eigenvalues of T, counted with multiplicities, is at most $2\kappa_+$.

IV. EIGENVALUE ESTIMATES

If additional information on the operator V is available, we can estimate the functionals $p_\pm$ and hence the eigenvalues of T as well as the numbers $\nu_\pm$. Further we compare the eigenvalues of T with eigenvalues of a certain abstract Schrödinger operator.

Proposition 4.1: Suppose that assumption (A1) *holds. Let $x \in \mathcal{D}(H_0^{1/2})$, $x \neq 0$, be such that $p_\pm(x) \neq \mp\infty$ and let a_3, $b_3 \geqslant 0$, $b_3 < 1$, be real constants such that (2.3) is satisfied.*

(i) *If V is bounded from above, $V \leqslant v_{\max}$, then*

$$p_-(x) \leqslant v_{\max} - \sqrt{\max\{0, \gamma^2 - a_3\}} \leqslant v_{\max}.$$

If, in addition, $v_{\max} \leqslant 0$, then

$$p_-(x) \leqslant v_{\max} - \sqrt{\max\{0, v_{\max}^2 + \gamma^2 - a_3\}} \leqslant v_{\max} \leqslant 0.$$

(ii) *If V is bounded from below, $V \geqslant v_{\min}$, then*

$$p_+(x) \geqslant v_{\min} + \sqrt{\max\{0, \gamma^2 - a_3\}} \geqslant v_{\min}.$$

(iii) *If V is bounded, $v_{\min} \leqslant V \leqslant v_{\max}$, then*

$$p_-(x) \leqslant v_{\max} - \sqrt{\max\{0, \gamma^2 - \|V\|^2\}} \leqslant v_{\max},$$

$$p_+(x) \geqslant v_{\min} + \sqrt{\max\{0, \gamma^2 - \|V\|^2\}} \geqslant v_{\min}.$$

If, in addition, $v_{\max} \leqslant 0$, then

$$p_-(x) \leqslant v_{\max} - \sqrt{\max\{0, v_{\max}^2 + \gamma^2 - \|V\|^2\}} \leqslant v_{\max} \leqslant 0,$$

$$p_+(x) \geqslant v_{\min} + \sqrt{\max\{0, v_{\max}^2 + \gamma^2 - \|V\|^2\}} \geqslant v_{\min}.$$

Proof: Let $x \in \mathcal{D}(H_0^{1/2}) = \mathcal{D}(A_0^{1/2})$, $\|x\| = 1$, be such that $p_-(x) \neq +\infty$. From (3.1) and (2.3) it follows that

$$\begin{aligned} p_-(x) &= (Vx,x) - \sqrt{(Vx,x)^2 - (Vx,Vx) + (A_0^{1/2}x, A_0^{1/2}x) + \gamma^2} \\ &\leqslant (Vx,x) - \sqrt{\max\{0, -\|Vx\|^2 + \|A_0^{1/2}x\|^2 + \gamma^2\}} \\ &\leqslant (Vx,x) - \sqrt{\max\{0, -a_3 + (1-b_3)\|A_0^{1/2}x\|^2 + \gamma^2\}} \\ &\leqslant (Vx,x) - \sqrt{\max\{0, -a_3 + \gamma^2\}}, \end{aligned}$$

where we have used that $b_3 < 1$ in (2.3). This proves the first inequality in (i); for the second inequality one additionally has to use the estimate $(Vx,x)^2 \geqslant v_{\max}^2$. The proof of (ii) is completely analogous. The claim in (iii) is an immediate consequence of (i) and (ii) since in this case we can choose $a_3 = \|V\|^2$ in (2.3). □

The above proposition together with the variational principle in Theorem 3.1 yields the following estimate for eigenvalues of T. We restrict ourselves to the case that V is bounded; the other cases are similar.

Corollary 4.2: Suppose that V is bounded, $v_{\min} \leqslant V \leqslant v_{\max}$ and that assumption (A2) *is satisfied. Then, using the notation of Theorem 3.1, we have*

$$\nu_- \leqslant v_{\max} - \sqrt{\max\{0, \gamma^2 - \|V\|^2\}} \leqslant v_{\max}$$

and

$$\lambda_k^+ \geqslant v_{\min} + \sqrt{\max\{0, \gamma^2 - \|V\|^2\}} \geqslant v_{\min}, \quad k = 1,2, \ldots, N_+.$$

If the operator V is bounded and has a definite sign, then assumption (A2) in Theorem 3.1 can be replaced by assuming that $\|V\| < 2\gamma$ (or even $v_{\max} - v_{\min} < 2\gamma$, cf. Ref. 9). In this case, the spectrum of T is real, the essential spectrum has a gap to the right of $-\gamma$ and there is no index shift in the variational principle.

Theorem 4.3: *Assume that* $-2\gamma \leqslant v_{\min} \leqslant V \leqslant 0$. *Then for* $x \in \mathcal{D}(H_0^{1/2})$, $x \neq 0$,

$$p_-(x) \leqslant -\gamma, \quad p_+(x) \geqslant \gamma + v_{\min} \geqslant -\gamma.$$

If, in addition, $v_{\min} > -2\gamma$, *then* $\sigma(T) \subset \mathbb{R}$, $(-\gamma, \gamma + v_{\min}) \subset \rho(T)$ *and the eigenvalues* $\lambda_1^+ \leqslant \lambda_2^+ \leqslant \cdots \leqslant \lambda_{N_+}^+$, $N_+ \in \mathbb{N}_0 \cup \{\infty\}$, *of* T *in* $(\gamma + v_{\min}, \lambda_e^+)$, $\lambda_e^+ = \min(\sigma_{\mathrm{ess}}(T) \cap (-\gamma, +\infty))$, *can be characterized by*

$$\lambda_n^+ = \min_{\substack{\mathcal{L} \subset \mathcal{D}(H_0^{1/2}) \\ \dim \mathcal{L} = n}} \max_{\substack{x \in \mathcal{L} \\ x \neq 0}} p_+(x), \quad n = 1,2, \ldots, N_+. \tag{4.1}$$

Proof: Let E_t be the spectral family of the self-adjoint operator V. Then

$$\|Vx\|^2 = \int_{v_{\min}}^0 t^2 \mathrm{d}(E_t x, x) \leqslant v_{\min} \int_{v_{\min}}^0 t \mathrm{d}(E_t x, x) = v_{\min}(Vx, x).$$

Using this estimate and the fact that the function $f(t) = t + \sqrt{(t+a)^2 + b}$, $t \in \mathbb{R}$, is increasing if $a \in \mathbb{R}$ and $b \geqslant 0$ we obtain

$$p_+(x) = (Vx,x) + \sqrt{(Vx,x)^2 - \|Vx\|^2 + \|A_0^{1/2}x\|^2 + \gamma^2} \geqslant (Vx,x) + \sqrt{(Vx,x)^2 - v_{\min}(Vx,x) + \gamma^2} \tag{4.2}$$

$$= (Vx,x) + \sqrt{\left((Vx,x) - \frac{v_{\min}}{2}\right)^2 - \frac{v_{\min}^2}{4} + \gamma^2} \geqslant v_{\min} + \sqrt{\left(v_{\min} - \frac{v_{\min}}{2}\right)^2 - \frac{v_{\min}^2}{4} + \gamma^2} = v_{\min} + \gamma. \tag{4.3}$$

Note that $b = -v_{\min}^2/4 + \gamma^2 \geqslant 0$ since $0 \geqslant v_{\min} \geqslant -2\gamma$. This also shows that the roots in (4.3) and hence in (4.2) are real. The proof for the estimate of $p_-(x)$ is similar.

Now assume that $v_{\min} > -2\gamma$. Then for $\lambda \in (-\gamma, \gamma + v_{\min})$ we have $\|V - \lambda\| < \gamma$ and hence the self-adjoint operator $T(\lambda) = H_0 - (V - \lambda)^2$ is strictly positive and $\kappa_-(T(\lambda)) = 0$. This implies that $(-\gamma, \gamma + v_{\min}) \subset \rho(T)$.

Further, we observe that for every $x \in \mathcal{D}(H_0^{1/2})$, $x \neq 0$, the equation $t(\lambda)[x] = 0$ has two real solutions $p_\pm(x)$ and hence

$$W(\mathfrak{t}) = \{p_\pm(x) : x \in \mathcal{D}(H_0^{1/2}), x \neq 0\} \subset (-\infty, -\gamma] \cup [\gamma + v_{\min}, +\infty).$$

Since $\rho(T) \neq \emptyset$, we have $\sigma(T) \subset \overline{W(T)} = \overline{W(\mathfrak{t})} \subset \mathbb{R}$ (cf. Ref. 8, Theorem 26.6).

Finally, it is not difficult to see that the proof of Theorem 3.1 carries over with $\lambda_0 \in (-\gamma, \gamma + v_{\min})$ and $\kappa_+ = \kappa_-(T(\lambda_0)) = 0$. □

The following theorem provides a comparison between the eigenvalues of the Klein–Gordon equation and a corresponding Schrödinger operator.

Theorem 4.4: *Suppose that assumptions* (A1) *and* (A2) *as well as the assumptions of Theorem 3.1 hold. Then the operator*

$$H_+ := \frac{1}{2\gamma}A_0 + V$$

is self-adjoint and bounded from below. If $\mu_1^+ \leqslant \mu_2^+ \leqslant \cdots \leqslant \mu_{M_+}^+$, $M_+ \in \mathbb{N}_0 \cup \{\infty\}$, *are the eigenvalues of* H_+ *below* $\sigma_{\mathrm{ess}}(H_+)$ *and* $\mu_n^+ := \min\sigma_{\mathrm{ess}}(H_+)$ *for* $n > M_+$, *then the eigenvalues* λ_n^+ *of* T *satisfy the estimate*

$$\lambda_n^+ \leqslant \mu_{n+\kappa_+}^+ + \gamma, \quad n = 1, \ldots, N_+.$$

Proof: It follows from (2.1) and the fact that $A_0^{1/2}$ is A_0-bounded with relative bound 0 that V is A_0-bounded with relative bound 0; hence H_+ is self-adjoint and bounded from below. Let $\mathfrak{h}_+$ be the quadratic form associated with H_+, i.e.,

$$\mathfrak{h}_+[x] := \frac{1}{2\gamma}(A_0^{1/2}x, A_0^{1/2}x) + (Vx, x), \quad x \in \mathcal{D}(A_0^{1/2}).$$

An elementary calculation shows that

$$\mathfrak{t}(\lambda)[x] = 2\gamma(\mathfrak{h}_+ + \gamma - \lambda)[x] - \|(V - \lambda + \gamma)x\|^2, \quad x \in \mathcal{D}(A_0^{1/2}). \tag{4.4}$$

Let $x \in \mathcal{D}(A_0^{1/2})$, $\|x\| = 1$. Then (4.4) implies that $\mathfrak{t}(\lambda)[x] \leqslant 0$ for all $\lambda \geqslant \mathfrak{h}_+[x] + \gamma$. Hence $p_+(x) \leqslant \mathfrak{h}_+[x] + \gamma$ since $\mathfrak{t}(\cdot)[x]$ is concave. Using Theorem 3.1 and the standard variational principle for semi-bounded self-adjoint operators, we obtain

$$\lambda_n^+ = \min_{\substack{\mathcal{L} \subset \mathcal{D}(H_0^{1/2}) \\ \dim \mathcal{L} = n + \kappa_+}} \max_{\substack{x \in \mathcal{L} \\ \|x\| = 1}} p_+(x) \leqslant \min_{\substack{\mathcal{L} \subset \mathcal{D}(H_0^{1/2}) \\ \dim \mathcal{L} = n + \kappa_+}} \max_{\substack{x \in \mathcal{L} \\ \|x\| = 1}} \mathfrak{h}_+[x] + \gamma = \mu_{n+\kappa_+}^+ + \gamma,$$

which completes the proof. □

Theorem 4.5: *Suppose that assumptions* (A1) *and* (A2) *as well as the assumptions of Theorem 3.3 hold. Then the operator*

$$H_- := -\frac{1}{2\gamma}A_0 + V$$

is self-adjoint and bounded from above. If $\mu_1^- \geqslant \mu_2^- \geqslant \cdots \geqslant \mu_{M_-}^-$, $M_- \in \mathbb{N}_0 \cup \{\infty\}$, *are the eigenvalues of* H_- *above* $\sigma_{\mathrm{ess}}(H_-)$ *and* $\mu_n^- := \max\sigma_{\mathrm{ess}}(H_-)$ *for* $n > M_-$, *then the eigenvalues* λ_n^- *of* T *satisfy the estimate*

$$\lambda_n^- \geqslant \mu_{n+\kappa_-}^- - \gamma, \quad n = 1, \ldots, N_-.$$

Proof: The proof is completely analogous to that of Theorem 4.4 if relation (4.4) is replaced by

$$\mathfrak{t}(\lambda)[x] = -2\gamma(\mathfrak{h}_- - \gamma - \lambda)[x] - \|(V - \lambda - \gamma)x\|^2, \quad x \in \mathcal{D}(A_0^{1/2}),$$

where $\mathfrak{h}_-$ is the quadratic form associated with H_-. □

Remark 4.6:

(i) For the Klein–Gordon equation in $\mathbb{R}^d$ we have $A_0 = c^2(-i\hbar\nabla - e/c\vec{A})^2$ and $\gamma = mc^2$, and the operator

$$H_+ = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2 + V$$

is the classical Schrödinger operator in $\mathbb{R}^d$.

(ii) In the particular case that $\vec{A} = 0$ the estimate

$$\lambda^+_{k-\kappa_+} - mc^2 \leqslant \mu^+_k \tag{4.5}$$

in Theorem 4.4 is sharp in the following sense. The Schrödinger operator $H_+ = -(\hbar^2/2m)\Delta + V$ and hence its eigenvalues on the right-hand side of (4.5) do not depend on c; one can show that $\kappa_+ = 0$ if c is large enough and that $\lim_{c\to\infty}(p_+(x) - mc^2) = (H_+x, x)/\|x\|^2$ uniformly on finite-dimensional spaces and hence

$$\lim_{c\to\infty}(\lambda^+_{k-\kappa_+} - mc^2) = \mu^+_k.$$

It was already proved in Ref. 12 that $\lambda^+_n - mc^2$ converges to some eigenvalue of H_+.

V. THE KLEIN–GORDON EQUATION IN $\mathbb{R}^d$

In this section we consider the Klein–Gordon equation in $\mathbb{R}^d$. Here $\mathcal{H} = L^2(\mathbb{R}^d)$,

$$A_0 = c^2\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2,$$

$$H_0 = c^2\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2 + m^2c^4,$$

and V is the multiplication operator by a function $V: \mathbb{R}^d \to \mathbb{R}$. Note that here and in the sequel $(-i\hbar\nabla - (e/c)\vec{A})^2$ denotes the self-adjoint operator $(-i\hbar\nabla - (e/c)\vec{A})^*(-i\hbar\nabla - (e/c)\vec{A})$.

Lemma 5.1: Assume that $(e/c)\vec{A}$ is $-i\hbar\nabla$-bounded with relative bound less than 1 and let $\hat{H}_0 := c^2(-i\hbar\nabla)^2 + m^2c^4$. Then $\hat{H}_0^{1/2}H_0^{-1/2}$ is bounded and $\mathcal{D}(H_0^{1/2}) = W^{1,2}(\mathbb{R}^d)$.

Proof: Obviously, $\hat{H}_0^{1/2}H_0^{-1/2}$ is closed. By the assumption on $\vec{A}$ it follows that $-i\hbar\nabla - (e/c)\vec{A}$ is closed and $\mathcal{D}(-i\hbar\nabla - (e/c)\vec{A}) = \mathcal{D}(-i\hbar\nabla)$. Hence we have the following chain of equalities of domains:

$$\begin{aligned}\mathcal{D}(H_0^{1/2}) = \mathcal{Q}(H_0) &= \mathcal{Q}\left(c^2\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2 + m^2c^4\right) = \mathcal{Q}\left(\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right)^2\right)\\ &= \mathcal{D}\left(-i\hbar\nabla - \frac{e}{c}\vec{A}\right) = \mathcal{D}(-i\hbar\nabla) = \mathcal{Q}((-i\hbar\nabla)^2) = \mathcal{Q}(c^2(-i\hbar\nabla)^2 + m^2c^4) = \mathcal{Q}(\hat{H}_0)\\ &= \mathcal{D}(\hat{H}_0^{1/2}) = W^{1,2}(\mathbb{R}^d).\end{aligned}$$

Thus $\hat{H}_0^{1/2}H_0^{-1/2}$ is everywhere defined and hence bounded. □

Note that in general $\mathcal{D}(H_0) \neq \mathcal{D}(\hat{H}_0)$.

Corollary 5.2: If $V\hat{H}_0^{-1/2}$ is bounded or compact, then so is $VH_0^{-1/2}$.

Now the following sufficient conditions for assumptions (A1) and (A2), proved in Ref. 6, Theorem 6.1 for the case $\vec{A} = 0$ carry over to the case $\vec{A} \neq 0$.

Proposition 5.3: Assume that $d \geqslant 3$ and that $(e/c)\vec{A}$ is $-i\hbar\nabla$-bounded with relative bound less than 1. Then the following assertions are true.

(i) *If $V \in L^p(\mathbb{R}^d)$ with $d \leqslant p < \infty$, then $VH_0^{-1/2}$ is compact.*

(ii) *There exists a constant $\eta_0 > 0$ (depending on $\vec{A}$) such that if $|V(x)| \leqslant \eta/|x|$, $\eta < \eta_0$, then assumptions* (A1) *and* (A2) *are satisfied with $S_0 = VH_0^{-1/2}$, $S_1 = 0$. If $\vec{A} = 0$, then we can choose $\eta_0 = c\hbar(d-2)/2$, and we have $\|S_0\| \leqslant 2\eta/c\hbar(d-2)$.*

As an illustration of Theorem 4.4 we consider two examples: the Klein–Gordon equation with Coulomb potential in $\mathbb{R}^3$ and with square-well potential in $\mathbb{R}$. In both cases we assume that there is no vector potential, i.e., $\vec{A}=0$.

Example 1: The Coulomb potential. The eigenvalues $\lambda_{n,l}$ of the Klein–Gordon equation in $\mathbb{R}^3$ with Coulomb potential are known explicitly, see, e.g., Ref. 12. In this case

$$V(x) = -\frac{Ze^2}{|x|},$$

where Z is the atomic number. If $Z \leqslant 1/2\alpha \approx 68.5$, where $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant, then V satisfies assumptions (A1) and (A2) according to Proposition 5.3. Since V is $-\Delta$-compact (cf. Ref. 3, Lemma V.5.8), the difference of the resolvents of $T(\lambda)$ and $H_0-\lambda^2$ is compact for every $\lambda \in \mathbb{R}$ and hence $\sigma_{\mathrm{ess}}(T) = (-\infty, -mc^2] \cup [mc^2, +\infty)$ (cf. also Ref. 13). The eigenvalues $\lambda_{n,l}$ all lie in the interval $(0, mc^2)$; they are given by the formula

$$\lambda_{n,l} = mc^2 \left[1 + \frac{(Z\alpha)^2}{\left(n-l-\frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 - (Z\alpha)^2} \right)^2} \right]^{-1/2}, \quad \begin{array}{l} n = 1,2,\ldots, \\ l = 0,1,\ldots,n-1, \end{array}$$

and have multiplicity $2l+1$. The eigenvalues $\lambda_{n,l}$ can be expanded as

$$\lambda_{n,l} = mc^2 - \frac{me^4Z^2}{2\hbar^2}\frac{1}{n^2} - \frac{me^8Z^4}{2\hbar^4}\frac{1}{n^4}\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4} \right)\frac{1}{c^2} + O\left(\frac{1}{c^4}\right), \quad c \to \infty;$$

here the second term is exactly an eigenvalue of the Schrödinger operator,

$$\mu_n = -\frac{me^4Z^2}{2\hbar^2}\frac{1}{n^2},$$

which has multiplicity n^2. In this case the estimate of the Klein–Gordon eigenvalues by the Schrödinger eigenvalues proved in Theorem 4.4 reads

$$\lambda_{n,l} - mc^2 \leqslant \mu_n, \quad l = 0,1,\ldots,n-1, \tag{5.1}$$

for $n=1,2,\ldots$. The values for $n=3$ and $Z=1$,

$$\lambda_{3,0} - mc^2 = -1.511\,79 \text{ eV},$$

$$\lambda_{3,1} - mc^2 = -1.511\,75 \text{ eV}, \quad \mu_3 = -1.511\,74 \text{ eV}$$

$$\lambda_{3,2} - mc^2 = -1.511\,75 \text{ eV},$$

show that the estimate (5.1) is rather tight.

Example 2: The square-well. It was noted already in Ref. 11 that the Klein–Gordon equation in $\mathbb{R}^3$ with square-well potential has complex eigenvalues if the potential is sufficiently deep. Here we consider a square-well potential in $\mathbb{R}$,

$$V(x) = \begin{cases} -v_1, & |x| \leqslant a \\ 0, & |x| > a, \end{cases} \tag{5.2}$$

where $a>0$ and $v_1>0$ are constants. The operator of multiplication by V in $L^2(\mathbb{R})$ satisfies assumption (A1) since it is bounded; it also satisfies assumption (A2). In fact, V is relatively compact with respect to A_0 and H_0 since V has compact support. By Theorem 2.8, this shows that the essential spectrum of the operator polynomial T is given by

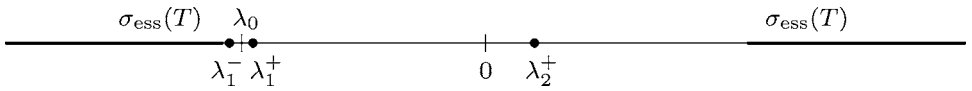

FIG. 1. Spectrum for $2mc^2<v_1=2.07<v_{\mathrm{crit}}$, $m=c=\hbar=a=1$.

$$\sigma_{\mathrm{ess}}(T)=(-\infty,-mc^2]\cup[mc^2,\infty).$$

Theorem 4.3 implies that if $v_1<2mc^2$, then the spectrum is real, $\nu_-\leqslant -mc^2$, the eigenvalues are confined to the interval (mc^2-v_1,mc^2) and all these eigenvalues, $\lambda_1^+\leqslant\lambda_2^+\leqslant\cdots\leqslant\lambda_{N_+}^+$, can be characterized by the variational principle (4.1).

If v_1 is increased such that $v_1>2mc^2$, then eigenvalues $\lambda_1^-\geqslant\lambda_2^-\geqslant\cdots$ start to emerge at $-mc^2$, the bottom of the gap in the essential spectrum. If we choose λ_0 in Theorem 3.1 between λ_1^- and λ_1^+, then we can characterize all eigenvalues λ_n^+ and λ_n^- to the right and left of λ_0, respectively, by the variational principles in Theorems 3.1 and 3.3 with $\kappa_\pm=0$.

If v_1 reaches some critical value v_{crit}, then the two eigenvalues λ_1^+ and λ_1^- meet; if $v_1>v_{\mathrm{crit}}$, they become a pair of nonreal complex conjugate eigenvalues. We can still characterize the real eigenvalues to the right of ν_- and the eigenvalues to the left of ν_+; in both cases the index shifts $\kappa_\pm$ are greater than or equal to the number of pairs of nonreal eigenvalues. Note that the enumeration of the real eigenvalues changes whenever a new pair of complex eigenvalues appears.

The index shift, say κ_+, can be determined exactly: it is equal to the number of negative eigenvalues of $T(\lambda_0)$. For example, if $m=c=\hbar=a=1$ and $v_1=2.11$, then there are no eigenvalues in the interval $(-mc^2,0]$, so we can choose $\lambda_0=0$, and the second sum in (3.5) is 0. Since the Schrödinger operator $T(0)$ has exactly one negative eigenvalue, it follows that $\kappa_+=1$. Now formula (3.5) implies that there is exactly one pair of nonreal complex conjugate eigenvalues, which are algebraically simple.

Finally, we illustrate the estimate of the Klein–Gordon eigenvalues λ_n^+ by the eigenvalues μ_k^+ of the Schrödinger operator $H_+=-\frac{1}{2}(\mathrm{d}^2/\mathrm{d}x^2)+V$ proved in Theorem 4.4, assuming that $m=c=\hbar=a=1$. We consider the two special values $v_1=2.07$ and $v_1=2.11$. In the first case, for which the spectrum is displayed in Fig. 1, there are two eigenvalues $\lambda_1^+<\lambda_2^+$ in the spectral gap $(-1,1)$ (and one eigenvalue λ_1^-), the index shift κ_+ is 0 and hence we obtain the estimates

$$\lambda_1^+\leqslant\mu_1^+ + mc^2,\quad \lambda_2^+\leqslant\mu_2^+ + mc^2;$$

in fact, the corresponding numerical values are

$$\lambda_1^+ = -0.887\,840,\quad \mu_1^+ + 1 = -0.532\,969, \tag{5.3}$$

$$\lambda_2^+ = 0.186\,578,\quad \mu_2^+ + 1 = 0.764\,013. \tag{5.4}$$

In the second case, for which the spectrum is displayed in Fig. 2, there is one eigenvalue λ_1^+ in the spectral gap $(-1,1)$, the index shift κ_+ is 1 and hence

$$\lambda_1^+\leqslant\mu_2^+ + mc^2;$$

here the numerical values are

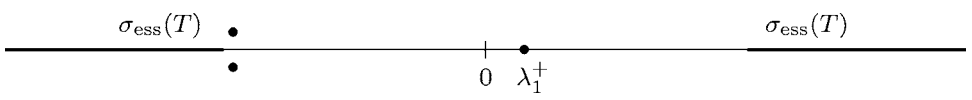

FIG. 2. Spectrum for $v_1=2.11>v_{\mathrm{crit}}$, $m=c=\hbar=a=1$.

$$\lambda_1^+ = 0.148\,517, \quad \mu_2^+ + 1 = 0.744\,769.$$

If c is increased to its physical value, then the Klein–Gordon eigenvalues λ_n^+ come much closer to the respective shifted Schrödinger eigenvalues.

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Classification of integrable Hamiltonian hydrodynamic chains associated with Kupershmidt's brackets

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We characterize a class of integrable Hamiltonian hydrodynamic chains, based on the necessary condition for the integrability provided by the vanishing of the Haantjes tensor. We prove that the vanishing of the first few components of the Haantjes tensor is already sufficiently restrictive, and allows a complete description of the corresponding Hamiltonian densities. In each of the cases we were able to explicitly construct a generating function for conservation laws, thus establishing the integrability. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2354590]

I. INTRODUCTION

We consider Hamiltonian systems of the form

$$\mathbf{u}_t = \left(B\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}B^t \right)\frac{\partial h}{\partial \mathbf{u}}, \tag{1}$$

where $\mathbf{u}=(u^1,u^2,u^3,\ldots)^t$ is an infinite-component column vector of the dependent variables, and the matrix B of the Hamiltonian operator $B(\mathrm{d}/\mathrm{d}x)+(\mathrm{d}/\mathrm{d}x)B^t$ is defined as $B^{ij}=(\alpha(i-1)+\beta)u^{i+j-1}$. Explicitly, one has

$$B = \begin{pmatrix} \beta u^1 & \beta u^2 & \beta u^3 & \ldots. \\ (\alpha+\beta)u^2 & (\alpha+\beta)u^3 & (\alpha+\beta)u^4 & \ldots. \\ (2\alpha+\beta)u^3 & (2\alpha+\beta)u^4 & (2\alpha+\beta)u^5 & \ldots. \\ \ldots. & \ldots. & \ldots. & \ldots. \end{pmatrix};$$

here α and β are arbitrary constants. Hamiltonian operators of this type first appeared in Ref. 8, and belong to the general class introduced in Ref. 2. The Hamiltonian density h is assumed to be a function of the first two independent variables u^1,u^2 only: $h=h(u^1,u^2)$. In this paper we address the problem of the classification of all densities $h(u^1,u^2)$ such that the corresponding Hamiltonian system is *integrable* (partial results were reported earlier in Ref. 8). The integrability of Hamiltonian chains of the type (1) can be defined by either of two properties:

(1) The existence of infinitely many additional conservation laws which Poisson commute with the Hamiltonian $\int h(u^1,u^2)\mathrm{d}x$, see Ref. 8.
(2) The existence of infinitely many hydrodynamic reductions, see Refs. 5, 6, and 3.

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To derive the integrability conditions we utilize the second approach, based on the calculation of the so-called Haantjes tensor.[7] Let us first represent the system (1) in a hydrodynamic form,

$$\mathbf{u}_t = V(\mathbf{u})\mathbf{u}_x,$$

where $V=v^i_j$ is an $\infty\times\infty$ matrix. This matrix has the following properties:

(a) each row of V contains *finitely many* nonzero elements;
(b) each matrix element of V depends on *finitely many* variables u^i.

Infinite systems of this type are known as "hydrodynamic chains." The properties (a) and (b) ensure that both the Nijenhuis tensor,

$$N^i_{jk} = v^p_j \partial_{u^p} v^i_k - v^p_k \partial_{u^p} v^i_j - v^i_p(\partial_{u^j} v^p_k - \partial_{u^k} v^p_j) \tag{2}$$

(the standard summation convention over repeated indices is adopted), and the Haantjes tensor,

$$H^i_{jk} = N^i_{pr} v^p_j v^r_k - N^p_{jr} v^i_p v^r_k - N^p_{rk} v^i_p v^r_j + N^p_{jk} v^i_r v^r_p, \tag{3}$$

are well-defined objects, so that the calculation of each particular component H^i_{jk} requires finitely many summations only. Moreover, for a fixed upper index i, one has *finitely many* nonzero components H^i_{jk}, see Ref. 3. According to the results of Tsarev,[15] the vanishing of the Haantjes tensor is necessary and sufficient for the integrability of finite-component Hamiltonian systems of hydrodynamic type by the generalized hodograph method. Thus, we formulate our main

Conjecture: The vanishing of the Haantjes tensor is a necessary and sufficient condition for the integrability of Hamiltonian hydrodynamic chains. In particular, it implies the existence of infinitely many Poisson commuting conservation laws, and infinitely many hydrodynamic reductions.

The necessity part of this conjecture follows from the general result of Ref. 3, according to which the vanishing of the Haantjes tensor is a necessary condition for the integrability of hydrodynamic chains (not necessarily Hamiltonian). The sufficiency is a far more delicate property and requires, as a subproblem, the classification of infinite-component Hamiltonian structures. The conjecture is supported by all examples of integrable Hamiltonian chains known to us. Since components of the Haantjes tensor can be calculated using computer algebra, this approach provides an effective classification criterion. The main goal of this paper is to demonstrate that the conjecture is indeed true for Hamiltonian chains of the type (1).

Upon setting the first components H^1_{jk} equal to zero we obtain the expressions for all third-order partial derivatives of the Hamiltonian density $h(u^1,u^2)$ in terms of lower order derivatives, see Eq. (4) in Sec. II. A complete list of integrable Hamiltonian densities is obtained in Sec. III by solving these equations for $h(u^1,u^2)$. In the general case ($\beta\neq 0$, $\alpha+2\beta\neq 0$) we have three essentially different examples,

$$h(u^1,u^2) = (u^2 + f(u^1))^{\beta/(\alpha+2\beta)},$$

where $f(u^1)=a(u^1+c)^{(\alpha+2\beta)/\beta}+b(u^1-c)^{(\alpha+2\beta)/\beta}$, as well as

$$h(u^1,u^2) = (u^1+c)^{-(\alpha+\beta)/\beta}u^2 + a(u^1-c)^{2+\alpha/\beta}(u^1+c)^{-1-\alpha/\beta}$$

and

$$h(u^1,u^2) = u^2 + c(u^1)^2;$$

here a,b,c are arbitrary constants. In the case $\beta=0$ we have two extra examples,

$$h(u^1,u^2) = \ln(u^2 + f(u^1)), \quad f'' = cf,$$

and

$$h(u^1,u^2)=e^{cu^1}u^2+e^{2cu^1}.$$

Finally, the case $\alpha+2\beta=0$ gives three extra examples,

$$h(u^1,u^2)=e^{au^2+f(u^1)},$$

here

$$f(u^1)=\frac{b}{2\sqrt{b^2+1}}\ln\frac{\sqrt{b^2+1}+cu^1}{\sqrt{b^2+1}-cu^1}+\frac{1}{2}\ln(b^2+1-c^2(u^1)^2),$$

as well as

$$h(u^1,u^2)=(u^1+c)u^2+b(u^1+c)\ln\frac{u^1+c}{u^1-c}$$

and

$$h(u^1,u^2)=u^1u^2+\frac{c}{u^1}.$$

These examples correct the list presented in Ref. 8.

We prove in Sec. IV that all remaining components of the Haantjes tensor of the corresponding Hamiltonian chains vanish identically by virtue of (4).

In Sec. V we demonstrate that the requirement of the existence of an additional conservation law of the form $p(u^1,u^2,u^3)_t=q(u^1,u^2,u^3,u^4)_x$ leads to the same relations (4).

As shown in Sec. VI, Eq. (4) implies the existence of a generating function of conservation laws and, hence, the infinity of conservation laws. This establishes the integrability of all examples constructed in Sec. III. In the general case the generating function is expressed in terms of a hypergeometric function of Gauss.

II. DERIVATION OF THE INTEGRABILITY CONDITIONS

There are two "trivial" cases which are to be excluded from the further analysis:

(i) $\alpha+\beta=0$. In this case the Haantjes tensor vanishes identically for any Hamiltonian density $h(u^1,u^2)$, indeed, the first two equations for u^1, u^2 form an independent subsystem, while the remaining equations become strictly lower-triangular.

(ii) $\Delta=(\alpha+\beta)h_2+(\alpha+2\beta)u^2h_{22}+2\beta u^1h_{12}=0$. In this case the first equation of the chain decouples from the rest, taking the form $u^1_t=\lambda(u^1)u^1_x$ where $\lambda(u^1)$ is a function of u^1. The Haantjes tensor is also identically zero.

Assuming in what follows that neither of the expressions in (i) and (ii) vanishes (they appear as denominators in the formulas to follow), calculating the components H^1_{jk} of the Haantjes tensor (one can use computer algebra to perform calculations of this type), and setting them equal to zero, we obtain the following expressions for third-order partial derivatives of the Hamiltonian density $h(u^1,u^2)$:

$$h_{222}=\frac{(2\alpha+3\beta)h_{22}^2}{(\alpha+\beta)h_2},$$

$$h_{122}=\frac{(2\alpha+3\beta)h_{22}h_{12}}{(\alpha+\beta)h_2},$$

$$h_{112}=\frac{(\alpha+2\beta)h_{12}^2+(\alpha+\beta)h_{22}h_{11}}{(\alpha+\beta)h_2},$$

$$h_{111}=\frac{-\alpha(\alpha+2\beta)u^2h_{12}^3+(\alpha+\beta)((2\alpha+3\beta)h_2+3(\alpha+2\beta)u^2h_{22})h_{11}h_{12}}{(\alpha+\beta)h_2\Delta}$$
$$+\frac{2\beta(\alpha+3\beta)u^1h_{12}^2h_{11}+2\alpha\beta u^1h_{22}h_{11}^2}{(\alpha+\beta)h_2\Delta}; \tag{4}$$

here $\Delta=(\alpha+\beta)h_2+(\alpha+2\beta)u^2h_{22}+2\beta u^1h_{12}$, and lower indices indicate differentiation with respect to u^1 and u^2. We have verified the involutivity of this system.

Remark 1: Since u^1 is the density of the momentum of the Hamiltonian structure (1), the addition of terms linear in u^1 to the Hamiltonian density h effects neither the integrability of the chain, nor the vanishing of the Haantjes tensor. Thus, the classification to follow is carried out up to transformations of the form

$$h\to ah+bu^1+c, \tag{5}$$

where a, b, c are arbitrary constants.

III. INTEGRABLE HAMILTONIAN DENSITIES

We begin with the general case when both β and $\alpha+2\beta$ are nonzero. The cases when either of them vanishes will be considered separately.

A. General case

If $h_{22}\neq 0$ then, using the first two equations (4), we obtain

$$h_{22}=ch_2^{(2\alpha+3\beta)/(\alpha+\beta)},\quad c=\text{const}.$$

This can be integrated twice to give $h=(u^2+f(u^1))^{\beta/(\alpha+2\beta)}+g(u^1)$. The substitution into the third equation implies $g''=0$. Thus, up to transformations (5), we have

$$h(u^1,u^2)=(u^2+f(u^1))^{\beta/(\alpha+2\beta)}. \tag{6}$$

Substituting this into the remaining expression for h_{111} we obtain an ODE for $f(u^1)$,

$$f'''=\alpha f''\frac{(\alpha+\beta)f'-2\beta u^1f''}{(\alpha+\beta)((\alpha+2\beta)f-2\beta u^1f')},$$

with the general solution

$$f=a(u^1+c)^{(\alpha+2\beta)/\beta}+b(u^1-c)^{(\alpha+2\beta)/\beta};$$

here a,b,c are arbitrary constants (we thank Sasha Veselov for this observation).

If $h_{22}=0$ then the first two equations (4) are satisfied identically, while the last two equations imply either

$$h(u^1,u^2)=(u^1+c)^{-(\alpha+\beta)/\beta}u^2+\tau(u^1), \tag{7}$$

where $\tau(u^1)$ satisfies an ODE

$$\tau'''=\frac{\tau''}{\beta}\left(\frac{\alpha}{u^1-c}-\frac{\alpha+3\beta}{u^1+c}\right)$$

with the general solution

$$\tau = a(u^1 - c)^{2+\alpha/\beta}(u^1 + c)^{-1-\alpha/\beta},$$

or

$$h(u^1,u^2) = u^2 + c(u^1)^2. \tag{8}$$

We point out that the integrability of the Hamiltonian chain with the density (8) was established in Ref. 8.

B. Case $\beta=0$

The equations for h take the form

$$h_{222} = \frac{2h_{22}^2}{h_2},$$

$$h_{122} = \frac{2h_{22}h_{12}}{h_2},$$

$$h_{112} = \frac{h_{11}h_{22} + h_{12}^2}{h_2},$$

$$h_{111} = \frac{-u^2h_{12}^3 + 2h_2h_{11}h_{12} + 3u^2h_{22}h_{12}h_{11}}{h_2(h_2 + u^2h_{22})}.$$

If $h_{22} \neq 0$ then, up to transformations (5), the first three equations imply

$$h(u^1,u^2) = \ln(u^2 + f(u^1)), \tag{9}$$

and the substitution of this ansatz into the fourth equation gives $f'''f - f'f'' = 0$, which integrates to $f'' = cf$, c=const. If $h_{22}=0$ then the first two equations (4) are satisfied identically, while the other two imply either

$$h(u^1,u^2) = e^{cu^1}u^2 + e^{2cu^1}, \tag{10}$$

or

$$h(u^1,u^2) = u^2 + c(u^1)^2, \tag{11}$$

c=const, the latter case coinciding with (8).

C. Case $\alpha+2\beta=0$

The equations for h take the form

$$h_{222} = \frac{h_{22}^2}{h_2},$$

$$h_{122} = \frac{h_{22}h_{12}}{h_2},$$

$$h_{112} = \frac{h_{11}h_{22}}{h_2},$$

$$h_{111} = \frac{h_2 h_{11} h_{12} + 2u^1 h_{12}^2 h_{11} - 4u^1 h_{22} h_{11}^2}{h_2(h_2 - 2u^1 h_{12})}.$$

If $h_{22} \neq 0$ then, up to transformations (5), the first three equations imply

$$h(u^1,u^2) = e^{au^2 + f(u^1)}. \tag{12}$$

The substitution of this ansatz into the fourth equation gives an ODE for f,

$$f''' + 2f'f'' = 2u^1(f'f''' - 2(f'')^2),$$

which can be solved as follows. Setting $f' = 1/w$ we obtain $w''(w - 2u^1) = 2w'(w' - 1)$. Introducing $w = v + 2u^1$ we arrive at an autonomous ODE $v''v = 2(v' + 2)(v' + 1)$ which integrates twice leading to the general solution

$$f = \frac{b}{2\sqrt{b^2+1}} \ln \frac{\sqrt{b^2+1} + cu^1}{\sqrt{b^2+1} - cu^1} + \frac{1}{2} \ln(b^2 + 1 - c^2(u^1)^2), \quad c, b = \text{const},$$

or its linear degeneration $f = cu^1$. Setting $b = \sinh a$ we can rewrite the above expression in the form

$$f = \frac{1}{2\cosh a}(e^a \ln(\cosh a + cu^1) + e^{-a} \ln(\cosh a - cu^1)).$$

The case $h_{22} = 0$ leads to either

$$h(u^1,u^2) = (u^1 + c)u^2 + b(u^1 + c) \ln \frac{u^1 + c}{u^1 - c}, \tag{13}$$

where c, b are arbitrary constants, or its degeneration,

$$h(u^1,u^2) = u^1 u^2 + \frac{c}{u^1}. \tag{14}$$

Further degeneration $h_{22} = h_{12} = 0$ results in

$$h(u^1,u^2) = u^2 + c(u^1)^2. \tag{15}$$

IV. THE VANISHING OF THE HAANTJES TENSOR

In this section we demonstrate that the relations (4), which were obtained from the requirement of the vanishing of the first few components H^1_{jk} of the Haantjes tensor, are already sufficiently restrictive and imply the vanishing of all other components. The proof utilizes an important property of Hamiltonian chains (1), namely, the existence of finite-component reductions for *any* (not necessarily integrable) Hamiltonian density h.[12] Let us parametrize u^i in terms of finitely many "moments" v^a, $a = 1, \ldots, n$, as follows:

$$u^k = \frac{1}{2 + \dfrac{\alpha}{\beta}(k-1)} \sum_1^n (v^a)^{2 + \alpha/\beta(k-1)},$$

$k = 1, 2, 3, \ldots$. (we consider the generic case when all expressions in the denominators are nonvanishing, see Ref. 12 for a discussion of the exceptional cases). Thus,

$$u^1 = \frac{1}{2}\sum_1^n (v^a)^2, \quad u^2 = \frac{1}{2+\frac{\alpha}{\beta}}\sum_1^n (v^a)^{2+\alpha/\beta}, \tag{16}$$

etc. One can verify that under this substitution the infinite chain (1),

$$u_t^k = (\alpha(k-1)+\beta)u^k(h_1)_x + (\alpha(k-1)+\beta)u^{k+1}(h_2)_x + \beta(u^k h_1)_x + (\alpha+\beta)(u^{k+1}h_2)_x,$$

reduces to an n-component "symmetric" conservative system for v^a,

$$v_t^a = \beta(v^a h_1 + (v^a)^{1+\alpha/\beta}h_2)_x, \tag{17}$$

$a=1,\ldots,n$, see Ref. 13. Here $h(u^1,u^2)$ is an *arbitrary* Hamiltonian density, not necessarily satisfying the integrability conditions (4), and u^1,u^2 are given by (16). Notice that the system (17) is manifestly Hamiltonian: $v_t^a = \beta(\partial h/\partial v^a)_x$. Similar formulas can be obtained if the density h depends on more than two u's. We have the following

Theorem 1: *For a Hamiltonian density $h(u^1,u^2)$ satisfying the integrability conditions (4), the Haantjes tensor of any finite-component reduction (17) is identically zero.*

The proof follows from the explicit formulas for the Nijenhuis tensor,

$$\begin{aligned}
N_{23}^1 = {} & \beta v^1v^2v^3((v^2)^{\alpha/\beta}-(v^3)^{\alpha/\beta})\Big[2\beta^2u^1(h_{11}h_{12}^2-h_{11}^2h_{22}) + \beta\Big(2+\frac{\alpha}{\beta}\Big)(\alpha u^2 - 2\beta(v^1)^{\alpha/\beta}u^1)(h_{11}h_{22}h_{12} \\
& - h_{12}^3) + (\alpha+\beta)\Big(2\Big(1+\frac{\alpha}{\beta}\Big)u^3 - \beta\Big(2+\frac{\alpha}{\beta}\Big)^2(v^1)^{\alpha/\beta}u^2\Big)(h_{11}h_{22}^2-h_{12}^2h_{22}) + (\alpha+\beta)h_2[(\alpha+2\beta) \\
& \times (h_{11}h_{12}+(v^1v^2v^3)^{\alpha/\beta}h_{22}^2) + ((v^1v^2)^{\alpha/\beta}+(v^1v^3)^{\alpha/\beta}+(v^2v^3)^{\alpha/\beta})h_{12}h_{22} + ((\alpha+\beta)((v^1)^{\alpha/\beta} \\
& + (v^2)^{\alpha/\beta}+(v^3)^{\alpha/\beta}) - (2\alpha+\beta)((v^1)^{\alpha/\beta})h_{11}h_{22} + (\beta((v^1)^{\alpha/\beta}+(v^2)^{\alpha/\beta}+(v^3)^{\alpha/\beta}) + (2\alpha+\beta) \\
& \times (v^1)^{\alpha/\beta})h_{12}^2)]\Big]
\end{aligned}$$

and

$$\begin{aligned}
N_{12}^1 = {} & \beta^2(v^1)^2v^2((v^1)^{\alpha/\beta}-(v^2)^{\alpha/\beta})\Big[\Big(2+\frac{\alpha}{\beta}\Big)(\alpha u^2 - 2\beta(v^1)^{\alpha/\beta}u^1)(h_{11}h_{22}h_{12}-h_{12}^3) + 2\beta^2u^1(h_{11}h_{12}^2 \\
& - h_{11}^2h_{22}) + \Big(\Big(2+\frac{\alpha}{\beta}\Big)(\alpha-2\beta)(v^1)^{\alpha/\beta}u^2 - 2(\alpha+\beta)\Big(1+\frac{\alpha}{\beta}\Big)u^3\Big)(h_{12}^2h_{22}-h_{22}^2h_{11})\Big] \\
& - \beta(\alpha+\beta)h_2v^2\Big[(v^1v^2)^{\alpha/\beta}\Big(2(\alpha+\beta)\Big(1+\frac{\alpha}{\beta}\Big)u^3 + (\alpha+2\beta)((v^2)^{\alpha/\beta}-(v^1)^{\alpha/\beta})(v^1)^{2+\alpha/\beta}\Big)h_{22}^2 \\
& + \Big(-\alpha(v^1)^{\alpha/\beta}\Big(-\Big(2+\frac{\alpha}{\beta}\Big)u^2 - 2(v^2)^{\alpha/\beta}u^1 + 2((v^1)^{\alpha/\beta}-(v^2)^{\alpha/\beta})(v^1)^2\Big) + \beta\Big(\Big(2+\frac{\alpha}{\beta}\Big) \\
& \times ((v^1)^{\alpha/\beta}+(v^2)^{\alpha/\beta})u^2 + 2(v^1v^2)^{\alpha/\beta}u^1 + 2\Big(1+\frac{\alpha}{\beta}\Big)u^3 + (v^1)^{2+\alpha/\beta}(2(v^2)^{\alpha/\beta}-3(v^1)^{\alpha/\beta}) \\
& + (v^2)^{\alpha/\beta}(v^1)^2\Big)\Big)h_{12}^2 + 2\beta u^1h_{11}^2 + \Big(2((\alpha+\beta)(v^1)^{\alpha/\beta}+\beta(v^2)^{\alpha/\beta})u^1 + \beta\Big(2+\frac{\alpha}{\beta}\Big)(((v^2)^{\alpha/\beta} \\
& - (v^1)^{\alpha/\beta}(v^1)^2+u^2)\Big)h_{11}h_{12} + \Big(2\Big(1+\frac{\alpha}{\beta}\Big)((\alpha+\beta)(v^1)^{\alpha/\beta}+\beta(v^2)^{\alpha/\beta})u^3 + \Big(2+\frac{\alpha}{\beta}\Big) \\
& \times (v^1)^{\alpha/\beta}(2(v^2)^{\alpha/\beta}(\alpha+\beta)u^3 + \beta(2(v^2)^{2\alpha/\beta}-(v^1)^{2\alpha/\beta}-(v^1v^2)^{\alpha/\beta})(v^1)^2)\Big)h_{12}h_{22}\Big] - (\alpha
\end{aligned}$$

$$+\beta)^2 h_2 v^2[((\alpha-\beta)(v^1)^{\alpha/\beta}+\beta(v^2)^{\alpha/\beta})h_{11}+((\alpha+\beta)(v^2)^{\alpha/\beta}-\beta(v^1)^{\alpha/\beta})(v^1v^2)^{\alpha/\beta}h_{22}$$
$$+(2\alpha(v^1v^2)^{\alpha/\beta}+\beta((v^2)^{2\alpha/\beta}-(v^1)^{2\alpha/\beta}))h_{12}],$$

which were obtained using the integrability conditions (4). Notice that, since (17) is invariant under permutations of v's, it is sufficient to specify N^1_{23} and N^1_{12} only. We emphasize that these expressions do not explicitly depend on the size n of the reduction (17): this dependence is hidden in the variables u^1,u^2,u^3. The vanishing of the Haantjes tensor (3) is now a straightforward algebraic calculation.

Thus, for the Hamiltonian densities $h(u^1,u^2)$ which satisfy the integrability conditions (4), the corresponding hydrodynamic chains possess diagonalizable n-component reductions (17) for any value of n. According to the results of Ref. 3, this implies that the full Haantjes tensor of the Hamiltonian chain vanishes identically.

V. CONSERVATION LAWS

For any Hamiltonian density $h(u^1,u^2)$ the system (1) necessarily possesses two conservation laws, namely,

$$u^1_t=(2\beta u^1h_1+(\alpha+2\beta)u^2h_2-\beta h)_x$$

and

$$h_t=((\alpha+\beta)u^3h_2^2+(\alpha+2\beta)u^2h_1h_2+\beta u^1h_1^2)_x,$$

which correspond to the conservation of the momentum and the Hamiltonian, respectively. Let us require that there exists an "extra" conservation law of the form

$$p(u^1,u^2,u^3)_t=q(u^1,u^2,u^3,u^4)_x. \tag{18}$$

Theorem 2: *The integrability conditions* (4) *are necessary and sufficient for the existence of an additional conservation law of the form* (18).

The proof is computational: substituting in for u^1_t,u^2_t,u^3_t,u^4_t into the left-hand side of (18), we collect coefficients at $u^1_x,\ldots,u^4_x$ and equate them to zero. This results in a system of first-order partial differential equations for the flux q,

$$q_1=(3\alpha+2\beta)u^4p_3h_{12}+(\alpha+2\beta)u^2(p_1h_{12}+p_2h_{11})+2(\alpha+\beta)u^3(p_3h_{11}+p_2h_{12})$$
$$+\beta h_1p_1+2\beta u^1p_1h_{11},$$

$$q_2=(3\alpha+2\beta)u^4h_{22}p_3+(\alpha+\beta)(2u^3(h_{12}p_3+h_{22}p_2)+h_2p_1)+(\alpha u^2p_2+2\beta(u^1p_1+u^2p_2))h_{12}$$
$$+u^2(\alpha+2\beta)p_1h_{22}+\beta h_1p_2,$$

$$q_3=\beta h_1p_3+(\alpha+\beta)h_2p_2,$$

$$q_4=(\alpha+\beta)h_2p_3.$$

Calculating the consistency conditions for the flux, $q_{ij}=q_{ji}$, we obtain all second-order partial derivatives of the density p,

$$p_{11}=\frac{2(2\alpha+\beta)((\alpha+\beta)u^3h_{12}^2+\beta u^1h_{11}^2)p_3+(2(2\alpha^2+5\alpha\beta+2\beta^2)u^2h_{12}p_3+(\alpha+\beta)^2p_2h_2)h_{11}}{(\alpha+\beta)^2h_2^2},$$

$$p_{12}=\frac{(\alpha+\beta)^2h_2h_{12}p_2+(2\alpha+\beta)(2\beta u^1h_{12}h_{11}+(\alpha+\beta)(2u^3h_{22}h_{12}+h_2h_{11}))p_3}{(\alpha+\beta)^2h_2^2}$$
$$+\frac{(2\alpha^2+5\alpha\beta+2\beta^2)u^2(h_{12}^2+h_{22}h_{11})p_3}{(\alpha+\beta)^2h_2^2},$$

$$p_{22}=\frac{(2\alpha+\beta)((\alpha+\beta)(2u^3p_3h_{22}^2+2h_{12}h_2p_3)+2((\alpha+2\beta)u^2h_{22}+\beta u^1h_{12})p_3h_{12})+(\alpha+\beta)^2h_{22}h_2p_2}{(\alpha+\beta)^2h_2},$$

$$p_{13}=\frac{(2\alpha+\beta)h_{12}p_3}{(\alpha+\beta)h_2},$$

$$p_{23}=\frac{(2\alpha+\beta)h_{22}p_3}{(\alpha+\beta)h_2},$$

$$p_{33}=0.$$

These equations imply, in particular, that p is linear in u^3, and q is linear in u^4. Upon imposing the consistency condition $(p_{ij})_k=(p_{ik})_j$ we get a system of third-order partial differential equations for the density $h(u^1,u^2)$, which is identical to (4). This finishes the proof.

We will demonstrate in Sec. VI that Eq. (4) imply the existence of a generating function for conservation laws. Thus, we can claim that the existence of one additional conservation law is already very restrictive and implies the existence of an infinity of conservation laws, thus manifesting the integrability.

Remark: Taking $p(u^1,u^2,u^3)$ defined by the above equations as a Hamiltonian density, one obtains a system (1) which commutes with the Hamiltonian system defined by the density $h(u^1,u^2)$, and also has the identically vanishing Haantjes tensor. We emphasize that the densities $p(u^1,u^2,u^3)$ arising in this way are necessarily linear in u^3. One can formulate a natural question: describe all Hamiltonian densities of the form $p(u^1,u^2,u^3)$ such that the associated chain (1) has the vanishing Haantjes tensor. A detailed analysis of this problem leads to the two possibilities: (i) the density p is linear in u^3. In this case one can show the existence of a lower order commuting flow with the Hamiltonian density $h(u^1,u^2)$, which brings us back to the situation discussed earlier.

(ii) The density p is such that the quantity $2\beta u^1p_1+(\alpha+2\beta)u^2p_2+2(\alpha+\beta)u^3p_3-\beta p$ is a function of the first coordinate u^1 only. In this case the first equation of the chain,

$$u_t^1=(2\beta u^1p_1+(\alpha+2\beta)u^2p_2+2(\alpha+\beta)u^3p_3-\beta p)_x,$$

decouples from the rest. The general form of all such densities is

$$p=\sqrt{u^1}F(u^2(u^1)^{-(\alpha+2\beta)/2\beta},u^3(u^1)^{-(\alpha+\beta)/\beta})+f(u^1),$$

where F and f are arbitrary functions. This result shows that, essentially, there exist no nontrivial "genuine" integrable densities of the form $p(u^1,u^2,u^3)$.

VI. GENERATING FUNCTIONS FOR CONSERVATION LAWS

The structure of reductions (17) suggests that one should seek a generating function for conservation laws in the form

$$\lambda=\lambda(p,u^1,u^2,u^3,\dots) \tag{19}$$

so that the following Gibbons-type relation holds:

$$\lambda_t - \beta(h_1 + (1+\alpha/\beta)p^{\alpha/\beta}h_2)\lambda_x = \lambda_p(p_t - \beta(ph_1 + p^{1+\alpha/\beta}h_2)_x); \tag{20}$$

this relation is required to be satisfied identically modulo (1). We will demonstrate the existence of a generating function of this form for any Hamiltonian density satisfying the integrability conditions (4). Suppose the relation (20) is already established. Then, setting $\lambda=\text{const}$, one has $\lambda_t=\lambda_x=0$, so that the relation (20) takes the form

$$p_t - \beta(ph_1 + p^{1+\alpha/\beta}h_2)_x = 0.$$

This provides an infinite sequence of conserved densities after one expands p as a series in λ by virtue of (19). The method of generating functions is standard, and can be traced back to, Refs. 1, 4, 9, and 10 see also Ref. 12 for recent developments. A detailed analysis of the relation (20) reveals that the dependence of λ on u^2,u^3,u^4, etc., is fixed uniquely,

$$\lambda = \sum_{k=2}^{\infty} q^{1-2\beta/\alpha-k}u^k + s(u^1,q), \quad q = p^{\alpha/\beta}, \tag{21}$$

while the function $s(u^1,q)$, which specifies the dependence of λ on u^1, satisfies

$$s_1 = q^{-1-2\beta/\alpha}F, \quad s_q = \frac{1}{\alpha}q^{-1-2\beta/\alpha}G. \tag{22}$$

Here F and G are the following rational expressions in q depending on the Hamiltonian density h:

$$F = \frac{(h_{11}+qh_{12})((\alpha+\beta)qh_2 - (\alpha+2\beta)u^2h_{12}) + (\alpha+2\beta)u^2h_{11}(h_{12}+qh_{22})}{(\alpha+\beta)h_2[q^2h_{22}+2qh_{12}+h_{11}] + (2\beta u^1q - (\alpha+2\beta)u^2)[h_{12}^2 - h_{11}h_{22}]},$$

$$G = \frac{(\alpha+\beta)^2qh_2 + 2\beta(\alpha+2\beta)u^1u^2(h_{12}^2 - h_{11}h_{22}) + (\alpha+\beta)h_2[(\alpha+2\beta)qu^2h_{22} - 2\beta u^1h_{11}]}{(\alpha+\beta)h_2[q^2h_{22}+2qh_{12}+h_{11}] + (2\beta u^1q - (\alpha+2\beta)u^2)[h_{12}^2 - h_{11}h_{22}]}.$$

With the ansatz (21), all terms in (20) containing $p_t,p_x,u_x^3,u_x^4,\ldots$, cancel identically, while the requirement of cancellation of coefficients at u_x^1 and u_x^2 results in (22). The functions F and G satisfy the relations

$$F_2 = 0, \quad G_2 = 0, \quad G_1 = \alpha F_q - (\alpha+2\beta)F/q, \tag{23}$$

which are the consistency conditions of Eq. (22). These relations are satisfied identically modulo the integrability conditions (4). Conversely, relations (23) imply the integrability conditions (4). Notice that, although the variable u^2 is seemingly present in the expressions for F and G, the right-hand sides of (22) do not depend on u^2. For each of the cases arising in the classification in Sec. III, Eq. (22) for $s(u^1,q)$ can be solved explicitly. Thus, the generating function λ can be reconstructed in closed form. This is mainly due to a simple dependence of the derivative s_q on q: integrating it with respect to q we obtain a closed form expression which, in most of the cases, automatically solves the equation for s_1. We consider the canonical forms (6)–(15) case by case in the following.

A. Generating functions in the general case: Densities (6)–(8)

For the Hamiltonian density (6) the function $s(u^1,q)$ is given by

$$s(u^1,q)=\frac{\beta^2 q^{1-2\beta/\alpha}((u^1)^2-c^2)^{-\alpha/\beta}}{4abc^2(\alpha^2-4\beta^2)}\left[a(u^1-c)^2(u^1+c)^{\alpha/\beta}F\left(\frac{\beta q(u^1-c)^{-\alpha/\beta}}{2bc(\alpha+2\beta)}\right)\right.$$
$$\left.+b(u^1-c)^{\alpha/\beta}(u^1+c)^2F\left(-\frac{\beta q(u^1+c)^{-\alpha/\beta}}{2ac(\alpha+2\beta)}\right)\right]+q^{-2\beta/\alpha}u^1;$$

here $F(t)={}_2F_1(1-2\beta/\alpha,1,2-2\beta/\alpha,t)$ is the hypergeometric function of Gauss. In the case (7) one has

$$s(u^1,q)=\frac{\beta^2 q^{1-2\beta/\alpha}(u^1-c)^{2-\alpha/\beta}}{4ac^2(\alpha^2-4\beta^2)}F\left(\frac{\beta q(u^1-c)^{-\alpha/\beta}}{2ac(\alpha+2\beta)}\right)+q^{-2\beta/\alpha}u^1;$$

here F is the same hypergeometric function as above. Finally, the case of (8) leads to

$$s(u^1,q)=\left(u^1+\frac{\alpha+\beta}{2c(\alpha-2\beta)}q\right)q^{-2\beta/\alpha}. \tag{24}$$

B. Generating functions in the case $\beta=0$: Densities (9)–(11)

Here the relation (20) takes the form

$$\lambda_t-e^p h_2\lambda_x=\lambda_p(p_t-(h_1+e^p h_2)_x)$$

where

$$\lambda=\sum_{k=2}^{\infty}q^{1-k}u^k+s(u^1,q),\quad q=e^p.$$

The function $s(u^1,q)$ satisfies

$$s_1=\frac{h_2(h_{11}+qh_{12})+u^2(h_{11}h_{22}-h_{12}^2)}{h_2h_{11}+u^2(h_{11}h_{22}-h_{12}^2)+2qh_2h_{12}+q^2h_2h_{22}},$$

$$s_q=\frac{h_2(u^2h_{22}+h_2)}{h_2h_{11}+u^2(h_{11}h_{22}-h_{12}^2)+2qh_2h_{12}+q^2h_2h_{22}},$$

which are consistent and define $s(u^1,q)$ explicitly: for the Hamiltonian density (9) one has

$$s(u^1,q)=\frac{1}{\sqrt{c}}\operatorname{arctanh}\left(\frac{q+f'}{\sqrt{c}f}\right);$$

recall that $f''=cf$. The density (10) leads to

$$s(u^1,q)=\frac{1}{2}u^1+\frac{1}{2c}\log(2ce^{cu^1}+q).$$

The density (11) gives

$$s(u^1,q)=u^1+q/2c;$$

notice that this expression can be obtained from (24) by setting $\beta=0$.

C. Generating functions in the case $\alpha+2\beta=0$: Densities (12)–(15)

Here the relation (20) takes the form (set $\beta=1,\alpha=-2$):

$$\lambda_t - (h_1 - p^{-2}h_2)\lambda_x = \lambda_p(p_t - (h_1 p + p^{-1}h_2)_x),$$

where

$$\lambda = \sum_{k=2}^{\infty} q^{2-k}u^k + s(u^1,q), \quad q = p^{-2}.$$

The function $s(u^1,q)$ satisfies

$$s_1 = -qh_2 \frac{h_{11} + qh_{12}}{(h_{11} + qh_{12})(2u^1 h_{12} - h_2) - (h_{12} + qh_{22})(2u^1 h_{11} + qh_2)},$$

$$s_q = -\frac{h_2}{2} \frac{2u^1 h_{11} + qh_2}{(h_{11} + qh_{12})(2u^1 h_{12} - h_2) - (h_{12} + qh_{22})(2u^1 h_{11} + qh_2)},$$

which are consistent and define $s(u^1,q)$ explicitly: for the Hamiltonian density (12) one has

$$s(u^1,q) = -\frac{b \operatorname{arctanh}\left(\frac{cu^1}{\sqrt{1+b^2}}\right)}{2\sqrt{1+b^2}} + \frac{b \operatorname{arctanh}\left(\frac{2q(1+b^2-c^2(u^1)^2)^2 - cb(b-cu^1)^2 - cb + 2c^2u^1}{c\sqrt{1+b^2}(1+(b-cu^1)^2)}\right)}{4\sqrt{1+b^2}}$$
$$+ \frac{1}{8}\log[-4cbq(1+b^2) + 4q^2(1+b^2)^2 - 4c^3bq(u^1)^2 + 4c^4q^2(u^1)^4 - c^2 + 8c^2qu^1(1+b^2)(1 - qu^1)].$$

The density (13) leads to

$$s(u^1,q) = \frac{1}{4c}q(u^1+c)^2 + \frac{b}{2}[1 - \log(q(u^1-c)^2 + 2cb)].$$

In the case of (14) one has

$$s(u^1,q) = qu^1 + \frac{1}{8c}q^2(u^1)^4.$$

Finally, the case of (15) gives

$$s(u^1,q) = qu^1 + \frac{1}{8c}q^2;$$

this follows from (24) when $\beta=1, \alpha=-2$.

We point out that the case $\alpha=0$ requires a special treatment: it corresponds to the chains which possess linearly degenerate hydrodynamic reductions. The approach of generating functions does not apply to this class, see, e.g., Ref. 11 for a discussion of a particular example of this type.

VII. CONCLUDING REMARKS

There exists a whole variety of approaches to the classification of integrable Hamiltonian hydrodynamic chains, based on seemingly different requirements, namely:

(1) the vanishing of the Haantjes tensor;
(2) the existence of infinitely many n-component hydrodynamic reductions for any n;
(3) the existence of one "extra" conservation law.
(4) the existence of a generating function for conservation laws.

All examples known to us support the evidence that these approaches are essentially equivalent, leading to the same integrability conditions and classification results. Among others, the approach based on the Haantjes tensor seems to be the most universal, leading to the required integrability conditions in a straightforward way. We emphasize that components of the Haantjes tensor can be calculated using computer algebra. Moreover, the vanishing of the first few components H^1_{jk} is already sufficiently restrictive and implies the identical vanishing of the Haantjes tensor.

It should be pointed out that, at present, there is no hope to *prove* the equivalence of the above listed approaches in the full generality: one first needs a classification of infinite-dimensional Poisson brackets of hydrodynamic type, which is an interesting and nontrivial problem on its own.[14] Some approaches in this direction were outlined recently in Ref. 12.

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An EDS approach to the inverse problem in the calculus of variations

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The inverse problem in the calculus of variations for a given set of second-order ordinary differential equations consists of deciding whether their solutions are those of Euler–Lagrange equations and whether the Lagrangian, if it exists, is unique. This paper discusses the exterior differential systems approach to this problem. In particular, it proposes an algorithmic procedure towards the construction of a certain differential ideal. The emphasis is not so much on obtaining a complete set of integrability conditions for the problem, but rather on producing a minimal set to expedite the differential ideal process. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2358000]

I. INTRODUCTION: THE INVERSE PROBLEM IN THE CALCULUS OF VARIATIONS

The inverse problem in the calculus of variations involves deciding whether for a given system of second-order ordinary differential equations,

$$\ddot{x}^a = F^a(t,x^b\dot{x}^b), \quad a,b = 1,\ldots,n,$$

a so-called multiplier matrix $g_{ab}(t,x^c,\dot{x}^c)$ can be found, such that

$$g_{ab}(\ddot{x}^b - F^b) \equiv \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}^a}\right) - \frac{\partial L}{\partial x^a},$$

for some Lagrangian function $L(t,x^b,\dot{x}^b)$, and to what extent such a multiplier, if it exists, is unique. Necessary and sufficient conditions for the existence of a Lagrangian are generally referred to as the *Helmholtz conditions*, but have been formulated in the literature in a variety of different ways. When regarded as conditions that a nonsingular multiplier must satisfy, a concise description of the Helmholtz conditions was derived by Douglas[6] and later recast in the following form by Sarlet:[14]

$$g_{ab} = g_{ba}, \quad \Gamma(g_{ab}) = g_{ac}\Gamma^c_b + g_{bc}\Gamma^c_a, \quad g_{ac}\Phi^c_b = g_{bc}\Phi^c_a, \quad \frac{\partial g_{ab}}{\partial \dot{x}^c} = \frac{\partial g_{ac}}{\partial \dot{x}^b}, \tag{1}$$

where

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$$\Gamma^a_b := -\frac{1}{2}\frac{\partial F^a}{\partial \dot{x}^b}, \quad \Phi^a_b := -\frac{\partial F^a}{\partial x^b} - \Gamma^c_b\Gamma^a_c - \Gamma(\Gamma^a_b),$$

and where

$$\Gamma := \frac{\partial}{\partial t} + \dot{x}^a\frac{\partial}{\partial x^a} + F^a\frac{\partial}{\partial \dot{x}^a}.$$

Douglas solved this problem for $n=2$ in the sense that he exhaustively classified all second-order ODEs according to the existence and multiplicity of solutions of the Helmholtz conditions. He did this essentially via the Jordan normal forms of the matrix Φ^a_b. The corresponding solution for $n=3$ remains unavailable although various subcases for arbitrary n have been elaborated.[5,15] Our principal purpose in this paper is to explore one of the key aspects in the analysis of the inverse problem using Exterior Differential Systems theory (EDS). The general structure of the EDS approach was set out in Anderson and Thompson,[2] although these authors only examined the case of arbitrary n when Φ is a multiple of the identity. As we will demonstrate, progress using EDS almost certainly relies on explicit use of the Jordan normal forms of Φ. This is the approach taken in the thesis.[1] The aspect that we will examine in detail is the so-called differential ideal step, in which there is an algorithmic search for the largest submodule of a certain module of 2-forms generating a differential ideal. We will explore the relation of this step to the hierarchies of integrability conditions for the Helmholtz conditions known in the literature. Importantly, we will expose the details of this step in the case where Φ is diagonalizable with distinct eigenfunctions. We give a nontrivial, three-dimensional example of the step and the way in which it leads directly to a solution of the Helmholtz conditions. A subsequent paper will deal with the remaining steps in the EDS process, and we will give a complete solution of a whole class of equations in the sense of Douglas.

We now outline the geometrical framework upon which progress over the last two or three decades has depended. In geometric terms, Γ is a second-order vector field (SODE) on the first-jet extension J^1E of a bundle $E\to\mathbb{R}$. For all practical purposes, E can be identified (choosing a "trivialization") with a product manifold $\mathbb{R}\times M$, and then $J^1E\equiv\mathbb{R}\times TM$. We shall denote adapted coordinates on $\mathbb{R}\times TM$ by (t,x^a,u^a) from now on, and use π for the projection $\mathbb{R}\times TM\to\mathbb{R}\times M$.

Every SODE equips $\mathbb{R}\times TM$ with a (nonlinear) connection, the connection coefficients being the functions Γ^a_b just introduced. As a result, an adapted local frame for decomposing arbitrary vector fields on $\mathbb{R}\times TM$ into their "horizontal" and "vertical" parts is given by $\{\Gamma,H_a,V_a\}$, where

$$H_a := \frac{\partial}{\partial x^a} - \Gamma^b_a\frac{\partial}{\partial u^b}, \quad V_a := \frac{\partial}{\partial u^a}.$$

The dual basis of 1-forms is given by $\{dt,\theta^a,\psi^a\}$, with

$$\theta^a := dx^a - u^a\,dt, \quad \psi^a := du^a - F^a\,dt + \Gamma^a_b\theta^b.$$

For a given regular Lagrangian function $L\in C^\infty(J^1E)$, we define the Poincaré-Cartan 1-form θ_L by

$$\theta_{\mathrm{L}} := L\,dt + dL\circ S = L\,dt + \frac{\partial L}{\partial u^a}\theta^a,$$

where $S=V_a\otimes dx^a$ is the vertical endomorphism, and the Euler-Lagrange equations come from the unique SODE, determined by (see, e.g., Goldschmidt and Sternberg[8])

$$i_\Gamma d\theta_{\mathrm{L}} = 0 \quad \text{and} \quad dt(\Gamma) = 1.$$

Inspired by the properties of the Poincaré-Cartan 2-form $d\theta_{\mathrm{L}}$, the following theorem from Ref. 4 gives a geometric version of the Helmholtz conditions.

Theorem 1.1: *Given a* SODE Γ, *the necessary and sufficient conditions for there to be a*

Lagrangian for which Γ *is the Euler-Lagrange field is that there should exist a 2-form* Ω, *of maximal rank, which further has the following properties:* Ω *vanishes on any two vertical vector fields,* $\Gamma \lrcorner \Omega = 0$ *and* $d\Omega = 0$.

Observe that the third and fourth conditions imply that $\mathcal{L}_\Gamma \Omega = 0$, and the first condition means that Ω has a one-dimensional kernel, which, as shown by the third condition, is spanned by Γ. Another important observation is that Ω, which if it exists, will become the Poincaré-Cartan 2-form $d\theta_{\mathrm{L}}$ of the corresponding Lagrangian, then has the following particularly simple representation in the adapted frame $\{dt, \theta^a, \psi^a\}$,

$$d\theta_{\mathrm{L}} = g_{ab}\psi^a \wedge \theta^b, \quad \text{with } g_{ab} = \frac{\partial^2 L}{\partial u^a \, \partial u^b}.$$

There are a number of geometrical ways of expressing this feature, one of which requires a brief discussion of the calculus of vector fields and forms along the projection π (see Ref. 17, or 11 for a slightly different approach).

Vector fields along π are sections of the pullback bundle $\pi^* TE$ over J^1E, and we let $\mathfrak{X}(\pi)$ denote the $C^\infty(J^1E)$ module of such vector fields. Similarly, $\wedge(\pi)$ denotes the graded algebra of forms along π. There is a canonical vector field along π, given by

$$\mathbf{T} := \frac{\partial}{\partial t} + u^a \frac{\partial}{\partial x^a}.$$

The natural bases for $\mathfrak{X}(\pi)$ and $\mathfrak{X}^*(\pi)$ are then $\{\mathbf{T}, \partial/\partial x^a\}$ and $\{dt, \theta^a\}$. We further write $\bar{\mathfrak{X}}(\pi)$ for the elements of $\mathfrak{X}(\pi)$ that have no time component, i.e., $\bar{\mathfrak{X}}(\pi) = \mathrm{Sp}\{\partial/\partial x^a\}$. Then, if

$$X := X^0 \mathbf{T} + X^a \frac{\partial}{\partial x^a}$$

is an arbitrary vector field along π, its horizontal and vertical lift give vector fields on J^1E, respectively, given by

$$X^H := X^0 \Gamma + X^a H_a, \quad X^V := X^a V_a.$$

In what follows, we will almost exclusively have to deal with horizontal and vertical lifts of vector fields along π that belong to the submodule $\bar{\mathfrak{X}}(\pi)$. So, in referring to vector fields on J^1E of the form $X^V, Y^H, \ldots$, it will be understood that $X, Y, \ldots$, belong to $\bar{\mathfrak{X}}(\pi)$. This is important, because it means that all the essential formulas are formally those of the time-independent calculus developed in Refs. 12 and 13, rather than the corresponding ones in Ref. 17. In particular, we will frequently use the commutator relations:

$$[X^V, Y^V] = (\mathrm{D}_X^V Y - \mathrm{D}_Y^V X)^V,$$

$$[X^H, Y^V] = (\mathrm{D}_X^H Y)^V - (\mathrm{D}_Y^V X)^H,$$

$$[X^H, Y^H] = (\mathrm{D}_X^H Y - \mathrm{D}_Y^H X)^H + R(X, Y)^V.$$

Here, D_X^V and D_X^H, the vertical and horizontal covariant derivative operators, are degree zero derivations on scalar and vector-valued forms along π, determined by $\mathrm{D}_X^H F = X^H(F)$, $\mathrm{D}_X^V F = X^V(F)$ for their action on functions $F \in C^\infty(J^1E)$:

$$\mathrm{D}_X^H \frac{\partial}{\partial x^a} = X^b \Gamma^c_{ba} \frac{\partial}{\partial x^c}, \quad \mathrm{D}_X^V \frac{\partial}{\partial x^a} = 0$$

(with $\Gamma^c_{ba} = \partial \Gamma^c_a / \partial u^b$), gives the action on $\bar{\mathfrak{X}}(\pi)$ and the standard duality rules give the action on 1-forms along π. The vector-valued 2-form R along π represents the curvature of the SODE connection with coordinate form,

$$R = \tfrac{1}{2} R^a_{bc} \theta^b \wedge \theta^c \otimes \frac{\partial}{\partial x^a}, \quad R^a_{bc} := H_c(\Gamma^a_b) - H_b(\Gamma^a_c).$$

We do not distinguish notationally the contact forms θ^a, as forms on J^1E from their counterparts along π. In fact, there is a dual process of lifting 1-forms along π giving (with an obvious slight abuse of notation),

$$\theta^{aH} = \theta^a, \quad \theta^{aV} = \psi^a.$$

The dynamical covariant derivative $\boldsymbol{\nabla}$ and the Jacobi endomorphism Φ that appear in (1) arise naturally through the following formulas:

$$[\Gamma, X^V] = -X^H + (\boldsymbol{\nabla} X)^V, \quad [\Gamma, X^H] = (\boldsymbol{\nabla} X)^H + \Phi(X)^V.$$

In coordinates,

$$\Phi = \Phi^a_b \frac{\partial}{\partial x^a} \otimes \theta^b,$$

with Φ^a_b as defined before, whereas $\boldsymbol{\nabla}$, defined to vanish on $\mathbf{T}$ and dually on dt, acts on $\bar{\mathfrak{X}}(\pi)$ (with dual action on contact forms) by

$$\boldsymbol{\nabla} F = \Gamma(F) \text{ on functions}, \quad \boldsymbol{\nabla} \frac{\partial}{\partial x^a} = \Gamma^b_a \frac{\partial}{\partial x^b}, \quad \boldsymbol{\nabla} \theta^a = -\Gamma^a_b \theta^b.$$

Now we can give the link we wanted between the geometric Helmholtz conditions of Theorem 1.1 with their coordinate form in (1). The observation we made about the simple structure of $d\theta_L$ in the adapted coframe means that the 2-form Ω on J^1E of Theorem 1.1 that we seek is completely determined by a symmetric type (0,2) tensor along π, of the form $g = g_{ab} \theta^a \otimes \theta^b$ (i.e., g vanishes on $\mathbf{T}$). To be precise, Ω is the so-called Kähler lift of g, $\Omega = g^K$, which vanishes on Γ and further is defined by

$$g^K(X^V, Y^V) = g^K(X^H, Y^H) = 0, \quad g^K(X^V, Y^H) = g(X, Y).$$

The intrinsic formulation of the conditions (1) (see Ref. 17, or 13 for the autonomous case) then reads as

$$\boldsymbol{\nabla} g = 0, \quad g(\Phi X, Y) = g(X, \Phi Y), \quad \mathrm{D}^V_X g(Y, Z) = \mathrm{D}^V_Y g(X, Z). \tag{2}$$

In the next section we briefly sketch the ideas of the exterior differential systems approach, specifically in the context of the inverse problem, and we identify our objectives concerning the construction of a differential ideal containing all possible two forms Ω.

II. EDS AND THE INVERSE PROBLEM

The inverse problem involves the search for a closed 2-form and so lends itself to analysis by EDS. For a general reference to EDS, we refer to Ref. 3. A thorough analysis of the inverse problem by means of such techniques (at least for autonomous differential equations) can be found in the work of Grifone and Muzsnay,[9,10] where the approach, however, starts from the partial differential equations that the Lagrangian itself has to satisfy, rather than equations such as (1) for the multiplier.

Anderson and Thompson in Ref. 2 describe the three components of the EDS process: finding a differential ideal, setting up a Pfaffian system for finding the closed 2-forms within that ideal, and finally analyzing this system, following the Cartan-Kähler theory to determine the generality of the solution (if any). We limit ourselves to a brief synopsis of the reasoning that underlies the first two steps here, with particular emphasis on the new elements involving the eigenspectrum of Φ that we want to bring to the differential ideal construction.

Given a SODE Γ, we know that the 2-form Ω we are looking for is going to be the Kähler lift of a symmetric $(0,2)$-tensor field g along the projection, i.e., $g=g_{ab}\theta^a\otimes\theta^b$, $g_{ab}=g_{ba}$. So we start by considering on J^1E the module Σ^0 of such Kähler lifts: intrinsically, ω belongs to Σ^0, if and only if

$$i_\Gamma\omega=0, \tag{3}$$

$$\omega(X^V,Y^V)=\omega(X^H,Y^H)=0, \tag{4}$$

$$\omega(X^V,Y^H)=\omega(Y^V,X^H). \tag{5}$$

(During the EDS process we will use lower case ω as the generic name for our 2-forms, reserving Ω for the 2-form of Theorem 1.1.) In coordinates, Σ^0 is spanned by the 2-forms

$$\omega^{ab}:=\frac{1}{2}(\psi^a\wedge\theta^b+\psi^b\wedge\theta^a). \tag{6}$$

Note however, that $\{dt,\theta^a,\psi^a\}$ may as well be any basis comprising of dt, n horizontal forms, and n vertical forms. In fact later we will use such a basis made up of the eigenforms of Φ.

The first step in the EDS approach produces from Σ^0 a sequence of submodules $\Sigma^0\supset\Sigma^1\supset\Sigma^2\supset\cdots$, arriving finally (or not at all) at a nontrivial submodule $\Sigma^l=\mathrm{Sp}\{\omega^k\}$ generating a differential ideal. Obtaining Σ^l consists of computing at each stage the exterior derivative of forms belonging to the submodule under consideration, and verifying whether they belong to the ideal generated by that submodule. In principle, whenever an obstruction is found, it is translated into a further restriction on the admissible 2-forms and the process is restarted from there. We shall be more specific about this in a moment. But, for the time being, assume that we have found $\Sigma^l=\mathrm{Sp}\{\omega^1,\ldots,\omega^d\}$, so that

$$d\omega^k=\xi^k_h\wedge\omega^h,\quad k=1,\ldots,d,$$

for some 1-forms ξ^k_h. In order to construct a closed 2-form in Σ^l we first identify a basis of d-tuples of 1-forms ρ^A_h such that $\rho^A_h\wedge\omega^h=0$. Then, if $r_k\omega^k\in\Sigma^l$ is required to be closed, the functions r_k must solve the Pfaffian system of equations (the notations are taken to conform with those in Ref. 2),

$$dr_k+r_h\xi^h_k+p_A\rho^A_k=0, \tag{7}$$

for some as yet arbitrary functions p_A. The freedom in the choice of p_A must then be exploited in the final part of the EDS procedure. This last part is by no means a straightforward matter; in fact, it is fair to say that it consists of several steps still and may even, if the involutivity test fails, lead to prolonging the system and starting again (see, e.g., Ref. 2 for a brief survey). We will argue in the final section that it may be better, therefore, to address the partial differential equations of the inverse problem in a more direct way, once the differential ideal procedure is complete. Our approach to specific examples should be contrasted with that of Anderson and Thompson,[2] who follow the formal EDS process.

Here are the details of the differential ideal process. At each step Σ^i, say, we will first identify the requirements for a 3-form ρ to be in $\langle\Sigma^i\rangle$, the ideal generated by Σ^i, because a large part of such an analysis does not depend on whether or not $\rho=d\omega\in\langle\Sigma^i\rangle$. Once we apply these requirements to such $d\omega$, the general formula,

$$d\omega(U,V,W) = \sum_{U,V,W} [U(\omega(V,W)) - \omega([U,V],W)], \tag{8}$$

(where a notation like $\Sigma_{\xi,\eta,\zeta}$ will always refer to a cyclic sum over the indicated arguments), produces algebraic restrictions on admissible 2-forms. If these are different from those already implemented, they are used to define the next submodule Σ^{i+1} in the sequence. But a couple of important remarks are in order here. First of all, the issue of algebraic conditions in the inverse problem is quite delicate. There are several infinite hierarchies of such conditions (see, e.g., Refs. 9 and 10), but it is impossible to tell in all generality which of these are more important, from which others possibly might follow, or simply which are more efficient in determining the existence or nonexistence of a multiplier. We therefore propose to integrate the decision about the usefulness of algebraic restrictions as much as possible into this differential ideal algorithm. That is to say, we shall attempt to obtain at each step in restricting to a submodule Σ^i, conditions for a 3-form ρ to belong to $\langle\Sigma^i\rangle$ which are both necessary and sufficient. It is, to some extent, the degree to which fresh conditions tend to be sufficient, which will guide the decision about the selection of further restrictions for defining the next submodule. It is precisely in this way that we will be able to push the EDS procedure beyond the level of results obtained in Ref. 2. However, as has always been the case in the study of the multiplier problem, there is no possibility of a general solution for an arbitrary dimension. At some point further progress relies on a classification of cases and subcases. Most notorious in this respect is the paper by Douglas[6] (see Ref. 16 for a geometrical account of Douglas' analysis). We should expect this to occur also in our current attempt.

III. THE FIRST STEP IN THE EDS ALGORITHM

Consider the module Σ^0, defined above, and let ρ be a 3-form in $\langle\Sigma^0\rangle$, so that $\rho=\beta_k\wedge\omega^k$ for some 1-forms β_k and $\omega^k\in\Sigma^0$. Then $i_\Gamma\rho=\beta_k(\Gamma)\omega^k$, so that $i_\Gamma\rho$ belongs to Σ^0 *if and only if*

$$\rho(\Gamma,X^V,Y^V) = 0, \tag{9}$$

$$\rho(\Gamma,X^H,Y^H) = 0, \tag{10}$$

$$\rho(\Gamma,X^V,Y^H) = \rho(\Gamma,Y^V,X^H). \tag{11}$$

Next, starting from the contraction of ρ with a vertical vector field,

$$i_{X^V}\rho = \beta_k(X^V)\omega^k - \beta_k\wedge i_{X^V}\omega^k,$$

we must have

$$\rho(X^V,Y^V,Z^V) = 0, \tag{12}$$

but how can we take other restrictions on Σ^0 into account, when further combinations of horizontal and vertical vector fields are inserted? For example, we can manipulate the right-hand side by using the properties of $\omega^k\in\Sigma^0$, until every appearance of the β_k has been eliminated and a condition about ρ emerges. We have

$$\begin{aligned}\rho(X^V,Y^V,Z^H) &= \beta_k(X^V)\omega^k(Y^V,Z^H) - \beta_k(Y^V)\omega^k(X^V,Z^H) = \beta_k(X^V)\omega^k(Z^V,Y^H) - \beta_k(Y^V)\omega^k(Z^V,X^H)\\ &= \rho(X^V,Z^V,Y^H) + \beta_k(Z^V)\omega^k(X^V,Y^H) - \beta_k(Y^V)\omega^k(Z^V,X^H) = \rho(X^V,Z^V,Y^H)\\ &\quad + \beta_k(Z^V)\omega^k(Y^V,X^H) - \beta_k(Y^V)\omega^k(Z^V,X^H) = \rho(X^V,Z^V,Y^H) + \rho(Z^V,Y^V,X^H).\end{aligned}$$

So it follows that ρ should satisfy

$$\sum_{X,Y,Z} \rho(X^V,Y^V,Z^H) = 0, \tag{13}$$

and in exactly the same way also

$$\sum_{X,Y,Z} \rho(X^V, Y^H, Z^H) = 0. \tag{14}$$

There remains the condition

$$\rho(X^H, Y^H, Z^H) = 0. \tag{15}$$

Details such as the way the cyclic sum condition (13) is obtained will not be repeated further on.

In total, we have obtained seven necessary conditions and, following the strategy deployed in the previous section, we now explore their sufficiency. But before we proceed, we remark that a number of the conditions to be encountered here, and in the subsequent sections, only have an effect when the number n of degrees of freedom of the system is at least 3. This is the case, for example, with the conditions (12) to (15), which are clearly void when $n=2$. As a result, each time a question of the sufficiency of conditions arises, we will say a few words about the case $n=2$. Besides, the case $n=2$ has been extensively studied already (see Refs. 6, 10, and 16) and therefore is not of prime interest for this paper.

Proposition 3.1: For an arbitrary 3-form ρ to belong to the ideal $\langle \Sigma^0 \rangle$, it is necessary and sufficient that ρ satisfies the conditions (9)–(15), where X, Y, Z are arbitrary vector fields along π.

Proof: It is easy to see that conditions (9)–(11) imply that ρ is of the form

$$\rho = dt \wedge \sigma + \bar{\rho}, \quad \text{with } \sigma \in \Sigma^0 \quad \text{and} \quad i_\Gamma \bar{\rho} = 0.$$

For $n \geq 3$, the remaining conditions then indicate that $\bar{\rho}$ is of the form

$$\bar{\rho} = \tfrac{1}{2} \mathcal{A}_{abc} \theta^a \wedge \psi^b \wedge \psi^c + \tfrac{1}{2} \mathcal{B}_{abc} \psi^a \wedge \theta^b \wedge \theta^c,$$

where $\mathcal{A}_{abc}$ and $\mathcal{B}_{abc}$ are skew-symmetric in their last two indices and satisfy [in view of (13) and (14)]

$$\sum_{abc} \mathcal{A}_{abc} = \sum_{abc} \mathcal{B}_{abc} = 0.$$

For $n=2$, $i_\Gamma \bar{\rho}=0$ is already enough to ensure that $\bar{\rho}$ is of the above form, but with two of the three indices the same. The skew symmetry of the coefficients in their last two indices then implies that they formally can be regarded as having this cyclic sum property as well.

The skew symmetry $\mathcal{A}_{abc}=-\mathcal{A}_{acb}$ and the cyclic sum property $\Sigma_{abc}\mathcal{A}_{abc}=0$ imply that

$$\begin{aligned}
\mathcal{A}_{abc} \theta^a \wedge \psi^b \wedge \psi^c &= \tfrac{1}{3} (\mathcal{A}_{abc} \theta^a \wedge \psi^b \wedge \psi^c + \mathcal{A}_{bca} \theta^b \wedge \psi^c \wedge \psi^a + \mathcal{A}_{cab} \theta^c \wedge \psi^a \wedge \psi^b) \\
&= \tfrac{1}{3} \mathcal{A}_{abc} (\psi^c \wedge \theta^a + \psi^a \wedge \theta^c) \wedge \psi^b - \tfrac{1}{3} \mathcal{A}_{bca} (\psi^c \wedge \theta^b + \psi^b \wedge \theta^c) \wedge \psi^a \\
&= -\tfrac{4}{3} \mathcal{A}_{abc} \omega^{ab} \wedge \psi^c,
\end{aligned}$$

where we have used the skew symmetry in the first and the cyclic sum property in the last term for the transition from the first to the second line. The same is also true for the other term in $\bar{\rho}$, so

$$\rho = dt \wedge \sigma - \tfrac{2}{3} \mathcal{A}_{abc} \omega^{ab} \wedge \psi^c + \tfrac{2}{3} \mathcal{B}_{abc} \omega^{ab} \wedge \theta^c, \tag{16}$$

or putting

$$A_{abc} = \mathcal{A}_{abc} + \mathcal{A}_{bac}, \quad B_{abc} = \mathcal{B}_{abc} + \mathcal{B}_{bac},$$

$$\rho = dt \wedge \sigma - \tfrac{1}{3} A_{abc} \omega^{ab} \wedge \psi^c + \tfrac{1}{3} B_{abc} \omega^{ab} \wedge \theta^c, \tag{17}$$

where the new coefficients now are symmetric in their first two indices and still have the cyclic sum property $\Sigma_{abc}A_{abc}=\Sigma_{abc}B_{abc}=0$. This manifestly exhibits that ρ belongs to $\langle \Sigma^0 \rangle$. □

Remark: An expression like $A_{abc}\omega^{ab} \wedge \psi^c$ with $A_{abc}=A_{bac}$ clearly belongs to $\langle \Sigma^0 \rangle$ without any further requirements. That the above necessary and sufficient conditions are not contradictory,

however, follows from the fact that one can assume that the coefficients further have the cyclic sum property without loss of generality. Verifying this is left to the reader.

From now on we will use the representation (17) of ρ.

To terminate the first step now, we apply the *necessary and sufficient conditions* (9)–(15) to an exact 3-form $d\omega$, for any $\omega \in \Sigma^0$ and use thereby the familiar identity (8). In doing that, only the second part that involves the Lie brackets can contribute; the list of bracket relations that are frequently used in these calculations has been given in Sec. I. It easily follows then that the conditions (9) and (11)–(14) are identically satisfied, whereas the remaining conditions (10) and (15) give rise to the following extra restrictions on admissible 2-forms (which are, in one form or another, well known in the literature):

$$\omega((\Phi X)^V, Y^H) = \omega((\Phi Y)^V, X^H), \tag{18}$$

$$\sum_{X,Y,Z} \omega(R(X,Y)^V, Z^H) = 0. \tag{19}$$

We could implement both of these new requirements to define the next submodule Σ^1, but it will be more convenient to continue in stages and start by implementing the Φ condition (18) only.

The first step has identified the structure of 3-forms in $\langle\Sigma^0\rangle$. When we apply the differential ideal algorithm to Σ^0 now, conditions on ρ that have Γ as one of the arguments will be easy to handle and merely impose that the 2-form σ in (17) belongs to the submodule under consideration. Other conditions must clearly come in pairs: for each condition that has two vertical and one horizontal argument and thus has an effect on the A part in ρ only, there will be a corresponding condition that has the "mirror" effect on the B part. The underlying reason for that is the basic symmetry property (5) of 2-forms in Σ^0, which makes that a condition like (18), for example, can equivalently be written in the form

$$\omega((\Phi X)^H, Y^V) = \omega((\Phi Y)^H, X^V). \tag{20}$$

Bearing this in mind avoids unnecessary duplications of conditions later on.

Finally, we examine the necessary and sufficient conditions that $\langle\Sigma^0\rangle$ is itself a differential ideal.

Theorem 3.2: *The module* Σ^0 *generates a differential ideal if and only* Φ *is a multiple of the identity*.

Proof: From the immediately preceding discussion, it follows that $\langle\Sigma^0\rangle$ is a differential ideal if and only if (18) and (19) are satisfied by all $\omega \in \Sigma^0$. If Φ is a multiple of the identity, the first of these is satisfied because of (5), and the second is true by virtue of the identity $V_a(\Phi^c_b) - V_b(\Phi^c_a) = 3R^c_{ab}$. Conversely, if (18) is true for all $\omega \in \Sigma^0$, then it is true for all ω^{ab} given by (6): using $X = \partial/\partial x^c$, $Y = \partial/\partial x^d$ yields

$$\Phi^a_c \delta^b_d + \Phi^b_c \delta^a_d = \Phi^a_d \delta^b_c + \Phi^b_d \delta^a_c.$$

Hence, $\Phi = \mu I$ and (19) follows automatically, again because of the stated identity. □

This is a stronger result than that obtained by Anderson and Thompson in Ref. 2, where it was shown that if Φ is a multiple of the identity then $\langle\Sigma^0\rangle$ is a differential ideal. Anderson and Thompson demonstrated that in this case the system is variational. However, in general there remain obstructions to variationality after a differential ideal has been obtained.

IV. A SECOND STEP IN THE PROCESS

We define Σ^1 to be the submodule of Σ^0 whose elements satisfy condition (18).

Let $\rho = \beta_k \wedge \omega^k$ be a 3-form in $\langle\Sigma^1\rangle$. Then, a contraction with Γ leads to the further restriction

$$\rho(\Gamma,(\Phi X)^V,Y^H)=\rho(\Gamma,(\Phi Y)^V,X^H), \tag{21}$$

which, as indicated before, says that σ in (17) must be in Σ^1 and plays further no role. When we take X^V as the first argument and follow the procedure that led to (13), but this time with $(\Phi Y)^V,Z^H$ as a further argument, we obtain

$$\sum_{X,Y,Z}(\rho(X^V,(\Phi Y)^V,Z^H)-\rho(X^V,(\Phi Z)^V,Y^H))=0.$$

But the left-hand side is $\Sigma_{X,Y,Z}(\rho(X^V,(\Phi Y)^V,Z^H)+\rho((\Phi Y)^V,Z^V,X^H))$ and then (13) gives the more transparent version

$$\sum_{X,Y,Z}\rho(X^V,Y^V,(\Phi Z)^H)=0. \tag{22}$$

Immediately we conclude that the "mirror" condition, which can, of course, independently be derived, will read as

$$\sum_{X,Y,Z}\rho(X^H,Y^H,(\Phi Z)^V)=0. \tag{23}$$

Unfortunately, this is not the end of the line, as there are other possible combinations of terms. For example, with $(\Phi X)^V$ as a first argument, rather than X^V,

$$i_{(\Phi X)^V}\rho=\beta_k((\Phi X)^V)\omega^k-\beta_k\wedge i_{(\Phi X)^V}\omega^k,$$

we can choose $(\Phi Y)^V,Z^H$ as second and third arguments. The by now familiar procedure of eliminating all terms involving the 1-forms β_k then leads to the new requirement

$$\sum_{X,Y,Z}\rho((\Phi X)^V,(\Phi Y)^V,Z^H)=0, \tag{24}$$

and its counterpart

$$\sum_{X,Y,Z}\rho((\Phi X)^H,(\Phi Y)^H,Z^V)=0. \tag{25}$$

We already reach a point here where it is difficult to say whether all such necessary conditions will generically be independent or whether perhaps there are still other ways of producing more conditions; hence our strategy to approximate, as best as possible, conditions that are also sufficient and demonstrate their utility in this way. So let us address the sufficiency question here.

Let ρ be of the form (17), where the A and B coefficients are symmetric in their first two indices and can, as argued before, without loss of generality be assumed to have the cyclic sum property $\Sigma_{abc}A_{abc}=\Sigma_{abc}B_{abc}=0$. The two conditions (22) and (24) affect only the A-term (23) and (25) will have the same sort of effect on the B term. Using a basis of horizontal and vertical vector fields, (H_i,V_j) say, we can compute the A-term of ρ acting on the triple $(V_r,V_t,\Phi_s^uH_u)$ and then take a cyclic sum over the indices (r,s,t). What remains (leaving out a numerical factor) is the following condition:

$$\sum_{rst}(A_{rut}-A_{tur})\Phi_s^u=0, \tag{26}$$

which, by recombining terms, can equivalently be written in the perhaps more appealing form

$$\sum_{rst}(A_{rut}\Phi_s^u-A_{sut}\Phi_r^u)=0. \tag{27}$$

Similarly, evaluating $\rho((\Phi X)^V,(\Phi Y)^V,Z^H)$ on $(\Phi_s^uV_u,\Phi_t^vV_v,H_r)$ and then taking the cyclic sum, the condition (24) is found to mean:

$$\sum_{rst} (A_{ruv} - A_{rvu})\Phi^u_s \Phi^v_t = 0. \tag{28}$$

Now, the 2-forms in Σ^1 we are talking about are of the form

$$\omega = h_{ab}\omega^{ab}, \quad \text{with} \quad h_{su}\Phi^u_r - h_{ru}\Phi^u_s = 0 \tag{29}$$

[we purposely avoid using g_{ab}, which we reserve for candidate multipliers satisfying (1)]. So the idea would be to prove that the requirements (26) [or (27)] and (28) force the functions A_{abc} to be of the form

$$A_{abc} = h_{ab}{}^k\, b_{kc}, \tag{30}$$

where, for each k, the $h_{ab}{}^k$ have the property (29) and the b_{kc} are arbitrary functions, representing the components of the 1-forms β_k in an expression like $\rho = \beta_k \wedge \omega^k$. Unfortunately, we were unable to prove that this is true in all generality, but we shall show now that it is a valid statement in an interesting (reasonably generic) special case.

As we know already from Douglas,[6] a classification into different cases where a multiplier g_{ab} for a given dynamics Γ does or does not exist, will largely be governed by properties of the Jacobi endomorphism Φ associated with Γ. A specific assumption about Φ that comes up in several situations (see, e.g., Ref. 5) is that of (algebraic) diagonalizability. So let us assume this, and that the (real) eigenvalues $\lambda_{(a)}$ are distinct, and let $\{\phi^a\}$ denote a complete set of eigenforms of Φ, so that

$$\Phi(\phi^a) = \lambda_{(a)}\phi^a \quad \text{(no sum)}.$$

These ϕ^a can be taken to be combinations of contact forms and are of course still semi-basic forms. We now have a new basis for $\mathfrak{X}(J^1E)$, namely $\{dt, \phi^{aH}, \phi^{aV}\}$ and new spanning 2-forms for Σ^0, namely,

$$\phi^{ab} := \tfrac{1}{2}(\phi^{aV} \wedge \phi^{bH} + \phi^{bV} \wedge \phi^{aH}).$$

It is important to realize that with this change of basis, nothing changes in our considerations of the first differential ideal step. For example, the 2-forms in Σ^0 are now of the form $\bar{h}_{ab}\phi^{ab}$ and 3-forms in the ideal $\langle\Sigma^0\rangle$ are of the form (17), with the ϕ^{aH} replacing the θ^a, and so on. Explicitly,

$$\rho = dt \wedge \sigma - \tfrac{1}{3}\bar{A}_{abc}\phi^{ab} \wedge \phi^{cV} + \tfrac{1}{3}\bar{B}_{abc}\phi^{ab} \wedge \phi^{cH}.$$

We will freely use the original basis formulas in the eigenform basis (and refer to their equation numbers) just by adding overbars and switching θ^a for ϕ^{aH} etc.

The additional restriction (18) that defines Σ^1, or equivalently (29), reduces to

$$(\lambda_{(b)} - \lambda_{(a)})\bar{h}_{ab} = 0, \tag{31}$$

and hence implies that the elements of Σ^1 must be diagonal in the eigenform basis, i.e., $\bar{h}_{ab}=0$ for $a \neq b$.

Proportion 4.1: Suppose that Φ *is diagonalizable with distinct (real) eigenvalues. Then, the necessary and sufficient conditions for a 3-form* ρ *to be in the ideal* $\langle\Sigma^1\rangle$ *are the conditions to be in* $\langle\Sigma^0\rangle$, *supplemented by* (21), (22), and (24), together with their counterparts (23) and (25).

Proof: What has to be proved is the sufficiency of the conditions. Using the eigenform basis of Φ, we already know that $\rho \in \langle\Sigma^0\rangle$ implies that it is of the form (17). The first extra condition (21) requires σ to belong to the smaller module Σ^1 now. As explained before, it suffices to study the effect of (22) and (24), or explicitly (26) and (28), on the A term in ρ. Under the present circumstances, this leads to the conditions

$$\sum_{abc} \bar{A}_{abc}(\lambda_{(a)} - \lambda_{(b)}) = 0, \tag{32}$$

$$\sum_{abc} \bar{A}_{abc}\lambda_{(c)}(\lambda_{(a)} - \lambda_{(b)}) = 0. \tag{33}$$

These conditions are identically satisfied whenever two of the indices are the same, so we begin by considering $n \geq 3$. For each set of three distinct indices, they produce, together with the given cyclic sum property, a homogeneous system of algebraic equations with coefficient matrix

$$\begin{pmatrix} 1 & 1 & 1 \\ \lambda_{(a)} - \lambda_{(b)} & \lambda_{(b)} - \lambda_{(c)} & \lambda_{(c)} - \lambda_{(a)} \\ \lambda_{(c)}(\lambda_{(a)} - \lambda_{(b)}) & \lambda_{(a)}(\lambda_{(b)} - \lambda_{(c)}) & \lambda_{(b)}(\lambda_{(c)} - \lambda_{(a)}) \end{pmatrix}.$$

The determinant of this matrix is proportional to $(\lambda_{(a)}-\lambda_{(b)})(\lambda_{(b)}-\lambda_{(c)})(\lambda_{(c)}-\lambda_{(a)})$ and hence is nonzero. Therefore, all $\bar{A}_{abc}$ with distinct indices must be zero. It further follows from the cyclic sum property that $\bar{A}_{aab}=-2\bar{A}_{baa}$. With these data, the A term of ρ becomes

$$\begin{aligned} -\tfrac{1}{3}\bar{A}_{abc}\phi^{ab} \wedge \phi^{cV} &= -\tfrac{1}{3}\left(\sum_{a\neq b} \bar{A}_{aab}\phi^{aa} \wedge \phi^{bV} + 2\sum_{a\neq b} \bar{A}_{baa}\phi^{ab} \wedge \phi^{aV} \right) \\ &= -\tfrac{1}{3}\left(\sum_{a\neq b} \bar{A}_{aab}\phi^{aa} \wedge \phi^{bV} - \sum_{a\neq b} \bar{A}_{aab}\phi^{ab} \wedge \phi^{aV} \right) = -\tfrac{1}{2}\sum_{a\neq b} \bar{A}_{aab}\phi^{aa} \wedge \phi^{bV}, \end{aligned}$$

where we have used the fact that $\phi^{ab}\wedge\phi^{aV}=-\frac{1}{2}\phi^{aa}\wedge\phi^{bV}$. But we know from (31) that the 2-forms in Σ^1 are diagonal in the basis of eigenforms, i.e., of the form $\bar{h}_{aa}\phi^{aa}$, and the above computation then shows that the A term of ρ is manifestly in $\langle\Sigma^1\rangle$. The effect of (23) and (25) on the B term is similar.

When $n=2$, only the condition (21) survives and implies as before that σ must belong to Σ^1. Moreover, it is easy to verify explicitly that for $n=2$, the $\bar{\rho}$ part of our 3-form in $\langle\Sigma^0\rangle$ automatically belongs to $\langle\Sigma^1\rangle$ as well, so the general claim is still valid. □

We now return once more to the general case with no assumptions about Φ. The final stage in our step 2 procedure is to apply the conditions on 3-forms again to the special case of exact 3-forms. This will determine possibly new restrictions on admissible 2-forms, which can then be used to identify further submodules. The computation related to condition (21) is straightforward and produces the new requirement,

$$\omega((\nabla\Phi(X))^V, Y^H) = \omega((\nabla\Phi(Y))^V, X^H), \tag{34}$$

When (22) is imposed on a 3-form $d\omega$, it merely reproduces the condition (19) we already have, in view of the general identity [see Ref. 13, remembering always that we are restricting to vector fields in $\bar{\mathfrak{X}}(\pi)$]

$$3R(X,Y) = D^V_X\Phi(Y) - D^V_Y\Phi(X). \tag{35}$$

But its counterpart (23) gives rise to the new condition,

$$\sum_{X,Y,Z} \omega(\nabla R(X,Y)^V, Z^H) = 0, \tag{36}$$

because we also have the identity

$$\nabla R(X,Y) = D^H_X\Phi(Y) - D^H_Y\Phi(X). \tag{37}$$

The computations for (24) and (25) run parallel and produce the following new requirements

$$\sum_{X,Y,Z} \omega((D^V_{\Phi X}\Phi(Y) - D^V_{\Phi Y}\Phi(X))^V, Z^H) = 0, \tag{38}$$

$$\sum_{X,Y,Z} \omega((D^H_{\Phi X}\Phi(Y) - D^H_{\Phi Y}\Phi(X))H, Z^V) = 0. \tag{39}$$

Conditions such as (34) and (36) are well known in the literature. It was pointed out in Ref. 14 that such conditions must hold for arbitrary ∇ derivatives of Φ and R and it is not difficult to see how this double hierarchy will emerge in the EDS process also, simply from the restrictions on ρ which have Γ in their arguments and will be produced step by step.

The conditions (38) and (39), however, have only been reported in the thesis[1] (though they must be related in some sense to requirements involving the Nijenhuis tensor of Φ in the approach adopted in Ref. 10). It is impossible to say in all generality which of the many algebraic restrictions are somehow the "more independent ones," but the message from our current algorithmic analysis is that it is likely to be more efficient in applications to impose the last mentioned requirements on admissible 2-forms first, before extracting all information, for example, from the double infinite hierarchy of $\nabla^k\Phi$ and $\nabla^k R$ conditions, which were the only conditions taken into consideration in Ref. 15.

But we must not yet embark on using any of these conditions to define a further submodule, as we have only dealt with half of the information that came out of the first step so far. We shall study the curvature condition (19) in the next section, but for the sake of applications it is worthwhile summing up what we now know about the termination of the differential ideal process at this level.

Proportion 4.2: Assume that Φ *is diagonalizable with distinct (real) eigenvalues. Then the necessary and sufficient conditions for* Σ^1 *to generate a differential ideal are that all 2-forms of the form* (29) *satisfy the algebraic conditions* (19), (34), (36), (38), and (39).

Proof: 2-forms in Σ^1 are characterized by (29). If Φ is diagonalizable, the necessary and sufficient conditions for their exterior derivative to belong to $\langle\Sigma^1\rangle$ (as identified by Proposition 4.1 and the subsequent analysis) are that they satisfy the supplementary restrictions (19), (34), (36), (38), and (39). But saying that Σ^1 generates a differential ideal already is the same as saying *that no further restrictions beyond those defining* Σ^1 *should be found* and thus that the five conditions just mentioned must hold for all 2-forms in Σ^1. □

Remark: as we observed in the proof of Proposition 4.1, only one of the five extra conditions survives when $n=2$ and this condition translates to the $\nabla\Phi$ condition (34) when applied to the exterior derivative of a 2-form in Σ^1. This is, therefore, the only condition to take into account when applying the above proposition to the case $n=2$.

V. A FURTHER STEP FOR DIAGONALIZABLE Φ

We return again to the general situation without assuming that Φ is diagonalizable. Define Σ^2 to be the module of 2-forms in Σ^1, which further satisfy the condition (19).

As before, if $\rho=\beta_k\wedge\omega^k$ is a 3-form in $\langle\Sigma^2\rangle$, a contraction with Γ, in view of (19), leads to the further restriction

$$\sum_{X,Y,Z} \rho(\Gamma, R(X,Y)^V, Z^H) = 0. \tag{40}$$

Likewise, when we contract first with an arbitrary vertical element and then proceed to eliminate all terms involving the β_k, a procedure that is more involved here (but we leave the details to the reader), the condition we obtain reads as

$$\sum_{X,Y,Z,U}^{e} \rho(X^V, R(Y,Z)^V, U^H) = 0, \tag{41}$$

where the upper index in the summation sign is meant to indicate that the sum extends over all even permutations of the indicated vector fields. Needless to say, there will be a mirror condition that can independently be derived, and reads as

$$\sum_{X,Y,Z,U}^{e} \rho(X^H, R(Y,Z)^H, U^V) = 0. \tag{42}$$

Obviously there are more possibilities as in the preceding section. For example, repeating the above computation, but with $(\Phi X)^V$ as first argument, rather than X^V, gives

$$\sum_{X,Y,Z,U}^{e} \rho((\Phi X)^V, R(Y,Z)^V, U^H) = 0, \tag{43}$$

and its analog with two horizontal and one vertical elements.

Once again, we have to try and find necessary conditions that are also sufficient for 3-forms to belong to $\langle \Sigma^2 \rangle$. Should we, for example, search for a condition also with two R-arguments in it? To begin with, here is a further infinite number of necessary conditions for ρ to be in $\langle \Sigma^2 \rangle$.

Lemma 5.1: Necessary conditions for a 3-form ρ to belong to $\langle \Sigma^2 \rangle$ are that

$$\sum_{X,Y,Z,U}^{e} \rho((\Phi^m X)^V, R(Y,Z)^V, U^H) = 0, \tag{44}$$

for all m.

Proof: Observe first that 2-forms that have the symmetry property (5) and satisfy (18), automatically also satisfy

$$\omega((\Phi^m X)^V, Y^H) = \omega((\Phi^m Y)^V, X^H), \tag{45}$$

for all m. Indeed, using successively the properties (18), (20), and (5), we have

$$\omega((\Phi^2 X)^V, Y^H) = \omega((\Phi Y)^V, (\Phi X)^H) = \omega(X^V, (\Phi^2 Y)^H) = \omega((\Phi^2 Y)^V, X^H).$$

The statement for general m follows by induction.

Replacing now ΦX by $\Phi^m X$ in the considerations that lead to (43), it is fairly straightforward to verify that we will arrive at (44) in view of (45). □

When a 2-form ω is in Σ^1 and so has the symmetry property (18) with respect to Φ, it makes no sense to impose symmetry with respect to powers Φ^m as further restrictions, because ω will automatically have these properties. Likewise, if we already knew that a 3-form ρ satisfying (41) and (43) belongs to the ideal $\langle \Sigma^2 \rangle$, there would be no sense in looking further at (44). But it is just because we do not have yet sufficiency, that extra requirements like (44) can have practical value.

Let us now first look at the impact of the curvature conditions we obtained so far, on the A part of ρ. Referring to the coordinate expression of R that was given in Sec. I, the condition (19) that further defines the module Σ^2, reads as

$$\sum_{abc} h_{ra} R^r_{bc} = 0. \tag{46}$$

One easily verifies that (41) and (43) imply that the A part of ρ must have the properties

$$\sum_{abcd}^{e} R^s_{bc}(A_{das} - A_{dsa}) = 0, \tag{47}$$

$$\sum_{abcd}^{e} \Phi_a^r R_{bc}^s (A_{drs} - A_{dsr}) = 0. \tag{48}$$

And (44), for $m=2$ for example, will require that

$$\sum_{abcd}^{e} \Phi_a^r \Phi_r^t R_{bc}^s (A_{dts} - A_{dst}) = 0. \tag{49}$$

It is of some interest to write out explicitly what such conditions mean. The first one, for example, making use of the skew-symmetry of the R_{bc}^a and the symmetry of the A_{abc} to recombine terms, can be written in the form

$$R_{bc}^s (A_{asd} - A_{dsa}) + R_{cd}^s (A_{asb} - A_{bsa}) + R_{db}^s (A_{asc} - A_{csa}) + R_{ad}^s (A_{bsc} - A_{csb}) + R_{ca}^s (A_{bsd} - A_{dsb}) + R_{ab}^s (A_{csd} - A_{dsc}) = 0. \tag{50}$$

Notice that the left-hand side of this expression is skew-symmetric in any pair of indices [the same can be verified for (48) and (49)]. Hence, these conditions are identically satisfied when the free indices are not distinct. In other words, for them to have any effect, the dimension must be at least 4.

We now return to the interesting case of diagonalizable Φ with distinct eigenvalues, as introduced in the previous section. Any further such assumption on Φ has an effect on curvature-type conditions, since Φ determines R according to (35). Let X_a denote a basis of eigenvectors of Φ, dual to the basis of eigenforms considered before; so we have $\Phi(X_a)=\lambda_{(a)}X_a$. With $\bar{R}_{bc}^a$ now denoting the components of R with respect to this adapted frame, we find from (35) and introducing the structure functions τ_{ab}^c, defined by

$$\mathrm{D}_{X_a}^V X_b = \tau_{ab}^c X_c, \tag{51}$$

that

$$3\bar{R}_{ab}^a = -(\mathrm{D}_{X_b}^V \lambda_{(a)} + (\lambda_{(a)} - \lambda_{(b)})\tau_{ab}^a), \tag{52}$$

$$3\bar{R}_{ab}^b = \mathrm{D}_{X_a}^V \lambda_{(b)} + (\lambda_{(b)} - \lambda_{(a)})\tau_{ba}^b, \tag{53}$$

$$3\bar{R}_{ab}^s = (\lambda_{(b)} - \lambda_{(s)})\tau_{ab}^s - (\lambda_{(a)} - \lambda_{(s)})\tau_{ba}^s, \quad s \neq a,b. \tag{54}$$

Now, when Φ is diagonalizable with distinct eigenvalues, we already know from the Σ^1-analysis that $\bar{A}_{abc}=0$ when all indices are distinct. Taking the condition (50) with a, b, c, d different, the summation in each of the terms gives rise to only two terms. Further simplifications arise from taking into account that $\Sigma_{abc}\bar{A}_{abc}=0$ implies $\bar{A}_{bba}=-2\bar{A}_{abb}$. Finally, using the R information, we find that only components of the type (54) enter. The condition is then

$$\sum_{abcd}^{e} (\lambda_{(b)} - \lambda_{(c)})(\bar{A}_{abb}\tau_{dc}^b + \bar{A}_{acc}\tau_{db}^c) = 0. \tag{55}$$

The corresponding condition (46) for the 2-forms defining Σ^2 (knowing that $\bar{h}_{ab}$ is diagonal) likewise reduces to

$$\sum_{abc} (\lambda_{(a)} - \lambda_{(b)})(\bar{h}_{aa}\tau^a_{cb} + \bar{h}_{bb}\tau^b_{ca}) = 0. \tag{56}$$

The similarity in structure between (55) and (56) becomes even clearer if we proceed as follows: for dealing with an expression such as (41), we write, for arbitrary $X_1, \ldots, X_4$,

$$\sum_{ijkl}^{e} \rho(X_i{}^V, R(X_j, X_k)^V, X_l{}^H) = \sum_{i=1}^{4} (-1)^i \sum_{jkl} \rho(X_i{}^V, R(X_j, X_k)^V, X_l{}^H). \tag{57}$$

The notation that is being used here on the right-hand side should be read as follows: for each $i = 1, \ldots, 4$, (i,j,k,l) is a cyclic permutation of (1), (2), (3), (4) and then with i being kept fixed, we perform a cyclic sum over the three other indices. Applying this idea to the explicit form of the condition (41) we are considering, (55) can be recast in the form:

$$\begin{aligned}\sum_{abcd}^{e} (\lambda_{(b)} - \lambda_{(c)})(\bar{A}_{abb}\tau^b_{dc} + \bar{A}_{acc}\tau^c_{db}) \equiv & \sum_{bcd} (\lambda_{(b)} - \lambda_{(c)})(\bar{A}_{abb}\tau^b_{dc} + \bar{A}_{acc}\tau^c_{db}) \\ & - \sum_{cda} (\lambda_{(c)} - \lambda_{(d)})(\bar{A}_{bcc}\tau^c_{ad} + \bar{A}_{bdd}\tau^d_{ac}) \\ & + \sum_{dab} (\lambda_{(d)} - \lambda_{(a)})(\bar{A}_{cdd}\tau^d_{ba} + \bar{A}_{caa}\tau^a_{bd}) \\ & - \sum_{abc} (\lambda_{(a)} - \lambda_{(b)})(\bar{A}_{daa}\tau^a_{cb} + \bar{A}_{dbb}\tau^b_{ca}) = 0. \end{aligned} \tag{58}$$

We can now be precise about what it is we should be able to prove to reach sufficiency of conditions for ρ to be in $\langle \Sigma^2 \rangle$. From the Σ^1 analysis we already know that the A part of ρ will be of the form:

$$\rho_A = \sum_{a \neq d} \bar{A}_{daa} \phi^{aa} \wedge \phi^{dV}. \tag{59}$$

To conclude that such a term "manifestly belongs" to the ideal generated by Σ^2 (or, in fact, to any further submodule of Σ^1) we must be able to show that for each fixed d, there exists a function α_d such that $\Sigma_{a \neq d} \bar{A}_{daa} \phi^{aa} + \alpha_d \phi^{dd}$ belongs to Σ^2 (or to the submodule under consideration). For the case at hand, assuming the dimension is at least 4, this 2-form should, in particular, have the property [see (56)] that for each set of three distinct indices a,b,c that are different from d: $\Sigma_{abc}(\lambda_{(a)} - \lambda_{(b)})(\bar{A}_{daa}\tau^a_{cb} + \bar{A}_{dbb}\tau^b_{ca}) = 0$. But the available data on ρ so far only tell us that a sum of four such terms is zero. So again, maybe, by throwing in more conditions, we might be able to ensure that all four parts in the expression (58) vanish separately.

Now consider the hierarchy (44) of further necessary conditions we have obtained. Following the different steps of the calculation that led from (47) to (55), one can show that (48) and (49) for diagonalizable Φ become

$$\sum_{abcd}^{e} \lambda_{(a)}(\lambda_{(b)} - \lambda_{(c)})(\bar{A}_{abb}\tau^b_{dc} + \bar{A}_{acc}\tau^c_{db}) = 0, \tag{60}$$

$$\sum_{abcd}^{e} \lambda^2_{(a)}(\lambda_{(b)} - \lambda_{(c)})(\bar{A}_{abb}\tau^b_{dc} + \bar{A}_{acc}\tau^c_{db}) = 0. \tag{61}$$

Lemma 5.2: If Φ is diagonalizable with distinct eigenvalues, then for ρ to satisfy the hierarchy of conditions (44), it is sufficient that these properties hold for $m = 0,1,2,3$.

Proof: The assumption is that we have for each set of four distinct indices a,b,c,d:

$$\sum_{abcd}^{e} \lambda_{(a)}^{n}(\lambda_{(b)}-\lambda_{(c)})(\bar{A}_{abb}\tau_{dc}^{b}+\bar{A}_{acc}\tau_{db}^{c})=0,$$

and this for $m=0,1,2,3$. Splitting the sum of 12 even permutations into four cyclic sum parts, as was done in (58), we get a homogeneous linear system of four equations for these sums, with the coefficient matrix

$$\begin{pmatrix} 1 & -1 & 1 & -1 \\ \lambda_{(a)} & -\lambda_{(b)} & \lambda_{(c)} & -\lambda_{(d)} \\ \lambda_{(a)}^{2} & -\lambda_{(b)}^{2} & \lambda_{(c)}^{2} & -\lambda_{(d)}^{2} \\ \lambda_{(a)}^{3} & -\lambda_{(b)}^{3} & \lambda_{(c)}^{3} & -\lambda_{(d)}^{3} \end{pmatrix}.$$

Its determinant, a Vandermonde-type determinant, is equal to the product

$$(\lambda_{(a)}-\lambda_{(b)})(\lambda_{(a)}-\lambda_{(c)})(\lambda_{(a)}-\lambda_{(d)})(\lambda_{(b)}-\lambda_{(c)})(\lambda_{(b)}-\lambda_{(d)})(\lambda_{(c)}-\lambda_{(d)}),$$

and hence is nonzero. It follows that for each set of four distinct indices a,b,c,d, we have

$$\sum_{abc}(\lambda_{(a)}-\lambda_{(b)})(\bar{A}_{daa}\tau_{cb}^{a}+\bar{A}_{dbb}\tau_{ca}^{b})=0. \tag{62}$$

This in turn implies that all further conditions in the hierarchy (44) are automatically satisfied.□

With this result, we are getting as close as we possibly can to concluding that we have sufficiency in this step of the differential ideal process. Indeed, we have now obtained with (62) all the properties that the 2-forms $\Sigma_{a\neq d}\bar{A}_{daa}\phi^{aa}+\alpha_d\phi^{dd}$ must have for belonging to Σ^2, except for those conditions of type (56) for which the cyclic sum over three indices will involve the undetermined function α_d (and this for each fixed d). These missing conditions may cause true obstructions to the existence of a solution for the inverse problem, as for each fixed d, there may, in principle, be three requirements to be satisfied, for only one unknown α_d. But there is no chance of getting more information about such possible obstructions at this level of generality, i.e., without breaking the discussion up into more subcases, because the 2-forms that interest us in an expression like (59) always appear in a wedge product with some ϕ^{dV}, so the functions we called α_d remain completely undetermined.

Let us summarize the situation now. For a 3-form ρ to be in the ideal $\langle\Sigma^2\rangle$, it must satisfy the requirement (40) and the curvature condition (41), but, in fact, also the infinite set of conditions (44) (plus corresponding analogs) that contain the one just mentioned for $m=0$. The special case of diagonalizable Φ has shown that imposing these conditions for $m=0,1,2,3$ is probably the closest we can get to having conditions that are also sufficient. So it is worthwhile exploring what comes out of such conditions when we apply them to exact forms, in terms of possibly new algebraic restrictions on admissible 2-forms.

Applying (40) to $d\omega$ is an easy computation: as already indicated, it reproduces the requirement (36) we obtained before. The other computations are a lot more involved, so we give a brief indication about the way to proceed. Starting with (44) for $m=0$, the bracket terms of the expansion of $\Sigma_{X,Y,Z,U}^{e}\, d\omega(X^V,R(Y,Z)^V,U^H)$ include, as terms in which X is fixed,

$$-\sum_{Y,Z,U}\{\omega([X^V,R(Z,U)^V],Y^H)+\omega([R(Z,U)^V,Y^H],X^V)+\omega([Y^H,X^V],R(Z,U)^V)\}$$

$$=-\sum_{Y,Z,U}\{\omega(\mathrm{D}_X^V(R(Z,U))^V-(\mathrm{D}_{R(Z,U)}^V X)^V,Y^H)+\omega((\mathrm{D}_{R(Z,U)}^V Y)^H,X^V)-\omega((\mathrm{D}_X^V Y)^H,R(Z,U)^V)\},$$

and there are similar terms in which one of the other vector fields is kept fixed each time. If, in the last term on the right, we make use of the property (19), it is easy to see that all terms that arise this way will directly cancel out the terms coming from the expansion of the first term on the right,

except those in which the tensor R itself is being derived. The second and third terms on the right will all disappear if the totality of all even sum permutations is taken into account. The only terms that remain then are those involving vertical derivatives of R. But they can be seen to cancel out as well in view of the Bianchi identity,

$$\sum_{X,Y,Z} \mathrm{D}^V R(X,Y,Z) = 0. \tag{63}$$

For the horizontal counterpart (42), something entirely similar happens in view of

$$\sum_{X,Y,Z} \mathrm{D}^H R(X,Y,Z) = 0. \tag{64}$$

We can now more or less see what will happen for the conditions (44) with $m \neq 0$. When, in the terms that have been made explicit above, X is replaced by ΦX, for example, most of the cancellations remain the same, but there will be extra terms in which derivatives of Φ appear; moreover, derivatives of R will now be taken with respect to arguments such as ΦX instead of X and that makes that the Bianchi identity does not directly help. In conclusion, we get the following new requirements:

$$\sum_{X,Y,Z,U}^{e} \omega(\mathrm{D}^V_{\Phi^m X} R(Z,U)^V - (\mathrm{D}^V_{R(Z,U)} \Phi^m)(X)^V, Y^H) = 0, \tag{65}$$

which in the context of the last lemma would be imposed only for $m=1,2,3$, plus analogous conditions with horizontal and vertical lifts or derivatives interchanged.

We have now obtained extra requirements more closely defining the module Σ^2, namely not only the ones just mentioned, but also those that came out of the analysis of the preceding section: (34), (36), and (38), (39). However, continuing further at this level of generality is not profitable.

VI. BEYOND THE DIFFERENTIAL IDEAL: EXAMPLES

In all practical situations, the algebraic conditions discussed so far will establish either that no nondegenerate multiplier exists, or that we have reached the stage of a differential ideal. In the latter case we then construct a Kähler lift g^{K} in the ideal that is closed. In principle, this means addressing the Pfaffian system of Eqs. (7), which is, of course, a particular way of representing a system of partial differential equations for the unknown functions r_k. While it is certainly true that the Cartan-Kähler theory is a powerful vehicle to decide about the integrability of such equations and the generality of their solutions, a drawback of (7) is that it is setup in such a general way as to lose contact with the specific geometrical structure of the inverse problem. For example, the symmetry relating to horizontal and vertical parts suggest splitting (7) into its horizontal and vertical components. But that inevitably must be equivalent to considering the partial differential equations of the inverse problem the way they were encoded geometrically in their most compact form in (2).

In other words, what we are advocating here is that, once we have reached a differential ideal, we go back to the partial differential equations in the original Helmholtz conditions, for example, in the representation

$$D^V_X g(Y,Z) = \mathrm{D}^V_Y g(X,Z), \quad \boldsymbol{\nabla} g = 0, \tag{66}$$

and specifically in that order. Indeed, by splitting the equations for the r_k in that way, we expect that they will become quite tractable: the first set of equations will determine the allowed velocity dependence of the unknown r_k, and $\boldsymbol{\nabla} g = 0$ will subsequently further restrict the arbitrary functions that may turn up in solving the first part. It may look rather disappointing that, after all the efforts of the differential ideal process, we now still have to address two of the three Helmholtz conditions (2). But we knew from the beginning that the differential ideal process was not going to solve these equations. The point is that, specifically by the way we have pursued obtaining

"efficient" algebraic conditions in that process, the algebraic freedom in the module of admissible 2-forms will likely be restricted in such a way that addressing the equations (66) directly will now become possible.

We will finish with two illustrations: one in which the differential ideal process leads to a negative result and one where we reach the final stage and subsequently solve the partial differential equations for the r_k. For these examples, we consider cases where Φ is diagonalizable with distinct eigenvalues and go back to the situation described at the end of Sec. IV. So, if the hope is that we will reach a decisive state at that point, it means that we are in the situation described by Proposition 4.2, so that Σ^1 generates a differential ideal, or that the conditions in that statement lead to the conclusion that no nondegenerate multiplier can exist.

The following is an important preliminary observation. Conditions that involve $\nabla\Phi$, ∇R, or other covariant derivatives of these tensors are likely to produce restrictions that contain the functions $\nabla\lambda_{(a)}$ and even $\nabla\tau^a_{bc}$ (or other derivatives of structure functions) and will prompt for further assumptions about $\nabla\Phi$, for example. The curvature condition (19) is more interesting to look at first, therefore, because it is purely algebraic in the structure functions τ^a_{bc}, as we have seen with (56). It turns out that also (38) is of such a nature in the case of diagonalizable Φ we are considering. Indeed, we have

$$(D^V_{\Phi X_a}\Phi)(X_b) = \lambda_{(a)}X_a{}^V(\lambda_{(b)})X_b + \lambda_{(a)}(\lambda_{(b)} - \lambda_{(c)})\tau^c_{ab}X_c,$$

from which it follows that for a 2-form of type $\omega = \bar{h}_{aa}\phi^{aa}$,

$$\omega((D^V_{\Phi X_a}\Phi(X_b) - D^V_{\Phi X_b}\Phi(X_a))^V, X_c{}^H) = \bar{h}_{bb}\lambda_{(a)}X_a{}^V(\lambda_{(b)})\delta_{bc} - \bar{h}_{aa}\lambda_{(b)}X_b{}^V(\lambda_{(a)})\delta_{ac} + \bar{h}_{cc}(\lambda_{(a)}(\lambda_{(b)} - \lambda_{(c)})\tau^c_{ab} - \lambda_{(b)}(\lambda_{(a)} - \lambda_{(c)})\tau^c_{ba}).$$

But for taking the cyclic sum (38), we need to take a,b,c distinct, so that derivatives of the eigenvalues will disappear. The condition in the end reduces to

$$\sum_{abc}\lambda_{(c)}(\lambda_{(a)} - \lambda_{(b)})(\bar{h}_{aa}\tau^a_{cb} + \bar{h}_{bb}\tau^b_{ca}) = 0, \tag{67}$$

which has a remarkable resemblance to (56). In fact, it is interesting to work out some conclusions from the combination of the conditions (56) and (67). To fix the idea, take $\{a,b,c\}=\{1,2,3\}$ and put, for example, $H_{12}=(\lambda_{(1)}-\lambda_{(2)})G_{12}$, with $G_{12}=(\bar{h}_{11}\tau^1_{32}+\bar{h}_{22}\tau^2_{31})$. Then, it is easy to see that the combination of both conditions is equivalent to requiring that $G_{12}=G_{23}=G_{31}$. So, for example, in dimension 3, we get the following two conditions of curvature type:

$$\bar{h}_{11}\tau^1_{32} + \bar{h}_{22}(\tau^2_{31} - \tau^2_{13}) - \bar{h}_{33}\tau^3_{12} = 0, \tag{68}$$

$$\bar{h}_{11}\tau^1_{23} - \bar{h}_{22}\tau^2_{13} + \bar{h}_{33}(\tau^3_{21} - \tau^3_{12}) = 0, \tag{69}$$

which actually only involve τ^a_{bc} with a,b,c distinct. In dimension 4, there will already be eight of such conditions, coming from the four combinations of three distinct indices: if these are not identically satisfied, chances are small that there will still be a nondegenerate ω.

Our first example is taken from Ref. 7 and is shown there to have no Lagrangian. We wish to confirm that we come to the same conclusion. Consider the four-dimensional system (b constant),

$$\ddot{x} = b\dot{x}\dot{w},$$

$$\ddot{y} = \dot{y}\dot{w},$$

$$\ddot{z} = (1-b)\dot{x}\dot{y} + by\dot{x}\dot{w} - bx\dot{y}\dot{w} + (b+1)\dot{z}\dot{w},$$

$$\ddot{w} = 0.$$

With u, v, s, t as the notation for the derivatives, we have

$$4\Phi = \begin{pmatrix} -b^2t^2 & 0 & 0 & b^2ut \\ 0 & -t^2 & 0 & vt \\ a_1 & a_2 & a_3 & a_4 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where

$$a_1 = (2b+1)(b+1)tv - (2b+1)byt^2,$$

$$a_2 = -(b+1)(b+2)ut + b(b+2)xt^2,$$

$$a_3 = -(b+1)^2t^2,$$

$$a_4 = b(2b+1)yut + (1-b^2)uv - b(b+2)xvt + (b+1)^2st.$$

The eigenvalues and corresponding eigenvectors are

$$-b^2t^2 \quad \text{and} \quad (t,0,(b+1)v - byt,0),$$

$$t^2 \quad \text{and} \quad (0,bt,bxt - (b+1)u,0),$$

$$-(b+1)^2t^2 \quad \text{and} \quad (0,0,1,0),$$

$$0 \quad \text{and} \quad (u,v,s,t).$$

It is easy to compute structure functions, as defined by (51); of the ones with distinct indices, only the following two appear to be nonzero:

$$\tau^3_{21} = (b+1)bt, \quad \tau^3_{12} = -(b+1)t.$$

For having distinct eigenvalues, we have to require that $b \neq 0$ and $b \neq -1$. The eight conditions coming from (56) and (67), applied to the multiplier g_{ab} we are now constructing, then reduce to 2, and they both require that $g_{33}=0$, so that there is indeed no nonsingular multiplier. Of course, it is a fact that, as shown in Ref. 7, the curvature condition by itself already leads to this conclusion, so that there is no real contribution from the extra condition (67).

To get beyond the differential ideal step we choose, as our second example, a three-dimensional system inspired by one of the favorable two-dimensional cases in Ref. 6. Consider the system

$$\ddot{x} = -x,$$

$$\ddot{y} = y^{-1}(1 + \dot{y}^2 + \dot{z}^2),$$

$$\ddot{z} = 0,$$

on an appropriate domain. Denoting the derivatives by u, v, w, Φ this time is given by

$$\Phi = \frac{1}{y^2}\begin{pmatrix} y^2 & 0 & 0 \\ 0 & 2(1+w^2) & -2vw \\ 0 & 0 & 0 \end{pmatrix}.$$

Eigenvalues and corresponding eigenvectors are

$$0 \quad \text{and} \quad (0, vw, 1+w^2),$$

$$1 \quad \text{and} \quad (1,0,0),$$

$$2y^{-2}(1+w^2) \quad \text{and} \quad (0,y,0).$$

The eigenvectors X_a are chosen in such a way that $\nabla X_a = 0$, which is possible because $\nabla\Phi$ commutes with Φ in this case. The corresponding dual basis of eigenforms is given by

$$\phi^1 = \frac{1}{1+w^2}\theta^3, \quad \phi^2 = \theta^1, \quad \phi^3 = \frac{1}{y}\theta^2 - \frac{vw}{y(1+w^2)}\theta^3.$$

Again, the structure functions τ^a_{bc} are easy to compute and they are zero, except the following:

$$\tau^3_{11} = \frac{v}{y}, \quad \tau^1_{11} = 2w, \quad \tau^3_{31} = w.$$

It is immediately clear that this implies that the conditions (68) and (69) are identically satisfied because all the τ's involved are zero. Going back to the result expressed in Proposition 4.2, we have just dealt with (19) and (38). Let us introduce also horizontal structure functions by $D^H_{X_a} X_b = \nu^c_{ab} X_c$, and observe now that in view of the similarity in structure between (35) and (37), and also between (38) and (39), the explicit form of the conditions (36) and (39), for example for $n=3$, will be the same as (68) and (69), with ν^c_{ab} replacing τ^c_{ab}. But in view of the commutator identity $[\nabla, D^V_X] = D^V_{\nabla X} - D^H_X$, and the fact that we chose the X_a to be ∇ invariant, we simply have $\nu^a_{bc} = -\Gamma(\tau^a_{bc})$ here and thus these two other conditions will be identically satisfied as well. It remains to look at (34), but this will hold trivially because $\nabla\Phi$ commutes with Φ. We conclude from Proposition 4.2 that Σ^1 generates a differential ideal.

The admissible g's are of the form $g = \Sigma_k r_k \phi^k \otimes \phi^k$ and following the scheme explained at the beginning of this section, we now start looking at the equations to be satisfied by the r_k. For the vertical closure conditions in (66), it is convenient to re-express g in the standard basis of θ^i, from which we learn that

$$g_{11} = r_2, \quad g_{22} = \frac{r_3}{y^2}, \quad g_{33} = \frac{1}{(1+w^2)^2}\left(r_1 + r_3\frac{v^2w^2}{y^2}\right),$$

$$g_{12} = g_{13} = 0, \quad g_{23} = -r_3\frac{vw}{y^2(1+w^2)}.$$

The vertical closure conditions then are

$$\frac{\partial g_{11}}{\partial v} = \frac{\partial g_{11}}{\partial w} = 0, \quad \frac{\partial g_{22}}{\partial u} = \frac{\partial g_{33}}{\partial u} = 0,$$

$$\frac{\partial g_{22}}{\partial w} = \frac{\partial g_{23}}{\partial v}, \quad \frac{\partial g_{33}}{\partial v} = \frac{\partial g_{23}}{\partial w},$$

or translated into equations for the r_k,

$$\frac{\partial r_2}{\partial v} = \frac{\partial r_2}{\partial w} = 0, \quad \frac{\partial r_3}{\partial u} = \frac{\partial r_1}{\partial u} = 0,$$

$$(1+w^2)\frac{\partial r_3}{\partial w} + vw\frac{\partial r_3}{\partial v} = -r_3 w,$$

and

$$y^2\frac{\partial r_1}{\partial v} = -v^2w^2\frac{\partial r_3}{\partial v} - vw(1+w^2)\frac{\partial r_3}{\partial w} - r_3 v(1+w^2).$$

The solution of these equations is quite straightforward. We have that r_2 can depend on u only and, of course, also arbitrarily on x,y,z,t for the moment. r_3, on the other hand, cannot depend on u and using the method of characteristics on the other equation that involves r_3 only gives

$$r_3 = \frac{1}{v}\chi(\xi), \quad \text{with } \xi = \frac{v}{\sqrt{1+w^2}},$$

where χ is an arbitrary function of the indicated argument, which again can further depend on x,y,z,t. The last equation and the fact that r_1 cannot depend on u either, then produces

$$r_1 = -\frac{\sqrt{1+w^2}}{y^2}\psi(\xi) + \zeta(w),$$

where $\psi' = \chi$ and, like ψ, the arbitrary ζ can further depend on x,y,z,t.

It remains to impose that ∇g must be zero. Since $\nabla\phi^a = 0$ by construction, this simply means that the r_k must be first integrals. The conclusion for r_2 is immediately that it cannot depend on y and z and simply must be a first integral of the equation $\ddot{x} = -x$. Equating $\Gamma(r_3) = 0$, we see that χ can no longer depend on x and further must satisfy

$$\left(\xi + \frac{1}{\xi}\right)\frac{\partial\chi}{\partial\xi} + y\frac{\partial\chi}{\partial y} + \frac{y}{v}\left(w\frac{\partial\chi}{\partial z} + \frac{\partial\chi}{\partial t}\right) - \left(1 + \frac{1}{\xi^2}\right)\chi = 0.$$

Now every function that depends on v and w through the variable ξ only, gives zero when acted upon by the vector field $(1+w^2)\,\partial/\partial w + vw\,\partial/\partial v$. Applying this operator to the left-hand side of the above equation, it follows that we must have

$$\frac{\partial\chi}{\partial z} - w\frac{\partial\chi}{\partial t} = 0,$$

and repeating the same process subsequently implies that χ cannot depend on z and t at all. The reduced equation for χ then can easily be solved by the method of characteristics again and yields

$$\chi(\xi, y) = \xi\chi_0\left(\frac{\sqrt{1+\xi^2}}{y}\right),$$

where χ_0 is an arbitrary function of the indicated single argument. With this further restriction, one can verify that the first term in the expression for r_1 is a first integral, and if the same must hold for ζ, this function cannot depend on x and y and simply has to be a first integral of the equation $\ddot{z} = 0$. In summary, the general solution for the r_k is given by

$$r_1 = -\frac{\sqrt{1+w^2}}{y^2}\psi(\xi, y) + \zeta(w, z, t),$$

$$r_2 = \sigma(u, x, t),$$

$$r_3 = \frac{1}{v}\chi(\xi, y) = \frac{\xi}{v}\chi_0\left(\frac{\sqrt{1+\xi^2}}{y}\right), \quad \xi = \frac{v}{\sqrt{1+w^2}},$$

where χ_0 is further arbitrary, $\partial\psi/\partial\xi = \chi$, ζ is a first integral of the equation $\ddot{z}=0$, and σ a first integral of the equation $\ddot{x}=-x$.

In a forthcoming paper, we plan to apply these techniques more systematically to the identification of a number of classes of three dimensional (and possibly higher dimensional) systems for which a multiplier exists. The last example here, for example, belongs to a class that is characterized by the fact that two of the eigenform codistributions of a diagonalizable Φ are integrable, and the third one is not, and this is one of the cases we shall be able to treat in all generality, even in any dimension.

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Integrable and superintegrable systems with spin

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A system of two particles with spin $s=0$ and $s=\frac{1}{2}$, respectively, moving in a plane is considered. It is shown that such a system with a nontrivial spin-orbit interaction can allow an eight dimensional Lie algebra of first-order integrals of motion. The Pauli equation is solved in this superintegrable case and reduced to a system of ordinary differential equations when only one first-order integral exists. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2360042]

I. INTRODUCTION

A Hamiltonian system with n degrees of freedom in classical mechanics is called integrable if it allows n functionally independent integrals of motion $\{X_1,\ldots,X_n\}$. These integrals must be well-defined functions on phase space and be in involution. The Hamiltonian H belongs to this set of n integrals. A "superintegrable system" is one that allows some additional integrals of motion, $\{Y_1,\ldots,Y_k\}$ such that the set $\{X_1,\ldots,X_n,Y_1,\ldots,Y_k\}$ is functionally independent. The integrals $\{Y_1,\ldots,Y_k\}$ are not necessarily in involution among each other, nor with the X_i. A system is maximally superintegrable if we have $k=n-1$, minimally superintegrable for $k=1$.

The concepts of integrability and superintegrability are also introduced in quantum mechanics. The only difference is that the integrals of motion are now well-defined linear quantum mechanical operators, assumed to be algebraically independent.[1,6–9,12,13,15,16,18,19,21]

The best known superintegrable systems are the Kepler, or Coulomb, system[1,8] and the harmonic oscillator.[12,16] They are characterized by the fact that all finite classical trajectories in these systems are periodic. In quantum mechanics these systems are exactly solvable, i.e., their bound state energy levels can be calculated algebraically and their wave function expressed in terms of polynomials.

The above properties are shared by all other known maximally superintegrable systems (see, for example, Ref. 19).

A systematic search for superintegrable systems and their properties was started quite some time ago.[6,7,9,15,21] Originally the approach concentrated on Hamiltonians of the type

$$H=-\frac{1}{2}\Delta+V(\vec{r}), \tag{1}$$

in two- and three- dimensional Euclidean spaces with the restriction that all integrals of motion should be first- or second-order polynomials in the momenta. More recently, the study of superintegrable systems with second-order integrals of motion was extended to curved spaces and also higher-dimensional ones (see Ref. 13 for some recent results and an extensive list of references).

For Hamiltonians of the type (1) with second-order integrals of motion there is a close relation between integrability and the separation of variables in the Schrödinger and Hamilton-Jacobi equations. Typically, superintegrable systems of this type are multiseparable: they allow the separation of variables in more than one system of coordinates.

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This relationship between integrability and separability breaks down in other cases. Thus for natural Hamiltonians of the type (1), the existence of third-order integrals of motion does not lead to the separation of variables.[4,5,10,11] Furthermore, if we consider velocity dependent potentials (e.g., related to a magnetic field),

$$H = -\frac{1}{2}\Delta + V(\vec{r}) + (\vec{A},\vec{p}), \tag{2}$$

then quadratic integrability no longer implies the separation of variables.[2,3,17,20]

In this paper we initiate the study of integrability and superintegrability in a different type of system, namely, one involving particles with spin. More specifically, we consider two nonrelativistic quantum particles, moving in a plane: one with spin $1/2$, the other with spin 0. In this case the Hamiltonian will be a matrix operator, acting on two component spinors, and we can decompose it in terms of the identity matrix I and the Pauli matrices σ_i $(i=1,2,3)$.

From the physical point of view, the most interesting Hamiltonian to consider would be

$$H = -\frac{\hbar^2}{2m}\Delta + V_0(\vec{r}) + \frac{1}{2}\{V_1(\vec{r}),(\vec{\sigma},\vec{L})\}, \tag{3}$$

in the three-dimensional Euclidean space E_3 (we drop the matrix I whenever this does not cause confusion). The curly bracket represents an anticommutator and $V_a(\vec{r})$, $a=0,1$ are real functions. The Hamiltonian is Hermitian and satisfies the requirements of parity and time reversal invariance. The spin-orbital interaction term $V_1(\vec{r})(\vec{\sigma},\vec{L})$ is the standard one in quantum mechanics.[14]

In this paper, the first one on integrability and superintegrability for particles with nonzero spin, we restrict to the two-dimensional space E_2. The orbital angular momentum $\vec{L}$ then only has one component, L_3, perpendicular to the xy plane E_2. The scalar product $(\vec{\sigma},\vec{L})$ reduces to $\sigma_3 L_3$ (since L_1 and L_2 are zero). We shall set the reduced mass m of the two particle system equal to $m=1$ and use units in which the Planck constant is $\hbar=1$ (we do not need to consider a classical limit here). Finally, the Hamiltonian to be considered in this paper is

$$H = \frac{1}{2}(p_1^2 + p_2^2) + V_0(x,y) + V_1(x,y)\sigma_3 L_3 + \frac{1}{2}\sigma_3(L_3 V_1(x,y)), \tag{4}$$

with

$$p_1 = -i\partial_x, \quad p_2 = -i\partial_y, \quad L_3 = i(y\partial_x - x\partial_y), \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5}$$

A priori, the functions $V_0(x,y)$ and $V_1(x,y)$ are arbitrary. In specific physical applications they may be related or they may both be specified. Our aim is to determine the conditions on these two functions under which one or more integrals of motion exist.

We request that at least one first-order integral of motion should exist, namely,

$$X = (A_0 p_1 + B_0 p_2 + \phi_0)I + (A_1 p_1 + B_1 p_2 + \phi_1)\sigma_3, \tag{6}$$

where A_μ, B_μ, and ϕ_μ $(\mu=0,1)$ are real functions of x and y. These functions as well as the potentials V_0 and V_1 are to be determined from the commutativity condition

$$[H,X] = 0. \tag{7}$$

The general formulation is set up in Sec. II, where we determine A_μ and B_μ and obtain the partial differential equations (PDE) that ϕ_0, ϕ_1, V_0, and V_1 must satisfy. In Sec. III we consider a special case when the Hamiltonian (4) allows six independent nontrivial integrals of the type (6). They generate an eight-dimensional symmetry group of the system. Section IV is devoted to more general integrable Hamiltonians, allowing just one first-order integral. The system of equations,

$$H\Psi = E\Psi, \quad X\Psi = \lambda\Psi, \tag{8}$$

is studied in Sec. V. We shall call the system (8) the Pauli system. Some conclusions and future directions are outlined in Sec. VI.

II. FORMULATION OF THE PROBLEM

In order to obtain determining equations for the coefficients A_μ, B_μ, and ϕ_μ ($\mu=0,1$) in the integral (6), we impose the commutation relation (7). The commutator will involve terms of the type p_1^2, $p_1^2\sigma_3$, p_2^2, $p_2^2\sigma_3$, p_1p_2, $p_1p_2\sigma_3$, p_1, $p_1\sigma_3$, p_2, $p_2\sigma_3$, I, and σ_3.We have $\sigma_3^2=I$, so no higher powers of σ_3 appear. We set the coefficients of each of the above terms equal to zero. This gives us 12 linear partial differential equations for A_μ, B_μ, and ϕ_μ. Those coming from the coefficients of second-order terms in the momentum imply that A_μ and B_μ are linear functions and we obtain, for any potentials V_0 and V_1,

$$A_\mu = \omega_\mu y + a_\mu, \quad B_\mu = -\omega_\mu x + b_\mu, \tag{9}$$

where ω_μ, a_μ, and b_μ are real constants. The coefficients of $\vec{p}$, $\vec{p}\sigma_3$, I, and σ_3 in the commutator provide an overdetermined system of six first-order PDEs for the four functions V_0, V_1, ϕ_0, and ϕ_1. They are

$$\phi_{\mu,x} = \delta_{\mu,1-\nu}[-b_\nu V_1 - (\omega_\nu y + a_\nu)yV_{1,x} + (\omega_\nu x - b_\nu)yV_{1,y}],$$

$$\phi_{\mu,y} = \delta_{\mu,1-\nu}[a_\nu V_1 + (\omega_\nu y + a_\nu)xV_{1,x} - (\omega_\nu x - b_\nu)xV_{1,y}], \tag{10}$$

$$(\omega_\mu y + a_\mu)V_{0,x} + (-\omega_\mu x + b_\mu)V_{0,y} = \delta_{\mu,1-\nu}(x\phi_{\nu,y} - y\phi_{\nu,x})V_1 \quad (\mu,\nu=0,1). \tag{11}$$

The coefficients of I and σ_3 *a priori* involve second-order derivatives of $V_1(x,y)$. These second-order terms cancel, once Eqs. (9) and (10) are taken into account. This leads to the two first-order equations (11).

Before solving this system, let us introduce "allowed transformations" that leave the Hamiltonian (4) form invariant, i.e., change only the functions $V_0(x,y)$ and $V_1(x,y)$. Such transformations will be used to simplify Hamiltonians, integrals of motion, and also the equations to be solved.

Allowed transformations for any potentials V_0 and V_1 are as follows.

(1) Rotations in the xy plane.
(2) Gauge transformations of the form

$$\tilde{H} = U^{-1}HU, \quad U = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}, \quad \alpha = \alpha(\xi), \quad \xi = \frac{y}{x}. \tag{12}$$

The transformation of the potentials is

$$\tilde{V}_1 = V_1 + \frac{\dot{\alpha}}{x^2}, \quad \tilde{V}_0 = V_0 + \left(1 + \frac{y^2}{x^2}\right)\left(\frac{1}{2}\frac{\dot{\alpha}^2}{x^2} + \dot{\alpha}V_1\right). \tag{13}$$

For certain specific potentials V_1, further allowed transformations exist (for any V_0), namely, simultaneous translations and gauge transformations.

(1) $V_1=\gamma=$ const. The allowed transformations are given by

$$\tilde{x} = x + x_0, \quad \tilde{y} = y + y_0, \quad \alpha = \gamma(y_0x - x_0y), \tag{14}$$

and the transformation of the potentials is

$$\tilde{V}_1 = V_1 = \gamma, \quad \tilde{V}_0(x,y) = V_0(x+x_0, y+y_0) - \frac{1}{2}\gamma^2(x_0^2 + y_0^2 + 2(xx_0 + yy_0)). \tag{15}$$

(2) $V_1 = V_1(x)$. The allowed transformation is

$$\tilde{x} = x, \quad \tilde{y} = y + y_0, \quad \alpha(x) = y_0 \int V_1(x)dx, \quad \tilde{V}_1 = V_1, \quad \tilde{V}_0(x,y) = V_0(x, y+y_0) - \frac{1}{2}V_1^2 y_0(y_0 + 2y). \tag{16}$$

Let us now return to Eq. (10). The compatibility conditions $\phi_{\mu,xy} = \phi_{\mu,yx}$ imply

$$(\omega_\mu y + a_\mu)(xV_{1,xx} + yV_{1,xy} + 3V_{1,x}) + (-\omega_\mu x + b_\mu)(yV_{1,yy} + xV_{1,xy} + 3V_{1,y}) = 0 \quad (\mu = 0,1). \tag{17}$$

In general, (17) represents an overdetermined system of two different equations for the potentials $V_1(x,y)$ and this system can be written as

$$xV_{1,xx} + yV_{1,xy} + 3V_{1,x} = 0,$$

$$yV_{1,yy} + xV_{1,xy} + 3V_{1,y} = 0. \tag{18}$$

An exception occurs if the two equations (17) coincide. This occurs if the constants figuring in Eq. (17) satisfy the three following equations:

$$\omega_0 a_1 - \omega_1 a_0 = 0, \quad \omega_0 b_1 - \omega_1 b_0 = 0, \quad a_1 b_0 - a_0 b_1 = 0. \tag{19}$$

We shall treat the case (18) in Sec. III. The case when (19) is satisfied and $V_1(x,y)$ satisfies only one equation (17) will be considered in Sec. IV.

III. SPIN ORBITAL INTERACTION WITH KINEMATICAL INVARIANCE GROUP

Let us now solve Eqs. (18). We transform the first equation to characteristic variables, solve and substitute into the second equation. The result is

$$V_1(x,y) = \gamma + \frac{G(\xi)}{x^2}, \quad \xi = \frac{y}{x}, \quad \gamma = \text{const}. \tag{20}$$

Comparing with Eq. (13) we see that we can annul the function $G(\xi)$ by a gauge transformation. Thus we have

$$V_1 = \gamma. \tag{21}$$

Substituting (21) into Eqs. (10) and (11), we obtain

$$V_0 = \frac{1}{2}\gamma^2(x^2 + y^2), \quad \phi_0 = -\gamma(b_1 x - a_1 y), \quad \phi_1 = -\gamma(b_0 x - a_0 y). \tag{22}$$

The Hamiltonian thus has the form

$$H = -\frac{1}{2}\Delta + \frac{1}{2}\gamma^2(x^2 + y^2) + \gamma\sigma_3 L_3, \quad \gamma \in R. \tag{23}$$

Since H does not depend on the constants ω_μ, a_μ, and b_μ we obtain six independent integrals of motion, generating the symmetry group of this Hamiltonian.

A basis for the symmetry algebra is given by the eight operators:

$$L_\pm = i(y\partial_x - x\partial_y)(I \pm \sigma_3),$$

$$X_\pm = (i\partial_x \mp \gamma y)(I \pm \sigma_3),$$

$$Y_\pm = (i\partial_y \pm \gamma x)(I \pm \sigma_3),$$

$$I_\pm = I \pm \sigma_3. \tag{24}$$

The nonzero commutation relations are

$$[L_\pm, X_\pm] = 2iY_\pm, \quad [L_\pm, Y_\pm] = -2iX_\pm, \quad [X_\pm, Y_\pm] = \pm 4i\gamma I_\pm. \tag{25}$$

The symmetry algebra is thus isomorphic to the direct sum of two central extensions of the Euclidean Lie algebra,

$$L \sim \tilde{e}_+(2) \oplus \tilde{e}_-(2) = \{L_+, X_+, Y_+, I_+\} \oplus \{L_-, X_-, Y_-, I_-\}. \tag{26}$$

The Casimir operators of L are

$$C_\pm = X_\pm^2 + Y_\pm^2 \pm 4\gamma L_\pm I_\pm, \quad I_\pm = I \pm \sigma_3, \tag{27}$$

and we have

$$H = \frac{1}{8}(C_+ + C_-). \tag{28}$$

The integral of motion X is a linear combination of the eight operators (24) with arbitrary real constant coefficients. Such operators X can be classified into conjugacy classes under the action of the group generated by the algebra (24). The conjugacy classes that lead to different types of solutions of the Pauli system (8) can be represented by

$$X_1 = L_+ + \alpha L_-, \quad X_2 = L_+ + \alpha X_-, \quad X_3 = X_+ + \alpha X_-, \quad \alpha \in R. \tag{29}$$

The Hamiltonian (23) is not only integrable, but actually "first-order superintegrable." For particles of spin 0 first-order superintegrability occurs only for free motion. Notice that if we set the spin-orbit interaction equal to zero in Eq. (23) (i.e., $\gamma=0$), we obtain free motion.

IV. HAMILTONIANS ALLOWING ONE FIRST-ORDER INTEGRAL

Let us now consider the case when Eqs. (19) are satisfied. The two equations (17) then coincide and the potential $V_1(x,y)$ satisfies just one second-order PDE. The equation (17) is of hyperbolic type. Its characteristic variables are

$$\xi = \frac{y}{x}, \quad \eta = \frac{1}{2}\omega_1(x^2 + y^2) - b_1 x + a_1 y. \tag{30}$$

Here we shall just consider two interesting special cases.

(a) $\omega_1 \neq 0$, $a_0 = b_0 = 0$, $a_1 = b_1 = 0$

We transform Eq. (17) to polar coordinates and obtain

$$\rho V_{1,\rho\theta} + 2V_{1,\theta} = 0, \quad x = \rho\cos\theta, \quad y = \rho\sin\theta. \tag{31}$$

The potential V_1 hence is

$$V_1 = f(\rho) + \frac{1}{\rho^2} g(\theta), \tag{32}$$

where $f(\rho)$ and $g(\theta)$ are arbitrary. Comparing with Eq. (13), we see that the function $g(\theta)$ can be set equal to $g=0$ by a gauge transformation. Solving (10) and (11), we obtain

$$V_0 = V_0(\rho), \quad V_1 = V_1(\rho), \quad \phi_0 = \phi_1 = 0, \tag{33}$$

$$X = (\omega_0 + \omega_1 \sigma_3) L_3. \tag{34}$$

(b) $\omega_0 = \omega_1 = 0$, $a_1^2 + b_1^2 \neq 0$
Equation (17) in characteristic variables (30) is

$$V_{1,\xi\eta} + \frac{2}{\eta} V_{1,\xi} = 0, \tag{35}$$

and we obtain

$$V_1 = F_1(a_1 y - b_1 x) + \frac{F_2\left(\frac{y}{x}\right)}{(a_1 y - b_1 x)^2}. \tag{36}$$

By a gauge transformation we set $F_2 = 0$ and rotate in the xy plane to obtain

$$V_1 = V_1(x). \tag{37}$$

From Eqs. (10) and (11) we obtain

$$V_0 = \frac{y^2}{2} V_1^2(x) + F(x), \tag{38}$$

$$\phi_0 = -b_1 \int V_1(x) dx, \quad \phi_1 = -b_0 \int V_1(x) dx. \tag{39}$$

Let us put $b_1 = 1$, $b_0 \neq 0$. We then have

$$\phi_1 = b_0 \phi_0, \quad V_1(x) = -\phi_0'(x),$$

$$V_0(x,y) = \frac{1}{2} y^2 [\phi_0'(x)]^2 + F(x), \tag{40}$$

and

$$X = -i b_0 \partial_y + \phi_0(x) + (-i \partial_y + b_0 \phi_0(x)) \sigma_3. \tag{41}$$

We shall call the case (33) the "polar" case, (37) and (38) the "Cartesian" one, because of the form of the operator X in (34) and (41), respectively.

V. SOLUTIONS OF THE PAULI EQUATION

In this section we shall analyze and solve the pair of equations (8) for the different superintegrable, or first-order integrable cases, found above.

A. The superintegrable Hamiltonian

Let us consider the Hamiltonian (23) with $\gamma \neq 0$, i.e., a constant spin-orbital potential and a harmonic oscillator spin-independent one. The Hamiltonian commutes with the entire kinematical algebra (24). We shall choose the operator X of Eq. (8) in the form of one of the different one-dimensional subalgebras shown in Eq. (29) and consider each of the three cases separately. The potentials $V_0(x,y)$ and $V_1(x,y)$ in this case have the form (33) and (40) simultaneously.

Hence, we can separate variables in polar coordinates, as well as in Cartesian ones. Moreover, we can consider a mixed case: separation in different coordinate systems for the upper and lower components of Ψ.

1. Polar case

We introduce polar coordinates (ρ,θ) and choose the operator X in the form

$$X=-i\begin{pmatrix}a_1 & 0\\ 0 & a_2\end{pmatrix}\partial_\theta,\quad a_i\neq 0. \tag{42}$$

The condition $X\Psi=\lambda\Psi$ provides a wave function in the form

$$\Psi(\rho,\theta)=\begin{pmatrix}F_1(\rho)e^{i(\lambda/a_1)\theta}\\ F_2(\rho)e^{i(\lambda/a_2)\theta}\end{pmatrix}. \tag{43}$$

Substituting into the Pauli equation with Hamiltonian (23) we find that the function $F_i(\rho)$ satisfies

$$\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{1}{\rho^2}\frac{\lambda^2}{a_i^2}\right)+\frac{1}{2}\gamma^2\rho^2\right\}F_i=\left(E\mp\gamma\frac{\lambda}{a_i}\right)F_i, \tag{44}$$

so both components satisfy radial harmonic oscillator type equations.

The solution of Eq. (44) is

$$F_i(\rho)=N_{n_i m_i}e^{-(\gamma/2)\rho^2}\rho^{|m_i|}L_{n_i}^{|m_i|}(\gamma\rho^2), \tag{45}$$

where $L_{n_i}^{|m_i|}(z)$ are Laguerre polynomials. The quantum number λ satisfies

$$\frac{\lambda}{a_1}=m_1,\quad \frac{\lambda}{a_2}=m_2; \tag{46}$$

hence we must choose

$$\frac{a_2}{a_1}=\frac{m_1}{m_2} \tag{47}$$

rational. The energy satisfies

$$E-\gamma m_1=\gamma(2n_1+|m_1|+1),$$

$$E+\gamma m_2=\gamma(2n_2+|m_2|+1), \tag{48}$$

so the two radial quantum numbers are constrained by

$$2(n_2-n_1)=m_1\left(\frac{a_1}{a_2}+1\right)-|m_1|\left(\left|\frac{a_1}{a_2}\right|-1\right). \tag{49}$$

If we normalize to have

$$\int_0^\infty\int_0^{2\pi}(|\Psi_1|^2+|\Psi_2|^2)\rho\,d\rho\,d\theta=1, \tag{50}$$

we must put the normalization constants in (45) equal to

$$N_{n_i m_i}=\sqrt{\frac{\gamma^{|m_i|+1}}{2\pi}}\sqrt{\frac{n_i!}{(n_i+|m_i|)!}}. \tag{51}$$

2. Cartesian case

We choose the operator to be diagonalized in the form

$$X=\begin{pmatrix} a_1(i\partial_y+\gamma x) & 0 \\ 0 & a_2(i\partial_y-\gamma x)\end{pmatrix}, \quad a_i\neq 0. \tag{52}$$

The equation $X\Psi=\lambda\Psi$ implies

$$\Psi=\begin{pmatrix} F_1(x)e^{-(i/a_1)(\lambda-a_1\gamma x)y} \\ F_2(x)e^{-(i/a_2)(\lambda+a_2\gamma x)y}\end{pmatrix}. \tag{53}$$

Substituting into the Pauli equation $H\Psi=E\Psi$ with H as in Eq. (23), we obtain

$$\ddot{F}_i-4\gamma^2\left(x\mp\frac{\lambda}{2a_i\gamma}\right)^2F_i+2EF_i=0, \quad i=1,2, \tag{54}$$

and hence

$$F_i=N_{n_i}e^{-\gamma\tilde{x}_i^2}H_{n_i}(\sqrt{2\gamma}\tilde{x}_i),$$

$$E=2\gamma\left(n_1+\frac{1}{2}\right)=2\gamma\left(n_2+\frac{1}{2}\right), \quad n_1=n_2=n,$$

$$N_{n_i}=\sqrt{\frac{\sqrt{2\gamma}}{\sqrt{\pi}n!\,2^n}}, \quad \tilde{x}_{1,2}=x\mp\frac{\lambda}{2a_i\gamma}, \tag{55}$$

where $H_n(z)$ is a Hermite polynomial.

3. Mixed case

Let us take the operator X in the form

$$X=\begin{pmatrix} -ia_1\partial_\theta & 0 \\ 0 & a_2(i\partial_y-\gamma x)\end{pmatrix}, \quad a_i\neq 0. \tag{56}$$

The wave function will then be

$$\Psi=\begin{pmatrix} F_1(\rho)e^{i(\lambda/a_1)\theta} \\ F_2(x)e^{-(i/a_2)(\lambda+a_2\gamma x)y}\end{pmatrix}, \tag{57}$$

where (ρ,θ) are polar coordinates; (x,y) Cartesian ones. The function $F_1(\rho)$ will satisfy Eq. (44) with $i=1$; $F_2(x)$ Eq. (54) with $i=2$. We hence obtain

$$F_1(\rho)=N_{n_1m_1}\,e^{-(\gamma/2)\rho^2}\rho^{|m_1|}L_{n_1}^{|m_1|}(\gamma\rho^2),$$

$$F_2(x)=N_{n_2}e^{-\gamma\tilde{x}_2^2}H_{n_2}(\sqrt{2\gamma}\tilde{x}_2), \tag{58}$$

with

$$E=\gamma(m_1+2n_1+|m_1|+1)=2\gamma\left(n_2+\frac{1}{2}\right). \tag{59}$$

B. Hamiltonians with one first order integral

1. Polar case

We consider the potential $V_0=V_0(\rho)$, $V_1=V_1(\rho)$ as in Eq. (33). We write the integral (34) in the form

$$X=-i\begin{pmatrix}a_1 & 0\\ 0 & a_2\end{pmatrix}\partial_\theta, \quad a_i\neq 0, \tag{60}$$

and the equation $X\Psi=\lambda\Psi$ implies

$$\Psi(\rho,\theta)=\begin{pmatrix}F_1(\rho)e^{i(\lambda/a_1)\theta}\\ F_2(\rho)e^{i(\lambda/a_2)\theta}\end{pmatrix}. \tag{61}$$

Substituting into the Pauli equation, we find that the radial functions F_1, F_2 satisfy

$$\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{1}{\rho^2}\frac{\lambda^2}{a_i^2}\right)+V_0\pm V_1\frac{\lambda}{a_i}\right\}F_i=EF_i, \quad i=1,2. \tag{62}$$

For instance, choosing

$$V_0=\frac{\alpha}{\rho}, \quad V_1=\frac{\beta}{\rho^2}, \tag{63}$$

we can solve Eq. (62) in terms of Coulomb wave functions.

2. Cartesian case

Let us now consider V_0, V_1 and the integral X as in (40) and (41). The equation $X\Psi=\lambda\Psi$ with X as in (41) implies

$$\Psi=\begin{pmatrix}\chi_1(x)e^{i\{[\lambda-(1+b_0)\phi_0(x)]/(1+b_0)\}y}\\ \chi_2(x)e^{i\{[\lambda-(1-b_0)\phi_0(x)]/(b_0-1)\}y}\end{pmatrix}. \tag{64}$$

The Pauli equation then reduces to the following two ODEs:

$$\ddot{\chi}_i-\left\{\frac{(\lambda\mp(b_0\pm1)\phi_0)^2}{(b_0\pm1)^2}\mp2x\phi_0'\frac{\lambda\mp(b_0\pm1)\phi_0}{(b_0\pm1)}+2F(x)-2E\right\}\chi_i=0, \quad i=1,2. \tag{65}$$

To solve these equations, or analyze further, we would have to specify the two functions $F(x)$, $\phi_0(x)$.

VI. CONCLUSIONS

Let us first of all compare the problem of integrability and superintegrability for particles with spin $s=0$ and spin $s\neq0$; in this case $s=\frac{1}{2}$. The spin zero case with a scalar potential in the two-dimensional Euclidean space E_2 corresponds to the Hamiltonian (1). First-order superintegrability is trivial: it requires $V(x)=$ const and corresponds to free motion. Superintegrability with one first-order and one second-order integral occurs for the potentials $V=\alpha r^2$, αr^{-1}, αx, and αx^{-2}.[18] Quadratic superintegrability leads to four families of potentials,[9,21] each depending on three significant constants and allowing the separation of variables in at least two coordinate systems.

By contrast, for $s=\frac{1}{2}$ first-order superintegrability leads to a nontrivial system, namely the Hamiltonian (23) with the symmetry algebra (24). The Hamiltonian allows the separation of variables in polar coordinates [see (43)] and "R separation" in Cartesian ones [see (53)]. Indeed, in Eq. (53) there is a term involving the product xy that does not depend on the separation constant λ. The same is true for Hamiltonians, allowing just one first-order integral. In the polar case we have separation [see (61)], in the Cartesian one R separation (64).

The next step in this research program will be to look for integrable and superintegrable systems with spin in Euclidean 3-space. This would provide a realistic and solvable model for pion-nucleon and possibly nucleon-nucleon interactions.

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When is negativity not a problem for the ultradiscrete limit?

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The "ultradiscrete limit" has provided a link between integrable difference equations and cellular automata displaying soliton-like solutions. In particular, this procedure generally turns *strictly positive* solutions of algebraic difference equations with *positive* coefficients into corresponding solutions to equations involving the "Max" operator. Although it certainly is the case that dropping these positivity conditions creates potential difficulties, it is still possible for solutions to persist under the ultradiscrete limit, even in their absence. To recognize when this will occur, one must consider whether a certain expression, involving a measure of the rates of convergence of different terms in the difference equation and their coefficients, is equal to zero. Applications discussed include the solution of elementary ordinary difference equations, a discretization of the Hirota Bilinear Difference Equation and the identification of integrals of motion for ultradiscrete equations.
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I. INTRODUCTION

Integrable nonlinear partial differential equations are of special interest in part because of their "soliton solutions" that exhibit particle-like behavior.[1,3,7,23] The link between these equations and the cellular automata that exhibit superficially similar solutions[2,11,13,18] was the observation in Ref. 20 that solutions to the discretizations of the soliton equations become solutions to these cellular automata under the "ultradiscrete limit." Loosely speaking, this works because of the fact that, for $a,b \in \mathbb{R}$

$$\lim_{\epsilon \to 0^+} \epsilon \ln(e^{a/\epsilon} + e^{b/\epsilon}) = \mathrm{Max}(a,b). \tag{1}$$

This formula can be understood intuitively by noting that the term corresponding to the smaller of the two exponents will be relatively insignificant when ϵ is very small and that with it eliminated the entire expression is simply equal to the numerator of the other exponent. It can also be easily verified using L'Hôpital's rule.

In applying (1) to difference equations, previous authors have been very cautious, allowing negative coefficients in front of the exponentials, and have not been concerned at all about the question of how allowing a and b in the formula above to depend on ϵ might affect the outcome. In fact, they are correct that letting those coefficients be negative may invalidate the prediction that the resulting limit will merely be given by the "Max." In this paper, we will be especially interested in the case in which the linear combination of exponential functions *does* involve negative coefficients. Our viewpoint is that it is worthwhile to investigate this situation to understand what can go wrong.

Theorem 2.1 demonstrates two surprising facts: (a) Even if negative coefficients are involved, a formula analogous to (1) continues to work "most of the time." (b) In determining when it might

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fail, it is necessary to explicitly consider the rate of convergence of the exponents under the limit in ϵ. This theorem is illustrated by an application to two simple, ordinary difference equations in Sec. III. In a more sophisticated application, the theorem is used to guarantee the production of a solution to an ultradiscrete limit of the Hirota Bilinear Difference Equation in Sec. IV. Finally, these results are applied to the question of when integrals of motion for difference equations survive the ultradiscrete limit in Sec. V.

Both to refer readers to other work that may be of interest and to emphasize the differences with this paper, we would like to conclude this Introduction with a discussion of three other papers. Equation (1) has been previously generalized in Ref. 21 to the case in which a and b are complex constants. This is of great interest, but clearly quite different from what we do below by allowing the argument of the logarithm to be an arbitrary linear combination of exponentials and letting the exponents be real functions of ϵ. Also, Ref. 8 presents work related to the goals of the present paper by addressing the question of how one can take an ultradiscrete limit of a solution to a difference equation that takes on negative values. Their approach involves an alternative method of introducing dependence on ϵ into the solution so that the new variable can be real, even in the case that the original variable was negative. However, in doing so, they are careful to be certain that they always apply (1) only in the case that the coefficients of the exponentials are equal to one and make no explicit mention of the possibility that the results may be affected by the dependence of the exponents on ϵ. So, that paper takes what might be viewed as an "orthogonal" approach to the question to the one that will be pursued later. It might be of interest to attempt to combine the two, by applying Theorem 2.1 to the *s-ultradiscrete limit* as defined in that paper. Finally, perhaps most closely related to this paper in spirit, Ref. 12 generalizes the procedure of ultradiscretization by formally extending the Max-Plus algebra through the introduction of an extra $\mathbb{Z}_2$ component. This extension of the Max-Plus semiring to a full ring, as is normally done in the Max-Plus community by moving to the symmetrized ring $\mathbb{S}_{\max}$,[4] means that the resulting equations are not ordinary ultradiscrete equations (the Max operator and even equality have slightly different meanings). In contrast, in this paper we address the question of when negativity fails to create any problems under the original definition of the ultradiscrete limit and integrable ultra-discrete equations.

A. Notation

In the following, a superscript of ϵ will indicate that the parameter depends *differentiably* on the real variable ϵ in some open interval $(0,\beta)$. Thus u_n^ϵ would be an ϵ dependent bi-infinite sequence and could be a solution to a difference equation in which the coefficients also depend on ϵ, and we would only call it a solution if the equation were true, not only for all n but also for all $\epsilon \in (0,\beta)$. [For example, $u_n^\epsilon = \epsilon n$ satisfies $u_{n+1}^\epsilon u_{n-1}^\epsilon = (u_n^\epsilon)^2 - \epsilon^2$].

B. An enlightening example

As we will see in Theorem 2.1, it is possible to generalize (1) to the case in which the argument of the logarithm is a more general linear combination of exponentials whose exponents depend on ϵ. As one might guess, the value of the limit turns out to be equal to the maximum of the limits of the numerators of the exponents. However, the theorem can only be applied subject to the condition that a certain expression involving the coefficients and the rates of convergence is not equal to zero. Following is a cautionary example whose purpose is to illustrate the fact that failing to consider this condition is liable to produce incorrect results.

If we consider the expression

$$\tau = e^{u_1^\epsilon/\epsilon} + \gamma e^{u_2^\epsilon/\epsilon}$$

then using the previously stated argument that the term with the lower power can simply be ignored, we may naively think that

$$\lim_{\epsilon\to 0^+} \epsilon \ln \tau = \mathrm{Max}(u_1,u_2), \quad \text{where } u_i = \lim_{\epsilon\to 0^+} u_i^\epsilon. \tag{2}$$

However, (2) may be false for some choices of u_i^ϵ and γ.

For instance, if we let

$$u_1^\epsilon = a + 2\epsilon \ln(e^{-k/\epsilon} + \sqrt{8 + e^{-2k/\epsilon}}), \quad u_2^\epsilon = a + \epsilon \ln 2 \quad \text{and } \gamma = -4$$

where $k>0$ and a is arbitrary, then

$$u_1 = u_2 = a.$$

However, despite the predictions of Eq. (2), one can check that, in fact,

$$\lim_{\epsilon\to 0^+} \epsilon \ln \tau = a - k.$$

The total avoidance of negativity in the literature on "ultradiscrete limits" might suggest that it is the fact that $\gamma<0$ that is causing a problem here, but that would be a drastic oversimplification. The fact is that for *any* choice of $\gamma\neq -4$ the prediction of (2) would have been correct and the limit would have the value a, as expected. So, an explanation of this phenomenon would have to shed light on the question of why this occurs only at $\gamma=-4$. (Such an explanation is provided in the following section.)

This example is not as artificial as it may at first seem since it will arise in a more general form as part of an investigation of a simple ordinary difference equation in Sec. III. It demonstrates that the coefficients in the linear combination of exponentials can have unexpected effects on the "ultradiscrete limit." It also demonstrates that the natural generalization of (1) provided by (2) is correct *generically* in the sense that it is only for rather specific choices of coefficient that it fails.

II. A MORE GENERAL LIMIT

In this section we state and prove a generalization of (1) that will later be applied to questions involving difference equations. We wish to consider instead the case in which the argument of the logarithm, τ, may be an arbitrary linear combination of exponentials and in which the numerator of the exponents can also depend upon ϵ. The following theorem gives conditions that are sufficient (but not necessary, as we will see in Sec. III A) to conclude that the limit of $\epsilon \ln \tau$ is still equal to the largest limit of the numerators of the exponents.

Theorem 2.1: *Let*

$$\tau = \sum_{i=1}^{n} \gamma_i e^{w_i^\epsilon/\epsilon}, \tag{3}$$

where $\gamma_i \in \mathbb{C}$ *are arbitrary, nonzero constants and* w_i^ϵ *are real valued functions such that the limits*

$$M_i = \lim_{\epsilon\to 0^+} w_i^\epsilon, \quad i = 1, \ldots, n,$$

are finite. Let

$$\mathfrak{M} = \mathrm{Max}(M_1, \ldots, M_n) \quad \text{and} \quad \mathfrak{I} = \{i | M_i = \mathfrak{M}\}$$

denote the largest value of these limits and the set of indices for which this maximum is achieved, respectively.

Then

$$\lim_{\epsilon\to 0^+} \epsilon \ln \tau = \mathfrak{M},$$

if either

(i) $|\mathfrak{I}|=1$ (*the maximum is achieved only once*) or
(ii) *the limits*

$$\mu_i = \lim_{\epsilon\to 0^+} (w_i^\epsilon - \mathfrak{M})/\epsilon, \quad for \quad i \in \mathfrak{I}$$

are finite and $D\neq 0$, *where*

$$D = \sum_{i\in\mathfrak{I}} \gamma_i e^{\mu_i}.$$

Proof: In the case $|\mathfrak{I}|=1$ let $\mathfrak{I}=\{i_0\}$ so that $M_{i_0}=\mathfrak{M}>M_i$ for $i\neq i_0$. Then

$$\begin{aligned}\lim_{\epsilon\to 0^+} \epsilon \ln \tau &= \lim_{\epsilon\to 0^+} \epsilon \ln(e^{\mathfrak{M}/\epsilon}\sum \gamma_i e^{(w_i^\epsilon-\mathfrak{M})/\epsilon})\\ &= \epsilon \ln e^{\mathfrak{M}/\epsilon} + \epsilon \ln \sum \gamma_i e^{(w_i^\epsilon-\mathfrak{M})/\epsilon}\\ &\quad \text{(then since } w_i^\epsilon - \mathfrak{M} < 0 \text{ for } i\neq i_0 \text{ and } \epsilon \text{ sufficiently small)}\\ &= \mathfrak{M} + \lim_{\epsilon\to 0^+} \epsilon \ln \gamma_{i_0} = \mathfrak{M}.\end{aligned}$$

The situation is more complicated in the case that $|\mathfrak{I}|>1$. We now assume that $D\neq 0$ and show that again the limit is simply equal to the maximum of the exponents.

First, we wish to show that $D\neq 0$ implies that τ is nonzero on a small open interval $(0,\beta)$ and so it makes sense to consider the function $\epsilon \ln \tau$. (There is no need to require $\tau>0$, however, since the proof to follow continues to be valid in the case that this function takes on complex values or even if it becomes multivalued as a consequence of analytic continuation.)

$$\begin{aligned}D = \sum_{i\in\mathfrak{I}} \gamma_i e^{\mu_i} &= \lim_{\epsilon\to 0^+} \sum_{i\in\mathfrak{I}} \gamma_i e^{(w_i^\epsilon-\mathfrak{M})/\epsilon}\\ &\quad \text{(then since } w_i^\epsilon - \mathfrak{M} < 0 \text{ for } i\notin\mathfrak{I} \text{ and } \epsilon \text{ sufficiently small)}\\ &= \lim_{\epsilon\to 0^+} \sum_{i=1}^{n} \gamma_i e^{(w_i^\epsilon-\mathfrak{M})/\epsilon} = \lim_{\epsilon\to 0^+} e^{-\mathfrak{M}/\epsilon}\tau.\end{aligned}$$

Suppose $\epsilon_i>0$ is a sequence that converges to 0 and with the property that $\tau=0$ for $\epsilon=\epsilon_i$. Then, since the limit above converges to D, it must be the case that $D=0$. Since $D\neq 0$, no such sequence of $\{\epsilon_i\}$ can exist.

Now, we simply compute that

$$\begin{aligned}\lim_{\epsilon\to 0^+} \epsilon \ln \tau &= \lim_{\epsilon\to 0^+} \epsilon \ln(e^{\mathfrak{M}/\epsilon}\sum \gamma_i e^{(w_i^\epsilon-\mathfrak{M})/\epsilon})\\ &= \lim_{\epsilon\to 0^+} \epsilon \ln e^{\mathfrak{M}/\epsilon} + \lim_{\epsilon\to 0^+} \epsilon \ln \sum_{i=1}^{n} e^{(w_i^\epsilon-\mathfrak{M})/\epsilon}\\ &= \mathfrak{M} + \lim_{\epsilon\to 0^+} \epsilon \ln\left(\sum_{i\in\mathfrak{I}} e^{(w_i^\epsilon-\mathfrak{M})/\epsilon} + \sum_{i\notin\mathfrak{I}} e^{(w_i^\epsilon-\mathfrak{M})/\epsilon}\right)\\ &= \mathfrak{M} + \lim_{\epsilon\to 0^+} \epsilon \ln(D+0) = \mathfrak{M}.\end{aligned}$$

□

Note that, apart from the restriction that $D\neq 0$, the value of the limit is independent of the choice of coefficients γ_i. We will take advantage of this feature in Secs. III–V to effectively apply

the procedure of ultradiscrete limits to integrable difference equations, even in the absence of any positivity restrictions. Furthermore, note that as a consequence of this lack of dependence on the value of the coefficients, the limit will be unaffected by an extra common factor of -1. In particular, we have the following corollary.

Corollary 2.2: If the conditions of Theorem 2.1 are met, then

$$\lim_{\epsilon\to 0^+} \epsilon \ln|\tau| = \lim_{\epsilon\to 0^+} \epsilon \ln \tau.$$

Again, this ability for us to take the absolute value prior to taking the ultra-discrete limit will be useful in our attempt to apply this result in the case of difference equations.

A. Continuation of earlier example

It is important to note that if neither conditions (i) or (ii) are met, then the value of the limit cannot necessarily be determined through knowledge of the limits M_i of the functions in the exponents. This is demonstrated by the example from Sec. I B in which the value of the limit of the entire expression, $a-k$, depends on the parameter k not appearing in the limits of the functions in the exponents when $\gamma=-4$.

We can now apply Theorem 2.1 to explain the significance of $\gamma=-4$ in that example. Again let

$$\tau = e^{u_1^\epsilon/\epsilon} + \gamma e^{u_2^\epsilon/\epsilon}, \quad u_1^\epsilon = a + 2\epsilon \ln(e^{-k/\epsilon} + \sqrt{8 + e^{-2k/\epsilon}}) \quad \text{and} \quad u_2^\epsilon = a + \epsilon \ln 2,$$

but consider γ arbitrary. The paramters μ_i measuring convergence are then

$$\mu_1 = \lim_{\epsilon\to 0^+} (u_1^\epsilon - a)/\epsilon = \ln 8 \quad \text{and} \quad \mu_2 = \lim_{\epsilon\to 0^+} (u_2^\epsilon - a)/\epsilon = \ln 2.$$

Hence, we find that

$$D = e^{\ln 8} + \gamma e^{\ln 2} = 2(4+\gamma).$$

Since this is only equal to zero at $\gamma=-4$, the "mystery" is resolved.

B. An example where *D* does not exist

To illustrate the role of condition (i) in Theorem 2.1, we briefly point out that for

$$\tau = e^{u_1^\epsilon/\epsilon} - e^{u_2^\epsilon/\epsilon} \quad u_1^\epsilon = \epsilon \sin(1/\epsilon) \quad u_2^\epsilon = -2 + 3\epsilon,$$

one has $\mathfrak{M}=\lim_{\epsilon\to 0^+} u_1^\epsilon = 0 > \lim_{\epsilon\to 0^+} u_2^\epsilon = -2$. Since $|\mathfrak{I}|=1$, we know that $\lim_{\epsilon\to 0^+}\epsilon \ln \tau = 0$, even though the limit defining μ_1 has no value.

III. APPLICATION: ORDINARY DIFFERENCE EQUATIONS

Consider the difference equation

$$\sum_{i=1}^{N} \left(\alpha_i^\epsilon \prod_{j=-d}^{d} (x_{n+j}^\epsilon)^{m_{ij}} \right) = \sum_{i=1}^{\hat{N}} \left(\hat{\alpha}_i^\epsilon \prod_{j=-d}^{d} (x_{n+j}^\epsilon)^{\hat{m}_{ij}} \right). \tag{4}$$

We will generally be interested in the case $m_{ij}, \hat{m}_{ij} \in \mathbb{Z}$ for the sake of preserving the integrality of solutions under the ultradiscrete limit.

Definition 3.1: *We say that a solution x_n^ϵ to (4) is a candidate for the ultradiscrete limit if the following conditions are met:*

- *$x_{n-d}^\epsilon, \ldots, x_{n+d}^\epsilon$, α_i^ϵ, and $\hat{\alpha}_i^\epsilon$ take non-zero real values for $\epsilon \in (0, \beta)$ for some small, positive number β.*

- The limits $u_n=\lim_{\epsilon\to 0^+}\epsilon\ln|x_n^\epsilon|$, $A_i=\lim_{\epsilon\to 0^+}\epsilon\ln|\alpha_i^\epsilon|$, *and* $\hat{A}_i=\lim_{\epsilon\to 0^+}\epsilon\ln|\hat{\alpha}_i^\epsilon|$ *exist and are finite*.
- The limits

$$\mu_i=\lim_{\epsilon\to 0^+}\frac{(\epsilon\ln|\alpha_i^\epsilon|+\epsilon\sum_{j=-d}^{d}m_{ij}\ln|x_{n+j}^\epsilon|)-\mathfrak{M}}{\epsilon},\quad \text{for } i\in\mathfrak{I}$$

and

$$\hat{\mu}_i=\lim_{\epsilon\to 0^+}\frac{(\epsilon\ln|\hat{\alpha}_i^\epsilon|+\epsilon\sum_{j=-d}^{d}\hat{m}_{ij}\ln|x_{n+j}^\epsilon|)-\hat{\mathfrak{M}}}{\epsilon},\quad \text{for } i\in\hat{\mathfrak{I}}$$

exist and are finite where

$$\mathfrak{M}=\operatorname*{Max}_{i=1}^{N}\left(A_i+\sum_{j=-d}^{d}m_{ij}u_{n+j}\right)$$

and

$$\mathfrak{I}=\left\{i\middle|A_i+\sum_{j=-d}^{d}m_{ij}u_{n+j}=\mathfrak{M}\right\}$$

is the set of indices for which this maximum is attained, and, similarly,

$$\hat{\mathfrak{M}}=\operatorname*{Max}_{i=1}^{\hat{N}}\left(\hat{A}_i+\sum_{j=-d}^{d}\hat{m}_{ij}u_{n+j}\right)\quad \textit{and}\ \hat{\mathfrak{I}}=\left\{i\middle|\hat{A}_i+\sum_{j=-d}^{d}\hat{m}_{ij}u_{n+j}=\hat{\mathfrak{M}}\right\}.$$

Theorem 3.2: *Suppose x_n^ϵ is a solution to the algebraic difference equation (4), which is a candidate for the ultradiscrete limit (see Definition 3.1 for terminology and notation). The ultradiscrete limit of x_n^ϵ,*

$$u_n=\lim_{\epsilon\to 0^+}\epsilon\ln|x_n^\epsilon|$$

is a solution to the equation

$$\operatorname*{Max}_{i=1}^{N}\left(A_i+\sum_{j=-d}^{d}m_{ij}u_{n+j}\right)=\operatorname*{Max}_{i=1}^{\hat{N}}\left(\hat{A}_i+\sum_{j=-d}^{d}\hat{m}_{ij}u_{n+j}\right)\tag{5}$$

if the maximum value on each side is never attained simultaneously for more than one value of the index, or as long as both

$$\sum_{i\in\mathfrak{I}}\sigma_i e^{\mu_i}\neq 0\quad\text{and}\ \sum_{i\in\hat{\mathfrak{I}}}\hat{\sigma}_i e^{\hat{\mu}_i}\neq 0,\tag{6}$$

where

$$\sigma_i=\frac{|\alpha_i^\epsilon\prod_{j=-d}^{d}(x_{n+j}^\epsilon)^{m_{ij}}|}{\alpha_i^\epsilon\prod_{j=-d}^{d}(x_{n+j}^\epsilon)^{m_{ij}}},\qquad \hat{\sigma}_i=\frac{|\hat{\alpha}_i^\epsilon\prod_{j=-d}^{d}(x_{n+j}^\epsilon)^{\hat{m}_{ij}}|}{\hat{\alpha}_i^\epsilon\prod_{j=-d}^{d}(x_{n+j}^\epsilon)^{\hat{m}_{ij}}},$$

are the signs of the corresponding term in the equation.

Proof: Letting

$$w_i^\epsilon = \epsilon \ln \left| \alpha_i^\epsilon \prod_{j=-d}^{d} (x_{n+j}^\epsilon)^{m_{ij}} \right|,$$

we can write the left side of (4) in the form

$$\tau = \sum_{i=1}^{N} \sigma_i e^{w_i^\epsilon/\epsilon}.$$

If $|\mathfrak{I}|=1$ or $D\neq 0$, then Theorem 2.1 tells us that the limit of $\epsilon \ln \tau$ will be

$$\max_{i=1}^{N}(\lim_{\epsilon\to 0^+} w_i^\epsilon).$$

But that D is nonzero is exactly the first of the two requirements in (6) and so

$$\lim_{\epsilon\to 0^+} w_i^\epsilon = \lim_{\epsilon\to 0^+}\left(\epsilon \ln \alpha_i^\epsilon + \epsilon \sum_{j=-d^d} m_{ij} \ln x_{n+j}^\epsilon\right) = A_i + \sum_{j=-d}^{d} m_{ij} u_{n+j},$$

and that $|\mathfrak{I}|=1$ is equivalent requiring that the maximum on the left hand side of (5) is achieved for a unique value of the index.

Similarly, we conclude that the limit of ϵ times the log of the right hand side of the equation is $\mathrm{Max}_i(\hat{A}_i+\Sigma_{j=-d}^{d}\hat{m}_{ij}u_{n+j})$. If x_n^ϵ is a solution, then these two sides are always equal and hence their limits are equal as well. □

A. Basic example

Consider the difference equation

$$x_{n+1}^\epsilon + e^{2b/\epsilon} x_{n-1}^\epsilon - e^{2c/\epsilon} x_{n-1}^\epsilon = 2e^{b/\epsilon} x_n^\epsilon. \tag{7}$$

Let $N=3$ because there are three terms on the left, $\hat{N}=1$ because there is one monomial on the right, and $d=1$ because we only see n shifted up and down by this much. The monomials on the left are given by letting

$$\alpha_1^\epsilon = \sigma_1 = 1, \quad m_{1,-1} = m_{1,0} = 0, \quad m_{1,1} = 1,$$

$$\alpha_2^\epsilon = e^{2b/\epsilon}, \quad \sigma_2 = 1, \quad m_{2,-1} = 1, \quad m_{2,0} = m_{2,1} = 0,$$

and

$$\alpha_3^\epsilon = e^{2c/\epsilon}, \quad \sigma_3 = -1, \quad m_{3,-1} = 1, \quad m_{3,0} = m_{3,1} = 0.$$

The monomial on the right is given by letting

$$\hat{\sigma}_1 = 1, \quad \hat{\alpha^\epsilon} = 2e^{b/\epsilon}, \quad \hat{m}_{1,-1} = \hat{m}_{1,1} = 0 \quad \text{and} \quad \hat{m}_{1,0} = 1.$$

A solution to this equation is given by

$$x_n^\epsilon = (e^{b/\epsilon} + e^{c/\epsilon})^n,$$

since expanding the left hand side of (7) with this definition for x_n^ϵ gives an expression equal to the right hand side for any n or ϵ.

Trivially, this same solution x_n^ϵ *also* solves the difference equation

$$e^{2b/\epsilon}x_{n-1}^{\epsilon} - e^{2c/\epsilon}x_{n-1}^{\epsilon} = 2e^{b/\epsilon}x_n^{\epsilon} - x_{n+1}^{\epsilon}. \tag{8}$$

In fact, in most circumstances one would want to consider this equation to be completely equivalent to (7) since one can simply add x_{n+1}^{ϵ} to both sides of one to make it into the other. *However*, for the purposes of this paper they are quite different.

Regardless of whether we are working with the difference equation in the form (7) or (8), the solution $x_n^{\epsilon}=(e^{b/\epsilon}+e^{c/\epsilon})^n$ is the same. Then our solution u_n to the ultradiscrete equation should take the form

$$u_n = \lim_{\epsilon\to 0^+} \epsilon \ln(e^{b/\epsilon}+e^{c/\epsilon})^n = n \lim_{\epsilon\to 0^+} \epsilon \ln(e^{b/\epsilon}+e^{c/\epsilon}) = n\,\mathrm{Max}(b,c).$$

Ignoring condition (6) of Theorem 3.2, we get from (7) that u_n should satisfy

$$\mathrm{Max}(u_{n+1}, 2b+u_{n-1}, 2c+u_{n-1}) = b+u_n, \tag{9}$$

and from (8) we get that it should satisfy

$$\mathrm{Max}(2b+u_{n-1}, 2c+u_{n-1}) = \mathrm{Max}(b+u_n, u_{n+1}). \tag{10}$$

However, it is *not* the case that u_n satisfies each of these equations, regardless of the choice of b and c. In particular, condition (6) may not be met and, as we will see, this causes u_n not to solve (9) when $b<c$.

Look at the arguments of Max on the left hand side of (9) and consider the question of which of them are *equal* to the maximum value. If $b>c$ then the terms have the values $(n+1)b$, $(n+1)b$ and $(n-1)b+2c$, respectively, so that the first two terms are equal to the maximum value. [Using the notation of the theorem, $\mathfrak{M}=(n+1)b$ and $\mathfrak{I}=1,2$.] All of the μ_i are zero (which means that these solutions converge quickly to their limits), and so all of the exponential terms are just equal to one. Now, we must look at the sum of σ_1 and σ_2 to make certain that it is not equal to zero. Since $\sigma_1+\sigma_2=2\neq 0$, the condition is met. And, in fact, one can easily verify that if $b>c$, then $u_n=nb$ *is* indeed a solution to (9). However, when $b<c$, then things are quite different. In that case, $\mathfrak{M}=(n+1)c$ and$\mathfrak{I}=\{1,3\}$, but $\sigma_1+\sigma_3=0$, and so Theorem 3.2 does *not* predict that u_n will solve the equation. In fact, it does not, because then the left hand side has the value $(n+1)c$ while the right side has the value $nc+b$.

In contrast, the theorem predicts that u_n will solve (10) when $b>c$ *and* when $b<c$. In particular, if $b>c$, then $\mathfrak{M}=\mathrm{Max}(2b+u_{n-1},2c+u_{n-1})=(n+1)b$ and $\mathfrak{I}=\{1\}$, while if $c>b$ then $\mathfrak{M}=(n+1)c$ and $\mathfrak{I}=\{2\}$. Thus, we conclude from the theorem that u_n should satisfy (10) as long as $b\neq c$. In fact, it can be checked explicitly that u_n is a solution to (10) in the case $b=c$ as well. This is true even though the conditions of the theorem fail to be satisfied in that case. This shows that the conditions of the theorem, while sufficient, are not necessary.

B. Another example: Demonstrating the role of rate of convergence

Consider the difference equation

$$x_{n+1}^{\epsilon} - 2x_{n-1}^{\epsilon} = e^{\lambda/\epsilon}x_n^{\epsilon}.$$

Considering the survival of solutions of this equation under the ultradiscrete limit illustrates the importance of the parameters μ_i, which measure the rate of convergence of the terms.

This has a solution of the form

$$x_n^{\epsilon} = \left(\frac{\sqrt{8+e^{2\lambda/\epsilon}}+e^{\lambda/\epsilon}}{2}\right)^n.$$

Consequently, we would expect

$$u_n = \lim_{\epsilon \to 0^+} \epsilon \ln x_n^\epsilon = \begin{cases} n\lambda, & \lambda > 0, \\ 0, & \lambda \le 0, \end{cases}$$

to solve

$$\mathrm{Max}(u_{n+1}, u_{n-1}) = \lambda + u_n.$$

And, indeed, if $\lambda > 0$ this is true. However, it fails when $\lambda < 0$. This could be predicted by the Theorem. Condition (6) is trivially met when $\lambda > 0$ because the exponents on the left do not have the same limit. However, when $\lambda < 0$ then both exponents go to 0 and $\mu_1 = \ln 2$, and hence the sum is $D = e^{\ln 2} - e^{\ln 2} = 0$.

IV. APPLICATION: HIROTA BILINEAR DIFFERENCE EQUATION

The Hirota Bilinear Difference Equation (HBDE)[10,17,22] for a function $x^\epsilon(a,b,c,d)$ of four variables is

$$\begin{aligned}(\lambda_4^\epsilon - \lambda_3^\epsilon)(\lambda_2^\epsilon - \lambda_1^\epsilon) x^\epsilon(a,b,c+1,d+1) x^\epsilon(a+1,b+1,c,d) \\ + (\lambda_4^\epsilon - \lambda_1^\epsilon)(\lambda_3^\epsilon - \lambda_2^\epsilon) x^\epsilon(a+1,b,c,d+1) x^\epsilon(a,b+1,c+1,d) \\ = (\lambda_4^\epsilon - \lambda_2^\epsilon)(\lambda_3^\epsilon - \lambda_1^\epsilon) x^\epsilon(a+1,b,c+1,d) x^\epsilon(a,b+1,c,d+1).\end{aligned}$$

As a consequence of the main result in Ref. 5, a solution to this equation can be constructed as

$$x^\epsilon(a,b,c,d) = \det(P \cdot (I - \lambda_1^\epsilon S)^a \cdot (I - \lambda_2^\epsilon S)^b \cdot (I - \lambda_3^\epsilon S)^c \cdot (I - \lambda_4^\epsilon S)^d \cdot \Omega),$$

where Ω is any $n \times k$ matrix ($k < n$), S is any $n \times n$ matrix such that the lower-left $k \times (n-k)$ block has rank one, I is the $n \times n$ identity matrix, and $P = (0 I_k)$ is the $k \times n$ matrix that has the $k \times k$ identity matrix as a block and all zeroes to the left of it.

It is interesting to note that even though $x^\epsilon(a,b,c,d)$ has dependence upon ϵ inherited from the presence of λ_i^ϵ in the formula, one is also free to choose S and Ω to depend upon ϵ and $x^\epsilon(a,b,c,d)$ would still solve the difference equation.

For example, let us consider

$$\lambda_1^\epsilon = e^{-2/\epsilon} - e^{2/\epsilon} + e^{3/\epsilon}, \quad \lambda_2^\epsilon = e^{3/\epsilon} - e^{2/\epsilon}, \quad \lambda_3^\epsilon = e^{3/\epsilon} + e^{-2/\epsilon}, \quad \lambda_4^\epsilon = e^{3/\epsilon},$$

so that

$$(\lambda_4^\epsilon - \lambda_3^\epsilon)(\lambda_2^\epsilon - \lambda_1^\epsilon) = e^{-4/\epsilon}, \quad (\lambda_4^\epsilon - \lambda_2^\epsilon)(\lambda_3^\epsilon - \lambda_1^\epsilon) = e^{4/\epsilon}.$$

[It is necessarily the case that $(\lambda_4^\epsilon - \lambda_1^\epsilon)(\lambda_3^\epsilon - \lambda_2^\epsilon)$ is the difference of the other two.]

Now, just for the sake of example, let us consider the solution that comes from using $k=2$, $n=4$,

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & e^{1/\epsilon} & 0 & 0 \\ 0 & 0 & e^{5/\epsilon} & 0 \\ 0 & e^{5/\epsilon} & 0 & e^{12/\epsilon} \end{pmatrix} \quad \text{and} \quad \Omega = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{pmatrix}.$$

This solution has the form (up to a common multiple independent of a, b, c, and d that does not matter due to the bilinear nature of the equation)

$$x^\epsilon(a,b,c,d) = x_1^\epsilon(a,b,c,d) - x_2^\epsilon(a,b,c,d) + x_3^\epsilon(a,b,c,d)$$

where

$$x_1^\epsilon(a,b,c,d) = e^{4/\epsilon}(1 - e^{4/\epsilon})^d (1 - e^{-1/\epsilon} - e^{4/\epsilon})^c (1 + e^{3/\epsilon} - e^{4/\epsilon})^b (1 - e^{-1/\epsilon} + e^{3/\epsilon} - e^{4/\epsilon})^a$$

$$(1-e^{8/\epsilon})^d(1-e^{3/\epsilon}-e^{8/\epsilon})^c(1+e^{7/\epsilon}-e^{8/\epsilon})^b(1-e^{3/\epsilon}+e^{7/\epsilon}-e^{8/\epsilon})^a,$$

$$x_2^\epsilon(a,b,c,d)=(1-e^{8/\epsilon})^d(1-e^{3/\epsilon}-e^{8/\epsilon})^c(1+e^{7/\epsilon}-e^{8/\epsilon})^b(1-e^{3/\epsilon}+e^{7/\epsilon}-e^{8/\epsilon})^a$$

$$(1-e^{15/\epsilon})^d(1-e^{10/\epsilon}-e^{15/\epsilon})^c(1+e^{14/\epsilon}-e^{15/\epsilon})^b(1-e^{10/\epsilon}+e^{14/\epsilon}-e^{15/\epsilon})^a,$$

and

$$x_3^\epsilon(a,b,c,d)=e^{11/\epsilon}(1-e^{8/\epsilon})^d(1-e^{3/\epsilon}-e^{8/\epsilon})^c(1+e^{7/\epsilon}-e^{8/\epsilon})^b(1-e^{3/\epsilon}+e^{7/\epsilon}-e^{8/\epsilon})^a$$

$$(1-e^{15/\epsilon})^d(1-e^{10/\epsilon}-e^{15/\epsilon})^c(1+e^{14/\epsilon}-e^{15/\epsilon})^b(1-e^{10/\epsilon}+e^{14/\epsilon}-e^{15/\epsilon})^a.$$

Before even worrying about the structure of the equation, one must worry that this solution itself will not have a well defined or simple ultradiscrete limit. In particular, if we define

$$u(a,b,c,d)=\lim_{\epsilon\to 0^+}\epsilon\ln x^\epsilon(a,b,c,d),$$

and we do not worry about the requirement that $D\neq 0$ in Theorem 2.1, then we would conclude that

$$u(a,b,c,d)=\mathrm{Max}(4+12a+12b+12c+12d,23a+23b+23c+23d,11+23a+23b+23c+23d). \tag{11}$$

(This is found by adding up for each factor in the expression of x_i^ϵ with $i=1,2,3$ the highest numerator of the exponent when viewed as a fraction having ϵ as the denominator. For instance, the first expression is found from x_1^ϵ as $4+4d+4c+4+4a+8d+8c+8b+8a$.) Yet, as the examples of the previous section demonstrate, we ought to be worried that this formula is not accurate in the case that $D=0$ when Theorem 2.1 is applied to this example.

In fact, it turns out that there is no need to worry about this since it is always the case here that $|\mathfrak{I}|=1$. Note first that the third is always 11 more than the second, and so there is no possibility that these would be equal. By the same argument, there would be no problem if the first two were equal since they could not be the maximum (with the third being 11 more all the time). Finally, we need only worry about the possibility that the first and third are equal. Certainly, it *is* possible for these two expressions to have the same value, but *never for integer values of* a,b,c, *and* d. In particular, they are only equal when

$$a=-\left(b+c+d+\frac{7}{11}\right).$$

A similar argument applies when we wish to compute the limit of the Hirota Bilinear Difference Equation to find the equation that this $u(a,b,c,d)$ satisfies. Rewriting the HBDE as

$$\sigma_1 e^{(u^\epsilon(a+1,b+1,c,d)+u^\epsilon(a,b,c+1,d+1)-4)/\epsilon}+\sigma_2 e^{(u^\epsilon(a+1,b,c,d+1)+u^\epsilon(a,b+1,c+1,d)+\epsilon\ln(e^{4/\epsilon}-e^{-4/\epsilon}))/\epsilon}$$

$$=\sigma_3 e^{(u^\epsilon(a+1,b,c+1,d)+u^\epsilon(a,b+1,c,d+1)+4)/\epsilon},$$

where $u^\epsilon(a,b,c,d)=\epsilon\ln|u(a,b,c,d)|$ and $\sigma_1=\pm 1$ as needed when u is negative, leads to its ultradiscretization as

$$\begin{aligned}&\mathrm{Max}(u(a+1,b+1,c,d)+u(a,b,c+1,d+1)-4,\ u(a+1,b,c,d+1)+u(a,b+1,c+1,d)+4),\\&=u(a+1,b,c+1,d)+u(a,b+1,c,d+1)+4.\end{aligned} \tag{12}$$

Then to show that (11) gives a solution, we apply Theorem 3.2 and note that since

$$u(a+1,b+1,c,d) = u(a,b,c+1,d+1) = u(a+1,b,c,d+1) = u(a,b+1,c+1,d),$$

the first argument of the Max operator is always 8 less than the second argument.

V. APPLICATION: FIRST INTEGRALS

In this section, we consider difference equations that admit first integrals and ask the following question: When does the ultradiscretization of the equation leave the ultradiscretization of the first integral invariant? The study performed in this section will be more algebraic than analytic: the results about first integrals will apply to the complete set of solutions as opposed to a particular solution, as considered before.

A. Preliminary examples

A well-known class of second order difference equations is given by the *QRT* mappings discovered by Quispel, Roberts, and Thompson.[14] The ultradiscrete limit of members of that class of mappings together with their first integrals was first performed in Ref. 19, but, each time this is done, one has to check explicitly that the resulting ultradiscretization of the first integral is indeed invariant.

Let us start with the following simple example of a difference equation,

$$x_{n+1} = \frac{\alpha^{\epsilon} x_n + 1}{x_n x_{n-1}}, \tag{13}$$

where α^{ϵ} is constant in n. Equation (13) is a member of the class of QRT mappings. As such, (13) admits the following first integral,

$$\iota^{\epsilon}(x_{n-1},x_n) = x_n + x_{n-1} + \frac{\alpha^{\epsilon}}{x_n} + \frac{\alpha^{\epsilon}}{x_{n-1}} + \frac{1}{x_n x_{n-1}}. \tag{14}$$

We say that ι^{ϵ} is a first integral for (13) because $\iota^{\epsilon}(x_{n-1},x_n) = \iota^{\epsilon}(x_n,x_{n+1})$ if x_n is a solution to (13). To obtain the ultradiscrete version of these two expressions, one writes $\alpha^{\epsilon} = e^{A/\epsilon}$ and $x_n = e^{u_n/\epsilon}$. Then we take the limit as $\epsilon \to 0^+$ of the equation using the identity (1) (note that in this particular example, we do not need the more general relation given by Theorem 2.1). We obtain

$$u_{n+1} = \mathrm{Max}(u_n + A, 0) - u_n - u_{n-1} \tag{15}$$

and

$$I = \mathrm{Max}(u_n, u_{n-1}, A - u_{n-1}, A - u_n, -u_n - u_{n-1}). \tag{16}$$

The quantity I defined in (16) is conserved by the equation (15). Following Ref. 9, this can be shown directly by substituting the expression for u_{n-1} in terms of u_n and u_{n+1} coming from (15) into the definition of I as follows:

$$\begin{aligned} I_n &= \mathrm{Max}(u_n, -u_{n+1} - u_n + (u_n + A)_+, A - u_n, A + u_{n+1} + u_n - (u_n + A)_+, u_{n+1} - (u_n + A)_+) \\ &= \mathrm{Max}(u_n, A - u_{n+1}, -u_n - u_{n+1}, A - u_n, \mathrm{Max}(A + u_{n+1} + u_n - (u_n + A)_+, u_{n+1} - (u_n + A)_+)) \\ &= \mathrm{Max}(u_n, A - u_{n+1}, -u_n - u_{n+1}, A - u_n, , u_{n+1}) = I_{n+1}, \end{aligned}$$

where we have introduced the notation $(k)_+ \equiv \mathrm{Max}(k,0)$.

Another more complex example is given by a difference equation that is related (through the process of deautonomization) to a discrete version of the third Painlevé equation,[6,15,16]

$$x_{n+1} = \frac{(\alpha_1^{\epsilon}\alpha_2^{\epsilon} + x_n)(\alpha_1^{\epsilon}/\alpha_2^{\epsilon} + x_n)}{x_{n-1}(\alpha_1^{\epsilon}\alpha_3^{\epsilon} x_n + 1)(\alpha_1^{\epsilon}/\alpha_3^{\epsilon} x_n + 1)}. \tag{17}$$

Again, as a member of the QRT family of mapping, (17) has a first integral given by

$$\iota^{\epsilon} = \alpha_1^{\epsilon}\alpha_3^{\epsilon}(1+\alpha_2^{\epsilon 2})\left(\frac{1}{x_{n-1}}+\frac{1}{x_n}\right) + \alpha_1^{\epsilon}\alpha_2^{\epsilon}(1+\alpha_3^{\epsilon 2})(x_n+x_{n-1}) + \alpha_1^{\epsilon 2}\alpha_2^{\epsilon}\alpha_3^{\epsilon}\left(x_n x_{n-1}+\frac{1}{x_n x_{n-1}}\right)$$
$$+ \alpha_2^{\epsilon}\alpha_3^{\epsilon}\left(\frac{x_n}{x_{n-1}}+\frac{x_{n-1}}{x_n}\right). \tag{18}$$

The ultradiscretization of these two expressions is performed the same way as before by setting $\alpha_i^{\epsilon}=e^{A_i/\epsilon}$ and $x_n=e^{u_n/\epsilon}$. In the limit as $\epsilon\to 0^+$, one gets

$$u_{n+1} = 2u_n + (A_1+A_2-u_n)_+ + (A_1-A_2-u_n)_+ - (A_1+A_3+u_n)_+ - (A_1-A_3+u_n)_+ - u_{n-1}, \tag{19}$$

with first integral

$$I = \mathrm{Max}(A_1+A_3-u_{n-1}, A_1+A_3-u_n, A_1+A_3+2A_2-u_{n-1}, A_1+A_3+2A_2-u_n, A_1+A_2+u_n, A_1+A_2$$
$$+u_{n-1}, A_1+A_2+2A_3+u_n, A_1+A_2+2A_3+u_{n-1}, 2A_1+A_2+A_3+u_n+u_{n-1}, 2A_1+A_2+A_3-u_n$$
$$-u_{n-1}, A_2+A_3+u_n-u_{n-1}, A_2+A_3+u_{n-1}-u_n). \tag{20}$$

Checking that I defined above is a first integral is quite a cumbersome task. Instead, we will rely on a general theorem that we prove later.

B. Main result about first integrals

Consider the difference equation

$$x_{n+d}^{\epsilon} = f(x_n^{\epsilon}, x_{n+1}^{\epsilon}, \ldots, x_{n+d-1}^{\epsilon}) \tag{21}$$

where f is a rational function on $\mathbb{R}^d$ of the form

$$f(a_0,a_1,\ldots,a_{d-1}) \equiv \frac{\sum_{i=1}^{N}\left(\alpha_i^{\epsilon}\prod_{j=0}^{d-1}(a_j)^{m_{ij}}\right)}{\sum_{i=1}^{\hat{N}}\left(\hat{\alpha}_i^{\epsilon}\prod_{j=0}^{d-1}(a_j)^{\hat{m}_{ij}}\right)}.$$

A first integral for (21) is defined to be a rational function ι^{ϵ} on $\mathbb{R}^d$ of the form

$$\iota^{\epsilon}(a_0,a_1,\ldots,a_{d-1}) = \frac{\sum_{i=1}^{M}\left(\beta_i^{\epsilon}\prod_{j=0}^{d-1}(a_j)^{l_{ij}}\right)}{\sum_{i=1}^{\hat{M}}\left(\hat{\beta}_i^{\epsilon}\prod_{j=0}^{d-1}(a_j)^{\hat{l}_{ij}}\right)}, \tag{22}$$

where $l_{ij},\hat{l}_{ij}\in\mathbb{N}$, which remains invariant when restricted to any solution to (21), that is, $\iota^{\epsilon}(a_1,a_2,\ldots,a_{d-1},f(a_0,a_1,\ldots,a_{d-1}))=\iota^{\epsilon}(a_0,a_1,\ldots,a_{d-1})$. Here, we assume the coefficients β_i^{ϵ} and $\hat{\beta}_i^{\epsilon}$ to be nonzero for ϵ in a certain interval $(0,\beta)$. In all our examples, these coefficients will be exponentials and thus never zero.

The following question arises: is the ultradiscretization of (22) a first integral for the ultradiscretization of (21)? Precisely, does the function

$$I(b_0,b_1,\ldots,b_{d-1}) = \operatorname*{Max}_{i=1}^{M}\left(B_i+\sum_{j=0}^{d-1}l_{ij}b_j\right) - \operatorname*{Max}_{i=1}^{\hat{M}}\left(\hat{B}_i+\sum_{j=0}^{d-1}\hat{l}_{ij}b_j\right),$$

where $B_i,\hat{B}_i$ are defined as $B_i=\lim_{\epsilon\to 0^+}\epsilon\ln|\beta_i^{\epsilon}|$ and $\hat{B}_i=\lim_{\epsilon\to 0^+}\epsilon\ln|\hat{\beta}_i^{\epsilon}|$, define a first integral for the equation

$$u_{n+d} = g(u_n,u_{n+1},\ldots,u_{n+d-1}) \tag{23}$$

where g a function on $\mathbb{R}^d$ defined by

$$g(b_0,b_1,\ldots,b_{d-1}) \equiv \underset{i=1}{\overset{N}{\mathrm{Max}}}\left(A_i + \sum_{j=0}^{d-1} m_{ij}b_j\right) - \underset{i=1}{\overset{\hat{N}}{\mathrm{Max}}}\left(\hat{A}_i + \textstyle\sum_{j=0}^{d-1} \hat{m}_{ij}b_j\right),$$

where A_i are defined in Definition (3.1).

Before stating the theorem, let us define the function D on $\mathbb{R}^d$ by

$$D(b_0,b_1,\ldots,b_{d-1}) \equiv \sum_{i\in\mathfrak{I}} \sigma_i e^{\mu_i},$$

where

$$\sigma_i = \frac{|\beta_i^{\epsilon}(f(e^{b_0/\epsilon},e^{b_1/\epsilon},\ldots,e^{b_{d-1}/\epsilon}))^{l_{id-1}}|}{\beta_i^{\epsilon}(f(e^{b_0/\epsilon},e^{b_1/\epsilon},\ldots,e^{b_{d-1}/\epsilon}))^{l_{id-1}}}$$

[σ_i is the sign of $\beta_i^{\epsilon}(f(e^{b_0/\epsilon},e^{b_1/\epsilon},\ldots,e^{b_{d-1}/\epsilon}))^{l_{id-1}}$ for ϵ close to zero] and

$$\mathfrak{M} = \underset{i=1}{\overset{M}{\mathrm{Max}}}\left(B_i + \sum_{j=0}^{d-2} l_{ij}b_{j+1} + l_{id-1}g(b_0,b_1,\ldots,b_{d-1})\right)$$

and

$$\mathfrak{I} = \left\{ i \middle| B_i + \sum_{j=0}^{d-2} l_{ij}b_{j+1} + l_{id-1}g(b_0,b_1,\ldots,b_{d-1}) = \mathfrak{M} \right\},$$

and

$$\mu_i = \lim_{\epsilon\to 0^+} \frac{\epsilon \ln|\beta_i^{\epsilon}| + \sum_{j=0}^{d-2} l_{ij}b_{j+1} + l_{id-1}h^{\epsilon}(b_0,b_1,\ldots,b_{d-1}) - \mathfrak{M}}{\epsilon}, \text{ for } i \in \mathfrak{I},$$

where

$$h^{\epsilon}(b_0,b_1,\ldots,b_{d-1}) = \epsilon \ln(|f(e^{b_0/\epsilon},e^{b_1/\epsilon},\ldots,e^{b_{d-1}/\epsilon})|).$$

Note that

$$\lim_{\epsilon\to 0^+} h^{\epsilon}(b_0,b_1,\ldots,b_{d-1}) = g(b_0,b_1,\ldots,b_{d-1}).$$

Furthermore, the function $\hat{D}$ is defined the same way by replacing $\sigma_i,\mu_i,\alpha_i^{\epsilon},B_i,l_{ij},M$ above by $\hat{\sigma}_i,\hat{\mu}_i,\hat{\alpha}_i^{\epsilon},\hat{B}_i,\hat{l}_{ij},\hat{M}$.

Theorem 5.1: *If D and $\hat{D}$ are nonzero almost everywhere in $\mathbb{R}^d$, then I is a first integral for (23).*

Proof: By definition of I, we have the equality

$$\lim_{\epsilon\to 0^+} \epsilon \ln(\iota^{\epsilon}(e^{b_0/\epsilon},e^{b_1/\epsilon},\ldots,e^{b_{d-1}/\epsilon})) = I(b_0,b_1,\ldots,b_{d-1}).$$

Furthermore, as a direct consequence of Theorem 2.1, since both D and $\hat{D}$ are nonzero almost everywhere in $\mathbb{R}^d$, the following equality must hold everywhere, except in a subset of measure zero,

$$\lim_{\epsilon\to 0^+} \epsilon \ln(\iota^{\epsilon}(e^{b_1/\epsilon},e^{b_2/\epsilon},\ldots,e^{b_{d-1}/\epsilon},e^{h^{\epsilon}(b_0,b_1,\ldots,b_{d-1})})) = I(b_1,b_2,\ldots,b_{d-1},g(b_0,b_1,\ldots,b_{d-1})).$$

Because both the argument of the limit and the right hand side of the equation are continuous in $\mathbb{R}^d$, the equality holds in all $\mathbb{R}^d$.

Since ι^ϵ is a first integral for (21), the arguments of the two limits above are equal. Hence, since both limits exist, the right sides are equal, which shows that I is a first integral for (23). □

C. Examples

Consider the difference equation

$$x_{n+2} = -x_n - x_{n+1} + \frac{\alpha^\epsilon}{x_{n+1}}, \tag{24}$$

which admits the first integral given by

$$\iota^\epsilon = x_{n+1}^2 x_n + x_{n+1} x_n^2 - \alpha^\epsilon (x_{n+1} + x_n) \tag{25}$$

[note that (24) was intentionally written so that x_{n+2} is a function of x_n and x_{n+1} in order to apply Theorem 5.1 directly with $d=2$]. Equation (24) is related to a discrete version of the first Painlevé equation.[6,15,16] For the ultradiscrete limit, we choose $\alpha^\epsilon = e^{A/\epsilon}$ and find

$$u_{n+2} = \mathrm{Max}(u_n, u_{n+1}, A - u_{n+1}) \equiv g(u_n, u_{n+1}), \tag{26}$$

$$I(u_n, u_{n+1}) = \mathrm{Max}(2u_{n+1} + u_n, u_{n+1} + 2u_n, A + u_{n+1}, A + u_n). \tag{27}$$

The quantity defined in (27) is not a first integral for (26). To see this, we consider the specific example with $A < 8$, in which we have that $I(3,5) = 13$ and $I(5, g(5,3)) = I(5,5) = 15 \neq I(3,5)$.

We now show that the conditions of Theorem 5.1 are not met. Specifically, it is not true that the function D is nonzero almost everywhere in $\mathbb{R}^2$. We first set

$$\beta_1^\epsilon = 1, \quad l_{1,0} = 2, \quad l_{1,1} = 1,$$

$$\beta_2^\epsilon = 1, \quad l_{2,0} = 1, \quad l_{2,1} = 2,$$

$$\beta_3^\epsilon = -e^{A/\epsilon}, \quad l_{3,0} = 1, \quad l_{3,1} = 0,$$

$$\beta_4^\epsilon = -e^{A/\epsilon}, \quad l_{4,0} = 0, \quad l_{4,1} = 1.$$

and

$$\mathfrak{M} = \mathrm{Max}(2g(b_1,b_2) + b_2, g(b_1,b_2) + 2b_2, A + g(b_1,b_2), A + b_2).$$

Furthermore, to apply Theorem 5.1, it is useful to write the following quantity explicitly:

$$f(e^{b_1/\epsilon}, e^{b_2/\epsilon}) = -e^{b_1/\epsilon} - e^{b_2/\epsilon} + e^{(A-b_2)/\epsilon}.$$

Consider the case where b_2 is greater than both b_1 and $A - b_1$. We obtain $g(b_1,b_2) = b_2$ and $\mathfrak{I} = \{1,2\}$. The sign of $f(e^{b_1/\epsilon}, e^{b_2/\epsilon})$ for small positive ϵ is negative, which means that $\sigma_1 = -\sigma_2 = 1$. Since $\mu_1 = \mu_2 = 0$, we finally get that $D = e^{\mu_1} - e^{\mu_2} = 0$. Thus, the function D is zero in the semi-infinite triangular region of the plane $b_2 > b_1$ and $b_2 > A - b_1$. The conditions of the Theorem 5.1 are thus not met.

Let us now consider the two examples of Sec. V A. In both cases, all the σ_i's are equal to one. Thus, this automatically implies that both D and $\hat{D}$ are nonzero. In particular, this shows that (20) is indeed a first integral for (19).

We now consider a last example,

$$x_{n+2} = \frac{x_{n+1}}{1 - x_{n+1}^2} - x_n \equiv f(x_n, x_{n+1}), \tag{28}$$

with first integral

$$\iota = x_{n+1}^2 + x_n^2 - x_{n+1}^2 x_n^2 - x_{n+1} x_n. \tag{29}$$

The ultradiscretization reads as

$$u_{n+2} = \mathrm{Max}(u_n + 2u_{n+1}, u_{n+1}, u_n) - \mathrm{Max}(2u_{n+1}, 0) \equiv g(u_n, u_{n+1}), \tag{30}$$

$$I = \mathrm{Max}(2u_{n+1}, 2u_n, 2u_{n+1} + 2u_n, u_{n+1} + u_n). \tag{31}$$

To apply Theorem 5.1, we set

$$\beta_1^\epsilon = 1, \quad l_{1,0} = 0, \quad l_{1,1} = 2,$$

$$\beta_2^\epsilon = 1, \quad l_{2,0} = 2, \quad l_{2,1} = 0,$$

$$\beta_3^\epsilon = -1, \quad l_{3,0} = l_{3,1} = 2,$$

$$\beta_4^\epsilon = -1, \quad l_{4,0} = l_{4,1} = 1,$$

and

$$\mathfrak{M} = \mathrm{Max}(2g(b_1, b_2), 2b_2, 2g(b_1, b_2) + 2b_2, g(b_1, b_2) + b_2).$$

Furthermore, it is useful to write the following explicitly:

$$f(e^{b_1/\epsilon}, e^{b_2/\epsilon}) = \frac{e^{b_2/\epsilon}}{1 - e^{2b_2/\epsilon}} - e^{b_1/\epsilon}.$$

To prove that the function D is nonzero almost everywhere in $\mathbb{R}^2$, we consider four cases. First, in the case $b_1, b_2 > 0$, we have that $g(b_1, b_2) = b_1$ and $\mathfrak{I} = \{3\}$ and, thus, because there is only one term in D, it cannot be zero. In the case $b_2 > 0, b_1 < 0$, $g(b_1, b_2) = \mathrm{Max}(b_1, -b_2)$ and $\mathfrak{I} = \{2\}$. Again, D cannot be zero. In the case $b_2 < 0, b_1 > b_2$, we have that $g(b_1, b_2) = b_1$ and $\mathfrak{I} = \{1\}$. Finally, in the case $b_1 < b_2 < 0$, $g(b_1, b_2) = b_2$ and $\mathfrak{I} = \{1, 2, 4\}$. Here, D is not trivially nonzero and a little more work is required. The sign of $f(e^{b_1/\epsilon}, e^{b_2/\epsilon})$ for small ϵ is positive, $\mu_i = 0$, $i = 1, 2, 4$ and $\sigma_1 = \sigma_2 = -\sigma_4 = 1$. Thus, $D = 1 + 1 - 1 = 1 \neq 0$. We thus have proven that D is nonzero almost everywhere in $\mathbb{R}^2$, which means, by Theorem 5.1, that (31) is a first integral for (30). Note, however, that D is not nonzero everywhere in $\mathbb{R}^2$. For example, in the case $b_1 = 0$ and $b_2 > 0$, we have that $g(b_1, b_2) = 0$, $\mathfrak{I} = \{2, 3\}$, the sign of $f(e^{b_1/\epsilon}, e^{b_2/\epsilon})$ is negative, $\sigma_2 = -\sigma_3 = 1$, and thus $D = 0$.

VI. CONCLUSIONS

Although it is the case that problems can arise in computing a limit of the form

$$\lim_{\epsilon \to 0^+} \epsilon \ln \tau$$

with τ of the form (3) when some terms are negative, it is not true that these problems arise "most of the time." Consequently, it is often still possible to use the procedure of ultradiscrete limits developed in Ref. 20 to produce integer solutions to equations involving the "Max" operator, even in the absence of positivity, as illustrated in Secs. III and IV. Furthermore, it is especially useful to apply the results of Theorem 2.1 to the question of which integrals of motion are preserved by an ultradiscrete limit since in that case one does not need to consider individual solutions (cf. Sec. V).

It should be noted that there are various different possibilities for the value of the limit in the case that $D=0$ and $|\mathfrak{I}|>1$, which we do not presently have the ability to differentiate, in general. For instance, in the example presented in Sec. III A the value of the limit is not the maximum of the exponents as usual, but rather the next largest of the exponents. (This happens here because the sum that forms D does not only vanish in the limit but actually is equal to zero for all ϵ, as briefly mentioned in Ref. 8.) On the other hand, in the case of the limit

$$\lim_{\epsilon\to 0^+} \epsilon \ln(e^{u_1^\epsilon/\epsilon} - e^{u_2^\epsilon/\epsilon} + e^{u_3^\epsilon/\epsilon}),$$

with $u_1^\epsilon=\sin(2\epsilon)/\epsilon$, $u_2^\epsilon=2\sin(\epsilon)/\epsilon$, and $u_3^\epsilon=1$, the limit yields the maximum value of 2, despite the fact that $D=0$. Most interestingly, in the example shown in Sec. I B it is evident that the value of the limit is not determined by the values of the limits of the functions in the exponents, since the ultradiscrete limit, $a-k$, could be varied arbitrarily by selecting k without affecting the limits of the individual exponents, all equal to a. It would be interesting to extend Theorem 2.1 to be able to predict the value of the limit in the case that neither conditions (i) nor (ii) are met.

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Representations of the quantum doubles of finite group algebras and spectral parameter dependent solutions of the Yang–Baxter equation

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Quantum doubles of finite group algebras form a class of quasitriangular Hopf algebras that algebraically solve the Yang–Baxter equation. Each representation of the quantum double then gives a matrix solution of the Yang–Baxter equation. Such solutions do not depend on a spectral parameter, and to date there has been little investigation into extending these solutions such that they do depend on a spectral parameter. Here we first explicitly construct the matrix elements of the generators for all irreducible representations of quantum doubles of the dihedral groups D_n. These results may be used to determine constant solutions of the Yang–Baxter equation. We then discuss Baxterization ansätze to obtain solutions of the Yang–Baxter equation with a spectral parameter and give several examples, including a new 21-vertex model. We also describe this approach in terms of minimal-dimensional representations of the quantum doubles of the alternating group A_4 and the symmetric group S_4. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Solutions of the Yang–Baxter equation [see (1)] provide a systematic way to construct exactly solvable models of two-dimensional statistical mechanics,[1] integrable quantum systems,[2–5] as well as having applications in other areas such as knot theory.[6] A great impetus to this field was given by Drinfeld,[7] who proposed the *quantum double construction*. This allows for any Hopf algebra A to be embedded in a larger Hopf algebra $D(A)$ in such a way that $D(A)$ is quasitriangular. A consequence of the quasitriangular property is that there exists a canonical element $R \in D(A) \otimes D(A)$, called the *universal R-matrix*, which solves the Yang–Baxter equation algebraically. Thus, for any representation of $D(A)$ a matrix solution of the Yang–Baxter equation is obtained. (Below we will abuse the notation and use R to denote both the universal R-matrix and its matrix representatives.) The seminal examples of quasitriangular Hopf algebras were given by both Drinfeld[7] and Jimbo,[8,9] who independently introduced the notion of quantum algebras, which are deformations of universal enveloping algebras of Lie algebras.

For applications to the areas mentioned above one is generally interested in solutions of the Yang–Baxter equation with a spectral parameter; i.e., for a vector space V one looks for $R(u,v) \in \mathrm{End}(V \otimes V)$ where u,v are complex variables such that

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$$R_{12}(u,v)R_{13}(u,w)R_{23}(v,w) = R_{23}(v,w)R_{13}(u,w)R_{12}(u,v), \tag{1}$$

holds on the threefold tensor product space $V \otimes V \otimes V$. The subscripts above refer to the way in which the action of $R(u,v)$ is embedded into the space of endomorphisms on $V \otimes V \otimes V$.

In the context of quantum algebras, the spectral parameter arises naturally when one considers the loop representations of affine algebras.[8,9] In such instances the solutions always satisfy the *difference property* $R(u,v)=R(u-v)$. However, it is worth mentioning that there are solutions that do not have the difference property, including the well-known cases of the solutions giving rise to the Hubbard model,[10] the Bariev model,[11] and the chiral Potts model.[12] Moreover, the spectral parameter need not necessarily be a scalar, but can be a complex vector variable.[13–17] Later we will only concern ourselves with cases of scalar spectral parameters where the difference property does hold.

For later use, we introduce the permutation operator P such that $P(x \otimes y)=y \otimes x$ and set $\check{R}(u)=PR(u)$. Then (1) can equivalently be expressed as

$$\check{R}_{12}(u)\check{R}_{23}(u+v)\check{R}_{12}(v) = \check{R}_{23}(v)\check{R}_{12}(u+v)\check{R}_{23}(u), \tag{2}$$

which we will refer to as the *braiding* Yang–Baxter equation. It is in this form that the Yang–Baxter equation is relevant to knot theory.[6] Indeed, setting

$$\check{\mathcal{R}} = \lim_{u \to -\infty} \check{R}(u)$$

gives us

$$\check{\mathcal{R}}_{12}\check{\mathcal{R}}_{23}\check{\mathcal{R}}_{12} = \check{\mathcal{R}}_{23}\check{\mathcal{R}}_{12}\check{\mathcal{R}}_{23}, \tag{3}$$

which can be recognized as a defining relation in the braid group.[6] In terms of

$$\mathcal{R} = \lim_{u \to -\infty} R(u),$$

we have

$$\mathcal{R}_{12}\mathcal{R}_{13}\mathcal{R}_{23} = \mathcal{R}_{23}\mathcal{R}_{13}\mathcal{R}_{12}, \tag{4}$$

which we will refer to as the *constant* Yang–Baxter equation. Finally, we mention that if

$$\check{R}(u)\check{R}(-u) \propto I \otimes I,$$

then the R-matrix is said to satisfy the *unitarity* condition, while if

$$\check{R}(0) \propto I \otimes I, \tag{5}$$

then it is said to satisfy the *regularity* condition. When the regularity condition holds, there is a standard procedure[1–4] for constructing an integrable quantum system on a one-dimensional lattice with periodic boundary conditions. The Hamiltonian is given by

$$H = \sum_{j=1}^{L-1} h_{j,j+1} + h_{L,1}, \tag{6}$$

where the two-site Hamiltonians are given by

$$h = \left. \frac{d}{du}\check{R}(u) \right|_{u=0}.$$

Models constructed in this manner, and other approaches, can be solved exactly using Bethe ansatz methods.[1–6]

One class of quasitriangular Hopf algebras is the set of quantum doubles of the group algebras of finite groups.[18,19] (Throughout we will refer to these as *finite group doubles*). Applications of finite group double representations to knot theory have been addressed in Ref. 20. These algebraic structures also underlie systems of *anyons* in two spatial dimensions. In cases where the global symmetry of the system is spontaneously broken to a discrete gauge group, the finite group double is the appropriate structure to describe the fusion properties and statistics. The fusion properties are essentially determined by the Clebsch-Gordan decomposition of tensor products into irreducible representations. The statistics associated with the interchange of two anyons is described by braiding. The consistency condition for the two ways in which three anyons may be interchanged by a sequence of three two-anyon exchanges is precisely (3), where $\check{R}_{jk}$ is the operation that interchanges the jth and kth anyons. For a comprehensive review of the salient features we refer to Refs. 21 and 22.

Such systems may exhibit topological order,[23] where quantum numbers are conserved for topological reasons, as opposed to the manifest symmetry. Due to the topological nature, excitations are resistant to decoherence. This property forms the basis of topological quantum computation that was first put forth by Kitaev[24] (see also, e.g., Refs. 25–28). When the symmetry is described by a finite group double, the braiding $\check{R}_{jk}$ is a unitary operator that can be employed as a quantum gate.

In view of the previous literature, it is surprising that there has been very little study on the role of finite group doubles in obtaining solutions for the spectral parameter dependent Yang–Baxter equation (1). Integrable systems constructed from such solutions via (6) realize models for interacting anyons with internal symmetries described by the finite group double. Even though the models are one-dimensional, there is a precedent, the Hubbard model, which leads us to believe that such models may have applications for understanding two-dimensional systems. One property that is evident from the analysis of the Bethe ansatz solution of the one-dimensional Hubbard model is spin-charge separation. The Hubbard model has an $so(4) \cong so(3) \oplus so(3)$ symmetry, where the two quantum numbers associated with the two copies of $so(3)$ can be assigned to spin and charge degrees of freedom. From this symmetry and the Bethe ansatz solution, it can be concluded that in one-dimension there exist excitations that carry spin but not charge, and *vice versa*, so spin-charge separation occurs.[29] It has been proposed that spin-charge separation is the mechanism responsible for high temperature superconductivity in two-dimensions.[30] Likewise, there may be insights gained into the properties of interacting anyons by studying one-dimensional models that can be solved exactly.

Our aim is to investigate the extent to which solutions of the spectral parameter dependent Yang–Baxter equation can be obtained using the Hopf algebra structure of finite group doubles. This is not straightforward, as there appears to be no obvious manner in which to consider the affine extension of a finite group double that affords loop representations. Using a different approach, some preliminary results in this regard have been obtained by Yang *et al.*[31] We believe these represent the tip of an iceberg, and there is ample scope for further work. Our aim here is to continue the advances in this direction.

Our starting point is to consider the quantum doubles of the dihedral groups D_n. Of all non-Abelian finite groups, the series of dihedral groups has the simplest representation theory. We will show that the representation theory for the quantum doubles is also readily tractable. Using the general results on the representation theory of finite group doubles given in Refs. 18 and 19, we begin by explicitly constructing *all* irreducible representations for the doubles $D(D_n)$[1] From these results it is straightforward to explicitly construct solutions R for the constant Yang–Baxter equation (4) that do not depend on the spectral parameter.

Our next goal is to determine if these constant solutions of the Yang–Baxter equation can be extended to spectral parameter dependent solutions. This is a procedure colloquially known as

[1]After completing this work, we learned that for odd n these representations have been constructed in the thesis by de Wild Propitius.[22] Results for even n have independently been obtained by Slingerland.[32]

Baxterization, as coined by Jones,[33] and there is sizable literature on this topic.[34–41] We begin by studying the case of the two-dimensional irreducible representations of $D(D_n)$ and find that Baxterization can be performed successfully. Our approach is based on an ansatz taken from Ref. 35, which is chosen by symmetry considerations. In all these cases we find that the resulting solution of the Yang–Baxter equation is a particular case of the well-known trigonometric six-vertex model in the symmetric gauge at a specific root of unity. We mention that this result is not obvious in the sense that the Baxterization is not underpinned by a Hecke algebra representation.

We then turn our attention to the three-dimensional irreducible representations of $D(D_n)$. We find that the only cases for which an irreducible three-dimensional representation exists are $D(D_3)$ and $D(D_6)$. All instances give unitarily equivalent constant solutions of the Yang–Baxter equation. Our Baxterization ansatz leads to a 21-vertex solution of the spectral parameter dependent Yang–Baxter equation, which as far as we can ascertain is new.

Rather than continuing on to investigate higher dimensional representations of the $D(D_n)$ series, we finish by considering minimal-dimensional representations of the double of the alternating group A_4 and the symmetric group S_4. Neither of these cases admit irreducible two-dimensional representations, but they both admit three-dimensional ones. Our ansatz for Baxterizing the constant solutions does lead us to spectral parameter dependent solutions. Remarkably though, we find in these latter examples that the infinite spectral parameter limit of the Baxterized solutions do not necessarily reproduce the original solutions of the constant Yang–Baxter equation.

II. THE DIHEDRAL GROUP D_n

Consider the dihedral group D_n. This has two generators σ, τ satisfying

$$\sigma^n = e, \quad \tau^2 = e, \quad \tau\sigma = \sigma^{n-1}\tau.$$

The properties of D_n vary according to whether n is odd or even, with the odd case being slightly simpler.

A. D_n where n is odd

When n is odd, there are $(n+3)/2$ conjugacy classes divided into three families, given by

$$\{e\},$$

$$\{\sigma^k, \sigma^{-k}\}, \quad \text{for } 1 \le k \le \frac{n-1}{2},$$

$$\{\sigma^i\tau, 0 \le i \le n-1\}.$$

There are $(n+3)/2$ irreducible representations (irreps), two of which are one-dimensional and the remaining $(n-1)/2$ which are two-dimensional. They are given by

$$\pi_\pm(\sigma) = 1, \quad \pi_\pm(\tau) = \pm 1$$

and

$$\pi_k(\sigma) = \begin{bmatrix} \omega^k & 0 \\ 0 & \omega^{-k} \end{bmatrix}, \quad \pi_k(\tau) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \omega = \exp\left(\frac{2\pi i}{n}\right), \quad 1 \le k \le \frac{n-1}{2}.$$

As required, the sum of the squares of the dimensions of the irreps is $2\times 1^2 + (n-1)/2 \times 2^2 = 2n = |D_n|$.[42]

B. D_n where n is even

When n is even, there are $(n+6)/2$ conjugacy classes divided into five families, given by

$$\{e\},$$

$$\{\sigma^{n/2}\},$$

$$\{\sigma^k,\sigma^{-k}\}, \quad \text{for } 1 \le k \le (n-2)/2,$$

$$\{\sigma^{2j}\tau, 0 \le j \le (n-2)/2\},$$

$$\{\sigma^{(2j+1)}\tau, 0 \le j \le (n-2)/2\}.$$

The $(n+6)/2$ irreps consist of 4 one-dimensional irreps and $(n-2)/2$ two-dimensional irreps. They are given by

$$\pi(\sigma) = (-1)^a, \quad \pi(\tau) = (-1)^b, \quad \text{for } a,b \in \{0,1\}$$

and

$$\pi_k(\sigma) = \begin{bmatrix} \omega^k & 0 \\ 0 & \omega^{-k} \end{bmatrix}, \quad \pi_k(\tau) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \omega = \exp\left(\frac{2\pi i}{n}\right), \quad 1 \le k \le \frac{n-2}{2}.$$

Again, the sum of the squares of the dimensions of the irreps is $2n$.

III. THE QUANTUM DOUBLE ALGEBRA $D(G)$

Here we give a brief survey of finite group doubles $D(G)$. Throughout, our approach follows that of Ref. 19. Let A be the group algebra of a finite group G over the complex field $\mathbb{C}$. Then A becomes a co-commutative Hopf algebra with coproduct, antipode, and counit, respectively, defined by

$$\Delta(g) = g \otimes g, \quad S(g) = g^{-1}, \quad \varepsilon(g) = e, \quad \forall\, g \in G.$$

Let A^* be the dual space of A, so $A^* = \{f | f: A \to \mathbb{C}\}$. Then A^* becomes an algebra on the dual elements g^* defined by

$$g^*(h) = \delta(g,h), \quad \forall\, g,h \in G,$$

which have the property

$$g^*h^* = \delta(g,h)h^*.$$

The resultant dual algebra is commutative and does not have an interesting representation theory. Now we follow the quantum double construction to obtain $D(G)$, which is a $|G|^2$-dimensional algebra spanned by the free products,

$$gh^*, \quad g,h \in G.$$

The elements h^*g are calculated using

$$h^*g = g(g^{-1}hg)^*.$$

Then $D(G)$ becomes a quasitriangular Hopf algebra with coproduct $\bar{\Delta}$, antipode $\bar{S}$, and counit $\bar{\varepsilon}$ given by

$$\bar{\Delta}(gh^*) = \sum_{k\in G} g(k^{-1}h)^* \otimes gk^* = \sum_{k\in G} gk^* \otimes g(kh^{-1})^*,$$

$$\bar{S}(gh^*) = g^{-1}(gh^{-1}g^{-1})^*,$$

$$\bar{\varepsilon}(gh^*) = \delta(h,e).$$

Note that we identify $g\varepsilon$ with g and eg^* with g^* for all $g \in G$. The universal R-matrix is given by

$$R = \sum_{g\in G} g \otimes g^*,$$

which can easily be shown to satisfy the defining relations for a quasitriangular Hopf algebra:

$$R\bar{\Delta}(a) = \bar{\Delta}^T(a)R, \quad \forall\, a \in D(G), \tag{7}$$

$$(\bar{\Delta} \otimes \mathrm{id})R = R_{13}R_{23}, \tag{8}$$

$$(\mathrm{id} \otimes \bar{\Delta})R = R_{13}R_{12}, \tag{9}$$

where $\bar{\Delta}^T$ is the opposite coproduct,

$$\bar{\Delta}^T(gh^*) = \sum_{k\in G} gk^* \otimes g(k^{-1}h)^* = \sum_{k\in G} g(kh^{-1})^* \otimes gk^*.$$

It follows from the relations (7)–(9) that R is a solution of the constant Yang–Baxter equation. We note that in any tensor product representation $\pi\otimes\pi$ we have that $\check{R}=PR$ commutes with the action of the finite group double; i.e.,

$$[\check{R}, (\pi \otimes \pi)\bar{\Delta}(a)] = 0, \quad \forall\, a \in D(G).$$

IV. REPRESENTATION THEORY OF *D*(*G*)

Several properties of group algebras extend to the quantum double. For example, the set

$$Q = \{gh^* | g,h \in G \text{ with } gh = hg\},$$

is stable under the adjoint action of G, i.e., $gQg^{-1}=Q$. Hence, Q can be partitioned into G-conjugacy classes, which implies[19] the following.

Theorem 4.1: *The number of nonisomorphic $D(G)$-modules equals the number of G-equivalence classes of Q.*

Moreover, a construction for these modules is known.[19] The general form is included in this section, with the explicit results for the odd and even dihedral groups given in the following two sections, respectively.

First, partition G into conjugacy classes,

$$G = \bigcup_k C_k.$$

Recall that the centralizer subgroup of an element h is defined by

$$Z(h) = \{g \in G | gh = hg\}.$$

Then, for each conjugacy class C_k choose a representative $g_k \in C_k$ and set $Z_k = Z(g_k)$ to be the centralizer subgroup of g_k, noting that $|Z_k||C_k| = |G|$. Denote the group algebra of Z_k by A_k. Also, for each $s \in C_k$ choose a fixed element $\alpha_s \in G$ satisfying

$$s = \alpha_s g_k \alpha_s^{-1}.$$

For simplicity, choose $\alpha_{g_k} = e, \forall g_k$.

Lemma 4.1: *We have the following properties of* α_s:

1. $G = \cup_{s \in C_k} \alpha_s Z_k$
2. *Given* $g \in G, s \in C_k, \exists t \in C_k$ *unique with the property* $\alpha_t^{-1} g \alpha_s \in Z_k$; *explicitly* $t = gsg^{-1}$.

Again, a proof can be found in Ref. 19.

The irreducible modules of $D(G)$ can be constructed from modules of the group algebras A_k. Let V_β^k denote an irreducible A_k-module. Then there is a corresponding induced A-module,[42]

$$V_{k,\beta} \subseteq A \otimes_{A_k} V_\beta^k,$$

spanned by vectors

$$v(s) = \alpha_s \otimes v, \quad v \in V_\beta^k, \quad s \in C_k,$$

where the action of G is given by

$$g(\alpha_s \otimes v) = \alpha_{gsg^{-1}} \otimes (\alpha_{gsg^{-1}}^{-1} g \alpha_s) v,$$

or, equivalently,

$$gv(s) = (\alpha_{gsg^{-1}}^{-1} g \alpha_s v)(gsg^{-1}).$$

Note $\dim V_{k,\beta} = |C_k| \dim V_\beta^k$. It follows from Lemma 4.1 that $V_{k,\beta}$ is an A-module under this definition.

The module $V_{k,\beta}$ can be decomposed according to

$$V_{k,\beta} = \underset{s \in C_k}{\oplus} V_{k,\beta}(s),$$

where

$$V_{k,\beta}(s) = \{v(s) | v \in V_\beta^k\}.$$

The latter becomes an irreducible module over the group algebra of $Z(s) = \alpha_s Z_k \alpha_s^{-1}$. When $s = g_k$, the module is isomorphic to V_α^k. Then $V_{k,\beta}$ becomes an irreducible $D(G)$-module with the action

$$h^* v(s) = \delta(h,s) v(s), \quad \forall h \in G.$$

Moreover, two $D(G)$-modules of this form, $V_{k,\beta}, V_{l,\gamma}$, are isomorphic iff $k = l$ and V_β^k, V_γ^k are isomorphic. Then using counting arguments the following can be shown.

Theorem 4.2: *Every irreducible* $D(G)$*-module is isomorphic to one of the* $V_{k,\beta}$.

V. REPRESENTATIONS OF $D(G)$, WHERE $G = D_n$, n EVEN

The conjugacy classes C_k of $G = D_n$, chosen representatives g_k, corresponding centralizer subgroups and the elements $\alpha_s, \forall s \in C_k$, are given in Table I.

Throughout the remainder of this paper, E_j^i denotes an elementary matrix with a 1 in the (i,j) position and zeros elsewhere. We also abuse notation by using g to denote both an element of the algebra $D(G)$ and its matrix representative in a given irrep, which should be clear from the context.

TABLE I. C_k, g_k, Z_k, and α_s for $G=D_n$, n even.

C_k	g_k	$Z_k=Z(g_k)$	$\alpha_s, \forall s \in C_k$
$\{e\}$	e	D_n	$\alpha_e=e$
$\{\sigma^{n/2}\}$	$\sigma^{n/2}$	D_n	$\alpha_{\sigma^{n/2}}=e$
$\{\sigma^k,\sigma^{-k}\}, 1\le k<n/2$	σ^k	$\{\sigma^i \mid 0\le i<n\}$	$\alpha_{\sigma^k}=e, \alpha_{\sigma^{-k}}=\tau$
$\{\sigma^{2i}\tau \mid 0\le i<n/2\}$	τ	$\{e,\tau,\sigma^{n/2},\sigma^{n/2}\tau\}$	$\alpha_{(\sigma^{2i}\tau)}=\sigma^i$
$\{\sigma^{2i+1}\tau \mid 0\le i<n/2\}$	$\sigma\tau$	$\{e,\sigma\tau,\sigma^{n/2},\sigma^{n/2+1}\tau\}$	$\alpha_{(\sigma^{2i+1}\tau)}=\sigma^i$

Representations induced by $C_k=\{e\}$. The module elements are of the form $e\otimes v$ where $v \in V$, V a D_n-module. In representation terms, there are 4 one-dimensional irreps and $(n/2-1)$ two-dimensional irreps. They are

$$\sigma=(-1)^a, \quad \tau=(-1)^b, \quad g^*=\delta(g,e)$$

where $a,b\in\{0,1\}$, and

$$\sigma=\begin{bmatrix}\omega^k & 0\\ 0 & \omega^{-k}\end{bmatrix}, \quad \tau=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad g^*=\delta(g,e)I_2,$$

where $1\le k<n/2$.

Representations induced by $C_k=\{\sigma^{n/2}\}$. The module elements are of the form $e\otimes v$, where $v \in V$, V a D_n-module. Again, there are 4 one-dimensional irreps and $(n-2)/2$ two-dimensional irreps. They are

$$\sigma=(-1)^a, \quad \tau=(-1)^b, \quad g^*=\delta(g,\sigma^{n/2}),$$

where $a,b\in\{0,1\}$, and

$$\sigma=\begin{bmatrix}\omega^k & 0\\ 0 & \omega^{-k}\end{bmatrix}, \quad \tau=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad g^*=\delta(g,\sigma^{n/2})I_2,$$

where $1\le k<n/2$.

Representations induced by $C_k=\{\sigma^k,\sigma^{-k}\}$, $1\le k<n/2$. The module elements are of the form $e\otimes v, \tau\otimes v$, where $v\in V$, V a module of the group algebra of $Z_k=\{\sigma^j \mid 0\le j<n\}$. There are n such A_k-modules, with the corresponding representations given by $\pi(\sigma)=\omega^j$, $0\le j<n$, where $\omega=\exp(2\pi i/n)$. Thus, we have $n(n-2)/2$ different irreducible representations of $D(D_n)$ induced by these conjugacy classes, given by

$$\sigma=\begin{bmatrix}\omega^j & 0\\ 0 & \omega^{-j}\end{bmatrix}, \quad \tau=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad (\sigma^k)^*=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}, \quad (\sigma^{-k})^*=\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}, \quad g^*=0, \quad \text{otherwise},$$

where $0\le j<n$, $1\le k<n/2$.

Representations induced by $C_k=\{\sigma^{2j}\tau \mid 0\le j<n/2\}$. The module elements are of the form $\sigma^j\otimes v$, $0\le j<n/2$, where $v\in V$, V a module of the group algebra of $Z_k=\{e,\tau,\sigma^{n/2},\sigma^{n/2}\tau\}$. Hence, there are 4 $(n/2)$-dimensional irreps of this form. They are

$$\sigma=A\in M_{n/2\times n/2}, \quad \text{where } [A]_{ij}=(-1)^{a\delta(i,1)}\delta(i,j+1), \quad \text{addition mod } n/2,$$

$$\tau=(-1)^{a+b}B\in M_{n/2\times n/2}, \quad \text{where } [B]_{ij}=(-1)^{a\delta(i,1)}\delta(i+j,2), \quad \text{addition mod } n/2,$$

$$(\sigma^j)^*=0, \quad (\sigma^{2j}\tau)^*=E_{j+1}^{j+1}, \quad (\sigma^{(2j+1)}\tau)^*=0, \quad 0\le i<n, \quad 0\le j<n/2,$$

where $a,b\in\{0,1\}$.

Example 5.1: *In* $D(D_6)$, σ *and* τ *are as follows:*

$$\sigma = \begin{bmatrix} 0 & 0 & (-1)^a \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad \tau = (-1)^b \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & (-1)^a \\ 0 & (-1)^a & 0 \end{bmatrix},$$

where $a,b \in \{0,1\}$, *giving 4 three-dimensional irreps.*

Representations induced by $C_k = \{\sigma^{2j+1}\tau | 0 \le j < n/2\}$. The module elements are of the form $\sigma^j \otimes v$, $0 \le j < n/2$, where $v \in V$, V a module of the group algebra of $Z_k = \{e, \sigma\tau, \sigma^{n/2}, \sigma^{(n+2)/2}\tau\}$. Hence, there are 4 $(n/2)$-dimensional irreps of this form. They are as follows:

$$\sigma = A \in M_{n/2\times n/2} \quad \text{where } [A]_{ij} = (-1)^{a\delta(i,1)}\delta(i,j+1), \quad \text{addition mod } n/2,$$

$$\tau = (-1)^{a+b}B \in M_{n/2\times n/2} \quad \text{where } [B]_{ij} = \delta(i+j,n/2+1), \quad \text{addition mod } n/2,$$

$$(\sigma^j)^* = 0, \quad (\sigma^{2j}\tau)^* = 0, \quad (\sigma^{(2j+1)}\tau)^* = E^{j+1}_{j+1}, \quad 0 \le i < n, \quad 0 \le j < n/2,$$

where $a,b \in \{0,1\}$.

Example 5.2: *In* $D(D_6)$, σ *and* τ *are as follows:*

$$\sigma = \begin{bmatrix} 0 & 0 & (-1)^a \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad \tau = (-1)^{a+b} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

where $a,b \in \{0,1\}$, *giving 4 three-dimensional irreps.*

Thus when n is even $D(D_n)$ has 8 one-dimensional irreps, 8 $(n/2)$-dimensional irreps, and $(n+2)(n/2-1)$ two-dimensional irreps. The sum of the squares of the dimension of the irreps is $|D_n|^2 = |D(D_n)|$, as required.[19]

Analogous results for odd n are given in the Appendix .

VI. SOLUTIONS OF THE YANG–BAXTER EQUATION ASSOCIATED WITH THE TWO-DIMENSIONAL IRREPS OF $D(D_n)$

As stated earlier, a solution to the constant Yang–Baxter equation in $D(G)$ is given by

$$R = \sum_{g \in G} g \otimes g^*.$$

In this section we will only consider the two-dimensional irreps of $D(G)$. Then, by inspection, the R-matrix will always be of the form

$$R = \mathrm{diag}(\omega^j, \omega^{-j}, \omega^{-j}, \omega^j),$$

where $\omega = \exp(2\pi i/n)$ and $0 \le j < n$, with the cases $j=0$ and $j=n/2$ being trivial. Thus $\check{R} = PR$ is given by

$$\check{R} = \begin{bmatrix} \omega^j & 0 & 0 & 0 \\ 0 & 0 & \omega^{-j} & 0 \\ 0 & \omega^{-j} & 0 & 0 \\ 0 & 0 & 0 & \omega^j \end{bmatrix}. \tag{10}$$

As remarked earlier, $\check{R}$ commutes with the action of $D(D_n)$. We seek a solution $\check{R}(x)$ of the braiding Yang–Baxter equation that has this symmetry. Now the matrix (10) has 3 different eigenvalues, namely $w^j, \pm w^{-j}$. Hence, for any k, $\check{R}^k$ can be written as a linear combination of $I \otimes I, \check{R}$ and $\check{R}^{-1}$. Making a change of variables $x = \exp(u)$, $z = \exp(v)$ in Eq. (2), we look for $\check{R}(x)$ in the following form:

$$\check{R}(x) = f(x)I \otimes I + g(x)\check{R} + h(x)\check{R}^{-1}.$$

Then

$$\check{R}(x) = \begin{bmatrix} A(x) & 0 & 0 & 0 \\ 0 & f(x) & B(x) & 0 \\ 0 & B(x) & f(x) & 0 \\ 0 & 0 & 0 & A(x) \end{bmatrix},$$

where

$$A(x) = f(x) + \omega^j g(x) + \omega^{-j} h(x),$$

$$B(x) = \omega^{-j} g(x) + \omega^j h(x).$$

We directly apply the braiding Yang–Baxter equation in the form

$$\check{R}_{12}(x)\check{R}_{23}(xz)\check{R}_{12}(z) = \check{R}_{23}(z)\check{R}_{12}(xz)\check{R}_{23}(x). \tag{11}$$

Although there are 20 nonzero entries on each side of the equation, there are only two independent nontrivial relations that must be satisfied. These are

$$A(z)f(xz)A(x) = f(x)A(xz)f(z) + B(x)f(xz)B(z), \tag{12}$$

$$A(z)B(xz)f(x) = f(x)A(xz)B(z) + B(x)f(xz)f(z). \tag{13}$$

Note that $f(x)=0$, $\forall x$ trivially satisfies the Yang–Baxter equation.

A proposal for constructing $\check{R}(x)$ when $\check{R}$ has three distinct eigenvalues λ_1, λ_2, and λ_3 has been discussed in Refs. 31 and 35, but it has not been proven to always be true. The conjecture is

$$\check{R}(x) = (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_1\lambda_3\lambda_2^{-1})xI \otimes I - (x-1)\check{R} + \lambda_1\lambda_3 x(x-1)\check{R}^{-1}.$$

Three distinct solutions are obtained by changing the ordering of the eigenvalues. We note that when the ansatz holds we have

$$\check{\mathcal{R}} = \lim_{x\to 0} R(x) = R.$$

Applying this ansatz to (10), we find that if $\lambda_2 = \pm\omega^{-j}$, then $f(x)=0$, which we have already shown gives a trivial result. Hence we consider the case when $\lambda_2 = \omega^j$. This gives

$$f(x) = (\omega^j - \omega^{-3j})x, \quad g(x) = -(x-1), \quad h(x) = -w^{-2j}x(x-1),$$

$$\Rightarrow A(x) = \omega^j - \omega^{-3j}x^2, \quad B(x) = -\omega^{-j}(x^2-1).$$

It can be easily shown that $f(x)$, $A(x)$, and $B(x)$ satisfy relations (12) and (13). Hence, we have solutions to the braiding Yang–Baxter equation, which are

$$\check{R}(x) = \begin{bmatrix} \omega^j - \omega^{-3j}x^2 & 0 & 0 & 0 \\ 0 & (\omega^j - \omega^{-3j})x & -\omega^{-j}(x^2-1) & 0 \\ 0 & -\omega^{-j}(x^2-1) & (\omega^j - \omega^{-3j})x & 0 \\ 0 & 0 & 0 & \omega^j - \omega^{-3j}x^2 \end{bmatrix},$$

where $\omega = \exp(2\pi i/n)$ and $0 \le j < n$. Rescaling by a factor of $\omega^j x^{-1}$, we can write

TABLE II. Possible solutions for $f(x)$, $g(x)$, and $h(x)$.

$f(x)$	$g(x)$	$h(x)$
x	$1-x$	$x(x-1)$
ωx	$1-x$	$\omega^2 x(x-1)$
$\omega^2 x$	$1-x$	$\omega x(x-1)$

$$\check{R}(x)=\begin{bmatrix} \omega^{2j}x^{-1}-\omega^{-2j}x & 0 & 0 & 0 \\ 0 & \omega^{2j}-\omega^{-2j} & x^{-1}-x & 0 \\ 0 & x^{-1}-x & \omega^{2j}-\omega^{-2j} & 0 \\ 0 & 0 & 0 & \omega^{2j}x^{-1}-\omega^{-2j}x \end{bmatrix}. \tag{14}$$

Note that the unitarity condition $\check{R}(x)\check{R}(x^{-1})=[\omega^{4j}+\omega^{-4j}-(x^2+x^{-2})]I\otimes I$ is satisfied. We can recognize (14) as specific cases of the six-vertex solution in the symmetric gauge, where the parameter q in the general solution is constrained to be a root of unity. We remark that the choice of gauge is related to the gradation chosen for the affine algebra (e.g., see Ref. 43). It is interesting to note that in the nonsymmetric gauge the constant solution $\check{\mathcal{R}}=\lim_{x\to 0} R(x)$ can be used to give rise to a representation of the Temperley-Lieb algebra. In this case there is a well known procedure for Baxterizing $\check{\mathcal{R}}$ to recover $\check{R}(x)$.[33,34] This is not the case for the symmetric gauge case described previously.

VII. SOLUTIONS OF THE YANG–BAXTER EQUATION ASSOCIATED WITH THE THREE-DIMENSIONAL IRREPS OF $D(D_3)$ AND $D(D_6)$

From the construction of the irreps of $D(D_n)$ given explicitly in Sec. V and the Appendix, we find that three-dimensional irreps only occur for $D(D_3)$ and $D(D_6)$. Moreover, the 2 three-dimensional irreps of $D(D_3)$ are also representations for the $D(D_3)$ subalgebra of $D(D_6)$, so these cases give identical R matrices. For any three-dimensional irrep of $D(D_6)$, we find $\check{R}=PR=P\Sigma_g g\otimes g^*$ is of the following form:

$$\check{R}=(-1)^b\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & (-1)^a & 0 \\ 0 & 0 & (-1)^a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & (-1)^a & 0 & 0 \\ 0 & (-1)^a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

where $a,b\in\{0,1\}$. Without loss of generality we take $b=0$, and find the eigenvalues of $\check{R}$ are 1, ω, and ω^2 with multiplicities 5, 2, and 2, respectively, where $\omega=\exp(2\pi i/3)$. As the two values of a give unitarily equivalent R matrices, we choose to take $a=0$. We can then write

$$\check{R}(x)=f(x)I\otimes I+g(x)\check{R}+h(x)\check{R}^{-1}.$$

Again we follow the procedure outlined in Refs. 31 and 35 to find possible solutions, which gives the following:

Using MATHEMATICA, we find only the first of these possible solutions satisfies the braiding Yang–Baxter equation (11) (see Table II):

$$\check{R}(x)=\begin{bmatrix} x^2-x+1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 1-x & x(x-1) & 0 & 0 \\ 0 & 0 & x & x(x-1) & 0 & 0 & 0 & 1-x & 0 \\ 0 & 0 & 1-x & x & 0 & 0 & 0 & x(x-1) & 0 \\ 0 & 0 & 0 & 0 & x^2-x+1 & 0 & 0 & 0 & 0 \\ 0 & x(x-1) & 0 & 0 & 0 & x & 1-x & 0 & 0 \\ 0 & 1-x & 0 & 0 & 0 & x(x-1) & x & 0 & 0 \\ 0 & 0 & x(x-1) & 1-x & 0 & 0 & 0 & x & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x^2-x+1 \end{bmatrix}.$$

The corresponding R-matrix $R(x)=P\check{R}(x)$ is given by

$$R(x)=\begin{bmatrix} x^2-x+1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-x & x & 0 & 0 & 0 & x(x-1) & 0 \\ 0 & 1-x & 0 & 0 & 0 & x(x-1) & x & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 1-x & x(x-1) & 0 & 0 \\ 0 & 0 & 0 & 0 & x^2-x+1 & 0 & 0 & 0 & 0 \\ 0 & 0 & x(x-1) & 1-x & 0 & 0 & 0 & x & 0 \\ 0 & 0 & x & x(x-1) & 0 & 0 & 0 & 1-x & 0 \\ 0 & x(x-1) & 0 & 0 & 0 & x & 1-x & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & x^2-x+1 \end{bmatrix}. \quad (15)$$

Note $\check{R}(x)\check{R}(x^{-1})=(x-1+1/x)^2 I\otimes I$, so the unitarity property holds.

The previous solution gives rise to a 21-vertex model, which appears to be new. It does not belong to the class of 21-vertex models discussed in Ref. 44. Viewed as a two-dimensional lattice statistical mechanics model though, it does not have real, non-negative Boltzmann weights. Since the regularity property (5) holds, we can, however, construct an integrable one-dimensional model. Even though $\check{R}(x)$ is not Hermitian, we obtain a Hermitian Hamiltonian in the following manner. We rescale $\check{R}(x)$ by a factor of i/x and define the two-site Hamiltonian h as

$$h=\frac{d}{dx}\left.\frac{i\check{R}(x)}{x}\right|_{x=1}=i\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

which can also be written as

$$h=\sum_{\gamma\in D_3} i(E^{\gamma(1)}_{\gamma(2)}\otimes E^{\gamma(2)}_{\gamma(3)}-E^{\gamma(2)}_{\gamma(3)}\otimes E^{\gamma(1)}_{\gamma(2)}), \quad (16)$$

where the elements γ of D_3 are written as permutations of $\{1,2,3\}$. The above integrable system describes a one-dimensional lattice of anyons with $D(D_3)$ or $D(D_6)$ symmetry and local interactions given by (16). The two-site Hamiltonian may also be expressed in terms of spin-1 operators:

$$-ih=-S_+^2\otimes(S_zS_-+S_-S_z)+(S_zS_-+S_-S_z)\otimes S_+^2$$

$$+S_-^2\otimes(S_zS_++S_+S_z)-(S_zS_++S_+S_z)\otimes S_-^2$$

$$+ S_+S_z \otimes S_zS_+ - S_zS_+ \otimes S_+S_z$$

$$+ S_-S_z \otimes S_zS_- - S_zS_- \otimes S_-S_z,$$

where $S_\pm = 1/2(S_x \pm iS_y)$. This Hamiltonian is not the same as other known integrable spin-1 Hamiltonians.[45–49]

In principle, the integrability of the previous model implies that algebraic Bethe ansatz methods may be used to obtain the exact solution. In the present case, however, there is no simple choice of reference state needed for the Bethe ansatz calculation, and a generalized algebraic Bethe ansatz similar to that employed for the XYZ model[50] is required. Because of the technical nature of such a calculation we defer it to a future publication.

VIII. SOLUTIONS OF THE YANG–BAXTER EQUATION ASSOCIATED WITH $D(A_4)$

The same procedure can be applied to the symmetric and alternating groups. The *symmetic group* S_n is the group of permutations of $\{1,2,\ldots,n\}$ where the operation is composition. The subgroup of S_n consisting of permutations that can be written as the product of an even number of transpositions is known as the *alternating group* and denoted A_n. Now $S_3 \cong D_3$ and $A_3 \cong Z_3$, so we only consider $n \geq 4$. In A_n the only conjugacy class with only one element is $\{e\}$, which always gives rise to the trivial R-matrix $R = I \otimes I$. Moreover, there are no conjugacy classes with two elements and only A_4 has a conjugacy class with three elements. Therefore only A_4 can give rise to a three-dimensional irrep, and we can never obtain a two-dimensional irrep.

Consider A_4, using the convention $(12)\circ(13) = (132)$. The relevent conjugacy class C_k and the details required to construct the representations are

$$C_k = \{(12)(34),(13)(24),(14)(23)\}, \quad g_k = (12)(34),$$

$$Z_k = \{e,(12)(34),(13)(24),(14)(23)\},$$

$$\alpha_{(12)(34)} = e, \quad \alpha_{(13)(24)} = (132), \quad \alpha_{(14)(23)} = (123).$$

This time $Z_k \cong \mathbb{Z}_2 \times \mathbb{Z}_2$, with the 4 one-dimensional irreps given by $(12)(34) = (-1)^a$, $(13)(24) = (-1)^b$, $a,b \in \{0,1\}$. We obtain

$$R = \mathrm{diag}((-1)^a,(-1)^{a+b},(-1)^b,(-1)^b,(-1)^a,(-1)^{a+b},(-1)^{a+b},(-1)^b,(-1)^a).$$

Applying the permutation operator, we find

$$\check{R} = \begin{bmatrix} (-1)^a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & (-1)^b & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & (-1)^{a+b} & 0 & 0 \\ 0 & (-1)^{a+b} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & (-1)^a & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & (-1)^b & 0 \\ 0 & 0 & (-1)^b & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & (-1)^{a+b} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & (-1)^a \end{bmatrix},$$

which has eigenvalues $1,-1$ with multiplicities $6,3$, respectively, when $a=0$, and eigenvalues $-1,i,-i$, each with multiplicity 3 when $a=1$. When $a=b=0$ this is the permutation matrix and gives rise to a representation of the Hecke algebra. Baxterization then leads to the known $su(3)$ invariant solution. In the case $a=0,b=1$, $\check{R}$ is again a Hecke algebra representation, which can be Baxterized as $\check{R}(u) = I \otimes I + u\check{R}$. This solution corresponds to the rational 15-vertex solution with a

Reshetikhin twist.[51] The last case is when $b=1$, in which case we can write without loss of generality:

$$\check{R}=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

We recognize this solution as belonging to the class of *nonstandard* solutions of the Yang–Baxter equation. However, it is curious that the origin of the nonstandard structure cannot be explained in terms of an underlying Lie superalgebra or colour Lie algebra structure,[52,53] nor is it due to a Reshetikhin twist.[51]

As $\check{R}$ has three eigenvalues, we try the ansatz $\check{R}(x)=f(x)I\otimes I+g(x)\check{R}+h(x)\check{R}^{-1}$. Applying the conjecture given in Refs. 31 and 35, we obtain three possible solutions. Two of these, however, have $f(x)=0$, which is undesirable if we want the regularity property to hold. The third possible case can be shown to not satisfy the braiding Yang–Baxter equation (11). Hence, we attempt to find another way to introduce a spectral parameter.

First we return to the original variables u,v instead of x,z. Writing $a(u)=f(u)+g(u)+h(u)$ and $b(u)=g(u)-h(u)$, we note $\check{R}(u)$ is

$$\check{R}(u)=\begin{bmatrix} a(u) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & f(u) & 0 & b(u) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & f(u) & 0 & 0 & 0 & -b(u) & 0 & 0 \\ 0 & -b(u) & 0 & f(u) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a(u) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & f(u) & 0 & b(u) & 0 \\ 0 & 0 & b(u) & 0 & 0 & 0 & f(u) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -b(u) & 0 & f(u) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a(u) \end{bmatrix}.$$

Substituting $\check{R}(u)$ into the braiding Yang–Baxter equation (2), we find $\check{R}(u)$ satisfies the Yang–Baxter equation if and only if the following conditions are met:

$$b(u+v)f(u)f(v)=f(u+v)[b(u)f(v)+b(v)f(u)], \tag{17}$$

$$a(u)b(u+v)f(v)=b(v)f(u)f(u+v)+a(u+v)b(u)f(v), \tag{18}$$

$$a(u+v)f(u)f(v)=f(u+v)[a(u)a(v)+b(u)b(v)]. \tag{19}$$

First, consider the case when $b(u)=0$. Then equations (17), (18) are automatically satisfied, and we need only consider Eq. (19). The solution $\check{R}(u)\propto I\otimes I$ is uninteresting, so we instead choose $f(u)=1$ and $a(u)=e^{u}$, giving

$$\check{R}(u) = \mathrm{diag}(e^u, 1, 1, 1, e^u, 1, 1, 1, e^u).$$

Observe that this solution has the following peculiar property:

$$\check{R} \neq \lim_{u \to -\infty} \check{R}(u). \tag{20}$$

Next consider $b(u) \neq 0$. We begin by choosing $f(u)=1$. Then we see that $b(u)=b_0 u$ is the only solution to (17). We substitute these into Eq. (18) to obtain

$$(u+v)a(u) = v + ua(u+v),$$

$$(u+v)a(v) = u + va(u+v).$$

Eliminating $a(u+v)$, we find

$$(u+v)\left(\frac{a(u)}{u} - \frac{a(v)}{v}\right) = \frac{v}{u} - \frac{u}{v} = \frac{v^2 - u^2}{uv}$$

$$\Rightarrow \left(\frac{a(u)}{u} - \frac{a(v)}{v}\right) = \frac{v-u}{uv} = \frac{1}{u} - \frac{1}{v}$$

$$\Rightarrow \frac{a(u)-1}{u} = \frac{a(v)-1}{v} = c$$

$$\Rightarrow a(u) = 1 + cu.$$

We find that this satisfies (19), provided $c = \pm i b_0$, so we have found a solution to the braiding Yang–Baxter equation (2). Note that b_0 is just a scaling factor on u, so we can choose any nonzero complex number. Choosing $b_0 = i$ and $c=1$, we have

$$\check{R}(u) = \begin{bmatrix} 1+u & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & iu & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -iu & 0 & 0 \\ 0 & -iu & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1+u & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & iu & 0 \\ 0 & 0 & iu & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -iu & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1+u \end{bmatrix}.$$

The previous solution again corresponds to the rational 15-vertex solution with a Reshetikhin twist.[51] We also note that the property (20) also holds for this solution.

IX. SOLUTIONS OF THE YANG–BAXTER EQUATION ASSOCIATED WITH $D(S_4)$

As with $D(A_n)$, the algebra $D(S_n)$ has no nontrivial two-dimensional irreps, and the only nontrivial three-dimensional irrep occurs when $n=4$. Then C_k, g_k, Z_k, and α_s, $s \in C_k$ are given by

$$C_k = \{(12)(34), (13)(24), (14)(23)\}, \quad g_k = (12)(34),$$

$$Z_k = \{e, (12), (34), (12)(34), (13)(24), (14)(23), (1324), (1423)\},$$

$$\alpha_{(12)(34)} = e, \quad \alpha_{(13)(24)} = (14), \quad \alpha_{(14)(23)} = (13).$$

Note that $Z_k \cong D_4$ with generators $\{(12),(1324)\}$, so we know it has exactly 4 one-dimensional reps given by $(12)=(-1)^a$, $(1324)=(-1)^b$, $a,b \in \{0,1\}$. Following the same procedure as earlier, we obtain

$$R = \sum_{g \in S_4} g \otimes g^* = \mathrm{diag}(1,(-1)^{a+b},(-1)^{a+b},(-1)^{a+b},1,(-1)^{a+b},(-1)^{a+b},(-1)^{a+b},1).$$

Both these solutions arose in $D(A_4)$ and were discussed in the previous section.

X. CONCLUSION

Our results show that for certain constant solutions of the Yang–Baxter equation obtained by using representations of finite group doubles, it is possible to Baxterize them to yield solutions of the spectral parameter Yang–Baxter equation. We have considered several examples where this is true and, in particular, we have found a new 21-vertex solution (15) from which we obtained an integrable model for a system of anyons with $D(D_3)$ or $D(D_6)$ symmetry. It is clearly of interest to determine if all constant solutions may be Baxterized. In contrast to the case of affine quantum algebras, where the spectral parameter has its origins in the loop representation, the origin of the spectral parameter for the above instances is unknown.

In all our examples we have only looked for cases where the spectral parameter has the difference property. For the case of the generalized chiral Potts model in Ref. 15, which does not have the difference property, an underlying finite group structure appears. This suggests that a Baxterization ansatz without the assumption of the difference property may also be fruitful. Certainly more work is needed to fully realize the potential of finite group doubles in solving the Yang–Baxter equation with spectral parameter.

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APPENDIX: REPRESENTATIONS OF $D(G)$, WHERE $G=D_n$, n ODD

The conjugacy classes C_k of $G=D_n$, chosen representatives g_k, corresponding centralizer subgroups Z_k and the elements α_s, $\forall s \in C_k$, are given in Table III.

1. Representations induced by $C_k=\{e\}$

The module elements are of the form $e \otimes v$, where $v \in V$, V a D_n-module. In representation terms, there are 2 one-dimensional irreps and $(n-1)/2$ two-dimensional irreps. They are as follows:

$$\sigma = 1, \quad \tau = \pm 1, \quad g^* = \delta(g,e)$$

and

TABLE III. C_k, g_k, Z_k and α_s for $G=D_n$, n odd.

C_k	g_k	$Z_k=Z(g_k)$	$\alpha_s, \forall s \in C_k$
$\{e\}$	e	D_n	$\alpha_e=e$
$\{\sigma^k,\sigma^{-k}\}, 1 \le k \le n-1/2$	σ^k	$\{\sigma^i\vert, 0 \le i < n\}$	$\alpha_{\sigma^k}=e, \alpha_{\sigma^{-k}}=\tau$
$\{\sigma^i\tau \vert 0 \le i < n\}$	τ	$\{e,\tau\}$	$\alpha_{\sigma^i\tau}=\sigma^{(n+1/2)i}$

$$\sigma = \begin{bmatrix} \omega^k & 0 \\ 0 & \omega^{-k} \end{bmatrix}, \quad \tau = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad g^* = \delta(g,e)I_2,$$

where $1 \leq k \leq (n-1)/2$.

2. Representations induced by $C_k = \{\sigma^k, \sigma^{-k}\}$, $1 \leq k \leq (n-1)/2$

The module elements are of the form $e \otimes v, \tau \otimes v$, where $v \in V$, V a module of the group algebra of $Z_k = \{\sigma^j | 0 \leq i < n\}$. There are n such A_k-modules, with the corresponding representations π_j given by $\pi_j(\sigma) = \omega^j$, $0 \leq j < n$, where $\omega = \exp(2\pi i/n)$. Thus, there are $n(n-1)/2$ different irreps of $D(D_n)$ induced by these conjugacy classes, given by

$$\sigma = \begin{bmatrix} \omega^j & 0 \\ 0 & \omega^{-j} \end{bmatrix}, \quad \tau = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (\sigma^k)^* = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad (\sigma^{-k})^* = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad g^* = 0 \text{ otherwise},$$

where $0 \leq j < n$, $1 \leq k \leq (n-1/2)$.

3. Representations induced by $C_k = \{\sigma^j \tau | 0 \leq i < n\}$

The module elements are of the form $\sigma^{j(n+1)/2} \otimes v$, $0 \leq j < n$, where $v \in V$, V a module of the group algebra of $Z_k = \{e, \tau\}$. Hence, there are two n-dimensional irreps of this form. They are as follows:

$$\sigma = A \in M_{n\times n}, \quad \text{where } [A]_{ij} = \delta(i, j+2), \quad \text{addition mod } n,$$

$$\tau = \pm B \in M_{n\times n}, \quad \text{where } [B]_{ij} = \delta(i+j, 2), \quad \text{addition mod } n,$$

$$(\sigma^i)^* = 0, \quad (\sigma^i \tau)^* = E^{i+1}_{i+1}, \quad 0 \leq i < n.$$

Example 10.1: *In $D(D_3)$, σ and τ are as follows:*

$$\sigma = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \tau = \pm \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Hence, when n is odd $D(D_n)$ has 2 one-dimensional irreps, 2 n-dimensional irreps and $(n^2-1)/2$ two-dimensional irreps, all of which are given above. Note that the sum of the squares of the dimensions is $4n^2 = |D_n|^2 = |D(D_n)|$, as we expect.[19]

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Isomorphisms between C^*-ternary algebras

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In this paper, we prove the Hyers-Ulam-Rassias stability of homomorphisms in C^*-ternary algebras and of derivations on C^*-ternary algebras for the following generalized Cauchy–Jensen additive mapping:

$$2f\left(\frac{\sum_{j=1}^{p} x_j}{2}+\sum_{j=1}^{d} y_j\right)=\sum_{j=1}^{p} f(x_j)+2\sum_{j=1}^{d} f(y_j).$$

This is applied to investigate isomorphisms between C^*-ternary algebras. The concept of Hyers-Ulam-Rassias stability originated from the Rassias stability theorem that appeared in his paper: On the stability of the linear mapping in Banach spaces, see Proc. Amr. Math. Soc. **72**, 297–300 (1978). © *2006 American Institute of Physics.* [DOI: 10.1063/1.2359576]

I. INTRODUCTION AND PRELIMINARIES

Ternary algebraic operations were considered in the 19th century by several mathematicians and physicists such as Cayley,[5] who introduced the notion of a *cubic matrix*, which in turn was generalized by Kapranov *et al.*[15] The simplest example of such nontrivial ternary operation is given by the following composition rule:

$$\{a,b,c\}_{ijk}=\sum_{l,m,n} a_{nil}b_{ljm}c_{mkn} \quad (i,j,k,\ldots=1,2,\ldots,N).$$

Ternary structures and their generalization, the so-called n-ary structures, raise certain hopes in view of their applications in physics. Some significant physical applications are as follows (see Refs. 16 and 17):

(1) The algebra of "*nonions*" generated by two matrices,

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \omega \\ \omega^2 & 0 & 0 \end{pmatrix} \quad (\omega=e^{2\pi i/3}),$$

was introduced by Sylvester as a ternary analog of Hamilton's quaternions (cf. Ref. 1).

(2) A natural ternary composition of four-vectors in the four-dimensional Minkowskian space-time M_4 can be defined as an example of a ternary operation:

$$(X,Y,Z)\to U(X,Y,Z)\in M_4,$$

with the resulting four-vector U^μ defined via its components in a given coordinate system as follows:

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$$U^{\mu}(X,Y,Z) = g^{\mu\sigma}\eta_{\sigma\nu\lambda\rho}X^{\nu}Y^{\lambda}Z^{\rho}, \quad \mu,\nu,\ldots = 0,1,2,3,$$

where $g^{\mu\sigma}$ is the metric tensor and $\eta_{\sigma\nu\lambda\rho}$ is the canonical volume element of M_4 (see Ref. 17).

(3) The quark model inspired a particular brand of ternary algebraic systems. The so-called "*Nambu mechnics*" is based on such structures (see Ref. 7).

There are also some applications, although still hypothetical, in the fractional quantum Hall effect, the nonstandard statistics, supersymmetric theory, and Yang-Baxter equation (cf. Refs. 1, 17, and 35).

Following the terminology of Ref. 2 a non-empty set G with a ternary operation $[\cdot,\cdot,\cdot]:G\times G\times G\to G$ is called a *ternary groupoid* and is denoted by $(G,[\cdot,\cdot,\cdot])$. The ternary groupoid $(G,[\cdot,\cdot,\cdot])$ is called *commutative* if $[x_1,x_2,x_3]=[x_{\sigma(1)},x_{\sigma(2)},x_{\sigma(3)}]$ for all $x_1,x_2,x_3\in G$ and all permutations σ of $\{1,2,3\}$.

If a binary operation $\circ$ is defined on G such that $[x,y,z]=(x\circ y)\circ z$ for all $x,y,z\in G$, then we say that $[\cdot,\cdot,\cdot]$ is derived from $\circ$. We say that $(G,[\cdot,\cdot,\cdot])$ is a *ternary semigroup* if the operation $[\cdot,\cdot,\cdot]$ is *associative*, i.e., if $[[x,y,z],u,v]=[x,[y,z,u],v]=[x,y,[z,u,v]]$ holds for all $x,y,z,u,v\in G$ (see Ref. 4).

A C^*-ternary algebra is a complex Banach space A, equipped with a ternary product $(x,y,z)\mapsto[x,y,z]$ of A^3 into A, which is $\mathbb{C}$ linear in the outer variables, conjugate $\mathbb{C}$-linear in the middle variable, and associative in the sense that $[x,y,[z,w,v]]=[x,[w,z,y],v]=[[x,y,z],w,v]$, and satisfies $\|[x,y,z]\|\le\|x\|\cdot\|y\|\cdot\|z\|$ and $\|[x,x,x]\|=\|x\|^3$ (see Refs. 2 and 36). Every left Hilbert C^* module is a C^*-ternary algebra via the ternary product $[x,y,z]:=\langle x,y\rangle z$.

If a C^*-ternary algebra $(A,[\cdot,\cdot,\cdot])$ has an identity, i.e., an element $e\in A$ such that $x=[x,e,e]=[e,e,x]$ for all $x\in A$, then it is routine to verify that A, endowed with $x\circ y:=[x,e,y]$ and $x^*:=[e,x,e]$, is a unital C^* algebra. Conversely, if $(A,\circ)$ is a unital C^* algebra, then $[x,y,z]:=x\circ y^*\circ z$ makes A into a C^*-ternary algebra.

A $\mathbb{C}$-linear mapping $H:A\to B$ is called a *C^*-ternary algebra homomorphism* if

$$H([x,y,z]) = [H(x),H(y),H(z)],$$

for all $x,y,z\in A$. If, in addition, the mapping H is bijective, then the mapping $H:A\to B$ is called a *C^*-ternary algebra isomorphism*. A $\mathbb{C}$-linear mapping $\delta:A\to A$ is called a *C^*-ternary derivation* if

$$\delta([x,y,z]) = [\delta(x),y,z]+[x,\delta(y),z]+[x,y,\delta(z)],$$

for all $x,y,z\in A$ (see Refs. 2 and 18).

In 1940, Ulam[34] gave a talk before the Mathematics Club of the University of Wisconsin in which he discussed a number of unsolved problems. Among these was the following question concerning the stability of homomorphisms.

We are given a group G and a metric group G' with metric $\rho(\cdot,\cdot)$. Given $\epsilon>0$, does there exist a $\delta>0$ such that if $f:G\to G'$ satisfies $\rho(f(xy),f(x)f(y))<\delta$ for all $x,y\in G$, then a homomorphism $h:G\to G'$ exists with $\rho(f(x),h(x))<\epsilon$ for all $x\in G$?

In 1941, Hyers[10] considered the case of approximately additive mappings $f:E\to E'$, where E and E' are Banach spaces and f satisfies *Hyers inequality*,

$$\|f(x+y)-f(x)-f(y)\|\le\epsilon,$$

for all $x,y\in E$. It was shown that the limit

$$L(x) = \lim_{n\to\infty}\frac{f(2^n x)}{2^n}$$

exists for all $x\in E$ and that $L:E\to E'$ is the unique additive mapping satisfying

$$\|f(x)-L(x)\|\le\epsilon.$$

In 1978, Rassias[26] provided a generalization of Hyers' Theorem that allows the *Cauchy difference to be unbounded*.

Theorem 1.1: (Rassias[26]) *Let $f:E\to E'$ be a mapping from a normed vector space E into a Banach space E', subject to the inequality*

$$\|f(x+y)-f(x)-f(y)\| \le \epsilon(\|x\|^p+\|y\|^p), \tag{1.1}$$

for all $x,y\in E$, where ϵ and p are constants with $\epsilon>0$ and $p<1$. Then the limit

$$L(x)=\lim_{n\to\infty}\frac{f(2^n x)}{2^n},$$

exists for all $x\in E$ and $L:E\to E'$ is the unique additive mapping that satisfies

$$\|f(x)-L(x)\| \le \frac{2\epsilon}{2-2^p}\|x\|^p, \tag{1.2}$$

for all $x\in E$. If $p<0$, then inequality (1.1) holds for $x,y\neq 0$ and (1.2) for $x\neq 0$.

In 1990, Rassias,[27] during the 27th International Symposium on Functional Equations, asked the question of whether such a theorem can also be proved for $p\ge 1$. In 1991, Gajda[8] following the same approach as in Rassias,[26] gave an affirmative solution to this question for $p>1$. It was shown by Gajda,[8] as well as by Rassias and Šemrl[32] that one cannot prove a Rassias' type theorem when $p=1$. The counterexamples of Gajda,[8] as well as of Rassias and Šemrl,[32] have stimulated several mathematicians to invent new definitions of *approximately additive* or *approximately linear* mappings; cf. Găvruta,[9] Jung,[14] who, among others, studied the Hyers-Ulam-Rassias stability of functional equations. The inequality (1.1) that was introduced for the first time by Rassias[26] provided a lot of influence in the development of a generalization of the Hyers-Ulam stability concept. This new concept is known as the *Hyers-Ulam-Rassias stability* of functional equations (cf. the books of Czerwik,[6] Hyers, Isac, and Rassias.[11])

Rassias,[24] following the spirit of the innovative approach of Rassias[26] for the unbounded Cauchy difference, proved a similar stability theorem in which he replaced the factor $\|x\|^p+\|y\|^p$ by $\|x\|^p\cdot\|y\|^q$ for $p,q\in\mathbb{R}$ with $p+q\neq 1$ (see also Ref. 25 for a number of other new results).

Găvruta[9] provided a further generalization of Rassias' Theorem. In 1996, Isac and Rassias[13] applied the Hyers-Ulam-Rassias stability theory to prove fixed point theorems and study some new applications in Nonlinear Analysis. In Ref. 12, Hyers, Isac, and Rassias studied the asymptoticity aspect of Hyers-Ulam stability of mappings. During the past few years several mathematicians have published on various generalizations and applications of Hyers-Ulam stability and Hyers-Ulam-Rassias stability to a number of functional equations and mappings, for example, quadratic functional equation, invariant means, multiplicative mappings—superstability, bounded nth differences, convex functions, generalized orthogonality functional equation, Euler-Lagrange functional equation, and Navier-Stokes equations. Several mathematicians have contributed works on these subjects; we mention a few: Baak and Moslehian,[3] Park,[19–23] Rassias,[28–31] and Skof.[33]

Throughout this paper, assume that p, d are non-negative integers with $p+d\ge 3$.

In Sec. II, we prove the Hyers-Ulam-Rassias stability of homomorphisms in C^*-ternary algebras for the generalized Cauchy-Jensen additive mapping.

In Sec. III, we investigate isomorphisms between unital C^*-ternary algebras associated with the generalized Cauchy-Jensen additive mapping.

In Sec. IV, we prove the Hyers-Ulam-Rassias stability of derivations on C^*-ternary algebras for the generalized Cauchy-Jensen additive mapping.

II. STABILITY OF HOMOMORPHISMS IN C^*-TERNARY ALGEBRAS

Throughout this section, assume that A is a C^*-ternary algebra with norm $\|\cdot\|_A$ and that B is a C^*-ternary algebra with norm $\|\cdot\|_B$.

For a given mapping $f:A\to B$, we define

$$C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d) := 2f\left(\frac{\sum_{j=1}^{p}\mu x_j}{2}+\sum_{j=1}^{d}\mu y_j\right)-\sum_{j=1}^{p}\mu f(x_j)-2\sum_{j=1}^{d}\mu f(y_j),$$

for all $\mu\in\mathbb{T}^1:=\{\lambda\in\mathbb{C}\,|\,|\lambda|=1\}$ and all $x_1,\ldots,x_p,y_1,\ldots,y_d\in A$.

One can easily show that a mapping $f:A\to B$ satisfies $C_1f(x_1,\ldots,x_p,y_1,\ldots,y_d)=0$ if and only if f is Cauchy additive, and that if a mapping $f:A\to B$ satisfies $C_1f(x_1,\ldots,x_p,y_1,\ldots,y_d)=0$ then $f(0)=0$.

We prove the Hyers-Ulam-Rassias stability of homomorphisms in C^*-ternary algebras for the functional equation $C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d)=0$.

Theorem 2.1: *Let $r>3$ and θ be non-negative real numbers, and let $f:A\to B$ be a mapping such that*

$$\|C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d)\|_B\le\theta\left(\sum_{j=1}^{p}\|x_j\|_A^r+\sum_{j=1}^{d}\|y_j\|_A^r\right),\tag{2.1}$$

$$\|f([x,y,z])-[f(x),f(y),f(z)]\|_B\le\theta(\|x\|_A^r+\|y\|_A^r+\|z\|_A^r),\tag{2.2}$$

for all $\mu\in\mathbb{T}^1$ and all $x,y,z,x_1,\ldots,x_p,y_1,\ldots,y_d\in A$. Then there exists a unique C^*-ternary algebra homomorphism $H:A\to B$, such that

$$\|f(x)-H(x)\|_B\le\frac{p+d}{2(p+2d)^r-(p+2d)2^r}\theta\|x\|_A^r,\tag{2.3}$$

for all $x\in A$.

Proof: Let us assume $\mu=1$ and $x_1=\cdots=x_p=y_1=\cdots=y_d=x$ in (2.1). Then we get

$$\left\|2f\left(\frac{p+2d}{2}x\right)-(p+2d)f(x)\right\|_B\le(p+d)\theta\|x\|_A^r,\tag{2.4}$$

for all $x\in A$. So

$$\left\|f(x)-\frac{p+2d}{2}f\left(\frac{2}{p+2d}x\right)\right\|_B\le\frac{p+d}{2(p+2d)^r}\theta\|x\|_A^r,$$

for all $x\in A$. Hence

$$\begin{aligned}&\left\|\frac{(p+2d)^l}{2^l}f\left(\frac{2^l}{(p+2d)^l}x\right)-\frac{(p+2d)^m}{2^m}f\left(\frac{2^m}{(p+2d)^m}x\right)\right\|_B\\&\le\sum_{j=l}^{m-1}\left\|\frac{(p+2d)^j}{2^j}f\left(\frac{2^j}{(p+2d)^j}x\right)-\frac{(p+2d)^{j+1}}{2^{j+1}}f\left(\frac{2^{j+1}}{(p+2d)^{j+1}}x\right)\right\|_B\\&\le\frac{(p+d)}{2(p+2d)^r}\sum_{j=l}^{m-1}\frac{2^{rj}(p+2d)^j}{2^j(p+2d)^{rj}}\theta\|x\|_A^r,\end{aligned}\tag{2.5}$$

for all non-negative integers m and l with $m>l$ and all $x\in A$. From this it follows that the sequence $\{[(p+2d)^n/2^n]f([2^n/(p+2d)^n]x)\}$ is a Cauchy sequence for all $x\in A$. Since B is complete, the sequence $\{[(p+2d)^n/2^n]f([2^n/(p+2d)^n]x)\}$ converges. Thus one can define the mapping $H:A\to B$ by

$$H(x) := \lim_{n\to\infty} \frac{(p+2d)^n}{2^n} f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x \in A$. Moreover, letting $l=0$ and passing the limit $m\to\infty$ in (2.5), we get (2.3).

It follows from (2.1) that

$$\begin{aligned}
&\left\| 2H\left(\frac{\sum_{j=1}^{p} x_j}{2} + \sum_{j=1}^{d} y_j\right) - \sum_{j=1}^{p} H(x_j) - 2\sum_{j=1}^{d} H(y_j)\right\|_B \\
&= \lim_{n\to\infty} \frac{(p+2d)^n}{2^n} \left\| 2f\left(\frac{2^n}{(p+2d)^n}\frac{\sum_{j=1}^{p} x_j}{2} + \frac{2^n}{(p+2d)^n}\sum_{j=1}^{d} y_j\right)\right. \\
&\quad \left. - \sum_{j=1}^{p} f\left(\frac{2^n}{(p+2d)^n}x_j\right) - 2\sum_{j=1}^{d} f\left(\frac{2^n}{(p+2d)^n}y_j\right)\right\|_B \\
&\le \lim_{n\to\infty} \frac{2^{nr}(p+2d)^n}{2^n(p+2d)^{nr}}\theta\left(\sum_{j=1}^{p}\|x_j\|_A^r + \sum_{j=1}^{d}\|y_j\|_A^r\right) = 0,
\end{aligned}$$

for all $x_1,\ldots,x_p,y_1,\ldots,y_d \in A$. Hence

$$2H\left(\frac{\sum_{j=1}^{p} x_j}{2} + \sum_{j=1}^{d} y_j\right) = \sum_{j=1}^{p} H(x_j) + 2\sum_{j=1}^{d} H(y_j),$$

for all $x_1,\ldots,x_p,y_1,\ldots,y_d \in A$. So the mapping $H:A\to B$ is Cauchy additive.

By the same reasoning as in the proof of Theorem 2.1 of Ref. 21, the mapping $H:A\to B$ is $\mathbb{C}$-linear.

It follows from (2.2) that

$$\begin{aligned}
\|H([x,y,z]) - [H(x),H(y),H(z)]\|_B &= \lim_{n\to\infty} \frac{(p+2d)^{3n}}{8^n}\left\| f\left(\frac{8^n[x,y,z]}{(p+2d)^{3n}}\right)\right. \\
&\quad \left. - \left[f\left(\frac{2^n x}{(p+2d)^n}\right), f\left(\frac{2^n y}{(p+2d)^n}\right), f\left(\frac{2^n z}{(p+2d)^n}\right)\right]\right\|_B \\
&\le \lim_{n\to\infty} \frac{2^{nr}(p+2d)^{3n}}{8^n(p+2d)^{nr}}\theta(\|x\|_A^r + \|y\|_A^r + \|z\|_A^r) = 0,
\end{aligned}$$

for all $x,y,z \in A$. Thus

$$H([x,y,z]) = [H(x),H(y),H(z)],$$

for all $x,y,z \in A$.

Now, let $T:A\to B$ be another generalized Cauchy-Jensen additive mapping satisfying (2.3). Then we have

$$\begin{aligned}\|H(x)-T(x)\|_B &= \frac{(p+2d)^n}{2^n}\left\|H\left(\frac{2^n x}{(p+2d)^n}\right)-T\left(\frac{2^n x}{(p+2d)^n}\right)\right\|_B \\ &\le \frac{(p+2d)^n}{2^n}\left(\left\|H\left(\frac{2^n x}{(p+2d)^n}\right)-f\left(\frac{2^n x}{(p+2d)^n}\right)\right\|_B\right. \\ &\quad \left.+\left\|T\left(\frac{2^n x}{(p+2d)^n}\right)-f\left(\frac{2^n x}{(p+2d)^n}\right)\right\|_B\right) \\ &\le \frac{p+d}{2(p+2d)^r-(p+2d)2^r}\cdot\frac{2^{nr+1}(p+2d)^n}{2^n(p+2d)^{nr}}\theta\|x\|_A^r,\end{aligned}$$

which tends to zero as $n\to\infty$ for all $x\in A$. So we can conclude that $H(x)=T(x)$ for all $x\in A$. This proves the uniqueness of H. Thus, the mapping $H:A\to B$ is a unique C^*-ternary algebra homomorphism satisfying (2.3).

Theorem 2.2: *Let $r<1$ and θ be non-negative real numbers, and let $f:A\to B$ be a mapping satisfying* (2.1) and (2.2). *Then there exists a unique C^*-ternary algebra homomorphism $H:A\to B$ such that*

$$\|f(x)-H(x)\|_B \le \frac{2^r(p+d)}{2^r(p+2d)-2(p+2d)^r}\theta\|x\|_A^r, \tag{2.6}$$

for all $x\in A$.

Proof: It follows from (2.4) that

$$\left\|f(x)-\frac{2}{p+2d}f\left(\frac{p+2d}{2}x\right)\right\|_B \le \frac{p+d}{p+2d}\theta\|x\|_A^r,$$

for all $x\in A$. So

$$\begin{aligned}&\left\|\frac{2^l}{(p+2d)^l}f\left(\frac{(p+2d)^l}{2^l}x\right)-\frac{2^m}{(p+2d)^m}f\left(\frac{(p+2d)^m}{2^m}x\right)\right\|_B \\ &\le \sum_{j=l}^{m-1}\left\|\frac{2^j}{(p+2d)^j}f\left(\frac{(p+2d)^j}{2^j}x\right)-\frac{2^{j+1}}{(p+2d)^{j+1}}f\left(\frac{(p+2d)^{j+1}}{2^{j+1}}x\right)\right\|_B \\ &\le \frac{p+d}{p+2d}\sum_{j=l}^{m-1}\frac{2^j(p+2d)^{jr}}{2^{jr}(p+2d)^j}\theta\|x\|_A^r,\end{aligned} \tag{2.7}$$

for all non-negative integers m and l with $m>l$ and all $x\in A$. From this it follows that the sequence $\{[2^n/(p+2d)^n]f([(p+2d)^n/2^n]x)\}$ is a Cauchy sequence for all $x\in A$. Since B is complete, the sequence $\{[2^n/(p+2d)^n]f([(p+2d)^n/2^n]x)\}$ converges. So one can define the mapping $H:A\to B$ by

$$H(x) := \lim_{n\to\infty}\frac{2^n}{(p+2d)^n}f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x\in A$. Moreover, letting $l=0$ and passing the limit $m\to\infty$ in (2.7), we get (2.6).

The rest of the proof is similar to the proof of Theorem 2.1. □

Theorem 2.3: *Let $r>1$ and θ be non-negative real numbers, and let $f:A\to B$ be a mapping such that*

$$\|C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d)\|_B \le \theta\prod_{j=1}^{p}\|x_j\|_A^r\cdot\prod_{j=1}^{d}\|y_j\|_A^r, \tag{2.8}$$

$$\|f([x,y,z])-[f(x),f(y),f(z)]\|_B \le \theta\cdot(\|x\|_A^r\cdot\|y\|_A^r\cdot\|z\|_A^r), \tag{2.9}$$

for all $\mu\in\mathbb{T}^1$ *and all* $x,y,z,x_1,\ldots,x_p,y_1,\ldots,y_d\in A$. *Then there exists a unique* C^**-ternary algebra homomorphism* $H:A\to B$ *such that*

$$\|f(x)-H(x)\|_B \le \frac{2^{(p+d)r}}{2(p+2d)^{(p+d)r}-2^{(p+d)r}(p+2d)}\theta\|x\|_A^{(p+d)r}, \tag{2.10}$$

for all $x\in A$.

Proof: Let us assume $\mu=1$ and $x_1=\cdots=x_p=y_1=\cdots=y_d=x$ in (2.8). Then we get

$$\left\|2f\left(\frac{p+2d}{2}x\right)-(p+2d)f(x)\right\|_B \le \theta\|x\|_A^{(p+d)r}, \tag{2.11}$$

for all $x\in A$.So

$$\left\|f(x)-\frac{p+2d}{2}f\left(\frac{2}{p+2d}x\right)\right\|_B \le \frac{2^{(p+d)r}}{2(p+2d)^{(p+d)r}}\theta\|x\|_A^{(p+d)r},$$

for all $x\in A$. Hence

$$\begin{aligned}&\left\|\frac{(p+2d)^l}{2^l}f\left(\frac{2^l}{(p+2d)^l}x\right)-\frac{(p+2d)^m}{2^m}f\left(\frac{2^m}{(p+2d)^m}x\right)\right\|_B\\&\le\sum_{j=l}^{m-1}\left\|\frac{(p+2d)^j}{2^j}f\left(\frac{2^j}{(p+2d)^j}x\right)-\frac{(p+2d)^{j+1}}{2^{j+1}}f\left(\frac{2^{j+1}}{(p+2d)^{j+1}}x\right)\right\|_B\\&\le\frac{2^{(p+d)r}}{2(p+2d)^{(p+d)r}}\sum_{j=l}^{m-1}\frac{2^{(p+d)rj}(p+2d)^j}{2^j(p+2d)^{(p+d)rj}}\theta\|x\|_A^{(p+d)r},\end{aligned} \tag{2.12}$$

for all non-negative integers m and l with $m>l$ and all $x\in A$. From this it follows that the sequence $\{[(p+2d)^n/2^n]f([2^n/(p+2d)^n]x)\}$ is a Cauchy sequence for all $x\in A$. Since B is complete, the sequence $\{[(p+2d)^n/2^n]f([2^n/(p+2d)^n]x)\}$ converges. Thus one can define the mapping $H:A\to B$ by

$$H(x):=\lim_{n\to\infty}\frac{(p+2d)^n}{2^n}f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x\in A$. Moreover, letting $l=0$ and passing the limit $m\to\infty$ in (2.12), we get (2.10).

The rest of the proof is similar to the proof of Theorem 2.1. □

Theorem 2.4: *Let* $r<1/(p+d)$ *and* θ *be non-negative real numbers, and let* $f:A\to B$ *be a mapping satisfying* (2.8) and (2.9). *Then there exists a unique* C^**-ternary algebra homomorphism* $H:A\to B$ *such that*

$$\|f(x)-H(x)\|_B \le \frac{2^{(p+d)r}}{2^{(p+d)r}(p+2d)-2(p+2d)^{(p+d)r}}\theta\|x\|_A^{(p+d)r}, \tag{2.13}$$

for all $x\in A$.

Proof: It follows from (2.11) that

$$\left\|f(x)-\frac{2}{p+2d}f\left(\frac{p+2d}{2}x\right)\right\|_B \le \frac{\theta}{p+2d}\|x\|_A^{(p+d)r},$$

for all $x\in A$. So

$$\begin{aligned}
&\left\|\frac{2^l}{(p+2d)^l}f\left(\frac{(p+2d)^l}{2^l}x\right)-\frac{2^m}{(p+2d)^m}f\left(\frac{(p+2d)^m}{2^m}x\right)\right\|_B\\
&\le\sum_{j=l}^{m-1}\left\|\frac{2^j}{(p+2d)^j}f\left(\frac{(p+2d)^j}{2^j}x\right)-\frac{2^{j+1}}{(p+2d)^{j+1}}f\left(\frac{(p+2d)^{j+1}}{2^{j+1}}x\right)\right\|_B\\
&\le\frac{\theta}{p+2d}\sum_{j=l}^{m-1}\frac{2^j(p+2d)^{j(p+d)r}}{2^{j(p+d)r}(p+2d)^j}\|x\|_A^{(p+d)r},
\end{aligned}\tag{2.14}$$

for all non-negative integers m and l with $m>l$ and all $x\in A$. From this it follows that the sequence $\{[2^n/(p+2d)^n]f([(p+2d)^n/2^n]x)\}$ is a Cauchy sequence for all $x\in A$. Since B is complete, the sequence $\{[2^n/(p+2d)^n]f([(p+2d)^n/2^n]x)\}$ converges. So one can define the mapping $H:A\to B$ by

$$H(x):=\lim_{n\to\infty}\frac{2^n}{(p+2d)^n}f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x\in A$. Moreover, letting $l=0$ and passing the limit $m\to\infty$ in (2.14), we get (2.13).

The rest of the proof is similar to the proof of Theorem 2.1. □

III. ISOMORPHISMS BETWEEN C^*-TERNARY ALGEBRAS

Throughout this section, assume that A is a unital C^*-ternary algebra with norm $\|\cdot\|_A$ and unit e, and that B is a unital C^*-ternary algebra with norm $\|\cdot\|_B$ and unit e'.

We investigate isomorphisms between C^*-ternary algebras associated with the functional equation $C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d)=0$.

Theorem 3.1: *Let $r>1$ and θ be non-negative real numbers, and let $f:A\to B$ be a bijective mapping satisfying* (2.1), *such that*

$$f([x,y,z])=[f(x),f(y),f(z)],\tag{3.1}$$

for all $x,y,z\in A$. If $\lim_{n\to\infty}[(p+2d)^n/2^n]f(2^ne/(p+2d)^n)=e'$, then the mapping $f:A\to B$ is a C^*-ternary algebra isomorphism.

Proof: By the same reasoning as in the proof of Theorem 2.1, there exists a unique $\mathbb{C}$-linear mapping $H:A\to B$ such that

$$\|f(x)-H(x)\|_B\le\frac{p+d}{2(p+2d)^r-(p+2d)2^r}\theta\|x\|_A^r,$$

for all $x\in A$. The mapping $H:A\to B$ is defined by

$$H(x):=\lim_{n\to\infty}\frac{(p+2d)^n}{2^n}f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x\in A$.

Since $f([x,y,z])=[f(x),f(y),f(z)]$ for all $x,y,z\in A$,

$$\begin{aligned}
H([x,y,z])&=\lim_{n\to\infty}\frac{(p+2d)^{3n}}{8^n}f\left(\left[\frac{2^nx}{(p+2d)^n},\frac{2^ny}{(p+2d)^n},\frac{2^nz}{(p+2d)^n}\right]\right)\\
&=\lim_{n\to\infty}\left[\frac{(p+2d)^n}{2^n}f\left(\frac{2^nx}{(p+2d)^n}\right),\frac{(p+2d)^n}{2^n}f\left(\frac{2^ny}{(p+2d)^n}\right),\frac{(p+2d)^n}{2^n}f\left(\frac{2^nz}{(p+2d)^n}\right)\right]\\
&=[H(x),H(y),H(z)],
\end{aligned}$$

for all $x,y,z\in A$. So the mapping $H:A\to B$ is a C^*-ternary algebra homomorphism.

It follows from (3.1) that

$$H(x) = H([e,e,x]) = \lim_{n\to\infty} \frac{(p+2d)^{2n}}{4^n} f\left(\frac{4^n}{(p+2d)^{2n}}[e,e,x]\right)$$
$$= \lim_{n\to\infty} \frac{(p+2d)^{2n}}{4^n} f\left(\left[\frac{2^n e}{(p+2d)^n}, \frac{2^n e}{(p+2d)^n}, x\right]\right)$$
$$= \lim_{n\to\infty} \left[\frac{(p+2d)^n}{2^n} f\left(\frac{2^n e}{(p+2d)^n}\right), \frac{(p+2d)^n}{2^n} f\left(\frac{2^n e}{(p+2d)^n}\right), f(x)\right] = [e',e',f(x)] = f(x),$$

for all $x \in A$. Hence the bijective mapping $f:A\to B$ is a C^*-ternary algebra isomorphism. □

Theorem 3.2: *Let $r<1$ and θ be non-negative real numbers, and let $f:A\to B$ be a bijective mapping satisfying* (2.1) and (3.1). *If* $\lim_{n\to\infty}[2^n/(p+2d)^n]f([(p+2d)^n/2^n]e)=e'$, *then the mapping $f:A\to B$ is a C^*-ternary algebra isomorphism.*

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.2, there exists a unique $\mathbb{C}$-linear mapping $H:A\to B$ such that

$$\|f(x)-H(x)\|_B \le \frac{2^r(p+d)}{2^r(p+2d)-2(p+2d)^r}\theta\|x\|_A^r,$$

for all $x \in A$. The mapping $H:A\to B$ is defined by

$$H(x) := \lim_{n\to\infty} \frac{2^n}{(p+2d)^n} f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proof of Theorem 3.1. □

Theorem 3.3: *Let $r>1/(p+d)$ and θ be non-negative real numbers, and let $f:A\to B$ be a bijective mapping satisfying* (2.8) and (3.1). *If* $\lim_{n\to\infty}[(p+2d)^n/2^n]f(2^n e/(p+2d)^n)=e'$, *then the mapping $f:A\to B$ is a C^*-ternary algebra isomorphism.*

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.3, there exists a unique $\mathbb{C}$-linear mapping $H:A\to B$ such that

$$\|f(x)-H(x)\|_B \le \frac{2^{(p+d)r}}{2(p+2d)^{(p+d)r}-2^{(p+d)r}(p+2d)}\theta\|x\|_A^{(p+d)r},$$

for all $x \in A$. The mapping $H:A\to B$ is defined by

$$H(x) := \lim_{n\to\infty} \frac{(p+2d)^n}{2^n} f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proofs of Theorems 2.3 and 3.1. □

Theorem 3.4: *Let $r<1/(p+d)$ and θ be non-negative real numbers, and let $f:A\to B$ be a bijective mapping satisfying* (2.8) and (3.1). *If* $\lim_{n\to\infty}[2^n/(p+2d)^n]f([(p+2d)^n/2^n]e)=e'$, *then the mapping $f:A\to B$ is a C^*-ternary algebra isomorphism.*

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.4, there exists a unique $\mathbb{C}$-linear mapping $H:A\to B$ such that

$$\|f(x)-H(x)\|_B \le \frac{2^{(p+d)r}}{2^{(p+d)r}(p+2d)-2(p+2d)^{(p+d)r}}\theta\|x\|_A^{(p+d)r},$$

for all $x \in A$. The mapping $H:A\to B$ is defined by

$$H(x) := \lim_{n\to\infty} \frac{2^n}{(p+2d)^n} f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proofs of Theorems 2.4 and 3.1. □

IV. STABILITY OF DERIVATIONS ON C^*-TERNARY ALGEBRAS

Throughout this section, assume that A is a C^*-ternary algebra with norm $\|\cdot\|_A$.

We prove the Hyers-Ulam-Rassias stability of derivations on C^*-ternary algebras for the functional equation $C_\mu f(x_1,\ldots,x_p,y_1,\ldots,y_d)=0$.

Theorem 4.1: *Let $r>3$ and θ be non-negative real numbers, and let $f:A\to A$ be a mapping satisfying (2.1) such that*

$$\|f([x,y,z]) - [f(x),y,z] - [x,f(y),z] - [x,y,f(z)]\|_A \le \theta(\|x\|_A^r + \|y\|_A^r + \|z\|_A^r), \tag{4.1}$$

for all $x,y,z \in A$. Then there exists a unique C^*-ternary derivation $\delta:A\to A$ such that

$$\|f(x) - \delta(x)\|_A \le \frac{p+d}{2(p+2d)^r - (p+2d)2^r}\theta\|x\|_A^r, \tag{4.2}$$

for all $x \in A$.

Proof: By the same reasoning as in the proof of Theorem 2.1, there exists a unique $\mathbb{C}$-linear mapping $\delta:A\to A$ satisfying (4.2). The mapping $\delta:A\to A$ is defined by

$$\delta(x) := \lim_{n\to\infty} \frac{(p+2d)^n}{2^n} f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x \in A$.

It follows from (4.1) that

$$\begin{aligned}
&\|\delta([x,y,z]) - [\delta(x),y,z] - [x,\delta(y),z] - [x,y,\delta(z)]\|_A \\
&= \lim_{n\to\infty} \frac{(p+2d)^{3n}}{8^n} \left\| f\left(\frac{8^n}{(p+2d)^{3n}}[x,y,z]\right) - \left[f\left(\frac{2^n x}{(p+2d)^n}\right), \frac{2^n y}{(p+2d)^n}, \frac{2^n z}{(p+2d)^n}\right] \right. \\
&\quad \left. - \left[\frac{2^n x}{(p+2d)^n}, f\left(\frac{2^n y}{(p+2d)^n}\right), \frac{2^n z}{(p+2d)^n}\right] - \left[\frac{2^n x}{(p+2d)^n}, \frac{2^n y}{(p+2d)^n}, f\left(\frac{2^n z}{(p+2d)^n}\right)\right] \right\|_A \\
&\le \lim_{n\to\infty} \frac{2^{nr}(p+2d)^{3n}}{8^n(p+2d)^{nr}} \theta(\|x\|_A^r + \|y\|_A^r + \|z\|_A^r) = 0,
\end{aligned}$$

for all $x,y,z \in A$. Hence

$$\delta([x,y,z]) = [\delta(x),y,z] + [x,\delta(y),z] + [x,y,\delta(z)],$$

for all $x,y,z \in A$. Thus the mapping $\delta:A\to A$ is a unique C^*-ternary derivation satisfying (4.2).□

Theorem 4.2: *Let $r<1$ and θ be nonnegative real numbers, and let $f:A\to A$ be a mapping satisfying (2.1) and (4.1). Then there exists a unique C^*-ternary derivation $\delta:A\to A$ such that*

$$\|f(x) - \delta(x)\|_A \le \frac{2^r(p+d)}{2^r(p+2d) - 2(p+2d)^r}\theta\|x\|_A^r, \tag{4.3}$$

for all $x \in A$.

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.2, there exists a unique $\mathbb{C}$-linear mapping $\delta:A\to A$ satisfying (4.3). The mapping $\delta:A\to A$ is defined by

$$\delta(x) := \lim_{n\to\infty} \frac{2^n}{(p+2d)^n} f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proof of Theorem 4.1. □

Theorem 4.3: *Let $r>1$ and θ be non-negative real numbers, and let $f:A\to A$ be a mapping satisfying (2.8) such that*

$$\|f([x,y,z]) - [f(x),y,z] - [x,f(y),z] - [x,y,f(z)]\|_A \le \theta \cdot \|x\|_A^r \cdot \|y\|_A^r \cdot \|z\|_A^r, \tag{4.4}$$

for all $x,y,z \in A$. Then there exists a unique C^*-ternary derivation $\delta:A\to A$ such that

$$\|f(x) - \delta(x)\|_A \le \frac{2^{(p+d)r}}{2(p+2d)^{(p+d)r} - 2^{(p+d)r}(p+2d)} \theta \|x\|_A^{(p+d)r}, \tag{4.5}$$

for all $x \in A$.

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.3, there exists a unique $\mathbb{C}$-linear mapping $\delta:A\to A$ satisfying (4.5). The mapping $\delta:A\to A$ is defined by

$$\delta(x) := \lim_{n\to\infty} \frac{(p+2d)^n}{2^n} f\left(\frac{2^n}{(p+2d)^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proof of Theorem 4.1. □

Theorem 4.4: *Let $r<1/(p+d)$ and θ be non-negative real numbers, and let $f:A\to A$ be a mapping satisfying (2.8) and (4.4). Then there exists a unique C^*-ternary derivation $\delta:A\to A$ such that*

$$\|f(x) - \delta(x)\|_A \le \frac{2^{(p+d)r}}{2^{(p+d)r}(p+2d) - 2(p+2d)^{(p+d)r}} \theta \|x\|_A^{(p+d)r}, \tag{4.6}$$

for all $x \in A$.

Proof: By the same reasoning as in the proofs of Theorems 2.1 and 2.4, there exists a unique $\mathbb{C}$-linear mapping $\delta:A\to A$ satisfying (4.6). The mapping $\delta:A\to A$ is defined by

$$\delta(x) := \lim_{n\to\infty} \frac{2^n}{(p+2d)^n} f\left(\frac{(p+2d)^n}{2^n}x\right),$$

for all $x \in A$.

The rest of the proof is similar to the proof of Theorem 4.1. □

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Bell-type inequalities for nonlocal resources

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We present bipartite Bell-type inequalities which allow the two partners to use some nonlocal resource. Such inequalities can only be violated if the parties use a resource which is more nonlocal than the one permitted by the inequality. We introduce a family of N-input nonlocal machines, which are generalizations of the well-known PR (Popescu-Rohrlich) box. Then we construct Bell-type inequalities that cannot be violated by strategies that use one of these new machines. Finally we discuss implications for the simulation of quantum states. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2352857]

I. INTRODUCTION

One of the most striking properties of quantum mechanics is nonlocality. It is well known that two separated observers, each holding half of an entangled quantum state and performing appropriate measurements, share correlations which are nonlocal, in the sense that they violate a Bell inequality.[1] Indeed, this has been demonstrated in many laboratory experiments.[2] A key feature of entanglement is that it does not allow the two distant observers to send information to each other faster than light, i.e., correlation from measurements on quantum states is no-signaling.

It is an interesting problem to quantify how powerful the nonlocal correlations of quantum mechanics are. In order to do that, one has to use some nonlocal resource. A quite natural choice is indeed classical communication. In 2003, Toner and Bacon showed that a single bit of communication is enough to reproduce the correlations of the singlet state.[3] In the last years another nonlocal resource, the PR (Popescu-Rohrlich) box, has also been proposed to study this problem. Introduced in 1994 by Popescu and Rohrlich,[4,5] the PR box was then proven to be a powerful resource for information theoretic tasks, such as communication complexity[6,7] and cryptography.[8] It was also recently suggested that the PR box is a unit of nonlocality.[9] The PR box has the appealing feature that it is intrinsically nonsignaling, which is of course not the case of classical communication.[10] Note that a PR box is a strictly weaker resource than a bit of communication.[11] Recently, Cerf *et al.* presented a model using a single PR box which simulates correlations from any projective measurement on the singlet.[12] It appears very natural to extend this study to other quantum states, but this turns out to be quite difficult, even for nonmaximally entangled pure states of two qubits. In a recent paper we showed a family of nonmaximally entangled states, whose correlations cannot be reproduced by a single PR box.[11] In other words, some nonmaximally entangled states require a strictly larger amount of nonlocal resources than the maximally entangled state to be simulated. This suggests that entanglement and nonlocality are different resources. To demonstrate this result we found a Bell-type inequality allowing some nonlocal resource; in this case a single use of a PR box. Then, it was proven that this inequality is violated by some nonmaximally entangled state.

In the present paper, we introduce N-input bipartite nonlocal machines (NLM), which appear as a natural extension of the two-input PR box. These machines, denoted PR_N, have a nice connection to a family of N-setting Bell inequalities known as I_{NN22},[13] similar to the one that relates the PR box to the Clauser-Horne-Shimony-Holt (CHSH) inequality,[14]

$$\text{CHSH} \Rightarrow \text{PR box}, \tag{1}$$

$$I_{NN22} \Rightarrow PR_N.$$

In fact, the structure of the N-input NLM can be directly deduced from the corresponding I_{NN22} inequality. Then, we present a family of N-setting inequalities, M_{NN22}, which allows one use of the PR_{N-1} machine. Again, the structure of these new inequalities is easily deduced from the structure of the I_{NN22} inequalities, i.e.,

$$I_{NN22} \Rightarrow M_{NN22}. \tag{2}$$

Thus, a nice construction appears: for any number of settings N, we have a Bell inequality I_{NN22} and the related NLM, PR_N, which reaches the upper (no-signaling) bound of the inequality. Adding one setting we find another inequality, $M_{(N+1)(N+1)22}$, which cannot be violated by strategies which require a single use of PR_N.

The organization of the paper is as follows. In Sec. II we present the mathematical tools and introduce the notations by reviewing the simplest case of two settings on each side. The link between the PR box and the CHSH inequality is pointed out. Section III is devoted to the case of three settings: we introduce a three-setting NLM and study an inequality for a single use of a PR box. In Sec. IV, the construction of Sec. III is extended to the case N settings. Section V concludes the paper by reviewing the main results about Bell inequalities with and without resources. Our present work is then clearly situated in this context.

II. TOOLS

Let us consider a typical Bell test scenario. Two distant observers, Alice and Bob, share some quantum state. Each of them chooses between a set of measurements (settings) $\{A_i\}_{i=1\ldots N_A}$, $\{B_j\}_{j=1\ldots N_B}$. The result of the measurement is noted r_A, r_B. Here we will focus on dichotomic observables and we will restrict Alice and Bob to use the same number of settings, i.e., $r_{A,B} \in \{0,1\}$ and $N_A = N_B \equiv N$. An "experiment" is fully characterized by the family of $4N^2$ probabilities $P(r_A, r_B | A_i, B_j) \equiv P_{ij}(r_A, r_B)$ and can be seen as a point in a $4N^2$-dimensional probability space. As probabilities must satisfy

(i) Positivity: $P_{ij}(r_A, r_B) \geq 0 \quad \forall\, i,j,r_A,r_B$

(ii) Normalization: $\sum_{r_A,r_B=0,1} P_{ij}(r_A, r_B) = 1 \quad \forall\, i,j,$

all relevant experiments are contained in a bounded region of this probability space. Since we want to restrict ourselves to no-signaling probability distributions, we impose also the no-signaling conditions

$$\begin{aligned} \sum_{r_A=0,1} P_{ij}(r_A, r_B) &= P_j(r_B) \quad \forall\, i, \\ \sum_{r_B=0,1} P_{ij}(r_A, r_B) &= P_i(r_A) \quad \forall\, j. \end{aligned} \tag{3}$$

Conditions (3) mean that Alice's output cannot depend on Bob's setting, and vice versa. This shrinks further the region of possible experiments, and the dimension of the probability space is now reduced to $d = N(N+2)$. So, each no-signaling experiment is represented by a point in a d-dimensional probability space. In fact, the region containing all relevant probability distributions (strategies), i.e., satisfying positivity, normalization, and no-signaling, forms a polytope, i.e., a convex set with a finite number of vertices. It is the no-signaling polytope.

One can restrict the probability distributions even further by requiring that these are built only by local means, such as shared randomness. We then obtain a smaller polytope: the local polytope. The facets of this polytope are Bell inequalities, in the sense that a probability distribution lying inside (outside) the local polytope satisfies (violates) a Bell inequality. The vertices (extremal

points) of this polytope are deterministic strategies obtained by setting the outputs r_A and r_B always to 0 or always to 1. Finding the facets of a polytope knowing its vertices is a computationally difficult task. In fact, Pitowsky has shown this problem to be NP-complete.[15] That is why all Bell inequalities have been listed for the case of two or three settings, whereas not much is known for a larger number of settings.

Let us start with a brief review of the simplest situation: two settings on each side.

This case has been largely studied, and both the local and the no-signaling polytope have been completely characterized.[16] The probability space has eight dimensions. We choose the eight probabilities $P_i(r_A=0)$, $P_j(r_B=0)$, and $P_{ij}(r_A=r_B=0)$ to characterize the space.

The local polytope. The local polytope has 16 vertices. Fine[17] showed that all nontrivial facets are equivalent to the CHSH inequality

$$\mathrm{CHSH} \equiv \begin{array}{c|cc} & -1 & 0 \\ \hline -1 & 1 & 1 \\ 0 & 1 & -1 \end{array} \leq 0. \tag{4}$$

Here, the notation represents the coefficients that are put in front of the probabilities, according to

$$\begin{array}{c|c} & P_i(r_A=0) \\ \hline P_j(r_B=0) & P_{ij}(r_A=r_B=0). \end{array} \tag{5}$$

The extremal points (vertices) of the local polytope are deterministic strategies, i.e., for each setting Alice and Bob always output 0 or always output 1. Let us do an example: Alice outputs bit 0 for the first setting A_0 and outputs 1 for the second setting A_1; Bob always outputs 0, for both settings. This strategy corresponds to the point in probability space

$$[\underbrace{0_d,1_d}_{\text{Alice}} ; \underbrace{0_d,0_d}_{\text{Bob}}] = \begin{array}{c|cc} & 1 & 0 \\ \hline 1 & 1 & 0 \\ 1 & 1 & 0 \end{array}. \tag{6}$$

All probability distributions lying outside this polytope are nonlocal.

The *quantum set* is the set of correlations that can be obtained by local measurements on quantum states. Inequality (4) can indeed be violated by quantum mechanics, and the maximal violation is $1/\sqrt{2}-1/2\approx 0.2071$, obtained by suitable measurements on the singlet state. Of course the quantum set is included in the no-signaling polytope, but the converse is not true. There are no-signaling correlations that are more nonlocal than those of quantum mechanics. The PR box is indeed among these correlations.

The no-signaling polytope. The no-signaling polytope has 24 vertices: 16 of them are the local vertices seen before and the eight others are the nonlocal vertices. Each one of these points corresponds to a PR box. Let us make this clear. The PR box is a two-input, two-output NLM. Alice inputs x into the machine and gets outcome a, while Bob inputs y and gets output b. The outcomes are correlated such that $a\oplus b=xy$. The local marginals are however completely random, i.e., $P(a=0)=P(b=0)=1/2$, which ensures no-signaling. In probability space, the PR box corresponds to the point

$$\mathrm{PR} = \frac{1}{2} \times \begin{array}{c|cc} & 1 & 1 \\ \hline 1 & 1 & 1 \\ 1 & 1 & 0 \end{array}. \tag{7}$$

According to the symmetries $x\to x+1$, $y\to y+1$, $a\to a+1$, there are eight "equivalent" PR boxes. As pointed out in Ref. 16 there is a strong correspondence between the eight CHSH facets of the local polytope and the eight PR boxes. Above each CHSH inequality lies one of the PR boxes. Each PR box violates its corresponding inequality up to 0.5, which is the maximal value for

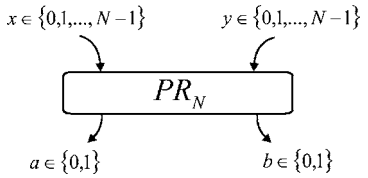

FIG. 1. An N-input NLM: generalization of the two-input PR box.

a no-signaling strategy. Formally, this correspondence is also pretty obvious by looking at Eqs. (4) and (7). To get the PR box from the CHSH inequality, proceed as follows:

Recipe. When the coefficient of a joint probability is +1 or 0 in the inequality, replace it with 0.5; when a coefficient is equal to −1, replace it with 0 in the machine.

In other words, when a joint probability appears with a coefficient +1 or 0, the outputs of the machine are correlated, and when the coefficient is −1, the outputs are anticorrelated. This simple recipe can be straightforwardly extended to Bell inequalities with more settings. For a Bell inequality with N settings, we then get a new NLM, denoted PR_N. This machine has N inputs and binary outcomes (see Fig. 1).

III. MAIN RESULT—THREE SETTINGS

In this paper we present Bell-type inequalities allowing the use of some nonlocal resource. This means that all strategies satisfying such inequalities can be simulated by local means (i.e., shared randomness, etc.) together with some nonlocal resource—for example, one NLM. In other words, any strategy violating such inequalities would require a strictly larger amount of nonlocal resource than is allowed by the inequality. In the case of two settings, described in the previous section, such inequalities cannot exist. This is because the most elementary nonlocal resource, the PR box, suffices already to generate all the nonlocal vertices of the no-signaling polytope.

Therefore we switch to the next case, i.e., three settings (with two outputs) on each side. Here, the situation becomes much more complicated but remains tractable. All facets of the local polytope have been listed.[13] No-signaling strategies are now living in a 15-dimensional space.

The local polytope. The local polytope has 64 vertices. Surprisingly, it turns out that each of the 648 nontrivial facets is equivalent to one of the two following Bell inequalities:

$$\mathrm{CHSH} \equiv \begin{array}{c|ccc} & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{array} \leq 0, \tag{8}$$

$$I_{3322} \equiv \begin{array}{c|ccc} & -1 & 0 & 0 \\ \hline -2 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{array} \leq 0. \tag{9}$$

The CHSH inequality is still a facet of the local polytope. This is a general property of Bell inequalities, known as "lifting"[18]: a facet Bell inequality, defined in a given configuration, remains a facet when the number of settings, outcomes, or parties is augmented.

Quantum mechanics indeed violates the three-setting CHSH inequality. The second inequality, I_{3322}, is also violated by quantum mechanics. Furthermore, this inequality is relevant, since it is violated by some quantum states which do not violate the CHSH inequality.[13]

The no-signaling polytope. The local polytope has 72 CHSH-type facets. Above each of these facets lies a PR box. This is clear since the CHSH inequality, while still being a facet of any local polytope with more settings, is a true two-input Bell inequality. Now, it is interesting to see that

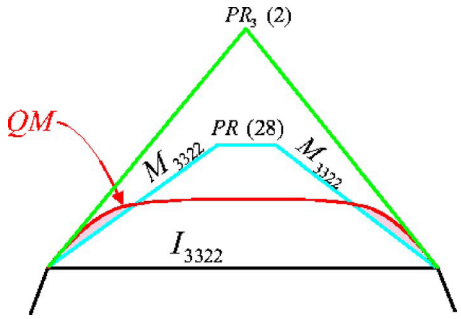

FIG. 2. A facet I_{3322} viewed in a simplified representation of the probability space. Above the facet, on the hyperplane $I_{3322}=0.5$, lie 28 strategies with a single PR. Above this hyperplane ($I_{3322}=1$) lie two strategies with a single PR_3. The local polytope is in black and the no-signaling in green. In blue is the polytope of all strategies using at most one PR; M_{3322} is a facet of this polytope. The quantum set is in red. Note that some quantum states violate M_{3322} (shaded area).

above each I_{3322} inequality (which is a true three-input Bell inequality) we find a no-signaling strategy which is more nonlocal than a PR box. This strategy is represented by a three-input NLM, defined by the relation $[xy/2]=a+b(\mathrm{mod}2)$, where $x,y\in\{0,1,2\}$ and $a,b\in\{0,1\}$. This machine will be referred to as PR_3. In probability space this new machine corresponds to the point

$$PR_3=\frac{1}{2}\times\begin{array}{c|ccc} & 1 & 1 & 1 \\ \hline 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{array}. \tag{10}$$

Note that $\langle I_{3322}|PR_3\rangle=1$, while $\langle I_{3322}|PR\rangle=0.5$ (see Fig. 2). Here, we have used a *scalar product-type* notation $\langle I|S\rangle=z$, which means that testing inequality I with strategy S gives a value z. The machine PR_3 can be simply obtained from the inequality I_{3322} using the Recipe mentioned at the end of Sec. II. One needs two PR boxes to simulate PR_3, as shown in Appendix A. PR_3 can also be rewritten in the elegant manner $x=y\Leftrightarrow a=b$, which corresponds to the probability point

$$\frac{1}{2}\times\begin{array}{c|ccc} & 1 & 1 & 1 \\ \hline 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{array}. \tag{11}$$

The distribution (11) is indeed equivalent to (10) up to local symmetries: here, both Alice and Bob flip their outputs for their first setting.

In a recent paper Jones and Masanes[19] gave a complete characterization of all the vertices of the no-signaling polytope for any number of settings and two outcomes—note that Barrett *et al.*studied the reversed case: two settings and any number of outcomes.[16] From their result it is clear that all vertices of the no-signaling polytope for three settings and two outputs can be constructed with a PR_3.

Numerically we find all the vertices of the no-signaling polytope. We proceed as follows. First we generate all strategies that use at most one PR_3. These are all the strategies where Alice and Bob can choose each of their three inputs in the set $\{0d,1d,0m,1m,2m,0mf,1mf,2mf\}$. Here $0d,1d$ means that they deterministically output the value 0 or 1; $0m,1m,2m$ means that they input $0,1,2$ in the machine PR_3; $0mf,1mf,2mf$ means that they input $0,1,2$ in PR_3 and flip the output of the machine. Second, we remove those strategies which are inside the local polytope by testing all the 648 Bell inequalities. Finally there are 1344 strategies left which are the nonlocal vertices

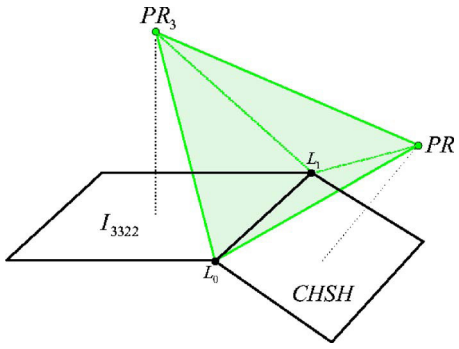

FIG. 3. Simplified three-dimensional view of a facet of the no-signaling polytope (green shaded surface). Among the extremal points of this facet are a PR-box strategy (38), a PR_3 (28) strategy, and a deterministic strategy, $L_0=[0_d,0_d,0_d;0_d,0_d,0_d]$. Behind this facet is another no-signaling facet which has a vertex $L_1=[1_d,1_d,1_d;1_d,1_d,1_d]$. Indeed, L_0,L_1 are extremal points of the local polytope. Note that PR and PR_3 are both above the CHSH and the I_{3322} facets.

of the (three-input, two-outcome) no-signaling polytope. We find four different classes of those vertices—given in Appendix B. A curious feature of those points is that each of them violates several inequalities of the local polytope. For example, the strategy

$$PR=\frac{1}{2}\times\begin{array}{c|ccc} & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{array} \tag{12}$$

violates the CHSH inequality (8). But, it clearly also violates eight I_{3322}-type inequalities, among which

$$\begin{array}{c|ccc} & -1 & 0 & 0 \\ \hline -2 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{array}\leq 0, \qquad \begin{array}{c|ccc} & -1 & 0 & -1 \\ \hline 0 & -1 & -1 & 1 \\ -1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{array}\leq 0. \tag{13}$$

Formally this is clear, since each of these eight I_{3322} inequalities [for example, (13)] reduces to the CHSH inequality (8) once Alice's third setting and Bob's first setting are discarded. Figure 3 gives some geometrical intuition of the situation.

Inequality with a PR box. We have just seen that, in the case of three settings on each side, there are two types of NLM, the PR box and the PR_3, generating different types of nonlocal vertices of the no-signaling polytope. As mentioned, the PR_3 is a stronger nonlocal resource than the PR box—it needs two PR boxes to be simulated. Thus there is a new polytope, sandwiched between the local and the no-signaling polytopes. It is formed by all strategies that can be simulated using at most one PR box (see Fig. 2). A facet of this polytope was recently found.[11] It corresponds to the inequality

$$M_{3322}\equiv\begin{array}{c|ccc} & -2 & 0 & 0 \\ \hline -2 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{array}\leq 0. \tag{14}$$

Although M_{3322} is not violated by the maximally entangled state, it is violated by a family of nonmaximally entangled states of two qubits.[11] Indeed, the maximally entangled state does not

violate this inequality, since its correlations can be simulated using a single PR box.[12] Note that the structure of M_{3322} is similar to I_{3322}, the only difference being the coefficient of Alice's first marginal.

We prove now that M_{3322} is a facet of the polytope of all strategies using at most one PR box. This result will be extended to the case of N settings in the next section.

The proof consists of two parts: first we show that no strategy with a single use of a PR box violates M_{3322}; then we show that there are (at least) $N(N+2)=15$ linearly independent strategies using at most one PR box which saturate M_{3322}. Here, we just sketch the idea of the proof; see Appendix C for details.

To prove the first part, we state a Lemma. Any no-signaling strategy S violating M_{3322}, also violates the two following inequalities:

$$C_1 \equiv \begin{array}{c|ccc} & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{array} \leq 0, \quad C_2 \equiv \begin{array}{c|ccc} & -1 & 0 & 0 \\ \hline -1 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{array} \leq 0.$$

The proof is straightforward. One needs only to note that, for no-signaling strategies, joint probabilities are smaller (or equal) than their respective marginals. Then by inverting the Lemma, we get the following proposition: if S does not violate both inequalities C_1 and C_2, then S does not violate M_{3322}. Finally, it is obvious that with a single PR box one can violate either C_1 or C_2, but not both at the same time.

For the second part of the proof, we find numerically eight local deterministic distributions which saturate M_{3322}. Then we find 57 other strategies with one PR box saturating M_{3322}. Altogether these strategies form a hyperplane of dimension 14. This completes the proof that M_{3322} is a facet of the polytope.

IV. *N* SETTINGS

In this section, the results of Sec. III are extended to the case of an arbitrary number of settings N. We use a family of Bell inequalities, known as I_{NN22}, which were proven to be facets of the local polytope.[13] These inequalities are generalization of the I_{3322} seen before. For N settings, the inequality reads

$$I_{NN22} \equiv \begin{array}{c|cccccc} & -1 & 0 & 0 & \cdots & 0 & 0 \\ \hline -(N-1) & 1 & 1 & 1 & \cdots & 1 & 1 \\ -(N-2) & 1 & 1 & 1 & \cdots & 1 & -1 \\ -(N-3) & 1 & 1 & 1 & \cdots & -1 & 0 \\ \vdots & \vdots & & & & & \vdots \\ -1 & 1 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 & 0 \end{array} \leq 0.$$

Using the Recipe of Sec. II, we construct a family of N-settings NLM

$$PR_N \equiv \frac{1}{2}\begin{array}{c|cccccc} & 1 & 1 & 1 & \cdots & 1 & 1 \\ \hline 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 1 & 1 & 1 & \cdots & 1 & 0 \\ 1 & 1 & 1 & 1 & \cdots & 0 & 1 \\ \vdots & \vdots & & & & & \vdots \\ 1 & 1 & 1 & 0 & \cdots & 1 & 1 \\ 1 & 1 & 0 & 1 & \cdots & 1 & 1 \end{array}. \tag{15}$$

TABLE I. Main results about Bell inequalities with and without nonlocal resources. We consider only the case of binary outcomes. N is the number of settings. The last line represents the vertices of the no-signaling polytope. The first column is almost empty since, for two settings, any no-signaling correlation can be generated with a PR box. The question marks mean that it is not known if there are more of these inequalities. For $N=3$, we are quite confident that M_{3322} is the only inequality for one use of a PR box, though we could not prove it rigorously.

Resource	$N=2$	$N=3$	$N\geq 4$
lhv	CHSH (Ref. 17)	CHSH+I_{3322} (Ref. 13)	CHSH+$\{I_{NN22}\}_{N\geq 3}$+ ?? (Ref. 13)
PR-box	…	M_{3322} (Ref. 11)	M_{3322}+ ??
1 bit	…	(Ref. 3)	??
PR_{N-1}	…	(Ref. 11)	M_{NN22} (this paper) + ??
No-signaling	PR (Ref. 16)	$PR+PR_3$ (Ref. 19)	$PR+\{PR_N\}_{N\geq 4}$ (Ref. 19)

One can simulate PR_N with $N-1$ PR-boxes. This is easily shown using a straightforward generalization of Appendix A. We think that PR_N cannot be simulated with fewer than $(N-1)$ PR-boxes, but we do not have a proof. The inequality

$$M_{(N+1)22} \equiv \begin{array}{c|ccccc} & -N & 0 & \cdots & 0 & 0 \\ \hline -N & 1 & 1 & \cdots & 1 & 1 \\ -(N-1) & 1 & 1 & \cdots & 1 & -1 \\ -(N-2) & 1 & 1 & \cdots & -1 & 0 \\ \vdots & \vdots & \vdots & & & \vdots \\ -1 & 1 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \end{array} \leq 0 \tag{16}$$

is an $(N+1)$-setting Bell inequality that cannot be violated by strategies which require a single use of PR_N, as proven in Appendix C. In (16) we have omitted a factor $(N+1)$ in the name of the inequality for practical reasons. Again the structure of M_{NN22} is similar to I_{NN22}, up to Alice's first marginal: in order to get M_{NN22} from I_{NN22}, one simply changes Alice's first marginal to $-(N-1)$.

So, finally we get the following nice construction. For any number of settings N we have a Bell inequality I_{NN22} and an N-input NLM (PR_N) which reaches the upper no-signaling bound of I_{NN22}. From there, we construct an $(N+1)$-setting inequality $(M_{(N+1)(N+1)22})$, which cannot be violated with one use of PR_N, i.e.,

$$(I_{NN22}, PR_N) \rightarrow (M_{(N+1)(N+1)22}, PR_{N+1}). \tag{17}$$

V. CONCLUSION

To conclude, we review briefly the main results concerning polytopes and Bell inequalities with and without nonlocal resources. We focus on two-outcome settings. Table I summarizes the situation. The oldest result is due to Fine, who showed that all (nontrivial) facets of the two-input, two-outcome local polytope are equivalent to the CHSH inequality.[17] Then Collins and Gisin completely characterized the case of three settings.[13] In particular, they showed that there is a single new inequality (I_{3322}) which is inequivalent to CHSH. They also found a family of facet inequalities I_{NN22} of the N setting local polytope, but for $N>3$ it is not known if there are other inequalities. The vertices of the no-signaling polytope for two settings and any number of outcomes have been characterized by Barrett *et al.*,[16] while Jones and Masanes studied the reversed case: an arbitrary number of settings with two outcomes.[19]

Not much is known about inequalities allowing nonlocal resources. In 2003 Toner and Bacon found inequalities allowing one bit of communication for the case of two and three settings.[20] They showed that the correlations from measurements on any quantum state satisfy those inequali-

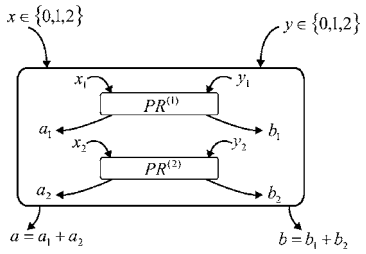

FIG. 4. A PR_3 with two PR's. The inputs of each PR, $x_{1,2}$ and $y_{1,2}$, are bits. For each ternary input $x(y)$, there is a combination of $x_{1,2}(y_{1,2})$. Finally, the output on each side is the sum (modulo 2) of the two binary outputs of the PR boxes.

ties. In the present paper we introduced a family of N-input NLMs ($\{PR_N\}_{N\geq 3}$), which are a generalization of the well-known PR box. These NLMs can be derived from Bell inequalities in the same way than the PR box is derived from the CHSH inequality. Then, we presented a new family of inequalities ($\{M_{NN22}\}_{N\geq 3}$) allowing one use of PR_N.

For $N=3$, we get an inequality which cannot be violated with a single PR box. This inequality, presented in a previous work,[11] is however violated by some nonmaximally entangled state of two qubits. Here, we checked numerically that no states of two qubits violates M_{4422} and M_{5522}, which suggests that these states could be simulated with two PR boxes, or even a PR_3 box. However such model has still not been found.

ACKNOWLEDGMENT

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APPENDIX A

Since $\langle M_{3322}|PR_3\rangle = 0.5$, PR_3 cannot be simulated with a single PR box. In this Appendix, we show how to construct a PR_3 with 2 PR boxes.

Alice and Bob each receive a trit. For each value of the trit they input one bit in each PR box. The strategy is the following:

x	x_1	x_2	y	y_1	y_2
0	0	0	0	0	0
1	0	1	1	1	0
2	1	0	2	0	1

, (A1)

where x,y denote the settings, and x_i,y_i are the binary inputs into PR-box number i. Finally, Alice and Bob output the sum (modulo 2) of both outputs of the PR boxes. See Fig. 4. Intuitively the strategy works as follows. The first machine introduces an anticorrelation of the outputs for the pair of settings $x=1,y=2$. The second PR box does the same for $x=2,y=1$. A nice way to show that this strategy works is by computing the parity of the outputs for each pair of settings. So, we compute a parity matrix P by multiplying Alice strategy by the transpose of Bob's strategy

$$P = S_A S_B^{\dagger} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{A2}$$

Note that matrix P has the same structure as the correlation terms of I_{3322}. So, Alice and Bob's outputs are identical when a 1 appears in the inequality and different when -1 is in the inequality.

This construction is easily generalized to N settings. Since I_{NN22} has $N-1$ correlation terms equal to -1, one simply uses a PR box to anticorrelate the outcomes for each of those terms. Thus it can be shown that a PR_N NLM is constructed with $N-1$ PR-boxes.

APPENDIX B

We find four classes of nonlocal vertices of the three-setting, two-outcome no-signaling polytope

$$S_1 = \begin{array}{c|ccc} & x & x & x \\ \hline x & x & x & x \\ x & x & x & 0 \\ x & x & 0 & x \end{array}, \quad S_2 = \begin{array}{c|ccc} & x & x & 0 \\ \hline 0 & 0 & 0 & 0 \\ x & x & x & 0 \\ x & x & 0 & 0 \end{array}, \tag{B1}$$

$$S_3 = \begin{array}{c|ccc} & x & x & 0 \\ \hline x & x & x & 0 \\ x & x & x & 0 \\ x & x & 0 & 0 \end{array}, \quad S_4 = \begin{array}{c|ccc} & x & x & x \\ \hline x & x & x & x \\ x & x & x & x \\ x & x & 0 & x \end{array}, \tag{B2}$$

where $x = 1/2$. Class S_1 corresponds to strategies with a PR_3. They violate maximally I_{3322}, i.e., up to 1. Classes S_2-S_4 are strategies which can be obtained with a PR box. In S_2, Alice and Bob have a deterministic output for one of their setting; in S_3, only Alice (or Bob) has a deterministic setting; in S_4, no one outputs deterministic values.

There are 192 vertices in class 1, 288 in class 2, 576 in class 3, and 288 in class 4. All strategies in the same class violate the same number of CHSH inequalities and the same number of I_{3322} inequalities. These numbers are summarized in the table below. For each class of vertices, the number of CHSH and I_{3322} inequalities violated is given:

Class	CHSH	I_{3322}
S_1	6	18
S_2	1	8
S_3	2	12
S_4	4	24

APPENDIX C

This Appendix is divided in two parts. In the first part, it is shown that inequality

$$M_{NN22} \equiv \begin{array}{c|cccccc} & -(N-1) & 0 & 0 & \cdots & 0 & 0 \\ \hline -(N-1) & 1 & 1 & 1 & \cdots & 1 & 1 \\ -(N-2) & 1 & 1 & 1 & \cdots & 1 & -1 \\ -(N-3) & 1 & 1 & 1 & \cdots & -1 & 0 \\ \vdots & \vdots & & & & & \vdots \\ -1 & 1 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 & 0 \end{array} \leq 0$$

cannot be violated by strategies using (at most) one PR_{N-1}. In the second part, we show that, for $N \leq 5$, inequality M_{NN22} is tight, i.e., it is a facet of the polytope containing all strategies that use (at most) one PR_{N-1}. We conjecture that this is also true for any number of settings N. To motivate our conjecture we show that there are 2^N deterministic strategies lying on the

$(d-1)$-dimensional hyperplane, where $d=N(N+2)$ is the dimension of the probability space.

Part 1. We start with a Lemma.

Lemma 1. Let us define the two inequalities

$$C_1^N \equiv \begin{array}{c|cccccc} & -(N-2) & 0 & 0 & \cdots & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -(N-2) & 1 & 1 & 1 & \cdots & 1 & 0 \\ -(N-3) & 1 & 1 & 1 & \cdots & -1 & 0 \\ \vdots & \vdots & & & & & \vdots \\ -1 & 1 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 & 0 \end{array} \leq 0,$$

$$C_2^N \equiv \begin{array}{c|cccccc} & -(N-2) & 0 & 0 & \cdots & 0 & 0 \\ \hline -(N-2) & 1 & 0 & 1 & \cdots & 1 & 1 \\ -(N-3) & 1 & 0 & 1 & \cdots & 1 & -1 \\ -(N-4) & 1 & 0 & 1 & \cdots & -1 & 0 \\ \vdots & \vdots & & & & & \vdots \\ 0 & 1 & 0 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{array} \leq 0.$$

Let S be a strategy with N settings for each of the two partners. S is in a probability space of dimension $N(N+2)$. If S violates inequality M_{NN22}, then S also violates both inequalities C_1^N and C_2^N.

Proof. S violates M_{NN22}, i.e.,

$$-(N-1)P(A_0)-\sum_{k=0}^{N-2}(N-k-1)P(B_k)+\sum_{k=0}^{N-1}P(A_kB_0)+\sum_{m=1}^{N-1}\left[\left(\sum_{k=0}^{N-m-1}P(A_kB_m)\right)-P(A_{N-m}B_m)\right] > 0. \tag{C1}$$

According to the no-signaling condition, we have

$$P(A_0) \geq P(A_0B_0), \tag{C2}$$

$$(N-1)P(B_0) \geq \sum_{k=1}^{N-1}P(A_kB_0), \tag{C3}$$

$$P(A_{N-1}B_1) \geq 0. \tag{C4}$$

Inserting these relations into (C1) we get

$$-(N-2)P(A_0)-\sum_{k=1}^{N-2}(N-k-1)P(B_k)+\sum_{k=0}^{N-2}P(A_kB_1)+\sum_{m=2}^{N-1}\left[\left(\sum_{k=0}^{N-m-1}P(A_kB_m)\right)-P(A_{N-m}B_m)\right] > 0,$$

which means S violates inequality C_1^N.

Again from to the no-signaling condition, we have

$$P(A_0) \geq P(A_0B_{N-1}), \tag{C5}$$

$$P(B_j) \geq P(A_1 B_j) \quad \forall\, j \in \{0, N-1\}, \tag{C6}$$

$$P(A_1 B_{N-1}) \geq 0, \tag{C7}$$

which inserted into (C1) gives

$$-(N-2)P(A_0) - \sum_{k=0}^{N-3} (N-k-2)P(B_k) + \sum_{k=0}^{N-2} P(A_0 B_k) + \sum_{k=2}^{N-1} P(A_k B_0) + \sum_{m=1}^{N-3} \left[\left(\sum_{k=2}^{N-m-1} P(A_k B_m) \right) - P(A_{N-m} B_m) \right] - P(A_2 B_{N-2}) > 0,$$

which means S violates inequality C_2^N.

This completes the proof.

Part 2. For $N \leq 5$, we checked numerically that all strategies using at most one PR_{N-1} form a subspace of dimension $d-1$, where $d=N(N+2)$ is the dimension of the probability space. This shows that inequality M_{NN22} is tight. We conjecture that this is also the case for any number of settings N. Below we show that there are 2^N deterministic strategies on the hyperplane $M_{NN22}=0$, which strongly supports our conjecture.

First we note that there are eight local strategies on the M_{3322} facet.

	0	1	1
1	0	1	1
0	0	0	0
0	0	0	0

	0	1	1
0	0	0	0
0	0	0	0
0	0	0	0

	0	1	0
0	0	0	0
1	0	1	0
0	0	0	0

	0	1	0
0	0	0	0
0	0	0	0
0	0	0	0

	0	0	1
0	0	0	0
0	0	0	0
1	0	0	1

	0	0	1
0	0	0	0
0	0	0	0
0	0	0	0

	0	0	0
0	0	0	0
0	0	0	0
1	0	0	0

	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0

(C8)

Obviously the marginals fix entirely a deterministic strategy. Then it is clear that if a three-setting strategy

	A_0	A_1	A_2
B_0			
B_1		⋯	
B_2			

(C9)

is on the facet M_{3322}, then both (four settings) strategies

	A_0	A_1	A_2	0
0	0	0	0	0
B_0				0
B_1		⋯		0
B_2				0

(C10)

$$S'' = \begin{array}{c|cccc} & A_0 & A_1 & A_2 & 1 \\ \hline B_0 & & & & \beta_0 \\ B_1 & & \cdots & & \beta_1 \\ B_2 & & & & \beta_2 \\ 0 & 0 & 0 & 0 & 0 \end{array}, \tag{C11}$$

are on the facet M_{4422}. The notation β_j for some correlation coefficients means that their value depends on Bob's marginal. Indeed, all these strategies are extremal since they are deterministic.

Then the argument is extended to the next case: for each of the 16 strategies (constructed above) which lie on M_{4422}, there are two strategies on M_{5522}. Thus there are 2^N deterministic strategies on M_{NN22}. Note that $2^N > N(N+2)$ for $N \geq 6$. In this case the number of local strategies on the hyperplane $M_{NN22}=0$ is larger than the dimension of the probability space. This suggests that M_{NN22} is a facet of the polytope of all strategies using at most one PR_{N-1}.

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On the Weyl algebras for systems with semibounded and bounded configuration space

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We define the Weyl algebra suitable to represent the quantization postulate for one-dimensional systems whose configuration space is semibounded. It consists of a group $\{V(\beta)=\exp(-i\beta q), \beta \in \mathbb{R}\}$ of unitary operators and a semigroup $\{U(\alpha), \alpha \geqslant 0\}$ of nonunitary isometries. We show that the spectrum $\sigma(q)$ is a half-line $[x_0, \infty)$, with an arbitrary $x_0 > -\infty$, and that the irreducible representations of the Weyl algebra with the same x_0 are equivalent. We also consider the case when the semigroup of translations is substituted with a semigroup of partial isometries of index 1 (particle confined to a segment of unit length). The uniqueness of the irreducible representations of the related Weyl algebra is proved also for this case by exploiting the result for the half-line. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2363256]

I. INTRODUCTION

In quantum mechanics the momentum (p) and position (q) operators obey the Heisenberg commutation relation

$$[p,q] = -i \tag{1}$$

which holds for a dense domain $\mathcal{D}$ of vectors where both pq and qp are defined. Since the spectrum of q is the range of positions accessible to the system, for unconstrained systems p and q can be represented in $L^2(-\infty, \infty)$ as the operators

$$qf = xf \quad \mathcal{D}_q = \{f: xf \in L^2\}, \tag{2}$$

$$pf = -if' \quad \mathcal{D}_p = \{f: f \text{ absolutely continuous}, f' \in L^2\}. \tag{3}$$

This representation is not unique: for example also $\tilde{p}=p+h(q)$ and $\tilde{q}=q$ obey Eq. (1).

The self-adjoint operators p, q in Eqs. (2) and (3) generate two strongly continuous groups of unitary operators $U(\alpha)=\exp(-i\alpha p)$ and $V(\beta)=\exp(-i\beta q)(\alpha_i, \beta_j \in \mathbb{R})$,

$$U(\alpha_1)U(\alpha_2) = U(\alpha_1+\alpha_2) \quad U(0)=I, \quad \lim_{\alpha\to 0}\|(U(\alpha)-I)f\| = 0, \tag{4}$$

$$V(\beta_1)V(\beta_2) = V(\beta_1+\beta_2) \quad V(0)=I, \quad \lim_{\beta\to 0}\|(V(\beta)-I)f\| = 0, \tag{5}$$

such that

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$$U(\alpha)f = f(x-\alpha), \quad V(\beta)f = \exp(-i\beta x)f(x), \tag{6}$$

which obey the following multiplication law:

$$U(\alpha)V(\beta) = \exp(i\alpha\beta)V(\beta)U(\alpha). \tag{7}$$

Equation (7) is referred to as the Weyl form of the commutation relations. A set of operators $U(\alpha)$, $V(\beta)$ which form two strongly continuous groups and obey Eq. (7) generate the Weyl algebra $\mathcal{W}_\infty$. von Neumann proved[1] that the irreducible representations of $\mathcal{W}_\infty$ are unitarily equivalent. Hence, they are equivalent to the representation given in Eqs. (2) and (3) (Schrödinger representation) which is easily seen to be irreducible.

In this paper we prove a similar result when the spectrum $\sigma(q)$ of q is bounded from below: $\sigma(q) \subset \{x : x \geqslant x_0\}$. This occurs, for example, when the Hilbert space $\mathcal{H}$ of the system is $L^2(0,\infty)$. While the self-adjoint operator q generates a group $V(\beta)$ of unitary operators, the momentum operator $p = -i\partial/\partial x$ does not possess self-adjoint extensions.[2,3] Only the right translations $U(\alpha)$ are isometric operators and constitute a continuous semigroup: Eq. (4) only holds for $\alpha_1, \alpha_2 \geqslant 0$, while Eqs. (5) and (7) still hold. Left translations are represented by the operators $U^\dagger(\alpha), \alpha \geqslant 0$, which do not conserve the norm of vectors. The $\{U^\dagger(\alpha)\}$ operators are properly a semigroup of contractions ($\|U^\dagger(\alpha)x\| \leqslant \|x\|$).

The relation of $U(\alpha)$ with its adjoint $U^\dagger(\alpha)$ is

$$U^\dagger(\alpha)U(\alpha) = I, \quad U(\alpha)U^\dagger(\alpha) = E_\alpha, \tag{8}$$

where E_α is the projection onto $\mathcal{H}_\alpha = U(\alpha)\mathcal{H}$. The algebra $\mathcal{W}_\infty$ is replaced by the algebra $\mathcal{W}_+$ generated by the positive translations, their adjoints and the unitary operators $V(\beta)$. The multiplication law between $U^\dagger(\alpha)$ and $V(\beta)$ is found by taking the adjoint of Eq. (7),

$$U^\dagger(\alpha)V(\beta) = \exp(-i\alpha\beta)V(\beta)U^\dagger(\alpha). \tag{9}$$

We will prove that, given an irreducible representation of the algebra $\mathcal{W}_+$, either all the operators $U(\alpha)$ are unitary, $\mathcal{H}_\alpha = \mathcal{H}$ and $E_\alpha = I$ for any α and $\mathcal{W}_+$ can be extended to the Weyl algebra $\mathcal{W}_\infty$ by defining $U(\alpha) = U^\dagger(-\alpha)$ for $\alpha \leqslant 0$, or the spectrum of the generator q of the group $\{V(\beta)\}$ is a half line $\{x : x \geqslant x_0\}$. In this latter case the irreducible representations of $\mathcal{W}_+$ with the same lower bound for the spectrum $\sigma(q)$ are proved to be unitarily equivalent. As a consequence the Schrödinger representation of $\mathcal{W}_+$ in $L^2(x_0,\infty)$,

$$U(\alpha)f = f(x-\alpha)\theta(x-\alpha), \quad V(\beta)f = \exp(-i\beta x)f(x), \tag{10}$$

which is irreducible (see below) is essentially unique.

Our approach is based on the construction, in Sec. IV, of a Hilbert space $\mathcal{K}$ where a Weyl algebra $\mathcal{W}_\infty = \{U_\mathcal{K}(\alpha), V_\mathcal{K}(\beta), \alpha, \beta \in \mathbb{R}\}$ is defined starting from the algebra $\mathcal{W}_+$ defined in $\mathcal{H}$. $\mathcal{K}$ can be seen as a direct sum $\mathcal{H} \oplus \mathcal{H}$, and the algebra $\mathcal{W}_+$ is recovered from $\mathcal{W}_\infty$ by projecting onto $\mathcal{H}$. For example, if $\mathcal{H} = L^2(0,\infty)$, then $\mathcal{K} = L^2(-\infty,\infty)$.

The representation of $\mathcal{W}_\infty$ in $\mathcal{K}$ is proved to be irreducible if the representation of $\mathcal{W}_+$ in $\mathcal{H}$ is irreducible, and equivalent representations of $\mathcal{W}_\infty$ give rise to equivalent representations of $\mathcal{W}_+$. We will rely on the property of irreducible representations of *algebras that the only bounded operators commuting with the operators of the *algebra are multiples of the identity operator.[3]

In this framework, whereas the definition of the group $V_\mathcal{K}(\beta)$ is immediate by a simple doubling of the group $V(\beta)$, the passage from a semigroup $U(\alpha)$ to a unitary group $U_\mathcal{K}(\alpha)$, such that the Weyl condition, Eq. (7), is satisfied depends on the existence of a family $\{R(\alpha), \alpha \geqslant 0\}$ of operators which fulfill conditions, given in detail in Sec. V, implying that the $U_\mathcal{K}(\alpha)$'s are a group and that with the $V_\mathcal{K}(\beta)$'s they obey Eq. (7).

The passage from a semigroup of isometries to a group of unitary operators in a larger space is not new. Cooper[4] first showed that a Hilbert space $\mathcal{H}$ where a semigroup of isometries is defined can be imbedded in a space $\mathcal{K}$ where a group of unitary operators exists whose components in the original space are the semigroup of isometries. His work relies on the use of the generator of the

semigroup and the definition of a homeomorphic and isometric mapping from $L^2(0,\infty)$ to $\mathcal{H}$. Instead, our approach is global in that we use the operators $U(\alpha)$, $V(\beta)$ directly, and show that the construction of $\mathcal{W}_\infty$ is reduced to the proof that a single operator $R(\alpha_0)$ exists, subject to appropriate conditions. This operator is shown to exist in Sec. VI, where we also give an explicit expression for it.

Later, building on an inspiring work by Sz.-Nagy,[5,6] who proved that any continuous one-parameter semigroup of contractions $\{T(\sigma),\sigma\geqslant 0\}$ in $\mathcal{H}$ can be dilated into a continuous unitary group in a space $\mathcal{K}\supset\mathcal{H}$, Foiaş and Gehér[7] showed that two continuous semigroups of contractions $\{U(\alpha),V(\beta),\alpha,\beta\geqslant 0\}$ obeying Eq. (7) can be simultaneously dilated into two continuous groups of unitary operators satisfying the Weyl condition for any $\alpha,\beta\in\mathbb{R}$ (see also Ref. 8, where the proof is somewhat simplified). The construction of Sz.-Nagy relies on a theorem on positive definite operator valued functions on a group, and Foiaş and Gehér show that the procedure of Sz.-Nagy can be iterated for any two semigroups of contractions $\{U(\alpha),V(\beta),\alpha,\beta\geqslant 0\}$ satisfying the Weyl form of the commutation relations in such a way that Eq. (7) still holds. Though Sz.-Nagy's technique is very elegant, we believe our construction of $\mathcal{K}$ and of the unitary group $\{U_{\mathcal{K}}(\alpha)\}$ is more intuitive and nearer to the physicists' approach to the problem.

Concerning the irreducible representations of $\mathcal{W}_+$, Cooper does not address the problem of the representation of this algebra, while Foiaş and Gehér do not consider the problem of the irreducible representations of $\mathcal{W}_+$. Although a lot of work has been made about the Heisenberg commutation relations (see Ref. 9, for example, and Ref. 10, where representations of the commutation relations intermediate between Heisenberg's and Weyl's are explored), as far as we know the proof presented in the paper is the first proof that all the irreducible representations of the algebra $\mathcal{W}_+$ with the same lower bound for the spectrum of q are unitarily equivalent. This is the ultimate reason why the use of the Schrödinger representation for systems with semibounded configuration space is not arbitrary.[14]

As a by-product of the aforementioned result, in Secs. VIII and IX we will also consider the representations of the algebra $\mathcal{W}_1$ generated by a semigroup of partial isometries $\{U(\alpha)\}$, $U(1)=0$, their adjoints and the operators $V(\beta)$, which obey the composition law Eq. (7). We will associate to a representation of $\mathcal{W}_1$ in a Hilbert space $\mathcal{H}_1$ a representation of $\mathcal{W}_+$ in a Hilbert space $\mathcal{H}\equiv\oplus_{n=1}^{\infty}\mathcal{H}_n,\mathcal{H}_n=\mathcal{H}_1$, and will derive the uniqueness of the irreducible representations of $\mathcal{W}_1$ from that of the irreducible representations of $\mathcal{W}_+$.

We aimed at writing a self-contained paper. This is why we did not refrain from giving space to some preliminary details and from writing expanded versions of the proofs of our statements in Secs. V and VI.

II. GENERAL PROPERTIES

Let $\mathcal{H}$ be a Hilbert space, $\{V(\beta),\beta\in\mathbb{R}\}$ a strongly continuous group of unitary operators, $\{U(\alpha),\alpha\geqslant 0\}$ a strongly continuous semigroup of isometries which obey the Weyl condition Eq. (7). We assume there is no Hilbert subspace invariant under all of them and the adjoints $U^\dagger(\alpha)$.

The $U(\alpha)$ operators obey $U^\dagger(\alpha)U(\alpha)=I$. The operators $E_\alpha=U(\alpha)U^\dagger(\alpha)$ are orthogonal projections: $E_\alpha^\dagger=E_\alpha=E_\alpha^2$. Hence, the operators $U^\dagger(\alpha)$ are contractions: $\|U^\dagger(\alpha)x\|^2\leqslant\|x\|^2$. The $U^\dagger(\alpha)$'s too are a continuous semigroup. Indeed, the composition law is seen to hold by taking the adjoint of Eq. (4). Moreover, we have

$$0\leqslant\|U^\dagger(\alpha)x-x\|^2\leqslant 2\|x\|^2-(x,U(\alpha)x)-(U(\alpha)x,x),$$

which shows that

$$\lim_{\alpha\to 0}\|U^\dagger(\alpha)x-x\|^2=0.$$

The semigroup condition implies strong continuity of $U^\dagger(\alpha)$ for any α.

The semigroup property fixes the composition law for $U^\dagger(\alpha)$ and $U(\beta)$. We have

$$U^\dagger(\alpha)U(\beta)=U^\dagger(\alpha-\beta),\quad U^\dagger(\beta)U(\alpha)=U(\alpha-\beta)\quad\alpha\geqslant\beta,\tag{11}$$

$$U(\beta)U^{\dagger}(\alpha) = U(\beta-\alpha)E_{\alpha} = E_{\beta}U(\beta-\alpha) \quad \alpha \leqslant \beta, \tag{12}$$

$$U(\alpha)U^{\dagger}(\beta) = E_{\alpha}U^{\dagger}(\beta-\alpha) = U^{\dagger}(\beta-\alpha)E_{\beta} \quad \alpha \leqslant \beta. \tag{13}$$

From the above equations we get

$$E_{\beta}U(\alpha) = U(\alpha) \quad \alpha \geqslant \beta, \tag{14}$$

$$E_{\beta}U(\alpha) = U(\alpha)E_{\beta-\alpha} \quad \alpha < \beta, \tag{15}$$

$$E_{\beta}U^{\dagger}(\alpha) = U^{\dagger}(\alpha)E_{\alpha+\beta}. \tag{16}$$

The projections $\{E_{\alpha}\}$ are strongly continuous:

$$\|E_{\alpha}x - E_{\beta}x\| = \|U(\alpha)[U^{\dagger}(\alpha) - U^{\dagger}(\beta)]x + [U(\alpha) - U(\beta)]U^{\dagger}(\beta)x\| \leqslant \|[U^{\dagger}(\alpha) - U^{\dagger}(\beta)]x\| + \|[U(\alpha) - U(\beta)]U^{\dagger}(\beta)x\| \overset{\alpha\to\beta}{\to} 0.$$

For the projections $\{E_{\alpha}\}$ we have

$$E_{\alpha}E_{\alpha+\beta} = E_{\alpha+\beta} = E_{\alpha+\beta}E_{\alpha} \quad \beta \geqslant 0, \tag{17}$$

since $E_{\alpha}E_{\alpha+\beta}=U(\alpha)[U^{\dagger}(\alpha)U(\alpha)]U(\beta)U^{\dagger}(\alpha+\beta)=E_{\alpha+\beta}$. Taking the adjoint one gets the latter of Eqs. (17). Hence, $E_{\alpha}-E_{\beta}, \beta \geqslant \alpha$, is a projection. Also, since $U(\alpha)E_{\beta}=E_{\alpha+\beta}U(\alpha)$, from Eqs. (16) and (17) we get

$$U(\alpha)E_{\beta}U^{\dagger}(\alpha) = E_{\alpha+\beta}, \tag{18}$$

$$U^{\dagger}(\alpha)E_{\beta}U(\alpha) = E_{\beta-\alpha} \quad \beta \geqslant \alpha. \tag{19}$$

The projections E_{α} either are constant, $E_{\alpha}=I \ \forall \alpha \geqslant 0$, or are a strictly decreasing family of operators. Indeed, if $E_{\alpha}=E_{\alpha+\gamma}$ and $0<\beta\leqslant\gamma$ we have

$$E_{\alpha} - E_{\alpha+\beta} = -[E_{\alpha+\beta} - E_{\alpha+\gamma}].$$

Since both $E_{\alpha}-E_{\alpha+\beta}$ and $E_{\alpha+\beta}-E_{\alpha+\gamma}$ are positive operators, we find $E_{\alpha+\beta}=E_{\alpha}, \beta\leqslant\gamma$. Equations (18) and (19) then imply that E_{α} is periodic with any period $\beta\leqslant\gamma$, so $E_{\alpha}=I\forall\alpha$. In this case the operators $U(\alpha)$ are unitary, the semigroup can be extended to a group by the obvious definition $U(\alpha)=U^{\dagger}(-\alpha)$ for $\alpha<0$ and we retrieve the Weyl algebra $\mathcal{W}_{\infty}$ which is the object of von Neumann's theorem. The case of interest to us is when the E_{α}'s are strictly decreasing and the operators $U^{\dagger}(\alpha)$ are genuine contractions.

In this latter case, the decreasing sequence of positive operators E_{α} has a strong limit E_{∞}, which is the projection onto the closed subspace $\mathcal{H}_{\infty}=\cap_{\alpha}\mathcal{H}_{\alpha}$. Indeed

$$E_{\alpha}E_{\infty}x = \lim_{\beta\to+\infty} E_{\alpha}E_{\beta}x = \lim_{\beta\to+\infty} E_{\beta}x = E_{\infty}x.$$

Because of Eq. (15), E_{∞} commutes with $U(\alpha)$, and, being self-adjoint, with $U^{\dagger}(\alpha)$. In addition, Eqs. (7) and (9) imply that $V(\beta)$ and E_{α} commute

$$[V(\beta), E_{\alpha}] = 0 \tag{20}$$

and consequently E_{∞} commutes with $V(\beta)$. In conclusion, since $\mathcal{H}_{\infty}$ is invariant under the operators $U(\alpha), U^{\dagger}(\alpha), V(\beta)$, in an irreducible representation of $\mathcal{W}_{+}$ for which $E_{\alpha}\neq I$ for $\alpha\neq 0$ we must have $\mathcal{H}_{\infty}=\{0\}$. In this case $\lim_{\alpha\to+\infty}E_{\alpha}x=0$ and the projections $\{P_{\alpha}\}=\{I-E_{\alpha}\}$ are a resolution of the identity, as can be verified taking into account the properties of the E_{α}'s. In the following we will only consider the case $\mathcal{H}_{\infty}=\{0\}$.

III. THE SPECTRAL RESOLUTION OF q

In this section we prove that, if $\mathcal{H}$ hosts an irreducible representation of the algebra $\mathcal{W}_+$, then the spectrum $\sigma(q)$ of the generator q of the group $\{V(\beta), \beta \in \mathbb{R}\}$ is $[x_0, \infty)$. To this purpose, we compare the operators $V(\beta)$ with the operators $V'(\beta)=\int_0^\infty \exp(-i\beta\gamma)dP_\gamma$. According to Stone's theorem[3] these latter operators constitute a group of unitary operators, due to the properties of the spectral family $\{P_\alpha\}$. $V(-\beta)V'(\beta)$ commutes with the operators $V(\alpha)$ (see Eq. (20)) as well as with the operators $U(\alpha)$ and $U^\dagger(\alpha)$. Indeed, we have

$$U(\alpha)V(-\beta)V'(\beta) = \exp(-i\alpha\beta)V(-\beta)U(\alpha)V'(\beta) = V(-\beta)\exp(-i\alpha\beta)\int_0^\infty \exp(-i\beta\gamma)dP_{\alpha+\gamma}U(\alpha)$$

$$= V(-\beta)\int_\alpha^\infty \exp(-i\beta\gamma)dP_\gamma U(\alpha) = V(-\beta)V'(\beta)U(\alpha),$$

where we used Eqs. (14) and (15). Similarly, $V(-\beta)V'(\beta)$ commutes with $U^\dagger(\alpha)$. Since the representation of $\mathcal{W}_+$ is irreducible, we have $V'(\beta)=V(\beta)f(\beta)$. Since both $V(\beta)$ and $V'(\beta)$ are groups of unitary operators we must have $f(\beta)=\exp(ix_0\beta)$. Hence,

$$V(\beta) = \exp(-ix_0\beta)\int_0^\infty \exp(-i\beta\gamma)dP_\gamma = \int_{x_0}^\infty \exp(-i\beta\gamma)dP_{\gamma-x_0}, \tag{21}$$

which shows that the generator q has the spectral representation

$$q = \int_0^\infty (x_0+\gamma)dP_\gamma = x_0 I + \int_0^\infty \gamma dP_\gamma = \int_{x_0}^\infty \gamma dF_\gamma \tag{22}$$

with $F_\gamma = P_{\gamma-x_0}$.

The above equation shows that for an irreducible representation of $\mathcal{W}_+$ (with $E_\alpha \neq I$ for any positive α) the situation is completely different from the case of the algebra $\mathcal{W}_\infty$. For $\mathcal{W}_+$ the generator of the group $\{V(\beta)\}$ is expressed in terms of the projections E_α, and the irreducibility of the representation depends only on the irreducibility with respect to the translations $U(\alpha)$ and $U^\dagger(\alpha)$. For an irreducible representation no proper subspace $\mathcal{H}'$ may be invariant with respect to the translations, since this would entail invariance also under the group $\{V(\beta)\}$. Conversely, if $\mathcal{H}$ is irreducible under translations, the group $\{\exp(-i\beta q)\}$, with q given by Eq. (22), together with the translations $U(\alpha)$ and $U^\dagger(\alpha)$, yields an irreducible representation in $\mathcal{H}$ of the algebra $\mathcal{W}_+$. The comparison between the representation of $\mathcal{W}_\infty$ in $\mathcal{H}_1=L^2(-\infty,\infty)$, Eq. (6), and that of $\mathcal{W}_+$ in $\mathcal{H}_2=L^2(x_0,\infty)$ (Eq. (10)) clarifies the situation. In $\mathcal{H}_1$ any subspace

$$\mathcal{H}'_A = \{f\text{: the Fourier transform of } f \text{ has support in a measurable set } A\}$$

is invariant under translations[11] (but not under the operators $V(\beta)$). Conversely, $\mathcal{H}_2$ has no subspace invariant with respect to (right and left) translations. Indeed, should such a subspace $\mathcal{H}'$ exist, given $f \in \mathcal{H}'$, for any γ, δ, and

$$g = [E_\gamma - E_{\gamma+\delta}]f = \chi_{[\gamma,\gamma+\delta]}f,$$

also $g \in \mathcal{H}'$. For any function $h \in \mathcal{H}_2 \ominus \mathcal{H}'$ (also invariant), any interval Δ and any positive α we have $(h, U(\alpha)\chi_\Delta f)=0$. This implies $h=0$ a.e., which means $\mathcal{H}'=\mathcal{H}_2$.

The most useful consequence of Eq. (22) is that we can limit our attention to the case that the generator q of $V(\beta)$ has spectrum $[0,\infty)$. In fact, when $\sigma(q)=[x_0,\infty)$ we can write $q=x_0 I + q_0, q_0=\int_0^\infty dP_\gamma$, with $\sigma(q_0)=[0,\infty)$. The (inequivalent) representations of the algebra $\mathcal{W}_+$ with $V(\beta)=\exp(-i\beta q)$ or $V'(\beta)=\exp(-iq_0\beta)$ are either both reducible or both irreducible, since they are related by the equation $V(\beta)=\exp(-ix_0\beta)V'(\beta)$.

IV. CONSTRUCTION OF $\mathcal{K}$

In this section we start with an irreducible representation of the algebra $\mathcal{W}_+$ in a Hilbert space $\mathcal{H}$, with $V(\beta)=\exp(-i\beta q), q=\int_0^\infty \gamma dP_\gamma$. We show how a Hilbert space $\mathcal{K}$ containing $\mathcal{H}$ can be introduced in such a way that the representation of $\mathcal{W}_+$ in $\mathcal{H}$ induces a representation of $\mathcal{W}_\infty$ in $\mathcal{K}$.

Let $\mathcal{K}$ be the vector space of pairs $\{x,y\}$, $x,y\in\mathcal{H}$, with scalar product $(\{x,y\},\{u,v\})=(x,u)+(y,v)$. $\mathcal{K}$ is a Hilbert space, and $\mathcal{H}$ can be identified with either of the subspaces

$$\mathcal{K}_1=\{\{x,0\}:\ x\in\mathcal{H}\},\quad \mathcal{K}_2=\{\{0,y\}:\ y\in\mathcal{H}\},$$

so that $\mathcal{K}_1=\mathcal{K}\oplus\mathcal{K}_2$ can be seen as the direct sum $\mathcal{H}\oplus\mathcal{H}$.

As hinted in Sec. I, we mimic the obvious procedure by which a representation of $\mathcal{W}_+$ in $\mathcal{H}=L^2(0,\infty)$ yields a representation of the Weyl algebra in $\mathcal{K}=L^2(-\infty,\infty)=\mathcal{H}\oplus\mathcal{H}$ according to the following equations:

$$U_\mathcal{K}(\alpha)\{f,g\}=\{U(\alpha)f+R(\alpha)g,U^\dagger(\alpha)g\}\quad \alpha\geqslant 0, \tag{23a}$$

$$U_\mathcal{K}(\alpha)\{f,g\}=\{U^\dagger(-\alpha)f,U(-\alpha)g+R^\dagger(-\alpha)f\}\quad \alpha\leqslant 0, \tag{23b}$$

$$V_\mathcal{K}(\beta)\{f,g\}=\{V(\beta)f,V(-\beta)g\}, \tag{23c}$$

where the operators $U(\alpha)$, $V(\beta)$ are defined in Eq. (10) and the "cut plus reflection" operator $R(\alpha)$ is defined as

$$R(\alpha)f=\theta(\alpha-x)f(\alpha-x).$$

It is obvious that the above defined operators $U_\mathcal{K}$ and $V_\mathcal{K}$ realize the Schrödinger representation of the Weyl algebra in $L^2(-\infty,\infty)$.

We want to translate Eqs. (23) into similar equations which yield a representation of the Weyl algebra in $\mathcal{K}=\mathcal{H}\oplus\mathcal{H}$ starting from a representation of $\mathcal{W}_+$ in $\mathcal{H}$. In matrix form the operators $U_\mathcal{K}(\alpha)$ and $V_\mathcal{K}(\beta)$ (as in Eqs. (23)) can be written as

$$U_\mathcal{K}(\alpha)=\begin{pmatrix} U(\alpha) & R(\alpha)\\ 0 & U^\dagger(\alpha)\end{pmatrix}\quad \alpha\geqslant 0,\quad U_\mathcal{K}(\alpha)=U^\dagger(-\alpha)\quad \alpha\leqslant 0, \tag{24}$$

$$V_\mathcal{K}(\beta)=\begin{pmatrix} V(\beta) & 0\\ 0 & V(-\beta)\end{pmatrix}. \tag{25}$$

The operators $V_\mathcal{K}(\beta)$ are obviously a continuous group of unitary operators in $\mathcal{K}$. They can be represented in terms of the generator $q_\mathcal{K}=\int_{-\infty}^\infty \alpha dG_\alpha$ as $V_\mathcal{K}(\beta)=\exp(-iq_\mathcal{K}\beta)$, with

$$G_\alpha=\theta(\alpha)(P_\alpha K_1+K_2)+\theta(-\alpha)E_{-\alpha}K_2,\quad G_0=K_2, \tag{26}$$

K_1 and K_2 being the projections onto $\mathcal{K}_1$ and $\mathcal{K}_2$, respectively. On the other hand, in order to ensure the group composition law (Eq. (4)) for the $U_\mathcal{K}(\alpha)$ operators as well as the Weyl composition law (Eq. (7)) we need to define an appropriate operator $R(\alpha)$. Note that we allow for a nonself-adjoint $R(\alpha)$, although the operator $R(\alpha)$ presented above for $L^2(0,\infty)$ is self-adjoint. Actually, $\tilde{R}(\alpha)=\exp(i\theta)R(\alpha)$ would work as well. As a matter of fact, it can be shown that the operator $R(\alpha)$ such that the $U_\mathcal{K}(\alpha)$'s obey the defining Eqs. (4) and (7) is unique up to a constant phase factor.

V. TOWARD THE CONSTRUCTION OF THE OPERATORS $R(\alpha)$

We report the conditions which the operators $R(\alpha)$ have to obey in order that Eq. (4) be satisfied, together with the composition law which forces them. The arguments α,α_i will be meant to be non-negative, with $\alpha_1\leqslant\alpha_2$,

$$U_{\mathcal{K}}(\alpha)U_{\mathcal{K}}(-\alpha)=I\Rightarrow\begin{cases}R(\alpha)R^{\dagger}(\alpha)=P_{\alpha} & (27a)\\ R(\alpha)U(\alpha)=0, & (27b)\end{cases}$$

$$U_{\mathcal{K}}(-\alpha)U_{\mathcal{K}}(\alpha)=I\Rightarrow\begin{cases}R^{\dagger}(\alpha)R(\alpha)=P_{\alpha} & (28a)\\ U^{\dagger}(\alpha)R(\alpha)=0, & (28b)\end{cases}$$

$$U_{\mathcal{K}}(\alpha_1)U_{\mathcal{K}}(\alpha_2)=U_{\mathcal{K}}(\alpha_1+\alpha_2)\Rightarrow U(\alpha_1)R(\alpha_2)+R(\alpha_1)U^{\dagger}(\alpha_2)=R(\alpha_1+\alpha_2), \quad (29)$$

$$U_{\mathcal{K}}(\alpha_2)U_{\mathcal{K}}(\alpha_1)=U_{\mathcal{K}}(\alpha_1+\alpha_2)\Rightarrow U(\alpha_2)R(\alpha_1)+R(\alpha_2)U^{\dagger}(\alpha_1)=R(\alpha_1+\alpha_2), \quad (30)$$

$$U_{\mathcal{K}}(\alpha_2)U_{\mathcal{K}}(-\alpha_1)=U_{\mathcal{K}}(\alpha_2-\alpha_1)\Rightarrow\begin{cases}R(\alpha_2)R^{\dagger}(\alpha_1)=U(\alpha_2-\alpha_1)P_{\alpha_1} & (31a)\\ R(\alpha_2)U(\alpha_1)=R(\alpha_2-\alpha_1) & (31b)\\ U^{\dagger}(\alpha_2)R^{\dagger}(\alpha_1)=0, & (31c)\end{cases}$$

$$U_{\mathcal{K}}(-\alpha_2)U_{\mathcal{K}}(\alpha_1)=U_{\mathcal{K}}(\alpha_1-\alpha_2)\Rightarrow\begin{cases}R^{\dagger}(\alpha_2)R(\alpha_1)=U(\alpha_2-\alpha_1)P_{\alpha_1} & (32a)\\ U^{\dagger}(\alpha_2)R(\alpha_1)=0 & (32b)\\ R^{\dagger}(\alpha_2)U(\alpha_1)=R^{\dagger}(\alpha_2-\alpha_1). & (32c)\end{cases}$$

The relations imposed by the remaining composition laws follow from the above equations.

The equations reported above are not independent. In fact, we have:

Theorem 1: *Eqs. (27a) and (28a) and either of Eqs. (29), (30) imply all the other equations reported above.*

Proof: Assume Eq. (29); nothing changes if Eq. (30) is assumed instead. By multiplying Eq. (27a) by $U^{\dagger}(\alpha)$ and $U(\alpha)$ at left and right, respectively, we find $R^{\dagger}(\alpha)U(\alpha)=0$, which implies Eq. (28b). Similarly, Eq. (27b) is obtained by multiplying Eq. (28a) by $U^{\dagger}(\alpha)$ (left) and $U(\alpha)$ (right). Equations (31c) and (32b) are a consequence. By right multiplying Eq. (29) by $U(\alpha_2)$ we find $R(\alpha_1)=R(\alpha_1+\alpha_2)U(\alpha_2)$, which is equivalent to Eq. (31b). By left multiplying Eq. (29) by $U^{\dagger}(\alpha_1)$ we get $R(\alpha_2)=U^{\dagger}(\alpha_1)R(\alpha_1+\alpha_2)$, which is equivalent to Eq. (32c). Using this equation in the form $R^{\dagger}(\alpha_1)=R^{\dagger}(\alpha_2)U(\alpha_2-\alpha_1)$ we find Eq. (31a). Using Eq. (31b) in the form $R(\alpha_1)=R(\alpha_2)U(\alpha_2-\alpha_1)$ we find Eq. (32a).

To prove Eq. (30) first note that $R(\alpha)=R(\alpha)P_{\alpha}=P_{\alpha}R(\alpha)$ as a consequence of Eqs. (27b) and (28b), respectively. This implies, by Eq. (31a), $R(\alpha_1+\alpha_2)P_{\alpha_1}=U(\alpha_2)R(\alpha_1)$. Hence, by Eq. (31b),

$$\begin{aligned}U(\alpha_2)R(\alpha_1)+R(\alpha_2)U^{\dagger}(\alpha_1)&=U(\alpha_2)R(\alpha_1)+R(\alpha_1+\alpha_2)U(\alpha_1)U^{\dagger}(\alpha_1)\\&=U(\alpha_2)R(\alpha_1)-R(\alpha_1+\alpha_2)P_{\alpha_1}+R(\alpha_1+\alpha_2)=R(\alpha_1+\alpha_2).\end{aligned}$$ □

For later use we prove the following Lemma.

Lemma 1: *If an operator $R(\alpha_0)$ is such that, if $\alpha\leqslant\alpha_0$,*

$$R(\alpha_0)R^{\dagger}(\alpha_0)=P_{\alpha_0}, \quad (33a)$$

$$R^{\dagger}(\alpha_0)R(\alpha_0)=P_{\alpha_0}, \quad (33b)$$

$$R(\alpha_0)U(\alpha)=U^{\dagger}(\alpha)R(\alpha_0), \quad (33c)$$

then

$$R(\alpha_0)U(\alpha_0)=0, \quad (34a)$$

$$R(\alpha_0)P_{\alpha_0} = R(\alpha_0), \tag{34b}$$

$$P_{\alpha_0}R(\alpha_0) = R(\alpha_0), \tag{34c}$$

$$P_{\alpha_0-\alpha}R(\alpha_0) = R(\alpha_0)E_\alpha, \tag{34d}$$

$$R(\alpha_0)P_\alpha = U(\alpha_0-\alpha)R(\alpha_0)U(\alpha_0-\alpha). \tag{34e}$$

Proof: Eq. (34a) follows from:

$$U^\dagger(\alpha_0)R^\dagger(\alpha_0)R(\alpha_0)U(\alpha_0) = U^\dagger(\alpha_0)P_{\alpha_0}U(\alpha_0) = 0.$$

Equations (34b) and (34c) are a consequence. Equation (34d) follows from:

$$\begin{aligned} R(\alpha_0)E_\alpha &= R(\alpha_0)P_{\alpha_0}E_\alpha = [R(\alpha_0)U(\alpha)][U^\dagger(\alpha)R^\dagger(\alpha_0)]R(\alpha_0) = U^\dagger(\alpha)R(\alpha_0)R^\dagger(\alpha_0)U(\alpha)R(\alpha_0) \\ &= U^\dagger(\alpha)P_{\alpha_0}U(\alpha)R(\alpha_0) = P_{\alpha_0-\alpha}R(\alpha_0). \end{aligned}$$

Equation (34e) follows by writing:

$$R(\alpha_0)P_\alpha = E_{\alpha_0-\alpha}R(\alpha_0) = U(\alpha_0-\alpha)[U^\dagger(\alpha_0-\alpha)R(\alpha_0)] = U(\alpha_0-\alpha)R(\alpha_0)U(\alpha_0-\alpha). \quad \square$$

We are now in the position to show that a family of operators $R(\alpha), \alpha \geqslant 0$, exists which satisfy Eqs. (27a), (28a), and (29) (and consequently the rest of the equations required by the group composition laws) provided an operator $R(\alpha_0)$ exists which satisfies the hypotheses of Lemma 1. First we prove this statement, and later we exhibit a suitable (nonunique) operator $R(\alpha_0)$.

The proof is achieved through the following steps.

Theorem 2: *Let $R(\beta)$ satisfy the hypotheses of Lemma 1. For $\alpha \leqslant \beta$ the operators $R(\alpha) \equiv R(\beta)U(\beta-\alpha)$ obey Eqs. (27a) and (28a). Given $\alpha_2 \geqslant \alpha_1 \geqslant 0, \alpha_1+\alpha_2 \leqslant \beta$, Eq. (29) is satisfied.*

Theorem 3: *If $R(\alpha_0)$ satisfies the hypotheses of Lemma 1 and $R(n\alpha_0)$ is defined recursively as follows*:

$$R(n\alpha_0) \equiv U((n-1)\alpha_0)R(\alpha_0) + R((n-1)\alpha_0)U^\dagger(\alpha_0),$$

then also $R(n\alpha_0)$ obeys the hypotheses of Lemma 1. Moreover,

$$R(n\alpha_0) = U(k\alpha_0)R((n-k)\alpha_0) + R(k\alpha_0)U^\dagger((n-k)\alpha_0) \quad k \leqslant (n-1). \tag{35}$$

Theorem 4: *For any $\alpha \geqslant 0$, choose n such that $n\alpha_0 \geqslant \alpha$. The operators $R(\alpha) \equiv R(n\alpha_0)U(n\alpha_0-\alpha)$ are independent of n and satisfy Eqs. (27a), (28a), and (29).*

Proof of Theorem 2:

$$R^\dagger(\alpha)R(\alpha) = U^\dagger(\beta-\alpha)R^\dagger(\beta)R(\beta)U(\beta-\alpha) = U^\dagger(\beta-\alpha)P_\beta U(\beta-\alpha) = P_\alpha.$$

Equation (27a) is proved in a similar way. Equation (29) is verified using Eq. (34d),

$$\begin{aligned} U(\alpha_1)R(\alpha_2) + R(\alpha_1)U^\dagger(\alpha_2) &= U(\alpha_1)U^\dagger(\beta-\alpha_2)R(\beta) + R(\beta)U(\beta-\alpha_1)U^\dagger(\alpha_2) \\ &= E_{\alpha_1}U^\dagger(\beta-\alpha_1-\alpha_2)R(\beta) + R(\beta)E_{\beta-\alpha_1}U(\beta-\alpha_1-\alpha_2) \\ &= [E_{\alpha_1}+P_{\alpha_1}]R(\alpha_1+\alpha_2) = R(\alpha_1+\alpha_2). \quad \square \end{aligned}$$

Proof of Theorem 3: The proof is by induction. If Eqs. (33) hold true up to $k=n$, then by Eq. (34a) we find

$$[U(n\alpha_0)R(\alpha_0)+R(n\alpha_0)U^\dagger(\alpha_0)]^\dagger[U(n\alpha_0)R(\alpha_0)+R(n\alpha_0)U^\dagger(\alpha_0)]=R^\dagger(\alpha_0)R(\alpha_0)$$
$$+U(\alpha_0)R^\dagger(n\alpha_0)R(n\alpha_0)U^\dagger(\alpha_0)=P_{\alpha_0}+P_{(n+1)\alpha_0}E_{\alpha_0}=P_{(n+1)\alpha_0}.$$

In a similar way Eq. (33a) is proved. In order to prove Eq. (35), suppose it is true for $k\leqslant n$. Then

$$R((n+1)\alpha_0)\equiv U(n\alpha_0)R(\alpha_0)+R(n\alpha_0)U^\dagger(\alpha_0)=U(k\alpha_0)U((n-k)\alpha_0)R(\alpha_0)+[U(k\alpha_0)R((n-k)\alpha_0)$$
$$+R(k\alpha_0)U^\dagger((n-k)\alpha_0)]U^\dagger(\alpha_0)=U(k\alpha_0)[U((n-k)\alpha_0)R(\alpha_0)+R((n-k)\alpha_0)U^\dagger(\alpha_0)]$$
$$+R(k\alpha_0)U^\dagger((n-k+1)\alpha_0)=U(k\alpha_0)R((n-k+1)\alpha_0)+R(k\alpha_0)U^\dagger((n-k+1)\alpha_0),$$

which shows that also $R((n+1)\alpha_0)$ can be seen as the result of the composition law Eq. (35) if this is true for $k\leqslant n$.

We now prove Eq. (33c) for $R(n\alpha_0)$. For a $\alpha\geqslant\alpha_0$ we have

$$R(n\alpha_0)U(\alpha)=[U((n-1)\alpha_0)R(\alpha_0)+R((n-1)\alpha_0)U^\dagger(\alpha_0)]U(\alpha)=R((n-1)\alpha_0)U(\alpha-\alpha_0)$$
$$=U^\dagger(\alpha-\alpha_0)R((n-1)\alpha_0)=U^\dagger(\alpha)[U(\alpha_0)R((n-1)\alpha_0)+R(\alpha_0)U^\dagger((n-1)\alpha_0)]$$
$$=U^\dagger(\alpha)R(n\alpha_0),$$

where we used the just proved independence of $R(n\alpha_0)$ on the way it is composed, and the inductive hypothesis that Eqs. (33) are satisfied up to $k=n-1$. For $\alpha<\alpha_0$, writing $R(n\alpha_0)=U((n-1)\alpha_0)R(\alpha_0)+R((n-1)\alpha_0)U^\dagger(\alpha_0)$ we find

$$D\equiv U^\dagger(\alpha)R(n\alpha_0)-R(n\alpha_0)U(\alpha)=U((n-1)\alpha_0-\alpha)R(\alpha_0)+R((n-1)\alpha_0)U(\alpha)U^\dagger(\alpha_0)$$
$$-U((n-1)\alpha_0)U^\dagger(\alpha)R(\alpha_0)-R((n-1)\alpha_0)U^\dagger(\alpha_0-\alpha)=U((n-1)\alpha_0-\alpha)P_\alpha R(\alpha_0)$$
$$-R((n-1)\alpha_0)P_\alpha U^\dagger(\alpha_0-\alpha).$$

Using Eq. (34e) for $R((n-1)\alpha_0)P_\alpha$, D can be written as

$$D=U((n-1)\alpha_0-\alpha)[P_\alpha R(\alpha_0)-R(\alpha_0)E_{\alpha_0-\alpha}]=0$$

since the term in bracket vanishes by Eq. (34d). □

Proof of Theorem 4: Taking into account Eq. (34a) we have

$$R((n+1)\alpha_0)U((n+1)\alpha_0-\alpha)=[U(n\alpha_0)R(\alpha_0)+R(n\alpha_0)U^\dagger(\alpha_0)]U((n+1)\alpha_0-\alpha)$$
$$=R(n\alpha_0)U(n\alpha_0-\alpha).$$

Thus the operators $R(\alpha)$ are uniquely defined, due to Theorem 3. Due to Lemma 1 and Theorem 2 they obey Eqs. (27a), (28a), and (29). □

We stress the gist of our argument to prove the existence of a family $\{R(\alpha),\alpha\geqslant 0\}$ such that all the Eqs. from (27) to (32) are satisfied: it suffices to exhibit an operator which satisfies the hypotheses of Lemma 1 for a definite value, say 2π, to conclude that the operators $R(\alpha)$ constructed according to Theorem 4 are uniquely defined and, by Theorem 2, satisfy Eqs. (27a), (28a), and (29). By Theorem 1, all the Eqs. from (27) to (32) are then satisfied, and consequently the group composition laws for the operators $U_{\mathcal{K}}(\alpha)$ are satisfied.

We note that in the language of Ref. 6 the operators $U_{\mathcal{K}}(\alpha)$ are a minimal dilation of $U(\alpha)$. Indeed, $\forall x\in\mathcal{H}=K_1\mathcal{K}$, $U(\alpha)x=K_1U_{\mathcal{K}}(\alpha)x$, and the vectors $U_{\mathcal{K}}(\alpha)x$, $\alpha\in\mathbb{R}$, $x\in K_1\mathcal{K}$, span the whole space $\mathcal{K}$. In fact, for any $\alpha=-\beta\leqslant 0$, $K_2U_{\mathcal{K}}(\alpha)x=R^\dagger(\beta)x$. Since $P_\beta=R^\dagger(\beta)R(\beta)$ we see that the vectors $R^\dagger(\beta)x$ are dense in $\mathcal{H}$, hence, $\{K_2U_{\mathcal{K}}(\alpha)x\}$ is dense in $K_2\mathcal{K}$. Our construction, however, is completely different from that of Ref. 6, and much more direct.

Now we consider the conditions imposed to the operators $R(\alpha)$ by the requirement that Eq. (7) holds for $U_{\mathcal{K}}(\alpha),V_{\mathcal{K}}(\beta)$. These conditions are

$$R(\alpha)V(-\beta)U(\alpha)=0, \tag{36a}$$

$$R(\alpha)V(-\beta)R^{\dagger}(\alpha) = \exp(i\alpha\beta)V(\beta)P_{\alpha}. \tag{36b}$$

They are equivalent to the single equation

$$V(-\beta)R(\alpha)V(-\beta) = \exp(i\alpha\beta)R(\alpha). \tag{37}$$

Indeed, by multiplying Eq. (36b) by $V(-\beta)$ (left) and by $R(\alpha)$ (right) we have Eq. (37), which can be transformed back into Eq. (36b) by multiplication by $V(\beta)$ (left) and $R^{\dagger}(\alpha)$ (right). Equation (36a) is obtained from Eq. (37) by multiplying by $V(\beta)$ (left) and by $U(\alpha)$ (right). It is useful to note that Eq. (37) holds for any α provided it holds for $R(\alpha_0)$. Indeed, we have:

Theorem 5: *If an operator $R(\alpha_0)$ obeys Eq. (37), then $\forall \alpha \geqslant 0$ the operators $R(\alpha)$ constructed according to Theorem 4 obey Eq. (37).*

Proof: By induction, using Eqs. (7) and (9), we check that $R(n\alpha_0)$ defined in Theorem 3 obeys Eq. (37). Likewise, the operators $R(\alpha) \equiv R(n\alpha_0)U(n\alpha_0 - \alpha)$ verify Eq. (37). □

VI. CONSTRUCTION OF THE OPERATOR $R(2\pi)$

Here again we mimic the situation which occurs in $\mathcal{H}=L^2(0,\infty)$. There in the basis $e_n = \exp(inx)/\sqrt{2\pi}$ of $L^2(0,2\pi)=P_{2\pi}\mathcal{H}=\oplus\mathcal{H}_n$, with $\mathcal{H}_n$ the subspaces generated by the vectors e_n, we have $R(2\pi)e_n=e_{-n}$. The subspaces $\mathcal{H}$ are connected to $\mathcal{H}_0$ by the equation

$$V(n)Q_0 = Q_n V(n), \tag{38}$$

where the Q_n's are the projections onto the subspaces $\mathcal{H}_n$.

In order to introduce a similar definition for $R(2\pi)$, first note that $R(2\pi)=R(2\pi)P_{2\pi}$ needs to be defined only in $\mathcal{H}_{2\pi}=P_{2\pi}\mathcal{H}$. Next, we resort to a well known lemma to Stone's theorem[12] which states that, given a strongly continuous one-parameter periodic group of unitary operators $\widetilde{U}(\alpha)$, $\widetilde{U}(\alpha)=\widetilde{U}(\alpha+2\pi)$, $\widetilde{U}(0)=I$, then the operators

$$Q_n = \int_0^{2\pi} \exp(-in\alpha)\widetilde{U}(\alpha)\frac{d\alpha}{2\pi} \tag{39}$$

are orthogonal projections such that $\Sigma_{-\infty}^{\infty} Q_n = I$. The inverse of Eq. (39) is

$$\widetilde{U}(\alpha) = \sum_{-\infty}^{\infty} Q_n \exp(in\alpha). \tag{40}$$

The operators

$$\widetilde{U}(\alpha) = U(\alpha)P_{2\pi-\alpha} + P_{\alpha}U^{\dagger}(2\pi-\alpha) \quad 0 \leqslant \alpha \leqslant 2\pi \quad \widetilde{U}(\alpha+2n\pi) = \widetilde{U}(\alpha) \tag{41}$$

verify the hypotheses of the lemma. By Eq. (7) they satisfy

$$V(n)\widetilde{U}(\alpha) = \exp(-in\alpha)\widetilde{U}(\alpha)V(n) \tag{42}$$

and by Eq. (15),

$$E(\alpha)\widetilde{U}(\alpha) = P_{2\pi}U(\alpha) \quad \alpha \leqslant 2\pi. \tag{43}$$

By integrating Eq. (42) over $[0,2\pi]$ we get Eq. (38), which implies that $V(n)$ is an invertible isometry from $\mathcal{H}_0=Q_0\mathcal{H}_{2\pi}=Q_0\mathcal{H}$ to $\mathcal{H}_n=Q_n\mathcal{H}_{2\pi}=Q_n\mathcal{H}$.

We define an operator $R(2\pi)$ in each $\mathcal{H}_n$ in the following way: if $x_n=V(n)x_0, x_0 \in \mathcal{H}_0$,

$$R(2\pi)x_n = R(2\pi)V(n)x_0 = V(-n)x_0. \tag{44}$$

$R(2\pi)$ satisfies the hypotheses of Lemma 1 and Eq. (37).

Equations (33a) and (33b) are obvious, since $R(2\pi)$ is self-adjoint and $R^2(2\pi)=P_{2\pi}$. To verify Eq. (33c) note that Eq. (44) is equivalent to

$$R(2\pi)V(n) = V(-n)R(2\pi), \tag{45a}$$

$$R(2\pi)Q_0 = Q_0 = Q_0R(2\pi). \tag{45b}$$

As a consequence, by Eq. (38) we get

$$R(2\pi)Q_n = Q_{-n}R(2\pi) \tag{46}$$

and by Eqs. (40) and (46),

$$R(2\pi)\widetilde{U}(\alpha) = \widetilde{U}^\dagger(\alpha)R(2\pi). \tag{47}$$

Hence, using Eq. (43), for $\alpha \leqslant 2\pi$ we have

$$\begin{aligned} R(2\pi)U(\alpha) &= R(2\pi)P_{2\pi}U(\alpha) = R(2\pi)E_\alpha\widetilde{U}(\alpha) = P_{2\pi-\alpha}R(2\pi)\widetilde{U}(\alpha) = P_{2\pi-\alpha}\widetilde{U}^\dagger(\alpha)R(2\pi) \\ &= U^\dagger(\alpha)P_{2\pi}R(2\pi) = U^\dagger(\alpha)R(2\pi), \end{aligned}$$

which proves Eq. (33c). The hypotheses of Lemma 1 are satisfied.

Finally, we prove that $R(2\pi)$ obeys Eq. (37). By Eqs. (34b), (34d) we have

$$\begin{aligned} R(2\pi)V(-\beta) &= R(2\pi)\int_0^\infty \exp(i\beta\lambda)dP_\lambda = \int_0^{2\pi} \exp(i\beta\lambda)d(R(2\pi)P_\lambda) = \int_0^{2\pi} \exp(i\beta\lambda)dE_{2\pi-\lambda}R(2\pi) \\ &= \int_0^{2\pi} \exp(i\beta(2\pi-\lambda))dP_\lambda R(2\pi) = \exp(2\pi i\beta)\int_0^\infty \exp(-i\beta\lambda)dP_\lambda R(2\pi) \\ &= \exp(2\pi i\beta)V(\beta)R(2\pi), \end{aligned}$$

which is equivalent to Eq. (37).

In conclusion, the operators $R(\alpha)$ constructed according to the procedure outlined in the previous section, starting from the operator $R(2\pi)$ defined in Eq. (44), obey equations from Eqs. (27) to (32) and (37). In this way we construct a representation of the Weyl algebra in the space $\mathcal{K}$ starting from a representation of $\mathcal{W}_+$ in the space $\mathcal{H}$.

We wish to stress that an explicit expression of the operators $R(\alpha)$ can be given in terms of P_λ, $U(\alpha)$, $U^\dagger(\alpha)$. Let

$$\widetilde{R}(\alpha) = \int_0^{\alpha/2} U(\alpha-2\lambda)dP_\lambda + \int_{\alpha/2}^{\alpha} U^\dagger(2\lambda-\alpha)dP_\lambda. \tag{48}$$

The (strong) convergence of the above integrals can be proved along the lines of Ref. 4. The $\widetilde{R}(\alpha)$'s are self-adjoint and their role as cut plus reflection operators is apparent when viewed in $L^2(0,\infty)$. We show that they satisfy Eqs. (27a), (28a), (29), and (37).

To this purpose, note the following identity:

$$P_\mu dP_\lambda = \theta(\mu-\lambda)dP_\lambda, \tag{49}$$

which implies

$$\widetilde{R}(\alpha)\widetilde{R}^{\dagger}(\alpha)=\widetilde{R}^{\dagger}(\alpha)\widetilde{R}(\alpha)$$
$$=\int_0^{\alpha/2}U(\alpha-2\lambda)dP_\lambda\int_0^{\alpha/2}dP_\mu U^{\dagger}(\alpha-2\mu)+\int_{\alpha/2}^{\alpha}U^{\dagger}(2\lambda-\alpha)dP_\lambda\int_{\alpha/2}^{\alpha}dP_\mu U(2\mu-\alpha)$$
$$=\int_0^{\alpha/2}U(\alpha-2\lambda)dP_\lambda U^{\dagger}(\alpha-2\lambda)+\int_{\alpha/2}^{\alpha}U^{\dagger}(2\lambda-\alpha)dP_\lambda U(2\lambda-\alpha).$$

By Eqs. (15) and (16), noting that $P_{\alpha-2\lambda}\,dP_{\alpha-\lambda}=0$ due to Eq. (49), we find

$$\widetilde{R}(\alpha)\widetilde{R}^{\dagger}(\alpha)=\int_0^{\alpha/2}E_{\alpha-2\lambda}dP_{\alpha-\lambda}+\int_{\alpha/2}^{\alpha}dP_{\alpha-\lambda}=P_\alpha.$$

As for Eq. (29), by recalling Eqs. (11)–(13) and (16) we have ($\alpha\leqslant\beta$):

$$U(\alpha)\widetilde{R}(\beta)+\widetilde{R}(\alpha)U^{\dagger}(\beta)=\int_0^{\beta/2}U(\alpha+\beta-2\lambda)dP_\lambda+\int_{\beta/2}^{(\alpha+\beta)/2}U(\alpha+\beta-2\lambda)E_{2\lambda-\beta}dP_\lambda$$
$$+\int_{(\alpha+\beta)/2}^{\beta}U^{\dagger}(2\lambda-\alpha-\beta)E_{2\lambda-\beta}dP_\lambda+\int_0^{\alpha}U^{\dagger}(2\lambda+\beta-\alpha)dP_{\lambda+\beta}.$$

Using Eq. (49) again and passing to a new variable $\sigma=\lambda+\beta$ in the last integral we conclude

$$U(\alpha)\widetilde{R}(\beta)+\widetilde{R}(\alpha)U^{\dagger}(\beta)=\int_0^{(\alpha+\beta)/2}U(\alpha+\beta-2\lambda)dP_\lambda+\int_{(\alpha+\beta)/2}^{\beta}U^{\dagger}(2\lambda-\alpha-\beta)dP_\lambda=\widetilde{R}(\alpha+\beta).$$

We prove Eq. (37) in the form $V(\beta)\widetilde{R}(\alpha)=\exp(-i\alpha\beta)\widetilde{R}(\alpha)V(-\beta)$. We note that, as a consequence of Eq. (49),

$$V(\beta)dP_\lambda=\int_0^{\infty}\exp(-i\beta\mu)dP_\mu dP_\lambda=\exp(-i\beta\lambda)dP_\lambda. \tag{50}$$

By Eqs. (7) and (9)

$$V(\beta)\widetilde{R}(\alpha)=\exp(-i\alpha\beta)\left\{\int_0^{\alpha/2}U(\alpha-2\lambda)\exp(2i\beta\lambda)dP_\lambda+\int_{\alpha/2}^{\alpha}U^{\dagger}(2\lambda-\alpha)\exp(2i\beta\lambda)dP_\lambda\right\}V(\beta).$$

Equation (50) implies

$$\exp(2i\beta\lambda)V(\beta)dP_\lambda=\exp(i\beta\lambda)dP_\lambda=V(-\beta)dP_\lambda,$$

which proves that Eq. (37) is satisfied.

VII. RELATION BETWEEN THE REPRESENTATIONS IN $\mathcal{H}$ AND IN $\mathcal{K}$

In this section we prove that:

(a) if the representation of the algebra $\mathcal{W}_+$ in $\mathcal{H}$ is irreducible, then the representation $U_{\mathcal{K}},V_{\mathcal{K}}$ in $\mathcal{K}$ is irreducible too; and
(b) if two representations of $\mathcal{W}_+$ in $\mathcal{H}$ generate equivalent representations of $\mathcal{W}_\infty$ in $\mathcal{K}$, then the representations of $\mathcal{W}_+$ are equivalent.

As a consequence, given two irreducible representations of $\mathcal{W}_+$, by (a) von Neumann's Theorem ensures that the representations of the Weyl algebra are equivalent. Hence, by (b) the representations of $\mathcal{W}_+$ are equivalent. In conclusion, the irreducible representations of $\mathcal{W}_+$ are unique, up to equivalence.

In order to prove (a), let T be a bounded operator in $\mathcal{K}=\mathcal{H}\oplus\mathcal{H}$,

$$T = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{51}$$

which commutes with the operators $U_{\mathcal{K}}(\alpha), V_{\mathcal{K}}(\beta)$ generated by an irreducible representation of $\mathcal{W}_+$ in $\mathcal{H}$. Since these operators are unitary in $\mathcal{K}$, also the adjoint $T^\dagger$ commutes with them, so we may assume T to be self-adjoint

$$A = A^\dagger, \quad D = D^\dagger, \quad B = C^\dagger. \tag{52}$$

We will prove $T = \lambda I$, which implies that the representation in $\mathcal{K}$ is irreducible.

Commutation of T with $V_{\mathcal{K}}(\beta)$ implies commutation with the projections G_α given in Eq. (26), in particular with G_0. This implies $B = C = 0$ and

$$AV(\beta) = V(\beta)A, \quad DV(\beta) = V(\beta)D. \tag{53}$$

Moreover, for $\alpha \geqslant 0$ we find

$$TU_{\mathcal{K}}(\alpha) = U_{\mathcal{K}}(\alpha)T \Rightarrow \begin{cases} AU(\alpha) = U(\alpha)A & \text{(54a)} \\ DU^\dagger(\alpha) = U^\dagger(\alpha)D & \text{(54b)} \\ AR(\alpha) = R(\alpha)D. & \text{(54c)} \end{cases}$$

Equations (53), (54a), and (54b), together with the irreducibility of the representation of $\mathcal{W}_+$, imply $A = \lambda I, D = \mu I$. Finally, Eq. (54c) implies $\lambda = \mu$, and consequently $T = \lambda I$. The representation in $\mathcal{K}$ is irreducible.

To prove (b), assume we have two equivalent representations of the Weyl algebra in $\mathcal{K}$, $\{V_{\mathcal{K}}^{(1)}, U_{\mathcal{K}}^{(1)}\}$ and $\{V_{\mathcal{K}}^{(2)}, U_{\mathcal{K}}^{(2)}\}$, induced by two representations $\{U_1, V_1\}, \{U_2, V_2\}$ in $\mathcal{H}$. Let S be the unitary operator such that

$$SU_{\mathcal{K}}^{(1)} = U_{\mathcal{K}}^{(2)}S, \quad SV_{\mathcal{K}}^{(1)} = V_{\mathcal{K}}^{(2)}S. \tag{55}$$

We represent S as

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{56}$$

The latter of Eqs. (55) implies $SG_\alpha^{(1)} = G_\alpha^{(2)}S$ for any α. In particular, for $\alpha = 0$ we find

$$B = C = 0, \tag{57}$$

which implies

$$AV_1 = V_2A, \quad DV_1^\dagger = V_2^\dagger D \tag{58}$$

and, by the unitarity of S,

$$AA^\dagger = A^\dagger A = DD^\dagger = D^\dagger D = I_{\mathcal{H}}. \tag{59}$$

The former of Eqs. (55) for $\alpha \geqslant 0$ implies $AU_1 = U_2A$, $DU_1^\dagger = U_2^\dagger D$, $AR_1 = R_2D$. Recalling Eqs. (58) and (59) we can conclude

$$U_2 = AU_1A^\dagger, \quad V_2 = AV_1A^\dagger. \tag{60}$$

The representations $\{U_1, V_1\}$ and $\{U_2, V_2\}$ are equivalent.

VIII. THE PARTICLE ON A SEGMENT: THE WEYL ALGEBRA

In this section we define the Weyl algebra appropriate to describe a particle on a segment and in the next section we shall prove also in this case the analogous of the von Neumann Theorem.

The algebra we are looking for differs from the algebra for the half-line $\mathcal{W}_+$ since right translations do not vanish only in an interval, say $0 \leqslant \alpha < 1$, and therefore they are no longer isometries: the isometric condition $U^\dagger(\alpha)U(\alpha)=I$ for the algebra $\mathcal{W}_+$ is now replaced by the assumption that $U^\dagger(\alpha)U(\alpha)$ is a projection. The defining equations of the algebra, that we shall denote by $\mathcal{W}_1$, are

$$U(0)=I; \quad U(\alpha)\neq 0 \quad \text{for} \quad 0 \leqslant \alpha < 1; \quad U(1)=0, \tag{61}$$

$$U(\alpha_1)U(\alpha_2)=U(\alpha_1+\alpha_2), \tag{62}$$

$$P_{1-\alpha} \equiv U^\dagger(\alpha)U(\alpha)=P_{1-\alpha}^2, \tag{63}$$

$$V(\beta_1)V(\beta_2)=V(\beta_1+\beta_2), \quad \beta_1,\beta_2 \in \mathbb{R}, \quad V(0)=I, \tag{64}$$

$$U(\alpha)V(\beta)=\exp(i\alpha\beta)V(\beta)U(\alpha), \tag{65}$$

where the $U(\alpha)$'s and the unitary operators $V(\beta)$ are assumed strongly continuous.

Equations (61)–(63) define what is called a semigroup of partial isometries of index 1; in particular Eq. (63) implies

$$U(\alpha)U^\dagger(\alpha)U(\alpha)=U(\alpha). \tag{66}$$

In fact, $U^\dagger U$ being a projection, for any $v \in \mathcal{H}$, $v=v_1+v_2$ with $U^\dagger U v_1=v_1, U^\dagger U v_2=0$, we have $Uv_2=0$, hence, $UU^\dagger Uv=Uv_1=Uv_1+Uv_2=Uv$. As a consequence $(UU^\dagger)^2=UU^\dagger$, i.e., also $UU^\dagger$ is a projection

$$E_\alpha \equiv U(\alpha)U^\dagger(\alpha)=E_\alpha^2. \tag{67}$$

The projections E_α commute among themselves. If $\alpha_1 \leqslant \alpha_2$, thanks to Eqs. (62) and (66),

$$E_{\alpha_1}E_{\alpha_2}=U(\alpha_1)U^\dagger(\alpha_1)U(\alpha_1)U(\alpha_2-\alpha_1)U^\dagger(\alpha_2)=E_{\alpha_2}=E_{\alpha_2}^\dagger=E_{\alpha_2}E_{\alpha_1}$$

and similarly

$$P_{\alpha_1}P_{\alpha_2}=P_{\alpha_2}P_{\alpha_1}=P_{\alpha_1} \quad (\alpha_1 \leqslant \alpha_2).$$

Moreover, the E_α's commute with the P_β's: since $(E_\alpha P_\beta)^2=E_\alpha P_\beta$ and $\|E_\alpha P_\beta\| \leqslant 1$, $E_\alpha P_\beta$ is a projection, hence, $E_\alpha P_\beta=(E_\alpha P_\beta)^\dagger=P_\beta E_\alpha$.

The algebra $\mathcal{W}_1$ could have been realized as the restriction of the algebra $\mathcal{W}_+$ to the interval $0 \leqslant \alpha \leqslant 1$ by the substitutions $U(\alpha) \to P_1 U(\alpha), V(\beta) \to P_1 V(\beta), P_1$ being the projection defined at the end of Sec. II. In this case, in addition to Eqs. (61)–(66), we have also $E_\alpha+P_\alpha \equiv U(\alpha)U^\dagger(\alpha)+U^\dagger(1-\alpha)U(1-\alpha)=I$. This equation obviously holds for the algebra of truncated shifts in $L^2(0,1)$. It can be proved[13] that, conversely, if the representation of the algebra $\mathcal{U}_1$ generated by $U(\alpha), U^\dagger(\alpha)$ is faithful and irreducible, the equation $E_\alpha+P_\alpha=I$ follows from the defining Eqs. (61)–(63). Thus, with these hypotheses, the algebra $\mathcal{U}_1$ is equivalent to the algebra of truncated shifts in $L^2(0,1)$. For the sake of completeness we outline the proof.

The operator $X(\alpha) \equiv E_\alpha+P_\alpha$ is a projection which obeys the following equations:

$$U(\alpha)X(\beta)=\begin{cases} X(\alpha+\beta)U(\alpha) & \alpha+\beta \leqslant 1 \\ U(\alpha) & \alpha+\beta \geqslant 1, \end{cases} \tag{68}$$

$$X(\alpha)U(\beta)=U(\beta) \quad \text{for} \quad \beta \geqslant \alpha. \tag{69}$$

As a consequence, the operator $Z \equiv \int_0^1 X(\alpha)d\alpha=Z^\dagger$ commutes with the operators $U(\alpha)$, $U^\dagger(\alpha)$ and in an irreducible representation is a multiple of the identity. Actually, $Z=I$ since, if $Z(\lambda)$

$\equiv \int_0^\lambda X(\alpha)d\alpha$, from Eqs. (68) and (69) we have $Z(\lambda)U(\lambda)=\lambda U(\lambda)$. Since $\|U(\lambda)\|\neq 0$ for $\lambda<1$ we find $\|Z(\lambda)\|\geqslant\lambda$. On the other hand, $\|Z(\lambda)\|\leqslant\int_0^\lambda\|X(\alpha)\|d\alpha=\lambda$, hence, $\|Z(\lambda)\|=\lambda$ for $\lambda<1$. Since $\lim_{\lambda\to 1}\|Z(\lambda)-Z(1)\|=0$, we conclude $\|Z(1)\|=1$. Thus $Z=I$, i.e., $\int_0^1(I-X(\alpha))d\alpha=0$. Since $I-X(\alpha)\geqslant 0$ we conclude $X(\alpha)=I$.

In the next section we show that the algebra $\mathcal{W}_1$ can always be considered as the restriction of the algebra $\mathcal{W}_+$ to the interval $0\leqslant\alpha\leqslant 1$.

IX. THE PARTICLE ON A SEGMENT: THE VON NEUMANN THEOREM

By the same arguments of Sec. III it can be shown that in an irreducible representation of $\mathcal{W}_1$ the spectrum $\sigma(q)$ of the generator q of the group $\{V(\beta),\beta\in\mathbb{R}\}$ is a segment $[x_0,x_0+1]$ and that, although representations with different values of x_0 are inequivalent, we can always limit our attention to the case $\sigma(q)=[0,1]$. Moreover, as for the algebra $\mathcal{W}_+$, the irreducibility of $\mathcal{W}_1$ entails the irreducibility of $\mathcal{U}_1$.

Suppose now that $\mathcal{H}_1$ hosts a representation of $\mathcal{W}_1$ and consider the space

$$\mathcal{H}\equiv\bigoplus_{n=1}^{\infty}\mathcal{H}_n,\quad \mathcal{H}_n=\mathcal{H}_1\quad x\in\mathcal{H}=(x_1,x_2,\cdots,x_n,\cdots):\ \sum_n\|x_n\|^2<\infty \tag{70}$$

and in $\mathcal{H}$ define $(0\leqslant\lambda\leqslant 1,\alpha\geqslant 0,\beta\in\mathbb{R})$,

$$U_{\mathcal{H}}(\lambda)x\equiv(U(\lambda)x_1,U^\dagger(1-\lambda)x_1+U(\lambda)x_2,\cdots,U^\dagger(1-\lambda)x_{n-1}+U(\lambda)x_n,\cdots), \tag{71a}$$

$$U_{\mathcal{H}}(n)\equiv[U_{\mathcal{H}}(1)]^n,\ U_{\mathcal{H}}(\alpha=n+\lambda)\equiv U_{\mathcal{H}}(n)U_{\mathcal{H}}(\lambda)=U_{\mathcal{H}}(\lambda)U_{\mathcal{H}}(n), \tag{71b}$$

$$V_{\mathcal{H}}(\beta)x\equiv(V(\beta)x_1,e^{-i\beta}V(\beta)x_2\cdots,e^{-i(n-1)\beta}V(\beta)x_n,\cdots). \tag{71c}$$

Using the properties of the $U(\lambda)$'s, and in particular $X(\lambda)=I$ (which ensures that the $U_{\mathcal{H}}(\alpha)$'s are isometries), it is easy to verify that $\{U_{\mathcal{H}}(\alpha),V_{\mathcal{H}}(\beta)\}$ generate the algebra $\mathcal{W}_+$.

As for the case of the half-line we show that if the representation of the algebra $\mathcal{W}_1$ in $\mathcal{H}_1$ is irreducible, then the representation of $\{U_{\mathcal{H}}(\alpha),V_{\mathcal{H}}\beta\}$ in $\mathcal{H}$ is irreducible too. Let T be a bounded operator in $\mathcal{H}$ commuting with the operators $U_{\mathcal{H}}(\alpha),U_{\mathcal{H}}^\dagger(\alpha)$ (hence with $V_{\mathcal{H}}(\beta)$) and let $T_{n,m}\equiv P_nTP_m$, where P_n is the projection on $\mathcal{H}_n$ $(P_n=U_{\mathcal{H}}(n-1)U_{\mathcal{H}}^\dagger(n-1)-U_{\mathcal{H}}(n)U_{\mathcal{H}}^\dagger(n))$. Since T commutes with the projections P_n, only the "diagonal" elements $T_{n,n}$ are different from zero. Moreover commutation with $U_{\mathcal{H}}(1)$ implies that $T_{n,n}$ is independent of n,

$$U_{\mathcal{H}}(1)Tx=(0,T_{1,1}x_1,T_{2,2}x_2,\cdots)=TU_{\mathcal{H}}(1)x=(0,T_{2,2}x_1,T_{3,3}x_2,\cdots).$$

Now, by imposing commutation with $U_{\mathcal{H}}(\lambda),U_{\mathcal{H}}^\dagger(\lambda)$ $(0\leqslant\lambda\leqslant 1)$, we conclude that $T=\mu I$.

Finally, we prove that all the irreducible representations of $\mathcal{W}_1$ are equivalent. Let $\{U_1(\lambda),V_1(\beta)\},\{U_2(\lambda),V_2(\beta)\}$ be two irreducible representations of $\mathcal{W}_1$ in $\mathcal{H}_1$ and $\{U_{\mathcal{H}}^{(1)}(\alpha),V_{\mathcal{H}}^{(1)}\times(\beta)\},\{U_{\mathcal{H}}^{(2)}(\alpha),V_{\mathcal{H}}^{(2)}(\beta)\}$ the induced irreducible representations of $\mathcal{W}_+$ in $\mathcal{H}$, according to Eqs. (71). Since we have proved that all the irreducible representations of $\mathcal{W}_+$ are equivalent, there exists a unitary operator S such that

$$SU_{\mathcal{H}}^{(1)}(\alpha)=U_{\mathcal{H}}^{(2)}(\alpha)S,\quad SV_{\mathcal{H}}^{(1)}(\beta)=V_{\mathcal{H}}^{(2)}(\beta)S. \tag{72}$$

Since $U_1(0)=U_2(0)=I$, $U_1(1)=U_2(1)=0$, S commutes with the projections P_n and, as before, only the diagonal element $S_n\equiv P_nSP_n$ are different from zero and independent of n. It is straightforward to conclude that $S_1U_1(\lambda)=U_2(\lambda)S_1$, with S_1 unitary in $\mathcal{H}_1$.

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Scattering and bound state Green's functions on a plane via so(2,1) Lie algebra

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We calculate the Green's functions for the particle-vortex system, for two anyons on a plane with and without a harmonic regulator and in a uniform magnetic field. These Green's functions which describe scattering or bound states (depending on the specific potential in each case) are obtained exactly using an algebraic method related to the SO(2,1) Lie group. From these Green's functions we obtain the corresponding wave functions and for the bound states we also find the energy spectra. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2363259]

I. INTRODUCTION

In this paper we study exactly solvable problems for one or two particles on a plane bound or not by external potentials by constructing algebraically their Green's functions. These Green's functions describe scattering or bound states, depending on the kind of interaction in each situation. The algebraic method used here is based on the Schwinger representation[1] for the inverse of an operator which is an integral representation involving the exponential of the operator. The operator is identified with the Hamiltonian of the problem which can be written as a linear combination of the generators of a Lie algebra. In particular, we are interested in the so(2,1) Lie algebra which describe some well known problems as the harmonic oscillator, the hydrogen atom, and the Morse potential.[2–16] Some other problems with more involved potentials can also be described by this algebra (see, for instance Refs. 17–32). Once the Hamiltonian is written in terms of the SO(2,1) generators one can use Baker–Campbell–Hausdorff (BCH) formulas[33–35] to split the exponential of the Hamiltonian into a convenient product of the so(2,1) generators. BCH formulas are also used to change the order of the product of the exponentials of generators to simplify the computation of the Green's functions. This method was used to describe the Dirac electron in a Coulomb potential[9] and the discussion presented here is a nonrelativistic version modified to include other potentials.[16,27] As we will see, for the simplest cases the Hamiltonian is identified simply with just one so(2,1) generator. In these particular cases just one BCH formula is used.

The two-dimensional problems we are going to discuss here have been studied before in Refs. 36–48 with other approaches, although for instance, in Ref. 43 the so(2,1) symmetry was invoked to construct the wave function for the particle-vortex system. The problem of particles moving on a plane is relevant to the studies of condensed matter systems as the fractional quantum Hall effect

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and anyonic superconductivity,[49–57] supersymmetry,[58,59] and fault-tolerant quantum computing.[60] Free anyon Green's functions have been recently used to study correlation functions of anyon interferometry.[61]

This paper is organized as follows: In Sec. II we discuss the particle-vortex system and its so(2,1) dynamical algebra and in Sec. III we use it to obtain its Green's function algebraically. From this Green's function we obtain the wave functions and find a continuous energy spectrum. In Sec. IV, we discuss the two anyon problem on a plane within a harmonic well and obtain its Green's function using the above mentioned algebraic method related to the SO(2,1) Lie group. From this Green's function we obtain the corresponding wave functions and the discrete energy spectrum. Then, in Sec. V, we obtain the Green's function for the problem of two anyons without any regulator from the results of the previous section. We also show that this problem is equivalent to the particle-vortex system, if one identifies the quantized flux of the particle-vortex with the anyon statistical parameter. Finally, in Sec. VI we obtain exactly the Green's function for two anyons in a uniform magnetic field and the corresponding wave functions and the discrete energy spectrum. In Sec. VII we present our conclusions.

II. THE PARTICLE-VORTEX SYSTEM

Let us start the discussion with the particle-magnetic vortex which is defined to be a two-dimensional system characterized by the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t}=H\Psi. \tag{1}$$

The Hamiltonian of interest is given by

$$H=\frac{1}{2M}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 \tag{2}$$

with an externally prescribed vector potential

$$\vec{A}=\frac{\Phi}{2\pi r^2}\mathbf{e}_3\wedge\vec{r}, \tag{3}$$

where $\mathbf{e}_3$ is a constant unit vector perpendicular to the plane in which $\vec{r}$ lies.

The vector potential gives rise to a magnetic field

$$B=\nabla\wedge\vec{A}=\Phi\delta^2(\vec{r}) \tag{4}$$

with flux $\Phi=\int B(\vec{r})d^2r$.

A simple example is given by the motion of a charged particle around a magnetic flux line when the force motion parallel to the flux line is ignored. If one solves the two-dimensional problem one may apply a boost along the direction of the flux line and get the description of the three-dimensional system. The experimental setup was considered in the Bohm–Aharonov effect.[36]

Clearly, the system is invariant under two-dimensional rotations whose generator is given by the conserved angular momentum

$$J=\vec{r}\wedge\vec{p}, \tag{5}$$

where $\vec{p}$ is the canonical momentum and J generates the O(2) group of rotations in a plane. Also, since H does not have an explicit time dependence it is a constant of motion. In principle we expect to have two more constants of motion. In an interesting paper Jackiw[43] constructed them in explicit form as

$$D = tH - \frac{1}{4}(\vec{r}\cdot\vec{p} + \vec{p}\cdot\vec{r}), \tag{6}$$

$$K = -t^2H + 2tD + \frac{Mr^2}{2}, \tag{7}$$

where the fact that $\vec{r}\cdot\vec{A}=0$ in Eq. (6) was used.

It may be noted that D and K are generators of scale and conformal transformations which change the Lagrangian by a total time derivative. One can verify that

$$[H,D] = -i\hbar H, \tag{8}$$

$$[D,K] = -i\hbar K, \tag{9}$$

$$[K,H] = +2i\hbar D, \tag{10}$$

which are the commutation relations of the generators of the algebra associated with the group SO(2,1).

Since J commutes with H, D, and K the symmetry group of the system is the direct product $\mathrm{SO}(2)\times\mathrm{SO}(2,1)$. In the following we consider the construction of the Green's function for the particle vortex system by making use of the BCH formulas for the exponentials of the generators of the algebra of SO(2,1) group. Since we separate the time variable we only need the form of the generators at $t=0$.

The Green's function associated with the particle-vortex system satisfies the equation

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)G(\vec{r},t;\vec{r}',t') = -\delta(\vec{r}-\vec{r}')\delta(t-t'). \tag{11}$$

Since H is time independent one may write

$$G(\vec{r},t;\vec{r}',t') = \frac{1}{2\pi}\int dE G_E(\vec{r},\vec{r}')e^{-iE(t-t')/\hbar} \tag{12}$$

and get

$$(-H+E)G_E(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}'). \tag{13}$$

Then, using the Schwinger[1] representation for the inverse of an operator one can write the Green's function as

$$G_E(\vec{r},\vec{r}') = \frac{i}{\hbar}\int_0^\infty ds e^{i(E-H+i\epsilon)s/\hbar}\delta(\vec{r}-\vec{r}'), \tag{14}$$

where s is usually known as the Schwinger's proper time and $\epsilon>0$ is included to assure the convergence of the above integral. Let us now calculate explicitly this Green's function algebraically.

III. GREEN'S FUNCTION FOR THE PARTICLE-VORTEX SYSTEM

Since H is invariant under rotations we may use the result

$$\delta(\vec{r}-\vec{r}') = \frac{1}{r}\delta(r-r')\delta(\phi-\phi'), \tag{15}$$

where

$$\delta(\phi-\phi')=\frac{1}{2\pi}\sum_m e^{im(\phi-\phi')}, \tag{16}$$

with integer m. Thus if we write

$$G_E(\vec{r},\vec{r}')=\frac{1}{2\pi}\sum_m e^{im(\phi-\phi')}G_{Em}(r,r') \tag{17}$$

then the one-dimensional Green's function is

$$G_{Em}(r,r')=\frac{i}{\hbar r'}\int_0^\infty e^{i(E-H_m)s/\hbar}\delta(r-r')ds, \tag{18}$$

where

$$H_m=-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{(m-\nu)^2}{r^2}\right) \tag{19}$$

is the radial Hamiltonian dependent on the integer angular momentum quantum number m and ν is the quantized flux

$$\nu=\frac{e\Phi}{2\pi\hbar c}. \tag{20}$$

In the following we use the set of differential operators given by:

$$T_1=\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{(m-\nu)^2}{r^2}, \tag{21}$$

$$T_2=-\frac{i}{2}\left(r\frac{\partial}{\partial r}+1\right), \tag{22}$$

$$T_3=-\frac{1}{8}r^2, \tag{23}$$

which can be easily related to the ones defined in the previous section. These operators satisfy the so(2,1) Lie algebra

$$[T_1,T_2]=-iT_1, \tag{24}$$

$$[T_2,T_3]=-iT_3, \tag{25}$$

$$[T_3,T_1]=+iT_2, \tag{26}$$

as well as the operators H, K, and D. Next we note the following representation for the delta function:

$$\delta(r-r')=\frac{M}{4\pi i r'^{\delta-1}}\int_{-i\infty}^{i\infty} e^{(1/4)qM(r^2-r'^2)}r^\delta dq, \tag{27}$$

where $r, r'\geqslant 0$, and the arbitrary parameter δ will be fixed later. Thus the one-dimensional Green's function can be written as

$$G_{Em}(r,r') = \frac{M}{4\pi\hbar\, r'^{\delta}} \int_0^{\infty} e^{iEs/\hbar} ds \int_{-i\infty}^{i\infty} e^{-(qM/4)r'^2} e^{(is\hbar/2M)T_1} e^{-2MqT_3} r^{\delta} dq. \tag{28}$$

Further, one can show that the following identity holds:

$$e^{(is\hbar/2M)T_1} e^{-2MqT_3} = e^{-i\zeta_3 T_3} e^{-i\zeta_2 T_2} e^{-i\zeta_1 T_1}, \tag{29}$$

where

$$e^{\zeta_2/2} = \frac{s\hbar}{2i}\left(q + \frac{2i}{s\hbar}\right) \tag{30}$$

$$-i\zeta_3 = -2M\left(\frac{2i}{s\hbar} + \frac{4}{(s\hbar)^2\left(q + \frac{2i}{s\hbar}\right)}\right). \tag{31}$$

The proof of the above relations is given, e.g., in Refs. 16 and 27 where ζ_1 is also calculated. Note however that the value of ζ_1 is not needed here since we will choose δ such that

$$T_1 r^{\delta} = 0, \tag{32}$$

which implies

$$\delta = |m - \nu|. \tag{33}$$

In fact the condition (32) also allows $\delta = -|m-\nu|$, but these negative values lead to unphysical solutions as will be seen in the following. Next, it is easy to verify that

$$e^{-ibT_2} f(r) = e^{-b/2} f(re^{-b/2}) \tag{34}$$

so that

$$G_{Em}(r,r') = \frac{Mr^{\delta}}{4\pi\hbar\, r'^{\delta}} \int_0^{\infty} ds \exp\left\{\frac{iEs}{\hbar}\right\} \exp\left\{\frac{iM}{2s\hbar} r^2\right\} \int_{-i\infty}^{i\infty} dq \exp\left\{-\frac{qM}{4} r'^2\right\} \times \exp\left\{\frac{Mr^2}{(s\hbar)^2\left(q + \frac{2i}{s\hbar}\right)}\right\} \left[\frac{s\hbar}{2i}\left(q + \frac{2i}{s\hbar}\right)\right]^{-(1+\delta)}. \tag{35}$$

Expanding the exponential as a power series and doing the integrations by repeatedly using the result

$$\frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dq \frac{\exp\left\{-\frac{qM}{4} r'^2\right\}}{\left(q + \frac{2i}{s\hbar}\right)^{\xi+1}} = \frac{\exp\left\{\frac{iM}{2s\hbar} r'^2\right\} \left(-\frac{M}{4} r'^2\right)^{\xi}}{\Gamma(\xi+1)}, \tag{36}$$

we find that the one-dimensional Green's function can be written as

$$G_{Em}(r,r') = -\frac{M}{\hbar} \int_0^{\infty} \frac{ds}{s} e^{iEs/\hbar} \exp\left\{\frac{iM}{2s\hbar}(r^2 + r'^2)\right\} e^{-(i\pi/2)\delta} J_{\delta}\left(\frac{Mrr'}{s\hbar}\right), \tag{37}$$

where we have used the definition of Bessel functions

$$J_{\delta}(z) = \left(\frac{z}{2}\right)^{\delta} \sum_n \frac{(-z^2/4)^n}{n!\,\Gamma(n+\delta+1)}. \tag{38}$$

Next using the result[62]

$$\int_0^\infty dz e^{-\xi z} J_\delta(2\beta\sqrt{z}) J_\delta(2\gamma\sqrt{z}) = \frac{1}{\xi} e^{-(1/\xi)(\beta^2+\gamma^2)} I_\delta\left(\frac{2\beta\gamma}{\xi}\right) \tag{39}$$

valid for $\Re(\delta) > -1$ and identifying $I_\delta(z) = i^{-\delta} J_\delta(iz)$ we get

$$G_{Em}(r,r') = \int_0^\infty dE' \frac{\mathcal{U}^m_{E'}(r)\mathcal{U}^m_{E'}(r')}{E - E' + i\epsilon}, \tag{40}$$

where

$$\mathcal{U}^m_{E'}(r) = \frac{\sqrt{M}}{\hbar} J_\delta\left(\sqrt{2ME'}\frac{r}{\hbar}\right). \tag{41}$$

Substituting this result into Eq. (17) we get

$$G_E(\vec{r},\vec{r}') = \int_0^\infty dE' \frac{1}{E - E' + i\epsilon} \sum_m \frac{e^{im(\phi-\phi')}}{2\pi} \mathcal{U}^m_{E'}(r)\mathcal{U}^m_{E'}(r'). \tag{42}$$

Note that Eq. (40) is the spectral representation of the one-dimensional Green's function (18), $\mathcal{U}^m_{E'}(r)$ are the corresponding one dimensional wave functions and the energy spectrum is continuous for energy $E > 0$ and angular momentum m, in agreement with Ref. 43. Note that this should be the case since the Hamiltonian (19) corresponds to a particle in a nonconfining potential of a centrifugal barrier $1/r^2$.

It is interesting to note that the above calculation leading to the wave functions (41) is rather different from Jackiw's[43] group theoretical discussion. To trace the main differences first we mention that he considered the operators

$$R = \frac{1}{2}\left(\frac{1}{a}K + aH\right), \tag{43}$$

$$S = \frac{1}{2}\left(\frac{1}{a}K - aH\right), \tag{44}$$

where a is a fixed parameter with time dimensionality. The operators R, S, and D also close the so(2,1) Lie algebra, analogous to Eqs. (8)–(10). Then, he calculated the eigenstates of R. Note that for any fixed time, as for instance $t=0$, the operator

$$R = \frac{1}{2}\left(\frac{1}{a}\frac{Mr^2}{2} + aH\right) \tag{45}$$

has a discrete spectrum because of the presence of the bounding potential r^2. Next, using further group theoretical methods he expressed the continuous eigenstates of H in terms of the eigenstates of R. This procedure can be understood as an infrared cutoff regularization of the continuous eigenstates of H. Our results are in agreement with those present by Jackiw.[43] In the next section we are going to discuss the problem of anyons in a harmonic well which, as we will discuss, can be interpreted as the particle-vortex problem with a harmonic regulator.

Before we move to the next section, let us comment that the Green's function (42) can also be written in terms of associated Laguerre's polynomials $L^\xi_n(x)$. Using the relation

$$J_\xi(2\sqrt{xz}) = e^{-z}(xz)^{\xi/2}\sum_{n=0}^{\infty}\frac{z^n L_n^\xi(x)}{\Gamma(n+\xi+1)} \tag{46}$$

valid for $\xi > -1$. Identifying $x = Mr^2/\hbar$, $z = E/2\hbar$ we get

$$\mathcal{U}_{E'}^m(r) = \frac{\sqrt{M}}{\hbar}e^{-E'/2\hbar}\left(\frac{E'Mr^2}{2\hbar^2}\right)^{\delta/2}\sum_{n=0}^{\infty}\left(\frac{E'}{2\hbar}\right)^n\frac{L_n^\delta\left(\frac{Mr^2}{\hbar}\right)}{\Gamma(n+\delta+1)}, \tag{47}$$

so that

$$G_E(\vec{r},\vec{r}') = \frac{M}{2\pi\hbar}\int_0^\infty \frac{dE'e^{-E'/\hbar}}{E-E'+i\epsilon}\sum_m e^{im(\phi-\phi')}\left(\frac{E'Mrr'}{2\hbar^2}\right)^\delta \times \sum_{n=0}^{\infty}\left(\frac{E'}{2\hbar}\right)^n\frac{L_n^\delta\left(\frac{Mr^2}{\hbar}\right)}{\Gamma(n+\delta+1)}\sum_{\ell=0}^{\infty}\left(\frac{E'}{2\hbar}\right)^\ell\frac{L_\ell^\delta\left(\frac{Mr'^2}{\hbar}\right)}{\Gamma(\ell+\delta+1)}. \tag{48}$$

Further, one can also perform the integration in E' so that this Green's function can be rewritten as

$$G_E(\vec{r},\vec{r}') = -\frac{M}{2\pi\hbar}e^{-E/\hbar}\sum_m e^{im(\phi-\phi')}\left(\frac{Mrr'}{\hbar}\right)^\delta\sum_{n=0}^{\infty}\sum_{\ell=0}^{\infty}L_n^\delta\left(\frac{Mr^2}{\hbar}\right)L_\ell^\delta\left(\frac{Mr'^2}{\hbar}\right) \times (-E)^{n+\ell+\delta}\frac{\Gamma(n+\ell+\delta+1)}{\Gamma(n+\delta+1)\Gamma(\ell+\delta+1)}\Gamma\left(-n-\ell-\delta,-\frac{E}{\hbar}\right), \tag{49}$$

where $\Gamma(a,x)$ is the incomplete gamma function.

IV. TWO ANYONS IN A HARMONIC WELL

Anyons are quasiparticles that obey fractional statistics, i.e., an intermediate statistics between the Bose–Einstein and Fermi–Dirac cases.[37–41] The boson and fermion wave functions differ by the interchange of two or more identical particles. The bosonic wave function is completely symmetric while the fermionic is completely antisymmetric. Then, the two-particle wave functions before and after the interchange of two particles are related by

$$\psi(\vec{r}_2,\vec{r}_1) = e^{i\theta}\psi(\vec{r}_1,\vec{r}_2), \tag{50}$$

where θ determines the statistics of the system. If $\theta = 0$ (modulo 2π) the system obeys Bose–Einstein (BE) statistics and if $\theta = \pi$ (modulo 2π) the system obeys Fermi–Dirac (FD) statistics. In three spatial dimensions these are the only allowed possibilities. However, if the particles are restricted to live in two spatial dimensions θ can assume any real value interpolating the BE and FD statistics.

Considering the path integral formulation of quantum mechanics, the transition amplitude between two states is proportional to $\exp\{iS/\hbar\}$, where S is the classical action. Then, to reproduce the above behavior we consider that a two anyon system (any θ) can be represented by a conventional Lagrangean L plus a topological term[57]

$$L \to L_\theta = L + \frac{\theta}{\pi}\dot{\phi}, \tag{51}$$

where ϕ is the relative angle between $\vec{r}_1$ and $\vec{r}_2$. This way, turning around one particle in respect to the other by an angle $\phi = \pi$ we obtain a phase

$$\exp\left\{\frac{i\theta}{\pi}\int_0^{\pi} d\phi\right\} = \exp\{i\alpha\pi\}, \tag{52}$$

where

$$\alpha = \frac{\theta}{\pi}, \tag{53}$$

is the statistical parameter of the two anyon system.

Here, in this section we consider a two anyon system characterized by the coordinates $\vec{r}_1$ and $\vec{r}_2$ moving on a plane subjected to a harmonic regulator $V(\vec{r}_1,\vec{r}_2)=\frac{1}{2}m_0\omega^2(r_1^2+r_2^2)$, where m_0 is the mass of each anyon. The use of a potential as a regulator is not mandatory but it is usual in the literature[41] since it simplifies the discussion once the spectrum becomes discrete. An alternative regulator procedure is to use boundary conditions as considered in Arovas *et al.*[40] to calculate the second virial coefficient of the two anyon system. Nonetheless, it is also possible to avoid the use of any regulator and consider the case of "free" anyons, as will be discussed in the next section. This situation is in fact related to the case of the magnetic vortex discussed in the previous section. The connection of these cases will be discussed in the next section.

Introducing the center of mass and relative coordinates $\vec{R}=\vec{r}_1+\vec{r}_2$, and $\vec{r}=\vec{r}_1-\vec{r}_2=(r,\phi)$, respectively, the Lagrangean for the two anyon system with a harmonic regulator can be written as

$$L_\alpha = \frac{1}{2}M\dot{R}^2 + \frac{1}{2}M\omega^2R^2 + \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\phi}^2 + \omega^2r^2) + \alpha\hbar\,\dot{\phi}, \tag{54}$$

where $M=2m_0$, $\mu=m_0/2$. The motion of the center of mass is described by the first part of the Lagrangean corresponding to a two-dimensional harmonic motion that does not contribute to the statistical behavior. From now on we will only consider the relative motion of the two anyon system. The canonical momenta are then given by

$$p_\phi = \frac{\partial L}{\partial\dot{\phi}} = \mu r^2\dot{\phi} + \alpha\hbar\,; \quad p_r = \mu\dot{r}, \tag{55}$$

and the Hamiltonian of the relative motion of the two particles is

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial\phi} - i\alpha\right)^2\right] + \frac{1}{2}\mu\omega^2r^2. \tag{56}$$

Here we are going to construct the Green's function for this problem using an algebraic method associated with the dynamical SO(2,1) Lie group.[16,27] The technique used here is a generalization of the one presented in the previous section, and we will recover that results in the following sections. The Green's functions for this problem satisfies the equation

$$(H-E)G_E(r,r',\phi,\phi') = \frac{\delta(r-r')}{r}\delta(\phi-\phi'), \tag{57}$$

where $G_E(\vec{r},\vec{r}')\equiv G_E(r,r',\phi,\phi')$. Decomposing this Green's function as we did in the previous section, Eq. (17), one can obtain the radial Hamiltonian H_r for this problem and we write the resolvent operator as

$$\Lambda_r = (H_r - E) = g_0 + g_1T_1(r) + g_3T_3(r), \tag{58}$$

where the operators T_i are given by Eqs. (21)–(23) which satisfy the so(2,1) Lie algebra Eqs. (24)–(26) and the parameters g_i are given by

$$g_0 = -E, \quad g_1 = -\frac{\hbar^2}{2\mu}, \quad g_3 = -4\mu\omega^2. \tag{59}$$

Note that $H_r = H_m + \frac{1}{2}\mu\omega^2 r^2$, with H_m given by Eq. (19), if we further identify α with ν. Using the Schwinger[1] representation as before we find

$$G_E(r,r') = i\int_0^\infty ds\, \exp[-is(g_0 + g_1 T_1(r) + g_3 T_3(r) - i\epsilon)]\frac{\delta(r-r')}{r}. \tag{60}$$

In addition to Eq. (29), here we need another BCH formula

$$\exp\left\{-i\frac{s}{\hbar}(g_1 T_1 + g_3 T_3)\right\} = \exp\{-iaT_3\}\exp\{-ibT_2\}\exp\{-icT_1\}, \tag{61}$$

where the parameters a, b, c, and k are given by

$$a = 2\frac{k}{g_1}\tan k\frac{s}{\hbar}, \quad b = 2\ln\left(\cos k\,\frac{s}{\hbar}\right), \quad c = \frac{g_1}{k}\tan k\,\frac{s}{\hbar}, \quad k = \sqrt{\frac{g_1 g_3}{2}}. \tag{62}$$

Following Ref. 16 we find

$$\exp\left\{-i\frac{s}{\hbar}(g_1 T_1 + g_3 T_3)\right\}\frac{\delta(r-r')}{r} = -\frac{ik\exp\{2i\pi\delta\}}{2g_1\sin(ks/\hbar)}r'\exp\left\{-\frac{ik}{4g_1}(r'^2 + r^2)\cot k\,\frac{s}{\hbar}\right\} \times I_\delta\left(-\frac{kr'r}{2ig_1\sin(ks/\hbar)}\right) \tag{63}$$

with δ given by

$$\delta = |m-\alpha|. \tag{64}$$

As before, $\delta = -|m-\alpha|$ would imply non-normalizable solutions and we will not consider this case.

Then we obtain the Green's function as

$$G_E(r,r') = -\frac{i}{\hbar}\int_0^\infty ds\,\exp\left\{-i\frac{s}{\hbar}(g_0 - i\epsilon)\right\}\frac{ik\exp(2i\pi\delta)}{2g_1\sin(ks/\hbar)}(rr')^{(1/2)} \times \exp\left\{-\frac{ik}{4g_1}(r^2 + r'^2)\cot(ks/\hbar)\right\}I_\delta\left[\frac{-krr'}{2ig_1\sin(ks/\hbar)}\right], \tag{65}$$

where I_δ is the modified Bessel function of order δ. This Bessel function is related to the associated Laguerre's polynomials L_n^δ by

$$I_\delta\left(2\frac{\sqrt{y'yz}}{1-z}\right)\exp\left\{-z\frac{y'+y}{1-z}\right\} = (y'yz)^{\delta/2}(1-z)\sum_{n=0}^{+\infty}\frac{n!}{\Gamma(n+\delta+1)}L_n^\delta(y)L_n^\delta(y')z^n. \tag{66}$$

Then integrating over the proper time s one finds for the Green's function of two anyons on a plane with a harmonic regulator

$$G_E(r,r',\phi,\phi') = -\frac{1}{\pi}\sum_{m=-\infty}^{+\infty}e^{2\pi i|m-\alpha|}\left(\frac{\mu\omega}{\hbar}\right)^{1+|m-\alpha|}(rr')^{|m-\alpha|} \times e^{im(\phi-\phi')}\sum_{n=0}^{\infty}\frac{n!\,L_n^{|m-\alpha|}\left(\frac{\mu\omega}{\hbar}r^2\right)L_n^{|m-\alpha|}\left(\frac{\mu\omega}{\hbar}(r')^2\right)}{\Gamma(n+|m-\alpha|+1)} \times \exp\left\{-\frac{\mu\omega}{2\hbar}(r^2+r'^2)\right\}\frac{1}{E-\hbar\,\omega(2n+|m-\alpha|+1)}. \tag{67}$$

If one writes the spectral representation for the Green's function as (Note that the obtained Green's function is real up to a complex phase $i\pi|m-\alpha|$. Then we are using a nonstandard definition for the spectral decomposition to preserve this nontrivial phase which is related to the statistics of the system.)

$$G(r,r',\phi,\phi') = \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} \frac{\psi_{n,m}(r,\phi)\psi_{n,m}(r',\phi')}{E-E_{n,m}}, \tag{68}$$

so that the wave functions are given by its residues

$$\psi^{\alpha}_{n,m}(r,\phi) = \frac{i}{\sqrt{\pi}} e^{\pi i|m-\alpha|} e^{im\phi} \left(\frac{\mu\omega}{\hbar}\right)^{(1/2)(1+|m-\alpha|)} r^{|m-\alpha|} \frac{\sqrt{n!} L_n^{|m-\alpha|}\left(\frac{\mu\omega}{\hbar} r^2\right)}{\sqrt{\Gamma(n+|m-\alpha|+1)}} \exp\left\{-\frac{\mu\omega}{2\hbar} r^2\right\} \tag{69}$$

and the poles correspond to the energy spectrum

$$E^{\alpha}_{nm} = \hbar\,\omega(2n+|m-\alpha|+1), \tag{70}$$

where $n=0,1,2,3,\ldots$ is the radial quantum number. This spectrum corresponds to that of a two-dimensional harmonic oscillator with angular momentum $|m-\alpha|$.

If we had started with particles identified with bosons then the allowed angular momentum values would be $m=0,\pm 2,\pm 4,\ldots$. Had we started with fermions then the values of the angular momentum should be $m=\pm 1,\pm 3,\pm 5,\ldots$. The quantized energy levels are periodic functions of the statistical parameter α with period 2, although the energy of a single state with quantum numbers (n,m) is not periodic. These conclusions are in agreement with Refs. 40 and 41 where the second virial coefficient for anyons has been calculated without a harmonic regulator, but considering boundary conditions on the wave functions.

V. TWO "FREE" ANYONS

In this section we are going to obtain the Green's function for two anyons as discussed above but without any regulator. Here, the relative motion Hamiltonian after separating the angular variable ϕ is

$$H = -\frac{\hbar^2}{2M}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{r} - \frac{1}{r^2}(m-\alpha)^2\right), \tag{71}$$

where $m=0,1,2,\ldots$ are again the eigenvalues of the angular momentum and $\alpha=\theta/\pi$. The so(2,1) Lie algebra here is analogous to the one discussed in the previous section with generators defined by Eqs. (21)–(23). Here the resolvent operator is simply

$$(H-E) = g_0 + g_1 T_1(r), \tag{72}$$

with g_0 and g_1 given by Eq. (59) (here $g_3=0$), so that the radial Green's function can be written as

$$G(r,r') = \frac{i}{\hbar}\int_0^{\infty} ds \exp\left\{-i\frac{s}{\hbar}(g_0 - i\epsilon)\right\} \exp\left\{-i\frac{s}{\hbar} g_1 T_1\right\} \frac{1}{r}\delta(r-r'). \tag{73}$$

It has been shown in Ref. 16 that

$$\exp\{icT_1\}\frac{\delta(r-r')}{r} = i(-i)^{|m-\alpha|}\frac{M}{s\hbar}\exp\left\{\frac{iM}{2s\hbar}(r^2-r'^2)\right\} J_{|m-\alpha|}\left(\frac{M}{s\hbar} rr'\right) \tag{74}$$

so that the radial Green's function is given by

$$G(r,r') = -\frac{M}{\hbar}(-i)^{|m-\alpha|}\int_0^\infty \frac{ds}{s}\exp\left\{i\frac{s}{\hbar}(E+i\epsilon)\right\}\exp\left\{\frac{iM}{2s\hbar}(r^2-r'^2)\right\}J_{|m-\alpha|}\left(\frac{M}{s\hbar}rr'\right). \quad (75)$$

Another way to approach the two anyon system without a regulator potential is to consider the two anyon system in the harmonic well, Eq. (56), and take the limit where the regulator vanishes $\omega \to 0$. This limit corresponds to take $k \to 0$ in Eq. (65), so that the above Green's function is reobtained.

This Green's function can be compared with the one obtained for the particle-vortex system, Eq. (37). One can note that they are identical if one identifies the quantized flux ν, Eq. (20), with the anyon statistical parameter α, Eq. (53).

VI. TWO ANYONS IN A UNIFORM MAGNETIC FIELD

The Hamiltonian of the relative motion of two anyons in a uniform and constant magnetic field B is given by[42–48]

$$H = \frac{1}{2\mu}\left(\vec{p} + \frac{1}{2}\mu\omega_c r\hat{\phi} + \frac{\alpha\hbar}{r}\hat{\phi}\right)^2, \quad (76)$$

where $\omega_c = eB/mc$ is the cyclotron frequency, the second term on brackets corresponds to the physical (external) magnetic vector potential $\vec{A} = Br\hat{\phi}/2$ and the third term is the statistical vector potential. This statistical term can be absorbed in the angular part of the kinetical term that contributes to the angular momentum of the particles. The radial part of this Hamiltonian can be written as before as

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{1}{r^2}(m-\alpha)^2\right] - \frac{m\hbar\,\omega_c}{4} + \frac{1}{8}\mu\omega_c^2 r^2. \quad (77)$$

The presence of the magnetic field B implies an r-independent term that contributes to the energy but the form of this Hamiltonian is similar to that of the problem of two anyons in a harmonic well, discussed in Sec. IV. This fact allows the use of the algebraic method as before to calculate the Green's functions. Then the so(2,1) generators that describe the two anyons in a magnetic field are the ones given by Eqs. (21)–(23). The resolvent operator is again given by Eq. (58) with the parameters

$$g_0 = -\left(E + \frac{1}{4}m\hbar\,\omega_c\right), \quad g_1 = -\frac{\hbar^2}{2\mu}, \quad g_3 = -\mu\omega_c^2. \quad (78)$$

Following the algebraic method as in Sec. IV with these parameters we find the Green's function:

$$\begin{aligned} G_E(r,r',\phi,\phi') = -\frac{1}{\pi}\sum_{m=-\infty}^{+\infty} & e^{2\pi i|m-\alpha|}\left(\frac{\mu\omega_c}{2\hbar}\right)^{1+|m-\alpha|}(rr')^{|m-\alpha|}e^{-im(\phi-\phi')} \\ & \times \sum_{n=0}^{\infty}\frac{n!\,L_n^{|m-\alpha|}\left(\frac{\mu\omega_c}{2\hbar}r^2\right)L_n^{|m-\alpha|}\left(\frac{\mu\omega_c}{2\hbar}(r')^2\right)}{\Gamma(n+|m-\alpha|+1)} \\ & \times \exp\left\{-\frac{\mu\omega_c}{4\hbar}(r^2+r'^2)\right\}\frac{1}{E-\frac{\hbar\omega_c}{2}\left(2n+|m-\alpha|+1+\frac{m}{2}\right)}. \end{aligned} \quad (79)$$

From this Green's function we obtain the normalized wave functions

$$\psi_{n,m}^{\alpha}(r,\phi)=\frac{i}{\sqrt{\pi}}e^{i\pi|m-\alpha|}e^{-im\phi}\left(\frac{\mu\omega_c}{2\hbar}\right)^{(1/2)(1+|m-\alpha|)}r^{|m-\alpha|}\frac{\sqrt{n!}L_n^{|m-\alpha|}\left(\frac{\mu\omega_c}{2\hbar}r^2\right)}{\sqrt{\Gamma(n+|m-\alpha|+1)}}\exp\left\{-\frac{\mu\omega_c}{4\hbar}r^2\right\} \tag{80}$$

and the corresponding energy levels

$$E_{nm}^{\alpha}=\frac{\hbar\omega_c}{2}\left(2n+|m-\alpha|+1+\frac{m}{2}\right). \tag{81}$$

These energy levels coincide with the Landau levels if the anyon statistical contribution vanishes ($m=\alpha=0$). In particular, the ground state wave function is obtained when one takes $m=n=0$,

$$\psi_{0,0}^{\alpha}(r)=\frac{i}{\sqrt{\pi}}e^{i\pi\alpha}\left(\frac{\mu\omega_c}{2\hbar}\right)^{(1/2)(1+\alpha)}\frac{r^{\alpha}}{\sqrt{\Gamma(1+\alpha)}}\exp\left\{-\frac{\mu\omega_c}{4\hbar}r^2\right\}. \tag{82}$$

VII. CONCLUSIONS

In this paper we have calculated algebraically the Green's functions for one and two particles confined on a plane, namely the particle-vortex system and a pair of anyons with and without external potentials. The external potentials considered were a harmonic well and a uniform magnetic field. In these problems we have identified the Hamiltonian operator in each case with the generators of the SO(2,1) Lie group satisfying the so(2,1) Lie algebra. From these algebraic properties we obtained all relevant dynamical quantities of each system. This means that these systems are described by the so(2,1) dynamical algebra.

In particular, we calculated the Green's function for particle-vortex system and the Green's function for a pair of free anyons and found that these Green's functions are equivalent, once one identifies the quantized flux ν of the particle-vortex system with the anyon statistical parameter α. These two Green's functions exhibit respectively the phase factors $(-i)^{|m-\nu|}$ and $(-i)^{|m-\alpha|}$ as a commom signature of fractional statistics for both systems.

We obtained also the Green's function for the two anyon system in a harmonic well as an integral representation of Bessel functions, and as a sum of product of Laguerre's generalized polynomials. This sum is recognized as the spectral representation of the Green's function from which we identify the normalized wave functions and energy spectrum.

It is interesting to note that in the particle-vortex discussion presented by Jackiw,[43] he obtained a discrete spectrum of the generator R (our Eq. (45)) of conformal transformations, and them, by a rotation in operators space he obtain the continuous spectrum calculated by standard methods to the particle-vortex system. This discrete spectrum is identical to one obtained for anyons in presence of an harmonic regulator. The eigenfunctions (up to a phase factor) and eigenvalues of this operator, (48) in Ref. 43 are equivalent to those ones we have obtained for the two anyon system in a harmonic well.

Regarding the Green's functions for the two anyon system in a harmonic well and two anyons in a uniform magnetic field both lead to bound states and we see that they are very similar to each other, although they differ in the energy spectrum. Charged anyons orbiting in a uniform magnetic field are equivalent to anyon bound states in the presence of a harmonic well. Note that wave functions (69) and (80), obtained from those Green's functions, are identical if we identify ω with $\omega_c/2$.

In particular the ground state wave function obtained for two charged particles in a magnetic field, Eq. (82), is similar to the two particle wave function used by Laughlin[54] to construct his ansatz for N-particles to describe the quantum Hall effect. In the problem discussed by Laughlin, there is also a Coulombic interaction which in general could not be disregarded. Then, he supposed that this interaction is infinitely short ranged and that the Landau levels energy is dominant

so $\hbar\omega_c \gg e^2/l$, where l is the magnetic length. Since the particles are separated by some finite length, this allows one to build an ansatz for the many particle ground state wave function as a superposition of single particle wave functions

$$\psi_{00}^{\alpha}(r_{p,q}) = e^{i\pi\alpha}\frac{i}{\sqrt{\pi\Gamma(1+\alpha)}}\left(\frac{\mu\omega_c}{2\hbar}\right)^{(1/2)(1+\alpha)}\prod_{p<q} r_{p,q}^{\alpha}\exp\left(-\frac{\mu\omega_c}{4\hbar}\sum_{p<q} r_{p,q}^2\right). \tag{83}$$

This is essentially the Laughlin's ansatz for N-particles.[54] Note that the interchange of particle positions adds a phase to the wave function in agreement with Ref. 57.

Let us now consider the excited states for the two anyon system in a uniform magnetic field. The wave functions (80), or equivalently (69), represent the excited states of this system. If we follow a similar reasoning as the ones that support (83), as discussed in Refs. 49, 50, and 54, we can superpose Eq. (80) to obtain an ansatz for the many particle excited state wave function

$$\psi_{n,m}^{\alpha}(r,\phi) = ie^{i\pi|m-\alpha|}\frac{\sqrt{n!}}{\sqrt{\pi}\sqrt{\Gamma(n+|m-\alpha|+1}}\left(\frac{\mu\omega_c}{2\hbar}\right)^{(1/2)(1+|m-\alpha|)} e^{-im\phi}\prod_{i<j} r_{ij}^{|m-\alpha|}L_n^{|m-\alpha|}\left(\frac{\mu\omega_c}{2\hbar}r_{ij}^2\right)$$
$$\times\exp\left\{-\frac{\mu\omega_c}{4\hbar}\sum_{i<j} r_{ij}^2\right\}. \tag{84}$$

This wave function is formally in agreement with the result for many anyons obtained by Dunne *et al.*[46]

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The Selberg trace formula for Dirac operators

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We examine spectra of Dirac operators on compact hyperbolic surfaces. Particular attention is devoted to symmetry considerations, leading to nontrivial multiplicities of eigenvalues. The relation to spectra of Maaß-Laplace operators is also exploited. Our main result is a Selberg trace formula for Dirac operators on hyperbolic surfaces. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2359578]

I. INTRODUCTION

Trace formulae play a prominent role in spectral geometry and in quantum chaos (see, e.g., Ref. 2). In spectral geometry, they relate spectra of certain (pseudo-) differential operators on manifolds to the geometry of that manifold. The prime example of such a trace formula, the classical Selberg trace formula,[33,19,20] is concerned with the Laplace-Beltrami operator on a hyperbolic manifold, i.e., a Riemannian manifold with constant negative sectional curvatures. This trace formula establishes a connection between the spectrum of the Laplacian and the length spectrum of closed geodesics on the manifold.

In a semiclassical context spectra of semiclassical operators are related to the periodic orbits of an associated Hamiltonian flow. In extensions of this procedure to operators acting on sections in vector bundles over the relevant phase space, it turned out that the Hamiltonian flow does not provide the entire input on the classical side of the trace formula (see, e.g., Ref. 8). In particular, for the Dirac operator on $\mathbb{R}^3$, the corresponding classical dynamics are given in terms of skew-product flows over Hamiltonian flows, with spin precessions as their cocycles. A similar result is found in the case of a trace formula for the Dirac operator on a graph.[7] A microlocal version of a trace formula for Dirac-type operators on compact manifolds was established in Ref. 31. Very recently, in the context of quantum ergodicity, Jakobson and Strohmaier[23] observed that (the square of) a Dirac operator on a compact Riemannian manifold is related to the associated frame flow, which is a geometric analog of the skew-product flows in the semiclassical setting. A previous approach to quantum ergodicity that uses representation-theoretic lifts for vector bundles can be found in Ref. 12.

In this paper, our goal is to investigate spectra of Dirac operators on compact hyperbolic surfaces in a geometric setting. On the way we exploit the well-known relation of the squared Dirac operator to a Laplacian that contains a coupling to a magnetic field (see, e.g., Ref. 28). In particular, we show that spectra of these Maaß-Laplacians, when they correspond to odd weights, possess multiplicities of at least two. This is a consequence of Kramers' degeneracy in the spectrum of the Dirac operator, which follows from quantum mechanical time reversal invariance. We further investigate the relation of the Dirac spectrum to a dynamical system that is associated with the surface in a geometric way. To this end we develop a Selberg trace formula in a classical approach, i.e., via Green's functions and point-pair invariants. This complements previous studies of related questions, which often focus on computations of eta invariants (see, e.g., Ref. 27) and employ a representation theoretic approach to trace formulae as, e.g., summarized in Ref. 11. The geometric side of the trace formula for the Dirac operator is primarily determined by the closed

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geodesics on the surface. In addition, we identify traces of the frame flow of the surface and its lift into the spin structure, which provides suitable phase factors associated with the closed geodesics. These factors are finally responsible for the differences in the eigenvalue distributions of Dirac and Laplace-Beltrami operators, respectively.

The paper is organized as follows: In Sec. II we review the definition of a Dirac operator on a Riemannian manifold and explicitly carry out the constructions in the case of the hyperbolic plane. Section III then is devoted to an identification of spinor bundles over compact hyperbolic surfaces via factors of automorphy. We then investigate symmetries of the Dirac operator on a compact surface and study their influence on the spectrum in Sec. IV. After having introduced point-pair invariants in Sec. V, we calculate traces of Hilbert-Schmidt operators to arrive at the desired trace formula in Sec. VI. Finally, in Sec. VII, we discuss some applications.

II. THE DIRAC OPERATOR

A Dirac operator is a first order, elliptic differential operator acting on sections in a spinor bundle over a Riemannian manifold. For its construction one first needs to supply an orientable, n-dimensional Riemannian manifold $(M,\mathbf{g})$ with a spin structure. To this end, let FM be the $\mathrm{SO}(n)$-principal bundle of oriented orthonormal frames of TM. A $\mathrm{Spin}(n)$-principal bundle Q is called spin structure on M if there exists a principal-bundle morphism $\phi: Q \to FM$ that is equivariant with respect to the two-fold covering $\Lambda: \mathrm{Spin}(n) \to \mathrm{SO}(n)$ (see, e.g., Refs. 15 and 4). Moreover, in even dimensions n the complexified Clifford algebra $\mathfrak{C}_n^c$ is isomorphic to $\mathrm{M}(2^{n/2},\mathbb{C})$, i.e., the algebra of complex $2^{n/2}\times 2^{n/2}$ matrices. The action of $\mathrm{M}(2^{n/2},\mathbb{C})$ on $\mathbb{C}^{2^{n/2}}$ defines the Clifford module Δ_n. As $\mathrm{Spin}(n)$ is contained in $\mathfrak{C}_n^c$, Δ_n is also a module for the spin group. This yields the spin representation $\rho: \mathrm{Spin}(n) \to \mathrm{Aut}(\Delta_n)$, which can be used to associate the spinor bundle $S := Q\times_\rho \Delta_n$ to a given spin structure.

The definition of the Dirac operator D rests on the canonical connection on Q that is given by the lift of the Levi-Civita connection on FM. Denoting the space of smooth sections of S by $C^\infty(S)$, this connection induces a covariant derivative $\boldsymbol{\nabla}^S: C^\infty(S) \to C^\infty(S\otimes T^*M)$. One then defines $D=\mu\circ\iota\circ\nabla^S$, where ι denotes the canonical isomorphism between T^*M and TM induced by the metric $\mathbf{g}$, and μ is the Clifford multiplication of a vector field and a smooth section in S.

The space $C_0^\infty(S)$ of smooth, compactly supported sections in S can be turned into a pre-Hilbert space by introducing the inner product,

$$\langle \Psi,\Phi\rangle_{L^2} := \int_M \langle \Psi(m),\Phi(m)\rangle_{\mathbb{C}^{2^{n/2}}}\, \mathrm{d}\mu(m),$$

where $\mathrm{d}\mu(m)$ denotes the volume form on M. The resulting Hilbert space will be denoted by $L^2(S)$. The Dirac operator D is elliptic and essentially self-adjoint on $C_0^\infty(S)$, thus its spectrum is real. Moreover, on a compact manifold M the spectrum is discrete.

In the sequel we will focus on compact surfaces of constant negative curvature. Their universal covering space is the upper half-plane $\mathbb{H}^2 := \{(x,y)\in\mathbb{R}^2 \,|\, y>0\}$ endowed with the Poincaré metric $\mathbf{g}=y^{-2}(\mathrm{d}x\otimes\mathrm{d}x+\mathrm{d}y\otimes\mathrm{d}y)$ of constant negative Gaussian curvature $K=-1$. The group of orientation-preserving isometries $\mathrm{PSL}(2,\mathbb{R})=\mathrm{SL}(2,\mathbb{R})/\{\pm\mathrm{Id}\}$ acts on $\mathbb{H}^2$ via fractional linear transformations,

$$z \mapsto \gamma z = \frac{az+b}{cz+d},$$

where $\gamma=\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}(2,\mathbb{R})$ is a representative for an element in $\mathrm{PSL}(2,\mathbb{R})$ and $z=x+\mathrm{i}y$ is viewed as a point in $\mathbb{H}^2$. Any compact hyperbolic surface can now be represented as $\Gamma\backslash\mathbb{H}^2$, where $\Gamma\subset\mathrm{PSL}(2,\mathbb{R})$ is a discrete, strictly hyperbolic subgroup (a cocompact Fuchsian group of the first kind).

On the simply connected upper half-plane the relevant bundles are trivial, i.e., $F\mathbb{H}^2 \simeq \mathbb{H}^2 \times \mathrm{SO}(n)$ and $Q \simeq \mathbb{H}^2 \times \mathrm{Spin}(n)$. This allows an immediate construction of the Dirac operator, which is explicitly given as the matrix-valued operator,

$$D = \mathrm{i}\begin{pmatrix} 0 & \mathrm{i}y\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} - \frac{1}{2} \\ -\mathrm{i}y\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} - \frac{1}{2} & 0 \end{pmatrix};$$

see, e.g., also Ref. 28. The operators appearing in the off-diagonals have been introduced by Maaß and have been further investigated by Roelcke (Refs. 25, 29, and 30). In fact, they considered the operators

$$K_k := \mathrm{i}y\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + \frac{k}{2},$$

$$\Lambda_k := \mathrm{i}y\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} + \frac{k}{2}.$$

It is therefore natural to introduce the weighted Dirac operators,

$$D_k := \mathrm{i}\begin{pmatrix} 0 & K_{k-2} \\ -\Lambda_k & 0 \end{pmatrix}, \tag{2.1}$$

which reduce to the Dirac operator for $k=1$. In physical terms the additional parameter k, which from now on will be called a weight, corresponds to a constant magnetic field on the surface. In normalized units the field strength is given by

$$B = \frac{k-1}{2e}. \tag{2.2}$$

On a compact surface the Dirac quantization condition for the magnetic flux implies that k must be an integer. Therefore, from now on we will only consider $k \in \mathbb{Z}$.

The weighted Dirac operator D_k is closely related to the weighted Maaß-Laplacian,

$$\Delta_k = -K_{k-2}\Lambda_k - \frac{k}{2}\left(1 - \frac{k}{2}\right) = y^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \mathrm{i}ky\frac{\partial}{\partial x},$$

since

$$D_k^2 = \begin{pmatrix} -\Delta_k - \frac{k}{2}\left(1 - \frac{k}{2}\right) & 0 \\ 0 & -\Delta_{k-2} - \frac{k}{2}\left(1 - \frac{k}{2}\right) \end{pmatrix}. \tag{2.3}$$

We remark that both the weighted Laplacians and the weighted Dirac operators are elliptic operators, as their principal symbols do not depend on k.

As yet, we have neither specified spaces of sections in spinor bundles S, nor have we introduced Dirac operators on compact surfaces. It turns out that both purposes can be conveniently achieved by identifying suitable automorphic forms. We devote the following section to this task.

III. AUTOMORPHIC FORMS

All relevant bundles over a compact surface $\Gamma\backslash\mathbb{H}^2$ correspond to trivial bundles over $\mathbb{H}^2$ (see Refs. 17 and 18). More specifically, given the canonical projection $p:\mathbb{H}^2 \to \Gamma\backslash\mathbb{H}^2$ and the vector

bundle $\zeta=(E,\Gamma\backslash\mathbb{H}^2,\pi,V)$ over the compact surface, its pullback $p^*(\zeta)$ is trivial, i.e., the total space is isomorphic to $\mathbb{H}^2\times V$. Now any covering translation $\gamma\in\Gamma$ extends to a bundle homomorphism $\tilde{\gamma}$ on $p^*(\zeta)$, and this can be written as

$$\tilde{\gamma}(z,v)=(\gamma z,\sigma(z,\gamma)v), \tag{3.1}$$

where $\sigma:\mathbb{H}^2\times\Gamma\to\mathrm{GL}(V)$.

For our purposes it will be useful to consider the subgroup $\bar{\Gamma}\subset\mathrm{SL}(2,\mathbb{R})$ that corresponds to the Fuchsian group $\Gamma\subset\mathrm{PSL}(2,\mathbb{R})$ via $\Gamma=\bar{\Gamma}/\{\pm\mathrm{Id}\}$. Instead of σ one hence considers a function $j:\mathbb{H}^2\times\bar{\Gamma}\to\mathrm{GL}(V)$, called factor of automorphy. To define the action of $\gamma\in\Gamma$ unambiguously, one therefore requires a suitable character χ of $\bar{\Gamma}$ (multiplier system) depending on the value of $j(z,-\mathrm{Id})$. Based on these observations, sections in ζ can be obtained from global sections in $p^*(\zeta)$: any vector-valued function $\psi:\mathbb{H}^2\to V$ with $\psi(\gamma z)=\chi(\gamma)j(z,\gamma)\psi(z)$, called automorphic form, yields a section in ζ, and vice versa.

Definition 1: Let $\Gamma\subset\mathrm{PSL}(2,\mathbb{R})$ be a strictly hyperbolic Fuchsian group, then a multiplier system of weight k is a unitary character χ of $\bar{\Gamma}$ with $\chi(-\mathrm{Id})=(-1)^k$. A factor of automorphy for the Maaß-Laplacian of weight k is defined by $j_\gamma(z,k):=(cz+d)^{k/2}/(c\bar{z}+d)^{k/2}$ when $\gamma=\begin{pmatrix}a & b\\ c & d\end{pmatrix}$. Then $\psi:\mathbb{H}^2\to\mathbb{C}$ is an automorphic form for the Maaß-Laplacian of weight k, if

$$\psi(\gamma z)=\chi(\gamma)j_\gamma(z,k)\psi(z),\quad \forall\ \gamma\in\bar{\Gamma}.$$

The space of all such automorphic forms is denoted by ${}^L\mathfrak{F}(\Gamma,k,\chi)$. Similarly, ${}^L\mathfrak{C}^l(\Gamma,k,\chi)$ and ${}^L\mathfrak{L}^2(\Gamma,k,\chi)$ are the spaces of differentiable and square-integrable automorphic forms, respectively. In the latter case, integrability is meant with respect to the measure $\mathrm{d}\mu(z)=\mathrm{d}x\,\mathrm{d}y/y^2$ over a fundamental domain $F\subset\mathbb{H}^2$ of Γ.

It is well known that Δ_k acting on a (twice differentiable) automorphic form of weight k yields again an automorphic form of weight k (see Refs. 29, 30, and 19). We denote the space of all eigenforms of $-\Delta_k$ with eigenvalue λ by ${}^L\mathfrak{F}_\lambda(\Gamma,k,\chi)$. In case $k\geq 2$ there exist certain special eigenvalues that are known explicitly,

$$\lambda_j^{(k)}=\frac{k-2j}{2}\left(1-\frac{k-2j}{2}\right),\quad j=0,1,2,\ldots,\left[\frac{k-1}{2}\right], \tag{3.2}$$

where $[x]$ is the integer part of $x\in\mathbb{R}$. For multiplier systems $\chi\neq 1$ the eigenvalue (3.2) has a multiplicity $(g-1)(k-2j-1)$; see Ref. 19; here $g\geq 2$ is the genus of the closed surface $\Gamma\backslash\mathbb{H}^2$.

The relations (2.1) and (2.3) now suggest the following definition of automorphic forms for the weighted Dirac operator.

Definition 2: Let

$$J_\gamma(z,k):=\begin{pmatrix} j_\gamma(z,k) & 0\\ 0 & j_\gamma(z,k-2)\end{pmatrix}.$$

Then we define the space $\mathfrak{F}(\Gamma,k,\chi)$ of automorphic forms for the Dirac operator with weight k to consist of the functions $\Psi:\mathbb{H}^2\to\Delta_2=\mathbb{C}^2$ that transform as

$$\Psi(\gamma z)=\chi(\gamma)J_\gamma(z,k)\Psi(z),\quad \forall\ \gamma\in\bar{\Gamma}. \tag{3.3}$$

The spaces $\mathfrak{C}^l(\Gamma,k,\chi)$, $\mathfrak{L}^2(\Gamma,k,\chi)$ are defined analogously, and $\mathfrak{F}_\rho(\Gamma,k,\chi)$ denotes the eigenspace of $-D_k$ corresponding to the eigenvalue ρ.

In order to demonstrate that the weighted Dirac operator D_k maps a differentiable automorphic form of the type (3.3) to a form of the same type, one has to show that under a covering translation γ the operator D_k behaves as

$$D_k \mapsto J_\gamma(z,k) D_k J_\gamma^{-1}(z,k). \tag{3.4}$$

This can be done in a straightforward calculation. Hence, the automorphic forms (3.3) represent sections in spinor bundles over the surface $\Gamma\backslash\mathbb{H}^2$.

We also note that D_k is essentially self-adjoint on $\mathfrak{C}^1(\Gamma,k,\chi)$. The proof is practically identical to the case of the Dirac operator ($k=1$), which is well-known (see, e.g., Ref. 15 where also Spin^C connections are considered). Thus, we conclude that the spectrum of D_k is real and discrete.

We are now able to establish a connection between the eigenforms of the Laplacian and of the Dirac operator. For this we recall that the spectrum of $-\Delta_k$ is bounded from below by $(k/2)(1-k/2)$.[29]

Proposition 1: Let $\Psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$ *be an eigenform of* $-D_k$ *with eigenvalue* ρ, *and let* $\lambda=\rho^2+(k/2)(1-k/2)$. *Then* $\psi_1 \in {}^L\mathfrak{F}_\lambda(\Gamma,k,\chi)$. *On the other hand, if* $\psi \in {}^L\mathfrak{F}_\lambda(\Gamma,k,\chi)$, *then* $\Psi=\begin{pmatrix}\rho\psi\\ i\Lambda_k\psi\end{pmatrix} \in \mathfrak{F}_\rho(\Gamma,k,\chi)$. *Moreover, if eigenforms of the Dirac operator* ($\rho\neq 0$) *are linearly independent, the same holds for the corresponding eigenforms of the Maaß-Laplacian, and vice versa.*

Proof: As both operators are elliptic, all eigenforms are smooth. The relation between ρ and λ can be obtained by using Eq. (2.3). To establish the desired transformation properties one has to write down the conditions on the components. The rest then follows from Ref. 29. The linear independence can be obtained from some straightforward manipulations using

$$-i\Lambda_k\psi_1 + \rho\psi_2 = 0,$$

which can be solved for ψ_2 if $\rho\neq 0$. □

IV. SYMMETRIES

Apart from the fact that spectra of weighted Dirac operators on compact surfaces are real and discrete, further spectral properties can be concluded from symmetry considerations.

Lemma 1: The weighted Dirac operator possesses a chiral symmetry, i.e., if $\Psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \in \mathfrak{F}_\rho(\Gamma,k,\chi)$, *then* $\begin{pmatrix}\psi_1\\ -\psi_2\end{pmatrix} \in \mathfrak{F}_{-\rho}(\Gamma,k,\chi)$. *Hence the spectrum of* D_k *is symmetric about zero.*

Proof: The proof amounts to a simple calculation that can be performed conveniently by using the relations in Ref. 29 once again. □

The symmetry statement extends to zero modes in that the Atiyah-Singer index theorem (see Refs. 21 and 1) implies that their number is even. From now on we will denote this number by $2N$.

A further symmetry is concerned with quantum mechanical time reversal. For the Dirac operators considered here, this is implemented through the antilinear operator $T:=i\sigma_2 C$ acting on automorphic forms of arbitrary weight, where C denotes complex conjugation and $\sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$ is one of the Pauli matrices. Hence $T^2=-\mathrm{Id}$. Moreover, on the Hilbert space $\mathfrak{L}^2(\Gamma,k,\chi)$ this operator is anti-unitary.

Lemma 2: Let $\Psi \in \mathfrak{F}_\rho(\Gamma,k,\chi)$; *then* $T\Psi \in \mathfrak{F}_\rho(\Gamma,2-k,\bar{\chi})$. *In particular, if* $k=1$ *and the multiplier system* χ *is real valued, every eigenvalue of D has a multiplicity of (at least) two.*

Proof: The first part of this lemma can be checked by straightforward calculations that we omit here. For the second part one merely has to use the fact that T is anti-unitary with $T^2=-\mathrm{Id}$. This immediately yields that the eigenforms Ψ and $T\Psi$ with eigenvalue ρ are linearly independent. □

At this point we add a few remarks.

(i) Above we have always assumed that Γ contains, apart from unity, only hyperbolic elements; hence there are no elements of finite order. Thus one can construct a real-valued multiplier system by simply assigning ± 1 to the generators of Γ and extending this to $\bar{\Gamma}$. If one also allows for elliptic elements this clearly will not work.

(ii) Lemma 2 says that D_k and D_{2-k} possess identical nonvanishing eigenvalues (including multiplicities). According to (2.2), the weights k and $2-k$, up to sign correspond to the same magnetic field strengths. We will therefore restrict subsequent discussions to the case $k \geq 1$.

(iii) In general, quantum systems with half-integer spin share the same behavior under time reversal as in the present case. For the respective quantum Hamiltonians, the multiplicity two of their eigenvalues due to time-reversal symmetry is known as Kramers' degeneracy.[24] Moreover, magnetic fields usually break time-reversal invariance. This is the reason for the special role played by the weight $k=1$.

(iv) In his tenfold-way scheme Zirnbauer classified quantum systems according to their behavior under basic symmetry operations like time-reversal, rotations, and chiral transformations.[36] The resulting symmetry classes are unambiguously linked with Cartan's ten classes of symmetric spaces. In this context the present case, with time-reversal symmetry, $T^2=-\mathrm{Id}$, and chiral symmetry is identified as the type *C*II and is related to the symmetric space $\mathrm{Sp}(p+q)/\mathrm{Sp}(p)\times\mathrm{Sp}(q)$ (of compact type).

(v) Following the conjecture of Bohigas, Giannoni, and Schmit,[6] one expects that, generically, correlations among the eigenvalues of geometric operators on manifolds of negative curvature can be described by random matrix theory. (See, however, exceptions when the Fuchsian group is arithmetic.[5,9]) The relevant random matrix ensemble for the present case is the chiral Gaussian symplectic ensemble (chGSE).

From supersymmetry considerations (see, e.g., Ref. 35) it is known that eigenvalues of the square of a Dirac operator have even multiplicities. We stress that this observation is unrelated to Lemma 2. Rather, this degeneracy stems from chiral symmetry (Lemma 1) combined with the squaring.

However, the degeneracy due to time reversal somewhat unexpectedly extends to the spectrum of D_k for odd weight. To this end we recall that the Maaß operator K_k raises the weight by two, without changing the eigenvalue of an eigenform of the appropriate Maaß-Laplacian.[29,30] It hence maps ${}^L\mathfrak{F}_\lambda(\Gamma,k,\chi)$ to ${}^L\mathfrak{F}_\lambda(\Gamma,k+2,\chi)$. The operator Λ_{k+2} is its formal adjoint from ${}^L\mathfrak{L}^2(\Gamma,k+2,\chi)$ to ${}^L\mathfrak{L}^2(\Gamma,k,\chi)$. As a consequence, up to the special eigenvalues (3.2) the spectrum of $-\Delta_k$ depends only on k mod 2.

Lemma 3: Let Γ *be a strictly hyperbolic group and* χ *a real-valued multiplier system. If the weight k is odd the eigenvalues of the Maaß-Laplacian* Δ_k *have a multiplicity of (at least) two.*

Proof: For odd $k=2m+1$, the multiplicities of the special eigenvalues (3.2) are known to be $(g-1)2(m-j)$; see Ref. 19 and after Eq. (3.2). In all other cases the statement follows immediately from Proposition 1 and Lemma 2. □

Apart from the special eigenvalues, a twofold degeneracy of the eigenvalues can also be obtained in a constructive way. To this end, one first lowers the weight from $k=2m+1$, $m \in \mathbb{N}_0$, to one by successive applications of operators Λ_l, then applies complex conjugation (i.e., time reversal for spin zero), and finally raises the weight back to $k=2m+1$. Altogether, one thus applies the antilinear operator

$$ {}^L S_{2m+1} := C\Lambda_{-2m+1}\Lambda_{-2m+3}\ldots\Lambda_{2m+1}. \tag{4.1}$$

Now some straightforward calculations show that this way an eigenform ψ is mapped to a linearly independent eigenform $\phi={}^L S_{2m+1}\psi$ of the same weight and with the same eigenvalue. In particular, ϕ may only vanish when its eigenvalue is of the special type (3.2).

We stress that this argument fails if k is even. In the case $k=0$ it is easy to see that if $\psi \in {}^L\mathfrak{F}_\rho(\Gamma,0,\chi)$, then $C\psi \in {}^L\mathfrak{F}_\rho(\Gamma,0,\chi)$, as long as χ is real. But it is well known that for $k=0$ the eigenforms can be chosen to be real valued, so ψ and $C\psi$ are not linearly independent.

Of course, according to Proposition 1, the degeneracy in the spectra of Maaß-Laplacians implies a corresponding degeneracy in the spectra of the Dirac operators D_k. Except for the eigenvalues that derive from the special eigenvalues (3.2) of the associated Maaß-Laplacian, one can again devise a constructive approach that reveals more clearly that the degeneracy is a consequence of a "generalized time reversal symmetry." To this end we introduce the operator

$$A_k^\dagger := \begin{pmatrix} \rho' K_k & 0 \\ \mathrm{i}k & \rho K_{k-2} \end{pmatrix}.$$

This maps $\mathfrak{F}_\rho(\Gamma,k,\chi)$ into $\mathfrak{F}_{\rho'}(\Gamma,k+2,\chi)$, where ρ' is determined by $\rho^2+k=\rho'^2$ and $\mathrm{sgn}(\rho')=\mathrm{sgn}(\rho)$. From Ref. 29, Satz 5.3 one can deduce that $A_k^\dagger$ indeed is an isomorphism between $\mathfrak{F}_\rho(\Gamma,k,\chi)$ and $\mathfrak{F}_{\rho'}(\Gamma,k+2,\chi)$ if $\rho\neq 0$. Its formal adjoint reads as

$$A_{k+2} := -\begin{pmatrix} \rho' \Lambda_{k+2} & \mathrm{i}k \\ 0 & \rho \Lambda_k \end{pmatrix}.$$

The analog to the operator (4.1) now is

$$S_{2m+1} := B_{2m-1}^\dagger \ldots B_1^\dagger T C_3 \ldots C_{2m+1},$$

where $B_k^\dagger := (1/\rho)A_k^\dagger$ and $C_k=(1/\rho')\mathrm{A}_k$. A direct calculation shows that S_{2m+1} does not depend on ρ.

Proposition 2: Let $k=2m+1$ and assume that the multiplier system χ is real valued. Then the eigenvalues of the weighted Dirac operator D_{2m+1} occur with multiplicities of at least two. Moreover,

$$S_{2m+1} = T\begin{pmatrix} \Lambda_{-2m+3}\Lambda_{-2m+5}\cdots\Lambda_{2m+1} & 0 \\ 0 & \Lambda_{-2m+1}\Lambda_{-2m+3}\cdots\Lambda_{2m-1} \end{pmatrix}$$

is identical on all spaces $\mathfrak{F}_\rho(\Gamma,2m+1,\chi)$ of eigenforms, and can therefore be extended to all of $\mathfrak{C}^\infty(\Gamma,2m+1,\chi)$. Then $\Psi\in\mathfrak{F}_\rho(\Gamma,2m+1,\chi)$ implies $\Phi := S_{2m+1}\Psi \in \mathfrak{F}_\rho(\Gamma,2m+1,\chi)$ and $\langle\Phi,\Psi\rangle_{L^2}=0$. For $m>0$ the form Φ vanishes identically iff ρ is related to one of the special eigenvalues (3.2) via $\lambda_j^{(k)}=\rho^2+(k/2)(1-k/2)$.

Proof: The statement about the multiplicities of eigenvalues is implied by Proposition 1 and Lemma 3. The conclusions $\Phi\in\mathfrak{F}_\rho(\Gamma,k,\chi)$ and $\langle\Phi,\Psi\rangle_{L^2}=0$ follow directly from the preceding considerations. One must only take care of the possibility that Φ may vanish. But evaluating $\|\Phi\|_{L^2}$ shows that this norm is zero, iff $\lambda=\rho^2+(k/2)(1-k/2)$ is of the form (3.2). □

V. POINT-PAIR INVARIANTS

From the case of the Laplacian it is well known that setting up a Selberg trace formula amounts to calculating traces of Hilbert-Schmidt operators L that commute with the Laplacian.[33,19,20] The kernels of such operators can be obtained from suitable Poincaré series over so-called point-pair invariants, whose construction will be briefly outlined in this section.

We first introduce two matrix-valued functions on the upper half-plane, which help to study transformation properties under fractional linear transformations,

$$A(z',z) := \begin{pmatrix} \dfrac{(z-\bar{z}')^{1/2}}{(z'-z)^{1/2}} & 0 \\ 0 & \dfrac{(z'-\bar{z})^{1/2}}{(\bar{z}-\bar{z}')^{1/2}} \end{pmatrix},$$

$$B(z',z) := \begin{pmatrix} \dfrac{(z'-z)^{1/2}}{(z'-\bar{z})^{1/2}} & 0 \\ 0 & \dfrac{(\bar{z}-\bar{z}')^{1/2}}{(z-\bar{z}')^{1/2}} \end{pmatrix}.$$

Definition 3: Let $\Phi=\begin{pmatrix}\Phi_1 & \Phi_2 \\ \Phi_3 & \Phi_4\end{pmatrix}:[1,\infty)\to\mathbb{R}^{2\times 2}$ be continuous. Assume, moreover, that $\Phi_2=\Phi_3$ and that there exists a constant C_ϵ such that each component satisfies

$$|\Phi_i(\sigma)| \leq C_\epsilon \sigma^{-1-\epsilon}, \tag{5.1}$$

for some $\epsilon > 0$. Then we call

$$K(z',z) = -\mathrm{i}A(z',z)\Phi\left(\frac{1}{2}(\cosh(d(z',z)+1))\right)B(z',z),$$

where $d(z',z)$ denotes the hyperbolic distance of two points $z,z' \in \mathbb{H}^2$, a point-pair invariant.

Applying any transformation $\gamma \in \mathrm{SL}(2,\mathbb{R})$ yields

$$K(\gamma z', \gamma z) = J_\gamma(z',1)K(z',z)J_\gamma^{-1}(z,1).$$

The restrictions on the components of Φ assure that K is Hermitian, i.e., $K(z',z)=K^\dagger(z,z')$. In order to proceed we need a technical lemma, which can be found in Ref. 19.

Lemma 4: Let $f:[1,\infty)\to\mathbb{C}$ *and* $\epsilon>0$. *Moreover, assume that*

$$f(\sigma) \leq C_\epsilon \sigma^{-1-\epsilon}$$

holds for all σ *and a constant* C_ϵ. *Then the sum*

$$\sum_{\gamma\in\bar{\Gamma}} f\left(\tfrac{1}{2}(\cosh(d(z',\gamma z))+1)\right)$$

converges absolutely and uniformly for all $z',z \in \mathbb{H}^2$.

Starting from the point-pair invariant, we can now construct automorphic kernels via Poincaré series. Due to our restrictions on Φ,

$$K_\Gamma(z',z) = \frac{1}{2}\sum_{\gamma\in\bar{\Gamma}} K(z',\gamma z)\chi(\gamma)J_\gamma(z,1) \tag{5.2}$$

is well defined. Some standard manipulations show that the behavior of K_Γ under transformations is given by

$$K_\Gamma(\gamma_1 z', \gamma_2 z) = \chi(\gamma_1)J_{\gamma_1}(z',1)K_\Gamma(z',z)J_{\gamma_2}^{-1}(z,1)\chi^{-1}(\gamma_2). \tag{5.3}$$

This allows us to define automorphic kernels.

Definition 4: Let F be a fundamental domain for the Fuchsian group Γ. We say that $K_\Gamma:\mathbb{H}^2\times\mathbb{H}^2\to\mathbb{C}^{2\times 2}$ is an element of $\mathfrak{L}^2(\Gamma\backslash\mathbb{H}^2,\Gamma\backslash\mathbb{H}^2,\chi)$, if (5.3) holds for all $\gamma\in\bar{\Gamma}$ and

$$\|K_\Gamma\|_{\mathrm{L}^2}^2 := \int_F\int_F \mathrm{tr}(K_\Gamma^\dagger(z',z)K_\Gamma(z',z))\mathrm{d}\mu(z)\mathrm{d}\mu(z') < \infty .$$

It is well known that such an automorphic kernel defines a Hilbert-Schmidt operator $L:\mathfrak{L}^2(\Gamma,1,\chi)\to\mathfrak{L}^2(\Gamma,1,\chi)$ via

$$[L\Psi](z') := \int_F K_\Gamma(z',z)\Psi(z)\mathrm{d}\mu(z).$$

If K_Γ is Hermitian there exists a basis $\{\Psi_n\}$ of orthonormal eigenforms of L in $\mathfrak{L}^2(\Gamma,1,\chi)$ such that $K_\Gamma(z',z)=\Sigma_n a_n\Psi_n(z')\Psi_n^\dagger(z)$. Furthermore, if K_Γ was constructed from a point-pair invariant via (5.2), then one can easily check that the operator L has a finite trace that is given by $\Sigma_n a_n$. In the following section we will construct point-pair invariants from a Green's function and then calculate such traces.

VI. THE TRACE FORMULA

Before we can proceed to introduce point-pair invariants, we have to identify Green's functions for Dirac operators on surfaces $\Gamma\backslash\mathbb{H}^2$. For this, and the following, we restrict our attention to the Dirac operator itself, i.e., to the weight $k=1$. The starting point will be a Green's function for D on the hyperbolic plane, from which the corresponding Green's function on the compact surface can be obtained in terms of a Poincaré series.

Since the resolvent of D is a bounded operator when $\mathrm{Im}(\rho)<0$, we can make the ansatz

$$(D+\rho)^{-1}\Psi(z') = \int_{\mathbb{H}^2} G(z',z;\rho)\Psi(z)\mathrm{d}\mu(z),$$

with $G(\cdot,\cdot;\rho):\mathbb{H}^2\times\mathbb{H}^2\to\mathbb{C}^{2\times 2}$. For the matrix entries of G, we use the notation $G=\begin{pmatrix} G_1 & G_2 \\ G_3 & G_4 \end{pmatrix}$. Then G can be uniquely characterized as a solution of the matrix-differential equation

$$(D+\rho)G(z',z;\rho) = 0, \quad \text{for } z\neq z', \tag{6.1}$$

with a specified behavior in a neighborhood of $z=z'$. That is, for the diagonal matrix entries

$$\lim_{d(z',z)\to 0}\left(G_i(z',z;\rho) - \frac{\rho}{4\pi}\log(d(z',z))\right) < \infty, \quad i=1,4,$$

is required, whereas the nondiagonal entries are regular in $z=z'$. In addition, $G_i(z',z;\rho)$ must approach zero as $d(z',z)\to\infty$.

Furthermore, the transformation property (3.4) implies the corresponding behavior,

$$G(z',z;\rho) = J_\gamma^{-1}(z',1)G(\gamma z',\gamma z;\rho)J_\gamma(z,1),$$

of the Green's function under an isometry $\gamma\in\mathrm{PSL}(2,\mathbb{R})$.

In order to solve for this Green's function we closely follow Refs. 29 and 30, where the corresponding problem for the Maaß-Laplacians is treated. We begin with introducing

$$\check{G}(z',z;\rho) := A^{-1}(z',z)G(z',z;\rho)B^{-1}(z',z),$$

which is invariant under $\mathrm{PSL}(2,\mathbb{R})$, and note that $\check{D}:=A^{-1}(z,\mathrm{i})DA(z,\mathrm{i})$ is invariant under the stability group $\mathrm{PSO}(2,\mathbb{R})$ of $z=\mathrm{i}$. Therefore, the differential equation for $\check{G}$ corresponding to (6.1) is transformed into polar coordinates (σ,ϕ) for $z\in\mathbb{H}^2$, where $\sigma=\frac{1}{2}(\cosh(d(z,z'))+1)$. With $H(\sigma;\rho)=\check{G}(z',z;\rho)$, this leads to a system of ordinary linear differential equations for $H=\begin{pmatrix} H_1 & H_2 \\ H_3 & H_4 \end{pmatrix}$,

$$\begin{pmatrix} \rho & \mathrm{i}\left[(\sigma(\sigma-1))^{1/2}\dfrac{\partial}{\partial\sigma}+\dfrac{1}{2}\left(\dfrac{\sigma-1}{\sigma}\right)^{1/2}\right] \\ \mathrm{i}\left[(\sigma(\sigma-1))^{1/2}\dfrac{\partial}{\partial\sigma}+\dfrac{1}{2}\left(\dfrac{\sigma-1}{\sigma}\right)^{1/2}\right] & \rho \end{pmatrix} H(\sigma;\rho)$$

$$= -\mathrm{i}\begin{pmatrix} \dfrac{1}{2}(\sigma(\sigma-1))^{-1/2}H_3(\sigma;\rho) & 0 \\ 0 & \dfrac{1}{2}(\sigma(\sigma-1))^{-1/2}H_2(\sigma;\rho) \end{pmatrix}. \tag{6.2}$$

The solution of (6.2) for $\sigma\to\infty$ is given by

$$H_1(\sigma;\rho) = -\frac{\rho}{4\pi}\sigma^{-\frac{1}{2}-i\rho}\frac{\Gamma(i\rho)\Gamma(i\rho+1)}{\Gamma(2i\rho+1)}F\left(i\rho,1+i\rho;1+2i\rho;\frac{1}{\sigma}\right)$$
$$= -\frac{\rho}{4\pi}\sigma^{-\frac{1}{2}}\int_0^1 t^{i\rho}(1-t)^{i\rho-1}(\sigma-t)^{-i\rho}\,dt, \tag{6.3}$$

and

$$H_2(\sigma;\rho) = -\frac{i}{4\pi}\sigma^{-1-i\rho}(\sigma-1)^{1/2}\frac{\Gamma^2(i\rho+1)}{\Gamma(2i\rho+1)}F\left(1+i\rho,1+i\rho;1+2i\rho;\frac{1}{\sigma}\right)$$
$$= \frac{\rho}{4\pi}(\sigma-1)^{1/2}\int_0^1 t^{i\rho}(1-t)^{i\rho-1}(\sigma-t)^{-i\rho-1}\,dt, \tag{6.4}$$

where $F(a,b;c;z)$ is a hypergeometric function (see, e.g., Ref. 14). Moreover, $H_3(\sigma;\rho) = H_2(\sigma;\rho)$ and $H_4(\sigma;\rho) = H_1(\sigma;\rho)$. From this representation we infer an upper bound for the components of the Green's function,

$$|G_i(z',z;\rho)| \le \text{const}|\rho|e^{-(1/2-\text{Im}(\rho))d(z',z)}, \quad \text{if } d(z',z) \ge d_0 > 0. \tag{6.5}$$

As the singularity of G for $d(z',z)\to 0$ is integrable, we obtain the following lemma.

Lemma 5: Let $f:\mathbb{H}^2\to\mathbb{C}^2$ *be bounded and continuous, then*

$$\int_{\mathbb{H}^2} G(z',z;\rho)f(z)d\mu(z)$$

converges absolutely and uniformly in $\text{Re}(\rho)$ *as long as* $\text{Im}(\rho) < -\frac{1}{2}$.

With Lemma 4 and the estimate (6.5), the Green's function for the Dirac operator on a compact surface can now be obtained in terms of a Poincaré series (5.2).

Lemma 6: Let $\text{Im}(\rho) < -\frac{1}{2}$; *then*

$$G_\Gamma(z',z;\rho) := \frac{1}{2}\sum_{\gamma\in\bar{\Gamma}} G(z',\gamma z;\rho)\chi(\gamma)J_\gamma(z,1)$$

converges for $z \ne z' \bmod \Gamma$, *and is the Green's function for D on* $\Gamma\backslash\mathbb{H}^2$.

We are now in a position to construct point-pair invariants as in Definition 3 through

$$\Phi(\sigma) := \frac{1}{\pi}\int_{-\infty}^{\infty} H(\sigma;\rho)h(\rho)d\rho,$$

where h is a function, as specified below.

Definition 5: A function $h:\mathbb{C}\to\mathbb{C}$ that satisfies the following:

- h is even, i.e. $h(\rho)=h(-\rho)$,
- h is complex analytic in the strip $|\text{Im}(\rho)| \le \beta$ for some fixed $\beta \ge \frac{1}{2}+\epsilon$,
- there exists $\delta > 0$, such that the bound

$$|h(\rho)| \le \text{const}(1+\text{Re}(\rho))^{-2-\delta}$$

holds uniformly for all ρ in the above mentioned strip, is called an admissible test function.

We denote the Fourier transform of an admissible test function by

$$g(u) := \frac{1}{2\pi}\int_{-\infty}^{\infty} h(\rho)\mathrm{e}^{-\mathrm{i}\rho u}\,\mathrm{d}\rho.$$

All that we have to check that this indeed leads to a point-pair invariant is the condition (5.1).

Lemma 7: Let $\sigma-1\geq\kappa>0$; *then the components* K_i *of* K *are bounded from above by*

$$|K_i(z',z)| \leq C_\kappa \mathrm{e}^{-(1/2+\beta)d(z',z)}, \quad i=1,\ldots,4, \tag{6.6}$$

with some $C_\kappa>0$. *Furthermore, the limit* $\lim_{d(z',z)\to 0}K(z',z)$ *is well defined. More precisely, we have*

$$\operatorname{tr} K(z,z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \rho h(\rho)\coth(\pi\rho)\mathrm{d}\rho.$$

Proof: To prove the first part one shifts the integral by $-i\beta$. Using the estimate (6.5) on G_i and shifting back, the bound (6.6) follows immediately. For the second part we note that

$$\lim_{\sigma\to 1^+}\frac{1}{4\pi}\int_{-\infty}^{\infty}\rho h(\rho)\log(\sigma-1)\mathrm{d}\rho = 0;$$

thus we can add this term to Φ. Then again shifting the integral by $-\mathrm{i}\epsilon$ and using Ref. 26, p. 44, one obtains

$$\lim_{d(z',z)\to 0} K_i(z',z) = \frac{1}{4\mathrm{i}\pi^2}\int_{-\infty-\mathrm{i}\epsilon}^{\infty-\mathrm{i}\epsilon}\rho h(\rho)[\psi(\mathrm{i}\rho)+\psi(\mathrm{i}\rho+1)]\mathrm{d}\rho, \quad i=1,4,$$

where $\psi(z)=(\mathrm{d}/\mathrm{d}z)\log\Gamma(z)$. After substituting ρ by $-\rho$ and using the fact that h is even, the statement follows immediately. □

Having shown that K is indeed a point-pair invariant, we can introduce the automorphic kernel,

$$K_\Gamma(z',z) := \frac{1}{2}\sum_{\gamma\in\bar{\Gamma}} K(z',\gamma z)\chi(\gamma)J_\gamma(z,1), \tag{6.7}$$

which by construction is in $\mathfrak{L}^2(\Gamma\backslash\mathbb{H}^2,\Gamma\backslash\mathbb{H}^2,\chi)$. The corresponding Hilbert-Schmidt operator on $\mathfrak{L}^2(\Gamma,1,\chi)$ is called L.

Lemma 8: Any $\Psi\in\mathfrak{F}_\rho(\Gamma,1,\chi)$ *is simultaneously an eigenform of the Hilbert-Schmidt operator* L,

$$[L\Psi](z') = \Lambda(\rho)\Psi(z'),$$

where the eigenvalue Λ *satisfies the equation*

$$\Lambda(\rho)+\Lambda(-\rho) = 2h(\rho). \tag{6.8}$$

Proof: With

$$[L\psi](z') = \frac{1}{2\pi\mathrm{i}}\int_F\left(\sum_{\gamma\in\bar{\Gamma}}\int_{-\infty}^{\infty} h(\rho)G(z',\gamma z;\rho)\chi(\gamma)J_\gamma(z,1)\mathrm{d}\rho\right)\Psi(z)\mathrm{d}\mu(z),$$

a standard calculation yields

$$[L\psi](z') = \frac{1}{\pi\mathrm{i}}\int_{-\infty-\mathrm{i}\beta}^{\infty-\mathrm{i}\beta} h(\rho')\left(\int_F G_\Gamma(z',z;\rho')\Psi(z)\mathrm{d}\mu(z)\right)\mathrm{d}\rho'.$$

From this we read off the eigenvalue of L as

$$\Lambda(\rho) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty-\mathrm{i}\beta}^{\infty-\mathrm{i}\beta} \frac{h(\rho')}{\rho' - \rho} \mathrm{d}\rho',$$

and this implies (6.8). □

As already noted in Sec. IV, the spectrum of the Dirac operator on a compact surface is real and discrete. Moreover, according to Lemma 1, the spectrum is symmetric with respect to zero. We hence denote the non-negative eigenvalues (listed with their respective multiplicities) by $0 \leq \rho_0 \leq \rho_1 \leq \cdots$, which include N of the $2N$ zero modes. The Hilbert space $\mathfrak{L}^2(\Gamma, 1, \chi)$ therefore has a basis of orthonormal eigenforms $\Psi_{n,\pm}$,

$$(D \pm \rho_n)\Psi_{n,\pm} = 0.$$

Thus the automorphic kernel possesses a spectral expansion of the form

$$K_\Gamma(z', z) = \sum_{n=0}^{\infty} \left(\Lambda(\rho_n)\Psi_{n,+}(z')\Psi_{n,+}^\dagger(z) + \Lambda(-\rho_n)\Psi_{n,-}(z')\Psi_{n,-}^\dagger(z)\right),$$

which immediately yields the spectral side of the desired trace formula.

Lemma 9: The Hilbert-Schmidt operator L has a finite trace, given by

$$\mathrm{tr}(L) = 2\sum_{n=0}^{\infty} h(\rho_n).$$

Next, we need to compute the geometric side of the trace formula, i.e.,

$$\mathrm{tr}(L) = \int_F K_\Gamma(z, z)\mathrm{d}\mu(z),$$

with the representation (6.7) of the automorphic kernel. Following a standard procedure, this yields

$$\mathrm{tr}(L) = \frac{1}{2}\sum_{\{\gamma\}} \chi(\gamma) \sum_{[g] \in \bar{Z}_\gamma \backslash \bar{\Gamma}} \mathrm{tr}\left(\int_{gF} K(z, \gamma z) J_\gamma(z, 1)\mathrm{d}\mu(z)\right), \tag{6.9}$$

where $\{\gamma\}$ denotes the $\bar{\Gamma}$-conjugacy classes of $\gamma \in \bar{\Gamma}$ and $\bar{Z}_\gamma$ is the centralizer of γ in $\bar{\Gamma}$. Next, we use the natural pairing of the disjoint conjugacy classes $\{\gamma\}$ and $\{-\gamma\}$, which cancels the factor $\frac{1}{2}$. Within these pairs we choose the conjugacy classes with $\mathrm{tr}(\gamma) > 0$. Moreover, it is well known that

$$D_\gamma := \bigcup_{[g] \in Z_\gamma \backslash \Gamma} g(F)$$

is a fundamental set for the centralizer $Z_\gamma \subset \Gamma$. Introducing primitive hyperbolic elements γ_p and their conjugacy classes, one can rewrite (6.9) as

$$\mathrm{tr}(L) = \mathrm{tr}\left(\int_F K(z, z)\mathrm{d}\mu(z)\right) + \sum_{\{\gamma_p\}} \sum_{n=1}^{\infty} \chi(\gamma_p^n)\mathrm{tr}\left(\int_{D_{\gamma_p}} K(z, \gamma_p^n z) J_{\gamma_p^n}(z, 1)\mathrm{d}\mu(z)\right).$$

Upon a conjugation with a matrix in $\mathrm{SL}(2, \mathbb{R})$, any hyperbolic element can be brought into the Jordan normal form

$$\gamma = \begin{pmatrix} e^{\frac{l_\gamma}{2}} & 0 \\ 0 & e^{-\frac{l_\gamma}{2}} \end{pmatrix}.$$

A fundamental domain for the group generated by γ is given by $\{z \in \mathbb{H}^2 | 1 < y < e^{l_\gamma}\}$. Note that $J_\gamma(z,1)=1$, so all that remains to be done is evaluating integrals of the form

$$I(\gamma^n) = \mathrm{tr}\left(\int_1^{e^l} \int_{-\infty}^{\infty} K(z, \gamma^n z) \mathrm{d}x \frac{\mathrm{d}y}{y^2} \right). \tag{6.10}$$

In order to calculate this integral, we introduce

$$\tau = \cosh^2 \frac{nl}{2} + \left(\frac{x}{y} \sinh \frac{nl}{2} \right)^2,$$

which allows us to perform the integration with respect to y. Inserting the explicit expressions (6.3) and (6.4) for the function H, the integral (6.10) reduces to

$$I(\gamma^n) = \frac{\mathrm{i} l_\gamma}{2\pi^2} \coth \frac{n l_\gamma}{2} \int_{-\infty}^{\infty} \rho h(\rho)$$
$$\times \int_{\cosh^2 \frac{n l_\gamma}{2}}^{\infty} \tau^{-1-\mathrm{i}\rho} \left(\tau - \cosh^2 \frac{n l_\gamma}{2} \right)^{-1/2} \sum_{m=0}^{\infty} \frac{\Gamma(\mathrm{i}\rho + m)\Gamma(\mathrm{i}\rho + m + 1)}{\Gamma(2\mathrm{i}\rho + m + 1) m!} \tau^{-m} \, \mathrm{d}\tau \, \mathrm{d}\rho.$$

Interchanging the order of integration and summation and employing the relation

$$\left(\frac{1}{2\cosh\left(\frac{a}{2}\right)} \right)^{-2q} \sum_{m=0}^{\infty} \frac{2q\Gamma(2q+2m)}{\Gamma(2q+m+1)m!} \left(\frac{1}{2\cosh\left(\frac{a}{2}\right)} \right)^{-2m} = e^{-qa},$$

which follows from Ref. 16, 1.114 for $a>0$ and $\mathrm{Re}(q)>0$, finally yields

$$I(\gamma^n) = \frac{l_\gamma}{\sinh \frac{n l_\gamma}{2}} \frac{1}{2\pi} \int_{-\infty}^{\infty} h(\rho) e^{-\mathrm{i}\rho n l_\gamma} \, \mathrm{d}\rho = \frac{l_\gamma g(n l_\gamma)}{\sinh\left(\frac{n l_\gamma}{2}\right)}. \tag{6.11}$$

Putting together Lemma 7, Lemma 9, and Eq. (6.11) then leads to the desired trace formula.

Theorem 1 (Selberg trace formula for the Dirac operator): *Let $\Gamma \subset \mathrm{PSL}(2,\mathbb{R})$ be a strictly hyperbolic Fuchsian group with fundamental domain F of area $A(F)$ and fix a multiplier system χ of weight one. Moreover, let $\{\rho_n\}_{n=0}^{\infty}$ be the non-negative eigenvalues of the Dirac operator D on $\mathfrak{L}^2(\Gamma,1,\chi)$, including half of the zero modes. Then, for any admissible test function h, see Definition 5, the following trace formula holds*:

$$\sum_{m=0}^{\infty} h(\rho_m) = \frac{A(F)}{4\pi} \int_{-\infty}^{\infty} \rho h(\rho) \coth(\pi\rho) \mathrm{d}\rho + \sum_{\{\gamma_p\}} \sum_{n=1}^{\infty} \chi(\gamma_p^n) \frac{l_{\gamma_p} g(n l_{\gamma_p})}{2 \sinh\left(\frac{n l_{\gamma_p}}{2}\right)}. \tag{6.12}$$

In accordance with Proposition 1, this trace formula is identical to the one for the Maaß-Laplacian $-\Delta_1$ on the same surface and with the same multiplier system. We stress, however, a difference in the interpretation of the geometric side. Both expressions can be viewed as sums over the closed geodesics on $\Gamma\backslash\mathbb{H}^2$, weighted with the factors $\chi(\gamma_p^n)$. For the Maaß-Laplacian, these factors stem from the nonvanishing magnetic fluxes that are necessarily present (see, e.g., Ref. 13), whereas for the Dirac operator with weight $k=1$ there is no magnetic field involved. Here the

factors $\chi(\gamma_p^n)$ reflect the fact that the classical dynamical system associated with the quantum dynamics generated by the Dirac operator is not the geodesic flow, but its associated frame flow; see also Ref. 23. This is analogous to Dirac operators on $\mathbb{R}^3$.[8]

The frame flow (see, e.g., Ref. 10) is a flow in the frame bundle FM over a Riemannian manifold M consisting of a parallel transport of oriented orthonormal frames along geodesics. To be precise, let $\{e_1(p),\ldots,e_n(p)\}$ be an orthonormal basis of T_pM. Then this frame is transported along the geodesic determined by e_1 with the Levi-Civita connection. This flow can be lifted into the spin structure by assigning an element $g(p)\in \mathrm{Spin}(n)$ to every point along the geodesic. This may also be done in the spin representation yielding $\rho(g(p))$. In the present case, where $M=\Gamma\backslash\mathbb{H}^2$, $\rho(g(z))$ must equal $\rho(g(\gamma z))$ for every $\gamma\in\bar{\Gamma}$. However, in the induced (trivial) bundle over the hyperbolic plane, the transformation property,

$$\rho(g(\gamma z))=\chi(\gamma)J_\gamma(z,1)\rho(g(z)),$$

applies; see (3.1) and (3.3). The factors $\chi(\gamma_p^n)$ in Eq. (6.12) therefore reflect the spin structure. Hence, although on two-dimensional manifolds the frame flow is not much different from the geodesic flow, only the latter is a natural dynamics that can be lifted into the spin structure. For $n\geq 3$ the situation will be different since in such a case a frame flow yields interesting classical dynamics beyond the geodesic flow.

VII. SOME APPLICATIONS

A first immediate application of the trace formula, which can be proved in the standard way (see, e.g., Ref. 19), concerns the asymptotic distribution of the eigenvalues.

Proposition 3 (Weyl's law): *Let $N(\rho)$ be the number of non-negative eigenvalues of D that are smaller than ρ. Then*

$$N(\rho)\sim\frac{A(F)}{4\pi}\rho^2,\quad \rho\to\infty.$$

This result also follows from Ref. 22.

Another application consists of determining properties of the related Selberg zeta function. If $\mathrm{Re}(s)$, $\mathrm{Re}(\sigma)>1$, the function

$$h(\rho):=\frac{1}{\rho^2+\left(s-\frac{1}{2}\right)^2}-\frac{1}{\rho^2+\left(\sigma-\frac{1}{2}\right)^2}$$

satisfies the criteria of Definition 5 to serve as an admissible test function. In the trace formula (6.12), it leads to a relation for the trace of a regularized resolvent,

$$\sum_{m=0}^{\infty}\left(\frac{1}{\rho_m^2+\left(s-\frac{1}{2}\right)^2}-\frac{1}{\rho_m^2+\left(\sigma-\frac{1}{2}\right)^2}\right)=-\frac{A(F)}{2\pi}\left(\psi\left(s-\tfrac{1}{2}\right)-\psi\left(\sigma-\tfrac{1}{2}\right)\right)+\frac{A(F)}{4\pi}\left(\frac{1}{\sigma-\frac{1}{2}}-\frac{1}{s-\frac{1}{2}}\right)$$
$$+\frac{1}{2s-1}\frac{Z'(s)}{Z(s)}-\frac{1}{2\sigma-1}\frac{Z'(\sigma)}{Z(\sigma)}.$$

Here $Z(s)$ is Selberg's zeta function, which is defined by

$$Z(s):=\prod_{\{\gamma_p\}}\prod_{k=0}^{\infty}(1-\chi(\gamma_p)\mathrm{e}^{-l_{\gamma_p}(k+s)}),\quad \mathrm{Re}(s)>1.$$

Now proceeding along the lines of Refs. 34 and 32, we find an analytic continuation of $Z(s)$ into the entire complex plane.

Proposition 4: The Selberg zeta function for the Dirac operator is an entire analytic function. Moreover, it can be represented as

$$Z(s)=\frac{Z^{(2N)}\left(\frac{1}{2}\right)}{(2N)!}\left(s-\frac{1}{2}\right)^{2N}\mathrm{e}^{(s-1/2)^2\gamma_D}\mathrm{e}^{(s-1/2)\frac{A(F)}{2\pi}}$$
$$\times\left[(2\pi)^{-(s-1/2)}\mathrm{e}^{(s^2-1/4)}G^2\left(s+\frac{1}{2}\right)\right]^{A(F)/2\pi}\prod_{m=N}^{\infty}\left[\left(1+\frac{\left(s-\frac{1}{2}\right)^2}{\rho_m^2}\right)\mathrm{e}^{-(s-1/2)^2/\rho_m^2}\right], \quad (7.1)$$

where G is Barnes' double Γ function (see Ref. 3) and $2N$ denotes the number of zero modes of D. The trivial zeros of $Z(s)$ are given by $s=-\frac{1}{2}-n$ with multiplicities $(2n)^{A(F)/2\pi}$, $n\in\mathbb{N}$. The nontrivial zeros are $s=\frac{1}{2}\pm\mathrm{i}\rho_m$, with the same multiplicities as the eigenvalues ρ_m of D.

In (7.1) the constant γ_D is a generalized Euler constant as introduced in Ref. 34 and $Z^{(2N)}$ denotes a derivative of the zeta function of order $2N$. Moreover, due to the Gauß-Bonnet theorem, $A(F)/2\pi=2(g-1)$ is a positive integer, where g is the genus of the surface $\Gamma\backslash\mathbb{H}^2$.

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Localization effects in a periodic quantum graph with magnetic field and spin-orbit interaction

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A general technique for the study of magnetic Rashba Hamiltonians in quantum graphs is presented. We use this technique to show how manipulating the magnetic and spin parameters can be used to create localized states in a certain periodic graph (T_3 lattice). © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this work, we discuss the creation of eigenvalues in periodic quantum graphs by certain external interactions, namely, by magnetic field and spin-orbit coupling.

The analysis of quantum graphs, i.e., of differential operators on singular one-dimensional manifolds, becomes one of the central topics in the mathematical physics during the last decades; see Refs. 28–33 and 35. This has many reasons; in particular, quantum graph Hamiltonians appear in the de Gennes-Alexander theory of superconductivity.[4,15,25] Some other fields of applications are described, e.g., in Ref. 31.

The spectral theory of compact quantum graphs has many common features, with the usual theory of differential operators; cf. Refs. 6, 42, and 48. Nevertheless, such an analogy is rather limited when considering noncompact structures. Some particular features of quantum graph models become obvious if one studies periodic configurations. For example, for a large class of periodic Schrödinger operators in Euclidian spaces, the spectrum is known to be absolutely continuous,[9,50] while even the simplest periodic quantum graphs can have eigenvalues.[12,33] Some other examples may include the sensibility of periodic quantum graphs to some arithmetic characteristics.[24]

Recently, in the physics literature one discussed the so-called extreme localization in the T_3 lattice (dice lattice).[1,54] From the mathematical point of view, it was shown that under certain magnetic fields the Hamiltonian of a quantum graph with the corresponding shape has no bands of a continuous spectrum, and the spectrum consists of infinitely degenerate eigenvalues. This effect was observed also experimentally by transport measuring in superconducting and metallic wire networks.[39–41] (It is worth emphasizing that bound states in the T_3 lattice appear without any external interactions;[51] the coexistence of the continuous and the point spectra is implied by the rich internal symmetry of the lattice and of its dual, Kagomé.[2]) Various aspects of this localization mechanism and its stability under disorder and external interactions are studied in a number of works.[8,38,52–54] In particular, it is shown that additional interactions, like the interparticle interaction, destroy the extreme localization mechanism, and a continuous spectrum appears.[53]

In Ref. 7 it was shown that in some periodic quantum graphs similar localization phenomena can be induced not only by magnetic fields, but also by the spin-orbit interaction at certain values of the Rashba constant.[14,47] Nevertheless, the numerical analysis of Ref. 8 shows that the Rashba localization does not appear in the T_3 lattice. In the present paper we consider the above situation

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with both the spin-orbit and magnetic interactions. We note that the quantum graph models with spin were studied previously, e.g., in Refs. 10, 11, 13, and 27, but the attention was mostly concentrated on Dirac- and Pauli-type operators. The theory of Rashba Hamiltonians is not developed, even in the Euclidian spaces, and the spin-orbit interaction promises to show effects that are absent in the scalar case, like embedded eigenvalues in short-range potentials or localization in crystals, hence giving possibilities for constructing new nanodevices.[17,34]

The aim in this paper is two-fold. First, we are going to describe the Schrödinger operators in two-dimensional networks with magnetic field and spin-orbit interaction. An essential part here is the reduction of the quantum graph Hamiltonian to a certain discrete equation. In the scalar case, an analogous procedure was done in Ref. 23 for the solutions of the stationary Schrödinger equation and recently in Ref. 44 for the spectra. Note that there is another approach to the relationship between the quantum graphs and tight-binding Hamiltonians coming from some asymptotic considerations.[36,37] Second, by considering the localization effects in the T_3 lattice we would like to attract the attention of researchers working on quantum graphs to potential applications in the study of superconducting networks. In Sec. II we give a mathematical formalism of quantum graphs with external interactions; essentially we describe rigorously the constructions of Refs.7 and 8. In Sec. III we use this machinery to study the spectrum of the T_3 lattice with a magnetic field and the Rashba interaction. We show that the spectral problem is of a supersymmetric type and that the study of some energy levels is equivalent to the study of zero modes in a certain discrete model. As a result, we give a rigorous justification of the extreme localization for the case of nontrivial scalar potentials on the edges and nonideal couplings at the nodes. We show that at zero spin-orbit interaction this effect is independent of the edge potential. At the same time, it appears that the generic Rashba interaction destroys the localization. We also show that at a certain combination of the magnetic and spin parameters a new localization effect appears, where one can localize one of the spin projections using the magnetic field.

II. QUANTUM GRAPHS WITH EXTERNAL INTERACTIONS

A. Schrödinger operator on a quantum graph embedded in Euclidian space

In this section we describe the construction of the Hamiltonian in a two-dimensional network with a magnetic field and Rashba interaction. Recall that the Rashba Hamiltonian of a two-dimensional system acts on two-component vector functions and takes the form[14,47]

$$H = (\mathbf{p} - \mathbf{A})^2 + 2k_{\mathrm{R}}\langle \boldsymbol{\sigma}, (\mathbf{p} - \mathbf{A}) \times \mathbf{n}\rangle + U, \tag{1}$$

where $\mathbf{A}$ is the magnetic vector potential, k_{R} is the Rashba constant expressing the strength of the spin-orbit interaction, U is a scalar potential, $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and $\mathbf{n}$ is the unit vector orthogonal to the plane of the system. The second term, which is the formal mixed product on the right-hand side of (1), takes into account the spin-orbit coupling. For $k_{\mathrm{R}}=0$ the problem splits into two identical scalar problems. The corresponding Hamiltonian for a network is obtained by projecting all the interactions onto each edge and by introducing suitable boundary conditions at the nodes, which will be described later. (We remark that some effects of the Rashba interaction and the magnetic field in a wire can be studied in other types of models.[19])

Let $\mathcal{V}$ be a uniformly discrete subset of the xy plane in $\mathbb{R}^3$, the set of nodes (vertices). The uniform discreteness means the existence of a constant $d>0$ such that $|\boldsymbol{\alpha}-\boldsymbol{\beta}| \geqslant d$ for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{V}$ with a $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$. Denote

$$l_{\boldsymbol{\alpha}\boldsymbol{\beta}} := |\boldsymbol{\alpha} - \boldsymbol{\beta}|, \quad \mathbf{e}_{\boldsymbol{\alpha}\boldsymbol{\beta}} := \frac{1}{l_{\boldsymbol{\alpha}\boldsymbol{\beta}}}(\boldsymbol{\beta} - \boldsymbol{\alpha}).$$

Some nodes are connected by a directed edge. The set of all edges will be denoted by $\mathcal{E}$, $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$. The edge with initial vertex $\boldsymbol{\alpha} \in \mathcal{V}$ and terminal vertex $\boldsymbol{\beta} \in \mathcal{V}$ will be denoted by $\boldsymbol{\alpha}\boldsymbol{\beta}$. For $\boldsymbol{\alpha} \in \mathcal{V}$ denote $\operatorname{indeg} \boldsymbol{\alpha} := \#\{\boldsymbol{\beta}\boldsymbol{\alpha} \in \mathcal{E}\}$, $\operatorname{outdeg} \boldsymbol{\alpha} = \#\{\boldsymbol{\alpha}\boldsymbol{\beta} \in \mathcal{E}\}$, $\deg \boldsymbol{\alpha} := \operatorname{indeg} \boldsymbol{\alpha} + \operatorname{outdeg} \boldsymbol{\alpha}$. We assume that the degrees satisfy the following conditions: that

$$\text{there exists } N \in \mathbb{Z} \text{ with} 1 \leqslant \deg \boldsymbol{\alpha} \leqslant N \text{ for all } \boldsymbol{\alpha} \in \mathcal{V}; \tag{2}$$

in particular, we assume that there are no isolated vertices. The configuration consisting of all segments $[\boldsymbol{\alpha}, \boldsymbol{\beta}]$, $\boldsymbol{\alpha\beta} \in \mathcal{E}$ will be referred to as a metric graph or as a (wire) network. We assume that the system has no self-intersections and that

$$0 < \inf\{l_{\boldsymbol{\alpha\beta}}\} \leqslant \sup\{l_{\boldsymbol{\alpha\beta}}\} < \infty . \tag{3}$$

The quantum state space corresponding to the metric graph is introduced as follows. Each edge $\boldsymbol{\alpha\beta}$ will be identified with the segment $[0, l_{\boldsymbol{\alpha\beta}}]$ such that $\boldsymbol{\alpha}$ is identified with 0 and $\boldsymbol{\beta}$ is identified with $l_{\boldsymbol{\alpha\beta}}$. The state space of each edge $\boldsymbol{\alpha\beta}$ is $\mathcal{H}_{\boldsymbol{\alpha\beta}} := L^2([0, l_{\boldsymbol{\alpha\beta}}], \mathbb{C}^2)$. The state space of the whole structure is $\mathcal{H} = \oplus_{\boldsymbol{\alpha\beta} \in \mathcal{E}} \mathcal{H}_{\boldsymbol{\alpha\beta}}$.

On each edge consider a real-valued scalar potential $U_{\boldsymbol{\alpha\beta}} \in L^2[0, l_{\boldsymbol{\alpha\beta}}]$. To avoid unnecessary technical difficulties we will assume that the scalar potentials are uniformly L^2 bounded,

$$\sup \|U_{\boldsymbol{\alpha\beta}}\|_{L^2} < \infty . \tag{4}$$

Assume that the system is subjected to an external magnetic field given by a vector potential $\mathbf{A} \in C^1(\mathbb{R}^3, \mathbb{R}^3)$. This induces magnetic potentials on each edge, $a_{\boldsymbol{\alpha\beta}}(t) := \langle \mathbf{A}(\boldsymbol{\alpha} + t\mathbf{e}_{\boldsymbol{\alpha\beta}}), \mathbf{e}_{\boldsymbol{\alpha\beta}} \rangle$.

Denote by k_{R} the Rashba constant. The spin-orbit interaction can be taken into account by adding the term $2k_R(-\mathrm{i}(\mathrm{d}/\mathrm{d}t) - a_{\boldsymbol{\alpha\beta}}(t))\langle \boldsymbol{\sigma} \times \mathbf{n}, \mathbf{e}_{\boldsymbol{\alpha\beta}} \rangle$ with $\mathbf{n} = (0, 0, 1)$. Therefore, the dynamics along each edge $\boldsymbol{\alpha\beta}$ is described by the differential expression

$$\begin{aligned} L_{\boldsymbol{\alpha\beta}} &= \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - a_{\boldsymbol{\alpha\beta}}(t) \right)^2 + 2k_{\mathrm{R}} \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - a_{\boldsymbol{\alpha\beta}}(t) \right) \langle \boldsymbol{\sigma} \times \mathbf{n}, \mathbf{e}_{\boldsymbol{\alpha\beta}} \rangle + U_{\boldsymbol{\alpha\beta}} \\ &\equiv \left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} + a_{\boldsymbol{\alpha\beta}}(t) + k_R \sigma_{\boldsymbol{\alpha\beta}} \right)^2 + U_{\boldsymbol{\alpha\beta}} - k_{\mathrm{R}}^2, \end{aligned}$$

where

$$\sigma_{\boldsymbol{\alpha\beta}} = \begin{pmatrix} 0 & e_{\boldsymbol{\alpha\beta}2+\mathrm{i}e_{\boldsymbol{\alpha\beta}1}} \\ e_{\boldsymbol{\alpha\beta}2-\mathrm{i}e_{\boldsymbol{\alpha\beta}1}} & 0 \end{pmatrix}.$$

For a uniform magnetic field with the strength $\mathbf{B} \in \mathbb{R}^3$ it is useful to use the symmetric gauge, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$. In this case the magnetic potentials $a_{\boldsymbol{\alpha\beta}}$ are constant, $a_{\boldsymbol{\alpha\beta}} = \frac{1}{2}\langle \mathbf{B} \times \boldsymbol{\alpha}, \mathbf{e}_{\boldsymbol{\alpha\beta}} \rangle$.

Denote by L an operator in $\mathcal{H}$, acting as

$$(\mathbf{f}_{\boldsymbol{\alpha\beta}}) \mapsto (\mathbf{L}_{\alpha\beta}\mathbf{f}_{\boldsymbol{\alpha\beta}}) \tag{5}$$

on functions $\mathbf{f}_{\boldsymbol{\alpha\beta}} \in H^2([0, l_{\boldsymbol{\alpha\beta}}], \mathbb{C}^2)$ satisfying, at each $\alpha \in \mathcal{V}$,

$$\mathbf{f}_{\boldsymbol{\alpha\beta}}(0) = \mathbf{f}_{\boldsymbol{\gamma\alpha}}(l_{\boldsymbol{\gamma}}\boldsymbol{\alpha}) =: \mathbf{f}(\boldsymbol{\alpha}), \quad \boldsymbol{\alpha\beta}, \boldsymbol{\gamma\alpha} \in \mathcal{E}, \tag{6a}$$

$$\begin{aligned} &\sum_{\boldsymbol{\alpha\beta} \in \mathcal{E}} \left(\frac{\mathrm{d}}{\mathrm{d}t} - \mathrm{i}(a_{\boldsymbol{\alpha\beta}} + k_R \sigma_{\boldsymbol{\alpha\beta}}) \right) \mathbf{f}_{\boldsymbol{\alpha\beta}}(0) \\ &\quad - \sum_{\boldsymbol{\beta\alpha} \in \mathcal{E}} \left(\frac{\mathrm{d}}{\mathrm{d}t} - \mathrm{i}(a_{\boldsymbol{\beta\alpha}} + k_R \sigma_{\boldsymbol{\beta\alpha}}) \right) \mathbf{f}_{\boldsymbol{\beta\alpha}}(l_{\boldsymbol{\beta\alpha}}) = \varepsilon(\boldsymbol{\alpha}) \mathbf{f}(\alpha), \end{aligned} \tag{6b}$$

where $\varepsilon(\boldsymbol{\alpha})$ are real-valued parameters. The case $\varepsilon(\boldsymbol{\alpha}) = 0$ may be considered as an ideal coupling, which is the analog of the Kirchhoff coupling in the scalar case. We are going to consider L as the Hamiltonian of the system, and our next aim is to show its self-adjointness.

B. Self-adjointness and spectral analysis

Denote by $\mathcal{D}$ the set of all functions $\mathbf{f}=(\mathbf{f}_{\boldsymbol{\alpha\beta}})$, with components $(\mathbf{f}_{\boldsymbol{\alpha\beta}}) \in \oplus H^2([0,l_{\boldsymbol{\alpha\beta}}]\mathbb{C}^2)$, $\boldsymbol{\alpha\beta} \in \mathcal{E}$, which are continuous at all nodes, i.e., such that the condition (6a) is satisfied. Clearly, for $\mathbf{f} \in \mathcal{D}$ the values $\mathbf{f}(\boldsymbol{\alpha})$, $\boldsymbol{\alpha} \in \mathcal{V}$, have the direct sense. Furthermore, for $\mathbf{f} \in \mathcal{D}$ and $\boldsymbol{\alpha} \in \mathcal{V}$ denote

$$\mathbf{f}'(\boldsymbol{\alpha}) := \sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}} \left(\frac{\mathrm{d}}{\mathrm{d}t} - \mathrm{i}(a_{\boldsymbol{\alpha\beta}} + k_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})\right)\mathbf{f}_{\boldsymbol{\alpha\beta}}(0) - \sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}} \left(\frac{\mathrm{d}}{\mathrm{d}t} - \mathrm{i}(a_{\boldsymbol{\beta\alpha}} + k_R\sigma_{\boldsymbol{\beta\alpha}})\right)\mathbf{f}_{\boldsymbol{\beta\alpha}}(l_{\boldsymbol{\beta\alpha}}).$$

Consider in $\mathcal{H}$ a linear operator Π with domain $\mathcal{D}$ acting by the rule (5).

Proposition 1: The operator Π *is closed. For any* $\mathbf{f} \in \operatorname{dom}\Pi \equiv \mathcal{D}$ *the vectors* $\Gamma\mathbf{f} := (\mathbf{f}(\boldsymbol{\alpha}))$ *and* $\Gamma'\mathbf{f} := (\mathbf{f}'(\boldsymbol{\alpha}))$ *belong to* $\ell^2(\mathcal{V},\mathbb{C}^2)$ *and the map* $(\Gamma,\Gamma'):\operatorname{dom} L \to \ell^2(\mathcal{V},\mathbb{C}^2)\oplus\ell^2(\mathcal{V},\mathbb{C}^2)$, *is surjective. For any* $\mathbf{f},\mathbf{g} \in \operatorname{dom}\Pi$ *there holds*

$$\langle \mathbf{f}, \Pi\mathbf{g}\rangle - \langle \Pi\mathbf{f}, \mathbf{g}\rangle = \langle \Gamma\mathbf{f}, \Gamma'\mathbf{g}\rangle - \langle \Gamma'\mathbf{f}, \Gamma\mathbf{g}\rangle. \tag{7}$$

Proof: Denote by $\Theta_{\boldsymbol{\alpha\beta}}$ the unitary transformation of $\mathcal{H}_{\boldsymbol{\alpha\beta}}$, given by

$$\Theta_{\boldsymbol{\alpha\beta}}\mathbf{f}(t) = \exp\left(\mathrm{i}\int_0^t (a_{\boldsymbol{\alpha\beta}}(s) + k_R\sigma_{\boldsymbol{\alpha\beta}})\mathrm{d}s\right)\mathbf{f}(t). \tag{8}$$

Denoting $\partial := \mathrm{d}/\mathrm{d}t$, we see $(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - \mathrm{i}k_R\sigma_{\boldsymbol{\alpha\beta}})\Theta_{\boldsymbol{\alpha\beta}} \equiv \Theta_{\boldsymbol{\alpha\beta}}\partial$.

By the Sobolev inequality, for any $c_1 > 0$ there exists $c_2 > 0$ such that for any $l > 0$ and $\varphi \in H^2[0,l]$ there holds that

$$\|\varphi\|_\infty \leqslant c_1 l^{3/2}\|\varphi''\|_{L^2[0,l]} + \frac{c_2}{l^{1/2}}\|\varphi\|_{L^2[0,l]},$$

$$\|\varphi'\|_\infty \leqslant c_1 l^{1/2}\|\varphi''\|_{L^2[0,l]} + \frac{c_2}{l^{1/2}}\|\varphi\|_{L^2[0,l]}.$$

Note that for any $t \in [0,l_{\boldsymbol{\alpha\beta}}]$ one has $\|\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\|_{\mathbb{C}^2} = \|\Theta_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\|_{\mathbb{C}^2}$. Therefore, using the above estimate, for any $\mathbf{f}_{\boldsymbol{\alpha\beta}} \in H^2([0,l_{\boldsymbol{\alpha\beta}}],\mathbb{C}^2)$, one has

$$\begin{aligned}\|\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\|_{\mathbb{C}^2} &= \|\Theta^*_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\|_{\mathbb{C}^2} \leqslant c_1 l_{\boldsymbol{\alpha\beta}}^{3/2}\|\partial^2\Theta^*_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}} + \frac{c_2}{l_{\boldsymbol{\alpha\beta}}^{1/2}}\|\Theta^*_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}}\\ &= c_1 l_{\boldsymbol{\alpha\beta}}^{3/2}\|\Theta^*_{\boldsymbol{\alpha\beta}}(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - ik_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})^2\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}} + \frac{c_2}{l_{\boldsymbol{\alpha\beta}}^{1/2}}\|\Theta^*_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}}\\ &= c_1 l_{\boldsymbol{\alpha\beta}}^{3/2}\|(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - ik_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})^2\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}} + \frac{c_2}{l_{\boldsymbol{\alpha\beta}}^{1/2}}\|\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}},\end{aligned}$$

and, in the same way,

$$\|(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - \mathrm{i}k_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\|_{\mathbb{C}^2} \leqslant c_1 l_{\boldsymbol{\alpha\beta}}^{1/2}\|(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - \mathrm{i}k_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})^2\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}} + \frac{c_2}{l_{\boldsymbol{\alpha\beta}}^{1/2}}\|\mathbf{f}_{\boldsymbol{\alpha\beta}}\|_{\mathcal{H}_{\boldsymbol{\alpha\beta}}}.$$

Using the assumptions (3) and (4), we conclude that there exist positive constants C_1 and C_2 such that for any $\boldsymbol{\alpha\beta} \in \mathcal{E}$, $\mathbf{f}_{\boldsymbol{\alpha\beta}} \in H^2([0,l_{\boldsymbol{\alpha\beta}}],\mathbb{C}^2), t \in [0,l_{\boldsymbol{\alpha\beta}}]$ one has

$$\|\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\| \leqslant C_1\|L_{\boldsymbol{\alpha\beta}}f_{\boldsymbol{\alpha\beta}}\| + C_2\|f_{\boldsymbol{\alpha\beta}}\|, \tag{9a}$$

$$\|(\partial - \mathrm{i}a_{\boldsymbol{\alpha\beta}} - \mathrm{i}k_{\mathrm{R}}\sigma_{\boldsymbol{\alpha\beta}})\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)\| \leqslant C_1\|L_{\boldsymbol{\alpha\beta}}f_{\boldsymbol{\alpha\beta}}\| + C_2\|f_{\boldsymbol{\alpha\beta}}\|. \tag{9b}$$

Here the norms are taken in $\mathbb{C}^2$ on the left-hand side and in $\mathcal{H}_{\boldsymbol{\alpha\beta}}$ on the right-hand side.

Denote by $\widetilde{\Pi}$ the operator acting in $\mathcal{H}$ by the rule (5) on the domain $\mathrm{dom}\,\Pi = \oplus_{\boldsymbol{\alpha\beta}\in\mathcal{E}} H^2([0,l_{\boldsymbol{\alpha\beta}}],\mathbb{C}^2)$. Clearly, $\widetilde{\Pi}$ is closed. By (9a), the linear maps

$$T_{\boldsymbol{\alpha\beta\gamma}}:\mathrm{dom}\,\widetilde{\Pi} \ni \mathbf{f} \mapsto \mathbf{f}_{\boldsymbol{\alpha\beta}}(0) - \mathbf{f}_{\boldsymbol{\gamma\alpha}}(l_{\boldsymbol{\gamma\alpha}}) \in \mathbb{C}^2, \quad \boldsymbol{\alpha\beta},\boldsymbol{\gamma\alpha} \in \mathcal{E},$$

are bounded with respect to the graph norm of $\widetilde{\Pi}$. Therefore, the restriction of $\widetilde{\Pi}$ to the subspace where all these functionals vanish is a closed operator. As this restriction is exactly Π, the operator Π is closed.

For $\mathbf{f}\in\mathcal{D}$ the inclusions $\Gamma\mathbf{f},\Gamma'\mathbf{f}\in\ell^2(\mathcal{V},\mathbb{C}^2)$ follow immediately from the estimates (9) and the assumption (2); and the identity (7) can be verified directly using the partial integration.

To prove the surjectivity condition, we fix first four functions $f_{jk}\in H^2[0,1]$ with $f_{jk}^{(i)}(l) = \delta_{ij}\delta_{kl}, i,j,k,l\in\{0,1\}$. Take arbitrary $\boldsymbol{\xi},\boldsymbol{\xi}'\in\ell^2(\mathcal{V},\mathbb{C}^2)$. Denote

$$\tau_{\boldsymbol{\alpha\beta}} := \exp\left(\mathrm{i}\int_0^{l_{\boldsymbol{\alpha\beta}}} (a_{\boldsymbol{\alpha\beta}}(s) + k_R\sigma_{\boldsymbol{\alpha\beta}})\mathrm{d}s\right) \equiv \exp\left(\mathrm{i}\int_0^{l_{\boldsymbol{\alpha\beta}}} a_{\boldsymbol{\alpha\beta}}(s)\mathrm{d}s\right)(\cos k_R l_{\boldsymbol{\alpha\beta}} + \mathrm{i}\,\sigma_{\boldsymbol{\alpha\beta}}\sin k_R l_{\boldsymbol{\alpha\beta}})$$
$$\in \mathbf{U}(2). \tag{10}$$

By direct calculation, the function $\mathbf{f}\in\mathcal{H}$ whose components are of the form $\mathbf{f}_{\boldsymbol{\alpha\beta}} = \Theta_{\boldsymbol{\alpha\beta}}\mathbf{g}_{\boldsymbol{\alpha\beta}}$, where

$$\mathbf{g}_{\boldsymbol{\alpha\beta}}(t) = f_{00}\left(\frac{t}{l_{\boldsymbol{\alpha\beta}}}\right)\boldsymbol{\xi}(\boldsymbol{\alpha}) + f_{01}\left(\frac{t}{l_{\boldsymbol{\alpha\beta}}}\right)\tau^*_{\boldsymbol{\alpha\beta}}\boldsymbol{\xi}(\boldsymbol{\beta}) + \frac{l_{\boldsymbol{\alpha\beta}}}{\deg\boldsymbol{\alpha}} f_{10}\left(\frac{t}{l_{\boldsymbol{\alpha\beta}}}\right)\boldsymbol{\xi}'(\boldsymbol{\alpha}) - \frac{l_{\boldsymbol{\alpha\beta}}}{\deg\boldsymbol{\beta}} f_{11}\left(\frac{t}{l_{\alpha\beta}}\right)\tau^*_{\boldsymbol{\alpha\beta}}\boldsymbol{\xi}'(\boldsymbol{\beta}),$$

lies in $\mathcal{D}$ and satisfies $(\Gamma\mathbf{f},\Gamma'\mathbf{f}) = (\boldsymbol{\xi},\boldsymbol{\xi}')$. □

Proposition 1 shows that the space $\mathcal{G} := \ell^2(\mathcal{V},\mathbb{C}^2)$ and the maps $\Gamma,\Gamma':\mathrm{dom}\,\Pi\to\mathcal{G}$ form a *boundary triple* for Π see e.g., [Refs. 21 and 46, for a detailed discussion. The self-adjointness of Π would follow from the following assertion:[21] if Π has at least one self-adjoint restriction (i.e., if Π^* is symmetric) and A is a self-adjoint operator in $\mathcal{G}$, then the restriction of Π to the vectors $\varphi\in\mathrm{dom}\,\Pi$ satisfying $\Gamma'\varphi = A\Gamma\varphi$ is self-adjoint in $\mathcal{H}$.

Consider the restriction D of Π to the functions $\mathbf{f}$ satisfying $\Gamma\mathbf{f} = \mathbf{0}$. Clearly, this restriction is nothing but the direct sum $\oplus_{\boldsymbol{\alpha\beta}\in\mathcal{E}} D_{\boldsymbol{\alpha\beta}}$, where $D_{\boldsymbol{\alpha\beta}}$ is an operator in $\mathcal{H}_{\boldsymbol{\alpha\beta}}$ acting as $\mathbf{f}_{\boldsymbol{\alpha\beta}}\mapsto L_{\boldsymbol{\alpha\beta}}\mathbf{f}_{\boldsymbol{\alpha\beta}}$ on functions satisfying $\mathbf{f}_{\boldsymbol{\alpha\beta}}(0) = \mathbf{f}_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}}) = \mathbf{0}$. As each $D_{\boldsymbol{\alpha\beta}}$ is self-adjoint, so is D. Note that L itself is the restriction of Π to the functions $\mathbf{f}$ satisfying $\Gamma'\mathbf{f} = T\Gamma\mathbf{f}, T = \mathrm{diag}(\varepsilon(\boldsymbol{\alpha}))$. This implies

Proposition 2: The spin-orbit Hamiltonian L is self-adjoint.

To carry out the spectral analysis of L, it is useful to relate the resolvents of L and D by Krein's resolvent formula,[21]

$$(D-E)^{-1} - (L-E)^{-1} = \gamma(E)[M(E)-T]^{-1}\gamma^*(\bar{E}), \tag{11}$$

where $E\notin\mathrm{spec}\,L\cup\mathrm{spec}\,D$ and the maps $\gamma(E)$ and $M(E)$ are defined as follows. For a given $E\notin\mathrm{spec}\,D$ and $\boldsymbol{\xi}\in\ell^2(\mathcal{V},\mathbb{C}^2)$, the function $\gamma(E)\boldsymbol{\xi} = (\mathbf{f}_{\boldsymbol{\alpha\beta}})$ is the solution to $(\Pi - E)\mathbf{f} = \mathbf{0}$ satisfying $\Gamma\mathbf{f} = \boldsymbol{\xi}$. The map $M(E):\ell^2(\mathcal{V},\mathbb{C}^2)\to\ell^2(\mathcal{V},\mathbb{C}^2)$ is given by $M(E) = \Gamma'\gamma(E)$. A direct consequence of Eq. (11) is the relationship

$$\mathrm{spec}\,L\setminus\mathrm{spec}\,D = \{E\notin\mathrm{spec}\,D : 0\in\mathrm{spec}(M(E)-T)\}. \tag{12}$$

Moreover, $E\notin\mathrm{spec}\,D$ is an eigenvalue of L iff 0 is an eigenvalue of $M(E)-T$, and $\gamma(E)\ker(M(E)-T)$ is the corresponding eigensubspace.[26]

Denote by $\widetilde{D}_{\boldsymbol{\alpha\beta}}$ the self-adjoint operator in $L^2[0,l_{\boldsymbol{\alpha\beta}}]$ acting as $g_{\boldsymbol{\alpha\beta}}\mapsto -g''_{\boldsymbol{\alpha\beta}} + (U_{\boldsymbol{\alpha\beta}} - k_R^2)g_{\boldsymbol{\alpha\beta}}$ on functions $g_{\boldsymbol{\alpha\beta}}\in H^2[0,l_{\boldsymbol{\alpha\beta}}]$ satisfying the Dirichlet boundary condition, $g_{\boldsymbol{\alpha\beta}}(0) = g_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}}) = 0$. Note that the operators $\Theta^*_{\boldsymbol{\alpha\beta}}D_{\boldsymbol{\alpha\beta}}\Theta_{\boldsymbol{\alpha\beta}}$ are of the form $\widetilde{D}_{\boldsymbol{\alpha\beta}}\oplus\widetilde{D}_{\boldsymbol{\alpha\beta}}$. In particular, the spectra of $D_{\boldsymbol{\alpha\beta}}$ coincide with those of $\widetilde{D}_{\boldsymbol{\alpha\beta}}$ and are discrete sets, and $\mathrm{spec}\,D = \overline{\cup_{\boldsymbol{\alpha\beta}\in\mathcal{E}}\mathrm{spec}\,D_{\boldsymbol{\alpha\beta}}}$.

Equation (12) shows that the spectrum of L outside spec D is completely described in terms of $M(E)$. The question whether spec D or some parts of it enter to the spectrum of L must be analyzed individually, taking into account the magnetic and spin parameters and the topological properties of the graph.

Therefore, to carry out the spectral analysis for L, it is useful to calculate the map $M(E)$. This can be done in terms of special (scalar) solutions to the equation

$$-y''+U_{\alpha\beta}y=zy,\quad z\in\mathbb{C}. \tag{13}$$

Namely, denote by $s_{\alpha\beta}$ and $c_{\alpha\beta}$ the uniquely determined solutions of (13) satisfying the boundary conditions

$$s_{\alpha\beta}(0;z)=c'_{\alpha\beta}(0;z)=0,\quad s'_{\alpha\beta}(0;z)=c_{\alpha\beta}(0;z)=1.$$

Now let $\boldsymbol{\xi}\in\ell^2(\mathcal{V},\mathbb{C}^2)$. To find $\gamma(E)\boldsymbol{\xi}=:(\mathbf{f}_{\alpha\beta})$, we need to solve the boundary value problems,

$$\left[\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}+a_{\alpha\beta}+k_{\mathrm{R}}\sigma_{\alpha\beta}\right)^2+U_{\alpha\beta}-k_R^2\right]\mathbf{f}_{\alpha\beta}=E\mathbf{f}_{\alpha\beta},$$

$$\mathbf{f}_{\alpha\beta}(0)=\boldsymbol{\xi}(\alpha),\quad \mathbf{f}_{\alpha\beta}(l_{\alpha\beta})=\boldsymbol{\xi}(\beta). \tag{14}$$

Writing $\mathbf{f}_{\alpha\beta}:=\Theta_{\alpha\beta}\mathbf{g}_{\alpha\beta}$, where $\Theta_{\alpha\beta}$ is the unitary transformation from (8), we rewrite (14) as a boundary value problem for $\mathbf{g}_{\alpha\beta}$,

$$-\mathbf{g}''_{\alpha\beta}+U_{\alpha\beta}\mathbf{g}_{\alpha\beta}=(E+k_{\mathrm{R}}^2)\mathbf{g}_{\alpha\beta},$$

$$\mathbf{g}_{\alpha\beta}(0)=\boldsymbol{\xi}(\alpha),\quad \mathbf{g}_{\alpha\beta}(l_{\alpha\beta})=\tau^*_{\alpha\beta}\boldsymbol{\xi}(\beta). \tag{15}$$

The solution to (15) takes the form

$$\mathbf{g}_{\alpha\beta}(t)=\frac{s_{\alpha\beta}(t;E+k_{\mathrm{R}}^2)}{s_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)}\cdot[\tau^*_{\alpha\beta}\boldsymbol{\xi}(\beta)-c_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)\boldsymbol{\xi}(\alpha)]+c_{\alpha\beta}(t;E+k_{\mathrm{R}}^2)\boldsymbol{\xi}(\alpha).$$

Now we have

$$\mathbf{g}'_{\alpha\beta}(0)=\frac{1}{s_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}^2})}[\tau^*_{\alpha\beta}\boldsymbol{\xi}(\beta)-c_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)\boldsymbol{\xi}(\alpha)], \tag{16}$$

$$\mathbf{g}'_{\alpha\beta}(l_{\alpha\beta})=\frac{1}{s_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)}[s'_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)\tau^*_{\alpha\beta}\boldsymbol{\xi}(\beta)-\boldsymbol{\xi}(\alpha)]. \tag{17}$$

Nothing that

$$\mathbf{f}'(\alpha)=\sum_{\alpha\beta\in\mathcal{E}}\mathbf{g}'_{\alpha\beta}-\sum_{\beta\alpha\in\mathcal{E}}\tau_{\beta\alpha}\mathbf{g}'_{\alpha\beta}(l_{\alpha\beta})$$

we arrive at

$$\begin{aligned}M(E)\boldsymbol{\xi}(\alpha)=&\sum_{\alpha\beta\in\mathcal{E}}\frac{1}{s_{\alpha\beta}(l_{\alpha\beta};E+k_R^2)}\tau^*_{\alpha\beta}\boldsymbol{\xi}(\beta)+\sum_{\beta\alpha\in\mathcal{E}}\frac{1}{s_{\beta\alpha}(l_{\beta\alpha};E+k_R^2)}\tau^*_{\beta\alpha}\boldsymbol{\xi}(\beta)\\&-\left(\sum_{\alpha\beta\in\mathcal{E}}\frac{c_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)}{s_{\alpha\beta}(l_{\alpha\beta};E+k_{\mathrm{R}}^2)}+\sum_{\beta\alpha\in\mathcal{E}}\frac{s'_{\beta\alpha}(l_{\beta\alpha};E+k_{\mathrm{R}}^2)}{s_{\beta\alpha}(l_{\beta\alpha};E+k_{\mathrm{R}}^2)}\right)\boldsymbol{\xi}(\alpha).\end{aligned} \tag{18}$$

Using Krein's resolvent formula (11) we come to the following theorem.

Theorem 3: *The set* spec $L\backslash$spec D *consists exactly of the real numbers* E *such that* 0

$\in \operatorname{spec}[M(E)-T]$, *where* $M(E)$ *and* T *are operators in* $\ell^2(\mathcal{V},\mathbb{C}^2)$, $M(E)$ *is given by* (18) *and* $T=\operatorname{diag}(\varepsilon(\boldsymbol{\alpha}))$. *Moreover, such* E *is an eigenvalue of* L *iff* 0 *is an eigenvalue of* $M(E)-T$, *and* $\gamma(E)\ker(M(E)-T)$ *is the corresponding eigenspace.*

We remark that in the above calculations it does not matter whether $\boldsymbol{\xi}$ is in ℓ^2 or not. Actually, all the construction hold for any set of vectors $\boldsymbol{\xi}(\boldsymbol{\alpha})\in\mathbb{C}^2, \boldsymbol{\alpha}\in\mathcal{V}$. This observation can be formulated as follows:

Theorem 4: *For* $E\notin \operatorname{spec} D$, *any continuous solution* $\mathbf{f}$ *to* $(L-E)\mathbf{f}=0$ *has the form*

$$\mathbf{f}_{\boldsymbol{\alpha\beta}}(t)=\frac{s_{\boldsymbol{\alpha\beta}}(t;E+k_R^2)}{s_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}};E+k_R^2)}\cdot\boldsymbol{\Theta}_{\boldsymbol{\alpha\beta}}[\tau^*_{\boldsymbol{\alpha\beta}}\mathbf{f}(\boldsymbol{\beta})-c_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}};E+k_{\mathrm{R}}^2)\mathbf{f}(\boldsymbol{\alpha})]+\boldsymbol{\Theta}_{\boldsymbol{\alpha\beta}}c_{\boldsymbol{\alpha\beta}}(t;E+k_{\mathrm{R}}^2)\mathbf{f}(\boldsymbol{\alpha}).$$

Such a function satisfies the boundary conditions (6b) *iff*

$$\sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}}\frac{1}{s_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}};E+k_{\mathrm{R}}^2)}\tau^*_{\boldsymbol{\alpha\beta}}\mathbf{f}(\boldsymbol{\beta})+\sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}}\frac{1}{s_{\boldsymbol{\beta\alpha}}(l_{\boldsymbol{\beta\alpha}};E+k_{\mathrm{R}}^2)}\tau_{\boldsymbol{\beta\alpha}}\mathbf{f}(\boldsymbol{\beta})$$
$$=\left(\sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}}\frac{c_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}};E+k_{\mathrm{R}}^2)}{s_{\boldsymbol{\alpha\beta}}(l_{\boldsymbol{\alpha\beta}};E+k_{\mathrm{R}}^2)}+\sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}}\frac{s'_{\boldsymbol{\beta\alpha}}(l_{\boldsymbol{\beta\alpha}};E+k_{\mathrm{R}}^2)}{s_{\boldsymbol{\beta\alpha}}(l_{\boldsymbol{\beta\alpha}};E+k_{\mathrm{R}}^2)}+\boldsymbol{\varepsilon}(\boldsymbol{\alpha})\right)\mathbf{f}(\boldsymbol{\alpha}).$$

Such an $\mathbf{f}$ *is an eigenfunction of* L (*i.e., belongs to* L^2) *iff* $(\mathbf{f}(\boldsymbol{\alpha}))_{\alpha\in\mathcal{V}}\in\ell^2(\mathcal{V},\mathbb{C}^2)$.

Note that similar formulas for more simple situations were obtained earlier, e.g., in Refs. 3, 5, 8, 22, 23, and 32.

The expression (18) can be simplified significantly if all the edges are the same, i.e., if $l_{\boldsymbol{\alpha\beta}}\equiv l$ and $U_{\boldsymbol{\alpha\beta}}\equiv U$, $s_{\boldsymbol{\alpha\beta}}=s, c_{\boldsymbol{\alpha\beta}}=c$ for all $\boldsymbol{\alpha\beta}\in\mathcal{E}$. Note that in this case the spectrum of D coincides with the Dirichlet spectrum of the operator $\widetilde{D}:=-\mathrm{d}^2/\mathrm{d}t^2+U-k_{\mathrm{R}}^2$ on the segment $[0,l]$ and hence is a discrete set. We have

$$M(E)\boldsymbol{\xi}(\boldsymbol{\alpha})=\frac{1}{s(l;E+k_{\mathrm{R}}^2)}\left\{\left[\sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}}\tau^*_{\boldsymbol{\alpha\beta}}\boldsymbol{\xi}(\boldsymbol{\beta})+\sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}}\tau_{\boldsymbol{\beta\alpha}}\boldsymbol{\xi}(\boldsymbol{\beta})\right]-[\operatorname{outdeg}\boldsymbol{\alpha}c(l;E+k_{\mathrm{R}}^2)\right.$$
$$\left.+\operatorname{indeg}\boldsymbol{\alpha}s'(l;E+k_{\mathrm{R}}^2)]\boldsymbol{\xi}(\boldsymbol{\alpha})\right.. \tag{19}$$

Even this expression admits further simplifications.

Proposition 5: Assume that all edges are identical, $l_{\boldsymbol{\alpha\beta}}\equiv l$, $U_{\boldsymbol{\alpha\beta}}\equiv U, U$ *is even,* $U(x)\equiv U(l-x)$, *and the coupling constants* $\varepsilon(\boldsymbol{\alpha})$ *are of the form* $\varepsilon(\boldsymbol{\alpha})=\deg\boldsymbol{\alpha}\varepsilon$, *then* $\operatorname{spec}L\setminus\operatorname{spec}\widetilde{D}=t_\varepsilon^{-1}(\operatorname{spec}\Delta)$, *where* $t_\varepsilon(E)=c(l;E+k_{\mathrm{R}}^2)+\varepsilon s(l;E+k_{\mathrm{R}}^2)$ *and* Δ *is the discrete Hamiltonian,*

$$\Delta\boldsymbol{\xi}(\boldsymbol{\alpha})=\frac{1}{\deg\boldsymbol{\alpha}}\left(\sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}}\tau^*_{\boldsymbol{\alpha\beta}}\boldsymbol{\xi}(\boldsymbol{\beta})+\sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}}\tau_{\boldsymbol{\beta\alpha}}\boldsymbol{\xi}(\boldsymbol{\beta})\right),$$

acting on the space $\ell^2(\mathcal{V},\mathbb{C}^2;\deg)$ *with the scalar product*

$$\langle\boldsymbol{\xi},\boldsymbol{\eta}\rangle_{\deg}=\sum_{\boldsymbol{\alpha}\in\mathcal{V}}\deg\boldsymbol{\alpha}\cdot\overline{\boldsymbol{\xi}(\boldsymbol{\alpha})}\,\boldsymbol{\eta}(\boldsymbol{\alpha}).$$

Proof: If the potential U is even, one has $c(l;E+k_{\mathrm{R}}^2)\equiv s'(l;E+k_{\mathrm{R}}^2):=t(E)$, see e.g., Ref. 44; hence

$$M(E)-T=\frac{1}{s(l;E+k_{\mathrm{R}}^2)}[\widetilde{\Delta}-t_\varepsilon(E)\deg],\quad \deg=\operatorname{diag}(\deg\boldsymbol{\alpha}),$$

where $\widetilde{\Delta}$ is the discrete Hamiltonian in $\ell^2(\mathcal{V},\mathbb{C}^2)$,

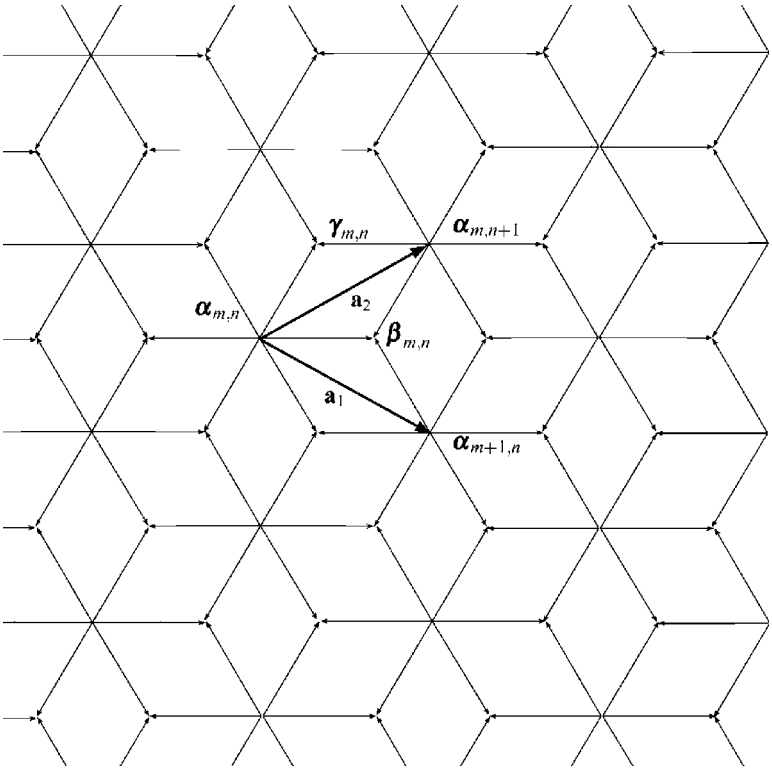

FIG. 1. A finite piece of a T_3 lattice.

$$\widetilde{\Delta}\boldsymbol{\xi}(\alpha) = \sum_{\boldsymbol{\alpha\beta}\in\mathcal{E}} \tau^*_{\alpha\beta}\boldsymbol{\xi}(\boldsymbol{\beta}) + \sum_{\boldsymbol{\beta\alpha}\in\mathcal{E}} \tau_{\beta\alpha}\boldsymbol{\xi}(\boldsymbol{\beta}).$$

The condition $0\in$ spec $[M(E)-T]$ takes the form $0\in\text{spec}[\widetilde{\Delta}-t_\varepsilon(E)\text{deg}]$ in $\ell^2(\mathcal{V},\mathbb{C}^2)$, which is equivalent to $0\in$ spec $[\Delta-t_\varepsilon(E)]$ in $\ell^2(\mathcal{V},\mathbb{C}^2;\text{deg})$. □

Proposition 5 shows that the spectral problem for a class of quantum graphs reduces to the study of the tight-binding Hamiltonian Δ. In the case $U\equiv 0$ and $\varepsilon(\boldsymbol{\alpha})\equiv 0$ one has $t_\varepsilon(E)=\cos\sqrt{E+k_\mathrm{R}^2}$, and we arrive at spec $L=\text{Arccos}^2$ spec $\Delta-k_\mathrm{R}^2$ (up to the discrete set spec $\widetilde{D}$), which is exactly the formula connecting the network and the tight-binding spectra in the de Gennes-Alexander model of superconductivity.[4] For the scalar situation, an analog of this correspondence was given, e.g., in Ref. 5 for the Laplacian on compact graphs, and in Ref. 16 for the Laplacian on noncompact graphs, and in Ref. 44 for more general Schrödinger operators. At the same time, Proposition 5 does not exhaust all possibilities of such a reduction, i.e., the reduction to a discrete Hamiltonian is possible also for some noneven U. (Such questions will be discussed in greater detail in Ref. 45.) One of such situations will be discussed in the next section.

III. SPECTRUM OF T_3 LATTICE

A. Description of the lattice

In this section, we consider the spectral problem for a quantum graph whose underlying structure is the so-called T_3 lattice (see Fig. 1). The nodes are the points $\boldsymbol{\alpha}_{m,n},\boldsymbol{\beta}_{m,n},\boldsymbol{\gamma}_{m,n}$, with $\boldsymbol{\alpha}_{m,n}=m\mathbf{a}_1+n\mathbf{a}_2,\mathbf{a}_1=\left(\frac{3}{2},-\sqrt{3}/2,0\right)$, $\mathbf{a}_2=\left(\frac{3}{2},\sqrt{3}/2,0\right),\boldsymbol{\beta}_{m,n}=\boldsymbol{\alpha}_{m,n}+(1,0,0),\boldsymbol{\gamma}_{m,n}=\boldsymbol{\alpha}_{m,n}+\left(\frac{1}{2},\frac{\sqrt{3}}{2},0\right),m,n\in\mathbb{Z}$, i.e.,

$$\boldsymbol{\alpha}_{m,n}=\left(\frac{3(m+n)}{2},\frac{\sqrt{3}(n-m)}{2},0\right),\quad \boldsymbol{\beta}_{m,n}=\left(\frac{3(m+n)+2}{2},\frac{\sqrt{3}(n-m)}{2},0\right),$$

$$\boldsymbol{\gamma}_{m,n} = \left(\frac{3(m+n)+1}{2}, \frac{\sqrt{3}(n-m+1)}{2}, 0 \right).$$

The edges are

$$e_{m,n,1} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\gamma}_{m,n}, \quad e_{m,n,2} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\beta}_{m-1,n}, \quad e_{m,n,3} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\gamma}_{m,n-1},$$

$$e_{m,n,4} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\beta}_{m,n-1}, \quad e_{m,n,5} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\gamma}_{m+1,n-1}, \quad e_{m,n,6} = \boldsymbol{\alpha}_{m,n}\boldsymbol{\beta}_{m,n}.$$

All the edges have the length 1. The direction vectors of $e_{m,n,j}$ are $\mathbf{e}_j = [\cos(\pi j/3), \sin(\pi j/3), 0], j = 1, \ldots, 6$.

B. Reduction to tight-binding Hamiltonian

We will assume that the system is subjected to the following external interactions. On each edge there is the same potential $U \in L^2[0,1]$. The lattice is subjected to the uniform magnetic field $\mathbf{B} = (0,0,2\pi\xi)$ orthogonal to the plane, and the magnetic vector potential in the symmetric gauge is $\mathbf{A}(\mathbf{x}) = (-\pi\xi x_2, \pi\xi x_1, 0)$. In what follows we use the magnetic parameter $\omega = \pi\xi\sqrt{3}/2$ expressing the magnetic flux through the elementary rhombus (for example, $\boldsymbol{\alpha}_{m,n}\boldsymbol{\beta}_{m,n}\boldsymbol{\alpha}_{m,n+1}\boldsymbol{\gamma}_{mn}$).

The external magnetic field implies nontrivial magnetic potentials on $e_{m,n,j}, a_{m,n,j} = 1/2\langle \mathbf{B} \times \boldsymbol{\alpha}_{m,n}, \mathbf{e}_j \rangle$,

$$a_{m,n,1} = \omega(2m+n), \quad a_{m,n,2} = \omega(m+2n), \quad a_{m,n,3} = \omega(n-m),$$

$$a_{m,n,4} = -\omega(2m+n), \quad a_{m,n,5} = -\omega(m+2n), \quad a_{m,n,3} = \omega(m-n).$$

The dynamics along $e_{m,n,j}$ is described by the differential expression

$$L_{m,n,j} = \left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} + a_{m,n,j} + k_{\mathrm{R}}\sigma_{m,n,j} \right)^2 + U - k_{\mathrm{R}}^2,$$

$$\sigma_{m,n,j} = \begin{pmatrix} 0 & e_{j2} + ie_{j1} \\ e_{j2} - ie_{j1} & 0 \end{pmatrix} \equiv \begin{pmatrix} 0 & \exp\left[\mathrm{i}\left(\frac{\pi}{2} - \frac{\pi j}{3} \right) \right] \\ \exp\left[\mathrm{i}\left(\frac{\pi j}{3} - \frac{\pi}{2} \right) \right] & 0 \end{pmatrix},$$

$$m,n \in \mathbb{Z} \quad j \in \{1, \ldots, 6\}.$$

Here e_{jk} are the components of the vectors $\mathbf{e}_j$ and k_{R} is the Rashba constant. We consider boundary conditions of the form (6) at all the nodes, assuming that there are only two types of coupling constants: $\lambda := \varepsilon(\boldsymbol{\alpha}_{m,n})$ and $\mu := \varepsilon(\boldsymbol{\beta}_{m,n}) = \varepsilon(\boldsymbol{\gamma}_{m,n})$.

The corresponding matrices $\tau_{m,n,j}$ from Eq. (10), $\tau_{m,n,j} = \exp[\mathrm{i}(a_{m,n,j} + k_R\sigma_{m,n,j})]$, are as follows:

$$\tau_{m,n,1} = \tau^*_{m,n,4} = \mathrm{e}^{\mathrm{i}\omega(2m+n)} \left\{ \cos k_{\mathrm{R}} + \mathrm{i} \sin k_{\mathrm{R}} \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}\pi/6} \\ \mathrm{e}^{-\mathrm{i}\pi/6} & 0 \end{pmatrix} \right\}, \tag{20a}$$

$$\tau_{m,n,2} = \tau^*_{m,n,5} = \mathrm{e}^{\mathrm{i}\omega(m+2n)} \left\{ \cos k_{\mathrm{R}} + \mathrm{i} \sin k_{\mathrm{R}} \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\pi/6} \\ \mathrm{e}^{\mathrm{i}\pi/6} & 0 \end{pmatrix} \right\}, \tag{20b}$$

$$\tau_{m,n,3} = \tau^*_{m,n,6} = \mathrm{e}^{\mathrm{i}\omega(n-m)} \left\{ \cos k_{\mathrm{R}} + \mathrm{i} \sin k_{\mathrm{R}} \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\pi/2} \\ \mathrm{e}^{\mathrm{i}\pi/2} & 0 \end{pmatrix} \right\}. \tag{20c}$$

Clearly, for any $m,n \in \mathbb{Z}$, one has

$$\text{outdeg}\,\boldsymbol{\alpha}_{m,n}=6,\quad \text{indeg}\,\boldsymbol{\beta}_{m,n}=\text{indeg}\,\boldsymbol{\gamma}_{m,n}=3,$$

$$\text{indeg}\,\boldsymbol{\alpha}_{m,n}=\text{outdeg}\,\boldsymbol{\beta}_{m,n}=\text{outdeg}\,\boldsymbol{\gamma}_{m,n}=0.$$

For the subsequent analysis, we use the fact that the lattice is bipartite. Represent the set of nodes as the disjoint union $\mathcal{V}=\mathcal{V}_0\cup\mathcal{V}_1, \mathcal{V}_0=\{\boldsymbol{\alpha}_{m,n}\}, \mathcal{V}_1=\{\boldsymbol{\beta}_{m,n}\}\cup\{\boldsymbol{\gamma}_{m,n}\}$. Clearly, for the set of edges one has $\mathcal{E}\subset\mathcal{V}_0\times\mathcal{V}_1$. With respect to the decomposition $\ell^2(\mathcal{V},\mathbb{C}^2)=\ell^2(\mathcal{V}_0,\mathbb{C}^2)\oplus\ell^2(\mathcal{V}_1,\mathbb{C}^2)$, the operator T in Theorem 3 takes the block-diagonal form

$$T=\begin{pmatrix}\lambda & 0\\ 0 & \mu\end{pmatrix}.$$

Using the above decomposition and Eq. (19), we rewrite $M(E)-T$ as

$$M(E)-T=\frac{1}{s(1;E+k_{\mathrm{R}}^2)}\begin{pmatrix}-a(E) & A^*\\ A & -b(E)\end{pmatrix},$$

$$a(E)=6c(1;E+k_{\mathrm{R}}^2)+\lambda s(1;E+k_{\mathrm{R}}^2),$$

$$b(E)=3s'(1;E+k_{\mathrm{R}}^2)+\mu s(1;E+k_{\mathrm{R}}^2),$$

where

$$A\mathbf{f}(\boldsymbol{\beta}_{m,n})=\tau_{m+1,n,2}\mathbf{f}(\boldsymbol{\alpha}_{m+1,n})+\tau_{m,n+1,4}\mathbf{f}(\boldsymbol{\alpha}_{m,n+1})+\tau_{m,n,6}\mathbf{f}(\boldsymbol{\alpha}_{m,n}),$$

$$A\mathbf{f}(\boldsymbol{\gamma}_{m,n})=\tau_{m,n,1}\mathbf{f}(\boldsymbol{\alpha}_{m,n})+\tau_{m,n+1,3}\mathbf{f}(\boldsymbol{\alpha}_{m,n+1})+\tau_{m-1,n+1,5}\mathbf{f}(\boldsymbol{\alpha}_{m-1,n+1}),$$

$$\begin{aligned}A^*\mathbf{f}(\boldsymbol{\alpha}_{m,n})=&\tau_{m,n,1}^*\mathbf{f}(\boldsymbol{\gamma}_{m,n})+\tau_{m,n,2}^*\mathbf{f}(\boldsymbol{\beta}_{m-1,n})+\tau_{m,n,3}^*\mathbf{f}(\boldsymbol{\gamma}_{m,n-1})\\&+\tau_{m,n,4}^*\mathbf{f}(\boldsymbol{\beta}_{m,n-1})+\tau_{m,n,5}^*\mathbf{f}(\boldsymbol{\gamma}_{m+1,n-1})+\tau_{m,n,6}^*\mathbf{f}(\boldsymbol{\beta}_{m,n}).\end{aligned}\tag{21}$$

The operator $A^*, A^*:\ell^2(\mathcal{V}_1,\mathbb{C}^2)\to\ell^2(\mathcal{V}_0,\mathbb{C}^2)$ is adjoint to $A, A:\ell^2(\mathcal{V}_0,\mathbb{C}^2)\to\ell^2(\mathcal{V}_1,\mathbb{C}^2)$. Using Theorem 3, we write the condition $E\in\operatorname{spec}L$ or, equivalently, $0\in\operatorname{spec}(M(E)-T)$, as

$$\frac{a(E)+b(E)}{2}\in\operatorname{spec}\left[\frac{b(E)-a(E)}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}+\begin{pmatrix}0 & A^*\\ A & 0\end{pmatrix}\right].\tag{22}$$

Note that $E\notin\operatorname{spec}\widetilde{D}$ in all the above constructions, where $\widetilde{D}$ is the Dirichlet realization of $-\mathrm{d}^2/\mathrm{d}t^2+U-k_{\mathrm{R}}^2$ on $[0,1]$. The question of whether spec $\widetilde{D}$ is a part of spec L or admits a simple answer in our case.

Lemma 6: For all ω and k_R one has $\operatorname{spec}\widetilde{D}\subset\operatorname{spec}L$.

Proof: Using the Schnol-type arguments, cf. Refs. 12 and 13, it is sufficient to show that for each $E\in\operatorname{spec}\widetilde{D}$ the equation $L\mathbf{f}=E\mathbf{f}$ has a bounded solution $\mathbf{f}$ satisfying the boundary conditions (6). Let $E\in\widetilde{D}$ and g be the corresponding eigenfunction of $\widetilde{D}$. Choose any infinite path $\mathcal{P}$ without intersection on the graph and any nonzero vector $\mathbf{z}\in\mathbb{C}^2$. For a fixed $e\in\mathcal{P}$ set $\mathbf{f}_e:=\Theta_e g\mathbf{z}$, where Θ_e is given by (8). Now extend $\mathbf{f}$ to the whole graph in such a way that (a) $\mathbf{f}_e=\mathbf{0}$ for $e\notin\mathcal{P}$ and (b) on each $b\in\mathcal{P}$ one has $\mathbf{f}_b=\Theta_b g\mathbf{z}_b$, where the vectors $\mathbf{z}_b$ are chosen in such a way that the boundary conditions (6) are satisfied. By construction, there holds $L\mathbf{f}=E\mathbf{f}$. At the same time, due to the unitarity of the matrices $\tau_{m,n,j}$ the obtained function $\mathbf{f}$ is bounded. This finishes the proof. □

C. Supersymmetric analysis

Equation (22) is a typical supersymmetric spectral problem. Using Proposition 11 and Corollary 12 in the Appendix , one easily sees that the set Σ of E for which the condition (22) is satisfied is the union $\Sigma=\Sigma_1\cup\Sigma_2\cap\Sigma_3$,

$$\Sigma_1=\{E\notin \operatorname{spec}\widetilde{D}: a(E)b(E)\neq 0 \text{ and } a(E)b(E)\in \operatorname{spec}A^*A\},$$

$$\Sigma_2=\begin{cases}\{E\notin \operatorname{spec}\widetilde{D}: a(E)=0\}, & \text{if } 0\in\operatorname{spec}A^*A,\\ \varnothing, & \text{otherwise;}\end{cases}$$

$$\Sigma_3=\begin{cases}\{E\notin \operatorname{spec}\widetilde{D}: b(E)=0\}, & \text{if } 0\in\operatorname{spec}AA^*,\\ \varnothing, & \text{otherwise.}\end{cases}$$

To summarize, we have the following.

Proposition 7: $\operatorname{spec}L=\Sigma_1\cup\Sigma_2\cup\Sigma_3\cup\operatorname{spec}\widetilde{D}$.

Note that the sets Σ_2,Σ_3, and $\operatorname{spec}\widetilde{D}$ are discrete. Therefore, only the set Σ_1 is responsible for the continuous spectrum. Writing $\mathbf{f}(\boldsymbol{\alpha}_{m,n})=:\mathbf{f}(m,n)$, we note that A^*A is an operator on $\ell^2(\mathbb{Z}^2,\mathbb{C}^2)$ of the form

$$\begin{aligned}A^*A\mathbf{f}(m,n)=&\,6\mathbf{f}(m,n)+(\tau^*_{m,n,1}\tau_{m,n+1,3}+\tau^*_{m,n,6}\tau_{m,n+1,4})\mathbf{f}(m,n+1)+(\tau^*_{m,n,3}\tau_{m,n-1,1}\\&+\tau^*_{m,n,4}\tau_{m,n-1,6})\mathbf{f}(m,n-1)+(\tau^*_{m,n,5}\tau_{m+1,n,3}+\tau^*_{m,n,6}\tau_{m+1,n,2})\mathbf{f}(m+1,n)+(\tau^*_{m,n,2}\tau_{m-1,n,6}\\&+\tau^*_{m,n,3}\tau_{m-1,n,5})\mathbf{f}(m-1,n)+(\tau^*_{m,n,1}\tau_{m-1,n+1,5}+\tau^*_{m,n,2}\tau_{m-1,n+1,4})\mathbf{f}(m-1,n+1)\\&+(\tau^*_{m,n,4}\tau_{m+1,n-1,2}+\tau^*_{m,n,5}\tau_{m+1,n-1,1})\mathbf{f}(m+1,n-1),\end{aligned}$$

i.e.,

$$\begin{aligned}A^*A=&\,6+\cos\omega\cdot\sin^2k_{\mathrm{R}}\cdot\widetilde{\Delta}+2\left[\cos\omega\cdot\cos^2k_{\mathrm{R}}-\sin^2k_{\mathrm{R}}\begin{pmatrix}\cos\left(\omega-\frac{\pi}{3}\right)&0\\0&\cos\left(\omega+\frac{\pi}{3}\right)\end{pmatrix}\right]\\&\times\begin{pmatrix}\Delta&0\\0&\Delta\end{pmatrix},\end{aligned}\tag{23}$$

where Δ is a spinless operator in $\ell^2(\mathbb{Z}^2)$,

$$\begin{aligned}\Delta f(m,n)=&\,\mathrm{e}^{-3\mathrm{i}\omega m}f(m,n+1)+\mathrm{e}^{3\mathrm{i}\omega m}f(m,n-1)+\mathrm{e}^{3\mathrm{i}\omega n}f(m+1,n)+\mathrm{e}^{-3\mathrm{i}\omega n}f(m-1,n)+\mathrm{e}^{-3\mathrm{i}\omega(m+n)}f(m\\&-1,n+1)+\mathrm{e}^{3\mathrm{i}\omega(m+n)}f(m+1,n-1),\end{aligned}$$

and

$$\begin{aligned}\widetilde{\Delta}\mathbf{f}(m,n)=&\,R_1\mathrm{e}^{-3\mathrm{i}\omega m}\mathbf{f}(m,n+1)+R_1^*\mathrm{e}^{3\mathrm{i}\omega m}\mathbf{f}(m,n-1)+R_2\mathrm{e}^{3\mathrm{i}\omega n}\mathbf{f}(m+1,n)+R_2^*\mathrm{e}^{-3\mathrm{i}\omega n}\mathbf{f}(m-1,n)\\&+R_3\mathrm{e}^{-3\mathrm{i}\omega(m+n)}\mathbf{f}(m-1,n+1)+R_3^*\mathrm{e}^{3\mathrm{i}\omega(m+n)}\mathbf{f}(m+1,n-1),\end{aligned}$$

with

$$R_1=\begin{pmatrix}0&\frac{3}{2}-\frac{\sqrt{3}}{2}\mathrm{i}\\-\frac{3}{2}-\frac{\sqrt{3}}{2}\mathrm{i}&0\end{pmatrix},\quad R_2=\begin{pmatrix}0&\frac{3}{2}+\frac{\sqrt{3}}{2}\mathrm{i}\\-\frac{3}{2}+\frac{\sqrt{3}}{2}\mathrm{i}&0\end{pmatrix},$$

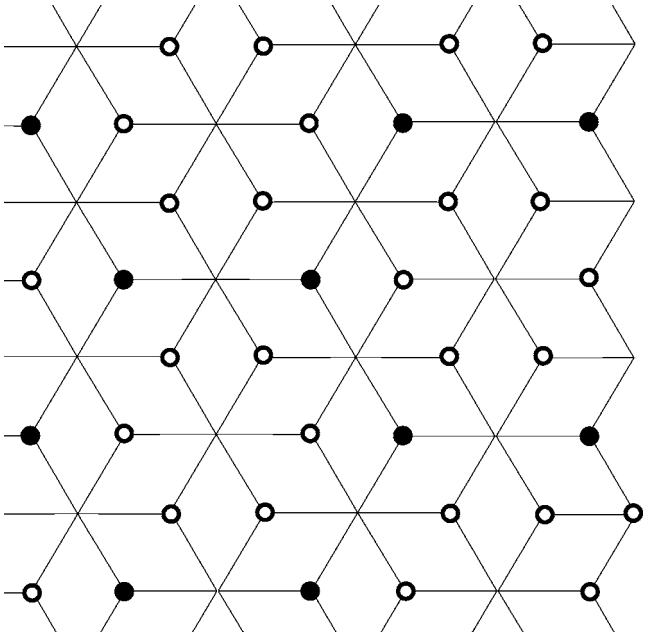

FIG. 2. Classification of the nodes $\boldsymbol{\beta}_{m,n}$ and $\boldsymbol{\gamma}_{m,n}$.

$$R_3 = \begin{pmatrix} 0 & -\sqrt{3}\mathrm{i} \\ -\sqrt{3}\mathrm{i} & 0 \end{pmatrix}.$$

The expression for A^*A shows explicitly the contribution of the magnetic and spin-orbit parameters to the spectrum. Let us discuss the situations where the spectrum shows certain localization phenomena.

D. Magnetic field induced extreme localization

If the spin-orbit interaction is not taken into account, $k_{\mathrm{R}}=0$, then one has $A^*A=6+2\cos\omega(\Delta\oplus\Delta)$. In particular, at $\omega-\pi/2\in\pi\mathbb{Z}$, one has $A^*A=6$, i.e., the spectrum of A^*A degenerates to a point. If $\omega-\pi/2\in\pi\mathbb{Z}$, but the spin-orbit interaction is nontrivial, similar phenomena occur only at certain values of the Rashba constant, i.e., $k_{\mathrm{R}}\in\pi\mathbb{Z}$. For generic values of k_{R}, obviously, there are some bands of continuous spectrum.

Let us analyze the sets Σ_2 and Σ_3 for this case, i.e., for $\omega-\pi/2\in\pi\mathbb{Z}$ and $k_{\mathrm{R}}\in\pi\mathbb{Z}$. Clearly, the set Σ_2 is empty, as $0\notin\operatorname{spec}A^*A$. Let us look at the operator AA^*.

Lemma 8: For $\omega-\pi/2\in\pi\mathbb{Z}$ and $k_R\in\mathbb{Z}$, one has $0\in\operatorname{spec}AA^*$.

Proof: In view of periodicity, it is sufficient to show that the equation $AA^*\psi=0$ has nontrivial bounded solutions, $\psi\in\ell^\infty(\mathcal{V}_1;\mathbb{C}^2)$.

Let us classify the nodes $\boldsymbol{\beta}_{m,n}$ and $\boldsymbol{\gamma}_{m,n}$ as shown in Fig. 2. Consider all vector-valued functions on $\mathcal{V}_1$ vanishing at the white marked nodes. For such a function ψ, the condition $A^*\psi=0$ is of very simple form, because in the expression (21) only two of the six terms on the right-hand side are nonzero. Therefore, fixing the value of ψ at a single black marked node, one uniquely extends ψ to a bounded solution of $A^*\psi=0$. The conditions $\omega\in\pi/2+\pi\mathbb{Z}$ and $k_{\mathrm{R}}\in\pi\mathbb{Z}$ guarantee that this solution is well defined, i.e., that the phase factor along each cycle on the hexagonal lattice of black nodes is 1. □

To summarize the previous considerations, we note that the set $\operatorname{spec}\widetilde{D}$ consists of the real E satisfying $s(1;E+k_{\mathrm{R}}^2)=0$. Proposition 7 reads as follows.

Theorem 9: *Let $\omega\in\pi/2+\pi\mathbb{Z}$ and $k_R\in\pi\mathbb{Z}$, then the spectrum of L consists of the real numbers E satisfying at least one of the following conditions:*

$$\left(c(1;E+k_{\mathrm{R}}^2)+\frac{\lambda}{6}(1;E+k_{\mathrm{R}}^2)\right)\cdot\left(s'(1;E+k_{\mathrm{R}}^2)+\frac{\mu}{3}s(1;E+k_{\mathrm{R}}^2)\right)=\frac{1}{3}, \tag{24a}$$

$$s'(1;E+k_{\mathrm{R}}^2)+\frac{\mu}{3}s(1;E+k_{\mathrm{R}}^2)=0, \tag{24b}$$

$$s(1;E+k_{\mathrm{R}}^2)=0. \tag{24c}$$

Each point of the spectrum is an infinitely degenerate eigenvalue.

Note that the eigenvalues (24a) are the most interesting ones, as they arise as the limit of the continuous spectrum. The Dirichlet eigenvalues (24c) are usually neglected in the physical works.

In the simplest case, when the scalar potential is zero and the couplings are trivial, i.e., $U=0,\lambda=\mu=0$, one has $s(x;E)=(1/\sqrt{E})\sin\sqrt{E}x, c(x;E)=\cos\sqrt{E}x$, and Eq. (24a) takes the form

$$\cos^2\sqrt{E+k_{\mathrm{R}}^2}\in\left\{0,\tfrac{1}{3},1\right\},$$

which was previously obtained in Ref. 54 for the case $k_{\mathrm{R}}=0$.

We remark that the presence of the extreme localization is periodic with respect to the shifts $k_{\mathrm{R}}\to k_{\mathrm{R}}+\pi$, but not the energy levels themselves, as the functions $s(\cdot;E+k_R^2)$, etc., are not periodic with respect to the Rashba constant. It is worthwhile to note that the above results hold for any potential U and any coupling constants λ and μ.

E. Magneto-spin induced localization

Another interesting situation appears at $\cos k_{\mathrm{R}}=0$, i.e., at $k_{\mathrm{R}}\in\pi/2+\pi\mathbb{Z}$. In this case one has

$$A^*A=6-2\begin{pmatrix}\cos\left(\omega-\frac{\pi}{3}\right)\Delta & 0\\ 0 & \cos\left(\omega+\frac{\pi}{3}\right)\Delta\end{pmatrix}.$$

For the values $\omega\in-\pi/6+\pi\mathbb{Z}$ the first component of A^*A degenerates. In particular, any function of the form $(f,0), f\in\ell^2(\mathbb{Z}^2)$ becomes an eigenfunction of A^*A. For $\omega\in\pi/6+\pi\mathbb{Z}$ the same holds for the functions $(0,f)$.

For a further analysis we calculate the spectrum of Δ.

Lemma 10: For $\omega\in\pm\pi/6+\pi\mathbb{Z}$ the spectrum of Δ is absolutely continuous and covers the segments $[-2\sqrt{3},-\sqrt{3}]$ and $[\sqrt{3},2\sqrt{3}]$.

Proof: Consider the unitary transformation

$$U:\ell^2(\mathbb{Z}^2)\ni(f(m,n))\mapsto(\mathrm{e}^{3\mathrm{i}\omega mn}f(m,n))\in\ell^2(\mathbb{Z}^2).$$

Clearly, U is unitary, and the operator $\hat{\Delta}:=U^*\Delta U$ has the form

$$\hat{\Delta}f(m,n)=\mathrm{e}^{-6\mathrm{i}\omega m}f(m,n+1)+\mathrm{e}^{6\mathrm{i}\omega m}f(m,n-1)+f(m+1,n)+f(m-1,n)+\mathrm{e}^{-3\mathrm{i}\omega(2m-1)}\times f(m-1,n+1)+\mathrm{e}^{3\mathrm{i}\omega(2m+1)}f(m+1,n-1).$$

The operator obtained has the same spectrum as Δ, but is periodic with respect to the shifts $n\mapsto n+1$ and can be studied using the Bloch analysis. Making the Bloch substitution $f(m,n)=\mathrm{e}^{\mathrm{i}nq}\xi_m$, where $q\in[0,2\pi)$ is the quasimomentum, we observe that the spectrum of $\hat{\Delta}$ is the union of the spectra of operators $H(q)$ acting in $\ell^2(\mathbb{Z})$ and defined by

$$(H(q)\xi)_m = 2\exp\left[-3\mathrm{i}\omega\left(m-\frac{1}{2}\right)+\mathrm{i}\frac{q}{2}\right]\cos\left[3\omega\left(m-\frac{1}{2}\right)-\frac{q}{2}\right]\xi_{m-1}+2\cos[6\omega m-q]\xi_m$$
$$+2\exp\left[3\mathrm{i}\omega\left(m+\frac{1}{2}\right)-\mathrm{i}\frac{q}{2}\right]\cos\left[3\omega\left(m+\frac{1}{2}\right)-\frac{q}{2}\right]\xi_{m+1}.$$

The operators $H(q)$ are nothing but the Harper operators for the triangular lattice.[18] Note that for $\omega\in\pm\pi/6+\pi\mathbb{Z}$, all these operators are invariant under the shift $m\mapsto m+2$. Therefore, substituting into the equation $H(q)\xi=E\xi$ a vector ξ satisfying $\xi_m=\mathrm{e}^{\mathrm{i}\theta}\xi_{m-2}$ for all m, where $\theta\in[0,2\pi)$ is another quasimomentum, one arrives at a 2×2 linear system for the components ξ_0 and ξ_1,

$$\mathrm{e}^{\mathrm{i}(3\omega/2+q/2)}\cos\left(\frac{3\omega}{2}+\frac{q}{2}\right)\mathrm{e}^{-\mathrm{i}\theta}\xi_1+\cos q\xi_0+\mathrm{e}^{-\mathrm{i}(3\omega/2-q/2)}\cos\left(\frac{3\omega}{2}-\frac{q}{2}\right)\xi_1=\frac{E}{2}\xi_0,$$

$$\mathrm{e}^{-\mathrm{i}(3\omega/2-q/2)}\cos\left(\frac{3\omega}{2}-\frac{q}{2}\right)\xi_0-\cos q\xi_1+\mathrm{e}^{-\mathrm{i}(3\omega/2+q/2)}\cos\left(\frac{3\omega}{2}+\frac{q}{2}\right)\mathrm{e}^{\mathrm{i}\theta}\xi_0=\frac{E}{2}\xi_1.$$

The condition for the determinants to vanish takes the form

$$\frac{E^2}{4}=1+\cos^2 q+\cos(q-\theta)\cos q=\frac{3}{4}+\left(\cos q+\frac{1}{2}\cos(q-\theta)\right)^2+\sin^2(q-\theta).$$

Here, taking all possible values of q and θ, we arrive at the conclusion. □

Lemma 10 means that for the values ω in question, the spectrum of A^*A has a continuous part, which is the union of the segments [0,3] and [9,12], and an infinitely degenerate eigenvalue 6.

Therefore, we arrive, as in Sec. III D, to a series of infinitely degenerate eigenvalues E satisfying the same Eq. (24a) (i.e., the *same* eigenvalues as in the extreme localization case), which are isolated in the spectrum, but we have additionally bands of continuous spectrum given by

$$\left(c(1;E+k_{\mathrm{R}}^2)+\frac{\lambda}{6}s(1;E+k_{\mathrm{R}}^2)\right)\cdot\left(s'(1;E+k_{\mathrm{R}}^2)+\frac{\mu}{3}s(1;E+k_{\mathrm{R}}^2)\right)\in\left[0,\frac{1}{6}\right]\cup\left[\frac{1}{2},\frac{2}{3}\right].$$

In particular, for the free case with zero coupling constants, one has the following characterization for E to be in the spectrum of L:

$$\cos^2\sqrt{E+k_R^2}\in\left[0,\frac{1}{6}\right]\cup\left\{\frac{1}{3}\right\}\cup\left[\frac{1}{2},\frac{2}{3}\right]\cup\{1\}.$$

The localization effect described in this section seems to be not covered by the existing works, and it would be interesting to know whether it can be really observed. As for different values of the magnetic paramteres we have completely different eigensubspaces of A^*A, we conjecture that this localization mechanism can be used to control the spin polarization by the magnetic field, but this needs a further analysis.

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Appendix: Supersymmetric spectral analysis

Here we prove the following proposition.

Proposition 11: Let $\mathcal{H}_1,\mathcal{H}_2$ are some Hilbert spaces, A be a bounded linear operator from $\mathcal{H}_1$ to $\mathcal{H}_2$, and $m\in\mathbb{R}$. On $\mathcal{H}_1\oplus\mathcal{H}_2$ consider the operator

$$L=\begin{pmatrix} m & A^* \\ A & -m \end{pmatrix}.$$

Then

$$\operatorname{spec} L=-\sqrt{\operatorname{spec}(AA^*+m^2)}\cup\sqrt{\operatorname{spec}(A^*A+m^2)}. \tag{A1}$$

This proposition is formulated (without proof) in Ref. 43 and is nothing but an abstract version of Proposition 2.5 in Ref. 49; we give here a complete proof just for the sake of completeness.

Proof: First, note that $\operatorname{spec} AA^*\setminus\{0\}=\operatorname{spec} A^*A\setminus\{0\}$.[20] Clearly,

$$L^2=\begin{pmatrix} A^*A+m^2 & 0 \\ 0 & AA^*+m^2 \end{pmatrix}. \tag{A2}$$

Therefore, $\operatorname{spec} L^2\setminus\{m^2\}=\operatorname{spec}(AA^*+m^2)\setminus\{m^2\}$, and for any $\lambda\in\operatorname{spec} AA^*\setminus\{0\}\equiv\operatorname{spec}AA^*\setminus\{0\}$, at least one of the numbers $-\sqrt{\lambda+m^2},\sqrt{\lambda+m^2}$ lies in spec L. Let us show that actually they both are in the spectrum of L.

Let $\lambda>0,\lambda\in\operatorname{spec} A^*A$; then there exists a sequence $(\phi_n),\phi_n\in\mathcal{H}_1$, such that $\|\phi_n\|\geqslant 1$ and $\lim(A^*A-\lambda)\phi_n=0$. Denote

$$\psi_n:=\left[\lambda+(\sqrt{\lambda+m^2}-m)\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}\right]\begin{pmatrix} \phi_n \\ 0 \end{pmatrix}. \tag{A3}$$

Clearly,

$$\begin{pmatrix} \phi_n \\ 0 \end{pmatrix}\perp\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}\begin{pmatrix} \phi_n \\ 0 \end{pmatrix},$$

which implies that

$$\|\psi_n\|\geqslant\lambda\|\phi_n\|\geqslant\lambda. \tag{A4}$$

By direct calculation,

$$(L-\sqrt{\lambda+m^2})\psi_n=(\sqrt{\lambda+m^2}-m)\begin{pmatrix} (A^*A-\lambda)\phi_n \\ 0 \end{pmatrix}.$$

Therefore, $\lim(L-\sqrt{\lambda+m^2})\psi_n=0$. Together with (A4), this implies that $\sqrt{\lambda+m^2}\in\operatorname{spec} L$.

To show $-\sqrt{\lambda+m^2}\in\operatorname{spec} L$ one has to consider the functions

$$\psi_n:=\left[\lambda-(\sqrt{\lambda+m^2}-m)\begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}\right]\begin{pmatrix} 0 \\ \phi_n \end{pmatrix},$$

where $\|\phi_n\|\geqslant 1$ and $\lim(AA^*-\lambda)\phi_n=0$, and to repeat the above steps. To finish the proof of Eq. (A1) it is necessary to study the points $\pm m$.

For $m=0$, Eq. (A2) reads as $\operatorname{spec} L^2=\operatorname{spec} AA^*\cup\operatorname{spec} A^*A$, and the conditions $0\in\operatorname{spec} L$ and $0\in\operatorname{spec} AA^*\cup\operatorname{spec} A^*A$ are equivalent.

Assume $m\neq 0$ and $m\in\operatorname{spec} L$, then there exist sequences $(\phi_n)\in\mathcal{H}_1,(\varphi_n)\in\mathcal{H}_2$ with

$$\|\phi_n\| + \|\varphi_n\| \geqslant 1 \tag{A5}$$

and

$$\lim(L-m)\begin{pmatrix}\phi_n\\ \varphi_n\end{pmatrix} \equiv \lim\begin{pmatrix}A^*\varphi_n\\ A\phi_n - 2m\varphi_n\end{pmatrix} = 0. \tag{A6}$$

Clearly, this implies $\lim A^*A\phi_n = 0$. Assume that $\lim \phi_n = 0$; then (A6) shows $\lim \varphi_n = 0$, which contradicts (A5). Therefore, there exists a subsequence (ϕ_n') of (ϕ_n) such that $\|\phi_n'\| \geqslant \varepsilon$ for some $\varepsilon > 0$. Together with $\lim A^*A\phi_n' = 0$, this implies $0 \in \operatorname{spec} A^*A$.

Assume now $0 \in \operatorname{spec} A^*A$, then there is a sequence $(\phi_n) \in \mathcal{H}_1$ with $\|\phi_n\| \geqslant 1$ and $\lim\langle A^*A\phi_n, \phi_n\rangle \equiv \lim\|A\phi_n\| = 0$. Then

$$\lim(L-m)\begin{pmatrix}\phi_n\\ 0\end{pmatrix} = \lim\begin{pmatrix}0\\ A\phi_n\end{pmatrix} = 0,$$

from which $m \in \operatorname{spec} L$.

The relationship between the conditions $-m \in L$ and $0 \in \operatorname{spec} AA^*$ can be proved in a completely similar way. □

It may be useful to have an alternative formulation of Proposition 11.

Corollary 12: There holds

$$\begin{aligned}\operatorname{spec} L \setminus \{-m, m\} &= -\sqrt{\operatorname{spec}(AA^* + m^2)} \cup \sqrt{\operatorname{spec}(AA^* + m^2)} \setminus \{-m, m\}\\ &\equiv -\sqrt{\operatorname{spec}(A^*A + m^2)} \cup \sqrt{\operatorname{spec}(A^*A + m^2)} \setminus \{-m, m\}.\end{aligned}$$

Furthermore, for $m \neq 0$, *one has* $m \in \operatorname{spec} L$ *iff* $0 \in \operatorname{spec} A^*A, -m \in \operatorname{spec} L$ *iff* $0 \in \operatorname{spec} AA^*$, *and for* $m = 0$ *there holds* $0 \in \operatorname{spec} L$ *iff* $0 \in \operatorname{spec} A^*A \cup \operatorname{spec} AA^*$.

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Basic properties of the current-current correlation measure for random Schrödinger operators

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The current-current correlation measure plays a crucial role in the theory of conductivity for disordered systems. We prove a Pastur-Shubin-type formula for the current-current correlation measure expressing it as a thermodynamic limit for random Schrödinger operators on the lattice and the continuum. We prove that the limit is independent of the self-adjoint boundary conditions and independent of a large family of expanding regions. We relate this finite-volume definition to the definition obtained by using the infinite-volume operators and the trace-per-unit volume. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2378618]

I. INTRODUCTION AND BASIC DEFINITIONS

The study of the transport properties of disordered systems requires an analysis of higher-order correlation measures of the spectral density operator $\rho_{H_\omega}(E) \equiv \pi^{-1} \lim_{\epsilon \to 0} \mathrm{Im}(H_\omega - E - i\epsilon)^{-1} \equiv \delta(H_\omega - E)$ of the one-particle random Schrödinger operator H_ω. The one-point correlation measure

$$\rho(E) = \mathbb{E}\{\langle x|\rho_{H_\omega}(E)|x\rangle\}, \tag{1}$$

which is independent of x by translational covariance [cf. Eq. (34)], is the density of states (DOS) measure. This measure has been extensively studied for random Schrödinger operators in recent years, and we refer the reader to the monographs.[1,2] The two-point correlation measure

$$K_2(x_1,y_1,x_2,y_2;E_1,E_2) = \mathbb{E}\{\langle x_1|\rho_{H_\omega}(E_1)|y_1\rangle\langle x_2|\rho_{H_\omega}(E_2)|y_2\rangle\}, \tag{2}$$

is related to, the current-current correlation measure that plays an important role in describing the conductivity of the system. In this note, we prove some fundamental properties of the current-current correlation measure such as the Pastur-Shubin formula. This formula expresses the function as the thermodynamic limit of quantities involving the system restricted to regions of finite volume.

Although this current-current correlation measure has been described in the literature, we could not find a complete proof of the Pastur-Shubin formula. Pastur[3] mentions the feasibility of a proof based on a perturbative expansion but this requires stronger conditions on the random potential than used here. The crucial point for continuum models is an estimate on the derivatives of the heat kernel. The necessary estimates on heat kernels associated with elliptic operators are proved by Eidelman and Ivasisen.[4] Shubin[5,6] considered the density of states and the current-current correlation measure for Schrödinger operators with uniformly almost periodic potentials, and more general elliptic operators with almost periodic coefficients. His results are similar to those we present here for random ergodic Schrödinger operators.

Our results apply to both lattice models with Hilbert space $\ell^2(\mathbb{Z}^d)$, and continuum models with Hilbert space $L^2(\mathbb{R}^d)$. For both of these settings, the random Hamiltonian H_ω, acting on $\ell^2(\mathbb{Z}^d)$ or $L^2(\mathbb{R}^d)$, is the self-adjoint operator given by

$$H_\omega = H_0 + V_\omega. \tag{3}$$

The Schrödinger operator $H_0 = L + V_0$ is the unperturbed, background operator, and V_ω is an ergodic, random, real-valued potential describing the disorder. Precise hypotheses on the deterministic potential V_0, and the random, ergodic potential V_ω, are given in Sec. II. We use the symbol L to denote either the finite-difference Laplacian on $\ell^2(\mathbb{Z}^d)$, or the non-negative Laplacian on $L^2(\mathbb{R}^d)$. The finite-difference Laplacian is defined by

$$(Lf)(n) = \sum_{m:|n-m|=1} f(m), \tag{4}$$

so that the spectrum is $[-2d, 2d]$. The non-negative Laplacian on $L^2(\mathbb{R}^d)$ is given by $L = -\Delta = -\Sigma_{\alpha=1}^d \partial^2/\partial x_\alpha^2 \geqslant 0$ and has spectrum $[0, \infty)$.

For one-particle quantum systems, the current operator J_α, describing the flow of charge in the x^α-direction, is proportional to the velocity operator ∇H_α. In order to define this observable, we let X_α denote the self-adjoint operator describing multiplication by the coordinate x_α, i.e., $X_\alpha f(x) = x_\alpha f(x)$, for $f \in C_0(\mathbb{R}^d)$. The *velocity operator* ∇H_α for direction x_α is the deterministic operator defined by

$$\nabla H_\alpha = i[H_\omega, X_\alpha] = i[L, X_\alpha], \tag{5}$$

so that $\nabla H_\alpha = -2i\,\partial/\partial x_\alpha$ on $L^2(\mathbb{R}^d)$. We describe ∇H_α on $\ell^2(\mathbb{Z}^d)$ in Sec. IV. Note that the velocity operator is independent of ω.

The *current-current correlation measure* can be described through either the trace-per-unit-volume formalism, in which one works directly with the infinite-volume operators, that is, with operators acting on $\ell^2(\mathbb{Z}^d)$ or on $L^2(\mathbb{R}^d)$, or through a limiting procedure of measures described by finite-volume observables acting on $\ell^2(\Lambda)$ or on $L^2(\Lambda)$, for bounded regions Λ. One of our results is that these two definitions define the same measure. In order to describe the finite-volume approach, we denote by H_Λ the restriction of H_ω to a finite volume $\Lambda \subset \mathbb{Z}^d$ or $\Lambda \subset \mathbb{R}^d$, with self-adjoint boundary conditions on the boundary $\partial\Lambda$. As H_Λ has discrete spectrum, we let $\psi_i^\Lambda(x) \in L^2(\Lambda)$ be the normalized eigenfunctions of the local Hamiltonian H_Λ with corresponding eigenvalues ϵ_i^Λ. We let $\nabla H_{i,j}^{(\alpha)}$ denote the matrix element of the velocity operator ∇H_α in the eigenstates ψ_j^Λ given by

$$\nabla H_{i,j}^{(\alpha)} = \langle \psi_i^\Lambda, \nabla H_\alpha \psi_j^\Lambda \rangle. \tag{6}$$

Note that these matrix-elements are well-defined although ∇H_α is not a self-adjoint operator when restricted to a finite volume region.

Definition 1.1: The *finite-volume current-current correlation measures* $m_\Lambda^{(\alpha)}$, *for current direction* α, *with* $\alpha = 1, \ldots, d$, *and for any bounded open region* $\Lambda \subset \mathbb{Z}^d$, *or* $\mathbb{R}^d$, *is the point measure on* $\mathbb{R}^2$ *defined, up to a constant prefactor, by*

$$m_\Lambda^\alpha(dE, dE') = \frac{1}{|\Lambda|} \sum_{i,j} \delta(E - \epsilon_i^\Lambda)\delta(E' - \epsilon_j^\Lambda)|\nabla H_{i,j}^{(\alpha)}|^2 dE dE', \tag{7}$$

with $\nabla H_{i,j}^{(\alpha)}$ *is the matrix element of the velocity operator in the direction* α *given in Eq.* (6), *and* $\{\epsilon_i^\Lambda\}_i$ *are the eigenvalues of the local Hamiltonian* H_Λ *corresponding to the eigenfunctions* ψ_i^Λ. *We write* $m_\Lambda(dE, dE') = \Sigma_{\alpha=1}^d m_\Lambda^\alpha(dE, dE')$ *for the total finite-volume current-current correlation measure*.

Of course, the point measures m_Λ^α depend on the configuration ω, the region Λ, and the boundary conditions on $\partial\Lambda$. One of our results is to prove that for a reasonable family of increasing regions $\Lambda_n \uparrow \mathbb{Z}^d$ or $\mathbb{R}^d$, and self-adjoint boundary conditions, the limit is independent of these, and almost surely independent of the configuration ω.

The physical significance of the limit measures $m_\alpha(dE, dE')$ is discussed thoroughly in Refs. 7–10, for example. These measures are directly related to the diagonal components of the finite-volume conductivity measures that we define as

$$\sigma_{\alpha\beta}(dE,dE') = \frac{\pi e^2}{|\Lambda|}\sum_{i\neq j}\delta(E-\epsilon_i^\Lambda)\,\delta(E'-\epsilon_j^\Lambda)\,\nabla H_{i,j}^{(\alpha)}\,\nabla H_{j,i}^{(\beta)}dEdE', \tag{8}$$

for $\alpha,\beta=1,\ldots,d$. The properties of these measures are basically unknown. In general, it is not known if the measures are absolutely continuous with respect to Lebesgue measure on $\mathbb{R}^2$ so that there exists a density $m(E,E')$. There has been some progress in understanding $m_\alpha(dE,dE')$ in the strong localization regime. Bellissard and Hislop[7] proved the existence of a smooth density in the strong disorder regime outside of the diagonal $E=E'$ for random Schrödinger operators with probability densities analytic in a strip. In Ref. 10, a density expansion for the correlation functions is developed based on the idea of Lifshitz emphasizing the role tunneling between deep and sparsely distributed potential wells that effectively trap the quantum particle in the strong localization regime. The authors apply this method to study the zero-temperature ac-conductivity tensor that is formally given by

$$\sigma_{\alpha\beta}(\nu,E_F) = \lim_{|\Lambda|\to\infty}\frac{\pi e^2}{|\Lambda|}\sum_{i\neq j}\delta(E_F+\nu-\epsilon_i^\Lambda)\,\delta(E_F-\epsilon_i^\Lambda)\,\nabla H_{i,j}^{(\alpha)}\,\nabla H_{j,i}^{(\beta)}, \tag{9}$$

where $\nu>0$ is the frequency of the external ac-field and E_F is the Fermi energy of the system. The goal is to study the low frequency behavior of the total ac-conductivity $\sigma(\nu,E_F)=\Sigma_\alpha\sigma_{\alpha\alpha}(\nu,E_F)$ in the strong localization regime. Mott[11] argued that the behavior is given by

$$\sigma(\nu,E_F) = C_0\rho^2(E_F)\,\nu^2(\log(1/\nu))^{d+1}, \tag{10}$$

now known as Mott's formula. The main result of[10] is an application of the density expansion method to give a heuristic derivation of Eq. (10). An upper bound on $\sigma(\nu,E_F)$, of the form given on the right in Eq. (10) but with an exponent $d+2$, has recently been proved in the strong localization regime by Klein, Lenoble, and Müller.[9]

II. PRELIMINARIES AND THE MAIN RESULTS

In this section, we first state the necessary hypotheses for the proof of the existence of the thermodynamic limit. As the techniques used in the continuum and lattice cases are different, the hypotheses on the potentials are different. For continuum models, we distinguish models that are $\mathbb{Z}^d$-ergodic or $\mathbb{R}^d$-ergodic, while for lattice models, the Hamiltonians are $\mathbb{Z}^d$-ergodic. We begin with the assumptions on the potentials for the continuum models. Let C_0 be the unit cube centered at the origin.

(H1C). For models that are $\mathbb{Z}^d$-ergodic, the background potential V_0 is a bounded, real-valued potential that is $\mathbb{Z}^d$-periodic and we assume $V_0\in C^{1,\beta}(C_0)$, for some $0<\beta$, where β is the Hölder continuity exponent. For models that are $\mathbb{R}^d$-ergodic, we take $V_0=0$.

(H2C). The potential V_ω is ergodic with respect to the group of translations $\mathbb{R}^d$ or the lattice translations $\mathbb{Z}^d$. It is lower semibounded and we assume that $V_\omega\in C^{1,\beta}(C_0)$, for some $0<\beta$, where β is the Hölder continuity exponent, and for almost every $\omega\in\Omega$.

For the lattice models, we make the following assumptions.

(H1L). The background potential V_0 is a bounded, real-valued potential that is $\Gamma_N\equiv N\mathbb{Z}^d$-periodic, for some $N\geqslant 1$.

(H2L). The potential V_ω is ergodic with respect to the group of lattice translations $\mathbb{Z}^d$. It is lower semibounded and has finite local expectation $\mathbb{E}\{|V_\omega(0)|\}<\infty$.

Note that if V_0 is $\Gamma_1=\mathbb{Z}^d$-periodic, it is simply a constant. We will denote by $C_0(N)$ a fundamental domain for the translation group Γ_N.

By shifting the energy, we may assume that the potentials V_0 and V_ω are non-negative. Under these assumptions, the Hamiltonians H_ω is self-adjoint for the lattice and continuum models, cf. Ref. 1, Chap. V. For a bounded region $\Lambda\subset\mathbb{R}^d$ or $\mathbb{Z}^d$, the local Hamiltonian H_Λ is obtained by taking the restriction of H_ω to Λ with some self-adjoint boundary conditions on $\partial\Lambda$, the boundary of Λ. *For continuum models, we may take either Dirichlet, Robin, or Neumann boundary conditions on the boundary $\partial\Lambda$ of the region Λ. For lattice models, we take Dirichlet boundary condi-*

tions. When not explicitly stated to the contrary, any result holds for any of the boundary conditions.

We also need some properties of the families of expanding regions Λ_n that we take to $\mathbb{Z}^d$ or $\mathbb{R}^d$. These conditions guarantee that the surface area of the boundary is vanishing small compared to the volume. We also need a mild regularity condition in the continuum case.

(vH). A sequence of bounded regions Λ_n converges to $\mathbb{Z}^d$ in the *sense of van Hove* if the following holds for any $a \in \mathbb{N}$. Consider a covering of $\mathbb{Z}^d$ by cubes Λ_a of side a centered at lattice points. For a bounded subset $\Lambda \subset \mathbb{Z}^d$, let $N_a^-(\Lambda) = \#\{\Lambda_a \cap \Lambda \neq \emptyset\}$ and let $N_a^+(\Lambda) = \#\{\Lambda_a \subset \Lambda\}$. Then, we require that

$$\lim_{n\to\infty} \frac{N_a^-(\Lambda_n)}{N_a^+(\Lambda_n)} = 1. \tag{11}$$

(F). A sequence of bounded regions Λ_n converges to $\mathbb{R}^d$ in the *sense of Fisher* if

$$\lim_{n\to\infty} \frac{|\partial\Lambda_n|}{|\Lambda_n|} = 0. \tag{12}$$

We assume that the boundary $\partial\Lambda_n \in C^{2,\beta}$, for $0 < \beta$ the Hölder exponent as in (H1C).

Let $E_{H_\omega}(\cdot)$ be the spectral family of the Hamiltonian H_ω (3), and for $x, y \in \mathbb{R}^d$, let $(\nabla H_\alpha E_H(dE) \nabla H_\alpha E_H(dE'))(x,y)$ represent the kernel of the operator defined, for any $f, g \in C_0(\mathbb{R})$ by

$$\nabla H_\alpha f(H_\omega) \nabla H_\alpha g(H) = \int_{\mathbb{R}} \int_{\mathbb{R}} f(E) g(E') m_\alpha(dE, dE'), \tag{13}$$

and described in Sec. V. The main results are the following theorems and representations of the current-current correlation measure. It proves the validity of a Pastur-Shubin formula for the current-current correlation measure. We begin with the continuum case.

Theorem 2.1: *We consider the continuum model (3) and the family of finite-volume current-current correlation measures* $m_\Lambda^\alpha(dE, dE')$, *defined in Eq.* (7), *for an increasing family of regions* Λ *satisfying condition* (*F*), *with Dirichlet*, *Robin*, *or Neumann boundary conditions*. *We assume hypotheses* (*H*1*C*) *and* (*H*2*C*). *Then*, *the sequence of finite-volume current-current correlation measures* $m_\Lambda^\alpha(dE, dE')$ *converges vaguely as* $|\Lambda| \to \infty$ *almost surely to a nonnegative measure* m_α. *The limit measure m is independent of the sequence of regions and the boundary conditions*. *Furthermore*, *the measure* m_α *admits the following representation*:

(1) *For the case with an* $\mathbb{R}^d$*-ergodic action*, *the limit measure* m_α *is given by*

$$\begin{aligned} m_\alpha(dE, dE') &= \lim_{|\Lambda|\uparrow\infty} m_\Lambda^\alpha(dE, dE') \\ &= \mathbb{E}\{(\nabla H_\alpha E_H(dE) \nabla H_\alpha E_H(dE'))(0,0)\}. \end{aligned} \tag{14}$$

(2) *For the case with a* $\mathbb{Z}^d$*-ergodic action*, *the limit measure* m_α *is given by*

$$\begin{aligned} m_\alpha(dE, dE') &= \lim_{|\Lambda|\uparrow\infty} m_\Lambda^\alpha(dE, dE') \\ &= \mathbb{E}\{Tr(\chi_{C_0} \nabla H_\alpha E_H(dE) \nabla H_\alpha E_H(dE') \chi_{C_0})\}. \end{aligned} \tag{15}$$

Consequently, the total current-current correlation measure $m = \sum_{\alpha=1}^d m_\alpha$ *exists and admits a representation as in Eqs.* (14) *or* (15).

The lattice case is different as we can use the Feynman-Kac formula directly. Because of this, we do not require any regularity on the potential.

Theorem 2.2: *We consider the* $\mathbb{Z}^d$*-ergodic lattice model given by Eqs.* (3) and (4), *and a family of finite-volume current-current correlation measures* $m_\Lambda^\alpha(dE, dE')$, *defined in Eq.* (7), *for*

an increasing family of regions Λ *satisfying condition* (vH), *with Dirichlet boundary conditions. We assume hypotheses* $(H1L)$ and $(H2L)$. *Then, the sequence of finite-volume current-current correlation measures* $m_\Lambda^\alpha(dE,dE')$ *converges vaguely as* $|\Lambda|\to\infty$ *almost surely to a nonnegative measure* m_α. *The limit measure* m *is independent of the sequence of regions. For a background potential* V_0 *that is* Γ_N*-periodic, for* $N\geqslant 1$, *the measure* m_α *admits the following representation*:

$$m_\alpha(dE,dE') = \lim_{|\Lambda|\uparrow\infty} m_\Lambda^\alpha(dE,dE')$$

$$= \frac{1}{N^d}\sum_{m\in C_0(N)} \mathbb{E}\{(\nabla H_\alpha E_H(dE)\,\nabla\, H_\alpha E_H(dE'))(m,m)\}. \tag{16}$$

The total current-current correlation measure $m=\sum_{\alpha=1}^d m_\alpha$ *exists and admits a representation as in Eq.* (16).

III. THE CURRENT-CURRENT CORRELATION MEASURE AS A THERMODYNAMIC LIMIT: CONTINUUM CASE

Introductory material in this section applies to both the lattice and continuum models. Details specific to the lattice models are given in Sec. IV. We will prove Theorem 2.1 using the two-variable Laplace transform, in analog with a standard proof of the Pastur-Shubin formula for the density of states (DOS) measure, cf. Ref. 12, and estimates on the convergence of finite-volume heat kernels[4]. We recall that in the study of the DOS measure, the convergence of the Laplace transform of the finite-volume DOS measure implies the vague convergence of the measures (cf. Ref. 12). We state and prove a similar result in Appendix A for a class of probability measures supported on the positive cone $(\mathbb{R}^+)^d$. The double Laplace transform of the finite-volume measure (7)), with $t>0$ and $p>0$, is given by

$$M_\Lambda^\alpha(t,p) = \int_{[0,\,\infty[^2} e^{-tE}e^{-pE'}\,m_\Lambda^\alpha(dE,dE') \tag{17}$$

$$= \frac{1}{|\Lambda|}\sum_{i,j} e^{-t\epsilon_i^\Lambda}e^{-p\epsilon_j^\Lambda}|\nabla H_{i,j}^{(\alpha)}|^2. \tag{18}$$

As above, we denote by ψ_i^Λ the normalized eigenvector of H_Λ associated with the energy ϵ_i^Λ. When Λ is fixed, we will occasionally omit the superscript Λ. We note that the integrals in Eq. (17) converge since

$$|\nabla H_{i,j}^{(\alpha)}|^2 \leqslant C_0|\mathrm{diam}\,\Lambda|^2|\epsilon_i^\Lambda-\epsilon_j^\Lambda|^2, \tag{19}$$

as follows from Eq. (5). Expanding these matrix elements in terms of the eigenfunctions for H_Λ, we find that

$$M_\Lambda^{(\alpha)}(t,p) = \frac{-4}{|\Lambda|}\int_{\Lambda^2} dxdy\sum_{i,j} e^{-t\epsilon_i}\partial_{x_\alpha}\psi_i(x)\bar{\psi}_i(y)e^{-p\epsilon_j}\partial_{y\alpha}\psi_j(y)\bar{\psi}_j(x). \tag{20}$$

The sums (20) can be expressed in terms of the local heat kernel and its derivatives. By Mercer's theorem, the local heat kernel can be expanded in the eigenfunctions of H_Λ and we write

$$K_\Lambda(t;x,y) = e^{-tH\Lambda}(x,y) = \sum_{i\geqslant 1} e^{-t\epsilon_i^\Lambda}\psi_i(x)\bar{\psi}_i(y), \tag{21}$$

for $t>0$, and $x,y\in\Lambda$. We then write $M_\Lambda^\alpha(t,p)$ in Eq. (20) as

$$M_\Lambda^{(\alpha)}(t,p) = \frac{-4}{|\Lambda|}\int_{\Lambda^2} dxdy\,\partial_{x_\alpha}K_\Lambda(t;x,y)\partial_{y_\alpha}K_\Lambda(t;y,x). \tag{22}$$

A. Heat kernels

Estimates on the heat kernels play an important role in evaluating the thermodynamic limit of Eq. (22). We will use the local heat kernels associated with H_Λ, and the nonrandom, unperturbed operator H_0^Λ on Λ, with the same self-adjoint boundary conditions. We denote these kernels by $K_\Lambda(t;x,y)$, and $K_\Lambda^{(0)}(t;x,y)$, respectively. We denote the heat kernel for the random operator $H_\omega(3)$, and the unperturbed operator H_0, both on $L^2(\mathbb{R}^d)$, by $K(t;x,y)$ and $K^{(0)}(t;x-y)$, respectively. Recall that $H_0=L$, the free operator, in the $\mathbb{R}^d$-ergodic case, and $H_0=L+V_0$, the unperturbed operator, in the $\mathbb{Z}^d$-ergodic case. In either case, we denote the free, translation-invariant, heat kernel associated with the Laplacian L by $K^{(\mathrm{free})}(t;x)$. These heat kernels are all real, nonnegative functions, and satisfy the following relationships:

$$0 \leqslant K_\Lambda(t;x,y) \leqslant K_\Lambda^{(0)}(t;x,y) \leqslant K^{(0)}(t;x,y) \leqslant K^{(free)}(t;x-y), \quad x,y \in \Lambda, \tag{23}$$

where the first inequality follows from the positivity assumptions (H1C) and (H2C), and the second follows from the Feynman-Kac representation (31). The free heat kernel associated with $H_0=L$ on $\mathbb{R}^d$ or $\mathbb{Z}^d$ is translation invariant and so a function of $(x-y)$ only. It is given by

$$K^{(\mathrm{free})}(t;x) = \frac{1}{(4\pi t)^{d/2}} e^{\frac{-\|x\|^2}{4t}}, \quad x \in \mathbb{R}^d, \tag{24}$$

with derivatives

$$\partial_{x_\alpha} K^{(\mathrm{free})}(t;x) = -\frac{2\pi x_\alpha}{(4\pi t)^{d/2+1}} e^{\frac{-\|x\|^2}{4t}}. \tag{25}$$

In the case when $H_0=L+V_0$, with a $\mathbb{Z}^d$-periodic operator, the heat kernel $K^{(0)}(t;x,y)$ is $\mathbb{Z}^d$-periodic. Finally, we note that the self-adjointness of the Hamiltonians implies that the corresponding heat kernels are symmetric $K^{(*)}(t;x,y)=K^{(*)}(t;y,x)$.

We now state a version of a general theorem for higher-order operators on smooth domains in $\mathbb{R}^d$ due to Eidelman and Ivasisen.[4] The version cited here also appears in the articles of Shubin[5,6] on the DOS measure for almost periodic operators.

Theorem 3.1: *Let $\Lambda \subset \mathbb{R}^d$ be a domain satisfying the regularity conditions stated in (F). We assume the local Hamiltonian H_Λ satisfies conditions (H1C) and (H2C) with Dirichlet, Robin, or Neumann boundary conditions on $\partial\Omega$. Let $K_\Lambda(t;x,y)$ denote the kernel of the local heat semigroup e^{-tH_Λ} on $L^2(\Lambda)$, and let $K(t;x,y)$ denote the kernel of the heat semigroup e^{-tH_ω} on $L^2(\mathbb{R}^d)$. We then have*

$$K_\Lambda(t;x,y) = K(t;x,y) + E_\Lambda(t;x,y), \quad \text{for } x,y \in \Lambda, \tag{26}$$

where, the difference E_Λ satisfies

$$|E_\Lambda(t;x,y)| \leqslant \frac{C_d}{t^{d/2}} e^{-(c_d/t)[\|x-y\| + d(w,\partial\Lambda)]^2}, \tag{27}$$

where w can be taken to be x or y, the constants C_d, $c_d>0$ are finite positive constants independent of Λ,t,x,y. The difference of the first partial derivatives of the heat kernels

$$\partial_{x_\alpha} K_\Lambda(t;x,y) = \partial_{x_\alpha} K(t;x,y) + F_\Lambda(t;x,y), \quad \text{for } x,y \in \Lambda, \tag{28}$$

satisfies

$$|F_\Lambda(t;x,y)| \leqslant \frac{\widetilde{C}_d}{t^{(d+1)/2}} e^{-(\tilde{c}_d/t)[\|x-y\| + d(w,\partial\Lambda)]^2}, \tag{29}$$

where w can be taken to be x or y, and the constants $\widetilde{C}_d, \tilde{c}_d>0$ are finite positive constants

independent of Λ, t, x, y. *The infinite-volume heat kernel and its first partial derivatives satisfy the following bound:*

$$|\partial_{x_\alpha}^j K(t;x,y)| \leqslant \frac{\widetilde{C}_{d,j}}{t^{(d+j)/2}} e^{-(\tilde{c}_{d,j}/t)\|x-y\|^2}, \tag{30}$$

for $j=0,1$.

Remark: Estimates on the difference of the Dirichlet heat kernels and the infinite volume heat kernel, as in Eqs. (26) and (27), *can be obtained from the Feynman-Kac formula. Using this representation, we have*

$$K_\Lambda(t;x,y) = K(t;x,y) + \mathbb{E}_{0,x}^{t,y}(e^{-\int_0^t (V_\omega(r(u))+V_0(r(u)))du}(1-\chi_\Lambda(r(\cdot)))), \tag{31}$$

where $\chi_\Lambda(r(u))=1$, *if* $r(u)\in\Lambda$ *for all* $u\in[0,t]$, *and zero otherwise. The difference term in Eq.* (31) *can be estimated as in Ref.* 12, *for example, and one obtains an upper bound like Eq.* (27). *This suffices for the DOS measure, but the higher-order correlation measures require estimates on the derivatives of the heat kernels that do not seem to be readily obtained from the Feynman-Kac formula.*

B. The Birkhoff Ergodic theorem for the continuum models

We now turn to the convergence of the sequence of the two-dimensional Laplace transforms $M_\Lambda^{(\alpha)}(t,p)$ defined in Eq. (22). We will use the estimates of Theorem 3.1 and the standard Birkhoff ergodic theorem in order to control the infinite volume limit. The form of the Birkhoff ergodic theorem depends upon whether the symmetry group is $\mathbb{Z}^d$ or $\mathbb{R}^d$. For models on $\mathbb{R}^d$, the random potential can either be $\mathbb{R}^d$ ergodic, such as a Gaussian random potential, or $\mathbb{Z}^d$-ergodic, such as the standard Anderson-type random potential. Suppose that the family $X_\omega(x)\in L^1(\Omega,\mathbb{P})$ is $\mathbb{R}^d$-ergodic. That is, there is an action τ_a for $\mathbb{R}^d$ on $(\Omega,\mathbb{P})$ so that the covariance property holds: $X_\omega(x+a) = X_{\tau_a\omega}(x)$. Then, the form of the Birkhoff ergodic theorem is

$$\mathbb{E}(X_\omega(0)) = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|}\int_\Lambda X_\omega(x)dx. \tag{32}$$

Let $C_0\subset\mathbb{R}^d$ denote the unit cube centered at the origin. In the $\mathbb{Z}^d$-ergodic case, we consider families of random variables $X_\omega(x)\in L^1(\Omega,\mathbb{P})$, satisfying the covariance property as above, but for $a\in\mathbb{Z}^d$, the Birkhoff ergodic theorem has the form

$$\int_{C_0} \mathbb{E}(X_\omega(x))dx = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|}\int_\Lambda X_\omega(x)dx. \tag{33}$$

We note that under our assumptions (H1C) and (H2C), the random potential V_ω is either $\mathbb{Z}^d$ or $\mathbb{R}^d$ ergodic, and that the Hamiltonian (3) satisfies

$$U_a H_\omega U_a^{-1} = H_{\tau_a\omega}, \tag{34}$$

for $a\mathbb{Z}^d$ or $a\in\mathbb{R}^d$, appropriately. As a consequence, the infinite-volume heat kernel $K_\omega(t;x,y)$ satisfies

$$K_\omega(t;x+a,y+a) = K_{\tau_a\omega}(t;x,y). \tag{35}$$

Furthermore, since the translations commute with differentiation, we have the following covariance property of the derivatives of the heat kernel:

$$U_a \partial_{x_\alpha} K_\omega(t;x,y) U_a^{-1} = \partial_{x_\alpha} K_\omega(t;x+a,y+a) = \partial_{x_\alpha} K_{\tau_a\omega}(t;x,y). \tag{36}$$

C. Convergence of the Laplace transform of the finite-volume measure

The main technical result is the convergence of the Laplace transforms of the finite-volume current-current correlation measure (7) in the continuous case.

Proposition 3.1: Let $K_\omega(t;x,y)$ denote the heat kernel for the Hamiltonian H_ω (3) on $L^2(\mathbb{R}^d)$. For every $t>0$ and $p>0$, the limit as $|\Lambda|\to\infty$ of $M_\Lambda^{(\alpha)}(t,p)$, with either Dirichlet, Robin, or Neumann boundary conditions, exists almost surely, for any $\alpha=1,\ldots,d$, and for any increasing sequence of domains satisfying condition (F). For $\mathbb{R}^d$ ergodic models on $\mathbb{R}^d$, the limit is equal to

$$M_\alpha(t,p) = \lim_{|\Lambda|\to\infty} M_\Lambda^{(\alpha)}(t,p) \tag{37}$$

$$= \mathbb{E}\left(-4 \int_{\mathbb{R}^d} dx \partial_{x_\alpha} K_\omega(t;x,0) \partial_{x_\alpha} K_\omega(p;0,x) \right). \tag{38}$$

For $\mathbb{Z}^d$-ergodic models on $\mathbb{R}^d$, the limit is equal to

$$M_\alpha(t,p) = \lim_{|\Lambda|\to\infty} M_\Lambda^{(\alpha)}(t,p) \tag{39}$$

$$= \mathbb{E}\left(-4 \int_{\mathbb{R}^d} dx \int_{C_0} dy \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x) \right). \tag{40}$$

Proof: We fix either Dirichlet, Robin, or Neumann boundary conditions and omit them from the notation. We always assume the regions satisfy (F). Recall that $M_\alpha(t,p)$ is given by

$$M_\alpha(t,p) = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_{\Lambda^2} dxdy \partial_{x_\alpha} K_\Lambda(t;x,y) \partial_{y_\alpha} K_\Lambda(p;y,x). \tag{41}$$

We first replace the derivatives of the finite-volume heat kernel K_Λ by the corresponding derivatives of the infinite-volume heat kernel K_ω in Eq. (41). We obtain

$$M_\alpha(t,p) = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_{\Lambda^2} dxdy \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x)$$

$$+ \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_{\Lambda^2} dxdy Q_\Lambda(t,p;x,y). \tag{42}$$

We estimate the remainder term involving Q_Λ using Theorem 3.1 and prove that this term converges to zero as $|\Lambda|\to\infty$. The details are given in Appendix B 1.

In order to apply the Birkhoff ergodic theorem, Eqs. (32) or (33), we replace the domain of $x\in\Lambda$ by $\mathbb{R}^d$ and obtain

$$M_\alpha(t,p) = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_{\mathbb{R}^d} dx \int_\Lambda dy \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x)$$

$$- \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_{\mathbb{R}^d\setminus\Lambda} dx \int_\Lambda dy \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x). \tag{43}$$

For the second term on the right of Eq. (43), we use estimate (30) and we prove that this term converges to zero in Appendix B 2. Let $X_\omega(t,p;y)$ be the family of random variables defined by

$$X_\omega(t,p;y) \equiv \int_{\mathbb{R}^d} dx \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x). \tag{44}$$

This family of random variable is $\mathbb{R}^d$ or $\mathbb{Z}^d$-covariant, as follows from Eq. (36), since

$$X_{\tau_a\omega}(t,p;y) = \int_{\mathbb{R}^d} dx \partial_{x_\alpha} K_\omega(t;x+a,y+a) \partial_{y_\alpha} K_\omega(p;y+a,x+a) = X_\omega(t,p;y+a). \tag{45}$$

Furthermore, we observe that $X_\omega(t,p;y) \in L^\infty(\Omega,\mathbb{P})$, uniformly in $y \in \mathbb{R}^d$. It follows from the translational invariance of the upper bound in Eq. (30) that

$$|X_\omega(t,p;y)| \leqslant \frac{(C_{d,1})^2}{t^{(d+1)/2} p^{(d+1)/2}} \int_{\mathbb{R}^d} dx e^{-2\tilde{c}_{d,1}(t+p)/tp\|x\|^2} \leqslant \frac{C_d}{(tp)^{1/2}(t+p)^{d/2}}. \tag{46}$$

Consequently, we apply Eq. (32) in the $\mathbb{R}^d$-ergodic case and obtain

$$\begin{aligned} M_\alpha(t,p) &= \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_\Lambda dy X_\omega(t,p;y) \\ &= \mathbb{E}\left\{ \int_{\mathbb{R}^d} dx \partial_{x_\alpha} K_\omega(t;x,0) \partial_{y_\alpha} K_\omega(p;0,x) \right\}. \end{aligned} \tag{47}$$

In the $\mathbb{Z}^d$-ergodic case, we apply Eq. (33) and obtain

$$\begin{aligned} M_\alpha(t,p) &= \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_\Lambda dy X_\omega(t,p;y) \\ &= \mathbb{E}\left\{ \int_{\mathbb{R}^d} dx \int_{C_0} dy \partial_{x_\alpha} K_\omega(t;x,y) \partial_{y_\alpha} K_\omega(p;y,x) \right\}. \end{aligned} \tag{48}$$

This proves the proposition. □

Corollary 3.1: From the definition of the velocity operator (5), we have

$$\partial_{x_\alpha} K_\omega(t;x,y) = \frac{-i}{2} (\nabla H_\alpha e^{-tH})(x,y), \tag{49}$$

so we can rewrite $M_\alpha(t,p)$ as given in Eq. (38) as

$$M_\alpha(t,p) = \mathbb{E}\{(\nabla H_\alpha e^{-tH} \nabla H_\alpha e^{-pH})(0,0)\}, \tag{50}$$

and as given in Eq. (40) as

$$M_\alpha(t,p) = \mathbb{E}\{Tr(\chi_{C_0} \nabla H_\alpha e^{-tH} \nabla H_\alpha e^{-pH} \chi_{C_0})\}. \tag{51}$$

D. Proof of Theorem 2.1

1. Proposition 3.1 shows that the limit of the double Laplace transform of the finite-volume current-current correlation measure exists almost surely. The limit is clearly independent of the family of expanding regions provided they satisfy condition (F). *A priori*, this limit depends on the boundary conditions, Dirichlet, Robin, or Neumann, used to define the finite-volume Hamiltonians. The independence of the boundary conditions follows from an estimate on the difference between pairs of heat kernels defined with the various boundary conditions. For example, the independence of Dirichlet or Neumann boundary conditions follow from estimating:

$$\partial_{x_\alpha}[K_\Lambda^D(t;x,y) - K_\Lambda^N(t;x,y)] = \partial_{x_\alpha}[K_\Lambda^D(t;x,y) - K(t;x,y)] + \partial_{x_\alpha}[K(t;x,y) - K_\Lambda^N(t;x,y)], \quad (52)$$

restricted to Λ. As each of the terms on the right in Eq. (52) are bounded above as in Eq. (27), we can show that

$$M_{\alpha,\Lambda}^D(t,p) - M_{\alpha,\Lambda}^N(t,p) \to 0, \quad (53)$$

as $\Lambda \to \mathbb{R}^d$ and for each $\alpha = 1, \ldots, d$. A similar estimate holds for any other pair of boundary conditions. Hence, the limit function $M_\alpha(t,p)$ is independent of the boundary conditions.

2. Given the convergence of the Laplace transforms, we prove in Appendix A, that there exists a unique measure $m_\alpha(dE, dE')$ such that

$$m_\alpha(dE, dE') = \lim_{|\Lambda| \uparrow \infty} m_\Lambda^\alpha(dE, dE'), \quad (54)$$

vaguely, and that

$$M_\alpha(t,p) = \int_{[0,\infty[^2} e^{-tE} e^{-pE'} m_\alpha(dE, dE'). \quad (55)$$

This expression of $M_\alpha(t,p)$ is given in Eq. (50) for the $\mathbb{R}^d$-ergodic case

$$M_\alpha(t,p) = \mathbb{E}_\omega((\nabla H_\alpha e^{-tH} \nabla H_\alpha e^{-pH})(0,0)), \quad (56)$$

and in Eq. (51) for the $\mathbb{Z}^d$-ergodic case

$$M_\alpha(t,p) = \mathbb{E}\{T_r(\chi C_0 \nabla H_\alpha e^{-tH} \nabla H_\alpha e^{-pH} \chi_{C_0})\}. \quad (57)$$

The spectral theorem allows us to write the semigroup e^{-mH} as $\int_\Sigma e^{-mE} E_H(dE)$, where Σ is the almost sure spectrum of the random family H_ω. In the case of a positive potential and $H_0 = -\Delta$, we have $\Sigma = [0, \infty[$. Using this representation in Eq. (56), we have

$$M_\alpha(t,p) = \int_{[0,\infty[^2} e^{-tE} e^{-pE'} \mathbb{E}\{(\nabla H_\alpha E_H(dE) \nabla H_\alpha E_H(dE'))(0,0)\}, \quad (58)$$

and the corresponding relation for Eq. (57). Comparing Eqs. (58) and (55), we obtain the result.□

IV. THE CURRENT-CURRENT CORRELATION MEASURE AS A THERMODYNAMIC LIMIT: LATTICE CASE

In this section, we prove Theorem 2.2 for the lattice case. The computation of the Pastur-Shubin formula for lattice models is different from the continuous case in two respects. First, the free heat kernel has sub-Gaussian, rather than Gaussian, decay. Second, the spatial derivative is a lattice translation so that estimates on the heat kernels only suffice for proving the existence of the thermodynamic limit.

A. Heat kernels

The lattice Laplacian defined in Eq. (4) has a Fourier transform given by $\mathcal{F}(L)(k) = \Sigma_{j=1}^d 2\cos(2\pi k_j)$, with $k \in T^d = [0,1]^d$. Using this to compute the $\mathbb{Z}^d$ -translation-invariant free heat kernel, one obtains

$$K^{(0)}(t;n) = e^{tL}(n) = \prod_{j=1}^d k^{(0)}(t;n_j), \quad n = (n_1, \ldots, n_d) \in \mathbb{Z}^d, \quad (59)$$

with $k^{(0)}(t;n_j)$, for $n_j \in \mathbb{Z}$, is the one-dimensional heat kernel given by

$$k^{(0)}(t;n_j) = i^{n_j} J_{n_j}(-2ti), \tag{60}$$

where $J_k(z)$ is the Bessel function of the first kind of order k given by

$$J_k(z) = \frac{1}{2\pi}\int_0^{2\pi} e^{iz\sin\theta} e^{-ik\theta} d\theta. \tag{61}$$

A simple calculation using the power series representation of $J_k(z)$ shows that $J_k(-2it) = i^{-k} P_k(t)$, where $P_k(t)$ is a positive function for $t \geqslant 0$. Consequently, the heat kernel $K^{(0)}(t;n)$ is a positive function for $t \geqslant 0$. The large $|n|$ behavior of this kernel is

$$K^{(0)}(t;n) \leqslant \frac{t^{C_d\|n\|}}{|n_1|!\ \ldots |n_d|!} e^{dt^2} \leqslant e^{dt^2} \prod_{j=1}^{d} (et)^{|n_j|} e^{-\alpha_d |n_j| \log(|n_j|+1)}. \tag{62}$$

This should be be compared with Eq. (24). In the case that $H_0 = L + V_0$, where V_0 satisfies (H1L), the free heat kernel is $\mathbb{Z}^d$-periodic. Inequalities (23) hold for the lattice model under hypotheses (H1L) and (H2L).

For the derivative in the x_α-direction, let e_α be the unit vector in that direction. There are actually two unitarily equivalent definitions of the derivative, one being

$$(\partial^+_{x_\alpha} f)(n) = f(n + e_\alpha), \tag{63}$$

and the other being

$$(\partial^-_{x_\alpha} f)(n) = f(n - e_\alpha). \tag{64}$$

We will work with the first definition $\partial^+_{x_\alpha}$, and drop the $+$ from the notation. With these definitions, the Laplacian defined in Eq. (4) is equal to $\Sigma_\alpha \partial^\pm_{x_\alpha}$, for either derivative. We compute, via Eq. (5), the αth-component of the velocity operator ∇H_α as i-times the partial derivative given in Eq. (63). The boundary $\partial\Lambda$ of the set $\Lambda \subset \mathbb{Z}^d$ is defined to be

$$\partial\Lambda = \left\{ n \in \Lambda^c; \quad \inf_{m\in\Lambda} |m-n| = 1 \right\}, \quad \partial\Lambda \subset \Lambda^c. \tag{65}$$

We present a version of Proposition 3.1 that holds for the lattice models with Dirichlet boundary conditions (DBC). The method of proof uses the Feynman-Kac formula (31). We refer the reader to Refs. 12 and 13 for a discussion of the Feynman-Kac formula and notation. Brownian motion on the lattice $\mathbb{Z}^d$ is discussed in the book of Carmona and Lacroix.[1] The proof given here in the lattice case is also applicable to the continuous models on $\mathbb{R}^d$ as remarked in Sec. III A. One has to use the Gaussian kernel (24) for $K^{(0)}$ and the Gaussian probability density in the calculation of the integral in Eq. (72) below. This will give the upper bound (27) for the difference of the heat kernels (26) in Theorem 3.1.

Proposition 4.1: *Let $K(t;m,n)$ and $K_\Lambda(t;m,n)$ be the infinite-volume and finite-volume heat kernels, respectively, for the Hamiltonian $H_\omega = L + V_0 + V_\omega$, on $\ell^2(\mathbb{Z}^d)$, respectively, on $\ell^2(\Lambda)$, with DBC and satisfying (H1L) and (H2L). We have*

$$K_\Lambda(t;m,n) = K(t;m,n) + E_\Lambda(t;m,n), \quad \text{for } m,n \in \Lambda, \tag{66}$$

where the difference E_Λ satisfies

$$|E_\Lambda(t;m,n)| \leqslant C_d e^{-c_d t} e^{-(\|m-n\|\log\|m-n\| + d(p,\partial\Lambda)\log d(p,\partial\Lambda))}, \tag{67}$$

where p can be taken to be either m or n, $d(\cdot,\cdot)$ denotes the distance function, and the constants $C_d, c_d > 0$ are finite positive constants independent of Λ, t, m, n.

Proof: The difference between the infinite volume heat kernel of the Hamiltonian $H = H_0 + V_\omega$ and the finite volume heat kernel (with Dirichlet boundary conditions) is given by the Feynman-Kac formula. Let $B(s)$ be d-dimensional Brownian motion on the lattice $\mathbb{Z}^d$ so that

$B(0)=0$. For $m,n \in \Lambda \subset \mathbb{Z}^d$ and $t>0$, let $b(s)$ be the Brownian bridge connecting m at $s=0$ to n at $s=t$. We then have

$$K(t;m,n) - K_\Lambda(t;m,n) = \mathbb{E}^{t,n}_{0,m}(e^{-\int_0^t (V_0+V_\omega)(b(u))du}) - \mathbb{E}^{t,n}_{0,m}(e^{-\int_0^t (V_0+V_\omega)(b(u))du}\chi_\Lambda(b(\cdot)))$$
$$= \mathbb{E}^{t,n}_{0,m}(e^{-\int_0^t (V_0+V_\omega)(b(u))du}(1-\chi_\Lambda(b(\cdot)))) \leqslant \mathbb{E}^{t,n}_{0,m}(1-\chi_\Lambda(b(\cdot))), \quad (68)$$

since the potential V_0+V_ω is nonnegative (actually, only lower semibounded is necessary). We recall that the measure corresponding to the expectation $\mathbb{E}^{t,n}_{0,m}$ in Eq. (68) satisfies

$$\mathbb{P}^{t,n}_{0,m}(\cdot) = K^{(0)}(t;n-m)\widetilde{\mathbb{P}}^{t,n}_{0,m}(\cdot), \quad (69)$$

where $\widetilde{\mathbb{P}}^{t,n}_{0,m}(\cdot)$ is the normalized probability measure on paths connecting m at $s=0$ to n at $s=t$. Because of the translation invariance and the nature of the integrand in the last term in Eq. (68), we have

$$\mathbb{E}^{t,n}_{0,m}(1-\chi_\Lambda(b(\cdot))) = \mathbb{E}^{t,n-m}_{0,0}(1-\chi_\Lambda(B(\cdot)+m)) = \mathbb{E}^{t,n-m}_{0,0}(B(s)+m \notin \Lambda, \quad \text{for some } 0 \leqslant s \leqslant t). \quad (70)$$

With reference to Eqs. (69) and (70), we note that the measure $\widetilde{\mathbb{P}}^{t,n-m}_{0,0}$ is the conditional probability measure for Brownian motion satisfying $B(0)=0$ and conditioned by $B(t)=n-m$. Bounding this above by the unconditioned probability measure $\bar{P}_{0,0}$, we obtain from Eq. (70)

$$\mathbb{E}^{t,n}_{0,m}(1-\chi_\Lambda(b(\cdot))) \leqslant K^{(0)}(t;m-n)\widetilde{\mathbb{P}}_{0,0}(B(s)+m \notin \Lambda, \quad \text{for some } 0 \leqslant s \leqslant t)$$
$$\leqslant K^{(0)}(t;m-n)\widetilde{\mathbb{P}}_{0,0}(|B(s)| \geqslant \operatorname{dist}(m,\partial\Lambda), \quad \text{for some } 0 \leqslant s \leqslant t). \quad (71)$$

The probability on the last line in Eq. (71) is calculated in Ref. 12 for the Gaussian case. The first line in Eq. (72) below, proven, for example, in Ref. 13, is called Lévy's inequality. We repeat this calculation here

$$\widetilde{\mathbb{P}}_{0,0}(|B(s)| \geqslant \operatorname{dist}(m,\partial\Lambda), \quad \text{for some } 0 \leqslant s \leqslant t)$$
$$\leqslant 2\widetilde{\mathbb{P}}_{0,0}(|B(t)| \geqslant \operatorname{dist}(m,\partial\Lambda))$$
$$\leqslant 2C(d,t) \sum_{\{n\in\mathbb{Z}^d : \|n\| > \operatorname{dist}(m,\partial\Lambda)\}} K^0(t;n), \quad (72)$$

where K^0 is defined in Eq. (59) and $C(d,t)>0$ is the normalization constant so that

$$C(d,t)\sum_{n\in\mathbb{Z}^d} K^0(t;n) = 1. \quad (73)$$

Using Eq. (62), we find that

$$\sum_{\{n\in\mathbb{Z}^d : \|n\| > \operatorname{dist}(m,\partial\Lambda)\}} K^{(0)}(t;n) \leqslant C_0 e^{-2t} e^{-C_1 d(m,\partial\Lambda)(\log d(m,\partial\Lambda) - |\log t|)}, \quad (74)$$

for some finite constants $C_0, C_1 > 0$. This estimate, along with the estimate (62) for the heat kernel prove bound (67). □

B. The Birkhoff Ergodic theorem for lattice models

For lattice models on $\ell^2(\mathbb{Z}^d)$, the translation group is $\mathbb{Z}^d$, or a subgroup $\Gamma_N = N\mathbb{Z}^d$, for $N \geqslant 1$. When $N=1$, we have $\Gamma_1 = \mathbb{Z}^d$. The operator $L+V_\omega$ is $\mathbb{Z}^d$-covariant, but the background potential V_0 may be only Γ_N-periodic. Consequently, the entire operator H_ω is Γ_N-covariant. In this case, the Birkhoff ergodic theorem that we will use is as follows. Let $X_\omega(m) \in L^1(\Omega,\mathbb{P})$ be a Γ_N-ergodic,

uniformly bounded, random variable such that $X_\omega(m+a)=X_{\tau_a\omega}(m)$, for any $a\in\Gamma_N$ and $m\in\mathbb{Z}^d$. Recall that τ_k is an ergodic action of Γ_N on the probability space $(\Omega,\mathbb{P})$. Let $C_0(N)$ denote a fundamental cell for Γ_N centered at the origin with volume $|C_0(N)|=N^d$. We then have

$$\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}(X_\omega(k))=\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|}\sum_{m\in\Lambda}X_\omega(m), \tag{75}$$

where the sequence of Γ_N-compatible regions Λ increases to $\mathbb{Z}^d$. When $N=1$, we obtain the usual expression

$$\mathbb{E}(X_\omega(0))=\lim_{|\Lambda|\uparrow\infty}\frac{1}{|\Lambda|}\sum_{j\in\Lambda}X_\omega(j). \tag{76}$$

C. Convergence of the Laplace transform of the finite-volume measure

We next present the analog of Proposition 3.1 for the lattice case.

Proposition 4.2: Let $K_\omega(t;x,y)$ denote the heat kernel for the Hamiltonian $H_\omega=L+V_0+V_\omega$ (3) on $\ell^2(\mathbb{Z}^d)$, with V_0 a Γ_N-periodic background potential. For every $t>0$ and $p>0$, the limit as $|\Lambda|\to\infty$ of $M_\Lambda^{(\alpha)}(t,p)$, with Dirichlet boundary conditions, exists almost surely, for any $\alpha=1,\ldots,d$, and for any increasing sequence of domains satisfying, condition (νH). The limit is equal to

$$M_\alpha(t,p)=\lim_{|\Lambda|\to\infty}M_\Lambda^{(\alpha)}(t,p) \tag{77}$$

$$=\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left(\sum_{m\in\mathbb{Z}^d}\partial_{m_\alpha}K_\omega(t;m,k)\partial_{m_\alpha}K_\omega(p;k,m)\right). \tag{78}$$

Proof: 1. In the lattice case, formula (22) reads

$$M_\Lambda(t,p)=\frac{1}{|\Lambda|}\sum_{m,n\in\Lambda}\partial_{m_\alpha}K_\Lambda(t;m,n)\partial_{n_\alpha}K_\Lambda(p;n,m). \tag{79}$$

From the definition (63), there are four terms involving the heat kernels K_Λ. We write $M_\Lambda=I+II+III+IV$, where

$$I=\frac{1}{|\Lambda|}\sum_{m,n\in\Lambda}K_\Lambda(t;m+e_\alpha,n)K_\Lambda(p;n+e_\alpha,m), \tag{80}$$

$$II=-\frac{1}{|\Lambda|}\sum_{m,n\in\Lambda}K_\Lambda(t;m,n)K_\Lambda(p;n+e_\alpha,m), \tag{81}$$

$$III=-\frac{1}{|\Lambda|}\sum_{m,n\in\Lambda}K_\Lambda(t;m+e_\alpha,n)K_\Lambda(p;n,m), \tag{82}$$

$$IV=\frac{1}{|\Lambda|}\sum_{m,n\in\Lambda}K_\Lambda(t;m,n)K_\Lambda(p;n,m). \tag{83}$$

2. We next replace each finite-volume heat kernel K_Λ by the infinite-volume heat kernel K_ω, restricted to Λ. As in the continuous case, the estimate of the difference E_Λ given in Proposition 4.1 is sufficient to repeat the arguments of Appendix B in the lattice case proving that the substitution can be performed.

3. We now use the Birkhoff ergodic theorem to control the resulting terms I,II,III,IV. For example, term I has the form

$$\frac{1}{|\Lambda|}\sum_{n,m\in\Lambda} K_\omega(t;m+e_\alpha,n)K_\omega(p;n+e_\alpha,m). \tag{84}$$

As in Sec. III, we replace the sum over $n\in\Lambda$ by the sum over $n\in\mathbb{Z}^d$. We now define

$$F_\omega(m)=\sum_{n\in Z^d} K_\omega(t;m+e_{\alpha,n})K_\omega(p;n+e_\alpha,m). \tag{85}$$

The covariance rule (35) and the translational invariance on the sum over n allow us to verify that

$$F_\omega(m+a)=F_{\tau_a\omega}(m), \tag{86}$$

for $a\in\Gamma_N$. As a consequence, the Birkhoff ergodic theorem (76) implies that

$$\lim_{\Lambda\to Z^d}\frac{1}{|\Lambda|}\sum_{m\in\Lambda} F_\omega(m)=\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\{F_\omega(k)\}, \tag{87}$$

so that term I has a limit

$$\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left\{\sum_{n\in Z^d} K_\omega(t;n+e_\alpha,k)K_\omega(p;e_\alpha,n)\right\}. \tag{88}$$

4. In the same way, we see that the limit of terms II–IV can be evaluated using the Birkhoff ergodic theorem and the invariance of the sum over Γ_N. We then find for these terms

$$-\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left\{\sum_{n\in Z^d} K_\omega(t;e_\alpha,n)K_\omega(p;n,k)\right\}, \tag{89}$$

$$-\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left\{\sum_{n\in Z^d} K_\omega(t;k,n)K_\omega(p;n+e_\alpha,k)\right\} \tag{90}$$

and

$$\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left\{\sum_{n\in Z^d} K_\omega(t;k,n)K_\omega(p;n,k)\right\}. \tag{91}$$

Combining the limits (88)–(91), we see that

$$\lim_{\Lambda\to Z^d} M_\Lambda^{(\alpha)}(t,p)=\frac{1}{N^d}\sum_{k\in C_0(N)}\mathbb{E}\left\{\sum_{n\in Z^d}\partial_{k_\alpha}K_\omega(t;k,n)\partial_{n_\alpha}K_\omega(p;n,k)\right\}. \tag{92}$$

The remaining parts of the proof proceed as in the continuum case. □

V. THE TRACE-PER-UNIT VOLUME APPROACH

There is another common, and equivalent, definition of the density of states measure using the infinite-volume Hamiltonian. We refer to this as the trace-per-unit volume definition. We refer the reader to Refs. 8 and 14 for further discussion. We extend this definition to the current-current

correlation measure. A covariant operator A_ω, for $\omega \in \Omega$, is a family of bounded, measurable operators satisfying $A_{\tau_j \omega} = U_j A_\omega U_j^{-1}$, for j in a translation group $\mathbb{R}^d$ or $\mathbb{Z}^d$.

Definition 5.1: *Let χ_Λ be the characteristic function on region $\Lambda \subset \mathbb{Z}^d$ or $\mathbb{R}^d$. The trace-per-unit volume of a covariant operator A_ω is defined as*

$$\mathcal{T}_{\mathbb{P}}(A) \equiv \lim_{\Lambda \to X} \frac{1}{|\Lambda|} Tr \chi_\Lambda A_\omega \chi_\Lambda, \tag{93}$$

where $X = \mathbb{Z}^d$ or $X = \mathbb{R}^d$.

Provided the limit in Eq. (93) exists, the ergodicity of the group action and the covariance property of A_ω imply that the limit is almost surely independent of ω. In order to obtain the integrated density of states $N(E)$, let $P_\omega(E)$ be the spectral projector for H_ω on the half-line $(-\infty, E]$. Then, we have $N(E) = \mathcal{T}_{\mathbb{P}}(P_\omega(E))$, and the DOS measure ν is defined through the relation

$$\int f(E) d\nu(E) = \mathcal{T}_{\mathbb{P}}(f(H_\omega)). \tag{94}$$

For the current-current correlation measures, we use standard notation for the velocity observable

$$\nabla H_\alpha \equiv i[H_\omega, X_\alpha] = i[H_0, X_\alpha], \tag{95}$$

as in the other sections. The infinite-volume *current-current correlation measures* $\tilde{m}_\alpha$, for $\alpha = 1, \ldots, d$, are defined directly using the infinite-volume operators H_ω. For two functions $f, g \in C_0(\mathbb{R})$, we define the bilinear mapping $\tilde{m}_\alpha$ by

$$f, g \in C_0(\mathbb{R}) \to \tilde{m}_\alpha(f, g) \equiv \mathcal{T}_{\mathbb{P}}\{\nabla H_\alpha f(H_\omega) \nabla H_\alpha g(H_\omega)\}. \tag{96}$$

This is the trace-per-unit volume of the covariant operator $\nabla H_\alpha f(H_\omega) \nabla H_\alpha g(H_\omega)$ and corresponds to the operator defined in Eq. (13).

Proposition 5.1: The map $\tilde{m}_\alpha$ defined on pairs of function as in Eq. (96) extends to a unique nonnegative linear functional on $C_0(\mathbb{R}^2)$ and hence determines a measure $\tilde{m}_\alpha$ on $\mathbb{R}^2$.

As a consequence, we note that for two intervals $\Delta_j \subset \mathbb{R}$, for $j = 1, 2$, the current-current correlation measure $\tilde{m}_\alpha$ is

$$\tilde{m}_\alpha(\Delta_1, \Delta_2) \equiv \mathcal{T}_{\mathbb{P}}\{\nabla H_\alpha E_H(\Delta_1) \nabla H_\alpha E_H(\Delta_2)\}. \tag{97}$$

The next theorem is the analog of a well-known result for the DOS. The DOS can be described through the thermodynamic limit as in Sec. II, or it can be described through the trace-per-unit volume approach as in Eq. (94). In most cases, these yield the same measure.

Theorem 5.1: *We assume the hypotheses of Theorems 2.1 or 2.2 and use the same increasing families of regions to construct $\tilde{m}_\alpha$. Then, the nonnegative measure $\tilde{m}_\alpha$, described in Proposition 5.1, is equal to the current-current correlation measure $\tilde{m}_\alpha$ constructed in Theorem 2.1, for continuum models, or in Theorem 2.2, for lattice models.*

Proof: We use the converse of Lemma 6.1 stating that if a uniformly bounded sequence of measures μ_n on $\mathbb{R}^d$ is such that the Laplace transforms converge pointwise, then the measures converge vaguely. We compare the Laplace transform of the local measure defined using H_Λ given by

$$\begin{aligned} L(\mu_\Lambda)(t,p) &= \frac{1}{|\Lambda|} Tr_\Lambda \nabla H_\alpha e^{-tH_\Lambda} \nabla H_\alpha e^{-pH_\Lambda} \\ &= \frac{1}{|\Lambda|} Tr_{\mathbb{R}^d} \chi_\Lambda \nabla H_\alpha e^{-tH_\Lambda} \nabla H_\alpha e^{-pH_\Lambda} \chi_\Lambda, \end{aligned} \tag{98}$$

with the expression involving the infinite-volume Hamiltonian H_ω restricted to Λ

$$L(\nu_\Lambda)(t,p) = \frac{1}{|\Lambda|} Tr_{\mathbb{R}^d} \chi_\Lambda \nabla H_\alpha e^{-tH_\omega} \nabla H_\alpha e^{-tH_\omega} \chi_\Lambda. \tag{99}$$

Note that the semigroups are smoothing operators. The convergence of the Laplace transforms requires that we prove the vanishing of the following two terms:

$$I = \frac{1}{|\Lambda|} Tr \chi_\Lambda (\nabla H_\alpha e^{-tH_\Lambda} - \nabla H_\alpha e^{-tH_\omega}) \nabla H_\alpha e^{-pH_\Lambda} \chi_\Lambda, \tag{100}$$

$$II = \frac{1}{|\Lambda|} Tr \chi_\Lambda \nabla H_\alpha e^{-tH_\omega} (\nabla H_\alpha e^{-pH_\Lambda} - \nabla H_\alpha e^{-pH_\omega}) \chi_\Lambda. \tag{101}$$

This follows directly from the estimates on the differences of the finite-volume and infinite-volume heat kernels and their derivatives as used in Secs. III and IV, and the arguments in Appendix B on the replacement of the finite-volume heat kernel by the infinite-volume one. □

It is, of course, an immediate consequence of the equality of m_α, constructed with some self-adjoint boundary condition, and $\tilde{m}_\alpha$, independent of any boundary conditions, that the current-current correlation measure is independent of the self-adjoint boundary conditions used to construct it.

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APPENDIX A: THE *d*-DIMENSIONAL LAPLACE TRANSFORM

We state the main results on the d-dimensional Laplace transform of positive measures supported on the positive cone $C_d^+ \equiv \{x \in \mathbb{R}^d | x_j > 0, \text{ for } j=1,\ldots,d\} \subset \mathbb{R}^d$ that we use in this paper. Let $\lambda=(\lambda_1,\ldots,\lambda_d)$ and $x=(x_1,\ldots,X_d)$ denote vectors in $\mathbb{R}^d$. Let μ be a d-dimensional positive measure defined on C_d^+ so that $\mu(C_d^+) \leqslant 1$. The d-dimensional Laplace transform of μ, denoted by $L(\mu)(\lambda)$, is given by

$$L(\mu)(\lambda) = \int_{C_d^+} e^{-\lambda \cdot x} d\mu(x), \tag{A1}$$

and we have $|L(\mu)(\lambda)| \leqslant 1$, for $\lambda \in C_d^+$. Of course, the Laplace transform exists for a much more general class of measures, but we do not deal with them here. We also need the following analyticity hypothesis on the Laplace transform.

Analyticity Hypothesis: The Laplace transform $L(\mu)(\lambda)$ *is analytic for* λ *in the product of half-planes* $\Pi^+ \equiv \{\lambda \in \mathbb{C}^d | \Re\lambda_j > 0, j=1,\ldots,d\}$.

It is clear from the representations (38) and (40), and the analyticity of the heat kernels in a half-plane, that this analyticity hypothesis is satisfied for the cases considered here.

We first recall the definition of vague convergence of measures, cf. Ref. 15. A sequence of measures μ_n on a measurable space Y *converges vaguely* to a measure μ if for any $f \in C_0(Y)$, we have $\mu_n(f) \to \mu(f)$, where $\mu(f) \equiv \int_Y f d\mu$. The main results that we use in this paper is the following theorem.

Theorem 6.1: *Let* $\{\mu_n\}$ *be a sequence of positive measures on* C_d^+ *such that* $\mu_n(C_d^+) \leqslant 1$ *and each measure* μ_n *satisfies the analyticity hypothesis. If the sequence of d-dimensional Laplace transforms* $L(\mu_n)$ *on* C_d^+ *converges pointwise to a finite function* ϕ, *also analytic on the product of half-planes* Π^+, *then there exists a unique positive measure* μ *on* C_d^+ *satisfying* $\mu(C_d^+) \leqslant 1$ *so that* $\phi(\lambda)=L(\mu)(\lambda)$, *and the measures* $\mu_n \to \mu$ *vaguely.*

We need two auxiliary lemmas.

Lemma 6.1: Suppose a sequence of nonnegative, normalized measures μ_n *on* C_d^+ *converges*

vaguely to a non-negative, normalized measure μ, *and the Laplace transforms* $L(\mu_n)(t)$ *converge pointwise for* $t \in C_d^+$ *to a function* $\phi(t)$. *Then, the Laplace transforms* $L(\mu_n)$ *converge pointwise to* $L(\mu)$, *that is,* $\phi(t)=L(\mu)(t)$.

Proof: Let f_n be a nonnegative function that is one for $t \in B_n(0) \cap C_d^+$, and zero otherwise. Because of the hypotheses on the measures, we note that for any n

$$\lim_{m\to\infty} L((1-f_m)\mu_n)(t) = 0, \quad t \in C_d^+. \tag{A2}$$

We also have uniformity in the sense that if $m>k$

$$0 \leqslant L(f_m\mu_n)(t) - L(f_k\mu_m)(t) \leqslant e^{-kt}, \quad t \in C_d^+. \tag{A3}$$

Using Eq. (A2), we have the following limits:

$$\lim_{n\to\infty}\lim_{m\to\infty} L(f_m\mu_n)(t) = \phi(t) \tag{A4}$$

and

$$\lim_{m\to\infty}\lim_{n\to\infty} L(f_m\mu_n)(t) = L(\mu)(t), \tag{A5}$$

for $t \in C_d^+$. Also, it is easy to show that

$$\lim_{m\to\infty} L(f_m\mu_m)(t) = \phi(t), \quad t \in C_d^+. \tag{A6}$$

If $m<n$, we have $0 \leqslant L(f_m\mu_n)(t) \leqslant L(f_n\mu_n)(t)$. Taking $n\to\infty$, we obtain from Eq. (A6) and vague convergence that $0 \leqslant L(f_m\mu)(t) \leqslant \phi(t)$, from which it follows that $0 \leqslant L(\mu)(t) \leqslant \phi(t)$. On the other hand, if $m>k$, we have

$$0 \leqslant L(f_m\mu_m)(t) = L((f_m - f_k)\mu_m)(t) + L(f_k\mu_m)(t) \leqslant e^{-kt} + L(f_k\mu_m)(t). \tag{A7}$$

Taking $m\to\infty$, it follows from Eq. (A3), Eq. (A6) and this inequality that $0 \leqslant \phi(t) \leqslant e^{-kt} + L(f_k\mu)(t)$. Now, taking $k\to\infty$, we obtain $0 \leqslant \phi(t) \leqslant L(\mu)(t)$. Hence, we have $\phi(t)=L(\mu)(t)$, for all $t \in C_d^+$. □

Lemma 6.2: (*Uniqueness*) *Distinct d-dimensional probability measures, satisfying the analyticity hypothesis, have distinct d-dimensional Laplace transforms.*

Proof: We use a multiple contour integral representation of the inverse Laplace transform (ILT) for contours $\gamma_j=\sigma_j+it_j$, with $t_j \in \mathbb{R}$ and $\sigma_j>0$. We first consider rectangles $R = \Pi_{j=1}^d [a_j,b_j] \subset C_d^+$, and compute the following limit:

$$\lim_{(t_j)\to\infty} \left(\frac{1}{2\pi i}\right)^d \int_{\sigma_1-it_1}^{\sigma_1+it_1} ds_1 \cdots \int_{\sigma_d-it_d}^{\sigma_d+it_d} ds_d \Pi_{k=1}^d \left(\frac{e^{s_k b_k} - e^{s_k a_k}}{s_k}\right) \mathcal{L}(\mu)(s_1, \ldots, s_d). \tag{A8}$$

We use the following identity:

$$\lim_{t_j\to\infty} \frac{1}{2\pi i} \int_{\sigma_j-it_j}^{\sigma_j+it_j} \frac{e^{s_j(b_j-x_j)} - e^{s_j(a_j-x_j)}}{s_j} ds_j = -[\Theta(x_j-b_j) - \Theta(x_j-a_j)], \tag{A9}$$

and the representation of the Laplace transform (A1). As a consequence, we see that the limit in Eq. (A8) is $\mu(R)$, for any rectangle $R \subset C_d^+$. Setting $a_j=0$, we recover a distribution function of the measure supported on C_d^+ and defined by $F_\mu(x_1,\ldots,x_d) \equiv \mu([0,x_1]\times[0,x_2]\times\cdots\times[0,x_d])$, Since the distribution function uniquely determines the measure, we see that if two measures μ_j, satisfying the above hypotheses, are such that $L(\mu_1)=L(\mu_2)$, their distribution functions, and hence the measures themselves, are equal. □

Proof of Theorem 6.1: 1. A normalized measure on C_d^+ is a positive measure with $\mu(C_d^+) \leqslant 1$.

Let μ_n be a sequence of normalized measures on $X=C_0(C_d^+)$ with the norm $\|f\|=\sup|f(x)|$. Each normalized measure defines a bounded linear functional on X since

$$|\mu(f)| \equiv \left| \int_{C_d^+} f d\mu \right| \leqslant \|f\|, \tag{A10}$$

for all $f \in X$. If $S^* \subset X^*$ denotes the unit ball of the dual X^*, then $\mu_n \in S^*$. Since S^* is compact in the weak* topology on X^*, there exists a weak* convergent subsequence μ_{n_j} in S^*. Let $\mu \in S^*$ be its limit point. By definition of weak* convergence, this means that $\mu_{n_j} \to \mu$ vaguely.

2. To prove that the sequence μ_n converges vaguely to μ, we use the Laplace transform $\phi_n \equiv L(\mu_n)$ defined in Eq. (A1). By hypothesis, the sequence $L(\mu_n)$ converges pointwise to a function ϕ on C_d^+. By Lemma 6.1, the vague convergence of measures implies the convergence of the Laplace transforms. Consequently, the subsequence $L(\phi_{n_j})$ converges to $L(\mu)$. But since the limit is unique, we have $L(\mu)=\phi=\lim_j L(\mu_j)$. By the uniqueness result Lemma 6.2, the function ϕ is the Laplace transform of μ.

3. Finally, we need to show that μ_n converges vaguely to μ. It follows that any vaguely convergent subsequence μ_{n_j} converges to μ. Since for any $f \in C_0(C_d^+)$, the sequence $\mu_n(f)$ is uniformly bounded, this implies $\mu_n(f) \to \mu(f)$. □

In order to apply Theorem 6.1 to the measures m_Λ^α, we need a renormalization since these positive measures are not probability measures. Since these measures grow at most polynomially in (E,E'), the Laplace transform exists and is pointwise bounded. Let $(t_0,p_0) \in C_2^+$ be a point at which the Laplace transform $L(m_{\Lambda_n}^\alpha)$ exists and is nonzero (such a point exists for all n). We define a sequence of renormalized measures by

$$\tilde{m}_{\Lambda_n}^\alpha(dE,dE') \equiv e^{-t_0 E - p_0 E'} \frac{m_{\Lambda_n}^\alpha(dE,dE')}{L(m_{\Lambda_n}^\alpha)(t_0,p_0)}. \tag{A11}$$

These positive measures satisfy

$$\tilde{m}_{\Lambda_n}^\alpha(C_2^+) = 1, \tag{A12}$$

and are hence probability measures. We can apply Theorem 6.1 to this sequence since, by Theorem 3.1, the Laplace transforms of m_Λ^α, and consequently of $\tilde{m}_\Lambda^\alpha$ converge pointwise. The Laplace transform of $\tilde{m}_\Lambda^\alpha$, dropping the subscript n, is then

$$L(\tilde{m}_\Lambda^\alpha)(t,p) = \int_{[0,\infty[^2} e^{-itE-pE'} \tilde{m}_\Lambda^\alpha(dE,dE') = \frac{L(m_\Lambda^\alpha)(t+t_0,p+p_0)}{L(m_\Lambda^\alpha)(t_0,p_0)}. \tag{A13}$$

As the Laplace transform is strictly positive, we know that $L(m_{\Lambda_n}^\alpha)(t_0,p_0) \to L(m_\alpha)(t_0,p_0) > 0$, so that the Laplace transforms $L(\tilde{m}_\Lambda^\alpha)(t,p)$ converge pointwise to

$$L(\tilde{m}_\Lambda^\alpha)(t,p) = \frac{L(m_\alpha)(t+t_0,p+p_0)}{L(m_\alpha)(t_0,p_0)}. \tag{A14}$$

So there exists a unique probability measure $\tilde{m}_\alpha(dE,dE')$ whose Laplace transform is $L(\tilde{m}_\alpha)$ and $\tilde{m}_\Lambda^\alpha \to \tilde{m}_\alpha$ vaguely. In order to remove the renormalization, we define a measure m_α by

$$m_\alpha(dE,dE') \equiv e^{t_0 E + p_0 E'} L(\tilde{m}_\alpha)(t_0,p_0) \tilde{m}_\alpha(dE,dE'). \tag{A15}$$

We have then the vague convergence

$$m_\alpha(dE,dE') = \lim_{\Lambda \to \mathbb{R}^d} m_\Lambda^\alpha(dE,dE'), \tag{A16}$$

completing the proof of Theorems 2.1 and 2.2.

APPENDIX B: SUBSTITUTION OF INFINITE-VOLUME HEAT KERNELS IN THE PROOF OF PROPOSITION 3.1

We present the technical details needed in the proof of Proposition 3.1. We work in the continuous case. Similar arguments work in the lattice case for the proof of Proposition 4.2, and we omit the details.

1. Replacement of finite-volume heat kernels by infinite-volume heat kernels

We provide the details of the replacement of the finite-volume heat kernels $\partial_{x_\alpha} K_\Lambda$ in Eq. (41) by the infinite-volume heat kernels $\partial_{x_\alpha} K$ restricted to the region Λ. Since these kernels should differ only on the boundary of the region, the difference should be of order of $|\partial\Lambda|$. We let $d(x,\partial\Lambda)$ denote the distance from $x \in \Lambda$ to the boundary of Λ, denoted by $\partial\Lambda$. In light of Eq. (29), the following integral plays a crucial role:

$$B(\Lambda) \equiv \int_\Lambda e^{-C_0(t)d(x,\partial\Lambda)^2} dx. \tag{B1}$$

We analyze this integral for families of increasing regions satisfying conditions (vH) or (F) in Appendix C and prove that

$$\lim_{n\to\infty} \frac{B(\Lambda_n)}{|\Lambda_n|_d} = 0, \tag{B2}$$

for a wide family of increasing regions Λ_n. We will always assume that we are working with a sequence Λ_n satisfying these conditions in this Appendix, and we will omit the index n from the notation. We consider the term in Eq. (41)

$$I_1 \equiv \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_\Lambda dy \int_\Lambda dx \partial_{x_\alpha} K_\Lambda(t;x,y) \partial_{y_\alpha} K_\Lambda((t;y,x)) \tag{B3}$$

$$\begin{aligned} &= \lim_{|\Lambda|\uparrow\infty} \left(\frac{1}{|\Lambda|} \int_\Lambda dy \int_\Lambda dx \partial_{x_\alpha} K(t;x,y) \partial_{y_\alpha} K(t;y,x) \right. \\ &\quad \left. + \frac{1}{|\Lambda|} \int_\Lambda dy \int_\Lambda dx Q_\Lambda(t,p;x,y) \right), \end{aligned} \tag{B4}$$

where we must control three terms

$$\begin{aligned} Q_\Lambda(t,p;x,y) &\equiv \partial_{x_\alpha} K_\Lambda(t;x,y) \partial_{y_\alpha} K_\Lambda(p;y,x) - \partial_{x_\alpha} K(t;x,y) \partial_{y_\alpha} K(p;y,x) \\ &= \partial_{x_\alpha} K(t;x,y) (\partial_{y_\alpha} K_\Lambda(p;y,x) - \partial_{y_\alpha} K(p;y,x)) \\ &\quad + (\partial_{x_\alpha} K_\Lambda(t;x,y) - \partial_{x_\alpha} K(t;x,y)) \partial_{y_\alpha} K(p;y,x) \\ &\quad + (\partial_{x_\alpha} K_\Lambda(t;x,y) - \partial_{x_\alpha} K(t;x,y)) (\partial_{y_\alpha} K_\Lambda(p;y,x) - \partial_{y_\alpha} K(p;y,x)) \\ &= J_1 + J_2 + J_3. \end{aligned} \tag{B5}$$

By Theorem 3.1, the differences can be written in terms of F_Λ described in Eqs. (28) and (29). To prove that the integral with $Q_\Lambda(t,p;x,y)$ in Eq. (B5) converges to zero, we first foucus on J_1, and note that J_2 is similar

$$J_1 = \lim_{|\Lambda|\uparrow\infty} \frac{1}{|\Lambda|} \int_\Lambda dy \int_\Lambda dx \partial_{x_\alpha} K(t;x-y) F_\Lambda(p;y,x). \tag{B6}$$

By using estimates (29) and (30), Eq. (B1), we easily obtain the upper bound

$$|J_1| \leq C(t,d)\frac{1}{|\Lambda|}\int_{\mathbb{R}^d} dy \int_\Lambda dx e^{-(\beta_d/t)\|x-y\|^2} e^{-(\bar{c}_d/t)d(x,\partial\Lambda)^2}$$

$$\leq \frac{C(t,d)}{|\Lambda|}\left(\int_{\mathbb{R}^d} du\ e^{-(\beta_d/t)\|u\|^2}\right)\left(\int_\Lambda dx e^{-(\bar{c}_d/t)d(x,\partial\Lambda)^2}\right) \leq C(t,d)\frac{B(\Lambda)}{|\Lambda|_d}. \tag{B7}$$

Because, of condition (F), this term vanishes as Λ increases to $\mathbb{R}^d$. The term J_3 in Eq. (B5) is treated in the same manner since

$$J_3 = \frac{1}{|\Lambda|}\int_\Lambda dy \int_\Lambda dx F_\Lambda(t;x,y)F_\Lambda(p;y,x) \leq \frac{C(t,d)}{|\Lambda|}\int_{\mathbb{R}^d} dy \int_\Lambda dx e^{-(\beta_d/t)\|x-y\|^2} e^{-(\bar{c}_d/t)d(x,\partial\Lambda)^2}$$

$$\leq C(t,d)\frac{B(\Lambda)}{|\Lambda|_d}. \tag{B8}$$

This proves the convergence to zero of the remainder integral in Eq. (42).

2. Convergence of the remainder integral in Eq. (43)

In this Appendix, we prove that the integral in the proof of the Proposition 3.1, obtained by replacing Λ by $\mathbb{R}^d\backslash\Lambda$, converges to zero as $\Lambda\to\mathbb{R}^d$. The term appearing in Eq. (43) is

$$\frac{1}{|\Lambda|}\int_{\mathbb{R}^d\backslash\Lambda} dx \int_\Lambda dy \partial_{x_\alpha} K_\omega(t;x,y)\partial_{y_\alpha} K_\omega(p;y,x). \tag{B9}$$

Since $x\in\mathbb{R}^d\backslash\Lambda$ and $y\in\Lambda$, we have $\|x-y\|\geq d(y,\Lambda)$. In view of estimate (30), we have the upper bound

$$\frac{C_{t,p}}{|\Lambda|}\int_{\mathbb{R}^d\backslash\Lambda} dx \int_\Lambda dy e^{-(\tilde{c}_d/t)\|x-y\|^2} e^{-(\tilde{c}_d/t)d(y,\partial\Lambda)^2}. \tag{B10}$$

Integrating first over x, the remaining integral over $y\in\Lambda$ is expressed in terms, of Eq. (B1). It then follows that the infinite-volume limit vanishes due to Eq. (B2).

APPENDIX C: INTEGRALS OVER BOUNDARY-DISTANCE FUNCTIONS

Let $\Lambda\subset\mathbb{R}^d$ or $\mathbb{Z}^d$ be a bounded set. As in Appendix B, for $x\in\Lambda$, we let $d(x,\partial\Lambda)\equiv\text{dist}(x,\partial\Lambda)$ be the distance function to the boundary of Λ. In the continuous case, we see from Proposition 3.1 that there are integrals of the type

$$B(\Lambda) \equiv \int_\Lambda e^{-c_0 d(x,\partial\Lambda)^2/t} d^d x, \tag{C1}$$

that we must evaluate. In particular, we must prove that

$$\lim_{|\Lambda|\to\infty} \frac{B(\Lambda)}{|\Lambda|_d} = 0, \tag{C2}$$

for a suitable sequence of increasing regions Λ_n, where $|A|_k$ denotes the k-dimensional Lebesgue measure of A. In order to verify this limit (C2), we assume that the sequence Λ_n satisfies either condition (vH) (11) in the lattice $\mathbb{Z}^d$ case, or condition (F) (12) in the continuous case. Furthermore, we assume the following property of the boundary-distance function:

Regularity: Given $\epsilon>0$, *there exists a constant* $0<R<\infty$ *so that*

$$|\{x\in\Lambda | d(x,\partial\Lambda)\leq\epsilon\}|_d \leq C\epsilon|\partial\Lambda|_{d-1}, \quad \text{for } 0<\epsilon<R \tag{C3}$$

and

$$|\{x \in \Lambda | d(x, \partial\Lambda) \leqslant \epsilon\}|_d \leqslant |\Lambda|_d, \quad for\ \epsilon > R. \tag{C4}$$

Proposition 8.1: Suppose Λ_n is an increasing sequence of bounded regions satisfying (vH) or (F), Eqs. (11) or (12), respectively, and conditions (C3) and (C4) with constants (C_n, R_n) and the constant C_n in Eq. (C3) is uniformly bounded $0 \leqslant C_n \leqslant C_0 < \infty$, and $R_n \to \infty$ as $|\Lambda_n| \to \infty$. Then, we have

$$\lim_{|\Lambda_n| \to \infty} \frac{B(\Lambda_n)}{|\Lambda_n|_d} = 0, \tag{C5}$$

where $B(\Lambda_n)$ is defined in (C1).

Proof: If Eq. (C5) holds true, the value of the parameter t is not important so we set $t=1$ for convenience. We estimate the integral (C1) for large n as follows:

$$\begin{aligned} B(\Lambda_n) &\leqslant \left\{ \int_{\{x \in \Lambda_n | d(x, \partial\Lambda_n) \leqslant 1\}} + \int_{\{x \in \Lambda_n | 1 < d(x, \partial_n) \leqslant R_n\}} \right\} e^{-c_0 d(x, \partial\Lambda_n)^2} d^d x \\ &\quad + \int_{\{x \in \Lambda_n | d(x, \partial\Lambda_n) \geqslant R_n\}} e^{-c_0 d(x, \partial\Lambda_n)^2} d^d x \\ &\leqslant C_n |\partial\Lambda_n|_{d-1} + \sum_{k=1}^{[\log R_n]+1} e^{-c_0 (1 + K_n (k-1))^2} |\{x \in \Lambda_n | C_k \\ &\quad \leqslant d(x, \partial\Lambda_n) \leqslant C_{k+1}\}|_d + e^{-c_0 R_n^2} |\Lambda_n|_d, \end{aligned} \tag{C6}$$

where $K_n = ((R_n - 1)/[\log R_n])$, with $[x]$ the greatest integer less than x, and $C_k = 1 + -K_n(k-1)$. The sum in Eq. (C6) is bounded above by

$$\begin{aligned} &\sum_{k=1}^{[\log R_n]+1} e^{-c_0 (1 + K_n (k-1))^2} |\{x \in \Lambda_n | C_k \leqslant d(x, \partial\Lambda_n) \leqslant C_{k+1}\}|_d \\ &\quad \leqslant D_0 \left(1 + \frac{1}{K_n}\right) (1 - e^{-c_0 K_n^2 ([\log R_n] - 1)^2}) |\partial\Lambda_n|_{d-1}, \end{aligned} \tag{C7}$$

for some finite constant $D_0 > 0$ independent of n. Consequently, we have

$$\frac{B(\Lambda_n)}{|\Lambda_n|_d} \leqslant D_1 \frac{|\partial\Lambda_n|_{d-1}}{|\Lambda_n|_d}, \tag{C8}$$

for some other finite constant $D_1 > 0$, independent of n, and the result follows. □

For what regions are conditions (C3) and (C4) satisfied? We state the following simple result. The proof follows from the existence of a boundary collar neighborhood.

Lemma 8.1: Let $\Lambda \subset \mathbb{R}^d$ be a bounded region with a piecewise C^1-boundary. Then conditions (C3) and (C4) are satisfied.

We can consider the family Λ_n obtained by dilations of a given region satisfying the hypothesis of Lemma 8.1 and easily check the hypotheses of Proposition 8.1.

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Equilibrium and eigenfunctions estimates in the semiclassical regime

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We establish eigenfunctions estimates, in the semiclassical regime, for critical energy levels associated to an isolated singularity. For Schrödinger operators, the asymptotic repartition of eigenvectors is the same as in the regular case, excepted in dimension one where a concentration at the critical point occurs. This principle extends to pseudo-differential operators and the limit measure is the Liouville measure as long as the singularity remains integrable. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2378619]

I. INTRODUCTION

The problem we consider here concerns the asymptotic behavior of eigenvectors of a self-adjoint operator and follows the works of Colin de Verdière[1] and Zelditch,[2] on the basis of a result stated first by Shnirel'man. We are more precisely interested in a proof of a microlocal concentration phenomena, in the semiclassical regime, as established in Refs. 3 and 4. The adaptation to semiclassical analysis was done in Ref. 5 following a technique proposed by Voros.[6] We also mention Ref. 7 for a more general approach in the scattering setting.

Consider a quantum operator P_h, realized as a self-adjoint operator acting on a dense subset of $L^2(\mathbb{R}^n)$. A typical example, studied in Sec. II, is the Schrödinger operator $P_h=-h^2\Delta+V$ where the potential V is smooth and bounded from below. If the spectrum of P_h is discrete in $[E-\varepsilon,E+\varepsilon]$, a sufficient condition for this is given below, we can enumerate the eigenvalues in this interval as a sequence $\lambda_j(h)$ with finite multiplicities. We note ψ_j^h the corresponding normalized eigenvectors, i.e.,

$$P_h\psi_j^h=\lambda_j(h)\psi_j^h, \quad \|\psi_j^h\|_{L^2}=1.$$

Our objective is to establish eigenfunctions estimates

$$\begin{cases} \nu_j(a)=\langle \mathrm{Op}_h^w(a)\psi_j^h,\psi_j^h\rangle, \\ \lambda_j(h)\to E,\ h\to 0^+, \end{cases}$$

where $a\in S^0(\mathbb{R}^{2n})$, so that by the Calderon-Vaillancourt theorem

$$f\mapsto \mathrm{Op}_h^w(a)f(x)=\frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}} a\left(\frac{x+y}{2},\xi\right)e^{(i/h)\langle x-y,\xi\rangle}f(y)dyd\xi,$$

is bounded on $L^2(\mathbb{R}^n)$. Note that the statement of the problem is local w.r.t. E and we are interested here in the case of $E=E_c$ critical. Let $\Phi_t=\exp(tH_p)$ be the Hamiltonian flow of the principal symbol p of P_h. Each $\nu_j(a)$ measures the observable $\mathrm{Op}_h^w(a)$ in the state ψ_j^h. Interpreted as distributions, these measures are Φ_t-invariant which easily follows from:

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$$\langle e^{-(it/h)P_h}\mathrm{Op}_h^w(a)e^{(it/h)P_h}\psi_j^h,\psi_j^h\rangle = \langle \mathrm{Op}_h^w(a)e^{(it/h)\lambda_j(h)}\psi_j^h, e^{(it/h)\lambda_j(h)}\psi_j^h\rangle = \nu_j(a).$$

By Egorov's theorem $e^{-(it/h)P_h}\mathrm{Op}_h^w(a)e^{(it/h)P_h}$ is an operator of principal symbol $(a\circ\Phi_t)$ and ν_j is invariant under Φ_t, up to $\mathcal{O}(h)$.

We recall that E is regular if $\nabla p \neq 0$ on the energy surface

$$\Sigma_E = \{(x,\xi) \in T^*\mathbb{R}^n / p(x,\xi) = E\},$$

and critical otherwise. When E_c is critical, Σ_{E_c} is not a smooth manifold. For E regular, Σ_E inherits a measure, invariant by Φ_t, given by

$$\mathrm{dLvol}(z) = \frac{dz}{\|\nabla p(z)\|}|_{\Sigma_E}, \quad z \in \Sigma_E,$$

where dz is the Riemannian surface element. We note $\mathcal{V}(E)$ the associated volume of Σ_E and we obtain a probability measure via

$$d\mu^E(z) = \frac{1}{\mathcal{V}(E)}\mathrm{dLvol}(z).$$

Note that if E_c is critical, $d\mu^{E_c}$ has a sense if and only if $1 \in L^1(\Sigma_{E_c}, \mathrm{dLvol})$. Via a wave equation approach, substituting here the heat equation strategy of Ref. 1 on a compact manifold, the problem is related at the first order to the geometry of the energy surfaces. Accordingly, the integrability of dLvol has a strong effect on the asymptotic behavior of the sequence ν_j.

First, we explain what is known in the presence of singularities. The micro-local concentration near a singularity was proven in Ref. 4 for one-dimensional Schrödinger operators with a nondegenerate instable equilibrium attached to a maximum of the potential. At the same time, in Ref. 3 several contributions of nondegenerate critical points are established in a more general setting. The case of critical energy level is specifically considered in Ref. 8 for several commuting elliptic operators and, more recently, in Refs. 9 and 10 these results have been generalized to the case of completely integrable Laplacians on compact Riemannian manifolds. In particular, precise estimates on the unboundedness of L^∞ and L^p norms of eigenfunctions attached to singular leaves are given. As concerns Schrödinger operators on $\mathbb{R}^n$, we mention Ref. 11 where the tunnel effect between degenerate minima of the potential is studied.

Next, we explain the contents of this article. Several results concerning the asymptotics of semiclassical spectral distributions, see Eq. (4), have been obtained in Refs. 12–15 following the approach of Ref. 3. For degenerate critical energy levels the existence of particular asymptotics are established and have been applied to the study of singularities of the distributional trace. The objective of this contribution is to complete these results by the study of the quantum probability $|\psi_j^h|^2$, attached to such critical energy levels, and the associated measures ν_j. As a corollary one obtains precise estimates for the microlocal counting function of eigenvalues. We are first interested in the case of Schrödinger operators, but a generalization to pseudo-differential operators is easy and provides more examples.

Finally, we recall that in Riemannian geometry, e.g., for Laplace operators on compact surfaces of negative curvature, the question to ask is if the full sequence ν_j converges to the invariant measure (quantum unique ergodicity) is still open and has attracted a lot of attention during the last years.

Definitions: We define now the objects used in Secs. II and III. If E_c is a critical energy level, we pick an h-dependant interval

$$I(h) = [E_c - dh, E_c + dh], \quad d > 0. \tag{1}$$

The associated counting function of eigenvalues is

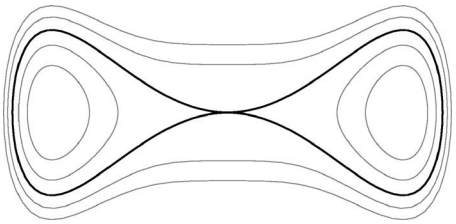

FIG. 1. Energy surfaces of $V(x)=-x^4+x^6$.

$$\Upsilon(h)=\sum_{\lambda_j(h)\in I(h)}\langle\psi_j^h,\psi_j^h\rangle=\#\{j/\lambda_j(h)\in I(h)\}. \tag{2}$$

For $A=\mathrm{Op}_h^w(a)$ a pseudo-differential operator of order zero, whose principal symbol is $a\in S^0(\mathbb{R}^{2n})$ we put

$$\Upsilon_a(h)=\sum_{\lambda_j(h)\in I(h)}\langle A\psi_j^h,\psi_j^h\rangle=\sum_{\lambda_j(h)\in I(h)}\nu_j(a). \tag{3}$$

Observe that $\Upsilon(h)=\Upsilon_1(h)$ since for every quantization used in this contribution the symbol of the identity is 1.

II. SCHRÖDINGER OPERATORS

Let $p(x,\xi)=\xi^2+V(x)$, where the potential $V\in C^\infty(\mathbb{R}^n)$ is a real value. To obtain a well defined spectral problem, we use

($\mathcal{H}_1$) There exists $C\in\mathbb{R}$ such that: $\liminf_\infty V>C$.

By a classical result, $P_h=-h^2\Delta+V(x)$ is essentially self-adjoint. Note that ($\mathcal{H}_1$) is always satisfied if V goes to infinity at infinity. Let $J=[E_1,E_2]$, with $E_2<\liminf_\infty V$. Since $p^{-1}(J)$ is compact, the spectrum $\sigma(P_h)\cap J$ is discrete and consists in a sequence $\lambda_1(h)\leqslant\lambda_2(h)\leqslant\cdots\leqslant\lambda_j(h)$ of eigenvalues of finite multiplicities, if h is small enough. Next, we impose the singularity:

($\mathcal{H}_2$) On Σ_{E_c} the symbol p has an isolated critical point $z_0=(x_0,0)$. This critical point can be degenerate but is associated to a local extremum of V

$$V(x)=E_c+V_{2k}(x)+\mathcal{O}(\|x-x_0^j\|^{2k+1}),\quad k\in\mathbb{N}^*,$$

where V_{2k}, homogeneous of degree $2k$, is definite positive or negative.

The case $k=1$, i.e., a nondegenerate singularity in dimension n, is treated in Ref. 3 without any extremum condition. In Fig. 1 the line in bold is the critical energy level attached to the top of a one-dimensional symmetric degenerate double well. Observe the instability near the recurrent critical point.

To simplify notations we write $z=(x,\xi)\in T^*\mathbb{R}^n$ and z_0 for a critical point. The first result concerns the statistical behavior of the sequence $\nu_j(a)$.

Theorem 1: *Assume ($\mathcal{H}_1$) and ($\mathcal{H}_2$) satisfied. If $n>1$ we have*

$$\lim_{h\to0^+}\frac{\Upsilon_a(h)}{\Upsilon(h)}=\int a d\mu^{E_c},$$

but in dimension 1 we obtain

$$\lim_{h\to 0^+}\frac{\Upsilon_a(h)}{\Upsilon(h)}=\langle\delta_{z_0},a\rangle=a(x_0,0).$$

These relations are statistical since when $h\to 0$ the number of eigenvalues in $I(h)$ tends to infinity, see Proposition 4. We define

$$K(h)=\{j\in\mathbb{N}/\lambda_j(h)\in I(h)\}.$$

Following the results of Refs. 1–3 and 5, for $n>1$ Theorem 1 implies that if Φ_t is ergodic on Σ_{E_c} there exists a density one subset $L(h)\subset K(h)$ such that for all integer valued function $h\to j(h)\in L(h)$ we have

$$\lim_{h\to 0}\langle\psi^h_{j(h)},\mathrm{Op}^w_h(a)\psi^h_{j(h)}\rangle=\int_{\Sigma_{E_c}}a d\mu^{E_c}.$$

Here, density one simply means that

$$\lim_{h\to 0}\frac{\#L(h)}{\#K(h)}=1.$$

Since there is nothing new to prove, we refer to Refs. 3 and 5 for a precise study. More interesting, is the generalization of the result of Ref. 4.

Corollary 2: In dimension one, assume that Σ_{E_c} is connected. Then, for the weak * topology, we have $\nu_{j(h)}\to\delta(z_0)$, $j(h)\in K(h)$, uniformly as $h\to 0$.

Hence, we obtain a concentration at z_0. Observe that $\delta(z_0)$ is Φ_t-invariant. If a is simply a function, the quantum probability satisfies

$$\lim_{h\to 0}\lambda_j(h)=E_c\Rightarrow\lim_{h\to 0}|\psi^h_{j(h)}|^2(x)=\delta_{x_0}.$$

The interpretation is as follows. In dimension one, the invariant measure on Σ_{E_c} has a singularity

$$d\mathrm{Lvol}(z)\sim c\frac{dz}{\|z-z_0\|},\quad \text{near } z_0=(x_0,0).$$

The measure is not integrable and the result has to be different. For $n>1$, the singularity is integrable and an isolated critical point has no effect. This reinforces the universality of the Liouville measure in quantum ergodicity. However, the case $n=1$ is important since many problems, with symmetries, can be reduced to the study of such a singular Schrödinger equation. See, e.g., Ref. 4 for an application in Riemannian-geometry.

Preliminary remarks: The case of a local minimum of V is not really deep. Since $\xi^2\geqslant 0$, z_0 is a local extremum of p and is an isolated point of Σ_{E_c}. According to the results of Ref. 13, the contribution of a minimum is significant only if $n=1$. We consider now the nontrivial case of a local maximum of V, corresponding to an unstable equilibrium of the flow. Finally, since we use the functional calculous below, p has to be a symbol. But with $(\mathcal{H}_1)$ we can eventually modify the potential V outside of a compact subset of $\mathbb{R}^n$, without modifying the main results. Hence no extra assumption is required. Similar comments apply for Sec. III.

Proof of Theorem 1: We use the semiclassical trace formula technique. This approach, analogous to the trace of the heat operator of Ref. 1, uses the propagator $e^{(it/h)P_h}$ and a generalization of the Poisson summation formula for this operator. Let $\varphi\in\mathcal{S}(\mathbb{R})$, a Schwartz function. To approximate Υ we define

$$\gamma(E_c,h,\varphi)=\sum_{|\lambda_j(h)-E_c|\leqslant\varepsilon}\varphi\left(\frac{\lambda_j(h)-E_c}{h}\right). \tag{4}$$

This object can be treated by mean of Fourier integral operators (FIO), see e.g., Ref. 16, and we refer to Refs. 3, 12, and 13 for a detailed study of the trace. We recall that the Tauberian approximation concerns expressions

$$\Upsilon^{\alpha}_{E,h}(\varphi)=\sum_j \alpha_j(h)\varphi\left(\frac{\lambda_j(h)-E}{h}\right).$$

Under our assumptions, the behavior of $\Upsilon^{\alpha}_{E,h}$ determines the behavior of the weighted counting functions

$$N^{\alpha}_{E,d}(h)=\sum_{|\lambda_j(h)-E|\leqslant dh}\alpha_j(h).$$

Precisely, we will apply the results of Sec. 6 of Ref. 3 for $\alpha_j(h)=1$ or $\nu_j(a)$. Strictly speaking, $\alpha_j(h)\geqslant 0$ is required but, by a standard result of pseudodifferential calculus, we can modify the quantization to have $\nu_j(a)\geqslant 0$. This does not change the main results, see Eq. (14) below.

To attain our objective, we can suppose that $\mathrm{supp}(\hat{\varphi})\subset[-M,M]$, $M>0$. Let $\Theta\in C_0^{\infty}(]E_c-\varepsilon,E_c+\varepsilon[)$, such that $\Theta=1$ in a neighborhood of E_c and $0\leqslant\Theta\leqslant 1$ on $\mathbb{R}$. We localize the problem near E_c by writing

$$\gamma(E_c,h,\varphi)=\gamma_1(E_c,h,\varphi)+\gamma_2(E_c,h,\varphi),$$

with

$$\gamma_2(E_c,h,\varphi)=\sum_{|\lambda_j(h)-E_c|\leqslant\varepsilon}\Theta(\lambda_j(h))\varphi\left(\frac{\lambda_j(h)-E_c}{h}\right)=\mathrm{Tr}\,\Theta(P_h)\varphi\left(\frac{P_h-E_c}{h}\right).$$

Where the last equality holds by support considerations. By a classical result, see, e.g., Ref. 12 Lemma 1, the term $\gamma_1=\gamma-\gamma_2$ satisfies

$$\gamma_1(E_c,h,\varphi)=\mathcal{O}(h^{\infty}),\quad \text{as } h\to 0. \tag{5}$$

The Fourier inversion formula for γ_2 and the previous estimate provide

$$\gamma(E_c,h,\varphi)=\frac{1}{2\pi}\mathrm{Tr}\int_{\mathbb{R}}e^{i(tE_c/h)}\hat{\varphi}(t)\exp\left(-\frac{i}{h}tP_h\right)\Theta(P_h)dt+\mathcal{O}(h^{\infty}). \tag{6}$$

Next, with a function $\Psi\in C_0^{\infty}(T^*\mathbb{R}^n)$, with $\Psi=1$ near z_0, we write

$$\gamma_2(E_c,h,\varphi)=\gamma_{z_0}(E_c,h,\varphi)+\gamma_{\mathrm{reg}}(E_c,h,\varphi),$$

where

$$\gamma_{z_0}(E_c,h,\varphi)=\frac{1}{2\pi}\mathrm{Tr}\int_{\mathbb{R}}e^{i(tE_c/h)}\hat{\varphi}(t)\Psi^w(x,hD_x)\exp\left(-\frac{i}{h}tP_h\right)\Theta(P_h)dt, \tag{7}$$

and γ_{reg} is simply the difference. The micro-local term γ_{z_0} contains the contribution of the singularity and the discussion below determines if this term is dominant. For finitely many critical point on Σ_{E_c}, we could repeat the procedure. For the convenience of the reader, we recall the contributions of an equilibrium to the trace formula.

Proposition 3: Assume $(\mathcal{H}_1)$, $(\mathcal{H}_2)$ *and that* $\hat{\varphi}\in C_0^{\infty}([-M,M])$, $M\leqslant M_0$. *If* x_0 *is a local maximum of V we have*

$$\gamma_{z_0}(E_c,h,\varphi) \sim h^{-n+n/2+n/2k} \sum_{m=0,1} \sum_{j,l\in\mathbb{N}^2} h^{j/2+l/2k} \log(h)^m \Lambda_{j,l,m}(\varphi).$$

If $n(k+1)/2k \in \mathbb{N}$ *and* n *is odd then the top-order term is*

$$C_{n,k} \log(h) h^{-n+n/2+n/2k} \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-n/2k} d\eta \int_{\mathbb{R}} |t|^{n[(k+1)/2k]-1} \varphi(t) dt.$$

Otherwise the first nonzero coefficient are given by

$$h^{-n+n/2+n/2k} \langle T_{n,k}, \varphi \rangle \int_{\mathbb{S}^{n-1}} |V_{2k}(\eta)|^{-n/2k} d\eta.$$

This result is the contribution of an equilibrium since the distributional coefficients have a non-discrete support, contrary to the Weyl-term supported in $t=0$ and the contributions of closed orbits supported by the length spectrum. The distributions $T_{n,k}$ and the universal constants $C_{n,k} \neq 0$ depend only on (n,k) and are explicitly determined in Ref. 14. Mainly, we need the order w.r.t. h of these contributions determined by the functions

$$w_c(h) = h^{-n+n/2+n/2k} \log(h)^j, \quad j = 0 \text{ or } 1.$$

First, we give a natural application of Proposition 3.

Proposition 4: The microlocal counting function satisfies

$$\Upsilon(h) = \begin{cases} 2d\mathcal{V}(E_c)(2\pi h)^{1-n} + o(h^{1-n}), & \text{if } n > 1, \\ \Lambda(\chi_{[-d,d]}) w_c(h) + o(w_c(h)), & \text{if } n = 1. \end{cases}$$

Here Λ *is the first nonzero distribution of Prop. 3 and* $\chi_{[-d,d]}$ *the characteristic function of* $[-d,d,]$.

Proof: By construction we have

$$\gamma_{\text{reg}}(E_c,h,\varphi) = \frac{1}{2\pi} \operatorname{Tr} \int_{\mathbb{R}} e^{i(tE_c/h)} \hat{\varphi}(t)(1 - \Psi^w(x,hD_x)) \exp\left(-\frac{i}{h} t P_h\right) \Theta(P_h) dt.$$

By the standard calculus on FIO and an easy application of the stationary phase method, as h tends to 0 we obtain

$$\gamma_{\text{reg}}(E_c,h,\varphi) \sim \frac{\hat{\varphi}(0)}{(2\pi h)^{n-1}} \operatorname{Lvol}(\Sigma_{E_c} \cap \operatorname{supp}(1-\Psi)) + \mathcal{O}(h^{2-n}).$$

Hence γ_{reg} always contributes at the order h^{1-n}.

Case of $n>1$*:* We have $w_c(h)=o(h^{1-n})$ and

$$\operatorname{Lvol}(\Sigma_{E_c} \cap \operatorname{supp}(1-\Psi)) \leqslant \mathcal{V}(E_c) < \infty, \quad \forall\, \Psi.$$

It follows easily by shrinking the support of the cut-off Ψ that

$$\gamma(E_c,\varphi,h) = (2\pi h)^{1-n} \hat{\varphi}(0) \mathcal{V}(E_c) + o(h^{1-n}). \tag{8}$$

Since the distributional factor is

$$\hat{\varphi}(0) = \int \varphi(t) dt = \langle 1, \varphi \rangle,$$

replacing φ by $\chi_{[-d,d]}$, via Theorem 6.3 of Ref. 3, provides

$$\Upsilon(h) = 2d\mathcal{V}(E_c)(2\pi h)^{1-n} + o(h^{1-n}).$$

Case of $n=1$: Here the contribution of the critical point has a bigger order than the regular one. We obtain

$$\gamma(E_c,\varphi,h) = w_c(h)\Lambda(\varphi) + o(w_c(h)). \tag{9}$$

To apply the Tauberian argument of Ref. 3, we observe that our distribution $\Lambda \in \mathcal{S}'(\mathbb{R})$ can be represented by an element of $L^1_{\mathrm{loc}}(\mathbb{R})$ and hence can be extended as a linear form on $C_0(\mathbb{R}) \cap L^\infty(\mathbb{R})$. We obtain

$$\Upsilon(h) \sim \Lambda(\chi_{[-d,d]})w_c(h). \tag{10}$$

Which provides the desired result for $n=1$. ■

As a matter of illustration, for $n=k=1$, we have

$$\log(h)|V_{2k}(x_0)|^{-1/2}\int_{-d}^{d} dt = \frac{2d\log(h)}{|V''(x_0)|^{\frac{1}{2}}}. \tag{11}$$

Which is the result established for $\Upsilon(h)$ in Refs. 3 and 4. Observe that for $n=1$, $k=1$ is the only case where a logarithm occurs and $\Upsilon(h)$ is slowly increasing w.r.t. k since for all $k>1$

$$\Upsilon(h) \sim Ch^{1/2k-1/2}|V^{(2k)}(x_0)|^{-1/2k}. \tag{12}$$

A. Eigenfunctions estimates

We recall how to derive eigenfunction estimates from the trace formula. First, to insert an observable A changes almost nothing. If Π is the spectral projector on $[E_c-\varepsilon, E+\varepsilon]$, computing the trace in the basis ψ_j^h and by cyclicity

$$\mathrm{Tr}\left(\Pi A\varphi\left(\frac{P_h - E_c}{h}\right)\right) = \sum_{|\lambda_j(h)-E_c|\leqslant\varepsilon} \langle A\psi_j^h, \psi_j^h\rangle \varphi\left(\frac{\lambda_j(h)-E_c}{h}\right).$$

Since A is a bounded operator, if $\varphi \in \mathcal{S}(\mathbb{R})$ we can again smooth the problem via an energy cut-off $\Theta(P_h)$, with an error of order $\mathcal{O}(h^\infty)$. Hence we can insert $A=\mathrm{Op}_h^w(a)$ in Eq. (7) and the results of Prop. 3 are the same after multiplication by $a(z_0)$. Similarly, the regular contribution changes via

$$\frac{\hat{\varphi}(0)}{(2\pi h)^{1-n}}\int_{\Sigma_{E_c}} a(z)(1-\Psi(z))\mathrm{dLvol}(z).$$

By evaluation of the trace, we have

$$\sum_{|\lambda_j(h)-E_c|\leqslant\varepsilon} \langle A\psi_j^h, \psi_j^h\rangle \varphi\left(\frac{\lambda_j(h)-E_c}{h}\right) \sim c_0(\varphi)w(h)m(a) + o(w(h)),$$

where $w(h)$ changes only if $n=1$. By Theorem 6.3 of Ref. 3 we obtain

$$\sum_{\lambda_j(h)\in I(h)} \langle A\psi_j^h, \psi_j^h\rangle = m(a)w(h) + o(w(h)).$$

In particular this implies that

$$\lim_{h\to 0^+}\frac{1}{\Upsilon(h)}\sum_{\lambda_j(h)\in I(h)} \langle A\psi_j^h, \psi_j^h\rangle = \lim_{h\to 0^+}\frac{\Upsilon_a(h)}{\Upsilon(h)} = \frac{m(a)}{m(1)}. \tag{13}$$

Substituting the correct expressions for these measures we obtain

(i) for $n>1$: m is a constant multiple of the Liouville measure;

(ii) for $n=1$: m is a multiple of the delta-Dirac distribution in z_0.

B. Extraction of a subsequence

We chose $a \geqslant 0$ and modify the quantization. Different choices are possible: Friedrichs quantization Op^F as in Ref. 3 or the anti-Wick quantization Op^{AW} as in Ref. 5. These quantization are positive, i.e.,

$$a \geqslant 0 \Rightarrow \langle f, \mathrm{Op}^{AW}(a) f \rangle \geqslant 0, \quad \forall f \in C_0^\infty(\mathbb{R}^n).$$

Since $\mathrm{Op}_h^w(a) - \mathrm{Op}_h^{AW}(a)$ is of order -1, we obtain

$$\langle \psi_j^h, (\mathrm{Op}_h^w(a) - \mathrm{Op}_h^{AW}(a)) \psi_j^h \rangle = \mathcal{O}(h), \tag{14}$$

and we can work with this positive operator. For $n>1$, under the condition that Φ_t is ergodic on Σ_{E_c}, the extraction of a convergent subsequence of density one is the same as in Refs. 1, 3, and 5 to which we refer for a detailed proof. For $n=1$, if Σ_{E_c} is connected, there is only one probability measure invariant by Φ_t and the full sequence converges to δ_{z_0}. Once the result is established for a positive symbol it can be extended by linearity to any $a \in S^0(\mathbb{R}^{2n})$.

III. PSEUDO-DIFFERENTIAL OPERATORS

The case of pseudo-differential operators provides more explicit examples. Let $P_h = \mathrm{Op}_h^w(p(x,\xi))$, obtained by Weyl quantization, where the symbol p is a real-valued smooth function on $T^*\mathbb{R}^n$. In a general position, one can also consider h-dependent symbols $\Sigma h^j p_j(x,\xi)$, see Ref. 5. However, to simplify, we consider only the homogeneous case. As above we impose

($\mathcal{A}_1$) There exists $\varepsilon_0 > 0$ such that $p^{-1}([E_c-\varepsilon_0, E_c+\varepsilon_0])$ is compact.

As in Sec. II, $\sigma(P_h) \cap [E_c-\varepsilon, E_c+\varepsilon]$ is discrete. *A fortiori*, ($\mathcal{A}_1$) ensures that Σ_{E_c} is compact. Next, we chose a homogeneous singularity

($\mathcal{A}_2$) On Σ_{E_c}, p has a unique critical point $z_0=(x_0,\xi_0)$ and near z_0:

$$p(z) = E_c + \mathfrak{p}_k(z) + \mathcal{O}(\|(z-z_0)\|^{k+1}), \quad k>2,$$

where $\mathfrak{p}_k$ is homogeneous of degree k w.r.t. $z-z_0$.

Strictly speaking, one could consider $k=2$. But this case is precisely treated in Ref. 3. The case of a critical point which is not an extremum is technical because the singularity is transferred on the blow up of z_0. To obtain a problem that can be explicitly solved, we consider the following hypothesis inspired by Hörmander's real principal condition:

($\mathcal{A}_3$) We have $\nabla \mathfrak{p}_k \neq 0$ on the set $C(\mathfrak{p}_k) = \{\theta \in \mathbb{S}^{2n-1} / \mathfrak{p}_k(\theta) = 0\}$.

For example, $\mathfrak{p}_3(x,\xi) = x^3 - \xi^3$ is admissible and $p(x,\xi) = x^3 - \xi^3 + x^4 + \xi^4$ satisfies all our hypothesis for $E_c = 0$.

Remark 5: With ($\mathcal{A}_3$), contrary to the case of a local extremum, z_0 is not an isolated point of Σ_{E_c} which imposes to study the classical dynamics in a neighborhood of z_0. The study of singularities as in ($\mathcal{A}_3$) is detailed in Ref. 17, Chap. 4 to which we refer concerning the integrability of dLvol.

As in Sec. II, it is sufficient to study the local problem γ_{z_0} defined in Eq. (7). The contributions to the trace formula are

Proposition 6: Under ($\mathcal{A}_1$) to ($\mathcal{A}_3$), we have an asymptotic expansion

$$\gamma_{z_0}(E_c,\varphi,h) \sim h^{\frac{2n}{k}-n} \sum_{m=0,1} \sum_{j=0}^{\infty} h^{j/k} \log(h)^m \Lambda_{j,m}(\varphi),$$

where the logarithms only occur when $(2n+j)/k \in \mathbb{N}^*$ *and* $\Lambda_{j,m} \in \mathcal{S}'(\mathbb{R})$. *For the leading term, we obtain, respectively:*

(1) If $k>2n$ *(nonintegrable singularity on* Σ_{E_c}*) we have*

$$\gamma_{z_0}(E_c,\varphi,h) \sim h^{2n/k-n}\Lambda_{0,0}(\varphi) + \mathcal{O}(h^{(2n+1)/k-n} \log(h)), \quad as\ h \to 0,$$

where $\Lambda_{0,0}$ *is a universal distribution.*

(2) If the ratio $2n/k \in \mathbb{N}$ *we obtain logarithmic contributions*

$$\gamma_{z_0}(E_c,\varphi,h) \sim h^{2n/k-n} \log(h)\Lambda_{0,1}(\varphi) + \mathcal{O}(h^{2n/k-n}), \quad as\ h \to 0,$$

(3) For $2n>k$, $2n/k \notin \mathbb{N}$ *the result is as in Eq.* (1) *with a different distribution.*

These results precisely describe the singularity at z_0. But this is not our purpose here and we refer to Ref. 15 for a detailed formulation of these contributions. For $n=1$, $k=2$, the case *(2)* agrees with Sec. II and allows us to recover some results established in Refs. 3 and 4.

A. Application to microlocal measures

The proof is exactly the same as in Sec. II. The main difference is that the singularity on Σ_{E_c} can be of arbitrary order. In our setting, according to Prop. 6 the top order coefficient changes if and only if we have

$$\frac{2n}{k} - n < 1 - n \Leftrightarrow \frac{2n}{k} < 1. \tag{15}$$

If $k<2n$ the singularity is integrable and contributes at a lower order compared to $h^{1-n}\mathcal{V}(E_c)$. But if $k \geqslant 2n$, which corresponds to a nonintegrable singularity for $d\mu^{E_c}$, the main term changes. To summarize, we obtain

$$\lim_{h\to 0} \frac{\Upsilon_a(h)}{\Upsilon(h)} = \begin{cases} \int a d\mu^{E_c}, & \text{for } k < 2n, \\ a(z_0), & \text{for } k \geqslant 2n. \end{cases}$$

Contrary to Sec. II, observe that for $k \geqslant 2n$ and if $n>1$ we do not obtain the convergence of the full sequence $\nu_{j(h)}$, $j(h) \in K(h)$, to the dirac-mass at the equilibrium. The obstruction is that an invariant probability measure can be supported by the closed orbits of Σ_{E_c}.

B. Comments

From these two examples the conclusion is that the limiting measure changes only if Σ_{E_c} carries a measure such that $1 \notin L^1_{\text{loc}}(\Sigma_{E_c}, \text{dLvol})$. Interpreted as a quantum measurement, one can obtain a very precise localization: If $a=0$ around z_0 the limit is the Liouville-measure but if $a(z_0) \neq 0$ the limit strongly differs.

An interesting problem would be to study the repartition in the presence of two equilibria z_1, z_2 on Σ_{E_c} of the same nature and with a nonintegrable singularity. In this case any convex combination

$$\nu = a\delta(z_1) + (1-a)\delta(z_2), \quad a \in [0,1], \tag{16}$$

provides an invariant probability measure. A natural question is to determine if the limiting measures are equally distributed between z_1 and z_2: This problem could be related with the approach proposed in Ref. 11.

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On Chern–Simons (super) gravity, E_8 Yang–Mills and polyvector-valued gauge theories in Clifford spaces

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It is shown how the E_8 Yang–Mills theory is a small sector of a Cl(16) algebra gauge theory and why the 11D Chern–Simons (super) gravity theory can be embedded into a Cl(11) algebra gauge theory. These results may shed some light into the origins behind the hidden E_8 symmetry of 11D supergravity. To finalize, we explain how the Clifford algebra gauge theory (that contains the Chern–Simons gravity action in $D=11$, for example) can itself be embedded into a more fundamental polyvector-valued gauge theory in Clifford spaces involving *tensorial* coordinates $x^{\mu_1\mu_2}, x^{\mu_1\mu_2\mu_3}, \ldots, x^{\mu_1\mu_2\cdots\mu_D}$ in addition to antisymmetric tensor gauge fields $A_{\mu_1\mu_2}, A_{\mu_1\mu_2\mu_3}, \ldots, A_{\mu_1\mu_2\cdots\mu_D}$. The polyvector-valued supersymmetric extension of this polyvector valued bosonic gauge theory in Clifford spaces may reveal more important features of a Clifford-algebraic structure underlying M, F theory. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2363257]

I. INTRODUCTION: WHY CLIFFORD ALGEBRAS

Ever since the discovery[1] that 11-dimensional (D) supergravity, when dimensionally reduced to an n-dim torus led to maximal supergravity theories with hidden exceptional symmetries E_n for $n \leqslant 8$, it has prompted intensive research to explain the higher dimensional origins of these hidden exceptional E_n symmetries.[2,3] More recently, there has been a lot of interest in the infinite-dim hyperbolic Kac–Moody E_{10} and non-linearly realized E_{11} algebras arising in the asymptotic chaotic oscillatory solutions of Supergravity fields close to cosmological singularities.[1,2]

The classification of symmetric spaces associated with the scalars of N extended supergravity theories (emerging from compactifications of 11D supergravity to lower dimensions), and the construction of the U-duality groups as spectrum-generating symmetries for four-dimensional BPS black-holes[6] also involved exceptional symmetries associated with the Jordan algebras $J_3[R,C,H,O]$. The discovery of the anomaly free 10-dim heterotic string for the algebra $E_8 \times E_8$ was another hallmark of the importance of exceptional Lie groups in physics.

Exceptional, Jordan, Division, and Clifford algebras are deeply related and essential tools in many aspects in Physics.[4–14] In this work we will focus mainly on the Clifford algebraic structures and show how the E_8 Yang–Mills theory can naturally be embedded into a Cl(16) algebra gauge theory and why the 11D Chern–Simons (super) gravity[15] is a very small sector of a more fundamental theory based on the Cl(11) algebra gauge theory. Polyvector-valued supersymmetries[16] in Clifford spaces[4] turned out to be more fundamental than the supersymmetries associated with M, F theory superalgebras.[17,18] For this reason we believe that Clifford structures may shed some light into the origins behind the hidden E_8 symmetry of 11D supergravity and reveal more important features underlying M, F theory.

In the remaining part of this introduction a very brief overview of the basic features of the extended relativity in Clifford spaces is presented along with the basic formulas involving the *polyvector* valued generalized supersymmety algebra in Clifford spaces. In Sec. II we show how

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the E_8 Yang–Mills theory can be obtained from a gauge theory based on the Clifford (16) algebra. In Sec. III the Chern–Simons gravity in 11-dim is embedded into a Clifford algebra gauge theory. This in itself is not much different than constructing a Chern–Simons gravity-theory based on a $gl(N,R)$ algebra, for example. However, the fundamental difference is shown in Sec. IV where we explain how the Clifford algebra gauge theory (that contains the Chern–Simons gravity action in $D=11$) is itself embedded into a more fundamental polyvector-valued gauge theory in Clifford spaces involving *tensorial* coordinates $x^{\mu_1\mu_2}$, $x^{\mu_1\mu_2\mu_3},\ldots$ in addition to antisymmetric tensor gauge fields. $A_{\mu_1\mu_2}, A_{\mu_1\mu_2\mu_3,\ldots}$. We leave for future work the explicit construction of the polyvector-valued generalized supersymmetric extension of our polyvector valued bosonic gauge theory in Clifford spaces and its implications for the further developments of M, F theory.

A. The extended relativity in Clifford spaces

The extended relativity theory in Clifford paces (C-spaces) is a natural extension of the ordinary relativity theory. A natural generalization of the notion of a space-time interval in Minkwoski space to C-space is

$$dX^2 = d\sigma^2 + dx_\mu dx^\mu + dx_{\mu\nu} dx^{\mu\nu} + \cdots . \tag{1.1}$$

The Clifford valued polyvector

$$X = X^M E_M = \sigma \mathbf{1} + x^\mu \gamma_\mu + x^{\mu\nu}\gamma_\mu \wedge \gamma_\nu + \ldots x^{\mu_1\mu_2\cdots\mu_D}\gamma_{\mu_1} \wedge \gamma_{\mu_2} \ldots \wedge \gamma\mu_D \tag{1.2a}$$

denotes the position of a polyparticle in a manifold, called Clifford space ro C-space. The series of terms in Eq. (1.2a) terminates at a *finite* value depending on the dimension D. A Clifford algebra $\mathrm{Cl}(r,q)$ with $r+q=D$ has 2^D basis elements. For simplicity, the gamma γ^μ correspond to a Clifford algebra associated with a flat spacetime

$$\frac{1}{2}\{\gamma^\mu, \gamma^\nu\} = \eta^{\mu\nu}\mathbf{1}, \tag{1.2b}$$

but in general one could extend this formulation to curved spacetimes with metric $g^{\mu\nu}$. The multigraded basis elements E_M of the Clifford-valued polyvectors are

$$E_M \equiv \mathbf{1}, \quad \gamma^\mu, \quad \gamma^{\mu_1} \wedge \gamma^{\mu_2}, \quad \gamma^{\mu_1} \wedge \gamma^{\mu_2} \wedge \gamma^{\mu_3}, \quad \gamma^{\mu_1} \wedge \gamma^{\mu_2} \wedge \gamma^{\mu_3} \wedge \cdots \wedge \gamma^{\mu D}. \tag{1.2c}$$

It is convenient to order the collective M indices as $\mu_1 < \mu_2 < \mu_3 < \cdots < \mu_D$.

The connection to strings and p-branes can be seen as follows. In the case of a closed string (a 1-loop) embedded in a target flat spacetime background of D-dimensions, one represents the projections of the closed string (1-loop) onto the embedding spacetime coordinate planes by the variables $x_{\mu\nu}$. These variables represent the respective *areas* enclosed by the projections of the closed string (1-loop) onto the corresponding embedding spacetime planes. Similary, one can embed a closed membrane (a 2-loop) onto a D-dim flat spacetime, where the projections given by the antisymmetric variables $x_{\mu\nu\rho}$ represent the corresponding *volumes* enclosed by the projections of the 2-loop along the hyperplanes of the flat target spacetime background.

This procedure can be carried to all closed p-branes (p-loops) where the values of p are $p=0,1,2,3,\ldots,D-2$. The $p=0$ value represents the center of mass and the coordinates $x^{\mu\nu}, x^{\mu\nu\rho}\ldots$ have been *coined* in the string-brane literature[19] as the *holographic* areas, volumes, … projections of the nested family of p-loops (closed p-branes) onto the embedding spacetime coordinate planes/hyperplanes. The classification of Clifford algebras $\mathrm{Cl}(r,q)$ in $D=r+q$ dimensions (modulo 8) for different values of the spacetime signature r,q is discussed, for example, in the book of Porteous.[20]

All Clifford algebras can be understood in terms of CL(8) and the CL(k) for k less than 8 due to the modulo 8 periodicity theorem $\mathrm{CL}(n)=\mathrm{CL}(8)\times\mathrm{Cl}(n-8)$, where $\mathrm{Cl}(r,q)$ is a matrix algebra for even $n=r+q$ or the sum of two matrix algebras for odd $n=r+q$. Depending on the signature, the matrix algebras may be real, complex, or quaternionic. For further details we refer to Ref. 20.

If we take the differential dX and compute the scalar product among two polyvectors $\langle dX^T dX\rangle_{\text{scalar}}$ we obtain the C-space extension of the particles proper time in Minkwoski space. The symbol X^T denotes the *reversion* operation and involves reversing the order of all the basis γ^μ elements in the expansion of X. The C-space proper time associated with a polyparticle motion is then

$$\langle dX^T dX\rangle_{\text{scalar}} = d\Sigma^2 = (d\sigma)^2 + \Lambda^{2D-2} dx_\mu dx^\mu + \Lambda^{2D-4} dx_{\mu\nu} dx^{\mu\nu} + \dots . \tag{1.3}$$

Here we have explicitly introduced the Planck scale Λ since a length parameter is needed in order to tie objects of different dimensionality together: 0-loops, 1-loops,…, p-loops. Einstein introduced the speed of light as a universal absolute invariant in order to "unite" space with time (to match units) in the Minkwoski space interval

$$ds^2 = c^2 dt^2 - dx_i dx^i . \tag{1.4}$$

A similar unification is needed here to unite objects of different dimensions, such as x^μ, $x^{\mu\nu}$, etc…. The Planck scale then emerges as another universal invariant in constructing an extended scale relativity theory in C-spaces.[4]

To continue along the same path, we consider the analog of Lorentz transformations in C-spaces which transform a polyvector X into another polyvector X' given by $X' = RXR^{-1}$ with

$$R = e^{\omega^A E_A} = \exp[(\omega \mathbf{1} + \omega^\mu \gamma_\mu + \omega^{\mu_1\mu_2} \gamma_{\mu_1} \wedge \gamma_{\mu_2} \dots)] \tag{1.5}$$

and

$$R^{-1} = e^{-\omega^A E_A} = \exp[-(\omega \mathbf{1} + \omega^\nu \gamma_\nu + \omega^{\nu_1\nu_2} \gamma_{\nu_1} \wedge \gamma_{\nu_2} \dots)], \tag{1.6}$$

where the ω parameters also belong to a Clifford-valued quantity

$$\omega; \omega^\mu; \omega^{\mu\nu}; \dots , \tag{1.7}$$

they are the C-space version of the Lorentz rotations/boosts parameters.

Since a Clifford algebra admits a matrix representation, one can write the norm of a polyvectors in terms of the trace operation as: $\|X\|^2 = \text{Trace} X^2$. Hence, under C-space Lorentz transformation the norms of polyvectors behave as follows:

$$\text{Trace} X'^2 = \text{Trace}[RX^2R^{-1}] = \text{Trace}[RR^{-1}X^2] = \text{Trace} X^2 . \tag{1.8}$$

These norms are invariant under C-space Lorentz transformations due to the cyclic property of the trace operation and $RR^{-1} = 1$. Another way of rewriting the inner product of polyvectors is by means of the reversal operation that reverses the order of the Clifford basis generators: $(\gamma^\mu \wedge \gamma^\nu)^T = \gamma^\nu \wedge \gamma^\mu$, etc…. Hence, the inner product can be rewritten as the scalar part of the geometric product $\langle X^T X\rangle_s$. The analog of an orthogonal matrix in Clifford spaces is $R^T = R^{-1}$ such that

$$\langle X'^T X'\rangle_s = \langle (R^{-1})^T X^T R^T R X R^{-1}\rangle_s = \langle R X^T X R^{-1}\rangle_s = \langle X^T X\rangle_s = \text{invariant}. \tag{1.9a}$$

This condition $R^T = R^{-1}$ of course, will *restrict* (constrain) the type of terms allowed inside the exponential defining the rotor R in Eq. (1.6) because the *reversal* of a p-vector obeys

$$(\gamma_{\mu_1} \wedge \gamma_{\mu_2} \dots \wedge \gamma_{\mu_p})^T = \gamma_{\mu_p} \wedge \gamma_{\mu_{p-1}} \dots \wedge \gamma_{\mu_2} \wedge \gamma_{\mu_1} = (-1)^{p(p-1)/2} \gamma_{\mu_1} \wedge \gamma_{\mu_2} \dots \wedge \gamma_{\mu_p} . \tag{1.9b}$$

Hence, only those terms that change sign (under the reversal operation) are permitted in the exponential defining $R = \exp[\omega^A E_A]$.

Another possibility is to *complexify* the C-space polyvector valued coordinates $= Z = Z^A E_A = X^A E_A + i Y^A E_A$ (which is *not* the same as *complexifying* the Clifford algebra) as well as the

boost/rotation parameters ω^A in order to allow the unitarity condition $U^\dagger \equiv U^{-1}$ to hold. The generalized Clifford unitary transformations $Z' = UZU^\dagger = UZU^{-1}$ associated with the complexified polyvector $Z = Z^A E_A$ must be such so the interval

$$\langle dZ^\dagger dZ \rangle_s = d\bar{\sigma} d\sigma + d\bar{z}^\mu dz_\mu + d\bar{z}^{\mu\nu} dz_{\mu\nu} + d\bar{z}^{\mu\nu\rho} dz_{\mu\nu\rho} + \ldots \tag{1.9c}$$

remains invariant under these unitary transformations above (upon setting the Planck scale $\Lambda = 1$).

The unitary condition $U^\dagger = U^{-1}$, under the *combined* reversal and complex-conjugate operation, will constrain the form of the complexified boosts/rotation parameters ω^A appearing in: $U = \exp[\omega^A E_A]$. The parameters ω^A must be either purely real, or purely imaginary, depending if the reversal $E_A^T = \pm E_A$, to ensure that an overall change of sign occurs in the terms $\omega^A E_A$ inside the exponential defining U so that $U^\dagger = U^{-1}$ actually holds, and the norm $\langle Z^\dagger Z \rangle_s$ remains invariant under the analog of unitary transformations in *complexified* C-spaces. These techniques are not very different from Penrose Twistor spaces. As far as we know a Clifford–Twistor space construction of C-spaces has not been performed so far.

Another alternative is to define the unitary transformations by $U = \exp(\Omega^{AB}[E_A, E_B])$ where the commutator $[E_A, E_B] = F_{AB}^C E_C$ is the C-space analog of the $i[\gamma_\mu, \gamma_\nu]$ commutator which is the generator of the Lorentz algebra, and the parameters Ω^{AB} are the C-space analogs of the rotation/boots parameters. The diverse parameters Ω^{AB} are purely real or purely imaginary depending whether the reversal $[E_A, E_B]^T = \pm [E_A, E_B]$ to ensure that $U^\dagger = U^{-1}$ such that the scalar part $\langle Z^\dagger Z \rangle_s$ remains invariant under the transformations $Z' = UZU^{-1}$. This last alternative seems to be more physical because a polyrotation should map the E_A direction into the E_B direction in C-spaces, hence, the meaning of the generator $[E_A, E_B]$ which is the extension of the $i[\gamma_\mu, \gamma_\nu]$ Lorentz generator. We refer to the review[4] for further details about the extended relativity theory in Clifford spaces. In particular, why relativity in *curved* Clifford spaces is equivalent to a higher derivative gravity with torsion associated with the underlying spacetime.[4]

B. Polyvector-valued super Poincare algebras and Clifford-space supersymmetry

Polyvector super-Poincare algebras as extensions of ordinary super-Poincare algebras have been studied by Ref. 18. The former Lie superalgebras (involving commutators and anticommutators) should not be confused with the Z_2-graded extensions of ordinary Lie algebras, in particular with Z_2-graded extensions of Clifford algebras involving only commutators. The polyvector super Poincare algebras have the form of $\mathbf{g} = \mathbf{g}_0 + \mathbf{g}_1$, where the even sector is $\mathbf{g}_0 = so(V) + W_0$ and the odd sector $\mathbf{g}_1 = W_1$ consists of a spinorial representation of $so(V) = so(p,q)$; i.e., W_1 is an $so(p,g)$-spinorial module, where V is a vector space of signature p,q.

The algebra of generalized translations $W = W_0 + W_1$ is the maximal solvable ideal of $\mathbf{g}$. W_0 is generated by W_1: $[W_1, W_1] \subseteq W_0$ and $[W_0, W_1] = 0$; $[W_0, W_0] = 0$. For example, in the ordinary super-Poincare algebra, the translations are generated by the supersymmetry generators: $\{Q, \bar{Q}\} \sim P$ and $[Q, P] = [P, P] = 0$. Choosing W_1 to be a spinorial $so(V)$-module consisting of a sum of spinors and semispinors (chiral spinors) the authors[18] proved that W_0 consists of *polyvectors*. They provided the classification of all polyvector Lie superalgebras, for all dimensions and signatures, after analyzing all the $so(V)$-invariant polyvector-valued bilinear forms that can be defined on the spinor modules. N-extended polyvector super Poincare algebras were also classified in Ref. 18.

The anticommutator is

$$\{S_\alpha, S_\beta\} = \sum_k (\mathcal{C}\Gamma^{\mu_1 \mu_2 \ldots \mu_k})_{\alpha\beta} W_{0 \mu_2 \mu_2 \ldots \mu_k}^{(k)}, \tag{1.10}$$

where α, β denote spinor indices and the summation over k must obey certain crucial restrictions to match degrees of freedom with the terms on the left-hand side (lhs). The matrix $\mathcal{C}$ is the charge conjugation matrix. Depending on the given spacetime and its signature there are at most two charge conjugation matrices $\mathcal{C}_S$, $\mathcal{C}_A$ given by the product of all symmetric and all antisymmetric gamma matrices, respectively. In special spacetime signatures they collapse into a single matrix.

These charge conjugation matrix $\mathcal{C}$ are essential in order to satisfy the nontrivial graded super Jacobi identities.

A Chern–Simons supergravity (CS-SUGRA) in $D=11$ involves the symplectic supergroup $OSp(32|1)$ and the connection[15]

$$\mathbf{A}_\mu = e_\mu^a \Gamma_a + \omega_\mu^{ab} \Gamma_{ab} + A_\mu^{a_1 a_2 \ldots a_5} \Gamma_{a_1 a_2 \ldots a_5} + \bar{\Psi}_\mu^\alpha Q_\alpha, \tag{1.11}$$

whereas the M theory superalgebra involve 32-component spinorial supercharges Q_α whose anticommutators are[17,18]

$$\{Q_\alpha, Q_\beta\} = (\mathcal{A}\Gamma_\mu)_{\alpha\beta} P^\mu + (\mathcal{A}\Gamma_{\mu_1\mu_2})_{\alpha\beta} Z^{\mu_1\mu_2} + (\mathcal{A}\Gamma_{\mu_1\mu_2\ldots\mu_5})_{\alpha\beta} Z^{\mu_1\mu_2\ldots\mu_5}. \tag{1.12}$$

There are 32×32 symmetric real matrices with at most $\frac{1}{2}(32\times 33)=528$ independent components that match the number of degrees of freedom associated with the translations P^μ and the antisymmetric rank 2, 5 abelian tensorial central charges $Z^{\mu_1\mu_2}$, $Z^{\mu_1\mu_2\ldots\mu_5}$ on the right-hand side (rhs) since $11+55+462=528$. The matrix $\mathcal{A}$ plays the role of the timelike γ^0 matrix in Minkowski spacetime and is used to introduce barred-spinors.[17,18]

The F theory $12D$ superalgebra involves the Majorana–Weyl spinors with 32 components whose anticommutators are[17]

$$\{Q_\alpha, Q_\beta\} = (\mathcal{A}\Gamma_{\mu\nu})_{\alpha\beta} Z^{\mu\nu} + (\mathcal{A}\Gamma_{\mu_1\mu_2\ldots\mu_6})_{\alpha\beta} Z^{\mu_1\mu_2\ldots\mu_6} \tag{1.13}$$

and the counting of components in $D=12$ yields also $32\times 33/2=528=66+462$. In $13D$ it requires the superalgebra $OSp(64|1)$ which is connected to a membrane, a 3-brane and a 6-brane, respectively, since antisymmetric tensors of ranks 2, 3, 6 in $13D$ have a total of $64\times 65/2=78+286+1716=2080$ components.

Therefore, by studying the polyvector super Poincare algebras, the M and F theory superalgebras ((1.10), (1.11), (1.12)) one concludes that these cannot be incorporated into Clifford superspaces because one cannot have a restricted summation in the k rank of the terms appearing in the $\{Q_\alpha, Q_\beta\}$ (anti)commutators. Unless one adds further spinorial degrees of freedom by introducing multispinor valued quantities $\theta^{\alpha_1\alpha_2}, \theta^{\alpha_1\alpha_2\alpha_3}, \ldots$, which are the fermionic partners of $x^{\mu_1\mu_2}, x^{\mu_1\mu_2\mu_3}, \ldots$, or by recurring to N extended supersymmetries, one will not be able to match the number of degrees of freedom in a satisfactory manner. N extended polyvector Super Lie Algebras which were also studied by Ref. 18. This means that the odd sector W_1 consists of N copies of the irreducible spinor module S. There are cases where there are two inequivalent copies (complex-even dimensional, or real with spatial signatures $s=0,4$) involving N_+ chiral generators and N_- antichiral ones. For further details we refer to Ref. 18.

Hence, by introducing a judicious number of extra spinorial degrees of freedom $\theta^{\alpha_1\alpha_2}, \theta^{\alpha_1\alpha_2\alpha_3}, \ldots$ in "Clifford superspace," depending on the dimensions and spacetime signatures, one can accommodate for the larger number of polyvector coordinates associated with C-spaces. For this reason we believe that polyvector-valued supersymmetries in Clifford superspaces[16] deserve to be investigated further since they are more fundamental than the supersymmetries associated with M, F theory superalgebras.

Nevertheless, there are instances, in particular when $D=4=3+1$, that the $\{Q_\alpha, Q_\beta\}$ is a symmetric matrix in α, β with ten independent components and which matches exactly the degrees of freedom of the momentum vector and bi-vector P^μ, $P^{\mu\nu}$ given by $4+6=10$. Therefore, in $D=4$, one may have the anticommutator written in terms of the charge conjugation matrix C as

$$\{Q_\alpha, Q_\beta\} = \frac{1}{2} C\gamma^\mu P_\mu + \frac{1}{2} C\gamma^{\mu\nu} P_{\mu\nu} \tag{1.14}$$

and the Jacobi indentities

$$\{[\mathcal{M}_{\mu_1\mu_2}, Q_\alpha], Q_\beta\} + \{[\mathcal{M}_{\mu_1\mu_2}, Q_\beta], Q_\alpha\} = [\mathcal{M}_{\mu_1\mu_2}, \{Q_\alpha, Q_\beta\}]. \tag{1.15a}$$

$$\{[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},Q_\alpha],Q_\beta\}+\{[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},Q_\beta],Q_\alpha\}=[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_2},\{Q_\alpha,Q_\beta\}] \tag{1.15b}$$

with the commutators

$$[M_{\mu_1\mu_2},P_{\rho_1\rho_2}]=-\eta_{\mu_1\rho_1}P_{\mu_2\rho_2}+\eta_{\mu_2\rho_1}P_{\mu_1\rho_2}\pm\ldots;\quad [\mathcal{M}_{\mu_1\mu_2},Q_\alpha]=-\frac{1}{2}(\gamma_{\mu_1\mu_2})_\alpha^\delta Q_\delta, \tag{1.15c}$$

where

$$\{Q_\alpha,Q_\beta\}=\frac{1}{2}C\gamma^\mu P_\mu+\frac{1}{2}C\gamma^{\mu\nu}P_{\mu\nu}, \tag{1.15d}$$

the spinorial charges Q_α behave under polyrotations as follows:

$$[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},Q_\alpha]=-\frac{1}{2}(\gamma_{\mu_1\mu_2\mu_3\mu_4})_\alpha^\delta Q_\delta, \tag{1.15e}$$

and the remaining commutators are

$$[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},P_{\nu_1\nu_2}]=\eta_{\mu_1\mu_2\nu_1\nu_2}P_{\mu_3\mu_4}+\eta_{\mu_3\mu_4\nu_1\nu_2}P_{\mu_1\mu_2}\pm\ldots;\quad [\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},P_{\nu_1}]=0, \tag{1.15f}$$

$$[M_{\mu_1\mu_2},M_{\nu_1\nu_2}]=-\eta_{\mu_1\nu_1}M_{\mu_2\nu_2}+\eta_{\mu_2\nu_1}M_{\mu_1\nu_2}\pm\ldots, \tag{1.15g}$$

$$[M_{\mu_1\mu_2\mu_3\mu_4},M_{\nu_1\nu_2\nu_3\mu_4}]=\eta_{\mu_1\mu_2\nu_1\nu_2}M_{\mu_3\mu_4\nu_3\nu_4}\pm\ldots, \tag{1.15h}$$

$$[M_{\mu_1\mu_2},M_{\nu_1\nu_2\nu_3\mu_4}]=-\eta_{\mu_1\nu_1}M_{\mu_2\nu_2\nu_3\nu_4}\pm\ldots \tag{1.15i}$$

In the Appendix we will prove that this algebra Eqs. (1.15) closes and satisfies the Jacobi identities. G_{MN} is the *flat* C-space generalized metric $\eta_{\mu_1\nu_1\mu_2\nu_2\ldots\mu_n\nu_n}$ given by the determinant of the $N\times N$ matrix $\mathbf{\Upsilon}_{mm}$ whose entries are $\eta_{\mu_m\nu_n}$. For instance

$$\eta_{\mu_1\nu_1\mu_2\nu_2\ldots\mu_n\nu_n}=\det\mathbf{\Upsilon}_{mm}=\frac{1}{N!}\boldsymbol{\epsilon}^{j_1i_2\ldots i_n}\boldsymbol{\epsilon}^{j_1j_2\ldots j_n}\eta_{\mu_{i_1}\nu_{j_1}}\eta_{\mu_{i_2}\nu_{j_2}}\cdots\eta_{\mu_{i_n}\nu_{j_n}}, \tag{1.16}$$

so that

$$\eta_{\mu_1\nu_1\mu_2\nu_2}=\eta_{\mu_1\nu_1}\eta_{\mu_2\nu_2}-\eta_{\mu_1\nu_2}\eta_{\mu_2\nu_1},\ \text{etc.} \tag{1.17}$$

Similar results apply to the definition of $\eta_{i_1j_1\ldots i_nj_n}$.

The graded super Jacobi identities (nontrivial matter) in C-space due to the nontrivial algebraic relations obtained from the (geometric) product of two polyvector basis elements $\Gamma^M\Gamma^N$ that involves a sum of terms with polyvectors of mixed grade

$$\langle\Gamma^M\Gamma^N\rangle_{m+n},\ \langle\Gamma^M\Gamma^N\rangle_{m+n-2},\ \langle\Gamma^M\Gamma^N\rangle_{m+n-4},\ \cdots\ \langle\Gamma^M\Gamma^N\rangle_{|m-n|}. \tag{1.18}$$

Using the standard notation

$$\gamma^{\nu_1\nu_2\ldots\nu_p}\equiv\gamma^{\mu_1}\wedge\gamma^{\mu_2}\wedge\cdots\wedge\gamma^{\mu_p}, \tag{1.19}$$

where the antisymmetrization of indices is performed with unit weight, one has for example

$$\gamma^\mu\gamma^\nu=\frac{1}{2}\{\gamma^\mu,\gamma^\nu\}+\frac{1}{2}[\gamma^\mu,\gamma^\nu]=\eta^{\mu\nu}\mathbf{1}+\frac{1}{2}\gamma^{\mu\nu}, \tag{1.20}$$

$$\gamma^{\mu_1\mu_2\cdots\mu_p}\gamma^{\mu_{p+1}} = \gamma^{\mu_1\mu_2\cdots\mu_p\mu_{p+1}} + p\,\gamma^{[\mu_1\mu_2\cdots\mu_{p-1}}\eta^{\mu_p]\mu_{p+1}}, \tag{1.21}$$

$$\gamma^{\mu}\gamma^{\nu_1\nu_2\cdots\nu_p} - (-1)^p\gamma^{\nu_1\nu_2\cdots\nu_p}\gamma^{\mu} = 2p\,\eta^{\mu[\nu_1}\gamma^{\nu_2\nu_3\cdots\nu_p]}. \tag{1.22}$$

Having outlined the basic features of the extended relativity theory in Clifford spaces and polyvector-valued supersymmetries we proceed with the main bulk of this work.

II. THE E_8 YANG–MILLS FROM A Cl(16) ALGEBRA GAUGE THEORY

It is well known among the experts that the E_8 algebra admits the SO(16) decomposition $\mathbf{248}\rightarrow\mathbf{120}\oplus\mathbf{128}$. The E_8 admits also a SL$(8,R)$ decomposition.[3] Due to the triality property, the SO(8) admits the vector $\mathbf{8}_v$ and spinor representations $\mathbf{8}_s,\mathbf{8}_c$. After a triality rotation, the SO(16) vector and spinor representations decompose as[3]

$$\mathbf{16}\rightarrow\mathbf{8}_s\oplus\mathbf{8}_c, \tag{2.1a}$$

$$\mathbf{128}_s\rightarrow\mathbf{8}_v\oplus\mathbf{56}_v\oplus\mathbf{1}\oplus\mathbf{28}\oplus\mathbf{35}_v, \tag{2.1b}$$

$$\mathbf{128}_c\rightarrow\mathbf{8}_s\oplus\mathbf{56}_s\oplus\mathbf{8}_c\oplus\mathbf{56}_c. \tag{2.1c}$$

To connect with (real) Clifford algebras,[6] i.e., how to fit E_8 into a Clifford structure, start with the 248-dim fundamental representation E_8 that admits a SO(16) decomposition given by the 120-dim bivector representation plus the 128-dim chiral-spinor representations of SO(16). From the modulo 8 periodicity of Clifford algebras one has $\mathrm{Cl}(16)=\mathrm{Cl}(2\times 8)=\mathrm{Cl}(8)\otimes\mathrm{Cl}(8)$, meaning, roughly, that the $2^{16}=256\times 256$ Cl(16)-algebra matrices can be obtained effectively by replacing each single one of the *entries* of the $2^8=256=16\times 16$ Cl(8)-algebra matrices by the 16×16 matrices of the second copy of the Cl(8) algebra. In particular, $120=1\times 28+8\times 8+28\times 1$ and $128=8+56+8+56$, hence, the 248-dim E_8 algebra decomposes into a $120+128$ dim structure such that E_8 can be represented indeed within a tensor product of Cl(8) algebras.

At the E_8 Lie algebra level, the E_8 gauge connection decomposes into the SO(16) vector $I,J=1,2,\ldots,16$ and (chiral) spinor $A=1,2,\ldots,128$ indices as follows:

$$\mathcal{A}_\mu = \mathcal{A}^{IJ}_\mu X_{IJ} + \mathcal{A}^{A}_\mu Y_A, \quad X_{IJ}=-X_{JI}, \quad I,J=1,2,3,\ldots,16. \quad A=1,2,\ldots,128, \tag{2.2}$$

where X_{IJ}, Y_A are the E_8 generators. The Clifford algebra $(\mathrm{Cl}(8)\otimes\mathrm{Cl}(8))$ structure behind the SO(16) decomposition of the E_8 gauge field $\mathcal{A}^{IJ}_\mu X_{IJ}+\mathcal{A}^{A}_\mu Y_A$ can be deduced from the expansion of the generators X_{IJ}, Y_A in terms of the Cl(16) algebra generators. The Cl(16) bivector basis admits the decomposition

$$X^{IJ} = \alpha^{IJ}_{ij}(\gamma_{ij}\otimes\mathbf{1}) + b^{IJ}_{ij}(\mathbf{1}\otimes\gamma_{ij}) + c^{IJ}_{ij}(\gamma_i\otimes\gamma_j), \tag{2.3}$$

where γ_i, are the Clifford algebra generators of the Cl(8) algebra present in $\mathrm{Cl}(16)=\mathrm{Cl}(8)\otimes\mathrm{Cl}(8)$; $\mathbf{1}$ is the unit Cl(8) algebra element that can be represented by a unit 16×16 diagonal matrix. The tensor products $\otimes$ of the 16×16Cl(8)-algebra matrices, like $\gamma_i\otimes\mathbf{1}$, $\gamma_i\otimes\gamma_j,\ldots$ furnish a 256×256 Cl(16)-algebra matrix, as expected. The Cl(8) algebra basis elements are

$$\gamma_M=\mathbf{1},\ \gamma_i, \quad \gamma_{i_1i_2}=\gamma_{i_1}\wedge\gamma_{i_2}, \quad \gamma_{i_1i_2i_3}=\gamma_{i_1}\wedge\gamma_{i_2}\wedge\gamma_{i_3},\ldots,\gamma_{i_1i_2\ldots i_8}=\gamma_{i_1}\wedge\gamma_{i_2}\wedge\cdots\wedge\gamma_{i_8}. \tag{2.4}$$

Therefore, the decomposition in Eq. (2.3) yields the $28+28+8\times 8=56+64=120$-dim bivector representation of SO(16); i.e., for each *fixed* values of IJ there are 120 terms on the rhs of Eq. (2.5), that match the number of *independent* components of the E_8 generators $X^{IJ}=-X^{JI}$, given by $\frac{1}{2}(16\times 15)=120$. The decomposition of Y_A is more subtle. A spinor Ψ in $16D$ has $2^8=256$ components and can be decomposed into a 128 component left-handed spinor Ψ^A and a 128 compo-

nent right-handed spinor $\Psi^{\dot{A}}$; The 256 spinor indices are $\alpha=A,\ \dot{A};\ \beta=B,\dot{B},\ldots$ with $A,B=1,2,\ldots,128$ and $\dot{A},\dot{B}=1,2,\ldots,128$, respectively.

Spinors are elements of right (left) ideals of the Cl(16) algebra and admit the expansion $\Psi=\Psi_\alpha\xi^\alpha$ in a 256-dim spinor basis ξ^α which in turn can be expanded as sums of Clifford polyvectors of *mixed* grade; i.e., into a sum of scalars, vectors, bivectors, trivectors, …. The chiral (left-handed, right-handed) 128-component spinors $\Psi^\pm$ are obtained via the projection operators

$$\Psi^\pm=\frac{1}{2}(1+\Gamma_{17})\Psi,\quad \Gamma^{17}=\Gamma^1\wedge\Gamma^2\wedge\cdots\wedge\Gamma^{16}, \tag{2.5}$$

such that $\xi^\alpha_+\equiv\xi^A$; $\xi^\alpha_-\equiv\xi^{\dot{A}}$, so the left-handed (right-handed) spinor basis $\xi_\pm$ can be represented by a column matrix (an element of the left ideal) with 128 nonvanishing upper (lower) components in the Weyl representation as

$$\xi^\alpha_\pm=\left(\frac{1\pm\Gamma_{17}}{2}\right)^{\alpha\beta}[(\mathbf{1}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}^\delta+(\gamma_i\otimes 1)^{\beta\delta}\mathcal{A}^\delta_i+(\gamma_{i_1i_2}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}_{i_1i_2}+\ldots\quad(\gamma_{i_1i_2\ldots i_7}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}^\delta_{i_1i_2\ldots i_7}$$
$$+(\gamma_{i_1i_2-_2\ldots i_8}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}_{i_1i_2\ldots i_8}], \tag{2.6}$$

where the numerical tensor-spinorial coefficients on the rhs of Eq. (2.6) are constrained to satisfy all the conditions imposed by the definition of an ideal element of the Cl(16) algebra; namely that *any* element of the ideal upon a multiplication from the left by any Clifford algebra element yields another element of the left ideal. Similar definitions apply to the right ideal elements upon multiplication from the right by any Clifford algebra element. The row matrix (an element of the right ideal) with 128 nonvanishing components is just given by $(\xi^\pm)^\dagger$.

The rigorous procedure to construct spinors as elements of right/left ideals of Clifford algebras using primitive idempotents can be found in Ref. 5, and references therein. The final outcome is the same as performing the expansion Eq. (2.6) and solving for the coefficients. In this fashion one can construct the 128-dim left-handed (right-handed) chiral spinor representations of SO(16) that match the number of 128 generators Y_A. Hence, the total number of E_8 generators is then $120+128=248$. What remains to be done is to enforce the E_8 commutation relations that in conjunction with the defining relations of a primitive ideal element of the Cl(16) algebra will fix the values of the coefficients appearing in (2.4) and (2.6). Based on the fact that the Clifford algebra commutators of even and odd grade satisfy the relations

$$[\text{Even},\text{Even}]=\text{Even},\ [\text{Odd},\text{Odd}]=\text{Even},\ [\text{Even},\text{Odd}]=[\text{Odd},\text{Even}]=\text{Odd}, \tag{2.7}$$

which are similar to the E_8 commutation relations described below, one can immediately choose to expand the spinor basis elements in Eq. (2.6) as sums of polyvectors of *odd* grade only, meaning that for each fixed value of δ, there are only 128 terms on the rhs of Eq. (2.6) given by the number of odd-grade elements of the Cl(8) algebra $8+56+56+8=128$. This is consistent with the fact that a chiral spinor in $16D$ has 128 nonvanishing components in a Weyl representation. Therefore, the generators $Y^A\equiv Y^\alpha_+$; $Y^{\dot{A}}=Y^\alpha_-$ must involve odd grade elements of the form

$$Y^\alpha_\pm=\left(\frac{1\pm\Gamma_{17}}{2}\right)^{\alpha\beta}[(\gamma_i\otimes\mathbf{1})^{\beta\delta}\mathcal{A}^\delta_i+(\gamma_{i_1i_2i_3}\otimes\mathbf{1})\beta\delta\mathcal{A}^\delta_{i_1i_2i_3}+(\gamma_{i_1i_2\ldots i_5}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}^\delta_{i_1i_2\ldots i_5}$$
$$+(\gamma_{i_1i_2\ldots i_7}\otimes\mathbf{1})^{\beta\delta}\mathcal{A}^\delta_{i_1i_2\ldots i_7}]. \tag{2.8}$$

The commutation relations of E_8 are[3]

$$[X^{IJ},X^{KL}]=4(\delta^{IK}X^{LJ}-\delta^{IL}X^{KJ}+\delta^{JK}X^{IL}-\delta^{JL}X^{IK}),\quad [X^{IJ},Y^{A}]=-\frac{1}{2}\Gamma^{IJ}_{AB}Y^{B};\quad [Y^{A},Y^{B}]=\frac{1}{4}\Gamma^{IJ}_{AB}X^{IJ}. \tag{2.9}$$

The combined E_8 indices are denoted by $\mathcal{A}\equiv[IJ],A$ $(120+128=248$ indices in total) that yield the Killing metric and the structure constants

$$\eta^{\mathcal{AB}}=\frac{1}{60}\,\mathrm{Tr}\,T^{\mathcal{A}}T^{\mathcal{B}}=-\frac{1}{60}f^{\mathcal{A}}_{\mathcal{CD}}f^{\mathcal{BCD}}, \tag{2.10a}$$

$$f^{IJ,KL,MN}=-8\,\delta^{JK}\delta^{LJ}_{MN}+\text{permutations};\quad f^{IJ,A,B}=-\frac{1}{2}\Gamma^{IJ}_{AB};\quad \eta^{IJKL}=-\frac{1}{60}f^{IJ}_{\mathcal{CD}}f^{KL,\mathcal{CD}}. \tag{2.10b}$$

Therefore, the odd grade expansion in Eq. (2.8) and the bivector grade expansion in Eq. (2.3) is consistent with the commutation relations of E_8. We shall proceed with the construction of a novel Cl(16) gauge theory that encodes the exceptional Lie algebra E_8 symmetry from the start. The E_8 gauge theory in $D=4$ is based on the E_8-valued field strengths

$$F^{IJ}_{\mu\nu}X_{IJ}=(\partial_\mu\mathcal{A}^{IJ}_\nu-\partial_\nu\mathcal{A}^{IJ}_\nu)X_{IJ}+\mathcal{A}^{KL}_\mu\mathcal{A}^{MN}_\nu[X_{KL},X_{MN}]+\mathcal{A}^{A}_\mu\mathcal{A}^{B}_\nu[Y_A,Y_B], \tag{2.11}$$

$$F^{A}_{\mu\nu}Y_A=(\partial_\mu\mathcal{A}^{A}_\nu-\partial_\nu\mathcal{A}^{A}_\mu)Y_A+\mathcal{A}^{A}_\mu\mathcal{A}^{IJ}_\nu[Y_A,X_{IJ}]. \tag{2.12}$$

The E_8 actions are

$$\begin{aligned}S_{\text{Topological}}[E_8]&=\int d^4x\frac{1}{60}\,\mathrm{Tr}[F^{\mathcal{A}}_{\mu\nu}F^{\mathcal{B}}_{\rho\tau}T_{\mathcal{A}}T_{\mathcal{B}}]\epsilon^{\mu\nu\rho\tau}=\int d^4xF^{\mathcal{A}}_{\mu\nu}F^{\mathcal{B}}_{\rho\tau}\eta_{\mathcal{AB}}\epsilon^{\mu\nu\rho\tau}\\&=\int d^4x[F^{IJ}_{\mu\nu}F^{KL}_{\rho\tau}\eta_{IJKL}+F^{A}_{\mu\nu}F^{B}_{\rho\tau}\eta_{AB}+2F^{IJ}_{\mu\nu}F^{B}_{\rho\tau}\eta_{IJB}]\epsilon^{\mu\nu\rho\tau},\end{aligned} \tag{2.13}$$

where $\epsilon^{\mu\nu\rho\tau}$ is the covariantized permutation symbol and

$$\begin{aligned}S_{YM}[E_8]&=\int d^4x\sqrt{g}\frac{1}{60}\,\mathrm{Tr}[F^{\mathcal{A}}_{\mu\nu}F^{\mathcal{B}}_{\rho\tau}T_{\mathcal{A}}T_{\mathcal{B}}]g^{\mu\rho}g^{\nu\tau}=\int d^4x\sqrt{g}F^{\mathcal{A}}_{\mu\nu}F^{\mathcal{B}}_{\rho\tau}\eta_{\mathcal{AB}}g^{\mu\rho}g^{\nu\tau}\\&=\int d^4x\sqrt{g}[F^{IJ}_{\mu\nu}F^{KL}_{\rho\tau}\eta_{IJKL}+F^{A}_{\mu\nu}F^{B}_{\rho\tau}\eta_{AB}+2F^{IJ}_{\mu\nu}F^{B}_{\rho\tau}\eta_{IJB}]g^{\mu\rho}g^{\nu\tau}.\end{aligned} \tag{2.14}$$

The above E_8 actions (are part of) can be embedded onto more general Cl(16) actions with a much larger number of terms given by

$$S_{\text{Topological}}[\mathrm{Cl}(16)]=\int d^4x\langle F^{\mathcal{M}}_{\mu\nu}F^{\mathcal{N}}_{\rho\tau}\Gamma_{\mathcal{M}}\Gamma_{\mathcal{N}}\rangle\epsilon^{\mu\nu\rho\tau}=\int d^4xF^{\mathcal{M}}_{\mu\nu}F^{\mathcal{N}}_{\rho\tau}G_{\mathcal{MN}}\epsilon^{\mu\nu\rho\tau} \tag{2.15}$$

and

$$S_{YM}[\mathrm{Cl}(16)]=\int d^4x\sqrt{g}\langle F^{\mathcal{M}}_{\mu\nu}F^{\mathcal{N}}_{\rho\tau}\Gamma_{\mathcal{M}}\Gamma_{\mathcal{N}}\rangle g^{\mu\rho}g^{\nu\tau}=\int d^4x\sqrt{g}F^{\mathcal{M}}_{\mu\nu}F^{\mathcal{N}}_{\rho\tau}G_{\mathcal{MN}}g^{\mu\rho}g^{\nu\tau}, \tag{2.16}$$

where $\langle\Gamma_{\mathcal{M}}\Gamma_{\mathcal{N}}\rangle=G_{\mathcal{MN}}\mathbf{1}$ denotes the *scalar* part of the Clifford geometric product, of the gammas. Notice that there are a total of 65 536 terms in

$$F^{\mathcal{M}}_{\mu\nu}F^{\mathcal{N}}_{\rho\tau}G_{\mathcal{MN}}=F_{\mu\nu}F_{\rho\tau}+F^{I}_{\mu\nu}F^{I}_{\rho\tau}+F^{I_1I_2}_{\mu\nu}F^{I_1I_2}_{\rho\tau}+\cdots+F^{I_1I_2\cdots I_{16}}_{\mu\nu}F^{I_1I_2\cdots I_{16}}_{\rho\tau}, \tag{2.17}$$

where the indices run as $I=1,2,\ldots,16$. The Clifford algebra Cl(16) has the graded structure (scalars, bivectors, trivectors,..., pseudoscalar) given by

$$1\ 16\ 120\ 560\ 1820\ 4368\ 8008\ 11\,440\ 12\,870$$

$$11\,440\ 8008\ 4368\ 1820\ 560\ 120\ 16\ 1, \tag{2.18}$$

consistent with the dimension of the Cl(16) algebra $2^{16}=256\times256=65\,536$. The possibility that one can accommodate another copy of the E_8 algebra within the Cl(16) algebraic structure warrants further investigation by working with the duals of the bivectors X_{IJ} and recurring to the remaining Y_A generators. The motivation is to understand the full symmetry of the $E_8\times E_8$ heterotic string from this Clifford algebraic perspective. A clear embedding is, of course, the following:

$$E_8\times E_8\subset \mathrm{Cl}(8)\otimes\mathrm{Cl}(8)\otimes\mathrm{Cl}(8)\otimes\mathrm{Cl}(8)\subset\mathrm{Cl}(16)\otimes\mathrm{Cl}(16)=\mathrm{Cl}(32), \tag{2.19}$$

where $\mathrm{SO}(32)\subset\mathrm{Cl}(32)$ and SO(32) is also an anomaly free group of the heterotic string that has the same dimension and rank as $E_8\times E_8$.

III. CHERN–SIMONS GRAVITY IN 11*D* FROM A CLIFFORD ALGEBRA GAUGE THEORY

The 11*D* Chern–Simons supergravity action is based on the smallest Anti de Sitter $\mathrm{OSp}(32|1)$ superalgebra. The Anti de Sitter group $\mathrm{SO}(10,2)$ must be embedded into a larger group $\mathrm{Sp}(32,R)$ to accomodate the fermionic degrees of freedom associated with the superalgebra $\mathrm{OSp}(32|1)$. The bosonic sector involves the connection[5]

$$\mathbf{A}_\mu=A^a_\mu\Gamma_a+A^{ab}_\mu\Gamma_{ab}+A^{a_1a_2\ldots a_5}_\mu\Gamma_{a_1a_2\ldots a_5}=e^a_\mu\Gamma_a+\omega^{ab}_\mu\Gamma_{ab}+A^{a_1a_2\ldots a_5}_\mu\Gamma_{a_1a_2\ldots a_5} \tag{3.1}$$

with $11+55+462=528$ generators. A Hermitian complex 32×32 matrix has a total of $32+2((32\times31)/2)=992+32=1024=32^2=2^{10}$ independent real components (parameters), the same number as the real parameters of the antisymmetric and symmetric real 32×32 matrices $496+528=1024$. The dimension of $\mathrm{Sp}(32)=(1/2)(32\times33)=528$. Notice that $2^{10}=1024$ is also the number of independent generators of the Cl(11) algebra since out of the 2^{11} generators, only half of them 2^{10}, are truly independent due to the duality conditions valid in odd dimensions only

$$\epsilon^{a_1a_2\ldots a_{2n+1}}\Gamma_{a_1}\wedge\Gamma_{a_2}\wedge\cdots\wedge\Gamma_{a_p}\sim\Gamma^{a_{p+1}}\wedge\Gamma^{a_{p+2}}\wedge\cdots\wedge\Gamma^{a_{2n+1}}. \tag{3.2}$$

This counting of components is the underlying reason why the Cl(11) algebra appears in this section. The generators of the Cl(11) algebra $\{\Gamma^a,\Gamma^b\}=2\eta^{ab}\mathbf{1}$ and the unit element $\mathbf{1}$ generate the Clifford polyvectors (including a scalar, pseudoscalar) of different grading

$$\Gamma^A=\mathbf{1},\Gamma^a,\Gamma^{a_1}\wedge\Gamma^{a_2},\Gamma^{a_1}\wedge\Gamma^{a_2}\wedge\Gamma^{a_3},\ldots,\Gamma^{a_1}\wedge\Gamma^{a_2}\wedge\cdots\wedge\Gamma^{a_{11}}, \tag{3.3}$$

obeying the conditions (3.2). The commutation relations (see Eqs. (3.4) below) involving the generators $\Gamma_a,\Gamma_{ab},\Gamma_{a_1a_2}\ldots a_5$ do in fact *close* due to the duality conditions (3.2). The Cl(11) algebra commutators, up to numerical factors, are

$$[\Gamma^a,\Gamma^b]=\Gamma^{ab},\quad [\Gamma^a,\Gamma^{bc}]=2\eta^{ab}\Gamma^c-2\eta^{ac}\Gamma^b, \tag{3.4a}$$

$$[\Gamma^{a_1a_2},\Gamma^{b_1b_2}]=-\eta^{a_1b_1}\Gamma^{a_2b_2}+\eta^{a_1b_2}\Gamma^{a_2b_1}-\cdots, \tag{3.4b}$$

$$[\Gamma^{a_1a_2a_3},\Gamma^{b_1b_2b_3}]=\Gamma^{a_1a_2a_3b_1b_2b_3}-(\eta^{a_1b_1a_2b_2}\Gamma^{a_3b_3}+\cdots), \tag{3.4c}$$

$$[\Gamma^{a_1a_2a_3a_4},\Gamma^{b_1b_2b_3b_4}]=-(\eta^{a_1b_1}\Gamma^{a_1a_2a_3a_4b_2b_3b_4}+\cdots)-(\eta^{a_1b_1a_2b_2a_3b_3}\Gamma^{a_4b_4}+\cdots), \tag{3.4d}$$

$$[\Gamma^{a_1a_2},\Gamma^{b_1b_2b_3b_4}] = -\eta^{a_1b_1}\Gamma^{a_2b_2b_3b_4} + \cdots, \tag{3.4e}$$

$$[\Gamma^{a_1},\Gamma^{b_1b_2b_3}] = \Gamma^{a_1b_1b_2b_3}[\Gamma^{a_1a_2},\Gamma^{b_1b_2b_3}] = -2\eta^{a_1b_1}\Gamma^{a_2b_2b_3} + \cdots, \tag{3.4f}$$

$$[\Gamma^{a_1},\Gamma^{b_1b_2b_3b_4}] = -\eta^{a_1b_1}\Gamma^{b_2b_3b_4} + \cdots, \tag{3.4g}$$

$$\begin{aligned}[\Gamma^{a_1a_2\ldots a_5},\Gamma^{b_1b_2\ldots b_5}] &= \Gamma^{a_1a_2\ldots a_5b_1b_2\ldots b_5} + (\eta^{a_1b_1a_2b_2}\Gamma^{a_3a_4a_5b_3b_4b_5} + \cdots) + (\eta^{a_1b_1a_2b_2a_3b_3a_4b_4}\Gamma^{a_5b_5} + \cdots)\\ &= \epsilon^{a_1a_2\ldots a_5b_1b_2\ldots b_5c}\Gamma_c + (\eta^{a_1b_1a_2b_2}\epsilon^{a_3a_4a_5b_3b_4b_5c_1c_2\ldots c_5}\Gamma_{c_1c_2\ldots c_5} + \cdots)\\ &\quad + (\eta^{a_1b_1a_2b_2a_3b_3a_4b_4}\Gamma^{a_5b_5} + \cdots),\end{aligned} \tag{3.4h}$$

etc, with

$$\eta_{a_1b_1a_2b_2} = \eta_{a_1b_1}\eta_{a_2b_2} - \eta_{a_2b_1}\eta_{a_1b_2}, \tag{3.5a}$$

$$\eta_{a_1b_1a_2b_2a_3b_3} = \eta_{a_1b_1}\eta_{a_2b_2}\eta_{a_3b_3} - \eta_{a_1b_2}\eta_{a_2b_1}\eta_{a_3b_3} + \cdots, \tag{3.5b}$$

$$\eta_{a_1b_1a_2b_2\ldots a_nb_n} = \frac{1}{n!}\epsilon_{i_1i_2\ldots i_n}\epsilon_{j_1j_2\ldots j_n}\eta_{a_{i_1}b_{j_1}}\eta_{a_{i_2}b_{j_2}}\cdots\eta_{a_{i_n}b_{j_n}}. \tag{3.5c}$$

The Cl(11) algebra gauge field is

$$\mathbf{A}_\mu = \mathcal{A}^A_\mu = \mathcal{A}_\mu\mathbf{1} + \mathcal{A}^a_\mu\Gamma_a + \mathcal{A}^{a_1a_2}_\mu\Gamma_{a_1a_2} + \mathcal{A}^{a_1a_2a_3}_\mu\Gamma_{a_1a_2a_3} + \cdots + \mathcal{A}^{a_1a_2\ldots a_{11}}_\mu\Gamma_{a_1a_2\ldots a_{11}}, \tag{3.6}$$

and the Cl(11)-algebra-valued field strength

$$\begin{aligned}\mathcal{F}^A_{\mu\nu}\Gamma_A &= \partial_{[\mu}A_{\nu]}\mathbf{1} + [\partial_{[\mu}A^a_{\nu]} + A^{b_2}_{[\mu}A^{b_1a}_{\nu]}\eta_{b_1b_2} + \cdots]\Gamma_a + [\partial_{[\mu}A^{ab}_{\nu]} + A^a_{[\mu}A^b_{\nu]} - A^{a_1a}_{[\mu}A^{b_1b}_{\nu]}\eta_{a_1b_1}\\ &\quad - A^{a_1a_2a}_{[\mu}A^{b_1b_2b}_{\nu]}\eta_{a_1b_1a_2b_2} - A^{a_1a_2a_3a}_{[\mu}A^{a_1b_2b_3b}_{\nu]}\eta_{a_1b_1a_2b_2a_3b_3} + \cdots]\Gamma_{ab} + [\partial_{[\mu}A^{abc}_{\nu]}\\ &\quad + A^{a_1a}_{[\mu}A^{b_1bc}_{\nu]}\eta_{a_1b_1} + \cdots]\Gamma_{abc} + [\partial_{[\mu}A^{abcd}_{\nu]} - A^{a_1a}_{[\mu}A^{b_1bcd}_{\nu]}\eta_{a_1b_1} + \cdots]\Gamma_{abcd}\\ &\quad + \cdots[\partial_{[\mu}A^{a_1a_2\ldots a_5b_1b_2\ldots b_5}_{\nu]} + A^{a_1a_2\ldots a_5}_{[\mu}A^{b_1b_2\ldots b_5}_{\nu]} + \cdots]\Gamma_{a_1a_2\ldots a_5b_1b_2\ldots b_5} + \cdots.\end{aligned} \tag{3.7}$$

The Chern–Simons actions rely on Stokes theorem

$$\int_{M^{12}}\epsilon^{\mu_1\mu_2\ldots\mu_{11}\mu_{12}}\partial_{\mu_{12}}(A_{\mu_1\mu_2\ldots\mu_{11}}) = \int_{\partial M^{12}=\Sigma^{11}}\epsilon^{\mu_1\mu_2\ldots\mu_{11}\mu_{12}}A_{\mu_1\mu_2\ldots\mu_{11}}d\Sigma^{11}_{\mu_{12}}, \tag{3.8}$$

which in our case reads

$$d(\mathcal{L}_{\text{Clifford}}) = \langle\mathcal{F}\wedge\mathcal{F}\wedge\cdots\wedge\mathcal{F}\rangle = \langle\mathcal{F}^{A_1}\wedge\mathcal{F}^{A_2}\wedge\cdots\wedge\mathcal{F}^{A_6}\Gamma_{A_1}\Gamma_{A_2}\ldots\Gamma_{A_6}\rangle, \tag{3.9}$$

where the bracket $\langle\cdots\rangle$ means taking the scalar part of the Clifford geometric product among the gammas. It involves products of the d_{ABC}, f_{ABC} structure constants corresponding to the (anti) commutators $\{\Gamma A,\Gamma_B\}=d_{ABC}\Gamma^C$ and $[\Gamma_A,\Gamma_B]=f_{ABC}\Gamma^C$.

One of the main results of this work is that the Cl(11) algebra based action (3.9) contains a *vast number* of *terms* among which is the Chern–Simons action of Ref. 15 $\mathcal{L}^{11}_{\text{CS}}(e,\omega,A_5)$,

$$\mathcal{L}_{\text{Clifford}}(\mathcal{A}^A_\mu\Gamma_A) = \mathcal{L}^{11}_{\text{CS}}(\omega,e,A_5) + \text{EXTRA TERMS}, \tag{3.10}$$

$$S_{\text{CS}}(\omega,e,A_5) = \int_{\partial M^{12}}\mathcal{L}^{11}_{\text{CS}} = \int_{\Sigma^{11}}\mathcal{L}^{11}_{\text{CS}}, \tag{3.11}$$

$$\mathcal{L}^{11}_{\rm CS}(\omega,e,A_5)=\mathcal{L}^{11}_{\rm Lovelock}(\omega,e)+\mathcal{L}^{11}_{\rm Pontryagin}(\omega,e)+\mathcal{L}^{11}(A_5,\omega,e). \tag{3.12}$$

In odd dimensions $D=2n-1$, the Lanczos–Lovelock Lagrangian is

$$\mathcal{L}^{D}_{\rm Lovelock}=\sum_{p=0}^{n-1}a_pL_p(D),\quad a_p=\kappa\frac{(\pm 1)^{p+1}l^{2p-D}}{(D-2p)}C_p^{n-1}\quad p=1,2,\ldots,n-1. \tag{3.13}$$

C_p^{n-1} is the binomial coefficient. The constants κ, l are related to the Newton's constant G and to the cosmological constant Λ through $\kappa^{-1}=2(D-2)\Omega_{D-2}G$ where Ω_{D-2} is the area of the $D-2$ -dim unit sphere and $\Lambda=\pm(D-1)(D-2)/2l^2$ for de Sitter (Anti de Sitter) spaces.[15] A derivation of the vacuum energy density of Anti de Sitter space (de Sitter) as the geometric mean between an upper and lower scale was obtained in Ref. 11 based on a BF–Chern–Simons–Higgs theory. Upon setting the lower scale to the Planck scale L_P and the upper scale to the Hubble radius (today) R_H, it yields the observed value of the cosmological constant $\rho=L_P^{-2}R_H^{-2}=L_P^{-4}(L_P/R_H)^2\sim 10^{-120}M_P^4$.

The terms inside the summand of Eq. (3.13) are

$$L_p(D)=\epsilon_{a_1a_2\ldots a_D}R^{a_1a_2}R^{a_3a_4}\ldots R^{a_{2p-1}a_{2p}}e^{a_{2p+1}}\ldots e^{a_D}, \tag{3.14}$$

where we have omitted the space-time indices $\mu_1,\mu_2,\ldots$. Despite the higher powers of the curvature (after eliminating the spin connection ω_μ^{ab} in terms of the e_μ^a field) the $\mathcal{L}^D_{\rm Lovelock}$ furnishes equations of motion for the e_μ^a field containing at most derivatives of *second* order, and not higher, due to the topological property of the Lovelock terms

$$d(\mathcal{L}^{11}_{\rm Lovelock})=\epsilon_{a_1a_2\ldots a_{11}}\left(R^{a_1a_2}+\frac{e^{a_1}e^{a_2}}{l^2}\right)\ldots\left(R^{a_9a_{10}}+\frac{e^{a_9}e^{a_{10}}}{l^2}\right)T^{a_{11}}=\text{Euler density in } 12D. \tag{3.15}$$

The exterior derivative of the Lovelock terms can be rewritten compactly as

$$d(\mathcal{L}^{11}_{\rm Lovelock})=\epsilon_{A_1A_2\ldots A_{12}}F^{A_1A_2}\ldots F^{A_{11}A_{12}}, \tag{3.16}$$

where $F^{A_1A_2}$ is the curvature field strength associated with the SO(10,2) connection $\Omega_\mu^{A_1A_2}$ in $12D$ and which can be decomposed in terms of the fields e_μ^a, ω_μ^{ab}, $a,b=1,2,\ldots,11$ by identifying $\Omega_\mu^{aD}=(1/l)e_\mu^a$ and $\Omega_\mu^{ab}=\omega_\mu^{ab}$ so that the Torsion and Lorenz curvature 2-forms are

$$T^a(\omega,e)=F^{aD}=d\Omega^{aD}+\Omega^a_b\wedge\Omega^{bD}=\frac{1}{l}(de^a-\omega^a_b\wedge e^b),$$
$$F^{ab}=(d\Omega^{ab}+\Omega^a_c\wedge\Omega^{cd})+(\Omega^a_D\wedge\Omega^{Db})=R^{ab}(\omega)+\frac{1}{l^2}e^a\wedge e^b,\quad R^{ab}(\omega)=d\omega^{ab}+\omega^a_c\wedge\omega^{cb}, \tag{3.17}$$

where a length parameter l must be introduced to match dimensions since the connection has units of $1/l$. This l parameter is related to the cosmological constant.

$\mathcal{L}^{11}_{\rm Pontryagin}(\omega,e)$ is the Chern–Simons 11-form whose exterior derivative

$$d(\mathcal{L}_{\rm Pontryagin})=F^{A_1}_{A_2}F^{A_2}_{A_3}\ldots F^{A_5}_{A_6}F^{A_6}_{A_1} \tag{3.18}$$

is the (one of the many) Pontryagin 12-form (up to numerical factors) for the SO(10,2) connection in $12D$. As mentioned above, the SO(10,2) connection Ω_μ^{AB} can be broken into the e_μ^a field and the SO(10,1) spin connection ω_μ^{ab} such that the number of components is $11+\frac{1}{2}(11\times 10)=66=\frac{1}{2}(12\times 11)$. Finally, the exterior derivative $d\mathcal{L}(A_5,\omega,e)$ is the 12-form (we are omitting space-time indices $\mu_1,\mu_2,\ldots,\mu_{12}$) that is comprised of terms of the form

$$(R^{a_1a_2\cdots a_5}R_{a_1a_2\cdots a_5})(R^{b_1b_2}R_{b_1b_2})(T^cT_c),(R^{a_1a_2\cdots a_5}R_{a_1a_2\cdots a_5})^2(R^{b_1b_2}R_{b_1b_2}),(R^{a_1a_2\cdots a_5}R_{a_1a_2\cdots a_5})^3, \tag{3.19}$$

the curvature 2-from associated with the field $A_\mu^{c_1c_2\cdots c_5}$ is given by

$$R_{\mu\nu}^{c_1c_2\cdots c_5} = \partial_{[\mu}A_{\nu]}^{c_1c_2\cdots c_5} + A_{[\mu}^{a_1a_2\cdots a_5}A_{\nu]}^{b_1b_2\cdots b_5}f_{a_1a_2\cdots a_5b_1b_2\cdots b_5}^{c_1c_2\cdots c_5}, \tag{3.20}$$

where the structure constants f_{ABC} in Eq. (3.18) are obtained from the Cl(11) algebra commutation relations in Eq. (3.4h).

IV. CONCLUSIONS: GENERALIZED CHERN–SIMONS GRAVITY IN CLIFFORD SPACES

The Cl(11) algebra based action [(3.9), (3.10)] can in turn be embedded into a more general expression in C-space (Clifford space) which is a generalized tensorial spacetime of coordinates $\mathbf{X}=\sigma,x^\mu,x^{\mu\nu},x^{\mu\nu\rho}\ldots$[4] involving a scalar $\Phi(\mathbf{X})$ and antisymmetric tensor gauge fields $A_\mu(\mathbf{X})$, $A_{\mu\nu}(\mathbf{X})$, $A_{\mu\nu\rho}(\mathbf{X})\ldots$ of higher rank (higher spin theories).[21] The most general action onto which the action (3.9), (3.10) itself can be embedded requires a tensorial gauge field theory[21] (generalized Yang–Mills theories) and an integration with respect to all the Clifford-valued coordinates $\mathbf{X}=X^M\Gamma_M$ corresponding to the 2^D-dim C-space associated with the underlying $Cl(2n)$-algebra in $D=2n$ dimensions

$$S = \int [d^{2^n}X]\langle(\mathcal{F}\wedge\mathcal{F}\wedge\cdots\wedge\mathcal{F})\rangle, \quad [d^{2^n}X] = (d\sigma)(dx^\mu)(dx^{\mu\nu})(dx^{\mu\nu\rho})\ldots. \tag{4.1}$$

A different sort of generalized Yang–Mills theories have been studied by Ref. 22 without the Clifford algebraic structure.

Given a Lie algebra $\mathbf{G}$ with generators T_a for $a=1,2,3,\ldots,dim\ \mathbf{G}$, it has for commutators $[T_a,T_b]=f_{ab}^cT_c$ and whose structure constants f_{abc} are fully antisymmetric in their indices. The Lie-algebra valued one-form is $\mathbf{A}=(A_M^a(\mathbf{X})T_a)dX^M$ and its generalized Lie-algebra valued field strength

$$\mathbf{F} = [F_{MN}^c(X)T_c]dX^M\wedge dX^N = [\partial_{[M}A_{N]}^c(X)T_c + gA_M^a(X)A_N^b(X)f_{ab}^cT_c]dX^M\wedge dX^N, \tag{4.2}$$

has for components

$$F_{[[\mu_1\mu_2\ldots\mu_m][\nu_1\nu_2\ldots\nu_n]]}^c = \partial_{[\mu_1\mu_2\ldots\mu_m]}A_{[\nu_1\nu_2\ldots\nu_n]}^c - \partial_{[\nu_1\nu_2\ldots\nu_n]}A_{[\mu_1\mu_2\ldots\mu_m]}^c + gA_{[\mu_1\mu_2\ldots\mu_m]}^aA_{[\nu_1\nu_2\ldots\nu_n]}^bf_{ab}^c. \tag{4.3}$$

The remaining components are of the form

$$F_{[0,N]}^c = F_{[0[\nu_1\nu_2\ldots\nu_n]]}^c = \partial_\sigma A_{[\nu_1\nu_2\ldots\nu_n]}^c - \partial_{x[\nu_1\nu_2\ldots\nu_n]}A_0^c + gA_0^aA_{[\nu_1\nu_2\ldots\nu_n]}^bf_{ab}^c, \tag{4.4}$$

where A_0^c is the Clifford-scalar part $\Phi(\mathbf{X})$ of the Lie-algebra valued Clifford polyvector and in general we must consider the $m=n$ and $m\neq n$ cases resulting from the mixing of different grades (ranks). The antisymmetry with respect the collective indices MN is explicit.

In order to raise, lower and contract polyvector indices in C-space it requires a generalized metric G^{MN}. In flat C-space it is defined by the components

$$G^{\mu\nu} = \eta^{\mu\nu}, \quad G^{\mu_1\mu_2\nu_1\nu_2} = \eta^{\mu_1\nu_1}\eta^{\mu_2\nu_2} - \eta^{\mu_1\nu_2}\eta^{\mu_2\nu_1}, \text{ etc}\,., \tag{4.5}$$

in addition to the scalar-scalar component $G^{\sigma\sigma}=1$. It can be recast as

$$G^{\mu_1\mu_2\cdots\mu_m\nu_1\nu_2\cdots\nu_m} = \det\mathbf{G}^{\mu_I\nu_J} = \frac{1}{m!}\epsilon_{i_1i_2\ldots i_m}\epsilon_{j_1j_2\ldots j_m}\eta^{\mu_{i_1}\nu_{j_1}}\eta^{\mu_{i_2}\nu_{j_2}}\ldots\eta^{\mu_{i_m}\nu_{j_m}}, \tag{4.6}$$

where $\mathbf{G}^{\mu_I\nu_J}$ is an $m\times m$ matrix whose entries are $\eta^{\mu_i\nu_j}$ for $i,j=1,2,3,\ldots,m\leq D$ and $\mu,\nu=1,2,3,\ldots,D$.

As a result of the expression for the flat C-space metric, given by sums of antisymmetrized products of $\eta^{\mu\nu}$, the Clifford-space generalized Yang–Mills action is of the form

$$S_{YM} = -\frac{1}{2}\int [\mathcal{D}X] \sum \text{trace}[F^{a}_{[[\mu_1\mu_2\ldots\mu_m][\nu_1\nu_2\ldots\nu_m]]} F^{[[\mu_1\mu_2\ldots\mu_m][\nu_1\nu_2\ldots\nu_m]]b} T_a T_b] +$$
$$-\frac{1}{2}\int [\mathcal{D}X] \sum \text{trace}[F^{a}_{[0[\nu_1\nu_2\ldots\nu_m]]} F^{[[0\nu_1\nu_2\ldots\nu_m]]b} T_a T_b], \tag{4.7}$$

where the C-space 2^D-dim measure associated with a Clifford algebra in D-dim is

$$[\mathcal{D}X] = [d\sigma][\mathbf{\Pi} dx^{\mu}][\mathbf{\Pi} dx^{\mu_1\mu_2}][\mathbf{\Pi} dx^{\mu_1\mu_2\mu_3}]\ldots[dx^{\mu_1\mu_2\cdots\mu_d}] \tag{4.8}$$

and the indices are ordered as $\mu_1 < \mu_2 < \mu_3 \ldots < \mu_m$, etc.

The action (4.7) is invariant under the infinitesimal gauge transformations

$$\delta_\xi A^c_M = \partial_M \xi^c + g f^c_{ab} A^a_M \xi^b, \quad \delta_\xi A^c_{\mu_1\mu_2\ldots\mu_n} = \partial_{x_{\mu_1\mu_2\ldots\mu_n}} \xi^c + g f^c_{ab} A^a_{\mu_1\mu_2\ldots\mu_n} \xi^b \tag{4.9}$$

associated with a Lie-algebra valued Clifford-scalar parameter $\xi(\mathbf{X}) = \xi^a(\mathbf{X}) T_a$.

In Sec. I A it was explained why another alternative to define the transformations in C-space was by writing the generators of polyrotations as $R = \exp(\Omega^{AB}[E_A, E_B])$ where the commutator $[E_A, E_B] = F^C_{AB} E_C$ is the C-space analog of the $i[\gamma_\mu, \gamma_\nu]$ commutator which is the generator of the Lorentz algebra, and the parameters Ω^{AB} are the C-space analogs of the rotation/boots parameters. This last alternative seems to be more physical because a polyrotation should map the E_A direction into the E_B direction in C-spaces, hence the meaning of the generator $[E_A, E_B]$ which is the generalization of the ordinary $i[\gamma_\mu, \gamma_\nu]$ Lorentz generator.

Therefore, when we recast the generators of polyrotations as $\mathcal{J}_{AB} = [\Gamma_A, \Gamma_B]$, an action of the form

$$S(C_{\text{space}}) = \int [\mathcal{D}X] F^{A_1B_1}_{M_1N_1} F^{A_2B_2}_{M_2N_2} \ldots F^{A_{2^{d-1}}B^2_{d-1}}_{M_{2^{d-1}}N_{2^{d-1}}} \epsilon_{A_1B_1A_2B_2\ldots A_{2^{d-1}}B_{2^{d-1}}} \epsilon^{M_1N_1M_2N_2\ldots M_{2^{d-1}}N_{2^{d-1}}} \tag{4.10}$$

is the natural generalization of the Euler density types of the D-dim ($D = 2n$) actions given by Eq. (3.16) in C-space.

This action $S(C_{\text{space}})$ (4.10) is more general than the action $S_{\text{Clifford}}(\mathcal{A}^A_\mu \Gamma_A)$ of Eq. (3.10), and which in turn, is more general than the Chern–Simons gravitational action $S_{\text{CS}}(\omega, e, A_5)$ given by Eq. (3.12). Therefore, we have the inclusions

$$S_{\text{CS}}(\omega, e, A_5) \subset S_{\text{Clifford}}[\mathcal{A}^A_\mu(x^\mu)\Gamma_A] \subset S(C_{\text{space}})[\mathcal{A}^{AB}_M(\sigma, x^\mu, x^{\mu_1\mu_2}, x^{\mu_1\mu_2\mu_3}, \ldots)\mathcal{J}_{AB}], \tag{4.11}$$

which should be very relevant in future developments of M, F theory upon the introduction of polyvector-valued supersymmetries in C-spaces.[16] These generalized supersymmetries deserve to be investigated further since they are more fundamental than the supersymmetries associated with M, F theory superalgebras and also span well beyond the N-extended supersymmetric field theories involving superalgebras like $\text{OS}_\text{p}(32|N)$ for example, which are related to a $\text{SO}(N)$ gauge theory coupled to matter fermions (besides the gravitinos). It is these polyvector-valued supersymmetries in C-spaces[16] that will permit the supersymmetrization of the most general action in C-spaces $S(C_{\text{space}})$ given by Eq. (4.10).

Finally, the results of this work may shed some light into the origins behind the hidden E_8 symmetry of $11D$ supergravity, the hyperbolic Kac–Moody algebra E_{10} and the nonlinearly realized E_{11} algebra related to chaos in M theory and oscillatory solutions close to cosmological singularities.[1–3]

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APPENDIX: CLOSURE OF THE CLIFFORD SPACE SUPERSYMMERTRY

The classification of the family of symmetric matrices $(C\gamma^{\mu_1\mu_1\cdots\mu_n})_{\alpha\beta}$ is what restricts the type of terms that appear in the $\{Q_\alpha, Q_\beta\}$ anticommutator and depends on the number of space time dimensions D, the signatures (s,t) and the rank n. A table of the allowed values of D,s,t,n can be found in Ref. 18. In particular, when $D=4=3+1$, the $\{Q_\alpha, Q_\beta\}$ is a symmetric matrix in α,β with ten independent components and which matches the degrees of freedom in P^μ, $P^{\mu\nu}$ given by $4+6=10$. Let us study the closure of

$$\{[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4}, O_\alpha], Q_\beta\} + \{[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4}, Q_\beta], Q_\alpha\} = [\mathcal{M}_{\mu_1\mu_2\mu_3\mu_2}, \{Q_\alpha Q_\beta\}], \tag{A1}$$

where

$$\{Q_\alpha, Q_\beta\} = \frac{1}{2} C\gamma^\mu P_\mu + \frac{1}{2} C\gamma^{\mu\nu} P_{\mu\nu}. \tag{A2}$$

In $D=4$, with signatures $-,+,+,+$ one can find a charge conjugation matrix C and its transpose C^T obeying the properties

$$(C\gamma^\mu)^T = (C\gamma^\mu), \quad (C\gamma^{\mu\nu})^T = (C\gamma^{\mu\nu}), \tag{A3}$$

$$C^T = -C, C\gamma_\mu C^{-1} = -\gamma_\mu^T, \quad C^\dagger C = CC^\dagger = 1, \quad C^{-1}\gamma_{\mu\nu} C = -\gamma_{\mu\nu}^T. \tag{A4}$$

It is convenient to use a Majorana representation where the charge conjugation matrix is given by $C=\gamma_0$ and $\gamma_5^T = -\gamma_5$ is a hermitian matrix that has zero entries along the diagonal and $-i\sigma_1$, $i\sigma_1$ off the diagonal.

We must verify that Eq. (A1) is obeyed. This requires that the spinorial charges Q_α behave under polyrotations as follows:

$$[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4}, Q_\alpha] = -\frac{1}{2}(\gamma_{\mu_1\mu_2\mu_3\mu_4})_\alpha^\delta Q_\delta \tag{A5}$$

and

$$[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4}, P_{\nu_1\nu_2}] = \eta_{\mu_1\mu_2\nu_1\nu_2} P_{\mu_3\mu_4} + \eta_{\mu_3\mu_4\nu_1\nu_2} P_{\mu_1\mu_2} \pm \cdots, \tag{A6}$$

the $\pm$ signs on the rhs of Eq. (A6) depend on the permutation of indices with respect to the initial combination $\mu_1\mu_2\mu_3\mu_4$, $\nu_1\nu_2$. There are six terms in Eq. (A6). The lhs of Eq. (A1) is

$$\begin{aligned} &-\frac{1}{4}\gamma_5(C\gamma^\mu P_\mu + C\gamma^{\mu\nu} P_{\mu\nu}) - \frac{1}{4}[\gamma_5(C\gamma^\mu P_\mu + C\gamma^{\mu\nu} P_{\mu\nu})]^T \\ &= -\frac{1}{4}\gamma_5(C\gamma^\mu P_\mu + C\gamma^{\mu\nu} P_{\mu\nu}) - \frac{1}{4}[(C\gamma^\mu)^T \gamma_5^T P_\mu + (C\gamma^{\mu\nu})\gamma_5^T P_{\mu\nu}] \\ &= -\frac{1}{4}\gamma_5(C\gamma^\mu P_\mu + C\gamma^{\mu\nu} P_{\mu\nu}) + \frac{1}{4}(C\gamma^\mu P_\mu + C\gamma^{\mu\nu} P_{\mu\nu})\gamma_5, \end{aligned} \tag{A7}$$

where we have used the conditions (A3) and $\gamma_5^T = -\gamma_5$.

Multiplying Eq. (A7) from the left by C^{-1} and using $C^{-1}\gamma_5 C = -\gamma_5$ yields

$$\frac{1}{4}(\gamma_5\gamma^{\mu}+\gamma^{\mu}\gamma_5)P_{\mu}+\frac{1}{4}(\gamma_5\gamma^{\mu\nu}+\gamma^{\mu\nu}\gamma_5)P_{\mu\nu}$$

$$=\frac{1}{4}(\gamma_5\gamma^{\mu\nu}+\gamma^{\mu\nu}\gamma_5)P_{\mu\nu}+\frac{1}{2}\gamma_5\gamma^{\mu\nu}P_{\mu\nu}=\frac{1}{2}\gamma_{[\mu_1}\gamma_{\mu_2}\gamma_{\mu_3}\gamma_{\mu_4}\gamma^{\nu_1\nu_2}P_{\nu_1\nu_2}$$

$$=\frac{1}{2}[\gamma_{[\mu_1\mu_2]}\eta^{\nu_1\nu_2}_{\mu_3\mu_4}+\cdots]P_{\nu_1\nu_2}$$

$$=\frac{1}{2}[\gamma_{[\mu_1\mu_2]}P_{\mu_3\mu_4}+\gamma_{[\mu_3\mu_4]}P_{\mu_1\mu_2}\pm\cdots]. \tag{A8}$$

One may notice that due to the condition $\{\gamma_5,\gamma_\mu\}=0$ there are no P_μ terms in Eq. (A8). The rhs of Eq. (A1) is

$$\frac{1}{2}[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},(C\gamma^{\nu_1}P_{\nu_1})+(C\gamma^{\nu_1\nu_2})P_{\nu_1\nu_2}]$$

$$=\frac{1}{2}(C\gamma^{\nu_1\nu_2})[\eta_{\nu_1\mu_2\nu_1\nu_2}P_{\mu_3\mu_4}+\eta_{\nu_2\mu_4\nu_1\nu_2}P_{\mu_1\mu_2}+\cdots], \tag{A9}$$

where

$$[\mathcal{M}_{\mu_1\mu_2\mu_3\mu_4},(C\gamma^{\nu_1}P_{\nu_1})]=C\gamma^{\nu_1}[\mathcal{M}\mu_1\mu_2\mu_3\mu_4,P_{\nu_1}]=0. \tag{A10}$$

Multiplying, Eq. (A9) on the left by C^{-1} yields

$$\frac{1}{2}\gamma^{\nu_1\nu_2}[\eta_{\mu_1\mu_2\nu_1\nu_2}P_{\mu_3\mu_4}+\eta_{\mu_3\mu_4\nu_1\nu_2}P_{\mu_1\mu_2}+\cdots]=\frac{1}{2}[\gamma_{[\nu_1\nu_2]}P_{\mu_3\mu_4}+\gamma_{[\mu_3\mu_4]}P_{\mu_1\mu_2}\pm\cdots]. \tag{A11}$$

We have seen that a left-multiplication of the rhs and lhs of Eq. (A1) by C^{-1}, leads to the equality of Eq. (A8) with Eq. (A11), which implies that Eq. (A1) is indeed satisfied.

The Jacobi identity

$$\{[\mathcal{M}_{\mu_1\mu_2},Q_\alpha],Q_\beta\}+\{[\mathcal{M}_{\mu_1\mu_2},Q_\beta],Q_\alpha\}=[\mathcal{M}_{\mu_1\mu_2},\{Q_\alpha,Q_\beta\}], \tag{A12}$$

when

$$[M_{\mu_1\mu_2},P_{\rho_1\rho_2}]=-\eta_{\mu_1\rho_1}P_{\mu_2\rho_2}\pm\cdots,[\mathcal{M}_{\mu_1\mu_1},Q_\alpha]$$

$$=-\frac{1}{2}(\gamma_{\mu_1\mu_2})^{\delta}_{\alpha}Q_\delta,\{Q_\alpha,Q_\beta\}=\frac{1}{2}C\gamma^{\nu}P^{\nu}+\frac{1}{2}C\gamma\nu_1\nu_2P_{\nu_1\nu_2} \tag{A13}$$

involves terms containing P_μ and $P_{\mu\nu}$. We know that the Jacobi identity is satisfied for the P_μ terms since this is what the ordinary supersymmetry algebra entails.

The $P_{\mu\nu}$ terms involve the commutator

$$-[\gamma_{\nu_1\nu_2},\gamma_{\nu_1\nu_2}]P^{\nu_1\nu_2}=(\eta_{\mu_1\nu_1}\gamma_{\mu_2\nu_2}\pm\cdots)P^{\nu_1\nu_2}. \tag{A14}$$

Each one of the four terms in Eq. (A14), for example, like the term $\eta_{\mu_1\nu_1}\gamma_{\mu_2\nu_2}P^{\nu_1\nu_2}$ can be rewritten as

$$\eta_{\mu_1\nu_1}\gamma_{\mu_2\nu_2}P^{\nu_1\nu_2} = \eta_{\mu_1\nu_1}\gamma^{\rho_1\rho_2}\eta_{\rho_1\rho_2\mu_2\nu_2}\eta^{\nu_1\nu_2\mu_2\rho_2}P_{\mu_2\rho_2} = -\eta_{\mu_1\nu_1}\delta^{\nu_1}_{\rho_1}\gamma^{\rho_1\rho_2}P_{\mu_2\rho_2} = -\eta_{\mu_1\rho_1}\gamma^{\rho_1\rho_2}P_{\mu_2\rho_2} \tag{A15}$$

and similarly one can rewrite the other three terms of Eq. (A14), so that the Jacobi identity (A12) is satisfied due to the equality in (A15)

$$\gamma^{\rho_1\rho_2}[M_{\mu_1\mu_2}, P_{\rho_1\rho_2}] = \gamma^{\rho_1\rho_2}(-\eta^{\mu_1\rho_1}P_{\mu_2\rho_2} \pm \cdots) = -[\gamma_{\mu_1\mu_2}, \gamma_{\nu_1\nu_2}]P^{\nu_1\nu_2} = P^{\nu_1\nu_2}(\eta_{\mu_1\nu_1}\gamma_{\mu_2\nu_2} \pm \cdots), \tag{A16}$$

i.e, the equality among the terms of Eq. (A16) can be seen effectively as exchanging $\gamma \leftrightarrow P$ and $(\nu_1, \nu_2) \leftrightarrow (\rho_1, \rho_2)$.

One must have as well

$$[Q_\alpha, P_\mu] = [Q_\alpha, P_{\mu\nu}] = 0, \quad [P_\mu, P_\nu] = [P_{\mu_1\mu_2}, P_{\nu_1\nu_2}] = 0 \ldots \tag{A17}$$

This example in $D=4$ should be valid in other dimensions and signatures provided we have the appropriate list of symmetric $(C\gamma^{\mu_1\mu_2\cdots\mu_n})_{\alpha\beta}$ matrices.

One has the remaining commutators

$$[M_{\mu_1\mu_2}, M_{\nu_1\nu_2}] = -\eta_{\mu_1\nu_1}M_{\mu_2\nu_2} + \eta_{\mu_2\nu_1}M_{\nu_1\nu_2} \pm \cdots, \tag{A18}$$

$$[M_{\mu_1\mu_2\mu_3\mu_4}, M_{\nu_1\nu_2\mu_3\mu_4}] = \eta_{\mu_1\nu_2\nu_1\mu_2}M_{\mu_3\nu_4\mu_3\mu_4} \pm \cdots, \tag{A19}$$

$$[M_{\mu_1\mu_2}, M_{\nu_1\nu_2\mu_3\mu_4}] = -\eta_{\mu_1\nu_1}M_{\mu_2\nu_2\nu_3\nu_4} \pm \cdots, \tag{A20}$$

which obey the Jacobi identities.

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Foundations of a spacetime path formalism for relativistic quantum mechanics

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Quantum field theory is the traditional solution to the problems inherent in melding quantum mechanics with special relativity. However, it has also long been known that an alternative first-quantized formulation can be given for relativistic quantum mechanics, based on the parametrized paths of particles in spacetime. Because time is treated similarly to the three space coordinates, rather than as an evolution parameter, such a spacetime approach has proved particularly useful in the study of quantum gravity and cosmology. This paper shows how a spacetime path formalism can be considered to arise naturally from the fundamental principles of the Born probability rule, superposition, and Poincaré invariance. The resulting formalism can be seen as a foundation for a number of previous parametrized approaches in the literature, relating, in particular, "off-shell" theories to traditional on-shell quantum field theory. It reproduces the results of perturbative quantum field theory for free and interacting particles, but provides intriguing possibilities for a natural program for regularization and renormalization. Further, an important consequence of the formalism is that a clear probabilistic interpretation can be maintained throughout, with a natural reduction to nonrelativistic quantum mechanics. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2375033]

I. INTRODUCTION

The idea of constructing quantum states as a "sum over histories" is well known in the form of the Feynman path integral formulation. However, this approach is best known in its application to nonrelativistic quantum mechanics,[1,2] in which particle paths are parametrized by coordinate time. A natural relativistic generalization is to consider parametrized paths in four-dimensional spacetime rather than time-parametrized paths in three-dimensional space. Feynman himself developed such an approach, and this conception seems to have informed much of Feynman's early view of relativistic quantum mechanics.[3–5]

At an even earlier date, Stueckelberg presented a detailed formulation of relativistic quantum mechanics in terms of parametrized spacetime paths.[6,7] A number of other authors (notably Refs. 8–18) have also developed related approaches involving an invariant "fifth parameter" governing the evolution of a quantum system, though not necessarily identifying this explicitly as a path parameter.

A key feature of these approaches is that time is treated comparably to the three space coordinates, rather than as an evolution parameter. This is particularly applicable to the study of quantum gravity and cosmology, in which the fundamental equations (such as the Wheeler–DeWitt equation) make no explicit distinction for the time coordinate (see, e.g., Refs. 19–25).

Also, in the infinite-tension limit, string theory reduces to a worldline formalism for relativistic quantum theory.[26–32] One would therefore expect a path formulation of relativistic quantum mechanics to provide a natural bridge to the typically first-quantized formulation of string theory.

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Despite the promise of the approach, spacetime path formalisms have often been presented in the literature as simply alternative formulations of results obtained from the more traditional quantum field theory formalism. The motivation of the present paper, however, is to construct a first-quantized spacetime path formalism that can be considered foundational in its own right. This means that many typical tools of field theory, such as Hamiltonian dynamics and the Lagrangian stationary action principle for fields, cannot be assumed to apply *a priori*.

Instead, we will begin with the fundamental principles of special-relativistic quantum theory—the Born probability rule, superposition, and Poincaré invariance—and introduce six additional, physically motivated postulates related to spacetime paths. (The perhaps even more fundamental question of why quantum probabilities are given via superpositions of probability amplitudes will not be addressed here.) Results deduced from these postulates then provide the basis for further physical interpretation.

Since this formalism is first quantized, particular care is given to properly handling particles and antiparticles and to developing a consistent probabilistic interpretation. The result is an approach that fully deals with the usual issues of negative energies and negative probabilities, but without necessitating the introduction of fields as fundamental entities. Rather, fields can be considered to be simply a convenient formalism for handling multiparticle states. The present work only discusses massive scalar particles, but the approach can be extended to handle nonscalar particles (e.g., Ref. 34).

Section II first introduces the formalism for free scalar particles, culminating in free multiparticle fields. Section III then extends the formalism to consider interacting states and scattering. In order to reduce clutter in the text, certain propositions resulting from purely mathematical, but somewhat involved, derivation are cited without proof in the main body of the text, with proofs given in appendices.

Natural units with $\hbar=1=c$ are used throughout the following and the metric has a signature of $(-+++)$.

II. FREE PARTICLES

For any path based approach, it is obviously critical to be clear on what is meant by the term *path*. In the present case, a path for a particle is an arbitrary curve through spacetime, that is, a continuous (though not necessarily differentiable), one-dimensional subspace of spacetime. Note that there is no *a priori* requirement that such a curve is timelike or lightlike. Indeed, the path may cross arbitrarily forwards and backwards in time. Since such a path is continuous, there is a one-to-one mapping between it and some interval of the real numbers. That is, a path may be given by functions $q^\mu(\lambda)$, for $\mu=0,1,2,3$, of a *path parameter* λ.

In this formulation, the path parameter λ serves a purpose similar to that of time in the traditional non-relativistic path integral approach.[2] For the restricted case of an everywhere-timelike path, this parameter is analogous to proper time. For the general case of an unrestricted path, there has been some debate as to the physical nature of the path parameter (see, for example, Refs. 35 and 36). In order not to presuppose any specific interpretation, we will consider, for each path, all possible parametrizations of the path.

To do this, choose a fiducial parametrization s, say over the interval $[0,1]$, and define any other parametrization as a monotonically increasing function $\lambda(s)$. Geometrically, the so called *lapse multiplier*

$$w(s) \equiv \frac{\mathrm{d}\lambda}{\mathrm{d}s} > 0$$

then gives an effective length metric $\mathrm{d}\lambda = w(s)\mathrm{d}s$ for the path, and the corresponding parametrization λ is an *intrinsic length* measure along the path.

Given this basic conception of a particle path, this section will review the fundamental postulates required for a path integral approach, derive the scalar free particle propagator, and carefully consider the corresponding probability interpretation.

A. The free particle propagator

The fundamental postulate of any spacetime path integral approach is that a particle's transition amplitude between two points in spacetime is a superposition of the transition amplitudes for all possible paths between those points. Let the functional $\Delta[q]$ give the transition amplitude for a path $q^\mu(\lambda)$. Then the total transition amplitude $\Delta(x,x_0)$ must be given by a path integral over $\Delta[q]$, for all paths q from x_0 to x.

Postulate 1: *For a free scalar particle, the transition amplitude* $\Delta(x,x_0)$ *is given by the superposition of path transition amplitudes* $\Delta[q]$, *for all possible four-dimensional path functions* $q^\mu(\lambda)$ *beginning at* x_0 *and ending at* x, *parametrized by all possible monotonically increasing functions* $\lambda(s)$. *That is*,

$$\Delta(x,x_0) = \int \mathrm{D}\lambda\, \theta\left[\frac{\mathrm{d}\lambda}{\mathrm{d}s}\right] F[\lambda]\Delta(x,x_0;[\lambda]), \tag{1}$$

where the real-valued functional $F[\lambda]$ *allows for the possibility of allowing different weights for different parametrizations, and*

$$\Delta(x,x_0;[\lambda]) \equiv \eta[\lambda] \int \mathrm{D}^4 q\, \delta^4(q(\lambda(1)) - x)\, \delta^4(q(\lambda(0)) - x_0)\Delta[q], \tag{2}$$

where $\eta[\lambda]$ *is a parametrization-dependent normalization factor as required to keep the path integral finite*.

Note that, in Eqs. (1) and (2), the notation $\mathrm{D}\lambda$ indicates a path integral over the parametrization function $\lambda(s)$ while $\mathrm{D}^4 q$ indicates a path integral over the four path functions $q^\mu(\lambda)$.

In the traditional Feynman sum-over-paths approach, the form of $\Delta[q]$ is simply assumed to be an exponential of the classical action.[2] This is justified because the resulting transition amplitudes agree with the results of the usual formulation of quantum mechanics. However, if the path-based formulation is to be considered foundational, one would prefer a more fundamental justification.

As a transition amplitude, $\Delta[q]$ strictly only applies to a particle on a specific path q from the starting position $q(\lambda_0)$ to the ending position $q(\lambda_1)$ (where the parameter range of q is $[\lambda_0,\lambda_1]$). However, by translational invariance in Minkowski spacetime, the particle propagation embodied in $\Delta[q]$ cannot depend on the absolute positions $q(\lambda)$, but only on the relative positions

$$\Delta q(\lambda) \equiv q(\lambda) - q(\lambda_0).$$

That is, we can take $\Delta[q]=\Delta[\Delta q]$.

Now, consider a *family* of parallel paths q_{x_0}, indexed by the starting position x_0, such that

$$q_{x_0}(\lambda) = x_0 + \Delta q(\lambda),$$

for a fixed relative position function Δq. Since all members of such a family have the same relative position function Δq, the amplitude $\Delta[q_{x_0}]=\Delta[\Delta q]$ must be the same for all members of the family.

Suppose that a probability amplitude $\psi(x_0)$ is given for a particle to be at an initial position x_0 and that the transition amplitude is known to be $\Delta[\Delta q]$ for a specific relative position function Δq. Then, the probability amplitude for the particle to traverse a specific path q_{x_0} from the family for relative position Δq is just $\Delta[q_{x_0}]\psi(x_0)=\Delta[\Delta q]\psi(x_0)$.

However, the very meaning of being on the specific path q_{x_0} is that the particle must propagate from the starting position at x_0 to the ending position at $q_{x_0}(\lambda_1)$. Therefore, the probability for reaching the end position $q_{x_0}(\lambda_1)$ must be the same as the probability for having started out at the position x_0. That is,

$$|\Delta[\Delta q]\psi(x_0)|^2 = |\psi(x_0)|^2.$$

But, since $\Delta[\Delta q]$ is independent of x_0, we must have $|\Delta[q]|^2 = 1$ in general.

Of course, this argument is really just a suggestive motivation rather than a proof, so we take the conclusion as a postulate, rather than a proposition.

Postulate 2: *For any path $q^\mu(\lambda)$, the transition amplitude $\Delta[q]$ preserves the position probability density for the particle along the path. That is, it satisfies*

$$|\Delta[q]|^2 = 1. \tag{3}$$

If the configuration space for a path is expanded to be a representation of the full Poincaré group—that is, to include a matrix representation of the (homogeneous) Lorentz group as well as the four spacetime coordinates—then members of a family of "parallel" paths are related by Poincaré transformations, not just translations. This can be used as the basis for extending the spacetime path formalism to cover nonscalar particles. If, further, the assumption of flat spacetime is dropped, then it is not generally possible to construct a family of parallel paths covering all spacetime. However, one can still consider infinitesimal variations along a path corresponding to arbitrary coordinate transformations. Such further generalizations of the spacetime path approach will be explored in future papers.

The requirements of Eq. (3) and translation invariance mean that $\Delta[q]$ must have the form

$$\Delta[q] = e^{iS[\Delta q]}, \tag{4}$$

for some phase functional S. Substituting Eq. (4) into Eq. (2) gives

$$\Delta(x,x_0;[\lambda]) = \eta[\lambda] \int D^4q\, \delta^4(q(\lambda(1)) - x)\, \delta^4(q(\lambda(0)) - x_0) e^{iS[\Delta q]}. \tag{5}$$

So far, we have made no assumption that the particle path functions $q^\mu(\lambda)$ are differentiable. Indeed, paths under a path integral will generally not be differentiable. Nevertheless, it is common practice to use (with some care) path derivatives in the integrand of a path integral. This is because a path integral is defined as the limit of discretized approximations in which path derivatives are approximated as the mean value $\Delta q/\Delta\lambda$, for finite differences Δq and $\Delta\lambda$. The limit $\Delta\lambda \to 0$ is then taken over the path integral as a whole, not each derivative individually. Thus, even though $\lim_{\Delta\lambda\to 0}\Delta q/\Delta\lambda$ may not be defined, the path integral has a well-defined value so long as the overall path integral limit is defined. (For a discussion of some of the issues involved here, see, for example, Sec. 7.3 of Ref. 2. See also the explicit example of the derivation in Appendix B.)

We are therefore justified in replacing the difference functions $\Delta q^\mu(\lambda)$ used in the phase functional under the path integral in Eq. (5) with the path derivatives $\dot{q}^\mu(\lambda) \equiv dq^\mu/d\lambda$, such that

$$\Delta q^\mu(\lambda) = \int_{\lambda_0}^{\lambda} d\lambda' \dot{q}^\mu(\lambda'),$$

letting the $q^\mu(\lambda)$ be considered as differentiable. This gives

$$\Delta(x,x_0;[\lambda]) = \eta[\lambda] \int D^4q\, \delta^4(q(\lambda(1)) - x)\, \delta^4(q(\lambda(0)) - x_0) e^{iS[\dot{q}]}, \tag{6}$$

which reflects the typical form of a Feynman sum over paths,[2] where each path is weighted by a phase determined by the action S. Unlike the usual nonrelativistic formulation, however, the path parameter here is λ, rather than time.[5,21]

Now, by dividing a path q into two paths at some arbitrary parameter value λ and propagating over each segment, we can see that

$$S[\dot{q};\lambda_1,\lambda_0] = S[\dot{q};\lambda_1,\lambda] + S[\dot{q};\lambda,\lambda_0], \tag{7}$$

where $S[\dot{q};\lambda',\lambda]$ denotes the value of $S[\dot{q}]$ for the parameter range of $\dot{q}$ restricted to $[\lambda,\lambda']$. Using this property to build the total value of $S[\dot{q}]$ from infinitesimal increments leads to the following result (proved in Appendix A).

Proposition A (Form of the Phase Functional): *The phase functional S must have the form*

$$S[\dot{q}] = \int_{\lambda_0}^{\lambda_1} d\lambda' L[\dot{q};\lambda'], \tag{8}$$

where the parametrization domain for $\dot{q}$ *is* $[\lambda_0,\lambda_1]$ *and* $L[\dot{q};\lambda]$ *depends only on* $\dot{q}$ *and its higher derivatives evaluated at* λ.

The question remains as to what form the function L should take. Traditionally, it is taken to be just the classical Langrangian, but, from a foundational viewpoint, one would like a better justification.

Of course, the simplest form for L would be a constant, independent of $\dot{q}$. However, this would result in a superficially divergent path integral in Eq. (6) which, when normalized, would leave to just a trivial phase. This would not give any appropriate particle dynamics. The next simplest form for L would be for it to depend only on $\dot{q}$ and no higher derivatives. Further, since L is a scalar quantity, it must then depend only on the Lorentz-invariant scalar function

$$\dot{q}^2(\lambda) \equiv \dot{q}^\mu(\lambda)\dot{q}_\mu(\lambda).$$

Taking L to further have the tractable form of a linear function of $\dot{q}^2$ gives

$$L[\dot{q};\lambda] = L(\dot{q}^2(\lambda)) = a\dot{q}^2(\lambda) + b,$$

for some a and b. Now, the factor a can be fixed arbitrarily, since any variation is effectively equivalent to a reparametrization of the path parameter λ. For a free particle, it is convenient to take $a=1/4$. If we further assume that b is always negative, we can set $b=-m^2$ and identifying m with the mass of the particle does, indeed, give a classical relativistic Lagrangian function.

As we will see in the following, evaluating the path integral in Eq. (6) with this Lagrangian function leads to the usual free-particle Feynman propagator. If, on the other hand, we take b to be positive, then the result is a similar propagator, but with an effective imaginary particle mass. Such particles are tachyons, which we will not consider further in this paper.

Postulate 3: *For a free scalar particle of mass m, the Lagrangian function is given by*

$$L(\dot{q}^2) = \tfrac{1}{4}\dot{q}^2 - m^2. \tag{9}$$

Substituting Eq. (8) into Eq. (6) gives

$$\Delta(x,x_0;[\lambda]) = \eta[\lambda]\int \mathrm{D}^4 q\,\delta^4(q(\lambda(1)) - x)\,\delta^4(q(\lambda(0)) - x_0)\exp\left(i\int_{\lambda(0)}^{\lambda(1)} d\lambda' L(\dot{q}^2(\lambda'))\right). \tag{10}$$

With the Lagrangian given by Eq. (9), it is well known that this path integral may be evaluated (see, for example, Ref. 21). However, in the present context, some care must be taken to mathematically evaluate the integral without making any further assumptions based on field equations or underlying traditional quantum mechanics. In any case, the result (proved in Appendix B) is as follows.

Proposition B (Evaluation of the Path Integral): *The path integral in Eq.* (10), *with the Lagrangian given by Eq.* (9), *may be evaluated to get*

$$\Delta(x,x_0;[\lambda]) = \Delta(x-x_0;\lambda(1)-\lambda(0)) \equiv (2\pi)^{-4}\int d^4p\, e^{ip(x-x_0)} e^{-i[\lambda(1)-\lambda(0)](p^2+m^2)}. \tag{11}$$

Note that the only dependency left of $\Delta(x-x_0;\lambda(1)-\lambda(0))$ on the parametrization $\lambda(s)$ is on

the total *intrinsic path length*

$$T = \lambda(1) - \lambda(0) = \int_0^1 \mathrm{d}s w(s) > 0.$$

If we were to take $F[\lambda]=1$ in Eq. (1) for all $\lambda(s)$, there would then be a parametrization gauge symmetry: all parametrizations that give the same intrinsic path lengths would be equivalent. Therefore, equivalent reparametrizations would be overcounted in the λ path integral of Eq. (1), so the integral would diverge.

If, on the other hand, the path integral over λ had not been included at all in Eq. (1), the result would have been to overspecify a specific path parametrization. The possible particle paths would then have been *undercounted*, missing the need to include paths of different intrinsic lengths. It is thus necessary to reduce the λ path integration in Eq. (1) to eliminate the overcounting due to the path gauge symmetry, without overspecifying the path parametrization.

In the usual fashion for a gauge symmetry, we retain the integration, but fix a specific gauge. This can be easily done by including a gauge fixing delta functional in $F[\lambda]$. The gauge typically chosen is to require that $w(s)=\mathrm{d}\lambda/\mathrm{d}s$ be constant,[21] which corresponds to setting

$$F[\lambda] = f(\lambda(1) - \lambda(0))\delta\left[\frac{\mathrm{d}\lambda}{\mathrm{d}s} - [\lambda(1) - \lambda(0)]\right],$$

for some real function $f(T)$. Using this in Eq. (1) gives

$$\Delta(x,x_0) = \int_0^\infty \mathrm{d}T f(T)\Delta(x - x_0;T).$$

In the following, we will generally assume equal weighting of all parametrizations, that is $f(T)=1$. However, in Sec. III D, we will see that an alternate choice provides a fruitful path for regularizing the infinite integrals that appear in the formalism for interacting particles. Nevertheless, assuming, for now, that $f(T)=1$, gives

$$\Delta(x,x_0) = \int_0^\infty \mathrm{d}T\Delta(x - x_0;T) = (2\pi)^{-4}\int \mathrm{d}^4 p \mathrm{e}^{ip\cdot(x-x_0)}\int_0^\infty \mathrm{d}T\mathrm{e}^{-iT(p^2+m^2)}. \tag{12}$$

This can be evaluated by introducing a convergence factor $\exp(-T\varepsilon)$, for infinitesimal ε, resulting in just the Feynman propagator

$$\Delta(x,x_0) = \Delta(x - x_0) \equiv -i(2\pi)^{-4}\int \mathrm{d}^4 p \frac{\mathrm{e}^{ip(x-x_0)}}{p^2 + m^2 - i\varepsilon}.$$

The integration of T from 0 to ∞ in Eq. (12) is similar to the integration carried out by Nambu,[9] based on previous work of Fock,[8] in order to obtain the Feynman propagator. Note, though, that this integration arises naturally here as the gauge-fixed reduction of the path parametrization integral in Eq. (1).

The relationship between the propagator $\Delta(x-x_0)$ and $\Delta(x-x_0;T)$ can be viewed in another way, which will also prove useful in Sec. III D. For $T>0$,

$$\Delta(x-x_0;T) = e^{-iTm^2}\int d^4p e^{ip(x-x_0)}\int_0^\infty dT' e^{-iT'p^2}\delta(T'-T)$$
$$= (2\pi)^{-1}e^{-iTm^2}\int d^4p e^{ip(x-x_0)}\int_0^\infty dT' e^{-iT'p^2}\int dm'^2 e^{-i(T'-T)m'^2}$$
$$= (2\pi)^{-1}e^{-iTm^2}\int dm'^2 e^{iTm'^2}\Delta(x-x_0;m'^2), \tag{13}$$

where

$$\Delta(x-x_0;m'^2) \equiv \int_0^\infty dT'\int d^4p e^{ip(x-x_0)}e^{-iT'(p^2+m'^2)} = -i(2\pi)^{-4}\int d^4p \frac{e^{ip(x-x_0)}}{p^2+m'^2-i\varepsilon}. \tag{14}$$

This form for $\Delta(x-x_0;T)$ is essentially that of the parametrized Green's function derived by Horwitz *et al.* for parametrized quantum field theory[37,38] as a superposition of propagators for different mass states (see also Refs. 39 and 40). Equation (13) differs from those references in the factor $\exp(-iTm^2)$. As a result of this factor, integrating Eq. (13) over T as in Eq. (12) effectively acts as a Fourier transform, resulting in a propagator with mass sharply defined at m.

B. Free particle position states

The path integral form for $\Delta(x-x_0;\lambda-\lambda_0)$ given in Eq. (2) is essentially the same as that of the path integral for the nonrelativistic *kernel*,[2] except that λ is used as the evolution parameter instead of t. Therefore, $\Delta(x-x_0;\lambda-\lambda_0)$ has similar properties as a propagation kernel in λ:

$$\int d^4x_1 \Delta(x-x_1;\lambda-\lambda_1)\Delta(x_1-x_0;\lambda_1-\lambda_0) = \Delta(x-x_0;\lambda-\lambda_0)$$

and

$$\Delta(x-x_0;\lambda-\lambda_0)^* = \Delta(x_0-x;\lambda_0-\lambda).$$

Given these properties, define a family of probability amplitude functions $\psi(x;\lambda)$, for which

$$\psi(x;\lambda) = \int d^4x_0 \Delta(x-x_0;\lambda-\lambda_0)\psi(x_0;\lambda_0), \tag{15}$$

for any λ and λ_0, normalized such that

$$\int d^4x |\psi(x;\lambda)|^2 = 1, \tag{16}$$

for each λ. Formally, these functions are probability amplitudes for the position x, with λ serving as an index identifying individual functions in the family. However, they can be interpreted as just the parametrized probability amplitude functions defined by Stueckelberg.[6] In this sense, the $\psi(x;\lambda)$ represent the probability amplitude for a particle to reach position x at the point along its path with parameter value λ.

Note that

$$i\frac{\partial}{\partial\lambda}\Delta(x-x_0;\lambda-\lambda_0) = (2\pi)^{-4}\int d^4p e^{ip(x-x_0)}(p^2+m^2)e^{-i(\lambda-\lambda_0)(p^2+m^2)}.$$

This means that $\psi(x;\lambda)$, as given by Eq. (15), satisfies

$$-i\frac{\partial}{\partial\lambda}\psi(x;\lambda)=\left(\frac{\partial^2}{\partial x^2}-m^2\right)\psi(x;\lambda). \tag{17}$$

Equation (17) is a generalized Schrödinger equation, such as proposed by Stueckelberg.[7] However, Stueckelberg and subsequent authors[4,12,15] used a Hamiltonian of the form $(2m)^{-1}\partial^2/\partial x^2$, by analogy with nonrelativistic mechanics, rather than the form of Eq. (17) (though Ref. 41 uses a Hamiltonian form similar to Eq. (17)). This difference is the origin of the extra factor $\exp(-iTm^2)$ in Eq. (13) relative to Refs. 37 and 38.

The properties of the kernel $\Delta(x-x_0;\lambda-\lambda_0)$ also allow for the definition of a consistent family of *position state* bases $|x;\lambda\rangle$, such that

$$\psi(x;\lambda)=\langle x;\lambda|\psi\rangle, \tag{18}$$

given a single Hilbert space state vector $|\psi\rangle$. These position states are normalized such that

$$\langle x';\lambda|x;\lambda\rangle=\delta^4(x'-x)$$

for each value of λ. Further, it follows from Eqs. (15) and (18) that

$$\Delta(x-x_0;\lambda-\lambda_0)=\langle x;\lambda|x_0;\lambda_0\rangle. \tag{19}$$

Thus, $\Delta(x-x_0;\lambda-\lambda_0)$ effectively defines a unitary transformation between the various Hilbert space bases $|x;\lambda\rangle$, indexed by the parameter λ.

Finally, the overall state for propagation from x_0 to x is given by the superposition of the states for paths of all intrinsic lengths. If we fix $q^\mu(\lambda_0)=x_0^\mu$, then $|x;\lambda\rangle$ already includes all paths of length $\lambda-\lambda_0$. Therefore, the overall state $|x\rangle$ for the particle to arrive at x should be given by the superposition of the states $|x;\lambda\rangle$ for all $\lambda>\lambda_0$:

$$|x\rangle\equiv\int_{\lambda_0}^{\infty}d\lambda|x;\lambda\rangle. \tag{20}$$

Then, using Eq. (19),

$$\langle x|x_0;\lambda_0\rangle=\int_{\lambda_0}^{\infty}d\lambda\Delta(x-x_0;\lambda-\lambda_0)=\int_0^{\infty}d\lambda\Delta(x-x_0;\lambda)=\Delta(x-x_0). \tag{21}$$

Now, the $|x\rangle$ are not actually proper Hilbert space states, since $\langle x|x_0\rangle$ is infinite (as can be seen by integrating Eq. (21) over λ_0). Nevertheless, via Eq. (12), the corresponding bras $\langle x|$ can be considered to be well-defined functions on proper, normalizable states $|\psi\rangle$ such that

$$\langle x|\psi\rangle=\int d^4x_0\Delta(x-x_0)\psi(x_0;\lambda_0)$$

is the transition amplitude for a particle with known probability amplitude $\psi(x_0;\lambda_0)$ at λ_0 to eventually reach position x at some $\lambda>\lambda_0$. We will thus continue to use $|x\rangle$ as a formal quantity, with the understanding that it is really just a shorthand for constructing propagators and transition amplitudes.

C. On-shell particle and antiparticle states

The states constructed so far have naturally been off-shell states. That is, they represent what are normally considered to be "virtual" particles. However, rather than simply imposing the on-shell mass condition to obtain "physical" states, on-shell states will be constructed in this subsection as the infinite time limit of off-shell states. That is, particles with paths that, in the limit, are unbounded in time will turn out to be naturally on-shell.

In order to take a time limit, it is necessary to make some distinction between past and future that can be used as the basis for taking the limit. For this purpose, divide the set of all possible paths q^μ that end at some specific $q^\mu(\lambda)=x^\mu$ into two subsets: those that begin (at $q^\mu(\lambda_0)=x_0^\mu$) in the *past* of x and those that begin in the *future* of x.

Outside of the light cone of x, the division into future and past is, of course, not Lorentz covariant and depends on the choice of a specific coordinate system. However, when we take the time limit, the light cone expands to cover all space, and, in this limit, the division into particle and antiparticle becomes fully coordinate system independent. The possibility of the particle/antiparticle distinction being coordinate system dependent in anything other than the infinite time limit is a subject for future exploration.

Now, particles are normally considered to propagate from the past to the future. On the other hand, antiparticles may be considered to propagate from the future into the past.[3,6,7]

Postulate 4: *Normal particle states* $|x_+\rangle$ *are such that*

$$\langle x_+|x_0;\lambda_0\rangle = \theta(x^0-x_0^0)\Delta(x-x_0).$$

Antiparticle states $|x_-\rangle$ *are such that*

$$\langle x_-|x_0;\lambda_0\rangle = \theta(x_0^0-x^0)\Delta(x-x_0).$$

Using the usual decomposition of the Feynman propagator (see, for example, Sec. 6.2 of Ref. 42)

$$\Delta(x-x_0) = \theta(x^0-x_0^0)\Delta_+(x-x_0) + \theta(x_0^0-x^0)\Delta_-(x-x_0), \tag{22}$$

where

$$\Delta_\pm(x-x_0) \equiv (2\pi)^{-3}\int \mathrm{d}^3p \frac{\mathrm{e}^{i[\mp\omega_{\boldsymbol{p}}(x^0-x_0^0)+\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}_0)]}}{2\omega_{\boldsymbol{p}}}, \tag{23}$$

with $\omega_{\boldsymbol{p}}\equiv\sqrt{\boldsymbol{p}^2+m^2}$, it is clear that

$$\langle x_\pm|x_0;\lambda_0\rangle = \theta(\pm(x^0-x_0^0))\Delta(x-x_0) = \theta(\pm(x^0-x_0^0))\Delta_\pm(x-x_0). \tag{24}$$

We would now like to take the time limits for future and past directed particle and antiparticle states. In doing this, one cannot expect to hold the three-position of the path end point constant. However, for a free particle, it is reasonable to take the particle *three-momentum* as being fixed. Therefore, consider the state of a particle or antiparticle with a three-momentum $\boldsymbol{p}$ at a certain time t. (The importance of the specific factor $\exp(\mp i\omega_{\boldsymbol{p}}t)$ in the definition below will become clear in a moment.)

Postulate 5: *The state of a particle* (+) *or antiparticle* (−) *with three-momentum* $\boldsymbol{p}$ *is given by*

$$|t,\boldsymbol{p}_\pm\rangle \equiv (2\pi)^{-3/2}\int \mathrm{d}^3x \mathrm{e}^{i(\mp\omega_{\boldsymbol{p}}t+\boldsymbol{p}\cdot\boldsymbol{x})}|t,\boldsymbol{x}_\pm\rangle = (2\pi)^{-1/2}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}t}\int \mathrm{d}p^0\mathrm{e}^{ip^0t}|p_\pm\rangle, \tag{25}$$

where

$$|p_\pm\rangle \equiv (2\pi)^{-2}\int \mathrm{d}^4x \mathrm{e}^{ip\cdot x}|x_\pm\rangle \tag{26}$$

is the corresponding four-momentum state.

Let

$$|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle \equiv (2\pi)^{-3/2}\int \mathrm{d}^3x \mathrm{e}^{i(\mp\omega_{\boldsymbol{p}}t_0+\boldsymbol{p}\cdot\boldsymbol{x})}|t_0,\boldsymbol{x};\lambda_0\rangle = (2\pi)^{-1/2}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}t_0}\int \mathrm{d}p^0\mathrm{e}^{ip^0t_0}|p;\lambda_0\rangle, \tag{27}$$

where

$$|p;\lambda_0\rangle \equiv (2\pi)^{-2}\int \mathrm{d}^4x \mathrm{e}^{ip\cdot x}|x;\lambda_0\rangle. \tag{28}$$

Substituting from Eqs. (26), (28), and (24),

$$\langle p_\pm|p_0;\lambda_0\rangle = (2\pi)^{-4}\int \mathrm{d}^4x\mathrm{d}^4x_0\mathrm{e}^{-ip\cdot x}\mathrm{e}^{ip_0\cdot x_0}\theta(\pm(x^0-x_0^0))\Delta_\pm(x-x_0) = \delta^4(p-p_0)\Delta_\pm(p), \tag{29}$$

where

$$\Delta_\pm(p) \equiv \int \mathrm{d}^4x\mathrm{e}^{-ip\cdot x}\theta(\pm x^0)\Delta_\pm(x). \tag{30}$$

Substituting Eq. (23) into Eq. (30) gives

$$\begin{aligned}\Delta_\pm(p) &= \int \mathrm{d}^4x\mathrm{e}^{-ip\cdot x}\theta(\pm x^0)(2\pi)^{-3}\int \mathrm{d}^3p'(2\omega_{\boldsymbol{p}'})^{-1}\mathrm{e}^{i(\mp\omega_{\boldsymbol{p}'}x^0+\boldsymbol{p}'\cdot\boldsymbol{x})}\\ &= \int \mathrm{d}t\mathrm{e}^{ip^0t}\theta(\pm t)\int \mathrm{d}^3p'(2\omega_{\boldsymbol{p}'})^{-1}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}'}t}(2\pi)^{-3}\int \mathrm{d}^3x\mathrm{e}^{i(\boldsymbol{p}'-\boldsymbol{p})\cdot\boldsymbol{x}}\\ &= \int \mathrm{d}t\mathrm{e}^{ip^0t}\theta(\pm t)\int \mathrm{d}^3p'(2\omega_{\boldsymbol{p}'})^{-1}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}'}t}\delta^3(\boldsymbol{p}'-\boldsymbol{p}) = (2\omega_{\boldsymbol{p}})^{-1}\int \mathrm{d}t\theta(\pm t)\mathrm{e}^{i(p^0\mp\omega_{\boldsymbol{p}})t}.\end{aligned} \tag{31}$$

Using Eq. (29) (and the completeness of the $|p;\lambda_0\rangle$ states) in Eq. (25), and substituting from Eq. (31) for $\Delta_\pm(p)$, then gives

$$\begin{aligned}|t,\boldsymbol{p}_\pm\rangle &= (2\pi)^{-1/2}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}t}\int \mathrm{d}p^0\mathrm{e}^{ip^0t}\Delta_\pm(p)^*|p;\lambda_0\rangle\\ &= (2\pi)^{-1/2}(2\omega_{\boldsymbol{p}})^{-1}\int \mathrm{d}t'\,\theta(\pm t')\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}(t-t')}\int \mathrm{d}p^0\mathrm{e}^{ip^0(t-t')}|p;\lambda_0\rangle.\end{aligned}$$

Change variables $t' \to t-t_0$ to get

$$|t,\boldsymbol{p}_\pm\rangle = (2\pi)^{-1/2}(2\omega_{\boldsymbol{p}})^{-1}\int dt_0\theta(\pm(t-t_0))\int \mathrm{d}p^0\mathrm{e}^{i(p^0\mp\omega_{\boldsymbol{p}})t_0}|p;\lambda_0\rangle = \begin{cases}(2\omega_{\boldsymbol{p}})^{-1}\displaystyle\int_{-\infty}^{t}\mathrm{d}t_0|t_0,\boldsymbol{p}_+;\lambda_0\rangle,\\ (2\omega_{\boldsymbol{p}})^{-1}\displaystyle\int_{t}^{+\infty}\mathrm{d}t_0|t_0,\boldsymbol{p}_-;\lambda_0\rangle.\end{cases} \tag{32}$$

It is then straightforward to take the time limit $t\to\pm\infty$. Note that

$$\begin{aligned}\int_{-\infty}^{+\infty}\mathrm{d}t_0|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle &= (2\pi)^{-1/2}\int \mathrm{d}p^0\int dt_0\mathrm{e}^{i(p^0\mp\omega_{\boldsymbol{p}})t_0}|p;\lambda_0\rangle = (2\pi)^{-1/2}\int \mathrm{d}p^0(2\pi)\,\delta(p^0\mp\omega_{\boldsymbol{p}})|p;\lambda_0\rangle\\ &= (2\pi)^{1/2}|\pm\omega_{\boldsymbol{p}},\boldsymbol{p};\lambda_0\rangle.\end{aligned}$$

Therefore

$$|\boldsymbol{p}_\pm\rangle \equiv \lim_{t\to\pm\infty}|t,\boldsymbol{p}_\pm\rangle = (2\pi)^{1/2}(2\omega_{\boldsymbol{p}})^{-1}|\pm\omega_{\boldsymbol{p}},\boldsymbol{p};\lambda_0\rangle. \tag{33}$$

Thus, a normal particle (+) or antiparticle (−) that has three-momentum $\boldsymbol{p}$ as $t\to\pm\infty$ is *on-shell*, with energy $\pm\omega_{\boldsymbol{p}}$. Such on-shell particles are unambiguously normal particles or antiparticles, independent of choice of coordinate system. (Note that these states are similar to the "mass representation" states of Ref. 12.)

Note also that the factor of $\exp(\mp i\omega_{\boldsymbol{p}}t)$ in the definition of $|t,\boldsymbol{p}_\pm\rangle$ (Eq. (25)) is not arbitrary. Without this, a factor of $\exp(\pm i\omega_{\boldsymbol{p}}t)$ would remain in Eq. (32), making it impossible to take the limit $t\to\pm\infty$.

D. On-shell probability interpretation

Unfortunately, the states defined in Eq. (33) are not normalizable using the usual inner product, since

$$\langle \boldsymbol{p}'_\pm|\boldsymbol{p}_\pm\rangle = 2\pi(2\omega_{\boldsymbol{p}})^{-2}\delta(0)\,\delta^3(\boldsymbol{p}'-\boldsymbol{p})$$

is infinite. In Ref. 12, this is handled by allowing the mass m to vary, even though the energy is fixed at $\sqrt{\boldsymbol{p}^2+m^2}$. Here we will take a different approach, noting that, from Eq. (28),

$$\langle p';\lambda|p;\lambda\rangle = \delta^4(p'-p).$$

Using this and Eq. (33), we clearly have

$$\langle \boldsymbol{p}_\pm|p_0;\lambda_0\rangle = (2\pi)^{1/2}(2\omega_{\boldsymbol{p}})^{-1}\,\delta(\pm\omega_{\boldsymbol{p}}-p_0^0)\,\delta^3(\boldsymbol{p}-\boldsymbol{p}_0). \tag{34}$$

Moreover, from this equation and Eq. (27),

$$\begin{aligned}\langle \boldsymbol{p}_\pm|t_0,\boldsymbol{p}_{0\pm};\lambda_0\rangle &= (2\pi)^{-1/2}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}t_0}\int \mathrm{d}p_0^0\mathrm{e}^{ip_0^0t_0}(2\pi)^{1/2}(2\omega_{\boldsymbol{p}})^{-1}\,\delta(\pm\omega_{\boldsymbol{p}}-p_0^0)\,\delta^3(\boldsymbol{p}-\boldsymbol{p}_0)\\ &= (2\omega_{\boldsymbol{p}})^{-1}\delta^3(\boldsymbol{p}-\boldsymbol{p}_0),\end{aligned} \tag{35}$$

for any value of t_0. This is essentially the basis for an "induced" inner product, in the sense of Refs. 23 and 43.

Let $\mathcal{H}$ be the Hilbert space of the $|x;\lambda_0\rangle$ and let $\mathcal{H}_t$ be the subspaces spanned by the $|t,\boldsymbol{x};\lambda_0\rangle$, for each t, forming a foliation of $\mathcal{H}$. Now, from Eq. (27), it is clear that the particle and antiparticle 3-momentum states $|t,\boldsymbol{p}_\pm;\lambda_0\rangle$ also each span $\mathcal{H}_t$. In these representations, states in $\mathcal{H}_t$ have the form

$$|t,\psi_\pm;\lambda_0\rangle = \int \mathrm{d}^3p\,\psi(\boldsymbol{p})|t,\boldsymbol{p}_\pm;\lambda_0\rangle, \tag{36}$$

for square-integrable functions $\psi(\boldsymbol{p})$. Conversely, it follows from Eq. (35) that a probability amplitude $\psi(\boldsymbol{p})$ is given by

$$\psi(\boldsymbol{p}) = (2\omega_{\boldsymbol{p}})\langle \boldsymbol{p}_\pm|t,\psi_\pm;\lambda_0\rangle. \tag{37}$$

Let $\mathcal{H}'_t$ be the space of linear functions dual to $\mathcal{H}_t$. Via Eq. (37), the bra states $\langle \boldsymbol{p}_\pm|$ can be considered to be members of $\mathcal{H}'_t$, for all t. Indeed, they span two common subspaces $\mathcal{H}'_\pm$ of the $\mathcal{H}'_t$, the states of which have the form

$$\langle\psi_\pm| = \int \mathrm{d}^3p\,\psi(\boldsymbol{p})^*\langle \boldsymbol{p}_\pm|.$$

Now, define an inner product on the functions $\psi(\boldsymbol{p})$ such that

$$(\psi_1,\psi_2) \equiv \langle\psi_{1\pm}|t,\psi_{2\pm};\lambda_0\rangle = \int \frac{\mathrm{d}^3p}{2\omega_{\boldsymbol{p}}}\psi_1(\boldsymbol{p})^*\psi_2(\boldsymbol{p}), \tag{38}$$

where the second equality follows from Eq. (35). Equipped with this inner product, each $\mathcal{H}_t$ is itself a Hilbert space of the wave functions $\psi(\boldsymbol{p})$. Note that it is the states of the *dual* spaces $\mathcal{H}'_\pm$ that naturally satisfy the on-shell constraint $\langle\psi_\pm|\hat{H}=0$ (as suggested by, for example, Ref. 44).

The operators $(2\omega_{\boldsymbol{p}})|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm|$ are self-adjoint under the inner product given in Eq. (38), in the sense that the conjugate of

$$(2\omega_{\boldsymbol{p}})\langle\psi_\pm|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm| = \psi(\boldsymbol{p})^*\langle\boldsymbol{p}_\pm|$$

is

$$(2\omega_{\boldsymbol{p}})|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm|t,\psi_\pm;\lambda_0\rangle = |t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\psi(\boldsymbol{p})$$

for that inner product. Further,

$$\int \mathrm{d}^3p(2\omega_{\boldsymbol{p}})\langle\psi_{1\pm}|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm|t,\psi_{2\pm};\lambda_0\rangle = \int \frac{\mathrm{d}^3p}{2\omega_{\boldsymbol{p}}}\psi_1(\boldsymbol{p})^*\psi_2(\boldsymbol{p}) = \langle\psi_{1\pm}|t,\psi_{2\pm};\lambda_0\rangle,$$

which gives the effective resolution of the identity

$$\int \mathrm{d}^3p(2\omega_{\boldsymbol{p}})|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm| = 1. \tag{39}$$

In fact, such a resolution of the identity generally holds for families of conjugate bra and ket states with a *biorthonormality relationship* such as Eq. (35) (see Ref. 45 and Appendix A.8.1 of Ref. 46). We can, therefore, take the operator $(2\omega_{\boldsymbol{p}})|t_0,\boldsymbol{p}_\pm;\lambda_0\rangle\langle\boldsymbol{p}_\pm|$ to represent the quantum proposition that an on-shell particle or antiparticle has the three-momentum $\boldsymbol{p}$. Then, with the normalization

$$(\psi,\psi) = \int \frac{\mathrm{d}^3p}{2\omega_{\boldsymbol{p}}}|\psi(\boldsymbol{p})|^2 = 1,$$

$|\psi(\boldsymbol{p})|^2$ is the corresponding probability density in three-momentum space.

Finally, consider that $|t,\boldsymbol{x};\lambda_0\rangle$ is an eigenstate of the three-position operator $\hat{\boldsymbol{X}}$, representing a particle localized at the three-position $\boldsymbol{x}$ at time t. From Eq. (37), and using the inverse Fourier transform of Eq. (28) with Eq. (33), its three-momentum wave function in $\mathcal{H}_t$ is

$$(2\omega_{\boldsymbol{p}})\langle\boldsymbol{p}_\pm|t,\boldsymbol{x};\lambda_0\rangle = (2\pi)^{-3/2}\mathrm{e}^{i(\pm\omega_{\boldsymbol{p}}t-\boldsymbol{p}\cdot\boldsymbol{x})}. \tag{40}$$

This is just a plane wave, and it is an eigenfunction of the operator

$$\mathrm{e}^{\pm i\omega_{\boldsymbol{p}}t}i\frac{\partial}{\partial\boldsymbol{p}}\mathrm{e}^{\mp i\omega_{\boldsymbol{p}}t},$$

which is the traditional momentum representation $i\partial/\partial\boldsymbol{p}$ of the three-position operator $\hat{\boldsymbol{X}}$, translated to time t.

This result contrasts with the well-known result of Newton and Wigner,[47] who conclude that a localized particle wave function satisfying the Klein–Gordon equation is an eigenfunction of

$$i\left(\frac{\partial}{\partial\boldsymbol{p}} - \frac{\boldsymbol{p}}{2\omega_{\boldsymbol{p}}^2}\right),$$

which has an extra term over the expected $i\partial/\partial\boldsymbol{p}$. The key reason for this difference is our use of the three-momentum basis $|t,\boldsymbol{p}_\pm;\lambda_0\rangle$. With the dual basis $(2\omega_{\boldsymbol{p}})\langle\boldsymbol{p}_\pm|$ from Eq. (35), this leads to the relation given in Eq. (37) and used in Eq. (40).

In contrast, the traditional formalism assumes that both bra and ket states are on-shell. Instead of the time-dependent spaces $\mathcal{H}_t$, the spaces $\mathcal{H}_\pm$ are used, with on-shell ket basis states $|\boldsymbol{p}_\pm\rangle$ that are dual to the bra states $\langle\boldsymbol{p}_\pm|$ under an inner product such that, instead of Eq. (35), one has

$$(2\omega_{\boldsymbol{p}'})^{1/2}\langle \boldsymbol{p}'_{\pm}|\boldsymbol{p}_{\pm}\rangle(2\omega_{\boldsymbol{p}})^{1/2} = \delta^3(\boldsymbol{p}'-\boldsymbol{p}),$$

where the factor of $(2\omega_{\boldsymbol{p}})^{1/2}$ is introduced symmetrically on dual bra and ket states in order provide an orthonormal basis. If we were to use the traditional dual basis $(2\omega_{\boldsymbol{p}})^{1/2}\langle \boldsymbol{p}_{\pm}|$, instead of $(2\omega_{\boldsymbol{p}}) \times\langle \boldsymbol{p}_{\pm}|$, the wave function of $|t,\boldsymbol{x};\lambda_0\rangle$ would be

$$(2\omega_{\boldsymbol{p}})^{1/2}\langle \boldsymbol{p}_{\pm}|t,\boldsymbol{x};\lambda_0\rangle = (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}})^{-1/2}e^{i(\pm\omega_{\boldsymbol{p}}t-\boldsymbol{p}\cdot\boldsymbol{x})}. \tag{41}$$

At $t=0$ this is exactly the Newton–Wigner wave function for a localized particle.[47]

Note that Eq. (40) is effectively related to Eq. (41) by a scalar Foldy–Wouthuysen transformation.[48,49] This makes sense, since the Foldy–Wouthuysen transformation produces a representation that separates positive and negative energy states (particles and antiparticles) and gives a reasonable non-relativistic limit.

Indeed, from Eq. (27) we can easily see that the time evolution of the three-momentum states $|t,\boldsymbol{p}_{\pm};\lambda_0\rangle$ is given by

$$e^{i\hat{P}^0\Delta t}|t,\boldsymbol{p}_{\pm};\lambda_0\rangle = e^{\pm i\omega_{\boldsymbol{p}}\Delta t}|t+\Delta t,\boldsymbol{p}_{\pm};\lambda_0\rangle = e^{\pm i\hat{H}_{\mathrm{FW}}\Delta t}|t+\Delta t,\boldsymbol{p}_{\pm};\lambda_0\rangle,$$

where

$$\hat{H}_{\mathrm{FW}} = (\hat{\boldsymbol{P}}\cdot\hat{\boldsymbol{P}}+m^2)^{1/2}$$

is the scalar Foldy–Wouthuysen Hamiltonian and the $\hat{P}^\mu$ are the generators of spacetime translations. Define the operation of time translation on the time-dependent states $|t,\psi;\lambda_0\rangle$ so that

$$|t+\Delta t,\psi_{\pm};\lambda_0\rangle = e^{i\hat{P}^0\Delta t}|t,\psi_{\pm};\lambda_0.$$

Substituting Eq. (36) then gives

$$\begin{aligned}|t+\Delta t,\psi_{\pm};\lambda_0\rangle &= \int d^3p\,\psi(t,\boldsymbol{p})e^{i\hat{P}^0\Delta t}|t,\boldsymbol{p}_{\pm};\lambda_0\rangle = \int d^3p\,\psi(t,\boldsymbol{p})e^{\pm i\omega_{\boldsymbol{p}}\Delta t}|t+\Delta t,\boldsymbol{p}_{\pm};\lambda_0\rangle \\ &= \int d^3p\,\psi(t+\Delta t,\boldsymbol{p})|t+\Delta t,\boldsymbol{p}_{\pm};\lambda_0\rangle,\end{aligned}$$

where the time dependence of the three-momentum wave function has been made explicit, with time evolution given by

$$\psi(t+\Delta t,\boldsymbol{p}) = e^{\pm i\omega_{\boldsymbol{p}}\Delta t}\psi(t,\boldsymbol{p}).$$

In the nonrelativistic limit, for positive-energy particles, $\omega_{\boldsymbol{p}}\approx m+\boldsymbol{p}^2/2m$, and this time evolution reduces to time evolution according to the usual nonrelativistic Hamiltonian (up to the momentum-independent phase factor $\exp(im\Delta t)$).

E. Free multiparticle states

The formalism introduced in the previous sections can be extended in a straightforward way to a Fock space of noninteracting multiparticle states. In order to allow for multiparticle states with different types of particles, extend the position state of each individual particle with a *particle type index n*, such that

$$\langle x',n';\lambda|x,n;\lambda\rangle = \delta_n^{n'}\delta^4(x'-x).$$

Then, construct a basis for the Fock space of multiparticle states as symmetrized products of N single particle states:

$$|x_1,n_1,\lambda_1;\ldots;x_N,n_N,\lambda_N\rangle \equiv (N!)^{-1/2}\sum_{\text{perms }\mathcal{P}}|x_{\mathcal{P}1},n_{\mathcal{P}1};\lambda_{\mathcal{P}1}\rangle\cdots|x_{\mathcal{P}N},n_{\mathcal{P}N};\lambda_{\mathcal{P}N}\rangle, \tag{42}$$

where the sum is over all permutations $\mathcal{P}$ of $1,2,\ldots,N$. (Since only scalar particles are being considered in the present work, only Bose–Einstein statistics need be accounted for.)

Define multiparticle states $|x_1,n_1;\ldots;x_N,n_N\rangle$ as similarly symmetrized products of $|x\rangle$ states. Then,

$$\langle x_1',n_1';\ldots;x_N',n_N'|x_1,n_1,\lambda_0;\ldots;x_N,n_N,\lambda_0\rangle = \sum_{\text{perms }\mathcal{P}}\prod_{i=1}^{N}\delta_{n_i}^{n_{\mathcal{P}i}'}\Delta(x_{\mathcal{P}i}'-x_i;m_i^2), \tag{43}$$

where m_i is the mass of particles of type n_i. Note that the use of the same parameter value λ_0 for the starting point of each particle path is simply a matter of convenience, using the path parametrization gauge freedom to choose this value arbitrarily. The intrinsic lengths of each particle path are still integrated over *separately* in $|x_1,n_1;\ldots;x_N,n_N\rangle$, which is important for obtaining the proper particle propagator factors in Eq. (43). Nevertheless, by using λ_0 as a common starting parameter value, we can make the small notational simplification of not repeating it multiple times in $|x_1,n_1,\lambda_0;\ldots;x_N,n_N,\lambda_0\rangle$, defining, instead,

$$|x_1,n_1;\ldots;x_N,n_N;\lambda_0\rangle \equiv |x_1,n_1,\lambda_0;\ldots;x_N,n_N,\lambda_0\rangle.$$

Following the same procedures as in Sec. II C for each particle in a multiparticle state, it is straightforward to construct the multiparticle three momentum states $|t_1,\boldsymbol{p}_{1\pm},n_1;\ldots;t_N,\boldsymbol{p}_{N\pm},n_N\rangle$ and $|t_1,\boldsymbol{p}_{1\pm},n_1;\ldots;t_N,\boldsymbol{p}_{N\pm},n_N;\lambda_0\rangle$. Note that each particle may be *either* a normal particle (+) or an antiparticle (−). Then, to obtain on-shell states we need to take $t_i\to+\infty$ in $|t_1,\boldsymbol{p}_{1\pm},n_1;\ldots;t_N,\boldsymbol{p}_{N\pm},n_N\rangle$ for particles, but $t_i\to-\infty$ for antiparticles. This results in the multiparticle on-shell states $|\boldsymbol{p}_{1\pm},n_1;\ldots;\boldsymbol{p}_{N\pm},n_N\rangle$.

Now, it can be seen that the $|\boldsymbol{p}_{1\pm},n_1;\ldots;\boldsymbol{p}_{N\pm},n_N\rangle$ states may not always be particularly convenient, since they describe normal particles at $t=+\infty$ and antiparticles at $t=-\infty$. For describing the asymptotic state of outgoing particles from a scattering process, for instance, we would like to take the limit for all particles and antiparticles together as $t\to+\infty$.

To do this, we can take the viewpoint of considering antiparticles to be positive energy particles traveling forwards in time, rather than negative energy particles traveling backwards in time. Since both particles and their antiparticles will then have positive energy, it becomes necessary to explicitly label antiparticles with separate (though related) types from their corresponding particles. Let n_+ denote the type label for a normal particle type and n_- denote the corresponding antiparticle type.

For normal particles of type n_+, position states are defined as in Eq. (24),

$$\langle x,n_+|x_0,n_+;\lambda_0\rangle = \theta(x^0-x_0^0)\Delta_+(x-x_0).$$

For antiparticles of type n_-, however, position states are now defined such that

$$\langle x,n_-|x_0,n_-;\lambda_0\rangle = \theta(x^0-x_0^0)\Delta_-(x_0-x). \tag{44}$$

Note the reversal with respect to Eq. (24) of x_0 and x on the righthand side of this equation.

Using Eq. (23), the Fourier transform of Eq. (44) is

$$\int \mathrm{d}^4x\mathrm{e}^{-ip\cdot x}\theta(x^0)\Delta_-(-x) = \int \mathrm{d}^4x\mathrm{e}^{-ip\cdot x}\theta(x^0)\Delta_+(x^0,-\boldsymbol{x}) = \int \mathrm{d}^4x\mathrm{e}^{\mathrm{i}(p^0x^0+\boldsymbol{p}\cdot\boldsymbol{x})}\theta(x^0)\Delta_+(x) = \Delta_+(p^0,-\boldsymbol{p}),$$

where $\Delta_+(p)$ is as given in Eq. (30). From this we can see that carrying through the derivation for antiparticle three-momentum states will, indeed, give positive energy states, but with reversed three momentum

$$|t,\boldsymbol{p},n_-\rangle = (2\omega_{\boldsymbol{p}})^{-1}\int_{-\infty}^{t} \mathrm{d}t_0 |t_0,\boldsymbol{p},n_-;\lambda_0\rangle,$$

where

$$|t_0,\boldsymbol{p},n_-;\lambda_0\rangle = |t_0,-\boldsymbol{p}_+,n;\lambda_0\rangle.$$

Further, taking the limit $t\to+\infty$ gives the on-shell states

$$|\boldsymbol{p},n_-\rangle \equiv \lim_{t\to+\infty}|t,\boldsymbol{p},n_-\rangle = (2\pi)^{1/2}(2\omega_{\boldsymbol{p}})^{-1}|+\omega_{\boldsymbol{p}},-\boldsymbol{p};\lambda_0\rangle.$$

We can now reasonably construct Fock spaces $\mathcal{F}_t$ with single time, multiparticle basis states

$$|t;\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle \equiv |t,\boldsymbol{p}_1,n_{1\pm};\ldots;t,\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle,$$

over all combinations of particle and antiparticle types. Similarly defining

$$|t;\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}\rangle \equiv |t,\boldsymbol{p}_1,n_{1\pm};\ldots;t,\boldsymbol{p}_N,n_{N\pm}\rangle,$$

we can now take $t\to+\infty$ for particles and antiparticles alike to get the multiparticle on-shell states $|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}\rangle$. The corresponding bra states $\langle\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}|$ then span a subspace of the dual space $\mathcal{F}_t'$, for any t. Analogously to the case for single particle states, this can be used to define a Hilbert space of multiparticle probability amplitudes for each time t.

Finally, since $|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}\rangle$ now uniformly represents particles and antiparticles in the $t\to+\infty$ limit, it can be used as the asymptotically free state of outgoing particles from a scattering process. The corresponding state for incoming particles is $|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle \equiv \lim_{t\to-\infty}|t;\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle$.

F. Fields

Even though the theory presented here is essentially first quantized, it is still often convenient to introduce the formalism of creation and annihilation fields on the Fock space of multiparticle states. Specifically, define the creation field $\hat{\psi}^\dagger(x,n;\lambda)$ by

$$\hat{\psi}^\dagger(x,n;\lambda)|x_1,n_1,\lambda_1;\ldots;x_N,n_N,\lambda_N\rangle = |x,n,\lambda;x_1,n_1,\lambda_1;\ldots;x_N,n_N,\lambda_N\rangle,$$

with the corresponding annihilation field $\hat{\psi}(x,n;\lambda)$ having the commutation relation

$$[\hat{\psi}(x',n';\lambda),\hat{\psi}^\dagger(x,n;\lambda_0)] = \delta_n^{n'}\Delta(x'-x;\lambda-\lambda_0).$$

Further define

$$\hat{\psi}(x,n) \equiv \int_{\lambda_0}^{\infty}\mathrm{d}\lambda\,\hat{\psi}(x,n;\lambda), \tag{45}$$

so that

$$[\hat{\psi}(x',n'),\hat{\psi}^\dagger(x,n;\lambda_0)] = \delta_n^{n'}\Delta(x'-x), \tag{46}$$

which is consistent with the multiparticle inner product as given in Eq. (43).

Note the asymmetry in Eq. (46): $\hat{\psi}^\dagger(x,n;\lambda_0)$ is at the reference value λ_0 of the path parameter (at the start of the path), while in $\hat{\psi}(x',n')$ the path parameter (at the end of the path) is integrated over. This results from the fact that it is the integrated position bra state $\langle x',n'|$, created by $\hat{\psi}(x',n')$, that generates complete particle transition amplitudes (as discussed at the end of Sec.

II A). It is thus convenient to consider $\langle x,n|$ to be "dual" to $|x,n;\lambda_0\rangle$, in a similar fashion to the states $\langle \boldsymbol{p}_\pm|$ and $|t,\boldsymbol{p}_\pm;\lambda_0\rangle$ in Sec. II C, even though, by Eq. (21), the position states are not orthogonal.

In the field operator notation, this duality can be captured by introducing a *special adjoint* $\hat{\psi}^\ddagger$ defined by

$$\hat{\psi}^\ddagger(x,n) = \hat{\psi}^\dagger(x,n;\lambda_0) \quad \text{and} \quad \hat{\psi}^\ddagger(x,n;\lambda_0) = \hat{\psi}^\dagger(x,n). \tag{47}$$

The commutation relation in Eq. (46) then takes on the more symmetric form

$$[\hat{\psi}(x',n'),\hat{\psi}^\ddagger(x,n)] = \delta_n^{n'}\Delta(x'-x).$$

We can also define field operators for explicit particle and antiparticle types, as considered in Sec. II E. Define the *normal particle field* $\hat{\psi}(x,n_+)$ by

$$\hat{\psi}(x,n_+) \equiv \int \mathrm{d}^4x_0 \Delta_+(x-x_0)\hat{\psi}(x_0,n_+;\lambda_0), \tag{48}$$

giving the commutation rule

$$[\hat{\psi}(x',n_+),\hat{\psi}^\dagger(x,n_+;\lambda_0)] = [\hat{\psi}(x',n_+),\hat{\psi}^\ddagger(x,n_+)] = \Delta_+(x'-x). \tag{49}$$

Substituting Eq. (23) into Eq. (48) gives the familiar expression

$$\hat{\psi}(x,n_+) = (2\pi)^{-3/2}\int \mathrm{d}^3p \mathrm{e}^{i(-\omega_{\boldsymbol{p}}x^0+\boldsymbol{p}\cdot\boldsymbol{x})}\hat{a}(\boldsymbol{p},n_+),$$

where

$$\hat{a}(\boldsymbol{p},n_+) \equiv (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}})^{-1}\int \mathrm{d}^4x_0 \mathrm{e}^{i(\omega_{\boldsymbol{p}}x_0^0-\boldsymbol{p}\cdot\boldsymbol{x}_0)}\hat{\psi}(x_0,n_+;\lambda_0)$$

is the *on-shell particle three-momentum field*.

For antiparticles, reverse the roles of the antiparticle creation and annihilation operators relative to increasing-λ propagation as defined for the normal particle type. Define the antiparticle *creation* field analogously to Eq. (48) for the corresponding normal particle *annihilation* field

$$\hat{\psi}^\dagger(x,n_-) \equiv \int \mathrm{d}^4x_0 \Delta_-(x-x_0)\hat{\psi}^\dagger(x_0,n_-;\lambda_0).$$

Now, $\Delta_-(x-x_0)^* = \Delta_-(x_0-x)$ (see Eq. (23)). Therefore,

$$\hat{\psi}(x,n_-) = \int \mathrm{d}^4x_0 \Delta_-(x_0-x)\hat{\psi}(x_0,n_-;\lambda_0), \tag{50}$$

giving the commutation rule (note the switching of x' and x on the right, relative to Eq. (49))

$$[\hat{\psi}(x',n_-),\hat{\psi}^\dagger(x,n_-;\lambda_0)] = [\hat{\psi}(x',n_-),\hat{\psi}^\ddagger(x,n_-)] = \Delta_-(x-x').$$

Substituting Eq. (23) into Eq. (50) and changing variables $\boldsymbol{p}\to-\boldsymbol{p}$ then gives

$$\hat{\psi}(x,n_-) = (2\pi)^{-3/2}\int \mathrm{d}^3p \mathrm{e}^{i(-\omega_{\boldsymbol{p}}x^0+\boldsymbol{p}\cdot\boldsymbol{x})}\hat{a}(\boldsymbol{p},n_-),$$

where

$$\hat{a}(\boldsymbol{p},n_-) \equiv (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}})^{-1}\int \mathrm{d}^4x_0 \mathrm{e}^{i(\omega_{\boldsymbol{p}}x_0^0-\boldsymbol{p}\cdot\boldsymbol{x}_0)}\hat{\psi}(x_0,n_-;\lambda_0)$$

is the *on-shell antiparticle three-momentum field*.

III. INTERACTING PARTICLES

In conventional second-quantized quantum field theory, interactions are introduced via the Lagrangian density into the Hamiltonian used to propagate the fields. The very conception of interacting particles and their paths then only arises at all as a result of the perturbative expansion of the Hamiltonian. Such an approach is thus not very natural for a foundational formalism based on spacetime paths.

Now, the actual traditional motivation for introducing fields in the first place is largely a heuristic response to the well known difficulties with negative energies and probabilities in relativistic quantum mechanics. However, as we have seen in Sec. II, these difficulties can also be handled in the context of the spacetime path formalism. Further, the spacetime path approach can very directly accommodate the creation and destruction of particles, as required in a relativistic theory. One simply considers particle paths with a finite length: a particle is created at the start of its path and destroyed at the end.

Taking this path viewpoint, an *interaction vertex* can then simply be considered as an event at which a set of particle paths all end together and another set of particle paths all begin. An *interaction graph* is a set of interaction vertices connected by particle paths. For a collection of interacting particles, it is essentially such graphs that act as the fundamental building blocks of the system state, rather than the individual particle paths themselves.

The natural spacetime path approach for interactions is therefore first quantized rather than second quantized. As we will see in this section, the first-quantized spacetime path formalism can duplicate the basic results of perturbative quantum field theory for Feynman diagrams and scattering. It is also consistent with the typically first-quantized geometric approach used in string theory.[50]

Of course, taking a first-quantized formalism as foundational requires that issues of consistency and convergence that appear in traditional perturbation theory be addressed directly, without recourse to a posited nonperturbative solution. We will return to this point at the end of Sec. III D, though a full discussion is beyond the scope of the present paper.

A. Interactions

Since incoming particles are destroyed at an interaction vertex, and outgoing particles are created, the vertex can be represented by an operator constructed as an appropriate product of the creation and annihilation operator fields introduced in Sec. II F. Note that "incoming" and "outgoing" are used here in the sense of the path evolution parameter λ, not time. That is, we are not separately considering particles and antiparticles at this point.

Postulate 6: *An interaction vertex, possibly occurring at any position in spacetime, with some number a of incoming particles and some number b of outgoing particles, is represented by the operator*

$$-\mathrm{i}\hat{V} \equiv h\int \mathrm{d}^4x \prod_{i=1}^{a}\hat{\psi}^{\ddagger}(x,n_i')\prod_{j=1}^{b}\hat{\psi}(x,n_j), \tag{51}$$

where the coefficient h represents the relative probability amplitude of the interaction and $\hat{\psi}^{\ddagger}$ *is the special adjoint defined in Eq.* (47).

The probability amplitude for a transition from an initial state $|x_1,n_1;\ldots;x_N,n_N;\lambda_0\rangle$ to a final state $|x_1',n_1';\ldots;x_{N'}',n_{N'}'\rangle$, with a single intermediate interaction, is then

$$G_1(x_1',n_1';\ldots;x_{N'}',n_{N'}'|x_1,n_1;\ldots;x_N,n_N) = \langle x_1',n_1';\ldots;x_{N'}',n_{N'}'|(-\mathrm{i})\hat{V}|x_1,n_1;\ldots;x_N,n_N;\lambda_0\rangle.$$

This is essentially the amplitude for a first-order *Wick diagram*.[51] That is, it is equivalent to the first-order terms in the Wick expansion of the Dyson series in conventional quantum field theory (including all permutations that may result from crossing symmetries if any of the incoming or outgoing particles in the interaction are of the same type).

The probability amplitude corresponding to multiple intermediate interactions can then be obtained by repeated applications of $\hat{V}$. Thus, the amplitude for m interactions is

$$G_m(x'_1,n'_1;\ldots;x'_{N'},n'_{N'}|x_1,n_1;\ldots;x_N,n_N) = \langle x'_1,n'_1;\ldots;x'_{N'},n'_{N'}|\frac{(-i)^m}{m!}\hat{V}^m|x_1,n_1;\ldots;x_N,n_N;\lambda_0\rangle,$$

where the $(m!)^{-1}$ factor accounts for all possible permutations of the m identical factors of $\hat{V}$. The *complete* interacting transition amplitude, with any number of intermediate interactions, is then

$$\begin{aligned} G(x'_1,n'_1;\ldots;x'_{N'},n'_{N'}|x_1,n_1;\ldots;x_N,n_N) &= \sum_{m=0}^{\infty} G_m(x'_1,n'_1;\ldots;x'_N,n'_N|x_1,n_1;\ldots;x_N,n_N) \\ &= \langle x'_1,n'_1;\ldots;x'_N,n'_N|\hat{G}|x_1,n_1;\ldots;x_N,n_N;\lambda_0\rangle, \end{aligned} \tag{52}$$

where

$$\hat{G} \equiv \sum_{m=0}^{\infty} \frac{(-i)^m}{m!}\hat{V}^m = e^{-i\hat{V}}. \tag{53}$$

Extend the operation of the special adjoint in the natural way to sums and products. Then it is clear, at least formally, that $\hat{G}$ is unitary relative to this adjoint (that is, $\hat{G}^{\ddagger}\hat{G}=\hat{G}\hat{G}^{\ddagger}=1$), so long as $\hat{V}$ is self-adjoint relative to it (that is, $\hat{V}^{\ddagger}=\hat{V}$).

From Eq. (51), there are two consequences to $\hat{V}$ being self-adjoint. First $ih=g$ must be real. Second, the interaction must involve the same number of incoming and outgoing particles, of the same types. This second consequence is a result of assuming so far that there is only one possible type of interaction. The formalism can be easily extended to allow for multiple types of interactions by adding additional terms to the definition of $\hat{V}$. In this case, only the overall operator $\hat{V}$ needs to be self-adjoint, not the individual interaction terms.

For example, consider the case of a three-particle interaction of the form $\hat{\psi}^{\ddagger}(x,n_A)\hat{\psi}(x,n_B)\hat{\psi}(x,n_A)$. Then, for the overall interaction operator $\hat{V}$ to be self-adjoint, there must also be a conjugate interaction term $\hat{\psi}^{\ddagger}(x,n_A)\hat{\psi}^{\ddagger}(x,n_B)\hat{\psi}(x,n_A)$. That is,

$$\hat{V} = g\int d^4x[\hat{\psi}^{\ddagger}(x,n_A)\hat{\psi}(x,n_B)\hat{\psi}(x,n_A) + \hat{\psi}^{\ddagger}(x,n_A)\hat{\psi}^{\ddagger}(x,n_B)\hat{\psi}(x,n_A)].$$

This corresponds to the case of the particle of type B being indistinguishable from its antiparticle. Defining the self-adjoint effective field

$$\hat{\psi}'(x,n_B) \equiv \hat{\psi}(x,n_B) + \hat{\psi}^{\ddagger}(x,n_B)$$

then allows $\hat{V}$ to be put back into the form of a single type of interaction:

$$\hat{V} = g\int d^4x\hat{\psi}^{\ddagger}(x,n_A)\hat{\psi}'(x,n_B)\hat{\psi}(x,n_A). \tag{54}$$

An alternate interpretation of a self-adjoint interaction vertex is to pair up incoming and outgoing particles of the same type and consider them to be the *same* particle before and after the interaction. For example, an interaction of the form given in Eq. (54) would be considered to represent a *single* particle of type A interacting with a self-adjoint particle of type B.

This viewpoint can be seen more explicitly by considering a first-order interaction matrix element and using Eq. (12) to expand the A-particle propagators

$$\begin{aligned}
&\langle x_A,n_A;x_B,n_B|\hat{V}|x_0,n_A;\lambda_0\rangle \\
&\quad = g\int \mathrm{d}^4x\Delta_A(x_A-x)\Delta_B(x_B-x)\Delta_A(x-x_0) \\
&\quad = g\int \mathrm{d}^4x\Delta_B(x_B-x)\int_{\lambda_0}^{\infty}\mathrm{d}\lambda\int_{\lambda_0}^{\infty}\mathrm{d}\lambda'\Delta_A(x_A-x;\lambda'-\lambda_0)\Delta_A(x-x_0;\lambda-\lambda_0) \\
&\quad = g\int \mathrm{d}^4x\Delta_B(x_B-x)\int_{\lambda_0}^{\infty}\mathrm{d}\lambda\int_{\lambda}^{\infty}\mathrm{d}\lambda'\Delta_A(x_A-x;\lambda'-\lambda)\Delta_A(x-x_0;\lambda-\lambda_0).
\end{aligned}$$

Substituting for the A-particle kernels from Eq. (6), the path integral for the first kernel ends at the same point x as the path integral for the second kernel begins. Therefore, the two path integrals can be combined into a single path integral, with the constraint that the paths always pass through the intermediate point x:

$$\begin{aligned}
&\langle x_A,n_A;x_B,n_B|\hat{V}|x_0,n_A;\lambda_0\rangle \\
&\quad = g\int \mathrm{d}^4x\Delta_B(x_B-x)\int_{\lambda_0}^{\infty}\mathrm{d}\lambda\int_{\lambda}^{\infty}\mathrm{d}\lambda'\,\eta\int \mathrm{D}^4q\,\delta^4(q(\lambda')-x_A)\,\delta^4(q(\lambda)-x)\,\delta^4(q(\lambda_0)-x_0)\mathrm{e}^{iS_A[q]} \\
&\quad = g\int_{\lambda_0}^{\infty}\mathrm{d}\lambda'\int_{\lambda_0}^{\lambda'}\mathrm{d}\lambda\,\eta\int \mathrm{D}^4q\,\delta^4(q(\lambda')-x_A)\,\delta^4(q(\lambda_0)-x_0)\mathrm{e}^{iS_A[q]}\Delta_B(x_B-q(\lambda)).
\end{aligned}$$

This form clearly reflects the viewpoint of a single A particle interacting with a B particle at the point $q(\lambda)$ in its path.

Now consider a second-order interaction in which the incoming and outgoing particles are all A particles

$$\begin{aligned}
&\langle x_1',n_A;x_2',n_A|\frac{1}{2}\hat{V}^2|x_1,n_A;x_2,n_A;\lambda_0\rangle \\
&\quad = \frac{g^2}{2}\int \mathrm{d}^4y_1\int \mathrm{d}^4y_2[\Delta_A(x_1'-y_2)\Delta_A(y_2-y_1)\Delta_A(y_1-x_1)\Delta_B(y_2-y_1)\Delta_A(x_2'-x_2) \\
&\qquad + \Delta_A(x_1'-y_1)\Delta_A(y_1-x_1)\Delta_B(y_2-y_1)\Delta_A(x_2'-y_2)\Delta_A(y_2-x_2)+\cdots],
\end{aligned} \tag{55}$$

where the additional terms not shown are the result of position interchanges from the terms given. The first term shown in Eq. (55) reflects a self-interaction of one A particle via the B particle, with the second A particle propagating freely. The self-interaction factor can be given the path integral representation

$$\begin{aligned}
&\int \mathrm{d}^4y_1\int \mathrm{d}^4y_2\Delta_A(x_1'-y_2)\Delta_A(y_2-y_1)\Delta_A(y_1-x_1)\Delta_B(y_2-y_1) \\
&\quad = \int_{\lambda_0}^{\infty}\mathrm{d}\lambda'\int_{\lambda_0}^{\lambda'}\mathrm{d}\lambda_2\int_{\lambda_0}^{\lambda_2}\mathrm{d}\lambda_1\,\eta\int \mathrm{D}^4q\,\delta^4(q(\lambda')-x_1')\,\delta^4(q(\lambda_0)-x_1)\mathrm{e}^{\mathrm{i}S_A[q]}\Delta_B(q(\lambda_2)-q(\lambda_1)),
\end{aligned} \tag{56}$$

reflecting an A particle interacting with the B particle at points λ_1 and λ_2. The second term shown in Eq. (55) reflects an interaction of two A particles via a B particle. It can be given the path integral representation

$$\int \mathrm{d}^4 y_1 \int \mathrm{d}^4 y_2 \Delta_A(x_1' - y_1)\Delta_A(y_1 - x_1)\Delta_A(x_2' - y_2)\Delta_A(y_2 - x_2)\Delta_B(y_2 - y_1)$$
$$= \int_{\lambda_0}^{\infty} \mathrm{d}\lambda_2' \int_{\lambda_0}^{\infty} \mathrm{d}\lambda_1' \int_{\lambda_0}^{\lambda_2'} \mathrm{d}\lambda_2 \int_{\lambda_0}^{\lambda_1'} \mathrm{d}\lambda_1 \eta^2 \int \mathrm{D}^4 q_2 \delta^4(q_2(\lambda_2') - x_2') \delta^4(q_2(\lambda_0) - x_2) \mathrm{e}^{iS_A[\dot{q}_2]}$$
$$\times \int \mathrm{D}^4 q_1 \delta^4(q_1(\lambda_1') - x_1') \delta^4(q_1(\lambda_0) - x_1) \mathrm{e}^{iS_A[\dot{q}_1]} \Delta_B(q_2(\lambda_2) - q_1(\lambda_1)),$$

showing the B particle propagating from the point at λ_1 on the path of the first A particle to the point at λ_2 on the path of the second A particle. If the B particle is taken to be a photon, then Barut and Duru have shown that expansions of just the form given above can be obtained from a general path integral formulation of quantum electrodynamics[52] (see also the similar result obtained in Ref. 33 using a parametrized perturbation series approach).

B. Feynman diagrams

Computing a scattering amplitude requires moving from the Wick diagram formulation of Eq. (52) to a Feynman diagram formulation. To do this, replace the initial and final states in Eq. (52) with on-shell multiparticle momentum states $|t_1, \boldsymbol{p}_{1\pm}, n_1; \ldots; t_N, \boldsymbol{p}_{N\pm}, n_N; \lambda_0\rangle$ and $|\boldsymbol{p}'_{1\pm}, n'_1; \ldots; \boldsymbol{p}'_{N'\pm}, n'_{N'}; \lambda_0\rangle$ (note that these are the on-shell multiparticle states defined early in Sec. II E, with antiparticles propagating *backwards* in time, not the single-time states defined at the end of that section):

$$G(\boldsymbol{p}'_{1\pm}, n'_1; \ldots; \boldsymbol{p}'_{N'\pm}, n'_{N'} | \boldsymbol{p}_{1\pm}, n_1; \ldots; \boldsymbol{p}_{N\pm}, n_N)$$
$$\equiv \left[\prod_{i=1}^{N'} 2\omega_{\boldsymbol{p}'_i} \prod_{i=1}^{N} 2\omega_{\boldsymbol{p}_i} \right]^{1/2} \langle \boldsymbol{p}'_{1\pm}, n'_1; \ldots; \boldsymbol{p}'_{N'\pm}, n'_{N'} | \hat{G} | t_1, \boldsymbol{p}_{1\pm}, n_1; \ldots; t_N, \boldsymbol{p}_{N\pm}, n_N; \lambda_0 \rangle. \quad (57)$$

The $2\omega_{\boldsymbol{p}}$ factors are required by the resolution of the identity for these multiparticle states, generalizing the single particle case of Eq. (39),

$$\sum_{N=0}^{\infty} \sum_{n_i \pm} \int \mathrm{d}^3 p_1 \cdots \mathrm{d}^3 p_N \left[\prod_{i=1}^{N} 2\omega_{\boldsymbol{p}_i} \right] |t_1, \boldsymbol{p}_{1\pm}, n_1; \ldots; t_N, \boldsymbol{p}_{N\pm}, n_N; \lambda_0 \rangle \langle \boldsymbol{p}_{1\pm}, n_1; \ldots; \boldsymbol{p}_{N\pm}, n_N | = 1, \quad (58)$$

where the summation over the $n_i\pm$ is over all particle types and particle/antiparticle states.

Note that use of the on-shell states in Eq. (57) requires specifically identifying external lines as particles and antiparticles. For each initial and final particle, + is chosen if it is a normal particle and − if it is an antiparticle. The result is a sum of Feynman diagrams, including all possible permutations of interaction vertices and crossing symmetries. The inner products of the on-shell states for individual initial and final particles with the off-shell states for interaction vertices give the proper factors for the external lines of a Feynman diagram.

For a final particle, the on-shell state $\langle \boldsymbol{p}'_+|$ is obtained in the limit $t' \to +\infty$. Such a particle is thus an *outgoing* particle from the scattering process. If the external line for this particle starts at an interaction vertex x, then the line contributes an appropriate factor

$$(2\omega_{\boldsymbol{p}'})^{1/2} \langle \boldsymbol{p}'_+ | x; \lambda_0 \rangle = (2\pi)^{-3/2} (2\omega_{\boldsymbol{p}'})^{-1/2} \mathrm{e}^{i(+\omega_{\boldsymbol{p}'} x^0 - \boldsymbol{p}' \cdot \boldsymbol{x})}.$$

For a final antiparticle, however, the on-shell state $\langle \boldsymbol{p}'_-|$ is obtained in the limit $t' \to -\infty$. This means that the antiparticle is *incoming* to the scattering process, even though it derives from a final vertex, reflecting the time-reversal of antiparticle paths. If the external line for this antiparticle starts at an interaction vertex x, then the line contributes the factor

$$(2\omega_{\boldsymbol{p}'})^{1/2}\langle \boldsymbol{p}'_-|x;\lambda_0\rangle = (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}'})^{-1/2}e^{i(-\omega_{\boldsymbol{p}'}x^0+\boldsymbol{p}'\cdot\boldsymbol{x})}.$$

Next, consider an initial particle on an external line ending at an interaction vertex x'. The factor for this line is (assuming $x'^0 > t$),

$$(2\omega_{\boldsymbol{p}})^{1/2}\langle x'|t,\boldsymbol{p}_+;\lambda_0\rangle = (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}})^{-1/2}e^{i(-\omega_{\boldsymbol{p}}x'^0+\boldsymbol{p}\cdot\boldsymbol{x}')}.$$

Note that this expression is independent of t, so we can take $t\to-\infty$ and treat the particle as incoming. For an initial antiparticle, the corresponding factor is (assuming $x'^0 < t$),

$$(2\omega_{\boldsymbol{p}})^{1/2}\langle x'|t,\boldsymbol{p}_-;\lambda_0\rangle = (2\pi)^{-3/2}(2\omega_{\boldsymbol{p}})^{-1/2}e^{i(+\omega_{\boldsymbol{p}}x'^0-\boldsymbol{p}\cdot\boldsymbol{x}')}.$$

Taking $t\to+\infty$, this represents the factor for an antiparticle that is outgoing.

If a particle or antiparticle both starts at an initial vertex x and ends at a final vertex x', then, by Eq. (35),

$$(2\omega_{\boldsymbol{p}'}2\omega_{\boldsymbol{p}})^{1/2}\langle \boldsymbol{p}'_\pm|t,\boldsymbol{p}_\pm;\lambda_0\rangle = \delta^3(\boldsymbol{p}'-\boldsymbol{p}).$$

Finally, particles that start and end on interaction vertices (i.e., internal edges) are "virtual" particles propagating between interactions, retaining the full Feynman propagator factor $\Delta(x'-x)$.

Thus, the effect of Eq. (57) is to remove the propagator factors from the external lines of the summed Feynman diagrams, retaining them on internal edges. Since, in the position representation, G is essentially a sum of Green's functions G_m, this procedure is effectively equivalent to the usual LSZ reduction of the Green's functions.[42,51,53]

C. Scattering

The formulation of Eq. (57) is still not that of the usual scattering matrix, since the initial state involves incoming particles but outgoing antiparticles, and vice versa for the final state. To construct the usual scattering matrix, it is necessary to have multiparticle states that involve either all incoming particles and antiparticles (that is, they are composed of individual asymptotic particle states that are all consistently for $t\to-\infty$) or all outgoing particles and antiparticles (with individual asymptotic states all for $t\to+\infty$). These are the states $|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle$ and $|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}\rangle$ defined at the end of Sec. II E.

Reorganizing the scattering amplitude of Eq. (57) in terms of these asymptotic states gives the more usual form using the scattering operator $\hat{S}$. Showing explicitly the asymptotic time limit used for each particle

$$\begin{aligned}&\langle +\infty,\boldsymbol{p}'_+,n';\ldots;-\infty,\bar{\boldsymbol{p}}'_-,\bar{n}';\ldots|\hat{G}|-\infty,\boldsymbol{p}_+,n;\ldots;+\infty,\bar{\boldsymbol{p}}_-,\bar{n};\ldots;\lambda_0\rangle\\ &\quad=\langle \boldsymbol{p}',n'_+;\ldots;\bar{\boldsymbol{p}},\bar{n}_-;\ldots|\hat{S}|\boldsymbol{p},n_+;\ldots;\bar{\boldsymbol{p}}',\bar{n}'_-;\ldots;\lambda_0\rangle.\end{aligned}\tag{59}$$

Using the resolution of the identity

$$\sum_{N=0}^{\infty}\sum_{n_{i\pm}}\int d^3p_1\cdots d^3p_N\left[\prod_{i=1}^{N}2\omega_{\boldsymbol{p}_i}\right]|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle\langle \boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm}| = 1,\tag{60}$$

expand the state $\hat{S}|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle$ as

$$\begin{aligned}\hat{S}|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle = \sum_{N'=0}^{\infty}\sum_{n_{i\pm}}\int d^3p'_1\cdots d^3p'_{N'}\left[\prod_{i=1}^{N'}2\omega_{\boldsymbol{p}'_i}\right]|\boldsymbol{p}'_1,n'_{1\pm};\ldots;\boldsymbol{p}'_{N'},n'_{N'\pm};\lambda_0\rangle\\ \times\langle \boldsymbol{p}'_1,n'_{1\pm};\ldots;\boldsymbol{p}'_{N'},n'_{N'\pm}|\hat{S}|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle.\end{aligned}$$

This shows how $\hat{S}|\boldsymbol{p}_1,n_{1\pm};\ldots;\boldsymbol{p}_N,n_{N\pm};\lambda_0\rangle$ is a superposition of possible out states, with the square

of the scattering amplitude, Eq. (59), giving the probability of a particular out state for a particular in state.

Next, use Eqs. (49) and (50) in Eq. (22) to write the propagator as

$$\Delta(x-x_0)=\theta(x^0-x_0^0)[\hat{\psi}(x,n_+),\hat{\psi}^\ddagger(x_0,n_+)]+\theta(x_0^0-x^0)[\hat{\psi}(x_0,n_-),\hat{\psi}^\ddagger(x,n_-)]. \tag{61}$$

Then, reversing the usual derivation for Feynman diagrams (see, for example, Ref. 42) gives the Dyson series expansion

$$\hat{S}=1+\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\cdots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\hat{V}(t_1)\hat{V}(t_2)\cdots\hat{V}(t_n) \tag{62}$$

in terms of the *time-dependent interaction operator*

$$\hat{V}(t)\equiv g\int\mathrm{d}^3x\prod_{i=1}^{a}\hat{\Psi}^\ddagger(t,\mathbf{x},n_i')\prod_{j=1}^{b}\hat{\Psi}(t,\mathbf{x},n_j),$$

where

$$\hat{\Psi}(x,n)\equiv\hat{\psi}(x,n_+)+\hat{\psi}^\ddagger(x,n_-). \tag{63}$$

Since $\hat{V}(t)$ represents an interaction with the same number of incoming and outgoing particles, of the same types, as $\hat{V}$, the self-adjointness of $\hat{V}$ implies the self-adjointness of $\hat{V}(t)$, from which it can be shown that $\hat{S}$ is unitary. The case of a self-adjoint effective field $\hat{\psi}'(x,n)$ in $\hat{V}$ (as discussed at the end of Sec. III A) corresponds to the requirement of self-adjointness for $\hat{\Psi}(x,n)$. As can be seen from Eq. (63), this requirement implies that particles of type n are indistinguishable from their (path-reversed) antiparticles (indeed, a working definition of "indistinguishable" in this sense might very well be "cannot be distinguished by any interaction").

D. Regularization and renormalization

Of course, the development given in the previous subsections is actually only formal, because of the usual problems with divergence of the series in Eq. (52). As in conventional field theory, it is necessary to regularize infinite integrals and renormalize the resulting amplitudes. For a first-quantized approach, though, these problems seem particularly severe, since Eq. (52) is taken as the fundamental definition for the interacting amplitude, rather than as a perturbation expansion.

Fortunately, there is a relatively straightforward way to approach regularization within the context of a spacetime path approach, inspired by the work of Frastai and Horwitz[37] (see also Refs. 54 and 55 for a similar approach in the context of off-shell electrodynamics). This is to make the interaction coupling dependent on the intrinsic path length. This can be naturally introduced into the spacetime path formalism by making a choice for the weight function $f(T)$ introduced in Sec. II A different than $f(T)=1$.

To see this, consider that replacing the field operator $\hat{\psi}(x,n)$ defined in Eq. (45) with

$$\hat{\psi}_f(x,n)\equiv\int_{\lambda_0}^{\infty}\mathrm{d}\lambda f(\lambda-\lambda_0)\hat{\psi}(x,n;\lambda)$$

gives the commutation relation

$$[\hat{\psi}_f(x',n),\hat{\psi}^\dagger(x,n;\lambda_0)]=\int_0^\infty \mathrm{d}T f(T)\Delta(x'-x;T),$$

resulting in a propagator including the weight factor $f(T)$. Using this new field operator for, say, particles of type n_A in the interaction vertex operator given in Eq. (54) produces the desired path-length-dependent coupling

$$\hat{V}=g\int \mathrm{d}^4x\int_{\lambda_0}^\infty \mathrm{d}\lambda f(\lambda-\lambda_0)\hat{\psi}^\dagger(x,n_A;\lambda_0)\hat{\psi}(x,n_A;\lambda)\hat{\psi}'(x,n_B). \tag{64}$$

For the purposes of the present section, an appropriate choice for $f(\lambda-\lambda_0)$ is the Gaussian

$$f(\lambda-\lambda_0)=\mathrm{e}^{-(\lambda-\lambda_0)^2/2\Delta\lambda^2},$$

where $\Delta\lambda$ is a *correlation length*. For $\Delta\lambda\to\infty$, $f(\lambda-\lambda_0)\to 1$, and Eq. (64) reduces to Eq. (54).

Now, consider again the self-interaction term from Eq. (55). Using the interaction vertex operator from Eq. (64), this becomes

$$\Delta_A(p)\int \mathrm{d}^4p'\int_{\lambda_0}^\infty \mathrm{d}\lambda_1\int_{\lambda_0}^\infty \mathrm{d}\lambda_2 f(\lambda_2-\lambda_0)\Delta_A(p';\lambda_2-\lambda_0)f(\lambda_1-\lambda_0)\Delta_B(p-p')\Delta_A(p;\lambda_1-\lambda_0).$$

For simplicity, the momentum representation has been used here, in which

$$\Delta_A(p;\lambda-\lambda_0)\equiv \mathrm{e}^{-i(\lambda-\lambda_0)(p^2+m_A^2)}$$

and

$$\Delta_A(p)\equiv\int_0^\infty \mathrm{d}T\Delta_A(p;T)=-i(p^2+m_A^2-i\varepsilon)$$

(and similarly for Δ_B). The propagator from λ_0 to λ_1 is not divergent, so we can let $f(\lambda_1-\lambda_0)\to 1$, giving $\Delta_A(p)T'(p)\Delta_A(p)$, where

$$T'(p)\equiv\int \mathrm{d}^4p'\int_{\lambda_0}^\infty \mathrm{d}\lambda f(\lambda-\lambda_0)\Delta_A(p';\lambda-\lambda_0)\Delta_B(p-p'). \tag{65}$$

Inserting Eq. (13) into Eq. (65) gives

$$T'(p)=\int \mathrm{d}m^2T(p;m^2)F(m^2), \tag{66}$$

where

$$T(p;m^2)\equiv\int \mathrm{d}^4p'\Delta(p';m^2)\Delta_B(p-p')$$

is the unregulated self-interaction amplitude (without the external legs), with

$$\Delta(p;m^2)\equiv\int_0^\infty \mathrm{d}\lambda'\mathrm{e}^{-i\lambda'(p^2+m^2)}=-i(p^2+m^2-i\varepsilon), \tag{67}$$

and

$$F(m^2) \equiv (2\pi)^{-1} \int_0^\infty d\lambda e^{i\lambda(m^2 - m_A^2)} f(\lambda).$$

The unregulated quantity $T(p;m_A^2)$ is divergent. However, Eq. (66) is exactly the Pauli-Villars regularization prescription in continuous form.[56] Adjust the Fourier transform of the coefficients $F(m^2)$ so that

$$\tilde{F}(\lambda) = \begin{cases} f(\lambda) e^{-i\lambda m_A^2}, & \text{if } \lambda > \delta; \\ 0, & \text{if } \lambda \leqslant \delta. \end{cases}$$

This then meets the Pauli–Villars conditions in Fourier space for cancellation of singularities:[10] $\tilde{F}(0)=0$ and $\tilde{F}'(0)=0$. For $\Delta\lambda \to \infty$ and $\delta \to 0$, $T'(p)$ reduces to the unregulated quantity $T(p;m_A^2)$. (For further discussion, see Ref. 37. In Refs. 54 and 55, a similar result is obtained for a photon mass spectrum cutoff for the renormalization of off-shell quantum electrodynamics.)

Once the divergent integrals have been regulated, one can apply the usual techniques of multiplicative renormalization in the context of the Feynman diagram formalism obtained in Sec. III B. However, further discussion of renormalization is beyond the scope of the present paper. An intriguing direction for future exploration is the development of a complete regularization and renormalization program based on a physically motivated formulation of spacetime interactions. This would be consistent with the first-quantized approach of considering the series expansion to be the primary representation of the physical situation of the scattering amplitude, rather than a perturbative approximation to a nonperturbative Lagrangian formulation.

A potentially more serious issue is whether, even after renormalization, series such as that in Eq. (52) converge at all. However, Dyson's classic argument against convergence[57] is based on the conception of traditional quantum electrodynamics, where such series result from perturbation expansion. In the present first-quantized formalism, Dyson's argument might simply imply that the traditional formalism, and arguments from it, are not always applicable.

Actually, it is not the convergence of series for probability amplitudes, such as Eq. (52), that is really important. Rather, the real issue is whether there is a well-defined limit as $N \to \infty$ for physically testable probabilities such as given by

$$\frac{|\langle \alpha_{\text{out}} | \hat{S}^{(N)} | \psi_{\text{in}} \rangle|^2}{\langle \psi_{\text{in}} | \hat{S}^{(N)\ddagger} \hat{S}^{(N)} | \psi_{\text{in}} \rangle},$$

where $\hat{S}^{(N)}$ is the result of summing Eq. (62) to Nth order, $|\psi_{\text{in}}\rangle$ is a properly normalized multiparticle in state and $|\alpha_{\text{out}}\rangle$ is a member of a complete basis for multiparticle out states. Quantities such as this for, say, QED produce values that agree with experiment for large N. If it turns out that they do diverge for very large N, this just means that there is some mechanism in the real universe that suppresses the interference effect of interaction graphs with very large N, producing a finite cutoff of the series in Eq. (62).

Indeed, from this perspective, the Lagrangian and Hamiltonian formulations could be viewed as the approximations, obtained by assuming the summing of series for $N \to \infty$. In the end, the problem of divergences might even be seen as an artifact of the conventional second-quantized Lagrangian formulation itself, rather than of its perturbation expansion. Clearly this is an area that bears continued exploration.

IV. CONCLUSION

Spacetime approaches to relativistic quantum mechanics have been developed along a number of different threads in the literature, from the early work on proper time formalisms by Schwinger and others,[8–10] to the equally early work of Stueckelberg[6,7] and the parametrized relativistic quantum theory it inspired,[12–16,18,36] to the path integral approach introduced by Feynman[4,11,17,52] and its application to quantum gravity,[19,21,25] to the worldline formalism obtained as the infinite-

tension limit of string theory[26–32] and its relation to the typically first-quantized approach to interaction taken in string theory.[50] The formalism presented in the previous sections can be seen as a foundation underlying all these approaches.

A particularly significant additional result is the derivation of on-shell particles and antiparticle states as the infinite time limit of free particle states. This provides a connection between off-shell parametrized spacetime quantum theories[33,37,41,58,59] and traditional on-shell quantum field theory. It also suggests the intriguing possibility that, while real particles are likely on-shell to a very high degree of approximation, there may be testable consequences to this approximation not being exact.

The foundation presented here provides a number of interesting avenues for exploration in future publications.

The approach can be readily extended to incorporate path integral representations for nonscalar particles.[60–64] It can also handle massless particles, though it is not so straightforward to deal properly with the resulting gauge symmetries[58] and non-Abelian interactions.

Further, an important payoff of the spacetime path formalism is the intuitive grounding it gives to the theory, as opposed to the somewhat arbitrary mathematical justifications for introducing fields in traditional quantum field theory. Moreover, the formalism for interacting spacetime paths provides interesting possibilities for addressing the issues of regularization and renormalization (which is all the more important because of the first-quantized nature of the formalism).

Finally, a natural interpretational framework for the formalism is the consistent histories approach to quantum theory.[65–69] Particle paths can be treated as fine-grained histories in the sense of this approach, with coarse-grained histories corresponding to the superposition of fine-grained states, including cosmological histories of the universe as a whole.[19,70–72]

For example, scattering probabilities can be considered to represent the probabilities of decohering alternative coarse-grained spacetime histories for the scattering process. Probabilities can even be given to decohering cosmological histories of the universe.[73] Such an interpretation also provides for a natural way to see how the macroscopic classical view of the universe emerges from the more detailed quantum description, rather than viewing quantum physics as a "quantization" of a classical description (see, for example, Ref. 74), just as one would wish from a foundational quantum theory.

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APPENDIX A: FORM OF THE PHASE FUNCTIONAL

Proposition: *The phase functional S must have the form*

$$S[\dot{q}] = \int_{\lambda_0}^{\lambda_1} d\lambda' L[\dot{q};\lambda'], \tag{A1}$$

where the parametrization domain for $\dot{q}$ *is* $[\lambda_0,\lambda_1]$ *and* $L[\dot{q};\lambda]$ *depends only on* $\dot{q}$ *and its higher derivatives evaluated at* λ.

Proof: In

$$S[\dot{q};\lambda',\lambda_0] = S[\dot{q};\lambda',\lambda] + S[\dot{q};\lambda,\lambda_0],$$

consider $\lambda' = \lambda + \delta\lambda$, for infinitesimal $\delta\lambda$:

$$S[\dot{q};\lambda+\delta\lambda,\lambda_0]=S[\dot{q};\lambda+\delta\lambda,\lambda]+S[\dot{q};\lambda,\lambda_0]\approx\delta\lambda\left.\frac{\partial S[\dot{q};\lambda',\lambda]}{\partial\lambda'}\right|_{\lambda'=\lambda}+S[\dot{q};\lambda,\lambda_0],$$

or

$$\frac{S[\dot{q};\lambda+\delta\lambda,\lambda_0]-S[\dot{q};\lambda,\lambda_0]}{\delta\lambda}\approx\left.\frac{\partial S[\dot{q};\lambda',\lambda]}{\partial\lambda'}\right|_{\lambda'=\lambda}.$$

Taking the limit $\delta\lambda\to 0$ then gives

$$\frac{\partial S[\dot{q};\lambda,\lambda_0]}{\partial\lambda}=L[\dot{q};\lambda], \tag{A2}$$

where

$$L[\dot{q};\lambda]\equiv\left.\frac{\partial S[\dot{q};\lambda',\lambda]}{\partial\lambda'}\right|_{\lambda'=\lambda}.$$

Now, the functional L depends only on $\dot{q}$ and λ, not λ_0. Therefore, integrate Eq. (A2) over λ, with the initial condition $S[\dot{q};\lambda_0,\lambda_0]=0$, to get

$$S[\dot{q};\lambda,\lambda_0]=\int_{\lambda_0}^{\lambda}d\lambda' L[\dot{q};\lambda'], \tag{A3}$$

which is just Eq. (A1).

Further, by definition $S[\dot{q};\lambda,\lambda_0]$ only depends on values of $\dot{q}^\mu$ between λ_0 and λ. Therefore, $S[\dot{q};\lambda+\delta\lambda,\lambda]\approx L[\dot{q};\lambda]\delta\lambda$ should only depend on $\dot{q}$ infinitesimally close to λ. As $\delta\lambda\to 0$, this effectively limits $L[\dot{q};\lambda]$ to depend only on $\dot{q}$ and its derivatives evaluated at λ.

APPENDIX B: EVALUATION OF THE PATH INTEGRAL

Proposition: *The path integral*

$$\Delta(x,x_0;[\lambda])=\eta[\lambda]\int \mathrm{D}^4q\,\delta^4(q(\lambda(1))-x)\,\delta^4(q(\lambda(0))-x_0)\exp\left(i\int_{\lambda_0}^{\lambda}d\lambda'\left[\tfrac{1}{4}\dot{q}^2(\lambda')-m^2\right]\right) \tag{B1}$$

may be evaluated to get

$$\Delta(x,x_0;[\lambda])=\Delta(x-x_0;\lambda-\lambda_0)\equiv(2\pi)^{-4}\int \mathrm{d}^4p\,\mathrm{e}^{ip(x-x_0)}\mathrm{e}^{-i(\lambda-\lambda_0)(p^2+m^2)}. \tag{B2}$$

Proof: The path integral in Eq. (B1) may be defined as

$$\Delta(x,x_0;[\lambda])=\lim_{N\to\infty}\bar{\Delta}^{(N)}(x,x_0;[\lambda]),$$

where

$$\bar{\Delta}^{(N)}(x,x_0;[\lambda])\equiv\bar{\eta}(\bar{\lambda}_0,\ldots,\bar{\lambda}_N)\int \mathrm{d}^4\bar{q}_0\cdots\mathrm{d}^4\bar{q}_N\,\delta^4(\bar{q}_N-x)\,\delta^4(\bar{q}_0-x_0)\exp\left(i\sum_{j=1}^{N}\Delta\bar{\lambda}_j\left(\tfrac{1}{4}\bar{q}_j^2-m^2\right)\right), \tag{B3}$$

$\bar{\eta}(\bar{\lambda}_0,\ldots,\bar{\lambda}_N)\to\eta[\lambda]$ as $N\to\infty$ and the N-point discrete approximations to the functions $\lambda(s)$ and $q(\lambda(s))$ are given by

$$\bar{\lambda}_j = \lambda(j/N)$$

and

$$\bar{q}_j = q(\bar{\lambda}_j), \tag{B4}$$

for $j=0,\ldots,N$. The λ integral is approximated by a summation with

$$\Delta\bar{\lambda}_j \equiv \bar{\lambda}_j - \bar{\lambda}_{j-1}$$

and

$$\dot{\bar{q}}_j \equiv (\bar{q}_j - \bar{q}_{j-1})/\Delta\bar{\lambda}_j, \tag{B5}$$

for $j=1,\ldots,N$.

To compute the path integral, insert the product of Gaussian integrals

$$\prod_{j=1}^{N} i\left(\frac{\Delta\bar{\lambda}_j}{\pi}\right)^2 \int \mathrm{d}^4\bar{p}_j \mathrm{e}^{-i\Delta\bar{\lambda}_j\bar{p}_j^2} = 1$$

into the N-point approximation of Eq. (B3) to get

$$\bar{\Delta}^{(N)}(x,x_0;[\lambda]) = \bar{\xi}(\bar{\lambda}_0,\ldots,\bar{\lambda}_N)\int \mathrm{d}^4\bar{q}_0\cdots\mathrm{d}^4\bar{q}_N \int \mathrm{d}^4\bar{p}_1\cdots\mathrm{d}^4\bar{p}_N \delta^4(\bar{q}_N - x)\,\delta^4(\bar{q}_0 - x_0)$$
$$\times \exp\left(i\sum_{j=1}^{N}\Delta\bar{\lambda}_j\left(-\bar{p}_j^2 + \tfrac{1}{4}\dot{\bar{q}}_j^2 - m^2\right)\right),$$

where

$$\bar{\xi}(\bar{\lambda}_0,\ldots,\bar{\lambda}_N) \equiv \left[\prod_{j=1}^{N} i\left(\frac{\Delta\bar{\lambda}_j}{\pi}\right)^2\right]\bar{\eta}(\bar{\lambda}_0,\ldots,\bar{\lambda}_N).$$

Inside the $\bar{p}_j$ integrals, make the change of variables $\bar{p}_j \to \bar{p}_j - (1/2)\dot{\bar{q}}_j$, so that

$$\sum_{j=1}^{N}\Delta\bar{\lambda}_j\left(-\bar{p}_j^2 + \tfrac{1}{4}\dot{\bar{q}}_j^2 - m^2\right) \to \sum_{j=1}^{N}\Delta\bar{\lambda}_j\left(-\bar{p}_j^2 + \bar{p}_j\cdot\dot{\bar{q}}_j - \tfrac{1}{4}\dot{\bar{q}}_j^2 + \tfrac{1}{4}\dot{\bar{q}}_j^2 - m^2\right) = \sum_{j=1}^{N}\Delta\bar{\lambda}_j[\bar{p}_j\cdot\dot{\bar{q}}_j - (\bar{p}_j^2 + m^2)]. \tag{B6}$$

Now, using Eq. (B5),

$$\sum_{j=1}^{N}\Delta\bar{\lambda}_j\bar{p}_j\dot{\bar{q}}_j = \sum_{j=1}^{N}\bar{p}_j\cdot(\bar{q}_j - \bar{q}_{j-1}) = \bar{p}_N\cdot\bar{q}_N - \bar{p}_1\cdot\bar{q}_0 - \sum_{j=1}^{N-1}(\bar{p}_{j+1} - \bar{p}_j)\cdot\bar{q}_j$$

(this is essentially just integration by parts within the approximation to the path integral). But, for each $\bar{q}_j$, $j=1,\ldots,N-1$,

$$\int \mathrm{d}^4\bar{q}_j \mathrm{e}^{-i(\bar{p}_{j+1}-\bar{p}_j)\bar{q}_j} = (2\pi)^4\delta^4(\bar{p}_{j+1} - \bar{p}_j),$$

so, integrating over the $\bar{p}_j$ for $j=2,3,\ldots,N$ gives $\bar{p}_{j+1}=\bar{p}_j$. Therefore,

$$\bar{\Delta}^{(N)}(x,x_0;[\lambda]) = \bar{\xi}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) \int \mathrm{d}^4\bar{q}_0 \mathrm{d}^4\bar{q}_N \delta^4(\bar{q}_N - x)\,\delta^4(\bar{q}_0 - x_0) \int \mathrm{d}^4\bar{p}_1 (2\pi)^{4(N-1)} \mathrm{e}^{i\bar{p}_1(\bar{q}_N - \bar{q}_0)}$$
$$\times \exp\left(-i \sum_{j=1}^{N} \Delta\bar{\lambda}_j (\bar{p}_1^2 + m^2) \right) = (2\pi)^{-4} \bar{\zeta}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) \int \mathrm{d}^4 p \mathrm{e}^{ip(x-x_0)} \mathrm{e}^{-i(\bar{\lambda}_N - \bar{\lambda}_0)(p^2+m^2)}, \tag{B7}$$

where

$$\bar{\zeta}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) \equiv (2\pi)^{4N} \bar{\xi}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) = \left[\prod_{j=1}^{N} i(4\pi\Delta\bar{\lambda}_j)^2 \right] \bar{\eta}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N).$$

Now set the normalization factor

$$\bar{\eta}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) = \prod_{j=1}^{N} (-i)(4\pi\Delta\bar{\lambda}_j)^{-2}.$$

Then $\bar{\zeta}(\bar{\lambda}_0, \ldots, \bar{\lambda}_N) = 1$, so we can take the limit $N \to \infty$ of Eq. (B7) to get Eq. (B2).

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Observers, observables, spinors, and the confusion of tongues

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Choquet-Bruhat was the first to give a proper physical definition of covariant spinors, taking into account the reference system and treating them as equivalence classes defined from the transformation laws of the representatives when the reference system is changed. Recently, Rodriguez *et al.*[Int. J. Theor. Phys. **35**, 1849 (1996)] have adapted this procedure from covariant spinors to the case of algebraic and operator spinors. These approaches are restrained in the sense that the type of spinor is chosen from the beginning, and it does not admit a general formulation. In this paper, we present a unified definition that is valid for any type of the space of representation, being independent of its particular properties. In our formulation the three types of spinors appear as particular cases of the general definition. Moreover, we stick out the importance of the bilinear covariants in the definition of spinors. From this, we recognize a completely different kind of spinor, characterized by the different nature of their bilinears. The unnoticed difference between this last one, which we have called right-operator spinors, and the previous (left-)operator spinors has been motive of a long time discussion. © *2006 American Institute of Physics.*

To Pertti Lounesto, in memoriam [DOI: 10.1063/1.2355688]

I. INTRODUCTION

Usually, for the same physical concept or for the same (in some sense) mathematical object, there exist different mathematical formalizations or constructions. Naturally, these different formalizations lead to or are based on different interpretations for the meaning of the object involved. This typically occurs for the concept of *vector*. Indeed, the word "vector" is especially polysemous. It is used in many different frameworks, where the unique common property is that vectors are, or can be, represented by ordered sets of numbers. It is not our intention to be so general. We restrict ourselves to some geometric frameworks, where the notion of vector is referred to a directional physical magnitude. In this context, the concept of observer or reference system plays a fundamental role. Most definitions of vectors include the *transformation* properties of their representatives when there is a change of reference system. There exist also alternative definitions where the transformation properties do not form part of the definition, but are a consequence of the defining properties.[1]

In order to be more concrete, we can think on some typical vectorial spaces in classical physics or in relativity. For instance, the space of translations or velocities in a flat Euclidean space, or the tangent space of a differential manifold at a point. We can mention here three different definitions of the tangent space of a manifold: the equivalence class of curves that are tangent at the point, the derivatives of scalar fields and, elements of $\mathbb{R}^n$ subject to a *contravariant*

transformation under a change of coordinates.[2–5] Of these three definitions, only the third includes the transformation properties. But all three are equivalent in the sense that, after having established some identifications, each one can be deduced from each other. However, each formalization suggests a different idea of the object, facilitating or obstructing the intuition or the obtainment of some properties.

Standard identifications are the assimilation of reference systems with a basis in the vector space, with coordinates in a manifold, or with fields of tetrads. The description of vectors in a reference system is fundamental for its numerical manipulation and for its relationship with experimental measures. Nevertheless, vectors themselves can be thought as independent of the observer and manipulated conceptually by giving one symbol to it. In the case of a definition based on the transformation properties, a proper formalization is the following. Each vector is defined as an equivalence class given by the set of pairs formed by each of its representatives and its corresponding reference system. The transformation properties define, in fact, the equivalence relation.

The most usual manner of representing vectors in a reference system is by the collection of its n components. This means that the representative of the vector is an element of the Cartesian product of n copies of $\mathbb{R}$, denoted by $\mathbb{R}^n$. However, this is not the unique type of representatives that can be used. One example of this is the use of complex numbers or quaternions to represent vectors in a bidimensional or a tridimensional space.[6] Typically, the reason for using these other representations is the possibility of using computational properties of the space of representation, which has some meaning for the vectors considered. For instance, the multiplication by a phase in the complex plane generates the rotation of the bidimensional vectors represented. This is especially the case when the vector representation is aimed to be related with some spinorial representation, usually linked to a Clifford algebra.

There are at least two different ways of defining vectors through equivalence classes. One of them is unavoidably attached to the representation of vectors in a reference system by its components, $(v^1,\ldots,v^n)\in\mathbb{R}^n$, and seems to be the most extended formalization and conceptualization for representing vectors. The other way, although less common, has the merit that it can be generalized to other types of representations of vectors. Moreover, in our opinion, this alternative formalization involves a more physical idea of vectors, since it makes explicit the *representation map* between the space of vectors represented and the space in which the vectors are represented. The identification and comparison of these two different, but generally unnoticed, approaches is one of the goals of this paper.

The concept of spinor is intimately related with the representations of groups of isometries. From a group theoretical point of view, they are the space of representation of the double covering group, $\mathrm{Spin}_{p,q}$, of the orthogonal group $\mathrm{SO}(p,q)$. In this approach, the idea of a reference system has no place. But, from a physical point of view, spinors are always representatives in a given reference system. Thus, an important defining property of spinors is their transformation properties when changing the reference system. In this sense, a *physical* formalization of spinors has to follow a construction analogous to the one described for vectors: each spinor will be an equivalence class of pairs formed by each of its representatives and the corresponding *spinorial* reference system. Again, different spaces of representation can be considered to represent spinors. From this point of view, in the literature,[7–11,6,12,13] there are essentially three types of spinors: classical spinors, algebraic spinors, and operator spinors. The most known of them, and the first ones that were introduced, are what we have called *classical* spinors. (Classical spinors have been previously called *covariant spinors*.[10,14,11] But this name is not appropriate since the three of them have the same properties of covariance.) They are characterized by being represented with a *column matrix*, which is an ordered collection of real or complex numbers arranged to be used with the matrix product. Algebraic spinors are defined by representatives on a minimal left ideal of the corresponding Clifford algebra, $\mathcal{C}\ell_{p,q}$. Thus, instead of the matrix product, it is the Clifford product that is used to act on spinors. Operator spinors use as a space of representation the even Clifford subalgebra, $\mathcal{C}\ell^+_{p,q}$; thus it also uses the Clifford product. The even subalgebra corresponds to the linear extension of the spin group inside the Clifford algebra, $\mathrm{Spin}_{p,q}\subset\mathcal{C}\ell_{p,q}$. There always exists

a clear correspondence between classical and algebraic spinors in any dimension and signature. However, operator spinors are clearly defined only for three and four dimensions. For higher dimensions, their definition is controversial since they are nonequivalent to classical and algebraic spinors. The use of different spaces of representation allows us to use different algebraic operations to perform physically meaningful operations, like the obtainment of the bilinear observables. This also suggests different images of the meaning of spinors. In addition, it leads to different formulation of the physical equation of motion, as, for instance, the Dirac equation.[15,16,12,17,18] This implies the possibility of using different techniques to solve the equation.[19–22,3]

Choquet-Bruhat introduced,[23,24] to the best of our knowledge, the first clear formalization of spinors as equivalence classes of pairs containing the reference system. In this treatment only the classical spinors are considered and the definitions are strongly dependent on the space of representation used. The same mechanism has been recently adapted by Rodrigues *et al.*[10,11] to the definition of the other types of spinors: algebraic and operator spinors. However, in this formalization, the definition of the two types of spinors is also dependent on the space of representation, forcing us to state an independent definition for each one. One of our main goals in this paper is to present a unique definition valid for the three types of spinors, since the particular properties of the space of representation are not involved in the definition itself. (A seed work, developed by the authors, was presented by D. M. in Ref. 25.) Thus, the different types appear simply by particularizing to the desired space of representation.

The definition of spinors requires the introduction of a spinorial frame. This structure includes the vectorial reference system, but is more complex than this one. This complicates particularly the definition of spinors. In previous formalizations of spinors the definition of the spinorial frames is mixed with the definition of spinors themselves, making the structure more obscure. Besides, this definition of the spinorial frame is also representation dependent. In our presentation, the definition of the spinorial frames is independent of the definition of the spinors, and is also completely independent of any representation. This considerably clarifies the structure.

The physical content of spinors is, if not completely included, a least strongly linked to the bilinear observables that they define. In fact, except the phase of the spin, the value of the spinor can be recovered from the value of the bilinears.[26–28] The bilinears are scalars, vectors, and tensors, in general. Thus, the formalism used to define vectors affects the way in which spinors are treated. In particular, if vectors and spinors are defined as equivalence classes of objects containing a representative for each reference system, then the two equivalence relations must be compatible. The formula for a vectorial bilinear of the representative of a spinor, has as output the representative of a vector. Then, it is required that the operation is well defined when translated to the quotient spaces. This is usually expressed by demanding the *covariance* of the bilinear observables of a spinor. This fact implies that the equivalence relation defining spinors is not independent of the equivalence relation defining vectors.

In contrast, we must remark that this is not the unique framework in which the relationship between spinors and vectors can be understood. We have observed that in the literature[12,17,13,3] there exist two essentially different kinds of operator spinors, which we will call *left operator* and *right operator spinors*. The left operator spinors are the type mentioned above as simply *operator spinors*. Thus, their relationship with vectors follows the scheme described in the previous paragraph. On the contrary, right operator spinors follow a completely different scheme. Their bilinears are not the representatives of the vectors in the corresponding reference system, but the vectors themselves. For this reason they are not, and cannot be, embraced by the definition unifying the other three types. This new type of spinor involves a different conceptualization of the role of the spinors, and has been used before especially by Parra.[12] However, it has never been formalized, especially confronted with the other types of spinors. In our opinion, this unnoticed different conceptualization has been the origin of many endless discussions. A comparison from another point of view can be found in Ref. 29. In the last section we introduce and formalize right operator spinors and discuss the nature of their bilinears.

II. VECTOR PASSIVE TRANSFORMATIONS

Consider a vector $X \in \mathcal{A}$ and a basis $\Sigma \equiv \{e_I\}$ in a vector space $\mathcal{A}$. We can write the vector in the basis Σ as $X = X^I e_I$. Another basis $\Sigma' \equiv \{e'_I\}$ is related to Σ by means of a linear transformation:

$$e'_I = M(e_I) = M^J{}_I e_J, \quad \text{where } M \in \mathrm{GL}(\mathcal{A}) \quad \text{and} \quad M^J{}_I \in \mathbb{R}(n). \tag{1}$$

This expression can be understood in two different ways:

- If the transformation is $M \in \mathrm{GL}(\mathcal{A})$, then two different changes of basis,

  $$e'_I = M(e_I) \quad \text{and} \quad e'''_I = N(e''_I),$$

  will be defined by the same transformation if $M = N \in \mathrm{GL}(\mathcal{A})$. This can be expressed in components

  $$e'_I = M^J{}_I e_J \quad \text{and} \quad e'''_I = N^{J''}{}_{I''} e''_J.$$

  The two transformations will be equal if $M^J{}_I = N^J{}_I$, but not if $M^J{}_I = N^{J''}{}_{I''}$, where $N^J{}_I$ is the transformation N written in the basis $\{e_I\}$ and $N^{J''}{}_{I''}$ is the same transformation N written in the basis $\{e''_I\}$.
- On the contrary, if we define the transformation by the matrix $M^J{}_I \in \mathbb{R}(n)$, then two different changes of basis,

  $$e'_I = M^J{}_{I'} e_J \quad \text{and} \quad e'''_I = N^{J''}{}_{I'''} e''_J,$$

  will be related by the same transformation if $M^J{}_{I'} = N^{J''}{}_{I'''}$.

These two clearly different ways of conceiving the basis transformation is the origin for correspondingly different ways of understanding vectors. As we will see, this difference also has implications in the manner of conceiving spinors. Observe that the different conceptualization affects also the meaning of the indices and, accordingly, the use of primes.

The two alternatives are explained in detail in Appendix. Our understanding of vectors corresponds to the first option, $M \in \mathrm{GL}(\mathcal{A})$, and will be the one followed in this paper. A more objective reason for this preference is that it is this unique one that can be generalized for any kind of space of representation. The second option is directly valid exclusively for the type of representation of vectors and spinors, which we call in this paper *Cartesian representation*, based on $\mathbb{R}^n$ (or $\mathbb{C}^n$) as a space of representation.

Now, we can relate the expression of X in Σ with its expression in Σ':

$$X = X^{I'} e'_I = X^{I'} M^J{}_I e_J = X^I e_I. \tag{2}$$

The last equality will be fulfilled iff $X^I = M^I{}_J X^{J'}$. It is important to make clear that the equal sign refers to the resulting expressions and not to them in a particular form. Thus, writing, for instance, $X^I e_I = X^{I'} e'_I$ does not mean that the components X^I and $X^{I'}$ are equal. Neither, writing $X = X^I e_I$ means that the vector X is attached to the reference frame $\{e_I\}$, or is necessarily expressed in it.

A. Cartesian representation

Let us denote by $\mathcal{B} \subset \mathcal{A}^n$ the set of basis of $\mathcal{A}$. The components of a vector in a particular basis, $\{X^I\}$, can be collected together as an element of $\mathbb{R}^n$. In order to make explicit the components and basis information in vectors, they can be displayed in an ordered pair,

$$X^I e_I \mapsto (\Sigma, \{X^I\}), \quad \text{where } \Sigma \equiv \{e_I\} \in \mathcal{B} \quad \text{and} \quad \{X^I\} \in \mathbb{R}^n. \tag{3}$$

In the set collecting all these pairs, $\mathcal{B} \times \mathbb{R}^n$, we can define the following equivalence relation:

$$\mathcal{R}_c:(\Sigma,\{X^I\}) \sim (\Sigma',\{Y^I\}) \Leftrightarrow \exists\, M \in \mathrm{GL}(\mathcal{A}) | \Sigma' = M\Sigma, \quad X^I = M^I{}_J Y^J, \tag{4}$$

where M^IJ are the components of the transformation M in the basis Σ. (They coincide with the components in Σ': $M^I{}_J = M^{I'}{}_{J'}$.) This implies that two pairs, $(\Sigma,\{X^I\})$ and $(\Sigma',\{Y^I\})$, are equivalent when they *generate* the same vector, i.e., $X^I e_I = Y^I e'_I$. Let us denote the equivalence class associated to the vector X by the symbol $[X]$. Then, the elements of $[X]$ are the *Cartesian representatives* of X. If the first element of a Cartesian representative pair is the basis Σ it is said the *representative in the basis* Σ. A *passive transformation* of a vector X is indeed a transformation from a representative to another, for the same vector X, i.e., a mapping between elements of the equivalence class $[X]$. On the contrary an *active transformation* is a correspondence between vectors (or between equivalence classes), where the concept of representative is not involved.

Let us observe that the equivalence relation (4) is based on considering the basis transformation $M \in \mathrm{GL}(\mathcal{A})$, and it involves the obtainment of the components of M in the basis Σ. Probably this is not the most popular formalization, which would be based on considering the transformation given by $M \in \mathbb{R}(n)$. The corresponding equivalence relation is

$$\mathcal{R}'_c:(\Sigma,\{X^I\}) \sim (\Sigma',\{Y^I\}) \Leftrightarrow \exists\, M \in \mathbb{R}(n) | e'_I = M^J{}_I e_J, \quad X^I = M^I{}_J Y^J. \tag{5}$$

Here $M^I{}_J$ are the components of the matrix $M \in \mathbb{R}(n)$ in the canonical basis of $\mathbb{R}(n)$, which is well defined and completely independent of the vector space $\mathcal{A}$ and the basis Σ and Σ'.

As commented above, this latter formalization (5) is fully attached to the representation of vectors in the space $\mathbb{R}^n$. Therefore, it can hardly be generalized for other representation spaces. However, the former formalization (4) is generalizable for using any vectorial space $\hat{\mathcal{A}}$ as the representation space. This generalization will be called the *vectorial representation* of vectors.

B. Vectorial representation

Let us consider a generic vector space $\hat{\mathcal{A}}$, with the same required properties as $\mathcal{A}$ (of the same dimension over the same field of scalars) but completely independent of it and devoided of any physical or geometrical meaning. It will play the same role as $\mathbb{R}^n$ in the Cartesian representation. Until now, only linear properties of $\mathcal{A}$ have been considered. But later the inclusion of a suitable geometric algebra for the linear space $\mathcal{A}$ will be essential.

Let $\mathcal{B}$ be the set of basis of $\mathcal{A}$. We establish the *representation function* as

$$f:\mathcal{B} \times \mathcal{A} \to \hat{\mathcal{A}}; \quad (\Sigma,X) \mapsto f(\Sigma,X) \equiv f_\Sigma(X),$$

where $f_\Sigma : \mathcal{A} \to \hat{\mathcal{A}}$ is a 1–1 mapping. We will interpret $f_\Sigma(X) \in \hat{\mathcal{A}}$ as a linear representation of $X \in \mathcal{A}$, as seen from the reference frame $\Sigma \in \mathcal{B}$. Then, considering the vectors X, Y and the linear frames Σ, Σ' related by the same linear active transformation $Y = M(X)$ and $\Sigma' = M(\Sigma)$, it seems natural to require that $f_\Sigma(X) = f_{\Sigma'}(Y)$. By linearity, this is equivalent to the condition

$$f_\Sigma(\Sigma) = f_{\Sigma'}(\Sigma'), \text{ or using composition } f_\Sigma = f_{\Sigma'} \circ M. \tag{6}$$

Note that this appoints a privileged basis in the generic space $\hat{\mathcal{A}}$,

$$\{\hat{e}_I\} \equiv \hat{\Sigma}_0 \equiv f_\Sigma(\Sigma). \tag{7}$$

Following the same structure as for the Cartesian representation, we define for the pairs $(\Sigma, \hat{X}) \in \mathcal{B} \times \hat{\mathcal{A}}$ the equivalence relation

$$\mathcal{R}_v:(\Sigma,\hat{X}) \sim (\Sigma',\hat{Y}) \Leftrightarrow f_\Sigma^{-1}(\hat{X}) = f_{\Sigma'}^{-1}(\hat{Y})$$

$$\text{or equivalently, } \Leftrightarrow \hat{Y} = f_{\Sigma'} \circ f_\Sigma^{-1}(\hat{X}) \equiv \hat{M}^{-1}(\hat{X}), \tag{8}$$

where $\hat{M}:\hat{\mathcal{A}} \to \hat{\mathcal{A}}$ is the endomorphism in $\hat{\mathcal{A}}$ corresponding to $M:\mathcal{A} \to \mathcal{A}$, as seen by the basis Σ or Σ':

$$\hat{M} = f_\Sigma \circ M \circ f_\Sigma^{-1} = f_{\Sigma'} \circ M \circ f_{\Sigma'}^{-1}.$$

This equivalence relation guarantees that two pairs $\mathbf{(\Sigma, f_\Sigma(X))}$ and $\mathbf{(\Sigma', f_{\Sigma'}(Y))}$ are equivalent iff $X=Y \in \mathcal{A}$.

It is interesting to note that taking $\hat{\mathcal{A}}=\mathbb{R}^n$ as the generic vector space, we recover the Cartesian representation. In this case, since $\mathbb{R}^n$ has a privileged *canonical basis*,

$$\hat{e}_1 = (1,0,\ldots,0), \quad \hat{e}_2 = (0,1,0,\ldots,0), \quad \ldots, \quad \hat{e}_n = (0,\ldots,0,1),$$

there exists a *canonical* representation function such that $f_\Sigma(\Sigma)=\{\hat{e}_I\}$, which implies that the representative of a vector $X \in \mathcal{A}$ in a basis $\Sigma=\{e_I\}$ is the collection of its components in this basis:

$$f_\Sigma(X) = f_\Sigma(X^I e_I) = X^I \hat{e}_I = (X^1, X^2, \ldots, X^n).$$

The introduction of the representation function f_Σ has two objectives. First, the generalization of the type of representatives considered for vectors and especially, as we will see, for spinors. Second, to make explicit that, even in the Cartesian representation, a concrete representation function is present, although it is concealed in the standard formalizations. This gives a more clear understanding of the representation of vectors.

III. CLIFFORD ALGEBRA AND SPIN GROUP

In the previous section we have treated the representation of vectors without considering any metric. Let us now consider the vectorial space $\mathcal{A}$ endowed with a nondegenerate metric g of signature (p,q) and the generic vectorial space also endowed with a metric $\hat{g}$ of the same signature. We will restrict ourselves to representation functions $f_\Sigma:\mathcal{A} \to \hat{\mathcal{A}}$ that are isometries,

$$g(a,b) = \hat{g}(f_\Sigma(a), f_\Sigma(b)).$$

The vector space $\mathcal{A}$ generates via the exterior product the exterior or Grassmann algebra $\wedge(\mathcal{A})$. When endowed with the metric g, it also generates the Clifford algebra $\mathcal{C}\ell_{p,q}$.[30] The two algebras share the same base linear space in such a way that the exterior product and the graduation of the exterior algebra is many times considered as an ingredient of the Clifford algebra. Analogously the generic $(\hat{\mathcal{A}},\hat{g})$ results in the *generic Clifford algebra* $\widehat{\mathcal{C}\ell}_{p,q}$. The function f_Σ can be then extended to the full Clifford algebra space[17] via the outermorphism, defined by the property of being a morphism of exterior algebras:

$$f_\Sigma:\mathcal{C}\ell_{p,q} \to \widehat{\mathcal{C}\ell}_{p,q}; \quad f_\Sigma(A \wedge B) = f_\Sigma(A) \wedge f_\Sigma(B). \tag{9}$$

The fact that $f_\Sigma:\mathcal{A} \to \hat{\mathcal{A}}$ is an isometry implies that its extension (9) is also an isomorphism of Clifford algebras: $f_\Sigma(AB)=f_\Sigma(A)f_\Sigma(B)$. (For the sake of simplicity we will use the same symbol f_Σ.)

The *spin group* $\mathrm{Spin}_{p,q}$ is a subset of the even Clifford subalgebra $\mathcal{C}\ell^+_{p,q}$,

$$\mathrm{Spin}_{p,q} = \{R \in \mathcal{C}\ell^+_{p,q} | RvR^{-1} \in \mathcal{A}, \ \forall v \in \mathcal{A}, \ R\tilde{R} = \pm 1\}. \tag{10}$$

$\mathrm{Spin}_{p,q}$ is the double covering group of the group of isometries $\mathrm{SO}(\mathcal{A})$. Let us denote $\mathcal{H}$ the mapping that relates both groups,

$$\mathcal{H}:\mathrm{Spin}_{p,q} \to \mathrm{SO}(\mathcal{A}); \quad R \mapsto \mathcal{H}(R), \tag{11}$$

where $\mathcal{H}(R) \in \mathrm{SO}(\mathcal{A})$ is the endomorphism,

$$\mathcal{H}(R):\mathcal{A} \to \mathcal{A}; \quad v \mapsto \mathcal{H}(R)(v) \equiv RvR^{-1}. \tag{12}$$

Analogously to (10), the *generic spin group* $\widehat{\mathrm{Spin}}_{p,q}$ is defined as the corresponding subset of the generic even Clifford subalgebra $\widehat{\mathcal{C}\ell}^{+}_{p,q}$. The restriction of $f_\Sigma:\mathcal{C}\ell_{p,q} \to \widehat{\mathcal{C}\ell}_{p,q}$ to the subset $\mathrm{Spin}_{p,q} \subset \mathcal{C}\ell_{p,q}$ is a group isomorphism that maps it to the generic $\widehat{\mathrm{Spin}}_{p,q}$,

$$f_\Sigma:\mathrm{Spin}_{p,q} \to \widehat{\mathrm{Spin}}_{p,q}; \quad f_\Sigma(R_1R_2) = f_\Sigma(R_1)f_\Sigma(R_2), \quad \forall\, R_1, R_2 \in \mathrm{Spin}_{p,q}.$$

We can also define the function $\hat{\mathcal{H}}:\widehat{\mathrm{Spin}}_{p,q} \to \mathrm{SO}(\hat{\mathcal{A}})$, where $\mathrm{SO}(\hat{\mathcal{A}}) \equiv \widehat{\mathrm{SO}}$, as the generic copy of (11) and (12).

IV. SPINORS AND SPINORIAL FRAMES

Using equivalence classes as presented above for vectors, we will introduce spinors following the well exposed presentation by Choquet-Bruhat found in Ref. 24. However, there, it has only been considered a type of linear space representation for spinors, which here we call *classical*. Recently, in Ref. 10 the Choquet-Bruhat presentation has been extended to other linear spaces of representation in order to connect with *algebraic and operator spinors*. Our presentation intends to be general in the sense that we do not fix a concrete linear space in the definition. Our discussion will allow us to contrast the three different cases mentioned above and give their relationships in this geometrical frame.

Let us consider a linear space S over which we have defined a left operation of the group $\widehat{\mathrm{Spin}}_{p,q}$:

$$\alpha:\widehat{\mathrm{Spin}}_{p,q} \times S \to S; \quad (\hat{R}, \psi) \mapsto \alpha(\hat{R}, \psi) \equiv \alpha_{\hat{R}}(\psi),$$

satisfying the property

$$\alpha(\hat{R}_1, \alpha(\hat{R}_2, \psi)) = \alpha(\hat{R}_1\hat{R}_2, \psi).$$

This product constitutes a representation of the group $\widehat{\mathrm{Spin}}_{p,q}$:

$$\tilde{\alpha}:\widehat{\mathrm{Spin}}_{p,q} \to \mathrm{End}(S); \quad \tilde{\alpha}(\hat{R}) \equiv \alpha_{\hat{R}}.$$

The space S is called *the space of representation*. The elements of this space, $\psi \in S$, are usually named *spinors*. However, this naming hides the fact that ψ is only the *representative* of the spinor in some *spinorial frame* Σ_S. A rigorous definition needs to specify how the representative ψ transforms when the spinorial frame is transformed.

Following the presentation of Ref. 24, a first attempt to define spinors is introducing them as equivalence classes of dyads where orthonormal vectorial frames are used as spinorial frames. If $\mathcal{B}_0 \subset \mathcal{B}$ is the set of proper[1] orthonormal basis of $\mathcal{A}$ then the dyads would be of the form

$$(\Sigma, \psi), \quad \text{where} \quad \Sigma = \{e_I\} \in \mathcal{B}_0 \quad \text{and} \quad \psi \in S.$$

The equivalence class would be defined by

$$(\Sigma, \psi) \sim (\Sigma', \psi') \Leftrightarrow \exists\, R \in \mathrm{Spin}(\mathcal{A}), \text{ so that } \Sigma' = \mathcal{H}(R)\Sigma \text{ and } \psi = \alpha(f_\Sigma(R), \psi').$$

This definition has as consequence that any two dyads of the form (Σ, ψ) and $(\Sigma, -\psi)$ are equivalent. This says that for the same observer Σ there are two possible representatives, ψ and $-\psi$, of

[1]Future and right-hand oriented.

the same spinor. This possibility is not usually considered. Instead, to avoid this problem the spinorial frame is introduced.

The spinorial frame will contain a vectorial frame Σ and a sign to distinguish the two representatives ψ and $-\psi$. The equivalence relation should allow us to relate different representatives continuously, while signs form a discrete set $\{+,-\}$. For this reason, the standard definition of the spinorial frame introduces a more sophisticated structure.

Definition 4.1: Any element (Σ,R) *of the set* $\mathcal{B}_0\times \mathrm{Spin}_{p,q}$ *will be called a* potential spinorial frame.

They have been called "potential" because this set contains much more elements than needed. The proper set of spinorial frames will be a restriction of this one.

Definition 4.2: Two potential spinorial frames are said to be compatibles *if they satisfy the equivalence relation*:

$$\mathcal{C}:(\Sigma,R)\bowtie(\Sigma',R')\Leftrightarrow \mathcal{H}(R'^{-1})\Sigma'=\mathcal{H}(R^{-1})\Sigma\equiv\Sigma_0,$$

where each compatibility class is characterized by a fiducial vectorial frame Σ_0, *since in every class there is a unique element of the form* $(\Sigma_0,1)$.

Each *compatibility* class is an element of the quotient set $(\mathcal{B}_0\times \mathrm{Spin}_{p,q})/\mathcal{C}$, which defines a foliation. The proper set of spinorial frames is the restriction of $\mathcal{B}_0\times \mathrm{Spin}_{p,q}$ to a chosen compatibility class. Observe that in each compatibility class $\mathcal{F}\in(\mathcal{B}_0\times \mathrm{Spin}_{p,q})/\mathcal{C}$, for every vectorial frame $\Sigma\in\mathcal{B}_0$, there are two and only two elements and they are different only by a change of sign: $(\Sigma,R)\bowtie(\Sigma,-R)$, that is,

$$\forall\Sigma\in\mathcal{B}_0\quad \exists\,!\,R\in \mathrm{Spin}_{p,q}\quad \text{(up to a sign), such that}\quad (\Sigma,R),(\Sigma,-R)\in\mathcal{F}.$$

Definition 4.3: The set of spinorial frames $\mathcal{F}$ *is a chosen element* $\mathcal{F}\in(\mathcal{B}_0\times \mathrm{Spin}_{p,q})/\mathcal{C}$.

Let us emphasize that the set of spinorial frames is NOT the quotient space, $\mathcal{F}\neq(\mathcal{B}_0\times \mathrm{Spin}_{p,q})/\mathcal{C}$, but only one equivalence class, $\mathcal{F}\in(\mathcal{B}_0\times \mathrm{Spin}_{p,q})/\mathcal{C}$. Thus, a spinorial frame is a single element of $\mathcal{B}_0\times \mathrm{Spin}_{p,q}$, and not an equivalence class. (Obviously, a construction based on the quotient space as the set of spinorial frames would be a more elegant mathematical construction. Unfortunately, such a construction cannot be consistently defined for spinorial frames.)

The set $\mathcal{F}$ is usually defined equivalently[24] through the fiducial vectorial frame Σ_0. The election of the compatibility class $\mathcal{F}$ is completely arbitrary. The definition of spinors that results will be equivalent whatever set $\mathcal{F}$ is chosen, but they will be well defined only if one $\mathcal{F}$ is fixed from the beginning. This is usually worded by "the fiducial frame is arbitrary but fixed."

Finally, we can enunciate the general definition for spinors, independently of the space of representation used.

Definition 4.4: An α spinor *is a class of equivalence of the set* $\mathcal{F}\times S$ *defined by the equivalence relation*

$$\mathcal{R}_s:(\Sigma_S,\psi)\sim(\Sigma'_S,\psi')\Leftrightarrow \alpha(f_\Sigma(R),\psi)=\alpha(f_{\Sigma'}(R'),\psi'),\tag{13}$$

where $\Sigma_S=(\Sigma,R)$ *and* $\Sigma'_S=(\Sigma',R')$.

The original content of our presentation is triple.

- First, we have tried to clarify the structure. Observe that by definition $\Sigma_S,\Sigma'_S\in\mathcal{F}$, which implies that they are compatible (see Definition 4.2):

$$\Sigma'=\mathcal{H}(R'R^{-1})\Sigma.\tag{14}$$

  This condition has generally appeared[24,10] as part of the definition of spinors, without defining previously the set of spinorial frames $\mathcal{F}$. Then, the problem of the redundancy of spinorial frames in $\mathcal{B}_0\times \mathrm{Spin}_{p,q}$, is blended into the definition of spinors. In contrast, segregating the discussion of spinorial frames from the definition of spinors helps to clarify the two concepts.
- Second, from properties (14) and (6), we have

$$f_{\Sigma'} = f_{\Sigma} \circ \mathcal{H}(RR'^{-1}),$$

which applied to Definition 4.4 gives us the expression of the "spinorial transformation:"

$$\psi' = \alpha(f_{\Sigma}(RR'^{-1}), \psi). \tag{15}$$

In the original definition presented in Ref. 24 and adapted in Ref. 10, the representation function f_{Σ} is not present. In the original form[24] the transformation of orthonormal basis (or spinorial frames) is considered as a matrix $M \in \mathbb{R}(n)$ (in the sense discussed at the beginning of Sec. II), so that the representation function is not necessary for the mathematical construction. However, let us comment that the abstract formalization in Ref. 24 led us to forget some element, which makes the relation defining the equivalence classes to be not really an equivalence relation, as is proved and discussed in Appendix. This error can be considered almost a misprint, but it has caused some confusion, since then the formulation seems to be applicable trivially to other representation spaces. In Ref. 10, the authors follow this construction for defining algebraic and operator spinors, translating the (likely) misprint in a more serious error, since there the representation function cannot be avoided. This defect in the definition of spinors has deep implications, because it hides a real conceptual and mathematical necessity of the representation function.

- Third, in contrast with other treatments, we have not fixed any concrete representation α and f_{Σ}. This means that, by specializing Definition 4.4 for different representation spaces S, it includes every type of spinor discussed in the literature: classical, algebraic, and operator.

It must be said that recently Rodrigues in Ref. 11 improved correctly the presentation of Ref. 10 that had motivated our interest about spinorial reference frames. We observe, however, that his definition of algebraic spinors in Ref. 11 does not correspond to the definition of algebraic spinor given in the present paper. In fact, they are a kind of *right* algebraic spinors since the nature of their bilinear covariants must coincide with the ones of the right operator spinors presented in Sec. VI. Also, it is worth mentioning here that in Ref. 31 a rigorous presentation of left and right algebraic spinor fields and also Dirac-Hestenes spinor fields and a thoughtful discussion of the Dirac-Hestenes equation using the theory of fiber bundles is given for the first time.

A. Classical spinors

The most extended treatment of spinors is based on representations of the group $\mathrm{Spin}_{p,q}$ over the space of representation $S=\mathbb{C}^n$ or $\mathbb{R}^n$. This representation is realized by considering a set of $p+q$ matrices, $\{\gamma_\mu\} \subset \mathbb{C}(n)$ or $\mathbb{R}(n)$, generators of a matricial Clifford algebra:

$$\widehat{\mathcal{C}\ell}_{p,q} \equiv \mathrm{gen}\{\gamma_\mu\}, \quad \gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\eta_{\mu\nu}\mathbf{1},$$

where $\eta_{\mu\nu}=\mathrm{diag}(\overset{p}{1,\ldots,1},\overset{q}{-1,\ldots,-1})$. These kinds of spinors will be called *classical spinors*. (The term *classical* has been employed because this is the first kind that was defined.[32,7] In addition, it is the only one that is considered by most groups in mathematics and theoretical physics.) The generic space is the vector space spanned by linear combinations of the generating matrices:

$$\hat{\mathcal{A}} \equiv \mathrm{span}\{\gamma_\mu\}.$$

Observe that for classical spinors, the generic spin group is a matricial group generated by the basis of matrices $\{\gamma_\mu\}$, $\widehat{\mathrm{Spin}}_{p,q}=\mathrm{Spin}\{\gamma_\mu\} \subset \mathbb{R}(n)$ or $\mathbb{C}(n)$.

A typical example is the case of Dirac matrices[7] $\{\gamma_0^D, \gamma_1^D, \gamma_2^D, \gamma_3^D\}$ with the representation function defined by this basis $\{\gamma_\mu^D\}=\hat{\Sigma}_0=f_{\Sigma}(\Sigma)$, that is,

$$\gamma_\nu^D = f_{\{e_\mu\}}(e_\nu), \quad \forall \{e_\mu\} \in \mathcal{B}_0.$$

Example 4.1: A classical Pauli spinor *is a* $\mathcal{P}$ *spinor, where*

$$\mathcal{P}:\mathrm{Spin}\{\sigma_i\}\times\mathbb{C}^2\to\mathbb{C}^2,\quad \mathcal{P}(\hat{R},\psi)=\hat{R}\psi,$$

where $\hat{R}\psi$ *denotes the standard matrix product and* σ_i *are the usual Pauli matrices*[7] *for the algebra* $\mathcal{C}\ell_{3,0}$. *Note that* $\mathrm{Spin}\{\sigma_i\}=\mathrm{SU}(2)$.

Example 4.2: A classical Dirac spinor *is a* $\mathcal{D}$ *spinor*, *where*

$$\mathcal{D}:\mathrm{Spin}\{\gamma_\mu^D\}\times\mathbb{C}^4\to\mathbb{C}^4,\quad \mathcal{D}(\hat{R},\psi)=\hat{R}\psi,$$

where γ_μ^D *are the usual Dirac matrices*[7] *for the algebra* $\mathcal{C}\ell_{1,3}$.

B. Algebraic spinors

Let us consider the generic Clifford algebra $\widehat{\mathcal{C}\ell}_{p,q}$ over the field $\mathbb{K}=\mathbb{R}$ or $\mathbb{C}$, denoted by $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{K})$. In general, the vector space $\hat{\mathcal{A}}$ is real, thus the natural Clifford algebra would be $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{R})$. However, we will consider in some cases its complexification $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{C})\equiv\mathbb{C}\otimes\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{R})$, although the vector space $\hat{\mathcal{A}}$ is still considered real. Let us also consider a minimal left-ideal $\hat{\mathcal{I}}$ of $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{K})$. Then, the restriction of the regular representation into the minimal left-ideal $\hat{\mathcal{I}}$ is an irreducible representation of $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{K})$:

$$\mathcal{L}_{p,q}^{\hat{\mathcal{I}}(\mathbb{K})}:\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{K})\times\hat{\mathcal{I}}\to\hat{\mathcal{I}},\quad (\hat{C},\hat{\psi})\mapsto\mathcal{L}_{p,q}^{\hat{\mathcal{I}}(\mathbb{K})}(\hat{C},\hat{\psi})=\hat{C}\hat{\psi},$$

where $\hat{C}\hat{\psi}$ denotes the Clifford product between $\hat{C}$ and $\hat{\psi}$.

The concept of algebraic spinors is based on considering a minimal left-ideal $\hat{\mathcal{I}}\subset\widehat{\mathcal{C}\ell}_{p,q}$, as the representation space S of spinors. Notice that using this representation for spinors is possible because any representation of the algebra $\widehat{\mathcal{C}\ell}_{p,q}$ is also a representation of the group $\widehat{\mathrm{Spin}}_{p,q}$, since this group is a subset of $\widehat{\mathcal{C}\ell}_{p,q}$.[33] (For Weyl spinors, a representation of only the even subalgebra is used instead. It sufices since $\widehat{\mathrm{Spin}}_{p,q}\subset\widehat{\mathcal{C}\ell}^+_{p,q}$. However, this restriction is the reason for which the parity operator cannot be included in the representation.)

If a matrix representation is used as the generic Clifford algebra $\widehat{\mathcal{C}\ell}_{p,q}(\mathbb{K})$, then the most typical example of representation space is provided by the left ideal $\hat{\mathcal{I}}$ consisting in the matrices with all the elements vanishing except the first column,

$$\hat{\mathcal{I}}=\left\{\left.\begin{pmatrix} m_{11} & 0 & \cdots & 0\\ m_{21} & 0 & \cdots & 0\\ \vdots & \vdots & & \vdots\\ m_{n1} & 0 & \cdots & 0\end{pmatrix}\right| m_{A1}\in\mathbb{K}\right\},$$

which is clearly isomorphic to the space of classical spinors, $S=\mathbb{K}^n$.

Example 4.3: An algebraic Pauli spinor is a $\mathcal{L}_{3,0}^{\hat{\mathcal{I}}(\mathbb{R})}$ *spinor. The typical case is obtained by considering the left ideal* $\hat{\mathcal{I}}=\widehat{\mathcal{C}\ell}_{3,0}P$ *generated by the idempotent* $P=\frac{1}{2}(1+\hat{e}_3)$. *Note that this privileges one vector in the generic space*, *which*, *in turn*, *privileges one direction*, $e_3=f_\Sigma^{-1}(\hat{e}_3)$, *for each reference frame* Σ.

Example 4.4: An algebraic Dirac spinor *is a* $\mathcal{L}_{1,3}^{\hat{\mathcal{I}}(\mathbb{C})}$ *spinor. The left ideal usually considered is generated by the idempotent* $\frac{1}{2}(1+\hat{e}_0)\frac{1}{2}(1+i\hat{e}_{12})$.

A very clear exposition treating deeply these kind of spinors can be found in Ref. 6.

C. Left operator spinors

As we commented on in the Introduction, we have found that, depending on the author the name of operator spinor is used for two objects of a different nature. And this difference is not remarked by the authors.

One of these two kinds of objects is embraced by Definition 4.4 and we will call them *left operator spinors*. In fact, this reflects that, beyond the representation space on which they are based, left operator spinors share with classical and algebraic spinors the same notion for the covariance of the bilinears, as we will see in the next section.

The other kind of operator spinors, which we will call *right operator spinor*, cannot be included in Definition 4.4 since their bilinears are of a totally different nature. These spinors will be studied in Sec. VI.

The representation space of left operator spinors is the real even subalgebra $S=\widehat{\mathcal{C}\ell}^{+}_{p,q}(\mathbb{R})$, on which the regular representation of itself, as an algebra on its own, is considered:[2]

$$\mathcal{L}^{+}_{p,q}:\widehat{\mathcal{C}\ell}^{+}_{p,q}\times\widehat{\mathcal{C}\ell}^{+}_{p,q}\to\widehat{\mathcal{C}\ell}^{+}_{p,q};\quad(\hat{C},\hat{\psi})\mapsto\mathcal{L}^{+}_{p,q}(\hat{C},\hat{\psi})\equiv\hat{C}\hat{\psi}$$

where $\hat{C}\hat{\psi}$ implies the Clifford product between them.

Example 4.5: A left operator Pauli *spinor is a* $\mathcal{L}^{+}_{3,0}$ *spinor.*

Example 4.6: A left operator Dirac spinor *is a* $\mathcal{L}^{+}_{1,3}$ *spinor. This operator spinor is usually known as Dirac-Hestenes spinor.*[13]

V. BILINEAR COVARIANTS

Physically, the bilinear covariants (scalars, vectors or tensors) are the observables of a spinor or spinor field. This fact implies, in particular, that the meaning that we attach to spinors is intimately tied to their bilinear covariants. In this section we will describe how the bilinear covariants of the three classes—classical, algebraic, and left-operator spinors—are obtained.

Given their physical relevance, we will concentrate in the case of the Dirac spinors. This case is sufficiently representative to illustrate the mechanisms involved in, and the differences between the three classes of spinors. Even more concretely, we will only consider the density current, i.e., the bilinear vector J. The consideration of the other bilinears does not involve any qualitative difference.

Recall that a spinor (Definition 4.4) is an equivalence class of pairs (Σ_S,ψ), where

$$\mathcal{R}_s:(\Sigma_S,\psi)\sim(\Sigma'_S,\psi')\Leftrightarrow\alpha(f_\Sigma(R),\psi)=\alpha(f_{\Sigma'}(R'),\psi').$$

In the definition of the equivalence relation $\mathcal{R}_s$, it is involved in the representation function f_Σ corresponding to a previously defined representation of vectors, given by the equivalence relation (see Sec. II B):

$$\mathcal{R}_v:(\Sigma,\hat{X})\sim(\Sigma',\hat{X}')\Leftrightarrow f^{-1}_{\Sigma}(\hat{X})=f^{-1}_{\Sigma'}(\hat{X}').$$

The key idea for the treatment of the bilinear covariants is that to each representative (Σ_S,ψ) of a spinor it corresponds to a representative of the observable, $(\Sigma,\hat{J})$, where $\hat{J}$ is constructed bilinearly from ψ. Then, the equivalence relation $\mathcal{R}_s$ for spinors induces an equivalence relation $\mathcal{R}_b$ between the representatives $(\Sigma,\hat{J})$ of observables. The covariant property of the bilinear $\hat{J}$ corresponds to the fact that the induced relation $\mathcal{R}_b$ coincides with the vectorial equivalent relation $\mathcal{R}_v$. Obviously, as we will see immediately, this requirement implies some condition on the bilinear function $\hat{J}(\psi)$.

Consider a representative of a spinor $((\Sigma,R),\psi)$. Its bilinear covariant $\hat{J}$ is defined as a quadratic function of ψ,

---

[2]For Weyl and Majorana spinors the *complete* regular representation is not used but it is used as a regular representation restricted to a particular left ideal:

$$\mathcal{L}^{+}_{p,q}|_{\hat{\mathcal{I}}}:\widehat{\mathcal{C}\ell}^{+}_{p,q}\times\hat{\mathcal{I}}\to\hat{\mathcal{I}},\quad\text{where}\quad\mathcal{L}^{+}_{p,q}|_{\hat{\mathcal{I}}}(\hat{C},\hat{\psi})\equiv\mathcal{L}^{+}_{p,q}(\hat{C},\hat{\psi})\ \ \forall\ \hat{\psi}\in\hat{\mathcal{I}}\subset\widehat{\mathcal{C}\ell}^{+}_{p,q}.$$

$$\hat{J} \equiv \hat{\beta}(\psi), \tag{16}$$

where $\hat{\beta}$ is independent of Σ and R. From the definition of an α spinor, two representatives are equivalent if and only if

$$\mathcal{R}_s:((\Sigma,R),\psi) \sim ((\Sigma',R'),\psi') \Leftrightarrow \Sigma' = \mathcal{H}(R'R^{-1})\Sigma \quad \text{and} \quad \psi' = \alpha_{\hat{R}}(\psi),$$

where $\hat{R} \equiv f_\Sigma(RR'^{-1})$. This induces the equivalence relation

$$\mathcal{R}_b:(\Sigma,\hat{J}) \sim (\Sigma',\hat{J}') \Leftrightarrow \hat{J} = \hat{\beta}(\psi), \quad \hat{J}' = \hat{\beta}(\psi') = \hat{\beta} \circ \alpha_{\hat{R}}(\psi). \tag{17}$$

The equivalence relation used to represent vectors is

$$\mathcal{R}_v:(\Sigma,\hat{J}) \sim (\Sigma',\hat{J}') \Leftrightarrow \hat{J}' = f_{\Sigma'} \circ f_\Sigma^{-1}(\hat{J}).$$

Since, here, the two vectorial frames are related by

$$\Sigma' = \mathcal{H}(R'R^{-1})\Sigma,$$

it follows that

$$f_{\Sigma'} = f_\Sigma \circ \mathcal{H}(RR'^{-1}) = \hat{\mathcal{H}}[f_\Sigma(RR'^{-1})] \circ f_\Sigma = \hat{\mathcal{H}}(\hat{R}) \circ f_\Sigma.$$

Hence

$$\mathcal{R}_v:(\Sigma,\hat{J}) \sim (\Sigma',\hat{J}'), \quad \Leftrightarrow \quad \hat{J}' = \hat{\mathcal{H}}(\hat{R})\hat{J}. \tag{18}$$

From expressions (17) and (18), we see that $\mathcal{R}_b$ and $\mathcal{R}_v$ are the same equivalence relation iff

$$\hat{\beta} \circ \alpha_{\hat{R}}(\psi) = \hat{\mathcal{H}}(\hat{R}) \circ \hat{\beta}(\psi), \quad \forall\, \psi \in S, \quad \forall\, R' \in \mathrm{Spin}_{1,3}.$$

That is, iff

$$\hat{\beta} \circ \alpha_{\hat{R}} = \hat{\mathcal{H}}(\hat{R}) \circ \hat{\beta}, \quad \forall\, \hat{R} \in \widehat{\mathrm{Spin}}_{1,3}. \tag{19}$$

We have found here the simplest expression for the condition of covariance for the bilinear $\hat{J} = \hat{\beta}(\psi)$. Let us check now that the three classes of Dirac spinors satisfy this condition.

Classical spinors: The bilinear covariant $\hat{J}$ is usually computed as[7]

$$\hat{J}_\mu = \bar{\psi}\gamma_\mu^D\psi = \psi^\dagger\gamma_0^D\gamma_\mu^D\psi,$$

where $\hat{J} \in \mathbb{R}^4$ and $\{\hat{J}_\mu\}$ are its four components. Here we must make a remark. For the definition of classical Dirac spinors we considered as generic space the linear space spanned by the four Dirac generating matrices $\hat{\mathcal{A}} = \mathrm{span}\{\gamma_\mu^D\}$, instead of the space $\mathbb{R}^4$. Then, as usually, for classical spinors we must consider $\hat{J}$ as *gammarized*,

$$\hat{\beta}(\psi) = \hat{J} = \hat{J}_\mu\gamma^{D\mu} = [\bar{\psi}\gamma_\mu^D\psi]\gamma^{D\mu} \in \hat{\mathcal{A}}.$$

Now we can check that (19) is satisfied,

$$\hat{\beta}[\mathcal{D}_{\hat{R}}(\psi)] = [\bar{\psi}\gamma_0^D\hat{R}^\dagger\gamma_0^D\gamma_\mu^D\hat{R}\psi]\gamma^{D\mu} = [\bar{\psi}\hat{R}^{-1}\gamma_\mu^D\hat{R}\psi]\gamma^{D\mu},$$

where we have used the property $\gamma_0^D\hat{R}^\dagger\gamma_0^D = \tilde{\hat{R}} = \hat{R}^{-1}$, where $\tilde{\ }$ denotes the reversion.[6] Using also that $\hat{R}^{-1}\gamma_\mu^D\hat{R} = \Lambda^\nu{}_\mu\gamma_\nu^D$ is an isometry and hence , we obtain that

$$\hat{\beta}[\mathcal{D}_{\hat{R}}(\psi)] = [\bar{\psi}\gamma_{\mu}^{D}\psi]\hat{R}\gamma^{D\mu}\hat{R}^{-1} = \hat{R}\hat{\beta}(\psi)\hat{R}^{-1}.$$

Algebraic spinors: The bilinear covariant $\hat{J} \in \hat{\mathcal{A}}$ is computed as[6]

$$\hat{\beta}(\hat{\psi}) = \hat{J} = \langle \hat{\psi}\hat{e}_0\widetilde{\hat{\psi}^*}\rangle_1,$$

where * denotes the complex conjugate. The condition (19) can be easily checked,

$$\hat{\beta}[\mathcal{L}_{1,3}^{\hat{I}(\mathbb{C})}(\hat{R},\hat{\psi})] = \langle \hat{R}\hat{\psi}\hat{e}_0\widetilde{\hat{\psi}^*}\hat{R}^{-1}\rangle_1 = \hat{R}\langle \hat{\psi}\hat{e}_0\widetilde{\hat{\psi}^*}\rangle_1\hat{R}^{-1} = \hat{R}\hat{\beta}(\hat{\psi})\hat{R}^{-1}.$$

Left operator spinors: In this case the bilinear covariant $\hat{J} \in \hat{\mathcal{A}}$ is[17]

$$\hat{\beta}(\hat{\psi}) = \hat{J} = \hat{\psi}\hat{e}_0\widetilde{\hat{\psi}}. \tag{20}$$

To check condition (19) is immediate,

$$\hat{\beta}[\mathcal{L}_{1,3}^{+}(\hat{R},\hat{\psi})] = \hat{R}\hat{\psi}\hat{e}_0\widetilde{\hat{\psi}}\hat{R}^{-1} = \hat{R}\hat{\beta}(\hat{\psi})\hat{R}^{-1}.$$

VI. RIGHT OPERATOR SPINORS

Right operator spinors are radically different from the spinors defined in Sec. IV. It is crucial that this new type does not fit Definition 4.4, and that this fact is intimately related to the different nature of the bilinear obtained from right operator spinors.

Definition 6.1: A right operator spinor is an equivalence class of the set $\mathcal{F}\times\mathcal{C}\ell_{p,q}^{+}$ *defined by the equivalence relation*,

$$\mathcal{R}_r{:}(\Sigma_S,\Psi) \sim (\Sigma_S',\Psi') \Leftrightarrow \Psi R = \Psi' R', \tag{21}$$

where $\Sigma_S=(\Sigma,R)$ and $\Sigma_S'=(\Sigma',R')$.

This definition has two differences with Definition 4.4. The first is merely technical. In (21) the action of the spin group,

$$\alpha_r{:}\mathrm{Spin}_{p,q}\times\mathcal{C}\ell_{p,q}^{+}\to\mathcal{C}\ell_{p,q}^{+};\quad \alpha_r(R,\Psi) = \Psi R$$

is not a representation but an *antirepresentation*:

$$\alpha_r(R_1,\alpha_r(R_2,\Psi)) = \alpha_r(R_2R_1,\Psi).$$

The second is more subtle and fundamental. Subtle since it is not usually noticed[24,10] that the equivalence relation defining α spinors is basis dependent. This dependence is carried by $f_{\Sigma}(R)$ in (13). In contrast, observe that α_r is independent of the basis Σ. Fundamental because α_r is a representation of the group $\mathrm{Spin}_{p,q}$, which is constructed directly from the vectorial space of interest $\mathcal{A}$, while α is a representation of $\widehat{\mathrm{Spin}}_{p,q}$ defined from the generic space $\hat{\mathcal{A}}$. This is the fact that takes relevance in the nature of the bilinear observables obtained.

We can particularize this type of spinors for the cases of Pauli or Dirac spinors simply by considering, respectively, the algebra of the tridimensional space, $\mathcal{C}\ell_{3,0}$, or the algebra of the four-dimensional space-time, $\mathcal{C}\ell_{3,1}$ or $\mathcal{C}\ell_{1,3}$.[12]

Example 6.1: A right operator Pauli spinor *is a right operator spinor for a tridimensional space*.

Example 6.2: A right operator Dirac spinor *is a right operator spinor for a four-dimensional space-time*.

The bilinear observables of right operator spinors have an expression similar to the one considered for left operator spinors. Taking, for instance, the density current vector J for Dirac spinor, the expressions for the left operator (20) and for the right operator are, respectively,

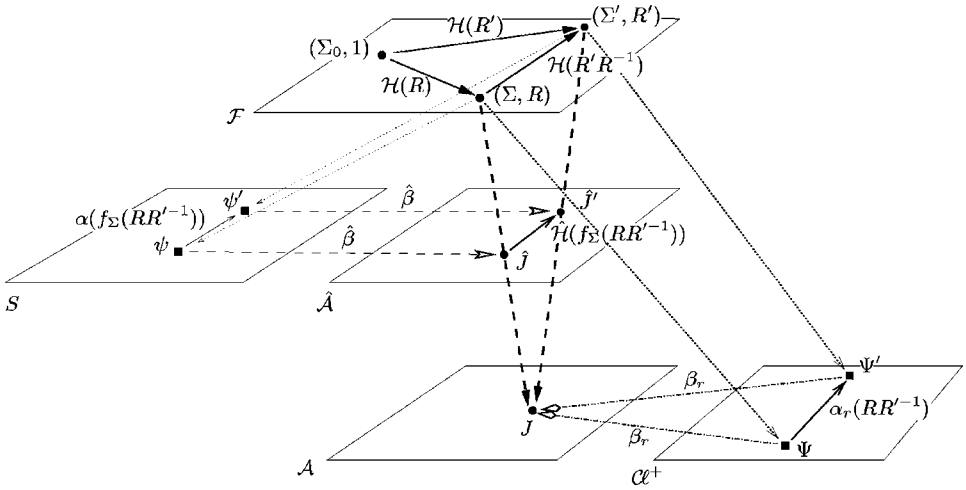

FIG. 1. Diagram representing the relationships between spinorial frames $\mathcal{F}$, vectors $\mathcal{A}$, vector representatives $\hat{\mathcal{A}}$ and spinor representatives S and $\mathcal{C}\ell^+$. Vector representatives are the bilinears of (left) α spinors, $\hat{J}=\hat{\beta}(\psi)$, while vectors are bilinears of right operator spinors, $J=\beta_r(\Psi,\Sigma)$. Observe that the bilinear function $\hat{\beta}$ does not depend on the reference frame Σ, but the transformation of spinorial representatives $\alpha(f_\Sigma(RR'^{-1})$ does. In contrast, the bilinear function β_r does depend on Σ, but the transformation of spinorial representatives $\alpha_r(RR'^{-1})$ does not.

$$\hat{J} = \hat{\psi}\hat{e}_0\tilde{\hat{\psi}} \tag{22a}$$

and

$$J = \Psi e_0 \tilde{\Psi}. \tag{22b}$$

Behind the similarity of these two formulas there is an essential difference. $\hat{J}$ belongs to the generic space $\hat{\mathcal{A}}$ and, together with the frame Σ, it forms a representative $(\hat{J},\Sigma)$ of the current vector. However, J belongs to the space $\mathcal{A}$ and is itself the current vector. Coherently, J does not transform when we change the frame Σ_S of the spinor with representative (Σ_S,Ψ). (See Fig. 1.)

In Eq. (22b), the vector e_0 is the time-like vector of the frame Σ. Hence, it changes when Σ changes:

$$e_0' = M(e_0) = \mathcal{H}(R'R^{-1})e_0,$$

where (Σ,R), $(\Sigma',R') \in \mathcal{F}$.

Accordingly to Definition 6.1, $\Psi \in \mathcal{C}\ell^+_{1,3}$ changes as

$$\Psi' = \Psi RR'^{-1}.$$

Therefore, a simple computation makes clear that the bilinear observable J is the same for both representants (Σ_S,Ψ) and (Σ_S',Ψ'):

$$J' = \Psi' e_0' \widetilde{\Psi'} = \Psi RR'^{-1}R'R^{-1}e_0 RR'^{-1}R'R^{-1}\tilde{\Psi} = \Psi e_0 \tilde{\Psi} = J. \tag{23}$$

As we announced in the Introduction, the interpretation of spinors that guides the whole of this paper is based on considering that a spinor does not describe objectively a physical particle but it describes how a physical particle is linked to the observer. It is for right operator spinors when this interpretation takes its most transparent expression[12]. This is clear from Eq. (23) since the spinor representative Ψ links the observer vector e_0 to the particle current field J. Equation (23) can be then paraphrased as *a transformation in the observer induces a transformation in the link so that the observable does not change*.

VII. CONCLUSIONS

Benn and Tucker in Ref. 34 manifested the *confusion of tongues* that it exists in the theory of spinors.

The theory of spinors was developed independently by physicist and mathematicians, and this historical apartheid has continued. […] Thus there is now a language, with many dialects, for discussing spinors in physics which makes little contact with the expositions of the theory to be found in mathematics literature.

Our aim in this paper has been to unify the definitions of spinors independently of their representations. Moreover, this goal has allowed us to identify and distinguish between two essential kinds of definitions as we showed in Secs. IV and VI. These definitions are intimately related with the bilinears and therefore with vectors. In fact, to demand covariance of the bilinear observables of spinors means that the equivalent relation defining spinors depends on the equivalence relation defining vectors, as we have seen in Sec. V.

Nowadays, we are working with a new kind of spinors.[35] They share with right operator spinors the property of generating directly the observables, instead of their representatives. However, their definition will not be necessarily constructed by means of an equivalent class, but they can be defined by a unique representative with no mention of observer tetrads or spinorial frames. This characteristic places those spinors close to being intrinsic spinors, in the sense of being defined independently of basis.

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APPENDIX: ABOUT THE NECESSITY OF THE REPRESENTATION FUNCTION ON THE DEFINITION OF VECTORS AND SPINORS

In the literature, there are few formal treatments for defining vectors and spinors as equivalent relation attending to their transformation properties in changing the reference frame.

A broadly accepted definition is the one found in Ref. 25. In this appendix we will discuss the correctness of this definition and two possible interpretations of it.

The definition of vectors in Ref. 25, p. 134 is the following.

A vector is a class of equivalence defined by

$$(u_{(i)},\rho_{(i)}) \sim (u_{(j)},\rho_{(j)}) \Leftrightarrow u_{(i)} = Lu_{(j)} \quad \text{and} \quad \rho_{(j)} = L\rho_{(i)}, \tag{A1}$$

where $u_{(i)} \in \mathbb{R}^n$, $\rho_{(i)}$ is a reference frame in V, and $L \in \mathrm{GL}(n)$.

This definition cannot be correct, at least without some explanatory complement. The reason is that the linear application L is applied to two different spaces: the representative space, $u_{(i)} \in \mathbb{R}^n$, and the space of reference frames $\rho_{(i)} \in \mathcal{B}$. Moreover, the guessing of an implicit canonical relation between the two different applications L affecting each of the two spaces, is misleading. Indeed, we present below two possible amendments of this definition.

A crucial point is that, even if the two spaces could be considered identified in some sense, so that the same application L could be applied to both, this definition would be incorrect because the relation $\sim$ introduced is not an equivalent relation. In concrete this relation does not satisfy transitivity. For three representatives we have

$$(u_{(1)},\rho_{(1)}) \sim (u_{(2)}\rho_{(2)}) \;\Leftrightarrow\; u_{(1)} = L_{12}u_{(2)} \quad \rho_{(2)} = L_{12}\rho_{(1)},$$

$$(u_{(2)},\rho_{(2)}) \sim (u_{(3)}\rho_{(3)}) \;\Leftrightarrow\; u_{(2)} = L_{23}u_{(3)} \quad \rho_{(3)} = L_{23}\rho_{(2)}, \tag{A2}$$

$$(u_{(1)},\rho_{(1)}) \sim (u_{(3)}\rho_{(3)}) \;\Leftrightarrow\; u_{(1)} = L_{13}u_{(3)} \quad \rho_{(3)} = L_{13}\rho_{(1)}.$$

But the two first relations imply that

$$u_{(1)} = L_{12}L_{23}u_{(3)} \quad \text{and} \quad \rho_{(3)} = L_{23}L_{12}\rho_{(1)}.$$

This is compatible with the third relation only if the two applications commute:

$$L_{12}L_{23} = L_{23}L_{12} = L_{13},$$

which is not true, in general.

Obviously, the theory of vectorial and spinorial transformations is not badly grounded. Thus, since the relation is not transitive, we are led to consider that the formal definition above does not recover properly or completely the actually utilized transformations. In order to reflect the actual transformations, we need to add an extra operation. Indeed, there are, at least, two different possibilities. They appear when we study more carefully the space of reference frames $\mathcal{B}$.

A reference frame ρ is a collection of n linearly independent vectors in V:

$$\rho = (\rho_1, \ldots, \rho_n), \quad \rho_I \in V.$$

Thus, we can write

$$\mathcal{B} = V \times \cdots \times V = V^n = \mathbb{R}^n \otimes V.$$

The last expression suggests two types of transformations for reference frames: acting on $\mathbb{R}^n$ or acting on V. The first possibility seems to be the one implied in definition (A1). However, in this case, the definition is misleading since the correct definition involves the operation of transposition. The second possibility is, in fact, the one considered in this work and it involves the representation function f_Σ.

(1) Consider that $L \in \mathrm{GL}(n)$ is a linear application on $\mathbb{R}^n$. Then, it seems natural to make it act on the $\mathbb{R}^n$ structure of $\mathcal{B}=\mathbb{R}^n \otimes V$. But then we will not have an equivalence relation. Let us write the usual operation of applying a linear transformation on components and basis in index notation:

$$\rho_{(2)}I = L^J{}_I\rho_{(1)J} \quad \text{and} \quad u^I_{(1)} = L^I{}_J u^J_{(2)}.$$

Observe that, in fact, the $\mathbb{R}^n$ in $\mathcal{B}=\mathbb{R}^n \otimes V$ is not the same as the $\mathbb{R}^n$ space of components, but the dual space of it, $\mathbb{R}^{n^*}$. Therefore, while $\mathbb{R}^n$ is transformed with the application $L:\mathbb{R}^n \to \mathbb{R}^n$, the space $\mathbb{R}^{n^*} \otimes V$ is transformed with the transposed application $L^{\mathsf{T}}:\mathbb{R}^{n^*} \to \mathbb{R}^{n^*}$,

$$(u_{(i)},\rho_{(i)}) \sim (u_{(j)},\rho_{(j)}) \quad \Leftrightarrow \quad u_{(i)} = Lu_{(j)} \quad \text{and} \quad \rho_{(j)} = L^{\mathsf{T}}\rho_{(i)}.$$

It is easy to see that with this transposition the relation is transitive. Taking three representatives as in (A2), we would obtain the conditions $L_{12}L_{23}=L_{13}$ and $L^{\mathsf{T}}_{23}L^{\mathsf{T}}_{12}=L^{\mathsf{T}}_{13}$, which are compatible. Hence, we have an equivalent relation.

This interpretation of the vectorial transformations is possibly the most extended one. Nevertheless, it is not the unique and, certainly, it was not the one primarily thought by the authors of this work. But, what is important to note is that it cannot be generalized for other types of representatives different from the Cartesian one.

(2) Let us consider L as an application on V, instead of one on $\mathbb{R}^n$. Then, it can be applied to reference frames $\rho_{(i)} \in \mathcal{B}=\mathbb{R}^{n^*} \otimes V$ by operating on the V structure. However, $L \in \mathrm{GL}(V)$ cannot be

applied to $u_{(i)} \in \mathbb{R}^n$. Thus, we need a way of relating the application $L \in \mathrm{GL}(V)$ with some application $\hat{L} \in \mathrm{GL}(\mathbb{R}^n)$. Let us express the application L by its components in the basis $\rho_{(i)}=\{e^{(i)}{}_I\}$:

$$e^{(2)}{}_I = L(e^{(1)}{}_I) = L^J{}_I\, e^{(1)}{}_J.$$

Now, these components can be used to define the application $\hat{L}$, which should relate the two representatives $u_{(i)}=\{u^I_{(i)}\} \in \mathbb{R}^n$:

$$u_{(1)}{}^I = [\hat{L}(u_{(2)})]^I \equiv L^I{}_J\, u_{(2)}{}^J.$$

This is formalized by considering the representation function $f_{\rho_{(i)}}: V \to \mathbb{R}^n$, which maps each vector $u \in V$ into its components in the corresponding reference frame $f_{\rho_{(i)}}(u)=u_{(i)}$, so that it satisfies

$$f_{\rho_{(i)}}(\rho_{(i)}) = f_{\rho_{(j)}}(\rho_{(j)}), \quad \forall\, i,j.$$

Then, the application $\hat{L}$ is defined by

$$\hat{L} \equiv f_{\rho_{(i)}} \circ L \circ f^{-1}_{\rho_{(i)}}. \tag{A3}$$

Let us remark that the relationship between L and $\hat{L}$ is frame dependent.

Now, we have the relation

$$(u_{(i)},\rho_{(i)}) \sim (u_{(j)},\rho_{(j)}) \quad \Leftrightarrow \quad u_{(i)} = \hat{L}_{ij} u_{(j)} \quad \text{and} \quad \rho_{(j)} = L_{ij}\rho_{(i)}.$$

Since $\hat{L}$ is frame dependent, we must check that the relation is symmetric, i.e., $\hat{L}_{ji}=\hat{L}^{-1}_{ij}$, provided that $L_{ji}=L^{-1}_{ij}$. The symmetry is obtained by taking into account Eq. (A3):

$$\rho_{(j)} = f^{-1}_{\rho_{(j)}} \circ f_{\rho_{(i)}}(\rho_{(i)}) \Rightarrow L_{ij} = f^{-1}_{\rho_{(j)}} \circ f_{\rho_{(i)}}$$

which implies the identity

$$\hat{L}_{ji} = f_{\rho_{(j)}} L_{ji} f_{\rho_{(j)}}{}^{-1} = f_{\rho_{(j)}} f_{\rho_{(i)}}{}^{-1} f_{\rho_{(j)}} f_{\rho_{(j)}}{}^{-1} = f_{\rho_{(i)}} f_{\rho_{(i)}}{}^{-1} f_{\rho_{(j)}} f_{\rho_{(i)}}{}^{-1}$$

$$= f_{\rho_{(i)}} L_{ji} f_{\rho_{(i)}}{}^{-1} = (\hat{L}_{ij})^{-1}.$$

This result is usually paraphrased as: "The transformation matrix is the same written in both reference frames, the original and the transformed one." The transitivity property is satisfied if $\hat{L}_{12}\hat{L}_{23}=\widehat{(L_{23}L_{12})}$. This is obtained by

$$\hat{L}_{12}\hat{L}_{23} = f_{\rho(1)} L_{12} f_{\rho(1)}{}^{-1} f_{\rho(2)} L_{23} f_{\rho(2)}{}^{-1} = f_{\rho(1)} L_{12} L_{12}{}^{-1} L_{23} f_{\rho(2)}{}^{-1}$$

$$= f_{\rho(1)} L_{23} f_{\rho(2)}{}^{-1} f_{\rho(1)} f_{\rho(1)}{}^{-1} = f_{\rho(1)} L_{23} L_{12} f_{\rho(1)}{}^{-1}$$

$$= \widehat{(L_{23}L_{12})}.$$

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Dimensional reduction of Seiberg-Witten monopole equations, $\mathcal{N}=2$ noncommutative supersymmetric field theories and Young diagrams

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We investigate the Seiberg-Witten monopole equations on noncommutative (N.C.) $\mathbb{R}^4$ at the large N.C. parameter limit, in terms of the equivariant cohomology. In other words, $\mathcal{N}=2$ supersymmetric U(1) gauge theories with a hypermultiplet on N.C.$\mathbb{R}^4$ are studied. It is known that after topological twisting partition functions of $\mathcal{N}>1$ supersymmetric theories on N.C. $\mathbb{R}^{2D}$ are invariant under the N.C. parameter shift; then the partition functions can be calculated by its dimensional reduction. At the large N.C. parameter limit, the Seiberg-Witten monopole equations are reduced to ADHM equations with the Dirac equation reduced to the 0 dimension. The equations are equivalent to the dimensional reduction of non-Abelian $U(N)$ Seiberg-Witten monopole equations in $N\to\infty$. The solutions of the equations are also interpreted as a configuration of a brane antibrane system. The theory has global symmetries under torus actions originated in space rotations and gauge symmetries. We investigate the Seiberg-Witten monopole equations reduced to the 0 dimension and the fixed point equations of the torus actions. We show that the Dirac equation reduced to the 0 dimension is automatically satisfied when the fixed point equations and the ADHM equations are satisfied. Then, we find that the Seiberg-Witten equations reduced to the 0 dimension and fixed point equations of the torus action are equivalent to just the ADHM equations with the fixed point equations. For finite N, it is known that the fixed points of the ADHM data are isolated and are classified by the Young diagrams. We also give a new proof of this statement by solving the ADHM equations and the fixed point equations concretely and by giving graphical interpretations of the field components and these equations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The Seiberg-Witten theory causes a revolution of nonperturbative analysis for $\mathcal{N}=2$ supersymmetric Yang-Mills theories.[1,2] In the Seiberg-Witten theory, the instanton effects of $\mathcal{N}=2$ supersymmetric Yang-Mills theories are encoded in the prepotential, which is defined by using the Seiberg-Witten curve. (See, for example, Ref. 3 and references therein.) The Seiberg-Witten theory

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also provides a powerful tool, the monopole equation, to investigate the topology of four dimensional manifolds.[4,5] The monopole equations are more tractable than the instanton equation, and yield many results in mathematics as well as physics.

Meanwhile, instanton calculus has developed by using ADHM data or *D*-instanton. (See, for example, Ref. 6.) Particularly, an important calculation technology for $\mathcal{N}=2$ supersymmetric Yang-Mills theories is brought by Nekrasov.[7] After Ref. 7, many related works have been made.[8–38] In Ref. 7 and so on, the localization theorem plays an essential role.[39–42] (See also Refs. 43 and 44.) The localization theorem is valid when the theory has symmetries that correspond to some group action and the group action has isolated fixed points. It is expected that many kinds of calculations of $\mathcal{N}>1$ supersymmetric gauge theory are carried out by using this theorem.

It is shown that partition functions of $\mathcal{N}>1$ supersymmetric gauge theories on noncommutative (N.C.) $\mathbb{R}^{2D}$ are invariant under the N.C. parameter change.[45] Therefore we can perform the calculation at the large N.C. parameter limit. As discussed in Refs. 45–48, taking this limit causes dimensional reduction, and we can calculate the partition functions by using the theory after dimensional reduction. For this reason, it is important to investigate the dimensional reduction.

In this paper, we will study a 0 dimensional model given by a dimensional reduction of Seiberg-Witten monopole equations derived from $\mathcal{N}=2$ supersymmetric $U(1)$ theory on N.C. $\mathbb{R}^4$. The equations are equivalent to the ADHM equations and the Dirac equation reduced to the 0 dimension. The equations are also equivalent to the dimensional reduction of non-Abelian $U(N)$ Seiberg-Witten monopole equations on commutative $\mathbb{R}^4$ at the large N limit. In this paper, we investigate both cases of finite N and infinite N. The finite N case is not only the toy model, but also the model that is possible to be implanted into the $N=\infty$ theory and the results are valid for some special cases of the $N=\infty$ model. We will find that the solutions of the equations are also interpreted as a configuration of the brane antibrane system. The theory has global symmetries under torus actions originated in space rotations and gauge symmetries. The torus actions define their fixed point equations. We will investigate the fixed point equations and the dimensional reduction of the Seiberg-Witten monopole equations. We will show that the Dirac equation is trivial when the fixed point equations and the ADHM equations are satisfied. For the finite N case, it is known that solutions satisfying the fixed point equations and the ADHM equations are isolated and classified by the Young diagrams.[49] We will give a new proof of this statement by solving the ADHM equations and the fixed point equations concretely and by giving a graphical interpretation of the field components and these equations.

Here is the organization of this paper. In Sec. II, we review the $\mathcal{N}=2$ supersymmetric gauge theory on $\mathbb{R}^4$ and N.C. $\mathbb{R}^4$ with a hypermultiplet. In Sec. III, a *D*-brane interpretation is discussed. In Sec. IV, we deform a BRS transformation defined as a topological twist of supersymmetric transformation by using the global symmetries of the theory. In Sec. V, we solve the Seiberg-Witten monopole equations reduced to a 0 dimension and the fixed point equations, and show our main claims. That is to say we show that the dimensional reduced Seiberg-Witten equations and fixed point equations of the torus action are equivalent to just the ADHM equations with the fixed point equations. We also give a new proof of the statement that solutions of the equations are localized and they are classified by Young diagrams. In Sec. VI, we briefly comment on the localization theorem. Section VII is a summary of this paper.

II. $\mathcal{N}=2$ SUPERSYMMETRIC $U(1)$ THEORY ON N.C. $\mathbb{R}^4$

In this section we review $\mathcal{N}=2$ supersymmetric theory and its topological twist on $\mathbb{R}^4$ and N.C. $\mathbb{R}^4$. We consider the case with a hypermultiplet.[50–54] For conventions in this paper, see Appendix A.

At first, we set up the model of the $\mathcal{N}=2$ supersymmetric theory on $\mathbb{R}^4$. $SO(4)$ spacetime rotation of four dimensional Euclidean space is locally equivalent to $SU(2)_L \otimes SU(2)_R$. $\mathcal{N}=2$ supersymmetric theories have $SU(2)_I$ R symmetry. The supersymmetry generators $Q_{\alpha i}$, $\bar{Q}_{\dot{\alpha} i}$ have indices $i=1,2$ for the R symmetry. $\mathcal{N}=2$ supersymmetric theories on $\mathbb{R}^4$ have the following symmetry:

$$H = SU(2)_L \otimes SU(2)_R \otimes SU(2)_I. \tag{1}$$

The supersymmetric gauge multiplet is given by

$$\begin{matrix} & A_\mu & \\ \psi^1 & & \psi^2. \\ & \phi & \end{matrix} \tag{2}$$

Here ψ_1 and ψ_2 are Weyl spinors. We denote $\bar{\psi}_1$ and $\bar{\psi}_2$ as their CPT conjugate. ϕ is a scalar field. We denote $\bar{\phi}$ as its complex conjugate. Their quantum number of H are assigned as

$$\psi^1 = (1/2,0,1/2), \quad \psi^2 = (1/2,0,1/2), \quad \phi = (0,0,0),$$

$$\bar{\psi}^1 = (0,1/2,1/2), \quad \bar{\psi}^2 = (0,1/2,1/2), \quad \bar{\phi} = (0,0,0). \tag{3}$$

The action functional is given by

$$L = -\frac{1}{4}F^a_{\mu\nu}F_a^{\mu\nu} - i\bar{\psi}^a_{\dot{\alpha}i}\,\bar{\sigma}^{\mu\dot{\alpha}\alpha}\,D_\mu\psi_{\alpha a}{}^i - D_\mu\bar{\phi}^a\,D^\mu\phi_a \tag{4}$$

$$-\frac{i}{\sqrt{2}}\psi^{\alpha ia}[\bar{\phi},\psi_{\alpha i}]_a - \frac{i}{\sqrt{2}}\bar{\psi}_{\dot{\alpha}}{}^{ia}[\phi,\bar{\psi}^{\dot{\alpha}}{}_i]_a - \frac{1}{2}[\bar{\phi},\phi]^2. \tag{5}$$

The supersymmetric transformation with parameter ξ and $\bar{\xi}$ are written as

$$\delta A_\mu = i\xi^{\alpha i}\sigma_{\mu\alpha\dot{\alpha}}\bar{\psi}^{\dot{\alpha}}{}_i - i\psi^{\alpha i}\sigma_{\mu\alpha\dot{\alpha}}\bar{\xi}^{\dot{\alpha}}{}_i,$$

$$\delta\psi_\alpha{}^i = \sigma_\alpha^{\mu\nu\beta}\xi_\beta{}^i F_{\mu\nu} + \sqrt{2}i\sigma^\mu_{\alpha\dot{\alpha}}\,D_\mu\phi\bar{\xi}^{\dot{\alpha}i} + [\phi,\bar{\phi}]\xi_\alpha{}^i,$$

$$\delta\bar{\psi}_{\dot{\alpha}i} = -\bar{\xi}_{\dot{\beta}i}\bar{\sigma}^{\mu\nu\dot{\beta}}_{\dot{\alpha}}F_{\mu\nu} + \sqrt{2}i\xi^{\alpha i}\sigma^\mu_{\alpha\dot{\alpha}}\,D_\mu\bar{\phi} - [\phi,\bar{\phi}]\bar{\xi}_{\dot{\alpha}i},$$

$$\delta\phi = \sqrt{2}\xi^{\alpha i}\psi_{\alpha i},$$

$$\delta\bar{\phi} = \sqrt{2}\bar{\xi}^{\dot{\alpha}}_i\bar{\psi}_{\dot{\alpha}}{}^i. \tag{6}$$

To classify the solutions of BPS equations by equivariant cohomology, let us introduce a topological twist here.[55,56] We use a diagonal subgroup $SU(2)_{R'}$ in $SU(2)_R \otimes SU(2)_I$ of H. We redefine the space time rotation group by

$$K' := SU(2)_L \otimes SU(2)_{R'}. \tag{7}$$

Then combinations of spinors whose quantum number of H are $(1/2,0,1/2)\oplus(0,1/2,1/2)$ have quantum number $(1/2,1/2)\oplus(0,1)\oplus(0,0)$ of K'. Particularly $(0,0)$ is scalar and $Q=\epsilon^{\dot{\alpha}i}\bar{Q}_{\dot{\alpha}i}$ is a BRS operator. Fermionic fields are similarly topological twisted as $\psi^i(\frac{1}{2},0,\frac{1}{2}) \to \psi_\mu(\frac{1}{2},\frac{1}{2})$ and $\bar{\psi}^i(0,\frac{1}{2},\frac{1}{2}) \to \chi_{\mu\nu}(0,1)\oplus\eta(0,0)$. BRS transformations are given as

$$\hat{\delta}A_\mu = i\psi_\mu, \quad \hat{\delta}\psi_\mu = -D_\mu\phi, \quad \hat{\delta}\phi = 0,$$

$$\hat{\delta}\chi_{\mu\nu} = H_{\mu\nu}, \quad \hat{\delta}\bar{\phi} = i\eta,$$

$$\hat{\delta}H_{\mu\nu} = i[\phi, \chi_{\mu\nu}], \quad \hat{\delta}\eta = [\phi, \bar{\phi}]. \tag{8}$$

Here we introduce auxiliary field $H_{\mu\nu}$.

As a next step, let us introduce hypermultiplets. The $\mathcal{N}=2$ hypermultiplet consists of two Weyl fermions λ_q and $\lambda_{\tilde{q}}^{\dagger}$ and two complex scalar bosons, q and $\tilde{q}^{\dagger}$,

$$\begin{matrix} & \lambda_q & \\ q & & \tilde{q}^{\dagger}. \\ & \lambda_{\tilde{q}}^{\dagger} & \end{matrix}$$

The definition of the symbol † is seen in Appendix A. Their supersymmetric transformations are given by

$$\begin{aligned} \delta q^i &= -\sqrt{2}\xi^{\alpha i}\lambda_{q\alpha} + \sqrt{2}\bar{\xi}_{\dot{\alpha}}{}^{i}\bar{\lambda}_{\tilde{q}}^{\dot{\alpha}}, \\ \delta\lambda_{q\alpha} &= -\sqrt{2}i\sigma^{\mu}_{\alpha\dot{\alpha}} D_{\mu} q^i \bar{\xi}^{\dot{\alpha}}{}_{i} - 2T_a q^i \bar{\phi}^a \xi_{\alpha i}, \\ \delta\bar{\lambda}_{\tilde{q}}^{\dot{\alpha}} &= -\sqrt{2}i\bar{\sigma}^{\mu\dot{\alpha}\alpha} D_{\mu} q^i \xi_{\alpha i} + 2T_a q^i \phi^a \bar{\xi}^{\dot{\alpha}}{}_{i}, \end{aligned} \tag{9}$$

where T_a is a generator of the gauge group. In the following, we consider the case that representation of the gauge group of the hypermultiplet is fundamental representation. After topological twisting, BRS transformations are given by

$$\begin{aligned} &\hat{\delta}q^{\dot{\alpha}} = \psi_q^{\dot{\alpha}}, \quad \hat{\delta}q_{\dot{\alpha}}^{\dagger} = \psi_{q\dot{\alpha}}^{\dagger}, \\ &\hat{\delta}\psi_q^{\dot{\alpha}} = -i\phi^a T_a q^{\dot{\alpha}}, \quad \hat{\delta}\psi_{q\dot{\alpha}}^{\dagger} = iq_{\dot{\alpha}}^{\dagger}\phi^a T_a, \\ &\hat{\delta}\chi_{q\alpha} = H_{q\alpha}, \quad \hat{\delta}\chi_q^{\dagger\alpha} = H_q^{\dagger\alpha} \\ &\hat{\delta}H_{q\alpha} = -i\phi^a T_a \chi_{q\alpha}, \quad \hat{\delta}H_q^{\dagger\alpha} = i\chi_q^{\dagger\alpha}\phi^a T_a, \end{aligned} \tag{10}$$

where fields are rescaled, $\phi \to (i/2\sqrt{2})\phi$, $\sqrt{2}\bar{\lambda}_q^{\dot{\alpha}} \to \bar{\lambda}_q^{\dot{\alpha}}$, $\sqrt{2}\bar{\lambda}_{q\dot{\alpha}} \to \bar{\lambda}_{q\dot{\alpha}}$, and also auxiliary field $H_{q\alpha}$ is introduced. After topological twisting, we rename the fermions as $\lambda_q \to \chi_q$ and $\bar{\lambda}_q \to \psi_q$.

Using these field contents, let us construct the action of Seiberg-Witten theory. The action with fundamental hypermultiplet terms are defined by

$$S = k - \hat{\delta}\Psi \tag{11}$$

where k is an instanton number,

$$k = \frac{1}{8\pi^2}\int \mathrm{Tr}(F_A \wedge F_A), \tag{12}$$

and Ψ is a gauge fermion;

$$\begin{aligned} \Psi = &-\chi_+^{\mu\nu a}\{H_{+\mu\nu}^a - s_{+\mu\nu}^a\} - \chi_q^{\dagger\alpha}\{H_{q\alpha} - s_{\alpha}\} - \{H_q^{\dagger\alpha} - s^{\dagger\alpha}\}\chi_{q\alpha} \\ &+ i[\phi, \bar{\phi}]^a \eta^a + D_{\mu}\bar{\phi}^a \psi^{\mu a} - (-iq_{\dot{\alpha}}^{\dagger}\bar{\phi})\psi_q^{\dot{\alpha}} - \psi_{q\dot{\alpha}}^{\dagger}(i\bar{\phi}q^{\dot{\alpha}}). \end{aligned} \tag{13}$$

Here

$$s^{\mu\nu}(A, q, q^{\dagger}) = F_a^{+\mu\nu} + q^{\dagger}\bar{\sigma}^{\mu\nu}T_a q,$$

$$s^{\alpha}(A,q) = \sigma^{\mu} D_{\mu} q = \not{D} q. \tag{14}$$

After integration of the auxiliary fields $H_{+\mu\nu}$ and H_q, the bosonic action are given as

$$S_B = \int d^4x \sqrt{g} \left[\frac{1}{4} |s^{\mu\nu}|^2 + \frac{1}{2} |s^{\alpha}|^2 \right] + \cdots . \tag{15}$$

Notice that when the gauge group is $U(1)$ and the theory is defined on simple type commutative manifolds, we get the Seiberg-Witten invariants as the partition function of this model.[4,5,50,51] From (15) we get the BPS equations,

$$s^{\mu\nu}(A,q,q^{\dagger}) = 0, \quad s^{\alpha}(A,q) = 0, \tag{16}$$

which is known as the non-Abelian Seiberg-Witten monopole equations.

In the following, we investigate some properties of $\mathcal{N}=2$ supersymmetric gauge theory on N.C. $\mathbb{R}^4$ whose noncommutativity is defined as

$$[x^{\mu}, x^{\nu}] = i\theta^{\mu\nu}, \tag{17}$$

where the $\theta^{\mu\nu}$ is an element of an antisymmetric matrix and called the N.C. parameter. For simplicity, we take

$$(\theta^{\mu\nu}) = \begin{pmatrix} 0 & \theta^1 & 0 & 0 \\ -\theta^1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \theta^2 \\ 0 & 0 & -\theta^2 & 0 \end{pmatrix}. \tag{18}$$

In the following, we only use operator formalisms to describe the N.C. field theory; therefore the fields are operators acting on the Hilbert space $\mathcal{H}$. Then differential operators ∂_{μ} are expressed by using commutation brackets $-i\theta^{-1}_{\mu\nu}[x^{\nu}, *] \equiv [\hat{\partial}_{\mu}, *]$ and $\int d^{2D}x$ is replaced with $\det(\theta)^{1/2}\mathrm{Tr}_{\mathcal{H}}$.

When we consider only the case of N.C. $\mathbb{R}^4$, field theories are expressed by the Fock space formalism. (See the appendix in Ref. 45.) In the Fock space representation, fields are expressed as $A_{\mu} = \Sigma A^{n_1 n_2}_{\mu_{m_1 m_2}} |n_1, n_2\rangle\langle m_1, m_2|$, $\psi_{\mu} = \Sigma \psi^{n_1 n_2}_{\mu_{m_1 m_2}} |n_1, n_2\rangle\langle m_1, m_2|$, etc. Therefore, the above BRS transformations are expressed as

$$\hat{\delta} A^{n_1 n_2}_{\mu_{m_1 m_2}} = \psi^{n_1 n_2}_{\mu_{m_1 m_2}}, \quad \hat{\delta} \psi^{n_1 n_2}_{\mu_{m_1 m_2}} = (D_{\mu}\phi)^{n_1 n_2}_{m_1 m_2}, \ldots , \tag{19}$$

where the covariant derivative is defined by $D_{\mu} * := [\hat{\partial}_{\mu} + iA_{\mu}, *]$ with $\hat{\partial}_{\mu} := -i\theta^{-1}_{\mu\nu} x^{\nu}$. The action functional is given by

$$S = \mathrm{Tr}_{\mathcal{H}} L(A_{\mu}, \ldots ; \hat{\partial}_{z_i}, \hat{\partial}_{\bar{z}_i}) = \mathrm{Tr}_{\mathcal{H}}\ \mathrm{tr}\ \hat{\delta}\Psi . \tag{20}$$

Let us change the dynamical variables as

$$A_\mu \to \frac{1}{\sqrt{\theta}}\tilde{A}_\mu, \quad \psi_\mu \to \frac{1}{\sqrt{\theta}}\tilde{\psi}_\mu, \quad \bar{\phi} \to \frac{1}{\theta}\tilde{\bar{\phi}}, \quad \eta \to \frac{1}{\theta}\tilde{\eta}, \quad q \to \frac{1}{\sqrt{\theta}}\tilde{q}, \quad q^\dagger \to \frac{1}{\sqrt{\theta}}\tilde{q}^\dagger$$

$$\chi^+_{\mu\nu} \to \frac{1}{\theta}\tilde{\chi}^+_{\mu\nu}, \quad H^+_{\mu\nu} \to \frac{1}{\theta}\tilde{H}^+_{\mu\nu}, \quad \phi \to \tilde{\phi} \quad \psi_q \to \frac{1}{\sqrt{\theta}}\tilde{\psi}_q, \quad \psi^\dagger_q \to \frac{1}{\sqrt{\theta}}\tilde{\psi}^\dagger_q, \tag{21}$$

$$\chi_q \to \frac{1}{\theta}\tilde{\chi}_q, \quad \chi^\dagger_q \to \frac{1}{\theta}\tilde{\chi}^\dagger_q, \quad H_q \to \frac{1}{\theta}\tilde{H}_q, \quad H^\dagger_q \to \frac{1}{\theta}\tilde{H}^\dagger_q.$$

Note that this changing does not cause nontrivial Jacobian from the path integral measure because of the BRS symmetry. Then, the action is rewritten as

$$S \to \frac{1}{\theta^2}\tilde{S}, \quad L(A_\mu, \ldots; \hat{\partial}_{z_i}, \hat{\partial}_{\bar{z}_i}) \to \frac{1}{\theta^2}L(\tilde{A}_\mu, \ldots; -a^\dagger_i, a_i). \tag{22}$$

Here the action on the left hand side (lhs) depends on θ because the derivative is given by $\partial_{z_i} = -\sqrt{\theta^{-1}}[a^\dagger_i,]$, and so on. In contrast, the action $\tilde{S}$ on the rhs does not depend on θ because all θ parameters are factorized out. Using the BRS symmetry, it is proved that the partition function is invariant under the deformation of θ, because $\delta_\theta Z = -2(\delta\theta)\theta^{-3}\langle\tilde{S}\rangle = 0$. As discussed in Ref. 45, the partition function of this theory is possible to be determined by using a lower dimension theory that is given by dimensional reduction. Therefore, the investigation of the dimensional reduction of the theories is important.

The dimensional reduction of Seiberg-Witten monopole equations (14) are expressed as

$$P^{\mu\nu\rho\tau}_+[A_\rho, A_\tau] + q\bar{\sigma}^{\mu\nu}q^\dagger = 0, \tag{23}$$

$$\sigma^\mu A_\mu q = 0, \tag{24}$$

where $P^{\mu\nu\rho\tau}_+$ is a self-dual projection operator. These expressions are valid for the dimensional reduction of the non-Abelian theory on commutative $\mathbb{R}^4$. Using $q_+ := (q_1 + q_2)/\sqrt{2}$ and $q_- := (q_1 - q_2)/\sqrt{2}$, if we start from the $U(1)$ theory on N.C.$\mathbb{R}^4$, the equation (23) is rewritten as ADHM equations:

$$[A_{z_1}, A^\dagger_{z_1}] + [A_{z_2}, A^\dagger_{z_2}] + q_- q_-^{*T} - q_+ q_+^{*T} = 0,$$

$$[A_{z_1}, A_{z_2}] + q_- q_+^{*T} = 0. \tag{25}$$

Note that these operators in (25) are expressed by infinite dimensional matrices and the ADHM equations correspond to the instanton of the $U(N)$ gauge group with instanton number N at the large N limit. We consider the finite N situation in the next section.

III. *D*-BRANE INTERPRETATION

In this paper, we study the details of the solution of (23) and (24). On the N.C. $\mathbb{R}^4$ the fields appearing in (23) and (24) are infinite dimensional matrices acting on Hilbert space. But the equations are important even if the dimension of the matrix is finite, because there is a corresponding physical model. In this section, we consider the correspondence between Seiberg-Witten monopole equations, the D-brane picture, and (23), (24).[57]

At first, we construct the physical model by using the similar manner of the article.[57] (See also Refs. 58–65.)

The generalized second order effective action of an N $D3$-brane N $\bar{D}3$-brane system without topological terms are given by

$$\int \mathrm{tr}\left\{\frac{1}{4}F^{(N)}_{\mu\nu}F^{(N)\mu\nu}+\frac{1}{4}F^{(\bar{N})}_{\mu\nu}F^{(\bar{N})\mu\nu}+|D^{\mu}\phi|^2+\frac{1}{2}(\tau^2-\phi\bar{\phi})^2\right\}. \tag{26}$$

Here the $F^{(N)}_{\mu\nu}$ and $F^{(\bar{N})}_{\mu\nu}$ are the curvature of the $A^{(N)}$ and $A^{(\bar{N})}$, respectively, where $A^{(N)}$ and $A^{(\bar{N})}$ correspond to open strings attached on the $D3$ brane and the $\bar{D}3$ brane. Up to topological terms, we can rewrite this action as

$$\int \mathrm{tr}\left\{\frac{1}{4}F^{(\bar{N})}_{\mu\nu}F^{(\bar{N})\mu\nu}+\frac{1}{2}|F^{(N)}_{z^1\bar{z}^1}+F^{(N)}_{z^2\bar{z}^2}+(\phi\bar{\phi}-\tau^2)|^2+8|F_{z^1z^2}|^2+2|D_{\bar{z}_1}\phi|^2+2|D_{\bar{z}_2}\phi|^2\right\}. \tag{27}$$

From this action, considering the case of $A^{(\bar{N})}_{\mu}=0$, stationary points are given by

$$F^{(N)}_{z^1\bar{z}^1}+F^{(N)}_{z^2\bar{z}^2}+q_-q_-^{*T}=\zeta, \tag{28}$$

$$F^{(N)}_{z^1z^2}=0, \tag{29}$$

$$D_{\bar{z}^1}q_-=0, \tag{30}$$

$$D_{\bar{z}^2}q_-=0, \tag{31}$$

where we replace ϕ by q_- and τ^2 by ζ. Then, this is the Seiberg-Witten monopole equations with $q_+=0$ condition and background constant field ζ. (See also the next section.) This case corresponds to the $\zeta>0$, as we will see in Sec. V. Note that q_- can be regarded as a complex scalar field when we consider the $\mathbb{R}^4$ case.

The solution of (23) and (24) of the finite matrix model is realized as some $D3$-$\bar{D}3$ configuration.

IV. DEFORMED BRS TRANSFORMATION

In this section, we will investigate the symmetry of the dimension reduction of (20) to 0 dimension, and deform the BRS symmetry as $\mathcal{G}\otimes T^{N+2}$ equivariant derivative, where $\mathcal{G}$ is the gauge transformation group of $U(N)$ and T^{N+2} is the torus action, in order to derive the fixed point equations. Note that the $U(N)$ symmetry is caused from the $U(1)$ symmetry if we consider the N.C. theory. As explained in Sec. II, the action functional is defined by infinite dimensional matrices when we start from N.C. theories; then N.C.$U(1)$ gauge symmetry is expressed by $U(\infty)$ symmetry. For simplicity, in some discussions of this paper, we restrict our analysis to the finite dimensional, $N\times N$, matrix case. (Only the proof of Theorem 3 in Sec. V and the calculations of the partition function of a toy model in Sec. VI are based on discussions of finite N.) All of the fields contents, A_μ, q, etc., are given by $N\times N$ matrices. Then the $U(\infty)$ symmetry is also truncated to $U(N)$. From the viewpoint of N.C. field theory, there might be another type of solutions that is not studied in this paper, and the following analysis might not be completed. On the other hand, as discussed in the previous section, the finite $N\times N$ theory has a $D3$-$\bar{D}3$ brane interpretation; then it has physical applications.

The path integral for cohomological field theories reduced to the integral over the moduli space of vacuum. In our case, the moduli space is defined by solutions of (23) and (24). As demonstrated in Ref. 7, the localization theorem is a powerful tool for path integrals of cohomological field theories. The localization theorem is valid when a theory under consideration has symmetries under some group actions, and the group actions have isolated fixed points. (For the localization theorem, also see Sec. VI.) Therefore, to investigate solutions of the fixed point equation is important. This is our main subject in this paper.

Adding to the $U(N)$ gauge symmetry and the Lorentz symmetry $SO(4)=SU(2)_L\otimes SU(2)_R$, the action reduced to 0 dimension has the next extra unitary symmetry, denoted by $\tilde{U}(N)$,

$$\delta^{\tilde{U}(N)} q_{\dot{\alpha}} = i q_{\dot{\alpha}} b, \tag{32}$$

where b is a generator of $\tilde{U}(N)$. When we consider the case that $q_{\dot{\alpha}}$ is a $N \times k$ matrix in the next section, then the symmetry becomes $\tilde{U}(k)$;

$$\delta^{\tilde{U}(k)} q_{\dot{\alpha}} = i q_{\dot{\alpha}} b, \quad b \in \tilde{u}(k). \tag{33}$$

Recall that q and $q^\dagger$ are fundamental representations of the gauge group. The gauge transformation of q is defined by left action of the $U(N)$. Notice that if we define the gauge transformation by using right action, we can define another gauge symmetry with the corresponding gauge field. We do not introduce this gauge field; then the symmetry appears only after the dimensional reduction. This is the origin of $\tilde{U}(N)$.

Now we use the Abelian subgroup $U(1)^2 \otimes U(1)^N$ of $SO(4) \otimes \tilde{U}(N)$. That is, we consider the following symmetry of the action:

$$\delta^{U(1)^2 \otimes U(1)^N} A_{z_i} = -i \epsilon_i A_{z_i}, \tag{34}$$

$$\delta^{U(1)^2 \otimes U(1)^N} q_{\dot{\alpha}} = +i M_{R\dot{\alpha}}{}^{\dot{\beta}} q_{\dot{\beta}} + i q_{\dot{\alpha}} b, \tag{35}$$

where $b = \mathrm{diag}.(b_1, \cdots, b_N)$ is a generator of an Abelian subgroup $U(1)^N$ of $\tilde{U}(N)$, and $\epsilon_i (i = 1, 2)$ is a generator of an Abelian subgroup $U(1)^2$ of $SO(4)$, defined by

$$\delta A_\mu = M_\mu{}^\nu A_\nu, \quad M_\mu{}^\nu = \begin{pmatrix} 0 & -\epsilon_1 & & \\ +\epsilon_1 & 0 & & \\ & & 0 & -\epsilon_2 \\ & & -\epsilon_2 & 0 \end{pmatrix}. \tag{36}$$

Also, $M_{R\dot{\alpha}}{}^{\dot{\beta}}$ is the generator of $U(1) \subset SU(2)_R$,

$$M_{R\dot{\alpha}}{}^{\dot{\beta}} = \begin{pmatrix} 0 & \epsilon_+ \\ \epsilon_+ & 0 \end{pmatrix}, \quad \epsilon_+ = \frac{\epsilon_1 + \epsilon_2}{2}. \tag{37}$$

By using $U(1)^2 \otimes U(1)^N$, let us deform the BRS symmetry from $\hat{\delta}$ to $\tilde{\delta}$. We define the deformation by replacing $\hat{\delta}^2 = \delta^{U(N)\text{gauge}}_{(-\phi)}$ to

$$\tilde{\delta}^2 = \delta^{U(N)\text{gauge}}_{(-\phi)} + \delta^{U(1)^N}_{(b)} + \delta^{U(1)^2}_{(\epsilon_1, \epsilon_2)}. \tag{38}$$

Here $\delta^G_{(\Delta)}$ is a gauge transformation operator with the group G and the transformation parameter Δ. Then, for ψ_{z_i} and $\psi_{q\dot{\alpha}}$, the BRS transformation rules are given by

$$\tilde{\delta}^2 A_{z_i} = \tilde{\delta} \psi_{z_i} = i[A_{z_i}, \phi] - i \epsilon_i A_{z_i}, \tag{39}$$

$$\tilde{\delta}^2 q_{\dot{\alpha}} = \tilde{\delta} \psi_{q\dot{\alpha}} = -i \phi q_{\dot{\alpha}} + M_{R\dot{\alpha}}{}^{\dot{\beta}} q_{\dot{\beta}} + i q_{\dot{\alpha}} b, \tag{40}$$

$$\tilde{\delta}^2 q^{\dagger \dot{\alpha}} = \tilde{\delta} \psi_q{}^{\dagger \dot{\alpha}} = q^{\dagger \dot{\alpha}} i \phi - M_{R\dot{\beta}}{}^{\dot{\alpha}} q^{\dagger \dot{\beta}} - i b q^{\dagger \dot{\alpha}}. \tag{41}$$

Now we list the equations, the solutions of which we will investigate. Some of them are the equations of motion, often called BPS equations. They are the same as (23) or (25), (24). However, we take some deformation of them, to remove singular solutions. We introduce a nonzero number ζ, and take

$$i([A_{z_1},A_{\bar{z}_1}]+[A_{z_2},A_{\bar{z}_2}])+q(\bar{\sigma}_{z_1\bar{z}_1}+\bar{\sigma}_{z_2\bar{z}_2})q^\dagger=i\zeta, \tag{42}$$

$$i[A_{z_1},A_{z_2}]+q\bar{\sigma}_{z_1z_2}q^\dagger=0, \tag{43}$$

$$(A_{z_1}\sigma^{z_1}+A_{\bar{z}_1}\sigma^{\bar{z}_1}+A_{z_2}\sigma^{z_2}+A_{\bar{z}_2}\sigma^{\bar{z}_2})q=0. \tag{44}$$

Here, (42), (43) are realized by the redefinition of $s^{\mu\nu}(A,q,q^\dagger)$,

$$s^{\mu\nu}(A,q,q^\dagger)\to F^{+\mu\nu}+q\bar{\sigma}^{\mu\nu}q^\dagger-\zeta^+_{\mu\nu},$$

$$\zeta_{z_1\bar{z}_1}+\zeta_{z_2\bar{z}_2}=i\zeta,\quad \zeta_{z_1z_2}=0. \tag{45}$$

This constant ζ is considered as a background field and we define its BRS transformation by $\tilde{\delta}\zeta=0$. Then, we find that all of the above discussions in previous sections are valid, although we add this background field. For later use, we rewrite them into

$$[A_{z_1},A_{\bar{z}_1}]+[A_{z_2},A_{\bar{z}_2}]-(q_{\dot{2}}q_{\dot{1}}^{*T}+q_{\dot{1}}q_{\dot{2}}^{*T})=\zeta, \tag{46}$$

$$[A_{z_1},A_{z_2}]+\frac{1}{2}(q_{\dot{1}}q_{\dot{1}}^{*T}-q_{\dot{2}}q_{\dot{2}}^{*T})+\frac{1}{2}(q_{\dot{1}}q_{\dot{2}}^{*T}-q_{\dot{2}}q_{\dot{1}}^{*T})=0, \tag{47}$$

$$(A_{\bar{z}_1}-A_{z_2})q_{\dot{2}}-(A_{\bar{z}_1}+A_{z_2})q_{\dot{1}}=0, \tag{48}$$

$$(A_{\bar{z}_2}+A_{z_1})q_{\dot{2}}-(A_{\bar{z}_2}-A_{z_1})q_{\dot{1}}=0. \tag{49}$$

The rest of the equations to be investigated are the fixed point equations of the deformed BRS transformation (39)–(41). They are given by

$$i[A_{z_i},\phi]-i\epsilon_iA_{z_i}=0, \tag{50}$$

$$-i\phi q_{\dot{\alpha}}+M^{\dot{\beta}}_{R\dot{\alpha}}q_{\dot{\beta}}+iq_{\dot{\alpha}}b=0. \tag{51}$$

In the next section, we will investigate solutions of (42), (43), (44), (50), (51), and will show that they have isolated solutions. This fact guarantees that the localization theorem is valid to our case.

V. SOLUTIONS OF (42), (43), (44), (50), (51)

In this section, we solve (42), (43), (44), (50), (51), and show that these equations have only isolated solutions, and the solutions are expressed by the Young diagrams. Notice that our analysis is also valid to a case where q_α's are $N\times k,(k\neq N)$ matrices, though we will treat q_α as $N\times N$ matrices in this section. If we take $q_{\dot{\alpha}}$ to be $N\times k$, $q^{*T}_{\dot{\alpha}}$ to be $k\times N$ and $b\in u(k)$, our proof in this section includes a new proof for Proposition 5.6. in Ref. 49.

First of all, we diagonalize ϕ by using the $U(N)$ gauge symmetry,

$$\phi=\mathrm{diag}(\phi_1,\phi_2,\ldots,\phi_N). \tag{52}$$

Next we tackle (50) and (51). From (50) we see immediately that if and only if

$$\phi_J-\phi_I=\epsilon_i, \tag{53}$$

A_{z_iIJ} could be nonzero,

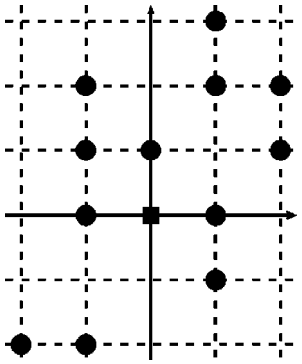

FIG. 1. $P_{[\hat{x_I}]}$.

$$A_{z_i IJ} \neq 0. \tag{54}$$

In this section, we use "$\neq 0$" as not "nonzero" but "not always zero." Also, from (51) we see that if and only if

$$\phi_I = b_J \pm \epsilon_+, \tag{55}$$

$q_{\dot{1}IJ}$ and $q_{\dot{2}IJ}$ could be nonzero,

$$q_{\dot{1}IJ} = \pm q_{\dot{2}IJ} \neq 0. \tag{56}$$

Notice $q_{\dot{1}IJ}$ and $q_{\dot{2}IJ}$ are not independent from one another.

These observations lead us to the following proposition.

Lemma 1: If (42), (50), (51) *have a solution, then* ϕ_I *takes any of* $\varphi^{(n_1,n_2)}_{[x_I^\wedge]}$, *given by*

$$\varphi^{(n_1,n_2)}_{[x_I^\wedge]} = x_I^\wedge + n_1\epsilon_1 + n_2\epsilon_2, \quad n_1, n_2 \in \mathbb{Z} \tag{57}$$

where

$$x_I^\wedge \in \{b_I^{(-)} \in \mathbb{R}, I = 1, \ldots, N | b_I^{(-)} := b_I - \epsilon_+\}, \tag{58}$$

or

$$x_I^\wedge \in \{y_{\bar{I}}^- \in \mathbb{R}, \bar{I} = 1, \ldots, \bar{N} | \forall I, n_1, n_2, y_{\bar{I}}^- \neq b_I^{(-)} + n_1\epsilon_1 + n_2\epsilon_2\}. \tag{59}$$

(proof)

Suppose that ϕ_I does not take any of $\varphi^{(n_1,n_2)}_{[x_I^\wedge]}$ given above. This implies that $\exists I, \forall J, q_{\dot{\alpha}IJ} = 0, A_{z_i IJ} = A_{z_i JI} = 0$. Consider (42). It is easy to see that the (I,I) component of the lhs of (42) is 0, whereas the (I,I) component of the rhs of (42) is $i\zeta \neq 0$. Therefore no solution to (42), (50), (51) is allowed. ■

For a set of all $\{\varphi^{(n_1,n_2)}_{[x_I^\wedge]} | x_I^\wedge$ is given $\}$, assign a graph $P_{[x_I^\wedge]}$. See Fig. 1. In Fig. 1, the origin, denoted by the black square, corresponds to the eigenvalue $\varphi^{(0,0)}_{[x_I^\wedge]} = x_I^\wedge$, and other lattice points (n_1, n_2), denoted by black dots, correspond to eigenvalues $\varphi^{(n_1,n_2)}_{[x_I^\wedge]}$. For given a set of $P_{[x_I^\wedge]}$, ϕ is written as

$$\phi = \bigoplus_I \begin{pmatrix} \varphi^{(n_1,n_2)}_{[b_I^{(-)}]}\mathbf{1}_{N^{(n_1,n_2)}_{[b_I^{(-)}]}} & & & \\ & \varphi^{(n_1',n_2')}_{[b_I^{(-)}]}\mathbf{1}_{N^{(n_1',n_2')}_{[b_I^{(-)}]}} & & \\ & & \varphi^{(n_1'',n_2'')}_{[b_I^{(-)}]}\mathbf{1}_{N^{(n_1'',n_2'')}_{[b_I^{(-)}]}} & \\ & & & \ddots \end{pmatrix}, \tag{60}$$

$$\bigoplus_{\bar{I}} \begin{pmatrix} \varphi^{(n_1,n_2)}_{[y_{\bar{I}}]}\mathbf{1}_{N^{(n_1,n_2)}_{[y_{\bar{I}}]}} & & & \\ & \varphi^{(n_1',n_2')}_{[y_{\bar{I}}]}\mathbf{1}_{N^{(n_1',n_2')}_{[y_{\bar{I}}]}} & & \\ & & \varphi^{(n_1'',n_2'')}_{[y_{\bar{I}}]}\mathbf{1}_{N^{(n_1'',n_2'')}_{[y_{\bar{I}}]}} & \\ & & & \ddots \end{pmatrix}. \tag{61}$$

In each Ith or $\bar{I}$th block, we suppose that eigenvalues $\varphi^{(n_1,n_2)}_{[b_I^{(-)}]}$ or $\varphi^{(n_1,n_2)}_{[y_{\bar{I}}]}$ are arranged by order,

$$\varphi^{(n_1,n_2)}_{[b_I^{(-)}]} < \varphi^{(n_1',n_2')}_{[b_I^{(-)}]} < \varphi^{(n_1'',n_2'')}_{[b_I^{(-)}]} < \cdots,$$

$$\varphi^{(n_1,n_2)}_{[y_{\bar{I}}]} < \varphi^{(n_1',n_2')}_{[y_{\bar{I}}]} < \varphi^{(n_1'',n_2'')}_{[y_{\bar{I}}]} < \cdots. \tag{62}$$

The index I is mapped to the triad of indices $(\hat{I},(n_1,n_2))$,

$$I \mapsto (\hat{I},(n_1,n_2)). \tag{63}$$

We denote the degeneracy of $\varphi^{(n_1,n_2)}_{[x_{\hat{I}}]}$ as $N^{(n_1,n_2)}_{[x_{\hat{I}}]}$,

$$^{\#}\{\phi_I | \phi_I = \varphi^{(n_1,n_2)}_{[x_{\hat{I}}]}\} = N^{(n_1,n_2)}_{[x_{\hat{I}}]} \geq 0, \tag{64}$$

$$\sum_{\hat{I}} \sum_{(n_1,n_2)} N^{(n_1,n_2)}_{[x_{\hat{I}}]} = N. \tag{65}$$

A_{z_i} takes a similar block structure,

$$A_{z_i} = \bigoplus_I \begin{pmatrix} & \vdots & \\ \cdots & A_{z_i(I,(n_1,n_2)),(I,(m_1,m_2))} & \cdots \\ & \vdots & \end{pmatrix} \bigoplus_{\bar{I}} \begin{pmatrix} & \vdots & \\ \cdots & E_{z_i(\bar{I},(n_1,n_2)),(\bar{I},(m_1,m_2))} & \cdots \\ & \vdots & \end{pmatrix}, \tag{66}$$

where

$$A_{z_i(I,(n_1,n_2)),(I,(m_1,m_2))} \quad \text{is a } N^{(n_1,n_2)}_{[b_I^{(-)}]} \times N^{(m_1,m_2)}_{[b_I^{(-)}]} \text{ complex matrix},$$

and

$$E_{z_i(\bar{I},(n_1,n_2)),(\bar{I},(m_1,m_2))} \text{ is a } N^{(n_1,n_2)}_{[y_{\bar{I}}]} \times N^{(m_1,m_2)}_{[y_{\bar{I}}]} \text{ complex matrix}.$$

A nontrivial component of A_{z_1} appears in $\{(\hat{I},(n_1,n_2)),(\hat{I},(n_1-1,n_2))\}$th block and, that of A_{z_2} appears in $\{(\hat{I},(n_1,n_2)),(\hat{I},(n_1,n_2-1))\}$th block,

$$A_{z_1(I,(n_1,n_2)),(I,(n_1-1,n_2))} \neq 0, \quad E_{z_1(\bar{I},(n_1,n_2)),(\bar{I},(n_1-1,n_2))} \neq 0, \tag{67}$$

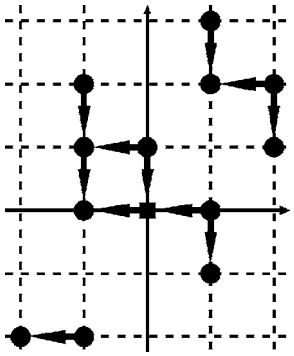

FIG. 2. $G_{[\hat{x}_{\hat{I}}]}$.

$$A_{z_2(I,(n_1,n_2)),(I,(n_1,n_2-1))} \neq 0, \quad E_{z_2(\bar{I},(n_1,n_2)),(\bar{I},(n_1,n_2-1))} \neq 0. \tag{68}$$

By adding left arrows connecting (n_1,n_2) and (n_1-1,n_2) and down arrows connecting (n_1,n_2) and (n_1,n_2-1) to the graph $P_{[x_{\hat{I}}]}$, we obtain a graph $G_{[x_{\hat{I}}]}$. For example, see Fig. 2. The left arrow corresponds to A_{z_1}'s nontrivial component, and the down arrow corresponds to A_{z_2}'s nontrivial component. Also, the nontrivial components of $q_{\dot{\alpha}}$ are

$$q_{\dot{1}(I,(0,0)),J} = -q_{\dot{2}(I,(0,0)),J} \neq 0, \quad \text{for } I,J, \text{ s.t. } \phi_I = b_J + \epsilon_+, \tag{69}$$

$$q_{\dot{1}(I,(1,1)),J} = +q_{\dot{2}(I,(1,1)),J} \neq 0, \quad \text{for } I,J, \text{ s.t. } \phi_I = b_J - \epsilon_+. \tag{70}$$

From (66), (69), (70), we obtain the next proposition.

Lemma 2: If ϕ_I takes any of $\varphi^{(n_1,n_2)}_{[y_{\bar{I}}]} = y_{\bar{I}} + n_1\epsilon_1 + n_2\epsilon_2$, then (42), (50), (51) have no solution.

(proof)

Suppose that some ϕ_I are given by

$$\phi_I = \varphi^{(n_1,n_2)}_{[y_{\bar{I}}]}. \tag{71}$$

Then, the lhs of (46), equivalent to (42), is given by the following:

$$\begin{aligned} \text{lhs of (46)} &= \sum_{i=1,2} [A_{z_i}, A_{\bar{z}_i}] - (q_{\dot{2}} q_{\dot{1}}^{*T} + q_{\dot{1}} q_{\dot{2}}^{*T}) \\ &= \begin{pmatrix} \oplus_I \sum_{i=1,2} [A^I_{z_i}, A^I_{\bar{z}_i}] - (q_{\dot{2}} q_{\dot{1}}^{*T} + q_{\dot{1}} q_{\dot{2}}^{*T}) & 0 \\ 0 & \oplus_{\bar{I}} \sum_{i=1,2} [E^{\bar{I}}_{z_i}, E^{\bar{I}}_{\bar{z}_i}] \end{pmatrix}, \end{aligned} \tag{72}$$

because the nontrivial components of $q_{\dot{\alpha}}$ are given by (69), (70). On the other hand, the rhs of (46) is proportional to a unit matrix,

$$\text{rhs of (46)} = \zeta \begin{pmatrix} \oplus_I \mathbf{1}^{I,I} & 0 \\ 0 & \oplus_{\bar{I}} \mathbf{1}^{\bar{I},\bar{I}} \end{pmatrix}. \tag{73}$$

The $(\bar{I},\bar{I})$ block of (72) is a traceless matrix, whereas the $(\bar{I},\bar{I})$ block of (73) has a nonzero trace. These are mutually exclusive. ■

When we consider the case of $N=\infty$, we cannot use the nature that the commutator is traceless; then this proof is not correct. But we can prove this statement even if $N=\infty$. Because, if $[E^{\bar{I}}_{z_i}, E^{\bar{I}}_{\bar{z}_i}]$ is not traceless, we can show that the curvature F does not converge to zero at infinity.

This means that if the set of the gauge fields is $\{A\,|\lim_{x\to\infty}|F(x)|=0\}$, then this theorem still holds. By the same reason, Theorem 1 in this section is valid for the $N=\infty$ case. That is why, all theorems in this section without Theorem 3 holds for the $N=\infty$ case.

Corollary 1: (42), (50), (51) *can have a solution, if and only if* ϕ *is given by*

$$\phi = \bigoplus_I \bigoplus_{(n_1,n_2)\in G_{[b_I^{(-)}]}} \varphi_{[b_I^{(-)}]}^{(n_1,n_2)} \mathbf{1}_{N_{[b_I^{(-)}]}^{(n_1,n_2)}}, \tag{74}$$

$$\varphi_{[b_I^{(-)}]}^{(n_1,n_2)} = b_I^{(-)} + n_1\epsilon_1 + n_2\epsilon_2, \tag{75}$$

and A_{z_i} *is given by*

$$A_{z_i} = \bigoplus_I A_{z_i}^I. \tag{76}$$

From now on, we suppose that the parameter ζ is a positive number,

$$\zeta > 0. \tag{77}$$

(If we assume $\zeta<0$, we have to change some statements in the following theorems, but essentially same theorems hold.) Then we obtain the next theorem.

Theorem 1: *Let* $G_{[b_I^{(-)}]}$ *be a graph defined from the eigenvalues* $\varphi_{[b_I^{(-)}]}^{(n_1,n_2)}$ *given by* (74). *Also let* ζ *be positive. The following three conditions are necessary for a solution of* (42), (50), and (51) *to exist.*

(1) $G_{[b_I^{(-)}]}$ *consists of one connected part.*
(2) $G_{[b_I^{(-)}]}$ *includes the origin* $(0,0)$.
(3) *All points* (n_1,n_2) *in* $G_{[b_I^{(-)}]}$ *must be in* $n_1\le 0, n_2\le 0$.

(proof)

First of all, notice that $A_{z_i}^I$ is a direct sum of upper triangle (block) matrices and $A_{\bar{z}_i}^I$ is of lower triangle (block) matrices [remember (62)],

$$A_{z_i}^I = \bigoplus_a A_{z_i}^{I(a)} = \bigoplus_a \begin{pmatrix} 0 & * & \cdots & * & * \\ 0 & 0 & \cdots & * & * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & * \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}, \tag{78}$$

$$A_{\bar{z}_i}^I = \bigoplus_a A_{\bar{z}_i}^{I(a)} = \bigoplus_a \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ * & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ * & * & \cdots & 0 & 0 \\ * & * & \cdots & * & 0 \end{pmatrix}, \tag{79}$$

where the index a labels connected diagrams $G_{[b_I^{(-)}]}^{(a)}$ in $G_{[b_I^{(-)}]}$. See Fig. 3. From (78) and (79), we obtain

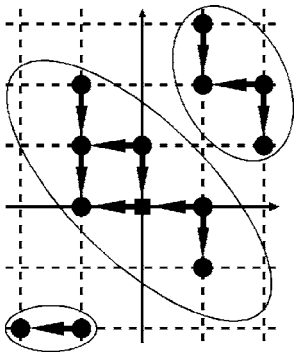

FIG. 3. $G_{[b_I^{(-)}]}$ consists of connected graphs $G^{(a)}_{[b_I^{(-)}]}$.

$$[A^{I(a)}_{z_i}, A^{I(a)}_{\bar{z}_i}] = \begin{pmatrix} M_{\min} & * & 0 \\ * & M_{\text{int}} & * \\ 0 & * & M_{\max} \end{pmatrix}, \tag{80}$$

where

$$M_{\min} = + \sum_{(m_1,m_2)} A^{I(a)}_{z_i(n_1^{\min},n_2^{\min}),(m_1,m_2)} A^{I(a)}_{\bar{z}_i(m_1,m_2),(n_1^{min},n_2^{\min})}, \tag{81}$$

$$M_{\max} = - \sum_{(m_1,m_2)} A^{I(a)}_{\bar{z}_i(n_1^{\max},n_2^{\max}),(m_1,m_2)} A^{I(a)}_{z_i(m_1,m_2),(n_1^{max},n_2^{\max})}, \tag{82}$$

and

$$M_{\text{int}} = \begin{pmatrix} M_{\text{int}}^{(n_1,n_2)} & * & * & \\ * & M_{\text{int}}^{(n_1',n_2')} & * & \\ * & * & M_{\text{int}}^{(n_1'',n_2'')} & \\ & & & \ddots \end{pmatrix}, \tag{83}$$

$$M_{\text{int}}^{(n_1,n_2)} = + \sum_{(m_1,m_2)} A^{I(a)}_{z_i(n_1,n_2),(m_1,m_2)} A^{I(a)}_{\bar{z}_i(m_1,m_2),(n_1,n_2)} - \sum_{(m_1,m_2)} A^{I(a)}_{\bar{z}_i(n_1,n_2),(m_1,m_2)} A^{I(a)}_{z_i(m_1,m_2),(n_1,n_2)}, \cdots . \tag{84}$$

$(n_1^{\min},n_2^{\min})$ in (81) denotes the point corresponding to the lowest eigenvalue in $G^{(a)}_{[b_I^{(-)}]}$, and $(n_1^{\max},n_2^{\max})$ in (82) denotes the point corresponding to the highest eigenvalue in $G^{(a)}_{[b_I^{(-)}]}$. Also $(n_1,n_2),\cdots$ in (83) denote other points corresponding to intermediate eigenvalues in $G^{(a)}_{[b_I^{(-)}]}$. Let us consider a $\{(I(a))(I(a))\}$ block of (46),

$$\sum_{i=1,2} [A^{I(a)}_{z_i}, A^{I(a)}_{\bar{z}_i}] - (q_2 q_1^{*T} + q_1 q_2^{*T})_{\{(I(a))(I(a))\}} = \zeta \mathbf{1}_{\{(I(a))(I(a))\}}. \tag{85}$$

If a connected part $G^{(a)}_{[b_I^{(-)}]}$ does not include $(0,0)$ or $(1,1)$, the second term on the lhs of (85) vanishes, since the nontrivial components of $q_{\dot{\alpha}}$ are given by (69), (70). We have supposed $\zeta > 0$, so (80)–(84) tell us that such $G^{(a)}_{[b_I^{(-)}]}$ does not exist.

Next, consider the $\{(I,(n_1^{\max},n_2^{\max}))(I,(n_1^{\max},n_2^{\max}))\}$ block of (46),

$$-\sum_{(m_1,m_2)} A^I_{\bar{z}_i(n_1^{\max},n_2^{\max}),(m_1,m_2)} A^I_{z_i(m_1,m_2),(n_1^{\max},n_2^{\max})} - (q_2 \dot{q}_1^{*T} + q_1 \dot{q}_2^{*T})_{\{(I,(n_1^{\max},n_2^{\max}))(I,(n_1^{\max},n_2^{\max}))\}}$$
$$= \zeta \mathbf{1}_{N^{(n_1^{\max},n_2^{\max})}_{[b_I^{(-)}]}}. \tag{86}$$

If

$$n_1^{\max} > 1 \quad \text{or} \quad n_2^{\max} > 1, \tag{87}$$

the second term on the lhs of (86) vanishes, since the nontrivial components of $q_{\dot{\alpha}}$ are given by (69), (70); then

$$\text{lhs of (86)} = -\sum_{(m_1,m_2)} A^I_{\bar{z}_i(n_1^{\max},n_2^{\max}),(m_1,m_2)} A^I_{z_i(m_1,m_2),(n_1^{\max},n_2^{\max})} \leq 0. \tag{88}$$

On the other hand,

$$\text{rhs of (86)} = \zeta > 0. \tag{89}$$

These are inconsistent from each other. Then, we conclude

$$n_1^{\max} \leq 1 \quad \text{and} \quad n_2^{\max} \leq 1. \tag{90}$$

Consider the maximal case, the $\{(I,(1,1))(I,(1,1))\}$ component of (46). The first term on the lhs is

$$-\sum_{(m_1,m_2)} A^I_{\bar{z}_i(1,1),(m_1,m_2)} A^I_{z_i(m_1,m_2),(1,1)} \leq 0, \tag{91}$$

and the second term is

$$-(q_2 \dot{q}_1^{*T} + q_1 \dot{q}_2^{*T}) = -2 q_1 \dot{q}_1^{*T} \leq 0. \tag{92}$$

Again, the rhs is $\zeta > 0$. Then we see that the $\{I(1,1)\}$ component does not exist. Repeating similar arguments, we conclude that

$$(n_1^{\max},n_2^{\max}) = (0,0). \tag{93}$$

We have finished the proof of Theorem 1. ■

Let us introduce such a map $\mathcal{I}$, that

$$\mathcal{I}:\{l|l=1,\cdots,M\} \to \{I|I=1,\cdots,N\}, \quad M \leq N, \tag{94}$$

$$N^{(0,0)}_{[b_{\mathcal{I}(l)}]} \neq 0. \tag{95}$$

For each l, assign a connected graph $C_{\mathcal{I}(l)}$. For example, see Fig. 4. For given $C_{\mathcal{I}(l)}$, nontrivial components of A_{z_i} are

$$A_{z_1\{l,(n_1-1,n_2)\}\{l,(n_1,n_2)\}} \neq 0, \quad (n_1-1,n_2),(n_1,n_2) \in C_{\mathcal{I}(l)}, \tag{96}$$

and

$$A_{z_2\{l,(n_1,n_2-1)\}\{l,(n_1,n_2)\}} \neq 0, \quad (n_1,n_2-1),(n_1,n_2) \in C_{\mathcal{I}(l)}. \tag{97}$$

Also nontrivial components of $q_{\dot{\alpha}}$ are

$$\dot{q}_{1I=\{l,(0,0)\},J=\mathcal{I}(l)} = -\dot{q}_{2I=\{l,(0,0)\},J=\mathcal{I}(l)} \neq 0. \tag{98}$$

For the nontrivial components (96)–(98), (42) and (43) are reduced to

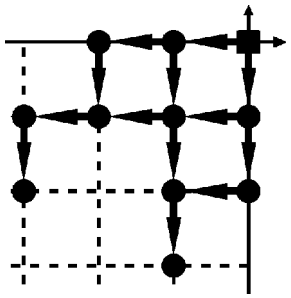

FIG. 4. $C_{\mathcal{I}(l)}$.

$$A_{z_1\{l,(n_1,n_2)\},\{l,(n_1+1,n_2)\}}A_{\bar{z}_1\{l,(n_1+1,n_2)\},\{l,(n_1,n_2)\}} - A_{\bar{z}_1\{l,(n_1,n_2)\},\{l,(n_1-1,n_2)\}}A_{z_1\{l,(n_1-1,n_2)\},\{l,(n_1,n_2)\}}$$
$$+ A_{z_2\{l,(n_1,n_2)\},\{l,(n_1,n_2+1)\}}A_{\bar{z}_2\{l,(n_1,n_2+1)\},\{l,(n_1,n_2)\}} - A_{\bar{z}_2\{l,(n_1,n_2)\},\{l,(n_1,n_2-1)\}}A_{z_2\{l,(n_1,n_2-1)\},\{l,(n_1,n_2)\}}$$
$$+ 2q_{\dot{1}_{\{l,(n_1,n_2)\},J}}q^{*T}_{\dot{1}J,\{l,(n_1,n_2)\}} = \zeta, \tag{99}$$

and

$$A_{z_1\{l,(n_1,n_2)\},\{l,(n_1+1,n_2)\}}A_{z_2\{l,(n_1+1,n_2)\},\{l,(n_1+1,n_2+1)\}} - A_{z_2\{l,(n_1,n_2)\},\{l,(n_1,n_2+1)\}}A_{z_1\{l,(n_1,n_2+1)\},\{l,(n_1+1,n_2+1)\}} = 0. \tag{100}$$

On the other hand, the Dirac equation reduced to 0 dimension (44) gives no constraint, which follows from the next theorem.

Theorem 2: *If A_{z_i} and $q_{\dot{\alpha}}$ satisfy Eqs.* (42), (43) *and Eqs.* (50), (51), *they satisfy the Dirac equation reduced to* 0 *dimension* (44) *automatically*.

(proof)

From (98), (44) is reduced to

$$A_{\bar{z}_1}q_{\dot{1}} = 0, \quad A_{\bar{z}_2}q_{\dot{1}} = 0. \tag{101}$$

Since we have taken the ordering (62), $A_{\bar{z}_i(l,(n_1,n_2)),(l,(m_1,m_2))}$ and $q_{\dot{1}\,(l,(n_1,n_2)),J=\mathcal{I}(l)}$ have the next structures,

$$A_{\bar{z}_i(l,(n_1,n_2)),(l,(m_1,m_2))} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ * & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ * & * & \cdots & 0 & 0 \\ * & * & \cdots & * & 0 \end{pmatrix}, \quad q_{\dot{1}(l,(n_1,n_2)),J=\mathcal{I}(l)} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ * \end{pmatrix}. \tag{102}$$

So, (101) always holds. ■

The above theorem means that the solutions of the dimensional reduction of the Seiberg-Witten monopole equations with the constant background under the fixed point conditions of the torus actions are equivalent to the solutions of the N.C. ADHM equations with the same fixed point conditions.

The above discussions and theorems are valid for infinite N as well as finite N. In the following, we consider only a finite N case to study more details. As we saw in Sec. III, the finite N case itself has a physical picture. Furthermore, solutions and their natures of finite N models are important, even if we consider the N.C. field theory, because such solutions are possible to be embedded in infinite N solutions.

From now on, we suppose that ϕ_I does not degenerate,

FIG. 5. A_{z_1}.

$$N_{[b_I^{(-)}]}^{(n_1,n_2)} \leq 1. \tag{103}$$

The reason is as follows. (We tried to prove the nondegeneracy of ϕ_I's by using a graphical consideration similar to one in the proof of Theorem 3. Although for several simple cases we succeeded in proving that the nondegeneracy is necessary for (42)–(44), (50), (51) to have a solution, we do not have a complete proof for general cases yet.)

(i) The solution of (42), (43) (44), (50), (51) is clearly included in solutions of (42), (43), (50), (51). The nondegeneracy of the solutions of (42), (43), (50), (51) is the very same one considered in Ref. 49. See the argument at the end of Sec. II and the above discussions. In this case, the nondegeneracy is certified.

(ii) It is clear that the degenerate solutions do not contribute to the path integral for the partition function, because the factor $\Pi_{I\neq J}(\phi_I-\phi_J)$ in (113) becomes zero if there are degenerate solutions of ϕ_I.[7]

Let us give graphical interpretations of (96), (97), (98).

• $A_{z_1\ \{l,(n_1,n_2)\}\{l,(n_1+1,n_2)\}}$ corresponds to a left arrow connecting (n_1,n_2) and (n_1+1,n_2) in $C_{\mathcal{I}(l)}$. See Fig. 5. The number of nontrivial real components, $^{\#}\{A_{z_1}\}$, is given by two times of the number of left arrows.

• $A_{z_2\ \{l,(n_1,n_2)\}\{l,(n_1,n_2+1)\}}$ corresponds to a down arrow connecting (n_1,n_2) and (n_1,n_2+1) in $C_{\mathcal{I}(l)}$. See Fig. 6. The number of nontrivial components, $^{\#}\{A_{z_2}\}$, is given by two times the number of the down arrows.

• $q_{I=\{l,(0,0)\}J=\mathcal{I}(l)}$ corresponds to the origin $(0,0)$ in $C_{\mathcal{I}(l)}$. See Fig. 7. The number of nontrivial components, $^{\#}\{q\}$, is given by 2.

The total number of undetermined real variables is $^{\#}\{A_{z_1}\}+^{\#}\{A_{z_2}\}+^{\#}\{q\}$.

Also graphical meanings of Eqs. (99), (100), and the residual gauge symmetry $U(1)^N$ are given as follows.

• Each equation of (99) corresponds to ending points of the left arrow or down arrow or the origin in $C_{\mathcal{I}(l)}$. In other words, each point $C_{\mathcal{I}(l)}$ corresponds to each equation of (99). See Fig. 8. The number of nontrivial constraints, $^{\#}\{\mathrm{Eq.}(49)\}$ is given by the number of points.

• Each equation of (100) corresponds to a hook connecting (n_1,n_2) and (n_1+1,n_2+1), which includes an intermediating point (n_1+1,n_2) or (n_1,n_2+1), in $C_{\mathcal{I}(l)}$. See Fig. 9. The number of nontrivial constraints, $^{\#}\{\mathrm{Eq.}(100)\}$, is given by two times the number of hooks.

• Each $U(1)$ factor of the residual gauge symmetry $U(1)^N$ corresponds to each point (n_1,n_2) in $C_{\mathcal{I}(l)}$. See Fig. 10. The number of degrees of the residual gauge symmetry $U(1)^N$, denoted by $^{\#}\{U(1)\}$, is given by the number of points.

The total number of real constraints is $^{\#}\{\mathrm{Eq.}(99)\}+^{\#}\{\mathrm{Eq.}(100)\}+^{\#}\{U(1)\}$.

Now let us prove the next theorem.

Theorem 3: *Let N be a finite natural number. If and only if* $C_{\mathcal{I}(l)}$ *is a Young diagram*, (42), (43), (44), (50), (51) *has a solution, and the solution is an isolated one.*

(proof)

From Theorem 1-2, it is enough to show that if and only if $C_{\mathcal{I}(l)}$ is a Young diagram, (99) and (100) has only an isolated solution. Consider a graph $C_{\mathcal{I}(l)}$ as a *quadrangulation* of a two dimensional surface. Here we admit *quadrangulations* to include some segments that do not make faces, like the graph in Fig. 11. (If one considers a dual graph, then one finds that the dual graph gives a quadrangulation of a two dimensional surface in the usual meaning. The dual graph is obtained from the original graph by replacing original points by dual faces and original segments connecting original points by dual segments gluing dual faces.) We start with cases where two dimensional surfaces have no hole. Recall the well-known formula for the Euler number χ of graphs,

FIG. 6. A_{z_2}.

$$\chi = 2 - 2h - b = {}^{\#}\{\text{points}\} - {}^{\#}\{\text{segments}\} + {}^{\#}\{\text{faces}\}, \tag{104}$$

where h denotes the number of handles of graphs, and b denotes the number of boundaries of graphs.

In our case, $h=0$ and $b=1$. Then we obtain

$$\chi = 1 = {}^{\#}\{\text{points}\} - {}^{\#}\{\text{segments}\} + {}^{\#}\{\text{faces}\}. \tag{105}$$

Notice that

$${}^{\#}\{\text{points}\} = {}^{\#}\{\text{Eq . (99)}\} = {}^{\#}\{U(1)\}, \tag{106}$$

and

$${}^{\#}\{\text{segments}\} = \frac{{}^{\#}\{A_{z_1}\} + {}^{\#}\{A_{z_2}\}}{2}. \tag{107}$$

Also, one sees that

$${}^{\#}\{\text{faces}\} \leq \frac{{}^{\#}\{\text{Eq . (100)}\}}{2}, \tag{108}$$

and that, in (108), the equation holds when the graph $C_{\mathcal{I}(l)}$ is a Young diagram. See Fig. 12. Then we obtain

$$({}^{\#}\{A_{z_1}\} + {}^{\#}\{A_{z_2}\} + {}^{\#}\{q\}) - ({}^{\#}\{\text{Eq . (99)}\} + {}^{\#}\{\text{Eq . (100)}\} + {}^{\#}\{U(1)\})$$

$$= 2{}^{\#}\{\text{segments}\} + 2 - 2{}^{\#}\{\text{points}\} - {}^{\#}\{\text{Eq . (100)}\}$$

$$\leq -2({}^{\#}\{\text{points}\} - {}^{\#}\{\text{segments}\} + {}^{\#}\{\text{faces}\}) + 2$$

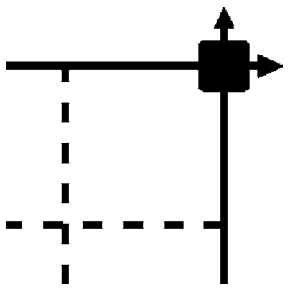

FIG. 7. q_i.

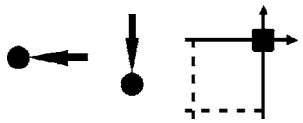

FIG. 8. Equation (99).

$$= -2 + 2$$

$$= 0. \tag{109}$$

From this, we find that if and only if $C_{\mathcal{I}(l)}$ is a Young diagram, we can have a solution to (99), (100), and that the solution is an isolated one.

Now let us turn to a case, where $C_{\mathcal{I}(l)}$ has some holes. A diagram with holes is constructed from one without holes by adding pieces of diagrams. For example, see Fig. 13. In Fig. 13, some white dots are added to make a hole. Under this operation, the number of undetermined variables increases by

$$\Delta^{\#}\{\text{undetermined variables}\} = \Delta^{\#}\{A_{z_1}\} + \Delta^{\#}\{A_{z_2}\} = 2 \times 4 + 2 \times 2 = 12. \tag{110}$$

On the other hand, the number of constraints increases by

$$\Delta^{\#}\{\text{constraints}\} = \Delta^{\#}\{\text{Eq. (99)}\} + \Delta^{\#}\{\text{Eq. (100)}\} + \Delta^{\#}\{U(1)\} = 5 + 2 \times 2 + 5 = 14. \tag{111}$$

As implied by the above example, one can show that "puncture" operations make the number of constraints greater than that of undetermined variables in general. We conclude that if $C_{\mathcal{I}(l)}$ has some holes, then (99), (100) have no solution.

We have finished the proof for Theorem 3. ■

As mentioned at the begining of this section, we have shown that (42), (43), (44), (50), (51) have only isolated solutions, and the solutions are expressed by the Young diagrams.

At the end of this section, we comment on the case that the q are not square matrices. Let us compare the above cases with the case of $\mathbb{C}^{[n]}$ and the ADHM data for a usual U(N) instanton. We have investigated the case that $q_{\dot{\alpha}}$ and $q^{\dagger}_{\dot{\alpha}}$ are $N \times N$ square matrices. It is clear that the above theorem is valid, even if $q_{\dot{\alpha}}$ and $q^{\dagger}_{\dot{\alpha}}$ are $N \times k$ and $k \times N$ for arbitrary $k \in \mathbb{Z}$, respectively. In this case, our equations (42) and (43) are ADHM equations corresponding to the U(N) instanton of the k instanton number with the Dirac equation reduced to 0 dimension. The Dirac equation (44) makes no nontrivial equations when we introduce ζ. Then, our models are completely equivalent to the case of ADHM equations with fixed point equations of torus action, that is discussed in Nakajima's lecture note[49] and others.[7,13,15] The proof for the correspondence with ADHM data and the Young diagrams is given by Ref. 49. In this light, our proof in this section is a new version for the Nakajima's theorem. We solved the fixed point equation of the torus action directly. By virtue of the concrete solution, the correspondence between fields components, ADHM equations, and Young diagrams are clarified.

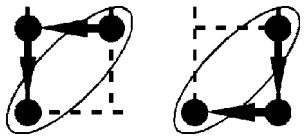

FIG. 9. Equation (100).

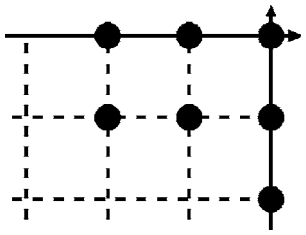

FIG. 10. $U(1)$ gauge symmetry.

VI. LOCALIZATION THEOREM

Although, in this paper, we do not perform the summation of the solutions nor obtain the partition function of our model, we make a comment on the localization theorem,[39,44] which is a powerful tool for the calculation of a path integral of cohomological field theories, in order to explain our motivation. To carry out the calculation of an infinite N case, that is the N.C. $\mathbb{R}^4$ case, is difficult. Therefore we consider the toy model that is given by the same type Lagrangian of Sec. II but its entire fields are finite $N\times N$ matrices.

For our purpose, one of the most suitable expression of the localization theorem is one given in Refs. 9 and 16. This is expressed as follows.

Let $\tilde{\delta}$ be the deformed BRS transformation defined in Sec. IV. As explained in Sec. II, the action S is given by a BRS exact function. Now we redefine the action as

$$S = \tilde{\delta}\Psi(\phi,\mathcal{B},\mathcal{F}). \tag{112}$$

The difference between $\hat{\delta}\Psi$ and $\tilde{\delta}\Psi$ causes no effect to the path integral, because the integral of equivariant cohomology is equal to that of original cohomology. Here we have used the notation $\mathcal{B},\mathcal{F}$ to denote the BRS doublet fields collectively. Then the localization theorem tells us that

$$Z = \int \frac{D\phi}{U(N)} D\mathcal{B}\, D\mathcal{F}\, e^{-\tilde{\delta}\Psi} = \int \prod_{I=1}^{N} d\phi_I \frac{\prod_{I\neq J}(\phi_I - \phi_J)}{S\det{}^{1/2}\,\mathcal{L}}. \tag{113}$$

ϕ_I are the eigenvalues of ϕ, and the superdeterminant $S\det\mathcal{L}$ is defined by

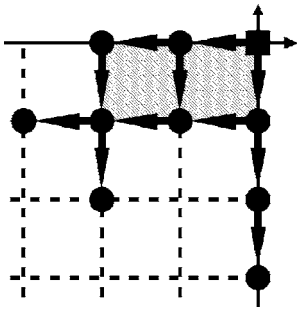

FIG. 11. A quadrangulation may include some segments that do not make faces.

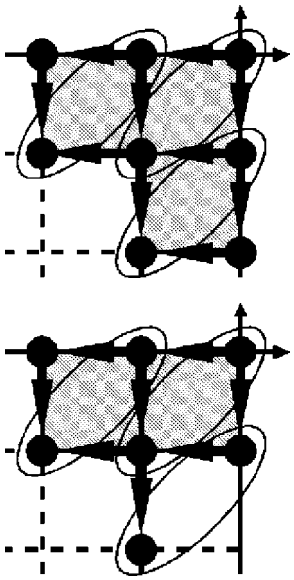

FIG. 12. Young diagram and variant diagram.

$$S\det\mathcal{L} = S\det\begin{pmatrix} \dfrac{\partial(Q)_{\mathcal{B}}}{\partial\mathcal{F}} & \dfrac{\partial(Q)_{\mathcal{B}}}{\partial\mathcal{B}} \\ \dfrac{\partial(Q)_{\mathcal{F}}}{\partial\mathcal{F}} & \dfrac{\partial(Q)_{\mathcal{F}}}{\partial\mathcal{B}} \end{pmatrix}, \tag{114}$$

where $(Q)_{\mathcal{B}}$ and $(Q)_{\mathcal{F}}$ are defined by the representation of the deformed BRS transformation $\tilde{\delta}$ on the fields $\mathcal{B},\mathcal{F}$,

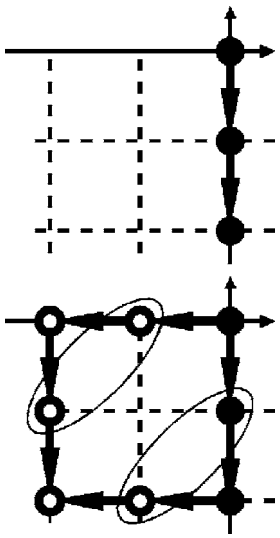

FIG. 13. Graph without a hole and graph with a hole.

$$Q = (Q)_{\mathcal{B}} \frac{\partial}{\partial \mathcal{B}} + (Q)_{\mathcal{F}} \frac{\partial}{\partial \mathcal{F}}. \tag{115}$$

Note that this expression is an analog of

$$\tilde{d} = d + i_X, \tag{116}$$

where X is a vector defining the Lie derivative $\mathcal{L}_X$ associated with $\mathcal{G} \otimes T^{N+2}$ action. See (39), (40), (41). In our case, we obtain

$$Z = \int \prod_{I=1}^{N} d\phi_I \prod_{I \neq J} (\phi_I - \phi_J) \prod_{I=1}^{N} \frac{(\epsilon_1 + \epsilon_2)\{-(\phi_I - b_I)^2 + \epsilon_-^2\}}{\epsilon_1 \epsilon_2 \{-(\phi_I - b_I)^2 + \epsilon_+^2\}}$$
$$\times \prod_{I \neq J} \frac{\{(\phi_I - \phi_J)^2 - 4\epsilon_+^2\}^{\frac{1}{2}} \{-(\phi_I - b_J)^2 + \epsilon_-^2\}}{\{-(\phi_I - b_J)^2 + \epsilon_+^2\}\{(\phi_I - \phi_J)^2 - \epsilon_1^2\}^{\frac{1}{2}} \{(\phi_I - \phi_J)^2 - \epsilon_2^2\}^{1/2}}$$

where $\epsilon_- = (\epsilon_1 - \epsilon_2)/2$.

Some comments might be necessary. This formula is derived by using a some version of localization theorem, which reduces the integral $\int D\mathcal{B}\, D\mathcal{F}$, and this is valid only if the BPS equations of the action (42), (43), (44) and the fixed point equations of the deformed BRS symmetry (50), (51) have isolated solutions for a given value of ϕ_I's. The integral $\int \Pi_I\, d\phi_I$ is remained, and this should be understood as the contour integral. In order to define an appropriate contour, we use $\epsilon_i \to \epsilon_i + i0$ prescription. The poles correspond to the isolated solutions.[39,42]

VII. CONCLUSION

The solutions of the Seiberg-Witten monopole equations reduced to 0 dimension that also satisfy the fixed point equations of torus actions were classified, where the torus action is induced from the global symmetries. More concretely speaking, we deformed the BRS transformation of the topological twisted $\mathcal{N}=2$ gauge theory on $\mathbb{R}^4$ with a hypermultiplet to the T-equivariant derivative by using the global symmetries. The global symmetries contain torus actions. Using these symmetries, the deformed BRS transformation was defined to satisfy the nilpotency up to the Lie derivative of the group actions. Then we classified the solutions of the fixed point equations of these deformed BRS transformations.

We showed that the Seiberg-Witten monopole equations are reduced to the ADHM equations with the Dirac equation reduced to 0 dimension at the large N.C. parameter limit. These equations are described by using infinite dimensional matrices. We showed that the Dirac equation reduced to 0 dimension is trivial when the ADHM equations and the fixed point equations are satisfied. It is known that the solutions of the ADHM equations with the fixed point equations are isolated ones, and are classified by the Young diagrams, when the matrix size is finite. We gave a new proof of this statement, too. Then, we found that we can perform the path integral by using the localization formula, in order to get the partition functions of the finite dimensional matrix model. This finite dimensional matrix model is given as reduced theory to 0 dimension from the topological twisted $\mathcal{N}=2$ non-Abelian gauge theory on $\mathbb{R}^4$ with a hypermultiplet, because the size of matrix is truncated to finite dimension from infinite dimension. We gave the result of the partition function of this toy model. The complete calculation of the partition function for the $\mathcal{N}=2$ $U(1)$ gauge theory on N.C. $\mathbb{R}^4$ remained. This calculation might reveal the relation between the Seiberg-Witten monopole and the instanton. We hope to report on this task elsewhere.

APPENDIX: CONVENTION

1. Complex coordinate

We define the complex coordinate $z^i, \bar{z}^i (i=1,2)$ as

$$z^1 = \frac{1}{\sqrt{2}}(x^1 + ix^2), \quad \bar{z}^1 = \frac{1}{\sqrt{2}}(x^1 - ix^2),$$

$$z^2 = \frac{1}{\sqrt{2}}(x^3 + ix^4), \quad \bar{z}^2 = \frac{1}{\sqrt{2}}(x^3 - ix^4). \tag{A1}$$

Also, $\partial_{z^i}, \partial_{\bar{z}^i}$ are given by

$$\partial_{z^1} = \frac{1}{\sqrt{2}}(\partial_1 - i\partial_2), \quad \partial_{\bar{z}^1} = \frac{1}{\sqrt{2}}(\partial_1 + i\partial_2),$$

$$\partial_{z^2} = \frac{1}{\sqrt{2}}(\partial_3 - i\partial_4), \quad \partial_{\bar{z}^2} = \frac{1}{\sqrt{2}}(\partial_3 + i\partial_4). \tag{A2}$$

Then, we obtain

$$\partial_{z^i} z^j = \delta_i^j, \quad \partial_{\bar{z}^i} \bar{z}^j = \delta_i^j. \tag{A3}$$

2. Spinor index

$\epsilon^{\alpha\beta}$, $\epsilon^{\dot{\alpha}\dot{\beta}}$ and $\epsilon_{\alpha\beta}$, $\epsilon_{\dot{\alpha}\dot{\beta}}$ are defined by

$$\epsilon^{\alpha\beta} = \epsilon^{\dot{\alpha}\dot{\beta}} = \begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix}, \quad \epsilon_{\alpha\beta} = \epsilon_{\dot{\alpha}\dot{\beta}} = \begin{pmatrix} 0 & -1 \\ +1 & 0 \end{pmatrix}. \tag{A4}$$

In other words, $\epsilon_{\alpha\beta}$, $\epsilon_{\dot{\alpha}\dot{\beta}}$ are defined to be the inverses of $\epsilon^{\alpha\beta}$, $\epsilon^{\dot{\alpha}\dot{\beta}}$,

$$\epsilon^{\alpha\beta}\epsilon_{\beta\gamma} = \delta^\alpha_\gamma \epsilon^{\dot{\alpha}\dot{\beta}}, \quad \epsilon_{\dot{\beta}\dot{\gamma}} = \delta^{\dot{\alpha}}_{\dot{\gamma}}. \tag{A5}$$

Then a spinor with upper indices and a spinor with lower indices are related as

$$\psi^\alpha = \epsilon^{\alpha\beta}\psi_\beta, \quad \psi_\alpha = \epsilon_{\alpha\beta}\psi^\beta,$$

$$\psi^{\dot{\alpha}} = \epsilon^{\dot{\alpha}\dot{\beta}}\psi_{\dot{\beta}}, \quad \psi_{\dot{\alpha}} = \epsilon_{\dot{\alpha}\dot{\beta}}\psi^{\dot{\beta}}. \tag{A6}$$

We use the following definition for the four dimensional Pauli matrix $\sigma^\mu (\mu=1,2,3,4)$,

$$(\sigma^\mu)_{\alpha\dot{\alpha}} = (\sigma^1, \sigma^2, \sigma^3, \sigma^4) = (i\mathbf{1}, -\vec{\tau}),$$

$$(\bar{\sigma}^\mu)^{\dot{\alpha}\alpha} = (\bar{\sigma}^1, \bar{\sigma}^2, \bar{\sigma}^3, \bar{\sigma}^4) = (i\mathbf{1}, +\vec{\tau}), \tag{A7}$$

where

$$\vec{\tau} = \left(\begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{A8}$$

We define $\sigma^{\mu\nu}$, $\bar{\sigma}^{\mu\nu}$ as

$$(\sigma^{\mu\nu})_\alpha{}^\beta = \frac{i}{4}(\sigma^\mu\bar{\sigma}^\nu - \sigma^\nu\bar{\sigma}^\mu)_\alpha{}^\beta,$$

$$(\bar{\sigma}^{\mu\nu})_{\dot\beta}{}^{\dot\alpha} = \frac{i}{4}(\bar{\sigma}^\mu\sigma^\nu - \bar{\sigma}^\nu\sigma^\mu)_{\dot\beta}{}^{\dot\alpha}. \tag{A9}$$

From this definition, $\sigma^{\mu\nu}$ and $\bar{\sigma}^{\mu\nu}$ satisfy the anti self-dual relation and the self-dual relation, respectively,

$$\sigma^{\mu\nu} = -*\sigma^{\mu\nu}, \quad \bar{\sigma}^{\mu\nu} = +*\bar{\sigma}^{\mu\nu}. \tag{A10}$$

3. † symbol

For a scalar matrix M and a vector matrix M_μ, the symbol † denotes the usual hermite conjugation for them,

$$M^\dagger = M^{*T}, \quad M_\mu{}^\dagger = M_\mu{}^{*T}, \tag{A11}$$

where the symbol * denotes the complex conjugation and the symbol T denotes the transposition. On the other hand, for an undotted spinor matrix M_α and a dotted spinor matrix $M_{\dot\alpha}$, $M_\alpha{}^\dagger$, and $M_{\dot\alpha}{}^\dagger$ are defined by,

$$M_\alpha{}^\dagger = \epsilon^{\alpha\beta}M_\beta{}^{*T}, \quad M_{\dot\alpha}{}^\dagger = \epsilon^{\dot\alpha\dot\beta}M_{\dot\beta}{}^{*T}. \tag{A12}$$

This definition makes $M_\alpha{}^\dagger$ and $M_{\dot\alpha}{}^\dagger$ transform in the same rules as M_α and $M_{\dot\alpha}$ under $SU(2)_L$ and $SU(2)_{R(R')}$, respectively.

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Type I vacuum solutions with aligned Papapetrou fields: An intrinsic characterization

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We show that Petrov type I vacuum solutions admitting a Killing vector whose Papapetrou field is aligned with a principal bivector of the Weyl tensor are the Kasner and Taub metrics, their counterpart with timelike orbits and their associated windmill-like solutions, as well as the Petrov homogeneous vacuum solution. We recover all these metrics by using an integration method based on an invariant classification which allows us to characterize every solution. In this way we obtain an intrinsic and explicit algorithm to identify them. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2363258]

I. INTRODUCTION

If ξ is a Killing vector, the *Killing 2-form* $\nabla\xi$ is closed and, in the vacuum case, it is a solution of the source-free Maxwell equations. Because this fact was pointed out by Papapetrou,[1] the covariant derivative $\nabla\xi$ has also been called the *Papapetrou field*.[2] In the Kerr geometry the principal directions of the Killing 2-form associated with the timelike Killing vector coincide with the two double principal null (Debever) directions of the Weyl tensor.[2] This means that the Killing 2-form is a Weyl principal bivector. This fact has been remarked upon by Mars[3] who has also shown that it characterizes the Kerr solution under an asymptotic flatness behavior.

A question naturally arises: can all the vacuum solutions with this property of the Kerr metric be determined? In other words, is it possible to integrate Einstein vacuum equations under the hypothesis that the spacetime admits an isometry whose Killing 2-form is a principal bivector of the Weyl tensor? Some partial results are known about this question. Thus, we have studied the case of Petrov type D spacetimes elsewhere[4] and we have shown that the Kerr-NUT solutions are the type D vacuum metrics with a timelike Killing 2-form aligned with the Weyl geometry.

Metrics admitting an isometry were studied by considering the algebraic properties of the associated Killing 2-form,[5,6] and this approach was extended to the spacetimes with an homothetic motion.[7,8] More recently Fayos and Sopuerta[2,9] have developed a formalism that improves the use of the Killing 2-form and its underlined algebraic structure for analyzing the vacuum solutions with an isometry. They consider two new viewpoints that permit a more accurate classification of these spacetimes: (i) the differential properties of the principal directions of the Killing 2-form, and (ii) the degree of alignment of the principal directions of the Killing 2-form with those of the Weyl tensor. The Fayos and Sopuerta approach uses the Newman–Penrose formalism and several extensions have been built for homothetic and conformal motions[10,11] and for nonvacuum solutions.[12]

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Some of the conditions on the Killing 2-form imposed in the literature quoted above could be very restrictive. Thus, in a previous paper[13] we have shown that the Petrov type I vacuum spacetimes admitting an isometry whose Killing 2-form is aligned with a Weyl principal bivector belong to two classes of metrics which admit a three-dimensional group of isometries of Bianchi types I or II. In the present work we show that a close relation between the Weyl principal directions and the isometry group exists in these classes. This fact allows us to achieve an integration of the vacuum equations with the aid of an invariant classification and, in this way, to obtain an intrinsic and explicit characterization of all the Petrov type I vacuum solutions that admit an aligned Papapetrou field. It is worth remarking that the integration method used here could be suitable in order to obtain other type I solutions.

The vacuum homogeneous Petrov solution[14] was found to be the only one satisfying: (i) vacuum, and (ii) existence of a simply transitive group G_4 of isometries. Although these two conditions characterize the Petrov metric, it is quite difficult to know when a metric tensor (given in an arbitrary coordinate system) satisfies them. Indeed, the first condition is intrinsic because it imposes a restriction on a metric concomitant, the Ricci tensor. Nevertheless, the second one imposes equations that mix up, in principle, elements other than the metric tensor (Killing vectors of the isometry group) and, consequently, it cannot be verified by simply substituting the metric tensor. In Ref. 13 we have changed this last nonintrinsic condition for an intrinsic one: the Weyl tensor is Petrov type I with constant eigenvalues. Moreover, as the Ricci and Weyl tensors are concomitants of the metric tensor, $\mathrm{Ric} \equiv \mathrm{Ric}(g)$, $\mathcal{W} \equiv \mathcal{W}(g)$, we have finally obtained the following *intrinsic* and *explicit* characterization of the Petrov solution:[13] *the necessary and sufficient conditions for g to be the Petrov homogeneous vacuum solution are*

$$\mathrm{Ric} = 0, \quad 6(\mathrm{Tr}\mathcal{W}^2)^3 \neq (\mathrm{Tr}\mathcal{W}^3)^2, \quad \mathrm{dTr}\mathcal{W}^2 = \mathrm{dTr}\mathcal{W}^3 = 0. \tag{1}$$

A whole intrinsic and explicit characterization of a metric or a family of metrics is quite interesting from a conceptual point of view and from a practical one because it can be tested by direct substitution of the metric tensor in arbitrary coordinates. Thus, it is an approach to the metric equivalence problem alternative to the usual one. This and other advantages have been pointed out elsewhere[15] where this kind of identification has been obtained for the Schwarszchild spacetime as well as for all the other type D static vacuum solutions. A similar study has been fulfilled for a family of Einstein–Maxwell solutions that include the Reissner–Nordström metric.[16]

In order to obtain intrinsic and explicit characterizations, as well as having an intrinsic labelling of the metrics, we need to express these intrinsic conditions in terms of explicit concomitants of the metric tensor. When doing this, the role played by the results on the covariant determination of the eigenvalues and eigenspaces of the Ricci tensor[17] and the principal 2-forms and principal directions of the Weyl tensor[18,19] is essential.

In this work we solve vacuum equations under the hypothesis that the spacetime is Petrov type I and there is a Killing vector whose associated Papapetrou field is a eigenbivector of the Weyl tensor. In this way, we recover the Petrov homogeneous vacuum solutions as well as the Kasner and Taub metrics, their counterpart with timelike orbits and their associated windmill-like solutions. Our integration method is based on an invariant classification which allows us to characterize the solutions intrinsically and explicitly. For every solution some properties of the isometry group and the aligned Killing 2-forms are given in terms of the Weyl principal directions.

The article is organized as follows. In Sec. II we present the Cartan formalism adapted to the Weyl principal frame that a Petrov type I spacetime admits. In Sec. III we summarize some results needed here about type I vacuum metrics admitting aligned Papapetrou fields. In Sec. IV we write vacuum Einstein equations for the families of Petrov type I metrics that, having a nonconstant Weyl eigenvalue, admit aligned Papapetrou fields. Sections V and VI are devoted to integrate these equations in different invariant subcases, as well as to determine, for every solution, the Killing vectors with an aligned Killing 2-form. In Sec. VII we present a similar study when all the Weyl eigenvalues are constant. Finally, in Sec. VIII, we summarize the results in an algorithmic form in order to make the intrinsic and explicit character of our results evident.

II. CARTAN FORMALISM IN THE WEYL FRAME OF A TYPE I SPACETIME

The algebraic classification of the Weyl tensor was first tackled by Petrov[20] considering the number of the invariant subespaces of the Weyl tensor regarded as an endomorphism of the 2-forms space. This classification was completed by Géhéniau[21] and Bel[22] considering also the eigenvalue multiplicity. In this framework appears the notion of *Weyl principal bivector* that we use here and which was widely analyzed by Bel[23] for the different algebraic types. In the 1960s many other authors presented alternative approaches to this classification, and in more recent studies[19,24] a wide bibliography on this subject can be found. For short, we refer the different classes of the Weyl tensor as the Petrov types. An algebraically general Weyl tensor is Petrov type I.

In a Petrov type I spacetime the Weyl tensor W determines four orthogonal principal directions which define the *Weyl principal frame* $\{e_\alpha\}$.[19,23] Then, the bivectors (self-dual 2-forms) $\mathcal{U}_i = 1/\sqrt{2}(U_i - i*U_i)$, with $U_i = e_0 \wedge e_i$, are eigenbivectors of the self-dual Weyl tensor $\mathcal{W} = 1/2(W - i*W)$, * being the Hodge dual operator. These bivectors satisfy $2\mathcal{U}_i \times \mathcal{U}_i = g$, where $\times$ denotes the contraction of adjacent index in the tensorial product. The tern $\{\mathcal{U}_i\}$ constitutes an orthonormal frame in the bivector space which has the induced orientation given by

$$\mathcal{U}_i \times \mathcal{U}_j = -\frac{i}{\sqrt{2}}\epsilon_{ijk}\mathcal{U}_k, \quad i \neq j. \tag{2}$$

If α_i is the eigenvalue associated with the eigenbivector $\mathcal{U}_i$, the self-dual Weyl tensor takes the canonical form

$$\mathcal{W} = -\sum_{i=1}^{3} \alpha_i \mathcal{U}_i \otimes \mathcal{U}_i. \tag{3}$$

The Cartan formalism can be referred to the Weyl principal frame $\{e_\alpha\}$ or, equivalently, to the *frame of eigenbivectors* $\{\mathcal{U}_i\}$. So, the six connection 1-forms ω_α^β defined by $\nabla e_\alpha = \omega_\alpha^\beta \otimes e_\beta$ can be collected into three complex ones Γ_i^j ($\Gamma_i^j = -\Gamma_j^i$), and the first structure equations take the expression

$$\nabla \mathcal{U}_i = \Gamma_i^j \otimes \mathcal{U}_j, \quad \Gamma_i^j = \omega_i{}^j - \epsilon_{ijk}\omega_0^k. \tag{4}$$

The second structure equations for a vacuum type I spacetime follow by applying the Ricci identities $\nabla_{[\alpha}\nabla_{\beta]}\mathcal{U}_{i\epsilon\delta} = \mathcal{U}_{i\epsilon}{}^{\mu}R_{\mu\delta\beta\alpha} + \mathcal{U}_i{}^{\mu}{}_{\delta}R_{\mu\epsilon\beta\alpha}$, and in terms of the eigenbivectors $\{\mathcal{U}_i\}$ they can be written as

$$\mathrm{d}\Gamma_i^k - \Gamma_i^j \wedge \Gamma_j^k = i\sqrt{2}\epsilon_{ikm}\alpha_m \mathcal{U}_m. \tag{5}$$

If we make the product of each of these second structure Eq. (5) with $\mathcal{U}_m$ we can obtain the following three complex scalar equations:

$$\nabla \cdot \lambda_i = \lambda_i^2 - (\lambda_j - \lambda_k)^2 - \alpha_i \quad (i,j,k \neq), \tag{6}$$

where $\lambda_i = -\mathcal{U}_i(\nabla \cdot \mathcal{U}_i)$, and we have denoted $\nabla \cdot \equiv \mathrm{Tr}\nabla$ and $\lambda_i^2 = g(\lambda_i, \lambda_i)$. The three complex 1-forms λ_i contain the 24 independent connection coefficients as the Γ_i^j do. In fact, by using Eq. (2) and the first structure Eqs. (4), both sets $\{\Gamma_i^j\}$ and $\{\lambda_i\}$ can be related by

$$\lambda_i \equiv -\mathcal{U}_i(\nabla \cdot \mathcal{U}_i) = -\frac{i}{\sqrt{2}}\epsilon_{ijk}\mathcal{U}_k(\Gamma_i^j). \tag{7}$$

And the inverse of these expressions say that for different i,j,k,

$$\mathcal{U}_k(\Gamma_i^j) = \frac{i}{\sqrt{2}}\epsilon_{ijk}(\lambda_i + \lambda_j - \lambda_k), \quad (i,j,k \neq). \tag{8}$$

The Bianchi identities in the vacuum case state that the Weyl tensor is divergence-free $\nabla \cdot \mathcal{W}=0$, and from Eq. (3) they can be written as

$$\mathrm{d}\alpha_i = (\alpha_j - \alpha_k)(\lambda_j - \lambda_k) - 3\alpha_i\lambda_i \quad (i,j,k \neq). \tag{9}$$

Equations (9) show the relation that exists between the gradient of the Weyl eigenvalues and the 1-forms λ_i in the vacuum case. This fact has suggested a classification of Petrov type I spacetimes taking into account the dimension of the space that $\{\lambda_i\}$ generate. More precisely,[13]

Definition 1: We say that a Petrov type I spacetime is of class I_a $(a=1,2,3)$ if the dimension of the space that $\{\lambda_i\}$ generate is a.

Differential conditions of this kind were imposed by Edgar[25] on the type I spacetimes, and he showed that in the vacuum case his classification also has consequences on the functional dependence of the Weyl eigenvalues. We have slightly modified the Edgar approach in order to obtain a classification that is symmetric in the principal structures of the Weyl tensor. We remark the invariant nature of this classification: it is based on the vector Weyl invariants λ_i.

We have been studied elsewhere the symmetries of the vacuum metrics of class I_1 and we have shown:[13]

Lemma 1: A vacuum metric of class I_1 admits at least a (simply transitive) group G_3 of isometries. It admits a G_4 if, and only if, it has constant eigenvalues.

III. ALIGNED KILLING 2-FORMS AND TYPE I VACUUM METRICS

If ξ is a (real) Killing vector its covariant derivative $\nabla\xi$ is named Killing 2-form or Papapetrou field.[1,2] The Papapetrou fields have been used to study and classify spacetimes admitting an isometry or an homothetic or conformal motion (see Refs. 2–12). In this way, some classes of vacuum solutions with a principal direction of the Papapetrou field aligned with a (Debever) null principal direction of the Weyl tensor have been considered.[9] Also, the alignment between the Weyl principal plane and the Papapetrou field associated with the timelike Killing vector has been shown in the Kerr geometry.[3,9]

Is it possible to determine all the vacuum solutions having this property of the Kerr metric? Elsewhere[4] we give an affirmative answer to this question for the case of Petrov type D spacetimes by showing that *the type D vacuum solutions with a timelike Killing 2-form aligned with the Weyl geometry are the Kerr-NUT metrics*. In this work we accomplish this study for the Petrov type I spacetimes by obtaining all the vacuum solutions with this property and by determining the Killing vectors with an aligned Killing 2-form. Moreover, we show the close relation between the Weyl tensor geometry and the geometries of ξ and $\nabla\xi$.

In order to clarify what kind of alignment between the Killing 2-form and the Weyl tensor is analyzed in this work we give the specific definition. If $\{\mathcal{U}_i\}$ is an orthonormal basis of the self-dual 2-forms space, the Papapetrou field $\nabla\xi$ associated to a Killing vector ξ has, generically, three independent complex components Ω_i:

$$\nabla\xi = \sum_{i=1}^{3} \Omega_i\mathcal{U}_i + \sum_{i=1}^{3} \tilde{\Omega}_i\tilde{\mathcal{U}}_i \tag{10}$$

where ~ means complex conjugate. Then:

Definition 2: We say that a Papapetrou field $\nabla\xi$ is aligned with a bivector $\mathcal{U}$ if both 2-forms have the same principal 2-planes, that is, $\nabla\xi=\Omega\mathcal{U}+\tilde{\Omega}\tilde{\mathcal{U}}$.

We say that a Papapetrou field $\nabla\xi$ is aligned (with the Weyl tensor) if it is aligned with a Weyl principal bivector.

When a Killing 2-form is aligned with a bivector of an orthonormal frame of invariants bivectors $\mathcal{U}_i$, the Killing vector is strongly restricted by the connection 1-forms. Thus, for type I metrics we have:[13]

Lemma 2: In a Petrov type I spacetime with a Killing vector ξ, the Papapetrou field $\nabla\xi$ is aligned with a Weyl principal 2-form $\mathcal{U}_i$ if, and only if, ξ is orthogonal to the two complex connection 1-forms Γ_i^j *(*defined by the Weyl principal frame $\{\mathcal{U}_i\}$*).*

The alignment between a Killing 2-form and a Weyl principal bivector of a type I vacuum solution has been partially analyzed[13] and the following necessary condition has been obtained:

Lemma 3: A vacuum Petrov type I spacetime which admits a Killing field with an aligned Papapetrou field belongs to class I_1.

As a consequence of Lemmas 1 and 3, we obtain that *a vacuum Petrov type I spacetime which admits a Killing field with an aligned Papapetrou field admits, at least, a three-dimensional group of isometries.* This means that a unique symmetry with an aligned Papapetrou field implies that other symmetries exist.

These results imply that in order to find all the type I vacuum solutions admitting an aligned Papapetrou field, we must analyze the vacuum solutions of class I_1. We shall start with the case where a non constant eigenvalue α_1 exists. After that we shall finish by dealing with the case of all the eigenvalues being constant.

IV. VACUUM EQUATIONS FOR THE CLASS I_1

As we know that every vacuum solution of class I_1 admits a (simply transitive) G_3 group of isometries, a real function τ exists such that $\alpha_i \equiv \alpha_i(\tau)$. Moreover, as we are in class I_1, it must be $\lambda_i \wedge \lambda_j = 0$ and so, from Bianchi identities (9), we obtain $\lambda_i \wedge \mathrm{d}\alpha_1 = 0$. So, taking into account Eq. (7) and that a G_3 is admitted, three functions $\varphi_i(\tau)$ exist such that

$$\Gamma_i^j = \mathrm{i}\epsilon_{ijk}\varphi_k \mathcal{U}_k(\mathrm{d}\tau). \tag{11}$$

On the other hand, it has also been shown in Ref. 13 that $\mathrm{d}\alpha_1$ cannot be a null vector and so, $(\mathrm{d}\tau)^2 \neq 0$. Thus, $\{\mathrm{d}\tau, u^i\}$, with $u^i = \mathcal{U}_i(\mathrm{d}\tau)$, is an orthogonal frame such that $2(u^i)^2 = -(\mathrm{d}\tau)^2$. Then, we can write the bivectors $\{\mathcal{U}_i\}$ as

$$\mathcal{U}_i = -\frac{1}{(\mathrm{d}\tau)^2}\left(\mathrm{d}\tau \wedge u^i + \frac{i}{\sqrt{2}}\epsilon_{ijk}u^j \wedge u^k\right). \tag{12}$$

We can use this expression to eliminate $\mathcal{U}_i$ in the second structure Eqs. (4) and then they become an exterior system for the orthonormal frame $\{\mathrm{d}\tau, u^i\}$,

$$\mathrm{d}u^i = \mu_i(\tau)\mathrm{d}\tau \wedge u^i + \nu_i(\tau)u^j \wedge u^k \tag{13}$$

for every cyclic permutation i, j, k, and where the functions μ_i and ν_i are given by

$$\mu_i = -(\ln \varphi_i)' + \frac{\sqrt{2}\alpha_i}{\varphi_i(\mathrm{d}\tau)^2}, \quad \nu_i = -\mathrm{i}\left(\frac{2\alpha_i}{\varphi_i(\mathrm{d}\tau)^2} + \frac{\varphi_j\varphi_k}{\varphi_i}\right), \tag{14}$$

where $'$ stands for the derivative with respect to the variable τ. But $\mathrm{d}\tau$ is proportional to the invariant 1-form $\mathrm{d}\alpha_1$ and a G_3 exists. Thus, it follows that $(\mathrm{d}\tau)^2$ and $\Delta\tau$ depend on τ. This fact allows us to choose τ such that $\Delta\tau = 0$. Then, τ is fixed up to an affine transformation $\tau \hookrightarrow \alpha\tau + \beta$. In terms of this harmonic function, the Eqs. (6) become

$$((\varphi_j + \varphi_k)' - \sqrt{2}\varphi_j\varphi_k)(\mathrm{d}\tau)^2 = 2\sqrt{2}\alpha_i \tag{15}$$

for every cyclic permutation of i, j, k. The Bianchi identities (9) can be stated as

$$\alpha_1' = \frac{1}{\sqrt{2}}(\varphi_3(\alpha_2 - \alpha_1) - \varphi_2(2\alpha_1 + \alpha_2)), \quad \alpha_2' = \frac{1}{\sqrt{2}}(\varphi_3(\alpha_1 - \alpha_2) - \varphi_1(\alpha_1 + 2\alpha_2)). \tag{16}$$

At this point, it is clear that the integration of the system (13) depends strongly on the number of the $u^i=\mathcal{U}_i(\mathrm{d}\tau)$ that are integrable 1-forms. Thus, it seems suitable to give a classification of type I_1 spacetimes that takes into account these restrictions. But these conditions lead to an invariant classification because of u^i is proportional to $\mathcal{U}_i(\mathrm{d}\alpha_1)$:

Definition 3: We will say that a Petrov type I_1 vacuum metric with $\mathrm{d}\alpha_1\neq 0$ is of class I_{1A} $(A=0,1,2,3)$ if there are exactly A integrable 1-forms in the set $\{\mathcal{U}_i(\mathrm{d}\alpha_1)\}$.

We have studied elsewhere[13] the symmetries that the different classes I_{1A} admit, as well as necessary conditions for the alignment of the associated Killing 2-forms with the Weyl tensor. Here we will make use of the following result:

Lemma 4: If a vacuum Petrov type I spacetime admits a Killing field with an aligned Papapetrou field then either it is the Petrov solution (that has constant eigenvalues) or it is of class I_{12} or I_{13}. These classes admit an isometry group G_3 of Bianchi types II and I, respectively.

Thus, in order to find the vacuum solutions with aligned Papapetrou fields, we must consider the Petrov solution that admits a G_4 or the classes I_{12} and I_{13}. Now we obtain the vacuum solutions for these two classes with non constant eigenvalues. To accomplish this goal, we will integrate the Bianchi identities (16) and the scalar Eqs. (15) taking into account that in class I_{13} all the functions ν_i given in Eq. (14) are zero and two of them vanish in class I_{12}. Finally, the second structure Eqs. (13) will be integrated to obtain the 1-forms u^i in terms of real coordinates. After that, the metric tensor will be obtained as

$$g=\frac{1}{(\mathrm{d}\tau)^2}\left[\mathrm{d}\tau\otimes\mathrm{d}\tau-2\sum_{i=1}^{3}u^i\otimes u^i\right] \tag{17}$$

It is worth pointing out that in the spacetimes of type I_1 that we are studying here there exist two outlined coframes, namely, the Weyl principal coframe $\{\theta^\alpha\}$ and that defined by $\{\mathrm{d}\tau,u^i\}$. We will see in following sections the close relation between both coframes for the spacetimes in classes I_{12} and I_{13}. This fact allows us to give intrinsic conditions that label every type I vacuum solution admitting an aligned Papapetrou field.

V. VACUUM SOLUTIONS OF CLASS I_{13}

In class I_{13} all of the 1-forms u^i are integrable. Then Eqs. (13) hold with $\nu_i=0$. Taking into account Eq. (14), we can solve the Eqs. (15) and (16) to obtain

$$\alpha_1=be^{2a\beta\tau},\quad \alpha_2=k\alpha_1,\quad (\mathrm{d}\tau)^2=\frac{be^{2a\beta\tau}}{a^2k(k+1)}, \tag{18}$$

$$\varphi_3=\sqrt{2}ka,\quad \varphi_2=-\sqrt{2}a(k+1),\quad \varphi_1=-\sqrt{2}k(k+1)a, \tag{19}$$

where a, b and $\beta=1+k+k^2$ are nonzero constants and k is different from 1, -2, and $-1/2$ because g is not of Petrov type D, and different from -1 and 0 because none of the Weyl eigenvalues vanishes as a consequence of the Szekeres–Brans theorem.[26,27] The second structure Eqs. (13) constitute an exterior system for the 1-forms $u^i\equiv\mathcal{U}_i(\mathrm{d}\tau)$. It implies that three complex functions $\{x^i\}$ exist such that

$$u^1=e^{a\tau}\mathrm{d}x^1,\quad u^2=e^{ak^2\tau}\mathrm{d}x^2,\quad u^3=e^{a(1+k)^2\tau}\mathrm{d}x^3. \tag{20}$$

From here and Eq. (17), we can obtain the metric tensor g in complex coordinates. In order to get real coordinates, another fact is needed. As τ is a real function, it follows that $\mathrm{d}\tau$, $(\mathrm{d}\tau)^2$ and $\nabla\mathrm{d}\tau$ must also be real. If we compute $\nabla\mathrm{d}\tau$ by using Eqs. (17)–(19) we obtain that, necessarily, either all of the coefficients are real and $\mathrm{d}\tau$ coincides with one of the principal directions θ^α, or two of the coefficients are conjugate and $\mathrm{d}\tau$ takes the direction of one of the bisectors $\theta^i\pm\theta^j$ of a spacelike principal plane. We shall analyze every case, but we must take into account that as $\mathrm{d}\tau\wedge\mathrm{d}\alpha_1=0$, these conditions can also be written in terms of the Weyl eigenvalue.

A. $d\alpha_1$ Is a Principal Direction

In this case a and k are real constants. We must remark that if $d\tau$ is a principal direction, then $u^i \equiv \mathcal{U}_i(d\tau)$ are so. But when $d\tau$ coincides with the timelike principal direction θ^0, every u^i is a real direction and, if $d\tau$ is a spacelike principal direction, some of them are purely imaginary. Now we will analyze each case in detail.

(i) Case $d\alpha_1 \wedge \theta^0 = 0$. We have $d\tau = e_0(\tau)\theta^0$. Then $u^i = (1/\sqrt{2})e_0(\tau)\theta^i$, and so dx^i of Eq. (20) are real. If we take into account that the harmonic coordinate τ is defined up to affine transformation, the metric tensor (17) in real coordinates takes the form of the Kasner metric

$$g = -e^{-2\tau}d\tau^2 + e^{2(1/\beta-1)\tau}(dx^1)^2 + e^{2(k^2/\beta-1)\tau}(dx^2)^2 + e^{2(((1+k)^2/\beta)-1)\tau}(dx^3)^2. \tag{21}$$

The coordinate transformation $e^{-\tau} = t$ changes the harmonic time to the proper time and gives us the usual expression for this solution.[24,28]

We must check whether there is a Killing field with an aligned Papapetrou field. We have established[13] that this condition is equivalent to a Killing field to be orthogonal to two of the complex connection 1-forms Γ_i^j (see Lemma 2). The real Killing fields of this metric are $\xi = k_1\partial_{x^1} + k_2\partial_{x^2} + k_3\partial_{x^3}$. As the connection 1-forms Γ_i^j are collinear with u^i it follows that every Killing field ∂_i satisfies this condition, and so, we have three Killing fields such that their Papapetrou fields are aligned with the three principal 2-forms.

(ii) Case $d\alpha_1 \wedge \theta^1 = 0$. Now, $d\tau = e_1(\tau)\theta^1$, and so $(d\tau)^2 > 0$. In order to get real coordinates we must take into account that in this case $\sqrt{2}u^1 = -e_1(\tau)\theta^0$, $\sqrt{2}u^2 = ie_1(\tau)\theta^3$ and $\sqrt{2}u^3 = ie_1(\tau)\theta^2$. And so, the coordinates adapted to u^2 and u^3 are purely imaginary $x^a = iy^a$ $(a=2,3)$, y^a being real functions. Then, for the metric tensor g we get a similar expression to the one in the previous case, the only change being the causal character of the gradient of the Weyl eigenvalue

$$g = e^{-2\tau}d\tau^2 - e^{2(1/\beta-1)\tau}(dx^1)^2 + e^{2(k^2/\beta-1)\tau}(dy^2)^2 + e^{2(((1+k)^2/\beta)-1)\tau}(dy^3)^2. \tag{22}$$

This is the static Kasner metric.[24]

This solution admits three Killing fields ∂_{x^1}, ∂_{y^2}, and ∂_{y^3} such that their Papapetrou fields are aligned with the three principal bivectors of the Weyl tensor. This finishes the study of the cases in which the gradient of the invariant $\alpha_1(\tau)$ is collinear with a principal direction of the Weyl tensor. The following proposition summarizes the main results.

Proposition 1: The Kasner metrics (21) and (22) are the only Petrov type I_{13} vacuum solutions where the gradient of the Weyl eigenvalue is a principal direction of the Weyl tensor.

The metrics of this family admit three Killing fields ξ_i which are collinear with the three principal directions $\mathcal{U}_i(d\alpha_1)$, such that their Papapetrou fields $\nabla\xi_i$ are aligned with the three principal bivectors $\mathcal{U}_i$ of the Weyl tensor.

B. $d\alpha_1$ Is Not a Principal Direction

As we have commented below, in this case $d\tau$ must take the direction of one of the bisectors of a spacelike principal plane, say $\theta^2 + \theta^3$, $d\tau \propto \theta^2 + \theta^3$. Then, $u^1 \propto \theta^3 - \theta^2$, $u^2 \propto \theta^0 + i\theta^1$ and $u^3 \propto \theta^0 - i\theta^1$. Moreover, $\nabla d\tau$ is real if, and only if, a is real and $2k = -1 + in$, n being a nonzero real constant because the metric is not of type D and $n^2 \neq 3$ because β cannot be zero. Then, the coordinate x^1 of Eq. (20) must be purely imaginary, $x^1 = ix$, and x^2 and x^3 must be conjugated functions, that is $x^2 = y - iz$, $x^3 = y + iz$. Thus we get a real coordinate system $\{\tau, x, y, z\}$ and, from Eq. (17), we find the following expression of the metric tensor:

$$g = \frac{1}{4}(3-n^2)^2 e^{(1/2)(3-n^2)\tau}d\tau^2 + e^{-(1/2)(1+n^2)\tau}dx^2 + e^{\tau}[\cos(n\tau)[dz^2 - dy^2] - 2\sin(n\tau)dydz]. \tag{23}$$

This is the so called *windmill solution*.[24,29]

To see if an aligned Killing 2-form can exist in this spacetime, we must look for a Killing field to be orthogonal to two of the connection 1-forms. The Killing fields of this solution are $\xi = k_1\partial_x + k_2\partial_y + k_3\partial_z$ and, as every connection 1-form is parallel to one of the directions u^i, the only Killing field which is orthogonal to a pair of connection 1-forms is ∂_x, that can be characterized as the Killing field that takes the direction of the bisector $\theta^2 - \theta^3$. Moreover, the Weyl tensor has just a real eigenvalue α_1 and if $\mathcal{U}_1$ is the associated eigenbivector, then $\mathcal{U}_1(\mathrm{d}\alpha_1)$ is collinear with the Killing field ∂_x. We can collect these results in the following:

Proposition 2: The windmill solution (23) is the only Petrov type I_{13} vacuum solution where the gradient of the Weyl eigenvalue α_1 is not a principal direction of the Weyl tensor.

In such spacetime a unique real eigenvalue α_1 exists. Then, if $\mathcal{U}_1$ is the associated eigenbivector, the field $\mathcal{U}_1(\mathrm{d}\alpha_1)$ is collinear with a Killing field that has a Papapetrou field aligned with $\mathcal{U}_1$.

VI. VACUUM SOLUTIONS OF CLASS I_{12}

Let us suppose now that only two directions, let us say u^2 and u^3, are integrable. So, we can take $\nu_2 = \nu_3 = 0$ in the second structure Eqs. (13). Taking into account the definition of ν_i from Eq. (14) we obtain

$$\varphi_3 = \frac{k}{\sqrt{2}} - \varphi_1, \quad \varphi_2 = \frac{a^2}{\sqrt{2}k} - \varphi_1, \quad \varphi_1 = \frac{a}{\sqrt{2}}\frac{be^{-a\tau}+1}{be^{-a\tau}-1}, \tag{24}$$

where a, b, and k are complex constants, $a^2 \neq k^2$. Then, by also using the Bianchi identities (16) we obtain

$$(\mathrm{d}\tau)^2 = \frac{-2\sqrt{2}c}{a} e^{-((a^2+ak+k^2)/k)\tau}(b^2e^{-2a\tau}-1)^{-1}, \tag{25}$$

where c is another complex constant.

As in the previous section, the only possibilities for $\nabla \mathrm{d}\tau$ to be real are that either $\mathrm{d}\tau$ is a principal direction θ^α or it is the bisector $\theta^i + \theta^j$ of a spacelike principal plane.

A. $\mathrm{d}\alpha_1$ Is a Principal Direction

In this case we have that k, a^2 and $\varphi_3'/\varphi_3 - \sqrt{2}\varphi_3$ are real. From Eq. (24) we obtain

$$\frac{\varphi_3'}{\varphi_3} - \sqrt{2}\varphi_3 = -a\frac{b^2 + e^{2\sqrt{2}\tau}}{b^2 - e^{2\sqrt{2}\tau}}. \tag{26}$$

So we can conclude that a and b^2 must be real constants. Now we shall go on the integration of Eq. (13). As in the previous section it will be useful to distinguish the cases of $\mathrm{d}\tau$ to be the timelike principal direction θ^0 or a spacelike principal direction θ^i. We will study these cases separately.

(i) Case $\mathrm{d}\alpha_1 \wedge \theta^0 = 0$. Here we have $\mathrm{d}\tau = e_0(\tau)\theta^0$, and so u^i must be real for every i. Consequently, if we take into account Eq. (13) with $\nu_2 = \nu_3 = 0$, real coordinates $\{x, y, z\}$ can be found such that

$$u^2 = \frac{e^{-(k/2)\tau}}{\sqrt{2}}\mathrm{d}x, \quad u^3 = \frac{e^{-(a^2/2k)\tau}}{\sqrt{2}}\mathrm{d}y, \quad u^1 = -\frac{\mathrm{i}\sqrt{2}abe^{-a\tau}}{b^2e^{-2a\tau}-1} e^{-((a^2+k^2)/2k)\tau}(\mathrm{d}z + x\mathrm{d}y). \tag{27}$$

As u^1 is real, we find that b is purely imaginary, $b = -i\beta$. Then, from Eq. (25) we can calculate $(\mathrm{d}\tau)^2$, and taking into account the freedom of an affine transformation in choosing the harmonic coordinate τ, we can take $\beta = 1$ and we can write the metric in the usual form of the Taub[30] metric

$$g = \frac{\cosh(a\tau)}{a}(-e^{((a^2+k^2)/k)\tau}\mathrm{d}\tau^2 + e^{(a^2/k)\tau}\mathrm{d}x^2 + e^{k\tau}\mathrm{d}y^2) + \frac{a}{\cosh(a\tau)}(\mathrm{d}z + x\mathrm{d}y)^2. \tag{28}$$

To see if a Killing field with an aligned Papapetrou field exists, we must look for a Killing field which is orthogonal to two of the connection 1-forms. The Killing fields of the Taub metric (28) are $\xi=k_1\partial_x+k_2\partial_y+(k_3-k_1y)\partial_z$ and, taking into account that the connection 1-forms Γ^j_i are collinear with u^k, from Eq. (27) we find that the only Killing field that is orthogonal to a pair of connection 1-forms is $\xi=\partial_z$, and it is orthogonal to Γ^2_1 and Γ^3_1. So, the principal 2-form aligned with a Papapetrou field is $\mathcal{U}_1$, and it is characterized by the fact that $\mathcal{U}_1(\mathrm{d}\tau)$ is not integrable.

(ii) Case $\mathrm{d}\alpha_1\wedge\theta^1=0$. Now, $\mathrm{d}\tau=e_1(\tau)\theta^1$ and we have $\sqrt{2}\,u^1=-e_1(\tau)\theta^0$, $\sqrt{2}u^2=ie_1(\tau)\theta^3$ and $\sqrt{2}\,u^3=ie_1(\tau)\theta^2$. So, we can consider real coordinates $\{x,y,z\}$ such that

$$u^2=\frac{\mathrm{i}e^{-(k/2)\tau}}{\sqrt{2}}\mathrm{d}x,\quad u^3=\frac{ie^{-(a^2/2k)\tau}}{\sqrt{2}}\mathrm{d}y,\quad u^1=\frac{-\sqrt{2}\beta ae^{-a\tau}}{\beta^2e^{-2a\tau}+1}e^{-((a^2+k^2)/2k)\tau}(\mathrm{d}z-x\mathrm{d}y). \tag{29}$$

Then, the same analysis of the previous case leads to the counterpart with timelike orbits of the Taub metric[24]

$$g=\frac{\cosh(a\tau)}{a}(e^{((a^2+k^2)/k)\tau}\mathrm{d}\tau^2+e^{(a^2/k)\tau}\mathrm{d}x^2+e^{k\tau}\mathrm{d}y^2)-\frac{a}{\cosh(a\tau)}(\mathrm{d}z-x\mathrm{d}y)^2. \tag{30}$$

The same property of the Taub metric concerned with the aligned Papapetrou fields holds in this case. We can summarize these results for the case that $\mathrm{d}\alpha_1$ is collinear with a principal direction in the following:

Proposition 3: The Taub metric (28) that has spacelike orbits, and its counterpart with timelike orbits (30) are the only type I_{12} vacuum solutions where the gradient of the Weyl eigenvalue α_1 is collinear with a principal direction of the Weyl tensor.

Both metrics admit a principal 2-form $\mathcal{U}_i$ such that $\mathcal{U}_i(\mathrm{d}\alpha_1)$ is not integrable. Then, the Killing field collinear with $\mathcal{U}_i(\mathrm{d}\alpha_1)$ is the only one whose Papapetrou field is aligned (with the principal 2-form $\mathcal{U}_i$).

B. $\mathrm{d}\alpha_1$ Is Not a Principal Direction

In this case $\mathrm{d}\tau$ must take the direction of one of the bisectors of a spacelike principal plane, say $\theta^2+\theta^3$, $\mathrm{d}\tau\propto\theta^2+\theta^3$. Then, a similar analysis to the one in the previous cases, leads to the metric

$$g=e^{2m\tau}\left[\frac{\cosh(a\tau)}{a}\mathrm{d}\tau^2+\frac{a}{\cosh(a\tau)}e^{-2m\tau}(\mathrm{d}z-u\mathrm{d}v)^2+\frac{\cosh(a\tau)}{a}e^{-m\tau}[\cos(n\tau)(\mathrm{d}v^2-\mathrm{d}u^2)\right.$$
$$\left.-2\sin(n\tau)\mathrm{d}u\mathrm{d}v]\right], \tag{31}$$

where $a^2=m^2+n^2$, $n\neq0$. This is an equivalent windmill-like metric for the Taub solution.

The real Killing fields of this metric in the previous coordinate system are $\xi=k_1\partial_u+k_2\partial_v+(k_1v+k_3)\partial_z$. As the complex connection 1-forms Γ^j_i are collinear with $u^k\equiv\mathcal{U}_k(\mathrm{d}\tau)$, we conclude that there is only one Killing field ∂_z which is orthogonal to two connection 1-forms, more precisely, to Γ^2_1 and Γ^3_1. So, this Killing field has a Papapetrou field which is aligned with the principal bivector $\mathcal{U}_1$. We summarize these results in the following:

Proposition 4: The metric (31) is the only vacuum solution of class I_{12} where the gradient of the Weyl eigenvalue α_1 is not a Weyl principal direction.

This solution admits a principal 2-form $\mathcal{U}_i$ such that $\mathcal{U}_i(\mathrm{d}\alpha_1)$ is not integrable. Then, the Killing field collinear with $\mathcal{U}_i(\mathrm{d}\alpha_1)$ is the only one whose Papapetrou field is aligned (with the principal 2-form $\mathcal{U}_i$).

VII. TYPE I VACUUM SOLUTIONS WITH CONSTANT EIGENVALUES

Elsewhere[13] we have shown that the only Petrov type I vacuum solution with constant eigenvalues is the homogeneous Petrov solution.[14,24] In real coordinates this metric writes as

$$k^2 g = \mathrm{d}x^2 + e^{-2x}\mathrm{d}y^2 + e^{x}(\cos\sqrt{3}x(\mathrm{d}z^2 - \mathrm{d}t^2) - 2\sin\sqrt{3}x\mathrm{d}z\mathrm{d}t). \tag{32}$$

The eigenvalues of this metric are proportional to the three cubic roots of -1, $\alpha_i = k^2\sqrt[3]{-1}$. So, a real eigenvalue, let us say α_3, exists. From the metric expression (32) we get that $\Gamma_1^3 \wedge \mathcal{U}_1(\Gamma_1^2) = 0$ and $\Gamma_2^3 \wedge \mathcal{U}_2(\Gamma_1^2) = 0$. Moreover, a straightforward calculation shows that $\mathrm{d}x$ takes the direction of one of the bisectors of the plane $^*U_3$, $\mathrm{d}x = e_1(x)(\theta^1 + \theta^2)$, and that the complex connection 1-forms Γ_i^j are given by

$$\Gamma_1^2 = e^{-x}\mathrm{d}y, \quad \mathcal{U}_3(\Gamma_1^2) = -\frac{i}{\sqrt{2}}\mathrm{d}x,$$

$$\mathcal{U}_1(\Gamma_1^2) = \frac{1}{2}e^{(1/2)(1+i\sqrt{3})x}(\mathrm{d}t - i\mathrm{d}z), \quad \mathcal{U}_2(\Gamma_1^2) = \frac{1}{2}e^{(1/2)(1-i\sqrt{3})x}(\mathrm{d}t + i\mathrm{d}z).$$

The Killing fields of this solution are $\{\partial_t, \partial_z, \partial_y, \partial_x + y\partial_y + 1/2(\sqrt{3}t - z)\partial_z - 1/2(t + \sqrt{3}z)\partial_t\}$ and so, it easily follows:

Proposition 5: The Petrov homogeneous vacuum solution (32) admits just a Killing field such that its Papapetrou field is aligned with a principal bivector. If α_3 is the real eigenvalue, this Killing field is proportional to Γ_1^2 and its Papapetrou field is aligned with $\mathcal{U}_3$.

VIII. SUMMARY IN ALGORITHMIC FORM

In this article we have found all the Petrov type I vacuum solutions admitting a Killing field whose Papapetrou field is aligned with a principal bivector of the Weyl tensor. We knew[13] that these solutions admit either a simply transitive group G_4 of isometries and then the metric must be the homogeneous Petrov solution (32), or a simply transitive G_3 group of isometries and then the spacetime belongs to one of the classes I_{13} and I_{12} in definition 3. Here we have shown that these necessary conditions given in Ref. 13 are also sufficient conditions.

The solutions can be characterized by a condition on the normal direction to the orbits group: for class I_{13}, (i) if it is a timelike principal direction we reach the Kasner metric (21), (ii) if it is a spacelike principal direction we reach the static Kasner metric (22), and (iii) if it is not a principal direction we obtain the windmill Kasner metric (23); for class I_{12}, under similar conditions, we obtain (i) the Taub metric (28), (ii) the timelike counterpart of the Taub metric (30), and (iii) the windmill-like metric for the Taub solution (31).

It is worth pointing out that the integration procedure is based on intrinsic conditions imposed on algebraic and differential concomitants of the Weyl tensor. On the other hand, these Weyl invariants can be obtained directly from the components of the metric tensor g in arbitrary local coordinates and without solving any equations.[18,19] Consequently, we get an intrinsic and explicit labeling of every solution (similar to that given for the Petrov metric in Ref. 13). Table I summarizes these results and enables us to obtain the directions of the Killing fields having aligned Papapetrou field. In the table we find the Weyl tensor invariants

$$\alpha_i \equiv \alpha_i(g), \quad \theta^\alpha \equiv \theta^\alpha(g), \quad \mathcal{U}_i \equiv \mathcal{U}_i(g), \tag{33}$$

$$\lambda_i \equiv \lambda_i(g) = -\mathcal{U}_i(\nabla \cdot \mathcal{U}_i), \tag{34}$$

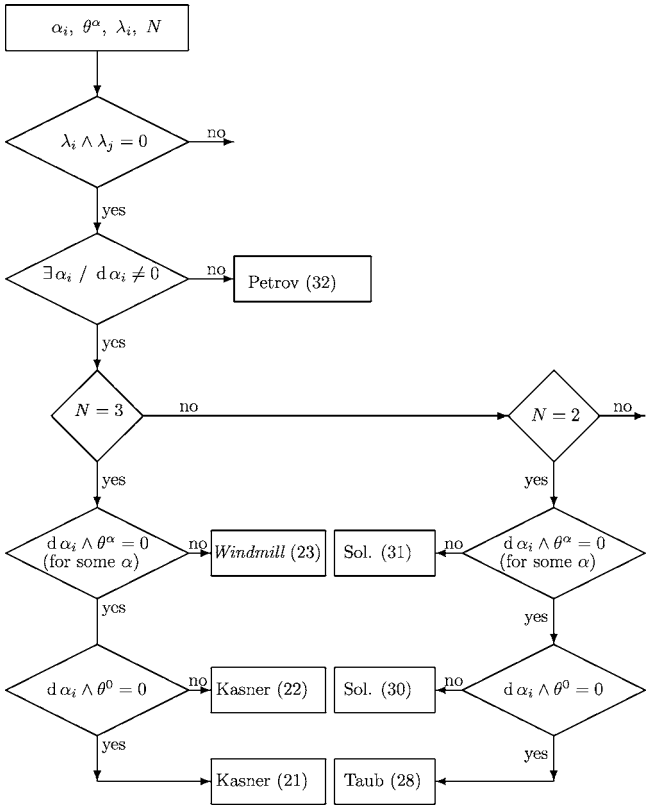
$$N \equiv N(g), \text{ number of integrable directions in the set } \{\mathcal{U}_j(\mathrm{d}\alpha_i)\}. \tag{35}$$

The metric concomitants (33) are, respectively, the Weyl eigenvalues $\alpha_i(g)$, the Weyl principal coframe $\theta^\alpha(g)$ and the unitary Weyl principal bivectors $\mathcal{U}_i(g)$. The explicit expressions of these Weyl invariants in terms of the Weyl tensor can be found elsewhere.[18,19]

TABLE I. Type I vacuum solutions with aligned Papapetrou fields.

SOLUTION	Intrinsic characterization $\lambda_i \wedge \lambda_j = 0$, Ric$=0$	Killing vectors with aligned Papapetrou field
Kasner (21)	$d\alpha_1 \neq 0$, $N=3$ $d\alpha_1 \wedge \theta^0 = 0$	$\xi_i \propto \mathcal{U}_i(d\alpha_1)$, $i=1,2,3$ $\nabla\xi_i$ aligned with $\mathcal{U}_i$
Kasner (22)	$d\alpha_1 \neq 0$, $N=3$ $d\alpha_1 \wedge \theta^j = 0$ for some j	
Windmill (23)	$d\alpha_1 \neq 0$, $N=3$ $d\alpha_1 \wedge \theta^\alpha \neq 0 \ \forall \alpha$	$\exists!\ \alpha_{i_0}$ real, $\xi \propto \mathcal{U}_{i_0}(d\alpha_1)$ $\nabla\xi$ aligned with $\mathcal{U}_{i_0}$
Taub (28)	$d\alpha_1 \neq 0$, $N=2$ $d\alpha_1 \wedge \theta^0 = 0$	$\exists!\ i_0/\mathcal{U}_{i_0}(d\alpha_1)$ is not integrable $\xi \propto \mathcal{U}_{i_0}(d\alpha_1)$ $\nabla\xi$ aligned with $\mathcal{U}_{i_0}$
Taub (30)	$d\alpha_1 \neq 0$, $N=2$ $d\alpha_1 \wedge \theta^j = 0$ for some j	
Windmill (31)	$d\alpha_1 \neq 0$, $N=2$ $d\alpha_1 \wedge \theta^\alpha \neq 0 \ \forall \alpha$	
Petrov (32)	$d\alpha_i = 0 \ \forall i$	$\exists!\ \alpha_3$ real, $\xi \propto \Gamma_1^2$ $\nabla\xi$ aligned with $\mathcal{U}_3$

Finally, to underline the intrinsic nature of our results we present a flow diagram that characterizes, among all the type I vacuum solutions, those having an aligned Papapetrou field. This operational algorithm can be useful from a computational point of view and also involves the Weyl invariants (33)–(35).



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On existence of matter outside a static black hole

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It is expected that matter composed of a perfect fluid cannot be at rest outside of a black hole if the spacetime is asymptotically flat and static (nonrotating). However, there has not been rigorous proof for this expectation without assuming spherical symmetry. In this paper, we provide a proof of nonexistence of matter composed of a perfect fluid in static black hole spacetimes under certain conditions, which can be interpreted as a relation between the stellar mass and the black hole mass. [DOI: 10.1063/1.2383009]

I. INTRODUCTION

The issue of the final state of gravitational collapse is important from various points of view. Usually we expect the black holes will eventually form after the gravitational collapse of a star and the spacetime is expected to asymptotically converge to a stationary or static state. The perturbation analysis[1] and numerical demonstrations support this picture. As a consequence, the limiting spacetime will be a stationary or static vacuum spacetime if all the matter is absorbed to the thus produced black hole. Nowadays we know that the uniqueness theorem for black holes holds in asymptotically flat, stationary (or static) and vacuum spacetimes and the resulting spacetimes are described by Kerr or Schwarzschild solutions.[2–4] Therefore we can have definite astrophysical predictions using these exact solutions.

While the uniqueness of the vacuum black hole has been established, it is interesting to ask if there is a uniqueness theorem for stationary or static spacetimes of a black hole plus matter. In the stationary case (i.e., time translation symmetry exists but their trajectories are not hypersurface orthogonal), clearly this is not the case because many spacetime solutions have been constructed. The perturbative solution of a slowly rotating black hole surrounded by an infinitesimal ring was constructed by Will.[5] There are numerical solutions of a black hole surrounded by an infinitely thin disk[6] or by an differentially rotating ring.[7] Recently, the black hole with a uniformly rotating ring around it has been calculated with high accuracy.[8]

On the other hand, we expect that there should be some kind of uniqueness theorem for static spacetimes (i.e., trajectories of time-translation symmetry are hypersurface orthogonal) of a black hole with matter. This is because if we try to put the matter at rest outside a black hole, it is expected to fall into the black hole because of the gravitational attraction. However, we would like to point out that this intuitive picture does not have a rigorous reasoning. In fact, one can easily provide a counterexample as follows. If an infinitely thin disk composed of counter-rotating particles exists on the equatorial plane of the black hole spacetime, there should exist a static configuration after a fine tuning of system parameters. This example indicates that the uniqueness

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of spacetimes of a black hole with matter depends not only on the energy condition but also the equation of state matter satisfies. As far as we know, there is Bekenstein's work[9] which proves the nonexistence of scalar fields outside a black hole in the static spacetime. However, without assuming the spherical symmetry, the question of nonexistence of matter composed of an ordinary perfect fluid outside a black hole in the static spacetime has not been addressed up to now.

As it turns out, proving the uniqueness in the setting above is rather a delicate problem. A similar situation is found for the proof of the spherical symmetry of a static isolated star composed of perfect fluid for a certain class of equations of state. This problem was solved relatively recently by Lindblom and Masood-ul-Alam[11] after a long history.[12,13] In the work of Ref. 11, the authors studied the condition that should hold inside of a star *without* assuming the spherical symmetry and proved the conformal flatness of the space that directly implies the spherical symmetry in turn.

Fortunately, many of the results in Ref. 11 can be used for our situation because much of their analysis was done in quite a general setting. In this paper we would like to reformulate the analysis of Ref. 11 for the goal of showing the uniqueness of the static spacetime of a black hole plus matter, taking care of the difference between the two setups. We will provide a partial proof for the nonexistence of matter outside a static black hole. The nonexistence we obtain here is conditional under an inequality between the black-hole mass and the stellar mass.

This paper is organized as follows. In the next section, we provide our setup concerning the Einstein equation. In Sec. III, we summarize the results of Lindblom and Masood-ul-Alam,[11] paying particular attention to the parts that are directly relevant to our argument. We prove our theorem in Sec. IV and summarize our paper with some discussion in Sec. V. We adopt the unit of $c=G=1$.

II. SETUP

We consider the static spacetime which has the metric

$$ds^2 = -V^2(x)dt^2 + g_{ij}(x)dx^i dx^j, \tag{1}$$

where $i=1,2,3$ and $g_{ij}(x)$ is the induced metric of $\{t=\text{const.}\}$ hypersurfaces Σ. In a static spacetime, its event horizon H is identified with Killing horizon $\{V=0\}$ and thus $V(x)$ vanishes on the horizon. We assume that there is a perfect fluid with energy density ρ and pressure P. The fluid is assumed to satisfy an equation of state $P=P(\rho)$. We assume the surface of the star/fluid is a two-dimensional closed connected equipotential surface $\{x: V(x)=V_s>0\}$ for some positive constant V_s.

The Einstein equation and equation for fluid are given by

$$D^2V = 4\pi V(\rho + 3P), \tag{2}$$

$$R_{ij} = \frac{1}{V}D_iD_jV + 4\pi(\rho - P)g_{ij}, \tag{3}$$

$$D_iP = -\frac{1}{V}(\rho + P)D_iV, \tag{4}$$

where D_i and R_{ij} are the covariant derivative and Ricci tensor of the metric $g_{ij}(x)$.

Equation (4) indicates that the surface $\{\rho=\text{const.}\}$ is identical to the surface $\{V=\text{const.}\}$ Let us suppose for the moment the condition $D_iV\neq 0$ at the horizon. Except for the extremal charged black holes, this condition is satisfied in all the known static black hole solutions. Then Eq. (4) says that the value of D_iP diverges at the horizon if matter exists at the horizon $\{V=0\}$, which is an unphysical situation. Hence, this would make the stellar surface disjoint from the horizon. We stress that the same conclusion can be obtained from Eq. (2) without any additional hypothesis. As Eq. (2) is elliptic, a standard boundary elliptic estimate (see, for example, Lemma 6.4 in Gilbarg–Trudinger[10]) says that near the horizon, the norm of the gradient of V is bounded by the

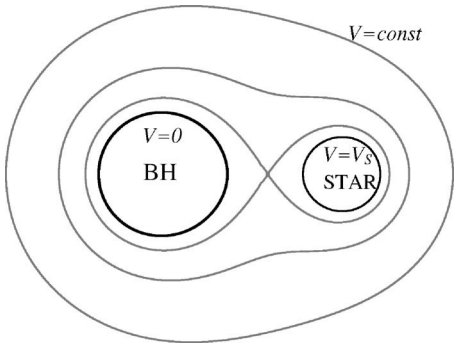

FIG. 1. Typical configuration of the system of a black hole (BH) and matter (STAR).

sup norm of the right-hand side of Eq. (2) as well as that of V, both of which are uniformly bounded in our case. As the horizon is the zero set of V, while the surface of the star is the level set $\{V=V_s(>0)\}$, the gradient bound for V provides a positive lower bound (dependent on V_s) for the distance between those two level sets, which in turn implies that the star is disjoint from the horizon.

At the moment pictures such as Fig. 1 are possible configurations of our setup. Although the star surface shown in this figure is spherical, note that its topology is arbitrary as long as it is specified as a connected equipotential surface $\{V=V_s\}$. Thus our theorem will hold also for, e.g., a barotropic perfect fluid ring. Note, however, that our theorem is not applicable to a ring composed of counter-rotating particles around a black hole, as mentioned in Sec. I. This is because such matter has anisotropic stress and its equation of state is not barotropic.

Here we stress that we will prove that such configurations as above do *not* occur under certain conditions. In doing so, we are also *not* assuming any symmetry of the spacelike slice.

Asymptotic flatness requires the following asymptotic behavior of V and the metric

$$V=\left(1-\frac{M}{r}\right)+O(r^{-2}) \tag{5}$$

and

$$g_{ij}=\left(1+\frac{2M}{r}\right)\delta_{ij}+O(r^{-2}), \tag{6}$$

where $r=:|\delta_{ij}x^ix^j|^{1/2}$ and M is the Arnowitt-Deser-Misner (ADM) mass.

Our strategy for the proof is as follows. We first show that the $\{t=\text{const.}\}$ hypersurface Σ is conformally flat. The main part of the proof is finding appropriate conformal transformations for Σ so that it becomes a hypersurface with zero ADM mass and non-negative Ricci scalar curvature. This wonderful idea was first introduced by Bunting and Masood-ul-Alam.[14] We then apply the positive energy theorem[15] to this surface to conclude that the surface is flat Euclidean space. In turn, the original hypersurface Σ is conformally flat and it will immediately follow that $\rho=P=0$. In order to find the appropriate conformal transformation, we will use the Lindblom and Masood-ul-Alam's theorems[11] that was used for proving the spherical symmetry of a static star. We review it in the next section.

III. THEOREMS OF STATIC STELLAR MODELS

In this section, we briefly review Lindblom and Masood-ul-Alam's results[11] where the spherical symmetry of static stellar models was obtained under a certain condition on the equation of state. We are able to transcribe their argument mostly because the techniques used in treating the *inside* of stars are identical.

Because the $\{V=\text{const.}\}$ surface is identical to $\{\rho=\text{const.}\}$ surface due to Eq. (4) and the equation of state $P=P(\rho)$, both ρ and P are regarded as functions of V. The minimum value of V in the star is denoted by $V=V_c$. Then quantities $r_\mu(V)$, $m_\mu(V)$ are defined as the solutions to the equations

$$\frac{dr_\mu}{dV}=\frac{r_\mu(r_\mu-2m_\mu)}{V(m_\mu+4\pi r_\mu^3 P)}, \tag{7}$$

$$\frac{dm_\mu}{dV}=\frac{4\pi r_\mu^3(r_\mu-2m_\mu)\rho}{V(m_\mu+4\pi r_\mu^3 P)}, \tag{8}$$

where the boundary conditions for Eqs. (7) and (8) are

$$r_\mu(V_s)=R_\mu := 2\mu/(1-V_s^2), \tag{9}$$

$$m_\mu(V_s)=\mu. \tag{10}$$

Here, μ is some constant suitably chosen in the proof. As we see from Eqs. (7) and (8), $dm_\mu/dr_\mu=4\pi r_\mu^2\rho$ holds and μ could be interpreted as the local mass of the star. Now $W_\mu(V)$ is defined by

$$W_\mu := \begin{cases} \dfrac{(1-V^2)^4}{16\mu^2} & \text{outside of the star,} \\ \left(1-\dfrac{2m_\mu}{r_\mu}\right)\left(\dfrac{dr_\mu}{dV}\right)^{-2} & \text{inside of the star.} \end{cases} \tag{11}$$

Various lemmas on $r_\mu(V)$, $m_\mu(V)$, and $W_\mu(V)$ are introduced, such as the existence of the solution on $(V_\mu, V_s]$ for some V_μ (Lemmas 1–3). In particular, assuming that the pressure is finite $P(V)<\infty$, W_μ can be made positive for somewhat small μ over the interval $(V_c, V_s]$ (Lemma 8).

We require that the equation of state satisfies at least one of the following constraints:

$$\frac{1}{5}\kappa^2+2\kappa+(\rho+P)\frac{d\kappa}{dP}\leqslant 0 \tag{12}$$

or

$$\frac{5\rho^2}{6P(\rho+3P)}\geqslant\kappa>\frac{10V_s^2}{e^{2h(P)}-V_s^2}, \tag{13}$$

where $\kappa := (d\rho/dP)(\rho+P)/(\rho+3P)$ and $h(P)=\log(V_s/V)$. The upper bound on κ in the condition (13) implies that the adiabatic index $\gamma := (dP/d\rho)(\rho+P)/P$ must be larger than or equal to $(6/5)\times(1+P/\rho)^2$. Under this assumption, the following quantity:

$$\Sigma_\mu := \frac{dW_\mu}{dV}-\frac{8\pi}{3}V(\rho+3P)+\frac{4W_\mu}{5V}\frac{\rho+P}{\rho+3P}\frac{d\rho}{dP} \tag{14}$$

is proved to be non-negative (Lemma 10 (Ref. 11)).

The most important technical result is Lemma 6 in Ref. 11: *Assuming that* $W_\mu>0$ *and* $\Sigma_\mu\geqslant 0$ *on* $(V_c, V_s]$, *then* $W_\mu\geqslant W := D_a V D^a V$ *on* (V_c, V_s) *holds everywhere*. In Lemma 6 of Ref. 11, it is stated that $W_\mu\geqslant W$ holds on $(V_c, V_s]$. However, we can easily see from the proof that it holds everywhere outside of the star *and* $\mu\leqslant M$. Because this lemma is relevant to our problem, we briefly review its proof. In, Ref. 11, a differential inequality of elliptic type in the exterior vacuum region is derived

$$D_a(V^{-1}D^a\Delta_\mu^+) \geqslant 0, \tag{15}$$

where

$$\Delta_\mu^+ := (W - W_\mu)\frac{(1-V_s^2)^3(1+b-V_s^2)}{(1-V^2)^3(1+b-V^2)}. \tag{16}$$

b is some positive constant to be chosen later. The appropriate boundary condition at infinity is $W-W_\mu=0$. From the maximum principle, Δ_μ^+ has the maximum value at the infinity or at the surface of the star $\{V=V_s\}$. The possibility of maximum value of $W-W_\mu$ occurring at $\{V=V_s\}$ is then removed by choosing b appropriately. Thus $\Delta_\mu^+ \leqslant 0$ holds everywhere and $W_\mu \geqslant W$. $\mu \leqslant M$ is directly derived from the asymptotic expansion of $W_\mu \geqslant W$. Note here that in our case where the black hole is additionally present, the possibility that Δ_μ^+ takes a maximal value at the event horizon cannot be removed, and we cannot use Lemma 6 in Ref. 11 without modifications. We will come back to this point in the next section.

They next introduce M^- and M^+ where M^- satisfies $M^- < M$ and $W_{\mu=M^-} > 0$ on $[V_c, V_s]$ while M^+ satisfies $M^+ > M$ with $W_{\mu=M^+}(V_{M_*^+})=0$ at a point $V_{M_*^+} \in (V_c, V_s)$. The existence of $M^\pm$ is guaranteed by, e.g., Lemma 6.[11] Then, they defined ν by $\nu=\inf_{\mu \in S_c}\mu$ where $S_c=\{\mu \in [M^-, M^+]: W_\mu > 0$ on $(V_c, V_s]$ and $W_\mu(V_c)=0\}$.

In their Lemma 14, they proved that $d^2\psi_\nu/dV^2$ is positive, where $\psi_\mu(V)$ is defined as the solution to the equation

$$\frac{d\psi_\mu}{dV} = \frac{\psi_\mu}{2r_\mu\sqrt{W_\mu}}\left(1 - \frac{2m_\mu}{r_\mu}\right), \tag{17}$$

with $\psi_\mu(V_s)=(1+V_s)/2$ at the surface of the star $\{V=V_s\}$. Finally they define a conformal metric $g_{ij}^+=\Omega_+^4 g_{ij}$, where

$$\Omega_+ = \begin{cases} (1+V)/2 & \text{outside of the star,} \\ \psi_\nu(V) & \text{inside of the star,} \end{cases} \tag{18}$$

and found that the Ricci scalar has the expression

$$R(g_{ij}^+) = (\tilde{W} - W)\frac{8}{\Omega_+^5}\frac{d^2\Omega_+}{dV^2}, \tag{19}$$

where $\tilde{W}=W_\nu$. In defining $\tilde{W}$ precisely, we must take care of the differential structure at the center of stars. As the argument is rather technical, we refer this point to Lemmas 11, 12, 13, 14 and the main theorem in Ref. 11. By Lemmas 6 and 14, this is positive, while the space has zero ADM mass. Here the case of equality in the positive energy theorem can be applied and we conclude that the space is conformally flat, which then implies that an isolated star is spherically symmetric.[16]

IV. PROOF OF NONEXISTENCE OF MATTER OUTSIDE A STATIC BLACK HOLE

Now we turn our attention to the proof of nonexistence of matter outside a static black hole. The various functions *inside* of a star, r_μ, m_μ, ψ_μ, W_μ, and Δ_μ^+ can be introduced without modifications. We adopt the same condition on the equation of state. However, the modification for Lemma 6 is required as mentioned in the previous section.

Lemma 6 in Ref. 11 says that $\tilde{W}-W \geqslant 0$ holds everywhere. In the case of Ref. 11 this inequality was proved by showing $\Delta_\mu^+ < 0$ at $V=V_s$ and by applying the maximum principle for the inequality $D_a(V^{-1}D^a\Delta_\mu^+) \geqslant 0$ which indicates that $\Delta_\mu^+=0$ at infinity is the maximum value. However, presently we have an additional boundary, which is the horizon $\{V=0\}$, and a possibility of $\Delta_\mu^+ > 0$ there remains. We thus have to *assume* $\Delta_\mu^+ < 0$ at the horizon or equivalently

$$(W - W_\mu)_{V=0} \leqslant 0. \tag{20}$$

We will discuss the physical meaning of this hypothesis in the last section. Under this assumption, $W_\mu - W \geqslant 0$ is guaranteed everywhere, and the results in Ref. 11 that were proven using Lemma 6 become available. In particular, the existence of ν is guaranteed.

Now we show the conformal flatness of this space. Consider the two conformal transformations defined by

$$g^{\pm}_{ij} = \Omega^4_{\pm} g_{ij}, \tag{21}$$

where Ω_+ is the same as Eq. (18) and

$$\Omega_- = \tfrac{1}{2}(1 - V). \tag{22}$$

Now we have two manifolds $(\Sigma^{\pm}, g^{\pm}_{ij})$. As in Bunting and Masood-ul-Alam,[14] we can make a smooth manifold out of $\Sigma^+ \cup \Sigma^-$ by gluing along $\{V=0\}$.

The asymptotic behavior of each metric is

$$g^{+}_{ij} = \delta_{ij} + O(r^{-2}) \tag{23}$$

and

$$g^{-}_{ij} dx^i dx^j = (M/2r)^4 (dr^2 + r^2 d\Omega_2^2) + O(r^{-5}). \tag{24}$$

In the manifold (Σ^-, g^-_{ij}), $\{r=\infty\}$ corresponds to a regular point in a three-dimensional surface. Indeed, introducing a new coordinate $R = M^2/4r$, the metric near $r=\infty$ can be written as

$$g^{-}_{ij} dx^i dx^j = dR^2 + R^2 d\Omega_2^2. \tag{25}$$

If the Ricci scalar of this space is non-negative, positive energy theorem tells us that $\Sigma^+ \cup \Sigma^-$ is the flat Euclidean space and thus Σ is conformally flat, because this manifold has the zero ADM mass and non-negative Ricci scalar. Hence, we want to show the non-negativity of the Ricci scalars $R(g^{\pm}_{ij})$.

The three-dimensional Ricci scalar becomes the same as Eq. (19) for Σ^+ and

$$R(g^{-}_{ij}) = 8\pi \Omega_-^{-5} [(1+V)\rho + 6VP] \geqslant 0, \tag{26}$$

for Σ^-. Since $R(g^-_{ij}) \geqslant 0$ holds as above, it remains to show the non-negativity of $R(g^+_{ij})$. $d^2\Omega_+/dV^2 \geqslant 0$ is guaranteed by Lemma 14 in Ref. 11 and $(\tilde{W} - W) \geqslant 0$ is guaranteed by the hypothesis (20). Then the conformally transformed space $\Sigma^+ \cup \Sigma^-$ has non-negative Ricci scalar [see Eq. (19)] and zero ADM mass, which implies that $\Sigma^+ \cup \Sigma^-$ is flat.

Now we have proven under the assumption (20) that the original space Σ is conformally flat. Going back to Eqs. (19) and (26), we find that $R(g^+_{ij}) = R(g^-_{ij}) = 0$ holds and they in turn imply $\tilde{W} = W$ and $\rho = P = 0$, respectively. The latter implies that the spacetime should be vacuum. Our result excludes any static configurations of a black hole with a star whose surface is given by $\{V = V_s\}$ as was suggested in Fig. 1.

We summarize what we have obtained as the following theorem.

Theorem: *In asymptotically flat static black hole spacetimes, the star, which is composed of a perfect fluid satisfying the dominant energy condition and has the surface of level surface set* $\{V = V_s (>0)\}$, *annot exist if (i) the equations of state* $P = P(\rho)$ *satisfies the condition* (12) or (13), *and (ii) for* W_μ *defined by Eq.* (11) *with Eqs.* (7) *and* (8), *the inequality* $W - W_\mu \leqslant 0$ *holds on the event horizon* $(V=0)$.

As a result, the ordinary uniqueness theorem[2] of vacuum spacetimes can be applied and then the spacetime in our setup is reduced to the Schwarzschild spacetime.

V. DISCUSSION

We have proven the nonexistence of matter composed of a perfect fluid under the hypothesis $(W-W_\mu)_{V=0}\leqslant 0$. Because the physical meaning of this hypothesis is still unclear, we examine it in this section. On the event horizon, the value of $\sqrt{W}$ coincides with the surface gravity κ_H of the black hole. We introduce the Komar integral on the event horizon $M_{\mathrm{BH}}=\kappa_H A_H/4\pi$ that indicates the local mass of the black hole, where A_H is the area of the horizon. Then, $(W-W_\mu)_{V=0}\leqslant 0$ corresponds to

$$\mu \leqslant \frac{1}{4\kappa_H} = \frac{A_H}{16\pi M_{\mathrm{BH}}}. \tag{27}$$

The first law of the black hole thermodynamics for the static spacetime $\delta M_{\mathrm{BH}}=\kappa_H \delta A_H/8\pi$ implies $A_H \propto M_{\mathrm{BH}}^2$. Hence, $A_H \sim 16\pi M_{\mathrm{BH}}^2$ and the right hand side of the inequality (27) is $O(M_{\mathrm{BH}})$. In order to find some upper bound on μ in terms of the quantities of the star, recall that $(W-W_\mu)_{V=V_s}\leqslant 0$ holds on the surface of the star as appeared in the proof of Lemma 6 of Ref. 11. This is rewritten as $\sqrt{W_s}\leqslant (1-V_s^2)^2/4\mu$. Integrating over the surface of the star, we find

$$\mu \leqslant \frac{(1-V_s^2)^2}{16\pi M_\star} A_s, \tag{28}$$

where $M_\star$ is the Komar mass of the star and A_s is the area of the surface of the star. Hence, $(W-W_\mu)_{V=0}\leqslant 0$ holds if

$$(1^*-V_s^2)^2 \frac{A_s}{16\pi M_\star} \leqslant \frac{A_H}{16\pi M_{\mathrm{BH}}} \sim M_{\mathrm{BH}}. \tag{29}$$

In order to simplify this inequality, let us consider the situation where a ball-shaped star exists outside a black hole and the distance between them is sufficiently large. In this case V_s^2 is approximated as $V_s^2 \simeq 1-2M_\star/r_s$ and $A_s \simeq 4\pi r_s^2$, where r_s is the radius of the star. Then the inequality becomes

$$M_\star \lesssim M_{\mathrm{BH}}. \tag{30}$$

Therefore the main theorem states that a star with smaller mass than a black hole mass cannot exist outside of the black hole in static spacetimes.

Intuitively, heavy stars are also not permitted to exist outside of black holes in static spacetimes. We hope to have a different argument for proving the statement because our current approach of adapting Lindblom and Masood-ul-Alam's results[11] is not expected to produce optimal statements.

Last, we note that the star surface is assumed to be a surface of one connected component. In order to exclude the configuration of a star whose surface has two or more components such as a shell surrounding the black hole, further considerations are needed.

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Domain walls on the surface of *q*-stars

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We study domain wall networks on the surface of *q*-stars in asymptotically flat or anti de Sitter spacetime. We provide numerical solutions for the whole phase space of the stable field configurations and find that the mass, radius, and particle number of the star is larger but the scalar field, responsible for the formation of the soliton, acquires smaller values when a domain wall network is entrapped on the star surface. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2363254]

I. INTRODUCTION

Planar domain wall networks in theories with three or more vacua have been investigated in a series of papers[1–4] Domain walls seem to have various applications especially in *D*-brane theories.[5,6]

The idea of three-dimensional networks on spherical surfaces has been established in Ref. 7 and applied to the spherical surface of a "large" soliton star.[8] Large soliton stars were investigated in a series of papers by Friedberg *et al.*[9–12] In Ref. 8 it was found that there exist stable with respect to fission into free particles field configurations, corresponding to soliton stars, with a domain wall network on their surface. The pressure of the soliton acts as a stabilizing force to the domain wall network. The star mass is, in general, slightly larger in the presence of the above network, when the particle number and the radius show a more complicated behavior, depending on the surface tension, the particle number, etc. In Ref. 13 the entrapment of the domain wall network on the surface of a soliton of any kind in the absence of gravity was discused. In the same article, another kind of "stability" was discussed, namely the stability of the domain walls. It was found that only two of the five Platonic solids, cube and octahedron, can be realized on a spherical surface. Networks forming other solids would collapse to a single vacuum. So, from now on, when discussing domain walls we restrict ourselves to these two solids.

In the present article we investigate the properties of *q*-stars[14–16] which are relativistic generalizations of *q*-balls[17] that seem to play a special role in baryogenesis through flat directions of supersymmetric extensions of the standard model.[18] Our purpose is to find numerical solutions to the coupled Einstein-scalar fields equations, and to calculate the mass, radius, particle number, and the value of the scalar field at the center of the soliton in the whole phase space (Figs. 1–4). We compare our results with those obtained in the absence of the domain wall network, including in our figures the relevant results, and to the results of Ref. 8, referring to the other family of solitonic stars, and Ref. 13. We also investigate the soliton stability with respect to gravitational collapse and to the decay to free particles.

II. DOMAIN WALL NETWORK ON THE SURFACE OF *q*-STARS

We consider a complex scalar field, ϕ, with a global $U(1)$ symmetry and a suitable potential U, coupled to a complex scalar field, ψ, able to generate a network of domain walls, and to gravity. In order for the ψ field to be able to generate a domain wall network, a

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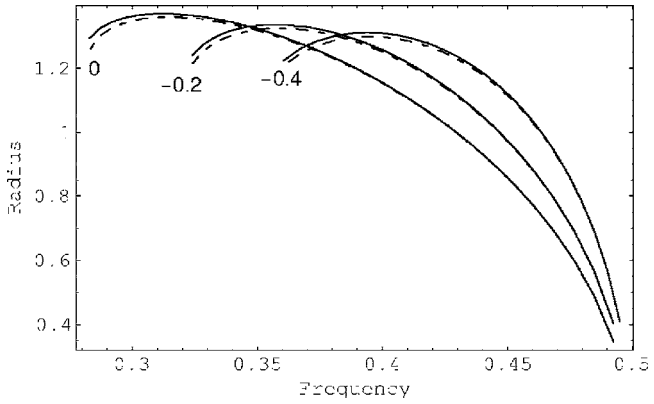

FIG. 1. The radius of the q-star as a function of the frequency. Solid lines correspond to the case with domain walls and dashed to the case without domain walls, i.e., $\beta=0$, included for comparison. The numbers within the figures denote the value of the cosmological constant Λ. The true cosmological constant is $\Lambda \times 8\pi G m^4$, according to Eq. (5).

$$\left| a - \frac{\psi^n}{v^n} \right|^2$$

term should be included in the action, where a is a constant.[1–6] The action of the above configuration is

$$S = \int d^4x\sqrt{-g}\left[\frac{R-2\Lambda}{16\pi G} + \partial_\mu\phi\partial^\mu\phi^* + \frac{1}{v^2}\partial_\mu\psi\partial^\mu\psi^* - U(\phi^*\phi) - \beta^2\left| c(f_0 - \phi^*\phi)\phi^*\phi - \frac{\psi^n}{v^n}\right|^2\right], \tag{1}$$

where Λ stands for the (negative or zero) cosmological constant and the constants β, c, and f_0 will be determined later, n is an integer, and v is a positive constant that can be absorbed in ψ and does not affect the solutions. A Lagrangian with a potential of the form

$$\left| 1 - \frac{\psi^n}{v^n} \right|^2$$

admits solutions corresponding to a domain wall network. In our case we choose

$$\phi(\vec{\rho},t) = \sigma(\rho)e^{-i\omega t}. \tag{2}$$

The field configuration is spherically symmetric, so we can choose a spherically symmetric metric

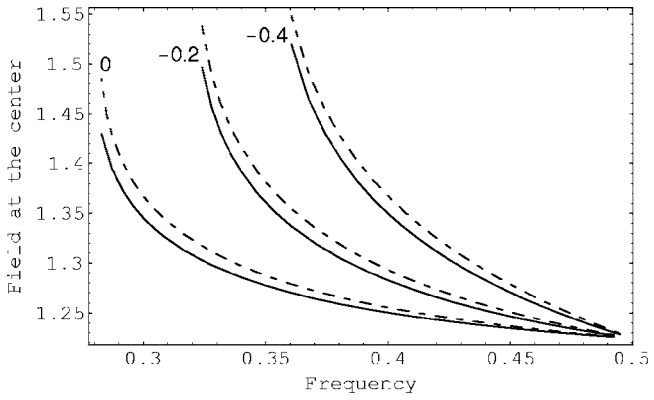

FIG. 2. The value of the scalar field at the center of the star as a function of its freaquency.

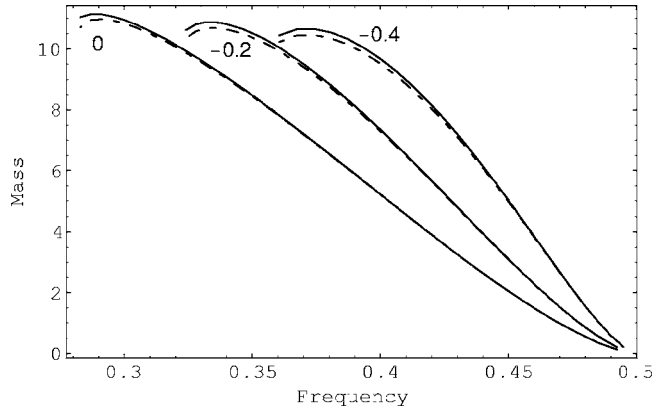

FIG. 3. The mass of a q-star as a function of its frequency.

$$ds^2 = -\frac{1}{B(\rho)}dt^2 + \frac{1}{A(\rho)}d\rho^2 + \rho^2 d\vartheta^2 + \rho^2 \sin^2 \vartheta d\varphi^2. \tag{3}$$

We define

$$W \equiv B\left(\frac{\partial \phi}{\partial t}\right)^*\left(\frac{\partial \phi}{\partial t}\right) = B\omega^2\sigma^2, \quad V \equiv A\left(\frac{\partial \phi}{\partial \rho}\right)^*\left(\frac{\partial \phi}{\partial \rho}\right) = A\sigma'^2 \tag{4}$$

and make the following rescalings:

$$\tilde{\rho} = \rho m, \quad \tilde{\omega} = \omega/m, \quad \tilde{\phi} = \phi/m, \quad \tilde{r} = \epsilon\tilde{\rho},$$

$$\tilde{\beta} = \beta/m^2, \quad \tilde{f}_0 = f_0/m^2, \quad \tilde{c} = cm^4$$

$$\tilde{U} = U/m^4, \quad \tilde{W} = W/m^4, \quad \tilde{V} = V/m^4, \quad \tilde{\Lambda} \equiv \frac{\Lambda}{8\pi G m^4}, \tag{5}$$

with

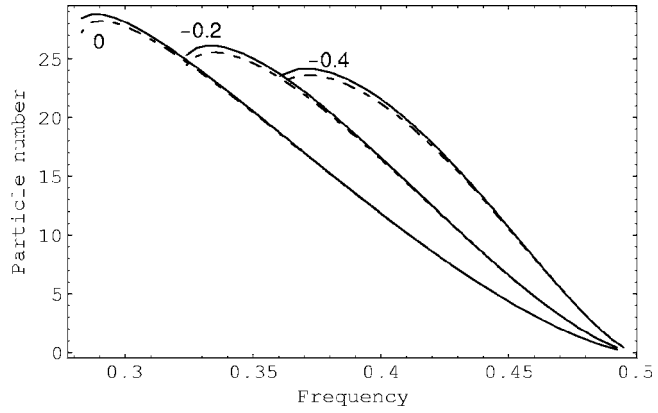

FIG. 4. The particle number of a q-star as a function of its frequency.

$$\epsilon \equiv \sqrt{8\pi G m^2},$$

a very small quantity for $m \sim GeV$. Quantities of the same order of magnitude as ϵ can be neglected. We also choose a rescaled potential

$$U = \phi^* \phi \left(1 - \phi^* \phi + \frac{1}{3} (\phi^* \phi)^2 \right) = \sigma^2 \left(1 - \sigma^2 + \frac{1}{3} \sigma^4 \right), \tag{6}$$

where we dropped tildes for simplicity.

We will now determine the proper values of f_0 and c regarding at present $\beta = 0$. Gravity becomes important when $R \sim GM$. If we regard that the scalar field σ varies very slowly with respect to the radial coordinate then $d\sigma / d\rho \sim \epsilon$ if we set $m = 1$. So, the Euler–Lagrange equation for the scalar field, dropping the tildes and the $O(\epsilon)$ quantities gives

$$\sigma^2 = 1 + \omega B^{1/2}. \tag{7}$$

The eigenvalue equation for the frequency can be obtained by integrating the equation of motion within the surface, where the scalar field varies rapidly from a σ_0 value at the inner edge of the surface, to a zero value at the outer edge. The result of integration is

$$V + W - U = 0, \tag{8}$$

which, in order to match with the interior solution, for which $\sigma' \sim \epsilon$, gives for the eigenfrequency

$$\omega = \frac{A_{\text{sur}}^{1/2}}{2} = \frac{B_{\text{sur}}^{-1/2}}{2}, \tag{9}$$

where A_{sur}, B_{sur} denote the value of the metrics at the surface of the star. In the absence of gravity $B(r) = 1$ and, as one can find from Eqs. (7) and (9), $\sigma^2 = 1.5$. When gravity is under consideration the situation is not too different, unless $B(r) \gg 1$. When $B(0) \to \infty$ the star collapses to a black hole. Excluding this case and regarding only stars in our discussion, we can set $f_0 = 1.5$, which means that the quantity $c(f_0 - \phi^* \phi)\phi^* \phi$ is zero inside and outside the soliton. The only region within which this quantity differs form zero is the very thin surface. The maximum value is at

$$\sigma^2 = \frac{3}{4}.$$

So we set

$$c = \frac{16}{9}$$

and the above quantity takes its proper maximum value: $c(f_0 - \phi^* \phi)\phi^* \phi|_{\max} = 1$. With these settings the field ψ is exactly zero outside the soliton, approximately zero in the interior and maximum within the surface.

We will now turn on the interactions between the two scalar fields. Let $\beta^2 = 0.01$ so as to treat the additional interaction as a perturbation, which does not disturb significantly the system. The equation of motion for the ϕ field, dropping the $O(\epsilon)$ quantities gives

$$\omega^2 B - (\sigma^2 - 1)^2 \left(1 + \frac{128}{9} \beta^2 \sigma^2 \right) + \frac{128}{81} \beta^2 \sigma^2 = 0. \tag{10}$$

The exact solution in the above equation is rather long and ugly, but if we substitute the value $\sigma^2 = 1.5$ (holding true when $B(r) \sim 1$ and $\beta^2 \ll$) in the $\beta^2 \sigma^2$ combination, we find for σ^2,

$$\sigma^2 = 1 + \sqrt{\frac{\omega^2 B + 16\beta^2/3}{1 + 64\beta^2/3}}, \tag{11}$$

which has the right limiting value for $\beta \to 0$ according to the Eq. (7). Integrating again the equation of motion within the surface, we find that the eigenvalue equation for the frequency, Eq. (9), remains valid.

Within the soliton, the ψ field is approximately zero. So, the total energy-momentum tensor is approximately the energy-momentum tensor for the ϕ field, which takes the form

$$T_{\mu\nu} = (\partial_\mu \phi)^* (\partial_\nu \phi) + (\partial_\mu \phi)(\partial_\nu \phi)^* - g_{\mu\nu}[g^{\alpha\beta}(\partial_\alpha \phi)^*(\partial_\beta \phi)] - g_{\mu\nu} U. \tag{12}$$

The Einstein equations are $G_{\mu\nu} = 8\pi G T_{\mu\nu} - \Lambda g_{\mu\nu}$. The independent components, 00 and 11, take the following form, dropping the tildes and the $O(\epsilon)$ quantities

$$\frac{A-1}{r^2} + \frac{A'}{r} = -W - U - \Lambda, \tag{13}$$

$$\frac{A-1}{r^2} - \frac{B'}{r}\frac{A}{B} = W - U - \Lambda, \tag{14}$$

where $U = \sigma^2 - \sigma^4 + 1/3\sigma^6$ and $W = B\omega^2\sigma^2$ and σ is given by Eq. (11). The mass of the field configuration is given by the relation

$$M = 4\pi r\left(1 - A(r) - \frac{1}{3}\Lambda r^3\right), \quad r \to \infty. \tag{15}$$

The particle number is defined as

$$N \equiv \int d^3x j^0, \tag{16}$$

with

$$j^\mu = \sqrt{-g} g^{\mu\nu}{}_1 (\phi^* \partial_\nu \phi - \phi \partial_\nu \phi^*). \tag{17}$$

For the interior, we take for the particle number

$$N = 8\pi \int_0^R r^2 dr \omega \sigma^2 \sqrt{\frac{B}{A}}, \tag{18}$$

where R is the radius of the q-star.

We will now prove that the energy and particle number contributions from the thin surface are negligible. At the exterior, the ϕ field is exactly zero, and consequently the ψ field is zero, and, thus, no energy or particle number contribution arises from the exterior. The surface is of width of order m^{-1}. For the moment we ignore our rescalings. Within the surface $|\phi| \sim m$ and consequently $U \sim W \sim m^4$. Also, the field ϕ varies from a certain value at the inner edge of the surface to a zero value at the outer, so $V \sim (|\phi| m)^2 \sim m^4$. ψ^n / v^n is of the same order of magnitude as $c|\phi^4|$. Because $\tilde{c} \sim 1$, then $c \sim m^{-4}$. Because $\tilde{\beta}^2 \sim 10^{-2}$, then $\beta^2 \sim m^4 10^{-2}$,which means that within the surface $\psi^n / v^n \sim 10^{-2} m^4$. The ψ field contributes to the total energy through the β^2 terms of potential energy and the kinetic terms. The energy density arising from the β^2 terms are of the same order of magnitude as $\beta^2 m^4$. If we repeat the discussion concerning the kinetic terms for the ϕ field, the kinetic terms for the ψ field are of the same order of magnitude as $\beta^2 m^4$. So, the total energy density from the surface (potential for both fields, kinetic from the temporal variation from the field ϕ and kinetic from the spatial variation from both fields) is $\sim m^4$ and the total energy stored within the surface is $\sim 1/(Gm)$. Within the interior the energy density is $\sim m^4$ and the total energy

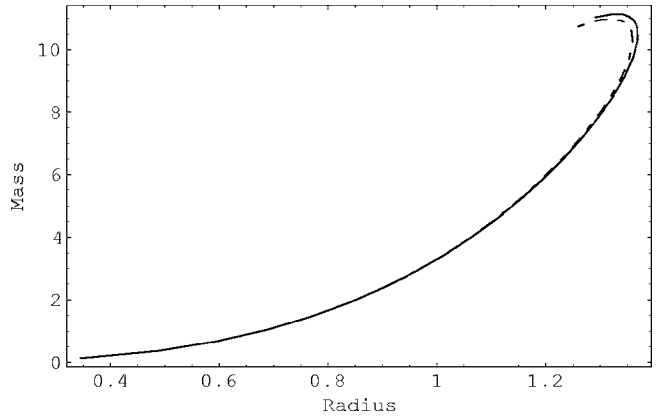

FIG. 5. The mass of the star as a function of its radius for asymptotically flat spacetime. The last stable field configurations with respect to gravitational collapse are at the top of the $M=M(R)$ curves.

is $\sim 1/(G^{3/2}m^2)$. One can see that $E_{\text{surface}} \sim \epsilon E_{\text{interior}}$ and thus the contribution of the surface to the total energy is negligible. The same discussion holds true for the particle number contribution of the surface. These steps reproduce the similar discussion holding true in the case of a "pure" q-star without any additional fields in the total action.

We numerically solve Eqs. (13) and (14) with boundary conditions $A(0)=1$, $A(r)=1/B(r)=1-(1/3)\Lambda r^2$, $r\to\infty$ and find the parameters of the q-star using relations (15)–(18) and (11).

III. CONCLUDING REMARKS

In the present work we investigated the formation of q-stars with a domain wall network on their surface. All the field configurations are stable with respect to fission into free particles because the energy of the free particles with the same charge is smaller than the star mass. They are also stable with respect to gravitational collapse, as one can see from Fig. 5.

We find that the radius, mass, and particle number of the q-star are slightly larger when domain walls are trapped on the star surface. These results agree with the estimation of Ref. 8, concerning the total energy of the soliton. Radius and particle number of large soliton stars, investigated in Ref. 8 show a more complicated dependence on β^2, which is the new parameter differentiating the stars with domain walls from usual, large soliton stars. The results of larger radii and smaller values of the scalar field at the center of the star agree with the similar ones, obtained in Ref. 13, despite the absence of gravity. The same results hold true in asymptotically flat, as well as in asymptotically anti de Sitter spacetime.

Unfortunately, one cannot find an analytical relation connecting the mass and the particle number of the star, due to the highly nonlinear character of the equations of motion. Instead, we use our numerical results, depicted in Fig. 6, in order to study the behavior of the soliton mass as a function of its particle number. From Fig. 6 one can see that our solutions are always stable with respect to fission into free particles, because the soliton energy is always smaller than the total energy of the free particles. For small values of the particle number, gravity is negligible. In the absence of gravity and for a large soliton the so called thin-wall approximation holds. It has been shown that for such solitons $M=\omega N$ plus some surface terms which are negligible in the above approximation, with $\omega \equiv (\sqrt{U/\sigma^2})_{\min}$. As one can see, for the potential 5, ω equals 0.5. Numerical results show clearly that, for small values of the particle number, when gravity is negligible, the ratio mass to particle number equals ω. For larger values of the particle number gravity becomes more important and the negative potential energy contributed by the attractive gravitational force decreases the ratio M to N. From Fig. 6 we also see that the above ratio is larger for smaller values of the (negative) cosmological constant. This reflects the repulsive character of a negative cosmological constant. The star decreases its mass so as to resist to the environment of the "negative" gravity induced by a negative cosmological constant.

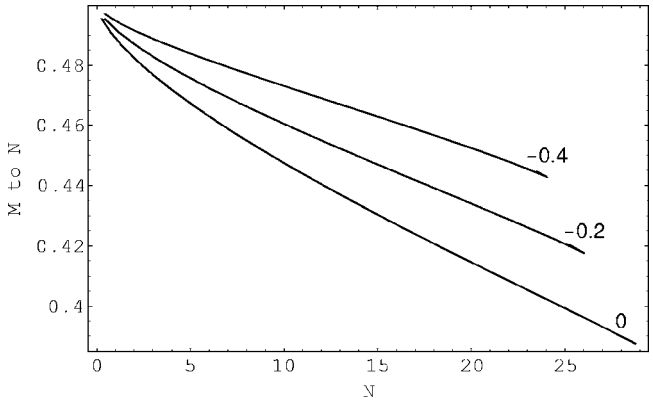

FIG. 6. The ratio mass to particle number of the star as a function of the particle number of the field configurations, for asymptotically flat or anti de Sitter spacetime. For any curve, $\beta^2=0.01$ holds.

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Propagating torsion in the Einstein frame

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The Einstein–Cartan–Saa theory of torsion modifies the spacetime volume element so that it is compatible with the connection. The condition of connection compatibility gives constraints on torsion, which are also necessary for the consistence of torsion, minimal coupling, and electromagnetic gauge invariance. To solve the problem of positivity of energy associated with the torsionic scalar, we reformulate this theory in the Einstein conformal frame. In the presence of the electromagnetic field, we obtain the Hojman–Rosenbaum–Ryan–Shepley theory of propagating torsion with a different factor in the torsionic kinetic term. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2365788]

I. INTRODUCTION

In the Einstein–Cartan theory, which extends general relativity to nonsymmetric connection, spin is the source of torsion.[1] The equations relating torsion and spin are algebraic and torsion does not propagate.[2] To allow such a propagation, we need a differential equation for the torsion tensor $S^{\rho}{}_{\mu\nu}$. This is usually achieved by modifying the Einstein–Hilbert action and introducing a scalar field related to the torsion vector $S_{\nu}=S^{\mu}{}_{\mu\nu}$.[3–6] There are also models in which the torsion vector is proportional to the electromagnetic potential.[7–9]

The Lagrangian density for a gravitational field can be, in principle, given by any scalar constructed from the curvature, connection, and metric. The standard Einstein–Hilbert Lagrangian of general relativity is linear in the curvature scalar R and torsion enters the dynamics through R. Such a Lagrangian is very natural from a physical point of view since it is linear in the second derivatives of the metric tensor. These derivatives can be taken out of the action using the Gauß theorem, making the Lagrangian a function of the metric and its first derivatives only.[10] The corresponding equations of field are thus second order. If the gravitational Lagrangian is a more general function of R or other curvature invariants, the field equations remain second order if we adopt the Palatini variational principle according to which the connection and metric are *a priori* independent quantities and we vary the action with respect to both of them.[11] In this approach, the connection arises from the field equations and is not metric compatible, $g_{\mu\nu;\rho}\neq 0$ (except the case where the Lagrangian is linear in R and there is no torsion).

The Palatini variation of connection imposes four algebraic constraints on the matter part of the action, which are caused by invariance of the curvature scalar under a projective transformation of the connection.[12,13] These constraints lead to inconsistencies that can be eliminated by replacing the connection with its projective-invariant part.[13] This procedure is equivalent to imposing the condition $S_{\mu}=0$.[14] In this case, we cannot associate the gradient of a scalar field with the torsion vector and induce the propagation of torsion. Therefore, we follow the metric variational principle and fix the connection by assuming its metricity, $g_{\mu\nu;\rho}=0$.

In the presence of torsion, we must modify the covariant volume element so that it remains parallel.[6,15] Such a modification is possible only if S_{μ} is the gradient of a scalar, which gives four equations of constraint on the torsion tensor.[16] This condition is also necessary for the compat-

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ibility of torsion and gauge invariance of the minimally coupled electromagnetic field (the Hojman–Rosenbaum–Ryan–Shepley or HRRS theory of propagating torsion).[3] (According to the Palatini principle of minimal coupling, the electromagnetic field tensor is defined as $F_{\mu\nu}=A_{\nu,\mu}-A_{\mu,\nu}$ and does not generate torsion.[14]) A generalization of the HRRS theory to non-Abelian gauge fields has been done in Ref. 17.

In this paper we point out that the equations of field resulting from the action with the torsion-modified volume element violate positivity of energy for the torsionic scalar. The solution to this problem is to apply a conformal transformation of the original metric into a new metric in which the field equations have the form of those in general relativity.[18,19] This new metric defines the *Einstein frame* while the original one defines the *Jordan frame*.[20] In Sec. II we review the Einstein–Cartan theory with the torsion-modified volume element. In Sec. III we reformulate this theory in the Einstein conformal frame and apply it to the gauge invariant electrodynamics in the presence of torsion. The results are briefly summarized in Sec. IV.

II. COVARIANT VOLUME IN THE PRESENCE OF TORSION

In general relativity, a minimally coupled theory is constructed by replacing the metric of special relativity $\eta_{\mu\nu}$ with the metric of general relativity $g_{\mu\nu}$, and by replacing ordinary derivatives with covariant derivatives (the comma–semicolon rule).[10] The covariant derivative of a vector V_μ is defined as

$$V_{\nu;\mu}=V_{\nu,\mu}-\left\{{}_{\mu}{}^{\rho}{}_{\nu}\right\}V_\rho. \tag{1}$$

The coefficients $\{{}_{\mu}{}^{\rho}{}_{\nu}\}$ are the Christoffel symbols:

$$\left\{{}_{\mu}{}^{\rho}{}_{\nu}\right\}=\frac{1}{2}g^{\rho\lambda}(g_{\nu\lambda,\mu}+g_{\mu\lambda,\nu}-g_{\mu\nu,\lambda}), \tag{2}$$

determined from the relation $g_{\mu\nu;\rho}=0$. The colon denotes a covariant derivative with respect to the Christoffel symbols, and the comma denotes a usual derivative. In the presence of torsion $S^{\rho}{}_{\mu\nu}=\Gamma_{[\mu}{}^{\rho}{}_{\nu]}$, the covariant derivative is given by

$$V_{\nu;\mu}=V_{\nu,\mu}-\Gamma_{\mu}{}^{\rho}{}_{\nu}V_\rho. \tag{3}$$

The semicolon denotes a covariant derivative with respect to the nonsymmetric connection, and the connection coefficients $\Gamma_{\mu}{}^{\rho}{}_{\nu}$ are now

$$\Gamma_{\mu}{}^{\rho}{}_{\nu}=\left\{{}_{\mu}{}^{\rho}{}_{\nu}\right\}+S^{\rho}{}_{\mu\nu}-2S_{(\mu\nu)}{}^{\rho}. \tag{4}$$

This relation results from the metric compatibility of the connection, $g_{\mu\nu;\rho}=0$. [In the presence of torsion, the relation $g_{\mu\nu;\rho}=0$ remains valid, which means that both covariant derivatives (with respect to $\{{}_{\mu}{}^{\rho}{}_{\nu}\}$ and $\Gamma_{\mu}{}^{\rho}{}_{\nu}$, respectively) are tensors.] The difference $\Gamma_{\mu}{}^{\rho}{}_{\nu}-\{{}_{\mu}{}^{\rho}{}_{\nu}\}$, which is a tensor, is called the contortion $K^{\rho}{}_{\mu\nu}$:

$$K^{\rho}{}_{\mu\nu}=S^{\rho}{}_{\mu\nu}-2S_{(\mu\nu)}{}^{\rho}. \tag{5}$$

In a spacetime without torsion, a covariant volume element is $\sqrt{-g}d^4x$, and the scalar density $\sqrt{-g}$ is connection compatible (parallel): $(\sqrt{-g})_{;\mu}=0$. When the spacetime is not torsionless, this element is not parallel since[21]

$$(\sqrt{-g})_{;\mu}=-2S_\mu\sqrt{-g}. \tag{6}$$

It is possible to find a parallel volume element if the torsion vector is the gradient of a scalar:[15,16]

$$S_\mu=\theta_{,\mu}. \tag{7}$$

In this case we have

$$(e^{2\theta}\sqrt{-g})_{;\mu}=0, \tag{8}$$

and the volume element becomes

$$dV_4=e^{2\theta}\sqrt{-g}d^4x. \tag{9}$$

The contortion tensor (5) can be split into a traceless part and a trace (the torsion vector):

$$K_{\rho\mu\nu}=C_{\rho\mu\nu}-\frac{2}{3}(S_\rho g_{\nu\mu}-S_\nu g_{\rho\mu}). \tag{10}$$

The Riemann–Cartan curvature tensor is given by

$$R^\sigma{}_{\mu\rho\nu}(\Gamma)=\Gamma_\nu{}^\sigma{}_{\mu,\rho}-\Gamma_\rho{}^\sigma{}_{\mu,\nu}+\Gamma_\nu{}^\kappa{}_\mu\Gamma_\rho{}^\sigma{}_\kappa-\Gamma_\rho{}^\kappa{}_\mu\Gamma_\nu{}^\sigma{}_\kappa, \tag{11}$$

and its contractions are the Ricci tensor $R_{\mu\nu}(\Gamma)=R^\rho{}_{\mu\rho\nu}(\Gamma)$ and the curvature scalar $R(\Gamma,g)=R_{\mu\nu}(\Gamma)g^{\mu\nu}$. The curvature scalar $R(\Gamma,g)$ can be split into the Riemannian curvature scalar $R(g)$ (constructed from $\{_\mu{}^\rho{}_\nu\}$ the same way as $R(\Gamma,g)$ is constructed from $\Gamma_\mu{}^\rho{}_\nu$) and the part that contains torsion:[6]

$$R(\Gamma,g)=R(g)-4S^\mu{}_{;\mu}+\frac{16}{3}S_\mu S^\mu+C_{\mu\nu\rho}C^{\mu\rho\nu}. \tag{12}$$

The Lagrangian density for the gravitational field in the Einstein–Cartan–Saa theory with the torsion-modified volume element is given by[6]

$$\mathcal{L}=\frac{1}{16\pi}R(\Gamma,g)\sqrt{-g}e^{2\theta}, \tag{13}$$

where we use the units in which $c=G=1$. The second term on the right-hand side of Eq. (12) is a total covariant divergence of a vector (with respect to the nonsymmetric connection $\Gamma_\mu{}^\rho{}_\nu$) and does not contribute to the field equations. [From Eq. (8) we obtain $\int S^\mu{}_{;\mu}\sqrt{-g}e^{2\theta}d^4x=\int(S^\mu\sqrt{-g}e^{2\theta})_{,\mu}\,d^4x$. The last integral can be transformed into an integral over a three-dimensional hypersurface, which vanishes when we use the principle of least action.] In the same equation we use the condition (7). For the reason explained in the next section, we replace the scalar field θ by another field ϕ such that

$$\theta=-\frac{3}{2}\phi. \tag{14}$$

The action for the gravitational field is thus

$$S_g=\int d^4x\sqrt{-g}e^{-3\phi}\left(-\frac{1}{16\pi}R(g)-\frac{3}{4\pi}\phi_{,\mu}\phi^{,\mu}-\frac{1}{16\pi}C_{\mu\nu\rho}C^{\mu\rho\nu}\right). \tag{15}$$

We note that if $C_{\mu\nu\rho}=0$, replacing the torsionic scalar by a new field $\varphi=e^{-3\phi}$ reproduces the Brans–Dicke action with $\omega=-\frac{4}{3}$.[22]

III. SCALAR TORSION IN THE EINSTEIN FRAME

In the action (15), the kinetic term of the torsionic scalar field has the negative sign. By a sufficiently rapid change of ϕ with time, this term can consequently be made as large as one likes. The action would then decrease without limit, that is, there could be no minimum. This is a feature of many scalar–tensor theories of gravity in the metric variational formalism.[19,20] To solve this problem, we need to apply a conformal transformation of the metric from the original Jordan frame to the Einstein frame. In the Einstein frame, the curvature scalar in the action is multiplied

by a constant only, and the equations of field have the form of the Einstein equations.[18] Let us make a conformal transformation from the Jordan metric $g_{\mu\nu}$ to a new metric $h_{\mu\nu}$:

$$h_{\mu\nu}=e^{\lambda}g_{\mu\nu}, \tag{16}$$

where λ is a function of the coordinates. The Jordan and Einstein curvature scalars are related by[23]

$$R(g)=e^{\lambda}\left(R(h)+3\lambda^{:\mu}{}_{\mu}-\frac{3}{2}\lambda_{,\mu}\lambda^{,\mu}\right), \tag{17}$$

and all the quantities of the right-hand side of this equation are calculated using the new metric $h_{\mu\nu}$.

To eliminate the exponential function multiplying $R(g)$ in Eq. (15), we put

$$\lambda=-3\phi. \tag{18}$$

The action for the gravitational field in the Einstein frame becomes

$$S_g=\int d^4x\sqrt{-h}\left(-\frac{1}{16\pi}R(h)+\frac{3}{32\pi}\phi_{,\mu}\phi^{,\mu}-\frac{1}{16\pi}C_{\mu\nu\rho}C^{\mu\rho\nu}\right), \tag{19}$$

where the traceless part of the contortion in the new action is given by

$$K_{\rho\mu\nu}=C_{\rho\mu\nu}-\frac{2}{3}(S_{\rho}h_{\nu\mu}-S_{\nu}h_{\rho\mu}). \tag{20}$$

[To obtain Eq. (19), we notice that we can rewrite (10) as $K_{\rho}{}^{\mu}{}_{\nu}=C_{\rho}{}^{\mu}{}_{\nu}-\frac{2}{3}(S_{\rho}\delta^{\mu}_{\nu}-S_{\nu}\delta^{\mu}_{\rho})$ that does not contain the metric, and that $C_{\mu\nu\rho}C^{\mu\rho\nu}$ scales under the conformal transformation (16) like R.] The sign of the kinetic term for the scalar field is now positive. The action (19) differs from the expression obtained without using the parallel volume element (9) by the factor $\frac{1}{4}$ in the scalar kinetic term.[24] (The action in Ref. 24 has $C_{\mu\nu\rho}=0$.)

Let us apply the obtained results to the case of the electromagnetic field coupled minimally to torsion. The electromagnetic field tensor is a spacetime without torsion given by

$$F_{\mu\nu}=A_{\nu:\mu}-A_{\mu:\nu}, \tag{21}$$

and is invariant under a gauge transformation $A_{\mu}\rightarrow A'_{\mu}=A_{\mu}+\Lambda_{,\mu}$. In the presence of torsion, the principle of minimal coupling requires the following definition:

$$F_{\mu\nu}=A_{\nu;\mu}-A_{\mu;\nu}=A_{\nu,\mu}-A_{\mu,\nu}-2S^{\rho}{}_{\mu\nu}A_{\rho}. \tag{22}$$

Such a tensor is invariant under a generalized gauge transformation,

$$A_{\mu}\rightarrow A'_{\mu}=A_{\mu}+e^{\phi}\,\delta^{\nu}_{\mu}\Lambda_{,\nu}, \tag{23}$$

provided that the torsion tensor is given by[3]

$$S^{\rho}{}_{\mu\nu}=\frac{1}{2}(\delta^{\rho}_{\nu}\phi_{,\mu}-\delta^{\rho}_{\mu}\phi_{,\nu}). \tag{24}$$

This relation means that the torsion tensor is fully determined in terms of the torsion vector $S_{\mu}=S^{\nu}{}_{\nu\mu}$, and this vector has a potential, $S_{\mu}=-\frac{3}{2}\phi_{,\mu}$. The above constraint on torsion contains the condition for the existence of a parallel volume element (7), but is stronger. The tensor (22) becomes

$$F_{\mu\nu}=A_{\nu,\mu}-A_{\mu,\nu}-A_{\nu}\phi_{,\mu}+A_{\mu}\phi_{,\nu}, \tag{25}$$

which looks more elegant if we use ϕ instead of θ.

The total gauge invariant action for the electromagnetic field and the gravitational field with torsion is given by

$$S=\int d^4x\sqrt{-h}\left(-\frac{1}{16\pi}R(h)+\frac{3}{32\pi}\phi_{,\mu}\phi^{,\mu}-\frac{3}{32\pi}m^2\phi^2-\frac{1}{16\pi}F_{\mu\nu}F^{\mu\nu}\right), \tag{26}$$

where we introduce a mass of the torsionic field[24,25] (see the next paragraph). The equations of field are obtained from variation of $h_{\mu\nu}$, ϕ, and A^{μ}:

$$G_{\mu\nu}(h)=\frac{3}{2}\left(\phi_{,\mu}\phi_{,\nu}-\frac{1}{2}\phi_{,\rho}\phi^{,\rho}h_{\mu\nu}\right)+\frac{3}{4}m^2\phi^2h_{\mu\nu}$$

$$+2\left(\frac{1}{4}F_{\rho\sigma}F^{\rho\sigma}h_{\mu\nu}-F_{\mu\rho}F_{\nu}{}^{\rho}\right), \tag{27}$$

$$\phi^{:\mu}{}_{\mu}+m^2\phi+\frac{4}{3}(F^{\mu\nu}A_{\nu})_{:\mu}=0, \tag{28}$$

$$F^{\mu\nu}{}_{:\nu}+F^{\mu\nu}\phi_{,\nu}=0, \tag{29}$$

where $G_{\mu\nu}(h)$ is the Einstein tensor. They differ from the equations derived in the HRRS theory[3,24] by the factor $\frac{1}{4}$ in the torsionic scalar field terms. The last two equations yield

$$\phi^{:\mu}{}_{\mu}+m^2\phi=-\frac{2}{3}F_{\mu\nu}F^{\mu\nu}. \tag{30}$$

The reason for the torsionic scalar field to be massive originates from the Eötvös–Dicke–Braginsky solar tests of the principle of equivalence[26] and the idea introduced in Ref. 25. For the scalar field of the Sun, Eq. (30) becomes

$$\nabla^2\phi-m^2\phi=\frac{1}{3}(\mathbf{B}^2-\mathbf{E}^2), \tag{31}$$

where **B** and **E** are the magnetic and electric field, respectively. The solution of Eq. (31) outside the Sun is

$$\phi=\frac{2}{3}\frac{e^{-mr}}{r}E_{ne}, \tag{32}$$

where E_{ne} is the total nuclear electric energy of the Sun and other energies are negligible. The data from Ref. 26 give

$$\phi=0.67\times10^{-4}U\cdot e^{-mr}, \tag{33}$$

where r is the distance from the Sun and U is the Newtonian potential. This expression modifies the relative acceleration between aluminum and gold/platinum[26] by the factor e^{-mR}, where R is the distance of the Earth from the Sun:

$$\mathbf{a}_{\mathrm{rel}}=2\times10^{-7}\ \nabla U\cdot e^{-mR}. \tag{34}$$

To avoid violations of the principle of equivalence in the solar system and obtain a theory compatible with experiment, we need

$$2\times10^{-7}\ \nabla U\cdot e^{-mR}<10^{-12}\ \nabla U. \tag{35}$$

This inequality gives the lower limit on the mass of the torsionic scalar field,[24]

$$m > 10^{-25}\ \mathrm{GeV}, \tag{36}$$

in agreement with Ref. 25.

IV. SUMMARY

In the presence of torsion, a covariantly conserved volume element can be found if the torsion vector equals the gradient of a scalar. This condition gives four equations of constraint on the torsion tensor. Remarkably, the condition for the compatibility of the gauge invariant electromagnetic field coupled minimally to torsion contains this constraint. Another condition for this compatibility is that the traceless part of the contortion tensor must vanish. The last requirement is a consequence of the equations of field in the Jordan frame, if we use the electromagnetic field that does not couple to torsion. It is not the case for the minimal coupling between torsion and photons. A possible solution would be to assume that the electromagnetic field couples to the trace part of the torsion tensor only. Ultimately, we should obtain this requirement as a result of a variational principle.

The action integral over the torsion-modified volume element contains the kinetic term of the torsionic scalar field with the negative sign. By a sufficiently rapid change of this field with time, this term can consequently be made arbitrarily large, and the action would have no minimum. To solve this problem, we applied a conformal transformation of the metric from the original Jordan frame to the Einstein frame in which the left side of the field equations is that of general relativity. The new action acquired the correct, positive sign in the kinetic term for the torsionic scalar. The obtained field equations differ from those in the original HRRS theory by the factor $\frac{1}{4}$ in the torsionic scalar field terms. This difference does not affect the order of the minimal value for the mass m of the torsionic scalar required for the theory to be compatible with experiment.

The minimal value of m is way below the masses of known elementary particles. There is no upper limit for m, and the Higgs boson could be a good candidate for the particle corresponding to the torsionic scalar. Since the lower limit on the mass of the Higgs boson is on the order of 100 GeV, the deviations from the principle of equivalence would be unnoticeable (below 10^{-27} of present experimental precision).

We emphasize that the question of whether the electromagnetic field couples to torsion or not should be ultimately answered by experiment. We assumed that the principle of minimal coupling holds in the presence of torsion, which leads to the appearance of the EM–torsion coupling and constraints on the torsion tensor. Otherwise, torsion does not affect the electromagnetic field and gauge invariance of the latter is compatible with nonsymmetric connection under no additional constraints.

We mentioned that the HRRS procedure of combining electromagnetic gauge invariance with minimal coupling between the EM field and torsion has been generalized to non-Abelian gauge fields such as the Yang–Mills field. A possible coupling between spin, which generates torsion in the Einstein–Cartan theory, and the non-Abelian chromomagnetic field of QCD would play an important role in objects composed of fermionic matter at large densities. Neutron stars would be ideal candidates to study this coupling and determine whether gauge fields interact with torsion.

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Variational approach to Robertson–Walker spacetimes with homogeneous scalar fields

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Existence of solutions between prescribed configurations is proved for spatially flat Robertson–Walker spacetimes coupled with homogeneous scalar field sources, using a modified version of the Euler–Maupertuis least action variational principle. The solutions are obtained as limits of approximating variational problems, solved using the techniques originally introduced by Rabinowitz. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2383068]

I. INTRODUCTION

Observational cosmology suggests that our universe has entered a stage of accelerated expansion (see Refs. 17 and 18, and references therein). The reason for that is the so called *dark energy*, that constitutes most of the energy density of the whole universe. The existence of a cosmological constant can be called as responsible for dark energy, but some physical problems arise from this interpretation. The most important alternative physical interpretation for dark energy origin calls into play scalar field models of spacetime (see Ref. 14, and references therein). In the latest years of theoretical physics, the belief for existence of *zero-spin* particles—whose description is given in terms of a wave *scalar* function—has gained supporters, although there is no observational evidence yet.

We shall concentrate here on the simple model of Robertson–Walker spacetimes with homogeneous scalar fields, and in this case the Einstein field equations read

$$(G_0^0 = 8\pi T_0^0): \quad -\frac{3\dot{a}^2}{a^2} = -(\dot{\phi}^2 + 2V(\phi)), \tag{1.1a}$$

$$(G_1^1 = 8\pi T_1^1): -\frac{\dot{a}^2 + 2a\ddot{a}}{a^2} = (\dot{\phi}^2 - 2V(\phi)), \tag{1.1b}$$

where the dot denotes differentiation with respect to t, $a(t)$ is the scale factor and $\phi(t)$ is the scalar field.

We will be interested in the problem of determining solutions of Eqs. (1.1a) and (1.1b) with fixed end points. The metric becomes singular when $a(t)$ vanishes in the past or in the future—corresponding to big-bang or big-crash singularity, respectively. In this paper we want to avoid this situation, so we will consider pieces of evolution where $a(t)$ keeps positive. The central result of the paper is the following theorem:

Theorem 1.1: *Let* $a_0, a_1 \in \mathbb{R}^+$, $\phi_0, \phi_1 \in \mathbb{R}$ *be such that*

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$$3\min\{a_0,a_1\}(a_1-a_0)^2 > \max\{a_0,a_1\}(\phi_1-\phi_0)^2, \tag{1.2}$$

and let $V\in\mathcal{C}^1(\mathbb{R},\mathbb{R})$ *such that*

$$V(\phi)>0, \quad \forall\ \phi\in\mathbb{R}. \tag{1.3}$$

Then, there exists $T>0$ *and* $[a(t),\phi(t)]\in\mathcal{C}^2([0,T],\mathbb{R}^2)$ *solutions of Eqs.* (1.1a) and (1.1b) *with the boundary conditions*

$$a(0)=a_0, \quad a(T)=a_1, \quad \phi(0)=\phi_0, \quad \phi(T)=\phi_1. \tag{1.4}$$

Note that the above result cannot be seen as a consequence of the well-known theory on the existence of solutions for Cauchy problems in general relativity (see pioneering work by Bruhat,[2] and the following literature). Here, indeed, we do not fix both fundamental forms on a Cauchy surface, and find evolution from it, but we show that, under the above condition, the set of initial data can be completed in order to reach a certain configuration from a given one. The solutions under our study stay regular in the interval $[0, T]$, since $a(t)>0$. Nevertheless, we believe that this approach may be useful to find the existence results for scalar field solutions evolving to singularity, a topic which is of relevant interest in the problems related to the cosmic censorship conjecture. In fact, although existence and causal structure of the singularities in matter-filled spacetimes has been so far widely investigated in the case of fluid-elastic matter (see Ref. 6, and references therein) for scalar fields the situation is fully understood only in the very special case of nonself-interacting, massless particles.[3,4] The homogeneous collapse with potential has been treated only in special cases, by Joshi *et al.* (who have also investigated on loop quantum gravity effects in Ref. 9) and in Ref. 5, where the collapse features are characterized by the dependence of the energy density on the scale factor a; an important open question in which models with potentials have been used is also that of cosmic censorship violation in AdS.[10,11]

We will cast the above problem into a suitable variational framework. The use of a variational approach in general relativity study is not a novelty, of course: for instance, some of the most important results in the relativistic gravitational lensing problem are reviewed in Ref. 15. In the present paper, actually, the variational approach is used to determine solutions of Einstein field equations, i.e., spacetimes. Hilbert–Palatini action,[13,19] indeed, provides a functional whose critical points with respect to variation of the metric g yields solutions of Einstein field equations. The particular case under our study produces the functional Eq. (2.2), which is an integral made on the interval $[0, T]$ of definition of the solutions. Of course, since T is let free in principle, it must be treated as an unknown for the system, but this problem may be circumvented by using the functional Eq. (2.15) in the space of curves reparameterized on the interval $[0, 1]$. Although the functional Eq. (2.15) seems in principle more complicated to deal with than Eq. (2.2), critical point existence can be obtained as a limit of a sequence of variational problems, for which Rabinowitz' saddle point theorem[16] techniques apply.

The outline of the paper is as follows. Section II is devoted to an exposition of the variational formulation for the problem; Section III briefly outlines the general theory that applies to the approximating variational problems introduced in Sec. IV, and studied in Sec. V. Section VI contains the proof of the main Theorem 1.1.

II. THE VARIATIONAL PRINCIPLE

In the case under study it can be easily shown that the action functional is the following:

$$\mathcal{L}(a,\phi)=\int_0^T 3(\dot{a}^2(t)+a(t)\ddot{a}(t))a(t)+a^3(t)(\dot{\phi}^2(t)-2V(\phi(t)))\ \mathrm{d}t. \tag{2.1}$$

We can integrate by parts the term in Eq. (2.1) containing $\ddot{a}(t)$. We ignore the contribution of the boundary term $3a^2\dot{a}|_0^T$ coming from the integration. This exactly amounts[19] to modify the functional Eq. (2.1), adding the contribution $(1/16\pi)\int_{\partial M}K$ of the trace of the extrinsic curvature K integrated along the boundary ∂M of the spacetime. All in all, we obtain

$$\mathcal{L}(a,\phi)=\int_0^T 3a(t)\dot{a}^2(t)-a^3(t)\dot{\phi}^2(t)+2a^3(t)V(\phi(t))\mathrm{d}t, \tag{2.2}$$

and the following proposition holds.

Proposition 2.1. If $(a,\phi)\in\mathcal{C}^2(\mathbb{R}^+,\mathbb{R})$ solves the Euler–Lagrange equation for $\mathcal{L}$, and

$$3\dot{a}(0)^2=a_0^2(\dot{\phi}(0)^2+2V(\phi_0)), \tag{2.3}$$

then it is a solution of Eqs. (1.1a) and (1.1b).

Proof: This is a standard result, consequence of Nöther's theorem, but an *ad hoc* proof can be easily given. Indeed, the Euler–Lagrange equations for the functional Eq. (2.2) read

$$\dot{a}^2+2a\ddot{a}=-a^2(\dot{\phi}^2-2V(\phi)), \tag{2.4a}$$

$$\ddot{\phi}+V'(\phi)=-3\frac{\dot{a}}{a}\dot{\phi}, \tag{2.4b}$$

where the condition $a\neq 0$ has also been used. Using these equations, the quantity $a(3\dot{a}^2-a^2(\dot{\phi}^2+2V))$ is easily seen to be constant with respect to t, and then if Eq. (1.1a) holds at the initial time—which is just condition (2.3)—then it vanishes during the whole evolution. Since $a\neq 0$, we therefore obtain Eq. (1.1a). Equation (1.1b) is equivalent to Eq. (2.4a). ■

Remark 2.2: A *partial* converse of Proposition above can be of course given, using the following identity:

$$T^{\mu}_{0;\mu}=-2\dot{\phi}\left(\ddot{\phi}+V'(\phi)+3\frac{\dot{a}}{a}\dot{\phi}\right). \tag{2.5}$$

The left hand side above is the zero-component of the divergence of T,[19] and it vanishes if the Einstein equations hold, due to the conservation of energy (Bianchi identity). Therefore, if $\dot{\phi}$ is everywhere nonzero, Eq. (2.4b) holds.

Actually, the converse result can be improved further.

Proposition 2.3: If $(a,\phi):[0,T]\to\mathbb{R}^+\times\mathbb{R}$ are $\mathcal{C}^2$ solutions of (1.1a) and (1.1b) with $\phi\equiv\phi_0$ on $[0, T]$, then they solve Eqs. (2.4a) and (2.4b). In particular Eq. (2.3) holds.

Proof: Only Eq. (2.4b) must be proved. Let $G(t)$ be the (continuous) function $G(t):=\ddot{\phi}(t)+V'(\phi(t))+3(\dot{a}(t)/a(t))\dot{\phi}(t)$, and assume by contradiction the existence of $t_0\in[0,T]$ such that $G(t_0)\neq 0$. Therefore, considered the (closed) set $C=\{t\in[0,T]:\dot{\phi}(t)=0\}\subsetneq[0,T]$, the Bianchi identity Eq. (2.5) implies the existence of a closed interval $[\alpha,\beta]$ such that

$$t_0\subset[\alpha,\beta]\subseteq C, \tag{2.6}$$

and that is maximal with respect to this property Eq. (2.6). We will show $G=0$ on $[\alpha,\beta]$, getting a contradiction. Since $[\alpha,\beta]$ is strictly contained in $[0, T]$ then $\alpha>0$ or $\beta<T$ (or both). Let us assume for instance $\alpha>0$. Since $\dot{\phi}_{|[\alpha,\beta]}=0$, and ϕ is $\mathcal{C}^2$, then $\ddot{\phi}_{|[\alpha,\beta]}=0$ and $\phi(t)=\phi(\alpha)$, $\forall t\in[\alpha,\beta]$. These facts imply

$$G(t)=V'(\phi(\alpha)),\quad \forall\, t\in[\alpha,\beta]. \tag{2.7}$$

Maximality of $[\alpha,\beta]$ with respect to Eq. (2.6) implies the existence of a sequence $\alpha_n\notin C$, $\alpha_n\to\alpha^-$. Then $\dot{\phi}(\alpha_n)\neq 0$ and therefore $G(\alpha_n)=0$ by Eq. (2.5), therefore the continuity of G and Eq. (2.7) finally imply

$$0=\lim_{n\to\infty}G(\alpha_n)=\lim_{t\to\alpha^-}G(t)=V'(\phi(\alpha)),$$

obtaining $G(t)=0$ on $[\alpha,\beta]$. ■

Remark 2.4: If ϕ is everywhere constant one can easily find counterexamples where Eqs. (1.1a) and (1.1b) hold but Eq. (2.4b) does not. This is a well known fact in relativistic elasticity theory, where equivalence between the Bianchi identity and the Euler–Lagrange equations (i.e., Nöther theorem) holds under the assumption that the deformation tensor has maximum rank. We refer the reader to Ref. 12 for further details on this topic. In the scalar field theory, the gradient $\nabla\phi$ plays the role of this deformation tensor. For our purposes here, anyway, we will only use Proposition 2.1.

The problem of finding the solutions of Eqs. (1.1a) and (1.1b) with fixed end points is brought to the study of critical points of the functional Eq. (2.2) with fixed end points and under the initial condition (2.3). Of course, since the arrival time T is left free so far, one can reparameterize the functions on the interval $[0, 1]$, with the obvious drawback to promote T as a new unknown of the problem. But this problem can be overcome, applying the following (general) variational principle.[1,7]

Theorem 2.5: *Let $(\mathfrak{M}, g)$ be a semi-Riemannian manifold, W a $\mathcal{C}^1$ function on $\mathfrak{M}$, $E \in \mathbb{R}$ and $p, q \in \mathfrak{M}$.*

(1) *If $y:[0,1]\to\mathfrak{M}$ is a critical point for the functional*

$$\mathfrak{F}(y) = \left(\int_0^1 \frac{1}{2} g\left(\frac{\mathrm{d}}{\mathrm{d}s} y(s), \frac{\mathrm{d}}{\mathrm{d}s} y(s)\right) \mathrm{d}s\right)\left(\int_0^1 E - W(y(s))\mathrm{d}s\right) \tag{2.8}$$

with positive critical value, in the space of $\mathcal{C}^2$ curves defined in $[0, 1]$, such that $y(0)=p$, $y(1)=q$, called

$$T_0 = \left(\frac{\displaystyle\int_0^1 \frac{1}{2} g\left(\frac{\mathrm{d}}{\mathrm{d}s} y, \frac{\mathrm{d}}{\mathrm{d}s} y\right) \mathrm{d}s}{\displaystyle\int_0^1 E - W(y(s))\mathrm{d}s}\right)^{1/2}, \tag{2.9}$$

then the curve $x:[0,T_0]\to\mathfrak{M}$, $x(t)=y(T_0 s)$ is a critical point for the functional

$$L(x) = \int_0^T \frac{1}{2} g\left(\frac{\mathrm{d}}{\mathrm{d}t} x(t), \frac{\mathrm{d}}{\mathrm{d}t} x(t)\right) - W(x(t))\mathrm{d}t, \tag{2.10}$$

with $T=T_0$, in the space of $\mathcal{C}^2$ curves satisfying the conditions

$$x(0) = p, \quad x(T) = q, \quad \frac{1}{2} g\left(\frac{\mathrm{d}}{\mathrm{d}t} x(t), \frac{\mathrm{d}}{\mathrm{d}t} x(t)\right) + W(x(t)) = E. \tag{2.11}$$

(2) *Vice versa, let us fix $T>0$, and let $x:[0,T]\to\mathfrak{M}$ be a critical point for the functional Eq. (2.10) in the space of $\mathcal{C}^2$ curves $\gamma:[0,T]\to\mathbb{R}$ satisfying conditions (2.11). If $\int_0^T (1/2) g((\mathrm{d}/\mathrm{d}t)x(t), (\mathrm{d}/\mathrm{d}t)x(t))\mathrm{d}t \neq 0$, then the reparameterization $y:[0,1]\to\mathfrak{M}$ of x on [0, 1], (i.e., $y(s)=x(Ts)$), is a critical point for the functional Eq. (2.8), with positive critical value, in the space of $\mathcal{C}^2$ curves defined in [0, 1], such that $y(0)=p$, $y(1)=q$.*

Proof: Let $y(s):[0,1]\to\mathfrak{M}$ be a critical point for $\mathfrak{F}$ (2.8). The fixed end point first variation of this functional and an integration by parts gives

$$\left(\int_0^1 E - W(y(s))\mathrm{d}s\right)\frac{\mathrm{D}^2}{\mathrm{d}s^2} y(s) + \left(\int_0^1 \frac{1}{2} g\left(\frac{\mathrm{d}}{\mathrm{d}s} y(s), \frac{\mathrm{d}}{\mathrm{d}s} y(s)\right) \mathrm{d}s\right) \nabla W(y(s)) = 0 \tag{2.12}$$

that is, using the value of T_0 given by (2.9) (well defined since the critical value is positive)

$$\frac{1}{T_0^2}\frac{\mathrm{D}^2}{\mathrm{d}s^2}y(s)+\nabla W(y(s))=0, \quad \forall\, s\in[0,1]. \tag{2.13}$$

Let $x:[0,T_0]\to\mathfrak{M}$ be the reparameterization of y on the interval $[0,\ T_0]$ (i.e., $x(t)=y(t/T_0)$). Therefore, Eq. (2.13) becomes nothing but the Euler–Lagrange equation for the functional Eq. (2.10) with $T=T_0$. Moreover, contracting the left hand side of Eq. (2.13) with $(\mathrm{d}/\mathrm{d}s)y(s)$, we obtain the existence of a constant K such that

$$\frac{1}{T_0^2}\frac{1}{2}g\left(\frac{\mathrm{d}}{\mathrm{d}s}y(s),\frac{\mathrm{d}}{\mathrm{d}s}y(s)\right)+W(y(s))=K, \quad \forall\, s\in[0,1]. \tag{2.14}$$

Integrating both sides above between 0 and 1, and using Eq. (2.9), we obtain $E=K$, and so

$$\frac{1}{2}g\left(\frac{\mathrm{d}}{\mathrm{d}t}x(t),\frac{\mathrm{d}}{\mathrm{d}t}x(t)\right)+W(x(t))=E, \quad \forall\, t\in[0,T_0].$$

Conversely, let $x(t):[0,T]\to\mathfrak{M}$ be a critical point for Eq. (2.10) in the space of $\mathcal{C}^2$ curves defined in $[0,\ T]$, satisfying Eq. (2.11), and $y(s):[0,1]\to\mathfrak{M}$ be its reparameterization: $y(s)=x(Ts)$. Since $\mathrm{d}/\mathrm{d}s=T(\mathrm{d}/\mathrm{d}t)$, Eq. (2.14) holds with T_0 and K replaced by T and E, respectively. Integrating both sides of Eq. (2.14) in $[0,\ 1]$ implies that T is equal to the value of T_0 given by Eq. (2.9). Moreover, $\mathrm{d}/\mathrm{d}s=T(\mathrm{d}/\mathrm{d}t)$ also implies Eq. (2.13), and substituting the value of T_0 given by Eq. (2.9) we find that $y(s)$ satisfies Eq. (2.12), that is the critical point equation for the functional Eq. (2.8), and the proof is complete. ■

Remark 2.6: The variational principle given above, is actually a sort of modified version of the classical Euler–Maupertuis least action principle. The above proof is an adaptation of the one given in Ref. 7 for the Euclidean case, and may not completely stress the link with the classical principle. For a deeper insight, we refer the reader to the review[8] by the same author.

Applying this variational principle to functional Eq. (2.2) (with $E=0$), the following problem provides solutions of homogeneous scalar field equation with fixed end points.

Problem: Let $a_0,\ a_1\in\mathbb{R}^+,\ \phi_0,\ \phi_1\in\mathbb{R}$, and $V\in\mathcal{C}^1(\mathbb{R},\mathbb{R})$.

Find the critical points of the functional

$$F(a,\phi)=\left(\int_0^1 3a(t)\dot{a}^2(t)-a^3(t)\dot{\phi}^2(t)\mathrm{d}t\right)\left(\int_0^1 2a^3(t)V(\phi(t))\mathrm{d}t\right), \tag{2.15}$$

with positive critical value, in the space of $\mathcal{C}^2$ curves $(a,\phi):[0,1]\to\mathbb{R}^+\times\mathbb{R}$ such that

$$a(0)=a_0, \quad a(1)=a_1, \quad \phi(0)=\phi_0, \quad \phi(1)=\phi_1. \tag{2.16}$$

III. THE FUNCTIONAL FRAMEWORK AND THE ABSTRACT CRITICAL POINTS THEORY

We first recall the classical notion of the Palais–Smale condition.

Definition 3.1: Let $\mathcal{X}$ a Hilbert manifold of class $\mathcal{C}^1$ and $f\in\mathcal{C}^1(\mathcal{X},\mathbb{R})$. We say that f satisfies the *Palais–Smale condition at level c* ($(PS)_c$) if any sequence $\{x_n\}_{n\in,\mathbb{N}}\subset\mathcal{X}$ such that

$$f(x_n)\to c, \quad \text{and} \quad \nabla f(x_n)\to 0$$

(where ∇f represents the gradient of f with respect to the Hilbert structure of $\mathcal{X}$) has a converging subsequence in $\mathcal{X}$. The sequence $\{x_n\}$ with properties above is called a *Palais–Smale sequence* for f.

Definition 3.2: We say that $x\in\mathcal{X}$ is a *critical point* of f if $\nabla f(x)=0$. A value $c\in\mathbb{R}$ such that there exists a critical point x with $f(x)=c$ is a *critical value* for f. A value $c\in\mathbb{R}$ which is not critical will be called *regular*.

Theorem 3.3: *Let* $\mathcal{X}=\Omega\times Y$, *where* Ω *is a Hilbert manifold and* Y *is a finite dimensional*

affine space. Let $\|\cdot\|$ *denote the norm on* Y, *and let* $f \in \mathcal{C}^1(\mathcal{X},\mathbb{R})$. *Assume that*

(1) *there exists* $\omega_0 \in \Omega$, $e_0 \in Y$, *and* $R>0$ *such that, called* $B_R(e_0)=\{e \in E: \|e-e_0\| \leqslant R\}$, *it is*

$$b_0 \equiv \sup_{e \in \partial B_R(e_0)} f(\omega_0,e) < b_1 \equiv \inf_{\omega \in \Omega} f(\omega,e_0);$$

(2) *if* $b_2=\sup_{e \in B_r(e_0)} f(\omega_0,e)$, *the strip* $\{x \in \mathcal{X}: b_1 \leqslant f(x) \leqslant b_2\} \subset \mathcal{X}$ *is complete; and*
(3) f *satisfies* $(PS)_c$ *at any* $c \in [b_1,b_2]$.

Then, there exists a critical value c *for* f *in* $[b_1,b_2]$.

The proof can be obtained adapting the scheme developed in Ref. 16. However, the idea behind is quite simple. If, by contradiction, $[b_1,b_2]$ is made by regular value only, using the gradient flow of the functional f one obtains the existence of a homotopy sending the sublevel $\{x \in \mathcal{X}: f(x) \leqslant b_2\}$ to the sublevel $\{x \in \mathcal{X}: f(x) \leqslant b_1\}$ letting $\{x \in \mathcal{X}: f(x) \leqslant b_1\}$ fixed. Therefore, using the projection on Y and the retraction of Y on $B_R(e_0)$, and observing that $b_0<b_1$, one can define a homotopy that sends $B_R(e_0)$ to its boundary $\partial B_R(e_0)$—recall that $b_2=\sup_{e \in B_R(e_0)} f(x_0,e)$—and that lets $\partial B_R(e_0)$ fixed, which is impossible in finite dimension.

IV. AN APPROXIMATION SCHEME

By assumption (1.2) of Theorem 1.1, we know that $a_0 \neq a_1$. To fix ideas, without loss of generality we can assume

$$a_0 > a_1, \tag{4.1}$$

so that Eq. (1.2) becomes

$$3a_1(a_1-a_0)^2 > a_0^3(\phi_1-\phi_0)^2.$$

We can choose constants m,M such that $0<m<a_1<a_0<M<+\infty$ and

$$3m(a_1-a_0)^2 - M^3(\phi_1-\phi_0)^2 > 0. \tag{4.2}$$

Consider the Hilbert manifold

$$\Omega = \{a \in H^1([0,1],\ ]m,M[\ ): a(0)=a_0, a(1)=a_1\}, \tag{4.3}$$

where $H^1([0,1],]m,M[)$ is the set of absolutely continuous functions defined on [0, 1], with values on $]m,M[$, such that $\int_0^1 \dot{a}^2 \mathrm{d}t < +\infty$. Let us observe that Ω is a *not* complete Hilbert manifold with Hilbert structure

$$\langle a_1,a_2\rangle = \int_0^1 \dot{a}_1(t)\dot{a}_2(t)\mathrm{d}t.$$

We denote by $\|a\|_\Omega$ the norm induced by the above inner product

$$\|a\|_\Omega = \left(\int_0^1 \dot{a}(t)\mathrm{d}t\right)^{1/2}. \tag{4.4}$$

Now set $\phi_*(t)=(1-t)\phi_0+t\phi_1$. Since $V>0$, we have

$$\inf_{t \in [0,1]} V(\phi_*(t)) \equiv v_* > 0. \tag{4.5}$$

Let us also consider the affine space

$$Y = \{\phi = \hat{\phi} + \phi_* : \hat{\phi} \in H_0^1([0,1],\mathbb{R})\}, \tag{4.6}$$

where $H_0^1([0,1],\mathbb{R}) = \{\phi \in H^1([0,1],\mathbb{R}) : \phi(0) = \phi(1) = 0\}$. Y is a closed affine subspace of $H^1([0,1],\mathbb{R})$, with norm

$$\|\phi\|_Y = \left(\int_0^1 \dot{\phi}^2(t) \mathrm{d}t \right)^{1/2}. \tag{4.7}$$

Since $\dim Y = +\infty$ we cannot apply Theorem 3.3 *as is* to our setting, and then we approximate Y by a sequence Y_k, defined as follows: for any $k \in \mathbb{N}$ set

$$W_k = \mathrm{span}\{\sin(\pi \ell t) : t \in [0,1], \ell = 1, \ldots, k\}, \tag{4.8}$$

and

$$Y_k = \{\phi = \hat{\phi}_k + \phi_* : \hat{\phi}_k \in W_k\}.$$

Remark 1: Since $\{\sqrt{2}\sin(\pi \ell t)\}_{\ell \in \mathbb{N}}$ is a complete orthonormal system of $H_0^1([0,1],\mathbb{R})$, if $\phi = \hat{\phi} + \phi_* \in Y$ and $\hat{\phi}_k$ denotes the projection of $\hat{\phi}$ on W_k, then $\hat{\phi}_k \to \hat{\phi}$ in H_0^1, with tejpect to the norm defined in Eq. (4.7).

We shall apply Theorem 3.3 to the space $\mathfrak{X}_k = \Omega \times Y_k$. Since Ω is not complete, and V is not bounded in general, we modify the functional F (2.5) and look for critical points $\mathfrak{x}_{\epsilon,\lambda}$, with positive critical value, of a suitable functional $F_{\epsilon,\lambda}$. Some estimates for the critical points $x_{\epsilon,\lambda}$ will show that they are critical points for F, whenever ϵ is sufficiently small, and λ sufficiently large.

Let $\chi: \mathbb{R}^+ \to \mathbb{R}^+$ of class $\mathbb{C}^1$, such that $\chi(s) = 0$ if $s \leqslant 0$ and $\chi(s) = s^2$ if $s > 0$. Fix $\epsilon \in]0,1]$, and define

$$U_\epsilon(a) = \chi\left(\frac{1}{a-m} - \frac{1}{\epsilon}\right) + \chi\left(\frac{1}{M-a} - \frac{1}{\epsilon}\right). \tag{4.9}$$

Moreover, consider $\psi: \mathbb{R} \to \mathbb{R}$ of class $\mathcal{C}^1$ such that $\psi(s) = s$ if $s \leqslant 0$, $\psi(s) = 1$ if $s \geqslant 1$, and ψ is strictly increasing on the interval $]0,1[$. Fix $\lambda > 0$ and define

$$V_\lambda(\phi) = \psi(V(\phi) - \lambda) + \lambda. \tag{4.10}$$

Observe that $V_\lambda = V$ whenever $V(\phi) \leqslant \lambda$. Finally, define

$$F_{\epsilon,\lambda}(a,\phi) = \int_0^1 [(3a + U_\epsilon(a))\dot{a}^2 - a^3\dot{\phi}^2]\mathrm{d}t \cdot \int_0^1 2a^3 V_\lambda(\phi)\mathrm{d}t. \tag{4.11}$$

It is a straightforward computation to show that the above functional is $\mathcal{C}^1$. In the next section we shall show how to apply Theorem 3.3 to $F_{\epsilon,\lambda}$ on the space $\Omega \times Y_k$.

V. CRITICAL POINTS FOR THE FUNCTIONAL $F_{\epsilon,\lambda}$.

The aim of this section is to prove the following result.

Proposition 1: For any $k \in \mathbb{N}$ there exists $x_k = (a_k, \phi_k)$ critical point of $F_{\epsilon,\lambda}$ on $\mathcal{X}_k$ such that

$$F_{\epsilon,\lambda}(x_k) \in [b_1, b_2],$$

where b_1, b_2 are positive, and independent of k.

We must first show that hypotheses (1)–(2) of Theorem 3.3 hold for $F_{\epsilon,\lambda}$ on $\mathcal{X}_k = \Omega \times Y_k$. The key point will be to show (3), namely the Palais–Smale condition (Definition 3.1). This will be done in Lemma 5.3. First, let us prove the validity of hypotheses (2).

Lemma 5.2: Denoted by F^c the sublevel $F^c = \{x \in \Omega \times E : F(x) \leqslant c\}$, then the set $F^c \cap \mathcal{X}_k$ is complete in $\mathfrak{X}_k$.

Proof: Take a Cauchy sequence $x_n = (a_n, \phi_n) \in \Omega \times E_k$. Since the closure of Ω is complete, and

so is E_k, then there exists $(a,\phi)\in\bar{\Omega}\times E_k$ such that $a_n\to a$ in H^1 and $\phi_n\to\phi$ in H^1. Now $\int_0^1 a_n^3 V_\lambda(\phi_n)\mathrm{d}t\to\int_0^1 a^3 V_\lambda(\phi)\mathrm{d}t$ which is strictly positive, and $\int_0^1(3a_n\dot{a}_n^2-a_n^3\dot{\phi}_n^2)\mathrm{d}t\to\int_0^1 3a\dot{a}^2-a^3\dot{\phi}^2\mathrm{d}t$.

If $a(t)\in\,]m,M[\,\forall t$, then (a_n,ϕ_n) converges in $\Omega\times E_k$. The proof is complete as one shows that there is no possibility that some $\bar{t}\in\,]0,1[$ exists such that either $a(\bar{t})=m$ or $a(\bar{t})=M$. By contradiction, suppose for instance

$$\exists\bar{t}\text{:}a(\bar{t})=m,\quad a(t)>m\ \forall\, t\in[0,\bar{t}[. \tag{5.1}$$

Observe that $F_{\epsilon,\lambda}(a_n,\phi_n)\leqslant c$, $\int_0^1 a^3 V_\lambda(\phi)\mathrm{d}t>0$, and $\int_0^1(3a\dot{a}^2-a^3\dot{\phi}^2)\mathrm{d}t$ is finite. We will show that the hypothesis (5.1) implies

$$\int_0^{\bar{t}} U_\epsilon(a_n)\dot{a}_n^2\mathrm{d}t\to+\infty,$$

obtaining a contradiction.

Since $a_n\to a$ uniformly, $\forall\epsilon>0$ there exists $\bar{s}<\bar{t}$ and $n_0\in\mathbb{N}$ such that

$$|a_n(t)-m|\leqslant\epsilon,\quad \forall\, t\in[\bar{s},\bar{t}],\quad \forall\, n\geqslant n_0.$$

Fix ϵ such that $m+\epsilon<M$. Then, recalling the definition of U_ϵ, it will suffice to show that

$$\lim_{n\to\infty}\int_{\bar{s}}^{\bar{t}}\frac{\dot{a}_n^2}{(a_n-m)^2}\mathrm{d}t=+\infty, \tag{5.2}$$

which easily follows from the following estimate:

$$\left(\int_{\bar{s}}^{\bar{t}}\frac{\dot{a}_n^2}{(a_n-m)^2}\mathrm{d}t\right)^{1/2}\geqslant\frac{1}{\sqrt{\bar{t}-\bar{s}}}\int_{\bar{s}}^{\bar{t}}\frac{|\dot{a}_n|}{a_n-m}\mathrm{d}t\geqslant\frac{1}{\sqrt{\bar{t}-\bar{s}}}\left|\int_{\bar{s}}^{\bar{t}}\frac{\dot{a}_n}{a_n-m}\mathrm{d}t\right|=\frac{1}{\sqrt{\bar{t}-\bar{s}}}\left|\log\left(\frac{a_n(\bar{t})-m}{a_n(\bar{s})-m}\right)\right|,$$

that diverges because $a_n(\bar{t})\to a(\bar{t})=m$ whereas $a_n(\bar{s})\to a(\bar{s})<m$ ■.

The lemma below show that the Palais–Smale condition actually holds in every closed interval of $\mathbb{R}$.

Lemma 5.3: Fixed two values c_1,c_2 such that $0<c_1<c_2<+\infty$, the functional $F_{\epsilon,\lambda}$ satisfies $(PS)_c$, $\forall c\in[c_1,c_2]$.

Proof: Let (a_n,ϕ_n) be a Palais–Smale sequence for $F_{\epsilon,\lambda}$ such that $F_{\epsilon,\lambda}(a_n,\phi_n)\in[c_1,c_2]$ for any n. Since $\nabla F_{\epsilon,\lambda}(a_n,\phi_n)$ is infinitesimal we have, $\forall\,\theta\in W_k$ (recall (4.8))

$$|\nabla F_{\epsilon,\lambda}(a_n,\phi_n)[0,\theta]|\leqslant\delta_n\|\theta\|_{H_0^1},\quad\text{with }\delta_n\to 0.$$

Therefore,

$$\left|\left(\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t\right)\int_0^1(-2a_n^3\dot{\phi}_n\dot{\theta})\mathrm{d}t+\left(\int_0^1(3a_n+U_\epsilon(a_n))\dot{a}_n^2-a_n^3\dot{\phi}_n^2\mathrm{d}t\right)\int_0^1 2a_n^3 V_\lambda'(\phi_n)[\theta]\mathrm{d}t\right|$$
$$\leqslant\delta_n\|\theta\|_{H_0^1}.$$

Multiplying end terms of the inequality chain above by the bounded and strictly positive quantity $\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t$ we have

$$\left|\left(\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t\right)^2\int_0^1(-2a_n^3\dot{\phi}_n\dot{\theta})\mathrm{d}t+F_{\epsilon,\lambda}(a_n,\phi_n)\int_0^1 2a_n^3 V_\lambda'(\phi_n)\theta\mathrm{d}t\right|\leqslant\hat{\delta}_n\|\theta\|_{H_0^1}, \tag{5.3}$$

where $\hat{\delta}_n:=\delta_n\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t\to 0$. Since $\phi_n-\phi_*\in W_k$ we can choose $\theta=\phi_n-\phi_*$, and observe the following facts:

- $\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t$ is bounded away from 0, independently of n,

- $F_{\epsilon,\lambda}(a_n,\phi_n)$ is bounded,
- $a_n^3 V_\lambda(\phi_n)$ is uniformly bounded, and
- $\|\phi_n-\phi_*\|L^\infty \leqslant \|\dot\phi-(\phi_1-\phi_0)\|L^1 \leqslant \|\dot\phi-(\phi_1-\phi_0)\|L^2$.

But $\int_0^1 a_n^3\dot\phi_n\dot\theta \mathrm{d}t=\int_0^1 a_n^3(\dot\phi_n^2-\dot\phi_n(\phi_1-\phi_0))\mathrm{d}t$ which behaves like $\int_0^1\dot\phi_n^2\mathrm{d}t$ if $\int_0^1\dot\phi_n^2\mathrm{d}t$ diverges—recall that $\|\theta\|_{H_0^1}=\|\dot\theta\|_{L^2}$. Then, by Eq. (5.3) we deduce the existence of a positive constant D_0 such that

$$\int_0^1 \dot\phi_n^2 \mathrm{d}t \leqslant D_0, \quad \forall\, n \in \mathbb{N}. \tag{5.4}$$

Since $m \leqslant a_n \leqslant M$, $F_{\epsilon,\delta}(a_n,\phi_n)\leqslant c$, and $\int_0^1 2a_n^3 V_\lambda(\phi_n)\mathrm{d}t$ is bounded away from zero we deduce, by Eq. (5.4), that $\int_0^1(3a_n+U_\epsilon(a_n))\dot a_n^2\mathrm{d}t$ is bounded; moreover, since $3a_n+U_\epsilon(a_n)\geqslant 3a_1>0\,\forall\, n\in,\mathbb{N}$, there exists a positive constant D_1 such that

$$\int_0^1 \dot a_n^2 \mathrm{d}t \leqslant D_1, \quad \forall\, n \in \mathbb{N}. \tag{5.5}$$

By Eqs. (5.4) and (5.5), there exists a and ϕ of class H^1 such that, up to subsequences

$$a_n \rightharpoonup a, \quad \phi_n \rightharpoonup \phi$$

weakly in H^1 and uniformly. Since $F(a_n,\phi_n)$ is bounded from above, arguing as in Lemma 5.2 one proves that $a(t)\in\,]m,M[,\forall\, t\in[0,1]$. Therefore, it remains to show

$$\dot a_n \to \dot a \quad \text{in } L^2([0,1],\mathbb{R}), \tag{5.6}$$

and

$$\dot\phi_n \to \dot\phi \quad \text{in } L^2([0,1],\mathbb{R}). \tag{5.7}$$

Observing that $\phi_n-\phi\in W_k$, we can choose $\theta=\phi_n-\phi$ in Eq. (5.3). Since $F_{\epsilon,\lambda}(a_n,\phi_n)$ is bounded by standard estimates it is not difficult to obtain Eqs. (5.6) and (5.7) ■.

Proof of Proposition 5.1: As already outlined, the aim is to apply Theorem 3 to the functional $F_{\epsilon,\lambda}$. In view of Lemmas 5.2 and 5.3, it still remains to show that hypothesis (3) holds. Take $a_*(t)=(1-t)a_0+ta_1$, and choose $\omega_0=a_*$, $e_0=\phi_*$. Note that, by Eq. (4.5) and the choice of m, we have

$$\int_0^1 a^3 V_\lambda(\phi_*)\mathrm{d}t \geqslant m^3 v_* > 0, \quad \forall\, a\in\Omega,\ \forall\,\lambda \geqslant \sup_{t\in[0,1]} V(\phi_*). \tag{5.8}$$

Moreover by assumption (4.2) we have, for any $a\in\Omega$,

$$\int_0^1 [(3a+U_\epsilon(a))\dot a^2 - a^3\dot\phi_*^2]\mathrm{d}t \geqslant \int_0^1 3m\dot a^2 - M^3(\phi_1-\phi_0)^2\mathrm{d}t \geqslant 3m(a_1-a_0)^2 - M^3(\phi_1-\phi_0)^2 > 0,$$

therefore, by Eq. (5.8),

$$b_1 := \inf F_{\epsilon,\lambda}(a,\phi_*) > 0. \tag{5.9}$$

Clearly, $b_1=b_1(m,M)$ and is independent of k. Actually, b_1 is independent of λ too, but this property won't be used here.

Since V_λ is bounded,

$$\sup_{\mathbb{R}} V_\lambda \equiv B_\lambda < +\infty,$$

and

$$\int_0^1 a_*^3 V_\lambda(\phi)\mathrm{d}t \leqslant a_0^3 B_\lambda.$$

Moreover, if ϵ is sufficiently small, $U_\epsilon(a_*(t))=0\,\forall\, t$, so

$$F_{\epsilon,\lambda}(a_*,\phi) = \int_0^1 (3a_*\dot{a}_*^2 - a_*^3\dot{\phi}^2)\mathrm{d}t \int_0^1 2a_*^3 V_\lambda(\phi)\mathrm{d}t,$$

but $\int_0^1(3a_*\dot{a}_*^2-a_*^3\dot{\phi}^2)\mathrm{d}t \leqslant \int_0^1(3a_*\dot{a}_*^2-m^3\dot{\phi}^2)\mathrm{d}t$, and then there exists $R>0$ independent of k such that

$$\sup_{\|\hat{\phi}\|_{E_k}=R} F_{\epsilon,\lambda}(a_*,\hat{\phi}+\phi_*) =: b_0 < b_1, \tag{5.10}$$

(note that b_0 depends on λ) and then hypothesis (1) of Theorem 3.3 also holds. This implies that there exists a critical value for the functional $F_{\epsilon,\lambda}$ on $\mathfrak{X}_k$ in the interval $[b_1,b_2]$, where

$$b_2 := \sup_{\|\hat{\phi}\|_{E_k}\leqslant R} F_{\epsilon,\lambda}(a_*,\hat{\phi}+\phi_*) \tag{5.11}$$

and since b_2, though depending on λ, is independent of k, the proof is complete. ■

VI. PROOF OF THE MAIN RESULT

To complete the proof of Theorem 1.1, using Proposition 5.1, we first need the following lemma. Recall the definitions of b_1, b_2 given in Eqs. (5.9) and (5.11).

Lemma 6.1: There exists a critical value of $F_{\epsilon,\lambda}$ on $\mathcal{X}=\Omega\times E$ in $[b_1,b_2]$.

Proof: Let $x_k=(a_k,\phi_k)$ the critical point given by Proposition 5.1. Arguing as in the proof of Lemma 3 we deduce the existence of $x=(a,\phi)\in\mathfrak{X}$ such that, up to subsequence

$$x_k \to x \quad \text{in } H^1.$$

We will show that x is a critical point of $F_{\epsilon,\lambda}$. Since $F_{\epsilon,\lambda}(x_k)\in[b_1,b_2]$ and $F_{\epsilon,\lambda}$ is continuous, it immediately will follow that $F_{\epsilon,\lambda}(x)\in[b_1,b_2]$.

Take (α,θ) in H_0^1, and consider θ_k, the orthogonal projection of θ on W_k. As observed in Remark 4.1, $\theta_k\to\theta$ in H^1. Since $\nabla F_{\epsilon,\lambda}(x_k)[\alpha,\theta_k]=0$ for any k, we have

$$\nabla F_{\epsilon,\lambda}(x)[\alpha,\theta] = \nabla F_{\epsilon,\lambda}(x)[\alpha,\theta-\theta_k] + (\nabla F_{\epsilon,\lambda}(x) - \nabla F_{\epsilon,\lambda}(x_k))[\alpha,\theta_k],$$

Let us observe that, since $[\alpha,\theta_k]$ is bounded in H^1, and—recalling that $F_{\epsilon,\lambda}$ is $\mathcal{C}^1$—$\nabla F_{\epsilon,\lambda}(x_k)\to\nabla F_{\epsilon,\lambda}(x)$, then $(\nabla F_{\epsilon,\lambda}(x)-\nabla F_{\epsilon,\lambda}(x_k))[\alpha,\theta_k]\to 0$. Moreover,

$$\nabla F_{\epsilon,\lambda}(x)[\alpha,\theta-\theta_k]\to 0,$$

, since $\theta_k\to\theta$ in H^1. Then $\nabla F_{\epsilon,\lambda}(x)[\alpha,\theta]=0,\forall\,\alpha,\theta$ in H_0^1, and the proof is complete. ■

Proof of Theorem 1.1: Recall first that, looking for solutions of Eqs. (1.1a) and (1.1b) in the space of curves (a,ϕ) defined on $[0,T]$ and with boundary conditions (1.4), amounts to find critical points for the functional Eq. (2.15) in the space of curves (a,ϕ) defined in [0, 1] with boundary conditions (2.16).

The above lemma ensures the existence of $(a_{\epsilon,\lambda},\phi_{\epsilon,\lambda})$, critical point of $F_{\epsilon,\lambda}$ in $\Omega\times E$, with critical value in $[b_1,b_2]$. First, let us observe that a simple bootstrap argument shows that both $a_{\epsilon,\lambda}$ and $\phi_{\epsilon,\lambda}$ are $\mathcal{C}^2$. Then the following conservation law follows from the variational principle:

$$(3a_{\epsilon,\lambda}+U_\epsilon(a_{\epsilon,\lambda}))\dot{a}_{\epsilon,\lambda}^2 - a_{\epsilon,\lambda}^3\dot{\phi}_{\epsilon,\lambda}^2 - 2a_{\epsilon,\lambda}^3 V_\lambda(\phi_{\epsilon,\lambda}) = 0. \tag{6.1}$$

Since $a_{\epsilon,\lambda}^3(\dot{\phi}_{\epsilon,\lambda}^2+2V_\lambda(\phi_{\epsilon,\lambda}))>0,\forall\, t$, then $\dot{a}_{\epsilon,\lambda}(t)\neq 0,\forall\, t$, and since we have supposed (see (4.1)) $a_0>a_1$ it is

$$\dot{a}_{\epsilon,\lambda}(t) < 0, \quad \forall\, t \in [0,1]$$

and

$$a_1 \leqslant a_{\epsilon,\lambda}(t) \leqslant a_0, \quad \forall\, t \in [0,1].$$

Then $a_{\epsilon,\lambda}(t)$ is bounded away from m and M. Taking a sufficiently small ϵ we have

$$m + \epsilon < a_{\epsilon,\lambda}(t) < M - \epsilon$$

so that $U_\epsilon(a_{\epsilon,\lambda})=0$, $U'_\epsilon(a_{\epsilon,\lambda})=0$ and therefore the couple $(a_\lambda, \phi_\lambda) := (a_{\epsilon,\lambda}, \phi_{\epsilon,\lambda})$ is a critical point of

$$F_\lambda(a,\phi) := \int_0^1 (3a\dot{a}^2 - a^3\dot{\phi}^2)\mathrm{d}t \cdot \int_0^1 2a^3 V_\lambda(\phi)\mathrm{d}t,$$

with the critical value in $[b_1, b_2]$. Moreover, the conservation law (6.1) takes the form

$$3a_\lambda \dot{a}_\lambda^2 - a_\lambda^3 \dot{\phi}_\lambda^2 - 2a_\lambda^3 V_\lambda(\phi_\lambda) = 0. \tag{6.2}$$

Recalling that $\dot{a}_\lambda$ is negative, that implies

$$\frac{\dot{a}_\lambda}{a_\lambda} = -\sqrt{\frac{\dot{\phi}_\lambda^2 + 2V_\lambda(\phi_\lambda)}{3}}.$$

Integrating the above relation in [0, 1] we obtain

$$a_\lambda(t) = a_0 e^{-(1/\sqrt{3})\int_0^t \sqrt{\dot{\phi}_\lambda^2 + 2V_\lambda(\phi_\lambda)}\mathrm{d}s},$$

and in particular

$$a_1 = a_0 e^{-(1/\sqrt{3})\int_0^1 \sqrt{\dot{\phi}_\lambda^2 + 2V_\lambda(\phi_\lambda)}\mathrm{d}s}.$$

But $a_1 > 0$ is of course fixed and therefore independent of λ, then there exists a positive constant D independent of λ such that

$$\int_0^1 |\dot{\phi}_\lambda|\mathrm{d}t \leqslant \int_0^1 \sqrt{\dot{\phi}_\lambda^2 + 2V_\lambda(\phi_\lambda)}\mathrm{d}s \leqslant D.$$

Since ϕ_0 is fixed, we see that, for any λ, the function ϕ_λ satisfies

$$|\phi_\lambda(t)| \leqslant |\phi_0| + D,$$

and therefore choosing $\lambda \geqslant \sup\{V(\phi) : |\phi| \leqslant |\phi_0 + D\}$ we have

$$V(\phi_\lambda) = V_\lambda(\phi_\lambda), \quad V'(\phi_\lambda) = V'_\lambda(\phi_\lambda).$$

This means that $(a_\lambda, \phi_\lambda)$ is also a critical point of F (2.15) with positive critical value. ■

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A new integrable equation with cuspons and W/M-shape-peaks solitons

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In this paper, we propose a new completely integrable wave equation: $m_t+m_x(u^2-u_x^2)+2m^2u_x=0$, $m=u-u_{xx}$. The equation is derived from the two dimensional Euler equation and is proven to have Lax pair and bi-Hamiltonian structures. This equation possesses new cusp solitons—cuspons, instead of regular peakons $ce^{-|x-ct|}$ with speed c. Through investigating the equation, we develop a new kind of soliton solutions—"W/M"-shape-peaks solitons. There exist no smooth solitons for this integrable water wave equation. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Solitons and integrable models are very attractive objects in nonlinear sciences. Originally found in experiments on shallow water wave propagations one and a half centuries ago, they have since then become an abundant and fascinating area of theoretical and mathematical study. Today, solitons and integrable systems are playing an increasingly important role in dynamical systems, harmonic analysis, and string theories.

There are well-known constructions of integrable systems. The idea of compatibility is the crucial of integrable systems theory. One is already at the very definition of the complete integrability of a Hamiltonian flow in the Liouville-Arnold sense, which means that the flow is able to be included into a complete family of commuting Hamiltonian flows.[2] Analogically, it is a symbolic feature of soliton (integrable) partial differential equations that they take on not separately but are always assigned in hierarchies of compatible systems. It is impossible to list all applications or adoptions of this idea. We mention only some that are relevant for our present purpose. A condition of the existence of a number of commuting systems may be taken as the basis of the bi-Hamiltonian structure and symmetry approach.[1,7–9,11] However, a key procedure is to figure out bi-Hamiltonian operators. In general, no universal method is available, and we have to work on concrete equations.

In the present paper, we use Hamiltonian methods to present a new completely integrable water wave equation:

$$u_t - u_{xxt} + 3u^2u_x - u_x^3 = (4u - 2u_{xx})u_xu_{xx} + (u^2 - u_x^2)u_{xxx}, \tag{1}$$

namely,

$$m_t + m_x(u^2 - u_x^2) + 2m^2u_x = 0, \quad m = u - u_{xx}, \tag{2}$$

where u is the fluid velocity and subscripts denote the partial derivatives. Actually, this equation can be reduced from the two-dimensional Euler equation by using the approximation procedure. In two dimensional Euler equations, $\mathbf{v}_t+\mathbf{v}\cdot\nabla\mathbf{v}=-\nabla p$, div $\mathbf{v}=0$ (p is a pressure), we take the velocity $\mathbf{v}=(-\psi_y,\psi_x)^T$, where ψ is a streamfunction. Then, the following equation:

$$r_t + \psi_x r_y - \psi_y r_x = 0, \quad r := \psi_{xx} + \psi_{yy},$$

is generated from the Euler equations, where r stands for the vorticity. Employing $\psi = \phi(\xi, y, \tau)$, $\xi = \epsilon(x - c_0 t)$, $\tau = \epsilon^3 t$, imposing $\phi(\xi, y, \tau) = \epsilon\phi_1(\xi, y, \tau) + \epsilon^2\phi_2(\xi, y, \tau) + \epsilon^3\phi_3(\xi, y, \tau)$ and $\phi_1(\xi, y, \tau) = B_1(y)F(\xi, \tau)$, $\phi_2(\xi, y, \tau) = B_2(y)F(\xi, \tau) + B_3(y)F(\xi, \tau)^2$, and picking up the coefficient of ϵ^4 term in the approximation expansion of the equation, we will eventually arrive at

$$F_\tau - a_1 F_{\xi\xi\tau} + (3a_2F^2 - a_3F_\xi^2)F_\xi - (2a_4F - 2a_5F_{\xi\xi})F_\xi F_{\xi\xi} - ((a_4 - a_3)F^2 - a_5F_\xi^2)F_{\xi\xi\xi} = 0, \quad (3)$$

where $a_1, \ldots, a_5$ are constants. If we take $a_1 = a_2 = a_3 = a_5 = 1$ and $a_4 = 2$, Eq. (3) exactly gives the new equation (1). So, Eq. (1) is a new nonlinear water wave equation.

In the paper, Eq. (1) is shown to have the bi-Hamiltonian structure and the Lax pair, which implies the integrability of the equation so that the initial value problem may be solved by the Inverse Scattering Transform (IST) method.[10,1] Our equation is proven to have new cusp solitons—cuspons, which are not peakons in the regular type of $ce^{-|x-ct|}$ (c is a wave speed)[3] and whose first order derivative is discontinuous at some point (see more mathematical studies about the Camassa-Holm equation in Refs. 5, 6, and 12). Furthermore, we develop a new kind of soliton solution, named "W-shape-peaks" or "M-shape-peaks" soliton, which is given in an explicit form for this water wave equation. We will take some graphs to show how these W/M-shape-peaks solitons look.

II. HAMILTONIAN STRUCTURE AND INTEGRABILITY

By using $m = u - u_{xx}$, $(1 - \partial^2)(\delta H_1/\delta m) = \delta H_1/\delta u$, the wave equation (2) can be rewritten as

$$m_t = -(m(u^2 - u_x^2))_x = J\frac{\delta H_0}{\delta m} = K\frac{\delta H_1}{\delta m}, \quad (4)$$

where

$$J = -\partial m\, \partial^{-1} m\, \partial, \quad (5)$$

$$K = \partial^3 - \partial, \quad (6)$$

$$H_0 = 2\int_\Omega mu\, dx,$$

$$H_1 = \frac{1}{4}\int_\Omega (u^4 + 2u^2u_x^2)dx,$$

$\Omega = (x_0, x_0 + T)$ or $\Omega = (-\infty, +\infty)$ is the domain of u that needs to be periodic with T or to approach a constant, and H_0, H_1 are two Hamiltonian functions. Apparently, both operator J and operator K are Hamiltonian. So, our equation is bi-Hamiltonian.

In order to show the integrability of this equation, let us consider the following spectral problem:

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_x = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\lambda m \\ -\frac{1}{2}\lambda m & \frac{1}{2}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \equiv U(m,\lambda)\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \quad (7)$$

where λ is a spectral parameter, m is a scalar potential function periodic or approaching the same constant at both infinities, and $\psi = (\psi_1, \psi_2)^T$ is the spectral function corresponding to the spectral parameter λ. Then, we have

$$K\nabla\lambda = \lambda^2 J\nabla\lambda, \tag{8}$$

where $\nabla\lambda = (\lambda/2)(\psi_1^2 + \psi_2^2)$.

Remark 1: Equation (8) plays a very important role in the discussions of the periodic solutions of the wave equation (2), which we will deal with in a subsequent paper.[14] *Actually, on the basis of these two operators, following our earlier method*[13] *we are able to generate a new integrable hierarchy.*

By a careful calculation, we can verify the following statement.

Equation (2) has the following Lax pair:

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_x = U(m,\lambda)\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{9}$$

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_t = V(m,u,\lambda)\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{10}$$

where

$$U(m,\lambda) = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\lambda m \\ -\frac{1}{2}\lambda m & \frac{1}{2}\end{pmatrix}, \quad m = u - u_{xx},$$

$$V(m,u,\lambda) = \begin{pmatrix} \lambda^{-2} + \frac{1}{2}(u^2 - u_x^2) & -\lambda^{-1}(u-u_x) - \frac{1}{2}\lambda m(u^2 - u_x^2) \\ \lambda^{-1}(u+u_x) + \frac{1}{2}\lambda m(u^2 - u_x^2) & -\lambda^{-2} - \frac{1}{2}(u^2 - u_x^2)\end{pmatrix}.$$

In fact, one just checks that the compatibility condition

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_{xt} = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_{tx},$$

namely,

$$U_t - V_x + [U,V] = 0$$

generates Eq. (2). A direct substitution of $U(m,\lambda)$ and $V(m,u,\lambda)$ is able to guarantee the truth of the above statement. One can also use maple to verify this procedure.

So the wave equation (2) is accordingly completely integrable by the Inverse Scattering Transformation.[1]

III. W/M-SHAPE-PEAKS SOLITONS

A. Traveling wave setting

Let us consider the traveling wave solution of our equation (2) through a generic setting $u(x,t) = U(x-ct)$, where c is the wave speed. Let $\xi = x - ct$, then $u(x,t) = U(\xi)$. Substituting it into Eq. (2) yields

$$(U^2 - U'^2 - c)(U - U'')' + 2U'(U - U'')^2 = 0, \tag{11}$$

where $U' = U_\xi$, $U'' = U_{\xi\xi}$, $U''' = U_{\xi\xi\xi}$.

Remark 2: (1) Our ODE (11), derived from our new PDE (2) through a traveling wave setting,

is different from the Camassa-Holm (CH) case. In the CH case (see Ref. 15), the traveling wave ODE reads as

$$(U-c)(U-U'')+2U'(U-U'')=0.$$

Here our new equation is more high order nonlinear terms than the CH case.

(2) The integrable CH equation has both peakon and smooth soliton solutions.[3,15] *However, our new integrable equation (2) has no smooth soliton solution, only cusp solitons and M/W-shape-peaks solitons solutions (see the following sections). This means that an integrable equation may have no smooth soliton, which may clue on a good idea to classify the integrable equations by the mathematical features of solitons.*

Generally, we have the following trivial facts.

(1) *Any constant function is a solution of Eq. (2) and the ODE (11).*
(2) *Any translation $U(\xi-\xi_0)$ of a solution $U(\xi)$ of ODE (11) is still a solution.*
(3) *If $u(x,t)$ is a solution of Eq. (2), then any translation $u(x-x_0,t-t_0)$ in space x and time t is a solution, too.*

Because of the translation invariance of the differential equation (11), without any loss of generality, we choose ξ_0 as vanishing, namely, $\xi_0=0$. If $U-U''=0$, then Eq. (11) has general solutions $U(\xi)=c_1e^{\xi}+c_2e^{-\xi}$ with any real constants c_1, c_2. Of course, they are the solutions of Eq. (2). This result is not interesting for us. Actually, there are general weak solutions to Eq. (2):

$$u(x,t)=c\cosh(|x-ct|)\pm\sqrt{c(c-1)}\sinh(|x-ct|), \tag{12}$$

where c ($c\geq 1$ or $c\leq 0$) is the wave speed.

Because the solution $u(x,t)$ defined by (12) approaches infinity as x goes to infinity, this solution is not a soliton, which is not so interesting, either. Let us now assume that U is NEITHER a constant solution of Eq. (11) NOR satisfies $U^2-U'^2=0$. Taking the integration on both sides of Eq. (11) leads to

$$(U-U'')[c-(U^2-U'^2)]=C_2, \tag{13}$$

where $C_2\neq 0\in\mathbb{R}$ is an integration constant.

Multiplying both sides of Eq. (13) by $-4U'$ and then taking another integration, we obtain

$$[c-(U^2-U'^2)]^2=-4C_2U+C_1, \tag{14}$$

namely,

$$U'^2=U^2-c\pm\sqrt{C_1-4C_2U}, \tag{15}$$

where $C_1\in\mathbb{R}$ is another integration constant.

Let us now impose the boundary condition

$$\lim_{\xi\to\pm\infty}U=A, \tag{16}$$

to figure out the two constants C_1, C_2. Substituting the boundary condition (16) into the ODEs (13) and (14) generates the following two constants:

$$C_1=(c-A^2)(c+3A^2), \tag{17}$$

$$C_2=A(c-A^2). \tag{18}$$

So the ODE (14) becomes

$$[c-(U^2-U'^2)]^2=(c-A^2)(c+3A^2-4AU). \tag{19}$$

Remark 3: There is no shock wave (or kink) solution for our equation (2) because we cannot

be allowed to set $\lim_{\xi\to+\infty} U \neq \lim_{\xi\to-\infty} U$. *In other words, the traveling wave solution of our equation, satisfying the boundary condition* (16), *is definitely a soliton!*

Let us solve Eq. (19) in the coming subsection.

B. W/M-shape-peaks solitons

Let us assume that $A\neq 0$ and $c\neq A^2$ (if $A=0$ or $c=A^2$, then $C_2=0$, which corresponds to $U-U''=0$. We already discussed it in Sec. III A. Actually, no solitons are found in this case). The fact that both sides of Eq. (19) are non-negative implies

$$(c-A^2)(c+3A^2-4AU)>0. \tag{20}$$

Let $V=\sqrt{(c-A^2)(c+3A^2-4AU)}$ and $s=c-A^2$, then $V>0, V=\sqrt{s(s+4A^2-4AU)}$, $U=A+(1/4sA)(s^2-V^2)$ and Eq. (19) becomes

$$\frac{VdV}{|s-\epsilon V|\sqrt{(s+\epsilon V)^2-8sA^2}}=\mp\frac{d\xi}{2},\quad \epsilon=\pm 1. \tag{21}$$

Let us discuss the cases of $\epsilon=1$ and $\epsilon=-1$ separately.

(1) *Case* $\epsilon=1$. If we chose $s<0$, then Eq. (21) can be integrated as

$$(V+s+\sqrt{(V+s)^2-8sA^2})\left[\frac{-V-s+4A^2+a\sqrt{(V+s)^2-8sA^2}}{V-s}\right]^{1/2a}=e^{-|\xi|/2-\ln(-4s)/2a}, \tag{22}$$

where $a=\sqrt{(s-2A^2)/s}=\sqrt{(3A^2-c)/(A^2-c)}$, $s-2A^2<0$, and $a>1$.

Because $V\nrightarrow\pm s$ as $\xi\to\infty$ whereas the right hand side of Eq. (22) goes to 0 as $\xi\to\infty$, the solution V determined by Eq. (22) does not exist. So, $s<0$ is not available for case $\epsilon=1$.

Therefore, s must be positive, namely, $s>0$, which assures that Eq. (21) can be integrated as

$$(V+s+\sqrt{(V+s)^2-8sA^2})\left[\frac{V-s}{V+s-4A^2+a\sqrt{(V-s)^2-8sA^2}}\right]^{1/2a}=e^{|\xi|/2+\ln(4s)/2a}, \tag{23}$$

where $a=\sqrt{(s-2A^2)/s}=\sqrt{(c-3A^2)/(c-A^2)}$, $s-2A^2>0$, and $0<a<1$.

In general, we cannot solve the equation (23) for V in an explicit form. But, for some very special a's, we do have the explicit solution V. For example, let us take $a=\frac{1}{2}$; then $c=\frac{11}{3}A^2$ and $s=\frac{8}{3}A^2$. Substituting it into Eq. (23) generates

$$V^2-bV+sb=0, \tag{24}$$

where

$$b=3se^{-\frac{|\xi|}{2}}+\frac{3s}{4}e^{\frac{|\xi|}{2}}+s=3s\cosh\left(\frac{|\xi|}{2}-\ln(2)\right)+s=s\left(3\cosh\left(\frac{|\xi|}{2}-\ln(2)\right)+1\right).$$

Therefore, solving Eq. (24) for V gives

$$V=\frac{1}{2}(b-\sqrt{b^2-4sb})=\frac{3s}{2}\left(\frac{2}{3}+z-\sqrt{z^2-\frac{4}{9}}\right)=s+\frac{3s}{2}\left(z-\sqrt{z^2-\frac{4}{9}}\right),$$

where $z=\cosh\left(|\xi|/2-\ln(2)\right)-\frac{1}{3}$. So, we arrive at explicit solutions $U(\xi)$ of Eq. (2),

$$U(\xi)=A\left(\frac{5}{3}-(3z+2)\left(z-\sqrt{z^2-\frac{4}{9}}\right)\right),$$

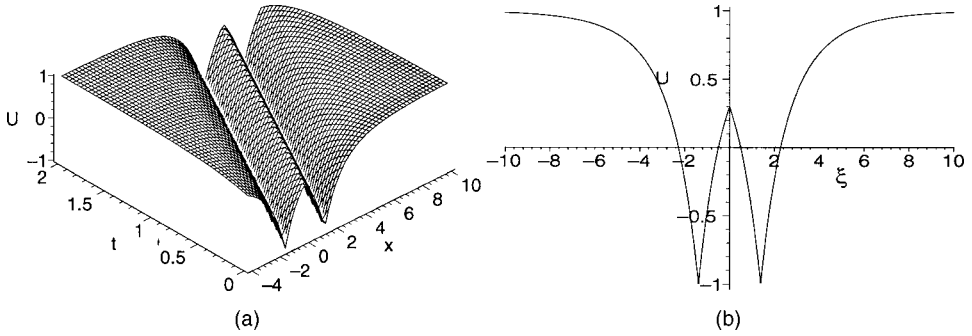

FIG. 1. (a) A three-dimensional (3-D) graph of the explicit solution $U(\xi)$ defined by (25), when $A=1$, $s=8/3$, wave speed $c=11/3$, and the range of x,t,u: $-4\le x\le 10$, $0\le x\le 2$, $-1\le u\le 1$. (b) A 2D graph of the explicit solution $U(\xi)$ defined by (25) when $A=1$, $s=8/3$, the wave speed $c=11/3$, and the range of ξ: $-10\le\xi\le 10$.

$$z=\cosh\left(\frac{|\xi|}{2}-\ln(2)\right)-\frac{1}{3},$$

$$\xi=x-\frac{11}{3}A^2t. \tag{25}$$

Apparently, $V(\xi)\to s$ and $U(\xi)\to A$ as $\xi\to\infty$. Since $A\neq 0$, there is no peaked soliton for a homogeneous boundary condition. Let us select a special $A=1$, then the solution $U(\xi)$ reads as

$$U(X)=2-3\cosh^2 X+\left(\cosh X+\frac{1}{3}\right)\sqrt{3(3\cosh X+1)(\cosh X-1)}.$$

$$X=\frac{\left|x-\frac{11}{3}t\right|}{2}-\ln 2.$$

Apparently, this solution has three peaks and looks like a "W" wave. So, we called it a "W-shape peaks" soliton. Three peaks occur at $x=\frac{11}{3}t_0$, $x=\frac{11}{3}t_0-2\ln(2)$, $x=\frac{11}{3}t_0+2\ln(2)$, for each time t_0. See Fig. 1 for more details.

If we select the boundary constant $A=-1$, we are able to get the anti-"W-shape-peaks" soliton, called an "M-shape-peaks" soliton. See a 3D and a 2D graph in Fig. 2 for more details.

For other a's, in a similar way we can also obtain the corresponding peaked soliton solutions, which are left for the readers' practice.

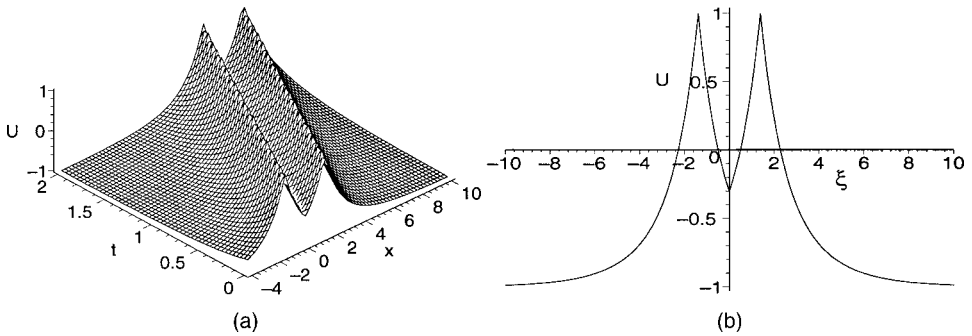

FIG. 2. (a) A 3D graph of the "M-shape-peaks" solution $U(\xi)$ defined by (25) with $A=-1$ and $c=11/3$. (b) 2D graph of the "M-shape-peaks" solution $U(\xi)$ defined by (25) with $A=-1$ and $c=11/3$.

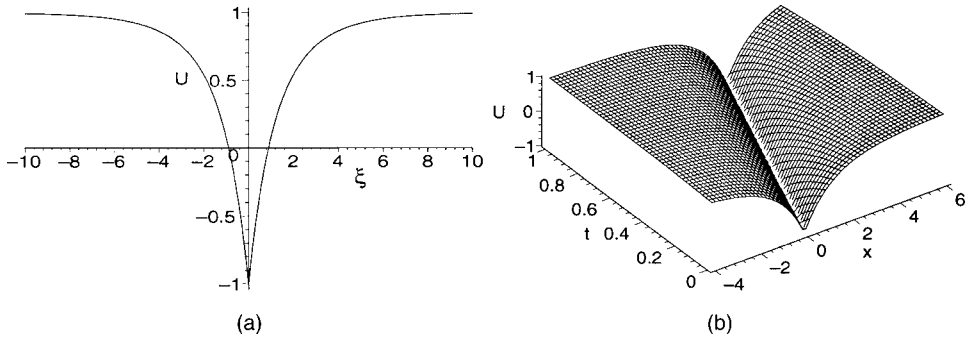

FIG. 3. (a) 2D graph of new cuspon solution $U(\xi)$ defined by (26) with amplitude $A=1$ and wave speed $c=11/3$. (b) 3D graph of new cuspon solution $U(\xi)$ defined by (26) with $A=1$ and $c=11/3$.

New cusp solitons-cuspons. In Eq. (22), we consider the solution V without the absolute value of ξ. Following the above procedure, in case of $a=\frac{1}{2}$ we may obtain

$$U(\xi)=A\left(\frac{5}{3}-(3z+2)\left(z-\sqrt{z^2-\frac{4}{9}}\right)\right),$$

$$z=\cosh\left(\frac{x}{2}-\frac{11}{6}A^2t\right)-\frac{1}{3}. \tag{26}$$

A direct verification shows us the following: (26) is indeed another explicit solutions of Eq. (2). Let us take $A=\pm 1$. Then the corresponding solutions read as

$$U(X)=\pm\left(2-3\cosh^2 X+\left(\cosh X+\frac{1}{3}\right)\sqrt{3(3\cosh X+1)(\cosh X-1)}\right),$$

$$X=\frac{x}{2}-\frac{11}{6}t,$$

which have the following characteristic features:

$$U(0)=\mp 1,\quad U'(0+)=\pm\infty,\quad U'(0-)=\mp\infty.$$

Apparently, they differ from the regular peakons.[3] So, both are new peaked solitons for our equation (2) (see Figs. 3, 4 for more details).

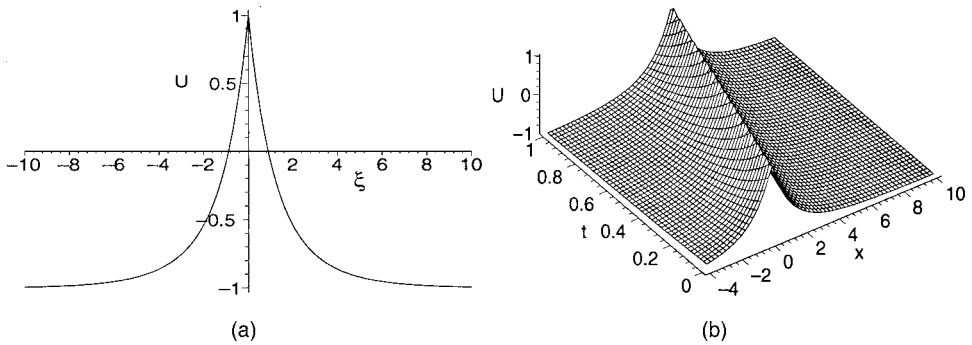

FIG. 4. (a) A 2D graph of new cuspon solution $U(\xi)$ defined by (25) when $A=-1$ and $c=11/3$. (b) A 3D graph of a new cuspon solution $U(\xi)$ defined by (25) when $A=-1$ and $c=11/3$.

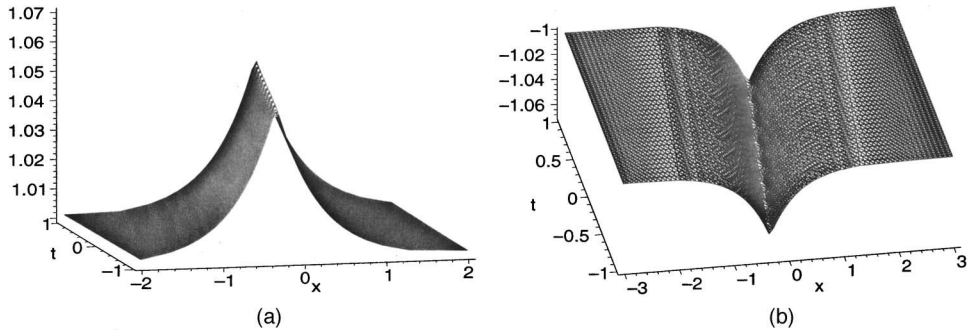

FIG. 5. (a) A 3D numerical graph of the cuspon solution $U(\xi)$ of Eq. (2) based on (28) with amplitude $A=1$ and wave speed $c=1/3$. (b) A 3D numerical graph of the cuspon solution $U(\xi)$ of Eq. (2) based on (28) with amplitude $A=-1$ and wave speed $c=1/3$.

(2) *Case* $\epsilon=-1$. If we chose $s>0$, then Eq. (21) can be integrated as

$$(V-s+\sqrt{(V-s)^2-8sA^2})\left[\frac{s-V-4A^2+a\sqrt{(V-s)^2-8sA^2}}{V+s}\right]^{1/2a}=e^{-|\xi|/2-\ln(4s)/2a}, \tag{27}$$

where $a=\sqrt{(s-2A^2)/s}=\sqrt{(c-3A^2)/(c-A^2)}$, $s-2A^2>0$, and $0<a<1$.

Because $V\nrightarrow\pm s$ as $\xi\to\infty$ whereas the right hand side of Eq. (27) goes to 0 as $\xi\to\infty$, the solution V determined by Eq. (27) does not exist. So, $s>0$ is not available for case $\epsilon=-1$. Therefore, s must be negative, namely, $s<0$, which gurantees that Eq. (21) can be integrated as

$$(V-s+\sqrt{(V-s)^2-8sA^2})\left[\frac{V+s}{V-s+4A^2+a\sqrt{(V-s)^2-8sA^2}}\right]^{1/2a}=e^{-|\xi|/2+\ln(-4s)/2a}, \tag{28}$$

where $\xi=x-ct$, $a=\sqrt{(s-2A^2)/s}=\sqrt{(3A^2-c)/(A^2-c)}$, $s-2A^2<0$, and $1<a$.

In general, we cannot solve Eq. (28) for V in an explicit form. But, we can numerically determine V from Eq. (28), and then according to the equation, $U=A+(1/4sA)(s^2-V^2)$ to figure out the solution $U(\xi)$ for our equation (2). For instance, in the case of $A=\pm1$, $c=1/3$, we have $a=2$ and $s=-2/3$, and numerically solve our equation (2) (see Fig. 5 for details).

For other a's (for instance, $a=3,4$), in a similar way we can also numerically obtain the corresponding cuspon solutions of Eq. (2).

IV. CONCLUSIONS AND OPEN PROBLEMS

In the paper, we present a new integrable water wave equation (2). Through studying the equation, we develop a new kind of soliton solution—"W-shape-peaks"/"M-shape-peaks" solutions (see Fig. 1, 2). Our equation is shown to possess not only "W-shape-peaks"/"M-shape-peaks" solitons, but new cuspon solution as well (see Figs. 3, 4 which are different from regular peakons).

Our new equation (2) naturally has a physical meaning since it is derived from the two dimensional Euler equation (see the Introduction). It can be cast into the following Newton equation $U'^2=P(U)-P(A^2)$ of a particle with a new potential $P(U)=U^2+\text{sign}(s)\sqrt{s(s+4A^2-4AU)}$, $s=c-A^2$, or $V'^2=Q(V)-Q(A)$ with $U=A+(1/4sA)(s^2-V^2)$, $Q(V)=V^2/4+4s|s|A^2/V+s^3(s-8A^2)/4V^2$. In the paper, we successfully solve this Newton equation with new cuspons and M-shape/W-shape-peaks solitons. Those peaked and cusped solutions may be applied to neuroscience for providing a mathematical model and explaining electrophysiological responses of visceral nociceptive neurons and sensitization of dorsal root reflexes.[4]

No smooth solitons are found for our equation, but our equation is completely integrable. Furthermore, we suggest a more general partial differential equation: $m_t+m_x(u^2-u_x^2)+km^2u_x=0$, $m=u-u_{xx}$ with any constant $k\in\mathbb{R}$. When $k=2$, the equation is integrable, which is already discussed in this paper. Any other integrable cases? We do not know yet.

ACKNOWLEDGMENTS

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The inverse problem for six-dimensional codimension two nilradical lie algebras

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Ado's theorem asserts that every real Lie Algebra $\mathfrak{g}$ of dimension n has a faithful representation as a subalgebra of $gl(p,\mathbb{R})$ for some p. The theorem offers no practical information about the size of p in relation to n and in principle p may be very large compared to n. This article is concerned with finding representations for a certain class of six-dimensional Lie algebras, specifically, real, indecomposable algebras that have a codimension two nilradical. These algebras were classified by Turkowski and comprise of 40 cases, some of which contain up to four parameters. Linear representations are found for each algebra in these classes: More precisely, a matrix Lie *group* is given whose Lie algebra corresponds to each algebra in Turkowski's list and can be found by differentiating and evaluating at the identity element of the group. In addition a basis for the right-invariant vector fields that are dual to the Maurer-Cartan forms are given thereby providing an effective realization of Lie's third theorem. The geodesic spray of the canonical symmetric connection for each of the 40 linear Lie group G is given. Thereafter the inverse problem of the calculus of variations for each of the geodesic sprays is investigated. In all cases it is determined whether the spray is of Euler-Lagrange type and in the affirmative case at least one concrete Lagrangian is written down. In none of the cases is there a Lagrangian of metric type. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2378620]

I. INTRODUCTION

In this article we study the inverse problem of Lagrangian dynamics for the canonical linear connection on a Lie group. More precisely we consider the inverse problem for solvable six-dimensional groups whose Lie algebras have a codimension two nilradical. A list of such algebras has been compiled by Turkowski (1990). In order to make the exposition reasonably self-contained, Secs. IV and V gives some background on the inverse problem. For more details we refer the reader to Anderson and Thompson (1992), Crampin (1981), Crampin *et al.* (1996), Douglas (1941), Ghanam *et al.* (2005), Grifone and Muzsnay (1999, 2000); Muzsnay and Thompson (2003), Sarlet (1982), Sarlet *et al.* (1998). It turns out that in order for the geodesics of the canonical connection to be variational a linear system of equations must have a nonsingular solution [Eqs. (12) and (13)]. If there is no nonsingular solution the inverse problem is answered in the negative. To proceed further using our methods, we need a local representation of the Lie algebra in terms of vector fields or preferably a linear representation for the corresponding Lie group.

A well-known theorem in the theory of Lie algebras due to Ado asserts that every real Lie algebra $\mathfrak{g}$ of dimension n has a faithful representation as a subalgebra of $gl(p,\mathbb{R})$ for some p. The

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theorem does not give much information about the value of p but leads one to believe that p may be very large in relation to the size of n and consequently it seems to be of limited practical value.

If the Lie algebra $\mathfrak{g}$ is semisimple there are well-known representations that are associated to the standard A_k, B_k, C_k, D_k series that are of the order of $\sqrt{n}$ where n is the dimension of $\mathfrak{g}$. On the other hand it is clear that semisimple algebras are very much the exception rather than the rule. For example, there are only two semisimples in dimension five or less. More generally if $\mathfrak{g}$ has a trivial center the adjoint representation furnishes a faithful representation of $\mathfrak{g}$ and in the notation used above $p=n$. Many of our representations are constructed in this way. We develop some theorems in Sec. III which explain how to obtain representations in the case where the algebra has a nontrivial center. In particular we will show that if $\mathfrak{g}$ has an abelian nilradical and abelian complement then it has a faithful linear representation. There are a few algebras for which we have obtained matrix representations by some experimentation. Ultimately we would like to have practical theorems that give the representations in all cases.

We refer to Patera *et al.* (1976) for a comprehensive list of the *indecomposable* algebras of dimension five or less, which in turn was based on Murozov (1958) and Mubarakzyanov (1963). However, in this article we are primarily concerned with the solvable six-dimensional algebras compiled by Turkowski (1990) and in Sec. VI we list linear representations for each of these algebras. In fact rather than giving representations for the Lie algebras we give in each case a matrix *group* whose Lie algebra coincides with a given algebra. It is straightforward then to construct the matrix representation of the algebra by differentiating and evaluating at the identity element of the group. We have also given a representation of the algebra in terms of the right invariant vector fields and the associated geodesic equations. For standard facts about Lie algebras and Lie groups we refer to Helgason (1978) and Jacobson (1962). We use $\langle e_1, e_2, \ldots, e_s \rangle$ to denote the s dimensional subspace of $\mathfrak{g}$ generated by $e_1, e_2, \ldots, e_s$.

The existence aspect of the inverse problem is solved in every case by either supplying at least one concrete Lagrangian or by checking that one cannot exist. It is to be noted that whenever one Lagrangian exists then so do many. We have not attempted in this article to find all possible Lagrangians in any of the forty cases nor special kinds of Lagrangians except to say that in none of the cases is there a metric Lagrangian.

The vast majority of work on the inverse problem is concerned with two degrees of freedom. There are very few examples or results in higher dimensions, the Kepler system being a rare example. The Lie group inverse problem is a much simpler version of the general problem but it already presents major difficulties. We believe that it will serve as a valuable guide to the kind of theory that one might expect in higher dimensions. We hope also that the results on representations may prove to be of independent interest.

Most of the calculations involving Maurer-Cartan one forms, vector fields and Euler-Lagrange equations were carried out using the symbolic manipulation program MAPLE. The fact that certain geodesic systems are not of Euler-Lagrange type follows from Eqs. (12) and (13) below. A routine written in MAPLE 9 was used that checks these conditions when a particular Lie algebra is used as input. In the interests of brevity and because a lot of similar arguments have been given previously [Ghanam *et al.* (2004)], we have chosen to suppress most details. However, we have supplied a short Appendix which should give the reader some insight as to how we construct our Lagrangians in six diverse cases. We must trust that this method is more efficient than trying to give hundreds of small routine calculations.

II. SIX-DIMENSIONAL LIE ALGEBRAS AND TURKOWSKI'S CLASSIFICATION

Let us explain how the indecomposable Lie algebras of dimension six are classified. First of all there is only one indecomposable simple algebra of dimension six, namely, the pseudo-orthogonal algebra $o(3,1)$ The next class of algebras to consider are the algebras that have a nontrivial Levi-decomposition. According to Turkowski there are up to isomorphism just four of them listed as $L_{6,1}$, $L_{6,2}$, $L_{6,3}$, and $L_{6,4}$ [Turkowski (1988)]. All the remaining indecomposable algebras in dimension six are solvable.

There is a general inequality that implies that the dimension of the nilradical of a solvable, indecomposable Lie algebra $\mathfrak{g}$ is at least $\frac{1}{2}\dim(\mathfrak{g})$ [Morozov (1958)]. According to Turkowski if the dimension of the nilradical of a solvable Lie algebra of dimension six is three, then the algebra is decomposable and hence there are just three classes to consider: The nilpotents and the algebras that have five-dimensional and four-dimensional nilradicals, respectively. We are concerned exclusively with this latter class of algebras in this article and they have been classified in Turkowski (1990). For a given algebra $\mathfrak{g}$ in Turkowski's list we always use a basis $\{e_1,e_2,e_3,e_4,e_5,e_6\}$ in which e_1 and e_2 are *not* in the nilradical of $\mathfrak{g}$.

Turkowski distinguishes 40 classes of algebras that have a codimension two nilradical [Turkowski (1990)]. Of course the situation is a good deal more complicated than that because most of the algebras have up to four parameters that vary in open intervals. Turkowski's method consists essentially of putting the two matrices $\mathrm{ad}(e_1)$ and $\mathrm{ad}(e_2)$ into simultaneous normal form, where e_1 and e_2 are basis vectors that lie outside of the nilradical. Turkowski arranges the 40 algebras into five tables as follows: Table 1 (algebras 1–19), algebras that have abelian nilradical and trivial center; Table 2 (algebras 20–27), algebras that have abelian nilradical and one-dimensional center; Table 3 (algebra 28), algebras that have nilradical isomorphic to the indecomposable four-dimensional nilpotent; Table 4 (algebras 29–37), algebras that have nilradical isomorphic to the direct sum of the indecomposable three-dimensional nilpotent with $\mathbb{R}$ and having trivial center; Table 5 (algebras 38–40), algebras that have nilradical isomorphic to the direct sum of the indecomposable three-dimensional nilpotent with $\mathbb{R}$ and having one-dimensional center.

III. REPRESENTATIONS FOR TURKOWSKI'S ALGEBRAS

Let us now consider the problem of constructing representations for the algebras in Turkowski's list. It is apparent that for algebras in Tables 1, 3, and 4 representations may be obtained from the adjoint representation. For the convenience of the reader we have given for each of these algebras the corresponding Lie subgroup of $GL(6,\mathbb{R})$ that we obtain by exponentiation or, Lie subgroup of $GL(5,\mathbb{R})$, that we obtain from Theorem 5.1 below. We give also in each case a collection of vector fields that are right-invariant and that are obtained by dualizing a collection of right-invariant Maurer-Cartan one-forms.

There are eleven classes of algebra in Table 2 and 5 for which faithful representations cannot be found by using the adjoint representation. Several of the algebras in Table 2 contain a parameter ϵ whose value is 0 or 1. The significance of ϵ is that when it is zero the nilradical has an *abelian* complement in the algebra g. For such algebras we can find faithful representations by appealing to the following proposition and theorem.

Proposition 3.1: Suppose that $\{e_1,e_2,\ldots,e_n\}$ *is a basis for a vector space* g *and there exists a skew bilinear map* $[,]$: $g\times g\to g$ *and* $[e_i,e_j]=0$, $[e_a,e_b]=0$, $[e_a,e_i]=C^j_{ai}e_j$, *where* $1\leqslant i,j\leqslant r$, $r+1\leqslant a,b,c\leqslant n$. *Then* g *is Lie algebra if* $C^j_{ai}C^k_{bj}=C^j_{bi}C^k_{aj}$.

Proof: If we consider the Jacobi identity we see that it is identically satisfied for each of the triples $\{e_i,e_j,e_k\}$, $\{e_i,e_j,e_a\}$, $\{e_a,e_b,e_c\}$. It remains to check $\{e_i,e_a,e_b\}$. Thus

$$[e_i,[e_a,e_b]]+[e_b,[e_i,e_a]]+[e_a,[e_b,e_i]]=-[e_b,C^j_{ai}e_j]+[e_a,C^j_{bi}e_j]=-C^j_{ai}C^k_{bj}e_k+C^j_{bi}C^k_{aj}e_k.$$

We deduce that the necessary and sufficient condition for obtaining a Lie algebra is

$$C^j_{bi}C^k_{aj}-C^j_{ai}C^k_{bj}=0.$$

□

Theorem 3.1. *Suppose that the n-dimensional Lie algebra* $\mathfrak{g}$ *has a basis* $\{e_1,e_2,\ldots,e_n\}$ *and only the following nonzero brackets:* $[e_a,e_i]=C^j_{ai}e_j$, *where* $(1\leqslant i,j\leqslant r,r+1\leqslant a,b,c\leqslant n)$. *Suppose that* $\mathfrak{g}$ *has an abelian nilradical for which a basis is* $\{e_1,e_2,\ldots,e_r\}$ *and* $\{e_{r+1},\ldots,e_n\}$ *is a basis for an abelian subalgebra complementary to the nitradical. Then* $\mathfrak{g}$ *has a faithful representation as a subalgebra of* $gl(r+1,\mathbb{R})$.

Proof: The endomorphism $ad(e_a)$ for $r+1\leqslant a\leqslant n$ correspond to $n\times n$ matrices in which there are nonzero entries only in the upper left $r\times r$ block: This $r\times r$ matrix is in fact $[C^i_{aj}]$. We denote

by E_a the $(r+1)\times(r+1)$ matrix whose upper left $r\times r$ block is $[C^i_{aj}]$ and whose remaining entries are zero. To obtain the representation, map e_a to E_a for $r+1\leqslant a\leqslant n$; for each vector $e_i(1\leqslant i\leqslant r)$ map it to the $(r+1)\times(r+1)$ matrix E_i whose only nonzero entry is a one in the $(i,r+1)$th position. Clearly the $E_i's$ commute. Note that the matrix product E_iE_a is zero and so

$$[E_a,E_i]=\sum_{k=1}^{r} C^k_{ai}E_k. \tag{1}$$

Finally, consider the Jacobi identity

$$[[e_a,e_b],e_i]+[[e_i,e_a],e_b]+[[e_b,e_i],e_a]=0.$$

On expanding we deduce that $C^k_{ai}C^j_{bk}-C^k_{bi}C^j_{ak}=0$. as in Proposition 3.1. It follows that $[E_a,E_b]=0$ and we have the required representation. □

Again we refer to the algebras in Turkowski's list [Turkowski (1990)]. It is possible to obtain representations, for example, for algebras 6.1–18 using Theorem 3.1 but for those particular algebras we have chosen to use the adjoint representation. On the other hand we do use Theorem 3.1 for algebras $6.22(\epsilon=0)$ and $6.23(\epsilon=0)$ in Sec. VI.

The next theorem is an improvement of a result that appears in Ghanam *et al.* (2005) and explains how under favorable circumstances the two-dimensional nonabelian Lie algebra can be used to extend a representation for an algebra of dimension n to a representation for an algebra of dimension $n+1$.

Theorem 3.2: *(i) Suppose that* $\mathfrak{g}$ *is an n-dimensional Lie algebra with structure equations* $[e_i,e_j]=C^k_{ij}e_k$ *with basis* $\{e_1,e_2,\ldots,e_n\}$ *and that* e_n *is not in the derived algebra* $[\mathfrak{g},\mathfrak{g}]$. *Suppose that* $\mathfrak{h}$ *is a space of dimension* $n+1$ *for which* $\mathfrak{g}$ *is an n-dimensional subspace and that* $\{e_1,e_2,\ldots,e_n,e_{n+1}\}$ *is a basis for* $\mathfrak{h}$. *Suppose that there is skew-bilinear map from* $\mathfrak{h}\times\mathfrak{h}$ *to* $\mathfrak{h}$ *defined on the basis for* $\mathfrak{h}$ *that satisfies* $[e_i,e_j]=C^k_{ij}e_k$, $[e_{n+1},e_i]=0$ $(1\leqslant i\leqslant n-1)$, $[e_{n+1},e_n]=be_{n+1}$ *for some nonzero* $b\in\mathbb{R}$. *Then* $\mathfrak{h}$ *is a Lie algebra, that is, the Jacobi identity holds on* $\mathfrak{h}$. *In fact* $\mathfrak{h}$ *is a one-dimensional split extension of* $\mathfrak{g}$ *and the subspace spanned by* $\{e_1,e_2,\ldots,e_{n-1}\}$ *is an ideal in* $\mathfrak{g}$ *as well as in* $\mathfrak{h}$.

(ii) In particular suppose that $\mathfrak{g}$ *is an n-dimensional solvable Lie algebra that is isomorphic to a subalgebra of* $gl(n,\mathbb{R})$ *and that* e_n *is not in the nilradical of* $\mathfrak{g}$. *Then* $\mathfrak{h}$ *as defined above is isomorphic to a subalgebra of* $gl(n+1,\mathbb{R})$.

We can use Theorem 3.2 to find, for example, representations for algebras 6.1, 6.2, 6.12, 6.19, 6.20, and 6.26 assuming that we have representations for the corresponding five-dimensional algebras.

IV. THE INVERSE PROBLEM FOR SECOND-ORDER ORDINARY DIFFERENTIAL EQUATION (ODE) SYSTEMS

There has been a great deal of activity in the inverse problem of Lagrangian dynamics during the past thirty years and we do not need to repeat all the theory here so we shall give a brief summary that is sufficient for our needs. Consider then a system of second-order ODE of the form

$$\ddot{x}^i=f^i(x^j,\dot{x}^j). \tag{2}$$

To simplify notation we shall denote $\dot{x}^i$ by u^i throughout. Douglas formulated an algebro-differential system which gives necessary and sufficient conditions for Eq. (2) to be the Euler-Lagrange equations of a regular first-order Lagrangian L.

To state Douglas' conditions we define the following $n\times n$ matrix of functions:

$$\Phi^i_j=\frac{1}{2}\frac{d}{dt}\left(\frac{\partial f^i}{\partial u^j}\right)-\frac{\partial f^i}{\partial x^j}-\frac{1}{4}\frac{\partial f^i}{\partial u^k}\frac{\partial f^k}{\partial u^j}. \tag{3}$$

Douglas obtained the following conditions known universally as the Helmholtz conditions whose role is explained in the theorem below

$$g\Phi = (g\Phi)^t, \tag{4}$$

$$\frac{dg_{ij}}{dt} + \frac{1}{2}\frac{\partial f^k}{\partial u^i}g_{kj} + \frac{1}{2}\frac{\partial f^k}{\partial u^j}g_{ki} = 0, \tag{5}$$

$$\frac{\partial g_{ij}}{\partial u^k} - \frac{\partial g_{ik}}{\partial u^j} = 0. \tag{6}$$

Theorem 4.1: (Douglas) *Necessary and sufficient conditions for there to exist a Lagrangian so that (2) are its Euler-Lagrange equations are that there should exist a nonsingular, symmetric matrix* g_{ij} *depending on* (x^i, u^i) *that satisfies Eqs. (4)–(6). To pass from the Hessian to the Lagrangian requires two integrations and the fact that appropriate linear and zeroth-order terms may be added is a consequence of the Helmholtz conditions; the only ambiguity in passing from Hessian to Lagrangian is the trivial one of scaling by a constant and adding a total time derivative.*

Let us consider the Helmholtz conditions as an algebro-differential system. It is always possible to solve Eq. (4) and it alone will not entail that the Lagrangian function is singular. As regards Eq. (5), it is in a sense a system of ODE's and it is possible, in principle, to solve them. Upon integration it is not constants that enter but rather arbitrary first integrals of the original ODE system (2). In practice this step becomes problematic unless Eq. (2) has sufficiently many explicit first integrals. Such integrals do exist for the geodesics of the canonical Lie group connection: See Proposition 5.2 below.

Thus, there is no obstruction to solving Eqs. (4) and (5) *in principle* and at this stage it is not possible to say definitively if the Lagrangian L exists or not. The final and most difficult step is to impose the so-called closure conditions (6). Even if we are fortunate enough to solve Eqs. (4) and (5) we are now faced with a daunting task: For n degrees of freedom (6) compromises a system of $2\binom{n+1}{3}$ PDE's on the components of g_{ij} and there are $2n$ independent variables. In the case at hand where $n=6$ we thus have a system of 70 PDE's. If one wants to construct the most general possible Lagrangian for Eq. (2) it is necessary to solve this system.

Fortunately, the situation confronting us in terms of solving the Helmholtz conditions is not as bad as one might imagine for two reasons. First of all, note that Eq. (4) are purely algebraic conditions on the unknown matrix g_{ij}. There are some auxiliary algebraic conditions that can be stated as follows. Define functions Ψ^i_{jk} by

$$\Psi^i_{jk} = \frac{1}{3}\left(\frac{\partial \Phi^i_j}{\partial u^k} - \frac{\partial \Phi^i_k}{\partial u^j}\right). \tag{7}$$

The extra conditions on g_{ij} are

$$g_{mi}\Psi^m_{jk} + g_{mk}\Psi^m_{ij} + g_{mj}\Psi^m_{ki} = 0. \tag{8}$$

In fact each of Eqs. (5) and (8) are the first in an infinite hierarchy of similar algebraic conditions. However, only Eqs. (5) and (8) are relevant in the present context because, since the curvature of the canonical Lie group connection is parallel, the higher order conditions in the hierarchy are identities. Notice that Eq. (8) comprises $\binom{n}{3}$ conditions whereas Eq. (5) comprises $\binom{n}{2}$ conditions. Thus it may well be the case that collectively Eqs. (5) and (8) entail that the Lagrangian function is singular. In this paper they are the only conditions that are obstructions to the existence of a regular Lagrangian although there is as yet no theoretical basis to conclude that a similar result is true in arbitrary dimensions. In the Appendix we have given a couple of examples for which we show that the Lagrangian is singular.

Secondly, in many cases it is very useful to know that at least one Lagrangian exists. After all, the best way to determine whether a particular system is variational is to give a Lagrangian! In fact even if one can find the general solution to Eq. (6) it will rarely be possible to find all possible

Lagrangians; it is impossible even for a free particle system. However, if system (2) admits submersions onto lower dimensional systems, it may be possible to lift Lagrangians to the higher dimensional systems. In the case of the geodesic equations of the canonical Lie group connection there are many such submersions: See Proposition (5.1) below.

V. THE INVERSE PROBLEM FOR THE CANONICAL LIE GROUP CONNECTION

Let us explain next how the general theory simplifies for the case of the geodesic equations associated to a linear connection. In this case the matrix Φ is of the form

$$\Phi^i_j = R^i_{kjl} u^k u^l \tag{9}$$

where R^i_{kjl} are the components of the curvature R of the connection relative to a coordinate system (x^i). For the case of a linear connection, one finds also that

$$\Psi^i_{jk} = R^i_{ljk} u^l. \tag{10}$$

The condition coming from Φ is

$$(g_{mi} R^i_{pjq} - g_{ji} R^i_{pmq}) u^p u^q = 0, \tag{11}$$

while the condition coming from Ψ is

$$(g_{mi} R^i_{pjq} + g_{qi} R^i_{pmj} + g_{ji} R^i_{pqm}) u^p = 0. \tag{12}$$

If we contract u^q into Eq. (12) we find from Eq. (11) that

$$g_{qi} R^i_{pmj} u^p u^q = 0. \tag{13}$$

Thus, for the special case of a linear connection, we can use Eqs. (12) and (13) instead of Eqs. (11) and (12).

Let us now consider the canonical symmetric connection ∇ on a Lie group G. In fact ∇ is defined on left invariant vector fields X and Y by [see Cartan and Schouten (1926)]

$$\nabla_X Y = \tfrac{1}{2}[X,Y], \tag{14}$$

and then extended to arbitrary vector fields by making ∇ tensorial in the X argument and satisfy the Leibnitz rule in the Y argument. It can be shown that ∇ is symmetric, bi-invariant and that the curvature tensor on left invariant vector fields is given by

$$R(X,Y)Z = \tfrac{1}{4}[Z,[X,Y]]. \tag{15}$$

Furthermore, G is a symmetric space in the sense that R is a parallel tensor field. The Ricci tensor R_{ij} of ∇ is symmetric and bi-invariant. In fact, if $\{E_i\}$ is a basis of left invariant vector fields then

$$[E_i, E_j] = C^k_{ij} E_k \tag{16}$$

where C^k_{ij} are the structure constants and relative to this basis the Ricci tensor R_{ij} is given by

$$R_{ij} = \tfrac{1}{4} C^l_{jm} C^m_{il}. \tag{17}$$

Since R^i_{jkl} is a parallel tensor field and R_{ij} is symmetric, it follows that Ricci gives rise to a quadratic Lagrangian which is not regular for solvable algebras because of Cartan's criterion. We shall also assume that G is indecomposable in the sense that the Lie algebra $\mathfrak{g}$ of G is not a direct sum of lower dimensional algebras. In terms of the Lie group inverse problem, if the algebra is indecomposable then we can obtain a Lagrangian on the product by adding Lagrangians on each component.

Since our starting point is the Lie algebra $\mathfrak{g}$ of a Lie group it is of interest to ask how the ideals of $\mathfrak{g}$ are related to ∇. To this end we shall quote the following result: see Kossowski and Thompson (1991) and Ghanam *et al.* (2004).

Proposition 5.1: Every ideal $\mathfrak{h}$ *of* $\mathfrak{g}$ *gives rise to a quotient space* Q *consisting of the leaf space of the integrable distribution determined by* $\mathfrak{h}$ *and* ∇ *on* G *projects to* Q. □

A very interesting situation occurs where a solvable algebra $\mathfrak{g}$ possesses two ideals $\mathfrak{h}_1$ and $\mathfrak{h}_2$ in the nilradical of $\mathfrak{g}$ such that $\mathfrak{h}_1 \cap \mathfrak{h}_2$ is zero and $\mathfrak{g}$ splits relative to both $\mathfrak{h}_1$ and $\mathfrak{h}_2$ [Ghanam *et al.* (2004)]. Denote the corresponding distributions on G by D_1 and D_2, respectively. Since we are always assuming that $\mathfrak{g}$ is indecomposable, $\mathfrak{g}$ cannot be the direct sum of $\mathfrak{h}_1$ and $\mathfrak{h}_2$ and hence $D_1 \cap D_2$ is nonzero. In fact $D_1 \cap D_2$ is the integrable distribution on G that corresponds to the ideal $\mathfrak{h}_1 + \mathfrak{h}_2$ of $\mathfrak{g}$ and similarly $D_1 + D_2$ corresponds to the ideal $\mathfrak{h}_1 \cap \mathfrak{h}_2$. This technique is very useful for constructing a single Lagrangian and many of the Lagrangians given in Sec. VI were obtained in this way.

We now quote a proposition that will be useful in the next chapter. For more details we refer the reader to Ghanam *et al.* (2004).

Proposition 5.2: Any left or right invariant one-form on G *gives rise to a linear first integral on* TG *when it is viewed as a linear function on* TG. □

The following Theorem is a continuation of Theorem 3.1.

Theorem 5.1: (i) *Suppose that the n-dimensional Lie algebra* $\mathfrak{g}$ *has a basis* $\{e_1, e_2, \ldots, e_n\}$ *and only the following nonzero brackets:* $[e_a, e_i] = C^j_{ai} e_j$, where $(1 \leqslant i, j \leqslant r,\ r+1 \leqslant a, b, c \leqslant n)$. *Suppose that* $\mathfrak{g}$ *has an abelian nilradical for which a basis is* $\{e_1, e_2, \ldots, e_r\}$ *and* $\{e_{r+1}, \ldots, e_n\}$ *is a basis for an abelian subalgebra complementary to the nilradical. Then there exists a coordinate system* (x^i, w^a) *on the local Lie group* G *associated to* $\mathfrak{g}$ *such that* $\mathfrak{g}$ *is faithfully represented by* $\{X_i, W_a\}$ *where* $X_i = \partial/\partial x$ *and* $W_a = \partial/\partial w^a + C^k_{aj} x^j (\partial/\partial x^k)$.

(ii) *In the coordinate system* (x^i, w^a) *of (i) the geodesic equations of the canonical connection are given by*

$$\ddot{x}^i = C^i_{bj} \dot{x}^j \dot{w}^b, \quad \ddot{w}^a = 0. \tag{18}$$

Proof: (i) It is clear that the coordinate representation for $\mathfrak{g}$ given above is faithful.

(ii) The one-forms dual to the vector fields of part (i) are given by $\{dx^i - C^i_{bj} x^j dw^b, dw^a\}$ and hence we find the geodesic equations are given as stated. □

VI. REPRESENTATIONS AND LAGRANGIANS

In this section we give matrix representations corresponding to the algebras in Turkowski's list [Turkowski (1990)]. In each case we give the nonzero brackets. Besides the representation we give also a basis for the right invariant vector fields. In those cases where the geodesic equations are of Euler-Lagrange type we give a specific Lagrangian. Finally we remind the reader that throughout this section we use (p, q, x, y, z, w) as the position coordinates and their dots for the corresponding velocities, respectively.

6.1 $(abcd: ab \neq 0,\ c^2 + d^2 \neq 0)$**:** $[e_1, e_3] = ae_3$, $[e_1, e_4] = ce_4$, $[e_1, e_6] = e_6$, $[e_2, e_3] = be_3$, $[e_2, e_4] = de_4$, $[e_2, e_5] = e_5$

$$S = \begin{bmatrix} e^w & 0 & 0 & 0 & 0 & p \\ 0 & e^z & 0 & 0 & q & 0 \\ 0 & 0 & e^{cw+dz} & 0 & dx & cx \\ 0 & 0 & 0 & e^{aw+bz} & by & ay \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right invariant vector fields

$$\{-(pD_p + cxD_x + ayD_y + D_w), -(qD_q + dxD_x + byD_y + D_z), D_y, D_x, D_q, D_p\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{y} = \dot{y}(b\dot{z} + a\dot{w}), \quad \ddot{x} = \dot{x}(d\dot{z} + c\dot{w}), \quad \ddot{q} = \dot{q}\dot{z}, \quad \ddot{p} = \dot{p}\dot{w}.$$

Lagrangian

$$L = \frac{e^{-w}\dot{p}^2}{\dot{w}} + \frac{e^{-z}\dot{q}^2}{\dot{z}} + \frac{e^{-(dz+cw)}\dot{x}^2}{d\dot{z} + c\dot{w}} + \frac{e^{-(bz+aw)}\dot{y}^2}{b\dot{z} + a\dot{w}} + \dot{w}^2 + \dot{z}^2.$$

6.2 $(abc: a^2+b^2 \neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_6$**,** $[e_2,e_3]=be_3$**,** $[e_2,e_4]=ce_4$**,** $[e_2,\overline{e_5}]=e_5$**,** $[e_2,e_6]=e_6$**.**

$$S = \begin{bmatrix} e^z & we^z & 0 & 0 & q & p \\ 0 & e^z & 0 & 0 & p & 0 \\ 0 & 0 & e^{w+cz} & 0 & cx & x \\ 0 & 0 & 0 & e^{aw+bz} & by & ay \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right invariant vector fields

$$\{-(pD_q + xD_x + ayD_y + D_w), -(pD_p + qD_q + cxD_x + byD_y + D_z), D_y, D_x, D_p, D_q\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{y} = \dot{y}(b\dot{z} + a\dot{w}), \quad \ddot{x} = \dot{x}(c\dot{z} + \dot{w}), \quad \ddot{p} = \dot{p}\dot{z}, \quad \ddot{q} = \dot{p}\dot{w} + \dot{q}\dot{z}.$$

Lagrangian

$$L = \frac{e^{-(cz+w)}\dot{x}^2}{c\dot{z} + \dot{w}} + \frac{e^{-(bz+aw)}\dot{y}^2}{b\dot{z} + a\dot{w}} + \dot{q}\ln\left(\frac{\dot{p}}{\dot{z}}\right) - \frac{\dot{p}\dot{w}}{\dot{z}} + \dot{z}\dot{w} + q\dot{z} + \dot{z}^2 - w\dot{p}.$$

6.3 (a)**:** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_6$**,** $[e_2,e_3]=ae_3+e_4$**,** $[e_2,e_4]=ae_4$**,** $[e_2,e_5]=e_5$**,** $[e_2,\overline{e_6}]=e_6$

$$S = \begin{bmatrix} e^z & we^z & 0 & 0 & q & p \\ 0 & e^z & 0 & 0 & 0 & q \\ 0 & 0 & e^{w+za} & ze^{w+za} & x & y+ax \\ 0 & 0 & 0 & e^{w+za} & y & ay \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right invariant vector fields

$$\{-(qD_p + xD_x + yD_y + D_w), -(pD_p + qD_q + (ax+y)D_x + ayD_y + D_z), D_y, D_x, D_q, D_p\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{y} = \dot{y}(a\dot{z} + \dot{w}), \quad \ddot{x} = \dot{x}(a\dot{z} + \dot{w}) + \dot{y}\dot{z}, \quad \ddot{q} = \dot{q}\dot{z}, \quad \ddot{p} = \dot{p}\dot{z} + \dot{q}\dot{w}.$$

Lagrangian

$$L = (a\dot{z} + \dot{w})^2 + \dot{x}\ln\left(\frac{\dot{y}}{a\dot{z} + \dot{w}}\right) - \frac{\dot{y}\dot{z}}{a\dot{z} + \dot{w}} + (x + \dot{z})(a\dot{z} + \dot{w}) - z\dot{y} + \dot{p}\ln\left(\frac{\dot{q}}{\dot{z}}\right) - \frac{\dot{q}\dot{w}}{\dot{z}} - w\dot{q} + p\dot{z}.$$

6.4 $(ab:a\neq 0)$**:** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_6$**,** $[e_2,e_3]=e_4$**,** $[e_2,e_4]=-e_3$**,** $[e_2,e_5]=ae_5+be_6$**,** $[e_2,e_6]=ae_6$

$$S=\begin{bmatrix} e^{az} & (w+bz)e^{az} & 0 & 0 & q & p \\ 0 & e^{az} & 0 & 0 & 0 & q \\ 0 & 0 & \cos(z)e^{w} & \sin(z)e^{w} & y & x \\ 0 & 0 & -\sin(z)e^{w} & \cos(z)e^{w} & x & -y \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(qD_p+xD_x+yD_y+D_w)D_p,-((ap+bq)D_p+aqD_q-yD_x+xD_y+D_z),D_x,D_y,D_q,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}\dot{w}-\dot{y}\dot{z},\quad \ddot{y}=\dot{x}\dot{z}+\dot{y}\dot{w},\quad \ddot{q}=a\dot{q}\dot{z},\quad \ddot{p}=\dot{z}(a\dot{p}+b\dot{q})+\dot{q}\dot{w}.$$

Lagrangian

$$L=\frac{e^{-w}((\dot{y}\cos(z)-\dot{x}\sin(z))(\dot{w}\dot{y}-\dot{x}\dot{z})-(\dot{x}\cos(z)+\dot{y}\sin(z))(\dot{z}\dot{y}+\dot{x}\dot{w}))}{\dot{z}^2+\dot{w}^2}+\dot{p}\ln\left(\frac{\dot{q}}{a\dot{z}}\right)-\frac{(\dot{w}+b\dot{z})\dot{q}}{a\dot{z}}$$
$$+a\dot{z}(\dot{w}+b\dot{z}+p)-(w+bz)\dot{q}.$$

6.5 $(ab:ab\neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_5]=e_5+e_6$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=be_3$**,** $[e_2,e_4]=e_4$**.**

$$S=\begin{bmatrix} e^{w} & we^{w} & 0 & 0 & 0 & p \\ 0 & e^{w} & 0 & 0 & 0 & q \\ 0 & 0 & e^{z} & 0 & y & 0 \\ 0 & 0 & 0 & e^{aw+bz} & bx & ax \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(axD_x+qD_q+(q+p)D_p+D_w),-(bxD_x+yD_y+D_z),D_x,D_y,D_q,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}(b\dot{z}+a\dot{w}),\quad \ddot{y}=\dot{y}\dot{z},\quad \ddot{q}=\dot{q}\dot{w},\quad \ddot{p}=\dot{w}(\dot{p}+\dot{q}).$$

Lagrangian

$$L=q\dot{w}+\frac{e^{-w}\dot{q}^2}{\dot{w}}+\dot{p}\left(-w+\ln\left(\frac{\dot{q}}{\dot{w}}\right)\right)+\frac{e^{-(aw+bz)}\dot{x}^2}{a\dot{w}+b\dot{z}}+\frac{e^{-z}\dot{y}^2}{\dot{z}}+\dot{z}^2+\dot{w}^2.$$

6.6 $(ab:a^2+b^2\neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_4]=ae_4$**,** $[e_1,e_5]=e_5+e_6$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=e_3+e_4$**,** $[e_2,e_4]=e_4$**,** $[e_2,e_5]=be_6$

$$S=\begin{bmatrix} e^{w} & (w+bz)e^{w} & 0 & 0 & bq & p \\ 0 & e^{w} & 0 & 0 & 0 & q \\ 0 & 0 & e^{aw+z} & ze^{aw+z} & x+y & ax \\ 0 & 0 & 0 & e^{aw+z} & y & ay \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((p+q)D_p+qD_q+axD_x+ayD_y+D_w),-(bqD_p+(x+y)D_x+yD_y+D_z),D_y,D_x,D_q,D_p\}.$$

Geodesics:

$$\ddot{w}=0,\ \ddot{z}=0,\ \ddot{y}=\dot{y}(\dot{z}+a\dot{w}),\ \ddot{x}=\dot{x}(\dot{z}+a\dot{w})+\dot{y}\dot{z},\ \ddot{q}=\dot{q}\dot{w},\ \ddot{p}=\dot{w}(\dot{p}+\dot{q})+b\dot{q}\dot{z}.$$

Lagrangian

$$L=\dot{p}\ln\left(\frac{\dot{q}}{\dot{w}}\right)-\frac{(b\dot{z}+\dot{w})\dot{q}}{\dot{w}}-(bz+w)\dot{q}+p\dot{w}+\dot{y}\ln\left(\frac{\dot{x}}{a\dot{w}+\dot{z}}\right)-\frac{\dot{x}\dot{z}}{a\dot{w}+\dot{z}}+(y+\dot{z})(a\dot{w}+\dot{z})-z\dot{x}.$$

6.7 $(abc:a^2+b^2\neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_4]=ae_4$**,** $[e_1,e_5]=e_5+e_6$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=ce_3+e_4$**,** $[e_2,e_4]=-e_3+ce_4$**,** $[e_2,e_5]=be_6$**.**

$$S=\begin{bmatrix} \cos(z)e^{aw+cz} & -\sin(z)e^{aw+cz} & 0 & 0 & cp-q & ap \\ \sin(z)e^{aw+cz} & \cos(z)e^{aw+cz} & 0 & 0 & cq+p & aq \\ 0 & 0 & e^{w} & (w+bz)e^{w} & bx & y \\ 0 & 0 & 0 & e^{w} & 0 & x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(apD_p+aqD_q+xD_x+D_w),-((cp-q)D_p+(cq-p)D_q+bxD_x+D_z),-D_p,D_q,D_x,D_y\}.$$

Geodesics

$$\ddot{w}=0,\ \ddot{z}=0,\ \ddot{p}=\dot{p}(c\dot{z}+a\dot{w})+\dot{q}\dot{z},\ \ddot{q}=\dot{z}(-\dot{p}+c\dot{q})+a\dot{q}\dot{w},\ \ddot{x}=\dot{x}\dot{w},\ \ddot{y}=\dot{x}(b\dot{z}+\dot{w})+\dot{y}\dot{w}.$$

Lagrangian

$$L=\frac{e^{-(aw+cz)}((\dot{p}\cos(z)-\dot{q}\sin(z))((a\dot{w}+c\dot{z})\dot{p}-\dot{q}\dot{z})-(\dot{q}\cos(z)+\dot{p}\sin(z))(\dot{z}\dot{p}+\dot{q}(a\dot{w}+c\dot{z})))}{\dot{z}^2+(a\dot{w}+c\dot{z})^2}$$

$$+\dot{y}\ln\left(\frac{\dot{x}}{\dot{w}}\right)-\frac{(b\dot{z}+\dot{w})\dot{x}}{\dot{w}}+(b\dot{z}+\dot{w})\dot{w}+y\dot{w}-(bz+w)\dot{x}+\dot{z}^2+\dot{w}^2.$$

6.8: $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_6$**,** $[e_2,e_5]=e_5+e_6$**,** $[e_2,e_6]=e_6$**,** $[e_2,e_4]=e_4$**:**

$$S=\begin{bmatrix} e^z & ze^z & we^z & 0 & q & p \\ 0 & e^z & 0 & 0 & 0 & y \\ 0 & 0 & e^z & 0 & 0 & q \\ 0 & 0 & 0 & e^w & x & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(qD_p+xD_x+D_w),-((y+p)D_p+qD_p+yD_y+D_z),D_x,D_q,D_y,D_p\}.$$

Geodesics

$$\ddot{w}=0,\ \ddot{z}=0,\ \ddot{x}=\dot{x}\dot{w},\ \ddot{q}=\dot{q}\dot{z},\ \ddot{y}=\dot{y}\dot{z},\ \ddot{p}=\dot{z}(\dot{p}+\dot{y})+\dot{q}\dot{w}.$$

No Lagrangian.

6.9 (*a*)**:** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_6$**,** $[e_2,e_4]=e_4+e_5$**,** $[e_2,e_5]=e_5+ae_6$**,** $[e_2,e_6]=e_6$

$$S=\begin{bmatrix} e^z & aze^z & \dfrac{(az^2+2w)e^z}{2} & 0 & q & p \\ 0 & e^z & ze^z & 0 & 0 & y \\ 0 & 0 & e^z & 0 & 0 & q \\ 0 & 0 & 0 & e^w & x & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(qD_p+xD_x+D_w),-((ay+p)D_p+qD_q+(q+y)D_y+D_z),D_x,D_q,D_y,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}\dot{w},\quad \ddot{q}=\dot{q}\dot{z},\quad \ddot{y}=\dot{z}(\dot{q}+\dot{y}),\quad \ddot{p}=\dot{z}(\dot{p}+a\dot{y})+\dot{q}\dot{w}.$$

Lagrangian

$$L=\frac{ae^{-z}(-2\dot{q}^2\dot{w}-2w\dot{q}^2\dot{z}+az^2\dot{q}^2\dot{z}+4\dot{p}\dot{q}\dot{z}-4az\dot{q}\dot{y}\dot{z}+2a\dot{y}^2\dot{z})}{4\dot{z}^2}-\frac{ae^{-w}\dot{x}^2}{\dot{w}}+\dot{z}\dot{w}.$$

6.10 (*ab*)**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_4]=e_4+be_6$**,** $[e_1,e_5]=e_5$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=e_3$**,** $[e_2,e_4]=e_5$**,** $[e_2,e_5]=e_6$

$$S=\begin{bmatrix} e^w & ze^w & \dfrac{(z^2+2bw)e^w}{2} & 0 & q & p \\ 0 & e^w & ze^w & 0 & x & q \\ 0 & 0 & e^w & 0 & 0 & x \\ 0 & 0 & 0 & e^{wa+z} & y & ay \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((bx+p)D_p+qD_q+x,D_x+ayD_y+D_w),-(qD_p+xD_q+yD_y+D_z),D_y,D_x,D_q,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{y}(\dot{z}+a\dot{w}),\quad \ddot{x}=\dot{x}\dot{w},\quad \ddot{q}=\dot{q}\dot{w}+\dot{x}\dot{z},\quad \ddot{p}=\dot{w}(\dot{p}+b\dot{x})+\dot{q}\dot{z}.$$

Lagrangian

$$L=\frac{(4\dot{w}^2\dot{p}\dot{x}+2\dot{w}^2\dot{q}^2-2bw\dot{w}^2\dot{x}^2-4\dot{w}^2\dot{x}z\dot{q}+\dot{w}^2\dot{x}^2z^2-4\dot{x}\dot{z}\dot{w}\dot{q}+2\dot{x}^2\dot{z}\dot{w}z+2\dot{z}^2\dot{x}^2)}{e^w\dot{w}^3}+\frac{e^{-(z+aw)}\dot{y}^2}{\dot{z}+a\dot{w}}+\dot{z}\dot{w}.$$

6.11 (a)**:** $[e_1,e_3]=e_4$**,** $[e_1,e_5]=e_5+e_6$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=e_3$**,** $[e_2,e_4]=e_4$**,** $[e_2,e_5]=ae_5$**,** $[e_2,e_6]=ae_6$**.**

$$S=\begin{bmatrix} e^{w+az} & we^{w+az} & 0 & 0 & ap & p+q \\ 0 & e^{w+az} & 0 & 0 & aq & q \\ 0 & 0 & e^z & we^z & y & x \\ 0 & 0 & 0 & e^z & x & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((p+q)D_p+qD_q+xD_y+D_w),-(apD_p+aqD_q+xD_x+yD_y+D_z),D_x,D_y,D_q,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}\dot{z},\quad \ddot{y}=\dot{x}\dot{w}+\dot{y}\dot{z},\quad \ddot{q}=\dot{q}(a\dot{z}+\dot{w}),\quad \ddot{p}=\dot{p}(a\dot{z}+\dot{w})+\dot{q}\dot{w}.$$

Lagrangian

$$L=(a\dot{z}+\dot{w})^2+\dot{p}\ln\left(\frac{\dot{q}}{a\dot{z}+\dot{w}}\right)-\frac{\dot{q}\dot{w}}{a\dot{z}+\dot{w}}+(a\dot{z}+\dot{w})(p+\dot{w})-w\dot{q}+\dot{z}^2+\dot{y}\ln\left(\frac{\dot{x}}{\dot{z}}\right)-\frac{\dot{x}\dot{w}}{\dot{z}}+\dot{z}\dot{w}+y\dot{z}-w\dot{x}.$$

6.12 (ab)**:** $[e_1,e_3]=e_3+e_4$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_5+e_6$**,** $[e_1,e_6]=e_6$**,** $[e_2,e_3]=ae_4+e_5-be_6$**,** $[e_2,e_4]=e_6$**,** $[e_2,e_5]=-e_3+be_4+ae_6$**,** $[e_2,e_6]=-e_4$**.**

$$S=\begin{bmatrix} \cos(w)e^z & \sin(w)e^z & ((z+aw)\cos(w)+bw\sin(w))e^z & ((z+aw)\sin(w)-bw\cos(w))e^z & p & q \\ -\sin(w)e^z & \cos(w)e^z & -((z+aw)\sin(w)-bw\cos(w))e^z & ((z+aw)\cos(w)+bw\sin(w))e^z & -q & p \\ 0 & 0 & \cos(w)e^z & \sin(w)e^z & x & y \\ 0 & 0 & -\sin(w)e^z & \cos(w)e^z & -y & x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((x+p)D_p+(y+q)D_q+xD_x+yD_y+D_z),(by-ax-q)D_p+(p-bx-ay)D_q-yD_x+xD_y+D_w,D_y,D_q,D_x,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}\dot{z}-\dot{y}\dot{w},\quad \ddot{y}=\dot{y}\dot{z}+\dot{x}\dot{w},\quad \ddot{p}=\dot{z}(\dot{p}+\dot{x})+\dot{w}(a\dot{x}+b\dot{y}-\dot{q}),\quad \ddot{q}=\dot{z}(\dot{q}+\dot{y})+\dot{w}(a\dot{y}-b\dot{x}+\dot{p}).$$

Lagrangian

$$L=\frac{\dot{p}}{2}(\ln(\dot{x}^2+\dot{y}^2)-\ln(\dot{z}^2+\dot{w}^2))+\dot{q}\left(\arctan\left(\frac{\dot{w}}{\dot{z}}\right)-\arctan\left(\frac{\dot{y}}{\dot{x}}\right)\right)+\frac{b\dot{w}(\dot{x}\dot{w}-\dot{y}\dot{w})-(\dot{z}+a\dot{w})(\dot{y}\dot{w}+\dot{x}\dot{z})}{\dot{z}^2+\dot{w}^2}$$

$$+r\dot{z}-q\dot{w}-(aw+z)\dot{x}-bw\dot{y}+\dot{z}\dot{w}.$$

6.13 $(abcd:a^2+b^2\neq 0,\ c^2+d^2\neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_4]=ce_4$**,** $[e_1,e_5]=e_6$**,** $[e_1,e_6]=-e_5$**,** $[e_2,e_3]=be_3$**,** $[e_2,e_4]=de_4$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=e_6$

$$S=\begin{bmatrix}\cos(z)e^w & \sin(z)e^w & 0 & 0 & q & p\\ -\sin(z)e^w & \cos(z)e^w & 0 & 0 & p & -q\\ 0 & 0 & e^{cw+dz} & 0 & cx & dx\\ 0 & 0 & 0 & e^{aw+bz} & ay & by\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{qD_p-pD_q-cxD_x-ayD_y-D_w,-(pD_p+qD_q+dxD_x+byD_y+D_z),D_y,D_x,D_p,D_q\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{y}(b\dot{z}+a\dot{w}),\quad \ddot{x}=\dot{x}(d\dot{z}+c\dot{w}),\quad \ddot{p}=\dot{p}\dot{z}-\dot{q}\dot{w},\quad \ddot{q}=\dot{p}\dot{w}+\dot{q}\dot{z}.$$

Lagrangian

$$L=\frac{e^{-w}((\dot{q}\dot{w}-\dot{p}\dot{z})(\dot{q}\cos(z)-\dot{p}\sin(z))-(\dot{z}\dot{q}+\dot{w}\dot{p})(\dot{p}\cos(z)+\dot{q}\sin(z)))}{\dot{w}^2+\dot{z}^2}+\frac{e^{-(cw+dz)}\dot{x}^2}{c\dot{w}+d\dot{z}}+\frac{e^{-(aw+bz)}\dot{y}^2}{a\dot{w}+b\dot{z}}$$

$$+\dot{w}^2+\dot{z}^2.$$

6.14 $(abc:ab\neq 0)$**:** $[e_1,e_3]=ae_3$**,** $[e_1,e_5]=ce_5+e_6$**,** $[e_1,e_6]=-e_5+ce_6$**,** $[e_2,e_3]=be_3$**,** $[e_2,e_4]=e_4$**.**

$$S=\begin{bmatrix}\cos(w)e^{cw} & \sin(w)e^{cw} & 0 & 0 & 0 & p\\ -\sin(w)e^{cw} & \cos(w)e^{cw} & 0 & 0 & 0 & q\\ 0 & 0 & e^z & 0 & x & 0\\ 0 & 0 & 0 & e^{aw+bz} & -y & y\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{-((cp+q)D_p+(cq-p)D_q+ayD_y+D_w),-(xD_x+byD_y+D_z),D_y,D_x,D_q,D_p\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{y}(b\dot{z}+a\dot{w}),\quad \ddot{x}=\dot{x}\dot{z},\quad \ddot{q}=\dot{w}(-\dot{p}+c\dot{q}),\quad \ddot{p}=\dot{w}(c\dot{p}+\dot{q}).$$

Lagrangian

$$L=\frac{e^{-cw}((\dot{p}^2-\dot{q}^2)\cos(w)-2\sin(w)\dot{p}\dot{q})}{2\dot{w}}+\frac{e^{-z}\dot{x}^2}{\dot{z}}+\frac{e^{-aw-bz}\dot{y}^2}{a\dot{w}+b\dot{z}}+\dot{z}^2+\dot{w}^2.$$

6.15 $(abcd:b\neq 0)$**:** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=ae_5+be_6$**,** $[e_1,e_6]=-be_5+ae_6$**,** $[e_2,e_3]=ce_3+e_4$**,** $[e_2,e_4]=-e_3+ce_4$**,** $[e_2,e_5]=de_5$**,** $[e_2,e_6]=de_6$**.**

$$S=\begin{bmatrix} \cos(z)e^{w+cz} & -\sin(z)e^{w+cz} & 0 & 0 & p-q & p \\ \sin(z)e^{w+cz} & \cos(z)e^{w+cz} & 0 & 0 & p+q & q \\ 0 & 0 & \cos(bw)e^{aw+dz} & -\sin(bw)e^{aw+dz} & \frac{x+y}{2} & x \\ 0 & 0 & \sin(bw)e^{aw+dz} & \cos(bw)e^{aw+dz} & \frac{y-x}{2} & y \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p+qD_q+(ax-by)D_x+(bx+ay)D_y+D_w),-((cp-q)D_p+(p+cq)D_q+dxD_x+dyD_y+D_z),D_p,D_q,-D_y,D_x\}.$$

Geodesics:

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{p}(c\dot{z}+\dot{w})-\dot{q}\dot{z},\quad \ddot{q}=\dot{z}(\dot{p}+c\dot{q})+\dot{q}\dot{w},\quad \ddot{y}=b\dot{x}\dot{w}+\dot{y}(d\dot{z}+q\dot{w}),\quad \ddot{x}=\dot{x}(d\dot{z}+a\dot{w})-b\dot{y}\dot{w}.$$

Lagrangian

$$L=\frac{e^{-(dz+aw)}((\dot{y}\cos(bw)-\dot{x}\sin(bw))((d\dot{z}+a\dot{w})\dot{y}-b\dot{x}\dot{w})-(\dot{x}\cos(bw)+\dot{y}\sin(bw))(b\dot{w}\dot{y}+\dot{x}(d\dot{z}+a\dot{w})))}{(d\dot{z}+a\dot{w})^2+b^2\dot{w}^2}$$
$$+\frac{e^{-(w+cz)}((\dot{q}\cos(z)-\dot{p}\sin(z))((\dot{w}+c\dot{z})\dot{q}-\dot{p}\dot{z})-(\dot{p}\cos(z)+\dot{q}\sin(z))(\dot{z}\dot{q}+\dot{p}(\dot{w}+c\dot{z})))}{(\dot{w}+c\dot{z})^2+\dot{z}^2}+\dot{w}^2+\dot{z}^2.$$

6.16 (ab)**:** $[e_1,e_3]=e_4$**,** $[e_2,e_4]=e_4$**,** $[e_1,e_5]=ae_5+e_6$**,** $[e_1,e_6]=-e_5+ae_6$**,** $[e_2,e_3]=e_3$**,** $[e_2,e_6]=be_6$**,** $[e_2,e_5]=be_5$

$$S=\begin{bmatrix} \cos(w)e^{aw+bz} & \sin(w)e^{aw+bz} & 0 & 0 & -bp & q-ap \\ -\sin(w)e^{aw+bz} & \cos(w)e^{aw+bz} & 0 & 0 & bq & p+aq \\ 0 & 0 & e^z & we^z & y & x \\ 0 & 0 & 0 & e^z & x & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((ap-q)D_p+(aq-p)D_q+xD_y+D_w),-(bpD_p+qbD_q+xD_x+yD_y+D_z),D_p,D_q,D_y,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{p}(b\dot{z}+a\dot{w})-\dot{q}\dot{w},\quad \ddot{q}=\dot{p}\dot{w}+\dot{q}(b\dot{z}+a\dot{w}),\quad \ddot{y}=\dot{y}\dot{z},\quad \ddot{x}=\dot{x}\dot{z}.$$

Lagrangian

$$L=\frac{e^{-bz-aw}((\dot{q}\cos(w)-\dot{p}\sin(w))(\dot{q}(b\dot{z}+a\dot{w})-\dot{w}\dot{p})-(\dot{p}\cos(w)+\dot{q}\sin(w))(\dot{p}(b\dot{z}+a\dot{w})\dot{w}\dot{q}))}{(b\dot{z}+a\dot{w})^2+\dot{w}^2}$$
$$+\frac{e^{-z}(\dot{x}^2+\dot{y}^2)}{\dot{z}}+\dot{z}\dot{w}.$$

6.17 (a)**:** $[e_1,e_3]=ae_3+e_4$**,** $[e_1,e_4]=ae_4$**,** $[e_1,e_5]=e_6$**,** $[e_1,e_6]=-e_5$**,** $[e_2,e_6]=e_6$**,** $[e_2,e_5]=e_5$**.**

$$S=\begin{bmatrix} \cos(w)e^z & \sin(w)e^z & 0 & 0 & q & p \\ -\sin(w)e^z & \cos(w)e^z & 0 & 0 & p & -q \\ 0 & 0 & e^{aw} & we^{aw} & 0 & x \\ 0 & 0 & 0 & e^{aw} & 0 & y \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_q - qD_p + (ax+y)D_x + ayD_y + D_w), -(pD_p + qD_q + D_z), D_y, D_x, D_p, D_q\}.$$

Geodesics

$$\ddot{w}=0, \quad \ddot{z}=0, \quad \ddot{y}=a\dot{y}\dot{w}, \quad \ddot{x}=\dot{w}(a\dot{x}+\dot{y}), \quad \ddot{p}=\dot{p}\dot{z}-\dot{q}\dot{w}, \quad \ddot{q}=\dot{p}\dot{w}+\dot{q}\dot{z}.$$

Lagrangian
$(a\neq 0)$.

$$L=2\dot{z}^2+a^2\dot{w}^2+\dot{x}\left(\ln\left(\frac{\dot{y}}{a^2\dot{w}}\right)-aw\right)+\frac{e^{-aw}\dot{y}^2}{a^3\dot{w}}+y\dot{w}+\dot{w}^2 + \frac{e^{-z}((\dot{q}\cos(w)-\dot{p}\sin(w))(\dot{q}\dot{z}-\dot{w}\dot{p})-(\dot{p}\cos(w)+\dot{q}\sin(w))(\dot{p}\dot{z}+\dot{w}\dot{q}))}{\dot{z}^2+\dot{w}^2}$$

$(a=0)$.

$$L=\frac{((\dot{q}\cos(w)-\dot{p}\sin(w))(\dot{q}\dot{z}-\dot{w}\dot{p})-(\dot{p}\cos(w)+\dot{q}\sin(w))(\dot{p}\dot{z}+\dot{w}\dot{q}))}{e^z(\dot{z}^2+\dot{w}^2)}+\dot{z}^2+\dot{w}^2 + \left(\dot{x}-\frac{y\dot{w}}{2}-\frac{w\dot{y}}{2}\right)^2+\dot{y}^2.$$

6.18 $(abc: b\neq 0)$**:** $[e_1,e_3]=e_4$**,** $[e_1,e_4]=-e_3$**,** $[e_1,e_5]=ae_5+be_6$**,** $[e_1,e_6]=-be_5+ae_6$**,** $[e_2,e_3]=e_3$**,** $[e_2,e_4]=e_4$**,** $[e_2,e_5]=ce_5$**,** $[e_2,e_6]=ce_6$

$$S=\begin{bmatrix} \cos(w)e^z & \sin(w)e^z & 0 & 0 & -q & p \\ -\sin(w)e^z & \cos(w)e^z & 0 & 0 & p & q \\ 0 & 0 & \cos(bw)e^{cz-aw} & \sin(bw)e^{cz-aw} & ax-by & cx \\ 0 & 0 & -\sin(bw)e^{cz-aw} & \cos(bw)e^{cz-aw} & ay+bx & cy \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{qD_p - pD_q + (by-ax)D_x - (ay+bx)D_y - D_w, -(pD_p + qD_q + cxD_x + cyD_y + D_z), D_q, -D_p, D_x, D_y\}.$$

Geodesics

$$\ddot{w}=0, \quad \ddot{z}=0, \quad \ddot{q}=-\dot{p}\dot{w}+\dot{q}\dot{z}, \quad \ddot{p}=\dot{p}\dot{z}+\dot{q}\dot{w}, \quad \ddot{x}=\dot{x}(c\dot{z}-a\dot{w})+b\dot{y}\dot{w}, \quad \ddot{y}=-b\dot{x}\dot{w}+\dot{y}(c\dot{z}-a\dot{w}).$$

Lagrangian

$$L=\frac{e^{-z}((\dot{p}\cos(w)-\dot{q}\sin(w))(\dot{p}\dot{z}-\dot{w}\dot{q})-(\dot{q}\cos(w)+\dot{p}\sin(w))(\dot{q}\dot{z}+\dot{w}\dot{p}))}{\dot{z}^2+\dot{w}^2}+(c\dot{z}-a\dot{w})^2+\dot{w}^2$$
$$+\frac{e^{-(cz-aw)}((\dot{x}\cos(bw)-\dot{y}\sin(bw))(\dot{x}(c\dot{z}-a\dot{w})-b\dot{w}\dot{y})-(\dot{y}\cos(bw)+\dot{x}\sin(bw))(\dot{y}(c\dot{z}-a\dot{w})+b\dot{w}\dot{x}))}{(c\dot{z}-a\dot{w})^2+b^2\dot{w}^2}.$$

6.19: $[e_1,e_3]=e_4+e_5$, $[e_1,e_4]=-e_3+e_6$, $[e_1,e_5]=e_6$, $[e_1,e_6]=-e_5$, $[e_2,e_3]=e_3$, $[e_2,e_4]=e_4$, $[e_2,e_5]=e_5$, $[e_2,e_6]=e_6$

$$S=\begin{bmatrix}\cos(w)e^z & \sin(w)e^z & w\cos(w)e^z & w\sin(w)e^z & p & q\\ -\sin(w)e^z & \cos(w)e^z & -w\sin(w)e^z & w\cos(w)e^z & -q & p\\ 0 & 0 & \cos(w)e^z & \sin(w)e^z & x & y\\ 0 & 0 & -\sin(w)e^z & \cos(w)e^z & -y & x\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{(x+q)D_p+(y-p)D_q+yD_x-xD_y+D_w,-(pD_q+qD_q+xD_x+yD_y+D_z),D_x,D_y,-D_p,-D_q\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{x}=\dot{x}\dot{z}-\dot{y}\dot{w},\quad \ddot{y}=\dot{y}\dot{z}+\dot{x}\dot{w},\quad \ddot{p}=\dot{p}\dot{z}+\dot{w}(\dot{x}-\dot{q}),\quad \ddot{q}=\dot{w}(\dot{y}-\dot{p})+\dot{q}\dot{z}.$$

Lagrangian

$$L=\frac{\dot{p}}{2}(\ln(\dot{x}^2+\dot{y}^2)-\ln(\dot{z}^2+\dot{w}^2))+\dot{q}\left(\arctan\left(\frac{\dot{w}}{z}\right)-\arctan\left(\frac{\dot{y}}{\dot{x}}\right)\right)-\frac{(\dot{w}\dot{y}+\dot{x}\dot{z})\dot{w}}{\dot{z}^2+\dot{w}^2}+p\dot{z}-w\dot{x}-q\dot{w}+\dot{z}\dot{w}.$$

6.20: $(ab:a^2+b^2\neq 0)$**:** $[e_1,e_4]=ae_4$, $[e_1,e_6]=e_6$, $[e_2,e_4]=be_4$, $[e_2,e_5]=e_5$, $[e_1,e_2]=e_3$

$$S=\begin{bmatrix}e^{az+bw} & 0 & 0 & 0 & 0 & p\\ 0 & e^z & 0 & 0 & 0 & q\\ 0 & 0 & e^w & 0 & 0 & x\\ 0 & 0 & 0 & 1 & w & y\\ 0 & 0 & 0 & 0 & 1 & z\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{-(apD_p+qD_q+D_z),-(bpD_p+xD_x+zD_y+D_w),D_y,D_p,D_x,D_q\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{z}\dot{w},\quad \ddot{p}=\dot{p}(a\dot{z}+b\dot{w}),\quad \ddot{x}=\dot{x}\dot{w},\quad \ddot{q}=\dot{q}\dot{z}.$$

Lagrangian

$$L=\frac{e^{-z}\dot{q}^2}{\dot{z}}+\frac{e^{-w}\dot{x}^2}{\dot{w}}+\frac{e^{-(az+bw)}\dot{p}^2}{a\dot{z}+b\dot{w}}+\dot{z}^2+\dot{w}^2+\left(\dot{y}-\frac{z\dot{w}}{2}-\frac{w\dot{z}}{z}\right)^2.$$

6.21: (a)**:** $[e_1,e_4]=e_4$, $[e_1,e_5]=e_6$, $[e_2,e_4]=ae_4$, $[e_2,e_5]=e_5$, $[e_2,e_6]=e_6$, $[e_1,e_2]=e_3$

$$S=\begin{bmatrix} e^{z+aw} & 0 & 0 & 0 & 0 & p \\ 0 & e^{w} & 0 & 0 & x & q \\ 0 & 0 & e^{w} & 0 & 0 & x \\ 0 & 0 & 0 & 1 & w & y \\ 0 & 0 & 0 & 0 & 1 & z \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(apD_p+qD_q+D_z),-(bpD_p+xD_x+zD_y+D_w),D_y,D_p,D_x,D_q\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{z}\dot{w},\quad \ddot{p}=\dot{p}(\dot{z}+a\dot{w}),\quad \ddot{x}=\dot{x}\dot{w},\quad \ddot{q}=\dot{w}(\dot{q}-x\dot{z})+\dot{z}\dot{x}.$$

Lagrangian

$$L=\dot{q}\ln\left(\frac{\dot{x}}{\dot{w}}\right)+\frac{\dot{x}\dot{z}}{\dot{w}}+q\dot{w}+z\dot{x}+\left(\dot{y}-\frac{w\dot{z}}{2}-\frac{z\dot{w}}{2}\right)^2+\frac{e^{-z-aw}\dot{p}}{\dot{z}+a\dot{w}}+\dot{z}\dot{w}.$$

6.22 ($a\epsilon: a^2+\epsilon^2\neq 0$, $\epsilon=0,1$)**:** $[e_1,e_3]=e_3$, $[e_1,e_5]=e_6$, $[e_2,e_4]=e_4$, $[e_2,e_3]=ae_3$, $[e_1,e_2]=\epsilon e_5$. ($\epsilon=\overline{0)}$

$$S=\begin{bmatrix} 1 & 0 & 0 & z & p \\ 0 & e^{w} & 0 & 0 & q \\ 0 & 0 & e^{z+aw} & 0 & x \\ 0 & 0 & 0 & 1 & y \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(yD_p+xD_x+D_z),-(qD_q+axD_x+D_w),D_x,D_q,D_y,D_p\}.$$

Geodesics

$$\ddot{z}=0,\quad \ddot{w}=0,\quad \ddot{x}=\dot{x}(\dot{z}+a\dot{w}),\quad \ddot{q}=\dot{q}\dot{w},\quad \ddot{y}=0,\quad \ddot{p}=\dot{y}\dot{z}.$$

Lagrangian

$$L=\frac{e^{-(az+w)}\dot{x}^2}{a\dot{z}+\dot{w}}+\frac{e^{-w}\dot{q}^2}{\dot{w}}+\left(\dot{p}-\frac{y\dot{z}}{2}-\frac{z\dot{y}}{2}\right)^2+\dot{z}^2+\dot{w}^2+\dot{y}^2.$$

($\epsilon=1$):

$$S=\begin{bmatrix} e^{az+w} & 0 & 0 & 0 & 0 & p \\ 0 & e^{z} & 0 & 0 & 0 & q \\ 0 & 0 & 1 & w & \frac{w^2}{2} & x \\ 0 & 0 & 0 & 1 & w & y \\ 0 & 0 & 0 & 0 & 1 & z \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p + yD_x + zD_y + D_w), -(apD_p + qD_q + D_z), D_p, D_q, D_y, D_x\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{p} = \dot{p}(a\dot{z} + \dot{w}), \quad \ddot{q} = \dot{q}\dot{z}, \quad \ddot{y} = \dot{z}\dot{w}, \quad \ddot{x} = \dot{y}\dot{w}.$$

Lagrangian

$$L = (2\dot{x} - w\dot{y} - y\dot{w})\ln\left(\frac{\dot{z}}{\dot{w}}\right) + \frac{w^2\dot{z}}{2} + \dot{w}^2 + \left(\dot{y} - \frac{z\dot{w}}{2} - \frac{w\dot{z}}{2}\right)^2 + \frac{e^{-z}\dot{q}^2}{\dot{z}} + \frac{e^{-(az+w)}\dot{p}^2}{a\dot{z} + \dot{w}}.$$

6.23 $(a\epsilon)$**:** $(a \geqslant 0,\ \epsilon = 0, 1)$**:** $[e_1, e_3] = e_3$**,** $[e_1, e_4] = e_4$**,** $[e_1, e_5] = e_6$**,** $[e_2, e_3] = e_4$**,** $[e_2, e_4] = -e_3$**,** $[e_2, \overline{e_5}] = ae_6$**,** $[e_1, e_2] = \epsilon e_5$**:**

$(\epsilon = 0)$

$$S = \begin{bmatrix} e^z\cos(w) & -e^z\sin(w) & 0 & 0 & p \\ e^z\sin(w) & e^z\cos(w) & 0 & 0 & q \\ 0 & 0 & 1 & aw + z & x \\ 0 & 0 & 0 & 1 & y \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p + qD_q + yD_x + D_z), -(-qD_p + pD_q + ayD_x + D_w), D_p, -D_q, D_y, D_x\}.$$

Geodesics

$$\ddot{z} = 0, \quad \ddot{w} = 0, \quad \ddot{p} = \dot{p}\dot{z} - \dot{q}\dot{w}, \quad \ddot{q} = \dot{p}\dot{w} + \dot{q}\dot{z}, \quad \ddot{y} = 0, \quad \ddot{x} = \dot{y}(\dot{z} + a\dot{w}).$$

Lagrangian

$$L = \frac{e^{-z}((-tb + sp)(\dot{q}\cos(w) - b\sin(w)) - (\dot{q}\dot{w} + \dot{p}\dot{z})(\dot{p}\cos(w) + \dot{q}\sin(w)))}{\dot{w}^2 + \dot{z}^2} + \dot{w}^2 + \dot{z}^2 + \dot{y}^2 + \left(\dot{x} - \frac{1}{2}\dot{y}(z + aw) - \frac{1}{2}(a\dot{w} + \dot{z})y\right)^2.$$

$(a = 0,\ \epsilon = 1)$

$$S = \begin{bmatrix} \cos(w)e^z & \sin(w)e^z & 0 & 0 & 0 & p \\ -\sin(w)e^z & \cos(w)e^z & 0 & 0 & 0 & q \\ 0 & 0 & 1 & z & \frac{z^2}{2} & x \\ 0 & 0 & 0 & 1 & z & y \\ 0 & 0 & 0 & 0 & 1 & w \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p + qD_q + yD_x + wD_y + D_z), qD_p - pD_q + D_w, D_p, -D_q, D_y, D_x\}.$$

Geodesics

$$\ddot{z} = 0, \quad \ddot{w} = 0, \quad \ddot{p} = \dot{p}\dot{z} + \dot{q}\dot{w}, \quad \ddot{q} = -\dot{p}\dot{w} + \dot{q}\dot{z}, \quad \ddot{y} = \dot{w}\dot{z}, \quad \ddot{x} = \dot{y}\dot{z}.$$

Lagrangian

$$L=\frac{e^{-z}((\dot{p}\cos(w)-\dot{q}\sin(w))(\dot{p}\dot{z}-\dot{w}\dot{q})-(\dot{q}\cos(w)+\dot{p}\sin(w))(\dot{q}\dot{z}+\dot{w}\dot{p}))}{\dot{z}^2+\dot{w}^2}$$
$$+2\dot{z}^2+(2\dot{x}-z\dot{y}-y\dot{z})\ln\left(\frac{\dot{w}}{\dot{z}}\right)+\frac{z^2\dot{w}}{2}+\left(\dot{y}-\frac{z\dot{w}}{2}-\frac{w\dot{z}}{2}\right)^2+\dot{w}^2.$$

$(a\neq 0,\ \epsilon=1)$:

$$S=\begin{bmatrix}\cos(w)e^z & \sin(w)e^z & 0 & 0 & 0 & p\\ -\sin(w)e^z & \cos(w)e^z & 0 & 0 & 0 & q\\ 0 & 0 & 1 & aw+z & \frac{(aw+z)^2}{2} & x\\ 0 & 0 & 0 & 1 & aw+z & y\\ 0 & 0 & 0 & 0 & 1 & z\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p+qD_q+yD_x+zD_y+D_z),-(qD_p-pD_q+ayD_x+azD_y+D_w),D_q,D_p,aD_y,aD_x\}.$$

Geodesics

$$\ddot{z}=0,\quad \ddot{w}=0,\quad \ddot{q}=-\dot{p}\dot{w}+\dot{q}\dot{z},\quad \ddot{p}=\dot{p}\dot{z}+\dot{q}\dot{w},\quad \ddot{y}=\dot{z}(\dot{z}+a\dot{w}),\quad \ddot{x}=\dot{y}(\dot{z}+a\dot{w}).$$

A Lagrangian is given by

$$L=\frac{e^{-z}((\dot{p}\cos(w)-\dot{q}\sin(w))(\dot{p}\dot{z}-\dot{w}\dot{q})-(\dot{q}\cos(w)+\dot{p}\sin(w))(\dot{q}\dot{z}+\dot{w}\dot{p}))}{\dot{z}^2+\dot{w}^2}+\dot{z}^2+(a\dot{w}+\dot{z})^2$$
$$+(2\dot{x}-(z+aw)\dot{y}-y(a\dot{w}+z\dot{x}))\ln\left(\frac{\dot{z}}{a\dot{w}+\dot{z}}\right)+\frac{(z+aw)^2\dot{z}}{2}+\left(\dot{y}-\frac{z(a\dot{w}+\dot{z})}{2}-\frac{(aw+z)\dot{z}}{2}\right)^2.$$

6.24: $[e_1,e_5]=e_5+e_6$, $[e_1,e_6]=e_6$, $[e_2,e_4]=e_4$, $[e_1,e_2]=e_3$

$$S=\begin{bmatrix}e^z & 0 & 0 & 0 & 0 & p\\ 0 & e^w & we^w & 0 & 0 & q\\ 0 & 0 & e^w & 0 & 0 & x\\ 0 & 0 & 0 & 1 & w & y\\ 0 & 0 & 0 & 0 & 1 & z\\ 0 & 0 & 0 & 0 & 0 & 1\end{bmatrix}.$$

Right-invariant vector fields

$$\{-((q+x)D_q+xD_x+zD_y+D_w),-(pD_p+D_z),D_y,D_p,D_x,D_q\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=\dot{z}\dot{w},\quad \ddot{p}=\dot{p}\dot{z},\quad \ddot{x}=\dot{x}\dot{w},\quad \ddot{q}=\dot{w}(\dot{q}+\dot{x}).$$

Lagrangian

$$L=\dot{q}\left(-w+\ln\left(\frac{\dot{x}}{\dot{w}}\right)\right)+\frac{e^{-z}\dot{p}^2}{\dot{z}}+\frac{e^{-w}\dot{z}^2}{\dot{w}}+x\dot{w}+\dot{z}^2+\dot{w}^2+\left(\dot{y}-\frac{w\dot{z}}{2}-\frac{z\dot{w}}{2}\right)^2.$$

6.25: $(ab:a^2+b^2\neq 0)$**:** $[e_1,e_4]=ae_4$**,** $[e_1,e_5]=e_6$**,** $[e_1,e_6]=-e_5$**,** $[e_2,e_4]=be_4$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=e_6$**,** $[e_1,e_2]=e_3$**.**

$$S=\begin{bmatrix} e^{aw+bz} & 0 & 0 & 0 & 0 & p \\ 0 & 1 & x & y & -z & q \\ 0 & 0 & \cos(w)e^{z} & \sin(w)e^{z} & 0 & 0 \\ 0 & 0 & -\sin(w)e^{z} & \cos(w)e^{z} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & w \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(apD_p+D_w),-(bpD_p+wD_q-D_z),D_q,D_p,e^{z}\cos(w)D_x+e^{z}\sin(w)D_y,-e^{z}\sin(w)D_x + e^{z}\cos(w)D_y\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{q}=-\dot{w}\dot{z},\quad \ddot{p}=\dot{p}(b\dot{w}+a\dot{z}),\quad \ddot{x}+\dot{y}\dot{w}-\dot{x}\dot{z}=0,\quad \ddot{y}-\dot{x}\dot{w}+\dot{y}\dot{z}=0.$$

Lagrangian

$$L=\frac{e^{-z}(\dot{y}\dot{z}-\dot{x}\dot{w})(\dot{y}\cos(w)-\dot{x}\sin(w))-(\dot{w}\dot{y}-\dot{x}\dot{z})(\dot{x}\cos(w)+\dot{y}\sin(w))}{\dot{z}^2+\dot{w}^2} + \frac{e^{-(az+bw)}\dot{p}^2}{a\dot{z}+b\dot{w}}+\dot{z}^2+\dot{w}^2+\left(\dot{q}+\frac{w\dot{z}}{2}+\frac{z\dot{w}}{2}\right)^2.$$

6.26 (a)**:** $[e_1,e_5]=ae_5+e_6$**,** $[e_1,e_6]=ae_6-e_5$**,** $[e_2,e_4]=e_4$**,** $[e_1,e_2]=e_3$

$$S=\begin{bmatrix} e^{z} & 0 & 0 & 0 & 0 & p \\ 0 & 1 & z & 0 & 0 & q \\ 0 & 0 & 1 & 0 & 0 & w \\ 0 & 0 & 0 & \cos(w)e^{aw} & \sin(w)e^{aw} & y \\ 0 & 0 & 0 & -\sin(w)e^{aw} & \cos(w)e^{aw} & x \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-((ay+x)D_y+(ax-y)D_x+D_w),-(pD_p+wD_q+D_z),D_q,D_p,-D_y,D_x\}$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{q}=\dot{w}\dot{z},\quad \ddot{p}=\dot{p}\dot{z},\quad \ddot{y}=\dot{w}(\dot{x}+a\dot{y}),\quad \ddot{x}=\dot{w}(a\dot{x}-\dot{y}).$$

Lagrangian

$$L=\left(\dot{q}-\frac{z\dot{w}}{2}-\frac{w\dot{z}}{2}\right)^2+\dot{z}^2+\dot{w}^2+\frac{e^{-z}\dot{p}^2}{\dot{z}}+\frac{\dot{z}^2}{\dot{w}}+\frac{e^{-aw}((\dot{x}^2-\dot{y}^2)\cos(w)+2\sin(w)\dot{x}\dot{y})}{2\dot{w}}$$

6.27 (ϵ)**:** $(\epsilon=0,1)$**:** $[e_1,e_3]=e_4$**,** $[e_1,e_5]=e_6$**,** $[e_1,e_6]=-e_5$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=e_6$**,** $[e_1,e_2]=\epsilon e_3$**,** $\epsilon=0$

$$S=\begin{bmatrix} \cos(z)e^{w} & -\sin(z)e^{w} & 0 & 0 & p \\ \sin(z)e^{w} & \cos(z)e^{w} & 0 & 0 & q \\ 0 & 0 & 1 & z & y \\ 0 & 0 & 0 & 1 & x \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-qD_p+pD_q+xD_y+D_z,-(pD_p+qD_q+D_w),D_x,D_y,D_p,D_q\}.$$

Geodesics

$$\ddot{z}=0,\quad \ddot{w}=0,\quad \ddot{x}=0,\quad \ddot{y}=\dot{x}\dot{z},\quad \ddot{p}=\dot{p}\dot{w}-\dot{q}\dot{z},\quad \ddot{q}=\dot{p}\dot{z}+\dot{q}\dot{w}.$$

Lagrangian

$$L=\frac{e^{-w}((\dot{q}\cos(z)-\dot{p}\sin(z))(\dot{w}\dot{q}-\dot{p}\dot{z})-(\dot{p}\cos(z)+\dot{q}\sin(z))(\dot{z}\dot{q}+\dot{p}\dot{w}))}{\dot{z}^2+\dot{w}^2}$$
$$+\dot{x}^2+\left(\dot{y}-\frac{z\dot{x}}{2}-\frac{x\dot{z}}{2}\right)^2+\dot{z}^2+\dot{w}^2$$

$\epsilon=1$:

$$S=\begin{bmatrix} 1 & w & \frac{w^2}{2} & p & x & y \\ 0 & 1 & w & q & 0 & 0 \\ 0 & 0 & 1 & z & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos(w)e^{z} & \sin(w)e^{z} \\ 0 & 0 & 0 & 0 & -\sin(w)e^{z} & \cos(w)e^{z} \end{bmatrix}.$$

Right-invariant vector fields

$$\{qD_p+zD_q+D_w,D_z,D_q,D_p,e^{z}\cos(w)D_x+e^{z}\sin(w)D_y,e^{z}\cos(w)D_y-e^{z}\sin(w)D_z\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{q}=\dot{z}\dot{w},\quad \ddot{p}=\dot{q}\dot{w},\quad \ddot{x}=\dot{z}\dot{x}-\dot{w}\dot{y},\quad \ddot{y}=\dot{z}\dot{y}+\dot{w}\dot{x}.$$

Lagrangian

$$L=\frac{e^{-z}((\dot{y}\cos(w)-\dot{x}\sin(w))(\dot{z}\dot{y}-\dot{x}\dot{w})-(\dot{x}\cos(w)+\dot{y}\sin(w))(\dot{w}\dot{y}+\dot{x}\dot{z}))}{\dot{z}^2+\dot{w}^2}$$
$$+(2\dot{p}-w\dot{q}-q\dot{w})\ln\left(\frac{\dot{z}}{\dot{w}}\right)+\frac{w^2\dot{z}}{2}+3\dot{w}^2+\left(\dot{q}-\frac{z\dot{w}}{2}-\frac{w\dot{z}}{2}\right)^2+\dot{z}^2.$$

6.28: $[e_4,e_6]=-e_3$, $[e_5,e_6]=-e_4$, $[e_1,e_3]=e_3$, $[e_1,e_5]=-e_5$, $[e_1,e_6]=e_6$, $[e_2,e_4]=e_4$, $[e_2,e_5]=2e_3$, $[e_2,e_6]=-e_6$:

$$S=\begin{bmatrix} e^{w} & -xe^{z} & \dfrac{x^{2}e^{2z-w}}{2} & ye^{w-z} & -yx & p \\ 0 & e^{z} & -xe^{2z-w} & qe^{w-z} & y-xq & xq \\ 0 & 0 & e^{2z-w} & 0 & 2q & -q \\ 0 & 0 & 0 & e^{w-z} & -x & x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p-qD_q+xD_x+D_w),-(2qD_q-xD_x+yD_y+D_z),-(xD_p+D_y),xqD_p-D_x+qD_y,D_q,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=-\dot{q}(\dot{x}+x\dot{z})+\dot{x}\dot{w}(q+y)+\dot{y}(\dot{z}+x\dot{w}),\quad \ddot{p}=\dot{p}\dot{w}+\dot{x}(\dot{y}-y\dot{z}-x\dot{q})+x^{2}(\dot{y}\dot{w}-\dot{q}\dot{z})$$
$$+x\dot{x}\dot{w}(y+q),\quad \ddot{q}=\dot{q}(2\dot{z}-\dot{w}),\quad \ddot{x}=-\dot{x}(\dot{z}+\dot{w}).$$

Note that there are no Lagrangians for cases 28–39.

6.29 $(ab:a^{2}+b^{2}\neq 0)$**:** $[e_4,e_5]=-e_3$**,** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_6]=ae_6$**,** $[e_2,e_3]=e_3$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=be_6$

$$S=\begin{bmatrix} e^{z+w} & -qe^{w} & ye^{z} & 0 & p-yq & p \\ 0 & e^{w} & 0 & 0 & y & 0 \\ 0 & 0 & e^{z} & 0 & 0 & q \\ 0 & 0 & 0 & e^{aw+bz} & ax & bx \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p+axD_x+yD_y+D_w),-(pD_p+qD_q+bxD_x+D_z),D_p,qD_p+D_y,D_q,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=(\dot{z}+\dot{w})+\dot{q}(\dot{y}-y\dot{w}),\quad \ddot{y}=\dot{y}\dot{w},\quad \ddot{q}=\dot{q}\dot{z},\quad \ddot{x}=\dot{x}(b\dot{z}+a\dot{w}).$$

6.30 (a)**:** $[e_4,e_5]=-e_3$**,** $[e_1,e_3]=2e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_5$**,** $[e_1,e_6]=ae_6$**,** $[e_2,e_4]=e_5$**,** $[e_2,e_6]=e_6$**.**

$$S=\begin{bmatrix} e^{2w} & ye^{w} & 0 & -qe^{w} & \dfrac{y^{2}}{2} & p \\ 0 & e^{w} & 0 & ze^{w} & y & zy+q \\ 0 & 0 & e^{aw+z} & 0 & x & ax \\ 0 & 0 & 0 & e^{w} & 0 & y \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(2pD_p+qD_q+axD_x+yD_y+D_w),-(xD_x+D_z),2D_p,(zy+q)D_p-zD_q+D_y,-yD_p+D_q,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{w}(2\dot{p}+q\dot{y}+y\dot{q})+y\dot{z}(\dot{y}-y\dot{w}),\quad \ddot{y}=\dot{y}\dot{w},$$
$$\ddot{q}=-\dot{q}\dot{w}-\dot{z}(\dot{y}+y\dot{w}),\quad \ddot{x}=\dot{x}(\dot{z}+a\dot{w}).$$

6.31: $[e_4,e_5]=-e_3$, $[e_1,e_4]=e_4$, $[e_1,e_5]=-e_5$, $[e_2,e_3]=e_3$, $[e_2,e_5]=e_5$, $[e_2,e_6]=e_6+e_3$

$$S=\begin{bmatrix} e^z & -qe^w & ye^{z-w} & ze^z & -yq & p \\ 0 & e^w & 0 & 0 & y & 0 \\ 0 & 0 & e^{z-w} & 0 & -q & q \\ 0 & 0 & 0 & e^z & 0 & x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(yD_y-qD_q+D_w),-((x+p)D_p+qD_q+xD_x+D_z),D_p,qD_p+D_y,D_q,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{z}(\dot{p}+\dot{x})+\dot{q}(\dot{y}-y\dot{w}),\quad \ddot{y}=\dot{y}\dot{w},\quad \ddot{q}=\dot{q}(\dot{z}-\dot{w}),\quad \ddot{x}=\dot{x}\dot{z}.$$

6.32 (a)**:** $[e_4,e_5]=-e_3$, $[e_1,e_4]=e_4$, $[e_1,e_5]=-e_5$, $[e_1,e_6]=e_3$, $[e_2,e_3]=e_3$, $[e_2,e_4]=ae_4$, $[e_2,e_5]=(1-a)e_5$, $[e_2,e_6]=e_6$

$$S=\begin{bmatrix} e^z & qe^{w+az} & ye^{-w+z-az} & we^z & x+yq & p \\ 0 & e^{w+az} & 0 & 0 & y & ya \\ 0 & 0 & e^{-w+z-az} & 0 & q & (a-1)q \\ 0 & 0 & 0 & e^z & 0 & x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(xD_p-qD_q+yD_y+D_w),-(pD_p+(1-a)qD_q+xD_x+ayD_y+D_z),D_p,(a-1)qD_p+D_y,-(ayD_p+D_q),D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{q}\dot{y}(1-2a)+y\dot{q}\dot{w}(a-1)+\dot{w}(\dot{x}-q\dot{y})+q(1-a^2)\dot{y}\dot{z},$$
$$\ddot{y}=(a+1)\dot{y}\dot{z},\quad \ddot{q}=-\dot{q}\dot{w},\quad \ddot{x}=\dot{x}\dot{z}.$$

6.33: $[e_4,e_5]=e_3$, $[e_1,e_3]=e_3$, $[e_1,e_4]=e_4$, $[e_2,e_3]=e_3$, $[e_2,e_5]=e_5+e_6$, $[e_2,e_6]=e_6$.

$$S=\begin{bmatrix} e^{w+z} & -qe^w & 0 & ye^z & p-yq & p \\ e & e^w & 0 & 0 & y & 0 \\ 0 & 0 & e^z & ze^z & 0 & x \\ 0 & 0 & 0 & e^z & 0 & q \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p+yD_y+D_w),-(pD_p+qD_q+(q+x)D_x+D_z),D_p,-(qD_p+D_y),D_q,D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{p}(\dot{w}+\dot{z})+\dot{q}(\dot{y}-y\dot{w}),\quad \ddot{y}=\dot{y}\dot{w},\quad \ddot{q}=\dot{q}\dot{z},\quad \ddot{x}=\dot{z}(\dot{q}+\dot{x}).$$

6.34 (a)**:** $[e_4,e_5]=e_3$**,** $[e_1,e_3]=e_3$**,** $[e_1,e_4]=e_4$**,** $[e_1,e_5]=e_6$**,** $[e_2,e_3]=(1+a)e_3$**,** $[e_2,e_4]=ae_4$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=e_6$**.**

$$S=\begin{bmatrix} e^{w+z+az} & -qe^{w+az} & 0 & ye^{z} & p+ap+yq & p\\ 0 & e^{w+az} & 0 & 0 & ay & y\\ 0 & 0 & e^{z} & we^{z} & x & q\\ 0 & 0 & 0 & e^{z} & q & 0\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p+qD_x+yD_y+D_w),-((ap+p)D_p+qD_q+xD_x+ayD_y+D_z),D_p,D_y,yD_p-D_q,-D_x\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{p}(a\dot{z}+\dot{z}+\dot{w})+\dot{q}(y\dot{z}-\dot{y})+q\dot{y}((1-a)\dot{z}-\dot{w}),\quad \ddot{y}=\dot{y}(a\dot{z}+\dot{w}),$$
$$\ddot{q}=\dot{q}\dot{z},\quad \ddot{x}=\dot{q}\dot{w}+\dot{x}\dot{z}.$$

6.35 $(ab:a^2+b^2\neq 0)$**:** $[e_4,e_5]=e_3$**,** $[e_1,e_4]=e_5$**,** $[e_1,e_5]=-e_4$**,** $[e_1,e_6]=ae_6$**,** $[e_2,e_3]=2e_3$**,** $[e_2,e_4]=e_4$**,** $[e_2,e_5]=e_5$**,** $[e_2,e_6]=be_6$

$$S=\begin{bmatrix} e^{2z} & -(x\cos(w)-\sin(w)q)e^{z} & (\cos(w)q+x\sin(w))e^{z} & 0 & \dfrac{(x^2+q^2)}{2} & p\\ 0 & \cos(w)e^{z} & -\sin(w)e^{z} & 0 & -x & q\\ 0 & \sin(w)e^{z} & \cos(w)e^{z} & 0 & q & x\\ 0 & 0 & 0 & e^{aw+bz} & ay & by\\ 0 & 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(D_w-xD_q+qD_x+ayD_y),-(2pD_p+qD_q+xD_x+byD_y+2D_z),-2D_p,xD_p+D_q,-qD_p+D_x,D_y\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=2\dot{p}(\dot{z}+p\dot{w})+\dot{q}(q\dot{w}+x\dot{z})-\dot{x}(x\dot{w}+q\dot{z}),\quad \ddot{q}=\dot{q}\dot{z}-\dot{x}\dot{w},$$
$$\ddot{x}=\dot{q}\dot{w}+\dot{x}\dot{z},\quad \ddot{y}=\dot{y}(b\dot{z}+a\dot{w}).$$

6.36: $[e_4,e_5]=e_3$, $[e_1,e_4]=e_5$, $[e_1,e_5]=-e_4$, $[e_2,e_3]=2e_3$, $[e_2,e_4]=e_4$, $[e_2,e_5]=e_5$, $[e_2,e_6]=2e_6+e_3$

$$S=\begin{bmatrix} e^{2z} & (x\cos(w)-\sin(w)q)e^{z} & (\cos(w)q+x\sin(w))e^{z} & ze^{2z} & \dfrac{x^2+q^2}{2} & p \\ 0 & \cos(w)e^{z} & \sin(w)e^{z} & 0 & x & q \\ 0 & -\sin(w)e^{z} & \cos(w)e^{z} & 0 & q & -x \\ 0 & 0 & 0 & e^{2z} & 0 & 2y \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(D_w-xD_q+qD_x),-((2p+2y)D_p+qD_q+xD_x+2yD_y+D_z),2D_p,-xD_p+D_q,qD_p+D_x,D_y\}.$$

Geodesics

$$\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{p}=\dot{z}(2\dot{y}-x\dot{q}+2\dot{p})-\dot{w}(q\dot{q}+x\dot{x}),\quad \ddot{q}=\dot{q}\dot{z}-\dot{x}\dot{w},\quad \ddot{x}=\dot{q}\dot{w}+\dot{x}\dot{z},\quad \ddot{y}=2\dot{y}\dot{z}.$$

6.37 (*a*)**:** $[e_4,e_5]=e_3$, $[e_1,e_4]=e_5$, $[e_1,e_5]=-e_5$, $[e_2,e_3]=2e_3$, $[e_2,e_4]=e_4+ae_5$, $[e_2,e_5]=-ae_4+e_5$, $[e_2,e_6]=2e_5$, $[e_1,e_6]=e_3$.

$$S=\begin{bmatrix} e^{2z} & -qe^{z} & pe^{z} & -we^{2z} & x+\dfrac{p^2+q^2}{2} & y \\ 0 & e^{z}\cos(w-az) & e^{z}\sin(w-az) & 0 & p\sin(w-az)-q\cos(w-az) & (p-aq)\cos(w-az)+(q+ap)\sin(w-az) \\ 0 & -e^{z}\sin(w-az) & e^{z}\cos(w-az) & 0 & p\cos(w-az)+q\sin(w-az) & (q+ap)\cos(w-az)+(aq-p)\sin(w-az) \\ 0 & 0 & 0 & e^{2z} & 0 & 2x \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\begin{aligned}\{&-2xD_y+D_w,-pD_p-qD_q-2xD_x-2yD_y-D_z,2D_y,-\sin(w-az)D_p-\cos(w-az)D_q-((p-aq)\\ &\times\cos(w-az)+(ap+q)\sin(w-az))D_y,-\cos(w-az)D_p-\sin(w-az)D_q-((ap+q)\\ &\times\cos(w-az)+(aq-p)\sin(w-az))D_y,D_x\}.\end{aligned}$$

Geodesics

$$\begin{aligned}&\ddot{w}=0,\quad \ddot{z}=0,\quad \ddot{y}=(p^2+q^2)(\dot{w}-a\dot{z})\dot{z}+(a^2-1)(p\dot{q}-q\dot{p})\dot{z}+(aq-p)\dot{w}\dot{p}-(ap+q)\dot{w}\dot{q},\quad \ddot{p}=\dot{p}\dot{z}\\ &\quad+(\dot{q}-q\dot{z})(a\dot{z}-\dot{w}),\quad \ddot{q}=\dot{q}\dot{z}+(\dot{p}-p\dot{z})(\dot{w}-a\dot{z}),\quad \ddot{x}=2\dot{x}\dot{z}.\end{aligned}$$

6.38: $[e_4,e_5]=e_3$, $[e_1,e_3]=e_3$, $[e_1,e_4]=e_4$, $[e_2,e_3]=e_3$, $[e_2,e_5]=e_5$, $[e_1,e_2]=e_6$

$$S=\begin{bmatrix} e^{z+w} & x & 0 & 0 & 0 & p \\ 0 & e^{z} & 0 & 0 & 0 & q \\ 0 & 0 & e^{w} & 0 & 0 & x \\ 0 & 0 & 0 & 1 & w & y \\ 0 & 0 & 0 & 0 & 1 & z \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{-(pD_p + xD_x + zD_y + D_w), -(pD_p + qD_q + xD_x + D_z), D_p, -(qD_p + e^z D_x), D_q, -D_y\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{p} = (\dot{z} + \dot{w})(\dot{p} - xe^{-z}\dot{q}) - e^{-z}\dot{q}\dot{x}, \quad \ddot{x} = \dot{x}(2\dot{z} + \dot{w}) - x\dot{z}(\dot{z} + \dot{w}), \quad \ddot{q} = \dot{q}\dot{z}, \quad \ddot{y} = \dot{z}\dot{w}.$$

6.39: $[e_4, e_5] = e_3$, $[e_1, e_4] = e_5$, $[e_1, e_5] = -e_4$, $[e_2, e_3] = 2e_3$, $[e_2, e_4] = e_4$, $[e_2, e_5] = e_5$, $[e_1, e_2] = e_6$.

$$S = \begin{bmatrix} 1 & z & 0 & 0 & 0 & p \\ 0 & 1 & 0 & 0 & 0 & w \\ 0 & 0 & e^{2w} & xe^w & ye^w & q \\ 0 & 0 & 0 & \cos(z)e^w & \sin(z)e^w & \cos(z)y - \sin(z)x \\ 0 & 0 & 0 & -\sin(z)e^w & \cos(z)e^w & -\cos(z)x - \sin(z)y \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{wD_p + D_z, -(2qD_q + xD_x + yD_y + D_w), -2D_q, -((y\cos(z) - x\sin(z))D_q + \sin(z)D_y + \cos(z)D_x), (x\cos(z) + y\sin(z))D_q + \sin(z)D_x - \cos(z)D_y, D_p\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{p} = \dot{w}\dot{z}, \quad \ddot{x} = \cos(2w)\dot{x}\dot{w} + (y(\sin^2(w) + 1) - x\sin(2w))\dot{z}\dot{w} - \dot{y}\dot{z}, \quad \ddot{y} = \dot{y}\dot{w} + \dot{x}\dot{z} + x\cos^2(w)\dot{z}\dot{w} + \sin(2w)\dot{x}\dot{w},$$

$$\ddot{q} = 2\dot{q}\dot{w} + (y^2 - x^2\cos(2w))\dot{z}\dot{w} + y\cos(2w)\dot{x}\dot{w} - x(\dot{y}\dot{w} + \dot{x}\dot{z}) - y\dot{y}\dot{z} - x\sin(2w)\dot{w}(y\dot{z} + \dot{x}).$$

6.40: $[e_4, e_5] = e_3$, $[e_1, e_4] = e_5$, $[e_1, e_5] = -e_4$, $[e_2, e_6] = e_6$, $[e_1, e_2] = e_3$.

$$S = \begin{bmatrix} e^z & 0 & 0 & 0 & 0 & p \\ 0 & 1 & -y\cos(w) + x\sin(w) & y\sin(w) + x\cos(w) & 2w & q \\ 0 & 0 & \cos(w) & -\sin(w) & 0 & x \\ 0 & 0 & \sin(w) & \cos(w) & 0 & y \\ 0 & 0 & 0 & 0 & 1 & z \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Right-invariant vector fields

$$\{2zD_q - yD_x + xD_y + D_w, -(pD_p + D_z), 2D_q, -xD_q + D_y, yD_q + D_x, D_p\}.$$

Geodesics

$$\ddot{w} = 0, \quad \ddot{z} = 0, \quad \ddot{q} = \dot{w}(x\dot{x} + y\dot{y}) + 2\dot{z}\dot{w}, \quad \ddot{y} = \dot{x}\dot{w}, \quad \ddot{x} = -\dot{y}\dot{w}, \quad \ddot{p} = \dot{p}\dot{z}.$$

Lagrangian

$$L = \dot{w}(\dot{q} - z\dot{w} - w\dot{z}) + (y\dot{x} - x\dot{y})\dot{w} + \dot{x}^2 + \dot{y}^2 + \dot{z}^2 + \dot{w}^2 + \frac{e^{-z}\dot{p}^2}{\dot{z}}.$$

APPENDIX: CONSTRUCTING LAGRANGIANS

We end with a brief Appendix that touches on six of the forty cases. We believe that this approach will offer the reader much more insight into our techniques rather than supplying a plethora of routine details, many of which in any case, have only been accomplished with the help of MAPLE. These six cases are quite representative and the reader should bear in mind that we have always considered our primary objective to be to find at least one Lagrangian by hook or crook.

The following sum of matrices constitutes a solution to Eqs. (12), (13), and (5). In fact we begin by finding a basis of solutions to Eqs. (12) and (13). These solutions themselves may not satisfy Eq. (5). However, we insert our basis of solutions of Eq. (4) with coefficients into Eq. (5) noting that the time derivative in Eq. (5) is taken with respect to the original ODE system (2). As such when Eq. (5) are integrated arbitrary first integrals of Eq. (2) occur instead of arbitrary constants, in this case represented by the functions A, B, C, D, E, F, and G. We have not given details of the actual integration in Eq. (5) but we advise the reader that it is elementary, the difficulties stemming only from the size of the matrices involved. The reader can see such concrete details in much simpler examples in Thompson (2003), for example.

The new basis will now satisfy both Eqs. (4) and (5)

$$
A\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
+B\begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
+C\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0\\
0 & 1 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
+\frac{e^{-w}D}{\dot{w}^2}\begin{bmatrix}
\frac{\dot{p}^2}{\dot{w}} & 0 & 0 & 0 & 0 & -\dot{p}\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
-\dot{p} & 0 & 0 & 0 & 0 & \dot{w}
\end{bmatrix}
$$

$$
+\frac{e^{-z}E}{\dot{z}^2}\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0\\
0 & \frac{\dot{q}^2}{\dot{z}} & 0 & 0 & -\dot{q} & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & -\dot{q} & 0 & 0 & \dot{z} & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
+\frac{e^{-(a\dot{w}+b\dot{z})}F}{(a\dot{w}+b\dot{z})^2}\begin{bmatrix}
a^2(a\dot{w}+b\dot{z}) & ab(a\dot{w}+b\dot{z}) & -a\dot{y} & 0 & 0 & 0\\
ab(a\dot{w}+b\dot{z}) & b^2(a\dot{w}+b\dot{z}) & -b\dot{y} & 0 & 0 & 0\\
-a\dot{y} & -b\dot{y} & a\dot{w}+b\dot{z} & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

$$
+\frac{e^{-(c\dot{w}+d\dot{z})}G}{(c\dot{w}+d\dot{z})^2}\begin{bmatrix}
c^2(c\dot{w}+d\dot{z}) & cd(c\dot{w}+d\dot{z}) & 0 & -c\dot{x} & 0 & 0\\
cd(c\dot{w}+d\dot{z}) & d^2(c\dot{w}+d\dot{z}) & 0 & -d\dot{x} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
-c\dot{x} & -d\dot{x} & 0 & c\dot{w}+d\dot{z} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
$$

If one requires now to find all possible Lagrangians for Eq. (2) it is necessary to solve the closure conditions (6), which as we have said compromises 70 conditions. We shall not write down Eq. (6). The system can be integrated explicitly in this case, however; each of $A, B, \ldots, G$ are first integrals. As such the general solution of Eq. (6) can be expressed in terms of first integrals. For example, it turns out that the function D can only depend on w, p, $\dot{p}/\dot{w}$. Thus if D is a first integral it can only depend on $e^{-w}(\dot{p}/\dot{w})$ and $\dot{p}/\dot{w}-p$. The reader can see more arguments of this type and in greater detail in Ghanam (2004).

The following matrix is the general solution of Eq. (6):

$$
\begin{bmatrix}
N_{\dot{w}\dot{w}} & N_{\dot{w}\dot{z}} & 0 & 0 & 0 & 0 \\
N_{\dot{w}\dot{z}} & N_{\dot{z}\dot{z}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
+ \frac{e^{-w}D}{\dot{w}^2}
\begin{bmatrix}
\frac{\dot{p}^2}{\dot{w}} & 0 & 0 & 0 & 0 & -\dot{p} \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-\dot{p} & 0 & 0 & 0 & 0 & \dot{w}
\end{bmatrix}
+ \frac{e^{-z}E}{\dot{z}^2}
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{\dot{q}^2}{\dot{z}} & 0 & 0 & -\dot{q} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\dot{q} & 0 & 0 & \dot{z} & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

$$
+
\begin{bmatrix}
\frac{a^2Fe^{-(aw+bz)}\dot{y}^2}{(a\dot{w}+b\dot{w})^3} + \frac{c^2Ge^{-((cw+dz))}\dot{x}^2}{(c\dot{w}+d\dot{w})^3} & \frac{abFe^{-(aw+bz)}\dot{y}^2}{(a\dot{w}+b\dot{w})^3} + \frac{cdGe^{-(cw+dz)}\dot{x}^2}{(c\dot{w}+d\dot{w})^3} & -\frac{aFe^{-(aw+bz)}\dot{y}}{(a\dot{w}+b\dot{w})^2} & -\frac{aGe^{-(cw+dz)}\dot{x}}{(c\dot{w}+d\dot{w})^2} & 0 & 0 \\
* & \frac{b^2Fe^{-(aw+bz)}\dot{y}^2}{(a\dot{w}+b\dot{w})^3} + \frac{d^2Ge^{-(cw+dz)}\dot{x}^2}{(c\dot{w}+d\dot{w})^3} & \frac{bFe^{-(aw+bz)}\dot{y}}{(a\dot{w}+b\dot{w})^2} & -\frac{dGe^{-(cw+dz)}\dot{x}}{(c\dot{w}+d\dot{w})^2} & 0 & 0 \\
* & * & \frac{Fe^{-(aw+bz)}}{(a\dot{w}+b\dot{w})} & 0 & 0 & 0 \\
* & * & * & \frac{Ge^{-(cw+dz)}}{(c\dot{w}+d\dot{w})} & 0 & 0 \\
* & * & * & * & 0 & 0 \\
* & * & * & * & * & 0
\end{bmatrix},
$$

where $D=D(e^{-w}\dot{p}/\dot{w},\dot{p}/\dot{w}-p)$, $E=E(e^{-z}\dot{q}/\dot{z},\dot{q}/\dot{z}-q)$, $F=F(e^{-(aw+bz)}\dot{y}/(a\dot{w}+b\dot{w}),\dot{y}/(a\dot{w}+b\dot{z})-y)$, $G=G(e^{-(cw+dz)}\dot{x}/(c\dot{w}+d\dot{z}),\dot{x}/c\dot{w}+d\dot{z}-x)$ and $N=N(\dot{w},\dot{z},z\dot{w}-w\dot{z})$.

It is not possible to integrate the Hessian above in complete generality, so to obtain a concrete Lagrangian it is necessary to choose specific forms for the functions D, E, F, G, and N. The Lagrangian given in Sec. VI is given by choosing $D=E=F=G=1/2$ and $N=\dot{w}^2+\dot{z}^2$. We have found it still to be a major practical problem to construct the Lagrangian from the Hessian and one that we have to do interactively. It seems likely to us that it will be quite some time before the symbolic manipulation programs are sufficiently powerful to enable us to automate these steps.

6.5 To construct a Lagrangian in this case we can make use of the remark that follows Proposition (5.1). In this case the subspaces spanned by $\{e_3,e_4\}$ and $\{e_5,e_6\}$, respectively, are ideals and each of them correspond to split extensions. As such we can combine two four-dimensional Lagrangians in the variables w, z, x, y and w, z, p, q (and their time derivatives), respectively. Similarly in case 6.9 we can extend a five-dimensional Lagrangian by using the subalgebra spanned by $\{e_1,e_3\}$, whereas the same trick would not work using the the subalgebra spanned by $\{e_2,e_6\}$, because the bracket $\{e_2,e_5\}$ involves e_6 on the left hand side.

6.8 In this example the matrix g_{ij} is singular. We use Eq. (15) to compute the nonzero components of the curvature R^i_{jkl}: Thus

$$
R^3_{113}=R^4_{224}=R^5_{225}=R^6_{214}=R^6_{124}=\tfrac{1}{2}R^6_{225}=R^6_{226}=\tfrac{1}{4}.
$$

Notice that this calculation is done entirely at the Lie algebra level: We do not need any representation here. If we do have a representation, such as is given in Sec. VI, we can also compute the curvature in coordinates though its components may not be constant. However, we could also do the calculation if we have a vector field representation of the Lie algebra because then we can compute the geodesics in coordinates.

Let us define generally, in dimension n, L_i to be u^jg_{ij} where there is a sum over j. Then Eq. (13) says in this case that $L_3=L_4=L_5=L_6=0$. Turning now to Eq. (12) we choose the following values for mjq: 126, 136, 145, 146, 245 and deduce that $g_{16}=g_{36}=g_{56}=g_{66}=g_{46}=0$, respectively. But now $L_6=0$ and hence it follows that the last column and bottom row of g_{ij} is zero.

6.19 A Lagrangian can be constructed in this example by identifying the group as a subgroup of $GL(3,\mathbb{C})$ and comparing it with the corresponding real subgroup of $GL(3,\mathbb{R})$. A Lagrangian in

the latter case was exhibited in Thompson (2003) and by complexifiying and taking the real part we can obtain the Lagrangian for case 6.19.

6.33 We consider another example where the matrix g_{ij} is singular. Again we use Eq. (15) to compute the nonzero components of the curvature R^i_{jkl}: Thus

$$R^3_{113}=R^3_{213}=R^3_{123}=R^3_{223}=R^3_{145}=R^3_{245}=R^3_{514}=R^3_{425}=R^4_{114}=R^5_{225}=\tfrac{1}{2}R^6_{225}=R^6_{226}=\tfrac{1}{4}.$$

Then just as in example 6.8, using the same notation, Eq. (13) says that $L_3=L_4=L_5=L_6=0$. As for Eq. (12) we choose the following values for mjq: 123, 134, 135, 136, 234 and deduce that $g_{13}-g_{23}=g_{33}=g_{35}=g_{36}=g_{34}=0$, respectively. Again since $L_3=0$ it follows that the third column and row of g_{ij} is zero.

One more remark about the cases where the matrix g_{ij} is singular is in order. Both of the algebras 6.8 and 6.33 do not contain parameters. However, there are some algebras that do depend on parameters and for which the matrix g_{ij} is singular. One has to take care, particularly when using symbolic manipulation programs such as MAPLE, not to exclude certain special values where the rank of a linear system can change. When running a routine, unless some special loop is included to track the possible values of the parameters, the routine is always going to assume that the parameters have generic values. In other words it is possible to exclude special values where, for example, the matrix g_{ij} may not be singular. This problem occurs in all questions that occur in the low-dimensional Lie algebras and at best they can be answered interactively.

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On the Hamiltonian reduction of geodesic motion on SU(3) to SU(3)/SU(2)

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The reduced Hamiltonian system on $T^*(SU(3)/SU(2))$ is derived from a Riemannian geodesic motion on the SU(3) group manifold parametrized by the generalized Euler angles and endowed with a bi-invariant metric. Our calculations show that the metric defined by the derived reduced Hamiltonian flow on the orbit space $SU(3)/SU(2) \simeq \mathbb{S}^5$ is not isometric or even geodesically equivalent to the standard Riemannian metric on the five-sphere $\mathbb{S}^5$ embedded into $\mathbb{R}^6$. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2358391]

I. INTRODUCTION

Symmetry plays a central role in our pursuit of a better understanding of nature. Through the preservation or artful breaking of symmetry, powerful models have been developed that describe the fundamental forces and that have, so far, withstood all tests. Indeed, any endeavor to go beyond this standard model also has, at its heart, an appropriate symmetry argument.

An immediate consequence of symmetry is that it permits for a reduction in the relevant degrees of freedom needed to describe a given problem. In a gauge theory this reduction implies that not all the degrees of freedom present in the formulation of the theory correspond to physical degrees of freedom. So, for example, in Quantum Electrodynamics, with its U(1) gauge symmetry, the potential A_μ, which naively has four degrees of freedom, describes the photon, which has just two physical degrees of freedom. Understanding how this type of reduction should best take place and how the process of quantizing a system interacts with the symmetry, has driven many of the important advances in our understanding of gauge theories.[1]

In many cases, the reduction to the true physical degrees of freedom in a field theory has been fruitfully studied through simpler, finite dimensional systems. In particular, coset spaces of the form G/H, where G and H are finite dimensional Lie groups, have provided much insight[2] into

how global and topological properties of these configuration spaces can be encoded into the quantization process via generalized notions of reduction to the true degrees of freedom.[3]

In all investigations to date, specific details on dynamical aspects of the reduction to G/H have been restricted to groups for which manageable parametrizations of the group elements exist. Essentially this has restricted attention to groups directly related to the rotation group and its covering, SU(2). However, recently there has been much progress in finding suitable parametrizations for the higher dimensional unitary groups[4–8] and particularly for the group SU(3).[9,10] These advances open the door to detailed investigations of dynamics on spaces such as the five-sphere, $\mathbb{S}^5$, now viewed as the reduction from SU(3) to SU(3)/SU(2). By exploiting our concrete description of this reduction we shall see a new phenomenon for this system: different metric structures emerge depending on whether the five sphere is viewed as the coset space or via its natural embedding in six dimensional Euclidean space. This is, to the best of our knowledge, the first explicit example of this metric property of reduction.

The plan of the paper is as follows. We will conclude this introduction with a brief summary of the classical Hamiltonian reduction procedure. Then, in Sec. II, we will see how this procedure is applied to the group SU(2). This section does not contain any new results, but fixes notation and introduces themes that will prepare us for the reduction on the configuration space SU(3) which will be presented in detail in Sec. III. Then, in Sec. IV we will investigate the possible Riemannian structures that arise on the quotient space $\mathbb{S}^5$ and discuss the possible metric and geodesic correspondences. In an Appendix, we will collect together the details of our consistent parametrization of SU(3).

A. Hamiltonian reduction

Consider the special class of Lagrangian systems whose configuration space is a compact matrix Lie group G. This means that the state of a system at fixed time $t=0$ is characterized by an element of the Lie group $g(0) \in G$, and the evolution is described by the curve $g(t)$ on the group manifold.[11,12] The "free evolution" on the semisimple group G is, by definition, the Riemannian geodesic motion on the group manifold with respect to the so-called Cartan-Killing metric,[13,14]

$$\mathrm{d}s_G^2 = \kappa\,\mathrm{Tr}(g^{-1}\,\mathrm{d}g \otimes g^{-1}\,\mathrm{d}g),$$

where κ is a normalization factor. The geodesies are given by the extremal curves of the action functional,

$$S[g] = \frac{\kappa}{2}\int_0^T \mathrm{d}t\,\mathrm{Tr}(g^{-1}\dot{g}g^{-1}\dot{g}). \tag{1.1}$$

This action is invariant under the continuous left translation,

$$g(t) \to g(\varepsilon)g(t), \quad \varepsilon = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_{\dim G}),$$

and therefore the system possesses the integrals of motion $\mathcal{I}_1, \mathcal{I}_2, \ldots, \mathcal{I}_{\dim G}$. The existence of these integrals of motion allows us to reduce the number of degrees of freedom of the system using the well-known method of Hamiltonian reduction.[11,12]

For a generic Hamiltonian system defined on the cotangent bundle T^*M with symmetry associated to the Lie group G action, the level set of the corresponding integrals of motion,

$$M_c = \mathcal{I}^{-1}(c). \tag{1.2}$$

where c is a set of arbitrary real constants $c=(c_1, \ldots, c_{\dim G})$, determines the reduced Hamiltonian system on the *reduced phase space* $F_c \subset M_c$. The subset F_c is described by the isotropy group, G_c, of the integrals level set M_c,

$$F_c = M_c/G_c.$$

Here we are interested in a special case when the manifold M is itself a group manifold and the symmetry transformations are group translations. Now the level set M_c is a subset of the trivial cotangent bundle T^*G that can be identified with the product of the group G and its algebra, $G \times g$. The level set given by the integrals $\mathcal{I}_1=c_1, \mathcal{I}_2=c_2, \ldots, \mathcal{I}_N=c_N, N \leq \dim \mathrm{G}$, defines the isotropy group $G_c \subset G$ and the so-called *orbit space*,

$$\mathcal{O} = G/G_c. \tag{1.3}$$

The relationship between the orbit space $\mathcal{O}$ and the reduced phase space F_c can be summarized as follows (see, e.g., Refs. 11 and 12):

- *the reduced phase space F_c is symplectic and diffeomorphic to the cotangent bundle $T^*\mathcal{O}$;*
- *the dynamics on the reduced degrees of freedom is Hamiltonian with a reduced Hamiltonian given by the projection of the original Hamiltonian function to F_c.*

These results are the modern generalizations of the classical theorems, proving that the collection of holonomic constraints defines a configuration manifold M as a submanifold of $\mathbb{R}^n$ and that, in the absence of forces, the trajectories of mechanical system are geodesies of the induced Riemannian metric.

Note that the above results do not claim that the reduced phase space and the dynamics on the orbit space are isometric. Indeed, we know that on the reduced phase space we can define, at least locally, an induced metric that arises from the kinetic energy part of the reduced Hamiltonian,

$$K_{\mathcal{O}} = \frac{1}{2}\mathbf{g}_{\mathcal{O}}(\xi_a, \xi_b)p_a p_b. \tag{1.4}$$

On the other hand the map $\pi: G \to G/G_c$ induces the metric

$$\overline{\mathbf{g}}_{\mathcal{O}} = \pi_* \mathbf{g}_G. \tag{1.5}$$

We now pose a question about the relation between these two metrics.

When are the metrics $\mathbf{g}_{\mathcal{O}}$ and $\overline{\mathbf{g}}_{\mathcal{O}}$ isometrically or, more weakly, geodesically equivalent?

We do not know the general answer to this question, so in this present paper we will focus our study on two examples: geodesic motion on the SU(2) and SU(3) group manifolds.

We start with a well-known example of Hamiltonian reduction $\mathrm{SU}(2) \to \mathrm{SU}(2)/\mathrm{U}(1)$ and show that the reduced space *is indeed in isometrical correspondence with the cotangent bundle* $T^*\mathbb{S}^2$ and the standard induced metric on the two-sphere $\mathbb{S}^2$. The case of the $\mathrm{SU}(3) \to \mathrm{SU}(3)/\mathrm{SU}(2)$ reduction gives an example of the opposite result: the metric defined by the Hamiltonian flow on the orbit space SU(3)/SU(2) *is not isometrically equivalent* to a standard round metric on the five-sphere $\mathbb{S}^5$. Furthermore, in this case, the stronger result is true: the reduced configuration space and the standard $\mathbb{S}^5$ are not even *geodesically equivalent*.

II. GEODESIC FLOW ON SU(2)

In this section we discuss the example of the reduction of free motion on the SU(2) group manifold. We start with a presentation of the key geometrical structures found on this group that are necessary for any further dynamical analysis.

A. The Euler angle parametrization

The special unitary group SU(2), considered as a subgroup of the general matrix group $\mathrm{GL}(2,\mathbb{C})$, is *topologically* the three-sphere $\mathbb{S}^3$ embedded into $\mathbb{C}^2$. This correspondence $\mathrm{SU}(2) \approx \mathbb{S}^3$ follows immediately from the standard identification of an arbitrary element $g \in \mathrm{SU}(2)$ as

$$g := \begin{pmatrix} z_1 & -\bar{z}_2 \\ z_2 & \bar{z}_1 \end{pmatrix}, \quad |z_1|^2 + |z_2|^2 = 1. \tag{2.1}$$

The three-sphere $\mathbb{S}^3$ is a manifold that requires more than one chart to cover it and therefore there is no global parametrization of the SU(2) group as a three-dimensional space. The local description usually adopted is given by the conventional symmetric *Euler representation*[15] for a group element,

$$g = \exp\left(i\frac{\alpha}{2}\sigma_3\right)\exp\left(i\frac{\beta}{2}\sigma_2\right)\exp\left(i\frac{\gamma}{2}\sigma_3\right), \tag{2.2}$$

with the appropriately chosen range for the Euler angles α, β, γ.

In this representation the generators of the one-parameter subgroups are the standard Pauli matrices σ_1, σ_2, and σ_3,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.3}$$

satisfying the $su(2)$ algebra

$$\sigma_a\sigma_b - \sigma_b\sigma_a = 2i\epsilon_{abc}\sigma_c. \tag{2.4}$$

Writing the complex numbers in (2.1) as $z_1 = x^1 + ix^2$ and $z_2 = x^3 + ix^4$ in polar form,

$$z_1 := e^{iu}\cos\theta, \quad z_2 := e^{iv}\sin\theta, \tag{2.5}$$

and comparing (2.1) with the explicit form of the Euler matrix (2.2),

$$g = \begin{pmatrix} e^{i\frac{\alpha+\gamma}{2}}\cos\left(\frac{\beta}{2}\right) & e^{i\frac{\alpha+\gamma}{2}}\sin\left(\frac{\beta}{2}\right) \\ -e^{-i\frac{\alpha-\gamma}{2}}\sin\left(\frac{\beta}{2}\right) & e^{-i\frac{\alpha+\gamma}{2}}\cos\left(\frac{\beta}{2}\right) \end{pmatrix}, \tag{2.6}$$

we have

$$u = \frac{\alpha+\gamma}{2}, \quad v = \frac{\alpha-\gamma}{2}, \quad \theta = \frac{\beta}{2}. \tag{2.7}$$

The Euler decomposition (2.2) corresponds to the following parametric representation of the three-sphere embedded in $\mathbb{R}^4$:

$$\begin{aligned} x^1 &= \cos\left(\frac{\alpha+\gamma}{2}\right)\cos\left(\frac{\beta}{2}\right), \quad x^2 = \sin\left(\frac{\alpha+\gamma}{2}\right)\cos\left(\frac{\beta}{2}\right), \\ x^3 &= -\cos\left(\frac{\alpha-\gamma}{2}\right)\sin\left(\frac{\beta}{2}\right), \quad x^4 = \sin\left(\frac{\alpha-\gamma}{2}\right)\sin\left(\frac{\beta}{2}\right). \end{aligned} \tag{2.8}$$

To be more precise, though, this is not a valid parametrization for the entire three-sphere. In particular, the neighborhood of the identity element of the group in this decomposition turns out to be degenerate. The identity element of SU(2) corresponds to the whole set: $\beta = 0$ and $\alpha + \gamma = 0$. In order to properly cover the whole group manifold, it is necessary to consider an atlas on the SU(2) group and used different parametrizations on the different charts. Bearing this in mind, we proceed by assuming that we are working in a chart $(\mathcal{U}, \phi)$, where α, β, and γ serve as good local coordinates on $\mathbb{S}^3$ and calculate the Maurer-Cartan forms on SU(2).

Using the following normalization:

$$g^{-1}\,\mathrm{d}g = \frac{i}{2}\sum_{a=1}^{3}\sigma_a \otimes \omega_L^a, \tag{2.9}$$

$$\mathrm{d}g\; g^{-1} = \frac{i}{2}\sum_{a=1}^{3}\sigma_a \otimes \omega_R^a, \tag{2.10}$$

and performing the straightforward calculations with the Eulerian representation (2.2) we arrive at the well-known expressions for left-invariant 1-forms:

$$\begin{aligned}\omega_L^1 &= \cos\gamma \sin\beta\, \mathrm{d}\alpha - \sin\gamma\, \mathrm{d}\beta,\\ \omega_L^2 &= \sin\beta \sin\gamma\, \mathrm{d}\alpha + \cos\gamma\, \mathrm{d}\beta,\\ \omega_L^3 &= \cos\beta\, \mathrm{d}\alpha + \mathrm{d}\gamma.\end{aligned} \tag{2.11}$$

and the corresponding dual vectors, $\omega_L^a(X_b^L) = \delta_b^a$, $a,b = 1,2,3$,

$$\begin{aligned}X_1^L &= \frac{\cos\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} - \sin\gamma\frac{\partial}{\partial\beta} - \cot\beta\cos\gamma\frac{\partial}{\partial\gamma},\\ X_2^L &= \frac{\sin\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} + \cos\gamma\frac{\partial}{\partial\beta} - \cot\beta\sin\gamma\frac{\partial}{\partial\gamma},\\ X_3^L &= \frac{\partial}{\partial\gamma}.\end{aligned} \tag{2.12}$$

The right invariant 1-forms and the corresponding dual vectors, $\omega_R^a(X_b^R) = \delta_b^a$, are

$$\begin{aligned}\omega_R^1 &= \sin\alpha\, \mathrm{d}\beta - \cos\alpha \sin\beta\, \mathrm{d}\gamma,\\ \omega_R^2 &= \cos\alpha\, \mathrm{d}\beta + \sin\alpha \sin\beta\, \mathrm{d}\gamma,\\ \omega_R^3 &= \mathrm{d}\alpha + \cos\beta\, \mathrm{d}\gamma.\end{aligned} \tag{2.13}$$

$$\begin{aligned}X_1^R &= \cos\alpha\cot\beta\frac{\partial}{\partial\alpha} + \sin\alpha\frac{\partial}{\partial\beta} - \frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma},\\ X_2^R &= -\sin\alpha\cot\beta\frac{\partial}{\partial\alpha} + \cos\alpha\frac{\partial}{\partial\beta} + \frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma},\\ X_3^R &= \frac{\partial}{\partial\alpha}.\end{aligned} \tag{2.14}$$

The vector fields X_a^L and X_a^R obey the $su(2)\otimes su(2)$ algebra with respect to the Lie brackets operation,

$$[X_a^L, X_b^L] = -\epsilon_{abc}X_c^L, \tag{2.15}$$

$$[X_a^R, X_b^R] = +\epsilon_{abc}X_c^R, \tag{2.16}$$

$$[X_a^L, X_b^R] = 0. \tag{2.17}$$

Any compact Lie group can be endowed with the bi-invariant Riemannian metric build uniquely (up to a normalization factor) from the Cartan-Killing form over the algebra. It is convenient to choose the following normalization for the bi-invariant metric on the SU(2) group:

$$\mathbf{g}_{\mathrm{SU}(2)} = -\frac{1}{2}\,\mathrm{Tr}(g^{-1}\,\mathrm{d}g \otimes g^{-1}\,\mathrm{d}g). \tag{2.18}$$

In terms of this left/right-invariant nonholonomic frame, (2.18) reads as

$$\mathbf{g}_{\mathrm{SU}(2)} = \frac{1}{4}(\omega_L^1 \otimes \omega_L^1 + \omega_L^2 \otimes \omega_L^2 + \omega_L^3 \otimes \omega_L^3), \tag{2.19}$$

$$= \frac{1}{4}(\omega_R^1 \otimes \omega_R^1 + \omega_R^2 \otimes \omega_R^2 + \omega_R^3 \otimes \omega_R^3). \tag{2.20}$$

Substitution of the expressions (2.11) and (2.13) for the Maurer-Cartan forms ω_L and ω_R yields the metric in the coordinate frame $\mathrm{d}\alpha, \mathrm{d}\beta, \mathrm{d}\gamma$ basis,

$$\mathbf{g}_{\mathrm{SU}(2)} = \frac{1}{4}(\mathrm{d}\alpha \otimes \mathrm{d}\alpha + \mathrm{d}\beta \otimes \mathrm{d}\beta + \mathrm{d}\gamma \otimes \mathrm{d}\gamma + 2\cos\beta\,\mathrm{d}\alpha \otimes \mathrm{d}\gamma). \tag{2.21}$$

In order to understand the *metrical* characteristics of a group manifold viewed as an embedded space, it is instructive to compare this invariant metric with the metric induced from the ambient four-dimensional Euclidian space on the *unit* three-sphere (2.8),

$$\mathbf{g}_{\mathrm{s}^3} = \mathrm{d}\bar{z}_1 \otimes \mathrm{d}z_1 + \mathrm{d}\bar{z}_2 \otimes \mathrm{d}z_2 = \frac{1}{4}(\mathrm{d}\alpha \otimes \mathrm{d}\alpha + \mathrm{d}\beta \otimes \mathrm{d}\beta + \mathrm{d}\gamma \otimes \mathrm{d}\gamma + 2\cos\beta\,\mathrm{d}\alpha \otimes \mathrm{d}\gamma). \tag{2.22}$$

Comparing the metrics, (2.21) and (2.22), we conclude that the bi-invariant metric on SU(2) is the same as the standard metric on the unit three-sphere $\mathbb{S}^3$ and its bi-invariant volume is

$$\mathrm{Vol}(\mathrm{SU}(2)) = \int \sqrt{\det \mathbf{g}_{\mathrm{SU}(2)}}\,\mathrm{d}\alpha \wedge \mathrm{d}\beta \wedge \mathrm{d}\gamma = \left(\frac{1}{2}\right)^3 \int_0^{2\pi} \mathrm{d}\alpha \int_0^{4\pi} \mathrm{d}\gamma \int_0^{\pi} \mathrm{d}\beta \sin(\beta) = 2\pi^2 = \mathrm{Vol}(\mathbb{S}^3). \tag{2.23}$$

As a Riemannian manifold, the SU(2) group endowed with the metric (2.21) is a 3-dimensional space of constant curvature with the Riemann scalar $\mathcal{R}_{\mathrm{SU}(2)} = 6$ and the Ricci tensor $\mathcal{R}_{ab}$ given by

$$\mathcal{R}_{ab} = \frac{\mathcal{R}_{\mathrm{SU}(2)}}{3} g_{ab} = 2g_{ab}. \tag{2.24}$$

The Gaussian curvature K of an n-dimensional manifold and the Riemann scalar are related via

$$K = \frac{\mathcal{R}}{n(n-1)}; \tag{2.25}$$

therefore $K_{\mathrm{SU}(2)} = 1$, in agreement with the volume calculation (2.23).

B. Quotient SU(2)/U(1)

Here we recall the key ingredients of the construction of a quotient space G/H by considering the transitive action of the group G on a certain base space M. We have the following[28] result.

If the group G acts transitively on a set M with $H \subset G$ being an isotropy subgroup leaving a point $x_0 \in M$ fixed,

$$H = \{g \in G | g \cdot x_0 = x_0\},$$

then the set M is in one-to-one correspondence with the left cosets gH of G.

The explicit form of this map for the SU(2) group is as follows. We identify the $su(2)$ algebra with $\mathbb{R}^3$ by the map $x^a \in \mathbb{R}^3 \to \mathbf{X} \in su(2)$,

$$\mathbf{X} = \sum_{a=1}^{3} x^a \sigma_a. \tag{2.26}$$

Consider now the *adjoint action* of SU(2) on an element of its algebra $\mathbf{X} \in su(2)$,

$$\mathrm{Ad}(g)(\mathbf{X}) = g\mathbf{X}g^{-1}.$$

The base point $x_0 = (0,0,1)$ (corresponding to the element σ_3) has a one-parameter isotropy subgroup,

$$\mathrm{H} = \exp\left(i\frac{\alpha}{2}\sigma_3\right).$$

The orbit space of σ_3,

$$\mathrm{Ad}(g)(\sigma_3) = g\sigma_3 g^{-1}$$

is the coset SU(2)/U(1). The proper atlas covering the SU(2) group manifold provides the coset space parametrization. When $\mathrm{SU}(2) \simeq \mathbb{S}^3$ is parametrized in terms of two complex coordinates z_1 and z_2, and the two-sphere is described by a unit vector $\mathbf{n} = (n^1, n^2, n^3)$, then the projection $\mathbb{S}^3 \to \mathbb{S}^2$ reads explicitly as

$$(z_1, z_2) \to (n^1, n^2, n^3) = (2\Re[\bar{z}_1 z_2],\ 2\Im[\bar{z}_1 z_2],\ |z_1|^2 - |z_2|^2). \tag{2.27}$$

This is the famous Hopf projection map $\pi: \mathrm{SU}(2) \to \mathbb{S}^2$, showing that SU(2) is a fiber bundle over $\mathbb{S}^2$ with nonintersecting circles $\mathrm{U}(1) \equiv \mathbb{S}^1$ as fibers,

$$\mathbb{S}^1 \hookrightarrow \mathrm{SU}(2) \xrightarrow{\pi} \mathbb{S}^2.$$

Using the Euler decomposition (2.6), the coset parametrization reads as

$$g\sigma_3 g^{-1} = n^a \sigma_a, \tag{2.28}$$

with the unit 3-vector,

$$\mathbf{n} = (-\sin\beta\cos\alpha,\ \sin\beta\sin\alpha,\ \cos\beta). \tag{2.29}$$

C. Lagrangian in Euler coordinates

The bi-invariant Lagrangian,

$$\mathrm{L}_{\mathrm{SU}(2)} = -\frac{1}{2}\,\mathrm{Tr}\left(g^{-1}(t)\frac{d}{dt}g(t)g^{-1}(t)\frac{d}{dt}g(t)\right), \tag{2.30}$$

in terms of left/right invariant Maurer-Cartan forms (2.9) reads as

$$\mathrm{L}_{\mathrm{SU}(2)} = \frac{1}{4}\sum_{a=1}^{3} i_{\dot{U}}\omega_L^a i_{\dot{U}}\omega_L^a = \frac{1}{4}\sum_{a=1}^{3} i_{\dot{U}}\omega_R^a i_{\dot{U}}\omega_R^a, \tag{2.31}$$

where $i_{\dot{U}}$ is the interior contraction of the vector field $\dot{U} = \dot{\alpha}(\partial/\partial\alpha) + \dot{\beta}(\partial/\partial\beta) + \dot{\gamma}(\partial/\partial\gamma)$.

Covering the group manifold with an atlas and considering the chart where the parameters α, β, γ in the Euler decomposition (2.2) serve as good coordinates, we arrive at

$$\mathrm{L}_{\mathrm{SU}(2)} = \frac{1}{4}(\dot{\alpha}^2 + \dot{\beta}^2 + \dot{\gamma}^2 + 2\cos(\beta)\dot{\alpha}\dot{\gamma}). \tag{2.32}$$

Comparing (2.32) with the expression (2.21) for the bi-invariant metric on SU(2), we conclude that

$$\mathrm{L}_{\mathrm{SU}(2)} = \mathbf{g}_{\mathrm{SU}(2)}(\dot{U}, \dot{U}). \tag{2.33}$$

D. Hamiltonian dynamics on T*SU(2)

The Hamiltonian dynamics on the SU(2) group is defined on the cotangent bundle $\mathrm{T}^*\mathrm{SU}(2)$ that can be identified with the trivialization $\mathrm{T}^*\mathrm{SU}(2) \approx \mathrm{SU}(2) \times su(2)_L$ or with $\mathrm{T}^*\mathrm{SU}(2) \approx \mathrm{SU}(2) \times su(2)_R$.

The canonical Hamiltonian describing geodesic motion on SU(2) can be obtained by a Legendre transformation of the Lagrangian function (2.31). Introducing the Poincare-Cartan symplectic one-form,

$$\Theta = p_\alpha \,\mathrm{d}\alpha + p_\beta \,\mathrm{d}\beta + p_\gamma \,\mathrm{d}\gamma,$$

with the canonically conjugated pairs,

$$\{\alpha, p_\alpha\} = 1, \quad \{\beta, p_\beta\} = 1, \quad \{\gamma, p_\gamma\} = 1,$$

the Hamiltonian on $\mathrm{T}^*\mathrm{SU}(2)$ is defined as

$$\mathrm{H}_{\mathrm{SU}(2)} = \sum_{a=1}^{3} \xi_a^L \xi_a^L, = \sum_{a=1}^{3} \xi_a^R \xi_a^R, \tag{2.34}$$

where ξ_a^L and ξ_a^R are the values of the one-form Θ on the left/right invariant vector fields X_a^L, X_a^R spanning the algebra $su(2)_{L,R}$,

$$\xi_a^L := \Theta(X_a^L), \quad \xi_a^R := \Theta(X_a^R).$$

The set of functions ξ_a^L and ξ_a^R obey the $su(2)_L \times su(2)_R$ relations with respect to the Poisson brackets,

$$\{\xi_a^L, \xi_b^L\} = -\epsilon_{abc}\xi_c^L, \tag{2.35}$$

$$\{\xi_a^R, \xi_b^R\} = \epsilon_{abc}\xi_c^R, \tag{2.36}$$

$$\{\xi_a^L, \xi_b^R\} = 0. \tag{2.37}$$

In the coordinate frame (2.32), the Hamiltonian (2.34) becomes

$$\mathrm{H}_{\mathrm{SU}(2)} = \frac{p_\alpha^2}{\sin^2(\beta)} + p_\beta^2 + \frac{p_\gamma^2}{\sin^2(\beta)} - \frac{2\cos(\beta)}{\sin^2(\beta)} p_\alpha p_\gamma. \tag{2.38}$$

Now noting that the components of the inverse of the bi-invariant metric (2.21) are

$$g^{-1}_{SU(2)} = \frac{4}{\sin^2(\beta)} \begin{pmatrix} 1 & 0 & -\cos(\beta) \\ 0 & \sin^2(\beta) & 0 \\ -\cos(\beta) & 0 & 1 \end{pmatrix}, \tag{2.39}$$

the Hamiltonian can be rewritten as

$$H_{SU(2)} = \frac{1}{4} \mathbf{g}^{-1}_{SU(2)}(\Theta, \Theta). \tag{2.40}$$

E. Hamiltonian reduction to the coset SU(2)/U(1)

The system with Hamiltonian function (2.38) has an obvious first integral,

$$p_\alpha = k, \quad \{p_\alpha, H_{SU(2)}\} = 0, \tag{2.41}$$

where k can be an arbitrary constant. The Hamiltonian on the level set $M_k := p_\alpha^{-1}(k)$ is, by definition, the projection of (2.38) onto this subspace:

$$H^{(k)} := H_{SU(2)}\big|_{p_\alpha = k} = p_\beta^2 + \frac{p_\gamma^2}{\sin^2(\beta)} - k\frac{2\cos(\beta)}{\sin^2(\beta)} p_\gamma + \frac{k^2}{\sin^2(\beta)}. \tag{2.42}$$

The inverse Legendre transformation gives

$$L_{SU(2)/SU(1)} = \frac{1}{4}(\dot\beta^2 + \sin^2(\beta)\dot\gamma^2) + k\cos(\beta)\dot\gamma. \tag{2.43}$$

The interpretation of the system so obtained is the following:[3] the first two terms correspond to a particle moving on the two-sphere $\mathbb{S}^2$ endowed with the standard embedding metric, while the last term describes the particle interaction with a Dirac monopole whose potential is

$$A_\phi := k(1 - \cos(\beta)).$$

III. GEODESIC FLOW ON SU(3) USING GENERALIZED EULER COORDINATES

A. Generalized Euler decomposition of SU(3)

Now we pass on to the description of the Euler decomposition of the SU(3) group element. The Euler angle parametrization of the three-dimensional rotation group has been generalized for the higher orthogonal SO(n) and special unitary SU(n) groups.[6–8,16–18] Special attention has been paid to the study of the SU(3)[19–22] and SU(4)[4,5] groups.

The starting point for the derivation[29] of the Euler angle representation of the SU(3) group is the so-called Cartan decomposition, which holds for a real semisimple Lie algebra $\mathcal{G}$. A decomposition of the algebra $\mathcal{G}$ into the direct sum of vector spaces $\mathcal{K}$ and $\mathcal{P}$,

$$\mathcal{G} = \mathcal{K} \otimes \mathcal{P}, \tag{3.1}$$

is a *Cartan decomposition of the algebra* $\mathcal{G}$ if

$$[\mathcal{K}, \mathcal{K}] \subset \mathcal{K}, \tag{3.2}$$

$$[\mathcal{K}, \mathcal{P}] \subset \mathcal{P}, \tag{3.3}$$

$$[\mathcal{P}, \mathcal{P}] \subset \mathcal{K}. \tag{3.4}$$

The Cartan decomposition for a Lie algebra induces a corresponding *Cartan decomposition of the group* G,

$$G = KP, \tag{3.5}$$

where K is a Lie subgroup of G with Lie algebra $\mathcal{K}$ and P is given by the exponential map $P = \exp(\mathcal{P})$.

An explicit realization of the Cartan decomposition for SU(3) can be achieved using the standard traceless 3×3 Hermitian Gell-Mann matrices $\lambda_a (a=1,\ldots,8)$ (the explicit form of the λ matrices is given in the Appendix). Indeed, from the expressions for the commutation relations,

$$[\lambda_a,\lambda_b] = 2i\sum_{c=1}^{8} f_{abc}\lambda_c, \tag{3.6}$$

where the structure constants f_{abc} are antisymmetric in all indices and have the nonzero values,

$$f_{123} = 1,$$

$$f_{147} = f_{246} = f_{257} = f_{345} = f_{516} = f_{637} = 1/2, \tag{3.7}$$

$$f_{458} = f_{678} = \sqrt{3/2},$$

it follows that the set of matrices $(\lambda_1,\lambda_2,\lambda_3,\lambda_8)$ can be used as the basis for the vector space $\mathcal{K}$ while the matrices $(\lambda_4,\lambda_5,\lambda_6,\lambda_7)$ span the Cartan subspace $\mathcal{P}$. Noting that the set of matrices $(\lambda_1,\lambda_2,\lambda_3,\lambda_8)$ comprise the generators $(\lambda_1,\lambda_2,\lambda_3)$ of the SU(2) group, one can locally represent K as the product of the SU(2) subgroup and a one-parameter subgroup,

$$K = \mathrm{SU}(2)e^{i\phi\lambda_8}. \tag{3.8}$$

The second factor, $P=\exp(\mathcal{P})$, in the Cartan decomposition (3.5) can be represented as a product of one-parameter subgroups. Moreover, based on the algebra (3.6), it can be represented as a product of a one-parameter subgroup generated by an element[23] from $\lambda_4,\ldots,\lambda_7$ "sandwiched" between two different copies of K. Fixing this generator to be, say λ_4, we have

$$P = K' e^{i\theta'\lambda_4} K''. \tag{3.9}$$

Now observing that $[\lambda_8,\lambda_4]=i\sqrt{3}\lambda_5$, the product KP can be reduced to

$$G = \mathrm{SU}(2)e^{i\theta\lambda_5}\mathrm{SU}(2)' e^{i\phi\lambda_8}. \tag{3.10}$$

Therefore, finally choosing the Euler representation for the elements of two subgroups $U \in SU(2)$ and $V \in \mathrm{SU}(2)'$ in terms of two sets of angles (α,β,γ) and (a,b,c),

$$U(\alpha,\beta,\gamma) = \exp\left(i\frac{\alpha}{2}\lambda_3\right)\exp\left(i\frac{\beta}{2}\lambda_2\right)\exp\left(i\frac{\gamma}{2}\lambda_3\right), \tag{3.11}$$

$$V(a,b,c) = \exp\left(i\frac{a}{2}\lambda_3\right)\exp\left(i\frac{b}{2}\lambda_2\right)\exp\left(i\frac{c}{2}\lambda_3\right), \tag{3.12}$$

we arrive at the generalized Euler decomposition of an element of $g \in SU(3)$,

$$g = U(\alpha,\beta,\gamma)Z(\theta,\phi)V(a,b,c), \tag{3.13}$$

with

$$Z(\theta,\phi) := e^{i\theta\lambda_5}e^{i\phi\lambda_8}. \tag{3.14}$$

Now it is necessary to fix the range of angles in (3.13). Just as in the case of the SU(2) group where the Euler parametrization was not a global one, the SU(3) group manifold cannot be covered by one chart. However, there is a range of parameters such that the parametrization covers

almost the whole manifold except the set whose measure in the integral quantities, e.g., such as the invariant volume, is zero.[23] The following ranges for the angles in (3.13):

$$0 \le \alpha,\ a \le 2\pi, \quad 0 \le \beta,\ b \le \pi, \quad 0 \le \gamma,\ c \le 4\pi, \tag{3.15}$$

$$0 \le \theta \le \frac{\pi}{2}, \quad 0 \le \phi \le \sqrt{3}\pi, \tag{3.16}$$

lead to the invariant volume for SU(3),

$$\mathrm{Vol}(SU(3)) = \int_{SU(3)} * 1 = \sqrt{3}\pi^5. \tag{3.17}$$

Below this result will be checked by an explicit calculation of the volume of the SU(3) manifold considered as the Riemannian space endowed with the bi-invariant metric,

$$\mathbf{g}_{\mathrm{SU(3)}} = -\frac{1}{2}\,\mathrm{Tr}(g^{-1}\,\mathrm{d}g \otimes g^{-1}\,\mathrm{d}g). \tag{3.18}$$

In terms of the nonholonomic frame built up from the left-/right-invariant forms,

$$g^{-1}\,\mathrm{d}g = \frac{i}{2}\sum_{A=1}^{8} \lambda_A \otimes \omega_L^A, \tag{3.19}$$

$$\mathrm{d}g\ g^{-1} = \frac{i}{2}\sum_{A=1}^{8} \lambda_A \otimes \omega_R^A, \tag{3.20}$$

the Cartan-Killing metric (3.18) has the diagonal form

$$\mathbf{g}_{\mathrm{SU(3)}} = \frac{1}{4}(\omega_L^1 \otimes \omega_L^1 + \omega_L^2 \otimes \omega_L^2 + \ \ldots\ + \omega_L^8 \otimes \omega_L^8) \tag{3.21}$$

$$= \frac{1}{4}(\omega_R^1 \otimes \omega_R^1 + \omega_R^2 \otimes \omega_R^2 + \ \ldots\ + \omega_R^8 \otimes \omega_R^8), \tag{3.22}$$

while in the corresponding coordinate frame, with the Eulerian coordinates $(\alpha,\beta,\gamma,a,b,c,\theta,\phi)$, presented in the Appendix, it becomes

$$\begin{aligned}
\mathbf{g}_{\mathrm{SU(3)}} = {} & \frac{1}{4}(\mathrm{d}\alpha \otimes \mathrm{d}\alpha + \mathrm{d}\beta \otimes \mathrm{d}\beta + \mathrm{d}\gamma \otimes \mathrm{d}\gamma + 2\cos\beta\,\mathrm{d}\alpha \otimes \mathrm{d}\gamma) + \frac{1}{4}(\mathrm{d}a \otimes \mathrm{d}a + \mathrm{d}b \otimes \mathrm{d}b + \mathrm{d}c \otimes \mathrm{d}c \\
& + 2\cos b\,\mathrm{d}a \otimes \mathrm{d}c) + \frac{1}{2}\cos\theta\,[\sin(a+\gamma)(\sin\beta\,\mathrm{d}\alpha \otimes \mathrm{d}b + \sin b\,\mathrm{d}\beta \otimes \mathrm{d}c) \\
& + \cos(a+\gamma)(\mathrm{d}\beta \otimes \mathrm{d}b - \sin\beta\sin b\,\mathrm{d}\alpha \otimes \mathrm{d}c)] - \frac{\sqrt{3}}{2}\sin^2\theta(\cos\beta\,\mathrm{d}\alpha + \mathrm{d}\gamma) \otimes \mathrm{d}\phi \\
& + \frac{1}{4}(1+\cos^2\theta)(\cos\beta\,\mathrm{d}\alpha + \mathrm{d}\gamma) \otimes (\mathrm{d}a + \cos b\,\mathrm{d}c) + \mathrm{d}\theta \otimes \mathrm{d}\theta + \mathrm{d}\phi \otimes \mathrm{d}\phi.
\end{aligned} \tag{3.23}$$

Fixing the range of the Euler angles according to (3.15) and noting that the determinant of the Cartan- Killing metric (3.23) is

$$\det \mathbf{g}_{\mathrm{SU}(3)} = \left(\frac{1}{2}\right)^{12} \sin^6(\theta)\cos^2(\theta)\sin^2(\beta)\sin^2(b),$$

one can check that the group invariant volume on SU(3) agrees with (3.17),

$$\begin{aligned}\mathrm{Vol}(\mathrm{SU}(3)) &= \int_{\mathrm{SU}(3)} \sqrt{\det \mathbf{g}_{\mathrm{SU}(3)}}\, \mathrm{d}\alpha \wedge \mathrm{d}\beta \wedge \mathrm{d}\gamma \wedge \mathrm{d}\theta \wedge \mathrm{d}a \wedge \mathrm{d}b \wedge \mathrm{d}c \wedge \mathrm{d}\phi \\ &= \left(\frac{1}{2}\right)^6 \int_0^{2\pi} \mathrm{d}\alpha \int_0^{4\pi} \mathrm{d}\gamma \int_0^{2\pi} \mathrm{d}a \int_0^{4\pi} \mathrm{d}c \int_0^{\sqrt{3}\pi} \mathrm{d}\phi \\ &\quad \times \int_0^{\pi} \mathrm{d}\beta \sin(\beta) \int_0^{\pi/2} \mathrm{d}\theta \cos(\theta)\sin^3(\theta) \int_0^{\pi} \mathrm{d}b \sin(b) = \sqrt{3}\pi^5. \end{aligned} \tag{3.24}$$

This volume is in accordance with the general formula established by Macdonald in Ref. 24 and expresses the volume element of a compact Lie group in terms of the product of volume elements of odd-dimensional unit spheres,

$$\mathrm{Vol}(\mathrm{SU}(3)) = \frac{\sqrt{3}}{2} \times \mathrm{Vol}(\mathbb{S}^5) \times \mathrm{Vol}(\mathbb{S}^3) = \frac{\sqrt{3}}{2} \times \pi^3 \times 2\pi^2. \tag{3.25}$$

In (3.25), the multiplier $\sqrt{3}/2$ comes from the volume of the maximal torus in SU(3), interpreted sometimes as the "*stretching*" factor.[25,26] This fact explicitly shows that the SU(3) group is not a trivial product of the two spheres, $\mathbb{S}^3$ and $\mathbb{S}^5$.

The SU(3) group endowed with the bi-invariant metric (3.23) has a constant positive Riemann scalar curvature,

$$\mathcal{R}_{\mathrm{SU}(3)} = 24,$$

and the Ricci tensor obeys the relations[27]

$$\mathcal{R}_{\mu\nu} = \frac{\mathcal{R}_{\mathrm{SU}(3)}}{8} \mathrm{g}_{\mu\nu} = 3\mathrm{g}_{\mu\nu}. \tag{3.26}$$

B. Geometry of the left coset SU(3)/SU(2)

The group SU(3) can be viewed as a *principal bundle over the base* $\mathbb{S}^5$ *with the structure group* SU(2),

$$SU(2) \hookrightarrow SU(3) \xrightarrow{\pi} \mathbb{S}^5,$$

with the canonical projection π from the SU(3) onto the left coset SU(3)/SU(2)$\simeq\mathbb{S}^5$. This map can be realized in the following manner. Consider the general linear group GL(3, $\mathbb{C}$).

An arbitrary element $M_{3\times 3}$ can be written in the block form

$$M_{3\times 3} = \left(\begin{array}{cc|c} & & z_3 \\ & M_{2\times 2} & z_2 \\ \hline y_1 & y_2 & z_1 \end{array}\right) = \left(\begin{array}{c|c} M_{2\times 2} & \mathbf{a} \\ \hline \mathbf{b} & z_1 \end{array}\right), \tag{3.27}$$

for complex 2×2 matrix $M_{2\times 2}$ and $z_1, z_2, z_3, y_1, y_2 \in \mathbb{C}$. The U(3) subgroup of the GL(3, $\mathbb{C}$) group is defined by the two matrix equations,

$$M_{3\times3}M_{3\times3}^{\dagger}=I_{3\times3},\quad M_{3\times3}^{\dagger}M_{3\times3}=I_{3\times3}. \tag{3.28}$$

When $M_{3\times3}$ is represented in block form (3.27), the conditions (3.28) reduce to the quadratic equations,

$$|z_1|^2+|z_2|^2+|z_3|^2=1, \tag{3.29}$$

$$|z_1|^2+|y_1|^2+|y_2|^2=1, \tag{3.30}$$

and to the set of 2×2 matrix equations,

$$M_{2\times2}M_{2\times2}^{\dagger}+\mathbf{a}\mathbf{a}^{\dagger}=I_{2\times2}, \tag{3.31}$$

$$M_{2\times2}^{\dagger}M_{2\times2}+\mathbf{b}^{\dagger}\mathbf{b}=I_{2\times2}, \tag{3.32}$$

$$z_1\mathbf{a}+M_{2\times2}\mathbf{a}=\mathbf{0}, \tag{3.33}$$

$$\bar{z}_1\mathbf{b}+M_{2\times2}^{\dagger}\mathbf{b}=\mathbf{0}. \tag{3.34}$$

Now let $\mathbb{S}^5$ be the five-sphere characterized by a unit complex vector $\mathbf{Z}:=(z_1,z_2,z_3)^T$

$$\mathbf{Z}^{\dagger}\mathbf{Z}=1.$$

The SU(3) group element g then acts on this through left translations:

$$\mathbf{Z}\rightarrow\mathbf{Z}'=g\mathbf{Z}. \tag{3.35}$$

Let $\mathbf{Z}_0$ be the base point on this five-sphere with coordinates $\mathbf{Z}_0=(0,0,1)^T$ whose isotropy group is

$$H_{3\times3}=\left(\begin{array}{c|c}\mathrm{SU(2)} & \mathbf{0}\\ \hline \mathbf{0} & 1\end{array}\right). \tag{3.36}$$

Then the coset SU(3)/SU(2) can be identified with the orbit

$$\mathbf{Z}=g\cdot(0,0,1)^T. \tag{3.37}$$

Using the explicit form of the representation (3.13), the subgroup SU(2) is embedded into SU(3) as follows:

$$SU(2)\rightarrow SU(3),\quad V=\begin{pmatrix} e^{-i(a+c)/2}\cos\left(\frac{b}{2}\right) & -e^{-i(a-c)/2}\sin\left(\frac{b}{2}\right) & 0\\ e^{i(a-c)/2}\sin\left(\frac{b}{2}\right) & e^{i(a+c)/2}\cos\left(\frac{b}{2}\right) & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{3.38}$$

So the parametrization of a group element is

$$g=UZV=WV,$$

where the factor W reads as

$$W=\begin{pmatrix} \cos\theta\cos\dfrac{\beta}{2}e^{i\left(u+\frac{1}{\sqrt{3}}\phi\right)} & \sin\dfrac{\beta}{2}e^{i(v+(1/\sqrt{3})\phi)} & \sin\theta\cos\dfrac{\beta}{2}e^{i(u-(2/\sqrt{3})\phi)} \\ -\cos\theta\sin\dfrac{\beta}{2}e^{-i\left(v-\frac{1}{\sqrt{3}}\phi\right)} & \cos\dfrac{\beta}{2}e^{-i(u-(1/\sqrt{3})\phi)} & -\sin\theta\sin\dfrac{\beta}{2}e^{-i(v+(2/\sqrt{3})\phi)} \\ -\sin\theta e^{\frac{i}{\sqrt{3}}\phi} & 0 & \cos\theta e^{-i(2/\sqrt{3})\phi} \end{pmatrix}$$

$$u=\frac{\alpha+\gamma}{2},\quad v=\frac{\alpha-\gamma}{2}.$$

Using these representations in (3.37), we easily identify the projection onto the left coset as a five-sphere:

$$\pi: g\in SU(3)\to(z_1,z_2,z_2)\in\mathbb{S}^5,$$

which explicitly reads as

$$z_1=\cos\theta e^{-i(2/\sqrt{3})\phi}, \tag{3.39}$$

$$z_2=-\sin\theta\sin\frac{\beta}{2}e^{-\frac{i}{2}(\alpha-\gamma+(4/\sqrt{3})\phi)}, \tag{3.40}$$

$$z_3=\sin\theta\cos\frac{\beta}{2}e^{(i/2)(\alpha+\gamma-(4/\sqrt{3})\phi)}. \tag{3.41}$$

Under this projection the Euclidean metric $\mathrm{tr}(\mathrm{d}M\,\mathrm{d}M^\dagger)$ on $\mathrm{GL}(3,\mathbb{C})$ induces the following metric on a unit $\mathbb{S}^5$:

$$\begin{aligned}\mathbf{g}_{\mathbb{S}^5}&=\mathrm{d}\bar{z}_1\otimes\mathrm{d}z_1+\mathrm{d}\bar{z}_2\otimes\mathrm{d}z_2+\mathrm{d}\bar{z}_3\otimes\mathrm{d}z_3\\&=\sin^2\theta\left(\frac{1}{4}(\mathrm{d}\alpha\otimes\mathrm{d}\alpha+\mathrm{d}\beta\otimes\mathrm{d}\beta+\mathrm{d}\gamma\otimes\mathrm{d}\gamma+2\cos\beta\,\mathrm{d}\alpha\otimes\mathrm{d}\gamma)-\frac{2}{\sqrt{3}}(\cos\beta\,\mathrm{d}\alpha+\mathrm{d}\gamma)\otimes\mathrm{d}\phi\right)\\&\quad+\mathrm{d}\theta\otimes\mathrm{d}\theta+\frac{4}{3}\mathrm{d}\phi\otimes\mathrm{d}\phi,\end{aligned} \tag{3.42}$$

whose determinant is

$$\det\mathrm{g}_{\mathbb{S}^5}=\frac{1}{48}\sin^6(\theta)\cos^2(\theta)\sin^2(\beta). \tag{3.43}$$

The metric (3.42) defines a unit five-sphere $\mathbb{S}^5$ as a constant curvature Riemann manifold,

$$\mathcal{R}_{\mathbb{S}^5}=20, \tag{3.44}$$

which is in accordance with its Gaussian curvature,

$$K_{\mathbb{S}^5}=\frac{\mathcal{R}_{\mathbb{S}^5}}{5(5-1)}=1,$$

as well as with its volume,

$$\mathrm{Vol}(\mathbb{S}^5) = \int_{\mathbb{S}^5} \sqrt{\det g_{\mathbb{S}^5}}\, d\alpha \wedge d\beta \wedge d\gamma \wedge d\theta \wedge d\phi$$
$$= \frac{1}{4\sqrt{3}} \int_0^{2\pi} d\alpha \int_0^{4\pi} d\gamma \int_0^{\sqrt{3}\pi} d\phi \int_0^{\pi} d\beta \sin(\beta) \int_0^{\pi/2} d\theta \cos(\theta)\sin^3(\theta) = \pi^3. \tag{3.45}$$

C. Lagrangian on SU(3) in terms of generalized Euler angles

Consider the Lagrangian describing the geodesic motion on the SU(3) group manifold with respect to the bi-invariant metric (3.18),

$$\mathrm{L}_{\mathrm{SU}(3)} = -\frac{1}{2}\,\mathrm{Tr}\left(g^{-1}(t)\frac{d}{dt}g(t)g^{-1}(t)\frac{d}{dt}g(t)\right). \tag{3.46}$$

Using the generalized Euler angles on SU(3) as the configuration space coordinates and (3.23) for the bi-invariant metric, one can write the Lagrangian (3.46) as

$$\mathrm{L}_{\mathrm{SU}(3)} = \frac{1}{4}(\dot{\alpha}^2 + \dot{\beta}^2 + \dot{\gamma}^2 + 2\cos\beta\dot{\alpha}\dot{\gamma} + \dot{a}^2 + \dot{b}^2 + \dot{c}^2 + 2\cos b\dot{a}\dot{c})$$
$$+ \frac{1}{2}\cos\theta(\sin(a+\gamma)(\sin\beta\dot{\alpha}\dot{b} + \sin b\dot{\beta}\dot{c}) + \cos(a+\gamma)(\dot{\beta}\dot{b} - \sin\beta\sin b\dot{\alpha}\dot{c}))$$
$$- \frac{\sqrt{3}}{2}\sin^2\theta(\cos\beta\dot{\alpha} + \dot{\gamma})\dot{\phi} + \frac{1}{4}(1+\cos^2\theta)(\cos\beta\dot{\alpha} + \dot{\gamma})(\dot{a} + \cos b\dot{c}) + \dot{\theta}^2 + \dot{\phi}^2. \tag{3.47}$$

From this expression and (3.23), it follows that

$$\mathrm{L}_{\mathrm{SU}(3)} = \mathbf{g}_{\mathrm{SU}(3)}(\dot{Z},\dot{Z}), \tag{3.48}$$

where $\dot{Z}$ is the vector field on the tangent bundle TSU(3),

$$\dot{Z} = \dot{\alpha}\frac{\partial}{\partial\alpha} + \dot{\beta}\frac{\partial}{\partial\beta} + \dot{\gamma}\frac{\partial}{\partial\gamma} + \dot{\theta}\frac{\partial}{\partial\theta} + \dot{\phi}\frac{\partial}{\partial\phi} + \dot{a}\frac{\partial}{\partial a} + \dot{b}\frac{\partial}{\partial b} + \dot{c}\frac{\partial}{\partial c}. \tag{3.49}$$

It is worth noting that the Euler decomposition (3.13) for elements of SU(3) in terms of the SU(2) subgroups,

$$\mathrm{SU}(3) = U(\alpha,\beta,\gamma)\exp(i\theta\lambda_5)V(a,b,c)\exp(i\phi\lambda_8),$$

allows for the expression of the SU(3) Lagrangian (3.47) in terms of the corresponding left and right invariant elements of the SU(2) Maurer-Cartan 1-forms:

$$\mathrm{L}_{\mathrm{SU}(3)} = \frac{1}{4}\sum_{a=1}^{3} i_{\dot{U}}\omega_L^a i_{\dot{U}}\omega_L^a + \frac{1}{4}\sum_{a=1}^{3} i_{\dot{V}}\omega_L^a i_{\dot{V}}\omega_L^a + \frac{1}{2}\cos\theta\sum_{a=1}^{3} i_{\dot{U}}\omega_L^a i_{\dot{V}}\omega_R^i - \frac{1}{4}(1+\cos^2\theta) i_{\dot{U}}\omega_L^3 i_{\dot{V}}\omega_R^3$$
$$- \frac{\sqrt{3}}{2}\sin^2\theta i_{\dot{U}}\omega_L^3\dot{\phi} + \dot{\theta}^2 + \dot{\phi}^2. \tag{3.50}$$

Here $i_{\dot{U}}$ and $i_{\dot{V}}$ denote the interior contraction of the vector field on each copy of the SU(2) group, U and V, respectively,

$$\dot{U}=\dot{\alpha}\frac{\partial}{\partial\alpha}+\dot{\beta}\frac{\partial}{\partial\beta}+\dot{\gamma}\frac{\partial}{\partial\gamma},\quad \dot{V}=\dot{a}\frac{\partial}{\partial a}+\dot{b}\frac{\partial}{\partial b}+\dot{c}\frac{\partial}{\partial c}. \tag{3.51}$$

D. Hamiltonian dynamics on SU(3)

Performing the Legendre transformation, we derive the canonical Hamiltonian generating the dynamics on the SU(3) group manifold:

$$\begin{aligned}H_{\mathrm{SU}(3)}=&\frac{1}{\sin^2\theta}\left[\frac{p_\alpha^2}{\sin^2\beta}+p_\beta^2+\left(\tan^2\theta+\frac{1}{\sin^2\beta}\right)p_\gamma^2-2\frac{\cos\beta}{\sin^2\beta}p_\alpha p_\gamma\right.\\&\left.+\sin^2\theta\left(1+\frac{1}{4}\cot^2\theta+\frac{1}{\sin^2 b}\right)p_a^2+p_b^2+\frac{1}{\sin^2 b}p_c^2-2\frac{\cos b}{\sin^2 b}p_a p_c\right]\\&+2\frac{\cos\theta}{\sin^2\theta\sin\beta\sin b}\{\cos(a+\gamma)[(p_\alpha-\cos\beta p_\gamma)(p_c-\cos b p_a)-\sin b p_\beta p_b]\\&-\sin(a+\gamma)[\sin b(p_\alpha-\cos\beta p_\gamma)p_b+\sin\beta(p_c-\cos b p_a)p_\beta]\}+\frac{1}{4}p_\theta^2\\&+\frac{1}{16}\left(1+\frac{3}{\cos^2\theta}\right)p_\phi^2+\frac{\sqrt{3}}{2}\frac{p_\gamma p_\phi}{\cos^2\theta}-\frac{\sqrt{3}}{4}\left(1+\frac{1}{\cos^2\theta}\right)p_a p_\phi.\end{aligned} \tag{3.52}$$

The Hamiltonian (3.52) can be rewritten in a compact form using the left- and right-invariant vector fields on the two SU(2) group copies, U and V, used in the Euler decomposition (3.13):

$$\begin{aligned}H_{\mathrm{SU}(3)}=&\sum_{a=1}^{3}\zeta_a^R\zeta_a^R+\frac{1}{\sin^2\theta}\sum_{a=1}^{2}(\xi_a^L-\cos\theta\zeta_a^R)^2+\frac{1}{\sin^2 2\theta}\left(2\xi_3^L-(1+\cos^2\theta)\zeta_3^R-\frac{\sqrt{3}}{2}\sin^2\theta p_\phi\right)^2\\&+\frac{1}{4}p_\theta^2+\frac{1}{4}p_\phi^2.\end{aligned} \tag{3.53}$$

Here ξ_a^b and ζ_α^R are functions defined through the relations

$$\xi_a^L:=\Theta(X_a^L),\quad \zeta_a^R:=\Theta(Y_a^R),$$

with the SU(2) left-invariant vector fields X_a^L on the tangent space to the U subgroup, TU, and the right-invariant fields Y_a^R on TV correspondingly.

E. Hamiltonian reduction to SU(3)/SU(2)

The representation (3.53) is very convenient for performing the reduction in degrees of freedom associated with the SU(2) symmetry transformation. Due to the algebra of Poisson brackets (2.35), the functions ζ_1^L,ζ_2^L, and ζ_3^L are the first integrals,

$$\{\zeta_a^L,H_{\mathrm{SU}(3)}\}=0.$$

Let us consider the zero level of these integrals

$$\zeta_1^L=0,\quad \zeta_2^L=0,\quad \zeta_3^L=0. \tag{3.54}$$

Noting the relation between the left and right invariant vector fields on a group, one can express the functions ζ_a^R entering in the Hamiltonian as

$$\zeta_c^R = \mathrm{Ad}(\mathrm{V})_{cb}\zeta_b^L,$$

where $\mathrm{Ad}(\mathrm{V})_{cb}$ is an adjoint matrix of an element $\mathrm{V} \in \mathrm{SU}(2)$. From this one can immediately find the reduced Hamiltonian on the integral level (3.54). Indeed, projecting the expression (3.53) on $\zeta_a^R = 0$, we find

$$H_{\mathrm{SU}(3)/\mathrm{SU}(2)} = \frac{1}{\sin^2\theta}\sum_{a=1}^{3}\xi_a^L\xi_a^L + \frac{1}{\sin^2 2\theta}\left(2\xi_3^L - \frac{\sqrt{3}}{2}\sin^2\theta p_\phi\right)^2 + \frac{1}{4}p_\theta^2 + \frac{1}{4}p_\phi^2, \tag{3.55}$$

or, more explicitly in terms of the canonical coordinates,

$$\begin{aligned}\mathrm{H}_{\mathrm{SU}(3)/\mathrm{SU}(2)} = {} & \frac{1}{\sin^2\theta}\left(\frac{p_\alpha^2}{\sin^2\beta} + p_\beta^2 + \left(\tan^2\theta + \frac{1}{\sin^2\beta}\right)p_\gamma^2 - 2\frac{\cos\beta}{\sin^2\beta}p_\alpha p_\gamma + \frac{\sqrt{3}}{2}\tan^2\theta p_\gamma p_\phi\right) \\ & + \frac{1}{4}p_\theta^2 + \frac{1}{16}\left(1 + \frac{3}{\cos^2\theta}\right)p_\phi^2.\end{aligned} \tag{3.56}$$

Performing the inverse Legendre transformation, we find the Lagrangian,

$$\begin{aligned}\mathrm{L}_{\mathrm{SU}(3)/\mathrm{SU}(2)} = {} & \frac{1}{4}\sin^2\theta\left[\left(1 - \frac{1}{4}\cos^2\beta\sin^2\theta\right)\dot{\alpha}^2 + \dot{\beta}^2 + \frac{1}{4}(3 + \cos^2\theta)\dot{\gamma}^2 + \frac{1}{2}\cos\beta(3 + \cos^2\theta)\dot{\alpha}\dot{\gamma}\right. \\ & \left. - 2\sqrt{3}(\cos\beta\dot{\alpha} + \dot{\gamma})\dot{\phi}\right] + \dot{\theta}^2 + \dot{\phi}^2.\end{aligned} \tag{3.57}$$

Now one can consider the bilinear form (3.57) as the metric $\mathbf{g}_{\mathcal{O}}$ on the orbit space $\mathcal{O} = \mathrm{SU}(3)/\mathrm{SU}(2)$,

$$\begin{aligned}\mathbf{g}_{\mathcal{O}} = {} & \frac{1}{4}\sin^2\theta\left[\left(1 - \frac{1}{4}\cos^2\beta\sin^2\theta\right)\mathrm{d}\alpha\otimes\mathrm{d}\alpha + \mathrm{d}\beta\otimes\mathrm{d}\beta + \frac{1}{4}(3 + \cos^2\theta)\mathrm{d}\gamma\otimes\mathrm{d}\gamma\right. \\ & \left. + \frac{1}{2}\cos\beta(3 + \cos^2\theta)\mathrm{d}\alpha\otimes\mathrm{d}\gamma - 2\sqrt{3}(\cos\beta\,\mathrm{d}\alpha + \mathrm{d}\gamma)\otimes\mathrm{d}\phi\right] + \mathrm{d}\theta\otimes\mathrm{d}\theta + \mathrm{d}\phi\otimes\mathrm{d}\phi.\end{aligned} \tag{3.58}$$

Using our previous calculations (3.45) of $\mathrm{Vol}(\mathbb{S}^5)$ with respect to the metric (3.42) induced by the canonical projection to the left coset $\pi:\mathrm{SU}(3)\to\mathrm{SU}(3)/\mathrm{SU}(2)$ and noting that the determinant of the new orbit metric (3.58) induced by the Hamiltonian reduction is

$$\det\mathbf{g}_{\mathcal{O}} = \frac{1}{64}\sin^6(\theta)\cos^2(\theta)\sin^2(\beta), \tag{3.59}$$

we find

$$\mathrm{Vol}(\mathrm{SU}(3)/\mathrm{SU}(2)) = \frac{\sqrt{3}}{2}\mathrm{Vol}(\mathbb{S}^5), \tag{3.60}$$

with the same *stretching* factor $\sqrt{3}/2$ as found in (3.25) for the bi-invariant volume of the SU(3) group.

IV. RIEMANNIAN STRUCTURES ON THE QUOTIENT SPACE

Now we are ready to answer the questions about the relation between metric (3.42) induced on the left coset SU(3)/SU(2) by canonical projection from the ambient Euclidian space and the metric (3.58) obtained as a result of performing the Hamiltonian reduction of the geodesic motion from SU(3) to SU(3)/SU(2).

Performing a straightforward calculation of the Riemannian curvature with respect to the metric (3.58) yields

$$\mathcal{R}\left(\mathbf{g}_{\frac{\mathrm{SU}(3)}{\mathrm{SU}(2)}}\right)=21, \tag{4.1}$$

while, from the embedding argumentation we used before, the Riemann scalar of the unit five-sphere $\mathbb{S}^5$ with standard metric induced from the Euclidean space is

$$\mathcal{R}\left(\mathbf{g}_{\mathbb{S}^5}\right)=20. \tag{4.2}$$

Furthermore, even though the Riemann scalar is a constant, calculations shows that the metric (3.57) *is not the metric of a space of constant curvature*.

So, we have found that the Lagrangian of the reduced system defines local flows on the configuration space which are not isometric to those on $\mathbb{S}^5$ with its standard round metric.

We have shown above that the orbit space SU(3)/SU(2) considered as a Riemannian space with metric $\mathbf{g}$ induced from the Cartan-Killing metric on SU(3) is not isometric to the $\mathbb{S}^5$ with the standard round metric $\mathbf{g}_{\mathbb{S}^5}$. The next natural question is whether the metrics $\mathbf{g}_{\mathcal{O}}$ and $\mathbf{g}_{\mathbb{S}^5}$ are *geodesically/projectively* equivalent.

There are several criteria on metrics to be geodesically equivalent. According to Eisenhart,[30] two metrics $\mathbf{g}$ and $\overline{\mathbf{g}}$ on an n-dimensional Riemann manifold are *geodesically equivalent if and only if*

$$2(n+1)\boldsymbol{\nabla}_i(\mathbf{g})\overline{\mathbf{g}}_{jk}=2\overline{\mathbf{g}}_{jk}\,\partial_i\Lambda+\overline{\mathbf{g}}_{ik}\partial_j\Lambda+\overline{\mathbf{g}}_{ji}\,\partial_k\Lambda, \tag{4.3}$$

where $\boldsymbol{\nabla}_i(\mathbf{g})$ is covariant with respect the metric $\mathbf{g}$ and the scalar function Λ is

$$\Lambda=\ln\left(\frac{\det(\overline{\mathbf{g}})}{\det(\mathbf{g})}\right). \tag{4.4}$$

According to our calculations,

$$\det(\mathbf{g}_{\mathcal{O}})=\frac{3}{4}\det(\mathbf{g}_{\mathbb{S}^5})$$

and

$$\boldsymbol{\nabla}_i(\mathbf{g}_{\mathbb{S}^5})\mathbf{g}_{\mathcal{O}_{jk}}\neq 0,$$

and therefore $\mathbf{g}_{\mathbb{S}^5}$ and $\mathbf{g}_{\mathcal{O}}$ are not *geodesically/projectively* equivalent.

V. CONCLUSION

In this paper we have presented, for the first time, the explicit Hamiltonian reduction from free motion on SU(3) to motion on the coset space $\mathrm{SU}(3)/\mathrm{SU}(2)\approx\mathbb{S}^5$. This has been made possible through a consistent parametrization of SU(3) that generalizes the Euler angle parametrization of SU(2). The full details for this parametrization of SU(3) are, for completeness, collected together in an Appendix to this paper. The results presented there have been checked independently using the computer algebra packages MATHEMATICA *5.0* and MAPLE *9.5*. (MATHEMATICA files are available at http://compalg.jinr.ru/CAGroup/Palii/math_prgr.php).

Through this analysis, we have seen that the resulting dynamics is not equivalent to the geodesic motion on $\mathbb{S}^5$ induced from its standard round metric. This result prompts the following questions.

- Is it possible to identify, *a priori*, the induced metric on the coset space in terms of the properties of SU(3)?
- Is it possible to formulate the dynamics on SU(3) so that the reduced dynamics *is* the expected geodesic motion on $\mathbb{S}^5$?

- What happens if we reduce to a nonzero level set of the integrals (3.54)?

Progress in answering these questions will, we feel, throw much light on the dynamical aspects of the Hamiltonian reduction procedure and hence lead to a deeper understanding of the quantization of gauge theories.

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APPENDIX: DETAILS OF CALCULATION

1. The su(3) algebra structure

The eight traceless 3×3 Gell-Mann matrices providing a basis for the su(3) algebra listed below:

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

$$\lambda_4=\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix},\quad \lambda_5=\begin{pmatrix}0&0&-i\\0&0&0\\i&0&0\end{pmatrix},\quad \lambda_6=\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix},\tag{A1}$$

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

Sometimes it is convenient to use instead of the Gell-Mann matrices the anti-Hermitian basis $\mathbf{t}_a:=(1/2i)\lambda_a$, obeying the relations

$$\mathbf{t}_a\mathbf{t}_b=-\frac{1}{6}\delta_{ab}\mathbf{I}+\frac{1}{2}\sum_{c=1}^{8}(f_{abc}-id_{abc})\mathbf{t}_c,\tag{A2}$$

where the structure constants d_{abc} are symmetric in their indices and nonvanishing values are given in Table I, the coefficients f_{abc} are skew symmetric in all indices. The constants f_{abc} determine the commutators between the basis elements (also see Table II)

$$[\mathbf{t}_a,\mathbf{t}_b]=\sum_{c=1}^{8}f_{abc}\mathbf{t}_c.\tag{A3}$$

TABLE I. The symmetric coefficients d_{abc}.

(abc)	(118)(228)(338)	(146)(157)(256)(344)(355)	(247)(366)(377)	(448)(558)(668)(778)	(888)
d_{abc}	$\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{\sqrt{3}}$

TABLE II. Structure of the su(3) algebra

	$\mathbf{t}_1$	$\mathbf{t}_2$	$\mathbf{t}_3$	$\mathbf{t}_4$	$\mathbf{t}_5$	$\mathbf{t}_6$	$\mathbf{t}_7$	$\mathbf{t}_8$
$\mathbf{t}_1$	0	$\mathbf{t}_3$	$-\mathbf{t}_2$	$\frac{1}{2}\mathbf{t}_7$	$-\frac{1}{2}\mathbf{t}_6$	$\frac{1}{2}\mathbf{t}_5$	$-\frac{1}{2}\mathbf{t}_4$	0
$\mathbf{t}_2$	$-\mathbf{t}_3$	0	$\mathbf{t}_1$	$\frac{1}{2}\mathbf{t}_6$	$\frac{1}{2}\mathbf{t}_7$	$-\frac{1}{2}\mathbf{t}_4$	$-\frac{1}{2}\mathbf{t}_5$	0
$\mathbf{t}_3$	$\mathbf{t}_2$	$-\mathbf{t}_1$	0	$\frac{1}{2}\mathbf{t}_5$	$-\frac{1}{2}\mathbf{t}_4$	$-\frac{1}{2}\mathbf{t}_7$	$\frac{1}{2}\mathbf{t}_6$	0
$\mathbf{t}_4$	$-\frac{1}{2}\mathbf{t}_7$	$-\frac{1}{2}\mathbf{t}_6$	$-\frac{1}{2}\mathbf{t}_5$	0	$\frac{1}{2}\mathbf{t}_3+\frac{\sqrt{3}}{t}\mathbf{t}_8$	$\frac{1}{2}\mathbf{t}_2$	$\frac{1}{2}\mathbf{t}_1$	$-\frac{\sqrt{3}}{2}\mathbf{t}_5$
$\mathbf{t}_5$	$\frac{1}{2}\mathbf{t}_6$	$-\frac{1}{2}\mathbf{t}_7$	$\frac{1}{2}\mathbf{t}_4$	$-\frac{1}{2}\mathbf{t}_3-\frac{\sqrt{3}}{2}\mathbf{t}_8$	0	$-\frac{1}{2}\mathbf{t}_1$	$\frac{1}{2}\mathbf{t}_2$	$\frac{\sqrt{3}}{2}\mathbf{t}_4$
$\mathbf{t}_6$	$-\frac{1}{2}\mathbf{t}_5$	$\frac{1}{2}\mathbf{t}_4$	$\frac{1}{2}\mathbf{t}_7$	$-\frac{1}{2}\mathbf{t}_2$	$\frac{1}{2}\mathbf{t}_1$	0	$-\frac{1}{2}\mathbf{t}_3+\frac{\sqrt{3}}{2}\mathbf{t}_8$	$-\frac{\sqrt{3}}{2}\mathbf{t}_7$
$\mathbf{t}_7$	$\frac{1}{2}\mathbf{t}_4$	$\frac{1}{2}\mathbf{t}_5$	$-\frac{1}{2}\mathbf{t}_6$	$-\frac{1}{2}\mathbf{t}_1$	$-\frac{1}{2}\mathbf{t}_2$	$\frac{1}{2}\mathbf{t}_3-\frac{\sqrt{3}}{2}\mathbf{t}_8$	0	$\frac{\sqrt{3}}{2}\mathbf{t}_6$
$\mathbf{t}_8$	0	0	0	$\frac{\sqrt{3}}{2}\mathbf{t}_5$	$-\frac{\sqrt{3}}{2}\mathbf{t}_4$	$\frac{\sqrt{3}}{2}\mathbf{t}_7$	$-\frac{\sqrt{3}}{2}\mathbf{t}_6$	0

2. The basis of invariant 1-forms on the SU(3) group

a. The left-invariant 1-forms

Using the generalized Euler decomposition (3.13) for the SU(3) group element, it is straightforward to calculate the left and right invariant 1-forms. The results are given below:

$$\omega_L^1 = \Big[\cos[\beta]\sin[b]\cos[c]\Big(1-\frac{1}{2}\sin^2[\theta]\Big)+\cos[\theta]\sin[\beta](\cos[b]\cos[c]\cos[a+\gamma] - \sin[c]\sin[a+\gamma])\Big]\mathrm{d}\alpha - \cos[\theta](\cos[a+\gamma]\sin[c]+\cos[b]\cos[c]\sin[a+\gamma])\mathrm{d}\beta + \cos[c]\sin[b]\Big(1-\frac{1}{2}\sin^2[\theta]\Big)\mathrm{d}\gamma+\cos[c]\sin[b]\mathrm{d}a-\sin[c]\mathrm{d}b,$$

$$\omega_L^2 = \Big[\cos[\beta]\sin[b]\sin[c]\Big(1-\frac{1}{2}\sin^2[\theta]\Big)+\cos[\theta]\sin[\beta](\cos[b]\cos[a+\gamma]\sin[c] + \cos[c]\sin[a+\gamma])\Big]\mathrm{d}\alpha + \cos[\theta](\cos[c]\cos[a+\gamma]-\cos[b]\sin[c]\sin[a+\gamma])\mathrm{d}\beta + \sin[b]\sin[c]\Big(1-\frac{1}{2}\sin^2[\theta]\Big)\mathrm{d}\gamma+\sin[b]\sin[c]\mathrm{d}a+\cos[c]\mathrm{d}b,$$

$$\omega_L^3 = \Big[\cos[b]\cos[\beta]\Big(1-\frac{1}{2}\sin^2[\theta]\Big)-\cos[a+\gamma]\cos[\theta]\sin[b]\sin[\beta]\Big]\mathrm{d}\alpha + \cos[\theta]\sin[b]\sin[a+\gamma]\mathrm{d}\beta+\cos[b]\Big(1-\frac{1}{2}\sin^2\theta\Big)\mathrm{d}\alpha+\cos[b]\mathrm{d}a+\mathrm{d}c,$$

$$\omega_L^4 = \sin[\theta]\Big(\cos[\beta]\cos[\theta]\cos\Big[\frac{b}{2}\Big]\cos\Big[\frac{a+c}{2}+\sqrt{3}\phi\Big]-\cos\Big[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\Big]\sin\Big[\frac{b}{2}\Big]\sin[\beta]\Big)\mathrm{d}\alpha + \sin\Big[\frac{b}{2}\Big]\sin[\theta]\sin\Big[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\Big]\mathrm{d}\beta+\frac{1}{2}\cos\Big[\frac{b}{2}\Big]\cos\Big[\frac{a+c}{2}+\sqrt{3}\phi\Big]\sin[2\theta]\mathrm{d}\gamma - 2\cos\Big[\frac{b}{2}\Big]\sin\Big[\frac{a+c}{2}+\sqrt{3}\phi\Big]\mathrm{d}\theta,$$

$$\omega_L^5 = \sin[\theta]\left(\sin\left[\frac{b}{2}\right]\sin[\beta]\sin\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]+\cos\left[\frac{b}{2}\right]\cos[\beta]\cos[\theta]\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\right)\mathrm{d}\alpha$$
$$+\cos\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]\sin[\theta]\mathrm{d}\beta+\frac{1}{2}\cos\left[\frac{b}{2}\right]\sin[2\theta]\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\mathrm{d}\gamma$$
$$+2\cos\left[\frac{b}{2}\right]\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\mathrm{d}\theta,$$

$$\omega_L^6 = \sin[\theta]\left(\cos[\beta]\cos[\theta]\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]+\sin[\beta]\cos\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\cos\left[\frac{b}{2}\right]\right)\mathrm{d}\alpha$$
$$-\cos\left[\frac{b}{2}\right]\sin[\theta]\sin\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\mathrm{d}\beta+\frac{1}{2}\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]\sin[2\theta]\mathrm{d}\gamma$$
$$-2\sin\left[\frac{b}{2}\right]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\mathrm{d}\theta,$$

$$\omega_L^7 = \sin[\theta]\left(\cos[\beta]\cos[\theta]\sin\left[\frac{b}{2}\right]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]-\cos\left[\frac{b}{2}\right]\sin[\beta]\sin\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\right)\mathrm{d}\alpha$$
$$-\cos\left[\frac{b}{2}\right]\cos\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\sin[\theta]\mathrm{d}\beta+\frac{1}{2}\sin\left[\frac{b}{2}\right]\sin[2\theta]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]d\gamma$$
$$+2\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]\mathrm{d}\theta,$$

$$\omega_L^8 = -\frac{\sqrt{3}}{2}\cos[\beta]\sin^2[\theta]\mathrm{d}\alpha-\frac{\sqrt{3}}{2}\sin^2[\theta]\mathrm{d}\gamma+2\,\mathrm{d}\phi.$$

b. The right-invariant 1-forms

$$\omega_R^1 = \sin[\alpha]\mathrm{d}\beta-\cos[\alpha]\sin[\beta]\mathrm{d}\gamma-\cos[\alpha]\sin[\beta]\left(1-\frac{1}{2}\sin^2[\theta]\right)\mathrm{d}a+\cos[\theta](\cos[a+\gamma]\sin[\alpha]$$
$$+\cos[\alpha]\cos[\beta]\sin[a+\gamma])\mathrm{d}b+\left(\cos[\theta]\sin[b](-\cos[\alpha]\cos[\beta]\cos[a+\gamma]+\sin[\alpha]\sin[a+\gamma])\right.$$
$$\left.-\cos[\alpha]\cos[b]\sin[\beta]\left(1-\frac{1}{2}\sin^2[\theta]\right)\right)\mathrm{d}c+\sqrt{3}\cos[\alpha]\sin[\beta]\sin^2[\theta]\mathrm{d}\phi,$$

$$\omega_R^2 = \cos[\alpha]\mathrm{d}\beta+\sin[\alpha]\sin[\beta]\mathrm{d}\gamma+\sin[\alpha]\sin[\beta]\left(1-\frac{1}{2}\sin^2[\theta]\right)\mathrm{d}a+\cos[\theta]\big(\cos[\alpha]\cos[a+\gamma]$$
$$-\cos[\beta]\sin[\alpha]\sin[a+\gamma]\big)\mathrm{d}b+\left[\cos[\theta]\sin[b](\cos[\beta]\cos[a+\gamma]\sin[\alpha]+\cos[\alpha]\sin[\alpha+\gamma])\right.$$
$$\left.+\cos[b]\sin[\alpha]\sin[\beta]\left(1-\frac{1}{2}\sin^2[\theta]\right)\right]\mathrm{d}c-\sqrt{3}\sin[\alpha]\sin[\beta]\sin^2[\theta]\mathrm{d}\phi$$

$$\omega_R^3 = \mathrm{d}\alpha + \cos[\beta]\mathrm{d}\gamma + \cos[\beta]\left(1 - \frac{1}{2}\sin^2\theta\right)\mathrm{d}a + \cos[\theta]\sin[\beta]\sin[a+\gamma]\mathrm{d}b$$
$$+ \left[\cos[b]\cos[\beta]\left(1 - \frac{1}{2}\sin^2[\theta]\right) - \cos[a+\gamma]\cos[\theta]\sin[b]\sin[\beta]\right]\mathrm{d}c - \sqrt{3}\cos[\beta]\sin^2[\theta]\mathrm{d}\phi,$$

$$\omega_R^4 = 2\cos\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\mathrm{d}\theta - \frac{1}{2}\cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha+\gamma}{2}\right]\sin[2\theta]\mathrm{d}a$$
$$- \sin\left[\frac{\beta}{2}\right]\sin\left[a - \frac{\alpha-\gamma}{2}\right]\sin[\theta]\mathrm{d}b + \sin[\theta]\left(\cos\left[a - \frac{\alpha-\gamma}{2}\right]\sin[b]\sin\left[\frac{\beta}{2}\right]\right.$$
$$\left. - \cos[b]\cos\left[\frac{\beta}{2}\right]\cos[\theta]\cos\left[\frac{\alpha+\gamma}{2}\right]\right)\mathrm{d}c - \sqrt{3}\cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha+\gamma}{2}\right]\sin[2\theta]\mathrm{d}\phi,$$

$$\omega_R^5 = \cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha+\gamma}{2}\right]\mathrm{d}\theta + \frac{1}{2}\cos\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\sin[2\theta]\mathrm{d}a + \cos\left[a - \frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\sin[\theta]\mathrm{d}b$$
$$+ \sin[\theta]\left(\sin[b]\sin\left[\frac{\beta}{2}\right]\sin\left[a - \frac{\alpha-\gamma}{2}\right] + \cos[b]\cos\left[\frac{\beta}{2}\right]\cos[\theta]\sin\left[\frac{\alpha+\gamma}{2}\right]\right)\mathrm{d}c$$
$$+ \sqrt{3}\cos\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\sin[2\theta]\mathrm{d}\phi,$$

$$\omega_R^6 = 2\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\mathrm{d}\theta + \frac{1}{2}\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\sin[2\theta]\mathrm{d}a$$
$$- \cos\left[\frac{\beta}{2}\right]\sin\left[a + \frac{\alpha+\gamma}{2}\right]\sin[\theta]\mathrm{d}b + \sin[\theta]\left(\cos\left[\frac{\beta}{2}\right]\cos\left[a + \frac{\alpha+\gamma}{2}\right]\sin[b]\right.$$
$$\left. + \cos[b]\cos[\theta]\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\right)\mathrm{d}c + \sqrt{3}\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\sin[2\theta]\mathrm{d}\phi,$$

$$\omega_R^7 = -2\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\mathrm{d}\theta + \frac{1}{2}\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\sin[2\theta]\mathrm{d}a$$
$$+ \cos\left[\frac{\beta}{2}\right]\cos\left[a + \frac{\alpha-\gamma}{2}\right]\sin[\theta]\mathrm{d}b + \sin[\theta]\left(\cos\left[\frac{\beta}{2}\right]\sin[b]\sin\left[a + \frac{\alpha+\gamma}{2}\right]\right.$$
$$\left. + \cos[b]\cos[\theta]\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\right)\mathrm{d}c + \sqrt{3}\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\sin[2\theta]\mathrm{d}\phi,$$

$$\omega_R^8 = -\frac{\sqrt{3}}{2}\sin^2[\theta]\mathrm{d}a - \frac{\sqrt{3}}{2}\cos[b]\sin^2[\theta]\mathrm{d}c + (2 - 3\sin^2[\theta])\mathrm{d}\phi.$$

3. The basis of the invariant vector fields on the SU(3) group

The expressions for the left-invariant vector fields basis in the Euler angles coordinate frame are given below

a. The left-invariant vector fields

$$X_1^L = \frac{\cos[c]}{\sin[b]}\frac{\partial}{\partial a} - \sin[c]\frac{\partial}{\partial b} - \cot[b]\cos[c]\frac{\partial}{\partial c},$$

$$X_2^L = \frac{\sin[c]}{\sin[b]}\frac{\partial}{\partial a} + \cos[c]\frac{\partial}{\partial b} - \cot[b]\sin[c]\frac{\partial}{\partial c},$$

$$X_3^L = \frac{\partial}{\partial c},$$

$$\begin{aligned}X_4^L = &-\frac{\sin\left[\frac{b}{2}\right]}{\sin[\beta]\sin[\theta]}\cos\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\alpha} + \frac{\sin\left[\frac{b}{2}\right]}{\sin[\theta]}\sin\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\beta}\\ &+\left(\frac{\sin\left[\frac{b}{2}\right]}{\sin[\theta]}\cot[\beta]\cos\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right] + \frac{2\cos\left[\frac{b}{2}\right]}{\sin[2\theta]}\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\right)\frac{\partial}{\partial\gamma}\\ &-\frac{1}{2}\cos\left[\frac{b}{2}\right]\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right] - \frac{1}{2}\left(\frac{\cot[\theta]}{\cos\left[\frac{b}{2}\right]} + \cos\left[\frac{b}{2}\right]\tan[\theta]\right)\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial a}\\ &+\cot[\theta]\sin\left[\frac{b}{2}\right]\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial b} - \frac{\cot[\theta]}{2\cos\left[\frac{b}{2}\right]}\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial c}\\ &+\frac{\sqrt{3}}{4}\cos\left[\frac{b}{2}\right]\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\tan[\theta]\frac{\partial}{\partial\phi},\end{aligned}$$

$$\begin{aligned}X_5^L = &\frac{\sin\left[\frac{b}{2}\right]}{\sin[\beta]\sin[\theta]}\sin\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\alpha} + \frac{\sin\left[\frac{b}{2}\right]}{\sin[\theta]}\cos\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\beta}\\ &+\left(\frac{\sin\left[\frac{b}{2}\right]}{\sin[\theta]}\cot[\beta]\sin\left[\frac{a-c}{2}+\gamma-\sqrt{3}\phi\right] - \frac{2\cos\left[\frac{b}{2}\right]}{\sin[2\theta]}\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\right)\frac{\partial}{\partial\gamma}\\ &+\frac{1}{2}\cos\left[\frac{b}{2}\right]\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial\theta} - \frac{1}{2}\left(\frac{\cot[\theta]}{\cos\left[\frac{b}{2}\right]} + \cos\left[\frac{b}{2}\right]\tan[\theta]\right)\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial a}\\ &-\cos\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\cot[\theta]\sin\left[\frac{b}{2}\right]\frac{\partial}{\partial b} - \frac{\cot[\theta]}{2\cos\left[\frac{b}{2}\right]}\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial c}\\ &+\frac{\sqrt{3}}{4}\cos\left[\frac{b}{2}\right]\sin\left[\frac{a+c}{2}+\sqrt{3}\phi\right]\tan[\theta]\frac{\partial}{\partial\phi},\end{aligned}$$

$$X_6^L = +\frac{\cos\left[\frac{b}{2}\right]}{\sin[\beta]\sin[\theta]}\cos\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\alpha}-\frac{\cos\left[\frac{b}{2}\right]}{\sin[\theta]}\sin\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\beta}$$
$$-\left(\frac{\cos\left[\frac{b}{2}\right]}{\sin[\theta]}\cot[\beta]\cos\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]-\frac{2\sin\left[\frac{b}{2}\right]}{\sin[2\theta]}\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\right)\frac{\partial}{\partial\gamma}$$
$$-\frac{1}{2}\sin\left[\frac{b}{2}\right]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial\theta}-\frac{1}{2}\left(\frac{\cot[\theta]}{\sin\left[\frac{b}{2}\right]}+\sin\left[\frac{b}{2}\right]\tan[\theta]\right)\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial a}$$
$$-\cos\left[\frac{b}{2}\right]\cot[\theta]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial b}+\frac{\cot[\theta]}{2\sin\left[\frac{b}{2}\right]}\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial c}$$
$$+\frac{\sqrt{3}}{4}\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_7^L = -\frac{\cos\left[\frac{b}{2}\right]}{\sin[\beta]\sin[\theta]}\sin\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\alpha}-\frac{\cos\left[\frac{b}{2}\right]}{\sin[\theta]}\cos\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]\frac{\partial}{\partial\beta}$$
$$+\left(\frac{\cos\left[\frac{b}{2}\right]}{\sin[\theta]}\cot[\beta]\sin\left[\frac{a+c}{2}+\gamma-\sqrt{3}\phi\right]+\frac{2\sin\left[\frac{b}{2}\right]}{\sin[2\theta]}\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\right)\frac{\partial}{\partial\gamma}$$
$$+\frac{1}{2}\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\sin\left[\frac{b}{2}\right]\frac{\partial}{\partial\theta}-\frac{1}{2}\left(\frac{\cot[\theta]}{\sin\left[\frac{b}{2}\right]}+\sin\left[\frac{b}{2}\right]\tan[\theta]\right)\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial a}$$
$$+\cos\left[\frac{b}{2}\right]\cos\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\cot[\theta]\frac{\partial}{\partial b}+\frac{\cot[\theta]}{2\sin\left[\frac{b}{2}\right]}\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\frac{\partial}{\partial c}$$
$$+\frac{\sqrt{3}}{4}\sin[b]\sin\left[\frac{a-c}{2}+\sqrt{3}\phi\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_8^L = \frac{1}{2}\frac{\partial}{\partial\phi}.$$

b. The right-invariant vector fields

$$X_1^R = \cos[\alpha]\cot[\beta]\frac{\partial}{\partial\alpha}+\sin[\alpha]\frac{\partial}{\partial\beta}-\frac{\cos[\alpha]}{\sin[\beta]}\frac{\partial}{\partial\gamma},$$

$$X_2^R = -\sin[\alpha]\cot[\beta]\frac{\partial}{\partial\alpha}+\cos[\alpha]\frac{\partial}{\partial\beta}+\frac{\sin[\alpha]}{\sin[\beta]}\frac{\partial}{\partial\gamma},$$

$$X_3^R = \frac{\partial}{\partial\alpha},$$

$$X_4^R = \frac{\cot[\theta]}{2\cos\left[\frac{\beta}{2}\right]}\cos\left[\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial\alpha} - \cot[\theta]\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial\beta} + \cos\left[\frac{\alpha+\gamma}{2}\right]\left(\frac{\cot[\theta]}{2\cos\left[\frac{\beta}{2}\right]}\right.$$
$$\left. - \cos\left[\frac{\beta}{2}\right]\tan[\theta]\right)\frac{\partial}{\partial\gamma} + \frac{1}{2}\cos\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial\theta} - \left(\frac{\cot[b]}{\sin[\theta]}\cos\left[a-\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\right.$$
$$\left. + \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[2\theta]}\cos\left[\frac{\alpha+\gamma}{2}\right](2-3\sin^2[\theta])\right)\frac{\partial}{\partial a} - \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[\theta]}\sin\left[a-\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial b}$$
$$+ \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[b]\sin[\theta]}\cos\left[a-\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial c} - \frac{\sqrt{3}}{4}\cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha+\gamma}{2}\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_5^R = -\frac{\cot[\theta]}{2\cos\left[\frac{\beta}{2}\right]}\sin\left[\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial\alpha} - \cos\left[\frac{\alpha+\gamma}{2}\right]\cot[\theta]\sin\left[\frac{\beta}{2}\right]\frac{\partial}{\partial\beta} - \sin\left[\frac{\alpha+\gamma}{2}\right]\left(\frac{\cot[\theta]}{2\cos\left[\frac{\beta}{2}\right]}\right.$$
$$\left. - \cos\left[\frac{\beta}{2}\right]\tan[\theta]\right)\frac{\partial}{\partial\gamma} + \frac{1}{2}\cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial\theta} - \left(\frac{\cot[b]}{\sin[\theta]}\sin\left[a-\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\right.$$
$$\left. - \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[2\theta]}\sin\left[\frac{\alpha+\gamma}{2}\right](2-3\sin^2[\theta])\right)\frac{\partial}{\partial a} + \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[\theta]}\cos\left[a-\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial b}$$
$$+ \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[b]\sin[\theta]}\sin\left[a-\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial c} + \frac{\sqrt{3}}{4}\cos\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha+\gamma}{2}\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_6^R = \frac{\cot[\theta]}{2\sin\left[\frac{\beta}{2}\right]}\cos\left[\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial\alpha} + \cos\left[\frac{\beta}{2}\right]\cot[\theta]\sin\left[\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial\beta} - \cos\left[\frac{\alpha-\gamma}{2}\right]$$
$$\times\left(\frac{\cot[\theta]}{2\sin\left[\frac{\beta}{2}\right]} - \sin\left[\frac{\beta}{2}\right]\tan[\theta]\right)\frac{\partial}{\partial\gamma} + \frac{1}{2}\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial\theta}$$
$$- \left(\frac{\cot[b]}{\sin[\theta]}\cos\left[a+\frac{\alpha+\gamma}{2}\right]\cos\left[\frac{\beta}{2}\right] - \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[2\theta]}\cos\left[\frac{\alpha-\gamma}{2}\right](2-3\sin^2[\theta])\right)\frac{\partial}{\partial a}$$
$$- \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[\theta]}\sin\left[a+\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial b} + \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[b]\sin[\theta]}\cos\left[a+\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial c}$$
$$+ \frac{\sqrt{3}}{4}\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_7^R = \frac{\cot[\theta]}{2\sin\left[\frac{\beta}{2}\right]}\sin\left[\frac{\alpha-\gamma}{2}\right]\frac{\partial}{\partial\alpha} - \cos\left[\frac{\beta}{2}\right]\cos\left[\frac{\alpha-\gamma}{2}\right]\cot[\theta]\frac{\partial}{\partial\beta} - \sin\left[\frac{\alpha-\gamma}{2}\right]\left(\frac{\cot[\theta]}{2\sin\left[\frac{\beta}{2}\right]}\right.$$

$$\left. - \sin\left[\frac{\beta}{2}\right]\tan[\theta]\right)\frac{\partial}{\partial\gamma} - \frac{1}{2}\cos\left[\frac{\alpha-\gamma}{2}\right]\sin\left[\frac{\beta}{2}\right]\frac{\partial}{\partial\theta} - \left(\frac{\cot[b]}{\sin[\theta]}\cos\left[\frac{\beta}{2}\right]\sin\left[a+\frac{\alpha+\gamma}{2}\right]\right.$$

$$\left. - \frac{\sin\left[\frac{\beta}{2}\right]}{\sin[2\theta]}\sin\left[\frac{\alpha-\gamma}{2}\right](2-3\sin^2[\theta])\right)\frac{\partial}{\partial a} + \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[\theta]}\cos\left[a+\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial b}$$

$$+ \frac{\cos\left[\frac{\beta}{2}\right]}{\sin[b]\sin[\theta]}\sin\left[a+\frac{\alpha+\gamma}{2}\right]\frac{\partial}{\partial c} + \frac{\sqrt{3}}{4}\sin\left[\frac{\beta}{2}\right]\sin\left[\frac{\alpha-\gamma}{2}\right]\tan[\theta]\frac{\partial}{\partial\phi},$$

$$X_8^R = \sqrt{3}\frac{\partial}{\partial\gamma} - \sqrt{3}\frac{\partial}{\partial a} + \frac{1}{2}\frac{\partial}{\partial\phi}.$$

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Nonequilibrium Glauber-type dynamics in continuum

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We construct the nonequilibrium Glauber dynamics as a Markov process in configuration space for an infinite particle system in continuum with a general class of initial distributions. This class we define in terms of correlation functions bounds and it is preserved during the Markov evolution we constructed. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2354589]

I. INTRODUCTION

The theory of stochastic lattice gases on the cubic lattice $\mathbb{Z}^d$, $d \in \mathbb{N}$ is one of the most important and well-developed areas in the theory of interacting particle systems. In the lattice gas model with spin space $S=\{0,1\}$, the configuration space is defined as $\mathcal{X}=\{0,1\}^{\mathbb{Z}^d}$. For a given $\sigma=\{\sigma(x)|x\in\mathbb{Z}^d\}\in\mathcal{X}$ we say that a lattice side $y\in\mathbb{Z}^d$ is free or occupied by a particle depending on $\sigma(y)=0$ or $\sigma(y)=1$, respectively.

In the Glauber-type stochastic dynamics of the lattice gas particles randomly disappear from occupied sites or appear at free places of the lattice. Obviously, this dynamics may be interpreted as a birth-and-death process on $\mathbb{Z}^d$. The generator of this dynamics is given by

$$(Lf)(\sigma)=\sum_{x\in\mathbb{Z}^d} a(x,\sigma)(\nabla_x f)(\sigma),$$

where

$$(\nabla_x f)(\sigma)=f(\sigma^x)-f(\sigma),$$

σ^x denoting the configuration σ in which the particle at site x has changed its spin value. The rate function $a(x,\sigma)$ is taken in such a way that an *a priori* given measure on $\mathcal{X}$ (say, a Gibbs measure for the Ising model) is a symmetrizing measure for the Glauber generator L, see, e.g., Ref. 17.

Let us consider a continuous particle system, i.e., a system of particles which can take any position in the Euclidean space $\mathbb{R}^d$. The configuration space Γ for such system is the set of all locally finite subsets $\gamma\subset\mathbb{R}^d$. An analog of the discussed lattice stochastic dynamics should be a process in which particles randomly appear and disappear in the space, i.e., a spatial birth-and-death process. The generator of such a process is informally given by the formula

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$$(LF)(\gamma) = \sum_{x \in \gamma} d(x,\gamma)(D_x^- F)(\gamma) + \int_{\mathbb{R}^d} b(x,\gamma)(D_x^+ F)(\gamma)\mathrm{d}x, \tag{1}$$

where

$$(D_x^- F)(\gamma) = F(\gamma \setminus x) - F(\gamma), \quad (D_x^+ F)(\gamma) = F(\gamma \cup x) - F(\gamma).$$

Here and in the following, for simplicity of notation, we just write x instead of $\{x\}$. The coefficient $d(x,\gamma)$ describes the rate at which the particle x of the configuration γ dies, while $b(x,\gamma)$ describes the rate at which, given the configuration γ, a new particle is born at x.

Spatial birth-and-death processes were first discussed by Preston in Ref. 19. Under some conditions on the birth and death rates, Preston proved the existence of such processes in a bounded domain in $\mathbb{R}^d$. Though the number of particles can be arbitrarily large in this case, the total number of particles remains finite at any moment of time. The study of the problem of construction of a spatial birth-and-death process in the infinite volume was initiated by Holley and Stroock in Ref. 5. In fact, in that paper, birth-and-death processes in bounded domains were analyzed in detail. Only in a very special case of nearest-neighbor birth-and-death processes on the real line was the existence of a corresponding process on the whole space proved and its properties were studied.

Glötzl[4] derived conditions on the coefficients $d(x,\gamma)$, $b(x,\gamma)$, under which the birth-and-death generators are symmetric in the space $\mathrm{L}^2(\mu)$, where μ is a given Gibbs measure. Such generators are natural to call Glauber dynamics generators (corresponding to the equilibrium state μ). However, the problem of the existence of such dynamics was left open. In Ref. 2, Bertini, Cancrini, and Cesi studied the problem of the existence of a spectral gap for the Glauber dynamics in a bounded domain in $\mathbb{R}^d$. Bertini *et al.* considered the Glauber dynamics with death coefficient $d(x,\gamma)=1$.

By using the theory of Dirichlet forms, an analog of the Glauber dynamics from Ref. 2, but on the whole space (thus, involving infinite configurations) and for quite general pair potentials, was constructed in Ref. 11. A general class of Glauber dynamics in continuum which admits a much wider family of birth and death rates (again in the framework of the Dirichlet forms theory) was considered in Ref. 12.

All papers mentioned deal with so-called equilibrium stochastic dynamics, which gives an existence result for almost all starting configurations with respect to the *a priori* given stationary measure. The latter means that we can start our Markov process with any initial measure which is absolutely continuous with respect to the symmetrizing one. In applications, however, we need to analyze the time development for different classes of initial states of the system. These states can be very far from the equilibrium ones and the equilibrium stochastic dynamics (coming from the Dirichlet forms method) is not enough for the construction of their evolution.

In the present paper we propose a construction of the nonequilibrium Glauber dynamics in continuum. Namely, we describe a set of initial distributions on Γ such that for any initial measure μ_0 from this class there exists a Markov process with considered Glauber generator $X_t^{\mu_0} \in \Gamma$ starting with μ_0. Moreover, the distribution μ_t of this process at the time $t>0$ is again in the same class of measures on Γ. Our construction is based on a general approach to the study of infinite particle dynamics using techniques of the harmonic analysis on configuration spaces developed in Ref. 8. More precisely, we start with the Kolmogorov equation corresponding to our Glauber dynamics. That is an evolutional equation on functions defined on the configuration space Γ which are called observables in the terminology of mathematical physics. An application of the combinatorial Fourier transform from Ref. 8 gives instead of this infinite dimensional evolution equation an infinite family of finite dimensional equations for so-called quasiobservables. This infinite system of equations admits a natural description in terms of a Fock-type structure. This structure is nothing but an L^1-Fock space with a fixed family of weight functions. Properly taking these weights we are able to apply perturbation techniques to the considered evolution equation in the L^1-Fock space and to construct a related semigroup. The dual semigroup gives then the time evolution of the correlation functions of the initial measure and due to a reconstruction theorem

from Ref.8 we can obtain an evolution of the initial measure. The latter solve the dual Kolmogorov equation and it is the main step in the construction of the nonequilibrium Glauber dynamics we are considering.

Let $\mathcal{M}_{\mathrm{corr}}$ be the class of probability measures on Γ whose correlation functions exist and satisfy Ruelle-type bound (the explicit description of this class of measures will be given in Sec. VI). Then, the main result of this paper can be formulated as follows

Theorem 1.1: *For any* $\mu \in \mathcal{M}_{\mathrm{corr}}$ *there exists a Markov process* $X_t^{\mu} \in \Gamma$ *with initial distribution* μ *associated with the generator* (1).

Note that the evolution of the correlation functions in the Glauber dynamics is described by a system of equations which give a dynamical version of the celebrated Kirkwood-Salsburg system of equations for an equilibrium state of the model. Solving this system we need to check a property of a positive definiteness for the solution in the sense of Refs. 1 and 8. This moment is usually outside of the attention in theoretical physics considerations of time evolutions for correlation functions. But this positive definiteness is a necessary (and together with a growth condition also sufficient) condition on correlation functions which relates them to a measure on Γ. Actually, the verification of this condition is one of the main difficulties in the above described approach.

II. GENERAL FACTS AND NOTATIONS

Let $\mathbb{R}^d$ be the d-dimensional Euclidean space. By $\mathcal{O}(\mathbb{R}^d)$, $\mathcal{B}(\mathbb{R}^d)$ we denote the family of all open and Borel sets, respectively. $\mathcal{O}_b(\mathbb{R}^d)$, $\mathcal{B}_b(\mathbb{R}^d)$ denote the system of all sets in $\mathcal{O}(\mathbb{R}^d)$, $\mathcal{B}(\mathbb{R}^d)$, respectively, which are bounded. The space of n-point configuration is

$$\Gamma_0^{(n)} = \Gamma_{0,\mathbb{R}^d}^{(n)} := \{\eta \subset \mathbb{R}^d \,|\, |\eta| = n\}, \quad n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\},$$

where $|A|$ denotes the cardinality of the set A. Analogously the space $\Gamma_{0,\Lambda}^{(n)}$ is defined for $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, which we denote for short by $\Gamma_{\Lambda}^{(n)}$.

For every $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ one can define a mapping $N_\Lambda : \Gamma_0^{(n)} \to \mathbb{N}_0$; $N_\Lambda(\eta) := |\eta \cap \Lambda|$. For short we write $\eta_\Lambda := \eta \cap \Lambda$. As a set, $\Gamma_0^{(n)}$ is equivalent to the symmetrization of

$$\widetilde{(\mathbb{R}^d)^n} = \{(x_1, \ldots, x_n) \in (\mathbb{R}^d)^n \,|\, x_k \neq x_l \quad \text{if } k \neq l\},$$

i.e., $\widetilde{(\mathbb{R}^d)^n}/S_n$, where S_n is the permutation group over $\{1, \ldots, n\}$. Hence $\Gamma_0^{(n)}$ inherits the structure of an $n \cdot d$-dimensional manifold. Applying this we can introduce a topology $\mathcal{O}(\Gamma_0^{(n)})$ on $\Gamma_0^{(n)}$. The corresponding Borel σ-algebra $\mathcal{B}(\Gamma_0^{(n)})$ coincides with $\sigma(N_\Lambda \,|\, \Lambda \in \mathcal{B}_b(\mathbb{R}^d))$.

The space of finite configurations

$$\Gamma_0 := \bigsqcup_{n \in \mathbb{N}_0} \Gamma_0^{(n)}$$

is equipped with the topology of disjoint union $\mathcal{O}(\Gamma_0)$. A set $B \in \mathcal{B}(\Gamma_0)$ (the corresponding Borel σ-algebra) is called bounded if there exists a $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ and an $N \in \mathbb{N}$ such that $B \subset \bigsqcup_{n=0}^{N} \Gamma_{\Lambda}^{(n)}$.

The configuration space

$$\Gamma := \{\gamma \subset \mathbb{R}^d \,|\, |\gamma \cap \Lambda| < \infty, \quad \text{for all } \Lambda \in \mathcal{B}_b(\mathbb{R}^d)\}$$

is equipped with the vague topology. The Borel σ-algebra $\mathcal{B}(\Gamma)$ is equal to the smallest σ-algebra for which all the mappings $N_\Lambda : \Gamma \to \mathbb{N}_0$, $N_\Lambda(\gamma) := |\gamma \cap \Lambda|$ are measurable, i.e.,

$$\mathcal{B}(\Lambda) = \sigma(N_\Lambda | \Lambda \in \mathcal{B}_b(\mathbb{R}^d))$$

and filtration on Γ given by

$$\mathcal{B}_\Lambda(\Gamma) := \sigma(N_{\Lambda'} | \Lambda' \in \mathcal{B}_b(\mathbb{R}^d), \Lambda' \subset \Lambda).$$

For every $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ one can define a projection $p_\Lambda : \Gamma \to \Gamma_\Lambda$,

$$p_\Lambda(\gamma) := \gamma_\Lambda$$

and with respect to this projection Γ is the projective limit of the spaces $\{\Gamma_\Lambda\}_{\Lambda \in \mathcal{B}_b(\mathbb{R}^d)}$.

In the sequel we will use the following classes of function: $\mathrm{L}^0(\Gamma_0)$ is the set of all measurable functions on Γ_0 and $\mathrm{L}^0_{\mathrm{ls}}(\Gamma_0)$ is the set of measurable functions which have additionally a local support, i.e., $G \in \mathrm{L}^0_{\mathrm{ls}}(\Gamma_0)$ if there exists $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ such that $G\restriction_{\Gamma_0 \setminus \Gamma_\Lambda} = 0$. $\mathrm{L}^0_{\mathrm{bs}}(\Gamma_0)$ denotes the class of measurable functions with bounded support, $B(\Gamma_0)$ the set of bounded measurable functions, and $B_{\mathrm{bs}}(\Gamma_0)$ the set of bounded functions with bounded support. For any $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, the class of functions $G \in B_{\mathrm{bs}}(\Gamma_0)$, whose support is a subset of Λ,will be denoted by $B^\Lambda_{\mathrm{bs}}(\Gamma_0)$. The class of continuous functions from $B^\Lambda_{\mathrm{bs}}(\Gamma_0)$ will be denoted by $CB^\Lambda_{\mathrm{bs}}(\Gamma_0)$.

On Γ we consider the set of a cylinder functions $\mathcal{F}\mathrm{L}^0(\Gamma)$, i.e., the set of all measurable functions $G \in \mathrm{L}^0(\Gamma)$ which are measurable with respect to $\mathcal{B}_\Lambda(\Gamma)$ for some $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$. These functions are characterized by the following relation: $F(\gamma) = F\restriction_{\Gamma_\Lambda}(\gamma_\Lambda)$.

Next we would like to describe some facts from harmonic analysis on configuration space based on Refs. 8 and 9.

The following mapping between functions on Γ_0, e.g., $\mathrm{L}^0_{\mathrm{ls}}(\Gamma_0)$, and functions on Γ, e.g., $\mathcal{F}L^0(\Gamma)$, plays a key role in our further considerations:

$$KG(\gamma) := \sum_{\xi \Subset \gamma} G(\xi), \quad \gamma \in \Gamma,$$

where $G \in \mathrm{L}^0_{\mathrm{ls}}(\Gamma_0)$, see, e.g., Refs. 15 and 16. The summation in the latter expression is extended over all finite subconfigurations of γ, in symbols $\xi \Subset \gamma$.

K is linear, positivity preserving, and invertible, with

$$K^{-1}F(\eta) := \sum_{\xi \subset \eta} (-1)^{|\eta \setminus \xi|} F(\xi), \quad \eta \in \Gamma_0. \tag{2}$$

It is easy to see that for all $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $F \in \mathcal{F}\mathrm{L}^0(\Gamma, \mathcal{B}_\Lambda(\Gamma))$,

$$K^{-1}F(\eta) = \mathbb{1}_{\Gamma_\Lambda}(\eta) K^{-1}F(\eta), \quad \forall\ \eta \in \Gamma_0. \tag{3}$$

One can introduce a convolution

$$\star : \mathrm{L}^0(\Gamma_0) \times \mathrm{L}^0(\Gamma_0) \to \mathrm{L}^0(\Gamma_0)$$

$$(G_1, G_2) \mapsto (G_1 \star G_2)(\eta) := \sum_{(\xi_1, \xi_2, \xi_3) \in \mathcal{P}^3_\emptyset(\eta)} G_1(\xi_1 \cup \xi_2) G_2(\xi_2 \cup \xi_3), \tag{4}$$

where $\mathcal{P}^3_\emptyset(\eta)$ denotes the set of all partitions (ξ_1, ξ_2, ξ_3) of η in three parts, i.e., all triples (ξ_1, ξ_2, ξ_3) with $\xi_i \subset \eta$, $\xi_i \cap \xi_j = \emptyset$ if $i \neq j$, and $\xi_1 \cup \xi_2 \cup \xi_3 = \eta$. It has the property that for $G_1, G_2 \in \mathrm{L}^0_{\mathrm{ls}}(\Gamma_0)$ we have $K(G_1 \star G_2) = KG_1 \cdot KG_2$. Due to this convolution we can interpret K transform as Fourier transform in configuration space analysis, see also Ref. 1.

Let $\mathcal{M}^1_{\mathrm{fm}}(\Gamma)$ be the set of all probability measures μ which have finite local moments of all orders, i.e., $\int_\Gamma |\gamma_\Lambda|^n \mu(\mathrm{d}\gamma) < +\infty$ for all $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ and $n \in \mathbb{N}_0$. A measure ρ on Γ_0 is called locally finite iff $\rho(A) < \infty$ for all bounded sets A from $\mathcal{B}(\Gamma_0)$, the set of such measures is denoted by $\mathcal{M}_{\mathrm{lf}}(\Gamma_0)$. One can define a transform $K^* : \mathcal{M}^1_{\mathrm{fm}}(\Gamma) \to \mathcal{M}_{\mathrm{lf}}(\Gamma_0)$, which is dual to the K-transform, i.e., for every $\mu \in \mathcal{M}^1_{\mathrm{fm}}(\Gamma)$, $G \in \mathcal{B}_{\mathrm{bs}}(\Gamma_0)$ we have

$$\int_\Gamma KG(\gamma) \mu(\mathrm{d}\gamma) = \int_{\Gamma_0} G(\eta) (K^*\mu)(\mathrm{d}\eta).$$

$\rho_\mu := K^*\mu$ we call the correlation measure corresponding to μ.

As shown in Ref. 8 for $\mu \in \mathcal{M}^1_{\mathrm{fm}}(\Gamma)$ and any $G \in \mathrm{L}^1(\Gamma_0, \rho_\mu)$ the series

$$KG(\gamma) := \sum_{\eta \Subset \gamma} G(\eta) \tag{5}$$

is μ-a.s. absolutely convergent. Furthermore, $KG \in \mathrm{L}^1(\Gamma, \mu)$ and

$$\int_{\Gamma_0} G(\eta)\rho_\mu(\mathrm{d}\eta) = \int_{\Gamma} (KG)(\gamma)\mu(\mathrm{d}\gamma). \tag{6}$$

Fix a nonatomic and locally finite measure σ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$. For any $n \in \mathbb{N}$ the product measure $\sigma^{\otimes n}$ can be considered by restriction as a measure on $\widetilde{(\mathbb{R}^d)^n}$ and hence on $\Gamma_0^{(n)}$. The measure on $\Gamma_0^{(n)}$ we denote by $\sigma^{(n)}$.

The *Lebesgue-Poisson measure* $\lambda_{z\sigma}$ on Γ_0 is defined as

$$\lambda_{z\sigma} := \sum_{n=0}^{\infty} \frac{z^n}{n!}\sigma^{(n)}.$$

Here $z > 0$ is the so-called activity parameter. The restriction of $\lambda_{z\sigma}$ to Γ_Λ will be also denoted by $\lambda_{z\sigma}$.

The *Poisson measure* $\pi_{z\sigma}$ on $(\Gamma, \mathcal{B}(\Gamma))$ is given as the projective limit of the family of measures $\{\pi_{z\sigma}^\Lambda\}_{\Lambda \in \mathcal{B}_b(\mathbb{R}^d)}$, where $\pi_{z\sigma}^\Lambda$ is the measure on Γ_Λ defined by $\pi_{z\sigma}^\Lambda := e^{-z\sigma(\Lambda)}\lambda_{z\sigma}$.

A measure $\mu \in \mathcal{M}_{\mathrm{fm}}^1(\Gamma)$ is called locally absolutely continuous with respect to $\pi_{z\sigma}$ iff $\mu_\Lambda := \mu \circ p_\Lambda^{-1}$ is absolutely continuous to $\pi_{z\sigma}^\Lambda = \pi_{z\sigma} \circ p_\Lambda^{-1}$ for all $\Lambda \in \mathcal{B}_\Lambda(\mathbb{R}^d)$. In this case $\rho_\mu := K^*\mu$ is absolutely with respect to $\lambda_{z\sigma}$. We denote by $k_\mu(\eta) := (\mathrm{d}\rho_\mu / \mathrm{d}\lambda_{z\sigma})(\eta)$, $\eta \in \Gamma_0$. For σ - Lebesgue measure on $\mathbb{R}^d$ we will write λ_z instead of $\lambda_{z\sigma}$.

The functions

$$k_\mu^{(n)} : (\mathbb{R}^d)^n \to \mathbb{R}_+,$$

$$k_\mu^{(n)}(x_1, \ldots, x_n) := \begin{cases} k_\mu(\{x_1, \ldots, x_n\}) & \text{if } (x_1, \ldots, x_n) \in \widetilde{(\mathbb{R}^d)^n} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

are well-known correlation functions of statistical physics, see, e.g. Refs. 22 and 21.

Let us now recall the so-called Minlos lemma which plays a very important role in our calculations (c.f. Ref. 13).

Lemma 2.1: *Let* $n \geqslant 2$, *and* $z > 0$ *be given. Then*

$$\int_{\Gamma_0} \cdots \int_{\Gamma_0} G(\eta_1 \cup \ldots \cup \eta_n) H(\eta_1, \ldots, \eta_n) \mathrm{d}\lambda_z(\eta_1) \cdots \mathrm{d}\lambda_z(\eta_n)$$
$$= \int_{\Gamma_0} G(\eta) \sum_{(\eta_1, \ldots, \eta_n) \in \mathcal{P}_n(\eta)} H(\eta_1, \ldots, \eta_n) \mathrm{d}\lambda_z(\eta)$$

for all measurable functions $G : \Gamma_0 \mapsto \mathbb{R}$ *and* $H : \Gamma_0 \times \ldots \times \Gamma_0 \mapsto \mathbb{R}$ *with respect to which both sides of the equality make sense. Here* $\mathcal{P}_n(\eta)$ *denotes the set of all partitions of* η *in n parts, which may be empty*.

III. POTENTIAL AND GIBBS MEASURES ON CONFIGURATION SPACES

A pair potential is a Borel, even function $\phi : \mathbb{R}^d \mapsto \mathbb{R} \cup \{+\infty\}$. We assume that ϕ satisfies the following conditions.

(**I**) (Integrability) For any $\beta > 0$,

$$C(\beta) := \int_{\mathbb{R}^d} |1 - \exp[-\beta\phi(x)]| \mathrm{d}x < \infty .$$

(**P**) (Positivity) $\phi(x) > 0$ for all $x \in \mathbb{R}^d$.

For $\gamma \in \Gamma$ and $x \in \mathbb{R}^d \setminus \gamma$, we define a relative energy of interaction as follows:

$$E(x,\gamma) := \begin{cases} \sum_{y\in\gamma} \phi(x-y) & \text{if } \sum_{y\in\gamma} |\phi(x-y)| < \infty \\ +\infty & \text{otherwise.} \end{cases}$$

The energy of configuration $\eta \in \Gamma_0$ or Hamiltonian $E^\phi: \Gamma_0 \to \mathbb{R} \cup \{+\infty\}$ which corresponds to potential ϕ is defined by

$$E^\phi(\eta) = \sum_{\{x,y\}\subset\eta} \phi(x-y), \eta \in \Gamma_0, |\eta| \geqslant 2.$$

The Hamiltonian $E^\phi_\Lambda: \Gamma_\Lambda \to \mathbb{R}$ for $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ which corresponds to potential ϕ is defined by

$$E^\phi_\Lambda(\eta) = \sum_{\{x,y\}\subset\eta} \phi(x-y), \eta \in \Gamma_\Lambda, |\eta| \geqslant 2.$$

For fixed ϕ we will write for short $E = E^\phi$ and $E_\Lambda = E^\phi_\Lambda$.

For given $\bar\gamma \in \Gamma$ define the interaction energy between $\eta \in \Gamma_\Lambda$ and $\bar\gamma_{\Lambda^c} = \bar\gamma \cap \Lambda^c$, $\Lambda^c = \mathbb{R}^d \setminus \Lambda$ as

$$W_\Lambda(\eta|\bar\gamma) = \sum_{x\in\eta, y\in\bar\gamma_{\Lambda^c}} \phi(x-y).$$

The interaction energy is said to be well-defined if for any $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $\eta \in \Gamma_\Lambda$ and $\bar\gamma \in \Gamma$ it is finite or $+\infty$.

For $\beta > 0$ we define

$$E_\Lambda(\eta|\bar\gamma) = E_\Lambda(\eta) + W_\Lambda(\eta|\bar\gamma)$$

and

$$Z_\Lambda(\bar\gamma) := \int_{\Gamma_\Lambda} \exp\{-\beta E_\Lambda(\eta|\bar\gamma)\} \lambda_z(\mathrm{d}\eta),$$

the so-called partition function.

Let $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $\beta > 0$ be arbitrary, and let $\bar\gamma \in \Gamma$. The finite volume Gibbs measure on the space Γ_Λ with boundary configuration $\bar\gamma$ is defined by

$$\mathrm{P}_{\Lambda,\bar\gamma}(\mathrm{d}\eta) = \frac{\exp\{-\beta E_\Lambda(\eta|\bar\gamma)\}}{Z_\Lambda(\bar\gamma)} \lambda_z(\mathrm{d}\eta).$$

When $\bar\gamma = \emptyset$, let $\mathrm{P}_{\Lambda,\emptyset}(\mathrm{d}\eta) =: \mathrm{P}_\Lambda(\mathrm{d}\eta)$.

Let $\{\pi_\Lambda\}$ denote the specification associated with z and the Hamiltonian E (see Ref. 18) which is defined by

$$\pi_{\Lambda,\bar\gamma}(A) = \int_{A'} \mathrm{P}_{\Lambda,\bar\gamma}(\mathrm{d}\eta),$$

where $A' = \{\eta \in \Gamma_\Lambda : \eta \cup (\bar\gamma_{\Lambda^c}) \in A\}$, $A \in \mathcal{B}(\Gamma)$ and $\bar\gamma \in \Gamma$.

A probability measure μ on Γ is called a Gibbs measure for E and z if

$$\mu(\pi_{\Lambda,\bar\gamma}(A)) = \mu(A)$$

for every $A \in \mathcal{B}(\Gamma)$ and every $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$.

This relation is the well-known (*DLR*)-equation (Dobrushin-Lanford-Ruelle equation), see Ref. 3 for more details.

The set of all Gibbs measures which corresponds to the potential ϕ, activity parameter $z>0$, and inverse temperature $\beta>0$ will be denoted by $\mathcal{G}(\phi,z,\beta)$. For fixed potential ϕ we will write $\mathcal{G}(z,\beta)$ instead of $\mathcal{G}(\phi,z,\beta)$.

Remark 3.1: *The set* $\mathcal{G}(\phi,z,\beta)$ *is nonempty for all* $z>0$, $\beta>0$ *and any potential* ϕ *satisfying* (**P**) *and* (**I**), *see Ref.* 14.

IV. GENERATORS: THE SYMBOL OF THE GLAUBER GENERATOR ON THE SPACE OF FINITE CONFIGURATIONS

We consider a Markov pregenerator on the configuration space Γ, the action of which is given by

$$(LF)(\gamma) := (L_{b,d}F)(\gamma) = \sum_{x\in\gamma} d(x,\gamma\setminus x)D_x^- F(\gamma) + \int_{\mathbb{R}^d} b(x,\gamma)D_x^+ F(\gamma)\mathrm{d}x,$$

where $D_x^- F(\gamma)=F(\gamma\setminus x)-F(\gamma)$ and $D_x^+ F(\gamma)=F(\gamma\cup x)-F(\gamma)$.

It is known that the Gibbs measure $\mu\in\mathcal{G}(z,\beta)$ is reversible with respect to the Markov process associated with the generator L (i.e., the operator L is symmetrical in $\mathrm{L}^2(\Gamma,\mu)$) iff the following condition on coefficients b and d (birth and death rates) holds:

$$b(x,\gamma) = ze^{-\beta E(x,\gamma)}d(x,\gamma). \tag{8}$$

In the sequel we will be interested only in particular cases of birth and death rates, which play an essential role in the study of some problems of mathematical physics:

$$b(x,\gamma) = ze^{-\beta E(x,\gamma)}, \quad d(x,\gamma) = 1.$$

Such model was investigated by many authors, see, e.g. Refs. 13 and 11. The corresponding Markov generator we denote by the same symbol L.

For technical reasons we will also be interested in the birth and death rates localized in some volume $\Lambda\in\mathcal{B}(\mathbb{R}^d)$. Namely,

$$b_\Lambda(x,\gamma) = z\mathbb{1}_\Lambda(x)e^{-\beta E(x,\gamma_\Lambda)}, \quad d_\Lambda(x,\gamma) = \mathbb{1}_\Lambda(x).$$

We denote the corresponding Markov generator by L_Λ.

In a recent paper,[13] the authors have shown that in the case of equilibrium Glauber dynamics with invariant measure $\mu\in\mathcal{G}(z,\beta)$, corresponding to the pair potential, the image of L under the K-transform (or symbol of the operator L) has the following form:

$$(\hat{L}G)(\eta) := (K^{-1}LKG)(\eta) = L_0G(\eta) + L_1G(\eta), \quad G\in B_{\mathrm{bs}}(\Gamma_0),$$

where

$$L_0G(\eta) := -|\eta|G(\eta)$$

and

$$L_1G(\eta) := z\sum_{\xi\subset\eta}\int_{\mathbb{R}^d} G(\xi\cup x)\prod_{y\in\eta\setminus\xi}(e^{-\beta\phi(x-y)}-1)\prod_{y'\in\xi}e^{-\beta\phi(x-y')}\mathrm{d}x.$$

Analogously, one can show that the symbol of L_Λ has form

$$(\widehat{L_\Lambda} G)(\eta) := (K^{-1} L_\Lambda K G)(\eta) = -|\eta_\Lambda| G(\eta) + z \sum_{\xi \subset \eta} \int_\Lambda G(\xi \cup x) \prod_{y \in \eta \setminus \xi} (e^{-\beta \phi(x-y) 1_\Lambda(y)} - 1) \times e^{-\beta E(x, \xi_\Lambda)} \mathrm{d}x, \quad G \in B_{\mathrm{bs}}(\Gamma_0).$$

V. CONSTRUCTION OF A SEMIGROUP OF THE SYMBOL

Let λ be the Lebesgue-Poisson measure on Γ_0 with activity parameter equal to 1. In the whole section we suppose that potential ϕ satisfies conditions (**P**) and (**I**).

For arbitrary and fixed $C>0$ and $\beta>0$, we consider operator $\hat{L}$ as a pregenerator of some nonequilibrium Markov process in the functional space

$$\mathcal{L}_{C,\beta} := \mathrm{L}^1(\Gamma_0, C^{|\eta|} e^{-\beta E(\eta)} \lambda(\mathrm{d}\eta)). \tag{9}$$

In this section, $\|\cdot\|$ stands for the norm of the space (9) and $\overset{s}{\to}$ denotes strong convergence in $\mathcal{L}_{C,\beta}$.

For any $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ we set

$$\mathcal{L}^\Lambda_{C,\beta} := \{G \in \mathcal{L}_{C,\beta} | \Gamma \restriction_{\Gamma_0 \setminus \Gamma_\Lambda} = 0\}. \tag{10}$$

It is not difficult to show that $\mathcal{L}^\Lambda_{C,\beta}$ is a closed linear subset in $(\mathcal{L}_{C,\beta}, \|\cdot\|)$. Therefore, $(\mathcal{L}^\Lambda_{C,\beta}, \|\cdot\|)$ is a subspace of $(\mathcal{L}_{C,\beta}, \|\cdot\|)$.

For any $\omega>0$ we introduce a set $\mathcal{H}(\omega,0)$ of all densely defined closed operators T on $\mathcal{L}_{C,\beta}$, the resolvent set $\rho(T)$ of which contains sector

$$\mathrm{Sect}\left(\frac{\pi}{2} + \omega\right) := \left\{\xi \in \mathbb{C} \middle| |\arg \zeta| < \frac{\pi}{2} + \omega\right\}, \quad \omega > 0$$

and for any $\varepsilon>0$,

$$\|(T - \zeta \mathbb{1})^{-1}\| \leqslant \frac{M_\varepsilon}{|\zeta|}, \quad |\arg \zeta| \leqslant \frac{\pi}{2} + \omega - \varepsilon,$$

where M_ε does not depend on ζ.

Let $\mathcal{H}(\omega, \theta)$, $\theta \in \mathbb{R}$ denote the set of all operators of the form $T = T_0 + \theta$ with $T_0 \in \mathcal{H}(\omega,0)$.

Remark 5.1: *It is well known (see e.g., Ref. 7), that any $T \in \mathcal{H}(\omega, \theta)$ is a generator of a semigroup $U(t)$ which is holomorphic in the sector $|\arg t| < \omega$. The function $U(t)$ is not necessary uniformly bounded, but it is quasibounded, i.e.*,

$$\|U(t)\| \leqslant \mathrm{const} |e^{\theta t}|$$

in any sector of the form $|\arg t| \leqslant \omega - \varepsilon$.

Proposition 5.1: *For any $C>0$ and $\beta>0$, the operator*

$$(L_0 G)(\eta) = -|\eta| G(\eta), \quad D(L_0) = \{G \in \mathcal{L}_{C,\beta} | |\eta| G(\eta) \in \mathcal{L}_{C,\beta}\}$$

is a generator of contraction semigroup on $\mathcal{L}_{C,\beta}$. Moreover, $L_0 \in \mathcal{H}(\omega,0)$, for all $\omega \in (0, \pi/2)$.

Proof: It is not difficult to show that L_0 is a densely defined and closed operator in $\mathcal{L}_{C,\beta}$.

Let $0 < \omega < \pi/2$ be arbitrary and fixed. It is clear that for all $\zeta \in \mathrm{Sect}(\pi/2 + \omega)$,

$$||\eta| + \zeta| > 0, \quad \eta \in \Gamma_0.$$

Therefore, for any $\zeta \in \mathrm{Sect}(\pi/2 + \omega)$ the inverse operator $(L_0 - \zeta \mathbb{1})^{-1}$, the action of which is given by

$$[(L_0-\zeta\mathbb{1})^{-1}G](\eta)=-\frac{1}{|\eta|+\zeta}G(\eta), \tag{11}$$

is well defined on the whole space $\mathcal{L}_{C,\beta}$. Moreover, it is bounded operator in this space and

$$\|(L_0-\zeta\mathbb{1})^{-1}\|\leqslant\begin{cases}\dfrac{1}{|\zeta|} & \text{if } \operatorname{Re}\zeta\geqslant 0\\[2ex] \dfrac{M}{|\zeta|} & \text{if } \operatorname{Re}\zeta<0,\end{cases} \tag{12}$$

where constant M does not depend on ζ.

The case $\operatorname{Re}\zeta\geqslant 0$ is a direct consequence of (11) and inequality

$$|\eta|+\operatorname{Re}\zeta\geqslant\operatorname{Re}\zeta\geqslant 0.$$

We prove now bound (12) in the case $\operatorname{Re}\zeta<0$. Using (11), we have

$$\|(L_0-\zeta\mathbb{1})^{-1}G\|=\left\|\frac{1}{||\cdot|+\zeta|}G(\cdot)\right\|=\frac{1}{|\zeta|}\left\|\frac{|\zeta|}{||\cdot|+\zeta|}G(\cdot)\right\|.$$

Since $\zeta\in\operatorname{Sect}(\pi/2+\omega)$,

$$|\operatorname{Im}\zeta|\geqslant|\zeta|\left|\sin\left(\frac{\pi}{2}+\omega\right)\right|=|\zeta|\cos\omega.$$

Hence,

$$\frac{|\zeta|}{||\eta|+\zeta|}\leqslant\frac{|\zeta|}{|\operatorname{Im}\zeta|}\leqslant\frac{1}{\cos\omega}=:M$$

and (12) is fulfilled.

The rest statement of the lemma now follows directly from the theorem of Hille-Yosida (see e.g., Ref. 7).

Let $\kappa>0$ be the parameter of the considered model.

We now consider the operator

$$(L_1G)(\eta)=(L_{1,\beta,\kappa}G)(\eta)=\kappa\sum_{\xi\subseteq\eta}\int_{\mathbb{R}^d}G(\xi\cup x)\prod_{y\in\eta\setminus\xi}(e^{-\beta\phi(x-y)}-1)e^{-\beta E(x,\xi)}\mathrm{d}x,\quad G\in D(L_1)$$

with domain $D(L_1):=D(L_0)$. The well-definiteness of this operator will be clear from the following lemma.

For the symbol of the operator L we will sometimes write $\widehat{L_{\beta,\kappa}}$ instead of $\hat{L}$ to stress the dependence of this operator on $\kappa>0$ and $\beta>0$.

Lemma 5.1: *For any* $\delta>0$ *there exists* $\kappa_0:=\kappa_0(\delta)>0$ *such that for all* $\kappa<\kappa_0$ *the following estimate holds*:

$$\|L_{1,\beta,\kappa}G\|\leqslant a\|L_0G\|+b\|G\|,\quad G\in D(L_0)=D(L_1), \tag{13}$$

with $a=a(\kappa)<\delta$ *and* $b=b(\kappa)<\delta$.

Proof: As 1 belongs to the resolvent set of L_0 we have

$$\|L_1(L_0-\mathbb{1})^{-1}G\|=\kappa\int_{\Gamma_0}|L_1(L_0-\mathbb{1})^{-1}G(\eta)|C^{|\eta|}e^{-\beta E(\eta)}\lambda(\mathrm{d}\eta). \tag{14}$$

Define

$$K(x,\eta) := \prod_{y\in\eta\setminus x} |e^{-\beta\phi(x-y)} - 1|,\ x \in \mathbb{R}^d, \quad \eta \in \Gamma_0,$$

then by modulus property (14) can be estimated by

$$\kappa \int_{\Gamma_0} \sum_{\xi\subseteq\eta} \int_{\mathbb{R}^d} \frac{|G(\xi\cup x)|}{|\xi\cup x|+1} K(x,\eta\setminus\xi) e^{-\beta E(x,\xi)} \mathrm{d}x C^{|\eta|} e^{-\beta E(\eta)} \lambda(\mathrm{d}\eta). \tag{15}$$

By the Minlos lemma, (15) is equal to

$$\kappa \int_{\Gamma_0}\int_{\Gamma_0}\int_{\mathbb{R}^d} \frac{|G(\xi\cup x)|}{|\xi\cup x|+1} K(x,\eta) e^{-\beta E(x,\xi)} \mathrm{d}x C^{|\eta\cup\xi|} e^{-\beta E(\eta\cup\xi)} \lambda(\mathrm{d}\xi)\lambda(\mathrm{d}\eta).$$

Using again the Minlos lemma we bound the latter expression by

$$\kappa \int_{\Gamma_0}\int_{\Gamma_0} \frac{|G(\xi)|}{|\xi|+1} \sum_{x\in\xi} K(x,\eta) e^{-\beta E(x,\xi\setminus x)} C^{|\eta\cup(\xi\setminus x)|} e^{-\beta E(\eta\cup(\xi\setminus x))} \lambda(\mathrm{d}\xi)\lambda(\mathrm{d}\eta).$$

Since

$$E(x,\xi\setminus x) = E(\xi) - E(\xi\setminus x)$$

and since positivity of ϕ implies

$$E(\eta\cup(\xi\setminus x)) - E(\xi\setminus x) \geqslant 0$$

we have

$$\begin{aligned}\|L_1(L_0-\mathbb{1})^{-1}G\| &\leqslant \kappa \int_{\Gamma_0} \frac{|G(\xi)|}{|\xi|+1} C^{|\xi|} e^{-\beta E(\xi)} \sum_{x\in\xi} \int_{\Gamma_0} K(x,\eta) C^{|\eta\cup(\xi\setminus x)|-|\xi|} \lambda(\mathrm{d}\eta)\lambda(\mathrm{d}\xi) \\ &\leqslant \kappa \int_{\Gamma_0} \frac{|G(\xi)|}{|\xi|+1} C^{|\xi|} e^{-\beta E(\xi)} \sum_{x\in\xi} \int_{\Gamma_0} K(x,\eta) C^{|\eta|-1} \lambda(\mathrm{d}\eta)\lambda(\mathrm{d}\xi).\end{aligned}$$

Finally,

$$\|L_1(L_0-1)^{-1}G\| \leqslant \kappa C^{-1} e^{C(\beta)C} \|G\|.$$

Therefore,

$$\|L_1 G\| \leqslant \kappa C^{-1} e^{C(\beta)C} \|(L_0-1)G\| \leqslant a\|L_0 G\| + b\|G\|,$$

where

$$a = b := \kappa C^{-1} e^{C(\beta)C}.$$

It is clear that taking

$$\kappa_0 = \delta C e^{-C(\beta)C}$$

we obtain that $a, b < \delta$. ■

Theorem 5.1: *For any $C>0$, and for all $\kappa,\beta>0$ which satisfy*

$$2\kappa \exp(C(\beta)C) < C, \tag{16}$$

the operator $\widehat{L_{\beta,\kappa}}$ a generator of a holomorphic semigroup in $\mathcal{L}_{C,\beta}$.

Proof: The statement of theorem follows directly from the theorem about perturbation of holomorphic semigroup (see, e.g. Ref. 7). For the reader's convenience, in the following we give its formulation:

for any $T \in \mathcal{H}(\omega,\theta)$ *and for any* $\varepsilon>0$ *there exists positive constants* ϵ, δ *such that if operator* A *satisfies*

$$\|Au\| \leqslant a\|Tu\| + b\|u\|, \quad u \in D(T) \subset D(A),$$

with $a<\delta, b<\delta$, *then* $T+A \in \mathcal{H}(\omega-\varepsilon,\epsilon)$.

In particular, if $\delta=0$ *and* $b=0$, *then* $T+A \in \mathcal{H}(\omega-\varepsilon,0)$. ■

Remark 5.2: *Due to Proposition* 5.1, *the operator* $L_0 \in \mathcal{H}(\omega,0)$, *for any* $\omega \in (0,\pi/2)$. *Since we are not interested yet in the domain of analyticity for the corresponding semigroup* (*which depends on* ω) *we consider* ω *close to* 0 *in order to get the best possible bound for the resolvent of* L_0. *Now, together with the proof of the theorem on holomorphic semigroups' perturbation* (*see, e.g., Ref.* 7), *one can conclude that the largest* δ *in this theorem applying to our case can be chosen to be* $\frac{1}{2}$.

For our further purposes we have to show that the holomorphic semigroup constructed in Theorem 5.1 can be approximated by the semigroups localized in bounded volumes.

Let $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ be arbitrary and fixed. Then all results proved in this section hold true for the operator $\widehat{L_\Lambda}$ acting in the functional space $\mathcal{L}^\Lambda_{C,\beta}$ with domain

$$D(\widehat{L_\Lambda}) := \{G \in \mathcal{L}_{C,\beta} \| \cdot_\Lambda | G(\cdot) \in \mathcal{L}^\Lambda_{C,\beta}\}.$$

Namely, the main result can be formulated as follows

Theorem 5.2: *For any* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, *and any triple of constants* $C,\kappa>0$, *and* $\beta>0$ *which satisfy*

$$2\kappa \exp(C(\beta)C) < C,$$

the operator $\widehat{L_\Lambda}$ *is a generator of a holomorphic semigroup in* $\mathcal{L}^\Lambda_{C,\beta}$.

Remark 5.3: *The arguments, analogous to those which were proposed in the proof of Lemma 5.1, imply the fulfilment of* (13) *for the operators*

$$\widehat{L_{0,\Lambda}} G(\eta) := -|\eta_\Lambda| G(\eta)$$

and

$$\widehat{L_{1,\Lambda}} G(\eta) := \kappa \sum_{\xi \subset \eta} \int_\Lambda G(\xi \cup x) \prod_{y \in \eta \setminus \xi} (e^{-\beta\phi(x-y)\mathbb{1}_\Lambda(y)} - 1) \prod_{y' \in \xi_\Lambda} e^{-\beta\phi(x-y')} \mathrm{d}x$$

with

$$D(\widehat{L_{0,\Lambda}}) = D(\widehat{L_{1,\Lambda}}) := \{G \in \mathcal{L}_{C,\beta} \| \cdot_\Lambda | G(\cdot) \in \mathcal{L}^\Lambda_{C,\beta}\}.$$

Moreover, bound (13) *in this case will be uniform with respect to the* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, *i.e., coefficients* $a>0$ *and* $b>0$ *in* (13) *can be chosen* Λ *independent.*

Fix any triple of positive constants C, κ, and β which satisfies (16) and any $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$.

Remark 5.4: *Let* $\widehat{U^\Lambda_t}(C,\beta,\kappa)$ *be holomorphic semigroup generated by operator* $(\widehat{L^\Lambda}, D(\widehat{L^\Lambda}))$ *on* $\mathcal{L}^\Lambda_{C,\beta}$. *Then* $\widehat{U^\Lambda_t}(C,\beta,\kappa)\circ P_\Lambda, t \geqslant 0$, *where*

$$P_\Lambda G(\eta) := \mathbb{1}_{\Gamma_\Lambda}(\eta) G(\eta), \quad G \in \mathcal{L}_{C,\beta}$$

is a semigroup on $\mathcal{L}_{C,\beta}$ *generated by the operator* $\widehat{L_\Lambda}\circ P_\Lambda$ *with domain*

$$D(\widehat{L_\Lambda}\circ P_\Lambda) := \{G \in \mathcal{L}_{C,\beta} \| \cdot_\Lambda | \mathbb{1}_{\Gamma_\Lambda}(\cdot) G(\cdot) \in \mathcal{L}_{C,\beta}\}.$$

Remark 5.5: *The theorem about perturbation of the generator of a holomorphic semigroup, mentioned before in this section* (*see also Ref.* 7), *implies that for any* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ *and* $\varepsilon>0$ *there*

exists $\epsilon>0$ *and constant* $M>0$ *which is not dependent on* Λ *such that for any* $\zeta>\epsilon$ *the following bound holds*:

$$\|(\widehat{L_\Lambda}\circ P_\Lambda-\zeta)^{-1}\|\leqslant\frac{M_\varepsilon}{|\zeta-\epsilon|},\quad |\arg(\zeta-\epsilon)|\leqslant\frac{\pi}{2}+\omega-\varepsilon.$$

Let $\{\Lambda_n\}_{n\geqslant 1}$ be a sequence of Borel sets such that $\Lambda_n\subset\Lambda_{n+1}$, for all $n\in\mathbb{N}$, and $\cup_{n\geqslant 1}\Lambda_n=\mathbb{R}^d$. Now, we formulate the following approximation theorem.

Theorem 5.3: *Let* $\hat{U}_t(C,\beta,\kappa)$ *and* $\{\widehat{U_t^{\Lambda_n}}(C,\beta,\kappa),n\geqslant 1\}$ *be holomorphic semigroups generated by* $\widehat{L_{\beta,\kappa}}$ *and* $\{\widehat{L_{\Lambda_n,\beta,\kappa}},n\geqslant 1\}$ *in the spaces* $\mathcal{L}_{C,\beta}$ *and* $\mathcal{L}^\Lambda_{C,\beta}$, *respectively. Then*,

$$\widehat{U_t^{\Lambda_n}}(C,\beta,\kappa)\circ P_{\Lambda_n}\overset{s}{\to}\hat{U}_t(C,\beta,\kappa),\quad n\to\infty$$

uniformly on any finite interval of $t\geqslant 0$.

Proof: Using approximation theorem for quasibounded semigroups (see, e.g., Ref. 7), it is enough to show that

$$(\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}-\zeta)^{-1}\overset{s}{\to}(\widehat{L_{\beta,\kappa}}-\zeta)^{-1}$$

for some $\zeta\in\mathbb{C}$ such that $\operatorname{Re}\zeta>\theta$.

Let $\zeta\in\mathbb{C}$, $\operatorname{Re}\zeta>\theta$ be arbitrary and fixed. For any $G\in\mathcal{L}_{C,\beta}$ it holds

$$\|(\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}-\zeta)^{-1}G-(\widehat{L_{\beta,\kappa}}-\zeta)^{-1}G\|=\|(\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}-\zeta)^{-1}[\widehat{L_{\beta,\kappa}}-\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}](\widehat{L_{\beta,\kappa}}-\zeta)^{-1}G\|. \tag{17}$$

For any $G\in D(\widehat{L_{\beta,\kappa}})=D(L_0)$,

$$\begin{aligned}[\widehat{L_{\beta,\kappa}}-\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}]G(\eta)=&-|\eta|[1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\eta)]G(\eta)+\kappa\sum_{\xi\subseteq\eta}\int_{\Lambda_n^c}G(\xi\cup x)\prod_{y\in\eta\setminus\xi}[e^{-\beta\phi(x-y)}-1]\\&\times\prod_{y'\in\xi}e^{-\beta\phi(x-y')}\mathrm{d}x+\kappa\sum_{\xi\subseteq\eta}\int_{\Lambda_n}G(\xi\cup x)\prod_{y\in\eta\setminus\xi}[e^{-\beta\phi(x-y)}-1]e^{-\beta E(x,\xi)}\\&\times[1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\xi\cup x)\mathbb{1}_{\Gamma_{\Lambda_n}}(\eta\setminus\xi)e^{\beta E(x,\xi_{\Lambda_n^c})}]\mathrm{d}x,\end{aligned}$$

where $\Lambda_n^c=\mathbb{R}^d\setminus\Lambda_n$.

Using the fact that for any $\xi\in\Gamma_0$ and $x\in\mathbb{R}^d$,

$$\mathbb{1}_{\Gamma_{\Lambda_n}}(\xi\cup x)e^{\beta E(x,\xi_{\Lambda_n^c})}=\mathbb{1}_{\Gamma_{\Lambda_n}}(\xi\cup x),$$

the simple inequality

$$|1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\xi)\mathbb{1}_{\Gamma_{\Lambda_n}}(\eta)|\leqslant|1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\xi)|+|1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\eta)|,\quad \xi,\eta\in\Gamma_0,$$

and estimates analogous to those which were proposed in Lemma 5.1 we obtain

$$\begin{aligned}\|[\widehat{L_{\beta,\kappa}}-\widehat{L_{\Lambda_n,\beta,\kappa}}\circ P_{\Lambda_n}]G(\eta)\|\leqslant&(1+\kappa\max\{1,C^{-1}\}e^{C(\beta)C})\|[1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\cdot)]\|\cdot|G(\cdot)\|\\&+\kappa\max\{1,C^{-1}\}e^{C(\beta)C}\|\cdot_{\Lambda_n^c}|G(\cdot)\|+\max\{1,C^{-1}\}\|\cdot_{\Lambda_n}|G(\cdot)\|\\&\times\int_{\Gamma_{\Lambda_n}}|1-\mathbb{1}_{\Gamma_{\Lambda_n}}(\eta)|K(0,\eta)C^{|\eta|}\lambda(\mathrm{d}\eta).\end{aligned}$$

All of the summands on the right-hand side of the last inequality definitely tend to zero, when $n \to \infty$.

Using Remark 5.5 and equality (17) we easily conclude that difference in (17) also tends to zero when $n \to \infty$. ■

VI. CONSTRUCTION OF A NONEQUILIBRIUM MARKOV PROCESS

Fix any triple of positive constants C, κ, and β which satisfies (16). Let $\hat{U}_t(C,\beta,\kappa)$ be holomorphic semigroup generated by $\widehat{L_{\beta,\kappa}}$ and let

$$\mathcal{K}_{C,\beta} := \{k:\Gamma_0 \to \mathbb{R}_+ |\ k(\cdot)C^{-|\cdot|}e^{\beta E(\cdot)} \in \mathrm{L}^\infty(\Gamma_0,\lambda)\} \tag{18}$$

be the set of "so-called correlation functions." Note that $\mathcal{K}_{C,\beta}$ is a Banach space.

We introduce the following duality between quasiobservables $G \in \mathcal{L}_{C,\beta}$ and functions $k \in \mathcal{K}_{C,\beta}$,

$$\langle\langle G,k\rangle\rangle := \langle G,k\rangle_{\mathrm{L}^2(\Gamma_0,\lambda)}. \tag{19}$$

Let us mention that $G \in \mathcal{L}_{C,\beta}$ means that $G(\cdot)C^{|\cdot|}e^{-\beta E(\cdot)} \in \mathrm{L}^1(\Gamma_0,\lambda)$. Therefore, the duality

$$\langle G,k\rangle_{\mathrm{L}^2(\Gamma_0,\lambda)} = \int_{\Gamma_0} G(\eta)C^{|\eta|}e^{-\beta E(\eta)}k(\eta)C^{-|\eta|}e^{\beta E(\eta)}\mathrm{d}\lambda(\eta) < \infty$$

is well-defined.

Note also that $k(\cdot)C^{-|\cdot|}e^{\beta E(\cdot)} \in \mathrm{L}^\infty(\Gamma_0,\lambda)$ means that function k satisfies the following bound

$$k(\eta) \leqslant \mathrm{const}\ C^{|\eta|}e^{-\beta E(\eta)}, \tag{20}$$

which is known as *generalized Ruelle bound*, see, e.g., Ref. 10.

Using duality (19) one can easily show that semigroup $\hat{U}_t(C,\beta,\kappa)$ determines corresponding semigroup $\widehat{U_t^\star}(C,\beta,\kappa)$ on $\mathcal{K}_{C,\beta}$.

Next, we solve the following problem: suppose that $k_0 \in \mathcal{K}_{C,\beta}$ is a correlation function which means that there exists a probability measure $\mu_0 \in \mathcal{M}^1_{\mathrm{fm}}(\Gamma)$, locally absolutely continuous with respect to Poisson measure, whose correlation function is exactly k_0. Does evolution of k_0 with respect to the semigroup $\widehat{U_t^\star}(C,\beta,\kappa)$ preserve the above-described property? Namely, will $\widehat{U_t^\star}(C,\beta,\kappa)k_0$, for any moment of time $t>0$, be a correlation function or not?

In order to answer this problem, one can apply, for example, the theorem about characterization of correlation functions, proposed in Ref. 8. In the model under consideration, the conditions of this theorem, which must to be checked are the following:

$$\textit{for any } t \geqslant 0\text{: } \langle\langle G \star G, \widehat{U_t^\star}(C,\beta,\kappa)k_0\rangle\rangle \geqslant 0, \quad \forall\, G \in B_{\mathrm{bs}}(\Gamma_0).$$

Further explanations will be devoted to verifying the latter condition.

Let $\mu \in \mathcal{G}(\beta,z)$ and $\{\pi_{\Lambda,\varnothing}\}_{\Lambda \in \mathcal{B}_b(\mathbb{R}^d)}$ denote the specification with empty boundary conditions corresponding to the Gibbs measure μ. We define

$$\mathcal{E}(F,G) := \int_\Gamma \sum_{x \in \gamma} D_x^- F(\gamma) D_x^- G(\gamma)\pi_\Lambda(\mathrm{d}\gamma, \varnothing), \quad F,G \in KCB^\Lambda_{\mathrm{bs}}(\Gamma_0),$$

where $KCB^\Lambda_{\mathrm{bs}}(\Gamma_0)$ is K-image of $CB^\Lambda_{\mathrm{bs}}(\Gamma_0)$.

Now we would like to list some facts the proofs of which are completely analogous to those proposed in Ref. 11.

Lemma 6.1: *The set* $KCB^\Lambda_{\mathrm{bs}}(\Gamma_0)$ *is dense in* $\mathrm{L}^2(\Gamma,\pi_{\Lambda,\varnothing})$ *for any* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$.

Lemma 6.2: *Let* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ *be arbitrary and fixed. Then* $(\mathcal{E}, KCB^\Lambda_{\mathrm{bs}}(\Gamma_0))$ *is a well-defined bilinear form on* $\mathrm{L}^2(\Gamma,\pi_{\Lambda,\varnothing})$.

Lemma 6.3: *Let* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ *be arbitrary and fixed. Suppose that conditions* (**I**) *and* (**P**) *are satisfied. Then* $(L_\Lambda, KCB^\Lambda_{\rm bs}(\Gamma_0))$ *is an operator associated with bilinear form* $(\mathcal{E}, KCB^\Lambda_{\rm bs}(\Gamma_0))$ *in* $\mathrm{L}^2(\Gamma, \pi_{\Lambda,\varnothing})$, *i.e.*,

$$\mathcal{E}(F,G) = \int_\Gamma L_\Lambda F(\gamma) G(\gamma)\, \pi_{\Lambda,\varnothing}(\mathrm{d}\gamma), \quad F,G \in KCB^\Lambda_{\rm bs}(\Gamma_0).$$

Lemma 6.4: *Let* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ *be arbitrary and fixed. Suppose that conditions* (**I**) *and* (**P**) *are satisfied and* $\mu \in \mathcal{G}(z,\beta)$. *Then there exists a self-adjoint positive Friedrichs' extension* $(\widetilde{L_\Lambda}, D(\widetilde{L_\Lambda}))$ *of the operator* $(L_\Lambda, KCB^\Lambda_{\rm bs}(\Gamma_0))$ *in* $\mathrm{L}^2(\Gamma, \pi_{\Lambda,\varnothing})$. *Moreover*, $(\widetilde{L_\Lambda}, D(\widetilde{L_\Lambda}))$ *is a generator of a contraction semigroup which preserves* 1 *in* $\mathrm{L}^2(\Gamma, \pi_{\Lambda,\varnothing})$, *associated with some Markov process*.

Remark 6.1: *It is well known* (*see, e.g., Ref.* 20) *that under condition of Lemma 6.4 the semigroup generated by* $(\widetilde{L_\Lambda}, D(\widetilde{L_\Lambda}))$ *can be extended to the* $\mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing})$. *For any* $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, *the extension of this semigroup in* $\mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing})$ *we will denote by* $(\widetilde{U^\Lambda_t})_{t\geqslant 0}$. *For the generator of this semigroup we will use notation* $(\widetilde{L_\Lambda}, D_1(\widetilde{L_\Lambda}))$, *where* $D_1(\widetilde{L_\Lambda}) \supset D(\widetilde{L_\Lambda})$ *is a domain of* $\widetilde{L_\Lambda}$ in $\mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing})$.

Now, we introduce one of the crucial lemmas about the evolution of the "so-called correlation function."

Lemma 6.5: *Let positive constants* C, κ, *and* β *which satisfy* (16) *be arbitrary and fixed. The semigroup* $\widehat{U^\star_t}(C,\beta,\kappa)$ *on* $\mathcal{K}_{C,\beta}$ *preserves positive semidefiniteness*, *i.e.*, *for any* $t \geqslant 0$,

$$\langle\langle G \star G, \widehat{U^\star_t}(C,\beta,\kappa) k\rangle\rangle \geqslant 0, \quad \forall\, G \in B_{\rm rs}(\Gamma_0)$$

iff

$$\langle\langle G \star G, k\rangle\rangle \geqslant 0, \tag{21}$$

for any $G \in B_{\rm bs}(\Gamma_0)$.

Remark 6.2: *Let* $\mathcal{M}_{C,\beta}$ *stand for the set of all probability measures on* Γ, *locally absolutely continuous with respect to Poisson measure*, *with locally finite moments*, *whose correlation functions satisfy bound* (20). *As it was pointed out at the beginning of this section*, *condition* (21) *on function* $k \in \mathcal{K}_{C,\beta}$, *ensures the existence of a unique measure* $\mu^k \in \mathcal{M}_{C,\beta}$ *whose correlation function is* k, *see Ref.* 8.

Proof of Lemma 6.5: Under assumptions of the lemma we have to show that for any $t \geqslant 0$,

$$\langle\langle \hat{U}_t(C,\beta,\kappa)(G \star G), k\rangle\rangle \geqslant 0, \quad \forall\, G \in B_{\rm bs}(\Gamma_0). \tag{22}$$

But $G \star G \in B_{\rm bs}(\Gamma_0)$ for any $G \in B_{\rm bs}(\Gamma_0)$. Therefore, due to Theorem 5.3 it is enough to show that for any $t \geqslant 0$ and any $G \in B_{\rm bs}(\Gamma_0)$ there exists $\Lambda' \in \mathcal{B}_b(\mathbb{R}^d)$ such that for all $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $\Lambda \supset \Lambda'$,

$$\langle\langle \widehat{U^\Lambda_t}(C,\beta,\kappa) \circ P_\Lambda(G \star G), k\rangle\rangle \geqslant 0. \tag{23}$$

Let $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$ be arbitrary and fixed. We set

$$U^\Lambda_t := K \widehat{U^\Lambda_t}(C,\beta,\kappa) K^{-1}, \quad t \geqslant 0.$$

$(U^\Lambda_t)_{t\geqslant 0}$ is a semigroup on

$$\left(\mathcal{L}^\Lambda_1 := K\mathcal{L}^\Lambda_{C,\beta}, \|\cdot\|_1 := \left\|K^{-1}\cdot\right\|_{\mathcal{L}_{C,\beta}}\right),$$

which is the Banach space. Moreover, it is not difficult to show that a generator of this semigroup coincides with $(L_\Lambda, KD(\widehat{L_\Lambda}))$.

Proposition 6.1: *For any* $F \in \mathcal{L}_1^\Lambda \subset \mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing})$,

$$U_t^\Lambda F = \widetilde{U_t^\Lambda} F, \quad t \geqslant 0 \text{ in } \mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing}).$$

Proof: The fact that $(L_\Lambda, KD(\widehat{L_\Lambda})$ is a generator of $(U_t^\Lambda)_{t\geqslant 0}$ in $(\mathcal{L}_1^\Lambda, \|\cdot\|_1)$ means the following (see, e.g., Ref. 6)

$$\left\| U_t^\Lambda F - \left(1 - \frac{t}{n} L_\Lambda\right)^{-n} F \right\|_1 \to 0, \quad n \to \infty \quad \text{for all } F \in \mathcal{L}_1^\Lambda.$$

Because $\|\cdot\|_1 \geqslant \|\cdot\|$, the latter fact implies

$$\left\| U_t^\Lambda F - \left(1 - \frac{t}{n} L_\Lambda\right)^{-n} F \right\| \to 0, \quad n \to \infty \quad \text{for all } F \in \mathcal{L}_1^\Lambda. \tag{24}$$

Analogously, the fact that $(\widetilde{L_\Lambda}, D_1(\widetilde{L_\Lambda}))$ is a generator of $(\widetilde{U_t^\Lambda})_{t\geqslant 0}$ gives us

$$\left\| \widetilde{U_t^\Lambda} F - \left(1 - \frac{t}{n} \widetilde{L_\Lambda}\right)^{-n} F \right\| \to 0, \quad n \to \infty \quad \text{for all } F \in \mathcal{L}_1^\Lambda. \tag{25}$$

As was shown before, there exists $\epsilon > 0$ such that for any real $\zeta > \varepsilon$ and any $F \in \mathcal{L}_1^\Lambda$,

$$(\widetilde{L_\Lambda} - \zeta 1)^{-1} F - (L_\Lambda - \zeta 1)^{-1} F = (\widetilde{L_\Lambda} - \zeta 1)^{-1} [L_\Lambda - \widetilde{L_\Lambda}](L_\Lambda - \zeta 1)^{-1} F.$$

The function $F_\zeta := (L_\Lambda - \zeta 1)^{-1} F \in KD(\widetilde{L_\Lambda})$. Hence, $[L_\Lambda - \widetilde{L_\Lambda}] F_\zeta = 0$. The latter fact means that

$$\left\| \widetilde{U_t^\Lambda} F - \left(1 - \frac{t}{n} \widetilde{L_\Lambda}\right)^{-n} F \right\| = \left\| \widetilde{U_t^\Lambda} F - \left(1 - \frac{t}{n} L_\Lambda\right)^{-n} F \right\| \to 0, \quad n \to \infty \quad \text{for all } F \in \mathcal{L}_1^\Lambda. \tag{26}$$

The convergence (24) and (25) imply the assertion of the proposition. ■

Corollary 6.1: *Lemma* 6.4 *implies that for any moment of time* $t \geqslant 0$,

$$U_t^\Lambda F \geqslant 0 \quad \textit{for all } F \geqslant 0 \text{ in } \mathrm{L}^1(\Gamma, \pi_{\Lambda,\varnothing}). \tag{27}$$

Let $t \geqslant 0$ and $G \in B_{\mathrm{bs}}(\Gamma_0)$ be arbitrary and fixed. Suppose that $N' \in \mathbb{N}$ and $\Lambda' \in \mathcal{B}_b(\mathbb{R}^d)$ are such that

$$G \star G \restriction_{\Gamma_0 \setminus \sqcup_{n=0}^{N'} \Gamma_{\Lambda'}^{(n)}} = 0.$$

Then, $K(G \star G) = |KG|^2 \in \mathcal{L}_1^\Lambda$ for all $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $\Lambda \subset \Lambda'$. Moreover, $P_\Lambda |KG|^2 = |KG|^2$.

Hence, the left-hand side of (23) for any $\Lambda \in \mathcal{B}_b(\mathbb{R}^d)$, $\Lambda \supset \Lambda'$ is equal to the following expression:

$$\langle\langle \widehat{U_t^\Lambda}(C, \beta, \kappa) \circ P_\Lambda (G \star G), k \rangle\rangle = \int_\Gamma K \widehat{U_t^\Lambda}(G \star G)(\gamma) \mu^k(\mathrm{d}\gamma) = \int_\Gamma U_t^\Lambda K(G \star G)(\gamma) \mu^k(\mathrm{d}\gamma)$$

$$= \int_{\Gamma_\Lambda} U_t^\Lambda |KG|^2(\gamma) \mu_\Lambda^k(\mathrm{d}\gamma),$$

where μ_Λ^k is a projection of μ^k on Γ_Λ. Let us mention that measure μ^k is locally absolutely continuous with respect to Poisson measure π. Therefore,

$$\langle\langle \widehat{U_t^\Lambda}(C, \beta, \kappa) \circ P_\Lambda (G \star G), k \rangle\rangle = \int_{\Gamma_\Lambda} U_t^\Lambda |KG|^2(\gamma) \frac{\mathrm{d}\mu_\Lambda^k}{\mathrm{d}\pi_\Lambda}(\gamma) \pi_\Lambda(\mathrm{d}\eta).$$

Corollary 6.1 implies that there exist set $S \subset \Gamma$, $\pi_{\Lambda,\varnothing}(S) = 0$ such that for all $\gamma \in \Gamma \setminus S$:

$$U_t^{\Lambda}|KG|^2(\gamma) \geqslant 0.$$

But $\pi_{\Lambda,\varnothing}$ is absolutely continuous with respect to π_Λ. Furthermore, the corresponding Radon-Nikodim derivative is positive almost surely with respect to π_Λ. Hence, $\pi_\Lambda(S_\Lambda)=0$, where S_Λ is a projection of the set S to Γ_Λ, and

$$\langle\langle \widehat{U_t^{\Lambda}}(C,\beta,\kappa)\circ P_\Lambda(G\star G),k\rangle\rangle = \int_{\Gamma_\Lambda\setminus S_\Lambda} U_t^{\Lambda}|KG|^2(\gamma)\frac{\mathrm{d}\mu_\Lambda^k}{\mathrm{d}\pi_\Lambda}(\gamma)\pi_\Lambda(\mathrm{d}\eta) \geqslant 0.$$

The latter proof the assertion of Lemma 6.5. ■

The result obtained in Lemma 6.5 and the fact about characterization of correlation functions from Ref. 8 imply the following corollary.

Corollary 6.2: *Let positive constants C, κ, and β which satisfy (16) be arbitrary and fixed. Let $k\in\mathcal{K}_{C,\beta}$ be such that $\langle\langle G\star G,k\rangle\rangle\geqslant 0$, for any $G\in B_{\mathrm{bs}}(\Gamma_0)$. Then for any $t\geqslant 0$ there exists unique measure $\mu_t\in\mathcal{M}_{C,\beta}$ whose correlation function is $\widehat{U_t^{\star}}(C,\beta,\kappa)k$.*

Let us denote in Corollary 6.2 the evolution of the measure μ in time by $U_t^{\star}(C,\beta,\kappa)\mu := \mu_t$. One can easily show that $(U_t^{\star}(C,\beta,\kappa))_{t\geqslant 0}$ is a semigroup on $\mathcal{M}_{C,\beta}$. This leads us directly to the construction of the nonequilibrium Markov process (or rather Markov function) on Γ.

Theorem 6.1 *Suppose that conditions* (**I**) *and* (**P**) *are satisfied. For any triple of positive constants C, κ, and β which satisfy (16) and any $\mu\in\mathcal{M}_{C,\beta}$ there exists Markov process $X_t^{\mu}\in\Gamma$ with initial distribution μ associated with generator $L_{\beta,\kappa}$.*

Proof: Let $n\in\mathbb{N}$, functions $0\leqslant F_0,F_1,\ldots,F_n\in \mathrm{L}^{\infty}(\Gamma)$ and moments of time $0\leqslant t_0\leqslant t_1\leqslant t_1\cdots\leqslant t_n$ be any and fixed. Then there exists a process, defined on some probability space $(\Omega,\mathcal{F},P)$, the finite-dimensional distribution of which is given by the following formula:

$$\int_\Omega F_0(X_{t_0}^{\mu})\ldots F_n(X_{t_n}^{\mu})\mathrm{d}P := \int_\Gamma \mathrm{d}F_n\ldots U_{t_1-t_0}^{*}(C,\kappa,\eta)(F_0\mu).$$

Eventually, we have constructed the nonequilibrium Markov process. ■

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Distant perturbation asymptotics in window-coupled waveguides. I. The nonthreshold case

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We consider a pair of straight adjacent quantum waveguides of constant, and in general different widths. These waveguides are coupled laterally by a pair of windows in the common boundary, not necessarily of the same length, at a distance $2l$. The Hamiltonian is the respective Dirichlet Laplacian. We analyze the asymptotic behavior of the discrete spectrum as the window distance tends to infinity for the generic case, i.e., for eigenvalues of the corresponding one-window problems separated from the threshold. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Quantum mechanics exhibits various effects which defy our intuition based on "classical" experience. A nice class of examples are bound states in hard-wall tubes induced solely by their geometric properties such as bends, protrusions, or "windows." Such systems are interesting not only *per se* but also from the practical point of view as models of various nanophysical devices, and in a reasonable approximation also of flat electromagnetic waveguides.

Among numerous questions such models pose, an important one concerns behavior of the spectra in the case of two distant perturbations. One can think of it as an analog of the exponential spectral shift for a pair of distant potential wells, despite the fact that the usual methods of the Schrödinger operator theory do not work here. The aim of the present paper is to study this problem in a model example of a pair of laterally coupled waveguides, or adjacent straight hard-wall strips in the plane, coupled by a pair of windows in the common boundary—we refer to Refs. 1–3 for a bibliography concerning such models. We concentrate mostly on the investigation of isolated eigenvalues of the considered system.

In our recent paper[2] we dealt with the symmetric situation where the widths d_1, d_2 of the two channels were the same and so were the window widths a_1, a_2. The technique used in this paper substantially employed the fact that the problem can be decomposed into parts with a definite parity, which allows one to study a single-window problem with a perturbation which consists of an additional Dirichlet or Neumann boundary condition at a perpendicular section far from the window.

The approach based on symmetry no longer works if $a_1 \neq a_2$. The main aim of the present work is to demonstrate a different technique, suitable for the general case, which reduces the question to analysis of a boundary perturbation at the distant window. This technique follows the

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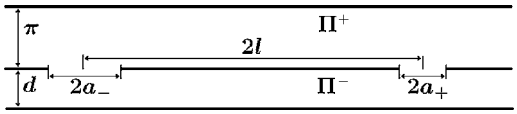

FIG. 1. Window-coupled waveguides.

main ideas of Ref. 4, where the Dirichlet Laplacian in an n-dimensional tube with a pair of distant perturbations described by two arbitrary operators was studied. It was assumed in Ref. 4 that the domains of these operators are preserved under the perturbation, and this assumption was employed substantially. This is obviously not true in the problem we study here, since the windows change the domain of the Laplacian (see, for instance, Ref. 5, Remark 1). At the same time, the general approach of Ref. 4 works in our case with the appropriate modifications. Moreover, since we restrict ourselves to the two-dimensional case and specify the nature of the distant perturbations, we are able to obtain a more detailed result in comparison with the general case in Ref. 4.

Let us describe briefly the main idea of our approach. The first key element is the fact that any eigenfunction of the two-window operator can be represented as the sum of two functions solving the eigenvalue equation for the Laplace operator in the one-window domains and vanishing at the boundary (see Lemma 4.1); one of these functions corresponds to the left window while the other does to the right one. The main feature of these functions is that their normal derivatives have a jump at the window. We show that the original eigenvalue problem is equivalent to a certain operator equation for the mentioned jumps of the normal derivatives. To solve this equation we employ the modification of the Birman-Schwinger approach suggested in Ref. 6; this is the second key ingredient of our technique. Finally, this approach reduces the equation to a search for nontrivial solutions to a finite system of linear equations, and the needed eigenvalues are roots of the determinant of the corresponding matrix. After such a reduction it is sufficient to study the behavior of these roots; in this way we obtain the main results presented in this paper.

Of course, the window-coupled waveguides are not the only, and by far, not the first, system in which distant perturbation asymptotics was studied. We have commented on that in the Introduction of the paper;[2] hence, we limit ourselves here to summarizing the three main points. First of all, our system has no classically closed trajectories, apart from a zero-measure set, so there is *no Agmon metric* on it. Despite this fact, however, the spectral behavior exhibits distinctive features common with one-dimensional Schrödinger operators—see, e.g., Refs. 7–9 and other papers quoted there and in Ref. 2. And finally, the just-mentioned analogy has to be taken *cum grano salis* as first illustrated in Ref. 10; in the two-window context this is clearly seen in the case of a threshold resonance.[2]

In order not to make this study too technical we concentrate in this paper on the generic case when the "unperturbed" energy is an *isolated* eigenvalue of the one-window problem, leaving the computationally involved discussion of threshold resonances to a sequel. The problem will be properly formulated and the results stated in the next section; the rest of the paper is devoted to the proofs.

II. STATEMENT OF THE PROBLEM AND THE RESULTS

Let $x=(x_1,x_2)$ be Cartesian coordinates in the plane $\Pi^+ := \{x: 0<x_2<\pi\}$ and $\Pi^- := \{x: -d<x_2<0\}$. With the natural scaling properties in mind, we may suppose without loss of generality that $d \leqslant \pi$. By $\gamma_\pm$ we denote two intervals $\gamma_\pm := \{x: |x_1 \mp l| < a_\pm, x_2=0\}$, from now on referred to as the *windows*. The numbers $a_\pm$ are assumed to be fixed throughout the paper, while the distance $2l$ between the windows will be changing playing the role of a large parameter.

We set $\Pi := \Pi^+ \cup \Pi^- \cup \gamma_+ \cup \gamma_-$ (cf. Fig. 1); the Hilbert space of our problem is $L_2(\Pi)$. We will employ the symbol H to denote Friedrichs extension of the negative Laplacian on the set $C_0^\infty(\Pi)$. As we have indicated in the Introduction, this work is devoted to the study of the asymptotic behavior of isolated eigenvalues of H as $l \to +\infty$. In order to formulate the main results we first have to introduce some more notations.

We denote $\gamma_a := \{x: |x_1| < a, x_2 = 0\}$ so that $\Pi_a := \Pi^+ \cup \Pi^- \cup \gamma_a$ is the double waveguide with a single window centered at $x_1 = 0$, and $\Gamma_a := \partial\Pi_a$. Furthermore, we introduce the corresponding cutoff sets $\Pi_a^b := \Pi_a \cap \{x: |x_1| < b\}$ and $\Gamma_a^b := \Gamma_a \cap \{x: |x_1| < b\}$. Consider the negative Laplacian in $L_2(\Pi_a)$ and call $H(a)$ its Friedrichs extension in $L_2(\Pi_a)$ from the set $C_0^\infty(\Pi_a)$ on which it is symmetric; by $\lambda_m(a)$, $m = 1, 2, \ldots$, we denote the isolated eigenvalues of this operator arranged in the ascending order with the multiplicity taken into account.

The following results were demonstrated in Refs. 1 and 3.

Proposition 2.1. For any $a > 0$ the essential spectrum of $H(a)$ equals $[1, +\infty)$ while the discrete spectrum of $H(a)$ is nonempty consisting of finitely many simple eigenvalues. The eigenfunction associated with an eigenvalue $\lambda_m(a)$ has a definite parity: it is even or odd with respect to x_1 if m is odd or even, respectively. In the particular case $d = \pi$ the eigenfunctions are even in the variable x_2.

Remark 2.1. The threshold of the essential spectrum of $H(a)$ equals the minimum of the thresholds corresponding to each of the strips. The latter are 1 and π^2/d^2, respectively; together with the normalization condition $d \leqslant \pi$ it explains the first part. The claims about the discrete spectrum are obtained by a variational estimate combined with bracketing bounds.

The eigenfunctions associated with the eigenvalues $\lambda_n(a)$ will be denoted as $\psi_n(\cdot, a)$ and assumed to be normalized, i.e., to be unit vectors in $L_2(\Pi_a)$. It is easy to check that $\psi_n(\cdot, a) \in C^\infty(\Pi_a)$. We will use the symbols $\sigma_{\mathrm{ess}}(\cdot)$ and $\sigma_{\mathrm{disc}}(\cdot)$ to indicate the essential and discrete spectrum, respectively. We set $\sigma_* := \sigma_{\mathrm{disc}} H(a_+) \cup \sigma_{\mathrm{disc}} H(a_-)$. Hereafter, the eigenvalues of H are assumed to be arranged in the nondecreasing order counting multiplicity.

With these preliminaries we can formulate the first main result of this paper.

Theorem 2.1. *For any $l > 0$, $a_\pm > 0$ the operator H has the essential spectrum equal to $[1, +\infty)$ and finitely many isolated eigenvalues. The number of the latter, counting multiplicity, is bounded uniformly with respect to the window distance. Each isolated eigenvalue of the operator H is a continuous function of l if the window distance is large enough, and in the limit $l \to +\infty$ it converges to one of the numbers from the set σ_* or to the threshold of the essential spectrum of H.*

The remaining part of the results describes the asymptotic behavior of the isolated eigenvalues and the associated eigenfunctions of H. In order to formulate these results we need to introduce auxiliary notations.

In Lemma 3.6 we will show that the eigenfunctions ψ_n of $H(a)$ behave for large values of $|x_1|$ as

$$\psi_n(x, a) = c(\lambda_n, a) \mathrm{e}^{-\sqrt{1-\lambda_n}x} \sin x_2 + \mathcal{O}(\mathrm{e}^{-\sqrt{4-\lambda_n}|x_1|}), \quad x_2 \in [0, \pi],$$

where $c(\lambda_n, a)$ are some constants. For any $\lambda \in (-\infty, 1) \setminus \sigma_{\mathrm{disc}}(H(a))$ we introduce that function U which is a unique solution of the boundary value problem,

$$\begin{gathered} (\Delta + \lambda) U = 0, \quad x \in \Pi_a \setminus \gamma_a, \quad U = 0, \quad x \in \partial\Pi_a, \\ \left.\frac{\partial U}{\partial x_2}\right|_{x_2=+0} - \left.\frac{\partial U}{\partial x_2}\right|_{x_2=-0} = \mathrm{e}^{\sqrt{1-\lambda}x_1}, \quad x \in \gamma_a, \end{gathered} \tag{2.1}$$

belonging to $W_2^1(\Pi_a)$. This function satisfies the relation

$$U(x, \lambda, a) = c(\lambda, a) \mathrm{e}^{-\sqrt{1-\lambda}x_1} \sin x_2 + \mathcal{O}(\mathrm{e}^{-\sqrt{4-\lambda}x_1}), \quad x_2 \in [0, \pi],$$

where $c(\lambda, a)$ is a constant. The unique solvability of (2.1) and the mentioned behavior of U at infinity will be proved in Lemma 3.7. We will also give formulas for the introduced constants c in Lemmas 3.6, 3.7 [see (3.15) and (3.18)].

We indicate by Ξ the set of all bounded domains $S \subset \Pi$ having smooth boundary and separated from the endpoints of $\gamma_\pm$ by a positive distance; the case $\partial S \cap \partial\Pi \neq \varnothing$ is not excluded. For brevity we introduce two-valued symbols, $\tau := 1$, $\rho = \rho(\lambda) := \min\{\sqrt{(\pi^2/d^2) - \lambda}, \sqrt{4-\lambda}\}$, $\lambda \in (-\infty, 1)$, if $d < \pi$ and $\tau := 2$, $\rho = \rho(\lambda) := \sqrt{4-\lambda}$, $\lambda \in (-\infty, 1)$, if $d = \pi$. An element $\lambda_* \in \sigma_*$ will be

called *simple* if it belongs to one of the sets $\sigma_{\mathrm{disc}}(H(a_\pm))$ only and *double* otherwise. Furthermore, we set $\boldsymbol{a} := (a_+, a_-)$.

Continuing the list of the main results we make the following claims.

Theorem 2.2. *Suppose that $\lambda_* \in \sigma_*$ is simple being an eigenvalue $\lambda_n(a_\pm)$ of the operator $H(a_\pm)$. Then, there is a unique eigenvalue $\lambda(l,\boldsymbol{a})$ of the operator H converging to λ_* as $l \to +\infty$. This eigenvalue is simple and behaves asymptotically as follows:*

$$\lambda(l,\boldsymbol{a}) = \lambda_* + \mu^\pm(l,\boldsymbol{a})\mathrm{e}^{-4l\sqrt{1-\lambda_*}} + \mathcal{O}(l^2\mathrm{e}^{-8l\sqrt{1-\lambda_*}} + \mathrm{e}^{-2l(\sqrt{1-\lambda_*}+\rho)}), \tag{2.2}$$

$$\mu^\pm(l,\boldsymbol{a}) := \tau\pi c(\lambda_*, a_\pm)c^2(\lambda_*, a_\mp)\sqrt{1-\lambda_*}. \tag{2.3}$$

The associated eigenfunction $\psi(x,l,\boldsymbol{a})$ satisfies the relation

$$\psi(x,l,\boldsymbol{a}) = \psi_n(x_1 \mp l, x_2, a_\pm) + \mathcal{O}(\mathrm{e}^{-2l\sqrt{1-\lambda_*}}) \tag{2.4}$$

in the norms of both the $W_2^1(\Pi)$ and $W_2^2(S)$ for each $S \in \Xi$.

This theorem describes the asymptotic behavior of the eigenvalues of H converging to a simple element of σ_*. In particular, it states that in this case exactly one eigenvalue of H converges to λ_*, this eigenvalue is simple, and the associated eigenfunction is localized around the left or right window subject to whether λ_* is an eigenvalue of $H(a_-)$ or $H(a_+)$.

The other possibility case is that λ_* is double. The next theorem describes the asymptotic behavior of the eigenvalues of H converging to such element of σ_*.

Theorem 2.3. *Suppose that $\lambda_* \in \sigma_*$ is double and $\lambda_* = \lambda_n(a_-) = \lambda_m(a_+)$. Then there exist, with the multiplicity taken into account, exactly two eigenvalues $\lambda^\pm(l,\boldsymbol{a})$ of H which converge to λ_* as $l \to +\infty$. The asymptotic expansions of these eigenvalues read as follows:*

$$\lambda^\pm(l,\boldsymbol{a}) = \lambda_* \pm |\mu(l,\boldsymbol{a})|\mathrm{e}^{-2l\sqrt{1-\lambda_*}} + \mathcal{O}(l\mathrm{e}^{-4l\sqrt{1-\lambda_*}} + \mathrm{e}^{-2l\rho(\lambda_*)}), \tag{2.5}$$

$$\mu(l,\boldsymbol{a}) = (-1)^{m+1}\tau\pi c(\lambda_*, a_-)c(\lambda_*, a_+)\sqrt{1-\lambda_*}. \tag{2.6}$$

In accordance with this theorem, in the case that λ_* is double the total multiplicity of the eigenvalues of H converging to λ_* is 2. In other words, for a fixed large value of l the operator H has either two simple or one double eigenvalue in the vicinity of λ_*. If $\mu(l,\boldsymbol{a}) \neq 0$, the asymptotics (2.5) implies that $\lambda^-(l,\boldsymbol{a}) \neq \lambda^+(l,\boldsymbol{a})$, and in this case we deal with two simple eigenvalues. We also observe that the leading terms in (2.5) are greater by order than ones in (2.2).

In the following theorem we describe the asymptotic behavior of the eigenfunctions associated with the mentioned eigenvalues.

Theorem 2.4 *Suppose the hypothesis of Theorem 2.3 holds true. If $\mu(l,\boldsymbol{a}) \neq 0$, the eigenvalues $\lambda^+(l,\boldsymbol{a})$, $\lambda^-(l,\boldsymbol{a})$ do not coincide and are simple, and the associated eigenfunctions $\psi^\pm(x,l,\boldsymbol{a})$ satisfy the relations*

$$\psi^\pm(x,l,\boldsymbol{a}) = \psi_n(x_1 + l, x_2, a_-) \mp \psi_m(x_1 - l, x_2, a_+)\operatorname{sgn}\mu(l,\boldsymbol{a}) + \mathcal{O}(\mathrm{e}^{-2l\sqrt{1-\lambda_*}}) \tag{2.7}$$

in the norms of $W_2^1(\Pi)$ and $W_2^2(S)$ for each $S \in \Xi$. If $\lambda^-(l,\boldsymbol{a}) = \lambda^+(l,\boldsymbol{a})$ is a double eigenvalue, the associated eigenfunctions $\psi^\pm(x,l,\boldsymbol{a})$ satisfy the relations

$$\begin{aligned} \psi^+(x,l,\boldsymbol{a}) &= \psi_n(x_1 + l, x_2, a_-) + \mathcal{O}(\mathrm{e}^{-2l\sqrt{1-\lambda_*}}), \\ \psi^-(x,l,\boldsymbol{a}) &= \psi_m(x_1 - l, x_2, a_-) + \mathcal{O}(\mathrm{e}^{-2l\sqrt{1-\lambda_*}}), \end{aligned} \tag{2.8}$$

in the norm of $W_2^1(\Pi)$ and $W_2^2(S)$ for each $S \in \Xi$. Finally, if $\mu(l,\boldsymbol{a}) = 0$ and $\lambda^-(l,\boldsymbol{a}) \neq \lambda^+(l,\boldsymbol{a})$, the eigenvalues $\lambda^\pm(l,\boldsymbol{a})$ *are simple and the associated eigenfunctions satisfy the relations*

$$\psi^\pm(x,l,\boldsymbol{a}) = c_+^\pm\psi_n(x_1 + l, x_2, a_-) + c_-^\pm\psi_m(x_1 - l, x_2, a_+) + \mathcal{O}(\mathrm{e}^{-2l\sqrt{1-\lambda_*}}), \tag{2.9}$$

where the vectors $\boldsymbol{c}^{\pm}:=\begin{pmatrix} c_+^{\pm} \\ c_-^{\pm} \end{pmatrix}$ *are nontrivial solutions to the system* (4.20) *with* $\lambda=\lambda^{\pm}$ *such that* $\|\boldsymbol{c}^{\pm}\|_{\mathbb{R}^2}=1$.

The leading terms of the asymptotics (2.2) and (2.5) are nonzero provided the corresponding coefficients $c(\lambda_*,a_\pm)$ are nonzero. We shall show in Lemmas 3.6 and 3.7 that this is true at least for $c(\lambda,a)$ if $\lambda\leqslant\lambda_1(a)$ or $\lambda=\lambda_2(a)$. For instance, if $\lambda_1(a_-)<\lambda_1(a_+)$, the eigenvalue of the operator H converging to $\lambda_1(a_-)$ has the asymptotic expansion (2.2), and the coefficient (2.3) of leading term is nonzero. Moreover, due to Lemma 3.7 this coefficient is negative. If $a_\pm$ are such that $\lambda_1(a_-)=\lambda_2(a_+)$, the eigenvalues of the operator H converging to $\lambda_*=\lambda_1(a_-)=\lambda_2(a_+)$ have the asymptotic expansions (2.5), and the coefficients of the leading terms are nonzero. By Theorem 2.4 the "perturbed" eigenvalues are simple and the associated eigenfunctions satisfy the identities (2.7) in this case. We also stress that in this case the leading terms of the asymptotic expansions (2.5) have the same modulus but different signs. This phenomenon is known for double-well problems with symmetric wells. It also occurs in the symmetric case, $a_-=a_+$ and $d_-=d_+$, as we have shown in Ref. 2. We also notice that the exponents in the leading terms in (2.5) are the same as for the symmetric case in Ref. 2 but the coefficients $\mu^{\pm}(\lambda,\boldsymbol{a})$ differ.

We conjecture that the coefficient $c(\lambda,a)$ is nonzero for all values a and $\lambda<1$. If it is true, this fact would imply that the leading terms in the asymptotics (2.2) and (2.5) are nonzero. In turn, this fact together with Theorem 2.4 would imply that a double $\lambda_*\in\sigma_*$ splits into two simple "perturbed" eigenvalues and the formulas (2.7) are valid for the associated eigenfunctions.

III. ANALYSIS OF THE ONE-WINDOW PROBLEM

In this section we shall study the following boundary value problem:

$$(\Delta+\lambda)u=0,\quad x\in\Pi_a\setminus\gamma_a,\quad u=0,\quad x\in\Gamma_a,$$
$$\left.\frac{\partial u}{\partial x_2}\right|_{x_2=+0}-\left.\frac{\partial u}{\partial x_2}\right|_{x_2=-0}=f,\quad x\in\gamma_a. \tag{3.1}$$

The function f is assumed to be an element of $L_2(\gamma_a)$. The parameter $\lambda\in\mathbb{C}$ is supposed to belong to $\mathbb{S}_\delta$ for a fixed $\delta>0$, where $\mathbb{S}_\delta$ is a set of all λ separated from the halfline $[1,+\infty)$ by a distance greater than δ. For any open set $\Omega\subset\mathbb{R}^2$ and $\gamma\subset\bar{\Omega}$ the symbol $W_2^1(\Omega,\gamma)$ will indicate the subset of the functions from $W_2^1(\Omega)$ having zero trace on γ.

We seek a generalized solution of the problem (3.1) belonging to $L_2(\Pi_a)$. More specifically, we are looking for a function belonging to $L_2(\Pi_a)$ and $W_2^1(\Pi_a^b,\Gamma_a^b)$ for each $b>0$ and satisfying the equation

$$-(\nabla u,\nabla\zeta)_{L_2(\Pi_a)}+\lambda(u,\zeta)_{L_2(\Pi_a)}-(f,\zeta)_{L_2(\gamma_a)}=0 \tag{3.2}$$

for any $\zeta\in C_0^\infty(\Pi_a)$. Our main aim is to study the dependence of this solution on the spectral parameter λ. In this section we will collect a series of preliminary results describing the mentioned dependence, while in the following sections these results will be employed to prove Theorems 2.1–2.4.

We construct the solution of (3.1) as a sum $u=u_1+u_2$, where the first function satisfies the boundary condition in (3.1), while the other is a value of the resolvent of $H(a)$ on some function. First we introduce the function u_1.

We fix $\beta>a$ and put $P:=\{x:|x_1|<a+\beta,0<x_2<d_0\}$. The number d_0 here is chosen so that $d_0<d$, and the lowest eigenvalue of the negative Laplacian in P subject to Dirichlet boundary condition on $\partial P\setminus\bar{\gamma}_a$ and to the Neumann one on γ_a exceeds 2. We consider the boundary value problem

$$(\Delta+\lambda)\tilde{u}=0,\quad x\in P,\quad \tilde{u}=0,\quad x\in\partial P,\quad \frac{\partial\tilde{u}}{\partial x_2}=\frac{1}{2}f,\quad x\in\gamma_a, \tag{3.3}$$

which is again treated in the weak sense,

$$-(\nabla\tilde{u},\nabla\zeta)_{L_2(P)}+\lambda(\tilde{u},\zeta)_{L_2(P)}-\frac{1}{2}(f,\zeta)_{L_2(\gamma_a)}=0 \tag{3.4}$$

for each function $\zeta\in C^\infty(P)$ vanishing in a neighborhood of $\partial P\setminus\bar{\gamma}_a$. The problem (3.3) is uniquely solvable in the space $W_2^1(P,\partial P\setminus\gamma_a)$ and the solution belongs to $C^\infty(\bar{P}\setminus\bar{\gamma}_a)$—see Ref. 12, Chap. II, Sec. 5, Remark 5.1 and Ref. 11, Chap. IV, Sec. 2.

Let a function $\chi_1=\chi_1(x)\in C^\infty(\mathbb{R}^2)$ be infinitely differentiable, even with respect to the variable x_2, equal to 1 if $|x_1|<a+\beta/6$ and $|x_2|<d_0/6$, and vanish for $|x_1|>a+\beta/3$ or $|x_2|>d_0/3$. We extend the function $\tilde{u}$ in an even way for $x_2<0$ setting $\tilde{u}(x):=\tilde{u}(x_1,-x_2)$ as $x_2<0$ and denote $u_1(x):=\chi_1(x)\tilde{u}(x)$.

By Ξ_a we indicate the set of all bounded domains $S\subset\Pi_a$ having smooth boundary and separated from the endpoints of γ_a by a positive distance; we stress that the case $\partial S\cap\partial\Pi_a\neq\varnothing$ is not excluded.

Lemma 3.1. The function u_1 belongs to $W_2^1(\Pi_a,\Gamma_a)$ and satisfies the equation

$$-(\nabla u_1,\nabla\zeta)_{L_2(\Pi_a)}+\lambda(u_1,\zeta)_{L_2(\Pi_a)}-(f,\zeta)_{L_2(\gamma_a)}=(F,\zeta)_{L_2(\Pi_a)} \tag{3.5}$$

for any $\zeta\in C_0^\infty(\Pi_a)$, where

$$F=T_1(\lambda,a)f:=2\nabla\tilde{u}\cdot\nabla\chi_1+\tilde{u}\Delta\chi_1.$$

The operator $T_1: L_2(\gamma_a)\to L_2(\{x:|x_1|<a+\beta/3,|x_2|<d_0/3\})$ is linear, bounded, and holomorphic in λ. The operator $T_2(\lambda,a)f:=u_1$ is linear, bounded, and holomorphic in λ as a map from $L_2(\gamma_a)$ into $W_2^1(\Pi_a,\Gamma_a)$, $W_2^2(S)$, and $W_2^2(\Pi^\pm\setminus\Pi_a^\beta)$, where $S\in\Xi_a$ is such that $S\subset\Pi^+$ or $S\subset\Pi^-$.

Proof. It is clear that $u_1\in W_2^1(\Pi_\pm,\partial\Pi_\pm\setminus\gamma_a)$. Since this function is even with respect to x_2, using integration by parts we obtain

$$\left(u_1,\frac{\partial\zeta}{\partial x_i}\right)_{L_2(\Pi_a)}=\left(u_1,\frac{\partial\zeta}{\partial x_i}\right)_{L_2(\Pi_+)}+\left(u_1,\frac{\partial\zeta}{\partial x_i}\right)_{L_2(\Pi_-)}=-\left(\frac{\partial u_1}{\partial x_i},\zeta\right)_{L_2(\Pi_+)}-\left(\frac{\partial u_1}{\partial x_i},\zeta\right)_{L_2(\Pi_-)},\quad i=1,2,$$

for each $\zeta\in C_0^\infty(\Pi_a)$. Hence, $u\in W_2^1(\Pi_a,\Gamma_a)$. Employing the parity of u_1 with respect to x_2 once again, we find that for each $\zeta\in C_0^\infty(\Pi_a)$ the left-hand side of (3.5) equals twice the expression

$$-(\nabla u_1,\nabla\zeta^+)_{L_2(P)}+\lambda(u_1,\zeta^+)_{L_2(P)}-(f,\zeta^+)_{L_2(\gamma_a)},$$

where $\zeta^+(x):=\zeta(x)+\zeta(x_1,-x_2)$. In view of (3.4) and the definition of χ_1, we get

$$\begin{aligned}
&-(\nabla u_1,\nabla\zeta)_{L_2(\Pi_a)}+\lambda(u_1,\zeta)_{L_2(\Pi_a)}-(f,\zeta)_{L_2(\gamma_a)}\\
&\quad=2\Big(-(\nabla\tilde{u},\nabla(\chi_1\zeta^+))_{L_2(P)}+\lambda(u_1,\chi_1\zeta^+)_{L_2(P)}-\frac{1}{2}(f,\chi_1\zeta^+)_{L_2(\gamma_a)}+(\nabla\tilde{u},\zeta^+\nabla\chi_1)_{L_2(P)}\\
&\quad\quad-(\tilde{u}\nabla\chi_1,\nabla\zeta^+)_{L_2(P)}\Big)\\
&\quad=2((\nabla\tilde{u},\zeta^+\nabla\chi_1)_{L_2(P)}-(\tilde{u}\nabla\chi_1,\nabla\zeta^+)_{L_2(P)})=2((\nabla\tilde{u},\zeta^+\nabla\chi_1)_{L_2(P)}+(\operatorname{div}\tilde{u}\nabla\chi_1,\zeta^+)_{L_2(P)})\\
&\quad=(F,\zeta)_{L_2(\Pi_a)}.
\end{aligned}$$

The boundedness of the operator $T_1(\lambda,a)$ follows from the smoothness-improving theorems of solutions to elliptic boundary value problems (see Ref. 11, Chap. II, Sec. 2).

In order to check that T_1 is holomorphic in the variable λ, we just need to show that the mapping $f \mapsto \tilde{u}$ is bounded and holomorphic as an operator family from $L_2(\gamma_a)$ into $W_2^1(P)$ and $W_2^2(S \cap P)$, where $S \in \Xi_a$ and $S \subset \overline{\Pi^+}$. To prove the last claim it is sufficient to reduce the boundary value problem to an operator equation in $W_2^1(P, \partial P \setminus \overline{\gamma}_a)$ in the standard way—see Ref. 11, Chap II, Sec. 2—and to apply then Proposition 4.5 of Ref. 13, Chap. XI, Sec. 4. □

As u_1 is compactly supported, the function u_2 has to be an element of $L_2(\Pi_a)$ and of $W_2^1(\Pi_a^b, \Gamma_a^b)$ for each $b > a$. It follows from (3.2) and (3.5) that the function u_2 must also obey the integral relation

$$-(\nabla u_2, \nabla \zeta)_{L_2(\Pi_a)} + \lambda (u_2, \zeta)_{L_2(\Pi_a)} = -(F, \zeta)_{L_2(\Pi_a)}$$

for any $\zeta \in C_0^\infty(\Pi_a)$. Thus u_2 has to solve the boundary value problem

$$-(\Delta + \lambda) u_2 = F, \quad x \in \Pi_a, \quad u = 0, \quad x \in \Gamma_a, \tag{3.6}$$

belonging to $L_2(\Pi_a)$ and $W_2^1(\Pi_a^b, \Gamma_a^b)$ for each $b > 0$. By Theorem 4.6.8 of Ref. 14, Chap. 4, Sec. 4.6 any solution of this problem belonging to $L_2(\Pi_a)$ is an element of the operator domain of $H(a)$. In this way the problem (3.6) can be cast into the form $(H(a) - \lambda) u_2 = F$, which in turn gives $u_2 = (H(a) - \lambda)^{-1} F$.

We denote the map $f \mapsto u$ as $T_3(\lambda, a)$. In fact, $T_3(\lambda, a) := T_2(\lambda, a) + (H(a) - \lambda)^{-1} T_1(\lambda, a)$.

Lemma 3.2. The linear operator $T_3(\lambda, a)$ is bounded and meromorphic in $\lambda \in \mathbb{S}_\delta$ as a map from $L_2(\gamma_a)$ into $W_2^1(\Pi_a, \Gamma_a)$ and into $W_2^2(S)$ for each $S \in \Xi_a$. Its poles coincide with the eigenvalues of the operator $H(a)$. For any λ close to an eigenvalue λ_n of $H(a)$, the representation

$$T_3(\lambda, a) = \frac{\psi_n}{\lambda - \lambda_n} T_4(a) + T_5(\lambda, a) \tag{3.7}$$

holds true. Here $T_4(a) f := (f, \psi_n)_{L_2(\gamma_a)}$, and the linear operator T_5 is bounded and holomorphic in $\lambda \in \mathbb{S}_\delta$ as a map from $L_2(\gamma_a)$ into $W_2^1(\Pi_a, \Gamma_a)$. The operator T_5 is also bounded and holomorphic as a map into $W_2^2(S)$ for each $S \in \Xi_a$.

Proof. In accordance with Ref. 15, Chap. 5, Sec. 3.5 the operator $(H(a) - \lambda)^{-1}$ is bounded and meromorphic in $L_2(\Pi_a)$, its poles coincide with the eigenvalues of $H(a)$, and for λ close to λ_n the representation

$$(H(a) - \lambda)^{-1} = -\frac{\psi_n}{\lambda - \lambda_n} (\cdot, \psi_n)_{L_2(\Pi_a)} + T_6(\lambda, a) \tag{3.8}$$

is valid, where the operator $T_6(\lambda, a)$ is bounded and holomorphic in λ in the vicinity of λ_n. The function $\hat{u} := T_6(\lambda, a) F$ is a solution to the boundary value problem (3.6) with F replaced by $\hat{F} := F - (F, \psi_n)_{L_2(\Pi_a)} \psi_n$; it means that

$$\|\nabla \hat{u}\|^2_{L_2(\Pi_a)} - \lambda \|\hat{u}\|^2_{L_2(\Pi_a)} = (\hat{F}, \hat{u})_{L_2(\Pi_a)}.$$

This relation, together with (3.8), implies that the operator T_6 is bounded and holomorphic as a map into $W_2^1(\Pi_a)$ as well. Using again the smoothness-improving theorems mentioned above, we conclude that the operator T_6 is also bounded and holomorphic in λ as a map into $W_2^2(S)$ for each $S \in \Xi_a$, $S \subset \Pi_+$ or $S \subset \Pi_-$.

Since the function ψ_n is an element of $W_2^1(\Pi_a, \Gamma_a)$, the relation (3.5) is valid for $\zeta = \psi_n$. For any $f \in L_2(\gamma_a)$ the function $T_1(\lambda, a) f$ is compactly supported; hence, we have

$$(T_1(\lambda_n, a) f, \psi_n)_{L_2(\Pi_a)} = -(\nabla u_1, \nabla \psi_n)_{L_2(\Pi_a)} + \lambda (u_1, \psi_n)_{L_2(\Pi_a)} - (f, \psi_n)_{L_2(\gamma_a)},$$

where $u_1 = T_2(\lambda_n, a) f$. According to Lemma 3.1, the function u_1 belongs to $W_2^1(\Pi_a, \Gamma_a)$, which allows us to proceed with the calculations,

$$-(\nabla u_1, \nabla \psi_n)_{L_2(\Pi_a)} + \lambda (u_1, \psi_n)_{L_2(\Pi_a)} = 0,$$

$$(T_1(\lambda_n, a) f, \psi_n)_{L_2(\Pi_a)} = -(f, \psi_n)_{L_2(\gamma_a)} = -T_4(a) f.$$

Substituting the relation thus obtained together with (3.8) into the definition of the operator T_3, and taking into account Lemma 3.1, we arrive finally at the statement of the lemma. □

For any numbers $b_1, b_2, b_3 \in \mathbb{R}$ we set $\Omega_\pm := \{x : \pm x_1 > b_1, b_2 < x_2 < b_3\}$ and $\omega_\pm := \partial\Omega_\pm \setminus \{x : x_1 = \pm b_1\}$.

Lemma 3.3. Let $v \in W_2^1(\Omega_\pm)$ be a solution to the problem

$$(\Delta + \lambda) v = 0, \quad x \in \Omega^\pm, \quad v = 0, \quad x \in \omega^\pm,$$

and $0 < b_2 - b_3 \leqslant \pi$, $\lambda \in \mathbb{S}_\delta$. Then the function v can be represented as

$$v(x, \lambda) = \sum_{j=1}^{\infty} \alpha_j(\lambda) \exp\left(- \sqrt{\frac{\pi^2 j^2}{(b_3 - b_2)^2} - \lambda} (\pm x_1 - b_1) \right) \sin \frac{\pi j}{b_3 - b_2} (x_2 - b_2), \tag{3.9}$$

where

$$\alpha_j(\lambda) := \frac{2}{b_3 - b_2} \int_{b_2}^{b_3} v(\pm b_1, x_2, \lambda) \sin \frac{\pi j}{b_3 - b_2} (x_2 - b_2) \mathrm{d}x_2.$$

The series (3.9) converges in the norms of $W_2^m(\{x : \pm x_1 > b_4, b_2 < x_2 < b_3\})$, $m \geqslant 0$, for any $b_4 > b_1$. The coefficients α_j satisfy the condition

$$\frac{\pi}{2} \sum_{j=1}^{\infty} |\alpha_j|^2 = \| v(\pm b_1, \cdot, \lambda) \|_{L_2(b_2, b_3)}.$$

This lemma is a particular case of Lemma 3.3 of Ref. 4 so we skip the proof.

Let us next fix a number $\widetilde{a} > 0$. For any $l \geqslant (a + \widetilde{a})$ we define operators $T_7^\pm(\lambda, l, a, \widetilde{a})$ which map an arbitrary $v \in W_2^1(\Pi_a^a)$ into the function

$$(T_7^\pm v)(x_1, \lambda, l) := \sum_{j=1}^{\infty} j \alpha_j^\pm \mathrm{e}^{\mp \kappa_j^+(\lambda)(x_1 \mp a)} \mathrm{e}^{-2\kappa_j^+(\lambda) l} - \sum_{j=1}^{\infty} \frac{\pi j}{d} \beta_j^\pm \mathrm{e}^{\mp \kappa_j^-(\lambda)(x_1 \mp a)} \mathrm{e}^{-2\kappa_j^-(\lambda) l},$$

$$\alpha_j^\pm = \frac{2}{\pi} \int_0^\pi v(a, x_2) \sin j x_2 \mathrm{d}x_2, \quad \beta_j^\pm = \frac{2}{d} \int_{-d}^0 v(a, x_2) \sin \frac{\pi j}{d} x_2 \mathrm{d}x_2,$$

$$\kappa_j^+(\lambda) := \sqrt{j^2 - \lambda}, \quad \kappa_j^-(\lambda) := \sqrt{\frac{\pi^2 j^2}{d^2} - \lambda}, \quad j \geqslant 1.$$

The branch of the root in the definition of the functions κ_j is specified by the requirement that the functions are analytic in $\mathbb{S}_\delta$ and $\sqrt{1} = 1$.

Lemma 3.4. The operators $T_7^\pm : W_2^1(\Pi_a^a) \to L_2(\gamma_{\widetilde{a}})$ are well defined, bounded, and holomorphic in $\lambda \in \mathbb{S}_\delta$. The estimates

$$\left\| \frac{\partial^i T_7^\pm}{\partial \lambda^i} \right\| \leqslant C l^i \mathrm{e}^{-(2l - a - \widetilde{a}) \operatorname{Re} \kappa_1^+(\lambda)}, \quad i = 0, 1, 2,$$

hold true uniformly with respect to $\lambda \in \mathbb{S}_\delta$ and $l \geqslant (a + \widetilde{a})$.

Proof. We will prove the lemma for T_7^+ only; the argument for T_7^- is similar. The function u belongs to $W_2^1(\Pi_a^a)$; hence, we have the estimate

$$\sum_{j=1}^{\infty}(|\alpha_j^{\pm}|^2+|\beta_j^{\pm}|^2)\leqslant C\|u\|^2_{W_2^1(\Pi_a)},$$

where the constant C is independent of $\lambda\in\mathbb{S}_\delta$ and $l\geqslant(a+\tilde{a})$. Employing this inequality, we infer that

$$\begin{aligned}\left\|\sum_{j=1}^{\infty} j\alpha_j^+ e^{-\kappa_j^+(\lambda)(\cdot-a)}e^{-2\kappa_j^+(\lambda)l}\right\|_{L_2(\gamma_{\tilde{a}})} &\leqslant \sum_{j=1}^{\infty} j|\alpha_j|e^{-2l\ \mathrm{Re}\ \kappa_j^+(\lambda)}\|e^{-\kappa_j^+(\lambda)(\cdot-a)}\|_{L_2(-\tilde{a},\tilde{a})}\\ &\leqslant C\sum_{j=1}^{\infty}\frac{j|\alpha_j^+|}{\sqrt{\mathrm{Re}\ \kappa_j^+(\lambda)}}e^{-(2l-a-\tilde{a})\mathrm{Re}\ \kappa_j^+(\lambda)}\\ &\leqslant C\left(\sum_{j=1}^{\infty}|\alpha_j|^2\right)^{1/2}\left(\sum_{j=1}^{\infty}\frac{j^2e^{-2(2l-a-\tilde{a})\mathrm{Re}\ \kappa_j^+(\lambda)}}{|\kappa_j^+(\lambda)|}\right)^{1/2}\\ &\leqslant C\|v\|_{W_2^1(\Pi_a^a)}e^{-(2l-a-\tilde{a})\mathrm{Re}\ \kappa_1^+(\lambda)}\\ &\quad\times\left(\sum_{j=1}^{\infty}\frac{j^2\exp(-2(2l-a-\tilde{a})\mathrm{Re}(\kappa_j^+(\lambda)-\kappa_1^+(\lambda)))}{\sqrt{|\mathrm{Im}\lambda|}}\right)^{1/2}\\ &\leqslant Ce^{-(2l-a-\tilde{a})\mathrm{Re}\ \kappa_1^+(\lambda)}\|v\|_{W_2^1(\Pi_a^a)},\end{aligned}$$

where C is independent of $\lambda\in\mathbb{S}_\delta$ and $\lambda\geqslant(a+\tilde{a})$. In the same way, one can prove that

$$\left\|\sum_{j=1}^{\infty}\frac{\pi j}{d}\beta_j^+e^{-\kappa_j^-(\lambda)(\cdot-a)}e^{-2\kappa_j^-(\lambda)l}\right\|_{L_2(\gamma_{\tilde{a}})}\leqslant Ce^{-(2l-a-\tilde{a})\mathrm{Re}\ \kappa_1^-(\lambda)}\|v\|_{W_2^1(\Pi_a^a)}.$$

The last two estimates imply that the operator $T_7^+:W_2^1(\Pi_a^a)\to L_2(\gamma_{\tilde{a}})$ is well defined and bounded. One can check easily that

$$\begin{aligned}\left(\frac{\partial T_7^+v}{\partial\lambda}\right)(x_1,\lambda,l) &:= \sum_{j=1}^{\infty}\frac{j\alpha_j^+}{2\kappa_j^+(\lambda)}(x_1-a+2l)e^{-\kappa_j^+(\lambda)(x_1-a)}e^{-2\kappa_j^+(\lambda)l}\\ &\quad-\sum_{j=1}^{\infty}\frac{\pi j\beta_j^+(x_1-a+2l)}{2\kappa_j^-(\lambda)d}e^{-\kappa_j^-(\lambda)(x_1-a)}e^{-2\kappa_j^-(\lambda)l}.\end{aligned}$$

Repeating the argument which yielded the estimate for T_7^+v, we can establish that

$$\left\|\frac{\partial T_7^{\pm}v}{\partial\lambda}\right\|_{L_2(\gamma_{\tilde{a}})}\leqslant Cle^{-(2l-a-\tilde{a})\mathrm{Re}\ \kappa_1^+(\lambda)}\|v\|_{W_2^1(\Pi_a^a)}$$

with the constant C independent of $\lambda\in\mathbb{S}_\delta$ and $l\geqslant(a+\tilde{a})$. Consequently, the operator $\partial T_7^+/\partial\lambda$ exists, it is bounded, and the stated estimate for its norm holds true. The norm estimate for $\partial^2T_7^+/\partial\lambda^2$ is obtained in a similar way. □

For any $l\geqslant(a+\tilde{a})$ we define operators $T_8^{\pm}(\lambda,l,a,\tilde{a})$ which map any $f\in L_2(\gamma_a)$ to the function

$$\frac{\partial u}{\partial x_2}(x_1\pm 2l,+0,\lambda)-\frac{\partial u}{\partial x_2}(x_1\pm 2l,-0,\lambda),\quad x_1\in(-\tilde{a},\tilde{a}).$$

Here u is a solution to the boundary value problem (3.1). Taking into account Lemma 3.2 together with the boundedness of the embedding $W_2^1(\Pi_a)$ into $L_2(\{x:|x_1\pm 2l|<\tilde{a},x_2=0\})$, we conclude that the operators $T_8^{\pm}:L_2(\gamma_a)\to L_2(\gamma_{\tilde{a}})$ are bounded and holomorphic in $\lambda\in\mathbb{S}_\delta$.

Lemma 3.5. The poles of the operators $T_8^{\pm}$ coincide with the eigenvalues of the operator $H(a)$.

For any compact set $K\subset\mathbb{S}_\delta$ separated from the discrete spectrum of $H(a)$ by a positive distance, the estimates

$$\left\|\frac{\partial^i T_8^\pm}{\partial\lambda^i}\right\| \leqslant C l^i \mathrm{e}^{-2l\ \mathrm{Re}\ \kappa_1^+(\lambda)}, \quad i=0,1, \tag{3.10}$$

hold true with C which is independent of $\lambda\in K$ and l. For any λ close to an eigenvalue λ_n of the operator $H(a)$ the representation

$$T_8^\pm(\lambda,l,a,\tilde{a}) = \frac{\phi_n^\pm}{\lambda-\lambda_n} T_4(a) + T_9^\pm(\lambda,l,a,\tilde{a}) \tag{3.11}$$

is valid, where

$$\phi_n^\pm(x_1,l,a) := \frac{\partial\psi_n}{\partial x_2}(x_1\pm 2l,+0,a) - \frac{\partial\psi_n}{\partial x_2}(x_1\pm 2l,-0,a), \quad x_1\in(-\tilde{a},\tilde{a}). \tag{3.12}$$

The operators $T_9^\pm: L_2(\gamma_a)\to L_2(\gamma_{\tilde{a}})$ are bounded and holomorphic with respect to λ in the vicinity of λ_n and satisfy the estimates

$$\left\|\frac{\partial^i T_9^\pm}{\partial\lambda^i}\right\| \leqslant C l^{i+1} \mathrm{e}^{-2l\ \mathrm{Re}\ \kappa_1^+(\lambda)}, \quad i=0,1, \tag{3.13}$$

where the constant C is independent of λ and l.

Proof. Due to Lemma 3.3 we have

$$T_8^\pm(\lambda,l,a,\tilde{a}) f = T_7^\pm(\lambda,l,a,\tilde{a}) u, \tag{3.14}$$

where u is a solution to the boundary value problem (3.1). Using this identity and the representation (3.7), we arrive at (3.11), where $T_9^\pm$ is a bounded operator holomorphic in λ. Moreover,

$$\begin{aligned} T_9^\pm(\lambda,l,a,\tilde{a}) &= \frac{T_7^\pm(\lambda,l,a,\tilde{a}) - T_7^\pm(\lambda_n,l,a,\tilde{a})}{\lambda-\lambda_n} T_4(a) + T_7^\pm(\lambda,l,a,\tilde{a}) T_5^\pm(\lambda,a) \\ &= \left(\frac{1}{\lambda-\lambda_n}\int_{\lambda_n}^{\lambda} \frac{\partial T_7^\pm}{\partial\lambda}(z,l,a,\tilde{a})\mathrm{d}z\right) T_4(a) + T_7^\pm(\lambda,l,a,\tilde{a}) T_5^\pm(\lambda,a), \end{aligned}$$

$$\frac{T_9^\pm}{\partial\lambda}(\lambda,l,a,\tilde{a}) = \left(\frac{1}{(\lambda-\lambda_n)^2}\int_{\lambda_n}^{\lambda}\int_{z_1}^{\lambda} \frac{\partial^2 T_7^\pm}{\partial\lambda^2}(z_2,l,a,\tilde{a})\mathrm{d}z_2\mathrm{d}z_1\right) T_4(a) + \frac{\partial}{\partial\lambda}(T_7^\pm(\lambda,l,a,\tilde{a}) T_5^\pm(\lambda,a)).$$

Applying now Lemma 3.4 we obtain the estimates (3.13).

The operators $\partial^i T_3/\partial\lambda^i$, $i=0,1$, are bounded uniformly in $\lambda\in K$, thus in view of the relation (3.14) and Lemma 3.4 we arrive readily at the estimates (3.10). □

Concluding this section we shall prove two auxiliary lemmas.

Lemma 3.6. In the limit $x_1\to\pm\infty$ the eigenfunction ψ_n of $H(a)$ behaves as

$$\psi_n(x,a) = (\pm 1)^{n+1} c(\lambda_n,a) \mathrm{e}^{-\kappa_1^+(\lambda_n)|x_1|} \sin x_2 + \mathcal{O}(\mathrm{e}^{-k_2^+(\lambda_n)|x_1|}), \quad x_2\in[0,\pi],$$

$$\nabla_x\psi_n(x,a) = (\pm 1)^{n+1} c(\lambda_n,a) \nabla_x \mathrm{e}^{-\kappa_1^+(\lambda_n)|x_1|} \sin x_2 + \mathcal{O}(\mathrm{e}^{-k_2^+(\lambda_n)|x_1|}), \quad x_2\in[0,\pi],$$

$$\psi_n(x,a) = \mathcal{O}(\mathrm{e}^{-\kappa_1^-(\lambda)|x_1|}), \quad \nabla_x\psi_n(x,a) = \mathcal{O}(\mathrm{e}^{-\kappa_1^-(\lambda)|x_1|}), \quad x_2\in[-d,0],$$

if $d<\pi$, and

$$\psi_n(x,a) = (\pm 1)^{n+1} c(\lambda_n,a) \mathrm{e}^{-\kappa_1^+(\lambda_n)|x_1|} \sin|x_2| + \mathcal{O}(\mathrm{e}^{-k_2^+(\lambda_n)|x_1|}), \quad x_2 \in [-\pi,\pi],$$

$$\nabla_x \psi_n(x,a) = (\pm 1)^{n+1} c(\lambda_n,a) \nabla_x \mathrm{e}^{-\kappa_1^+(\lambda_n)|x_1|} \sin|x_2| + \mathcal{O}(\mathrm{e}^{-k_2^+(\lambda_n)|x_1|}), \quad x_2 \in [-\pi,\pi],$$

in the case of equal-width channels, $d=\pi$. In these relations

$$c(\lambda_n,a) = \frac{1}{\pi\kappa_1^+(\lambda_n)} \int_{\gamma_a} \psi_n(x,a) \mathrm{e}^{\kappa_1^+(\lambda_n)x_1} \mathrm{d}x_1 = \frac{(-1)^{n+1}}{\pi\kappa_1^+(\lambda_n)} \int_{\gamma_a} \psi_n(x,a) \mathrm{e}^{-\kappa_1^+(\lambda_n)x_1} \mathrm{d}x_1, \tag{3.15}$$

and $c(\lambda_i,a) \neq 0$, $i=1,2$.

Proof. Applying Lemma 3.3 to ψ_n with $b_1=\pm a$, $b_2=0$, $b_3=\pi$ and $b_2=-d$, $b_3=0$, we obtain the needed asymptotic behavior of ψ_n. The factor $(\pm 1)^{n+1}$ in these formulas is due to the definite parity of ψ_n with respect to x_1. The formula (3.15) for $c_1^{(n)}$ follows from the chain of relations obtained by integration by parts,

$$0 = \int_{\Pi^+} \mathrm{e}^{\pm\kappa_1^+(\lambda_n)x_1} \sin x_2 (\Delta + \lambda_n) \psi_n(x,a) \mathrm{d}x = \int_{\gamma_a} \mathrm{e}^{\pm\kappa_1^+(\lambda_n)x_1} \psi_n(x,a) \mathrm{d}x - (\pm 1)^{n+1} \pi\kappa_1^+(\lambda_n) c(\lambda_n,a).$$

It remains to check the inequalities $c(\lambda_i,a) \neq 0$, $i=1,2$. Since

$$\lambda_1 = \frac{\|\nabla\psi_1\|^2_{L_2(\Pi_a)}}{\|\psi_1\|^2_{L_2(\Pi_a)}} = \frac{\|\nabla\widetilde{\psi}_1\|^2_{L_2(\Pi_a)}}{\|\widetilde{\psi}_1\|^2_{L_2(\Pi_a)}},$$

where $\widetilde{\psi}_1 := |\psi_1|$, we conclude that $\widetilde{\psi}_1$ is an eigenfunction associated with λ_1. This eigenvalue being simple, we infer that $\widetilde{\psi}_1 = \psi_1$. Hence, $\psi_1 \geqslant 0$. Moreover, ψ_1 is not identically zero at γ_a, since otherwise it would be an eigenfunction of the negative Dirichlet Laplacian in Π^+ and would correspond to the eigenvalue $\lambda_1 < 1$. At the same time, the spectrum of the mentioned operator is the halfline $[1,+\infty)$. The described properties of ψ_1 and the formula (3.15) imply that $c(\lambda_1,a) \neq 0$.

According to Proposition 2.1 the eigenfunction ψ_2 is odd with respect to x_1. Thus, the eigenvalue λ_2 is the ground state of the negative Dirichlet Laplacian in $\Pi_a \cap \{x : x_1 > 0\}$. Completely by analogy with how it was done for ψ_1, one can make sure that $\psi_2 \geqslant 0$ on $\Pi_a \cap \{x : x_1 > 0\}$, and $\psi_2(x_1,0,a) \not\equiv 0$ for $x_1 \in (0,a)$. The parity of ψ_2 allows us to modify the formula (3.15),

$$c(\lambda_2,a) = \frac{1}{\pi\kappa_1^+(\lambda_2)} \int_{\gamma_a} \psi_2(x,a) \sinh \kappa_1^+(\lambda_2) x_1 \mathrm{d}x_1 = \frac{2}{\pi\kappa_1^+(\lambda_2)} \int_0^a \psi_2(x_1,0,a) \sinh \kappa_1^+(\lambda_2) x_1 \mathrm{d}x_1.$$

Together with the non-negativity of ψ_2 on $\gamma_a \cap \{x : x_1 > 0\}$, it implies that $c_2(\lambda,a) \neq 0$. □

Lemma 3.7. For any $\lambda \in (-\infty,1) \setminus \sigma_{\mathrm{disc}}(H(a))$ there exists a unique solution of the boundary value problem (2.1) belonging to $W_2^1(\Pi_a)$. For large values of $|x_1|$ this function is infinitely differentiable and in the limit $x_1 \to +\infty$ it behaves as

$$U(x,\lambda,a) = c(\lambda,a)\mathrm{e}^{-\kappa_1^+(\lambda)x_1}\sin x_2 + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,\kappa_2^+(\lambda)x_1}), \quad x_2 \in [0,\pi],$$

$$\nabla_x U(x,\lambda,a) = c(\lambda,a)\nabla_x \mathrm{e}^{-\kappa_1^+(\lambda)x_1}\sin x_2 + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,\kappa_2^+(\lambda)x_1}), \quad x_2 \in [0,\pi], \tag{3.16}$$

$$U(x,\lambda,a) = \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,\kappa_1^-(\lambda)x_1}), \quad \nabla_x U(x,\lambda,a) = \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,\kappa_1^-(\lambda)x_1}), \quad x_2 \in [-d,0],$$

if $d<\pi$, *and*

$$U(x,\lambda,a) = c(\lambda,a)\mathrm{e}^{-\kappa_1^+(\lambda_n)x_1}\sin|x_2| + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,\kappa_2^+(\lambda)x_1}), \quad x_2 \in [-\pi,\pi],$$

$$\nabla_x U(x,\lambda,a) = c(\lambda,a)\nabla_x \mathrm{e}^{-\kappa_1^+(\lambda_n)x_1}\sin|x_2| + \mathcal{O}(\mathrm{e}^{-\mathrm{Re}\,k_2^+(\lambda)x_1}), \quad x_2 \in [-\pi,\pi], \tag{3.17}$$

in the case $d=\pi$ *where the coefficient is given by*

$$c(\lambda,a) = \frac{1}{\pi\kappa_1^+(\lambda)}\int_{\gamma_a} U(x,\lambda,a)\mathrm{e}^{\kappa_1^+(\lambda)x_1}\mathrm{d}x_1. \tag{3.18}$$

This coefficient is negative for $\lambda<\lambda_1(a)$.

Proof. The unique solvability of the problem (2.1) is ensured by Lemma 3.2. Moreover, we have $U=T_3(\lambda,a)\mathrm{e}^{\kappa_1^+(\lambda)x_1}$. The relations (3.16) and (3.17) follow from Lemma 3.3, and the formula (3.18) is proved in the same way as (3.15).

Integrating by parts and employing the formula (3.18), we obtain a chain of identities,

$$\begin{aligned} 0 = \int_\Pi U(\Delta+\lambda)U\mathrm{d}x &= \lambda\|U\|^2_{L_2(\Pi)} - \|\nabla U\|^2_{L_2(\Pi)} - \int_{\gamma_a} U\left(\left.\frac{\partial U}{\partial x_2}\right|_{x_2=+0} - \left.\frac{\partial U}{\partial x_2}\right|_{x_2=-0}\right)\mathrm{d}x_1 \\ &= \lambda\|U\|^2_{L_2(\Pi)} - \|\nabla U\|^2_{L_2(\Pi)} - \pi\kappa_1^+(\lambda)c(\lambda,a), \end{aligned}$$

which implies

$$c(\lambda,a) = \frac{\lambda\|U\|^2_{L_2(\Pi)} - \|\nabla U\|^2_{L_2(\Pi)}}{\pi\kappa_1^+(\lambda)}. \tag{3.19}$$

Since $U\in W_2^1(\Pi,\partial\Pi)$, the minimax principle yields the inequality

$$\|U\|^2_{L_2(\Pi)} \leqslant \frac{1}{\lambda_1(a)}\|\nabla U\|^2_{L_2(\Pi)}.$$

We substitute this inequality into the formula (3.19) and obtain

$$c(\lambda,a) \leqslant \frac{1}{\pi\kappa_1^+(\lambda)}\left(\frac{\lambda}{\lambda_1(a)} - 1\right)\|\nabla U\|^2_{L_2(\Pi)} < 0,$$

if $\lambda<\lambda_1(a)$.

IV. REDUCTION OF THE PERTURBED PROBLEM

In this section we shall transform the eigenvalue equation for H to another operator equation. The main advantage of such transformation is that the final equation involves only the resolvents of one-window operators $H(a_\pm)$. More specifically, the presented approach allows us to *decouple* two-window system and to reduce it to a small perturbation of a direct sum of left- and right-window operators.

We are looking for eigenvalues of the operator H, i.e., nontrivial $L_2(\Pi)$ solutions to the boundary value problem

$$-\Delta\psi=\lambda\psi,\quad x\in\Pi,\quad \psi=0,\quad x\in\partial\Pi. \tag{4.1}$$

We denote $Q^b:=\{x:-b<x_1<b,-d<x_2<\pi\}$ and introduce the cutoff regions $\Pi^b:=\Pi\cap Q^b$, $\Gamma^b:=\partial\Pi\cap Q^b$. Solutions to the problem (4.1) are functions belonging to $W_2^1(\Pi^b,\Gamma^b)$ for any $b>0$ such that

$$(\nabla\psi,\nabla\zeta)_{L_2(\Pi)}=\lambda(\psi,\zeta)_{L_2(\Pi)} \tag{4.2}$$

holds for each $\zeta\in C_0^\infty(\Pi)$; it follows from the smoothness-improving theorem mentioned above that such a ψ belongs to $C^\infty(\Pi)$.

We assume that $\lambda\in\mathbb{S}_\delta$, with $\delta>0$ is chosen in such a way that $\sigma_*\subset\mathbb{S}_\delta$. Let $f_\pm=f_\pm(\cdot,l)\in L_2(\gamma_{a_\pm})$ be an arbitrary pair of functions. Denote by $u_\pm$ the solutions of the problem (3.1) with $a=a_\pm$ and $f=f_\pm\in L_2(\gamma_{a_\pm})$ and assume that $u_\pm\in L_2(\Pi_{a_\pm})$. We will seek a solution to the problem (4.1) in the form

$$\psi(x,\lambda,l)=u_+(x_1-l,x_2,\lambda,l)+u_-(x_1+l,x_2,\lambda,l). \tag{4.3}$$

Suppose for a moment that the function ψ defined in this way solves the problem (4.1). In such a case the function ψ is infinitely differentiable at the points of the intervals $\gamma_{a_\pm}$, and therefore

$$\frac{\partial\psi}{\partial x_2}(x_1,+0,\lambda,l)-\frac{\partial\psi}{\partial x_2}(x_1,-0,\lambda,l)=0,\quad x\in\gamma_\pm.$$

Substituting from (4.3) into this identity, we obtain a pair of equations,

$$f_\pm(x_1)+\frac{\partial u_\mp}{\partial x_2}(x_1\pm 2l,+0,\lambda,l)-\frac{\partial u_\mp}{\partial x_2}(x_1\pm 2l,-0,\lambda,l)=0,\quad x\in\gamma_{a_\pm}. \tag{4.4}$$

Denote $\mathbf{f}=(f_+,f_-)\in L_2(\gamma_{a_+})\oplus L_2(\gamma_{a_-})$. The following lemma is the main ingredient of our technique and it states that the last equation is equivalent to the original problem (4.1).

Lemma 4.1. For any solution $\mathbf{f}\in L_2(\gamma_{a_+})\oplus L_2(\gamma_{a_-})$ *of* (4.4) *and functions* $u_\pm$ *solving* (3.1) *for* $a=a_\pm$, $f=f_\pm$ *there exists a unique* $L_2(\Pi)$ *solution of* (4.1) *given by* (4.3). *Reversely, for any solution* ψ *of* (4.1) *there are unique* $\mathbf{f}\in L_2(\gamma_{a_+})\oplus L_2(\gamma_{a_-})$ *solving* (4.4) *and unique functions* $u_\pm\in L_2(\Pi_{a_\pm})$ *satisfying* (3.1) *with* $a=a_\pm$, $f=f_\pm$ *such that* ψ *is given by* (4.3). *This equivalence holds for any* $\lambda\in\mathbb{S}_\delta$ *and* $l\geqslant\max\{a_-,a_+\}+1$.

Proof. Suppose that $\mathbf{f}\in L_2(\gamma_{a_+})\oplus L_2(\gamma_{a_-})$ is a solution to the equations (4.4), where the functions $u_\pm\in L_2(\Pi_{a_\pm})$ solve the problem (3.1) for $a=a_\pm$ and $f=f_\pm$. We define ψ in accordance with (4.3). The functions $u_\pm$ are elements of $L_2(\Pi)$; hence, the same is true for ψ. Moreover, the function ψ belongs obviously to $W_2^1(\Pi^b,\Gamma^b)$ for each $b>0$ and vanishes on Γ.

Let us check that the function ψ satisfies Eq. (4.2). To this purpose, we indicate by $\chi_2=\chi_2(x_1)$ an infinitely differentiable cutoff function being equal to 1 if $|x_1+l|<\max\{a_+,a_-\}+1/2$ and vanishing if $|x_1+l|>\max\{a_+,a_-\}+1$. For any $\zeta\in C_0^\infty(\Pi)$ we have

$$\begin{aligned}(\nabla u_+,\nabla\zeta)_{L_2(\Pi)}-\lambda(u_+,\zeta)_{L_2(\Pi)}&=(\nabla u_+,\nabla(\zeta\chi_2))_{L_2(\Pi)}-\lambda(u_+,\zeta\chi_2)_{L_2(\Pi)}+(\nabla u_+,\nabla(\zeta(1-\chi_2)))_{L_2(\Pi)}\\&\quad-\lambda(u_+,\zeta(1-\chi_2))_{L_2(\Pi)},\end{aligned} \tag{4.5}$$

where the arguments of u_+ are (x_1-l,x_2,λ,l). Since $u_+(\cdot)$ is an element of $C^\infty(\Pi_{a_+}\setminus\bar{Q}^{a_+})$, we can integrate by parts,

$$(\nabla u_+,\ \nabla\zeta\chi_2))_{L_2(\Pi)} - \lambda(u_+,\zeta\chi_2)_{L_2(\Pi)} = -\int_{\gamma_-}\left(\frac{\partial u_+}{\partial x_2}(\cdot - l,+0,\lambda,l) - \frac{\partial u_+}{\partial x_2}(\cdot - l,-0,\lambda,l)\right)\zeta \mathrm{d}x_1$$
$$-\int_\Pi \zeta\chi_2(\Delta+\lambda)u_+ \mathrm{d}x = \int_{\gamma_-} f_-(\cdot + l)\zeta \mathrm{d}x_1,$$

where $u_+ = u_+(x_1 - l, x_2, \lambda, l)$. We have employed here the equation satisfied by u_+ as well as Eq. (4.4) for f_+. Since $\zeta(x_1+l,x_2)(1-\chi_2(x_1+l)) \in C_0^\infty(\Pi_{a_+})$, we can use the identity (3.2) to infer that

$$(\nabla u_+, \nabla\zeta(1-\chi_2))_{L_2(\Pi)} - (u_+, \zeta(1-\chi_2))_{L_2(\Pi)} = -\int_{\gamma_+} f_+(\cdot - l)\zeta \mathrm{d}x_1,$$

where $u_+ = u_+(x_1 - l, x_2, \lambda, l)$. We substitute now the last two relations into (4.5) and arrive at the identity

$$(\nabla u_+, \nabla\zeta)_{L_2(\Pi)} - \lambda(u_+,\zeta)_{L_2(\Pi)} = (f_-(\cdot + l),\zeta)_{L_2(\gamma_-)} - (f_+(\cdot - l),\zeta)_{L_2(\gamma_+)},$$

where $u_+ = u_+(x_1 - l, x_2, \lambda, l)$. In the same way, one can check that

$$(\nabla u_-, \nabla\zeta)_{L_2(\Pi)} - \lambda(u_-,\zeta)_{L_2(\Pi)} = (f_+(\cdot - l),\zeta)_{L_2(\gamma_+)} - (f_-(\cdot + l),\zeta)_{L_2(\gamma_-)},$$

where $u_- = u_-(x_1 + l, x_2, \lambda, l)$. Summing the last two relations we arrive at the relation (4.2) for the function ψ.

Let ψ be a solution to the problem (4.1) belonging to $L_2(\Pi)$. By smoothness-improving theorems the function ψ belongs to $C^\infty(\{x: -1 \leqslant x_1 \leqslant 1, 0 \leqslant x_2 \leqslant \pi\})$ and to $C^\infty(\{x: -1 \leqslant x_1 1 \leqslant, -d \leqslant x_2 \leqslant 0\})$. This allows us to define the numbers

$$\alpha_j^\pm = \alpha_j^\pm(\lambda,l) := \frac{2}{\pi}\int_0^\pi \left(\psi(0,x_2,\lambda,l) \pm \frac{1}{\kappa_j^+(\lambda)}\frac{\partial\psi}{\partial x_1}(0,x_2,\lambda,l)\right)\sin jx_2 \mathrm{d}x_2,$$

$$\beta_j^\pm = \beta_j^\pm(\lambda,l) := \frac{2}{d}\int_0^\pi \left(\psi(0,x_2,\lambda,l) \pm \frac{1}{\kappa_j^-(\lambda)}\frac{\partial\psi}{\partial x_1}(0,x_2,\lambda,l)\right)\sin\frac{\pi j}{d}x_2 \mathrm{d}x_2.$$

Using these numbers, we introduce the functions $u_\pm$ in the following way:

$$u_\pm(x_1 \mp l, x_2, \lambda, l) := \sum_{j=1}^\infty \alpha_j^\pm(\lambda,l)\mathrm{e}^{\pm\kappa_j^+(\lambda)x_1}\sin jx_2, \quad \pm x_1 \leqslant 0, \quad x_2 \in (0,\pi),$$

$$u_\pm(x_1 \mp l, x_2, \lambda, l) := \sum_{j=1}^\infty \beta_j^+(\lambda,l)\mathrm{e}^{\pm\kappa_j^-(\lambda)x_1}\sin\frac{\pi j}{d}x_2, \quad \pm x_1 \leqslant 0, \quad x_2 \in (-d,0),$$

$$u_\pm(x_1 \mp l, x_2, \lambda, l) := \psi(x,\lambda,l) - u_\pm(x_1 \pm l, x_2, \lambda), \quad \pm x_1 > 0, \quad x_2 \in (-d,\pi).$$

Proceeding in the same way as in the proof of Lemma 4.1 in Ref. 4, we check that the functions $u_\pm$ are well defined and

$$u_\pm \in W_2^1(\Pi_{a_\pm},\Gamma_{a_\pm}) \cap W_2^2(S), \quad S \in \Xi_a, \tag{4.6}$$

$$(\Delta+\lambda)u_\pm(x_1 \mp l, x_2, \lambda, l) = 0, \quad x \in \Pi \setminus \{x: x_1 = 0\}. \tag{4.7}$$

The relation (4.3) follows from the definition of the functions $u_\pm$. Now, we set

$$f_\pm(x_1,l) := -\frac{\partial u_\mp}{\partial x_2}(x_1 \pm 2l, +0,\lambda,l) + \frac{\partial u_\mp}{\partial x_2}(x_1 \pm 2l,-0,\lambda,l), \quad x_1 \in (-a_\pm,a_\pm); \tag{4.8}$$

in view of (4.6) we can conclude that $f_\pm(\cdot,l) \in L_2(\gamma_{a_\pm})$. We also note that the definition of $u_\pm$ and the smoothness of ψ at $\gamma_\pm$ imply

$$f_\pm(x_1,l) = \frac{\partial u_\pm}{\partial x_2}(x_1, +0,\lambda,l) - \frac{\partial u_\pm}{\partial x_2}(x_1,-0,\lambda,l), \quad x_1 \in (-a_\pm,a_\pm). \tag{4.9}$$

Let us check the integral equation (3.2) for the function $u_+ = u_+(x,\lambda)$. Taking into account (4.7) and (4.9), and integrating by parts, we get

$$-(\nabla u_+,\nabla\zeta)_{L_2(\Pi_a)} + \lambda(u_+,\zeta)_{L_2(\Pi_a)} = \left(\frac{\partial u_+}{\partial x_2}(x_1, +0,\lambda) - \frac{\partial u_+}{\partial x_2}(x_1,-0,\lambda),\zeta\right)_{L_2(\gamma_{a_+})} = (f_+,\zeta)_{L_2(\gamma_{a_+})}$$

for any $\zeta \in C_0^\infty(\Pi_{a_+})$. In the same way one can check that

$$-(\nabla u_-,\nabla\zeta)_{L_2(\Pi_a)} + \lambda(u_-,\zeta)_{L_2(\Pi_a)} = (f_-,\zeta)_{L_2(\gamma_{a_-})}$$

for any $\zeta \in C_0^\infty(\Pi_{a_-})$; thus, $u_\pm$ are solutions to the problem (3.1) for $a = a_\pm$ and $f = f_\pm$. Equations (4.4) follow from (4.8).

Suppose that $\lambda \in \mathbb{S}_\delta \setminus \sigma_*$. In that case the functions $u_\pm$ introduced above can be represented as $u_\pm = T_3(\lambda,a_\pm) f_\pm$; thus, Eq. (4.4) become

$$\boldsymbol{f} + T_8(\lambda,l,\boldsymbol{a})\boldsymbol{f} = 0, \tag{4.10}$$

where the operator $T_8 : L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-}) \to L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-})$ is defined by

$$T_8(\lambda,l,\boldsymbol{a})\boldsymbol{f} := (T_8^+(\lambda,l,a_-,a_+)f_-, T_8^-(\lambda,l,a_+,a_-)f_+).$$

Now we are ready to demonstrate the first of our main results.

Proof of Theorem 2.1. If $a_\pm = 0$ the essential spectrum of the operator H is obviously $[1,+\infty)$, and an elementary argument using Dirichlet-Neumann bracketing (Ref. 16 Chap. XIII, Sec. 15) and the minimax principle (Ref. 16 Chap. XIII, Sec. 1) shows that the threshold of the essential spectrum of H is 1, i.e., $\sigma_{\mathrm{ess}}(H) \subseteq [1,+\infty)$. The opposite inclusion can be shown easily; one needs to employ Weyl's criterion (see, for instance, proof of Lemma 2.1 in Ref. 4).

The operator H being self-adjoint, its isolated eigenvalues are real, and in view of the above observation they are smaller than 1. To prove the uniform bound on their total multiplicity we use bracketing in a way analogous to Ref. 1; without loss of generality we may suppose that $l \geqslant \max\{a_-,a_+\}$. We add Neumann boundaries at segments corresponding to x_1 at the endpoints of $\gamma_\pm$ and $x_2 \in (-d,\pi)$; in this way we get an operator estimating H from below. To be completely explicit, we get a lower bound $H \geqslant H_{\mathrm{left}} \oplus H_{\mathrm{lw}} \oplus H_{\mathrm{middle}} \oplus H_{\mathrm{rw}} \oplus H_{\mathrm{right}}$, and since only the window part $H_{\mathrm{windows}} = H_{\mathrm{lw}} \oplus H_{\mathrm{rw}}$ contributes to the spectrum below 1, being obviously independent of l, we infer by minimax that H has finitely many eigenvalues for any $l > 0$ and their number counting multiplicity has a bound independent of l.

The eigenvalue continuity can be established using a simple perturbation argument. The operator H' with the window distance $2l'$ can be mapped unitarily into an operator on $L_2(\Pi)$ with the same boundary condition as H by means of the longitudinal coordinate change, $x_1 \to x_1' := x_1 + \varepsilon\int_0^x \varphi(y)\mathrm{d}y$ with an arbitrary $\varphi \in C_0^\infty(\mathbb{R})$ of nonzero mean such that $\operatorname{supp}\varphi \in \left(-\frac{1}{2}l,-\frac{1}{2}l\right)$; for large enough l the region where the coordinates are changed is clearly disjoint with the windows. The variation of the window distance is in this way expressed through the operator coefficients on a fixed domain, and since $l' - l = \varepsilon\int_{-l/2}^{l/2}\varphi(y)\mathrm{d}y$, the sought continuity for $\varepsilon \to 0$ follows easily by analytic perturbation theory.

Let $K \subset \mathbb{S}_\delta$ be any compact set separated from σ_* by a positive distance. By the estimates (3.10) the operator T_8 has a norm being strictly less than 1 for $\lambda \in K$ and l large enough. For such

λ and l Eq. (4.10) has thus a trivial solution only, and in view of Lemma 4.1 this implies that the operator H has no eigenvalues in the set K if l is large enough. This means that each eigenvalue of the operator H has to converge to one of the numbers from the set σ_* or to the threshold of the essential spectrum.

The eigenvalues of H, i.e., those λ for which the problem (4.1) has a nontrivial $L_2(\Pi)$ solution, coincide in view of Lemma 4.1 with the values of λ for which Eq. (4.4) has a nontrivial solution. In the case considered here we deal only with the eigenvalues of H which converge to a value $\lambda_* \in \sigma_*$ separated from the threshold, in other words, being smaller than 1.

Our aim is to solve Eq. (4.4) and to obtain in this way an equation for the aforementioned values of λ. Consider a $\lambda_* \in \sigma_*$; if $\lambda_*=\lambda_n$ is an eigenvalue of the operator $H(a_+)$ we set

$$\boldsymbol{\phi}_*^+(\cdot,l) := (0,\phi_n^-(\cdot,l,a_+)) \in L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-}), \quad T_4^+\boldsymbol{f} := (f_+,\psi_n)_{L_2(\gamma_{a_+})},$$

where ϕ_n^- is determined by ψ_n in accordance with (3.12) and ψ_n is an eigenfunction associated with λ_n. In the opposite case we set

$$\boldsymbol{\phi}_*^+(\cdot,l) := (0,0) \in L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-}), \quad T_4^+\boldsymbol{f} := 0.$$

Analogously, if $\lambda_*=\lambda_n$ is an eigenvalue of $H(a_-)$, we set

$$\boldsymbol{\phi}_*^-(\cdot,l) := (\phi_n^+(\cdot,l,a_-),0) \in L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-}), \quad T_4^-\boldsymbol{f} := (f_-,\psi_n)_{L_2(\gamma_{a_-})},$$

where ϕ_n^+ corresponds to ψ_n in accordance with (3.12) and ψ_n is an eigenfunction associated with λ_n; otherwise,

$$\boldsymbol{\phi}_*^-(\cdot,l) := (0,0) \in L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-}), \quad T_4^-\boldsymbol{f} := 0.$$

Given a number $\lambda_* \in \sigma_*$, we consider Eq. (4.4) for λ in the vicinity of λ_*. Assume first that $\lambda \neq \lambda_*$, in which case Eq. (4.4) is equivalent to (4.10). In view of Lemma 3.5 the operator T_8 is bounded and meromorphic as a function of $\lambda \in \mathbb{S}_\delta$, and the numbers $\lambda_* \in \sigma_*$ are poles of T_8. For any λ close to λ_* the operator T_8 can be thus represented as

$$T_8(\lambda,l,\boldsymbol{a}) = \boldsymbol{\phi}_*^+(\cdot,l)\frac{T_4^+}{\lambda-\lambda_*} + \boldsymbol{\phi}_*^-(\cdot,l)\frac{T_4^-}{\lambda-\lambda_*} + T_9(\lambda,l,\boldsymbol{a}), \tag{4.11}$$

where the operator T_9 acts as

$$T_9(\lambda,l,\boldsymbol{a})\boldsymbol{f} := (T_8^+(\lambda,l,a_-,a_+)f_-, T_9^-(\lambda,l,a_+,a_-)f_+)$$

if $\lambda_* \in \sigma_{\mathrm{disc}}(H(a_+))\setminus\sigma_{\mathrm{disc}}(H(a_-))$,

$$T_9(\lambda,l,\boldsymbol{a})\boldsymbol{f} := (T_9^+(\lambda,l,a_-,a_+)f_-, T_8^-(\lambda,l,a_+,a_-)f_+)$$

if $\lambda_* \in \sigma_{\mathrm{disc}}(H(a_-))\setminus\sigma_{\mathrm{disc}}(H(a_+))$, and finally,

$$T_9(\lambda,l,\boldsymbol{a})\boldsymbol{f} := (T_9^+(\lambda,l,a_-,a_+)f_-, T_9^-(\lambda,l,a_+,a_-)f_+)$$

if $\lambda_* \in \sigma_{\mathrm{disc}}(H(a_-)) \cap \sigma_{\mathrm{disc}}(H(a_+))$. The operator T_9 on $L_2(\gamma_{a_+}) \oplus L_2(\gamma_{a_-})$ is bounded and holomorphic with respect to λ in the vicinity of λ_*, and the estimate

$$\left\| \frac{\partial^i T_9}{\partial \lambda^i} \right\| \leqslant C l^{i+1} \mathrm{e}^{-2l \operatorname{Re} \kappa_1^+(\lambda)}, \quad i=0,1, \tag{4.12}$$

holds true with a constant C which is independent on λ and l.

We substitute the representation (4.11) into (4.10) to obtain

$$\boldsymbol{f}+\frac{T_4^+\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\phi}_*^+ + \frac{T_4^-\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\phi}_*^- + T_9\boldsymbol{f}=0.$$

Since the norm of T_9 is small for large l due to (4.12), the operator $(\mathrm{I}+T_9)^{-1}$ is well defined being bounded in $L_2(\gamma_{a_+})\oplus L_2(\gamma_{a_-})$. We apply this operator to the last equation, arriving at

$$\boldsymbol{f}+\frac{T_4^+\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\Phi}_*^+ + \frac{T_4^-\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\Phi}_*^- = 0, \tag{4.13}$$

where $\boldsymbol{\Phi}_*^\pm(\cdot,\lambda,l)=(\mathrm{I}+T_9(\lambda,l,\boldsymbol{a}))^{-1}\boldsymbol{\phi}_*^\pm(\cdot,l)$. The last equation implies that

$$\boldsymbol{f}=c_+\boldsymbol{\Phi}_*^+ + c_-\boldsymbol{\Phi}_*^- \tag{4.14}$$

for some numbers $c_\pm$. We substitute from here into (4.13), obtaining

$$\boldsymbol{\Phi}_*^+\left(c_+\left(1+\frac{A_{11}}{\lambda-\lambda_*}\right)+c_-\frac{A_{12}}{\lambda-\lambda_*}\right)+\boldsymbol{\Phi}_*^-\left(c_+\frac{A_{21}}{\lambda-\lambda_*}+c_-\left(1+\frac{A_{22}}{\lambda-\lambda_*}\right)\right)=0, \tag{4.15}$$

where the quantities $A_{ij}=A_{ij}(\lambda,l)$ are defined by

$$A_{11}(\lambda,l) := T_4^+\Phi_*^+(\cdot,\lambda,l), \quad A_{12}(\lambda,l) := T_4^+\Phi_*^-(\cdot,\lambda,l),$$

$$A_{21}(\lambda,l) := T_4^-\Phi_*^+(\cdot,\lambda,l), \quad A_{22}(\lambda,l) := T_4^-\Phi_*^-(\cdot,\lambda,l).$$

The definition of $\boldsymbol{\Phi}_*^\pm$, together with the estimate (4.12), implies for l large enough

$$\boldsymbol{\Phi}_*^\pm=\boldsymbol{\phi}_*^\pm+\mathcal{O}(\mathrm{e}^{-2l\ \mathrm{Re}\ \kappa_1^+(\lambda)}\|\boldsymbol{\phi}_*^\pm\|). \tag{4.16}$$

If $\boldsymbol{\phi}_*^+\neq 0$, and $\boldsymbol{\phi}_*^-=0$, in particular, we have

$$\boldsymbol{\Phi}_*^+\neq 0, \quad \boldsymbol{\Phi}_*^-=0, \quad A_{12}=A_{22}=0, \tag{4.17}$$

and in this case Eq. (4.15) holds if and only if

$$c_+\left(1+\frac{A_{11}}{\lambda-\lambda_*}\right)=0.$$

If $\boldsymbol{f}$ corresponds to an eigenfunction ψ of the problem (4.1) by (4.3), the number c_+ is nonzero. Indeed, in the opposite case the identities (4.14) and (4.17) would imply that $\boldsymbol{f}=0$, which by Lemma 4.1 results in $\psi=0$. Consequently, Eq. (4.10) has in this case a nontrivial solution if and only if

$$\lambda-\lambda_*+A_{11}(\lambda,l)=0. \tag{4.18}$$

If λ is a root of this equation, the corresponding nontrivial solution of (4.10) can be expressed as (4.14) with $c_+\neq 0$ and $c_-=0$.

In the case $\boldsymbol{\phi}_*^+=0$ and $\boldsymbol{\phi}_*^-\neq 0$, similar arguments lead us to the conclusion that Eq. (4.10) has a nontrivial solution if and only if

$$\lambda-\lambda_*+A_{22}(\lambda,l)=0, \tag{4.19}$$

and the corresponding nontrivial solution can be written as (4.14) with the coefficients $c_+=0$ and $c_-\neq 0$.

Finally, if both the vectors $\boldsymbol{\phi}_*^\pm$ are nonzero, they are linearly independent by definition and the same is true for the vectors $\boldsymbol{\Phi}_*^\pm$. Hence Eq. (4.10) holds if and only if

$$((\lambda-\lambda_*)\mathrm{E}+\mathrm{A}(\lambda,l))\boldsymbol{c}=0, \tag{4.20}$$

where E is the unit matrix, and

$$\mathrm{A}(\lambda,l):=\begin{pmatrix} A_{11}(\lambda,l) & A_{12}(\lambda,l) \\ A_{21}(\lambda,l) & A_{22}(\lambda,l) \end{pmatrix}, \quad \boldsymbol{c}:=\begin{pmatrix} c_+ \\ c_- \end{pmatrix}.$$

The column $\boldsymbol{c}$ is nonzero, since otherwise (4.14) and (4.17) would imply $\boldsymbol{f}=0$; thus, the system (4.20) of linear equations has a nontrivial solution if and only if

$$\det((\lambda-\lambda_*)\mathrm{E}+\mathrm{A}(\lambda,l))=0, \tag{4.21}$$

which can be rewritten as

$$(\lambda-\lambda_*)^2+(\lambda-\lambda_*)\mathrm{tr}\mathrm{A}(\lambda,l)+\det \mathrm{A}(\lambda,l)=0; \tag{4.22}$$

the corresponding nontrivial solution of Eq. (4.10) is given by (4.14), where $\binom{c_+}{c_-}$ is a nontrivial solution of (4.20).

Assume now that $\lambda=\lambda_*$. Let λ_* coincide with an eigenvalue λ_n of the operator $H(a_+)$ being not at the same time an eigenvalue of $H(a_-)$. In this case we again can claim that $u_-=T_3(\lambda_*,a_-)f_-$, on the other hand, the boundary value problem for u_+ with $\lambda=\lambda_*$ is solvable if and only if

$$0=\int_{\gamma_{a_+}} f_+\psi_n(x,a_+)\mathrm{d}x=T_4^+\boldsymbol{f}. \tag{4.23}$$

This follows from Lemma 3.2. The function u_+ is given by $u_+=T_5(\lambda_*,a_+)f_+-c_+\psi_+$, where c_+ is a constant. We can substitute now the described $u_\pm$ into (4.4) and obtain

$$\begin{gathered} \boldsymbol{f}+T_9(\lambda,l,\boldsymbol{a})\boldsymbol{f}=c_+\boldsymbol{\phi}_*^+, \\ \boldsymbol{f}=c_+\boldsymbol{\Phi}_*^+. \end{gathered} \tag{4.24}$$

This function will generate a solution to the problem (4.1) if and only if (4.18) holds true. Substituting (4.24) into (4.23), we arrive at Eq. (4.18) with $\lambda=\lambda_*$. If $c_+\neq 0$ holds in (4.24) we see that the formula (4.23) coincides with (4.14) with $c_-=0$. Consequently, in the case $\lambda_* \in \sigma(H(a_-))\setminus\sigma(H(a_+))$ Eq. (4.18) determines all the values of λ in the vicinity of λ_* for which Eq. (4.4) has a nontrivial solution; these nontrivial solutions are given by (4.14) with $c_+\neq 0$ and $c_-=0$.

In the same way one can check that Eq. (4.19) determines the sought values of λ in the case when λ_* is an eigenvalue of the operator $H(a_-)$ and not of $H(a_+)$. The corresponding nontrivial solutions of (4.4) have $c_+=0$ and $c_-\neq 0$.

Finally, if $\lambda_*\in\sigma_*$ is double and $\lambda=\lambda_*$, the solvability conditions of the boundary value problems for u are $T_4^\pm\boldsymbol{f}=0$. If this holds true, the functions $u_\pm$ are given by $u_\pm=T_5(\lambda,a_\pm)-c_\pm\psi_\pm(\cdot)$, where $c_\pm$ are constants and $\psi_\pm$ are the eigenfunctions of $H(a_\pm)$ associated with λ_*. Equation (4.4) becomes

$$\boldsymbol{f}+T_9(\lambda_*,l,\boldsymbol{a})\boldsymbol{f}=c_+\boldsymbol{\phi}_*^+ + c_-\boldsymbol{\phi}_*^-,$$

which yields the relation (4.14). The solvability conditions $T_4^\pm\boldsymbol{f}=0$ are nothing else than the system of linear equations (4.20). In this way (4.14), (4.20), and (4.21) describe the sought values of λ in the vicinity of λ_* and the corresponding nontrivial solutions of (4.4).

V. PROOFS OF THEOREMS 2.2–2.4

Now we are going to demonstrate the remaining part of our claims. In order to do it, we employ the results of the previous section. More specifically, we analyze the behavior of the roots of Eqs. (4.18), (4.19), and (4.22).

Proof of Theorem 2.2. We will give the proof for the case $\lambda_*=\lambda_n(a_-)$; the argument for $\lambda_*=\lambda_n(a_+)$ is similar. In accordance with the results of the previous section, if the eigenvalue $\lambda^-(a,l)$ exists, it must be a root of the Eq. (4.19). Let us prove first that there is a unique root which converges to λ_* as $l\to+\infty$. Lemma 3.6 implies that the relation

$$\phi_n^+(x_1,l,a_-)=\tau c(\lambda_*,a_-)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}), \tag{5.1}$$

holds in the norm of $L_2(\gamma_{a_+})$; hence, by the definition of $\boldsymbol{\phi}_*^-$ we have

$$\boldsymbol{\phi}_*^-(x_1,l)=\tau c(\lambda_*,a_-)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1},0)+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}). \tag{5.2}$$

This formula, in combination with the estimate (4.12), leads to the relation

$$A_{22}(\lambda,l)=\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}). \tag{5.3}$$

Since T_9 is holomorphic with respect to λ and has a small norm for large l, we infer that the left-hand side of the last equation is holomorphic in λ. In view of (5.3) for a small δ the function A_{22} satisfies the estimate $|A_{22}|<\delta$ if l is large enough and $|\lambda-\lambda_*|=\delta$; by Rouché theorem it implies that the function $\lambda\mapsto\lambda-\lambda_*+A_{22}(\lambda,l)$ has the same number of zeros in the disk $\{\lambda:|\lambda-\lambda_*|<\delta\}$ as the function $\lambda\mapsto\lambda-\lambda_*$ does. The number δ is arbitrary, so we can conclude that there is a unique root of Eq. (4.19) converging to λ_* as $l\to+\infty$. As a consequence, there exists a unique eigenvalue of the operator H converging to λ_* as $l\to+\infty$; we will denote this eigenvalue as $\lambda(l,\boldsymbol{a})$. The estimate (5.3) implies at the same time that

$$\lambda(l,\boldsymbol{a})-\lambda_*=\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}). \tag{5.4}$$

Let us derive the asymptotic expansion (2.2) for the eigenvalue $\lambda(l,\boldsymbol{a})$. In order to do it, we will need to know the asymptotic behavior for A_{22} in a way more precise than (5.3). For the sake of brevity we will write simply λ instead of $\lambda(l,\boldsymbol{a})$. The relations (5.2) together with the estimates (4.12) and (5.4) imply that

$$\begin{aligned}
A_{22}(\lambda,l)&=T_4^-(\mathrm{I}+T_9(\lambda,l,\boldsymbol{a}))^{-1}\boldsymbol{\phi}_*^-(\cdot,l)\\
&=T_4^-\boldsymbol{\phi}_*^-(\cdot,l)-T_4^-T_9(\lambda,l,\boldsymbol{a})\boldsymbol{\phi}_*^-(\cdot,l)+\mathcal{O}(\|T_9\|^2\|\boldsymbol{\phi}_*^-\|)\\
&=-T_4^-T_9(\lambda_*,l,\boldsymbol{a})\boldsymbol{\phi}_*^-(\cdot,l)+\mathcal{O}\left(|\lambda-\lambda_*|\left\|\frac{\partial T_9}{\partial\lambda}\right\|\|\boldsymbol{\phi}_*^-\|+\|T_9\|^2\|\boldsymbol{\phi}_*^-\|\right)\\
&=-T_4^-T_8^-(\lambda,l,\boldsymbol{a})\phi_n^+(\cdot,l,a_-)+\mathcal{O}(|\lambda-\lambda_*|l^2\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}+l\mathrm{e}^{-6\kappa_1^+(\lambda_*)l}).
\end{aligned} \tag{5.5}$$

Taking into account the estimate (3.10) for $\|T_8^-\|$ and the relation (5.1), we can proceed with the calculations, obtaining

$$\begin{aligned}
A_{22}(\lambda,l)=&-\tau c(\lambda,a_-)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(T_8^-(\lambda_*,l,a_+,a_-)\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1},\psi_*)_{L_2(\gamma_{a_-})}+\mathcal{O}(|\lambda-\lambda_*|l^2\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}\\
&+\mathrm{e}^{-2l(\kappa_1^+(\lambda_*)+\rho(\lambda_*))}),
\end{aligned} \tag{5.6}$$

where we have denoted $\psi_*(x)=\psi_n(x,a_-)$. In view of the relation (3.14) the function $T_8^-(\lambda_*,l,a_+,a_-)\mathrm{e}^{\kappa_1^+(\lambda_*)x_1}$ coincides with $T_7^-(\lambda,l,a_+,a_-)u$, where u is the solution to the problem (3.1) with $a=a_+$, $\lambda=\lambda_*$, and $f=\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1}$. It is clear that $u(x)=U(-x_1,x_2,\lambda_*,a_+)$, and in view of (3.15)–(3.17) we obtain

$$\begin{aligned}
(T_8^-(\lambda_*,l,a_+,a_-)\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1},\psi_*)_{L_2(\gamma_{a_-})}&=c(\lambda_*,a_+)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(\mathrm{e}^{\kappa_1^+(\lambda_*)x_1},\psi_*)_{L_2(\gamma_{a_-})}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l})\\
&=\pi c(\lambda_*,a_+)c(\lambda_*,a_-)\kappa_1^+(\lambda_*)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}).
\end{aligned}$$

Substituting these identities into (5.6), we finally arrive at the following formula:

$$A_{22}(\lambda,l)=\mu^-(l,\boldsymbol{a})\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}+\mathcal{O}(|\lambda-\lambda_*|l^2\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}+\mathrm{e}^{-2l(\kappa_1^+(\lambda_*)+\rho(\lambda_*))}),$$

where $\mu^-(l,\boldsymbol{a})$ is defined by (2.3). It allows us to rewrite Eq. (4.19) as

$$(\lambda-\lambda_*)(1+\mathcal{O}(l^2\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}))=\mu^-(l,\boldsymbol{a})\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}+\mathcal{O}(\mathrm{e}^{-2l(\kappa_1^+(\lambda_*)+\rho(\lambda_*))});$$

expressing $(\lambda-\lambda_*)$ from here we get the asymptotic expansion (2.2) and the formula (2.3).

Next, we have to prove the asymptotic expansion for the eigenfunction associated with λ. The nontrivial solution of Eq. (4.4) is given by (4.14) with $c_+=0$ and $c_-=1$, i.e., as $\boldsymbol{f}=\boldsymbol{\Phi}_*^-$. We substitute it into the relation $u_+=T_3(\lambda(l,\boldsymbol{a}),a_+)f_+$ and take into account (5.2) and (4.16); this yields

$$u_+=T_3(\lambda(l,\boldsymbol{a}),a_+)f_+=\mathcal{O}(\|\boldsymbol{\phi}_*^-\|)=\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}),$$

which holds true in $W_2^1(\Pi_{a_+})$ and in $W_2^2(S)$ for each $S\in\Xi_{a_+}$. If $\lambda(l,\boldsymbol{a})\neq\lambda_*$, we obtain similarly with the help of Lemma 3.2

$$u_-=T_3(\lambda(l,\boldsymbol{a}),a_-)f_-=\frac{\psi_*}{\lambda(l,\boldsymbol{a})-\lambda_*}T_4^-\boldsymbol{\Phi}_*^-+T_5^-(\lambda(l,\boldsymbol{a}),a_-)f_-=\frac{A_{22}(\lambda(l,\boldsymbol{a}),l)\psi_*}{\lambda(l,\boldsymbol{a})-\lambda_*}+\mathcal{O}(\|\boldsymbol{\phi}_*^-\|). \tag{5.7}$$

Due to Eq. (4.19) it follows that

$$u_-=-\psi_*+\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l})$$

holds in $W_2^1(\Pi_a)$ and $W_2^2(S)$ for each $S\in\Xi_{a_-}$. If $\lambda(l,\boldsymbol{a})=\lambda_*$, the last relation holds again; in order to prove it, it is sufficient to employ the identity

$$u_-=T_5(\lambda_*,a_-)f_--c_-\psi_*=T_5(\lambda_*,a_-)f_--\psi_*.$$

The relations obtained in this way together with (4.3) lead to (2.4). ■

Proof of Theorem 2.3. The general lines of the proof are similar to those of the previous one. According to the results of the previous section the eigenvalues of H converging to λ_* are roots of Eq. (4.22). First we will check that the function at the left-hand side of this equation has two zeros, the order taken into account, which converge to λ_* as $l\to+\infty$.

To this aim, we need to estimate the functions A_{ij}. Lemma 3.6 implies

$$\phi_m^-(x_1,l,a_+)=(-1)^m\pi c(\lambda_*,a_+)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}). \tag{5.8}$$

This formula, together with (5.1), allows us to conclude that

$$A_{ij}(\lambda,l)=\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}), \tag{5.9}$$

hence for any small δ we have the inequality

$$|(\lambda-\lambda_*)\mathrm{tr}A(\lambda,l)+\det A(\lambda,l)|<\delta^2\quad\text{as } |\lambda-\lambda_*|=\delta,$$

if l is large enough. Since the functions A_{ij} are holomorphic, by Rouché theorem this inequality implies that the function $\lambda\mapsto D(\lambda,l):=\det((\lambda-\lambda_*)\mathrm{E}+\mathrm{A}(\lambda,l))$ has the same number of zeros (with the order taken into account) as the function $\lambda\mapsto(\lambda-\lambda_*)^2$ does. The last function has λ_* as a second-order zero, of course, so it follows that the function $D(\cdot,l)$ has two zeros, with the order taken into account, which converge to λ_* as $l\to+\infty$. In what follows we denote these roots as $\lambda^\pm$; the case of the second-order zero corresponds to the equality $\lambda^+=\lambda^-$.

As it was established in the previous section, the nontrivial solutions of Eq. (4.4) associated with the roots of (4.22) are given by (4.14) with the coefficients $c_\pm$ solving the system of linear equations (4.20). If the numbers $\lambda^\pm$ solve (4.21), the system (4.20) has at least one nontrivial solution corresponding to λ^+ and λ^-.

Suppose that $\lambda^+ \neq \lambda^-$. Then $\lambda^\pm$ are simple zeros of the function $D(\cdot,l)$, and in view of the above discussion the system (4.20) has exactly one nontrivial solution for $\lambda=\lambda^+$ and $\lambda=\lambda^-$. Hence, in the case $\lambda^+ \neq \lambda^-$ the operator H has exactly two simple eigenvalues converging to λ_* as $l \to +\infty$.

Let us check that if the system (4.20) has two linear independent solutions referring to $\lambda=\lambda^\pm$, it follows that $\lambda^\pm$ is a second-order zero of the function $D(\cdot,l)$. Indeed, two linear independent solutions exist if and only if

$$A_{11}(\lambda^\pm,l) = A_{22}(\lambda^\pm,l) = \lambda_* - \lambda^\pm, \quad A_{12}(\lambda^\pm,l) = A_{21}(\lambda^\pm,l) = 0. \tag{5.10}$$

The derivative of $D(\lambda,l)$ with respect to λ equals

$$\frac{\partial D}{\partial \lambda}(\lambda,l) = 2(\lambda-\lambda_*) + (A_{11}(\lambda,l)+A_{22}(\lambda,l)) + (\lambda-\lambda_*)\left(\frac{\partial A_{11}}{\partial \lambda}(\lambda,l) + \frac{\partial A_{22}}{\partial \lambda}(\lambda,l)\right) + A_{11}(\lambda,l)\frac{\partial A_{22}}{\partial \lambda}(\lambda,l)$$
$$- A_{12}(\lambda,l)\frac{\partial A_{21}}{\partial \lambda}(\lambda,l) + A_{22}(\lambda,l)\frac{\partial A_{11}}{\partial \lambda}(\lambda,l) - A_{21}(\lambda,l)\frac{\partial A_{12}}{\partial \lambda}(\lambda,l).$$

Substituting from (5.10) into this expression, we see that

$$\frac{\partial D}{\partial \lambda}(\lambda,l) = 0 \quad \text{as } \lambda = \lambda^\pm,$$

thus $\lambda^\pm$ is a second-order zero.

It is more complicated to check existence of a double eigenvalue of the operator H if $\lambda^+ = \lambda^- =: \tilde{\lambda}$. It is equivalent to the fact that for $\lambda=\tilde{\lambda}$ the system (4.20) has two linear independent solutions, and this in turn is equivalent to the relations (5.10). Let us prove that they hold. Consider the boundary value problem

$$\begin{gathered}(\Delta+\lambda)u = 0, \quad x \in \Pi_a \setminus (\gamma_+ \cup \gamma_-), \quad u = 0, \quad x \in \partial\Pi, \\ \left.\frac{\partial u}{\partial x_2}\right|_{x_2=+0} - \left.\frac{\partial u}{\partial x_2}\right|_{x_2=-0} = -g_\pm, \quad x \in \gamma_\pm.\end{gathered} \tag{5.11}$$

Here $g_\pm \in L_2(\gamma_\pm)$ are arbitrary functions, and the parameter λ is supposed to range in a small neighborhood of λ_* without coinciding with λ_* and $\tilde{\lambda}$. This problem is uniquely solvable provided we seek a generalized solution to (5.11) belonging to $L_2(\Pi)$. In a complete analogy with the proof of Lemma 1 one can check easily that the problem (5.11) is equivalent to the equation

$$\boldsymbol{f} + T_8(\lambda,l,\boldsymbol{a})\boldsymbol{f} = \boldsymbol{g}, \tag{5.12}$$

where $\boldsymbol{g}=(g_+,g_-) \in L_2(\gamma_{a_-}) \oplus L_2(\gamma_{a_+})$, while the solution u of (5.11) is given by

$$u(x,\lambda,l) = u_+(x_1-l,x_2,\lambda,l) + u_-(x_1+l,x_2,\lambda,l), \quad u_\pm := T_3(\lambda,a_\pm)f_\pm.$$

We can solve Eq. (5.12) in the same way as Eq. (4.10), obtaining as a result that

$$\boldsymbol{f} + \frac{T_4^+\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\Phi}_*^+ + \frac{T_4^-\boldsymbol{f}}{\lambda-\lambda_*}\boldsymbol{\Phi}_*^- = \boldsymbol{G}, \quad \boldsymbol{G} := (\mathrm{I} + T_9(\lambda,l,\boldsymbol{a}))^{-1}\boldsymbol{g}. \tag{5.13}$$

Hence the function $\boldsymbol{f}$ is of the form

$$\boldsymbol{f} = C_+\boldsymbol{\Phi}_*^+ + C_-\boldsymbol{\Phi}_*^- + \boldsymbol{G}, \tag{5.14}$$

where $C_\pm = C_\pm(\lambda,l)$ are constants to be found. Denoting $\boldsymbol{C} := \binom{C_+}{C_-}$ and substituting (5.14) into (5.13), we obtain an equation for $\boldsymbol{C}$,

$$((\lambda-\lambda_*)\mathrm{E}+\mathrm{A}(\lambda,l))\boldsymbol{C}=\boldsymbol{h},\quad \boldsymbol{h}:=\begin{pmatrix}-T_4^+\boldsymbol{G}\\ -T_4^-\boldsymbol{G}\end{pmatrix}. \tag{5.15}$$

The solution of this system is given by Cramer's formula,

$$C_+(\lambda,l)=\frac{A_{12}(\lambda,l)T_4^-\boldsymbol{G}-(\lambda-\lambda_*+A_{22}(\lambda,l))T_4^+\boldsymbol{G}}{D(\lambda,l)},$$

$$C_-(\lambda,l)=\frac{A_{21}(\lambda,l)T_4^+\boldsymbol{G}-(\lambda-\lambda_*+A_{11}(\lambda,l))T_4^-\boldsymbol{G}}{D(\lambda,l)}. \tag{5.16}$$

Using now (5.15) and Lemma 3.2, we infer that

$$\begin{aligned}u_+(\cdot,\lambda,l)&=-C_+(\lambda,l)\psi_m(\cdot,a_+)+C_+(\lambda,l)T_5(\lambda,a_+)\Phi_{*,+}^++C_-(\lambda,l)T_5(\lambda,a_+)\Phi_{*,+}^-+T_5(\lambda,a_+)G_+,\\ u_-(\cdot,\lambda,l)&=-C_-(\lambda,l)\psi_n(\cdot,a_-)+C_-(\lambda,l)T_5(\lambda,a_-)\Phi_{*,-}^++C_-(\lambda,l)T_5(\lambda,a_-)\Phi_{*,-}^-+T_5(\lambda,a_-)G_-,\end{aligned} \tag{5.17}$$

where $\Phi_{*,\pm}^\pm$ and $G_\pm$ are the components of the vectors $\boldsymbol{\Phi}_*^\pm$ and $\boldsymbol{G}$,

$$\boldsymbol{\Phi}_*^\pm=(\Phi_{*,+}^\pm,\Phi_{*,-}^\pm),\quad \boldsymbol{G}=(G_+,G_-).$$

Since the number $\tilde\lambda$ is a second-order zero of $D(\cdot,l)$, we conclude from (5.16) that the coefficients $C_\pm$ have, in general, a second-order pole at $\tilde\lambda$, and the same is true for $u_\pm$. Taking into account (5.17), we conclude that the solution of (5.11) can be represented as

$$u(x,\lambda,l)=u_{-1}^+(x,\lambda,l)C_+(\lambda,l)+u_{-1}^-(x,\lambda,l)C_-(\lambda,l)+\mathcal{O}(1),\quad \lambda\to\tilde\lambda.$$

In a complete analogy with the proof of Lemma 3.2, one can check easily that the solution of the problem (5.11) has a simple pole at $\tilde\lambda$. Hence the function $u_{-1}^+(x,\lambda,l)C_+(\lambda,l)+u_{-1}^-(x,\lambda,l)C_-(\lambda,l)$ has a simple pole at $\tilde\lambda$. For x from a neighborhood of γ_+ this function satisfies due to (5.16) and (5.17) the relation

$$\begin{aligned}&D(\lambda,l)(u_{-1}^+(x,\lambda,l)C_+(\lambda,l)+u_{-1}^-(x,\lambda,l)C_-(\lambda,l))\\ &\quad=((\lambda-\lambda_*+A_{22}(\lambda,l))T_4^+\boldsymbol{G}-A_{12}(\lambda,l)T_4^-\boldsymbol{G})\psi_m^+(x_1-l,x_2)+\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}).\end{aligned}$$

Since $\tilde\lambda$ is by assumption a second-order zero of $D(\cdot,l)$, the obtained identity yields

$$\tilde\lambda-\lambda_*+A_{22}(\tilde\lambda,l)=A_{12}(\tilde\lambda,l)=0.$$

Observing the behavior of the function u for x in the vicinity of γ_-, one can prove in the same way that

$$\tilde\lambda-\lambda_*+A_{11}(\tilde\lambda,l)=A_{21}(\tilde\lambda,l)=0.$$

This completes the check of the relations (5.10) for $\lambda^+=\lambda^-$, showing that in this case the operator H has a double eigenvalue converging to λ_* as $l\to+\infty$.

We proceed to calculation of the asymptotic expansions for the root(s) of Eq. (4.22). Substituting the estimates (5.9) into (4.22), we obtain

$$\lambda-\lambda_*=o(\mathrm{e}^{-\kappa_1^+(\lambda_*)l}). \tag{5.18}$$

This relation, in combination with (5.1) and (5.5) and the estimate (3.10), implies that

$$A_{22}(\lambda,l)=\mathcal{O}(l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}). \tag{5.19}$$

It is easy to establish an expression for A_{11} similar to (5.5), which together with (5.8) and (5.18) yield

$$A_{11}(\lambda,l)=\mathcal{O}(l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}). \tag{5.20}$$

Proceeding in the same way as in (5.5) we obtain a chain of relations,

$$\begin{aligned}A_{12}(\lambda,l)=T_4^+(\mathrm{I}+T_9(\lambda,l,\boldsymbol{a}))^{-1}\boldsymbol{\phi}_*^-(\cdot,l)&=T_4^+\boldsymbol{\phi}_*^-(\cdot,l)+\mathcal{O}(\|T_9\|\|\boldsymbol{\phi}_*^-\|)\\&=(\phi_n^+(\cdot,l,a_-),\psi_m(\cdot,a_+))_{L_2(\gamma_{a_+})}+\mathcal{O}(l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}).\end{aligned}$$

Due to (5.1) and (3.15) we have

$$\begin{aligned}(\phi_n^+(\cdot,l,a_-),\psi_m(\cdot,a_+))_{L_2(\gamma_{a_+})}&=c(\lambda_*,a_-)\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(\mathrm{e}^{-\kappa_1^+(\lambda_*)x_1},\psi_m(\cdot,a_+))_{L_2(\gamma_{a_+})}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l})\\&=\mu(l,\boldsymbol{a})\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}),\end{aligned}$$

where $\mu(l,\boldsymbol{a})$ is given by (2.6). Consequently,

$$A_{12}(\lambda,l)=\mu(l,\boldsymbol{a})\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}+l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}), \tag{5.21}$$

and in the same way one can show that

$$A_{21}(\lambda,l)=\mu(l,\boldsymbol{a})\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}+\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}+l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}). \tag{5.22}$$

Equation (4.22) is equivalent to the following pair of the equations:

$$\lambda-\lambda_*=\frac{-\mathrm{tr}A(\lambda,l)\pm\sqrt{(A_{11}(\lambda,l)-A_{22}(\lambda,l))^2+4A_{12}(\lambda,l)A_{21}(\lambda,l)}}{2}. \tag{5.23}$$

If $c(\lambda_*,a_-)c(\lambda_*,a_+)=0$, these equations together with (5.19)–(5.22) imply that

$$\lambda-\lambda_*=\mathcal{O}(\mathrm{e}^{-2\rho(\lambda_*)l}+l\mathrm{e}^{-4\kappa_1^+(\lambda_*)l}),$$

which proves the asymptotic expansion (2.5) in the case $\mu(l,\boldsymbol{a})=0$.

Suppose on the contrary that $c(\lambda_*,a_-)c(\lambda_*,a_+)\neq 0$. In this case the function $(A_{11}-A_{22})^2+4A_{12}A_{21}$ is nonzero as $\lambda=\lambda_*$, and therefore its square root is holomorphic with respect to λ. Using this fact and the relations (5.19)–(5.22), one can show easily, in analogy with the similar argument for Eq. (4.22), that each of the equations (5.23) has a unique root converging to λ_* as $l\to+\infty$. Hence one of the roots of (4.22) satisfies the first of Eqs. (5.23), while the other satisfies the other one. Substituting now from (5.19)–(5.22) into (5.23), we arrive immediately at the asymptotics (2.5) and (2.6) in the case $\mu(l,\boldsymbol{a})\neq 0$. □

Proof of Theorem 2.4. Let $\boldsymbol{c}$ be a nontrivial solution to the system (4.20), where λ is λ^+ or λ^-. Without loss of generality we may assume that $\|\boldsymbol{c}\|_{\mathbb{R}^2}=1$. Modifying (4.14), we choose the corresponding nontrivial solution of Eq. (4.4) as $\boldsymbol{f}=-c_+\boldsymbol{\Phi}_*^+-c_-\boldsymbol{\Phi}_*^-$. In analogy with (5.7), we then obtain

$$u_-=\frac{\psi_n(\cdot,a_-)}{\lambda-\lambda_*}T_4^-\boldsymbol{f}+\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l})=-\frac{c_+A_{21}(\lambda,l)+c_-A_{22}(\lambda,l)}{\lambda-\lambda_*}\psi_n(\cdot,a_-)+\mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}),$$

which holds true in $W_2^1(\Pi_{a_-})$ and $W_2^2(S)$ for each $S\in\Xi_{a_-}$. Employing now the system (4.20) we can write

$$c_+A_{21}(\lambda,l)+c_-A_{22}(\lambda,l)=-c_-(\lambda-\lambda_*),$$

hence

$$u_- = c_-\psi_n(\cdot, a_-) + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}),$$

and in the same way one can prove that

$$u_+ = c_+\psi_m(\cdot, a_+) + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}).$$

in the norm of $W_2^1(\Pi_{a_-})$ and $W_2^2(S)$ for each $S \in \Xi_{a_-}$. The last two relations prove the sought formulas (2.9).

Suppose that $\lambda^+ = \lambda^-$, then (4.20) has two nontrivial solutions, which means that $(\lambda - \lambda_*)\mathrm{E} + \mathrm{A}(\lambda, l) = 0$; we can choose these solutions as $(c_+, c_-) = (-1, 0)$ and $(c_+, c_-) = (0, -1)$. Substituting these values into (2.9), we arrive at (2.8).

Suppose that $\mu(l, \boldsymbol{a}) \neq 0$. In view of (2.5) it implies that $\lambda^+(l, \boldsymbol{a}) \neq \lambda^-(l, \boldsymbol{a})$, i.e., that $\lambda^\pm(l, \boldsymbol{a})$ are simple eigenvalues. In this case the relations (2.5), (5.20), and (5.21) yield

$$\begin{aligned} \lambda^\pm - \lambda_* + A_{11}(\lambda^\pm, l) &= \pm\,|\mu(l, \boldsymbol{a})|\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(1 + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l})) \neq 0, \\ A_{12}(\lambda^\pm, l) &= \mu(l, \boldsymbol{a})\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}(1 + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l})) \neq 0. \end{aligned} \tag{5.24}$$

Since the matrix $(\lambda^\pm - \lambda_*)\mathrm{E} + \mathrm{A}(\lambda^\pm, l)$ has rank one, we can choose nontrivial solutions of (4.20) as

$$c_+^\pm := \pm \frac{\sqrt{2}(\lambda^\pm - \lambda_* + A_{11}(\lambda^\pm, l))}{\sqrt{(\lambda^\pm - \lambda_* + A_{11}(\lambda^\pm, l)^2 + A_{12}^2(\lambda^\pm, l)}},$$

$$c_-^\pm := \pm \frac{\sqrt{2}A_{12}(\lambda^\pm, l)}{\sqrt{(\lambda^\pm - \lambda_* + A_{11}(\lambda^\pm, l)^2 + A_{12}^2(\lambda^\pm, l)}}.$$

In view of (5.24) we then have

$$c_+^\pm = 1 + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}), \quad c_-^\pm = \mp\,\mathrm{sgn}\,\mu(l, \boldsymbol{a}) + \mathcal{O}(\mathrm{e}^{-2\kappa_1^+(\lambda_*)l}).$$

Substituting from here into (2.9) we arrive immediately at (2.7). ■

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Construction of basis functions for the spin-cluster expansion of the magnetic energy on the atomic scale in rotationally invariant systems

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The recently introduced spin-cluster expansion (SCE) is a powerful tool to represent on the atomic scale the adiabatic magnetic energy for each magnetic configuration of a system with N sites. In the present paper the theory is worked out for the very important case of rotationally invariant magnets. Appropriate basis functions for this SCE are rotationally invariant and exhibit time-reversal symmetry, are real, and constitute a complete orthonormal set for the representation of any rotationally invariant observable. It is also shown how generalized Heisenberg-type models of the magnetic energy of an isotropic magnet are represented in this symmetry-adapted SCE basis. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The investigation of noncollinear spin systems is very important because of the following reasons. First, there are many systems which exhibit noncollinear magnetic ground-state configurations, e.g., fcc Fe,[1] or amorphous Fe-B alloys.[2] Second, there are physically and technologically important noncollinear topological defects in magnets with collinear ground states, e.g., domain walls on the atomic scale in quasi-one-dimensional Fe nanostripes[3] on W(110) or magnetization singularities in the interior of magnetic vortex structures.[4] Finally, thermal magnetic excitations are of noncollinear nature, e.g., small-amplitude spin waves[5] at low temperatures or strongly noncollinear excitations in the paramagnetic temperature regime.

For a theoretical modeling of noncollinearities on an atomic scale, the coarse graining inherent in the continuum approach of micromagnetism[6] is not appropriate and has to be replaced by a microscopic approach. The use of the *ab initio* density functional electron theory for noncollinear spin systems[5,7–9] thereby yields highly accurate results but is often too costly. An alternative approach therefore models the spin interactions on the scale of atomic magnetic moments rather than on the electronic scale, e.g., by means of the classical Heisenberg model for the exchange interactions between "classical" magnetic moments $\mathbf{M}_i = M_i \mathbf{e}_i$ at the atomic sites i with orientations $\mathbf{e}_i$ and magnitudes M_i,

$$E_{\mathrm{H}} = -\sum_{i<j} J_{\mathrm{H}}(\mathbf{M}_i \cdot \mathbf{M}_j), \tag{1}$$

where J_{H} is the nearest-neighbor exchange coupling. Unfortunately, Eq. (1) in general fails badly for the case of atomic-scale noncollinearity because of the following reasons. First, it assumes that the magnitudes M_i do not depend on the magnetic configurations, whereas in reality this is not at all the case[9] (there are configurations for which in some materials M_i even vanishes). Finally, the

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Heisenberg model neglects the influence of multispin interactions,[10] which may become important for strong noncollinearities on an atomic scale.

Because of these deficiencies of the Heisenberg model, two other parametrizations of the magnetic energy on the atomic scale have been introduced recently.[11,12] Both parametrizations are based on the adiabatic approximation where it is assumed that the electronic system is at any instant in its ground state with respect to the momentary orientational configuration $\{\mathbf{e}_i\}$ so that the magnitudes M_i are "slaved," i.e., completely determined by $\{\mathbf{e}_i\}$, $M_i=M_i[\{\mathbf{e}_j\}]$. In the first parametrization[11] the part of the magnetic energy which is invariant with respect to a rotation and inversion of the coordinate system is modeled by an in principle infinite series in terms of all the relative angles $(\mathbf{e}_i\cdot\mathbf{e}_j)$. This method classifies the classical Heisenberg model as a first approximation. Extensions of the Heisenberg model discussed in the literature are shown to be of second order in this parametrization, and explicit third-order expressions are derived. The second parametrization, the so-called spin-cluster expansion[12] (SCE), may be in general applied to systems with arbitrary symmetry, i.e., it is not confined to systems which are rotationally invariant. To achieve this, the SCE for a system with N sites is evaluated in terms of product functions invoking N one-spin basis functions $\phi_\nu(\mathbf{e}_i)$ rather than in terms of the two-spin functions $(\mathbf{e}_i\cdot\mathbf{e}_j)$. Of course, the SCE in general encompasses also the case of a rotationally invariant system, but due to its generality it is yet too undetermined for practical calculations. Because in many magnets the magnetic energy is strongly dominated by the isotropic exchange interactions, it is very often justified to approximate them by a rotationally and time-reversal invariant system. In the present paper it will be shown how rotationally and time-reversal invariant basis functions for the SCE of an isotropic magnetic system can be constructed from product basis functions of the general SCE, which is very important for practical computations. Furthermore, the above-mentioned general Heisenberg-type parametrization is also expanded in this symmetry-adapted SCE basis.

II. THE SPIN-CLUSTER EXPANSION

By the SCE,[12] the adiabatic magnetic energy surface, including all relevant magnetic interactions in the solid (exchange energy, anisotropy energy, dipolar, and Zeeman energy), are represented in principle exactly in terms of one-spin basis functions. The expansion coefficients appearing in the SCE may be obtained by fitting the SCE to the energies of magnetic reference configurations, which in turn may be calculated by the highly accurate *ab initio* density functional electron theory for noncollinear spin systems,[5,7–9] and a carefully constructed SCE therefore will have near-*ab initio* accuracy. Having obtained the SCE it is possible to calculate very quickly the energy of any magnetic configuration $\{\mathbf{e}_i\}=(\mathbf{e}_1,\ldots,\mathbf{e}_N)$. Therefore, the SCE can be used to determine the ground-state configuration of systems with complex magnetic interactions, it can be combined, e.g., with a Monte Carlo simulation method to determine the thermodynamic properties, or it can be combined[13] with an adiabatic equation of motion for the variables $\{\mathbf{e}_i\}$ in order to explore the magnetization dynamics.

The construction of the SCE represents a step-by-step generalization of the arguments given in the conventional cluster expansion of alloy theory.[14] Because it is described in more detail in Ref. 12, we confine ourselves to a short summary. The first step is to parametrize the orientation vectors $\mathbf{e}_i$ by the angles ϑ_i and φ_i with $\vartheta_i\in[0,\pi]$ and $\varphi_i\in[0,2\pi[$ describing the continuous direction of the unit vector in a global coordinate system. In a second step a complete set of orthogonal one-spin basis functions is introduced. For expedience in later developments, we determine these one-spin basis functions to be the set of spherical harmonics $\sqrt{4\pi}Y_L(\mathbf{e})\equiv\sqrt{4\pi}Y_L(\vartheta(\mathbf{e}),\varphi(\mathbf{e}))$ with $L=(l,m)$, the integral order $l=0,1,2,\ldots$, and the respective projection $m=-l,(-l+1),\ldots,l$. Hence, the one-spin basis of order l spanned by the $\sqrt{4\pi}Y_L$ is $(2l+1)$-dimensional. In a third step the complete set of orthogonal basis functions for the full N-site system is constructed from a direct product of one-spin basis functions,

$$\tilde{\mathbf{\Phi}}_{\ell\mathbf{m}}(\{\mathbf{e}_i\}) = (4\pi)^{-N/2} Y_{L_1}(\mathbf{e}_1) Y_{L_2}(\mathbf{e}_2) \cdots Y_{L_N}(\mathbf{e}_N), \tag{2}$$

where $\ell = (l_1, l_2, \ldots, l_N)$ labels the orders of the corresponding one-spin basis functions attached to the single sites and $\mathbf{m} = (m_1, \ldots, m_N)$ is the tuple of respective projection indices. By the appropriate definition of a scalar product,

$$\langle \tilde{\mathbf{\Phi}}_{\ell\mathbf{m}} | \tilde{\mathbf{\Phi}}_{\ell'\mathbf{m}'} \rangle \equiv \frac{1}{(4\pi)^N} \int \mathrm{d}\mathbf{e}_1 \cdots \int \mathrm{d}\mathbf{e}_N \tilde{\mathbf{\Phi}}^*_{\ell\mathbf{m}} \tilde{\mathbf{\Phi}}_{\ell'\mathbf{m}'}, \tag{3}$$

where $\mathrm{d}\mathbf{e}_i$ denotes the integration over the corresponding unit sphere, the orthogonality of the N-site basis follows immediately,

$$\langle \tilde{\mathbf{\Phi}}_{\ell\mathbf{m}} | \tilde{\mathbf{\Phi}}_{\ell'\mathbf{m}'} \rangle = \delta_{\ell\ell'} \delta_{\mathbf{m}\mathbf{m}'}. \tag{4}$$

Since this basis is also complete,

$$\sum_{\ell} \sum_{\mathbf{m}} \tilde{\mathbf{\Phi}}^*_{\ell\mathbf{m}}(\{\mathbf{e}_i\}) \tilde{\mathbf{\Phi}}_{\ell\mathbf{m}}(\{\mathbf{e}'_i\}) = (4\pi)^N \delta(\mathbf{e}_1 - \mathbf{e}'_1) \cdots \delta(\mathbf{e}_N - \mathbf{e}'_N), \tag{5}$$

the configuration dependent magnetic energy E (or any other configuration-dependent quantity) can be exactly expanded into

$$E(\{\mathbf{e}_i\}) = \sum_{\ell} \sum_{\mathbf{m}} \tilde{J}_{\ell\mathbf{m}} \tilde{\mathbf{\Phi}}_{\ell\mathbf{m}}(\{\mathbf{e}_i\}). \tag{6}$$

Recognizing $\sqrt{4\pi} Y_{00}(\mathbf{e}) = 1$, Eq. (6) can be recast[11,14] into a sum running over contributions from all conceivable spin clusters α, which are defined as mere subsets of $1 \leq M \leq N$ sites $i_1, \ldots, i_M$, i.e., $\alpha = (i_1, i_2, \ldots, i_M)$. Hence,

$$E(\{\mathbf{e}_i\}) = J_0 + \sum_{\alpha} \sum_{\ell} \sum_{\mathbf{m}} J_{\alpha\ell\mathbf{m}} \mathbf{\Phi}_{\alpha\ell\mathbf{m}}(\{\mathbf{e}_i\}), \tag{7}$$

where the cluster basis functions $\mathbf{\Phi}_{\alpha\ell\mathbf{m}}$ only depend on the cluster variables $(\mathbf{e}_{i_1}, \ldots, \mathbf{e}_{i_M})$,

$$\mathbf{\Phi}_{\alpha\ell\mathbf{m}}(\{\mathbf{e}_i\}) = (4\pi)^{M/2} Y_{L_{i_1}}(\mathbf{e}_{i_1}) \cdots Y_{L_{i_M}}(\mathbf{e}_{i_M}), \tag{8}$$

and the respective order tuple $\ell = (l_{i_1}, \ldots, l_{i_M})$ is restricted to $l_i > 0$ for all sites i constituting the cluster α. In this recast notion the orthogonality, Eq. (4), reads

$$\langle \mathbf{\Phi}_{\alpha\ell\mathbf{m}} | \mathbf{\Phi}_{\alpha'\ell'\mathbf{m}'} \rangle = \delta_{\alpha\alpha'} \delta_{\ell\ell'} \delta_{\mathbf{m}\mathbf{m}'}, \tag{9}$$

which means that basis functions of different clusters and different order are orthogonal. In the same fashion the completeness relation, Eq. (5), rewrites

$$1 + \sum_{\gamma \subseteq \alpha} \sum_{\ell} \sum_{\mathbf{m}} \mathbf{\Phi}^*_{\gamma\ell\mathbf{m}}(\{\mathbf{e}_i\}) \mathbf{\Phi}_{\gamma\ell\mathbf{m}}(\{\mathbf{e}'_i\}) = \delta(\mathbf{e}_{i_1} - \mathbf{e}'_{i_1}) \cdots \delta(\mathbf{e}_{i_M} - \mathbf{e}'_{i_M}), \tag{10}$$

where the sum runs over all subclusters γ of $K \leq M$ sites contained in the cluster α.

In a practical calculation the SCE, Eq. (7), has to be terminated with respect to the number and type of clusters α which are taken into account and with respect to the order of the entering one-spin basis functions. Such a termination is physically justified because in general the contributions to Eq. (7) will decrease with increasing cluster size and with increasing order l of Y_{lm}. The expansion coefficients $J_{\alpha\ell\mathbf{m}}$ then are obtained by fitting Eq. (7) to the energies $E(\{\mathbf{e}_{i,\mathrm{ref}}\})$ of appropriately chosen reference configurations $\{\mathbf{e}_{i,\mathrm{ref}}\}$, which in turn may be calculated by the highly accurate *ab initio* density functional electron theory (for details of the fitting see Ref. 12). The bare SCE, Eq. (7), is the starting point for all our further considerations.

III. TRANSFORMATION TO SYMMETRY ADAPTED BASIS FUNCTIONS

In the following we consider isotropic magnetic systems for which the magnetic energy is invariant with respect to rotations of the global coordinate system. Because the simple product functions, Eq. (8), are not scalar-rotationally invariant, it is essential to construct a new set of basis functions which exhibit the following properties:

(1) In isotropic systems the magnetic energy is invariant under a global rotation of the coordinate system. Thus, we have to identify the scalar-rotationally invariant part of the full SCE basis and then restrict the SCE basis accordingly.
(2) The magnetic energy must be invariant with respect to time reversal. To guarantee this, the basis functions have to be invariant with respect to the simultaneous inversion of all $\mathbf{e}_i$.
(3) Because the magnetic energy is a physical observable, the basis functions should be real.
(4) Even under the above restrictions the basis functions should be orthonormal and complete in the sense that every rotationally invariant magnetic energy function can be uniquely represented in this basis. As already sketched in Sec. II, orthogonality and completeness are important for the SCE formalism.

A. Construction of rotationally invariant basis functions

In order to meet the first restriction of scalar-rotational invariance, we have to reduce the direct product basis functions, Eq. (8), using concepts of group theory.[15] We start by noting that the spherical harmonics form the basis of the irreducible representation $D^{(l)}$ of the group $SO(3)$ of proper rotations $\mathcal{R}$ in three-dimensional space $\mathbb{R}^3$. Conseqently, the product functions, Eq. (8), of the shape $Y_{L_1}(\mathbf{e}_1)\cdots Y_{L_M}(\mathbf{e}_M)$ are the natural basis of a direct product representation $D^{(l_1)}\otimes\cdots\otimes D^{(l_M)}$ of the M-fold direct product group $SO(3)\otimes\cdots\otimes SO(3)$. This direct product representation in general is reducible, which means that it can be in turn decomposed into a direct sum of irreducible representations of the $SO(3)$. The order l of the irreducible representations $D^{(l)}$ contained in this decomposition is in the range of

$$l_{\max}=\sum_{i=1}^{M} l_i \geq l \geq \max\left(2l_{i'}-\sum_{i=1}^{M} l_i, 0\right)=l_{\min}, \tag{11}$$

where $l_{i'}$ has to be chosen out of the $\{l_i\}$ such that the lower bound for l is minimum. In general an irreducible representation $D^{(l)}$ may occur multiple times in this decomposition, which is referred to as multiplicity t_l.

Concerning the corresponding bases, this decomposition is achieved by the transformation,

$${}^{B}Y_{lm}^{(\mathbf{k},\ell)}(\{\mathbf{e}_i\})=\sum_{\mathbf{m}} C_{\square\square}^{K_1}C_{\square\square}^{K_2}\cdots C_{\square\square}^{L}Y_{L_1}(\mathbf{e}_1)\cdots Y_{L_M}(\mathbf{e}_M), \tag{12}$$

from the direct product basis to the basis of the irreducible representation which is a straightforward generalization of the decomposition of the basis of the direct product representation of $D^{(l_1)}\otimes D^{(l_2)}$ mediated by the Clebsch-Gordan transformation

$$Y_L^{(l_1l_2)}(\mathbf{e}_1,\mathbf{e}_2)=\sum_{m_1m_2} C_{L_1L_2}^{L}Y_{L_1}(\mathbf{e}_1)Y_{L_2}(\mathbf{e}_2). \tag{13}$$

As it is well known, the Clebsch-Gordan coefficients $C_{L_1L_2}^{L}$ are only nonzero if

$$|l_1-l_2|\leq l\leq l_1+l_2 \tag{14}$$

$$m=m_1+m_2 \tag{15}$$

holds. For the case of a multiple direct product of irreducible representations $D^{(l_i)}$ the decomposition transformation is constructed by a successive application of Clebsch-Gordan transforma-

tions resulting in the general scheme, Eq. (12). This succession inherently introduces bases $K_i=(k_i,\mu_i)$ of intermediate representations $D^{(k_i)}$, which are denoted by the tuple $\mathbf{k}=(k_1,\ldots,k_{M-2})$, whereas the μ_i are summed over implicitly by means of Eq. (15). Naturally, within this construction scheme a twofold ambiguity arises:[16] the sequence of both the L_i and the K_i constituting the subscripts of the Clebsch-Gordan coefficients in Eq. (12) is widely undetermined. This is indicated by the boxes $\square$ in Eq. (12). The freedom concerning the intermediate basis indices arises because each index K_i appears twice in the product of Clebsch-Gordan coefficients. Thus, the relative arrangement of the K_i actually determines the sequence of Clebsch-Gordan transformations and with it the virtual transformation. Every sequence of filling the K_i to the boxes $\square$ in the product of Clebsch-Gordan coefficients in Eq. (12) generates a distinct binary bracketing scheme[16] and is symbolically designated by the index B. After the specification of the binary bracketing scheme, the freedom of distributing the L_i in the M remaining boxes in Eq. (12) persists, whereas every sequence of the L_i also generates a distinct transformation. In order to eliminate this indeterminacy, we introduce the convention of identical sequence of entries in the tuple of representation orders, $\boldsymbol{\ell}$, and in the sequence filling the L_i in the free subscripts in the product of Clebsch-Gordan coefficients. Obviously, the complete filling of the boxes $\square$ in the right hand side of Eq. (12) is then uniquely determined by the coupling scheme represented by $(B,\boldsymbol{\ell})$.

Finally, basis sets $\{{}^{B}Y_{lm}^{(\mathbf{k},\boldsymbol{\ell})}\}$ and $\{{}^{B'}Y_{lm}^{(\mathbf{k},\tilde{\boldsymbol{\ell}})}\}$ obtained by different coupling schemes $(B,\boldsymbol{\ell})$ and $(B',\tilde{\boldsymbol{\ell}})$ with $\tilde{\boldsymbol{\ell}}$ being a nontrivial permutation of $\boldsymbol{\ell}$ are equivalent but not necessarily identical. Thus, for practical calculations one has to agree on a certain coupling scheme $(B,\boldsymbol{\ell})$. A simple choice for a coupling scheme would be, e.g., the ordered tuple $\boldsymbol{\ell}=(l_1,\ldots,l_M)$ with

$$l_1 \geq l_2 \geq \cdots \geq l_M, \tag{16}$$

and the linear binary bracketing scheme where every K_i is taken as the lower-left subscript of the Clebsch-Gordan coefficient succeeding the one with the same K_i as superscript.

The decomposition transformation, Eq. (12), in general is unitary, because it is constructed from unitary Clebsch-Gordan transformations. Hence, the dimensionality of the direct product of spherical harmonics of orders $\{l_1,\ldots,l_M\}$ must equal the dimensionality of the irreducible representations of order l and multiplicity t_l,

$$\prod_{j=1}^{M}(2l_j+1)=\sum_{l=l_{\min}}^{l_{\max}} t_l(2l+1). \tag{17}$$

The multiplicity reflects in the different numerical values of the intermediate representation orders k_i governed by Eq. (14), which lead in total to a set of t_l numerically different $\mathbf{k}$-tuples for a given order tuple $\boldsymbol{\ell}$. Therefore, by means of the $\mathbf{k}$-tuple the bases of the inequivalent irreducible representations $D^{(l)}$ can be distinguished.

Now coming back to restriction (1) of scalar-rotational invariance, the key advantage of the transition to the irreducible representation is the well-known transformation behavior under the action of proper rotations $\mathcal{R}$,

$${}^{B}Y_{lm}^{(\mathbf{k},\boldsymbol{\ell})}(\{\mathbf{R}^{-1}(\mathcal{R})\mathbf{e}_i\})=\sum_{m'} D_{m'm}^{(l)}(\mathcal{R})\,{}^{B}Y_{lm'}^{(\mathbf{k},\boldsymbol{\ell})}(\{\mathbf{e}_i\}). \tag{18}$$

Herein $D_{m'm}^{(l)}$ is the irreducible representation matrix of order l and $\mathbf{R}^{-1}$ is the corresponding rotation matrix in $\mathbb{R}^3$. Because $D_{00}^{(0)}=1$ always holds regardless of the coupling scheme, the scalar-rotationally invariant part of the full basis $\{{}^{B}Y_{lm}^{(\mathbf{k},\boldsymbol{\ell})}\}$ is uniquely given by the subset $\{{}^{B}Y_{00}^{(\mathbf{k},\boldsymbol{\ell})}\}$. Introducing the generalized Wigner coefficients[15,17,18]

$$\begin{pmatrix} l_1 & \cdots & l_M \\ m_1 & \cdots & m_M \end{pmatrix}^B_{(\mathbf{k})} \equiv C^{K_1}_{L_1 L_2} \cdots C^{00}_{K_{M-2} L_M} = \frac{(-1)^{l_M - m_M}}{\sqrt{2l_M + 1}} C^{K_1}_{L_1 L_2} \cdots C^{l_M - m_M}_{K_{M-3} L_{M-1}}, \tag{19}$$

and using Eqs. (8) and (12), we arrive at

$$\mathcal{Y}^{(\mathbf{k},\ell)}_{\alpha}(\{\mathbf{e}_i\}) \equiv (4\pi)^{M/2}\ {}^B Y^{(\mathbf{k},\ell)}_{00}(\{\mathbf{e}_i\}) = \sum_{\mathbf{m}} \begin{pmatrix} l_1 & \cdots & l_M \\ m_1 & \cdots & m_M \end{pmatrix}^B_{(\mathbf{k})} \mathbf{\Phi}_{\alpha \ell \mathbf{m}}(\{\mathbf{e}_i\}), \tag{20}$$

which directly shows the decomposition transformation from the bare product basis, Eq. (8), to the rotationally symmetry adapted basis postulated by constraint (1) of this section. Please note that because of Eq. (19) there are only $(M-3)$ entries in the $\mathbf{k}$-tuple. For $M \leq 3$ the following special cases emerge from Eq. (19):

$$\begin{pmatrix} l_1 & l_2 \\ m_1 & m_2 \end{pmatrix} = (-1)^{l_1 - m_1} \frac{\delta_{l_1 l_2} \delta_{m_1 - m_2}}{\sqrt{2l_1 + 1}} \quad \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{l_3 - m_3}}{\sqrt{2l_3 + 1}} C^{l_3 - m_3}_{l_1 m_1 l_2 m_2}, \tag{21}$$

and the point function naturally turns out to be constant. Finally, we want to remark that the generalized Wigner coefficients are only nonzero, if the irreducible $l=0$ representation is contained in the product representation, i.e., if $l_{\min}=0$ holds in Eq. (11). This marks some boundary for the l_i which obviously cannot be chosen arbitrarily.

B. Consideration of time-reversal symmetry and basis properties

Next, we have to fulfill the criterion (2) of time-reversal symmetry, i.e., invariance with respect to simultaneous inversion of all variables, $\{\mathbf{e}_i\} \to \{-\mathbf{e}_i\}$. From the well-known property $Y_L(-\mathbf{e}) = (-1)^l Y_L(\mathbf{e})$ we immediately get the behavior under time reversal,

$$\mathcal{Y}^{(\mathbf{k},\ell)}_{\alpha}(\{-\mathbf{e}_i\}) = (-1)^{l_1 + l_2 + \ldots + l_M}\ \mathcal{Y}^{(\mathbf{k},\ell)}_{\alpha}(\{\mathbf{e}_i\}). \tag{22}$$

The postulate for invariance with respect to time reversal consequently translates into the restriction of even total parity, i.e.,

$$l_1 + l_2 + \ \ldots\ + l_M = \text{even}. \tag{23}$$

Criterion (3) of real-valuedness can be proven by using the general property[15]

$$\begin{pmatrix} l_1 & \cdots & l_M \\ -m_1 & \cdots & -m_M \end{pmatrix}^B_{(\mathbf{k})} = (-1)^{l_1 + l_2 + \cdots + l_M} \begin{pmatrix} l_1 & \cdots & l_M \\ m_1 & \cdots & m_M \end{pmatrix}^B_{(\mathbf{k})} \tag{24}$$

of the real-valued generalized Wigner coefficients. Together with $Y^*_{lm} = (-1)^m Y_{l-m}$, the condition, Eq. (23), of even parity and the nonzero criterion[15]

$$m_1 + m_2 + \cdots + m_M = 0 \tag{25}$$

of the generalized Wigner coefficients, it can be seen from Eq. (20) that the imaginary parts of the terms characterized by any tuple $(m_1, \ldots, m_M)$ cancel with those of the conjugated tuple $(-m_1, \ldots, -m_M)$. Thus, the SCE basis functions turn out to be real by means of criteria (1) and (2), and the demand for real-valuedness constitutes no further restriction.

Finally, we have to prove the orthonormality and completeness, demand (4). With Eq. (9) we get

$$\langle \mathcal{Y}^{(\mathbf{k},\ell)}_{\alpha} | \mathcal{Y}^{(\mathbf{k}',\ell')}_{\alpha'} \rangle = \delta_{\alpha\alpha'} \delta_{\ell\ell'} \sum_{\mathbf{m}} \begin{pmatrix} l_1 & \cdots & l_M \\ m_1 & \cdots & m_M \end{pmatrix}^B_{(\mathbf{k})} \begin{pmatrix} l_1 & \cdots & l_M \\ m_1 & \cdots & m_M \end{pmatrix}^B_{(\mathbf{k}')} = \delta_{\alpha\alpha'} \delta_{\ell\ell'} \delta_{\mathbf{k}\mathbf{k}'}, \tag{26}$$

where in the last step we used the orthonormality of the generalized Wigner coefficients.[15] Hence, the SCE basis functions of different clusters α, order ℓ, and component $\mathbf{k}$ are orthogonal. Con-

cerning completeness, we recall the completeness, Eq. (10), of the product basis $\{\mathbf{\Phi}_{\alpha\ell\mathbf{m}}\}$. Because the transformation, Eq. (12), to the irreducible representation generated by the basis set $\{Y_L^{(\mathbf{k},\ell)}\}$ is unitary, the latter one must be also complete if we consider all orders l in the limits of Eq. (11). By the restrictions of scalar-rotational and time-reversal invariance the whole set of basis functions is reduced to the part of the complete basis whose expansion coefficients are not forced to be zero by symmetry restrictions. Together with the feature of linear independence we conclude that this subset $\{\mathcal{Y}_\alpha^{(\mathbf{k},\ell)}\}$ is complete in view of the representation of rotationally and time-reversal invariant functions.

After having implemented all symmetry restrictions, we can expand the magnetic energy of a rotationally invariant system uniquely,

$$E(\{\mathbf{e}_i\}) = J_0 + \sum_\alpha \sum_\ell {}' \sum_{\mathbf{k}} J_\alpha^{(\mathbf{k},\ell)} \mathcal{Y}_\alpha^{(\mathbf{k},\ell)}(\{\mathbf{e}_i\}), \tag{27}$$

where the prime denotes that only ℓ-tuples with even total parity, Eq. (23), are taken into account, and where the cluster summation starts from pairs on. Please note that the extensive $\mathbf{m}$ summation of the bare SCE, Eq. (7), is now already incorporated in the basis functions, Eq. (20).

IV. RELATION BETWEEN SCE AND $(\mathbf{e}_i \cdot \mathbf{e}_j)$ BASIS FUNCTIONS

It has been mentioned in Sec. I that there are alternative approaches[11] for the parametrization of the isotropic magnetic energy in terms of two-spin arguments $(\mathbf{e}_i \cdot \mathbf{e}_j)$, i.e.,

$$E(\{\mathbf{e}_i\}) = \sum_\alpha \sum_K \sum_{\lambda_1 \cdots \lambda_K} J_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)} V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}(\{\mathbf{e}_i\}). \tag{28}$$

Thereby the M-point configuration functions,

$$V_{\lambda_1 \cdots \lambda_K}^{(M)}(\mathbf{e}_1, \ldots, \mathbf{e}_M) = P_{\lambda_1}(\mathbf{e}_{i_{1,1}} \cdot \mathbf{e}_{i_{1,2}}) \cdots P_{\lambda_K}(\mathbf{e}_{i_{K,1}} \cdot \mathbf{e}_{i_{K,2}}), \tag{29}$$

are defined as product of K polynomials, P_λ, of order $\lambda \geq 1$ in the pair scalar products $(\mathbf{e}_{i_{\kappa,1}} \cdot \mathbf{e}_{i_{\kappa,2}})$ chosen out of the variables $\{\mathbf{e}_1, \ldots, \mathbf{e}_M\}$ forming the M-point cluster α. Thus, the number of pairs, K, can be

$$M/2 \leq K \leq M(M-1)/2. \tag{30}$$

Obviously, this parametrization is a systematic generalization of the Heisenberg model, Eq. (1), and the $J_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ are the expansion coefficients of the respective configuration functions. Please note that for the polynomials P_λ in Ref. 11 simple power functions are used, whereas in the present paper we will consider Legendre polynomials instead. Because they are related by one-to-one mappings these two polynomial sets are equivalent. Furthermore, we skip the permutation symmetrization performed in Ref. 11, because in atomistic nonquantum modeling there are no physical reasons for it.

From a closer look at Eq. (29) it can be easily seen that the configuration functions $V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ are also invariant under proper rotations of the coordinate system and time reversal, as every scalar product $(\mathbf{e}_{i_{\kappa,1}} \cdot \mathbf{e}_{i_{\kappa,2}})$ is so. Because for each M-point cluster the basis set $\{\mathcal{Y}_\alpha^{(\mathbf{k},\ell)}\}$ is complete with respect to these restrictions, the $V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ can be expanded into this SCE basis. In contrast, the inverse expansion of the SCE basis functions into the $V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ does not necessarily have to exist because neither the linear independence nor the completeness of the $V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ parametrization has been investigated so far.

The general route to expand the $V_{\alpha,\lambda_1 \cdots \lambda_K}^{(M)}$ in the $\mathcal{Y}_\alpha^{(\mathbf{k},\ell)}$ is the following. First, the expansion[18]

$$P_\lambda(\mathbf{e}_1\cdot\mathbf{e}_2)=\frac{4\pi}{2\lambda+1}\sum_\eta(-1)^\eta Y_{\lambda-\eta}(\mathbf{e}_1)Y_{\lambda\eta}(\mathbf{e}_2) \tag{31}$$

is inserted into Eq. (29). Because every site variable $\mathbf{e}_i$ enters in ν_i different scalar products, with $1\le\nu_i\le K-1$, this leads to a product of ν_i spherical harmonics of the same argument $\mathbf{e}_i$, respectively. Recursive application of the expansion[18]

$$Y_{\lambda_1\eta_1}(\mathbf{e}_i)Y_{\lambda_2\eta_2}(\mathbf{e}_i)=\sum_{lm}\sqrt{\frac{(2\lambda_1+1)(2\lambda_2+1)}{4\pi(2l+1)}}C^{l0}_{\lambda_1 0\lambda_2 0}C^{lm}_{\lambda_1\eta_1\lambda_2\eta_2}Y_{lm}(\mathbf{e}_i) \tag{32}$$

allows one to expand every product of spherical harmonics of the same argument into a linear combination of single spherical harmonics of the same argument. Applying these expansions for each cluster variable $\mathbf{e}_i$, Eq. (29) becomes an expansion of $V^{(M)}_{\alpha,\lambda_1\cdots\lambda_K}$ into the basis $\mathbf{\Phi}_{\alpha\ell\mathbf{m}}$ of the same cluster α, while the expansion coefficients essentially turn out to be sums of products of Clebsch-Gordan coefficients. Performing all the summations over internal projection indices, with the help of graphical methods[15,18] it is possible to rewrite the expansion of the $V^{(M)}_{\alpha,\lambda_1\cdots\lambda_K}$ in terms of the SCE basis $\mathcal{Y}^{(\mathbf{k},\ell)}_\alpha$, and it can be shown that the condition of even total parity, Eq. (23), in general is fulfilled.

Performing this scheme of calculation explicitly for the $V^{(M\le4)}_{\alpha,\lambda_1\cdots\lambda_K}$ functions, using the abbreviations $C^c_{ab}\equiv C^{c0}_{a0b0}$ and $[\lambda_1\cdots\lambda_i]=(2\lambda_1+1)\cdots(2\lambda_i+1)$, and with the $6j$ ($9j$ resp.) symbols $\{\cdots\}$ common in the recoupling theory of angular momenta, we finally obtain

$$V^{(2)}_\lambda(\mathbf{e}_1,\mathbf{e}_2)\equiv P_\lambda(\mathbf{e}_1\cdot\mathbf{e}_2)=(-)^\lambda[\lambda]^{-1/2}\mathcal{Y}^{(\lambda\lambda)}_\alpha(\mathbf{e}_1,\mathbf{e}_2), \tag{33}$$

$$V^{(3)}_{\lambda_1\lambda_2}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)\equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)=[\lambda_1\lambda_2]^{-1/2}\sum_l(-)^l C^l_{\lambda_1\lambda_2}\mathcal{Y}^{(\lambda_1\lambda_2 l)}_\alpha(\mathbf{e}_1,\mathbf{e}_3,\mathbf{e}_2), \tag{34}$$

$$\begin{aligned}V^{(3)}_{\lambda_1\lambda_2\lambda_3}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)&\equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)P_{\lambda_3}(\mathbf{e}_3\cdot\mathbf{e}_1)\\&=(-)^{\lambda_1+\lambda_2+\lambda_3}\sum_{l_1l_2l_3}C^{l_1}_{\lambda_1\lambda_3}C^{l_2}_{\lambda_1\lambda_2}C^{l_3}_{\lambda_2\lambda_3}\begin{Bmatrix}l_1&l_3&l_2\\\lambda_2&\lambda_1&\lambda_3\end{Bmatrix}\mathcal{Y}^{(l_1l_3l_2)}_\alpha(\mathbf{e}_1,\mathbf{e}_3,\mathbf{e}_2),\end{aligned} \tag{35}$$

$$V^{(4)}_{\lambda_1\lambda_2}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4)\equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_3\cdot\mathbf{e}_4)=[\lambda_1\lambda_2]^{-1/2}(-)^{\lambda_1+\lambda_2}\mathcal{Y}^{(0,\lambda_1\lambda_1\lambda_2\lambda_2)}_\alpha(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4), \tag{36}$$

$$\begin{aligned}V^{(4)}_{\lambda_1\lambda_2\lambda_3}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4)&\equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)P_{\lambda_3}(\mathbf{e}_3\cdot\mathbf{e}_4)\\&=[\lambda_1\lambda_2\lambda_3]^{-1/2}\sum_{l_1l_2}(-)^{l_1+l_2+\lambda_2}C^{l_1}_{\lambda_1\lambda_2}C^{l_2}_{\lambda_2\lambda_3}\mathcal{Y}^{(\lambda_2,l_1\lambda_1\lambda_3l_2)}_\alpha(\mathbf{e}_2,\mathbf{e}_1,\mathbf{e}_4,\mathbf{e}_3),\end{aligned} \tag{37}$$

$$\begin{aligned}V^{(4)}_{\lambda_1\lambda_2\lambda_3\lambda_4}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4)&\equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)P_{\lambda_3}(\mathbf{e}_3\cdot\mathbf{e}_4)P_{\lambda_4}(\mathbf{e}_4\cdot\mathbf{e}_1)\\&=\sum_{l_1l_2l_3l_4}(-)^{\lambda_1+\lambda_3-l_1-l_2}C^{l_1}_{\lambda_4\lambda_1}C^{l_2}_{\lambda_1\lambda_2}C^{l_3}_{\lambda_2\lambda_3}C^{l_4}_{\lambda_3\lambda_4}\\&\quad\times\sum_x\sqrt{[x]}\begin{Bmatrix}l_1&\lambda_1&\lambda_4\\x&l_2&l_4\\l_3&\lambda_2&\lambda_3\end{Bmatrix}\mathcal{Y}^{(x,l_3l_1l_2l_4)}_\alpha(\mathbf{e}_3,\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_4),\end{aligned} \tag{38}$$

$$V^{(4)}_{\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4) \equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)P_{\lambda_3}(\mathbf{e}_3\cdot\mathbf{e}_4)P_{\lambda_4}(\mathbf{e}_4\cdot\mathbf{e}_1)P_{\lambda_5}(\mathbf{e}_1\cdot\mathbf{e}_3)$$
$$= \sum_{l_1\cdots l_6} \sqrt{[l_1 l_4]}(-)^{\lambda_2+\lambda_4-l_2-l_6} C^{l_1}_{\lambda_4\lambda_1} C^{l_2}_{l_1\lambda_5} C^{l_3}_{\lambda_1\lambda_2} C^{l_4}_{\lambda_2\lambda_3} C^{l_5}_{l_4\lambda_5} C^{l_6}_{\lambda_3\lambda_4}$$
$$\times \sum_x \sqrt{[x]} \begin{Bmatrix} l_2 & x & l_5 \\ l_4 & \lambda_5 & l_1 \end{Bmatrix} \begin{Bmatrix} l_6 & x & l_3 \\ \lambda_4 & l_1 & \lambda_1 \\ \lambda_3 & l_4 & \lambda_2 \end{Bmatrix} \mathcal{Y}^{(x,l_3 l_6 l_5 l_2)}_{\alpha}(\mathbf{e}_2,\mathbf{e}_4,\mathbf{e}_3,\mathbf{e}_1), \tag{39}$$

$$V^{(4)}_{\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5\lambda_6}(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4) \equiv P_{\lambda_1}(\mathbf{e}_1\cdot\mathbf{e}_2)P_{\lambda_2}(\mathbf{e}_2\cdot\mathbf{e}_3)P_{\lambda_3}(\mathbf{e}_3\cdot\mathbf{e}_4)P_{\lambda_4}(\mathbf{e}_4\cdot\mathbf{e}_1)P_{\lambda_5}(\mathbf{e}_1\cdot\mathbf{e}_3)P_{\lambda_6}(\mathbf{e}_2\cdot\mathbf{e}_4)$$
$$= \sum_{l_1\cdots l_8} \sqrt{[l_1 l_3 l_5 l_7]}(-)^{l_3+l_4+l_5+l_6+l_7+l_8+\lambda_1+\lambda_3+\lambda_6}$$
$$\times C^{l_1}_{\lambda_4\lambda_1} C^{l_2}_{l_1\lambda_5} C^{l_3}_{\lambda_1\lambda_2} C^{l_4}_{l_3\lambda_6} C^{l_5}_{\lambda_2\lambda_3} C^{l_6}_{l_5\lambda_5} C^{l_7}_{\lambda_3\lambda_4} C^{l_8}_{l_7\lambda_6}$$
$$\times \sum_x \sqrt{[x]} \begin{Bmatrix} l_5 & x & l_1 \\ l_2 & \lambda_5 & l_6 \end{Bmatrix} \begin{Bmatrix} l_7 & x & l_3 \\ l_4 & \lambda_6 & l_8 \end{Bmatrix} \begin{Bmatrix} l_5 & x & l_1 \\ \lambda_2 & l_3 & \lambda_1 \\ \lambda_3 & l_7 & \lambda_4 \end{Bmatrix}$$
$$\times \mathcal{Y}^{(x,l_2 l_6 l_4 l_8)}_{\alpha}(\mathbf{e}_1,\mathbf{e}_3,\mathbf{e}_2,\mathbf{e}_4) \tag{40}$$

Herein the $\mathcal{Y}^{(\mathbf{k},\ell)}_{\alpha}$ are defined on basis of the linear binary bracketing scheme mentioned in Sec. II. In principle, the basis properties of the $V^{(M)}_{\alpha,\lambda_1\cdots\lambda_K}$ also would reflect in an analysis of the regularity of these expansion coefficients, but this is far beyond the scope of the present paper.

V. CONCLUSIONS

The SCE is a powerful representation of the adiabatic magnetic energy hypersurface of a magnetic system on the scale of atomistic modeling. In the present paper we have worked out the theory of the SCE for the very important limit of rotationally and time-reversely invariant systems. Because the basis of the SCE is complete and orthogonal, the magnetic energy $E(\{\mathbf{e}_i\})$ as function of the orientations of the moments of all atomic sites i in the system can be systematically expanded into contributions from clusters $\alpha=\{i_1,\ldots,i_M\}$ of different size M and shape. Finally, it is shown both, generally and explicitly, how the widely used Heisenberg-type modeling in terms of pair contributions $(\mathbf{e}_i\cdot\mathbf{e}_j)$ is covered by the SCE with rotationally and time-reversal invariant basis functions.

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Harmonic oscillators coupled by springs: Discrete solutions as a Wigner quantum system

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We consider a quantum system consisting of a one-dimensional chain of M identical harmonic oscillators with natural frequency ω, coupled by means of springs. Such systems have been studied before, and appear in various models. In this paper, we approach the system as a Wigner quantum system, not imposing the canonical commutation relations, but using instead weaker relations following from the compatibility of Hamilton's equations and the Heisenberg equations. In such a setting, the quantum system allows solutions in a finite-dimensional Hilbert space, with a discrete spectrum for all physical operators. We show that a class of solutions can be obtained using generators of the Lie superalgebra $\mathfrak{gl}(1|M)$. Then we study – from a mathematical point of view – the properties and spectra of the physical operators in a class of unitary representations of $\mathfrak{gl}(1|M)$. These properties are both interesting and intriguing. In particular, we can give a complete analysis of the eigenvalues of the Hamiltonian and of the position and momentum operators (including multiplicities). We also study probability distributions of position operators when the quantum system is in a stationary state, and the effect of the position of one oscillator on the positions of the remaining oscillators in the chain. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2364183]

I. INTRODUCTION

In recent years quantum information theory has known an enormous expansion. This has boosted new interest in probabilistic and geometric aspects of state spaces of simple quantum systems. In this context, the dynamics of entanglement in a chain of coupled harmonic oscillators has been the subject of many papers.[1–5] One of the systems for which entanglement dynamics is being studied consists of a large chain of harmonic oscillators coupled by some nearest neighbor interaction.[5] In a popular model this coupling is represented by springs obeying Hooke's law. Then the Hamiltonian of the system is given by

$$\hat{H} = \sum_{k=1}^{M} \left(\frac{\hat{p}_k^2}{2m} + \frac{m\omega^2}{2}\hat{q}_k^2 + \frac{cm}{2}(\hat{q}_k - \hat{q}_{k+1})^2 \right). \tag{1.1}$$

In other words, the quantum system consists of a string or chain of M identical harmonic oscillators, each having the same mass m and natural frequency ω. The position and momentum operator for the kth oscillator are given by $\hat{q}_k$ and $\hat{p}_k$; more precisely $\hat{q}_k$ measures the displacement of the kth mass point with respect to its equilibrium position (see Fig. 1). The last term in Eq. (1.1)

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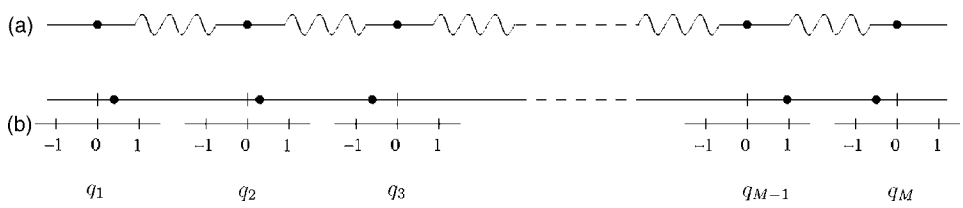

FIG. 1. Illustration of the quantum system: (a) the M masses in equilibrium position and (b) certain displacements q_k for each oscillator.

represents the nearest neighbor coupling by means of "springs," with a coupling strength c ($c>0$). Finally, we shall assume periodic boundary conditions, i.e.,

$$\hat{q}_{M+1} \equiv \hat{q}_1. \tag{1.2}$$

Such quantum systems are also relevant in quantum optics (photonic crystals), or for describing phonons in a crystal.[5,6]

In the standard approach for the quantum system governed by Eq. (1.1), one assumes the canonical commutation relations (CCRs),

$$[\hat{q}_k,\hat{q}_l]=0, \quad [\hat{p}_k,\hat{p}_l]=0, \quad [\hat{q}_k,\hat{p}_l]=i\hbar\,\delta_{kl}. \tag{1.3}$$

Then, reformulating the problem in normal coordinates, the eigenstates of $\hat{H}$ can be described in some infinite-dimensional Fock space.[5]

The approach of the present paper is more general. Instead of postulating the CCRs, we shall start from a more general quantization procedure. This procedure is based upon the compatibility of Hamilton's equations with the Heisenberg equations. Such systems are called Wigner quantum systems (WQSs).[7] The idea is based on Wigner's observation – for the simple example of a one-dimensional harmonic oscillator – that this quantum system also allows solutions for which both Hamilton's equations and the Heisenberg equations are satisfied, but not the CCRs.[8] In other words, the CCRs are sufficient but not necessary conditions for Hamilton's equations and the Heisenberg equations to be compatible. Wigner's work led to the theory of parabosons and parafermions in quantum field theory,[9–11] and because of this attention its impact for ordinary quantum systems was somewhat overlooked. Another reason why WQSs did not receive immediate attention was because no general solutions could be constructed for the compatibility conditions of simple WQSs (apart from the one-dimensional harmonic oscillator). It was only much later – after the theory of Lie superalgebra's was completed – that Palev[12] observed that classes of WQS solutions for the n-dimensional harmonic oscillator are described by means of representations of the Lie superalgebras $\mathfrak{osp}(1|2n)$ and $\mathfrak{sl}(1|n)$ or $\mathfrak{gl}(1|n)$. This algebraic or representation theoretic approach to quantum systems has revived the interest in WQSs.[13–15] The WQS approach has so far been applied to simple systems of free harmonic oscillators, with some interesting and surprising results.[16–20] Here it is, for the first time, applied to a more realistic quantum system.

In this paper, we shall study the system described by Eq. (1.1) as a WQS. This implies that, apart from the standard solutions for which the CCRs hold, we shall also discover noncanonical solutions. In particular, we shall show that the quantum system allows solutions in a finite-dimensional Hilbert space, thus with a discrete spectrum not only for $\hat{H}$ but also for the position and momentum operators $\hat{q}_k$ and $\hat{p}_k$. The class of solutions considered here is related to a $\mathfrak{gl}(1|M)$ solution of the quantization or compatibility conditions, and we consider then a simple class of $\mathfrak{gl}(1|M)$ representations in which the physical properties of the quantum system are analyzed.

It should be emphasized that our work is essentially mathematical. Whether WQS solutions offer an appropriate extension to those of canonical quantum mechanics is a question of discussion. We do not enter this discussion in this paper. But we hope that our results might be stimulating for further research in the areas of noncanonical commutation relations and, more general, noncommutative space geometry.

In Sec. II we analyze the compatibility conditions for the system Eq. (1.1) as a WQS. This leads to an expression of the Hamiltonian $\hat{H}$ in terms of a set of $2M$ operators $a_r^{\pm}$ $(r=1,\ldots,M)$, which are themselves certain linear combinations of the $\hat{q}_k$ and $\hat{p}_k$. These operators $a_r^{\pm}$ should satisfy certain triple relations, see Eq. (2.29). The task is then to construct operator solutions (constructions for the $a_r^{\pm}$ as operators acting in some Hilbert space) satisfying these triple relations. Although a complete set of solutions cannot be given, we show in Sec. III that certain generators of the Lie superalgebra $\mathfrak{gl}(1|M)$ satisfy the triple relations. In other words, we present algebraic solutions of the compatibility condition (or quantization condition) in terms of a Lie superalgebra. In order to have algebraic solutions that also satisfy the required unitarity conditions, the coupling constant c is bounded by a critical value c_0, depending upon M. Since the problem has a $\mathfrak{gl}(1|M)$ solution, the unitary representations of $\mathfrak{gl}(1|M)$ serve as Hilbert space representations for the operators of the quantum system. In principle, all unitary representations of $\mathfrak{gl}(1|M)$ are allowed for this purpose. In this paper, however, we shall concentrate on a particular class of unitary representations $W(p)$, mainly for computational purposes. For these representations $W(p)$, the actions of the $\mathfrak{gl}(1|M)$ generators, and in particular of the operators $a_r^{\pm}$, are very simple expressions, see Sec. IV. On the other hand, the class of representations $W(p)$ is already sufficiently rich to exhibit intriguing physical properties of the quantum system under consideration. These properties are examined in the remaining sections. In Sec. V we study the energy spectrum of the quantum system in $W(p)$. If $c=0$ (absence of coupling), the system consist of M independent (or free) identical one-dimensional oscillators, and it is easy to see that there are $M+1$ equidistant energy levels in $W(p)$, with multiplicities $\binom{M}{k}$ according to the level k $(k=0,1,\ldots,M)$. For $0<c<c_0$, these energy levels split: we can give a closed formula for the energy levels themselves, for their multiplicities, and for the total number of energy levels (which grows like $3^{M/2}$). Section VI is devoted to the investigation of spatial properties of the chain of coupled oscillators, if the system is in one of the representations $W(p)$. Clearly, since the representations considered here are finite-dimensional, the spectrum of position operators $\hat{q}_k$ and momentum operators $\hat{p}_k$ is discrete. We manage to give the spectrum of these operators in closed form, but so far an analytic expression for a set of orthonormal eigenvectors is missing. Finally, we examine numerically for a simple example $(M=4)$ some position probability distributions of the oscillator system. The case of *atypical* representations $W(p)$ (i.e., $p\leqslant M-1$) is examined in Sec. VII, followed by some concluding remarks in Sec. VIII.

II. THE QUANTIZATION PROCEDURE

In our approach we shall require that Hamilton's equations

$$\dot{\hat{q}}_k=\frac{\partial\hat{H}}{\partial\hat{p}_k},\quad \dot{\hat{p}}_k=-\frac{\partial\hat{H}}{\partial\hat{q}_k}\quad (k=1,2,\ldots,M) \tag{2.1}$$

and the Heisenberg equations

$$\dot{\hat{p}}_k=\frac{i}{\hbar}[\hat{H},\hat{p}_k],\quad \dot{\hat{q}}_k=\frac{i}{\hbar}[\hat{H},\hat{q}_k]\quad (k=1,2,\ldots,M) \tag{2.2}$$

should be identical as operator equations. Since Hamilton's equations for the Hamiltonian (1.1) take the explicit form

$$\dot{\hat{q}}_k=\frac{1}{m}\hat{p}_k, \tag{2.3}$$

$$\dot{\hat{p}}_k=cm\hat{q}_{k-1}-m(\omega^2+2c)\hat{q}_k+cm\hat{q}_{k+1}, \tag{2.4}$$

the compatibility conditions read

$$[\hat{H},\hat{q}_k] = -\frac{i\hbar}{m}\hat{p}_k, \tag{2.5}$$

$$[\hat{H},\hat{p}_k] = -i\hbar\, cm\hat{q}_{k-1} + i\hbar\, m(\omega^2+2c)\hat{q}_k - i\hbar\, cm\hat{q}_{k+1}, \tag{2.6}$$

where $k=1,2,\ldots,M$, and – extending Eq. (1.2) – $\hat{q}_0$ stands for $\hat{q}_M$, or more generally

$$\hat{q}_k = \hat{q}_{k \bmod M}, \quad \hat{p}_k = \hat{p}_{k \bmod M}, \tag{2.7}$$

whenever k is out of the range $\{1,2,\ldots,M\}$. In other words, the task is to find operator solutions for $\hat{q}_k$ and $\hat{p}_k$ such that the compatibility conditions (2.5) and (2.6), together with Eq. (1.1), are satisfied. Furthermore, since $\hat{q}_k$ and $\hat{p}_k$ correspond to physical observables, the operators should be self-adjoined

$$\hat{q}_k^\dagger = \hat{q}_k, \quad \hat{p}_k^\dagger = \hat{p}_k \quad (k=1,2,\ldots,M). \tag{2.8}$$

Just as in the canonical treatment of the problem,[5,6] it will be useful to introduce "normal coordinates" and reformulate the problem in terms of these new coordinates. So let us consider the finite Fourier transforms of $\hat{q}_k$ and $\hat{p}_k$,

$$\hat{Q}_r = \frac{1}{\sqrt{M}}\sum_{k=1}^{M} e^{-(2\pi irk/M)}\hat{q}_k, \tag{2.9}$$

$$\hat{P}_r = \frac{1}{\sqrt{M}}\sum_{k=1}^{M} e^{(2\pi irk/M)}\hat{p}_k. \tag{2.10}$$

The inverse relations are given by

$$\hat{q}_k = \frac{1}{\sqrt{M}}\sum_{r=1}^{M} e^{(2\pi ikr/M)}\hat{Q}_r, \tag{2.11}$$

$$\hat{p}_k = \frac{1}{\sqrt{M}}\sum_{r=1}^{M} e^{-(2\pi ikr/M)}\hat{P}_r. \tag{2.12}$$

As for $\hat{q}_k$ and $\hat{p}_k$, see Eq. (2.7), it will sometimes be useful to extend the indices by

$$\hat{Q}_k = \hat{Q}_{k \bmod M}, \quad \hat{P}_k = \hat{P}_{k \bmod M}. \tag{2.13}$$

Note that the conditions (2.8) imply

$$\hat{Q}_r^\dagger = \hat{Q}_{M-r}, \quad \hat{P}_r^\dagger = \hat{P}_{M-r} \quad (r=1,2,\ldots,M), \tag{2.14}$$

and in particular, following the convention Eq. (2.13), $\hat{Q}_M^\dagger = \hat{Q}_M$ and $\hat{P}_M^\dagger = \hat{P}_M$. An essential part is now to substitute Eqs. (2.11) and (2.12) in the Hamiltonian $\hat{H}$, given by Eq. (1.1), and simplify this expression without assuming any commutation relations between the operators. For the term $\Sigma_k \hat{p}_k^2 = \Sigma_k \hat{p}_k \hat{p}_k^\dagger$, one can, after the substitution, use the identity

$$\sum_{k=1}^{M} e^{(2\pi ik(r-s)/M)} = M\delta_{rs},$$

and thus $\Sigma_k \hat{p}_k^2 = \Sigma_r \hat{P}_r \hat{P}_r^\dagger$. Similarly, $\Sigma_k \hat{q}_k^2 = \Sigma_r \hat{Q}_r \hat{Q}_r^\dagger$. The coupling terms can be written as

$$\sum_k (\hat{q}_k - \hat{q}_{k+1})(\hat{q}_k - \hat{q}_{k+1})^\dagger = \sum_k \hat{q}_k \hat{q}_k^\dagger + \sum_k \hat{q}_{k+1}\hat{q}_{k+1}^\dagger - \sum_k (\hat{q}_k \hat{q}_{k+1}^\dagger + \hat{q}_{k+1}\hat{q}_k^\dagger). \tag{2.15}$$

On the right hand side, the first two sums are of the same form as before; the last sum yields

$$\sum_k (\hat{q}_k \hat{q}_{k+1}^\dagger + \hat{q}_{k+1}\hat{q}_k^\dagger) = \sum_r (e^{(-2\pi ir/M)} \hat{Q}_r \hat{Q}_r^\dagger + e^{(2\pi ir/M)} \hat{Q}_r \hat{Q}_r^\dagger) = \sum_r 2\cos\left(\frac{2\pi r}{M}\right) \hat{Q}_r \hat{Q}_r^\dagger. \tag{2.16}$$

Thus we obtain, just as in the canonical case[5,6]

$$\hat{H} = \sum_{r=1}^{M} \left(\frac{1}{2m} \hat{P}_r \hat{P}_r^\dagger + \frac{m\omega_r^2}{2} \hat{Q}_r \hat{Q}_r^\dagger \right), \tag{2.17}$$

where, for $r=1,2,\ldots,M$, the quantities ω_r are positive numbers with

$$\omega_r^2 = \omega^2 + 2c - 2c\cos\left(\frac{2\pi r}{M}\right) = \omega^2 + 4c\sin^2\left(\frac{\pi r}{M}\right), \tag{2.18}$$

and clearly

$$\omega_{M-r} = \omega_r. \tag{2.19}$$

Substituting Eqs. (2.11) and (2.12) in Eqs. (2.5) and (2.6) yields the set of compatibility conditions for the new operators

$$[\hat{H}, \hat{Q}_r] = -\frac{i\hbar}{m} \hat{P}_r^\dagger, \quad [\hat{H}, \hat{Q}_r^\dagger] = -\frac{i\hbar}{m} \hat{P}_r, \tag{2.20}$$

$$[\hat{H}, \hat{P}_r] = i\hbar\, m\omega_r^2 \hat{Q}_r^\dagger, \quad [\hat{H}, \hat{P}_r^\dagger] = i\hbar\, m\omega_r^2 \hat{Q}_r. \tag{2.21}$$

The task is now reduced to finding operator solutions for $\hat{Q}_r$ and $\hat{P}_r$ such that the compatibility conditions (2.20) and (2.21), together with Eq. (2.17), are satisfied.

As a final step it is convenient to introduce linear combinations of the unknown operators $\hat{Q}_r$ and $\hat{P}_r$, say a_r^+ and a_r^- $(r=1,2,\ldots,M)$, by

$$a_r^- = \sqrt{\frac{m\omega_r}{2\hbar}} \hat{Q}_r + \frac{i}{\sqrt{2m\omega_r\hbar}} \hat{P}_r^\dagger, \tag{2.22}$$

$$a_r^+ = \sqrt{\frac{m\omega_r}{2\hbar}} \hat{Q}_r^\dagger - \frac{i}{\sqrt{2m\omega_r\hbar}} \hat{P}_r, \tag{2.23}$$

with

$$(a_r^\pm)^\dagger = a_r^\mp. \tag{2.24}$$

Observe that the inverse relations take the form

$$\hat{Q}_r = \sqrt{\frac{\hbar}{2m\omega_r}} (a_{M-r}^+ + a_r^-), \quad r = 1, \ldots, M-1; \quad \hat{Q}_M = \sqrt{\frac{\hbar}{2m\omega_M}} (a_M^+ + a_M^-), \tag{2.25}$$

$$\hat{P}_r = i\sqrt{\frac{m\omega_r\hbar}{2}}(a_r^+ - a_{M-r}^-), \quad r = 1, \ldots, M-1; \quad \hat{P}_M = i\sqrt{\frac{m\omega_M\hbar}{2}}(a_M^+ - a_M^-), \tag{2.26}$$

with similar expressions for $\hat{Q}_r^\dagger$ and $\hat{P}_r^\dagger$. In terms of the new set of unknown operators $a_r^\pm$ $(r = 1,2,\ldots,M)$, the Hamiltonian (2.17) becomes

$$\hat{H} = \sum_{r=1}^{M} \frac{\hbar\omega_r}{2}\{a_r^-, a_r^+\} = \sum_{r=1}^{M} \frac{\hbar\omega_r}{2}(a_r^- a_r^+ + a_r^+ a_r^-). \tag{2.27}$$

It is essential – and the reader should verify this – that in going from Eq. (2.17) to Eq. (2.27), no commutation relations among the operators $\hat{Q}_r$ and $\hat{P}_r$ are used, but only identities like Eqs. (2.13), (2.14), and (2.19). A final and simple calculation, using Eqs. (2.22) and (2.23), shows that Eqs. (2.20) and (2.21) is equivalent to

$$[\hat{H}, a_r^\pm] = \pm\hbar\,\omega_r a_r^\pm, \quad (r = 1,2\ldots,M). \tag{2.28}$$

Thus

Proposition 1: In the approach of Eq. (1.1) as a Wigner quantum system, the problem is reduced to finding $2M$ operators $a_r^\pm$ $(r=1,\ldots,M)$, acting in some Hilbert space, such that $(a_r^\pm)^\dagger = a_r^\mp$ and

$$\left[\sum_{j=1}^{M} \omega_j(a_j^- a_j^+ + a_j^+ a_j^-), a_r^\pm\right] = \pm 2\omega_r a_r^\pm, \quad (r = 1,2\ldots,M). \tag{2.29}$$

The operators corresponding to physical observables $\hat{q}_k$ and $\hat{p}_k$ are then known linear combinations of $a_r^\pm$, and the Hamiltonian $\hat{H}$ is given by Eq. (2.27).

As we shall see in the following section, this is an algebraic problem that has a class of solutions in terms of the Lie superalgebra $\mathfrak{gl}(1|M)$.

Before concentrating on an algebraic solution, let us end this section with a few words about the time dependency of the operators. The time dependency of $\hat{q}_k$ and $\hat{p}_k$ is determined by Eqs. (2.3) and (2.4). From these equations and Eqs. (2.9) and (2.10) it follows that:

$$\dot{\hat{Q}}_r = \frac{1}{m}\hat{P}_r^\dagger, \quad \dot{\hat{P}}_r = -m\omega_r^2\hat{Q}_r^\dagger. \tag{2.30}$$

Using Eqs. (2.22) and (2.23) yields

$$\dot{a}_r^- = -i\omega_r a_r^-, \quad \dot{a}_r^+ = i\omega_r a_r^+, \tag{2.31}$$

with the evident solution

$$a_r^\pm(t) = e^{\pm i\omega_r t}a_r^\pm(0). \tag{2.32}$$

So it is sufficient to have solutions for the operators $a_r^\pm$ at time 0, $a_r^\pm \equiv a_r^\pm(0)$. The time dependence for $a_r^\pm(t)$ is given by Eq. (2.32), and since all operators of the quantum system can be expressed in terms of $a_r^\pm$, their time dependence follows. As a consequence, we shall concentrate on solutions of the system Eqs. (2.27) and (2.28) at time $t=0$.

For completeness, it should also be mentioned that if the CCRs Eq. (1.3) hold, then the operators $a_r^\pm$ satisfy the usual boson relations $[a_r^\pm, a_s^\pm]=0$, $[a_r^-, a_s^+]=\delta_{rs}$. In that case Eq. (2.28) follows automatically from Eq. (2.27).

III. ALGEBRAIC SOLUTIONS OF THE COMPATIBILITY CONDITIONS

The set of relations (2.29), together with the conditions (2.24), are reminiscent of the algebraic relations satisfied by a set of $\mathfrak{gl}(1|M)$ generators.[12] We shall show that our problem has indeed a

solution in terms of the Lie superalgebra $\mathfrak{gl}(1|M)$ or $\mathfrak{sl}(1|M)$. Let us first recall the definition of $\mathfrak{gl}(1|M)$: it is a Lie superalgebra with basis elements e_{jk}, with $j,k=0,1,\ldots,M$. The elements e_{k0} and e_{0k} $(k=1,\ldots,M)$ are *odd* elements, having degree $\deg(e_{k0})=\deg(e_{0k})=1$; the remaining basis elements are *even* elements, having degree 0. The Lie superalgebra bracket is determined by[21–23]

$$[\![e_{ij},e_{kl}]\!]=\delta_{jk}e_{il}-(-1)^{\deg(e_{ij})\deg(e_{kl})}\delta_{il}e_{kj}. \tag{3.1}$$

In a representation, or in the enveloping algebra of $\mathfrak{gl}(1|M)$, the bracket $[\![x,y]\!]$ (where x and y are homogeneous elements of $\mathfrak{gl}(1|M)$) stands for an anti-commutator if x and y are both odd elements, and for a commutator otherwise. The Lie superalgebra $\mathfrak{sl}(1|M)$ is the subalgebra of $\mathfrak{gl}(1|M)$ consisting of elements with supertrace 0, or also $\mathfrak{sl}(1|M)=[\![\mathfrak{gl}(1|M),\mathfrak{gl}(1|M)]\!]$.

For a Lie superalgebra one can also fix a star condition, i.e., an antilinear anti-involution. For $\mathfrak{gl}(1|M)$ or $\mathfrak{sl}(1|M)$ such a star condition is fixed by a signature σ, i.e., a sequence of plus or minus signs $\sigma=(\sigma_1,\ldots,\sigma_M)$ and

$$(e_{0k})^{\dagger}=\sigma_k e_{k0},\quad (k=1,\ldots,M), \tag{3.2}$$

thus with each σ_k equal to $+1$ or -1. We are particularly interested in the case where all σ_k's are $+1$ since this corresponds to the "compact form" $\mathfrak{u}(1|M)$ of $\mathfrak{gl}(1|M)$ (Ref. 24), for which finite-dimensional unitary representations exist.[25]

We shall now show that there exist solutions of the form

$$a_k^-=\sqrt{\frac{2}{\omega_k}}\alpha_k e_{k0},\quad a_k^+=\sqrt{\frac{2}{\omega_k}}\alpha_k^*\sigma_k e_{0k},\quad (k=1,\ldots,M) \tag{3.3}$$

with α_k certain complex constants to be determined. First of all, note that by Eq. (3.2), the Hermiticity condition (2.24) is automatically satisfied. With Eq. (3.3), the Hamiltonian (2.27) becomes

$$\hat{H}=\hbar\left(\sum_{j=1}^{M}\sigma_j|\alpha_j|^2\right)e_{00}+\hbar\sum_{k=1}^{M}\sigma_k|\alpha_k|^2e_{kk}, \tag{3.4}$$

and the commutator of the above with Eq. (3.3) yields

$$[\hat{H},a_k^{\pm}]=\pm\hbar\left(\sum_{j=1}^{M}\sigma_j|\alpha_j|^2-\sigma_k|\alpha_k|^2\right)a_k^{\pm}\quad (k=1,\ldots,M). \tag{3.5}$$

These should coincide with the compatibility conditions (2.28). Thus we get a system of M equations in the unknown coefficients α_k,

$$\sum_{j=1}^{M}\sigma_j|\alpha_j|^2-\sigma_k|\alpha_k|^2=\omega_k\quad (k=1,2,\ldots,M). \tag{3.6}$$

It is easy to verify that a solution for this set of equations is determined by

$$\sigma_k|\alpha_k|^2=-\omega_k+\frac{1}{M-1}\sum_{j=1}^{M}\omega_j. \tag{3.7}$$

For further use, it will be convenient to introduce the following numbers:

$$\beta_k=-\omega_k+\frac{1}{M-1}\sum_{j=1}^{M}\omega_j, \tag{3.8}$$

with ω_j the values fixed by Eq. (2.18). Note that

TABLE I. Critical values c_0/ω^2.

M	c_0/ω^2	M	c_0/ω^2
4	0.9873724357	13	0.10546881460
5	0.7500000000	14	0.09256321610
6	0.3457442295	15	0.08687882025
7	0.2982653656	16	0.07814800074
8	0.2061705212	17	0.07388896853
9	0.1851128402	18	0.06760983697
10	0.1464642846	19	0.06429500840
11	0.1343028683	20	0.05957194222
12	0.1134651313	21	0.05691629341

$$\beta_{M-k}=\beta_k, \quad \beta \equiv \sum_{j=1}^{M} \beta_j = \sum_{j=1}^{M} \omega_j, \tag{3.9}$$

and thus $\hat{H}$ can be rewritten as

$$\hat{H} = \hbar \left(\beta e_{00} + \sum_{k=1}^{M} \beta_k e_{kk} \right). \tag{3.10}$$

Remember that we are primarily interested in the signature with all σ_k's equal to +1. Since $\sigma_k |\alpha_k|^2 = \beta_k$, the question is whether there exist solutions such that all β_k's are positive. At first sight, Eq. (3.8) indicates that β_k is equal to $-\omega_k$ plus "some average value" of the ω_j's, and hence, one would expect half of the β_k's to be negative and half of them to be positive. We shall show, however, that under certain conditions ("weak coupling," i.e., a small value for c), all β_k's are indeed positive. First of all, note that for $c>0$,

$$\beta_1 > \beta_2 > \cdots > \beta_{\lfloor M/2 \rfloor}, \quad \beta_{\lfloor M/2 \rfloor} \leqslant \beta_{\lfloor M/2 \rfloor + 1} < \cdots < \beta_M, \tag{3.11}$$

since a similar property holds for the values ω_k. Thus if $\beta_{\lfloor M/2 \rfloor} > 0$, then all β_k's are positive. The value of $\beta_{\lfloor M/2 \rfloor}$ depends on the value of c; if $c=0$ then indeed all $\beta_k = \omega/(M-1)$ are positive. So by continuity as a function of c there will be a certain interval $]0, c_0[$ where all β_k's are positive. This critical value c_0 is the c-value for which $\beta_{\lfloor M/2 \rfloor}=0$. For general M, this is a complicated transcendental equation that can be solved only numerically. Table I gives the numerical solutions for this equation, for M ranging from 4 to 21 (for $M=2$ or $M=3$ the β_k's are always positive). The following proposition gives a lower bound for the critical value c_0, such that all β_k's are positive.

Proposition 2: An upper bound for c is determined by

$$0 \leqslant c \leqslant \frac{\omega^2}{2(M-2)} \Rightarrow \beta_k \geqslant 0, \quad \text{for } 1 \leqslant k \leqslant M. \tag{3.12}$$

Proof: By definition Eq. (3.8) $\beta_k \geqslant 0$ if and only if

$$\omega_k \leqslant \frac{1}{M-1} \sum_{j=1}^{M} \omega_j \Leftrightarrow (M-1)^2 \omega_k^2 \leqslant \sum_{j=1}^{M} \omega_j^2 + 2 \sum_{i>j} \omega_i \omega_j. \tag{3.13}$$

We write the right hand side of Eq. (3.13) as a series with respect to c. For the first sum, we find

$$\sum_{j=1}^{M} \omega_j^2 = \sum_{j=1}^{M} \left(\omega^2 + 4c \sin^2\left(\frac{j\pi}{M}\right)\right) = M\omega^2 + 2c \sum_{j=1}^{M} \left(1 - \cos\left(\frac{2j\pi}{M}\right)\right) = M(\omega^2 + 2c).$$

Here, we used the Lagrange identity

$$1+\cos(x)+\cos(2x)+\cdots+\cos(nx)=\frac{1}{2}+\frac{\sin\left(\frac{(2n+1)x}{2}\right)}{2\sin\left(\frac{x}{2}\right)}.$$

In order to evaluate the second sum in Eq. (3.13), let

$$F(c)\equiv\sum_{i>j}\omega_i\omega_j=\sum_{i>j}\sqrt{\omega^2+4c\sin^2\left(\frac{i\pi}{M}\right)}\sqrt{\omega^2+4c\sin^2\left(\frac{j\pi}{M}\right)}. \tag{3.14}$$

It is then clear that

$$F(0)=\omega^2\frac{M(M-1)}{2}.$$

One can write the derivate of ω_k with respect to c as

$$\omega_k'=\frac{d\omega_k}{dc}=\frac{2}{\omega_k}\sin^2\left(\frac{k\pi}{M}\right),$$

and one finds that

$$F'(c)=\sum_{j>i}(\omega_i'\omega_j+\omega_i\omega_j')\geqslant 0,$$

since $\omega_k'\geqslant 0$. This implies that $F(0)\leqslant F(c)$ for $c\geqslant 0$. Thus it follows from Eq. (3.13) that

$$(M-1)^2\omega_k^2\leqslant\sum_{j=1}^{M}\omega_j^2+2F(0) \tag{3.15}$$

is a sufficient condition for $\beta_k\geqslant 0$. Since $\omega_k^2\leqslant\omega_{[M/2]}^2\leqslant\omega^2+4c$ for $1\leqslant k\leqslant M$, it is sufficient to solve the following inequality:

$$(M-1)^2(\omega^2+4c)\leqslant M(\omega^2+2c)+\omega^2M(M-1)\Leftrightarrow c\leqslant\frac{\omega^2}{2(M-2)},$$

leading to Eq. (3.12). □

Note that for $M=2$ or $M=3$ there are no conditions: for $M=2$, $\beta_1=\omega_2>0$ and $\beta_2=\omega_1>0$; for $M=3$, $\beta_1=\beta_2=\omega/2>0$ and $\beta_3=(\omega^2+3c)^{1/2}-\omega/2>0$.

We can now summarize the main result of this section in the following.

Proposition 3: For fixed M, let c satisfy

$$c\leqslant\frac{\omega^2}{2(M-2)}(\leqslant c_0)$$

(no condition if $M=2$ or $M=3$). Then the compatibility conditions (2.27) and (2.28) have a solution for the operators $a_k^{\pm}$ in terms of $\mathfrak{gl}(1|M)$ generators

$$a_k^-=\sqrt{\frac{2\beta_k}{\omega_k}}e_{k0},\quad a_k^+=\sqrt{\frac{2\beta_k}{\omega_k}}e_{0k},\quad (k=1,\ldots,M) \tag{3.16}$$

with β_k given by Eq. (3.8). The Hermiticity conditions (2.24) are equivalent with the star condition

$$(e_{0k})^{\dagger}=e_{k0}. \tag{3.17}$$

IV. A CLASS OF $\mathfrak{gl}(1|M)$ REPRESENTATIONS

In order to study properties of the given quantum system related to the $\mathfrak{gl}(1|M)$ solution of the previous section, one should consider representations of $\mathfrak{gl}(1|M)$ for which Eq. (3.17) holds. These are known as the unitary representations (or star representations), and have been classified by Gould and Zhang.[25] For the explicit actions of the $\mathfrak{gl}(1|M)$ generators on a Gel'fand-Zetlin basis for these unitary representations, see Ref. 26. These actions becomes fairly complicated, so in this paper we will concentrate on a particular class of representations, the so-called Fock type representations $W(p)$.

Without going into the details of the construction of such representations, we briefly summarize their main features here. Further details can be found in Refs. 27 and 28.

The representations $W(p)$ are labeled by a number p, with either $p \in \{0,1,2,\ldots,M-1\}$ or else $p \in \mathbb{R}$ with $p > M-1$. We describe the representation by giving the basis vectors of the representation space $W(p)$ and the action of the $\mathfrak{gl}(1|M)$ generators on these basis vectors.

For $p \in \{0,1,2,\ldots,M-1\}$, the basis vectors of $W(p)$ are given by:

$$w(\theta) \equiv w(\theta_1,\theta_2,\ldots,\theta_M), \quad \theta_i \in \{0,1\}, \quad \text{and } |\theta| = \theta_1 + \cdots + \theta_M \leqslant p. \tag{4.1}$$

Note that in this case the dimension of $W(p)$ is given by

$$\dim W(p) = \sum_{k=0}^{p} \binom{M}{k}. \tag{4.2}$$

For p real and $p > M-1$, the basis vectors of $W(p)$ are all vectors $w(\theta) \equiv w(\theta_1,\theta_2,\ldots,\theta_M)$ with each $\theta_i \in \{0,1\}$. Clearly, for $p > M-1$, the dimension of $W(p)$ is given by 2^M.

The action of the $\mathfrak{gl}(1|M)$ generators on the basis vectors of $W(p)$ is now given by

$$e_{00}w(\theta) = (p - |\theta|)w(\theta); \tag{4.3}$$

$$e_{kk}w(\theta) = \theta_k w(\theta), \quad (1 \leqslant k \leqslant M); \tag{4.4}$$

$$e_{k0}w(\theta) = (1-\theta_k)(-1)^{\theta_1+\cdots+\theta_{k-1}}\sqrt{p-|\theta|}\,w(\theta_1,\ldots,\theta_k+1,\ldots,\theta_M), \quad (1 \leqslant k \leqslant M); \tag{4.5}$$

$$e_{0k}w(\theta) = \theta_k(-1)^{\theta_1+\cdots+\theta_{k-1}}\sqrt{p-|\theta|+1}\,w(\theta_1,\ldots,\theta_k-1,\ldots,\theta_M), \quad (1 \leqslant k \leqslant M). \tag{4.6}$$

The action of the remaining $\mathfrak{gl}(1|M)$ basis elements can be determined from the above formulas, and one finds (for $1 \leqslant j < k \leqslant M$),

$$e_{jk}w(\theta) = \theta_k(1-\theta_j)(-1)^{\theta_j+\cdots+\theta_{k-1}}w(\theta_1,\ldots,\theta_j+1,\ldots,\theta_k-1,\ldots,\theta_M), \tag{4.7}$$

$$e_{kj}w(\theta) = -\theta_j(1-\theta_k)(-1)^{\theta_j+\cdots+\theta_{k-1}}w(\theta_1,\ldots,\theta_j-1,\ldots,\theta_k+1,\ldots,\theta_M). \tag{4.8}$$

With respect to the inner product

$$\langle w(\theta)|w(\theta')\rangle = \delta_{\theta,\theta'}, \tag{4.9}$$

the representation $W(p)$ is unitary for the star condition

$$e_{jk}^{\dagger} = e_{kj}.$$

The representations $W(p)$ with $p > M-1$ are *typical* irreducible $\mathfrak{gl}(1|M)$ representations; those with $p \in \{0,1,2,\ldots,M-1\}$ are *atypical* irreducible $\mathfrak{gl}(1|M)$ representations.[22,29] In Secs. V and VI we shall develop results for the typical representations; the atypical case is treated in Sec. VII.

Note, by Eq. (3.16) and Eq. (4.5) and (4.6) the action of the operators $a_k^{\pm}$ on the basis vectors $w(\theta)$ of $W(p)$ $(k=1,\ldots,M)$ is given by

$$a_k^- w(\theta) = \sqrt{\frac{2\beta_k}{\omega_k}}(1-\theta_k)(-1)^{\theta_1+\cdots+\theta_{k-1}}\sqrt{p-|\theta|}\,w(\theta_1,\ldots,\theta_k+1,\ldots,\theta_M), \tag{4.10}$$

$$a_k^+ w(\theta) = \sqrt{\frac{2\beta_k}{\omega_k}}\theta_k(-1)^{\theta_1+\cdots+\theta_{k-1}}\sqrt{p-|\theta|+1}\,w(\theta_1,\ldots,\theta_k-1,\ldots,\theta_M). \tag{4.11}$$

So the operators $a_k^\pm$ raise or lower θ_k by one unit (if allowed). This means that, for $p>M-1$, the basis vectors $w(\theta)$ of $W(p)$ have a Fock basis construction, by letting $|0\rangle=w(1,1,\ldots,1)$. Then $a_k^-|0\rangle=0$ and

$$w(\theta) \sim (a_1^+)^{1-\theta_1}(a_2^+)^{1-\theta_2}\cdots(a_M^+)^{1-\theta_M}|0\rangle. \tag{4.12}$$

This is the reason why $W(p)$ is referred to as a Fock representation.

V. ON THE SPECTRUM OF $\hat{H}$ IN THE REPRESENTATIONS $W(p)$

For any $p>M-1$, the representation $W(p)$ is of dimension 2^M. Under the solution (3.16), the Hamiltonian $\hat{H}$ takes the form (3.10),

$$\hat{H} = \hbar\left(\beta e_{00} + \sum_{k=1}^{M}\beta_k e_{kk}\right),$$

with $\beta=\Sigma_{k=1}^M\beta_k=\Sigma_{k=1}^M\omega_k$. Since the actions of e_{kk} $(k=0,1,\ldots,M)$ are diagonal in the basis $w(\theta)$, see Eqs. (4.3) and (4.4), it follows that the vectors $w(\theta)$ are eigenvectors for $\hat{H}$:

$$\hat{H}w(\theta) = \hbar\, E_\theta w(\theta), \tag{5.1}$$

with eigenvalues

$$E_\theta = \beta(p-|\theta|) + \sum_{k=1}^{M}\theta_k\beta_k = \beta\left(p-\frac{M-2}{M-1}|\theta|\right) - \sum_{k=1}^{M}\theta_k\omega_k. \tag{5.2}$$

In this expression, $\theta=(\theta_1,\ldots,\theta_M)$, with each $\theta_k\in\{0,1\}$, and $|\theta|=\Sigma_{k=1}^M\theta_k$.

In the case without coupling $(c=0)$, all β_k's are the same: $\beta_k=\omega/(M-1)$ and $\beta=(M/(M-1))\omega$. The eigenvalues of $\hat{H}$ are then

$$\hbar\,\omega\left(p\frac{M}{M-1}-|\theta|\right).$$

The multiplicity of this eigenvalue is $\binom{M}{|\theta|}$. In other words, there are $M+1$ distinct energy levels, equally spaced with steps of unit $\hbar\omega$. The lowest energy level corresponds to $E_{(1,\ldots,1)}=\omega pM/(M-1)-\omega M$, and the highest to $E_{(0,\ldots,0)}=\omega pM/(M-1)$.

We are mainly interested in the weak coupling case $(c>0$, but $c<c_0)$. Also in this case, it is easy to describe the energy levels through Eq. (5.2), but the analysis of their multiplicity requires some further attention. For this purpose, observe that by Eq. (3.9)

$$\sum_{k=1}^{M}\theta_k\beta_k = \sum_{k=1}^{M}\theta_k\beta_{M-k} = \sum_{k=0}^{M-1}\theta_{M-k}\beta_k = \sum_{k=1}^{M}\theta_{M-k}\beta_k, \tag{5.3}$$

where in the last step we have followed the convention that $\beta_0=\beta_M$, and we have set $\theta_0=\theta_M$. Let $w(\theta)$ be an arbitrary eigenvector $\hat{H}$ with eigenvalue $\hbar E_\theta$. Obviously, by Eqs. (5.2) and (5.3) all basis vectors $w(\theta')$ which are obtained by swapping θ_i and θ_{M-i} for arbitrary indices i yield the same eigenvalue $\hbar E_\theta$. The multiplicity of this eigenvalue is thus (at least)

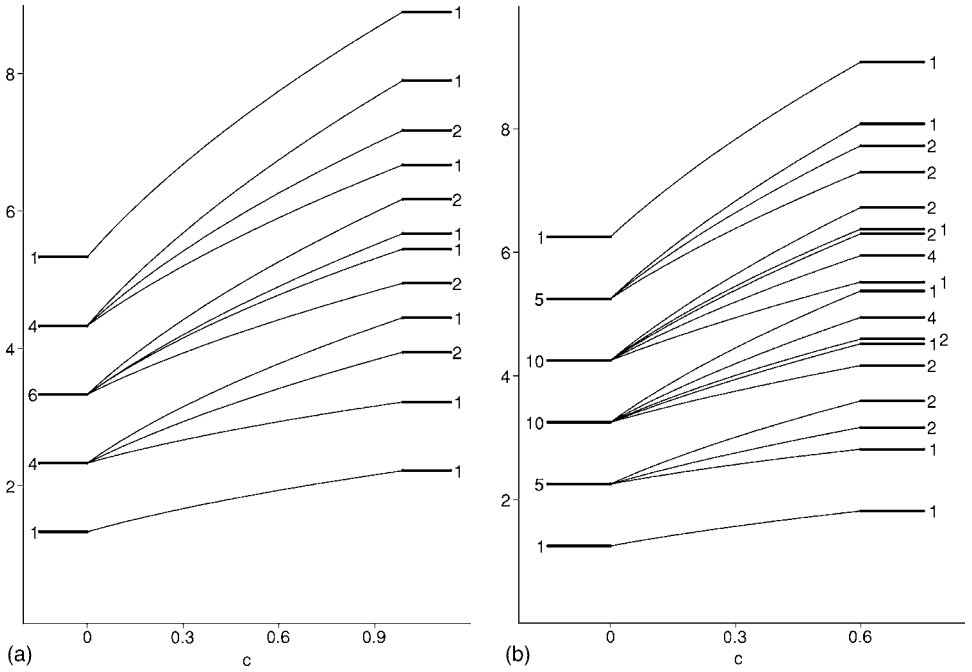

FIG. 2. (a) The energy levels of the quantum system for $M=4$ in $W(p)$, where we have taken $\hbar=\omega=1$, $p=M$, and c varies from 0 to c_0. The vertical axis gives the energy values. The numbers next to the levels refer to the multiplicity. When $c=0$ there are $M+1=5$ energy levels, with multiplicities (1,4,6,4,1). When $0<c<c_0$, the energy levels split up in 12 levels, with multiplicities 1 or 2. (b) The same illustration for $M=5$. There are six levels for $c=0$ with multiplicities (1,5,10,10,5,1), and there are 18 levels for $0<c<c_0$, with multiplicities 1, 2, or 4.

$$2^{\Sigma_{k=1}^{M}(\theta_k-\theta_{M-k})^2/2}. \tag{5.4}$$

Further inspection of the last expression in Eq. (5.2) shows that this is indeed the multiplicity of the eigenvalue, for $0<c<c_0$.

In Fig. 2 we give a plot of the energy levels for $M=4$ and $M=5$, as an illustration of the above. As c increases, the $M+1$ equidistant energy levels for $c=0$ split up in different levels, with smaller degeneracies.

It is worth noting that one can say something extra about the number of energy levels, for arbitrary M, also when $c\neq 0$. For $M=4$, the five levels $1+1+1+1+1$ at $c=0$ become $1+3+4+3+1$ levels for $c>0$ [just counting the energy levels, disregarding their multiplicities], see Fig. 2(a). We list here the number of levels for a few M values, when $c>0$:

M	Number of levels	Total number of levels
1	1+1	2
2	1+2+1	4
3	1+2+2+1	6
4	1+3+4+3+1	12
5	1+3+5+5+3+1	18
6	1+4+8+10+8+4+1	36
7	1+4+9+13+13+9+4+1	54
8	1+5+13+22+26+22+13+5+1	108

Let $T(M,k)$ $(k=0,1,\ldots,M)$ be the number of levels "per split" (the numbers in the middle column), and $L(M)=\Sigma_{k=0}^{M}T(M,k)$ be the total number of energy levels for $c>0$. $T(M,k)$ is also the number of distinct energy levels for all θ with $|\theta|=k$. Analysing this, using Eq. (5.4), one finds

$$T(M,k) = T(M-2,k) + T(M-2,k-1) + T(M-2,k-2). \tag{5.5}$$

Summing now over all k yields a simple recursion for the number of levels $L(M)$,

$$L(M) = 3L(M-2). \tag{5.6}$$

So we obtain the following result for the number of energy levels when $0 < c < c_0$, depending on whether M is even or odd

$$L(2n+1) = 2 \times 3^n, \quad L(2n+2) = 4 \times 3^n, \quad (n = 0,1,2,\dots). \tag{5.7}$$

Note that the numbers $L(M)$ belong to a known sequence, see entry A068911 in Ref. 30, with a simple generating function

$$G(x) = \sum_{M=0}^{\infty} L(M)x^M = \frac{(1+x)^2}{1-3x^2}. \tag{5.8}$$

VI. ON THE SPECTRUM OF POSITION OPERATORS IN THE REPRESENTATIONS $W(\boldsymbol{p})$ AND SPATIAL PROPERTIES

The purpose of the present section is to consider some geometric aspects of the given quantum system. In the first instance, we shall analyze the spectrum of the position operators $\hat{q}_r$ in the representations $W(p)$. By construction, these Hilbert spaces $W(p)$ are finite dimensional, so the position operators have a discrete spectrum.

The determination of the spectrum for general M and p requires a lot of work. This goes in two steps: first the operators $\hat{q}_r^2$ will be considered; this is the difficult part. Once the spectrum of $\hat{q}_r^2$ is analyzed, that of $\hat{q}_r$ follows rather easily. The spectrum of the momentum operators $\hat{p}_r^2$ and $\hat{p}_r$ is completely similar. In fact, we shall see that the structure of $\hat{p}_r^2$ and $\hat{q}_r^2$ as operators in $\mathfrak{gl}(1|M)$ is equivalent, and they can be treated simultaneously.

Note that, due to the symmetry of the system (1.1) and (1.2), the spectrum of $\hat{q}_r^2$ and $\hat{q}_r$ will be independent of r.

A. Eigenvalues and eigenvectors for $\hat{q}_r^2$

We start by writing the operator $\hat{q}_r^2$ in terms of the $\mathfrak{gl}(1|M)$ basis elements. Using Eq. (2.11), one finds

$$\hat{q}_r^2 = \frac{1}{2}\{\hat{q}_r, \hat{q}_r^\dagger\} = \frac{1}{2M}\sum_{k=1}^{M}\sum_{l=1}^{M} e^{(2\pi i r(k-l)/M)}\{\hat{Q}_k, \hat{Q}_l^\dagger\}.$$

Using Eq. (2.25) and the solution (3.16), this yields

$$\hat{q}_r^2 = \frac{\hbar}{mM}\left(\sum_{k=1}^{M}\frac{\beta_k}{\omega_k^2}e_{00} + \sum_{k=1}^{M}\sum_{l=1}^{M} e^{(2\pi i r(l-k)/M)}\frac{\sqrt{\beta_l\beta_k}}{\omega_l\omega_k}e_{lk}\right). \tag{6.1}$$

In a similar way, one finds

$$\hat{p}_r^2 = \frac{\hbar m}{M}\left(\sum_{k=1}^{M}\beta_k e_{00} + \sum_{k=1}^{M}\sum_{l=1}^{M} e^{(2\pi i r(l-k)/M)}\sqrt{\beta_l\beta_k}e_{lk}\right). \tag{6.2}$$

As operators of $\mathfrak{gl}(1|M)$, these two expressions are structurally equivalent: $\hat{q}_r^2$ is obtained from the expression of $\hat{p}_r^2$ by formally replacing every parameter β_k by β_k/ω_k^2, and multiplying by an overall factor $1/m^2$. So their spectral analysis is equivalent. Since the expression of $\hat{p}_r^2$ is somewhat simpler from the point of view of notation (no denominators in the factors), we shall first concentrate on the analysis for $\hat{p}_r^2$.

Following Eq. (6.2), it will be useful to introduce the even $\mathfrak{gl}(1|M)$ operators

$$\hat{s}_r = \sum_{k=1}^{M} \sum_{j=1}^{M} e^{(2\pi ir(j-k)/M)} \sqrt{\beta_j \beta_k} e_{jk}. \tag{6.3}$$

The main ingredient of our analysis is the following technical lemma.

Lemma 4: In the representation $W(p)$, the operator $\hat{s}_r$ has only two eigenvalues, namely $\beta = \Sigma_{k=1}^{M} \beta_k$ and 0, each with multiplicity 2^{M-1}.

Proof: Consider a vector of the form

$$v_r \equiv \sum_{k=1}^{M} e^{(2\pi irk/M)} \sqrt{\beta_k} w(1^k), \tag{6.4}$$

where $w(1^k)$ denotes the basis vector of $W(p)$ with $|\theta| = 1$ and the "1" occurring in position k (counting from left, and starting from one). For instance, if $M=4$ then

$$w(1^1) = w(1,0,0,0), \quad w(1^2) = w(0,1,0,0), \quad w(1^3) = w(0,0,1,0), \quad w(1^4) = w(0,0,0,1).$$

We extend the notation to $w(1^{k_1} \cdots 1^{k_n})$ which denotes the basis vector with $|\theta| = n$ and with 1's in the positions k_1 up to k_n.

It is easy to verify that v_r is an eigenvector of $\hat{s}_r$ with eigenvalue β.

In $\mathfrak{gl}(1|M)$, one can see that

$$[e_{l0}, \hat{s}_r] = -\sqrt{\beta_l} e^{-(2\pi irl/M)} \sum_{j=1}^{M} \sqrt{\beta_j} e^{(2\pi irj/M)} e_{j0}, \tag{6.5}$$

and thus the action (4.5) implies that

$$[e_{l0}, \hat{s}_r] v_r = 0. \tag{6.6}$$

This means that $e_{l0} v_r$ (provided it does not vanish) is also an eigenvector of $\hat{s}_r$, with the same eigenvalue β. Our goal is now to show that

$$e_{l_n 0} e_{l_{n-1} 0} \cdots e_{l_1 0} v_r \tag{6.7}$$

is also an eigenvector of $\hat{s}_r$ with the same eigenvalue β, provided all l_i are different (and different from M). If one would apply the same e_{l0} twice, the resulting vector vanishes since $\{e_{l0}, e_{k0}\} = 0$, by Eq. (3.1). This means that we can also assume, without loss of generality, that $M > l_n > l_{n-1} > \cdots > l_1 > 0$.

Using Eq. (4.5), one can write

$$e_{l_n 0} e_{l_{n-1} 0} \cdots e_{l_1 0} v_r \sim \sum_{t=0}^{n} (-1)^t \sum_{k=l_t+1}^{l_{t+1}-1} \sqrt{\beta_k} e^{(2\pi irk/M)} w(1^{l_1} \cdots 1^{l_t} 1^k 1^{l_{t+1}} \cdots 1^{l_n}), \tag{6.8}$$

with $l_0 = 0$ and $l_{n+1} = M+1$. Using Eq. (6.5), this implies that

$$[e_{l0}, \hat{s}_r] e_{l_n 0} e_{l_{n-1} 0} \cdots e_{l_1 0} v_r \sim \sum_{j=1}^{M} \sqrt{\beta_j} e^{(2\pi irj/M)} \sum_{t=0}^{n} (-1)^t \sum_{k=l_t+1}^{l_{t+1}-1} \sqrt{\beta_k} e^{(2\pi irk/M)} e_{j0} w(1^{l_1} \cdots 1^{l_t} 1^k 1^{l_{t+1}} \cdots 1^{l_n}). \tag{6.9}$$

Keeping in mind the action of e_{j0} on a basis vector $w(\theta)$, one sees that this expression is a linear combination of basis vectors $w(\theta)$ for which $|\theta| = n+2$, having a 1 in the positions l_1, l_2 up to l_n and in two extra positions x and y. Consider such a vector

$$w(1^{l_1}\cdots 1^{l_{i_x}}1^{x}1^{l_{i_x+1}}\cdots 1^{l_{i_y}}1^{y}1^{l_{i_y+1}}\cdots 1^{l_n}).$$

In expression (6.9) this vector will appear twice, once with k and j playing the role of x and y respectively, and one vice versa. In the first case the coefficient of this vector is

$$\sqrt{p-(n+1)}\sqrt{\beta_x\beta_y}e^{(2\pi ir(x+y)/M)}(-1)^{i_x}(-1)^{i_y+1},$$

while in the second case it is

$$\sqrt{p-(n+1)}\sqrt{\beta_x\beta_y}e^{(2\pi ir(x+y)/M)}(-1)^{i_x}(-1)^{i_y}.$$

Since these two coefficients cancel, we can conclude that

$$[e_{l0},\hat{s}_r]e_{l_n0}e_{l_{n-1}0}\cdots e_{l_10}v_r=0. \tag{6.10}$$

Following Eqs. (6.6) and (6.10), all vectors of the form (6.7) are eigenvectors of $\hat{s}_r$ for the eigenvalue β. It remains to find the number of linearly independent eigenvectors, i.e., the multiplicity of the eigenvalue β.

For n fixed, consider the $\binom{M-1}{n}$ vectors (6.7) with $1\leqslant l_1<l_2<\cdots<l_n\leqslant M-1$. Expressing these in the $w(\theta)$ basis by Eq. (6.8), in total $\binom{M}{n+1}$ basis vectors are involved. Each basis vector $w(\theta)$ occurs $\binom{n+1}{n}=n+1$ times, *except* those vectors that have a 1 in position M. There are $\binom{M-1}{n}$ such vectors. Next, let A be the $\binom{M-1}{n}\binom{M}{n+1}$ matrix, consisting of the coefficients of the $\binom{M-1}{n}$vectors (6.7) written in terms of the $\binom{M}{n+1}$ basis vectors. Select in A those columns that correspond to basis vector having a 1 in position M. This submatrix is equivalent with a diagonal matrix of which the diagonal elements are proportional to $\sqrt{\beta_M}$. So, the vectors (6.7) with $1\leqslant l_1<\cdots<l_n\leqslant M-1$ are linearly independent.

Furthermore, it is immediately clear that the vectors

$$e_{l_n0}e_{l_{n-1}0}\cdots e_{l_10}v_r \quad \text{and } e_{l_t0}e_{l_{t-1}0}\cdots e_{l_10}v_r$$

are linearly independent if $n\neq t$ (they are linear combinations of basis vectors with different $|\theta|$).

The conclusion is that we have found

$$\sum_{n=0}^{M-1}\binom{M-1}{n}=2^{M-1}$$

linearly independent eigenvectors of $\hat{s}_r$ with eigenvalue β. Note that for some fixed $|\theta|$, there are $\binom{M-1}{|\theta|-1}$ linearly independent eigenvectors of $\hat{s}_r$ with eigenvalue β.

The eigenvalue 0 of $\hat{s}_r$ also has multiplicity 2^{M-1}. This is seen in a completely similar way, starting with the vector

$$\tilde{v}_r\equiv\sum_{k=1}^{M}e^{-(2\pi irk/M)}(-1)^k\sqrt{\beta_k}w(0^k)$$

and acting repeatedly with e_{0l} (with $1\leqslant l\leqslant M-1$) on this vector. Herein we have extended the notation of Eq. (6.4): $w(0^k)$ denotes a basis vector where every $\theta_j=1$ $(j\neq k)$ except $\theta_k=0$. For fixed $|\theta|$, there are thus $\binom{M-1}{|\theta|}$ linearly independent eigenvectors with eigenvalue 0. □

We can now describe the eigenvalues of $\hat{p}_r^2$. Since

$$e_{00}w(\theta)=(p-|\theta|)w(\theta),$$

it follows from Eq. (6.2) that an eigenvector of $\hat{s}_r$ which is a linear combination of basis vectors with fixed $|\theta|$ will also be an eigenvector of $\hat{p}_r^2$. The eigenvalues of $\hat{p}_r^2$ are thus given by

$\hbar m(p-K)\beta/M$, for $0 \leqslant K \leqslant M-1$, with multiplicities $2\binom{M-1}{K}$. More in particular, the eigenvectors of $\hat{p}_r^2$ with eigenvalue $\hbar m(p-K)\beta/M$ arise in two ways, one set having $|\theta|=K+1$ and containing vectors of the form

$$e_{l_K 0} e_{l_{K-1} 0} \cdots e_{l_1 0} v_r.$$

The other set has $|\theta|=K$ and contains vectors of the form

$$e_{0 l_{M-K-1}} \cdots e_{0 l_1} \tilde{v}_r.$$

Unfortunately, the vectors (for a given eigenvalue) constructed here are not orthogonal. For any fixed M, one can construct a set of orthogonal eigenvectors by Gram–Schmidt orthogonalization. But so far we cannot give a closed analytic expression for some set of orthogonal eigenvectors.

Let us also state the result for the squared position operators $\hat{q}_r^2$. Recall from the beginning of this subsection that every β_k should be replaced by β_k/ω_k^2, thus β should be replaced by

$$\gamma = \sum_{k=1}^{M} \frac{\beta_k}{\omega_k^2}. \tag{6.11}$$

Proposition 5: The operator $\hat{q}_r^2$ has M distinct eigenvalues given by $x_K^2 = \hbar(p-K)\gamma/mM$, where $0 \leqslant K \leqslant M-1$. The multiplicity of each x_K^2 is $2\binom{M-1}{K}$. The eigenvectors of $\hat{q}_r^2$ with eigenvalue x_K^2 arise in two ways: there are $\binom{M-1}{K}$ vectors with $|\theta|=K+1$ of the form

$$e_{l_K 0} e_{l_{K-1} 0} \cdots e_{l_1 0} u_r;$$

and there are $\binom{M-1}{M-K-1} = \binom{M-1}{K}$ vectors with $|\theta|=K$ of the form

$$e_{0 l_{M-K-1}} \cdots e_{0 l_1} \tilde{u}_r.$$

Herein

$$u_r = \sum_{k=1}^{M} e^{(2\pi i r k/M)} \frac{\sqrt{\beta_k}}{\omega_k} w(1^k), \quad \tilde{u}_r = \sum_{k=1}^{M} e^{-(2\pi i r k/M)} (-1)^k \frac{\sqrt{\beta_k}}{\omega_k} w(0^k). \tag{6.12}$$

B. Eigenvalues for $\hat{q}_r$

We have shown that the eigenvectors of $\hat{q}_r^2$ with eigenvalue x_K^2 have either $|\theta|=K$ or $|\theta|=K+1$. Let ψ_{r,x_K} be an eigenvector of $\hat{q}_r$ with eigenvalue x_K. Such an eigenvector necessarily has the form

$$\psi_{r,x_K} = \sum_{|\theta|=K} C_{\theta,r,x_K} w(\theta) + \sum_{|\theta|=K+1} C_{\theta,r,x_K} w(\theta), \tag{6.13}$$

with C some constants. Thus one can write

$$\sum_{|\theta|=K} C_{\theta,r,x_K} \hat{q}_r w(\theta) + \sum_{|\theta|=K+1} C_{\theta,r,x_K} \hat{q}_r w(\theta) = x_K \sum_{|\theta|=K} C_{\theta,r,x_K} w(\theta) + x_K \sum_{|\theta|=K+1} C_{\theta,r,x_K} w(\theta). \tag{6.14}$$

But the action of $\hat{q}_r$ on a basis vector $w(\theta)$ is necessarily a linear combination of basis vectors $w(\theta')$ with $|\theta'|=|\theta|-1$ and $|\theta'|=|\theta|+1$: this follows from Eqs. (2.11), (2.25) and Eqs. (4.10) and (4.11). Thus the first sum on the left hand side of Eq. (6.14) is a linear combination of basis vectors with $|\theta|=K-1$ and $|\theta|=K+1$, while the second sum on the left hand side of Eq. (6.14) is a linear combination of basis vectors with $|\theta|=K$ and $|\theta|=K+2$. Of these four linear combinations

the first and the last vanish (since they do no occur on the right hand side), and it follows that

$$\sum_{|\theta|=K} C_{\theta,r,x_K}\hat{q}_r w(\theta) = x_K \sum_{|\theta|=K+1} C_{\theta,r,x_K} w(\theta). \tag{6.15}$$

Combining this with Eq. (6.14) implies

$$\sum_{|\theta|=K+1} C_{\theta,r,x_K}\hat{q}_r w(\theta) = x_K \sum_{|\theta|=K} C_{\theta,r,x_K} w(\theta). \tag{6.16}$$

We will now show that, given Eq. (6.13),

$$\psi_{r,-x_K} \equiv \sum_{|\theta|=K} C_{\theta,r,x_K} w(\theta) - \sum_{|\theta|=K+1} C_{\theta,r,x_K} w(\theta) \tag{6.17}$$

is an eigenvector of $\hat{q}_r$ with eigenvalue $-x_K$. In fact, the action of $\hat{q}_r$ on $\psi_{r,-x_K}$ follows directly from Eqs. (6.15) and (6.16) and yields $\hat{q}_r\psi_{r,-x_K}=-x_K\psi_{r,-x_K}$.

Thus we have shown:

Proposition 6: The operator $\hat{q}_r$ has $2M$ distinct eigenvalues given by $\pm x_K = \pm\sqrt{\hbar(p-K)\gamma/mM}$, where $0\leqslant K\leqslant M-1$. The multiplicity of the eigenvalue $\pm x_K$ is $\binom{M-1}{K}$. The eigenvectors of $\hat{q}_r$ for the eigenvalue $\pm x_K$ contain, when expanded in the standard basis $w(\theta)$, only vectors with $|\theta|=K$ or $|\theta|=K+1$.

So far, we have no simple analytic expression of the (orthogonal) eigenvectors of $\hat{q}_r$ in terms of the standard basis vectors $w(\theta)$.

C. Position probability distributions for stationary states $w(\theta)$

Consider the eigenvectors $\psi_{r,x,g}$ of the position operator $\hat{q}_r$ for the eigenvalue x expanded in the $w(\theta)$ basis

$$\psi_{r,x,g} = \sum_{\theta} C_{\theta,r,x,g} w(\theta), \tag{6.18}$$

and assume that these vectors are orthonormal, i.e.,

$$\langle \psi_{r,x,g} | \psi_{r,y,h} \rangle = \sum_{\theta} C^*_{\theta,r,x,g} C_{\theta,r,y,h} = \delta_{x,y}\delta_{g,h}. \tag{6.19}$$

In the above, g (or h) stands for a multiplicity label for vectors with the same eigenvalue x: e.g., when $x=\pm x_K$ then g runs from 1 to $\binom{M-1}{K}$. We know from the previous subsection that for $x=\pm x_K$, only coefficients $C_{\theta,r,x,g}$ with $|\theta|=K$ or $|\theta|=K+1$ will appear.

Let us now suppose that the quantum system is in a fixed eigenstate $w(\theta)$ of $\hat{H}$ (a stationary state). The expression

$$P(\theta, r, \pm x_K) = \sum_{g=1}^{\binom{M-1}{K}} |C_{\theta,r,\pm x_K,g}|^2 \tag{6.20}$$

yields the probability of "measuring" the value $\pm x_K$ for the position of the rth oscillator when the system is in the state $w(\theta)$. Plotting all these values $P(\theta, r, \pm x_K)$ for $K=0,\ldots,M-1$ yields the probability distribution of oscillator r in the stationary state $w(\theta)$.

It will be interesting to look at an explicit example of such probability distributions. First of all, due to the earlier mentioned symmetry of the system, these probability distributions will be independent of r; so we need to plot it for one r-value only (say $r=1$). We have considered the example $M=4$, with $\hbar=m=\omega=1$ and $c=0.5$. Then the eight eigenvalues $\pm x_K$ are given by $\pm(\sqrt{\gamma}/2)\sqrt{p-K}$, $K=0$, 1, 2, 3, with $p>3$ and $\gamma=(5\sqrt{2}+4\sqrt{3}-2)/9$ follows from Eq. (6.11). Let us

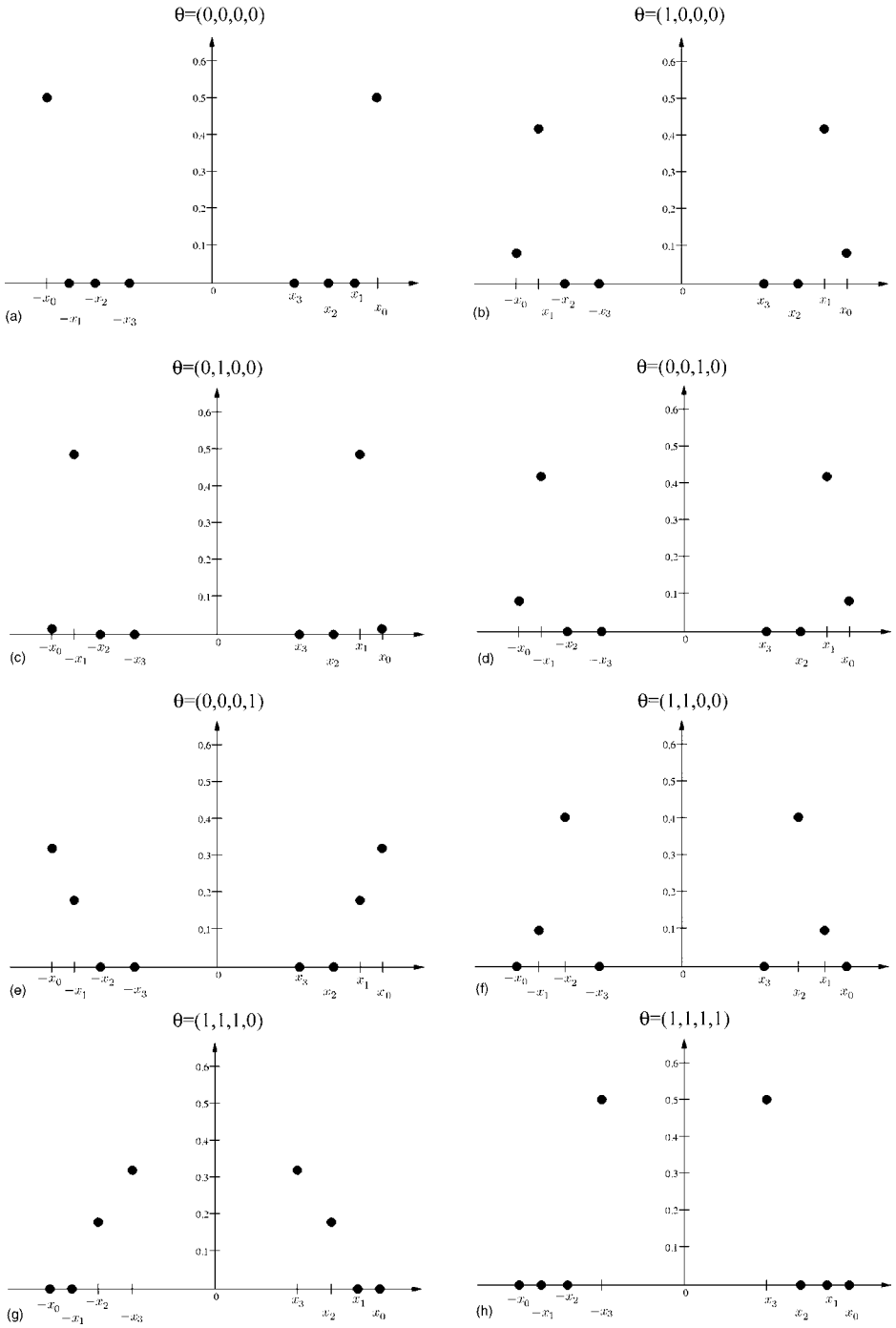

FIG. 3. Position probability distributions $P(\theta,1,\pm x_K)$ for a number of θ-values, for $M=4$. The vertical axis gives the values of $P(\theta,1,\pm x_K)$. On the horizontal axis one finds the possible eigenvalues $\pm x_K$ with $K=0$, 1, 2, 3. The values of the parameters are described in the text.

also choose a value for the representation label p: $p=M=4$. In Fig. 3 we give the position probability distributions for a number of stationary states $w(\theta)$, namely for $\theta=(0,0,0,0)$, $(1,0,0,0)$,$(0,1,0,0)$, $(0,0,1,0)$, $(0,0,0,1)$, $(1,1,0,0)$, $(1,1,1,0)$, and $(1,1,1,1)$.

Note in these plots that – in agreement with the previous paragraph – only the probabilities for $\pm x_K$ with $K=|\theta|$ or $K=|\theta|-1$ are nonzero. For $\theta=(0,0,0,0)$, corresponding to the highest energy

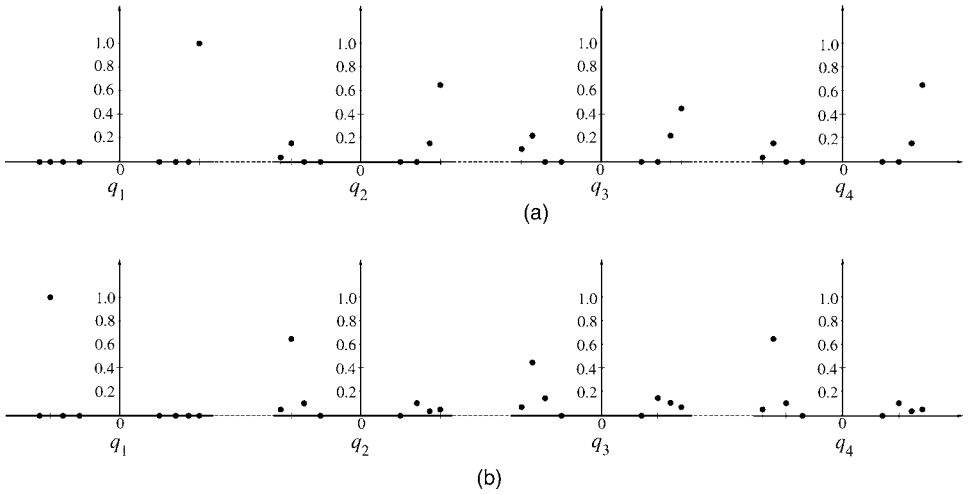

FIG. 4. Position probability distributions for all oscillators when the system is in the state (a) $\psi_{1,+x_0,1}$ and (b) $\psi_{1,-x_1,g}$.

state, the oscillators can be detected only in positions corresponding to the largest eigenvalues x_0 or $-x_0$. For $\theta=(1,1,1,1)$, corresponding to the lowest energy state, the oscillators can be detected only in positions corresponding to the smallest eigenvalues x_3 or $-x_3$. The four plots with $|\theta|=1$ give some probability distributions in which $\pm x_0$ and $\pm x_1$ are involved. Note that for $w(1,0,0,0)$ and $w(0,0,1,0)$, two stationary states for which the energy level is the same by Eq. (5.2) and Eq. (5.3), also the probability distributions coincide. According to Eq. (5.2), $E_{(0,0,0,1)}>E_{(0,0,1,0)}=E_{(0,1,0,0)}>E_{(1,0,0,0)}$. For the highest of these three energy levels, the probability of detecting the oscillator in $\pm x_0$ is larger than detecting it in $\pm x_1$; for the lowest of these three levels, it is vice versa. As $|\theta|$ increases (thus E_θ decreases), the probabilities indicate that the oscillator deviation from its equilibrium position also decreases.

D. Coupling of position probability distributions

In the previous subsection we considered, for a fixed stationary state $w(\theta)$, the position probabilities of the rth oscillator. Due to the symmetry of the system, these probability distributions are independent of r. It will be interesting to approach the position probabilities from a different point of view. For this purpose, let us assume that the system is in a fixed eigenstate of $\hat{q}_1$ with eigenvalue x, say $\psi_{1,x,g}$. Let us also consider another oscillator $r\neq 1$, and the expansion of $\psi_{1,x,g}$ in terms of the eigenvectors of $\hat{q}_r$:

$$\psi_{1,x,g}=\sum_{y,h} A_{1,x,g}^{r,y,h}\psi_{r,y,h}. \tag{6.21}$$

Then

$$\sum_{h} |A_{1,x,g}^{r,y,h}|^2 \tag{6.22}$$

is the probability of detecting the rth oscillator in the position y (corresponding to the eigenvalue y of $\hat{q}_r$) when the first oscillator is in the state $\psi_{1,x,g}$. Averaging this out over the multiplicities g (if present), thus yields the probability of detecting the rth oscillator in position y when the first oscillator is in position x.

Let us again look at an example of such probability distributions. We shall consider the same data as before: $M=4$, $\hbar=m=\omega=1$, and $c=0.5$. First, assume that oscillator 1 is in its highest possible position $+x_0$, so the system is in the state $\psi_{1,+x_0,1}$. Then, we can compute the probabilities (6.22), for $r=2$, 3, 4 and for $y=\pm x_K$ $(K=0,1,2,3)$. These probabilities are plotted in Fig. 4(a).

Note that the extreme position of oscillator 1 has a strong influence on the possible positions of oscillator 2, a weaker influence on the possible positions of oscillator 3, and again a stronger one on those of oscillator 4 (this last is due to the periodic boundary conditions (1.2), oscillator 4 behaves as if it is just to the left of oscillator 1).

We have also considered a second example, when the first oscillator is in an eigenstate with eigenvalue $-x_1$, i.e., the system is in a state $\psi_{1,-x_1,g}$. The position probability distributions for the other oscillators $r=2$, 3, 4 are plotted in Fig. 4(b), where we have averaged out over g ($g=1$, 2, 3). Thus in Fig. 4(b) an answer is given to the following question: suppose we make a measurement of the position of the first oscillator, and detect it in $-x_1$, what are in that case the probabilities of finding the other oscillators 2, 3, and 4 in one of their positions $\pm x_K$?

VII. ON THE SPECTRUM OF $\hat{H}$ AND POSITION OPERATORS IN ATYPICAL REPRESENTATIONS $W(p)$

In this section, we very briefly discuss what happens when working with atypical representations $W(p)$, i.e., when $p \in \{0,1,\ldots,M-1\}$. We concentrate on the spectrum of the Hamiltonian $\hat{H}$ and on that of the operators $\hat{q}_r^2$ and $\hat{q}_r$. Recall that the representation space in the atypical case is a truncation of that in the typical case, discarding basis vectors $w(\theta)$ for which $|\theta| > p$. Thus one expects a close connection between the spectra of the different operators in the typical and atypical case.

It is clear that each basis vector $w(\theta)$ is still an eigenvector of $\hat{H}$, with eigenvalue $\hbar E_\theta$, with E_θ given by Eq. (5.2). So the spectrum of $\hat{H}$ in the atypical case is nothing but a truncation of that in the typical case where the higher eigenvalues are retained (of course, the actual values are different because of the different value for p). As an example, for $M=4$ and $p=1$ the dimension of the representation space is

$$\binom{4}{0} + \binom{4}{1} = 5,$$

and the only four eigenvalues $\hbar E_\theta$ of $\hat{H}$ are

$$E_{(0,0,0,0)} = \beta = \beta_1 + \beta_2 + \beta_3 + \beta_4, \quad E_{(0,0,0,1)} = \beta_4,$$

$$E_{(1,0,0,0)} = \beta_1 = E_{(0,0,1,0)} = \beta_3, \quad \text{and } E_{(0,1,0,0)} = \beta_2,$$

where $\beta_4 > \beta_3 = \beta_1 > \beta_2$ for $0 < c < c_0$. These are the four topmost energy levels depicted in Fig. 2(a).

In the typical case $\hat{q}_r^2$ has eigenvalues $x_K^2 = \hbar(p-K)\gamma/mM$, with $0 \leqslant K \leqslant M-1$. From Eqs. (6.1), (4.3), (4.7), and (4.8) it follows immediately that an eigenvector of $\hat{q}_r^2$ in the typical case is also an eigenvector of $\hat{q}_r^2$ in the atypical case provided that it is a linear combination of basis vectors $w(\theta)$ with $|\theta| \leqslant p$. When $K<p$ one has the same set of eigenvectors as in the typical case, arising from both u_r and $\tilde{u}_r$ and the multiplicity of x_K^2 is $2\binom{M-1}{K}$. However, when $K=p$, $x_p=0$ and only the vectors arising from $\tilde{u}_r$ remain (the vectors arising from u_r would have $|\theta| = p+1$ which is impossible in an atypical representation). The multiplicity of eigenvalue $x_p=0$ is thus $\binom{M-1}{P}$. Consider the case $M=4$ and $p=1$; each operator $\hat{q}_r^2$ has two eigenvalues namely 0, with multiplicity $\binom{4-1}{1}=3$ and $\hbar(1)\gamma/4m$ with multiplicity $2\binom{3}{0}=2$.

For the position operators $\hat{q}_r$ finally, it is seen as before that $\pm x_K$ with $0 \leqslant K \leqslant p-1$ are eigenvalues of $\hat{q}_r$ each with multiplicity $\binom{M-1}{K}$. Besides these eigenvalues, there is also the eigenvalue $x_p=0$ with multiplicity $\binom{M-1}{P}$. So in the atypical case it is possible to "detect" an oscillator in its equilibrium position, in contrast with the typical case.

It is worth giving some further details for the representation $W(1)$ (so $p=1$), for general M-values. This representation has dimension $M+1$, with basis vectors $w(0)$ and $w(1^j)$ (in the notation of Eq. (6.4)), with $j=1,\ldots,M$. Each position operator $\hat{q}_r$ has spectrum $\{-x_0,0,+x_0\}$, with multiplicities $\{1,M-1,1\}$ respectively, where $x_0=\sqrt{\hbar\gamma/mM}$. Herein, γ is given by Eq. (6.11); in fact it will be useful to introduce the notation

$$\gamma_k=\frac{\sqrt{\beta_k}}{\omega_k},\quad k=1,\ldots,M, \tag{7.1}$$

and thus $\gamma=\Sigma_{k=1}^{M}\gamma_k^2$.

In this case, it is not difficult to construct explicitly a set of orthonormal eigenvectors of $\hat{q}_r$. In the notation of Sec. VI C, it is given by

$$\psi_{r,+x_0,1}=\frac{1}{\sqrt{2}}w(0)+\sum_{j=1}^{M}\frac{\gamma_j}{\sqrt{2\gamma}}e^{(2\pi irj/M)}w(1^j), \tag{7.2}$$

$$\psi_{r,-x_0,1}=\frac{1}{\sqrt{2}}w(0)-\sum_{j=1}^{M}\frac{\gamma_j}{\sqrt{2\gamma}}e^{(2\pi irj/M)}w(1^j), \tag{7.3}$$

$$\psi_{r,0,g}=\frac{1}{\sqrt{\dfrac{1}{\gamma_1^2+\cdots+\gamma_g^2}+\dfrac{1}{\gamma_{g+1}^2}}}\left(\sum_{j=1}^{g}\frac{\gamma_j}{\gamma_1^2+\cdots+\gamma_g^2}e^{(2\pi irj/M)}w(1^j)-\frac{1}{\gamma_{g+1}}e^{(2\pi ir(g+1)/M)}w(1^{g+1})\right), \tag{7.4}$$

where $g=1,2,\ldots,M-1$.

Now it becomes simple to compute some position probabilities. Following Eq. (6.20), one finds for the state $w(0)$ with $\theta=(0)=(0,\ldots,0)$,

$$P((0),r,+x_0)=P((0),r,-x_0)=\frac{1}{2},\quad P((0),r,0)=0.$$

Hence, in the highest energy state of $W(1)$, the oscillators can be detected only in the positions $\pm x_0$ and not in 0. Similarly

$$P((1^j),r,+x_0)=P((1^j),r,-x_0)=\frac{\gamma_j^2}{2\gamma},\quad P((1^j),r,0)=1-\frac{\gamma_j^2}{\gamma}.$$

Also the probabilities (6.22) can be computed. One finds, for example

$$A_{1,+x_0,1}^{r,+x_0,1}=\frac{1}{\gamma}\sum_{j=1}^{M}\gamma_j^2\cos^2\left(\frac{\pi(r-1)j}{M}\right),\quad A_{1,+x_0,1}^{r,-x_0,1}=\frac{1}{\gamma}\sum_{j=1}^{M}\gamma_j^2\sin^2\left(\frac{\pi(r-1)j}{M}\right), \tag{7.5}$$

and thus

$$\sum_g|A_{1,+x_0,1}^{r,0,g}|^2=\frac{2}{\gamma^2}\left(\sum_{j=1}^{M}\gamma_j^2\cos^2\left(\frac{\pi(r-1)j}{M}\right)\right)\left(\sum_{j=1}^{M}\gamma_j^2\sin^2\left(\frac{\pi(r-1)j}{M}\right)\right).$$

As before, the quantities $|A_{1,+x_0,1}^{r,+x_0,1}|^2$, $\Sigma_g|A_{1,+x_0,1}^{r,0,g}|^2$, and $|A_{1,+x_0,1}^{r,-x_0,1}|^2$ describe the probabilities of detecting the rth oscillator in the position $+x_0$, 0, or $-x_0$ respectively, when the first oscillator is in its highest position $+x_0$.

With the given probabilities, one can consider a final illustration. If the system is in the state $\psi_{1,+x_0,1}$, the average position of each oscillator r is given by

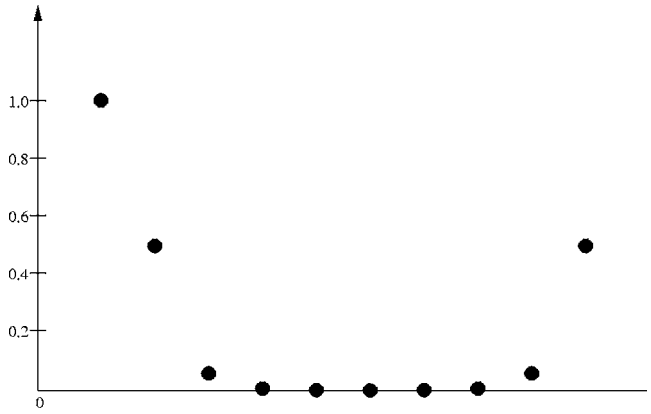

FIG. 5. Average positions of the M oscillators, $M=10$, when the first oscillator is in the position $+x_0$, in the representation $W(1)$. Here, we have taken $c=0.12\omega^2$. The horizontal axis labels the M oscillators; the vertical axis gives the average position in units of x_0.

$$+x_0|A^{r,+x_0,1}_{1,+x_0,1}|^2+0\sum_g|A^{r,0,g}_{1,+x_0,1}|^2-x_0|A^{r,-x_0,1}_{1,+x_0,1}|^2.$$

Using Eq. (7.5), this simplifies to

$$\langle\hat{q}_r\rangle_{\psi_{1,+x_0,1}}=x_0\frac{1}{\gamma}\sum_{j=1}^{M}\gamma_j^2\cos\left(\frac{2\pi(r-1)j}{M}\right).$$

In Fig. 5 we plot the average position of each oscillator r in this state. So in this figure one can see the effect of having the first oscillator in its highest position $+x_0$ on the average position of the other oscillators.

VIII. CONCLUSION AND OUTLOOK

We have examined some properties of noncanonical solutions of the quantum system determined by the Hamiltonian (1.1). These solutions arise from a WQSs approach, where the quantization conditions are weaker than the canonical commutation relations, thus allowing more types of solutions.

The solutions studied here are found by identifying certain linear combinations of position and momentum operators with generators of the Lie superalgebra $\mathfrak{gl}(1|M)$. We have shown that this is always possible, but that the solutions are corresponding to the compact form $\mathfrak{u}(1|M)$ of $\mathfrak{gl}(1|M)$ only if the coupling constant c is sufficiently small.

The physical Hilbert spaces in which the states of the system are described then correspond to unitary representations of $\mathfrak{gl}(1|M)$. In this paper, we have considered only a simple class of such unitary representations, the so-called Fock spaces $W(p)$. This class of representations turns out to be already sufficiently resourceful in order to exhibit some fascinating physical properties of the solutions. Of special interest is the feature of having only a discrete spectrum for each oscillator position operator. At first sight, this is somewhat unusual. On the other hand, our analysis of probability distributions for position operators has shown effects that are reminiscent of canonical results.

This paper presents only the first results for this quantum system consisting of a one-dimensional chain of coupled harmonic oscillators in the WQSs approach. There are still many open problems or new aspects to be studied. For example, it is clear that the system (2.29) has also solutions outside $\mathfrak{gl}(1|M)$. For instance, if $M=2n$ is even, then one can construct an algebraic solution by means of the direct sum Lie superalgebra $\mathfrak{gl}(1|2)\oplus\cdots\oplus\mathfrak{gl}(1|2)$ (n copies). In this case, the unitarity conditions following from the form $\mathfrak{u}(1|2)\oplus\cdots\oplus\mathfrak{u}(1|2)$ imply no conditions

on the coupling constant c, and it would be interesting to study the system from this point of view. Furthermore, it would be worth investigating whether Eq. (2.29) has also solutions related to orthosymplectic Lie superalgebras.[31]

But even if we restrict for the moment our attention to the $\mathfrak{gl}(1|M)$ solutions given here in Sec. III, work remains to be done. In particular, one should also consider other classes of unitary $\mathfrak{gl}(1|M)$ representations[26] and investigate the corresponding physical properties.

Finally, and this a more technical question, the explicit construction of orthonormal eigenvectors of the position operators $\hat{q}_k$ is lacking. Although this can be done numerically for any given M and a given set of parameters, we have at the moment no closed form expressions for these eigenvectors. We hope to find such forms, as they would allow us to draw some general conclusions regarding position probability distributions. At this moment, the last conclusions in Sec. VI are based upon observations of examples rather than upon analytic formulas. We expect to return to some of these remaining questions in future publications.

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Framework for nonlocally related partial differential equation systems and nonlocal symmetries: Extension, simplification, and examples

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Any partial differential equation (PDE) system can be effectively analyzed through consideration of its tree of nonlocally related systems. If a given PDE system has n local conservation laws, then each conservation law yields potential equations and a corresponding nonlocally related potential system. Moreover, from these n conservation laws, one can directly construct 2^n-1 independent nonlocally related systems by considering these potential systems individually (n singlets), in pairs ($n(n-1)/2$ couplets),..., taken all together (one n-plet). In turn, any one of these 2^n-1 systems could lead to the discovery of new nonlocal symmetries and/or nonlocal conservation laws of the given PDE system. Moreover, such nonlocal conservation laws could yield further nonlocally related systems. A theorem is proved that simplifies this framework to find such extended trees by eliminating redundant systems. The planar gas dynamics equations and nonlinear telegraph equations are used as illustrative examples. Many new local and nonlocal conservation laws and nonlocal symmetries are found for these systems. In particular, our examples illustrate that a local symmetry of a k-plet is not always a local symmetry of its "completed" n-plet ($k<n$). A new analytical solution, arising as an invariant solution for a potential Lagrange system, is constructed for a generalized polytropic gas. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2349488]

I. INTRODUCTION

For any given system of partial differential equations (PDEs), one can systematically construct an extended tree of nonlocally related potential systems and subsystems.[1] All systems within a tree have the same solution set as the given system.

The analysis of a system of PDEs through consideration of nonlocally related systems in an extended tree can be of great value. In particular, using this approach, through Lie's algorithm one can systematically calculate nonlocal symmetries (which in turn are useful for obtaining new exact solutions from known ones), construct invariant and nonclassical solutions, as well as obtain linearizations, etc. (Examples are found in Ref. 1.) Perhaps more importantly, as all such related systems contain all solutions of the given system, any general method of analysis (qualitative, numerical, perturbation, conservation laws, etc.) considered for a given PDE system may be tried again on any nonlocally related potential system or subsystem. In this way, new results may be obtained for any method of analysis that is not coordinate-dependent as the systems within a tree are related in a nonlocal manner.

In Ref. 1, a tree construction algorithm is described. First, local conservation laws for the given system are found (through the direct construction method (DCM) or other method).[2–4] For each conservation law, one or several potentials are introduced.[5] Consequently, a potential system

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is obtained. Next, for each potential system, its conservation laws are computed, and further potential systems are constructed. This procedure terminates when no more new conservation laws are found. After potential systems are determined, for each potential system, new subsystems may be generated when one is able to reduce the number of dependent variables (including a reduction after a point transformation of dependent and independent variables of a potential system in a tree). At any step, all locally related potential systems and subsystems are excluded from the tree.

In this article we further extend the tree construction algorithm presented in Ref. 1. In particular, if a given system of PDEs has n conservation laws, one can directly construct 2^n-1 independent nonlocally related systems by considering their corresponding potential systems individually (n singlets), in pairs ($n(n-l)/2$ couplets),…, taken all together (one n-plet). In turn, any one of these 2^n-1 systems could lead to the discovery of new nonlocal symmetries and/or nonlocal conservation laws of the given PDE system. Moreover, such nonlocal conservation laws could yield further nonlocally related systems and subsystems as described earlier. Hence, for a given system of PDEs, the construction of its tree of nonlocally related PDE systems through our extended tree framework can be complex. Most importantly, we introduce and prove a theorem that simplifies this construction to find such extended trees by eliminating redundant systems. The work presented in this paper also simplifies and extends to within an algorithmic framework the heuristic approaches presented in Refs. 9 and 10.

This article gives a comprehensive analysis of trees of nonlocally related systems for classes of constitutive functions, including a systematic search of corresponding nonlocal symmetries and nonlocal conservation laws. In particular, new nonlocal symmetries and new conservation laws are found for planar gas dynamics (PGD) equations and nonlinear telegraph (NLT) equations, extending work in Refs. 6–10, respectively, and in references therein. Moreover, we extend and simplify the tree construction framework presented in Ref. 1 through further elimination of redundant systems. In a related work,[11] for a class of diffusion-convection equations, Popovych and Ivanova[11] completely classified its potential conservation laws and, correspondingly, constructed (hierarchical) trees of inequivalent potential systems.

This article is organized as follows. In Sec. II, we review the DCM for finding conservation laws for a given system of PDEs. We show how a related potential system arises from each local conservation law of the given system and, further, how to construct the corresponding 2^n-1 nonlocally related systems for a given system of PDEs with n local conservation laws. As examples, we consider systems of PGD equations. We find local conservation laws and corresponding nonlocally related systems for the PGD system in Lagrangian coordinates.

In Sec. III, we prove a fundamental theorem on finding conservation laws of PDE systems. In particular, for *any* given PDE system **F** with two independent variables (x and t) with precisely n local conservation laws, we show that from consideration of all combinations of the n corresponding *potential systems of PDEs* arising from the given system, no nonlocal conservation laws can be obtained for **F** through potential systems arising from multipliers that depend only on x and t. In particular, for such multipliers, all conservation laws of potential systems must be linear combinations of the n local conservation laws of the given system **F**. Consequently, for such multipliers, all further potential systems are equivalent to all possible couplets, triplets,…,n-plets of potential systems obtained from a given system **F**—a total of 2^n-1 systems for consideration. Hence for a given PDE system **F**, in order to find additional inequivalent potential systems as well as nonlocal conservation laws for **F**, it is necessary to seek conservation laws through multipliers having an essential dependence on dependent variables. The fundamental theorem is also shown to hold for PDE systems with any number of independent variables.

In Sec. IV, as a prototypical example, we consider NLT equations. We give a complete classification of local conservation laws arising from multipliers that are functions of independent and dependent variables. As a consequence, we find five new local conservation laws arising from three distinguished cases. We then use the simplified procedure introduced in Sec. III to construct corresponding trees of nonlocally related PDE systems. Nonlocal symmetries are found for corresponding NLT systems with constitutive functions involving power law nonlinearities, including all nonlocal symmetries found in Ref. 6 as well as a new one. Moreover, six new nonlocal

conservation laws are constructed for such power law NLT equations through a search of multipliers (which have an essential dependence on potential variables) for the potential systems arising from its conservation laws.

In Sec. V, we consider PGD equations, with a generalized polytropic equation of state, in Lagrangian coordinates. We give the point symmetry classification of the seven potential systems resulting from its three local conservation laws. Two new nonlocal symmetries are found which arise as point symmetries for only one of these potential systems (a couplet). We observe that these new nonlocal symmetries also arise as point symmetries of a subsystem of the Lagrange system and give the symmetry classification of this subsystem. This yields one more new nonlocal symmetry of the PGD equations. We consider invariant solutions that essentially arise from new nonlocal symmetries.

In Sec. VI, we summarize the new results presented in this article. In particular, we outline the procedure to construct a tree of nonlocally related PDE systems for a given PDE system.

In this work, a recently developed package GeM for MAPLE[12] is used for automated symmetry and conservation law analysis and classifications.

II. CONSTRUCTION OF CONSERVATION LAWS AND NONLOCALLY RELATED PDE SYSTEMS

A. Direct construction method for finding conservation laws

We first present the DCM to find the conservation laws for a general PDE system.

Let $\mathbf{G}\{\mathbf{x},\mathbf{u}\}=0$ be a system of m partial differential equations

$$\mathbf{G}\{\mathbf{x},\mathbf{u}\}=0:\begin{cases} G_1\{\mathbf{x},\mathbf{u}\}=0 \\ \vdots \\ G_m\{\mathbf{x},\mathbf{u}\}=0 \end{cases} \tag{2.1}$$

with M independent variables $\mathbf{x}=(x^1,\ldots,x^M)$, and N dependent variables $\mathbf{u}=(u^1,\ldots,u^N)$. Let $\partial^l\mathbf{u}$ denote the set of all partial derivatives of $\mathbf{u}$ of order l.

A set of multipliers $\{\Lambda_k(\mathbf{x},\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})\}_{k=1}^m$ yields a conservation law

$$\Lambda_k(\mathbf{x},\mathbf{u},\partial\mathbf{u},\ldots,\partial^l\mathbf{u})G_k\{\mathbf{x},\mathbf{u}\}=D_i\Phi^i(\mathbf{x},\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})=0 \tag{2.2}$$

of system (2.1) if and only if the linear combination $\Lambda_k(\mathbf{x},\mathbf{U},\partial\mathbf{U}\ldots,\partial^l\mathbf{U})G_k\{\mathbf{x},\mathbf{U}\}$ is annihilated by the *Euler operators*

$$E_{U^s}\frac{\partial}{\partial U^s}-D_i\frac{\partial}{\partial U_i^s}+\cdots+(-1)^jD_{i_1}\cdots D_{i_j}\frac{\partial}{\partial U^s_{i_1\ldots i_j}}+\cdots, \tag{2.3}$$

i.e., the N determining equations

$$E_{U^s}(\Lambda_k(\mathbf{x},\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})G_k\{\mathbf{x},\mathbf{U}\})=0,\quad s=1,\ldots,N, \tag{2.4}$$

must hold for an arbitrary set of functions $\mathbf{U}=(U^1,\ldots,U^N)$. Here and for the rest of this article, we assume summation over a repeated index.

After solving the determining equations (2.4) and finding a set of multipliers $\{\Lambda_k(\mathbf{x},\mathbf{U},\partial\mathbf{U},\ldots,\partial^l\mathbf{U})\}_{k=1}^m$ that yield a conservation law, one can obtain the fluxes $\Phi^i(\mathbf{x},\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})$ by using integral formulas arising from homotopy operators (see Refs. 2 and 3).

A conservation law $D_i\Phi^i(\mathbf{x},\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})=0$ is called *trivial* if its fluxes are of the form $\Phi^i=M^i+H^i$, where M^i and H^i are smooth functions such that M^i vanishes on the solutions of the system (2.1), and $D_iH^i\equiv 0$. Two conservation laws $D_i\Phi^i[\mathbf{u}]=0$ and $D_i\Psi^i[\mathbf{u}]=0$ are *equivalent* if $D_i(\Phi^i[\mathbf{u}]-\Psi^i[\mathbf{u}])=0$ is a trivial conservation law. The more general "triviality" idea is the notion of linear dependence of conservation laws. A set of conservation laws is *linearly dependent* if there exists a linear combination of them which is a trivial conservation law.

B. Construction of nonlocally related systems from local conservation laws

Case A: Two independent variables. Suppose a PDE system with two independent variables

$$\mathbf{F}\{x,t,\mathbf{u}\}=0:\quad \begin{cases} F_1\{x,t,\mathbf{u}\}=0,\\ \vdots\\ F_m\{x,t,\mathbf{u}\}=0, \end{cases} \tag{2.5}$$

possesses n local conservation laws $\{\mathcal{R}^s\}_{s=1}^n$ of the form

$$\mathcal{R}^s:\quad D_xX_s(x,t,\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})+D_tT_s(x,t,\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})=0,\quad s=1,\ldots,n, \tag{2.6}$$

where T_s and X_s are differentiable functions of their arguments. Each conservation law $\mathcal{R}^s$ (2.6) of the system (2.5) yields a pair of potential equations of the form

$$\mathcal{P}^s:\quad \begin{cases} (v_s)_x=T_s(x,t,\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u}),\\ (v_s)_t=-X_s(x,t,\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u}). \end{cases} \tag{2.7}$$

For each conservation law (2.6), the corresponding set of potential equations $\mathcal{P}^s$ (2.7) can be *appended* to the given system $\mathbf{F}$ (2.5) to yield a nonlocally related *potential system* $\mathbf{F}^s_{\mathbf{P}}$. (Alternatively, if at least one of the factors of the conservation law does not vanish outside of the solution space, the potential equations $\mathcal{P}^s$ can *replace* one of the equations of the given system $\mathbf{F}$.)

From the n conservation laws (2.6), one can obtain further inequivalent nonlocally related systems, by considering not only potential systems $\mathbf{F}^s_{\mathbf{P}}$ arising from single conservation laws $\mathcal{R}^s$, but also couplets $\{\mathbf{F}^i_{\mathbf{P}},\mathbf{F}^j_{\mathbf{P}}\}^n_{i,j=1}$, triplets $\{\mathbf{F}^i_{\mathbf{P}},\mathbf{F}^j_{\mathbf{P}},\mathbf{F}^k_{\mathbf{P}}\}^n_{i,j,k=1},\ldots$, and finally the n-plet of potential systems $\{\mathbf{F}^1_{\mathbf{P}},\ldots\mathbf{F}^n_{\mathbf{P}}\}$. Hence one obtains as many as 2^n-1 potential systems of equations nonlocally related to $\mathbf{F}$ (2.5) through the n conservation laws (2.6).

Case B: Several independent variables. Now consider a general PDE system $\mathbf{G}$ (2.1) with $M\geq 2$ independent variables. Suppose it possesses n local conservation laws $\{\mathcal{K}^s\}_{s=1}^n$ of the form

$$\mathcal{K}^s:\quad D_i\Phi^i_s(\mathbf{x},\mathbf{u},\partial\mathbf{u},\ldots,\partial^r\mathbf{u})=0,\quad s=1,\ldots,n, \tag{2.8}$$

with fluxes $\Phi^{(s)i}$ that are differentiable functions of their arguments. Each conservation law (2.8) yields a set of M potential equations of the form (see Refs. 5 and 14)

$$\mathcal{Q}^s:\quad \Phi^i_s=\sum_{i<j}(-1)^j\frac{\partial}{\partial x^j}v_{ij}+\sum_{j<i}(-1)^{i-1}\frac{\partial}{\partial x^j}v_{ji},\quad i=1,\ldots,M, \tag{2.9}$$

where the potentials $\mathbf{v}=\{v_{ij}(\mathbf{x})\}$ are the $\frac{1}{2}M(M-1)$ nonrepeating components of an $M\times M$ antisymmetric tensor.

For every s, by appending potential equations $\mathcal{Q}^s$ to the given system $\mathbf{G}$ (or replacing an equation of $\mathbf{G}$ by potential equations $\mathcal{Q}^s$, whatever is appropriate), one obtains a *potential system* $\mathbf{G}^s_{\mathbf{P}}$ which is nonlocally related to the given system $\mathbf{G}$ (2.1).

In the same manner as for the case of two independent variables, by considering singlets, couplets, triplets, $\ldots,n$-plet of potential systems $\mathbf{G}^s_{\mathbf{P}}$, one can obtain as many as 2^n-1 independent PDE systems nonlocally related to the given system $\mathbf{G}$, whose solution sets are equivalent to that of $\mathbf{G}$.

We now illustrate the use of 2^n-1 independent potential systems to study symmetries of a system of polytropic gas dynamics equations.

C. Conservation laws, nonlocally related PDE systems and nonlocal symmetry analysis of planar gas dynamics equations

1. Conservation laws and nonlocally related systems

In Lagrangian mass coordinates $s=t, y=\int_{x_0}^x\rho(\xi)d\xi$, planar one-dimensional gas motion is described by the equations

TABLE I. Local conservation laws of (2.10) with $\Lambda_i=\Lambda_i(y,s)$.

CL	Multipliers $(\Lambda_1,\Lambda_2,\Lambda_3)$	Conservation law	Potential	Potential equations
(W_1)	$(1,0,0)$	$D_s(q)-D_y(v)=0$	w_1	$w_{1y}=q,\ w_{1s}=v$
(W_2)	$(0,1,0)$	$D_s(v)+D_y(p)=0$	w_2	$w_{2y}=v,\ w_{2s}=-p$
(W_3)	$(y,s,0)$	$D_s(sv+yq)+D_y(sp-yv)=0$	w_3	$w_{3y}=sv+yq,\ w_{3s}=-sp+yv$

$$\mathbf{L}\{y,s,v,p,q\}=0:\quad \begin{cases} q_s-v_y=0 \\ v_s+p_y=0 \\ p_s+B(p,q)v_y=0. \end{cases} \tag{2.10}$$

Here x is a Cartesian space coordinate, t is time, v is the gas velocity, $q=1/\rho$ where ρ is the gas density, and p is the gas pressure. In terms of the entropy density $S(p,q)$, the constitutive function $B(p,q)$ is given by

$$B(p,q)=\frac{S_q}{S_p}.$$

We note that system (2.10) admits the group of equivalence transformations

$$s=a_1\tilde{s}+a_4,\quad y=a_2\tilde{y}+a_5,\quad v=a_3\tilde{v}+a_6,$$

$$p=\frac{a_2a_3}{a_1}\tilde{p}+a_7,\quad q=\frac{a_1a_3}{a_2}\tilde{q}+a_8,\quad B(p,q)=\frac{a_2^2}{a_1^2}\tilde{B}(\tilde{p},\tilde{q}) \tag{2.11}$$

for arbitrary constants $a_1\ldots,a_8$ with $a_1a_2a_3\neq 0$.

We first construct the simplest conservation laws and all corresponding inequivalent potential systems for the Lagrange system (2.10). Using the DCM (Sec. II A), for an arbitrary constitutive function $B(p,1/\rho)$, we find that for multipliers of the form $\Lambda_i=\Lambda_i(y,s)$, the Lagrange system (2.10) has the conservation laws exhibited in Table I.

The potential equations that arise from the conservation law (W_1) can be used to replace the first equation of the Lagrange system (2.10); potential equations arising from the conservation law (W_2), can replace the second equation of (2.10); finally, potential equations arising from the conservation law (W_3), can equivalently replace either the first or second equation of (2.10).

The independent set of nonlocally related (potential) systems of the Lagrange system (2.10) consists of the following:

- Three singlets (potential systems involving a single nonlocal variable w_i)

$$\mathbf{LW}_1\{y,s,v,p,q,w_1\}=0:\quad \begin{cases} w_{1y}=1, \\ w_{1s}=v, \\ v_s+p_y=0, \\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.12}$$

$$\mathbf{LW}_2\{y,s,v,p,q,w_2\}=0:\quad \begin{cases} q_s-v_y=0, \\ w_{2y}=v, \\ w_{2s}=-p, \\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.13}$$

$$\mathbf{LW}_3\{y,s,v,p,q,w_3\}=0:\quad \begin{cases} w_{3y}=sv+yq,\\ w_{3s}=-sp+yv,\\ v_s+p_y=0,\\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.14}$$

- Three couplets

$$\mathbf{LW}_1\mathbf{W}_2\{y,s,v,p,q,w_1,w_2\}=0:\quad \begin{cases} w_{1y}=q,\\ w_{1s}=v,\\ w_{2y}=v,\\ w_{2s}=-p,\\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.15}$$

$$\mathbf{LW}_1\mathbf{W}_3\{y,s,v,p,q,w_1,w_3\}=0:\quad \begin{cases} w_{1y}=q,\\ w_{1s}=v,\\ w_{3y}=sv+yq,\\ w_{3s}=-sp+yv,\\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.16}$$

$$\mathbf{LW}_2\mathbf{W}_3\{y,s,v,p,q,w_2,w_3\}=0:\quad \begin{cases} w_{2y}=v,\\ w_{2s}=-p,\\ w_{3y}=sv+yq,\\ w_{3s}=-sp+yv,\\ p_s+B(p,q)v_y=0; \end{cases} \tag{2.17}$$

- One triplet involving all three conservation laws:

$$\mathbf{LW}_1\mathbf{W}_2\mathbf{W}_3\{y,s,v,p,q,w_1,w_2,w_3\}=0:\quad \begin{cases} w_{1y}=q,\\ w_{1s}=v,\\ w_{2y}=v,\\ w_{2s}=-p,\\ w_{3y}=sv+yq,\\ w_{3s}=-sp+yv,\\ p_s+B(p,q)v_y=0. \end{cases} \tag{2.18}$$

The Lagrange system (2.10) has also a nonlocally related *subsystem* obtained by excluding v (See Ref. 1):

$$\underline{\mathbf{L}}\{y,s,p,q\}=0:\quad \begin{cases} q_{ss}+p_{yy}=0,\\ p_s+B(p,q)q_s=0. \end{cases} \tag{2.19}$$

2. Nonlocal symmetry analysis for polytropic gas flows

We consider the polytropic equation of state

$$B(p,q) = \gamma \frac{p}{q}.$$

Applying group analysis to the triplet potential system (2.18), for arbitrary γ, one finds the basis of the ten-dimensional point symmetry algebra admitted by the given Lagrange system (2.10):

$$X_1 = \frac{\partial}{\partial s} + w_2 \frac{\partial}{\partial w_3}, \quad X_2 = \frac{\partial}{\partial y} + w_1 \frac{\partial}{\partial w_3},$$

$$X_3 = s\frac{\partial}{\partial s} + v\frac{\partial}{\partial v} + 2q\frac{\partial}{\partial q} + 2w_1\frac{\partial}{\partial w_1} + w_2\frac{\partial}{\partial w_2} + 2w_3\frac{\partial}{\partial w_3},$$

$$X_4 = \frac{\partial}{\partial v} + s\frac{\partial}{\partial w_1} + y\frac{\partial}{\partial w_2} + ys\frac{\partial}{\partial w_3}, \quad X_5 = s\frac{\partial}{\partial s} + y\frac{\partial}{\partial y} + w_1\frac{\partial}{\partial w_1} + w_2\frac{\partial}{\partial w_2} + 2w_3\frac{\partial}{\partial w_3},$$

$$X_6 = v\frac{\partial}{\partial v} + p\frac{\partial}{\partial p} + q\frac{\partial}{\partial q} + w_1\frac{\partial}{\partial w_1} + w_2\frac{\partial}{\partial w_2} + w_3\frac{\partial}{\partial w_3},$$

$$X_7 = \frac{\partial}{\partial w_1}, \quad X_8 = \frac{\partial}{\partial w_2}, \quad X_9 = \frac{\partial}{\partial w_3},$$

$$X_{10} = y^2\frac{\partial}{\partial y} + (w_2 - yv)\frac{\partial}{\partial v} + yp\frac{\partial}{\partial p} - 3yq\frac{\partial}{\partial q} + (sw_2 - w_3)\frac{\partial}{\partial w_1} + yw_2\frac{\partial}{\partial w_2} + ysw_2\frac{\partial}{\partial w_3}. \tag{2.20}$$

In particular, the operators $X_1,\ldots,X_9$ project onto point symmetries of the given Lagrange system (2.10); the operator X_{10} yields a *nonlocal symmetry* of the Lagrange system **L**.[1,10]

If $\gamma=3$, system (2.10) admits one additional symmetry[9]

$$X_{11} = s^2\frac{\partial}{\partial s} + (w_1 - sv)\frac{\partial}{\partial v} - 3sp\frac{\partial}{\partial p} + sq\frac{\partial}{\partial q} + sw_1\frac{\partial}{\partial w_1} + (yw_1 - w_3)\frac{\partial}{\partial w_2} + ysw_1\frac{\partial}{\partial w_3},$$

which also yields a nonlocal symmetry of the Lagrange system **L**.

If $\gamma=-1$, system (2.10) corresponds to Chaplygin gas and is linearizable, as will be shown in Sec. II C 3.

Remark 1: Among all of these constructed potential systems of **L**, symmetries $X_1\ldots,X_{10}$ (or their projections) are obtained *simultaneously* as point symmetries only for the triplet potential system $\mathbf{LW}_1\mathbf{W}_2\mathbf{W}_3$, which in this sense is a *grand system* for the Lagrange system **L**. [All other potential systems admit the corresponding projected proper subalgebras of the Lie algebra arising from (2.20).] The practical value of such a grand system is evident—possessing the largest known symmetry group, it allows the construction of a maximal possible set of invariant solutions of the given system.

Note that it does not automatically follow that the potential system with the maximum number of potential variables is a "grand system" for determining symmetries, as is the case in this example. Counterexamples will be presented in Secs. IV and V.

3. Further conservation laws for a general constitutive function

We now look for conservation law multipliers for the Lagrange system **L** (2.10) in terms of the more general form $\Lambda_i=\Lambda_i(y,s,V,P,Q)$, $i=1,2,3$.

The solution of the conservation law determining equations (2.4) yields the following multipliers:

$$\Lambda_1 = \alpha y - \beta P + B(P,Q)\Lambda_3 + \delta,$$

$$\Lambda_2 = \alpha s + \beta V + \nu,$$

$$\Lambda_3 = \Lambda_3(y,P,Q), \tag{2.21}$$

where α, β, ν, and δ are arbitrary real constants, and $\Lambda_3(y,P,Q)$ is any solution of the PDE

$$(\Lambda_3)_Q = (B(P,Q)\Lambda_3)_P - \beta. \tag{2.22}$$

Conservation laws corresponding to $\beta=0$, $\Lambda_3=0$ and $\delta,\nu,\alpha\neq 0$ are, respectively, the conservation laws (W_1), (W_2), and (W_3) listed in Table I. Additional conservation laws arise when $\Lambda_3 \neq 0$. It is possible to show that from multipliers (2.21) only two new linearly independent conservation laws follow. The first conservation law corresponds to $\beta=1$ and represents conservation of energy. It is given by

$$\left[\left(\frac{v^2}{2} + K(p,q)\right)_s + (pv)_y\right] = 0, \tag{2.23}$$

where $K(p,q)$ is a solution of the equation $K_q(p,q)=B(p,q)K_p(p,q)-p$.

The second conservation law ($\beta=0$) defines the adiabatic process in Lagrangian coordinates:

$$(S(p,q))_s = 0, \tag{2.24}$$

where the entropy $S(p,q)$ is a solution of the equation $S_q(p,q)=B(p,q)S_p(p,q)$.

For forms of $B(p,q)$ for which the functions $K(p,q)$, $S(p,q)$ can be explicitly evaluated, the conservation laws (2.23) and (2.24), respectively, yield explicit potential systems with potentials w_4, w_5.

For the polytropic case $B(p,q)=\gamma p/q$, we find that $S(p,q)=q^\gamma p$. The conservation law $(S(p,q))_s=0$ (2.24) can equivalently replace the last equation of the given system **L** (2.10). This leads to the potential system

$$\mathbf{LW}_5\{y,s,v,p,q,w_5\} = 0: \begin{cases} (w_5)_y(y,s) = q^\gamma p, \\ (w_5)_s(y,s) = 0, \\ q_s - v_y = 0, \\ v_s + p_y = 0 \end{cases} \tag{2.25}$$

Noting that $w_5(y,s)=w_5(y)$ and expressing $q=k(y)p^{-1/\gamma}$, for an arbitrary $k(y)$, we find a subsystem

$$\underline{\mathbf{LW}_5}\{y,s,v,p,k\} = 0: \begin{cases} v_y - (k(y)p^{-1/\gamma})_s = 0, \\ v_s + p_y = 0 \end{cases} \tag{2.26}$$

nonlocally related to the given system **L** (2.10).

Remark 2: For the case of a Chaplygin gas $\gamma=-1$, the Lagrange PGD system **L** (2.10) is nonlinear as it stands, and *cannot* be linearized by a point transformation. But the equivalent system $\underline{\mathbf{LW}_5}$ for $\gamma=-1$ becomes *linear*. Thus in the Chaplygin gas case, the Lagrange PGD system **L** is *linearized by a nonlocal transformation*.

Remark 3: Excluding the variable v from (2.26), we see that the Lagrange polytropic PGD system is equivalent to

$$\underline{\underline{\mathbf{LW}_5}}\{y,s,p\} = 0: \quad p_{yy} + (k(y)p^{-1/\gamma})_{ss} = 0, \tag{2.27}$$

which is a nonlinear elliptic equation for $k(y)>0$, $\gamma>-1$, $\gamma\neq 0$, and a nonlinear hyperbolic equation for $k(y)>0$, $\gamma<-1$.

Remark 4: The solutions of (2.26) for a particular form of $k(y)$ correspond to a subset of the

solutions of the given system **L** (2.10). In particular, for $k(y)=\text{const}$, the system $\underline{\underline{\mathbf{LW}_5}}$ (2.26) can be mapped into a linear system by a hodograph transformation (e.g., Ref. 18). Thus it is possible to obtain a special class of solutions of the given nonlinear system **L** (2.10) through solving this *linear PDE system*.

III. LINEAR DEPENDENCE OF CONSERVATION LAWS AND LOCAL EQUIVALENCE OF POTENTIAL SYSTEMS

For a given PDE system, its conservation laws can be constructed systematically (through the Direct Construction Method or other method[2–4]). For each conservation law, one or several potentials are introduced, and the corresponding potential system is constructed. Next, for each such nonlocally related system, its conservation laws are computed, and from these, more potentials are introduced, which in turn lead to the construction of further potential systems, etc. Together with subsystems (obtained by a reduction of the number of dependent variables for a potential system, which includes consideration of reductions after an interchange of dependent and independent variables), this systematic procedure yields an extended tree of PDE systems nonlocally related to the given one (see Ref. 1 and Sec. II B).

In this section, we present theorems which simplify the tree construction through elimination of redundant systems.

A. Linear dependence of conservation laws and tree simplification. Two-dimensional case

Definition 1: Suppose the system of PDEs (2.5) has precisely n local conservation laws. Its *general potential system* **P** is the set of 2^n-1 potential systems arising from these n local conservation laws.

We now prove the following fundamental theorem concerned with the construction of further potential systems arising from **P**.

Theorem 1: *Each conservation law of any potential system in* **P**, *arising from multipliers that depend only on x and t, is linearly dependent on the n local conservation laws of the given system* (2.5).

Proof: Each conservation law of any system in **P**, constructed from multipliers depending only on x and t, must be of the form

$$D_x(b^i(t,x)v_i+\beta(t,x,\mathbf{u}))+D_t(a^i(t,x)v_i+\alpha(t,x,\mathbf{u}))=0, \tag{3.1}$$

for some functions $b^i(t,x),a^i(t,x),\beta(t,x,\mathbf{u}),\alpha(t,x,\mathbf{u})$.

From the compatibility conditions for multipliers of conservation laws, we immediately obtain $D_ta^i+D_xb^i=0$. Hence

$$\int a^i dx+\int b^i dt=f^i(t)+g^i(x), \tag{3.2}$$

for some functions $f^i(t)$ and $g^i(x)$.

Now consider a conservation law (3.1) on the solution manifold of the system in **P** that it was constructed from. We have

$$\begin{aligned}D_x[b^iv_i+\beta]+D_t[a^iv_i+\alpha]&=D_x\left[b^iv_i+\beta+D_t\left(\left(\int a^i dx-\int b^i dt\right)v_i\right)\right]+D_t\left[a^iv_i+\alpha\right.\\&\quad\left.-D_x\left(\left(\int a^i dx-\int b^i dt\right)v_i\right)\right]=D_x\left[\beta-(v_i)_t\int b^i dt\right]+D_t\left[\alpha\right.\\&\quad\left.-(v_i)_x\int a^i dx\right]+D_xD_t\left[\left(\int b^i dt+\int a^i dx\right)v_i\right]=D_x\left[\beta\right.\end{aligned}$$

$$-(v_i)_t\int b^i dt\Big]+D_t\Big[\alpha-(v_i)_x\int a^i dx\Big]+D_xD_t[(f_i(t)+g_i(x))v_i]$$
$$=D_x\Big[\beta-(v_i)_t\int b^i dt+g_i(x)(v_i)_t\Big]+D_t\Big[\alpha-(v_i)_x\int a^i dx+f_i(t)(v_i)_x\Big]. \tag{3.3}$$

As all derivatives of potentials v_i can be expressed in terms of local variables x, t and $\mathbf{u}$, it follows that a conservation law (3.1) is linearly dependent on local ones constructed from the given system (2.5). □

Remark 5: From Theorem 1 it follows that a conservation law of any system in **P** related to the given system (2.5), arising from multipliers that depend only on x and t, is trivial on the solution manifold of **P**.

The next theorem immediately follows from Theorem 1.

Theorem 2: *Suppose one finds the set of n local conservation laws for a given system* (2.5) *and then constructs the corresponding general potential system* **P**. *It follows that if one starts with any one of the* 2^n-1 *potential systems in* **P** *and seeks conservation laws from multipliers depending only on x and t, each of the resulting potential systems is locally equivalent to one of the* 2^n-1 *potential systems in* **P**.

B. Linear dependence of conservation laws and tree simplification. General case: $M \geq 2$ independent variables

We now consider the general case for $M \geq 2$ independent variables. Suppose the system of PDEs (2.1) has a set of n conservation laws $\{\mathcal{K}^s\}_{s=1}^n$ of the form (2.8). Each conservation law $\mathcal{K}^s$ yields a set of M potential equations $\mathcal{Q}^s$ of the form (2.9) (Sec. II B).

Definition 1: Suppose the system of PDEs (2.1) has precisely n local conservation laws of the form (2.8). Its *general potential system* **Q** is the set of 2^n-1 potential systems arising from combinations of these n local conservation laws.

The following theorems generalize Theorems 1 and 2 for the case of $M \geq 2$ independent variables.

Theorem 3: *Each conservation law of any potential system in* **Q**, *arising from multipliers that depend only on independent variables* **x**, *is linearly dependent on the n local conservation laws of the given system* (2.1).

The proof of Theorem 3 is presented in the Appendix. The following theorem holds.

Theorem 4: *Suppose one finds the set* $\{\mathcal{K}^s\}_{s=1}^n$ *of n local conservation laws for the given system* **G** (2.1), *and then constructs the corresponding general potential system* **Q**. *It follows that if one starts with any one of the potential systems in* **Q** *and seeks conservation laws from multipliers depending only on the independent variables* **x**, *each of the resulting potential systems is locally equivalent to one of the potential systems in* **Q**.

Remark 6: From Theorem 4 it follows that no new nonlocally related potential systems of a given system **G** (2.1) can arise from conservation laws constructed from known potential systems of **G** with multipliers depending only on independent variables **x**.

Remark 7: Note that for any potential system in **Q**, one can allow gauge constraints relating the potentials $\{v_{ij}(\mathbf{x})\}$. In order to find nonlocal symmetries of the given system (2.1) from point symmetries of a potential system in **Q** it is necessary to adjoin such gauge constraints.[15–17]

IV. EXTENDED TREES OF NONLOCALLY RELATED PDE SYSTEMS, NONLOCAL SYMMETRIES AND NONLOCAL CONSERVATION LAWS FOR NONLINEAR TELEGRAPH EQUATIONS

As a prototypical example, for classes of NLT equations, we use the simplified procedure introduced in Sec. III to construct trees of nonlocally related PDE systems and, as a consequence, find new nonlocal symmetries and new nonlocal conservation laws.

A. Local conservation laws for the NLT equation

We consider NLT equations of the form

$$\mathbf{U}\{x,t,u\}=0: \quad u_{tt}-(F(u)u_x)_x-(G(u))_x=0. \tag{4.1}$$

Equation (4.1) and its potential versions, including

$$\mathbf{UV}\{x,t,u,v\}=0: \quad \begin{cases} u_t-v_x=0, \\ v_t-F(u)u_x-G(u)=0, \end{cases} \tag{4.2}$$

are known to possess rich conservation law and symmetry structure for various classes of constitutive functions $F(u),G(u)$.[6–8,13] In particular, the point symmetry classification of (4.1) appears in Ref. 13; the point symmetry and local conservation law classification of (4.2) appear in Refs. 6 and 7, respectively.

Using the DCM, we now construct nontrivial linearly independent local conservation laws for the NLT equations **U** (4.1). First we note that Eq. (4.1) admits the group of equivalence transformations

$$x=a_1\tilde{x}+a_4, \quad t=a_2\tilde{t}+a_5, \quad u=a_3\tilde{u}+a_6,$$

$$F(u)=a_1^2a_2^{-2}\tilde{F}(\tilde{u}), \quad G(u)=a_1a_2^{-2}a_3\tilde{G}(\tilde{u})+a_7, \tag{4.3}$$

where $a_1,\ldots,a_7$ are arbitrary constants, $a_1a_2a_3\neq 0$. We classify the local conservation laws and point symmetries of (4.1) modulo the equivalence transformations (4.3). A multiplier of the form $A(x,t,U)$ yields a local conservation law

$$D_x(X(x,t,u,u_x,u_t))+D_t(T(x,t,u,u_x,u_t))=0$$

of (4.1) if and only if the equation

$$E_U(\Lambda(x,t,U)(U_{tt}-(F(U)U_x)_x-(G(U))_x))=0 \tag{4.4}$$

holds for an arbitrary function $U(x,t)$.

Solving determining equation (4.4), one obtains an overdetermined system of linear PDEs in terms of the unknown multiplier $\Lambda(x,t,U)$. It is easy to show that $\Lambda=\Lambda(x,t)$. Three cases are distinguished. For arbitrary functions $F(u)$ and $G(u)$, one has two conservation laws (V_1) and (V_2); for the case $G'=F$, there are two additional conservation laws (B_1) and (B_2); for the case $G=u$, there are also two additional conservation laws (C_1) and (C_2). The classification is presented in Table II. [Note that the case where G is linear in u and $F=$const is the linear case and hence is not considered. The case $G=$const (with arbitrary F) is linearizable and hence also is not considered.]

The local conservation laws (V_2), (B_3), (B_4), (C_3), and (C_4) have not previously appeared in the literature.

The following potential systems result from the conservation laws listed in Table II.

Case (a): Arbitrary $F(u),G(u)$.

$$\mathbf{UV}_1\{x,t,u,v_1\}=0:\begin{cases} v_{1x}-u_t=0, \\ v_{1t}-F(u)u_x-G(u)=0; \end{cases} \tag{4.5}$$

$$\mathbf{UV}_2\{x,t,u,v_2\}=0:\begin{cases} v_{2x}-(tu_t-u)=0, \\ v_{2t}-t(F(u)u_x+G(u))=0. \end{cases} \tag{4.6}$$

Case (b): $G'(u)=F(u),F(u)$ arbitrary. In addition to potential systems (4.5) and (4.6), here we also have

TABLE II. Local conservation laws of (4.1).

$F(u)$	$G(u)$	CL	Multipliers	T	$-X$
Arbitrary	Arbitrary	(V_1)	$\Lambda=1$	u_t	$F(u)u_x+G(u)$
		(V_2)	$\Lambda=t$	tu_t-u	$t(F(u)u_x+G(u))$
Arbitrary	$G'(u)=F(u)$	(B_3)	$\Lambda=e^x$	e^xu_t	$e^xF(u)u_x$
		(B_4)	$\Lambda=te^x$	$e^x(tu_t-u)$	$te^xF(u)u_x$
Arbitrary $(F(u)\neq\text{const})$	u	(C_3)	$\Lambda=x-\frac{t^2}{2}$	$\left(x-\frac{t^2}{2}\right)u_t+ut$	$\left(x-\frac{t^2}{2}\right)(F(u)u_x+u)-\int F(u)du$
		(C_4)	$\Lambda=xt-\frac{t^3}{6}$	$\left(tx-\frac{t^3}{6}\right)u_t-\left(x-\frac{t^2}{2}\right)u$	$\left(tx-\frac{t^3}{6}\right)(F(u)u_x+u)-t\int F(u)du$

$$\mathbf{UB}_3\{x,t,u,b_3\}=0:\begin{cases}b_{3x}-e^xu_t=0,\\ b_{3t}-e^xF(u)u_x=0;\end{cases} \tag{4.7}$$

$$\mathbf{UB}_4\{x,t,u,b_4\}=0:\begin{cases}b_{4x}-e^x(tu_t-u)=0,\\ b_{4t}-te^xF(u)u_x=0.\end{cases} \tag{4.8}$$

Case (c): $G(u)=u, F(u)$ arbitrary. In addition to potential systems (4.5) and (4.6), here we also have

$$\mathbf{UC}_3\{x,t,u,c_3\}=0:\begin{cases}c_{3x}-\left(\left(x-\frac{t^2}{2}\right)u_t+tu\right)=0,\\ c_{3t}-\left(\left(x-\frac{t^2}{2}\right)(F(u)u_x+u)-\int F(u)du\right)=0;\end{cases} \tag{4.9}$$

$$\mathbf{UC}_4\{x,t,u,c_4\}=0:\begin{cases}c_{4x}-\left(\left(tx-\frac{t^3}{6}\right)u_t-\left(x-\frac{t^2}{2}\right)u\right)=0,\\ c_{4t}-\left(\left(tx-\frac{t^3}{6}\right)(F(u)u_x+u)-t\int F(u)du\right)=0.\end{cases} \tag{4.10}$$

We now apply Theorem 2 to find inequivalent nonlocally related potential systems for the NLT equation (4.1). The following statements hold.

Corollary 1: *In terms of multipliers depending only on x and t, the set of locally inequivalent potential systems for the NLT equation (4.1) with general nonlinearities $F(u)$ and $G(u)$ is exhausted by the following PDE systems*:

- *Two potential systems* (4.5) and (4.6), *involving single potentials*;
- *One couplet* {(4.5), (4.6)}.

Corollary 2: *In terms of multipliers depending only on x and t, the set of locally inequivalent potential systems for Eq. (4.1) with $G'(u)=F(u)$ is exhausted by the following systems*:

- *Four potential systems* (4.5)–(4.8) *involving single potentials*;
- *Six couplets* {(4.5), (4.6)}, {(4.5), (4.7)}, {(4.5), (4.8)}, {(4.6), (4.7)}, {(4.6), (4.8)}, and {(4.7), (4.8)} *involving pairs of potentials*;
- *Four triplets* {(4.5), (4.6), (4.7)}, {(4.5), (4.6), (4.8)}, {(4.5), (4.7), (4.8)}, and {(4.6), (4.7),

TABLE III. Symmetries of the NLT equation (4.1) and its potential systems (4.5), (4.6), (4.11) for the general case (a): $F(u)=u^{\alpha}$, $G(u)=u^{\beta}(\alpha,\beta,\neq 0)$.

System	Symmetries
$\mathbf{UV_1V_2}$, $\mathbf{UV_1}$, $\mathbf{UV_2}$, $\mathbf{U}$	$X_1=(\alpha-\beta+1)x\frac{\partial}{\partial x}+\left(\frac{\alpha}{2}-\beta+1\right)t\frac{\partial}{\partial t}+u\frac{\partial}{\partial u}$ $+\frac{\alpha+2}{2}v_1\frac{\partial}{\partial v_1}+(\alpha-\beta+2)v_2\frac{\partial}{\partial v_2}$, $X_2=\frac{\partial}{\partial x}$, $X_3=\frac{\partial}{\partial t}+v_1\frac{\partial}{\partial v_2}$, $X_4=\frac{\partial}{\partial v_1}$, $X_5=\frac{\partial}{\partial v_2}$.

(4.8)} *for combinations involving three potentials*;
- *One quadruplet* {(4.5), (4.6), (4.7), (4.8)} *involving all four potentials*.

Corollary 3: *In terms of multipliers depending only on x and t, the set of locally inequivalent potential systems for Eq.* (4.1) *with arbitrary* $F(u)$ *and* $G(u)=u$ *is exhausted by the following systems*:

- *Four potential systems* (4.5), (4.6), (4.9), and (4.10) *involving single potentials*;
- *Six couplets* {(4.5), (4.6)}, {(4.5), (4.9)}, {(4.5), (4.10)}, {(4.6), (4.9)}, {(4.6), (4.10)}, *and* {(4.9), (4.10)} *involving pairs of potentials*;
- *Four triplets* {(4.5), (4.6), (4.9)}, {(4.5), (4.6), (4.10)}, {(4.5), (4.9), (4.10)}, *and* {(4.6), (4.9), (4.10)} *for combinations involving three potentials*;
- *One quadruplet* {(4.5), (4.6), (4.9), (4.10)} *involving all four potentials*.

B. Point and nonlocal symmetry analysis of NLT equations with power nonlinearities

We now apply the results of Sec. III to seek point and nonlocal symmetries of the NLT equation (4.1) with power nonlinearities $F(u)=u^{\alpha}, G(u)=u^{\beta}(\alpha,\beta\neq 0)$ by considering its locally inequivalent potential systems.

Case (a): Arbitrary power nonlinearities $F(u), G(u)$. We first consider general power nonlinearities: $F(u)=u^{\alpha}$, $G(u)=u^{\beta}$ ($\alpha,\beta\neq 0$ arbitrary constants.) In this case, the given system (4.1) has two conservation laws (V_1) and (V_2) exhibited in Table II. From Corollary 1, the set of inequivalent nonlocally related potential systems of the PDE **U** (4.1) is exhausted by the systems $\mathbf{UV_1}$ (4.5), $\mathbf{UV_2}$ (4.6), and the couplet $\mathbf{UV_1V_2}$:

$$\mathbf{UV_1V_2}\{x,t,u,v_1,v_2\}=0:\begin{cases} v_{1x}-u_t=0,\\ v_{1t}-F(u)u_x-G(u)=0,\\ v_{2x}-(tu_t-u)=0,\\ v_{2t}-t(F(u)u_x+G(u))=0. \end{cases} \tag{4.11}$$

Symmetry generators of the given NLT equation (4.1), its potential systems (4.5) and (4.6) and the couplet (4.11) are given in Table III.

From the form of the symmetries in Table III it follows that no nonlocal symmetries arise for systems **U** and $\mathbf{UV_1}$. The generator X_3 is a nonlocal symmetry for the system $\mathbf{UV_2}$ (i.e., the system $\mathbf{UV_2}$ is not invariant under translations in t) and a point symmetry for the other systems. All other generators define point symmetries for all systems in Table III.

Case (b): $G'(u)=F(u)$. We now consider power nonlinearities $F(u)=(\alpha+1)u^{\alpha}$, $G(u)=u^{\alpha+1}$, $\alpha\neq 0,-1$. From the equivalence relation (4.3), this case is equivalent to $F(u)=u^{\alpha}$, $G(u)=u^{\alpha+1}$.

TABLE IV. Symmetries of the potential NLT systems for case for case (b): $F(u)=(\alpha+1)u^{\alpha}$, $G(u)=u^{\alpha+1}(\alpha\neq 0,-1)$.

System	$F(u)$	$G(u)$	Symmetries
$\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_3\mathbf{B}_4$, $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_3$, $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_4$, $\mathbf{UV}_1\mathbf{B}_3\mathbf{B}_4$, $\mathbf{UV}_2\mathbf{B}_3\mathbf{B}_4$, $\mathbf{UV}_1\mathbf{V}_2, \mathbf{UV}_1\mathbf{B}_3$, $\mathbf{UV}_1\mathbf{B}_4, \mathbf{UV}_2\mathbf{B}_3$, $\mathbf{UV}_2\mathbf{B}_4, \mathbf{UB}_3\mathbf{B}_4$, $\mathbf{UV}_1, \mathbf{UV}_2$, $\mathbf{UB}_3, \mathbf{UB}_4$, $\mathbf{U}$	$(\alpha+1)u^{\alpha}$	$u^{\alpha+1}$	$Y_1=-\frac{\alpha}{2}t\frac{\partial}{\partial t}+u\frac{\partial}{\partial u}+v_2\frac{\partial}{\partial v_2}+\frac{\alpha+2}{2}v_1\frac{\partial}{\partial v_1}+\frac{\alpha+2}{2}b_3\frac{\partial}{\partial b_3}+b_4\frac{\partial}{\partial b_4}$, $Y_2=\frac{\partial}{\partial x}+b_3\frac{\partial}{\partial b_3}+b_4\frac{\partial}{\partial b_4}$, $Y_3=\frac{\partial}{\partial t}+b_3\frac{\partial}{\partial b_4}+v_1\frac{\partial}{\partial v_2}$, $Y_4=\frac{\partial}{\partial v_1}$, $Y_5=\frac{\partial}{\partial v_2}$, $Y_6=\frac{\partial}{\partial b_3}$, $Y_7=\frac{\partial}{\partial b_4}$
	$-3u^{-4}$	u^{-3}	$Y_8=t^2\frac{\partial}{\partial t}+tu\frac{\partial}{\partial u}-v_2\frac{\partial}{\partial v_1}-b_4\frac{\partial}{\partial b_3}$
$\mathbf{UV}_1\mathbf{V}_2$	$3u^2$	u^3	$Y_9=3v_1\frac{\partial}{\partial x}+(tv_1-v_2+3u)\frac{\partial}{\partial t}-uv_1\frac{\partial}{\partial u}-v_1^2\frac{\partial}{\partial v_1}-v_1v_2\frac{\partial}{\partial v_2}$

From Corollary 2, the set of inequivalent nonlocally related potential systems of the PDE **U** (4.1) is exhausted by the potential systems $\mathbf{UV}_1$ (4.5), $\mathbf{UV}_2$ (4.6), $\mathbf{UB}_3$ (4.7), $\mathbf{UB}_4$ (4.8), their six couplets, four triplets and one quadruplet. The corresponding classification of symmetry generators is presented in Table IV.

A point symmetry of any of these potential systems, where the symmetry generator components for u, x or t have an essential dependence on at least one of the potentials v_1, v_2, b_3, b_4, is a *nonlocal* (potential) symmetry of the given NLT equation (4.1).

The case $\alpha=-2$ is not considered in Table IV as here the system $\mathbf{UV}_1$ is linearizable by a point transformation.[18,19]

The point symmetries of PDE **U** (4.1) and system $\mathbf{UV}_1$ (4.5) were completely classified in Refs. 13 and 6, respectively. In Ref. 6, many new nonlocal symmetries of **U** (4.1) for other than power nonlinearities were found from the point symmetries of corresponding $\mathbf{UV}_1$ systems.

Most importantly, from Table IV, we see that for the case when $F(u)=3u^2, G(u)=u^3$, through the potential system $\mathbf{UV}_1\mathbf{V}_2$, we have discovered a new nonlocal symmetry Y_9 for the scalar PDE **U**.

Note that Y_3 is a nonlocal symmetry for the systems $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_4$, $\mathbf{UV}_2\mathbf{B}_3\mathbf{B}_4$, $\mathbf{UV}_1\mathbf{B}_4$, $\mathbf{UV}_2\mathbf{B}_3$, $\mathbf{UV}_2\mathbf{B}_4$, $\mathbf{UV}_2$, and $\mathbf{UB}_4$, and a point symmetry for the other nine systems; Y_8 is a nonlocal symmetry for the systems $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_3$, $\mathbf{UV}_1\mathbf{B}_3\mathbf{B}_4$, $\mathbf{UV}_1\mathbf{B}_3$, $\mathbf{UV}_1\mathbf{B}_4$, $\mathbf{UV}_2\mathbf{B}_3$, $\mathbf{UV}_1$, $\mathbf{UB}_3$ and a point symmetry for the other nine systems; Y_9 is a point symmetry for $\mathbf{UV}_1\mathbf{V}_2$ and a nonlocal symmetry for the other listed 15 inequivalent systems, which include $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_3$, $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_4$, and $\mathbf{UV}_1\mathbf{V}_2\mathbf{B}_3\mathbf{B}_4$!

Case (c): $F(u)=u^{\alpha}, G(u)=u$. In this case, similarly to case (b), the set of independent nonlocally related potential systems of (4.1) is exhausted by the potential systems $\mathbf{UV}_1$ (4.5), $\mathbf{UV}_2$ (4.6), $\mathbf{UC}_3$ (4.9), $\mathbf{UC}_4$ (4.10), their six couplets, four triplets and one quadruplet. The corresponding classification of symmetry generators is found in Table V. The linear cases $\alpha=0,1$ are not considered.

As the simplification of overdetermined systems of linear determining equations in classification problems involving triplets $\mathbf{UV}_1\mathbf{C}_3\mathbf{C}_4$, $\mathbf{UV}_2\mathbf{C}_3\mathbf{C}_4$ and couplets $\mathbf{UV}_1\mathbf{C}_4$, $\mathbf{UC}_3\mathbf{C}_4$ presented a computational difficulty, the corresponding entries in Table V are not known.

From the form of the symmetries in Table V, it follows that no nonlocal symmetries arise for systems **U** and $\mathbf{UV}_1$; Z_2 is a nonlocal symmetry for the systems $\mathbf{UV}_2\mathbf{C}_3$, $\mathbf{UC}_3$, and $\mathbf{UC}_4$ and a point symmetry for the other listed systems; Z_3 is a nonlocal symmetry for the systems $\mathbf{UV}_1\mathbf{V}_2\mathbf{C}_4$, $\mathbf{UV}_1\mathbf{C}_3$, $\mathbf{UV}_2\mathbf{C}_3$, $\mathbf{UV}_2\mathbf{C}_4$, $\mathbf{UV}_2$, $\mathbf{UC}_3$, and $\mathbf{UC}_4$ and a point symmetry for the other listed systems. All other generators define point symmetries for the systems listed in Table V.

TABLE V. Symmetries of the potential NLT systems for case (c): $F(u)=u^{\alpha}, G(u)=u(\alpha\neq 0,1)$.

System	Case	Symmetries
$\mathbf{UV}_1\mathbf{V}_2\mathbf{C}_3\mathbf{C}_4$, $\mathbf{UV}_1\mathbf{V}_2\mathbf{C}_3$, $\mathbf{UV}_1\mathbf{V}_2\mathbf{C}_4$ $\mathbf{UV}_1\mathbf{V}_2$, $\mathbf{UV}_1\mathbf{C}_3$, $\mathbf{UV}_2\mathbf{C}_3$, $\mathbf{UV}_2\mathbf{C}_4$, $\mathbf{UV}_1, \mathbf{UV}_2$, $\mathbf{UC}_3, \mathbf{UC}_4$ $\mathbf{U}$,	$\alpha\neq -1$	$Z_1=\frac{\alpha}{2}t\frac{\partial}{\partial t}+\alpha x\frac{\partial}{\partial x}+u\frac{\partial}{\partial u}+\frac{\alpha+2}{2}v_1\frac{\partial}{\partial v_1}+v_2(a+1)\frac{\partial}{\partial v_2}+\frac{3\alpha+2}{2}c_3\frac{\partial}{\partial c_3}+(2\alpha+1)c_4\frac{\partial}{\partial c_4}$, $Z_2=\frac{\partial}{\partial x}+v_1\frac{\partial}{\partial c_3}+v_2\frac{\partial}{\partial c_4}$, $Z_3=\frac{\partial}{\partial t}+v_1\frac{\partial}{\partial v_2}-v_2\frac{\partial}{\partial c_3}+c_3\frac{\partial}{\partial c_4}$, $Z_4=\frac{\partial}{\partial v_1}$, $Z_5=\frac{\partial}{\partial v_2}$, $Z_6=\frac{\partial}{\partial c_3}$, $Z_7=\frac{\partial}{\partial c_4}$.
	$\alpha=-1$	$Z_8=-\frac{1}{2}t\frac{\partial}{\partial t}-x\frac{\partial}{\partial x}+u\frac{\partial}{\partial u}+\frac{1}{2}v_1\frac{\partial}{\partial v_1}-\left(t+\frac{1}{2}c_3\right)\frac{\partial}{\partial c_3}-\left(\frac{t^2}{2}+c_4\right)\frac{\partial}{\partial c_4}$ $Z_2, Z_3, Z_4, Z_5, Z_6, Z_7$.
$\mathbf{UV}_1\mathbf{C}_3\mathbf{C}_4, \mathbf{UV}_2\mathbf{C}_3\mathbf{C}_4$ $\mathbf{UV}_1\mathbf{C}_4, \mathbf{UC}_3\mathbf{C}_4$		?

C. New nonlocal conservation laws for NLT equations with power nonlinearities

In this section, new nonlocal conservation laws are constructed for NLT equations (4.1) with power nonlinearities. We use the DCM for all singlet potential systems of the NLT equation (4.1) in each of cases (a), (b), and (c), allowing multipliers to have an essential dependence on dependent variables. We obtain new conservation laws for particular classes of constitutive functions. The classification is presented in the following.

For power nonlinearities $F(u)=u^{\alpha}$, $G(u)=u^{\beta}$, the set of nonlocal conservation laws is given in Table VI.

The computations were done for all systems: $\mathbf{UV}_1$, $\mathbf{UV}_2$, $\mathbf{UB}_3$, $\mathbf{UB}_4$, $\mathbf{UC}_3$, and $\mathbf{UC}_4$. No nonlocal conservation laws were found for the $\mathbf{UC}_4$ system.

The nonlocal conservation laws for PDE **U** (4.1) arising from analysis of the system $\mathbf{UV}_1$ were first found in Ref. 6. All other nonlocal conservation laws for PDE **U** (4.1) found in Table VI are new.

The case (b) with $\alpha=-2$ is not considered in Table VI as here the system $\mathbf{UV}_1$ is linearizable by a point transformation.[18,19]

V. NONLOCAL SYMMETRY CLASSIFICATION FOR GENERALIZED POLYTROPIC GAS FLOWS

We now consider the Lagrange PGD system **L** (2.10) with a generalized polytropic equation of state

$$B(p,q)=\frac{M(p)}{q},\quad M''(p)\neq 0. \tag{5.1}$$

To construct a corresponding tree of nonlocally related potential systems, first we search for local conservation laws with multipliers of the form

$$\Lambda_i=\Lambda_i(y,s),\quad i=1,2,3.$$

The classification with respect to the constitutive function $M(p)$ reveals no special case and thus the conservation laws listed in Table I are exhaustive. According to Theorem 2, from these conservation laws we obtain the following inequivalent potential systems for the generalized polytropic Lagrange PGD system **L** (2.10):

- Three potential systems (2.12)–(2.14) involving single potentials;
- Three couplets (2.15)–(2.17) involving pairs of potentials;

TABLE VI. Nonlocal conservation laws of (4.1).

Case	System	Subcase	Multipliers	Fluxes
(a)	$\mathbf{UV}_1$	$\beta=-1$	$\Lambda_1=x+\frac{v_1^2}{2}+\frac{u^{\alpha+2}}{\alpha+2}, \Lambda_2=uv_1$	$X=-\left(\frac{u^{\alpha+2}}{\alpha+2}+\frac{v_1^2}{6}+x\right)v_1,$ $T=\left(\frac{u^{\alpha+2}}{(\alpha+2)(\alpha+3)}+\frac{v_1^2}{2}+x\right)u.$
$F(u)=u^\alpha$			$\Lambda_1=v_1, \Lambda_2=u.$	$X=-\frac{u^{\alpha+2}}{\alpha+2}-\frac{v_1^2}{2},$ $T=uv_1-t.$
$G(u)=u^\beta$		$\alpha=-1$ $\beta=-1$	$\Lambda_1=\frac{v_1^3}{3}+2(x+u)v_1+t,$ $\Lambda_2=(v_1^2+u+2x)u.$	$X=-\frac{v_1^4}{12}-(x+u)v_1^2-tv_1-\frac{u^2}{2}-2xu,$ $T=\left(u+\frac{v_1^2}{3}\right)uv_1+2xuv_1+t(u-2x).$
			$\Lambda_1=v_1^4/12+(u+x)v_1^2+tv_1+2xu+x^2+\frac{u^2}{2},$ $\Lambda_2=\left(\frac{v_1^3}{3}+t+uv_1+2xv_1\right)u.$	$X=-\frac{v_1^5}{60}-\frac{(x+u)v_1^3}{3}-\frac{(tv_1+u^2)v_1}{2}-(2u+x)xv_1-tu,$ $T=-\frac{t^2}{2}+\left(\frac{u}{3}+v_1^2+2x\right)\frac{u^2}{2}+\frac{uv_1^4}{12}+(xv_1+t)uv_1+x^2u.$
	$\mathbf{UV}_2$	$\beta=-1$	$\Lambda_1=-\frac{v_2}{t^2}, \Lambda_2=\frac{u}{t}.$	$X=-\frac{v_2^2}{2t^2}-\frac{u^{\alpha+2}}{\alpha+2}, T=\frac{uv_2-t^2}{t}.$
(b) $F(u)=(\alpha+1)u^\alpha$	$\mathbf{UV}_1$	$\alpha\neq-1$ $\alpha\neq-2$	$\Lambda_1=e^xu^{\alpha+1}, \Lambda_2=e^xv_1,$	$X=-e^xu^{\alpha+1}v_1,$ $T=e^x\left(\frac{u^{\alpha+2}}{\alpha+2}+\frac{v_1^2}{2}\right).$
$G(u)=u^{\alpha+1}$	$\mathbf{UV}_2$	$\alpha=-4$	$\Lambda_1=-e^x\frac{t}{u^3}, \Lambda_2=e^xv_2.$	$X=e^x\frac{tv_2}{u^3}, T=e^x\left(\frac{t^2}{u^2}-v_2^2\right).$
	$\mathbf{UB}_3$	$\alpha\neq-1$	$\Lambda_1=-u^{\alpha+1}, \Lambda_2=e^{-x}b_3.$	$X=-u^{\alpha+1}b_3, T=e^x\frac{u^{\alpha+2}}{\alpha+2}+e^{-x}\frac{b_3^2}{2}.$
	$\mathbf{UB}_4$	$\alpha=-4$	$\Lambda_1=-\frac{t}{u^3}, \Lambda_2=e^{-x}b_4.$	$X=-\frac{tb_4}{u^3}, T=\frac{1}{2}e^{-x}b_4^2-e^x\frac{t^2}{2u^2}.$
(c) $F(u)=u^\alpha$ $G(u)=u$	$\mathbf{UV}_1$	$\alpha=1$	$\Lambda_1=\frac{t^4}{12}-xt^2+tv_1-\frac{u^2}{2}+x^2,$ $\Lambda_2=-\frac{t^3}{3}+t(u+2x)-v_1.$	$X=\left(\frac{v_1}{2}-xt+\frac{t^3-2tu}{6}\right)u^2$ $-\left(tv_1+\frac{t^4}{12}-xt^2+x^2\right)v_1,$ $T=-\frac{u^3}{6}+\left(\frac{t^4}{12}+x^2-xt^2+tv_1\right)u$ $+\left(2xt-\frac{v}{2}-\frac{t^3}{3}\right)v_1.$
			$\Lambda_1=\frac{t^3}{6}-xt+v_1$ $\Lambda_2=-\frac{t^2}{2}+u+x.$	$X=\left(\frac{t^2}{2}-\frac{u}{3}-x\right)u^2+\left(2xt-\frac{t^3}{3}-\frac{v_1}{2}\right)v_1,$ $T=\left(\frac{t^3}{3}-2xt\right)u+(u+2x-t^2)v_1.$
	$\mathbf{UV}_2$	$\alpha=1$	$\Lambda_1=\frac{t^2}{4}-x+\frac{v_2-x^2}{t^2},$ $\Lambda_2=t-\frac{u+2x}{t}.$	$X=\frac{u^3}{3}+\frac{2x-t^2}{2}u^2+\frac{v_2^2}{2t^2}+\frac{(t^4-4x(t^2+x))v_2}{4t^2},$ $T=-\frac{uv_2}{t}-\frac{(t^4-4x(t^2+x))u}{4t}-\frac{(2x-t^2)v_2}{t}.$
	$\mathbf{UC}_3$	$\alpha=1$	$\Lambda_1=-\frac{t^2-2x}{80}+\frac{2xt^2+5u^2}{40(t^2-2x)}+\frac{4x^3+5tc_3}{10(t^2-2x)^2},$ $\Lambda_2=\frac{3t^5-20c_3}{40(t^2-2x)^2}-\frac{t(2x+u)}{4(t^2-2x)}.$	$X=-\frac{(t^2-2x)(tu^2+2c_3)}{64}+\frac{t(u^3+3tc_3)}{48}+\frac{t^4(tu^2-10c_3)+20u^2c_3}{160(t^2-2x)}+\frac{t(t^5+5c_3)c_3}{40(t^2-2x)^2},$ $T=\frac{(t^4-4x^2)u}{64}+\frac{u^3-3t^4u-6tc_3}{96}+\frac{t(t^5+10c_3)u}{80(t^2-2x)}+\frac{(t^5+5c_3)c_3}{40(t^2-2x)^2}.$

- One triplet (2.18) involving all three potentials.

TABLE VII. Symmetries of the generalized polytropic PGD system (2.10), (5.1).

System	$M(p)$	Symmetries
L, **LW**$_1$,**LW**$_2$,**LW**$_3$, **LW**$_1$**W**$_2$,**LW**$_1$**W**$_3$, **LW**$_2$**W**$_3$, **LW**$_1$**W**$_2$**W**$_3$	(i) Arbitrary	$Z_1=\frac{\partial}{\partial s}+w_2\frac{\partial}{\partial w_3}$, $Z_2=\frac{\partial}{\partial y}+w_1\frac{\partial}{\partial w_3}$, $Z_3=\frac{\partial}{\partial v}+s\frac{\partial}{\partial w_1}+y\frac{\partial}{\partial w_2}+sy\frac{\partial}{\partial w_3}$, $Z_4=-y\frac{\partial}{\partial y}+2q\frac{\partial}{\partial q}+v\frac{\partial}{\partial v}+w_1\frac{\partial}{\partial w_1}$, $Z_5=s\frac{\partial}{\partial s}+y\frac{\partial}{\partial y}+w_1\frac{\partial}{\partial w_1}+w_2\frac{\partial}{\partial w_2}+2w_3\frac{\partial}{\partial w_3}$, $Z_6=\frac{\partial}{\partial w_1}$, $Z_7=\frac{\partial}{\partial w_2}$, $Z_8=\frac{\partial}{\partial w_3}$,
L,**LW**$_2$	(ii) $-p\ln p$	$Z_9=y\frac{\partial}{\partial y}+2p\frac{\partial}{\partial p}+\frac{2q}{\ln p}\frac{\partial}{\partial q}+v\frac{\partial}{\partial v}+2w_2\frac{\partial}{\partial w_2}$.
	(iii) $\gamma p+\alpha p^{(\gamma+1)/\gamma}$ $\gamma\neq 0,-1$	$Z_{10}=\frac{(\gamma+1)y}{2\gamma}\frac{\partial}{\partial y}+p\frac{\partial}{\partial p}-\frac{q}{\delta p^{1/\gamma+\gamma}}\frac{\partial}{\partial q}+\frac{(\gamma-1)v}{2\gamma}\frac{\partial}{\partial v}+w_2\frac{\partial}{\partial w_2}$.
	(iv) $1+\alpha e^p$, $\alpha=\pm 1$	$Z_{11}=\frac{\partial}{\partial p}+\frac{\alpha e^p}{1+\alpha e^p}q\frac{\partial}{\partial q}-s\frac{\partial}{\partial w_2}$, $Z_{12}=y\frac{\partial}{\partial p}+\frac{\alpha e^p}{1+\alpha e^p}yq\frac{\partial}{\partial q}-s\frac{\partial}{\partial v}-sy\frac{\partial}{\partial w_2}$.
LW$_2$	(ii) $-p\ln p$	$Z_{13}=y^2\frac{\partial}{\partial y}+yp\frac{\partial}{\partial p}-\left(3-\frac{1}{\ln p}\right)yq\frac{\partial}{\partial q}-(yv-w_2)\frac{\partial}{\partial v}+yw_2\frac{\partial}{\partial w_2}$.
	(iii) $\gamma p+\delta p^{(\gamma+1)/\gamma}$ $\gamma\neq 0,-1$	$Z_{14}=y^2\frac{\partial}{\partial y}+yp\frac{\partial}{\partial p}-\left(3-\frac{\delta}{\gamma}\frac{p^{1/\gamma}}{\delta p^{1/\gamma+\gamma}}\right)yq\frac{\partial}{\partial q}-(yu-w_2)\frac{\partial}{\partial v}+yw_2\frac{\partial}{\partial w_2}$.

A. Classification of point and nonlocal symmetries

The classification of point symmetries of the seven potential systems (2.12)–(2.18) [modulo the equivalence transformations (2.11)] yields Table VII of point symmetries and nonlocal symmetries for the Lagrange PGD system (2.10) with the equation of state (5.1).

From Table VII, we observe that Z_{13},Z_{14} are point symmetries for the system **LW**$_2$ and nonlocal symmetries for all other systems, including the given system **L**; $Z_9,\ldots,Z_{12}$ are point symmetries for systems **L** and **LW**$_2$ and nonlocal symmetries for all other systems.

Most importantly, we have shown that for cases (ii) and (iii), when $M(p)=-p\ln p$ and $M(p)=\gamma p+\delta p^{(\gamma+1)/\gamma}$, respectively, through the potential system **LW**$_2$ we have discovered *new nonlocal symmetries* Z_{13} and Z_{14} for the generalized polytropic Lagrange PGD system **L** (2.10), (5.1). Note that all other generators in Table VII project onto point symmetries of the Lagrange PGD system **L** (2.10) and thus were found from point symmetry analysis of **L** in Ref. 9.

Note that the newly discovered nonlocal symmetries Z_{13} and Z_{14} of the Lagrange system **L** (2.10), (5.1) with $M(p)=-p\ln p$ and $M(p)=\gamma p+\delta p^{(\gamma+1)/\gamma}$ project onto point symmetries of the corresponding Lagrange subsystem $\underline{\mathbf{L}}$ (2.19). In other words, the point symmetries $\underline{Z}_{13}=y^2(\partial/\partial y)+py(\partial/\partial p)-(3-(1/\ln p))yq(\partial/\partial q)$, $\underline{Z}_{14}=y^2(\partial/\partial y)+yp(\partial/\partial p)-(3-(\delta/\gamma)[p^{1/\gamma}/(\delta p^{1/\gamma}+\gamma)])yq(\partial/\partial q)$ of $\underline{\mathbf{L}}$ yield nonlocal symmetries of $\underline{\mathbf{L}}$.[1] It can be shown that symmetries Z_{13} and Z_{14} also yield nonlocal symmetries of the corresponding system written in terms of Eulerian coordinates.[1] The classification of point symmetries of $\underline{\mathbf{L}}$ (2.19) yields Table VIII with respect to the equation of state given by (5.1).

From Table VIII we observe that point symmetries of the Lagrange subsystem $\underline{\mathbf{L}}$ (2.19) include all corresponding point symmetries of **LW**$_2$, and additionally for $M(p)=3p+\delta p^{4/3}$ one *new symmetry* $\underline{Z}_{15}$ is obtained. The new symmetry $\underline{Z}_{15}$ is a nonlocal symmetry of the Lagrange system **L** (2.10) and all its potential systems (2.12)–(2.18).

TABLE VIII. Point symmetries of the subsystem $\underline{\mathbf{L}}$ (2.19) of the generalized polytropic PGD system (2.10), (5.1).

$M(p)$	Symmetries
(i) Arbitrary	$\underline{Z_1}=\frac{\partial}{\partial s}$, $\underline{Z_2}=\frac{\partial}{\partial y}$, $\underline{Z_4}=-y\frac{\partial}{\partial y}+2q\frac{\partial}{\partial q}$, $\underline{Z_5}=s\frac{\partial}{\partial s}+y\frac{\partial}{\partial y}$.
(ii) $-p\ln p$	$\underline{Z_9}=y\frac{\partial}{\partial y}+2p\frac{\partial}{\partial p}+\frac{2q}{\ln p}\frac{\partial}{\partial q}$, $\underline{Z_{13}}=y^2\frac{\partial}{\partial y}+yp\frac{\partial}{\partial p}-\left(3-\frac{1}{\ln p}\right)yq\frac{\partial}{\partial q}$.
(iii) $\gamma p+\delta p^{(\gamma+1)/\gamma}$	$\underline{Z_{10}}=\frac{(\gamma+1)y}{2\gamma}\frac{\partial}{\partial y}+p\frac{\partial}{\partial p}-\frac{q}{\delta p^{1/\gamma+\gamma}}\frac{\partial}{\partial q}$, $\underline{Z_{14}}=y^2\frac{\partial}{\partial y}+yp\frac{\partial}{\partial p}-\left(3-\frac{\alpha}{\gamma}\frac{p^{1/\gamma}}{\delta p^{1/\gamma+\gamma}}\right)yq\frac{\partial}{\partial q}$.
$\gamma=3$	$\underline{Z_{15}}=\frac{1}{3}s^2\frac{\partial}{\partial s}-sp\frac{\partial}{\partial p}+\frac{1}{\delta p^{4/3+3}}spq\frac{\partial}{\partial q}$.
(iv) $1+\alpha e^p$	$\underline{Z_{11}}=\frac{\partial}{\partial p}+\frac{\alpha e^p}{1+\alpha e^p}q\frac{\partial}{\partial q}$, $\underline{Z_{12}}=y\frac{\partial}{\partial p}+\frac{\alpha e^p}{1+\alpha e^p}yq\frac{\partial}{\partial q}$.

B. Nonlocally related systems and invariant solutions

1. Construction of invariant solutions for generalized polytropic PGD equations

For any given form of the constitutive function $M(p)$, different combinations of corresponding point and nonlocal symmetry generators can be used to construct families of invariant solutions of the Lagrange system **L** (2.10). As an example, we consider the case $M(p)=-p\ln p$.

The potential system $\mathbf{LW}_2$ has the largest algebra of symmetry generators. Thus it has the largest set of invariant solutions. The algebra $\mathcal{A}$ of symmetry generators for the constitutive function of interest is spanned by projections of the eight operators $Z_1,\ldots,Z_5,Z_7,Z_9,Z_{13}$ on the space of variables $\{y,s,v,p,q,w_2\}$ of $\mathbf{LW}_2$:

$$\mathcal{A}=\mathrm{Span}\{Z_1,Z_2,Z_3,Z_4,Z_5,Z_7,Z_9,Z_{13}\}. \tag{5.2}$$

The simplest way to find all solutions of $\mathbf{LW}_2$ invariant with respect to elements of $\mathcal{A}$ consists of two steps[20]:

1. Finding optimal systems of one-dimensional invariant subalgebras $\mathcal{A}_i\subset\mathcal{A}$ and constructing solutions invariant with respect to each subalgebra $\mathcal{A}_i$;
2. Using the transformation groups corresponding to symmetry generators in $\mathcal{A}$ to extend the set of solutions.

The solutions of the Lagrange system **L** (2.10) are obtained from solutions of the potential system $\mathbf{LW}_2$ by excluding the potential variable w_2.

Following the above procedure, we first find the optimal system of one-dimensional subalgebras of $\mathcal{A}$ (5.2) (see Ref. 20.) This optimal system consists of the invariant subalgebras given by

$$\mathcal{A}_1=Z_2+\varepsilon_1Z_3,$$

$$\mathcal{A}_2=Z_2+\varepsilon_1Z_1+\varepsilon_2Z_3,$$

$$\mathcal{A}_3=Z_4+\varepsilon_1Z_1+\varepsilon_2Z_7,$$

$$\mathcal{A}_4=Z_4+\varepsilon_1Z_1+\varepsilon_2Z_2+\varepsilon_3Z_3,$$

$$\mathcal{A}_5 = Z_4 + \varepsilon_1 Z_1 + \alpha Z_9,$$

$$\mathcal{A}_6 = Z_5 + \alpha Z_4,$$

$$\mathcal{A}_7 = Z_5 + \varepsilon_1 Z_3,$$

$$\mathcal{A}_8 = Z_{13} + \varepsilon_1 Z_1 + \varepsilon_2 Z_2 + \varepsilon_3 Z_7 + \alpha Z_9. \tag{5.3}$$

Here $\varepsilon_i = 0, \pm 1$, $\alpha \in \mathbb{R}$.

The set of all resulting invariant solutions of the potential system $\mathbf{LW}_2$ [and, consequently, corresponding solutions of the Lagrange system $\mathbf{L}$ (2.10)] is obtained from solutions invariant with respect to each of the subalgebras $\mathcal{A}_1, \ldots, \mathcal{A}_8$ by means of the group transformations corresponding to the operators $Z_1, \ldots, Z_9, Z_{13}$. These group transformations are as follows:

$$\begin{aligned}
&Z_1: \quad y' = y, \quad s' = s + \epsilon_1, \quad v' = v, \quad p' = p, \quad q' = q, \quad w_2 = w_2;\\
&Z_2: \quad y' = y + \epsilon_2, \quad s' = s, \quad v' = v, \quad p' = p, \quad q' = q, \quad w_2 = w_2;\\
&Z_3: \quad y' = y, \quad s' = s, \quad v' = v + \epsilon_3, \quad p' = p, \quad q' = q, \quad w_2' = w_2 + \epsilon_3 y;\\
&Z_4: \quad y' = e^{-\epsilon_4} y, \quad s' = s, \quad v' = v, \quad p' = p, \quad q' = a^{2\epsilon_4} q, \quad v' = w_2 + \epsilon_4 y;\\
&Z_5: \quad y' = e^{\epsilon_5} y, \quad s' = e^{\epsilon_5} s, \quad v' = v, \quad p' = p, \quad q' = q, \quad w_2' = e^{\epsilon_5} w_2,\\
&Z_7: \quad y' = y, \quad s' = s, \quad v' = v, \quad p' = p, \quad q' = q, \quad w_2' = w_2 + \epsilon_7;\\
&Z_9: \quad y' = e^{\epsilon_9} y, \quad s' = s, \quad v' = e^{\epsilon_9} v, \quad p' = e^{2\epsilon_9} p, \quad q' = (1 + 2\epsilon_9/\ln p) q, \quad w_2' = e^{2\epsilon_9} w_2;\\
&Z_{13}: \quad y' = \frac{y}{1 - \epsilon_{13} y}, \quad s' = s, \quad v' = v + \epsilon_{13}(w_2 - yv),\\
&\qquad p' = \frac{p}{1 - \epsilon_{13} y}, \quad q' = \frac{1 - \epsilon_{13} y}{\ln p} q \ln \frac{p}{1 - \epsilon_{13} y}, \quad w_2' = \frac{w_2}{1 - \epsilon_{13} y}.
\end{aligned} \tag{5.4}$$

Particular solutions of the Lagrange system $\mathbf{L}$ (2.10) are obtained as solutions invariant with respect to any linear combination of generators $Z_1, \ldots, Z_5, Z_7, Z_9, Z_{13}$, possibly transformed further by using one or more Lie groups (5.4).

2. An invariant solution from a nonlocal symmetry

For the case $M(p) = -p \ln p$, we construct a solution of the Lagrange system $\mathbf{L}$ (2.10) arising from a solution of the potential system $\mathbf{LW}_2$ (2.13) invariant with respect to the subalgebra $\mathcal{A}_8$ (5.3) with $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 0, \alpha = 1$, i.e., from operator

$$X = Z_{13} + \alpha Z_9 = (y^2 + y)\frac{\partial}{\partial y} + (y + 2)p\frac{\partial}{\partial p} - \left(3y - \frac{y - 2}{\ln p}\right) q \frac{\partial}{\partial q} - (yv - v - w_2)\frac{\partial}{\partial v} + (y + 2) w_2 \frac{\partial}{\partial w_2}.$$

One can show that this solution of $\mathbf{L}$ (2.10) does not arise as an invariant solution of an admitted point symmetry of $\mathbf{L}$. In particular, this solution has the form

$$p(y,s) = \frac{\gamma\beta^2}{\alpha^2} \frac{y^2}{y + \alpha} (1 - \tanh^2(\beta s)),$$

$$q(y,s) = -\frac{\gamma}{(y + \alpha)^3} \ln \left[\frac{\gamma\beta^2}{\alpha^2} \frac{y^2}{y + \alpha} (1 - \tanh^2(\beta s)) \right],$$

$$v(y,s) = -\frac{\gamma\beta}{\alpha^2}\frac{y(y+2\alpha)}{(y+\alpha)^2}\tanh(\beta s), \tag{5.5}$$

where α, β, and γ are arbitrary constants.

For $\alpha=1$, $\beta=1$, $\gamma=-2$, after the application of the equivalence transformation (2.11) with $a_1=a_3=1$, $a_2=a_4=a_6=0$, $a_5=-1$, $a_7=p_0$, $a_8=q_0$, this yields the solution

$$p = \tilde{p}(y,s) = p_0 - \frac{2y^2}{y+1}\frac{1}{\cosh^2 s},$$

$$q = \tilde{q}(y,s) = q_0 - \frac{2}{(y+1)^3}\ln\left[\frac{2y^2}{y+1}\frac{1}{\cosh^2 s}\right],$$

$$v = \tilde{v}(y,s) = 2\frac{y(y+2)}{(y+1)^2}\tanh s \tag{5.6}$$

of the Lagrange system **L** (2.10) for the constitutive function

$$B(p,q) = -\frac{(p_0-\tilde{p})\ln(p_0-\tilde{p})}{q_0-q}.$$

For $p_0=9, q_0=1$, the pressure $p=\tilde{p}(y,s)$, density $p=1/\tilde{q}(y,s)$ and velocity $v=\tilde{v}(y,s)$ profiles at times $s=0.1, 0.8, 1.3$ are shown in Figure 1 with thin, medium and thick lines, respectively. The solution is regular, bounded and satisfies physical conditions $p>0, \rho>0$ for all times $s\geq 0$ for the material space interval $0\leq y\leq 5$.

VI. CONCLUDING REMARKS

In this article, we extended the procedure presented in Ref. 1 to construct a tree of nonlocally related systems for a given PDE system **G** (2.1). In summary, the extended procedure is as follows.

1. **Construction of conservation laws**. Using the DCM (Sec. II A) or other method, construct local conservation laws of the given system **G**. Note that some conservation laws can be present in the given system as it stands.
2. **Construction of potential systems**. For each of the n known conservation laws $\{\mathcal{K}^s\}_{s=1}^n$ of the given system **G**, introduce potential(s) and construct a potential system $G^s_{\mathbf{P}}(s=1,\ldots,n)$. Let $\mathcal{T}_1$ denote the set of systems that consists of the given system **G**, potential systems $\mathbf{G}^s_{\mathbf{P}}$ and all possible couplets, triplets,…, n-plets of the potential systems $\mathbf{G}^s_{\mathbf{P}}$. The tree $\mathcal{T}_1$ includes a total of 2^n inequivalent systems.
3. **Construction of subsystems**. For each system in the tree $\mathcal{T}_1$, exclude where possible, one by one, dependent variables (including exclusions following interchanges of independent and dependent variables, i.e., where an independent variable becomes a dependent variable and vice versa through a point transformation), to generate all subsystems of the systems in the tree $\mathcal{T}_1$. Eliminate subsystems that are locally related to existing systems. This yields a possibly larger tree $\mathcal{T}_2$.
4. **Continuation**. In the tree $\mathcal{T}_2$, first distinguish the systems that arise from multipliers depending only on independent variables. For each such system, use the DCM or other method to construct the conservation laws for multipliers with an essential dependence on dependent variables. Construct all combinations of further potential systems arising from these conservation laws (i.e., couplets, triplets, etc.). For the other systems in the tree $\mathcal{T}_2$, construct all possible conservation laws (these can even arise from multipliers that depend only on the independent variables) and, correspondingly, construct all combinations of further potential systems. Find all nonlocally related subsystems by reduction of dependent variables. This yields an extended tree $\mathcal{T}_3$.

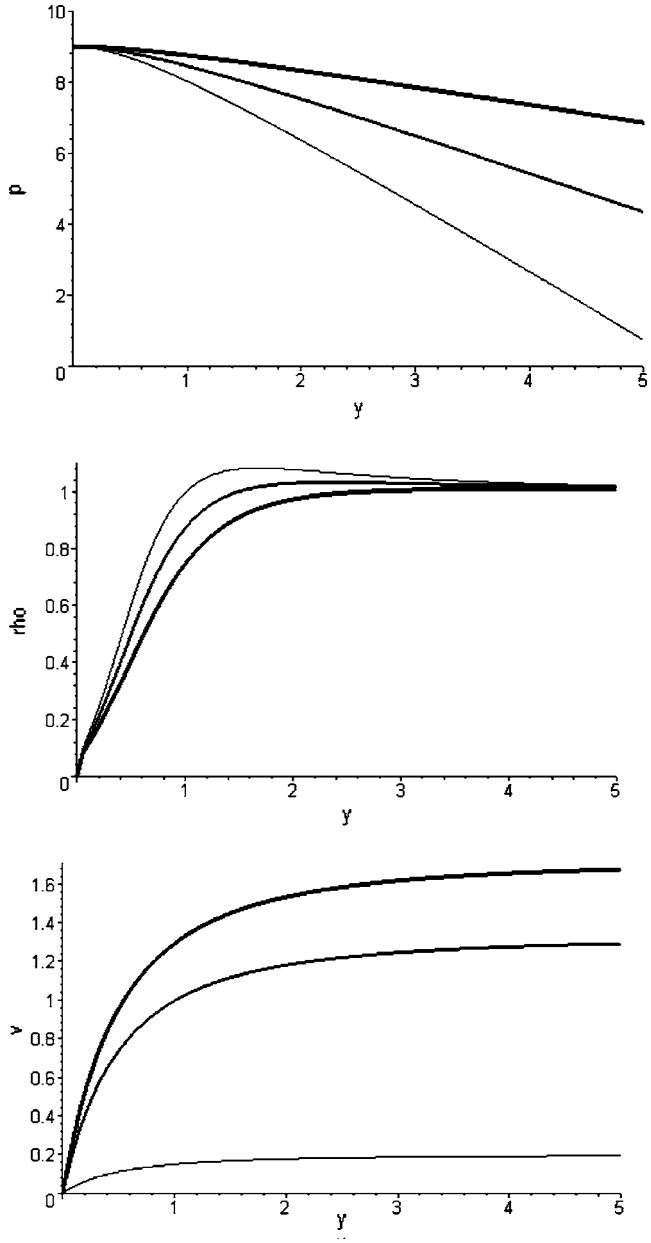

FIG. 1. Profiles of pressure p, density ρ, and velocity v at times $s=0.1$, 0.8, and 1.3.

Where possible, repeat step 4 to obtain a further tree extension (growth), etc.

The new theorem presented in Sec. III simplifies the construction of a tree of nonlocally related inequivalent systems for a given system of PDEs through elimination of redundant systems. To illustrate this theorem, as a prototypical example, we considered the nonlinear telegraph equations. Five new local conservation laws were constructed. Specializing to NLT equations with constitutive functions having power law nonlinearities, we found one nonlocal symmetry not found in Ref. 6. Further, from nonlocally related potential systems arising from new conservation laws for such NLT equations, we have found six new nonlocal conservation laws in addition to the nine nonlocal conservation laws found in Ref. 7.

For a system of planar gas dynamics equations, with a generalized polytropic equation of state, we found three new symmetries which are nonlocal for this system written in either Lagrangian or Eulerian coordinates.

It still remains a challenge to solve the overdetermined linear systems of PDEs for the symmetry classifying problems corresponding to the two couplet systems $\mathbf{UV}_1\mathbf{C}_4$, $\mathbf{UC}_3\mathbf{C}_4$ and the two triplet systems $\mathbf{UV}_1\mathbf{C}_3\mathbf{C}_4$, $\mathbf{UV}_2\mathbf{C}_3\mathbf{C}_4$ as we have been unable to solve any of these four systems.

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APPENDIX: PROOF OF THEOREM 3

Proof: Each conservation law of any k-plet potential system $\{\mathbf{G}^{i_1}_{\mathbf{P}},\dots,\mathbf{G}^{i_k}_{\mathbf{P}}\}$ in $\mathbf{Q}$, arising from multipliers that depend only on independent variables $\mathbf{x}$, is a linear combination of terms involving potential equations in $\{\mathbf{G}^{i_1}_{\mathbf{P}},\dots,\mathbf{G}^{i_k}_{\mathbf{P}}\}$ and, possibly, equations of the given system (2.1).

For simplicity, we prove the theorem for the case when the new conservation law is obtained as a linear combination of potential equations of a *singlet* potential system $\mathbf{G}^{s}_{\mathbf{P}}$ in $\mathbf{Q}$ arising from the given system (2.1) and a single conservation law (2.8), and involving M potential equations $\mathcal{Q}^s$ (2.9). The proof directly carries over to the case when the new conservation law involves a linear combination of potential and non-potential equations of *any k-plet potential system* in $\mathbf{Q}$, $1\le k\le n$.

A new conservation law obtained using the DCM from a set of M potential equations $\mathcal{Q}^s$ has the form

$$D_k A^k(\mathbf{x},\mathbf{u},\partial\mathbf{u},\dots,\partial^r\mathbf{u},\mathbf{v},\partial\mathbf{v},\dots,\partial^s\mathbf{v}) = \Lambda_i(\mathbf{x})\Bigg(\sum_{i<j}(-1)^j\frac{\partial}{\partial x^j}v_{ij}(\mathbf{x}) + \sum_{j<i}(-1)^{i-1}\frac{\partial}{\partial x^{ji}}v_{ji}(\mathbf{x}) - \Phi^i(\mathbf{x},\mathbf{u},\partial\mathbf{u},\dots,\partial^r\mathbf{u})\Bigg) = 0. \tag{A1}$$

where $A^k(\mathbf{x},\mathbf{u},\mathbf{v},\partial\mathbf{u},\dots,\partial^r\mathbf{u})$ are fluxes of the new conservation law, and $\Lambda_i(\mathbf{x})(i=1,\dots,M)$ are multipliers. [Note that for the case of M independent variables, from a given conservation law (2.8), one obtains M potential equations (2.9). Hence, when one seeks a new conservation law, the number of multipliers is the same as the number of independent variables.]

It is evident that the dependence of fluxes of the new conservation law (A1) on the potentials $\mathbf{v}$ is as follows:

$$A^k = \sum_{i<k}(-1)^k\Lambda_i v_{ik} + \sum_{k<i}(-1)^{i-1}\Lambda_i v_{ki} + \alpha_k(\mathbf{x},\mathbf{u}). \tag{A2}$$

We substitute (A2) in the conservation law (A1), and deduce the following compatibility conditions for multipliers:

$$\frac{\partial\Lambda_q}{\partial x^p} - \frac{\partial\Lambda_p}{\partial x^q} = 0, \quad 1\le p,q\le n. \tag{A3}$$

This means the differential form $\omega_\Lambda=\Lambda_i dx^i$ is closed. A closed form is locally exact within an open domain, and hence for some sufficiently smooth $\phi(\mathbf{x}):\omega_\Lambda=d\phi(\mathbf{x})$. Equivalently $\Lambda_i=\partial\phi(\mathbf{x})/\partial x^i$, $i=1,\dots,M$.

We now demonstrate that the conservation law (A1) with fluxes A^k is equivalent to a conservation law whose fluxes do not contain the nonlocal variables v^{ik}, but only their derivatives.

Indeed,

$$
\begin{aligned}
D_k A^k &= D_k\left(\sum_{i<k}(-1)^k \Lambda_i v_{ik} + \sum_{k<i}(-1)^{i-1}\Lambda_i v_{ki} + \alpha_k(\mathbf{x},\mathbf{u})\right)\\
&= D_k\left(\sum_{i<k}(-1)^k \frac{\partial \phi}{\partial x^i} v_{ik} + \sum_{k<i}(-1)^{i-1}\frac{\partial \phi}{\partial x^i} v_{ki} + \alpha_k(\mathbf{x},\mathbf{u})\right)\\
&= D_k\left(\left[\sum_{i<k}(-1)^k \frac{\partial(\phi v_{ik})}{\partial x^i} + \sum_{k<i}(-1)^{i-1}\frac{\partial(\phi v_{ki})}{\partial x^i}\right]\right.\\
&\quad \left. - \phi\left[\sum_{i<k}(-1)^k \frac{\partial v_{ik}}{\partial x^i} + \sum_{k<i}(-1)^{i-1}\frac{\partial v_{ki}}{\partial x^i}\right] + \alpha^k(\mathbf{x},\mathbf{u})\right).
\end{aligned}
$$

The divergence of the flux part involving the first rectangular bracket is identically zero [see (2.8), (2.9)].

As all derivatives of potentials v_{ik} can be expressed in terms of local variables $\mathbf{x}$ and $\mathbf{u}$ on the solution manifold of $\mathbf{G}^s_{\mathbf{p}}$, it follows that the flux part involving the second rectangular bracket and $\alpha_k(\mathbf{x},\mathbf{u})$ contains only local variables of the given system (2.1). Hence the conservation law (A1) is linearly dependent on local ones constructed from the given system (2.5), and hence is trivial on the solution manifold of $\mathbf{G}^s_{\mathbf{p}}$. This concludes the proof. □

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Gabor Schauder bases and the Balian-Low theorem

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The Balian-Low Theorem is a strong form of the uncertainty principle for Gabor systems that form orthonormal or Riesz bases for $L^2(\mathbb{R})$. In this paper we investigate the Balian-Low Theorem in the setting of Schauder bases. We prove that new weak versions of the Balian-Low Theorem hold for Gabor Schauder bases, but we constructively demonstrate that several variants of the BLT can fail for Gabor Schauder bases that are not Riesz bases. We characterize a class of Gabor Schauder bases in terms of the Zak transform and product $\mathcal{A}_2$ weights; the Riesz bases correspond to the special case of weights that are bounded away from zero and infinity. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2360041]

I. INTRODUCTION

A *Gabor* or *Weyl-Heisenberg system* consists of a discrete set of time-frequency shifts of a fixed *window function* or *atom* $g \in L^2(\mathbb{R})$. Often, the indexing set is required to possess some structure. For example, we will consider *lattice Gabor systems* of the form

$$\mathcal{G}(g,\alpha,\beta) = \{M_{\beta n}T_{\alpha k}g\}_{k,n\in\mathbb{Z}} = \{e^{2\pi i\beta nt}g(t-\alpha k)\}_{k,n\in\mathbb{Z}}, \tag{1.1}$$

where T_x is the translation operator $T_xg(t)=g(t-x)$, M_ξ is the modulation operator $M_\xi g(t) = e^{2\pi i\xi t}g(t)$, and the compositions T_xM_ξ or $M_\xi T_x$ are called *time-frequency shift operators*. Gabor systems can also be defined in higher dimensions and on general lattices or even completely irregular sets of time-frequency shifts. One may also consider continuous Gabor transforms. For background on the theory and applications of Gabor systems, we refer to Refs. 1–3.

Gabor[4] proposed using the Gaussian function $\varphi(t)=e^{-t^2}$ as a window, with respect to the unit time-frequency shift lattice ($\alpha=\beta=1$). However, while this Gaussian Gabor system $\mathcal{G}(\varphi,1,1)$ is complete in $L^2(\mathbb{R})$ and remains complete if any single element of $\mathcal{G}(\varphi,1,1)$ is removed (cf. Ref. 5, p. 168), it is not an orthonormal basis, a Riesz basis, a frame, or a Schauder basis for $L^2(\mathbb{R})$ (even if the "extra" element is removed).

However, completeness alone is too weak a property to be useful in practice. A *Schauder basis* allows unique representations of elements of $L^2(\mathbb{R})$ in terms of the basis elements, i.e., $\mathcal{G}(g,\alpha,\beta)$ is a Schauder basis if for each $f \in L^2(\mathbb{R})$ there exist unique scalars $c_{kn}(f)$ such that

$$f = \sum_{k,n\in\mathbb{Z}} c_{kn}(f)M_{\beta n}T_{\alpha k}g, \tag{1.2}$$

with convergence of the series in the norm of L^2 with respect to some fixed ordering of the series. However, for a Schauder basis there need not be any direct relation between the size of the coefficients $c_{kn}(f)$ and the norm of f. In contrast, if $\mathcal{G}(g,\alpha,\beta)$ is a *frame* (defined precisely in Sec.

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II A), then it follows not merely that $\mathcal{G}(g,\alpha,\beta)$ is complete, but that every $f \in L^2(\mathbb{R})$ can be written as in (1.2) for a canonical choice of scalars $c_{kn}(f)$ whose ℓ^2 norm forms an equivalent norm for $L^2(\mathbb{R})$. Moreover, for a frame the series (1.2) converges *unconditionally* in the L^2 norm, i.e., regardless of ordering. However, a frame need not provide unique expansions—the scalars $c_{kn}(f)$ need not be unique in general. The canonical choice of scalars is determined by the canonical dual frame, which for a lattice Gabor frame $\mathcal{G}(g,\alpha,\beta)$ is another lattice Gabor frame $\mathcal{G}(\widetilde{g},\alpha,\beta)$ generated by a dual window $\widetilde{g} \in L^2(\mathbb{R})$. A *Riesz basis* is both a frame and a Schauder basis, and thus provides unique unconditionally convergent expansions whose coefficients stably encode the norm of f.

The Density Theorem for Gabor systems provides necessary (but not sufficient) conditions for $\mathcal{G}(g,\alpha,\beta)$ to be complete, a frame, a Riesz basis, or a Riesz sequence [a sequence that need not be complete but forms a Riesz basis for its closed span within $L^2(\mathbb{R})$]. Moreover, these conditions are formulated solely in terms of the lattice $\alpha\mathbb{Z}\times\beta\mathbb{Z}$.

Theorem 1.1 (Density Theorem): *Let* $g \in L^2(\mathbb{R})$ *and* $\alpha, \beta > 0$ *be given.*

(a) *If* $\mathcal{G}(g,\alpha,\beta)$ *is complete in* $L^2(\mathbb{R})$, *then* $\alpha\beta \leqslant 1$. *In particular, if* $\mathcal{G}(g,\alpha,\beta)$ *is a frame, then* $\alpha\beta \leqslant 1$.
(b) *If* $\mathcal{G}(g,\alpha,\beta)$ *is a Riesz basis in* $L^2(\mathbb{R})$, *then* $\alpha\beta = 1$.
(c) *If* $\mathcal{G}(g,\alpha,\beta)$ *is a Riesz sequence in* $L^2(\mathbb{R})$, *then* $\alpha\beta \geqslant 1$.

The Density Theorem has a long and involved history, including extensions to general lattices, to irregular Gabor frames in higher dimensions, and beyond Gabor frames to the setting of abstract "localized frames." Some of the main references include Refs. 6–12. We refer to Ref. 13 for a detailed survey of the Density Theorem, with extensive references to the original literature.

By the Density Theorem, there is a clear separation between "overcomplete" frames and "undercomplete" Riesz sequences, with the Riesz bases corresponding to the *critical density lattices* that satisfy $\alpha\beta = 1$. Moreover, there exists a simple exact characterization, in terms of the Zak transform, of those g such that $\mathcal{G}(g,\alpha,\beta)$ is a Riesz basis for $L^2(\mathbb{R})$ (see Theorem 2.8).

Unfortunately, the *Balian-Low Theorem* (BLT) is a classical result that implies that if $\mathcal{G}(g,\alpha,\beta)$ is a Riesz basis, then the window g must have poor joint localization in the time-frequency plane. Specifically, the localization integrals

$$\int |t|^2 |g(t)|^2 \, dt \quad \text{and} \quad \int |\xi|^2 |\hat{g}(\xi)|^2 \, d\xi$$

cannot both be finite. These same localization integrals appear in the Heisenberg uncertainty principle and, indeed, the BLT may be viewed as a strong form of the uncertainty principle for functions that generate a Gabor Riesz basis (we refer to Ref. 14 for a survey of uncertainty principles).

As with the Density Theorem the BLT has a long and involved history. Stated independently by Balian[15] and Low[16] for the case of orthonormal bases, a complete proof, and an extension to Riesz bases was given by Coifman, Daubechies, and Semmes.[7] Battle[17] gave an elegant new proof for the orthonormal basis case, which shows the intimate connection between the BLT and the operator theory associated with the Heisenberg uncertainty principle. This proof was further extended by Daubechies and Janssen in Ref. 18. Related theorems that relate distinct uncertainty principles to Riesz basis properties have been proved in Refs. 19–22, and extensions of the BLT to higher dimensions appear in Refs. 23–25. We collectively refer to these results as Balian-Low Theorems. Surveys of the Balian-Low Theorems appear in Refs. 19 and 26, and we also note the related results in the papers in Refs. 27–30.

In this paper we determine the extent to which the class of Balian-Low Theorems extend to Gabor systems $\mathcal{G}(g,\alpha,\beta)$ that form Schauder bases but that need not be Riesz bases. Despite the large literature on Gabor systems, very little has been known to date about Gabor Schauder bases. The initial work in this direction[31] proved the existence of a particular Gabor Schauder basis that is not a Riesz basis, and also provided partial results suggesting that the Density Theorem applies

to Gabor Schauder bases; cf. also Ref. 32 for the setting of windowed exponentials in $L^2(\Omega)$. However, these papers clearly indicate that all results become more delicate and difficult for Schauder bases, with the consequence that open questions abound.

In this paper, we accomplish several goals, as follows.

(a) We prove that the Density Theorem does hold for lattice Gabor Schauder bases. Specifically, if $\mathcal{G}(g,\alpha,\beta)$ is a Schauder basis, then $\alpha\beta=1$. We prove that the dual basis is also a Gabor system of the form $\mathcal{G}(\tilde{g},\alpha,\beta)$ for a unique dual window $\tilde{g}$.
(b) We give a characterization of a class of Gabor Schauder bases $\mathcal{G}(g,\alpha,\beta)$ in terms of the Zak transform of the window g and product $\mathcal{A}_2$ weights.
(c) We prove that several variants of the Balian-Low Theorems fail to hold for Gabor Schauder bases.
(d) We prove new weak versions of the BLT for Gabor Schauder bases, and show that as a consequence, if the window g of a Gabor Schauder basis $\mathcal{G}(g,\alpha,\beta)$ is well concentrated in the time-frequency plane, then the dual window $\tilde{g}$ is poorly concentrated.

Thus, counterintuitively, the window of a Gabor Schauder basis can have much better joint time-frequency localization than the generator of a Riesz basis. At the same time, the weak BLT for Gabor Schauder bases implies a striking difference from the behavior of Gabor frames. To discuss this more precisely, let us quantify time-frequency localization by the behavior of the *short-time Fourier transform* (STFT) of g:

$$V_\varphi g(x,\xi)=\langle g,M_\xi T_x\varphi\rangle=\int g(t)\varphi(t-x)e^{-2\pi i\xi t}\,dt,\quad (x,\xi)\in\mathbb{R}^2.$$

If we normalize as $\varphi(t)=(\pi/2)^{-1/4}e^{-t^2}$, then we have $\|\varphi\|_2=1$ and $\|V_\varphi g\|_2=\|g\|_2$. We define the *modulation space* $M^1(\mathbb{R})$ to be the function space consisting of all $g\in L^2(\mathbb{R})$ whose STFT is integrable, i.e.,

$$M^1(\mathbb{R})=\left\{g\in L^2(\mathbb{R}):\|g\|_{M^1}=\|V_\varphi g\|_1=\int\int|V_\varphi g(x,\xi)|dx\,d\xi<\infty\right\}. \tag{1.3}$$

Thus, a function $g\in M^1(\mathbb{R})$ possesses an L^1-type of joint localization in the time-frequency plane. We refer to Ref. 20, Chaps. 11–13 for a detailed background on the class of modulation spaces (of which M^1 is the prototypical example). In particular, we note that the choice of Gaussian window φ above is only for convenience; any nonzero Schwartz-class window, or indeed any nonzero window in M^1, may be used to define the modulation spaces, with each choice of window defining the same space under an equivalent norm.

In Gabor analysis, it is essential to jointly understand the behavior of a frame $\mathcal{G}(g,\alpha,\beta)$ and its dual frame $\mathcal{G}(\tilde{g},\alpha,\beta)$. For a Riesz basis, the Balian-Low Theorems imply that both the window and the dual window must have poor localization:

$$\text{For a Gabor Riesz basis:}\quad g\notin M^1(\mathbb{R})\quad\text{and}\quad\tilde{g}\notin M^1(\mathbb{R}).$$

In contrast, Gröchenig and Leinert[63] proved that if the window of a Gabor frame is well localized, then the dual window is as well, and, conversely:

$$\text{For a Gabor frame:}\quad g\in M^1(\mathbb{R})\Leftrightarrow\tilde{g}\in M^1(\mathbb{R}).$$

The Gröchenig and Leinert proof used deep results on symmetric C^* algebras. A new proof, based on a type of noncommutative Wiener's lemma, that extends to irregular Gabor frames and abstract localized frames, was given in Refs. 33 and 12.

In this paper, we constructively demonstrate the following:

For a Gabor Schauder basis: $g \in M^1(\mathbb{R})$, $\widetilde{g} \notin M^1(\mathbb{R})$ is possible.

Moreover, we show that whenever the window of a Gabor Schauder basis is well localized, then the dual window must be poorly localized, specifically the following:

$$\text{For a Gabor Schauder basis:} \quad g \in M^1(\mathbb{R}) \Rightarrow \widetilde{g} \notin M^1(\mathbb{R}). \tag{1.4}$$

We note that many types of weight functions play important roles in many aspects of time-frequency analysis (see Gröchenig's recent survey[34] for details and references). However, to date the Muckenhoupt, or $\mathcal{A}_p$, weights have had no application within time-frequency analysis. Our results show that the Muckenhoupt weight class is important in time-frequency analysis as a window class via the Zak transform. This is in contrast to the usual use of weights, which normally are used in time-frequency analysis in the quantification of time-frequency concentration.

Overview: Our paper is organized as follows. In Sec. II A we present background information on Schauder bases, Riesz bases, and the Zak transform. In Sec. III we recall the classical Balian-Low Theorem and several of its variants. These results, which are all stated in terms of Riesz bases for $L^2(\mathbb{R})$, form the backdrop for our investigation into the Balian-Low Theorem for Schauder bases. In Sec. IV we investigate some basic properties of Gabor Schauder bases, including the structure of the dual basis, and we present a short proof of a weak Balian-Low Theorem for Gabor Schauder bases. In Sec. V we show how to use product $\mathcal{A}_2$ weights to give a characterization of a class of Gabor Schauder bases for $L^2(\mathbb{R})$. In Sec. VI we show that several versions of the Balian-Low Theorem do not extend to the setting of Schauder bases. In Sec. VII, we prove that weak versions of the M^1 BLT and Amalgam BLT hold for Gabor Schauder bases and exact systems.

II. BACKGROUND AND PRELIMINARIES

A. Schauder bases, frames, and Riesz bases

We recall the definition and basic facts regarding Schauder bases, frames, and Riesz bases in Hilbert spaces. We refer to Refs. 35–38 for additional background.

Definition 2.1: An ordered collection $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ in a Hilbert space H is a *Schauder basis* for H if for each $f \in H$ there exist unique scalars $c_n(f)$ such that

$$f = \sum_{n=0}^{\infty} c_n(f) f_n, \tag{2.1}$$

where the series converges in the norm of H.

It is important to point out that Schauder basis expansions may converge conditionally, i.e., the order of summation in (2.1) matters.

The linear functionals c_n in (2.1) can be shown to be continuous. Therefore there exist $\widetilde{f}_n \in H$ such that $c_n(f)=\langle f, \widetilde{f}_n \rangle$. Further, $\widetilde{\mathcal{F}}=\{\widetilde{f}_n\}_{n=0}^{\infty}$ is the unique sequence in H that is *biorthogonal* to $\mathcal{F}$, i.e.,

$$\langle f_m, \widetilde{f}_n \rangle = \delta_{mn}.$$

Every Schauder basis has an associated biorthogonal sequence, but the converse is not true, i.e., the existence of a biorthogonal system does not imply that the original sequence is a Schauder basis. The existence of a biorthogonal sequence is equivalent to the statement that $\mathcal{F}$ is *minimal*, i.e., no element of $\mathcal{F}$ lies in the closed linear span of the remaining elements. A system that is both complete and minimal is said to be *exact*. There exist complete and minimal systems that are not Schauder bases.

Given a sequence $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ that has a biorthogonal sequence $\widetilde{\mathcal{F}}=\{\widetilde{f}_n\}_{n=0}^{\infty}$, we define the *partial sum operators* $S_N: H \to H$ by

$$S_N(f) = \sum_{n=0}^{N} \langle f, \tilde{f}_n \rangle f_n.$$

There are several equivalent definitions of a Schauder basis, of which we will need the following.

Theorem 2.2: *Given a collection* $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ *in a Hilbert space* H, *the following statements are equivalent*.

(a) $\mathcal{F}$ *is a Schauder basis*.

(b) *There exists a biorthogonal sequence* $\tilde{\mathcal{F}}=\{\tilde{f}_n\}_{n=0}^{\infty}$ *such that the partial sum operators* S_N *converge in the strong operator topology to the identity map, i.e.,*

$$\forall f \in H, \quad f = \sum_{n=0}^{\infty} \langle f, \tilde{f}_n \rangle f_n. \tag{2.2}$$

(c) *There exists a biorthogonal sequence* $\tilde{\mathcal{F}}=\{\tilde{f}_n\}_{n=0}^{\infty}$ *such that the partial sum operators are uniformly bounded in operator norm, i.e.,*

$$\sup_N \|S_N\| < \infty.$$

The number $C=\sup_N\|S_N\|$ is called the *basis constant* for $\mathcal{F}$. The biorthogonal sequence $\tilde{\mathcal{F}}$ is itself a Schauder basis for H, and is called the *dual basis* to $\mathcal{F}$.

In contrast to Schauder bases, frames are defined in terms of a norm-equivalence criterion.

Definition 2.3: A collection $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ in a Hilbert space H is a *frame* for H if there exist constants $A, B>0$, called *frame bounds*, such that

$$\forall f \in H, \quad A\|f\|^2 \leqslant \sum_{i=0}^{\infty} |\langle f, f_i \rangle|^2 \leqslant B\|f\|^2. \tag{2.3}$$

A sequence for which the upper inequality in (2.3) is satisfied, but not necessarily the lower inequality, is called a *Bessel sequence*.

If $\mathcal{F}$ is a frame, then the *frame operator* $Sf=\Sigma_{n=0}^{\infty}\langle f, f_n\rangle f_n$ is a bounded, positive, and invertible mapping of H onto itself. The *canonical dual frame* $\tilde{\mathcal{F}}=\{\tilde{f}_n\}_{n=0}^{\infty}$ defined by $\tilde{f}_n=S^{-1}(f_n)$ yields frame expansions exactly of the form in (2.2). Moreover, those series converge unconditionally for each f. However, in general, a frame need not be a Schauder basis. In particular, the scalars $\langle f, \tilde{f}_n \rangle$ in (2.2) need not be unique.

Definition 2.4: A collection $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ in a Hilbert space H is a *Riesz basis* for H if it is the image of an orthonormal basis for H under a continuous, invertible map of H onto itself.

Among other characterizations, the following theorem shows that a Riesz basis is precisely a sequence that is both a frame and a Schauder basis.

Theorem 2.5: *Given a collection* $\mathcal{F}=\{f_n\}_{n=0}^{\infty}$ *in a Hilbert space* H, *the following statements are equivalent*.

(a) $\mathcal{F}$ *is a Riesz basis*.

(b) $\mathcal{F}$ *is a bounded unconditional basis, i.e.,* $\mathcal{F}$ *is a Schauder basis, the basis expansions in* (2.1) *converge unconditionally for each* $f \in H$, *and* $0<\inf_n\|f_n\| \leqslant \sup_n\|f_n\|<\infty$.

(c) $\mathcal{F}$ *is an exact frame, i.e., it is a frame and is biorthogonal to its canonical dual frame*.

(d) $\mathcal{F}$ *is complete and there exist constants* $A, B>0$, *such that*

$$\forall c_0, \ldots, c_N, \quad A\sum_{n=0}^{N} |c_N|^2 \leqslant \left\| \sum_{n=0}^{N} c_n f_n \right\|^2 \leqslant B\sum_{n=0}^{N} |c_n|^2.$$

(e) *$\mathcal{F}$ is a complete Bessel sequence and possesses a biorthogonal sequence that is also a complete Bessel sequence.*

The dual basis of a Riesz basis coincides with its canonical dual frame, and is itself a Riesz basis for H.

We say that a sequence is a *Riesz sequence* if it forms a Riesz basis for its closed span within H.

Example 2.6: Let $\varphi(t)=e^{-t^2}$. von Neumann (Ref. 39, p. 406) claimed (without proof) that $\mathcal{G}(\varphi,1,1)$ is complete in $L^2(\mathbb{R})$. Gabor conjectured in Ref. 4, Eq. 1.29 that every function in $L^2(\mathbb{R})$ can be represented in the form

$$f=\sum_{k,n\in\mathbb{Z}} c_{kn}(f)M_nT_k\varphi, \tag{2.4}$$

for some scalars $c_{kn}(f)$. von Neumann's claim of completeness was proved in Refs. 40 and 41. Janssen proved in Ref. 42 that Gabor's conjecture is true, but he showed that the series in (2.4) converges only in the sense of tempered distributions—not in the norm of L^2. Thus the Gabor system $\mathcal{G}(\varphi,1,1)$ fits none of the definitions given previously in this section.

On the other hand, Lyubarskii[43] and Seip and Wallstén[44,45] proved that $\mathcal{G}(\varphi,\alpha,\beta)$ is a frame for $L^2(\mathbb{R})$ whenever $0<\alpha\beta<1$. Moreover, $\mathcal{G}(\varphi,\alpha,\beta)$ is an incomplete Riesz sequence in $L^2(\mathbb{R})$ whenever $\alpha\beta>1$.

B. The Zak transform

The Zak transform was introduced by Gelfand[46] and goes by several names. It is often called the *Weil-Brezin map* in representation theory and abstract harmonic analysis. Zak rediscovered this transform, which he called the *k-q transform*, in his work on quantum mechanics, e.g., Ref. 47. For more information, we refer to Janssen's influential paper[48] and survey,[49] or to Gröchenig's text.[1]

The Zak transform is an extremely useful tool for analyzing Gabor systems at the critical density $\alpha\beta=1$. Because the unitary dilation $D_\alpha f(t)=\alpha^{1/2}f(\alpha t)$ maps the Gabor system $\mathcal{G}(g,\alpha,1/\alpha)$ to the Gabor system $\mathcal{G}(D_\alpha g,1,1)$, when working at the critical density we always can, by a change of variables, reduce to the case $\alpha=\beta=1$. This is what we will do throughout, i.e., when we are at the critical density we will only consider Gabor systems of the form

$$\mathcal{G}(g,1,1)=\{M_nT_kg\}_{k,n\in\mathbb{Z}}.$$

The Zak transform is the unitary operator Z: $L^2(\mathbb{R})\to L^2(Q)$, where $Q=[0,1)^2$, formally defined for $f\in L^2(\mathbb{R})$ by

$$Zf(t,\xi)=\sum_{k\in\mathbb{Z}} f(t-k)e^{2\pi ik\xi},\quad (t,\xi)\in[0,1)^2. \tag{2.5}$$

It can be shown that the series above converges in the norm of $L^2(Q)$, and that Z is a unitary map of $L^2(\mathbb{R})$ onto $L^2(Q)$. The utility of the Zak transform is made apparent by the following theorem, where we use the notation

$$E_{n,k}(t,\xi)=e^{2\pi int}e^{-2\pi ik\xi}. \tag{2.6}$$

Theorem 2.7: *Let $g\in L^2(\mathbb{R})$ be given. Then*

$$Z(M_nT_kg)(t,\xi)=(E_{n,k}\cdot Zg)(t,\xi)=E_{n,k}(t,\xi)Zg(t,\xi).$$

In other words, the Zak transform diagonalizes time-frequency shifts.

Since $\{E_{n,k}\}_{k,n\in\mathbb{Z}}$ forms an orthonormal basis for $L^2(Q)$ and since Z is unitary, the following characterization follows easily; cf. Ref. 50 Theorem 4.3.3.

Theorem 2.8: *Let $g\in L^2(\mathbb{R})$ be given.*

(a) $\mathcal{G}(g,1,1)$ *is complete if and only if* $Zg \neq 0$ *a.e.*
(b) $\mathcal{G}(g,1,1)$ *is minimal if and only if* $1/Zg \in L^2(Q)$. *In this case* $\mathcal{G}(g,1,1)$ *is also complete, i.e., it is exact.*
(c) $\mathcal{G}(g,1,1)$ *is a frame for* $L^2(\mathbb{R})$ *if and only if there exist* $0<A\leqslant B<\infty$ *such that* $A\leqslant|Zg|^2 \leqslant B$ *a.e. In this case* $\mathcal{G}(g,1,1)$ *is a Riesz basis for* $L^2(\mathbb{R})$, *and* A, B *are frame bounds for* $\mathcal{G}(g,1,1)$.
(d) $\mathcal{G}(g,1,1)$ *is an orthonormal basis for* $L^2(\mathbb{R})$ *if and only if* $|Zg|^2=1$ *a.e.*

C. Modulation spaces

In addition to the modulation space $M^1(\mathbb{R})$ defined in (1.3), we will need the following particular modulation spaces. We refer to Ref. 1 for details.

Definition 2.9: Let $\varphi(t)=(\pi/2)^{-1/4}e^{-t^2}$. For $1\leqslant p<\infty$ and $s\geqslant 0$, the modulation space $M^p_s(\mathbb{R})$ consists of all tempered distributions $g\in S'(\mathbb{R})$ for which the norm

$$\|g\|_{M^p_s}=\|V_\varphi g\|_{L^p_s}=\left(\int\int |V_\varphi g(x,\xi)|^p(1+|x|+|\xi|)^{ps}\,dx\,d\xi\right)^{1/p}$$

is finite.

For any α, β with $0<\alpha\beta<1$, the following is an equivalent norm for $M^p_s(\mathbb{R})$:

$$|||g|||_{M^p_s}=\left(\sum_{k\in\mathbb{Z}}\sum_{n\in\mathbb{Z}}|\langle g,M_{\beta n}T_{\alpha k}\varphi\rangle|^p(1+|\alpha k|+|\beta n|)^{ps}\right)^{1/p}. \tag{2.7}$$

For $s\geqslant 0$, we have $M^2_s(\mathbb{R})=L^2_s(\mathbb{R})\cap H^s(\mathbb{R})$, where

$$L^2_s(\mathbb{R})=\left\{f\in L^2(\mathbb{R}):\int |f(t)|^2(1+|t|)^{2s}\,dt<\infty\right\}$$

and

$$H^s(\mathbb{R})=\left\{f\in L^2(\mathbb{R}):\int |\hat{f}(\xi)|^2(1+|\xi|)^{2s}\,d\xi\right\}.$$

It follows from the discrete-type norm given in (2.7) that $M^2_s(\mathbb{R})\subseteq M^1(\mathbb{R})$ if $s>1$. However, $M^2_1(\mathbb{R})$ does not embed into $M^1(\mathbb{R})$, nor conversely.

III. THE BALIAN-LOW THEOREMS

In this section we recall the precise statement of several variants of the Balian-Low Theorem. We use the Fourier transform normalized by $\hat{f}(\xi)=\int f(t)e^{-2\pi i\xi t}\,dt$. Recall that, by the Density Theorem, if a lattice Gabor system is a Riesz basis, then necessarily we are at the critical density, and hence it suffices to consider $\alpha=\beta=1$. The first part of the following theorem is the classical wording of the BLT; we also give an equivalent wording in terms of modulation spaces.

Theorem 3.1 (Classical Balian-Low Theorem): *If* $g\in L^2(\mathbb{R})$ *and*

$$\int |t|^2|g(t)|^2\,dt<\infty \quad \textit{and} \quad \int |\xi|^2|\hat{g}(\xi)|^2\,d\xi<\infty,$$

then $\mathcal{G}(g,1,1)$ *is not a Riesz basis for* $L^2(\mathbb{R})$. *Equivalently, if* $g\in M^2_1(\mathbb{R})$, *then* $\mathcal{G}(g,1,1)$ *is not a Riesz basis for* $L^2(\mathbb{R})$.

The following theorem summarizes four variations of the Balian-Low Theorem that involve different quantifications of time-frequency localization. Part (a) is formulated in terms of the modulation space $M^1(\mathbb{R})$ that was defined in (1.3). Part (b) is formulated in terms of the *Wiener amalgam space*,

$$W(\mathcal{C},\ell^1)=\left\{f\colon \mathbb{R}\to\mathbb{C}\colon f \text{ is continuous and } \sum_{n\in\mathbb{Z}}\|f\cdot\chi_{[n,n+1)}\|_\infty<\infty\right\}.$$

For details on the amalgam spaces, with extensive references to the original literature, we refer to the survey in Ref. 62.

Theorem 3.2: *Fix $g\in L^2(\mathbb{R})$: If any of the following hypotheses hold:*

(a) $g\in M^1(\mathbb{R})$;
(b) $g\in W(\mathcal{C},\ell^1)$;
(c) $1<q<2<p<\infty$, $\frac{1}{p}+\frac{1}{q}=1$, $0<\varepsilon<2-q$,

$$\int |t|^{p+\varepsilon}|g(t)|^2\,dt<\infty, \quad \text{and} \quad \int |\xi|^{q+\varepsilon}|\hat{g}(\xi)|^2\,d\xi<\infty;$$

(d) $\sup_{N>0}\int |t|^N|g(t)|^2\,dt<\infty$ *and* $\int|\xi||\hat{g}(\xi)|^2\,d\xi<\infty$,

then $\mathcal{G}(g,1,1)$ is not a Riesz basis for $L^2(\mathbb{R})$.

The theorem corresponding to the hypothesis in part (a) of Theorem 3.2 was proved in Ref. 23, and it extends to Gabor systems on arbitrary lattices in higher dimensions. We will refer to this theorem as the M^1 BLT. Since M^1 does not embed into $M^2_1(\mathbb{R})$ nor conversely, this result is distinct from Theorem 3.1.

The theorem corresponding to part (b) is known as the *Amalgam BLT*.[51,19] It extends to rectangular lattices of the form $\alpha\mathbb{Z}^d\times\beta\mathbb{Z}^d$ in higher dimensions. For rectangular lattices, the Amalgam BLT implies the M^1 BLT. However, it is not known if the Amalgam BLT extends to arbitrary lattices, so in that setting these two results are distinct. Furthermore, it was shown in Ref. 19 that the Amalgam BLT and the Classical BLT are distinct.

Part (c) follows from part (a) and Ref. 52, Theorem 1; see Ref. 30, Eq. (2.6).

Part (d) was proved in Ref. 22. It is worth mentioning that part (c) actually holds for all $\varepsilon>0$, but we shall only deal with the case where ε is sufficiently small. We refer to parts (c) and (d) as *nonsymmetric (p,q) BLTs*.

IV. SCHAUDER BASES AND A WEAK BALIAN-LOW THEOREM

In this section we will prove some basic facts about Gabor Schauder bases, and establish that a weak version of the BLT holds for Schauder bases.

Gabor systems are naturally indexed by $\mathbb{Z}\times\mathbb{Z}$, but do not come equipped with a standard enumeration. Since Schauder basis expansions may depend critically on ordering any discussion of Gabor Schauder bases must specify a particular enumeration of $\mathbb{Z}\times\mathbb{Z}$. Therefore, whenever we say that $G(g,\alpha,\beta)$ is a Gabor Schauder basis, we shall implicitly mean that there exists an enumeration of the Gabor system $G(g,\alpha,\beta)$, which is a Schauder basis. When necessary we shall explicitly define the enumeration.

A. The Density Theorem and the Dual Basis

We first observe that the existing results for Gabor Schauder bases implicitly contain a Density Theorem. We make this explicit as follows (we refer to Ref. 11 for the definition of Beurling density). As a consequence, for lattice Gabor Schauder bases, we will always be able to reduce to the case $\alpha=\beta=1$.

Theorem 4.1 (Density Theorem for Lattice Gabor Schauder Bases): *Let $g\in L^2(\mathbb{R})$ and $\alpha,\beta>0$ be given. If $\mathcal{G}(g,\alpha,\beta)$ is a Schauder basis for $L^2(\mathbb{R})$, then $\alpha\beta=1$.*

Proof: First, if $\mathcal{G}(g,\alpha,\beta)$ is a Schauder basis, then it is complete, so Theorem 1.1 implies that $\alpha\beta\leqslant 1$. On the other hand, see Ref. 31, Corollary 4.6, which gives partial necessary conditions for an irregular Gabor system to form a Schauder basis, and implies that the lower and upper Beurling densities of the index set $\alpha\mathbb{Z}\times\beta\mathbb{Z}$ must satisfy $D^{\pm}(\alpha\mathbb{Z}\times\beta\mathbb{Z})\leqslant 1$. The Beurling density of the lattice $\alpha\mathbb{Z}\times\beta\mathbb{Z}$ is $D^{\pm}(\alpha\mathbb{Z}\times\beta\mathbb{Z})=1/(\alpha\beta)$, so this implies that $\alpha\beta\geqslant 1$. □

It was conjectured in Ref. 31 that if $\mathcal{G}(g,\Lambda)=\{M_\xi T_x g\}_{(x,\xi)\in\Lambda}$ is a Gabor Schauder basis with respect to an arbitrary sequence of time-frequency shifts Λ, then we must have $D^{\pm}(\Lambda)=1$. This conjecture remains open for non-lattice Gabor Schauder bases.

It is well known that the dual basis to a Gabor Riesz basis $\mathcal{G}(g,\alpha,\beta)$ is itself a Gabor Riesz basis $\mathcal{G}(\tilde{g},\alpha,\beta)$. This follows from the fact that if $\mathcal{G}(g,\alpha,\beta)$ is a frame, then the frame operator S commutes with the time-frequency shifts $M_{\beta n}T_{\alpha k}$. For a Gabor Schauder basis, the frame operator need not be a bounded or even a well-defined map. Nonetheless, we show next that the dual of a lattice Gabor Schauder basis is also a lattice Gabor Schauder basis. By Theorem 4.1, it suffices to consider $\alpha=\beta=1$.

Theorem 4.2: *If $g\in L^2(\mathbb{R})$ and $\mathcal{G}(g,1,1)$ is an exact system in $L^2(\mathbb{R})$, then the biorthogonal system has the form $\mathcal{G}(\tilde{g},1,1)$, where the dual window $\tilde{g}\in L^2(\mathbb{R})$ is defined by the condition*

$$Z\tilde{g}=1/\overline{Zg}.$$

In particular, this determines the dual basis for a Gabor Schauder basis.

Proof: By Theorem 2.8 we have that the function $G=1/\overline{Zg}$ belongs to $L^2(\mathbb{R})$. Therefore, by the unitarity of the Zak transform we may define $\tilde{g}=Z^{-1}G\in L^2(\mathbb{R})$.

If (k,n), $(j,m)\in\mathbb{Z}^2$ then by Theorem 2.7, we have that

$$\langle M_nT_kg,M_mT_j\tilde{g}\rangle=\langle ZM_nT_kg,ZM_mT_j\tilde{g}\rangle=\int_0^1\int_0^1 E_{n,k}(t,\xi)Zg(t,\xi)\overline{E_{m,j}(t,\xi)Z\tilde{g}(t,\xi)}dt\,d\xi$$

$$=\int_0^1\int_0^1 E_{n,k}(t,\xi)\overline{E_{m,j}(t,\xi)}dt\,d\xi=\langle E_{n,k},E_{m,n}\rangle=\delta_{jk}\delta_{mn}.$$

Thus, $\mathcal{G}(\tilde{g},1,1)$ is biorthogonal to $\mathcal{G}(g,1,1)$. Since an exact system has a unique biorthogonal system, it follows that $\mathcal{G}(\tilde{g},1,1)$ is the biorthogonal system. □

The following elementary lemma will be used later.

Lemma 4.3: Let $g\in L^2(\mathbb{R})$. Let $\{(k_j,n_j)\}_{j=1}^\infty$ be an enumeration of $\mathbb{Z}\times\mathbb{Z}$. If $\mathcal{G}(g,1,1)$ is a Gabor Schauder basis with respect to this enumeration, then it is also a Gabor Schauder basis with respect to the enumeration $\{(-k_j,-n_j)\}_{j=1}^\infty$.

Equivalently, if $\{M_{n_j}T_{k_j}g\}_{j=1}^\infty$ is a Schauder basis for $L^2(\mathbb{R})$ with dual basis $\{M_{n_j}T_{k_j}\tilde{g}\}_{j=1}^\infty$, then $\{M_{-n_j}T_{-k_j}g\}_{j=1}^\infty$ is a Schauder basis for $L^2(\mathbb{R})$ with dual basis $\{M_{-n_j}T_{-k_j}\tilde{g}\}_{j=1}^\infty$.

B. A weak classical Balian-Low Theorem for Gabor Schauder bases

Daubechies and Janssen proved in Ref. 18 that a weak version of the BLT holds for Gabor systems $\mathcal{G}(g,1,1)$ that are exact in $L^2(\mathbb{R})$. In particular, all Schauder bases are exact. As the proof is simpler for Gabor Schauder bases than general exact systems, we include it here. It will be convenient to state this result in terms of the unbounded operators P and X on $L^2(\mathbb{R})$, defined by

$$Pf(t)=tf(t)\quad\text{and}\quad Xf(t)=(\hat{Pf})^\vee(t),$$

where $h^\vee$ denotes the inverse Fourier transform.

Theorem 4.4 (Weak BLT): *Let $g\in L^2(\mathbb{R})$. If $\mathcal{G}(g,1,1)$ is a Schauder basis for $L^2(\mathbb{R})$ with dual basis $\mathcal{G}(\tilde{g},1,1)$, then at least one of the functions,*

$$Pg,\quad Xg,\quad P\tilde{g},\quad X\tilde{g},$$

does not belong to $L^2(\mathbb{R})$. Equivalently, if $g,\tilde{g}\in M_1^2(\mathbb{R})$, then $\mathcal{G}(g,1,1)$ is not a Schauder basis for $L^2(\mathbb{R})$.

Proof: Although the proof is formally similar to that in Ref. 17, extra care must be taken since Schauder basis expansions converge only conditionally in general. To this end, suppose that $\mathcal{G}(g,1,1)$ is a Schauder basis for $L^2(\mathbb{R})$ with respect to a specific enumeration $\{(k_j,n_j)\}_{j=1}^\infty$ of $\mathbb{Z}\times\mathbb{Z}$.

We proceed by contradiction. Assume that Pg, Xg, $P\widetilde{g}$, $X\widetilde{g}$ all belong to $L^2(\mathbb{R})$. By direct calculation, for each k, $n \in \mathbb{Z}$ we have

$$\langle Xg, M_n T_k \widetilde{g}\rangle = \langle M_{-n} T_{-k} g, X\widetilde{g}\rangle \quad \text{and} \quad \langle M_n T_k g, P\widetilde{g}\rangle = \langle Pg, M_{-n} T_{-k}\widetilde{g}\rangle. \tag{4.1}$$

Next, using (4.1) and Lemma 4.3, we compute that

$$\begin{aligned}\langle Xg, P\widetilde{g}\rangle &= \left\langle \lim_{N\to\infty} \sum_{j=1}^{N} \langle Xg, M_{n_j} T_{k_j}\widetilde{g}\rangle M_{n_j} T_{k_j} g, P\widetilde{g}\right\rangle = \lim_{N\to\infty} \sum_{j=1}^{N} \langle M_{-n_j} T_{-k_j} g, X\widetilde{g}\rangle \langle Pg, M_{-n_j} T_{-k_j}\widetilde{g}\rangle \\ &= \left\langle Pg, \lim_{N\to\infty} \sum_{j=1}^{N} \langle X\widetilde{g}, M_{-n_j} T_{-k_j} g\rangle M_{-n_j} T_{-k_j}\widetilde{g}\right\rangle = \langle Pg, X\widetilde{g}\rangle. \end{aligned} \tag{4.2}$$

Because the commutator $[X,P]=XP-PX=-1/(2\pi i)I$ is a multiple of the identity operator I (on the domain of $[X,P]$), we have by Ref. 19, Lemma 7.2 that

$$\frac{1}{2\pi i}\langle g, \widetilde{g}\rangle = \langle Pg, X\widetilde{g}\rangle - \langle Xg, P\widetilde{g}\rangle. \tag{4.3}$$

Therefore, $\langle g, \widetilde{g}\rangle = 0$ by (4.2). But this is a contradiction, because the definition of biorthogonality implies that $\langle g, \widetilde{g}\rangle = 1$. □

V. $\mathcal{A}_2$ WEIGHTS AND CHARACTERIZATIONS OF GABOR SCHAUDER BASES

Theorem 2.8 shows that the Zak transform can be used to characterize many properties of a Gabor system. In this section we address this issue of whether Gabor Schauder bases also admit a simple characterization in the Zak transform domain.

First, let us give a basic equivalent reformulation of the definition of Gabor Schauder bases. This reformulation, which is an immediate consequence of Theorems 2.2 and 2.7, reveals the issues that must be addressed in order to find the desired characterization.

Lemma 5.1: Let $g \in L^2(\mathbb{R})$ be given, and let $\{(k_j, n_j)\}_{j=1}^{\infty}$ be an enumeration of $\mathbb{Z}\times\mathbb{Z}$. Then the following statements are equivalent.

(a) $\mathcal{G}(g,1,1)$ *is a Schauder basis for* $L^2(\mathbb{R})$ *with respect to the enumeration* $\{(k_j,n_j)\}_{j=1}^{\infty}$.
(b) $1/|Zg| \in L^2(Q)$, *and the partial sum operators* $S_N: L^2(Q) \to L^2(Q)$, *defined by*

$$S_N F = \sum_{j=1}^{N} \langle F, E_{n_j,k_j}\overline{/Zg}\rangle (E_{n_j,k_j}\cdot Zg), \tag{5.1}$$

are uniformly bounded in operator norm, i.e., $\sup_N \|S_N\| < \infty$.

The boundedness of partial sum operators in higher dimensions is, in general, a delicate issue, e.g., Ref. 53. However, for rectangular partial sums the problem is well understood, using $\mathcal{A}_2$ weights as a tool.

A. Background on $\mathcal{A}_2$ weights

We give here some background and basic results on $\mathcal{A}_2$ weights. We let $L^1(\mathbb{T})$ denote the space of 1-periodic functions on $\mathbb{R}$ that are integrable on $[0,1]$. We use the convention that $0\cdot\infty = 0$, and the symbol $\mathbf{1}_S$ will denote the characteristic function of a set $S \subseteq \mathbb{R}$. We use the notation $A \lesssim B$ to mean that there exists an absolute constant C, such that $A \leq CB$.

Definition 5.2 ($\mathcal{A}_2$ weight): A non-negative function $w \in L^1(\mathbb{T})$ is an $\mathcal{A}_2(\mathbb{T})$ *weight*, denoted $w \in \mathcal{A}_2(\mathbb{T})$, if there exists a constant $C>0$ such that for every interval $I \subset \mathbb{R}$ we have

$$\left(\frac{1}{|I|}\int_I w(t)dt\right)\left(\frac{1}{|I|}\int_I \frac{1}{w(t)}dt\right) \leqslant C.$$

We refer to the smallest such C as the $\mathcal{A}_2(\mathbb{T})$ characteristic of w, denoted $\|w\|_{\mathcal{A}_2(\mathbb{T})}$. Note that every $w \in \mathcal{A}_2(\mathbb{T})$ satisfies $1 \leqslant \|w\|_{\mathcal{A}_2(\mathbb{T})}$.

Now define

$$e_n(t) = e^{2\pi i n t}.$$

The following fundamental theorem of Hunt, Muckenhoupt, and Wheeden addresses the uniform boundedness of the Fourier partial sum operators,

$$T_N f = \sum_{n=-N}^{N} \langle f, e_n\rangle e_n, \tag{5.2}$$

in weighted L^2 spaces. In particular, the equivalence of statements (a) and (b) in the following theorem is a special case of Ref. 54, Theorem 8. We let $L^2_w(D)$ be the space of all complex-valued functions f on D for which

$$\|f\|_{2,w} = \left(\int_D |f(x)|^2 w(x)dx\right)^{1/2} < \infty.$$

Theorem 5.3 (Hunt, Muckenhoupt, Wheeden): *Let w be a non-negative function in $L^1(\mathbb{T})$. For $N \geqslant 0$, let $T_N: L^2_w(\mathbb{T}) \to L^2_w(\mathbb{T})$ be the operator formally defined by (5.2), and let $\|T_N\|_{2,w}$ denote its operator norm. Then the following statements are equivalent.*

(a) $\sup_N \|T_N\|_{2,w} < \infty$.
(b) $w \in \mathcal{A}_2(\mathbb{T})$.

Furthermore,

$$\|w\|_{\mathcal{A}_2(\mathbb{T})} \lesssim \sup_N \|T_N\|^2_{2,w} \lesssim \|w\|^2_{\mathcal{A}_2(\mathbb{T})}. \tag{5.3}$$

Along with the explicit equivalence of (a) and (b), the first inequality in (5.3) is implicit in the proof of Ref. 54, Theorem 8. For the second inequality in (5.3), the proof of Ref. 54, Thm. 8, along with the fact that $1 \leqslant \|w\|_{\mathcal{A}_2(\mathbb{T})}$, shows that

$$\sup_N \|T_N\|^2_{2,w} \lesssim (C_w)^2 + \|w\|_{\mathcal{A}_2(\mathbb{T})} \lesssim (C_w)^2 + \|w\|^2_{\mathcal{A}_2(\mathbb{T})},$$

where C_w is the norm bound for the conjugate function on $L^2_w(\mathbb{T})$ (see Ref. 54, Theorem 1). It therefore suffices to know that C_w is controlled from above by $\|w\|_{\mathcal{A}_2(\mathbb{T})}$. This is a consequence of the corresponding sharp result for the Hilbert transform proved in Ref. 55. For our purposes, the full strength of (5.3) is not needed, and any reasonable relation between $\sup_N \|T_N\|^2_{2,w}$ and $\|w\|_{\mathcal{A}_2(\mathbb{T})}$ is enough for our subsequent results. In this regard, the weaker estimates given by Refs. 56 and 57 would also suffice.

Rewriting Theorem 5.3 in terms of the partial sum operators for windowed systems of exponentials gives the following. Here $\langle\cdot,\cdot\rangle$ denotes the usual inner product on $L^2(\mathbb{T})$.

Corollary 5.4: Let $w \in L^2(\mathbb{T})$ be nonzero a.e., and define $\tilde{w} = 1/\bar{w}$. Let $\{n_j\}_{j=1}^{\infty}$ be the enumeration $\{0,1,-1,2,-2,3,-3,\ldots\}$ of $\mathbb{Z}$. For $N \geqslant 1$, let $S_N: L^2(\mathbb{T}) \to L^2(\mathbb{T})$ be the operator, formally defined by

$$S_N f = \sum_{j=1}^{N} \langle f, e_{n_j}\cdot \tilde{w}\rangle (e_{n_j}\cdot w),$$

and let $\|S_N\|$ *denote its operator norm. Then the following statements are equivalent.*

(a) $\sup_N \|S_N\| < \infty$.
(b) $|w|^2 \in \mathcal{A}_2(\mathbb{T})$.

Proof: Let $T_N: L^2_{|w|^2}(\mathbb{T}) \to L^2_{|w|^2}(\mathbb{T})$ be defined by (5.2). By Theorem 5.3, it suffices to show that $\sup_N \|T_N\|_{2,|w|^2} < \infty$ if and only if $\sup_N \|S_N\| < \infty$.

Suppose that $C = \sup_N \|T_N\|_{2,|w|^2} < \infty$. Then for $f \in L^2(\mathbb{T})$, we have

$$\|S_{2N+1} f\|_2 = \|T_N(f/w)\|_{2,|w|^2} \leq C\|f/w\|_{2,|w|^2} = C\|f\|_2.$$

Since $|w|^2 \in \mathcal{A}_2(\mathbb{T})$, we have $A = \|\widetilde{w}\|_2 \|w\|_2 < \infty$. Therefore

$$\|S_{2N} f\|_2 \leq \|S_{2N-1} f\|_2 + |\langle f, e_N \widetilde{w}\rangle| \|e_N w\|_2 \leq C\|f\|_2 + \|f\|_2 \|\widetilde{w}\|_2 \|w\|_2 = (C + A)\|f\|_2.$$

Hence $\sup_N \|S_N\| \leq C + A < \infty$.

For the converse, suppose that $\sup_N \|S_N\| < \infty$. If $f \in L^2_{|w|^2}(\mathbb{T})$ then

$$\|T_N(f)\|_{2,|w|^2} = \|S_{2N+1}(fw)\|_2 \leq C\|fw\|_2 = C\|f\|_{2,|w|^2}.$$

Hence $\sup_N \|T_N\|_{2,|w|^2} < \infty$. □

B. Product domains and enumerations of $\mathbb{Z} \times \mathbb{Z}$

The results of the preceding section readily extend to product domains. In fact, many related results are true more generally in the setting of singular integral operators and maximal functions on product domains, e.g., Refs. 58 and 59.

We let $L^1(\mathbb{T} \times \mathbb{T})$ denote the space of functions on $\mathbb{R}^2$ that are 1-periodic in each variable and integrable on $[0,1]^2$.

Definition 5.5 (product $\mathcal{A}_2$ weight): A non-negative function $w \in L^1(\mathbb{T} \times \mathbb{T})$ is an $\mathcal{A}_2(\mathbb{T} \times \mathbb{T})$ weight if there exists $C > 0$ such that for all intervals $I, J \subset \mathbb{R}$, we have

$$\left(\frac{1}{|I||J|}\int_J \int_I w(x,y)\,dx\,dy\right)\left(\frac{1}{|I||J|}\int_I \int_J \frac{1}{w(x,y)}\,dx\,dy\right) \leq C.$$

The above definition of product $\mathcal{A}_2$ weights is equivalent to requiring that w satisfies a uniform $\mathcal{A}_2$ condition in each variable, e.g., see Ref. 59, p. 15. More precisely, $w \in \mathcal{A}_2(\mathbb{T} \times \mathbb{T})$ if and only if for almost every $x \in \mathbb{T}$ and for every interval $J \subset \mathbb{R}$,

$$\left(\frac{1}{|J|}\int_J w(x,y)\,dy\right)\left(\frac{1}{|J|}\int_J \frac{1}{w(x,y)}\,dy\right) \leq C,$$

and likewise for the y variable. For perspective, recall that the product weights in $\mathcal{A}_2(\mathbb{T} \times \mathbb{T})$ differ from classical $\mathcal{A}_2(\mathbb{T}^2)$ weights in that they involve averages over rectangles instead of just squares.

For our purposes, formally define

$$T_{M,N} F = \sum_{m=-M}^{M} \sum_{n=-N}^{N} \langle F, E_{n,k}\rangle E_{n,k},$$

where $E_{n,k}(t,\xi) = e^{2\pi i n t} e^{-2\pi i k \xi}$ is as defined in (2.6).

Theorem 5.6: *Let* $w \in L^2(\mathbb{T} \times \mathbb{T})$ *be non-negative. Then the following statements are equivalent.*

(a) $\sup_{M,N} \|T_{M,N}\|_{2,w} < \infty$.
(b) $w \in \mathcal{A}_2(\mathbb{T} \times \mathbb{T})$.

Proof (b)⇒(a): This direction follows Ref. 58, p. 128. Assume that $w \in \mathcal{A}_2(\mathbb{T} \times \mathbb{T})$. Let

$T_N f=\Sigma_{n=-N}^{N}\langle f,e_n\rangle e_n$ be as defined in (5.2). Then since $w_t=w(t,\cdot)$ and $w^\xi=w(\cdot,\xi)$ satisfy uniform $\mathcal{A}_2$ conditions, we have by Theorem 5.3 that there exists a constant C such that for a.e. t and ξ we have

$$\int_0^1 |T_N f(\xi)|^2 w_t(\xi)d\xi \leqslant C\int_0^1 |f(\xi)|^2 w_t(\xi)d\xi, \quad f\in L^2_{w_t}(\mathbb{T}),$$

$$\int_0^1 |T_N f(t)|^2 w^\xi(t)dt \leqslant C\int_0^1 |f(t)|^2 w^\xi(t)dt, \quad f\in L^2_{w^\xi}(\mathbb{T}).$$

Choose any $F\in L^2_w(\mathbb{T}\times\mathbb{T})$. By Fubini's Theorem, $F_t=F(t,\cdot)\in L^2_{w_t}(\mathbb{T})$ and $F^\xi=F(\cdot,\xi)\in L^2_{w^\xi}(\mathbb{T})$ for a.e. t and ξ. Define

$$T_N^1 F(t,\xi)=T_N F^\xi(t)=\sum_{-N}^{N}\langle F^\xi,e_n\rangle e_n(t), \quad T_M^2 F(t,\xi)=T_M F_t(\xi)=\sum_{-N}^{N}\langle F_t,e_n\rangle e_n(\xi).$$

Then $T_{M,N}F=T_N^1 T_M^2 F$, so

$$\|T_{M,N}F\|_2^2=\int_0^1\int_0^1 |T_N^1 T_M^2 F(t,\xi)|^2 w(t,\xi)dt\,d\xi \leqslant C\int_0^1\int_0^1 |T_M^2 F(t,\xi)|^2 w(t,\xi)dt\,d\xi$$
$$\leqslant C^2\int_0^1\int_0^1 |F(t,\xi)|^2 w(t,\xi)d\xi\,dt=C^2\|F\|_{2,w}^2.$$

(a)$\Rightarrow$(b): This direction is similar to the proof of Theorem 8 in Ref. 54. Suppose that $C=\sup_{M,N}\|T_{M,N}\|_{2,w}<\infty$. Write

$$T_{M,N}F(t,\xi)=\int_0^1\int_0^1 F(u,\eta)D_N(t-u)D_M(\xi-\eta)du\,d\eta,$$

where

$$D_N(t)=\frac{\sin 2\pi\left(N+\frac{1}{2}\right)t}{\sin \pi t}.$$

Choose any rectangle $I\times J$. Without loss of generality, we may assume that $|I|$, $|J|$ are small, e.g., $|I|$, $|J|\leqslant\frac{1}{16}$. Choose any integer N such that $1/(32N)\leqslant|I|\leqslant 1/(16N)$. If t, $u\in I$ then $t-u\in I-I\subset[-1/(8N),1/(8N)]$, so

$$D_N(t-u)\geqslant D_N(1/(8N))\gtrsim N.$$

Similarly, choose M so that $1/(32M)\leqslant|J|\leqslant 1/(16M)$.

Let $H\geqslant 0$ be any non-negative 1-periodic function that is supported in the 1-periodic extension of $I\times J$. Then, for $(t,\xi)\in I\times J$ we have

$$|T_{M,N}(t,\xi)|=\int\int_{I\times J} H(u,\eta)D_N(t-u)D_M(\xi-\eta)du\,d\eta \gtrsim MN\int\int_{I\times J} H(u,\eta)du\,d\eta$$
$$\gtrsim\frac{1}{|I||J|}\int\int_{I\times J} H(u,\eta)du\,d\eta.$$

Consequently,

$$\frac{1}{|I|^2|J|^2}\left(\int\int_{I\times J} H\right)^2 \int\int_{I\times J} w(t,\xi)dt\,d\xi \lesssim \int\int_{I\times J} |T_{M,N}(t,\xi)|w(t,\xi)dt\,d\xi = \|T_{M,N}H\|_{2,w}^2 \lesssim \|H\|_{2,w}^2. \tag{5.4}$$

In particular, if H is the 1-periodic extension of $(1/w)\mathbf{1}_{I\times J}$, then $\|H\|_{2,w}^2 = \int\int_{I\times J}(1/w)$, so

$$\left(\frac{1}{|I||J|}\int\int_{I\times J}\frac{1}{w}\right)\left(\frac{1}{|I||J|}\int\int_{I\times J} w\right)\left(\int\int_{I\times J}\frac{1}{w}\right) \lesssim \left(\int\int_{I\times J}\frac{1}{w}\right).$$

Consequently, if $0<\int\int_{I\times J}(1/w)<\infty$, then we conclude that

$$\left(\frac{1}{|I||J|}\int\int_{I\times J}\frac{1}{w}\right)\left(\frac{1}{|I||J|}\int\int_{I\times J} w\right) \lesssim 1. \tag{5.5}$$

This estimate also follows trivially if $\int\int_{I\times J}(1/w)=0$. So, it only remains to consider the case $\int\int_{I\times J}(1/w)=\infty$. In this case there must be some $F\in L^2(I\times J)$ such that $F/w^{1/2}\notin L^1(I\times J)$. Set $H=|F|/w^{1/2}$. Then $\int\int_{I\times J}H=\infty$, while $\|H\|_{2,w}=\|F\|_2$ is finite. Equation (5.4) therefore implies that $\int\int_{I\times J}w=0$, and hence (5.5) holds trivially in this case as well. Therefore $w\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. □

Corollary 5.7: Let $W\in L^2(\mathbb{T}\times\mathbb{T})$ be nonzero a.e., and define $\widetilde{W}=1/\overline{W}$. For M, $N\geqslant 0$ let $S_{M,N}:L^2(\mathbb{T}\times\mathbb{T})\to L^2(\mathbb{T}\times\mathbb{T})$ be the operator formally defined by

$$S_{M,N}F = \sum_{n=-N}^{N}\sum_{m=-M}^{M}\langle F, E_{n,k}\cdot\widetilde{W}\rangle(E_{n,k}\cdot W), \tag{5.6}$$

and let $\|S_{M,N}\|$ denote its operator norm. Then the following statements are equivalent.

(a) $\sup_{M,N}\|S_{M,N}\|<\infty$.
(b) $|W|^2\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$.

Proof: Using Theorem 5.6, the proof is similar to that of Corollary 5.4. □

It will be convenient to work with the following set of enumerations of $\mathbb{Z}\times\mathbb{Z}$, which are well suited for dealing with rectangular partial sums.

Definition 5.8: Let Λ be the set containing all enumerations $\{(k_j,n_j)\}_{j=1}^{\infty}$ of $\mathbb{Z}\times\mathbb{Z}$ constructed in the following recursive manner.

(a) The initial terms $(k_1,n_1),\ldots,(k_{J_1},n_{J_1})$ are either

$$(0,0),(1,0),(-1,0),\ldots,(A_1,0),(-A_1,0)$$

or

$$(0,0),(0,1),(0,-1),\ldots,(0,B_1),(0,-B_1),$$

for some positive integers A_1 or B_1.

(b) If $\{(k_j,n_j)\}_{j=1}^{J_k}$ has been constructed to be of the product form $\{-A_k,\ldots,A_k\}\times\{-B_k,\ldots,B_k\}$ for some non-negative integers A_k,B_k, then terms are added to either the top and bottom or the left and right sides to obtain either the rectangle

$$\{-A_k,\ldots,A_k\}\times\{-(B_k+1),\ldots,B_k+1\}$$

or

$$\{-(A_k+1),\ldots,A_k+1\}\times\{-B_k,\ldots,B_k\}.$$

For example, terms would first be added to the top ordered as

$$(0,B_k+1),(1,B_k+1),(-1,B_k+1),\ldots,(A_k,B_k+1),(-A_k,B_k+1),$$

and then likewise for the bottom. The left and right sides proceed analogously.

Corollary 5.9: Suppose $W\in L^2(\mathbb{T}\times\mathbb{T})$ *is such that* $\widetilde{W}=1/\overline{W}\in L^2(\mathbb{T}\times\mathbb{T})$. *For each enumeration* $\sigma=\{(k_j,n_j)\}_{j=1}^{\infty}\in\Lambda$, *let* $S_N^\sigma: L^2(\mathbb{T}\times\mathbb{T})\to L^2(\mathbb{T}\times\mathbb{T})$ *be the operator formally defined by*

$$S_N^\sigma F=\sum_{j=1}^{N}\langle F,E_{n_j,k_j}\cdot\widetilde{W}\rangle(E_{n_j,k_j}\cdot W),$$

and let $\|S_N^\sigma\|$ *denote its operator norm. Then the following statements are equivalent.*

(a) $\sup_{N,\sigma}\|S_N^\sigma\|<\infty$.
(b) $|W|^2\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$.

Proof (a)⇒(b): Assume that $\sup_{N,\sigma}\|S_N^\sigma\|<\infty$. By the definition of Λ, it follows that $\sup_{M,N}\|S_{M,N}\|<\infty$, with $S_{M,N}$ as in (5.6). By Corollary 5.7 we conclude that $|W|^2\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$.

(b)⇒(a): Assume that $|W|^2\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. Then, by definition, we have that $A=\|W\|_2\|\widetilde{W}\|_2<\infty$, and by Corollary 5.7 we have that $C=\sup_{M,N}\|S_{M,N}\|<\infty$.

Choose any enumeration $\sigma\in\Lambda$ and any positive integer N. Let M_N be the largest integer $M_N<N$ for which $S_{M_N}^\sigma F=S_{J,K}F$ for some integers J, K. Note that

$$\|S_N^\sigma F\|_2\leq\|S_{J,K}F\|_2+\|(S_N^\sigma-S_{M_N}^\sigma)F\|_2\leq C\|F\|_2+\|(S_N^\sigma-S_{M_N}^\sigma)F\|_2.$$

Thus we must estimate the norm of

$$(S_N^\sigma-S_{M_N}^\sigma)F=\sum_{j=M_N+1}^{N}\langle F,E_{n_j,k_j}\cdot\widetilde{W}\rangle(E_{n_j,k_j}\cdot W).\tag{5.7}$$

This series corresponds to terms that have been added to a rectangle according to the algorithm given in Definition 5.8. For example, if terms have been added to the top of the rectangle, then (5.7) has one of the following two forms:

$$\sum_{n=-L}^{L}\langle F,E_{n,K+1}\cdot\widetilde{W}\rangle(E_{n,K+1}\cdot W)\quad\text{or}\quad\sum_{n=-L}^{L+1}\langle F,E_{n,K+1}\cdot\widetilde{W}\rangle(E_{n,K+1}\cdot W).\tag{5.8}$$

The first sum is bounded by

$$\left\|\sum_{n=-L}^{L}\langle F,E_{n,K+1}\cdot\widetilde{W}\rangle(E_{n,K+1}\cdot W)\right\|_2=\left\|\sum_{n=-L}^{L}\langle F\cdot E_{0,-K-1},E_{n,0}\cdot\widetilde{W}\rangle(E_{n,0}\cdot W)\right\|_2=\|S_{L,0}(F\cdot E_{0,-K-1})\|_2$$
$$\leq C\|F\cdot E_{0,-K-1}\|_2=C\|F\|_2.\tag{5.9}$$

The second sum in (5.8) is bounded by

$$\left\|\sum_{n=-L}^{L+1}\langle F,E_{n,K+1}\cdot\widetilde{W}\rangle(E_{n,K+1}\cdot W)\right\|_2\leq\left\|\sum_{n=-L}^{L}\langle F,E_{n,K+1}\cdot\widetilde{W}\rangle(E_{n,K+1}\cdot W)\right\|_2+|\langle F,E_{L+1,K+1}\cdot\widetilde{W}\rangle|$$
$$\times\|E_{L+1,K+1}\cdot W\|_2\leq C\|F\|_2+A\|F\|_2.\tag{5.10}$$

Substituting each of (5.9) and (5.10) into (5.7), we conclude that for this case we have $\|S_N^\sigma F\|_2\leq(2C+A)\|F\|_2$. The same estimate applies if terms have been added only to the bottom, left, or right of the rectangle. If terms have been added either to both the top and bottom, or to both the left and right sides of the rectangle, then we end with the estimate $\|S_N^\sigma F\|_2\leq(3C+2A)\|F\|_2$. In any case, we conclude that $\sup_{N,\sigma}\|S_N^\sigma\|\leq(3C+2A)<\infty$. □

C. A Zak transform characterization of Gabor Schauder bases

Using the machinery that we have developed in the previous sections, we can now give a simple Zak transform characterization of lattice Gabor Schauder bases for $L^2(\mathbb{R})$. We then construct examples of Gabor Schauder bases that have interesting properties.

Note that while Z_g has a natural quasiperiodic extension from $[0,1)^2$ to $\mathbb{R}^2$, the definition of $\mathcal{A}_2$ weight only depends on the absolute value of the weight, and $|Zg|$ is 1-periodic in each variable.

Theorem 5.10: *Let $g \in L^2(\mathbb{R})$ be given. Then the following statements are equivalent.*

(a) *The Gabor system $\mathcal{G}(g,1,1)$ is a Schauder basis for $L^2(\mathbb{R})$ with respect to every enumeration $\sigma=\{(k_j,n_j)\}_{j=1}^{\infty} \in \Lambda$. Further, if C_σ is the basis constant associated to the enumeration σ, then $\sup_{\sigma\in\Lambda} C_\sigma < \infty$.*
(b) $|Zg|^2 \in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$.

Proof (a)$\Rightarrow$(b): Suppose that statement (a) holds. Then by Lemma 5.1 we have that $1/Zg \in L^2(\mathbb{T}\times\mathbb{T})$. Further, by hypothesis, $\sup_{N,\sigma}\|S_N^\sigma\| \leqslant \sup_{\sigma\in\Lambda} C_\sigma < \infty$, so Corollary 5.9 implies that $|Zg|^2 \in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$.

(b)$\Rightarrow$(a): Assume $|Zg|^2 \in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. Then, by definition of $\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$, we have that $1/Zg \in L^2(\mathbb{T}\times\mathbb{T})$. Further, we have by Corollary 5.9 that $\sup_{N,\sigma}\|S_N^\sigma\| < \infty$. Lemma 5.1 therefore implies that $\mathcal{G}(g,1,1)$ is a Schauder basis with respect to each $\sigma \in \Lambda$. □

While Theorem 5.10 implies that if $|Zg|^2 \in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$ then $\mathcal{G}(g,1,1)$ is a Schauder basis with respect to every enumeration $\sigma \in \Lambda$, this does not imply that it is a Schauder basis with respect to every possible enumeration of $\mathbb{Z}\times\mathbb{Z}$, since that would imply that $\mathcal{G}(g,1,1)$ is a Riesz basis. In fact, by Theorem 2.8, the Riesz bases correspond to the subclass of weights in $\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$ that are essentially bounded, i.e., bounded away from zero and infinity. The following example is inspired by Babenko's example from Ref. 60; cf. Ref. 36, Example 11.2, pp. 351–354, and gives examples of Gabor Schauder bases that are not Riesz bases.

Example 5.11. Fix $0<\alpha<1/2$. Assume that $g=g_\alpha \in L^2(\mathbb{R})$ satisfies the following:

(a) g is real-valued;
(b) $\mathrm{supp}(g) \subseteq [0,1]$;
(c) g is infinitely differentiable on every subinterval $(\delta, 1-\delta)$, $0<\delta<1/2$;
(d) $g(t)=t^\alpha$ on $[0,1/4]$;
(e) $g(t)=(1-t)^\alpha$ on $[3/4,1]$;
(f) $g(t-1/2)$ is even;
(g) $g(t) \geqslant C>0$ for $1/4<t<3/4$.

Since g is supported in [0,1], a direct calculation shows that $|Zg(t,\xi)|^2=|g(t)|^2 \in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. Therefore, Theorem 5.10 implies that $\mathcal{G}(g,1,1)$ is a Schauder basis for $L^2(\mathbb{R})$ with respect to every enumeration $\sigma \in \Lambda$. However, since $|Zg|$ is not bounded away from zero, Theorem 2.8 implies that $\mathcal{G}(g,1,1)$ is not a Riesz basis for $L^2(\mathbb{R})$.

We make some additional remarks concerning the windows constructed in Example 5.11. Note that since Zg is bounded, $\mathcal{G}(g,1,1)$ is a Bessel sequence, i.e., it has an upper frame bound. Since g is supported in [0,1], the dual window is easily seen to be the function that is $\widetilde{g}=1/\overline{g}$ on [0,1] and zero elsewhere. The dual basis $\mathcal{G}(\widetilde{g},1,1)$ possesses a lower frame bound but not an upper frame bound (compare Theorem 7.1).

Theorem 5.10 allows one to generate other interesting examples. Building on Example 5.11, the following example provides a Gabor Schauder basis that has neither an upper frame bound nor a lower frame bound. In other words, e.g., Ref. 36, this Gabor Schauder basis is neither Besselian nor Hilbertian.

Example 5.12: Fix $0<\alpha<1/2$ and let $g=g_\alpha$ be the function from Example 5.11. Define

$$f(t)=\begin{cases} g(2t), & \text{if } 0\leqslant t\leqslant 1/2,\\ \dfrac{1}{g(2t-1)}, & \text{if } 1/2<t<1,\\ 0, & \text{if } t\notin[0,1). \end{cases}$$

As in Example 5.11, we have that $Zf(t,\xi)=f(t)$ for $(t,\xi)\in Q$. Further, Zf, $1/Zf\in L^2(\mathbb{R})$, so we at least have that $\mathcal{G}(f,1,1)$ is complete and minimal. However, one can check that $|Zf|^2\in \mathcal{A}_2(\mathbb{T}\times\mathbb{T})$, so, in fact, we have that $\mathcal{G}(f,1,1)$ is a Schauder basis with respect to every enumeration $\sigma\in\Lambda$. However, since $|Zg|$ is not bounded away from zero or infinity, we conclude that $\mathcal{G}(f,1,1)$ has neither an upper frame nor a lower frame bound.

For perspective, note that $f\notin M^1(\mathbb{R})$ since any Gabor system generated by a window in $M^1(\mathbb{R})$ is a Bessel sequence, Ref. 1, Theorem 12.2.3. By contrast, we shall later prove (see Theorem 6.1) that the example g from Example 5.11 does belong to $M^1(\mathbb{R})$.

Example 5.13: The two preceding examples were both compactly supported. However, we can easily create noncompactly supported examples. For example, since the Fourier transform is unitary, if g is one of the functions constructed in Example 5.11 or 5.12, then $\mathcal{G}(\hat{g},1,1)$ is a Gabor Schauder basis with respect to every enumeration in Λ, but it is not a Riesz basis, and $\hat{g}$ is not compactly supported.

We can also work directly in the Zak transform domain. Again, let g be any function constructed in Example 5.11 or 5.12, and let h be any function supported in $[0,1]$ such that $|h|^2\in\mathcal{A}_2(\mathbb{T})$. Then $G(t,\xi)=g(t)h(\xi)$ is such that $|G|^2\in\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. Hence $f=Z^{-1}G\in L^2(\mathbb{R})$, and, for every enumeration in Λ, $\mathcal{G}(f,1,1)$ is a Gabor Schauder basis that is not a Riesz basis. By definition of the Zak transform, if h is not a trigonometric polynomial, then f cannot be compactly supported.

In general, while every Schauder basis is complete and minimal, the converse need not be true. If $\varphi(t)=e^{-t^2}$, then we know that a proper subset of $\mathcal{G}(\varphi,1,1)$ is complete and minimal but is not a Schauder basis. The following example shows that it is possible for a lattice Gabor system $\mathcal{G}(g,1,1)$ (not just a subset) to be complete and minimal yet not form a Schauder basis for $L^2(\mathbb{R})$.

Example 5.14: For $n=1,2,3,\ldots$, set $A_n=(3/2)^{n/2}$ and $B_n=(2/3)^{n/2}$. Define disjoint intervals,

$$L_n=[1-2^{-n+1},1-2^{-n}-2^{-n-1}],\quad R_n=[1-2^{-n}-2^{-n-1},1-2^{-n}],$$

and set $I_n=L_n\cup R_n$. Then $|I_n|=2^{-n}=2|R_n|=2|L_n|$ and $\cup_{n=1}^{\infty}I_n=[0,1)$. For $t\in\mathbb{R}$, let g be the following non-negative function supported in $[0,1]$:

$$g=\sum_{n=1}^{\infty}(A_n\mathbf{1}_{L_n}+B_n\mathbf{1}_{R_n}).$$

We compute that

$$\int_0^1|g(t)|^2\,dt=\frac{1}{2}\sum_{n=1}^{\infty}|I_n|(A_n^2+B_n^2)=\frac{1}{2}\sum_{n=1}^{\infty}2^{-n}\left(\left(\frac{3}{2}\right)^n+\left(\frac{2}{3}\right)^n\right)<\infty,$$

and

$$\int_0^1\frac{1}{|g(t)|^2}dt=\frac{1}{2}\sum_{n=1}^{\infty}|I_n|\left(\frac{1}{A_n^2}+\frac{1}{B_n^2}\right)=\int_0^1|g(t)|^2\,dt<\infty.$$

Further, since g is supported in $[0,1]$, we have that $|Zg(t,\xi)|=g(t)$ for $(t,\xi)\in Q$. Therefore Zg, $1/Zg\in L^2(Q)$, so by Theorem 2.8, $\mathcal{G}(g,1,1)$ is complete and minimal in $L^2(\mathbb{R})$.

Next, note that

$$\left(\frac{1}{|I_n|}\int_{I_n}|g(t)|^2\,dt\right)\left(\frac{1}{|I_n|}\int_{I_n}\frac{1}{|g(t)|^2}dt\right)=\frac{1}{4}(A_n^2+B_n^2)\left(\frac{1}{A_n^2}+\frac{1}{B_n^2}\right)=\frac{1}{4}\left(2+\left(\frac{9}{4}\right)^n+\left(\frac{4}{9}\right)^n\right).$$

Letting $n\to\infty$, we see that $|Zg|^2\notin\mathcal{A}_2(\mathbb{T}\times\mathbb{T})$. Therefore, by Theorem 5.10 there exists at least one enumeration $\sigma\in\Lambda$ with respect to which the Gabor system $\mathcal{G}(g,1,1)$ is not a Schauder basis for $L^2(\mathbb{R})$.

VI. COUNTEREXAMPLES TO THE BALIAN-LOW THEOREMS FOR GABOR SCHAUDER BASES

In this section we investigate the extent to which the variants of the Balian-Low Theorem hold in the setting of Schauder bases. It was conjectured in Ref. 31 that if hypothesis (a) of Theorem 3.2 holds, then the conclusion of that theorem remains true if the words "Riesz basis" are replaced by "Schauder basis." In other words, it was conjectured that there do not exist any Gabor Schauder bases whose window function belongs to $M^1(\mathbb{R})$. We will provide counterexamples to that conjecture in this section. Moreover, our counterexamples apply to each of the four hypotheses appearing in Theorem 3.2.

Theorem 6.1: *The conclusion of Theorem 3.2 is false if the words* "Riesz basis" *are replaced by* "Schauder basis."

Specifically, if $g=g_\alpha$ *with* $0<\alpha<1/2$ *is one of the functions constructed in Example 5.11, then* $\mathcal{G}(g,1,1)$ *is a Schauder basis for* $L^2(\mathbb{R})$ *with respect to any enumeration* $\sigma\in\Lambda$, *but it is not a Riesz basis for* $L^2(\mathbb{R})$. *Further, the following statements hold.*

(a) $g\in M^1(\mathbb{R})$.
(b) $g,\ \hat{g}\in W(\mathcal{C},\ell^1)$.
(c) *If* $1<q<2<p<\infty$, $1/p+1/q=1$, $0<\varepsilon<2-q$, *and* $(q+\varepsilon-1)/2<\alpha$, *then*

$$\int|t|^{p+\varepsilon}|g(t)|^2\,dt<\infty\quad\text{and}\quad\int|\xi|^{q+\varepsilon}|\hat{g}(\xi)|^2\,d\xi<\infty.$$

(d) $\sup_{N>0}\int|t|^N|g(t)|^2dt<\infty$ *and* $\int|\xi||\hat{g}(\xi)|^2\,d\xi<\infty$.

Proof: (c) Assume that p, q, ε, and α satisfy the given conditions, and define

$$I_{p+\varepsilon}(g)=\int|t|^{p+\varepsilon}|g(t)|^2\,dt\quad\text{and}\quad I_{q+\varepsilon}(\hat{g})=\int|\xi|^{q+\varepsilon}|\hat{g}(\xi)|^2\,d\xi.\tag{6.1}$$

Since g is continuous and compactly supported, we certainly have that $I_{p+\varepsilon}(g)<\infty$. Therefore, we just have to show that $I_{q+\varepsilon}(\hat{g})<\infty$.

Let φ be a $C^\infty(\mathbb{R})$ function that equals 1 on $[-2\nu,2\nu]$ and is supported in $[-3\nu,3\nu]$ for some sufficiently small fixed $\nu>0$. Let ψ be a $C^\infty(\mathbb{R})$ function that equals 1 on $[3\nu,1-3\nu]$ and is compactly supported in $[2\nu,1-2\nu]$. Finally, suppose that the partition of unity property $\varphi(t)+\psi(t)+\varphi(t-1)=1$ holds for all $t\in[0,1]$. Since $\psi(t)g(t)$ is $C^\infty(\mathbb{R})$ and is compactly supported, it suffices to show that $I_{q+\varepsilon}(\hat{h}_1)<\infty$ and that $I_{q+\varepsilon}(\hat{h}_2)<\infty$, where $h_1(t)=\varphi(t)g(t)$ and $h_2(t)=\varphi(t-1)g(t)$. Both estimates are similar, so we only prove the estimate for $h=h_1$.

To estimate $I_q(h)$, we use Ref. 61, Proposition 4, p. 139, which implies that for any $0<s<1$ there exists $0<C_s$ such that

$$\int|\xi|^{2s}|\hat{h}(\xi)|^2\,d\xi=C_s\int\int\frac{|h(x+t)-h(x)|^2}{|t|^{1+2s}}dx\,dt.$$

Begin by noting that

$$\int_{\mathbb{R}\setminus[-\nu,\nu]} \int \frac{|h(x+t)-h(x)|^2}{|t|^{1+q+\varepsilon}} dx\, dt \lesssim \int_{\mathbb{R}\setminus[-\nu,\nu]} \frac{\|h\|_2^2}{|t|^{1+q+\varepsilon}} dt < \infty.$$

It remains to estimate the analogous two integrals over the domains $[0,\nu]\times\mathbb{R}$ and $[-\nu,0]\times\mathbb{R}$. Since both proceed similarly, we shall only show the estimates for the first of these, which we, in turn, break up into the following integrals:

$$J_1 = \int_0^\nu \int_{-\infty}^{-t}, \quad J_2 = \int_0^\nu \int_{-t}^{t}, \quad J_3 = \int_0^\nu \int_t^\nu, \quad J_4 = \int_0^\nu \int_\nu^{3\nu}, \quad J_5 = \int_0^\nu \int_{3\nu}^\infty.$$

Since h is supported on $[0,3\nu]$, it follows that $J_1=J_5=0$.

Note that since $q+\varepsilon-2\alpha<1$, we have

$$J_2 \lesssim \int_0^\nu \frac{1}{t^{q+\varepsilon+1}} \int_0^{2t} |h(x)|^2\, dx\, dt = \int_0^\nu \int_0^{2t} \frac{x^{2\alpha}}{t^{q+\varepsilon+1}} dx\, dt \lesssim \int_0^\nu \frac{t^{2\alpha+1}}{t^{q+\varepsilon+1}} dt < \infty.$$

Next, since $|(x+t)^\alpha - x^\alpha| \lesssim \alpha t x^{\alpha-1}$ for all $0<x$, t, we have that

$$J_3 \lesssim \int_0^\nu \int_t^\nu \frac{t^2 x^{2\alpha-2}}{t^{q+\varepsilon+1}} dx\, dt \lesssim \int_0^\nu \frac{t^{2\alpha+1}}{t^{q+\varepsilon+1}} dt < \infty.$$

Finally, the smoothness properties of h on $[\nu,\infty)$ and the Mean Value Theorem imply that if $x+t$ and x are both greater than ν then $|h(x+t)-h(x)| \lesssim |t|$. Therefore, since $q+\varepsilon<2$,

$$J_4 \lesssim \int_0^\nu \int_\nu^{3\nu} \frac{t^2}{|t|^{q+\varepsilon+1}} dx\, dt = \int_0^\nu \frac{1}{t^{q+\varepsilon-1}} dt < \infty,$$

which completes the proof.

(d) The estimates in the proof of part (c) together with the fact that g is compactly supported in $[0,1]$ yields the result.

(a) This follows from part (c) and the following modulation space embedding of Gröchenig:[52] If $1/p+1/q=1$, $1<p,q,<\infty$, and $0<\varepsilon$, then

$$\|g\|_{M^1} \lesssim \left(\int |t|^{p+\varepsilon} |g(t)|^2\, dt \right)^{1/2} + \left(\int |\xi|^{q+\varepsilon} |\hat{g}(\xi)|^2\, d\xi \right)^{1/2}.$$

(b) By part (a), we have $g \in M^1(\mathbb{R}) \subset W(\mathcal{C},\ell^1)$. Since $M^1(\mathbb{R})$ is invariant under the Fourier transform, we also have $\hat{g} \in M^1(\mathbb{R}) \subset W(\mathcal{C},\ell^1)$.

Note that the integrals in (6.1) are also finite when $\varepsilon=0$.

VII. WEAK BLT's FOR GABOR SCHAUDER BASES

We close by proving some new Weak BLTs for exact Gabor systems, including Gabor Schauder bases, in particular. Parts (a) and (b) of the following theorem can be, respectively, viewed as weak versions of the M^1 BLT and Amalgam BLT in the setting of exact Gabor systems.

Theorem 7.1 (weak BLTs for exact Gabor systems): *Let $g \in L^2(\mathbb{R})$ be such that $\mathcal{G}(g,1,1)$ is exact in $L^2(\mathbb{R})$ and let $\widetilde{g}=Z^{-1}(1/\overline{Zg})$ be the dual window.*

(a) *If $g \in M^1(\mathbb{R})$ then $\widetilde{g} \notin M^1(\mathbb{R})$.*
(b) *If $g \in W(\mathcal{C},\ell^1)$ then $\widetilde{g} \notin W(\mathcal{C},\ell^1)$.*
(c) *If $\mathcal{G}(g,1,1)$ is a Bessel sequence, then $\mathcal{G}(\widetilde{g},1,1)$ is Bessel if and only if $\mathcal{G}(g,1,1)$ is a Riesz basis.*

Proof: (b) If $g \in W(\mathcal{C},\ell^1)$, then Zg has a continuous extension to all of $\mathbb{R}^2$ by Ref. 19, Theorem 3.2. But the quasiperiodicity of Zg then forces Zg to have a zero.[1] Hence $Z\widetilde{g}=1/\overline{Zg}$ is not continuous, so $\widetilde{g} \notin W(\mathcal{C},\ell^1)$.

(a) This follows immediately from part (b) and the fact that $M^1(\mathbb{R}) \subset W(\mathcal{C}, \ell^1)$.

(c) This follows from Theorem 2.5(e). □

Remark 7.2: In Ref. 18, Daubechies and Janssen proved that (in equivalent modulation space terminology) if $g \in M^2_2(\mathbb{R})$, then $\mathcal{G}(g,1,1)$ is not exact. Hence, if $\mathcal{G}(g,1,1)$ is to be a Schauder basis and $g \in M^2_s(\mathbb{R})$, then we must have $0<s<2$. For $1<s<2$ we will have $g \in M^2_s(\mathbb{R}) \subset M^1(\mathbb{R})$, and hence $\widetilde{g} \notin M^1(\mathbb{R})$.

In particular, the function $g=g_\alpha$ constructed in Example 5.11 can be shown to lie in $M^2_s(\mathbb{R})$ for $0<s<1$. While this does not imply that $g \in M^1(\mathbb{R})$, the stronger embeddings of Gröchenig[52] imply that $g \in M^1(\mathbb{R})$.

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Noncommutative geometry, topology, and the standard model vacuum

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As a ramification of a motivational discussion for previous joint work, in which equations of motion for the finite spectral action of the standard model were derived, we provide a new analysis of the results of the calculations therein, switching from the perspective of spectral triple to that of Fredholm module and thus from the analogy with Riemannian geometry to the premetrical structure of the noncommutative geometry. Using a suggested noncommutative version of Morse theory together with algebraic K theory to analyze the vacuum solutions, the first two summands of the algebra for the finite triple of the standard model arise up to Morita equivalence. We also demonstrate a new vacuum solution whose features are compatible with the physical mass matrix. © *2006 American Institute of Physics.*
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I. INTRODUCTION

This article is a continuation of previous work joint with Barrett and Dawe Martins[1] in which field equations were calculated for the full set of internal space metric fluctuations allowed by the noncommutative geometry axioms in the spectral triple formulation of the standard model. We begin with a development of the discussion begun in the previous work and then provide a new analysis of the results of the calculations therein from the perspective of Fredholm module instead of spectral triple. Studying these Fredholm modules using algebraic K theory and K homology leads to a suggested noncommutative version of Morse theory—a well-known tool for studying the topology of manifolds—which is applied to the finite spectral action.

As this work ramifies from Ref. 1, for this article to make sense it is necessary to give an explanation of the key concepts of the previous work before the main analysis in this article can begin. Furthermore, discussion given in the previous work is brief and so one of the purposes of this article is to explain how it highlights an open question about the noncommutative framework. This explanation leads into a detailed introduction to the main analysis given at the beginning of the main section, entitled "Fredholm module solutions."

II. CONTEXT

More details about the tools and formalisms referred to below are provided in Sec. III.

The context of Ref. 1 and this its "second chapter," is on the spectral action principle by Connes and Chamseddine,[2] where the standard model is formulated with a product (whose image is called the total space) of two spectral triples—one that represents the Euclidean space-time manifold and the other the zero-dimensional internal space of particle charges. The space-time coordinate functions remain commutative but the internal space is a noncommutative "manifold." The spectral action principle is an important step towards the unification of gravity with particle physics; the Einstein–Hilbert action plus Weinberg–Glashow–Salam theory all result from a cal-

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culation of the eigenvalues of the Dirac operator on the total space and since the Dirac operator encodes the metric, the spectral action principle is a purely geometrical theory.

The scope of this study involves irreducible finite real spectral triples over the complex numbers; irreducible in the sense that there is no proper invariant subspace of the Hilbert space for which the triple restricted to that space is itself a (nondegenerate) triple.[3] For example, the standard model finite triple of three fermion families is reducible whereas the one family triple is irreducible. By finite, we mean a finite dimensional Hilbert space over a semisimple algebra. A caveat is that calculations carried out in this and the previous article apply only in the context of these zero-dimensional geometries with Euclidean signature. This means that at present, no direct physical inference can be made.

Currently concerned with the internal space triple by itself and not the full standard model tensor product triple, we consider a single point of space time: we remove all terms that do not depend solely on the fluctuations of the internal space Dirac operator D_F. The finite spectral action corresponds to the Higgs potential: $\mathrm{Tr}(D_F^4 - 2D_F^2)$.

The extra Einstein's equations for internal space were calculated by Schücker *et al.*[3,17] (for one generation of elementary fermions) by minimizing the Higgs potential with respect to the "fluctuated Dirac operator."[4] They found that the standard model Dirac operator was a solution. The construction of the fluctuated Dirac operator is carried out by beginning with a choice of initial Dirac operator (to correspond to the standard model fermion mass matrix) to satisfy the noncommutative geometry axioms, and in analogy with the equivalence principle, fluctuating it with the standard model's internal space algebra of coordinates. In this way, the Higgs force is treated as an internal space version of gravity.

III. BACKGROUND

A. Standard model finite spectral triple

A spectral triple $(\mathcal{A},\mathcal{H},\mathcal{D})$ provides the analog of a Riemannian (note: Riemannian not pseudo-Riemannian; applications are to Euclidean not Lorentzian space times) spin manifold to noncommutative geometry.[4,5] It consists of a involutive, not necessarily commutative algebra $\mathcal{A}$, a Hilbert space $\mathcal{H}$: a finitely generated projective module, on which the algebra is represented, and a Dirac operator $\mathcal{D}$ that gives a notion of distance, and from which is built a differential algebra.

The geometry of any closed (even dimensional) Riemannian spin manifold can be fully described by a (real and even) spectral triple (according to the reconstruction theorem) and a noncommutative geometry is essentially the same structure but with the generalization that the algebra of coordinates are allowed to be noncommuting.[6,7]

For the standard model the internal Hilbert space is: $\mathcal{H}=\mathcal{H}_L\oplus\mathcal{H}_R\oplus\mathcal{H}_L^c\oplus\mathcal{H}_R^c$, where

$$\mathcal{H}_L = (\mathbb{C}^2\otimes\mathbb{C}^N\otimes\mathbb{C}^3)\oplus(\mathbb{C}^2\otimes\mathbb{C}^N),$$

$$\mathcal{H}_R = ((\mathbb{C}\oplus\mathbb{C})\otimes\mathbb{C}^N\otimes\mathbb{C}^3)\oplus(\mathbb{C}\otimes\mathbb{C}^N)$$

and whose basis is labeled by the elementary fermions and their antiparticles.[8] The symbol c is used to indicate the section represented by the antiparticles. The even triple has the $\mathbb{Z}$/two-grading operator χ, the chirality (eigenvalues $+1$ or -1). In either case of $\mathcal{H}_L$ and $\mathcal{H}_R$, the first direct summand is the quarks and the second, the leptons. N stands for the number of generations. For example, the left-handed up and down quarks form an isospin doublet and their right-handed counterparts are singlets and there are three colors for quarks and none for leptons. The charges on the particles are identified by the faithful representation of the algebra on the Hilbert space.

In the definition of $\mathcal{H}$ above we see a second $\mathbb{Z}$/two-grading that splits the Hilbert space into two orthogonal subspaces for particles and antiparticles: $\mathcal{H}^+\oplus\mathcal{H}^-$ or $\mathcal{H}\oplus\mathcal{H}^c$.[9] This is called S^o reality and is not an axiom but applies to the standard model as it excludes Majorana masses. The S^o reality grading operator ϵ satisfies: $[\mathcal{D},\epsilon]=0$, $[J,\epsilon]_+=0$, $\epsilon^*=\epsilon$, $\epsilon^2=1$. (Compare with reality operator J explanation below.)

Let D_F denote the Dirac operator that acts on the finite dimensional internal Hilbert space; it is the internal space counterpart of the Dirac operator that acts on space time. D_F is a matrix whose parameters are given by the Higgs field, Cabbibo–Kobayashi–Maskawa family mixing matrix and the Yukawa couplings.[2] In other words, it provides the fermion mass matrix.

The *choice* made for D_F in order that the spectral action principle reproduces the standard model is

$$D_F = \begin{pmatrix} 0 & M^* & 0 & 0 \\ M & 0 & 0 & 0 \\ 0 & 0 & 0 & M^T \\ 0 & 0 & \overline{M} & 0 \end{pmatrix} \tag{1}$$

with basis left, right, then antiparticles left and right. $M = M_Q \otimes 1_3 \oplus M_L$, and

$$M_Q = \begin{pmatrix} k_u \phi_1 & k_d \phi_2 \\ -k_u \bar{\phi}_2 & k_d \bar{\phi}_1 \end{pmatrix},$$

$$M_L = \begin{pmatrix} k_e \phi_1 & k_e \phi_2 \\ 0 & 0 \end{pmatrix}.$$

(An extra row is added to M_L here so that the matrices are square, this is not normally done and relative to other literature, the labeling M is swapped with M^*.) with

$$k_u = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_c & 0 \\ 0 & 0 & m_t \end{pmatrix} \quad k_d = V_{\mathrm{CKM}} \begin{pmatrix} m_d & 0 & 0 \\ 0 & m_s & 0 \\ 0 & 0 & m_b \end{pmatrix}$$

$$k_e = \begin{pmatrix} m_e & 0 & 0 \\ 0 & m_\mu & 0 \\ 0 & 0 & m_\tau \end{pmatrix}.$$

T denotes transposition, * denotes hermitian conjugation, the bar denotes complex conjugation, m_x are the Yukawa couplings of the elementary fermions, V_{CKM} is the Cabibbo–Kobayashi–Maskawa generation mixing matrix. $(\phi_1, \phi_2)^T$ is the (Higgs) scalar doublet.

The finite spectral action corresponds to the Higgs potential: $\mathrm{Tr}(D_F^4 - 2D_F^2)$. If the $\mathrm{Tr}(I)$ term is included,[2] which obviously does not affect the equations of motion, then the action can be written $\mathrm{Tr}(MM^* - I)^2$.

The spectral triple algebra $\mathcal{A}$ is a subalgebra of the bounded operators on the Hilbert space, it is a *-algebra not necessarily a C^*-algebra but its norm closure in the Hilbert space is a C^*-algebra. The standard model tensor product algebra is "almost commutative"

$$\mathcal{A} = C^\infty(M) \otimes (\mathbb{H} \oplus \mathbb{C} \oplus M_3(\mathbb{C})), \tag{2}$$

where the first factor is the (commutative) algebra of function on (Euclidean) space time and the second factor is the internal space (real) algebra of particle charges.

The (faithful) representation ρ of the finite space algebra has been worked out by Connes to correspond to the particle charges, see Ref. 2. The first and second summand acts on the particles while the third summand acts on the antiparticles. The basis is given by the Hilbert space above

$$\rho := \begin{pmatrix} \rho_L & 0 & 0 & 0 \\ 0 & \rho_R & 0 & 0 \\ 0 & 0 & \rho^c & 0 \\ 0 & 0 & 0 & \rho^c \end{pmatrix}. \tag{3}$$

B. Real structure and Poincaré duality

Instead of splitting $\mathbb{C}$ into two copies of $\mathbb{R}$ as its name suggests, J forms two subspaces of the Hilbert space (not orthogonal as in S^o reality), which are interpreted as fermions and antifermions, in which case J is given by the composition of the charge conjugation operator with complex conjugation. The mathematical purpose of the J operator entering the axioms is to provide Connes' notion of a "noncommutative manifold." That is, by turning the Hilbert space into a bimodule, the "real" structure (Ref. 9) allows the generalization of Poincaré duality to the spectral triple; $a \in \mathcal{A}$ and the opposite algebra, $b^o \in \mathcal{A}^o$ (or $\mathcal{A}^{\mathrm{op}}$) where a acts on the left of $\mathcal{H}$ and b^o acts on the right

$$[a,b^o] = 0, \quad b^o = Jb^*J^{-1} \quad \forall\, a,b \in \mathcal{A}.$$

The opposite algebra provides the "dual" to the algebra. The pairing of the K theories of these two algebras provides a noncommutative geometric version of Poincaré duality. This structure is also important in the notion of first order differential operator in noncommutative geometry. The tangent space over any manifold is real, and the reality structure gives rise to the real-K theory of the enveloping algebra $\mathcal{A} \otimes \mathcal{A}^o$.

The action of J on $\mathcal{H}$ as given by the composition of charge conjugation and complex conjugation

$$J\begin{pmatrix} \psi_1 \\ \bar{\psi}_2 \end{pmatrix} = \begin{pmatrix} \psi_2 \\ \bar{\psi}_1 \end{pmatrix} \quad (\psi_1, \bar{\psi}_2) \in \mathcal{H} \oplus \mathcal{H}^c,$$

where the bar indicates complex conjugation.

C. *K* theory

K theory is a generalized cohomology theory. Topological K theory is the topological invariant that classifies the vector bundles over a given field, over a compact topological space X up to stable equivalence. It is an Abelian group $K^0(X)$ generated by the isomorphism classes of vector bundles over a given field. Addition is given by $[E]+[F]=[E \oplus F]$ where $[E]$ and $[F]$ are isomorphism classes of vector bundles E and F. Every element of the group is a difference: $[E]-[F]$. The Serre–Swan theorem provides the identification of topological with algebraic K theory. That is, $K^0(X)$ is isomorphic to the algebraic K-theory group $K_0(C^0(X))$. The group $K_0(A)$ for a C^*-algebra A is generated by the projections (self-adjoint idempotents) in A. These projections form an Abelian semigroup rather than a group, but the Grothendieck construction turns them into an Abelian group using an equivalence relation, which is very much analogous to the process of constructing the integers from the natural numbers.[10,11]

Some rules for K theory include $K_0(M_n(A))=K_0(A)$ (Morita equivalent algebras have the same K theory), $K_0(A \oplus B)=K_0(A) \oplus K_0(B)$, where A and B are C^*-algebras.

D. Fredholm modules and *K* homology

The Fredholm module is the "premetric" structure that is used to define the noncommutative calculus.[5] A spectral triple can be thought of as an unbounded (unless the Hilbert space is finite dimensional) Fredholm module with Dirac operator providing a notion of distance.

1. Definition: Fredholm operator

A Fredholm operator is a bounded operator on a Hilbert space whose kernel and cokernel are finite dimensional and is invertible modulo compact operators.

2. Definition: Fredholm module

Let A be an involutive algebra (over $\mathbb{C}$). Then a Fredholm module (H,F) over A is given by: (1) an involutive representative ρ of A in a Hilbert space H and (2) a Fredholm operator $F=F^*$, $F^2=I$ on H such that $[F,\rho(a)]$ is a compact operator for any $a\in A$. (After some trivial changes that we do not need to go into details of here, Connes ensures that the Fredholm module makes sense in finite dimensions.[5])

If there is a $\mathbb{Z}/2$ grading χ, such that $\chi=\chi^*$, $\chi^2=1$ of the Hilbert space such that (a) $[\chi,\rho]=0\ \forall a\in A$ and (b) the anticommutator $[\chi,F]_+=0$ then the Fredholm is *even*.

There is a natural assignment of a Fredholm module to a spectral triple. To be precise, an observation given in Ref. 5 is that there is a canonical assignment of a Fredholm module to a spectral triple given by $F=\text{sign}(\mathcal{D})$ (that is, $\mathcal{D}=F|\mathcal{D}|$) outside the kernel of $\mathcal{D}$. (On the finite dimensional kernel of $\mathcal{D}$, one takes an arbitrary isometry.[12])

Kasparov's K homology is the Poincaré dual theory to K theory—the K homology (Abelian) group of a Fredholm module is given by the homotopy classes of its Fredholm operator F. Let F be an elliptic operator on a compact space X (all such are Fredholm), then there is an isomorphism, index: $[X,F]\to K_0(X)$ where $[,]$ denotes homotopy equivalence classes. Due to Connes' construction of Poincaré duality for noncommutative spaces, in which the dual to $\mathcal{A}$ is its opposite algebra $\mathcal{A}^{\text{op}}$, one can write that $[F]\in\rho(A^{\text{op}})$ because the Abelian group $K^0(A^{\text{op}})$ is generated by the minimal rank projections of the opposite algebra A^{op}.[13]

E. Index and intersection form

We recall that every finite dimensional real involutive algebra on a finite dimensional Hilbert space[14] over the complex numbers is isomorphic to the direct summand $M_{n_1}(\mathbb{C})\oplus\cdots\oplus M_{n_k}(\mathbb{C})$ for some integers n_1 to n_k. Consider the Hilbert space to be made up of separate "chunks" where each is acted upon by a different algebra summand[12]

$$H_{ij}=P_i\mathcal{H}P_j,\quad \mathcal{H}=\underset{i,j}{\oplus}H_{ij} \tag{4}$$

where the P_i or p_i are projections in $\mathcal{A}$ and the P_j or Jp_jJ^{-1} are projections in $\mathcal{A}^o$. The action on H_{ij} from the left is $a_i\otimes 1\otimes 1$ and the action from the right is $1\otimes 1\otimes a_j^T$. Let r_{ij} be the number of particles represented by H_{ij} and χ. The intersection form is

$$\mu_{ij}=r_{ij}\chi, \tag{5}$$

which has nonzero determinant.

The matrix $\mu_{ij}=r_{ij}\chi$ is the same thing as the tensor product pairing of the K-theory groups of the algebra $\mathcal{A}$ with its opposite algebra

$$\mu_{ij}=\text{Tr}(\chi(\rho(p_i)J\rho(p_j)J^{-1})) \tag{6}$$

and we also see that

$$\mu_{ij}=r_{ij}\chi=\dim H_{ij}^R-\dim H_{ij}^L, \tag{7}$$

and then by summing over all the H_{ij} one arrives at right-hand side of the Fredholm index formula

$$\text{Index}(P\mathcal{D}^+P)=\dim\mathcal{H}_R-\dim\mathcal{H}_L, \tag{8}$$

where $\mathcal{D}^+=M^*$ in our conventions for the finite triple.

F. The axioms

Axioms 1, 3, and 5 are identical with those of commutative geometry. See Ref. 4 for a full statement and explanation of the axioms.

(1) $n>0$ $ds=\mathcal{D}^{-1}$ is an infinitesimal of order $1/n$ where n is the dimension of the space.
(2) $[[\mathcal{D},a],b^0]=0$ $\forall a,b\in\mathcal{A}$. By axiom 7 we also have: $[[\mathcal{D},b^0],a]=0$ $b^o\in\mathcal{A}^o$ opposite algebra.
(3) (Smoothness) This is the algebraic formulation of smoothness of coordinates.
(4) (Orientability) There is a Hochschild cycle c. For n even, its representation on $\mathcal{H}$ is $\pi(c)=a^0[\mathcal{D},a^1]\cdots[\mathcal{D},a^n]$. This defines the construction of the analog of the differential form that does not require a previous knowledge of the tangent bundle. If n is odd, require $\pi(c)=1$. If n is even, $\pi(c)=\chi$ satisfies: $\chi=\chi^*$, $\chi^2=1$, $\chi D=-D\chi$.
(5) (Finiteness and absolute continuity) The Hilbert space is a finite, projective $\mathcal{A}$ module possessing a Hermitian structure.
(6) There is the Poincaré duality isomorphism $K_*(\mathcal{A})\to K^*(\mathcal{A})$ where the intersection form is nondegenerate.
(7) (Reality) There is an antilinear isometry $J:\mathcal{H}\to\mathcal{H}$ with $b^0=Jb^*J^{-1}$ and $[a,b^0]=0$. The operator J must satisfy a set of further conditions, which for 0-dimensions are the following: $J^2=I$, $JD=DJ$, $J\chi=\chi J$.

IV. GRAVITY AND INTERNAL SPACE

In order to motivate the main analysis of this article we give an outline of the previous work in Ref. 1 and discuss some of its implications. We also prove a new result.

The article (Ref. 1) highlights the following issue. Einstein's equations involve all fluctuations of the space-time metric, and so if we believe that noncommutataive spectral triples are analogous to Riemannian spin manifolds, then we should vary the finite action with respect to the most general internal space Dirac operator allowed by the noncommutative geometry axioms. In other words, since Riemannian geometry gives rise to the study of gravity, we should continue to treat the Higgs force as an internal space version of gravity by calculating the extra Einstein's equations for the entire set of metric fluctuations. A feature of this approach is that the element of choice is removed; the hypothesis was that the standard model fermion mass matrix would arise as a solution of these equations of motion, just as Newton's laws of motion are selected through an action minimization principle, and thus the existence of classical mechanics can be explained mathematically. The physical mass matrix did not turn out to be a solution, in fact the additional fluctuations overconstrained the vacuum so that the solutions were completely degenerate. However, given the logic of this idea (of Barrett's (Ref. 1)), despite giving an unphysical result, it deserves further attention.

In response to the result, we may consider:

(a) abandoning the paradigm that noncommutative spectral triples be completely analogous to Riemannian geometry, and taking the Yukawa couplings to be derived from "finely tuned" constants,

(b) proposing that the extra fluctuations are physical, in which case additional scalar field terms in the action are needed (in order that the mass matrix vacuum be non-degenerate) (one replaces the action $\mathrm{Tr}(MM^*-I)^2$ with $\mathrm{Tr}(MM^*+XX^*-I)^2$ for some matrix X), together with an additional internal space discrete version of gravity. Such a new interaction might arise from a background source term or a twisting of the Dirac operator, and

(c) proposing an eighth axiom for noncommutative geometry to act as a further geometric constraint on the Dirac operator, which might involve a definition of curvature of internal space.

Even by leaving out the S^o-reality condition to increase the number of degrees of freedom in the Dirac operator (connecting antiparticles with particles) and imposing the first order condition as a geometric constraint upon it, did not lead to a vacuum M for the physical mass matrix because the extra fields all had zero vacuum expectation values as shown in Ref. 1. There is another side

of the coin revealed by modifying this calculation such that those new fields are treated as constant numbers, which means that the Yukawa couplings determine from constants, or are constants as in the standard model: while the fermion mass ratios are not determined of course, the vacuum solution is a non-degenerate matrix and the product MM^* is diagonal whereas M^*M is not diagonal. These features are compatible with the physical mass matrix and with consideration (a) above. After defining some notation we give the proof.

We label the additional degrees of freedom in the standard model Dirac operator on internal space when S^o-reality condition is omitted: g,u,x,h,v,y. In Ref. 15 these "leptoquarks" are variable fields and effect spontaneous breaking of color symmetry, whereas we are treating them as constants, so here color symmetry remains intact. There are also two more fields j,l that arise and exist when ν_R is included,[1] which was done to allow the neutrino a mass.

We use the notation: $M=M_Q\otimes 1_3\oplus M_L$ with

$$M_Q=\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad M_L=\begin{pmatrix} q & r \\ s & t \end{pmatrix}.$$

If M is a diagonal matrix then a,d,q,t are interpreted as Dirac masses for the up, down, electron, and neutrino respectively.

The field equations (Ref. 1) for the Dirac operator with leptoquarks held constant are given in the Appendix. With M_Q invertible (substituting $ad-bc=0$ into the equations for M_Q (A1) to (A4) gives $g=u=x=h=v=y=0$) and with all of the additional fields held constant and $r=s=0$ by gauge freedom the equations[1] reduce to

$$3|a|^2+3|b|^2+|g|^2+|u|^2+|x|^2+|h|^2+|v|^2+|y|^2-3=0, \tag{9}$$

$$|d|^2+|c|^2-1=0, \tag{10}$$

$$a\overline{c}+\overline{b}d=0, \tag{11}$$

$$|q|^2+|g|^2+|u|^2+|x|^2+|j|^2-1=0, \tag{12}$$

$$|t|^2+|h|^2+|v|^2+|y|^2+3|l|^2+|j|^2-1=0, \tag{13}$$

$$\overline{g}h+\overline{u}v+\overline{x}y=0, \quad lj=0. \tag{14}$$

As claimed above, these equations give M a nondegenerate set of eigenvalues with MM^* diagonal and M^*M not diagonal. In the case of the standard model where $\nu_R=0$, the equations are the above minus the equation involving t, and with $j=l=0$. (In the previous work $g=u=x=h=v=y$ were allowed to vary, thus there were more equations and the solution was a fully degenerate mass matrix.)

Since $|a|^2+|b|^2$ is identified with $m_u(|\phi_1|^2+|\phi_2|^2)$, when g,u,x,h,v,y are constants means that the Yukawa couplings are determined from numbers that are constant. The conclusion is that we have found equations of motion for which there exists a solution that is not demonstrably incompatible with experiment by means of an action principle in which an element of human choice is removed. The result ironically provides a mathematical reason for the Yukawa couplings to require fine tuning, however, options (b) and (c) are open and there is the caveat that these results apply only to the zero-dimensional, Euclidean case. Also, there are the extra particle-antiparticle mixing action terms.[15]

There is also a set of equations where j and l are allowed to vary while the leptoquarks remain constant. These are the first three equations above Eq. (9) together with

$$j=0,$$

$$|q|^2 + |g|^2 + |u|^2 + |x|^2 - 1 = 0,$$

$$|t| = |l| = \tfrac{1}{2},$$

$$\overline{g}\overline{h} + \overline{u}\overline{v} + \overline{x}\overline{y} = 0.$$

The conclusion is the same as above.

V. FREDHOLM MODULE SOLUTIONS

The final discussion point we would like to make with regard to Ref. 1 will motivate the calculations that follow. Below we make the observation that the vacuum solutions to the field equations for the full set of metric fluctuations do not pertain to the spectral triple, but rather to the premetric structure of the spectral triple, namely the Fredholm module. Rather than the standard model Dirac operator being a solution, its sign is a solution. We refer to the observation of Connes that any spectral triple has a Fredholm module associated to it where the Fredholm operator F of the Fredholm module is identified with the sign of the Dirac operator (outside its kernel) of the spectral triple.[5] In switching the focus from spectral triple to Fredholm module, one zooms out from the geometry to the topology. Hence, instead of hypothesizing that the equations of motion single out the correct *metric*, in this section we ask if the equations of motion can give solutions which relate to *topological invariants*, that is, K theory and K homology.

Since the K homology of a Fredholm module is isomorphic to the K theory of the algebra it is over, we should observe a relationship between a given algebra and the vacuum solution. Connes' realization of Poincaré duality in noncommutative geometry is to define the Poincaré dual to be the opposite algebra. This means that the homotopy classes of the projections in the dual algebra are identified with the K homology, which we recall is given by the homotopy classes of the Fredholm module $[F]$. For a given algebra, one may identify a corresponding Fredholm module solution, and below we demonstrate this for the standard model and for one other algebra. This is only an observation, but to use this framework to obtain topological data from the vacua, we need to make the procedure unique, so that there is a one-to-one relationship between algebra and vacuum solution. To this end, tools from Morse theory are borrowed from commutative geometry and a way to generalize them for this noncommutative work is suggested.

A. S^o-real standard model finite triple vacuum

First we recall that the most general internal space Dirac operator given the appropriate constraints of self-adjointness, same dynamics for particles and antiparticles, orientability, S^o reality and first order condition

$$\mathcal{D} = \mathcal{D}^*, \quad [\mathcal{D}, J] = 0, \quad [\mathcal{D}, \chi]_+ = 0,$$

$$[\mathcal{D}, \epsilon] = 0, \quad [[\mathcal{D}, a], b^o] = 0, \quad [[\mathcal{D}, b^o], a] = 0,$$

(where $[,]_+$ denotes the anticommutator) is

$$D_F = \begin{pmatrix} 0 & M^* & 0 & 0 \\ M & 0 & 0 & 0 \\ 0 & 0 & 0 & M^T \\ 0 & 0 & \overline{M} & 0 \end{pmatrix}, \tag{15}$$

where $M = M_Q \otimes 1_3 \oplus M_L$, and we have allowed for the inclusion of ν_R. To exclude ν_R as in the standard model, we simply delete the final column from M^* (or row from M).

From the first order condition

$$(M\rho^c - \rho^c M)\rho_L^{T'} - \rho_R^{T'}(M\rho^c - \rho^c M) = 0, \tag{16}$$

when $\rho_L^{T'}=0$ and $\rho_R^{T'}=1$ we find that $[M,\rho^c]=0$ (the Higgs has no color charge) and with the standard model representation this splits M up into the direct sum of quark and lepton masses. Further than this, the mass matrix M is not constrained by the first order condition. This means that the action does not know how the algebra is represented, and hence, it is missing some geometrical information about the manifold. When S^o reality is omitted some of this information becomes available to the action and, hence, (when the extra fields are kept constant) the nondegenerate mass matrix solution of the previous section arises.

As in the previous work, we drop the S^o-reality condition, and allow degrees of freedom in D_F to vary but we leave the first order condition until after the equations of motion have been derived; since we are to aim to develop a method to identify the algebra given a vacuum solution, we had better omit any axioms that involve the algebra. However, we retain the condition that $[M,\rho^c]=0$.

The result is

$$D_F = \begin{pmatrix} Y & Z \\ \overline{Z} & \overline{Y} \end{pmatrix} = \begin{pmatrix} 0 & M^* & 0 & G \\ M & 0 & G^T & 0 \\ 0 & \overline{G} & 0 & M^T \\ G^* & 0 & \overline{M} & 0 \end{pmatrix}, \tag{17}$$

(where G having the same dimensionality as M, was not a general matrix in Ref. 1 but was constrained by the first order condition.) Alternate blocks are zero due to the condition $[D_F,\chi]_+=0$. Here we are not using the first order condition, so G and M are both general matrices with complex coefficients and having dimensionality depending on the number of fermions considered.

To calculate the equations of motion we vary the finite spectral action with respect the degrees of freedom in D_F as given above, first for the S^o-real case and then for the non-S^o-real triple. The result of the former is the same as that given in Ref. 1 but we make a new interpretation of it.

1. S^o-real triple

The action is

$$S = \mathrm{Tr}[(D_F)^4 - 2D_F^2] \tag{18}$$

or, with the $\mathrm{Tr}(I)$ term included

$$S = \mathrm{Tr}(MM^* - I)^2, \tag{19}$$

(where I denotes the unit matrix.)

Minimizing the (19) with respect to M gave the very definition of partial isometry

$$M^*(MM^* - I) = 0 \tag{20}$$

and Hermitian conjugate.

This result means that the mass matrix that minimizes the action gives each fermion an identical mass. The new interpretation we give is that the standard model finite triple's Dirac operator is a solution only up to its sign, and hence, only up to the conformal structure of the spectral triple, where $\mathrm{sign}\, D_F = D_F/|D_F|$. Specifically, the vacuum solution M^*_{vac} is the partial isometry in the polar decomposition of D^+. This operator sign D_F is the Fredholm operator for the Fredholm module associated to the standard model finite spectral triple outside the kernel of the Dirac operator (Ref. 5).

2. Non-S^o-real triple

The action is

$$S = \mathrm{Tr}[(D_F)^4 - 2D_F^2] \tag{21}$$

with D_F given by (17).

Simplifying the action by using cyclicity of trace and the fact that $\mathrm{Tr}(X)=\mathrm{Tr}(X^T)$:

$$S = \mathrm{Tr}(-2(G^*G + MM^*) + (MM^*)^2 + (G^*G)^2 + 2(MGG^*M^* + MM^*G^T\overline{G} + MG\overline{MG})) \tag{22}$$

or

$$S = \mathrm{Tr}(-2(GG^* + M^*M) + (M^*M)^2 + (GG^*)^2 + 2(GG^*M^*M + G\overline{M}M^TG^* + G\overline{MG}M)). \tag{23}$$

We vary the first of the above Eq. (22) with respect to M and the result is

$$M^*(MM^* + G^T\overline{G} - I) + G\overline{MG} + GG^*M^* = 0 \tag{24}$$

and the second with respect to G and the result is

$$G^*(GG^* + M^*M - I) + \overline{MG}M + \overline{M}M^TG^* = 0. \tag{25}$$

The field equations for G^T, M^T, G^*, M^*, $\overline{G}$, and $\overline{M}$ are just the transpose, Hermitian conjugate or complex conjugate, respectively, of the above equations for M and G.

Although there are zeros in D_F due to orientability, the equation below is the same thing as that above, due to there being no linear terms in M or G:

$$D_F^3 = D_F,$$

which is of course the result of differentiating (18) with respect to D_F. In other words, simply by substituting for D_F with (17) into $D_F^3=D_F$, precisely the equations of motion obtained above together with all their conjugate counterparts, appear.

The conclusion in this non-S^o-real case is the same as that in the S^o-real one, namely that the solutions are partial isometries. Here is the proof:

First we check if the equations of motion do have any Fredholm module solutions. To do this, we must look for solutions such that $D_{F,\mathrm{vac}}^2=I$:

$$D_{F,\mathrm{vac}}^2 = \begin{pmatrix} M^*M + GG^* & 0 & M^*G^T + G\overline{M} & 0 \\ 0 & MM^* + G^T\overline{G} & 0 & MG + G^TM^T \\ \overline{G}M + M^TG^* & 0 & \overline{G}G^T + M^T\overline{M} & 0 \\ 0 & G^*M^* + \overline{MG} & 0 & G^*G + \overline{M}M^T \end{pmatrix}. \tag{26}$$

Equations (24) and (25) (and conjugates) are equivalent to the equation $D_F^3=D_F$, and therefore we can state that the eigenvalues of the vacuum solution for D_F are all in the set $\{-1,0,1\}$. Then we see that $D_{F,\mathrm{vac}}^2$ has eigenvalues all 1 or 0, which means that assuming it is diagonalizable, $D_{F,\mathrm{vac}}^2=UpU^*$ for some unitary matrix U and where p is a projection, that is, p satisfies $p=p^2$ and $p=p^*$. Clearly, UpU^* is a projection, in other words $D_{F,\mathrm{vac}}^2$ is a projection, and since the Dirac operator is self-adoint, we may conclude that all the vacuum solutions are that $D_{F,\mathrm{vac}}$ is a partial isometry: $(D_{F,\mathrm{vac}}^*D_{F,\mathrm{vac}})(D_{F,\mathrm{vac}}^*D_{F,\mathrm{vac}})=D_{F,\mathrm{vac}}^*D_{F,\mathrm{vac}}$. A simpler way to see this is to multiply on both sides of the equation $D_{F,\mathrm{vac}}^3=D_{F,\mathrm{vac}}$ by $D_{F,\mathrm{vac}}$ while recalling that the Dirac operator is self-adjoint. Notice also that for the eigenvalues of $D_{F,\mathrm{vac}}$ that are 1, Eq. (26) shows that the sum of the two types of masses for each particle add up to 1 and so even if G can lift the degeneracy of the Dirac mass matrix, the total mass ends up being the same. To summarize, the Fredholm module interpretation Sec. V A 1 is again valid in this, the non-S^o-real case.

B. Orthogonal complements

Although the orthogonal complement relationship between M and G can already be seen from the result of the last part, below we demonstrate it explicitly and analyze Eqs. (25) and (24). This data will be used in the next part.

Since a partial isometry is just a projection multiplied by a unitary matrix, we let M be a diagonal projection of dimensionality n. (For a partial isometry v, $v\mathcal{H}=vv^*\mathcal{H}$.) We do not assume that G is diagonal. In any calculation we assume that the dimensionalities of the matrices M and G are the same.

From Eqs. (24) and (25) it is immediately clear that when $M=0$, G is a partial isometry and vice versa.

With M a diagonal projection inserted, the equation of motion for M simplifies to

$$M^*G^T\overline{G}+G\overline{M}\overline{G}+GG^*M^*=0. \tag{27}$$

If $M=I$ it simplifies further to

$$G^T\overline{G}+G\overline{G}+GG^*=0, \tag{28}$$

and whereas if M is a diagonal projection of dimensionality n and rank m then the bottom $n-m$ rows of Eq. (27) disappear.

We show below that Eq. (28) gives $G=0$ for $n=2$ while explaining the procedure in words to make clear that this method can be applied to the general case of arbitrary n and m—consider the top left elements of GG^* and $G^T\overline{G}$ where $n=2$—all terms are positive and all elements of the top row of G are present. The equations containing the top left and bottom right elements of $G\overline{G}$ may be combined as shown below to find that $G=0$.

For $n=2$ let

$$G=\begin{pmatrix} z & y \\ x & w \end{pmatrix},$$

the top left and bottom right equations are

$$3|z|^2+2|x|^2+y\overline{x}=0$$

$$3|w|^2+2|y|^2+x\overline{y}=0,$$

and their combination is

$$3|z|^2+3|w|^2+|x|^2+|y|^2+|x+y|^2,$$

which means that $x=y=w=z=0$ in other words $G=0$.

As mentioned, if $M=0$ then G is a partial isometry. Equivalently, GG^* and G^*G are Murray–von-Neumann equivalent projections. And in the same way, we see for general n, m the bottom $n-m$ rows of Eq. (28) show that the nonzero part of G is a partial isometry.

Notice the simple relationship between M and G; when M^*M and G^*G are diagonal projections and when $D^2_{F,\mathrm{vac}}=I$, they are the orthogonal complement of one another. The simultaneous matrix equations below simplify the statements: If $G=0$ then M is a partial isometry and vice versa, and if $M=I$ then $G=0$ and vice versa, and if M is a diagonal projection and if $D_{F,\mathrm{vac}}$ is invertible, then G is a partial isometry orthogonal to M,

$$M(M^*M+G^*G-I)=0,$$

$$G(G^*G+M^*M-I)=0.$$

C. Poincaré duality

Given the standard model algebra and using Connes' realization of Poincaré duality in noncommutative geometry, we may write down the sign of the standard model Dirac operator. This is just the matrix (15) with eigenvalue "1" for each particle mass. An aim of the previous work was to answer the question, "Is the standard model fermion mass matrix (internal space Dirac operator) a solution to the additional Einstein's equations?," whereas here we are considering the similar question, "Is the sign of the standard model internal space Dirac operator a solution to the equations?" If the direction of this arrow is reversed, that is if the K-theory group is identified for a given vacuum solution, then topological information has been retrieved about the manifold from the minimization procedure, and hence, there would be a mathematical reason for the choice of the algebra up to Morita equivalence. We begin by exploring the relationship between vacuum solution and algebra. We only study the first two summands of the algebra, that is, the algebra for the Electroweak force. The matrix M commutes with ρ^c as the Higgs has no color charge and we do not involve color charge at all in the remainder of this article.

We study the standard model and one other solution.

Above a set of solutions was found where for a given projection G, the vacuum solution for M, or M_{vac}, is determined via the simple relationship found in the equations of motion. Let us consider one such solution, namely the one in which $G=0$, that is, the one pertaining to the standard model. Then the M^*_{vac} is

$$M^*_{\text{vac}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \tag{29}$$

which is a rectangular matrix because the two direct summands of the chirality $\mathbb{Z}$/two-graded Hilbert space have different dimensions. The basis may be labeled $(u_R, d_R, e_R)^T$. We can add a final column of zeros to M^*_{vac} and the basis becomes $(u_R, d_R, e_R, \nu_R)^T$.

Recall that $[F] \in \rho(\mathcal{A}^{\text{op}})$ where $\rho(\mathcal{A})$ is given by Eq. (3). The opposite algebra is represented by $J\rho(a)J^{-1}$. The generators of the K-homology group are the homotopy classes of the minimal rank projections of the opposite algebra $\mathcal{A}^o$, that is, $J\rho_L(p_1)J^{-1}$, which is the 2 by 2 unit matrix $\text{diag}(1,1)$ and $J\rho_R(p_2)J^{-1}$, which is given by the number 1. The former is a projection of the algebra of the quaternions $\mathbb{H}$ and the latter is simply a projection of the complex numbers $\mathbb{C}$. So the vacuum solution (29) is consistent with the element b^o of the opposite algebra being

$$b^o = \begin{pmatrix} \rho^{cT} & 0 & 0 & 0 \\ 0 & \rho^{cT} & 0 & 0 \\ 0 & 0 & q^T & 0 \\ 0 & 0 & 0 & \Lambda^T \end{pmatrix}, \tag{30}$$

where q is a quaternion and $\Lambda = \text{diag}(\bar{\lambda}, \lambda)$, $\lambda \in \mathbb{C}$. Using the reality operator we find that an element b of $\mathcal{A}$ can be given by

$$b = \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & \Lambda & 0 & 0 \\ 0 & 0 & \rho^c & 0 \\ 0 & 0 & 0 & \rho^c \end{pmatrix} \tag{31}$$

from which we see that the first two summands of the algebra may be: $\mathbb{H} \oplus \mathbb{C}$.

Note that this is not a unique answer because the projection $\text{diag}(1,1)$ is also in $K_0(\mathbb{C})$.

A Fredholm module to be associated to a spectral triple must have algebra and Fredholm operator compatibility such that the first order condition is satisfied. In order to check that a

spectral triple can be assigned to the Fredholm module, we check that the first order condition is satisfied. It is satisfied because $G=0$ and $[M,\rho^c]=0$ where M is given by the direct sum.

We can generalize this procedure by choosing any other projective solution for G. For example let alternate eigenvalues of G be nonzero beginning with the first eigenvalue zero. Then by the orthogonal complement relationship we have the solution for M^*_{vac}:

$$M^*_{\text{vac}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{32}$$

and by the same procedure as above, we find that this solution is compatible with the algebra $M_2(\mathbb{C})\oplus\mathbb{C}$. $M_2(\mathbb{C})$ is Morita equivalent to $\mathbb{C}$ and so the first two summands of the algebra of this spectral triple are Morita equivalent to $\mathbb{C}\oplus\mathbb{C}$.

A point of clarification is that the two solutions considered above are unitary (and homotopy) (unitary and homotopy equivalence are the same thing for stable algebras) equivalent, and so one expects them to lead to the same topological invariants. However, in the part to follow, we will restrict this homotopy freedom to separate "nodes"; one for each of ρ_L, ρ_R, and ρ^c.

D. Morse theory and the Witten complex

The projection $\text{diag}(1,1)$ is in the K theory of both algebras $\mathbb{C}$ and $\mathbb{H}$, but to obtain topological information from the vacuum solutions the relationship between the vacuum solutions and the algebra must be one to one. We need a reason why the solutions should correspond only to the generators of the $K_0(\mathcal{A})$ group and not to any other element of the group. For example we need the matrix $\text{diag}(1,1)$ to be associated only with $\mathbb{H}$ and algebras Morita equivalent to it.

In this section we generalize a theorem involving the Morse theory and the Witten complex to suggest a method for finding topological information from the equations of motion about the S^o-real ($G=0$) spectral triple pertaining to the standard model. The theorem is that a chain complex called the Witten complex, which is constructed from the critical points of the Morse function has the same homology groups as the manifold that the Morse function is defined on. Atiyah and Bott have proven that the Yang-Mills action is an equivariant Morse function and since the Higgs is a gauge field component in the internal space direction, we ask whether the finite spectral action is also a Morse function in a proposed noncommutative sense described below. To do this, we make a straightforward generalization of the theorem to noncommutative geometry (which comes down to little more than the usual replacement of the commutative with the noncommutative algebra) by proposing a noncommutative generalization to the definition of Morse function, equivariant Morse function (or Morse–Bott function), Hessian matrix, and Witten complex.

A Morse function is a real-valued function on a (smooth) manifold N, $f:N\to\mathbb{R}$ such that every one of its critical points is nondegenerate. The way to check for nondegeneracy is to calculate the Hessian matrix of the critical point and if this has no zero eigenvalues then the point is nondegenerate. Of course the Higgs vacuum is an entire three-sphere of nondegenerate solutions, so in order to use Morse theory in physics problems where there is a gauge symmetry, the equivariant Morse function was defined where the gauge symmetry is just divided out. (There are more complicated cases.)

The Hessian matrix of a Morse function f for a critical point is given by

$$a_{ij} = \left(\frac{\partial^2 f}{\partial x_i\,\partial x_j}\right)\Big|_c, \tag{33}$$

where c is the critical point, x_i are the coordinates on N, and i runs from 1 to the dimension of N. The "index" of the critical point is the number of negative eigenvalues of this matrix.

The action we want to consider is the finite spectral action with $G=0$:

$$S = \mathrm{Tr}((MM^*)^2 + - 2MM^*). \tag{34}$$

To proceed from here, we need to make some generalizations of the above definitions to the context of noncommutative geometry. To begin with, the notion of a critical *point* is no longer valid, and differentiating with respect to each of the commuting coordinates x_i on N goes over to differentiating with respect to the matrix M. Consider the Fredholm operator F ingredient of the Fredholm module over a noncommutative C^*-algebra. Recalling that F is the generalization to noncommutative geometry of an elliptic operator on a compact manifold in commutative geometry, we understand that F is parametrized by the underlying space pertaining to the Fredholm module. Moreover, the homotopy classes of F, $[F] \in \rho(\mathcal{A}^{\mathrm{op}})$. With in mind the Fredholm module picture of the underlying space on which the Morse function acts, we replace the x_i with the M as 2 by 2 matrices over $\mathbb{C}$. We use 2 by 2 matrices because each direct summand of the standard model algebra is viewed as a node (not quite a point) upon which the vector bundle is built, and the representation ρ is separated into 2 by 2 chunks; one for each algebra summand. Obviously the critical points will be replaced by the vacuum solutions M_{vac}. Finally, we need to write down a condition corresponding to Eq. (33) that will give meaning to a noncommutative version of a Morse function (or at least equivariant Morse function) and check that the action S satisfies that condition. We continue this chapter's focus on the Fredholm module as the underlying space.

The index i does not run very far because we are working in zero dimensions and the action only depends on M and its hermitian conjugate. The Hessian matrix can only be as follows:

$$a = \left(\frac{\partial^2 S}{\partial M^* \, \partial M} \right)\Big|_c. \tag{35}$$

S is real-valued and we do not need to worry about smoothness as this is already covered in the noncommutative geometry axioms. Differentiating the action S with respect to M and afterwards with respect to M^* and evaluating at $M=0$ produces the Hessian of S. The resulting matrix is: MM^*+M^*M-I evaluated at the vacuum solution which is that MM^* and M^*M are "initial" and "final" projections. Since in some solutions this matrix can have zero eigenvalues, we differentiate twice with respect to MM^*, so that MM^* becomes the field to vary instead of M. The resulting matrix is $2I$, which has no zero eigenvalues. We suggest then that S is a noncommutative version of a Morse function. Since the degeneracies due to the vacuum manifold exist and may be associated with the finding of zero eigenvalues above, it may be more accurate to designate the function as an equivariant Morse function in keeping with the analogy with Yang–Mills theory.

In (commutative) Morse theory, the Witten complex is defined as follows (Ref. 16). To begin, the free Abelian group C_i generated by the set of critical points of index i is constructed. If C_{i-1} is defined in the same way for index $i-1$, it is possible to define a map from C_i to C_{i-1}, that is, the boundary map. This defines a chain complex called the Witten complex. It is a proven theorem that *the homology groups of this chain complex are isomorphic to the homology groups of the manifold.*

Classifying the vacuum solutions according to homotopy class, where each solution is homotopic to one of the following two diagonal projections:

$$M_{v1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad M_{v2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{36}$$

This is equivalent to dividing out the degenerate solutions as in equivariant theory and to considering the homotopy classes of the projections $(MM^*)_v$ where the action is varied with respect to MM^* instead of M.

Since the two solutions share the same Hessian, they have the same index and therefore the Witten complex for this particular function has only one component C_i so the homology groups are simply C_i. Since the Witten chain complex in the case studied above is made out of only one term C_i, the kernel of the boundary map is C_i, and the image of the boundary map for the next term in the sequence takes the identity to the identity, therefore the homology group is simply

given by C_i. The Abelian group C_i is generated by the two projections M_{v1} and M_{v2}, which is exactly the K-homology group $K^0(\mathcal{A}^o)$, that is, the K-homology group of the underlying Fredholm module. (The other elements of the Abelian group arise from the other generations—of which this framework implies there are an arbitrary number, and of course it is a mystery that we have to stop at 3—in analogy to the Abelian group $\mathbb{Z}$ where $S^1=\mathbb{R}/\mathbb{Z}$.) The K-theory group of the standard model algebra is isomorphic to $\mathbb{Z}\oplus\mathbb{Z}\oplus\mathbb{Z}$ (though here we have only studied the first two summands). Since one counts only a limited number of generations, the algebra is associated to the punctured torus.

The two critical nodes can be identified with the first two direct summands (up to Morita equivalence) on the internal space, one for $\mathbb{H}$ and the other $\mathbb{C}$, an example of the noncommutative generalization of the two point space (left and right) as follows. We associate M_{v1} with left and M_{v2} with right. So $M_{v1}\in\rho_L(\mathcal{A}^o)$ and $M_{v2}\in\rho_R(\mathcal{A}^o)$. Removing ν_R from the Hilbert space and a row and column from D_F means that the vacuum solution is: $M_Q=\mathrm{diag}(1,1)$ and $M_L=1$. These are the minimal rank projections of $\mathbb{H}$ and $\mathbb{C}$ and Morita equivalent algebras. And by Poincaré duality (as shown in the previous part), the noncommutative space can be described by the quaternions over the right 'node' and the complex numbers over the left.

VI. CONCLUSIONS

Although the solutions to the field equations calculated in our previous work yielded an unphysical result, we have argued that the reasoning for their derivation deserves further attention and we explained why Ref. 1 has highlighted an open question in the noncommutative framework. A solution was found to the equations of motion calculated previously with the leptoquarks held constant whose features are compatible with the physical fermion mass matrix. Ironically, this result provides a mathematical reason for the Yukawa couplings to need fine tuning.

The solutions to the field equations for D_F both with and without the S^o-reality condition were shown to be partial isometries. These were interpreted as the phase or sign of D_F. The relationship between the vacuum solutions and the topology of the internal space was explored using K theory and K homology and a method inspired by Morse theory to extract topological information from the vacuum about the underlying noncommutative space was developed. Instead of finding a mathematical reason in the action principle for the *geometry* of the standard model to be what it is known to be by experiment, we have claimed that the vacuum provides information on its *topology* in terms of K homology. Rather than the vacuum picking out just one of a myriad of possible answers, all partial isometries are solutions. The study was limited to the first two of three summands, that is, the Electroweak part of the standard model algebra.

We also note that with $D_F^2=I$, we can consider solutions in the case without S^o reality in which M_{v2} is associated with its orthogonal complement matrix $G_{v2}=\mathrm{diag}(0,1)$. Applying these solutions to the standard model basis, where $\nu_R=0$, $G=0$ and the bottom row vanishes from M_{v2} and the outcome is the same as above. Also, a similar analysis can be carried out with M having arbitrary dimensionalities and arbitrary numbers of algebra direct summands. This involves either an unwanted prediction of new massless particles, or cutting the matrices down as above to fit the standard model Hilbert space. For example, in the dimensionality 3 case, there is an additional solution, $M_{v3}=\mathrm{diag}(1,1,1)\in\mathrm{SU}(3)$. Algebras with a greater number of summands cannot be identified using this method if there are repeated summands, for example the algebra $\mathbb{H}\oplus\mathbb{H}\oplus\mathbb{C}\oplus\mathbb{C}$ cannot be distinguished from $\mathbb{H}\oplus\mathbb{C}$ because they have the same critical nodes.

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APPENDIX

The equations of motion for one generation and three colored quarks with leptoquarks held constant. These were calculated for Ref. 1 using the computer package MAPLE

$$\overline{a}(3|a|^2+3|c|^2+3|b|^2+|g|^2+|u|^2+|x|^2+|h|^2+|v|^2+|y|^2-3)+3\overline{cb}d=0, \tag{A1}$$

$$\overline{b}(3|b|^2+3|d|^2+|g|^2+|u|^2+|x|^2+|h|^2+|v|^2+|y|^2+3|a|^2-3)+3\overline{ad}c=0, \tag{A2}$$

$$\overline{c}(|a|^2+|c|^2+|d|^2-1)+\overline{ad}b=0, \tag{A3}$$

$$\overline{d}(|b|^2+|d|^2+|c|^2-1)+\overline{cb}a=0, \tag{A4}$$

$$\overline{q}(|q|^2+|s|^2+|r|^2+|g|^2+|u|^2+|x|^2+|j|^2-1)+\overline{r}(\overline{hg}+\overline{vu}+\overline{yx}+\overline{lj}+\overline{st})=0, \tag{A5}$$

$$\overline{r}(|r|^2+|t|^2+|q|^2+|h|^2+|v|^2+|y|^2+|l|^2-1)+\overline{q}(\overline{gh}+\overline{uv}+\overline{xy}+\overline{jl}+\overline{ts})=0, \tag{A6}$$

$$\overline{s}(3|j|^2+|q|^2+|s|^2+|t|^2+|g|^2+|u|^2+|x|^2+|l|^2-1)+\overline{t}(\overline{hg}+\overline{vu}+\overline{yx}+2\overline{lj}+\overline{qr})=0, \tag{A7}$$

$$\overline{t}(3|l|^2+|r|^2+|t|^2+|s|^2+|h|^2+|v|^2+|y|^2+|j|^2-1)+\overline{s}(\overline{gh}+\overline{uv}+\overline{xy}+2\overline{jl}+\overline{rq})=0, \tag{A8}$$

$$\overline{j}(3|s|^2+|j|^2+|g|^2+|u|^2+|x|^2+|l|^2+|t|^2+|q|^2-1)+\overline{l}(\overline{rq}+2\overline{ts}+\overline{gh}+\overline{uv}+\overline{xy})=0, \tag{A9}$$

$$\overline{l}(3|t|^2+|h|^2+|v|^2+|y|^2+|j|^2+|l|^2+|r|^2+|s|^2-1)+\overline{j}(\overline{qr}+2\overline{st}+\overline{hg}+\overline{vu}+\overline{yx})=0. \tag{A10}$$

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On the structure of (2+1)-dimensional commutative and noncommutative integrable equations

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We develop the symbolic representation method to derive the hierarchies of (2+1)-dimensional integrable equations from the scalar Lax operators and to study their properties globally. The method applies to both commutative and noncommutative cases in the sense that the dependent variable takes its values in $\mathbb{C}$ or a noncommutative associative algebra. We prove that these hierarchies are indeed quasi-local in the commutative case as conjectured by Mikhailov and Yamilov [J. Phys. A **31**, 6707 (1998)]. We propose a ring extension in the noncommutative case based on the symbolic representation. As examples, we give noncommutative versions of Kadomtsev-Petviashvili (KP), modified Kadomtsev-Petviashvili (mKP), and Boussinesq equations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Integrable (1+1)-dimensional nonlinear evolution equations, i.e., equations of the form

$$u_t = F(u, u_x, u_{xx}, \ldots, u_{xx\ldots x})$$

possess rich algebraic and geometrical structures such as Lax representations, a bi-Hamiltonian formulation, infinitely many symmetries and conservation laws, etc. A lot of work has been devoted to the study of such equations and comprehensive classification results have been obtained.

The extension of these remarkable structures to the (2+1)-dimensional case is not straightforward. It was proved in Ref. 1 that there is no bi-Hamiltonian formulation for (2+1)-dimensional integrable equations of the same type as those for the (1+1)-dimensional case like the Korteweg–de Vries (KdV) equation

$$u_t = u_{xxx} + 6uu_x.$$

In 1988, Fokas and Santini, cf. Refs. 2 and 3, constructed a bi-Hamiltonian structure for the Kadomtsev-Petviashvili (KP) equation

$$u_t = u_{xxx} + 6uu_x + 3D_x^{-1}u_{yy}$$

by considering it as a reduction of (3+1)-dimensional system. Meanwhile, Magri and his coauthors,[4] explained this structure from the geometric point of view by developing the concept of Nijenhuis G-manifolds, which amazingly works for both one and two space dimensions. Dorfman and her coauthors introduced the noncommutative ring of formal pseudo-differential operators, cf. Refs. 5 and 6. They proved that the Fokas-Santini bi-Hamiltonian structure of the KP can be obtained from the Adler-Gel'fand-Dikii (AGD) scheme by considering the second-order Lax operator

$$L = D_x^2 + u - \partial_y.$$

The bi-Hamiltonian structure naturally leads to a recursion operator for the equation. However, the operator (so-called operand) takes its value in the ring of formal differential operators and is of a different type from the one for KdV (and therefore does not contradict the result of Ref. 1). A hierarchy of infinitely many symmetries can only be produced by making suitable combinations of the operator acting on distinct seeds.[4]

One of the main obstacles to extend the spectacular results of $(1+1)$-dimensional integrable equations to the $(2+1)$-dimensional case is that the equations themselves, their higher symmetries, and conservation laws are nonlocal, i.e., the appearance of the formal integral D_x^{-1} or D_y^{-1}. In 1998, Mikhailov and Yamilov,[7] introduced the concept of quasi-local functions based on the observation that the operators D_x^{-1} and D_y^{-1} never appear alone but always in pairs like $D_x^{-1}D_y$ and $D_y^{-1}D_x$ for all known integrable equations and their hierarchies of symmetries and conservation laws, which enables them to extend the symmetry approach of testing integrability[8] to the $(2+1)$-dimensional case.

In this paper, we develop the symbolic representation method to produce hierarchies of $(2+1)$-dimensional integrable equations from scalar Lax operators and to study their properties globally. The method applies both to the commutative and noncommutative case in the sense that the dependent variable takes its values in $\mathbb{C}$ or in a noncommutative associative algebra. We prove that these hierarchies are indeed quasi-local in the commutative case as conjectured by Mikhailov and Yamilov in 1998.[7] This concept of quasi-locality has to be extended in the noncommutative case. Here we propose a ring extension based on the symbolic representation. As examples, we give noncommutative versions of the KP, mKP, and Boussinesq equations.

II. QUASI-LOCAL POLYNOMIALS AND SYMBOLIC REPRESENTATION

The symbolic method was introduced by Gel'fand and Dikii in 1975.[9] However, its basic idea can be dated back to the middle of 19th century. Recently, we successfully applied this method to the classification of both commutative and noncommutative $(1+1)$-dimensional homogeneous evolution equations in a series of papers, cf. Refs. 10–12. With the help of number theory, it enables us to give a global description of their integrable hierarchies.[13] The symbolic method is also powerful in dealing with differential (cf. Ref. 14) and pseudo-differential (cf. Ref. 15) operators. The authors of Ref. 15 generalized the standard symmetry approach[8] and made it suitable for the study of nonlocal and nonevolutionary equations; see also Ref. 16.

In this section, we will extend the symbolic method to the case of two spatial variables x and y. For simplicity, we restrict our attention to a single dependent variable u. Extensions to several independent variables and dependent variables are straightforward.

A. Quasi-local polynomials

We begin with basic definitions and notations of the ring of commutative and noncommutative differential polynomials. The derivatives of dependent variable u with respect to its independent variables x and y are denoted by $u_{ij}=\partial_x^i\partial_y^j u$. For smaller i and j, we sometimes write the indices out explicitly, that is, u_{xxy} and u instead of u_{21} and u_{00}. A differential monomial takes the form

$$u_{i_1j_1}u_{i_2j_2}\cdots u_{i_kj_k}.$$

We call k the degree of the monomial. We let $\mathcal{U}^k$ denote the set of differential polynomials of degree k. The ring of differential polynomials is denoted by $\mathcal{U}=\oplus_{k\geqslant 1}\mathcal{U}^k$. Notice that $1\notin\mathcal{U}$ and it is a differential ring with total x-derivation and y-derivation

$$D_x = \sum_{i=0}^{+\infty}\sum_{j=0}^{+\infty} u_{i+1,j}\frac{\partial}{\partial u_{ij}} \text{ and } D_y = \sum_{i=0}^{+\infty}\sum_{j=0}^{+\infty} u_{i,j+1}\frac{\partial}{\partial u_{ij}}.$$

The ring $\mathcal{U}$ is commutative if the dependent variable u takes its values in a commutative algebra, for example the ring of smooth functions in x and y. Let us denote

$$\Theta = D_x^{-1}D_y, \quad \Theta^{-1} = D_y^{-1}D_x. \tag{1}$$

The concept of quasi-local (commutative) polynomials $\mathcal{U}(\Theta)$ was introduced in Ref. 7 to test integrability of a given equation. To define it, we consider a sequence of extensions of $\mathcal{U}$. Let $\Theta\mathcal{U}=\{\Theta f: f\in\mathcal{U}\}$ and $\Theta^{-1}\mathcal{U}=\{\Theta^{-1}f: f\in\mathcal{U}\}$. We define $\mathcal{U}_0(\Theta)=\mathcal{U}$ and $\mathcal{U}_k(\Theta)$ is the ring closure of the union

$$\mathcal{U}_{k-1}(\Theta)\cup\Theta\mathcal{U}_{k-1}(\Theta)\cup\Theta^{-1}\mathcal{U}_{k-1}(\Theta).$$

Here the index k indicates the maximal depth of nesting the operator $\Theta^{\pm 1}$ in the expression. Clearly, we have $\mathcal{U}_{k-1}(\Theta)\subset\mathcal{U}_k(\Theta)$. We now define $\mathcal{U}(\Theta)=\lim_{k\to\infty}\mathcal{U}_k(\Theta)$. However, for a given $f\in\mathcal{U}(\Theta)$, there exists k such that $f\in\mathcal{U}_k(\Theta)$. The extension $\mathcal{U}(\Theta)$ has a natural gradation according to the number of u and its derivatives

$$\mathcal{U}(\Theta)=\oplus_{l\geqslant 1}\mathcal{U}^l(\Theta), \quad \mathcal{U}^p(\Theta)\mathcal{U}^q(\Theta)\in\mathcal{U}^{p+q}(\Theta).$$

Note that $\mathcal{U}_k(\Theta)$ is not invariant under transformation of variables. For example, a simple transformation

$$x' = x+y, \quad y' = y \tag{2}$$

transforms $\Theta=D_{x'}^{-1}D_{y'}\mapsto 1-\Theta=1-D_x^{-1}D_y$. Hence $\Theta^{-1}\mapsto(1-\Theta)^{-1}$, which is not in $\mathcal{U}_k(\Theta)$.

If u takes its value in a noncommutative associative algebra, the ring $\mathcal{U}$ is noncommutative. Typical examples are the algebras of $n\times n$ matrices and Clifford algebras (see Ref. 17 for more examples and noncommutative (1+1)-dimensional integrable evolution equations). For any element f, g, and h in a noncommutative associative algebra, we use the notation

$$L_f(g)=fg, \quad R_f(g)=gf \tag{3}$$

for the operators of left and right multiplication, and

$$C_f(g)=L_f(g)-R_f(g)=fg-gf \tag{4}$$

for the commutator (notation ad_f is also commonly used). It is a derivation since it satisfies the Leibniz rule: $C_f(gh)=C_f(g)h+gC_f(h)$.

So far there is no proper extension from noncommutative differential polynomials to quasi-local noncommutative polynomials, mainly because the study of noncommutative (2+1)-dimensional integrable equations is a new and challenging topic. We can take the corresponding extension of $\mathcal{U}(\Theta)$ as the starting point. However, this turns out to be too restrictive. This will be discussed further in Sec. IV B.

B. Symbolic representation

The basic idea of the symbolic representation is to replace u_{ij} by $u\xi^i\eta^j$, where ξ and η are symbols. Now the total differentiation with respect to x, that is, mapping u_{ij} to $u_{i+1,j}$, is replaced by multiplication with ξ, as in the Fourier transform. Similarly, the total differentiation with respect to y mapping u_{ij} to $u_{i,j+1}$, is replaced by multiplication with η. For higher degree terms with multiple u's, one uses different symbols to denote each of them. Its symbolic representation depends on where u takes its value, i.e., whether it is commutative or not. For example, the noncommutative binomial $u_{ij}u_{kl}$ has symbolic representation $u^2\xi_1^i\eta_1^j\xi_2^k\eta_2^l$. In the commutative case, one has $u_{ij}u_{kl}=u_{kl}u_{ij}$. We therefore need to average its symbolic representation over the permutation group Σ_2 so

that $u_{ij}u_{kl}$ and $u_{kl}u_{ij}$ have the same symbolic form. So the symbolic representation of $u_{ij}u_{kl}$ is $(u^2/2)(\xi_1^i\eta_1^j\xi_2^k\eta_2^l+\xi_2^i\eta_2^j\xi_1^k\eta_1^l)$. Symmetrization makes the symbol representation of monomials unique.

Let $\mathcal{A}^k$ be the space of algebraic polynomials f in $2k$ variables, ξ_i and η_i, where $i=1,\ldots,k$.

The symbolic representation defines a linear isomorphism between the space $\mathcal{U}^k$ of (non)-commutative differential polynomials of degree k and the space $\mathcal{A}^k$. It is uniquely defined by its action on monomials.

Definition 1: *The symbolic representation of a differential monomial is defined as*

$$u_{i_1,j_1}u_{i_2,j_2}\cdots u_{i_k,j_k}\mapsto\begin{cases}u^k\xi_1^{i_1}\eta_1^{j_1}\xi_2^{i_2}\eta_2^{j_2}\cdots\xi_k^{i_k}\eta_k^{j_k}, & (\textit{noncommutative});\\ \dfrac{u^k}{k!}\displaystyle\sum_{\sigma\in\Sigma_k}\xi_{\sigma(1)}^{i_1}\eta_{\sigma(1)}^{j_1}\cdots\xi_{\sigma(k)}^{i_k}\eta_{\sigma(k)}^{j_k}, & (\textit{commutative}).\end{cases}$$

There are two parts in the symbolic representation of a monomial: the first part, u^k, indicating its degree; the second part being in $\mathcal{A}^k$. The symbols of Gel'fand and Dikii only contain the second part. We emphasize that the first part is very important in dealing with the monomials u^l and the case of several noncommutative dependent variables.

In general, we denote the symbolic representation of $P\in\mathcal{U}^k$, whether it is commutative or not, by $\hat{P}$ and $Q\in\mathcal{U}^l$ by $\hat{Q}$. The multiplication of P and Q corresponds to the symbol

$$\widehat{PQ}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k,\xi_{k+1},\eta_{k+1},\ldots,\xi_{k+l},\eta_{k+l})=\hat{P}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k)\hat{Q}(\xi_{k+1},\eta_{k+1},\ldots,\xi_{k+l},\eta_{k+l});\tag{5}$$

when P and Q are commutative differential polynomials, the right-hand side needs to be symmetrized

$$\begin{aligned}&\widehat{PQ}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k,\xi_{k+1},\eta_{k+1},\ldots,\xi_{k+l},\eta_{k+l})\\&\quad=\frac{1}{(k+l)!}\sum_{\sigma\in\Sigma_{k+l}}\hat{P}(\xi_{\sigma(1)},\eta_{\sigma(1)},\ldots,\xi_{\sigma(k)},\eta_{\sigma(k)})\hat{Q}(\xi_{\sigma(k+1)},\eta_{\sigma(k+1)},\ldots,\xi_{\sigma(k+l)},\eta_{\sigma(k+l)}).\end{aligned}\tag{6}$$

The total derivatives D_x and D_y have the following representations:

$$\widehat{D_xP}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k)=(\xi_1+\cdots+\xi_k)\hat{P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k);$$

$$\widehat{D_yP}(\xi_1,\eta_1,\xi_2,\eta_2,\cdots,\xi_k,\eta_k)=(\eta_1+\cdots+\eta_k)\hat{P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k).$$

Naturally, the actions of $\Theta=D_x^{-1}D_y$ and Θ^{-1} on $P\in\mathcal{U}^k$ can be represented as

$$\widehat{\Theta P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k)=\frac{\eta_1+\cdots+\eta_k}{\xi_1+\cdots+\xi_k}\hat{P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k);$$

$$\widehat{\Theta^{-1}P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k)=\frac{\xi_1+\cdots+\xi_k}{\eta_1+\cdots+\eta_k}\hat{P}(\xi_1,\eta_1,\xi_2,\eta_2,\ldots,\xi_k,\eta_k).$$

Similar to the multiplication of P and Q, we have

Definition 2: *Let $P\in\mathcal{U}^k$ and $Q\in\mathcal{U}^l$. Then*

$$\widehat{P\Theta Q}=\hat{P}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k)\frac{\eta_{k+1}+\cdots+\eta_{k+l}}{\xi_{k+1}+\cdots+\xi_{k+l}}\hat{Q}(\xi_{k+1},\eta_{k+1},\ldots,\xi_{k+l},\eta_{k+l}).$$

When P and Q are commutative differential polynomials, the right-hand side needs to be symmetrized.

In the same way, we can uniquely define the symbol of $P\Theta^{-1}Q$. Together with the multiplication rule (5) or (6), we have now completely determined the symbolic representations of the elements in $\mathcal{U}_1(\Theta)$. By induction, we can define the symbolic representation of any element in $\mathcal{U}(\Theta)$, which is a rational function with its denominator being the products of the linear factors. The expression of the denominator uniquely determines how the operator $\Theta^{\pm 1}$ is nested.

Example 1: The expressions $u^3\xi_1(\eta_2+\eta_3)/(\xi_2+\xi_3)(\xi_3/\eta_3)$ *and* $u^3\xi_1(\eta_2/\xi_2)(\xi_3/\eta_3)$ *are the symbolic representations of* $u_x\Theta(u\Theta^{-1}u)\in\mathcal{U}_2(\Theta)$ *and* $u_x(\Theta u)\Theta^{-1}u\in\mathcal{U}_1(\Theta)$, *respectively*.

Let us define the symbolic representations of pseudo-differential operators motivated by their Fourier transforms. First we assign a special symbol X to the operator D_x. Its formal inverse D_x^{-1} has the symbol $1/X$. Then we have the following rules for $f\in\mathcal{U}^k(\Theta)$ with symbol $\hat{f}$ and $g\in\mathcal{U}^l(\Theta)$ with symbol $\hat{g}$:

$$X\circ\hat{f}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k)=(\xi_1+\cdots+\xi_k+X)\hat{f}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k),$$

which represents the Leibniz rule $D_x\circ f=D_x(f)+f\circ D_x$; and the composition rule

$$\hat{f}X^p\circ\hat{g}X^q=\hat{f}(\xi_1,\eta_1,\ldots,\xi_k,\eta_k)(\xi_{k+1}+\cdots+\xi_{k+l}+X)^p\hat{g}(\xi_{k+1},\eta_{k+1},\ldots,\xi_{k+l},\eta_{k+l})X^q.$$

This composition rule is valid for both positive and negative powers p and q. For positive powers, it is a polynomial of X. For negative powers, one can expand it at $X=\infty$ to identify it.

Example 2: The symbol of $D_x^{-1}u$ *is* $u/(X+\xi)$ *if we assign* ξ *as the symbol for* u. *Then in the noncommutative case we have*

$$D_x^{-1}uD_x^{-1}u=u^2D_x^{-2}-(2uu_x+u_xu)D_x^{-3}+(3uu_{xx}+3u_x^2+u_{xx}u)D_x^{-4}+\cdots.$$

Symbolically, we can compute it by

$$\frac{u}{X+\xi}\circ\frac{u}{X+\xi}=\frac{u^2}{(X+\xi_1+\xi_2)(X+\xi_2)}=u^2\left(\frac{1}{X^2}-\frac{\xi_1+2\xi_2}{X^3}+\frac{\xi_1^2+3\xi_1\xi_2+3\xi_2^2}{X^4}+\cdots\right).$$

To extend the symbolic representation from one dependent variable to several noncommutative dependent variables is straightforward. We need to assign new symbols for each of them such as assigning $\xi^{(1)},\eta^{(1)}$ for u and $\xi^{(2)},\eta^{(2)}$ for v, and so on. As one can imagine, the abstract formulas for arbitrary n-dependent variables get very long and it is difficult to present them in a compact way. We have no problems in handling small n or given expressions.

Example 3: The symbolic representation of u_xv_y *is* $uv\xi^{(1)}\eta^{(2)}$ *and that of* v_yu_x *is* $vu\xi^{(1)}\eta^{(2)}$.

Notice that the only difference in the symbolic representations for u_xv_y and v_yu_x is uv instead of vu, that is, the noncommutativity of dependent variables lies in the first part of the symbolic representation indicating the degree of the expression.

III. LAX FORMULATION OF (2+1)-DIMENSIONAL INTEGRABLE EQUATIONS

In this section, we give a short description of construction of (2+1)-dimensional integrable equations from a given scalar Lax operator based on the well-known Sato approach. For details on the Sato approach, see the recent books[18,19] and related references therein.

Consider an mth-order formal pseudo-differential operator

$$A=a_mD_x^m+a_{m-1}D_x^{m-1}+\cdots+a_0+a_{-1}D_x^{-1}+\cdots,\quad m\geqslant 0,$$

where the coefficients a_k are functions of x and D_x^{-1} is the formal inverse of the total x-derivative D_x. Here the functions a_k take their values in commutative (for instance complex numbers $\mathbb{C}$) or noncommutative (for instance the algebra of $n\times n$ matrices) associative algebras.

To define the product of two pseudo-differential operators requires the action of differential operator D_x^n on a multiplication operator f (given by a function of x),

$$D_x^n \circ f = \sum_{i\geqslant 0} \frac{n(n-1)\cdots(n-i+1)}{i!}(D_x^i f)D_x^{n-i}.$$

Let the commutator be the bracket on the set of pseudo-differential operators. Thus, the set of pseudo-differential operators forms a Lie algebra. For an integer $k<m$, we introduce notations

$$A_{\geqslant k} = a_m D_x^m + a_{m-1}D_x^{m-1} + \cdots + a_k D_x^k$$

$$A_{<k} = A - A_{\geqslant k} = a_{k-1}D_x^{k-1} + \cdots .$$

When $k \in \{0,1\}$, the Lie algebra decomposes as a direct sum of two subalgebras in both commutative and noncommutative cases. We denote the projections onto these subalgebras by $\mathcal{P}_{\pm}$. Such decompositions are naturally related with integrability and lead to admissible scalar Lax operators for $(1+1)$-dimensional Lax dynamics (cf. Ref. 18, p. 270 for the commutative case), namely

$$k=0\text{: } \widetilde{L} = D_x^n + u^{(n-2)}D_x^{n-2} + u^{(n-3)}D_x^{n-3} + \cdots + u^{(0)}, \quad n \geqslant 2;$$

$$k=1\text{: } \widetilde{L} = D_x^n + u^{(n-1)}D_x^{n-1} + u^{(n-2)}D_x^{n-2} + \cdots + u^{(0)} + D_x^{-1}u^{(-1)}, \quad n \geqslant 2;$$

where $u^{(i)}$ are functions of a spatial variable x.

We know every pseudo-differential operator of order $n>0$ has an nth root. This allows us to define the fractional powers $\widetilde{L}^{i/n}, i \in \mathbb{N}$. Let $\widetilde{B}_i = \mathcal{P}_+(\widetilde{L}^{i/n})$. For each choice of i, we introduce a different time variable t_i. Thus, the flows defined by

$$\frac{\partial \widetilde{L}}{\partial t_i} = [B_i, \widetilde{L}], \quad i \in \mathbb{N}$$

commute.[20]

This setting up can be generalized into the $(2+1)$-dimensional case as follows: An mth-order pseudo-differential operator of two spatial variables is of the form

$$H = -D_y + a_m D_x^m + a_{m-1}D_x^{m-1} + \cdots + a_0 + a_{-1}D_x^{-1} + \cdots, \quad m \geqslant 0,$$

where coefficients a_k are functions of x, y and for an integer $k<m$, we split into

$$H_{\geqslant k} = a_m D_x^m + a_{m-1}D_x^{m-1} + \cdots + a_k D_x^k$$

$$H_{<k} = H - H_{\geqslant k} = -D_y + a_{k-1}D_x^{k-1} + \cdots .$$

Similar to the $(1+1)$-dimensional case, this operator algebra decomposes as a direct sum of two subalgebras in both commutative and noncommutative cases when $k \in \{0,1\}$. The admissible types of scalar Lax operators for the case of $(2+1)$ dimensions are $\widetilde{L} - D_y$, i.e.,

(a) $k=0$: $L = D_x^n + u^{(n-2)}D_x^{n-2} + u^{(n-3)}D_x^{n-3} + \cdots + u^{(0)} - D_y, \quad n \geqslant 2;$

(b) $k=1$: $L = D_x^n + u^{(n-1)}D_x^{n-1} + u^{(n-2)}D_x^{n-2} + \cdots + u^{(0)} + D_x^{-1}u^{(-1)} - D_y, \quad n \geqslant 2;$

(c) $k=1$: $L = u^{(0)} + D_x^{-1}u^{(-1)} - D_y;$

where $u^{(i)}$ are functions of two spatial variables x, y. We often use $u, v, w, \ldots$ in the examples. When $n=1$ for case (b), we have $L = D_x + u^{(0)} + D_x^{-1}u^{(-1)} - D_y$, which can be transformed into case (c) by transformation (2). Therefore, we exclude it from our consideration.

Let $S = D_x + a_0 + a_{-1}D_x^{-1} + \cdots$. For any operator L as listed in cases (a), (b), and (c), the relation

$$[S,L] := SL - LS = 0, \tag{7}$$

uniquely determines the operator S by taking the integration constants as zero. Furthermore, we have $[S^n,L]=0$ for any $n \in \mathbb{N}$. For each choice of i, we introduce a different time variable t_i and define the Lax equation by

$$\frac{\partial L}{\partial t_i} = [S^i{}_{\geqslant k}, L], \tag{8}$$

where k is determined by the operator L as listed in cases (a), (b), and (c).

Theorem 1: *For the operator S uniquely determined as above by (7), the flows defined by Lax equations (8) commute, that is,* $\partial_{t_j}\partial_{t_i}L=\partial_{t_i}\partial_{t_j}L$.

Proof: Using Lax equations, we have

$$\partial_{t_j}\partial_{t_i}L = [\partial_{t_j}S^i{}_{\geqslant k}, L] + [S^i{}_{\geqslant k}, \partial_{t_j}L] = [\partial_{t_j}S^i{}_{\geqslant k}, L] + [S^i{}_{\geqslant k}, [S^j{}_{\geqslant k}, L]].$$

Hence

$$\partial_{t_j}\partial_{t_i}L - \partial_{t_i}\partial_{t_j}L = [\partial_{t_j}S^i{}_{\geqslant k} - \partial_{t_i}S^j{}_{\geqslant k} - [S^j{}_{\geqslant k}, S^i{}_{\geqslant k}], L].$$

Meanwhile, from formula (7), we get

$$[\partial_{t_i}S, L] = -[S, \partial_{t_i}L] = -[S, [S^i{}_{\geqslant k}, L]] = [[S^i{}_{\geqslant k}, S], L],$$

implying

$$\partial_{t_i}S = [S^i{}_{\geqslant k}, S]. \tag{9}$$

Thus

$$\begin{aligned}
\partial_{t_j}S^i{}_{\geqslant k} - \partial_{t_i}S^j{}_{\geqslant k} - [S^j{}_{\geqslant k}, S^i{}_{\geqslant k}] &= (\partial_{t_j}S^i)_{\geqslant k} - (\partial_{t_i}S^j)_{\geqslant k} - [S^j{}_{\geqslant k}, S^i{}_{\geqslant k}] \\
&= [S^j{}_{\geqslant k}, S^i]_{\geqslant k} - [S^i{}_{\geqslant k}, S^j]_{\geqslant k} - [S^j{}_{\geqslant k}, S^i{}_{\geqslant k}] \\
&= -[S^j{}_{<k}, S^i{}_{\geqslant k} + S^i{}_{<k}]_{\geqslant k} - [S^i{}_{\geqslant k}, S^j{}_{\geqslant k} + S^j{}_{<k}]_{\geqslant k} - [S^j{}_{\geqslant k}, S^i{}_{\geqslant k}] \\
&= -[S^j{}_{<k}, S^i{}_{<k}]_{\geqslant k} = 0.
\end{aligned}$$

This leads to $\partial_{t_j}\partial_{t_i}L=\partial_{t_i}\partial_{t_j}L$. ◇

Remark 1: In the commutative case, there is one more admissible type of scalar Lax operator, that is,

$$k=2: \quad L = u^{(n)^n}D_x^n + u^{(n-1)}D_x^{n-1} + u^{(n-2)}D_x^{n-2} + \cdots + u^{(0)} + D_x^{-1}u^{(-1)} + D_x^{-2}u^{(-2)} - D_y.$$

Theorem 1 is also valid for this type by taking $S=u^{(n)}D_x+a_0+a_{-1}D_x^{-1}+\cdots$ instead.

Example 4: Consider the Lax operator $L=u^2D_x^2+vD_x+w+D_x^{-1}p+D_x^{-2}q-D_y$, *where all dependent variables take their values in* $\mathbb{C}$. *Using formula (7), we have* $S=uD_x+a_0+a_{-1}D_x^{-1}+\cdots$ *with*

$$a_0 = -\frac{1}{2}\left(u_x - \frac{v}{u} + \Theta\frac{1}{u}\right)$$

$$a_{-1} = \frac{1}{8}\left(2u_{xx} - \frac{u_x^2}{u} - \frac{2v_x}{u} + \frac{4u_xv}{u^2} - \frac{v^2}{u^3} - \frac{4u_y}{u^2} + \frac{2}{u}\Theta\frac{v}{u^2} + \frac{4w}{u} - \frac{2}{u}\Theta\left(\frac{1}{u}\Theta\frac{1}{u}\right) + \frac{1}{u}\left(\Theta\frac{1}{u}\right)^2\right).$$

and $S^1{}_{\geqslant 2}=0$, $S^2{}_{\geqslant 2}=u^2D_x^2$, $S^3{}_{\geqslant 2}=u^3D_x^3+3u^2(u_x+a_0)D_x^2$. *By the Lax equation, we obtain*

$$\begin{cases} u_{t_3} = \frac{1}{4}\left(u^3 u_{xxx} - 6u_y \Theta \frac{1}{u} - 3u\left(\Theta \frac{1}{u} \right)_y + 3u^2 v_{xx} + 3u^2 w_x + 3v_y + 3v v_x - 3\frac{u_x}{u} v^2 - 6(uv)_x \Theta \frac{1}{u} \right) \\ v_{t_3} = u^3 v_{xxx} + 3u^2 (w_{xx} + u p_x + u_x p + (v_{xx} + 2w_x)(u_x + a_0)) \\ w_{t_3} = u^3 w_{xxx} + 3u^2 (w_{xx} + p_x)(u_x + a_0) + 3p(u^2 a_0)_x + 3u^2 (u q_x - 2u_x p_x + 2u_x q) \\ p_{t_3} = (u^3 p)_{xxx} - 3([u^2 (u_x p + a_0 p + q)]_{xx} + 2[u^2 q (u_x + a_0)]_x) \\ q_{t_3} = (u^3 q)_{xxx} - 3[u^2 q (u_x + a_0)]_{xx}. \end{cases}$$

Notice that the reduction of $v=w=p=q=0$ *leads to the well-known* $(2+1)$*-Harry-Dym equation*

$$u_{t_3} = \frac{1}{4}\left(u^3 u_{xxx} - 6u_y \Theta \frac{1}{u} - 3u\left(\Theta \frac{1}{u} \right)_y \right).$$

IV. LAX FORMULATION IN SYMBOLIC REPRESENTATION

In this section, we carry out the formalism of Sec. III in symbolic form. We first consider noncommutative dependent variables to simplify our formulas. The strategy for the commutative case is to do the calculation as much as possible by treating it as noncommutative and only do symmetrization at the last stage to get the uniqueness of the symbolic representation since the symmetrization complicates the calculation dramatically.

Let us assign the symbols $\xi^{(i)}$, $\eta^{(i)}$ for dependent variable $u^{(i)}$ and the symbol Y for the operator D_y. The symbolic representations of the admissible scalar Lax operators are

(a) $k=0$: $\hat{L} = X^n - Y + u^{(n-2)} X^{n-2} + u^{(n-3)} X^{n-3} + \cdots + u^{(0)}, \quad n \geqslant 2;$

(b) $k=1$: $\hat{L} = X^n - Y + u^{(n-1)} X^{n-1} + u^{(n-2)} X^{n-2} + \cdots + u^{(0)} + u^{(-1)} \frac{1}{X + \xi^{(-1)}}, \quad n \geqslant 2;$

(c) $k=1$: $\hat{L} = -Y + u^{(0)} + u^{(-1)} \frac{1}{X + \xi^{(-1)}}.$

We first treat case (a). It is convenient to consider formal series in the form, for $n \geqslant 2$,

$$S = X + \sum_{i=0}^{n-2} u^{(i)} a_1^{(i)}(\xi_1^{(i)}, \eta_1^{(i)}, X) + \sum_{i_1=0}^{n-2} \sum_{i_2=0}^{n-2} u^{(i_1)} u^{(i_2)} a_2^{(i_1 i_2)}(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \xi_{j_2}^{(i_2)}, \eta_{j_2}^{(i_2)}, X) + \cdots, \tag{10}$$

where a_i are functions of their specific arguments and j_k is defined by the number of i_k in the list of $[i_1, i_2, \ldots, i_l]$, which implies that $j_1=1$ and $j_k \geqslant 1$, $k=1,2,\ldots,l$. For example, when $i_1=i_2$, the arguments of function $a_2^{i_1 i_1}$ are $\xi_1^{(i_1)}$, $\eta_1^{(i_1)}$, $\xi_2^{(i_1)}$, $\eta_2^{(i_1)}$, and X.

It is easy to check that

$$[X^n - Y, \phi(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X)] = N_l(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X)\phi, \tag{11}$$

where the polynomial N_l is defined by

$$N_l(x_1, y_1, x_2, y_2, \ldots, x_l, y_l; X) = \left(\sum_{i=1}^{l} x_i + X \right)^n - X^n - \sum_{i=1}^{l} y_i. \tag{12}$$

Proposition 1: For any operator L *in case* (a)*, if the formal series (10) satisfies the relation* $[S,L]=0$ *[cf. (7)], we have for* $l \geqslant 1$,

$$a_l^{(i_1 i_2 \cdots i_l)} = a_l(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X) = \prod_{r=1}^{l} \left(X + \sum_{s=r+1}^{l} \xi_{j_s}^{(i_s)} \right)^{i_r} b_l(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X), \tag{13}$$

where the superindex $i_s \in \{0,1,2,\ldots,n-2\}$ *and the subindex* j_k *is defined by the number of* i_k *in the list of* $[i_1,i_2,\ldots,i_k]$. *The function* b_l, $l \geqslant 1$, *is defined by*

$$b_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)=\frac{c_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}{N_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)} \tag{14}$$

with $l>1$

$$\begin{aligned} c_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X) &= b_{l-1}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)}\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)}) \\ &\quad - b_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X) \end{aligned} \tag{15}$$

and the initial function $c_1(\xi_1^{(i)},\eta_1^{(i)},X)=\xi_1^{(i)}$.

Proof: We compute $[L,S]$ symbolically and collect the coefficients of each algebraically independent monomial of the dependent variables. For the linear terms, we have for any $i \in \{0,\ldots,n-2\}$,

$$a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)=\frac{\xi_1^{(i)}X^i}{N_1(\xi_1^{(i)},\eta_1^{(i)},X)}=b_1(\xi_1^{(i)},\eta_1^{(i)},X)X^i. \tag{16}$$

For the quadratic terms, when $i \neq j$, we need to compute

$$\begin{aligned} A^{ij} &:= -X^i \circ a_1^{(j)}(\xi_1^{(j)},\eta_1^{(j)},X)+a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)\circ X^j \\ &= -\frac{(X+\xi_1^{(j)})^i\xi_1^{(j)}X^j}{N_1(\xi_1^{(j)},\eta_1^{(j)},X)}+\frac{\xi_1^{(i)}(X+\xi_1^{(j)})^iX^j}{N_1(\xi_1^{(i)},\eta_1^{(i)},X+\xi_1^{(j)})} \\ &= (X+\xi_1^{(j)})^iX^j\left(\frac{\xi_1^{(i)}}{N_1(\xi_1^{(i)},\eta_1^{(i)},X+\xi_1^{(j)})}-\frac{\xi_1^{(j)}}{N_1(\xi_1^{(j)},\eta_1^{(j)},X)}\right) \\ &= (X+\xi_1^{(j)})^iX^j(b_1(\xi_1^{(i)},\eta_1^{(i)},X+\xi_1^{(j)})-b_1(\xi_1^{(j)},\eta_1^{(j)},X))=(X+\xi_1^{(j)})^iX^jc_2(\xi_1^{(i)},\eta_1^{(i)},\xi_1^{(j)},\eta_1^{(j)},X), \end{aligned}$$

and when $i=j$, we have

$$\begin{aligned} A^{ii} &:= -[X^i,a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)]=-X^i\circ a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)+a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)\circ X^i \\ &= -\frac{(X+\xi_2^{(i)})^i\xi_2^{(i)}X^i}{N_1(\xi_2^{(i)},\eta_2^{(i)},X)}+\frac{\xi_1^{(i)}(X+\xi_2^{(i)})^iX^i}{N_1(\xi_1^{(i)},\eta_1^{(i)},X+\xi_2^{(i)})}. \end{aligned}$$

This can be obtained by substituting $\xi_1^{(j)}=\xi_2^{(i)}$ and $\eta_1^{(j)}=\eta_2^{(i)}$ in A^{ij}. It follows that

$$a_2^{(i_1i_2)}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},X)=\frac{A^{i_1i_2}}{N_2(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},X)}=(X+\xi_{j_2}^{(i_2)})^{i_1}X^{i_2}b_2(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},X). \tag{17}$$

Assume that formula (13) is valid for degree $l-1$. Let us compute $a_l^{(i_1i_2\cdots i_l)}$ in the same way as computing the quadratic terms. Then we have

$$\begin{aligned} &N_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)a_l^{(i_1i_2\cdots i_l)} \\ &\quad = -X^{i_1}\circ a_{l-1}^{(i_2\cdots i_l)}+a_{l-1}^{(i_1i_2\cdots i_{l-1})}\circ X^{i_l} \\ &\quad = -\left(X+\sum_{p=2}^{l}\xi_{j_p}^{(i_p)}\right)^{i_1}\prod_{r=2}^{l}\left(X+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}\right)^{i_r}b_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X) \end{aligned}$$

$$
\begin{aligned}
&+\prod_{r=1}^{l-1}\left(X+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}\right)^{i_r} X^{i_l} b_{l-1}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})\\
&=\prod_{r=1}^{l}\left(X+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}\right)^{i_r}(b_{l-1}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})\\
&\quad-b_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X))\\
&=\prod_{r=1}^{l}\left(X+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}\right)^{i_r} c_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X).
\end{aligned}
$$

According to definition (14), we proved that formula (13) is valid for degree l. ◇

Similarly, we prove the following result for any operator L in cases (b) and (c).

Proposition 2: For any operator L in case (b), *consider a formal series of the form for* $n\geqslant 2$,

$$
S=X+\sum_{i=-1}^{n-1}u^{(i)}a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)+\sum_{i_1,i_2=-1}^{n-1}u^{(i_1)}u^{(i_2)}a_2^{(i_1i_2)}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},X)+\cdots . \tag{18}
$$

Here a_i *are functions of their specific arguments, the superindex* $i_s\in\{-1,0,1,\ldots,n-1\}$ *and the subindex* j_k *is defined by the number of* i_k *in the list of* $[i_1,i_2,\ldots,i_k]$. *If it satisfies the relation* $[S,L]=0$ *[cf. (7)], we have for* $l\geqslant 1$,

$$
a_l^{(i_1i_2\cdots i_l)}=a_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)=\prod_{r=1}^{l}\left(h(i_r)+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}\right)^{i_r} b_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X), \tag{19}
$$

where $h(i_r)=X+\xi_{j_r}^{(-1)}$ *if* $i_r=-1$, *otherwise* $h(i_r)=X$. *The functions* b_l *are defined in Proposition 1; cf. formula (14) and (15).*

Notice that for operator L listed in case (c), we have $N_l(x_1,y_1,x_2,y_2,\ldots,x_l,y_l;X)=-\Sigma_{i=1}^{l}y_i$, cf. (11), which corresponds to the action of total y-derivative D_y. Thus

Proposition 3: For operator L listed in case (c), *if a formal series of the form*

$$
S=X+\sum_{i=-1}^{0}u^{(i)}a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)+\sum_{i_1,i_2=-1}^{0}u^{(i_1)}u^{(i_2)}a_2^{(i_1i_2)}(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},X)+\cdots , \tag{20}
$$

where the superindex $i_s\in\{-1,0\}$ *and the subindex* j_k *is defined by the number of* i_k *in the list of* $[i_1,i_2,\ldots,i_k]$, *satisfies the relation* $[S,L]=0$ *[cf. (7)], we have for* $l\geqslant 1$, *the functions* a_l *are defined in Proposition 2, cf. formula (19) with* $N_l(x_1,y_1,x_2,y_2,\ldots,x_l,y_l;X)=-\Sigma_{i=1}^{l}y_i$.

To construct the hierarchy of the Lax equations we need to expand the coefficients of operator (10) or (18) or (20) at $X=\infty$ and truncate at the required degree.

Definition 3: *We say that a function* $h(x_1,y_1,x_2,y_2,\ldots,x_l,y_l,X)$ *is kth (quasi-local) polynomial if the first k coefficients of its expansion at* $X=\infty$ *are symbols of (quasi-local) polynomials. If a function is kth (quasi-local) polynomial for any k, we say it is (quasi-local) polynomial.*

When $n\geqslant 2$, that is, operator L in cases (a) and (b), the expansion of $N_l(x_1,y_1,x_2,y_2,\ldots,x_l,y_l;X)$ at $X=\infty$ is of the form

$$
\begin{aligned}
&N_l(x_1,y_1,x_2,y_2,\ldots,x_l,y_l;X)^{-1}\\
&=\frac{1}{nX^{n-1}\left(\sum_{i=1}^{l}x_i\right)}\sum_{j\geqslant 0}\left[\frac{\sum_{i=1}^{l}y_i}{nX^{n-1}\left(\sum_{i=1}^{l}x_i\right)}-\frac{1}{n}\sum_{k=0}^{n-2}\binom{n}{k}X^{k+1-n}\left(\sum_{i=0}^{l}x_i\right)^{n-k-1}\right]^{j},\quad n\geqslant 2.
\end{aligned}
$$

For operator L listed in case (c), we know $N_l(x_1,y_1,x_2,y_2,\ldots,x_l,y_l;X)=-\Sigma_{i=1}^{l}y_i$. Therefore, if we

want to prove that the coefficients of operators (10), (18), and (20), i.e., the functions a_l, are quasi-local, we need to show that the functions c_l can be split into the sum of the image of D_x and the image of D_y. It is clear from formula (16) that $a_1^{(i)}(\xi_1^{(i)},\eta_1^{(i)},X)$ are quasi-local since we have $c_1(\xi_1^{(i)},\eta_1^{(i)},X)=\xi_1^{(i)}$. Now we concentrate on the cases when $l>1$.

Proposition 4: The functions $c_l(\xi_{j_1}^{(i_1)},\eta_{j_1}^{(i_1)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)$ *for* $l>1$ *vanish after substitution*

$$\xi_{j_1}^{(i_1)}=-\xi_{j_2}^{(i_2)}-\cdots-\xi_{j_{l-1}}^{(i_{l-1})} \text{ and } \eta_{j_1}^{(i_1)}=-\eta_{j_2}^{(i_2)}-\cdots-\eta_{j_{l-1}}^{(i_{l-1})}.$$

We give its proof in the Appendix. In fact, this proposition does not lead to our intended conclusion that b_l and thus a_l are quasi-local since the objects are rational, not polynomial. For example, the expression $u^2((\eta_2/\xi_2)-(\eta_1/\xi_1))$ representing $u\Theta u-(\Theta u)u$ satisfies the above proposition. However, we cannot write $u\Theta u-(\Theta u)u=D_xf_1+D_yf_2$, where both f_1 and f_2 are in $\mathcal{U}(\Theta)$.

We first have a close look at the quadratic terms. For any operator L in cases (a) and (b), let $\eta_{j_r}^{i_r}=\theta_{j_r}^{i_r}\xi_{j_r}^{i_r}$. Then the function $c_2(\xi_{j_1}^{i_1},\eta_{j_1}^{i_1},\xi_{j_2}^{i_2},\eta_{j_2}^{i_2},X)$, where $\xi_{j_1}^{i_1}\neq 0$ and $\xi_{j_2}^{i_2}\neq 0$, is a polynomial of $\theta_{j_r}^{i_r},\xi_{j_r}^{i_r}$, $r=1,2$. Notice that

$$(\eta_{j_1}^{i_1}+\eta_{j_2}^{i_2})=\theta_{j_1}^{i_1}\xi_{j_1}^{i_1}+\theta_{j_2}^{i_2}\xi_{j_2}^{i_2}=(\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})\xi_{j_1}^{i_1}+\theta_{j_2}^{i_2}(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2})=\theta_{j_1}^{i_1}(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2})-(\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})\xi_{j_2}^{i_2}. \tag{21}$$

The affine variety (cf. Ref. 21) defined by $\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2}$ and $\eta_{j_1}^{i_1}+\eta_{j_2}^{i_2}$ is

$$V(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2},\eta_{j_1}^{i_1}+\eta_{j_2}^{i_2})=V(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2},(\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})\xi_{j_1}^{i_1},(\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})\xi_{j_2}^{i_2})=V(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2},\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})\cup V(\xi_{j_1}^{i_1},\xi_{j_2}^{i_2}).$$

From Proposition 4, it can be written as

$$c_2(\xi_{j_1}^{i_1},\theta_{j_1}^{i_1}\xi_{j_1}^{i_1},\xi_{j_2}^{i_2},\theta_{j_2}^{i_2}\xi_{j_2}^{i_2},X)=(\xi_{j_1}^{i_1}+\xi_{j_2}^{i_2})f_1+(\theta_{j_1}^{i_1}-\theta_{j_2}^{i_2})f_2,$$

where both f_1 and f_2 are polynomials of $\theta_{j_r}^{i_r},\xi_{j_r}^{i_r}$, $r=1,2$. From formula (21), the part that is not in the image of D_x or D_y only depends on $\theta_{j_r}^{i_r}$, $r=1,2$.

For operator L listed in case (c) since the function $N_l(x_1,y_1,\ldots,x_l,y_l,X)=-\Sigma_{i=1}^{l}y_i$, cf. Proposition 3, we let $\xi_{j_r}^{i_r}=\theta_{j_r}^{i_r}\eta_{j_r}^{i_r}$ instead. Then the function $c_2(\xi_{j_1}^{i_1},\eta_{j_1}^{i_1},\xi_{j_2}^{i_2},\eta_{j_2}^{i_2},X)$, where $\eta_{j_1}^{i_1}\neq 0$ and $\eta_{j_2}^{i_2}\neq 0$, is a polynomial of $\theta_{j_r}^{i_r},\xi_{j_r}^{i_r}$, $r=1,2$. The above discussion is valid.

Setting $\xi_{j_1}^{i_1}=\xi_{j_2}^{i_2}=0$, we obtain the function $c_2(\xi_{j_1}^{i_1},\eta_{j_1}^{i_1},\xi_{j_2}^{i_2},\eta_{j_2}^{i_2},X)$ equals

$$\frac{1}{nX^{n-1}-\theta_{j_1}^{i_1}}-\frac{1}{nX^{n-1}-\theta_{j_2}^{i_2}} \quad \text{for cases (a) and (b)}; \quad \theta_{j_2}^{i_2}-\theta_{j_1}^{i_1} \quad \text{for case (c)}, \tag{22}$$

which is zero after we symmetrize it with the permutation group Σ_2. This implies that the functions b_2 and thus a_2 are quasi-local in the commutative case.

A. The commutative case

We first give the formulas to compute the high degree terms of operator S for the commutative case directly from the formulas we obtained in Propositions 1, 2, and 3.

We denote the list $(i_1,i_2,\ldots,i_l)$ by I and $I_1=(i_{s_1},i_{s_2},\ldots,i_{s_r})$, where $1\leqslant s_1<s_2<\cdots<s_r\leqslant l$ and $1\leqslant r\leqslant l-1$. We use $I_2=(i_{p_1},i_{p_2},\ldots,i_{p_{l-r}})$ to denote the list by removing the elements of list I_1 from list I. For any element i_r in the set $\{i_1,i_2,\ldots,i_l\}$, we denote the number of i_r in the list I by $\#i_r$. Then the coefficient of $\Pi_{i_r\in\{i_1i_2\cdots i_l\}}(u^{(i_r)})^{\#i_r}$ in operator S, cf. formula (10), (18), and (20), can be computed by

$$\frac{1}{\prod_{i_r\in\{i_1i_2\cdots i_l\}}(\#i_r)!}\sum_{\sigma\in\Sigma_l}a_l(\xi_{j_{\sigma(1)}}^{(i_{\sigma(1)})},\eta_{j_{\sigma(1)}}^{(i_{\sigma(1)})},\ldots,\xi_{j_{\sigma(l)}}^{(i_{\sigma(l)})},\eta_{j_{\sigma(l)}}^{(i_{\sigma(l)})},X). \tag{23}$$

We denote it by

$$\frac{d_l^{i_1 i_2 \cdots i_l}}{N_l(\xi_{j_1}^{(i_1)}, \eta_{j_1}^{(i_1)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X)}.$$

In particular, for any operator L in case (a), the numerator $d_l^{i_1 i_2 \cdots i_l}$ equals

$$\frac{1}{\prod_{i_r \in \{i_1 i_2 \cdots i_l\}} (\#i_r)!} \sum_{\sigma \in \Sigma_l} \prod_{r=1}^{l} \left(X + \sum_{s=r+1}^{l} \xi_{j_{\sigma(s)}}^{(i_{\sigma(s)})} \right)^{i_{\sigma(r)}} c_l(\xi_{j_{\sigma(1)}}^{(i_{\sigma(1)})}, \eta_{j_{\sigma(1)}}^{(i_{\sigma(1)})}, \ldots, \xi_{j_{\sigma(l)}}^{(i_{\sigma(l)})}, \eta_{j_{\sigma(l)}}^{(i_{\sigma(l)})}, X). \quad (24)$$

For cases (b) and (c) the expression $(X+p)^{-1}$, where $p=\xi_{j_r}^{(-1)}+\sum_{s=r+1}^{l}\xi_{j_s}^{(i_s)}$, appears in formula (19). Its expansion at $X=\infty$ is of the form

$$(X+p)^{-1} = \frac{1}{X} \sum_{j=0}^{+\infty} \left(-\frac{p}{X} \right)^s, \quad (25)$$

whose coefficients are polynomials in p. This does not affect the proof and result. For case (c), we need to exchange the symbols $\xi_{j_r}^{i_r}$ and $\eta_{j_r}^{i_r}$ in the proof as the discussion we did for quadratic terms. Therefore, we will only give the proof for case (a).

The immediate consequence of the previous discussion on the quadratic terms is the following statement.

Proposition 5: All quadratic terms in operator S are quasi-local.

In fact, we can prove this statement is valid for all $l>0$.

Theorem 2: *Every term in the operator S, cf. formula* (10), (18), and (20), *obtained via* (23) *is quasi-local.*

Proof: We proved the linear and quadratic terms in S are quasi-local, that is, the statement is true for $l=1,2$. Assume it is also true for $l-1$. By induction, the function $d_l^{i_1 i_2 \cdots i_l}$, cf. (24), is polynomial of $\xi_{j_r}^{(i_r)}$ and $\theta_{I_1}=(\eta_{j_{s_1}}^{(i_{s_1})}+\cdots\eta_{j_{s_r}}^{(i_{s_r})})/(\xi_{j_{s_1}}^{(i_{s_1})}+\cdots\xi_{j_{s_r}}^{(i_{s_r})})$, $r=1,2,\ldots,l-1$, which obviously satisfies Proposition 4. This implies that the function $d_l^{i_1 i_2 \cdots i_l}$ is the sum of the parts with factors $\xi_{j_1}^{(i_1)}+\xi_{j_2}^{(i_2)}+\cdots+\xi_{j_l}^{(i_l)}$ or $\theta_{I_1}-\theta_{I_2}$ using the argument of the affine variety. From the recurrent relation in Proposition 1, we can compute the factor for any $\theta_{I_1}-\theta_{I_2}$ (without symmetrization), which equals

$$\prod_{q=1}^{r}(X+\xi_{j_{s_{q+1}}}^{(i_{s_{q+1}})}+\cdots+\xi_{j_{s_r}}^{(i_{s_r})}+\xi_{j_{p_1}}^{(i_{p_1})}+\cdots+\xi_{j_{p_{l-r}}}^{(i_{p_{l-r}})})^{i_{s_q}}\prod_{q=1}^{l-r}(X+\xi_{j_{p_{q+1}}}^{(i_{p_{q+1}})}+\cdots+\xi_{j_{p_{l-r}}}^{(i_{p_{l-r}})})^{i_{p_q}}$$
$$-\prod_{q=1}^{l-r}(X+\xi_{j_{p_{q+1}}}^{(i_{p_{q+1}})}+\cdots+\xi_{j_{p_{l-r}}}^{(i_{p_{l-r}})}+\xi_{j_{s_1}}^{(i_{s_1})}+\cdots+\xi_{j_{s_r}}^{(i_{s_r})})^{i_{p_q}}\prod_{q=1}^{r}(X+\xi_{j_{s_{q+1}}}^{(i_{s_{q+1}})}+\cdots+\xi_{j_{s_r}}^{(i_{s_r})})^{i_{s_q}}.$$

This expression is zero under the substitution $\Xi_{I_2}=\xi_{j_{p_1}}^{(i_{p_1})}+\cdots+\xi_{j_{p_{l-r}}}^{(i_{p_{l-r}})}=0$ and $\Xi_{I_1}=\xi_{j_{s_1}}^{(i_{s_1})}+\cdots+\xi_{j_{s_r}}^{(i_{s_r})}=0$, implying we have either $\Xi_{I_2}(\theta_{I_1}-\theta_{I_2})$ or $\Xi_{I_1}(\theta_{I_1}-\theta_{I_2})$ as a factor. We know

$$\Xi_{I_2}(\theta_{I_1}-\theta_{I_2})=\theta_{I_1}(\xi_{j_1}^{(i_1)}+\cdots+\xi_{j_l}^{(i_l)})-(\eta_{j_1}^{(i_1)}+\cdots+\eta_{j_l}^{(i_l)});$$

$$\Xi_{I_1}(\theta_{I_1}-\theta_{I_2})=(\eta_{j_1}^{(i_1)}+\cdots+\eta_{j_l}^{(i_l)})-\theta_{I_2}(\xi_{j_1}^{(i_1)}+\cdots+\xi_{j_l}^{(i_l)}).$$

Thus, the lth degree term of S is quasi-local. ◇

This theorem implies that every terms in S^n is quasi-local. From Theorem 1, we have

Theorem 3: *The hierarchies of* $(2+1)$*-integrable equation with scalar Lax operators are quasi-local.*

As mentioned in Remark 1, there is one more type of scalar Lax operator in the commutative case. The same result can be proved by extending the symbolic approach used in Ref. 22 for the $(1+1)$-dimensional case.

B. The noncommutative case

The extension of the concept of quasi-locality to the noncommutative case is rather complicated. D_x and D_y are the only derivations for the commutative differential ring. The extension simply enables us to apply D_x^{-1} and D_y^{-1} on the derivations. We know that the C_f, cf. (4), are also derivations for a noncommutative associative algebra and we need to take them into consideration. Based on Proposition 4, we propose the following extension using the symbolic representation. We start with $\mathcal{A}^k$, the space of polynomials in $2k$ variables, ξ_i and η_i, $i=1,\ldots,k$. Let $\xi_i=\lambda z_i$ and $\eta_i=\mu z_i$, where λ, μ are constants. We define $I(\mathcal{A}^k)$ as a set of all $f\in\mathcal{A}^k$ satisfying $f|_{z_1+\cdots z_k=0}=0$. For the elements in $g\in I(\mathcal{A}^k)$, we compute $g/(\xi_1+\cdots+\xi_k)$ and $g/(\eta_1+\cdots\eta_k)$ and collect them in the set $\mathcal{E}xt(\mathcal{A}^k)$. Now we define a sequence of extensions of $\mathcal{A}=\cup_k\mathcal{A}^k$. Let $\mathcal{A}_0^{ext}=\mathcal{A}$ and $\mathcal{A}_1^{ext}$ be the ring closure of the union $\mathcal{A}_0^{ext}\cup(\cup_k\mathcal{E}xt(\mathcal{A}^k))$. The number of variables is a natural grade on $\mathcal{A}_1^{ext}$ and again denote $\mathcal{A}_1^{ext^k}$ the space of elements in $\mathcal{A}_1^{ext}$ with $2k$ variables, ξ_i and η_i, $i=1,\ldots,k$. In general, we can define $\mathcal{A}_l^{ext}$ is the ring closure of the union $\mathcal{A}_{l-1}^{ext}\cup(\cup_k\mathcal{E}xt(\mathcal{A}_{l-1}^{ext^k}))$. Clearly, we have $\mathcal{A}_{l-1}^{ext}\subset\mathcal{A}_l^{ext}$. We now define $\mathcal{A}^{ext}=\lim_{l\to\infty}\mathcal{A}_l^{ext}$.

The above ring extension is bigger than we require. For example, the expression $(\eta_2/\xi_2)-(\eta_1/\xi_1)$ is not equal to zero under the substitution $\xi_1+\xi_2+\xi_3=0$ and $\eta_1+\eta_2+\eta_3=0$, that is, not satisfying Proposition 4. But it is in $I(\mathcal{A}_1^{ext^3})$. If we start from the symmetric polynomial, we hope to end up with the extension of commutative differential polynomial, i.e., quasi-local polynomials we defined in Sec. II. It is not difficult to notice that this extension is bigger than the concept of quasi-local commutative polynomials. However, we can not formulate such extension either via symbolic representation or from noncommutative differential polynomials as in the commutative case. It is still an open problem.

Here we compute explicitly some Lax flows for lower order scalar Lax operators of noncommutative dependent variable, which will help the reader to see the structures.

1. Noncommutative Boussinesq equation

Let us compute the hierarchy of Lax operator $L=D_x^3+uD_x+v-D_y$. From Proposition 1, we have

$$
\begin{aligned}
S=&X+u\frac{\xi_1^{(1)}X}{(X+\xi_1^{(1)})^3-X^3-\eta_1^{(1)}}+v\frac{\xi_1^{(0)}}{(X+\xi_1^{(0)})^3-X^3-\eta_1^{(0)}}+\frac{u^2(X+\xi_2^{(1)})X}{(X+\xi_1^{(1)}+\xi_2^{(1)})^3-X^3-\eta_1^{(1)}-\eta_2^{(1)}}\\
&\times\left(\frac{\xi_1^{(1)}}{(X+\xi_1^{(1)}+\xi_2^{(1)})^3-(X+\xi_2^{(1)})^3-\eta_1^{(1)}}-\frac{\xi_2^{(1)}}{(X+\xi_2^{(1)})^3-X^3-\eta_2^{(1)}}\right)\\
&+\frac{uv(X+\xi_1^{(0)})}{(X+\xi_1^{(1)}+\xi_1^{(0)})^3-X^3-\eta_1^{(1)}-\eta_1^{(0)}}\left(\frac{\xi_1^{(1)}}{(X+\xi_1^{(1)}+\xi_1^{(0)})^3-(X+\xi_1^{(0)})^3-\eta_1^{(1)}}\right.\\
&\left.-\frac{\xi_1^{(0)}}{(X+\xi_1^{(0)})^3-X^3-\eta_1^{(0)}}\right)+\frac{vuX}{(X+\xi_1^{(1)}+\xi_1^{(0)})^3-X^3-\eta_1^{(1)}-\eta_1^{(0)}}\\
&\times\left(\frac{\xi_1^{(0)}}{(X+\xi_1^{(1)}+\xi_1^{(0)})^3-(X+\xi_1^{(1)})^3-\eta_1^{(0)}}-\frac{\xi_1^{(1)}}{(X+\xi_1^{(1)})^3-X^3-\eta_1^{(1)}}\right)+\cdots\\
=&X+\frac{u}{3X}+\frac{v-u\xi_1^{(1)}}{3X^2}+\left(\frac{2u\xi_1^{(1)^2}}{9}+\frac{u\eta_1^{(1)}}{9\xi_1^{(1)}}-\frac{v\xi_1^{(0)}}{3}-\frac{u^2}{9}\right)\frac{1}{X^3}\\
&+\left(\frac{-u\xi_1^{(1)^3}}{9}-\frac{2u\eta_1^{(1)}}{9}+\frac{2v\xi_1^{(0)^2}}{9}+\frac{v\eta_1^{(0)}}{9\xi_1^{(0)}}-\frac{uv}{9}-\frac{vu}{9}+u^2\left(\frac{7\xi_2^{(1)}}{27}+\frac{5\xi_1^{(1)}}{27}+\frac{\frac{\eta_1^{(1)}}{27\xi_1^{(1)}}-\frac{\eta_2^{(1)}}{27\xi_2^{(1)}}}{\xi_1^{(1)}+\xi_2^{(1)}}\right)\right)\frac{1}{X^4}
\end{aligned}
$$

$$+\cdots,$$

which corresponds to

$$S = D_x + \frac{u}{3}D_x^{-1} + \left(\frac{v}{3} - \frac{u_x}{3}\right)D_x^{-2} + \left(\frac{2u_{xx}}{9} + \frac{\Theta u}{9} - \frac{v_x}{3} - \frac{u^2}{9}\right)D_x^{-3} + \left(\frac{2v_{xx}}{9} - \frac{u_{xxx}}{9} - \frac{2u_y}{9} + \frac{\Theta v}{9} - \frac{uv}{9} - \frac{vu}{9} + \frac{7uu_x}{27} + \frac{5u_x u}{27} + \frac{D_x^{-1}((\Theta u)u)}{27} - \frac{D_x^{-1}(u\Theta u)}{27}\right)D_x^{-4} + \cdots.$$

This leads to

$$S_{\geqslant 0} = D_x; \quad S^2_{\geqslant 0} = D_x^2 + \frac{2}{3}u; \quad S^3_{\geqslant 0} = D_x^3 + uD_x + v;$$

$$S^4_{\geqslant 0} = D_x^4 + \frac{4}{3}uD_x^2 + \frac{2}{3}(u_x + 2v)D_x + \frac{4}{9}\Theta u + \frac{2}{9}u^2 + \frac{2}{9}u_{xx} + \frac{2}{3}v_x;$$

$$S^5_{\geqslant 0} = D_x^5 + \frac{5}{3}uD_x^3 + \frac{5}{3}(u_x + v)D_x^2 + \left(\frac{5}{9}\Theta u + \frac{5}{9}u^2 + \frac{10}{9}u_{xx} + \frac{5}{3}v_x\right)D_x + \frac{10}{9}v_{xx} + \frac{5}{9}(\Theta v + uv + vu) + \frac{5}{27}(uu_x - u_x u + D_x^{-1}((\Theta u)u - u\Theta u)).$$

And we have

$$\begin{cases} u_{t_2} = -u_{xx} + 2v_x \\ v_{t_2} = v_{xx} + \frac{2}{3}(u_y - u_{3x} - uu_x + uv - vu). \end{cases}$$

Eliminating the dependent variable v from this equation and writing $t_2 = t$, we can derive the $(2+1)$-dimensional Boussinesq equation

$$u_{tt} = -\frac{1}{3}u_{4x} + \frac{4}{3}u_{xy} - \frac{2}{3}(u^2)_{xx} + \frac{2}{3}D_x[u, D_x^{-1}u_t].$$

Under the scaling transformation $x \mapsto \sqrt{6}x$, $y \mapsto \sqrt{\frac{3}{2}}y$, $u \mapsto 3u$, $t \mapsto 2t$, it can be rewritten as

$$u_{tt} = -u_{4x} + u_{xy} - 3(u^2)_{xx} + D_x[u, D_x^{-1}u_t].$$

Let $w = D_x^{-1}u$. We get the $(2+1)$-dimensional noncommutative potential Boussinesq equation

$$w_{tt} = -w_{4x} + w_{xy} - 3(w_x^2)_x + [w_x, w_t].$$

2. Noncommutative KP equation

Let us compute the hierarchy of the Lax operator $L = D_x^2 + u - D_y$. Since the order of L is low, it is easier to compute the operator S directly order by order as in Example 4 than to apply Proposition 2. Let

$$S = D_x + a_{-1}D_x^{-1} + a_{-2}D_x^{-2} + a_{-3}D_x^{-3}\cdots.$$

Using formula (10), we obtain

$$a_{-1} = \frac{u}{2}$$

$$a_{-2} = -\frac{u_x}{4} + \frac{\Theta u}{4}$$

$$a_{-3} = \frac{\Theta^2 u}{8} + \frac{u_{xx}}{8} - \frac{u_y}{4} - \frac{u^2}{8} - \frac{1}{8} D_x^{-1} C_u \Theta u.$$

This leads to

$$S^3_{\geqslant 0} = D_x^3 + \frac{3u}{2} D_x + \frac{3}{4}(u_x + \Theta u)$$

$$S^4_{\geqslant 0} = D_x^4 + 2uD_x^2 + (2u_x + \Theta u)D_x + \frac{u_y}{2} + u^2 + u_{xx} + \frac{\Theta^2 u}{2} - \frac{1}{2} D_x^{-1} C_u \Theta u$$

$$= 2D_x^2 D_y - D_y^2 + 2uD_y + \Theta u D_x + \frac{3u_y}{2} + \frac{\Theta^2 u}{2} - \frac{1}{2} D_x^{-1} C_u \Theta u + L^2.$$

And we have

$$u_{t_3} = \frac{1}{4}(u_{xxx} + 3uu_x + 3u_x u + 3\Theta u_y - 3C_u \Theta u),$$

which is the noncommutative KP equation and can be obtained from the recursion operator of KP, cf., Ref. 5, and

$$u_{t_4} = \frac{1}{2}(u_{xxy} + \Theta^2 u_y + 2uu_y + 2u_y u + u_x \Theta u + (\Theta u)u_x + C_u D_x^{-1} C_u \Theta u - \Theta C_u \Theta u - C_u \Theta^2 u).$$

3. Noncommutative mKP equation

Let us compute the hierarchy of the Lax operator $L = D_x^2 + uD_x + v + D_x^{-1} w - D_y$. Let

$$S = D_x + a_0 + a_{-1} D_x^{-1} + \cdots .$$

Using formula (10), we obtain

$$a_0 = \frac{u}{2}$$

$$a_{-1} = -\frac{u_x}{4} - \frac{u^2}{8} + \frac{v}{2} + \left(D_x + \frac{C_u}{2}\right)^{-1} \frac{u_y}{4}.$$

This leads to

$$S^2_{\geqslant 1} = D_x^2 + uD_x; \quad S^3_{\geqslant 1} = D_x^3 + \frac{3u}{2} D_x^2 + \frac{3}{8}\left(2u_x + u^2 + 4v + 2\left(D_x + \frac{C_u}{2}\right)^{-1} u_y\right) D_x.$$

And we have

$$\begin{cases} u_{t_2} = u_y + 2v_x + uv - vu \\ v_{t_2} = v_x + 2w_x + uv_x + uw - wu \\ w_{t_2} = -w_{xx} + (wu)_x \end{cases}$$

$$\begin{cases} u_{t_3}=\frac{1}{4}u_{xxx}+\frac{3}{8}C_u u_{xx}-\frac{3}{8}uu_x u+\frac{3}{4}u_{xy}+\frac{3}{8}(u^2)_y+\frac{3}{2}v_{xx}+\frac{3}{2}v_y+\frac{3}{2}uv_x+\frac{3}{2}vu_x-\frac{3}{8}C_v u^2-\frac{3}{4}C_v u_x+3w_x+\frac{3}{2}C_u w \\ \quad +\frac{3}{4}(D_y-D_x^2-uD_x+R_{u_x}-C_v)\left(D_x+\frac{C_u}{2}\right)^{-1}u_y \\ v_{t_3}=v_{xxx}+\frac{3}{2}uv_{xx}+\frac{3}{4}u_x v_x+\frac{3}{8}u^2 v_1+\frac{3}{2}vv_1+\frac{3}{2}uw_x+\frac{3}{2}w_x u+\frac{3}{4}wu_x+\frac{3}{4}u_x w-\frac{3}{8}C_w u^2-\frac{3}{2}C_w v+\frac{3}{4}(R_{v_x}-C_w)\left(D_x+\frac{C_u}{2}\right)^{-1}u_y \\ w_{t_3}=w_{xxx}-(wa_0)_{xx}+(wa_{-1})_x. \end{cases}$$

The reduction $v=w=0$ leads to the noncommutative mKP equation

$$u_{t_3}=\frac{1}{4}u_{xxx}+\frac{3}{8}C_u u_{xx}-\frac{3}{8}uu_x u+\frac{3}{4}u_{xy}+\frac{3}{8}(u^2)_y+\frac{3}{4}(D_y-D_x^2-L_u D_x+R_{u_x})\left(D_x+\frac{C_u}{2}\right)^{-1}u_y. \tag{26}$$

If we introduce new variable p satisfying $u_y=p_x+\frac{1}{2}C_u p$, the system for u and p is equivalent to the matrix mKP in Ref. 23.

If u does not depend on y, i.e., $u_y=0$, this gives us the noncommutative mKdV equation,[17,12]

$$u_{t_3}=\frac{1}{4}u_{xxx}+\frac{3}{8}C_u u_{xx}-\frac{3}{8}uu_x u.$$

If u takes its value over $\mathbb{C}$ (commutative), this gives us the well-known mKP equation

$$u_{t_3}=\frac{1}{4}u_{xxx}-\frac{3}{8}u^2u_x+\frac{3}{4}\Theta u_y+\frac{3}{4}u_x\Theta u. \tag{27}$$

We know Miura transformation $V=u_x-(u^2/2)+\Theta u$ transforms the mKP equation (27) into the KP equation $V_{t_3}=\frac{1}{4}V_{xxx}+\frac{3}{4}VV_x+\frac{3}{4}\Theta V_y$. However, we do not know a Miura transformation for noncommutative mKP (26).

4. Nonsymmetric Novikov-Veselov equation

Consider the Lax operator $L=u+D_x^{-1}v-D_y$ [case (c)]. In the commutative case, this worked out in Ref. 24 by both central extension approach and the operand approach. Let $S=D_x+a_0+a_{-1}D_x^{-1}+\cdots$. Using formula (7), we have

$$a_0=(C_u-D_y)^{-1}u_x;$$

$$a_{-1}=(C_u-D_y)^{-1}(v_x+C_v a_0),$$

leading to $S^1{}_{\geqslant 1}=D_x$, $S^1{}_{\geqslant 2}=D_x^2+2a_0D_x$, $S^3{}_{\geqslant 1}=D_x^3+3a_0D_x^2+3(a_{0x}+a_{-1}+a_0^2)D_x$. From the Lax equation, we obtain

$$\begin{cases} u_{t_2}=u_{xx}+2v_x+2a_0u_x+2a_0v-2va_0 \\ v_{t_2}=-v_{xx}+2(va_0)_x \end{cases}$$

$$\begin{cases} u_{t_3}=u_{xxx}+3(a_0u_x)_x+3a_{-1}u_x+3a_0^2u_x+3a_0v_x+3(va_0)_x-3C_v(a_{0x}+a_{-1}+a_0^2) \\ v_{t_3}=v_{xxx}-3(v_xa_0)_x+3(va_{-1})_x+3(va_0^2)_x. \end{cases}$$

The reduction $v=0$ leads to

$$u_{t_2}=u_{xx}-2\{(D_y-C_u)^{-1}u_x\}u_x.$$

Let $w=(D_y-C_u)^{-1}u_x$. This equation transforms into the noncommutative Burgers equation $w_{t_2}=w_{xx}-2ww_x$, which is linearizable, that is, we obtain $p_t=p_{xx}$ by $pw=-p_x$.

There is no reduction $u=0$ in noncommutative case. In the commutative case, the reduction $u=0$ leads to the nonsymmetric Novikov-Veselov equation.[25]

$$v_{t_3} = v_{xxx} - 3(v\Theta^{-1}v)_x.$$

V. CONCLUSION

We have demonstrated the power of the symbolic representation in the study of (2+1)-dimensional integrable equations. It enables us to produce the hierarchies of (2+1)-dimensional integrable equations from the scalar Lax operators and to study their properties globally. We proved the conjecture of Mikhailov and Yamilov on the ring extension for (2+1)-dimensional commutative integrable equations derived from these scalar Lax operators.

There exist other types of scalar Lax operators such as the Lax pair of Eq. (2.14) in Ref. 26, i.e. $L_t=[B,L]$, where

$$L = D_x^2 + u, \quad B = D_y L + \tfrac{1}{2}\Theta u D_x - \tfrac{1}{4}u_y - \tfrac{1}{4}D_x^{-1}C_u\Theta u.$$

In fact, Eq. (2.14) shares the same L operator as noncommutative KdV,

$$u_t = \frac{1}{4}(u_{xxx} + 3uu_x + 3u_x u),$$

and hence it can be obtained by a recursion operator of noncommutative KdV acting on u_y. The same ring extension results can be proved by either adapting the proof in this paper or deriving from the structure of recursion operators of the corresponding (1+1)-dimensional integrable equations.[12,27]

The method can easily be applied to the case of (2+1)-dimensional differential-difference integrable equation with scalar Lax operators.[24] This is an ongoing research topic.

Recently, there was an attempt at constructing noncommutative integrable equations in the framework of the Sato theory motivated by noncommutative gauge theories, cf. Refs. 26 and 28 and references therein. However, the authors had imposed an ansatz to derive the equations from certain scalar Lax operators in the case (a) instead of the systematical approach proposed in this paper. Noncommutative (2+1)-dimensional integrable equations derived from the scalar Lax operators in the cases (b) and (c) have not been well studied mainly due to the appearance of a new type of nonlocal terms such as $(D_x+(C_u/2))^{-1}u_y$ and $(D_y-C_u)^{-1}u_x$.

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APPENDIX: PROOF OF PROPOSITION 4

Proof. We need to show [cf. (14)] for all $l\geqslant 2$ that

$$b_{l-1}\left(-\sum_{s=2}^{l}\xi_{j_s}^{(i_s)}, -\sum_{s=2}^{l}\eta_{j_s}^{(i_s)}, \xi_{j_2}^{(i_2)}, \eta_{j_2}^{(i_2)}, \ldots, \xi_{j_{l-1}}^{(i_{l-1})}, \eta_{j_{l-1}}^{(i_{l-1})}, X+\xi_{j_l}^{(i_l)}\right) = b_{l-1}(\xi_{j_2}^{(i_2)}, \eta_{j_2}^{(i_2)}, \ldots, \xi_{j_l}^{(i_l)}, \eta_{j_l}^{(i_l)}, X). \tag{A1}$$

We prove it by induction. It is true for $l=2$ since

$$b_1(-\xi_{j_2}^{(i_2)}, -\eta_{j_2}^{(i_2)}, X+\xi_{j_2}^{(i_2)}) = \frac{-\xi_{j_2}^{(i_2)}}{N_1(-\xi_{j_2}^{(i_2)}, -\eta_{j_2}^{(i_2)}, X+\xi_{j_2}^{(i_2)})} = \frac{\xi_{j_2}^{(i_2)}}{N_1(\xi_{j_2}^{(i_2)}, \eta_{j_2}^{(i_2)}, X)}.$$

Assume that formula (A1) is valid for $l-1$. Then its left-hand side equals

$$
\begin{aligned}
&\frac{b_{l-2}\left(-\sum_{s=2}^{l}\xi_{j_s}^{(i_s)},-\sum_{s=2}^{l}\eta_{j_s}^{(i_s)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)}\right)}{N_{l-1}\left(-\sum_{s=2}^{l}\xi_{j_s}^{(i_s)},-\sum_{s=2}^{l}\eta_{j_s}^{(i_s)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)}\right)}\\
&\quad-\frac{b_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})}{N_{l-1}\left(-\sum_{s=2}^{l}\xi_{j_s}^{(i_s)},-\sum_{s=2}^{l}\eta_{j_s}^{(i_s)},\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)}\right)}\\
&=-\frac{b_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)},\eta_{j_{l-1}}^{(i_{l-1})}+\eta_{j_l}^{(i_l)},X)}{N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&\quad+\frac{b_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})}{N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&=\frac{b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)})-b_{l-3}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\ldots,\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})}{N_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&\quad-\frac{b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)})}{N_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)},\eta_{j_{l-1}}^{(i_{l-1})}+\eta_{j_l}^{(i_l)},X)N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&\quad+\frac{b_{l-3}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)},\eta_{j_{l-1}}^{(i_{l-1})}+\eta_{j_l}^{(i_l)},X)}{N_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)},\eta_{j_{l-1}}^{(i_{l-1})}+\eta_{j_l}^{(i_l)},X)N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}.
\end{aligned}
$$

Meanwhile, the right side gives us

$$
\begin{aligned}
&\frac{b_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})-b_{l-2}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}{N_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&=\frac{b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)})}{N_1(\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})N_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&\quad-\frac{b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_{l-2}}^{(i_{l-2})}+\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-2}}^{(i_{l-2})}+\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})}{N_1(\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})N_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}\\
&\quad-\frac{b_{l-3}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\ldots,\eta_{j_{l-1}}^{(i_{l-1})},X+\xi_{j_l}^{(i_l)})-b_{l-3}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\ldots,\xi_{j_{l-1}}^{(i_{l-1})}+\xi_{j_l}^{(i_l)},\eta_{j_{l-1}}^{(i_{l-1})}+\eta_{j_l}^{(i_l)},X)}{N_1(\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)N_{l-1}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\ldots,\xi_{j_l}^{(i_l)},\eta_{j_l}^{(i_l)},X)}.
\end{aligned}
$$

The difference between the above two expression vanishes due to the induction assumption, which implies that

$$
\begin{aligned}
&\frac{N_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})})b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-2}}^{(i_{l-2})},\eta_{j_{l-2}}^{(i_{l-2})},X+\xi_{j_{l-1}}^{(i_{l-1})})}{N_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X)N_1(\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X)}\\
&=\frac{b_{l-3}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\xi_{j_{l-2}}^{(i_{l-2})}+\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-2}}^{(i_{l-2})}+\eta_{j_{l-1}}^{(i_{l-1})},X)}{N_1(\xi_{j_{l-1}}^{(i_{l-1})},\eta_{j_{l-1}}^{(i_{l-1})},X)}-\frac{b_{l-3}(\xi_{j_3}^{(i_3)},\eta_{j_3}^{(i_3)},\cdots,\eta_{j_{l-1}}^{(i_{l-1})},X)}{N_{l-2}(\xi_{j_2}^{(i_2)},\eta_{j_2}^{(i_2)},\cdots,\eta_{j_{l-1}}^{(i_{l-1})},X)}.
\end{aligned}
$$

By now we have proved our proposition. ◇

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Quantum Stratonovich calculus and the quantum Wong-Zakai theorem

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We extend the Itō-to-Stratonovich analysis or quantum stochastic differential equations, introduced by Gardiner and Collett for emission (creation), absorption (annihilation) processes, to include scattering (conservation) processes. Working within the framework of quantum stochastic calculus, we define Stratonovich calculus as an algebraic modification of the Itō one and give conditions for the existence of Stratonovich time-ordered exponentials. We show that conversion formula for the coefficients has a striking resemblance to Green's function formulas from standard perturbation theory. We show that the calculus conveniently describes the Markov limit of regular open quantum dynamical systems in much the same way as in the Wong-Zakai approximation theorems of classical stochastic analysis. We extend previous limit results to multiple-dimensions with a proof that makes use of diagrammatic conventions. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Quantum stochastic calculus[1–4] was developed as a framework to construct concrete models of irreversible quantum dynamical systems. Prior to this, models tended to consider a system couple to an environment, but with only the system being accessible to physical measurement: as a result the environment observables were often relegated to a secondary status, leaving one with a master equation for the state of the system only.[5,6]

Hudson and Parthasarathy[3] in 1984 presented a rigorous theory of integration with respect to processes on bosonic (later fermionic) Fock spaces generalizing the Itō-Doob theory of stochastic integration. In addition to integrals with respect to time, they also introduced integrals with respect to creation, annihilation, and number (more generally, scattering) processes. Motivated by noncommutative Feynman-Kac formulas, they were able to describe unitary dynamical evolutions of a system coupled to the Fock space environment which reduced to an irreversible Markov dynamics for the system when averaged over the partial expectation with respect to the Fock vacuum. Here the Schrödinger equation is replaced by a quantum stochastic differential equation (QSDE) driven by the creation, annihilation, and scattering processes, as well as time.

Independently, Gardiner and Collett[4] in 1985 gave the version of quantum stochastic integration for the bosonic creation and annihilation that is best known amongst the physics community. Although they did not include the scattering processes, they did introduce several important physical concepts, in particular, they gave to the noise the status of a physical observable. This has been vital in subsequent analysis of quantum filtering and feedback where the environment can act as an apparatus/communication channel.[7–9] In their analysis, they also introduced the Stratonovich version of the theory by extending the usual midpoint definition to noncommuting processes.[10] This is a natural physical choice for two reasons: unlike the Itō form, the Leibniz rule of differential calculus holds for Stratonovich differentials and so physical symmetries are more apparent;

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second, in classical analysis it is generally the case that if the model can be obtained as a singular limit of regular dynamical models, then it is the Stratonovich form that resembles the prelimit equations the most. Historically, it was actually the latter reason that led to Stratonovich initially introducing his modification of the Itō theory. In ordinary stochastic analysis, such results involving a central limit effect for stochastic processes are known as Wong-Zakai theorems. Our original motivation stems from quantum Markov limits[11–16] and the desire to understand the limit processes in a Stratonovich sense.

To give a concrete mathematical account, we start from the quantum Itō theory developed by Hudson and Parthasarathy, and deduce quantum Stratonovich calculus as an algebraic modification of the quantum Itō one which restores the Leibniz rule. An approach starting from Gardiner and Collett's input processes would have been more appealing from a physical point of view, however, we do not want to bypass questions of the mathematical status of the objects considered. Traditionally, the Stratonovich integral is defined through a midpoint Riemann sum approximation: this has been extended by Chebotarev[12,13] to quantum stochastic integrals, however, we emphasize that our formulation here is to define Stratonovich integrals as combinations of well-defined Itō integrals where possible. Rather than there being an unique version, we find that there are degrees of freedom in how we actually achieve this—we refer to this as a "gauge" freedom—and that the standard (symmetric) choice, corresponding to the midpoint rule, is just one possibility. We give the self-consistency formula $\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{V}\mathbf{G}$ relating the matrix of Itō coefficients $\mathbf{G}$ to the matrix of Stratonovich coefficients $\mathbf{G}_0$. (Here the "potential" $\mathbf{V}$ is half the noise covariance matrix plus the gauge.) Rather surprisingly, this has the same algebraic form as the one relating the free and perturbed Green's functions in scattering theory: a fact that we readily exploit. It is shown that the Itō coefficients of a unitary process are related to Hamiltonian Stratonovich coefficients ($\mathbf{G}_0^\dagger=-\mathbf{G}_0$) and that this is true for any gauge so long as the self-consistency formula can be solved. This allows the interpretation that the Stratonovich calculus can be viewed as a perturbation of the Itō calculus, and vice versa.

A major motivation here is the results of Ref. 16 for a quantum Markov limit involving emission, absorption, and scattering. We formulate the limit as a Wong-Zakai result where the Stratonovich QSDE resembles the prelimit Schrödinger equation (with gauge set by the imaginary part of the complex damping). Our key requirement is convergence of the "Neumann series" $\mathbf{G}=\sum_{n=0}^{n}\mathbf{G}_0(\mathbf{V}\mathbf{G}_0)^n$. We generalize the result to multiple channel noise sources and make the proof more accessible by means of diagrammatic conventions which make the connections with the Dyson series expansion transparent. We also present the results in a fluxion notation, as an alternative to the differential increment language, which is closer to the formulation employed by Gardiner and Collett[4] and effectively generalizes their results to include scattering. This also reveals a new representation (Lemma 3) for the Evans-Hudson flow maps.

II. QUANTUM STOCHASTIC CALCULUS

A. Quantum processes

Given a Hilbert space $\mathfrak{h}_1$, the Fock space over $\mathfrak{h}_1$ is the Hilbert space $\Gamma(\mathfrak{h}_1)$ generated by symmetrized n-particle vectors $\varphi_1\hat{\otimes}\cdots\hat{\otimes}\varphi_n:=(n!)^{-1}\Sigma_{\sigma\in\mathfrak{S}_n}\varphi_{\sigma(1)}\otimes\cdots\otimes\varphi_{\sigma(n)}$ for $n\geqslant 0$ arbitrary, $\varphi_j\in\mathfrak{h}_1$ and $\mathfrak{S}_n$ the group of permutations on n labels. The special case $n=0$ requires the introduction of unit vector Ω called the Fock vacuum vector. The inner product on $\Gamma(\mathfrak{h}_1)$ is given by $\langle\varphi_1\hat{\otimes}\cdots\hat{\otimes}\varphi_n|\psi_1\hat{\otimes}\cdots\hat{\otimes}\psi_n\rangle=\delta_{nm}(n!)^{-1}\Sigma_{\sigma\in\mathfrak{S}_n}\langle\varphi_1|\psi_{\sigma(1)}\rangle\cdots\langle\varphi_n|\psi_{\sigma(n)}\rangle$.

The exponential vector with test function $\varphi\in\mathfrak{h}_1$ is defined to the Fock space vector

$$\varepsilon(\varphi)=\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\underbrace{\varphi\otimes\cdots\otimes\varphi}_{n\text{ fold}}, \tag{1}$$

and we have $\langle\varepsilon(\varphi)|\varepsilon(\psi)\rangle=\exp\langle\varphi|\psi\rangle$. If S is a dense subset of $\mathfrak{h}_1$ then the vectors $\varepsilon(\varphi)$, with $\varphi\in S$, are total in $\Gamma(\mathfrak{h}_1)$, that is, the closure of the span of these vectors gives the whole Fock space.

We now take the one-particle space to be the Hilbert space of $\mathbb{C}^N$-valued square-integrable functions of positive time: this consists of measurable functions $\mathbf{f}=(f_1,\ldots,f_n)$ with $\int_0^\infty \Sigma_{i=1}^n |f_i(t)|^2 < \infty$. An orthogonal projection Π_s is defined on the one-particle space for each $s>0$ by taking $\Pi_s\mathbf{f}=(\chi_{[0,s]}f_1,\ldots,\chi_{[0,s]}f_n)$ where $\chi_{[0,s]}$ is the indicator function for the interval $[0,s]$. An N-channel quantum noise source is modeled by operators processes $\{A_t^{\alpha\beta}: t>0\}$ acting on the corresponding Fock space $\mathfrak{F}$. For $\alpha,\beta\in\{0,1,\ldots,n\}$, these processes are defined on the domain of exponential vectors by

$$\langle \varepsilon(\mathbf{f}) \left| \left\{ A_t^{\alpha\beta} - \int_0^t f_\alpha^*(s) g_\beta(s) ds \right\} \varepsilon(\mathbf{g}) \right\rangle = 0, \tag{2}$$

where we include the index zero by setting $f_0=g_0=1$. We shall adopt the convention that lower case Latin indices (with the exception of t and s which we reserve for time!) range over the values $1,\ldots,N$ while lower case Greek indices range over $0,1,\ldots,N$. We also apply an Einstein summation convention for repeated indices over the appropriate range.

We also fix a Hilbert space $\mathfrak{h}$, called the initial space. Let D be a domain in $\mathfrak{h}$ and take S to be the space of bounded $\mathbb{C}^N$-valued functions. A family $X_\cdot=\{X_t: t\geqslant 0\}$ of operators on $\mathfrak{h}\otimes\mathfrak{F}$ is said to be an adapted quantum stochastic process based on (D,S) if, for each $t\geqslant 0$, $X_t u\otimes\varepsilon(\mathbf{f})$ is defined for each $u\in D$ and $\mathbf{f}=(f_1,\ldots,f_n)\in S$ and is independent of the values $f_i(s)$ for $s>t$. If $X_\cdot^{\alpha\beta}$ are adapted processes, their stochastic integral $X_\cdot$ may be written as (implied summation!) $X_t=\int_0^t a_\alpha^\dagger(s) X_s^{\alpha\beta} a_\beta(s)\mathrm{d}s$, with the meaning that

$$\langle u\otimes\varepsilon(\mathbf{f}) \left| \int_0^t a_\alpha^\dagger(s) X_s^{\alpha\beta} a_\beta(s)\mathrm{d}s v\otimes\varepsilon(\mathbf{g})\right\rangle := \int_0^t f_\alpha^*(s)\langle u\otimes\varepsilon(\mathbf{f})|X_s^{\alpha\beta}v\otimes\varepsilon(\mathbf{g})\rangle g_\beta(s)\mathrm{d}s.$$

The stochastic integral is more often written in the form $X_t=\int_0^t X_s^{\alpha\beta}\mathrm{d}A_s^{\alpha\beta}$ or equivalently $\int_0^t \mathrm{d}A_s^{\alpha\beta}X_s^{\alpha\beta}$ with these integrals making sense as Riemann-Itō limits for locally square-integrable integrands. The stochastic integral will again be an adapted process. At the moment, the symbols $a_\alpha^\dagger(t)$, $a_\beta(t)$ have no meaning other than notational, however $a_0^\dagger(t)$ and $a_0(t)$ are easily interpreted as the identity operator and $a_i(t)$ as a pointwise Malliavin gradient. What is crucial is that they appear in Wick order: that is, $a_\alpha^\dagger(t)$ to the left of $a_\beta(t)$. Let $Y_t=\int_0^t a_\alpha^\dagger(s) Y_s^{\alpha\beta} a_\beta(s)\mathrm{d}s$ be a second integral, with the $Y_\cdot^{\alpha\beta}$ adapted, then we have the formula[3]

$$X_tY_t = \int_0^t a_\alpha^\dagger(s) X_s^{\alpha\beta} Y_s a_\beta(s)\mathrm{d}s + \int_0^t a_\alpha^\dagger(s) X_s Y_s^{\alpha\beta} a_\beta(s)\mathrm{d}s + \int_0^t a_\alpha^\dagger(s) X_s^{\alpha\mu} P_{\mu\nu} Y_s^{\nu\beta} a_\beta(s)\mathrm{d}s,$$

where we introduce

$$P^{\mu\nu} = \begin{cases} 1, & \mu=\nu\neq 0 \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

(As is well-known to the quantum probability community, the components $P^{\mu\nu}$ are just the Evans Kronecker-delta[17] usually denoted $\hat{\delta}^{\mu\nu}$.)

Introducing the differential notation $\mathrm{d}X_t=X_t^{\alpha\beta}\mathrm{d}A_t^{\alpha\beta}$, etc., we may write the quantum Itō formula in the more familiar guise as

$$\mathrm{d}(X_tY_t) = (\mathrm{d}X_t)Y_t + X_t(\mathrm{d}Y_t) + (\mathrm{d}X_t)(\mathrm{d}Y_t), \tag{4}$$

where the Itō correction is $(\mathrm{d}X_t)(\mathrm{d}Y_t)=X_t^{\alpha i}Y_t^{i\beta}\mathrm{d}A_t^{\alpha\beta}\equiv X_t^{\alpha\mu}P^{\mu\nu}Y_t^{\nu\beta}\mathrm{d}A_t^{\alpha\beta}$. Let us define iterated integrals in the natural way:

$$\langle \varepsilon(\mathbf{f}) \left| \int_{\Delta_n(t)} \mathrm{d}A_{t_n}^{\alpha_n\beta_n} \cdots \mathrm{d}A_{t_1}^{\alpha_1\beta_1} \varepsilon(\mathbf{g}) \right\rangle = \int_{\Delta_n(t)} f_{\alpha_n}^*(t_n) \cdots f_{\alpha_1}^*(t_1) g_{\beta_n}(t_n) \cdots g_{\beta_1}(t_1) \langle \varepsilon(\mathbf{f}) | \varepsilon(\mathbf{g}) \rangle, \tag{5}$$

where $\Delta_n(t)$ is the simplex $t \geqslant t_n > \cdots \geqslant t_1 > 0$.

B. Quantum Markov evolutions

Let $\{G_{\alpha\beta}\}$ be bounded operators on a fixed initial space $\mathfrak{h}$, then there exists a unique solution $U_\cdot$ to the equation $U_t = 1 + \int_0^t G_{\alpha\beta} U_s \mathrm{d}A_s^{\alpha\beta}$ which we can naturally interpret as the QSDE $\mathrm{d}U_t = G_{\alpha\beta} U_t \mathrm{d}A_t^{\alpha\beta}$, with $U_0 = 1$. In such cases, we may write $U_\cdot$ as the *Dyson-Itō time-ordered exponential* $U_t = \vec{\mathbf{T}}_{\mathrm{ID}} \exp \int_0^t G_{\alpha\beta} \mathrm{d}A^{\alpha\beta}$.

Proposition 1: *Let $U_\cdot$ be the solution to the QSDE $\mathrm{d}U_t = G_{\alpha\beta} U_t \mathrm{d}A_t^{\alpha\beta}$, with $U_0 = 1$, where the $\{G_{\alpha\beta}\}$ are bounded operators on $\mathfrak{h}$. Necessary and sufficient conditions*[3] *for $U_\cdot$ to be unitary process are that $G_{\alpha\beta} + G_{\beta\alpha}^\dagger + G_{i\alpha}^\dagger G_{i\beta} = 0 = G_{\alpha\beta} + G_{\beta\alpha}^\dagger + G_{i\alpha} G_{i\beta}^\dagger$ with the general solution*

$$G_{ij} = W_{ij} - \delta_{ij}, \quad G_{i0} = L_i,$$

$$G_{0j} = -L_k^\dagger W_{kj}, \quad G_{00} = -\tfrac{1}{2} L_k^\dagger L_k - iH,$$

where W_{ij}, L_i, and H are bounded operators on the initial space with H self-adjoint and $W_{ij}^\dagger W_{jk} = \delta_{ik} = W_{ij} W_{jk}^\dagger$.

Proposition 2: Let $U_\cdot$ be the unitary process described above. The corresponding flow map is given by $J_t(X) := U_t^\dagger (X \otimes 1) U_t$ for bounded X on the initial space. We find that $J_t(X)$ satisfies the QSDE

$$\mathrm{d}J_t(X) = J_t(\mathcal{L}_{\alpha\beta}(X)) \mathrm{d}A_t^{\alpha\beta},$$

where the Evans-Hudson maps[17] *are given by $\mathcal{L}_{\alpha\beta}(X) := XG_{\alpha\beta} + G_{\beta\alpha}^\dagger X + G_{i\alpha}^\dagger X G_{i\beta}$.*

Following Lindblad,[18] the dissipation of a linear map $\mathcal{L}$ on the algebra of bounded operators on $\mathfrak{h}$ is defined to be the bilinear mapping $\mathcal{D}\mathcal{L} : (X, Y) \mapsto \mathcal{L}(XY) - \mathcal{L}(X)Y - X\mathcal{L}(Y)$.

Proposition 3: The Evans-Hudson maps for a unitary flow satisfy $\mathcal{L}_{\alpha\beta}(X)^\dagger = \mathcal{L}_{\beta\alpha}(X^\dagger)$ and their dissipation is described by

$$\mathfrak{D}\mathcal{L}_{\alpha\beta}(X, Y) = \mathcal{L}_{\alpha\mu}(X) P^{\mu\nu} \mathcal{L}_{\nu\beta}(Y).$$

C. Approximations

For each $\lambda > 0$, we set $a_0^\#(t, \lambda) = 0$ and take $a_i^\#(t, \lambda) = A^\#(\varphi(i, t, \lambda))$ where $\varphi(i, t, \lambda)$ is a $\mathbb{C}^N$-valued square-integrable function on $[0, \infty)$: we also take $t \to \varphi(i, t, \lambda)$ to be strongly differentiable. We assume that $\langle \varphi(i, t, \lambda) | \varphi(j, s, \lambda) \rangle \equiv C_{ij}(t - s, \lambda)$ where $C_{ij}(\tau, \lambda) = C_{ji}(-\tau)^*$ is integrable in τ, and that we have the convergence $\lim_{\lambda \to 0} C_{ij}(\tau, \lambda) = \delta_{ij} \delta(\tau)$ in the sense of Schwartz distributions. We set $\kappa_{ij} = \lim_{\lambda \to 0} \int_0^\infty C_{ij}(\tau, \lambda) \mathrm{d}\tau$ and note the identity $\kappa_{ij} + \kappa_{ji}^* = \delta_{ij}$.

The $a_i^\#(t, \lambda)$ are approximations to quantum white noises. We may introduce integrated processes $A_t^{\alpha\beta}(\lambda) := \int_0^t a_\alpha^\dagger(s, \lambda) a_\beta(s, \lambda) \mathrm{d}s$ which serve as approximations to the fundamental processes. The approximation will be termed symmetric if $\kappa_{ij} = \frac{1}{2} \delta_{ij}$, but this is only a special case. Defining smeared exponential vectors by

$$\varepsilon_\lambda(\mathbf{f}) = \exp\left\{ \int_0^\infty \sum_{i=1}^N f_i(t) a_i^\dagger(t) \mathrm{d}t \right\} \Omega, \tag{6}$$

we see that the limit

$$\lim_{\lambda\to 0}\langle \varepsilon_\lambda(\mathbf{f})\left|\int_{\Delta_n(t)} a^*_{\alpha_n}(t_n,\lambda)\cdots a^*_{\alpha_1}(t_1,\lambda)a_{\beta_n}(t_n,\lambda)\cdots a_{\beta_1}(t_1,\lambda)\varepsilon_\lambda(\mathbf{g})\right\rangle$$

coincides with (5). Therefore, whenever we consider the limit of Wick ordered expressions, it does not matter whether we have the symmetric approximation or not.

A term such as $\int_{\Delta_2(t)} a_i(t_2,\lambda)a_j^\dagger(t_1,\lambda)$ must, however, be put in to Wick order as $\int_{\Delta_2(t)} a_j^\dagger(t_1,\lambda)\alpha_i(t_2,\lambda)$ plus an additional term $\int_{\Delta_2(t)} C_{ij}(t_2-t_2,\lambda)$ which converges to $\kappa_{ij}t$. As a rule, expressions violating of Wick order will have a limit that depends on the constants κ_{ij}.[19,20]

D. Notation and conventions

Let $\mathbf{X}=\{X_{\alpha\beta}\}$ be an $(N+1)\times(N+1)$ matrix of bounded operators on some Hilbert space. (Previously, we had the Itō coefficients which were operators on $\mathfrak{h}\otimes\mathfrak{F}$.) We shall adopt the matrix representation

$$\mathbf{X}=\left(\begin{array}{c|c} X_{00} & X_{01},X_{02},\ldots \\ \hline X_{10} & \\ X_{20} & \mathsf{X} \\ \vdots & \end{array}\right) \tag{7}$$

where X is the $N\times N$ submatrix consisting of the entries $\{X_{ij}\}$.

For instance, $\mathbf{P}=\{P^{\alpha\beta}\}$ will be a projection operator:

$$\mathbf{P}=\left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & 1 \end{array}\right),\quad \mathbf{Q}=\mathbf{1}-\mathbf{P}=\left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & 0 \end{array}\right). \tag{8}$$

The quantum Itō correction is therefore described by the matrix $\mathbf{X}(t)\mathbf{P}\mathbf{Y}(t)\equiv\{X_{\alpha\mu}(t)P^{\mu\nu}Y_{\nu\beta}(t)\}$.

Let $\{G_{\alpha\beta}\}\equiv\mathbf{G}$ be a matrix with bounded operators on $\mathfrak{h}$ as entries, then the Dyson-Itō time-ordered exponential $U_t=\vec{\mathbf{T}}_{\mathrm{DI}}\{\exp\int_0^t G_{\alpha\beta}\mathrm{d}A^{\alpha\beta}\}$ will be unitarity if, from Proposition 1,

$$\mathbf{G}+\mathbf{G}^\dagger+\mathbf{G}^\dagger\mathbf{P}\mathbf{G}=\mathbf{0},\quad \mathbf{G}+\mathbf{G}^\dagger+\mathbf{G}\mathbf{P}\mathbf{G}^\dagger=\mathbf{0}. \tag{9}$$

It is relatively easy to see that the Itō coefficients then take the general form

$$\mathbf{PGP}=\mathbf{W}-\mathbf{P},$$

$$\mathbf{QGP}=-(\mathbf{PGQ})^\dagger\mathbf{W},$$

$$\mathbf{QGQ}=-\frac{1}{2}(\mathbf{PGQ})^\dagger(\mathbf{PGQ})-\mathrm{i}\left(\begin{array}{c|c} H & 0 \\ \hline 0 & 0 \end{array}\right), \tag{10}$$

where $\mathbf{W}^\dagger\mathbf{W}=\mathbf{P}=\mathbf{W}\mathbf{W}^\dagger$ (i.e., the restriction of $\mathbf{W}$ to $\mathfrak{h}\otimes\mathbb{C}^N$ is unitary) and H is self-adjoint on $\mathfrak{h}$.

More explicitly, we may set

$$\mathbf{W}=\left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathsf{W}=\{W_{ij}\} \end{array}\right),\quad \mathbf{PGQ}=\left(\begin{array}{c|c} 0 & 0,0,\cdots \\ \hline L_1 & \\ L_2 & 0 \\ \vdots & \end{array}\right),$$

where W_{ij}, L_i, and H are the operators on $\mathfrak{h}$ introduced in Proposition 1.

We should remark that the restriction to a finite number N of channels is not essential and that the unitary process exists under certain conditions on the boundedness of $\mathbf{G}$ as a matrix operator.[22]

III. QUANTUM STRATONOVICH CALCULUS

We wish to write the quantum Itō formula in the form

$$\mathrm{d}(X_t Y_t) = (\mathrm{d}X_t) \circ Y_t + X_t \circ (\mathrm{d}Y_t). \tag{11}$$

This can be achieved by formally defining

$$\begin{aligned} (\mathrm{d}X_t) \circ Y &:= (\mathrm{d}X_t) Y_t + X_t^{\alpha\mu} V_t^{\mu\nu} Y_t^{\nu\beta} \mathrm{d}A_t^{\alpha\beta}, \\ X_t \circ (\mathrm{d}Y_t) &:= X_t (\mathrm{d}Y_t) + X_t^{\alpha\mu} (V_t^{\nu\mu})^\dagger Y_t^{\nu\beta} \mathrm{d}A_t^{\alpha\beta}, \end{aligned} \tag{12}$$

where the $\{V_t^{\alpha\beta}\}$ may in general be taken as adapted processes, however, we shall take them to be just scalar coefficients. It follows that $[(\mathrm{d}X_t) \circ Y_t]^\dagger = Y_t^\dagger \circ \mathrm{d}X_t^\dagger$, and we recover the Itō formula provided we have the condition $V^{\mu\nu} + (V^{\nu\mu})^* = P^{\mu\nu}$. (It should be noted that the differential maps considered here are not actions. For instance, $((\mathrm{d}X_t) \circ Y_t) \circ Z_t$ is not the same as $(\mathrm{d}X_t) \circ (Y_t Z_t)$—this is also the case for the classical notion of Stratonovich differential! In contrast, the Leibniz rule can be restored by absorbing the Itō correction completely onto either the left or right action of the algebra of integrands on the algebra of differentials. This has been recently carried out by Hudson,[23] who was able to construct a Woronowicz first-order differential calculus[24] by this device.

The simplest solution possible is to take $V^{\mu\nu} = \frac{1}{2} P^{\mu\nu}$ and this corresponds algebraically to the traditional Stratonovich definition of a differential. The general solution however takes the form $V^{\mu\nu} = \frac{1}{2} P^{\mu\nu} + \mathrm{i} Z^{\mu\nu}$, where the constants $\{Z^{\mu\nu}\}$ satisfy $(Z^{\mu\nu})^* = Z^{\nu\mu}$. The appearance of these constants is similar to the ambiguity in the Tomita-Takesaki theory, and we refer to them as a gauge freedom. We shall identify the V^{ij} with the constants κ_{ij} occurring in the approximation scheme. Let us take $\mathbf{V} \equiv \{V^{\alpha\beta}\}$ to be the family of constants, then the requirement is $\mathbf{V} + \mathbf{V}^\dagger = \mathbf{P}$ with general solution $\mathbf{V} \equiv \frac{1}{2}\mathbf{P} + \mathrm{i}\mathbf{Z}$ where $\mathbf{Z}^\dagger = \mathbf{Z}$. We shall take the $\{Z^{\alpha\beta}\}$ to be scalar constants and set $Z^{00} = Z^{i0} = Z^{0j} = 0$. This implies that $\mathbf{Z} = \mathbf{Z}\mathbf{P} = \mathbf{P}\mathbf{Z}$ and so $\mathbf{V} = \mathbf{V}\mathbf{P} = \mathbf{P}\mathbf{V}$:

$$\mathbf{V} = \tfrac{1}{2}\mathbf{P} + \mathrm{i}\mathbf{Z} \equiv \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathsf{V} \end{array} \right).$$

where $\mathsf{V} = \frac{1}{2} + \mathrm{i}\mathsf{Z}$ with $\mathsf{Z}^\dagger = \mathsf{Z}$. Note that V is a normal operator with $\mathsf{V}\mathsf{V}^\dagger = \mathsf{V}^\dagger \mathsf{V} = 4^{-1} + \mathsf{Z}^2$.

It should be pointed out that we have the relation

$$\mathrm{d}J_t(XY) = (\mathrm{d}J_t(X)) \circ J_t(Y) + J_t(X) \circ (\mathrm{d}J_t(Y)),$$

which we can get either from taking differentials of the homomorphic property $J_t(XY) = J_t(X) J_t(Y)$, or explicitly by noting that $(\mathrm{d}J_t(X)) \circ J_t(Y) \equiv J_t(\mathcal{L}_{\alpha\beta}(X) Y + \mathcal{L}_{\alpha\mu}(X) V^{\mu\nu} \mathcal{L}_{n\beta}(Y)) \mathrm{d}A_t^{\alpha\beta}$, etc., and using Proposition 3.

A. Stratonovich-Dyson time ordered exponentials

Let us now suppose that $U_\cdot$ is simultaneously the solution to the Itō QSDE $\mathrm{d}U = (\mathrm{d}G)U$, with $\mathrm{d}G = G_{\alpha\beta} \mathrm{d}A^{\alpha\beta}$ as before, and a Stratonovich QSDE (for a fixed gauge!)

$$\mathrm{d}U_t = (\mathrm{d}G_0(t)) \circ U_t, \quad U_0 = 1, \tag{13}$$

with $\mathrm{d}G_0 = G^0_{\alpha\beta} \mathrm{d}A^{\alpha\beta}$. In such cases, we may write $U_\cdot$ as the *Dyson-Stratonovich time-ordered exponential* $U_t = \vec{\mathbf{T}}_{\mathrm{SD}}\{\exp \int_0^t G^0_{\alpha\beta} \mathrm{d}A^{\alpha\beta}\}$ and shall refer to $\mathbf{G}_0 \equiv \{G^0_{\alpha\beta}\}$ as the matrix of *Stratonovich coefficients*.

Self-consistency requires that $\mathrm{d}U = (\mathrm{d}G^0) \circ U = (\mathrm{d}G)U$ and so we should have that $\mathrm{d}U = (\mathrm{d}G^0)U + G^0_{\alpha\mu} V^{\mu\nu} G_{\nu\beta} U \mathrm{d}A^{\alpha\beta} = (G^0_{\alpha\beta} + G^0_{\alpha\mu} V^{\mu\nu} G_{\nu\beta}) U \mathrm{d}A^{\alpha\beta}$. This means that the Itō coefficients $\mathbf{G} = \{G_{\alpha\beta}\}$ are related to the Stratonovich coefficients $\mathbf{G}_0 = \{G^0_{\alpha\beta}\}$ by

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \mathbf{V} \mathbf{G}. \tag{14}$$

As we shall see, so long as $\mathbf{1}+\mathbf{VGP}$ is invertible, we may solve for $\mathbf{G}_0$ in terms of $\mathbf{G}$. Similarly, invertibility of $\mathbf{1}-\mathbf{PG}_0\mathbf{V}$ implies that we may write $\mathbf{G}$ in terms of $\mathbf{G}_0$. It might be remarked that the relation (14) also applies if we consider matrices $\mathbf{G},\mathbf{G}_0$ of adapted processes.

What is rather astonishing is that relation (14) is precisely of the form relating free and perturbed Green's functions. Let us recall briefly that if $H=H_0+V$ is a Hamiltonian considered as a perturbation of the free Hamiltonian H_0 then the resolvent operator $\mathcal{G}(z)=(z-H)^{-1}$ is related to the free resolvent $\mathcal{G}_0(z)=(z-H_0)^{-1}$ by the algebraic identity

$$\mathcal{G}=\mathcal{G}_0+\mathcal{G}_0V\mathcal{G} \tag{15}$$

for all z outside of the spectra of H and H_0. The identity may be rewritten as $\mathcal{G}=(1-\mathcal{G}_0V)^{-1}\mathcal{G}_0$ and iterated to give the formal expansion $\mathcal{G}=\mathcal{G}_0+\mathcal{G}_0V\mathcal{G}_0+\mathcal{G}_0V\mathcal{G}_0V\mathcal{G}_0+\cdots$ which, when convergent, is the Neumann series. The details of the actual scattering are contained in the operator $\mathcal{T}:=V+V\mathcal{G}V$ and we have the identity $\mathcal{G}=\mathcal{G}_0+\mathcal{G}_0\mathcal{T}\mathcal{G}_0$.

B. The *T*-matrix

We now exploit the similarity between (14) and (15). We begin by introducing the operator

$$\mathbf{T}:=\mathbf{V}+\mathbf{VGV}\equiv\left(\begin{array}{c|c}0&0\\\hline 0&\mathsf{T}\end{array}\right). \tag{16}$$

Assuming that $\mathbf{1}-\mathbf{VG}_0\mathbf{P}$ is again invertible, we obtain the following identities:

$$\mathbf{T}=\frac{1}{\mathbf{1}-\mathbf{VG}_0\mathbf{P}}\mathbf{V}, \tag{17}$$

$$\mathbf{G}_0\mathbf{T}=\mathbf{GV}, \tag{18}$$

$$\mathbf{TG}_0=\mathbf{VG}, \tag{19}$$

$$\mathbf{G}=\mathbf{G}_0+\mathbf{GVG}_0, \tag{20}$$

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{TG}_0. \tag{21}$$

The proof of (17) comes from writing

$$\mathbf{T}=\mathbf{V}+\mathbf{T}(\mathbf{G}_0+\mathbf{G}_0\mathbf{TG})\mathbf{V}=\mathbf{V}+\mathbf{VG}_0\mathbf{T}$$

so that $(\mathbf{1}-\mathbf{VG}_0\mathbf{P})\mathbf{T}=\mathbf{V}$. The remaining identities are just precise analogues of well-known relations for resolvent operators.[25]

Combining (17) and (21) we see that $\mathbf{G}$ can be expressed in terms of $\mathbf{G}_0$ as

$$\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0(\mathbf{1}-\mathbf{PVG}_0\mathbf{P})^{-1}\mathbf{VG}_0. \tag{22}$$

In particular, we see that $\mathbf{G}$ is bounded. We may then invert to get

$$\mathbf{G}_0=\mathbf{G}-\mathbf{G}(\mathbf{1}+\mathbf{PVGP})^{-1}\mathbf{VG}. \tag{23}$$

Equations (22) and (23) reveal a remarkable duality between the Itō and Stratonovich coefficients. (Of course this just means that we may view either as a "perturbation" of the other!)

If $\mathbf{PVG}_0\mathbf{P}$ is a strict contraction, then we may develop a Neumann series expansion $\mathbf{G}=\mathbf{G}_0+\mathbf{G}_0\mathbf{VG}_0+\mathbf{G}_0\mathbf{VG}_0\mathbf{VG}_0+\cdots=\mathbf{G}_0\Sigma_{n=0}^{\infty}(\mathbf{VG}_0)^n$.

It is convenient to introduce a related matrix

$$\mathbf{F} = \mathbf{1} + \mathbf{T}\mathbf{G}_0 = \mathbf{1} + \mathbf{V}\mathbf{G} \tag{24}$$

so that $\mathbf{G} = \mathbf{G}_0\mathbf{F}$.

C. An "optical theorem"

Let us next suppose that the Stratonovich coefficients take the *Hamiltonian* form

$$\mathbf{G}_0 = -\mathrm{i}\mathbf{E}, \tag{25}$$

where $\mathbf{E}$ is a bounded, self-adjoint operator on $\mathfrak{h} \otimes \mathbb{C}^{N+1}$. We then have the relation $\mathbf{G}_0^\dagger = -\mathbf{G}_0$ and set

$$\mathbf{P}\mathbf{E}\mathbf{P} = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathsf{E} \end{array}\right)$$

so that E is self-adjoint on $\mathfrak{h} \otimes \mathbb{C}^N$. When our invertibility condition is met, it is easy to see that matrix T exists and can be written as

$$\mathsf{T} = [1 + \mathrm{i}\mathsf{V}\mathsf{E}]^{-1}\mathsf{V} \equiv \frac{1}{\mathsf{V}^{-1} + \mathrm{i}\mathsf{E}}. \tag{26}$$

(In the special case where $\mathsf{Z} = 0$, the self-adjointness of E ensures that $\mathsf{V} = 1 + \mathrm{i}\frac{1}{2}\mathsf{E}$ is invertible by von Neumann's theorem.[26] Therefore the existence of matrix T is guaranteed. More generally, so long as the value 1 lies in the resolvent set of $\mathsf{Z}\mathsf{E}$, this theorem implies the existence of T.)

The related matrix $\mathbf{F}$ then takes the form

$$\mathbf{F} = \left(\begin{array}{c|c} 1 & 0, 0, \ldots \\ \hline -\mathrm{i}T_{1j}E_{j0} & \\ -\mathrm{i}T_{2j}E_{j0} & \mathsf{F} \\ \vdots & \end{array}\right)$$

with $\mathsf{F} = 1 - \mathrm{i}\mathsf{T}\mathsf{E} = \mathsf{T}\mathsf{V}^{-1}$, so that $\mathsf{F} \equiv [1 + \mathrm{i}\mathsf{V}\mathsf{E}]^{-1}$.

Lemma 1 ("Optical Theorem"): $\mathrm{Re}\,\mathsf{T} \geqslant 0$ *and in particular* T *satisfies the identity*

$$\mathsf{T} + \mathsf{T}^\dagger = \mathsf{F}\mathsf{F}^\dagger = \mathsf{F}^\dagger\mathsf{F}.$$

Proof: We have that $\mathsf{T} + \mathsf{T}^\dagger$ may be written as

$$\mathsf{F}\mathsf{V} + \mathsf{V}^\dagger\mathsf{F}^\dagger = \mathsf{F}[\mathsf{V}(1 - \mathrm{i}\mathsf{E}\mathsf{V}^\dagger) + (1 + \mathrm{i}\mathsf{V}\mathsf{E})\mathsf{V}^\dagger]\mathsf{F}^\dagger = \mathsf{F}[\mathsf{V} + \mathsf{V}^\dagger]\mathsf{F}^\dagger = \mathsf{F}\mathsf{F}^\dagger.$$

It is then relatively straightforward to show that

$$\mathsf{F}\mathsf{F}^\dagger = \frac{1}{(1 - \mathrm{i}\mathsf{V}^\dagger\mathsf{E})(1 + \mathrm{i}\mathsf{E}\mathsf{V})} = [1 - \mathsf{E}\mathsf{Z} - \mathsf{Z}\mathsf{E} + \mathsf{E}\mathsf{V}(\mathsf{V}^\dagger)\mathsf{E}]^{-1} = \frac{1}{(1 + \mathrm{i}\mathsf{E}\mathsf{V})(1 - \mathrm{i}\mathsf{V}^\dagger\mathsf{E})} = \mathsf{F}^\dagger\mathsf{F}.$$

□

A similar calculation shows that $\mathrm{Im}\,\mathsf{T} = -\mathsf{T}\mathsf{E}\mathsf{T}^\dagger$.

D. Unitarity

We now wish to show that the choice of Hamiltonian Stratonovich coefficients naturally leads to unitary processes.

Lemma 2: Let $\mathbf{G}_0^\dagger = -\mathbf{G}_0$ *be bounded with* $\mathbf{1} - \mathbf{V}\mathbf{G}_0\mathbf{P}$ *invertible, and set* $G^0(t) = \int_0^t G^0_{\alpha\beta}\mathrm{d}A^{\alpha\beta}$. *Then the solution to the Stratonovich QSDE* $\mathrm{d}U = (\mathrm{d}G^0) \circ U$, $U_0 = 1$ *will be unitary.*

Proof: This fact is an immediate consequence of the optical theorem (27). To establish the

isometric property for the Itō coefficients, first observe that $\mathbf{G}+\mathbf{G}^\dagger=-\mathbf{G}_0(\mathbf{T}+\mathbf{T}^\dagger)\mathbf{G}_0$ while

$$\mathbf{GPG}^\dagger = \mathbf{G}_0\mathbf{FVF}^\dagger\mathbf{G}_0^\dagger = \mathbf{G}_0\left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathsf{FF}^\dagger \end{array}\right)\mathbf{G}_0^\dagger = -\mathbf{G}_0(\mathbf{T}+\mathbf{T}^\dagger)\mathbf{G}_0.$$

The isometry condition in (9) then follows from the first part of (27). The co-isometric property likewise follows from the second part. ■

E. Changing gauge

Let $\mathbf{G}$ be a fixed Itō coefficient matrix related to the Stratonovich coefficient matrices $\mathbf{G}_0^{(a)}$ and $\mathbf{G}_0^{(a)}$ with gauges $\mathbf{Z}^{(a)}$ and $\mathbf{Z}^{(a)}$, respectively. The two matrices will then be related by the perturbative formula

$$\mathbf{G}_0^{(a)} = \mathbf{G}_0^{(a)} + \mathrm{i}\mathbf{G}_0^{(a)}(\mathbf{Z}^{(a)} - \mathbf{Z}^{a})\mathbf{G}_0^{(a)}.$$

In particular, we can relate $\mathbf{G}_0^{(a)}$ for a nonzero gauge to the symmetric (gauge zero) form $\mathbf{G}_0^{(a)}$. As we shall see, the gauge $\mathbf{Z}$ has the physical interpretation as the imaginary part in the complex damping and in many applications this may be small.[21]

F. The "midpoint rule" construction

We wish to indicate briefly that the traditional midpoint rule construction of Stratonovich integrals agrees with the symmetric $\left(\mathbf{V}=\frac{1}{2}\mathbf{P}\right)$ situation considered here. This was shown to be at least plausible for integrals with respect to creation and annihilation process by Gardiner and Collett.[4] However, we describe in the following some rigorous results due to Chebotarev[13] using the notations of that paper.

A map M from the Borel sets of $\mathbb{R}^+$ to operators on $\mathfrak{h}\otimes\Gamma(L^2(\mathbb{R}^+))$ is said to be *interval-adapted* if $M(T)$ acts trivially on the factor $\Gamma(L^2(T^c))$ with respect to the continuous tensor product decomposition $\Gamma(L^2(\mathbb{R}^+))=\Gamma(L^2(T))\otimes\Gamma(L^2(T^c))$ with $T^c=\mathbb{R}^+/T$. The operators may be assumed to act on some dense domain $\mathcal{D}$. The prototypical integrators are then σ-additive interval adapted processes. An interval-adapted process U is said to be a cocycle if $U(t,s)=U(t,r)U(r,s)$ for $t\geqslant r\geqslant s$ where $U:[t_1,t_2)\mapsto U(t_2,t_1)$.

Suppose now that an interval adapted cocycle U is a weak solution to the QSDE

$$\mathrm{d}U(t,s) = U(t,s)M(\mathrm{d}t_+),$$

where $M(\mathrm{d}t_+)\equiv M(t+\mathrm{d}t,t)$ is the forward pointing Itō differential; that is, the following weak limit is assumed over increasingly fine partitions $S=t_0<t_1<\cdots<t_n=T$,

$$\int_S^T U(t,s)M(\mathrm{d}t_+)\phi := \lim_{\max|t_{j+1}-t_j|\to 0}\sum_j U(t_j,s)M(t_{j+1},t_j)\phi,$$

for all $\phi\in\mathcal{D}$, and $U(t,s)\phi=\phi+\int_s^t U(r,s)M(\mathrm{d}r_+)\phi$. Then, under mild conditions on a second interval adapted σ-additive process L, we have from Theorem 2.1[13]

$$\int_S^T U(t,s)L(\mathrm{d}t)\phi = \int_S^T U(t,s)\left\{L(\mathrm{d}t_+) + \frac{1}{2}M(\mathrm{d}t_+)L(\mathrm{d}t_+)\right\}\phi$$

for all $\phi\in\mathcal{D}$, where

$$\int_S^T U(t,s)L(\mathrm{d}t)\phi = \lim_{\max|t_{j+1}-t_j|\to 0}\sum_j U(t_j^*,s)L(t_{j+1},t_j)\phi$$

where $t_j^*=(t_{j+1}+t_j)/2$ is the midpoint of the interval $[t_j,t_{j+1})$.

In particular, the theorem is valid when the interval adapted σ-additive processes take the specific $[t_1,t_2)\mapsto M(t_2,t_1)=M_{\alpha\beta}\otimes(A_{t_2}^{\alpha\beta}-A_t^{\alpha\beta})$ for bounded operators $\{M_{\alpha\beta}\}$ on $\mathfrak{h}$: That is, $M(\mathrm{d}t_+)=M_{\alpha\beta}\otimes A_t^{\alpha\beta}$ and $L(\mathrm{d}t_+)=L_{\alpha\beta}\otimes A_t^{\alpha\beta}$. The situation that $\int_S^T U(t,s)L(\mathrm{d}t)\phi$ will equal $\int_S^T U(t,s)M(\mathrm{d}t_+)\phi$ occurs when

$$L(T,S)+\frac{1}{2}\int_S^T M(\mathrm{d}t_+)+L(\mathrm{d}t_+)=M(T,S).$$

The requirement on the coefficients, Eq. (2.23) of Ref. 13 can the, be rewritten as $M_{\alpha\beta}=L_{\alpha\beta}+\frac{1}{2}M_{\alpha 1}L_{1\beta}$ which is a special case of our relation (14).

IV. WICK ORDERING RULE

Let $X_\cdot$ and $Y_\cdot$ be quantum stochastic integrals with adapted integrands as before. In terms of our notation involving the $a_\alpha^\dagger(t),a_\beta(t)$, the product $X_tY_t=\int_0^t\mathrm{d}s_1\int_0^t\mathrm{d}s_2a_\alpha^\dagger(s_1)X_{s_1}^{\alpha\beta}a_\beta(s_1)a_\mu^\dagger(s_2)Y_{s_2}^{\mu\nu}a_\nu(s_2)$ is not immediately interpreted as an iterated integral since it is out of Wick order. However, the rule for achieving this is formally equivalent to the kinematic relations

$$[a_\alpha(t),Y_s]=\begin{cases}P^{\alpha\mu}Y_t^{\mu\nu}a_\nu(t), & t<s\\ V^{\alpha\mu}Y_t^{\mu\nu}a_\nu(t), & t=s\\ 0, & t>s,\end{cases}\tag{27}$$

under the integral sign, along with its adjoint $[X_t,a_\beta^\dagger(t)]=[a_\beta(t),X_s^\dagger]^\dagger$. These relations can be viewed as the formal commutation relations $[a_\alpha(t),a_\beta^\dagger(s)]=V^{\alpha\beta}\delta_+(t-s)+(V^{\beta\alpha})^*\delta_-(t-s)$ at work, where the $\delta_\pm$ are one-sided delta-functions: $\int\delta_\pm(f)f(t)=f(0^\pm)$, see e.g., Refs. 27 and 28. It is possible to interpret the $a_\alpha^\#(t)$ as quantum white noise operators, but we do not stress this point further here. At this stage, we could switch to a fluxion notation such as $\dot{X}_t=\mathrm{d}X_t/\mathrm{d}t=a_\alpha^\dagger(t)X_t^{\alpha\beta}a_\beta(t)$, etc., and write the Itō formula as $(\mathrm{d}/\mathrm{d}t)(X_tY_t)=\dot{X}_t\circ Y_t+X_t\circ\dot{Y}_t$ with the convention that

$$\dot{X}_t\circ Y_t\equiv a_\alpha^\dagger(t)X_t^{\alpha\beta}a_\beta(t)Y_t=a_\alpha^\dagger(t)X_t^{\alpha\beta}Y_ta_\beta(t)+a_\alpha^\dagger(t)X_t^{\alpha\mu}V^{\mu\nu}Y_t^{\nu\beta}a_\beta(t).$$

In particular, we have the following interpretation of the results of the previous section: The equation $\dot{U}_t=\dot{G}_0(t)U_t$ with $\dot{G}_0(t)=a_\alpha^\dagger(t)G_{\alpha\beta}^0a_\beta(t)$ is out of Wick order, but can be put to Wick order as $\dot{U}_t=a_\alpha^\dagger(t)G_{\alpha\beta}U_ta_\beta(t)$. The relation $[a_\alpha(t),U_t]=V^{\alpha\mu}G^{\mu\nu}U_ta_\nu(t)$ implies that

$$a_\alpha(t)U_t=(\delta_{\alpha\beta}+V^{\alpha\mu}G_{\mu\beta})U_ta_\beta(t)=F_{\alpha\beta}U_ta_\beta(t),\tag{28}$$

where $\{F_{\alpha\beta}\}$ are the components of the matrix $\mathbf{F}$ introduced in (24).

The QSDE for the unitary $U_\cdot$, with $G_{\alpha\beta}^0=-\mathrm{i}E_{\alpha\beta}$, will then be

$$\dot{U}_t=-\mathrm{i}a_\alpha^\dagger(t)E_{\alpha\beta}a_\beta(t)U_t=-\mathrm{i}a_\alpha^\dagger(t)E_{\alpha\beta}F_{\beta\nu}U_ta_\nu(t)\tag{29}$$

and likewise the QSDE for the flow will be

$$\frac{\mathrm{d}}{\mathrm{d}t}J_t(X)=\dot{U}_t^\dagger(X)U_t+U_t^\dagger(X)\dot{U}_t=-\mathrm{i}U_t^\dagger a_\alpha^\dagger(t)[X,E_{\alpha\beta}]a_\beta(t)U_t=-\mathrm{i}a_\mu^\dagger(t)U_t^\dagger F_{\alpha\mu}^\dagger[X,E_{\alpha\beta}]F_{\beta\nu}U_ta_\nu(t).\tag{30}$$

Comparison with Proposition 2 suggests that $\mathcal{L}_{\mu\nu}(X)=F_{\alpha\mu}^\dagger[X,E_{\alpha\beta}]F_{\beta\nu}$. As this is an entirely new relation, we give an independent derivation in Appendix A using only the Itō calculus.

Lemma 3: Under the conventions and notations of the previous sections, the Evans-Hudson maps take the form

$$\mathcal{L}_{\alpha\beta}(X) = -\mathrm{i}F^{\dagger}_{\mu\alpha}[X,E_{\mu\nu}]F_{\nu\beta}. \tag{31}$$

V. QUANTUM WONG-ZAKAI THEOREM

The following is the multidimensional version of a result first established in Ref. 16.

Theorem: *Let* $a^{\#}_{\alpha}(t,\lambda)$, $\alpha=0,1,\ldots,N$, *be creation/annihilation fields continuous in t for each* $\lambda>0$ *with* $A^{\alpha\beta}_t(\lambda)=\int^t_0 a^{\dagger}_{\alpha}(s,\lambda)a_{\beta}(s,\lambda)\mathrm{d}s$ *approximating fundamental quantum stochastic processes with internal space* $\mathbb{C}^N$ *as before, with fixed gauge matrix* $\mathbf{V}=\{V^{\alpha\beta}\}$. *If* $\Upsilon^{(\lambda)}_t=E_{\alpha\beta}\otimes a^{\dagger}_{\alpha}(t,\lambda)a_{\beta}(t,\lambda)$ *with* $E^{\dagger}_{\alpha\beta}=E_{\beta\alpha}$ *bounded operators on a fixed Hilbert space* $\mathfrak{h}$ *such that* VE *is a strict contraction, then the unitary family* $U^{(\lambda)}_{\cdot}$ *and the Heisenberg dynamical map* $J^{(\lambda)}_{\cdot}(X)=U^{(\lambda)\dagger}_{\cdot}XU^{(\lambda)}_{\cdot}$, *determined by the Schrödinger equation* $\dot{U}^{(\lambda)}_t=-\mathrm{i}\Upsilon^{(\lambda)}_t U^{(\lambda)}_t$, $U^{(\lambda)}_0=1$, *converge in the sense of weak matrix limits to the unitary quantum stochastic process* $U_{\cdot}$ *and corresponding quantum stochastic flow* $J_{\cdot}(X)$. *The limit process* $U_{\cdot}$ *is unitary adapted and satisfies the Stratonovich QSDE* $\mathrm{d}U_t=-\mathrm{i}E_{\alpha\beta}U_t\circ\mathrm{d}A^{\alpha\beta}_t$, $U_0=1$, *with gauge determined by* $\mathbf{V}=\{V^{\alpha\beta}\}$.

The proof is given in Appendix B. We remark that the condition $\|\mathsf{VE}\|<1$ gives convergence of the Neumann series. It also implies that $\mathbf{1}+\mathbf{VEP}$ will be invertible and therefore the Stratonovich QSDE makes sense. We will sketch the proof of this theorem in Appendix B. Provided that the strict contractivity conditions hold, we could replace E, and indeed V, by suitably continuous adapted processes.

It might be remarked that there exists an analogue of this result using Fermi fields in place of Bose fields.[32] The limit QSDE changes insofar as the noises must now be fermionic processes, however, the coefficients are exactly as before.

Examples: Classical Wong Zakai theorem. As a very special example of theorem, let us take the one-dimensional case with the prelimit Hamiltonian $\Upsilon^{(\lambda)}_t$ determined by $E_{00}=H$, $E_{01}=E_{10}=R$ and $E_{11}=0$ with $\kappa=\frac{1}{2}$. Then the limit flow is characterized by the maps $\mathcal{L}_{11}(X)=0$, $\mathcal{L}_{10}(X)=\mathcal{L}_{01}(X)=-i[X,R]$ and $\mathcal{L}_{00}(X)=-i[X,H]-\frac{1}{2}[[X,R],R]$. For the choices $H=\frac{1}{2}(pv(q)+v(q)p)$ and $R=\frac{1}{2}(p\sigma(q)+\sigma(q)p)$, where $v(\cdot)$ and $\sigma(\cdot)$ are Lipschitz continuous with $|v(x)|,|\sigma(x)|<C(1+|x|)$ for some constant $0<C<\infty$, and q and p are canonical position and momentum observables, we have that $q_t:=J_t(q)$ satisfies the essentially classical SDE $\mathrm{d}q_t=[v(q_t)+\sigma(q_t)\sigma'(q_t)]\mathrm{d}t+\sigma(q_t)\mathrm{d}Q_t$ or equivalently $\mathrm{d}q_t=v(q_t)\mathrm{d}t+\sigma(q_t)\circ\mathrm{d}Q_t$, where $Q_t=A^{10}_t+A^{01}_t$ is a copy of the Wiener process.

As a result, the theorem reduces to a classical Wong-Zakai approximation theorem which states that, since $Q^{(\lambda)}_t=\int^t_0(a^{\dagger}(s,\lambda)+a(s,\lambda))\mathrm{d}s$ is an essentially classical stochastic process that is differentiable in time t and converges almost always uniformly on compact time-intervals to a Wiener process Q_t, the solution to the random ODE $\dot{X}^{(\lambda)}_t=v(X^{(\lambda)}_t,t)+\sigma(X^{(\lambda)}_t,t)\dot{Q}^{(\lambda)}_t$, $X^{(\lambda)}_0=x_0$ similarly converges to the diffusion process X. satisfying the Stratonovich SDE

$$\mathrm{d}X_t=v(X_t,t)\mathrm{d}t+\sigma(X_t,t)\circ\mathrm{d}Q_t,\quad X_0=x_0.$$

Quantum diffusions. Taking $\Upsilon^{(\lambda)}_t=R\otimes a^{\dagger}(t,\lambda)+R^{\dagger}\otimes a(t,\lambda)+H$ leads to the limit QSDE

$$\mathrm{d}U_t=-\mathrm{i}(R\otimes\mathrm{d}A^{\dagger}_t+R^{\dagger}\otimes\mathrm{d}A_t+H)\circ U_t\equiv-\mathrm{i}(R\otimes\mathrm{d}A^{\dagger}_t+R^{\dagger}\otimes\mathrm{d}A_t+H)U_t-\kappa R^{\dagger}RU_t\mathrm{d}t.$$

Note that $\mathrm{Re}\,\kappa=\frac{1}{2}$ so that $\mathrm{d}J_t(X)=-\mathrm{i}J_t([X,R])\mathrm{d}A^{\dagger}_t-\mathrm{i}J_t([X,R^{\dagger}])\mathrm{d}A_t+J_t(\mathcal{L}(X))\mathrm{d}t$ where we set $A_t=A^{01}_t$, $A^{\dagger}_t=A^{10}_t$ and $\mathcal{L}(X)=\mathcal{L}_{00}(X)=-\mathrm{i}[X,H']+\frac{1}{2}[R^{\dagger},X]R+\frac{1}{2}R^{\dagger}[X,R]$. The new operator H' is $H+\mathrm{Im}\{\kappa\}R^{\dagger}R$ which includes an energy shift coming from the complex damping κ. The theorem then reduces to a long line of results dealing with broadband noise limits, weak coupling limits, etc., in quantum physics.

It is straightforward to extend this to describe coherent states, thermal states, and squeezed states.[29]

Counting processes. Let us consider the choice $\Upsilon^{(\lambda)}_t=E\otimes\{a(t,\lambda)+f(t)\}^{\dagger}\{a(t,\lambda)+f(t)\}$. This is what we could consider in the vacuum as an equivalent of studying $E\otimes a(t,\lambda)^{\dagger}a(t,\lambda)$ in a coherent of intensity f. Here we have $E_{\alpha\beta}=Ef^{*}_{\alpha}(t)f_{\beta}(t)$ and the one-dimensional form of the theorem yields the Itō coefficients

$$G_{\alpha\beta} = -iE_{\alpha\beta} - \kappa E_{\alpha 1}\frac{1}{1+\mathrm{i}\kappa E_{11}}E_{1\beta},$$

which in this case reduce to

$$G_{\alpha\beta}(t) = \frac{-\mathrm{i}E}{1+\mathrm{i}\kappa E}f_\alpha^*(t)f_\beta(t).$$

The Itō form of the limit QSDE is then

$$\mathrm{d}U_t = \frac{-\mathrm{i}E}{1+\mathrm{i}\kappa E}\mathrm{d}N_t(f)U_t$$

and we introduce $N_t(f)=\int_0^t(\mathrm{d}A_s^{11}+f(s)\mathrm{d}A_s^{10}+f^*(s)\mathrm{d}A_s^{01}+|f(s)|^2\mathrm{d}s)$ which is essentially classical and corresponds to a time-inhomogeneous Poisson process with instantaneous rate of change $\nu(t)=|f(t)|^2$.

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APPENDIX A (PROOF OF LEMMA 3)

We restrict ourselves to the $N=1$ case, as this is already somewhat involved. The multidimensional case does not present any more technical difficulties. Here the Evans-Hudson maps are given by

$$\mathcal{L}_{11}(X) = W^\dagger XW - X,$$

$$\mathcal{L}_{10}(X) = W^\dagger[X,L]; \quad \mathcal{L}_{01}(X) = -[X,L^\dagger]W, \tag{A1}$$

$$\mathcal{L}_{00}(X) = \tfrac{1}{2}[L^\dagger,X]L + \frac{1}{2}L^\dagger[X,L] - \mathrm{i}[X,H],$$

where the operators W,H,L have the explicit forms

$$W = \frac{1-\mathrm{i}\kappa^* E_{11}}{1+\mathrm{i}\kappa E_{11}}, \quad L = -\mathrm{i}\frac{1}{1+\mathrm{i}\kappa E_{11}}E_{10}, \quad H = E_{00} + E_{01}\,\mathrm{Im}\left\{\frac{\kappa}{1+\mathrm{i}\kappa E_{11}}\right\}E_{10}. \tag{A2}$$

The components of the matrix F can also be written out in detail:

$$F_{11} = \frac{1}{1+\mathrm{i}\kappa E_{11}}, \quad F_{10} = -\mathrm{i}\kappa\frac{1}{1+\mathrm{i}\kappa E_{11}}E_{10}, \quad F_{01}=0, \quad F_{00}=1. \tag{A3}$$

We now check that the relation (A1) is correct by direct substitution.

For $\alpha=\beta=1$, we find after a little algebra that

$$\mathcal{L}_{11}(X) = \frac{1+\mathrm{i}\kappa E_{11}}{1-\mathrm{i}\kappa^* E_{11}}X\frac{1-\mathrm{i}\kappa^* E_{11}}{1+\mathrm{i}\kappa E_{11}} - X = -\mathrm{i}\frac{1}{1-\mathrm{i}\kappa^* E_{11}}[X,E_{11}]\frac{1}{1+\mathrm{i}\kappa E_{11}} = -\mathrm{i}F_{\mu 1}^\dagger[X,E_{\mu\nu}]F_{\nu 1}.$$

For $\alpha=1$, $\beta=0$, we have

$$\mathcal{L}_{10}(X) = \frac{1+\mathrm{i}\kappa E_{11}}{1-\mathrm{i}\kappa^* E_{11}}\left[X, -\mathrm{i}\frac{1}{1+\mathrm{i}\kappa E_{11}}E_{10}\right]$$

and to compute this we need the observation that

$$\left[X, \frac{1}{1+\mathrm{i}\kappa E_{11}}\right] = -\mathrm{i}\kappa\frac{1}{1+\mathrm{i}\kappa E_{11}}[X,E_{11}]\frac{1}{1+\mathrm{i}\kappa E_{11}} \tag{A4}$$

to write

$$\mathcal{L}_{10}(X) = i\kappa\frac{1}{1-\mathrm{i}\kappa^* E_{11}}[X,E_{11}]\frac{1}{1+\mathrm{i}\kappa E_{11}} - \mathrm{i}\frac{1}{1-\mathrm{i}\kappa^* E_{11}}[X,E_{10}] = -\mathrm{i}F^\dagger_{\mu 1}[X,E_{\mu\nu}]F_{\nu 0}.$$

As we have $\mathcal{L}_{\alpha\beta}(X)^\dagger = \mathcal{L}_{\beta\alpha}(X^\dagger)$, this gives the $\mathcal{L}_{01}(X)$ result also.

The final case is the Lindbladian map $\mathcal{L}_{00}$. Substituting in gives

$$\mathcal{L}_{00}(X) = -\mathrm{i}[X,E_{00}] - \mathrm{i}[X,E_{01}\,\mathrm{Im}\{T\}E_{10}] + \frac{1}{2}\left[E_{01}\frac{1}{1-\mathrm{i}\kappa^* E_{11}}, X\right]\frac{1}{1+\mathrm{i}\kappa E_{11}}E_{10} + \frac{1}{2}E_{01}\frac{1}{1-\mathrm{i}\kappa^* E_{11}}\left[X, \frac{1}{1+\mathrm{i}\kappa E_{11}}E_{10}\right]$$

and again we use (B1) along with the observation that

$$\mathrm{Re}\,T = \frac{1}{2}\frac{1}{1-\mathrm{i}\kappa^* E_{11}}\frac{1}{1+\mathrm{i}\kappa E_{11}}$$

to obtain

$$\mathcal{L}_{00}(X) = -\mathrm{i}[X,E_{00}] - [X,E_{01}]TE_{10} + E_{01}T^\dagger[X,E_{10}] - \mathrm{i}E_{01}[X,\mathrm{Im}\,T]E_{10} - \mathrm{i}E_{01}T^\dagger[X,E_{11}]\mathrm{Re}\{T\}E_{10} - \mathrm{i}E_{01}\,\mathrm{Re}\{T^\dagger\}[X,E_{11}]TE_{10}.$$

The first three terms are $-\mathrm{i}F^\dagger_{\alpha 0}[X,E_{\alpha\beta}]F_{\beta 0}$, for $(\alpha,\beta)=(0,0)$, (0, 1), and (1, 0), respectively. To tidy up the last term, we note the identities

$$[X,T] = -\mathrm{i}T[X,E_{11}]T, [X,T^\dagger] = +\mathrm{i}T^\dagger[X,E_{11}]T^\dagger$$

so that

$$[X,\mathrm{Im}\,T] + T^\dagger[X,E_{11}]\mathrm{Re}\,T + \mathrm{Re}\,T[X,E_{11}]T = -\tfrac{1}{2}T[X,E_{11}]T - \tfrac{1}{2}T^\dagger[X,E_{11}]T + T^\dagger[X,E_{11}]\mathrm{Re}\,T + \mathrm{Re}\,T[X,E_{11}]T \equiv T^\dagger[X,E_{11}]T$$

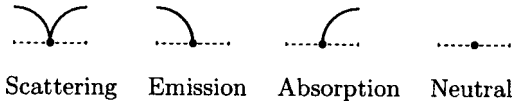
and therefore the last term is $-\mathrm{i}E_{01}T^\dagger[X,E_{11}]TE_{10} \equiv -\mathrm{i}F^\dagger_{10}[X,E_{10}]F_{10}$. This gives the desired form.

APPENDIX B (PROOF OF THE THEOREM)

We now sketch briefly the proof of limit using diagrams. Essentially, this is a form of the van Kampen cumulant expansion[21] which can be described explicitly. The Heisenberg evolution limit is similar though more involved.[16]

Step 1: Wick ordering the Dyson series. For finite λ, the mapping $t \mapsto U_t^{(\lambda)}$ is differentiable, and we may formally expand as the Dyson series $U_t^{(\lambda)} = \Sigma_{n\geqslant 0}(-\mathrm{i})^n \int_{\Delta_n(t)} \Upsilon^{(\lambda)}_{t_n}\cdots\Upsilon^{(\lambda)}_{t_1}$. Here $\Delta_n(t)$ is the simplex consisting of multi-times $(t_n,\ldots,t_1)$ with $t \geqslant t_n \geqslant \cdots \geqslant t_1 \geqslant 0$.

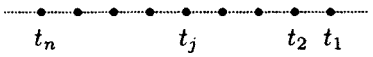
It is convenient to put the Dyson series to Wick order using the commutation relations. The most convenient way to describe this is to expand in terms of diagrammatic series and we borrow some standard techniques from field theory. To this end, we introduce four vertices corresponding to the four components of $\Upsilon_t^{(\lambda)}$:[30]



The Wick-ordered Dyson series is then given by the sum

$$U_t^{(\lambda)} = \sum_{\mathfrak{D}} \hat{\mathfrak{D}}_t(\lambda) \tag{B1}$$

which we now describe. We sum over all diagrams $\mathfrak{D}$ obtained by writing n vertices in a line $(n=0,1,2,\ldots)$ as below



taking each of the vertices to be one of the four shown above, connecting up some of the creation/annihilation pairs and leaving the rest as external lines.

With each such diagram $\mathfrak{D}$ we associate the operator

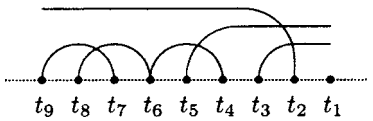
$$\hat{\mathfrak{D}}_t(\lambda) = (-\mathrm{i})^n E_n \cdots E_1 \otimes \int_{\Delta_n(t)} \Pi a^\dagger(\lambda) \Pi C(\lambda) \Pi a(\lambda) \tag{B2}$$

where, depending on the type of vertex at t_j,

$$E_j = \begin{cases} E_{ij}, \text{ scattering} \\ E_{i0}, \text{ emission} \\ E_{0j}, \text{ absorption} \\ E_{00}, \text{ neutral} \end{cases}$$

and in the simplex integral $\Pi a^\dagger(\lambda)$ is the product over all external lines going out, $\Pi a(\lambda)$ is the product over all external lines coming in and $\Pi C(\lambda)$ is a product over all contraction pairs.

For instance the nine vertex diagram below



corresponds to the operator

$$-\mathrm{i}E_{0j_9}E_{0j_8}E_{i_70}E_{i_6j_6}E_{0j_5}E_{i_40}E_{0j_3}E_{i_20}E_{00}$$
$$\otimes \int_{\Delta_9(t)} a^\dagger_{i_2}(t_2,\lambda)a_{j_5}(t_5,\lambda)a_{j_3}(t_3,\lambda)C_{j_9i_7}(t_9-t_7,\lambda)C_{j_8i_6}(t_8-t_6,\lambda)C_{j_6i_4}(t_6-t_4,\lambda).$$

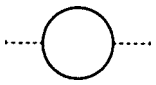
The diagrams we are considering are Goldstone diagrams, or time-ordered Feynman diagrams.[31] The vertices however carry an operator weight $E_{\alpha\beta}$ and, even in the absence of external lines, the diagrams will not generally be scalars!

Step 2: The Markov limit of individual diagrams. Let us consider the effect of the Markov limit $\lambda \to 0$ on individual diagrams. If we have a contraction

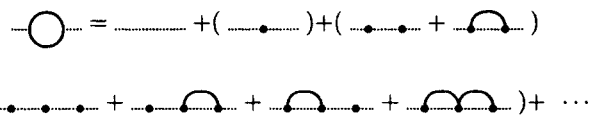
over consecutive times $t_{j+1} > t_j$, then we will have $t_{j+1} - t_j \to 0^+$ in the limit. The effect of each such contraction is to reduce the order of the simplex by one degree and to introduce a multiplication factor V^{ij}. (Remember, we only get a partial contribution from the delta-function since $t_{j+1} > t_j$.) On the other hand, if any of the contracted time pairs are not time consecutive then the contribution converges weakly to zero! The reason is essentially that not just the emission and absorption times, but all the intermediate times are forced to be equal, and we get a collapse of the integral to zero.

We therefore say that a diagram is time-consecutive (TC) if each contraction appearing is between time consecutive vertices only.

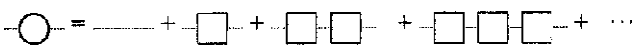
Step 3: The vacuum limit. We now fix u, $v \in \mathfrak{h}$ and investigate the limit $\lim_{\lambda \to 0} \langle u \otimes \Omega | U_t^{(\lambda)} | v \otimes \Omega \rangle$ which we denote by the single vertex



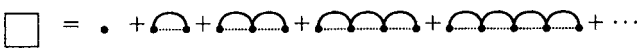
We now argue that this limit will consist of the TC diagrams having no external lines which we can express as



The diagrams have been grouped by vertex number, however, it also possible to group them by effective vertex number which is the actual number minus the number of contractions and which gives reduced degree of the simplex. The series can be partially re-summed as



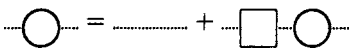
where each box is a sum over all effective one-vertex contributions:



which is analogous to the expression of the self-energy in quantum field theory:as a sum over irreducible terms. (Note that series terminates at second order when there is no scattering: as this is a form of cumulant expansion, the emission/absorption problem is then Gaussian while allowing scattering means that we have cumulant moments to all orders!) Explicitly, the box at time vertex t corresponds to the sum

$$
\begin{aligned}
&-\mathrm{i}E_{00}\mathrm{d}t + (-\mathrm{i})^2 E_{0i_1} E_{i_1 0}\mathrm{d}t + (-\mathrm{i})^3 E_{0i_4} V^{i_4 i_3} E_{i_3 i_2} V^{i_2 i_1} E_{i_1,0}\mathrm{d}t + \cdots \\
&\quad = \left(-\mathrm{i}E_{00} - E_{0i} V^{ij} \left(\frac{1}{1 + \mathrm{i}\mathsf{VE}} \right)_{jk} E_{k0} \right) \mathrm{d}t \equiv -\mathrm{i}G_{00}\mathrm{d}t
\end{aligned}
$$

and we have summed the geometric series, convergent since $\|\mathrm{VE}\| < 1$, to get the required coefficient G_{00}. We can write the expansion in the recursive form



and this is interpreted as the integrodifferential equation

$$\int_0^t \langle u\otimes\Omega|\mathrm{d}U_{t_1}|v\otimes\Omega\rangle = \langle u\otimes\Omega|v\otimes\Omega\rangle - \mathrm{i}\int_0^t \mathrm{d}t_2 \left\langle u\otimes\Omega \left| G_{00}\int_0^{t_2}\mathrm{d}U_{t_1}\right| v\otimes\Omega\right\rangle$$

with decaying exponential solution

$$\langle u\otimes\Omega|U(t)|v\otimes\Omega\rangle = \langle u|e^{-\mathrm{i}tG_{00}}|v\rangle.$$

The interpretation is intended to suggest that there is a limit object U_t which we interpret as a unitary quantum stochastic process on a noise space with initial space $\mathfrak{h}$.

Step 4: Limit of exponential vector matrix elements. Calculating $\lim_{\lambda\to 0}\langle u\otimes\varepsilon_\lambda(\mathbf{f})|U(t,\lambda)|v\otimes\varepsilon_\lambda(\mathbf{g})\rangle$ does not require too much machinery beyond that used in the vacuum case. Indeed, we can convert the new matrix elements to vacuum ones using the relation

$$\langle u\otimes\varepsilon_\lambda(\mathbf{f})|U_f^{(\lambda)}|v\otimes\varepsilon_\lambda(\mathbf{g})\rangle = \langle u\otimes\Omega|\widetilde{U}_t^{(\lambda)}|v\otimes\Omega\rangle,$$

where $\widetilde{U}_t^{(\lambda)}$ is the solution to the Schrödinger equation determined by the "Hamiltonian" $\widetilde{\Upsilon}_t^{(\lambda)}$ obtained by replacing the fields $a(t,\lambda)$ and $a^\dagger(t,\lambda)$ with

$$\widetilde{a}_i(t,\lambda) = a_i(t,\lambda) + \int C_{ij}(t-s,\lambda)g_j(s),$$

$$\widetilde{a}_i^\dagger(t,\lambda) = a_i^\dagger(t,\lambda) + \left[\int C_{ij}(t-s)f_j(\lambda)\right]^*.$$

The new interaction $\widetilde{\Upsilon}_t^{(\lambda)}$ is not necessarily self-adjoint, however, that does not effect things. We may rearrange $\widetilde{\Upsilon}_t^{(\lambda)}$ in terms of the original fields as $\widetilde{E}_{\alpha\beta}\otimes a_\alpha^\dagger(t,\lambda)a_\beta(t,\lambda)$ where, suppressing the λ and t dependencies, the $\widetilde{E}_{\alpha\beta}$ are the operators

$$\widetilde{E}_{ij} = E_{ij},$$

$$\widetilde{E}_{i0} = E_{i0} + E_{ij}\int C_{jl}(t-s,\lambda)g_l(s),$$

$$\widetilde{E}_{0j} = E_{0j} + E_{jk}\left[\int C_{kl}(t-s)f_l(t)\right]^*,$$

$$\widetilde{E}_{00} = E_{00} + E_{i0}\left[\int C_{il}(t-s)f_l(t)\right]^* + E_{0j}\int C_{jl}(t-s,\lambda)g_l(s) + E_{jk}\left[\int C_{il}(t-s)f_l(t)\right]^*\int C_{jm}(t-s,\lambda)g_m(s).$$

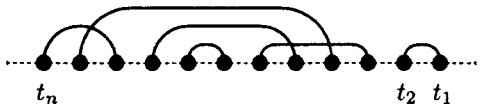
Therefore we only have to repeat our previous argument, but with the original coefficients now replaced by the modified ones $\widetilde{E}_{\alpha\beta}$, taking care with the t and λ dependencies. This time the box at time vertex t corresponds to the sum $-\mathrm{i}f_\alpha^* g_\beta G_{\alpha\beta}\mathrm{d}t$ where now

$$G_{\alpha\beta} = E_{\alpha\beta} - E_{\alpha i}(\mathsf{V} - \mathrm{i}\mathsf{VEV} + (-i)^2\mathsf{VEVEV} + \cdots)_{ij}E_{j\beta} = \left(-\mathrm{i}E_{\alpha\beta} - E_{\alpha i}V^{ij}\left(\frac{1}{1+\mathrm{i}\mathsf{VE}}\right)_{jk}E_{k\beta}\right)$$

and this gives the required result.

Step 5: Convergence of the series. What we have done so far has been to expand the Dyson series, determine the asymptotic limit of each diagram term (only the TC ones survived), to replace the terms by their respective limits and to re-sum the series. To complete the proof, we need to establish that the series is absolutely and uniformly convergent. Fortunately we are able to extend the proof for estimating that these types of series exist for emission-absorption interactions[33] to the general case.

Let us start with the case where we have emission and absorption only in the interaction. The order must be even say, $n=2n_2$, as the vacuum diagrams consist of n_2 pair contractions only. There will then be $(2n_2)!/2^{n_2}n_2!$ such diagrams with $2n_2$ vertices. A typical diagram, having $n_2=6$ is sketched in the following:



There exists a permutation σ of the $n=2n_2$ time indices which re-orders to the diagram $\mathfrak{D}_0(n)$ shown in the following:

The permutation is moreover unique if it has the induced ordering of the emission times. Not all permutations arise this way, the ones that do are termed admissible. We now consider an estimate of the nth term in the Dyson series. Let $E=\max\|E_{\alpha\beta}\|$, then

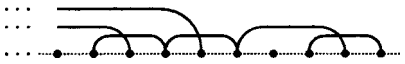
$$\sum_{\mathfrak{D}} E^n \int_{\Delta_n(t)} \prod |C(\lambda)| \Big|_{\mathfrak{D}} = \sum_{\text{Admissible perms.}} E^n \int_{\Delta_n(t)} \prod |C(\lambda)\circ\sigma| \Big|_{\mathfrak{D}_0(n)}$$

$$= E^n \int_{R(t)} \prod_{k=1}^{n_2} |C(t_{2k}-t_{2k-1},\lambda)|,$$

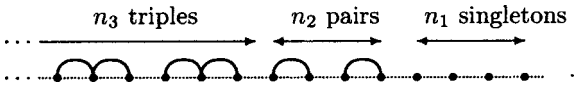
where $R(t)$ is the union of simplices $\{(t_n,\ldots,t_1): t>t_{\sigma^{-1}(n)}>\ldots>t_{\sigma^{-1}(1)}>0\}$ over all admissible permutations Z. $R(t)$ will be a subset of $[0,t]^{2n_2}$ and if we introduce variables t_{2k} and $s_{2k}=t_{2k}-t_{2k-1}$ for $k=1,\ldots,n_2$, it is easily seen that the above is majorized by $E^{2n_2}C^{n_2}\times\max(t,1)^{n_2}/n_2!$, where $C=\max V^{ij}$. This is the Pulè inequality[33] and clearly gives the uniform absolute estimate required to sum the series.

We now consider scattering, and constant, terms in the interaction. This time, the number of diagrams with n vertices will be given by the nth Bell number B_n. To see why this is so, we recall that if we have a reservoir quanta created at a vertex, then perhaps scattered, and finally reabsorbed then we can think of it as the same quantum and treat all the vertices it has been at as being linked. Each such diagram is then described by these subsets of linked vertices (we should also count the neutral vertices as these are singleton sets): in this way we have a one-to-one correspondence between the diagrams and partitions of vertices into nonempty subsets. The Bell numbers grow rapidly and have a complicated asymptotic behavior. The proliferation of diagrams is due mainly to the multiple scattering that now takes place.

Let us consider a typical diagram. We shall assume that within the diagram there are n_1 singleton vertices $[\cdots \bullet \cdots]$, n_2 contraction pairs $[\cdots \overset{\frown}{\bullet\cdots\bullet} \cdots]$, n_3 contraction triples $[\cdots \overset{\frown}{\bullet\cdots\bullet\cdots\bullet} \cdots]$ etc. That is the diagram has a total of $n=\Sigma_j jn_j$ vertices which are partitioned into $m=\Sigma_j n_j$ connected subdiagrams. For instance, we might have an initial segment of a diagram looking like the following:



There will exist a permutation σ of the n vertices which will reorder the vertices so that we have the singletons first, then the pair contractions, then the triples, etc., so that we obtain a picture of the following type:



The permutation is again unique if we retain the induced ordering of the first emission times for each connected block. We now wish to find a uniform estimate for the nth term in the Dyson series, we have

$$\sum_{\mathfrak{D}} \int_{\Delta_n(t)} \prod |C(\lambda)| \times \text{“ weights”}$$

where the weights are the operator norms of various products of the type $E_{\alpha_n\beta_n}\cdots E_{\alpha_1\beta_1}$. Each connected diagram of $j\geqslant 2$ vertices will typically have one emission and one absorption, and $j-2$ scattering vertices. The Pulè argument of rearranging the sum over diagrams into a single integral over a region $R(t)$ of $[0,t]^n$ again applies and by similar reason we arrive at the upper bound, this time of the type

$$\sum_{n_1,n_2,n_3,\ldots}{}' \|\mathsf{VE}\|^{n_1+2n_2+3n_3+\cdots} E^{n_1+n_2+n_3+\cdots} \times \frac{\max(t,1)^{n_1+n_2+n_3+\cdots}}{n_1!n_2!n_3!\cdots}.$$

Here the sum is restricted so that $\Sigma_j jn_j=n$. An uniform estimate for the entire series is then given by removing this restriction:

$$\Xi(A,B)=\sum_{n_1,n_2,n_3,\cdots} \frac{\exp\{\sum_j (A_j+B)n_j\}}{n_1!n_2!n_3!\ldots}$$

where $e^A=\|\mathsf{VE}\|$ and $e^B=E\max(t,1)$. Again we use the trick to convert a sum of products into a product of sums

$$\Xi(A,B)=\prod_j \sum_n \frac{\exp\{(Aj+B)n\}}{n!}=\exp\left\{\frac{e^{A+B}}{1-e^A}\right\},$$

where we need $e^A<1$ to sum the geometric series—this however, is precisely our condition that $\|\mathsf{VE}\|<1$.

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Bayesian analog of Gleason's theorem

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We introduce a novel notion of probability within quantum history theories and give a Gleasonesque proof for these assignments. This involves introducing a tentative novel axiom of probability. We also discuss how we are to interpret these generalized probabilities as partially ordered notions of preference, and we introduce a tentative generalized notion of Shannon entropy. A Bayesian approach to probability theory is adopted throughout; thus the axioms we use will be minimal criteria of rationality rather than *ad hoc* mathematical axioms. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2390658]

I. INTRODUCTION AND SUMMARY

In Ref. 1 we postulated a novel notion of probability by generalizing Cox's axioms of probability[2,3] in a manner appropriate to quantum theory. In this paper we wish to go one step further; we will present a uniqueness proof analogous to Gleason's theorem for our postulated generalized probabilities. We will be helped considerably by another analog of Gleason's theorem in the literature[4] which is applied to the decoherence functional in the history projection operator (HPO) formulation of the consistent histories program.[5] First we will review results previously discussed[1] and then we will outline the relevant Gleason-like theorem, its interpretation, and, for completeness, its proof. We will then propose a generalized entropy.

We will adopt a Bayesian approach to probability theory and we will use Cox's approach in particular.[3] Probabilities are usually considered real numbers because of an association with relative frequencies. As soon as we adopt an approach to probability theory where we merely assign probabilities as an ordered notion of preference, then there is absolutely no *a priori* reason to consider probabilities as real numbers. One might try to design "zeroth" axioms of probability theory which end up ensuring that probabilities are, in fact, real numbers, and then one might introduce further axioms to constrain how we assign these real numbers to propositions. Such an approach is, however, problematic because such zeroth axioms are rather *ad hoc*.

Consider some arbitrary propositions α, β, and γ to which we are to assign probabilities. Consider also a notion of ordering "$>$" to be defined on the probability space. Two possible zeroth axioms,[6] which constrain how this ordering notion is to behave, are "universal transitivity:"
Axiom 0a,

$$\text{if } p(\alpha|I) > p(\beta|I) \text{ and } p(\beta|I) > p(\gamma|I) \text{ then } p(\alpha|I) > p(\gamma|I), \tag{1}$$

and "universal comparability:"
Axiom 0b,

$$\text{for all } \alpha \text{ and } \beta \text{ we have that either } p(\alpha|I) > p(\beta|I) \text{ or } p(\alpha|I) < p(\beta|I) \text{ or } p(\alpha|I) = p(\beta|I). \tag{2}$$

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Given these zeroth axioms it would seem natural (although it is still not strictly necessary) to use real numbers for probability assignments. Axiom 0a is often considered desirable because probabilities are intended to represent transitive notions of preference in some sense. Axiom 0b is, however, far more dubious and there is a history in the literature of people trying not to assume it (see Appendix A.3 of Ref. 6 for references and also see Refs. 7 and 8). Why presume that we can probabilistically compare all propositions universally, especially in quantum theory where some propositions are considered "incompatible" or "complimentary?" It is prudent not to assume Axiom 0b from the outset (it might be that we are forced to adopt it later). If we were to adopt Axiom 0b, then it might be that we will be introducing relationships between probabilities that we are not justified in invoking—and any problems such as nonadditivity and so forth might be due to such a mistaken assumption.

Rather than adopt these two controversial zeroth axioms let us, for the time being, use a weaker zeroth axiom that we can all surely agree on:
Axiom 0′,

$$\text{if } \alpha \preccurlyeq \beta \text{ then, presumably, } p(\alpha|I) \leqslant p(\beta|I), \tag{3}$$

where "$\preccurlyeq$" is, in the least, a partial order in the context of both the proposition space and the space of generalized probabilities (in the context of standard probability theory, we could use Venn diagrams to define $\alpha \preccurlyeq \beta$ using subset inclusion and we would define $p(\alpha|I) \leqslant p(\beta|I)$ using the total ordering of real numbers). We call this axiom "monoticity."[9] So as to avoid confusion with standard probability theory (theories which obey Axioms 0a and 0b), it is prudent to call any assignment which merely obeys the weaker zeroth axiom [Eq. (3)] by another name: we will call them "pedagogical examples" or "pegs." Probabilities are then special examples of pegs.

Our task in this paper is then to find a peg theory for a histories algebra. We will use the histories propositional algebra $\mathcal{P}(\mathcal{V})$, where $\mathcal{V}=\otimes^n\mathcal{H}$, which was originally introduced by Isham.[5] The natural connectives on this space of projection operators are the standard $\wedge$, $\vee$, and $\neg$ connectives and we use the standard partial order $\preccurlyeq$ upon it.[5] A homogeneous history proposition α is defined as a time ordered tensor product of projection operators $\hat{\alpha}_{t_m} \in \mathcal{P}(\mathcal{H})$:

$$\alpha := \hat{\alpha}_{t_n}(t_n) \otimes \hat{\alpha}_{t_{n-1}}(t_{n-1}) \otimes \cdots \otimes \hat{\alpha}_{t_1}(t_1). \tag{4}$$

We stay in the Heisenberg picture such that each projection operator has the dynamics already implicit such that $\hat{\alpha}_{t_m}(t_m)=\hat{U}^\dagger(t_m-t_{m-1})\hat{\alpha}_{t_m}\hat{U}(t_m-t_{m-1})$, where $\hat{\alpha}_{t_m}$ are Schrödinger picture operators. Our novel peg assignments, those that we suggested in Ref. 1, are

$$p(\alpha|I) := \mathrm{tr}_{\mathcal{H}}(C_\alpha \hat{\rho}), \tag{5}$$

where $C_\alpha=\hat{\alpha}_{t_n}(t_n)\hat{\alpha}_{t_{n-1}}(t_{n-1})\cdots\hat{\alpha}_{t_1}(t_1)$ and $\hat{\rho}$ is a density operator on $\mathcal{H}$. We keep an explicit hypothesis I in the notation because such a thing is natural when discussing probabilities from a Bayesian perspective,[10] and it avoids us confusing peg assignments that are made given different prior information. Clearly these pegs might obey Eq. (3) by relating the natural partial order on $\mathcal{P}(\mathcal{V})$ to some partial order on $\mathbb{C}$. Once we introduce further axioms that these pegs ought to obey—other than Eq. (3)—then we will be able to speculate what this partial order on the peg space might be.

We proposed these pegs for the history algebra $\mathcal{P}(\mathcal{V})$ because they are additive for disjoint homogeneous history propositions;[1] thus these complex pegs seem to *behave* something like we expect probabilities should. Now we aim to show that we can *derive* these pegs from axioms analogous to Cox's axioms of probability theory applied to the HPO algebra using an analog of Gleason's theorem.

II. A GLEASON ANALOG

So, let us remind ourselves of what Gleason's theorem[11] tells us. Gleason's theorem is about trying to assign probabilities to a quantum propositional algebra. In standard quantum theory the

relevant propositional algebra is taken to be $\mathcal{P}(\mathcal{H})$, the set of projection operators upon a Hilbert space $\mathcal{H}$, where the natural logical connectives on $\mathcal{P}(\mathcal{H})$ are $\wedge$, $\vee$, and $\neg$, and we denote the standard partial order relation $\leqslant$. So, naturally, a probability assignment should obey certain rules which we shall use to define what is often, perhaps confusingly, called a state (we call it a state more because of what we end up proving). A state $\sigma \in \mathcal{S}$ is a real valued function on $\mathcal{P}(\mathcal{H})$ which has the following properties:

1. Positivity: $\sigma(\hat{P}) \geqslant 0$ for all $\hat{P} \in \mathcal{P}(\mathcal{H})$,
2. Additivity: if $\hat{P}$ and $\hat{R}$ are disjoint—$\hat{P} \wedge \hat{R} = \hat{\mathbf{0}}$—then $\sigma(\hat{P} \vee \hat{R}) = \sigma(\hat{P}) + \sigma(\hat{R})$, and
3. Normalization: $\sigma(\hat{1}) = 1$,

where $\hat{\mathbf{0}} \in \mathcal{P}(\mathcal{H})$ is the proposition that is always false and $\hat{\mathbf{1}} \in \mathcal{P}(\mathcal{H})$ is the proposition that is always true. Gleason's theorem is simply that states assigned to $\mathcal{P}(\mathcal{H})$, for $\dim \mathcal{H} > 2$, are in one-to-one correspondence with density matrices on $\mathcal{H}$ such that

$$\sigma_\rho(\hat{P}) = \mathrm{tr}(\hat{P}\hat{\rho}) \quad \text{for all } \hat{P} \in \mathcal{P}(\mathcal{H}). \tag{6}$$

One takes the propositional algebra of projection operators, makes basic assumptions about how probabilities ought to behave, and derives that such probability assignments are in one-to-one correspondence with density matrices. The axioms of probability theory ensure the density matrix structure of quantum theory.

In analogy with Gleason's theorem, we should list a set of axioms that our pegs should obey and then try and derive the theorem from there. For these axioms, we argue, we should look to Cox's axioms of probability theory which ensure that we do not introduce functional relationships between peg assignments that are not rationally justified. Cox's $\wedge$-axiom is simply that the pegs we peg to propositions conjoined using the AND operation should be limited to be functionally dependent only on some very specific pegs:

$$p(\alpha \wedge \beta | I) := F[p(\alpha|\beta I), p(\beta|I)], \tag{7}$$

where F is an arbitrary function that is sufficiently well behaved for our purposes. Similarly, Cox's $\neg$-axiom is that the peg we peg to the negation of a proposition should only functionally depend upon the peg of the proposition before it was negated:

$$p(\neg\alpha|I) := G[p(\alpha|I)]. \tag{8}$$

These two axioms are criteria of rationality that are at the heart of Cox's approach to probability theory and these are all he needed (except for the additional assumption that probabilities are real numbers) in order to prove the basics of probability theory as applied to a Boolean algebra of propositions.

Cox's two axioms suggest we should use a peg that is additive for disjoint history propositions and that is normalized.[3] It turns out that this will not be sufficient for our peg theory; we will need a further axiom. Luckily one is forthcoming. Note that in the HPO formulation of history theories, we have the three natural logical connectives $\wedge$, $\vee$, and $\neg$ which correspond roughly to AND, OR, and "negation" operations (although with the standard nondistributivity issue we have in quantum theory). Clearly, however, when going from projection operators defined at a single time to explicitly history orientated propositions, there is another natural connective, namely, changing the temporal order. As such we can define an operator M which reverses the order on any tensor product vector, $M(v_1 \otimes v_2 \otimes \cdots v_m) := (v_m \otimes v_{m-1} \otimes \cdots v_1)$. Thus the temporal reversal of the Heisenberg picture history proposition α is given by

$$\alpha := M\alpha M = \hat{\alpha}_{t_1}(t_1) \otimes \hat{\alpha}_{t_2}(t_2) \otimes \cdots \otimes \hat{\alpha}_{t_n}(t_n). \tag{9}$$

Note that $\lhd$ reverses both the kinematical and the dynamical temporal orderings because we are in the Heisenberg picture (cf. Ref. 12). Applying $\lhd$ twice in this manner obviously gives back the same history proposition, behavior that is analogous to the negation operation. Hence we should introduce a third peg axiom analogous to Eq. (8):

$$p(\lhd\alpha|I) := H[p(\alpha|I)], \tag{10}$$

where H is an arbitrary function that is sufficiently well behaved for our purposes. The peg we assign to such a proposition should be assigned in a noncontextual manner according to Eq. (10). Clearly, by Youssef's argument,[7] we could use complex numbers and still keep consistency with analogs of Cox's two axioms. Our tentative third axiom seems to give our pegs an "extra degree of freedom." Using real numbers would not be a possibility for a peg that also obeys Eq. (10), and luckily we are using the uncontroversial weaker zeroth axiom [Eq. (3)]. Hence it might be that we can find a peg which obeys Eqs. (3), (7), (8), and (10).

In analogy with how we define states in Gleason's theorem, let us define complex assignments as maps $l:\mathcal{P}(\mathcal{V})\rightarrow\mathbb{C}$ which obey the following rules:

1. Conjugation: $l(\alpha)^*=l(\lhd\alpha)$ for all α,
2. Additivity: if α and β are disjoint then $l(\alpha\vee\beta)=l(\alpha)+l(\beta)$, and
3. Normalization: $l(\mathbf{1})=1$.

We use the similar notation as we used for the Hilbert space $\mathcal{H}$ because $\mathcal{V}$ is still a Hilbert space (although we leave the "hats" off operators in $\mathcal{V}$). This is an advantage of using Isham's HPO formulation of the history algebra.[5]

Note that the peg axioms (7), (8), and (10) do not uniquely ensure that we *must* use the complex assignments l—just as Cox's axioms in standard probability theory do not ensure that we must use real numbers *per se*. The peg axioms ensure that, whatever assignments we do use for convenience, such assignments at least obey the relevant criteria of rationality. Hence we do not argue that the complex assignments l are uniquely the only pegs we could use, but clearly the maps l do obey Eqs. (7), (8), and (10) and might yet obey Eq. (3) for some partial order on $\mathbb{C}$. One might even argue that it is not the particular assignments that matter; it is the catalog of functional relationships between them that is important (this we categorize axiomatically using analog of Cox's axioms). Nonetheless, it is convenient to use particular representations (just as it is convenient to use real numbers in standard Bayesian probability theory).

Can we now start to tackle a proof of a Gleason-like theorem for these complex assignments l? In fact, the result follows from an analog of Gleason's theorem for decoherence functionals already in the literature.[4]

Let us first review some identities.[4] Note that

$$\mathrm{tr}_{\mathcal{H}}(\hat{A}_1\hat{A}_2\cdots\hat{A}_n)=\mathrm{tr}_{\otimes^n\mathcal{H}}(\hat{A}_1\otimes\hat{A}_2\otimes\cdots\hat{A}_nS), \tag{11}$$

where $\hat{A}_m$ are arbitrary self-adjoint operators on $\mathcal{H}$ and S is a linear operator $S:\otimes^n\mathcal{H}\rightarrow\otimes^n\mathcal{H}$ defined on product vectors by

$$S(v_1\otimes v_2\otimes\cdots\otimes v_n) := v_2\otimes v_3\otimes\cdots\otimes v_n\otimes v_1 \tag{12}$$

and extended by linearity and continuity to give a unitary operator on $\otimes^n\mathcal{H}$.

We can swap between the Heisenberg and Schrödinger pictures using

$$\mathrm{tr}_{\mathcal{H}}(C_\alpha)=\mathrm{tr}_{\otimes^n\mathcal{H}}(\hat{\alpha}_{t_n}\otimes\hat{\alpha}_{t_{n-1}}\otimes\cdots\hat{\alpha}_{t_1}S^U), \tag{13}$$

where the $\hat{\alpha}_{t_m}$ are Schrödinger picture projection operators and $S^U := (\hat{U}_1^\dagger\otimes\cdots\otimes\hat{U}_n^\dagger)S(\hat{U}_1\otimes\cdots\otimes\hat{U}_n)$.

In an analogous way,[4] we can absorb the initial state into an operator defined on $\mathcal{V}=\otimes^n\mathcal{H}$ using the identity (11). Note that

$$\mathrm{tr}_{\mathcal{H}}(\hat{A}_1\hat{A}_2\cdots\hat{A}_n)=\mathrm{tr}_{\otimes^n\mathcal{H}}((\hat{A}_1\otimes\hat{A}_2\otimes\cdots\hat{A}_{n-1}\otimes\mathbf{1}_n)(\mathbf{1}_1\otimes\mathbf{1}_2\otimes\cdots\mathbf{1}_{n-1}\otimes\hat{A}_n)S) \tag{14}$$

$$=\mathrm{tr}_{\otimes^n\mathcal{H}}((\hat{A}_1\otimes\hat{A}_2\otimes\cdots\hat{A}_{n-1}\otimes\mathbf{1}_n)Y) \tag{15}$$

$$=\mathrm{tr}_{\otimes^{n-1}\mathcal{H}}((\hat{A}_1\otimes\hat{A}_2\otimes\cdots\hat{A}_{n-1}Y')\ , \tag{16}$$

where Y' is obtained from Y by tracing over a complete set of states for the nth Hilbert space. The form of Eq. (11) is preserved under removing an operator by the action of a partial tracing and is also preserved when removing the dynamics from around each single-time proposition in the history proposition.

So, using these identities we can absorb all the dynamics and initial state into some operator Z such that

$$\mathrm{tr}_{\mathcal{H}}(C_\alpha\hat{\rho})=\mathrm{tr}_{\otimes^n\mathcal{H}}(\hat{\alpha}_{t_n}\otimes\hat{\alpha}_{t_{n-1}}\cdots\otimes\hat{\alpha}_{t_1}Z_{\rho,H}). \tag{17}$$

Note that the left-hand side (LHS) of Eq. (17) is in the Heisenberg picture, whereas the right-hand side (RHS) is in the Schrödinger picture; we have split the dynamics and kinematics into distinct entities. There are good reasons for doing this as it would allow us to investigate the distinction between the two forms of temporal orderings.[12] But note that we can stay within the Heisenberg picture if we wish (for it is, by far, the preferable picture[13]); we keep the dynamics around the corresponding projection operators and absorb just the initial state into an operator Y:

$$\mathrm{tr}_{\mathcal{H}}(C_\alpha\hat{\rho})=\mathrm{tr}_{\otimes^n\mathcal{H}}(\hat{\alpha}_{t_n}(t_n)\otimes\hat{\alpha}_{t_{n-1}}(t_{n-1})\otimes\cdots\hat{\alpha}_{t_1}(t_1)Y_\rho). \tag{18}$$

The above ensures that we can put our tentative assignment into "Gleason" form. Now we can prove an analog of Gleason's theorem for such operators Y_ρ. The theorem and proof follow the analysis in Ref. 4 almost word for word. There are, however, distinguishing features and, for completeness, we repeat the analysis here since the proof is so short.

Theorem: If $\dim\mathcal{V}>2$, the complex assignments l are in one-to-one correspondence with operators Y on $\mathcal{V}=\otimes^n\mathcal{H}$ according to the rule

$$l(\alpha)=\mathrm{tr}_{\mathcal{V}}(\alpha Y), \tag{19}$$

with the restrictions that

$$Y^\dagger=MYM, \tag{20}$$

$$\mathrm{tr}_{\mathcal{V}}(Y)=1, \tag{21}$$

where M is an operator that reverses the order of the entries in a tensor product vector; $M(v_1\otimes v_2\otimes\cdots v_m):=(v_m\otimes v_{m-1}\otimes\cdots v_1)$.

Proof: In one direction, the theorem is trivial; if a function l is *defined* by the right-hand side of Eq. (19) it clearly obeys the crucial additivity condition. The extra requirements (20) and (21) ensure normalization and conjugation requirements.

Conversely, let $l:\mathcal{P}(\mathcal{V})\to\mathbb{C}$ be a complex assignment. The proof that it must have the form (19) exploits Gleason's theorem applied to $\mathcal{P}(\mathcal{V})$.

Let $\mathrm{Re}\,l$ and $\mathrm{Im}\,l$ denote the real and imaginary parts of l so that

$$l(\alpha)=\mathrm{Re}\,l(\alpha)+\mathrm{Im}\,l(\alpha) \tag{22}$$

where $\mathrm{Re}\,l(\alpha)\in\mathbb{R}$ and $\mathrm{Im}\,l(\alpha)\in\mathbb{R}$. The additivity condition on l means that $\mathrm{Re}\,l(\alpha)$ and $\mathrm{Im}\,l(\alpha)$ are additive functions on $\mathcal{P}(\mathcal{V})$, i.e., $\mathrm{Re}\,l(\alpha_1\vee\alpha_2)=\mathrm{Re}\,l(\alpha_1)+\mathrm{Re}\,l(\alpha_2)$ for any disjoint pair α_1, α_2 of projectors and similarly for $\mathrm{Im}\,l$. We have that $l(\alpha)$ is a continuous function of its argument and hence $\alpha\mapsto l(\alpha)$ is a continuous function on $\mathcal{P}(\mathcal{V})$, as are its real and imaginary parts. However, the

set of all projectors in the finite dimensional space $\mathcal{V}$ is a finite disjoint union of Grassman manifolds and is hence compact. It follows that the functions $\alpha \mapsto \mathrm{Re}\, l(\alpha)$ and $\alpha \mapsto \mathrm{Im}\, l(\alpha)$ are bounded below and above. On the other hand, for any $r \in \mathrm{R}$, the quantity

$$\kappa_r(\alpha) := r \dim(\alpha) = r\mathrm{tr}(\alpha) \tag{23}$$

is a real additive function of α, and hence so are $\mathrm{Re}\, l + \kappa_r$ and $\mathrm{Im}\, l + \kappa_s$ for any $r, s \in \mathbb{R}$. We can choose an r such that $\mathrm{Re}\, l + \kappa_r \geqslant 0$ for all α (and s such that $\mathrm{Im}\, l + \kappa_s \geqslant 0$), and due to an upper bound we can choose positive real scale factors μ and ν such that for all α we have that

$$0 \leqslant \mu(\mathrm{Re}\, l + \kappa_r)(\alpha) \leqslant 1, \tag{24}$$

$$0 \leqslant \nu(\mathrm{Im}\, l + \kappa_s)(\alpha) \leqslant 1. \tag{25}$$

These inequalities plus the additivity property show that, for each $\alpha \in \mathcal{P}(\mathcal{V})$, the quantities $\alpha \mapsto \mu(\mathrm{Re}\, l + \kappa_r)(\alpha)$ and $\alpha \mapsto \nu(\mathrm{Im}\, l + \kappa_s)(\alpha)$ are states on the lattice $\mathcal{P}(\mathcal{V})$. Then Gleason's theorem shows that there exists a pair of density matrices ρ^1 and ρ^2 on $\mathcal{V}$ such that for all $\alpha \in \mathcal{P}(\mathcal{V})$,

$$\mu(\mathrm{Re}\, l + \kappa_r)(\alpha) = \mathrm{tr}_{\mathcal{V}}(\rho^1 \alpha), \tag{26}$$

$$\nu(\mathrm{Im}\, l + \kappa_s)(\alpha) = \mathrm{tr}_{\mathcal{V}}(\rho^2 \alpha), \tag{27}$$

and so

$$\mathrm{Re}\, l(\alpha) = \mathrm{tr}_{\mathcal{V}}\left(\left(\frac{1}{\mu}\rho^1 - r\right)\alpha\right) = \mathrm{tr}_{\mathcal{V}}(Y^1 \alpha), \tag{28}$$

$$\mathrm{Im}\, l(\alpha) = \mathrm{tr}_{\mathcal{V}}\left(\left(\frac{1}{\nu}\rho^2 - s\right)\alpha\right) = \mathrm{tr}_{\mathcal{V}}(Y^2 \alpha), \tag{29}$$

where $Y^1 := (1/\mu)\rho^1 - r$ and $Y^2 := (1/\nu)\rho^2 - s$. Thus we have shown the existence of a family of operators $Y := Y^1 + iY^2$ on $\mathcal{V}$ such that

$$l_\rho(\alpha) = \mathrm{tr}_{\mathcal{V}}(\alpha Y_\rho). \tag{30}$$

This completes the proof of the theorem because the conditions (20) and (21) follow at once from the conjugation and normalization conditions on complex assignments. ■

We do not discuss any extensions to infinite dimensional cases. We add the subscript ρ to Y to emphasize that it depends upon the initial state; it is anticipated that Y_ρ can be decomposed into some operators on $\mathcal{V}$ which are universally defined (through relations between traces of products of operators and traces of tensor product operators) and some operators that are related to the initial state. Clearly the Y operators on $\mathcal{V}$ and density operators on $\mathcal{H}$ are intimately related; the task is now to investigate the properties and interpretation of these pegs. But, in the least, we can put our assignment (5) into the form (30) for which we have an analog of Gleason's theorem.

One issue that we have to identify is that we have promoted the operation to $\lhd$ a connective on par with $\vee$, $\wedge$, and $\neg$, and it may not seem natural to some to do this. We considered it natural because we were going from a space $\mathcal{P}(\mathcal{H})$ which identified propositions at a single time to a space $\mathcal{P}(\mathcal{V})$ which explicitly identified history propositions. So we need a connective that can relate different temporal orderings. One might then query, why specifically $\lhd$? Why not some other operation, such as making any permutation of single-time entries? Staying in the Heisenberg picture ensures that the dynamics are already taken care of, and permuting the entries would mess up this fact; hence we only discuss a connective that maintains the dynamical relationships between single-time propositions.

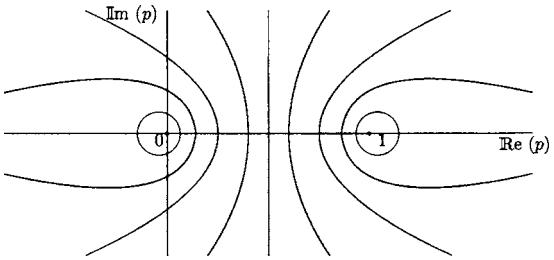

FIG. 1. Contour lines of pegs of equivalent size by a suggested partial order on $\mathbb{C}$. The "height" of each contour gets larger starting from the circle around 0 until we reach the circle around 1.

Note that we do not need to use the monoticity axiom [Eq. (3)] for Gleason-like proofs; it is, in some sense, redundant. Nonetheless, how might our pegs obey monoticity? In $\mathcal{P}(\mathcal{V})$ we have the following condition:

$$\mathbf{0} \leqslant \alpha \leqslant \mathbf{1} \quad \text{for all } \alpha \in \mathcal{P}(V). \tag{31}$$

For our pegs we have that $p(\mathbf{0}|I)=0$ and $P(\mathbf{1}|I)=1$ and hence, by monoticity, we must, in the least, demand that

$$0 \leqslant p(\alpha|I) \leqslant 1 \quad \text{for all } \alpha \in \mathcal{P}(V). \tag{32}$$

One tentative partial order might look something like Fig. 1. This partial order has the added advantage as we are unable to relate $p(\lhd\alpha|I)$ and $p(\alpha|I)$ using it (the partial ordering is symmetric in the real axis and complex conjugation represents time reversal). [Equivalently, one can picture the same partial order as allowing many different paths from uncertainty to certainty such that these paths are symmetric in the real axis. These paths would look like the lines of magnetic flux between north (0) and south (1) magnetic poles in two dimensions (2D) (not illustrated). This absolves us of Jaynes' argument against comparative probability theories—ones that do not obey Axiom 0b—by allowing many dense paths from 0 to 1, see the Appendix of Ref. 6]. Since, by the partial order on $\mathcal{P}(\mathcal{V})$, α NR $\lhd\alpha$ (where NR stands for "not related to by the relevant partial order"), we ought to demand this of the peg space as well, such that $p(\lhd\alpha|I)$ NR $p(\alpha|I)$. Also, this partial order reduces to the standard probabilities when we move to the real line between 0 and 1.

Note, however, that there are many partial orders on $\mathbb{C}$ and there might be another applicable one; we introduce the partial order represented by Fig. 1 to emphasize that monoticity will provide constraints for the partial orders that we can use. For disjoint propositions α and β, we have that $\alpha \leqslant \neg\beta$; hence the monoticity requirement ensures that $p(\alpha|I) \leqslant 1-p(\beta|I)$ which is satisfied as long as Eq. (32) is. The constraint (32) thus ensures a class of partial orders that might be useful and Fig. 1 seems the most apt.

Even obeying all the peg axioms we have to hand it is still very difficult to interpret these pegs as "probabilities" *per se* because we are taught again and again that probabilities are real numbers. However, remember that there is no *a priori* reason to regard probabilities as real numbers; they are merely magnitudes that we use in order to assign a partially ordered notion of preference to propositions.

III. DISCUSSION

Having an analog of Gleason's theorem for our pegs is not enough; we now need to argue why we should use such complex pegs in the first place. We have given an argument based on rejecting Axiom 0b; so now it is important to discuss the factitious problems that are solved by rejecting it. If we keep Axiom 0b then, by the very fact that we will be comparing propositions in a manner

that is not justified rationally, we will be introducing relations within the probability space that are not underpinned by relations in the proposition space. Hence we call such relations in the probability space "factitious."

The language we have used here is perhaps quite telling. Our use of the term factitious harks back to Einstein's use of the term. Clearly, if we adopt a relational approach to theory building (one which obeys Leibniz's principles of relationalism[14]), we do not want to introduce factitious elements in any theory. Cox adopted a rationalist approach analogous to relationalism—he gave a formulation of probability theory which ensures that factitious functional relations between propositions, quantified using pegs, are never introduced. Instead we only maintain those functional relationships that we can justify. Clearly this peg approach might therefore be useful in the quantum gravity domain where an explicitly relational approach is often considered a requirement. One might naïvely argue that, in addition to a relational notion of space-time, one needs a relational notion of probability. In the least it would be prudent to adopt an approach to probability theory based upon criteria of rationality rather than ad hoc axioms.

Hence it is plausible that problems such as nonlocality are factitious problems that are caused by invoking a probability theory which does not have sufficient structure. Thus a Bayesian approach may bring locality back to quantum theory, just as Einstein bought locality back to gravitational theories in building general relativity[15]—in fact, this is the major reason many invoke Bayesian reasoning within quantum theory[16] (although one does not need to adopt as drastic a peg theory as we adopt here in order to tentatively deny nonlocality).

Similarly, the problem of hidden variables might also be factitious. The Kochen-Specker theorem[17] seems[18] to prove that we cannot assign definitive values to variables prior to measurement in quantum theory. This is obviously compatible with a Bayesian approach to ignorance—we cannot assign such values because we are explicitly *presuming we are ignorant of them.*

These complex pegs are intimately related to the approaches of Feynman[19] and Hartle[20] who invoke real probabilities that can lie outside of [0, 1]. Hartle's virtual probabilities are explicitly found using the real parts of our complex pegs [Eq. (5)] which, in turn, were originally introduced by Goldstein and Page[21] in their linearly positive histories approach. Thus the linearly positive histories and the consistent histories programs appear naturally within this peg framework. If we wish to discuss real Bayesian probabilities, we could follow the linearly positive histories program and take the real parts of our pegs and ensure a linearly positive condition.[22] Similarly, if we wish to discuss relative frequencies, we could follow the consistent histories program and take the real parts of our complex pegs and define a consistency condition stronger than linear positivity.[23] Even so, we are still wary of invoking complex pegs because they are so alien to our usual notion of relative frequency. Note, however, that we are not wholly uncomfortable as such complex pegs appear naturally in quantum theory—the generalized Berry phase is derived from such complex pegs[24] and is an experimentally verifiable quantity (using ensembles of experiments). As such, we can combine such phases and frequentist notions into one probabilistic entity using axioms that were outlined over 60 years ago by Cox.[2]

In the history of science we have been rather ambiguous about what the word "probability" means. Some call relative frequencies probabilities even though they do not behave in the same manner as the term in common parlance. Similarly we have called certain nonadditive numbers in quantum theory probabilities even when they do not obey axioms of probability—nor axioms of relative frequency (which are necessarily additive). We might call our complex pegs probabilities because at least they do obey rational probabilistic axioms, but perhaps we would make a similar category error or confuse the issue by doing so; hence, for the want of a better name, we have resorted to calling them pegs—at least it begins with a "p" so we do not need to change our notation. So far we have two different kinds of pegs but there may be more. We have objects that obey Cox's two axioms which are real; we might call these "round pegs." We also have these objects that obey analogs of Cox's two axioms and our tentative third, which are complex. Let us call these "square pegs." These names lead naturally to a playful, albeit unfortunately sardonic, metaphor for what we are trying to do. A baby metaphor for science perhaps. We

are trying to find the right-shaped peg for the corresponding hole and we must reject the pegs that do not fit snugly. When dealing with a histories algebra, we argue that these complex pegs fit rather snugly.

IV. ENTROPY

With a generalization of probability to hand, we must also begin to discuss a generalization of entropy—a complimentary concept that is often just as important as a good notion of probability. Perhaps we do not have to search very far for such a generalization.

First of all, how should a notion of entropy behave? It should behave, in part, like a probability. It should probably be a transitive or monotonic notion of preference in some sense.[25] It should reflect the space of pegs in a natural way. Hence the first naïve object to suggest is simply a generalization of Shannon's entropy:

$$S[P(\mathbf{1}_\alpha|I)] := -K_S\sum_{i=1}^{n} p(\alpha^i|I)\ln p(\alpha^i|I), \tag{33}$$

where $P(\mathbf{1}_\alpha|I) := \{p(\alpha_i|I): i=1,2\ldots N_\alpha\}$ and K_S is a constant. Does this object $S[\cdot]$ behave like an entropy should? Does it, for example, obey the grouping property,[26] a property that Shannon suggests is natural for any notion of entropy?[27] Consider the complete—disjoint and exhaustive—set $\{\alpha^i\}$ split up into groups labeled by an integer g. We could consider the peg entropy (33) of the original set as split up into the peg entropy of each of the groups and the peg entropy as to which group $g=1,2,\ldots,N_G$ one should use; this alternative way of looking at the peg entropy (33) of the set should be equivalent to not splitting $\{\alpha^i\}$ into groups (this is the grouping property). How we split the entropy into groups should not make a difference. We can split up the peg entropy as follows:

$$S[P(\mathbf{1}_\alpha|I)] := -K_S\sum_{g}^{N_G}\sum_{i\in g} p(\alpha^i|I)\ln p(\alpha^i|I). \tag{34}$$

The complex peg we assign to a group g is simply

$$p(g|I) = \sum_{i\in g} p(\alpha^i|I). \tag{35}$$

So now we must ask ourselves whether

$$S[P(\mathbf{1}_\alpha|I)] = S[P(\mathbf{1}_G|I)] + \sum_g p(g|I)S_g, \tag{36}$$

where

$$S[P(\mathbf{1}_G|I)] := -K_S\sum_{g}^{N_G} p(g|I)\ln p(g|I) \tag{37}$$

and

$$S_g := -K_S\sum_{i\in g} p(\alpha^i|gI)\ln p(\alpha^i|gI). \tag{38}$$

In order to work this out, we need to work out what pegs we should assign to the histories $\{\alpha^i: i\in g\}$ upon the knowledge that the group g is the correct group. Thus we need a notion of conditioning. We need to work out what conditional pegs we should use and whether it allows Eq. (33) to obey the grouping property.

Using Bayes' rule in our complex peg framework is quite interesting:

$$p(\alpha^i|gI) = \frac{p(g|\alpha^i I)p(\alpha^i)}{p(g|I)}. \tag{39}$$

It is natural to assign $p(g\,|\,\alpha^i I)=1$ if we know that α^i is in the group g [we are normalizing due to Eq. (8), cf. Ref. 3]. Hence we should assign

$$p(\alpha^i|gI) = \frac{p(\alpha^i|I)}{p(g|I)} \tag{40}$$

to conditional grouping pegs. Does this allow the grouping property to be satisfied? Note that for $y,z\in\mathbb{C}$ we do not necessarily have that $\ln(y/z)=\ln y-\ln z$ because of different branches of the logarithm function; it only works if $-\pi<(\arg(x)-\arg(y))<\pi$. Complex logarithms behave as follows:

$$\ln(r\,\mathrm{e}^{i\theta}) = \ln r + i\theta, \tag{41}$$

where we may choose the principle value of θ. Renaming the index i with j so as not to confuse it with imaginary components, it is therefore clear that

$$\sum_j \ln\frac{p(\alpha^j|I)}{p(g|I)} = \sum_j \left(\ln\frac{|p(\alpha^j|I)|}{|p(g|I)|} + i\theta_j - i\theta_g\right), \tag{42}$$

where $\theta_j=\arg[p(\alpha^j\,|\,I)]$ and $\theta_g=\arg[p(g\,|\,I)]$.

So, using the definition of the complex logarithm, we have that

$$-\sum_{j\in g} p(\alpha^j|I)\ln p(\alpha^j|I) = -p(g|I)\sum_{j\in g}\frac{p(\alpha^j|I)}{p(g|I)}\ln\frac{p(\alpha^j|I)}{p(g|I)} - p(g|I)\ln p(g|I). \tag{43}$$

Thus we do have the grouping property for our test entropy functional (33), i.e., we have that

$$S[P(\mathbf{1}_\alpha|I)] = S[P(\mathbf{1}_G|I)] + \sum_g p(g|I)S_g + 2m\pi i, \tag{44}$$

where m is an integer—Eq. (33) is satisfied as long as we identify the different branches of the logarithm.

What, other than the grouping property, should an entropy functional obey so as to be a useful definition of uncertainty or information? According to Shannon,[27] $S[\cdot]$ should be continuous in the pegs. When all the pegs are equal (and hence real $p_i=1/n$), then it should be a monotonic increasing function of n. Hence $S[\cdot]$ should correspond to the standard Shannon entropy for the real subset of complex pegs. Clearly Eq. (33) is very plausible as a generalization of Shannon entropy that is apt for quantum histories. But, like the Shannon entropy for real probabilities, is it possible to prove that we must use Eq. (33) because it is the only functional that fits the required desiderata up to some equivalence of functionals? This we cannot yet answer.

Are strong additivity and concavity also satisfied by this peg entropy? In order to find out, we need to define a conditional peg entropy; presumably this involves Bayes' rule which is satisfied by our complex pegs since the $\wedge$-operation is associative.[3] Let us define the conditional peg entropy in an analogous way to how we define conditional Shannon entropies:

$$S[P(\mathbf{1}_\alpha|\mathbf{1}_\beta I)] := \sum_j p(\beta^j|I)S[P(\mathbf{1}_\alpha|\beta^j I)] \tag{45}$$

$$= -K_S\sum_j p(\beta^j|I)\sum_i p(\alpha^i|\beta^j I)\ln p(\alpha^i|\beta^j I). \tag{46}$$

And thus we can check whether the following "strong additivity" condition is satisfied by $S[\cdot]$:

$$S[P(\mathbf{1}_\alpha \wedge \mathbf{1}_\beta|I)] = S[P(\mathbf{1}_\alpha|I)] + S[P(\mathbf{1}_\beta|\mathbf{1}_\alpha I)] = S[P(\mathbf{1}_\beta|I)] + S[P(\mathbf{1}_\alpha|\mathbf{1}_\beta I)]. \tag{47}$$

We can also check whether the following "concavity" condition is satisfied:

$$S[P(\mathbf{1}_\alpha|I)] \geqslant S[P(\mathbf{1}_\alpha|\mathbf{1}_\beta I)]. \tag{48}$$

Note that $P(\mathbf{1}_\alpha \wedge \mathbf{1}_\beta|I) := \{p(\alpha^i \wedge \beta^j|I) : i = 1,2,\ldots,n_\alpha \text{ and } j = 1,2,\ldots n_\beta\}$. So we can work out the LHS of Eq. (47) to be

$$S[P(\mathbf{1}_\alpha \wedge \mathbf{1}_\beta|I)] = -K_S \sum_i \sum_j p(\alpha^i \wedge \beta^j|I) \ln p(\alpha^i \wedge \beta^j|I). \tag{49}$$

We can also work out the RHS (second decomposition) of Eq. (47):

$$-K_S \sum_j p(\beta^j|I) \ln p(\beta^j|I) - K_S \sum_j p(\beta^j|I) \sum_i p(\alpha^i|\beta^j I) \ln p(\alpha^i|\beta^j I). \tag{50}$$

Now, $p(\alpha^i \wedge \beta^j|I) = p(\alpha^i|\beta^j I) p(\beta^j|I)$ because Cox's axioms ensure that this is the case. Note that $\Sigma_i p(\alpha^i|\beta^j I) = 1$ for each j as long as α^i all commute with β^j. Hence we can identify the LHS and RHS, and thus Eq. (47) is satisfied for sets of commuting histories. Clearly it is natural that strong additivity applies for commuting histories because, in such cases, we can easily interpret the two sets of history propositions to be compatible. If they do not commute then there is no *a priori* reason we should demand strong additivity, just as there is no *a priori* reason we should demand comparability (by the dubious Axiom 0b) of probabilities in such cases.

In order to work out when Eq. (48) is also satisfied by our novel notion of entropy, we would have to decide what partial order on the space $\mathbb{C}$ we ought to use. Monoticity provides significant constraints upon what partial orders we can use and, as we argued above, it seems we should use the partial order illustrated in Fig. 1 for pegs. The partial order on the peg space will inform the partial order on the peg-entropy space (although perhaps scaled by the K_S constant). Concavity might then be satisfied, at least for a subset of histories. Having shown that our tentative notion (33) obeys the grouping property (albeit identifying branches of the logarithm), it is a matter only of mathematical consequence whether our peg entropy also obeys other convenient identities such as strong additivity and concavity (these identities are not axioms *per se*). It is clear, then, that Eq. (33) is a plausible generalization of entropy for quantum history theories but we have not yet proven whether all peg entropies that obey the grouping property for complex pegs must be of this form.

V. CONCLUSION

In quantum theory we use Gleason's theorem to justify the probabilistic assignments we give to projection operators. However, as soon as we begin to discuss more than one single projection operator—when we begin to discuss history propositions—we have to postulate a notion of state collapse in order to define probabilities. However, such postulated probabilities are nonadditive and many problems or issues arise because of this. From a Bayesian perspective it is even dubious to call such things "probabilities" because they are nonadditive and thus alien to our normal notion of probability.[28] Problems with nonlocality also arise by discussing propositions that involve two or more times (in a given frame of reference). Hence it is natural to tackle this problem head-on and define a propositional space that includes multitime propositions. Since we do not want to give any causal bias to the peg or probability theory that we use,[29] it seems prudent to put timelike and spacelike separated propositions on the same footing;[30] hence we might naïvely like to use tensor products to produce history propositions (this is the HPO algebra). Of course, in full generality, one would prefer to use a fully relational algebra. Rather than postulate dubious notions of state collapse, one can then *derive* a monotonic peg for such history propositions, and one can do such a thing without getting into the problems of nonadditivity and, tentatively, nonlocality. There also exists a plausible generalization of Shannon entropy for such pegs. Of course such complex pegs are alien to our standard notion of probability. However, our standard notion of probability is

rather alien too; when you get down to it, what really does the term "probability" mean? The interpretation of probabilities is clearly, historically speaking, a debatable issue and hence it is necessary to axiomatize and formalize a relational approach. Such an approach will ensure that, even if we do not know with full clarity what such concepts mean, we will, in the least, not introduce functional relationships between pegs that we are not justified in introducing.

So we cannot yet give a clear answer to the question: What are probabilities? One can, however, begin to answer another quite daunting question: Why do we naturally find complex numbers in quantum theory?

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Pauli-Hamiltonian in the presence of minimal lengths

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We construct the Pauli-Hamiltonian on a space where the position and momentum operators obey generalized commutation relations leading to the appearance of a minimal length. Using the momentum space representation we determine exactly the energy eigenvalues and eigenfunctions for a charged particle of spin half moving under the action of a constant magnetic field. The thermal properties of the system in the regime of high temperatures are also investigated, showing a magnetic behavior in terms of the minimal length. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2393151]

I. INTRODUCTION

In a series of papers Kempf[1–3] and Hinrichsen and Kempf[4] introduced a deformed quantum mechanics based on a modified commutation relation between position and momentum operators $[X_i, P_j]=i\hbar[(1+\beta P^2)\delta_{ij}+\beta' P_i P_j]$, where β and β' are small parameters. This commutation relation leads to a generalized Heisenberg uncertainty principle (GUP) which defines a nonzero minimum length in position. Other similar constructions leading to the same GUP have been also initiated by some authors.[5–8] The concept of minimal length is a common feature of string theory,[9] loop quantum gravity,[10] and noncommutative field theories.[11] One major consequence of the GUP is the appearance of a UV/IR "bootstrap," which allows to probe short distance physics (UV) from long distance ones (IR). This mixing between UV and IR divergences, first noticed in the Anti-deSitter/Conformal Filed Theory (AdS/CFT) correspondence,[12] is also a feature of noncommutative quantum field theories.[13] Recently, some scenarios have been proposed where the minimal length is related to large extra dimensions,[5] to the running coupling constant,[6] and to the physics of black hole production.[7]

Recently, numerous studies of quantum mechanical problems in the presence of minimal lengths have been carried out, among them we cite the solution of the Schrodinger equation in momentum space for the harmonic oscillator in D dimensions;[2,3,14] the cosmological constant problem and the classical limit of the physics with minimal lengths have been investigated in Refs. 15 and 16; the effect of the minimal length on the energy spectrum and momentum wave functions of the Coulomb potential in one dimension and three dimensions has been studied, respectively, in Ref. 17 and Refs. 18–20; the high temperature properties of the one dimensional Dirac oscillator has been recently investigated by the author in Ref. 21; the three dimensional Dirac oscillator with minimal lengths has been solved in Ref. 22 using supersymmetric quantum mechanics; the Casimir force for the electromagnetic field in the presence of the minimal length has been also computed.[23,24]

In this paper we are interested by the new kind of interactions that the incorporation of the minimal length into a quantum model can reveal. To this aim we construct the analog of the Pauli-Hamiltonian on a space where the position and momentum operators obey generalized commutation relations and determine exactly the energy eigenvalues and momentum eigenfunctions of a charged particle of spin half under the action of a constant magnetic field. The rest of the

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paper is organized as follows. In Sec. II, we give a brief review of quantum mechanics with generalized uncertainty principle. In Sec. III, we solve exactly the Pauli equation in the presence of a minimal length for a charged particle with spin half in the potential of a constant magnetic field. In Sec. IV the magnetic moment and the magnetic susceptibility of the system are examined in the regime of high temperatures. Section V is left for concluding remarks.

II. THE PAULI-HAMILTONIAN IN THE PRESENCE OF MINIMAL LENGTHS

Let us start with the following D-dimensional realization of the position and momentum operators[2]

$$X_i = i\hbar\left[(1+\beta P^2)\frac{\partial}{\partial p_i} + \beta' P_i P_j \frac{\partial}{\partial p_j} + \gamma P_i\right], \tag{1}$$

$$P_i = p_i, \tag{2}$$

where β and β' are two very small non-negative parameters. This realization leads to the following generalized commutation relations:

$$[X_i, P_j] = i\hbar(\delta_{ij} + \delta_{ij}\beta P^2 + \beta' P_i P_j), \tag{3}$$

$$[X_i, X_j] = -i\hbar[(2\beta - \beta') + (2\beta + \beta')\beta P^2]\epsilon_{ijk} L_k, \tag{4}$$

$$[P_i, P_j] = 0, \tag{5}$$

where the components of the angular momentum are given by

$$L_i = \frac{1}{1+\beta P^2}\epsilon_{ijk} X_j P_k \tag{6}$$

and satisfy the usual algebra

$$[L_i, X_j] = i\hbar\epsilon_{ijk} X_k, \quad [L_i, P_j] = i\hbar\epsilon_{ijk} P_k. \tag{7}$$

Using states for which $\langle P_i\rangle = 0$ and that (ΔP_i) do not depend on i, we easily obtain the GUP,

$$(\Delta X_i)(\Delta P_i) \geqslant \frac{\hbar}{2}(1 + \beta D(\Delta P_i)^2 + \beta'(\Delta P_i)^2). \tag{8}$$

A minimization of the saturated GUP with respect to ΔP_i gives an isotropic minimal length,

$$(\Delta X_i)_{\min} = \hbar\sqrt{D\beta + \beta'}, \quad i = 1,2,3,\ldots,D. \tag{9}$$

We note also that the constant γ in the definition of the position operator does not affect the observable quantities and enters only in the definition of a squeezed weighting factor of the momentum measure,

$$\int \frac{\mathrm{d}^D p}{(1+(\beta+\beta')p^2)^{1-\alpha}}|p\rangle\langle p|, \quad \alpha = \frac{\gamma - \beta'[(D-1)/2]}{\beta + \beta'}. \tag{10}$$

In the rest of our calculations we use the simple algebra where $\beta' = 0$ and $\gamma = 0$.

In order to obtain the Pauli-Hamiltonian in the framework of quantum mechanics in the presence of the minimal length defined above, we start from the nonrelativistic limit of the Dirac-Hamiltonian and then use the representation (1), instead of using directly the well known Pauli-Hamiltonian. Ignoring the scalar potential, the nonrelativistic limit of the Dirac equation is given by

$$H = \frac{(\sigma\mathbf{\Pi})^2}{2m} = \frac{1}{2m}(\mathbf{\Pi}\mathbf{\Pi} + i\sigma\mathbf{\Pi}\wedge\mathbf{\Pi}), \tag{11}$$

where $\mathbf{\Pi}=\mathbf{P}-(q/c)\mathbf{A}$, $\sigma=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices, and $\mathbf{A}$ is the potential vector. Using the algebra defined by Eqs. (1)–(3) we show that

$$\mathbf{\Pi}\wedge\mathbf{\Pi} = \frac{i\hbar q}{c}(1+\beta P^2)\mathbf{B} + \frac{q^2}{c^2}(\mathbf{A}\wedge\mathbf{A}), \tag{12}$$

with $\mathbf{B}=\nabla\wedge\mathbf{A}$ the magnetic field. Then substituting in Eq. (11) we obtain

$$H = \frac{1}{2m}\left(\mathbf{P}-\frac{q}{c}\mathbf{A}\right)^2 - \frac{q\hbar}{2mc}(1+\beta P^2)\sigma\mathbf{B} + \frac{iq^2}{2mc^2}\sigma(\mathbf{A}\wedge\mathbf{A}). \tag{13}$$

We observe that, besides the usual magnetic interaction, the Hamiltonian contains other interactions coming essentially from the presence of the minimal length. The second term in Eq. (13) shows a correction to the usual magnetic moment of the electron. The third term in Eq. (13) is different from zero and proportional to the angular momentum as a consequence of the noncommutativity of the position operators. It generates a spin-orbit interaction. At this stage we note that, in the undeformed case, the spin-orbit interaction is generated by the scalar potential. Then in our case such a scalar potential is the gravitational field generated by the perturbation of the space by the presence of the minimal length. This allows us to interpret the correction to the magnetic moment of the electron, in the second term, as an electric-dipole-magnetic-moment-like interaction. Finally, it is interesting to note that, at the quantum mechanical level, an electric dipole–magnetic interaction appears. However, this result is a consequence of the UV/IR bootstrap which allows to probe high energy effects by low energy physics.

III. CONSTANT MAGNETIC FIELD

In this section we illustrate the effect of the minimal length on the energy eigenvalues and eigenfunctions of a charged spinning particle in a constant magnetic field. Let us consider the vector potential in the symmetric gauge,

$$\mathbf{A} = \frac{B_0}{2}(-y\mathbf{i}+x\mathbf{j}), \tag{14}$$

where B_0 is the magnitude of the magnetic field. Then it is easy to show that the spin-orbit interaction in Eq. (13) is given by

$$\mathbf{A}\wedge\mathbf{A} = 2i\hbar\beta(1+\beta p^2)\left(\frac{B_0}{2}\right)^2 L_z\mathbf{k}, \tag{15}$$

where we have used the definition of the angular momentum given by Eq. (6).

Finally, we arrive to the following expression of the Pauli Hamiltonian in the presence of the minimal length:

$$H = H_0 + \frac{P_z^2}{2m} + \omega(1+\beta p^2)(L_z+\hbar\sigma_z) + \beta m\omega^2\hbar(1+\beta p^2)L_z\sigma_z, \tag{16}$$

where H_0, given by

$$H_0 = \frac{P_x^2+P_y^2}{2m} + \frac{m\omega^2}{2}(X^2+Y^2), \tag{17}$$

is the Hamiltonian of a two dimensional isotropic harmonic oscillator of frequency $\omega=(qB_0/2mc)$. To solve the eigenvalue equation $H\Psi_\epsilon(\mathbf{p})=E_{nl}\Psi_\epsilon(\mathbf{p})$ in the momentum space representation, we exploit the rotational invariance of Eq. (16) by setting

$$\Psi_{\epsilon}(\mathbf{p}) = \frac{e^{-il\phi}}{\sqrt{2\pi\hbar}} R_{nl}(p)\chi_{\epsilon}, \tag{18}$$

where n is the radial quantum number, l and $\epsilon = \pm 1$ are, respectively, the eigenvalues of angular momentum and spin operators, and $\chi_{+1}^{T} = (1,0)$, $\chi_{-1}^{T} = (0,1)$ are the spin functions.

Using the two dimensional representation of the position operators given by Eq. (1), we obtain the following differential equation for the radial part of the wave function:

$$\left\{(1+\beta p^2)^2\left(\frac{\partial^2}{\partial p_x^2} + \frac{\partial^2}{\partial p_y^2}\right) + 2\beta(1+\beta p^2)\left(p_x\frac{\partial}{\partial p_x} + p_y\frac{\partial}{\partial p_y}\right) - \frac{2}{m\omega\hbar}(l+\epsilon+m\omega\hbar\beta l\epsilon)(1+\beta p^2) - \frac{p^2}{(m\hbar\omega)^2} + \mathcal{E}_{nl}\right\} R_{nl}(p) = 0, \tag{19}$$

with $\mathcal{E}_{nl}$ given by

$$\mathcal{E}_{nl} = \frac{2E_{nl}}{m\hbar^2\omega^2} - \frac{p_z^2}{(m\hbar\omega)^2}. \tag{20}$$

In the terms of the radial coordinate p, Eq. (19) is given by

$$\left\{\left((1+\beta p^2)\frac{\partial}{\partial p}\right)^2 + (1+\beta p^2)^2\left(\frac{1}{p}\frac{\partial}{\partial p} - \frac{l^2}{p^2}\right) - \left(\frac{2}{m\omega\hbar}(l+\epsilon+m\omega\hbar\beta l\epsilon)(1+\beta p^2) - \frac{p^2}{(m\hbar\omega)^2} + \mathcal{E}_{nl}\right)\right\} R_{nl}(p) = 0. \tag{21}$$

We simplify this equation by introducing the variable ρ defined by

$$\rho = \frac{1}{\sqrt{\beta}}\arctan(p\sqrt{\beta}). \tag{22}$$

Then we obtain

$$R_{nl}''(\rho) + \sqrt{\beta}(\cot\sqrt{\beta}\rho + \tan\sqrt{\beta}\rho)R_{nl}'(\rho) - \beta l^2(\cot\sqrt{\beta}\rho + \tan\sqrt{\beta}\rho)^2 R_{nl}(\rho) - \left(\Omega_{l\epsilon} + \frac{1}{\beta(m\omega\hbar)^2}\right)\tan^2\sqrt{\beta}\rho R_{nl}(\rho) + (\mathcal{E}_{nl} - \Omega_{l\epsilon})R_{nl}(\rho) = 0, \tag{23}$$

with $\Omega_{l\epsilon}$ given by

$$\Omega_{l\epsilon} = \frac{2}{m\omega\hbar}(l+\epsilon+m\omega\hbar\beta l\epsilon). \tag{24}$$

We simplify Eq. (23) by setting $R_{nl}(\rho) = c^{\lambda} f(s)$ with c and s defined by

$$c = \cos\sqrt{\beta}\rho, \quad s = \sin\sqrt{\beta}\rho. \tag{25}$$

A straightforward calculation gives the following differential equation for $f(s)$:

$$(1-s^2)f''(s) + \left(\frac{1}{s} - (2\lambda+1)\right)f'(s) + \left(\left(\lambda(\lambda-2) - \frac{\Omega_{l\epsilon}}{\beta} - \frac{1}{\kappa^4} - l^2\right)\frac{s^2}{c^2} + \left(\frac{\mathcal{E}_{nl} - \Omega_{l\epsilon}}{\beta} - 2\lambda - l^2\right) - \frac{l^2}{s^2}\right) f(s) = 0, \tag{26}$$

where we have set $\kappa = \sqrt{m\omega\hbar\beta}$.

Then we cancel the term proportional to (s^2/c^2) by choosing λ such that

$$\lambda^2 - 2\lambda - \frac{\Omega_{l\epsilon}}{\beta} - l^2 - \frac{1}{\kappa^4} = 0. \tag{27}$$

The solutions of this equation are given by

$$\lambda = 1 \pm \sqrt{1 + \frac{\Omega_{l\epsilon}}{\beta} + \frac{1}{\kappa^4} + l^2}. \tag{28}$$

The relevant sign in Eq. (28) will be fixed later by appealing to the generalized uncertainty principle.

A further step in our calculation consists in canceling the centrifugal barrier in Eq. (26) by setting $f(s)=s^{|l|}g(s)$. Then $g(s)$ verify the following differential equation:

$$(1-s^2)g''(s) + \left(\frac{2|l|+1}{s} - (2\lambda + 2|l| + 1)s\right)g'(s) + \left(\frac{\mathcal{E}_{nl} - \Omega_{l\epsilon}}{\beta} - 2l^2 - 2\lambda(|l|+1)\right)g(s) = 0. \tag{29}$$

At this stage we use the variable $z=2s^2-1$ to obtain

$$(1-z^2)g''(z) + [(|l| - \lambda + 1) - (|l| + \lambda + 1)z]g'(z) + \frac{1}{4}\left(\frac{\mathcal{E}_{nl} - \Omega_{l\epsilon}}{\beta} - 2l^2 - 2\lambda(|l|+1)\right)g(z) = 0. \tag{30}$$

Defining two new parameters

$$a = \lambda - 1, \quad b = |l|, \tag{31}$$

and imposing the following condition:

$$\frac{\mathcal{E}_{nl} - \Omega_{l\epsilon}}{\beta} - 2l^2 - 2\lambda(|l|+1) = 4n(n + a + b + 1), \tag{32}$$

with n a non-negative integer, we reduce Eq. (30) to the following form:

$$(1-z^2)g''(z) + [(b-a) - (a+b+2)z]g'(z) + n(n+a+b+1)g(z) = 0. \tag{33}$$

The condition given by Eq. (32) suffices to obtain polynomial solutions to Eq. (33) given by the Jacobi polynomials

$$g(z) = P_n^{(a,b)}(z). \tag{34}$$

Using the old variable p, the radial part of the wave function $R_{nl}(p)=c^\lambda s^{|l|}g(s)$ is then given by

$$R_{nl}(p) = \mathcal{N}(1+\beta p^2)^{-(\lambda+|l|)/2}(\beta p^2)^{|l|/2} P_n^{(\lambda-1,|l|)}\left(\frac{\beta p^2 - 1}{\beta p^2 + 1}\right). \tag{35}$$

The normalization constant $\mathcal{N}$ is obtained by employing the normalization condition $\int[d^3p/(1+\beta p^2)]|R_{nl}(p)|^2=1$ and the Jacobi polynomial orthogonality relation.[25] Finally, the normalized momentum radial wave functions are given by

$$R_{nl}(p) = \sqrt{\beta}\sqrt{\frac{2(n!)(2n+\lambda+|l|)\Gamma(n+\lambda+|l|)}{\Gamma(n+\lambda)\Gamma(n+|l|+1)}}(1+\beta p^2)^{-(\lambda+|l|)/2}(\beta p^2)^{|l|/2} P_n^{(\lambda-1,|l|)}\left(\frac{\beta p^2 - 1}{\beta p^2 + 1}\right). \tag{36}$$

However, as pointed in Ref. 2, the normalization condition alone does not guarantee physically relevant wave functions but the latter must be in the domain of p, which physically means that it should have a finite uncertainty in momentum. This leads to the condition

$$\langle p^2\rangle = \int_0^\infty \frac{d\mathbf{p}}{(1+\beta p^2)} p^2 |R_{nl}(p)|^2 < \infty. \tag{37}$$

In our case the integrand in Eq. (37) behaves like $p^{-2\lambda+2}$ which requires $\lambda > 1$. Then we choose the upper sign in the expression of λ. However, the condition $\lambda > 1$ can be also obtained from physical considerations. Let us take λ with the minus and work with $l=0$,

$$\lambda = 1 - \sqrt{1 + \frac{2\epsilon}{m\omega\hbar\beta} + \frac{1}{(m\omega\hbar\beta)^2}}. \tag{38}$$

Using the fact that $\hbar\sqrt{2\beta} \leqslant l_c$ where $l_c = \sqrt{2\hbar/m\omega}$ is the characteristic length of the oscillator we have $m\omega\hbar\beta < 1$. Then

$$\lambda = 1 - \frac{1}{m\omega\hbar\beta} < 0, \tag{39}$$

leading to $(\Delta X)_{\min} > l_c$ which contradicts the fundamental requirement stipulating that we cannot probe the physics below the minimal length.

The energy spectrum is now derived from Eq. (32),

$$\frac{\mathcal{E}_{nl} - \Omega_{l\epsilon}}{\beta} = 2(N+1)(\lambda - 1) + (N^2 + l^2 + 2N + 2), \tag{40}$$

where $N = 2n + |l|$ is the principal quantum number. Using the expressions of κ, $\mathcal{E}_{nl}$, and $\Omega_{l\epsilon}$ we finally obtain

$$E_{Nl} = \frac{p_z^2}{2m} + \hbar\omega\left[(N+1)\sqrt{1 + 2\beta m\hbar\omega(l + \epsilon + m\hbar\omega\beta l\epsilon) + (m\hbar\omega\beta)^2(l^2+1)}\right.$$
$$\left. + \frac{m\hbar\omega\beta}{2}(N^2 + l^2 + 2N + 2) + (l + \epsilon + m\hbar\omega\beta l\epsilon)\right]. \tag{41}$$

Ignoring the spin and the spin-orbit contributions and the last term in Eq. (41) we reproduce exactly, besides the term $p_z^2/2m$, the energy spectrum of the two dimensional harmonic oscillator with minimal length.[14]

Let us in the following discard the spin contributions. The energy spectrum in this case is given by

$$E_{Nl} = \frac{p_z^2}{2m} + \hbar\omega\left[(N+1)\sqrt{1 + 2\beta m\hbar\omega l + (m\hbar\omega\beta)^2(l^2+1)} + \frac{m\hbar\omega\beta}{2}(N^2 + l^2 + 2N + 2) + l\right]. \tag{42}$$

As noted above, the quantity $\sqrt{m\hbar\omega\beta}$ expresses the ratio between the minimal length and the characteristic length of the oscillator $(\Delta X)_{\min}/l_c$, which is by virtue of the GUP, a small parameter. Then to first order in $m\hbar\omega\beta$ we have

$$E_{Nl} = \frac{p_z^2}{2m} + \hbar\omega\left[(N + l + 1) + \frac{m\hbar\omega\beta}{2}(N^2 + l^2 + 2N + 2 + 2(N+1)l)\right]. \tag{43}$$

In terms of n and l we write this expression as

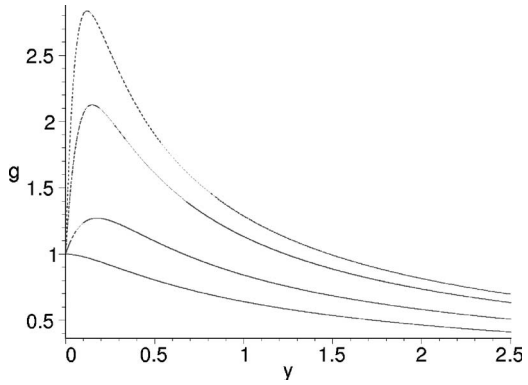

FIG. 1. Plot of the one particle state density vs $y=\beta m\mu_B B_0$ for $n_d=0,1,5,10$.

$$E_{Nl}=\frac{p_z^2}{2m}+2\hbar\omega\left[n+\frac{|l|+l+1}{2}\right]+\frac{1}{2}\hbar\omega\left(\frac{(\Delta X)_{\min}}{l_c}\right)^2\left[4\left(n+\frac{|l|+l}{2}\right)^2+4\left(n+\frac{|l|+l+1}{2}\right)\right]. \tag{44}$$

Using the numbers n_d and n_g defined by

$$n_d=n+\frac{|l|+l}{2},\quad n_g=n+\frac{|l|-l}{2}, \tag{45}$$

we obtain

$$E_{n_d}=\frac{p_z^2}{2m}+2\hbar\omega\left[n_d+\frac{1}{2}\right]+2\hbar\omega\left(\frac{(\Delta X)_{\min}}{l_c}\right)^2\left[n_d^2+n_d+\frac{1}{2}\right]. \tag{46}$$

We observe that we have the usual infinite degeneracy.

IV. THERMODYNAMICAL PROPERTIES

In this section we are interested by the thermodynamical properties of the system at high temperatures. In the following we set $z=e^{\tilde{\beta}\mu}$, where $\tilde{\beta}=1/kT$ and μ is the chemical potential. Let us start by computing the one particle state density $g(n_d)$ given by

$$g(n_d)=\frac{V^{2/3}}{4\pi\hbar^2}\int_{E_{n_d}\leq E<E_{n_d+1}}\frac{dp_x dp_y}{(1+\beta p^2)}, \tag{47}$$

with $V^{2/3}$ a surface. Using polar coordinates we obtain

$$g(n_d)=\frac{V^{2/3}}{2\pi\hbar^2}\int_{p_{n_d}}^{p_{n_d+1}}\frac{pdp}{(1+\beta p^2)}=\frac{V^{2/3}}{4\pi\beta\hbar^2}\ln\frac{1+\beta p_{n_d+1}^2}{1+\beta p_{n_d}^2}. \tag{48}$$

Using $p_{n_d}=[4m\mu_B B_0(n_d+yn_d^2)]^{1/2}$, where $y=((\Delta X)_{\min}/l_c)^2=\beta m\mu_B B_0$ and $\mu_B=\hbar q/2mc$ is the Bohr magneton, the density of states is given by

$$g(n_d)=\frac{V^{2/3}}{4\pi\beta\hbar^2}\ln[1+4y(2yn_d+1)]. \tag{49}$$

In the last derivations we have used the fact that $y+1\approx 1$, by virtue of the GUP. We note that the density of states, unlike the standard expression without the minimal length, is now a function of the quantum number n_d. In Fig. 1 we show the behavior of $g=g(n_d)/(V^{2/3}m\mu_B B_0/\pi\hbar^2)$ in terms of

$y=\beta m\mu_B B_0$ for different values of n_d.

It is interesting to note that the density of states reaches a maximum for a critical value of the minimal length and then decreases rapidly for higher values of the minimal length corresponding to strong gravitational field.

The grand canonical thermodynamical potential is defined by the following expression:

$$\Phi = -\frac{V^{1/3}}{2\pi\tilde{\beta}\hbar}\int_{-\infty}^{+\infty}\frac{dp_z}{1+\beta p_z^2}\sum_{n_d=0}^{\infty} g(n_d)\ln[1+z\exp(-\tilde{\beta}E_{n_d})]. \tag{50}$$

Using the density of states and the energy spectrum given, respectively, by Eqs. (49) and (46) and $y+1\approx 1$, we obtain

$$\Phi \approx -\frac{V}{8\pi^2\tilde{\beta}\beta\hbar^3}\int_{-\infty}^{+\infty}\frac{dp_z}{1+\beta p_z^2}\sum_{n_d=0}^{\infty}\ln[1+4y(2yn_d+1)] \times\ln\left[1+ze^{-\tilde{\beta}\mu_B B_0}\exp\left(-\tilde{\beta}\left[\frac{p_z^2}{2m}+2\mu_B B_0(n_d+yn_d^2)\right]\right)\right]. \tag{51}$$

At this stage, in the regime of high temperatures, we use the assumption that $|\mu-\mu_B B_0|\gg\tilde{\beta}$. With the aid of the approximation $\ln(1+ua)\approx ua$, we obtain

$$\Phi \approx -\frac{ze^{-\tilde{\beta}\mu_B B_0}m\mu_B B_0 V}{2\pi^2\tilde{\beta}\hbar^3}\int_{-\infty}^{+\infty}\frac{dp_z}{1+\beta p_z^2}\sum_{n_d=0}^{\infty}(1+2yn_d)\times\exp\left(-\tilde{\beta}\left[\frac{p_z^2}{2m}+2\mu_B B_0(n_d+yn_d^2)\right]\right). \tag{52}$$

The integration over p_z gives

$$\Phi \approx -\frac{ze^{-\tilde{\beta}\mu_B B_0}m\mu_B B_0 V}{4\pi\hbar^3\sqrt{\tilde{\beta}}\tilde{\beta}}e^{\tilde{\beta}/2m\beta}\left[1-\mathrm{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]\sum_{n_d=0}^{\infty}(1+2yn_d)\times\exp(-2\mu_B B_0\tilde{\beta}(n_d+yn_d^2)), \tag{53}$$

where $\mathrm{erf}(x)$ is the error function. The computation of the summation over n_d is now performed with the aid of Euler's formula given by

$$\sum_{n_d=0}^{\infty} f(n) = \frac{1}{2}f(0)+\int_0^{\infty} f(x)dx-\sum_{p=1}^{\infty}\frac{1}{(2p)!}B_{2p}f^{(2p-1)}(0), \tag{54}$$

where B_{2p} are Bernoulli's numbers and $f^{(2p-1)}(0)$ are the derivatives of the function $f(x)$ at $x=0$. In the high temperature regime the contribution of the sum in Eq. (54) is neglected.

Using $y=\beta m\mu_B B_0$ and the following integrals:

$$\int_0^{\infty} e^{-2\mu_B B_0\tilde{\beta}(x+\beta m\mu_B B_0 x^2)}dx = \frac{1}{2\mu_B B_0\sqrt{\tilde{\beta}\beta m}}e^{\tilde{\beta}/4m\beta}D_{-1}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right), \tag{55}$$

$$\int_0^{\infty} xe^{-2\mu_B B_0\tilde{\beta}(x+\beta m\mu_B B_0 x^2)}dx = \frac{1}{2\mu_B^2 B_0^2\tilde{\beta}\beta m}e^{\tilde{\beta}/4m\beta}D_{-2}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right), \tag{56}$$

where $D_\nu(x)$ is the cylindrical function, we finally obtain the thermodynamical potential

$$\Phi \approx -\frac{ze^{-\tilde{\beta}\mu_B B_0}\sqrt{m}V}{8\pi\hbar^3\beta\tilde{\beta}^{3/2}}e^{3\tilde{\beta}/4m\beta}\left[1-\operatorname{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]\left[D_{-1}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right)+\sqrt{\frac{\beta m}{\tilde{\beta}}}D_{-2}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right)\right]$$
$$-\frac{ze^{-\tilde{\beta}\mu_B B_0}m\mu_B B_0 V}{8\pi h^3\sqrt{\beta}\tilde{\beta}}e^{\tilde{\beta}/2m\beta}\left[1-\operatorname{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]. \tag{57}$$

The magnetic moment of the system defined by $M_\beta=-(\partial/\partial B)\Phi$ and the magnetic susceptibility $\chi_\beta=\partial M/\partial B$ are then easily obtained,

$$M_\beta=\frac{zm\mu_B V}{8\pi\hbar^3\sqrt{\beta}\tilde{\beta}}e^{\tilde{\beta}/2m\beta}[1-2z\tilde{\beta}\mu_B B_0]\left[1-\operatorname{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]$$
$$+\frac{z\mu_B\sqrt{m}V}{8\pi\hbar^3\beta\tilde{\beta}^{1/2}}e^{3\tilde{\beta}/4m\beta}\left[1-\operatorname{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]\left[D_{-1}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right)+\sqrt{\frac{\beta m}{\tilde{\beta}}}D_{-2}\left(\sqrt{\frac{\tilde{\beta}}{\beta m}}\right)\right], \tag{58}$$

and

$$\chi_\beta=-\frac{z\mu_B^2 mV}{4\pi\hbar^3\sqrt{\beta}}e^{\tilde{\beta}/2m\beta}\left[1-\operatorname{erf}\left(\sqrt{\frac{\tilde{\beta}}{2m\beta}}\right)\right]. \tag{59}$$

Let us exploit the fact that $m\beta/\beta$ is a small parameter. Indeed we have

$$\sqrt{\frac{m\beta}{\tilde{\beta}}}=\sqrt{\pi}\frac{(\Delta X)_{\min}}{\lambda}, \tag{60}$$

where $(\Delta X)_{\min}=\hbar\sqrt{2\beta}$ and $\lambda=\sqrt{2\pi\beta\hbar^2/m}$ is the thermal wavelength. Since λ is a physical characteristic length of the system and in order to be experimentally accessible it must be greater than the minimal length.

An asymptotic expansion in terms of $\tilde{\beta}/m\beta$ gives

$$\chi_\beta=-\frac{zV}{\lambda^3}\mu_B^2\tilde{\beta}\left[1-\pi\left(\frac{(\Delta X)_{\min}}{\lambda}\right)^2\right]. \tag{61}$$

This relation shows that we have the usual Landau diamagnetism at high temperatures in terms of the minimal length if the later verify

$$(\Delta X)_{\min}\leqslant\frac{\sqrt{\pi}}{\lambda}. \tag{62}$$

It is interesting to note that this upper bound for the minimal length does not depend on the magnitude of the applied external magnetic field.

The susceptibility given by Eq. (61) is weaker than in the ordinary case. A similar result has been recently obtained for the Dirac oscillator with minimal length in one dimension in a thermal bath.[21] On the other hand the new result in Eq. (61) clearly shows the effect of the perturbation of the space by the presence of the minimal. In fact, the contribution of the minimal length to the magnetic susceptibility is of a paramagnetic nature. This can be interpreted as if the minimal length generates magnetic moments aligned in the direction of the applied external magnetic field. We note also that the limit $T\to\infty$ is forbidden by the condition (62) and the susceptibility is always finite. This effect does not appear neither in the case without the minimal length[26] nor in the canonical noncommutative case characterized by the parameter θ.[27] In this paper the author has obtained the susceptibility at high temperatures for the Landau system with a confining

harmonic potential of frequency ω_0. However, for $\theta \neq 0$, the susceptibility becomes infinite in the limit $\omega_0 \to 0$. Our result reflects clearly the regularizing effect of the minimal length which is directly related to the existence of a minimal thermal wavelength given by

$$\lambda_{\min} = \sqrt{\pi}(\Delta X)_{\min}, \tag{63}$$

which in turn define a maximal temperature

$$kT_{\max} = \frac{2}{mc^2}\left(\frac{\hbar c}{(\Delta X)_{\min}}\right)^2. \tag{64}$$

The appearance of a maximal temperature seems to be a common feature of noncommutative theories. Indeed we have found recently an upper bound for the deconfinement temperature of a quark gluon plasma.[21] On the other hand the existence of a minimal length may have important consequences on the thermodynamics of black holes. In the context of canonical noncommutative theories[28] and generalized uncertainty principle,[29] it was shown that during the evaporation process the black hole reaches a maximal temperature before cooling down to a nonsingular remnant at zero temperature.

We close this section by pointing out that the results derived in this paper can be used to obtain experimental values of the minimal length using available data for the magnetic susceptibility at high temperatures. Following Ref. 30, another interesting approach is to consider the quantum Hall effect in the presence of the minimal length and interpret it as the usual fractional quantum Hall effect. The work in this direction is in progress.

V. CONCLUSION

In this paper starting from the nonrelativistic Dirac-Hamiltonian without the scalar potential, we have constructed the Pauli-Hamiltonian in the framework of quantum mechanics with minimal lengths, which besides the usual terms contains additional interaction terms revealing the rich structure of the space at short distances. Particularly we obtained a spin-orbit-like interaction term suggesting that the noncommutativity of the position operators generates a scalar field which can be related to the gravitational field. Then the problem of a charged particle with spin half under the action of a constant magnetic field is solved exactly in the momentum representation. The energy spectrum and the corresponding wave functions are then obtained. We have also investigated the magnetic behavior of the system at high temperatures where we have shown that the magnetic susceptibility in terms of the minimal length remains finite, while it is infinite in the case without the minimal length. This important result reflects the regularizing effect of the minimal length.

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On bipartite pure-state entanglement structure in terms of disentanglement

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Schrödinger's disentanglement [E. Schrödinger, Proc. Cambridge Philos. Soc. **31**, 555 (1935)], i.e., remote state decomposition, as a physical way to study entanglement, is carried one step further with respect to previous work in investigating the qualitative side of entanglement in any bipartite state vector. Remote measurement (or, equivalently, remote orthogonal state decomposition) from previous work is generalized to remote linearly independent complete state decomposition both in the nonselective and the selective versions. The results are displayed in terms of commutative square diagrams, which show the power and beauty of the physical meaning of the (antiunitary) correlation operator inherent in the given bipartite state vector. This operator, together with the subsystem states (reduced density operators), constitutes the so-called correlated subsystem picture. It is the central part of the antilinear representation of a bipartite state vector, and it is a kind of core of its entanglement structure. The generalization of previously elaborated disentanglement expounded in this article is a synthesis of the antilinear representation of bipartite state vectors, which is reviewed, and the relevant results of [Cassinelli *et al.*, J. Math. Anal. Appl. **210**, 472 (1997)] in mathematical analysis, which are summed up. Linearly independent bases (finite or infinite) are shown to be almost as useful in some quantum mechanical studies as orthonormal ones. Finally, it is shown that linearly independent remote pure-state preparation carries the highest probability of occurrence. This singles out linearly independent remote influence from all possible ones. © *2006 American Institute of Physics.*
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I. INTRODUCTION

There are different *measures of the amount* of entanglement in bipartite states. In pure states they all coincide. Hence, this is well understood. But one may wonder the measure of what is at issue; i.e., what is the structure of entanglement, or what is its *qualitative side*.

According to Schrödinger, the natural way to investigate entanglement is to perform *disentanglement*:[1] It consists in *measurements on the nearby subsystem*. Since it is simultaneously a measurement on the composite system, the bipartite state becomes a mixed one. As a consequence, one has an *actual decomposition* (as opposed to a potential or mathematical one) *of the remote subsystem state*.

In previous work,[2] complete remote measurement or, equivalently, complete remote orthogonal state decomposition, was studied as a first step in carrying out Schrödinger's program, and the concept of twin observables was introduced. They gave physical meaning to the so-called correlated subsystem picture.[3]

Mathematically, the optimal way to study pure-state bipartite entanglement is to use the antilinear operator representation of the state vector. As it is well known, in theoretical physics mathematics is inextricably connected with physics. In the mentioned previous work it turned out

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that the antiunitary polar factor, the so-called *correlation operator*, plays a central role in establishing the concepts of twin observables and remote measurement. Naturally, this operator is endowed with basic physical meaning.

The antilinear operator representation of bipartite state vectors and the polar factorizations of these operators are summed up and shortly reviewed in Sec. II. Delving into the antilinear approach may require some effort on part of some readers, but it is pure-state bipartite entanglement and not this author who made it optimal. Eventually, the insight gained should make it worth the effort.

In this article the physical content of the correlated subsystem picture is extended one step beyond remote measurement.

The organization of the rest of the article is as follows. In Sec. III the relevant purely mathematical results on classification of all linearly independent complete decompositions of any given density operator (that with an infinite-dimensional range included)[4] are shortly stated. Besides, they are, to some extent, elaborated in order to show that linearly independent bases can be almost as useful as orthonormal ones (to encourage their use at least in entanglement studies in quantum mechanics). In Sec. IV the first result of this article, the generalized twin observables, consisting of twin observables and of extended twin observables, are presented in the form of Theorem 1 and a commutative square diagram. In Sec. V selective (or specific-result) nearby-subsystem measurement that gives rise to so-called remote pure-state preparation is paid special attention to in terms of Theorem 2 and another square commutative diagram. Besides, in Theorem 3 the physical meaning of linearly independent remote pure-state preparation is clarified. In Sec. VI concluding remarks point out the essential features of the results.

As a technical remark, it should be noted that by a basis (without further specification) in a subspace is meant a complete orthonormal set, i.e., one spanning the subspace. We will also deal with linearly-independent bases in linear manifolds (cf. Corollaries 1 and 3).

II. THE CORRELATED SUBSYSTEM PICTURE

The correlated subsystem picture is based on the role of the antiunitary correlation operator U_a inherent in any bipartite state vector $|\Phi\rangle_{12}$. The correlation operator is the antiunitary polar factor of the antilinear Hilbert–Schmidt operator A_a that maps the state space of subsystem 1 into that of subsystem 2. Such an operator, in turn, gives an antilinear representation of any given bipartite state vector $|\Phi\rangle_{12}$.

Antilinear operators were introduced in physics from the mathematical literature[5] by Jauch.[6] They were utilized in Ref. 7 and in the first-step bipartite pure-state studies.[2,8] The main result of these was establishing the correlated subsystem picture of $|\Phi\rangle_{12}$ (with the twin observables) as a core of its structure.

A. The mathematical part

Let $|\Phi\rangle_{12}$ be a given state vector of an arbitrary bipartite pure state with a nearby (1) and a remote (2) subsystem. Naturally, $|\Phi\rangle_{12} \in (\mathcal{H}_1 \otimes \mathcal{H}_2)$, where the tensor factors are complex separable Hilbert spaces.

The first notion that is being utilized is that of the *partial scalar product*: If $|\psi\rangle_1$ is an arbitrary vector of the nearby subsystem, then the partial scalar product

$$\langle\psi|_1|\Phi\rangle_{12} \in \mathcal{H}_2 \tag{1}$$

gives a vector in the state space $\mathcal{H}_2$ of the remote subsystem. It can be defined and evaluated by introducing bases $\{|j\rangle_1 : \forall j\} \subset \mathcal{H}_1$ and $\{|k\rangle_2 : \forall k\} \subset \mathcal{H}_2$ and expanding $|\Phi\rangle_{12}$ in them

$$|\Phi\rangle_{12} = \sum_j \sum_k f_{jk}|j_1\rangle|k\rangle_2. \tag{2a}$$

Then $\langle\psi|_1|\Phi\rangle_{12}$ is obtained in terms of the ordinary scalar product in $\mathcal{H}_1$:

$$\langle\psi|_1|\Phi\rangle_{12} = \sum_j \sum_k [f_{jk}(\langle\psi|_1|j\rangle_1)]|k\rangle_2. \tag{2b}$$

The point is, of course, that, as it is straightforward to show, the right-hand side (rhs) is always defined (in case of infinite sums, one has convergence), and the left-hand side (lhs) is *independent* of the choice of the subsystem bases, and thus a well-defined element of $\mathcal{H}_2$.

The next notion is that of the *antilinear operator representation* of a bipartite state vector $|\Phi\rangle_{12}$: Relation (1) is actually an antilinear, i.e., expansion-coefficients complex-conjugating, map A_a of the entire space $\mathcal{H}_1$ into $\mathcal{H}_2$:

$$(A_a|\psi\rangle_1)_2 \equiv \langle\psi|_1|\Phi\rangle_{12} \in \mathcal{H}_2. \tag{3}$$

The operator A_a defines its *adjoint* $A_a^\dagger$, which maps in the antilinear way $\mathcal{H}_2$ into $\mathcal{H}_1$. This is done via the pair of scalar products, that in $\mathcal{H}_1$ and that in $\mathcal{H}_2$:

$$\forall\,\psi_1 \in \mathcal{H}_1, \forall\,\chi_2 \in \mathcal{H}_2: \quad (\chi_2,(A_a\psi_1)_2)_2 = ((A_a^\dagger\chi_2)_1,\psi_1)_1^*, \tag{4}$$

where the asterisk denotes complex conjugation. It is easy to see that Eq. (4) defines adjoining as a linear operation.

The operators A_a and $A_a^\dagger$ are called Hilbert–Schmidt ones because

$$\mathrm{tr}(A_a^\dagger A_a)_1 < \infty\,, \tag{5a}$$

$$\mathrm{tr}(AA_a^\dagger)_2 < \infty\,. \tag{5b}$$

The set of *all* antilinear Hilbert–Schmidt operators mapping $\mathcal{H}_1$ into $\mathcal{H}_2$ is a complex separable Hilbert space, in which the *scalar product* is defined as

$$\forall A_a, A_a': \quad (A_a, A_a') \equiv \mathrm{tr}(A_a'^\dagger A_a)_1. \tag{6}$$

It is straightforward to show that Eq. (3) constitutes an *isomorphism* of the complex separable Hilbert space of all ordinary bipartite vectors $|\Phi\rangle_{12}$ onto that of all antilinear Hilbert–Schmidt operators mapping $\mathcal{H}_1$ into $\mathcal{H}_2$.

In the sense of this isomorphism, one can speak of A_a as *the antilinear operator representative* of $|\Phi\rangle_{12}$.

It is known that the reduced density operators $\rho_1 \equiv \mathrm{tr}_2(|\Phi\rangle_{12}\langle\Phi|_{12})$ and $\rho_2 \equiv \mathrm{tr}_1(|\Phi\rangle_{12}\langle\Phi|_{12})$ of any given bipartite state vector $|\Phi\rangle_{12}$, which describe the respective subsystem states, have *equal positive parts of their spectra*, i.e., their positive eigenvalues, together with their multiplicities, coincide. Further, it is known that if one expands $|\Phi\rangle_{12}$ in any eigensubbasis $\{|r_i\rangle_1 : \forall\, i\}$ of ρ_1 spanning its range, then one obtains the so-called *biorthogonal Schmidt expansion*

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2}|r_i\rangle_1|r_i\rangle_2, \tag{7}$$

where $\{r_i : \forall\, i\}$ are the positive eigenvalues of ρ_1 corresponding to its mentioned eigenvectors, and $\{|r_i\rangle_2 : \forall\, i\}$ turn out necessarily to be eigenvectors of ρ_2 spanning its (equally dimensional) range. Actually, one can write the spectral forms as follows:

$$\rho_1 = \sum_i r_i|r_i\rangle_1\langle r_i|_1, \tag{8a}$$

$$\rho_2 = \sum_i r_i|r_i\rangle_2\langle r_i|_2. \tag{8b}$$

What the standard approach is lacking is any expression of the *correlations* between the two subsystems that the bipartite state implies. This is where the *antilinear* operator representation of the bipartite state has a marked *advantage*.

If one writes down the *polar factorizations* of A_a, one obtains

$$A_a = U_a \rho_1^{1/2}, \tag{9a}$$

$$A_a = \rho_2^{1/2} U_a Q_1, \tag{9b}$$

where U_a is the antilinear unitary (or antiunitary) *correlation operator*, which maps the (topologically) closed range $\bar{\mathcal{R}}(\rho_1)$ of ρ_1 onto $\bar{\mathcal{R}}(\rho_2)$, that of ρ_2 (preserving the scalar product up to complex conjugation). The Hermitian polar factors are the positive-operator roots of the corresponding reduced density operators, and Q_1 is the range projector of ρ_1. The operator U_a is uniquely determined by A_a (i.e., by $|\Phi\rangle_{12}$), e.g., by $U_a Q_1 = \tilde{\rho}_2^{-1/2} A_a$ [as follows from Eq. (9b)], where $\tilde{\rho}_2$ is the reducee of ρ_2 in $\bar{\mathcal{R}}(\rho_2)$. [See also remark beneath relation (12c).] (An elementary discussion of polar factorization of linear operators in one space is given in Ref. 9, and a more general one in Appendix 4 of Ref. 2. The polar factorizations (9a) and (9b) of A_a differ very little from this.)

It turns out that

$$\rho_2 = (U_a \rho_1 U_a^{-1})_2 Q_2 \tag{10}$$

is valid, where Q_2 is the range projector of ρ_2. Utilizing U_a, the above Schmidt expansion and the spectral forms can be rewritten as follows:

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2} |r_i\rangle_1 (U_a |r_i\rangle_1)_2 \tag{11}$$

and

$$\rho_1 = \sum_i r_i |r_i\rangle_1 \langle r_i|_1, \tag{12a}$$

$$\rho_2 = \sum_i r_i (U_a |r_i\rangle_1)_2 (\langle r_i|_1 U_a^\dagger)_2. \tag{12b}$$

(Note that $U_a^\dagger = U_a^{-1}$.) Actually,

$$\forall i: \quad |r_i\rangle_2 = U_a |r_i\rangle_1. \tag{12c}$$

Thus, the correlation operator U_a can be read off from the Schmidt biorthogonal expansion (11) when the latter is explicitly evaluated.

If $\{|j\rangle_1; \forall j\}$ is a basis in $\mathcal{H}_1$, one can uniquely expand the bipartite state, and, as easily seen, one obtains

$$|\Phi\rangle_{12} = \sum_j |j\rangle_1 (A_a |j\rangle_1)_2. \tag{13a}$$

The antilinear representation A_a of $|\Phi\rangle_{12}$ can be read off from this because the antilinear operator A_a is continuous (cf. Appendix 2 in Ref. 2); hence, it is determined by its action on a basis.

Relation (13a) can also be understood as giving the inverse of isomorphism (3), i.e., as determining the map $A_a \to |\Phi\rangle_{12}$. (It is straightforward to show that the lhs of (13a) does not depend on the choice of the basis.)

If the basis in Eq. (13a) is an *eigenbasis* of ρ_1, *then, and only then*, as immediately seen from Eq. (9a), the general expansion (13a) takes on the special form of the biorthogonal Schmidt expansion (7).

Returning to the general expansion (13a), it can be completed by

$$\rho_2 = \sum_j (A_a |j\rangle_1)_2 (\langle j|_1 A_a^\dagger)_2 = \sum_j p_j |\phi_j\rangle_2 \langle \phi_j|_2, \tag{13b}$$

$$\forall j: \quad p_j \equiv \|(A_a|j\rangle_1)_2\|^2, \tag{13c}$$

$$\forall j,\ p_j > 0: \quad |\phi_j\rangle_2 \equiv p_j^{-1/2}(A_a|j\rangle_1)_2. \tag{13d}$$

Here p_j is the probability that the event $(|j\rangle_1\langle j|_1 \otimes 1)$ occurs in nearby-subsystem measurement in $|\Phi\rangle_{12}$, and $|\phi_j\rangle_2$ is the state of the remote subsystem thus obtained, i.e., it is the result of so-called *remote preparation*. From the nonselective (or entire-ensemble) point of view, the physical meaning of Eqs. (13a)–(13d) consists in the fact that these relations express a *remote complete state decomposition* in the antilinear representation. (In remote incomplete state decomposition also mixed states of the remote subsystem are obtained. Such a remote decomposition is given rise to by incomplete nearby-subsystem measurement, i.e., by measurement of an observable with degenerate eigenvalues.)

The adjoint antilinear Hilbert–Schmidt operators $A_a^\dagger$ also form a complex separable Hilbert space in their turn with the scalar product

$$(A_a^\dagger, (A_a^\dagger)') \equiv \mathrm{tr}(A_a' A_a^\dagger)_2. \tag{14}$$

They give the second antilinear operator representation for bipartite vectors via the isomorphism

$$\forall |\Phi\rangle_{12}: \to A_a^\dagger: \quad \forall\, |\chi\rangle_2 : (A_a^\dagger|\chi\rangle_2)_1 \equiv \langle\chi|_2|\Phi\rangle_{12} \in \mathcal{H}_1. \tag{15}$$

Associating $A_a^\dagger$ with A_a [cf. Eq. (4)] is also an isomorphism. (Any two of the mentioned three isomorphisms of bipartite state spaces multiply, i.e., give, when taken one after the other, the third one.)

One has the following relations that are symmetric to Eqs. (9a)–(13a) in terms of the adjoint antilinear operator representation of $|\Phi\rangle_{12}$:

$$A_a^\dagger = U_a^{-1}\rho_2^{1/2}, \tag{16a}$$

$$A_a^\dagger = \rho_1^{1/2} U_a^{-1} Q_2. \tag{16b}$$

Further

$$\rho_1 = U_a^{-1}\rho_2 U_a Q_1, \tag{17}$$

$$|\Phi\rangle_{12} = \sum_i r_i^{1/2}(U_a^{-1}|r_i\rangle_2)_1|r_i\rangle_2, \tag{18}$$

where $\{|r_i\rangle_2 : \forall i\}$ is any eigensubbasis of ρ_2 spanning the range of the latter, and $\{r_i : \forall i\}$ are the corresponding (positive) eigenvalues

$$\rho_1 = \sum_i r_i (U_a^{-1}|r_i\rangle_2)_1 (\langle r_i|_2 U_a)_1 = \sum_i r_i (U_a^{-1}(|r_i\rangle_2\langle r_i|_2)U_a)_1, \tag{19a}$$

$$\rho_2 = \sum_i r_i |r_i\rangle_2\langle r_i|_2. \tag{19b}$$

In general

$$|\Phi\rangle_{12} = \sum_k (A_a^\dagger|k\rangle_2)_1|k\rangle_2, \tag{20a}$$

where $\{|k\rangle_2 : \forall k\}$ is any basis in $\mathcal{H}_2$. Again, it is clear from Eq. (16a) that if this basis is an eigenbasis of ρ_2, then and only then, the general expansion (20a) takes the special form of the biorthogonal Schmidt expansion (18).

Finally, one has

$$\rho_1 = A_a^\dagger A_a, \tag{20b}$$

$$\rho_2 = A_a A_a^\dagger. \tag{20c}$$

The correlation operator U_a establishes a striking *mathematical symmetry* and close connection between the two closed ranges $\bar{\mathcal{R}}(\rho_s)$, $s=1,2$, for any bipartite state vector $|\Phi\rangle_{12}$. The pair of entities ρ_1, U_a, which is equivalent to $|\Phi\rangle_{12}$ [cf. Eqs. (9a) and (3)], is called *the correlated subsystem picture* of the given bipartite state vector. (Note that when one takes a state vector $|\Phi\rangle_{12}$ instead of a state $|\Phi\rangle_{12}\langle\Phi|_{12}$, the former is informationally richer by the choice of a fixed phase factor $e^{i\lambda}$, $\lambda \in \mathbf{R}$, which is arbitrary in the latter. This choice is carried by A_a or U_a. Thus, U_a and $e^{i\lambda}U_a$ with the same ρ_1,correspond to $|\Phi\rangle_{12}$ and $e^{i\lambda}|\Phi\rangle_{12}$, respectively.)

We have summed up in this subsection the mathematical part of the antilinear representation of $|\Phi\rangle_{12}$, and of the correlated subsystem picture. The basic physical meaning of these was studied in previous articles.[2,8] A summary is given in the next subsection.

B. The physical part—detectably complete state-compatible observables

A detectably complete (see below) nearby subsystem observable A_1 that is compatible with the nearby subsystem state, i.e., that satisfies $[A_1,\rho_1]=0$, shortly, a *state-compatible* observable, has, on account of this relation, as it is well known, a common eigenbasis with ρ_1. Let its subbasis spanning $\bar{\mathcal{R}}(\rho_1)$ be $\{|r_i\rangle_1 : \forall i\}$ [cf. Eqs. (7) and (8a)]. Then the relevant partial spectral form of A_1 is

$$A_1 = \sum_i a_i |r_i\rangle_1\langle r_i|_1 + Q_1^\perp A_1, \quad i \neq i' \Rightarrow a_i \neq a_{i'}, \tag{21a}$$

where $Q_1=\Sigma_i |r_i\rangle_1\langle r_i|_1$ is the range projector of ρ_1, $Q_1^\perp$ is the orthocomplementary projector, and the sum in Eq. (21a) is the *detectable part* [in $\bar{\mathcal{R}}(\rho_1)$] of A_1.

By *detectably complete* is meant the requirement in Eq. (21a), i.e., completeness of the reducee $\widetilde{A_1}=\Sigma_i a_i \widetilde{|r_i\rangle\langle r_i|}$ of A_1 in $\bar{\mathcal{R}}(\rho_1)$. [For the use of tilde cf $\tilde{\rho}_2$ in the passage beneath Eqs. (9a) and (9b).]

When A_1 is measured (in an ideal way, e.g.), it gives rise to the actual state decomposition (empirically ensemble decomposition)

$$\rho_2 = \sum_i r_i |r_i\rangle_2\langle r_i|_2 \tag{21b}$$

[special case of Eqs. (13a)–(13d)]. Since the state vectors $\{|r_i\rangle_2 : \forall i\}$ are orthogonal [cf. Eqs. (7) and (8b)], Eq. (21b) amounts to the same as if a detectably complete remote-subsystem observable (Hermitian operator)

$$A_2 = \sum_i a_i' |r_i\rangle_2\langle r_i|_2 + Q_2^\perp A_2, \quad i \neq i' \Rightarrow a_i' \neq a_{i'}' \tag{21c}$$

had been measured in an ideal way. Here $Q_2=\Sigma_i |r_i\rangle_2\langle r_i|_2$ is the range projector of ρ_2.

The pairs of observables (A_1,A_2) are called (physical) *twin observables*, the indirect measurement of A_2 by measuring A_1 directly is called *remote measurement*, and the twin observables satisfy the symmetric relations

$$[A_1,\rho_1] = 0, \tag{22a}$$

$$[A_2,\rho_2] = 0; \tag{22b}$$

$$A_2 = \sum_i a_i' (U_a(|r_i\rangle_1\langle r_i|_1)U_a^{-1})_2 Q_2 + Q_2^{\perp} A_2, \tag{22c}$$

$$A_1 = \sum_i a_i (U_a^{-1}(|r_i\rangle_2\langle r_i|_2)U_a)_1 Q_1 + Q_1^{\perp} A_1. \tag{22d}$$

In Eq. (22c) it is assumed that $A_1 = \Sigma a_i |r_i\rangle_1\langle r_i|_1 + Q_1^{\perp} A_1$ is given, and A_2 is determined by it (at least as far as the eigenvectors of the detectable part of A_2 are concerned). In Eq. (22d) the symmetrical assumption is made. One should note that the undetectable parts $Q_1^{\perp} A_1$ and $Q_2^{\perp} A_2$ are completely arbitrary (and so are the distinct detectable eigenvalues of the twin operator).

In Refs. 2 and 8, it was assumed that *the detectable spectra coincide*

$$\forall i: \quad a_i' = a_i. \tag{23a}$$

Then

$$A_2 = (U_a A_1 U_a^{-1})_2 Q_2 + Q_2^{\perp} A_2, \tag{23b}$$

and

$$A_1 = (U_a^{-1} A_2 U_a)_1 Q_1 + Q_1^{\perp} A_1 \tag{23c}$$

are valid. In later work,[10] twin observables with the stronger requirement Eq. (23a) were called *algebraic twin observables*. *Relaxation* of the stronger requirement led to the wider and more useful class of *physical twin observables*.

If one exchanges the roles of subsystems 1 and 2, one can measure A_1 remotely by a direct measurement of A_2.

Thus, part of the *physical meaning* of the *correlation operator* U_a inherent in $|\Phi\rangle_{12}$ is in the following: When a detectably complete nearby-subsystem observable A_1 [cf. Eq. (21a)] that is compatible with the nearby-subsystem state is measured in an ideal way in selective measurement and a_i is obtained as a result, then the nearby subsystem is found in the state $|r_i\rangle_1$, and the remote subsystem is in the state $|r_i\rangle_2 \equiv (U_a|r_i\rangle_1)_2$ (conditional state). It is obvious from Eqs. (18) and (19a), that also the symmetrical argument is valid. The correlation operator (and its inverse) gives the corresponding *conditional states* when selective ideal measurement of state-compatible subsystem observables is performed.

The remote measurement of a twin observable A_2, selective or nonselective, is one and the same in every kind of measurement of A_1: in ideal measurement and in second-kind (synonym: non-repeatable) measurement [cf. subsection 6(B) in Ref. 2].

III. LINEARLY INDEPENDENT COMPLETE DECOMPOSITIONS OF DENSITY OPERATORS

Definition 1: A finite or countably infinite set of vectors $\{|\phi_i\rangle: \forall i\}$ is said to be *linearly independent* if

$$\forall i: \quad |\phi_i\rangle \notin \overline{\text{span}}\{|\phi_{i'}\rangle: \forall i', i' \neq i\}, \tag{24}$$

where by "$\overline{\text{span}}$" is meant the algebraic and topological span, i.e., the set of all linear combinations together with all their limiting points. (It is a subspace.)

One can define linear independence of a finite sequence $\{|\phi_i\rangle: i = 1, 2, \ldots, d < \infty\}$ of vectors by the weaker requirement:

$$\forall k, \quad k \geqslant 2: |\phi_k\rangle \notin \text{span}\{|\phi_1\rangle, \ldots, |\phi_{(k-1)}\rangle\}. \tag{25}$$

Proof is given in Appendix A. (Note that finite-dimensional linear manifolds are subspaces, i.e., span$=\overline{\text{span}}$ in this case.)

Definition 2: If $\{|\phi_i\rangle: i = 1, 2, \ldots, d \leqslant \infty\}$ is a linearly independent finite or infinite sequence, ρ

a density operator with a d-dimensional closed range, and if one can write

$$\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|, \tag{26a}$$

where $\forall i : p_i > 0$, $\Sigma_i p_i = 1$, then one speaks of a *linearly independent complete decomposition* of the density operator. (It is called "irreducible decomposition" in Refs. 11 and 4.)

We call "complete" those decompositions of a density operator that cannot be continued by further decomposing any term. These are the pure-state decompositions quantum mechanically. In a followup to this article we turn to "incomplete" decompositions, i.e., to mixed-or-pure state decompositions quantum mechanically.

For Eq. (26a) the relation

$$\bar{\mathcal{R}}(\rho) = \overline{\text{span}}\{|\phi_i\rangle : \forall\, i\} \tag{26b}$$

is valid (cf. Proposition 1 in Ref. 11).

Corollary 1: Obviously, orthonormal sets are special cases of linearly independent ones. The latter possess some important properties of the former. One of them is the following. If $\{|\phi_i\rangle : i = 1,2,\ldots,d \leqslant \infty\}$ is a linearly independent sequence, k is an integer not larger than d, and $\{|\phi_1\rangle,\ldots,|\phi_k\rangle\}$ is a subset of arbitrary elements in arbitrary order, then it spans a k-dimensional subspace $\mathcal{S}_k$, and each vector in it can be uniquely expanded in the set. This is why the latter is called a *linearly independent basis* in $\mathcal{S}_k$. (See also Corollary 3 below.)

Proof is given in Appendix B.

Now we sum up those results on density-operator decomposition from Ref. 4 the application of which forms the basis of this work. They are further elaborated in this section with a view to help applications in quantum-mechanical studies. (No heed is paid to the extent to which the elaborations are possibly new with respect to the mathematical literature, cf., e.g., Ref. 12.)

Lemma: (A) Let ρ be an arbitrary given density operator, and let d be the dimension of its (finite or infinite dimensional) closed range. Then *all* linearly independent sequences $\{|\phi_i\rangle : i = 1,2,\ldots,d\}$ that determine a complete decomposition

$$\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i| \tag{27}$$

of ρ stand in a *one-to-one relation* with the set of *all* bases in $\bar{\mathcal{R}}(\rho)$ each vector of which is within $\mathcal{R}(\rho^{1/2})$:

$$\{|e_i\rangle : i = 1,2,\ldots,d \leqslant \infty\} \subset \mathcal{R}(\rho^{1/2}), \tag{28}$$

where d is the dimension of $\bar{\mathcal{R}}(\rho)$.

(B) The bijection from the set of all bases Eq. (28) to all linearly independent sequences that give decompositions Eq. (27)—we call it the Cassinelli–Vito–Levrero (CVL) bijection—reads as follows:

$$p_i = \langle e_i|\rho|e_i\rangle = ||\rho^{1/2}|e_i\rangle||^2 > 0, \quad |\phi_i\rangle = p_i^{-1/2}\rho^{1/2}|e_i\rangle, \tag{29a}$$

$$i = 1,2,\ldots,d \leqslant \infty\,. \tag{29b}$$

The *inverse* CVL bijection is

$$|e_i\rangle = p_i^{1/2}\tilde{\rho}^{-1/2}|\phi_i\rangle, \quad i = 1,2,\ldots,d \leqslant \infty\,, \tag{30}$$

where the tilde denotes the reducee in $\bar{\mathcal{R}}(\rho)$.

(C) Finally, a state vector $|\phi\rangle$ can appear in a linearly independent complete decomposition of ρ if and only if

$$|\phi\rangle \in \mathcal{R}(\rho). \tag{31}$$

For proof see Theorem 1, Proposition 1, and Remark 8 in Ref. 4.

In connection with the Lemma, one should keep in mind the well-known (and easily proved) relations

$$\mathcal{R}(\rho) \subseteq \mathcal{R}(\rho^{1/2}) \subseteq \bar{\mathcal{R}}(\rho^{1/2}) = \bar{\mathcal{R}}(\rho). \tag{32}$$

In the case of finite-dimensional range, one has equality all over. Contrarily, in the case of infinite-dimensional range, both subset relations in Eq. (32) are *proper*.

Corollary 2: The CVL bijection is *nontrivial* if and only if the basis Eq. (28) is *not* an eigensubbasis of ρ (otherwise, it is the identity map).

Corollary 3: Another property of linearly independent sequences parallelling that of orthonormal ones is the following. If Eq. (27) is a linearly independent complete decomposition of a density operator, then each element $|\chi\rangle$ from the range $\mathcal{R}(\rho^{1/2})$ can be *uniquely expanded* in the sequence $\{|\phi_i\rangle : i=1,2,\ldots,d\leqslant\infty\}$:

$$|\chi\rangle = \sum_i \alpha_i |\phi_i\rangle, \tag{33a}$$

[cf. Eq. (32)]. Further, utilizing the scalar product, one has the following *compact* formula for the expansion coefficients:

$$\alpha_i = p_i[(\langle\phi_i|\tilde{\rho}^{-1})|\chi\rangle], \quad i=1,2,\ldots,d\leqslant\infty \tag{33b}$$

(cf. Lemma C). In this sense, the sequence at issue is a *linearly independent basis* in $\mathcal{R}(\rho^{1/2})$.

Note that the uniqueness of expansion (33a) allows an arbitrary (hence, if desired, a suitable) choice of the probability distribution $\{p_i : i=1,2,\ldots,d\leqslant\infty; p_i>0; \Sigma_{i=1}^{d} p_i=1\}$, and the definition of ρ via Eq. (27). [But care must be taken that $\mathcal{R}(\rho^{1/2})$ contain $|\chi\rangle$.] Note, further, that all d probabilities p_i must be positive. Otherwise, $|\chi\rangle$ would not be expanded in the linearly independent basis $\{|\phi_i\rangle : i=1,2,\ldots,d\leqslant\infty\}$.

Corollary 3 is proved in Appendix C.

Corollary 4: If Eq. (27) is a linearly independent complete decomposition of a given density operator, then the weight p_i can also be expressed in the following two ways:

$$p_i = (\langle\phi_i|\tilde{\rho}^{-1}|\phi_i\rangle)^{-1}, \quad i=1,2,\ldots,d\leqslant\infty, \tag{34}$$

and

$$p_i = 1/\left(\sum_k (|\langle k||\phi_i\rangle|^2 r_k^{-1})\right), \quad i=1,2,\ldots,d\leqslant\infty, \tag{35a}$$

where

$$\rho = \sum_k r_k |k\rangle\langle k|, \quad \forall\, k: \quad r_k>0 \tag{35b}$$

is a complete spectral decomposition of ρ.

Further, one has

$$\inf\{r_k : |\langle\phi_i||k\rangle|^2>0\} \leqslant p_i \leqslant \max\{r_k : |\langle\phi_i||k\rangle|^2>0\}, \quad i=1,2,\ldots,d\leqslant\infty, \tag{36}$$

where the "infimum" can be replaced by "minimum" if the range of ρ is finite dimensional.

Proof: Expression (34) is obtained by taking the square norm of both sides of Eq. (30). Expression (35a) follows from Eq. (34) when $|\phi_i\rangle$ is expanded in the eigensubbasis $\{|k\rangle : \forall\, k\}$ of ρ (and eigenbasis of $\tilde{\rho}$.) Finally, inequalities (36) are an immediate consequence of Eq. (35a). □

Remark 1: When a density operator ρ is given and a state vector satisfies $|\phi\rangle \in \mathcal{R}(\rho)$ (cf. Lemma C), then, in whatever linearly independent complete decomposition of the former the latter

appears, it has a *unique* weight p, which depends only on ρ and $|\phi\rangle$ [cf. Eq. (34)].

Definition 3: We call the weight p from Remark 1 the *characteristic weight* of $|\phi\rangle$ in ρ. If $|\phi\rangle \notin \mathcal{R}(\rho)$, then $p \equiv 0$.

Note that if $|\phi\rangle \in \mathcal{R}(\rho)$, then $p > 0$ [cf. Eq. (29a)]. Note, further, that Remark 1 and Corollary 4 are a completion of Lemma C.

Remark 2: For a possible positive value of the characteristic weight p, there may be more than one corresponding state vector $|\phi\rangle$ in a linearly independent complete state decomposition (27) as seen from Eq. (29a), because more than one state vector $|f\rangle$ can give one and the same expectation value of ρ, and each can be the first $|e_1\rangle \equiv |f\rangle$ in a basis etc. (cf. the Lemma).

Corollary 5: The characteristic weight p of a given state vector $|\phi\rangle \in \mathcal{R}(\rho)$ satisfies the inequality

$$p \leqslant \langle\phi|\rho|\phi\rangle. \tag{37}$$

One has $p = \langle\phi|\rho|\phi\rangle$ if and only if $|\phi\rangle$ is an eigenvector of ρ, and then p equals the corresponding eigenvalue of the density operator.

Proof: The inequality (37) follows from Eq. (27) when one puts $|\phi_1\rangle \equiv |\phi\rangle$ in Eq. (27), and one obtains

$$\rho = p|\phi\rangle\langle\phi| + \sum_{i=2} p_i|\phi_i\rangle\langle\phi_i|, \tag{38a}$$

one applies $|\phi\rangle\langle\phi|$ to both sides, and one takes the trace (keeping in mind, of course, that $\mathrm{tr}(|\phi\rangle \times \langle\phi|\rho) = \langle\phi|\rho|\phi\rangle$):

$$\langle\phi|\rho|\phi\rangle = p + \sum_{i=2} p_i|\langle\phi||\phi_i\rangle|^2 \geqslant p. \tag{38b}$$

One can see from Eq. (34) that if $|\phi\rangle$ is an eigenvector of ρ corresponding to the eigenvalue r, then $p = r$, and also $\langle\phi|\rho|\phi\rangle = r = p$. Conversely, if $p = \langle\phi|\rho|\phi\rangle$, then one can see from Eq. (38b) that all vectors $\{|\phi_i\rangle : i = 2, 3, \ldots\}$ must be orthogonal to $|\phi\rangle$. Hence, applying Eq. (38a) to $|\phi\rangle$, it is seen that the latter is an eigenvector of ρ corresponding to the eigenvalue $r = p$. □

IV. REMOTE LINEARLY INDEPENDENT COMPLETE STATE DECOMPOSITION

Let $|\Phi\rangle_{12}$ be an arbitrary bipartite state vector. Owing to the Cassinelli *et al.* theory, summed up in the Lemma, we can now easily sort out what kind of local, i.e., subsystem measurement gives rise to a linearly independent complete decomposition of the opposite-subsystem state.

Definition 4: Since subsystem measurement, by definition, excludes any interaction between the measuring instrument and the remote subsystem, we call any influence of the former on the latter, which is due exclusively to the quantum correlations inherent in the bipartite state, *remote* influence.

Definition 5: We call a nearby subsystem observable A_1 *relevant* (for remote linearly independent complete state decomposition) if the following three conditions are satisfied:

(i)

$$[A_1, Q_1] = 0, \tag{39}$$

where Q_1 is the range projector of $\rho_1 \equiv \mathrm{tr}_2(|\Phi\rangle_{12}\langle\Phi|_{12})$. If Eq. (39) is satisfied, then A_1 will be said to be *range compatible*.

(ii) $\tilde{A}_1$, the reducee of A_1 in $\bar{\mathcal{R}}(\rho_1)$ if Eq. (39) is satisfied, has a purely discrete and nondegenerate spectrum.

(iii) The eigenbasis $\{|e_i\rangle_1 : \forall i\}$ of $\tilde{A}_1$ in $\bar{\mathcal{R}}(\rho_1)$ (which is uniquely determined by $\tilde{A}_1$ up to arbitrary phase factors and ordering) is within $\mathcal{R}(\rho_1^{1/2})$. (This requirement is always satisfied if the dimension d of ρ_1 is finite.)

Further, we call a *basis* $\{|e_i\rangle_1 : \forall i\}$ in $\bar{\mathcal{R}}(\rho_1)$ that is entirely within $\mathcal{R}(\rho_1^{1/2})$ *relevant*. Finally, we

call a *class of observables* A_1 relevant if it consists of relevant observables that have *one and the same* relevant basis $\{|e_i\rangle_1 : \forall i\}$ (up to phase factors and ordering) as their eigensubbasis in $\bar{\mathcal{R}}(\rho_1)$.

Evidently, the set of all relevant classes of observables A_1 is in a simple one-to-one relation with the set of all relevant bases in $\mathcal{R}(\rho_1^{1/2})$.

If A_1 is *state compatible*, i.e., $[A_1,\rho_1]=0$, then A_1 commutes also with every eigenprojector of ρ_1, and hence, Eq. (39) is satisfied. Namely, Q_1 is the sum of the eigenprojectors corresponding to positive eigenvalues. [If $\mathcal{R}(\rho_1)$ is infinite dimensional, we can assume that A_1 is bounded, or, equivalently, continuous, or equivalently, that its spectrum is within a finite interval. We can do this because the spectrum of A_1 is arbitrary within the relevant class of observables, i.e., it is irrelevant for remote state decomposition.]

In this case the reducee $\tilde{A}_1$ has necessarily a purely discrete spectrum (because it reduces in every eigensubspace of ρ_1, and these are necessarily finite dimensional due to the fact that the corresponding eigenvalues add up to 1). Thus, in this case, requirement (i) is necessarily fulfilled, and (ii) reads that A_1 is a detectably complete observable, i.e., that $\tilde{A}_1$ is complete. Requirement (iii) is necessarily satisfied because $[A_1,\rho_1]=0$ entails a common eigenbasis of $\tilde{A}_1$ and $\tilde{\rho}_1$. Further, the corresponding spectral form of $\tilde{\rho}_1$ is simultaneously a complete decomposition of it. Hence, according to the known result of Hadjisavvas,[11] each of the eigenvectors necessarily belongs to $\mathcal{R}(\rho_1^{1/2})$.

Theorem 1: (A) If a relevant observable $(A_1\otimes 1)$ is measured in the state $|\Phi\rangle_{12}$, it gives rise to a remote linearly independent complete decomposition of the state $\rho_2\equiv \mathrm{tr}_1(|\Phi\rangle_{12}\langle\Phi|_{12})$:

$$\rho_2=\sum_i p_i|\phi_i\rangle_2\langle\phi_i|_2. \tag{40}$$

Conversely, each mathematically possible linearly independent complete decomposition of ρ_2 can be obtained in this way.

(B) The mathematical way how A_1 determines Eq. (40) can be understood as a bijection of the set of all classes of detectably equivalent observables A_1, or, equivalently, of all relevant bases $\{|e_i\rangle_1 : \forall i\}$, onto the set of all linearly independent complete decompositions Eq. (40) (A$\searrow$D on Diagram 1 below) that reads:

$$\forall i:\quad p_i=\langle\Phi|_{12}(|e_i\rangle_1\langle e_i|_1\otimes 1)|\Phi\rangle_{12}>0, \tag{41a}$$

$$\forall i:\quad |\phi_i\rangle_2=p_i^{-1/2}\rho_2^{1/2}(U_a|e_i\rangle_1)_2, \tag{41b}$$

where $|e_i\rangle_1$ are the eigenbasis vectors of $\tilde{A}_1=\Sigma_{i'}a_{i'}|e_{i'}\rangle_1\langle e_{i'}|_1$. Further, U_a is the antiunitary correlation operator determined by $|\Phi\rangle_{12}$ [cf. Eqs. (9a) and (9b) and the passage beneath it, as well as the passage beneath Eq. (12c)].

(C) The inverse bijection (A$\nwarrow$D on the diagram) has the form

$$\forall i:\quad |e_i\rangle_1=(U_a^{-1}(p_i^{1/2}\tilde{\rho}_2^{-1/2}|\phi_i\rangle_2))_1. \tag{42}$$

All claims symmetric to those in (A)–(C) are also valid.

(D) If $(1\otimes A_2)=\Sigma_j a_j'(1\otimes|f_j\rangle_2\langle f_j|_2)+(1\otimes Q_2^{\perp}A_2)$ is the relevant partial spectral form of an arbitrary relevant observable A_2 [Q_2 being the range projector of $\rho_2\equiv\mathrm{tr}_1(|\Phi\rangle_{12}\langle\Phi|_{12})$], its (nonselective) measurement causes a remote linearly independent complete state decomposition

$$\rho_1\equiv\mathrm{tr}_2(|\Phi\rangle_{12}\langle\Phi|_{12})=\sum_j q_j|\chi_j\rangle_1\langle\chi_j|_1,\quad \forall j:\quad q_j>0,\quad \sum_j q_j=1. \tag{43}$$

Each linearly independent complete decomposition of ρ_1 can be obtained in this way.

(E) The bijection (C$\swarrow$B on the diagram) taking the set of all relevant classes of second-subsystem observables onto that of all linearly independent complete first-subsystem state decompositions reads

$$\forall j: \quad q_j \equiv \langle\Phi|_{12}(1 \otimes |f_j\rangle_2\langle f_j|_2)|\Phi\rangle_{12} > 0, \tag{44a}$$

$$\forall j: \quad |\chi_j\rangle_1 \equiv q_j^{-1/2}\rho_1^{1/2}(U_a^{-1}|f_j\rangle_2)_1. \tag{44b}$$

(F) The inverse bijection (C$\nearrow$B) is

$$\forall j: \quad |f_j\rangle_2 \equiv (U_a(q_j^{1/2}\widetilde{\rho_1}^{-1/2}|\chi_j\rangle_1))_2. \tag{45}$$

(G) A bijection mapping all relevant classes of observables $(A_1 \otimes 1)$ onto that of all relevant classes of observables $(1 \otimes A_2)$ (A$\rightarrow$B on the diagram) is

$$\forall i: \quad |f_i\rangle_2 \equiv (U_a|e_i\rangle_1)_2. \tag{46a}$$

The inverse bijection (A$\leftarrow$B on the diagram) is

$$\forall j: \quad |e_j\rangle_1 \equiv (U_a^{-1}|f_j\rangle_2)_1. \tag{46b}$$

(H) The product bijection (C$\swarrow$B)$\circ$(A$\rightarrow$B) ("$\circ$" meaning "after") is the corresponding CVL bijection $(A \downarrow C)$; and symmetrically, the product bijection (A$\searrow$D)$\circ$(A$\leftarrow$B) is the corresponding CVL bijection $(B \downarrow D)$.

(I) A bijection taking all linearly independent complete decomposition of ρ_1 onto those of ρ_2 (C$\rightarrow$D) is

$$\left[U_a\left(\rho_1 = \sum_i q_i|\chi_i\rangle_1\langle\chi_i|_1\right)U_a^{-1}\right]_2 Q_2,$$

giving, due to Eq. (10),

$$\rho_2 = \sum_j p_j|\phi_j\rangle_2\langle\phi_j|_2,$$

where

$$\forall j: \quad p_j \equiv q_j, \tag{47a}$$

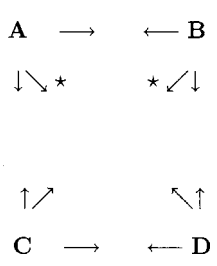
$$\forall j: \quad |\phi_j\rangle_2 \equiv (U_a|\chi_j\rangle_1)_2. \tag{47b}$$

The inverse bijection (C$\leftarrow$D on the diagram) is symmetric to this (under the exchange of the two subsystems) mutatis mutandis.

(J) The square Diagram 1 summing up the preceding items of Theorem 1 is *commutative*, i.e., any two successive bijections multiply into the corresponding bijection on the diagram.

Commutative Square Diagram 1.
A Mathematical Framework for Remote
Linearly Independent Complete State Decompositions

A $\equiv$ {all relevant classes of A_1} **B** $\equiv$ {all relevant classes of A_2}



C $\equiv$ {all linearly-independent complete decompositions of ρ_1}

$\mathbf{D} \equiv \{\text{all linearly-independent complete decompositions of } \rho_2\}$

Each arrow goes from one of the sets (A,B,C,D) towards another. It stands for the corresponding bijection. Oppositely oriented arrows denote mutually inverse bijections. The diagram is *commutative*, i.e., the successive bijections combine into the displayed corresponding one. For instance, taking the bijection $\mathbf{B} \downarrow \mathbf{D}$ after the bijection $\mathbf{A} \rightarrow \mathbf{B}$ gives the bijection $\mathbf{A} \searrow \mathbf{D}$. The bijections are given in detail in Theorem 1. The imaginary vertical line cutting the square into two equally wide halves makes these completely symmetric (due to the symmetry between the two subsystems in $|\Phi\rangle_{12}$).

⋆ The downward diagonal bijections $\mathbf{A} \searrow \mathbf{D}$ and $\mathbf{C} \swarrow \mathbf{B}$ have the *physical meaning* of *remote linearly-independent state decompositions*.

Proof of Theorem 1.

(B) To prove claim B, we take resort to the relations (13a)–(13d), which express the general remote complete state decomposition. Relation (13c) and (3) imply in our case

$$\forall i: \quad 0 < p_i = ||(A_a|e_i\rangle_1)_2||^2 = ||\langle e_i|_1|\Phi\rangle_{12}||^2 = ((\langle\Phi|_{12}|e_i\rangle_1)_2, (\langle e_i|_1|\Phi\rangle_{12})_2)$$
$$= \langle\Phi|_{12}(|e_i\rangle_1\langle e_i|_1 \otimes 1)|\Phi\rangle_{12}.$$

Further, Eqs. (13d) and (9b) give $\forall i: |\phi_i\rangle_2 = p_i^{-1/2}\rho_2^{1/2}(U_a|e_i\rangle_1)_2$.

(C) Claim C obviously follows from B in view of the facts that both U_a and $\tilde{\rho}_2^{1/2}$ are nonsingular on $\bar{\mathcal{R}}(\rho_1)$ and in $\bar{\mathcal{R}}(\rho_2)$, respectively.

(A) The proof of claim A is a consequence of part of the commutativity of the square Diagram, viz., of the fact that $(A \searrow D) = (B \downarrow D) \circ (A \rightarrow B)$. To see this, one should keep in mind that $\rho_2 = (U_a\rho_1 U_a^{-1})_2 Q_2$ [cf. Eq. (10)] implies $U_a\mathcal{R}(\rho_1^{1/2}) = \mathcal{R}(\rho_2^{1/2})$ because the definition $\rho_1^{1/2}\rho_1^{1/2} = \rho_1$ of the square root, Eq. (10) and the well known uniqueness of the square root lead to $(U_a\rho_1^{1/2}U_a^{-1})_2 Q_2 (U_a\rho_1^{1/2}U_a^{-1})_2 Q_2 = \rho_2$, and finally to $(U_a\rho_1^{1/2}U_a^{-1})_2 Q_2 = \rho_2^{1/2}$. Therefore, $\{|e_i\rangle_1 : \forall i\} \subset \mathcal{R}(\rho_1^{1/2})$ implies $\{(U_a|e_i\rangle_1)_2 : \forall i\} \subset \mathcal{R}(\rho_2^{1/2})$.

Further, let us rewrite Eq. (41a) as

$$\forall i: \quad p_i = \langle e_i|_1\rho_1|e_i\rangle_1 = (\langle e_i|_1 U_a^\dagger)_2 (U_a\rho_1 U_a^{-1})_2 (U_a|e_i\rangle_1)_2 = (\langle e_i|_1 U_a^\dagger)\rho_2(U_a|e_i\rangle_1)_2.$$

(Complex conjugation due to applying an antilinear operator to the left is omitted because the scalar product is a positive number.)

Comparing the last relation with Eq. (29a), and Eq. (41b) with Eq. (29b), we see that the claimed product of maps holds true. Since the factors in the product are bijections, so is the product itself (and its inverse is the reverse product of the inverses).

Finally, on account of the fact that the CVL bijection $(B \downarrow D)$ maps onto the set of all linearly independent complete state decompositions [in $\mathcal{R}(\rho_2)$], the same is valid for the remote state decompositions $(A \searrow D)$ as claimed.

The symmetric claims D, E, and F can be proved symmetrically. Claim G is obviously valid.

(H) Claim H is an immediate consequence of the products $(C \swarrow B) = (A \downarrow C) \circ (A \leftarrow B)$, which is the symmetric relation of $(A \searrow D) = (B \downarrow D) \circ (A \rightarrow B)$ (see proof of claim C).

Claim I is obviously valid. The final claim J easily follows from the multiplications proved for claim C. □

Remark 3: In the special case when a pair of range-compatible observables A_s $s = 1, 2$, are state compatible, then the CVL bijections $(A \downarrow C)$ and $(B \downarrow D)$ become mathematically most simple, and are endowed with physical meaning of actual orthogonal decomposition of the states $\rho_s, s = 1, 2$, due to ideal measurement. If the range-compatible observables are state incompatible, then the CVL bijections are formal.

The *remote linearly independent complete decomposition* Eq. (40), caused by the direct subsystem measurement of $(A_1 \otimes 1)$, *has the physical meaning of actual decomposition* of ρ_2. This is so because, when the measurement interaction is over, the tripartite pure state vector has undergone the change

$$|0\rangle_{MA}|\Phi\rangle_{12}=|0\rangle_{\mathrm{MA}}\left[\sum_i |e_i\rangle_1[\rho_2^{1/2}(U_a|e_i\rangle_1)_2]\right]\rightarrow\sum_i |i\rangle_{\mathrm{MA}}|e_i'\rangle_1[\rho_2^{1/2}(U_a|e_i\rangle_1)_2]=\sum_i p_i|i\rangle_{\mathrm{MA}}|e_i'\rangle_1|\phi_i\rangle_2, \tag{48}$$

where $|0\rangle_{\mathrm{MA}}$ is the initial state vector of the *measuring apparatus*, and $\{|i\rangle_{\mathrm{MA}}:\forall i\}$ is the orthonormal set of so-called "pointer positions": the state vectors in it display the results $\{a_i:\forall i\}$ in the measurement of A_1. The state vectors $|e_i'\rangle_1$ equal the initial state vectors $|e_i\rangle_1$ if the measurement is a nondemolition (repeatable) one, and they differ otherwise. (Remember that we have complete measurement.) Anyway, according to Eqs. (13a)–(13d) [where now "1" is to be replaced by "(MA+1)"], the final tripartite state gives rise to the remote state decomposition $\rho_2=\Sigma_i p_i|\phi_i\rangle_2\langle\phi_i|_2$. After reading the results on the measuring apparatus, i.e., after so-called *objectivization*,[13] this decomposition becomes *actual* (in contrast to the infinitely many mathematically possible so-called "potential" decompositions).

Returning to Theorem 1, and the square Diagram 1, we can say that the latter displays an extended physical meaning (with respect to that in Sec. II B) of the correlated subsystem picture.

Definition 6: Pairs of opposite subsystem observables (A_1,A_2) satisfying $[A_s,Q_s]=0,s=1,2$, that are relevant (cf. Definition 5) and can be written either as A_1 and $A_2=\Sigma_i a_i'(U_a|e_i\rangle_1)_2(\langle e_i|_1U_a^\dagger)_2+Q_2^\perp A_2$ or as $A_1=\Sigma_i a_i(U_a^{-1}|f_i\rangle_2)_1(\langle f_i|_2U_a)_1+Q_1^\perp A_1$ and A_2 (depending on the choice of the nearby and the remote subsystems), which amount to the same, can be called *generalized twin observables*. If $[A_s,\rho_s]=0,s=1,2$, are *not valid*, then one is dealing with *extended twin observables*.

Diagram 1 displays the physical meaning of the correlated subsystem picture that includes the extended twin observables (in addition to the special case of twin observables).

Corollary 6: The relevant classes of nearby-subsystem observables give an *alternative classification* of all linearly independent complete decompositions of ρ_2. This can be extended to any density operator ρ, if it becomes ρ_2 by so-called purification, i.e., by constructing a bipartite state vector $|\Phi\rangle_{12}$ that implies the initial density operator as its second-subsystem reduced density operator.

One should note that, from the point of view of mathematical physics, this classification has an *advantage* over that of Cassinelli *et al.*[4] (cf. the Lemma above) consisting in the fact that the classifying entities and the details of the connection between them and the linearly independent complete decompositions has a clear physical meaning in terms of the antilinear operator representation of $|\Phi\rangle_{12}$, and its polar factorization (cf. Sec. II).

Remark 4: In Ref. 14, the approach of this section was indicated (without the antilinear operator representation) for finite-dimensional ranges. It was pointed out that this can lead to generating linearly independent complete decomposition of states even at spacelike separation.

V. THE SELECTIVE ASPECT OF REMOTE LINEARLY INDEPENDENT COMPLETE STATE DECOMPOSITION: REMOTE STATE PREPARATION

The selective or one-result subensemble aspect of complete subsystem measurement that gives remote linearly independent complete state decomposition was only implicitly given so far. Now we make it explicit. It is an immediate consequence of Theorem 1.

Theorem 2: Also the selective (or the one-result subensemble) aspect, i.e., the *remote preparations* of pure states that are part of a linearly independent complete state decomposition, can be displayed in a commutative square diagram as below. The symbols on Diagram 2 have the following meaning.

A is the set of all state vectors $|e_k\rangle_1$ from $\mathcal{R}(\rho_1^{1/2})$ (equivalently, the set of all corresponding atomic events or ray projectors $|e_k\rangle_1\langle e_k|_1$). **B** is the set of all state vectors $|f_n\rangle_2$ from $\mathcal{R}(\rho_2^{1/2})$. **C** is the set of all state vectors $|\chi_n\rangle_1$ from $\mathcal{R}(\rho_1)$. Finally, **D** is the set of all state vectors $|\phi_k\rangle_2$ from $\mathcal{R}(\rho_2)$.

The bijection $\mathbf{A}\rightarrow\mathbf{B}$ comes about by application of the antiunitary correlation operator U_a, which is determined by the given bipartite state vector $|\Phi\rangle_{12}$. The inverse bijection $\mathbf{B}\leftarrow\mathbf{A}$ is U_a^{-1}.

$\mathbf{A}\downarrow\mathbf{C}$ is $p_k^{-1/2}\rho_1^{1/2}$. The inverse is $\mathbf{C}\uparrow\mathbf{A}=p_k^{1/2}\tilde{\rho}_1^{-1/2}$, where the tilde denotes the reducee to the range. $\mathbf{B}\downarrow\mathbf{D}$ is $p_n^{-1/2}\rho_2^{1/2}$. The inverse is $\mathbf{D}\uparrow\mathbf{B}=p_n^{1/2}\tilde{\rho}_2^{-1/2}$. $\mathbf{C}\rightarrow\mathbf{D}$ is U_a. The inverse bijection $\mathbf{C}\leftarrow\mathbf{D}$ is U_a^{-1}.

The diagonal arrows, which have the physical meaning of remote state preparation, are the following. $\mathbf{A}\searrow\mathbf{D}$ is $p_k^{-1/2}\rho_2^{1/2}U_a$, or, equivalently, $p_k^{-1/2}A_a$. The inverse is $\mathbf{A}\nwarrow\mathbf{D}=p_k^{1/2}\tilde{\rho}_1^{-1/2}U_a^{-1}$.

$\mathbf{C}\swarrow\mathbf{B}$ is $p_n^{-1/2}\rho_1^{1/2}U_a^{-1}$, or, equivalently, $p_n^{-1/2}A_a^{\dagger}$. The inverse is $\mathbf{C}\nearrow\mathbf{B}=p_n^{1/2}\tilde{\rho}_2^{-1/2}U_a$.

Commutative Square Diagram 2.
Remote Pure-State Preparation.
(The Selective Aspect of
Remote Linearly Independent Complete State
Decompositions)

$\mathbf{A}\equiv\{\text{all state vectors } |e_k\rangle_1\in\mathcal{R}(\rho_1^{1/2})\}$ $\mathbf{B}\equiv\{\text{all state vectors } |f_n\rangle_2\in\mathcal{R}(\rho_2^{1/2})\}$

$$\begin{array}{ccc} \mathbf{A} & \longrightarrow & \longleftarrow \mathbf{B} \\ \downarrow\searrow\star & & \star\swarrow\downarrow \\ \uparrow\nearrow & & \nwarrow\uparrow \\ \mathbf{C} & \longrightarrow & \longleftarrow \mathbf{D} \end{array}$$

$\mathbf{C}\equiv\{\text{all state vectors } |\chi_n\rangle_1\in\mathcal{R}(\rho_1)\}$
$\mathbf{D}\equiv\{\text{all state vectors } |\phi_k\rangle_2\in\mathcal{R}(\rho_2)\}$

Each arrow goes from one of the sets (A,B,C,D) towards another. It stands for the corresponding bijection specified in Theorem 2. Oppositely oriented arrows denote mutually inverse bijections. The diagram is *commutative*, i.e., the successive bijections combine into the displayed corresponding one. For instance, taking the bijection $\mathbf{B}\downarrow\mathbf{D}$ after the bijection $\mathbf{A}\rightarrow\mathbf{B}$ gives the bijection $\mathbf{A}\searrow\mathbf{D}$, etc. The imaginary vertical line cutting the square into two equally wide halves makes these completely symmetric (due to the symmetry between the two subsystems in $|\Phi\rangle_{12}$).

$\star$ The downward diagonal bijections $\mathbf{A}\searrow\mathbf{D}$ and $\mathbf{C}\swarrow\mathbf{B}$ have the *physical meaning* of *remote state preparations*.

Theorem 2 completes previous work on remote preparation (or "steering," to use Schrödinger's term) begun by Schrödinger,[1] and continued in Ref. 15. To make the completion more precise, the following theorem clarifies the issue.

Theorem 3: (A) A state vector $|\phi\rangle_2$ is obtainable by remote preparation in $|\Phi\rangle_{12}$ if and only if $|\phi\rangle_2\in\mathcal{R}(\rho_2^{1/2})$.

(B) *The set of all* atomic events $|j\rangle_1\langle j|_1$ the occurrence of which in nearby-subsystem measurement in $|\Phi\rangle_{12}$ remotely prepares a given state vector $|\phi\rangle_2$ is (in terms of state vectors $|f\rangle_1$ and $|g\rangle_1$):

$$\{|j\rangle_1\langle j|_1 : |j\rangle_1=\alpha|f\rangle_1+\beta|g\rangle_1\}, \tag{49a}$$

where

$$|f\rangle_1\equiv U_a^{-1}\rho_2^{-1/2}|\phi\rangle_2, \tag{49b}$$

$$|\alpha|>0, \quad |\alpha|^2+|\beta|^2=1, \tag{49c}$$

and

$$|g\rangle_1=Q_1^{\perp}|g\rangle_1, \tag{49d}$$

(Q_1 being the range projector of ρ_1, and $Q_1^{\perp}$ being its orthocomplementary projector, i.e., the null projector), otherwise $|g\rangle_1$ is arbitrary.

(C) If the occurrence of the atomic event $|j\rangle_1\langle j|_1$ remotely prepares $|\phi\rangle_2$, then the *probability* of occurrence is *proportional* to $|\alpha|^2$ [cf. Eq. (49a)]. It is *maximal* if and only if $|j\rangle_1=|f\rangle_1$ [cf. Eq. (49b)].

(D) If $|\phi\rangle_2 \in \mathcal{R}(\rho_2)$ [cf. Eq. (32)], then $|f\rangle_1 \in \mathcal{R}(\rho_1^{1/2})$, where $|f\rangle_1$ is given by Eq. (49b). Thus, one has linearly independent remote preparation in this case, where the maximal probability is the *characteristic weight* of $|\phi\rangle_2$ (cf. Definition 3).

(E) If $|\phi\rangle_2 \in (\mathcal{R}(\rho_2^{1/2})-\mathcal{R}(\rho_2))$, where, "–" denotes set-theoretical subtraction (of a subset), then $|f\rangle_1 \in (\bar{\mathcal{R}}(\rho_1)-\mathcal{R}(\rho_1^{1/2}))$, where $|f\rangle_1$ is given by Eq. (49b).

If the ranges of ρ_s, $s=1,2$ are finite dimensional, then the largest probability is always the characteristic weight corresponding to linearly independent remote preparation [cf. Eq. (32)].

Proof of Theorem 3: (A) The most general case of remote pure-state preparation in a bipartite state vector $|\Phi\rangle_{12}$ is given by Eq. (13d). Replacing A_a by its polar-factorized form $\rho_2^{1/2}U_aQ_1$ [cf. Eq. (9b)], one can see that it is necessary that $|\phi\rangle_2 \in \mathcal{R}(\rho_2^{1/2})$. That this is also sufficient is obvious from the fact that $|\phi\rangle_2$ is obtained by remote preparation when the atomic event $|f\rangle_1\langle f|_1$ occurs, where $|f\rangle_1$ is given by Eq. (49b). [We again utilize the above polar-factorized form Eq. (9b) of A_a in Eq. (13d).]

(B) Since $|\phi\rangle_2=p^{-1/2}U_a\rho_1|j\rangle_1=p^{-1/2}U_a\rho_1Q_1|j\rangle_1$ [cf. Eqs. (13d) and (9a)], where p is the probability of occurrence, it is obvious that the occurrence of each of the atomic events $|j\rangle_1\langle j|_1$ [cf. Eqs. (49a)–(49d)] remotely prepares $|\phi\rangle_2$. On the other hand, Eq. (49a) with $|f\rangle_1 \in \bar{\mathcal{R}}(\rho_1)$ is the general form of a state vector from $\mathcal{H}_1$, and $A_a=U_a\rho_1^{1/2}$ [cf. (9a)] is nonsingular on $\bar{\mathcal{R}}(\rho_1)$, hence, it follows from Eq. (13d) that if $|j\rangle_1$is not in the set Eq. (49a), then the occurrence of $|j\rangle_1\langle j|_1$ remotely prepares a state vector $|\phi'\rangle_2$ that is distinct from $|\phi\rangle_2$.

(C) Substituting in Eq. (13c) A_aQ_1 instead of A_a and $|j\rangle_1$ by its form in Eq. (49a), one obtains

$$p=|\alpha|^2\|\rho_1^{1/2}|f\rangle_1\|^2, \tag{50}$$

which is independent of $|g\rangle_2$ [cf. Eq. (49a)]. Both claims in Theorem 3C are obvious from Eq. (50).

(D) and (E) The claims of Theorem 3D and 3E follow from the following set-theoretical insight. One has

$$\bar{\mathcal{R}}(\rho_1)=\mathcal{R}(\rho_1^{1/2})+(\bar{\mathcal{R}}(\rho_1)-\mathcal{R}(\rho_1^{1/2})), \tag{51}$$

and

$$\mathcal{R}(\rho_1^{1/2})=\mathcal{R}(\rho_1)+(\mathcal{R}(\rho_1^{1/2})-\mathcal{R}(\rho_1)), \tag{52}$$

where "+" denote the set-theoretical union of disjoint sets. The operator $\rho_1^{1/2}$ maps the first term on the rhs of Eq. (51) *into* the first term on the rhs of Eq. (52). This is seen from the fact that if $|j\rangle_1 \in \mathcal{R}(\rho_1^{1/2})$, then $\exists:|k\rangle_1,\langle k|_1|k\rangle_1>0,\rho_1^{1/2}|k\rangle_1=|j\rangle_1$. Then $\rho_1^{1/2}|j\rangle_1=\rho_1|k\rangle_1 \in \mathcal{R}(\rho_1)$.

Actually, $\rho_1^{1/2}$ maps $\mathcal{R}(\rho_1^{1/2})$ *onto* $\mathcal{R}(\rho_1)$. Namely, if $0\neq|k\rangle_1 \in \mathcal{R}(\rho_1)$, then $\exists:0\neq|j\rangle_1$ such that $|k\rangle_1=\rho_1|j\rangle_1=\rho_1^{1/2}(\rho_1^{1/2}|j\rangle_1)$.

Finally, since $\rho_1^{1/2}$ maps the lhs of Eq. (51) *onto* the lhs of Eq. (52) *in a nonsingular way*, one easily concludes that this operator maps the second term on the rhs of Eq. (51) onto the second term on the rhs of Eq. (52). □

VI. CONCLUDING REMARKS

There is a very basic and elementary general claim: Every statement valid for all bipartite state vectors $|\Phi\rangle_{12} \in (\mathcal{H}_1 \otimes \mathcal{H}_2)$ is either symmetric in the two subsystems, or if not, then also the statement symmetrical to it is always valid. This comes from the essential symmetry between $\mathcal{H}_1$ and $\mathcal{H}_2$ (in spite of the fact that one has to use the two factor spaces in an ordered way).

The results of this article confirm the claim that at the very core of entanglement in any $|\Phi\rangle_{12}$ is the *correlated subsystem picture* (see Sec. II). It consists of statements that appear in symmetrical pairs: the two reducees $\tilde{\rho}_1$ and $\tilde{\rho}_2$ are symmetric [cf. Eq. (10)] and so are the reducees of twin

observables $\tilde{A}_1$ and $\tilde{A}_2$ (if one takes algebraic twin observables, i.e., ones with equal relevant spectra). The symmetry is in terms of the *antiunitary correlation operator* U_a inherent in $|\Phi\rangle_{12}$, which establishes a sort of duality (like between kets and bras) between the closed ranges $\bar{\mathcal{R}}(\rho_1)$ and $\bar{\mathcal{R}}(\rho_2)$.

The correlation operator connects the orthogonal decompositions (or spectral forms) $\tilde{\rho}_1 = \Sigma_i r_i \widetilde{|i\rangle_1\langle i|_1}$, $\tilde{\rho}_2 = \Sigma_i r_i \widetilde{|i\rangle_2\langle i|_2}$, to which correspond the spectral forms of (physical) twin observables $\tilde{A}_1 = \Sigma_i a_i \widetilde{|i\rangle_1\langle i|_1}$ and $\tilde{A}_2 = \Sigma_i a_i' \widetilde{|i\rangle_2\langle i|_2}$. (One should remember that the tilde denotes that the corresponding operator is reduced to the range of $\rho_s, s=1,2$.)

In the wider view, when also extended twin observables are taken into account, or, equivalently, when one considers generalized twin observables, which has been elaborated in this article, one treats the wider class of linearly independent subsystem state decompositions $\rho_1 = \Sigma_n q_n |\chi_n\rangle_1\langle\chi_n|_1$ and $\rho_2 = \Sigma_k p_k |\phi_k\rangle_2\langle\phi_k|_2$ along with the relevant generalized twin observables A_1 and A_2 the measurement of either of which gives rise to the mentioned state decomposition on the *opposite* subsystem (remote linearly independent complete decomposition of state), but *not* to the decomposition on the same subsystem (except in the special case of proper twin observables). The full mathematical details and beauty of the generalized physical meaning of the correlated subsystem picture is expressed via the commutative diagrams.

If, following Schrödinger,[1] one tries to understand entanglement solely in terms of disentanglement, i.e., in terms of remote state decomposition, then one wonders what is left out from this article.

Restricting ourselves first to the (more important) complete state decompositions and pure-state preparation, the following is omitted.

If the bipartite state vector has infinite entanglement, i.e., if the dimension of the two ranges of the respective reduced density operators is infinite, then even among the observables for which the basic commutation $[A_s, Q_s]=0$, $s=1,2$, is valid (range-compatible observables), those for which the eigenbases of the reducees $\tilde{A}_s$, $s=1,2$ are not entirely within $\mathcal{R}(\rho_s^{1/2})$ $s=1,2$ are left out from remote linearly independent complete state decomposition. Further, equally for finite and for infinite entanglement, if at least one of the reduced density operators is singular, then the corresponding commutation $[A_s, Q_s]=0$, $s=1,2$ can be violated by some A_s, and the remote state decompositions caused by the measurement of such violating observables are also outside our treatment except in Theorem 3, which addresses the general case.

Considering only the nonselective aspect of remote influence, from the physical point of view it may not be clear why one should attach more importance to linearly independent remote complete state decomposition than to the rest mentioned above. The answer lies in the selective aspect, when one considers remote linearly independent pure-state preparation. Theorem 3C makes it clear that these are the nearby-subsystem occurrences that in measurement in $|\Phi\rangle_{12}$ have *the highest probability*. This fact singles them out in importance.

In Theorem 2 and Diagram 2 we have treated linearly independent remote pure-state preparation as part of linearly independent remote complete state decomposition. This is methodologically quite correct. But in view of the mentioned result in Theorem 3C, physically it is more satisfactory to reverse the roles of the nonselective and the selective aspects, and to consider the former as composed out of the latter. In other words, perhaps it is physically more correct to consider remote linearly independent complete state decomposition as consisting of remote linearly independent pure-state preparations. Then the physical importance of the latter is shared by the former.

One should point out that we have not considered incomplete remote linearly independent state decomposition or remote linearly independent mixed-or-pure state preparation. This is much used in practice as a step towards complete state decomposition (towards pure-state preparation).

We may repeat the remark from the Sec. I that in theoretical physics mathematics and physics are inextricably connected and the optimal form of the former, as a rule, gives physical insight, often in terms of new physical concepts. The correlated subsystem picture, by itself a mathematical concept, which has been further applied to disentanglement in this article, leads to insight into

the structure of pure-state entanglement in terms of generalized (proper and extended) twin observables. In particular, linearly independent remote pure-state preparation appears as the maximal-probability way of such a remote effect.

Finally, the largest-probability requirement in remote pure-state preparation leads to the conclusion (cf. Theorem 3C) that, from the physical point of view, in case of infinite-dimensional ranges of ρ_s, $s=1,2$, one should generalize "relevant" (for linearly independent influence) observables by the weaker requirement of only range-compatible and detectably complete ones (cf. Definition 5).

APPENDIX A

Proof that

$$\{|\phi_k\rangle \notin \mathrm{span}\{|\phi_1\rangle, \ldots, |\phi_{(k-1)}\rangle, |\phi_{(k+1)}\rangle, \ldots, |\phi_d\rangle\}, \quad k=1,2,\ldots d; d \in \mathbf{N}\}$$
$$\Leftrightarrow \{\forall k: |\phi_k\rangle \notin \mathrm{span}\{|\phi_1\rangle, \ldots, |\phi_{(k-1)}\rangle\}, \tag{A1.1}$$

where **N** is the set of all natural numbers.

The first requirement on the set $\{|\phi_i\rangle : i=1,\ldots,d\}$ obviously implies the second one. To prove the inverse implication, we assume *ab contrario* that the first requirement is not valid, but the second is. Then there exists $k \in \mathbf{N}$, $1 \leqslant k \leqslant d$ such that

$$|\phi_k\rangle = \sum_{i=1}^{(k-1)} \alpha_i |\phi_i\rangle + \sum_{j=(k+1)}^{d} \alpha_j |\phi_j\rangle, \tag{A1.2}$$

all α_i and all α_j complex numbers. On account of the assumed validity of the second requirement in Eq. (A1.1), not all α_j can be zero. We define $\bar{j} \equiv \max\{j : \alpha_j \neq 0\}$. Then Eq. (A1.2) implies

$$|\phi_{\bar{j}}\rangle = \alpha_{\bar{j}}^{-1}\left(|\phi_k\rangle - \sum_{i=1}^{(k-1)} \alpha_i |\phi_i\rangle - \sum_{j=(k+1)}^{(\bar{j}-1)} \alpha_j |\phi_j\rangle\right)$$

in contradiction to the assumed validity of the second requirement. □

APPENDIX B

Proof (of Corollary 1) that every finite subset $\{|\phi_1\rangle, \ldots, |\phi_k\rangle\}$ of a linearly independent set (finite or infinite) is a linearly independent basis in the k-dimensional subspace $\mathcal{S}_k$ that it spans. First we prove the claimed dimensionality of the span.

Total induction. We assume that the dimensionality claim is true for $(n-1)<k$: span $\{|\phi_1\rangle, \ldots, |\phi_{(n-1)}\rangle\} = \mathcal{S}_{(n-1)}$. Let $|\phi_n\rangle$ be linearly independent of the mentioned preceding state vectors. Let P project onto $\mathcal{S}_{(n-1)}$. One has

$$|\phi_n\rangle = P|\phi_n\rangle + P^{\perp}|\phi_n\rangle, \tag{A2.1}$$

where $P^{\perp} \equiv (1-P)$, and $P^{\perp}|\phi_n\rangle$ cannot be zero (cf. Definition 1). We define $|f_n\rangle \equiv cP^{\perp}|\phi_n\rangle$, where c is a normalization constant, and

$$\mathcal{S}_n \equiv \mathrm{span}\{\mathcal{S}_{(n-1)}, |f_n\rangle\} \tag{A2.2}$$

is a subspace of n dimensions. Since $|f_n\rangle = c(|\phi_n\rangle - P|\phi_n\rangle)$, $\mathcal{S}_n \subset \mathrm{span}\{|\phi_1\rangle, \ldots, |\phi_n\rangle\}$. It is obvious from Eq. (A2.1) that $|\phi_n\rangle \in \mathcal{S}_n$. Hence, $\mathrm{span}\{|\phi_1\rangle, \ldots, |\phi_n\rangle\} \subset \mathcal{S}_n$, and, finally, $S_n = \mathrm{span}\{|\phi_1\rangle, \ldots, |\phi_n\rangle\}$.

Since the claim that the span is a subspace of that many dimension as the number of linearly independent state vectors is true for $n=1$, total induction implies that it is true for any $n \leqslant k$.

The uniqueness of the expansion follows from Corollary 3 is one takes an arbitrary probability distribution $\{p_i : i=1,2,\ldots,k; p_i>0; \Sigma_{i=1}^k p_i = 1\}$ and one defines $\rho \equiv \Sigma_{i=1}^k p_i |\phi_i\rangle\langle\phi_i|$.

APPENDIX C

Proof of Corollary 3. We show that assuming Eq. (27), each element $|\chi\rangle$ from the range $\mathcal{R}(\rho^{1/2})$ can be expanded in the linearly independent sequence $\{|\phi_i\rangle : i=1,2,\ldots,d\leqslant\infty\}$.

Let

$$\tilde{\rho}^{-1/2}|\chi\rangle = \sum_i \beta_i |e_i\rangle. \tag{A3.1}$$

Applying the continuous operator $\rho^{1/2}$, one obtains (cf. Lemma B):

$$|\chi\rangle = \sum_i \beta_i \rho^{1/2}|e_i\rangle = \sum_i \beta_i p_i^{1/2}|\phi_i\rangle,$$

$$|\chi\rangle = \sum_i \alpha_i |\phi_i\rangle, \tag{A3.2}$$

where $\forall i$: $\alpha_i = \beta_i p_i^{1/2}$. On account of Eqs. (A3.1) and (28), one has

$$\forall i: \quad \alpha_i = p_i^{1/2}[(\langle e_i|\tilde{\rho}^{-1/2})|\chi\rangle].$$

Substituting $\langle e_i|$ from Eq. (30), the last relation enables us to rewrite Eqs. (A3.2) as follows:

$$|\chi\rangle = \sum_i p_i[(\langle\phi_i|\tilde{\rho}^{-1})|\chi\rangle]|\phi_i\rangle. \tag{A3.3}$$

Finally, the uniqueness of the expansion Eq. (A3.3) is easily proved by bringing the opposite assumption into contradiction with the definition of linear independence (cf. Definition 1). □

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Shape invariance through Crum transformation

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We show in a rigorous way that Crum's result regarding the equal eigenvalue spectrum of Sturm-Liouville problems can be obtained iteratively by successive Darboux transformations. Furthermore, it can be shown that all neighboring Darboux-transformed potentials of higher order, u_k and u_{k+1}, satisfy the condition of shape invariance provided the original potential u does so. Based on this result, we prove that under the condition of shape invariance, the nth iteration of the original Sturm-Liouville problem defined solely through the shape invariance is equal to the nth Crum transformation. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Supersymmetric quantum mechanics,[1,2] the factorization method,[3] the Darboux transformation,[4] Crum's generalization of the former results,[5] the isospectral Hamiltonians based on the Gelfand-Levitan equation[6–9] or the Marchenko equation,[10,11] and the shape invariance condition on the potentials[12] together with a transformation defined through this condition have been in the last two decade an active area of mathematical physics[13–18] and pure mathematics.[19–21] The main concern of these areas has been the construction of isospectral Schrödinger operators and the analytical solvability of the Sturm-Liouville problem. The field allowed a deeper insight into the eigenvalue problem and served as a source for many new ideas and generalizations.[22–25] Indeed, it is almost impossible to quote all research papers on the subject (suffices to note that one review[26] and several books have been devoted to the subject[27–31]). The applications range from constructing new solvable potentials in quantum mechanics, differential equations,[32] atomic physics,[33] nuclear physics,[34] classical mechanics,[35] acoustic spectral problems[36] to quantum gravitation,[37,38] and neutrino oscillation[39] to mention a few important areas.

Mathematically, not all these transformations mentioned above are equal, or at least this is not apparent at first sight. For instance, the usual Darboux transformation is not the most general solution of the Riccati equation and as such does not give us the most general transformation in connection with the isospectral eigenvalue spectrum. On the other hand, the generalization of the Darboux transformations, namely, the so-called Crum transformation appears to be much more complicated than the original Darboux result and as such seems to offer us new avenues to construct new potentials. The third transformation of a Hamiltonian which we have in mind [defined here in Eq. (90)] is closely related to the condition of shape invariance. Hence, without doubt, there is some need to at least classify these transformations according to the complexity or generality and to uncover their relations between them. One such result in this direction is the nonequivalence of the Abraham-Moses[7] and Darboux constructions shown in Ref. 9. Two remarks are in order here. Firstly, it is understood that unlike the Darboux transformation, any transforma-

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tion in connection with the shape invariance is, of course, limited to the set of shape invariant Hamiltonians. Secondly, for completeness it is worth noting that the level of complexity of isospectral quantum systems can be increased by considering nonlinear and higher order supersymmetric transformations.[40–43] These are transformations which cannot be reached by iterative Darboux transformations. In this work, however, we will not consider these kinds of transformations and restrict ourselves to the Darboux case. After some preparatory statements we will show that the undertaking to uncover relationships between the transformations gives a simple result, namely, allowing the use of higher order Darboux transformations, we can state that all three transforms of the original Sturm-Liouville problem are equal. This result is based on a theorem which we prove in the present paper concerning higher order Darboux transformations of shape invariant potentials denoted by $u^D[k]$. The theorem states that provided the original potential satisfies the shape invariance conditions, all pairs $u^D[k]$, $u^D[k+1]$ are also mutually shape invariant. The theorem can be proved by induction. Interestingly, it intertwines this induction with another statement, this time for the wave functions. We illustrate the theorems by two examples.

II. CRUM'S RESULT

In this section, we briefly present Crum's result and comment on one identity on which Crum's result is partly based. This identity is crucial for the subsequent results which we will elaborate upon in the next section.

Let

$$W_k \equiv W(\psi_1, \psi_2, \ldots, \psi_k) = \det A, \quad A_{ij} = \frac{d^{i-1}\psi_j}{dx^{i-1}}, \quad i,j = 1,2, \ldots, k \tag{1}$$

be the Wronskian determinant of the functions $\psi_1, \psi_2, \ldots, \psi_k$, and

$$W_{k,s} = W(\psi_1, \psi_2, \ldots, \psi_k, \psi_s). \tag{2}$$

Theorem 2.1 (Crum): *If $\psi_1, \psi_2, \ldots, \psi_n$ are the solutions of the regular Sturm-Liouville problem*

$$-\frac{\mathrm{d}^2\psi_s}{\mathrm{d}x^2} + u\psi_s = \lambda_s\psi_s, \tag{3}$$

then $\psi^C[n]_s$ satisfies the Sturm-Liouville equation,

$$-\frac{\mathrm{d}^2\psi^C[n]_s}{\mathrm{d}x^2} + u^C[n]\psi^C[n]_s = \lambda_s\psi^C[n]_s, \tag{4}$$

with $\psi^C[n]_s$ and $u^C[n]_s$ given by

$$\psi_s \to \psi^C[n]_s \equiv \frac{W_{n,s}}{W_n} \tag{5}$$

and

$$u \to u^C[n] = u - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln W_n. \tag{6}$$

Note that the Crum transforms of ψ and u are not defined iteratively. By $[C]$ we wish to distinguish the Crum transformation from other transforms (like Darboux) which will be defined later in the text. The proof of Crum's theorem can be found in Refs. 5 and 29. We comment here only on one cornerstone of the original proof given by Crum[5] which we will also use later. The first step in the proof of Crum's result on the Wronskian determinant is to consider the derivative of W_k. Taking the derivative of

$$W_2 = \begin{vmatrix} \psi_1 & \psi_2 \\ \mathrm{d}\psi_1/\mathrm{d}x & \mathrm{d}\psi_2/\mathrm{d}x \end{vmatrix}, \tag{7}$$

we find the rather obvious result,

$$\frac{\mathrm{d}W_2}{\mathrm{d}x} = \begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1'' & \psi_2'' \end{vmatrix}, \tag{8}$$

where we used the notation ψ_i'' for $\mathrm{d}^2\psi_i/\mathrm{d}x^2$, $i=1,2$. This result can be readily generalized for the $n\times n$ case.

Lemma 2.2: *For the derivative of a Wronskian determinant we have*

$$W_n' = \{\psi_1^{(n)} M_{(1,n)}^{(1)} + \psi_2^{(n)} M_{(2,n)}^{(1)} + \cdots + \psi_{n-1}^{(n)} M_{(n-1,n)}^{(1)} + \psi_n^{(n)} M_{(n,n)}^{(1)}\}. \tag{9}$$

Assume the result to be valid for $n-1$. Using the Laplace expansion according to the last line of the Wronskian W_n we get

$$\begin{aligned} W_n' = {} & \{\psi_1^{(n)} M_{(1,n)}^{(1)} + \psi_2^{(n)} M_{(2,n)}^{(1)} + \cdots + \psi_{n-1}^{(n)} M_{(n-1,n)}^{(1)} + \psi_n^{(n)} M_{(n,n)}^{(1)}\} \\ & + \{\psi_1^{(n-1)} (M_{(1,n)}^{(1)})' + \cdots + \psi_{n-1}^{(n-1)} (M_{(n-1,n)}^{(1)})' + \psi_n^{(n-1)} (M_{(n,n)}^{(1)})'\}, \end{aligned} \tag{10}$$

where every $(n-1)\times(n-1)$ determinant $M_{(i,n)}^{(1)}$ is a Wronskian for which, by assumption, the theorem is valid. Hence

$$\det B \equiv \{\psi_1^{(n-1)} (M_{(1,n)}^{(1)})' + \cdots + \psi_{n-1}^{(n-1)} (M_{(n-1,n)}^{(1)})' + \psi_n^{(n-1)} (M_{(n,n)}^{(1)})'\} \tag{11}$$

is a determinant whose two last lines are equal and therefore $\det B=0$. The result [Eq. (10)] can be written as

$$W_n' = \begin{vmatrix} \psi_1 & \psi_2 & \cdots & \psi_{n-1} & \psi_n \\ \psi_1' & \psi_2' & \cdots & \psi_{n-1}' & \psi_n' \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ \psi_1^{(n-2)} & \psi_2^{(n-2)} & \cdots & \psi_{n-1}^{(n-2)} & \psi_n^{(n-2)} \\ \psi_1^{(n)} & \psi_2^{(n)} & \cdots & \psi_{n-1}^{(n)} & \psi_n^{(n)} \end{vmatrix}. \tag{12}$$

We can now state a result which will be of some importance later and which is one of the important ingredients in proving Theorem 2.1 of Crum.

Lemma 2.3 (Crum): *The Wronski determinant of the two Wronskians*, W_n and $W_{n-1,s}$, *is equal to* $W_{n,s}W_{n-1}$. *In other words*

$$W(W_n, W_{n-1,s}) = W_{ns} W_{n-1}. \tag{13}$$

The proof relies on the Jacobi theorem for determinants (see the Appendix). We refer the reader to the Appendix for the proof of this Lemma too.

It is well known that for $n=1$ the Crum transformations reduce to the Darboux transformation when $W_1=\psi_1$ and $W_{1,s}=W(\psi_1,\psi_s)$. Specifically, we have

$$\psi^D[1]_s \equiv \psi^C[1]_s = \frac{W_{1,s}}{\psi_1} = \psi_s' - \frac{\psi_1'}{\psi_1}\psi_s, \quad s>1, \tag{14}$$

$$u^D[1] \equiv u^C[1] = u - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2} \ln W_1 = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi_1'}{\psi_1}. \tag{15}$$

We can define higher order Darboux transformations iteratively by

$$u^D[k-1] \to u^D[k] = u[k-1] - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[k-1]_k)'}{\psi^D[k-1]_k},$$
$$\psi^D[k-1]_s \to \psi^D[k]_s = \frac{W(\psi^D[k-1]_k, \psi^D[k-1]_s)}{\psi^D[k-1]_k}, \qquad s > k. \tag{16}$$

Obviously, the last equation can be written also in a way which resembles more the first Darboux transformation, i.e.,

$$\psi^D[k]_s = (\psi^D[k-1]_s)' - \frac{(\psi^D[k-1]_k)'}{\psi^D[k-1]_k}\psi^D[k-1]_s. \tag{17}$$

It is *a priori* not clear as to what connection the kth Darboux transformation has with the kth Crum transformation and if they can be related at all, except for the definition at the lowest order of Crum's transformation. The answer is provided in the next section.

III. THE CONNECTION BETWEEN HIGHER ORDER DARBOUX AND CRUM TRANSFORMATION

To this end, let us first examine the simplest case of $k=2$,

$$u^D[2] = u^D[1] - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[1]_2)'}{\psi^D[1]_2}. \tag{18}$$

Since $u[D]_{[1]}$ is the Darboux transformed potential the above equation reads

$$u^D[2] = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi_1'}{\psi_1} + \frac{(\psi^D[1]_2)'}{\psi^D[1]_2}\right). \tag{19}$$

According to Eq. (19), $\psi^D[1]_2 = W_{1,2}/\psi_1$ and on account of the simple identity $W_{n,n+1} = W_{n+1}$, we can write

$$u^D[2] = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi_1'}{\psi_1} + \frac{(W_2/\psi_1)'}{W_2/\psi_1}\right), \tag{20}$$

which finally gives

$$u^D[2] = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{W_2'}{W_2}\right) = u^C[2]. \tag{21}$$

Similarly, the eigenfunctions

$$\psi^D[2]_s = \frac{\begin{vmatrix} \psi^D[1]_2 & \psi^D[1]_s \\ (\mathrm{d}/\mathrm{d}x)\psi^D[1]_2 & (\mathrm{d}/\mathrm{d}x)\psi^D[1]_s \end{vmatrix}}{\psi^D[1]_2} \tag{22}$$

can be cast into the form

$$\psi^D[2]_s = \frac{1/\psi_1 \begin{vmatrix} W_2 & W_{1,s} \\ (W_2/\psi_1)' & (W_{1,s}/\psi_1)' \end{vmatrix}}{\frac{W_2}{\psi_1}} = \frac{\begin{vmatrix} W_2 & W_{1,s} \\ (W_2/\psi_1)' & (W_{1,s}/\psi_1)' \end{vmatrix}}{W_2}. \tag{23}$$

With the help of the standard property of determinants, namely, $\det(\mathbf{z}_1, \ldots, \mathbf{z}_i, \ldots, \mathbf{z}_n) = \det(\mathbf{z}_1, \ldots, \mathbf{z}_i + \alpha\mathbf{z}_k, \ldots, \mathbf{z}_n)$ the last equation reduces to

$$\psi^D[2]_s = \frac{1/\psi_1 \begin{vmatrix} W_2 & W_{1,s} \\ W_2' & W_{1,s}' \end{vmatrix}}{W_2}. \tag{24}$$

Applying the result of Lemma 2.3 and remembering that $W_1 = \psi_1$, one finally finds

$$\psi^D[2]_s = \frac{W_{2,s}}{W_2} = \psi^C[2]_s. \tag{25}$$

The steps above will serve as a beginning of the induction proof of the following general statement,

Theorem 3.1: *The n*th *Crum transformation is equivalent to the n*th *higher order Darboux transformation. This is to say, any Crum transformation can be reached iteratively by successive Darboux transformations, i.e.*,

$$\begin{aligned} u^C[n] &= u^D[n], \\ \psi^C[n]_s &= \psi^D[n]_s. \end{aligned} \tag{26}$$

Proof: Assuming the theorem to be valid for n means that the statement

$$\begin{aligned} u^D[n] &= u^D[n-1] - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[n-1]_n)'}{\psi^D[n-1]_n}, \\ \psi^D[n]_s &= \frac{W(\psi^D[n-1]_n, \psi^D[n-1]_s)}{\psi^D[n-1]_n}, \end{aligned} \qquad s > n \tag{27}$$

is equivalent to

$$\begin{aligned} u^D[n] &= u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{W_n'}{W_n}\right), \\ \psi^D[n]_s &= \frac{W_{n,s}}{W_n}. \end{aligned} \qquad s > n. \tag{28}$$

Based on that, we have to show

$$u^C[n+1] = u^D[n+1] = u^D[n] - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[n]_{n+1})'}{\psi^D[n]_{n+1}} = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{W_{n+1}'}{W_{n+1}} \tag{29}$$

and

$$\psi^D[n+1]_s = \frac{W(\psi^D[n]_{n+1}, \psi^D[n]_s)}{\psi^D[n]_{n+1}} = \frac{W_{n+1,s}}{W_{n+1}}. \tag{30}$$

The validity of the hypothesis of the induction for n allows us to write

$$u^D[n+1] = u^D[n] - 2\frac{d}{dx}\frac{(\psi^D[n]_{n+1})'}{\psi^D[n]_{n+1}} = u - 2\frac{d}{dx}\left(\frac{W_n'}{W_n} + \frac{(\psi^D[n]_{n+1})'}{\psi^D[n]_{n+1}}\right). \tag{31}$$

Using the validity of the hypothesis for n, but this time for the wave functions, implies

$$u^D[n+1] = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{W_n'}{W_n} + \frac{\left(\frac{W_{n+1}}{W_n}\right)'}{\frac{W_{n+1}}{W_n}}\right) = u - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{W_{n+1}'}{W_{n+1}}\right) = u^C[n+1]. \tag{32}$$

Similarly, the result for the eigenfunctions may be written as

$$\psi^D[n+1]_s = \frac{\begin{vmatrix} \psi^D[n]_{n+1} & \psi^D[n]_s \\ \psi'^D[n]_{n+1} & \psi'^D[n]_s \end{vmatrix}}{\psi^D[n]_{n+1}} = \frac{\begin{vmatrix} W_{n+1}/W_n & W_{n,s}/W_n \\ (W_{n+1}/W_n)' & (W_{n,s}/W_n)' \end{vmatrix}}{W_{n+1}/W_n}. \tag{33}$$

One easily proceeds now to verify the validity of the following equation:

$$\psi^D[n+1]_s = \frac{\begin{vmatrix} W_{n+1} & W_{n,s} \\ W_{n+1}'/W_n - W_n'W_{n+1}/W_n^2 & W_{n,s}'/W_n - W_n'W_{n,s}/W_n^2 \end{vmatrix}}{W_{n+1}} = \frac{1/W_n \begin{vmatrix} W_{n+1} & W_{n,s} \\ W_{n+1}' & W_{n,s}' \end{vmatrix}}{W_{n+1}}. \tag{34}$$

By virtue of Lemma 2.3 we can assure that

$$\psi^D[n+1]_s = \frac{W_{n+1,s}}{W_{n+1}} = \psi^C[n+1]_s \tag{35}$$

is true which completes the proof.

It is instructive to follow this theorem by an explicit example.

IV. TWO EXAMPLES

In this section we will demonstrate the above theorems by two examples. We choose first a potential which satisfies the condition of shape invariance (Morse potential) followed by the example of Ginnochio potential, which falls into the class of nonshape invariant, but solvable potentials.

Let us consider, as an example, the Sturm Liouville problem with the Morse potential, i.e.,

$$u(x;A) = 2\left[A^2 - A\left(A + \frac{\alpha}{\sqrt{2}}\right)\mathrm{sech}^2(\alpha x)\right]. \tag{36}$$

The superpartner of this potential corresponding to ψ_1 and λ_1 is

$$u^C[1] = u^D[1] = 2[A^2 - AA_1\,\mathrm{sech}^2(\alpha x)], \tag{37}$$

and the first three eigenfunctions are given by the following:

$$1.\ \ \psi_1 = c_1[\mathrm{sech}(\alpha x)]^{\sqrt{2}A/\alpha}.$$

$$2.\ \ \psi_2 = c_2\sinh(\alpha x)\psi_1.$$

$$3.\ \ \psi_3 = c_3\left(-\cosh^2(\alpha x) + \frac{(2\sqrt{2}A - \alpha)}{\alpha}\sinh^2(\alpha x)\right)\psi_1.$$

In the following we will not determine the constants c_i as they are of minor importance for our results. Secondly, the results become increasingly complicated. For instance, to calculate c_1 we can use

$$\int_0^\infty \operatorname{sech}(ax)^{2\sqrt{2}A/\alpha}\mathrm{d}x = -\frac{1}{\sqrt{2}A}{}_2F_1\left(\frac{\sqrt{2}A}{\alpha},\frac{1}{2},1+\frac{\sqrt{2}A}{\alpha},\frac{\alpha}{\sqrt{2}A}\right), \tag{38}$$

where ${}_2F_1$ is the hypergeometric function. The corresponding eigenvalues can be compactly written as

$$\lambda_n = 2\left(A^2 - \left(A - \frac{(n-1)\alpha}{\sqrt{2}}\right)^2\right). \tag{39}$$

It is convenient to define A_n as

$$A_n \equiv A - \frac{n\alpha}{\sqrt{2}}, \tag{40}$$

such that the eigenvalues read now

$$\lambda_n = 2(A^2 - A_{n-1}^2), \quad n = 1,2,3,\ldots. \tag{41}$$

The first three are explicitly given as follows:

$$\lambda_1 = 0, \quad \lambda_2 = 2\sqrt{2}A\alpha - \alpha^2, \quad \lambda_3 = 4\sqrt{2}A\alpha - 4\alpha^2. \tag{42}$$

Besides Eq. (37) we will also need the following results:

$$\psi^C[1]_2 = \psi^D[1]_2 = c_2\alpha\cosh(\alpha x)\psi_1, \tag{43}$$

$$\psi^C[1]_3 = \psi^D[1]_3 = 4\sqrt{2}c_3A_1\sinh(\alpha x)\cosh(\alpha x)\psi_1. \tag{44}$$

To show explicitly the equality $u^C[2]=u^D[2]$, we start with $u^C[2]$, i.e.,

$$u^C[2] = u - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln W_2. \tag{45}$$

Since $W_{1,2}=W_2$ and using

$$\frac{W_{1,2}}{W_1} = c_2\alpha\cosh(\alpha x)\psi_1, \tag{46}$$

we have,

$$\ln W_2 = \ln c_2\alpha + \ln\cosh(\alpha x) + 2\ln\psi_1, \tag{47}$$

but also

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln W_2 = \alpha(\alpha - 2\sqrt{2}A)\operatorname{sech}^2(\alpha x). \tag{48}$$

Finally, with Eq. (36) we arrive at

$$u^C[2] = 2[A^2 - A_1A_2\operatorname{sech}^2(\alpha x)]. \tag{49}$$

Next we turn to the expression for $u^D[2]$, namely,

$$u^D[2] = u^D[1] - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[1]_2)'}{\psi^D[1]_2}. \tag{50}$$

Taking into account Eq. (43) we obtain

$$\frac{(\psi^D[1]_2)'}{\psi^D[1]_2} = -\sqrt{2}A_1 \tanh(\alpha x), \tag{51}$$

and therefore

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{(\psi^D[1]_2)'}{\psi^D[1]_2} = -\sqrt{2}\alpha A_1 \operatorname{sech}^2(\alpha x). \tag{52}$$

From this we conclude [see Eq. (50)] that

$$u^D[2] = 2[A^2 - A_1 A_2 \operatorname{sech}^2(\alpha x)], \tag{53}$$

and hence

$$u^C[2] = u^D[2]. \tag{54}$$

The transformed potentials here have almost identical functional form. This is, of course, due to the choice of the potential and need not be so in other cases.

To demonstrate that $\psi^C[2]_s = \psi^D[2]_s$, we calculate $\psi^C[2]_3$ to be

$$\psi^C[2]_3 = \frac{W_3}{W_2} = \frac{\begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1' & \psi_2' & \psi_3' \\ -\lambda_1\psi_1 & -\lambda_2\psi_2 & -\lambda_3\psi_3 \end{vmatrix}}{\begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix}} = \lambda_2\psi_2\frac{W_{1,3}}{W_2} - \lambda_3\psi_3. \tag{55}$$

Making use of

$$\lambda_2\psi_2\frac{W_{1,3}}{W_2} = \left(\frac{4\sqrt{2}\lambda_2 c_3 A_1}{\alpha}\right)\sinh^2(\alpha x)\psi_1, \tag{56}$$

this becomes

$$\psi^C[2]_3 = \lambda_3 c_3 \cosh^2(\alpha x)\psi_1(x). \tag{57}$$

On the other hand

$$\psi^D[2]_3 = \frac{\begin{vmatrix} \psi[1]_2 & \psi[1]_3 \\ (\psi[1]_2)' & (\psi[1]_3)' \end{vmatrix}}{\psi[1]_2} = \frac{(\psi[1]_3/\psi[1]_2)'(\psi[1]_2)^2}{\psi[1]_2} = \left(\frac{\psi[1]_3}{\psi[1]_2}\right)'\psi[1]_2 = \lambda_3 c_3 \cosh^2(\alpha x)\psi_1, \tag{58}$$

where on the right hand side we already dropped the distinction between D and C [see Eqs. (43) and (44)]. The simple conclusion that we can draw is

$$\psi^C[2]_3 = \psi^D[2]_3. \tag{59}$$

It is instructive to consider also a case of a solvable, but nonshape invariant potential. Many such cases are known (see Refs. 44–46 and the discussion in Ref. 26) and explicit proofs that these potentials fail to satisfy the shape invariance condition were given. For instance, for the case of the Natanzon potential this was shown in Ref. 47. Many of these potentials are complicated and some, like the Natanzon case, only known in implicit form. Therefore, for the sake of efficient

calculations, it is recommendable to develop first a fast algorithm to perform the desired calculations. We will do exactly that before giving the explicit example of the Ginocchio case. Imagine we would like to calculate $\psi^D[2]_3$. In turns out that the calculation can be greatly simplified by invoking the ratios $h_n=\psi_n'/\psi_n$, where ψ_n is, as usual, the eigenfunction to the ϵ_n eigenvalue. It is now a straightforward exercise to show that

$$\psi^D[2]_3=\frac{\begin{vmatrix}\psi^D[1]_2 & \psi^D[1]_3\\ (\psi^D[1]_2)' & (\psi^D[1])_3)'\end{vmatrix}}{(\psi^D[1]_2)} \tag{60}$$

is equal to

$$\frac{1}{(h_1-h_0)\psi_1}[(h_1-h_0)\{(h_2-h_0)'+(h_2-h_0)h_2\}\psi_1\psi_2-(h_2-h_0)\{(h_1-h_0)'+(h_1-h_0)h_1\}\psi_1\psi_2]. \tag{61}$$

Using the Schrödinger equation the latter simplifies to

$$\psi^D[2]_3=\frac{[\epsilon_0\{h_2-h_1\}-\epsilon_1\{h_2-h_0\}+\epsilon_2\{h_1-h_0\}]}{(h_1-h_0)}\psi_2. \tag{62}$$

It is obvious that, provided we know the functions h_0, h_1, h_2, and ψ_2, this expression allows a fast calculation or the wave function $\psi^D[2]_3$ for arbitrary potential. Crum's result gives

$$\psi^C[2]_3=\frac{W_{2,3}}{W_2}=\frac{W_3}{W_2}=\frac{W_3}{(h_1-h_0)\psi_0\psi_1}, \tag{63}$$

where W_3 is

$$\begin{aligned}W_3&=\begin{vmatrix}\psi_0 & \psi_1 & \psi_2\\ \psi_0' & \psi_1' & \psi_2'\\ \psi_0'' & \psi_1'' & \psi_2''\end{vmatrix}=\begin{vmatrix}\psi_0 & \psi_1 & \psi_2\\ h_0\psi_0 & h_1\psi_1 & h_2\psi_2\\ \psi_0'' & \psi_1'' & \psi_2''\end{vmatrix}\\ &=\begin{vmatrix}\psi_0 & \psi_1 & \psi_2\\ h_0\psi_0 & h_1\psi_1 & h_2\psi_2\\ u-\epsilon_0\psi_0 & u-\epsilon_1\psi_1 & u-\epsilon_1\psi_2\end{vmatrix}=-\begin{vmatrix}\psi_0 & \psi_1 & \psi_2\\ h_0\psi_0 & h_1\psi_1 & h_2\psi_2\\ \epsilon_0\psi_0 & \epsilon_1\psi_1 & \epsilon_2\psi_2\end{vmatrix}.\end{aligned} \tag{64}$$

Hence, taking Eq. (63) into account, we can show that

$$\psi^C[2]_3=\frac{[\epsilon_0\{h_2-h_1\}-\epsilon_1\{h_2-h_0\}+\epsilon_2\{h_1-h_0\}]\psi_0\psi_1\psi_2}{(h_1-h_0)\psi_1\psi_0}, \tag{65}$$

which obviously implies that $\psi^D[2]_3=\psi^C[2]_3$. This, as it stands, is a general proof for a subcase of our general theorem. On purpose above we have used different steps than in the proof of our general theorem. The idea behind it is to demonstrate that in an explicit example we would be only repeating the very same steps as above. It is therefore sufficient to calculate every time only the right hand side of Eq. (65). The equality $\psi^D[2]_3=\psi^C[2]_3$ is guaranteed by Eqs. (62) and (65). We can now apply the results for $\psi^D[2]_3$ by choosing the Ginocchio potential,

$$V(x)=\left\{-\beta^2\upsilon(\upsilon+1)+\frac{1}{4}(1-\beta^2)[5(1-\beta^2)y^4-(7-\beta^2)y^2+2]\right\}(1-y^2), \tag{66}$$

where $y(x)$ satisfies the following differential equation:

$$\frac{dy}{dx} = (1-y^2)[1-(1-\beta^2)y^2], \tag{67}$$

and β and υ are parameters.

The wave functions of this problem are known to be expressible through Gegenbauer polynomials $C_n^{(a)}(x)$, namely,

$$\psi_n = (1-\beta^2)^{\mu_n/2}[g(y)]^{-(2\mu_n+1)/4} C_n^{(\mu_n+1/2)}(f(y)), \tag{68}$$

where

$$g(y) = 1-(1-\beta^2)y^2, \quad f(y) = \frac{\beta y}{\sqrt{g(y)}}. \tag{69}$$

The value of μ_n is connected to the eigenvalue ϵ_n by $\epsilon_n = -\mu_n^2\beta^4$ such that

$$\mu_n\beta^2 = \sqrt{\beta^2(\upsilon+1/2)^2 + (1-\beta^2)(n+1/2)^2} - (n+1/2). \tag{70}$$

The first four Gegenbauer polynomials are given as follows:

$$\begin{gathered} C_0^{(\mu_0+1/2)}(f(y)) = 1, \\ C_1^{(\mu_1+1/2)}(f(y)) = 2(\mu_1+1/2)[f(y)], \\ C_2^{(\mu_2+1/2)}(f(y)) = 2(\mu_2+1/2)(\mu_2+3/2)[f(y)]^2 - (\mu_2+1/2), \\ C_3^{(\mu_3+1/2)}(f(y)) = \frac{4}{3}(\mu_3+1/2)(\mu_3+3/2)(\mu_3+5/2)[f(y)]^3 - 2(\mu_3+1/2)(\mu_3+3/2)[f(y)]. \end{gathered} \tag{71}$$

These functions can be used, in the next step, to compute explicitly the ratios $h_i = \psi_i'/\psi_i$. We obtain

$$\begin{gathered} h_0 = \frac{\psi_0'}{\psi_0} = \frac{[g(y)]'}{g(y)} = -2(1-\beta^2)y(1-y^2), \\ h_1 = \frac{\psi_1'}{\psi_1} = \frac{[g(y)]'}{[g(y)]} + \frac{[f(y)]'}{[f(y)]} = \frac{(1-y^2)}{y}\{1-2(1-\beta^2)y^2\}, \\ h_2 = \frac{\psi_2'}{\psi_2} = \left(\frac{[g(y)]'}{[g(y)]} + \frac{2[f(y)][f(y)]'}{([f(y)]^2 - [1/(2\mu_2+3)])}\right), \end{gathered} \tag{72}$$

where we have used

$$\frac{[f(y)]'}{[f(y)]} = \frac{1}{y}(1-y^2). \tag{73}$$

Noting that the h_i are proportional $(1-y^2)$ and that $h_1 - h_0 = (1-y^2)/y$, we can insert our results into Eq. (65) to obtain

$$\begin{aligned} \psi^C[2]_3 = {} & (1-\beta^2)^{\mu_2/2}(\mu_2+1/2)(2\mu_2+3)[g(y)]^{-(2\mu_2+1)/4} \\ & \times\left\{(\epsilon_2-\epsilon_0)\left([f(y)]^2 - \frac{1}{(2\mu_2+3)}\right) - (\epsilon_1-\epsilon_0)2[f(y)]^2\right\}. \end{aligned} \tag{74}$$

Turning our attention to the potential the superpartner of V in Eq. (66) it is not difficult to see that the superpartner is given by

$$V^D[1] = V^C[1] = V - 2\frac{d^2}{dx^2} \ln W_1$$

$$= V - 2\frac{d}{dr}\frac{[g(y)]'}{g(y)} = V + 4(1-\beta^2)(1-3y^2)^2(1-y^2)[1-(1-\beta^2)y^2]. \tag{75}$$

The second Crum iteration yields

$$V^C[2] = V - 2\frac{d^2}{dx^2} \ln W_2 = V - 2[\{-2 + (1-\beta^2)[5y^2-3]\} + 10y^2(1-\beta^2)](1-y^2)[1-(1-\beta^2)y^2]. \tag{76}$$

To proof that this is equivalent to the second Darboux transformations it is convenient, as was the case with the wave functions, to provide first a general proof for this subcase. Starting with the definition, it is straightforward to show that

$$\psi^D[1]_2 = (h_1 - h_0)\psi_1, \tag{77}$$

which leads to

$$V^D[2] = V^D[1] - 2\frac{d}{dr}\frac{(\psi^D[1]_2)'}{\psi^D[1]_2} = V - 2\frac{d^2}{dr^2} \ln \psi_0 - 2\frac{d^2}{dr^2} \ln(h_1 - h_0)\psi_1$$

$$= V - 2\frac{d^2}{dr^2}\{\ln(h_1 - h_0)\psi_0\psi_1\} = V - 2\frac{d^2}{dr^2} \ln W_2 = V^C[2]. \tag{78}$$

In taking explicit examples we would be only repeating the very same steps as above. This demonstration concludes our two examples.

V. THE CONNECTION BETWEEN SHAPE INVARIANCE AND CRUM TRANSFORMATIONS

In view of the results of the previous section we can now drop the distinction between higher order Darboux (D) and Crum (C) transformations.

Let a denote a set of parameters in the original potential, i.e.,

$$u = u(x;a). \tag{79}$$

The condition for shape invariance of u is given by

$$u[1](x;a) = u(x;f(a)) + R(f(a)), \tag{80}$$

where $u[1](x;a)$ is the first Darboux transform of the original potential, f transforms a into another set $f(a)$, and $R(f(a))$ is a function of the parameters. In the following, we use the usual notation $a_m \equiv f^m(a)$, where m indicates the function f applied m times.

In the preceding section we established an equivalence between higher order Darboux transformation and the Crum result. Since the shape invariance is given in terms of the first order Darboux transformation, it is legitimate to ask if higher order Darboux transformations (Crum transformations) play a role in the Schrödinger equation with shape invariant potentials. As a first step we will prove the following theorem.

Lemma 5.1: *Under the condition of shape invariance one has*

$$\psi_s(x;a_1) = \psi[1]_{s+1}(x;a), \tag{81}$$

up to a multiplicative constant and

$$\lambda_s(a_1) + R(a_1) = \lambda_{s+1}(a). \tag{82}$$

In the above $\psi_s(x;a)$ denotes the eigenfunction to the Hamiltonian with the potential $u(x;a)$ with the eigenvalue λ_s.

These results are not new. But since we will make use of them, we offer here a short proof. We start with initial Sturm-Liouville problem,

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+u(x;a)\right)\psi_s(x;a)=\lambda_s(a)\psi_s(x;a) \tag{83}$$

and

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+u[1](x;a)\right)\psi[1]_s(x;a)=\lambda_s(a)\psi[1]_s(x;a),\quad s>1. \tag{84}$$

Equation (83) is valid for any a, hence we may write

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+u(x;a_1)\right)\psi_s(x;a_1)=\lambda_s(a_1)\psi_s(x;a_1), \tag{85}$$

and add $R(f(a))\psi_s(x;f(a))$ on both sides implying the following identity:

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+u(x;a_1)+R(a_1)\right)\psi_s(x;a_1)=(\lambda_s(a_1)+R(a_1))\psi_s(x;a_1). \tag{86}$$

Due to the shape invariance condition (for the sake of formulating the next Lemma we can say that $u[1]$ and u are pairwise shape invariant) this becomes

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+u[1](x;a)\right)\psi_s(x;a_1)=(\lambda_s(a_1)+R(a_1))\psi_s(x;a_1). \tag{87}$$

Without loss of generality, the spectrum can be ordered as $\lambda_1<\lambda_2<\lambda_3<\cdots$. Hence, $\{\lambda_s(a)\}$, $\{\lambda_s(a_1)\}$, and $\{\lambda_s(a_1)+R(a_1)\}$ are similarly ordered sets. $\psi[1]_{s+1}$ is then an eigenfunction to the ordered spectrum $\lambda_2<\lambda_3<\cdots$. We can conclude that up to a multiplicative factor

$$\psi_s(x;a_1)=\psi[1]_{s+1}(x,a) \tag{88}$$

and

$$\lambda_s(a_1)+R(a_1)=\lambda_{s+1}(a). \tag{89}$$

In preparation of the main theorem of this section we prove the next Lemma.

Lemma 5.2: *By virtue of the the above Lemma and under the condition that u and $u[1]$ are pairwise shape invariant, $u[1]$ and $u[2]$ are also pairwise shape invariant i.e.,*

$$u[2](x;a)=u[1](x;a_1)+R(a_1). \tag{90}$$

The proof can be done in two steps.

1. The condition of shape invariance and the definition of the Darboux transformation allows us to write

$$u(x;a)-2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi_1'(x;a)}{\psi_1(x;a)}=u[1](x;a)=u(x;a_1)+R(a_1), \tag{91}$$

which remains valid if we replace a by a_1, i.e.,

$$u(x;a_1)-2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi_1'(x;a_1)}{\psi_1(x;a_1)}=u[1](x;a_1)=u(x;a_2)+R(a_2). \tag{92}$$

Hence, we easily obtain

$$u(x;a_1) = u[1](x;a_1) + 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi_1'(x;a_1)}{\psi_1(x;a_1)}. \tag{93}$$

2. Applying the Darboux transformation [Eq. (16)], once again on $u[1](x;a)$, gives

$$u[2](x;a) = u[1](x;a) - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi'[1]_2(x;a)}{\psi[1]_2(x;a)}. \tag{94}$$

On the other hand, using the shape invariance condition leads to

$$u[2](x;a) = u(x;a_1) + R(a_1) - 2\frac{\mathrm{d}}{\mathrm{d}x}\frac{\psi'[1]_2(x;a)}{\psi[1]_2(x;a)}. \tag{95}$$

The result in the first step of the proof, [Eq. (93)] can be used to derive the following equation:

$$u[2](x;a) = u[1](x;a_1) + R(a_1) + 2\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{\psi_1'(x;a_1)}{\psi_1(x;a_1)} - \frac{\psi'[1]_2(x;a)}{\psi[1]_2(x;a)}\right\}. \tag{96}$$

If we now apply Eq. (88) from Lemma 5.1 for $s=1$, i.e.,

$$\psi[1]_2(x;a) = \psi_1(x;a_1), \tag{97}$$

we obtain the desired final expression which we wanted to prove, namely,

$$u[2](x;a) = u[1](x;a_1) + R(a_1). \tag{98}$$

For the sake of a more compact notation of the properties of the potential and wave functions, let us now call the property (88) *shape invariance for eigenfunctions* (or better *the two eigenfunctions involved are pairwise shape invariant*) and property (82) *shape invariance for the eigenvalues*. Note that the shape invariance of the wave functions follows from the shape invariance of the potentials. From the shape invariance of the eigenfunction we can, in turn, conclude that the next two pairs of Darboux transformations of the potential are pairwise shape invariant. One is led to the conjecture that the chain continues: from Lemma 5.2 one can show that the next pair of higher order Darboux transformations of eigenfunctions are also pairwise shape invariant, from which it follows that the next higher order pair of Darboux transformed potentials is also pairwise shape invariant. Indeed, we can prove the following theorem extending hereby the notion of shape invariance.

Theorem 5.3: *All neigbouring higher order Darboux transformed potentials and eigenfunctions are pairwise shape invariant. This is to say*,

$$u[k](x;a) = u[k-1]\ (x;a_1) + R(a_1)) \tag{99}$$

and

$$\psi[k]_{s+1}(x;a) = \psi[k-1]_s(x;a_1), \tag{100}$$

up to a multiplicative factor. In more detail, Eq. (99) *implies* Eq. (100) *which, in turn, implies*

$$u[k+1](x;a) = u[k](x;a_1) + R(a_1). \tag{101}$$

The proof proceeds via induction whose first step consists in Lemmas 5.2 and 5.1 or in Eqs. (88) and (98). We assume the hypothesis of the induction to be [Eq. (99) $\Rightarrow$ (100)]. This is sufficient since we start with the original shape invariance condition for potentials and the first step of induction is presented in Lemmas 5.1 and 5.2. We have to show that under this condition

$$\psi[k+1]_{s+1}(x;a) = \psi[k]_s(x;a_1) \tag{102}$$

holds, from which, in turn,

$$u[k+2](x;a) = u[k+1](x;a_1) + R(a_1) \tag{103}$$

follows.

1. We have

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u[k](x;a)\right)\psi[k]_s(x;a) = \lambda_s(a)\psi[k]_s(x;a), \quad s > k. \tag{104}$$

2. Since the above equation is valid for any a, it is also valid when a is replaced by $f(a)$. If we add $R(a_1)\psi[k]_s(x;a_1)$ on both sides and make use of the induction hypothesis we arrive, for $s>k$, at

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u[k+1](x;a)\right)\psi[k]_s(x;a_1) = (\lambda_s(a_1) + R(a_1))\psi[k]_s(x;a_1). \tag{105}$$

   Equation (82) then tells us that

$$\psi[k]_s(x;a_1) = \psi[k+1]_{s+1}(x;a), \tag{106}$$

   up to a multiplicative factor.
3. By definition we have

$$u[k+1](x;a) = u[k](x;a) - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi'[k]_{k+1}(x;a)}{\psi[k]_{k+1}(x;a)}\right), \tag{107}$$

   for any a. Hence also

$$u[k+1](x;a_1) = u[k](x;a_1) - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi'[k]_{k+1}(x;a_1)}{\psi[k]_{k+1}(x;a_1)}\right). \tag{108}$$

   Taking $u[k](x;a_1)$ from this equation and inserting the result in the induction hypothesis, one can easily show that

$$u[k+1](x;a) = u[k+1](x;a_1) + 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi'[k]_{k+1}(x;a_1)}{\psi[k]_{k+1}(x;a_1)}\right) + R(a_1). \tag{109}$$

4. Again per definition we know that

$$u[k+2](x;a) = u[k+1](x;a) - 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi'[k+1]_{k+2}(x;a)}{\psi[k+1]_{k+2}(x;a)}\right). \tag{110}$$

5. Combining the last two equations yields

$$u[k+2](x;a) = u[k+1](x;a_1) + R(a_1) + 2\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\psi'[k]_{k+1}(x;a_1)}{\psi[k]_{k+1}(x;a_1)} - \frac{\psi'[k+1]_{k+2}(x;a)}{\psi[k+1]_{k+2}(x;a)}\right). \tag{111}$$

6. The last step consists in using the already established result [Eq. (106)] to obtain

$$u[k+2](x;a) = u[k+1](x;a_1) + R(a_1), \tag{112}$$

   which completes the proof.

The shape invariance condition (more accurately, the shape invariance between u and $u[1]$) allows one to define a new Hamiltonian of the order s,

$$H_s^{\mathrm{SI}} \equiv -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u(x;a_s) + \sum_{k=1}^{s} R(a_k). \tag{113}$$

Note that this definition makes no reference to higher order Darboux (or Crum) transformations. However, by virtue of the Theorem V.3 we can iterate

$$H_s^{\mathrm{SI}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u[1](x;a_{s-1}) + \sum_{k=1}^{s-1} R(a_k) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u[2](x;a_{s-2}) + \sum_{k=1}^{s-2} R(a_k)$$

$$= \cdots = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + u[s](x;a) = H_s^D. \tag{114}$$

Hence, in view of the above and Theorem 3.1 we can state as a corollary.

Collary 5.4. *Under the condition of shape invariance all three transformations are equal, i.e.,*,

$$H_s^{\mathrm{SI}} = H_s^D = H_s^C. \tag{115}$$

VI. EXAMPLE

We will continue here with our example of the Morse potential, now, however, emphasizing the aspect of shape invariance around Lemmas 5.1 and 5.2 and Theorem 5.3. Indeed, the Morse potential is shape invariant. One defines the action of f as

$$f(A) \equiv A_1 = A - \frac{\alpha}{\sqrt{2}}, \tag{116}$$

in accordance with the notation in Eq. (40). R is identified with

$$R(A_1) = 2(A^2 - A_1^2). \tag{117}$$

Note that

$$\psi_1(x;A_1) = c_1(A_1)[\mathrm{sech}(\alpha x)]^{\sqrt{2}A_1/\alpha} = c_1(A_1)[\mathrm{sech}(\alpha x)]^{(\sqrt{2}A/\alpha)-1} = c\cosh(\alpha x)\psi_1(x;A) \tag{118}$$

immediately leads to

$$\psi[1]_2(x;A) = \psi_1(x;A_1), \tag{119}$$

which is valid up to a multiplicative constant. One also verifies that the equality below

$$\psi_2(x;A_1) = c_2(A_1)\sinh(\alpha x)\psi_1(x;A_1) \tag{120}$$

$$= c_2(A_1)\sinh(\alpha x)\cosh(\alpha x)\psi_1(x;A), \tag{121}$$

together with Eq. (44) has as a consequence the following identity (again up to a constant multiplicative value):

$$\psi[1]_3(x;A) = \psi_2(x;A_1). \tag{122}$$

Equations (119) and (122) are explicit examples of the result [Eq. (81) in Lemma 5.1. Regarding the eigenvalues, i.e., the property (82) in the same lemma, let us first note that another compact notation for Eq. (41) is

$$\lambda_n(A_1) = 2(A_1^2 - A_n^2), \tag{123}$$

which leaves us with the identity

$$\lambda_n(A_1) + R(A_1) = \lambda_{n+1}(A), \tag{124}$$

as it should be according to Lemma 5.1. Finally, we can also give explicit examples regarding Theorem 5.1. Due to the results from Sec. V, we can write

$$u[1](x;A_1) + R(A_1) = 2\left[A_1^2 - A_1\left(A_1 - \frac{\alpha}{\sqrt{2}}\right)\mathrm{sech}^2(\alpha x)\right] + 2(A^2 - A_1^2)$$
$$= 2[A^2 - A_1 A_2\ \mathrm{sech}^2(\alpha x)] = u[2](x;A). \tag{125}$$

This demonstrates in an explicit example the result [Eq. (99)] from Theorem 5.1. Last but not the least, one sees that Eq. (43) can be written as

$$\psi[1]_2(x;A_1) = c_2(A_1)\alpha\cosh(\alpha x)\psi_1(x;A_1), \tag{126}$$

which, according to Eq. (119) can be cast into the following form:

$$\psi[1]_2(x;A_1) = \frac{c_2(A_1)}{c}\alpha\cosh(\alpha x)\psi[1]_2(x;A) = \frac{c_2(A_1)c_2(A)}{c}\alpha^2\cosh^2(\alpha x)\psi_1(x;A) = \bar{c}\psi[2]_3(x;A), \tag{127}$$

with $\bar{c}$ a constant. To arrive at the last result we have used Eq. (57) from which one can also determine the constant $\bar{c}$ in terms of λ_3, $c_2(A)$, $c_2(A_1)$, and $c_3(A)$. Obviously, the above equation falls into the category of explicit examples of Eq. (100). Note that in none of the above examples we have used the actual lemmas or theorems to be exemplified (as it should be if an example carries some meaning).

VII. CONCLUSIONS

In the present work, we have clarified the relations between the Darboux and Crum transformations. We have shown that the latter can be reached iteratively by higher order Darboux transformations. This is valid for the potential as well as the eigenfunctions. If we subject the potential to the condition of shape invariance, another transform (not making use of Crum transformation for $n>1$) is possible [Eq. (113)]. We prove that this is also equivalent to the Crum transform. The main steps of this proof involved establishing Eqs. (99), (100), and (82). The first result, namely Eq. (99), is a generalization of the original shape invariance condition. Note that Eqs. (100) and (82) could be called shape invariance for the wave functions and eigenvalues. The results of the paper help to understand the relation between the different transformations of the Hamiltonian operator. Indeed, in view of our results, one could say that the Crum transformation which appears much more complex than the original Darboux result is essentially an iterative higher order Darboux transformation and therefore not more complex than the former.

APPENDIX: AN APPLICATION OF JACOBI THEOREM

The identity $W(W_n, W_{n-1,s}) = W_{ns}W_{n-1}$ has been used by Crum in the proof of his theorem. We have also made use of it several times in the present paper. It therefore makes sense to sketch a proof of the same.

Let us first establish some notations and definitions. Let $A=[a_{ij}]$ be an $n\times n$ matrix. The determinant of A will be denoted by $|A|$ as usual. We call the minor M_r, the determinant obtained by retaining from A the r lines $i_1, i_2, \ldots, i_r$ and the r columns $k_1, k_2, \ldots, k_r$. One defines the complement of the minor M_r as the determinant obtained from A by dropping the r lines $i_1, i_2, \ldots, i_r$ and the r columns $k_1, k_2, \ldots, k_r$. This complement will be denoted by M_r^c. One then defines $M^{(r)}$

$$M^{(r)} = (-1)^{i_1+i_2+\ldots+i_r+k_1+k_2+\ldots+k_r}M_r^c. \tag{A1}$$

Furthermore, let Δ be the matrix of the cofactors of A,

$$\Delta = \begin{vmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{vmatrix}, \tag{A2}$$

and M_r and M_r' the minors of $|A|$ and Δ, respectively.

Theorem (Jacobi): *With these notations, the theorem of Jacobi asserts that*

$$M_r' = |A|^{r-1} M^{(r)}. \tag{A3}$$

Before proceeding we make a small diversion to an example of the application of the above theorem starting with a Wronskian composed of ψ_1, ψ_2, ψ_3, and ψ_s, i.e.,

$$|A| \equiv W_{3,s} = \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 & \psi_s \\ \psi_1' & \psi_2' & \psi_3' & \psi_s' \\ \psi_1'' & \psi_2'' & \psi_3'' & \psi_s'' \\ \psi_1''' & \psi_2''' & \psi_3''' & \psi_s''' \end{vmatrix}. \tag{A4}$$

The matrix of the cofactors is then given by

$$\Delta = \begin{vmatrix} + \begin{vmatrix} \psi_2' & \psi_3' & \psi_s' \\ \psi_2'' & \psi_3'' & \psi_s'' \\ \psi_2''' & \psi_3''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1' & \psi_3' & \psi_s' \\ \psi_1'' & \psi_3'' & \psi_s'' \\ \psi_1''' & \psi_3''' & \psi_s''' \end{vmatrix} & + \begin{vmatrix} \psi_1' & \psi_2' & \psi_s' \\ \psi_1'' & \psi_2'' & \psi_s'' \\ \psi_1''' & \psi_2''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1' & \psi_2' & \psi_3' \\ \psi_1'' & \psi_2'' & \psi_3'' \\ \psi_1''' & \psi_2''' & \psi_3''' \end{vmatrix} \\ - \begin{vmatrix} \psi_2 & \psi_3 & \psi_s \\ \psi_2'' & \psi_3'' & \psi_s'' \\ \psi_2''' & \psi_3''' & \psi_s''' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_3 & \psi_s \\ \psi_1'' & \psi_3'' & \psi_s'' \\ \psi_1''' & \psi_3''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1 & \psi_2 & \psi_s \\ \psi_1'' & \psi_2'' & \psi_s'' \\ \psi_1''' & \psi_2''' & \psi_s''' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1'' & \psi_2'' & \psi_3'' \\ \psi_1''' & \psi_2''' & \psi_3''' \end{vmatrix} \\ + \begin{vmatrix} \psi_2 & \psi_3 & \psi_s \\ \psi_2' & \psi_3' & \psi_s' \\ \psi_2''' & \psi_3''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1 & \psi_3 & \psi_s \\ \psi_1' & \psi_3' & \psi_s' \\ \psi_1''' & \psi_3''' & \psi_s''' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_2 & \psi_s \\ \psi_1' & \psi_2' & \psi_s' \\ \psi_1''' & \psi_2''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1' & \psi_2' & \psi_3' \\ \psi_1''' & \psi_2''' & \psi_3''' \end{vmatrix} \\ - \begin{vmatrix} \psi_2 & \psi_3 & \psi_s \\ \psi_2' & \psi_3' & \psi_s' \\ \psi_2'' & \psi_3'' & \psi_s'' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_3 & \psi_s \\ \psi_1' & \psi_3' & \psi_s' \\ \psi_1'' & \psi_3'' & \psi_s'' \end{vmatrix} & - \begin{vmatrix} \psi_1 & \psi_2 & \psi_s \\ \psi_1' & \psi_2' & \psi_s' \\ \psi_1'' & \psi_2'' & \psi_s'' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1' & \psi_2' & \psi_3' \\ \psi_1'' & \psi_2'' & \psi_3'' \end{vmatrix} \end{vmatrix}.$$

We choose as lines and columns: $(i_1, i_2) = (3,4) = (k_1, k_2)$. Applying the Jacobi theorem gives us

$$\begin{vmatrix} + \begin{vmatrix} \psi_1 & \psi_2 & \psi_s \\ \psi_1' & \psi_2' & \psi_s' \\ \psi_1''' & \psi_2''' & \psi_s''' \end{vmatrix} & - \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1' & \psi_2' & \psi_3' \\ \psi_1''' & \psi_2''' & \psi_3''' \end{vmatrix} \\ - \begin{vmatrix} \psi_1 & \psi_2 & \psi_s \\ \psi_1' & \psi_2' & \psi_s' \\ \psi_1'' & \psi_2'' & \psi_s'' \end{vmatrix} & + \begin{vmatrix} \psi_1 & \psi_2 & \psi_3 \\ \psi_1' & \psi_2' & \psi_3' \\ \psi_1'' & \psi_2'' & \psi_3'' \end{vmatrix} \end{vmatrix} = W_{3,s} \begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix}. \tag{A5}$$

Using Lemma 2.2 the left hand side takes the form

$$\begin{vmatrix} (\mathrm{d}/\mathrm{d}x) W_{2,s} & (\mathrm{d}/\mathrm{d}x) W_3 \\ W_{2,s} & W_3 \end{vmatrix}, \tag{A6}$$

such that we can write

$$\begin{vmatrix} (\mathrm{d}/\mathrm{d}x)W_{2,s} & -(\mathrm{d}/\mathrm{d}x)W_3 \\ -W_{2,s} & W_3 \end{vmatrix} = W_{3,s}W_2. \tag{A7}$$

Explicitly, this implies the following equality:

$$W_{3,s}W_2 = W_3\frac{\mathrm{d}}{\mathrm{d}x}W_{2,s} - W_{2,s}\frac{\mathrm{d}}{\mathrm{d}x}W_3 = W(W_3, W_{2,s}). \tag{A8}$$

The proof of the general case does not require any new procedure and follows essentially the steps outlined in the example. Let W_{ns} be the Wronskian of the $n+1$ functions $\psi_1, \ldots, \psi_n, \psi_s$, namely,

$$|A| = W_{n,s} = \begin{vmatrix} \psi_1 & \psi_2 & \cdots & \psi_n & \psi_s \\ \psi_1' & \psi_2' & \cdots & \psi_n' & \psi_s' \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \psi_1^{(n-1)} & \psi_2^{(n-1)} & \cdots & \psi_n^{(n-1)} & \psi_s^{(n-1)} \\ \psi_1^{(n)} & \psi_2^{(n)} & \cdots & \psi_n^{(n)} & \psi_s^{(n)} \end{vmatrix}, \tag{A9}$$

and Δ the matrix of the cofactors of $W_{n,s}$. We would like to apply the Jacobi theorem for the choice

$$(i_1, i_2) = (n, n+1) = (k_1, k_2), \tag{A10}$$

such that $r=2$. In this case we need

$$M_r' = \begin{vmatrix} +W_{n-1,s}' & -W_n' \\ -W_{n-1,s} & +W_n \end{vmatrix} = W(W_n, W_{n-1,s}), \tag{A11}$$

where we have used explicitly the result of Lemma 2.2. Clearly, we have,

$$M^{(r)} = W_{n-1}, \tag{A12}$$

such that the Jacobi theorem for the Wronskian A can be stated as

$$W(W_n, W_{n-1,s}) = W_{ns}W_{n-1}, \tag{A13}$$

which proves Lemma 2.3.

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Parametric-time coherent states for the generalized MIC-Kepler system

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In this study, we construct the parametric-time coherent states for the negative energy states of the generalized MIC-Kepler system, in which a charged particle is in a monopole vector potential, a Coulomb potential, and a Bohm-Aharonov potantial. We transform the system into four isotropic harmonic oscillators and construct the parametric-time coherent states for these oscillators. Finally, we compactify these states into the physical time coherent states for the generalized MIC-Kepler system. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2399362]

I. INTRODUCTION

First, Schrödinger derived the coherent states for the one-dimensional linear harmonic oscillator and also pointed out the construction of the localized nonspreading wave packets for the electrons in a Coulomb potential.[1] The coherent states are eigenstates of the lowering operator of the harmonic oscillator with complex eigenvalues. The expectation values of the dynamical variables, i.e., the position and the momentum, satisfy the classical equations of motion. These states are the most classical ones, with minimum uncertainty and nondispersion in the physical time, and have time dependent probabilities. In this respect, they are the most useful states to discuss the time dependent process and the classical limit of the quantum systems. The coherent states have been used in the quantum theory of the electrodynamics in 1963 which is known as the Glauber states.[2] Recently, Robinett reviewed the theoretical and numerical studies on the wave packets.[3] Earlier, Brown, and later Nieto and Simmons, developed a general formalism to construct coherent states for the different potentials.[4,5] In 1986, Bhaumik *et al.* constructed coherent states for the Kepler problem and showed that these states are dispersed.[6] Here, the authors discuss the dynamical symmetries of the problem, $SU(2) \times SU(2)$ and try to construct the eigenstates of the lowering operators of this group. They transform the problem into the four harmonic oscillators which evolve in the physical time. ten Wolde *et al.* observed a radially localized electron wave packet.[7]

Since the dynamical symmetry groups are related to the stationary states of a problem, they do not give the (physical) time evolution of the related eigenstates. Even in the classical mechanics, we do not know the time evolution of the physical systems explicitly, except for the free particle and for the particle in a linear or a quadratic potential. Therefore, the time evolution of the classical Kepler problem is given in terms of a parametric time or the eccentric anomaly.[8] In 1967, Kustaanheimo-Stiefel (KS) developed a mapping technique in order to transform the 3D classical Kepler problem into the four isotropic harmonic oscillators which evolve in a parametric time.[9] However, this mapping is nonholonomic and a highly technical one.

Later, KS transformation is used by Duru and Kleinert to find the solution of the Kepler problem via the Feynman path integrals.[10] In this formulation, they introduce a new nondynamical, free particle coordinate for the particle and map this system into the four harmonic oscillators which evolve in a parametric time. They also add the (physical) time as another coordinate of the particle.

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Recently, Toyoda and Wakayama transformed the Kepler problem into the four harmonic oscillators, which evolve in the parametric time, by using the squared parabolic coordinates and investigated coherent states for the Kepler problem.[11]

Generally, the Feynman path integrals are used to evaluate the transition amplitudes between the configuration space eigenstates. In 1998, we derived the transition amplitudes of the linear harmonic oscillator between the eigenstates of its lowering operator, by using a complementary formulation of the Feynman path integrals, and defined the coherent states in terms of these amplitudes.[12] Recently, the coherent states of the Kepler problem have been derived by using the mapping technique given in Ref. 10 and consider the transition amplitudes of the four harmonic oscillators between the eigenstates of their lowering operators.[13] Here, it is also shown that the expectation values for the coordinates of the electron satisfy the Kepler laws and oscillate in the parametric time. The uncertainties in these expectation values are not constant, but they oscillate in the parametric time. Later, this technique has been applied to derive the coherent states for a particle in the Morse potential or in a 5D Coulomb potential.[14,15] The coherent states in Ref. 11 have been improved during the same period[16] and these states are the same with the coherent states in Refs. 13 and 17.

A natural generalization of the Coulomb problem is given by Zwanziger and rediscovered by McIntosh and Cisneros.[18] It is known as the MIC-Kepler system and described by the Hamiltonian in a Coulomb field as well as a Dirac's monopole field

$$H_1 = \frac{(\mathbf{p} - s\mathbf{A})^2}{2M} + \frac{s^2}{2Mr^2} - \frac{Ze^2}{r},$$

where s is the monopole number and the vector potential, $\mathbf{A}$ is given by

$$\mathbf{A} = \frac{1}{r(r-z)}(y,-x,0) \quad \text{with rot } \mathbf{A} = \frac{\hat{r}}{r^2}.$$

The MIC-Kepler system gives the generalizations of the conserved angular momentum and of the Runge-Lenz vectors.

Another generalization of the Coulomb problem is the particle in the Coulomb and Bohm-Aharonov potential.[19] This system is described by the Hamiltonian

$$H_2 = \frac{1}{2M}\mathbf{p}^2 - \frac{Ze^2}{r} + \frac{C_1}{2Mr(r-z)} + \frac{C_2}{2Mr(r+z)},$$

where C_1 and C_2 are non-negative constants.

The following noncentral Hamiltonian is proposed as one of the generalization of these two type of potentials and known as the generalized MIC-Kepler system:[20]

$$H = \frac{1}{2M}(\mathbf{p} - s\mathbf{A})^2 + \frac{s^2}{2Mr^2} - \frac{Ze^2}{r} + \frac{C_1}{2Mr(r-z)} + \frac{C_2}{2Mr(r+z)}.$$

The Hamiltonian, H, is written in the spherical coordinates as

$$H = \frac{1}{2M}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta}\right) + V(r,\theta),$$

where the noncentral potential, $V(r,\theta)$, is

$$V(r,\theta) = -\frac{f}{r} + \frac{B + C\cos\theta}{r^2 \sin^2\theta}, \tag{1}$$

$$f = Ze^2, \quad B = \frac{(C_1 + C_2) - 2s(p_\phi - s)}{2M}, \quad C = \frac{(C_1 - C_2) - 2s(p_\phi - s)}{2M}.$$

The Hartmann potential is an example of the special cases of this potential with

$$f = 2a_0 \eta\sigma^2 \epsilon_0, \quad B = q\epsilon_0 (a_0 \eta\sigma)^2, \quad C = 0,$$

where a_0 is the Bohr radius, ϵ_0 is the ground state energy of the hydrogen atom, q is a real parameter, and η and σ are positive real numbers with values ranging from about 1 to 10. It is proposed as a model for the ring-shaped organic molecules like cyclic polyenes and benzene.[21] The combined Coulomb and Aharonov-Bohm potential is another example of this noncentral potential[19] and it can be obtained by taking $C=0$ and $s=0$ in Eq. (1), respectively. Both $B=0$ and $C=s=0$ give the Coulomb potential.

The Schrödinger equation for the particle in the Hartmann potential is discussed by using the separation of the variables method,[22,23] KS transformation and the path integral method, the supersymmetry and shape invariance, the usual methods,[24–35] or the Nikiforov-Uvarov method.[36] The "accidental" degeneracy of the spectrum and "hidden" symmetry of the Hartmann potential are also discussed.[37–39] The coherent states for the Hartmann potential have been derived.[40]

The aim of this study is to construct the coherent states for the generalized MIC-Kepler system by using the path integral formalism proposed in Ref. 13. Instead of the KS transformation, we use the squared parabolic coordinates, in order to transform the problem into the four isotropic harmonic oscillators, which evolve in a parametric time.[41] We notice that, the configuration spaces of the four oscillators for noncentral potentials are different from those for the Kepler problem. We can construct the coherent states of these oscillators and compactify these states into the three-dimensional generalized MIC-Kepler system. For the completeness, we also find the expressions of the wave functions in terms of the energy eigenfunctions of the system for both the parabolic and the spherical coordinates.

The paper is organized as follows: In Sec. II, we discuss the transformation of the action for the classical particle in the noncentral potential into the four isotropic harmonic oscillators. In Sec. III, we derive the coherent states in terms of the energy eigenstates of the four oscillators in the parametric time. In Sec. IV, we give the wave function of the coherent states in configuration space by using the energy eigenstates of the system for the parabolic and the spherical coordinates.

II. ACTION FOR THE GENERALIZED MIC-KEPLER SYSTEM

The parabolic coordinates are given as

$$\xi = r(1 - \cos\theta),$$

$$\eta = r(1 + \cos\theta),$$

$$\phi = \phi.$$

First, we express $V(r,\theta)$, in the parabolic coordinates, (ξ, η, ϕ),

$$V(\zeta,\eta) = -\frac{2f}{\zeta+\eta} + \frac{B}{\zeta\eta} - \frac{C(\zeta-\eta)}{\zeta\eta(\zeta+\eta)}. \tag{2}$$

Hence, the classical Hamiltonian can be written in the parabolic coordinates as

$$H(\zeta,\eta,\phi) = \frac{4}{2M(\zeta+\eta)}[\zeta p_\zeta^2 + \eta p_\eta^2] + \frac{1}{2M\eta\zeta} p_\phi^2 + V(\zeta,\eta). \tag{3}$$

Using Eq. (3) we write the action as

$$A=\int \mathrm{d}t\left[p_\xi\dot{\xi}+p_\eta\dot{\eta}+p_\phi\dot{\phi}-\frac{4}{2M(\xi+\eta)}(p_\xi^2\xi+p_\eta^2\eta)-\frac{1}{2M\eta\zeta}p_\phi^2+\frac{2f}{\zeta+\eta}-\frac{B}{\zeta\eta}+\frac{C(\zeta-\eta)}{\zeta\eta(\zeta+\eta)}\right]. \tag{4}$$

Next, we perform the following canonical transformation in Eq. (4),

$$\zeta=\frac{\alpha^2}{2}u^2,\ \ 0\le u<\infty,$$

$$\eta=\frac{\alpha^2}{2}v^2,\ \ 0\le v<\infty. \tag{5}$$

Here, a parameter, α, is introduced in order to obtain the dimensionless units for u and v. This implies the following relations for the canonical conjugate momenta,

$$p_u=\alpha\sqrt{2\zeta}p_\zeta,$$

$$p_v=\alpha\sqrt{2\eta}p_\eta. \tag{6}$$

We use Eqs. (5) and (6), and rewrite Eq. (4) as

$$A=\int \mathrm{d}t\left\{p_u\dot{u}+p_v\dot{v}+p_\phi\dot{\phi}-\frac{4}{\alpha^2(u^2+v^2)}\times\left[\frac{1}{2M\alpha^2}\left(p_u^2+p_v^2+\frac{p_\phi^2+2M(B-C)}{u^2}+\frac{p_\phi^2+2M(B+C)}{v^2}\right)-f\right]\right\}. \tag{7}$$

In Eq. (8), the term

$$\left(p_u^2+p_v^2+\frac{p_\phi^2+2M(B-C)}{u^2}+\frac{p_\phi^2+2M(B+C)}{v^2}\right),$$

is similar to the Hamiltonian of the particle in the four-dimensional space with the azimuthal momenta as $[p_\phi^2+2M(B\mp C)]^{1/2}$. We introduce two dummy momenta, p_{ϕ_1} and p_{ϕ_2}, into the action by Lagrange multipliers, $\frac{\mathrm{d}\phi_1}{\mathrm{d}t}$ and $\frac{\mathrm{d}\phi_2}{\mathrm{d}t}$, and transform the system into four dimensions:

$$A=\int \mathrm{d}t\left\{p_u\dot{u}+p_v\dot{v}+p_\phi\dot{\phi}+\frac{\mathrm{d}\phi_1}{\mathrm{d}t}[p_{\phi_1}-\sqrt{p_\phi^2+2M(B-C)}]+\frac{\mathrm{d}\phi_2}{\mathrm{d}t}[p_{\phi_2}-\sqrt{p_\phi^2+2M(B+C)}]-\frac{4}{\alpha^2(u^2+v^2)}\left[\frac{1}{2M\alpha^2}\left(p_u^2+p_v^2+\frac{p_{\phi_1}^2}{u^2}+\frac{p_{\phi_2}^2}{v^2}\right)-f\right]\right\}. \tag{8}$$

To eliminate the $[4/\alpha^2(u^2+v^2)]$ term in Eq. (8), we introduce a new time parameter, s, defined as

$$\frac{\mathrm{d}t}{\mathrm{d}s}=\frac{\alpha^2(u^2+v^2)}{4}. \tag{9}$$

We also add the physical time, t, into the physical coordinates of the particle and represent the dynamics of the particle in terms of the parametric time, s. Then we rewrite the action in terms of the parametric time as the following:

$$A=\int \mathrm{d}s\left\{p_u\frac{\mathrm{d}u}{\mathrm{d}s}+p_v\frac{\mathrm{d}v}{\mathrm{d}s}+ +p_\phi\frac{\mathrm{d}\phi}{\mathrm{d}s}+(-p_o)\left(\frac{\mathrm{d}t}{\mathrm{d}s}-\frac{\alpha^2(u^2+v^2)}{4}\right)+\frac{\mathrm{d}\phi_1}{\mathrm{d}s}[p_{\phi_1}-\sqrt{p_\phi^2+2M(B-C)}]\right.$$
$$\left.+\frac{d\phi_2}{ds}[p_{\phi_2}-\sqrt{p_\phi^2+2M(B+C)}]-\left[\frac{1}{2M\alpha^2}\left(p_u^2+p_v^2+\frac{p_{\phi_1}^2}{u^2}+\frac{p_{\phi_2}^2}{v^2}\right)-f\right]\right\}, \tag{10}$$

where p_o is another Lagrange multiplier corresponding to the momentum, which is a conjugate to physical time, t. Here, we only consider the bound states, $p_o<0$. We represent the position of the particle in the four dimensional space by the two sets of the polar coordinates

$$\mathbf{u}=(u\cos\phi_1,\ u\sin\phi_1,\ v\cos\phi_2,\ v\sin\phi_2). \tag{11}$$

We notice that ϕ_1 and ϕ_2 are two dummy coordinates in the interval of $-\infty<\phi_1,\ \phi_2<+\infty$. Then the action in Eq. (9), becomes

$$A=\int \mathrm{d}s\left\{\mathbf{p_u}\cdot\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}s}+p_\phi\frac{\mathrm{d}\phi}{\mathrm{d}s}+(-p_o)\frac{\mathrm{d}t}{\mathrm{d}s}-H_4-\left[\frac{\mathrm{d}\phi_1}{\mathrm{d}s}\sqrt{p_\phi^2+2M(B+C)}+\frac{\mathrm{d}\phi_2}{\mathrm{d}s}\sqrt{p_\phi^2+2M(B-C)}\right]\right\}, \tag{12}$$

where the terms in the square bracket are the total derivatives, as p_o and p_ϕ are the conserved quantities. In Eq. (12), H_4 is given as

$$H_4=\frac{1}{2M\alpha^2}[(\mathbf{p_u})^2+(M\omega)^2\alpha^4(\mathbf{u})^2]-f. \tag{13}$$

Here ω is the frequency of the four isotropic oscillators and are given as $\sqrt{-p_o/2M}$. We choose the scale factor α^2 such that $M\omega\alpha^2=1$. The term (H_4+f) corresponds to the Hamiltonian of the four isotropic harmonic oscillators. Hence, we consider them separately and discuss the action of the four oscillator system:

$$A_\omega=\int \mathrm{d}s\left\{\mathbf{p_u}\cdot\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}s}-\frac{\omega}{2}\left[(\mathbf{p_u})^2+(\mathbf{u})^2-\frac{2f}{\omega}\right]\right\}. \tag{14}$$

We define the holomorphic coordinates

$$\mathbf{a}=\begin{pmatrix}a_1\\a_2\\a_3\\a_4\end{pmatrix}$$

as

$$a_i=\frac{1}{\sqrt{2}}(u_i+ip_{u_i}),\quad i=1,\ldots,4. \tag{15}$$

We also define the conjugate dynamical variables $\mathbf{a}^*=(a_1^*,\ ,a_4^*)$ as

$$a_i^*=\frac{1}{\sqrt{2}}(u_i-ip_{u_i}). \tag{16}$$

Then, we rewrite the action A_ω in terms of the holomorphic coordinates $\mathbf{a}$ and $\mathbf{a}^*$ as

$$A_\omega[\mathbf{a}^*(s_b),\ s_b;\mathbf{a}(s_a),s_a]=f(s_b-s_a)+\int_{s_a}^{s_b}\mathrm{d}s\left[\frac{1}{2i}\left(\frac{\mathrm{d}\mathbf{a}^*}{\mathrm{d}s}\cdot\mathbf{a}-\mathbf{a}^*\cdot\frac{\mathrm{d}\mathbf{a}}{\mathrm{d}s}\right)-\omega(\mathbf{a}^*\cdot\mathbf{a})\right], \tag{17}$$

where we omitted the total derivative term, $\frac{1}{2}\Sigma_{i=1}^2\mathbf{p}_u\cdot\mathbf{u}|_a^b$, in the action, A_ω.

In Eq. (12), H_4 is the new Hamiltonian or the energy of the particle in parametric time, s. H_4 is constant, even taking the value of zero. The physical energy of the classical particle is

$$p_o = -2Mf^2(\mathbf{a}^* \cdot \mathbf{a})^{-2}.$$

III. COHERENT STATES FOR THE FOUR OSCILLATORS

The kernel of the four oscillator system is defined in Ref. 13 as

$$K_\omega[\mathbf{a}^*(s_b), s_b; \mathbf{a}(s_a), s_a] = e^{i(f-2\omega)(s_b-s_a)} \int \frac{D\mathbf{a}^* \cdot D\mathbf{a}}{[2\pi i]^4} \times e^{i\left\{\int_{s_a}^{s_b} ds\left[\frac{1}{2i}\left(\frac{d\mathbf{a}^*}{ds}\cdot\mathbf{a} - \mathbf{a}^*\cdot\frac{d\mathbf{a}}{ds}\right) - \omega(\mathbf{a}^*\cdot\mathbf{a})\right]\right\}}, \quad (18)$$

where we take $\hbar = 1$ and the term 2ω in the exponential comes from the quantum ordering terms between the operators $\hat{a}_i^*$ and $\hat{a}_i$. We perform a_i^* and a_i integrations by the method developed in Ref. 12. Then the kernel K_ω becomes

$$K_\omega[\mathbf{a}^*(s_b),\ \mathbf{a}(s_a); (s_b - s_a)] = e^{i(f-2\omega)(s_b-s_a)} \times e^{\mathbf{a}^*(s_b)\cdot\mathbf{a}(s_a)e^{-i\omega(s_b-s_a)}}. \quad (19)$$

The coordinate transformation in Eq. (5) is double valued. Hence, we also consider the kernel $K_\omega[-\mathbf{a}^*(s_b),\ \mathbf{a}(s_a); (s_b - s_a)]$. Since we are interested in a spinless system, the total transition amplitude, $K_\omega^{(+)}$, is the symmetric sum of these two kernels:

$$K_\omega^{(+)}[\mathbf{a}^*(s_b),\ \mathbf{a}(s_a); (s_b - s_a)] = 2e^{i(f-2\omega)(s_b-s_a)} \times \cosh[\mathbf{a}^*(s_b)\cdot\mathbf{a}(s_a)e^{-i\omega(s_b-s_a)}]. \quad (20)$$

We can represent the kernel $K_\omega^{(+)}$ by expanding the exponential terms in Eq. (21) into a power series of $a_i^*(s_b)a_i(s_a)$ for each value of i:

$$K_\omega^{(+)}[\mathbf{a}^*(s_b), \boldsymbol{\lambda}(s_a); (s_b - s_a)] = \sum_{n_{1,2,3,4}=0}^{\infty} [1 + (-1)^{n_1+n_2+n_3+n_4}] \times e^{-i[(n_1+n_2+n_3+n_4+2)\omega - f](s_b-s_a)} \prod_{i=1}^{4} \frac{(a_i^*\lambda_i)^{n_i}}{\Gamma(n_i+1)}, \quad (21)$$

where $n_1+n_2+n_3+n_4$ is an even number. We omit the s_b dependence of the final eigenvalues a_i^* and s_a dependence of the eigenvalues λ_i. If we parametrize the quantum numbers n_i in terms of the radial and angular quantum numbers of the four oscillators as

$$n_1 = (n_r)_1 + \frac{1}{2}(|m_1| + m_1),$$

$$n_2 = (n_r)_1 + \frac{1}{2}(|m_1| - m_1),$$

$$n_3 = (n_r)_2 + \frac{1}{2}(|m_2| + m_2),$$

$$n_4 = (n_r)_2 + \frac{1}{2}(|m_2| - m_2),$$

and denote the final eigenstates by $a_\pm^*$ and $b_\pm^*$ and initial eigenstates by $\kappa_\pm$ and $\lambda_\pm$,

$$a_{\pm}^{*}=\frac{(a_1^{*}\mp ia_2^{*})}{\sqrt{2}},\quad b_{\pm}^{*}=\frac{(a_3^{*}\mp ia_4^{*})}{\sqrt{2}},$$

$$\kappa_{\pm}=\frac{(a_1\pm ia_2)}{\sqrt{2}},\quad \lambda_{\pm}=\frac{(a_3\pm ia_4)}{\sqrt{2}},\tag{22}$$

then

$$K_{\omega}^{(+)}[a_{\pm}^{*},\,b_{\pm}^{*},s_b;\kappa_{\pm},\lambda_{\pm},s_a]=\sum_{(n_r)_{1,2}=0}^{\infty}\sum_{m_{1,2}=-\infty}^{+\infty}[1+(-1)^{|m_1|+|m_2|}]\times e^{-2i\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1-\frac{f}{2}\right]\omega(s_b-s_a)}$$
$$\times\Pi_{\epsilon=+,-}\frac{(a_{\pm}^{*}\kappa_{\pm})^{(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)}}{\Gamma\left[(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)+1\right]}\times\frac{(b_{\pm}^{*}\lambda_{\pm})^{(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)}}{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)+1\right]}.\tag{23}$$

Here, $(n_r)_{1,2}$ and $m_{1,2}$ are the radial and angular quantum numbers of the oscillators. In the derivation of Eq. (24), we assume that $-\pi\leq\phi_{1,2}<+\pi$. However, for the physical problem, there is no periodicity in $\phi_{1,2}$ and therefore, $-\infty<\phi_1,\ \phi_2<+\infty$. If we perform the scale transformation $\phi_{1,2}\rightarrow\frac{2\pi}{2L}\phi_{1,2}$ and $p_{\phi_{1,2}}\rightarrow\frac{2L}{2\pi}p_{\phi_{1,2}}$ and then evaluate the limit $L\rightarrow\infty$ in Eq. (24) by considering the present physical problem,

$$K_{\omega}^{(+)}[a_{\pm}^{*},\,b_{\pm}^{*},s_b;\kappa_{\pm},\lambda_{\pm},s_a]=\sum_{(n_r)_{1,2}=0}^{\infty}\int_{-\infty}^{+\infty}dm_1\int_{-\infty}^{+\infty}dm_2F_{(n_r)_1,m_1,(n_r)_2,m_2}$$
$$\times e^{-2i\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1-\frac{f}{2}\right]\omega(s_b-s_a)},\tag{24}$$

where

$$F_{(n_r)_1,m_1,(n_r)_2,m_2}(a_{\pm}^{*}\kappa_{\pm},b_{\pm}^{*}\lambda_{\pm})=(1+(-1)^{|m_1|+|m_2|})\times\Pi_{\epsilon=+,-}\frac{(a_{\epsilon}^{*}\kappa_{\epsilon})^{(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)}}{\Gamma\left[(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)+1\right]}$$
$$\times\frac{(b_{\epsilon}^{*}\lambda_{\epsilon})^{(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)}}{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)+1\right]}.$$

For the four oscillators, the energy eigenstates are

$$|(n_r)_{1,2},m_{1,2}\rangle=\Pi_{\epsilon=+,-}\frac{(a_{\pm}^{\dagger})^{(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)}}{\sqrt{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_1|+\epsilon m_1)+1\right]}}\times\frac{(b_{\pm}^{\dagger})^{(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)}}{\sqrt{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)+1\right]}}|0\rangle.\tag{25}$$

$K_{\omega}^{(+)}$ is the matrix elements of the parametric-time evolution operator, U between the initial eigenstates of the operators $\hat{\mathbf{a}}_i$, $\kappa_{\pm}$, $\lambda_{\pm}$, and the final eigenstates of the operators $\hat{\mathbf{a}}_i$, $a_{\pm}$, $b_{\pm}$. If we expand $K_{\omega}^{(+)}$ in terms of the oscillator energy eigenstates $|(n_r)_{1,2},m_{1,2}\rangle$ as

$$K_{w}^{(+)}[a_{\pm}^{*},\,b_{\pm}^{*},s_b;\kappa_{\pm},\lambda_{\pm},s_a]=\sum_{(n_r)_{1,2}=0}^{\infty}\int_{-\infty}^{+\infty}dm_1\int_{-\infty}^{+\infty}dm_2\langle(n_r)_{1,2},m_{1,2}|a_{\pm}b_{\pm}\rangle^{*}$$
$$\times\langle(n_r)_{1,2},m_{1,2}|U(s_b-s_a)|\kappa_{\pm},\lambda_{\pm}\rangle.$$

Here, $|a_{\pm},b_{\pm}\rangle$ is the final coherent state and $U(s_b-s_a)|\kappa_{\pm},\lambda_{\pm}\rangle$ is the time evolution of the initial coherent state for the four symmetric oscillators. These are given by

$$|a_{\pm},b_{\pm}\rangle = \sum_{(n_r)_{1,2}=0}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}m_1 \int_{-\infty}^{+\infty} \mathrm{d}m_2 \times U_{(n_r)_1,m_1,(n_r)_2,m_2}(a_{\pm},b_{\pm})|(n_r)_{1,2},m_{1,2}\rangle \tag{26}$$

and

$$U(s_b-s_a)|\kappa_{\pm},\lambda_{\pm}\rangle = \sum_{(n_r)_{1,2}=0}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}m_1 \int_{-\infty}^{+\infty} \mathrm{d}m_2 \times e^{-2i\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1-\frac{f}{2}\right]\omega(s_b-s_a)} \times U_{(n_r)_1,m_1,(n_r)_2,m_2}(\kappa_+,\kappa_-,\lambda_+,\lambda_-)|(n_r)_{1,2},m_{1,2}\rangle,$$

where

$$U_{(n_r)_1,m_1,(n_r)_2,m_2}(a_{\pm},b_{\pm}) = [1+(-1)^{|m_1|+|m_2|}] \times \Pi_{\epsilon=+,-} \frac{(a_{\epsilon})^{(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)}}{\sqrt{\Gamma\left[(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)+1\right]}} \times \frac{(b_{\epsilon})^{(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)}}{\sqrt{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)+1\right]}}.$$

In order to derive the other physical conditions for the coherent states, we consider the integration of the kernel over the all values of s_b from s_a to $+\infty$. It gives the Green's function of the four oscillators as

$$G_{\omega}^{(+)}(a_{\pm}^*,\, b_{\pm}^*;\kappa_{\pm},\lambda_{\pm}) = \sum_{(n_r)_{1,2}=0}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}m_1 \int_{-\infty}^{+\infty} \mathrm{d}m_2 \times \frac{iF_{(n_r)_1,m_1,(n_r)_2,m_2}(a_{\pm}^*\kappa_{\pm},b_{\pm}^*\lambda_{\pm})}{f-2\omega\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1\right]}. \tag{27}$$

The poles of the Green's function are at

$$f = 2\omega\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1\right],$$

which give the energy eigenvalues of the physical system as

$$p_o = -\frac{Mf^2}{2\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1\right]^2}. \tag{28}$$

To derive the Green's function or the matrix elements for the physical particle we consider the elimination of the dummy coordinates, ϕ_1 and ϕ_2. There are two methods of the elimination: In the path integration formalism, we integrate over all the possible final values of these variables. In the wave function formalism, we consider the physical eigenvalues of the corresponding conjugate momenta

$$\hat{p}_{\phi_1}\Psi^{\mathrm{phys}} = \sqrt{m^2+2M(B-C)}\Psi^{\mathrm{phys}},$$

$$\hat{p}_{\phi_2}\Psi^{\mathrm{phys}} = \sqrt{m^2+2M(B+C)}\Psi^{\mathrm{phys}}, \tag{29}$$

where m is the azimuthal quantum number corresponding to the operator $\hat{p}_{\phi}$. Then the Green's function at p_o becomes

$$G_{\omega}^{\text{phys}}(a_{\pm}^{*},\, b_{\pm}^{*};\kappa_{\pm},\lambda_{\pm}) = G_{\omega}^{(+)}\,(a_{\pm}^{*},\, b_{\pm}^{*};\kappa_{\pm},\lambda_{\pm})\big|_{|m_{1,2}|=\sqrt{m^2+2M(B\mp C)}}$$

$$= \sum_{(n_r)_{1,2}=0}^{\infty} V_{(n_r)_1,(n_r)_2}(a_{+}^{*},a_{-}^{*},b_{+}^{*},b_{-}^{*}) \times V_{(n_r)_1,(n_r)_2}(\kappa_{+},\kappa_{-},\lambda_{+},\lambda_{-}),$$

where

$$V_{(n_r)_1,(n_r)_2}(a_{\pm}^{*},b_{\pm}^{*}) = [1+(-1)^{|m_1|+|m_2|}] \times \Pi_{\epsilon=+,-} \frac{(a_{+}^{*}a_{-}^{*})^{(n_r)_1+|m_1|}\left(\frac{a_{+}^{*}}{a_{-}^{*}}\right)^{m_1}}{\sqrt{\Gamma\left[(n_r)_1+\frac{1}{2}(|m_1|+\epsilon m_1)+1\right]}}$$

$$\times \frac{(b_{+}^{*}b_{-}^{*})^{(n_r)_2+|m_2|}\left(\frac{b_{+}^{*}}{b_{-}^{*}}\right)^{m_2}}{\sqrt{\Gamma\left[(n_r)_2+\frac{1}{2}(|m_2|+\epsilon m_2)+1\right]}}. \tag{30}$$

In Eq. (30) we take the values of $|m_{1,2}|$ as $\sqrt{m^2+2M(B\mp C)}$. Thus, we derive the physical coherent states by evaluating $|a_{\pm},b_{\pm}\rangle$ at the poles of the $|m_{1,2}|=\sqrt{m^2+2M(B\mp C)}$ and p_0,

$$|a_{\pm},b_{\pm}\rangle = (n_r)_{1,2} = \sum_{(n_r)_{1,2}=0}^{\infty} V_{(n_r)_1,(n_r)_2}(a_{\pm}^{*},b_{\pm}^{*})|(n_r)_{1,2},\, m_{1,2}\rangle. \tag{31}$$

The coherent states are parametrized by three quantum numbers $[(n_r)_1+|m_1|]$, $[(n_r)_2+|m_2|]$, and m as $|m_{1,2}|=\sqrt{m^2+2M(B\mp C)}$.

IV. GREEN'S FUNCTION AND COHERENT STATES IN CONFIGURATION SPACE

In Sec. III, we derive the Green's function between the initial and final coherent states. However, in this section, we write the Green's function between the final eigenstates of the configuration space and the initial coherent states as

$$G_{\omega}^{\text{phys}}(u,\phi_1,v,\phi_2;\kappa_{\pm},\lambda_{\pm}) = \Pi_{\epsilon=+,-}\int \frac{da_{\epsilon}^{*}\,da_{\epsilon}}{2\pi i}\int \frac{db_{\epsilon}^{*}\,db_{\epsilon}}{2\pi i} e^{-a_{\epsilon}^{*}a_{\epsilon}-b_{\epsilon}^{*}b_{\epsilon}} \times \langle u,\phi_1|a_{+},a_{-}\rangle$$

$$\times\langle v,\phi_2|b_{+},b_{-}\rangle G_{\omega}^{\text{phys}}(a_{\pm}^{*},\, b_{\pm}^{*};\kappa_{\pm},\lambda_{\pm}). \tag{32}$$

The matrix elements, $\langle u,\phi_1|a_{+},a_{-}\rangle$ and $\langle v,\phi_2|b_{+},b_{-}\rangle$ can be calculated by using the representation of $a_{\pm}$ and $b_{\pm}$ in terms of $u,\phi_1,(v,\phi_2)$ and $p_u,p_{\phi_1},(p_v,p_{\phi_2})$, in Eqs. (15) and (16). Since the volume element of the four-dimensional space is $2(uv)^3\,du\,dv\,d\phi_1\,d\phi_2$, the normalized wave functions will be

$$\langle u,\phi_1,v,\phi_2|a_{\pm},b_{\pm}\rangle = Ne^{-(u^2+v^2)/2} \times e^{[u(a_{+}e^{-i\phi_1}+a_{-}e^{i\phi_1})+v(b_{+}e^{-i\phi_2}+b_{-}e^{i\phi_2})]-\frac{1}{2}(a^2+b^2)}, \tag{33}$$

where the normalization constant, N, is given by

$$N = \frac{2\sqrt{2}e^{-\frac{1}{2}(aa^{*}+bb^{*})}}{[1+(a+a^{*})^2]^{1/2}[1+(b+b^{*})^2]^{1/2}}. \tag{34}$$

If we substitute $\langle u,\phi_1,v,\phi_2|a_{\pm},b_{\pm}\rangle$ into Eq. (32) and integrate over $a_{\pm}^{*}$, $a_{\pm}$ and $b_{\pm}^{*}$, $b_{\pm}$, the result will be

$$G_{\omega}^{\text{phys}}(u,\phi_2,v,\phi_2;\kappa_{\pm},\lambda_{\pm}) = iNe^{-(u^2+v^2)/2} \times e^{[u(\kappa_{+}e^{-i\phi_1}+\kappa_{-}e^{i\phi_1})+v(\lambda_{+}e^{-i\phi_2}+\lambda_{-}e^{i\phi_2})]-\frac{1}{2}(\kappa^2+\lambda^2)}. \tag{35}$$

To derive the coherent states of the particle, we consider the path integrations over the conjugate variables t and p_0 and ϕ and p_{ϕ}. The integrations of t and p_0 are discussed in Ref. 13 and the result of these integrations is given as

$$\int \frac{\mathrm{d}(-p_0)}{2\pi i} e^{i(-p_0)(t_b-t_a)}.$$

The integrations of ϕ and p_ϕ are given in Ref. 10 and the result of these integrations is

$$\sum_{m=-\infty}^{+\infty} \frac{e^{im(\phi_b-\phi_a)}}{2\pi},$$

where m is the azimuthal quantum number of the particle. Then the Green's function of the particle is

$$\widetilde{G}_\omega^{(+)}(u,\, v, \phi, t;\, \kappa_\pm, \lambda_\pm, \phi_a, t_a) = \sum_{m=-\infty}^{+\infty} \frac{e^{im(\phi-\phi_a)}}{2\pi} \times \int \frac{\mathrm{d}(-p_0)}{2\pi i} e^{i(-p_0)(t-t_a)} \widetilde{G}_\omega^{phys}(u, v; \kappa_\pm, \lambda_\pm),$$

where $\widetilde{G}_\omega^{\mathrm{phys}}(u, v; \kappa_\pm, \lambda_\pm)$ will be derived from $G_\omega^{\mathrm{phys}}(u, \phi_1, v, \phi_2; \kappa_\pm, \lambda_\pm)$ by performing the integrations over ϕ_1 and ϕ_2.

In order to derive coherent states in the parabolic coordinates, we rewrite Eq. (35) as follows:

$$G_\omega^{\mathrm{phys}}(u, \phi_1, v, \phi_2; \kappa_\pm, \lambda_\pm) = 2iNe^{-(u^2+v^2)/2+(i\kappa)^2+(i\lambda)^2} \times \cosh\left\{ \sqrt{u^2\frac{\kappa^2}{2}}[(e^{-i(\phi_1-\Delta_1)} + e^{i(\phi_1-\Delta_1)})] + \sqrt{v^2\frac{\lambda^2}{2}}[(e^{-i(\phi_2-\Delta_2)} + e^{i(\phi_2-\Delta_2)})] \right\}, \tag{36}$$

where the complex phases, $\Delta_{1,2}$, are

$$\frac{(\kappa_1 \pm i\kappa_2)}{\sqrt{2}} = \sqrt{\frac{\kappa^2}{2}} e^{\pm i\Delta_1}, \quad \frac{(\lambda_1 \pm i\lambda_2)}{\sqrt{2}} = \sqrt{\frac{\lambda^2}{2}} e^{\pm i\Delta_2}.$$

Then we can expand the Green's function, in terms of Bessel functions, as

$$G_\omega^{\mathrm{phys}}(u, \phi_1, v, \phi_2; \kappa_\pm, \lambda_\pm) = iNe^{-(u^2+v^2)/2-\kappa^2-\lambda^2} \sum_{m_1,m_2=0}^{+\infty\prime} [1 + (-1)^{m_1+m_2}] \times J_{m_1}\left(-2i\sqrt{u^2\frac{\kappa^2}{2}}\right) \cos m_1(\phi_1 - \Delta_1) \times J_{m_2}\left(-2i\sqrt{v^2\frac{\lambda^2}{2}}\right) \cos m_2(\phi_2 - \Delta_2). \tag{37}$$

Here, the prime on the summation shows that we can take the half of this term for $m_1 = m_2 = 0$. In Eq. (37), we change the range of the variables, ϕ_1 and ϕ_2 from $]-\pi, +\pi[$ to the interval $]-\infty, +\infty[$. As a consequence of this change, we can convert the summation into the integrals over m_1 and m_2. If we perform the integrations over ϕ_1 and ϕ_2 by considering the Lagrange multipliers for p_{ϕ_1} and p_{ϕ_2}, the Green's function becomes

$$G_\omega^{\mathrm{phys}}(u, v, ; \kappa_\pm, \lambda_\pm) = iNe^{-(u^2+v^2)/2-(\kappa^2+\lambda^2)/2}[1 + (-1)^{m_1+m_2}] \times J_{m_1}\left(-2i\sqrt{u^2\frac{\kappa^2}{2}}\right) \cos m_1\Delta_1 \times J_{m_2}\left(-2i\sqrt{v^2\frac{\lambda^2}{2}}\right) \cos m_2\Delta_2, \tag{38}$$

where

$$\begin{pmatrix} |m_1| \\ |m_2| \end{pmatrix} = \sqrt{m^2 + 2M(B \mp C)}.$$

To derive the coherent state wave functions in parabolic coordinates we expand the Bessel functions in terms of the associate Laguerre polynomials[42]

$$J_\alpha(2\sqrt{xz}) = e^{-z}(xz)^{\frac{\alpha}{2}} \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n+\alpha+1)} L_n^\alpha(x). \tag{39}$$

Then the Green's function is

$$G_\omega^{\text{phys}}(u,v;\kappa_\pm,\lambda_\pm) = i \sum_{(n_r)_{1,2}=0}^{\infty} [1+(-1)^{m_1+m_2}] N_{(n_r)_1,m_1} N_{(n_r)_2,m_2} \times \widetilde{R}_{(n_r)_1,m_1}(u) \left(-\frac{\kappa^2}{2}\right)^{(n_r)_1+\frac{m_1}{2}} \cos m_1\Delta_1$$
$$\times \widetilde{R}_{(n_r)_2,m_2}(v) \left(-\frac{\lambda^2}{2}\right)^{(n_r)_2+\frac{m_2}{2}} \cos m_2\Delta_2, \tag{40}$$

where

$$\widetilde{R}_{n_r,m}(u) = e^{-u^2/2}(u^2)^{\frac{m}{2}} L_{n_r}^m(u^2) \tag{41}$$

and

$$N_{(n_r),m}^2 = \frac{1}{\sqrt{\pi}\Gamma[(n_r)+m+1]}. \tag{42}$$

The reduced Green's function, $\widetilde{G}_\omega^{(+)}$, is the scalar product of the coherent states with configuration space eigenstates. We identify them as the configuration space dependent coherent state wave functions, $\Psi_{\kappa,\lambda,m,p_0}(u,v,\phi,t)$,

$$\Psi_{\kappa,\lambda,m,p_0}(u,\, v, \phi-\phi_0, t) = \widetilde{G}_\omega^{(+)}(u,\, v, \phi, t;\, \kappa_\pm, \lambda_\pm, \phi_0, t_0)$$
$$= \sum_{(n_r)_{1,2}=0}^{\infty} \sum_{m=-\infty}^{\infty} \psi_{(n_r)_1,(n_r)_2,m}(\xi,\eta,\phi) \times e^{i(-p_0)(t-t_0)} [\psi_{(n_r)_1,(n_r)_2,m}(\kappa^*,\lambda^*,\phi_0)]^*, \tag{43}$$

where

$$p_0 = 2M\omega^2 = -\frac{Mf^2}{2\left[(n_r)_1 + (n_r)_2 + \frac{1}{2}(m_1+m_2)+1\right]^2} = -\frac{Mf^2}{2\tilde{n}^2}. \tag{44}$$

In Eq. (43), $\psi_{(n_r)_1,(n_r)_2,m}(\xi,\eta,\phi)$ and $\psi(\kappa^*,\lambda^*,\phi_0)$ are the energy eigenstates in parabolic coordinates and holomorphic coordinates, respectively. They are given as

$$\psi_{(n_r)_1,(n_r)_2,m}(\xi,\eta,\phi) = \left(\frac{4[1+(-1)^{m_1+m_2}]M^3f^3}{\tilde{n}^4\Pi_{i=1}^2\Gamma[(n_r)_i+m_i+1]}\right)^{1/2}$$
$$\times \frac{e^{im\phi}}{\sqrt{2\pi}} R_{(n_r)_1,m_1}(\xi) R_{(n_r)_2,m_2}(\eta), \psi_{(n_r)_1,(n_r)_2,m}(\kappa^*,\lambda^*,\phi_0)$$
$$= (-1)^{(n_r)_1+(n_r)_2} \times \left(\frac{4[1+(-1)^{m_1+m_2}]M^3f^3}{\tilde{n}^4\Pi_{i=1}^2\Gamma[(n_r)_i+m_i+1]}\right)^{1/2} \frac{e^{im\phi_0}}{\sqrt{2\pi}}$$

$$\times \frac{e^{-(a+a^*)^2}}{[1+(a+a^*)^2]^{1/2}}(\kappa^2)^{(n_r)_1+\frac{m_1}{2}}\cos m_1\Delta_1$$
$$\times \frac{e^{-(b+b^*)^2}}{[1+(b+b^*)^2]^{1/2}}(\lambda^2)^{(n_r)_2+\frac{m_2}{2}}\cos m_2\Delta_2$$

and

$$R_{n_r,m}(\xi)=e^{-\frac{1}{2}\sqrt{-2Mp_0}\xi}(\sqrt{-2Mp_0}\xi)^{m/2}L_{n_r}^{m}(\sqrt{-2Mp_0}\xi).$$

$\Psi_{\kappa,\lambda,m,p_0}(u,v,\phi-\phi_0,t)$ is the coherent state for the particle in the potential given by Eq. (1) in terms of the normalized energy eigenstates in parabolic coordinates.

In order to find the coherent state wave functions in spherical coordinates, we write the product of two modified Bessel functions in terms of one modified Bessel function:

$$\frac{z}{2}I_\mu(z\sin\alpha\sin\beta)I_\nu(z\cos\alpha\cos\beta)=(\sin\alpha\sin\beta)^\mu(\cos\alpha\cos\beta)^\nu\sum_{l=0}^{\infty}\frac{l!\,\Gamma(\mu+\nu+l+1)}{\Gamma(\mu+l+1)\Gamma(\nu+l+1)}$$
$$\times I_{\mu+\nu+2l+1}(z)P_l^{(\mu,\nu)}(\cos 2\alpha)P_l^{(\mu,\nu)}(\cos 2\beta).$$

The product of two modified Bessel functions is

$$I_{m_1}\left(2\sqrt{\frac{M\omega u^2}{2}(\kappa)^2}\right)I_{m_2}\left(2\sqrt{\frac{M\omega v^2}{2}(\lambda)^2}\right)=I_{m_1}\left(2\sqrt{2(a^2+b^2)}\sqrt{2M\omega r}\sin\frac{\theta}{2}\sin\frac{\Theta}{2}\right)$$
$$\times I_{m_2}\left(2\sqrt{2(a^2+b^2)}\sqrt{2M\omega r}\cos\frac{\theta}{2}\cos\frac{\Theta}{2}\right),$$

where

$$\kappa=\frac{\sqrt{a^2+b^2}}{\sqrt{2}}\sin\frac{\Theta}{2}\quad\text{and}\quad\lambda=\frac{\sqrt{a^2+b^2}}{\sqrt{2}}\cos\frac{\Theta}{2}.$$

Then, we combine them as

$$I_{m_2}\left(2\sqrt{4M\omega r(a^2+b^2)}\cos\frac{\theta}{2}\cos\frac{\Theta}{2}\right)\times I_{m_1}\left(2\sqrt{4M\omega r(a^2+b^2)}\sin\frac{\theta}{2}\sin\frac{\Theta}{2}\right)$$
$$=\sum_{k=0}^{\infty}\frac{2k!\,\Gamma(k+m_1+m_2+1)}{\Gamma(k+m_1+1)\Gamma(k+m_2+1)}\times\frac{I_{2k+m_1+m_2+1}(2\sqrt{4M\omega r(a^2+b^2)})}{2\sqrt{4M\omega r(a^2+b^2)}}$$
$$\times d_{k,m_1,m_2}(\cos\theta)d_{k,m_1,m_2}(\cos\Theta),\tag{45}$$

where the angular wave function $d_{k,m_1,m_2}(\cos\theta)$ is defined in terms of Jacobi polynomials, $P_k^{(m_1,m_2)}(\cos\theta)$, as

$$d_{k,m_1,m_2}(\cos\theta)=\left(\sin\frac{\theta}{2}\right)^{m_1}\left(\cos\frac{\theta}{2}\right)^{m_2}P_k^{(m_1,m_2)}(\cos\theta).\tag{46}$$

We can expand the modified Bessel function in Eq. (45), in terms of Laguerre polynomials by using Eq. (39). Then we substitute this result into Eq. (45),

$$G_{\omega}^{\mathrm{phys}}[r,\theta;(a^2+b^2)^{1/2},\Theta]=\sum_{n_r,k=0}^{\infty}\sum_{m=-\infty}^{\infty}\psi_{n_r,k,m}(r,\theta,\phi)\times[\psi_{n_r,k,m}((a^{*2}+b^{*2})^{1/2},\Theta^*,\phi_a)]^*, \tag{47}$$

where $\psi_{n_r,k,m}(r,\theta,\phi)$ and $\psi_{n_r,k,m}((a^{*2}+b^{*2})^{1/2},\Theta*,\phi)$ are the normalized energy eigenfunctions in spherical coordinates and holomorphic coordinates, respectively. They are given in terms of the Jacobi polynomials as

$$\psi_{n_r,k,m}(r,\theta,\phi,t)=N_{n_r,k,m}\times e^{-2M\omega r}(\sqrt{4M\omega r})^{2k+m_1+m_2}L_{n_r}^{2k+m_1+m_2+1}(4M\omega r)\times e^{im\phi}d_{k,m_1,m_2}(\cos\,\theta) \tag{48}$$

and

$$\begin{aligned}\psi_{n_r,k,m}((a^{*2}+b^{*2})^{1/2},\Theta^*,\phi)=(-1)^{n_r}N_{n_r,k,m}\times(\sqrt{(a^{*2}+b^{*2})})^{2k+m_1+m_2+2n_r}e^{im\phi}\\ \times d_{k,m_1,m_2}(\cos\,\Theta^*)\cos\,m_1\Delta_1\,\cos\,m_2\Delta_2,\end{aligned} \tag{49}$$

where the normalization constant, $N_{n_r,k,m}$, is

$$N_{n_r,k,m}=\left(\frac{4M^3f^3}{2\pi\tilde{n}^4}\right)^{1/2}\times\left[\frac{(1+(-1)^{m_1+m_2})(2k+m_1+m_2+1)}{2\pi\Gamma(k+m_1+1)\Gamma(k+m_2+1)}\right]^{1/2}\times\frac{\Gamma(k+m_1+m_2+1)k!}{\Gamma(n+2k+m_1+m_2+2)}\Bigg]. \tag{50}$$

Then, coherent states in spherical coordinates are given by

$$\begin{aligned}\Psi_{(a^2+b^2)^{1/2},\Theta,\Delta}(r,\theta,\phi,t)=\tilde{G}_{\omega}^{(+)}(r,\theta,\phi,t;\,\kappa_{\pm},\lambda_{\pm},\phi_0,t_0)=\sum_{n_r,k=0}^{\infty}\sum_{m=-\infty}^{\infty}\exp\left[i\frac{Mf^2}{2\tilde{n}^2}(t-t_0)\right]\\ \times\psi_{n_r,k,m}(r,\theta,\phi)\left[\psi_{n_r,k,m}(a^{*2}+b^{*2})^{1/2},\Theta^*,\phi_0\right]^*,\end{aligned} \tag{51}$$

where the principal quantum number, $\tilde{n}$, is introduced as

$$\tilde{n}=n_r+\check{l}+1, \tag{52}$$

with

$$\check{l}=k+\frac{1}{2}(m_1+m_2)=k+\sqrt{m^2+2M(B+C)}+\sqrt{m^2+2M(B-C)}. \tag{53}$$

V. CONCLUSION

In this paper, we discuss the negative energy coherent states for the generalized MIC-Kepler system. First, we transform the system into the four isotropic harmonic oscillators, which evolve in a parametric time. Second, we construct the coherent states for the four oscillators. Third, we compactify the four oscillator system into a 3D generalized MIC-Kepler system. We also express the wave functions of these states in terms of the normalized energy eigenstates in the parabolic coordinates and in the spherical coordinates. The special cases of this system are the combined Coulomb and Aharonov-Bohm potentials, the Hartmann potential, and the Coulomb potential.

The four harmonic oscillators have 16 conserved quantities. These are constructed as follows: We expand the bilinear $aa^{\dagger}$ in terms of the Euclidian Dirac matrices. The coefficients of these expansion denote the conserved quantities corresponding to the four isotropic oscillators. The coefficient of the diagonal matrices, $1\otimes 1$, $\sigma^3\otimes 1$, $1\otimes\sigma^3$, and $\sigma^3\otimes\sigma^3$, give the complete commuting set of the operators for the four oscillators. These are related to the quantum numbers of the oscillators. Half of these coefficients are related to the conserved quantities of the generalized

MIC-Kepler system. In the case of the Kepler problem, one of these generators is exactly zero and the residual 7 generators correspond to the Hamiltonian, angular momentum and Runge-Lenz vectors and they satisfy the algebra $SU(2)\times SU(2)$. In the case of the generalized MIC-Kepler system, this generator is not zero and the classical orbits are not closed. In some extend these variables measure the precession of the orbits. In the Kepler problem, there is no precession and the orbits are closed. In the noncentral potential cases, the orbits are not closed and parametrized by the angles ϕ_1 and ϕ_2 ranging between $-\infty$ and $+\infty$.

The expectation values for the dynamical variables, i.e., the position and the momentum can be derived by using the parametric time coherent states given in Eq. (26). The center of the localized states follows finite trajectories. Since the azimuthal quantum numbers m_1 and m_2, and the principal quantum number, $\left[(n_r)_1+(n_r)_2+\frac{1}{2}(|m_1|+|m_2|)+1\right]$ are not integers, these trajectories are not closed, except for the Coulomb potential: In this case, $m_1=m_2=m$ and the trajectories are Keplerian ellipses. In all cases, the uncertainties are finite.

Here, we do not discuss the positive energy coherent states. They can be easily derived from the negative energy coherent states given in Eq. (43) by the analytic continuation discussed in Ref. 13. In this case, the trajectories and the uncertainties are not finite.

The coherent states for the generalized Aharonov-Bohm and Coulomb potential were discussed for the constant values of the quantum number, m.[43] These states correspond to the eigenvalues of the lowering operators for $(n_r)_i+|m_i|$ for $i=1,2$, which are denoted by the quadratic combinations of the lowering operators $a_\pm$ and $b_\pm$. However, they are different than the coherent states discussed in our paper.

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Time-of-arrival probabilities and quantum measurements

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In this paper we study the construction of probability densities for time of arrival in quantum mechanics. Our treatment is based upon the facts that (i) time appears in quantum theory as an external parameter to the system, and (ii) propositions about the time of arrival appear naturally when one considers histories. The definition of time-of-arrival probabilities is straightforward in stochastic processes. The difficulties that arise in quantum theory are due to the fact that the time parameter of the Schrödinger's equation does not naturally define a probability density at the continuum limit, but also because the procedure one follows is sensitive on the interpretation of the reduction procedure. We consider the issue in Copenhagen quantum mechanics and in history-based schemes like consistent histories. The benefit of the latter is that it allows a proper passage to the continuous limit—there are, however, problems related to the quantum Zeno effect and decoherence. We finally employ the histories-based description to construct Positive-Operator-Valued-Measures (POVMs) for the time-of-arrival, which are valid for a general Hamiltonian. These POVMs typically depend on the resolution of the measurement device; for a free particle, however, this dependence cancels in the physically relevant regime and the POVM coincides with that of Kijowski. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The probabilities provided by quantum mechanics usually refer to measurements that take place at specific moments of time. However, there are physically realizable measurements that do not fall in this category. One such example involves the determination of a particle's time-of-arrival (or time-of-flight) measurement. If the quantum mechanical system is described by a wave function $\psi(x,t)$, its modulus square $|\psi(x,t)|^2$ is a probability density with respect to x at any time t. If ψ describes a particle beam, the probability density describes the particles' distribution in space, as if a snapshot were taken at a moment t. However, the setup for particle detection is slightly different. The time interval between the emission of the beam and its detection is not fixed; rather, one places a detector at a fixed distance L from the source. This is *not* a single-time measurement of the particle's position. Therefore, the object $|\psi(x,t)|^2$ is not immediately relevant, because it is not a probability distribution with respect to t. Only if one assumes that the initial wave packet is narrowly concentrated around a specific momentum value p and that it remains so at all times until detection, is it possible to state that this measurement is equivalent to a single-time measurement at time $t=mL/p$ (m being the particle mass). But even for small momentum spreads of the initial state, the assumptions above are valid only for free particles.

In the general case, the detector registers particles at different times t. One therefore needs to construct a probability $p(t)$ for the time of arrival. This would have been an elementary problem,

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if there existed an operator representing time in the system's Hilbert space. In that case one would use the Born rule to determine a probability density for the time of arrival. Unfortunately, the existence of a time operator $\hat{T}$, conjugate to the Hamiltonian (so that the Hamiltonian generates time translations: $e^{i\hat{H}s}\hat{T}e^{-i\hat{H}s}=\hat{T}+s$) is ruled out by the requirement that the Hamiltonian is bounded from below.[1,2] Nonetheless, one may still define a quantum time variable by choosing some degrees of freedom of the system (or of a measuring apparatus) as defining an internal "clock." The simplest example for the time-of-arrival is the quantum version of the classical function mx/p, for a free particle of mass $m-x$, p being the position and momentum, respectively. Still, clock times fail to be conjugate to the Hamiltonian of the system, with the result that they do not forward under Hamiltonian evolution. In simpler language, quantum fluctuations invariably force clocks to move occasionally "backward in time." For time-of-arrival operators, see, for example, Refs. 3 and 4 and the extensive bibliography in the review.[5]

This discussion brings us invariably to the issue of the role of time in quantum theory. Time enters the quantum mechanical formalism as the *external* evolution parameter in Schrödinger's equation; it is not an intrinsic variable of a physical system. Indeed, outside the realm of general relativity, time is assumed to be part of a background structure—both in nonrelativistic or special relativistic physics. For Bohr, time is a part of the classical description of physics that is "complementary" to the quantum description, and is needed if the measurement theory of the later is to make sense.

In this paper we identify different candidates for the time-of-arrival probability, by treating time as a parameter external to the quantum system under consideration. This assumption is not only forced on us by the quantum mechanical formalism, but also corresponds to the way time is taken into account in experiments. When an event occurs (say a detector clicks), we record the time it took place by "looking" at a clock in the laboratory. Clocks are classical systems that do not interact with either the quantum system or with the measurement device– their degrees of freedom are not correlated to the physical processes that take place in the act of measurement. In effect, the time parameter we consider is the reading of the clock that is simultaneous with the detector's click. Since in any laboratory the relative speeds involved are much smaller than the speed of light, there is no problem in assuming a synchronization of events. Hence, in this paper, we construct a probability distribution for the clock reading that are simultaneous with the realization of a specific quantum event (usually a particle detection). It is important to emphasize that the determination of the time of arrival involves only *a single act of measurement*, which corresponds to the particle being registered by the detector.

In each individual run of the experiment, we record the moment the particle entered the measuring device. The only way to do so is by checking at every single moment of time which of the two alternatives holds: the particle having been detected or not. We then identify the time of arrival as the moment of transition from the event of no detection to the event of detection. For this purpose, we need to consider a (continuous) history of alternatives of detection. This suggests that a framework based on histories (path integrals or the consistent histories approach) is particularly suitable for that purpose. Indeed, an important feature of the history's formalism is that it distinguishes the role of the causal ordering of events in quantum theory from that of evolution (see Ref. 6 or the more general discussion in Ref. 7). This allows us to set up the problem of the time-of-arrival probabilities at a kinematical level, i.e., without specific reference to the system's Hamiltonian.

A key feature of the constructions we present here is that they are not tied to a specific choice of the Hamiltonian that describes the quantum system's dynamics. From the experimentalist's point of view, this is perhaps the most natural procedure. One may measure the time of arrival for any system without any prior knowledge about the system's dynamics. All that is needed is a particle detector and an external clock. We would use the same detector for a free particle, for a particle moving in a potential, for a particle in presence of an environment, or even when we have complete ignorance about the particle's dynamical behavior. The procedure one follows to measure the time of arrival should not depend, in principle, on the system's dynamics, only the results (namely the probabilities) should.

The histories description provides an important technical advantage. While the time of arrival does not define a function on the space of single-time alternatives of the system, it becomes one in the space of histories. In fact, the problem of defining a time-of-arrival probability is a special case of defining probabilities for histories. We shall exploit this fact in Sec. V, in order to construct a Positive-Operator-Valued-Measure for histories, by mirroring the corresponding construction of probabilities in sequential measurements.

To demonstrate unambiguously that time of arrival is naturally defined in a history framework, we consider an analogous construction, namely the time of arrival in stochastic processes (Sec. II). At this level a probability density for the time of arrival can be simply constructed. However, when we pass to quantum theory, a problem appears. The probabilities obtained from Born's rule depend on the time variable in a way that does not allow the straightforward definition of a probability density. As a result, there is a strong ambiguity in the implementation of the continuous-time limit.

The second complication involved in quantum theory is the fact that the construction depend strongly on the interpretation of the "wave-packet reduction" rule. One possible interpretation is that the wave-packet reduction is a physical process that takes place only after the measured system has interacted with a measuring device. Another interpretation is that the reduction rule can be applied to any circumstance, in which we have obtained information about the quantum system. For example, if a particle detector did not click at a specific moment of time, then we can infer that the particle has been outside the region of detection at that time.

The first interpretation allows us to construct time-of-arrival probabilities by applying *classical reasoning* to the quantum mechanical probabilities. The corresponding probability density is not a linear functional of the initial density matrix, because the assumption we employed violates the "logic" of quantum mechanical propositions. Nonetheless, it has the correct classical limit and physically reasonable properties. Its main drawback is that it is ambiguous with respect to the continuous-time limit, and depends on the procedure one employs for its implementation.

The second interpretation of the reduction procedure lends itself to constructions that emphasize the "logic" of quantum events. All information we obtain for a quantum system, whether this arises from a concrete experimental datum or from inference from the lack of such a datum (i.e., the detector not having clicked) are treated in the same footing. An important example is the consistent histories approach, which we examine in Sec. IV. Time-of-arrival histories are a special case of the so-called "spacetime coarse grainings" that have been studied before by Hartle[8] and others.[9] The advantage conferred to us by this approach is that the continuous-time limit *is naturally obtained at the level of amplitudes* (which essentially correspond to restricted path integrals). The problem arises at the level of combining the amplitudes in order to obtain a probability density. In effect, there is strong interference between different values of arrival times that are mutually exclusive in the classical context.

The quantum Zeno effect[10] poses another problem for the determination of probabilities; it can be partially evaded but it remains troublesome at the fundamental level. It seems that the only information we can obtain unambiguously in this framework is the classical deterministic limit for the time of arrival.

In Sec. V, we apply the results obtained from the analysis of histories in a different context, namely the construction of a Positive-Operator-Valued Measure that provides probabilities for the time of arrival. The key idea is that the construction of a probability density for the time of arrival is not fundamentally different from that of probabilities for sequential measurements. Hence, we follow a procedure developed for the study sequential measurements.[11,12] The resulting time-of-arrival probabilities, like those of sequential measurements, are contextual; they depend strongly on the resolution of the measurement device. However, in the physically relevant regime for the free particle the dependence on τ drops out, and the constructed POVM coincides with that of Kijowski.[4]

The approach to the time-of-arrival developed in Sec. V involves acting with the projection operator corresponding to no detection on the system's wave function at every moment of time. This action loosely corresponds to the fact that we have obtained information from the quantum

system. It is important to emphasize that it does not refer to a physical act of measurement. It cannot be described in the language of standard quantum measurement theory: a von Neumann measurement, for example, involves a finite time interval during which the interaction Hamiltonian between system and measuring device dominates over the system's self-Hamiltonian. This is clearly not happening in the time-of-arrival setup, at any moment prior to the system entering the measuring device. In quantum measurement theory, a physical measurement involves premeasurement and reduction, and here the former part is missing. In physical terms, the time-of-arrival measurement involves a single measuring device, a single act of detection, a single irreversible change in the device, and a single moment of time at which the interaction Hamiltonian becomes dominant. The only difference from the case of standard measurements is that the time of detection is unknown.

II. TIME OF ARRIVAL IN STOCHASTIC PROCESSES

We first study the time-of-arrival probability in the theory of stochastic processes. This allows us to demonstrate the procedure we will follow in quantum theory, without the complications arising from the interpretations of the quantum measurement process.

We consider for simplicity a one-dimensional system, the state of which is fully specified at a moment of time by the position variable x. The sample space Ω is then identified with $\mathbf{R}$. An ensemble of such systems is described at $t=0$ by the probability density $\rho_0(x)$. This probability density evolves according to the law

$$\frac{\partial \rho}{\partial t} = \mathcal{L}\rho, \tag{2.1}$$

where $\mathcal{L}$ is a linear, positive, trace-preserving operator on the space of probability densities.

We next construct the stochastic process corresponding to the system described by Eq. (2.1). We assume that the measurements take place in the time interval $I=[0,T]$, where T may be eventually taken to infinity. The sample space Ω^I for the stochastic process is the space of all continuous paths $x(\cdot)$ from I to $\mathbf{R}$. The relevant random variables are the function X_t on Ω defined as $X_t(x(\cdot))=x(t)$. There exists a probability measure on Ω^I given by the "continuum limit" of discrete-time paths $(t_1,x_1;t_2,x_2;\ldots;t_n,x_n)$,

$$d\mu_{\{t_1,t_2,\ldots,t_n\}}(x_1,x_2,\ldots,x_n) = \rho_0(x_0)g(x_0,0;x_1,t_1)g(x_1,t_1;x_2,t_2)\ldots g(x_{n-1},t_{n-1};x_n,t_n),dx_0\,dx_1\,dx_2\ldots dx_n, \tag{2.2}$$

where $g(x,t;x',t')$ represents the propagator associated to Eq. (2.1). We assume that ρ_0 has support only for values of $x<0$.

From the probability measure (2.2) we construct the probability for the proposition that the particle is detected at $x=0$ at a specific time t, $0<t<T$. For this purpose, we split the interval $[0,T]$ into N time steps of width $\delta t=T/N$. We assume also that $t=n\,\delta t$ for an integer $n<N$ and write $m=N-n$. We denote by $\chi_\pm$ the characteristic functions of the intervals $-\infty<x<0$ and $0<x<\infty$, respectively.

If the particle crosses the surface $x=0$ for the first time within the time interval $[t,t+\delta t]$, then it must have been in the region $(-\infty,0)$ for all times less or equal to t and in the region $(0,\infty)$ at time $t+\delta t$. There is no reason to make any assumption about where it will be at times larger than $t+\delta t$, because in time-of-arrival measurements we are interested only in the time of the first detection. The particle may be, for example, absorbed by the detector at time t.

With the above considerations in mind, we see that the probability that the particle is measured during the interval $[t,t+\delta t]$ equals

$$p(x=0|[t,t+\delta t]) = \mu(D_{[t,t+\delta t]}), \tag{2.3}$$

where μ is the stochastic probability measure and

$$D_{[t,t+\delta t]} = \chi_- \otimes \chi_- \otimes \cdots \chi_- \otimes \chi_+ \otimes 1 \otimes \cdots 1. \tag{2.4}$$

The function $D_{[t,t+\delta t]}$ is a characteristic function on $\times_{t_i}\Omega_{t_1}$, and depends only on the value of n, namely the time step that corresponds to detection. We may then also write $D_{[t,t+\delta t]}$ as D_n. If we also define by $\bar{D}$ the characteristic function

$$\bar{D} = \chi_- \otimes \chi_- \otimes \cdots \otimes \chi_- \tag{2.5}$$

that corresponds to the particle never crossing $x=0$ within the time interval $[0,T]$, the following relations hold:

$$D_n D_m = D_n \delta_{nm}, \tag{2.6}$$

$$D_n \bar{D} = 0, \tag{2.7}$$

$$\sum_{n=0}^{N} D_n + \bar{D} = 1. \tag{2.8}$$

The variables $D_n, \bar{D}$ then define an exclusive and exhaustive set of alternatives, hence the restriction of the probability measure to the algebra they generate defines a proper normalized probability measure for the time of arrival in discrete time. (This decomposition is a special case of the Path-Decomposition expansion and has been used in the context of restricted path integrals in Ref. 19).

We next construct the continuous limit of this probability as $N \to \infty$. We use an operator notation, representing the action of the integral kernel as $e^{\mathcal{L}t}$. Using Eq. (2.2), we write

$$p(x=0|[t,t+\delta t]) = \int dx [\chi_+ e^{\mathcal{L}\,\delta t} [\chi_- e^{\mathcal{L}\,\delta t}]^n \rho_0](x). \tag{2.9}$$

If we denote by K_t the limit

$$K_t = \lim_{n\to\infty} [\chi_- e^{\mathcal{L}t/n} \chi_-]^n, \tag{2.10}$$

we obtain

$$p(x=0|[t,t+\delta t]) = \delta t \int dx [\chi_+ \mathcal{L} \chi_-(x) K_t \rho_0](x). \tag{2.11}$$

The fact that the probability of the first crossing is proportional to δt implies that we can pass to the continuum limit defining a probability density on $[0,T]$,

$$p(t|x=0) = \int dx [\chi_+ \mathcal{L} K_t \rho_0](x). \tag{2.12}$$

This probability density is not normalized to one as there is a no-zero residual probability $p(N)$ that the particle is not detected at all within $[0,T]$:

$$\int_0^T dt\, p(t|x=0) = 1 - \int dx [K_T \rho_0](x) := 1 - p(N). \tag{2.13}$$

For generic initial states and dynamics the residual probability does not vanish as $t \to \infty$.

Using the probability density $p(t|x=0)$, we define the probability of detection within any interval $[t_1,t_2]$ by integrating $p(t|x=0)$ in this interval. The definition of average values of quantities is slightly more intricate. The sample space for the time of arrival (at the continuum limit) is

not the interval $[0,T]$, but the set $[0,T]\cup\{N\}$, where N refers to the event of no detection. Strictly speaking, physical observables are functions on $[0,T]\cup\{N\}$. Hence there is an ambiguity in the definition of a function representing time t, because there is no natural numerical value it can take when evaluated on N.

In effect, a time function is defined unambiguously as a *conditional expectation*, namely after the assumption that the particle has actually been detected. This implies that we restrict (condition) the sample space to $[0,T]$. The conditional probability p_c density is then

$$p_c(t|x=0)=\frac{p(t|x=0)}{1-p(N)}. \tag{2.14}$$

A. Examples

1. Two-level system

In the derivation of the probability of time of arrival, we referred to the variable x as position. However, the derivation is completely general and Eq. (3.15) may be applied to any sample space. If the latter is discrete, we have to exchange the integral with a summation. We may consider, for example, a stochastic two-level system (a bit) and determine the probability for the time of transition. In this case the sample space then consists of two alternatives: 0 and 1. We assume that initially the system is found at state 0. The most general operator $\mathcal{L}$ consistent with the positivity and normalization of probabilities is

$$\mathcal{L}=\begin{pmatrix}-a & b\\ a & -b\end{pmatrix}. \tag{2.15}$$

The corresponding transition matrix for a small time interval δt is

$$\begin{pmatrix}1-a\,\delta t & b\,\delta t\\ a\,\delta t & 1-b\,\delta t\end{pmatrix}, \tag{2.16}$$

which is the most general stochastic map for a two-level system.

It is then easy to compute the probability density for the time of the transition $0\to 1$,

$$p(0\to 1;t)=be^{-bt}. \tag{2.17}$$

The probability $p(N)$ that no transition took place within the time interval $[0,T]$ equals e^{-bT}. As $T\to\infty$, $p(\infty)=0$, and we may compute the mean time of transition,

$$\langle t\rangle=b^{-1}, \tag{2.18}$$

which are the standard results for decay processes.

2. Wiener process

We next consider the case of the Wiener process, defined by the evolution operator,

$$\mathcal{L}\rho=\frac{D}{2}\partial^2\rho, \tag{2.19}$$

where D is a diffusion constant. We assume that the particle is initially localized at $x=-L$, namely $\rho_0(x)=\delta(x+L)$.

The operator K_t is the propagator corresponding to $\mathcal{L}$ with the Dirichlet boundary conditions at $x=0$. [This is, in fact, a more general result. A quick but not fully rigorous way to see this is by writing the characteristic function of a set C as $\chi_C(x)=e^{-V_C(x)\delta t}$, where $V_C(x)$ is a "confining

potential" that takes value 0 within C and ∞ outside C. We may then use the Trotter product formula $\lim_{n\to\infty}(e^{\mathcal{L}t/n}e^{-V_-t/n})^n=(\mathcal{L}-V_-)t$, which is exactly the propagator for $\mathcal{L}$ with Dirichlet conditions at the boundaries of C.]

The integral kernel $K(x,x';t)$ corresponding to K_t is

$$K(x,x';t)=\chi_-(x)\chi_-(x')\sqrt{\frac{1}{2\pi Dt}}(e^{-(x-x')^2/2Dt}-e^{-(x+x')^2/2Dt}), \tag{2.20}$$

yielding

$$p(t|x=0)=\sqrt{\frac{1}{2\pi Dt}}\frac{L}{2t}e^{-L^2/2Dt}, \tag{2.21}$$

while

$$p(N)=\mathrm{erf}(L/\sqrt{2DT})-\mathrm{erf}(-L/\sqrt{2DT}), \tag{2.22}$$

where erf is the error function.

III. THE COPENHAGEN DESCRIPTION

A. The standard construction and its problems

We next attempt to construct the time-of-arrival probability for quantum theory within the Copenhagen interpretation.

We split the time interval $[0,T]$ into n time steps of width $\delta t=T/n$. We represent the projection operators that correspond to the particle lying within $(-\infty,0]$ and in $[0,\infty)$ as $\hat{P}_-$ and $\hat{P}_+$, respectively. The time of arrival is defined as the moment the particle crosses from $(-\infty,0)$ to $[0,\infty)$. We assume that at $t=0$ the particle is described by a density matrix $\hat{\rho}_0$.

The probability that the particle crossed $x=0$ at time t_1 equals $p_1=\mathrm{Tr}(\hat{\rho}e^{i\hat{H}t_1}\hat{P}_+e^{-i\hat{H}t_1})$. The probability that the particle crossed $x=0$ at the next moment t_2 is then equal to

$$p_1p(-,t_1;+,t_2), \tag{3.1}$$

where $p(-,t_1;+t_2)$ is the conditional probability that the particle was found within $(-\infty,0]$ at t_1 and within $(0,\infty)$ at t_2. According to the standard "reduction" rule this equals

$$p(-,t_1;+t_2)=\frac{\mathrm{Tr}(\hat{P}_+e^{-i\hat{H}(t_2-t_1)}\hat{P}_-e^{-i\hat{H}t_1}\hat{\rho}_0e^{i\hat{H}t_1}\hat{P}_-e^{i\hat{H}(t_2-t_1)})}{\mathrm{Tr}(\hat{\rho}e^{i\hat{H}t_1}\hat{P}_-e^{-i\hat{H}t_1})}, \tag{3.2}$$

yielding

$$p_2=\mathrm{Tr}(\hat{P}_+e^{-i\hat{H}(t_2-t_1)}\hat{P}_-e^{-i\hat{H}t_1}\hat{\rho}_0e^{i\hat{H}t_1}\hat{P}_-e^{i\hat{H}(t_2-t_1)}). \tag{3.3}$$

Following the same procedure, we obtain the probability that the particle crossed $x=0$ at the kth time step,

$$p_k=\mathrm{Tr}(\hat{P}_+e^{-i\hat{H}(t_k-t_{k-1})}\ldots\hat{P}_+e^{-i\hat{H}(t_2-t_1)}\hat{P}_-e^{-i\hat{H}t_1}\hat{\rho}_0\times e^{i\hat{H}t_1}\hat{P}_-e^{i\hat{H}(t_2-t_1)}\hat{P}_-\ldots e^{i\hat{H}(t_k-t_{k-1})}). \tag{3.4}$$

As we take the continuum limit $n\to\infty$, assuming that the initial state has support only in $(-\infty,0)$, we obtain the probability that the particle was found between t and $t+\delta t$,

$$p([t,t+\delta t])=\delta t^2\,\mathrm{Tr}((\hat{C}_t\hat{H}\hat{\rho}_0\hat{C}_t^\dagger\hat{H}\hat{P}_+), \tag{3.5}$$

where

$$\hat{C}_t=(\hat{P}_-e^{-i\hat{H}t/n}\hat{P}_-)^n. \tag{3.6}$$

There are two severe problems in this result. First, the probability $p([t,t+\delta t])$ is proportional to δt^2, and hence does not define a probability density. If we tried to construct the probability for the detection within a finite time interval $[t_1,t_2]$ by integration, we would, strictly speaking, obtain zero, i.e., we would find that the particle is never detected.

Second, the probability that the particle never crosses $x=0$ within the time interval $[0,T]$ equals

$$p(N)=\mathrm{Tr}(\hat{C}_T\hat{\rho}_0\hat{C}_T^\dagger). \tag{3.7}$$

The operator $\hat{C}_t$ is a degenerate unitary operator with a support in the range of $\hat{P}_-$[10]—this is the well-known quantum Zeno paradox. It follows that $\hat{C}_t\hat{C}_t^\dagger=\hat{P}_-$, hence

$$p(N)=\mathrm{Tr}(\hat{\rho}_0\hat{P}_-)=1. \tag{3.8}$$

It seems as though the particle can never cross $x=0$, which is clearly a mistake. This problem can be addressed by noticing that the probabilities $p([t,t+\delta t])$ are, by definition, nonadditive with respect to the projectors and hence do not satisfy the Kolmogorov additivity condition, i.e., they are not probabilities at all. It is therefore no surprise that they do not define a probability density. One should employ for the continuum limit a probabilistic object that is additive with respect to the projectors. This is the decoherence functional of the consistent histories approach. The problem of the quantum Zeno effect is also partially alleviated in consistent histories, since the quantity $p(N)$ is not a genuine probability, unless a decoherence condition is satisfied. There are other problems, however, that appear in the implementation of the theory's classical limit. We will discuss this issue in more detail in the next section.

B. A different interpretation of the reduction procedure

An objection that can be raised to the derivation above has to do with the use of the conditional probability rule in Eq. (3.2). One may argue that since the particle has not been detected at time t_2, it has not interacted with the measuring device, and for this reason, one should not employ the "reduction of the wave packet" rule, because no measurement has actually taken place. (See the discussion in the Introduction). Instead of the conditional probability, one should use the full probability of detection at t_2, namely

$$\mathrm{Tr}(\hat{P}_+e^{-i\hat{H}t_2}\hat{\rho}_0e^{i\hat{H}t_2}) := \mathrm{Tr}(\hat{P}_+\rho_{t_2}); \tag{3.9}$$

hence the probability of detection at the kth time step equals

$$p_k=\left(1-\sum_{i=0}^{k-1}p_i\right)\mathrm{Tr}(\hat{\rho}_{t_k}\hat{P}_+), \tag{3.10}$$

This is a recursive equation with the following solution:

$$p_k=\mathrm{Tr}(\hat{\rho}_{t_k}\hat{P}_+)\prod_{-=0}^{k-1}[1-\mathrm{Tr}(\hat{\rho}_{t_i}\hat{P}_+)]=\mathrm{Tr}(\hat{\rho}_{t_k}\hat{P}_+)\exp\left[\sum_{i=0}^{k-1}\log(1-\mathrm{Tr}(\hat{\rho}_{t_i}\hat{P}_+))\right]. \tag{3.11}$$

The expression above does not have a natural continuum limit. The sum in the exponential does not define an integral, because a δt term is missing. Again, we face the problem that the dependence of the quantum mechanical probabilities on time does not correspond to the existence of a genuine probability measure—hence a continuous limit does not exist naturally.

One way to obtain a probability measure is to introduce a time step τ, which is a measure of the temporal resolution of the measuring device. For any time scales much larger than τ, one may substitute the sum in Eq. (3.11) with an integral, thus obtaining a probability measure on $[0,T]$,

$$p(t) = \frac{1}{\tau}\,\mathrm{Tr}(\hat{\rho}_t \hat{P}_+)\exp\left[\frac{1}{\tau}\int_0^t ds\ \mathrm{Tr}(\hat{\rho}_s \hat{P}_-)\right] = -\,e^{t/\tau}\frac{d}{dt}e^{-F(t)}, \tag{3.12}$$

where $F(t)=(1/\tau)\int_0^t ds\ \hat{\rho}_s \hat{P}_-$.

The probability density above has a physically reasonable behavior for a time-of-arrival probability. For a wave function whose center follows approximately a classical path, the probability density (3.12) is peaked around the classical time of arrival for this path. To see this one may consider Eq. (3.12) for a free particle of mass m. Considering an initial Gaussian state,

$$\psi_0(x) = \frac{1}{[\pi\sigma^2]^{1/4}} e^{-(x+L)^2/2\sigma^2 + ipx}, \tag{3.13}$$

peaked at $t=0$ around $x=-L$ with mean momentum p, we obtain for the function $F(t)$,

$$F(t) = \frac{1}{2\tau}\int_0^t ds\left[1 + \mathrm{Erf}\left(\frac{\left(L - \frac{p}{m}t\right)}{\sqrt{\sigma^2 + \frac{t^2}{m^2\sigma^2}}}\right)\right], \tag{3.14}$$

which implies that (3.12) has a strong peak around the classical time of arrival $t_{\mathrm{cl}}=Lm/p$.

The problem lies in the strong dependence of these probabilities on the parameter τ. While it is reasonable to assume that the probabilities will be dependent on parameters that characterize the method of detection, we would intuitively expect that this dependence would be insignificant when we consider sufficiently large intervals of time. This is definitely not the case here, as the probabilities are very sensitive on the value of τ.

Since quantum theory does not provide a natural way to pass into the continuum limit (at least in the scheme we consider in this section), it is natural to expect that different procedures will lead to different results. We may consider, for example, the following alternative.

In Eq. (3.11) we may substitute in place of $\hat{P}_+$ a projector $\hat{P}_{\delta x}$ in position of width δx around $x=0$, and the projector $\hat{1}-\hat{P}_{\delta x}$ in place of $\hat{P}_-$. This corresponds to a setup by which the particle is detected only if it crosses the region $[-\delta x/2, \delta x/2]$. We next assume that the size δx decreases with δt, so that, as $\delta t \to 0$, the area of detection also shrinks to zero. We therefore write $\delta x = v\ \delta t$, for some unspecified constant v with dimensions of velocity. This way of taking the limit essentially implies that the actual detection of a particle needs a finite time interval, since at the limit $\delta t \to 0, \hat{P}_{\delta x}=\hat{1}$.

Writing $\rho_t(0)=\langle x=0|\hat{\rho}_t|x=0\rangle$, we obtain at the limit $\delta t \to 0$ the probability that the particle is detected between time t and $t+\delta t$ as

$$p(t)\,\delta t = \delta t\, v\rho_t(0)e^{-v\int_0^t ds\ \rho_s(0)} = -\,\delta t\frac{d}{dt}e^{-v\int_0^t ds\ \rho_s(0)}. \tag{3.15}$$

Hence, the probability that the particle is detected within the time interval $[t_1,t_2]$ equals

$$p([t_1,t_2]) = e^{-v\int_0^{t_1} ds\ \rho_s(0)} - e^{-v\int_0^{t_2} ds\ \rho_s(0)}, \tag{3.16}$$

while the probability that the particle is not detected within the time interval $[0,T]$ equals

$$p(N) = e^{-v\int_0^T ds\ \rho_s(0)}. \tag{3.17}$$

The probability density (3.15) has the correct behavior at the classical limit, but again it depends on an unspecified parameter v, which this time has dimensions of velocity. One has to assume that v has to be identified with a characteristic property of the measuring device.

It follows that with the interpretation of the reduction rule we employed here, a probability distribution for the time of arrival cannot be constructed without making reference to the specific setup through which it is determined. Whatever scheme one might employ, one has to introduce additional parameters in the description.

It would be mistaken, however, to consider the derivation leading to Eqs. (3.15) or (3.12) as inherently faulty. The only assumption we employed is that the reduction rule can only be applied when an actual measurement has actually taken place, and not when we make an *inference* about the system by the fact that no detection has occurred. This implies, in particular, that the quantum Zeno effect is irrelevant for the time of arrival, because we do not have a continuous act of measurement (only a continuous inference). With this assumption the proof leading to (3.11) only employs the classical rules of probability theory. In that sense, the key mathematical problem is that the dependence of the quantum mechanical probabilities on time does not allow the definition of a stochastic process—see the related discussion in Ref. 12. Quantum probabilities *are not naturally densities with respect to time*; one can make them densities by introducing additional parameters.

It is important to note that this fundamental difficulty does not go away, when we enlarge the system by including degrees of freedom of the measurement device. The problem of finding a suitable continuous expression for (3.11) does not depend on specific features of the system's Hilbert space. The density matrix may include degrees of freedom of the measuring device or of an environment. The problem lies with the way time appears in the formalism of quantum theory.

In any case, Eqs. (3.15) and (3.12) provide interesting candidates for a probability distribution for a time of arrival. They have a proper classical limit and they are mathematically unambiguous. In principle, they could be checked by any precision measurement of times of arrival.

IV. THE HISTORIES DESCRIPTION

In this section, we follow a different approach from that of Sec. III B. We assume that the reduction rule can be applied in any case we have obtained information about a quantum system. This allows us to preserve the "logical" structure of quantum mechanical propositions. The natural scheme to explore the time-of-arrival problem is then the consistent histories approach. However, the results we obtain here are of a more general character. The mathematical objects employed in the consistent histories approach are essentially path integrals and the amplitudes defined by these path integrals can be employed for the study of the time of arrival in different schemes. (We do that in Sec. V). The most important gain from this approach is that the continuous-time limit can be obtained unambiguously, because it is implemented at the level of amplitudes and not at that of probabilities.

A. Consistent histories

The consistent histories approach to quantum theory was developed by Griffiths,[13] Omnés,[14] and Gell-Mann and Hartle.[15,16] The basic object is a history that corresponds to properties of the physical system at successive instants of time. A discrete-time history α will then correspond to a string $\hat{P}_{t_1}, \hat{P}_{t_2}, \ldots, \hat{P}_{t_n}$ of projectors, each labeled by an instant of time. From them, one can construct the class operator,

$$\hat{C}_\alpha = \hat{U}^\dagger(t_1)\hat{P}_{t_1}\hat{U}(t_1)\cdots\hat{U}^\dagger(t_n)\hat{P}_{t_n}\hat{U}(t_n), \tag{4.1}$$

where $\hat{U}(s)=e^{-i\hat{H}s}$ is the time-evolution operator. The probability for the realisation of this history is

$$p(\alpha) = \mathrm{Tr}(\hat{C}_\alpha^\dagger \hat{\rho}_0 \hat{C}_\alpha), \tag{4.2}$$

where $\hat{\rho}_0$ is the density matrix describing the system at time $t=0$.

However, the expression above does not define a probability measure in the space of all histories, because the Kolmogorov additivity condition cannot be satisfied: if α and β are exclusive histories, and $\alpha \vee \beta$ denotes their conjunction as propositions, then it is not true that

$$p(\alpha \vee \beta) = p(\alpha) + p(\beta). \tag{4.3}$$

The histories formulation of quantum mechanics does not, therefore, enjoy the status of a genuine probability theory.

However, an additive probability measure *is* definable, when we restrict to particular sets of histories. These are called *consistent sets*. They are more conveniently defined through the introduction of a new object: the decoherence functional. This is a complex-valued function of a pair of histories given by

$$d(\alpha,\beta) = \mathrm{Tr}(\hat{C}_\beta^\dagger \hat{\rho}_0 \hat{C}_\alpha). \tag{4.4}$$

A set of exclusive and exhaustive alternatives is called consistent, if for all pairs of different histories α and β, we have

$$\mathrm{Re}\, d(\alpha,\beta) = 0. \tag{4.5}$$

In that case one can use Eq. (2.2) to assign a probability measure to this set.

B. Time-of-arrival histories

Histories and propositions about histories may be represented by projection operators on a Hilbert space $\mathcal{V} = \otimes_t H_t$, which the tensor product of the single time Hilbert spaces of standard theory—this is the History Projection Operator (HPO) formulation of the history theory.[17] The merit of this description is that the logical structure of history propositions is preserved (they form a lattice that corresponds with the lattice of subspaces of $\mathcal{V}$), and in the present context allows the arguments used for the time-of-arrival description of stochastic processes to be transferred into the quantum level. In particular, the continuum limit in time may be taken in an unambiguous manner. Note that in this scheme the decoherence functional is a Hermitian, bilinear functional on $\mathcal{V} \times \mathcal{V}$ that satisfies the following properties:

$$d(1,1) = 1, \tag{4.6}$$

$$d(0,\alpha) = 0, \tag{4.7}$$

$$d(\alpha,\alpha) \geq 0. \tag{4.8}$$

We next consider a description of time-of-arrival histories with n time steps. One defines the projectors $\hat{\alpha}_n$ corresponding to the proposition that the particle crossed $x=0$ for the first time between the mth and the $m+1$-th time step,

$$\hat{\alpha}_m = \hat{P}_- \otimes \hat{P}_- \otimes \cdots \otimes \hat{P}_+ \otimes \hat{1} \otimes \cdots \otimes \hat{1}, \tag{4.9}$$

as well as the projector $\hat{\bar{\alpha}}$ corresponding to the proposition that the particle does not cross $x=0$ within the n time steps,

$$\hat{\bar{\alpha}} = \hat{P}_- \otimes \hat{P}_- \otimes \cdots \otimes \hat{P}_-. \tag{4.10}$$

Clearly these projectors satisfy

$$\hat{\alpha}_n \hat{\alpha}_m = \delta_{nm} \hat{\alpha}_n, \tag{4.11}$$

$$\hat{\alpha}_n \hat{\bar{\alpha}} = 0, \tag{4.12}$$

$$\sum_m \hat{\alpha}_m + \hat{\bar{\alpha}} = 1. \tag{4.13}$$

Thus they form a exhaustive and exclusive set of histories, hence a sublattice of the lattice of history propositions. (One should note that the n time histories we study here should not be viewed as discretizations of continuous time paths, but as histories corresponding to genuinely discrete time. The consideration of discretized alternatives in a continuous-time theory is conceptually problematic because at any time between t_i and t_{i+1} the particle may have crossed $x=0$, and this fact will not be captured in the resulting propositions. Our approach is that we first consider alternatives of detection in a discrete-time theory, and we then identify a suitable continuous limit for the decoherence functional. This involves a choice on the way we *define* the continuous histories. This choice allows us to recover known results.[8,22] However, this procedure may not be unique–see the discussion on alternative treatments of the quantum Zeno effect.) One can therefore pullback the decoherence functional to this lattice, thereby obtaining a decoherence functional on a sample space consisting of the points $(t_1,\ldots,t_n)$ together with the point N corresponding to no crossing,

$$d(t_n,t_m) = d(\hat{\alpha}_n,\hat{\alpha}_m), \tag{4.14}$$

$$d(N,t_n) = d(\hat{\bar{\alpha}},\hat{\alpha}_n), \tag{4.15}$$

$$d(N,N) = d(\hat{\bar{\alpha}},\hat{\bar{\alpha}}). \tag{4.16}$$

In analogy to the stochastic case, one may define a self-adjoint time-of-arrival operator $\hat{T}$ on $\mathcal{V}$ modulo its value on the subspace corresponding to $\hat{\bar{\alpha}}$, namely one may define

$$\hat{T}_{x=0} = \sum_i t_i \hat{\alpha}_i, \tag{4.17}$$

which is unambiguously defined on $\mathcal{V}-\mathrm{Ran}(\hat{\bar{\alpha}})$ – $\mathrm{Ran}(\hat{\bar{\alpha}})$ is the closed linear subspace corresponding to $\hat{\bar{\alpha}}$.

We next consider two discretizations $\{t_0=0,t_1,t_2,\ldots,t_N=T\}$ and $\{t'_0=0,t'_1,t'_2,\ldots,t'_{N'}=T\}$ of the time interval $[0.T]$ with time step $\delta t=T/N$, and $\delta t'=T/N'$. We construct the decoherence functional $d([t,t+\delta t],[t',t'+\delta t'])$, where $n=tN/T$ and $m=t'N'/T$. This reads as

$$d([t,t+\delta t],[t',t'+\delta t']) = \mathrm{Tr}(\hat{\rho}_0[e^{i\hat{H}\,\delta t'}\hat{P}_-]^n e^{i\hat{H}\,\delta t'}\hat{P}_+ \times e^{i\hat{H}(t'-t)}\hat{P}_+ e^{-i\hat{H}\,\delta t}[\hat{P}_- e^{-i\hat{H}\,\delta t}]^m). \tag{4.18}$$

We take then the limit $N,N'\to\infty$, while keeping t and t' fixed. Assuming that ρ_0 lies within the range of $\hat{P}_-$, i.e., $\hat{P}_-\hat{\rho}_0\hat{P}_-=\hat{\rho}_0$ we obtain

$$d([t,t+\delta t],[t',t'+\delta t']) = \delta t\ \delta t'\ \mathrm{Tr}(e^{-i\hat{H}(t'-t)}\hat{P}_+\hat{H}\hat{P}_-\hat{C}_t^\dagger\hat{\rho}_0\hat{C}_{t'}\hat{P}_-\hat{H}\hat{P}_+), \tag{4.19}$$

where $\hat{C}_t=\lim_{n\to\infty}(\hat{P}_- e^{-i\hat{H}t/n}\hat{P}_-)^n$. Writing

$$\rho(t,t') = \mathrm{Tr}(e^{-i\hat{H}(t'-t)}\hat{P}_+\hat{H}\hat{P}_-\hat{C}_{t'}^\dagger\hat{\rho}_0\hat{C}_t\hat{P}_-\hat{H}\hat{P}_+), \tag{4.20}$$

we see that the decoherence functional corresponds to a complex-valued density on $[0,T]\times[0,T]$. The additivity of the decoherence functional (which reflects the additivity of quantum mechanical amplitudes) allows us to obtain a continuum limit, something that could not be done if we worked at the level of probabilities. Consequently, one may obtain its values on coarse-grained histories corresponding to a time-of-arrival lying within the subsets $[t_1,t'_2]$ and $[t'_1,t'_2]$ of $[0,T]$ by integrating over $\rho(t,t')$,

$$d([t_1',t_2'],[t_1,t_2]) = \int_{t_1}^{t_2} dt \int_{t_1'}^{t_2'} dt'\ \rho(t,t'). \tag{4.21}$$

We then obtain the values of the decoherence functional for any pair of measurable subsets of $[0,T]$. However, the decoherence functional on $[0,T]$ is not properly normalized, because the actual space of time-of-arrival propositions is not the space of subsets of $[0,T]$, but rather the space of subsets of $[0,T]\cup\{N\}$, where N corresponds to the event of no detection. The values of the decoherence functional, when at least one of its entries is N are easily computed

$$d([t_1,t_2],N) = \int_{t_1}^{t_2} dt\ \mathrm{Tr}(e^{-i\hat{H}(T-t)}\hat{C}_T^\dagger\hat{\rho}_0\hat{C}_t\hat{P}_-\hat{H}\hat{P}_+), \tag{4.22}$$

$$d(N,N) = \mathrm{Tr}(\hat{C}_T^\dagger\hat{\rho}_0\hat{C}_T) = 1. \tag{4.23}$$

The last equation is due to the fact that the operator $\hat{C}_t$ is a degenerate unitary operator with support on the range of $\hat{P}_-$ (the quantum Zeno effect).

The normalization condition for the decoherence functional implies that

$$d([0,T],[0,T]) + d([0,T],N) + d(N,[0,T]) + d(N,N) = 1, \tag{4.24}$$

which leads to

$$d([0,T],[0,T]) = -2\ \mathrm{Re}\ d([0,T],N). \tag{4.25}$$

It is important to note that in the context of consistent histories, the fact that $d(N,N)=1$ does not imply that the event N (never crossing $x=0$) will be realized, because $d(N,N)$ does not correspond to a probability, unless the consistency condition $\mathrm{Re}\ d[0,T],N)=0$ is satisfied. In this case, however, $d([0,T],[0,T])=0$, and hence that crossing $x=0$ never takes place. This implies that the event of the particle not crossing the surface $x=0$ can only be a member of a consistent set in which the probability for crossing $x=0$ is zero. This is rather counterintuitive, because it fails to give a correct classical limit—see the related discussion in Ref. 21. One would expect that at some level of coarse graining, one would obtain the classical result, namely a probability distribution sharply peaked around the classical time of arrival t_{cl}, similar to the one we derived in the last section.

1. Possible treatments of the quantum Zeno effect

A key feature of the quantum Zeno effect is that it is not robust. When one employs a positive operator $\hat{E}$ in the definition of the operator $\hat{C}_t$ (instead of a projector), the result is no more a degenerate unitary operator. This is true even if the operator $\hat{E}$ is very close to a true projector $\mathrm{Tr}|\hat{E}^2-\hat{E}| = \epsilon\,\mathrm{Tr}\,\hat{E}$, for a number $\epsilon \ll 1$. In that case the matrix elements of $\hat{C}_t$ fall with $e^{-\epsilon t}$, as we demonstrate in a simple example in the Appendix. This implies that even a very small deviation from a true projector leads to a qualitatively different result.

If our calculation of probabilities refers to actual measurements then the quantum Zeno effect should not pose a problem. Realistic measurements should be represented by POVMs rather than projection-valued-measures, in which case the quantum Zeno effect does not arise. However, this would spoil the continuous-time limit, which depends crucially on the fact that the operators $\hat{P}_+$ and $\hat{P}_-$ correspond to exclusive alternatives. A naive substitution of the operators $\hat{P}_+$ and $\hat{P}_-$, by partially overlapping approximate projectors would introduce extra terms in the expression of the decoherence functional. It is easy to verify that these terms would be of the order of $||\hat{P}_+\hat{P}_-||$ and not dependent on δt, hence they would remain nonzero even at the limit $\delta t \to 0$. One could entertain the possibility that the approximate projectors could be dependent on δt, and that at the

limit of δt their overlap becomes zero, i.e., they become true projectors. We have explored this possibility, but it does not seem to work. The Zeno effect still persists at the continuum limit. (This can easily be seen in the example we provide in theAppendix A.)

While the continuous-time limit we constructed here leads invariably to a quantum Zeno effect, this is not the only way that this limit can be taken in the histories formalism. The construction of the decoherence functional we presented here is obtained from a limit of discrete time expression. We have not constructed actual continuous time histories and defined the decoherence functional straightforwardly on them. To do that one should proceed in the logic of the HPO approach and construct a history Hilbert space that would correspond in some sense to a "continuous-tensor product" of single-time Hilbert spaces. Such Hilbert spaces have been constructed before;[18,6] they are not genuine continuous tensor products, but they share many of their features, and they are obtained from group-theoretical arguments. A key property of this construction is that propositions have support on finite time intervals $[t_1,t_2]$ and not on sharp points of the real line. The operator structure is then quite different at the kinematical level, and it raises the possibility that one could define a decoherence functional as a genuinely continuum object, in a way that does not suffer from the Zeno effect. For example, it is plausible that the operators entering the definition of the operator $\hat{C}_t$ as the limit of $\delta t \to 0$, should also be dependent on δt, as they should refer to finite intervals of the real line rather than sharp points. As we argued earlier, even a small change might be sufficient to remove the undesirable properties of $\hat{C}_t$; the real issue is to justify such changes from first principles within the continuous-time-histories formalism. We shall elaborate on this construction in a follow-up paper.

2. Conditioning

As we showed in Sec. II, it is possible in classical probability to reduce the probability measure from the full algebra of subsets in $[0,T]\times\{N\}$ to the algebra of events on $[0,T]$. This reduction results from the use of conditional probability. We defined a probability for the time of arrival conditioned upon the premise that the particle did cross $x=0$ at some time within the interval $[0,T]$.

This reasoning may be partially transferred to the quantum case. We cannot speak, however, for a conditional probability because this involves the consideration of consistent sets. Classical conditional probability is defined through a natural mathematical procedure, which employs the additivity of the probability measure over the space of functions on the sample space, to reduce the level of description into a subalgebra of events. Quantum probabilities are not additive over the lattice of events, but the decoherence functional is. In Refs. 20 the procedure of conditioning at the level of decoherence functional has been developed in detail, by generalizing the classical notion of conditional expectation to the quantum level. One may define a decoherence functional over a subalgebra of events (namely propositions about histories), thus incorporating any information we may have obtained for the system. For the details of the procedure, we refer the reader to Ref. 20, but for the simple case that the subalgebra with respect to which we implement the conditioning is generated by a single history proposition β, such that $d(\beta,\beta)\neq 0$, the conditioned decoherence functional is given by the intuitively simple expression

$$d_c(\alpha,\alpha') = \frac{d(\alpha\wedge\beta,\alpha'\wedge\beta_i)}{d(\beta,\beta)}. \tag{4.26}$$

The resulting decoherence functional is the mathematical object that should be used in the derivation of probabilities, provided we know that events corresponding to the subalgebra have been realized.

In the present case, we need to condition the decoherence functional from the algebra of events corresponding to the sample space $[0,T]\times\{N\}$ to the subalgebra of events corresponding to a sample space $[0,T]$, namely assuming that the particle has actually been detected. Since this operation involves "discarding" only a simple point of the sample space, the result is very simple. The conditioned decoherence functional d_c is obtained by a conditioned density,

$$\rho_c(t,t') = \frac{\rho(t,t')}{d([0,T],[0,T])} = \frac{\rho(t,t')}{-2\,\mathrm{Re}\,d([0,T],N)}. \tag{4.27}$$

Since the event of no detection is removed from the resulting subalgebra, we may pretend that we have avoided the quantum Zeno effect. This is, however, an evasion and not a solution to the problem. It only allows one to differentiate the problem of defining a probability for the time of arrival, from the more general issue of properly defining a continuum limit, that avoids the quantum Zeno effect.

C. The free particle

For the simple case of a particle at a line with Hamiltonian $\hat{H}=\hat{p}^2/2M+V(\hat{x})$, where the potential is bounded from below, we may employ a result in Refs. 8 and 22 that the restricted propagator $\hat{C}_t$ is obtained from the Hamiltonian $\hat{H}$ by Dirichlet boundary conditions. (The result cited is valid for bounded intervals of the real line; the generalization to semibounded intervals, however, is straightforwardly obtained using their method.) If we also denote by $G_0(x,x'|t)$ the full propagator in the position basis (corresponding to $e^{-i\hat{H}t}$), we obtain

$$\rho(t,t') = \frac{1}{4M^2}\partial_x(\hat{C}_{t'}\psi_0)^*(0)\partial_x(\hat{C}_t\psi_0)(0)G_0(0,0|t'-t), \tag{4.28}$$

$$d(t,N) = -\frac{1}{2M}\int_{-\infty}^{0} dx(\hat{C}_T\psi_0)^*(x)\partial_x(\hat{C}_t\psi_0)(0)G_0(x,0|T-t), \tag{4.29}$$

where $\hat{\rho}_0=|\psi_0\rangle\langle\psi_0|$, with ψ_0 having support in $(-\infty,0]$.

Note that in the derivation of the equations above, the derivative ∂_x arises from the presence of a term $\hat{P}_+\hat{H}\hat{P}_-$ in the operator product in Eq. (4.20). The contribution of the potential $V(x)$ vanishes, and the only contribution comes from the $\hat{p}^2$ of the kinetic energy.

For a free particle of mass M,

$$G_0(x,x',t) = \sqrt{\frac{M}{2\pi it}}e^{iM(x-x')^2/2t}, \tag{4.30}$$

$$C_t(x,x') = \chi_-(x)\chi_-(x')\sqrt{\frac{M}{2\pi it}}[e^{iM(x-x')^2/2t} - e^{iM(x+x')^2/2t}], \tag{4.31}$$

leading to

$$\partial_x(\hat{C}_t\psi_0)(0) = \sqrt{\frac{M}{2\pi it}}\int_{-\infty}^{0} dx\frac{-2iMx}{t}e^{i(Mx^2/2t)}\psi_0(x) := -2\partial_x(\hat{U}_t\psi_0)(0), \tag{4.32}$$

where we assumed that $\hat{P}_-\psi_0=\psi_0$.

It follows that

$$\rho(t,t') = \left(\frac{\hat{p}}{M}\hat{U}_t\psi_0\right)(0)\left(\frac{\hat{p}}{M}\hat{U}_{t'}\psi_0\right)^*(0)\sqrt{\frac{M}{2\pi i(t'-t)}}. \tag{4.33}$$

D. The classical limit

To verify that the decoherence functional for the free particle has the correct classical limit, we consider a Gaussian initial state centered around $x=-L$ and with mean momentum equal to p,

$$\psi_0(x) = (\pi\sigma_0^2)^{-1/4} e^{-(x+L)^2/2\sigma_0^2 + ipx}. \tag{4.34}$$

This state is localized within $[-\infty, 0]$ within an error of order e^{-L^2/σ^2}. We then obtain

$$\partial_x(\hat{C}_t\psi_0)(0) = \frac{2p}{\pi^{1/4}}\sqrt{\frac{\sigma_0}{\sigma^2(t)}}\left(\frac{t-t_{\mathrm{cl}}}{M\sigma^2(t)} + i\right) e^{-\left(p^2/2m^2\sigma^2(t)(t-t_{\mathrm{cl}})^2 - i\frac{p^2}{M}(t-t_{\mathrm{cl}})\right)}, \tag{4.35}$$

where

$$\sigma^2(t) = \sigma_0^2\left(1 + i\frac{t}{M\sigma_0^2}\right), \tag{4.36}$$

and $t_{\mathrm{cl}} = LM/p$ is the classical time of arrival.

Choosing T very large ($T \to \infty$), so that the classical time of arrival lies well within $[0,T]$ we see that the bidensity $\rho(t,t')$ has a singularity for $t=t'$ and that it is sharply peaked in each of its arguments around $t_{\mathrm{cl}} = LM/p$, with a width δ of the order of

$$\delta = \frac{M|\sigma(t_{\mathrm{cl}})|}{p} = \frac{M\sigma_0}{p}\sqrt{1 + \frac{L^2}{\sigma_0^4 p^2}}. \tag{4.37}$$

Note that for large values of L/p, the width δ also becomes very large. This is due to the fact that the free time evolution causes the wave packet to spread in time. A very small value of σ_0 (hence a large initial momentum uncertainty) leads to large values of δ.

Hence, if we consider a coarse-grained history α_{cl} for the time of crossing, which is centered around t_{cl} and has a width of $\Delta t \gg \delta$, and we denote as α'_{cl} the complement of α_{cl}, we obtain for the conditioned decoherence functional,

$$|d_c(\alpha_{\mathrm{cl}}, \alpha'_{\mathrm{cl}})| = O(e^{-(\Delta t/\delta)^2}), \tag{4.38}$$

$$d_c(\alpha_{\mathrm{cl}}, \alpha_{\mathrm{cl}}) = 1 - O(e^{-(\Delta t/\delta)^2}); \tag{4.39}$$

hence we conclude that history α_{cl} will almost definitely be realized, provided the particle crosses $x=0$ at some time within $[0,T]$.

Clearly there exists no classical limit, if either the initial state is not sufficiently localized in position, or if it is too localized so that the momentum uncertainty is very large, or if it is a superposition of states with a distinct value of momentum.

E. Inclusion of measurement device

In the consistent histories interpretation probabilities are only defined, if the consistency condition is satisfied. For time-of-arrival propositions, this occurs for coarse-grained histories like α_{cl} of Sec. IV D, which essentially correspond to the classical result. (Note that this result is obtained after conditioning the decoherence functional upon arrival.) However, consistent histories refer to closed systems—hence, to obtain a prediction for the time-of-arrival probabilities in the general case, we have to model the interaction of the particle with the measuring device.

There are various models for such an interaction with various degrees of complexity[23] (or for a more general case see Ref. 24). We consider here a very simple one, which will allow us to analyze some basic features of this procedure. We model the pointer of the measuring device with a two-level system. The pointer is found in the state of lower energy, while the state of higher energy corresponds to the detector having clicked. The combined Hamiltonian of the system + apparatus is then

$$\hat{H} = \frac{\Omega}{2}(1 - \sigma_3) + \hat{H}_0 + \epsilon \hat{P}_+ \sigma_1, \tag{4.40}$$

where $\hat{H}_0$ is the particle's Hamiltonian, and the interaction characterized by a coupling constant ϵ is switched on, only when the particle enters the region $x > 0$. We next construct histories similar to the ones of Sec. IV, only that they would refer to the properties of the pointer, i.e., they would be constructed from projectors of the form

$$\hat{E}_+ = \hat{1}_{\text{particle}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{E}_- = \hat{1}_{\text{particle}} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.41}$$

inserted into the definition of histories of the form (4.9) and (4.10). Hence, we seek the moment of transition from the lowest energy state of the detector to the higher energy state.

We assume that the initial state is factorized

$$\hat{\rho} = \hat{\rho}_0 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

where $\hat{\rho}_0$ is the particle's density matrix. Using similar arguments, we obtain the following expressions for the densities defining the decoherence functional:

$$\rho(t,t') = \epsilon^2 \operatorname{Tr}(e^{-i\hat{H}_0(t'-t)} \hat{P}_+ e^{-i\hat{H}_0 t} \hat{\rho}_0 e^{i\hat{H}_0 t'} \hat{P}_+) + O(\epsilon^4), \tag{4.42}$$

$$d(t,N) = \epsilon \operatorname{Tr}(e^{-i\hat{H}_0(T-t)} \hat{P}_+ e^{-i\hat{H}_0 t} \hat{\rho}_0), \tag{4.43}$$

while $d(N,N) = 1$. Again we can define the conditioned decoherence functional on $[0,T]$ as $\rho_c(t,t') = \rho(t,t')/d([0,T],[0,T])$.

This model does not solve the fundamental problem of defining a probability density—one can easily check that the consistency condition is approximately satisfied only for highly coarse-grained histories centered around the classical time of arrival. On one hand, this is not a surprise. Realistic measurement devices are much more complex than the system described by the Hamiltonian (4.40). Moreover, they involve by necessity a degree of irreversibility, which is incompatible with a unitary evolution law (see, for example, a model in Ref. 25): the states of detection and no detection are asymmetric, because the latter involves an amplification procedure that leads to a macroscopic designation that the particle has been detected. Such an asymmetry is incompatible with unitary evolution.

On the other hand, the present model demonstrates a rather generic feature associated with the measurement problem, that makes its present felt in all interpretations of quantum theory that attempt to describe the measurement process unitarily. In the consistent histories approach measurement devices are thought of as quantum systems, which are characterized by a consistent set of histories for the pointer device, so that the values of the pointer can be ascertained individually (and assigned probabilities) for a large class of initial states of the measured system.[14,16] This is equivalent with obtaining a density matrix diagonalized in a basis factorized with respect to the degrees of freedom of the system and the measuring device, which is necessary in order to attribute definite values to the macroscopic pointer.

In the model we presented here, this is clearly not the case. There exist also very general theorems that state that such a factorization is, in general, not possible,[27] (see also the discussion in Refs. 28–30 and in a different but related context the theorems of Ref. 31). The general argument is rather simple and in the present context takes the following form. The derivation of the decoherence functional for time-of-arrival histories remains the same, whether the Hilbert space is that of a single quantum system, or if it includes the degrees of freedom of a measurement device or of an environment. The nonzero value of the off-diagonal elements of the decoherence functional would then still persist, except possibly for the case of sufficient coarse graining

corresponding to the classical results. Hence, it seems that, unless we introduce additional assumptions, the consistent histories scheme cannot produce more detailed information about the time-of-arrival probability, beyond the determination of the classical limit.

The situation is different when the evolution of the particle (rather than that of the measurement device) involves a degree of irreversibility.[26] Indeed, in the presence of a decohering environment, the evolution of the particle is closely approximated (after a typically short decoherence time) by a stochastic process, in which case one may employ the construction of time-of-arrival probabilities sketched in Sec. II. However, the time of arrival seems to depend rather crucially on properties of the environment, which seems to destroy much "more" interference than what is necessary to define a consistent set of histories. [There is a rather paradoxical situation in the presence of environment. If the full quantum mechanical treatment of system+environment is taken into account, in which case the full evolution law is unitary, we are faced with the quantum Zeno effect. Any proposition about the system will be represented by projection operators, and the operator $\hat{C}_t$ will still be a degenerate unitary operator. If, however, one describes the effect of the environment in terms of a nonunitary evolution (or a stochastic process), an excellent approximation in many cases, no such problem seems to arise. This suggests again that the quantum Zeno effect is not robust.]

Another possibility would be to consider a different measuring apparatus interacting with the particle at each moment of time. This, however, would describe a different physical circumstance than the one we consider in this paper. Here we consider the case that the only information we can obtain from the system is a signal that the particle has been detected at a specific moment of time, i.e., there is a single event of measurement. Inserting multiple measuring devices would be equivalent to letting the particle move within a material that records its track (like a bubble chamber). In that case our datum is a continuous history of the particle, and can be treated within the theory of continuous time measurement. Such an interaction inevitably causes the particle to decohere, and as such its evolution can be well approximated by a stochastic process. The derivation of the time of arrival would the be much simpler in this case and would follow the general scheme of Ref. 26. This is, however, different from the issue taken up in this paper.

V. AN OPERATIONAL DESCRIPTION FOR TIME-OF-ARRIVAL MEASUREMENTS

The derivation of the decoherence functional for the time-of-arrival propositions does not answer the question we asked at the beginning of this paper: it is, in principle, possible to measure the time of arrival in individual runs of an experiment, therefore constructing the relative frequencies for a detection of the particle within any time interval $[t_i, t_f]$. From these frequencies of events we can construct in the limit of a large number of runs a probability for the detection of the particle within any time interval. One then is entitled to ask how to obtain this operationally meaningful probability density from the rules of quantum theory.

The main contribution of the histories formalism to the final result is that it allows one to implement the continuous-time limit. However, this passage refers not to a probability density, but to the decoherence functional, and one needs further assumptions in order to construct genuine probabilities. As the expression (4.20) for the decoherence functional demonstrates, there is persistent interference between the different alternatives for the time of arrival.

This problem is not specific to the time-of-arrival measurements. It is a special case of a more general problem, that of defining a probability density for the outcomes of measurement that take place at more than one moment of time. This issue has been analyzed in Refs. 11 and 12. In sequential measurements it is possible to obtain the probabilities in terms of a Positive-Operator-Valued Measure, whose mathematical form is markedly similar to the "probabilities" constructed by the consistent histories approach. We shall attempt to do the same here for the time-of-arrival probabilities, thus exploiting the convenient continuous-time limit incorporated in the decoherence functional.

Note that the considerations in this section are purely operational and employ the Copenhagen interpretation: we do not consider closed, individual systems, but are only interested in probabili-

ties obtained in specific measurement situations, which we assume refer to a statistical ensemble. Hence, even though we shall use the mathematical apparatus of consistent histories, the context in which we work is markedly distinct.

A. Probabilities for sequential measurements

1. Discrete spectrum

Let us consider the two-time measurement of an observable $\hat{x}=\Sigma_i \lambda_i \hat{P}_i$ with a discrete spectrum. Writing $\hat{Q}_i=e^{i\hat{H}t}\hat{P}_i e^{-i\hat{H}t}$, we construct the probabilities for the most-fine grained two-time results,

$$p(i,0;j,t)=\mathrm{Tr}(\hat{Q}_j\hat{P}_i\hat{\rho}_0\hat{P}_i)=|\langle|\hat{\rho}_0|i\rangle|^2|\langle i|e^{-i\hat{H}t}|j\rangle|^2. \tag{5.1}$$

Irrespective of the interpretation of the measurement process, the probabilities (5.1) refer to the most elementary alternatives that can be unambiguously determined in the experimental setup corresponding to the sequential measurement of $\hat{x}$. Therefore, they can be employed to construct probabilities for general sample sets U_1, U_2 on the spectrum Ω of $\hat{x}$, namely,

$$p(U_1,0;U_2,t)=\sum_{i\in U_1}\sum_{j\in U_2} p(i,0;j,t). \tag{5.2}$$

The total probability is normalized,

$$p(\Omega,0;\Omega,t)=\sum_{ij}\mathrm{Tr}(\hat{Q}_j\hat{P}_i\hat{\rho}_0\hat{P}_i)=1, \tag{5.3}$$

a property that follows from the fact that $\Sigma_i\hat{P}_i=\Sigma_j\hat{Q}_j=\hat{1}$.

Equation (5.2) defines a POVM for two-time measurements. Note the difference from Eq. (4.2). Equation (4.2) is valid only for the most fine-grained alternatives. Any further coarse graining is done by summing only the elementary probabilities that correspond to the value of the decoherence functional for the most fine-grained histories. This result implies that we can use the decoherence functional to construct POVMs for sequential measurements and may expect to repeat do the same for the case of time-of-arrival.

2. Continuous spectrum

When we consider the case of an operator with a discrete spectrum, a problem appears. There are no fine-grained projectors, and the choice of the elementary quantum probabilities, from which one may build the general probabilities for measurement outcomes, cannot be made uniquely.

The immediate generalization of Eq. (5.1) for the measurement of an operator with a continuous spectrum is

$$p(x_1,0;x_2,t)=|\langle x_1|\hat{\rho}_0|x_1\rangle|^2|\langle x_1|e^{-i\hat{H}t}|x_2\rangle|^2. \tag{5.4}$$

However, this does not define a proper probability density, because it is not normalized to unity,

$$\int dx_1 \int dx_2\, p(x_1,0;x_2,t)=\infty. \tag{5.5}$$

This is due to the fact that there can be no measurements of infinite accuracy. One has, therefore, to take into account the finite width of any position measurement, say δ. This quantity depends on the properties of the measuring device—for example, the type of the material that records the particle's position.

The simplest procedure is to consider the measurement of a self-adjoint operator $\hat{x}_\delta=\Sigma_i x_i \hat{P}_i^\delta$, where $\hat{P}_i^\delta$ is a projection operator corresponding to the interval $[x_i-\delta/2, x_i+\delta/2]$. In that case we may immediately construct the fine-grained probabilities,

$$p_\delta(i,0;j,t) = \mathrm{Tr}(\hat{Q}_j^\delta \hat{P}_i^\delta \hat{\rho}_0 \hat{P}_i^\delta), \tag{5.6}$$

from which we may construct probabilities for general sample sets U_1 and U_2:

$$p_\delta(U_1,0;U_2,t) = \sum_{i\in U_1}\sum_{j\in U_2} \mathrm{Tr}(\hat{Q}_j^\delta \hat{P}_i^\delta \hat{\rho}_0 \hat{P}_i^\delta). \tag{5.7}$$

Strictly speaking, one may only consider sample sets that are unions of the elementary sets that define our lattice. If, however, the size of the sample sets L is much larger than δ, we may approximate the summation with an integral. This amounts to defining the continuous version of probabilities (5.6),

$$p_\delta(x_1,t_1;x_2,t_2) = \mathrm{Tr}(e^{i\hat{H}(t_2-t_1)}\hat{P}_{x_2}^\delta e^{-i\hat{H}(t_2-t_1)}\hat{P}_{x_1}^\delta \hat{\rho}(t_1)\hat{P}_{x_1}^\delta), \tag{5.8}$$

where we denoted $\hat{P}_x^\delta = \int_{x-\delta/2}^{x+\delta/2} dy\,|y\rangle\langle y|$.

The important result of this analysis is that the probabilities for sequential measurements (5.6) depend strongly on the resolution δ of the measuring device. This dependence is very strong: even probabilities of sample sets coarse grained at a scale much larger than δ exhibit a very strong dependence on δ. From a mathematical point of view this dependence is a consequence of the fact that the off-diagonal elements of the decoherence functional between fine-grained multitime measurement outcomes do not vanish and are generically of the order of magnitude of the probabilities themselves. Hence, when we compare a probability corresponding to a value δ, with another one corresponding to 2δ, they differ by an amount proportional to the corresponding off-diagonal terms of the decoherence functional, which is, in general, substantially large. The reader is referred to Ref. 12 for extensive discussion and generalizations.

The construction probabilities for the outcomes of sequential measurements consists of two steps. First, we identify the most fine-grained alternatives compatible with the measuring device at hand, and we construct the corresponding elementary quantum probabilities by using the rule (4.2). These fine-grained alternatives (referred to by the index a) correspond to specific functions $F_a[x(\cdot)]$ on the space of paths Ω^I. The elementary probabilities will be

$$p(a) = d(F_a,F_a). \tag{5.9}$$

In the equation above the decoherence functional is viewed as a bilinear functional on Ω^I. For example, in the two-time measurement of position, the functions take the form $F_{ij}[x(\cdot)] = \chi_i^\delta(X_{t_1})\chi_j^\delta(X_{t_2})$, and

$$p_\delta(i,0;j,t) = d(F_{ij},F_{ij}). \tag{5.10}$$

The next step involves the summation over those elementary probabilities to construct an additive measure that assigns probabilities to every sample set obtained by the coarse graining of the elementary alternatives. We shall apply this procedure to the construction of time-of-arrival probabilities.

B. POVMs for time-of-arrival probabilities

Our contention is that the analysis of sequential measurements above may be transferred to the case of time-of-arrival measurements, because they share the crucial feature that they do not refer to the properties of a physical system at a single moment of time. This implies that the decoherence functional (4.20) may be employed for the construction of a POVM on $[0,T]$ for the time of arrival probabilities, in analogy to that of (5.6).

The diagonal elements $\rho(t,t)\delta t^2$ of the decoherence functional (4.20) is essentially the modulus square of the amplitude that is obtained by the sum over all paths that cross the surface $x=0$ within the interval $t+\delta t$. While the amplitude is obtained unambiguously through path integrals, its square cannot define a proper probability density, because of the presence of a term δt^2 rather than a δt one, but also because $\rho(t,t)$ diverges. (It is interesting to note that the δt^2

dependence disappears if the decoherence condition for histories holds—see Ref. 21.) This divergence is analogous to that of (5.4) for sequential measurements of position, and can be removed in a similar manner by assuming a finite temporal resolution τ. Hence, we consider elementary intervals $[t_i,t_{i+1}]$ of width τ, τ corresponding to the temporal resolution of our measurement device. The elementary probabilities will be

$$\rho_i^\tau = \int_0^T dt \int_0^T dt' \rho(t,t') \chi_i^\tau(t) \chi_i^\tau(t'), \tag{5.11}$$

where χ_i^τ is the characteristic function of the set $[t_i,t_{i+1}]$. One then may employ these probabilities to construct any probability corresponding to a set U constructed from the elementary cells $[t_i,t_{i+1}]$. By definition $\Sigma_i \chi_i^\tau = \chi_{[0,T]}$, hence the set of all i together with the event of no detection form a proper resolution of the unity.

The reader may object at this point that this leads us back to the discrete-time expression for the diagonal elements of the decoherence functional. This is not the case, because the probabilities (5.11) involve the sum over *all* continuous paths that are detected in the time interval $[t_i,t_{i+1}]$—hence it involves the contribution of any discretization within $[t_i,t_{i+1}]$.

It is more convenient to avoid the discretization procedure and construct a POVM on the continuous sample space $[0,T]$—see Ref. 12 for the analogous procedure in sequential measurements. For this purpose we introduce a family of smeared delta functions $f_\tau(s,s')$ characterized by the parameter τ, which satisfy the following properties:

$$\int_0^T ds\, f^\tau(s,s') = \chi_{[0,T]}(s'). \tag{5.12}$$

One may consider, for example, the following functions:

$$f_\tau(s,s') = \frac{1}{T} \sum_{n=-[T/\tau]}^{[T/\tau]} e^{i(n\pi/T)(s-s')}. \tag{5.13}$$

For practical purposes these are well approximated by the Gaussians (as long as $T \gg \tau$),

$$f^\tau(s,s') = \frac{1}{\sqrt{2\pi\tau}} e^{-(s-s')^2/2\tau^2}. \tag{5.14}$$

Thus, we may define the elementary probabilities in analogy to (5.6) as

$$p^\tau(t) = \int ds\, ds' \sqrt{f^\tau(t,s)} \sqrt{f^\tau(t,s')} \rho(s,s'), \tag{5.15}$$

and construct from them the probabilities for any set $U \subset [0,T]$ as

$$p^\tau(U) = \int_U dt\, p^\tau(t). \tag{5.16}$$

Up to an error of order τ, this is equivalent with the probabilities obtained by coarse graining the elementary discrete-time probabilities (5.11). [The use of the square root in (5.15) is necessary in order to guarantee the proper dimensions of the probability density (dimensions of $[T]^{-1}$). Another way to see this is by noticing that $\sqrt{\sqrt{2\pi\tau} f^\tau(t)}$, for the Gaussian (5.14) is a smeared characteristic function for the interval $[t-\sqrt{2\pi\tau}, t+\sqrt{2\pi\tau}]$, thus corresponding to a smeared version of (5.11), which needs to be divided by $\sqrt{2\pi\tau}$ in order to define a probability density. Note also that if the decoherence condition holds, Eq. (5.15) becomes, as it must, the Gaussian smearing of the probability distribution for arrival times.]

In effect, we associate to each set U the positive operator,

$$\hat{\Pi}(U) = \int_U dt\, \hat{R}_t \hat{R}_t^\dagger, \tag{5.17}$$

where

$$\hat{R}_t = \int ds \sqrt{f^\tau(t,s)} \hat{C}_s \hat{P}_- \hat{H} \hat{P}_+ e^{i\hat{H}s} \tag{5.18}$$

is an operator that corresponds to the sum over all paths that lie within $[-\infty, 0]$ and cross through to $[0, \infty)$ within a time interval of width τ around t.

These positive operators do not yet define a POVM, because the corresponding probabilities do not add up to unity. We have to also include the event N of no detection. The normalization condition implies that a positive operator $\hat{\Pi}(N)$ should be defined as

$$\hat{\Pi}(N) = \hat{1} - \int_0^T dt\, \hat{R}_t \hat{R}_t^\dagger. \tag{5.19}$$

The operator $\hat{\Pi}(N)$ is indeed positive, because

$$\int_0^T dt\, p^\tau(t) \leq \sup_{s,s' \in [0,T]} \left(\int_0^T dt \sqrt{f^\tau(t,s)} \sqrt{f^\tau(t,s')} \right) \int_0^T ds\, ds'\, \rho(s,s'). \tag{5.20}$$

Since f^τ is a smeared delta function, the term $\int_0^T dt \sqrt{f^\tau(t,s)} \sqrt{f^\tau(t,s')}$ is maximized for $s=s'$, in which case it equals $\int_0^T dt\, f^\tau(t,s) = \chi_{[0,T]}(s) \leq 1$. Hence, $\int_0^T dt\, p^\tau(t) \leq \int_0^T ds\, ds'\, \rho(s,s') = d([0,T],[0,T]) \leq 1$. Hence

$$p(N) = \mathrm{Tr}(\hat{\rho}\hat{\Pi}(N)) = 1 - \int_0^T dt\, p^\tau(t) \geq 0, \tag{5.21}$$

for all $\hat{\rho}$.

We have thus constructed a POVM for the time of arrival essentially by summing over all possible paths that correspond to crossing the $x=0$ surface within a time interval of width τ; τ was essentially introduced as a "regularization" parameter. In general, the POVM is expected to depend strongly upon its value. The key idea employed in this derivation is that time-of-arrival probabilities are not fundamentally different from the probabilities that correspond to measurements that take place at more than one moment of time. Whenever the measured quantity is continuous, it is necessary to introduce a parameter that determines the resolution of the measuring device, and it turns out that the constructed probabilities depend strongly on this parameter. Measurements of the time-of-arrival-like sequential measurements of position seem to be strongly contextual, namely, to depend strongly on the specific measurement device employed in their determination.[12]

Our derivation relied on two assumptions. The first one is that the reduction rule may be employed consistently for the incorporation of *any information* we may obtain about a quantum system (and not only for the results of actual measurements as in Sec. III B). The second assumption is that the construction of probabilities for sequential measurements may be applied in the context of time-of-arrival measurements through a generalization of Eq. (5.10). The key mathematical input arises from the histories description, namely, the fact that it is possible to construct a sample space for the values of the time of arrival by considering continuous-time histories of the system.

C. An explicit calculation: The free particle

We shall now compute the POVM (5.17) explicitly for the case of a free particle. This case is particularly interesting, because it allows the comparison with a well-established result, namely,

the POVM constructed by Kijowski.[4] Kijowski's POVM for the time of arrival of a free particle assigns to any pure state ψ_0 a probability density $p(t,\psi_0)$, which is normalized to unity in the interval $(-\infty,\infty)$,

$$p(t,\psi_0)=\left|\int_0^\infty dp\left(\frac{p}{2\pi m}\right)^{1/2}e^{-ip^2t/2M}\psi(p)\right|^2+\left|\int_{-\infty}^0 dp\left(\frac{-p}{2\pi m}\right)^{1/2}e^{-ip^2t/2M}\psi(p)\right|^2. \tag{5.22}$$

To construct the POVM (5.17) for a free particle we use Eq. (4.33) for the decoherence functional. Since the integration in (5.15) involves the square roots of the smeared delta-functions, which have a width of order τ, we may within an error of order $O(\tau/T)$ substitute the range of integration $\int_0^T ds\int_0^T ds'\to\int_{-\infty}^\infty ds\int_{-\infty}^\infty ds'$ and employ the Gaussian smearing functions (5.14).

The probability density associated with (5.17) can be written in the momentum representation as follows:

$$p(t)=\frac{1}{2\pi}\int dp\int dp'\frac{pp'}{M^2}R(p,p',t)\tilde{\psi}_0(p)\tilde{\psi}_0^*(p'), \tag{5.23}$$

where $\tilde{\psi}_0$ is the Fourier transform of ψ_0 and

$$R(p,p',t)=\int_{-\infty}^\infty ds\int_{-\infty}^\infty ds'\sqrt{f^\tau(t,s)}\sqrt{f^\tau(t,s')}e^{-i(p^2/2M)s+i(p'^2/2M)s'}\sqrt{\frac{M}{2\pi i(s-s')}}. \tag{5.24}$$

Changing variables to $u=1/2(s+s')$ and $v=s-s'$, we note that

$$\sqrt{f^\tau(t,s)}\sqrt{f^\tau(t,s')}=f_\tau(u-t)e^{-v^2/8\tau^2}. \tag{5.25}$$

Within an error of order $O(\tau/T)$, the function $f_\tau(u-t)$ behaves as a delta function when integrated over u, thus leading to

$$p(t)\simeq\frac{1}{2\pi}\int dp\int dp'\frac{pp'}{M^2}e^{-i(p^2/2M-p^2/2M)t}r\left(\frac{E_p+E_{p'}}{2}\right)\tilde{\psi}_0(p)\tilde{\psi}_0^*(p'), \tag{5.26}$$

where $E_p=p^2/2M$ and

$$r(\epsilon)=\sqrt{\frac{M}{2\pi}}\int_{-\infty}^\infty dv\frac{e^{-v^2/8\tau^2-i\epsilon v}}{\sqrt{iv}}=\sqrt{\frac{2M\tau}{\pi}}\int_0^\infty dy\frac{e^{-y^2/2}[\cos(2\epsilon\tau y)+\sin(2\epsilon\tau y)]}{\sqrt{y}}. \tag{5.27}$$

The integral in Eq. (5.27) can be computed explicitly in terms of modified Bessel functions; however, the physically interesting information is found in specific regimes for which $r(\epsilon)$ takes a simple form. For $\epsilon\tau\ll 1$, the leading contribution to the integral is a constant, leading to

$$r(\epsilon)=\frac{\Gamma\left(\frac{1}{4}\right)}{2^{3/4}}\sqrt{\frac{M\tau}{2\pi}}, \tag{5.28}$$

which implies that the probability density $p(t)$ is proportional to $\tau^{1/2}$, when $\tau\to 0$. Hence, at the limit that the temporal resolution tends to zero the particle is never detected, crossing the surface $x=0$.

The physically interesting regime corresponds to $\epsilon\tau\gg 1$. The parameter ϵ appears in (5.26) as the particle's energy, while τ is the temporal resolution of the measurement device. According to a common interpretation of the time-energy uncertainty principle, τ cannot be smaller than $(\Delta E)^{-1}$, where ΔE is the energy spread of the wave functions. Hence for any wave function with relatively small energy spread ($\Delta E/E\ll 1$), one expects that $\tau E\gg 1$. In general, it suffices that the wave-function has support only for values of energy much larger than $1/\tau$. The resolution τ is, by assumption, much smaller than t_{cl}, hence this range of energies is well defined whenever $Et_{\mathrm{cl}}\gg 1$.

Since $t_{\rm cl}=ML/\bar{p}$, where $\bar{p}$ is the initial state's mean momentum, the condition above is equivalent to $\bar{p}L\gg\hbar$, which is always satisfied in any macroscopic configuration for the measurement of the time of arrival.

At the limit $\epsilon\tau\gg 1$,

$$\int_0^\infty dy \frac{e^{-y^2/2}[\cos(2\epsilon\tau y)+\sin(2\epsilon\tau y)]}{\sqrt{y}} \simeq \sqrt{\frac{\pi}{\epsilon\tau}}; \tag{5.29}$$

hence the dependence on τ drops from the probability density (5.26),

$$p(t) \simeq \frac{1}{\pi}\int dp \int dp' \frac{pp'}{M\sqrt{\frac{1}{2}(p^2+p'^2)}} e^{-i(p^2/2M-p^2/2M)t}\tilde{\psi}_0(p)\tilde{\psi}_0^*(p'). \tag{5.30}$$

The POVM (5.30) is defined for positive values of time, and for wave functions that satisfy $\hat{P}_+|\psi_0\rangle=0$. To compare (5.30) with Kijowski's POVM of Eq. (5.22), which is normalized to unity by integration over for all times $t\in(-\infty,\infty)$, it is convenient to also extend the domain of the probability distribution (5.30) to the whole real axis for time, by requiring that the extended POVM is invariant under the combined action of the parity and time-reversal transformations.[4] We employ the convention that the negative times correspond to the crossing of $x=0$ from the right, i.e., to initial states that have support on values of position $x\in[0,\infty)$. We then construct an equal-weight convex combination of the probability distribution (5.30) for positive t with its counterpart for negative t. We thus obtain the extension of the probability distribution (5.30) for all real values of time and all initial wave functions $\tilde{\psi}_0(p)$,

$$p_{\rm ext}(t) \simeq \frac{1}{2\pi}\int dp \int dp' \frac{pp'}{M\sqrt{\frac{1}{2}(p^2+p'^2)}} e^{-i(p^2/2M-p^2/2M)t}\tilde{\psi}_0(p)\tilde{\psi}_0^*(p'). \tag{5.31}$$

If the wave function is sharply concentrated around the mean value $\bar{p}$, i.e., if $\Delta p\ll|\bar{p}|$, then $p^2+p'^2=2pp'+O((\Delta p/\bar{p})^2)$ within the integration in (5.30). The probability density (5.31) is then identical to (5.22). Integrating $p_{\rm ext}(t)$ over $t\in(-\infty,\infty)$, we obtain

$$\int_{-\infty}^{\infty} dt\, p_{\rm ext}(t) = 1 - \int dp\ \tilde{\psi}_0^*(-p)\tilde{\psi}_0(p). \tag{5.32}$$

We see therefore that $p_{\rm ext}(t)$ is normalized to unity, if the state $\tilde{\psi}_0(p)$ has support only on positive (or only on negative) values of momentum. In this case, $\hat{\Pi}(N)=0$, i.e., all particles are eventually detected. In general, a nonzero probability $p(N)$ of nondetection is due to the fraction of particles in the statistical ensemble, which move away from the crossing surface $x=0$.

We conclude therefore that the POVM (5.17) leads to the same probability distributions for the time of arrival with Kijowski's POVM (5.22) for all initial wave functions that (i) have support in values of momentum $|p|\gg\sqrt{2m/\tau}$, and (ii) satisfy $\Delta p\ll|\bar{p}|$. This regime includes the classical limit (e.g., wave functions of the form (4.34) with $\sigma_0 p\gg 1$), but also states that are not sharply localized in position, like superpositions of macroscopically distinct wave packets, or even superpositions of states with different value of momentum—as long as Δp remains much smaller than p. Outside this regime, the POVMs (5.17) and (5.22) provide different predictions.

To make the points above more explicit, we consider an initial Gaussian state,

$$\tilde{\psi}_0(p) = (a^2/2\pi)^{1/4}\exp\left(-\frac{a^2}{4}(p-\bar{p})^2+ipL\right) \tag{5.33}$$

of mean position $-L$ and mean momentum $\bar{p}$. The momentum spreads are equal to a. In leading order to $1/a\bar{p}$ the probability distributions for the time-of-arrival predicted by the POVMs (5.30) and (5.22) coincide,

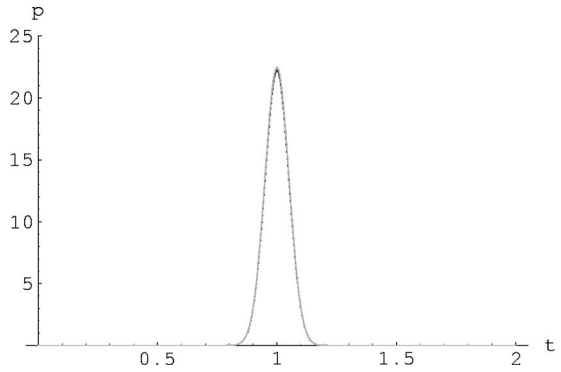

FIG. 1. The probability distribution of the time of arrival for a Gaussian initial state (5.33) of mean position $-L$ and mean momentum $\bar{p}$. It is sharply peaked around the value $t_{\mathrm{cl}}=ML/\bar{p}$. In fact, this plot contains the probability distributions provided by both POVMs (5.30) and (5.22), but even for the relatively large value of $\Delta p=0.1\bar{p}$ we employed here the two curves almost coincide.

$$p(t) \simeq \frac{\bar{p}}{\mathrm{Ma}\sqrt{8\pi}} e^{-(2/a^2)(L-\bar{p}t/M)^2}. \tag{5.34}$$

The difference between the two POVMs is of order $1/(\bar{p}a)^2$, and even for a relatively large value $1/\bar{p}a \simeq 0.1$ as in Fig. 1 their graphs are practically indistinguishable.

We next consider an initial state, which is a superposition of two Gaussians with the same mean position $-L$, but different mean momenta $\bar{p}_1$ and $\bar{p}_2$,

$$\tilde{\psi}_0(p) = \left(\frac{a^2}{4\pi}\right)^{1/4} [e^{-(a^2/4)(p-\bar{p}_1)^2+ipL} + e^{-(a^2/4)(p-\bar{p}_2)^2+ipL}]. \tag{5.35}$$

For $a\bar{p}_1 \gg 1$, $a\bar{p}_2 \gg 1$ and $a|\bar{p}_1-\bar{p}_2| \gg 1$, the leading contribution to the probability distribution obtained by the POVM (5.22) is

$$p(t) \simeq \frac{1}{\mathrm{Ma}\sqrt{8\pi}} \left[\frac{\bar{p}_1}{2} e^{-\frac{2}{a^2}(L-\bar{p}_1 t/M)^2} + \frac{\bar{p}_2}{2} e^{-\frac{2}{a^2}(L-\bar{p}_1 t/M)^2} + \sqrt{\bar{p}_1\bar{p}_2}\, e^{-(2/a^2)\left(L-\frac{1}{2}(\bar{p}_1+\bar{p}_2)t/M\right)^2} \right.$$
$$\left. \times \cos\left(\frac{\bar{p}_1^2 t}{2M} - \frac{\bar{p}_2^2 t}{2M}\right) \right], \tag{5.36}$$

and the leading contribution to the probability contribution obtained by the POVM (5.30) is

$$p(t) \simeq \frac{1}{\mathrm{Ma}\sqrt{8\pi}} \left[\frac{\bar{p}_1}{2} e^{-(2/a^2)(L-\bar{p}_1 t/M)^2} + \frac{\bar{p}_2}{2} e^{-(2/a^2)(L-\bar{p}_1 t/M)^2} \right.$$
$$\left. + \frac{\bar{p}_1\bar{p}_2}{\sqrt{\frac{1}{2}(\bar{p}_1^2+\bar{p}_2^2)}} e^{-(2/a^2)\left(L-\frac{1}{2}(\bar{p}_1+\bar{p}_2)t/M\right)^2} \cos\left(\frac{\bar{p}_1^2 t}{2M} - \frac{\bar{p}_2^2 t}{2M}\right) \right]. \tag{5.37}$$

We see that near the two classical values of the time of arrival that correspond to each of the two wave packets; the two probability distributions coincide. However, for intermediate values of time, they differ. They both manifest an oscillatory behavior there, which is characteristic of interference between the two classical values of the time of arrival. From Eqs. (5.36) and (5.37), we readily see that the oscillation amplitudes are different in this regime, and their ratio is given by the quantity $\frac{1}{2}(\bar{p}_1/\bar{p}_2+\bar{p}_2/\bar{p}_1)$. When this becomes appreciably larger than unity, i.e., if the

difference in mean momentum between the two Gaussians becomes comparable with the mean momenta themselves, the behavior of the two distributions in the oscillatory region becomes substantially different.

It is important to emphasize that the domain of applicability of the POVM (5.17) is much larger than that of the free particle case (for a generalization of Kijowski's distribution see also Ref. 32). It can be, in principle, applied for systems described by arbitrary Hamiltonians. Moreover, it is constructed through a general argumentation that does not refer only to the time of arrival and it can be easily generalized to systems with finite-dimensional Hilbert spaces, for which there is no analog of (5.22). To see this, one may consider Eqs. (5.17) and (5.18). The only objects appearing in the definition of the POVM is the Hamiltonian (together with its propagator $\hat{C}_t$) and the projection operators corresponding to the two alternatives of detection. The POVM (5.17) is therefore completely general. It can be applied, for example, the description of the particle being coupled to a measuring device, in which case the alternatives will correspond to projectors of the device's Hilbert space, and the Hamiltonian will contain an interaction term between the particle and the measurement device. It can also accommodate interactions with the environment i.e., further terms in the Hamiltonian. Its more immediate application would be the study of tunneling probabilities. This POVM may also refer to systems other than particles (e.g., multilevel atoms). Its derivation is only based on properties of Hilbert space operators and for this reason it can be applied to any physical context.

We chose to elaborate on the free particle case and ignore the effects of any measuring devices. The reason is that this system contains no other parameters other than the particle's mass (no couplings), and for this reason the only relevant time scale is t_{cl}. This allowed us to identify a physically relevant regime in which the time-of-arrival probabilities do not depend strongly on τ. Thus, we were able to compare our result with Kijowski's POVM. This, however, cannot be expected to hold for general systems, which may involve time scales of the same order of magnitude or smaller than τ. In the general case, the POVM (5.17) is expected to have a strong dependence on τ, even in physically relevant regimes.

D. The problem of contextuality

We saw that in the free particle case there exists a regime, in which the time-of-arrival probabilities are rather insensitive to τ, but this simple behavior cannot be expected to hold for systems with more complicated Hamiltonians that involve additional time scales. The POVM (5.17) will, in general, be strongly dependent on τ, and hence the probabilities for time will be strongly dependent upon the measurement scheme employed for their determination.

This contextuality of time measurements in quantum theory has been emphasized by Landauer in his study of tunneling times[33] (see also a related discussion with reference to the quantum Zeno effect[10]). However, this result is not a consequence of time being a special or distinguished variable. This type of contextuality is generic in quantum theory, once we consider measurements that do not refer to a single moment of time—e.g., sequential measurements of a continuous variable. This is a necessary consequence of the formalism of quantum theory: the evolution of the quantum state involves a linear law, while probabilities are quadratic with respect to the state. Hence, it is (in general) impossible to construct a natural probability measure for the outcomes of any measurement that reveals information that pertain to a system's dynamics (sequential, time-of-arrival, continuous measurements). This problem can be seen from different angles: from the fact that the dependence on time of the quantum probabilities do not define a probability measure and hence the continuous-time limit is not well defined (as in Sec. V B); from the fact that the natural measure for histories (4.2) is nonadditive; from the necessity to regularize the path integral amplitudes for the time of arrival in order to define probabilities; from the fact that there is interference between different alternatives for the value of the time of arrival. One therefore has to introduce an additional structure (external to the physical parameters of the system). The simplest such structure is the specification of the most fine-grained outcomes that can be recorded by a

measurement device. In the case of observables with a discrete spectrum, this is provided naturally by the formalism. For continuous variables, however, it is not, and this brings inevitably the introduction of a scale for the fine-grained alternatives.

We cannot evade this problem by enlarging our system, including, for example, a quantum measuring device or an environment. The problem is a consequence of the interplay between the quantum probability rule and the unitary dynamics. It will appear in any closed system (and will be accompanied by the quantum Zeno effect). Indeed, our arguments here were very general and hold with few modifications for an arbitrary Hilbert space and with reference to the detection of any quantum event. To avoid this problem (which can take a rather extreme form[12]) we have to abandon either the probability rule or the dynamics, and neither one of these steps is easy to take.

On the other hand, the acceptance of this contextuality is very disturbing. The devices that determine the time of arrival are not different in nature from the ones that measure a particle's position. (This is reflected in the fact that the histories for the time of arrival are written in terms of spectral elements of the position operator.) The only distinctive character in the time-of-arrival measurements is that the "observable" quantity is the reading of the clock, which is associated to the time of detection. In position measurements, however, the fuzziness due to the finite resolution of the measurement device is relatively small, when the sampling of the measurement results are sufficiently coarse grained. On physical grounds, one would expect that coarse graining at a scale much larger than the temporal resolution of the measurement device would give results independent of the device. Unlike the case of the free particle there is no reason to expect this for a general Hamiltonian—unless one considers the highly coarse-grained samplings around the classical equations of motion.

VI. CONCLUSIONS

We have considered the problem of constructing a probability density for the time of arrival. Our main guideline was the fact that time appears as an external parameter in quantum theory. We relied on the histories formalism, because they allow the natural definition of probabilities about the time of arrival.

In our perspective, the most severe problem in the determination of the time-of-arrival probability is the fact that the quantum states do not correspond to densities with respect to time. For this reason it is very difficult to obtain the continuous-time limit in a natural way. The naive way of taking the continuous-time limit gives very bad results, as it is plagued by the quantum Zeno effect. The first alternative we tried is to employ a more strict operational interpretation of the wave packet reduction, namely, that it can only be applied as a result of a system's *physical* interaction with a measurement device, and not when we obtain information about the system through inference from the lack of a detection signal. Again, the continuous-time limit was pathological and involved the introduction of an arbitrary temporal resolution.

We then considered this problem in light of the consistent histories approach. This suggests that the continuous-time limit should be taken at the level of amplitudes and not of probabilities, and for this reason it can be taken unambiguously. The consistent histories framework, however, is not sufficient for the definition of probabilities—there is "interference" between different values of the time of arrival. This problem is aggravated by the presence of the quantum Zeno effect.

Nonetheless, the mathematical benefits conveyed by the histories techniques are very important and prove essential for the construction of a POVM for the time of arrival (working, however, within the operational formulation of quantum mechanics). The consideration of measurements smeared in time allows us to construct a POVM of general validity for the time of arrival, in analogy with POVMs for the probabilities of sequential measurements. For free particles, this POVM reduces to one obtained by Kijowski. For a general system, however, the constructed POVM also depends strongly on the resolution of the measurement device. This seems to imply that the measurement of the time of arrival is highly contextual within standard quantum theory.

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APPENDIX A: THE QUANTUM ZENO EFFECT IS NOT ROBUST

We provide here a simple example demonstrating the quantum Zeno effect is not robust, in the sense that even a small deviation from a projection operator in the definition (3.6) of the operator $\hat{C}_t$ yields to a qualitatively different behavior.

We consider a spin system: the Hilbert space is $\mathbf{C}^2$, and we choose the Hamiltonian $\hat{H}$ and projector $\hat{E}$ to correspond to the matrices,

$$H=\begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}, \quad E=\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{A1}$$

We consider the self-adjoint operator,

$$\hat{V}=\begin{pmatrix} x & 0 \\ 0 & y \end{pmatrix}, \tag{A2}$$

from which we define the positive operator,

$$e^{-V\,\delta t}=\begin{pmatrix} e^{-x\,\delta t} & 0 \\ 0 & e^{-y\,\delta t} \end{pmatrix} \tag{A3}$$

This operator can be seen as a regularized expression for $\hat{E}$,

$$\lim_{x\to\infty}\lim_{y\to 0} e^{-V\,\delta t}=\hat{E}. \tag{A4}$$

We may then write a regularized version $\hat{K}_t^y$ of the operator $\hat{C}_t=(\hat{E}e^{-i\hat{H}t/n})^n$, such that.

$$\hat{C}_t=\lim_{y\to 0}\hat{K}_t^y, \tag{A5}$$

The operator $\hat{K}_t^y$ reads explicitly as

$$\hat{K}_t^y=\lim_{x\to\infty}\lim_{n\to\infty}(e^{-i\hat{H}t/n}e^{-\hat{V}t/n})^n=\lim_{x\to\infty} e^{-iHt-Vt}. \tag{A6}$$

We easily find that

$$\hat{K}_t^y=e^{-yt}\hat{E}, \tag{A7}$$

has the exponential fall behavior that characterizes Fermi's golden rule.

When the limit $y\to 0$ is also taken, we obtain the familiar result $\hat{C}_t=\hat{E}$, which is trivially a degenerate unitary operator. However, even a small deviation from $\hat{E}$ in the definition of $\hat{C}_t$ leads to a different (and intuitively more physical) qualitative behavior.

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Hudson's theorem for finite-dimensional quantum systems

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We show that, on a Hilbert space of odd dimension, the only pure states to possess a non-negative Wigner function are stabilizer states. The Clifford group is identified as the set of unitary operations which preserve positivity. The result can be seen as a discrete version of Hudson's theorem. Hudson established that for continuous variable systems, the Wigner function of a pure state has no negative values if and only if the state is Gaussian. Turning to mixed states, it might be surmised that only convex combinations of stabilizer states give rise to non-negative Wigner distributions. We refute this conjecture by means of a counterexample. Further, we give an axiomatic characterization which completely fixes the definition of the Wigner function and compare two approaches to stabilizer states for Hilbert spaces of prime-power dimensions. In the course of the discussion, we derive explicit formulas for the number of stabilizer codes defined on such systems. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2393152]

I. INTRODUCTION

A. General introduction

The Wigner distribution establishes a correspondence between quantum mechanical states and real pseudoprobability distributions on phase space. "Pseudo" refers to the fact that while the Wigner function resembles many of the properties of probability distributions, it can take on negative values. This phenomenon has been linked to nonclassical features of such quantum states (see Ref. 1 for an exposition of literature on that problem). It is naturally of interest to characterize those quantum states that are classical in the sense of giving rise to non-negative phase space distributions.

For the case of pure states described by vectors in $\mathcal{H}=L^2(\mathbb{R})$, the resolution of this problem was given by Hudson in Ref. 2. Later, Soto and Claverie generalized Hudson's result to states of multiparticle systems (Ref. 3).

Theorem 1 *(Hudson, Soto, Claverie): Let $\psi \in L^2(\mathbb{R}^n)$ be a state vector. The Wigner function of ψ is non-negative if and only if ψ is a* Gaussian state.

By definition, a vector is Gaussian if and only if it is of the form

$$\psi(q) \propto \mathrm{e}^{2\pi i(q\theta q + xq)},$$

where $q,x \in \mathbb{R}^n$ and θ is a symmetric matrix with entries in $\mathbb{C}$ [Note that the boundedness of $\psi \in L^2(\mathbb{R}^n)$ implies that θ has positive semidefinite imaginary part].

It is our objective to prove that the situation for discrete quantum systems is very similar, at least when the dimension of the Hilbert space is odd. Before stating the result, we pause for a brief overview of its main ingredients: discrete Wigner functions and stabilizer states.

The Wigner function[4] of a pure state $\psi \in L^2(\mathbb{R})$ is computed as

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$$W_\psi(p,q) = \pi^{-1} \int_{\xi \in \mathbb{R}} \mathrm{e}^{-2\pi i \xi p} \bar{\psi}\left(q - \frac{1}{2}\xi\right) \psi\left(q + \frac{1}{2}\xi\right). \tag{1}$$

Equivalently, W_ψ is the (symplectic) Fourier transform of the *characteristic function* Ξ_ψ, which in turn is defined by

$$\Xi_\psi(p,q) = \mathrm{tr}(w(p,q)^\dagger |\psi\rangle\langle\psi|).$$

Here, $w(p,q) = \mathrm{e}^{i(p\hat{X} - q\hat{P})}$ are the well-known *Weyl or displacement operators*.[5,6] Partly triggered by the advent of quantum information theory, considerable work has been undertaken to explore Wigner functions for finite-dimensional quantum systems.[7–16] Two approaches might be identified in the literature on that subject. The first one aims to cast the *definition* of the Wigner function into a form that can be interpreted for both continuous variable and discrete systems.[9–11,15] The second approach—introduced by Gibbons *et al.* in Ref. 16—focuses on the *properties* of Eq. (1). The authors imposed a set of axioms which a candidate definition of a discrete Wigner function would have to fulfill in order to resemble the well-known continuous counterpart.

We will argue that, for odd dimensions d,

$$W_\psi(p,q) = d^{-1} \sum_{\xi \in \mathbb{Z}_d} \mathrm{e}^{-(2\pi/d) i \xi p} \bar{\psi}(q - 2^{-1}\xi) \psi(q + 2^{-1}\xi)$$

is the most sensible analogue of Eq. (1), judged in terms of either of these approaches. Here, p,q are elements of $\mathbb{Z}_d = \{0, \ldots, d-1\}$ and $2^{-1} = (d+1)/2$ is the multiplicative inverse of 2 modulo d. Indeed, the definition given above is the discrete symplectic Fourier transform of the discrete characteristic function and will be shown to be the *unique* choice to mimic certain desirable properties of the continuous Wigner function.

Stabilizer states were originally defined by Gottesman in Ref. 17 as the joint eigenvectors of certain sets of elements of the qubit Pauli group. Exceeding the case of qubits, stabilizer states for higher-dimensional quantum systems have been treated in the literature (see, e.g., Refs. 18–21). Such states find manifold applications in quantum information theory, ranging from quantum error correction[22] to cluster state quantum computation.[23] Although displaying complex features such as multi-particle entanglement,[24] stabilizer states allow for an efficient classical description. In particular, a quantum computer that operates only with stabilizer states can offer no principal advantage over classical methods of computing.[22] The latter statement is sometimes called *Gottesman-Knill theorem*.

Using that language, we intend to show the following theorem.

Theorem 2 *(Discrete Hudson's theorem): Let d be odd and* $\psi \in L^2(\mathbb{Z}_d^n)$ *be a state vector. The Wigner function of* ψ *is non-negative if and only if* ψ *is a* stabilizer state.

Given that $\psi(q) \neq 0$ *for all q, a vector* ψ *is a stabilizer state if and only if it is of the form*

$$\psi(q) \propto \mathrm{e}^{(2\pi/d) i (q\theta q + xq)},$$

where $q,x \in \mathbb{Z}_d^n$ *and* θ *is a symmetric matrix with entries in* $\mathbb{Z}_d$.

Theorem 2 should convey two central messages. First, if the right definitions are employed, the continuous and the discrete case behave very similarly (even though the methods of proof are completely different). Second, it adds further evidence to what might be called a piece of folk knowledge in the field of quantum information theory: namely, that stabilizer states are the natural finite-dimensional analog of Gaussian states.

This paper is organized as follows. We survey previous work on the subject in Sec. I B. Section II is devoted to a superficial, yet self-contained introduction to Weyl operators, characteristic functions, Wigner distributions and stabilizer states. The main theorem is proven in Sec. III. Sections V–VII address various related topics. The results of these last three sections do not rely on each other. Concretely, we comment on the relation between stabilizer states and Gaussian states in Sec. IV; we consider mixed states with positive Wigner functions in Sec. V; and use Sec. VII for a discussion of Hilbert spaces whose dimension is the power of a prime.

B. Previous results

Recently, Galvao and co-workers, took a first step into the direction of classifying the quantum states with positive Wigner function.[26] To explain the relationship of their results to the present paper, we have to comment on an axiomatic approach to discrete Wigner functions and, further, on stabilizer states in dimensions that are the power of a prime number.

In Ref. 16, Gibbons *et al.* listed a set of requirements which should be met by any definition of a discrete Wigner function W. Denoting the dimension of the Hilbert space by d, their axioms amount as follows:

1. *(Phase space)* W is a linear mapping sending operators to functions on a $d\times d$ lattice, called the *phase space*.
2. *(Translational covariance)* The Wigner function is covariant under the action of the Weyl operators (in the sense of Theorem 7).
3. *(Marginal probabilities)* There exists a function $Q(\lambda)$ that assigns a pure quantum state to every line λ in phase space. If ψ is state vector, then the sum of its Wigner function along λ must be equal to the overlap $|\langle Q(\lambda)|\psi\rangle|^2$.

Let us call functions that fall into this class *generalized Wigner functions*. This term is justified, as the characterization does not specify a unique solution: for a d-dimensional Hilbert space, there exist d^{d+1} distinct generalized Wigner functions. Note also that the construction has been described only for the case where $d=p^n$ is the power of a prime, because only then the notion of a *line* in phase space has a well-defined meaning.

We turn to the second remark, concerning stabilizer states. Consider a composite system, built of n d-level particles. We are free to conceive it as a single d^n-dimensional object. The two points of view give rise to different definitions of stabilizer states, the "single-particle" one being starkly reduced as compared to the multiple-particle one. In Sec. VII, we show that the set of single-particle stabilizer states is strictly contained in the set of multiparticle ones. Indeed, the ratio of the respective cardinalities of the two sets grows super-exponentially in n. As an example, the generalized Bell and GHZ states

$$d^{-n/2}\sum_i |i\rangle\otimes|i\rangle, \quad d^{-n/2}\sum_i |i\rangle\otimes|i\rangle\otimes|i\rangle,$$

arguably the best-known multiparticle stabilizer states, do not belong to the respective single-particle sets.

The result of Ref. 26 concerns quantum states in prime-power dimensions that are nonnegative with respect to *all* possible definitions of generalized Wigner functions. These states are shown to be mixtures of single-particle stabilizer states, as described above. The authors aim to establish necessary requirements for quantum computational speedup. Indeed, if the Wigner function of a quantum computer is positive at all times, then it operates only with stabilizer states and hence offers no advantage over classical computers, by the Gottesman-Knill theorem.

Thus for the case of nonqubit pure states, Theorem 2 implies the results of Ref. 26 and goes further in two essential ways. Firstly, it suffices to look at a single definition of the Wigner function, as opposed to $d^{n(d^n+1)}$ generalized ones. Second, quantum computation and the Gottesman-Knill theorem are naturally set in the context of *multiple* particles. Our definition assigns positive Wigner functions to all multiple-particle stabilizer states, while Ref. 26 effectively relies on the single-particle definition (up to equivalence under Clifford operations). On the other hand, our main theorem does not address qubits or mixed states, which Galvao and co-workers do.

II. PHASE SPACE FORMALISM

The term *phase space formalism* encompasses the ideas and tools in relation to the *Weyl representation* to be defined shortly. We will give a concise introduction in this section. Many of the results presented can be found in the literature, but some, e.g., the Clifford covariance of the Wigner function in nonprime dimensions, seem to be new.

A. Weyl representation

We start by considering a d-dimensional quantum system d odd. In its Hilbert space $\mathcal{H}$, we choose a basis $\{|0\rangle, \ldots, |d-1\rangle\}$, labeled by elements of $\mathbb{Z}_d$. Henceforth, $\mathbb{Z}_d$ will be referred to as the *configuration space* and abbreviated by Q.

The pivotal objects in the phase space formalism are the *Weyl operators* (also known as the *generalized Pauli operators*), as constructed below. Let $\chi(q)=e^{(2\pi/d)iq}$. The relations

$$\hat{x}(q)|x\rangle = |x+q\rangle, \quad \hat{z}(p)|x\rangle = \chi(px)|x\rangle \tag{2}$$

define the *shift* and *boost* operators, respectively. The Weyl operators are given by

$$w(p,q) = \chi(-2^{-1}pq)\hat{z}(p)\hat{x}(q), \tag{3}$$

for $p,q,t \in Q$. The specific choice of phases will prove useful later on. The set of Weyl operators is closed under multiplication up to phase factors. Direct computation shows that the composition law is given by

$$w(p,q)w(p',q') = \chi\left(2^{-1}\left[\begin{pmatrix} p \\ q \end{pmatrix}, \begin{pmatrix} p' \\ q' \end{pmatrix}\right]\right) w(p+p', q+q'). \tag{4}$$

The square brackets denote the standard *symplectic inner product* on $\mathbb{Z}_d^2$,

$$\left[\begin{pmatrix} p \\ q \end{pmatrix}, \begin{pmatrix} p' \\ q' \end{pmatrix}\right] := \begin{pmatrix} p \\ q \end{pmatrix}^T J \begin{pmatrix} p' \\ q' \end{pmatrix}, \tag{5}$$

where

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{6}$$

We write $w(v)=w(v_p,v_q)$ for elements $v=(v_p,v_q)\in\mathbb{Z}_d^2$. The space $V:=Q\times Q$ with inner product given by Eq. (5) will be called phase space in the sequel, owing to its analogy to the phase space known in classical mechanics.

The preceding constructing generalizes naturally to multiple particles. Indeed, the configuration space of an n-particle system is given by $Q=\mathbb{Z}_d^n$. Multiplication between two elements $p,q \in Q$ is understood as the usual inner product $pq=\Sigma_i p_i q_i$. The Hilbert space is again spanned by $\{|q\rangle\}_{q\in Q}$ and the Weyl operators are defined to be the tensor products,

$$w(p,q) = w(p_1, \ldots, p_n, q_1, \ldots, q_n) = w(p_1,q_1) \otimes \cdots \otimes w(p_n,q_n). \tag{7}$$

Equations (4) and (5) remain valid in the multiple-particle setting, if we substitute the matrix J by its multidimensional version,

$$J = \begin{pmatrix} 0_{n\times n} & \mathbb{1}_{n\times n} \\ -\mathbb{1}_{n\times n} & 0_{n\times n} \end{pmatrix}.$$

We end this section with some miscellaneous remarks.

A state vector $|\psi\rangle$ can be identified with a complex function on configuration space by setting $\psi(q)=\langle q|\psi\rangle$. We will use both representations interchangeably.

The continuous Weyl operators $w(p,q)=e^{i(p\hat{X}-q\hat{P})}$, $p,q\in\mathbb{R}$ fulfill exactly the same composition law as stated in Eq. (4), if χ is set to $\chi(q)=e^{iq}$ and the other symbols are interpreted in the obvious way. In fact, Eq. (4) is then equivalent to the fundamental *Weyl commutation relations*.[6] Having this analogy in mind, p and q will sometimes be called *momentum* and *position* coordinates, respectively.

For future reference, note the two simple relations,

$$(w(p,q)\psi)(x) = \chi(-2^{-1}pq + px)\psi(x-q), \tag{8}$$

$$\operatorname{tr} w(p,q) = d^n \delta_{p,0}\delta_{q,0}. \tag{9}$$

It remains yet to justify the name Weyl *representation*. For $v \in V$, $t \in \mathbb{Z}_d$, define $w(v,t) = \chi(t)w(v)$. Equation (4) takes on the form

$$w(v_1,t_1)w(v_2,t_2) = w(v_1+v_2, t_1+t_2+2^{-1}[v_1,v_2]).$$

The set $V \times \mathbb{Z}_d$, equipped with the above composition law is called the *Heisenberg group* $H(\mathbb{Z}_d^n)$, the Weyl matrices constituting a unitary representation of $H(\mathbb{Z}_d^n)$.[6] This point of view on Weyl operators will be needed only in Appendix A.

B. Clifford group

The Clifford group is the subset of the unitary operators that map Weyl operators to multiples of Weyl operators under conjugation,

$$Uw(v)U^\dagger = c(v)w(S(v)), \tag{10}$$

for some maps $c: V \to \mathbb{C}$ and $S: V \to V$.[17] The structure of the Clifford group is described in the following theorem. Note that the Clifford group appearing in quantum information theory has no connection to the Clifford group used in the representation theory of SO(n).

Before stating the theorem, we have to comment on a re-appearing issue: namely, that things are more involved if d is not a prime number. For prime values of d, $\mathbb{Z}_d$ has the structure of a *finite algebraic field*, $\mathbb{Z}_d^n$ is a *finite vector space*, and most of the intuitions we have about vector spaces continue to be true. Among the more severe deficiencies of the general case is the fact that not every element a of $\mathbb{Z}_d$ possesses a multiplicative inverse modulo d. But even if the analog of a theorem about vector spaces holds for nonprime values of d, it is often difficult to find a proof in the literature. Appendices C and D contain a collection of statements of this kind. Less technically inclined readers will not loose much by skipping these sections.

For the sake of clarity of language, we call functions f on Q which fulfill $f(\lambda a+b)=\lambda f(a)+f(b)$ *linear*, disregarding the fact that Q might fail to be a linear space. Similarly, a subset S of Q that is closed under addition and multiplication by elements of $\mathbb{Z}_d$ is referred to as a *subspace*. We define a function S to be *symplectic* if it is linear and preserves the symplectic form: $[S\cdot, S\cdot]=[\cdot,\cdot]$.

Theorem 3 *(Structure of the Clifford group):*

1. *For any symplectic S, there is a unitary operator $\mu(S)$ such that*

$$\mu(S)w(v)\mu(S)^\dagger = w(Sv).$$

2. *μ is a* projective representation *of the symplectic group, that is,*

$$\mu(S)\mu(T) = e^{i\phi}\mu(ST),$$

for some phase factor $e^{i\phi}$.

3. *Up to a phase, any Clifford operation is of the form*

$$U = w(a)\mu(S),$$

for a suitable $a \in V$ and symplectic S.

The representation μ is called the *Weil* or *metaplectic* representation.[6,27] Theorem 3 could be called a discrete version of the celebrated *Stone-von Neumann theorem*.[6] Its proof is not essential for understanding the further argument and has therefore been moved to Appendix A.

Note that a Clifford operation is connected to a vector a and a linear mapping S. This should remind us of a well-known structure on linear spaces: *affine transformations*. An affine mapping A

is of the form $A(b)=Sb+a$ where S is an invertible linear operator and a is a vector. Let us call A symplectic if its linear part S is.

We will frequently use the "dot notation" to define functions of one parameter; for example, writing $S\cdot+a$ for A.

Lemma 4 (Clifford group and affine transformations): The mapping

$$S\cdot+a\mapsto w(a)\mu(S)$$

is a projective representation of the group of symplectic affine transformations.

Proof: All we need to do is to compare the composition law of the affine group

$$(S\cdot+a)\circ(T\cdot+b)=S(T\cdot+b)+a=ST\cdot+(Sb+a)$$

to the composition law of the representation

$$w(a)\mu(S)w(b)\mu(T)=w(a)\mu(S)w(b)\mu(S)^{\dagger}\mu(S)\mu(T)=w(a)w(Sb)\mu(S)\mu(T)\propto w(Sb+a)\mu(ST),$$

which proves the assertion. ■

The correspondence established by the last lemma will find a very tangible manifestation in Sec. II D, when we will see that the Clifford group induces affine transformations of the Wigner function.

C. Fourier transforms

Let $Q=\mathbb{Z}_d^n$ and $f:Q\to\mathbb{C}$ be a complex function on Q. The Fourier transform of f is

$$(\mathcal{F}f)(p)=\hat{f}(p)=|Q|^{-1/2}\sum_{q\in Q}\bar{\chi}(pq)f(q). \tag{11}$$

In the course of the main proof we will be confronted with Fourier transforms of functions which are defined only on a subspace of Q. If d is prime, then any subspace of $Q=\mathbb{Z}_d^n$ is of the form $\mathbb{Z}_d^{n'}$, for some $n'\leqslant n$, so no new situation arises.

For nonprime dimensions, however, subspaces may not be as well behaved. Consider as an example $\{0,3,6\}\subset\mathbb{Z}_9^1$. The set is closed under addition and multiplication, but can clearly not be written as $\mathbb{Z}_9^{n'}$.

To cope with this problem, we will cast Eq. (11) into a form that is well defined for functions f on more general spaces. The construction is presented below. It can be found in any textbook on harmonic analysis (e.g., Ref. 28).

A *character* of Q is a function $\zeta:Q\to\mathbb{C}$ such that $\zeta(a+b)=\zeta(a)\zeta(b)$. Any character of Q is of the form $\zeta(q)=\bar{\chi}(xq)$ for an appropriate $x\in Q$ (see Appendix C). We can hence conceive the Fourier transformation defined in Eq. (11) as a function of the characters of Q,

$$\hat{f}(\zeta)=|Q|^{-1/2}\sum_{q}\zeta(q)f(q). \tag{12}$$

We denote the set of characters of Q by Q^*. With these notions, Eq. (12) defines a function $Q^*\to\mathbb{C}$. If, now, S is any subspace of Q and f a function on S, the Fourier transform

$$\hat{f}:S^*\to S,\quad \hat{f}(\zeta)=|S|^{-1/2}\sum_{s}\zeta(s)f(s)$$

is well defined.

For $f:V\to\mathbb{C}$, we define the *symplectic Fourier transform* as

$$(\mathcal{F}_S f)(a)=|V|^{-1/2}\sum_{b\in V}\bar{\chi}([a,b])f(b). \tag{13}$$

Finally, take note that the normalization in Eqs. (11) and (12) has been chosen in such a way that *Parzeval's theorem* $\|f\|=\|\hat{f}\|$ holds, where $\|f\|^2=\Sigma_q|f(q)|^2$.

D. Definition and properties of the Wigner function

Employing Eq. (9) in conjunction with the composition law [Eq. (4)], one finds that the Weyl operators $\{w(p,q)\}$ form an orthonormal basis in the space of operators on $\mathcal{H}$ with respect to the trace scalar product $d^{-n}\,\mathrm{tr}(\cdot^{\dagger}\cdot)$. The *characteristic function* Ξ_ρ of an operator ρ is given by its expansion coefficients with respect to the Weyl basis,

$$\Xi_\rho(\xi,x)=d^{-n}\mathrm{tr}(w(\xi,x)^{\dagger}\rho). \tag{14}$$

We mentioned in the introduction that the continuous Wigner function is the symplectic Fourier transform of the characteristic function.[5,6] The two latter concepts have been defined for finite-dimensional systems in the preceding paragraphs. We can now state in complete analogy to the continuous case.

Definition 5 (*Wigner function*): *Let d be odd,* $Q=\mathbb{Z}_d^n$ *for some n. Let* $V,\mathcal{H}$ *be as usual and let* ρ *be a quantum state on* $\mathcal{H}$.

The Wigner function W_ρ *associated with* ρ *is the symplectic Fourier transformation of the characteristic function* Ξ_ρ.

An explicit calculation yields, for all $a\in V$,

$$(\mathcal{F}_S\Xi_\rho)(a)=d^{-2n}\sum_{b\in V}\bar{\chi}([a,b])\mathrm{tr}(w(b)^{\dagger}\rho)=d^{-n}\mathrm{tr}\left(\left(d^{-n}\sum_b\bar{\chi}([a,b])w(b)^{\dagger}\right)\rho\right)=:d^{-n}\mathrm{tr}(A(a)\rho), \tag{15}$$

where we have implicitly defined the *phase space point operator* $A(a)$.[16]

Theorem 6 lists a selection of properties of the Wigner function. For a more thorough discussion, the reader is deferred to Refs. 9 and 15.

Theorem 6 (*properties of the Wigner function*):

1. *The phase space point operators have unit trace and form an orthonormal basis in the space of Hermitian operators on* $\mathcal{H}$. *Hence the Wigner function of a Hermitian operator is real, and further, the* overlap

$$d^{-n}\mathrm{tr}(\rho\sigma)=\sum_{v\in V}W_\rho(v)W_\sigma(v)$$

and normalization *relations*

$$\sum_v W_\rho(v)=\mathrm{tr}\rho$$

hold.

2. *For a pure state* ψ, *the Wigner function* $W_\psi:=W_{|\psi\rangle\langle\psi|}$ *equals*

$$W_\psi(p,q)=d^{-n}\sum_{\xi\in Q}\bar{\chi}(\xi p)\bar{\psi}(q-2^{-1}\xi)\psi(q+2^{-1}\xi).$$

3. *When computing marginal probabilities, the Wigner function behaves like a classical probability distribution*,

$$\sum_{p\in Q}W_\psi(p,q)=|\psi(q)|^2.$$

4. *The multiparticle phase space point operators factor*,

$$A(p_1,\ldots,p_n,q_1,\ldots,q_n)=\bigotimes_i^n A^{(i)}(p_i,q_i)$$

(*and hence so does the Wigner function*).

5. *It holds that* $A(0)|q\rangle=|-q\rangle$. *In other words, the phase space point operator at the origin equals the* parity operator.
6. *The Wigner function* $W_{\rho\sigma}$ *of an operator product is given by the* * product (*also known as the* Groenewold *or* Moyal product,[29])

$$W_{\rho\sigma}(u)=(W_\rho\star W_\sigma)(u):=d^{-n}\sum_{v,w}W_\rho(u+v)W_\sigma(u+w)\bar{\chi}([v,w]).$$

Proof: The proofs are all straightforward; we give only hints on how to conduct them. It will be essential to recall the well-known relation

$$\sum_{x\in\mathbb{Z}_d^n}\chi(xy)=d^n\delta_{y,0}, \tag{16}$$

for all $y\in\mathbb{Z}_d^n$.

Indeed, the first claim can be proven by using Eq. (16) together with the definition of the phase space point operators Eq. (15). Employ Definition 5 and Eq. (16) to establish the second assertion, which in turn implies the third one. Theorem 6.4 makes use of the fact that $\bar{\chi}(pq)=\prod_i\bar{\chi}(p_iq_i)$ (see also Sec. VII for a very similar and more explicit calculation). The validity of the fifth statement is best shown using Eqs. (8) and (16).

Let us lastly turn to Claim 6. We have noted that the phase space point operators form an orthonormal system. Hence we can expand an operator ρ in terms of its Wigner function as $\rho=\Sigma_v W_\rho(v)A(v)$. Substituting ρ and σ by their respective expansions in $W_{\rho\sigma}(v)=d^{-n}\,\mathrm{tr}(A(v)\rho\sigma)$ yields the desired formula with the help of Lemma 29. □

The following statement will be vital to the proof of the main theorem. It assigns an elegant geometric interpretation to the Clifford group.

Theorem 7 (*Clifford covariance*): *Let* $U=w(a)\mu(S)$ *be a Clifford operation. Let* $\rho':=U\rho U^\dagger$ *for some Hermitian operator* ρ. *The Wigner function is* covariant *in the sense that*

$$W_\rho(v)=W_{\rho'}(Sv+a).$$

Proof: We compute the action of the Clifford group on the phase space point operators.

$$\begin{aligned}
w(a)\mu(S)A(b)\mu(S)^\dagger w(a)^\dagger &= d^{-n}\sum_{v\in V}\bar{\chi}([b,v])w(a)\mu(S)w(v)\mu(S)^\dagger w(a)^\dagger\\
&= d^{-n}\sum_v\bar{\chi}([b,v])w(a)w(Sv)w(a)^\dagger = d^{-n}\sum_v\bar{\chi}([b,v])\chi([a,Sv])w(Sv)\\
&= d^{-n}\sum_{v':=Sv}\bar{\chi}([b,S^{-1}v'])\bar{\chi}([a,v'])w(v') = d^{-n}\sum_{v'}\bar{\chi}([Sb+a,v'])w(v')\\
&= A(Sb+a).
\end{aligned}$$

The claim follows by use of Eq. (15). □

Our definition of the discrete Wigner function coincides with the ones used in Refs. 7, 9, 11, and 15. It is further equal to Leonhardt's version,[8] up to a permutation of points in phase space; it corresponds to choice (a) in Ref. 12 and lastly to $G=\mathbb{Z}_d^n$ in Ref. 14. One can show that W, as defined here, fulfills the axioms of Ref. 16 which had been laid out in Sec. I B. Put differently, it is an element of the set of generalized Wigner functions. Gibbons *et al.* remarked in Ref. 16 that among the generalized Wigner functions, some stand out by their high degree of symmetry. In our language, this symmetry is an incarnation of the Clifford covariance established in Theorem 7.

Naturally, it is now interesting to ask how much freedom is left in the definition of a Wigner function, once one requires Clifford covariance to hold. We show in Appendix B that the definition used here is virtually unique in that regard.

E. Stabilizer states

Using the composition law of the Heisenberg group [Eq. (4)], it is easy to see that two Weyl operators $w(v_1)$ and $w(v_2)$ commute if and only if $[v_1,v_2]=0$. Now consider the image of an entire subspace M under the Weyl representation w. The set

$$w(M)=\{w(m)|m\in M\}$$

consists of mutually commuting operators if and only if the symplectic form vanishes on M

$$[m_1,m_2]=0 \quad \text{for all } m_i\in M.$$

Spaces of that kind are called *isotropic*. Clearly, if M is isotropic, then the operators $w(M)$ can be simultaneously diagonalized. We will see that if $|M|=d^n$, the eigenspaces become nondegenerate and can thus be used to single out state vectors in the Hilbert space. A subspace M of V is said to be *maximally isotropic* if its cardinality equals d^n. See Appendix C for a justification of that nomenclature.

Lemma 8 (Stabilizer States): Let M *be a maximally isotropic subspace of* V. *Let* $v\in V$. *Up to a global phase, there is a unique state vector* $|M,v\rangle$ *that fulfills the eigenvalue equations*

$$\chi([v,m])w(m)|M,v\rangle=|M,v\rangle,$$

for all $m\in M$.

Proof: Existence. It is elementary to check that

$$|M|^{-1}\sum_{m\in M}\chi([v,m])w(m) \tag{17}$$

is a rank one projection operator fulfilling the eigenvalue equations.

Uniqueness. According to Appendix C, there are p^n characters of M, each giving rise to a distinct projection operator as defined in the last paragraph. Two distinct operators of that kind are mutually orthogonal, because they belong to different eigenvalues of at least one of the Weyl operators. But $\dim\mathcal{H}=|Q|=p^n$ and thus there is no space for more than one-dimensional solutions to the given set of equations. □

The state vector $|M,v\rangle$ is called the *stabilizer state* associated with M and v. For obvious reasons, one refers to the set of operators $\{\chi([v,m])w(m)|m\in M\}$ as the *stabilizer* of $|M,v\rangle$. Due to the isotropicity of M, the stabilizer is closed under multiplication and thus constitutes a group. Occasionally, we write $|M\rangle$ for $|M,0\rangle$. To specify a stabilizer state, we need to specify a maximally isotropic space M. This is best done by giving a basis $\{m_1,\ldots,m_k\}$ of M. It is convenient to assemble the basis vectors as the columns of a $2n\times k$ matrix, which is generally referred to as the *generator matrix*. As the choice of a basis is nonunique, so is the form of the generator matrix.

A stabilizer state $|M\rangle$ is a *graph state* if it possesses a generator matrix of the form

$$\begin{pmatrix}\vartheta\\ \mathbb{1}_{n\times n}\end{pmatrix}, \tag{18}$$

where ϑ is a symmetric $n\times n$ matrix.[24] The designation stems from the fact that ϑ can be interpreted as the adjacency matrix of a graph. Many properties of $|M\rangle$ are describable in terms of that graph alone.[24] Some authors require the diagonal elements $\vartheta^i{}_i$ to vanish (equivalently, no vertex of the graph should be linked to itself), but we will not impose that restriction. Note that there exist considerably more general definitions of graph states.[19]

Obviously, we will be concerned with Wigner functions of stabilizer states. Lemma 9 clarifies their structure.

Lemma 9 (Wigner functions of stabilizer states): The Wigner function of a stabilizer state $|M,v\rangle$ *is the* indicator function *on* $M+v$. *More precisely*,

$$W_{|M,v\rangle}(a) = \frac{1}{d^n}\delta_{M+v}(a) = \frac{1}{d^n}\begin{cases} 1 & a \in M+v \\ 0 & \text{else.} \end{cases}$$

Proof: The representation given in Eq. (17) of $|M,v\rangle$ determines the characteristic function

$$\Xi_{|M,v\rangle}(b) = d^{-n}\chi([v,b])\,\delta_M(b).$$

We compute the symplectic Fourier transformation,

$$(\mathcal{F}_S\Xi_{|M,v\rangle})(a) = d^{-2n}\sum_{b\in V}\bar{\chi}([a,b])\chi([v,b])\,\delta_M(b) = d^{-2n}\sum_{b\in M}\bar{\chi}([a-v,b]) = d^{-n}\delta_{M^\perp}(a-v),$$

where

$$M^\perp = \{v \in V | [m,v] = 0 \text{ for all } m \in M\}$$

is the *symplectic complement* of M in V. But M is a maximally isotropic space and hence $M = M^\perp$ (see Appendix C). □

In particular, we know now that the Wigner function of stabilizer states is non-negative. The next sections are devoted to the proof of the converse.

III. DISCRETE HUDSON'S THEOREM

A. Bochner's theorem

Define the *self-correlation function*

$$K_\psi(q,x) = \psi(q+2^{-1}x)\bar{\psi}(q-2^{-1}x),$$

and note that the Wigner function fulfills

$$W(p,q) = \frac{1}{d^n}\sum_{x\in Q}\bar{\chi}(px)K_\psi(q,x). \tag{19}$$

Fix a $q_0 \in Q$. Designating the function $p \mapsto W(p,q_0)$ by $W(\cdot,q_0)$, Eq. (19) says that $W(\cdot,q_0)$ is the Fourier transform of $K(q_0,\cdot)$. Therefore, W is non-negative if and only if the d^n functions $K(q_0,\cdot)$ have non-negative Fourier transforms.

In harmonic analysis, the set of functions with non-negative Fourier transforms is characterized via a theorem due to Bochner. It is usually proven either in the context of Fourier analysis on the real line or else, in full generality, for harmonic analysis on—not necessarily Abelian—locally compact groups. While the former statement is not general enough for our purpose, the latter is not easily accessible. However, it turns out that in the discrete Abelian setting an elementary proof can be given. It is stated in the next theorem, along with a variation for subsequent use.

Theorem 10 *(Variations of Bochner's Theorem): Let* M *be a subspace of* Q. *Let* $f: M \to \mathbb{C}$. *The following holds*.

1. *The Fourier transform of* f *is non-negative if and only if the matrix*

$$A^x{}_q = f(x-q) \quad (x,q \in M)$$

is positive semidefinite.

2. *The Fourier transform of* f *has constant modulus (i.e.,* $|\hat{f}(x)| = \text{const}$*) if and only if* f *is orthogonal to its translations*,

$$\langle f, \hat{x}(q) f\rangle = \sum_{x\in M}\bar{f}(x)f(x-q) = 0,$$

for all nonzero $q \in M$.

Proof: The following computation is a variant of a well-known fact concerning circulant matrices. We claim that any character ζ of M is an eigenvector of A with eigenvalue $\lambda = |M|^{-1/2}\hat{f}(\zeta)$. Indeed, plugging in the definitions yields

$$(A\zeta)(x) = \sum_q A^x{}_q \zeta(q) = \sum_q f(x-q)\zeta(q) = \sum_q f(q)\bar{\zeta}(q)\zeta(x) = \sqrt{|M|}\hat{f}(\zeta)\zeta(x).$$

There exist $|M|$ characters and thus equally many eigenvectors of A. Therefore, A can diagonalized. All its eigenvalues are non-negative if and only if $\hat{f}$ is non-negative.

By the same argument, A is proportional to a unitary matrix if and only if $|\hat{f}(q)|$ is constant. But a matrix is unitary if and only if its rows form an orthonormal set of vectors. □

From here, the proof proceeds in two steps. Section III B harvests Theorem 10.1 to gain information on the pointwise modulus $|\psi(q)|$ of a vector with non-negative Wigner function. Building on these findings, we will analyze the properties of such Wigner functions in Sec. III C.

B. Supports and moduli

Lemma 11 (Modulus inequality): Let ψ *be a state vector with non-negative Wigner function. It holds that*

$$|\psi(q)|^2 \geqslant |\psi(q-x)||\psi(q+x)|,$$

for all $q,x \in Q$.

Proof: Fix a $q \in Q$. As W_ψ is non-negative, so is the Fourier transform of $K_\psi(q,\cdot)$. Bochner's theorem implies that the matrix $A^x_y = K(x-y,q)$ is positive semidefinite (psd) which in turn implies that all principal submatrices are psd. In particular the determinant of the 2×2 principal submatrix

$$\begin{pmatrix} K_\psi(q,0) & K_\psi(q,2x) \\ K_\psi(q,-2x) & K_\psi(q,0) \end{pmatrix} = \begin{pmatrix} |\psi(q)|^2 & \psi(q+x)\bar{\psi}(q-x) \\ \bar{\psi}(q+x)\psi(q-x) & |\psi(q)|^2 \end{pmatrix}$$

must be non-negative. But this means

$$|\psi(q)|^4 - |\bar{\psi}(q+x)\psi(q-x)|^2 \geqslant 0,$$

which proves the theorem. □

We will call the set supp ψ of points where a state vector is nonzero its *support*. $S = \text{supp}\ \psi$ has the property to contain the *midpoint* of any two of its elements. Indeed, if $a,b \in S$, then setting $q = 2^{-1}(a+b)$ and $x = 2^{-1}(a-b)$ in the modulus inequality shows that

$$|\psi(2^{-1}(a+b))| \geqslant |\psi(a)||\psi(b)| > 0,$$

hence $2^{-1}(a+b) \in S$. Let us refer to sets possessing this quality as being *balanced*.

The following lemma clarifies the structure of balanced sets. Recall that a subset A of V is *affine* if $A = M + v$ for a subspace M and some vector v. An affine space is a subspace if and only if it contains the origin 0.

Lemma 12 (Balanced sets): A subset S of Q *is balanced if and only if* S *is an affine space.*

Proof: We show the "only if" part, the other one being simple.

As both the characterizations of balance and affinity are invariant under translation, there is no loss of generality in assuming that $0 \in S$. We have to establish that S is closed under both addition and scalar multiplication.

Let $a \in S$. We claim that

$$2^{-l}\lambda a \in S, \tag{20}$$

for all $l \in \mathbb{N}$ and $\lambda \leqslant 2^l$. The proof is by induction on l. Suppose Eq. (20) holds for some l. If $\lambda \leqslant 2^{l+1}$ is even, then $2^{-l-1}\lambda a = 2^{-l}(\lambda/2)b \in S$. Else,

$$2^{-l-1}\lambda a = 2^{-1}\left(2^{-l}\frac{\lambda-1}{2}a + 2^{-l}\frac{\lambda+1}{2}a\right) \in S,$$

which shows the validity of Eq. (20).

There exists an integer $l > d$ such that $2^l = 1 \bmod d$. Indeed, by Euler's theorem, $2^{\phi(d)} = 1 \bmod d$, where ϕ is Euler's totient function. So $l = d\phi(d)$ satisfies the requirements. Inserting l into Eq. (20), we conclude that $\lambda a \in S$ for all $\lambda \leqslant 2^d$. Thus certainly $\lambda a \in S$ for all $\lambda \in \mathbb{Z}_d$ and we have proved closure under scalar multiplication.

If $a, b \in S$ then, by the last paragraph $2a, 2b \in S$ and hence $2^{-1}(2a+2b) \in S$, establishing closure of S under addition. □

Lemma 13 (Constant modulus): Let ψ be a state vector with non-negative Wigner function. Then $|\psi(\cdot)|$ is constant on the support of ψ.

Proof: Pick two points $x, q \in \operatorname{supp}\psi$ and suppose $|\psi(q)| > |\psi(x)|$.

Letting $z = x - q$, the assumption reads $|\psi(q)| > |\psi(q+z)|$. The modulus inequality, centered at $q+z$, gives

$$|\psi(q+z)|^2 \geqslant |\psi(q)||\psi(q+2z)|. \tag{21}$$

As supp ψ is affine, we know that $\psi(q+kz) \neq 0$ for all $k \in \mathbb{Z}_d$. Hence Eq. (21) together with the assumption implies

$$|\psi(q+z)|^2 > |\psi(q+z)||\psi(q+2z)| \Leftrightarrow |\psi(q+z)| > |\psi(q+2z)|.$$

By inducting on this scheme, we arrive at

$$|\psi(q)| > |\psi(q+z)| > |\psi(q+2z)| > \cdots$$

and therefore $|\psi(q)| > |\psi(q+dz)| = |\psi(q)|$, which is a contradiction.

Thus $|\psi(q)| \leqslant |\psi(x)|$. Swapping the roles of x and q proves that equality must hold. □

At this point, we have full knowledge of the pointwise *modulus* of a state vector with non-negative Wigner function. The *phases* of $\psi(\cdot)$ are, however, completely unknown. The section to come addresses this problem indirectly by studying non-negative Wigner functions.

C. Non-negative Wigner functions

To motivate the following, assume for a moment that ψ has a non-negative Wigner function and further that $\psi(q) \neq 0$ for all q. Choose a $q_0 \in Q$ and consider the function $W(\cdot, q_0)$. Lemma 13 implies that $K_\psi(q_0, \cdot)$ has constant modulus and hence—by Theorem 10.2—$W(\cdot, q_0)$ must be orthogonal to its translations. Clearly, a non-negative function possesses this property if and only if it is supported on at most a single point.

There hence exists a $p_0 \in Q$ such that $W(p, q_0) \propto \delta_{p,p_0}$. This observation starkly reduces the possible forms of positive Wigner functions; it will be generalized to state vectors with arbitrary support in the next lemma.

Lemma 14: Let ψ be a state vector. If W_ψ is non-negative, then it is of the form

$$W_\psi(v) = d^{-n}\delta_T(v),$$

where $T \subset V$ is a set of cardinality d^n.

What is more, if $0 \in T$, then the set of elements of T with vanishing position coordinates

$$\{(p,0) \in T | p \in Q\}$$

is a subspace of V.

Proof: Let $S=\operatorname{supp}\psi$. Again, we may assume that S is a subspace of Q, for else we replace ψ by $w(-s)\psi$ for some $s\in S$. It follows that $\operatorname{supp}K_\psi=S\times S$. Indeed,

$$K_\psi(q,x)\neq 0\Leftrightarrow q\pm 2^{-1}x\in S\Leftrightarrow q\in S\wedge x\in S.$$

Denote by $S^\perp=\{q\in Q|sq=0 \text{ for all } s\in S\}$ the orthogonal complement of S. (For subsets S of Q, $S^\perp$ denotes the orthogonal complement, while for subsets S of V the same symbol refers to the *sympectic* complement. This notation is natural, as for both Q and V only one respective inner product has been defined). We will adopt the common notation $[p]=p+S^\perp$ for cosets of $S^\perp$. It should be clear that $[p]$ is nothing other but the *affine space* with directional vector space given by $S^\perp$ and base vector p. The set S^* of characters of S can be identified with $Q/S^\perp$. Certainly, $s\mapsto\chi(ps)$ defines a character of S for every $p\in Q$. Further, $\chi(ps)=\chi(p's)$ for all $s\in S$ if and only if $p-p'\in S^\perp$. That indeed all elements of S^* can be obtained this way is shown in Corollary 26.

Define K'_ψ to be the restriction of K_ψ to its support $S\times S$. For the rest of the proof, we fix a $q_0\in S$. Now consider

$$W(p,q_0)=d^{-n}\sum_{x\in Q}\bar{\chi}(px)K(q_0,x)=d^{-n}\sum_{x\in S}\bar{\chi}(px)K'(q_0,x).$$

Viewed as a function in p, $W(p,q_0)$ has constant values on cosets of $S^\perp$. Therefore,

$$W'([p],q):=d^n|S|^{-1/2}W(p,q) \tag{22}$$

is a well-defined function on S^*. The considerations of the previous paragraph allow us to identify $W'([\cdot],q_0)$ as the Fourier transform of $K'(q_0,\cdot)$.

We can now repeat the argumentation presented just before the current lemma. Indeed, the modulus of $K'(q_0,[\cdot])$ is constant and W' is non-negative. Furthermore, by definition of q_0, $K'(q_0,[\cdot])$ is nonzero and we may thus conclude that $p\mapsto W'([p],q_0)$ is supported on exactly one coset $[p_0]$.

Normalization of ψ implies $|\psi(\cdot)|=|S|^{-1/2}$. Hence $|K'_\psi(q_0,\cdot)|=|S|^{-1}$ and

$$\|K'_\psi(q_0,\cdot)\|^2=\sum_x|K'_\psi(q_0,x)|^2=|S|^{-1}.$$

By Parzeval's theorem, $\|W'([\cdot],q_0)\|^2=|S|^{-1}$ as well. It follows that $W'([p_0],q_0)=|S|^{-1/2}$.

Inverting Eq. (22) gives

$$W(p,q)=d^{-n}\begin{cases}1 & [p]=[p_0]\\ 0 & \text{else},\end{cases} \tag{23}$$

which proves the first claim of the lemma. The cardinality of T is fixed by the normalization of the Wigner function (Theorem 6.6).

Now suppose $W(0,0)=W'([0],0)\neq 0$. Clearly, then $W(p,0)$ is nonzero if and only if $p\in[0]\Leftrightarrow p\in S^\perp$. The last assertion of the lemma follows, since $S^\perp$ is a subspace of Q. □

So a non-negative Wigner function is the indicator functions of some set T. This finding is compatible with Lemma 9, which describes the structure of Wigner functions of stabilizer states. The next two lemmas verify that T has indeed all the properties of the sets that appear in Lemma 9.

Lemma 15: Let ψ *be a state vector. If* W_ψ *is of the form*

$$W_\psi(v)=d^{-n}\delta_T(v),$$

then T *is an affine space*.

Proof: The proof proceeds similar to the one of Lemma 12. There is no loss of generality in assuming that $0\in T$.

First, we show that T is closed under scalar multiplication. To this end, pick a point $a\in T$. There exists a symplectic mapping S that sends a to a vector a' of the form $(a'_p,0)$ where a'_p

$\in Q$ (see Appendix D). The set $T'=ST$ is the support of the Wigner function of $\mu(S)\psi$. By the second assertion of Lemma 14, $\lambda a' \in ST$ for every $\lambda \in \mathbb{Z}_d$. Hence $S^{-1}(\lambda a')=\lambda a \in T$.

Turning to closeness under addition, let $a,b \in T$. By the last paragraph, $2a,2b \in T$. Arguing as before, note that the set $T-2a$ is the support of the Wigner function of $w(-2a)\psi$ and thus closed under multiplication. As $2b-2a \in T-2a$, we know that $b-a \in T-2a$ and hence $b+a \in T$. □

Lemma 16: Let ψ be a state vector such that W_ψ is of the form

$$W_\psi(v) = d^{-n}\delta_T(v).$$

If T is a subspace, then it is isotropic.

Proof: The vector ψ describes a pure state, hence $W_\psi \star W_\psi = W_\psi$ (recall the Moyal product, introduced in Theorem 6). Let $u \in T$. Plugging in the definitions gives

$$W_\psi \star W_\psi(u) = d^{-n} \sum_{v,w \in V} W_\psi(u+v) W_\psi(u+w) \overline{\chi}([v,w]) = d^{-3n} \sum_{v,w \in T} \overline{\chi}([v,w]).$$

Note that $\Sigma_{w \in T} \overline{\chi}([v,w]) \leqslant |T| = d^n$ with equality if and only if $[v,w]=0$ for all w. Hence

$$W_\psi \star W_\psi(u) \leqslant d^{-n} = W_\psi(u).$$

For the left-hand and the right-hand side to be equal, T must be isotropic. □

Therefore T, as defined above, is of the form $T=M+v$ where M is an isotropic space of cardinality d^n. But then, W_ψ is the Wigner function of a stabilizer state by Lemma 9. We have proven the following.

Theorem 17 (*Main theorem*): *Let $\psi \in L^2(\mathbb{Z}_d^n)$ be a state vector. If the Wigner function of ψ is non-negative, then ψ is a stabilizer state.*

IV. DISCRETE GAUSSIANS

It has long been realized that the coefficients of stabilizer state vectors are described by quadratic forms. However, the current literature either neglects the nonprime case (Refs. 19, 20, and 25) or is less explicit (Ref. 21) than the following lemma in showing the tight relation between Gaussian states and stabilizer states.

We will concentrate on stabilizer states with full support. This constitutes only a modest restriction of generality. Indeed, let ψ be a general stabilizer state, let $Q' := \operatorname{supp} \psi$. Let us for the sake of simplicity assume that d is prime and Q' is a subspace of Q. The restriction of the coordinate function $\psi(q)$ to Q' can be thought of as defining a vector ψ' of a quantum state of an $n' := \dim Q'$ particle system. It is now possible to check that ψ' is a stabilizer state. In this way any stabilizer state can be viewed as one with full support, possibly on a smaller system. We will, however, not take the time to make this construction precise nor will we rely on it in this paper.

Lemma 18: Let ψ be a state vector. The following statements are equivalent.

1. *ψ is a stabilizer state and $\psi(q) \neq 0$ for all $q \in Q$.*
2. *Up to the action of a Weyl operator, ψ is a graph state.*
3. *There exists a symmetric $n \times n$ matrix θ and an $x \in Q$ such that*

$$\psi(q) = \omega^{q\theta q + xq}.$$

Proof: (1 $\Rightarrow$ 2) By assumption $|\psi\rangle = |M,v\rangle$ for some maximal isotropic space M and a vector v. We claim that there is no nonzero $p \in Q$ such that $(p,0) \in M$.

Suppose there exists such a p. Then

$$\langle q|w(p,0)|M\rangle = \chi(-pq)\langle q|M\rangle.$$

On the other hand,

$$\langle q|w(p,0)|M\rangle = \bar{\chi}([v,(p,0)])\langle q|M\rangle,$$

by the definition of $|M,v\rangle$. Hence supp $|M\rangle$ must be contained within a hypersurface of Q specified by $pq=$const, which contradicts the assumption that supp $\psi=Q$.

There are d^n elements in M. By the last paragraph, no two of them have the same position coordinates. As there exist only $d^n=|Q|$ possible choices for the position coordinates, one can find for every $q\in Q$ a $p\in Q$ such that $(p,q)\in M$. Let $e_1,\ldots,e_n$ denote the canonical basis of $\mathbb{Z}_d^n$. Choose $m_1,\ldots,m_n\in M$ such that the position part of m_i equals e_i. The span of $\{m_i\}_{i=1,\ldots,n}$ has clearly cardinality d^n, so we have found a basis of M. By construction, the generator matrix composed of these basis vectors has the form shown in Eq. (18) with some $n\times n$ matrix θ. It is not hard to see that M is isotropic if and only if θ is symmetric, establishing that $|M\rangle$ is a graph state. Theorem 7 and Lemma 9 show that $w(v)|M\rangle=|M,v\rangle=|\psi\rangle$.

$(2\Rightarrow 3)$. Let M be an isotropic space which possesses a generator matrix of the form given in Eq. (18). Let $m_i=(\vartheta_i,e_i)$ be the ith column of that matrix. We need to establish the existence of a symmetric matrix θ and an $x\in Q$ such that

$$\langle q|M,v\rangle = \omega^{q\theta q+xq} =: \psi(q).$$

Indeed, choose

$$\theta = 2^{-1}\vartheta, \quad x_i=[v,m_i].$$

Using Eq. (8), one can then check by direct computation that ψ fulfills the defining eigenvalue equations

$$\chi([v,m_i])w(m_i)\psi=\psi,$$

and hence $|\psi\rangle=|M,v\rangle$ by Lemma 8.

$(3\Rightarrow 1)$. Reverting the previous proof shows that ψ is a graph state. It has maximal support by definition. □

The claimed analogy between stabilizer states and Gaussian states is apparent when comparing statement 3 to Theorem 1.

V. MIXED STATES

It is natural to ask how the results obtained before generalize to mixed states. Certainly, mixtures of stabilizer states are non-negative on phase space and it might be surmised that all such quantum states are convex combinations of stabilizer ones. In the context of continuous variable systems, Bröcker and Werner refuted an analogous conjecture by giving a counterexample.[30] Again, the situation is similar in the finite setting, as will be shown now.

As a consequence of Theorem 6.5, $A(0)$ can be decomposed as $A(0)=P_+ + P_-$, where $P_\pm$ denotes the projector onto the symmetric and antisymmetric state vectors, respectively (see Fig. 1). Since $P_+ + P_- = \mathbb{1}$, we have that $P_- = 1/2(\mathbb{1}-A(0))$. Because we know the Wigner functions of both $\mathbb{1}$ $(W(v)=d^{-n})$ and of $A(0)$ $(W(v)=\delta_{v,0})$, we immediately obtain

$$W_{P_-}(v) = \frac{1}{2}\begin{cases} d^{-n}-1 & v=0 \\ d^{-n} & \text{else}. \end{cases} \tag{24}$$

For a single three-dimensional quantum system there exists a unique antisymmetric state vector $|\psi_-\rangle=2^{-1/2}(|+1\rangle-|-1\rangle)$, hence $P_-=|\psi_-\rangle\langle\psi_-|$. Figure 2 depicts the Wigner function of the state ρ, obtained by mixing the pure states $|\psi_-\rangle, w(-1,0)|\psi_-\rangle$, and $w(-1,-1)|\psi_-\rangle$ with equal weights.

The Wigner function of a single-particle stabilizer state is a line in the two-dimensional phase space, according to Lemma 9. There are $d(d+1)$ such lines and hence equally many stabilizer states. Assume these states have been brought into some order and denote the associated projection operators by $P_1,\ldots,P_{d(d+1)}$. Let $\rho=\sum_i^{d(d+1)}\lambda_i P_i$ be a convex decomposition of ρ in terms these

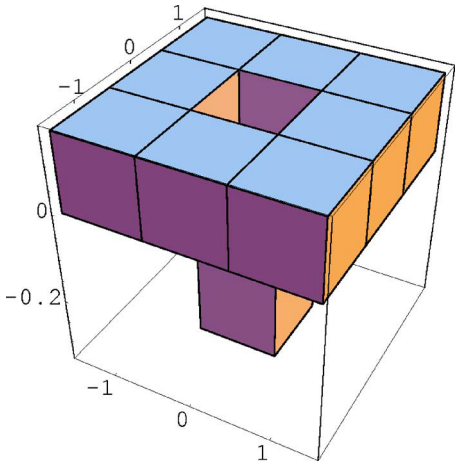

FIG. 1. Wigner function of the antisymmetric vector $|\psi_-\rangle$.

operators. If there is a point v in phase space where $W_\rho(v)=0$ and $W_{P_i}(v)\neq 0$, then clearly λ_i must vanish. By exhaustively listing all 12 lines in $\mathbb{Z}_3^2$, one finds that ρ can have nonzero coefficients only with respect to the stabilizer states whose Wigner functions are shown in Fig. 3.

But ρ admits no convex decomposition in terms of these three lines. Indeed, no two of them cover all the points in the support of W_ρ, so only a mixture of all three lines could potentially suffice. Now notice that the point $(1,-1)$ is an element only of the third line, while $(1, 0)$ is contained in both the second and the third one. Therefore any mixture of these three lines takes on a higher value on $(1, 0)$ than on $(1,-1)$. The distribution W_ρ, on the other hand, is constant on its support.

VI. DYNAMICS

Having established which quantum states give rise to non-negative phase space distributions, the next step is to characterize the set of operations that preserve this property. We have seen in Sec. II D that Clifford unitaries implement permutations in phase space and thus manifestly preserve positivity. They are unique in that regard, as will be shown now.

By the results of Sec. III, it is apparent that a unitary operation U can preserve positivity only if it sends stabilizer states to stabilizer states. One can reasonably conjecture that only Clifford

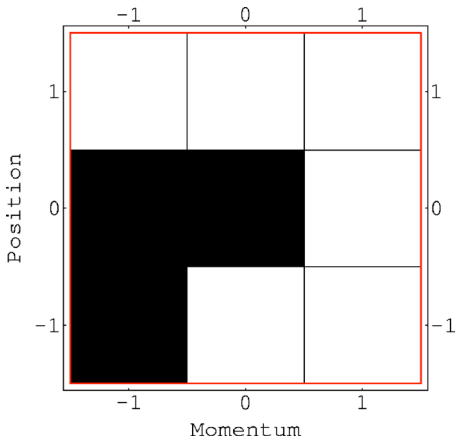

FIG. 2. Wigner function of the equal mixture of the vectors $|\psi-\rangle$, $w(-1,0)|\psi_-\rangle$, and $w(-1,-1)|\psi_-\rangle$. White squares stand for a value of $1/6$ and black squares for 0.

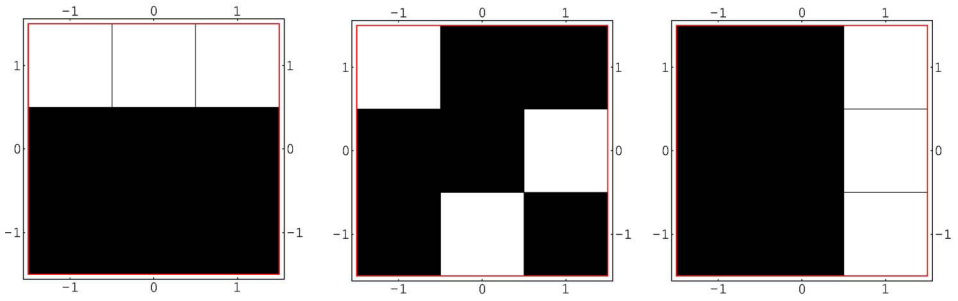

FIG. 3. The white squares mark all lines in $\mathbb{Z}_3^2$ that do not intersect any point where the Wigner function shown in Fig. 2 vanishes.

operations possess this feature and in the case of single particles in prime-power dimensions, a proof of this fact has been given in Ref. 26. The general case, however, poses surprising difficulties which have forced us to take a less direct route.

Let us shortly pause to clarify our objectives. We aim to characterize the set of unitaries U that satisfy statements of the kind: $W_{U\rho U^\dagger}$ is non-negative whenever W_ρ is. We can require the above statement to hold for *any* Hermitian operator ρ or just whenever ρ is a *quantum state*. In the former case the restrictions on U are much stronger than in the latter one. Indeed, by considering the image of the phase space point operators $A(a)$ under the action of U and making use of Lemma 29, it is straightforward to prove that only Clifford operations can preserve positivity of the Wigner functions of general Hermitian operators. The following theorem is slightly more ambitious in considering only the action of U on quantum states.

Theorem 19 *(Only permutations preserve positivity): Let U be unitary. If, for all quantum states ρ with non-negative Wigner function, it holds that* $W_{U\rho U^\dagger}$ *is non-negative, then U is Clifford.*

Proof: First, take note that substituting "quantum state" by "positive operator" in the above theorem, only amounts to a change of normalization and does not alter the statement. Set

$$\mu(\rho) := \min_{v \in V} W_\rho(v),$$

$$\nu(\rho) := \operatorname{minarg} W_\rho := \{v \in V | W_\rho(v) = \mu(v)\}.$$

Let ρ be such that $\mu(\rho) < 0$. We claim that $\mu(\rho) = \mu(\rho')$, where $\rho' = U_\rho U^\dagger$. In other words, U preserves minimal values.

Indeed, there exists positive constants $\lambda_{1,2}$ such that

$$\lambda_1 \mu(\rho') + \lambda_2 d^{-n} = 0.$$

Hence $\sigma := \lambda_1 \rho + \lambda_2 \mathbb{I}$ has a non-negative Wigner function. The assumption $\mu(\rho') < \mu(\rho)$ yields

$$W_{U\sigma U^\dagger}(v) = \lambda_1 \mu(\rho') + \lambda_2 d^{-n} < 0,$$

for every $v \in \nu(\rho')$, which contradicts the defining property of U. Thus $\mu(\rho') \leqslant \mu(\rho)$. Substituting U by U^{-1} shows that equality of $\mu(\rho)$ and $\mu(\rho')$ must hold.

Now set

$$\rho(a) := (1 - d^{-n})^{-1} w(a) P_- w(a)^\dagger,$$

for all $a \in V$. We have $\mu(\rho(a)) = \mu(\rho'(a)) = -1$ and $\nu(\rho) = \{a\}$. The crucial observation lies in the fact that $\nu(\rho')$ contains only a single point as well. So, U preserves the "pointed" shape of $W_\rho(a)$. To see why that is the case, suppose there is a a_0 such that $|\nu(\rho(a_0)')| > 1$. There are d^{2n} operators $\rho(a)'$ and equally many points in phase space, so there exists an a_1 such that $\nu(a_0)$ and $\nu(a_1)$ intersect in at least one point v. Define $\sigma = 1/2(\rho(a_0) + \rho(a_1))$. It holds that $\mu(\sigma) > -1/2$, whereas

$W_{\sigma'}(v)=-1$ which is a contradiction. There is hence a well-defined function S which sends a to the unique element of $\nu(\rho(a)')$.

Finally, let σ be any density matrix. The idea is to mix σ very weakly to $\rho(a)$, so that the positions of the minima of the mixture are still determined by $\rho(a)$. Indeed, there exists an $\epsilon > 0$ such that

$$\nu(\rho(a) + \epsilon\sigma) = \{a\},$$

$$\mu(\rho(a) + \epsilon\sigma) = -1 + \epsilon W_\sigma(a),$$

$$\nu(\rho(a)' + \epsilon\sigma') = \{S(a)\},$$

$$\mu(\rho(a)' + \epsilon\sigma') = -1 + \epsilon W_\sigma(S(a)).$$

Hence $W_{\sigma'}(Sa)=W_\sigma(a)$. We have established that U acts as a permutation in phase space and is therefore Clifford by Lemma 29. □

VII. PRIME POWER DIMENSIONS

Wigner functions for quantum systems with prime power dimensions have received particular attention in the literature (most prominently in Ref. 16). Once again, this is due to the fact that a finite field of order d exists exactly when d is the power of a prime and that the field's well-behaved geometrical properties facilitate many constructions. The present section briefly addresses the relationship between three natural approaches to Wigner functions for such systems. We assume the reader is already familiar with the definition of Weyl operators over Galois fields; a thorough introduction can be found in Refs. 15 and 16.

Let $d=p^k$ for some prime number p. There are three natural ways of associating a configuration space to $\mathcal{H}$. These are the following:

1. an n-dimensional vector space over $\mathbb{Z}_p$,
2. a one-dimensional module over $\mathbb{Z}_{p^n}$, or
3. a one-dimensional vector space over the Galois field $\mathbb{F}_{p^n}$ of order p^n.

The first and the second of these points of view have manifestly been covered in this paper. So far we neglected case 3, because—as we will see—it can be completely reduced to the first one.

Let us quickly gather some well-known facts on finite fields. If p is prime and n a positive integer, $\mathbb{F}_{p^n}$ denotes the unique finite field of order $d=p^n$. The simplest case occurs for $n=1$, when $\mathbb{F}_p \simeq \mathbb{Z}_p$. For $n>1$, fields $\mathbb{F}_{p^n}$ are realized by *extending* $\mathbb{F}_p$, which is then referred to as the *base field*. Extension fields contain the base field as a subset. The extension field possesses the structure of an n-dimensional vector space over the base field. A set of elements of F_{p^n} is a *basis* if it spans the entire field under addition and $\mathbb{F}_p$ multiplication. After having chosen a basis $\{b_1,\ldots,b_n\}$, we can specify any element $f=\Sigma_i f^i b_i$ by its expansion coefficients $\{f^i\}$. The operation

$$\mathrm{Tr}\, f = \sum_{k=0}^{n-1} f^{p^k}$$

takes on values in the base field and is $\mathbb{F}_p$ linear. Therefore,

$$\langle f,g\rangle \mapsto \mathrm{Tr}(fg)$$

defines an $\mathbb{F}_p$-bilinear form. For any basis $\{b_i\}$, there exists a *dual basis* $\{b^i\}$ fulfilling the relation $\mathrm{Tr}(b^i b_j)=\delta_{i,j}$ (we do not use Einstein's summation convention). From now on, we assume that a basis b_i and a dual one b^i have been fixed.

Repeating the construction put forward in Sec. II, we introduce the Hilbert space $\mathcal{H}=L^2(\mathbb{F}_{p^n})$, in other words, $\mathcal{H}$ is the span of $\{|q\rangle|q\in\mathbb{F}_{p^n}\}$. The choice of a basis induces a tensor structure on $\mathcal{H}$ via

$$|q\rangle=\left|\sum_i q^i b_i\right\rangle\mapsto\bigotimes_i|q^i\rangle.$$

We obtain a character of $\mathbb{F}_{p^n}$ by setting $\chi_{p^n}(f)=\chi_p(\mathrm{Tr}\,f)$. Note that for $n=1$, $\chi_{p^n}=\chi_p$. Expanding momentum coordinates $p=\Sigma_j p_j b^i$, the character factors,

$$\chi(pq)=\chi_p\left(\sum_{i,j}p_j q^i\,\mathrm{Tr}(b_i b^j)\right)=\prod_i\chi_p(p_i q^i).$$

Similarly, the shift and multiply operators factor with respect to this tensor structure,

$$x\left(\sum_i q^i b_i\right)\left|\sum_j x^j b_j\right\rangle=\bigotimes_i x^{(i)}(q^i)|x^i\rangle,$$

$$z\left(\sum_i p_i b^i\right)\left|\sum_j x^j b_j\right\rangle=\prod_i\chi_p(p_i x^i)\left|\sum_j x^j b_j\right\rangle=\bigotimes_i z^{(i)}(p_i)|x^i\rangle,$$

where $x^{(i)}$ and $z^{(i)}$ act on the ith p-dimensional subsystem. A straightforward computation along the lines just presented shows that both the Weyl operators and the phase space point operators factor,

$$w(p,q)=\bigotimes_i w^{(i)}(p_i,q^i)=w(p_1,\ldots,p_n,q^1,\ldots,q^n)$$

$$A(p,q)=\bigotimes_i A^{(i)}(p_i,q^i)=A(p_1,\ldots,p_n,q^1,\ldots,q^n).$$

The above result thus states that the Wigner function induced by the choice $Q=\mathbb{F}_{p^n}$ coincides—up to relabeling of the phase space points—with the one for $Q=\mathbb{F}_p^n$. In particular, both definitions give rise to the same set of states with a non-negative phase space distribution.

For stabilizer states, however, the situation is not as easy, as will be discussed subsequently. The preceding discussion suggests defining a map $\iota:\mathbb{F}_{p^n}^2\to\mathbb{F}_p^{2n}$ by

$$(p,q)\mapsto(p_1,\ldots,p_n,q^1,\ldots,q^n)$$

(see Refs. 15 and 31). Let M be a maximal isotropic subspace of $\mathbb{F}_{p^n}^2$. It is readily verified that $\iota(M)\subset\mathbb{F}_p^{2n}$ is again isotropic and a subspace. Further, we have shown that the sets of Weyl operators $w(M)$ and $w(\iota(M))$ coincide and hence so do the stabilizer states $|M\rangle$ and $|\iota(M)\rangle$.

The converse is not true. ι^{-1} does not necessarily map $\mathbb{F}_p^{2n}$ subspaces to those of $\mathbb{F}_{p^n}^2$. More precisely, if $M\subset\mathbb{F}_p^{2n}$ is a subspace, then $\iota^{-1}(M)$ can easily be proven to be closed under addition, but will in general fail to be closed under $\mathbb{F}_{p^n}$-scalar multiplication. This proves the remark made in the introduction, namely, that the set of "single-particle" (i.e., $\mathbb{F}_{p^n}^2$) stabilizer states is a true subset of corresponding "multiparticle" set. The following subsection gives a quantitative account of the relation of the sets.

A. Counting stabilizer codes

We are going to count the number of stabilizer states of a system composed of n d-level particles. In fact, the computation given below is slightly more general in that it gives the number of k-dimensional *stabilizer codes*.[17]

Stabilizer codes are generalizations of stabilizer states. Recall Eq. (17), where we showed that summing Weyl operators $w(m)$ over the elements m of a maximal isotropic subspace M of V yields a one-dimensional projection operator. It can be shown that if the requirement of maximality is dropped, the sum still evaluates to a projector. The range of this operator is the *stabilizer code*

defined by M. The dimension m of M and the dimension k of the stabilizer code are related by $k=d^{n-m}$.

Theorem 20 *(Number of isotropic subspaces): Let V be a $2n$-dimensional symplectic vector space over $\mathbb{F}_d$, where d is the power of a prime. The number of m-dimensional isotropic subspaces of V is given by*

$$\mathrm{Iso}(n,m,d) = \begin{bmatrix} n \\ m \end{bmatrix}_d \prod_{i=0}^{m-1} (d^{n-i}+1),$$

where the square brackets denote the Gaussian coefficients,

$$\begin{bmatrix} n \\ m \end{bmatrix}_d = \prod_{i=0}^{m-1} \frac{d^{n-i}-1}{d^{m-i}-1}.$$

Proof: The proof is inspired by a method employed in Ref. 32 to solve a related problem. We count the number of linearly independent m tuples consisting of mutual orthogonal vectors. Indeed, as the first vector v_1 we are free to choose any nonzero element of V. There are $d^{2n}-1$ such choices. The second vector must lie in the symplectic complement of the span of the first vector $\langle v_1\rangle^{\perp}$. Hence, v_2 can be chosen from a $2n-1$-dimensional vector space, the only restriction being that $v_2 \notin \langle v_1\rangle$. It follows that there exist $d^{2n-1}-d^1$ possibilities for v_2. Inducting on this scheme gives

$$\prod_{i=0}^{m-1} (d^{2n-i}-d^i) \tag{25}$$

such tuples.

However, since two different tuples might correspond to the same isotropic space, Eq. (25) overcounted the subspaces. To take that fact into account, we must divide by the number of bases within an m-dimensional space. Arguing in a similar fashion as before, we arrive at $\Pi_{i=0}^{m-1}(d^m-d^i)$ for the sought-after number (see also Ref. 32). Division gives

$$\mathrm{Iso}(n,m,d) = \prod_{i=0}^{m-1} \frac{d^{2n-i}-d^i}{d^m-d^i} = \prod_{i=0}^{m-1} \frac{d^{2(n-i)}-1}{d^{m-i}-1}.$$

Expanding $d^{2(n-i)}-1=(d^{n-i}-1)(d^{n-i}+1)$ and using the definition of the Gaussian coefficients concludes the proof. □

Corollary 21; The number of d^{n-m}-dimensional stabilizer codes defined on n d-level systems is

$$\mathrm{Stabs}(n,m,d) = d^m \begin{bmatrix} n \\ m \end{bmatrix}_d \prod_{i=0}^{m-1} (d^{n-i}+1).$$

In particular, the number of stabilizer states is

$$\mathrm{Stabs}(n,n,d) = d^n \prod_{i=1}^{n} (d^i+1).$$

Proof: We only need to justify the prefactor d^m. The defining Eq. (17) generates a projector onto a stabilizer code given an isotropic space M and a character $\chi([v,\cdot])$ on M. If $\dim M=m$, then there are $|M|=d^m$ distinct such characters (see Appendix C). □

We can now compare the number of stabilizer states for n particles of dimension d to the corresponding number for a single d^n-dimensional system,

$$\frac{\mathrm{Stabs}(n,n,d)}{\mathrm{Stabs}(1,1,d^n)} = \frac{\prod_{i=1}^{n}(d^i+1)}{d^n+1} = \prod_{i=1}^{n-1}(d^i+1) \geqslant d^{\sum_{i=1}^{n-1} i} = d^{1/2(n^2-n)}.$$

This is the superexponential scaling mentioned in the introduction.

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APPENDIX A: DISCRETE STONE–VON NEUMANN THEOREM

This section generalizes well-known results for prime-power dimensions (see, e.g., Ref. 33 and citations therein) to all odd d. The proof is based on some simple observations employing group representation theory. We state a preparing lemma beforehand.

Lemma 22: The Weyl representation is irreducible.

Proof: We compute

$$\frac{1}{|H(\mathbb{Z}_d^n)|}\sum_{\substack{a\in V,\\ t\in\mathbb{Z}_d}} |\mathrm{tr}\, w(a,t)|^2 = d^{-(2n+1)}\sum_t |\mathrm{tr}\, w(0,t)|^2 = d^{-(2n+1)}\sum_t d^{2n} = 1,$$

which establishes irreducibility by a well-known criterion from group representation theory (see any textbook on that topic, e.g., Ref. 34). □

Proof (of Theorem 3): By the composition law Eq. (4) it is clear that $w'(p,q,t) := w(S(p,q),t)$ is a representation of the Heisenberg group which affords the same character (i.e., $\mathrm{tr}\, w(a,t)=\mathrm{tr}\, w'(a,t)$). The preceding lemma yields that w and w' are equivalent and thus the existence of $\mu(S)$ follows. Further,

$$\mu(S)\mu(T)w(p,q)\mu(T)^\dagger\mu(S)^\dagger = \mu(S)w(T(p,q))\mu(S)^\dagger = w(ST(p,q)) = \mu(ST)w(p,q)\mu(ST)^\dagger.$$

Because the Weyl matrices span the set of all operators, the last line fixes $\mu(ST)$ modulo a phase and we have proven the second assertion.

We turn to the last claim. Let S and c be as defined in Eq. (10). Using the commutation relations Eq. (4) and the fact that conjugation by unitaries leaves the center $\chi(t)\mathbb{1}$ of the Weyl representation invariant, it is easy to see that S must be an isometry in the sense that $[Sa,Sb]=[a,b]$. To proceed, consider the following calculation. On the one hand,

$$Uw(a)w(b)U^\dagger = Uw(a+b,2^{-1}[a,b])U^\dagger = w(S(a+b),2^{-1}[a,b])c(a+b), \tag{26}$$

while on the other hand,

$$Uw(a)w(b)U^\dagger = Uw(a)U^\dagger Uw(b) = w(Sa)w(Sb)c(a)c(b) = w(Sa+Sb,2^{-1}[Sa,Sb])c(a)c(b). \tag{27}$$

Comparing the last lines of Eqs. (26) and (27) one finds that S must be compatible with addition in $\mathbb{Z}_d^{2n}$ meaning that $S(a+b)=Sa+Sb$. Because $\mathbb{Z}_d$ is *cyclic* the preceding property implies that S is also compatible with scalar multiplication,

$$S(\lambda a) = S(a + \cdots + a) = S(a) + \cdots + S(a) = \lambda S(a).$$

Hence S is linear and therefore symplectic. Last, again using lines (26) and (27), we have that $c(a+b)=c(a)c(b)$ and conclude that c is a character. By Lemma 24, there exists an $a_0 \in V$ such that $c(\cdot)=\chi([a_0,S\cdot])$. Thus,

$$w(a_0)\mu(S)w(a)\mu(S)^\dagger w(a_0)^\dagger = w(a_0)w(Sa)w(-a_0) = \chi([a_0,Sa])w(Sa) = c(a)w(Sa).$$

□

APPENDIX B: AXIOMATIC CHARACTERIZATION OF THE WIGNER FUNCTION

The discussion in Sec. II D should suggest that Definition 5 yields the natural analog of the original continuous Wigner function. However, to bolster that claim with more objective arguments, we establish that—at least in prime dimensions—the form is virtually determined by the property of Clifford covariance (Theorem 7).

Theorem 23 *(Uniqueness): Let d be an odd prime. Let $Q,V,\mathcal{H}$ be as usual. Consider a mapping W' that fulfills the following axioms.*

1. (Phase space) *W' is a linear mapping sending operators to functions on the phase space V.*
2. (Clifford covariance) *W' is covariant under the action of the Clifford group, in the sense of Theorem 7.* Then $W'_\rho(p,q)=\lambda_1 W_\rho(p,q)+\lambda_2$ *for two constants* $\lambda_{1,2}$. *If further,*
3. (Marginal probabilities) *W' gives the correct marginal probabilities, as stated in Theorem 6.43,*

then $W'(p,q)=W(p,q)$.

Proof: Consider an alternative definition $\rho \mapsto W'_\rho$ of a Wigner function. Linearity implies the existence of a set of operators $\{A'(v)\}$ such that $W'(v)=d^{-n}\operatorname{tr}(A'(v)\rho)$. W' is covariant under the action of the Weyl operators if and only if $A'(v)=w(v)A'(0)w(v)^\dagger$. So the only degree of freedom left in the definition of W' is the choice of $A'(0)$. Again, one must require $A'(Sv)=\mu(S)A(v)\mu(S)$ if Theorem 7 is to hold. In particular, because the origin 0 is a fixed point of any linear operation, $A'(0)$ must commute with all $\mu(S)$.

As a consequence, the old, unprimed Wigner function $W_{A'(0)}$ of $A'(0)$ stays fixed under any symplectic operation S. Since any two non-zero points of V can be mapped onto each other by a suitable symplectic matrix S, $W_{A'(v)}$ must be constant on all such points. So there are only two parameters free to be chosen: $W_{A'(0)}(0)$ and $W_{A'(0)}(v), v \neq 0$. Clearly, the set of all operators that comply with these constraints is spanned by $\mathbb{1}$ and $A(0)$,

$$A'(0) = \lambda_1 \mathbb{1} + \lambda_2 A(0). \tag{28}$$

The above decomposition implies the first statement of the theorem.

As for the second claim, choose an $a \in V$. The projection operator $|a\rangle\langle a|$ is invariant under the action of Weyl operators of the form $w(p,0)$. Thus, due to Clifford covariance, the Wigner function $W'_{|a\rangle}$ must be p-shift invariant: $W'_{|a\rangle}(p+p',q)=W'_{|a\rangle}(p,q)$. We required Theorem 6.3 to hold, hence

$$\sum_{p\in Q} W'_{|a\rangle}(p,0) = d^n W'(0,0) = \delta_{a,0}.$$

By Eq. (28) and Theorem 6.5 it follows that $W'(0,0)=d^{-n}(\lambda_1+\lambda_2\delta_{a,0})$, yielding $\lambda_1=0,\lambda_2=1$. □

APPENDIX C: CHARACTERS AND COMPLEMENTS

Consider a space $R=\mathbb{Z}_d^n$ with a bilinear form $\langle\cdot,\cdot\rangle: R\times R\to\mathbb{Z}_d$. For any $s\in R$ the function $r\mapsto\chi(\langle s,r\rangle)$ defines a character of R. The form is said to be *nondegenerate* if $\langle s,\cdot\rangle \neq \langle s',\cdot\rangle$ for distinct s,s'. The two spaces we are concerned with are Q with the canonical scalar product and V with the symplectic scalar product. Both can easily be checked to be nondegenerate.

The following lemma states a basic fact about spaces with nondegenerate forms. We repeat it for completeness.

Lemma 24: Let $R=\mathbb{Z}_d^n$ with nondegenerate bilinear form $\langle\cdot,\cdot\rangle$. Any character ζ of R is of the form $\zeta(r)=\chi([s,r])$ for some unique $s\in R$.

Proof: Addition gives V the structure of a finite Abelian group. Therefore, $V\simeq V^*$, as is well-known (see, e.g., Ref. 28). So there are $|V|$ different characters of V, but equally many of the form $\chi([v,\cdot])$. □

If d is prime and M a subspace of V, the well-known relation $\dim M+\dim M^\perp=\dim V$ holds.[35] It is, however, no longer true in the general case. A counterexample can be constructed along the same lines as in Sec. II C. Still, an analog exists as demonstrated below.

Theorem 25: *Let $R=\mathbb{Z}_d^n$ with nondegenerate bilinear form $\langle\cdot,\cdot\rangle$. If M denotes a subspace of R, then the "complementarity relation" $|M||M^\perp|=|R|$ holds.*

Proof: We will show that

$$M^\perp\simeq(V/M)^*. \tag{29}$$

For $m\in M^\perp$, the relation $[v]\mapsto\chi([m,v])$ defines a character of V/M, as can easily be verified. Let us denote the map $m\mapsto\chi([m,\cdot])$ by ι_1.

Conversely, given an element ζ of $(V/M)^*$, $v\mapsto\zeta([v])$ is a character of V. By Lemma 24 there exists a unique $w\in V$ such that $\zeta([v])=\chi([w,v])$. If $m\in M$, then $\zeta([m])=\zeta([0])=1$ and hence $w\in M^\perp$. Using the notions just introduced, we can define $\iota_2:(V/M)^*\to M^\perp$ by $\zeta\mapsto w$.

It is simple to check that $\iota_2=\iota_1^{-1}$. In particular, ι_1 is invertible and Eq. (29) follows.

With the help of Lagrange's theorem, we can compute

$$|M^\perp|=|(V/M)^*|=|V/M|=|V|/|M|,$$

which concludes the proof. □

Corollary 26: Let V,Q be defined as usual. Let M be an isotropic subspace of V and S be any subspace of Q.

1. (Maximally isotropic spaces) *M is equal to its symplectic complement $M^\perp$ if and only if $|M|=d^n$.*
2. (Characters of subspaces) *Any character ζ of S can be written as $\zeta(s)=\chi(qs)$ for a suitable $q\in Q$.*

Proof: Claim 1 follows immediately from Theorem 25 and the fact that isotropic spaces are contained in their symplectic complement: $M\subset M^\perp$.

We turn to the second statement. In Lemma 14 we have argued that the characters of S which are expressable as $\chi(qs)$ stand in one-to-one correspondence to cosets in $Q/S^\perp$. But $|Q/S^\perp|=|S|$ and hence all characters are of that form. □

APPENDIX D: A GEOMETRIC NOTE

The proof of the main theorem makes use of the fact that for any vector $v\in V$, there exists a symplectic operation S that sends v to a vector of the form $(p,0)$. Indeed, if d is prime, any two vectors are similar, in the sense that they can be mapped onto each other by a symplectic matrix. Technically, this is a trivial incarnation of Witt's lemma (see Ref. 36 for a formulation that is applicable in our context).

Once again the nonprime case poses additional difficulties. Recall that the *order* of a $v\in V$ is the least positive $\lambda\in\mathbb{Z}_d$ such that $\lambda v=0$. It is easy to see that the order of a vector is left invariant by the action of invertible linear mappings. If d is a composite number (i.e., not prime), then $V=\mathbb{Z}_d^{2n}$ contains elements of different orders which cannot be related by a linear operation. However, one might conjecture that any two vectors of equal order are similar. This is the content of the following lemma. Some concepts used in the proof can be found in Refs. 35 and 37.

Lemma 27 (Similarity): Let $V=\mathbb{Z}_d^{2n}$. Let $a_1,a_2\in V$ be two vectors with the same order. Then there exists a symplectic matrix S such that $Sa_1=a_2$.

Proof: We can slightly weaken the assumptions made about V. All we require for this proof is that V is a finite $\mathbb{Z}_d$ module with nondegenerate symplectic form $[\cdot,\cdot]$. It need not be of the form $\mathbb{Z}_d^{2n}$.

Let $v \in V$ be a vector of order d. As $v \mapsto \chi([v,\cdot])$ implements an isomorphism, $V \to V^*$, ord $(\chi([v,\cdot]))=\mathrm{ord}(v)=d$. There hence exists a $w \in V$ such that $[v,w]=\lambda$ has order d. Any such number possesses a multiplicative inverse λ^{-1} modulo $\mathbb{Z}_d$ and hence $w'=\lambda^{-1}$ fulfills $[v,w']=1$. Vectors satisfying such a relation are said to be *hyperbolic couples*. Denote their span $\langle\{v,w'\}\rangle$ as H.

Set $V' := H^\perp$. By Theorem 25 $|V|=|H||V'|$. Further, it is easy to see that $H^\perp \cap H=\{0\}$ and hence $V=HV'$, where $\oplus$ denotes the *orthogonal direct Sum*. We claim that the symplectic inner product is nondegenerate on V'. Indeed, supose there is a nonzero $v' \in V'$ such that $[v',w']=0$ for all $w' \in V'$. Then, by definition of V', $[h,w']=0$ for all $h \in H$ and therefore v' would be orthogonal on all vectors of V. Hence such a v' cannot exist by the nondegeneracy of $[\cdot,\cdot]$.

Note that V' fulfills the assumptions made about V at the beginning of the proof and has strictly smaller cardinality. Thus, we can induct on $|V|$ to obtain a decomposition

$$V = H_1 \oplus \ldots \oplus H_n$$

of V in terms of two-dimensional subspaces spanned by hyperbolic couples $\{v_i,w_i'\}$. We arrange these vectors as the columns of a matrix $S=(v_1,\ldots,v_n,w_1',\ldots,w_n')$. The construction of the couples $\{v_i,w_i'\}$ ensures that S is symplectic, as can easily be verified.

Now let $a_1,a_2 \in V$ be two vectors with maximal order. By the preceding discussion, there exists symplectic matrices S_i having a_i as their respective first column. Clearly, then $S_2 S_1^{-1} a_1 = a_2$.

Last, suppose $\mathrm{ord}(a_i)=k \leqslant d$. It is easy to see that $a_i'=ka_i/d$ are elements of V with maximal order. Further, if S maps a_1 to a_2, then also a_1 to a_2. □

Corollary 28 (Transitive action): Let $|M_1,v_1\rangle$, $|M_2,v_2\rangle$ be stabilizer states. If their respective associated isotropic subspaces M_1 and M_2 are spanned by vectors of maximal order, then there exists a Clifford operation relating these state vectors.

Proof: Let $\{m_1^{(i)},\ldots,m_n^{(i)}\}$, $i=1,2$ be bases of M_1 and M_2, respectively. Assume that all vectors have maximal order. It is simple to adapt the previous proof for constructing a symplectic matrix S sending $m_i^{(1)}$ to $m_i^{(2)}$. □

APPENDIX E: SOME PROPERTIES OF THE PHASE SPACE POINT OPERATORS

Lemma 29 (Properties of the phase space point operators): The phase space point operators fulfill the following relations:

$$A(a) = w(2a)A(0),$$

$$A(a)A(b) = w(2a-2b),$$

$$tr(A(u)A(v)A(w)) = \chi([v,u]+[u,w]+[w,v]).$$

Further, if U permutes the phase space point operators under conjugation

$$UA(v)U^\dagger = A(v'),$$

for all $v \in V$, then U is Clifford.

Proof: Clifford covariance (Theorem 7) implies $A(a)=w(a)A(0)w(a)\dagger$. Using Theorem 6.5 it is easy to see that $A(0)w(a)A(0)=w(-a)$ and $A(0)^2=\mathbb{1}$. Hence,

$$A(a) = w(a)A(0)w(-a)A(0)A(0) = w(2a)A(0),$$

proving the first relation. The second one follows.

For the proof of the third equation, we abbreviate $A(0)$ as A. Then

$$\begin{aligned}\mathrm{tr}(A(u)A(v)A(w)) &= \mathrm{tr}(w(2u)Aw(2v)Aw(2w)A) = \mathrm{tr}(w(2u)w(-2v)w(2w)A^3)\\ &= \chi([u,-v]+[u-v,w])\mathrm{tr}(w(2(u-v+w))A)\\ &= \chi([v,u]+[u,w]+[w,v])\mathrm{tr}(A(u-v+w)).\end{aligned}$$

It has been noted in Theorem 6.6 that phase space point operators have unit trace, which concludes the proof.

Last, suppose the action of U permutes phase space point operators. For any $a \in V$, we have

$$Uw(a)U^\dagger = Uw(22^{-1}(a-0))U^\dagger = UA(a)UU^\dagger A(0)U^\dagger = A(a')A(0') = w(2(a'-0')),$$

for suitable $a', 0' \in V$. Hence U maps Weyl operators to Weyl operators and is thus Clifford by definition. □

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Fractional supersymmetry and hierarchy of shape invariant potentials

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Fractional supersymmetric quantum mechanics is developed from a generalized Weyl-Heisenberg algebra. The Hamiltonian and the supercharges of fractional supersymmetric dynamical systems are built in terms of the generators of this algebra. The Hamiltonian gives rise to a hierarchy of isospectral Hamiltonians. Special cases of the algebra lead to dynamical systems for which the isospectral supersymmetric partner Hamiltonians are connected by a (translational or cyclic) shape invariance condition. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Supersymmetry was initially introduced in high energy physics, as a kind of symmetry between bosons and fermions, to describe fundamental interactions of Nature in an unified way (e.g., see Ref. 1). Supersymmetry cannot be an exact symmetry. In order to understand supersymmetry breaking in quantum field theory, Witten studied supersymmetric quantum mechanics (SUSYQM).[2] Presently, SUSYQM turns out to be a powerful tool to investigate integrability in quantum mechanics.[3–5] In this connection, the concept of shape invariant potential was introduced by Gendenshtein.[6] This concept is especially useful to determine the spectrum of exactly solvable potentials. Indeed, for a given solvable potential, shape invariance implies integrability. It is now well known there are three kinds of shape invariant potentials, namely, translational shape invariant potentials,[7,8] scaling shape invariant potentials,[9,10] and cyclic shape invariant potentials.[11,12]

For any exactly solvable Hamiltonian (shape invariant or not), SUSYQM provides us with a process to generate a supersymmetric partner Hamiltonian. This process can be used successively to span a hierarchy of isospectral Hamiltonians.[5]

The aim of this work is to study shape invariant potentials together with the generation of a hierarchy of isospectral superpartner Hamiltonians in the framework of *fractional* SUSYQM of order k ($k=3,4,\ldots$).

In general, to pass from *ordinary* SUSYQM to *fractional* SUSYQM of order k (abbreviated as k-SUSYQM in the following), it is necessary to replace the Z_2-grading of the relevant Hilbert space by a Z_k-grading. This amounts either to replace a fermionic degree of freedom by a para-fermionic[13–18] one, of order $k-1$, or to introduce k-fermions,[19–22] which are objects interpolating between bosons and fermions. Quantum groups, with the deformation parameter being a root of unity, play also an important role in the development of k-SUSYQM.[23–31] On the other hand, a realization of bosonized k-SUSYQM can be developed owing to the introduction of a Klein operator of order k ($K^k=1$) which induces a Z_k-grading.[18,32] In this direction, a relation exists between k-SUSYQM and hidden supersymmetric structures.[33–36]

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The approach of k-SUSYQM developed in the present paper took its origin in Ref. 22 (see also Refs. 37–39 for some similar developments). It is based on a Z_k-graded Weyl-Heisenberg algebra W_k. Section III deals with algebra W_k and its use for generating a family of k isospectral Hamiltonians. In Secs. IV and V, some specific Hamiltonians (with translational shape invariant potentials or cyclic shape invariant potentials) corresponding to particular cases of the algebra W_k are studied. We will start in Sec. II with some preliminaries and motivations.

Throughout the present paper, $[A,B]$ and $\{A,B\}$ stand for the commutator and the anticommutator of the operators A and B, respectively. The operator $A^\dagger$ denotes the adjoint of A. The symbol δ is the Kronecker delta. Many quantities are defined modulo k ($\Pi_k \equiv \Pi_0$, $H_k \equiv H_0$, $F_k \equiv F_0$ and $V_k \equiv V_0$). As usual, $f \circ g(x) = f(g(x))$ for two functions f and g. We shall use the convention according to which $\Sigma_{i=a}^{b} x(i) = 0$ when $b < a$ and the symbols S_0 and S_1 for denoting the sets $\{0,1,\cdots,k-1\}$ and $\{1,2,\cdots,k\}$, respectively.

II. PRELIMINARIES AND MOTIVATIONS

For the purpose to establish our notations and to present our motivations, we shall begin with a brief review of *ordinary* SUSYQM, corresponding to $k=2$, and of shape invariance (for more details, see Refs. 3–5).

A. Ordinary supersymmetric quantum mechanics

Let us start with ordinary SUSYQM. A supersymmetric dynamical system is defined by a triplet $(H, Q_+, Q_-)_2$ of linear operators acting on a Z_2-graded Hilbert space $\mathcal{H}$ and satisfying the following relations:

$$H = H^\dagger, \quad Q_- = Q_+^\dagger, \quad Q_\pm^2 = 0,$$

$$\{Q_-, Q_+\} = H, \quad [H, Q_\pm] = 0.$$

The operators Q_+ and Q_- are the supercharges of the system. The self-adjoint operator H, the supersymmetric Hamiltonian for the (one-dimensional) system, can be written as

$$H = H_0 + H_1,$$

where H_0 and H_1 act on the states $|n,0\rangle$ and $|n,1\rangle$ of grading 0 and 1, respectively. These states span the Hilbert space

$$\mathcal{H} = \{|n,s\rangle : n \text{ ranging}; \ s = 0,1\}.$$

We shall assume that there is no supersymmetry breaking. In this situation, the Hamiltonians H_0 and H_1 are isospectral except that the ground state of H_0 has no supersymmetric partner in the spectrum of H_1.

Now suppose that H_0 has p states $|n,0\rangle$ with $n=0,1,\cdots,p-1$ ($p \geq 2$). From the Hamiltonian H_1 with $p-1$ states $|n,1\rangle$ ($n=1,2,\cdots,p-1$), we can find a supersymmetric partner H_2 with $p-2$ states $|n,2\rangle$ ($n=2,3,\cdots,p-1$) and we can repeat this process to generate a hierarchy of p Hamiltonians H_0, H_1, $\cdots$, H_{p-1}. The Hamiltonian H_m ($0 < m < p$) has the same energy spectrum than H_0 except that the $m-1$ first energies of H_0 do not occur in the spectrum of H_m. This result remains valid when p goes to infinity.

We can then ask the following question. What happens when we go from ordinary SUSYQM to k-fractional SUSYQM (with $k=3,4,\cdots$)? We shall answer this question by showing that a hierarchy of isospectral Hamiltonians H_0, H_1, $\cdots$, H_{k-1} can be constructed from a single Hamiltonian H_0 by making use of a Z_k-graded Weyl-Heisenberg algebra. This construction shall be achieved without a repetition process of the type $H_0 \to H_1$, $H_1 \to H_2$, $\cdots$, $H_{k-2} \to H_{k-1}$ as used in ordinary SUSYQM.

B. Shape invariance

It is known that there exists a set of exactly solvable potentials characterized by an integrability condition known as shape invariance condition.[3,5,6] In connection with ordinary SUSYQM, this shape invariance condition leads in an easy way to the spectrum of any invariant shape potential.

More precisely, let us consider the partner potentials $V_0(x,a_0)$ and $V_1(x,a_0)$ associated with the supersymmetric Hamiltonians H_0 and H_1 such that

$$H_s = -\frac{d^2}{dx^2} + V_s(x,a_0), \quad s=0,1,$$

where a_0 is a set of real parameters. The shape invariance condition is defined by

$$V_1(x,a_0) = V_0(x,a_1) + R(a_0), \tag{1}$$

where $a_1=h(a_0)$ corresponds to a reparametrization in V_0 and $R(a_0)$ is a constant. The shape invariance condition immediately yields the energies and wave functions of H_0.[3,5] One obtain the energies $E_{n,0}$ of H_0

$$E_{n,0} = \sum_{l=0}^{n-1} R(a_l), \quad n \geq 1,$$

where

$$a_l = h^{(l)}(a_0) = h \circ h \circ \cdots \circ h(a_0), \quad l \text{ times}.$$

(We take $E_{0,0}=0$.) The three kinds of shape invariance mentioned in the introduction correspond to $a_1=a_0+\alpha$ with $\alpha \in \mathbf{R}$, $a_1=\beta a_0$ with $0<\beta<1$, and $a_1=h(a_0)$ with $h^{(l)}(a_0)=a_0$ for translational,[7,8] scaling,[9,10] and cyclic[11,12] shape invariance, respectively.

Another motivation for this work is to show that the isospectral Hamiltonians obtained from k-SUSYQM are connected through shape invariance. In this respect, we shall use some specific realizations of the Z_k-graded Weyl-Heisenberg algebra W_k in order to generate a hierarchy of Hamiltonians subjected to translational or cyclic shape invariance.

III. FRACTIONAL SUPERSYMMETRIC QUANTUM MECHANICS

A. Definition

Let us go now to k-SUSYQM. A k-fractional supersymmetric dynamical system is defined by a triplet $(H,Q_+,Q_-)_k$ of operators satisfying the following relations[13–16,22]

$$H = H^\dagger, \quad Q_- = Q_+^\dagger, \quad Q_\pm^k = 0,$$

$$\sum_{s=0}^{k-1} Q_-^{k-1-s} Q_+ Q_-^s = Q_-^{k-2} H, \quad [H,Q_\pm] = 0, \tag{2}$$

where $k=3,4,\cdots$. The Hamiltonian H and the supercharges $Q_\pm$ of the dynamical system are linear operators acting on a Hilbert space $\mathcal{H}$,

$$\mathcal{H} = \bigoplus_{s=0}^{k-1} \mathcal{H}_s,$$

which is Z_k-graded in view of the relations $Q_\pm^k=0$. It is to be observed that Eq. (2) works equally well in the case $k=2$ corresponding to ordinary SUSYQM.

B. Generalized Weyl-Heisenberg algebra

Following Ref. 22, we consider the generalized Weyl-Heisenberg algebra W_k, with $k \in \mathbf{N}\backslash\{0,1\}$, spanned by the four linear operators X_+, X_-, N, and K acting on the space $\mathcal{H}$ and satisfying

$$X_- = X_+^\dagger, \quad N = N^\dagger, \quad KK^\dagger = K^\dagger K = 1, \quad K^k = 1,$$

$$[X_-, X_+] = \sum_{s=0}^{k-1} f_s(N)\Pi_s, \quad [N, X_-] = -X_-, \quad [N, X_+] = X_+,$$

$$KX_+ - qX_+K = 0, \quad KX_- - pX_-K = 0, \quad [K, N] = 0, \tag{3}$$

where q and p are roots of unity with

$$q = e^{2\pi i/k}, \quad p = e^{-(2\pi i/k)}.$$

In Eq. (3), the functions $f_s: N \mapsto f_s(N)$ of the number operator N are such that

$$f_s(N) = f_s(N)^\dagger.$$

Furthermore, the operators Π_s are defined in terms of the Klein or grading operator K as

$$\Pi_s = \frac{1}{k}\sum_{t=0}^{k-1} p^{st}K^t, \quad s \in S_0.$$

It is easy to check that

$$\Pi_s = \Pi_s^\dagger, \quad \sum_{s=0}^{k-1} \Pi_s = 1, \quad \Pi_s\Pi_t = \delta_{s,t}\Pi_s.$$

Consequently, the operators Π_s are projection operators for the cyclic group Z_k. It can be proved that they satisfy

$$\Pi_s X_+ = X_+\Pi_{s-1} \Leftrightarrow X_-\Pi_s = \Pi_{s-1}X_-.$$

Note that the operators X_+ and X_- can be considered as generalized creation and annihilation operators, respectively.

It should be realized that, for fixed k, Eq. (3) defines indeed a family of generalized Weyl-Heisenberg algebras W_k. The various members of the family are distinguished by the various sets $\{f_s\} \equiv \{f_s(N): s \in S_0\}$.

C. Realization of *k*-SUSYQM

We can use the generators of W_k for obtaining a realization of $(H, Q_+, Q_-)_k$.

First, we take the supercharge operators $Q_\pm$ [see Eq. (2)] in the form

$$Q_- = X_-(1 - \Pi_1), \quad Q_+ = X_+(1 - \Pi_0). \tag{4}$$

It can be proved that they satisfy the Hermitean conjugation property $Q_- = Q_+^\dagger$ and the k-nilpotency property $Q_\pm^k = 0$. Note that there are k equivalent definitions of type (4) corresponding to the k circular permutations of $0, 1, \cdots, k-1$.

Second, the k-fractional supersymmetric Hamiltonian H, satisfying (2) and compatible with (4), takes the form[22]

$$H=(k-1)X_+X_- -\sum_{s=3}^{k}\sum_{t=2}^{s-1}(t-1)f_t(N-s+t)\Pi_s-\sum_{s=1}^{k-1}\sum_{t=s}^{k-1}(t-k)f_t(N-s+t)\Pi_s,$$

in terms of X_+X_-, Π_s, and f_s. In addition, it can be shown that the operator H can be decomposed as

$$H=\sum_{s=1}^{k}H_s\Pi_s=\sum_{s=0}^{k-1}H_{k-s}\Pi_{k-s}, \tag{5}$$

where

$$H_s=(k-1)X_+X_- -\sum_{t=2}^{k-1}(t-1)f_t(N-s+t)+(k-1)\sum_{t=s}^{k-1}f_t(N-s+t),\quad s\in S_1. \tag{6}$$

As an important result, it can be proved, from $[H,Q_\pm]=0$, that the k operators $H_k\equiv H_0$, H_{k-1}, $\cdots$, H_1 constitute a hierarchy of isospectral Hamiltonians. Therefore, the spectra of $H_1,H_2,\cdots,H_{k-1}$ can be deduced from the spectrum of H_0.

D. Representation of W_k

Let us now examine the action of X_+, X_-, N, and K on each subspace

$$H_s=\{|n,s\rangle:n \text{ ranging}\}$$

of $\mathcal{H}$ (n can take a finite or infinite number of values according to whether as $\mathcal{H}_s$ is of finite or infinite dimension). For this purpose, we introduce the structure functions $F_s:N\mapsto F_s(N)$ through

$$X_+X_-=\sum_{s=0}^{k-1}F_s(N)\Pi_s,\quad X_-X_+=\sum_{s=0}^{k-1}F_{s+1}(N+1)\Pi_s.$$

In view of Eq. (3), we have the recurrence relation

$$F_{s+1}(n+1)-F_s(n)=f_s(n),\quad F_s(0)=0. \tag{7}$$

Then, we can take[22]

$$X_+|n,s\rangle=\sqrt{F_{s+1}(n+1)}|n+1,s+1\rangle,\quad s\neq k-1,$$

$$X_+|n,s\rangle=\sqrt{F_{s+1}(n+1)}|n+1,0\rangle,\quad s=k-1,$$

$$X_-|n,s\rangle=\sqrt{F_s(n)}|n-1,s-1\rangle,\quad s\neq 0,$$

$$X_-|n,s\rangle=\sqrt{F_s(n)}|n-1,k-1\rangle,\quad s=0,$$

$$N|n,s\rangle=n|n,s\rangle,\quad K|n,s\rangle=q^s|n,s\rangle \tag{8}$$

for the action of X_+, X_-, N, and K on space $\mathcal{H}_s$. Relations (8) define a representation of W_k.

In the following, we shall consider two special cases of W_k: (i) The case where $f_s(N)$ is independent of s (see Sec. IV) and (ii) the case where $f_s(N)$ is independent of N (see Sec. V).

IV. TRANSLATIONAL SHAPE INVARIANT POTENTIALS

A. Structure function

In this section, we assume that $f_s(N)$ is independent of s and linear in N. More precisely, we take

$$f_s(N) = aN + b \Rightarrow [X_-, X_+] = aN + b,$$

with strictly positive eigenvalues, where a and b are two real parameters. Thus, from Eq. (7) we have

$$X_+X_- \equiv F(N,a,b),$$

where

$$F(N,a,b) = \frac{1}{2}aN(N-1) + bN.$$

The nonlinear spectrum of X_+X_- is then given by

$$X_+X_-|n,s\rangle = \left[\frac{1}{2}an(n-1) + bn\right]|n,s\rangle.$$

For either $a=0$ and $b>0$ or $a>0$ and $b\geq 0$, the spectrum of X_+X_- is infinite-dimensional and does not present degeneracies. For $a<0$ and $b\geq 0$, the spectrum of X_+X_- is finite-dimensional with $n=0,1,\cdots,E(-b/a)$ and all the states are nondegenerate.

It is possible to find a realization of each of the three cases just described in terms of an exactly solvable dynamical system in a one-dimensional space, with coordinate x, and characterized by a potential $V(x,a,b)$. As a matter of fact, we have the following:

(i) $a=0$ and $b=1$ correspond to the harmonic oscillator potential

$$V_{ho}(x,0,1) = x^2, \tag{9}$$

with an infinite nondegenerate spectrum ($n\in\mathbf{N}$).

(ii) $a=2$ and $b=u+v+1$, with $u>1$ and $v>1$, correspond to the Pöschl-Teller potential

$$V_{PT}\left(x,2,\left\{u+\frac{1}{2},v+\frac{1}{2}\right\}\right) = \frac{1}{4}\left[\frac{u(u-1)}{\sin^2(x/2)} + \frac{v(v-1)}{\cos^2(x/2)}\right] - \frac{1}{4}(u+v)^2, \tag{10}$$

with an infinite nondegenerate spectrum ($n\in\mathbf{N}$).

(iii) $a=-2$ and $b=2l+1$, with $l\in\mathbf{N}$, correspond to the Morse potential

$$V_M(x,-2,2l+1) = e^{-2x} - (2l+3)e^{-x} + (l+1)^2, \tag{11}$$

with an finite nondegenerate spectrum ($n=0,1,\cdots,l$).

B. Isospectral Hamiltonians

The various isospectral Hamiltonians occurring in (5) are easily deduced from Eq. (6). This gives

$$H_{k-s} \equiv H_{k-s}(N,a,b) = (k-1)\left[F\left(N,a,b-\frac{1}{2}ka+a+sa\right) + \frac{1}{6}(k-2)(ka-3b) + \frac{1}{2}s(s-k+1)a + sb\right], \quad s\in S_0.$$

Thus, the isospectral Hamiltonians are linked by

$$H_{k-s}(N,a,b) = H_0(N,a,b+sa) + \frac{1}{2}(k-1)s(sa-a+2b), \quad s \in S_0, \tag{12}$$

a relation of central importance, in the k-SUSYQM context, for the derivation of the translational shape invariance condition.

Let us denote by $V_k \equiv V_0$, V_{k-1}, $\cdots$, V_1 the potentials (in x-representation) associated with the isopectral Hamiltonians H_0, H_{k-1}, $\cdots$, H_1, respectively. In other words, we set

$$H_{k-s}(N,a,b) \equiv -\frac{d^2}{dx^2} + V_{k-s}(x,a,b), \quad s \in S_0.$$

By using Eq. (12), we immediately get the recurrence relation

$$V_{k-s}(x,a,b) = V_0(x,a,b+sa) + \frac{1}{2}(k-1)s(sa-a+2b), \quad s \in S_0, \tag{13}$$

which may be considered as the k-SUSYQM version of the translational shape invariance condition for ordinary SUSY [see Eq. (1)].

By way of illustration, Eq. (13) yields the following results.

(i) For the harmonic oscillator system:

$$V_{k-s}(x,0,1) = x^2 + \frac{1}{2}(k-1)(2s-k+2). \tag{14}$$

(ii) For the Pöschl-Teller system:

$$\begin{aligned} V_{k-s}\left(x,2,\left\{u+\frac{1}{2},v+\frac{1}{2}\right\}\right) = \frac{1}{4}\Bigg[& \frac{(u+s+1-(k/2))(u+s-(k/2))}{\sin^2(x/2)} \\ & + \frac{(v+s+1-(k/2))(v+s-(k/2))}{\cos^2(x/2)}\Bigg] - \frac{1}{4}(u+v+2s+2-k)^2 \\ & + \frac{1}{6}(k-1)(k-2)(2k-3u-3v-3) + (k-1)s(s-k+u+v+2). \end{aligned} \tag{15}$$

(iii) For the Morse system:

$$\begin{aligned} V_{k-s}(x,-2,2l+1) = {} & e^{-2x} - (2l+k+1-2s)e^{-x} + \frac{1}{4}(2l+k-2s)^2 - \frac{1}{6}(k-1)(k-2)(2k+6l+3) \\ & + (k-1)s(k-s+2l). \end{aligned} \tag{16}$$

In the case $k=2$ and $s=0$, Eqs. (14)–(16) reduce to Eqs. (9)–(11), respectively.

V. CYCLIC SHAPE INVARIANT POTENTIALS

A. Structure function

In this section, we assume that $f_s(N)$ is independent of N, i.e.,

$$f_s(N) = f_s \Rightarrow [X_-,X_+] = \sum_{s=0}^{k-1} f_s \Pi_s.$$

(The paradigmatic case of the harmonic oscillator corresponds to f_s=const for any s in S_0.)

It is convenient to write the integer n occurring in $|n,s\rangle$ as $n=kp+t$ with $p \in \mathbf{N}$ and $t \in S_0$. Here, to adapt our construction to one-dimensional periodic potentials, we restrict the Hilbert-Fock

space $\mathcal{H}$ to its subspace $\mathcal{G}=\{|kp+s,s\rangle: p \text{ ranging}; s\in S_0\}$. In addition, it is appropriate to denote the state $|kp+s,s\rangle$ as $|kp+s)$. Hence, the action of the number operator N on the states $|kn+s)$ is given by

$$N|kn+s) = (kn+s)|kn+s)$$

and the grading operator K can be identified, on the subspace $\mathcal{G}$, with the operator q^N since

$$K|kn+s) = q^s|kn+s) = q^{kn+s}|kn+s) = q^N|kn+s).$$

From Eq. (7), it can be shown

$$F_s(N) = g_0 N + \sum_{t=1}^{k-1} g_t \frac{1-q^{st}}{1-q^t},$$

where

$$g_t = \frac{1}{k}\sum_{s=0}^{k-1} p^{st} f_s, \quad t \in S_0.$$

Thus, the action of

$$X_+X_- = \sum_{t=0}^{k-1} g_t \frac{1-q^{Nt}}{1-q^t}$$

on the space $\mathcal{G}$ reads

$$X_+X_-|kn+s) = \left(n\sum_{i=0}^{k-1} f_i + \sum_{i=0}^{s-1} f_i \right)|kn+s). \tag{17}$$

The spectrum of X_+X_- is periodic and can be seen as a superposition of identical blocks. For a given block, the various gaps between the consecutive eigenvalues are

$$f_0, f_1, \cdots, f_{k-1}.$$

The first block (corresponding to $n=0$) has the following nonzero eigenvalues,

$$E_1 = f_0, E_2 = f_0 + f_1, \cdots, E_k = f_0 + f_1 + \cdots + f_{k-1},$$

while the second block (corresponding to $n=1$) has the eigenvalues

$$E_{k+1} = E_k + f_0, E_{k+2} = E_k + f_0 + f_1, \cdots, E_{2k} = E_k + f_0 + f_1 + \cdots + f_{k-1},$$

and so on for the subsequent blocks corresponding to $n=2,3,\cdots$ (the eigenvalue for the ground state is $E_0=0$). In other words, in the $(n+1)$th block the parameter f_s is the difference between the eigenvalues for $|kn+s+1)$ and $|kn+s)$. According to Eq. (17), the various eigenvalues are given by

$$E_{kn+s} = nkg_0 + \sum_{i=0}^{s-1} f_i, \quad n \in \mathbf{N};\ s \in S_0.$$

Thus, each block has the length kg_0, which can be considered as the period of the cyclic spectrum.

At this level, it should be emphasized that our approach covers the one of Ref. 11 concerning the two-body Calogero-Sutherland model. The latter model corresponds to $k=2$. Consequently, the relevant Hilbert-Fock space is

$$\mathcal{G} = \{|2n+s): n \in \mathbf{N};\ s = 0,1\}$$

and X_+X_- reads

$$X_+X_- = \frac{1}{2}(f_0 + f_1)N + \frac{1}{2}(f_0 - f_1)\Pi_1.$$

Equation (17) can then be particularized as

$$X_+X_-|2n) = n(f_0 + f_1)|2n),$$

$$X_+X_-|2n+1) = [n(f_0 + f_1) + f_0]|2n+1),$$

in accordance with the results of 11. (Our parameters f_0 and f_1 read $f_0 = \omega_0$ and $f_1 = \omega_1$ in the notations of 11.)

It is interesting to note that the spectrum of X_+X_- coincides with one of the Hamiltonian corresponding to the potential (in x-representation)

$$V_0(x, f_0, f_1) = \frac{1}{16}(f_0 + f_1)^2x^2 + \frac{1}{4}\frac{(f_0 - f_1)(3f_0 + f_1)}{(f_0 + f_1)^2}\frac{1}{x^2} - \frac{1}{2}f_1. \tag{18}$$

Furthermore, using the standard tools of ordinary SUSYQM, we get

$$V_1(x, f_0, f_1) = \frac{1}{16}(f_0 + f_1)^2x^2 + \frac{1}{4}\frac{(f_1 - f_0)(3f_1 + f_0)}{(f_0 + f_1)^2}\frac{1}{x^2} + \frac{1}{2}f_0, \tag{19}$$

which corresponds to the operator X_-X_+.

For $k > 2$, the derivation of analytical forms of the potentials exhibiting a cyclic spectrum was discussed in Ref. 12.

B. Isospectral Hamiltonians

Going back to the general case, the expressions for the isospectral Hamiltonians in (6) can be obtained from (5). This yields the relations

$$H_s \equiv H_s(N, \{f_s\}) = (k-1)X_+X_- + \sum_{t=2}^{k-1}(1-t)f_t + (k-1)\sum_{t=s}^{k-1} f_t, \quad s \in S_1.$$

These relations show that the spectra of the supersymmetric partner Hamiltonians $H_0, H_1, \cdots, H_{k-1}$ can be deduced from the one of X_+X_- given by Eq. (17). By combining the latter two relations, we obtain

$$H_{k-s}(N, \{f_s\}) = H_0(N+s, \{f_s\}), \quad s \in S_0, \tag{20}$$

an important relation for the derivation of the cyclic shape invariance condition.

From (20), we can prove that

$$H_{k-s}(N, \{f_s\}) = H_0(N, h^{(s)}\{f_s\}) + \sum_{i=0}^{s-1} f_i, \quad s \in S_0 \tag{21}$$

with

$$h^{(s)} = h \circ h \circ \cdots \circ h, \quad s \text{ times},$$

where h is the circular permutation

$$h\{f_s\} = h\{f_0, f_1, \cdots, f_{k-2}, f_{k-1}\} = \{f_1, f_2, \cdots, f_{k-1}, f_0\}$$

such that $h^{(k)}$ is the identity.

We continue with dynamical systems in one-dimensional space (coordinate x). Let us note $V_0(x,\{f_s\})$ the potential associated with $H_0(N,\{f_s\})$:

$$H_0(N,\{f_s\}) \equiv -\frac{d^2}{dx^2} + V_0(x,\{f_s\}).$$

From Eq. (21), it is easy to check that the potential $V_{k-s}(x,\{f_s\})$ associated with the Hamiltonian $H_{k-s}(N,\{f_s\})$ can be obtained via

$$V_{k-s}(x,\{f_s\}) = V_0(x,h^{(s)}\{f_s\}) + \sum_{i=0}^{s-1} f_i, \quad s \in S_0, \tag{22}$$

to be compared with the cyclic shape invariance condition for ordinary SUSY (see Eq. (1) and Refs. 11 and 12).

As an example, for $k=2$, Eq. (22) leads to

$$V_1(x,\{f_0,f_1\}) = V_0(x,\{f_1,f_0\}) + f_0,$$

a relation satisfied by Eqs. (18) and (19) for the Calogero-Sutherland potential.

VI. CONCLUDING REMARKS

It was shown in the present paper how to tackle k-fractional SUSYQM through a Z_k-graded Weyl-Heisenberg algebra, noted W_k with $k=3,4,\cdots$ (the case $k=2$ corresponding to ordinary SUSYQM). From the generators of this algebra, it was possible to find several realizations of k-fractional supersymmetric dynamical systems. Each system was characterized by a k-fractional supersymmetric Hamiltonian which gave rise to a hierarchy of k isospectral Hamiltonians H_{k-s} with $s \in S_0$. Two special cases of algebra W_k were examined. They both led to k-fractional isospectral Hamiltonians, the potentials of which are connected by a recurrence relation that reflects a (translational or cyclic) shape invariance condition.

As a conclusion, k-fractional SUSYQM developed in the framework of algebra W_k turns out to be a useful tool to generate a hierarchy of k isospectral Hamiltonians linked by a translational or cyclic invariance condition.

A brief comparison with the results given by ordinary SUSYQM is in order. For $k=2$, the hierarchy of Hamiltonians reduces to a pair of isospectal Hamiltonians. Therefore, in order to generate a hierarchy of k isospectal Hamiltonians, it is necessary to apply ordinary SUSYQM repeatedly. This is no longer the case for k-fractional SUSYQM since the hierarchy of k isospectral Hamiltonians is generated at once. The equivalence between the approaches via ordinary SUSYQM applied repeatedly and k-fractional SUSYQM is ensured by the fact that k-SUSYQM can be seen as a superpostion of $k-1$ copies of ordinary SUSYQM.[22]

To close this paper, let us offer two remarks. First, it is worthwhile to mention that our approach to k-SUSYQM by means of algebra W_k can be applied to other potentials. For instance, by taking $X_+X_- \equiv F(N,a,b,c)$, where the structure function F is given by

$$F(N,a,b,c) = \frac{1}{2}aN(N-1) + bN + c\frac{1}{(N+1)^2},$$

it might be possible to describe potentials involving a Coulombic part. Along this vein, a k-SUSYQM study to the effective screened potential,[40] singular inverse-power potentials,[41] and noncentral potentials[42] could be fruitful. Second, it would interesting to examine the hidden supersymmetries exhibited by the Aharanov-Bohm, Dirac delta, and Pöschl-Teller potentials[34–36] in the light of our approach to k-fractional SUSYQM. For this purpose, the connection between

ordinary SUSYQM, possibly in a q-deformed approach,[43] and k-SUSYQM[22] should play a central role.

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Propagator for finite range potentials

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The Schrödinger equation in integral form is applied to the one-dimensional scattering problem in the case of a general finite range, nonsingular potential. A simple expression for the Laplace transform of the transmission propagator is obtained in terms of the associated Fredholm determinant, by means of matrix methods; the particular form of the kernel and the peculiar aspects of the transmission problem play an important role. The application to an array of delta potentials is shown.
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I. INTRODUCTION

The space-time propagator is a very important object in quantum physics; it governs the time evolution of a dynamical state and naturally enters any kind of time dependent problem.[1] It is more fundamental than the wave function itself, since it is a characteristic of the physical system and does not depend on initial conditions. However, its calculation is more difficult; suffice it to consider the square potential: the wave functions are well known, but the propagator cannot be expressed in a simple form. On the other hand, the knowledge of the propagator helps to the insight into the physics of a quantum system. For example, let us think about the tunneling time for a potential barrier: in a basic paper on this argument, it is shown that a satisfactory definition of the tunneling time can be given just by the propagator;[2] considering coupling effects in quantum tunneling, it makes it possible to go beyond the perturbative expansion;[3] studying the interaction of a system with a thermal bath, it accounts in a simple way for the oscillatory degrees of freedom, so leading to the concept of effective action.[4]

The nonrelativistic quantum mechanical propagator can be expressed in several ways. The most widely known one is the "spectral decomposition" method, but it is often used also the path-integral approach. We refer to the literature for a complete discussion about this subject.[5,6]

In this paper we show that the integral Schrödinger equation allows us to find an interesting expression for the Laplace transform (LT) of the one-dimensional transmission propagator, since in this case the associated Fredholm equation of the second kind has a simple solution in terms of the Fredholm determinant.

In Sec. II we derived the integral equation for the Laplace transform of the one-dimensional propagator. In Sec. III the fundamental equation of quantum scattering is solved for a general finite range, nonsingular potential, in order to obtain the LT in the case of a transmitted particle. Section IV shows some properties of Fredholm determinant and in Sec. V we apply our results to an array of delta potentials.

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II. THE INTEGRAL EQUATION

Let H_0 be a Hamiltonian for which the propagator G_0 is known and V a general potential. The Schrödinger equation for the system with Hamiltonian $H=H_0+V$ is

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{1}$$

where $|\psi(t)\rangle$ is the vector representing the dynamical state of our system. A standard procedure leads to

$$|\psi(t)\rangle = \mathrm{e}^{-(i/\hbar)H_0 t}|\psi(0)\rangle - \frac{i}{\hbar}\int_0^t \mathrm{d}\tau \mathrm{e}^{-(i/\hbar)H_0(t-\tau)}V|\psi(\tau)\rangle, \tag{2}$$

that is, the Schrödinger equation in integral form. Using the representation where the position variables are diagonal,[7] and performing Wick rotation to imaginary time $t\to -it$ (Ref. 8) (in view of the future use of the LT), this equation is easily written in terms of the propagators G and G_0,

$$G(x,t;\eta) = G_0(x,t;\eta) - \frac{1}{\hbar}\int_0^t \mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\xi G_0(x,t-\tau;\xi)V(\xi)G(\xi,\tau;\eta), \tag{3}$$

where

$$G(x,t;\eta) = \langle x|\mathrm{e}^{-(i/\hbar)Ht}|\eta\rangle, \quad G_0(x,t;\eta) = \langle x|\mathrm{e}^{-(i/\hbar)H_0 t}|\eta\rangle \tag{4}$$

and η and x are the space coordinates at the times 0 and t, respectively.

After a LT,[9]

$$\mathcal{L}\{\psi(x,t)\} = \int_0^{\infty}\mathrm{d}t\psi(x,t)\mathrm{e}^{-st} = \psi(x,s),$$

we are led to

$$G(x,s;\eta) = G_0(x,s;\eta) - \frac{1}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}\xi G_0(x,s;\xi)V(\xi)G(\xi,s;\eta). \tag{5}$$

Let us suppose that H_0 corresponds to the free particle. In imaginary time,[7]

$$G_0(x,t;\eta) = \sqrt{\frac{m}{2\pi\hbar t}}\exp\left[-\frac{m}{2\hbar}\frac{(x-\eta)^2}{t}\right] \tag{6}$$

and therefore

$$G_0(x,s;\eta) = \frac{c}{2}\frac{\mathrm{e}^{-c|x-\eta|\sqrt{s}}}{\sqrt{s}}, \quad c=\sqrt{\frac{2m}{\hbar}}. \tag{7}$$

With the definitions,

$$G_0(x,s;\eta)=\phi(x), \quad G(x,s;\eta)=\psi(x), \quad \lambda = \frac{c}{2\hbar}\frac{1}{\sqrt{s}}, \quad k=c\sqrt{s}. \tag{8}$$

Equation (5) can be written in short, assuming that V has a finite range $(0,a)$,

$$\psi(x) + \lambda \int_0^a \mathrm{d}\xi \mathrm{e}^{-k|x-\xi|} V(\xi)\psi(\xi) = \phi(x), \tag{9}$$

where the variable s, considered as a parameter, is omitted, since we are now mainly interested in the space coordinates. We would like to point out that $\psi(x)$ is nothing but Green's function, whose poles represent the energies of the system;[6] the inverse LT is quite equivalent to an integration over the energy.

III. THE SOLUTION OF THE INTEGRAL EQUATION FOR THE TRANSMISSION PROPAGATOR G_T

Equation (9) is a Fredholm integral equation of the second kind, with kernel

$$K(x,\xi) = \mathrm{e}^{-k|x-\xi|} V(\xi). \tag{10}$$

We will show that an appealing expression for the solution can be obtained in the case of the transmission of a particle initially localized on the left of the barrier; i.e., when

$$\eta < 0, \quad x > a. \tag{11}$$

In this case, to obtain the required result, Eq. (9) must be solved first for $x \in (0,a)$, then reintroducing the solution in the initial equation with $x > a$. To this aim, N steps discretization on the interval $(0,a)$ leads to[10]

$$\psi_j + \lambda \sum_{i=1}^{N} \mathrm{e}^{-kx_{ij}} V_i \psi_i \mathrm{d}x = \phi_j, \quad x_{ij} = |x_i - x_j|, \quad \mathrm{d}x = \frac{a}{N}, \quad x_i = i\mathrm{d}x, \quad f_i = f(x_i). \tag{12}$$

In vectorial form (here and in the following, it is understood that the limit $N \to \infty$ will be performed at the end),

$$\mathbf{A}\vec{\psi} = \vec{\phi} \Rightarrow \vec{\psi} = \mathbf{A}^{-1}\vec{\phi}, \tag{13}$$

where

$$\vec{\psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_N \end{pmatrix}, \quad \vec{\phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_N \end{pmatrix} \tag{14}$$

and

$$\mathbf{A} = \begin{pmatrix} 1 + \mathrm{d}\lambda_1 & \mathrm{d}\lambda_2 \mathrm{e}^{-kx_{12}} & \mathrm{d}\lambda_3 \mathrm{e}^{-kx_{13}} & \dots & \mathrm{d}\lambda_N \mathrm{e}^{-kx_{1N}} \\ \mathrm{d}\lambda_1 \mathrm{e}^{-kx_{12}} & 1 + \mathrm{d}\lambda_2 & \mathrm{d}\lambda_3 \mathrm{e}^{-kx_{23}} & \dots & \mathrm{d}\lambda_N \mathrm{e}^{-kx_{2N}} \\ \mathrm{d}\lambda_1 \mathrm{e}^{-kx_{13}} & \mathrm{d}\lambda_2 \mathrm{e}^{-kx_{23}} & 1 + \mathrm{d}\lambda_3 & \dots & \mathrm{d}\lambda_N \mathrm{e}^{-kx_{3N}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}\lambda_1 \mathrm{e}^{-kx_{1N}} & \mathrm{d}\lambda_2 \mathrm{e}^{-kx_{2N}} & \mathrm{d}\lambda_3 \mathrm{e}^{-kx_{3N}} & \dots & 1 + \mathrm{d}\lambda_N \end{pmatrix}, \quad \mathrm{d}\lambda_i = \lambda V_i \mathrm{d}x, \tag{15}$$

assuming that $\det \mathbf{A} \neq 0$ (this assumption does not give rise to difficulties; see the end of this section). Now, in the transmission case Eq. (9) can be written as

$$\psi(x) + \lambda \mathrm{e}^{-kx} \int_0^a \mathrm{d}\xi \mathrm{e}^{k\xi} V(\xi)\psi(\xi) = \phi(x) \tag{16}$$

and, after discretization,[11]

$$\psi(x) + \lambda e^{-kx} \sum_{i=1}^{N} e^{kx_i} V_i \psi_i dx = \phi(x). \tag{17}$$

Recalling that, by Eq. (7),

$$\phi(x) = \frac{c}{2} \frac{e^{-c(x-\eta)\sqrt{s}}}{\sqrt{s}},$$

and introducing the vectors

$$\vec{\varphi} = \begin{pmatrix} e^{-kx_1} \\ e^{-kx_2} \\ e^{-kx_3} \\ \vdots \\ e^{-kx_N} \end{pmatrix}, \quad \vec{v} = \begin{pmatrix} d\lambda_1 e^{kx_1} \\ d\lambda_2 e^{kx_2} \\ d\lambda_3 e^{kx_3} \\ \vdots \\ d\lambda_N e^{kx_N} \end{pmatrix} \tag{18}$$

Eq. (17) becomes

$$\psi(x) = \phi(x) - e^{-kx}(\vec{v}^T \cdot \vec{\psi}) = \phi(x) - \frac{c}{2} \frac{e^{-k(x-\eta)}}{\sqrt{s}} \vec{v}^T (\mathbf{A}^{-1} \vec{\varphi}) = \phi(x)(1 - \vec{v}^T \mathbf{A}^{-1} \vec{\varphi}) \tag{19}$$

where T denotes the transposematrix or vector. Since

$$\vec{v}^T \mathbf{A}^{-1} \vec{\varphi} = \sum_{i,j} v_i (\mathbf{A}^{-1})_{ij} \varphi_j = \sum_{i,j} (\mathbf{A}^{-1})_{ij} (v_i \varphi_j) \tag{20}$$

and defining the matrix

$$\mathbf{V} = \vec{\varphi} \vec{v}^T = \begin{pmatrix} d\lambda_1 & d\lambda_2 e^{kx_{12}} & d\lambda_3 e^{kx_{13}} & \dots & d\lambda_N e^{kx_{1N}} \\ d\lambda_1 e^{-kx_{12}} & d\lambda_2 & d\lambda_3 e^{kx_{23}} & \dots & d\lambda_N e^{kx_{2N}} \\ d\lambda_1 e^{-kx_{13}} & d\lambda_2 e^{-kx_{23}} & d\lambda_3 & \dots & d\lambda_N e^{kx_{3N}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d\lambda_1 e^{-kx_{1N}} & d\lambda_2 e^{-kx_{2N}} & d\lambda_3 e^{-kx_{3N}} & \dots & d\lambda_N \end{pmatrix}, \tag{21}$$

it follows at once

$$\vec{v}^T \mathbf{A}^{-1} \vec{\varphi} = \sum_{i,j} (\mathbf{A}^{-1})_{ij} (\mathbf{V}^T)_{ij} = \mathrm{Tr}[\mathbf{A}^{-1} \mathbf{V}]. \tag{22}$$

Let R be the rank of a matrix; it is easy to recognize that $R(\mathbf{V}) = 1$ and therefore also $R(\mathbf{A}^{-1}\mathbf{V}) = 1$.[12] If $|\mathbf{A}| = \det \mathbf{A} = \Delta$, we can write

$$|\mathbf{A} - \mathbf{V}| = \Delta |\mathbf{I} - \mathbf{A}^{-1} \mathbf{V}|.$$

Expanding the last factor by the diagonal minors[13] and using $R(\mathbf{A}^{-1}\mathbf{V}) = 1$, one has

$$|\mathbf{I} - \mathbf{A}^{-1} \mathbf{V}| = 1 - \mathrm{Tr}[\mathbf{A}^{-1} \mathbf{V}]. \tag{23}$$

On the other hand, $\mathbf{A} - \mathbf{V}$ is a triangular matrix in which every diagonal element is 1, so that

$$|\mathbf{A} - \mathbf{V}| = 1. \tag{24}$$

Therefore

$$\frac{1}{\Delta} = 1 - \mathrm{Tr}[\mathbf{A}^{-1}\mathbf{V}], \tag{25}$$

and from Eqs. (19) and (22) we eventually obtain

$$\psi(x) = \frac{\phi(x)}{\Delta} \tag{26}$$

or, recalling Eq. (8),

$$G_T(x,s;\eta) = \frac{G_0(x,s;\eta)}{\Delta(\lambda)}, \tag{27}$$

Δ depending on s through $\lambda(s)$ and $k(s)$ [see definitions (8)]. In Eq. (27) poles represent the discrete energy levels, while cuts represent the continuous ones; the contour of the inverse LT to obtain G_T passes around these singularities, avoiding the values of s for which $\Delta(\lambda)=0$.[9]

IV. EVALUATION OF THE FREDHOLM DETERMINANT Δ

We see therefore that the problem is completely solved by the knowledge of Δ, that is the *Fredholm determinant* relative to the integral equation [Eq. (9)]. The result [Eq. (26)] represents an important simplification, considering that for $x \in (0,a)$ the solution has a much more complicated form,[10]

$$\psi(x) = \phi(x) - \frac{\lambda}{\Delta(\lambda)} \int \mathrm{d}\xi \Delta(x,\xi;\lambda)\phi(\xi), \tag{28}$$

where $\Delta(x,\xi;\lambda)$ is similar to $\Delta(\lambda)$; however, its explicit expression is not necessary here.

Rewriting Δ as

$$\Delta(\lambda) = \begin{vmatrix} 1+\lambda K_{11}\mathrm{d}x & \lambda K_{12}\mathrm{d}x & \lambda K_{13}\mathrm{d}x & \dots & \lambda K_{1N}\mathrm{d}x \\ \lambda K_{21}\mathrm{d}x & 1+\lambda K_{22}\mathrm{d}x & \lambda K_{23}\mathrm{d}x & \dots & \lambda K_{2N}\mathrm{d}x \\ \lambda K_{31}\mathrm{d}x & \lambda K_{32}\mathrm{d}x & 1+\lambda K_{33}\mathrm{d}x & \dots & \lambda K_{3N}\mathrm{d}x \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda K_{N1}\mathrm{d}x & \lambda K_{N2}\mathrm{d}x & \lambda K_{N3}\mathrm{d}x & \dots & 1+\lambda K_{NN}\mathrm{d}x \end{vmatrix}, \tag{29}$$

where

$$K_{ij} = K(x_i,x_j) = V(x_j)\mathrm{e}^{-k|x_i-x_j|} = V(x_j)\mathrm{e}^{-kx_{ij}}, \tag{30}$$

the following expansion can be used:[11,13]

$$\Delta(\lambda) = 1 + \lambda \sum_{p_1=1}^{N} K_{p_1p_1}\mathrm{d}x + \frac{\lambda^2}{2} \sum_{p_1,p_2=1}^{N} \begin{vmatrix} K_{p_1p_1} & K_{p_1p_2} \\ K_{p_2p_1} & K_{p_2p_2} \end{vmatrix} + \cdots + \frac{\lambda^N}{N!} \sum_{p_1,p_2,\dots,p_N=1}^{N} \begin{vmatrix} K_{p_1p_1} & K_{p_1p_2} & \cdots & K_{p_1p_N} \\ K_{p_2p_1} & K_{p_2p_2} & \cdots & K_{p_2p_N} \\ \vdots & \vdots & \ddots & \vdots \\ K_{p_Np_1} & K_{p_Np_1} & \cdots & K_{p_Np_N} \end{vmatrix}. \tag{31}$$

Now we can perform explicitly the limit $N \to \infty$ and obtain the everywhere convergent series [in other terms, $\Delta(\lambda)$ is an entire function of λ],

$$\Delta(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} D_n, \tag{32}$$

$$\begin{aligned} D_n &= \int_0^a dx_n \cdots \int_0^a dx_2 \int_0^a dx_1 \begin{vmatrix} K(x_1,x_1) & K(x_1,x_2) & \cdots & K(x_1,x_n) \\ K(x_2,x_1) & K(x_2,x_2) & \cdots & K(x_2,x_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(x_n,x_1) & K(x_n,x_2) & \cdots & K(x_n,x_n) \end{vmatrix} \\ &= \int_0^a dx_n \cdots \int_0^a dx_2 \int_0^a dx_1 \begin{vmatrix} 1 & e^{-kx_{12}} & \cdots & e^{-kx_{1n}} \\ e^{-kx_{12}} & 1 & \cdots & e^{-kx_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-kx_{1n}} & e^{-kx_{2n}} & \cdots & 1 \end{vmatrix} V(x_1)V(x_2)\cdots V(x_n). \end{aligned} \tag{33}$$

Among the interesting analytical properties of Δ, the following is remarkable:[11]

$$\frac{\Delta'(\lambda)}{\Delta(\lambda)} = \sum_{n=0}^{\infty} (-1)^n A_{n+1} \lambda^n, \tag{34}$$

where the A_n are the traces of iterated kernels,

$$A_n = \int_0^a dx \int_0^a dx_{n-1} \cdots \int_0^a dx_2 \int_0^a dx_1 K(x,x_{n-1}) K(x_{n-1},x_{n-2}) \cdots K(x_2,x_1) K(x_1,x). \tag{35}$$

This alternative expression for Δ follows

$$\Delta(\lambda) = e^{-F(\lambda)}, \quad F(\lambda) = \sum_{n=1}^{\infty} (-1)^n A_n \frac{\lambda^n}{n}. \tag{36}$$

For example, in the case of a delta potential

$$V(x) = V\delta(x-y), \quad 0 < y < a, \tag{37}$$

it is easily obtained $A_n = V^n$, so that

$$F(\lambda) = \sum_{n=1}^{\infty} (-1)^n V^n \frac{\lambda^n}{n} = -\ln(1+\lambda V) \Rightarrow \Delta(\lambda) = 1 + \lambda V, \tag{38}$$

and Eq. (27) gives the well known formula for the propagator of a delta potential.[14,15] This result can be obtained in a much easier way if one starts from expansion (32), as it is shown in the next section.

V. APPLICATION: AN ARRAY OF DELTA POTENTIALS

Atomic and molecular systems are often approximately represented by models involving zero-range potentials; for example, to calculate exchange forces in hydrogen molecular ion,[16] to describe valence transfer during nuclear collisions,[17] to obtain a closed form expression for phase and dwell tunneling times,[18] etc. So, the knowledge of the propagator in the general case of an array of delta potentials can be useful,

$$V(x) = \sum_{i=1}^{N} V_i \delta(x - y_i), \quad 0 < y_1 < y_2 < \cdots < y_N < a. \tag{39}$$

It is a simple task to recognize that, introducing this expression of V into Eq. (33), one has

$$D_n = 0 \quad \text{for } n > N, \tag{40}$$

$$D_n = \begin{vmatrix} 1 & e^{-ky_{12}} & \cdots & e^{-ky_{1n}} \\ e^{-ky_{12}} & 1 & \cdots & e^{-ky_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ e^{-ky_{1n}} & e^{-ky_{2n}} & \cdots & 1 \end{vmatrix} V_1 V_2 \cdots V_n \quad \text{for } n \leqslant N, \tag{41}$$

with $y_{ij} = |y_i - y_j|$. In this way, the series (32) stops to $n=N$ and represents a finite expansion by principal minors; i.e.,

$$\Delta_N = 1 + \sum_{n=1}^{N} \frac{\lambda^n}{n!} D_n = \begin{vmatrix} 1+\lambda_1 & \lambda_2 e^{-ky_{12}} & \lambda_3 e^{-ky_{13}} & \ldots & \lambda_N e^{-ky_{1N}} \\ \lambda_1 e^{-ky_{12}} & 1+\lambda_2 & \lambda_3 e^{-ky_{23}} & \ldots & \lambda_N e^{-ky_{2N}} \\ \lambda_1 e^{-ky_{13}} & \lambda_2 e^{-ky_{23}} & 1+\lambda_3 & \ldots & \lambda_N e^{-ky_{3N}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_1 e^{-ky_{1N}} & \lambda_2 e^{-ky_{2N}} & \lambda_3 e^{-ky_{3N}} & \ldots & 1+\lambda_N \end{vmatrix}, \quad \lambda_i = \lambda V_i. \tag{42}$$

Of course, this result could be achieved directly substituting the potential [Eq. (39)] into Eq. (9), automatically obtaining a (nonuniform) discretization in the interval $(0,a)$, and following the same steps of Sec. III.

For $N=1$, $\Delta_1 = 1+\lambda V_1$; for $N=2$,

$$\Delta_2 = 1 + \lambda(V_1 + V_2) + \lambda^2 V_1 V_2 (1 - e^{-2ky_{12}}), \tag{43}$$

and the results of Ref. 19 are found (in particular, the symmetry under the exchange of barriers is remarkable). For $N=3$,

$$\begin{aligned} \Delta_3 = 1 &+ \lambda(V_1 + V_2 + V_3) + \lambda^2 [V_1 V_2 (1 - e^{-2ky_{12}}) + V_1 V_3 (1 - e^{-2ky_{13}}) + V_2 V_3 (1 - e^{-2ky_{23}})] \\ &+ \lambda^3 V_1 V_2 V_3 (e^{-2ky_{13}} - e^{-2ky_{12}} - e^{-2ky_{23}} + 1) \end{aligned} \tag{44}$$

and Eq. (27) can be Laplace inverted by the same approximation methods of Ref. 19, getting the space-time propagator $G_T(x,t;\eta)$.

VI. CONCLUSIONS

The main result of the paper is given by Eq. (27), representing a solution of the scattering integral equation [Eq. (9)]. We were able to obtain this solution since, in the transmission case, the coordinate x is on the right of the integration interval $(0,a)$. It is far from a general, closed form expression for the space-time propagator, since an inverse LT must be performed, but it can be the starting point for approximate calculations, using the expansions (32) and (36) for $\Delta(\lambda)$. It is worth to point out that the calculations of Sec. III do not hold for reflected particles, showing in this way a substantial and problematic difference between the quantum physics of transmission and the one of reflection.

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Relativistic quaternionic wave equation

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We study a one-component quaternionic wave equation which is relativistically covariant. Bilinear forms include a conserved four-vector current and an antisymmetric second rank tensor. Waves propagate within the light cone and there is a conserved quantity which looks like helicity. The principle of superposition is retained in a slightly altered manner. External potentials can be introduced in a way that allows for gauge invariance. There are some results for scattering theory and for two-particle wave functions as well as the beginnings of second quantization. However, we are unable to find a suitable Lagrangian or an energy-momentum tensor. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2397555]

I. INTRODUCTION

Many attempts have been made to consider the extension of the usual quantum theory, based on the field of complex numbers, to quaternions. The 1936 paper by Birkhoff and von Neumann[1] opened the door to this possibility, and the 1995 book by Adler[2] covers many aspects that have been studied.

Here is a wave equation that appears to have escaped previous recognition:

$$\frac{\partial \psi}{\partial t} i = \mathbf{u} \cdot \boldsymbol{\nabla} \psi + m \psi j. \tag{1.1}$$

The single wave function ψ is a function of the space time coordinates $\mathbf{x}, t$. The usual elementary quaternions i, j, k, are defined by

$$i^2 = j^2 = k^2 = ijk = -1 \tag{1.2}$$

and

$$\mathbf{u} \cdot \boldsymbol{\nabla} = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}. \tag{1.3}$$

Boldface type is used to designate a three-vector.

This combination Eq. (1.3) of elementary quaternions and space derivatives was originated by Hamilton[3] in 1846; its square is the negative of the Laplacian operator.

What one should note about Eq. (1.1) is that it employs quaternions which multiply the wave function on *both* the right side and the left side. This distinction arises from the noncommutativity of quaternion algebra and is central to the present study.

II. OTHER EQUATIONS

There are other quaternionic wave equations one can consider, based on the apparent structural similarities between quaternions and relativity. The simplest is

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$$\frac{\partial \psi}{\partial t} = \mathbf{u} \cdot \boldsymbol{\nabla} \psi, \tag{2.1}$$

which, when squared, appears as a four-dimensional Laplace equation, and not a wave equation.

Going to two-dimensions we construct

$$\begin{pmatrix} \frac{\partial}{\partial t} & \mathbf{u} \cdot \boldsymbol{\nabla} \\ \mathbf{u} \cdot \boldsymbol{\nabla} & -\frac{\partial}{\partial t} \end{pmatrix} \boldsymbol{\Psi} = m \boldsymbol{\Psi}. \tag{2.2}$$

When this equation is squared, we do get a wave equation, but it is for a tachyon. If one sets $m = 0$ in this equation, it can be revised to appear as either two copies of the Weyl equation or the Maxwell equations (keeping only the imaginary components).

Various authors have shown that the familiar Dirac equation can be put into quaternionic form. This may be done by putting an i to the right of Ψ on one side of Eq. (2.2) (Ref. 4) or by the use of biquaternions in a one-component equation.[5] All of those representations involve eight real functions—as does the usual Dirac equation—while the basic equation of the current study [Eq. (1.1)] involves only four real functions.

There are two other known relativistic equations with four real components. One of these is the Majorana representation of the Dirac equation,

$$i \gamma^{\mu} \partial_{\mu} \psi = m \psi, \tag{2.3}$$

where all four of the gamma matrices can be made purely imaginary, so that one can take all four components of the Dirac wave function to be real functions of space-time. Indeed, if we write our quaternionic wave function as

$$\psi = \psi_0 + i\psi_1 + j\psi_2 + k\psi_3, \tag{2.4}$$

and arrange these four real functions as a column vector, then our Eq. (1.1) can be put in exactly this Majorana-Dirac form. One awkward feature of that formalism is that the usual Dirac Lagrangian becomes useless for an action principle, since every single term is identically zero.

The other comparison involves the Weyl equation (two complex components), which is usually reserved for massless particles. One can map quaternions onto a two-dimensional space of complex numbers. The correspondence can be expressed in terms of the familiar Pauli matrices $\mathbf{u} \rightarrow -i\boldsymbol{\sigma}$, and the wave equation (1.1) can be written in a pseudo-Weyl form as

$$i \frac{\partial \boldsymbol{\Psi}}{\partial t} = -i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \boldsymbol{\Psi} + m \sigma_2 \boldsymbol{\Psi}^*. \tag{2.5}$$

In this second example, one also has trouble with the usual Lagrangian in that the mass term is identically zero.

Both of these equations, Majorana-Dirac and modified Weyl, are used in building supersymmetry theories (see, for example, Ref. 6), but only after one introduces a second set of wave functions—with "dotted" spinor indices. Thus, they do return to eight real functions, which are, furthermore, not simply real functions but elements of a Grassmann algebra.

These comparisons leave me without a definitive answer to the question of whether the focal equation of this paper [Eq. (1.1)] is truly something new in theoretical physics. The work presented here will be to explore this quaternionic wave equation on its own terms and see what interesting things arise.

III. SOME PROPERTIES

In the usual quantum mechanics there is "gauge invariance of the first kind:" we can replace the complex wave function ψ by $\exp(i\theta)\psi$. This freedom is also noted by saying that there is a ray,

not just one vector, in Hilbert space corresponding to each physical state. (The reader will note that this paper focuses entirely on the wave function approach to quantum theory and not the Hilbert space version.) For the quaternionic wave function we have a larger set of freedoms: $\psi \rightarrow q_1 \psi q_2$, where the two numbers q_1, q_2 are quaternions of unit magnitude. The one on the left induces a change of basis in the elementary quaternions $\mathbf{u}$ seen in Eq. (1.1), while the one on the right changes the particular choice of i and j acting to the right of ψ in that equation. Thus, instead of the usual $U(1)$ group, we appear to have $SU(2) \times SU(2)/Z_2$.

A first calculation is to take another time derivative of Eq. (1.1) and arrive at the second-order wave equation,

$$\frac{\partial^2 \psi}{\partial t^2} = \boldsymbol{\nabla}^2 \psi - m^2 \psi, \tag{3.1}$$

which is the ordinary Klein-Gordon equation for a relativistic particle of mass m.

Now we look at some bilinear forms. The first is $\rho = \psi^* \psi$, where the complex conjugation operator $(^*)$ changes the sign of each imaginary quaternion (and requires the reversal of order in multiplication of any expression upon which it operates). The second is the vector $\mathbf{U} = \psi^* \mathbf{u} \psi$. While ρ is real, $\mathbf{U}$ is purely imaginary, and we can write $\mathbf{U} = i\mathbf{U}_1 + j\mathbf{U}_2 + k\mathbf{U}_3$ in terms of three real three-vectors.

Making use of the wave equation [Eq. (1.1)], we then calculate

$$\frac{\partial \rho}{\partial t} = \boldsymbol{\nabla} \cdot \mathbf{U}_1, \tag{3.2}$$

which is the familiar statement of a conserved current. We shall return to $\mathbf{U}_2$ and $\mathbf{U}_3$ shortly. [If you ask what singled out $\mathbf{U}_1$ as the conserved current, it is the choice of the imaginary i sitting beside the time derivative in the wave equation (1.1).]

IV. SPACE-TIME SYMMETRIES

Now we look at the behavior of the wave equation (1.1) under familiar symmetry transformations. To achieve rotation of the spatial coordinates $\mathbf{x}$, we make the transformation

$$\psi \rightarrow \mathrm{e}^R \psi, \quad R = \mathbf{u} \cdot \theta/2, \tag{4.1}$$

where θ is the axis and the angle of rotation.

For the Lorentz transformation, we start with the infinitesimal form

$$\psi \rightarrow \psi + B\psi i, \quad B = \mathbf{u} \cdot \mathbf{v}/2, \tag{4.2}$$

where $\mathbf{v}$ is the direction and amount of the velocity boost. Note the appearance of the imaginary i acting on the right of ψ in this transformation. I leave it as an exercise for the reader to show that this transformation of ψ does indeed induce the familiar Lorentz transformation of the space-time coordinates in the wave equation (1.1).

One can now readily show that the components of the conserved current (ρ and $\mathbf{U}_1$) tansform as a Lorentz four-vector. With a bit more work, one can also see that the other two vectors $\mathbf{U}_2$ and $\mathbf{U}_3$ transform as the components of an antisymmetric second rank tensor in four dimensions (also called a six-vector).

A useful notation for operators that may multiply quaternionic functions on the right or on the left is the following:[1]

$$(a||b)\psi = a\psi b, \quad (a||b)(c||d) = (ac||db), \tag{4.3}$$

which allows us to write the finite Lorentz transformation operator as $e^{(B||i)}$.

[1] A similar notation was introduced by the authors of Ref. 4.

The generators of the Lorentz group may be constructed as

$$\mathbf{J} = \mathbf{x} \times \boldsymbol{\nabla} - \frac{1}{2}\mathbf{u}, \quad \mathbf{K} = \mathbf{x}\frac{\partial}{\partial t} + t\,\boldsymbol{\nabla} - \frac{1}{2}\mathbf{u}||i. \tag{4.4}$$

One can extend this to the full Poincare group by adding the displacement operators: $\partial_\mu = (\partial_t, \nabla)$.

In the Appendix is a more extensive study of various tensors that can be built from solutions of the wave equation.

V. MORE BILINEAR FORMS

Start by defining the derivative operator which acts in both directions, $\mathrm{d}_\mu = (\mathrm{d}_0, \mathbf{d}) = \frac{1}{2}(\vec{\partial}_\mu - \overleftarrow{\partial}_\mu)$. This is a covariant four-vector, but let us now see how things behave when we combine it with the Lorentz transformation of the wave function:

$$D_\mu \equiv \psi^* \mathrm{d}_\mu \psi \rightarrow D_\mu + \frac{1}{2}\{i, \psi^* \mathrm{d}_\mu \mathbf{v} \cdot \mathbf{u}\psi\}. \tag{5.1}$$

The expression D_μ is purely imaginary, and so we can write $D_\mu = D_{1,\mu}\, i + D_{2,\mu}\, j + D_{3,\mu} k$. I hope that the use of the subscripts (1,2,3), denoting which imaginary component they come from, does not cause confusion with the vector or tensor subscripts μ. The expression inside the anticommutator brackets (next to i) is real. This leads us to conclude that under the Lorentz transformation of ψ

$$D_{2,\mu} \text{ and } D_{3,\mu} \text{ are } \textit{unchanged}, \tag{5.2}$$

$$D_{1,\mu} \rightarrow D_{1,\mu} + \textit{more complicated} \text{ stuff}. \tag{5.3}$$

This means that under the full Lorentz transformation of both coordinates and wave function D_2 and D_3 behave simply as four-vectors. The quantity D_1, however, will be shown in the Appendix to be part of a higher rank tensor.

Before proceeding, we note that $D_{\mu=0}$ can be reexpressed by using the wave equation (1.1):

$$D_{\mu=0} = -i\tau - \frac{j}{2}\,\boldsymbol{\nabla} \cdot \mathbf{U}_3 + k\left[m\rho + \frac{1}{2}\,\boldsymbol{\nabla} \cdot \mathbf{U}_2\right], \tag{5.4}$$

where $\tau \equiv \psi^* \mathbf{u} \cdot \mathbf{d}\psi$ is a real three-scalar. Under the Lorentz transformation of the wave function, we calculate $\tau \rightarrow \tau + \mathbf{v} \cdot \mathbf{D}_1$.

We have the identity

$$\partial^\mu D_\mu = 0; \tag{5.5}$$

and we will be interested in the following time derivatives, which are derived by using the wave equation (1.1):

$$\frac{\partial}{\partial t}\tau = -\boldsymbol{\nabla} \cdot \mathbf{D}_1, \tag{5.6}$$

$$\frac{\partial}{\partial t} D_\mu = i[2mD_{2,\mu} - \boldsymbol{\nabla} \cdot (\psi^* \mathbf{u} \mathrm{d}_\mu \psi)] - 2mjD_{1,\mu} + [i, \psi^* \mathrm{d}_\mu \mathbf{u} \cdot \mathbf{d}\psi], \tag{5.7}$$

$$\frac{\partial}{\partial t}\mathbf{U} = i[\boldsymbol{\nabla}\rho + 2\psi^* \mathbf{u} \times \mathbf{d}\psi + 2m\mathbf{U}_2] + j[-2m\mathbf{U}_1 + 2\mathbf{D}_3 - \boldsymbol{\nabla} \times \mathbf{U}_3] + k[-2\mathbf{D}_2 + \boldsymbol{\nabla} \times \mathbf{U}_2]. \tag{5.8}$$

See the Appendix for a more systematic discussion of tensor quantities.

VI. PLANE WAVES

One way of representing "plane-wave" solutions of the wave equation (1.1) is

$$\psi(\mathbf{x},t) = \exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot\mathbf{x})\phi\exp((i\eta p + km)t), \tag{6.1}$$

where $\eta = \pm 1$. The set of possible momentum vectors $\mathbf{p} = \hat{p}p$ should cover only one-half of space to avoid overcounting of solutions. With this, one can construct the solution for the general initial value problem:

$$\psi(\mathbf{x},t) = \int \mathrm{d}^3\mathbf{x}' \sum_{\eta} \int_H \frac{\mathrm{d}^3 p}{(2\pi)^3} \exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}'))\psi(\mathbf{x}',t'=0)\exp((i\eta p + km)t), \tag{6.2}$$

where the subscript H reminds us that the integral covers only half of momentum space.

With the expansions

$$\exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')) = \cos(\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')) + \eta\mathbf{u}\cdot\hat{p}\sin(\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')), \tag{6.3}$$

$$\exp((i\eta p + km)t) = \cos(\omega t) + (i\eta p + km)\sin(\omega t)/\omega, \tag{6.4}$$

where $\omega = \sqrt{p^2+m^2}$, we sum over η and reduce Eq. (6.2) to the following:

$$\begin{aligned}\psi(\mathbf{x},t) = \int \mathrm{d}^3\mathbf{x}' \int_H \frac{\mathrm{d}^3 p}{(2\pi)^3} 2[&\cos(\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}'))\psi(\mathbf{x}',0)(\cos(\omega t) + km\sin(\omega t)/\omega) \\ &+ \mathbf{u}\cdot\mathbf{p}\sin(\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}'))\psi(\mathbf{x}',0)i\sin(\omega t)/\omega].\end{aligned} \tag{6.5}$$

Here we can recognize that the results of the integrals over $\mathbf{p}$ (which now may be extended to cover the full momentum space) give us functions of the invariant $R^2 = t^2 - (\mathbf{x}-\mathbf{x}')^2$, which vanish outside the light cone ($R^2 > 0$). Thus we do have relativistic causality for this quaternionic wave equation; something which we could have expected because the solutions satisfy the Klein-Gordon equation.

The Klein-Gordon equation also has the property that positive (negative) frequency solutions propagate only to positive (negative) frequency solutions. For the quaternionic equation, we have no way to talk about this distinction between positive and negative frequencies; however, we do find a substitute "selection rule" for wave propagation here.

First, we note the orthogonality relation

$$\int \frac{\mathrm{d}^3 x}{(2\pi)^3} \exp(-\eta'\mathbf{u}\cdot\hat{p}'\mathbf{p}'\cdot\mathbf{x})\exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot\mathbf{x}) = \delta_{\eta,\eta'}\delta(\mathbf{p}\pm\mathbf{p}'), \tag{6.6}$$

where I have not required that both sets of momentum variables belong to the same half-space. Next, we use this orthogonality in Eq. (6.2), where we represent $\psi(\mathbf{x}',0)$ as any superposition of plane wave solutions with exclusively $\eta' = +1$ (or exclusively -1). The resulting $\psi(\mathbf{x},t)$ will contain only that same value for η. It is tempting to call this "helicity conservation" in the propagation of these quaternionic waves.

This interpretation is bolstered by the following observations. The operator $\mathbf{u}\cdot\nabla$, acting on a plane wave solution [Eq. (6.1)], has eigenvalue $-\eta p$. Furthermore, one can readily show, from Eq. (1.1), that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3 x \psi^* \mathbf{u}\cdot\boldsymbol{\nabla}\psi = 0. \tag{6.7}$$

VII. SUPERPOSITION

In the usual (complex) quantum theory, if we have two solutions to the Schrodinger (time dependent) equation, ψ_1 and ψ_2, then any linear combinmation $c_1\psi_1+c_2\psi_2$ is also a solution for arbitrary complex numbers c_1 and c_2. With our quaternionic wave equation (1.1), the idea of superposition requires a slightly different wording.

Note that the general plane wave solution [Eq. (6.1)] has an arbitrary amplitude ϕ positioned in the midst of certain quaternionic functions of space and time. Given any such solution, we find another solution by changing the amplitude: $\phi \rightarrow q\phi q'$, where q and q' are arbitrary quaternionic numbers. Furthermore, if we have one solution of Eq. (1.1)—ψ_1 with amplitude ϕ_1—and another solution—ψ_2 with amplitude ϕ_2—then we also have a solution by simply adding these two: $\psi_1 + \psi_2$. This version of the principle of superposition is implicit in Eq. (6.2).

VIII. ADDING POTENTIALS

The original wave equation (1.1) can be extended by the introduction of external potentials, as follows:

$$\frac{\partial \psi}{\partial t} i = \mathbf{u} \cdot \boldsymbol{\nabla} \psi + \mathrm{e}\varphi\psi - \mathrm{e}\mathbf{u} \cdot \mathbf{A}\psi i + m\psi \mathrm{e}^{ieW} j, \tag{8.1}$$

where φ, $\mathbf{A}$, W are real functions of space-time. The gauge transformation that leaves this equation invariant is

$$\psi \rightarrow \psi \mathrm{e}^{ie\chi}, \tag{8.2}$$

$$\varphi \rightarrow \varphi - \frac{\partial \chi}{\partial t}, \tag{8.3}$$

$$\mathbf{A} \rightarrow \mathbf{A} + \boldsymbol{\nabla}\chi, \tag{8.4}$$

$$W \rightarrow W - 2\chi. \tag{8.5}$$

One can show that the previously discussed symmetries still hold, with $(\varphi, \mathbf{A})$ a Lorentz four-vector and W a scalar. This appearance of the four-vector potentials is (almost) exactly like the usual way of introducing electromagnetism into quantum theory; however, the explicit appearance of a gauge quantity W is something different.

The reflection symmetries of Eq. (8.1) are

$$\psi \rightarrow \psi j, \quad t, \mathbf{A}, W \textit{ change } \text{sign } (T), \tag{8.6}$$

$$\psi \rightarrow \psi k, \quad \mathbf{x}, \varphi, W \textit{ change } \text{sign } (CP), \tag{8.7}$$

$$\psi \rightarrow \psi i, \quad t, \mathbf{x}, \mathbf{A}, \varphi \textit{ change } \text{sign } (TCP). \tag{8.8}$$

The current conservation equation (3.2) is still true for this extended wave equation (8.1), however, Eq. (6.7) must be modified. For the situation where $W=0$, we calculate

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}(\psi^* \mathbf{u} \cdot \mathbf{d}\psi) = -\boldsymbol{\nabla} \cdot \mathbf{D}_1 + \mathrm{e}\rho\, \boldsymbol{\nabla} \cdot \mathbf{A} - 2\mathrm{e}\mathbf{A} \cdot (\psi^* \mathbf{u} \times \mathbf{d}\psi), \tag{8.9}$$

where we have used the notations from Sec. V. From this we see that in the case where the only external potential is φ, then the space integral of τ, which we identified with helicity, is conserved.

IX. MORE ON PLANE WAVES

The plane wave solutions to the wave equation (1.1), which we set out in Sec. VI, contain an amplitude ϕ which we should study some more:

$$\psi(\mathbf{x},t) = \exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot\mathbf{x})\phi\exp(\Omega t), \tag{9.1}$$

where $\Omega = \hat{\Omega}\omega = (i\eta p + km)$, $\omega = \sqrt{p^2+m^2}$.

We can ask to evaluate the various bilinear forms discussed earlier in the case of this plane wave solution. The easiest are

$$\rho = \phi^*\phi, \quad \tau = -\eta p\rho, \quad D_0 = \Omega\rho, \tag{9.2}$$

but to do more we must be able to evaluate $\phi^*\mathbf{u}\cdot\hat{p}\phi$.

I now propose to classify the constants ϕ in a particular way. The set ϕ_α is defined such that it performs a specific rotation, as follows:

$$\hat{p}\cdot\mathbf{u}\phi_\alpha = \phi_\alpha\hat{\Omega}, \tag{9.3}$$

which sends one unit imaginary quaternion into another. With this type, the solution can be written as

$$\psi = \phi_\alpha\exp(\hat{\Omega}(\omega t + \eta\mathbf{p}\cdot\mathbf{x})), \tag{9.4}$$

which looks like the sort of plane waves we are used to. It should be noted that this definition of ϕ_α is not unique but leaves us with a $U(1)$ class of equivalent amplitudes,

$$\phi_\alpha \to \phi_\alpha\exp(\theta\hat{\Omega}), \tag{9.5}$$

just as in ordinary (complex) quantum theory.

With this α type of amplitude, we can now evaluate the plane wave values for the following bilinears:

$$\mathbf{U}\cdot\hat{p} = i\rho\eta\frac{p}{\omega} + k\rho\frac{m}{\omega}, \quad \mathbf{D} = \eta\mathbf{p}(\mathbf{U}\cdot\hat{p}). \tag{9.6}$$

Components of the vector $\mathbf{U}$ which are orthogonal to $\mathbf{p}$ will oscillate rapidly in space, thus any space average of them will be vanishingly small.

Two other categories for the amplitudes ϕ, called β and γ, can be defined as

$$\mathbf{u}\cdot\hat{p}\phi_\beta = \phi_\beta j, \tag{9.7}$$

$$\mathbf{u}\cdot\hat{p}\phi_\gamma = \phi_\gamma j\hat{\Omega}. \tag{9.8}$$

Note that the three numbers $\hat{\Omega}, j, j\hat{\Omega}$ are mutually anticommuting quaternions. If we calculate any of the bilinears involving $\mathbf{u}\cdot\hat{p}$ with either the β or γ type of amplitude, the result will be rapidly oscillating in time, thus any time average will be vanishingly small.

If we stay with the α type amplitudes, we get the following values, in the plane wave states, for various four-vectors that are defined in Sec. V or the Appendix:

$$j_\mu = \rho(1, \eta\mathbf{p}/\omega), \tag{9.9}$$

$$V_\mu = \rho(\eta p, \omega\hat{p}), \tag{9.10}$$

$$D_{2,\mu} = 0, \tag{9.11}$$

$$D_{3,\mu} = \rho m(1, \eta \mathbf{p}/\omega). \tag{9.12}$$

The four-vectors j and D_3 look like what we would expect for the usual energy-momentum. The four-vector V, however, is spacelike, not timelike; it is similar to the spin vector $s_\mu = \epsilon_{\mu,\nu,\kappa,\lambda} P^\nu S^{\kappa,\lambda}$ in the usual theories, where s_0 is the helicity.

The plane wave solutions are characterized by a parameter **p** which we sometimes call "momentum." This is merely a linguistic habit carried over from conventional quantum theory (following de Broglie's rule that momentum equals Planck's constant divided by wavelength) and should not be confused with the physical quantity called momentum until and unless that connection is established.

X. SCATTERING

Lets start with the wave equation plus a source,

$$\frac{\partial}{\partial t}\psi i = \mathbf{u} \cdot \nabla \psi + m\psi j + s(\mathbf{x},t) i, \tag{10.1}$$

and write the retarded solution as

$$\psi(\mathbf{x},t) = \int_{-\infty}^{t} \mathrm{d}t' \int \mathrm{d}^3x' \int_H \frac{\mathrm{d}^3p}{(2\pi)^3} \sum_\eta \exp(\eta \mathbf{u} \cdot \hat{p}\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')) s(\mathbf{x}',t') \exp(\Omega(t-t')). \tag{10.2}$$

For the general scattering problem, we replace the source s with $V\psi$ and add in the initial (free particle) solution $\psi_0(\mathbf{x},t)$. If the interaction V is independent of time, then we have an integral equation,

$$\psi(\mathbf{x},t) = \psi_0(\mathbf{x},t) + \int_{-\infty}^{t} \mathrm{d}t' \int \mathrm{d}^3x' \int_H \frac{\mathrm{d}^3p}{(2\pi)^3} \sum_\eta \exp(\eta \mathbf{u} \cdot \hat{p}\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')) \times V(\mathbf{x}') \psi(\mathbf{x}',t') \exp(\Omega(t-t')). \tag{10.3}$$

Now we make the "Born approximation" that $\psi = \psi_0$ under the integral and let the time t go to $+\infty$. Then, we find that the integral over t' gives us $\delta(\omega - \omega_0)$, which is usually read as conservation of energy. This result appears to be generally true, not just in the first Born approximation. One can now project this solution onto any plane wave solution and achieve the quaternionic version of the S matrix.

In the special case when the scattering potential V comes from the term φ in the extended wave equation (8.1), we also find—as a result of the integral over t'—that we have the selection rule $\eta = \eta_0$. This is consistent with the result noted after Eq. (8.9).

XI. SOME OTHER SOLUTIONS

We can write solutions for the extended wave equation (8.1) in some special cases.

One may ask whether there is a central potential, $\varphi(r)$, which leads to bound states. The easiest way to explore this is through "reverse engineering:" write down a plausible wave function and see what potential fits the wave equation. The form

$$\psi = [f(r) + \mathbf{u} \cdot \hat{r} g(r)] \phi(t) \tag{11.1}$$

leads to the requirements

$$r^4 \frac{\mathrm{d}}{\mathrm{d}r} f^2 = -\frac{\mathrm{d}}{\mathrm{d}r}(r^4 g^2), \quad \mathrm{e}\varphi = -f'/g, \quad \phi(t) = \phi_0 \mathrm{e}^{kmt}. \tag{11.2}$$

If we try the asymptotic ($r \to \infty$) behavior, $g \to \alpha r^{-\beta}$, we find a similar behavior for f, provided that $0 < \beta < 2$. The wave function is then normalizable for $\beta > 1.5$, and the potential is $\mathrm{e}\varphi(r) = \sqrt{\beta(2-\beta)}/r$ at large r. Looking instead at $r \to 0$, one can do the same analysis and require $\beta < 1.5$; this suggests that we are dealing with something like a shielded Coulomb potential.

There are familiar procedures for taking the nonrelativistic limit of the Klein-Gordon or Dirac equation. Here is the best I could do with the present relativistic equation. First, write $\psi = \psi_{nr} \exp(k\omega t)$, where $\omega = \sqrt{m^2 + p^2} \approx m - \boldsymbol{\nabla}^2/2m$. Next, multiply the equation from the right with $i \exp(-k\omega t)$. Finally, drop all terms that oscillate rapidly in time, as $\exp(\pm 2k\omega t)$. The resulting version of the full extended Eq. (8.1) is

$$\frac{\partial \psi_{nr}}{\partial t} k \approx H_{nr} \psi_{nr}, \tag{11.3}$$

$$H_{nr} = -\nabla^2/2m + m(1 - \cos(\mathrm{e}W)) - \mathrm{e}\mathbf{u} \cdot \mathbf{A} \| k, \tag{11.4}$$

which looks like an ordinary Schrodinger equation except that the single imaginary is called k instead of i, and there is also the unfamiliar term with $\mathbf{A}$. What looks like an effective potential energy term (coming from the gauge quantity W) is positive, thus incapable of producing bound states, although it might conceivably yield metastable states through the oscillation of the cosine function.

XII. TWO-PARTICLE EQUATION

Previous studies of quaternionic quantum theory have gotten into trouble when they try to write wave functions for multiparticle systems. In the ordinary (complex) theory, one simply makes a direct product of one-particle wave functions, and because all the numbers there commute, one can manipulate such a product to achieve various sensible results. In the quaternion case, that approach leads to a horrid mess. (See, for example, Ref. 2, Chap. 9.)

The present work suggests a somewhat different approach. Consider this construction with plane waves:

$$\psi(1,2) = \exp(\eta_1 \mathbf{u} \cdot \hat{p}_1 \mathbf{p}_1 \cdot \mathbf{x}_1) \psi(2) \exp(\Omega_1 t_1), \tag{12.1}$$

$$\psi(2) = \exp(\eta_2 \mathbf{u} \cdot \hat{p}_2 \mathbf{p}_2 \cdot \mathbf{x}_2) \phi \exp(\Omega_2 t_2), \tag{12.2}$$

which might be described as a "nested" product. The symbol ϕ here is a quaternionic constant, which can depend on all the parameters of this two-particle wave function. Note that we have written this with independent time variables for the two particles.

These two-particle wave functions, with all their momentum-helicity labels, form a complete orthogonal set of functions in the space of $\mathbf{x}_1$ and $\mathbf{x}_2$. Note, however, that this product is ordered in a way that was meaningless in ordinary (complex) quantum theory but requires some extra bookkeeping in the quaternionic case.

Let us introduce some more compact notation for such wave functions:

$$\psi^{\mathrm{op}}(1) \equiv \exp(\eta_1 \mathbf{u} \cdot \hat{p}_1 \mathbf{p}_1 \cdot \mathbf{x}_1) \| \exp(\Omega_1 t_1) \ , \tag{12.3}$$

where the $\|$ symbol separates those things that are to act on the left from what is to act on the right of whatever follows. Then the two-particle wave function Eq. (12.1) can be written simply as

$$\psi(1,2) = \psi^{\mathrm{op}}(1) \psi^{\mathrm{op}}(2) \phi; \tag{12.4}$$

and we can also write the operator of the wave equation as

$$\mathcal{D} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \| i - m \| k. \tag{12.5}$$

Next we have the propagators,

$$G(\mathbf{x}-\mathbf{x}', t-t') \equiv \sum_{p,\eta} \exp(\eta \mathbf{u} \cdot \hat{p}\mathbf{p} \cdot (\mathbf{x}-\mathbf{x}')) \| \exp((i\eta p + km)(t-t')) \ , \tag{12.6}$$

where $\Sigma_{p,\eta} = \int_H [\mathrm{d}^3 p/(2\pi)^3] \Sigma_\eta$, and this leads to

$$\mathcal{D}G(\mathbf{x}-\mathbf{x}', t-t') = 0, \quad G(\mathbf{x}-\mathbf{x}', 0) = \delta^3(\mathbf{x}-\mathbf{x}'), \tag{12.7}$$

$$G_+(x-x') \equiv \theta(t-t') G(\mathbf{x}-\mathbf{x}', t-t'), \tag{12.8}$$

$$\mathcal{D}G_+(x-x') = \delta^4(x-x'). \tag{12.9}$$

The coordinate x stands for the full space-time coordinates $t, \mathbf{x}$. Now Eq. (10.2) can be briefly written as

$$\psi(x) = \int \mathrm{d}^4 x' G_+(x-x') s(x'). \tag{12.10}$$

Following that construction, we now write down a general two-particle quaternionic wave function as follows:

$$\psi(x_1, x_2) = \int \mathrm{d}^4 x_1' G_+(x_1 - x_1') \int \mathrm{d}^4 x_2' G_+(x_2 - x_2') s(x_1', x_2'). \tag{12.11}$$

Acting on this with two of those differential operators gives

$$\mathcal{D}_2 \mathcal{D}_1 \psi(x_1, x_2) = s(x_1, x_2). \tag{12.12}$$

This is a two-particle wave equation of the Bethe-Salpeter type, involving separate times as well as separate space coordinates. The term s might be left as an external source or might be used to represent some interaction, such as $V(1,2)\psi(1,2)$. Note that the order in which the two differential operators are applied is significant.

It seems easy now to extend this to any number of particles. This appears to be a significant advance over previous studies of quaternionic wave equations, although there are still many issues to be faced.

XIII. NO LAGRANGIAN

If I use the interacting wave equation (8.1), and think that ψ^* is something independent of ψ, then the following would be suggested as a Lagrangian density:

$$\mathcal{L} = i\psi^* \frac{\partial \psi}{\partial t} i - i\psi^* \mathbf{u} \cdot \boldsymbol{\nabla} \psi - i\psi^* \mathrm{e} \varphi \psi + i\psi^* \mathrm{e} \mathbf{u} \cdot \mathbf{A} \psi i - im\psi^* \psi \mathrm{e}^{\mathrm{i}\mathrm{e}W} j. \tag{13.1}$$

Varying $i\psi^*$ gives immediately the full wave equation for ψ. Before varying ψi on the right, we do a few things: partially integrate in space and time; and move i from left side to right side in the second and third terms and rearrange the i and j coefficients in the last term (this is justified because those $\psi^* \cdots \psi$ expressions are real). Then we get the adjoint wave equation.

But that prescription is not what the usual action principle allows. The familiar game from complex qm does not work here. If one varies each of the four real functions which make up both

quaternionic functions ψ and ψ^*, then we actually get 12 equations from the action principle. This is due to the fact that this Lagrangian is imaginary, that is, it consists of three imaginary parts and each of those parts must vanish after the variation. If we write

$$\mathcal{L} = i\mathcal{L}_1 + j\mathcal{L}_2 + k\mathcal{L}_3, \tag{13.2}$$

we find that the first term, $\mathcal{L}_1$, is Lorentz invariant [see Eq. (A9)]; but what should we do with the other two terms?

Our difficulty with a Lagrangian is different from the difficulty noted earlier for the Dirac-Majorana equation or for the pseudo-Weyl equation. But we do have a problem here.

XIV. DISCUSSION

Several advances have been made in trying to develop a sensible quantum theory based on quaternions, rather than complex numbers. So far, this work has been limited to the wave equation formalism.

We have noted the lack of a conserved energy-momentum tensor (see the Appendix) as well as the lack of a Lagrangian. Nevertheless, we can write down the time-development operator as

$$U(t) = \mathrm{e}^{Ht}, \quad H = -\mathbf{u}\cdot\boldsymbol{\nabla}\|i + m\|k. \tag{14.1}$$

This operator H commutes with the angular momentum operator $\mathbf{J}$, but whether we want to call it the Hamiltonian is unclear. Perhaps these questions wait for a full model of how this quaternionic wave system interacts with other physical systems.

Another approach that may be relevant to that problem, as well as to improving our treatment of many-particle systems, is the method of second quantization. We are led to write down a quaternionic quantum field operator as

$$\psi(\mathbf{x},t) = \sum_{p,\eta} \exp(\eta\mathbf{u}\cdot\hat{p}\mathbf{p}\cdot\mathbf{x})a_{p,\eta}\exp((i\eta p + km)t) \tag{14.2}$$

involving some kind of annihilation/creation operators $a_{p,\eta}$. With this we immediately get

$$N = \frac{1}{(2\pi)^3}\int \mathrm{d}^3x\rho = \sum_{p,\eta} a^\dagger_{p,\eta}a_{p,\eta}, \tag{14.3}$$

$$h = \frac{1}{(2\pi)^3}\int \mathrm{d}^3x\tau = -\sum_{p,\eta} a^\dagger_{p,\eta}a_{p,\eta}\eta p. \tag{14.4}$$

Can one be sure that the matrix product $a^\dagger a$ is real? If these are matrices in a Fock space of the sort we are familiar with, with nonzero elements only on one line parallel to the central diagonal, then this product is real.

It remains unclear to this author whether the equation studied in this paper is merely an alternative mathematical formulation of things already well known or whether it may have consequential applications to some as-yet unidentified physics.

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APPENDIX: GENERAL TENSORS

We can construct Lorentz covariant tensors of any rank, as follows. Start with the direct product of the "two-way" derivative operators:

$$\mathrm{d}_\mu^n = \mathrm{d}_{\mu_1}\mathrm{d}_{\mu_2}\cdots\mathrm{d}_{\mu_n}, \tag{A1}$$

where the subscript μ now stands for the set of indices $\mu_1\cdots\mu_n$. This expression is manifestly a covariant tensor of rank n as far as the coordinate transformations are concerned, and our task is to package these between the wave functions, which transform under infinitesimal Lorentz transformations as given in Eq. (4.2).

We note that the packages $\psi^*\mathrm{d}_\mu^n\psi$ are real for n even and imaginary for n odd, while these conditions are reversed when we add the quaternions $\mathbf{u}$ inside the package.

We find the following constructions for covariant tensors of rank $n+1$, $Q_{\mu,\nu}^{(n+1)}=Q_{\mu,\nu}=(Q_{\mu,0},\mathbf{Q}_\mu)$:

$$Q_{\mu,\nu} = \left(\psi^*\mathrm{d}_\mu^n\psi, \left\{\frac{-i}{2}, \psi^*\mathrm{d}_\mu^n\mathbf{u}\psi\right\}\right) \quad \text{for } n \text{ even}, \tag{A2}$$

$$Q_{\mu,\nu} = \left(\left\{\frac{-i}{2}, \psi^*\mathrm{d}_\mu^n\psi\right\}, -\psi^*\mathrm{d}_\mu^n\mathbf{u}\psi\right) \quad \text{for } n \text{ odd}. \tag{A3}$$

In the case $n=0$ this is just the four-vector current, previously written as $j_\mu=(\rho,\mathbf{U}_1)$. All these tensors are real.

In addition, for n odd, we have the tensors of rank n,

$$R_{2,\mu} = \left\{\frac{-j}{2}, \psi^*\mathrm{d}_\mu^n\psi\right\}, \quad R_{3,\mu} = \left\{\frac{-k}{2}, \psi^*\mathrm{d}_\mu^n\psi\right\}, \tag{A4}$$

which generalize the previously noted four-vectors D_2, D_3. For n even, we have the tensors of rank $n+2$, $S_{\mu,\nu,\lambda}=-S_{\mu,\lambda.\nu}$:

$$S_{\mu,0,\alpha} = -S_{\mu,\alpha,0} = \left\{\frac{-j}{2}, \psi^*\mathrm{d}_\mu^n\mathbf{u}_\alpha\psi\right\}, \quad S_{\mu,\alpha,\beta} = \epsilon_{\alpha,\beta,\gamma}\left\{\frac{-k}{2}, \psi^*\mathrm{d}_\mu^n\mathbf{u}_\gamma\psi\right\}, \tag{A5}$$

where $\alpha,\beta,\gamma=1,2,3$. This generalizes the previously noted six-vector $(\mathbf{U}_2,\mathbf{U}_3)$.

We can make lower rank tensors by contracting indices:

$$g^{\mu_1,\mu_2}Q_{\mu,\nu}^{(n+1)} = -\left(m^2 + \frac{1}{4}\partial^\lambda\partial_\lambda\right)Q_{\mu',\nu}^{(n-1)}, \tag{A6}$$

where μ_1 and μ_2 are in the set μ, and the set μ' has these two indices removed. An alternative is to contract one of the μ indices with the ν index. We find, for solutions of the free wave equation (1.1), the following:

$$g^{\mu_1,\nu}Q_{\mu,\nu}^{(n+1)} = -mR_{3,\mu'}^{(n-1)} \quad \text{for } n \text{ even}, \tag{A7}$$

$$g^{\mu_1,\nu}Q_{\mu,\nu}^{(n+1)} = 0 \quad \text{for } n \text{ odd}. \tag{A8}$$

If we are looking to find a Lorentz scalar, a tensor of rank zero, take a closer look at the second rank tensor $Q_{\mu,\nu}$. The contraction is

$$Q_\mu^\mu = \left\{\frac{-i}{2}, \psi^*\mathrm{d}_0\psi\right\} + \psi^*\mathbf{u}\cdot\mathbf{d}\psi = D_{1,0} + \tau \tag{A9}$$

and this is exactly zero for the free equation (1.1) but not for the extended Eq. (8.1), where it equals $-ej_\mu A^\mu$.

Now we look at the contraction of such tensors with the derivative operator. In what follows we shall limit ourselves to solutions of the free equation (1.1). It is transparent that $\partial^{\mu_1} Q_{\mu,\nu}=0$ for any μ_1 in the set of labels μ. The same holds true for the tensors R and S. Furthermore, by using the wave equation, one can show that

$$\partial^{\nu} Q_{\mu,\nu} = 0 \quad \text{for } n \text{ even}, \tag{A10}$$

$$\partial^{\nu} Q_{\mu,\nu} = 2mR^{(n)}_{2,\mu} \quad \text{for } n \text{ odd}. \tag{A11}$$

For tensors of rank 1, we have just the previously identified j_μ, $D_{2,\mu}$, and $D_{3,\mu}$, all of which are conserved.

At rank 2, the usual desire is for a conserved symmetric tensor, which one can call the energy-momentum tensor. The closest we come here is the $Q_{\mu,\nu}$, which is not symmetric and is conserved only on the first index. Nevertheless, this does allow us to write integral quantities which are conserved (their time derivatives vanish), as follows:

$$V_\nu = (V_0, \mathbf{V}) \equiv \int \mathrm{d}^3 x Q^{(2)}_{0,\nu}, \tag{A12}$$

$$V_0 = -\int \mathrm{d}^3 x \psi^* \mathbf{u} \cdot \mathbf{d}\psi, \tag{A13}$$

$$\mathbf{V} = \int \mathrm{d}^3 x \left(\mathbf{D}_1 + m\mathbf{U}_3 - \frac{1}{2} \nabla \times \mathbf{U}_1 \right). \tag{A14}$$

This is not what we would identify as the energy-momentum, as noted at the end of Sec. IX.

For the second rank antisymmetric tensor we have

$$\partial^{\mu} S_{\mu,\nu} = -2mj_\nu + 2D_{3,\nu}, \tag{A15}$$

$$\widetilde{S}_{\mu,\nu} = \epsilon_{\mu,\nu,\kappa,\lambda} S^{\kappa,\lambda}/2, \tag{A16}$$

$$\partial^{\mu} \widetilde{S}_{\mu,\nu} = -2D_{2,\nu}. \tag{A17}$$

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Generating loop graphs via Hopf algebra in quantum field theory

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We use the Hopf algebra structure of the time-ordered algebra of field operators to generate all connected weighted Feynman graphs in a recursive and efficient manner. The algebraic representation of the graphs is such that they can be evaluated directly as contributions to the connected n-point functions. The recursion proceeds by loop order and vertex number. © *2006 American Institute of Physics.*
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The combinatorics of perturbative quantum field theory is traditionally dealt with via functional methods and generating functions. However, it is possible to use a more intrinsic algebraic approach instead, rooted directly at the level of n-point functions and pioneered in the 1960s, see Ref. 1.

More recently, it was realized that the Hopf algebra structure of the algebra of field operators (with the normal or with the time-ordered product) can be fruitfully exploited. In particular, using the Hopf algebra and its cohomology it was shown (among other things) how different products of the algebra of field operators are related by Drinfeld twists and how interactions correspond to 2-cocycles.[2]

Relations between different types of n-point functions and the associated combinatorics of Feynman graphs via the Hopf algebra structure of the time-ordered algebra of field operators were established in Ref. 3. More precisely, the relations between complete and connected n-point functions on the one hand and between connected and 1-particle irreducible n-point functions on the other hand were described in this way. At the center of that work stands an algorithm to recursively generate all tree graphs and their values as Feynman graphs. The underlying structure in this is an algebraic representation of graphs in terms of certain generalized monomials in field operators.

In the present paper we extend this algorithm to recursively generate all connected graphs using this algebraic representation. The recursion proceeds by loop number (and by vertex number). The special case of vanishing loop number precisely recovers the algorithm of Ref. 3. Crucially, and as in the special case of tree graphs, the correct weights of graphs are obtained so as to allow for their direct evaluation in terms of the Feynman graph expansion of the connected n-point function of a quantum field theory. Note, however, that no type of renormalization procedure is taken into account. In this sense the computed n-point functions may be considered as bare ones.

As in the previous work[3] all results apply to bosonic as well as fermionic fields and the algorithm is amenable to direct implementation and should allow efficient calculations.

Section I reviews basics about certain graphs and their symmetries, n-point functions, Feynman graphs, the algebraic representation of graphs, and the Hopf algebra structure of the time-ordered field operator algebra. Section II contains the main result with the algorithmic construction of connected graphs and its proof. Section III presents an alternative recursive algorithm to

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construct connected graphs that can be applied directly on the level of n-point functions. Section IV offers some discussion, especially concerning the efficient algorithmic implementation and the inclusion of fermions. The Appendix lists all connected graphs without external edges and with up to three internal edges together with their weight factors.

I. BASIC CONCEPTS AND DEFINITIONS

The basic setup in this paper is substantially similar to that of Ref. 3. Hence, the present section has substantial overlap with Sec. II and a part of Sec. IV of that paper. Nevertheless, there are important differences, most notably a more extensive treatment of abstract graphs and their symmetries.

A. Graphs

We introduce certain kinds of graphs and elementary properties of them. The graphs will be later interpreted as Feynman graphs. Here we are only interested in them as abstract graphs.

Definition 1: A graph *is a finite collection of* vertices *and* edges, *such that any end of an edge may be connected to a vertex. Edges that are connected to vertices at both ends are called* internal, *while edges with at least one free end are called* external. *Internal edges with both ends connected to the same vertex are also called* self-loops. *The* valence *of a vertex is the number of ends of edges connected to the vertex. The* loop number *of a graph is its number of cycles. A graph is* connected *if it is connected as a topological space*.

We recall the well known relation between vertex number, edge number, and loop number of connected graphs.

Lemma 2: *Consider a connected graph with at least one vertex. Let* v, e, and l *be its number of vertices, internal edges, and loops, respectively. Then*,

$$l = e - v + 1. \tag{1}$$

Definition 3: *A* labeled *graph is a graph whose free ends of external edges are labeled with labels from a label set. Labels on different ends of edges are required to be distinct*.

In the following we shall consider only such labeled graphs, i.e., from now on *graph* means *labeled graph*. The label set is fixed from the outset and will later be identified with an appropriate set of field operator labels.

Definition 4: *A graph is said to be* vertex ordered *if its vertices are ordered. That is, the vertices are numbered* $1,\ldots,n$, *where n is the total number of vertices. A graph is said to be* edge ordered *if the ends of its internal edges are ordered. That is, the ends of internal edges are numbered* $1,\ldots,2m$, *where m is the total number of internal edges (each edge having two ends). A graph is called* ordered *if it is both vertex ordered and edge ordered*.

Definition 5: *Consider an ordered graph* γ. *A* symmetry *of* γ *is a permutation of the numbering of the vertices and of the end points of the internal edges that yields combinatorially the same ordered (and labeled) graph. The number of symmetries, i.e., the order of the group of permutations leaving the graph invariant, is called the* symmetry factor *of the graph. It will be denoted by* S^γ.

Since the symmetry factor is the same for any ordering of the vertices and ends of internal edges of a graph, the concept is well defined for unordered graphs as well.

Definition 6: *Consider a vertex ordered graph* γ. *A* vertex symmetry *of* γ *is a permutation of the numbering of its vertices, which yields combinatorially the same vertex ordered (and labeled) graph. The order of the group of vertex symmetries is called the* vertex symmetry factor *of the graph. It will be denoted by* S^γ_{vertex}.

Definition 7: *Consider an ordered graph* γ. *An* edge symmetry *of* γ *is a permutation of the numbering of the ends of its internal edges that yields combinatorially the same ordered (and labeled) graph while the order of the vertices is held fixed. The order of the group of edge symmetries is called the* edge symmetry factor *of the graph. It will be denoted by* S^γ_{edge}.

Clearly, the concepts of vertex and edge symmetry factors also make sense for unordered graphs as the vertex and edge symmetry factors are the same for any ordering of the vertices and of the ends of the internal edges of a graph, respectively.

Lemma 8: *Let γ denote an ordered graph. The orders of the associated symmetry groups satisfy $S^\gamma = S^\gamma_{\text{vertex}} \cdot S^\gamma_{\text{edge}}$.*

Proof: Denote the group of symmetries, vertex symmetries, and edge symmetries of γ by G^γ, G^γ_{vertex}, and G^γ_{edge}, respectively. Note that an edge symmetry is merely a particular type of symmetry. Hence, the group G^γ_{edge} may be seen as a subgroup of G^γ via an injective group homomorphism $G^\gamma_{\text{edge}} \to G^\gamma$. Furthermore, a symmetry defines a vertex symmetry by forgetting its action on the numbering of ends of edges. On the other hand, any vertex symmetry can be augmented to a symmetry. Hence, there is a surjective group homomorphism $G^\gamma \to G^\gamma_{\text{vertex}}$. It is easy to see that the group homomorphisms form an exact sequence of groups

$$0 \to G^\gamma_{\text{edge}} \to G^\gamma \to G^\gamma_{\text{vertex}} \to 0.$$

Hence, as the groups are finite their orders satisfy $S^\gamma = S^\gamma_{\text{vertex}} \cdot S^\gamma_{\text{edge}}$. □

Lemma 9: *Consider a connected graph γ. Let v be its number of vertices. For each vertex $1 \leqslant i \leqslant v$ let p_i be the number of self-loops connected to it. Let t be the number of pairs of vertices which are directly connected through at least one edge. For each pair $1 \leqslant j \leqslant t$ of such vertices let q_j be the number of edges connecting it. Then, the edge symmetry factor of γ is given by $S^\gamma_{\text{edge}} = (\Pi_{i=1}^{v} 2^{p_i} p_i!)(\Pi_{j=1}^{t} q_j!)$.*

The proof is straightforward combinatorics.

B. *n*-point functions and Feynman graphs

The physical content of a quantum field theory is usually extracted from its n-point functions. In perturbation theory, these are computed as sums of values of Feynman graphs. We briefly review here the essentials. More details can be found in any standard textbook on quantum field theory such as Ref. 4.

We denote by $G^{(n)}(x_1, \ldots, x_n)$ the *complete* n-point function. This is the vacuum expectation value of the time-ordered product of n field operators, i.e.,

$$G^{(n)}(x_1, \ldots, x_n) = \langle 0 | T\phi(x_1) \cdots \phi(x_n) | 0 \rangle.$$

The notation we use here suggests a scalar field theory on Minkowski space time. In general there would be internal field indices as well and possibly other modifications (other space time, etc.). The real nature of the fields is completely irrelevant for our treatment as long as the standard perturbative treatment applies. Therefore, we shall continue with our present notation for simplicity. Hence, we denote field operators generically by $\phi(x)$, where x is from a label set (here suggestive of points in Minkowski space). Furthermore, we shall assume all fields to be bosonic. The fermionic case is also straightforward, but includes extra factors, see Sec. IV.

Let V be the complex vector space of linear combinations of field operators $\phi(x)$. The algebra generated by the field operators with the *time-ordered* product is commutative and can be identified with the *symmetric algebra* $\mathsf{S}(V)$ over V. More precisely, $\mathsf{S}(V) = \oplus_{k=0}^{\infty} V^k$, where V^k is the space of linear combinations of monomials of degree k in the field operators and V^0 is the one-dimensional vector space spanned by the identity element $\mathbf{1}$. We may now express ensembles of n-point functions as functions $\mathsf{S}(V) \to \mathbb{C}$. In particular, we may set

$$\rho(\phi(x_1) \cdots \phi(x_n)) := G^{(n)}(x_1, \ldots, x_n).$$

In perturbation theory, the n-point functions can be computed as a sum over values of Feynman graphs. For the complete n-point functions we may write

$$G^{(n)}(x_1, \ldots, x_n) = \sum_{\gamma \in \Gamma_n} w_\gamma \gamma(x_1, \ldots, x_n). \tag{2}$$

Here Γ_n is the set of Feynman graphs. These are graphs γ in the sense of Sec. I A with n external edges labeled by field operator labels $x_1, \ldots, x_n$. (Note that usually Feynman graphs involve lines of different types depending on particle species. In our treatment lines correspond to sums over all particle species. The information about which particle species can interact resides completely in the vertex functions.) Indeed, from here onward we fix the label set to be the label set of the field operators. The value of a graph γ labeled by $x_1, \ldots, x_n$ is denoted above by $\gamma(x_1, \ldots, x_n)$. The set Γ_n may be taken to be precisely the set of all graphs with n external legs (up to topological equivalence). The weight factor w_γ is precisely the inverse of the symmetry factor S^γ of a graph in the sense of Definition 5.

We should emphasize that the discussion here applies to bare n-point functions. Renormalization is outside the scope of the present paper.

The type of n-point functions we shall be interested in in the following are the *connected* ones, denoted $G_c^{(n)}$. These may be defined in the same way as (2), but with the restriction that only connected graphs are considered. We define $\sigma: \mathsf{S}(V) \to \mathbb{C}$ via

$$\sigma(\phi(x_1) \cdots \phi(x_n)) := G_c^{(n)}(x_1, \ldots, x_n).$$

We now turn to the calculation of the value of a Feynman graph. The Feynman propagator $G_F(x,y)$ is the value of the graph that consists of an edge only, its two ends labeled by x and y, respectively. The value of a graph that consists of a vertex with external edges labeled by $x_1, \ldots, x_k$ is given by the vertex function $F(x_1, \ldots, x_k)$. Note that we can encode the ensemble of vertex functions in a way analogous to n-point functions as a function $\nu: \mathsf{S}(V) \to \mathbb{C}$ via

$$\nu(\phi(x_1) \cdots \phi(x_n)) := F(x_1, \ldots, x_n). \tag{3}$$

For more general graphs we also need the inverse Feynman propagator, G_F^{-1}, determined by the equation

$$\int dy G_F(x,y) G_F^{-1}(y,z) = \delta(x,z). \tag{4}$$

The value of a general graph may then be computed as follows: Associate a label with each internal edge and form the product over a vertex function associated with each vertex and an inverse Feynman propagator associated with each internal edge. Finally, integrate over all possible assignments of internal labels.

C. Algebraic representation of graphs

We introduce an algebraic representation of graphs based on the time-ordered operator algebra $\mathsf{S}(V)$ and allowing straightforward evaluation of graphs in the above sense. More precisely, we associate a given graph with v vertices with a certain element in $\mathsf{S}(V)^{\otimes v}$, the v-fold tensor product of $\mathsf{S}(V)$.

Each vertex of the graph corresponds to one tensor factor. A product $\phi(x_1) \cdots \phi(x_n)$ in a given tensor factor corresponds to external edges of the associated vertex whose end points are labeled by $x_1, \ldots, x_n$. To represent internal edges, we define the formal elements $R_{i,j} \in \mathsf{S}(V)^{\otimes v}$ with $1 \leqslant i \leqslant j \leqslant v$ using the inverse Feynman propagator (4). [$R_{i,j}$ is formal insofar as it really lives in a completion of the tensor product $\mathsf{S}(V)^{\otimes v}$. However, this fact is largely irrelevant for our purposes.] For $i \neq j$ the definition is

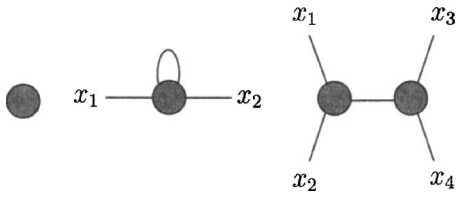

FIG. 1. Examples of the algebraic representation of graphs in terms of elements of $\mathsf{S}(V)^{\otimes v}$.

$$R_{i,j} := \int dxdy G_F^{-1}(x,y)(\mathbf{1}^{\otimes i-1} \otimes \phi(x) \otimes \mathbf{1}^{\otimes j-i-1} \otimes \phi(y) \otimes \mathbf{1}^{\otimes v-j}), \tag{5}$$

with the field operators $\phi(x)$ and $\phi(y)$ inserted at the ith and jth positions, respectively. For $i=j$ the definition is

$$R_{i,i} := \int dxdy G_F^{-1}(x,y)(\mathbf{1}^{\otimes i-1} \otimes \phi(x)\phi(y) \otimes \mathbf{1}^{\otimes v-i}). \tag{6}$$

The element $R_{i,j} \in \mathsf{S}(V)^{\otimes v}$ corresponds to one internal edge connecting the vertices which occupy the positions i and j. In particular, the element $R_{i,i} \in \mathsf{S}(V)^{\otimes v}$ for $1 \leqslant i \leqslant v$ is interpreted as an internal edge connecting the ith vertex to itself. That is, it corresponds to a self-loop.

Combining several internal edges (which can be self-loops) and their products with external edges by multiplying the respective expressions in $\mathsf{S}(V)^{\otimes v}$ allows to build arbitrary graphs with v vertices. Figure 1 shows some examples. It is then obvious that applying the vertex functions ν defined by Eq. (3) to each tensor factor yields precisely the value of the respective graph as a Feynman graph. Thus, the graphs we just discussed are exactly those that are to enter in the v-vertex contribution to an n-point function.

The ordering of the tensor factors of $\mathsf{S}(V)^{\otimes v}$ induces an ordering of the vertices of the graphs in the sense of Definition 4. However, when applying $\nu^{\otimes v}$ the ordering is "forgotten." Indeed, it is not relevant for the interpretation of graphs as Feynman graphs, but only plays a role at the level of their algebraic representation here. In the following, we will encounter elements of $\mathsf{S}(V)^{\otimes v}$ that are linear combinations of expressions corresponding to graphs. In this context, we call the scalar multiplying the expression for a given graph the *weight* of the graph. Clearly, if we are interested in unordered graphs, the weight of such a graph is the sum of the weights of all vertex ordered graphs that correspond to it upon forgetting the vertex order.

D. The field operator algebra as a Hopf algebra

A crucial ingredient of our setting is the fact that the algebra $\mathsf{S}(V)$ of time-ordered field operators is not only an algebra but a *Hopf algebra*. That is, $\mathsf{S}(V)$ carries a coproduct $\Delta: \mathsf{S}(V) \to \mathsf{S}(V) \otimes \mathsf{S}(V)$ and a counit $\epsilon: \mathsf{S}(V) \to \mathbb{C}$ that are compatible with its algebra structure and unit. [$\mathsf{S}(V)$ also carries an antipode map, but this will not be used in the following.] We refer the reader to Ref. 5 for a classical treatment of Hopf algebras and to Ref. 6 for the Hopf algebra structure of the symmetric algebra. The significance of this Hopf algebra structure for quantum field theory was developed in Ref. 2. (Note, however, that the product taken there is the normal product and not the time-ordered one.)

At this point we will only mention the explicit form of the coproduct on $\mathsf{S}(V)$. On monomials this takes the form

$$\Delta(\phi(x_1) \cdots \phi(x_n)) = \sum_{I_1 \cup I_2 = \{\phi(x_1), \ldots, \phi(x_n)\}} T(I_1) \otimes T(I_2), \tag{7}$$

and is extended to all of $\mathsf{S}(V)$ by linearity. Here the sum runs over partitions of the set of field operators $\{\phi(x_1), \ldots, \phi(x_n)\}$ into two sets I_1 and I_2. T denotes the time-ordered product of the field

operators in the corresponding partition. The coproduct may be extended (by suitable composition with itself) to a map (on monomials and extended by linearity),

$$\Delta^k(\phi(x_1)\cdots\phi(x_n)) = \sum_{I_1\cup\cdots\cup I_{k+1}=\{\phi(x_1),\ldots,\phi(x_n)\}} T(I_1)\otimes\cdots\otimes T(I_{k+1}). \tag{8}$$

The difference to the single coproduct is that the set of field operators is now split into $k+1$ partitions. Note also that the partitions are *ordered*, i.e., the sets $I_1,\ldots,I_{k+1}$ are distinguishable. An important property of the coproduct is that it is multiplicative, i.e., it is an algebra map with respect to the algebra structure of $\mathsf{S}(V)$ (and the induced algebra structure on the tensor product). A more extensive discussion of the Hopf algebra structure, adapted to the present context, can be found in Ref. 3.

II. GENERATING LOOP GRAPHS

A. Statement of result

The main result of this paper, which is the subject of the present section, may be described as an efficient algorithm that recursively generates all connected graphs γ. The graphs are generated together with the correct weights w_γ, explained in Sec. I B. In particular, the recursion is such that it may be organized in ascending loop order. Also, the graphs are generated directly in the algebraic representation introduced in Sec. I C. This allows their direct evaluation as Feynman graphs.

More precisely, we shall construct recursively a set of maps $\Omega^{l,v}:\mathsf{S}(V)\to\mathsf{S}(V)^{\otimes v}$ indexed by integers l and v such that the following theorem holds.

Theorem 10: *Fix integers* l, $n\geqslant 0$, $v\geqslant 1$, *and operator labels* $x_1,\ldots,x_n$. *Then*, $\Omega^{l,v}(\phi(x_1)\ldots\phi(x_n))\in\mathsf{S}(V)^{\otimes v}$ *corresponds to the weighted sum over all connected graphs with* l *loops*, v *vertices, and* n *external edges whose end points are labeled by* $x_1,\ldots,x_n$, *each with weight being the inverse of its symmetry factor*.

This specializes for $l=0$ to Lemma 10 of Ref. 3, with $\Lambda^{v-1}=\Omega^{0,v}$.

We may conclude with the interpretation in terms of Feynman graphs and n-point functions. Denote the l-loop and v-vertex contributions to the ensemble σ of connected n-point functions by $\sigma^{l,v}$. In particular, the l-loop order contribution σ^l to σ and σ itself are given by

$$\sigma^l = \sum_{v=0}^{\infty}\sigma^{l,v}, \quad \sigma = \sum_{l=0}^{\infty}\sigma^l.$$

There is only one contribution with zero vertex number. This is the Feynman propagator contributing to the 2-point function. Hence $\sigma^{l,v}$ is zero if $v=0$ and $l\neq 0$, while $\sigma^{0,0}$ is nonzero only on $V\otimes V$ and coincides there with the Feynman propagator. All nonzero vertex number contributions are captured by the following corollary.

Corollary 11: *For* $v\geqslant 1$,

$$\sigma^{l,v} = \nu^{\otimes v}\circ\Omega^{l,v}.$$

Restricting to the $l=0$ (tree level) contribution recovers Corollary 18 of Ref. 3. Note, however, that the contribution corresponding to the Feynman propagator was missing there as well as in Theorem 5 of that paper.

The Appendix lists all connected graphs without external edges as weighted contributions to $\Omega^{l,v}(\mathbf{1})$, for edge number $e=l+v-1\leqslant 3$.

B. Construction and proof

The proof proceeds in a manner very analogous to the proof in Ref. 3. Indeed, each intermediate lemma in this section specializes to a corresponding lemma in Sec. IV of that paper when restricted to the case $l=0$. We do not point this out explicitly in the following, but refer the reader to that paper for comparison.

In order to construct $\Omega^{l,v}$ we introduce certain auxiliary maps. Using the componentwise product in $\mathsf{S}(V)^{\otimes v}$, we may view the elements $R_{i,j}$, defined by Eq. (5) and (6), as operators on this space by multiplication. In particular, these elements are used to define the following maps.

- $T_i:\mathsf{S}(V)^{\otimes v}\to\mathsf{S}(V)^{\otimes v}$, with $1\leqslant i\leqslant v$, as the operator $R_{i,i}$ together with the factor $1/2$:

$$T_i := \frac{1}{2}R_{i,i}. \tag{9}$$

- $Q_i:\mathsf{S}(V)^{\otimes v}\to\mathsf{S}(V)^{\otimes v+1}$, with $1\leqslant i\leqslant v$, given by the composition of $R_{i,i+1}$ with the coproduct applied to the ith component of $\mathsf{S}(V)^{\otimes v}$, i.e., $\Delta_i := \mathrm{id}^{\otimes i-1}\otimes\Delta\otimes\mathrm{id}^{\otimes v-i}:\mathsf{S}(V)^{\otimes v}\to\mathsf{S}(V)^{\otimes v+1}$, together with a factor of $1/2$:

$$Q_i := \frac{1}{2}R_{i,i+1}\circ\Delta_i. \tag{10}$$

The map T_i given by Eq. (9) endows the ith vertex of a vertex ordered graph with a self-loop together with a factor of $1/2$. The latter is the inverse of the edge symmetry factor of a single self-loop (see Lemma 9). The action of the map Q_i given by Eq. (10) is less simple. Consider the coproduct Δ_i applied to the ith component of $\mathsf{S}(V)^{\otimes v}$. Recalling formula (7), we see that Δ_i converts a graph with v vertices into a sum over graphs with $v+1$ vertices by *splitting* the ith vertex into two in all possible ways. That is, the ith vertex is replaced by two vertices (numbered i and $i+1$) and the edges ending on it (considered as distinguishable) are distributed between the two new vertices in all possible ways. Note that the two new vertices are distinguished due to the ordering of the tensor factors. Thus, to obtain the corresponding operation for unordered graphs we need to divide by a factor of 2. This factor corresponds to the two different relative orderings of the new vertices with which each unordered configuration occurs. The only exception to this is the case when the split vertex has no edges at all. No overcounting happens in this case. The meaning of the map Q_i given by Eq. (10) becomes clear now in terms of graphs. Namely, it splits the ith vertex into two and subsequently reconnects the two new vertices with an edge. Dividing by 2 compensates for the double counting as described above if we are interested in unordered graphs (assuming the set of endings of edges of the split vertex is not empty).

We remark that the maps T_i increase both the loop and edge numbers of a graph by one unit, leaving the vertex number invariant, while the maps Q_i increase both the edge and vertex numbers by one unit, leaving the loop number invariant.

We use the maps T_i and Q_i, given by Eq. (9) and (10), respectively, to define recursively maps $\Omega^{l,v}:\mathsf{S}(V)\to\mathsf{S}(V)^{\otimes v}$ for $l\geqslant 0$ and for $v\geqslant 1$ as follows:

$$\begin{aligned}\Omega^{0,1} &:= \mathrm{id},\\ \Omega^{l,v} &:= \frac{1}{l+v-1}\left(\sum_{i=1}^{v-1} Q_i\circ\Omega^{l,v-1}+\sum_{i=1}^{v} T_i\circ\Omega^{l-1,v}\right).\end{aligned} \tag{11}$$

Note that in the recursion equation above the T and Q summands do not appear when $l=0$ or when $v=1$, respectively. Figure 2 shows the recursive dependencies of $\Omega^{l,v}$ for different l, v with $l+v\leqslant 4$.

We notice that $\Omega^{l,v}$ satisfies the following factorization property.

Lemma 12: *Fix integers* l, n, $m\geqslant 0$, $v\geqslant 1$, *and operator labels* $x_1,\ldots,x_n$, $y_1,\ldots,y_m$. *Then*, $\Omega^{l,v}$ *satisfies the factorization property*

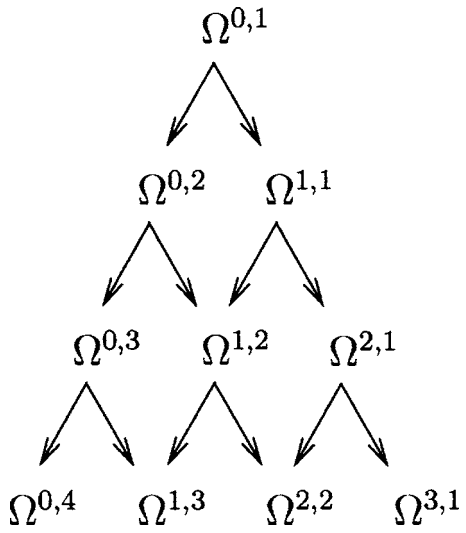

FIG. 2. Recursive dependencies of the maps $\Omega^{l,v}$ up to order $l+v\leqslant 4$. The right directed arrows correspond to T_i maps while the left directed ones correspond to Q_i maps.

$$\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n)\phi(y_1)\cdots\phi(y_m))=\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))\Delta^{v-1}(\phi(y_1)\cdots\phi(y_m)). \tag{12}$$

Proof: This follows from the multiplicativity of the coproduct and the recursive definition (11), noticing that each time the vertex number increases by 1, one coproduct is applied as part of the operator Q_i. □

We now turn to the proof of Theorem 10. We begin with weaker lemmas, increasing their strength stepwise until reaching the desired result.

Lemma 13: *Fix integers* l, $n\geqslant 0$, $v\geqslant 1$ *as well as field operator labels* $x_1,\ldots,x_n$. *(a)* $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ *corresponds to a weighted sum of connected graphs with* l *loops*, v *vertices, and* n *external edges whose end points are labeled by* $x_1,\ldots,x_n$. *(b) Any connected graph with* l *loops*, v *vertices, and the given external edges occurs in* $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ *with some positive weight*.

Proof: First, it is clear that $\Omega^{0,1}(\phi(x_1)\cdots\phi(x_n))$ corresponds to the connected graph with one single vertex with no self-loops and the external edges whose end points are labeled by $x_1,\ldots,x_n$. Moreover, $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ is generated from this by sums of multiple applications of the maps T_i and Q_i with scalar factors according to recursion formula (11). Both T_i and Q_i convert a term corresponding to a connected graph to a sum over terms corresponding to connected graphs. Thus, $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ is a sum of terms each of which corresponds to a connected graph (with some weight). Second, the fact that every graph contained in $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ has l loops and v vertices follows from noticing that the maps T_i increase the loop number by one unit, while the vertex number remains fixed, and the maps Q_i increase the vertex number by one unit, leaving the loop number unchanged. This concludes the proof of (a).

To prove (b) we proceed by induction on the internal edge number $e=l+v-1$ (recall Lemma 2). The result is evidently valid for $e=0$, corresponding to $l=0$ and $v=1$. We assume that the result holds for $e-1$. Let γ denote a graph with l loops and v vertices so that $l+v-1=e$. We show that it is generated by applying the maps T_i or Q_i to graphs contained in $\Omega^{l-1,v}(\phi(x_1)\cdots\phi(x_n))$ or in $\Omega^{l,v-1}(\phi(x_1)\cdots\phi(x_n))$, respectively. Since both T_i and Q_i produce graphs with positive weight from graphs with positive weight, the weight of a graph γ occurring in $\Omega^{l,v}$, being given by a sum over positive contributions according to formula (11), is positive. Now, suppose the graph γ has at least one vertex with one or more self-loops. Let this vertex occupy the ith position, for instance. Shrinking one of these self-loops yields a graph that corresponds by assumption to a term in $\Omega^{l-1,v}(\phi(x_1)\cdots\phi(x_n))$ with some positive weight so that applying the map T_i to the vertex i produces the graph γ with (positive) weight. Thus, by formula (11) the graph γ occurs in $\Omega^{l,v}$.

Finally, suppose the graph γ does not contain vertices with self-loops. Choose an arbitrary internal edge. Shrinking this edge and fusing the vertices it connects yield a graph that corresponds by assumption to a term in $\Omega^{l,v-1}(\phi(x_1)\cdots\phi(x_n))$. Say, the fused vertex has position i. Applying Q_i to this term will yield a sum over terms one of which will correspond to the original. By the recursive definition of $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ it thus contains this term with positive weight. This completes the proof of (b). □

What remains in order to prove Theorem 10 is to show that the term corresponding to each graph has weight given exactly by the inverse of its symmetry factor. We start with a more restricted result.

Lemma 14: *Fix integers* $l\geqslant 0$, $v\geqslant 1$, *and* $n\geqslant v$ *as well as field operator labels* $x_1,\ldots,x_n$. *Consider a connected graph* γ *with* l *loops*, v *vertices*, n *external edges whose end points are labeled by* $x_1,\ldots,x_n$, *and the property that each vertex has at least one external edge ending on it. Then, the term in* $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ *corresponding to that graph has weight given by the inverse of its symmetry factor* S^γ.

Proof: We proceed by induction on the number of internal edges e. Clearly, the statement is true for $e=0$ so that we assume it holds for a general number of internal edges $e-1$. Let γ be a connected graph with e internal edges. Let l be its loop number and let v be its vertex number. By Lemma 13, this graph occurs in $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ with positive weight α. We proceed to show that $\alpha=1/S^\gamma$. We pick an ordering of the vertices and also order the set of pairs of vertices which are connected by at least one edge. Denote the number of self-loops of the vertex i by p_i, with $1\leqslant i\leqslant v$. Denote the number of edges connecting the pair j of vertices by q_j, with $1\leqslant j\leqslant t$, where t is the total number of connected pairs of vertices. By Lemma 9 the edge symmetry factor of γ is given by $S^\gamma_{\text{edge}}=(\Pi_{i=1}^v 2^{p_i}p_i!)(\Pi_{j=1}^t q_j!)$, with $e=\Sigma_{i=1}^v p_i+\Sigma_{j=1}^t q_j$. Since the graph γ has the property that each vertex has at least one external edge, its vertices are distinguishable and it has no nontrivial vertex symmetries: $S^\gamma_{\text{vertex}}=1$ and $S^\gamma_{\text{edge}}=S^\gamma$ (as any symmetry is an edge symmetry). We check from which graphs with $e-1$ internal edges γ is generated by recursion formula (11) and how many times it is generated. It turns out that we can think of each internal edge of γ as contributing with a factor of $1/(e\cdot S^\gamma)$ as follows.

(i) Consider the ith vertex of γ endowed with p_i self-loops. Shrinking one of these self-loops yields a graph γ' whose ith vertex has p_i-1 self-loops. Consequently, by Lemma 9, the symmetry factor of γ' is related to that of γ via $S^{\gamma'}=S^\gamma/(2p_i)$. By assumption, the graph γ' corresponds to a term in $\Omega^{l-1,v}(\phi(x_1)\cdots\phi(x_n))$ which occurs with weight given by the inverse of its symmetry factor: $1/S^{\gamma'}=2p_i/S^\gamma$. Applying the map T_i, which carries the factor of $1/2$, to the vertex i of γ' produces the graph γ from the graph γ' exactly with factor p_i/S^γ. Thus, the contribution to Eq. (11) is $p_i/(e\cdot S^\gamma)$. Distributing this factor between the p_i edges considered yields $1/(e\cdot S^\gamma)$ for each edge considered.

(ii) Consider the jth pair of vertices of γ connected by q_j edges. We assume now the indices of the vertices forming this pair to be consecutive, given by k and $k+1$. (Note that this merely amounts to a particular vertex ordering of the graph γ. Since γ is *a priori* unordered this does not imply any loss of generality.) Shrinking one of the edges and fusing the vertices it connects yield a graph γ'' whose fused vertex has $r:=p_k+p_{k+1}+q_j-1$ self-loops. Consequently, by Lemma 9, the symmetry factor of γ'' is related to that of γ as follows:

$$\frac{1}{2^r}\frac{1}{r!}S^{\gamma''}=\frac{1}{2^{p_k}p_k!}\frac{1}{2^{p_{k+1}}p_{k+1}!}\frac{1}{q_j!}S^\gamma.$$

By assumption, the graph γ'' corresponds to a term in $\Omega^{l,v-1}(\phi(x_1)\cdots\phi(x_n))$ which occurs with weight given by the inverse of its symmetry factor, i.e.,

$$\frac{1}{S^{\gamma''}}=\frac{p_k!p_{k+1}!q_j!}{r!}\frac{1}{2^{q_j-1}S^\gamma}. \tag{13}$$

The map Q_k, when applied to the fused vertex, produces a pair of vertices occupying the positions k and $k+1$, distributes the $2r$ endings of edges between the two vertices in all

possible ways, and attaches them together by an edge. The action of Q_k on the fused vertex k (leaving out external edges) reads explicitly as

$$Q_k R^r_{k,k} = \frac{1}{2} R_{k,k+1}(R_{k,k} + 2R_{k,k+1} + R_{k+1,k+1})^r \tag{14}$$

$$= \sum_{a=0}^{r} \sum_{b=0}^{a} \binom{r}{a} \binom{a}{b} 2^{a-b-1} R^{r-a}_{k,k} R^{a-b+1}_{k,k+1} R^b_{k+1,k+1}. \tag{15}$$

Taking into account the external edges, there are two terms in Eq. (15) corresponding to the graph γ: one with $r-a=p_k$ and $b=p_{k+1}$ and one with $r-a=p_{k+1}$ and $b=p_k$. The sum of the coefficients of these two contributions is

$$2^{q_j-1} \frac{r!}{p_k! p_{k+1}! (q_j-1)!}. \tag{16}$$

Multiplying Eq. (13) with Eq. (16), we see that Q_j produces γ from γ' exactly with a factor q_j/S^γ and the contribution to Eq. (11) is $q_j/(e \cdot S^\gamma)$. In other words, we get a factor of $1/(e \cdot S^\gamma)$ for each of the q_j edges considered.

Since each of the $e=l+v-1$ internal edges contributes with a factor of $1/(e \cdot S^\gamma)$ to the weight of the graph γ, the overall contribution is exactly $1/S^\gamma$. This completes the proof. □

To complete the proof of Theorem 10, we show that the term in $\Omega^{l,v}(\phi(x_1)\cdots\phi(x_n))$ corresponding to a connected graph γ with l loops, v vertices, and external edges whose end points are labeled by $x_1,\ldots,x_n$ has weight given by $1/S^\gamma$. If γ has external edges attached to every one of its vertices we simply recall Lemma 14. Thus, we may now assume that γ has m vertices to which no external leg is attached. Consider a graph γ' which is constructed from γ by attaching an external edge to every vertex without external edges, choosing arbitrary but fixed labels $y_1,\ldots,y_m$ for the end points of external edges in the process. By Lemma 14, the graph γ' occurs in the term on the left hand side of Eq. (12) with weight $1/S^\gamma$. By Lemma 13, the graph γ occurs in the first factor on the right hand side with some nonzero weight, say α. Every summand of $\Delta^{v-1}(\phi(y_1)\cdots\phi(y_m))$ [recall formula (8)] which places the end points of external edges at the designated vertices of γ to produce γ' contributes to the weight of γ' in terms of that of γ. Any different ways this can happen define a vertex symmetry of γ. Furthermore, γ can have no more than these vertex symmetries, since its vertices that already carry external edges are distinguishable and thus held fixed under any symmetry. Therefore, using Lemma 12 we obtain the formula $1/S^{\gamma'} = \alpha \cdot S^\gamma_{\text{vertex}}$ by extracting the weights from the corresponding terms in Eq. (12). Moreover, $S^{\gamma'} = S^{\gamma'}_{\text{edge}} = S^\gamma_{\text{edge}}$. Thus, using $S^\gamma = S^\gamma_{\text{vertex}} \cdot S^\gamma_{\text{edge}}$ (Lemma 8), we find $\alpha = 1/S^\gamma$. This completes the proof.

III. FURTHER RECURSION RELATIONS

Generalizing the case with trees (Sec. V in Ref. 3) we present an alternative recursion relation satisfied by $\Omega^{l,v}$. This has the advantage over Eq. (11) that it may be translated directly into a recursion relation of the resulting n-point functions $\sigma^{l,v}$, related via Corollary 11.

Proposition 15: *Let $v \geqslant 1$ and $l \geqslant 0$, but not $v=1$ and $l=0$. Then,*

$$\Omega^{l,v} = \frac{1}{l+v-1} \left(\Omega^{l-1,v} \circ T + \sum_{a=0}^{l} \sum_{b=1}^{v-1} (\Omega^{a,b} \otimes \Omega^{l-a,v-b}) \circ Q \right).$$

It is understood that the first summand does not contribute if $l=0$ while the second does not contribute if $v=1$.

Before proceeding with the proof we note that this formula has a straightforward interpretation in terms of sums over weighted graphs following the correspondence of Sec. I C. Namely, the formula states that the weighted sum over graphs with l loops and v vertices is given by a sum of two terms divided by the edge number $e=l+v-1$. The first term is the sum over all weighted graphs with $l-1$ loops and v vertices which have an extra edge attached, its end points being connected to vertices in all possible ways. The second term is a sum over all ordered pairs of weighted graphs with total number of vertices equal to v and total number of loops equal to l, connected in all possible ways with an edge.

Proof: The proof proceeds by induction on the number of edges $e=l+v-1$ (recall Lemma 2). It is straightforward to check its validity for $e=1$ by reducing the cases $l=0$, $v=2$ and $l=1$, $v=1$ to Eq. (11), remembering that $\Omega^{0,1}$ is the identity.

We now assume the formula to hold for any edge number smaller than a fixed $e\geqslant 2$. Then for loop number l and vertex number v such that $e=l+v-1$ we use Eq. (11) to show the following equality and hence complete the proof:

$$
\begin{aligned}
\Omega^{l,v} &= \frac{1}{l+v-1}\left(\sum_{j=1}^{v-1} Q_j \circ \Omega^{l,v-1} + \sum_{j=1}^{v} T_j \circ \Omega^{l-1,v}\right) \\
&= \frac{1}{(l+v-1)(l+v-2)}\left(\sum_{j=1}^{v-1} Q_j \circ \left(\Omega^{l-1,v-1}\circ T + \sum_{a=0}^{l}\sum_{b=1}^{v-2}(\Omega^{a,b}\otimes\Omega^{l-a,v-1-b})\circ Q\right)\right. \\
&\quad \left. + \sum_{j=1}^{v} T_j \circ \left(\Omega^{l-2,v}\circ T + \sum_{a=0}^{l-1}\sum_{b=1}^{v-1}(\Omega^{a,b}\otimes\Omega^{l-1-a,v-b})\circ Q\right)\right) \\
&= \frac{1}{(l+v-1)(l+v-2)}\left(\sum_{j=1}^{v-1} Q_j \circ \Omega^{l-1,v-1}\circ T + \sum_{j=1}^{v} T_j \circ \Omega^{l-2,v}\circ T\right. \\
&\quad + \sum_{a=0}^{l}\sum_{b=1}^{v-2}\left(\sum_{j=1}^{b} Q_j\circ\Omega^{a,b}\otimes\Omega^{l-a,v-1-b} + \sum_{j=1}^{v-1-b}\Omega^{a,b}\otimes Q_j\circ\Omega^{l-a,v-1-b}\right)\circ Q \\
&\quad \left. + \sum_{a=0}^{l-1}\sum_{b=1}^{v-1}\left(\sum_{j=1}^{b} T_j\circ\Omega^{a,b}\otimes\Omega^{l-1-a,v-b} + \sum_{j=1}^{v-b}\Omega^{a,b}\otimes T_j\circ\Omega^{l-1-a,v-b}\right)\circ Q\right) \\
&= \frac{1}{(l+v-1)(l+v-2)}\left(\left(\sum_{j=1}^{v-1} Q_j\circ\Omega^{l-1,v-1} + \sum_{j=1}^{v} T_j\circ\Omega^{l-2,v}\right)\circ T\right. \\
&\quad + \left(\sum_{b=1}^{v-2}\left(\sum_{j=1}^{b}(Q_j\circ\Omega^{0,b})\otimes\Omega^{l,v-1-b} + \sum_{j=1}^{v-1-b}\Omega^{l,b}\otimes(Q_j\circ\Omega^{0,v-1-b})\right)\right. \\
&\quad + \sum_{a=0}^{l-1}\left((T\circ\Omega^{a,1})\otimes\Omega^{l-1-a,v-1} + \Omega^{a,v-1}\otimes(T\circ\Omega^{l-1-a,1})\right) \\
&\quad + \sum_{a=1}^{l}\sum_{b=2}^{v-1}\left(\sum_{j=1}^{b-1} Q_j\circ\Omega^{a,b-1} + \sum_{j=1}^{b} T_j\circ\Omega^{a-1,b}\right)\otimes\Omega^{l-a,v-b} \\
&\quad \left.\left. + \sum_{a=0}^{l-1}\sum_{b=1}^{v-2}\Omega^{a,b}\otimes\left(\sum_{j=1}^{v-1-b} Q_j\circ\Omega^{l-a,v-1-b} + \sum_{j=1}^{v-b} T_j\circ\Omega^{l-1-a,v-b}\right)\right)\circ Q\right) \\
&= \frac{1}{(l+v-1)(l+v-2)}\left((l+v-2)\Omega^{l-1,v}\circ T\right.
\end{aligned}
$$

$$
\begin{aligned}
&+\Bigg(\sum_{b=2}^{v-1}(b-1)\Omega^{0,b}\otimes\Omega^{l,v-b}+\sum_{b=1}^{v-2}(v-b-1)\Omega^{l,b}\otimes\Omega^{0,v-b}\\
&+\sum_{a=1}^{l}a\Omega^{a,1}\otimes\Omega^{l-a,v-1}+\sum_{a=0}^{l-1}(l-a)\Omega^{a,v-1}\otimes\Omega^{l-a,1}\\
&+\sum_{a=1}^{l}\sum_{b=2}^{v-1}(a+b-1)\Omega^{a,b}\otimes\Omega^{l-a,v-b}\\
&+\sum_{a=0}^{l-1}\sum_{b=1}^{v-2}(l-a+v-b-1)\Omega^{a,b}\otimes\Omega^{l-a,v-b}\Bigg)\circ Q\Bigg)\\
=&\frac{1}{(l+v-1)(l+v-2)}\Bigg((l+v-2)\Omega^{l-1,v}\circ T\\
&+\Bigg(\sum_{a=0}^{l}\sum_{b=1}^{v-1}(a+b-1)\Omega^{a,b}\otimes\Omega^{l-a,v-b}\\
&+\sum_{a=0}^{l}\sum_{b=1}^{v-1}(l-a+v-b-1)\Omega^{a,b}\otimes\Omega^{l-a,v-b}\Bigg)\circ Q\Bigg)\\
=&\frac{1}{l+v-1}\Bigg(\Omega^{l-1,v}\circ T+\sum_{a=0}^{l}\sum_{b=1}^{v-1}\left(\Omega^{a,b}\otimes\Omega^{l-a,v-b}\right)\circ Q\Bigg).
\end{aligned}
$$

□

Combining this result with Corollary 11 yields the corresponding recursion equation for $\sigma^{l,v}$.

Corollary 16: *Let* $v\geqslant 1$ *and* $l\geqslant 0$, *but not* $v=1$ *and* $l=0$. *Then*,

$$
\sigma^{l,v}=\frac{1}{l+v-1}\Bigg(\sigma^{l-1,v}\circ T+\sum_{a=0}^{l}\sum_{b=1}^{v-1}(\sigma^{a,b}\otimes\sigma^{l-a,v-b})\circ Q\Bigg).
$$

It is understood that the first summand does not contribute if $l=0$ *while the second does not contribute if* $v=1$.

IV. DISCUSSION AND CONCLUSION

The results of the present paper can be seen as an extension of those of Ref. 3, where only tree graphs were generated. Accordingly, many points in the discussion of the main result in that paper extend to the present setting. In particular, this applies to the algorithmic aspects and to the inclusion of fermions. We refer the reader to Secs. VI C and VI D of Ref. 3 for details. Here we shall only touch these points briefly and highlight differences arising through the inclusion of graphs with loops.

The generation of the graphs in their algebraic representation via recursion formula (11) has the structure of an algorithm. Indeed, this algorithmic structure can be used directly and efficiently in implementing concrete calculations of (loop) graphs. In doing so, external edges may be fixed from the beginning and $\Omega^{l,v}$ as applied to the external edges is calculated recursively rather than as an abstract map. An important aspect for the efficiency of concrete calculations is to discard graphs that do not contribute. In typical quantum field theoretic calculations, the vertex function is such that only vertices with a minimum valence (usually three) contribute. In the case of tree graphs this allows the restriction of the coproduct implicit in the operator Q_i in recursion formula (11).[3] Concretely, coproduct (7) may be replaced by a *truncated* coproduct $\Delta_{\geqslant k}$ with $k\geqslant 1$. This is defined by removing from the right hand side of Eq. (7) all terms where the number of elements in I_1 or I_2 is smaller than k. This will prevent graphs from being generated who have vertices with

valence smaller than $k+1$. If only tree graphs are considered this is consistent with the recursion process. More precisely, a graph with all vertices of valence at least $k+1$ cannot be generated by Q_i from a graph with at least one vertex having valence smaller than $k+1$. The analogous statement is not true for the operator T_i. Hence, considering loop graphs as well (recall that T_i increases loop number), we can no longer globally restrict the coproduct. However, if we are interested in graphs only up to a maximal loop number m, we may still restrict the coproduct in Q_i in certain instances. These are precisely the instances when a later application of T_i to a graph cannot occur, i.e., when the graph has already the maximal loop number m.

The restriction on the valence of vertices to be at least a, where $a \geqslant 3$, leads to another obvious limit we can impose on the algorithm. Namely, for a given number of loops m and a given number of external edges n there is an upper bound $b=(n+2m-2)/(a-2)$ on the number of vertices a graph can have. Thus, in this case we only need to compute $\Omega^{l,v}$ for $l \leqslant m$ and $v \leqslant b$.

We now turn to the question of the implementation of fermions. Here the situation is not at all changed by the extension to loop graphs. Namely, the whole formalism is completely functorial and carries over immediately to the case that the vector space V of field operators is a $\mathbb{Z}_2$-graded space. (Recall that this means that V is a direct sum of a bosonic and fermionic part.) Concretely, certain field operators will anticommute which introduces minus signs in front the summands in Eqs. (7) and (8) which correspond to odd permutations of such field operators. In contrast, all formulas appearing in Secs. II and III remain unchanged as the $\mathbb{Z}_2$ grading is completely implicit there.

The algorithm to generate tree graphs was applied in two contexts in Ref. 3: To relate connected n-point functions with 1-particle irreducible ones and to generate all tree graphs using the vertex functions. In both cases renormalization does not introduce any alteration. This is different in the present situation where we interpret the algorithms of Secs. II and III as generating all connected graphs using the vertex functions. Renormalization, via counterterms, alters this process considerably. Thus, it would be highly desirable to include the renormalization process into the present framework. At this point we have very little to say about this, except to point out that the algorithms of Secs. II and III are naturally organized as a recursion by loop order, which might facilitate the task.

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APPENDIX

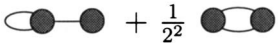
This appendix shows all graphs without external edges and with up to three edges computed as contributions to $\Omega^{l,v}(\mathbf{1})$ via Eq. (11). The factors in front of the graphs are the inverses of their symmetry factors of Definition 5, see Theorem 10.

$$\Omega^{0,1}(\mathbf{1}) = \bullet$$

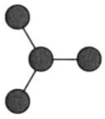
$$\Omega^{0,2}(\mathbf{1}) = \tfrac{1}{2}\ \bullet\!\!-\!\!\bullet$$

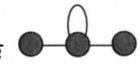
$$\Omega^{1,1}(\mathbf{1}) = \tfrac{1}{2}$$ 

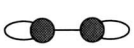
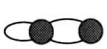
$$\Omega^{0,3}(\mathbf{1}) = \tfrac{1}{2}\ \bullet\!\!-\!\!\bullet\!\!-\!\!\bullet$$

$$\Omega^{1,2}(\mathbf{1}) = \tfrac{1}{2}$$  $$+ \tfrac{1}{2^2}$$

$$\Omega^{2,1}(\mathbf{1}) = \tfrac{1}{2^3}$$ 

$$\Omega^{0,4}(\mathbf{1}) = \tfrac{1}{2}$$ $$+ \tfrac{1}{3!}$$ 

$$\Omega^{1,3}(\mathbf{1}) = \tfrac{1}{3!}$$  $$+ \tfrac{1}{2^2}$$  $$+ \tfrac{1}{2}$$  $$+ \tfrac{1}{2}$$ 

$$\Omega^{2,2}(\mathbf{1}) = \tfrac{1}{2^3}$$  $$+ \tfrac{1}{2^3}$$  $$+ \tfrac{1}{2^2}$$  $$+ \tfrac{1}{2\cdot 3!}$$ 

$$\Omega^{3,1}(\mathbf{1}) = \tfrac{1}{2^3\cdot 3!}$$ 

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Endomorphisms on half-sided modular inclusions

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In algebraic quantum field theory we consider nets of von Neumann algebras indexed over regions of the space time. Wiesbrock ["Conformal quantum field theory and half-sided modular inclusions of von Neumann algebras," Commun. Math. Phys. **158**, 537–543 (1993)] has shown that strongly additive nets of von Neumann algebras on the circle are in correspondence with standard half-sided modular inclusions. We show that a finite index endomorphism on a half-sided modular inclusion extends to a finite index endomorphism on the corresponding net of von Neumann algebras on the circle. Moreover, we present another approach to encoding endomorphisms on nets of von Neumann algebras on the circle into half-sided modular inclusions. There is a natural way to associate a weight to a Möbius covariant endomorphism. The properties of this weight have been studied by Bertozzini *et al.* ["Covariant sectors with infinite dimension and positivity of the energy," Commun. Math. Phys. **193**, 471–492 (1998)]. In this paper we show the converse, namely, how to associate a Möbius covariant endomorphism to a given weight under certain assumptions, thus obtaining a correspondence between a class of weights on a half-sided modular inclusion and a subclass of the Möbius covariant endomorphisms on the associated net of von Neumann algebras. This allows us to treat Möbius covariant endomorphisms in terms of weights on half-sided modular inclusions. As our aim is to provide a framework for treating endomorphisms on nets of von Neumann algebras in terms of the apparently simpler objects of weights on half-sided modular inclusions, we lastly give some basic results for manipulations with such weights. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Algebraic quantum field theory is an approach to quantum field theory in which the basic objects of the theory are local algebras of observables associated with bounded regions of space time. A local algebra associated with a given bounded region of space time is an algebra of operators corresponding to the physical measurements that can be performed in that region of space time. Standard introductions to the subject include Refs. 12, 1, and 4.

Commonly we consider states corresponding to particularly simple physical systems in order to obtain a more amenable theory. The Doplicher-Haag-Roberts (DHR) superselection criterion[7] has proven to be fruitful in this respect. In essence it picks out states corresponding to spatially bounded physical systems with no long-range forces. The representations of the net of local algebras whose folia satisfy the DHR superselection criterion are unitarily equivalent to endomorphisms of the local algebras. These endomorphisms are known as DHR endomorphisms and the study of them is central to algebraic quantum field theory.

To model the physical world as we presently understand it, the natural choice of space time is the four-dimensional Minkowski space. However, theories in lower-dimensional space times have

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proven to be both physically and mathematically interesting in their own right. Especially nets of local algebras on the circle have been of growing interest recently. Wiesbrock showed in 1993 that one-dimensional nets of local algebras on the circle satisfying an assumption known as strong additivity could be completely described by half-sided modular inclusions of factors;[19] a gap in the proof was later filled by Araki and Zsidó.[2]

Wiesbrock's result opens the door to the study of algebraic quantum field theories on the circle in terms of half-sided modular inclusions of factors. In this paper we take the first steps towards developing a theory for Möbius covariant DHR endomorphisms on half-sided modular inclusions.

We present two main results. Firstly we show an extension theorem for endomorphisms with finite index. Specifically we show that normal, injective endomorphisms with finite index on a half-sided modular inclusion extend to endomorphisms with finite index on the associated net of von Neumann algebras under some light assumptions. Secondly we present a way of treating Möbius covariant endomorphisms in terms of weights on half-sided modular inclusions. To any Möbius covariant endomorphism there is a naturally occurring cocycle satisfying the conditions for being the Connes cocycle derivative of some weight with respect to the vacuum state. Properties of this weight for endomorphisms with finite index have been studied by Longo[14] and Bertozzini *et al.*[5] In this paper we construct a method for passing the other way, that is, from weights to endomorphisms. This gives us a correspondence between a class of weights on a half-sided modular inclusion and a subclass of the Möbius covariant endomorphisms on the net of von Neumann algebras associated with the half-sided modular inclusion. Finally, we give the analog for weights of some basic constructions for endomorphisms; e.g., unitary equivalence, direct sums, and weak conjugates.

Sectionwise the paper breaks down as follows. In Sec. II we recall the basic notions of nets of von Neumann algebras, Möbius covariant endomorphisms, and half-sided modular inclusions. Next we show in Sec. III that any finite index endomorphism on the larger factor of a half-sided modular inclusion extends to a finite index endomorphism on the net of local algebras associated with the half-sided modular inclusion as per Wiesbrock's result.

In Refs. 14 and 5, Longo and Bertozzini *et al.* studied for a given Möbius covariant endomorphism ρ, the weight ψ whose Connes cocycle derivative relative to the vacuum state ω satisfies

$$(D\psi:D\omega)_t = U_\rho(D(t))U(D(t))^*, \tag{1}$$

where $D(t)$ denotes the dilations and U_ρ and U are the usual (projective) representations of the Möbius group such that $\mathrm{Ad}U_\rho(g)\circ\rho=\rho\circ\mathrm{Ad}U(g)$. In Sec. IV we take a different tack and show conversely that for a suitable weight ψ on the larger factor of a half-sided modular inclusion, we can associate a Möbius covariant endomorphism ρ on the net of local algebras such that Eq. (1) holds true. We also establish a correspondence between weights and endomorphisms allowing us to treat the latter in terms of weights on half-sided modular inclusions.

Finally in Sec. V we give the equivalents of basic operations pertaining to endomorphisms in terms of weights including unitary equivalence, direct sums, subrepresentations, and weak conjugates. Also we give criteria for finite index and positivity for an endomorphism associated with a weight.

II. PRELIMINARIES

Below we present the basic objects and results that will form the foundation for later sections. Most notably we introduce nets of von Neumann algebras and their relation with half-sided modular inclusions.

A. Nets of von Neumann algebras

We will identify $S^1 := \{z \in \mathbb{C} \,|\, |z|=1\}$ with the one-point compactification of $\mathbb{R}$, $\mathbb{R}\cup\{\infty\}$, through the stereographic projection,

$$S^1 \ni z \mapsto x(z) := \frac{1}{i}\frac{z-1}{z+1} \in \mathbb{R} \cup \{\infty\}.$$

The Möbius group $\mathsf{PSU}(1,1)$ acts on S^1 by

$$\begin{pmatrix} \alpha & \beta \\ \bar{\beta} & \bar{\alpha} \end{pmatrix} \cdot z := \frac{\alpha z + \beta}{\bar{\beta} z + \bar{\alpha}}.$$

Two types of elements of note are the translations and dilations.

$$\text{Translations:} \quad T(a) := \begin{pmatrix} 1 + ia/2 & ia/2 \\ -ia/2 & 1 - ia/2 \end{pmatrix}, \quad a \in \mathbb{R}.$$

$$\text{Dilations:} \quad D(t) := \begin{pmatrix} \cosh(\pi t) & \sinh(\pi t) \\ \sinh(\pi t) & \cosh(\pi t) \end{pmatrix}, \quad t \in \mathbb{R}.$$

By a *proper interval* on S^1 we will mean a nonempty, nondense, open, connected subset of S^1. For convenience we will often refer to proper intervals simply as intervals when no confusion can occur. If I is an interval, we write $I^\perp$ for the interior of its complement in S^1. If I and J are intervals such that $I \cap J = \emptyset$, we write $I \perp J$.

Definition 2.1 (Net of von Neumann Algebras): A *net of von Neumann algebras on* S^1 is an assignment for each interval I on S^1 of a von Neumann algebra $\mathcal{A}(I)$ on a fixed Hilbert space $\mathfrak{H}$ satisfying the following axioms.

- **Isotony:** For intervals $I \subseteq J$ we have $\mathcal{A}(I) \subseteq \mathcal{A}(J)$.
- **Locality:** If I and J are disjoint intervals, then $\mathcal{A}(I) \subseteq \mathcal{A}(J)'$.
- **Möbius covariance:** There exists a unitary representation $(U, \mathfrak{H})$ of the Möbius group $\mathsf{PSU}(1,1)$ such that $U(g)\mathcal{A}(I)U(g)^* = \mathcal{A}(gI)$. We write α_g for $\mathsf{Ad}U(g)$.
- **Positive energy:** The generator of the one-parameter group $\theta \mapsto U(R(\theta))$ is positive.
- **Existence and uniqueness of vacuum vector:** The subspace of U-invariant vectors in $\mathfrak{H}$ is one dimensional. We single out one such vector Ω of norm one, which will be referred to as the *vacuum vector*. We also require that $\cup_I \mathcal{A}(I)\Omega$ is dense in $\mathfrak{H}$, where I ranges over the intervals on S^1.

We will write $\mathcal{A}$ for the family $(\mathcal{A}(I))_I$.

The above defined concept of a net of von Neumann algebras also appears in the literature under the names of *conformal precosheaf*[10] and *local conformal net*[13] amongst others. The individual von Neumann algebras $\mathcal{A}(I)$ are called *local algebras* and elements of $\mathbb{B}(\mathfrak{H})$ belonging to a local algebra are called *local elements*.

We will denote the vector state associated with Ω by $\omega(\cdot) := (\cdot\Omega|\Omega)$. Usually we will think of this as a vector state on $\mathcal{A}(S_+)$, where $S_+ := \{z \in S^1 | \mathrm{Im}(z) > 0\}$. For notational ease we will write its restriction to a local algebra $\omega_I := \omega|\mathcal{A}(I)$.

Remark 2.2: If $\mathcal{A}$ is a net of von Neumann algebras, it is often practical to be able to speak of $\mathcal{A}(\mathcal{O})$ for general open sets $\mathcal{O}$. We define $\mathcal{A}(\mathcal{O})$ as follows.

$$\mathcal{A}(\mathcal{O}) := \vee\{\mathcal{A}(I) | I \text{ is a proper interval and } I \subseteq \mathcal{O}\}.$$

By isotony of the net $\mathcal{A}$, there is no ambiguity when speaking of $\mathcal{A}(I)$ for a proper interval.

We mention some important consequences of the axioms. All proofs can be found in Ref. 4.

Theorem 2.3 (Irreducibility): *If* $\mathcal{A}$ *is a net of von Neumann algebras on the Hilbert space* $\mathfrak{H}$ *then* $\vee_I \mathcal{A}(I) = \mathbb{B}(\mathfrak{H})$.

Theorem 2.4: *Every local algebra in a net of von Neumann algebras is a type* III_1 *factor.*

Theorem 2.5: (Haag Duality): *If* $\mathcal{A}$ *is a net of von Neumann algebras then* Haag duality *holds*,

$$\mathcal{A}(I^{\perp}) = \mathcal{A}(I)', \quad I \text{ is an interval on } S^1.$$

Theorem 2.6 (Reeh-Schlieder): *The vacuum vector* Ω *is cyclic and separating for each local algebra* $\mathcal{A}(I)$.

We write r for the reflection $S^1 \ni z \mapsto \bar{z} \in S^1$. For any interval I on S^1 we define the *reflection associated with* I to be $r_I := grg^{-1}$, where g is an element of the Möbius group such that $gS_+ = I$. It is easily checked that r_I is well defined. We write $\mathsf{PSU}(1,1)_{\pm}$ for the extended Möbius group generated by the Möbius group and the reflections.

Also for any interval I we define the dilations associated with I by $D_I(t) := gD(t)g^{-1}$ for any $g \in \mathsf{PSU}(1,1)$ such that $gI = S_+$. As with the reflections, it is easy to check that D_I is well defined.

Theorem 2.7 (Bisognano-Wichmann): *Let* $\mathcal{A}$ *be a net of von Neumann algebras. The representation* U *of the Möbius group can be extended to the extended Möbius group in such a way that the net* $\mathcal{A}$ *is covariant under this representation and*

$$U(D_I(t)) = \Delta_{\mathcal{A}(I)}^{it},$$

$$U(r_I) = J_{\mathcal{A}(I)},$$

where the modular operator and conjugation for $\mathcal{A}(I)$ *are with respect to the vacuum state* $\omega(\cdot) = (\cdot\Omega|\Omega)$.

Finally we mention an important axiom that we will be needing.

Definition 2.8 (Strong Additivity): *A net of von Neumann algebras* $\mathcal{A}$ is *strongly additive* if for any interval I and point $z \in I$, we have $\mathcal{A}(I) = \mathcal{A}(I_1) \vee \mathcal{A}(I_2)$, where I_1 and I_2 are the two connected components of $I \backslash \{z\}$.

To any net of von Neumann algebras $\mathcal{A}$, we can associate the *global* C^**-algebra* $C^*(\mathcal{A})$ with the following properties:[8,9]

(1) There is an embedding of every local algebra $\mathcal{A}(I)$ into $C^*(\mathcal{A})$, $i_I : \mathcal{A}(I) \to C^*(\mathcal{A})$ such that $i_J|_{\mathcal{A}(I)} = i_I$ whenever $I \subseteq J$.
(2) If (π_I) is a family of representations, $\pi_I : \mathcal{A}(I) \to \mathbb{B}(\mathfrak{H}_\pi)$, then there exists a unique representation $(\pi, \mathfrak{H}_\pi)$ of $C^*(\mathcal{A})$ such that $\pi \circ i_I = \pi_I$.

B. Endomorphisms on nets of von Neumann algebras

Let $\mathcal{A}$ be a fixed net of von Neumann algebras on $\mathfrak{H}$. A family of $*$-homomorphisms $\rho = (\rho_I)$, $\rho_I : \mathcal{A}(I) \to \mathbb{B}(\mathfrak{H})$ is said to be *consistent* if $\rho_J|_{\mathcal{A}(I)} = \rho_I$ whenever $I \subseteq J$. By the universal property of the global C^* algebra, ρ induces a representation of $C^*(\mathcal{A})$.

If there exists an interval I such that $\rho_{I^{\perp}} = \mathsf{id}_{\mathcal{A}(I^{\perp})}$, then ρ is said to be *localized in* I. If ρ is consistent and localized in I, then ρ_J is an endomorphism of $\mathcal{A}(J)$ whenever $J \supseteq I$ and ρ is an endomorphism of the global algebra $C^*(\mathcal{A})$.

A consistent, localized endomorphism is said to be *transportable* if for every interval J there exists a unitary u such that $\mathsf{Ad}u \circ \rho$ is localized, in J. Such a unitary is called a *transporter*. A consistent, localized, and transportable endomorphism is called a *Doplicher-Haag-Roberts endomorphism*, or simply a DHR *endomorphism*. A unitary equivalence class of DHR endomorphisms is called a *sector*.

The requirement of transportability can be strengthened to a requirement of covariance. If G is a subgroup of the Möbius group, we say that ρ is *covariant with respect to* G if there is a projective representation $(U_\rho, \mathfrak{H})$ of G such that

$$U_\rho(g)\rho(a)U_\rho(g)^* = \rho(U(g)aU(g)^*), \quad g \in G, \quad a \in C^*(\mathcal{A}).$$

If G is either the translation-dilation subgroup of the Möbius group or the Möbius group itself, we say that ρ is *translation-dilation covariant or Möbius covariant*, respectively. As projective unitary representations of connected semi-simple Lie groups, such as the Möbius group, lift to true unitary

representations of the universal covering groups,[3] we will instead of projective representations of the Möbius group $\mathsf{PSU}(1,1)$ often consider unitary representations of the universal covering group $\overline{\mathsf{PSU}(1,1)}$ of the Möbius group. As the translation-dilation group is connected and contractible, it is its own universal covering group. Hence, any projective representation of the translation-dilation group stems from a true unitary representation.

A DHR endomorphism ρ localized in some interval I will restrict to an endomorphism ρ_J of $\mathcal{A}(J)$ for any interval $J \supseteq I$. As ρ_J is given by conjugation with a unitary, the inclusion $\rho_J(\mathcal{A}(J)) \subseteq \mathcal{A}(J)$ is a subfactor. We write the (minimal) index of this $\mathrm{Ind}(\rho_J)$. If ρ is covariant, it is easy to check that $\mathrm{Ind}(\rho_J)=\mathrm{Ind}(\rho_{gJ})$ if $J, gJ \supseteq I$.[10] Thus, we will speak merely of the *index of* ρ and write this $\mathrm{Ind}(\rho)$.

C. Half-sided modular inclusions

The concept of half-sided modular inclusions and how to construct nets of von Neumann algebras based on these was first introduced by Wiesbrock in 1993.[19] The article, however, contained a gap which was finally filled by Araki and Zsidó in 2004.[2] Following Ref. 11 we give some basic definitions and results.

Definition 2.9 (Half-Sided Modular Inclusion): Suppose that $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ is a triple, where $\mathcal{N} \subseteq \mathcal{M}$ is an inclusion of von Neumann algebras on some Hilbert space $\mathfrak{H}$ and that $\Omega \in \mathfrak{H}$ is cyclic and separating for both $\mathcal{N}$ and $\mathcal{M}$.

(1) The triple $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ is said to be *standard* if Ω is cyclic for the relative commutant of $\mathcal{N}$ in $\mathcal{M}$, $\mathcal{N}^c = \mathcal{N}' \cap \mathcal{M}$.
(2) The triple $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ is said to be $+$ *half-sided modular* ($-$ *half-sided modular*) *if* $\sigma_t^{\mathcal{M}}(\mathcal{N}) \subseteq \mathcal{N}$ for all $t \leqslant 0$ ($t \geqslant 0$), where $\sigma^{\mathcal{M}}$ denotes the modular automorphism associated with $(\mathcal{M}, \Omega)$.

For brevity, we will refer to a triple $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ which is $\pm$ half-sided modular, as a $\pm$ *half-sided modular inclusion*.

Theorem 2.10 Ref. 11: *Suppose that* $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ *is a standard* $+$ *half-sided modular inclusion*. Then there exists a unique strongly additive net of von Neumann algebras $\mathcal{A}$ *on* S^1 *for which* $\mathcal{A}(]0;\infty[) = \mathcal{M}$, $\mathcal{A}(]0;\infty[) = \mathcal{N}$ *and* Ω *is the vacuum vector.*

III. EXTENDING FINITE INDEX ENDOMORPHISMS

If $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ is a standard half-sided modular inclusion and $\mathcal{A}$ is the associated net of von Neumann algebras as per Theorem 2.10, it can be difficult to determine the endomorphisms on $\mathcal{M}$ that extend to DHR endomorphisms on the net $\mathcal{A}$. To extend a given endomorphism on $\mathcal{M}$ to a DHR endomorphism, we would be forced to come up with transporters for all proper intervals on S^1. This can be difficult as there need be no particular relation between the transporters associated with different intervals, and the half-sided modular inclusion is only directly linked to the intervals $]0;\infty[$ and $]1;\infty[$.

The situation is easier if we are lucky enough to deal with a translation-dilation covariant endomorphism which is localized in some interval, say, $]a;b[$, such that the translation-dilation group alone gives all the necessary transporters. A simple way of making sure that the endomorphism has such covariance is by requiring it to have finite index. This even gives Möbius covariance.

The basic idea will be to use a finite index condition to obtain two one-parameter groups through the Takesaki theorem. We will then show that these together generate a representation U_ρ of the translation-dilation group such that $\mathsf{Ad}U_\rho(g) \circ \rho = \rho \circ \mathsf{Ad}U(g)$, allowing us to extend the given endomorphism ρ to a translation-dilation covariant endomorphism on the net $\mathcal{A}$. Using the finite index condition once again will finally yield Möbius covariance of the extended endomorphism.

A. Endomorphisms and α-cocycles

As mentioned above, a DHR endomorphism is completely known by its transporters. As a special case, a translation-dilation covariant endomorphism ρ localized in some interval I_0 for which $\infty \in I_0^{\perp}$ is completely known by the unitary representation U_ρ of the translation-dilation group $\mathcal{P}$ satisfying

$$\mathrm{Ad}U_\rho(g) \circ \rho = \rho \circ \alpha_g, \quad g \in \mathcal{P}.$$

Below we make precise the connection between such transporters and translation-dilation covariant endomorphisms. The basic idea and techniques are borrowed from Guido and Longo[9] where the case of Möbius covariant endomorphisms is treated. Having only the translation-dilation group and not the full Möbius group at our disposal engenders some technical problems, as two arbitrarily given intervals are not in general connected by an element of the translation-dilation group.

Remark 3.1 (A Comment on the Global C^*-algebra): Recall that $\alpha_g = \mathrm{Ad}U(g)$ satisfies $\alpha_g(\mathcal{A}(I)) = \mathcal{A}(gI)$. Thus by the universal property of the global C^*-algebra $C^*(\mathcal{A})$, α_g induces an automorphism of $C^*(\mathcal{A})$. We will denote this automorphism α_g as well.

As a technical aside we note that when embedding a local element x of $\mathcal{A}$ into the global algebra $C^*(\mathcal{A})$, we need to specify the interval in which x is localized. If $I \subseteq J$ and x is localized in I, associating x with either I or J leads to the same embedding in $C^*(\mathcal{A})$, as can be seen directly from the definition of the global C^* algebra.

Thus if x is localized in intervals I and J and there exists a third interval $K \subseteq I \cap J$ in which x is likewise localized, then the embedding of x into the global C^* algebra is the same whether one considers x associated with I or J. There are, however, cases where no such interval K can be found and these have to be treated with more care.

Definition 3.2 (α-Cocycle): A family of unitaries $(z_g)_g$ in the universal C^*-algebra $C^*(\mathcal{A})$ indexed by a subset $\mathcal{O}$ of the Möbius group is said to be an α-cocycle on $\mathcal{O}$ with values in $C^*(\mathcal{A})$ localized in the proper interval I_0 if (1) z_g is localized in $I_0 \cup gI_0$ whenever this is a proper interval. and (2) $z_{gh} = z_g \alpha_g(z_h)$ when g, h, and gh belong to $\mathcal{O}$.

We will refer to the second requirement as *the cocycle condition*.

Our main interest will be α-cocycles indexed either over the translation-dilation group or the full Möbius group.

Given a translation-dilation covariant endomorphism, we can define $z_g = U_\rho(g)U(g)^*$ for any $g \in \mathcal{P}$. While (z_g) satisfies the cocycle condition the elements will not all have a unique embedding into the universal C^*-algebra $C^*(\mathcal{A})$ as mentioned in Remark 3.1. The next proposition shows how to get around this problem.

Proposition 3.3: *Let I_0 be a subinterval of S^1 whose complement contains ∞ and let $\mathcal{O} \subseteq \{g \in \mathcal{P} | I_0 \cup gI_0$ is a proper interval$\}$ be an open set containing the identity.*

If $(w_g)_{g \in \mathcal{O}}$ is an α-cocycle on $\mathcal{O}$ with values in $C^*(\mathcal{A})$ then it extends uniquely to an α-cocycle on $\mathcal{P}$ with values in $C^*(\mathcal{A})$.

Proof: Our first step is to choose an open subset $\mathcal{U}$ of $\mathcal{O}$ which contains the identity and satisfies $\mathcal{U}^2 \subseteq \mathcal{O}$. This ensures that whenever we have elements g and h of $\mathcal{U}$, the α-cocycle condition makes sense and is satisfied: $w_{gh} = w_g \alpha_g(w_h)$.

The next step is to note that any element of $\mathcal{P}$ can be written as a finite product of elements in $\mathcal{U}$. That is, for a given $g \in \mathcal{P}$ we can choose a decomposition

$$g = \prod_{i=1}^{n} g_i \quad (g_i \in \mathcal{U}).$$

To extend the cocycle to all of $\mathcal{P}$ we will define w_g as

$$w_g = w_{g_1}\alpha_{g_1}(w_{g_2})\cdots\alpha_{g_1\cdots g_{n-1}}(w_{g_n}).$$

To show that this is independent of the choice of g_i's and thus well-defined, it is enough to show that the change $g_i \rightsquigarrow g_i h$, $g_{i+1} \rightsquigarrow h^{-1}g_{i+1}$ for $h \in \mathcal{U}$ leaves the right-hand side of the above equation unchanged. This will follow if we can show that $w_{g_i}\alpha_{g_i}(w_{g_{i+1}}) = w_{g_i h}\alpha_{g_i h}(w_{h^{-1}g_{i+1}})$. We compute

$$\begin{aligned} w_{g_i h}\alpha_{g_i h}(w_{h^{-1}g_{i+1}}) &= w_{g_i}\alpha_{g_i}(w_h)\alpha_{g_i h}(w_{h^{-1}}\alpha_{h^{-1}}(w_{g_{i+1}})) = w_{g_i}\alpha_{g_i}(w_h\alpha_h(w_{h^{-1}})w_{g_{i+1}}) \\ &= w_{g_i}\alpha_{g_i}(w_{hh^{-1}})\alpha_{g_i}(w_{g_{i+1}}) = w_{g_i}\alpha_{g_i}(w_{g_{i+1}}). \end{aligned}$$

Hence, w_g is well-defined on all of $\mathcal{P}$. The cocycle property follows directly from the definition

$$w_{gh} = w_{g_1}\alpha_{g_1}(w_{g_2})\cdots\alpha_{g_1\cdots g_{n-1}}(w_{g_n})\alpha_g(w_{h_1})\alpha_{gh_1}(w_{h_2})\cdots\alpha_{gh_1\cdots h_{m-1}}(w_{h_m}) = w_g\alpha_g(w_h).$$

The question remains whether w_g will be localized in $I_0 \cup gI_0$ whenever this is a proper interval. Let $g \in \mathcal{P}$ be given such that $I_0 \cup gI_0$ is a proper interval and choose another proper interval J extending $I_0 \cup gI_0$ slightly on both sides. It is then possible to choose a decomposition $g = \Pi g_i$ such that $I_0 \cup g_1 I_0 \cup \cdots \cup (g_1 \cdots g_n)I_0$ is contained in J. Consequently,

$$w_g = w_{g_1}\alpha_{g_1}(w_{g_2})\cdots\alpha_{g_1\cdots g_{n-1}}(w_{g_n})$$

belongs to $\mathcal{A}(J)$. By taking the intersection over such intervals J it follows by continuity from the outside that w_g is localized in $I_0 \cup gI_0$. □

The above proposition tells us that whenever we have a translation-dilation covariant endomorphism suitably localized, we obtain a unique α-cocycle on $\mathcal{P}$ with values in $C^*(\mathcal{A})$ similarly localized. This situation is similar to the case of Möbius covariant endomorphisms presented in Ref. 9 where we would get α-cocycles on the Möbius group.

In the latter case there is a bijective correspondence between cocycles and endomorphisms but in the case of α-cocycles on the translation-dilation group, which concerns us, we will need to add an extra assumption to counter the problem that the translation-dilation group cannot transform a given interval into any other arbitrary interval. Colloquially put, the problem is that the translation-dilation group "cannot move points through infinity."

The extra assumption and its use will be elaborated below.

Proposition 3.4: *Let I_0 be an interval whose complement contains ∞. Suppose that (w_g) is an α-cocycle on $\mathcal{P}$ with values in $C^*(\mathcal{A})$ localized in I_0 and that $w_{D(t)}$ is localized in the smallest proper subinterval J of S^1 containing I_0, $D(t)I_0$, and the connected component of $S^1 \setminus (I_0 \cup D(t)I_0)$ containing ∞ whenever $\bar{I}_0 \cap D(t)\bar{I}_0 = \emptyset$. Then there exists a unique translation-dilation covariant endomorphism ρ on S^1 localized in I_0 such that*

$$\rho|_{\mathcal{A}(gI_0^\perp)} = \mathrm{Ad}\, w_g|_{\mathcal{A}(gI_0^\perp)}.$$

Proof: For each proper interval J on S^1 containing ∞ there is exactly one $g \in \mathcal{P}$ such that $gI_0^\perp = J$ and we can therefore define ρ on all such intervals by $\rho_{gI_0^\perp} := \mathrm{Ad}w_g$. Any proper interval not containing ∞ is a subinterval of a proper interval which *does* contain ∞ so we will define ρ on the former intervals by restriction. To show that this is well-defined, we assume that $J \subseteq gI_0^\perp \cap hI_0^\perp$ and attempt to show that $\mathrm{Ad}w_g|_{\mathcal{A}(J)} = \mathrm{Ad}w_h|_{\mathcal{A}(J)}$. This will be accomplished by showing that $w_g^* w_h \in \mathcal{A}(J^\perp)$.

We compute

$$w_g^* w_h = \alpha_g(w_{g^{-1}})w_h = \alpha_g(w_{g^{-1}}\alpha_{g^{-1}}(w_h)) = \alpha_g(w_{g^{-1}h}).$$

As w_g is localized in $I_0 \cup gI_0$ whenever this is a proper interval, it follows that $w_{g^{-1}h}$ is localized in any proper subinterval of $\mathbb{R}$ containing $I_0 \cup g^{-1}hI_0$. Consequently, $\alpha_g(w_{g^{-1}h})$ is localized in any proper subinterval of $\mathbb{R}$ containing $gI_0 \cup hI_0$. Thus, in the case that J is a subinterval of the connected component of $gI_0^\perp \cap hI_0^\perp$ containing ∞, it follows that $\mathrm{Ad}w_g|_{\mathcal{A}(J)} = \mathrm{Ad}w_h|_{\mathcal{A}(J)}$.

The fact that we do not have the full Möbius group available but only the translation-dilation group forces us to consider separately the case where J is a subinterval of a component of $gI_0^\perp \cap hI_0^\perp$ *not* containing ∞. In light of the previous arguments, it is enough to show for $t \in \mathbb{R}$ such that $\bar{I}_0 \cap D(t)\bar{I}_0 = \emptyset$ that if J is a subinterval in the connected component of $I_0^\perp \cap D(t)I_0^\perp$ not containing ∞, then $\mathrm{Ad}w_{D(t)}(x) = x$ for any $x \in \mathcal{A}(J)$. This follows directly by the assumptions in the proposition. Thus, we have a well-defined, consistent endomorphism ρ.

The translation-dilation covariance of ρ easily follows from the definition

$$\mathrm{Ad}(w_g^*)\,\rho|_{A(hI_0^\perp)} = \mathrm{Ad}\,(w_g^* w_h)|_{A(hI_0^\perp)} = \mathrm{Ad}\,(\alpha_g(w_{g^{-1}})w_h)|_{A(hI_0^\perp)} = \alpha_g \circ \mathrm{Ad}(w_{g^{-1}h}) \circ\ \alpha_{g^{-1}}|_{A(hI_0^\perp)}$$
$$= \alpha_g \circ\ \rho|_{A(g^{-1}hI_0^\perp)} \circ \alpha_{g^{-1}}.$$

The covariance of the ρ_I's which are defined by restriction of some $\rho_{gI_0^\perp}$ is also settled by the above calculation. □

Corollary 3.5: *Suppose that I_0 is a proper interval on S^1 whose complement contains ∞.*

Then each translation-dilation covariant endomorphism on $\mathcal{A}$ localized in I_0 gives rise to an α-cocycle (w_g) localized in I_0 and satisfying the assumptions of Proposition 3.4 such that

$$\rho_{gI_0^\perp} = \mathrm{Ad}w_g, \quad g \in \mathcal{P}. \tag{2}$$

Conversely, any α-cocycle (w_g) localized in I_0 and satisfying the assumptions of Proposition 3.4 gives rise to an endomorphism ρ on $\mathcal{A}$ localized in I_0 and satisfying Eq. (2).

B. Extending finite index endomorphisms

Recall that we have a standing assumption that $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ is a standard+half-sided modular inclusion and that $\mathcal{A}$ is the net of von Neumann algebras associated with $(\mathcal{N} \subseteq \mathcal{M}, \Omega)$ as per Theorem 2.10.

Our goal in this section is to give sufficient criteria for endomorphisms on $\mathcal{M}$ to extend to DHR endomorphisms on the net $\mathcal{A}$. We will focus on endomorphisms which are translation-dilation covariant. This, in particular, includes endomorphisms of finite index, as these are automatically Möbius covariant.[9] The main element in the approach is to construct an α-cocycle on the translation-dilation group and use the results of the previous section to associate a translation-dilation covariant endomorphism to it.

Remark 3.6 (Localization): In general we will not distinguish between $\mathcal{N} \subseteq \mathcal{M}$ and its embedding in $\mathcal{A}$, $\mathcal{A}(]1;\infty[) \subseteq \mathcal{A}(\mathbb{R}_+)$ and will therefore continue speaking of $\mathcal{A}(I)$ as a sub-von Neumann algebra of $\mathcal{M}$ whenever $I \subseteq \mathbb{R}_+$. In this spirit we can say that an element $x \in \mathcal{M}$ is localized in an interval I if $x \in \mathcal{A}(I)$ under the usual embedding.

Similarly we will call an endomorphism $\rho \in \mathrm{End}(\mathcal{M})$ localized in $I \subseteq \mathbb{R}_+$ if its restriction to $\mathcal{A}(\mathbb{R}_+) \cap \mathcal{A}(I)'$ is identity.

To properly formulate our results completely within the framework of the half-sided modular inclusion we will introduce notation for ρ being localized in some interval I for which $\bar{I} \subseteq S_+$ as follows.

Definition 3.7 (Localization Strictly Within $\mathcal{M}$): An endomorphism ρ on $\mathcal{M}$ is *localized strictly within $\mathcal{M}$* if ρ is localized in an interval whose closure is contained in S_+.

Lemma 3.8: *Suppose that $\rho \in \mathrm{End}(M)$ is an irreducible endomorphism localized strictly within $\mathcal{M}$, say, in I_0. Suppose furthermore that (v_t) and (w_t) are unitary one-parameter groups such that*

(1) $\mathrm{Ad}v_s(\rho(x)) = \rho(\alpha_{D(s)}(x))$ *for* $s \in R$ *and* $x \in \mathcal{M}$,
(2) $\mathrm{Ad}w_t(\rho(y)) = \rho(\alpha_{D_{]1;\infty[}(t)}(y))$ *for* $t \in \mathbb{R}$ *and* $y \in \mathcal{M} \cap \alpha_{D_{]1;\infty[}(-t)}(\mathcal{M})$,
(3) $v(s)U(D(s))^*$ *belongs to* $\mathcal{A}(I_0 \cup D(s)I_0)$ *for t belonging to some neighborhood of zero, and*
(4) $w(t)U(D_{]1;\infty[}(t))^*$ *belongs to* $\mathcal{A}(I_0 \cup D_{]1;\infty[}(t)I_0)$ *for s belonging to some neighborhood of zero. Then ρ extends to an irreducible translation-dilation covariant endomorphism on $\mathcal{A}$*

localized in I_0.

Proof: By standard arguments, ρ is an endomorphism of $\mathcal{A}(J)$ whenever $J \subseteq \mathbb{R}_+$ is a proper interval containing I_0 and as usual irreducibility implies that $\rho(\mathcal{A}(J))' \cap \mathcal{A}(J) = \mathbb{C}1$.

The key to proving this lemma is to turn the question of extendability into a question of the existence of a suitable α-cocycle. To demonstrate the existence of such an α-cocycle we will use the two given one-parameter unitary groups (v_s) and (w_t) to construct a cocycle satisfying the assumptions of Proposition 3.3 and then invoke Proposition 3.4 to obtain the desired endomorphism on $\mathcal{A}$.

The first step will be to show that the one-parameter groups (v_s) and (w_t) generate a projective representation of the translation-dilation group $\mathcal{P}$ in which (v_s) is identified with the dilations associated with $\mathbb{R}_+$ and (w_t) with the dilations associated with $]1;\infty[$.

To do this it will be enough to show that (v_s) and (w_t) satisfy the proper commutation relations for small s and t. The equivalent of the commutation relation

$$T(a)D(t) = D(t)T(\exp(2\pi t)a) \tag{3}$$

takes the shape

$$\begin{aligned} w(s)v(t-s) = v(t)w(-\log(1-\exp(2\pi t)+\exp(2\pi(t-s)))/2\pi) \\ \times v(\log(1-\exp(2\pi t)+\exp(2\pi(t-s)))/2\pi) \end{aligned} \tag{4}$$

for sufficiently small s and t. In this particular case "sufficiently small" means $\exp(2\pi t)(1-\exp(2\pi(s))) \leqslant 1$ which is satisfied for (s,t) in a neighborhood of (0,0). This requirement ensures that both a and $\exp(2\pi t)a$ appearing in the former commutation relation are strictly less than 1, making it possible to use the equation $T(1-\exp(2\pi t)) = D(t)D_{]1;\infty[}(-t)$.

We set $V(D(t)) := v(t)$ and $V(D_{]1;\infty[}(s)) := w(s)$. If $g_i \in \mathcal{P}$, $i=1,\ldots,n$, is a collection of elements of the form $D(t)$ or $D_{]1;\infty[}(s)$, where t and s may depend on the index, then we write by abuse of notation $z(g_1\cdots g_n)$ for the element $V(g_1)\cdots V(g_n)U(g_1\cdots g_n)^*$. We will show in a moment that $z(g)$ does not depend on the choice of decomposition of g. For now we note by the assumptions of the lemma that $z(g_1\cdots g_n)$ is localized in $I_0 \cup g_1 I_0 \cup g_1 g_2 I_0 \cup \cdots \cup g_1\cdots g_n I_0$.

Now, choose a neighborhood $\mathcal{O}$ of $(0,0) \in \mathbb{R}^2$ and a proper interval $J \supseteq I_0$ such that the manipulations in Eq. (3) keep I_0 inside J and J inside $\mathbb{R}_+$ for $(s,t) \in \mathcal{O}$. For convenience, let z_1 denote the $z(g_1 g_2)$ corresponding to the left-hand side of Eq. (4) and let z_2 denote the $z(g_3 g_4 g_5)$ corresponding to the right-hand side. As the manipulations will map $\mathcal{A}(I_0)$ into $\mathcal{A}(J)$, the element $z_1^* z_2$ is localized in J. Therefore to show the validity of Eq. (4) we need only to show that $z_1^* z_2$ belongs to $\rho(\mathcal{A}(J))'$.

But by our choice of J and the assumptions of the lemma, it follows that $\mathsf{Ad}(z_1^* z_2)\rho(x) = \rho(x)$ for $x \in \mathcal{A}(J)$.

In conclusion, we get a projective representation $g \mapsto V(g)$ of the translation-dilation group $\mathcal{P}$. As $\mathcal{P}$ is its own universal covering group we can assume that the representation is a unitary representation. Then defining $z(g) = V(g)U(g)^*$ as before, but this time without abuse of notation, gives us an α-cocycle localized in I_0 by Proposition 3.3.

Finally, we want to employ Proposition 3.4 to obtain a translation-dilation covariant endomorphism on S^1 localized in I_0. To do so we must first check that $z(D(t))$ is localized in the smallest subinterval J of S^1 containing I_0, $D(t)I_0$, and ∞ whenever $\bar{I}_0 \cap D(t)\bar{I}_0 = \varnothing$. This, however, is an immediate consequence of the third assumption of this lemma.

Hence, Proposition 3.4 provides us with a translation-dilation covariant endomorphism on $\mathcal{A}$ localized in I_0. As it obviously coincides with ρ on I_0, it is an extension of ρ as desired. □

Remark 3.9: While the former lemma is phrased for unitary one-parameter groups (v_t) and (w_t) corresponding to dilations for the intervals $]0;\infty[$ and $]1;\infty[$, respectively, obviously we can get an analogous result for unitary one-parameter groups corresponding to two intervals $I \subset J$ with one common boundary point. We omit a rephrasing of the lemma.

The assumptions of the above lemma may not be trivial to check and we will be focusing our attention on a class of endomorphisms which satisfy these assumptions automatically, namely, endomorphisms with finite index.

Theorem 3.10: *Suppose that* $\rho \in \mathsf{End}(\mathcal{M})$ *is a finite index endomorphism strictly localized within* $\mathcal{M}$. *Then* ρ *extends to a Möbius covariant endomorphism on* S^1.

Proof: First off, as ρ is assumed to have finite index, it can be written as the direct sum of irreducible endomorphisms similarly localized and we may therefore assume without loss of generality that ρ is, in fact, irreducible. Moreover, ρ is normal and injective as $\mathcal{M}$ is a type III factor (Ref. 17, Theorem V.5.1).

Call the interval in which ρ is localized I_0 and choose a proper interval $I \subseteq \mathbb{R}_+$ containing I_0. As $\rho(\mathcal{A}(I)) \subseteq \mathcal{A}(I)$ has finite index we can find a faithful, normal conditional expectation $E: \mathcal{A}(I) \to \rho(\mathcal{A}(I))$. We then choose a faithful, normal state ϕ_0 on $\mathcal{A}(I)$, say, the vacuum state, and let $\phi := \phi_0 \circ E$. This is then a faithful, normal state on $\mathcal{A}(I)$ whose modular group σ^ϕ leaves $\rho(A(I))$ globally invariant by Takesaki's theorem.

Moreover, the restriction of σ^ϕ to $\rho(A(I))$ is σ^{ϕ_0} (Ref. 18, Lemma IX.4.21). Thus, on $\mathcal{A}(I)$ we have that (Ref. 18, Corollary VIII.1.4),

$$\sigma_t^{\phi\circ\rho}(x) = \rho^{-1} \circ \sigma_t^{\phi_0} \circ \rho(x), \quad x \in \mathcal{A}(I)$$

or equivalently

$$\rho \circ \sigma_t^{\phi\circ\rho}(x) = \sigma_t^{\phi_0} \circ \rho(x), \quad x \in \mathcal{A}(I).$$

Let $u_t := (D\phi : D\omega_I)_t$ and $w_t := (D(\phi\circ\rho) : D\omega_I)_t$. The usual property of Connes cocycles implies that

$$\rho \circ \mathsf{Ad}(w_t) \circ \sigma_t^{\omega_I}(x) = \mathsf{Ad}(u_t) \circ \sigma_t^{\omega_I} \circ \rho(x), \quad x \in \mathcal{A}(I).$$

Letting $z_t := \rho(w_t)^* u_t$ and $\alpha_t := \mathsf{Ad}(U(D_I(t)))$, where D_I is the dilation associated with the interval I, then the above can be simplified to the expression

$$\alpha_t \circ \rho \circ \alpha_{-t}(x) = z_t^* \rho(x) z_t.$$

Next, defining $v_t := U(D_I(t)) z_{-t}^*$ gives us a unitary satisfying

$$\mathsf{Ad}v_t \circ \rho(x) = \rho \circ \alpha_t(x), \quad x \in \mathcal{A}(I).$$

As ρ is irreducible (v_t) is a projective unitary representation of $\mathbb{R}$. As usual this lifts to a unitary representation of $\mathbb{R}$ for which we use the same notation. We also note in passing that if $x \in \mathcal{A}(I) \cap \mathcal{A}(I_0 \cup D_I(t) I_0)'$ then

$$\mathsf{Ad}(v_t U(D_I(t))^*)(x) = \mathsf{Ad}v_t \circ \rho(\alpha_t(x)) = \rho(x) = x,$$

so $v_t U(D_I(t))^*$ belongs to $\mathcal{A}(I) \cap \mathcal{A}(I_0 \cup D_I(t) I_0)'$. In particular, the covariance property $\mathsf{Ad}v_t \circ \rho = \rho \circ \alpha_t$ holds on all of $\alpha_{-t}(\mathcal{M})$.

Finally, to wrap up the proof, we take the intervals $]0;\infty[$ and $]a;\infty[$ where $a \in \mathbb{R}_+$ is chosen such that $I_0 \subseteq]a;\infty[$ and consider the two corresponding unitary one-parameter groups. We have seen above that these satisfy the assumptions of Lemma 3.8 and we therefore get an extension of ρ to a translation-dilation covariant endomorphism on $\mathcal{A}$. As ρ has finite index, it is automatically Möbius covariant. □

The construction of v_t in the proof of Theorem 3.10 is borrowed from Ref. 9 where DHR endomorphisms on the Minkowski space with finite statistics and only countably many sectors are shown to be Poincaré covariant.

Corollary 3.11: *If* $\rho \in \mathsf{End}(\mathcal{M})$ *is an endomorphism localized strictly within* $\mathcal{M}$ *and which is a direct sum of endomorphisms with finite index, then* ρ *extends to a Möbius covariant endomorphism on* S^1 *with the same localization.*

C. Basic observations for finite index endomorphisms

Corollary 3.11 gives us a correspondence between finite index endomorphisms on the circle localized in some interval I satisfying $\bar{I}\subseteq S_+$ and injective, normal endomorphisms localized strictly within $\mathcal{M}$. As the correspondence is given simply by restriction of ρ to $\mathcal{A}(S_+)$, it follows that all manipulations of ρ which can be carried out within S_+ are preserved by the correspondence.

In particular, unitary equivalence, direct sums, subrepresentations, left inverses, permutators, and the like carry over from the net $\mathcal{A}$ to the half-sided modular inclusion $(\mathcal{N}\subseteq\mathcal{M},\Omega)$ unchanged.

When considering α-induction for a quantum field theoretical net of subfactors $\mathcal{A}\subseteq\mathcal{B}$,[6,16] where both nets are strongly additive nets of von Neumann algebras, the net of subfactors can instead be described by a commuting square of subfactors in which the corners are made up by the factors of the half-sided modular inclusions $\mathcal{A}(]1;\infty[)\subseteq\mathcal{A}(]0;\infty[)$ and $\mathcal{B}(]1;\infty[)\subseteq\mathcal{B}(]0;\infty[)$. As such it is in principle possible to perform α-induction within the framework of half-sided modular inclusions. However, the fact that the endomorphisms lifted by α-induction are not necessarily well-behaved DHR endomorphisms may complicate matters.

IV. ENDOMORPHISMS FROM WEIGHTS

As in the previous section, our goal is to find a workable equivalent of Möbius covariant endomorphisms on a strongly additive net of von Neumann algebras $\mathcal{A}$ in the framework of a half-sided modular inclusion $(\mathcal{N}\subseteq\mathcal{M},\Omega)$ inducing the net of von Neumann algebras as per Theorem 2.10. While we focused on the endomorphism ρ itself in the previous section, in this section we will try a different tack, instead focusing on a subgroup of the transporters of the endomorphism, specifically $t\mapsto U_\rho(D(t))$.

Assume that a Möbius covariant endomorphism ρ on the net $\mathcal{A}$ is given. Assume furthermore that ρ is localized in some interval I satisfying $\bar{I}\subseteq S_+$. By strong additivity of the net $\mathcal{A}$, the endomorphism ρ is completely determined by its restriction to $\mathcal{A}(I)$. By the assumption $\bar{I}\subseteq S_+$, there exists $t\in\mathbb{R}_+$ such that $D(t)I\perp I$. For such a t the covariance property of ρ implies that $\rho_I=\mathrm{Ad}z_\rho(D(t))|_{\mathcal{A}(I)}$ where as usual $z_\rho(g):=U_\rho(g)U(g)^*$. Hence, knowledge of a subinterval I of $\mathbb{R}_+$ in which ρ is localized together with knowledge of the one-parameter group $t\mapsto U_\rho(t)$ give complete knowledge of ρ.

More natural than considering $t\mapsto U_\rho(D(t))$ might be to consider the associated transporters themselves, $t\mapsto z_\rho(D(t))=U_\rho(D(t))U(D(t))^*$. It is easy to check that $t\mapsto z_\rho(D(t))$ satisfies the condition of being a Connes cocycle derivative of some weight ψ relative to ω, $(D\psi:D\omega)_t=z_\rho(D(t))$. The properties of the weight ψ, which contains all information about ρ, have been studied by Longo[16] and Bertozzini *et al.*[5] with the main focus on weights associated with endomorphisms with finite index.

In this section we will be taking the opposite approach. That is, starting with a weight ψ we will construct a Möbius covariant endomorphism ρ such that $(D\psi:D\omega)_t=z_\rho(D(t))$. Two of the most fundamental problems in this approach are determining the class of weights that are associated with Möbius covariant endomorphisms and the level of redundancy there is, that is, when will two weights give rise to the same endomorphism.

As always we fix a standard half-sided modular inclusion $(\mathcal{N}\subseteq\mathcal{M},\Omega)$ and associate to it a net of von Neumann algebras $\mathcal{A}$ as per Theorem 2.10.

A. Weak Möbius covariance

In Sec. III A we gave a correspondence between translation-dilation covariant endomorphisms and α-cocycles on the translation-dilation group $\mathcal{P}$ based on the work by Guido and Longo.[9] Given an endomorphism ρ on $\mathcal{M}$ with finite index, we were then able to associate to it an α-cocycle on the translation-dilation group, and the correspondence of α-cocycles with endomorphisms then provided us with an extension of ρ to the net $\mathcal{A}$ with finite index.

A key element in the above argument was that we knew *a priori* that ρ had finite index;

wherefore it could be written as a direct sum of irreducible endomorphisms. The irreducibility was necessary to get an α-cocycle. In this section, however, we will not have finite index *a priori* and will therefore not be able to reduce the problem to the case of irreducible endomorphisms. Thus when faced with a family of unitaries $(v_g)_{g\in\mathcal{P}}$ satisfying

$$\mathrm{Ad}v_g \circ \rho = \rho \circ \alpha_g,$$

we can no longer conclude that $g\mapsto v_g$ is a projective representation of the translation-dilation group $\mathcal{P}$.

The properties that concern us, however, are unaffected by the lack of continuity of $g\mapsto v_g$ as we will see in this and the following section.

Definition 4.1 (Weak Möbius Covariance): A DHR endomorphism ρ on S^1 is said to be *weakly Möbius covariant* if there exists a family of unitaries $(U_\rho(g))_g$ indexed over the Möbius group such that $\mathrm{Ad}U_\rho(g)\circ\rho=\rho\circ\alpha_g$.

Replacing the Möbius group with the translation-dilation group in the definition above instead gives us what we will call *weak translation-dilation covariance*.

Remark 4.2: If ρ is a weakly Möbius covariant endomorphism localized in I_0 then for any elements g and h of the Möbius group, $\mathrm{Ad}U_\rho(gh)\circ\rho=\mathrm{Ad}(U_\rho(g)U_\rho(h))\circ\rho$. Consequently, the element $U_\rho(gh)^*U_\rho(g)U_\rho(h)$ commutes with the image of ρ, i.e.,

$$U_\rho(gh)^*U_\rho(g)U_\rho(h) \in \rho(\mathcal{A}(I_0))' \cap \mathcal{A}(I_0).$$

Thus, U_ρ is a unitary representation of the Möbius group modulo $\rho(\mathcal{A}(I_0))' \cap \mathcal{A}(I_0)$ in the sense that

$$U_\rho(gh) = x_{g,h}U_\rho(g)U_\rho(h) \quad \text{for some } x_{g,h} \in \rho(\mathcal{A}(I_0))' \cap \mathcal{A}(I_0).$$

For irreducible endomorphisms, the notion of weak Möbius covariance coincides with that of ordinary Möbius covariance.

We found in Sec. III A that there is a bijective correspondence between α-cocycles and Möbius covariant endomorphisms. In this section we will find a similar correspondence with one part being played by the weakly Möbius covariant endomorphisms. The other part will be played by α-cocycle modulo some von Neumann algebra, to be defined next.

Definition 4.3 (α-Cocycle Modulo $\mathcal{B}$): Let $I_0\subseteq S^1$ be a proper interval and $\mathcal{B}$ a sub-von Neumann algebra of $\mathcal{A}(I_0)$. An *α-cocycle modulo $\mathcal{B}$ localized in I_0* is a family of unitaries (z_g) indexed over the Möbius group satisfying

(1) $z_g \in \mathcal{A}(I_0)\vee\mathcal{A}(gI_0)$,
(2) $z_{gh}=x_{g,h}z_g\alpha_g(z_h)$ for some $x_{g,h}\in\mathcal{B}$, and
(3) $\mathrm{Ad}z_g(\mathcal{A}(I_0))=\mathcal{B}'\cap\mathcal{A}(I_0)$ for some g for which $gI_0\perp I_0$.

Lemma 4.4: *Suppose that (z_g) is an α-cocycle modulo $\mathcal{B}$ localized in I_0. Then $\mathrm{Ad}z_g(\mathcal{A}(I_0))=\mathcal{B}'\cap\mathcal{A}(I_0)$ for every g satisfying $gI_0\perp I_0$.*

Proof: Straightforward. □

The two following propositions will detail how to move back and forth between weakly Möbius covariant endomorphisms and α-cocycles modulo a given von Neumann algebra.

Proposition 4.5: *Suppose that ρ is a weakly Möbius covariant endomorphism localized in I_0. Then $z_g:=U_\rho(g)U(g)^*$ defines an α-cocycle localized in I_0 modulo $\rho(\mathcal{A}(I_0))'\cap\mathcal{A}(I_0)$.*

Proof: Given $x\in\mathcal{A}(I_0)'\cap\mathcal{A}(gI_0)'$; then

$$\mathrm{Ad}z_g(x) = \mathrm{Ad}U_\rho(g)(\alpha_{g^{-1}}(x)) = \mathrm{Ad}U_\rho(g)\rho(\alpha_{g^{-1}}(x)) = \rho(x) = x.$$

Thus, z_g belongs to $(\mathcal{A}(I_0)'\cap\mathcal{A}(gI_0)')'=\mathcal{A}(I_0)\vee\mathcal{A}(gI_0)$.

To show that the second requirement of the definition is met, let g and h be elements of the Möbius group. A quick calculation shows for any local element x that

$$\mathrm{Ad}(z_{gh}\alpha_g(z_h)^* z_g^*)\rho(x) = \mathrm{Ad}z_{gh}(\alpha_{gh}\circ\rho\circ\alpha_{(gh)^{-1}}(x)) = \mathrm{Ad}U_\rho(gh)(\rho\circ\alpha_{(gh)^{-1}}(x)) = \rho(x).$$

Hence, $z_{gh}=xz_g\alpha_g(z_h)$ for some $x\in\rho(\mathcal{A}(I_0))'\cap\mathcal{A}(I_0)$.

Finally we note that for any g such that $gI_0\perp I_0$, we have $\mathrm{Ad}z_g(\mathcal{A}(I_0))=\rho(\mathcal{A}(I_0))$ $=(\rho(\mathcal{A}(I_0))'\cap\mathcal{A}(I_0))'\cap\mathcal{A}(I_0)$. □

Proposition 4.6: *Suppose that* (z_g) *is an* α*-cocycle modulo* $\mathcal{B}\subseteq\mathcal{A}(I_0)$ *localized in* I_0. *Then there exists a weakly Möbius covariant* ρ *localized in* I_0 *giving rise to* (z_g) *as in Lemma 4.5*.

Proof: We aim to define $\rho|_{\mathcal{A}(gI_0^\perp)}=\mathrm{Ad}z_g|_{\mathcal{A}(gI_0^\perp)}$. To show that this gives a well-defined consistent endomorphism on S^1 we need to show that $z_h^* z_g$ belongs to $\mathcal{A}(gI_0)\vee\mathcal{A}(hI_0)$ for all elements of the Möbius group g and h.

The cocycle condition implies that $z_h^*=\alpha_h(xz_{h^{-1}})$ for some $x\in\mathcal{B}$. Using that $z_{h^{-1}}\alpha_{h^{-1}}(z_g)$ $=yz_{h^{-1}g}$ for some $y\in\mathcal{B}$ we find that

$$z_h^* z_g = \alpha_h(xz_{h^{-1}})z_g = \alpha_h(xz_{h^{-1}}\alpha_{h^{-1}}(z_g)) = \alpha_h(xyz_{h^{-1}g}),$$

which belongs to $\mathcal{A}(hI_0)\vee\mathcal{A}(gI_0)$. Hence, we obtain a consistent endomorphism ρ on S^1.

That ρ is weakly Möbius covariant can be demonstrated by reapplying the above equation as follows:

$$\mathrm{Ad}z_h^*\circ\rho|_{\mathcal{A}(gI_0^\perp)} = \mathrm{Ad}(z_h^* z_g)|_{\mathcal{A}(gI_0^\perp)} = \alpha_h\circ\mathrm{Ad}(xy)\circ\mathrm{Ad}z_{h^{-1}g}\circ\ \alpha_{h^{-1}}|_{\mathcal{A}(gI_0^\perp)} = \alpha_h\circ\ \rho|_{\mathcal{A}(h^{-1}gI_0^\perp)}\circ\alpha_{h^{-1}}.$$

Note that Lemma 4.4 is used to eliminate $\mathrm{Ad}(xy)$ in the above computation. □

Remark 4.7 (The Case for the Translation-Dilation Group): If instead of considering α-cocycles indexed over the entire Möbius group, we consider α-cocycles indexed over the translation-dilation group satisfying the requirements of Definition 4.3, then we find a result similar to that of Proposition 4.6. The proof can be applied unchanged except that for the translation-dilation covariant case, we have to work with an interval I_0 whose complement contains ∞.

B. Weak conjugates

In Ref. 9 it is shown how to obtain a weak conjugate of a Möbius covariant endomorphism based on its associated α-cocycle. Following the exposition given in Ref. 9 closely, we will make the necessary generalizations to obtain an equivalent result for weakly Möbius covariant endomorphisms. We start out by recalling some facts about conjugate endomorphisms.

Remark 4.8 (Conjugate Endomorphisms): Assume that $\mathcal{B}\subseteq\mathcal{C}$ is an inclusion of properly infinite von Neumann algebras. Then there exists a normal faithful state ω on $\mathcal{C}$ represented by a vector in the Gel'fand-Naimark-Segal (GNS) representation which is cyclic and separating for both $\mathcal{B}$ and $\mathcal{C}$.[15] Letting $j_\mathcal{B}$ and $j_\mathcal{C}$ denotes the modular conjugations of $\mathcal{B}$ and $\mathcal{C}$, respectively, with respect to the aforementioned cyclic and separating vector, we define the *canonical endomorphism* $\gamma:\mathcal{C}\to\mathcal{B}$ by $\gamma:=j_\mathcal{B}j_\mathcal{C}$.

Now suppose that ρ is a unital, injective endomorphism of $\mathcal{C}$ and let γ_ρ be the canonical endomorphism associated with $\rho(\mathcal{C})\subseteq\mathcal{C}$. A conjugate of ρ is then given by $\bar{\rho}=\rho^{-1}\circ\gamma_\rho$.

If U is a unitary that implements ρ, that is, $\rho=\mathrm{Ad}U$, then $\bar{U}=j_\mathcal{C}(U)$ implements a conjugate $\bar{\rho}$ of ρ, $\bar{\rho}=\mathrm{Ad}\bar{U}$. Moreover, every conjugate of ρ is of this form.[9]

Definition 4.9 (Weak Conjugate Endomorphism): Suppose that ρ is a consistent endomorphism on the net of von Neumann algebras $\mathcal{A}$ localized in the proper interval I_0. A *weak conjugate endomorphism of* ρ is a consistent endomorphism $\bar{\rho}$ localized in I_0 such that $\bar{\rho}_I$ is conjugate of ρ_I for every interval $I\supseteq I_0$.

As usual we extend the Möbius group and the unitary representation $(U,\mathfrak{H})$ to include reflections associated with proper intervals. In general we will use the notation r or s for such reflections, adding a subscript, r_I, if necessary to emphasize the interval with which the reflection is associated. We write J_I for the modular conjugation associated with $(\mathcal{A}(I),\Omega)$ and note that $U(r_I)=J_I$.

Proposition 4.10: *Suppose that* (z_g) *is an* α*-cocycle modulo* $\mathcal{B}$ *localized in* I_0*. If* h *is an element of the Möbius group and* r *a reflection associated with some interval, then* $g \mapsto \bar{z}_g^{h,r} := \alpha_h j_r(z_{rh^{-1}ghr})$ *defines an* α*-cocycle modulo* $\alpha_h j_r(\mathcal{B})$ *localized in* hrI_0*.*

Proof: We fix an element h of the Möbius group and a reflection r and consider the mapping $g \mapsto \bar{z}_g^{h,r}$.

Firstly, we will deal with the localization. Let g be an arbitrary element of the Möbius group. Then

$$\bar{z}_g^{h,r} = \alpha_h j_r(z_{rh^{-1}ghr}) \in \alpha_h j_r(\mathcal{A}(I_0) \vee \mathcal{A}(rh^{-1}ghrI_0)) = \mathcal{A}(hrI_0) \vee \mathcal{A}(g(hrI_0)).$$

Secondly, as concerns the cocycle condition for $\bar{z}^{h,r}$ we make the following computation:

$$\begin{aligned}\bar{z}_{g_1g_2}^{h,r} = \alpha_h j_r(z_{rh^{-1}g_1hrrh^{-1}g_2hr}) &\in \alpha_h j_r(\mathcal{B} z_{rh^{-1}g_1hr}\alpha_{rh^{-1}g_1hr}(z_{rh^{-1}g_2hr})) \\ &= \alpha_h j_r(\mathcal{B})\bar{z}_{g_1}^{h,r}\alpha_{g_1}(\alpha_h j_r(z_{rh^{-1}g_2hr})) = \alpha_h j_r(\mathcal{B})\bar{z}_{g_1}^{h,r}\alpha_{g_1}(\bar{z}_{g_2}^{h,r}).\end{aligned}$$

Finally, choose a g such that $ghrI_0 \perp hrI_0$. This clearly implies that $rh^{-1}ghrI_0 \perp I_0$ and we therefore have

$$\mathrm{Ad}(\bar{z}_g^{h,r})\mathcal{A}(hrI_0) = \mathrm{Ad}(\alpha_h j_r(z_{rh^{-1}ghr}))\alpha_h j_r\mathcal{A}(I_0) = \alpha_h j_r(\mathrm{Ad}(z_{rh^{-1}ghr})\mathcal{A}(I_0)) = \alpha_h j_r(\mathcal{B}' \cap \mathcal{A}(I_0))$$

as desired. □

Definition 4.11: For a given weakly Möbius covariant endomorphism ρ localized in I or equivalently the corresponding α-cocycle (z_g) modulo $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$, we denote the weakly Möbius covariant endomorphism associated with $(\bar{z}_g^{h,r})$ by $\bar{\rho}^{h,r}$.

We fix a weakly Möbius covariant endomorphism ρ localized in an interval I_0 whose complement contains ∞.

Lemma 4.12: *For any element* h *of the Möbius group and reflection* r*, it holds that*

$$\bar{\rho}^{h,r} = \alpha_h \circ j_r \circ \rho \circ j_r \circ \alpha_{h^{-1}}.$$

Proof:

$$\begin{aligned}\bar{\rho}_{ghrI_0^\perp}^{h,r} = \mathrm{Ad}(\alpha_h j_r(z_{rhg^{-1}hr}))|_{\mathcal{A}(ghrI_0^\perp)} &= \alpha_h j_r \circ \mathrm{Ad}(z_{rh^{-1}ghr})|_{\mathcal{A}(rh^{-1}ghrI_0^\perp)} \circ j_r\alpha_{h^{-1}} \\ &= \alpha_h j_r \circ \rho_{rh^{-1}ghrI_0^\perp} \circ j_r\alpha_{h^{-1}}.\end{aligned}$$

□

Proposition 4.13: *The endomorphisms* $\bar{\rho}^{h,r}$ *with* h *ranging over the Möbius group and* r *over the reflections are all in the same sector.*

Proof: Let g and h be elements of the Möbius group and let r and s be reflections. Then

$$\bar{\rho}^{h,r} = \alpha_h j_r\rho j_r\alpha_h^{-1} = \alpha_h j_r j_s\alpha_g^{-1}\bar{\rho}^{g,s}\alpha_g j_s j_r\alpha_h^{-1} = \alpha_{hrsg^{-1}} \circ \bar{\rho}^{g,s} \circ \alpha_{(hrsg^{-1})^{-1}} = \mathrm{Ad}((\bar{z}_{hrsg^{-1}}^{g,s})^*) \circ \bar{\rho}^{g,s}.$$

Proposition 4.14: *For each proper interval* $I \supseteq I_0$ *there exists a* $\bar{\rho}^{h,r}$ *such that* $\bar{\rho}_I^{h,r}$ *is a conjugate of* ρ_I*.*

Proof: Let a proper interval $I \supseteq I_0$ be given. As outlined in Remark 4.8, the proof will be done if we can produce a unitary u such that $\rho_I = \mathrm{Ad}u$ and show that $\bar{\rho}_I^{h,r} = \mathrm{Ad}j_I(u)^*$ for some h and r. Let $r := r_I$ and choose h such that $hrI_0 = I_0$. It then follows that $\mathrm{Ad}z_{rhr}|\mathcal{A}(rhrI_0^\perp) = \rho_{rhrI_0^\perp} = \rho_{rI_0^\perp}$. Noting that $rI_0^\perp \supseteq I$ we define $u := z_{rhr}$ and consequently obtain $\rho_I = \mathrm{Ad}u|\mathcal{A}(I)$.

By the cocycle condition for ρ there exists an $x \in \rho(\mathcal{A}(I_0))' \cap \mathcal{A}(I_0)$ such that $z_{rhr}^* = \alpha_{rhr}(z_{rh^{-1}r})x$. Using this we compute

$$j_r(u^*) = j_r(z_{rhr}^*) = j_r(\alpha_{rhr}(z_{rh^{-1}r})x) = \alpha_h j_r(z_{rh^{-1}h^{-1}hr})j_r(x) = \bar{z}_{h^{-1}}^{h,r} j_r(x).$$

For any $a \in \mathcal{A}(I)$ we have $\mathrm{Ad}(j_r(x))(a) \in \mathcal{A}(I) \subseteq \mathcal{A}(rI_0^\perp) = \mathcal{A}(h^{-1}I_0^\perp)$. Therefore,

$$\mathrm{Ad}j_r(u)^*(a) = \mathrm{Ad}(\bar{z}^{h,r}_{h^{-1}}j_r(x))(a) = \mathrm{Ad}(\bar{z}^{h,r}_{h^{-1}})\mathrm{Ad}(j_r(x))(a) = \bar{\rho}^{h,r}(\mathrm{Ad}(j_r(x))a) = \alpha_h j_r \rho j_r \alpha_h^{-1}(\mathrm{Ad}j_r(x)a)$$
$$= \mathrm{Ad}(\alpha_h j_r \rho(\alpha_{rh^{-1}r}(x)))\bar{\rho}^{h,r}(a).$$

Now, as $x \in \mathcal{A}(I_0)$ and $rh^{-1}rI_0 \perp rh^{-1}I_0 = I_0$, we have $\rho(\alpha_{rh^{-1}r}(x)) = \alpha_{rh^{-1}r}(x)$. Consequently,

$$\mathrm{Ad}(\alpha_h j_r \rho(\alpha_{rh^{-1}r}(x)))\bar{\rho}^{h,r}(a) = \mathrm{Ad}(j_r(x))\bar{\rho}^{h,r}(a) = \bar{\rho}^{h,r}(a),$$

as $j_r(x) \in \mathcal{A}(rI_0) \subseteq \mathcal{A}(I)'$ and $\bar{\rho}^{h,r}(a) \in \mathcal{A}(I)$.

In conclusion, $\mathrm{Ad}j_r(u)^* | \mathcal{A}(I) = \bar{\rho}^{h,r}_I$ and $\bar{\rho}^{h,r}_I$ is therefore a conjugate of ρ_I. □

Lemma 4.15: *If h is an element of the Möbius group and r a reflection chosen such that $hrI_0 = I_0$, then for any proper interval $I \supseteq I_0$ the endomorphism $\bar{\rho}^{h,r}$ is unitarily equivalent to $j_I \circ \rho \circ j_I$.*

Proof: As in the previous proof we find a unitary $u := z_{rhr}$ such that

$$\rho = \begin{cases} \mathrm{Ad}u \text{ on } \mathcal{A}(I) \\ \mathrm{id} \text{ on } \mathcal{A}(I^\perp). \end{cases}$$

Hence, $j_I \circ \rho \circ j_I$ is given by

$$j_I \circ \rho \circ j_I = \begin{cases} \mathrm{id} \text{ on } \mathcal{A}(I) \\ \mathrm{Ad}j_I \text{ on } \mathcal{A}(I^\perp). \end{cases}$$

Conjugating $j_I \circ \rho \circ j_I$ with $j_I(u)^*$ then gives

$$\mathrm{Ad}(j_I(u)^*) \circ j_I \circ \rho \circ j_I = \begin{cases} \mathrm{Ad}j_I(u)^* \text{ on } \mathcal{A}(I) \\ \mathrm{id} \text{ on } \mathcal{A}(I^\perp), \end{cases}$$

which we recognize as $\bar{\rho}^{h,r}$. □

Lemma 4.16: *For any interval I and any element g of the Möbius group, $j_I \circ \rho \circ j_I$ is unitarily equivalent to $j_{gI} \circ \rho \circ j_{gI}$.*

Proof:

$$j_{gI} \circ \rho \circ j_{gI} = \alpha_g \circ j_I \circ \alpha_g^{-1} \circ \rho \circ \alpha_g \circ j_I \circ \alpha_g^{-1} = \alpha_g \circ j_I \circ \mathrm{Ad}z_g^* \circ \rho \circ j_I \circ \alpha_g^{-1} \sim j_I \circ \rho \circ j_I \circ \alpha_g^{-1} \sim j_I \circ \rho \circ j_I.$$

□

We sum up our findings in the following proposition.

Proposition 4.17: *Suppose that ρ is a weakly Möbius covariant endomorphism localized in I_0. Then ρ has a weakly Möbius covariant weak conjugate and for any interval I, $j_I \circ \rho \circ j_I$ is in the sector of that weak conjugate.*

C. Endomorphisms from weights

We have now come to the part where we construct Möbius covariant endomorphisms from weights. While we ultimately want to formulate the results in terms of half-sided modular inclusions, it is convenient, especially in the proofs, to keep working in the setting of nets of von Neumann algebras.

The construction falls in two parts. The first part is to construct a weakly Möbius covariant endomorphism associated with a given weight. This part uses techniques similar to those employed in Sec. III where we were able to extend an endomorphism ρ on $\mathcal{A}(S_+)$ to the entire net $\mathcal{A}$ provided that there existed a conditional expectation $E: \mathcal{A}(S_+) \to \rho(\mathcal{A}(S_+))$ with finite index. We will construct an endomorphism on some local algebra $\mathcal{A}(]a;\infty[)$ along with a conditional expectation onto its image. The fact that this conditional expectation may not have finite index is the reason we are only able to obtain *weak* Möbius covariance *a priori*.

The second part of the construction consists of showing that the obtained weakly Möbius covariant endomorphism is a direct sum of endomorphisms with finite index and thus *a fortiori*

Möbius covariant. This part relies on proof techniques developed by Bertozzini *et al.*[5] in which the existence of a weak conjugate, proven in the previous section, will play a central role.

Definition 4.18 [Localized Weight]: Let ψ be semifinite, normal, faithful weight on $\mathcal{M}$. We say that ψ *is localized in the proper interval* $I_0 \subseteq \mathbb{R}_+$ if (1) $(D\psi:D\omega)_t \in \mathcal{A}(I_0) \vee \mathcal{A}(D(t)I_0)$ for all $t \in \mathbb{R}$ and (2) The restriction of ψ to $\mathcal{M}(\psi) := \vee_{t\in\mathbb{R}} \mathrm{Ad}((D\psi:D\omega)_t)(\mathcal{A}(D(t)I_0)' \cap \mathcal{M})$ is semifinite.

Note that $\mathcal{M}(\psi) \subseteq \mathcal{A}(I_0)$.

Remark 4.19 ($\mathcal{M}(\psi)$ Globally Invariant under σ^ψ): By its very definition $\mathcal{M}(\psi)$ is globally invariant under the modular automorphism group of ψ:

$$\sigma_s^\psi(\vee_t \mathrm{Ad}(D\psi:D\omega)_t \mathcal{A}(D(t)I_0)' \cap \mathcal{M}) = \sigma_s^\psi(\vee_t \sigma_t^\psi \mathcal{A}(I_0)' \cap \mathcal{M}) = \vee_t \sigma_t^\psi \mathcal{A}(I_0)' \cap \mathcal{M}$$
$$= \vee_t \mathrm{Ad}((D\psi:D\omega)_t)(\mathcal{A}(D(t)I_0)' \cap \mathcal{M}).$$

The existence of a conditional expectation from $\mathcal{M}$ onto $\mathcal{M}(\psi)$ follows from the remark above. It is, however, difficult to construct an endomorphism on $\mathcal{M}$ with image $\mathcal{M}(\psi)$. Instead we will construct an endomorphism on some $\mathcal{A}(]a;\infty[) \subseteq \mathcal{M}$ by conjugation with $(D\psi:D\omega)_{t_0}$ for some suitable t_0. The following lemma asserts that this endomorphism has the proper image, i.e., $\mathcal{M}(\psi) \cap \mathcal{A}(]a;\infty[)$.

Lemma 4.20: *Suppose that ψ is a weight localized in the interval $I_0 \subseteq \mathbb{R}_+$ and that $I \subseteq \mathbb{R}_+$ is an interval containing the closure of I_0. In that case, if $t_0 \in \mathbb{R}$ is chosen such that $D(t_0)I_0 \perp I$, then* $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I) = \mathcal{M}(\psi) \cap \mathcal{A}(I)$.

Proof: We start by showing the inclusion $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I) \subseteq \mathcal{M}(\psi) \cap \mathcal{A}(I)$.

It is useful to note that $(D\psi:D\omega)_t^*(D\psi:D\omega)_s$ belongs to $\mathcal{A}(D(t)I_0) \vee \mathcal{A}(D(s)I_0)$ as seen by the following calculation:

$$(D\psi:D\omega)_t^*(D\psi:D\omega)_s = ((D\psi:D\omega)_s \sigma_s^\omega((D\psi:D\omega)_{t-s}))^*(D\psi:D\omega)_s = \sigma_s^\omega((D\psi:D\omega)_{t-s})^*$$
$$\in \mathcal{A}(D(t)I_0) \vee \mathcal{A}(D(s)I_0).$$

Consequently, the von Neumann algebra $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I)$ is independent of the choice of t_0 as long as $D(t_0)I_0 \perp I$. As it is contained in $\mathcal{A}(I) \vee \mathcal{A}(D(t_0)I_0)$ we conclude by the independence of t_0 that it is, in fact, contained in the smaller von Neumann algebra $\mathcal{A}(I)$, that is, $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I) \subseteq \mathcal{A}(I)$. Secondly, that $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I)$ is contained in $\mathcal{M}(\psi)$ is an immediate consequence of I being contained in $D(s)I_0^\perp$ for some $s \in \mathbb{R}$. Hence, we have shown the inclusion $\mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I) \subseteq \mathcal{M}(\psi) \cap \mathcal{A}(I)$.

The converse inclusion will follow if we can simply show that

$$(\mathrm{Ad}((D\psi:D\omega)_s)\mathcal{A}(D(s)I_0^\perp)) \cap \mathcal{A}(I) \subseteq \mathrm{Ad}(D\psi:D\omega)_{t_0}\mathcal{A}(I)$$

for all $s \in \mathbb{R}$. As the only elements of $\mathcal{A}(D(s)I_0^\perp)$ to be mapped into $\mathcal{A}(I)$ by conjugation with $(D\psi:D\omega)_s$ are those localized in I, it suffices to show that conjugation with $(D\psi:D\omega)_s$ and $(D\psi:D\omega)_{t_0}$, respectively, is identical to $\mathcal{A}(D(s)I_0^\perp \cap I)$. This, however, is a consequence of the aforementioned fact that $(D\psi:D\omega)_t^*(D\psi:D\omega)_s$ belongs to $\mathcal{A}(D(t)I_0) \vee \mathcal{A}(D(s)I_0)$. Thus, we find that $\mathcal{M}(\psi) \cap \mathcal{A}(I) \subseteq \mathrm{Ad}((D\psi:D\omega)_{t_0})\mathcal{A}(I)$. □

As shown as a step in the previous proof,

$$(D\psi:D\omega)_t^*(D\psi:D\omega)_s \in \mathcal{A}(D(t)I_0) \vee \mathcal{A}(D(s)I_0).$$

This has the consequence that not only the image of the endomorphism $\mathrm{Ad}(D\psi:D\omega)_{t_0}|_{\mathcal{A}(I)}$ but also the endomorphism itself is independent of t_0 as long as $D(t_0)I_0 \perp I$.

Proposition 4.21: *Let I_0 be an interval such that $\bar{I}_0 \subseteq S_+$. For any weight ψ on $\mathcal{M}$ localized in I_0 there exists a unique weakly Möbius covariant endomorphism ρ localized in I_0 such that $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$ on $\mathcal{M}$.*

Many aspects of the proof will closely parallel arguments presented in Sec. III. Instead of giving the same arguments again, we will refer back to the relevant proofs and restrict ourselves to dealing with the differences.

Proof: As ψ by assumption is semifinite on both $\mathcal{M}$ and $\mathcal{M}(\psi)$ and the latter as noted in Remark 4.19 is globally invariant under the modular automorphism group of ψ, the Takesaki theorem supplies us with a faithful conditional expectation E from $\mathcal{M}$ onto $\mathcal{M}(\psi)$.

We choose a proper interval I such that $\bar{I}_0 \subseteq I \subseteq]\delta;\infty[$ for some $\delta > 0$. We also choose a t_0 such that $D(t_0)I_0 \perp I$. From the previous lemma it follows that we can define an endomorphism ρ on $\mathcal{A}(I)$ with image $\mathcal{M}(\psi) \cap \mathcal{A}(I)$ by $\rho := \mathrm{Ad}(D\psi : D\omega)_{t_0}$. As $\mathcal{A}(I_0)' \cap \mathcal{M} \subseteq \mathcal{M}(\psi)$, it follows that the restriction of E to $\mathcal{A}(I)$ is a faithful conditional expectation of $\mathcal{A}(I)$ onto $\mathcal{M}(\psi) \cap \mathcal{A}(I)$.

We are now in the situation where we have an endomorphism on $\mathcal{A}(I)$ along with a conditional expectation onto its image. If the endomorphism was irreducible we could apply the proof of Theorem 3.10 to extend ρ to a Möbius covariant endomorphism on S^1. That ρ might be reducible will present some problems but the basic techniques used in the previous section can still be used. Our first goal is to construct an α-cocycle on the translation-dilation group modulo $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ and use this to extend ρ to all of S^1 as per Remark 4.7.

As in the proof of Theorem 3.10 we can find a one-parameter group (v_t) such that $\mathrm{Ad}v_t \circ \rho = \rho \circ \sigma_t^{\omega_I}$. Taking a proper subinterval J of I with one end point in common with I and which contains the closure of I_0, we can find another one-parameter unitary group w_t such that $\mathrm{Ad}w_t \circ \rho|_{\mathcal{A}(J)} = \rho|_{\mathcal{A}(J)} \circ \sigma_t^{\omega_J}$. We can assume without loss of generality that the end point shared by I and J is ∞. It is important to note that $v_t \Delta_{\omega_I}^{-it}$ belongs to $\mathcal{A}(I)$ and that $w_t \Delta_{\omega_J}^{-it}$ belongs to $\mathcal{A}(J)$.

We want to show that the one-parameter unitary groups (v_t) and (w_t) together generate a representation of the translation-dilation group up to left multiplication by elements of $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$. As in the proof of Lemma 3.8, it is enough to show that (v_t) and (w_s) satisfy a commutation relation of the shape (4),

$$w(s)v(t-s) = v(t)w(-\log(1-\exp(2\pi t)+\exp(2\pi(t-s)))/2\pi) \times v(\log(1-\exp(2\pi t)+\exp(2\pi(t-s)))/2\pi), \tag{5}$$

up to left multiplication by elements of $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ for small s and t.

For convenience we will write $U_\rho(D_I(t))$ for v_t and $U_\rho(D_J(t))$ for w_t. Let $g_1, \ldots, g_5$ denote the elements of the group generated by $D_I(s)$ and $D_J(t)$, $s,t \in \mathbb{R}$, corresponding to Eq. (5). With argumentation similar to that of the proof of Lemma 3.8 we find for a suitably chosen "small" interval $K \supseteq I_0$ that

$$U_\rho(g_5)^* U_\rho(g_4)^* U_\rho(g_3)^* U_\rho(g_1) U_\rho(g_2) \in \rho(\mathcal{A}(K))'.$$

As in the proof of Lemma 3.8, the interval K is chosen such that the successive application of the concerned elements of the Möbius group, $g_1, \ldots, g_5$, keeps I_0 within K and K within S_+. Also with argumentation like in the proof of Lemma 3.8, we find that $U_\rho(g_5)^* U_\rho(g_4)^* U_\rho(g_3)^* U_\rho(g_1) U_\rho(g_2)$ belongs to $\mathcal{A}(K)$. By considering smaller and smaller intervals $K \supseteq I_0$ we can conclude that $U_\rho(g)$ is well defined up to right multiplication with $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ for g in the group generated by $D_I(s)$ and $D_J(t)$. It is easy to check that conjugation by $U_\rho(g)$ defines an automorphism on $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$; wherefore $U_\rho(g)$ is well defined up to left multiplication of elements in $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$. That is, for given g_1 and g_2 in the group generated by $D_I(s)$ and $D_J(t)$,

$$U_\rho(g_1)U_\rho(g_2) = x_{g_1,g_2} U_\rho(g_1 g_2) \quad \text{for some } x_{g_1,g_2} \in \rho(\mathcal{A}(I))' \cap \mathcal{A}(I).$$

We now define $z_g := U_\rho(g)U(g)^*$. The aim is to show that (z_g) defines an α-cocycle modulo $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ localized in I_0 such that we can apply Remark 4.7 to extend ρ to all of S^1. The previous arguments show that (z_g) satisfies the cocycle requirement of Definition 4.18. By the very definition of the endomorphism ρ and the weight ψ, it is clear that (z_g) also satisfies the third requirement of the definition, namely, that $\mathrm{Ad}(z_g)\mathcal{A}(I_0) = \rho(\mathcal{A}(I_0))$ for some g such that $gI_0 \perp I_0$.

For the last requirement, i.e., $z_g \in \mathcal{A}(I_0) \vee \mathcal{A}(gI_0)$, we encounter the same problem that we did in Lemma 3.8 stemming from the translation-dilation group being unable to "move points through ∞." With the same argument as in Proposition 3.4 it is enough to show that $z_{D_I(t)} \in \mathcal{A}(I_0) \vee \mathcal{A}(D_I(t)I_0)$ for some t such that $\bar{I}_0 \cap D(t)\bar{I}_0 = \emptyset$. But this is a direct consequence of the definition of $z_{D_I(t)}$. Let a suitable t be given. Then we have for $x \in \mathcal{A}(I \setminus (I_0 \cup D_I(t)I_0))$ that

$$\mathrm{Ad} z_{D_I(t)}(x) = \mathrm{Ad} z_{D_I(t)} \rho(x) = \alpha_{D_I(t)} \circ \rho \circ \alpha_{D_I(-t)}(x) = \alpha_{D_I(t)} \circ \alpha_{D_I(t)}(x) = x.$$

In conclusion, (z_g) is an α-cocycle on the translation-dilation group modulo $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ localized in I_0. By Remark 4.7, ρ extends to a weakly translation-dilation covariant endomorphism on S^1 localized in I_0.

Having defined ρ on all of S^1, it is easy to see that it is, in fact, weakly Möbius covariant. Take a third subinterval L of S_+ containing the closure of I_0 such that $D_L(r)$, $D_I(s)$, and $D_J(t)$ together generate the Möbius group. As before we can construct a one-parameter unitary group $t \mapsto U_\rho(D_L(t))$ such that $\mathrm{Ad} U_\rho(D_L(t)) \circ \rho = \rho \circ \alpha_{D_L(t)}$. Checking that $U_\rho(D_L(t))$ together with the previously defined representation U_ρ of the group generated by $D_I(s)$ and $D_J(t)$ generate a representation of the Möbius group up to left multiplication with $\rho(\mathcal{A}(I))' \cap \mathcal{A}(I)$ is trivial.

Lastly we show that $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$. Let $t \in \mathbb{R}$ be given. For any t_0 such that $D(t_0)I_0 \perp I$ we have $\rho_{D(t_0)I_0^\perp} = \mathrm{Ad}(D\psi : D\omega)_{t_0}$ by the definition of ρ. Therefore, if $x \in \mathcal{A}(D(t_0)I_0^\perp) \cap \mathcal{A}(D(t_0 - t)I_0^\perp) \cap \mathcal{A}(S_+)$, then

$$\begin{aligned}
\sigma_t^\psi \circ \rho(x) = \sigma_t^\psi \circ \mathrm{Ad}(D\psi : D\omega)_{t_0 - t}(x) &= \mathrm{Ad}(D\psi : D\omega)_t \circ \sigma_t^\omega \circ \mathrm{Ad}(D\psi : D\omega)_{t_0 - t}(x) \\
&= \mathrm{Ad}((D\psi : D\omega)_t \sigma_t^\omega((D\psi : D\omega)_{t_0 - t}))\sigma_t^\omega(x) \\
&= \mathrm{Ad}(D\psi : D\omega)_{t_0} \circ \sigma_t^\omega(x) = \rho \circ \sigma_t^\omega(x).
\end{aligned}$$

This shows that the equation $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$ holds on $X_{t_0} := \mathcal{A}(S_+ \setminus (D(t_0)I_0 \cup D(t_0 - t)I_0))$. As we can make X_{t_0} cover all of $\mathcal{A}(S_+)$ by varying t_0 and ρ does not depend on t_0, we conclude that $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$ holds on all of $\mathcal{A}(S_+)$. The equality $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$ also ensures uniqueness of ρ. □

Having constructed a weakly Möbius covariant endomorphism on the basis of a weight, we have completed the first part of the program described in the Introduction to this section. For the second part we will use proof elements from Ref. 5 to show that the endomorphism is a direct sum of finite index endomorphisms. A key element will be played by the following result due to Longo.

Proposition 4.22 Ref. 14: *If $\mathcal{B} \subseteq \mathcal{C}$ is an inclusion of factors and if there exists normal, faithful conditional expectations $E : \mathcal{C} \to \mathcal{B}$ and $E' : \mathcal{C}' \to \mathcal{B}'$, then $\mathcal{B}' \cap \mathcal{C}$ is a direct sum of type I factors. Moreover, for each minimal projection p in $\mathcal{B}' \cap \mathcal{C}$, the inclusion $\mathcal{B}p \subseteq p\mathcal{C}p$ has finite index.*

Theorem 4.23: *Suppose that ψ is a semifinite, normal, faithful weight on $\mathcal{M}$ localized in the interval I_0, $\bar{I}_0 \subseteq S_+$. There exists a unique consistent endomorphism ρ on S^1 localized in I_0 such that $\sigma_t^\psi \circ \rho = \rho \circ \sigma_t^\omega$ on $\mathcal{M}$. This ρ is a (possibly infinite) direct sum of finite index endomorphisms. In particular, ρ is Möbius covariant.*

Proof: From Proposition 4.21 we obtain a weakly Möbius covariant endomorphism ρ localized in $I_0 \subseteq S_+$. Also, as argued in the beginning of the proof of Proposition 4.21, the Takesaki theorem provides us with a normal, faithful conditional expectation E of $\mathcal{A}(S_+)$ onto $\rho(\mathcal{A}(S_+))$. We want to construct a normal, faithful conditional expectation from $\mathcal{A}(S_+)'$ onto $\rho(\mathcal{A}(S_+))'$ such that we can utilize Proposition 4.22.

We will write S_R for the right half of the circle S^1 corresponding to the interval $]-1;1[$. As the reflection associated with S_R maps S_+ bijectively onto S_+, the operator j_{S_R} is an antiautomorphism of $\mathcal{A}(S_+)$. Let $\bar{\rho} := j_{S_R} \circ \rho \circ j_{S_R}$. From Proposition 4.17 we know this to be in the sector of a weak conjugate of ρ. As $\bar{\rho}$ is localized in S_+, there exists a unitary $u \in \mathcal{A}(S_+)$ such that $\mathrm{Ad} u \circ \bar{\rho} = \rho^{-1} \circ j_{\rho(\mathcal{M})} j_{\mathcal{M}}$ on $\mathcal{A}(S_+)$. Thus, if we define $\bar{E} := j_{S_R} \circ E \circ j_{S_R}$ we get a normal, faithful conditional expectation of $\mathcal{M}$ onto $\bar{\rho}(\mathcal{M})$. The inclusion $\bar{\rho}(\mathcal{M}) \subseteq \mathcal{M}$ can be written as $\mathrm{Ad}(u^*) \circ \rho^{-1} \circ j_{\rho(\mathcal{M})} j_{\mathcal{M}}(\mathcal{M}) \subseteq \mathcal{M}$ which by simple rearrangements is seen to be unitarily equivalent to

$\mathcal{M}' \subseteq \rho(\mathcal{M})'$. In this way we obtain a normal, faithful conditional expectation of $\rho(\mathcal{M})'$ onto $\mathcal{M}'$ and Proposition 4.22 then tells us that ρ is a (possibly infinite) direct sum of finite index endomorphisms. As each of these is automatically Möbius covariant, so is ρ. □

Definition 4.24: *Let ψ be a semifinite, normal, faithful weight on $\mathcal{M}$ localized in some interval I_0, $\bar{I}_0 \subseteq S_+$. The unique weakly Möbius covariant endomorphism ρ on S^1 such that $\sigma_t^{\psi} \circ \rho = \rho \circ \sigma_t^{\omega}$ is called the endomorphism associated with ψ and written ρ_ψ.*

D. Freedom of choice of weights

The characterizing equation for an endomorphism ρ associated with a weight ψ is $\sigma_t^{\psi} \circ \rho = \rho \circ \sigma_t^{\omega}$ or equivalently,

$$\mathrm{Ad}((D\psi:D\omega)_t) \circ \rho = \sigma_t^{\omega} \circ \rho \circ \sigma_{-t}^{\omega}.$$

As this only determines the Connes cocycle $(D\psi:D\omega)_t$ up to left multiplication with $\rho(\mathcal{A}(I_0))' \cap \mathcal{A}(I_0)$, assuming ρ localized in I_0, many weights will give rise to the same endomorphism. In fact, the following holds.

Proposition 4.25: *Let I_0 be an interval such that $\bar{I}_0 \subseteq S_+$ and suppose that ϕ and ψ are semifinite, normal, faithful weights on $\mathcal{M}$ localized in I_0. Then the following conditions are equivalent:*

(1) $(D\psi:D\phi)_t \in \rho_\phi(\mathcal{M})' \cap \mathcal{M}$, $t \in \mathbb{R}$.
(2) $(D\psi:D\phi)_t \in \rho_\psi(\mathcal{M})' \cap \mathcal{M}$, $t \in \mathbb{R}$.
(3) $\sigma_t^{\psi}(x) = \sigma_t^{\phi}(x)$, $x \in \rho_\phi(\mathcal{M})$.
(4) $\sigma_t^{\psi}(x) = \sigma_t^{\phi}(x)$, $x \in \rho_\psi(\mathcal{M})$.
(5) $\rho_\phi = \rho_\psi$.

Proof. As the last condition is symmetric in ϕ and ψ, it is enough to show that (1)⇒(5)⇒(3)⇒(1). Assuming Eq. (5), then

$$\sigma_t^{\psi}(\rho_\phi(y)) = \sigma_t^{\psi}(\rho_\psi(y)) = \rho_\psi(\sigma_t^{\omega}(y)) = \rho_\phi(\sigma_t^{\omega}(y)) = \sigma_t^{\phi}(\rho_\phi(y)).$$

Assuming Eq. (3), clearly $(D\psi:D\phi)_t$ commutes with $\rho_\phi(\mathcal{M})$ as stated in Eq. (1). Finally, we assume Eq. (1). As both ρ_ϕ and ρ_ψ are localized in I_0, it is enough to show that they coincide on $\mathcal{A}(I_0)$. Choose t_0 such that $D(t_0)I_0 \perp I_0$. Then

$$\rho_\phi|_{\mathcal{A}(I_0)} = \mathrm{Ad}(D\psi:D\phi)_{t_0} \circ \rho_\phi|_{\mathcal{A}(I_0)} = \mathrm{Ad}(D\psi:D\phi)_{t_0} \circ \mathrm{Ad}\,(D\phi:D\omega)_{t_0}|_{\mathcal{A}(I_0)} = \mathrm{Ad}(D\psi:D\omega)_{t_0}|_{\mathcal{A}(I_0)}$$
$$= \rho_\psi|_{\mathcal{A}(I_0)}$$

as per condition (5). □

In case the endomorphism ρ_ψ is irreducible, the weight ψ is unique up to a scalar.

Corollary 4.26: *Let ρ be an irreducible Möbius covariant endomorphism localized in I_0, $\bar{I}_0 \subseteq S_+$. If ψ and ρ are weights localized in I_0 such that $\rho_\psi = \rho_\phi = \rho$ then $\psi = \lambda\phi$ for some positive real λ.*

Proof: As $(D\psi:D\phi)_t \in \rho(\mathcal{M})' \cap \mathcal{M} = \mathbb{C}$, there exists a positive scalar λ such that $\lambda^{it} = (D\psi:D\phi)_t$ for all $t \in \mathbb{R}$. By the defining properties of the Connes cocycle derivative, $\psi = \lambda\phi$. □

While in general there is a certain amount of freedom in the choice of the weight inducing a given endomorphism ρ, we want to single out the weight ψ satisfying $(D\psi:D\omega)_t = z_\rho(D(t))$. Bertozzini *et al.* have given a criterion for when this is satisfied for finite index endomorphisms.

Proposition 4.27 Refs. 14 and 5: *Let ρ be a Möbius covariant endomorphism localized in I_0, $\bar{I}_0 \subseteq S_+$ and ψ a positive linear functional on $\mathcal{M}$. Then the following conditions are equivalent.*

(1) *ψ is normal and faithful and its Connes cocycle derivative relative to ω satisfies $(D\psi:D\omega)_t = z_\rho(D(t))$, $t \in \mathbb{R}$.*
(2) *$\psi = \mathrm{Ind}(\rho)\omega \circ \rho^{-1} \circ E_\rho$, where E_ρ is the minimal conditional expectation of $\mathcal{M}$ onto $\rho(\mathcal{M})$.*

(3) $\psi(xy^*)=(\exp(-D_\rho/2)x\Omega|\exp(-D_\rho/2)y\Omega)$, *where* D_ρ *is the infinitesimal generator of* $t\mapsto U_\rho(D(t))$.
(4) ψ *is normal, faithful, satisfies* $\sigma_t^\psi\circ\rho=\rho\circ\sigma_t^\omega$, $t\in\mathbb{R}$, *and* $\psi|_{\rho(\mathcal{M})'\cap\mathcal{M}}$ *is a trace whose value on a central projection* p *is given by* $\psi(p)=\mathrm{Ind}(\rho_p)$, *where* ρ_p *is the subrepresentation of* ρ *associated with* p.

The condition that ψ is a trace on $\rho(\mathcal{M})'\cap\mathcal{M}$ is equivalent to $\rho(\mathcal{M})'\cap\mathcal{M}$ being a subset of the centralizer of ψ. This can be restated as the condition that the modular automorphism group of the conditional expectation E_ρ is trivial.

For later use we also mention that condition (2) can be rewritten as $\psi\circ\rho=\mathrm{Ind}(\rho)\omega$, suggesting that it may be useful to think of ψ as the vacuum state for the net $(\rho(\mathcal{A}(I)))$.

V. BASIC CONSTRUCTIONS WITH WEIGHTS

In order to work with weights instead of endomorphisms, we need to establish the analogs of unitary equivalence, direct sums, conjugate endomorphisms, and the like within the framework of weights. In this section we take the first basic steps in that direction.

As usual we fix a standard half-sided modular inclusion $(\mathcal{N}\subseteq\mathcal{M},\Omega)$ and denote the associated net of von Neumann algebras by $\mathcal{A}$.

A. Unitary equivalence, subrepresentations, and direct sums

We introduce the notions of unitary equivalence, subrepresentations, and direct sums for weights. Similar considerations appear in Ref. 14.

Remark 5.1 (The Connes Cocycle Derivative): We briefly recall some facts and notation concerning the Connes cocycle derivative. Define $\mathbb{D}:=\{z\in\mathbb{C}|0\leqslant\mathrm{Im}\,z\leqslant 1\}$ and let $A(\mathbb{D})$ denote the set of bounded, continuous functions on $\mathbb{D}$ that are analytic in the interior. If ψ is a weight on $\mathcal{M}$ we define $\mathfrak{n}_\psi:=\{x\in\mathcal{M}|\psi(x^*x)<\infty\}$.

For given normal, semifinite, faithful weights ψ and ϕ on $\mathcal{M}$, the Connes cocycle derivative $(D\psi:D\phi)_t$ is uniquely determined by the following condition.[18] For each $x\in\mathfrak{n}_\psi\cap\mathfrak{n}_\phi^*$ and $y\in\mathfrak{n}_\psi^*\cap\mathfrak{n}_\phi$, there exists a function $F_{x,y}\in A(\mathbb{D})$ such that

$$F(t)=\psi((D\psi:D\phi)_t\sigma_t^\phi(y)x),\quad F(t+i)=\phi(x(D\psi:D\phi)_t\sigma_t^\phi(y)),\quad t\in\mathbb{R}.$$

.

Proposition 5.2: *Suppose that* ψ *is a semifinite, normal, faithful weight localized in the interval* I_0, $\bar{I}_0\subseteq S_+$ *and that* u *is a unitary localized in some interval whose closure is contained in* S_+. *Then* ρ_ψ *is unitarily equivalent to* ρ_{ψ_u}, *where* $\psi_u:=\psi\circ\mathrm{Ad}u^*$.

Proof. We will write ρ for the endomorphism ρ_ψ and ρ_u for the endomorphism $\mathrm{Ad}u\circ\rho$. Defining $U_{\rho_u}(g)=uU_\rho(g)u^*$ gives a representation of the universal covering group of the Möbius group satisfying $\mathrm{Ad}U_{\rho_u}(g)\circ\rho_u=\rho_u\circ\alpha_g$. We define ψ_u to be the weight whose Connes cocycle derivative with respect to ω satisfies $(D\psi_u:D\omega)_t=U_{\rho_u}(D(t))U(D(t))^*$. Thus, $(D\psi_u:D\omega)_t=u(D\psi:D\omega)_t\sigma_t^\omega(u)^*$.

For $x\in\mathfrak{n}_{\psi_u}\cap\mathfrak{n}_\omega^*$ and $y\in\mathfrak{n}_\omega\cap\mathfrak{n}_{\psi_u}^*$ we have an $F_{x,y}\in A(\mathbb{D})$ such that

$$F_{x,y}(t)=\psi_u(u(D\psi:D\omega)_t\sigma_t^\omega(u^*y)x),\quad F_{x,y}(t+i)=\omega(xu(D\psi:D\omega)_t\sigma_t^\omega(u^*y)).$$

We recognize $F_{x,y}(t+i)$ as being equal to the function $G_{xu,u^*y}(t+i)$, where $G\in A(\mathbb{D})$ is the unique function determining $(D\psi:D\omega)_t$, i.e., $G_{xu,u^*y}(t)=\omega((D\psi:D\omega)_t\sigma_t^\omega(u^*y)xu)$. In particular,

$$\psi_u(yx)=F_{x,y}(0)=G_{xu,u^*y}(0)=\psi(u^*yxu)$$

and we conclude that $\psi_u=\psi\circ\mathrm{Ad}u^*$ □.

The proof above would work just as well, were the unitary u to be replaced by an isometry. This observation leads to the following two propositions.

Proposition 5.3: *Suppose that* ψ *is a semifinite, normal, faithful weight localized in the*

interval I_0, $\bar{I}_0 \subseteq S_+$. *If* ρ *is a subrepresentation of* ρ_ψ, $\rho = \mathrm{Ad}v \circ \rho_\psi$, *then* $\rho = \rho_{\psi \circ \mathrm{Ad}v^*}$.

Proof: The proof is identical to that of Proposition 5.2. □

Proposition 5.4: *Suppose that* $\psi_1, \ldots, \psi_n$ *are semifinite, normal, faithful weights localized in* I_0. *For any choice of isometries* $v_1, \ldots, v_n \in \mathcal{A}(I_0)$ *such that* $\Sigma v_i v_i^* = 1$, *the weight* $\psi := \Sigma \psi_i \circ \mathrm{Ad}v_i^*$ *satisfies* $\rho_\psi = \Sigma \mathrm{Ad}v_i \circ \rho_{\psi_i}$.

Proof: The proof is a slight variation of that of Proposition 5.2. □

In case we are considering weights of the form described in Proposition 4.27, i.e., weights ψ satisfying $(D\psi : D\omega)_t = z_{\rho_\psi}(D(t))$, it is easy to check that forming unitary equivalence, subrepresentations, and direct sums preserves this form.

B. Weak conjugates for weights

While several representatives of a weak conjugate of a given endomorphism ρ localized in S_+ exists, we focus on the most obvious one which is likewise localized in S_+, namely, $j_{S_+} \circ \rho \circ j_{S_+}$. Longo presents similar considerations in Ref. 14.

Proposition 5.5: *Suppose that* ψ *is a semifinite, normal, faithful weight localized in the interval* I_0, $\bar{I}_0 \subseteq S_+$, *and that* r *is the reflection associated with the right half-circle* S_R. *Then the endomorphism associated with the weight* $\bar{\psi} := \psi \circ j_r$ *localized in* $rI_0 \subseteq S_+$ *is a weak conjugate of* ρ_ψ, *in fact*, $\rho_{\bar{\psi}} = j_r \circ \psi \circ j_r$.

Proof: By Proposition 4.17, the endomorphism $j_r \circ \rho_\psi \circ j_r$ is a weak conjugate of ρ_ψ, and clearly $j_r \circ \rho_\psi \circ j_r$ is localized in $rI_0 \subseteq S_+$. The α-cocycle associated with $j_r \circ \rho_\psi \circ j_r$ is $\bar{z}_g = j_r(z_{rgr})$. We seek the weight $\bar{\psi}$ whose Connes cocycle derivative with respect to ω is $\bar{z}_{D(t)}$. As usual we do this by computing the function $F^{\bar{\psi}} \in A(\mathbb{D})$ satisfying the following for $x \in \mathbf{n}_{\bar{\psi}} \cap \mathbf{n}_\omega^*$ and $y \in \mathbf{n}_\omega \cap \mathbf{n}_{\bar{\psi}}^*$:

$$F^{\bar{\psi}}_{x,y}(t) = \bar{\psi}(\bar{z}(D(t))\sigma_t^\omega(y)x), \quad F^{\bar{\psi}}_{x,y}(t+i) = \omega(x\bar{z}(D(t))\sigma_t^\omega(y)).$$

It is easy to calculate that $rD(t)r = D(-t)$ and that consequently $j_r \circ \sigma_t^\omega \circ j_r = \sigma_{-t}^\omega$. Using this and the fact that $\omega = \omega \circ j_r$, we can rewrite $F^{\bar{\psi}}_{x,y}(t+i)$ as

$$F^{\bar{\psi}}_{x,y}(t+i) = \omega(xj_r(z_{D(-t)})\sigma_t^\omega(y)) = \omega(j_r(xj_r(z_{D(-t)})j_r(\sigma_{-t}^\omega(j_r(y))))) = \omega(j_r(x)z_{D(-t)}\sigma_{-t}^\omega(j_r(y)))$$
$$= F^{\psi}_{j_r(x),j_r(y)}(-t+i).$$

Thus we find that

$$\bar{\psi}(yx) = F^{\bar{\psi}}_{x,y}(0) = F^{\psi}_{j_r(x),j_r(y)}(0) = \psi(j_r(yx))$$

and conclude that $\bar{\psi} = \psi \circ j_r$. □

We note in passing that if the weight ψ is of the form given in Proposition 4.27, then $\bar{\psi}$ is likewise of that form.

C. Criteria for finite index

It is possible for a given weight ψ to determine whether or not ρ_ψ has finite index on the basis of the weight alone. In fact, Longo has shown that if the weight ψ is of the form given in Proposition 4.27, then the index of ρ_ψ is $\mathrm{Ind}(\rho_\psi) = \psi(1)$.[14] In particular, ρ_ψ has finite index if and only if ψ is a functional.

For a general weight ψ localized in an interval I_0 it is more difficult to determine the index of ρ_ψ directly. It is easy to construct a weight ψ such that ρ_ψ has infinite index but $\psi(1) < \infty$.

Proposition 5.6: *Let* ψ *be a normal, semifinite, faithful weight localized in* I_0, $\bar{I}_0 \subseteq S_+$. *The following holds.*

(1) *If any normal, semifinite, faithful weight* ϕ *localized in* I_0 *for which* $\sigma^\phi|_{\rho_\psi(\mathcal{M})} = \sigma^\psi|_{\rho_\psi(\mathcal{M})}$ and $\rho(\mathcal{M})' \cap \mathcal{M} \subseteq \mathcal{M}_\phi$ *is a functional, then* ρ_ψ *has finite index.*

(2) *If ψ is a functional and $\psi\circ\rho_\psi$ is proportional to ω, then ρ_ψ has finite index.*

Proof: If ψ_0 is the weight for which the Connes cocycle derivative satisfies $(D\psi_0:D\omega)_t = U_{\rho_\psi}(D(t))$ then ρ_ψ has finite index if and only if ϕ_0 is a functional.[14] Condition (2) is simply a restatement of ψ_0 being a functional, see the comment after Proposition 4.27.

As concerns the first condition, if ϕ is a normal, semifinite, faithful weight localized in I_0 such that $\sigma^\phi|_{\rho_\psi(\mathcal{M})} = \sigma^\psi|_{\rho_\psi(\mathcal{M})}$ and $\rho_\psi(\mathcal{M})' \cap \mathcal{M} \subseteq M_\phi$, then $\rho_\phi = \rho_\psi$ and $\sigma^\phi = \sigma^{\psi_0}$. The latter equality is equivalent to $\phi = \lambda\psi_0$ for some real number $\lambda > 0$. Hence, ϕ is a functional if and only if ψ_0 is a functional, and ψ_0 is a functional if and only if $\rho_\psi = \rho_{\psi_0}$ has finite index.[14] □

D. Positive energy

As any endomorphism ρ_ψ associated with a weight as per Theorem 4.23 is a direct sum of finite index endomorphisms, and any endomorphism of finite index has positive energy we can make the following easy observations.

Proposition 5.7: *Suppose that ψ is a normal, semifinite, faithful weight localized in I_0, $\bar{I}_0 \subseteq S_+$. Then the associated endomorphism ρ_ψ has positive energy.*

Corollary 5.8: *Suppose that ρ is a Möbius covariant endomorphism localized in I_0, $\bar{I}_0 \subseteq S_+$ and that ψ is the weight on $\mathcal{M}$ for which $(D\psi:D\omega)_t = z_\rho(D(t))$. If it holds that $\psi|_{\rho(\mathcal{M})}$ is semifinite, then ρ has positive energy.*

Other criteria for a Möbius covariant endomorphism having positive energy can be found in Ref. 5.

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Minimal redefinition of the OSV ensemble

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In the interesting conjecture, $Z_{BH}=|Z_{top}|^2$, proposed by Ooguri, Strominger, and Vafa (OSV), the black hole ensemble is a mixed ensemble. So if working in the complex polarization, the black hole degeneracy of states as obtained from the ensemble inverse-Laplace integration, generically receives prefactors that do not respect the electric-magnetic duality. One way to handle this, as claimed recently, is working instead of the complex polarization in the real polarization. The other idea would be imposing nontrivial measures for the ensemble sum in the complex polarization. We address this problem in the complex polarization, which is canonical, and upon a redefinition of the OSV ensemble with variables as numerous as the electric potentials, show that for restoring the symmetry no non-Euclidean measure is needed. In detail, applying the electric-magnetic duality as a constraint governing the proper definition of the ensemble variables, we rewrite the OSV free energy as a function of new variables that are combinations of the electric potentials and the black hole charges. Subsequently the Legendre transformation, which bridges between the entropy and the black hole free energy in terms of these variables, points to a generalized ensemble that is well behaved in the complex polarization. In this context, we will consider all the cases of relevance: small and large black holes, with or without $D6$-brane charge. For the case of vanishing $D6$-brane, the new ensemble is purely canonical and the electric-magnetic duality is restored exactly, leading to proper results for the black hole degeneracy of states to all orders in an asymptotic expansion. For more general cases as well, the construction does the job as far as the violation of the duality by the corresponding OSV result is restricted to a prefactor. In the case of black holes with nonvanishing $D6$-brane charge, in a concrete example, we shall show that there are cases where the duality violation goes beyond this restriction and imposing nontrivial measures is incapable of restoring the duality. © *2006 American Institute of Physics.*
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I. INTRODUCTION

The theory of topological strings is a beautiful, smart, and powerful mathematics to probe the various aspects of the superstring theories. From the time of its invention,[1–3] it has been an active field of new discoveries. The reader may refer to Ref. 4 as an excellent textbook on the topological strings, or consult Refs. 5–7 as quick introductions to the subject and Ref. 5 for a nice view of recent developments.

On the other hand, one of the most striking outcomes of the string theory has been the microscopic derivation of the black hole entropy.[8] Recently Ooguri, Strominger, and Vafa (OSV), in Ref. 9, have proposed a deep and promising connection between the topological free energy and the microstate ensemble of the four-dimensional BPS black holes in the CY_3 compactifications of

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type-II strings. This conjecture roots from earlier works on the black hole entropy,[10–12] which made a consistent generalization of the Bekenstein-Hawking formula, incorporating the F-term corrections to the supergravity action as encoded in the prepotential. The evidence for the fact that a generalization to the standard area-law formula for the black hole entropy is needful in the context of string-M theory had been provided in Ref. 13. A detailed review on the results about the black hole entropy from the string theory is found in Ref. 14.

In Ref. 9, OSV observe that the Bekenstein-Hawking-Wald entropy of the black holes, as derived in Refs. 11 and 12, can be reexpressed as the Legendre transformation of a real function $\mathcal{F}$, called the OSV free energy, with respect to the half of its variables,

$$S(p^\Lambda,q_\Lambda)=\mathcal{F}(p^\Lambda,\phi^\Lambda)+q_\Lambda\phi^\Lambda;\quad \mathcal{F}(p^\Lambda,\phi^\Lambda)\equiv-\pi\,\Im F(CX^\Lambda,C^2W^2=2^8), \tag{1.1}$$

with

$$CX^\Lambda=p^\Lambda+i\,\phi^\Lambda \tag{1.2}$$

as obtained from the magnetic part of the attractor equations, and $F(X^\Lambda)=F(X^0,X^A)$ being the full holomorphic prepotential. Independently, a very close relation is established between the asymptotic expansion of the prepotential and the free energy of topological strings.[15,16] In all, the OSV conjecture states that, given a BPS black hole of electric-magnetic charge-multiplet (p^Λ,q_Λ), arising in $\mathcal{N}=2$ compactification of IIA(B) string theory on $CY_3=\mathcal{M}$, the topological $A-A(B-\overline{B})$ models on $\mathcal{M}$ define a mixed ensemble as

$$Z_{\text{mix}}\equiv e^{\mathcal{F}(p^\Lambda,\phi^\Lambda)}=\sum_{q_\Lambda}\Omega(p^\Lambda,q_\Lambda)e^{-\pi\,q_\Lambda\phi^\Lambda}, \tag{1.3}$$

where the black hole free energy is given by

$$F_{\text{BH}}=\mathcal{F}(p^\Lambda,\phi^\Lambda)=F_{\text{top}}+\overline{F}_{\text{top}}, \tag{1.4}$$

with $\Omega(p^\Lambda,q_\Lambda)$ proposed as (index) degeneracy of the black hole states and ϕ^Λ being the electric potential corresponding to q_Λ.[1] This proposal has been successfully tested in Refs. 18 and 21 from different points of view and further developed in Ref. 17. Remarkably, using the OSV conjecture, Dabholker[21] was able for the first time to derive, from the macroscopic side, the exact coefficient of the leading term in the asymptotic expansion of the degeneracy of states for the small black hole of type IIA on $K_3\times T^2$, dual to Heterotic on T^6, where both the prepotential and the microscopic degeneracy counting are known exactly. For a review lecture on Refs. 9, 17, and 18, see Ref. 22. For a recent and extensive review see Ref. 23. There are, however, examples in Refs. 24 and 25 where a naive application of this conjecture sounds problematic. For example, Ref. 24 mainly focuses on $\mathcal{N}=4$ models where in some cases the string coupling is strong. Before concentrating on the concern of this paper, it is worth pointing out that before any attempt is made to apply the proposal, one may note that the OSV conjecture, in the form of Refs. 9 and 17 in its strong version, is a statement about the full free energy of the topological string theory, including all the perturbative quantum corrections as well as the nonperturbative contributions. Therefore, regarding the fact that the nonperturbative completion of the topological free energy is not as yet known, what the OSV conjecture provides is a nonperturbative definition of the topological strings, parallel to the program of topological M-theory as proposed in Refs. 26 and 27.

A distinguished ambiguity in (1.3) originates from the electric-magnetic duality considerations, that is, the requirement of the invariance of $\Omega(p^I,q_I)$ under the (relevant subgroup) of the

[1]For a nonperturbative completion of the original conjecture see Ref. 17; also there are suggestions concerning the holomorphic anomaly in Refs. 18–20.

symplectic transformations. Actually if one works in the complex polarization, as concrete examples in Refs. 24, 25, and 28 show us using the relevant terms of the topological free energy, the inverse Laplace transformation corresponding to (1.3)[2],

$$\Omega(p^\Lambda,q^\Lambda) \doteq \int [d\phi^\Lambda] e^{\mathcal{F}+\pi q_\Lambda \phi^\Lambda} \equiv \int [d\phi^\Lambda] e^G, \tag{1.5}$$

does generically lead to the results that are duality violating by some unwanted prefactors (for a highlighted example, see the next section). As we will argue later, this property is not restricted to a specific subset of prepotentials but it is a general fact about (1.5), if working in the complex polarization. Understanding and handling this fact has been a matter of some investigations. For example, for an attempt within an independent and, by construction, duality-invariant formulation see Ref. 29, where the proposed modification works for the dyonic black holes relatively well but it is not applicable to the case of $\frac{1}{2}$BPS states for which the proposed measure vanishes (for details and recent improvements see Ref. 30). Alternatively Refs. 31–33 propose a black hole ensemble that sums over a single duality-invariant charge, and so by construction respects the expected symmetries. The application of this approach, where the nonholomorphic corrections to the free energy should necessarily be considered, is so far limited to $\frac{1}{2}$BPS black holes. So there is not yet any overlap between these two approaches. Another idea to improve the duality violations, being closer to the OSV proposal, is assuming that the OSV free energy intrinsically lives in a curved space; accordingly (1.5) is redefined via a non-Euclidean measure,[20,25]

$$\overline{\Omega}(p^\Lambda,q_\Lambda) \doteq \int [d\phi^\Lambda] \sqrt{|g(p,\phi)|}\, e^{\mathcal{F}+\pi q_\Lambda \phi^\Lambda}. \tag{1.6}$$

This measure, which differs from case to case, is responsible for removing the mentioned prefactors.

A new claim in the literature, being argued generally although not yet materialized in concrete examples, is working in the real polarization instead of the complex polarization. This is so because the former polarization is expected to be protected against such duality violations (for details see Refs. 19 and 30, and especially Ref. 23).

In this paper we focus on this problem, that is, the duality aspects of the OSV conjecture, while in the whole work we will choose to keep working in the complex polarization, which is canonical, in contrast to the real polarization, which depends on the symplectic basis that one chooses.[23][3] We shall prove that the curvature of the space where the OSV free energy is defined, in the case of vanishing $D6$-brane charge, is asymptotically zero and as such, to all orders in the asymptotic expansion, no nontrivial measure is needed to be imposed. To show this we shall follow a direct approach: explicit construction of a proper flat ensemble, based on the OSV free energy, which is canonic in as many variables as the original OSV ensemble. In different examples, also within general arguments, we observe that the ensemble leads to the proper results for the black hole degeneracy of states. In fact, the construction works properly for all types of the known BPS black holes in CY_3 compactifications of type-IIA(B) theories and to all orders in the saddle-point asymptotic expansion of the inverse Laplace integral, as far as the duality violation is restricted to a prefactor. This is done via a simple change of variables, which, being linear in the electric potentials, preserves the Legendre transformation from the free energy to the entropy. The new variables have the advantage that the corresponding ensemble is potentially protected against the duality-violating prefactors. For the cases with a vanishing $D6$-brane charge, where the prepotential takes a simplified form and the construction is readable from the form of the prepotential, the new ensemble is purely canonical and restores the electric magnetic exactly. The idea still works quite well for the most general case, of course, up to nonholomorphic corrections, which are

[2]The sign $\doteq$ means "equality" up to an arbitrary constant, which is independent of the black hole charges.

[3]We understand that from now on the reader is aware of the frame of polarization in which we handle the problem.

missed also in the original OSV proposal. For the most general case, considering the leading term of the saddle-point approximation, we obtain a general constraint on the Jacobian from the new variables to the old ones. This constraint equation admits an infinite number of solutions; in principle, all the solutions are equally well, but practically we can pick up the simplest choices. In fact, the exact choice of these variables is not needed. The job they do is just removing the duality-violating prefactor of the corresponding OSV result, which could be done by hand from the first. In this sense it is an existence problem.

It is worth asking about higher orders of the saddle-point approximation for the most general case. The question is whether the duality violation appears just as a prefactor in higher orders. Indeed, for the black holes with a vanishing $D6$-brane charge the answer is positive to all orders of the asymptotic expansion, however, we will show that in case of nonvanishing $D6$-brane charge, the violation can become more complicated than a simple prefactor. This implies that, in higher orders, a simple measure factor is not sufficient to restore the duality generally and deeper modifications/investigations are necessary.

Finally as an alternative, motivated by manifest symplectic-invariant construction, we try a different ensemble that from the beginning treats both of the magnetic and electric charges at the same footing. This enlarged ensemble is related to the ensemble of Sec. IV via an effective integration over the magnetic potentials and asymptotically reproduces the same results for the black hole degeneracy of states.

The outline of the paper is as follows. In the next section, to clarify the main problem within a concrete example, we review one result from Refs. 24 and 25. In Sec. III we redefine the OSV ensemble for the large and small black holes in the absence of $D6$-brane, respectively, and show how it leads to proper results for the degeneracy of states. In Sec. IV we lift the idea for the most general case of BPS black holes in the context of CY_3 compactifications of type-IIA(B) string theories. In Sec. V we check out the procedure for higher orders in the saddle-point approximation and show that in some special cases the duality violation cannot be fixed by a single prefactor. In Sec. VI we introduce an effective that asymptotically reproduces the same results of Sec. IV. We end the paper with a conclusion.

II. ELECTRIC-MAGNETIC DUALITY IN THE OSV CONJECTURE

Let us start by addressing the duality invariance of the proposal of Ref. 9 in the complex polarization. To do that, we quickly repeat a result from Refs. 21, 24, and 25.[4] The prepotential of type-II string theory on a CY_3 is given by the free energy of the corresponding topological string theory as follows:

$$F_{\mathrm{II}} = -\frac{i\pi}{2} F_{\mathrm{top}}, \quad F_{\mathrm{top}} = F_{\mathrm{top}}^{\mathrm{pert.}} + F_{\mathrm{top}}^{\mathrm{GW}} + F_{\mathrm{top}}^{\text{non-pert. completion}}, \tag{2.1}$$

where

$$F^{\mathrm{pert.}} = \sum_h F_h W^{2h}, \tag{2.2}$$

with F_h being the genus-h amplitude of the topological theory and W^2 includes the graviphoton field strength. For the case of IIA on $K_3 \times T^2$, $F_{h>1}$ vanishes and the prepotential is given by

$$F(X^I, W^2) = -\frac{1}{2} C_{ab} \frac{X^a X^b X^1}{X^0} - \frac{W^2}{128\pi i} \log \Delta(e^{2\pi i \frac{X^1}{X^0}}), \tag{2.3}$$

where $C_{ab} \equiv C_{1ab}$ with $a, b = 2, \ldots, b_2$, $b_2 = 23$, and C_{ABC} being the intersection numbers of the CY_3. Δ stands for the Dedekind function. Taking $p^0 = 0$, the OSV free energy is given by

[4]This example is in the context of $\mathcal{N}=4$, but for $\mathcal{N}=2$, where the OSV conjecture is originally formulated, this is the case as well. For example, see the next section.

$$\mathcal{F}(p^\Lambda,\phi^\Lambda)=\frac{\pi}{2\phi^0}C_{ab}(p^1\phi^a\phi^b+p^a\phi^b\phi^1+p^b\phi^a\phi^1-p^ap^bp^1)-\log|\Delta(e^{2\pi\frac{p^1}{\phi^0}}e^{2\pi i\frac{\phi^1}{\phi^0}})|^2. \quad (2.4)$$

For the small black hole we set $p^a=0$,

$$\mathcal{F}(p^\mathrm{I},\phi^\mathrm{I})=\frac{1}{2}C_{ab}\frac{\phi^a\phi^bp^1}{\phi^0}-\log(|\Delta(e^{2\pi^2\frac{p^1}{\phi^0}}e^{2\pi i\frac{\phi^1}{\phi^0}})|^2). \quad (2.5)$$

Accordingly the inverse Laplace transformation, with the Euclidean measure, calculates the degeneracy of states as

$$\Omega(p^1,\vec{q})\doteq\int[d\phi^0d\phi^1d\phi^a]\,e^{\mathcal{F}+q_a\phi^a+q_0\phi^0+q_1\phi^1} \quad (2.6)$$

$$\doteq\int \mathrm{d}x\,\mathrm{d}\theta\left(\frac{-x^{12}(p^1)^2}{\sqrt{\det C}}\right)\times\frac{e^{\left(\frac{1}{2}C^{ab}q_aq_b-p^1q_0\right)x-p^1q_1x\theta}}{|\Delta(e^{-\frac{2\pi^2}{x}}e^{2\pi i\theta})|}, \quad (2.7)$$

where, in the second line, we have taken the integration over ϕ^a's and used the change of variables $x=-\phi^0/p^1$ and $\theta=\phi^1/\phi^0$ with $\mathrm{d}\phi^0\,\mathrm{d}\phi^1=(p^1)^2x\,\mathrm{d}x\,\mathrm{d}\theta$. For the two-charge case, we set $q_A=0$ for $A\neq0$. Defining the T-duality-invariant charge $N\equiv-p^1q_0$, integrating over ϕ^a gives

$$\Omega(p^1,q_0)\doteq\frac{-(p^1)^2}{\sqrt{\det C}}\int \mathrm{d}x\,x^{12}e^{Nx}\int\mathrm{d}\theta\frac{1}{|\Delta(e^{-\frac{2\pi^2}{x}}e^{2\pi i\theta})|}. \quad (2.8)$$

In this form, beside the prefactor $(p^1)^2$, everything is in a duality-invariant form. The presence of this p-dependent factor violates the duality invariance of the degeneracy of states.

In the large N limit, $|\Delta(q)|\approx|q|$, so that Ω approaches

$$\Omega(p^1,q_0)\doteq\frac{-(p^1)^2}{\sqrt{\det C}}\hat{I}_{13}(4\pi\sqrt{N}), \quad (2.9)$$

where[24]

$$\hat{I}_\nu(Q)\equiv\frac{(2\pi)^\nu}{i}\int \mathrm{d}t\,t^{-\nu-1}e^{t+\frac{Q^2}{4t}}. \quad (2.10)$$

Note that at the above limit, the genus 0 and 1 terms of prepotential read as

$$F_0(X^\Lambda)=-\frac{1}{2}C_{ab}\frac{X^1X^aX^b}{X^0}, \quad (2.11)$$

$$F_1(X^\Lambda)=-\frac{1}{64}\frac{X^1}{X^0}, \quad (2.12)$$

with the OSV free energy being

$$\mathcal{F}^{\mathrm{pert}}_{\mathrm{IIA}/K_3\times T^2}=\frac{C_{ab}}{2}\phi^a\phi^b\frac{p^1}{\phi^0}-4\,\pi^2\frac{p^1}{\phi^0}. \quad (2.13)$$

We mention that any attempt to remove the prefactor of (2.9), and similar prefactors, should be done in a way to keep the correct results for the entropy and degeneracy of states. In the following sections we redefine the black hole ensemble to do this job.

III. REDEFINITION OF THE OSV ENSEMBLE FOR A CLASS OF LARGE AND SMALL BLACK HOLES

In this section we consider black holes with vanishing $D6$-brane charge, where $p^0=0$ and the prepotential takes a simplified form. We start with the case of large black holes. The perturbative OSV free energy for a general CY_3 compactification in the large volume is given by

$$\mathcal{F}=-\frac{\pi}{6}\frac{\hat{C}(p)}{\phi^0}+\frac{\pi}{2}\frac{C_{AB}\phi^A\phi^B}{\phi^0}, \tag{3.1}$$

where

$$C_{AB}(p)=C_{ABC}p^C,\ \ C(p)=C_{ABC}p^Ap^Bp^C;\ \ \hat{C}(p)=C(p)+C_{2A}p^A, \tag{3.2}$$

and the indices $A,B,\ldots$ take the integers $1,\ldots,h$.

Let us change the variables of the free energy as follows:

$$\psi^0\equiv\frac{6}{\hat{C}(p)}\phi^0;\ \ \frac{C_{AB}(p)\phi^A\phi^B}{\phi^0}\equiv\frac{\psi^A\psi^A}{\psi^0}, \tag{3.3}$$

where $\psi^A=M^A{}_B(p)\phi^B$.[5]

The free energy is now redefined as a new function,

$$\mathcal{F}=\grave{\mathcal{F}}(\psi^0,\psi^A)=-\pi\frac{1}{\psi^0}+\frac{\pi}{2}\frac{\psi^A\psi^B}{\psi^0}. \tag{3.4}$$

Noting that

$$-\phi^0\frac{\partial\mathcal{F}}{\partial\phi^0}=-\psi^0\frac{\partial\grave{\mathcal{F}}}{\partial\psi^0};\ \ -\phi^A\frac{\partial\mathcal{F}}{\partial\phi^A}=-\psi^A\frac{\partial\grave{\mathcal{F}}}{\partial\psi^A}, \tag{3.5}$$

and defining

$$N\equiv\frac{1}{6}\hat{C}(p)q_0;\ \ N_A\equiv q_B(M^{-1})^B{}_A, \tag{3.6}$$

the Legendre transformation reads as

$$S(N,N_A)=\grave{\mathcal{F}}-\pi\psi^0\frac{\partial\grave{\mathcal{F}}}{\partial\psi^0}-\pi\psi^A\frac{\partial\grave{\mathcal{F}}}{\partial\psi^A}, \tag{3.7}$$

$$N=-\frac{\partial\grave{\mathcal{F}}}{\partial\psi^0};\ \ N_A=-\frac{\partial\grave{\mathcal{F}}}{\partial\psi^A}. \tag{3.8}$$

Motivated by the above observation we introduce the correct black hole ensemble to use as

$$Z\equiv e^{\grave{\mathcal{F}}(\psi^0,\psi^A)}=\sum_N\sum_{N_A}\tilde{\Omega}(N,N_A)\ e^{-\pi\psi^0N-\pi\psi^AN_A}. \tag{3.9}$$

Note that the ensemble defined above, unlike the OSV ensemble, is purely canonical. Now the black hole degeneracy of states is proposed to be

[5] $M^A{}_B(p)$ is a transformation matrix which first diagonalizes $C_{AB}(p)$, then rescales the variables appropriately.

$$d(p,q) \doteq \tilde{\Omega}(N,N_A). \tag{3.10}$$

Let us now consider (3.1) and calculate the corresponding degeneracy of states in the light of the definition (3.9):

$$\tilde{\Omega}(N,N_A) \doteq \int \mathrm{d}\psi^0\, \mathrm{d}\psi^A\, e^{\grave{\mathcal{F}}(\psi^0,\psi^A)+\pi N\psi^0+\pi N_A\psi^A}. \tag{3.11}$$

The integral over the variables ψ^A's is Gaussian and yields

$$\tilde{\Omega}(N,N_A) \doteq \hat{N}^{-\frac{h}{2}-1} \int \mathrm{d}\mu\, \mu^{\frac{h}{2}} e^{\mu-\pi^2\frac{\hat{N}}{\mu}}, \tag{3.12}$$

where

$$\hat{N} \equiv N - \frac{1}{2}N_A N_A. \tag{3.13}$$

A simple algebra shows that

$$\hat{N} = \frac{1}{6}\hat{C}(p)\hat{q}_0;\quad \hat{q}_0 \equiv q_0 - \frac{1}{2}C^{AB}q_A q_B, \tag{3.14}$$

where C^{AB} denotes the inverse of C_{AB}. Thus the degeneracy of the large black hole states as calculated via the ensemble (3.9) is given by

$$d(p,q) \doteq \hat{I}_{\frac{h}{2}+1}(S);\quad S = 2\pi\sqrt{\frac{1}{6}\hat{C}(p)\hat{q}_0}. \tag{3.15}$$

This is indeed the correct result. In contrast, the result by the standard OSV ensemble receives a duality-noninvariant prefactor of the form $|\det C_{AB}(p)|^{-\frac{1}{2}}\left(\frac{\hat{C}(p)}{6}\right)^{\frac{h}{2}+1}$.[24,25]

Now we come to the case of small black holes following the same idea: rewriting the OSV free energy and the macroscopic entropy in terms of new variables and new charges, respectively, leads to a new ensemble for the black holes that by construction is purely canonical. For the interesting case of $K3$ fibrations with Heterotic duals, of which the most well-known example is $\frac{\text{IIA}}{K_3\times T^2} \equiv \frac{\text{Het.}}{T^6}$, the OSV free energy is (2.5). Defining

$$\alpha \equiv -\frac{\phi^0}{p^1};\quad \beta \equiv \frac{\phi^1}{p^1} \tag{3.16}$$

and

$$N \equiv -p^1 q_0;\quad N' \equiv -p^1 q_1, \tag{3.17}$$

we obtain

$$\grave{\mathcal{F}}(\alpha,\beta,\phi^a) = -\frac{C_{ab}\phi^a\phi^b}{2\alpha} - 2\log|\Delta(e^{\frac{2\pi^2}{\alpha}}e^{\frac{-2\pi i\beta}{\alpha}})|, \tag{3.18}$$

where

$$S(N,N',q^a) = \grave{\mathcal{F}} - \pi\alpha\frac{\partial\grave{\mathcal{F}}}{\partial\alpha} - \pi\beta\frac{\partial\grave{\mathcal{F}}}{\partial\beta} - \pi\phi^a\frac{\partial\grave{\mathcal{F}}}{\partial\phi^a} \tag{3.19}$$

and

$$N = -\frac{\partial \grave{\mathcal{F}}}{\partial \alpha};\quad N' = -\frac{\partial \grave{\mathcal{F}}}{\partial \beta};\quad q_a = -\frac{\partial \grave{\mathcal{F}}}{\partial \phi^a}. \tag{3.20}$$

Subsequently we define

$$\grave{Z} \equiv e^{\grave{\mathcal{F}}(\alpha,\beta,\phi^a)} = \sum_N \sum_{N'} \sum_{q_a} \grave{\Omega}(N,N',q_a)\, e^{-\pi\alpha N - \pi\beta N' - \pi\phi^a q_a} \tag{3.21}$$

as the correct black hole ensemble.

The corresponding degeneracy of states is given by

$$\grave{\Omega}(N,N',q_a) \doteq \int \mathrm{d}\alpha\, \mathrm{d}\beta\, \mathrm{d}\phi^a \frac{e^{-\frac{C_{ab}\phi^a\phi^b}{2\alpha} + \pi N\alpha + \pi N'\beta + \pi q_a \phi^a}}{|\Delta(e^{\frac{2\pi^2}{a}} e^{\frac{-2\pi i\beta}{\alpha}})|^2}. \tag{3.22}$$

Doing the Gaussian integration and changing the variables of the remaining integrals from (α,β) to $\left(\alpha, \theta \equiv -\frac{\beta}{\alpha}\right)$, we obtain

$$\grave{\Omega}(N,N',q_a) \doteq \int \mathrm{d}\alpha\, \alpha^{12}\, e^{\pi\alpha\hat{N}} \int \mathrm{d}\theta \frac{e^{-\pi N'\theta\alpha}}{|\Delta(e^{\frac{2\pi^2}{\alpha}} e^{2\pi i\theta})|^2}, \tag{3.23}$$

where

$$\hat{N} \equiv N + \frac{1}{2} q_a C^{ab} q_b = \frac{1}{2} Q_e^2. \tag{3.24}$$

For the two-charge case where $\hat{N}=N$ and $N'=0$, taking the large-volume limit, for which $|\Delta(x)| \approx |x|$, simplifies (3.24) as

$$\tilde{\Omega}(N) \doteq \int \mathrm{d}\alpha\, \alpha^{12}\, e^{\pi\alpha\hat{N} + \frac{4\pi}{\alpha}} = \hat{I}_{13}(4\pi\sqrt{\hat{N}}), \tag{3.25}$$

which is the well-known result for the degeneracy of states, as known from its duality with Heterotic string theory by direct counting of the DH fundamental stringy states.[21]

IV. BLACK HOLES WITH NONVANISHING *D*6-brane CHARGE: SADDLE-POINT EVALUATION

In this section we are concerned with the most general case, $p^0 \neq 0$, and as the central idea follow what we did before. We introduce a generalized OSV ensemble as

$$\grave{Z} \equiv e^{\grave{\mathcal{F}}(p^\Lambda,\psi^\Lambda)} = \sum_{\grave{q}_\Lambda} \grave{\Omega}(p^\Lambda,\grave{q}_\Lambda)\, e^{-\pi \grave{q}_\Lambda \psi^\Lambda}, \tag{4.1}$$

$$\grave{\mathcal{F}}(p^\Lambda,\psi^\Lambda) = \mathcal{F}(p^\Lambda,\phi^\Lambda), \tag{4.2}$$

where the new variables ψ^Λ, which preserve the entropy-defining Legendre transformation,

$$S(p^\Lambda,\grave{q}_\Lambda) = \grave{\mathcal{F}} + \pi \grave{q}_\Lambda \psi^\Lambda, \tag{4.3}$$

are defined from the electric potentials via the linear relations[6]r

[6]The sign * over or below a quantity stands for the saddle-point value of that quantity.

$$\psi^{\Lambda} = U^{\Lambda}{}_{\Gamma}(p^{\Sigma}, \phi_{*}^{\Sigma})\phi^{\Gamma} = V^{\Lambda}{}_{\Gamma}(p^{\Sigma}, q_{\Sigma})\phi^{\Gamma}. \tag{4.4}$$

The fact that, unlike the previous cases, here we let the matrix U depend on ϕ_{*}^{Λ} as well as p^{Λ}, is rooted in the observation that for the cases with a nonvanishing $D6$-brane charge, the OSV prefactors are functions of both the magnetic and electric charges.[25,28]

We now require that the corresponding inverse Laplace integration, as defined via the Euclidean measure,

$$\grave{\Omega}(p^{\Lambda}, \grave{q}_{\Lambda}) \doteq \int [\mathrm{d}\psi^{\Lambda}]\, e^{\grave{\mathcal{F}} + \pi \grave{q}_{\Lambda}\psi^{\Lambda}}, \tag{4.5}$$

be duality invariant, exactly or at least at the saddle-point approximation. Subsequently the black hole degeneracy of states is recognized as

$$d(p^{\Lambda}, q_{\Lambda}) \doteq \grave{\Omega}(p^{\Lambda}, \grave{q}_{\Lambda}), \tag{4.6}$$

where, as implied by (4.4),

$$\grave{q}_{\Lambda} = q_{\Gamma}(V^{-1})^{\Gamma}{}_{\Lambda}. \tag{4.7}$$

From (4.2) and (4.4), the relation between the ensemble (4.1) and (1.3) reads from[7]

$$\grave{\Omega} \doteq \int [\mathrm{d}\phi^{\Lambda}] J(\psi \to \phi)\, e^{\mathcal{F} + \pi q_{\Lambda}\phi^{\Lambda}} = \det[V] \int [\mathrm{d}\phi^{\Lambda}]\, e^{\mathcal{F} + \pi q_{\Lambda}\phi^{\Lambda}} = \det[V]\Omega. \tag{4.8}$$

Obviously a proper choice of the Jacobian matrix V can remove any unwanted prefactor as obtained by the evaluation of (1.5). So we consider the cases where the result by (1.5) is duality violating only by a (single) prefactor besides the proper result[8] Then, for the duality invariance in the saddle-point asymptotic expansion of (4.8),a constraint equation on $U^{\Lambda}{}_{\Gamma}$ is formed as a necessary and sufficient condition. The exact form of this constraint may depend on the order of the saddle-point approximation. Here we write it for the first order. The saddle-point evaluation of (4.8) results at

$$\grave{\Omega}^{*} = \det(V)\Omega^{*}. \tag{4.9}$$

Thus at the first order,

$$\grave{\Omega}^{*} \doteq \det\big[V\big]\, \det[H_{*}]^{-\frac{1}{2}}\, e^{S}, \tag{4.10}$$

$$H_{\Lambda\Gamma} \equiv \frac{\partial^{2}\mathcal{F}}{\partial\phi^{\Lambda}\,\partial\,\phi^{\Gamma}}. \tag{4.11}$$

Remembering that what we want to do is just to get rid of the unwanted prefactor appearing in Ω and to get a proper result, we define

$$\det[H_{*}] \equiv S^{m}\, \det[H'_{*}], \tag{4.12}$$

where m denotes a convenient power of the entropy that is factorized out from the Hessian, so that $\det[H'_{*}]$ is the pure duality-violating prefactor. To remove this prefactor by the matrix V, we arrive at the constraint

[7]Since the matrices U and V differ from each other just by a change of variable $q \leftrightarrow \phi_{*}$, hereafter both of them are denoted as V.

[8]Whether this is a general property of the OSV results is a question that we address in the next section.

$$\det[V^2] \doteq \det[H'_*]. \tag{4.13}$$

Equation (4.13) admits an infinite number of solutions, any solution of which is, in principle, as good as other ones. One choice is taking $V=v\,1$, where

$$v \doteq (\det[H'_*])^{\frac{1}{2h+2}}. \tag{4.14}$$

As a different choice for V we can take a diagonal matrix with elements v_Λ such that

$$v_\Lambda \doteq \sqrt{h'_\Lambda}, \tag{4.15}$$

where

$$\prod_\Lambda h'_\Lambda = \det[H'_*]. \tag{4.16}$$

Equivalently, we can solve the constraint (4.13) by defining the new ensemble to be

$$\hat{X}^0 \equiv \det[V]\, X^0; \quad \hat{X}^A \equiv X^A. \tag{4.17}$$

This solution might be of particular physical interest since X^0 controls the coupling of topological strings via the relation

$$g = \frac{4\pi i}{X^0}. \tag{4.18}$$

In conclusion, we shall briefly speculate on a possible physical interpretation of the ensemble (4.17).

As a specific example in the sector $p^0 \neq 0$, let us consider the case of a large black hole in type IIA on a $K3$ fibered CY_3, for which $C_{abc}=C_{2A}=0$, $a,b\in 2,\ldots,h$, as discussed in Refs. 25 and 28. The prepotential is

$$\mathcal{F} = \frac{1}{2}[\Im(t^1)C_{ab}(p^a p^b - \phi^a \phi^b) + 2\Re(t^1)p^a q_a], \tag{4.19}$$

with $t^A = \frac{X^A}{X^0}$ being flat coordinates for the Kähler moduli. The Hessian determinant of (4.19) at the attractor point is evaluated as

$$\det[H_*] \doteq B^2 (C_{ab}p^a p^b - 2p^0 q_1)^{\frac{h}{2}-1} S^{-\frac{h}{2}-2} \equiv S^{-\frac{h}{2}-2} \det[H'_*], \tag{4.20}$$

where

$$B = \sqrt{(C_{ab}p^a p^b - 2p^0 q_1)[(p^1)^2 C_{ab}p^a p^b + (p^0)^2 C^{ab} q_a q_b - 2p^0 p^1 p^a q_a]}; \quad C^{an}C_{nb} = \delta^a_b. \tag{4.21}$$

Regarding (4.13), the new variables are defined via the constraint

$$\det[V] \doteq B(C_{ab}p^a p^b - 2p^0 q_1)^{\frac{h-2}{4}}, \tag{4.22}$$

from which, in case of interest, one can exactly specify a new set of variables.

Finally we want to show how in a simple way the variables of (3.4) can be deduced from (4.15). The attractor point of the prepotential (3.1) is

$$(\phi^0_*)^2 = -\frac{1}{6}\frac{\hat{C}(p)}{\hat{q}_0}; \quad \phi^A_* = -C^{AB}(p)\, q_B\, \phi^0_*, \tag{4.23}$$

so that

$$\det[H_*]; \doteq \det[C_{AB}(p)]\frac{\hat{C}(p)}{\phi_*^0} \Rightarrow \det[H'_*] \doteq \det\left[\frac{C_{AB}(p)}{\hat{C}(p)}\right]\hat{C}^{-2}(p), \tag{4.24}$$

and then from (4.15) we obtain

$$v^0 \doteq \frac{1}{\hat{C}(p)}; \; v^A \doteq \left[\frac{\omega_A(p)}{\hat{C}(p)}\right]^{\frac{1}{2}}, \tag{4.25}$$

with $\omega_A(p)$ being the eigenvalues of $C_{AB}(p)$. Thus for the ψ variables we obtain

$$\psi^0 \doteq \frac{\phi^0}{\hat{C}(p)}; \; \frac{C_{AB}(p)\phi^A\phi^B}{\phi^0} = \frac{\omega_A(p)\hat{\phi}^A\hat{\phi}^A}{\phi^0} \doteq \frac{\psi^A\psi^A}{\psi^0}, \tag{4.26}$$

where $\hat{\phi}^A$ form a diagonal basis for $C_{AB}(p)$. The result (4.26) is in accordance with (3.3).

V. BEYOND THE SADDLE POINT WITH *D*6-branes?

The electric-magnetic duality is restored by the ensemble (4.1) as long as the result by (1.5) admits the general form

$$\Omega(p,q) \doteq N(p,q)f(S). \tag{5.1}$$

We naturally ask if a violation of the duality in the results of (1.5) is restricted only to a prefactor, $N(p,q)$. Of course for a vanishing $D6$-brane charge, this is always true, at least for the large CY_3-volume limit. In these cases the prepotential is quadratic with respect to ϕ^A, so the exact evaluation of (1.5) results in the form (5.1) with $f(S)$ being a modified Bessel function. Now we come to the cases for which $p^0 \neq 0$. The prepotential, at the genus zero and one terms, is of the general form

$$\mathcal{F} = \frac{p^0}{(\phi^0)^2 + (p^0)^2}[E(\phi) - 3E_{AB}(\phi)p^Ap^B - E_{2A}\phi^A] + \frac{\phi^0}{(\phi^0)^2 + (p^0)^2}[E(p) - 3E_{AB}(p)\phi^A\phi^B + E_{2A}p^A], \tag{5.2}$$

where

$$E(z) \equiv E_{ABC}\, z^A z^B z^c; \; E_{AB}(z) \equiv E_{ABC}\, z^c,$$

with

$$E_{ABC} \equiv -\frac{\pi}{6}C_{ABC}; \; E_{2A} \equiv -\frac{\pi}{6}C_{2A}.$$

To address the above-mentioned question for the case of nonvanishing p^0, we evaluate the OSV result for the black hole degeneracy of states in concrete examples by incorporating all the terms that appear in the saddle-point asymptotic expansion of the integral (1.5),

$$G = S + \sum_{n=2}^{\infty}\frac{1}{n!}H^*_{\Lambda_1\ldots\Lambda_n}\,\eta^{\Lambda_1}\ldots\eta^{\Lambda_n},$$

$$H_{\Lambda_1\ldots\Lambda_n} \equiv \frac{\partial^n\mathcal{F}}{\partial\phi^{\Lambda_1}\ldots\partial\phi^{\Lambda_n}},$$

$$\eta^{\Lambda} \equiv \phi^{\Lambda} - \phi^{\Lambda}_{*}, \tag{5.3}$$

for the two extreme limits $p^0 \to \infty$ and $p^0 \to 0$.

A. An example in the large-p^0 limit

The prepotential (5.2) is expanded over $\frac{\phi^0}{p^0}$ as

$$\mathcal{F} = \frac{1}{p^0}\left\{ [E(\phi) - 3E_{AB}(\phi)p^A p^B - E_{2A}\phi^A] + \frac{\phi^0}{p^0}[E(p) - 3E_{AB}(p)\phi^A\phi^B + E_{2A}p^A] + O\left(\frac{\phi^0}{p^0}\right)^2 \right\}.$$

We require that the contribution to (1.5) from the regions of integration far away from the attractor point is not major, and so ignoring terms of higher orders in the above expansion is satisfactory if $O\left(\left|\frac{\phi^0_*}{p^0}\right|\right) \ll 1$. As we will see, this would be the case for $\left|\frac{E(p)}{p^0}\right| \gg 1$. For the limit under consideration, the prepotential is linear with respect to ϕ^0, so (5.3) is easily evaluated as

$$G(\eta) = S - \frac{6}{(p^0)^2}E_{AB}(p)p^B\eta^0\eta^A + \frac{3}{p^0}\left[E_{AB}(\phi_*) - \frac{\phi^0_*}{p^0}E_{AB}(p) - \frac{\eta^0}{p^0}E_{AB}(p) \right]\eta^A\eta^B + \frac{1}{p^0}E_{ABC}\eta^A\eta^B\eta^C$$

$$\equiv S + g_A\eta^A + \frac{1}{2}g_{AB}\eta^A\eta^B + g_{ABC}\eta^A\eta^B\eta^C.$$

Accordingly (1.5) leads to

$$\Omega \doteq e^S \int \mathrm{d}\eta^0 \int [\mathrm{d}\eta^A] e^{g_A\eta^A + \frac{1}{2}g_{AB}\eta^A\eta^B + g_{ABC}\eta^A\eta^B\eta^C} = e^S \int \mathrm{d}\eta^0 \int [\mathrm{d}\eta^A] e^{g_A x^A + \frac{1}{2}g_{AB}\eta^A\eta^B} \left[1 + g_{ABC}\eta^A\eta^B\eta^C + O\left(\frac{1}{(p^0)^2}\right) \right].$$

Now, as a specific example of the case under consideration, we consider a charge configuration for which

$$\phi^A_* = p^A; \quad \phi^0_* = 0,$$

which is in line with the attractor equations for

$$q_A = \frac{1}{p^0}E_{2A},$$

$$q_0 = \frac{1}{(p^0)^2}[2E(p) - E_{2A}p^A],$$

with the entropy obtained as

$$S = -2\frac{E(p)}{p^0}.$$

Given this ansatz, (1.5) is given by

$$\Omega \doteq e^S \int \mathrm{d}\eta^0 [\mathrm{d}\eta^A] \exp\left\{ \frac{1}{2}\left[\frac{6}{p^0}\left(1 - \frac{\eta^0}{p^0}\right)E_{AB}(p) \right]\eta^A\eta^B - \left[\frac{6}{p^0}\frac{\eta^0}{p^0}E_{AB}(p)p^B \right]\eta^A \right\} \left[1 + \frac{1}{p^0}E(\eta) \right]$$

$$\equiv \Omega_0 + \Omega_1,$$

where $\doteq$ differs from $\doteq$ by higher order corrections. A simple algebra leads to the result

$$\Omega_1 \doteq \frac{(p^0)^{\frac{h}{2}+1}}{\sqrt{\det[E_{AB}]}} e^{-2S} I_{\frac{h}{2}-1}(3S),$$

$$\Omega_2 \doteq \frac{(p^0)^{\frac{h}{2}+1}}{\sqrt{\det[E_{AB}]}} e^{-2S} \int \mathrm{d}t\, t^{-\frac{h}{2}} \left[\left(1+\frac{1}{t}\right)^3 \frac{S}{2} - \frac{h}{2}\frac{1-t}{t^2} \right] e^{\frac{3}{2}\left(t+\frac{1}{t}\right)S},$$

so in this example Ω is of the form (5.1).

B. The infinitesimal p^0 limit

Here considering black holes with infinitesimal $D6$-brane charge, $|p^0| \ll 1$, we evaluate the OSV degeneracy of states up to $O(|p^0|^2)$. To do that, we do not restrict ourselves to any finite order of the saddle-point approximation and sum over all the terms of the series (5.3). However, we still assume that the integral (1.5) is essentially localized around the saddle point of the integrand, so that in the power expansion of the prepotential (5.2) over $\frac{p^0}{\phi^0}$, we can ignore the terms $O\left(\frac{p^0}{\phi^0}\right)^2$ as far as $\kappa \equiv \frac{p^0}{\phi^0_*} \ll 1$. As the attractor-point equations will show us below, this assumption is consistent with the infinitesimal-p^0 limit.

The prepotential (5.2), up to $O\left(\frac{p^0}{\phi^0}\right)^2$, reads as

$$\mathcal{F} = \frac{1}{\phi^0}\left\{ \frac{p^0}{\phi^0}[E(\phi) - 3E_{AB}(\phi)p^A p^B - E_{2A}\phi^A] + [E(p) - 3E_{AB}(p)\phi^A\phi^B + E_{2A}p^A] \right\} \equiv p^0 \frac{K}{(\phi^0)^2} + \frac{L}{\phi^0}. \tag{5.4}$$

Regarding that the prepotential is a polynomial of degree three with respect to ϕ^A's, we can explicitly evaluate the sum (5.3). Using

$$H^*_{(n)} = (-1)^n \left[(n+1)!\ p^0 \frac{K^*}{(\phi^0_*)^{n+2}} + n!\ \frac{L^*}{(\phi^0_*)^{n+1}} \right],$$

$$H^*_{A(n)} = (-1)^n \left[(n+1)!\ p^0 \frac{K^*_A}{(\phi^0_*)^{n+2}} + n!\ \frac{L^*_A}{(\phi^0_*)^{n+1}} \right],$$

$$H^*_{AB(n)} = (-1)^n \left[(n+1)!\ p^0 \frac{K^*_{AB}}{(\phi^0_*)^{n+2}} + n!\ \frac{L^*_{AB}}{(\phi^0_*)^{n+1}} \right],$$

$$H^*_{ABC(n)} = (-1)^n \left[(n+1)!\ p^0 \frac{K^*_{ABC}}{(\phi^0_*)^{n+2}} + n!\ \frac{L^*_{ABC}}{(\phi^0_*)^{n+1}} \right],$$

where

$$\{K,L\}_{\{A_1 \ldots A_m\}} \equiv \frac{\partial\{K,L\}}{\partial\{A_1 \ldots A_m\}}$$

and the index (n) denotes the number of derivatives with respect to ϕ^0. Accordingly $G(\eta)$ is evaluated as

$$G(\eta) = S + (\eta^0)^2 \left[\sum_0^\infty \frac{(\eta^0)^n}{(n+2)!} H^*_{(n+2)} \right] + \eta^0 \eta^A \left[\sum_0^\infty \frac{(\eta^0)^n}{(n+1)!} H^*_{A(n+1)} \right] + \frac{1}{2}\eta^A \eta^B \left[\sum_0^\infty \frac{(\eta^0)^n}{n!} H^*_{AB(n)} \right]$$
$$+ \frac{1}{6}\eta^A \eta^B \eta^C \left[\sum_0^\infty \frac{(\eta^0)^n}{n!} H^*_{ABC(n)} \right]$$

$$=S+\frac{(\eta^0)^2}{(\phi_*^0)^2}\left[\frac{p^0K^*}{(\phi_*^0)^2}R_3\left(\frac{\eta^0}{\phi_*^0}\right)+\frac{L^*}{\phi_*^0}R\left(\frac{\eta^0}{\phi_*^0}\right)\right]-\frac{\eta^0\eta^A}{(\phi_*^0)^2}\left[\frac{p^0K_A^*}{\phi_*^0}R_2\left(\frac{\eta^0}{\phi_*^0}\right)+L_A^*R\left(\frac{\eta^0}{\phi_*^0}\right)\right]$$
$$+\frac{1}{2}\frac{\eta^A\eta^B}{(\phi_*^0)^2}\left[p^0K_{AB}^*\,R_1\left(\frac{\eta^0}{\phi_*^0}\right)+\phi_*^0L_{AB}^*\,R\left(\frac{\eta^0}{\phi_*^0}\right)\right]+\frac{1}{6}\frac{\eta^A\eta^B\eta^C}{(\phi_*^0)^3}p^0\phi_*^0K_{ABC}^*\,R_1\left(\frac{\eta^0}{\phi_*^0}\right),$$

where

$$R(z)\equiv\sum_0^\infty(-1)^nz^n=\frac{1}{1+z};\;\; R_m(z)\equiv\sum_0^\infty(-1)^n(n+m)z^n=\frac{(m-1)\,z+m}{(1+z)^2}.$$

Defining

$$x\equiv\frac{\eta^0}{\phi_*^0},\;\; x^A\equiv\frac{\eta^A}{\phi_*^0},$$

together with

$$g_{ABC}\equiv\kappa\frac{(\phi_*^0)^2}{(1+x)^2}E_{ABC},$$

$$g_{AB}\equiv\frac{6\phi_*^0}{(1+x)^2}[\kappa\,E_{AB}(\phi_*)-(1+x)E_{AB}(p)],$$

$$g_A\equiv-\frac{3\,x}{(1+x)^2}\left[\kappa(x+2)\{E_{AB}(\phi_*)\phi_*^B-E_{AB}(p)p^B\}-2(1+x)E_{AB}(p)\phi_*^B-\kappa\frac{x+2}{3}E_{2A}\right],$$

$$g\equiv\frac{x^2}{(1+x)^2}\frac{1}{\phi_*^0}[\{\,E(p)(1+x)+\kappa\,E(\phi_*)(3+2\,x)\}-3\{(1+x)E_{AB}(p)\phi_*^A\phi_*^B$$
$$+\kappa(3+2\,x)E_{AB}(\phi_*)p^Ap^B\}+\{(1+x)E_{2A}p^A-\kappa(3+2\,x)E_{2A}\phi_*^A\}],$$

we obtain

$$G(\eta)=S+g+g_A\,x^A+\frac{1}{2}g_{AB}\,x^Ax^B+g_{ABC}\,x^Ax^Bx^C.$$

Subsequently, (1.5) is given by

$$\Omega\doteq e^S(\phi_*^0)^{h+1}\int\mathrm{d}x\,e^g\int[\mathrm{d}x^A]\,e^{g_Ax^A+\frac{1}{2}g_{AB}x^Ax^B+g_{ABC}x^Ax^Bx^C}$$

$$=e^S(\phi_*^0)^{h+1}\int\mathrm{d}x\,e^g\int[\mathrm{d}x^A]e^{g_Ax^A+\frac{1}{2}g_{AB}x^Ax^B}$$
$$\times[1+g_{ABC}x^Ax^Bx^C+O(\kappa^2)]$$

$$\doteq e^S(\phi_*^0)^{h+1}\int\mathrm{d}x\frac{1}{\sqrt{\det[g_{AB}]}}e^g\left(1+g_{ABC}\frac{\partial^3}{\partial g_C\,\partial g_B\,\partial g_A}\right)$$
$$\times e^{-\frac{1}{2}g_Ag^{AB}g_B}$$

$$\ddot{=} e^S (\phi_*^0)^{h+1} \int \mathrm{d}x \frac{1}{\sqrt{\det[g_{AB}]}} e^{T_1}(1 + T_2 + T_3),$$

where

$$T_1 = g - \frac{1}{2} g_A g^{AB} g_B,$$

$$T_2 = 3 g_{ABC} g^{AB} g^{CV} g_V,$$

$$T_3 = - g_{ABC} g^{AM} g^{BN} g^{CV} g_M g_N g_V,$$

and the sign "$\ddot{=}$" meaning "$\doteq$" up to $O(\kappa^2)$. Now to proceed further and check whether the above result is of the form (5.1), we need to know some concrete information about how g^{AB} and S depend on E_{ABC}, E_{2A}, and the black hole charges. In that respect, a helpful choice for us is to set

$$\phi_*^A = p^A$$

according to which the attractor equations are equivalent to

$$q_A = \frac{6}{\phi_*^0} p_A + \frac{p^0}{(\phi_*^0)^2} E_{2A},$$

$$q_0 = - \frac{1}{(\phi_*^0)^2} [2(1 + 2\kappa) E(p) - (1 - 2\kappa) E_{2A} p^A],$$

and the entropy reads as

$$S = \frac{2}{\phi_*^0} [(1 - 3\kappa) E(p) + (1 - \kappa) E_{2A} p^A]. \tag{5.5}$$

Now $\{g, g_A, g_{AB}, T_1, T_2, T_3\}$ is given by

$$g_{AB} = - 6 \ \phi_*^0 \frac{1 + x - \kappa}{(1 + x)^2} E_{AB},$$

$$g = \frac{x^2}{(1 + x)^2} \frac{1}{\phi_*^0} [- 2 \ E(p) \{1 + x + 3\kappa + 2\kappa x\} + E_{2A} p^A \{1 + x - 3\kappa - 2\kappa x\}],$$

$$T_1 \ddot{=} \frac{x^2}{1 + x} \left[\left\{ 1 - \kappa \frac{3 + 4x}{1 + x} \right\} + (1 - \kappa) E_{2A} p^A \right] \frac{1}{\phi_0^*}, \tag{5.6}$$

$$T_2 \ddot{=} \kappa \frac{x}{1 + x} \frac{h}{2},$$

$$T_3 \ddot{=} \kappa \frac{x^3}{(1 + x)^2} \frac{E(p)}{\phi_*^0}.$$

Thus the final expression for Ω is obtained as

$$\Omega \ddot{=} e^S (\phi_*^0)^{\frac{h}{2}+1} \frac{1}{\sqrt{\det[E_{AB}]}} \int \mathrm{d}x (1 + x)^{\frac{h}{2}} \ e^{T_1} \left[1 + \kappa \frac{h}{2(1 + x)} + T_2 + T_3 \right]$$

$$\ddot{=} e^{S}(\phi_*^0)^{\frac{h}{2}+1}\frac{1}{\sqrt{\det[E_{AB}]}}\int \mathrm{d}x(1+x)^{\frac{h}{2}}\, e^{T_1}\left[1+\kappa\left\{\frac{h}{2}+\frac{x^2}{(1+x)^2}\frac{E(p)}{\phi_0^*}\right\}\right]. \tag{5.7}$$

Now from (5.5) and (5.6) it is obvious that (5.7) does not admit the form (5.1). Indeed, if it were the case, it would be so for any h, implying that

$$\int \mathrm{d}x(1+x)^{\frac{h}{2}}\, e^{T_1}$$

itself is of the form (5.1), which is not the case![9]

As we learn from the above examples, for black holes with nonvanishing p^0 there is no guarantee that the result of (1.5) be of the form (5.1), if one incorporates the subleading terms of the saddle-point asymptotic expansion. As a consequence, even a generalization of type (1.6) or (4.8) does not restore the electric-magnetic duality. That is so because if the corresponding metric/Jacobian determinant does not change the saddle point of the integrand in (1.5), then it cannot remove more than one noninvariant factor from the OSV result, and if it changes the saddle point of the integrand, then the leading term of the asymptotic expansion does not match microcanonically with the Bekenstein-Hawking-Wald entropy. It seems that this observation opens the possibility of deeper modifications.

VI. AN EFFECTIVE APPROACH

The ensemble defined through (4.1) and (4.4) is canonic in as many variables as the OSV ensemble, that is, by construction the set of electric potentials is mapped one to one to the set of new variables ψ^Λ. However, since the multiplet (CX^Λ, CF_Λ) defines a vector under the symplectic transformations, it is more natural for a black hole ensemble to treat both the magnetic and the electric charges at the same footing, if it is requested to produce symplectic invariant results. In that direction, the simplest generalization of (1.5) is an inverse Laplace transformation from $Z_{\text{invari}} \equiv e^G$, which integrates over both the $\Re X \equiv \mu$ and $\Im X \equiv \phi$ with an appropriate Jacobian/measure, such that

$$[\mathrm{d}\mu_\Lambda][\mathrm{d}\phi^\Lambda]\, J(\mu,\phi) \tag{6.1}$$

defines a symplectic invariant measure. In (6.1), $J(\mu,\phi)$ appears either as a Jacobian when we change variables from those that originally define the ensemble to (μ,ϕ) or as an intrinsic measure. As it is well known, one choice for the measure of (6.1) that is invariant under the symplectic transformations is

$$[\mathrm{d}\mu_\Lambda][\mathrm{d}\phi^\Lambda]\det(\Im F_{\Lambda\Gamma}), \tag{6.2}$$

where

$$F_{\Lambda\Gamma} \equiv \frac{\partial^2 F}{\partial X^\Lambda\, \partial X^\Gamma}. \tag{6.3}$$

(6.2) is used, for example, as the intrinsic measure of the ensemble introduced in Ref. 29. However, this measure vanishes for the case of $\frac{1}{2}$BPS black holes, so is not universally applicable. In fact, a satisfactory universal measure has not been presented so far. Moreover, even if we apply such a measure, to respect the electric-magnetic duality we need to introduce a symplectic invariant free energy G. Thus regarding the fact that the OSV free energy, which, as given by (1.3) and (1.4), forms the essence of the OSV proposal, and is only symplectic invariant at the attractor point, we take a more conservative approach in what follows. That is, to enjoy the proposed relationship between the topological-string free energy and the black hole physics within a mani-

[9]The saddle point is $x=0$. At the leading order, the saddle approximation of (5.7) takes the form of (5.1), but this fails in the subleading orders.

fest symmetric approach, we keep the OSV free energy unchanged but introduce an enlarged ensemble which is twice the OSV ensemble big, in phase space terminology. This is done by associating to each doublet $(\mu^\Lambda, \phi^\Lambda)$, two canonical variables $(\chi_\Lambda, \zeta^\Lambda)$, which preserve the Legendre transformation from the OSV free energy to the black hole entropy. Obviously the simplest choice of such variables is to take them to be linear in ϕ^Λ. Thus we define an invertible change of variables as

$$\chi_\Lambda \equiv A(p,q)\phi^\Lambda f_\Lambda(\mu^\Lambda), \quad \xi^\Lambda \equiv A(p,q)\phi^\Lambda g^\Lambda(\mu^\Lambda), \quad \forall\, \Lambda, \tag{6.4}$$

with

$$\widetilde{\mathcal{F}}(\chi_\Lambda, \xi^\Lambda) = \mathcal{F}(\mu^\Lambda, \phi^\Lambda), \tag{6.5}$$

so that the Bekenstein-Hawking-Wald entropy is given by

$$S(p^\Lambda, q_\Lambda) = \widetilde{S}(\alpha^\Lambda, \beta_\Lambda) = \widetilde{\mathcal{F}}(\chi_\Lambda, \xi^\Lambda) + \pi\alpha^\Lambda\chi_\Lambda + \pi\beta_\Lambda\xi^\Lambda, \tag{6.6}$$

$$-\alpha^\Lambda = \frac{\partial\widetilde{\mathcal{F}}}{\partial\chi_\Lambda}, \quad -\beta_\Lambda = \frac{\partial\widetilde{\mathcal{F}}}{\partial\xi^\Lambda}, \tag{6.7}$$

where the exact dictionary for translating the expressions in terms of the new charges (α, β) to those in terms of the black hole electric magnetic charges will be given a bit later in this section.

Based on (6.6) and (6.7), a black hole ensemble is defined as

$$\widetilde{Z} \equiv e^{\widetilde{\mathcal{F}}(\chi_\Lambda, \xi^\Lambda)} = \sum_{\alpha^\Lambda, \beta_\Lambda} \widetilde{\Omega}(\alpha^\Lambda, \beta_\Lambda) e^{-\pi\alpha^\Lambda\chi_\Lambda - \pi\beta_\Lambda\xi^\Lambda}. \tag{6.8}$$

As before we use the Euclidean measure for the ensemble (6.8), so that

$$d(p^\Lambda, q_\Lambda) \doteq \widetilde{\Omega}(\alpha^\Lambda, \beta_\Lambda) \doteq \int [\mathrm{d}\chi_\Lambda][\mathrm{d}\xi^\Lambda] e^{\widetilde{\mathcal{F}} + \pi\alpha^\Lambda\chi_\Lambda + \pi\beta_\Lambda\xi^\Lambda}. \tag{6.9}$$

Although the measure of (6.9),

$$\prod_\Lambda \mathrm{d}\chi_\Lambda\, \mathrm{d}\xi^\Lambda = A^2(p,q) \prod_\Lambda \phi^\Lambda (f_\Lambda g'^\Lambda - f'_\Lambda g^\Lambda) \mathrm{d}\mu^\Lambda\, \mathrm{d}\phi^\Lambda, \tag{6.10}$$

is not universally symplectic invariant, unlike (6.2), we can follow the idea of Sec. IV: we require the asymptotic symplectic invariance of (6.9). More precisely, given an arbitrary order in the saddle-point asymptotic expansion of (6.9), we choose the function $A(p,q)$, in the definition (6.4), such that the unwanted prefactor of the corresponding OSV result is removed.

The integral (6.9) in terms of (μ, ϕ) takes the form

$$d(p,q) \doteq A^2(p,q) \int \prod_\Lambda [\mathrm{d}\phi^\Lambda\ \phi^\Lambda] \int \prod_\Lambda [\mathrm{d}\mu^\Lambda (f_\Lambda g'^\Lambda - f'_\Lambda g^\Lambda)] Z(\mu,\phi) e^{\pi A \phi^\Lambda (\alpha^\Lambda f_\Lambda + \beta_\Lambda g^\Lambda)}, \tag{6.11}$$

where $Z(\mu,\phi) = e^{\mathcal{F}(\mu,\phi)}$. Now to bridge between (6.11) and (1.5), we should effectively integrate over μ^Λ, which fixes the value of μ^Λ at μ^Λ_*. Here one important constraint on the functions f_Λ and g^Λ comes into play. First of all, in accordance with (1.2), we require that the saddle-point values of μ^Λ's coincide with the corresponding black hole magnetic charges,

$$\mu^\Lambda_* = p^\Lambda, \quad \forall\, \Lambda. \tag{6.12}$$

Regarding the saddle-point equation for (6.11), (6.12) implies that

$$\alpha^{\Lambda} f'_{\Lambda}(p) + \beta_{\Lambda} g'^{\Lambda}(p) = 0, \quad \forall\, \Lambda. \tag{6.13}$$

Next we require that the saddle-point evaluation of (6.11) takes the form of

$$\Omega(p^{\Lambda}, q^{\Lambda}) \doteq \int [\mathrm{d}\phi^{\Lambda}] M(p,q,\phi) e^{\mathcal{F}+\pi q_{\Lambda}\phi^{\Lambda}}, \tag{6.14}$$

which together with (6.12) implies that

$$\frac{q_{\Lambda}}{A(p,q)} = \alpha^{\Lambda} f_{\Lambda}(p) + \beta_{\Lambda} g^{\Lambda}(p), \quad \forall\, \Lambda. \tag{6.15}$$

The dictionary between (α,β) and (p,q) is now given by the solution to the Eqs. (6.13) and (6.15), which reads as

$$\alpha^{\Lambda} = \frac{q_{\Lambda}}{A(p,q)} \frac{g'^{\Lambda}(p)}{f_{\Lambda}(p) g'^{\Lambda}(p) - f'_{\Lambda}(p) g^{\Lambda}(p)}, \tag{6.16}$$

$$\beta_{\Lambda} = \frac{q_{\Lambda}}{A(p,q)} \frac{-f'^{\Lambda}(p)}{f_{\Lambda}(p) g'^{\Lambda}(p) - f'_{\Lambda}(p) g^{\Lambda}(p)}. \tag{6.17}$$

Now as a constraint on the functions f and g, we require that Eqs. (6.16) and (6.17) are consistent with the attractor equations of (6.7), for $A(p,q)$ treated as an arbitrary given function. That is, the following two equations should hold:

$$\frac{\partial \widetilde{\mathcal{F}}}{\partial \chi^{*}_{\Lambda}} = -\frac{q_{\Lambda}}{A(p,q)} \frac{g'^{\Lambda}(p)}{f_{\Lambda}(p) g'^{\Lambda}(p) - f'_{\Lambda}(p) g^{\Lambda}(p)}, \tag{6.18}$$

$$\frac{\partial \widetilde{\mathcal{F}}}{\partial \xi^{\Lambda}_{*}} = \frac{q_{\Lambda}}{A(p,q)} \frac{f'^{\Lambda}(p)}{f_{\Lambda}(p) g'^{\Lambda}(p) - f'_{\Lambda}(p) g^{\Lambda}(p)}, \tag{6.19}$$

with $\chi^{*}_{\Lambda} = A\phi^{\Lambda}_{*} f_{\Lambda}(p^{\Lambda})$, $\xi^{\Lambda}_{*} = A\phi^{\Lambda}_{*} g^{\Lambda}(p^{\Lambda})$ and $q_{\Lambda} = -\frac{1}{\pi}\frac{\partial \mathcal{F}}{\partial \phi^{\Lambda}_{*}}$.

Given these requirements, the first order saddle-point evaluation of (6.11) takes the form of (6.14) with

$$M(p,q,\phi) = A^{2h+2}(p,q) \prod_{\Lambda} \left[\left(\frac{\phi^{\Lambda}}{q_{\Lambda}} \right)^{\frac{1}{2}} \frac{\left(f_{\Lambda}(p) g'^{\Lambda}(p) - g^{\Lambda}(p) f'_{\Lambda}(p) \right)^{\frac{3}{2}}}{\left(f''_{\Lambda}(p) g'^{\Lambda}(p) - g''^{\Lambda}(p) f'_{\Lambda}(p) \right)^{\frac{1}{2}}} \right]. \tag{6.20}$$

So, the effective inverse Laplace transformation, (6.14), differs from the original OSV formula, (1.5), by a measure M, which in form is something between the metric measure of (1.6) and the Jacobian matrix in (4.8).

Now given a specific prepotential and an arbitrary order of the saddle-point asymptotic expansion of (6.14), the measure (6.20) equals

$$\grave{M}(p,q) \equiv M(p,q,\phi_{*}) = A^{2h+2}(p,q) \prod_{\Lambda} \left[\frac{\left(f_{\Lambda}(p) g'^{\Lambda}(p) - g^{\Lambda}(p) f'_{\Lambda}(p) \right)^{\frac{3}{2}}}{\left(f''_{\Lambda}(p) g'^{\Lambda}(p) - g''^{\Lambda}(p) f'_{\Lambda}(p) \right)^{\frac{1}{2}}} \sqrt{\frac{\phi^{\Lambda}_{*}}{q_{\Lambda}}} \right], \tag{6.21}$$

$$\tilde{\Omega}_* = \grave{M}(p,q)\Omega_*. \tag{6.22}$$

It is obvious that $\grave{M}(p,q)$ plays the same role as $\det[V]$ of Sec. IV and protects the resulting black hole degeneracy of states against the electric-magnetic duality violations by removing the unwanted prefactors, with a proper choice of the function $A(p,q)$.

VII. CONCLUSION

We studied the issue of electric-magnetic duality in the OSV proposal, as it appears as itself in the complex polarization. The main conclusion of the work is as follows:

Applying the duality invariance of the degeneracy of states as a constraint to the definition of the ensemble variables, there are proper redefinitions of the OSV mixed ensemble in the complex polarization, in the form of a generalized purlye canonical ensemble of new variables such that the results of the inverse Laplace transformation with a flat measure of integration respect the electric-magnetic duality and match properly the known microscopic results, to all orders in the asymptotic expansion, as far as the D6-brane charge vanishes. With a nonvanishing D6-brane charge, however, the duality restoration is limited to the saddle-point evaluation.

Here we would like to mention an independent and equivalent way to define these new variables more systematically. We note the fact that the integrand of (1.5), $[\mathrm{d}\phi]e^G$, is not invariant under the symplectic transformations, and this noninvariance depends on the detail of the charge configuration. So we look for $\det[V] \doteq J(p,q,\phi_*)$, which, up to vanishing boundary terms, solves the equation

$$\delta_T\{[d\phi]J(p,q,\phi)e^{G(p,q,\phi)}\} = 0 \Leftrightarrow \det\left[\frac{\partial \breve{\phi}^\Lambda}{\partial \phi^\Gamma}\right]\breve{J}e^{\breve{G}} = Je^G \Rightarrow \det\left[\frac{\partial \breve{\phi}^\Lambda}{\partial \phi^\Gamma}\right]_* = \frac{J_*}{\breve{J}_*}, \tag{7.1}$$

with T denoting a general member of the relevant symplectic transformations that brings (X^Λ, F_Λ) to $(\breve{X}^\Lambda, \breve{F}_\Lambda)$. For example, if we consider the large black hole of section 3 in the specific case of $K3$ fiberation where T-duality holds as the symmetry of the action, taking for simplicity the only nonvanishing intersection numbers to be $C_{ABC}=C_{1ab}\equiv C_{ab}$, it is easy to see that, for an infinitesimal transformation T, (7.1) leads to the result

$$J_* = \frac{1}{(p^1)^2} f(|\vec{p}|),$$

where $\vec{p}\equiv(p^2,\ldots,p^h)$ and $|\vec{P}|^2 \equiv C_{ab}p^a p^b$. We note that the inverse of the OSV prefactor for this example exactly matches with this result.

We would like to finally bring the reader's attention to the following possibility.

To define the ensemble of Secs. III and IV, one can absorb the unwanted OSV prefactor within the redefinition of a single X variable. Among the X variables, X^0, which controls the topological-string coupling via (4.18), plays a distinguished role in the prepotential (5.2). It is physically natural to think about a redefinition of the OSV ensemble as $\hat{X}^0 = M(p,q)X^0$, according to (4.17), and ask if for a given black hole charge multiplet (p^Λ, q_Λ), the requirement of the electric-magnetic duality gives an effective sense to the topological-string coupling as seen by the black hole ensemble through the identification $\hat{g} \equiv \frac{4\pi i}{\hat{X}^0}$.

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Fractional Israel layers

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A fractional Lie derivative, valid in the thin shell limit, is developed. The nonlocal nature of the fractional derivative allows the inclusion of shell thickness in the stress energy description of zero thickness Israel layers. The method is applied to several examples. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Derivatives of fractional order, first described in 1695 by Leibnitz,[1,2] have been successful in modeling transport processes with anomalous microscopic time and/or spatial structures.[3–6] Among the transport applications are diffusion equations fractional in both time and spatial coordinates[7–9] and fractional Schrödinger equations;[10,11] there are applications in biophysics and thermodynamics[12] as well as texts[13,14] on solving the fractional differential equations arising in transport. Other areas of application are the inclusion of dissipative processes in a Lagrangian formalism by introducing fractional derivatives as generalized coordinates[15,16] and the use of a fractional derivative in the metric match over a boundary layer[17,18] in general relativity.

The field equations of general relativity are not easily fractionally generalized because of the covariance requirement on derivatives. The general relativity (GR) applications in Refs. 17 and 18 did not modify the field equations or any of the usual GR tensors in any way; the fractional match simply provided a broader set of metric relations across a boundary. It was used to create a family of Israel layers parametrized by the noninteger order of the fractional derivative. There are, however, geometric objects used in general relativity, which can be fractionalized without altering the basic covariant structure of the theory. One of these is the Lie derivative, defined only with partial derivatives. The Lie derivatives take into account the difference between a tensor that is Taylor transported to a point and coordinate transformed at the same point. It is a local derivative. Fractional derivatives are intrinsically nonlocal, involving an integral over some region of space time. A fractional Lie derivative, while it also evaluates functional differences at a point, since it is nonlocal in its definition, could be a useful way of including nonlocal effects in single layer calculations. For example, the Israel formalism calculates the stress energy content of a single layer in terms of the jump in extrinsic curvatures across a boundary. Using a fractional Lie derivative to define a fractional extrinsic curvature would allow the inclusion of shell thickness in the standard Israel formalism. In the next section we develop a fractional Lie derivative valid to first order in a thin shell thickness. The formalism is used to describe the stress energy content of some simple fractional layers. A brief list of notation is included in the Appendix.

II. LIE DERIVATIVE

A. The integer Lie derivative

The Lie derivative compares the value of a function under transport from x to x' and under a coordinate transform from a system of coordinates (x) to a primed system (x'). The difference $V^i(x')-V'^i(x')$ defines the Lie derivative. Consider a vector V^i at a point x. Under a coordinate transform, $x^{i\prime}=x^i+\xi^i d\lambda$, its value transforms as

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$$V'^{i}(x') = \frac{\partial x'^{i}}{\partial x^{a}} V^{a}(x) = \left(\delta^{i}_{a} + \frac{\partial \xi^{i}}{\partial x^{a}} d\lambda \right) V^{a}(x), \tag{1}$$

where ξ^i is the tangent to the transport path. The vector is assumed to be analytic and we have

$$V^{i}(x') = V^{i}(x) + \left(\frac{\partial V^{i}}{\partial x'^{a}} \right)_{x} (x'^{a} - x^{a}) + \cdots . \tag{2}$$

Using Eq. (1), the Lie derivative to first order in ξ^i is

$$(\mathcal{L}_{\xi} V^{i}) = \lim_{d\lambda \to 0} \frac{V^{i}(x') - V'^{i}(x')}{d\lambda},$$

$$(\mathcal{L}_{\xi} V^{i}) = \left(\frac{\partial V^{i}}{\partial x'^{a}} \right)_{x} \xi^{a} - \left(\frac{\partial \xi^{i}}{\partial x'^{a}} \right)_{x} V^{a}(x).$$

Similar expressions exist for covariant vectors and tensors of higher order. For a scalar function, F, the Lie derivative is a simple directional derivative.

$$(\mathcal{L}_{\xi} F) = \xi^{a} \left(\frac{\partial F}{\partial x'^{a}} \right)_{x}.$$

B. Fractional generalization

1. Fractional derivative

There are several choices to make in developing a fractional Lie derivative. The first is to choose the type of fractional derivative from among the many available. We will use the Caputo form of the fractional derivative. The Caputo fractional derivative integrates the derivative of the function while other forms take the derivative of the function integral. Among the many fractional derivative operators, the Caputo form is the closest generalization of the classical derivative.[13] We generalize the usual form by using partial derivatives. With q as the fractional parameter, the Caputo derivative is defined for $0 < q \leqslant 1$ as

$$D^{q}_{x} V^{i}(x') = \frac{\partial^{q} V^{i}(x')}{\partial (x' - x)^{q}} = \frac{1}{\Gamma(1-q)} \int_{x}^{x'} dy \frac{\partial V^{i}(y)}{\partial y} (x' - y)^{-q}. \tag{3}$$

The derivative can be extended to values of $q > 1$; this is discussed in the Appendix. The indices, (q,x), on D^q_x are not tensor indices. q is the fractional parameter and x is the lower limit in the integral definition. The choice of limits depends on the application being made. Our development will be for applications to thin layers of thickness Δ. The coordinates near the shell are (t, η, x^3, x^4). The spatial coordinates in the layer are (x^3, x^4). The radial coordinate, η, is measured to the outer shell boundary, $\eta = R_o$. The integration will run from the bottom of the layer, $x = \eta - \Delta$, to the top, $x' = \eta$, with $\eta = R_o$ when the outer boundary size is set. With these choices, the fractional derivative definition that will be used is

$$D^{q}_{\eta - \Delta} V^{i}(\eta) = \frac{1}{\Gamma(1-q)} \int_{\eta - \Delta}^{\eta} dy \frac{\partial V^{i}(y)}{\partial y} (\eta - y)^{-q}. \tag{4}$$

The other parts of the fractional generalization to consider are the tensor transformation rule and the first terms of a fractional expansion of the tensor. These parts depend on the fractional replacement for the partial derivative.

2. Partial derivative and fractional derivative

A relation between a partial derivative and a fractional derivative can be obtained by integrating Eq. (3) by parts. We have

$$D_x^q V^i(x') = \frac{(x'-x)^{1-q}}{\Gamma(2-q)}\left(\frac{\partial V^i(y)}{\partial y}\right)_x + \frac{(x'-x)^{2-q}}{\Gamma(3-q)}\left(\frac{\partial^2 V^i(y)}{\partial y^2}\right)_x + \cdots \tag{5}$$

In the limit, $x'-x \ll 1 (\Delta \ll 1)$, the first term will dominate and we have the relation between the fractional derivative and the partial derivative to lowest order in shell thickness.

$$\frac{(\Delta)^{1-q}}{\Gamma(2-q)}\left(\frac{\partial V^i(y)}{\partial y}\right)_{\eta-\Delta} \to D_{\eta-\Delta}^q V^i(\eta). \tag{6}$$

For convenience, we define a fractional operator Đ_x^q,

$$D_x^q(\,) = \frac{(x'-x)^{1-q}}{\Gamma(2-q)}\text{Đ}_x^q(\,). \tag{7}$$

In the $q=1$ limit, the usual derivative is obtained. The Đ_x^q derivative used over a nonthin shell region, for some functions, can divide out much of the usual fractional behavior and will be used to provide the direct replacement for the partial derivative for layer examples.

3. The first order fractional expansion

For analytic V^i, the regular Taylor expansion is

$$V^i(x') = V^i(x) + \left(\frac{\partial V^i(y)}{\partial y}\right)_x (x'-x) + \cdots \tag{8}$$

Using the fractional replacement the expansion can be written to first order as

$$V^i(x') = V^i(x) + \text{Đ}_x^q(V^i)(x'-x) + \cdots \tag{9}$$

Note that this is not a replacement for the regular Taylor expansion, complete to all orders. It will be used only to first order in the shell thickness. A complete fractional expansion was developed by Taylor and Riemann.[19] Their expansion, including both fractional integrals and derivatives, is difficult to implement. Kolwankar[20] have also developed a local fractional expansion.

4. A notation addition

The general fractional derivative

$$D_x^q V^i(x') = \frac{\partial^q V^i(x')}{\partial(x'-x)^q} = \frac{1}{\Gamma(1-q)}\int_x^{x'} dy \frac{\partial V^i(y)}{\partial y}(x'-y)^{-q}$$

is not written with tensor functions in mind. For example, if $V^i(x')=x'^i$ we have

$$D_x^q x'^i = \frac{\partial^q x'^i}{\partial(x'-x)^q} = \frac{1}{\Gamma(1-q)}\int_x^{x'} dy \frac{\partial y^i}{\partial y}(x'-y)^{-q},$$

where i has the usual coordinate index range (1, 2, 3, 4) but the coordinate identification of x' and its integral counterpart, y, is not clear. To clarify this an index k is added to the fractional derivative notation, allowing the partial derivative to be written in index notation

$$D_{x,k}^q x'^i = \frac{\partial^q x'^i}{\partial(x'^k - x^k)^q} = \frac{1}{\Gamma(1-q)}\int_x^{x'} dy \frac{\partial y^i}{\partial y^k}(x'-y)^{-q}. \tag{10}$$

A similar notation is used by Samko *et al.*[2] With this notation and using the incomplete beta function, the integral in Eq. (10) is

$$D^q_{x,k}x'^i = \frac{\partial^q x'^i}{\partial(x'^k - x^k)^q} = \frac{\delta^i_k}{\Gamma(1-q)}\int_x^{x'} dy(x'-y)^{-q} = \frac{\delta^i_k(x'-x)^{1-q}}{\Gamma(2-q)}. \tag{11}$$

5. The coordinate transformation

The remaining step is to consider the transport as a coordinate transformation. The usual tensor transformation rule can be written as

$$V^i(x) = \frac{\partial(x^i - x^i_o)}{\partial(x'^k - x'^k_o)}V'^k(x'), \tag{12}$$

where x^i_o and x'^i_o are the initial points in the two systems. The partial derivative in the transformation rule generalizes to

$$\frac{\partial(x^i)}{\partial(x'^k - x^k)} \to Đ^q_{x,k}(x^i) \tag{13}$$

and we have

$$V^i(x) = D^q_{x,k}(x^i)V'^k(x') = \frac{\Gamma(2-q)}{(x'-x)^{1-q}}\frac{\partial^q(x^i)}{\partial(x'^k - x^k)^q}V'^k(x'). \tag{14}$$

Substituting from the coordinate transformation one obtains

$$V^i(x) = \frac{\Gamma(2-q)}{(x'-x)^{1-q}}\left\{\frac{\partial^q(x'^i)}{\partial(x'^k - x^k)^q} - \frac{\partial^q(\xi^i d\lambda)}{\partial(x'^k - x^k)^q}\right\}V'^k(x'). \tag{15}$$

The first integral is evaluated above giving

$$V^i(x) = V'^i(x') - Đ^q_{x,k}(\xi^i)d\lambda V'^k(x').$$

For the layer application this becomes

$$V^i(\eta - \Delta) = V'^i(\eta) - Đ^q_{\eta-\Delta,k}(\xi^i)d\lambda V'^k(\eta). \tag{16}$$

A fractional coordinate transformation has been considered by Cotrill-Shepherd and Naber.[21] Their transformation takes a fractional coordinate differential $d^q x^i$ to another $d^q y^i$ in n dimensions. For $q \leqslant 1$ their transformation can be written as

$$dx^{q,k} = \sum_{i=1}^{n} dy^{q,i}\frac{1}{\Gamma(1+q)}\frac{1}{\prod_{p=1 p\neq k}^{n}(x^p - x^p_o)^{q-1}}\frac{\partial\left\{\prod_{j=1 j\neq k}^{n}(x^j - x^j_o)^{q-1}(x^k - x^k_o)^q\right\}}{\partial(y^i - x'^i_o)^q}, \tag{17}$$

where x^i_o and x'^i_o are the initial points for the coordinate systems. In addition to the obvious term differences, this transformation is not an approximation but an exact transformation for a fractional differential defined on a fractional tangent space. The transformation used to develop the fractional Lie derivative in this paper is the fractional derivative of a regular function; it is not complete but only considers the first order terms in the shell thickness.

6. The fractional Lie derivative

Using Eqs. (8) and (16) and equating $V^i(x)$ we have

$$V^i(x') - \mathcal{D}^q_{x,k}(V^i)(x'^k - x^k) = V'^i(x') - \mathcal{D}^q_{x,k}(\xi^i)d\lambda V'^k(x'). \tag{18}$$

The Lie derivative comes from the difference $V^i(x') - V^{i'}(x')$. Forming the difference we have

$$V^i(x') - V'^i(x') = d\lambda\{\mathcal{D}^q_{x,k}(V^i)\xi^k - \mathcal{D}^q_{x,k}(\xi^i)V^k\}. \tag{19}$$

The fractional Lie derivative ${}^q\mathcal{L}_\xi(V^i)$ is

$${}^q\mathcal{L}_\xi V^i = \mathcal{D}^q_{x,k}(V^i)\xi^k - \mathcal{D}^q_{x,k}(\xi^i)V^k. \tag{20}$$

Similar development results in the fractional Lie derivative forms for covariant vectors and higher order tensors. The fractional Lie derivative of V_i is

$${}^q\mathcal{L}_\xi V_i = \mathcal{D}^q_{x,k}(V_i)\xi^k + \mathcal{D}^q_{x,i}(\xi^k)V_k. \tag{21}$$

The simplest case, a scalar function, has fractional Lie derivative

$${}^q\mathcal{L}_\xi f = \xi^k\mathcal{D}^q_{x,k}(f). \tag{22}$$

Some properties of the fractional Lie derivative are discussed in the Appendix.

III. A FRACTIONAL THIN LAYER

A. Describing the layer

Many of the thin shell examples considered in the literature[22–34] are descriptions of a boundary layer between two space times, $M^\pm$. Boundary layers are often treated in the Israel formalism[35] which models a thin shell as a layer of zero thickness. The basic input into this description is the extrinsic curvature of the boundary layer as seen by the bounding space times.

$$K^\pm_{cd} = \frac{1}{2}\mathcal{L}_N(g^\pm_{ij})h^{\pm i}_c h^{\pm j}_d, \tag{23}$$

where c,d range over the coordinates of the boundary layer, N^i is the normal to the layer, and h_{ij} is the projection operator onto the layer,

$$h^\pm_{ij} = g^\pm_{ij} - N^\pm_i N^\pm_j. \tag{24}$$

The jump in the extrinsic curvatures, $\langle K_{ab}\rangle = K^+_{cd} - K^-_{cd}$, and their trace $\langle K\rangle = K^+ - K^-$ are related to the stress energy of the single boundary layer.[35]

$$-8\pi S_{ab} = \langle K_{ab}\rangle - \langle K\rangle h_{ab}. \tag{25}$$

The fractional extrinsic curvature is defined in terms of the fractional Lie derivative.

$${}^qK_{cd} = \frac{1}{2}{}^q\mathcal{L}_N(g_{ij})h^i_c h^j_d, \tag{26}$$

where

$${}^q\mathcal{L}_N(g_{ij}) = N^k\mathcal{D}^q_{x,k}(g_{ij}) + g_{kj}\mathcal{D}^q_{x,i}(N^k) + g_{ik}\mathcal{D}^q_{x,j}(N^k) \tag{27}$$

and Eq. (7) relates $\mathcal{D}^q_{x,k}$ to the fractional derivative form. The fractional stress energy is defined through jumps in the fractional extrinsic curvature,

$$-8\pi {}^qS_{ab} = \langle {}^qK_{ab}\rangle - \langle {}^qK\rangle h_{ab}. \tag{28}$$

B. Using the fractional extrinsic curvature

The fractional extrinsic curvature is defined as an integral over a shell of thickness Δ. Because of this nonlocal integral structure, one might assume that the usual Israel jump in extrinsic curvature could be replaced by a single extrinsic curvature calculation. However, just as for the regular Lie derivative, the fractional Lie derivative, while it includes a thickness component, only provides the value of the derivative at a single space-time point. For example, consider a shell bounded by two Minkowski space times. We would expect no jump discontinuities across such a boundary.

$$M^{\pm}: ds^2 = -dt^2 + dr^2 + r^2 d\Omega^2. \tag{29}$$

The unit normal to the shell is $N^i=(0,1,0,0)$. ${}^qK_{\theta\theta}$ and ${}^qK_{\phi\phi}$ will be nonzero for each of Minkowski boundaries. Using Eqs. (7), (26), and (27), with $\eta=r$, the fractional extrinsic curvature is

$${}^qK_{cd} = \frac{\Gamma(2-q)}{2(\Delta)^{1-q}} N^r D^q_{r-\Delta,r}(g_{ij}) h^i_c h^j_d. \tag{30}$$

For Minkowski we have

$$\begin{aligned} {}^qK^M_{\theta\theta} &= \frac{\Gamma(2-q)}{2\Gamma(1-q)(\Delta)^{1-q}} \int_{r-\Delta}^{r} dy 2y(r-y)^{-q}, \\ {}^qK^M_{\theta\theta} &= \frac{\Gamma(2-q)2R_o^{2-q}}{2\Gamma(1-q)(\Delta)^{1-q}} B_{\Delta/R_o}(1-q,2), \end{aligned} \tag{31}$$

where $B_{\Delta/R}(1-q,2)$ is the incomplete beta function and r was set equal to the boundary value, R_o.

$$B_x(a,b) = \int_0^x t^{a-1}(1-t)^{b-1}.$$

Using the beta function expansion[36]

$$B_x(a,b) = x^a\left(\frac{1}{a} + \frac{1-b}{a+1}x + \frac{(1-b)(2-b)}{2!(a+2)}x^2 + \cdots\right), \tag{32}$$

we have

$${}^qK^M_{\theta\theta} = \frac{\Gamma(2-q)2R_o^{2-q}}{2\Gamma(1-q)(\Delta)^{1-q}}\left(\frac{\Delta}{R_o}\right)^{1-q}\left(\frac{1}{1-q} - \frac{1}{2-q}\frac{\Delta}{R_o} + \cdots\right),$$

$${}^qK^M_{\theta\theta} \sim R_o\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right). \tag{33}$$

Because of the integral over the shell, this single extrinsic curvature might be regarded as the entire jump contribution. However, if there were no boundary layer between the two space times, one would expect the jump in the extrinsic curvatures to be zero. Instead, the fractional extrinsic curvature, in the $\Delta->0$ limit, is simply the regular extrinsic curvature evaluated over the outer bounding surface. The expression above is only the extrinsic curvature evaluated with one of the bounding space times. In order to use the fractional extrinsic curvature in an Israel layer calculation, it has to be calculated for both interior and exterior boundaries, just as in the nonfractional case. In this example, there is no jump in the extrinsic curvatures across the boundary as expected.

IV. TWO EXAMPLES

In this section two examples of fractional shells are considered. One layer has cylindrical symmetry and is bounded by Levi-Civita and Minkowski. The second layer has spherical symmetry and separates Schwarzschild and Minkowski. Dynamic shells have broad applications as reflected by the large literature dealing with their evolution.[22–34] The two examples considered in this section are static and are presented as examples of the use of the fractional Lie derivative in the Israel formalism. Dynamic fractional shells will be considered elsewhere.

A. A layer between Minkowski and Levi-Civita

A simple cylindrical example is a layer separating an interior Minkowski and a vacuum Levi-Civita with angular deficit factor δ,

$$M^+: ds^2 = -dt^2 + dr^2 + \delta^2 r^2 d\phi^2 + dz^2, \tag{34}$$

$$M^-: ds^2 = -dt^2 + d\rho^2 + \rho^2 d\phi^2 + dz^2. \tag{35}$$

Using the result from the previous section, Eq. (33), the nonzero fractional extrinsic curvatures are ${}^qK_{\theta\theta}$,

$${}^qK_\theta^{\theta M-} \simeq R_o\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right), \tag{36}$$

$${}^qK_\theta^{\theta M+} \simeq \delta R_o\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right). \tag{37}$$

Calculating the jumps we find

$$\langle {}^qK\rangle \simeq R_o(\delta-1)\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right), \tag{38}$$

$$\langle {}^qK_\theta^\theta\rangle \simeq R_o(\delta-1)\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right), \tag{39}$$

$$\begin{aligned} -8\pi S_j^i &= \langle {}^qK_j^i\rangle - \langle {}^qK\rangle h_j^i, \\ 8\pi S_t^t &\simeq -R_o(1-\delta)\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right). \end{aligned} \tag{40}$$

The stress energy in the layer has positive density and no pressure. In a perfect fluid model this could be dust. The method of including a fractional parameter in the regular Israel layer[17,18] by matching fractional derivatives across the boundary would require no angular deficit, $\delta=1$, for these two space times. In this example, the stress energy of the layer only includes a thin layer contribution for $q \neq 1$, the fractional case. The Δ dependence was included by using the nonlocality of the fractional derivative. In the $q->1$ limit, the fractional derivative becomes a regular local derivative and the effect vanishes.

B. A layer between Minkowski and Schwarzschild

1. The fractional extrinsic curvature

Consider a shell bounded by the an exterior Schwarzschild space time and an interior Minkowski at $r=R_o$,

$$M^+: ds^2 = -\left(1 - \frac{2m}{r}\right)dt^2 + \frac{dr^2}{1-(2m/r)} + r^2 d\Omega^2, \tag{41}$$

$$M^-: ds^2 = -\left(1 - \frac{2m}{R_o}\right)dt^2 + dr^2 + r^2 d\Omega^2. \tag{42}$$

For this calculation the normal vectors have only radial components and we have

$${}^q\mathcal{L}_N(g_{ij}) = N^r \text{Đ}^q_{r-\Delta,r}(g_{ij}) + g_{rj}\text{Đ}^q_{r-\Delta,i}(N^r) + g_{ir}\text{Đ}^q_{r-\Delta,j}(N^r)$$

with

$$\text{Đ}^q_{r-\Delta,r}(g_{ij}) = \frac{\Gamma(2-q)}{\Gamma(1-q)(\Delta)^{1-q}}\int_{r-\Delta}^{r}\frac{\partial g_{ij}(w)}{\partial w}(r-w)^{-q}dw$$

and $q \leqslant 1$, $r->R_o$ on the boundary. For the interior Minkowski space time, $N^i=(0,1,0,0)$ and only ${}^qK_{\theta\theta}$ and ${}^qK_{\phi\phi}$ will contribute and the result has been calculated above. From Eq. (33) we have

$${}^qK^\theta_\theta = {}^qK^\phi_\phi = \frac{1}{R_o}\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right). \tag{43}$$

For the exterior Schwarzschild (SC) space time, $N^i=(0,\sqrt{1-(2m/r)},0,0)$ and ${}^qK_{\theta\theta}$, ${}^qK_{\phi\phi}$, and ${}^qK_{tt}$ will contribute. Except for the structure of the normal, the angular extrinsic curvatures will be the same as in Minkowski and we have at the boundary

$${}^qK^\theta_\theta = {}^qK^\phi_\phi = \frac{\sqrt{1-(2m/R_o)}}{R_o}\left(1 - \frac{1-q}{2-q}\frac{\Delta}{R_o} + \cdots\right). \tag{44}$$

Calculating ${}^qK_{tt}$ and letting $r->R_o$ we have

$${}^qK_{tt} = \frac{N^r}{2}\text{Đ}^q_{r-\Delta,r}(g_{tt}) = 2m\frac{\sqrt{1-(2m/R_o)}}{2}\text{Đ}^q_{r-\Delta,r}(r^{-1}),$$

$${}^qK_{tt} = -2m\frac{\sqrt{1-(2m/R_o)}}{2}\frac{\Gamma(2-q)R_o^{-1-q}}{\Gamma(1-q)\Delta^{1-q}}B_{\Delta/R_o}(1-q,-1).$$

The negative one beta function parameter is permitted for $\Delta/R_o \neq 1$.[36] This expression is most easily expanded in terms of the hypergeometric function ${}_2F_1(a,b,c;x)$,

$$B_{\Delta/R_o}(1-q,-1) = \frac{(\Delta/R_0)^{1-q}}{1-q}{}_2F_1\left(1-q,2,2-q;\frac{\Delta}{R_o}\right) = \frac{(\Delta/R_o)^{1-q}}{1-q}\left(1 + \frac{1-q}{2-q}2\frac{\Delta}{R_o} + \cdots\right)$$

and we have

$${}^qK^t_t = \frac{m}{\sqrt{1-(2m/R_o)}R_o^2}\left(1 + \frac{1-q}{2-q}2\frac{\Delta}{R_o} + \cdots\right). \tag{45}$$

2. The layer stress energy

Using the ${}^{q}K_{ab}$ calculated in the previous section, the jumps are

$$\langle {}^{q}K_{\theta}^{\theta}\rangle = \langle {}^{q}K_{\phi}^{\phi}\rangle = \frac{(\sqrt{1-(2m/R_o)}-1)}{R_o}\left(1-\frac{1-q}{2-q}\frac{\Delta}{R_o}+\cdots\right)$$
$$\langle {}^{q}K_{t}^{t}\rangle = \frac{m}{\sqrt{1-(2m/R_o)}R_o^2}\left(1+2\frac{1-q}{2-q}\frac{\Delta}{R_o}+\cdots\right). \tag{46}$$

With these jumps, the layer energy density, σ, and stress, P, are

$$8\pi S_t^t = -8\pi\sigma = -\langle {}^{q}K_{\theta}^{\theta} + {}^{q}K_{\phi}^{\phi}\rangle,$$

$$8\pi S_{\theta}^{\theta} = 8\pi P = \langle {}^{q}K_{t}^{t} + {}^{q}K_{\phi}^{\phi}\rangle.$$

Substituting we have

$$8\pi\sigma = 2\frac{(1-\sqrt{1-(2m/R_o)})}{R_o}\left(1-\frac{1-q}{2-q}\frac{\Delta}{R_o}+\cdots\right), \tag{47}$$

$$8\pi P = \frac{1}{R_o\sqrt{1-(2m/R_o)}}\left\{+1-\frac{m}{R_o}-\sqrt{1-\frac{2m}{R_o}}+\frac{1-q}{2-q}\frac{\Delta}{R_o}\left(\frac{4m}{R_o}-1+\sqrt{1-\frac{2m}{R_o}}\right)\cdots\right\}. \tag{48}$$

In the $m \ll R_o$ limit the stress energy becomes

$$\sigma \approx \frac{m}{4\pi R_o^2}\left(1-\frac{1-q}{2-q}\frac{\Delta}{R_o}\right),$$
$$P \approx \frac{3m}{8\pi R_o^2}\frac{1-q}{2-q}\frac{1}{R_o}. \tag{49}$$

For $q=1$, the density is simply the SC mass parameter over the surface area of the sphere and the fluid is dust. For $q<1$ the reduction in density, for the same mass, means the same mass is distributed over a larger region. Since the size of the sphere is set, the reduction in the areal density is possible if the mass is being distributed in an annular volume rather than totally over an area. In addition, the appearance of the fractional correction factor suggests that the thickness of the shell is parametrized by q. One could define a parametrized shell thickness,

$$\Delta_q = \frac{1-q}{2-q}\Delta. \tag{50}$$

With this parametrization, a family of shells is created with the thickest shells occurring for q close to zero.

V. DISCUSSION

The Israel formalism models a thin shell of matter as a zero thickness layer. The stress energy of the layer is related to jumps in the extrinsic curvature across the single boundary. In this paper, a fractional Lie derivative was developed and used to calculate a fractional extrinsic curvature which was input into the Israel formalism. The layer being described still has zero thickness; a single coordinate boundary is used to calculate the curvature jumps, but the nonlocal fractional derivative used to define the fractional extrinsic curvature allows the inclusion of a contribution

from a thin layer thickness as well as a fractional parameter, q, in the layer stress energy. The fractional parameter can be used to parametrize the shell thickness, creating a family of shells of varying thickness. The development is for $q \leqslant 1$ but can be extended to higher values of the fractional parameter. As an example of the use of the fractional Lie derivative within the Israel formalism, the method was applied to a cylindrical layer between a Minkowski interior and a Levi-Civita exterior and a spherical Schwarschild-Minkowski shell. The inclusion of the shell thickness is a fractional effect and vanishes as the fractional parameter approaches one.

There are choices to be made in the development of fractional formalisms applicable in general relativity. There are many fractional derivative definitions, Caputo, Riesz, Riemann-Liouville, etc., and the choice of derivative will depend on the application. The layers discussed here involve one-dimensional fractional Lie transport in a spatial variable but multidimensional transport processes will be important in the dynamics of fractional layers. Fractional derivatives have successfully described random walk processes that are heavy tailed in either jump size or jump timing and this has provided avenues for higher dimensional generalizations of the fractional derivative. Umarov and Gorenflo[37] have discussed a multispace dimension random walk model that is related to diffusion that is fractional in its spatial derivatives. Gorenflo and Mainardi have presented some random walk models discrete in both space and time.[38] Meerschaert and co-workers,[39,40] have begun to develop a fractional derivative operator that may be used when space and time variables are linked. Generalizing the formalism to describe the dynamic fractional layers with plane and spherical symmetries in general relativity[41–43] would be both useful and interesting.

APPENDIX: FRACTIONAL DETAILS

1. The Caputo derivative

The Caputo derivative of a scalar function can generally be written as[4]

$$D_x^q f(x') = \frac{1}{\Gamma(m-q)} \int_x^{x'} f^{(m)}(z)(x'-z)^{m-1-q} dz,$$

where $m-1 < q \leqslant m$, m integer. $f^{(m)} = d^m f / dz^m$. The development in the text was for $m=1$. The fractional derivative is an interpolator between regular integer derivatives. To move to $q>1$ would require $m=2$ and we would have

$$D_x^q f(x') = \frac{1}{\Gamma(2-q)} \int_x^{x'} \frac{d^2 f(z)}{dz^2} (x'-z)^{1-q} dz.$$

Integrating by parts we have

$$D_x^q f(x') = -\left(\frac{df}{dz}\right)_x (x'-x)^{1-q} + \frac{1}{\Gamma(1-q)} \int_x^{x'} \frac{df(x)}{dz} (x'-z)^{-q} dz. \tag{A1}$$

Remembering that for $m=2$, $q>1$, one can see the interpolating term.

2. Notation

This section contains a list of the notations used. The starting point is the Caputo derivative discussed in the previous section, $D_x^q(\ )$ with an additional index, k, to define the coordinate partial occurring in the definition.

$$D_{x,k}^q V^i(x') = \frac{\partial^q x'^i}{\partial (x'^k - x^k)^q} = \frac{1}{\Gamma(1-q)} \int_x^{x'} dy \frac{\partial V^i(y)}{\partial y^k} (x'-y)^{-q}. \tag{A2}$$

The integral is over the thickness of the layer with $x = \eta - \Delta$, $x' = \eta$. The $\mathcal{D}_x^q$ derivative is defined in terms of the Caputo derivative,

$$D^q_{x,k}() = \frac{(x'-x)^{1-q}}{\Gamma(2-q)} Đ^q_{x,k}(). \tag{A3}$$

An example of its use are found in the next section. The fractional Lie derivative is defined in terms of $Đ^q_{x,k}(\ )$,

$${}^q\mathcal{L}_\xi V^i = Đ^q_{x,k}(V^i)\xi^k - Đ^q_{x,k}(\xi^i)V^k, \tag{A4}$$

$${}^q\mathcal{L}_\xi V_i = Đ^q_{x,k}(V_i)(\xi^k) + V_k Đ^q_{x,i}(\xi^k), \tag{A5}$$

$${}^q\mathcal{L}_\xi f = \xi^k Đ^q_{x,k}(f). \tag{A6}$$

The fractional extrinsic curvature is defined in terms of the fractional Lie derivative generated by the normal to the layer. g_{ij} is the metric of the bounding space time and h_{ij} is the projection operator onto the layer,

$${}^qK_{cd} = \frac{1}{2}{}^q\mathcal{L}_N(g_{ij})h^i_c h^j_d. \tag{A7}$$

Jumps across the layer are described by

$$\langle {}^qK_{cd}\rangle. \tag{A8}$$

3. The $Đ^q$ derivative

The $Đ^q$ derivative defined in Eq. (7) in the text as a replacement for the regular partial derivative divides out some of the usual fractional derivative behavior. Consider the Caputo derivative of r^2 over a spherical region from the origin to r. We have

$$D^q_r r^2 = \frac{1}{\Gamma(1-q)}\int_0^r 2z(r-z)^{-q}dz = \frac{2r^{2-q}}{\Gamma(1-q)}\int_0^1 w(1-w)^{-q}dw = \frac{2r^{2-q}}{\Gamma(1-q)}\frac{\Gamma(1-q)\Gamma(2)}{\Gamma(2-q)} = \frac{2r^{2-q}}{\Gamma(3-q)}.$$

The $Đ^q$ derivative is

$$D^q_x(\ ) = \frac{(x'-x)^{1-q}}{\Gamma(2-q)} Đ^q_x(),$$

$$Đ^q r^2 = \frac{2r}{2-q}.$$

4. Some properties of the fractional Lie derivative

a. Defining the fractional commutator

The regular Lie derivative defines the commutator as

$$\mathcal{L}_U V = [U,V] = \nabla_U V - \nabla_V U,$$

where $\nabla_U = U^k\nabla_k$ is the standard directional derivative. The fractional Lie derivative generalizes the commutator,

$$\begin{aligned} {}^q\mathcal{L}_U V^i &= U^k Đ^q_{x,k}V^i - V^k Đ^q_{x,k}U, \\ {}^q[U,V]^i &= U^k Đ^q_{x,k}V^i - V^k Đ^q_{x,k}U^i. \end{aligned} \tag{A9}$$

Product of derivatives

The product of two regular Lie derivatives is related to the Lie derivative of the commutator.

$$\mathcal{L}_{[U,V]} = \mathcal{L}_U \mathcal{L}_V - \mathcal{L}_V \mathcal{L}_U.$$

Consider the fractional Lie derivative acting on a scalar function f,

$${}^q\mathcal{L}_{[U,V]} f = \{U^k \text{Đ}^q_{x,k} V^i - V^k \text{Đ}^q_{x,k} U^i\} \text{Đ}^q_{x,i} f = U^k \text{Đ}^q_{x,k} V^i \text{Đ}^q_{x,i} f - V^k \text{Đ}^q_{x,k} U^i \text{Đ}^q_{x,i} f = {}^q\mathcal{L}_U {}^q\mathcal{L}_V f - {}^q\mathcal{L}_V {}^q\mathcal{L}_U f$$

and the fractional derivative has the same structure.

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Infinitely many periodic orbits for the rhomboidal five-body problem

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We prove the existence of infinitely many symmetric periodic orbits for a regularized rhomboidal five-body problem with four small masses placed at the vertices of a rhombus centered in the fifth mass. The main tool for proving the existence of such periodic orbits is the analytic continuation method of Poincaré together with the symmetries of the problem. © *2006 American Institute of Physics.*
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I. INTRODUCTION

In this paper we consider a particular case of the planar five-body problem defined as follows. We consider a mass $m_0=1$ at the origin of coordinates with zero initial velocity, two small masses $m_1=m_2=\mu\nu_1$ with initial positions and velocities on the x axis symmetric with respect to the origin, and two small masses $m_3=m_4=\mu\nu_2$ with initial positions and velocities on the y axis also symmetric with respect to the origin (see Fig. 1). Our five-body problem consists of describing the motion of the five masses under their mutual Newtonian gravitational attraction. Due to the symmetry of the initial conditions and velocities, the four small bodies form a rhombus with center at m_0 at any time and the mass m_0 remains at rest at the origin. The description of the motion of this five-body problem is called the *rhomboidal five-body problem*.

Although this is a five-body problem it can be formulated as a Hamiltonian system of two degrees of freedom, one is the distance $x\geqslant 0$ of m_1 to the origin and the other is the distance $y\geqslant 0$ of m_3 to the origin (the distances of m_2 and m_4 to the origin are obtained by symmetry). The system has three singularities, the triple collision between m_0, m_1, and m_2, the triple collision between m_0, m_3, and m_4, and the total collision of the five bodies. Due to the symmetries doing a double Levi-Civita transformation we regularize both triple collisions.

When $\mu=0$ the problem is reduced to two collision two-body problems, the collision two-body problem with m_0 and m_1 and the collision two-body problem with m_0 and m_3. Note that if we take into account the five bodies, then really for $\mu=0$ we have instead of the binary collisions m_0 with m_1, and m_0 with m_3, the triple collisions m_0, m_1, and m_2, and m_0, m_3, and m_4. Since the solutions of the collision two-body problem are known we can compute the periodic solutions of the regularized system for $\mu=0$ in a fixed energy level $h<0$. The objective of this paper is to prove that the symmetric periodic orbits of the regularized rhomboidal five-body problem for $\mu=0$ can be continued to symmetric periodic orbits of the regularized rhomboidal five-body problem for $\mu>0$ sufficiently small. The main tool for proving this result is the classical analytic continuation method of Poincaré.

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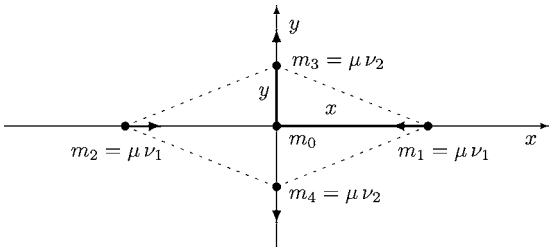

FIG. 1. The rhomboidal five-body problem.

The paper is structured as follows. In Sec. II we give the equations of motion of the rhomboidal five-body problem and we apply a double Levi-Civita transformation to regularize the triple collision between m_0, m_1, and m_2 and the triple collision between m_0, m_3, and m_4. Notice that the total collision of the five bodies is not regularized. In Sec. III we analyze the discrete symmetries of the regularized problem. In particular we see that there are three different symmetries that provide symmetric periodic solutions of the problem. We characterize these symmetric periodic solutions, and the double symmetric periodic solutions which are the main objective of this work. In Sec. IV we compute the periodic solutions of the regularized rhomboidal five-body problem for $\mu=0$ and in particular we analyze the double symmetric periodic solutions. Finally in Sec. V we apply the analytic continuation method of Poincaré to continue the double symmetric periodic orbits of the regularized rhomboidal five-body problem for $\mu=0$ to double-symmetric periodic orbits of the regularized rhomboidal five-body problem for $\mu>0$ sufficiently small.

II. EQUATIONS OF MOTION FOR THE RHOMBOIDAL FIVE-BODY PROBLEM

We consider five point particles with masses $m_0=1$, $m_1=m_2=\mu\nu_1$, $m_3=m_4=\mu\nu_2$, positions $\mathbf{q}_0=(0,0)$, $\mathbf{q}_1=(x,0)$, $\mathbf{q}_2=(-x,0)$, $\mathbf{q}_3=(0,y)$, and $\mathbf{q}_4=(0,-y)$, respectively, and velocities $\mathbf{v}_0=(0,0)$, $\mathbf{v}_1=(v_x,0)$, $\mathbf{v}_2=(-v_x,0)$, $\mathbf{v}_3=(0,v_y)$, and $\mathbf{v}_4=(0,-v_y)$, respectively (see Fig. 1). Our five-body problem consist of describing the motion of these particles under their mutual Newtonian gravitational attraction. We note that due to the symmetry of the problem the mass m_0 is at rest at the origin and the motion of the masses m_1 and m_2 (respectively, m_3 and m_4) is confined to the x axis (respectively, y axis). Since the configuration of the four bodies in motion is always a rhombus with center at m_0, we call the five-body problem the *rhomboidal five-body problem*.

Without loss of generality we can assume that the gravitational constant is $G=1$. Then the kinetic energy of the rhomboidal five-body problem is

$$T = \mu\nu_1\dot{x}^2 + \mu\nu_2\dot{y}^2,$$

where the dot denotes derivative with respect to the time t and the potential energy is

$$U = -\frac{\mu\nu_1(4+\mu\nu_1)}{2x} - \frac{\mu\nu_2(4+\mu\nu_2)}{2y} - \frac{4\mu^2\nu_1\nu_2}{\sqrt{x^2+y^2}}.$$

The Lagrangian of the problem is given by $L=T-U$. By the Legendre transformation (see, for instance, Refs. 1–3) the Hamiltonian of the problem is

$$H = \frac{p_x^2}{4\mu\nu_1} + \frac{p_y^2}{4\mu\nu_2} - \frac{\mu\nu_1(4+\mu\nu_1)}{2x} - \frac{\mu\nu_2(4+\mu\nu_2)}{2y} - \frac{4\mu^2\nu_1\nu_2}{\sqrt{x^2+y^2}},$$

where p_x and p_y are the conjugate momenta. The equations of motion associated to the Hamiltonian H are

$$\dot{x} = \frac{p_x}{2\mu\nu_1}, \quad \dot{p}_x = -\frac{\mu\nu_1(4+\mu\nu_1)}{2x^2} - \frac{4\mu^2\nu_1\nu_2 x}{(x^2+y^2)^{3/2}},$$

$$\dot{y} = \frac{p_y}{2\mu\nu_2}, \quad \dot{p}_y = -\frac{\mu\nu_2(4+\mu\nu_2)}{2y^2} - \frac{4\mu^2\nu_1\nu_2 y}{(x^2+y^2)^{3/2}}. \tag{1}$$

Doing the rescaling of the variables $x=\mu^2 X$, $y=\mu^2 Y$, and $t=\mu^3 T$, and denoting the new variables (X,Y,T) again by (x,y,t) system (1) becomes

$$\dot{x} = \frac{p_x}{2\nu_1}, \quad \dot{p}_x = -\frac{\nu_1(4+\mu\nu_1)}{2x^2} - \frac{4\mu\nu_1\nu_2 x}{(x^2+y^2)^{3/2}},$$

$$\dot{y} = \frac{p_y}{2\nu_2}, \quad \dot{p}_y = -\frac{\nu_2(4+\mu\nu_2)}{2y^2} - \frac{4\mu\nu_1\nu_2 y}{(x^2+y^2)^{3/2}}. \tag{2}$$

This system is also Hamiltonian with Hamiltonian

$$H = \frac{p_x^2}{4\nu_1} + \frac{p_y^2}{4\nu_2} - \frac{\nu_1(4+\mu\nu_1)}{2x} - \frac{\nu_2(4+\mu\nu_2)}{2y} - \frac{4\mu\nu_1\nu_2}{\sqrt{x^2+y^2}},$$

We note that system (2) has three singularities: $x=0$, that corresponds to triple collision between m_0, m_1, and m_2, $y=0$ that corresponds to triple collision between m_0, m_3, and m_4, and finally $x^2+y^2=0$ that corresponds to the total collision of the five bodies. We regularize both triple collisions applying a double Levi-Civita transformation (see Refs. 4–6)

$$x = \xi_1^2, \quad y = \xi_2^2, \quad p_x = \frac{\eta_1}{2\xi_1}, \quad p_y = \frac{\eta_2}{2\xi_2}, \quad dt = 4\xi_1^2\xi_2^2 ds.$$

The regularized system of the rhomboidal five-body problem (2) on the level energy $H=h$ for some constant h is the Hamiltonian system

$$\frac{d\xi_1}{ds} = \frac{\eta_1\xi_2^2}{2\nu_1},$$

$$\frac{d\xi_2}{ds} = \frac{\eta_2\xi_1^2}{2\nu_2},$$

$$\frac{d\eta_1}{ds} = -\frac{\xi_1\eta_2^2}{2\nu_2} + 8h\xi_1\xi_2^2 + 4\nu_2(4+\mu\nu_2)\xi_1 + \frac{32\mu\nu_1\nu_2\xi_1\xi_2^6}{(\xi_1^4+\xi_2^4)^{3/2}}, \tag{3}$$

$$\frac{d\eta_2}{ds} = -\frac{\xi_2\eta_1^2}{2\nu_1} + 8h\xi_1^2\xi_2 + 4\nu_1(4+\mu\nu_1)\xi_2 + \frac{32\mu\nu_1\nu_2\xi_1^6\xi_2}{(\xi_1^4+\xi_2^4)^{3/2}}$$

with Hamiltonian

$$K = \frac{\eta_1^2\xi_2^2}{4\nu_1} + \frac{\eta_2^2\xi_1^2}{4\nu_2} - 2\nu_2(4+\mu\nu_2)\xi_1^2 - 2\nu_1(4+\mu\nu_1)\xi_2^2 - 4h\xi_1^2\xi_2^2 - \frac{16\mu\nu_1\nu_2\xi_1^2\xi_2^2}{\sqrt{\xi_1^4+\xi_2^4}},$$

and satisfying the energy relation $K=0$; i.e., $H=h$.

We note that system (3) is analytic with respect to its variables except when $\xi_1^4+\xi_2^4=0$ which corresponds to the total collision.

The regularization of the triple collisions allows us to look for periodic orbits of the rhomboidal five-body problem containing triple collisions between m_0, m_1, and m_2 and between m_0 and m_3 and m_4. Our aim is to find periodic orbits of the rhomboidal five-body problem (3) for $\mu>0$ sufficiently small, satisfying the energy relation $K=0$. In fact, we look only for symmetric periodic orbits which are easier to study than the general periodic orbits.

III. SYMMETRIES

It is easy to check that system (3) is invariant under the discrete symmetries

$$Id: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (\xi_1, \xi_2, \eta_1, \eta_2, s),$$

$$S_1: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (-\xi_1, \xi_2, \eta_1, -\eta_2, -s),$$

$$S_2: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (\xi_1, -\xi_2, -\eta_1, \eta_2, -s),$$

$$S_3: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (\xi_1, \xi_2, -\eta_1, -\eta_2, -s),$$

$$S_4: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (-\xi_1, -\xi_2, -\eta_1, -\eta_2, s),$$

$$S_5: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (-\xi_1, \xi_2, -\eta_1, \eta_2, s),$$

$$S_6: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (\xi_1, -\xi_2, \eta_1, -\eta_2, s),$$

$$S_7: \quad (\xi_1, \xi_2, \eta_1, \eta_2, s) \to (-\xi_1, -\xi_2, \eta_1, \eta_2, -s).$$

The invariance under these symmetries means that if $\varphi(s)=(\xi_1(s), \xi_2(s), \eta_1(s), \eta_2(s))$ is a solution of system (3), then also $S_i(\varphi(s))$ is a solution for $i=1,\ldots,7$. An orbit $\varphi(s)$ is called *S_i-symmetric* if $S_i(\varphi(s))=\varphi(s)$.

We note that $\{Id, S_1, \ldots, S_7\}$ with the usual composition forms an abelian group isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$. This discrete group of symmetries appeared in many Hamiltonian systems as, for instance, the anisotropic Kepler problem,[7] the Manev anisotropic problem,[8] or the collinear three-body problem.[9]

Using the uniqueness theorem of a solution of an ordinary differential system, it follows easily that $\varphi(s)$ is a S_1-symmetric solution if and only if $\varphi(s)$ intersects the plane $\xi_1=\eta_2=0$ at least in one point. Now, it is clear that a periodic solution is S_1-symmetric if and only if it has exactly two intersection points with the plane $\xi_1=\eta_2=0$. So, clearly the half-period of such a S_1-symmetric periodic orbit is the time which the orbit needs for travel from one of the intersection points to the other. Using similar arguments for the other symmetries, we obtain the following proposition.

Proposition 1: Let $\varphi(s)=(\xi_1(s), \xi_2(s), \eta_1(s), \eta_2(s))$ *be a solution of system* (3).

(a) *If* $\xi_1(s)$ *and* $\eta_2(s)$ *are zero at* $s=s_0$ *and at* $s=s_0+S/2$ *but they are not simultaneously zero at any value of* $s \in (s_0, s_0+S/2)$, *then* $\varphi(s)$ *is a* S_1*-symmetric periodic solution of period* S.

(b) *If* $\xi_2(s)$ *and* $\eta_1(s)$ *are zero at* $s=s_0$ *and at* $s=s_0+S/2$ *but they are not simultaneously zero at any value of* $s \in (s_0, s_0+S/2)$, *then* $\varphi(s)$ *is a* S_2*-symmetric periodic solution of period* S.

(c) *If* $\eta_1(s)$ *and* $\eta_2(s)$ *are zero at* $s=s_0$ *and at* $s=s_0+S/2$ *but they are not simultaneously zero at any value of* $s \in (s_0, s_0+S/2)$, *then* $\varphi(s)$ *is a* S_3*-symmetric periodic solution of period* S.

Since in system (3) the total collision is not regularized, in our study we must avoid the orbits of the rhomboidal five-body problem which start or end in total collision. In the variables that we are working the total collision takes place when $\xi_1=\xi_2=0$. Therefore, the symmetries S_4 and S_7 are not considered because their symmetric orbits present total collision. Due to the fact that $S_5=S_1 \circ S_3$ and $S_6=S_2 \circ S_3$, studying the symmetric periodic orbits with respect to S_1, S_2, and S_3 we shall get also the symmetric periodic orbits with respect to S_5 and S_6.

There could be periodic solutions of system (3) that are simultaneously S_1- and S_2-symmetric periodic solutions. These periodic solutions will be called *S_{12}-symmetric periodic solutions*. In a similar way we can define the *S_{13}-symmetric periodic solutions* and the *S_{23}-symmetric periodic solutions*. These kinds of symmetric periodic solutions are characterized in the following result.

Proposition 2: Let $\varphi(s)=(\xi_1(s),\xi_2(s),\eta_1(s),\eta_2(s))$ *be a solution of rhomboidal five-body problem* (3).

(a) *The solution* $\varphi(s)$ *is a* S_{12}*-symmetric periodic solution of period* S *if and only if either* $\xi_1(s_0)=\eta_2(s_0)=0$, *and* $\xi_2(s_0+S/4)=\eta_1(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\xi_2(s)=\eta_1(s)=0$; *or* $\xi_2(s_0)=\eta_1(s_0)=0$, *and* $\xi_1(s_0+S/4)=\eta_2(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\xi_1(s)=\eta_2(s)=0$.

(b) *The solution* $\varphi(s)$ *is a* S_{13}*-symmetric periodic solution of period* S *if and only if either* $\xi_1(s_0)=\eta_2(s_0)=0$, *and* $\eta_1(s_0+S/4)=\eta_2(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\eta_1(s)=\eta_2(s)=0$; *or* $\eta_1(s_0)=\eta_2(s_0)=0$, *and* $\xi_1(s_0+S/4)=\eta_2(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\xi_1(s)=\eta_2(s)=0$.

(c) *The solution* $\varphi(s)$ *is a* S_{23}*-symmetric periodic solution of period* S *if and only if either* $\xi_2(s_0)=\eta_1(s_0)=0$, *and* $\eta_1(s_0+S/4)=\eta_2(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\eta_1(s)=\eta_2(s)=0$; *or* $\eta_1(s_0)=\eta_2(s_0)=0$, *and* $\xi_2(s_0+S/4)=\eta_1(s_0+S/4)=0$, *and there is no* $s\in(s_0,s_0+S/4)$ *such that* $\xi_2(s)=\eta_1(s)=0$.

The next result shows that there are no symmetric periodic orbits with respect more than two symmetries.

Proposition 3: There are no periodic solutions of the rhomboidal five-body problem (3), *which are simultaneously* S_i*-symmetric for* $i=1,2,3$.

Proof: Assume that $\varphi(s)$ is a S_i-symmetric periodic solution of period S for $i=1,2,3$. Then there exist times s_1, s_2, and s_3 with $s_1,s_2,s_3\in[0,S/2)$ such that

$$\xi_1(s_1)=\eta_2(s_1)=0,\quad \xi_2(s_2)=\eta_1(s_2)=0,\quad \eta_1(s_3)=\eta_2(s_3)=0.$$

We assume that $s_1=0$. This is not restrictive because system (3) is autonomous, and consequently the origin of time can be chosen arbitrarily. Then, since the orbit is in particular S_{12}-symmetric, from Proposition 2, $s_2=S/4$. Similarly, since it is also S_{13}-symmetric, again from Proposition 2, $s_3=S/4$. The fact that $s_2=s_3$ is a contradiction, so we have proved the result. ■

IV. SYMMETRIC PERIODIC SOLUTIONS FOR $\mu=0$

For $\mu=0$ system (3) becomes

$$\frac{d\xi_1}{ds}=\frac{\eta_1\xi_2^2}{2\nu_1},\quad \frac{d\eta_1}{ds}=-\frac{\xi_1\eta_2^2}{2\nu_2}+8h\xi_1\xi_2^2+16\nu_2\xi_1,$$

$$\frac{d\xi_2}{ds}=\frac{\eta_2\xi_1^2}{2\nu_2},\quad \frac{d\eta_2}{ds}=-\frac{\xi_2\eta_1^2}{2\nu_1}+8h\xi_1^2\xi_2+16\nu_1\xi_2, \tag{4}$$

and the Hamiltonian K goes over to

$$K=\frac{\eta_1^2\xi_2^2}{4\nu_1}+\frac{\eta_2^2\xi_1^2}{4\nu_2}-8\nu_2\xi_1^2-8\nu_1\xi_2^2-4h\xi_1^2\xi_2^2.$$

The Hamiltonian H for $\mu=0$ can be written as

$$H=H_1(x,p_x)+H_2(y,p_y)=\left(\frac{p_x^2}{4\nu_1}-\frac{2\nu_1}{x}\right)+\left(\frac{p_y^2}{4\nu_2}-\frac{2\nu_2}{y}\right).$$

We note that $H_1(x,p_x)$ and $H_2(y,p_y)$ are two fist integrals of the nonregularized problem, so they are constant along the solutions in the intervals between two consecutive zeros of x and y.

The flow of the rhomboidal five-body problem on the energy level $H=h$ for some constant h is obtained from the flow of the Hamiltonian $H_1(x,p_x)$ on the energy level $H_1=h_1$ and the flow of the Hamiltonian $H_2(y,p_y)$ on the energy level $H_2=h_2$ with $h=h_1+h_2$.

The Hamiltonian $H_1(x,p_x)$ in the Levi-Civita coordinates (ξ_1,η_1) is given by

$$H_1 = \frac{\eta_1^2}{16\nu_1\xi_1^2} - \frac{2\nu_1}{\xi_1^2} = h_1,$$

and the Hamiltonian $H_2(y, p_y)$ in the Levi-Civita coordinates (ξ_2, η_2) is

$$H_2 = \frac{\eta_2^2}{16\nu_2\xi_2^2} - \frac{2\nu_2}{\xi_2^2} = h_2.$$

Let $(\xi_1, \xi_2, \eta_1, \eta_2)$ be a solution of system (4) satisfying the energy relation $K=0$ (i.e., $H=h$), we define a new time variable σ as follows:

$$\frac{d\sigma}{ds} = \xi_2^2, \quad \text{or equivalently} \quad \frac{dt}{d\sigma} = 4\xi_1^2. \tag{5}$$

The Hamiltonian K in the new time variable σ can be written as

$$K_1 = \frac{1}{\xi_2^2}K = \frac{\eta_1^2}{4\nu_1} - 8\nu_1 - 4h_1\xi_1^2 + \left(\frac{\eta_2^2}{4\nu_2\xi_2^2} - \frac{8\nu_2}{\xi_2^2} - 4h_2\right)\xi_1^2 = \frac{\eta_1^2}{4\nu_1} - 8\nu_1 - 4h_1\xi_1^2.$$

Then ξ_1, η_1 satisfy the system of differential equations associated to the Hamiltonian K_1

$$\frac{d\xi_1}{d\sigma} = \frac{\eta_1}{2\nu_1}, \quad \frac{d\eta_1}{d\sigma} = 8h_1\xi_1. \tag{6}$$

We are only interested in the periodic solutions of system (6). Thus we must consider only negative values of h_1. Then, fixed $h_1<0$, system (6) can be integrated directly and the solution $(\xi_1(\sigma), \eta_1(\sigma))$ of system (6) with initial conditions

$$\xi_1(0) = \xi_{10}^*, \quad \eta_1(0) = \eta_{10}^*, \tag{7}$$

is

$$\xi_1(\sigma) = \xi_{10}^* \cos(w_1\sigma) + \frac{\eta_{10}^*}{2w_1\nu_1}\sin(w_1\sigma), \quad \eta_1(\sigma) = \eta_{10}^* \cos(w_1\sigma) - 2w_1\nu_1\xi_{10}^* \sin(w_1\sigma), \tag{8}$$

where $w_1 = 2\sqrt{-h_1/\nu_1}$.

We note that the solution (8) is a periodic solution of system (6) with period $\bar{\sigma} = 2\pi/w_1$. Since we are interested in the periodic solution (8) satisfying the energy relation $K_1=0$, by Eq. (5), its period in the real time t is given by

$$T_1(h_1, \nu_1) = \int_0^{\bar{\sigma}} 4\xi_1^2(\sigma)d\sigma = 4\pi\left(-\frac{\nu_1}{h_1}\right)^{3/2}.$$

Now we introduce a new time τ with

$$\frac{d\tau}{ds} = \xi_1^2, \quad \text{or equivalently} \quad \frac{dt}{d\tau} = 4\xi_2^2. \tag{9}$$

Then ξ_2, η_2 are functions of the new time τ via the Hamiltonian system

$$\frac{d\xi_2}{d\tau} = \frac{\eta_2}{2\nu_2}, \quad \frac{d\eta_2}{d\tau} = 8h_2\xi_2, \tag{10}$$

with Hamiltonian

TABLE I. Period of $\varphi(s)$.

Time t	Time σ	Time τ	Time s
$T=pT_1(h_1,\nu_1)=qT_2(h_2,\nu_2)$	$\sigma^*=p\bar{\sigma}$	$\tau^*=q\bar{\tau}$	$S^*=s(T)$
$T/4$	$\sigma^*/4$	$\tau^*/4$	$S^*/4$

$$K_2=\frac{1}{\xi_1^2}K=\frac{\eta_2^2}{4\nu_2}-8\nu_2-4h_2\xi_2^2.$$

Moreover, fixed $h_2<0$, the solution $(\xi_2(\tau),\eta_1(\tau))$ of system (10) with initial conditions

$$\xi_2(0)=\xi_{20}^*,\quad \eta_2(0)=\eta_{20}^*, \tag{11}$$

is given by

$$\xi_2(\tau)=\xi_{20}^*\cos(w_2\tau)+\frac{\eta_{20}^*}{2w_2\nu_2}\sin(w_2\tau),\quad \eta_2(\tau)=\eta_{20}^*\cos(w_2\tau)-2w_2\nu_2\xi_{20}^*\sin(w_2\tau), \tag{12}$$

where $w_2=2\sqrt{-h_2/\nu_2}$.

The solution (12) is periodic of period $\bar{\tau}=2\pi/w_2$. Moreover, if the solution (12) satisfies the energy relation $K_2=0$, then, by Eq. (9), the period of the solution (12) in the real time t is given by

$$T_2(h_2,\nu_2)=\int_0^{\bar{\tau}}4\xi_2^2(\tau)d\tau=4\pi\left(-\frac{\nu_2}{h_2}\right)^{3/2}.$$

Proposition 4: Let $(\xi_1(\sigma),\eta_1(\sigma))$ *be a periodic solution of system* (6), *for a fixed* $h_1<0$, *with initial conditions* (7) *and period* $\bar{\sigma}=2\pi/w_1$ *that satisfies* $K_1=0$. *Let* $(\xi_2(\tau),\eta_2(\tau))$ *be the periodic solution of system* (10), *for a fixed* $h_2<0$, *with initial conditions* (11) *and period* $\bar{\tau}=2\pi/w_2$ *that satisfies* $K_2=0$. *Assume that* $h=h_1+h_2$, *and that* $\sigma(s)$ *and* $\tau(s)$ *are given by Eqs.* (5) and (9), *respectively*, *where we choose* $\sigma(0)=\tau(0)=0$. *Suppose that there is no* $s\in\mathbb{R}$ *such that* $\xi_1(\sigma(s))=\xi_2(\tau(s))=0$. *Then the following statements hold*:

(a) $\varphi(s)=(\xi_1(\sigma(s)),\xi_2(\tau(s)),\eta_1(\sigma(s)),\eta_2(\tau(s))$ *is a solution of system* (4) *with initial conditions* $\xi_1(0)=\xi_{10}^*$, $\xi_2(0)=\xi_{20}^*$, $\eta_1(0)=\eta_{10}^*$, *and* $\eta_2(0)=\eta_{20}^*$ *that satisfies* $K=0$.

(b) *If* $h_1=(p/q)^{2/3}\nu_1h_2/\nu_2$ *for some* $p,q\in\mathbb{N}$ *coprime*, *then* $\varphi(s)$ *is a periodic solution of system* (4).

(c) *Assume that* $s(t)$ *is given by the inverse function of* $t=\int_0^s 4\xi_1^2(\rho)\xi_2^2(\rho)d\rho$. *Under the hypotheses of statement* (b), *the period and the quarter of the period of the periodic solution* $\varphi(s)$ *using the different times* t, σ, τ, *and* s *is given in* Table I.

Proof: Statement (a) follows easily from the definitions of $(\xi_1(\sigma),\eta_1(\sigma))$ and $(\xi_2(\tau),\eta_2(\tau))$ together with the definitions of $\sigma(s)$ and $\tau(s)$.

We have seen that, in the time t, $(\xi_1(\sigma),\eta_1(\sigma))$ and $(\xi_2(\tau),\eta_2(\tau))$ are periodic solutions of periods $T_1(h_1,\nu_1)$ and $T_2(h_2,\nu_2)$, respectively. Thus, in order to have a periodic solution of system (4) we need that

$$pT_1(h_1,\nu_1)=qT_2(h_2,\nu_2), \tag{13}$$

for some $p,q\in\mathbb{N}$ coprime. Solving Eq. (13) with respect to h_1, we get that $h_1=(p/q)^{2/3}\nu_1h_2/\nu_2$. So, statement (b) is proved.

Now we see that the time $t=T/4$ corresponds to the time $\sigma=\sigma^*/4$. In a similar way we can see that the time $t=T/4$ corresponds to the time $\tau=\tau^*/4$ and $s=S^*/4$.

We note that system (6) is invariant under the symmetry $(\xi_1, \eta_1, \sigma) \to (-\xi_1, \eta_1, -\sigma)$. This means that $\xi_1(\sigma) = -\xi_1(-\sigma)$. So $\xi_1^2(\sigma)$ is an even function. On the other hand, it is easy to see that $\xi_1^2(\sigma)$ is a periodic function of period $\bar{\sigma}/2$. Then, from Eq. (5), we have that

$$T_1 = \int_0^{\bar{\sigma}} 4\xi_1^2(\sigma)d\sigma = 2\int_0^{\bar{\sigma}/2} 4\xi_1^2(\sigma)d\sigma = 4\int_0^{\bar{\sigma}/4} 4\xi_1^2(\sigma)d\sigma.$$

Moreover, it is clear that

$$\int_0^{\bar{\sigma}/4} 4\xi_1^2(\sigma)d\sigma = \int_{\bar{\sigma}/4}^{\bar{\sigma}/2} 4\xi_1^2(\sigma)d\sigma = \frac{T_1}{4}.$$

Consequently

$$t(\sigma^*/4) = \int_0^{p\bar{\sigma}/4} 4\xi_1^2(\sigma)d\sigma = p\int_0^{\bar{\sigma}/4} 4\xi_1^2(\sigma)d\sigma = p\frac{T_1}{4} = \frac{T}{4}.$$

Therefore, the time $t = T/4$ corresponds to $\sigma = \sigma^*/4$. In short, statement (c) is proved. ■

We remark that the number p in Proposition 4 represents the number of triple collisions between m_0, m_1, and m_2 during a period, whereas q represents the number of triple collisions between m_0, m_3, and m_4.

We are interested in symmetric periodic solutions of system (4) satisfying the energy relation $K = 0$ with $h = h_1 + h_2$. In the next proposition we give initial conditions for those symmetric periodic solutions.

Proposition 5: The following statements hold:

(a) *If p and q are odd, then the solution $\varphi(s)$ given by Proposition 4 with initial conditions*

$$\text{either } \xi_{10}^* = 0,\ \xi_{20}^* = \sqrt{-2\nu_2/h_2},\ \eta_{10}^* = 4\sqrt{2}\nu_1,\ \eta_{20}^* = 0;$$

$$\text{or } \xi_{10}^* = \sqrt{-2\nu_1/h_1},\ \xi_{20}^* = 0,\ \eta_{10}^* = 0,\ \eta_{20}^* = 4\sqrt{2}\nu_2;$$

is a S_{12}-symmetric periodic solution.

(b) *If p is odd and q is even, then the solution $\varphi(s)$ given by Proposition 4 with initial conditions*

$$\text{either } \xi_{10}^* = 0,\ \xi_{20}^* = \sqrt{-2\nu_2/h_2},\ \eta_{10}^* = 4\sqrt{2}\nu_1,\ \eta_{20}^* = 0;$$

$$\text{or } \xi_{10}^* = \sqrt{-2\nu_1/h_1},\ \xi_{20}^* = \sqrt{-2\nu_2/h_2},\ \eta_{10}^* = 0,\ \eta_{20}^* = 0;$$

is a S_{13}-symmetric periodic solution.

(c) *If p is even and q is odd, then the solution $\varphi(s)$ given by Proposition 4 with initial conditions*

$$\text{either } \xi_{10}^* = \sqrt{-2\nu_1/h_1},\ \xi_{20}^* = 0,\ \eta_{10}^* = 0,\ \eta_{20}^* = 4\sqrt{2}\nu_2;$$

$$\text{or } \xi_{10}^* = \sqrt{-2\nu_1/h_1},\ \xi_{20}^* = \sqrt{-2\nu_2/h_2},\ \eta_{10}^* = 0,\ \eta_{20}^* = 0;$$

is a S_{23}-symmetric periodic solution.

Proof: Solving $K_1 = 0$ and $K_2 = 0$ for the initial conditions of the S_{12}-symmetric periodic orbits given in Proposition 2(a) we get the initial conditions of statement (a). In these initial conditions we have only considered the positive determination in the squareroots due to the fact that the Levi-Civita transformation duplicates the orbits. The proof follows from the evaluation of the solution $\varphi(s) = (\xi_1(\sigma(s)), \xi_2(\tau(s)), \eta_1(\sigma(s)), \eta_2(\tau(s))$ with these initial conditions at times $s = 0$ and

$s=S^*/4$. We note that by Table I $\varphi(S^*/4)=(\xi_1(p\bar{\sigma}/4),\xi_2(q\bar{\tau}/4),\eta_1(p\bar{\sigma}/4),\eta_2(q\bar{\tau}/4))$. This completes the proof of statement (a). The other statements follow similarly. ■

V. CONTINUATION OF SYMMETRIC PERIODIC SOLUTIONS

In this section using the continuation method of Poincaré (see, for instance, Ref. 10) we shall continue the symmetric periodic orbits of the rhomboidal five-body problem (3) from $\mu=0$ to symmetric periodic orbits of system (3) for $\mu>0$ sufficiently small.

A. The S_{12}-symmetric periodic solutions

We denote by $\varphi(s;0,\xi_{20},\eta_{10},0,\mu)=(\xi_1(s;\xi_{20},\eta_{10},\mu),\xi_2(s;\xi_{20},\eta_{10},\mu),\eta_1(s;\xi_{20},\eta_{10},\mu),\eta_2(s;\xi_{20},\eta_{10},\mu))$ the solution of (3), for fixed values of $\nu_1>0$, $\nu_2>0$, and $h<0$, with initial conditions $\xi_1(0)=0$, $\xi_2(0)=\xi_{20}$, $\eta_1(0)=\eta_{10}$, and $\eta_2(0)=0$. From Proposition 2(a), $\varphi(s;0,\xi_{20},\eta_{10},0,\mu)$ is a S_{12}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation$K=0$ if and only if

$$\xi_2(S/4;\xi_{20},\eta_{10},\mu)=0,\quad \eta_1(S/4;\xi_{20},\eta_{10},\mu)=0,\quad K(\xi_{20},\eta_{10},\mu)=0.$$

We solve equation $K(\xi_{20},\eta_{10},\mu)=0$ with respect the variable η_{10} obtaining in this way

$$\eta_{10}=2\sqrt{2}\nu_1\sqrt{4+\mu\nu_1}. \tag{14}$$

So $\varphi(s;0,\xi_{20},\eta_{10},0,\mu)$ is a S_{12}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation $K=0$ if and only if

$$\xi_2(S/4;\xi_{20},\mu)=0,\quad \eta_1(S/4;\xi_{20},\mu)=0. \tag{15}$$

Notice that we have omitted the dependence with respect to η_{10}, which is given by Eq. (14).

Assume that $p=2\ell+1$, $q=2k+1$ for some $\ell,k\in\mathbb{N}\cup\{0\}$ and that h_1^* and h_2^* verify that $h=h_1^*+h_2^*$ and $h_1^*=(p/q)^{2/3}\nu_1h_2^*/\nu_2$. By Propositions 4 and 5(a), we see that $S=S^*=s(pT_1(h_1^*))=s(qT_2(h_2^*))$, $\xi_{20}=\xi_{20}^*=\sqrt{-2\nu_2/h_2^*}$, is a solution of system (15) for $\mu=0$. This solution correspond to the known S_{12}-symmetric periodic solution $\varphi(s;0,\xi_{20}^*,\eta_{10}^*,0,0)$ of system (3), for $\mu=0$ where $\eta_{10}^*=4\sqrt{2}\nu_1$. Our aim is to continue this solution of system (15) for $\mu=0$ to $\mu>0$ sufficiently small.

Applying the implicit function theorem to system (15) in a neighborhood of the known solution we have that if

$$\left.\begin{vmatrix} \dfrac{\partial\xi_2}{\partial s} & \dfrac{\partial\xi_2}{\partial\xi_{20}} \\ \dfrac{\partial\eta_1}{\partial s} & \dfrac{\partial\eta_1}{\partial\xi_{20}} \end{vmatrix}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*\\ \mu=0}}\neq 0, \tag{16}$$

then we can find unique analytic functions $\xi_{20}=\xi_{20}(\mu)$, $S=S(\mu)$ defined for $\mu\geqslant 0$ sufficiently small, such that

(i) $\xi_{20}(0)=\xi_{20}^*$, $S(0)=S^*$,
(ii) $\varphi(s;0,\xi_{20},\eta_{10},0,\mu)$ with $\xi_{20}=\xi_{20}(\mu)$ and η_{10} given by (14) is a S_{12}-symmetric periodic solution of system (3) with period $S=S(\mu)$ that satisfies the energy relation $K=0$.

The derivatives $\partial\xi_2/\partial s$ and $\partial\eta_1/\partial s$ evaluated at $s=S^*/4$, $\xi_{20}=\xi_{20}^*$ and $\mu=0$ can be obtained directly from system (3) for $\mu=0$ [i.e., system (4)], evaluating the right hand of the system at the solution $\varphi(s;0,\xi_{20}^*,\eta_{10}^*,0,0)$ at time $s=S^*/4$. Then

$$\left.\frac{\partial \xi_2}{\partial s}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*\\ \mu=0}} = \left.\frac{1}{2\nu_2}\eta_2\xi_1^2\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*\\ \mu=0}} = \frac{4(-1)^k\sqrt{2}\nu_2}{h_2^*}\left(\frac{q}{p}\right)^{2/3} \neq 0$$

and

$$\left.\frac{\partial \eta_1}{\partial s}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*\\ \mu=0}} = \left.8h_1^*\xi_1\xi_2^2\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*\\ \mu=0}} = 0.$$

It only remains to compute the value of $\partial\eta_1/\partial\xi_{20}$ evaluated at $s=S^*/4$, $\xi_{20}=\xi_{20}^*$, $\mu=0$. This value is given by the derivative, evaluated at $s=S^*/4$ and $\xi_{20}=\xi_{20}^*$, of the solution $\eta_1(\sigma(s);0,\xi_{20},\eta_{10}^*,0,0)$ with respect to ξ_{20}, where $\eta_1(\sigma(s);0,\xi_{20},\eta_{10}^*,0,0)$ is the solution of system (4) with initial conditions $\xi_1(0)=0$, $\xi_2(0)=\xi_{20}$, $\eta_1(0)=\eta_{10}^*$, and $\eta_2(0)=0$ satisfying the energy relation $K=0$ [see Proposition 4(a)]. Then

$$\left.\frac{\partial \eta_1(\sigma(s);0,\xi_{20},\eta_{10}^*,0,0)}{\partial \xi_{20}}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = \left.\left(\frac{\partial \eta_1}{\partial \sigma}\frac{\partial \sigma(s)}{\partial \xi_{20}} + \frac{\partial \eta_1}{\partial \xi_{20}}\right)\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}}.$$

From Eqs. (5) and (9), we have that the times σ and τ are related by

$$\xi_1^2(\sigma)d\sigma = \xi_2^2(\tau)d\tau.$$

Integrating this equation over the solutions (8) and (12) with the corresponding initial conditions and assuming that when $\sigma(0)=\tau(0)=0$, we have that $\sigma(s)$ and $\tau(s)$ are related by the equation

$$\frac{4\sigma(s)}{w_1^2} - \frac{\xi_{20}^2\tau(s)}{2} - \frac{2\sin(2w_1\sigma(s))}{w_1^3} - \frac{\xi_{20}^2\sin(2w_2\tau(s))}{4w_2} = 0. \tag{17}$$

Since $\varphi(s;0,\xi_{20},\eta_{10}^*,0,0)$ must be a solution of system (4), by Proposition 4 we have that $K_1=0$ and $K_2=0$, so

$$w_2 = 2\sqrt{-h_2/\nu_2}, \quad \text{with} \quad h_2 = -2\nu_2/\xi_{20}^2$$

and

$$w_1 = 2\sqrt{-h_1/\nu_1}, \quad \text{with} \quad h_1 = h - h_2.$$

Then derivating implicitly Eq. (17) with respect to ξ_{20} we obtain

$$\left.\frac{\partial \sigma(s)}{\partial \xi_{20}}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = \frac{\pi q}{8\sqrt{2}\nu_1}\left(3\left(\frac{p}{q}\right)^{2/3}\nu_1 + \nu_2\right).$$

On the other hand, from systems (6) and (8) we have that

$$\left.\frac{\partial \eta_1}{\partial \sigma}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = \left.8h_1\xi_1\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = 8(-1)^{\ell+1}\sqrt{2}\nu_1\left(\frac{p}{q}\right)^{1/3}\sqrt{-\frac{h_2^*}{\nu_2}}$$

and

$$\left.\frac{\partial \eta_1}{\partial \xi_{20}}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = 2(-1)^{\ell}ph_2^*\pi\left(\frac{q}{p}\right)^{2/3}\sqrt{-\frac{\nu_2}{h_2^*}}.$$

Hence

$$\left.\frac{\partial \eta_1(\sigma(s);0,\xi_{20},\eta_{10}^*,0,0)}{\partial \xi_{20}}\right|_{\substack{s=S^*/4\\ \xi_{20}=\xi_{20}^*}} = 3(-1)^{\ell+1}\pi\sqrt{-\frac{h_2^*}{\nu_2}}\left(p\nu_1+\left(\frac{p}{q}\right)^{1/3}q\nu_2\right).$$

So, this derivative is different from zero. Hence, the determinant (16) is not zero. In short, we have proved the following result.

Theorem 6: *Given* $\nu_1>0$, $\nu_2>0$, $h<0$ *and* p *and* q *odd positive integers, the* S_{12}*-symmetric periodic solution of the rhomboidal five-body problem* (3) *for* $\mu=0$ *with initial conditions* $\xi_1(0)=0$, $\xi_2(0)=\sqrt{-2\nu_2/h_2^*}$, $\eta_1(0)=4\sqrt{2}\nu_1$, *and* $\eta_2(0)=0$ *where* $h_2^*=h\nu_2/((p/q)^{2/3}\nu_1+\nu_2)$, *can be continued to a* μ*-parameter family of* S_{12}*-symmetric periodic orbits of the rhomboidal five-body problem* (3) *for* $\mu>0$ *sufficiently small.*

B. The S_{23}-symmetric periodic solutions

We denote by $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)=(\xi_1(s;\xi_{10},\xi_{20},\mu),\xi_2(s;\xi_{10},\xi_{20},\mu),\eta_1(s;\xi_{10},\xi_{20},\mu),\eta_2(s;\xi_{10},\xi_{20},\mu))$ the solution of system (3), for fixed values of $\nu_1>0$, $\nu_2>0$, and $h<0$, with initial conditions $\xi_1(0)=\xi_{10}$, $\xi_2(0)=\xi_{20}$, $\eta_1(0)=0$, and $\eta_2(0)=0$. From Proposition 2(c), $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ is a S_{23}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation $K=0$ if and only if

$$\xi_2(S/4;\xi_{10},\xi_{20},\mu)=0,\quad \eta_1(S/4;\xi_{10},\xi_{20},\mu)=0,\quad K(\xi_{10},\xi_{20},\mu)=0.$$

We solve equation $K(\xi_{10},\xi_{20},\mu)=0$ with respect to the variable ξ_{20} obtaining in this way $\xi_{20}=\xi_{20}(\xi_{10},\mu)$. In particular, $\xi_{20}(\xi_{10},0)=\sqrt{2\nu_2}\xi_{10}/\sqrt{-2\nu_1-h\xi_{10}^2}$. So $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ is a S_{23}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation $K=0$ if and only if

$$\xi_2(S/4;\xi_{10},\mu)=0,\quad \eta_1(S/4;\xi_{10},\mu)=0. \tag{18}$$

Assume that $p=2\ell$, $q=2k+1$ for some $\ell\in\mathbb{N}$ and $k\in\mathbb{N}\cup\{0\}$ and that h_1^* and h_2^* verify that $h=h_1^*+h_2^*$ and $h_1^*=(p/q)^{2/3}\nu_1h_2^*/\nu_2$. By Propositions 4 and 5(c), we see that $S=S^*=s(pT_1(h_1^*))=s(qT_2(h_2^*))$, $\xi_{10}=\xi_{10}^*=\sqrt{-2\nu_1/h_1^*}$ is a solution of system (18) for $\mu=0$. This solution corresponds to the known S_{23}-symmetric periodic solution $\varphi(s;\xi_{10}^*,\xi_{20}^*,0,0,0)$ of system (3), for $\mu=0$ where $\xi_{20}=\xi_{20}^*=\sqrt{-2\nu_2/h_2^*}$. Our aim is to continue this solution of system (18) for $\mu=0$ to $\mu>0$ sufficiently small.

Applying the implicit function theorem to system (18) in a neighborhood of the known solution we have that if

$$\left.\begin{vmatrix}\frac{\partial\xi_2}{\partial s} & \frac{\partial\xi_2}{\partial\xi_{10}}\\ \frac{\partial\eta_1}{\partial s} & \frac{\partial\eta_1}{\partial\xi_{10}}\end{vmatrix}\right|_{\substack{s=S^*/4\\ \xi_{10}=\xi_{10}^*\\ \mu=0}}\neq 0, \tag{19}$$

then we can find unique analytic functions $\xi_{10}=\xi_{10}(\mu)$, $S=S(\mu)$ defined for $\mu\geqslant 0$ sufficiently small, such that

(i) $\xi_{10}(0)=\xi_{10}^*$, $S(0)=S^*$,
(ii) $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ with $\xi_{10}=\xi_{10}(\mu)$ and $\xi_{20}=\xi_{20}(\xi_{10}(\mu),\mu)$ is a S_{23}-symmetric periodic solution of system (3) with period $S=S(\mu)$ that satisfies the energy relation $K=0$.

Working as for the S_{12}-symmetry we get that

$$\left.\frac{\partial \xi_2}{\partial s}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^* \\ \mu=0}} \neq 0, \quad \text{and} \quad \left.\frac{\partial \eta_1}{\partial s}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^* \\ \mu=0}} = 0.$$

It only remains to compute the value of $\partial\eta_1/\partial\xi_{10}$ evaluated at $s=S^*/4$, $\xi_{10}=\xi_{10}^*$, $\mu=0$. This value is given by the derivative, evaluated at $s=S^*/4$ and $\xi_{10}=\xi_{10}^*$, of the solution $\eta_1(\sigma(s);\xi_{10},\xi_{20},0,0,0)$ with respect to ξ_{10}, where $\eta_1(\sigma(s);\xi_{10},\xi_{20},0,0,0)$ is the solution of system (4) with initial conditions $\xi_1(0)=\xi_{10}$, $\xi_2(0)=\xi_{20}(\xi_{10},0)$, $\eta_1(0)=0$, and $\eta_2(0)=0$ satisfying the energy relation $K=0$ [see Proposition 4(c)]. Then

$$\left.\frac{\partial \eta_1(\sigma(s);0,\xi_{10},\xi_{20},0,0,0)}{\partial \xi_{10}}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^*}} = \left.\left(\frac{\partial \eta_1}{\partial \sigma}\frac{\partial \sigma(s)}{\partial \xi_{10}} + \frac{\partial \eta_1}{\partial \xi_{10}}\right)\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^*}}$$
$$= \frac{3(-1)^{\ell+1}h_2^* p\pi\nu_1}{q\nu_2^2}\left(p\nu_1 + \left(\frac{p}{q}\right)^{1/3} q\nu_2\right),$$

so this derivative is different from zero. Hence, the determinant (19) is not zero. In short, we have proved the following result.

Theorem 7: *Given $\nu_1>0$, $\nu_2>0h<0$, p even and q odd positive integers, the S_{23}-symmetric periodic solution of the rhomboidal five-body problem (3) for $\mu=0$ with initial conditions $\xi_1(0)=\sqrt{-2\nu_1/h_1^*}$, $\xi_2(0)=\sqrt{-2\nu_2/h_2^*}$, $\eta_1(0)=0$, and $\eta_2(0)=0$, where $h_2^*=h\nu_2/((p/q)^{2/3}\nu_1+\nu_2)$, $h_1^*=h(p/q)^{2/3}\nu_1/((p/q)^{2/3}\nu_1+\nu_2)$, can be continued to a μ-parameter family of S_{23}-symmetric periodic orbits of the rhomboidal five-body problem (3) for $\mu>0$ sufficiently small.*

C. The S_{13}-symmetric periodic solutions

Let $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ be the solution of system (3), for fixed values of $\nu_1>0$, $\nu_2>0$, and $h<0$, defined as in Sec. V B. From Proposition 2(b), $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ is a S_{13}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation $K=0$ if and only if

$$\xi_1(S/4;\xi_{10},\xi_{20},\mu)=0, \quad \eta_2(S/4;\xi_{10},\xi_{20},\mu)=0, \quad K(\xi_{10},\xi_{20},\mu)=0.$$

Let $\xi_{20}=\xi_{20}(\xi_{10},\mu)$ be the function defined in Sec. V B. Then $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ is a S_{13}-symmetric periodic solution of the rhomboidal five-body problem with period S satisfying the energy relation $K=0$ if and only if

$$\xi_1(S/4;\xi_{10},\mu)=0, \quad \eta_2(S/4;\xi_{10},\mu)=0. \tag{20}$$

Assume that $p=2\ell+1$, $q=2k$ for some $\ell\in\mathbb{N}\cup\{0\}$ and $k\in\mathbb{N}$ and that h_1^* and h_2^* verify that $h=h_1^*+h_2^*$ and $h_1^*=(p/q)^{2/3}\nu_1 h_2^*/\nu_2$. By Propositions 4 and 5(b), we see that $S=S^*=s(pT_1(h_1^*))=s(qT_2(h_2^*))$, $\xi_{10}=\xi_{10}^*=\sqrt{-2\nu_1/h_1^*}$ is a solution of system (20) for $\mu=0$. This solution correspond to the known S_{13}-symmetric periodic solution $\varphi(s;\xi_{10}^*,\xi_{20}^*,0,0,0)$ of system (3), for $\mu=0$ where $\xi_{20}=\xi_{20}^*=\sqrt{-2\nu_2/h_2^*}$. Our aim is to continue this solution of system (20) for $\mu=0$ to $\mu>0$ sufficiently small.

Applying the implicit function theorem to system (20) in a neighborhood of the known solution we have that if

$$\left.\begin{vmatrix} \dfrac{\partial \xi_1}{\partial s} & \dfrac{\partial \xi_1}{\partial \xi_{10}} \\ \dfrac{\partial \eta_2}{\partial s} & \dfrac{\partial \eta_2}{\partial \xi_{10}} \end{vmatrix}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^* \\ \mu=0}} \neq 0, \tag{21}$$

then we can find unique analytic functions $\xi_{10}=\xi_{10}(\mu)$, $S=S(\mu)$ defined for $\mu \geqslant 0$ sufficiently small, such that

(i) $\xi_{10}(0)=\xi_{10}^*$, $S(0)=S^*$,

(ii) $\varphi(s;\xi_{10},\xi_{20},0,0,\mu)$ with $\xi_{10}=\xi_{10}(\mu)$ and $\xi_{20}=\xi_{20}(\xi_{10}(\mu),\mu)$ is a S_{13}-symmetric periodic solution of system (3) with period $S=S(\mu)$ that satisfies the energy relation $K=0$.

Working as for the S_{12}-symmetry we get that

$$\left.\frac{\partial \xi_1}{\partial s}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^* \\ \mu=0}} \neq 0, \quad \text{and} \quad \left.\frac{\partial \eta_2}{\partial s}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^* \\ \mu=0}} = 0.$$

It only remains to compute the value of $\partial \eta_2/\partial \xi_{10}$ evaluated at $s=S^*/4$, $\xi_{10}=\xi_{10}^*$, $\mu=0$. This value is given by the derivative, evaluated at $s=S^*/4$ and $\xi_{10}=\xi_{10}^*$, of the solution $\eta_2(\tau(s);\xi_{10},\xi_{20},0,0,0)$ with respect to ξ_{10}, where $\eta_2(\tau(s);\xi_{10},\xi_{20},0,0,0)$ is the solution of system (4) with initial conditions $\xi_1(0)=\xi_{10}$, $\xi_2(0)=\xi_{20}(\xi_{10},0)$, $\eta_1(0)=0$, and $\eta_2(0)=0$ satisfying the energy relation $K=0$ [see Proposition 4(b)]. Then

$$\begin{aligned} \left.\frac{\partial \eta_2(\tau(s);\xi_{10},\xi_{20},0,0,0)}{\partial \xi_{10}}\right|_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^*}} &= \left(\frac{\partial \eta_2}{\partial \tau}\frac{\partial \tau(s)}{\partial \xi_{10}} + \frac{\partial \eta_2}{\partial \xi_{10}}\right)_{\substack{s=S^*/4 \\ \xi_{10}=\xi_{10}^*}} \\ &= \frac{(-1)^k h_2 \pi}{\nu_2}\left(p\nu_1 + \left(\frac{p}{q}\right)^{1/3} q(2\nu_1+3\nu_2)\right), \end{aligned}$$

so this derivative is different from zero. Hence, the determinant (21) is not zero. In short, we have proved the following result.

Theorem 8: *Given $\nu_1>0$, $\nu_2>0$, $h<0$, p odd and q even positive integers, the S_{13}-symmetric periodic solution of the rhomboidal five-body problem (3) for $\mu=0$ with initial conditions $\xi_1(0)=\sqrt{-2\nu_1/h_1^*}$, $\xi_2(0)=\sqrt{-2\nu_2/h_2^*}$, $\eta_1(0)=0$, and $\eta_2(0)=0$ where $h_2^*=h\nu_2/((p/q)^{2/3}\nu_1+\nu_2)$, $h_1^*=h(p/q)^{2/3}\nu_1/((p/q)^{2/3}\nu_1+\nu_2)$, can be continued to a μ-parameter family of S_{13}-symmetric periodic orbits of the rhomboidal five-body problem (3) for $\mu>0$ sufficiently small.*

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Perturbed block circulant matrices and their application to the wavelet method of chaotic control

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Controlling chaos via wavelet transform was proposed by Wei *et al.* [Phys. Rev. Lett. **89**, 284103.1–284103.4 (2002)]. It was reported there that by modifying a tiny fraction of the wavelet subspace of a coupling matrix, the transverse stability of the synchronous manifold of a coupled chaotic system could be dramatically enhanced. The stability of chaotic synchronization is actually controlled by the second largest eigenvalue $\lambda_2(\alpha,\beta)$ of the (wavelet) transformed coupling matrix $C(\alpha,\beta)$ for each α and β. Here β is a mixed boundary constant and α is a scalar factor. In particular, $\beta=1$ (0) gives the nearest neighbor coupling with periodic (Neumann) boundary conditions. In this paper, we obtain two main results. First, the reduced eigenvalue problem for $C(\alpha,0)$ is completely solved. Some partial results for the reduced eigenvalue problem of $C(\alpha,\beta)$ are also obtained. Second, we are then able to understand behavior of $\lambda_2(\alpha,0)$ and $\lambda_2(\alpha,1)$ for any wavelet dimension $j\in\mathbb{N}$ and block dimension $n\in\mathbb{N}$. Our results complete and strengthen the work of Shieh *et al.* [J. Math. Phys. **47**, 082701.1–082701.10 (2006)] and Juang and Li [J. Math. Phys. **47**, 072704.1–072704.16 (2006)]. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2400828]

I. INTRODUCTION

Of concern here is the eigencurve problem for a class of "perturbed" block circulant matrices.

$$C(\alpha,\beta)\mathbf{b}=\lambda(\alpha,\beta)\mathbf{b}. \tag{1.1a}$$

Here $C(\alpha,\beta)$ is an $n\times n$ block matrix of the following form:

$$C(\alpha,\beta)=\begin{pmatrix} C_1(\alpha,\beta) & C_2(\alpha,1) & 0 & \cdots & 0 & C_2^T(\alpha,\beta) \\ C_2^T(\alpha,1) & C_1(\alpha,1) & C_2(\alpha,1) & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & C_2^T(\alpha,1) & C_1(\alpha,1) & C_2(\alpha,1) \\ C_2(\alpha,\beta) & 0 & \cdots & 0 & C_2^T(\alpha,1) & \hat{I}C_1(\alpha,\beta)\hat{I} \end{pmatrix}_{n\times n}. \tag{1.1b}$$

Here

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$$C_1(\alpha,\beta)=\begin{pmatrix} -1-\beta & 1 & 0 & \cdots & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & \cdots & 0 & 1 & -2 \end{pmatrix}_{2^j\times 2^j} - \frac{\alpha(1+\beta)}{2^{2j}}ee^T =: A_1(\beta,2^j) - \frac{\alpha(1+\beta)}{2^{2j}}ee^T, \tag{1.1c}$$

where $e=(1,1,\ldots,1)^T$, j is a positive integer, $\alpha>0$ is a (wavelet) scalar factor, and $\beta\in\mathbb{R}$ represents a mixed boundary constant. Moreover,

$$C_2(\alpha,\beta)=\begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & & & 0 \\ \beta & 0 & \cdots & 0 \end{pmatrix} + \frac{\alpha\beta}{2^{2j}}ee^T =: A_2(\beta,2^j) + \frac{\alpha\beta}{2^{2j}}ee^T, \tag{1.1d}$$

$$\hat{I}=\begin{pmatrix} 0 & 0 & \cdots & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ \vdots & & \cdot & \cdot & \cdot & \vdots \\ \vdots & \cdot & \cdot & \cdot & & \vdots \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & \cdots & 0 & 0 \end{pmatrix}. \tag{1.1e}$$

The dimension of $C(\alpha,\beta)$ is $n2^j\times n2^j$. From here on, we shall call n and j the block and the wavelet dimensions of $C(\alpha,\beta)$, respectively. $C(\alpha,\beta)$ is a block circulant matrix (see, e.g., Ref. 1) only if $\beta=1$. It is well known, see, e.g., Theorem 5.6.4 of Ref. 1, that for each α the eigenvalues of $C(\alpha,1)$ consist of eigenvalues of a certain linear combinations of its block matrices. Such results are called the reduced eigenvalue problem for $C(\alpha,1)$.

This problem arises in the wavelet method for a chaotic control.[7] It is found there that the modification of a tiny fraction of wavelet subspaces of a coupling matrix could lead to a dramatic change in chaos synchronizing properties. We begin with describing their work. Let there be N nodes (oscillators). Assume $\mathbf{u}_i$ is the m-dimensional vector of dynamical variables of the ith node. Let the isolated (uncoupling) dynamics be $\dot{\mathbf{u}}_i=f(\mathbf{u}_i)$ for each node. Used in the coupling, $h:\mathbb{R}^m\to\mathbb{R}^m$ is an arbitrary function of each node's variables. Thus, the dynamics of the ith node is

$$\dot{\mathbf{u}}_i=f(\mathbf{u}_i)+\epsilon\sum_{j=1}^{N}a_{ij}h(\mathbf{u}_j),\quad i=1,2,\ldots,N, \tag{1.2a}$$

where ϵ is a coupling strength. The sum $\Sigma_{j=1}^{N}a_{ij}=0$. Let $\mathbf{u}=(\mathbf{u}_1,\mathbf{u}_2,\ldots,\mathbf{u}_N)^T$, $F(\mathbf{u})=(f(\mathbf{u}_1),f(\mathbf{u}_2),\ldots,f(\mathbf{u}_N))^T$, $H(\mathbf{u})=(h(\mathbf{u}_1),h(\mathbf{u}_2),\ldots,h(\mathbf{u}_N))^T$, and $A=(a_{ij})$. We may write Eq. (1.1a) as

$$\dot{\mathbf{u}}=F(\mathbf{u})+\epsilon A\times H(\mathbf{u}). \tag{1.2b}$$

Here $\times$ is the direct product of two matrices B and C defined as follows. Let $B=(b_{ij})_{k_1\times k_2}$ be a $k_1\times k_2$ matrix and $C=(C_{ij})_{k_2\times k_3}$ be a $k_2\times k_3$ block matrix. Then

$$B \times C = \left(\sum_{l=1}^{k_2} b_{il} C_{lj} \right)_{k_1 \times k_3}.$$

Many coupling schemes are covered by Eq. (1.2b). For example, if the Lorenz system is used and the coupling is through its three components x, y, and z, then the function h is just the matrix

$$I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.3}$$

The choice of A will provide the connectivity of nodes. For instance, the nearest neighbor coupling with periodic, Neumann boundary conditions and mixed boundary conditions are, respectively, given as $A=A_1(1,N)+A_2(1,N)+A_2^T(1,N)=:A_P$, $A=A_1(0,N)+A_2(1,N)\hat{I}=:A_N$ and $A=A_1(\beta,N)+A_2(\beta,N)+A_2^T(\beta,N)+(1-\beta)A_2(1,N)\hat{I}=:A_M$, where those A_i's, $i=1,2$, are defined in Eqs. (1.1c) and (1.1d).

Mathematically speaking,[5] the second largest eigenvalue λ_2 of A is dominant in controlling the stability of chaotic synchronization, and the critical strength ϵ_c for synchronization can be determined in terms of λ_2,

$$\epsilon_c = \frac{L_{\max}}{-\lambda_2}. \tag{1.4}$$

The eigenvalues of $A=A_P$ are given by $\lambda_i=-4\sin^2[\pi(i-1)/N]$, $i=1,2,\ldots,N$. In general, a larger number of nodes give a smaller nonzero eigenvalue λ_2 in magnitude and, hence, a larger ϵ_c. In controlling a given system, it is desirable to reduce the critical coupling strength ϵ_c. The wavelet method in Ref. 7 will, in essence, transform A into $C(\alpha,\beta)$. Consequently, it is of great interest to study the second eigencurve of $C(\alpha,\beta)$ for each β. By the second largest eigencurve $\lambda_2(\alpha,\beta)$ of $C(\alpha,\beta)$ for fixed β, we mean that for given $\alpha>0$, $\lambda_2(\alpha,\beta)$ is the second largest eigenvalue of $C(\alpha,\beta)$. We remark that 0 is the largest eigenvalue of $C(\alpha,\beta)$ for any $\alpha>0$ and $\beta\in\mathbb{R}$. This is to say that for fixed β, $\lambda_2(\alpha,\beta)=0$ is the first eigencurve of $C(\alpha,\beta)$. A numerical simulation[7] of a coupled system of $N=512$ Lorenz oscillators shows that with $h=I_3$ and $A=A_P$, the critical coupling strength ϵ_c decreases linearly with respect to the increase of α up to a critical value α_c. The smallest ϵ_c is about 6, which is about 10^3 times smaller than the original critical coupling strength, indicating the efficiency of the proposed approach.

The mathematical verification of such phenomena is first achieved by Shieh *et al.*[6] Specifically, they solved the second eigencurve problem of $C(\alpha,1)$ with n being a multiple of 4 and j being any positive integer. Subsequently, in Ref. 4 the second eigencurve problem for $C(\alpha,0)$ and $C(\alpha,1)$ with n being any positive integer and $j=1$ are solved without touching on the reduced eigenvalue problem. In this paper, we obtain two main results. First, the reduced eigenvalue problem for $C(\alpha,0)$ is completely solved. Some partial results for the reduced eigenvalue problem of $C(\alpha,\beta)$ are also obtained. Second, we are then able to understand the behavior of $\lambda_2(\alpha,0)$ and $\lambda_2(\alpha,1)$ for any j and $n\in\mathbb{N}$.

II. REDUCED EIGENVALUE PROBLEMS

Writing the eigenvalue problem $C(\alpha,\beta)\mathbf{b}=\lambda\mathbf{b}$, where $\mathbf{b}=(\mathbf{b}_1,\mathbf{b}_2,\ldots,\mathbf{b}_n)^T$ and $\mathbf{b}_i\in\mathbb{C}^{2^j}$, in block component form, we get

$$C_2^T(\alpha,1)\mathbf{b}_{i-1} + C_1(\alpha,1)\mathbf{b}_i + C_2(\alpha,1)\mathbf{b}_{i+1} = \lambda\mathbf{b}_i, \quad 1 \leqslant i \leqslant n. \tag{2.1a}$$

Mixed boundary conditions would yield that

$$C_2^T(\alpha,1)\mathbf{b}_0 + C_1(\alpha,1)\mathbf{b}_1 + C_2(\alpha,1)\mathbf{b}_2 = \lambda\mathbf{b}_1 = C_1(\alpha,\beta)\mathbf{b}_1 + C_2(\alpha,1)\mathbf{b}_2 + C_2^T(\alpha,\beta)\mathbf{b}_n$$

and

$$C_2^T(\alpha,1)\mathbf{b}_{n-1} + C_1(\alpha,1)\mathbf{b}_n + C_2(\alpha,1)\mathbf{b}_{n+1} = \lambda\mathbf{b}_n = C_2(\alpha,\beta)\mathbf{b}_1 + C_2^T(\alpha,1)\mathbf{b}_{n-1} + \hat{I}C_1(\alpha,\beta)\hat{I}\mathbf{b}_n,$$

or, equivalently,

$$\begin{aligned} C_2^T(\alpha,1)\mathbf{b}_0 &= (C_1(\alpha,\beta) - C_1(\alpha,1))\mathbf{b}_1 + C_2^T(\alpha,\beta)\mathbf{b}_n \\ &= \left[\begin{pmatrix} 1-\beta & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} + \frac{\alpha(1-\beta)}{2^{2j}} ee^T\right]\mathbf{b}_1 + \left[\begin{pmatrix} 0 & \cdots & 0 & \beta \\ 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \end{pmatrix} + \frac{\alpha\beta}{2^{2j}} ee^T\right]\mathbf{b}_n \\ &= (1-\beta)C_2^T(\alpha,1)\hat{I}\mathbf{b}_1 + \beta C_2(\alpha,1)\mathbf{b}_n \end{aligned} \tag{2.1b}$$

and

$$C_2(\alpha,1)\mathbf{b}_{n+1} = (\hat{I}C_1(\alpha,\beta)\hat{I} - C_1(\alpha,1))\mathbf{b}_n + C_2(\alpha,\beta)\mathbf{b}_1 = (1-\beta)C_2^T(\alpha,1)\hat{I}\mathbf{b}_n + \beta C_2(\alpha,1)\mathbf{b}_1. \tag{2.1c}$$

To study the block difference equation [Eq. (2.1)], we set

$$\mathbf{b}_j = \delta^j v, \tag{2.2}$$

where $\boldsymbol{v} \in \mathbb{C}^{2^j}$ and $\delta \in \mathbb{C}$.

Substituting Eq. (2.2) into Eq. (2.1a), we have

$$[C_2^T(\alpha,1) + \delta(C_1(\alpha,1) - \lambda I) + \delta^2 C_2(\alpha,1)]\mathbf{v} = 0. \tag{2.3}$$

To have a nontrivial solution $\boldsymbol{v}$ satisfying Eq. (2.3), we need to have

$$\det[C_2^T(\alpha,1) + \delta(C_1(\alpha,1) - \lambda I) + \delta^2 C_2(\alpha,1)] = 0. \tag{2.4}$$

Definition 2.1: Equation (2.4) is to be called the characteristic equation of the block difference equation [Eq. (2.1a)]. Let $\delta_k = \delta_k(\lambda) \neq 0$ and $\boldsymbol{v}_k = \boldsymbol{v}_k(\lambda) \neq 0$ be complex numbers and vectors, respectively, satisfying Eq. (2.3). Here $k = 1,2,\ldots,m$ and $m \leqslant 2^j$. Assume that there exists a $\lambda \in \mathbb{C}$, such that $\mathbf{b}_j = \Sigma_{k=1}^m c_k \delta_k^j(\lambda)\boldsymbol{v}_k(\lambda)$, $j = 0,1,\ldots,n+1$, satisfy Eqs. (2.1b) and (2.1c), where $c_k \in \mathbb{C}$. If, in addition, $\mathbf{b}_j$, $j = 1,2,\ldots,n$, are not all zero vectors, then such $\delta_k(\lambda)$ is called a characteristic value of Eq. (2.1a), (2.1b), and (2.1c) or (1.1a) with respect to λ and $\boldsymbol{v}_k(\lambda)$ its corresponding characteristic vector.

Remark 2.1: Clearly, for each α and β, λ in Definition 2.1 is an eigenvalue of $C(\alpha,\beta)$.

Should no ambiguity arises, we will write $C_2^T(\alpha,1) = C_2^T$, $C_1(\alpha,1) = C_1$, and $C_2(\alpha,1) = C_2$. Likewise, we will write $A_2(\beta,2^j) = A_2(\beta)$ and $A_1(\beta,2^j) = A_1(\beta)$.

Proposition 2.1: *Let* $\rho(\lambda) = \{\delta_i(\lambda) : \delta_i(\lambda)$ *is a root of Eq. (2.4)*$\}$, *and let* $\bar{\rho}(\lambda) = \{1/\delta_i(\lambda) : \delta_i(\lambda)$ *is a root of Eq. (2.4)*$\}$. *Then* $\rho(\lambda) = \bar{\rho}(\lambda)$. *Let* δ_i *and* δ_k *be in* $\rho(\lambda)$. *We further assume that* δ_i *and* $\boldsymbol{v}_i = (v_{i1},\ldots,v_{i2^j})^T$ *satisfy Eq. (2.3). Suppose* $\delta_i \cdot \delta_k = 1$. *Then* δ_k *and* $\boldsymbol{v}_k = (v_{i2^j}, v_{i2^j-1},\ldots,v_{i2},v_{i1})^T =: \boldsymbol{v}_i^s$ *also satisfy Eq. (2.3). Conversely, if* $\delta_i \cdot \delta_k \neq 1$, *then* $\boldsymbol{v}_k \neq \boldsymbol{v}_i^s$.

Proof: To prove $\rho(\lambda) = \bar{\rho}(\lambda)$, we see that

$$\begin{aligned} \det[C_2^T + \delta(C_1 - \lambda I) + \delta^2 C_2] &= \delta^2 \det\left[\frac{1}{\delta^2}C_2^T + \frac{1}{\delta}(C_1 - \lambda I) + C_2\right] \\ &= \delta^2 \det\left[\frac{1}{\delta^2}C_2^T + \frac{1}{\delta}(C_1 - \lambda I) + C_2\right]^T \\ &= \delta^2 \det\left[C_2^T + \frac{1}{\delta}(C_1 - \lambda I) + \frac{1}{\delta^2}C_2\right]. \end{aligned}$$

Thus, if δ is a root of Eq. (2.4), then so is $1/\delta$. To see the last assertion of the proposition, we write Eq. (2.3) with $\delta=\delta_i$ and $\boldsymbol{v}=\boldsymbol{v}_i$ in component form.

$$\sum_{m=1}^{2^j}[(C_2^T)_{lm}v_{im}+\delta_i(\bar{C}_1)_{lm}v_{im}+\delta_i^2(C_2)_{lm}v_{im}]=0,\quad l=1,2,\ldots,2^j. \tag{2.5}$$

Here $\bar{C}_1=C_1-\lambda I$. Now the right hand side of Eq. (2.5) becomes

$$\left(\frac{1}{\delta_k}\right)^2\left\{\sum_{m=1}^{2^j}[(C_2)_{l(2^j+1-m)}v_{i(2^j+1-m)}+\delta_k(\bar{C}_1)_{l(2^j+1-m)}v_{i(2^j+1-m)}+\delta_k^2(C_2^T)_{l(2^j+1-m)}v_{i(2^j+1-m)}]\right\}$$
$$=\left(\frac{1}{\delta_k}\right)^2\left\{\sum_{m=1}^{2^j}[(C_2^T)_{(2^j+1-l)m}v_{i(2^j+1-m)}+\delta_k(\bar{C}_1)_{(2^j+1-l)m}v_{i(2^j+1-m)}+\delta_k^2(C_2)_{(2^j+1-l)m})v_{i(2^j+1-m)}]\right\},$$
$$l=1,2,\ldots,2^j. \tag{2.6}$$

We have used the fact that

$$(A)_{(2^j+1-l)m}=(A^T)_{l(2^j+1-m)}, \tag{2.7}$$

where $A=C_2^T$ or $\bar{C}_1$ or C_2 to justify the equality in Eq. (2.6). However, Eq. (2.7) follows from Eqs. (1.1c) and (1.1d). Letting $v_{i(2^j+1-m)}=v_{km}$, we have that the pair $(\delta_k,\boldsymbol{v}_k)$ satisfies Eq. (2.3). Suppose $\boldsymbol{v}_k=\boldsymbol{v}_i^s$, we see, similarly, that the pair $(1/\delta_i,\boldsymbol{v}_k)$ also satisfies Eq. (2.3). Thus $1/\delta_i=\delta_k$. □

Remark 2.2: Equation (2.4) is a palindromic equation. That is, for each λ, δ and δ^{-1} are both the roots of Eq. (2.4). However, the eigenvalue problem discussed here is not a palindromic eigenvalue problem.[3]

Definition 2.2: We shall call $\boldsymbol{v}^s$ and $-\boldsymbol{v}^s$, the symmetric vector and antisymmetric vector of $\boldsymbol{v}$, respectively. A vector $\boldsymbol{v}$ is symmetric (antisymmetric) if $\boldsymbol{v}=\boldsymbol{v}^s$ ($\boldsymbol{v}=-\boldsymbol{v}^s$).

Theorem 2.1: *Let* $\delta_k=e^{(\pi k/n)i}$, k *is an integer and* $i=\sqrt{-1}$, *then* δ_{2k}, $k=0,1,\ldots,n-1$, *are characteristic values of Eq.* (2.1a), (2.1b), and (2.1c) *with* $\beta=1$. *For each* α, *if* $\lambda\in\mathbb{C}$ *satisfies*

$$\det[C_2^T+\delta_{2k}(C_1-\lambda I)+\delta_{2k}^2C_2]=0,$$

for some $k\in\mathbb{Z}$, $0\leqslant k\leqslant n-1$, *then* λ *is an eigenvalue of* $C(\alpha,1)$.

Proof: Let λ be as assumed. Then there exists a $\boldsymbol{v}\in\mathbb{C}^{2^j}$, $\boldsymbol{v}\neq\mathbf{0}$ such that

$$[C_2^T+\delta_{2k}(C_1-\lambda I)+\delta_{2k}^2C_2]\mathbf{v}=\mathbf{0}.$$

Let $\mathbf{b}_j=\delta_{2k}^j\boldsymbol{v}$, $0\leqslant j\leqslant n+1$. Then such $\mathbf{b}_j$'s satisfy Eqs. (2.1a), (2.1b), and (2.1c). We just proved the assertion of the theorem. □

Corollary 2.1: *Set*

$$\Gamma_k=C_1+\delta_{2n-k}C_2^T+\delta_kC_2. \tag{2.8}$$

Then the eigenvalues of $C(\alpha,1)$, *for each* α, *consist of eigenvalues of* Γ_k, $k=0,2,4,\ldots,2(n-1)$. *That is*, $\rho(C(\alpha,1))=\cup_{k=0}^{n-1}\rho(\Gamma_{2k})$. Here $\rho(A)=$ *the spectrum of the matrix* A.

Remark 2.3: $C(\alpha,1)$ is a block circulant matrix. The assertion of Corollary 2.1 is not new (see, e.g., Theorem 5.6.4 of Ref. 1). Here we merely gave a different proof.

To study the eigenvalue of $C(\alpha,0)$ for each α, we begin with considering the eigenvalues and eigenvectors of $C_2^T+C_1+C_2$ and $C_2^T-C_1+C_2$.

Proposition 2.2: *Let* $T_1(C)$ $(T_2(C))$ *be the set of linearly independent eigenvectors of the matrix* C *that are symmetric (antisymmetric). Then* $|T_1(C_2^T+C_1+C_2)|=|T_2(C_2^T+C_1+C_2)|=|T_1(C_2^T-C_1+C_2)|=|T_2(C_2^T-C_1+C_2)|=2^{j-1}$. *Here* $|A|$ *denote the cardinality of the set* A.

Proof: We will only illustrate the case for $C_2^T-C_1+C_2=:C$. We first observe that $|T_1(C)|$ is less than or equal to 2^{j-1}. So is $|T_2(C)|$. We also remark that the cardinality of the set of all linearly

independent eigenvectors of C is 2^j. If $0<|T_1(C)|<2^{j-1}$, there must exist an eigenvector $\boldsymbol{v}$ for which $\boldsymbol{v}\neq\boldsymbol{v}^s$, $\boldsymbol{v}\neq-\boldsymbol{v}^s$, and $\boldsymbol{v}\notin\text{span}\{T_1(C),T_2(C)\}$, the span of the vectors in $T_1(C)$ and $T_2(C)$. It then follows from Proposition 2.1 that $\boldsymbol{v}+\boldsymbol{v}^s$, a symmetric vector, is in the span$\{T_1(C)\}$. Moreover, $\boldsymbol{v}-\boldsymbol{v}^s$ is in span$\{T_2(C)\}$. Hence $\boldsymbol{v}\in\text{span}\{T_1(C),T_2(C)\}$, a contradiction. Hence, $|T_1(C)|=2^{j-1}$. Similarly, we conclude that $|T_2(C)|=2^{j-1}$. □

Theorem 2.2: *Let* $\delta_k=e^{(\pi k/n)i}$, *where* k *is an integer and* $i=\sqrt{-1}$. *For each* α, *if* $\lambda\in\mathbb{C}$ *satisfies*

$$\det[C_2^T+\delta_k(C_1-\lambda I)+\delta_k^2C_2]=0,$$

for some $k\in\mathbb{Z}$, $1\leqslant k\leqslant n-1$, *then* λ *is an eigenvalue of* $C(\alpha,0)$. *Let* λ *be the eigenvalue of* $C_2^T+C_1+C_2$ $(-C_2^T+C_1-C_2)$ *for which its associated eigenvector* $\boldsymbol{v}$ *satisfies* $\hat{I}\boldsymbol{v}=\boldsymbol{v}$ $(\hat{I}\boldsymbol{v}=-\boldsymbol{v})$, *then* λ *is also an eigenvalue of* $C(\alpha,0)$.

Proof: For any $1\leqslant k\leqslant n-1$, let δ_k be as assumed. Let λ_k and ν_k be a number and a nonzero vector, respectively, satisfying

$$[C_2^T+\delta_k(C_1-\lambda_kI)+\delta_k^2C_2]\boldsymbol{v}_k=\boldsymbol{0}. \tag{2.9}$$

Using Proposition 2.1, we see that λ_k satisfies

$$\det[C_2^T+\delta_{2n-k}(C_1-\lambda_kI)+\delta_{2n-k}^2C_2]=0. \tag{2.10}$$

Let $\boldsymbol{v}_{2n-k}$ be a nonzero vector satisfying $[C_2^T+\delta_{2n-k}(C_1-\lambda_kI)+\delta_{2n-k}^2C_2]\boldsymbol{v}_{2n-k}=\boldsymbol{0}$. Letting

$$\mathbf{b}_i=\delta_k^i\boldsymbol{v}_k+\delta_k\delta_{2n-k}^i\boldsymbol{v}_{2n-k},\quad i=0,1,\ldots,n+1,$$

we conclude, via Eqs. (2.9) and (2.10), that $\mathbf{b}_i$ satisfy Eq. (2.1a) with $\lambda=\lambda_k$. Moreover,

$$\hat{I}\mathbf{b}_1=\delta_k\hat{I}\boldsymbol{v}_k+\hat{I}\boldsymbol{v}_{2n-k}=\delta_k\boldsymbol{v}_{2n-k}+\boldsymbol{v}_k=\mathbf{b}_0.$$

We have used Proposition 2.1 to justify the second equality above. Similarly, $\mathbf{b}_{n+1}=\hat{I}\mathbf{b}_n$. To see $\lambda=\lambda_k$, $1\leqslant k\leqslant n-1$, is indeed an eigenvalue of $C(\alpha,0)$ for each α, it remains to show that $\mathbf{b}_i\neq\mathbf{0}$ for some i. Using Proposition 2.1, we have that there exists an m, $1\leqslant m\leqslant 2^j$ such that $v_{km}=v_{(2n-k)(2^j-m+1)}\neq0$. We first show that $\mathbf{b}_0\neq\mathbf{0}$. Let m be the index for which $v_{km}\neq0$. Suppose $\mathbf{b}_0=\mathbf{0}$. Then

$$v_{km}+\delta_kv_{(2n-k)m}=0$$

and

$$v_{k(2^j-m+1)}+\delta_kv_{(2n-k)(2^j-m+1)}=v_{(2n-k)m}+\delta_kv_{km}=0.$$

And so, $v_{km}=\delta_k^2v_{km}$, a contradiction. Let λ and $\boldsymbol{v}$ be as assumed in the last assertion of theorem. Letting $\mathbf{b}_i=\boldsymbol{v}$ $(\mathbf{b}_i=(-1)^i\boldsymbol{v})$, we conclude that λ is an eigenvalue of $C(\alpha,0)$ with corresponding eigenvector $(\mathbf{b}_1,\mathbf{b}_2,\ldots,\mathbf{b}_n)^T$. Thus, λ_k is an eigenvalue of $C(\alpha,0)$ for each α. □

Corollary 2.2: *Let* $\delta_k=e^{(\pi k/n)i}$, *where* k *is an integer and* $i=\sqrt{-1}$. *Then, for each* α, $\rho(C(\alpha,0))=\cup_{k=1}^{n-1}\rho(\Gamma_k)\cup\rho^S(\Gamma_0)\cup\rho^{AS}(\Gamma_n)$, *where* $\rho^S(A)$ $(\rho^{AS}(A))$ *the set of eigenvalues of* A *for which their corresponding eigenvectors are symmetric (antisymmetric).*

We next consider the eigenvalues of $C(\alpha,\beta)$.

Theorem 2.3: *Let* $\delta_k=e^{(\pi k/n)i}$, *where* k *is an integer and* $i=\sqrt{-1}$. *Then, for each* α,

$$\rho(C(\alpha,\beta))\supset\begin{cases}\bigcup_{k=1}^{[n/2]}\rho(\Gamma_{2k})\cup\rho^S(\Gamma_0), & n\text{ is odd}\\ \bigcup_{k=1}^{(n/2)-1}\rho(\Gamma_{2k})\cup\rho^S(\Gamma_0)\cup\rho^{AS}(\Gamma_n), & n\text{ is even.}\end{cases}$$

Here $[n/2]$ *is the greatest integer that is less than or equal to* $n/2$.

Proof: We illustrate only the case that n is even. Assume that k is such that $1 \leqslant k \leqslant n/2-1$. Let $\mathbf{b}_i = \delta^i_{2k}\boldsymbol{v}_{2k} + \delta_{2k}\delta^i_{2n-2k}\boldsymbol{v}_{2n-2k}$, we see clearly that such $\mathbf{b}_i$, $i=0,1,n,n+1$, satisfy both Neumann and periodic boundary conditions, respectively. And so

$$\mathbf{b}_0 = (1-\beta)\mathbf{b}_0 + \beta\mathbf{b}_0 = (1-\beta)\hat{I}\mathbf{b}_1 + \beta\mathbf{b}_n$$

and

$$\mathbf{b}_{n+1} = (1-\beta)\mathbf{b}_{n+1} + \beta\mathbf{b}_{n+1} = (1-\beta)\hat{I}\mathbf{b}_n + \beta\mathbf{b}_1.$$

Here, δ_{2k}, $1 \leqslant k \leqslant (n/2)-1$, are characteristic values of Eq. (2.1a), (2.1b), and (2.1c). Thus, if $\lambda \in \rho(\Gamma_{2k})$, then λ is an eigenvalue of $C(\alpha,\beta)$. The assertions for Γ_0 and Γ_n can be done similarly.□

Remark 2.4: If n is an even number, for each α and β, half of the eigenvalues of $C(\alpha,\beta)$ are independent of the choice of β. The other characteristic values of Eq. (2.1) seem to depend on β. It is of interest to find them.

III. THE SECOND EIGENCURVE OF $C(\alpha,0)$ AND $C(\alpha,1)$

We begin with considering the eigencurves of Γ_k, as given in Eq. (2.8). Clearly,

$$\Gamma_k = \begin{pmatrix} -2 & 1 & 0 & \cdots & \cdots & \delta_{2n-k} \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ \delta_k & \cdots & \cdots & 0 & 1 & -2 \end{pmatrix}_{m\times m} - \frac{\alpha(2-2\cos(\pi k/n))}{m} ee^T =: D_1(k) - \alpha(k)ee^T, \tag{3.1}$$

where $m=2^j$. We next find a unitary matrix to diagonalize $D_1(k)$.

Remark 3.1: Let $(\lambda(k),\mathbf{v}(k))$ be the eigenpair of $D_1(k)$. If $e^T\boldsymbol{v}(k)=0$, then $\lambda(k)$ is also an eigenvalue of Γ_k.

Proposition 3.1: *Let*

$$\theta_{l,k} = \frac{2l\pi}{m} + \frac{k\pi}{nm}, \quad l=0,1,\ldots,m-1, \tag{3.2a}$$

$$\boldsymbol{p}_l(k) = (e^{i\theta_{l,k}}, e^{i2\theta_{l,k}}, \cdots, e^{im\theta_{l,k}})^T, \tag{3.2b}$$

and

$$P(k) = \left(\frac{p_0(k)}{\sqrt{m}}, \ldots, \frac{p_{m-1}(k)}{\sqrt{m}}\right). \tag{3.2c}$$

(i) *Then $P(k)$ is a unitary matrix and $P^H(k)D_1(k)P(k)=\mathrm{diag}(\lambda_{0,k}\cdots\lambda_{m-1,k})$, where P^H is the conjugate transpose of P, and*

$$\lambda_{l,k} = 2\cos\theta_{l,k} - 2, \quad l=0,1,\ldots,m-. \tag{3.2d}$$

(ii) *Moreover, for $0 \leqslant k \leqslant 2n$, the eigenvalues of $D_1(k)$ are distinct if and only if $k \neq 0$, n, or $2n$.*

Proof: Let $\mathbf{b}=(b_1,\ldots,b_m)^T$. Writing the eigenvalue problem $D_1(k)\mathbf{b}=\lambda\mathbf{b}$ in component form, we get

$$b_{j-1} - (2+\lambda)b_j + b_{j+1} = 0, \quad j=2,3,\ldots,m-1, \tag{3.3a}$$

$$-(2+\lambda)b_1 + b_2 + \delta_{2n-k}b_m = 0, \tag{3.3b}$$

$$\delta_k b_1 + b_{m-1} - (2+\lambda) b_m = 0. \tag{3.3c}$$

Set $b_j = \delta^j$, where δ satisfies the characteristic equation $1-(2+\lambda)\delta+\delta^2=0$ of the system $D_1(k)\mathbf{b}=\lambda\mathbf{b}$. Then the boundary conditions (3.3b) and (3.3c) are reduced to

$$\delta^m = \delta_k. \tag{3.4}$$

Thus, the solutions $e^{i\theta_{l,k}}$, $l=0,1,\ldots,m-1$, of Eq. (3.4) are the candidates for the characteristic values of Eq. (3.3). Substituting $e^{i\theta_{l,k}}$ into Eq. (3.3a) and solving for λ, we see that $\lambda=\lambda_{l,k}$ are the candidates for the eigenvalues of $D_1(k)$. Clearly, $(\lambda,\mathbf{b})=(\lambda_{l,k},\boldsymbol{p}_l(k))$ satisfies $D_1(k)\mathbf{b}=\lambda\mathbf{b}$ and $\mathbf{b}=\boldsymbol{p}_l(k)\neq 0$. Thus, $\lambda=\lambda_{l,k}$ are, indeed, the eigenvalues of $D_1(k)$. To complete the proof of the proposition, it suffices to show that $P(k)$ is unitary. To this end, we need to compute $\boldsymbol{p}_l^H(k)\cdot\boldsymbol{p}_{l'}(k)$. Clearly, $\boldsymbol{p}_l^H(k)\cdot\boldsymbol{p}_l(k)=m$. Now, let $l\neq l'$, we have that

$$\boldsymbol{p}_l^H(k)\cdot\boldsymbol{p}_{l'}(k) = \sum_{j=1}^{m} e^{ij(\theta_{l,k}-\theta_{l',k})} = \sum_{j=1}^{m} e^{ij([2(l-l')/m]\pi)} = \frac{r(1-r^m)}{1-r} = 0,$$

where $r=e^{i([2(l-l')/m]\pi)}$. Hence, $P(k)$ is unitary. The last assertion of the proposition is obvious. □

To prove the main results in this section, we also need the following proposition. Some assertions of the proposition are from Theorem 8.6.2 of Ref. 2.

Proposition 3.2: *Suppose* $D=\mathrm{diag}(d_1,\ldots,d_m)\in\mathbb{R}^{m\times m}$ *and that the diagonal entries satisfy* $d_1>\cdots>d_m$. *Let* $\gamma\neq 0$ *and* $\mathbf{z}=(z_1,\ldots,z_m)^T\in\mathbb{R}^n$. *Assume that* $(\lambda_i(\gamma),\boldsymbol{v}_i(\gamma))$ *are the eigenpairs of* $D+\gamma\mathbf{z}\mathbf{z}^T$ *with* $\lambda_1(\gamma)\geqslant\lambda(\gamma)\geqslant\cdots\geqslant\lambda_m(\gamma)$. *(i) Let* $A=\{k:1\leqslant k\leqslant m, z_k=0\}$, $A^c=\{1,\ldots,m\}-A$. *If* $k\in A$, *then* $d_k=\lambda_k$. *(ii) Assume* $\alpha>0$. *Then the following interlacing relations hold* $\lambda_1(\gamma)\geqslant d_1\geqslant\lambda_2(\gamma)\geqslant d_2\geqslant\cdots\geqslant\lambda_m(\gamma)\geqslant d_m$. *Moreover, the strict inequality holds for these indices* $i\in A^c$. *(iii) Let* $i\in A^c$, $\lambda_i(\gamma)$ *are strictly increasing in* γ *and* $\lim_{\alpha\to\infty}\lambda_i(\gamma)=\bar{\lambda}_i$ *for all* i, *where* $\bar{\lambda}_i$ *are the roots of* $g(\lambda)=\Sigma_{k\in A^c}z_i^2/(d_k-\lambda)$ *with* $\bar{\lambda}_i\in(d_i,d_{i-1})$. *In the case that* $1\in A^c$, $d_0=\infty$.

Proof: The proof of interlacing relations in (*ii*) and the assertion in (*i*) can be found in Theorem 8.6.2 of Ref. 2. We only prove the remaining assertions of the proposition. Rearranging $\mathbf{z}$ so that $\mathbf{z}^T=(0,0,\ldots,0,z_{i_1},\ldots,z_{i_k}):=(0,\ldots,0,\underline{\mathbf{z}}^T)$, where $i_1<i_2<\cdots<i_k$ and $i_j\in A^c$, $j=1,\ldots,k$. The diagonal matrix D is rearranged accordingly. Let $D=\mathrm{diag}(D_1,D_2)$, where $D_2=\mathrm{diag}(d_{i_1},\ldots,d_{i_k})$. Following Theorem 8.6.2 of Ref. 2, we see that $\lambda_{i_j}(\gamma)$ are the roots of the scalar equation $f_\gamma(\lambda)$, where

$$f_\gamma(\lambda_{i_j}(\gamma)) = 1+\gamma\sum_{j=1}^{k}\frac{z_j^2}{d_{i_j}-\lambda_{i_j}(\gamma)} = 0. \tag{3.5}$$

Differentiating the equation above with respect to γ, we get

$$\sum_{j=1}^{k}\frac{z_{i_j}^2}{d_{i_j}-\lambda_{i_j}(\gamma)} + \left(\gamma\sum_{j=1}^{k}\frac{z_{i_j}^2}{(d_{i_j}-\lambda_{i_k}(\gamma))^2}\right)\frac{d\lambda_{i_j}(\gamma)}{d\gamma} = 0.$$

Thus,

$$\frac{d\lambda_{i_j}(\gamma)}{d\gamma} = \frac{1}{\gamma^2}\sum_{j=1}^{k}\frac{z_{i_j}^2}{(d_{i_j}-\lambda_{i_j}(\gamma))^2} > 0.$$

Clearly, for each i_j, the limit of $\lambda_{i_j}(\gamma)$ as $\gamma\to\infty$ exists, say, $\bar{\lambda}_{i_j}$. Since, for $d_{i_j}<\lambda<d_{i_j-1}$,

$$\sum_{j=1}^{k}\frac{z_{i_j}^2}{d_{i_j}-\lambda_{i_j}(\gamma)} = \frac{1}{\gamma}.$$

Taking the limit as $\alpha\to\infty$ on both sides of the equation above, we get

$$\sum_{j=1}^{k} \frac{z_{i_j}^2}{d_{i_j} - \bar{\lambda}_{i_j}} = 0. \tag{3.6}$$

as desired. □

We are now in the position to state the following theorems.

Theorem 3.1: *Let n and $m=2^j$ be given positive integers. For each k, $k=1,2,\ldots,n-1$, and α, we denote by $\lambda_{l,k}(\alpha)$, $l=0,1,\ldots,2^j-1$, the eigenvalues of Γ_k. For $k=1,2,\ldots,n-1$, we let $(\lambda_{l,k},u_{l,k})$, $l=0,1,\ldots,2^j-1$, be the eigenpairs of $D_1(k)$, as defined in* Eq. (3.1). *Then the following hold true.*

(i) $\lambda_{l,k}(\alpha)$ *is strictly decreasing in* α, $l=0,1,\ldots,2^j-1$ *and* $k=1,2,\ldots,n-1$.

(ii) *There exist* $\lambda_{l,k}^*$ *such that* $\lim_{\alpha\to\infty}\lambda_{l,k}(\alpha)=\lambda_{l,k}^*$. *Moreover,* $g_k(\lambda_{l,k}^*)=0$, *where*

$$g_k(\lambda) = \sum_{l=1}^{m} \frac{1}{(\lambda_{l-1,k})(\lambda_{l-1,k}+\lambda)}. \tag{3.7}$$

Proof: The first assertion of the theorem follows from Proposition 3.2 (iii). Let k be as assumed. Set, for $l=0,1,\ldots,m-1$,

$$z_{l+1} = \boldsymbol{p}_l^H(k)e = \sum_{j=1}^{m} e^{ij\theta_{l,k}} = \frac{e^{-\theta_{l,k}}(1-e^{-im\theta_{l,k}})}{1-e^{-\theta_{l,k}}} = \frac{e^{-\theta_{l,k}}(1-e^{-ik(\pi/n)})}{1-e^{-\theta_{l,k}}}.$$

Then

$$\bar{\mathbf{z}}_{l+1}\mathbf{z}_{l+1} = \frac{2-2\cos m\theta_{l,k}}{2-2\cos\theta_{l,k}} = \frac{2\cos(k\pi/n)-2}{\lambda_{l,k}} \neq 0. \tag{3.8}$$

Let $P(k)$ be as given in Eq. (3.2c). Then

$$-P^H(k)\cdot\Gamma_k\cdot P(k) = \mathrm{diag}(-\lambda_{0,k},\ldots,-\lambda_{m-1,k}) + \alpha(k)P_l^H(k)e(P_l^H(k)e)^H.$$

Note that if k is as assumed, it follows from Proposition 3.1(ii) that $\lambda_{l,k}$, $l=0,\ldots,m-1$, are distinct. Thus, we are in the position to apply Proposition 3.2. Specifically, by noting $A^c=\phi$, we see that $\lambda_{0,k}^*$ satisfies $g(\lambda)=0$, where

$$g(\lambda) = \sum_{l=1}^{m} \frac{1}{(\lambda_{l-1,k})(\lambda_{l-1,k}+\lambda)}.$$

We have used Eqs. (3.2d), (3.6), and (3.8), to find $g(\lambda)$. □

We next give an upper bound for $\lambda_{0,k}^*$, $k=1,2,\ldots,n-1$.

Theorem 3.2: *The following inequalities hold true:*

$$\lambda_{0,k}^* < \lambda_{0,n}, \quad k=1,2,\ldots,n-1. \tag{3.9}$$

Proof: To complete the proof of Eq. (3.9), it suffices to show that $g_k(-\lambda_{0,n})<0$. Now,

$$\begin{aligned} &g_k(-\lambda_{0,n}) \\ &\quad= \sum_{l=1}^{m} \frac{1}{[2\cos([2(l-1)\pi/m]+(k\pi/nm))-2][2\cos([2(l-1)\pi/m]+(k\pi/nm))-2\cos(\pi/m)]} \\ &\quad=: h(m,n,k) = h(2^j,n,k). \end{aligned} \tag{3.10}$$

We shall prove that $h(2^j,n,k)<0$ by the induction on j. For $j=1$, $h(2,n,k)=\frac{1}{2}[[1/\cos^2(k\pi/2n)-1]]<0$, $k=1,2,\ldots,n-1$. Assume $h(2^j,n,k)<0$. Here, $n\in\mathbb{N}$ and $k=1,2,\ldots,n-1$. We first note that

$$\cos\left(\frac{2(2^j+i-1)\pi}{2^{j+1}}+\frac{k\pi}{2^{j+1}n}\right)=-\cos\left(\frac{2(i-1)\pi}{2^{j+1}}+\frac{k\pi}{2^{j+1}n}\right)=:-\cos\,\theta_{i-1,k,j+1},\quad i=1,2,\ldots,2^j. \tag{3.11}$$

Moreover, upon using Eq. (3.11), we get that

$$\begin{aligned}
&\frac{1}{(\cos\,\theta_{i-1,k,j+1}-1)(\cos\,\theta_{i-1,k,j+1}-\cos\,\theta_{0,n,j+1})}+\frac{1}{(\cos\,\theta_{2j+i-1,k,j+1}-1)(\cos\,\theta_{2j+i-1,k,j+1}-\cos\,\theta_{0,n,j+1})}\\
&=\frac{1}{(\cos\,\theta_{i-1,k,j+1}-1)(\cos\,\theta_{i-1,k,j+1}-\cos\,\theta_{0,n,j+1})}+\frac{1}{(\cos\,\theta_{i-1,k,j+1}+1)(\cos\,\theta_{i-1,k,j+1}+\cos\,\theta_{0,n,j+1})}\\
&=\frac{2\cos^2\,\theta_{i-1,k,j+1}+2\cos\,\theta_{0,n,j+1}}{(\cos^2\,\theta_{i-1,k,j+1}-1)(\cos^2\,\theta_{i-1,k,j+1}-\cos^2\,\theta_{0,n,j+1})}\\
&=\frac{8(\cos^2\,\theta_{i-1,k,j+1}+\cos\,\theta_{0,n,j+1})}{(\cos\,2\theta_{i-1,k,j+1}-1)(\cos\,2\theta_{i-1,k,j+1}-\cos\,2\theta_{0,n,j+1})}=\frac{2(\cos^2\,\theta_{i-1,k,j+1}+\cos\,\theta_{0,n,j+1})}{(\cos\,\theta_{i-1,k,j}-1)(\cos\,\theta_{i-1,k,j}-\cos\,\theta_{0,n,j})}.
\end{aligned} \tag{3.12}$$

We are now in a position to compute $h(2^{j+1},n,k)$. Using Eq. (3.12), we get that

$$\begin{aligned}
h(2^{j+1},n,k)&=\sum_{l=1}^{2^{j+1}}\frac{1}{4(\cos\,\theta_{l-1,k,j+1}-1)(\cos\,\theta_{l-1,k,j+1}-\cos\,\theta_{0,n,j+1})}\\
&=\sum_{l=1}^{2^j}\frac{2(\cos^2\,\theta_{l-1,k,j+1}+\cos\,\theta_{0,n,j+1})}{(\cos\,\theta_{l-1,k,j}-1)(\cos\,\theta_{i-1,k,j}-\cos\,\theta_{0,n,j})}\leqslant 8(\cos^2\,\theta_{0,k,j+1}+\cos\,\theta_{0,n,j+1})h(2^j,n,k).
\end{aligned} \tag{3.13}$$

We have used the facts that $\cos^2\,\theta_{0,k,j+1}>\cos^2\,\theta_{i-1,k,j+1}$, $i=2,\ldots,2^j$, and that the first term ($i=1$) of the summation in Eq. (3.13) is negative while all the others are positive to justify the inequality in Eq. (3.13). It then follows from Eq. (3.13) that $h(2^{j+1},n,k)<0$. We just complete the proof of the theorem. □

Theorem 3.3: *Let n and j be the block and wavelet dimensions of* $C(\alpha,1)$, *respectively. Assume n and j are any positive integers. Let* $\lambda_2(\alpha)$ *be the second eigencurve of* $C(\alpha,1)$. *Then the following hold.*

(i) $\lambda_2(\alpha)$ *is a nonincreasing function of* α.
(ii) *If n is an even number, then* $\lambda_2(\alpha)=\lambda_{0,n}$ *whenever* $\alpha\geqslant\alpha^*$ *for some* $\alpha^*>0$.
(iii) *If n is an odd number, then* $\lambda_2(\alpha)<\lambda_{0,n}$ *whenever* $\alpha\geqslant\bar{\alpha}$ *for some* $\bar{\alpha}>0$.

Proof: We first remark that in the case of $\beta=1$, the set of the indices k's in Eq. (3.1) is $\{0,2,4,\ldots,2(n-1)\}:=I_n$. Suppose n is an even number. Then $n\in I_n$. Thus, $\delta_n=-1$, $\theta_{0,n}=\pi/m$, and $\boldsymbol{p}_0(n)=(e^{i(\pi/m)},e^{i(2\pi/m)},\ldots,e^{i\pi})^T$. Applying Proposition 3.1, we see that $\boldsymbol{p}_0(n)-\boldsymbol{p}_0^s(n)$, an antisymmetric vector, is also an eigenvector of $D_1(n)$. And so $e^T(\boldsymbol{p}_0(n)-\boldsymbol{p}_0^s(n))=0$. It then follows from Remark 3.1 that $\lambda_{0,n}$ is an eigenvalue of $\Gamma_n=D_1(n)-\rho(n)ee^T$ for all α. The first and second assertions of the theorem now follow from Theorems 3.1 and 3.2. Let n be an odd number. Then $\delta_i\cdot\delta_i\neq 1$ for any $i\in I_n$. Thus, if the pair $(\delta_i,\boldsymbol{v}_i)$ satisfy Eq. (2.3), then $\boldsymbol{v}_i\neq-\boldsymbol{v}_i^s$. Otherwise, the pair $(\delta_i,\boldsymbol{v}_i-(-\boldsymbol{v}_i)^s)=(\delta_i,\boldsymbol{v}_i+\boldsymbol{v}_i^s)$ also satisfy Eq. (2.3). This is a contradiction to the last assertion in Proposition 2.1. Thus, $\boldsymbol{v}_i^H\cdot e\neq 0$ for any $i\in I_n$. We then conclude, via Proposition 3.2 (iii) and Theorem 3.2, that the last assertion of the theorem holds. □

Remark 3.2: (i) Let the number of uncoupled (chaotic) oscillators be $N=2^jn$. If n is an odd number, then the wavelet method for controlling the coupling chaotic oscillators work even better in the sense that the critical coupling strength ϵ can be made even smaller. (ii) For n being a

multiple of 4 and $j \in \mathbb{N}$, the assertions in Theorem 3.3 were first proved in Ref. 6 by a different method.

Theorem 3.4: *Let n and j be the block and wavelet dimensions of* $C(\alpha,0)$, *respectively. Assume n and j are any positive integers. Let* $\lambda_2(\alpha)$ *be the second eigencurve of* $C(\alpha,0)$. *Then for any n, there exists a* $\tilde{\alpha}$ *such that* $\lambda_2(\alpha)=\lambda_{0,n}$ *whenever* $\alpha \geqslant \tilde{\alpha}$.

Remark 3.3: For $n \in \mathbb{N}$ and $j=1$, the explicit formulas for the eigenvalues of $C(\alpha,0)$ were obtained in. Ref. 4 Such results are possible due to the fact that the dimension of the matrices in Eq. (2.4) is 2×2.

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Existence and uniqueness for the reflection and transmission problem in stratified electromagnetic media

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The reflection-transmission problem of time-harmonic waves in a stratified electromagnetic medium is investigated. The waves are sent from upward or downward with oblique incidence. By means of the energy flux, up-going and down-going waves are distinguished and the reflection and transmission matrices are introduced. When the solid occupies a strip between two homogeneous media, the existence and uniqueness of the reflected and transmitted waves are proved. The same conclusions are obtained for a dielectric without memory extended in the whole space. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2401751]

I. INTRODUCTION

The aim of this paper is to study the reflection-transmission problem in electromagnetic media occupying the whole space. More precisely, we consider an incident wave and discuss the existence and uniqueness of the scattering matrix resulting from the corresponding reflection and transmission coefficients.

Following Refs. 2, 12, and 13, we consider electromagnetic fields with a time-harmonic dependence. Accordingly, it turns out that the whole procedure is highly dependent on this assumption. Alternative approaches can be found in Refs. 6, 8, and 9, where the scattering problem is examined in the time domain.

The solid is supposed to be linear, anisotropic, dissipative, and stratified along the direction of a given unit vector $\mathbf{n}$. The last assumption implies that the material parameters are constant on planes perpendicular to $\mathbf{n}$. Maxwell's equations lead to a system of first-order ordinary differential equations of the form

$$\mathbf{w}'(z) = \mathbb{N}(z)\mathbf{w}(z), \tag{1}$$

where z is the running parameter along the direction of $\mathbf{n}$, $\mathbb{N}$ is a 4×4 complex-valued matrix depending on the material parameters and the frequency, and the vector $\mathbf{w}$ is formed by the components of the electric displacement and the magnetic field orthogonal to $\mathbf{n}$ and $\mathbf{w}' = d\mathbf{w}/dz$.

The system (1) decouples into two systems of two first-order ordinary differential equations, provided that the solid is isotropic and the incidence is normal. By means of a particular transformation of the dependent and independent variables, the scattering problem of the decoupled systems can be shown to be equivalent to the scattering problem for a linear Schrödinger equation. As it is well known, within this framework the Jost solutions allow a natural identification of the reflection and transmission coefficients, that is, of the scattering matrix. In the present paper, the procedure followed for the Schrödinger equation is suitably generalized so that it can be applied to the system (1).

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Hence we consider two suitable sets of four independent solutions of (1). Each set is partitioned into two up-going and two down-going waves, according as they propagate in the direction of **n** or in the opposite direction. As in Ref. 2, the direction of propagation of a wave is determined by looking at the sign of the component of the corresponding energy flux along the vector **n**, which we denote by $\mathcal{F}$. The scattering matrix is determined by the two bases.

The formulation (1) of Maxwell's equations for time-harmonic fields in stratified solids is discussed in Sec. II. The properties of the energy flux component $\mathcal{F}$ are examined in Sec. III. In particular, it is shown that $\mathcal{F}$ is nonincreasing in the direction **n** of the stratification, as a consequence of the second law of Thermodynamics. This property is crucial for the proof of existence and uniqueness.

In Sec. IV, we consider an anisotropic stratified layer between two homogeneous half-spaces. In each homogeneous region we introduce a suitable basis consisting of two up-going and two down-going waves, which are regarded as the generators of incident, reflected, and transmitted waves. The existence and uniqueness of the reflection and transmission matrices are then proved under the assumption that any linear superposition of the up-going (down-going) generators inherits the property of being up-going (down-going).

A dielectric without memory extended in the whole space is considered in Sec. V. The material parameters are allowed to depend on z, but tend to constant values as $z \to \pm\infty$. The asymptotic generators of incident, reflected, and transmitted waves are then introduced and the existence and uniqueness of the reflection and transmission matrices are shown.

The particular case of normal incidence in isotropic media is considered in Sec. VI.

II. WAVE PROPAGATION IN ELECTROMAGNETIC SOLIDS

An electromagnetic solid occupying the whole space $\mathbb{R}^3$ is considered. We denote by **E**, **H**, **D**, **B** the electric field, the magnetic field, the electric displacement, and the magnetic induction, respectively. For time-harmonic fields, whose time dependence is given by the factor $e^{-i\omega t}$ with $\omega > 0$, Maxwell's equations assume the form

$$\nabla \times \mathbf{E} = i\omega \mathbf{B}, \quad \nabla \times \mathbf{H} = -i\omega \mathbf{D} + \mathbf{J}, \tag{2}$$

$$\nabla \cdot \mathbf{D} = \rho, \quad \nabla \cdot \mathbf{B} = 0, \tag{3}$$

where the current density **J** and the free charge density ρ satisfy the continuity equation

$$\nabla \cdot \mathbf{J} - i\omega\rho = 0. \tag{4}$$

We suppose that the solid is linear and anisotropic, namely the constitutive equations

$$\mathbf{B} = \boldsymbol{\mu}\mathbf{H}, \quad \mathbf{D} = \boldsymbol{\varepsilon}\mathbf{E}, \quad \mathbf{J} = \boldsymbol{\sigma}\mathbf{E}$$

hold, where $\boldsymbol{\mu}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ are second-order complex-valued tensors depending on the position vector **x**. Hence, Eqs. (2) assume the form

$$\nabla \times \mathbf{H} = -i\omega \bar{\boldsymbol{\varepsilon}}\mathbf{E}, \quad \nabla \times \mathbf{E} = i\omega \boldsymbol{\mu}\mathbf{H}, \tag{5}$$

where $\bar{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon} + (i/\omega)\boldsymbol{\sigma}$.

By applying the divergence operator to Eqs. (5) and by using the continuity Eq. (4), we deduce (3). Therefore we take only Eqs. (5) into account.

We assume that the solid is stratified along a direction **n** and we introduce a system of Cartesian axes x_1, x_2, x_3, with unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, such that $\mathbf{e}_3 = \mathbf{n}$. Accordingly, the tensors $\boldsymbol{\mu}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ are constant on planes perpendicular to $\mathbf{e}_3$. Here and in the sequel we denote by z the independent variable x_3.

Owing to the stratification, we look for solutions of (5) in the form

$$\mathbf{H}(\mathbf{x},t)=\boldsymbol{\mathcal{H}}(z)e^{i(\mathbf{k}_\parallel\cdot\mathbf{x}-\omega t)},\quad \mathbf{E}(\mathbf{x},t)=\boldsymbol{\mathcal{E}}(z)e^{i(\mathbf{k}_\parallel\cdot\mathbf{x}-\omega t)}, \tag{6}$$

where $\mathbf{k}_\parallel$ is a real vector perpendicular to $\mathbf{e}_3$. The exponential dependence on $\mathbf{k}_\parallel\cdot\mathbf{x}$ agrees with Snell's law. Substitution of (6) into (5) yields

$$\mathbf{e}_3\times\boldsymbol{\mathcal{H}}'_\parallel+i\mathbf{k}_\parallel\times\boldsymbol{\mathcal{H}}+i\omega\bar{\varepsilon}\boldsymbol{\mathcal{E}}=0,\quad \mathbf{e}_3\times\boldsymbol{\mathcal{E}}'_\parallel+i\mathbf{k}_\parallel\times\boldsymbol{\mathcal{E}}-i\omega\boldsymbol{\mu}\boldsymbol{\mathcal{H}}=0, \tag{7}$$

where the prime indicates differentiation with respect to z and

$$\boldsymbol{\mathcal{H}}_\parallel=\mathcal{H}_1\mathbf{e}_1+\mathcal{H}_2\mathbf{e}_2,\quad \boldsymbol{\mathcal{E}}_\parallel=\mathcal{E}_1\mathbf{e}_1+\mathcal{E}_2\mathbf{e}_2.$$

Since $\mathbf{k}_\parallel$ is real, it is not restrictive to assume $\mathbf{k}_\parallel=k_1\mathbf{e}_1$. Then, inner product of (7) with $\mathbf{e}_3$ leads to the equations

$$\mathbf{e}_3\cdot(\mathbf{k}_\parallel\times\boldsymbol{\mathcal{H}}+\omega\bar{\varepsilon}\boldsymbol{\mathcal{E}})=0,\quad \mathbf{e}_3\cdot(\mathbf{k}_\parallel\times\boldsymbol{\mathcal{E}}-\omega\boldsymbol{\mu}\boldsymbol{\mathcal{H}})=0,$$

which imply

$$\mathcal{E}_3=-\frac{1}{\omega\bar{\varepsilon}_{33}}(k_1\mathcal{H}_2+\omega\bar{\varepsilon}_{13}\mathcal{E}_1+\omega\bar{\varepsilon}_{23}\mathcal{E}_2), \tag{8}$$

$$\mathcal{H}_3=\frac{1}{\omega\mu_{33}}(k_1\mathcal{E}_2-\omega\mu_{13}\mathcal{H}_1-\omega\mu_{23}\mathcal{H}_2). \tag{9}$$

By projecting (7) along $\mathbf{e}_1$, $\mathbf{e}_2$ and taking (8) and (9) into account, we obtain the linear system

$$\mathbf{w}'=\mathbb{N}\mathbf{w}, \tag{10}$$

where $\mathbf{w}=(\mathcal{H}_1,\mathcal{H}_2,\mathcal{E}_1,\mathcal{E}_2)^T$ and $\mathbb{N}$ is a complex valued matrix whose block structure is given by

$$\mathbb{N}=i\begin{pmatrix}\mathbb{N}_1 & \mathbb{N}_2\\ \mathbb{N}_3 & \mathbb{N}_4\end{pmatrix}, \tag{11}$$

with

$$\mathbb{N}_1=-k_1\begin{pmatrix}\dfrac{\mu_{13}}{\mu_{33}} & \dfrac{\mu_{23}}{\mu_{33}}-\dfrac{\bar{\varepsilon}_{23}}{\bar{\varepsilon}_{33}}\\ 0 & \dfrac{\bar{\varepsilon}_{13}}{\bar{\varepsilon}_{33}}\end{pmatrix},$$

$$\mathbb{N}_2=\omega\begin{pmatrix}\dfrac{\bar{\varepsilon}_{13}\bar{\varepsilon}_{23}}{\bar{\varepsilon}_{33}}-\bar{\varepsilon}_{12} & \dfrac{\bar{\varepsilon}_{23}^2}{\bar{\varepsilon}_{33}}-\bar{\varepsilon}_{22}+\dfrac{k_1^2}{\omega^2\mu_{33}}\\ \bar{\varepsilon}_{11}-\dfrac{\bar{\varepsilon}_{13}^2}{\bar{\varepsilon}_{33}} & \bar{\varepsilon}_{12}-\dfrac{\bar{\varepsilon}_{13}\bar{\varepsilon}_{23}}{\bar{\varepsilon}_{33}}\end{pmatrix},$$

$$\mathbb{N}_3=\omega\begin{pmatrix}\mu_{12}-\dfrac{\mu_{13}\mu_{23}}{\mu_{33}} & \mu_{22}-\dfrac{\mu_{23}^2}{\mu_{33}}-\dfrac{k_1^2}{\omega^2\bar{\varepsilon}_{33}}\\ \dfrac{\mu_{13}^2}{\mu_{33}}-\mu_{11} & \dfrac{\mu_{13}\mu_{23}}{\mu_{33}}-\mu_{12}\end{pmatrix},$$

$$\mathbb{N}_4 = -k_1 \begin{pmatrix} \dfrac{\overline{\varepsilon}_{13}}{\overline{\varepsilon}_{33}} & \dfrac{\overline{\varepsilon}_{23}}{\overline{\varepsilon}_{33}} - \dfrac{\mu_{23}}{\mu_{33}} \\ 0 & \dfrac{\mu_{13}}{\mu_{33}} \end{pmatrix}.$$

Since $\mathcal{H}_3$ and $\mathcal{E}_3$ are expressed in terms of the $\mathcal{H}_\parallel$ and $\mathcal{E}_\parallel$ through (8) and (9), we restrict our attention to the system (10).

The material parameters $\boldsymbol{\mu}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ (and hence the matrix $\mathbb{N}$) are supposed to be continuous or are allowed to suffer jump discontinuities at planes orthogonal to $\mathbf{e}_3$, when different solids in contact are considered. At such planes, the continuity of the electric and magnetic fields $\boldsymbol{\mathcal{E}}_\parallel$, $\boldsymbol{\mathcal{H}}_\parallel$ is required as usual.

III. ENERGY FLUX

In this section we recall the definition and the properties of the energy flux which is involved in the formulation of the reflection-transmission problem.

For complex-valued fields, the time-averaged energy flux vector $\mathbf{S}$, i.e. the Poynting vector, is defined by[7]

$$\mathbf{S} = \frac{1}{2}\mathrm{Re}(\mathbf{E} \times \mathbf{H}^*),$$

where the symbol * denotes the complex conjugate. Since $\mathbf{k}_\parallel$ is real, by using (6) $\mathbf{S}$ is expressed in terms of $\boldsymbol{\mathcal{E}}$, $\boldsymbol{\mathcal{H}}$ as

$$\mathbf{S} = \frac{1}{2}\mathrm{Re}(\boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}}^*). \tag{12}$$

Thus the Poynting vector depends only on the independent variable z.

The second law of Thermodynamics implies the relation

$$\nabla \cdot \mathbf{S} < 0, \quad (\mathbf{E},\mathbf{H}) \neq (0,0), \tag{13}$$

which is equivalent to

$$\omega\ \mathrm{Im}\ \boldsymbol{\mu} > 0, \quad \omega\ \mathrm{Im}\ \overline{\varepsilon} > 0, \quad \forall\ \omega \in \mathbb{R} \setminus \{0\} \tag{14}$$

in case of harmonic fields (see Ref. 1). In the relations (13) and (14), the equalities hold if the material is without memory.

We denote by $\mathcal{F}$ the projection of the energy flux vector $\mathbf{S}$ along the direction of the stratification, namely

$$\mathcal{F} = \mathbf{S} \cdot \mathbf{e}_3 = S_3.$$

In view of (12), $\mathcal{F}$ assumes the form

$$\mathcal{F} = \frac{1}{4}(\boldsymbol{\mathcal{E}}^* \times \boldsymbol{\mathcal{H}} + \boldsymbol{\mathcal{E}} \times \boldsymbol{\mathcal{H}}^*) \cdot \mathbf{e}_3.$$

Since $\mathcal{F}$ depends only on $\mathcal{E}_1$, $\mathcal{E}_2$, $\mathcal{H}_1$, $\mathcal{H}_2$, it follows that $\mathcal{F}$ is continuous at the common boundary between two different solids.

If we denote by $\mathbb{J}$ the matrix defined as

$$\mathbb{J} = \frac{1}{4}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

we write the energy flux in terms of $\mathbf{w}$, i.e.,

$$\mathcal{F} = \mathbf{w}^{\dagger}\mathbb{J}\mathbf{w}, \tag{15}$$

where the symbol † means the conjugate transpose.

The theorem of existence and uniqueness for the reflection-transmission problem is based on the following property of the energy flux.

Proposition. 3.1: *The energy flux $\mathcal{F}$ is nonincreasing in $\mathbb{R}$.*

Proof: Since the vector $\mathbf{S}$ depends only on the variable z, we have

$$\mathcal{F}' = \partial_3 S_3 = \nabla \cdot \mathbf{S}.$$

The thermodynamic restrictions (13) and the continuity of $\mathcal{F}$ guarantee that $\mathcal{F}$ is nonincreasing for each $z \in \mathbb{R}$. □

IV. REFLECTION AND TRANSMISSION PROBLEM IN A STRATIFIED LAYER

In this section we study wave propagation in a stratified solid constituted by a nonhomogeneous layer in the strip $0<z<L$, between two homogeneous media occupying the half-spaces $z<0$ and $z>L$. The matrix $\mathbb{N}$ of system (10) is written as

$$\mathbb{N} = \begin{cases} \mathbb{N}^- & z<0, \\ \widetilde{\mathbb{N}} & 0<z<L, \\ \mathbb{N}^+ & z<L, \end{cases} \tag{16}$$

where $\mathbb{N}^-$ and $\mathbb{N}^+$ denote the constant matrices in the homogeneous regions $z<0$ and $z>L$, respectively, while $\widetilde{\mathbb{N}}$ depends continuously on z.

We assume that $\mathbb{N}^-$ and $\mathbb{N}^+$ are simple matrices and denote by $i\nu_k^{\pm}$, $\mathbf{p}_k^{\pm}$, $k=1,\ldots,4$, the related eigenvalues and corresponding independent eigenvectors. No normalization condition on the eigenvectors $\mathbf{p}_k^{\pm}$, $k=1,\ldots,4$, is required. Moreover, we define by $\mathbb{P}^-$, $\mathbb{P}^+$ the matrices whose columns are the eigenvectors $\mathbf{p}_1^-,\ldots,\mathbf{p}_4^-$ and $\mathbf{p}_1^+,\ldots,\mathbf{p}_4^+$, respectively, i.e.,

$$\mathbb{P}^- = (\mathbf{p}_1^-,\ldots,\mathbf{p}_4^-), \quad \mathbb{P}^+ = (\mathbf{p}_1^+,\ldots,\mathbf{p}_4^+).$$

In order to describe the reflection-transmission problem, we need to characterize the direction of propagation of a wave. Following Ref. 2, we make use of the energy flux to distinguish between waves propagating in the increasing and decreasing z direction. More precisely, we say that a wave $\mathbf{w}$ is up-going or down-going across the plane $z=c$, with $c \in (-\infty,0) \cup (L,+\infty)$, if

$$\mathcal{F}_{\mathbf{w}}(c) > 0 \quad \text{or} \quad \mathcal{F}_{\mathbf{w}}(c) < 0,$$

where the notation $\mathcal{F}_{\mathbf{w}}$ emphasizes the dependence of the flux $\mathcal{F}$ on $\mathbf{w}$.

Consider a solution $\mathbf{w}$ of the system (10). In the half-space $z<0$, $\mathbf{w}$ is written in the form

$$\mathbf{w}(z) = \sum_{k=1}^{4} c_k^- \mathbf{p}_k^- e^{i\nu_k^- z},$$

where c_k^-, $k=1,\ldots,4$, are suitable complex coefficients. In view of (15), the energy flux of $\mathbf{w}$ is given by

$$\mathcal{F}_{\mathbf{w}}(z) = \sum_{k,h=1}^{4} c_k^{-*} c_h^- (\mathbf{p}_k^-)^\dagger \mathbb{J} \mathbf{p}_h^- e^{i(\nu_h^- - \nu_k^{-*})z}$$

$$= \sum_{k,h=1}^{4} c_k^{-*} c_h^- \mathbf{\Phi}_{kh}^- e^{i(\nu_h^- - \nu_k^{-*})z} \tag{17}$$

in the half-space $z<0$, where $\mathbf{\Phi}^-$ is the matrix defined as

$$\mathbf{\Phi}^- = (\mathbb{P}^-)^\dagger \mathbb{J} \mathbb{P}^-. \tag{18}$$

As $\mathbb{P}^-$ is nonsingular, the matrices $\mathbf{\Phi}^-$ and $\mathbb{J}$ are congruent and hence they have the same number of positive, negative, and zero eigenvalues.[11] In particular, since the eigenvalues of $\mathbb{J}$ are

$$\lambda_{1,2} = \frac{1}{4}, \quad \lambda_{3,4} = -\frac{1}{4},$$

And $\mathbf{\Phi}^-$ has two positive and two negative eigenvalues.

This condition is not sufficient to guarantee that a linear combination of up-going (down-going) waves is up-going (down-going). Therefore, further conditions on the matrix $\mathbf{\Phi}^-$ are required.

For convenience, we represent $\mathbf{\Phi}^-$ in the form

$$\mathbf{\Phi}^- = \begin{pmatrix} \mathbf{\Phi}_p^- & \mathbf{\Phi}_1^- \\ \mathbf{\Phi}_2^- & \mathbf{\Phi}_n^- \end{pmatrix}.$$

Henceforth, we assume that $\mathbf{\Phi}_p^-$ and $\mathbf{\Phi}_n^-$ are positive and negative definite, respectively.

Let $\mathbf{w}$ and $\tilde{\mathbf{w}}$ be two solutions of the system (10) such that

$$\mathbf{w} = c_1^- \mathbf{p}_1^- e^{i\nu_1^- z} + c_2^- \mathbf{p}_2^- e^{i\nu_2^- z}, \quad \tilde{\mathbf{w}} = c_3^- \mathbf{p}_3^- e^{i\nu_3^- z} + c_4^- \mathbf{p}_4^- e^{i\nu_4^- z},$$

in the half-space $z<0$ with (c_1^-, c_2^-), $(c_3^-, c_4^-) \in \mathbb{C}^2 \setminus \{(0,0)\}$. From (17) and the assumptions on the definiteness, we obtain

$$\mathcal{F}_{\mathbf{w}}(z) = \sum_{k,h=1}^{2} c_k^{-*} c_h^- \mathbf{\Phi}_{p,kh}^- e^{i(\nu_h^- - \nu_k^{-*})z} > 0,$$

$$\mathcal{F}_{\tilde{\mathbf{w}}}(z) = \sum_{k,h=1}^{2} c_{k+2}^{-*} c_{h+2}^- \mathbf{\Phi}_{n,kh}^- e^{i(\nu_{h+2}^- - \nu_{k+2}^{-*})z} < 0,$$

for every $z<0$. In particular, $\mathbf{p}_1^- e^{i\nu_1^- z}$, $\mathbf{p}_2^- e^{i\nu_2^- z}$ are up-going waves while $\mathbf{p}_3^- e^{i\nu_3^- z}$, $\mathbf{p}_4^- e^{i\nu_4^- z}$ are down-going waves in the half-space $z<0$.

Similarly, we introduce the matrix

$$\mathbf{\Phi}^+ = (\mathbb{P}^+)^\dagger \mathbb{J} \mathbb{P}^+ = \begin{pmatrix} \mathbf{\Phi}_p^+ & \mathbf{\Phi}_1^+ \\ \mathbf{\Phi}_2^+ & \mathbf{\Phi}_n^+ \end{pmatrix},$$

and we assume that $\mathbf{\Phi}_p^+$ and $\mathbf{\Phi}_n^+$ are positive and negative definite, respectively. Therefore, $\mathbf{p}_1^+ e^{i\nu_1^+(z-L)}$, $\mathbf{p}_2^+ e^{i\nu_2^+(z-L)}$ and $\mathbf{p}_3^+ e^{i\nu_3^+(z-L)}$, $\mathbf{p}_4^+ e^{i\nu_4^+(z-L)}$ are waves propagating upwards and downwards, respectively, in the half-space $z>L$.

A. Uniqueness

Let us consider an incident wave $\mathbf{w}^i$ coming from the homogeneous region $z<0$. The corresponding reflected and transmitted waves, $\mathbf{w}^r$ and $\mathbf{w}^t$, occur in the half-spaces $z<0$ and $z>L$, respectively.

We represent the incident, reflected and transmitted waves in the form

$$\mathbf{w}^i = c_1^i \mathbf{p}_1^- e^{i\nu_1^- z} + c_2^i \mathbf{p}_2^- e^{i\nu_2^- z}, \quad \mathbf{w}^r = c_3^r \mathbf{p}_3^- e^{i\nu_3^- z} + c_4^r \mathbf{p}_4^- e^{i\nu_4^- z}$$

in the half-space $z<0$ and

$$\mathbf{w}^t = c_1^t \mathbf{p}_1^+ e^{i\nu_1^+ z} + c_2^t \mathbf{p}_2^+ e^{i\nu_2^+ z}$$

in $z>L$. The assumptions on the matrices $\mathbf{\Phi}^+$ and $\mathbf{\Phi}^-$ guarantee that $\mathbf{w}^i, \mathbf{w}^r$ are up-going and down-going waves, respectively, in the half-space $z<0$, while $\mathbf{w}^t$ propagates upwards in the region $z>L$.

We define

$$\mathbf{w} = \begin{cases} \mathbf{w}^i + \mathbf{w}^r & z \in (-\infty, 0), \\ \tilde{\mathbf{w}} & z \in (0, L), \\ \mathbf{w}^t & z \in (L, +\infty), \end{cases} \tag{19}$$

where $\tilde{\mathbf{w}}$ is a solution of (10) in the open set $(0,L)$.

The reflection-transmission problem is to determine $\mathbf{w}^r$, $\mathbf{w}^t$, $\tilde{\mathbf{w}}$ from the knowledge of the incident wave $\mathbf{w}^i$ such that the function $\mathbf{w}$ is continuous for every $z \in \mathbb{R}$. More precisely, we have to determine $\tilde{\mathbf{w}}$ and the coefficients c_3^r, c_4^r, c_1^t, c_2^t, such that the function $\mathbf{w}$ defined in (19) satisfies (10) with $\mathbb{N}$ given by (16) and is continuous at $z=0$ and $z=L$.

Theorem 4.1: If $\mathbf{\Phi}_n^-$ is negative definite and $\mathbf{\Phi}_p^+$ is positive definite, then the solution $\mathbf{w}$ of the reflection-transmission problem is unique.

Proof: Consider two different solutions $\mathbf{w}$ and $\overline{\mathbf{w}}$ of the reflection-transmission problem. Denote by c_3^r, c_4^r, c_1^t, c_2^t and $\overline{c}_3^r$, $\overline{c}_4^r$, $\overline{c}_1^t$, $\overline{c}_2^t$ the reflection and transmission coefficients related to $\mathbf{w}$ and $\overline{\mathbf{w}}$. By letting $\mathbf{v} = \mathbf{w} - \overline{\mathbf{w}}$, we have

$$\mathbf{v}(z) = \begin{cases} (c_3^r - \overline{c}_3^r)\mathbf{p}_3^- e^{i\nu_3^- z} + (c_4^r - \overline{c}_4^r)\mathbf{p}_4^- e^{i\nu_4^- z} & z \in (-\infty, 0), \\ \tilde{\mathbf{v}}(z) & z \in (0, L), \\ (c_1^t - \overline{c}_1^t)\mathbf{p}_1^+ e^{i\nu_1^+ z} + (c_2^t - \overline{c}_2^t)\mathbf{p}_2^+ e^{i\nu_2^+ z} & z \in (L, +\infty), \end{cases}$$

where $\tilde{\mathbf{v}}$ is defined by $\tilde{\mathbf{v}} = \tilde{\mathbf{w}} - \tilde{\overline{\mathbf{w}}}$.

The assumptions on the matrices $\mathbf{\Phi}_n^-$ and $\mathbf{\Phi}_p^+$ assure that $\mathcal{F}_{\mathbf{v}}(z) \leq 0$ in the half-space $z<0$ and $\mathcal{F}_{\mathbf{v}}(z) \geq 0$ in the region $z>L$. Since the energy flux is non-increasing, we deduce that

$$\mathcal{F}_{\mathbf{v}}(z) \equiv 0$$

for every $z \in \mathbb{R}$. The definiteness of the matrices $\mathbf{\Phi}_n^-$ and $\mathbf{\Phi}_p^+$ guarantees that

$$\mathbf{v}(z) = 0, \quad z \in (-\infty, 0] \cup (L, +\infty].$$

Furthermore, since $\tilde{\mathbf{v}}$ is the unique solution of the Cauchy problem,

$$\mathbf{w}' = \tilde{\mathbb{N}}\mathbf{w}, \quad 0 < z < L,$$

$$\tilde{\mathbf{w}}(0) = 0,$$

$\tilde{\mathbf{v}}$ vanishes identically in $(0,L)$. Thus $\mathbf{w} = \overline{\mathbf{w}}$. □

If we consider incident waves coming from the half-space $z>L$, we have

$$\mathbf{w}^i = c_3^i \mathbf{p}_3^+ e^{i\nu_3^+ z} + c_4^i \mathbf{p}_4^+ e^{i\nu_4^+ z}, \quad \mathbf{w}^r = c_1^r \mathbf{p}_1^+ e^{i\nu_1^+ z} + c_2^r \mathbf{p}_2^+ e^{i\nu_2^+ z}$$

in $z > L$ and

$$\mathbf{w}^t = c_3^t \mathbf{p}_3^- e^{i\nu_3^- z} + c_4^t \mathbf{p}_4^- e^{i\nu_4^- z}$$

in $z < 0$. The corresponding reflection-transmission problem is formulated straightforwardly and the following result can be proved.

Theorem 4.2: If $\mathbf{\Phi}_p^-$ is positive definite and $\mathbf{\Phi}_n^+$ is negative definite, then the solution $\mathbf{w}$ of the reflection-transmission problem is unique.

B. Existence

In order to prove the existence of the solutions of the reflection-transmission problem, we introduce two suitable sets of four independent solutions of the system (10).

Since the matrix $\mathbb{N}$ is constant in the half-space $z < 0$, $\mathbf{p}_1^- e^{i\nu_1^- z}, \ldots, \mathbf{p}_4^- e^{i\nu_4^- z}$ are four independent solutions of the system $\mathbf{w}' = \mathbb{N}^- \mathbf{w}$ in the region $z < 0$. Let $\tilde{\psi}_1^-, \ldots, \tilde{\psi}_4^-$ be the solutions of the Cauchy problems

$$\mathbf{w}' = \tilde{\mathbb{N}}\mathbf{w}, \quad 0 < z < L,$$

$$\mathbf{w}(0) = \mathbf{p}_h^-, \quad h = 1, \ldots, 4.$$

Next consider the half-space $z > L$ and denote by $\alpha_{hk}^+ \in \mathbb{C}$, $h, k = 1, \ldots, 4$, the unique coefficients such that $\Sigma_{k=1}^4 \alpha_{hk}^+ \mathbf{p}_k^+ e^{i\nu_k^+ (z-L)}$ are the solutions of (10) with initial value $\tilde{\psi}_h^-(L)$ at $z = L$. Accordingly, the vectors $\psi_1^-, \ldots, \psi_4^-$, defined by

$$\psi_h^- = \begin{cases} \mathbf{p}_h^- e^{i\nu_h^- z} & z \le 0, \\ \tilde{\psi}_h^- & 0 < z < L, \quad h = 1, \ldots, 4, \\ \displaystyle\sum_{k=1}^4 \alpha_{hk}^+ \mathbf{p}_k^+ e^{i\nu_k^+ (z-L)} & z \ge L, \end{cases}$$

are continuous in $\mathbb{R}$ and satisfy the system (10) in the open set $(-\infty, 0) \cup (0, L) \cup (L, +\infty)$.

Similarly, we introduce the functions $\psi_1^+, \ldots, \psi_4^+$ defined by

$$\psi_h^+ = \begin{cases} \displaystyle\sum_{k=1}^4 \alpha_{hk}^- \mathbf{p}_k^- e^{i\nu_k^- z} & z \le 0, \\ \tilde{\psi}_h^+ & 0 < z < L, \quad h = 1, \ldots, 4 \\ \mathbf{p}_h^+ e^{i\nu_h^+ (z-L)} & z \ge L, \end{cases}.$$

For any incident wave

$$\mathbf{w}^i = c_1^i \mathbf{p}_1^- e^{i\nu_1^- z} + c_2^i \mathbf{p}_2^- e^{i\nu_2^- z}, \quad z < 0,$$

coming from below, we define the corresponding continuous extension $\hat{\mathbf{w}}^i$ of $\mathbf{w}^i$ as

$$\hat{\mathbf{w}}^i = c_1^i \psi_1^- + c_2^i \psi_2^-.$$

Furthermore, we denote by $\hat{\mathbf{w}}^r, \hat{\mathbf{w}}^t$ the continuous extensions of $\mathbf{w}^r$ and $\mathbf{w}^t$, respectively, i.e.,

$$\hat{\mathbf{w}}^r = c_3^r \psi_3^- + c_4^r \psi_4^-, \quad \hat{\mathbf{w}}^t = c_1^t \psi_1^+ + c_2^t \psi_2^+.$$

On determining the coefficients c_3^r, c_4^r, c_1^t, c_2^t in terms of c_1^i, c_2^i by the equation

$$\hat{\mathbf{w}}^i + \hat{\mathbf{w}}^r = \hat{\mathbf{w}}^t, \tag{20}$$

we obtain a solution of the reflection-transmission problem. Indeed, the vector $\mathbf{w}$ defined as

$$\mathbf{w} = \hat{\mathbf{w}}^i + \hat{\mathbf{w}}^r = \hat{\mathbf{w}}^t$$

solves (10) with $\mathbb{N}$ given by (16), is continuous in $\mathbb{R}$ and satisfies (19).

For the sake of simplicity, we let $\mathbf{w}^i = \psi_h^-$, $h=1,2$. Then Eq. (20) reduces to

$$\psi_h^- + \mathbb{R}_{1h}^- \psi_3^- + \mathbb{R}_{2h}^- \psi_4^- = \mathbb{T}_{1h}^+ \psi_1^+ + \mathbb{T}_{2h}^+ \psi_2^+, \quad h=1,2, \tag{21}$$

where R^- and T^+ are the unknown reflection and transmission matrices, respectively.

The equations governing the reflection-transmission process for incident waves coming from upward are

$$\psi_{h+2}^+ + \mathbb{R}_{1h}^+ \psi_1^+ + \mathbb{R}_{2h}^+ \psi_2^+ = \mathbb{T}_{1h}^- \psi_3^- + \mathbb{T}_{2h}^- \psi_4^-, \quad h=1,2. \tag{22}$$

Theorem 4.3 (Existence): *If $\mathbf{\Phi}_p^+$ and $\mathbf{\Phi}_p^-$ are positive definite and $\mathbf{\Phi}_n^+$ and $\mathbf{\Phi}_n^-$ are negative definite, there exist unique $\mathbb{T}^+$, $\mathbb{T}^-$, $\mathbb{R}^+$, $\mathbb{R}^-$, which solve (21) and (22).*

It is sufficient to prove that ψ_1^+, ψ_2^+, ψ_3^-, ψ_4^- constitute a basis for the solutions of system (10).

Let us suppose

$$c_1\psi_1^+ + c_2\psi_2^+ + c_3\psi_3^- + c_4\psi_4^- = 0$$

and define

$$\mathbf{v} = c_1\psi_1^+ + c_2\psi_2^+ = -c_3\psi_3^- - c_4\psi_4^-.$$

The assumption on the matrices $\mathbf{\Phi}^-$ and $\mathbf{\Phi}^+$ ensures that the inequalities

$$\mathcal{F}_{\mathbf{v}}(z) \geq 0, \quad \forall\, z \geq L,$$

$$\mathcal{F}_{\mathbf{v}}(z) \leq 0, \quad \forall\, z \leq 0,$$

hold.

Since $\mathcal{F}$ is nonincreasing, we deduce

$$0 \leq \mathcal{F}_{\mathbf{v}}(L) \leq \mathcal{F}_{\mathbf{v}}(0) \leq 0,$$

which implies

$$c_k = 0, \quad \forall\, k = 1,\ldots,4,$$

thanks to the definiteness of the matrices $\mathbf{\Phi}_n^-$ and $\mathbf{\Phi}_p^+$. Therefore, the independence of ψ_1^+, ψ_2^+, ψ_3^-, ψ_4^- is proved. □

V. REFLECTION AND TRANSMISSION PROBLEM IN $\mathbb{R}^3$

This section is devoted to an analysis of the reflection and transmission problem in a nonhomogeneous medium occupying the whole space $\mathbb{R}^3$. We assume that the solid is a dielectric without memory, namely the matrices $\boldsymbol{\varepsilon}$, $\boldsymbol{\mu}$ have real entries and $\boldsymbol{\sigma}$ vanishes identically. Furthermore, we suppose that $\boldsymbol{\varepsilon}$, $\boldsymbol{\mu}$, and hence $\mathbb{N}$ are continuous.

The definition of the reflection and transmission coefficients depends on the asymptotic behavior of the solutions of the system (10). Therefore, we need to introduce some requirements on the asymptotic behavior of $\mathbb{N}$.

We assume the existence of the limits of $\mathbb{N}$ as $z \to -\infty$ and $z \to +\infty$, denoted by $\mathbb{N}^-$ and $\mathbb{N}^+$, respectively. The matrices $\mathbb{N}^-$ and $\mathbb{N}^+$ are supposed to be simple and are not required to be equal.

We denote by $i\nu_k^{\pm}$, $\mathbf{p}_k^{\pm}$, $k=1,\dots,4$, the eigenvalues and the corresponding independent eigenvectors of $\mathbb{N}^{\pm}$. From the relation (11), we deduce that the blocks $\mathbb{N}_1,\dots,\mathbb{N}_4$ of the matrix $\mathbb{N}$ have real entries. Therefore, ν_k^+ and ν_k^-, $k=1,...,4$, are either real or occur in conjugate pairs. We assume that $\nu_k^{\pm}\in\mathbb{R}$ for every $k=1,\dots,4$.

Moreover, we suppose that there exist $a,b\in\mathbb{R}$ such that the conditions

$$\int_{-\infty}^{a}\|\mathbb{N}-\mathbb{N}^-\|dz<+\infty,\quad \int_{b}^{+\infty}\|\mathbb{N}-\mathbb{N}^+\|dz<+\infty$$

hold, where $\|\cdot\|$ denotes any norm in the fourth-order square matrices.

Under these assumptions,[10] there exist two sets of four solutions $\psi_1^-,\dots,\psi_4^-$ and $\psi_1^+,\dots,\psi_4^+$ of the system (10) such that

$$\psi_k^{\pm}=(\mathbf{p}_k^{\pm}+\mathbf{v}_k^{\pm})e^{i\nu_k^{\pm}z},\quad k=1,\dots,4, \tag{23}$$

where $\mathbf{v}_k^-$ and $\mathbf{v}_k^+$ satisfy the condition

$$\lim_{z\to-\infty}\mathbf{v}_k^-=\lim_{z\to+\infty}\mathbf{v}_k^+=0,\quad k=1,\dots,4. \tag{24}$$

Moreover, since the conditions

$$\text{Im }\nu_1^-=\dots=\text{Im }\nu_4^-=0,\quad \text{Im }\nu_1^+=\dots=\text{Im }\nu_4^+=0$$

are satisfied, the solutions $\psi_1^-,\dots,\psi_4^-$ and $\psi_1^+,\dots,\psi_4^+$ are determined uniquely[10] by the asymptotic behaviors (24).

The functions $\psi_1^-,\dots,\psi_4^-$ and $\psi_1^+,\dots,\psi_4^+$ are related to the Jost solutions of the Schödinger equation (see Refs. 3 and 4).

By denoting by $\mathbb{E}^{\pm}$ and $\mathbb{V}^{\pm}$ the matrices defined as

$$\mathbb{E}^{\pm}=\text{diag}(e^{i\nu_1^{\pm}z},\dots,e^{i\nu_4^{\pm}z}),\quad \mathbb{V}^{\pm}=(\mathbf{v}_1^{\pm},\dots,\mathbf{v}_4^{\pm}),$$

we write the conditions (23) in the form

$$\boldsymbol{\Psi}^{\pm}=(\psi_1^{\pm},\dots,\psi_4^{\pm})=(\mathbb{P}^{\pm}+\mathbb{V}^{\pm})\mathbb{E}^{\pm}.$$

The independence of the vectors $\mathbf{p}_1^-,\dots,\mathbf{p}_4^-$ and $\mathbf{p}_1^+,\dots,\mathbf{p}_4^+$ guarantees that the functions $\psi_1^-,\dots,\psi_4^-$ and $\psi_1^+,\dots,\psi_4^+$ are independent solutions of the system (10), i.e., any solution $\mathbf{w}$ of (10) may be written in the form

$$\mathbf{w}=\sum_{k=1}^{4}c_k^-\psi_k^-=\sum_{k=1}^{4}c_k^+\psi_k^+,$$

where $c_k^+,c_k^-\in\mathbb{C}$, $k=1,\dots,4$ are suitable complex coefficients.

As in the previous section, we make use of the energy flux to select waves propagating in the increasing and decreasing z direction. More precisely, we say that a wave $\mathbf{w}$ is asymptotically up-going (down-going) when $z\to-\infty$ if $\mathbf{w}$ is definitively up-going (down-going), namely if there exists $Z_{\mathbf{w}}$ such that

$$\mathcal{F}_{\mathbf{w}}(z)>0,\quad [\mathcal{F}_{\mathbf{w}}(z)<0],\quad \forall\, z\le -Z_{\mathbf{w}}.$$

We introduce the matrix $\mathbb{F}^-$ defined as

$$\mathbb{F}^-=(\boldsymbol{\Psi}^-)^{\dagger}\,\mathbb{J}\boldsymbol{\Psi}^-=\begin{pmatrix}\mathbb{F}_p^- & \mathbb{F}_1^-\\ \mathbb{F}_2^- & \mathbb{F}_n^-\end{pmatrix},$$

so that the energy flux of a wave $\mathbf{w}=\Sigma_{k=1}^4c_k^-\psi_k^-$ is given by

$$\mathcal{F} = (\mathbf{c}^-)^\dagger \mathbb{F}^- \mathbf{c}^-,$$

where $\mathbf{c}^- = (c_1^-, \ldots, c_4^-)^T$.

Proposition 5.1: Suppose that the matrices $\mathbf{\Phi}_p^-, \mathbf{\Phi}_n^-$, defined in (18), are positive and negative definite, respectively. Then there exists $Z > 0$ such that $\mathbb{F}_p^-$, $\mathbb{F}_n^-$ are positive and negative definite for all $z \leq -Z$.

Proof: From the relation (18), we deduce that $\mathbf{\Phi}$ and hence $\mathbf{\Phi}_p^-$ are Hermitian. The hypothesis on the definiteness of the matrix $\mathbf{\Phi}_p^-$ guarantees that $\mathbf{\Phi}_p^-$ has two positive eigenvalues λ_1, λ_2 (see Ref. 11).

Let $\mathbb{A}^-$ be the matrix, depending on z, defined as

$$\mathbb{A}^- = (\mathbb{P}^- + \mathbb{V}^-)^\dagger \mathbb{J} (\mathbb{P}^- + \mathbb{V}^-). \tag{25}$$

For convenience, we represent $\mathbb{A}^-$ in the form

$$\mathbb{A}^- = \begin{pmatrix} \mathbb{A}_p^- & \mathbb{A}_1^- \\ \mathbb{A}_2^- & \mathbb{A}_n^- \end{pmatrix}.$$

Since $\mathbb{A}^-$ is Hermitian, $\mathbb{A}_p^-(z)$ is also Hermitian and has two real eigenvalues, $\mu_1(z)$, $\mu_2(z)$.

The definitions (18) and (25) and the condition (24) yield

$$\mathbb{A}_p^-(z) z \underset{z \to -\infty}{\to} \mathbf{\Phi}_p^-$$

and hence

$$\mu_1(z) z \underset{z \to -\infty}{\to} \lambda_1, \quad \mu_2(z) z \underset{z \to -\infty}{\to} \lambda_2.$$

Therefore, there exists $Z_p > 0$ such that $\mu_1(z)$, $\mu_2(z) > 0$ for all $z \leq -Z_p$, namely, the matrix $\mathbb{A}_p^-(z)$ is positive definite for all $z \leq -Z_p$.

The identity

$$\mathbb{F}^- = (\mathbb{E}^-)^\dagger \mathbb{A}^- \mathbb{E}^-$$

leads to the equality

$$\mathbb{F}_p^- = (\mathbb{E}_p^-) \mathbb{A}_p^- \mathbb{E}_p^-,$$

where $\mathbb{E}_p^- = \mathrm{diag}(e^{i\nu_1^- z}, e^{i\nu_2^- z})$, namely, $\mathbb{F}_p^-$ and $\mathbb{A}_p^-$ are congruent. Therefore, $\mathbb{F}_p^-$ is positive definite for all $z \leq -Z_p$.

By repeating the same arguments, we prove that there exists $Z_n > 0$ such that $\mathbb{F}_n^-$ is negative definite for all $z \leq -Z_n$. The theorem is proved with $Z = \max\{Z_p, Z_n\}$. □

The previous proposition assures that linear combinations of ψ_1^-, ψ_2^- represent asymptotically up-going waves, when $z \to -\infty$, whereas linear combinations of ψ_3^-, ψ_4^- represent waves propagating in the decreasing z direction.

Following a similar procedure, we define the matrix $\mathbb{F}^+$ as

$$\mathbb{F}^+ = (\mathbf{\Psi}^+) \mathbb{J} \mathbf{\Psi}^+ = \begin{pmatrix} \mathbb{F}_p^+ & \mathbb{F}_1^+ \\ \mathbb{F}_2^+ & \mathbb{F}_n^+ \end{pmatrix},$$

and we assume that $\mathbf{\Phi}_p^+$ and $\mathbf{\Phi}_n^+$ are positive and negative definite respectively. It follows that ψ_1^+, ψ_2^+ and ψ_3^+, ψ_4^+ represent waves propagating upwards and downwards, respectively, as $z \to +\infty$.

As in the previous section, the equations ruling the reflection-transmission problem are

$$(\psi_1^+, \psi_2^+)\mathbb{T}^+ = (\psi_1^-, \psi_2^-) + (\psi_3^-, \psi_4^-)\mathbb{R}^- \tag{26}$$

for incident waves coming from downward and

$$(\psi_3^-, \psi_4^-)\mathbb{T}^- = (\psi_3^+, \psi_4^+) + (\psi_1^+, \psi_2^+)\mathbb{R}^+ \tag{27}$$

for incident waves coming from upward.

The reflection-transmission problem consists in proving existence and uniqueness of the matrices $\mathbb{R}^\pm$, $\mathbb{T}^\pm$ (and hence of the reflected and transmitted waves) satisfying (26) and (27).

Theorem 5.2: *Suppose that* $\mathbf{\Phi}_p^+$, $\mathbf{\Phi}_p^-$ *are positive definite and* $\mathbf{\Phi}_n^+$ *and* $\mathbf{\Phi}_n^-$ *are negative definite. Then, given the incident waves* ψ_h^-, ψ_{h+2}^+, $h=1,2$ *, there exist unique* $\mathbb{T}^+$, $\mathbb{T}^-$, $\mathbb{R}^+$, $\mathbb{R}^-$ *that solve the reflection-transmission problem (26) and (27).*

Proof: The procedure followed in the proof of Theorem 3 and application of Proposition 1 show that ψ_1^+, ψ_2^+, ψ_3^-, ψ_4^- constitute a basis for the solutions of the system (10). Therefore, there exist unique matrices $\mathbb{R}^\pm$, $\mathbb{T}^\pm$ satisfying (26) and (27) in correspondence with the incident waves ψ_h^-, ψ_{h+2}^+, $h=1,2$. □

Remark: Consider a hereditary medium occupying the whole space. In this case, $\nu_1^\pm, \ldots, \nu_4^\pm$ are allowed to be complex.

The relations (15) and (23) lead to the equality

$$\mathcal{F}_{\psi_k^\pm}(z) = (\mathbf{p}_k^\pm + \mathbf{v}_k^\pm)^\dagger \mathbb{J}(\mathbf{p}_k^\pm + \mathbf{v}_k^\pm) e^{-2\,\mathrm{Im}\,\nu_k^\pm z}, \quad k = 1, \ldots 4.$$

Since only waves with bounded energy flux are physically admissible,[5] we have to consider only media satisfying the conditions

$$\mathrm{Im}\ \nu_k^+ \leq 0, \quad \mathrm{Im}\ \nu_k^- \geq 0, \quad k = 1, \ldots, 4$$

for layer of infinite amplitude.

Moreover, if the conditions

$$\mathrm{Im}\ \nu_1^- = \ldots = \mathrm{Im}\ \nu_4^- \quad \mathrm{Im}\ \nu_1^+ = \ldots = \mathrm{Im}\ \nu_4^+$$

are not satisfied, the functions $\psi_1^\pm, \ldots, \psi_4^\pm$ are not uniquely determined by the asymptotic conditions (24) (see Ref. 10). Therefore, for hereditary media the generators of the incident, reflected, and transmitted waves are not defined uniquely and the uniqueness of the reflection-transmission problem is lost.

VI. ISOTROPIC MEDIA

In general, the matrices $\mathbf{\Phi}_p^\pm$ and $\mathbf{\Phi}_n^\pm$ depend on the material parameters, the wave vector $\mathbf{k}_\parallel$, and the frequency ω. Moreover, the assumptions on the definiteness of the blocks of these matrices are not necessarily satisfied. In this section we give an example of medium verifying these requirements.

For definiteness, consider a homogeneous isotropic solid occupying the half-space $z<0$. The same conclusions can be obtained for the half-space $z>L$ or for isotropic dielectric without memory occupying the whole space. The tensors $\boldsymbol{\varepsilon}$, $\boldsymbol{\mu}$, $\boldsymbol{\sigma}$ assume the form

$$\boldsymbol{\varepsilon} = \varepsilon\mathbb{I}, \quad \boldsymbol{\mu} = \mu\mathbb{I}, \quad \boldsymbol{\sigma} = \sigma\mathbb{I}, \quad z < 0.$$

Moreover, suppose that the incidence is normal, namely $k_1=0$. Hence the matrix $\mathbb{N}^-$ is written as

$$\mathbb{N}^- = i\begin{pmatrix} 0 & 0 & 0 & -\omega\bar{\varepsilon} \\ 0 & 0 & \omega\bar{\varepsilon} & 0 \\ 0 & \omega\mu & 0 & 0 \\ -\omega\mu & 0 & 0 & 0 \end{pmatrix}.$$

Notice that if the solid is isotropic for all $z\in\mathbb{R}$, the system (10) decouples into two systems of first-order differential equations that can be reduced to linear Schrödinger equations.

It is easy to check that the eigenvalues of the matrix $\mathbb{N}^-$ are the complex square roots of $-\omega^2\bar{\varepsilon}\mu$ with multiplicity two. Moreover, the matrix $\mathbb{P}^-$ is given by

$$\mathbb{P}^-=\begin{pmatrix}-\alpha & 0 & \alpha & 0\\ 0 & \alpha & 0 & -\alpha\\ 0 & 1 & 0 & 1\\ 1 & 0 & 1 & 0\end{pmatrix},$$

where α and $-\alpha$ are the complex square roots of $\bar{\varepsilon}\mu^{-1}$. It is not restrictive to assume Re $\alpha>0$, in that Re $\alpha\neq 0$. This is easily seen for dielectrics without memory, since $\bar{\varepsilon}=\varepsilon\neq 0$, and may be shown by contradiction for material with memory. Accordingly, consider the latter case and suppose that Re$\alpha=0$. This condition is equivalent to

$$\mathrm{Im}\left(\bar{\varepsilon}\mu^{-1}\right)=0,\quad \mathrm{Re}\left(\bar{\varepsilon}\mu^{-1}\right)<0, \tag{28}$$

since $\bar{\varepsilon}$ does not vanish.

The thermodynamic restrictions (14) lead to

$$\mathrm{Im}\ \mu\ \mathrm{Im}\ \bar{\varepsilon}>0,\quad \forall\ \omega\neq 0. \tag{29}$$

By using the identities

$$\mathrm{Re}(\bar{\varepsilon}\mu^{-1})=\frac{1}{|\mu|^2}(\mathrm{Re}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu+\mathrm{Im}\ \bar{\varepsilon}\ \mathrm{Im}\ \mu),$$

$$\mathrm{Im}(\bar{\varepsilon}\mu^{-1})=\frac{1}{|\mu|^2}(\mathrm{Im}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu-\mathrm{Im}\ \mu\ \mathrm{Re}\ \bar{\varepsilon}),$$

and in view of the conditions (28) and (29), we deduce the relations

$$\mathrm{Re}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu<0, \tag{30}$$

$$\mathrm{Im}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu-\mathrm{Im}\ \mu\ \mathrm{Re}\ \bar{\varepsilon}=0, \tag{31}$$

for all $\omega\neq 0$. By multiplying (31) for Im μ, we obtain the equality

$$\mathrm{Im}\ \mu\ \mathrm{Im}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu-(\mathrm{Im}\ \mu)^2\mathrm{Re}\ \bar{\varepsilon}=0.$$

Comparison with the condition (29) shows that

$$\mathrm{Re}\ \bar{\varepsilon}\ \mathrm{Re}\ \mu\geq 0,$$

which is a contradiction with (30). Therefore, Re $\alpha\neq 0$.

In view of (18), we deduce

$$\mathbf{\Phi}^-=(\mathbb{P}^-)\mathbb{J}\mathbb{P}^-=\frac{1}{4}\begin{pmatrix}\alpha^*+\alpha & 0 & -\alpha^*+\alpha & 0\\ 0 & \alpha^*+\alpha & 0 & -\alpha^*+\alpha\\ \alpha^*-\alpha & 0 & -\alpha^*-\alpha & 0\\ 0 & \alpha^*-\alpha & 0 & -\alpha^*-\alpha\end{pmatrix}.$$

Therefore the matrices $\mathbf{\Phi}_p^-$, $\mathbf{\Phi}_n^-$ given by

$$\mathbf{\Phi}_p^- = -\mathbf{\Phi}_n^- = \frac{1}{2}\begin{pmatrix} \mathrm{Re}\ \alpha & 0 \\ 0 & \mathrm{Re}\ \alpha \end{pmatrix},$$

are positive and negative definite, respectively.

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Green functions for wave propagation on a five-dimensional manifold and the associated gauge fields generated by a uniformly moving point source

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Gauge fields associated with the manifestly covariant dynamics of particles in (3,1) space time are five dimensional (5D). We provide solutions of the classical 5D gauge field equations in both (4,1) and (3,2) flat space-time metrics for the simple example of a uniformly moving point source. Green functions for the 5D field equations are obtained, which are consistent with the solutions for uniform motion obtained directly from the field equations with free asymptotic conditions. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2401692]

I. INTRODUCTION

Maxwell electrodynamics arises in a natural way in the study of quantum dynamical evolution of particles in three-dimensional (3D) space. The nonrelativistic Schrödinger equation has a form that is invariant under the transformation

$$\Psi_t(x) \to e^{i\Lambda(x,t)}\Psi_t(x) \tag{1}$$

when the so-called gauge compensation fields are added to the space and time derivation. One finds in this method how the 3D dynamics associated with nonrelativistic theory results in a four-dimensional (4D) gauge field, which has an $O(3,1)$ invariance for the *homogeneous* field equations.

In a similar way, the manifestly covariant Stueckelberg-Schrödinger[1] equation (discussed below in Sec. II) induces five gauge fields. Some applications and results of the covariant theory are discussed in Sec. II. The motivation for discussing the gauge fields associated with the Stueckelberg-Schrödinger equation follows from the necessity for constructing a logically complete theory. The generalized classical electrodynamics is a direct consequence of the gauge covariant forms of the quantum equations of motion, and it is therefore essential to investigate the implications of this generalized electrodynamics. In this paper we consider the simplest problem of computing the field due to a point source moving with constant velocity in space time. The classical form of the Stueckelberg dynamics has the property that the particles are in principle "off shell," that is, the particle mass defined by $p^\mu p_\mu = -m^2c^2$ is not constrained to have a given numerical value. In this theory, the particle attains its observed mass, to a good approximation, according to the state of the system,[2] and we assume generally that the particle mass lies in this neighborhood. We define the "mass shell" values of m as the value obtained in the nonrelativistic (Galilean) limit of the theory (only a definite value of mass is admissible by Galilean invariance).

What we find is that the qualitative nature of the fields is very different when the source has values above, below, or equal to the mass shell values. We also discuss both timelike and spacelike motion for the source (both types of motion are admitted by the Stueckelberg classical mechanics). These results are important ingredients for the construction of a theory that provides a good phenomenological description for actual laboratory experiments, a subject of current research. For

example, it was shown by Land[3] that scattering of a test particle in the fields produced by a timelike on-shell source does not agree with the Rutherford result. However, an integration over a small section of the orbit of the same particle regularizes some of the singularities of the fields produced, and brings the scattering of the test particle arbitrarily close to the Rutherford form. Thus, as we discuss below, a partial concatenation of the source motion appears to be important for the construction of such a theory. Nevertheless, it is essential to investigate carefully the results of the direct pointwise application of the theory.

We study then, the mathematical and physical properties of these five-dimensional (5D) gauge fields. The work is divided as follows.

In Sec. II, an overview of the 5D off-mass-shell gauge field theory based on the framework of Stueckelberg[1,2,4] is given. 5D gauge theories also arise in other studies, such as a special case of higher dimensional relativistic dynamics and electrodynamics (cf. Refs. 5 and 6), or modern Kaluza-Klein type theories (cf. Ref. 7 and references therein). In this paper, we concentrate on the construction that is based on the Stueckelberg framework (cf. Refs. 2 and 4).

Previous studies of the fields have been conducted (cf. Refs. 3 and 8–11) using certain types of Green functions (GF's). Since the field equation in higher dimension admits many types of GF's, in order to gain some insight into criteria for selecting useful ones, here we study a direct solution by Fourier transform for the special case of a uniformly moving point source (UMS).

In Sec. III, a derivation of 5D gauge fields generated by a uniformly moving point source is given for both (4,1) and (3,2) metrics, followed by classification to regions of source motion, namely, spacelike and timelike. The wave equations are solved with asymptotically free conditions in which the boundary value of the fields at infinity vanish pointwise.

In Sec. IV, a derivation is given of the principal part GF's consistent with the fields generated by a uniformly moving source of Sec. III.

The GF's obtained agree with a particular form of fundamental solutions of 5D wave equations, found in, for example Refs. 12 and 13, i.e.,

$$g(x,\tau) = \lim_{\varepsilon \to 0^+} 14\pi^2 G_\varepsilon(x^2 + \sigma_5 \tau^2), \tag{2}$$

$$G_\varepsilon(y) = \frac{\partial}{\partial \varepsilon} \frac{\theta(-\sigma_5 y + \varepsilon)}{\sqrt{-\sigma_5 y + \varepsilon}}, \tag{3}$$

where σ_5 determines the metric signature, ± 1, for (4,1) and (3,2) metrics, respectively.

Our present study differs from the previous literature as follows:

- The GF's carry the group symmetry in all coordinates, whereas normally only the t retarded solutions are considered.
- The GF's are treated in a unified manner in both (4,1) and (3,2) metrics.
- We shall show that the derivative present in (3) is useful in regularizing the fields, whereas nonderivative forms (cf. Ref. 5 and references therein) have an additional infinite part, which may be removed by other methods such as Hadamard's *finite part* (cf. Ref. 14).
- We study, in particular, the properties of the gauge fields, derived both from the GF's and a more direct method, generated by a uniformly moving point source.

II. FUNDAMENTALS

An off-shell classical and quantum electrodynamics has been constructed[4] from a fundamental theory of relativistic dynamics of 4D particles, termed *events*, in a framework first derived by Stueckelberg.[1,2]

Stueckelberg defined a Lorentz invariant Hamiltonian-like generator of evolution, over an eight-dimensional (8D) phase space, parametrized by a Lorentz invariant τ, in both classical and quantum relativistic mechanics. Solutions of the relativistic quantum two-body bound state problem agree, up to relativistic corrections,[15] with solutions of the nonrelativistic Schrödinger equa-

tion. The experiments of Lindner *et al.*,[16] moreover, showing quantum interference in time, can be explained in a simple and consistent way in the framework of this theory,[17] which also provides strong evidence that the time t is a quantum observable, as required in this framework.

In the classical manifestly covariant theory, the Hamiltonian of a free particle is given by

$$K = \frac{p_\mu p^\mu}{2M}, \tag{4}$$

where $x^\mu = [ct, \mathbf{x}]$ and $p^\mu = [E/c, \mathbf{p}]$. A simple model for an interacting system is provided by the potential model

$$K = \frac{p_\mu p^\mu}{2M} + V(x). \tag{5}$$

The equations are

$$\dot{x}^\mu = \frac{\partial K}{\partial p_\mu} = \frac{1}{M} p^\mu, \quad \dot{p}^\mu = -\frac{\partial K}{\partial x_\mu} = -\frac{\partial V}{\partial x^\mu}. \tag{6}$$

It follows from (6) that

$$\boldsymbol{v} = \frac{d\boldsymbol{x}}{dt} = \frac{\dot{\boldsymbol{x}}}{\dot{t}} = \frac{\boldsymbol{p}}{E},$$

which is the standard formula obtained for velocity in special relativity (we take $c=1$ in the following).

Horwitz and Piron[2] generalized the framework to many-body systems, and gave τ the physical meaning of a *universal historical time*, correlating events in space time.

A general many-body, τ-invariant, classical evolution function may be defined as

$$K = \sum_{n=1}^{N} \frac{1}{2M_n} \eta_{\mu\nu} P_n^\mu P_n^\nu + V(x_1, x_2, \ldots, x_N), \tag{7}$$

where $\eta_{\mu\nu} = \mathrm{diag}(-,+,+,+)$ and n sums over all particles of the system, and, in this case, we have taken the potential function V not to be a function of momenta or τ. The classical equations of motion, for a single particle system in an external potential $V(x)$, are similar to the nonrelativistic Hamilton equations, with, in addition, motion and "momentum" along the t axis:

$$\dot{x}_n^\mu = \frac{\partial K}{\partial p_{n\,\mu}} = \frac{1}{M_n} p_n^\mu, \quad \dot{p}_{n\,\mu} = -\frac{\partial K}{\partial x_n^\mu} = -\frac{\partial V}{\partial x_n^\mu}. \tag{8}$$

In the usual formulation of relativistic dynamics (cf. Ref. 18), the energy momentum is constrained to a *mass shell* defined as

$$p^\mu p_\mu = \mathbf{p}^2 - E^2 = -m^2, \tag{9}$$

where m is a given fixed quantity, a property of the particle. In the Stueckelberg formulation, however, the event mass is generally unconstrained. Since in (5), the value of K is absolutely conserved, $p_\mu p^\mu = -m^2$ is constant only in the special case where

$$\frac{d}{d\tau} V(x) = \left[\dot{x}^\mu \frac{\partial}{\partial x^\mu} + \frac{\partial}{\partial \tau} \right] V(x) = 0.$$

In this case, the particle remains in a specific mass shell, which may or may not coincide with its so-called *Galilean target mass*, usually denoted by M. In the nonrelativistic limit, the mass dis-

tribution converges to a single point; one may choose the parameter M to have this *Galilean target mass value*.[19] We shall assume that M has this value in the following.

In the general case, however, $p^\mu p_\mu \equiv -m^2$ is a dynamical (Lorentz invariant) property, which may depend on τ. The relation between τ and the proper time s, in the model of Eq. (7), is given by

$$ds^2 \equiv -dx^\mu dx_\mu = -\dot{x}^\mu \dot{x}_\mu d\tau^2 = -\frac{1}{M^2} p^\mu p_\mu d\tau^2 = \frac{m^2}{M^2} d\tau^2. \tag{10}$$

Thus, the proper time ds and *universal time* $d\tau$ are related through the ratio between the dynamical Lorentz invariant mass m, and the *Galilean target mass* M. If $V(x)$ goes to zero asymptotically, then it becomes constant. Since this asymptotic value is usually what is measured in experiment, we may assume that it takes on the value of the Galilean target mass. Although there are no detailed models at present, one assumes that there is a stabilizing mechanism (for example, self-interaction or, in terms of statistical mechanics and condensation phenomenon[19]) which brings the particle, at least to a good approximation, to a defined mass value,[19] such that

$$K = \frac{1}{2M} p^\mu p_\mu = \frac{-m^2}{2M} = -\frac{M}{2}.$$

For the quantum case, for which p^μ is represented by $-i\partial/\partial x_\mu$, the Stueckelber Schrödinger equation is taken to be (we take $\hbar = 1$ in the following)

$$i\frac{\partial \Psi_\tau(x)}{\partial \tau} = K\Psi_\tau(x). \tag{11}$$

The Stueckelberg classical and quantum relativistic dynamics have been studied for various systems in some detail, including the classical relativistic Kepler problem[2] and the quantum two-body problem for the central potential.[15]

A. Off-shell electrodynamics

Pre-Maxwell off-shell electrodynamics (OSE) is constructed in a similar fashion to the construction of Maxwell electrodynamics from the Schrödinger equation.[4]

Under the local gauge transformation

$$\Psi'_\tau(x) = e^{-ie_0\chi(x,\tau)}\Psi_\tau(x), \tag{12}$$

five compensation fields $a^\alpha(x,\tau)$ $(\alpha \in \{0,1,2,3,5\})$ are implied, such that with the transformation

$$a'_a(x,\tau) = a_\alpha(x,\tau) - \partial_\alpha \chi(x,\tau),$$

the following modified Stueckelberg-Schrödinger equation remains form invariant:

$$\left[i\frac{\partial}{\partial\tau} + e_0 a_5(x,\tau)\right]\Psi_\tau(x) = \frac{1}{2M}[(p^\mu - e_0 a^\mu)(p_\mu - e_0 a_\mu)]\Psi_\tau(x), \tag{13}$$

under the transformation (12).

We can see this by observing the following relations:

$$[p_\mu - e_0 a'_\mu]\Psi' = \left[-i\frac{\partial}{\partial x^\mu} - e_0\left(a_\mu - \frac{\partial}{\partial x^\mu}\chi\right)\right]e^{-ie_0\chi}\Psi$$
$$= \left[-e_0\frac{\partial}{\partial x^\mu}\chi - i\frac{\partial\Psi}{x^\mu} - e_0\left(a_\mu - \frac{\partial\chi}{\partial x^\mu}\right)\right]e^{-ie_0\chi}\Psi$$
$$= e^{-ie_0\chi}[P_\mu - e_0 a_\mu]\Psi,$$

$$\left[i\frac{\partial}{\partial\tau} + e_0\left(a_5 - \frac{\partial\chi}{\partial\tau}\right)\right]e^{-ie_0\chi}\Psi = \left[e_0\frac{\partial\chi}{\partial\tau} + i\frac{\partial\Psi}{\partial\tau} + e_0\left(a_5 - \frac{\partial\chi}{\partial\tau}\right)\right]e^{-ie_0\chi}\Psi = e^{-ie_0\chi}\left[i\frac{\partial}{\partial\tau} + e_0 a_5\right]\Psi.$$

The result is then of the same form as for the usual $U(1)$ gauge compensation argument for the nonrelativistic Schrödinger equation. Thus, the classical (and quantum) evolution function for a particle, under an external field, assumed to be given by

$$K = \frac{1}{2M}[p - e_0 a(x,\tau)]^2 - e_0 a^5(x,\tau) \tag{14}$$

(where we have used the shorthand notation of $x^2 = x_\mu x^\mu$) and the corresponding Hamilton equations are

$$\dot{x}^\mu(\tau) = \frac{\partial K}{\partial p_\mu} = \frac{1}{M}[p^\mu - e_0 a^\mu], \tag{15}$$

$$\dot{p}^\mu(\tau) = -\frac{\partial K}{\partial x_\mu} = \frac{e_0}{M}(p - e_0 a(x,\tau))_\nu \partial^\mu a^\nu(x,\tau) + e_0\partial^\mu a^5(x,\tau). \tag{16}$$

Here, e_0 is proportional to the Maxwell charge e through a dimensional constant, which is derived below. Second-order equations of motion for $x^\mu(\tau)$, a generalization of the usual Lorentz force, follow from the Hamilton Eqs. (15) and (16) (Ref. 4)

$$M\ddot{x}^\mu = e_0\dot{x}^\nu f^\mu{}_\nu + e_0 f^\mu{}_5, \tag{17}$$

where, for $\alpha,\beta = 0,1,2,3,5$, the antisymmetric tensor

$$f^{\alpha\beta} \equiv \partial^\alpha a^\beta - \partial^\beta a^\alpha \tag{18}$$

is the 5D field tensor. Moreover, the second-order wave equation for the fields $f^{\alpha\beta}$ can be derived from a Lagrangian density as follows[4]:

$$\mathcal{L} = -\frac{\lambda}{4}f_{\alpha\beta}f^{\alpha\beta} - e_0 a_\alpha j^\alpha, \tag{19}$$

which produces the wave equation

$$\lambda\partial_\alpha f^{\alpha\beta} = e_0 j^\beta. \tag{20}$$

λ is a dimensional constant, which will be shown below to have dimensions of length. The sources $j^\beta(x,\tau)$ depend both on space time and on τ, and obey the continuity equation

$$\partial_\alpha j^\alpha = \partial_\mu j^\mu + \partial_\pi \rho = 0, \tag{21}$$

where $j^5 \equiv \rho$ is a Lorentz scalar *space-time density of events*. This equation follows from (13) for

$$\rho_\tau(x) = \Psi^*_\tau(x)\Psi_\tau(x),$$

$$j^{\mu}_{\tau}(x) = -\frac{i}{2M}[\Psi^{*}_{\tau}(x)(i\partial^{\mu} - e_0 a^{\mu}(x,\tau))\Psi_{\tau}(x) + \text{c.c.}],$$

as we discuss below, and also for the classical case from the argument given below.

1. Currents of point events

Maxwell current conservation, for point charges, can be derived (cf. Refs. 20 and 21) by defining the current of a point charge as

$$J^{\mu}(x) = e\int_{-\infty}^{+\infty} ds\, \dot{z}^{\mu}(s)\,\delta^4[x - z(s)]. \tag{22}$$

In that case, s is the proper time, $z^{\mu}(s)$ is the world-line of the point charge (for free motion, s may coincide with τ), and $\dot{z}^{\mu}(s) = (d/ds)z^{\mu}(s)$. Then,

$$\partial_{\mu}J^{\mu} = -e\int_{-\infty}^{+\infty} ds\frac{d}{ds}\delta^4[x - z(s)] = -e\lim_{L\to+\infty}\delta^4[x - z(s)]_{-L}^{+L}, \tag{23}$$

which vanishes if $z^{\mu}(s)$ [or, for example, just the time component $z^0(s)$] becomes infinite for $s \to \pm\infty$, and the observation point x^{μ} is restricted to a bounded region of space time, e.g., the laboratory. Therefore, with Jackson,[20] we identify J^{μ} as the Maxwell current. We see that this current is a functional on the world line, and the usual notion of a "particle" corresponds to this functional on the world line.

If we identify $\delta^4[x-z(s)]$ with a density $\rho_s(x)$ and the local (in τ) current $\dot{z}^{\mu}(s)\,\delta^4[x-z(s)]$ with a local current $j^{\mu}_s(x)$,

$$\rho_s(x) = \delta^4[x - z(s)],\quad j^{\mu}(x,s) = \dot{z}^{\mu}(s)\,\delta^4[x - z(s)], \tag{24}$$

then the relation

$$\frac{d}{ds}\delta^4[x - z(s)] = -\dot{z}^{\mu}(s)\partial_{\mu}\delta^4[x - z(s)]$$

used in the above demonstration in fact corresponds to the conservation law (reverting to the more general parameter τ in place of the proper time s) (21):

$$\partial_{\mu}j^{\mu}(x,\tau) + \partial_{\tau}\rho(x,\tau) = 0. \tag{25}$$

What we call the *pre-Maxwell* current of a point *event* is then defined as

$$j^{\alpha}(x,\tau) = \dot{z}^{\alpha}(\tau)\,\delta^4[x - z(\tau)], \tag{26}$$

where $j^5(x,\tau) \equiv \rho(x,\tau)$ and $\dot{z}^5(\tau) \equiv 1$ [since $z^5(\tau) \equiv \tau$]. Integrating (20) over τ, we recover the standard Maxwell equations for Maxwell fields defined by

$$A^{\mu}(x) = \int a^{\mu}(x,\tau)d\tau. \tag{27}$$

We therefore call the fields $a^{\mu}(x,\tau)$ *pre-Maxwell fields*. Thus, the Maxwell theory is properly contained in the more general pre-Maxwell theory.

For the quantum theory, a real positive definite density function $\rho_{\tau}(x)$ can be derived from the Stueckelberg-Schrödinger Eq. (11)

$$\rho_{\tau}(x) = |\Psi_{\tau}|^2 = \Psi^{*}_{\tau}(x)\Psi_{\tau}(x), \tag{28}$$

which can be identified with the $\rho(x,\tau) = \delta^4[x-z(\tau)]$ in the classical (relativistic) limit. The continuity Eq. (25) is then satisfied for the gauge invariant currents

$$j_\tau^\mu(x) = -\frac{1}{2M}[\Psi_\tau^*(x)(i\partial^\mu - e_0 a^\mu(x,\tau))\Psi_\tau(x) + \text{c.c.}]. \tag{29}$$

Combining (22) with (24), we obtain

$$J^\mu(x) = e\int_{-\infty}^{+\infty} j^\mu(x,\tau)d\tau. \tag{30}$$

This is a restatement of the 5D continuity Eq. (25) and provides a connection between pre-Maxwell OSE and Maxwell electrodynamics. It also follows from (11) that

$$\frac{\partial\rho}{\partial t} + \partial_\mu j^\mu = 0, \tag{31}$$

where $\rho = |\Psi_\tau(x)|^2$, as for the classical case.

2. The wave equation

From Eqs. (20) and (18) one can derive the wave equation for the potentials $a^\alpha(x,\tau)$:

$$\lambda\partial_\beta\partial^\beta a^\alpha - \lambda\partial^\alpha(\partial_\beta a^\beta) = e_0 j^\alpha. \tag{32}$$

Under the generalized Lorentz gauge $\partial_\beta a^\beta = 0$, the wave equation takes the simpler form

$$\lambda\partial_\beta\partial^\beta a^\alpha = \lambda\left[\Box^2 a^\alpha + \sigma_5\frac{\partial^2 a^\alpha}{\partial\tau^2}\right] = e_0 j^\alpha(x,\tau). \tag{33}$$

where a fifth diagonal metric component can take either signs $\sigma_5 = \pm 1$, corresponding to $O(4,1)$ and $O(3,2)$ symmetries of the homogeneous field equations, respectively.

Integrating (33) with respect to τ, and assuming that $\lim_{\tau\to\pm\infty}\partial_\tau a^\alpha(x,\tau) = 0$, we obtain

$$\lambda\int_{-\infty}^{+\infty} d\tau\left[\Box^2 a^\alpha + \sigma_5\frac{\partial^2 a^\alpha}{\partial\tau^2}\right] = \frac{e_0}{e}J^\alpha(x).$$

Identifying

$$A^\mu(x) = \int_{-\infty}^{+\infty} d\tau a^\mu(x,\tau), \tag{34}$$

we obtain

$$\lambda\Box^2 A^\mu(x) = \frac{e_0}{e}J^\mu(x)$$

(where we have restricted our attention to $\mu = 0,1,2,3$), from which a relation between e_0, λ, and the Maxwell charge e can be obtained:

$$e = \frac{e_0}{\lambda}. \tag{35}$$

Therefore, the Maxwell electrodynamics is properly contained in the 5D electromagnetism.

3. A note about units

In natural units ($\hbar = c = 1$), the Maxwell potentials A^μ have units of $1/L$. Therefore, the pre-Maxwell OSE potentials a^α have units of $1/L^2$, and in order to maintain the action integral

$$S = \int_{-\infty}^{+\infty} \mathcal{L}\, d\tau\, d^4x \tag{36}$$

dimensionless, the coefficient λ in (19) must have units of L, forcing e_0 to have units of L as well.

The Fourier transform of the pre-Maxwell OSE fields

$$\tilde{a}^\mu(x,s) = \int_{-\infty}^{+\infty} e^{is\tau} a^\mu(x,\tau) d\tau \tag{37}$$

and Eq. (34) suggest that the Maxwell potentials and fields are the *zero mode* of the pre-Maxwell OSE fields, with respect to the τ axis, i.e.,

$$A^\mu(x) = \tilde{a}^\mu\,(x,s)\big|_{s=0}. \tag{38}$$

B. Solutions of the wave equation

The classical 5D wave Eq. (33) can be solved by the method of Green functions. Such GF's have been found[10,22] through a fivefold Fourier transform of the wave equation. The GF obeys the wave equation of a point source

$$\partial_\beta \partial^\beta g(x,\tau) = \delta^4(x)\,\delta(\tau). \tag{39}$$

After transformation to momentum space, (39) becomes ($k^2 = k_\mu k^\mu$)

$$(k^2 + \sigma_5 k_5^2)\tilde{g}(k,k_5) = 1, \tag{40}$$

i.e., in terms of the inverse transform

$$g(x,\tau) = \frac{1}{(2\pi)^5} \int d^4k\, dk_5 \frac{1}{k^2 + \sigma_5 k_5^2} e^{i[k\cdot x + \sigma_5 k_5 \tau]}. \tag{41}$$

Although (41) is not a well-defined integral, there are, as for GF's in 4D, several ways of defining the integral, which result in GF's, all of which satisfy (39). These different forms of solutions have physical consequences and it is part of the motivation of our work to obtain criteria that could determine this choice.

For example, Land and Horwitz[22] found what they called the *Principal-Part* GF to be

$$g_P(x,\tau) = -\frac{1}{4\pi}\delta(x^2)\,\delta(\tau) - \frac{1}{2\pi^2}\frac{\partial}{\partial x^2}\frac{\theta(-\sigma x^2 - \tau^2)}{\sqrt{-\sigma x^2 - \tau^2}}, \tag{42}$$

where $\sigma = \sigma_5 = \pm 1$ is the signature of the fifth dimension, τ.

A later work by Oron and Horwitz[10] found another, τ-retarded GF of the form

$$g(x,\tau) = \frac{2\theta(\tau)}{(2\pi)^3} \begin{cases} \dfrac{1}{(-x^2-\tau^2)^{3/2}} \tan^{-1}\left(\dfrac{1}{\tau}\sqrt{-x^2-\tau^2}\right) - \dfrac{\tau}{x^2(x^2+\tau^2)} & x^2+\tau^2 < 0, \\ \dfrac{1}{2}\dfrac{1}{(x^2+\tau^2)^{3/2}} \ln\left|\dfrac{\tau - \sqrt{\tau^2+x^2}}{\tau+\sqrt{\tau^2+x^2}}\right| - \dfrac{\tau}{x^2(x^2+\tau^2)} & x^2+\tau^2 > 0, \end{cases} \tag{43}$$

where only the $(4,1)$ case was explicitly given.

GF's of $(n,1)$ wave equations are well known in the mathematical literature (this is taken from Ref. 12; cf. also Refs. 5, 6, and 13):

$$g(x,t)=\begin{cases}\dfrac{\theta(t)}{2\pi}\left(\dfrac{1}{\pi}\dfrac{d}{dt^2}\right)^{(n-3)/2}\delta(t^2-\mathbf{x}^2), & n=3,5,7,\ldots,\\ \dfrac{1}{2\pi}\left(\dfrac{1}{\pi}\dfrac{d}{dt^2}\right)^{(n-2)/2}\dfrac{\theta(t-|\mathbf{x}|)}{\sqrt{t^2-\mathbf{x}^2}}, & n=4,6,8,\ldots,\end{cases}\tag{44}$$

where $n=4$ is the case of $(4,1)$ metric. These well-known GF's, which are *retarded* in t, can be made *symmetric* by the proper choice of the contour of integration on the original Fourier integral representation.

Once the GF's have been found, the general field generated by a given source can then be found by integration on its support

$$a^{\alpha}(x,\tau)=e_0\int d^4x'\,d\tau'\;g(x-x',\tau-\tau')j^{\alpha}(x',\tau'),\tag{45}$$

and applying it on a point particle given by (24). The potentials of point events can then be found from

$$a^{\alpha}(x,\tau)=e_0\int_{-\infty}^{+\infty}d\tau'\;g(x-z(\tau'),\tau-\tau')\dot{z}^{\alpha}(\tau').\tag{46}$$

In order to get some insight into the criteria for choosing appropriate GF's, we study solutions of the differential Eq. (33) (for the particular choice of uniformly moving point source) without using the GF, i.e., we compute directly

$$a^{\alpha}(x,\tau)=\frac{e}{(2\pi)^5}\int_{-\infty}^{+\infty}d\tau'\;\dot{z}^{\alpha}(\tau')\int d^4k\,dk_5\frac{e^{i[k\cdot(x-z(\tau'))+\sigma_5k_5(\tau-\tau')]}}{k^2+\sigma_5k_5^2}.\tag{47}$$

Solutions of the integral (47) are the subject of the next section.

III. FIELDS OF A UNIFORMLY MOVING POINT CHARGE

A. Solutions of the wave equation

Let us seek a solution to the field equation generated by a uniformly moving point source. Such a source has a general world-line description

$$z^{\alpha}(\tau)=z_0^{\alpha}+b^{\alpha}(\tau-\tau_0)\equiv D^{\alpha}+b^{\alpha}\tau,\quad \dot{z}^{\alpha}(\tau)=b^{\alpha},\quad \alpha\in\{0,1,2,3,5\},\tag{48}$$

where for $z^5\equiv\tau$ we have $b^5=1$. However, we leave b^5 unspecified, leaving the possibility for a 5D symmetry of the solution to emerge, as indeed we find. Without loss of generality, we can eliminate D^{α} by choosing a coordinate system in which $D^{\alpha}=0$. The current of such a source is then given by

$$j^{\alpha}(x,\tau)=b^{\alpha}\delta^4[x-b\tau].\tag{49}$$

Substituting (48) into (47) we obtain an integral representation of the uniform motion fields, which could be called *pre-Coulomb fields*:

$$\begin{aligned}a^{\alpha}(x,\tau)&=\frac{e}{(2\pi)^5}\int_{-\infty}^{+\infty}d\tau'\;b^{\alpha}\int d^4k\,dk_5\frac{e^{i[k\cdot(x-b\tau')+\sigma_5k_5(\tau-b^5\tau')]}}{k^2+\sigma_5k_5^2}=\frac{eb^{\alpha}}{(2\pi)^5}\int_{-\infty}^{+\infty}d\tau'\int d^5k\frac{e^{ik_{\beta}[x^{\beta}-b^{\alpha}\tau']}}{k_{\beta}k^{\beta}}\\&=\frac{eb^{\alpha}}{(2\pi)^5}\int d^5k\int_{-\infty}^{+\infty}d\tau'\frac{e^{ik_{\beta}[x^{\beta}-b^{\alpha}\tau']}}{k_{\beta}k^{\beta}}=\frac{eb^{\alpha}}{(2\pi)^5}\int d^5k\frac{e^{ik_{\beta}x^{\beta}}}{k_{\beta}k^{\beta}}\int_{-\infty}^{+\infty}d\tau'\;e^{-ik_{\beta}b^{\alpha}\tau'}\\&=\frac{eb^{\alpha}}{(2\pi)^4}\int d^5k\frac{e^{ik_{\beta}x^{\beta}}}{k_{\beta}k^{\beta}}\delta(k_{\beta}b^{\beta}).\end{aligned}\tag{50}$$

The argument $k_\beta b^\beta$ of the δ function causes the fivefold integration to be constrained to a 5D hyperplane,

$$S[b]=\{k\in\mathbb{R}^5|k_\alpha b^\alpha=0\},$$

whose normal is just b^β.

In order to proceed, we select a pivot axis for which integration would put the remaining fourfold integral to be in that hyperplane. Naturally, we select k^5, since we will take $b^5>0$:

$$k_\beta b^\beta=k\cdot b+\sigma_5 k^5 b^5=b^5[k\cdot b'+\sigma_5 k^5],$$

where $\mu\in\{0,1,2,3\}$ and

$$b'^\mu=\frac{b^\mu}{b^5},$$

b'^μ is the (3,1) *velocity* of the source relative to its motion in the τ direction.

We then have

$$\delta(k_\beta b^\beta)=\frac{1}{|b^5|}\delta(k\cdot b'+\sigma_5 k^5)\Rightarrow k^5=-\frac{1}{\sigma_5}k\cdot b',$$

$$k_\beta k^\beta=k^2+\sigma_5(k^5)^2=k^2+\sigma_5\left[\frac{-1}{\sigma_5}(k\cdot b')\right]^2=k^2+\sigma_5(k\cdot b')^2,$$

$$k_\beta x^\beta=k\cdot x+\sigma_5 k^5\tau=k\cdot x+\sigma_5\frac{-1}{\sigma_5}[k\cdot b']\tau=k\cdot(x-b'\tau). \tag{51}$$

And thus we obtain

$$a^\alpha(x,\tau)=\frac{eb^\alpha}{2\pi^4|b^5|}\int d^4k\frac{e^{ik\cdot(x-b'\tau)}}{k^2+\sigma_5(k\cdot b')^2}. \tag{52}$$

The integral (52) can be solved by introducing a rotation in k space in which b' takes a particularly simple form, namely, along one of the axes. Aside from the special case of $b'^2=0$, b' can be rotated to be along one of the axes by an $SO(3,1)$ transformation. We shall now divide our discussion to the *spacelike* case where $b'^2>0$ and the *timelike* case where $b'^2<0$, and to avoid complications, we shall solve the zero measure case of $b'^2=0$ by a limiting procedure.

B. *a*-fields due to a (3,1) timelike source

Since $b'^2<0$, we can find $\Lambda\in SO(3,1)$ such that

$$b'=\Lambda b''\ \text{ such that }\ b''=[b''^0;\mathbf{0}],$$

$$b''^0\equiv s=\varepsilon(b'^0)\sqrt{-b'^2},$$

and since $|\Lambda|=1$, we have $d^4k''=d^4k$. Replacing b' with b'' and k with k'', we obtain

$$a^\alpha(x,\tau)=\frac{eb^\alpha}{2\pi^4|b^5|}\int d^4k''\frac{e^{i[\mathbf{k}''\cdot\mathbf{x}''-k''^0(x''^0-s\tau)]}}{k''^2+\sigma_5(-k''^0 s)^2}=\frac{eb^\alpha}{2\pi^4|b^5|}\int d^4k''\frac{e^{i[\mathbf{k}''\cdot\mathbf{x}''-k''^0(x''^0-s\tau)]}}{\mathbf{k}''^2+(k''^0)^2(\sigma_5 s^2-1)}, \tag{53}$$

where $x''=\Lambda^{-1}x$. We follow the convention of boldface corresponding to the space part of a four-vector. Since $b''\tau$ is a four-vector along the time axis, we can find simple closed form expressions for x'' as follows:

TABLE I. Types of source motion.

Source motion	Description
$\sigma_5 b_2' > 1$	*Supershell* case, where the integral (53) has a well-defined solution, essentially the Laplace GF in 4D.
$\sigma_5 b_2' < 1$	*Undershell* case, where the integral is not well defined. The integral is essentially the Maxwell GF.

$$x''^0 = \frac{x''^0 s}{s} = \frac{-x''\cdot b''}{\sqrt{-b'^2}} = \frac{-x\cdot b'}{\sqrt{-b'^2}},$$

$$(\boldsymbol{x}''^0)^2 = x''^2 + (x''^0)^2 = x^2 + \frac{(b'\cdot x)^2}{-b'^2} = x^2 - \frac{(b'\cdot x)^2}{b'^2}.$$

The integral (53) depends on the value of the denominator along the path of integration, where two types of source motion emerge. The types are given as follows in Table I.

In the following we describe the properties of these cases.

1. Undershell timelike *a-fields* $\sigma_5 b'^2 > -1$

As mentioned, the denominator of the integral is not positive definite. Nevertheless, we shall proceed first by absorbing the coefficient $1-\sigma_5 s^2$ into k^0:

$$k^0 \to \frac{k^0}{\sqrt{1-\sigma_5 s^2}}.$$

Equation (53) becomes

$$a^\alpha(x,\tau) = \frac{eb^\alpha}{2\pi^4|b^5|\sqrt{1-\sigma_5 s^2}}\int d^4k \frac{\exp^{i\left[\boldsymbol{k}\cdot\boldsymbol{x}'' - k^0\frac{(x''^0 - s\tau)}{\sqrt{1-\sigma_5 s^2}}\right]}}{\boldsymbol{k}^2-(k^0)^2} = \frac{eb^\alpha}{|b^5|\sqrt{1-\sigma_5 s^2}}\left\{\frac{1}{(2\pi^4)}\int d^4k\frac{e^{ik\cdot y}}{k^2}\right\},$$

where

$$y^\mu \equiv \left[\frac{x''^0 - s\tau}{\sqrt{1-\sigma_5 s^2}}; \boldsymbol{x}''\right].$$

The last integral inside the braces is the well-known Fourier integral form for Maxwell wave equations's GF in four dimensions, and, although it is ill defined, it has many well-known solutions, corresponding to different limits of the integration contour chosen. We shall choose the *Principal Part* solution for our present study:

$$G_P(x) = \frac{1}{(2\pi)^4} P\int_{\mathbb{R}^4} d^4k \frac{e^{ik\cdot x}}{k^2} = \frac{\delta(x^2)}{4\pi}, \tag{54}$$

corresponding to the sum of retarded and advanced GF's. Using the G_P above, we arrive at the undershell a-fields:

$$\begin{aligned} a^\alpha(x,\tau) &= \frac{eb^\alpha}{4\pi|b^5|\sqrt{1-\sigma_5 s^2}}\delta\left[\boldsymbol{x}''^2 - \frac{(x''^0 - s\tau)^2}{1-\sigma_5 s^2}\right] \\ &= \frac{eb^\alpha}{4\pi|b^5|\sqrt{1+\sigma_5 b'^2}}\delta\left[x^2 - \frac{(b'\cdot x)^2}{b'^2} + \frac{(-b'\cdot x + b'^2\tau)^2}{b'^2(1+\sigma_5 b'^2)}\right]. \end{aligned} \tag{55}$$

We call these *undershell solutions* because they correspond to the off-shell mass of the source below its Galilean target mass. Equation (55) has $O(3,1)$ symmetry, with respect to the first four

coordinates of x^α. It can be further broken to a sum of δ functions with linear arguments in τ as follows:

$$p(\tau_{1,2}) \equiv x^2 - \frac{(b'\cdot x)^2}{b'^2} + \frac{(-b'\cdot x + b'^2\tau_{1,2})^2}{b'^2(1+\sigma_5 b'^2)} = 0,$$

$$\tau_{1,2} = \frac{b'\cdot x}{b'^2} \pm \frac{1}{b'^2}\sqrt{1+\sigma_5 b'^2}\sqrt{(b'\cdot x)^2 - b'^2 x^2}.$$

Using the linearity of the δ function,

$$\delta(p(\tau)) = \left|\frac{b'^2(1+\sigma_5 b'^2)}{(b'^2)^2}\right| \delta[(\tau-\tau_1)(\tau-\tau_2)] = \frac{(1+\sigma_5 b'^2)}{b'^2|\tau_1-\tau_2|}[\delta(\tau-\tau_1)+\delta(\tau-\tau_2)],$$

we then have

$$a^\alpha(x,\tau) = \frac{eb^\alpha \Delta_+}{8\pi|b^5|\sqrt{(b'\cdot x)^2 - b'^2x^2}},$$

where

$$\Delta_+(x,\tau) = \delta(\tau-\tau_1)+\delta(\tau-\tau_2).$$

The a-field depends on the fifth metric component, σ_5, only through $\tau_{1,2}$, i.e., the coefficient is independent of the signature of the 5D space. However, the values $\tau=\tau_{1,2}$ correspond to a 4D surface in 5D space where the a-fields are nonzero, and therefore the metric appears, to some extent, in the *geometry* of the nonzero surfaces.

After some algebra, the a-fields can gain yet another, 5D covariant form. We start by rewriting the δ-function argument in 5D form:

$$p(\tau) = x^2 - \frac{(b'\cdot x)^2}{b'^2} + \frac{(-b'\cdot x + b'^2\tau_{1,2})^2}{b'^2(1+\sigma_5 b'^2)} = x_\beta x^\beta - \frac{b_\beta x^\beta}{b_\beta b^\beta}, \tag{56}$$

where the metric signature of (4,1) or (3,2) is used in the contraction products, e.g.,

$$b_\beta x^\beta = b\cdot x + \sigma_5 b^5 x^5 = b\cdot x + \sigma_5 b^5 \tau.$$

For the (4,1) case, we have

$$b_\alpha b^\alpha = b^2 + (b^5)^2 = \frac{1}{(b^5)^2}[b'^2+1] > 0,$$

since $\sigma_5 b^2 > -1$ in the present case. Thus, in the (4,1) metric, the *undershell* motion corresponds to the 5D *spacelike* region in the b^α velocity space. As shall be observed later, this region is not limited to 4D timelike source motion $b'^2<0$, and it includes $b'^2\geq 0$ as well. For the (3,2) metric, on the other hand, the motion is in the 5D timelike region $b_\alpha b^\alpha < 0$.

Furthermore, one can define

$$n^\alpha = \frac{b^\alpha}{\sqrt{\sigma_5 b_\beta b^\beta}}. \tag{57}$$

Substituting Eqs. (56) and (57) into (55), we arrive at the 5D covariant form:

$$a^\alpha(x,\tau) = \frac{en^\alpha}{4\pi}\delta[x_\beta x^\beta - \sigma_5(n_\beta x^\beta)^2]. \tag{58}$$

The term *undershell source motion* stems from the mass shell equation

$$P_\alpha P^\alpha = M^2 \dot{x}_\alpha \dot{x}^\alpha = M^2\left[-\frac{m^2}{M^2}+\sigma_5\right] = \sigma_5 M^2\left[-\sigma_5\frac{m^2}{M^2}+1\right] \tag{59}$$

$$= M^2 b_\alpha b^\alpha \tag{60}$$

or

$$b_\alpha b^\alpha = \sigma_5\left[-\sigma_5\frac{m^2}{M^2}+1\right]. \tag{61}$$

For the (4,1) metric, $\sigma_5=1$, where the undershell timelike motion leads to $|m|<M$. Hence, undershell motion refers to the *mass shell of the source* being *less* than its nonrelativistic mass-shell M.

2. Supershell timelike *a-fields* $\sigma_5 b'^2<-1$

As the name suggests, in the (4,1) metric of the source motion, the *supershell* case is determined by $|m|>M$, i.e., the relativistic mass $|m|$ being greater than the its nonrelativistic Galilean target mass M. In this case, however, only $\sigma_5=1$ is applicable, since there is no timelike motion $b'^2<0$ such that $(-1)b'^2+1<0$, unless $b'^2>1$, which is no longer timelike. Such a case will be investigated later. In this case, the integral (53) is well defined, as the zeros in the denominator are no longer real. By following a similar procedure of absorbing the coefficient of k^0 in the denominator into k^0, we obtain ($\sigma_5=1$)

$$\begin{aligned}
a^\alpha(x,\tau) &= \frac{eb^\alpha}{2\pi^4|b^5|\sqrt{s^2-1}}\int d^4k \frac{e^{i[\mathbf{k}\cdot\mathbf{x}''-k^0(x''^0-s\tau)/\sqrt{s^2-1}]}}{\mathbf{k}^2+(k^0)^2}\\
&= \frac{4\pi eb^\alpha}{(2\pi)^4|b^5||\mathbf{x}'|\sqrt{s^2-1}}\int_0^{+\infty} k\,dk\,\sin(k|\mathbf{x}''|)\int_{-\infty}^{+\infty} dk^0 \frac{e^{-ik^0[x''^0-s\tau]/\sqrt{s^2-1}}}{k^2+(k^0)^2}\\
&= \frac{eb^\alpha}{4\pi^3|b^5||\mathbf{x}'|\sqrt{s^2-1}}\int_0^{+\infty} kdk\,\sin(k|\mathbf{x}''|)(-1)\frac{\pi}{k}e^{-k[x''^0-s\tau]/\sqrt{s^2-1}}\\
&= \frac{eb^\alpha}{4\pi^2|b^5||\mathbf{x}''|\sqrt{s^2-1}}\frac{1}{2i}\left[\frac{0-1}{-|x''^0-s\tau|/\sqrt{s^2-1}+i|\mathbf{x}''|}-\frac{0-1}{-|x''^0-s\tau|/\sqrt{s^2-1}-i|\mathbf{x}''|}\right]\\
&= \frac{eb^\alpha}{4\pi^2|b^5|\sqrt{-b'^2-1}}\left[\mathbf{x}''^2+\frac{(x''^0-s\tau)^2}{-b'^2-1}\right]\\
&= \frac{eb^\alpha}{4\pi^2|b^5|\sqrt{-b'^2-1}}\left[x^2-\frac{(b'\cdot x)^2}{b'^2}+\frac{(-b'\cdot x+b'^2\tau)^2}{b'^2(b'^2+1)}\right]\\
&= \frac{en^\alpha}{4\pi^2}\frac{1}{[x_\beta x^\beta+(n_\beta x^\beta)^2]},
\end{aligned}$$

where we have defined $n^\alpha \equiv b^\alpha/\sqrt{-b_\beta b^\beta}$.

The supershell *a*-field is found to be a *smooth* function on 5D space time; it is the 5D analog of the well-known (cf. Ref. 20) on-shell 4D Maxwell *a*-field of a uniformly moving charge

$$A^{\mu}(x) = \frac{en^{\mu}}{4\pi\sqrt{x^2 + (n\cdot x)^2}},$$

where $n^{\mu}=dz^{\mu}(s)/ds$ is the constant four-velocity obeying the mass-shell constraint $n^2=-1$. Clearly, the 5D a-field, proportional to r^{-2}, as opposed to the Maxwell A-field being proportional to r^{-1}, is a consequence of the additional dimension.

The supershell a-field has the same form as the GF for the 4D *Laplace operator*

$$\nabla^2 G_L(x) = \delta^4(x), \tag{62}$$

where $x\in\mathbb{R}^4$, $r^2=(x^1)^2+(x^2)^2+(x^3)^2+(x^4)^2$, and the GF $G_L(x)$ is given by (cf. Ref. 12)

$$G_L = \frac{1}{(2\pi)^4}\int \frac{e^{ik_c x^c}}{k_c k^c} = \frac{1}{2\pi^2 r^2}, \tag{63}$$

where in this case

$$k_c x^c = k^1x^1 + k^2x^2 + k^3x^3 + k^4x^4.$$

This is far from being coincidental, as the 5D scalar $x_{\beta}x^{\beta}+(n_{\beta}x^{\beta})^2$ reduces to r^2 in 4D, when the source's uniform velocity is purely *temporal* $n^{\beta}=[1;0,0,0,0]$.

C. *a*-fields due to a spacelike source

We now solve the integral (52) for spacelike source motion, $b'^2>0$, which may not be regarded as a possible physical source, since it implies faster than light motion of the source particle. Once again, we choose to integrate in a k-frame such that $b''=[0;0,0,b''^3]$ is along one of the spatial axes, e.g., the z axis, and we now define

$$b''^3 \equiv s = \sqrt{b''^2} = \sqrt{b'^2}, \quad b'^2>0. \tag{64}$$

The current in the b'' frame can be expressed by

$$j''^{\mu}(x'',\tau) = b''^{\mu}\delta^4[x - z''(\tau)] = b'^3\delta^{\mu}_3\delta(t'')\delta(x'')\delta(y'')\delta(z'' - b''^3\tau). \tag{65}$$

Returning to pre-Maxwell a-field integral (52),

$$a^{\alpha}(x,\tau) = \frac{eb^{\alpha}}{|b^5|(2\pi)^4}\int d^4k'' \frac{e^{i[k''^1x''+k''^2y''+k''^3(z''-s\tau)-k''^0t'']}}{(k''^1)^2+(k''^2)^2+(k''^3)^2-(k''^0)^2+\sigma_5(sk^3)^2} \tag{66}$$

$$= \frac{eb'^{\alpha}}{|b^5|(2\pi)^4}\int d^4k \frac{e^{i[k^1x+k^2y+k^3(z-s\tau)-k^0t]}}{(k^1)^2+(k^2)^2+(k^3)^2(1+\sigma_5 s^2)-(k^0)^2}, \tag{67}$$

where we have renamed k'' as k and x'' as x.

The coefficient of $(k^3)^2$ changes sign when $1+\sigma_5 s^2=1+\sigma b'^2=0$, which can only occur when $\sigma_5=-1$ (since for spacelike motion, $b'^2>0$) and $|s|\geq 1$ $[s=\varepsilon(b'^0)\sqrt{b'^2}]$, causing the denominator to obtain a (2,2) quadratic form.

Once again, the form of the fields are characterized by the types of source motion. In the following, we shall treat both possible types of source motion separately.

1. Under spacelike motion $1+\sigma_5 b'^2>0$

Rescaling $k^3\rightarrow k^3/\sqrt{1+\sigma_5 s^2}$, the spacelike a-field integral (66) can be expressed by

$$a^{\alpha}(x,\tau) = \frac{eb^{\alpha}}{|b^5|(2\pi)^4\sqrt{1+\sigma_5 s^2}}\int d^4k \frac{e^{ik\cdot y}}{k^2} = \frac{eb^{\alpha}\delta(y^2)}{4\pi|b^5|\sqrt{1+\sigma_5 s^2}},$$

where $y^\mu=\left[x^0;x^1,x^2,x^3-s\tau/\sqrt{1+\sigma_5 s^2}\right]$, $k^2=k_\mu k^\mu$, and we have chosen the *Principal Part* contour.

However:

$$y^2=(x^1)^2+(x^2)^2+\frac{(x^3-s\tau)^2}{1+\sigma_5 s^2}-(x^0)^2=x_\mu x^\mu-(x^3)^2+\frac{(x^3-\sqrt{b'^2}\tau)^2}{1+\sigma_5 b'^2}.$$

We can furthermore put x^3 into an invariant form:

$$x^3=\frac{x^3 s}{s}=\frac{x\cdot b'}{\sqrt{b'^2}},$$

$$y^2=x^2-\frac{(b'\cdot x)^2}{b'^2}+\frac{(-b'\cdot x+b'^2\tau)^2}{b'^2(1+\sigma_5 b'^2)}.$$

The spacelike a-fields then obtain a 4D covariant form:

$$a^\alpha(x,\tau)=\frac{eb^\alpha}{4\pi|b^5|\sqrt{1+\sigma_5 b'^2}}\delta\left[x^2-\frac{(b'\cdot x)^2}{b'^2}+\frac{(-b'\cdot x+b'^2\tau)^2}{b'^2(1+\sigma_5 b'^2)}\right]=\frac{eb^\alpha\Delta_+}{8\pi|b^5|\sqrt{(b'\cdot x)^2-b'^2x^2}},$$

where we have, as before,

$$\Delta_+\equiv\delta(\tau-\tau_1)+\delta(\tau-\tau_2),$$

$$\tau_{1,2}=\frac{b'\cdot x}{b'^2}\pm\frac{1}{b'^2}\sqrt{1+\sigma_5 b'^2}\sqrt{(b'\cdot x)^2+b'^2x^2}.$$

Thus, the *under* spacelike motion fields are of the same form as their timelike *under-shell* counterparts.

2. Super spacelike motion $1+\sigma_5 b'^2>0$

As mentioned above, in this case we have $b'^2>1$ and the choice $\sigma_5=-1$ is therefore necessary. Therefore, the integral (66) takes the form

$$a^\alpha(x,\tau)=\frac{eb^\alpha}{|b^5|(2\pi)^4}\int d^4k\frac{e^{i[k^1x+k^2y+k^3(z-s\tau)-k^0t]}}{(k^1)^2+(k^2)^2-(s^2-1)(k^3)^2-(k^0)^2}.$$

Rescaling $k^3\to k^3/\sqrt{s^2-1}$,

$$=\frac{eb^\alpha}{(2\pi)^4|b^5|\sqrt{s^2-1}}\int d^4k\frac{e^{ik\cdot y}}{(k^1)^2+(k^2)^2-(k^3)^2-(k^0)^2}. \tag{68}$$

We shall solve this integral by transforming the integrand to a Gaussian form:

$$\int_{-\infty}^{+\infty}\frac{e^{iax}}{x^2}dx=\frac{1}{2i}\int_{-\infty}^{+\infty}\varepsilon(q)dq\int_{-\infty}^{+\infty}e^{iax+iqx^2}dx,$$

where $\varepsilon(q)$ is the sign function. Using this relation in (68) we obtain

$$a^{\alpha}(x,\tau)=\frac{eb^{\alpha}}{(2\pi)^4|b^5|\sqrt{s^2-1}}\frac{1}{2i}\int_{-\infty}^{+\infty}dq\varepsilon(q)\int d^4k\,\exp[ik\cdot y+iq[(k^1)^2+(k^2)^2-(k^3)^2-(k^0)^2]]$$

$$=\frac{eb^{\alpha}}{(2\pi)^4|b^5|\sqrt{s^2-1}}\frac{1}{2i}\int_{-\infty}^{+\infty}dq\varepsilon(q)\left(\sqrt{\frac{\pi}{q}}\right)^4\exp\left[\frac{i}{4q}((y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2)\right]$$

$$=\frac{eb^{\alpha}|b^5|}{(2\pi)^4\sqrt{s^2-1}}\frac{\pi^2}{2i}(-1)\int_0^{+\infty}du\left\{\exp\left[\frac{iu}{4}((y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2)\right]\right.$$

$$\left.-\exp\left[-\frac{iu}{4}((y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2)\right]\right\},$$

where we have put $u=1/q$. Here, the singularity at $q=0$ is controlled by the oscillation in the exponent (although one can find the same result by other methods).

Using

$$\int_0^{+\infty}\exp[iax]dx=P\left[\frac{i}{a}\right]+\pi\delta(a),$$

we find the fields to be

$$a^{\alpha}(x,\tau)=-\frac{eb^{\alpha}}{(2\pi)^4|b^5|\sqrt{s^2-1}}\frac{1}{2}\frac{8\pi^2}{[(y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2]}$$

$$=-\frac{eb^{\alpha}}{4\pi^2|b^5|\sqrt{s^2-1}}\frac{1}{[(y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2]}.$$

We have

$$y^{\mu}=\left[x^0;x^1,x^2,\frac{x^3-s\tau}{\sqrt{s^2-1}}\right],$$

$$(y^1)^2+(y^2)^2-(y^3)^2-(y^0)^2=(x^1)^2+(x^2)^2-\frac{(x^3-s\tau)^2}{s^2-1}-(x^0)^2=x^2-\frac{(b'\cdot x)^2}{b'^2}-\frac{(b\cdot x-b^2\tau)^2}{(b'^2-1)b'^2}.$$

Thus we obtain the final form

$$a^{\alpha}(x,\tau)=-\frac{eb^{\alpha}}{4\pi^2|b^5|\sqrt{b'^2-1}}\frac{1}{\left[x^2-\frac{(b\cdot x)^2}{b^2}-\frac{(b\cdot x-b^2\tau)^2}{b^2(b^2-1)}\right]},\tag{69}$$

The corresponding 5D covariant form is then

$$a^{\alpha}(x,\tau)=\frac{en^{\alpha}}{4\pi^2}\frac{1}{[(n_{\alpha}x^{\alpha})^2-x_{\alpha}x^{\alpha}]},\tag{70}$$

where $n^{\alpha}=b^{\alpha}/\sqrt{b_{\beta}b^{\beta}}$

TABLE II. Regions of source velocity summary.

Metric	σ_5	Velocity region	Mass shell	$\varepsilon(b_\alpha b^\alpha)$	ζ
(4,1)	+1	Undershell	$m^2<M^2$	+1	+1
(4,1)	+1	Supershell	$m^2>M^2$	−1	−1
(3,2)	−1	Under-spacelike	$-m^2<M^2$	−1	+1
(3,2)	−1	Super-spacelike	$-m^2>M^2$	+1	−1

D. Summary of fields generated by a uniformly moving source

We present a short summary of the results obtained in this section:

$$a^\alpha(x,\tau)=\begin{cases} en^\alpha 4\pi\delta[x_\beta x^\beta-(n_\beta x^\beta)^2] & \text{Undershell } \sigma_5=+1,\ n_\alpha n^\alpha=+1,\\ \dfrac{en^\alpha}{4\pi^2}\dfrac{1}{[x_\beta x^\beta+(n_\beta x^\beta)^2]} & \text{Supershell } \sigma_5=+1,\ n_\alpha n^\alpha=-1,\\ \dfrac{en^\alpha}{4\pi}\delta[x_\beta x^\beta+(n_\beta x^\beta)^2] & \text{Under-spacelike } \sigma_5=-1,\ n_\alpha n^\alpha=-1,\\ \dfrac{en^\alpha}{4\pi^2}\dfrac{1}{[(n_\beta x^\beta)^2-x_\beta x^\beta]} & \text{Super-spacelike } \sigma_5=-1,\ n_\alpha n^\alpha=+1. \end{cases} \tag{71}$$

In a more general compact representation, we have

$$a^\alpha(x,\tau)=\begin{cases} \dfrac{en^\alpha}{4\pi}\delta[(n_\beta x^\beta)^2-\sigma_5 x_\beta x^\beta] & \zeta=+1,\\ \dfrac{en^\alpha}{4\pi^2}\dfrac{1}{[(n_\beta x^\beta)^2+\sigma_5 x_\beta x^\beta]} & \zeta=-1, \end{cases} \tag{72}$$

where

$$\zeta=\sigma_5\cdot\varepsilon[b_\alpha b^\alpha]=\sigma_5\cdot\varepsilon[b^2+\sigma_5(b^5)^2],$$

$$n^\alpha=\frac{b^\alpha}{|b_\beta b^\beta|}.$$

The various values for σ_5 and ζ are given in Table II.

E. Concatenation

As we have pointed out above, the pre-Maxwell theory can be contracted to Maxwell form by integration [as in (34)] over τ (called *concatenation*). Applying this procedure to the 5D pre-Maxwell fields that we have obtained above, we find

$$A^\mu(x)=\int_{-\infty}^{+\infty}a^\mu(x,\tau)d\tau=\frac{en^\mu}{4\pi}\frac{\theta[(n\cdot x)^2-n^2x^2]}{\sqrt{(n\cdot x)^2-n^2x^2}}, \tag{73}$$

where

$$n^2=n_\mu n^\mu=n_\alpha n^\alpha-\sigma_5(n^5)^2$$

and $n_\alpha n^\alpha=\pm1$ according to the velocity regions of source motion (see Table II). It should be emphasized that (73) is a *general* Maxwell field for all values of n^2. The solutions can be put into a more specific form for the three regions of (3,1) space time:

$$A^{\mu}(x)=\begin{cases}\dfrac{en'^{\mu}}{4\pi\sqrt{(n'\cdot x)^2+x^2}} & n'^2=-1,\\ \dfrac{en'^{\mu}}{4\pi}\dfrac{\theta[(n'\cdot x)^2-x^2]}{\sqrt{(n'\cdot x)^2-x^2}} & n'^2=+1,\\ \dfrac{en'^{\mu}}{4\pi|n'\cdot x|} & n'^2=0,\end{cases} \tag{74}$$

where

$$n'^{\mu}=\frac{n^{\mu}}{|n_{\nu}n^{\nu}|}.$$

We will discuss the possibility of integrating on a smaller interval of τ (Land regularization[3]) adequate in some cases to reproduce the results of ordinary Maxwell scattering.

IV. GREEN FUNCTIONS

In this section, Green functions for both (4,1) and (3,2) wave equations are given. Green functions for equations of this type have been discussed.[12,13,23] In particular, two distinct versions of the fundamental solution for (4,1) wave equation have been given:

$$G_{4,1}(\mathbf{x},t)=-\frac{1}{4\pi^2}\frac{\theta(t-|\mathbf{x}|)}{[t^2-\mathbf{x}^2]^{3/2}} \tag{75}$$

[cf. Ref. 23, based on Ref. 24],

$$H_{4,1}(\mathbf{x},t)=\frac{1}{2\pi^2}\frac{d}{dt^2}\frac{\theta(t-|\mathbf{x}|)}{\sqrt{t^2-\mathbf{x}^2}} \tag{76}$$

(cf. Ref. 12).

The difference expression $(H_{4,1}-G_{4,1})(\mathbf{x},t)$ is a distribution

$$(H_{4,1}-G_{4,1})(\mathbf{x},t)=\frac{\delta(t-|\mathbf{x}|)}{2t\sqrt{t^2-\mathbf{x}^2}}.$$

In the analysis below, on the other hand, we shall provide a distinct derivation of the GF's for both (4,1) and (3,2), which are similar to $H_{4,1}(x,t)$, as follows:

$$g_{\sigma_5}(x,\tau)=\lim_{\varepsilon\to 0^+}\frac{\sigma_5}{4\pi^2}\frac{\partial}{\partial\varepsilon}\frac{\theta[-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon]}{\sqrt{-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon}}.$$

$g_{\sigma_5}(x,\tau)$ contains a singular distribution term as well:

$$\Delta_{\sigma_5}=-\lim_{\varepsilon\to 0^+}\frac{\sigma_5}{4\pi^2}\frac{\delta[-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon]}{\sqrt{-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon}}.$$

In the following sections, GF's are derived for the (4,1) and (3,2) wave equations, which are *symmetric* in t. Then, we apply the GF's to the current of a uniformly moving point source, and rederive the results of Sec. III. We shall describe the importance of the form of Δ_{σ_5} in the derivation of the fields.

A. (4,1) Green function

With $\sigma_5=+1$ in (41), we have

$$g_+(x,\tau)=\frac{1}{(2\pi)^5}\int d^4k d\,k_5\frac{1}{k^2+k_5^2}e^{i[k\cdot x+k_5\tau]}=\frac{1}{(2\pi)^5}\int d^3\mathbf{k}d\,k_5 e^{i[\mathbf{k}\cdot\mathbf{x}+k_5\tau]}\int_{-\infty}^{+\infty}\frac{dk_0}{\mathbf{k}^2+k_5^2-k_0^2}e^{-ik_0t}. \tag{77}$$

The *Cauchy Principal Part* of the k_0 integral is

$$P\int_{-\infty}^{+\infty}\frac{dk_0}{\mathbf{k}^2+k_5^2-k_0^2}e^{-ik_0t}=\pi i\varepsilon(-t)\frac{1}{2\sqrt{\mathbf{k}^2+k_5^2}}[+e^{+it\sqrt{\mathbf{k}^2+k_5^2}}-e^{-it\sqrt{\mathbf{k}^2+k_5^2}}]=\varepsilon(t)\frac{\pi\sin(t\sqrt{\mathbf{k}^2+k_5^2})}{\sqrt{\mathbf{k}^2+k_5^2}}.$$

We then have

$$g_+(x,\tau)=\frac{\pi\varepsilon(t)}{(2\pi)^5}\int d^3\mathbf{k}dk_5\frac{\sin(t\sqrt{\mathbf{k}^2+k_5^2})}{\sqrt{\mathbf{k}^2+k_5^2}}e^{i[\mathbf{k}\cdot\mathbf{x}+k_5\tau]}.$$

We now orient the $\mathbf{k}$, k_5 space such the 4D "observation" vector $(\mathbf{x},\tau)$ is along k_3 (one observes at time τ on the laboratory clock at the point $\mathbf{x}$). Defining $l=\sqrt{\mathbf{k}^2+k_5^2}$ and $R=\sqrt{\mathbf{x}^2+\tau^2}$, and using α, θ, and ϕ as the 4D polar angles we find

$$k_5=l\cos\alpha,$$

$$k_3=l\sin\alpha\cos\theta,$$

$$\mathbf{k}\cdot\mathbf{x}+k_5\tau=Rk_3=Rl\sin\alpha\cos\theta,$$

$$d^3\mathbf{k}dk_5=l^3\sin^2\alpha\sin\theta dl\,d\alpha\,d\theta\,d\phi.$$

In terms of these variables,

$$\begin{aligned}g_+(x,\tau)&=\frac{\pi\varepsilon(t)}{(2\pi)^5}\int_0^{+\infty}l^3dl\int_0^{\pi}\sin^2\alpha\,d\alpha\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}d\varphi\frac{\sin(tl)}{l}e^{ilR\sin\alpha\cos\theta}\\&=\frac{\varepsilon(t)4\pi^2}{R(2\pi)^5}\int_0^{+\infty}l^3dl\int_0^{\pi}\sin^2\alpha\,d\alpha\frac{\sin(lR\sin\alpha)}{l\sin\alpha}\frac{\sin(tl)}{l}\\&=\frac{\varepsilon(t)4\pi^2}{R(2\pi)^5}\int_0^{+\infty}dl\int_0^{\pi}d\alpha\sin(lt)\sin(lR\sin\alpha)l\sin\alpha\\&=-\frac{\varepsilon(t)4\pi^2}{R(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\int_0^{+\infty}dl\int_0^{\pi}d\alpha\sin(lt)\cos(lR\sin\alpha).\end{aligned}$$

The choice of orientation in k-space resulted in a first-order derivative with respect to the "4D observation point" R. This form is important in convergence of the UMS solution. The α integral is simply $\pi J_0(lR)$ and using the *sine transform* of $J_0(x)$ (cf. Ref. 25),

$$J_0(x)=\frac{2}{\pi}\int_1^{+\infty}\frac{\sin(xs)}{\sqrt{s^2-1}}ds, \tag{78}$$

we find

$$g_+(x,\tau) = -\frac{8\pi^2\varepsilon(t)}{(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\int_0^{+\infty} dl \int_1^{+\infty} ds\, \sin(lt)\frac{\sin(lRs)}{\sqrt{s^2-1}}.$$

Changing the order of integration and noting that the l integrand is symmetric under $l\to -l$, we have

$$g_+(x,\tau) = -\frac{8\pi^2\varepsilon(t)}{(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\int_1^{+\infty}\frac{ds}{\sqrt{s^2-1}}\frac{1}{2}\int_{-\infty}^{+\infty} dl\, \sin(lt)\sin(lRs)$$

$$= -\frac{4\pi^2\varepsilon(t)}{(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\int_1^{+\infty}\frac{ds}{\sqrt{s^2-1}}\frac{2\pi}{(-4)}[2\delta(t+Rs)-2\delta(t-Rs)].$$

Since $Rs>0$, then using

$$\delta(t+Rs)-\delta(t-Rs) = -\varepsilon(t)[\delta(t+Rs)+\delta(t-Rs)],$$

we find

$$g_+(x,\tau) = \frac{4\pi^3\varepsilon^2(t)}{(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\int_1^{+\infty}\frac{ds}{\sqrt{s^2-1}}[\delta(t+Rs)+\delta(t-Rs)]$$

$$= \frac{4\pi^3}{(2\pi)^5}\frac{1}{R}\frac{\partial}{\partial R}\frac{1}{R}\frac{1}{\sqrt{t^2/R^2-1}}[\theta(-t/R-1)+\theta(+t/R-1)]$$

$$= \frac{1}{8\pi^2}\frac{1}{R}\frac{\partial}{\partial R}\frac{\theta(t^2-R^2)}{\sqrt{t^2-R^2}}.$$

We have $t^2-R^2=t^2-\mathbf{x}^2-\tau^2=-x_\alpha x^\alpha$, and since $R>0$, we can use $1/R\,\partial/\partial R=2\,\partial/\partial R^2$, which is *linear* in $x_\alpha x^\alpha$, thus

$$g_+(x,\tau) = -\lim_{\varepsilon\to 0^+}\frac{1}{4\pi^2}\frac{\partial}{\partial\varepsilon}\frac{\theta(-x_\alpha x^\alpha+\varepsilon)}{\sqrt{-x_\alpha x^\alpha+\varepsilon}}. \tag{79}$$

B. (3,2) Green function

We shall repeat the procedure for $\sigma_5=-1$ as follows:

$$g_-(x,\tau) = \frac{1}{(2\pi)^5}\int d^4k dk_5 \frac{1}{k^2-k_5^2}e^{i[k\cdot x-k_5\tau]} = \frac{1}{(2\pi)^5}\int_{\mathbb{R}^3} d^3\mathbf{k}e^{i[\mathbf{k}\cdot\mathbf{x}]}\int_{\mathbb{R}^2}\frac{dk_5\,dk_0}{\mathbf{k}^2-k_5^2-k_0^2}e^{-i[k_0t+k_5\tau]}. \tag{80}$$

The integration is separated into the two subspaces $\mathbb{R}^3$ for the spatial coordinates, and R^2 for the temporal coordinates. We shall use polar coordinates in *both* spaces, using the following substitutions:

$$k^2 = k_1^2+k_2^2+k_3^2,\ \ d^3\mathbf{k} = k^2\sin\theta dk\, d\theta\, d\varphi,$$

$$r^2 = x^2+y^2+x^2,\ \ \mathbf{k}\cdot\mathbf{x} = kr\cos\theta,$$

$$l^2 = k_0^2+k_5^2,\ \ dk_0\,dk_5 = l\,dl\,d\alpha,$$

$$s^2 = t^2+\tau^2,\ \ k_0t+k_5\tau = sl\cos\alpha.$$

The integral then takes the form

$$g_-(x,\tau)=\frac{1}{(2\pi)^5}\int_0^{+\infty}k^2\,dk\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}d\phi e^{ikr\cos\theta}\int_0^{+\infty}l\,dl\int_0^{2\pi}d\alpha\frac{e^{ils\cos\alpha}}{k^2-l^2}.$$

We can integrate immediately on ϕ, θ, and α as follows:

$$\int_0^{2\pi}d\phi=2\pi,\quad \int_0^{\pi}d\theta=\frac{2\sin(kr)}{kr},\quad \int_0^{2\pi}d\alpha=2\pi J_0(ls),$$

and thus

$$g_-(x,\tau)=\frac{1}{(2\pi)^5}\frac{8\pi^2}{r}\int_0^{+\infty}k\,dk\sin(kr)\int_0^{+\infty}l\,dl\,\frac{J_0(ls)}{k^2-l^2}=-\frac{1}{(2\pi)^3}\frac{2}{r}\frac{\partial}{\partial r}\int_0^{+\infty}l\,dl\,J_0(ls)\int_0^{+\infty}dk\,\frac{\cos(kr)}{k^2-l^2}$$

$$=-\frac{1}{(2\pi)^3}\frac{1}{r}\frac{\partial}{\partial r}\int_0^{+\infty}l\,dl\,J_0(ls)\int_{-\infty}^{+\infty}dk\,\frac{\cos(kr)}{k^2-l^2}.$$

The *Principal Part* value of the k integral is

$$P\int_{-\infty}^{+\infty}\frac{\cos(kr)}{k^2-l^2}dk=P\,.\,P\,.\,\Re\left[\int_{-\infty}^{+\infty}\frac{e^{ikr}}{k^2-l^2}dk\right]=\Re\left\{\frac{i\pi}{2l}[e^{ilr}-e^{-ilr}]\right\}=-\frac{\pi}{l}\sin(lr).$$

Thus, as the expression for $g_-(x,\tau)$, one obtains the form

$$g_-(x,\tau)=\frac{\pi}{(2\pi)^3}\frac{1}{r}\frac{\partial}{\partial r}\int_0^{+\infty}l\,dl\,J_0(ls)\frac{\sin(lr)}{l}=\frac{\pi}{(2\pi)^3}\frac{1}{r}\frac{\partial}{\partial r}\int_0^{+\infty}dl\,J_0(ls)\sin(lr).$$

Once again, using the sine transform of $J_0(x)$ [see (78)], we have

$$g_-(x,\tau)=\frac{\pi}{(2\pi)^3}\frac{2}{\pi}\frac{1}{r}\frac{\partial}{\partial r}\int_1^{+\infty}\frac{du}{\sqrt{u^2-1}}\frac{1}{2}\int_{-\infty}^{+\infty}dl\,\sin(lsu)\sin(lr)$$

$$=\frac{1}{(2\pi)^3}\frac{1}{r}\frac{\partial}{\partial r}\int_1^{+\infty}\frac{du}{\sqrt{u^2-1}}\frac{2\pi}{(-4)}[2\delta(su+r)-2\delta(su-r)]$$

$$=-\frac{\pi}{(2\pi)^3}\frac{1}{r}\frac{\partial}{\partial r}\int_1^{+\infty}\frac{du}{\sqrt{u^2-1}}\varepsilon(-s)[\delta(su+r)+\delta(su-r)].$$

However, $su\geq 0$ and $r\geq 0$, and thus the first term $\delta(su+r)$ vanishes identically, leaving

$$g_-(x,\tau)=\frac{1}{2(2\pi)^2}\frac{1}{r}\frac{\partial}{\partial r}\frac{1}{s}\frac{\theta(r/s-1)}{\sqrt{r^2/s^2-1}}=\frac{1}{2(2\pi)^2}\frac{1}{r}\frac{\partial}{\partial r}\frac{\theta(r-s)}{\sqrt{r^2-s^2}}.$$

Using the same arguments that were made for the (4,1) case, we have

$$g_-(x,\tau)=\lim_{\varepsilon\to 0^+}\frac{1}{4\pi^2}\frac{\partial}{\partial\varepsilon}\frac{\theta(x_\alpha x^\alpha+\varepsilon)}{\sqrt{x_\alpha x^\alpha+\varepsilon}},\tag{81}$$

where $x_\alpha x^\alpha=x^2-\tau^2$ in this case.

Combining both (4,1) and (3,2) cases, we obtain

$$g_{\sigma_5}(x,\tau)=\lim_{\varepsilon\to 0^+}\frac{\sigma_5}{4\pi^2}\frac{\partial}{\partial\varepsilon}\frac{\theta[-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon]}{\sqrt{-\sigma_5(x^2+\sigma_5\tau^2)+\varepsilon}}=\lim_{\varepsilon\to 0^+}\frac{\sigma_5}{4\pi^2}\frac{\partial}{\partial\varepsilon}\frac{\theta[-\sigma_5 x_\alpha x^\alpha+\varepsilon]}{\sqrt{-\sigma_5 x_\alpha x^\alpha+\varepsilon}}.\tag{82}$$

The factor 2 between (82) and (76) stems from the fact that *both* retarded and advanced t are used,

picking up an additional contribution from the future of t. An attempt to provide GF's that are τ retarded in (4,1) and (3,2) is currently under study.

C. Fields solution through GF's

We shall now apply the GF's (82) to the current generated by a uniformly moving point source. Recalling the UMS path (48), and generating the current (26), we shall use (45) to find the fields

$$a^{\alpha}_{\sigma_5}(x,\tau)=\lim_{\varepsilon\to 0^+}\frac{e\sigma_5}{4\pi^2}\frac{\partial}{\partial\varepsilon}\int_{-\infty}^{+\infty}d\tau'\; b^{\alpha}\frac{\theta[-\sigma_5((x-b\tau')+\sigma_5(\tau-b^5\tau')^2)+\varepsilon]}{\sqrt{-\sigma_5((x-b\tau')+\sigma_5(\tau-b^5\tau')^2)+\varepsilon}}. \tag{83}$$

Clearly, the limits of integration depend on the coefficients of the quadratic argument

$$\begin{aligned}p(\tau')&=-\sigma_5((x-b\tau')+\sigma_5(\tau-b^5\tau')^2)+\varepsilon\\&=-\sigma_5[(b^2+\sigma_5(b^5)^2)\tau'^2-2(b\cdot x+\sigma_5 b^5\tau)\tau'+x^2+\sigma_5\tau^2]+\varepsilon\\&=-\sigma_5 b_\alpha b^\alpha\tau'^2+2\sigma_5(b_\alpha x^\alpha)\tau'-\sigma_5[x_\alpha x^\alpha-\sigma_5\varepsilon].\end{aligned}$$

Thus, the polarity of the quadratic form $p(\tau)$ depends on the sign of $\zeta\equiv\sigma_5\varepsilon(b_\alpha b^\alpha)$, which we shall treat individually.

D. UMS fields for $\zeta=+1$

We have $-\sigma_5 b_\alpha b^\alpha<0$. The condition $p(\tau')>0$ is then limited to $\tau_1<\tau<\tau_2$, where $\tau_{1,2}$ are the *roots* of $p(\tau')$:

$$\tau'_{1,2}=\frac{-b_\alpha x^\alpha\pm\sqrt{(b_\alpha x^\alpha)^2-b_\alpha b^\alpha(x_\alpha x^\alpha-\sigma_5\varepsilon)}}{-b_\alpha b^\alpha}, \tag{84}$$

the fields become

$$a^{\alpha}_{\sigma_5}(x,\tau)=\lim_{\varepsilon\to 0^+}\frac{e\sigma_5 b^\alpha}{4\pi^2}\frac{\partial}{\partial\varepsilon}\int_{\tau_1}^{\tau_2}d\tau'\frac{\theta[p(\tau')]}{\sqrt{p(\tau')}}. \tag{85}$$

Clearly, the integral would be become zero *identically* if $\tau_{1,2}$ are *complex*, thus

$$(\tau'_1-\tau'_2)^2=\frac{4}{(b_\alpha b^\alpha)^2}[(b_\alpha x^\alpha)^2-b_\alpha b^\alpha(x_\alpha x^\alpha-\sigma_5\varepsilon)]>0.$$

We can now write $p(\tau')$ as follows:

$$p(\tau')\equiv\frac{\sigma_5}{b_\alpha b^\alpha}R^2-A^2(\tau'-B)^2, \tag{86}$$

where

$$R^2=(b_\alpha x^\alpha)^2-b_\alpha b^\alpha(x_\alpha x^\alpha-\sigma_5\varepsilon),\quad A=\sqrt{\sigma_5 b_\alpha b^\alpha},\quad B=\frac{b_\alpha x^\alpha}{b_\alpha b^\alpha}, \tag{87}$$

where $R^2>0$ is a requirement for the integral to be nonzero, and $A^2>0$ in this case. After making the substitution

$$\sqrt{\frac{\sigma_5}{b_\alpha b^\alpha}}R\tanh\beta=A(\tau'-B),$$

we have

$$a^{\alpha}_{\sigma_5}(x,\tau) = \lim_{\varepsilon\to 0^+} \sqrt{\frac{e\sigma_5}{b_\alpha b^\alpha}} \frac{\sigma_5 b^\alpha}{4\pi^2} \frac{\partial}{\partial\varepsilon}\theta(R^2) \int_{-\infty}^{+\infty} \frac{Rd\beta}{A\cosh^2\beta} \frac{1}{\sqrt{(\sigma_5/b_\alpha b^\alpha)R^2[1-\tanh^2\beta]}}$$

$$= \lim_{\varepsilon\to 0^+} \frac{1}{\sqrt{\sigma_5 b_\alpha b^\alpha}} \frac{e\sigma_5 b^\alpha}{4\pi^2} \frac{\partial}{\partial\varepsilon}\theta(R^2) \int_{-\infty}^{+\infty} \frac{d\beta}{\cosh\beta}.$$

The remaining β integral is a constant and equal to π (easily verified by substituting $u=e^{\beta}$). Thus

$$a^{\alpha}_{\sigma_5}(x,\tau) = \lim_{\varepsilon\to 0^+} \frac{e\sigma_5 b^\alpha}{4\pi\sqrt{b_\alpha b^\alpha}} \frac{\partial}{\partial\varepsilon}\theta(R^2),$$

where $\partial_\varepsilon\theta(R^2)=\sigma_5 b_\alpha b^\alpha \delta(R^2)$, which gives the final form for $a_{\sigma_5}(x,\tau)$ for this case:

$$a^{\alpha}_{\sigma_5}(x,\tau) = \frac{eb^\alpha(\sigma_5 b_\beta b^\beta)}{4\pi\sqrt{\sigma_5 b_\alpha b^\alpha}} \delta[(b_\alpha x^\alpha)^2 - b_\alpha b^\alpha x_\alpha x^\alpha], \tag{88}$$

where the limit of $\varepsilon\to 0^+$ was taken explicitly. Defining the normalized 5D velocity $n^\alpha = b^\alpha/\sqrt{\sigma_5 b_\beta b^\beta}$, we obtain the solution consistent with $\zeta=1$ of (72),

$$a^{\alpha}_{\sigma_5}(x,\tau) = \frac{en^\alpha}{4\pi}\delta[(n_\alpha x^\alpha)^2 - \sigma_5 x_\alpha x^\alpha], \tag{89}$$

where it is stressed again that σ_5 appears implicitly in the scalar products such as $n_\alpha x^\alpha$.

E. UMS fields for $\zeta=+1$

We shall repeat the analysis of the last section for the case of $-\sigma_5 b_\alpha b^\alpha > 0$. The roots (84) are applicable in the present case as well. However, the range of integration of (83) now reveals that $p(\tau')>0$ for the *exterior* region $\tau' \in (-\infty,\tau_1')\cup(\tau_2',+\infty)$. Therefore, (86) now becomes:

$$p(\tau') = (-\sigma_5 b_\alpha b^\alpha)\left(\tau' - \frac{b_\alpha x^\alpha}{b_\alpha b^\alpha}\right)^2 - \left(-\frac{\sigma_5}{b_\alpha b^\alpha}\right)[(b_\alpha x^\alpha)^2 - b_\alpha b^\alpha(x_\alpha x^\alpha - \sigma_5\varepsilon)]$$

$$= A^2(\tau' - B)^2 - \left(-\frac{\sigma_5}{b_\alpha b^\alpha}\right)R^2, \tag{90}$$

where in this case

$$A = \sqrt{-\sigma_5 b_\alpha b^\alpha}.$$

However, in order that the field integral (85) converges, we shall define $p_\lambda(\tau')$ as follows:

$$p_\rho(\tau') = p(\tau') + \rho^2. \tag{91}$$

The field integral (85) obtains the form

$$a^{\alpha}_{\sigma_5}(x,\tau) = \frac{e\sigma_5 b^\alpha}{4\pi^2} \lim_{\substack{\rho\to 0^+\\ \varepsilon\to 0^+}} \frac{\partial}{\partial\varepsilon} \int_{-\infty}^{+\infty} \frac{\theta(p(\tau'))}{\sqrt{p_\rho(\tau')}} d\tau' = \frac{e\sigma_5 b^\alpha}{4\pi^2} \lim_{\substack{\rho\to 0^+\\ \varepsilon\to 0^+}} \int_{-\infty}^{+\infty} \left[\frac{\delta(p(\tau'))}{\sqrt{p_\rho(\tau')}} - \frac{1}{2}\frac{\theta(p(\tau'))}{[p_\rho(\tau')]^{3/2}}\right]\frac{\partial p(\tau')}{\partial\varepsilon}, \tag{92}$$

where we used that fact that $\partial_\varepsilon p(\tau')=\partial_\varepsilon p_\rho(\tau')$. The first $\delta(p(\tau'))$ term breaks up over the roots of $p(\tau')$:

$$\frac{\delta(p(\tau'))}{\sqrt{p_\rho(\tau')}} = \frac{1}{A^2}\frac{\delta(\tau-\tau_1')+\delta(\tau-\tau_2')}{|\tau_1'-\tau_2'|}\frac{1}{\sqrt{p_\rho(\tau')}}. \tag{93}$$

We also have

$$\partial_\varepsilon p(\tau') = \partial_\varepsilon p_\rho(\tau') = 1. \tag{94}$$

Integrating the first δ-term, and combining (94) with (93) and (92), we obtain

$$\int_{-\infty}^{+\infty} \frac{\delta(p(\tau'))}{\sqrt{p_\rho(\tau')}} \frac{\partial p(\tau')}{\partial \varepsilon} d\tau' = \frac{1}{A^2} \frac{|b_\alpha b^\alpha|}{2R} \left[\frac{1}{\sqrt{p_\rho(\tau')}} \right|_{\tau'=\tau_1'} + \frac{1}{\sqrt{p_\rho(\tau')}}{}_{\tau'=\tau_2'} = \frac{1}{R} \frac{1}{\rho}, \tag{95}$$

which diverges as $1/\rho$. The second term can be integrated with the substitution

$$C \cosh \beta = A(\tau' - R) \quad \text{where } C = \left[\sqrt{\frac{-\sigma_5}{b_\alpha b^\alpha} R^2 - \lambda^2} \right].$$

Thus

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{\theta(p(\tau'))}{[p_\rho(\tau')]^{3/2}} d\tau' &= \frac{2C}{A} \theta(R^2) \int_{\beta_0}^{+\infty} \sinh \beta d\beta \frac{1}{[C^2(\cosh^2 \beta - 1)]^{3/2}} \\ &= 2 \frac{\theta(R^2)}{AC^2} \int_{\beta_0}^{+\infty} \frac{d\beta}{\sinh^2 \beta} = 2 \frac{\theta(R^2)}{AC^2} (-1) \coth \beta_{\beta_0}^{+\infty} = 2 \frac{\theta(R^2)}{AC^2} [\coth \beta_0 - 1]. \end{aligned} \tag{96}$$

The β_0 lower bound is given by

$$\sinh^2 \beta_0 = \frac{\rho^2}{C^2} \Rightarrow \coth \beta_0 = \sqrt{1 + \frac{1}{\sinh^2 \beta_0}} = \frac{1}{\rho} \sqrt{C^2 + \rho^2} = \frac{C}{\rho} + O(\rho),$$

which provides the complete solution for the second term

$$\int_{-\infty}^{+\infty} \frac{\theta(p(\tau'))}{[p_\rho(\tau')]^{3/2}} d\tau' = 2 \frac{\theta(R^2)}{AC^2} \left[\frac{C}{\rho} - 1 \right] \tag{97}$$

$$= 2\theta(R^2) \left[\frac{1}{\sqrt{R^2 + \sigma_5 \rho^2 b_\alpha b^\alpha}} \frac{1}{\rho} - \frac{1}{\sqrt{-\sigma_5 b_\alpha b^\alpha}(-\sigma_5 R^2 / b_\alpha b^\alpha - \rho^2)} \right]. \tag{98}$$

The sum of the δ-term and the smooth term becomes

$$\begin{aligned} a_{\sigma_5}^\alpha(x,\tau) &= \frac{e\sigma_5 b^\alpha}{4\pi^2} \lim_{\substack{\rho \to 0^+ \\ \varepsilon \to 0^+}} \theta(R^2) \left[\frac{1}{R} \frac{1}{\rho} - \left(\frac{1}{\sqrt{R^2 + \sigma_5 \rho^2 b_\alpha b^\alpha}} \frac{1}{\rho} - \frac{1}{\sqrt{-\sigma_5 b_\alpha b^\alpha}(-\sigma_5 R^2 / b_\alpha b^\alpha - \rho^2)} \right) \right] \\ &= \frac{e b^\alpha}{4\pi^2 \sqrt{-\sigma_5 b_\alpha b^\alpha}} \frac{b_\alpha b^\alpha}{[(b_\alpha x^\alpha)^2 - (b_\alpha b^\alpha)(x_\alpha x^\alpha)]}. \end{aligned}$$

Once again, defining $n^\alpha = b^\alpha / |b_\alpha b^\alpha|$, we obtain the final result for $\zeta = -1$:

$$a_{\sigma_5}^\alpha(x,\tau) = \frac{e n^\alpha}{4\pi^2} \frac{\theta((n_\alpha x^\alpha)^2 + \sigma_5 x_\alpha x^\alpha)}{[(n_\alpha x^\alpha)^2 + \sigma_5 x_\alpha x^\alpha]}. \tag{99}$$

V. CONCLUSIONS

The a-fields [see (72)] generated by a uniformly moving point source in (4,1) and (3,2) off-shell electrodynamics clearly resemble the expected UMS fields in a 5D Maxwell electrodynamics. However, the latter, generally in a framework of relativistic dynamics, are normally

regarded as producing fields from *timelike* sources only. Stueckelberg-based off-shell electrodynamics, on the other hand, that are based on a 4D dynamics parametrized along an invariant parameter, have no apparent limit on the region of the source velocity, though normally, the equations are set with constant $z^5(\tau)\equiv\tau\Rightarrow b^5\equiv 1$. Moreover, the 4D dynamics place no *a priori* restriction on $b'_\mu\equiv b^\mu/b^5$, and all cases of $b'^2<0$ or $b'^2>0$ were shown. However, the two forms of the fields given in (72) differ dramatically, and in particular, one is required to explain the δ-functions fields found for the 5D spacelike and timelike regions of source velocity for the (4,1) and (3,2) flat metric equations, respectively.

The δ-function fields ($\zeta=-1$) have support on a 4D null surface given by $x_\alpha x^\alpha-\sigma_5(n_\alpha x^\alpha)^2=0$, which is orthogonal to the direction of motion of the source n^α. Thus, this null surface is actually the (3,1) light cone, as can easily be observed in the frame $n^\alpha=[0;0,0,0,1]$, in which case both (4,1) and (3,2) fields reduce to the Maxwell time-symmetric GF $\delta(x^2)$. This reflects the choice of Principal Part, which was taken in the derivation of those fields. These singular fields are in fact the analog for a 4D UMS field of a spacelike moving source.

In a subsequent study, we plan to show that when a Lorentz force derived from those fields is applied to a test particle, it produces a finite force in an infinitesimally short τ interval, and thus has no noticeable effect on test particles. The reason for this is that the field tensor $f_{\alpha\beta}=\partial_\alpha a_\beta-\partial_\beta a_\alpha$contains derivatives of the δ-functions, and when integrated by parts, a coupling of the δ to acceleration terms is obtained, causing a large mass renormalization effect when the test particle hits the surface of singular support. This effect actually reduces the impact to a finite value, causing it to behave as a zero-measure force.

The smooth fields, on the other hand, obey a $1/r^2$ decay power-law. However, the (4,1) and (3,2) fields differ dramatically in this case. For the (4,1) metric case, the denominator is positive definite, which can easily be observed when a nonphysical frame of $n^\alpha=[1;0,0,0,0]$ is taken ($b^5=0$ in this case, contradicting the theory). In fact, for any $n^5\neq 0$, it causes the field to be a transient phenomenon, decaying as $1/\tau^2$ for large $\tau\gg\sqrt{\mathbf{x}^2+t^2}$.

On the other hand, for the (3,2) case, the fields follow an $O(2,2)$ symmetry as well, which can be seen when $n^\alpha=\delta^\alpha_i$ for one of $i\in\{1,2,3\}$. When this field is integrated over τ, it produces the $O(2,1)$ GF (proportional to $[t^2-x^2-y^2]^{-1/2}$), which is also the Maxwell field produced by a uniformly moving 3D point source in spacelike motion.

In Ref. 3, Land studied the equations of motion of a test particle in a field with similar singular support behavior. In particular, the scattering problem in the nonrelativistic limit was derived, in which he noted a failure in matching the well-known Rutherford scattering formula. Land then used the mass-τ uncertainty relations, similar to the time-energy uncertainty in nonrelativistic QM, to argue that a true pointwise 4D particle is insufficient to describe a physical source, and thus defined a *distribution of events* along the τ parameter, acting coherently as a single particle. He chose the following distribution,

$$j^\alpha(x,\tau)=\frac{b^\alpha}{2\lambda}\int_{-\infty}^{+\infty}d\tau' e^{-|\tau-\tau'|/\lambda}\delta^4[x-b\tau'], \tag{100}$$

which approaches the pointwise distribution for $\lambda\to 0^+$, and the Maxwell worldline [see Eq. (22)] for $\lambda\to+\infty$. Since the fields are linear, the cumulative contribution smoothed out the δ-function fields. Using a numerical computation, Land found a constraint on λ.

We shall show in a subsequent study how this method of regularization applies to the type of fields we have found here, and make comparison with observed phenomena.

It was found that the GF's (82) are consistent with the UMS fields. The ε derivative is used to indicate derivation with respect to the argument, which is maintained even once the fields are applied on a test particle. Although the derivative seems to contain a strong distribution $\delta(y)/\sqrt{y}$, this term has proved essential in the derivation of $\zeta=-1$ smooth fields (99), in which it counterbalanced an infinite contribution from the bounds $\tau\to\tau'^+_2,\tau'^-_1$. Geometrically, it regularized the singular support at the 5D light cone.

The GF's obtained could be used for subsequent studies of radiation-reaction, two-particle systems and various models of regularizations.

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New class $\hat{o}_N$ of statistical models: Transfer matrix eigenstates, chain Hamiltonians, factorizable S matrix

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Statistical models corresponding to a new class of braid matrices $(\hat{o}_N; N \geqslant 3)$ presented in a previous paper are studied. Indices labeling states spanning the N^r dimensional base space of $T^{(r)}(\theta)$, the rth order transfer matrix are so chosen that the operators W (the sum of the state labels) and (CP) (the circular permutation of state labels) commute with $T^{(r)}(\theta)$. This drastically simplifies the construction of eigenstates, reducing it to solutions of relatively small number of simultaneous linear equations. Roots of unity play a crucial role. Thus for diagonalizing the 81 dimensional space for $N=3$, $r=4$, one has to solve a maximal set of five linear equations. A supplementary symmetry relates invariant subspaces pairwise $[W=(r,Nr)$ and so on] so that only one of each pair needs study. The case $N=3$ is studied fully for $r=(1,2,3,4)$. Basic aspects for all (N,r) are discussed. Full exploitation of such symmetries lead to a formalism quite different from, possibly generalized, algebraic Bethe ansatz. Chain Hamiltonians are studied. The specific types of spin flips they induce and propagate are pointed out. The inverse Cayley transform of the YB matrix giving the potential leading to factorizable S matrix is constructed explicitly for $N=3$ as also the full set of $\hat{R}tt$ relations. Perspectives are discussed in a final section. © *2006 American Institute of Physics.*
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I. INTRODUCTION

New classes of braided matrices were presented in recent papers.[1,2] Statistical models corresponding to Ref. 1 have been presented in Ref. 3. Here we present those corresponding to Ref. 2. Different types of statistical models thus obtained will be compared at the end (Sec. VII). In Ref. 2 two distinct classes of braid matrices $(\hat{o}_N, \hat{p}_N)$ were presented. Here we consider only the $\hat{o}_N$ $(N \geqslant 3)$. For real, positive values of the parameter q and a certain domain (depending on q and N) of the spectral parameter θ, one obtains $N^2 \times N^2$ braid matrices with all nonzero elements real, positive giving non-negative Boltzmann weights. For the class $\hat{p}_N$ one encounters both positive and negative elements and thus one would need suitable reinterpretation of the corresponding Boltzmann weights.

We first recapitulate briefly the $\hat{o}_N$ braid matrices.[2] The $N^2 \times N^2$ baxterized braid matrices satisfying (in standard notations)

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$$\hat{R}_{12}(\theta)\hat{R}_{23}(\theta+\theta')\hat{R}_{12}(\theta') = \hat{R}_{23}(\theta')\hat{R}_{12}(\theta+\theta')\hat{R}_{23}(\theta) \tag{1.1}$$

are given by

$$\hat{R}(\theta) = I - \frac{\sinh\,\theta}{\sinh(\eta+\theta)}P_0', \tag{1.2}$$

where

$$e^{\eta}+e^{-\eta} = [N-1]+1 \equiv \frac{q^{N-1}-q^{-N+1}}{q-q^{-1}}+1 \tag{1.3}$$

and

$$P_0' = \sum_{i,j=1}^{N} q^{\rho_{j'}-\rho_j}(ij)\otimes(i'j') \tag{1.4}$$

with the following notations:

1. The $N\times N$ matrix (ij) has only one nonzero element, unity, on row i and column j and

$$(i',j') = (N-i+1,N-j+1). \tag{1.5}$$

2. The N tuple $(\rho_1,\rho_2,\ldots,\rho_N)$ is defined as

$$\left(n-\tfrac{1}{2},n-\tfrac{3}{2},\ldots,\tfrac{1}{2},0,-\tfrac{1}{2},\ldots,-n+\tfrac{1}{2}\right) \tag{1.6}$$

for $N=2n+1$ and

$$(n-1,n-2,\ldots,1,0,0,-1,\ldots,-n+1) \tag{1.7}$$

for $N=2n$.

Of the three projectors (P_+,P_-,P_0) providing a spectral resolution of $SO_q(N)$ braid matrices only

$$P_0' = ([N-1]+1)P_0 \tag{1.8}$$

appears in our class. To signal this provenance (along with crucial differences) our class is designated as $\hat{o}_N$. More relevant discussions can be found in Ref. 2.

We now introduce the permutation matrix

$$P = \sum_{i,j}(ij)\otimes(ji), \quad P^2 = I, \tag{1.9}$$

the Yang–Baxter matrix

$$R(\theta) = P\hat{R}(\theta), \tag{1.10}$$

and the monodromy matrices satisfying

$$\hat{R}(\theta-\theta')(t(\theta)\otimes t(\theta')) = (t(\theta')\otimes t(\theta))\hat{R}(\theta-\theta'). \tag{1.11}$$

The t matrix satisfying Eq. (1.11) is $N\times N$ in terms of the blocks

$$t_{ij,} \quad (i,j=1,\ldots,N), \tag{1.12}$$

each t_{ij} being itself a matrix whose dimension is prescribed as follows. One starts with $N\times N$ blocks t_{ij} obtained from the standard prescription [satisfying Eq. (1.11)]

$$t^{(1)}(\theta) = P\hat{R}(\theta) = R(\theta) \tag{1.13}$$

and then a hierarchy is obtained implementing the coproduct prescription

$$t_{ij}^{(r)}(\theta) = \sum_{k_1,\ldots,k_{r-1}} t_{ik_1}^{(1)}(\theta) \otimes t_{k_1k_2}^{(1)}(\theta) \otimes \cdots \otimes t_{k_{r-1},j}^{(1)}(\theta). \tag{1.14}$$

Starting with Eq. (1.13), this prescription assures that $t^{(r)}(\theta)$ satisfies Eq. (1.11).

Now the transfer matrix is defined, for each order r, as

$$T^{(r)}(\theta) = \sum_{i=1}^{N} t_{ii}^{(r)}(\theta). \tag{1.15}$$

The trace and more generally the eigenstates and the eigenvalues of $T^{(r)}(\theta)$ provide crucial properties of the statistical mechanical model associated with $\hat{R}(\theta)$. In particular, Eqs. (1.1), (1.11), and (1.13)–(1.15) all together assure the commutativity

$$[T(\theta), T(\theta')] = 0. \tag{1.16}$$

Commutative transfer matrices provide the crucial feature of exactly solvable models of statistical mechanics, the braid matrices encoding star-triangle relations.[4] For our specific case ($\hat{o}_N$) we illustrate, in the following section, some basic features for the simplest case ($N=3$). Certain aspects for $N>3$ will be presented afterwards (Sec. V).

Define

$$K(\theta) = -\frac{\sinh\theta}{\sinh(\eta+\theta)}, \tag{1.17}$$

where [setting $N=3$ in Eq. (1.3)]

$$e^{\eta} + e^{-\eta} = q + q^{-1} + 1. \tag{1.18}$$

For

$$-\eta < \theta < 0, \quad K(\theta) > 0. \tag{1.19}$$

For

$$\theta = 0, \quad K(0) = 0,$$

$$\theta = -\frac{\eta}{2}, \quad K\left(-\frac{\eta}{2}\right) = 1,$$

$$\theta \to -\eta, \quad K(\theta) \to +\infty. \tag{1.20}$$

Henceforward we consider the domain (1.19).

II. TRACE OF THE TRANSFER MATRIX FROM ITERATIVE STRUCTURE

The standard prescription (1.13) yields for $\hat{o}_3$

$$t^{(1)}(\theta) = P\hat{R}(\theta) = P(I + K(\theta)P_0'), \tag{2.1}$$

and hence, (suppressing now the argument θ for simplicity)

$$t_{11}^{(1)}=\begin{vmatrix}1&0&0\\0&0&0\\0&0&K\end{vmatrix},\quad t_{12}^{(1)}=\begin{vmatrix}0&0&0\\1&0&0\\0&q^{1/2}K&0\end{vmatrix},\quad t_{13}^{(1)}=\begin{vmatrix}0&0&0\\0&0&0\\1+qK&0&0\end{vmatrix},$$

$$t_{21}^{(1)}=\begin{vmatrix}0&1&0\\0&0&q^{-1/2}K\\0&0&0\end{vmatrix},\quad t_{22}^{(1)}=\begin{vmatrix}0&0&0\\0&1+K&0\\0&0&0\end{vmatrix},\quad t_{23}^{(1)}=\begin{vmatrix}0&0&0\\q^{1/2}K&0&0\\0&1&0\end{vmatrix},$$

$$t_{31}^{(1)}=\begin{vmatrix}0&0&1+q^{-1}K\\0&0&0\\0&0&0\end{vmatrix},\quad t_{32}^{(1)}=\begin{vmatrix}0&q^{-1/2}K&0\\0&0&1\\0&0&0\end{vmatrix},\quad t_{33}^{(1)}=\begin{vmatrix}K&0&0\\0&0&0\\0&0&1\end{vmatrix}. \tag{2.2}$$

All θ dependence is contained in the parameter K, as defined in Eq. (1.17). Starting with the 3×3 blocks the prescription Eq. (1.14) gives $3^r\times 3^r$ blocks $t_{ij}^{(r)}$. The recursion relations for our case $(N=3)$ are (for $j=1,2,3$),

$$t_{1j}^{(r+1)}=\begin{vmatrix}t_{1j}^{(r)}&0&0\\t_{2j}^{(r)}&0&0\\(1+qK)t_{3j}^{(r)}&q^{1/2}Kt_{2j}^{(r)}&Kt_{1j}^{(r)}\end{vmatrix}, \tag{2.3}$$

$$t_{2j}^{(r+1)}=\begin{vmatrix}0&t_{1j}^{(r)}&0\\q^{1/2}Kt_{3j}^{(r)}&(1+K)t_{2j}^{(r)}&q^{-1/2}Kt_{1j}^{(r)}\\0&t_{3j}^{(r)}&0\end{vmatrix}, \tag{2.4}$$

$$t_{3j}^{(r+1)}=\begin{vmatrix}Kt_{3j}^{(r)}&q^{-1/2}Kt_{2j}^{(r)}&(1+q^{-1}K)t_{1j}^{(r)}\\0&0&t_{2j}^{(r)}\\0&0&t_{3j}^{(r)}\end{vmatrix}. \tag{2.5}$$

The transfer matrix is iterated as

$$\begin{aligned}T^{(r+1)}&=t_{11}^{(r+1)}+t_{22}^{(r+1)}+t_{33}^{(r+1)}\\&=\begin{vmatrix}t_{11}^{(r)}+Kt_{33}^{(r)}&t_{12}^{(r)}+q^{1/2}Kt_{23}^{(r)}&(1+q^{-1}K)t_{13}^{(r)}\\t_{21}^{(r)}+q^{-1/2}Kt_{32}^{(r)}&(1+K)t_{22}^{(r)}&q^{-1/2}Kt_{12}^{(r)}+t_{23}^{(r)}\\(1+qK)t_{31}^{(r)}&q^{1/2}Kt_{21}^{(r)}+t_{32}^{(r)}&Kt_{11}^{(r)}+t_{33}^{(r)}\end{vmatrix}.\end{aligned} \tag{2.6}$$

Hence,

$$\begin{aligned}\mathrm{Tr}(T^{(r+1)})&=\mathrm{Tr}(t_{11}^{(r)}+Kt_{33}^{(r)}+(1+K)t_{22}^{(r)}+Kt_{11}^{(r)}+t_{33}^{(r)})\\&=(1+K)\mathrm{Tr}(t_{11}^{(r)}+t_{22}^{(r)}+t_{33}^{(r)})\\\mathrm{Tr}(T^{(r+1)})&=(1+K)\mathrm{Tr}(T^{(r)}).\end{aligned} \tag{2.7}$$

But from Eq. (2.2)

$$\mathrm{Tr}(T^{(1)})=\mathrm{Tr}(t_{11}^{(1)}+t_{22}^{(1)}+t_{33}^{(1)})=3(1+K). \tag{2.8}$$

Hence,

$$\mathrm{Tr}(T^{(r)})=3(1+K)^r. \tag{2.9}$$

Thus we obtain the trace of $T^{(r)}$ for all r directly without constructing explicitly the eigenstates and the 3^r eigenvalues. But the latter being of crucial interest we now turn to their systematic explicit constructions.

III. EIGENSTATES AND EIGENVALUES ($N=3$)

For $N=3$ the transfer matrix $T^{(r)}(\theta)$ of order r acts on a dimension 3^r. Construction of eigenstates corresponds to diagonalization of $T^{(r)}$ on such a base space. But basic symmetries of $T^{(r)}$ (Sec. I) for our case have profound consequences. They reduce the problem so that one has effectively to diagonalize subspaces whose dimensions increase polynomially with r (rather than according to the power law 3^r). To formulate these features conveniently we introduce the following conventions for state labels.

For the fundamental case, $r=1$, the three-dimensional basis is denoted as

$$|1\rangle \equiv \begin{vmatrix} 1 \\ 0 \\ 0 \end{vmatrix}\rangle, \quad |2\rangle \equiv \begin{vmatrix} 0 \\ 1 \\ 0 \end{vmatrix}\rangle, \quad |3\rangle \equiv \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix}\rangle. \tag{3.1}$$

For $r>1$, the order of the indices (1,2,3) represents the tensored structure. Thus, for example, for $r=5$,

$$|11231\rangle \equiv |1\rangle \otimes |1\rangle \otimes |2\rangle \otimes |3\rangle \otimes |1\rangle. \tag{3.2}$$

The fundamental realizations $t_{ij}^{(1)}$ of Eq. (2.2) implemented in the tensored structure Eq. (1.14) of $t_{i,j}^{(r)}$ lead to the following major consequences.

(I) Each set of states corresponding to a given sum of the indices (state labels 1,2,3) forms a closed subspace under the action of $T^{(r)}(\theta)$. Define with [with $a_i=(1,2,3)$]

$$W|a_1 a_2 \ldots a_r\rangle = (a_1 + a_2 + \cdots + a_r)|a_1 a_2 \ldots a_r\rangle. \tag{3.3}$$

Then

$$[T^{(r)}(\theta), W] = 0 \tag{3.4}$$

implying for each state on the right of

$$T^{(r)}(\theta)|a_1 a_2 \ldots a_r\rangle = \sum_{b_i} f_{(a,b)}(\theta)|b_1 b_2 \ldots b_r\rangle, \quad (b_1 + b_2 + \cdots + b_r) = (a_1 + a_2 + \cdots + a_r). \tag{3.5}$$

Thus the 3^r dimensional base space of $T^{(r)}$ splits into $(2r+1)$ closed subspaces under the action of $T^{(r)}$ as

$$S_r, S_{r+1}, \ldots, S_{2r-1}, S_{2r}, S_{2r+1}, \ldots, S_{3r}, \tag{3.6}$$

where S_n corresponds to $a_1+a_2+\ldots+a_r=n$. In constructing eigenstates of $T^{(r)}$ each S_n can be treated separately simplifying the problem considerably. The simplest subspaces are the extreme ones, namely

$$S_r = |11 \ldots 1\rangle \tag{3.7}$$

and

$$S_{3r} = |33 \ldots 3\rangle, \tag{3.8}$$

[the index 1(3) being repeated r times]. These are already automatically eigenstates. The highest dimensional subspace is obtained for $n=2r$ which includes the state $|22\ldots2\rangle$. Special feature of some subspaces will be displayed below.

(II) Within each subspace again $T^{(r)}(\theta)$ commutes with circular permutations of states labels. Thus (CP) representing a circular permutation

$$[T^{(r)}(\theta),(\mathrm{CP})]=0 \tag{3.9}$$

in the sense

$$(\mathrm{CP})^2 T^{(r)}|a_1a_2a_3,\ldots,a_{r-1}a_r\rangle=(\mathrm{CP})T^{(r)}|a_ra_1a_2,\ldots,a_{r-2}a_{r-1}\rangle=T^{(r)}|a_{r-1}a_ra_1,\ldots,a_{r-3}a_{r-2}\rangle \tag{3.10}$$

and so on for all successive (CP) of the indices $(a_1a_2,\ldots,a_r)$.

(III) As a consequence the states in each invariant subspace can again be grouped together implementing roots of unity as follows. Let ω be any rth root of unity, i.e.,

$$\omega=\left(1,e^{i(2\pi/r)},e^{i(2\pi/r)\cdot 2},\ldots,e^{i(2\pi/r)\cdot(r-1)}\right) \tag{3.11}$$

and (for each possible value of ω, separately)

$$|a_1a_2a_3,\ldots,a_{r-1}a_r\rangle_\omega\equiv|a_1a_2a_3,\ldots,a_{r-1}a_r\rangle+\omega|a_ra_1a_2,\ldots,a_{r-2}a_{r-1}\rangle+\omega^2|a_{r-1}a_ra_1,\ldots,a_{r-3}a_{r-2}\rangle$$
$$+\cdots+\omega^{r-1}|a_2a_3a_4,\ldots,a_ra_1\rangle. \tag{3.12}$$

The components states are, evidently, all in the same invariant subspace. For r different values of ω these provide a mutually orthogonal set of r states diagonalizing CP since

$$(\mathrm{CP})|a_1a_2a_3,\ldots,a_{r-1}a_r\rangle_\omega=\omega|a_1a_2a_3,\ldots,a_{r-1}a_r\rangle_\omega. \tag{3.13}$$

The action of $T^{(r)}$ on, say, $|a_1a_2,\ldots,a_{r-1}a_r\rangle$ gives directly, due to Eq. (3.10), that on $|a_1a_2,\ldots,a_{r-1}a_r\rangle_\omega$ for all values of ω. Thus one can effectively reduce the dimension of the relevant subspace S_n for a given sum of state labels, $(a_1+a_2+\cdots+a_{r-1}+a_r)=n$. Such a "two-step reduction," firstly, restriction to invariant subspaces S_n, second, introduction of roots of unity to form eigenstates of (CP) will be shown to lead to a much slower increase with r (as compared to $e^{(\ln 3)r}$) of the dimension of the spaces on which one has to diagonalize $T^{(r)}$. This will be first displayed through particular examples. The general formulation will be given at the end of this section.

(IV) But another symmetry is appropriately mentioned at this stage (to be illustrated later explicitly). Interchanging the indices as

$$(1,2,3)\rightarrow(3,2,1). \tag{3.14}$$

The action of $T^{(r)}$ is directly obtained via the inversion

$$q\rightarrow q^{-1} \tag{3.15}$$

in each coefficient. Thus the invariant subspaces related through Eq. (3.14) need not be studied separately. The corresponding eigenstates and eigenvalues are related through Eq. (3.15). It is sufficient to study the first $(r+1)$ subspaces since under Eqs. (3.14) and (3.15),

$$S_{2r}\rightarrow S_{2r},\quad (S_r,S_{r+1},\ldots,S_{2r-1})\rightleftharpoons(S_{3r},S_{3r-1},\ldots,S_{2r+1}). \tag{3.16}$$

Explicit examples for $r=(3,4)$ will follow. Our $\hat{o}_N$ braid matrices remain nontrivial for $q=1$ as pointed out in Ref. 2. Now Eq. (3.14) becomes a full symmetry. The degeneracy thus induced is of interest.

(V) A final crucial feature is due to Eq. (1.16),

$$[T^{(r)}(\theta),T^{(r)}(\theta')]=0. \tag{3.17}$$

Suppose that for, say, $r=4$ in some subspace one obtains a closed subset of states (A,B,C,D) with

$$T^{(4)}(\theta)A = a_{11}A + a_{12}B + a_{13}C + a_{14}D, \ldots, T^{(4)}(\theta)D = d_{11}A + d_{12}B + d_{13}C + d_{14}D. \quad (3.18)$$

The coefficients $(a_{11}, \ldots, d_{14})$ are in general polynomials in $K(\theta)$, the maximal degree being $r=4$ for this case. Define eigenstates as

$$T^{(4)}(\theta)(\alpha A + \beta B + \gamma C + \delta D) = v(\alpha A + \beta B + \gamma C + \delta D), \quad (3.19)$$

which are to be solved for by implementing Eq. (3.18) on the left. Consistency with Eq. (3.17) imposes θ independence (K independence) of $(\alpha, \beta, \gamma, \delta)$. Hence, on the right only v can be K dependent. All K dependence of $(a_{11}, \ldots, d_{14})$ on the left must thus factorize as a polynomial (here for $r=4$)

$$v = f_4K^4 + f_3K^3 + f_2K^2 + f_1K + f_0 \quad (3.20)$$

for suitable $(f_4, f_3, f_2, f_1, f_0)$ which can depend on (q, ω) only. In general this leads to a set of overdetermined set of coupled linear equations (for our case) in

$$(\alpha, \beta, \gamma, \delta; f_4, f_3, f_2, f_1, f_0). \quad (3.21)$$

Varied illustrations will follow. Moreover, while all eigenvalues are, in general, K and q dependent, all explicit q dependence [except for the implicit one through K of Eqs. (1.17) and (1.18)] must cancel in the overall trace (summing over all subspaces) to give Eq. (2.9), i.e.,

$$\mathrm{Tr}(T^{(r)}) = 3(1 + K)^r. \quad (3.22)$$

This provides a stringent check (Appendix A).

Special features of the subspaces $(S_r, S_{3r}), (S_{r+1}, S_{3r-1}), S_{2r}$

• (S_r, S_{3r}): As mentioned following Eqs. (3.7) and (3.8) these two are one-dimensional subspaces. One obtains immediately, for all r,

$$T^{(r)}(\theta)|11 \ldots 1\rangle = (1 + K^r)|11 \ldots 1\rangle, \quad (3.23)$$

$$T^{(r)}(\theta)|33 \ldots 3\rangle = (1 + K^r)|33 \ldots 3\rangle. \quad (3.24)$$

These eigenstates of (CP), singlets, provide the simplest illustrations of Eqs. (3.14) and (3.15).

• (S_{r+1}, S_{3r-1}): For arbitrary r, with

$$\omega = (1, e^{i(2\pi/r)}, e^{i(2\pi/r)2}, \ldots, e^{i(2\pi/r)(r-1)}) \quad (3.25)$$

define

$$X_\omega = |111 \ldots 12\rangle + \omega|211 \ldots 11\rangle + \omega^2|121 \ldots 11\rangle + \omega^{r-1}|111 \ldots 21\rangle, \quad (3.26)$$

$$Y_\omega = |333 \ldots 32\rangle + \omega|233 \ldots 33\rangle + \omega^2|323 \ldots 33\rangle + \omega^{r-1}|333 \ldots 23\rangle. \quad (3.27)$$

One easily obtains

$$T^{(r)}(\theta)X_\omega = (K^r\omega + \omega^{r-1})X_\omega, \quad (3.28)$$

$$T^{(r)}(\theta)Y_\omega = (K^r\omega + \omega^{r-1})Y_\omega. \quad (3.29)$$

For the r values of ω one obtains thus, in a single stroke, all the requisite r eigenstates for these two r-dimensional subspaces. Note that

$$\sum_{\omega} (K^r\omega + \omega^{r-1}) = \sum_{\omega} (K^r\omega + \omega^{-1}) = 0. \tag{3.30}$$

Hence, (S_{r+1}, S_{3r-1}) do not contribute to the total trace $\mathrm{Tr}(T^{(r)}(\theta))$.

For $S_{r+2}(S_{3r-2})$ already the structure of eigenstates and eigenvalues are not so simple. (See Appendix A for $r=3,4$.) Some special features of S_{2r} are, however, worth mentioning, particularly to compare the structures of r prime and non-prime.

• (S_{2r}): Like $|11\ldots1\rangle$ and $|33\ldots3\rangle, |22\ldots2\rangle$ is also a singlet under (CP). But unlike the former the latter one does not form an 1-dimensional subspace. It can get coupled with the other states of S_{2r} (for $\omega=1$) as follows. When r is prime, apart from $|22\ldots2\rangle$, S_{2r} is composed of r-plets (formed using ω with $\omega^r=1$). When r is factorizable there can be intermediate multiplets corresponding to factors $(n_1, n_2, \ldots, n_k)$ of $r=(n_1 n_2 \ldots n_k)$. Thus for $r=4$ (the first factorizable r) there are doublets corresponding to $r=2\times2$. For $r=6$, there are doublets and triplets between 1- and 6-plets. Let us illustrate the situation using the simplest nontrivial cases $r=3,4$.

◇ $(r=3, S_6)$: Define

$$A_1 = |222\rangle, \quad B_\omega = |123\rangle + \omega|312\rangle + \omega^2|231\rangle, \quad C_\omega = |321\rangle + \omega|132\rangle + \omega^2|213\rangle, \tag{3.31}$$

where $\omega=(1, e^{i(2\pi/3)}, e^{i(2\pi/3)2})$. In our notation A_1 indicates that here (for singlet) one has only $\omega=1$. Correspondingly (B_1, C_1) will denote the latter for $\omega=1$. Consistently with Eq. (3.9) set

$$T^{(3)}(\theta)(\alpha A_1 + \beta B_1 + \gamma C_1) = \upsilon(\alpha A_1 + \beta B_1 + \gamma C_1) \tag{3.32}$$

for $\omega=1$ and

$$T^{(3)}(\theta)(\mu B_\omega + \nu C_\omega) = w(\mu B_\omega + \nu C_\omega) \tag{3.33}$$

for $\omega=(e^{i(2\pi/3)}, e^{-i(2\pi/3)})$. Here (ν, w) are assumed to be cubic polynomials in K and $(\alpha, \beta, \gamma), (\mu, \nu)$ to be K independent. Note also that

$$(1 \rightleftharpoons 3) B_\omega = C_\omega. \tag{3.34}$$

Hence, [consistently with Eqs. (3.14) and (3.15)] one obtains the coefficient in $T^{(3)}(\theta)C_\omega$ by inverting q to q^{-1} in those of $T^{(3)}(\theta)B_\omega$. Explicit solutions are given in Appendix A. Here we only note that the decoupling of A_1 in Eq. (3.33) is assured via the structure

$$T^{(3)}(\theta)A_1 = a_{11}A_1 + a_{12}B_1 + a_{13}C_1,$$

$$T^{(3)}(\theta)B_\omega = (1 + \omega + \omega^2)b_{11}A_1 + b_{12}B_\omega + b_{13}C_\omega,$$

$$T^{(3)}(\theta)C_\omega = (1 + \omega + \omega^2)c_{11}A_1 + c_{12}B_\omega + c_{13}C_\omega. \tag{3.35}$$

◇ $(r=4, S_8)$: Here, after the (CP)- singlet

$$A_1 = |2222\rangle \tag{3.36}$$

one has also that doublets

$$B_{\pm1} = |1313\rangle \pm |3131\rangle \tag{3.37}$$

and then the quartets completing the 19-dimensional S_8 for all values of ω, namely,

$$\omega = (1, e^{i(2\pi/4)}, e^{i(2\pi/4)\cdot2}, e^{i(2\pi/4)\cdot3}) = (1, i, -1, -i), \tag{3.38}$$

$$C_\omega = |1133\rangle + \omega|3113\rangle + \omega^2|3311\rangle + \omega^3|1331\rangle,$$

$$D_\omega = |1223\rangle + \omega|3122\rangle + \omega^2|2312\rangle + \omega^3|2231\rangle,$$

$$E_\omega = |3221\rangle + \omega|1322\rangle + \omega^2|2132\rangle + \omega^3|2213\rangle,$$

$$F_\omega = |1232\rangle + \omega|2123\rangle + \omega^2|3212\rangle + \omega^3|2321\rangle. \tag{3.39}$$

Note also that

$$(1 \rightleftharpoons 3)(C_\omega, D_\omega, E_\omega, F_\omega) = (\omega^2 C_\omega, E_\omega, D_\omega, \omega^2 F_\omega), \tag{3.40}$$

which simplifies computations according to Eqs. (3.14) and (3.15). The set F_ω alone has a distinctive feature. The two indices 2 remain separated (unlike for D_ω, E_ω) under (CP). This singles it out directly as an eigenstate of $T^{(4)}(\theta)$ (Appendix A). As for $(C_\omega, D_\omega, E_\omega)$ decouplings, analogous to Eq. (3.35) but in two stages

(1) from A_1 for $\omega=(-1, \pm i)$,
(2) and also from $B_{\pm 1}$ for $\omega=(\pm i)$

are assured through factors of the type (Appendix A),

$$(1 + \omega + \omega^2 + \omega^3), (1 + \omega^2)(1 \pm \omega). \tag{3.41}$$

The maximal set of five coupled linear equations arises for $(\omega=1)$

$$T^{(4)}(\theta)(aA_1 + bB_1 + cC_1 + dD_1 + eE_1) = v_1(aA_1 + bB_1 + cC_1 + dD_1 + eE_1). \tag{3.42}$$

To conclude we emphasize again that for $r=(3,4)$ in base spaces respectively of dimensions (27,81) the maximal set of coupled linear equations encountered are sets of (3,5) respectively. This is the slow growth with r signaled before [end of (III)].

For $r=(1,2,3,4)$ we have studied the invariant subspaces S_n explicitly. Let us now indicate the general situation. Associate the variables (x_1, x_2, x_3) to the states $(|1\rangle, |2\rangle, |3\rangle)$ respectively. In the expansion

$$(x_1 + x_2 + x_3)^r = \sum_{n_1, n_2, n_3} C_{n_1, n_2, n_3} x_1^{n_1} x_2^{n_2} x_3^{n_3} \tag{3.43}$$

for each term

$$n_1 + n_2 + n_3 = r \tag{3.44}$$

and

$$\sum_{n_1, n_2, n_3} C_{n_1, n_2, n_3} = 3^r. \tag{3.45}$$

Imposing an additional constraint one obtains the subsets

$$\dim S_n = \sum_{n_1, n_2, n_3} C_{n_1, n_2, n_3}, \quad (n_1 + 2n_2 + 3n_3 = n) \tag{3.46}$$

for $n=(r, r+1, \ldots, 2r, \ldots, 3r)$. The dimension of the total base space for order r is given by Eq. (3.45).

Let us consider as an example the central subspace S_{10} for $r=5$. From Eq. (3.46) one easily finds

$$\dim S_{10} = 51 \quad (r = 5). \tag{3.47}$$

The states can be grouped into multiplets as follows with:

$$\omega^5 = 1, \tag{3.48}$$

$$V_1^{(1)} = |22222\rangle,$$

$$V_2^{(\omega)} = (|13222\rangle + \omega|21322\rangle + \omega^2|22132\rangle + \omega^3|22213\rangle + \omega^4|32221\rangle) \equiv ((\mathrm{CP})|13222\rangle)_\omega,$$

$$V_3^{(\omega)} = ((\mathrm{CP})|12322\rangle)_\omega,$$

$$V_4^{(\omega)} = ((\mathrm{CP})|13132\rangle)_\omega,$$

$$V_5^{(\omega)} = ((\mathrm{CP})|13312\rangle)_\omega,$$

$$V_6^{(\omega)} = ((\mathrm{CP})|13321\rangle)_\omega,$$

$$(V_7^{(\omega)}, \ldots, V_{11}^{(\omega)}) = (1 \rightleftharpoons 3)(V_2^{(\omega)}, \ldots, V_6^{(\omega)}), \tag{3.49}$$

i.e., $V_7^{(\omega)} = ((\mathrm{CP})|31222\rangle)_\omega$ and so on. For $\omega = 1$, now one has to solve a set of 11 (coupling $V_1^{(1)}, \ldots V_{11}^{(1)}$) linear equations. This is the maximal such set for $r=5$ where the total dimension is 243.

Whenever r is a prime number, i.e., $r=(1,3,5,7,11,13,\ldots)$, the multiplet structure is relatively simple. Thus for S_{2r} apart from $|22\ldots2\rangle$ there are only r-plets in terms of the roots $\omega^r=1$. When r is factorizable lower multiplets can arise corresponding to factors of r. We have illustrated this for $r=4$.

IV. CHAIN HAMILTONIANS ($N=3$)

The Hamiltonian for order r is defined as

$$H^{(r)} = (T^{(r)}(\theta))^{-1}_{\theta=0}(\partial_\theta(T^{(r)}(\theta)))_{\theta=0}. \tag{4.1}$$

Instead of using the standard formulation as a sum (see the basic references in Sec. IV of Ref. 3)

$$H^{(r)} = \sum_{k=1}^{r} I \otimes I \otimes \cdots \otimes \dot{\hat{R}}_{k,k+1}(0) \otimes I \otimes \cdots \otimes I, \tag{4.2}$$

where

$$\dot{\hat{R}}_{k_1,k+1}(0) = (\partial_\theta \hat{R}_{k,k+1}(\theta))_{\theta=0} \tag{4.3}$$

with the circular boundary condition for $k=r$ $(r+1 \approx 1)$ we will use Eq. (4.1) directly, as explained below, in a fashion particularly well adapted to our formalism for constructing eigenstates.

Define starting from Eq. (1.17), i.e.,

$$K(\theta) = -\frac{\sinh\,\theta}{\sinh(\eta+\theta)}, \tag{4.4}$$

$$\dot{K}_0 \equiv (\partial_\theta K(\theta))_{\theta=0} = -(\sinh\,\eta)^{-1} \tag{4.5}$$

with $K_0=(K(\theta))_{\theta=0}=0$. We start with eigenstate of $T^{(r)}(\theta)$,

$$|V\rangle_\omega = (c_1A_1 + c_2A_2 + \cdots + c_mA_m)_\omega, \tag{4.6}$$

where the subscript ω indicates that each A_i $(i=1,\ldots,m)$ is an eigenstate of (CP), circular permutation of r state labels corresponding to a subspace S_n $(n=r,\ldots,3r)$ (see Sec. III and Appendix

A). Thus for example, for $r=3$ and $S_n=S_5$ [see Eqs. (A13) and (A18)–(A20)] $|V\rangle_\omega = aA_\omega + bB_\omega$, where

$$A_\omega = (|113\rangle + \omega|311\rangle + \omega^2|131\rangle), \quad B_\omega = (|122\rangle + \omega|212\rangle + \omega^2|221\rangle), \tag{4.7}$$

with $\omega^3=1$. Quite generally, if for Eq. (4.6),

$$T^{(r)}(\theta)|V\rangle = v|V\rangle = v\left(\sum_k c_k A_k\right) \tag{4.8}$$

then as explained and emphasized (in Sec. III and Appendix A) the coefficients c_k can depend on q (but not on θ) the only θ dependence on the right is in v, a polynomial of order r in $K(\theta)$,

$$v = f_r(K(\theta))^r + f_{r-1}(K(\theta))^{r-1} + \cdots + f_1(K(\theta)) + f_0, \tag{4.9}$$

where the coefficients f_i are each θ independent. Thus for Eq. (4.7) the solutions (for each value of ω) are

(1)
$$(a,b) = (q^{1/2} + \omega q^{-1/2}, 1),$$
$$v = \omega^2 K^3 + ((q+q^{-1})\omega^2 + (1+\omega+\omega^2))K^2 + ((q+q^{-1})\omega + (1+\omega+\omega^2))K + \omega, \tag{4.10}$$

(2)
$$(a,b) = (1, -(q^{1/2} + \omega^2 q^{-1/2})), \quad v = \omega^2 K^3 + \omega. \tag{4.11}$$

From Eqs. (4.5), (4.8), and (4.9) one obtains (since $K_0=0$) the general result (with $\dot{T}_0^{(r)} \equiv (\partial_\theta T^{(r)}(\theta))_{\theta=0}, T_0^{(r)} = (T^{(r)}(\theta))_{\theta=0}$)

$$\dot{T}_0^{(r)}|V\rangle = \dot{K}_0 f_1|V\rangle, \tag{4.12}$$

$$T_0^{(r)}|V\rangle = f_0|V\rangle = \omega|V\rangle \tag{4.13}$$

and hence,

$$(T_0^{(r)})^{-1}|V\rangle = \omega^{r-1}|V\rangle. \tag{4.14}$$

The result $f_0=\omega$ (and $f_0^{-1}=\omega^{r-1}$ for $\omega^r=1$) is a general one. This corresponds to our use of eigenstates (CP) as basis states since for our class T_0 coincides with (CP). Hence, finally

$$H^{(r)}|V\rangle = T_0^{-1}\dot{T}_0|V\rangle = (\dot{K}_0\omega^{r-1}f_1)|V\rangle. \tag{4.15}$$

Thus starting with an eigenstate of $T^{(r)}(\theta)$ in our formalism it remains one of $H^{(r)}$ and the eigenvalue of $H^{(r)}$ is extracted, as above from that of $T^{(r)}$. Note that for

$$f_1 = 0, \quad H^{(r)}|V\rangle = 0. \tag{4.16}$$

Thus for Eq. (4.11),

$$H^{(3)}(A_\omega - (q^{-1/2} + \omega^2 q^{-1/2})B_\omega) = 0. \tag{4.17}$$

From Eqs. (3.23)–(3.29) it follows that, for all r:

$$H^{(r)}(S_r, S_{3r}; S_{r+1}, S_{3r-1}) \approx 0, \tag{4.18}$$

i.e., each eigenstate belonging to these subspaces is annihilated by $H^{(r)}$.

For $r=2$, the explicit form of the Hamiltonian is

$$(\dot{K}_0)^{-1}H^{(2)} = (q+q^{-1})(11)\otimes(33) + (q^{1/2}+q^{-1/2})(12)\otimes(32) + 2(13)\otimes(31) + (q^{1/2}+q^{-1/2})(21) \otimes(23) + 2(22)\otimes(22) + (q^{1/2}+q^{-1/2})(23)\otimes(21) + 2(31)\otimes(33) + (q^{1/2}+q^{-1/2})(32) \otimes(12) + (q+q^{-1})(33)\otimes(11). \tag{4.19}$$

Consistently with Eq. (4.18)

$$H^{(2)}(|11\rangle,|33\rangle;|12\rangle,|21\rangle;|23\rangle,|32\rangle) = 0. \tag{4.20}$$

For the only remaining subspace S_4, setting

$$H^{(2)}(a|13\rangle + b|22\rangle + c|31\rangle) = v_H(a|13\rangle + b|22\rangle + c|31\rangle). \tag{4.21}$$

One obtains the solutions

$$(1) \qquad (a,b,c) = (1,-(q^{1/2}+q^{-1/2}),1);\ v_H = 0,$$

$$(2) \qquad (a,b,c) = (1,0,-1);\ v_H = \dot{K}_0(q+q^{-1}-2),$$

$$(3) \qquad (a,b,c) = (1,2(q^{1/2}+q^{-1/2})^{-1},1);\ v_H = \dot{K}_0(q+q^{-1}+4). \tag{4.22}$$

Combining Eqs. (4.15) with Eqs. (A4)–(A6) one consistently reproduces the results Eqs. (4.20)–(4.22) obtained using the explicit form Eq. (4.19). Note that for $r=2$ and $\omega=-1$, Eq. (4.15) gives

$$H^{(2)}|V\rangle = -\dot{K}_0 f_1|V\rangle. \tag{4.23}$$

This corresponds to the positive sign in solution (2) of Eq. (4.22) since in Eq. (A6) the corresponding factor is

$$f_1 = -(q+q^{-1}-2). \tag{4.24}$$

Such changes of sign introduce a qualitative change: $\mathrm{Tr}(T^{(r)})$ in Eq. (2.9) has no explicit dependence on q (only an implicit one though K). But $\mathrm{Tr}(H^{(r)})$ can have explicit q dependence. For the simple example above $(N=3, r=2)$,

$$\mathrm{Tr}(H^{(2)}) = 2\dot{K}_0(q+q^{-1}+1). \tag{4.25}$$

Selection rules for transitions

Adopting the convention of attaching to the states $(|1\rangle,|2\rangle,|3\rangle)$ respectively the "spins"

$$(+,0,-) \tag{4.26}$$

it is seen from Eq. (4.19) that the action of the Hamiltonian on neighboring sites, induces transitions only when the sum of the two spins is zero, i.e., for

$$(+-),\quad (00),\quad (-+). \tag{4.27}$$

The final states corresponding again to zero sum. Thus one has nonzero matrix elements for a neighboring pair $|ij\rangle \overset{H}{\rightarrow} |kl\rangle$ only when for the corresponding spins

$$\sigma_i + \sigma_j = 0 = \sigma_k + \sigma_l. \tag{4.28}$$

Such matrix elements depend on $(\dot{K}_0, q)$. The structure of $H^{(r)}$ in Eq. (4.2) indicates that Eq. (4.21) is a generic feature. Any pair of the type Eq. (4.27) somewhere in the chain can start transitions which can propagate along the chain since the three possibilities in Eq. (4.27) can create such a pair with the next neighboring site and so on.

V. $N>3$

Three basic features displayed and studied at length for $N=3$ are

(1) A simple recursion relation yielding the trace of the transfer matrix for any order r [see Eqs. (2.2)–(2.9)].
(2) Invariant subspaces corresponding to the sum of the state labels [see Eqs. (3.1)–(3.6) and Appendix A).
(3) Role of (CP) circular permutation of state labels within each invariant subspace S_n [see Eqs. (3.9)–(3.13) and Appendix A).

It was shown (for $N=3$) how (2) and (3) greatly simplify the construction of eigenstates and eigenvalues of $T^{(r)}(\theta)$ for successive values of r.

We now indicate how these features are carried over for $N>3$ via the simplest possibilities, namely $N=4$, $r=(1,2)$. Now, as compared to Eqs. (1.17) and (1.18),

$$K(\theta) = -\frac{\sinh\theta}{\sinh(\eta+\theta)}, \tag{5.1}$$

where $e^{\eta}+e^{-\eta}=(q^2+1+q^{-2})+1=(q+q^{-1})^2$. As compared to Eq. (2.2) [writing t_{ij} for $t_{ij}^{(1)}(\theta)$, $i=(1,2,3,4)$ and K for $K(\theta)$]

$$t_{11} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & K \end{vmatrix} \equiv (11) + K(44)$$

and similarly,

$$t_{12} = (21) + Kq(43),\ t_{13} = (31) + Kq(42),\ t_{14} = (1 + Kq^2)(41),$$

$$t_{21} = (12) + Kq^{-1}(34),\ t_{22} = (22) + K(33),\ t_{23} = (1 + K)(32),\ t_{24} = Kq(31) + (42),$$

$$t_{31} = (13) + Kq^{-1}(24),\ t_{32} = (1 + K)(23),\ t_{33} = K(22) + (33),\ t_{34} = Kq(21) + (43),$$

$$t_{41} = (1 + Kq^{-2})(14),\ t_{42} = Kq^{-1}(13) + (24),\ t_{43} = Kq^{-1}(12) + (34),\ t_{44} = K(11) + (44). \tag{5.2}$$

As compared to Eqs. (2.3)–(2.9) recursion relations are now (suppressing arguments θ)

$$t_{ij}^{(r+1)} = t_{i1}^{(1)} \otimes t_{1j}^{(r)} + t_{i2}^{(2)} \otimes t_{2j}^{(r)} + t_{i3}^{(1)} \otimes t_{3j}^{(r)} + t_{i4}^{(1)} \otimes t_{4j}^{(r)}, \quad (i,j = 1,2,3,4) \tag{5.3}$$

giving [due to Eq. (5.2)]

$$t_{1j}^{(r+1)} = ((11) + K(44)) \otimes t_{1j}^{(r)} + ((21) + Kq(43)) \otimes t_{2j}^{(r)} + ((31) + Kq(42)) \otimes t_{3j}^{(r)} + (1 + Kq^2)(41) \otimes t_{4j}^{(r)},$$

$$t_{2j}^{(r+1)} = ((12) + Kq^{-1}(34)) \otimes t_{1j}^{(r)} + ((22) + K(33)) \otimes t_{2j}^{(r)} + (1 + K)(32) \otimes t_{3j}^{(r)} + (Kq(31) + (42)) \otimes t_{4j}^{(r)},$$

$$t_{3j}^{(r+1)} = ((13) + Kq^{-1}(24)) \otimes t_{1j}^{(r)} + (1 + K)(23) \otimes t_{2j}^{(r)} + (K(22) + (33)) \otimes t_{3j}^{(r)} + (Kq(21) + (43)) \otimes t_{4j}^{(r)},$$

$$t_{4j}^{(r+1)} = (1 + Kq^{-2})(14) \otimes t_{1j}^{(r)} + (Kq^{-1}(13) + (24)) \otimes t_{2j}^{(r)} + (Kq^{-1}(12) + (34)) \otimes t_{3j}^{(r)} + (K(11) + (44)) \otimes t_{4j}^{(r)}. \tag{5.4}$$

Hence, for the transfer matrix

$$T^{(r+1)} = t_{11}^{(r+1)} + t_{22}^{(r+1)} + t_{33}^{(r+1)} + t_{44}^{(r+1)} = \begin{vmatrix} t_{11}^{(r)} + Kt_{44}^{(r)} & t_{12}^{(r)} + Kq^{-1}t_{34}^{(r)} & t_{13}^{(r)} + Kq^{-1}t_{34}^{(r)} & (1+Kq^{-2})t_{14}^{(r)} \\ t_{21}^{(r)} + Kt_{43}^{(r)} & t_{22}^{(r)} + Kt_{33}^{(r)} & (1+K)t_{23}^{(r)} & Kq^{-1}t_{13}^{(r)} + t_{24}^{(r)} \\ t_{31}^{(r)} + Kqt_{42}^{(r)} & (1+K)t_{32}^{(r)} & Kt_{22}^{(r)} + t_{33}^{(r)} & Kq^{-1}t_{12}^{(r)} + t_{34}^{(r)} \\ (1+kq^2)t_{41}^{(r)} & t_{42}^{(r)} + Kqt_{31}^{(r)} & Kqt_{21}^{(r)} + t_{43}^{(r)} & Kt_{11}^{(r)} + t_{44}^{(r)} \end{vmatrix}. \tag{5.5}$$

One now obtains

$$\mathrm{Tr}(T^{(r+1)}) = (K+1)\mathrm{Tr}(T^r), \tag{5.6}$$

but

$$T^{(1)} = (K+1)I_4. \tag{5.7}$$

Hence,

$$\mathrm{Tr}(T^{(r)}) = 4(K+1)^r. \tag{5.8}$$

It is not difficult to obtain the general result (following from the fact that only the diagonal blocks $t_{ii}^{(r)}$ have diagonal terms)

$$\mathrm{Tr}(T^{(r)}) = N(K+1)^r. \tag{5.9}$$

For $N=(3,4)$ the particular solutions are given by Eqs. (2.9) and (5.8), respectively.

Now let us consider the eigenstates of $T^{(r)}(\theta)$ for $N=4$, $r=1,2$. As compared to Eq. (3.1) we now have the fundamental state vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{5.10}$$

and, as before, we denote tensor products as

$$|ijk\ldots\rangle = |i\rangle \otimes |j\rangle \otimes |k\rangle \otimes \ldots. \tag{5.11}$$

For a given n, as before, the set of states with

$$i + j + k + \cdots = n \tag{5.12}$$

will constitute the basis of the subspace S_n. For $r=1$ the situation is trivial. From Eq. (5.2)

$$T^{(1)} = t_{11} + t_{22} + t_{33} + t_{44} = (K+1)I_4, \tag{5.13}$$

$$T^{(1)}|i\rangle = (K+1)|i\rangle, \quad (i=1,2,3,4). \tag{5.14}$$

For $r=2$, from Eqs. (5.2) and (5.5),

$$\begin{aligned} T^{(2)} = {} & (K^2+1)P + 2K((11)\otimes(44) + (22)\otimes(33) + (33)\otimes(22) + (44)\otimes(11))K(q+q^{-1})((12) \\ & \otimes(43) + (13)\otimes(42) + (21)\otimes(34) + (24)\otimes(31) + (31)\otimes(24) + (34)\otimes(21) + (42)\otimes(13) \\ & + (43)\otimes(12)) + K(q^2+q^{-2})((14)\otimes(41) + (41)\otimes(14)), \end{aligned} \tag{5.15}$$

where

$$P = \sum_{ij} (ij)\otimes(ji), \quad (i,j=1,2,3,4). \tag{5.16}$$

Implementing the definitions Eqs. (5.10)–(5.12) one obtains from Eq. (5.15) for the subspaces $(S_2,\ldots,S_8)$ the following results (with $\epsilon=\pm 1$),

$$S_2: \quad T^{(2)}|11\rangle = (K^2+1)|11\rangle,$$

$$S_8: \quad T^{(2)}|44\rangle = (K^2+1)|44\rangle,$$

$$S_3: \quad T^{(2)}(|12\rangle + \epsilon|21\rangle = \epsilon(K^2+1)(|12\rangle + \epsilon|21\rangle,$$

$$S_7: \quad T^{(2)}(|43\rangle + \epsilon|34\rangle) = \epsilon(K^2+1)(|43\rangle + \epsilon|34\rangle),$$

$$S_4: \quad T^{(2)}|22\rangle = (K^2+1)|22\rangle,$$

$$T^{(2)}(|13\rangle + \epsilon|31\rangle) = \epsilon(K^2+1)(|13\rangle + \epsilon|31\rangle),$$

$$S_6: \quad T^{(2)}|33\rangle = (K^2+1)|33\rangle,$$

$$T^{(2)}(|42\rangle + \epsilon|24\rangle) = \epsilon(K^2+1)(|42\rangle + \epsilon|24\rangle), \tag{5.17}$$

$$S_5: \quad T^{(2)}(|14\rangle - |41\rangle) = -((K^2-2K+1) + K(q^2+q^{-2}))(|14\rangle - |41\rangle) \tag{5.18}$$

$$T^{(2)}(|23\rangle - |32\rangle) = -(K^2-2K+1)(|23\rangle - |32\rangle). \tag{5.19}$$

Finally, denoting

$$|A\rangle = (|14\rangle + |41\rangle), \quad |B\rangle = (|23\rangle + |32\rangle) \tag{5.20}$$

and setting

$$T^{(2)}(a|A\rangle + b|B\rangle) = v(a|A\rangle + b|B\rangle), \tag{5.21}$$

where

$$v = K^2 + 1 + Kf, \tag{5.22}$$

f begin K independent [a function $f(q)$ of q only], one obtains the constraints

$$a((q+q^{-1})^2 - f) + 2b(q+q^{-1}) = 0, \quad 2a(q+q^{-1}) + b(2-f) = 0. \tag{5.23}$$

Hence,

$$f = \tfrac{1}{2}(q^2+q^{-2}+4) \pm \tfrac{1}{2}\sqrt{(q+q^{-1})^4 + 12(q+q^{-1})^2 + 4} \tag{5.24}$$

with corresponding K-independent values of (a,b). The sum of the eigenvalues given by Eqs. (5.17)–(5.24) is

$$4(K+1)^2, \tag{5.25}$$

consistently with Eq. (5.8) for $r=2$. Our explicit results for $r=2$ not only shows how the basic properties (1), (2), (3) stated at the beginning of this section are all realized systematically but also how Eq. (3.14) is carried over, the subspaces now being paired via

$$(1,2,3,4) \to (4,3,2,1). \tag{5.26}$$

The chain Hamiltonian for any N is given by Eqs. (4.1)–(4.3) with Eqs. (1.4)–(1.7) giving P_0' in $\dot{\hat{R}}_0=\dot{K}_0P_0'$. In $\dot{K}_0$ of Eq. (4.5) now, from Eq. (1.3), $e^{\eta}+e^{-\eta}=[N-1]+1$. For $r=2$, one obtains for example

$$H^{(2)}=\dot{K}_0(P_0'+PP_0'P)=\dot{K}_0\left(\sum_{i,j=1}^{N}(q^{\rho_{i'}-\rho_j}+q^{\rho_i-\rho_j'})(ij)\otimes(i'j')\right). \tag{5.27}$$

For $N=4$ this corresponds to

$$\begin{aligned}(\dot{K}_0)^{-1}H^{(2)}=&(q^{-2}+q^2)(11)\otimes(44)+(q^{-1}+q)(12)\otimes(43)+(q^{-1}+q)(13)\otimes(42)+2(14)\otimes(41)\\&+(q^{-1}+q)(21)\otimes(34)+2(22)\otimes(33)+2(23)\otimes(32)+(q^{-1}+q)(24)\otimes(31)\\&+(q^{-1}+q)(31)\otimes(24)+2(32)\otimes(23)+2(33)\otimes(22)+(q^{-1}+q)(34)\otimes(21)+2(41)\\&\otimes(14)+(q^{-1}+q)(42)\otimes(13)+(q^{-1}+q)(43)\otimes(12)+(q^{-2}+q^2)(44)\otimes(11).\end{aligned} \tag{5.28}$$

Generalizations for $r>2$ can be written down systematically. If the spin associated with the state $|i\rangle$ is denoted as σ_i then Eq. (4.1) along with structures analogous to Eq. (5.27) implies transitions (if the states of two neighboring sites have spins σ_j, $\sigma_{j'}$)

$$(\sigma_j,\sigma_{j'})\rightarrow(\sigma_i,\sigma_{i'}) \tag{5.29}$$

with evident q-dependent transition amplitudes corresponding to the matrix elements of $H^{(r)}$ for order r. In particular if, for example,

$$(\sigma_1,\sigma_2,\ldots,\sigma_{N-1},\sigma_N)=\left(\frac{N-1}{2},\frac{N-2}{2},\ldots,-\frac{N-2}{2},-\frac{N-1}{2}\right) \tag{5.30}$$

then

$$\sigma_i+\sigma_{i'}=0\quad(i'=N-i+1). \tag{5.31}$$

For $N=3$ [as discussed in Eqs. (4.26)–(4.28)],

$$(\sigma_1,\sigma_2,\sigma_3)=(1,0,-1) \tag{5.32}$$

and for $N=4$

$$(\sigma_1,\sigma_2,\sigma_3,\sigma_4)=\left(\tfrac{3}{2},\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{3}{2}\right) \tag{5.33}$$

and so on.

If for two adjacent sites (including circular boundary constraints) one has states $(|i\rangle,|i'\rangle)$ they can be flipped to any pair $(|j\rangle,|j'\rangle)$. Thus such a flip can propagate along the chain for any state $|j\rangle$ of the next site.

A thorough investigation of our class of models for arbitrary N is beyond the scope of the present paper. We have, however, indicated how the basic features studied for $N=3$ are carried over as N increases. Such properties are conserved due to the specific structure of P_0' as defined in Eqs. (1.4)–(1.7).

We just mention finally that features parallel to those discussion for $N=3$ in Eqs. (3.43)–(3.49) can be carried over starting with the multimonial expansion of

$$(x_1+x_2+x_3+\cdots+x_N)^r. \tag{5.34}$$

Dimensions of invariant subspaces are obtained entirely analogously.

VI. POTENTIAL FOR FACTORIZABLE *S* MATRIX (*N*=3)

As in Sec. V of Ref. 3 we construct the inverse Cayley transform of the YB matrix which is also the $t^{(1)}(\theta)$ matrix (2.1) and given by Eq. (2.2) for $N=3$ for the class studied in this paper. The role of this in providing the potential for factorizable S matrices can be found in various sources.[5,6] As explained and emphasized in Sec. V of Ref. 3 an arbitrary normalization factor (denoted $\gamma^{-1}(\theta)$] of $R(\theta)$ must be introduced to start with for the inversion involved in the transform to be well-defined. The explicit inversion in the first factor of

$$-iV=(R(\theta)-\lambda(\theta)I)^{-1}(R(\theta)+\lambda(\theta)I) \tag{6.1}$$

will display admissible choices of $\lambda(\theta)$. Defining

$$X(R(\theta)-\lambda(\theta)I)=I, \quad -iV=X(X^{-1}+2\lambda(\theta)I)=I+2\lambda(\theta)X, \tag{6.2}$$

for $N=3$, Eq. (2.1) leads to (suppressing the argument θ in notation below)

$$X\begin{vmatrix} 1-\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\lambda & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & K-\lambda & 0 & q^{1/2}K & 0 & 1+qK & 0 & 0 \\ 0 & 1 & 0 & -\lambda & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q^{-1/2}K & 0 & 1+K-\lambda & 0 & q^{1/2}K & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\lambda & 0 & 1 & 0 \\ 0 & 0 & 1+q^{-1}K & 0 & q^{-1/2}K & 0 & K-\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1-\lambda \end{vmatrix} = I, \tag{6.3}$$

Only the nonzero elements of X will be given below. One obtains easily

$$(X_{11},X_{99})=(1-\lambda)^{-1}, \quad (X_{22},X_{44},X_{66},X_{88})=\frac{\lambda}{(1-\lambda^2)}, \quad (X_{24},X_{42},X_{68},X_{86})=\frac{1}{(1-\lambda^2)}. \tag{6.4}$$

These already show $\lambda\neq\pm1$. For $i=(3,5,7)$ one obtains the equations

$$(-X_{i3}\lambda+X_{i7})+q^{-1/2}KZ_i=\delta_{i3}, \quad X_{i5}(1-\lambda)+KZ_i=\delta_{i5}, \quad (X_{i3}-\lambda X_{i7})+Kq^{1/2}Z_i=\delta_{i7}, \tag{6.5}$$

where

$$Z_i\equiv q^{1/2}X_{i3}+X_{i5}+q^{-1/2}X_{i7}. \tag{6.6}$$

The solutions for $i=(3,5,7)$ are, respectively, the following ones. For $i=3$, (X_{33},X_{35},X_{37}) are given by

$$X_{33}=\frac{\lambda}{1-\lambda^2}+q^{-1/2}\left(\frac{q+\lambda}{1+\lambda}\right)X_{35}, \tag{6.7}$$

$$X_{37}=\frac{1}{1-\lambda^2}+q^{-1/2}\left(\frac{1+q\lambda}{1+\lambda}\right)X_{35}, \tag{6.8}$$

$$Z_3=\frac{q^{-1/2}(1+q\lambda)}{1-\lambda^2}+\left(\frac{q+q^{-1}+1+3\lambda}{1+\lambda}\right)X_{35}, \tag{6.9}$$

$$X_{35}(1-\lambda)+KZ_3=0. \tag{6.10}$$

The K dependence is now explicit. The case $i=3,7$ are related though the exchange of indices and inversion of q, namely

$$(3,7;q)\rightleftharpoons(7,3;q^{-1}). \tag{6.11}$$

For $i=5$,

$$X_{53}(1+q\lambda)=X_{57}(q+\lambda), \tag{6.12}$$

$$X_{53}=-\frac{q^{-1/2}(q+\lambda)}{1-\lambda^2}+\frac{(q+\lambda)q^{-1/2}}{1+\lambda}X_{55}, \tag{6.13}$$

$$X_{57}=-\frac{q^{-1/2}(1+q\lambda)}{1-\lambda^2}+\frac{(1+q\lambda)q^{-1/2}}{1+\lambda}X_{55}, \tag{6.14}$$

$$Z_5=-\frac{q+q^{-1}+2\lambda}{1-\lambda^2}+\frac{3\lambda+1+q+q^{-1}}{1+\lambda}X_{55}, \tag{6.15}$$

$$X_{55}(1-\lambda)+KZ_5=1. \tag{6.16}$$

Now Eqs. (6.19) and (6.20) give directly X_{55}. Next Eqs. (6.17) and (6.18) give X_{53} and X_{57}. Finally, we obtain

$$X=\begin{vmatrix}
\frac{1}{1-\lambda} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & \frac{1}{1-\lambda^2} & 0 & \frac{1}{1-\lambda^2} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & \mathsf{A} & 0 & \mathsf{B} & 0 & \mathsf{C} & 0 & 0\\
0 & \frac{1}{1-\lambda^2} & 0 & \frac{\lambda}{1-\lambda^2} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & \mathsf{D} & 0 & \mathsf{E} & 0 & \mathsf{B} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \frac{\lambda}{1-\lambda^2} & 0 & \frac{1}{1-\lambda^2} & 0\\
0 & 0 & \mathsf{F} & 0 & \mathsf{D} & 0 & \mathsf{A} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \frac{1}{1-\lambda^2} & 0 & \frac{\lambda}{1-\lambda^2} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{1-\lambda}
\end{vmatrix} \tag{6.17}$$

where

$$\mathsf{A}=\frac{(\lambda^2-\lambda-2K\lambda+K)q}{(1-\lambda)(q\lambda^2-3qK\lambda-q^2K-K-qK-q)}=X_{33}=X_{77},$$

$$\mathsf{B}=\frac{(q\lambda+1)q^{1/2}K}{(1-\lambda)(q\lambda^2-3qK\lambda-q^2K-K-qK-q)}=X_{35}=X_{57},$$

$$\mathsf{C} = \frac{(\lambda + qK\lambda - qK - 1 - K)q}{(1-\lambda)(q\lambda^2 - 3qK\lambda - q^2K - K - qK - q)} = X_{37},$$

$$\mathsf{D} = \frac{K(\lambda + q)q^{1/2}}{(1-\lambda)(q\lambda^2 - 3qK\lambda - q^2K - K - qK - q)} = X_{53} = X_{75},$$

$$\mathsf{E} = \frac{q\lambda^2 - 2Kq\lambda - q^2K - K - q}{(1-\lambda)(q\lambda^2 - 3qK\lambda - q^2K - K - qK - q)} = X_{55},$$

$$\mathsf{F} = \frac{-q - qK + q\lambda - K + K\lambda}{(1-\lambda)(q\lambda^2 - 3qK\lambda - q^2K - K - qK - q)} = X_{73}, \tag{6.18}$$

where $\lambda \neq \pm 1$, $\frac{1}{2}[3K \pm \sqrt{9K^2+4(q+1+q^{-1})K+4}]$.

From X, V is obtained as indicated in Eq. (6.2). Expressing it as

$$V = \sum_{ab,cd} V_{(ab,cd)}(ab) \otimes (cd). \tag{6.19}$$

The corresponding fermionic Lagrangian should be

$$\mathcal{L} = \int dx(i\bar{\psi}_a \gamma_\nu \partial_\nu \psi_a - g(\bar{\psi}_a \gamma_\nu \psi_c) V_{ab,cd}(\bar{\psi}_b \gamma_\nu \psi_d)). \tag{6.20}$$

The scalar Lagrangian can be obtained analogously. Such Lagrangians correspond to S matrices factorizable into two particles scattering independently of the chosen order of the latter ones.

VII. DISCUSSION

In Ref. 3 and in the present paper we have studied two different classes of statistical models. Certain aspects of the respective transfer matrices are strikingly contrasted. Such a major difference is in the number of parameters. The first model is indeed multiparameter. One has $\frac{1}{2}(N+3) \times (N-1)$ free parameters ($N=3,4,\ldots$). Here the only parameter is q appearing in the braid matrix given by Eqs. (1.2)–(1.7) and in $K(\theta)$ as defined by Eqs. (1.17)–(1.20). The structures of the eigenvalues of the respective transfer matrices are also quite different. In Ref. 3 we obtained single exponentials as eigenvalues, the exponent being a sum of the free parameters multiplied by θ. Here we have rth order polynomials in $K(\theta)$ for the eigenvalues of $T^{(r)}(\theta)$. There are other differences. But analogies and common features are also remarkable.

(a) In both case Tr $(T^{(r)}(\theta))$ is obtained quite simply for all r (though the structures are different). In (6.1) of Ref. 3 we obtained (for $N=2p-1$)

$$\mathrm{Tr}(T^{(r)}(\theta)) = 2(e^{rm_{11}^{(+)}\theta} + e^{rm_{22}^{(+)}\theta} + \cdots + e^{rm_{p-1,p-1}^{(+)}\theta}) + 1 \tag{7.1}$$

the $m_{ii}^{(+)}$ being a subset of the free parameters. Here (for $N=3,4,\ldots$) the corresponding result Eq. (5.9) is

$$\mathrm{Tr}(T^{(r)}(\theta)) = N(K(\theta)+1)^r, \tag{7.2}$$

where $K(\theta)$ is given by Eqs. (1.3) and (1.17).

(b) In both cases the N^r dimensional base space of $T^{(r)}(\theta)$ breaks up into closed subspaces of lower dimensions. The definitions of these subspaces have some differences however. The relevant definitions in Ref. 3 should be compared to Eqs. (3.2)–(3.6) here and their generalization in Sec. V.

(c) In each subspace S_n the circular permutation of states labels as formulated in Eqs. (3.9)–(3.19) leads to a further reduction of dimension in constructing eigenstates by splitting S_n

again into subsets corresponds to the eigenstates of the operator (CP) of circular permutations. This involves a crucial role of the roots of unity, $[\omega^r=1$ for $T^{(r)}(\theta)]$ in the construction of eigenstates. The role of roots of unity was also crucial in Ref. 3 though they were implemented in a slightly different fashion (corresponding to the difference in labeling states).

In both cases the "two-step reduction" [via (b) and (c)] in the effective dimension of the basis in construction of eigenstates has been emphasized (see the formulation of Sec. III). The exponential increase in dimension with r ($e^{(\ln N)r}$) is replaced in actual construction by a relatively moderate polynomial one. Thus for $N=3$ and $r=4$ we have to solve here at most a set of 5 simultaneous linear equations (Appendix A) though now N^r is $3^4=81$. This reduction of the problem to a relatively low number of linear equations should be constrasted to the implementation of algebraic Bethe ansatz.[6–8] For the latter one has to solve complex nonlinear equations whose number increases along with N.

In the preceding sections (particularly in Sec. III for $N=3$ and in Sec. V for $N>3$), we have formulated carefully the crucial properties, basic features of models corresponding to the braid matrices presented in Ref. 2. Exploiting such properties we have constructed eigenstates and eigenvalues of $T^{(r)}(\theta)$ for $N=3$, $r=(1,2,3,4)$ (Appendix A). Certain related features for all r have been formulated at the end of Sec. III. Chain Hamiltonians and potentials for factorizable S matrices have been studied (Secs. IV and VI).

Further explorations in several directions are evidently desirable. Reflection equations[9,10] and correlation functions[11,12] should be studied. More basically one may try to elucidate the relevance of the star-triangle relations[4] encoded in our class of braid matrices to specific contexts. We hope to undertake such studies elsewhere.

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APPENDIX A: EIGENSTATES AND EIGENVALUES OF $T^{(r)}(\theta)$ FOR $r=1,2,3,4$ ($N=3$)

We start by noting the following points:

(1) For each case the subscript n of S_n denotes the sum of the state labels [see discussion from Eqs. (3.3) to (3.6)].
(2) For each r we present results only up to S_{2r}. The remaining subspaces $(S_{2r+1},\ldots,S_{3r})$ are then obtained implementing Eqs. (3.14)–(3.16).
(3) For different subspaces we often repeat the same notations for states. Since $T^{(r)}$ does not couple such spaces no confusion is likely.
(4) The notation K and ω correspond to Eqs. (1.17) and (3.11), respectively. (CP) denotes circular permutations.

1. $r=1$

The three states directly furnish the spectrum, each being a one-dimensional subspace

$$T^{(1)}(\theta)(|1\rangle,|2\rangle,|3\rangle)=(1+K)(|1\rangle,|2\rangle,|3\rangle), \tag{A1}$$

$$\mathrm{Tr}(T^{(1)}(\theta))=3(1+K). \tag{A2}$$

2. $r=2$

The (CP) eigenstates constructed as in Eqs. (3.10)–(3.13), with $\omega^2=1$, give

$$S_2: \quad A_1=|11\rangle,$$

$$S_3: \quad A_{\pm 1}=|12\rangle+|21\rangle,$$

$$S_4: \quad A_1=|22\rangle, \quad B_{\pm 1}=|13\rangle\pm|31\rangle. \tag{A3}$$

One obtains [K being $K(\theta)$],

$$S_2{:}T^{(2)}(\theta)A_1=(K^2+1)A_1, \tag{A4}$$

$$S_3{:}T^{(2)}(\theta)A_{\pm 1}=\pm(K^2+1)A_{\pm 1}, \tag{A5}$$

$$S_4{:}T^{(2)}(\theta)B_{-1}=-(K^2+(q+q^{-1}-2)K+1)B_{-1},$$

$$T^{(2)}(\theta)(B_1-(q^{1/2}+q^{-1/2})A_1)=(K^2+1)(B_1-(q^{1/2}+q^{-1/2})A_1),$$

$$T^{(2)}(\theta)((q^{1/2}+q^{-1/2})B_1+2A_1)=(K^2+(q+q^{-1}+4)K+1)((q^{1/2}+q^{-1/2})B_1+2A_1). \tag{A6}$$

Also

$$(S_5,S_6)\rightleftharpoons(S_3,S_2) \tag{A7}$$

according to Eqs. (3.14)–(3.16). Summing over all subspaces $(S_2,\ldots,S_6)$,

$$\mathrm{Tr}(T^{(1)}(\theta))=3(1+K)^2 \tag{A8}$$

consistently with Eq. (2.9). We have not uniformly normalized the states. Thus $\langle A_1|A_1\rangle=1$ and $\langle B_{\pm 1}|B_{\pm 1}\rangle=2$. This is crucial to the orthogonality

$$\langle B_1-(q^{1/2}+q^{-1/2})A_1|(q^{1/2}+q^{-1/2})B_1+2A_1\rangle=0. \tag{A9}$$

This point displayed here for this simple case will not be repeated in cases to follow.

3. $r=3$

Here

$$\omega=(1,e^{(2\pi/3)},e^{(2\pi/3)2}) \tag{A10}$$

and (CP) eigenstates for (S_3,S_4,S_5,S_6) are

$$S_3: \quad A_1=|111\rangle, \tag{A11}$$

$$S_4: \quad A_\omega=|112\rangle+\omega|211\rangle+\omega^2|121\rangle, \tag{A12}$$

$$S_5: \quad A_\omega=|113\rangle+\omega|311\rangle+\omega^2|131\rangle,\ B_\omega=|122\rangle+\omega|212\rangle+\omega^2|221\rangle, \tag{A13}$$

$$S_6: \quad A_1=|222\rangle,\ B_\omega=|123\rangle+\omega|312\rangle+\omega^2|231\rangle,$$

$$C_\omega=|321\rangle+\omega|132\rangle+\omega^2|213\rangle=(1\rightleftharpoons 3)B_\omega. \tag{A14}$$

Also

$$(1 \rightleftharpoons 3)(S_3,S_4,S_5) = (S_9,S_8,S_7). \tag{A15}$$

The $T^{(3)}(\theta)$ eigenstates are now obtained as follows:

$$S_3: \quad T^{(3)}(\theta)A_1 = (K^3+1)A_1, \tag{A16}$$

$$S_4: \quad T^{(3)}(\theta)A_\omega = (K^2\omega+\omega^2)A_\omega, \tag{A17}$$

$$S_5: \quad T^{(3)}(\theta)(aA_\omega + bB_\omega) = v(aA_\omega + bB_\omega). \tag{A18}$$

Solutions:

(1)
$$(a,b) = (q^{1/2}+\omega q^{-1/2},1),$$
$$v = \omega^2K^3 + (q+q^{-1})(\omega^2K^2+\omega K) + (1+\omega+\omega^2)(K^2+K) + \omega, \tag{A19}$$

(2)
$$(a,b) = (1,-(q^{1/2}+\omega^2q^{-1/2})), \quad v = K^3\omega^2+\omega. \tag{A20}$$

$\diamond S_6$: For $\omega = e^{\pm(2\pi/3)}$, A_1 is decoupled. Set

$$T^{(3)}(\theta)(bB_\omega + cC_\omega) = v(bB_\omega + cC_\omega). \tag{A21}$$

Solutions:

(1)
$$(b,c) = (q,-1), \quad v = K^3\omega^2+\omega \tag{A22}$$

(2)
$$(b,c) = (1,q), \quad v = K^3\omega^2+\omega+(q+q^{-1})(K^2\omega^2+K\omega). \tag{A23}$$

For the values of $\omega(\neq 1)$, with $\omega+\omega^2=-1$ the sum of eigenvalues

$$\Sigma v = -2(K^3+1) - (q+q^{-1})(K^2+K). \tag{A24}$$

For $\omega-1$, $T^{(3)}$ couples (A_1,B_1,C_1). Set

$$T^{(3)}(\alpha A_1 + \beta B_1 + \gamma C_1) = v_1(\alpha A_1 + \beta B_1 + \gamma C_1). \tag{A25}$$

Solutions:

(1)
$$(\alpha,\beta,\gamma) = (0,q^{1/2},-q^{-1/2}), \quad v_1 = (K+1)(K^2-K+1), \tag{A26}$$

(2)
$$(\alpha,\beta,\gamma) = (-(q+q^{-1}),q^{-1/2},q^{1/2}), \quad v_1 = (K+1)(K^2-K+1), \tag{A27}$$

(3)
$$(\alpha,\beta,\gamma) = (3,q^{-1/2},q^{1/2}), \quad v_1 = (K+1)((K^2-K+1)+K(q+q^{-1}+3)). \tag{A28}$$

Concerning orthogonality note that

$$\langle A_1|A_1\rangle = 1, \quad \langle B_1|B_1\rangle = \langle C_1|C_1\rangle = 3. \tag{A29}$$

The sum of the eigenvalues over S_6 is

$$(\Sigma v)_{S_6} = K^3+1+3K(K+1). \tag{A30}$$

The results for (S_7,S_8,S_9) are obtained, as usual, directly from those of (S_5,S_4,S_3), respectively.

Summing over all the subspaces $(S_3,\ldots,S_9)$ one obtains [all explicit q dependence canceling consistently with Eq. (2.9)],

$$\mathrm{Tr}(T^{(3)}(\theta)) = (K^3+1)+(K^3+1)+3(K^2+K)+3(K^2+K)+(K^3+1)+3(K^2+K) = 3(K+1)^3. \tag{A31}$$

4. $r=4$

Here

$$\omega = (1, e^{i(2\pi/4)}, e^{i(2\pi/4)2}, e^{i(2\pi/4)3}) = (1, i, -1, i). \tag{A32}$$

Of the invariant subspaces we consider $(S_4, S_5, S_6, S_7, S_8)$. One obtains the results of the remaining ones via $(1,2,3;q) \leftrightarrow (3,2,1;q^{-1})$ as

$$(S_9, S_{10}, S_{11}, S_{12}) \rightleftarrows (S_7, S_6, S_5, S_4). \tag{A33}$$

For brevity and simplicity, we will recapitulate our results in Tables I and II.

TABLE I. CP eigenstates for $r=4$.

Subspace	(CP) eigenstates	Dimension
S_4	$\|1111\rangle$	1
S_5	$A_\omega = \|1112\rangle + \omega\|2111\rangle + \omega^2\|1211\rangle + \omega^3\|1121\rangle$	4
S_6	$A_{\pm 1} = \|1212\rangle \pm \|2121\rangle$	10
	$B_\omega = \|1113\rangle + \omega\|3111\rangle + \omega^2\|1311\rangle + \omega^3\|1131\rangle$	
	$C_\omega = \|1122\rangle + \omega\|2112\rangle + \omega^2\|2211\rangle + \omega^3\|1221\rangle$	
S_7	$A_\omega = \|1222\rangle + \omega\|2122\rangle + \omega^2\|2212\rangle + \omega^3\|2221\rangle$	16
	$B_\omega = \|1123\rangle + \omega\|3112\rangle + \omega^2\|2311\rangle + \omega^3\|1231\rangle$	
	$C_\omega = \|1132\rangle + \omega\|2113\rangle + \omega^2\|3211\rangle + \omega^3\|1321\rangle$	
	$D_\omega = \|1213\rangle + \omega\|3121\rangle + \omega^2\|1312\rangle + \omega^3\|2131\rangle$	
S_8	$A_1 = \|2222\rangle$	19
	$B_{\pm 1} = \|1313\rangle \pm \|3131\rangle$	
	$C_\omega = \|1133\rangle + \omega\|3113\rangle + \omega^2\|3311\rangle + \omega^3\|1331\rangle$	
	$D_\omega = \|1223\rangle + \omega\|3122\rangle + \omega^2\|2312\rangle + \omega^3 2231\rangle$	
	$E_\omega = \|3221\rangle + \omega\|1322\rangle + \|\omega^2\|2132\rangle + \omega^3\|2213\rangle$	
	$F_\omega = \|1232\rangle + \omega\|2123\rangle + \omega^2\|3212\rangle + \omega^3\|2321\rangle$	

TABLE II. Eigenstates and eigenvalues for $r=4$.[a]

	Eigenvalues	Eigenstates
S_4:	K^4+1	$\|1111\rangle$
S_5:	$\omega^3K^4+\omega$	A_ω
S_6:	$\pm(K^4+1)$	$A_{\pm 1}$
	$\omega^3K^4+\omega$	$B_\omega-(q+\omega^3)C_\omega/\sqrt{q}$
	$\omega^3[K^4+(q+1+\omega+\omega^3+q^{-1})K^3$	
	$+\omega^3(q+1+\omega+\omega^3+q^{-1})K^2$	$B_\omega+\sqrt{q}C_\omega/(q+\omega)$
	$+\omega^2(q+1+\omega+\omega^3+q^{-1})K+\omega^2]$	
S_7:	$\omega^3K^4+\omega$	$A_\omega-\omega\sqrt{q}B_\omega-C_\omega/\sqrt{q}$,
		$-(q^3+\omega^2)A_\omega+q\sqrt{q}(q+1+q^{-1})D_\omega$
		$+\omega\sqrt{q}(\omega^2-q^2-q)B_\omega+\sqrt{q}(q^2-\omega^2q-\omega^2)C_\omega$
	$\omega^3K^4+\omega+(\omega^3K^3+\omega K)(q+1+\omega+\omega^3+q^{-1})$	$(1+\omega)A_\omega/\sqrt{q}+\omega^2B_\omega/q+C_\omega+\omega(q+\omega)D_\omega/q$
	$+K^2\omega^2(q+1+\omega+\omega^3+q^{-1})$	
	$\omega^3K^4+\omega+(\omega^3K^3+\omega K)(q+1+\omega+\omega^3+q^{-1})$	$(1-\omega)A_\omega/\sqrt{q}-\omega^2B_\omega/q+C_\omega-\omega(q-\omega)D_\omega/q$
	$+K^2\omega^2(q+1-\omega-\omega^3+q^{-1})$	
S_8:	K^4+1	F_1, $2A_1+C_1-\sqrt{q}D_1-E_1/\sqrt{q}$,
		$2\sqrt{q}(q^2+q-2+q^{-1}+q^{-2})A_1$
		$+2\sqrt{q}(q+2+q^{-1})B_1-\sqrt{q}(q+4+q^{-1})C_1$
		$+(q^2+2q-3-2q^{-1}-3)D_1$
		$-(2q^2+3q-2-q^{-1})E_1$
	$-K^4-1$	F_{-1},
		$B_{-1}+(q^2-1)C_{-1}/2q-(q^2+1)D_{-1}/(2\sqrt{q})$
		$+(q^2+1)E_{-1}/(2q\sqrt{q})$
	$\mp iK^4\pm i$	$F_{\pm i}$, $\sqrt{q}C_{\pm i}-D_{\pm i}+E_{\pm i}$
	$\mp i[K^4+(q+1+q^{-1})K^3\pm 3iK^2$	$-(q+1)C_{\pm i}/\sqrt{q}-D_{\pm i}+E_{\pm i}$
	$-(q+1+q^{-1})K-1]$	
	$\mp i[K^4+(q+1+q^{-1})K^3\mp i(q+1+q^{-1})K^2$	$C_{\pm i}+(1+2q)D_{\pm i}/(q-1)\sqrt{q}+(q+2)\sqrt{q}E_{\pm i}/(q-1)$
	$-(q+1+q^{-1})K-1]$	
	$K^4+(q+3+q^{-1})K^3+(q+3+q^{-1})K^2$	$-4A_1+2B_1+C_1-D_1/((q+1)\sqrt{q})-q\sqrt{q}E_1/(q+1)$
	$+(q+3+q^{-1})K+1$	
	$-[K^4+(q-1+q^{-1})K^3-(q-1+q^{-1})K^2$	$-2(q-1)B_{-1}/(q+1)+C_{-1}-D_{-1}/((q+1)\sqrt{q})$
	$+(q-1+q^{-1})K+1]$	$-q\sqrt{q}E_{-1}/(q+1)$

[a]For S_8, there exist also four others eigenvectors $aA_1+bB_1+cC_1+dD_1+eE_1$, $\alpha A_1+\beta B_1+\gamma C_1+\delta D_1+\eta E_1$, $b'B_{-1}+c'C_{-1}+d'D_{-1}+e'E_{-1}$, $\beta'B_{-1}+\gamma'C_{-1}+\delta'D_{-1}+\eta'E_{-1}$ associated, respectively, to the eigenvalues v_1, v_2, v_1', and v_2', which have complicated forms (these results have been obtained by using a MAPLE program),

$$v_1=\tfrac{1}{2}(2K^4+3K^3(q+1+q^{-1})+K^2(q^2+2q+13+2q^{-1}+q^{-2})+3K(q+1+q^{-1})+2$$
$$+K(K^2+(q+1+q^{-1})K+1)\sqrt{q^2+2q+43+2q^{-1}+q^{-2}})$$

$$v_2=\tfrac{1}{2}(2K^4+3K^3(q+1+q^{-1})+K^2(q^2+2q+13+2q^{-1}+q^{-2})+3K(q+1+q^{-1})+2$$
$$-K(K^2+(q+1+q^{-1})K+1)\sqrt{q^2+2q+43+2q^{-1}+q^{-2}}),$$

$$v_1'=\tfrac{1}{2}(-2K^4-3K^3(q+1+q^{-1})-K^2(q^2+2q+1+2q^{-1}+q^{-2})-3K(q+1+q^{-1})-2$$
$$+K(K^2+(q+1+q^{-1})K+1)\sqrt{q^2+2q-5+2q^{-1}+q^{-2}}),$$

$$v_2'=\tfrac{1}{2}(-2K^4-3K^3(q+1+q^{-1})-K^2(q^2+2q+1+2q^{-1}+q^{-2})-3K(q+1+q^{-1})-2$$
$$-K(K^2+(q+1+q^{-1})K+1)\sqrt{q^2+2q-5+2q^{-1}+q^{-2}}), \tag{A34}$$

The sums of the eigenvalues over S_4, S_5, S_6, S_7, and S_8 are, respectively,

$$\sum_{S_4} v = K^4 + 1,$$

$$\sum_{S_5} v = 0,$$

$$\sum_{S_6} v = 4K^3 + 4K,$$

$$\sum_{S_7} v = 0,$$

$$\sum_{S_8} v = K^4 + 4K^3 + 18K^2 + 4K + 1. \tag{A35}$$

The results for $(S_9, S_{10}, S_{11}, S_{12})$ are obtained directly from the those of (S_7, S_6, S_5, S_4), respectively. Summing over all subspaces $(S_4, \ldots, S_{12})$ one obtains

$$\mathrm{Tr}(T^{(4)}(\theta)) = 2(K^4 + 1) + 2(4K^3 + 4K) + 1(K^4 + 4K^3 + 18K^2 + 4K + 1) = 3(K + 1)^4. \tag{A36}$$

APPENDIX B: $\hat{R}tt$ ALGEBRA

We present below, for $N=3$, the constraints on the blocks $t_{ij}(\theta)$ of the transfer matrix following from:

$$\hat{R}(\theta - \theta')t(\theta) \otimes t(\theta') = t(\theta') \otimes t(\theta)\hat{R}(\theta - \theta'). \tag{B1}$$

We use the notations below

$$(t(\theta), t(\theta'), K(\theta - \theta')) \equiv (t, t', K''). \tag{B2}$$

In terms of P_0' defined by Eq. (1.4) with (i,j) and (ρ_i, ρ_j) corresponding to $N=3$ and $K(\theta)$ of Eqs. (1.17) and (1.18), Eq. (B1) now is (maintaining the notation P_0' unrelated to θ, θ'),

$$(I + K''P_0')(t \otimes t') = (t' \otimes t)(I + K''P_0'), \tag{B3}$$

where

$$P_0' = q^{-1}(11) \otimes (33) + q^{-1/2}(12) \otimes (32) + (13) \otimes (31) + q^{-1/2}(21) \otimes (23) + (22) \otimes (22) + q^{1/2}(23) \otimes (21) + (31) \otimes (13) + q^{1/2}(32) \otimes (12) + q(33) \otimes (11). \tag{B4}$$

This leads to a set of 36 relations independent of K'', namely

$$t_{ij}t'_{kl} = t'_{ij}t_{kl}, \tag{B5}$$

where for $(ij) = (11), (12), (13)$, respectively,

$$(kl) = (11,12,21,22), (11,13,21,23), (12,13,22,23) \tag{B6}$$

and similarly for $(ij) = (21), (22), (23)$,

$$(kl) = (11,12,31,32),(11,13,31,33),(12,13,32,33) \tag{B7}$$

and for $(ij)=(31),(32),(33)$,

$$(kl) = (21,22,31,32),(21,23,31,33),(22,23,32,33). \tag{B8}$$

To present the K'' dependent constraints we first define

$$X_1 = q^{-1/2}t_{11}t'_{31} + t_{21}t'_{21} + q^{1/2}t_{31}t'_{11}, \quad X_2 = q^{-1/2}t_{11}t'_{32} + t_{21}t'_{22} + q^{1/2}t_{31}t'_{12},$$

$$X_3 = q^{-1/2}t_{11}t'_{33} + t_{21}t'_{23} + q^{1/2}t_{31}t'_{13}, \quad X_4 = q^{-1/2}t_{12}t'_{31} + t_{22}t'_{21} + q^{1/2}t_{32}t'_{11},$$

$$X_5 = q^{-1/2}t_{12}t'_{32} + t_{22}t'_{22} + q^{1/2}t_{32}t'_{12}, \quad X_6 = q^{-1/2}t_{12}t'_{33} + t_{22}t'_{23} + q^{1/2}t_{32}t'_{13},$$

$$X_7 = q^{-1/2}t_{13}t'_{31} + t_{23}t'_{21} + q^{1/2}t_{33}t'_{11}, \quad X_8 = q^{-1/2}t_{13}t'_{32} + t_{23}t'_{22} + q^{1/2}t_{33}t'_{12},$$

$$X_9 = q^{-1/2}t_{13}t'_{33} + t_{23}t'_{23} + q^{1/2}t_{33}t'_{13}, \tag{B9}$$

and a set

$$(Y_1, Y_2, \ldots, Y_9), \tag{B10}$$

which is obtained by transposing the indices of each term on the right of Eq. (B9) and also the order of (θ, θ'). Thus

$$Y_1 = q^{-1/2}t'_{11}t_{13} + t'_{12}t_{12} + q^{1/2}t'_{13}t_{11} \tag{B11}$$

and so on. The constraints involving K'' only through X_i are the following ones:

$$q^{1/2}(t_{11}t'_{31} - t'_{11}t_{31}) = (t_{21}t'_{21} - t'_{21}t_{21}) = q^{-1/2}(t_{31}t'_{11} - t'_{31}t_{11}) = -K''X_1,$$

$$q^{1/2}(t_{11}t'_{32} - t'_{11}t_{32}) = (t_{21}t'_{22} - t'_{21}t_{22}) = q^{-1/2}(t_{31}t'_{12} - t'_{31}t_{12}) = -K''X_2,$$

$$q^{1/2}(t_{12}t'_{31} - t'_{12}t_{31}) = (t_{22}t'_{21} - t'_{22}t_{21}) = q^{-1/2}(t_{32}t'_{11} - t'_{32}t_{11}) = -K''X_4,$$

$$q^{1/2}(t_{12}t'_{33} - t'_{12}t_{33}) = (t_{22}t'_{23} - t'_{22}t_{23}) = q^{-1/2}(t_{32}t'_{13} - t'_{32}t_{13}) = -K''X_6,$$

$$q^{1/2}(t_{13}t'_{32} - t'_{13}t_{32}) = (t_{23}t'_{22} - t'_{23}t_{22}) = q^{-1/2}(t_{33}t'_{12} - t'_{33}t_{12}) = -K''X_8,$$

$$q^{1/2}(t_{13}t'_{33} - t'_{13}t_{33}) = (t_{23}t'_{23} - t'_{23}t_{23}) = q^{-1/2}(t_{33}t'_{13} - t'_{33}t_{13}) = -K''X_9. \tag{B12}$$

There are six corresponding sets involving K'' only through Y_i. As for Eq. (B11) they are obtained by transposing indices in the first three terms of each equation of Eq. (B12) and changing the sign before K''. Thus

$$q^{1/2}(t_{11}t'_{13} - t'_{11}t_{13}) = (t_{12}t'_{12} - t'_{12}t_{12}) = q^{-1/2}(t_{13}t'_{11} - t'_{13}t_{11}) = K''Y_1 \tag{B13}$$

and so on.

Finally there is a set involving K'' through both X_i, and Y_i,

$$(t_{11}t'_{33} - t'_{11}t_{33}) = -K''q^{-1/2}(X_3 - Y'_3),$$

$$(t_{12}t'_{32} - t'_{12}t_{32}) = -K''(q^{-1/2}X_5 - Y'_3),$$

$$(t_{13}t'_{31} - t'_{13}t_{31}) = -K''(q^{-1/2}X_7 - q^{1/2}Y'_3),$$

$$(t_{21}t'_{23} - t'_{21}t_{23}) = -K''(X_3 - q^{-1/2}Y'_5),$$

$$(t_{22}t'_{22} - t'_{22}t_{22}) = -K''(X_5 - Y'_5),$$

$$(t_{23}t'_{21} - t'_{23}t_{21}) = -K''(X_7 - q^{1/2}Y'_5),$$

$$(t_{31}t'_{13} - t'_{31}t_{13}) = -K''(q^{1/2}X_3 - q^{-1/2}Y'_7),$$

$$(t_{32}t'_{12} - t'_{32}t_{12}) = -K''(q^{1/2}X_5 - Y'_7),$$

$$(t_{33}t'_{11} - t'_{33}t_{11}) = -K''q^{1/2}(X_7 - Y'_7). \tag{B14}$$

An alternative approach to the $\hat{R}tt$ relations is via the diagonalization of P'_0. The diagonalizer is given in Ref. 13. Such an approach was presented for our multiparameter ("nested-sequence") class in Appendix C of Ref. 3.

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Localization at low temperature and infrared bounds

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We consider a class of classical lattice spin systems, with $\mathbb{R}^n$-valued spins and two-body interactions. Our main result states that the associated Gibbs measure localizes in certain cylindrical neighborhoods of the global minima of the unperturbed Hamiltonian. As an application we establish existence of a first order phase transition at low temperature, for a reflection positive mexican hat model on $\mathbb{Z}^d$, $d \geqslant 3$, with a nonferromagnetic interaction. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2364180]

I. ASSUMPTIONS AND MAIN RESULT

Let $n \in \mathbb{N}$ and Λ be a finite set. Elements of Λ are denoted by x, y, and z. We pick and fix one element $o \in \Lambda$ which plays the distinguished role of an origin. We write $\Omega = (\mathbb{R}^n)^\Lambda$ for the vector space of spin configurations $\varphi = \{\varphi_x\}_{x \in \Lambda}$ over Λ, where $\varphi_x \in \mathbb{R}^n$. We use the symbols ψ and φ for elements of Ω. The letters u and v are used for vectors in $\mathbb{R}^n$, and $|u|$ denotes the Euclidean norm of u. It is assumed that Λ comes equipped with a metric ρ which satisfies

$$\max_{x \in \Lambda} \sum_{y \in \Lambda} e^{-\rho(x,y)} \leqslant C_\rho < \infty . \tag{1.1}$$

We study a Hamiltonian function $H_\Lambda \in C^1(\Omega; \mathbb{R})$ of the form

$$H_\Lambda(\varphi) = \sum_{x \in \Lambda} f_x(\varphi_x) + J \sum_{x,y \in \Lambda, x \neq y} w_{xy}(\varphi_x, \varphi_y).$$

The self-energies $\{f_x\}_{x \in \Lambda}$ and the interactions $\{w_{xy}\}_{x,y \in \Lambda, x \neq y}$ should satisfy assumptions specified in the following Conditions (1.1) and (1.2), respectively.

We introduce some notation. We write $\partial_{|u|} = |u|^{-1} u \cdot \nabla_u$ for the radial derivative with respect to the $\mathbb{R}^n$-valued variable u, and $B_r(u) := \{v \in \mathbb{R}^n \,|\, |u - v| \leqslant r\}$, for the closed ball of radius r and centered at u.

Condition 1.1. *There are positive constants $R, c_f, C_f > 0$ such that the family $\{f_x\}_{x \in \Lambda}$ of functions $f_x \in C^1(\mathbb{R}^n; \mathbb{R})$ satisfy (i)–(iv) as follows*:

(i) $f_x \geqslant 0$ *and* $\min_{u \in \mathbb{R}^n} f_x(u) = 0$.
(ii) *The set* $\mathcal{G}_0 := \{u \in \mathbb{R}^n \,|\, f_o(u) = 0\}$ *of global minima satisfies* $\mathcal{G}_0 \subset B_R(0)$.
(iii) *For all* $x \in \Lambda$ *and* $u \in \mathbb{R}^n$, *with* $|u| \geqslant R$, *we have* $\partial_{|u|} f_x(u) \geqslant c_f$.
(iv) *For all* $x, y \in \Lambda$ *and* $u, v \in \mathbb{R}^n$, *with* $|v| \geqslant |u| \geqslant R$, *we have*

$$\partial_{|u|} f_x(u) \leqslant C_f \partial_{|v|} f_y(v).$$

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For $j \in \{1,2\}$, we write $\nabla_j w_{xy}$ for the gradient of w_{xy} with respect to the jth variable. The w_{xy}'s are required to be dominated by the f_x's, as specified by the next condition

Condition 1.2. *There exist constants* $C_a^\rho > 0$ *and* $\{a_{xy}\}_{x,y\in\Lambda}$, *with* $a_{xy}=a_{yx}\geqslant 0$, $a_{xx}=0$, *and*

$$\max_{x\in\Lambda}\left\{\sum_{y\in\Lambda} a_{xy}e^{\rho(x,y)}\right\} \leqslant C_a^\rho, \tag{1.2}$$

such that the family $\{w_{xy}\}_{x,y\in\Lambda}$ *of functions* $w_{xy}\in C^1(\mathbb{R}^n\times\mathbb{R}^n;\mathbb{R})$, *with* $w_{xx}\equiv 0$, *obeys the following bounds*:

$$\max\{|\nabla_1 w_{xy}(u,v)|,|\nabla_2 w_{xy}(u,v)|\} \leqslant a_{xy}(1+\mathbb{1}_{[|u|\geqslant 4R]}\partial_{|u|}f_x(u)+\mathbb{1}_{[|v|\geqslant 4R]}\partial_{|v|}f_y(v)). \tag{1.3}$$

Equation (1.2) expresses exponential decay of the interaction with respect to the metric ρ. Let $C_a^0 \leqslant C_a^\rho$ be such that

$$\max_{x\in\Lambda}\left\{\sum_{y\in\Lambda} a_{xy}\right\} \leqslant C_a^0. \tag{1.4}$$

For polynomially bounded, measurable functions $u:\Omega\to\mathbb{C}$, we use the following notation for expectations with respect to the Gibbs state in finite volume Λ and inverse temperature β:

$$\mathbb{E}_\Lambda[u] := \mathcal{Z}_\Lambda^{-1}\int_\Omega u(\varphi)e^{-\beta H_\Lambda(\varphi)}d^\Lambda\varphi. \tag{1.5}$$

Here $\mathcal{Z}_\Lambda=\int_\Omega e^{-\beta H_\Lambda(\varphi)}d^\Lambda\varphi$ is the partition function. For the integral in Eq. (1.5) to exist under Conditions 1.1 and 1.2, we require $|J|<\Gamma_0^{-1}$, where

$$\Gamma_0 := 2C_a^0(1+C_f+c_f^{-1}). \tag{1.6}$$

See Lemma A.1. We note that for many examples, including the example in Sec. II, the f_x's grow at a faster rate than the w_{xy}'s such that no assumption on $|J|$ is needed to make polynomially bounded observables integrable. For the probability of a (measurable) event $\mathcal{A}\subset\Omega$, we write

$$\mathbb{P}_\Lambda[\mathcal{A}] := \mathbb{E}_\Lambda[\mathbb{1}_\mathcal{A}].$$

For $\zeta>0$, we introduce level sets for f_o,

$$\mathcal{G}_\zeta := \{u\in\mathbb{R}^n | f_o(u)\leqslant\zeta\}.$$

We are now ready to formulate the main result of the paper.

Theorem 1.1. *Assume Eq. (1.1). Let* $\{f_x\}_{x\in\Lambda}$ *satisfy Condition 1.1 and* $\{w_{xy}\}_{x,y\in\Lambda}$ *satisfy Condition 1.2. Let*

$$\Gamma_1 := 4RC_a^0\left(\tfrac{1}{3}C_\rho+3\right),\quad \Gamma_2=\Gamma_0+\tfrac{102}{5}C_a^\rho,\quad \Gamma_3 := \tfrac{2}{3}c_fR, \tag{1.7}$$

and

$$J_0 := \Gamma_3\min\left\{\frac{3}{4\Gamma_1},\frac{1}{\Gamma_1+\Gamma_2\Gamma_3}\right\}. \tag{1.8}$$

For $|J|<J_0$, $\beta>0$ *and* $\delta>2|J|\Gamma_1$, *we have*

$$\mathbb{P}_\Lambda[\{\varphi\in\Omega|\varphi_o\notin\mathcal{G}_\delta\}] \leqslant Ce^{-\beta\sigma}, \tag{1.9}$$

where

$$C = 2\max\left\{\left[\frac{4R}{\min\left\{\delta,\frac{3}{2}\Gamma_3\right\}}\sup_{|u|\leqslant 2R}|\nabla f_o(u)|\right]^n,\left(\frac{3}{5}\right)^n\right\}e^{nC_\rho/2}, \tag{1.10}$$

and σ is a strictly positive constant given by

$$\sigma = \min\left\{\tfrac{1}{2}\delta, \tfrac{3}{4}\Gamma_3, \Gamma_3(1-|J|\Gamma_2)\right\} - |J|\Gamma_1. \tag{1.11}$$

Remark 1.2.

(1) We stress that the constants J_0, $\{\Gamma_j\}_{j=1,2,3}$, C, and σ, only depend on ρ, $\{f_x\}_{x\in\Lambda}$ and $\{w_{xy}\}_{x,y\in\Lambda}$ through the constants C_ρ, c_f, C_f, R, C_a^0, and C_a^ρ. In particular, they are independent of Λ and the choice of origin o.

(2) The set of φ's with $\varphi_o \in \mathcal{G}_\delta$ is a cylinder set containing the global minima of the unperturbed (that is, $J=0$) Hamiltonian. The condition $\delta > 2|J|\Gamma_1$, ensures that the global minima of the perturbed Hamiltonian remain contained in this cylinder set.

(3) The proof goes through without modifications if $\mathbb{R}^n$ is replaced by a convex subset thereof containing 0.

(4) A choice was made here to present the method for a class of Hamiltonians without any special symmetry. For models with $O(n)$ symmetry, like the example discussed in Sec. II, one can tweak the proof to get better constants.

(5) The restriction to two-body interactions is made for simplicity. The method extends to models with many-body interactions.

The derivation of the bound Eq. (1.9) follows a scheme used in Ref. 1, Sec. 3, to derive low temperature localization bounds for models with a unique global minimum at 0. The method developed in Ref. 1 was in turn inspired by work going back to Sjöstrand,[2] see also Refs. 3 and 4. The common idea in the papers cited in this paragraph is to systematically shift points in the set of φ's with $\varphi_o \notin \mathcal{G}_\delta$, towards the global mimima and measure the resulting decrease in energy. In this paper and in Ref. 1 the shift is implemented by a single transformation T, with the property that $\inf_{\varphi,\varphi_o\notin\mathcal{G}_\delta}[H(\varphi)-H(T(\varphi))] \geqslant \sigma > 0$. It is this σ which contributes to the exponential localization in Eq. (1.9). In the papers[2–4] the idea is slightly different: The configuration space is cut up into pieces, each of which is translated into a neighborhood of a unique global minimum, and the contributions are then summed up. We remark that in Ref. 4, the interaction does not shift the global minimum away from 0, which makes it possible to localize arbitrarily close to 0 while keeping the coupling constant J fixed (see Remark 1.2 (2)).

II. MOTIVATING EXAMPLE

Let $\Lambda =]-L,L]^d \cap \mathbb{Z}^d$, be the d-dimensional hypercubic lattice of sidelength $2L$, for some $d \geqslant 3$ and $L \in \mathbb{N}$. We view Λ as the torus $\mathbb{Z}^d/2L\mathbb{Z}^d$, equipped with the metric $\rho(x,y) = \min_{z\in\mathbb{Z}^d}|x-y-2Lz|_1$, where $|z|_p$, is the p-norm of $z \in \mathbb{R}^d$. As self-energies we take

$$f_x(u) = |u|^4 - 2|u|^2 + 1, \tag{2.1}$$

and as interaction we take

$$w_{xy}(u,v) = -\mathcal{J}_\Lambda(x-y)u\cdot v, \tag{2.2}$$

where $\mathcal{J}_\Lambda$ is periodic and defined from an underlying interaction $\mathcal{J} \in \ell^1(\mathbb{Z}^d;\mathbb{R})$ by

$$\mathcal{J}_\Lambda(x) := \sum_{y\in\mathbb{Z}^d} \mathcal{J}(x+2Ly). \tag{2.3}$$

In general, one should take a reflection positive interaction, with respect to a suitable reflection, in order to get an infrared bound. Here we specialize to the following example:

$$\mathcal{J}(x) := \begin{cases} 1, & |x|_2 = 1, \\ -b, & |x|_2 = \sqrt{2}. \end{cases} \tag{2.4}$$

In order to obtain a reflection positive interaction, we impose the restriction

$$J > 0, \quad 0 < b < \frac{1}{2(d-1)}.$$

Note that the ferromagnetic case $-b \geqslant 0$, can be treated by methods already established. We introduce the correlation function $F_\Lambda : \Lambda \to \mathbb{R}$ by

$$F_\Lambda(x) := \mathbb{E}_\Lambda[\varphi_0 \cdot \varphi_x].$$

Let $\Lambda^* =]-\pi, \pi]^d \cap (\pi/L)\mathbb{Z}^d$ be the dual lattice and $\hat{F}_\Lambda : \Lambda^* \to \mathbb{R}$ the Fourier transform of F_Λ. That is, $\hat{F}_\Lambda(\xi) = \Sigma_{x\in\Lambda} \exp(-ix\cdot\xi) F_\Lambda(x)$. Similarly, for $\xi \in \Lambda^*$,

$$\hat{\mathcal{J}}_\Lambda(\xi) = \hat{\mathcal{J}}(\xi) = 2a \sum_{j=1}^{d} \cos(\xi_j) - 4b \sum_{1\leqslant i<j\leqslant d} \cos(\xi_i)\cos(\xi_j)$$

is the Fourier transform of $\mathcal{J}_\Lambda$. Here $\hat{\mathcal{J}}(\xi) = \Sigma_{x\in\mathbb{Z}^d} e^{-ix\cdot\xi} \mathcal{J}(x)$. The model defined by Eqs. (2.1) and (2.4) is translation invariant and reflection positive, cf. Refs. 5 and 6, and hence, it satisfies an infrared bound of the form

$$0 \leqslant \hat{F}_\Lambda(\xi) \leqslant \frac{n}{J\beta} (\hat{\mathcal{J}}(0) - \hat{\mathcal{J}}(\xi))^{-1}, \tag{2.5}$$

for $\xi \in \Lambda^* \setminus \{0\}$. Here n is the dimension of the single spin space. For a proof of this bound see [Ref. 6, Proposition 20.12]. See Ref. 7 for a discussion of the critical case, where $2(d-1)b = 1$.

As usual, Eq. (2.5) implies that

$$\begin{aligned}\mathbb{E}_\Lambda[\varphi_0 \cdot \varphi_x] &= \mathbb{E}_\Lambda[|\varphi_0|^2] + F_\Lambda(x) - F_\Lambda(0) \\ &= \mathbb{E}_\Lambda[|\varphi_0|^2] + \frac{1}{|\Lambda|} \sum_{\xi\in\Lambda^*} (e^{ix\cdot\xi} - 1)\hat{F}_\Lambda(\xi) \geqslant \mathbb{E}_\Lambda[|\varphi_0|^2] - \frac{2n}{J\beta|\Lambda|} \sum_{\xi\in\Lambda^*\setminus\{0\}} (\hat{\mathcal{J}}(0) - \hat{\mathcal{J}}(\xi))^{-1}.\end{aligned} \tag{2.6}$$

Note that $\hat{\mathcal{J}}(0) = \hat{\mathcal{J}}(\xi)$ if, and only if, $\xi = 0$, and

$$\hat{\mathcal{J}}(0) - \hat{\mathcal{J}}(\xi) \sim (1 - 2(d-1)b)\xi^2,$$

near $\xi = 0$. In dimension $d \geqslant 3$ this implies the existence of a first order phase transition at low temperature (large β), provided one can verify the following moment inequality:

$$\mathbb{E}_\Lambda[|\varphi_0|^2] \geqslant c > 0. \tag{2.7}$$

Here c should be independent of L. The estimate Eq. (2.6) then says that a (necessarily translation invariant) limit state $\mathbb{E}_\infty = \mathrm{w}-\lim_{\Lambda\to\mathbb{Z}^d} \mathbb{E}_\Lambda$ is not ergodic, hence, not a pure phase. See Refs. 5, 8, and 9 and in particular Ref. 6, Theorem 20.15, for a reference dealing with possibly unbounded spins. For models constrained to the unit sphere (or in general to closed subsets of $\mathbb{R}^n$ not containing 0) the bound Eq. (2.7) is trivial.

If $\mathcal{J}(x) \geqslant 0$, for all x, i.e., the model is ferromagnetic, there are two general methods one can use to verify Eq. (2.7) for models with interaction of the type Eq. (2.2). If $n = 1$ one can use the FKG inequalities,[10] which imply monotonicity of the second moment in $\mathcal{J}(x)$ (for any fixed x). This can be used to reduce the moment inequality to a one-dimensional problem which can be analyzed explicitly. See Ref. 11 for a discussion of this idea. Another argument applies under the additional assumption of reflection positivity of the interaction Eq. (2.2). Then the so-called chessboard estimate (Ref. 6, Chap. 17.1) applies (a key ingredient in the proof of Eq. (2.5) and the reason for the choice of a reflection positive model as our example). The chessboard estimate together with ferromagnetism, i.e., positivity of $\mathcal{J}$, also leads to a moment inequality; no restrictions on n are needed. See. Ref. 6, Lemma 20.8.

If the interaction is not ferromagnetic there seems to be no method available in the literature to deal with the innocuous looking moment inequality Eq. (2.7). This is where our main result comes in. Clearly, Theorem 1.1 gives explicit J_0 and α_0 such that, for $0<J<J_0$ and $J\beta>\alpha_0$, we have $\mathbb{E}_\Lambda[|\varphi_0|^2]\geqslant c>0$, for an equally explicit constant c. Here one should take $0<\delta<1$, such that $\mathcal{G}_\delta$ is an annulus. Moreover, as opposed to the methods of the preceding paragraph, Theorem 1.1 is robust and does not rely on correlation inequalities or indeed on any nontrivial properties of the underlying Gibbs measure. We have thus extended the applicability of Georgii's result (Ref. 6, Theorem 20.15) to interactions $\mathcal{J}$, which need not be ferromagnetic. (Recall that Georgii in this case requires the single spin space to be bounded away from 0, cf. Ref. 6, Comments 20.18 (3)).

For the above concrete model, we estimated the constant J_0, fixed a $J<J_0$ and estimated σ and C, for which the bound Eq. (1.9) is valid. As for J_0 we got $J_0\sim 10^{-4}$, which seems small, but is in fact only a factor of 10 smaller than Γ_0^{-1}. Recall that Γ_0^{-1} was the upper limit for coupling strengths such that all models satisfying the conditions, with the same constants, are well-defined. This also serves to illustrate Remark 1.2 (4). We then took $J=10^{-4}/2$ and found $\sigma\sim 1/20$ and $C\sim e^{60}$. To get a probability less than 1 in Eq. (1.9), one has to take $\beta>\beta_0$ with $\beta_0\sim 1200$. We note that we did not try to optimize carefully over possible choices of metric and the constant R. (For R we chose $R=1.03$. For the metric we chose $\kappa\rho$, with $\kappa=\ln(2)$. Here ρ is the metric given at the beginning of this section.)

III. TRANSFORMATION T^ζ

The purpose of this section is to construct a transformation of the space Ω, and estimate its Jacobian.

We begin by analyzing the size of the level sets $\mathcal{G}_\zeta$. Let $\zeta\geqslant 0$ and $u\in\mathbb{R}^n$ be such that $|u|>2\zeta c_f^{-1}+R$, where the constants c_f and R are taken from Condition 1.1. Let $u':=Ru/|u|$, and for $0\leqslant t\leqslant 1$,

$$u_t := tu+(1-t)u' = \left(\frac{R}{|u|}+t\left(1-\frac{R}{|u|}\right)\right)u.$$

Then, using that $\dot{u}_t/|\dot{u}_t|=u_t/|u_t|$, we estimate

$$f_o(u)\geqslant f_o(u)-f_o(u')=\int_0^1 \dot{u}_t\cdot\nabla f_o(u_t)dt=(|u|-R)\int_0^1(\partial_{|u|}f_o)(u_t)dt\geqslant 2\zeta c_f^{-1}\int_0^1 c_f dt=2\zeta.$$

This implies that

$$\mathcal{G}_{2\zeta}\subset B_{R+2\zeta c_f^{-1}}(0). \tag{3.1}$$

We shall henceforth assume that $0<\zeta\leqslant(1/2)c_fR$, which is equivalent to

$$R<R_\zeta := R+\frac{2\zeta}{c_f}\leqslant 2R. \tag{3.2}$$

We introduce the size r_ζ, of the largest ball contained in $\mathcal{G}_\zeta$;

$$r_\zeta := \sup\{r\geqslant 0\,|\,\exists\, u\in\mathcal{G}_\zeta\colon B_r(u)\subset\mathcal{G}_\zeta\}. \tag{3.3}$$

Fix an $\eta_\zeta\in\mathcal{G}_\zeta$, for which $B_{r_\zeta}(\eta_\zeta)\subset\mathcal{G}_\zeta$. Such an η_ζ exists by the choice Eq. (3.3) of r_ζ. By Eq. (3.1) we get a bound from below on r_ζ,

$$r_\zeta\geqslant \operatorname{dist}(\mathcal{G}_\zeta^c,\mathcal{G}_0)=\operatorname{dist}(B_{R_\zeta}(0)\cap\mathcal{G}_\zeta^c,\mathcal{G}_0).$$

Let $u\in\mathcal{G}_0$ and $v\in B_{R_\zeta}(0)\cap\mathcal{G}_\zeta^c$. Then

$$\zeta \leqslant f_o(v) - f_o(u) \leqslant |v-u| \sup_{u \in B_{R_\zeta}(0)} |\nabla f_o(u)|.$$

This implies

$$r_\zeta \geqslant \frac{\zeta}{\sup_{u \in B_{R_\zeta}(0)} |\nabla f_o(u)|}. \tag{3.4}$$

We pick a function $\theta \in C^\infty(\mathbb{R};[0,1])$ with $\theta \equiv 0$ on $(-\infty, 1/2]$, $\theta \equiv 1$ on $[1,\infty)$, and $\theta' \geqslant 0$. Note that $\mathrm{supp}(\theta') \subset (1/2,1)$.

The final input is a family of scaling factors $\{\epsilon_x\}_{x \in \Lambda}$. We choose them to be of the form

$$\epsilon_x := \epsilon_o e^{-\rho(x,o)}. \tag{3.5}$$

Here ϵ_o is chosen such that

$$0 < \epsilon_o < \tfrac{1}{2}(1 + \|\theta'\|_\infty)^{-1}, \tag{3.6}$$

where $\|\theta'\|_\infty = \max_{t \in [1/2,1]} |\theta'(t)| > 2$. (We will optimize over ϵ_o and θ in Sec. VI.)

We define a transformation $T^\zeta : \Omega \to \Omega$ as follows: $(T^\zeta(\varphi))_x := T^\zeta_x(\varphi_x)$ and

$$\forall x \neq o : T^\zeta_x(u) := \left(1 - \epsilon_x \theta\left(\frac{|u|}{4R}\right)\right) u, \tag{3.7}$$

$$T^\zeta_o(u) := \begin{cases} (1-\epsilon_o)u, & |u| \geqslant 4R, \\ \left(\dfrac{r_\zeta}{4R}\right) u + \eta_\zeta, & |u| < 4R. \end{cases} \tag{3.8}$$

The transformation T^ζ is not a global diffeomorphism, but we work below in the sectors $\{\varphi : |\varphi_o| < 4R\}$ and $\{\varphi : |\varphi_o| > 4R\}$ separately, and T^ζ restricted to these sectors is a smooth transformation.

We end this section with an estimate on the determinant of $\mathrm{Jac}(T^\zeta)$, the Jacobian of T^ζ.

Lemma 3.1 Let T^ζ be the transformation defined in (3.7) and (3.8). We have the bound

$$|\det \mathrm{Jac}(T^\zeta)(\varphi)| \geqslant \min\left\{ \frac{\zeta}{4R \sup_{|u| \leqslant R_\zeta} |\nabla f_o(u)|}, 1 - \epsilon_o \right\}^n \exp[-n\epsilon_o(1 + \|\theta'\|_\infty) C_\rho], \tag{3.9}$$

for all $\varphi \in \Omega$, with $|\varphi_o| \neq 4R$.

Proof: The Jacobian of T^ζ (away from $|\varphi_o| = 4R$) is a block diagonal matrix with $n \times n$ blocks given by

$$\forall x \neq o : \mathrm{Jac}(T^\zeta)_{xx}(\varphi) = \left(1 - \epsilon_x \theta\left(\frac{|\varphi_x|}{4R}\right)\right) I_n - \frac{\epsilon_x |\varphi_x}{4R} \theta'\left(\frac{|\varphi_x|}{4R}\right) P_{\varphi_x},$$

$$\mathrm{Jac}(T^\zeta)_{oo}(\varphi) = \begin{cases} (1-\epsilon_o) I_n, & |\varphi_o| > 4R, \\ \left(\dfrac{r_\zeta}{4R}\right) I_n, & |\varphi_o| < 4R. \end{cases}$$

Here I_n is the identity matrix in $\mathbb{R}^n$, and $P_u := |u|^{-2} |u\rangle\langle u|$, is the orthogonal projection onto $\mathrm{span}\{u\}$, for $u \in \mathbb{R}^n \setminus \{0\}$.

Note that, for $x \neq o$,

$$\frac{\epsilon_x|\varphi_x|}{4R}\theta'\left(\frac{|\varphi_x|}{4R}\right)P_{\varphi_x} \leqslant \epsilon_x\|\theta'\|_\infty I_n.$$

Using this observation, we estimate the determinant of the Jacobian as follows:

$$\text{for } |\varphi_o| < 4R: |\text{detJac}(T^\zeta)(\varphi)| \geqslant \left[\frac{r_\zeta}{4R}\prod_{x(\neq o)}\{1-\epsilon_x(1+\|\theta'\|_\infty)\}\right]^n,$$

$$\text{for } |\varphi_o| > 4R: |\text{detJac}(T^\zeta)(\varphi)| \geqslant \left[(1-\epsilon_o)\prod_{x(\neq o)}\{1-\epsilon_x(1+\|\theta'\|_\infty)\}\right]^n.$$

Using the bound $\ln(1-t)\geqslant -2t$, for $0\leqslant t\leqslant 1/2$, together with Eqs. (1.1), (3.5), and (3.6), we arrive at Eq. (3.9). □

IV. ESTIMATING THE INTERACTION

In this section we estimate the effect of the transformation T^ζ on the interaction $W(\varphi)=\Sigma_{x\neq y}w_{xy}(\varphi_x,\varphi_y)$. We prove the following lemma which is the central technical step in the proof of Theorem 1.1. The constant Γ_0 below is defined in Eq. (1.6).

Lemma 4.1: For $0<\zeta\leqslant c_f R/2$, we have, for all $\varphi\in\Omega$, the bound

$$|W(\varphi)-W(T^\zeta(\varphi))| \leqslant C_W^1 + C_W^2\sum_{x\in\Lambda}\mathbb{1}_{[|\varphi_x|\geqslant 4R]}(f_x(\varphi_x)-f_x(T_x^\zeta(\varphi_x))), \tag{4.1}$$

where

$$C_W^1 := 4RC_a^0(2\epsilon_o C_\rho+3), \quad C_W^2 := \Gamma_0 + C_a^\rho(3\epsilon_o^{-1}+2(1-\epsilon_o)^{-1}). \tag{4.2}$$

Proof: Let $\varphi\in\Omega$, $x,y\in\Lambda$ with $x\neq y$. For $z\in\{x,y\}$ we abbreviate $u_z(t)=t\varphi_z+(1-t)T_z^\zeta(\varphi_z)$.

Using the fundamental theorem of calculus, together with Condition 1.2, we estimate

$$\begin{aligned}
&|w_{xy}(\varphi_x,\varphi_y)-w_{xy}((T^\zeta(\varphi))_x,(T^\zeta(\varphi))_y)|\\
&\quad=\left|\int_0^1\{(\varphi_x-T_x^\zeta(\varphi_x))\cdot\nabla_1 w_{xy}(u_x(t),u_y(t))+(\varphi_y-T_y^\zeta(\varphi_y))\cdot\nabla_2 w_{xy}(u_x(t),u_y(t))\}dt\right|\\
&\quad\leqslant a_{xy}(|\varphi_x-T_x^\zeta(\varphi_x)|+|\varphi_y-T_y^\zeta(\varphi_y)|)\left[1+\int_0^1\{\mathbb{1}_{[|u_x(t)|\geqslant 4R]}(\partial_{|u|}f_x)(u_x(t))\right.\\
&\quad\left.+\mathbb{1}_{[|u_y(t)|\geqslant 4R]}(\partial_{|u|}f_y)(u_y(t))\}dt\right]\\
&\quad= a_{xy}(S_1^x(\varphi)+S_1^y(\varphi)+S_2^{xy}(\varphi)+S_2^{yx}(\varphi)),
\end{aligned}\tag{4.3}$$

where

$$S_1^z(\varphi)=|\varphi_z-T_z^\zeta(\varphi_z)|\left[1+\int_0^1\mathbb{1}_{[|u_z(t)|\geqslant 4R]}(\partial_{|u|}f_z)(u_z(t))dt\right],$$

$$S_2^{zz'}(\varphi)=|\varphi_z-T_z^\zeta(\varphi_z)|\int_0^1\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]}(\partial_{|u|}f_{z'})(u_{z'}(t))dt.$$

We proceed to estimating $S_1^z(\varphi)$ and $S_2^{zz'}(\varphi)$, for all $\varphi\in\Omega$.

To estimate S_1^z we recall Eq. (3.7), and observe the bound

$$|\varphi_z - T_z^\zeta(\varphi_z)| \leqslant \epsilon_z |\varphi_z|, \tag{4.4}$$

which holds true if $z \neq o$, or $z=o$ and $|\varphi_o| \geqslant 4R$. To deal with the complementary case, where $z=o$ and $|\varphi_o| < 4R$, we note that in this case Eq. (3.8) implies $|T_o^\zeta(\varphi_0)| \leqslant R_\zeta \leqslant 2R$, and hence,

$$|u_o(t)| < 4R \quad \text{and} \quad |\varphi_o - T_o^\zeta(\varphi_o)| \leqslant 6R. \tag{4.5}$$

Combining Eqs. (4.4) and (4.5) yields for all z and $\varphi \in \Omega$,

$$S_1^z(\varphi) \leqslant 6R\delta_{zo} + \epsilon_z|\varphi_z|\left[1 + \int_0^1 \mathbb{1}_{[|u_z(t)|\geqslant 4R]}(\partial_{|u|}f_z)(u_z(t))dt\right]. \tag{4.6}$$

Here we used that $|\varphi_o| \geqslant 4R$ on the support of $\mathbb{1}_{[|u_o(t)|\geqslant 4R]}$.

As for $S_2^{zz'}$ we split Ω into two regions

$$\Omega_{\mathrm{I}}^{zz'} := \{\varphi \in \Omega \,||\varphi_z| \geqslant |\varphi_{z'}|/(1-\epsilon_z)\} \quad \text{and} \quad \Omega_{\mathrm{II}}^{zz'} = \Omega \setminus \Omega_{\mathrm{I}}^{zz'}.$$

From Condition 1.1 (iv) we get the bound

$$\mathbb{1}_{[\varphi\in\Omega_{\mathrm{I}}^{zz'}]}\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]}(\partial_{|u|}f_{z'})(u_{z'}(t)) \leqslant C_f \mathbb{1}_{[|u_z(t)|\geqslant 4R]}(\partial_{|u|}f_z)(u_z(t)), \tag{4.7}$$

because on the support of the indicator functions we have

$$|u_z(t)| \geqslant (1-\epsilon_z)|\varphi_z| \geqslant |\varphi_{z'}| \geqslant |u_{z'}(t)| \geqslant 4R.$$

Complementing Eq. (4.7) we now consider the region $\Omega_{\mathrm{II}}^{zz'}$. We obtain, for $z \neq o$, or $z=o$ and $|\varphi_o| \geqslant 4R$,

$$|\varphi_z - T_z^\zeta(\varphi_z)|\mathbb{1}_{[\varphi\in\Omega_{\mathrm{II}}^{zz'}]}\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]} \leqslant \frac{\epsilon_z}{1-\epsilon_z}|\varphi_{z'}|\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]}. \tag{4.8}$$

Here Eq. (4.4) was used. We note that, for $|\varphi_o| \leqslant 4R$, we have from Eq. (4.5),

$$|\varphi_o - T_o^\zeta(\varphi_o)|\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]} \leqslant 6R\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]} \leqslant \tfrac{3}{2}|\varphi_{z'}|\mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]}. \tag{4.9}$$

Combining Eqs. (4.7)–(4.9) yields for $z \neq z'$ and $\varphi \in \Omega$,

$$S_2^{zz'}(\varphi) \leqslant \epsilon_z|\varphi_z|C_f\int_0^1 \mathbb{1}_{[|u_z(t)|\geqslant 4R]}(\partial_{|u|}f_z)(u_z(t))dt + \epsilon_{z'}|\varphi_{z'}|\left\{\frac{\epsilon_z}{(1-\epsilon_z)\epsilon_{z'}} + \frac{3}{2\epsilon_{z'}}\delta_{oz}\right\}\int_0^1 \mathbb{1}_{[|u_{z'}(t)|\geqslant 4R]}$$
$$\times(\partial_{|u|}f_{z'})(u_{z'}(t))dt. \tag{4.10}$$

Inserting the bounds Eqs. (4.6) and (4.10) into Eq. (4.3), we get the following estimate for all $x \neq y$ and $\varphi \in \Omega$:

$$\begin{aligned}
&|w_{xy}(\varphi_x,\varphi_y) - w_{xy}((T^\zeta(\varphi))_x,(T^\zeta(\varphi))_y)| \\
&\quad\leqslant a_{xy}\epsilon_x|\varphi_x|\left(1 + \left\{1 + C_f + \frac{3}{2\epsilon_x}\delta_{yo} + \frac{\epsilon_y}{(1-\epsilon_y)\epsilon_x}\right\}\int_0^1 \mathbb{1}_{[|u_x(t)\geqslant 4R]}(\partial_{|u|}f_x)(u_x(t))dt\right) \\
&\qquad + a_{xy}\epsilon_y|\varphi_y|\left(1 + \left\{1 + C_f + \frac{3}{2\epsilon_y}\delta_{xo} + \frac{\epsilon_x}{(1-\epsilon_x)\epsilon_y}\right\}\int_0^1 \mathbb{1}_{[|u_y(t)\geqslant 4R]}(\partial_{|u|}f_y)(u_y(t))dt\right) \\
&\qquad + a_{xy}6R(\delta_{xo} + \delta_{yo}).
\end{aligned} \tag{4.11}$$

Observe that

$$|\varphi_x| \geqslant |u_x(t)| \geqslant 4R \text{ implies } T_x^\zeta(\varphi_x) = (1-\epsilon_x)\varphi_x, \tag{4.12}$$

and hence,

$$\begin{aligned}\epsilon_x|\varphi_x| \int_0^1 \mathbb{1}_{[|u_x(t)|\geqslant 4R]}(\partial_{|u|}f_x)(u_x(t))dt &\leqslant \mathbb{1}_{[|\varphi_x|\geqslant 4R]}\int_0^1 \epsilon_x|\varphi_x|(\partial_{|u|}f_x)(u_x(t))dt \\ &= \mathbb{1}_{[|\varphi_x|\geqslant 4R]}\int_0^1 \left(\frac{d}{dt}[f_x(u_x(t))]\right)dt = \mathbb{1}_{[|\varphi_x|\geqslant 4R]}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x))).\end{aligned} \tag{4.13}$$

As an application we get the bound, cf. Condition I.1 (iii) and Eq. (4.12),

$$\epsilon_x|\varphi_x| = \epsilon_x|\varphi_x|\mathbb{1}_{[|\varphi_z|<4R]} + \epsilon_x|\varphi_x|\mathbb{1}_{[|\varphi_x|\geqslant 4R]} \leqslant \epsilon_x 4R\mathbb{1}_{[|\varphi_x|<4R]} + c_f^{-1}\mathbb{1}_{[|\varphi_x|\geqslant 4R]}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x))). \tag{4.14}$$

Inserting Eqs. (4.13) and (4.14) into Eq. (4.11) we get, for $\varphi \in \Omega$,

$$\begin{aligned}|w_{xy}(\varphi_x,\varphi_y) - w_{xy}((T^\zeta(\varphi))_x,(T^\zeta(\varphi))_y)| \leqslant a_{xy}\Bigg[&\epsilon_x 4R + 6R\delta_{xo} + \left\{1 + c_f^{-1} + C_f + \frac{3}{2\epsilon_x}\delta_{yo} + \frac{\epsilon_y}{(1-\epsilon_y)\epsilon_x}\right\} \\ &\times \mathbb{1}_{[|\varphi_x|\geqslant 4R]}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x)))\Bigg] + a_{xy}\Bigg[\epsilon_y 4R + 6R\delta_{yo} \\ &+ \left\{1 + c_f^{-1} + C_f + \frac{3}{2\epsilon_y}\delta_{xo} + \frac{\epsilon_x}{(1-\epsilon_x)\epsilon_y}\right\} \\ &\times \mathbb{1}_{[|\varphi_y|\geqslant 4R]}(f_y(\varphi_y) - f_y(T_y^\zeta(\varphi_y)))\Bigg].\end{aligned}$$

We now recall Eqs. (1.1), (1.2), (1.4), and (3.5), before we sum up and obtain, for $\varphi \in \Omega$,

$$\begin{aligned}|W(\varphi) - W(T^\zeta(\varphi))| \leqslant 8\epsilon_o R C_a^0 C_\rho + 12RC_a + 2\sum_{x\in\Lambda}\Bigg\{ &C_a^0(1 + c_f^{-1} + C_f) + \tfrac{3}{2}C_a^\rho \epsilon_o^{-1} + \sum_{y\in\Lambda}\frac{a_{xy}\epsilon_y}{(1-\epsilon_o)\epsilon_x}\Bigg\} \\ &\times \mathbb{1}_{[|\varphi_x|\geqslant 4R]}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x))).\end{aligned} \tag{4.15}$$

The following bound is a consequence of Eq. (1.2) and the triangle inequality for ρ:

$$\sum_{y\in\Lambda}\frac{a_{xy}\epsilon_y}{(1-\epsilon_o)\epsilon_x} \leqslant \frac{C_a^\rho}{1-\epsilon_o}. \tag{4.16}$$

See also the proof of Ref. 1, Lemma 3.2.

From Eqs. (4.15) and (4.16) we conclude the lemma with the constants given in Eq. (4.2). □

V. ESTIMATING THE HAMILTONIAN

Lemma 5.1: Let $0 < \zeta \leqslant c_f R/2$, $|J| < \tilde{J}_0(\zeta)$, and

$$\sigma_T^\zeta := \min\{\zeta, 4\epsilon_o c_f R(1 - |J|C_W^2)\} - |J|C_W^1, \tag{5.1}$$

where

$$\tilde{J}_0(\zeta) := \min\left\{\frac{\zeta}{C_W^1}, \frac{4\epsilon_o c_f R}{C_W^1 + 4\epsilon_o c_f R C_W^2}\right\}. \tag{5.2}$$

Then, for all $\varphi \in \Omega$, with $\varphi_o \notin \mathcal{G}_{2\zeta}$, we have the bound

$$H_\Lambda(\varphi) - H_\Lambda(T^\zeta(\varphi)) \geqslant \sigma_T^\zeta. \tag{5.3}$$

Proof: We begin by analyzing the self-energy difference between φ and $T^\zeta(\varphi)$.

For $x \neq o$ we get by definition of T_x^ζ, cf. Eq. (3.7), and Condition 1.1 *(iii)* that $f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x)) \geqslant 0$. In particular we get

$$f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x)) \geqslant \mathbb{1}_{[|\varphi_x| \geqslant 4R]}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x))) \geqslant 0. \tag{5.4}$$

For $x=o$, we distinguish two cases. First consider $|\varphi_o| \geqslant 4R$. Here $|T_o^\zeta(\varphi_o)| = (1-\epsilon_o)|\varphi_o| \geqslant R$, and hence, by Condition 1.1 *(iii)*,

$$f_o(\varphi_o) - f_o(T_o^\zeta(\varphi_o)) \geqslant \epsilon_o c_f |\varphi_o| \geqslant 4\epsilon_o c_f R. \tag{5.5}$$

Second, consider the case $|\varphi_o| < 4R$ and $\varphi_o \notin \mathcal{G}_{2\zeta}$. Then $T_o^\zeta(\varphi_o) \in \mathcal{G}_\zeta$ and thus

$$f_o(\varphi_o) - f_o(T_o^\zeta(\varphi_o)) \geqslant \zeta. \tag{5.6}$$

Putting Eqs. (4.1) and (5.4)–(5.6) together, we obtain the desired lower bound on $H(\varphi) - H_\Lambda(T^\zeta(\varphi))$,

$$\begin{aligned} H_\Lambda(\varphi) - H_\Lambda(T^\zeta(\varphi)) &\geqslant \left[\sum_{x \neq o} \mathbb{1}_{[|\varphi_x| \geqslant 4R]}\{1 - |J|C_W^2\}(f_x(\varphi_x) - f_x(T_x^\zeta(\varphi_x)))\right] - |J|C_W^1 + \{\mathbb{1}_{[|\varphi_o| < 4R]} \\ &\quad + \mathbb{1}_{[|\varphi_o| \geqslant 4R]}(1 - |J|C_W^2)\}(f_o(\varphi_o) - f_o(T_o^\zeta(\varphi_o))) \\ &\geqslant \min\{\zeta, 4\epsilon_o c_f R(1 - |J|C_W^2)\} - |J|C_W^1, \end{aligned} \tag{5.7}$$

where we use $\varphi_o \notin \mathcal{G}_{2\zeta}$ and also $|J|C_W^2 < \tilde{J}_0(\zeta)C_W^2 \leqslant 1$. □

VI. LOCALIZATION

In this section we prove the main result, Theorem 1.1.

We begin separating into two regions

$$\begin{aligned} \mathbb{P}_\Lambda[\varphi_o \notin \mathcal{G}_{2\zeta}] &= \mathbb{P}_\Lambda[|\varphi_o| \geqslant 4R] + \mathbb{P}_\Lambda[\varphi_o \in B_{4R}(0) \setminus \mathcal{G}_{2\zeta}] \\ &= \mathcal{Z}_\Lambda^{-1}\left(\int_{\{|\varphi_o| \geqslant 4R\}} e^{-\beta H_\Lambda(\varphi)} d^\Lambda\varphi + \int_{\{\varphi_o \in B_{4R}(0) \setminus \mathcal{G}_{2\zeta}\}} e^{-\beta H_\Lambda(\varphi)} d^\Lambda\varphi\right). \end{aligned} \tag{6.1}$$

Let $\mathcal{A}_1 = \{|\varphi_o| \geqslant 4R\}$ and $\mathcal{A}_2 = \{\varphi_o \in B_{4R}(0) \setminus \mathcal{G}_{2\zeta}\}$. We estimate using Lemma 5.1, for $j=1,2$,

$$\begin{aligned} \int_{\mathcal{A}_j} e^{-\beta H_\Lambda(\varphi)} d^\Lambda\varphi &\leqslant \sup_{\varphi \in \mathcal{A}_j}\{e^{-\beta[H_\Lambda(\varphi) - H_\Lambda(T^\zeta(\varphi))]}\} \int_{\mathcal{A}_j} e^{-\beta H_\Lambda(T^\zeta(\varphi))} d^\Lambda\varphi \\ &= e^{-\beta \inf_{\varphi \in \mathcal{A}_j}[H_\Lambda(\varphi) - H_\Lambda(T^\zeta(\varphi))]} \int_{T^\zeta(\mathcal{A}_j)} e^{-\beta H_\Lambda(\psi)} \frac{d^\Lambda\psi}{|(\det \mathrm{Jac} T^\zeta)(T^{\zeta-1}(\psi))|} \\ &\leqslant \frac{e^{-\beta\sigma_T^\zeta}}{\inf_{\varphi \in \mathcal{A}_j}|(\det \mathrm{Jac} T^\zeta)(T^{\zeta-1}(\varphi))|} \mathcal{Z}_\Lambda, \end{aligned} \tag{6.2}$$

provided $|J| < \tilde{J}_0(\zeta)$ and $0 < \zeta \leqslant c_f R/2$. Inserting Eqs. (6.2) into (6.1), together with the estimate Eq. (3.9) on the determinant of the Jacobian of T^ζ, we get

$$\mathbb{P}_\Lambda[\varphi_o \notin \mathcal{G}_{2\zeta}] \leqslant \max\left\{\left[4R\zeta^{-1} \sup_{|u| \leqslant R_\zeta} |\nabla f_o(u)|\right]^n, (1-\epsilon_o)^{-n}\right\} \exp[n\epsilon_o(1 + \|\theta'\|_\infty)C_\rho] e^{-\beta\sigma_T^\zeta}. \tag{6.3}$$

Taking infimum over admissible θ's and ϵ_o's, yields the estimate with $\|\theta'\|_\infty$ replaced by 2 and ϵ_o replaced by 1/6 (see Eq. (3.6)). We have thus obtained the bound

$$\mathbb{P}_\Lambda[\varphi_o \notin \mathcal{G}_{2\zeta}] \leqslant 2\max\left\{\left[4R\zeta^{-1}\sup_{|u|\leqslant R_\zeta}|\nabla f_o(u)|\right]^n, \left(\tfrac{6}{5}\right)^n\right\} e^{(1/2)nC_\rho} e^{-\beta\sigma_T^\zeta}. \tag{6.4}$$

We recapitulate: The constants in Eqs. (4.2), (5.1), and (5.2), with $\|\theta'\|_\infty = 2$ and $\epsilon_o = 1/6$, become

$$C_W^1 = 4RC_a^0\left(\tfrac{1}{3}C_\rho + 3\right), \quad C_W^2 = \Gamma_0 + \tfrac{102}{5}C_a^\rho, \tag{6.5}$$

$$\tilde{J}_0(\zeta) = \min\left\{\frac{\zeta}{C_W^1}, \frac{\frac{2}{3}c_f R}{C_W^1 + \frac{2}{3}c_f R C_W^2}\right\}, \tag{6.6}$$

$$\sigma_T^\zeta = \min\left\{\zeta, \tfrac{2}{3}c_f R(1 - |J|C_W^2)\right\} - |J|C_W^1. \tag{6.7}$$

With these constants and for $|J| < \tilde{J}_0(\zeta)$, $0 < \zeta/2 \leqslant c_f R$, and $\beta > 0$ the localization bound Eq. (6.3) holds true.

We end by explaining how to derive the assertion of Theorem 1.1 from here. Note that $\Gamma_1 = C_W^1$ and $\Gamma_2 = C_W^2$. Comparing Eq. (6.6) to Eq. (1.8), we further notice that $\tilde{J}_0(c_f R/2) = J_0$ and that $\tilde{J}_0(\zeta) \leqslant J_0$, whenever $\zeta \leqslant c_f R/2$. By assumption, we have $|J| \leqslant \min\{J_0, \delta/(2\Gamma_1)\}$. We distinguish the cases $\delta \geqslant c_f R$ and $\delta < c_f R$.

If $\delta \geqslant c_f R$ then we choose $\zeta := c_f R/2$ and observe that $|J| \leqslant J_0 = \tilde{J}_0(\zeta)$. The claim now follows from Eq. (6.3), the trivial bound $\mathbb{P}_\Lambda[\varphi_o \notin \mathcal{G}_\delta] \leqslant \mathbb{P}_\Lambda[\varphi_o \notin \mathcal{G}_{c_f R}]$, and the fact that $\min\{\delta, 3\Gamma_3/2\} = \min\{\delta, c_f R\} = c_f R = 2\zeta$.

Conversely, if $\delta < c_f R$ then we choose $\zeta := \delta/2 < c_f R/2$. Since $\delta > 2|J|\Gamma_1$, also this choice insures that $|J| \leqslant \tilde{J}_0(\zeta)$, namely, $|J| < \zeta/(2\Gamma_1) \leqslant \tilde{J}_0(\zeta)$. Now the claim follows directly from Eq. (6.3) and $\min\{\delta, 3\Gamma_3/2\} = \min\{\delta, c_f R\} = \delta = 2\zeta$.

This completes the proof of Theorem 1.1. □

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APPENDIX A. CONTROLLING THE INTERACTION

In this appendix we prove a basic bound on the interaction, which shows that it can be dominated by the self-energy. This is only used to ensure that polynomially bounded observables are integrable, and in particular that the partition function is finite.

Lemma A.1: Suppose Conditions 1.1 and 1.2. There exists a constant A, which may depend on Λ, such that for all $\varphi \in \Omega$,

$$\left|\sum_{x \neq y, x, y \in \Lambda} \omega_{xy}(\varphi_x, \varphi_y)\right| \leqslant A + 2C_a^0(1 + C_f + c_f^{-1})\sum_{x \in \Lambda} f_x(\varphi_x).$$

Proof: Let $u, v \neq 0$. In the following A_j, $j \in \{1,2,3\}$, denote non-negative constants, which contribute to the A in the lemma. We estimate using Conditions 1.1 and 1.2,

$$
\begin{aligned}
|w_{xy}(u,v)| &\leqslant A_1 + |w_{xy}(u,v) - w_{xy}(0,0)| \leqslant A_1 + \int_0^1 |u \cdot (\nabla_1 w_{xy})(tu,tv) + v \cdot (\nabla_2 w_{xy})(tu,tv)| dt \\
&\leqslant A_1 + a_{xy} \int_0^1 (|u| + |v|)[1 + \mathbb{1}_{[t|u| \geqslant 4R]} (\partial_{|u|} f_x)(tu) + \mathbb{1}_{[t|v| \geqslant 4R]} (\partial_{|v|} f_y)(tv)] dt \\
&\leqslant A_1 + a_{xy} \left\{ |u| + |v| + (1 + C_f) \int_0^1 [\mathbb{1}_{[t|u| \geqslant 4R]} |u| (\partial_{|u|} f_x)(tu) + \mathbb{1}_{[t|v| \geqslant 4R]} |v| (\partial_{|v|} f_y)(tv)] dt \right\} \\
&= A_1 + a_{xy} \left\{ |u| + |v| + (1 + C_f) \int_0^1 \left[\mathbb{1}_{[t|u| \geqslant 4R]} \frac{d}{dt} f_x(tu) + \mathbb{1}_{[t|v| \geqslant 4R]} \frac{d}{dt} f_y(tv) \right] dt \right\} \\
&= A_1 + a_{xy} \left\{ |u| + |v| + (1 + C_f) \left[\mathbb{1}_{[|u| \geqslant 4R]} \int_{\frac{4R}{|u|}}^1 \frac{d}{dt} f_x(tu) dt + \mathbb{1}_{[|v| \geqslant 4R]} \int_{\frac{4R}{|v|}}^1 \frac{d}{dt} f_y(tv) dt \right] \right\} \\
&\leqslant A_2 + a_{xy} \{ |u| + |v| + (1 + C_f)[f_x(u) + f_y(v)] \}.
\end{aligned}
$$

To conclude the proof we observe the following bound:

$$
|u| \leqslant A_3 + \mathbb{1}_{[|u| \geqslant R]} |u| \leqslant A_3 + c_f^{-1} \mathbb{1}_{[|u| \geqslant R]} f_x(u) \leqslant A_3 + c_f^{-1} f_x(u),
$$

and sum up, using Eq. (1.4). □

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Feynman cycles in the Bose gas

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We study the lengths of the cycles formed by trajectories in the Feynman-Kac representation of the Bose gas. We discuss the occurrence of infinite cycles and their relation to Bose-Einstein condensation. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2383008]

I. INTRODUCTION

Bose and Einstein understood 80 years ago that a curious phase transition occurs in a gas of noninteracting bosons; it is now commonly referred to as the Bose-Einstein condensation. Real particles interact, however, and for many years there were doubts that this transition takes place in natural systems. London suggested in 1938 that superfluid helium undergoes a Bose-Einstein condensation, and this idea is largely accepted nowadays. Bogoliubov considered interacting systems; careful approximations allowed him to get back to a noninteracting gas but with a different dispersion relation. See Refs. 16 and 8 for more discussion and partial justifications of the Bogoliubov theory.

In 1953 Feynman studied the system in the Feynman-Kac representation.[5] The partition function can be expanded as a gas of trajectories living in $(d+1)$ dimensions. The extra dimension is commonly referred to as "the time," although it is not related to physical time. The situation is illustrated in Fig. 1. A finite system with N particles induces a probability on the group S_N of permutations of N elements. Feynman considered the probability for a given particle to belong to a cycle of length n. In the thermodynamic limit, there may be strictly positive probability for infinite cycles to be present, and Feynman suggested to use this as an order parameter for Bose-Einstein condensation.

A few years later, in 1956, Penrose and Onsager introduced the concept of "off-diagonal long-range order."[9] Formally, it is a correlation between positions x and y given by $\sigma(x,y) = \langle c^\dagger(x)c(y)\rangle$. The system displays off-diagonal long-range order when this correlation is strictly positive, uniformly in the size of the system and in $|x-y|\to\infty$. One can write a Feynman-Kac version of this correlation, and it involves a special cycle starting at x and ending at y; this cycle may wind many times around the imaginary time direction. In the limit where x and y are infinitely distant there corresponds a notion of infinite open cycle that is reminiscent of Feynman's approach.

Feynman's order parameter is simpler; it is often used in numerical simulations or in order to gain heuristic understanding. On the other hand, everybody agrees that the Penrose and Onsager order parameter is the correct one. Surprisingly, the question of their equivalence is usually eluded, and many physicists implicitly assume equivalence to hold. The first mathematical investigation of this question is due to Sütő, who showed that equivalence holds in the ideal gas. Indeed, he proved that infinite cycles occur in the presence of condensation,[12] and that no infinite cycles occur in the absence of condensation;[13] the latter result uses probabilistic methods from the theory of large deviations. These results have been extended to mean-field systems in Refs. 1 and 3.

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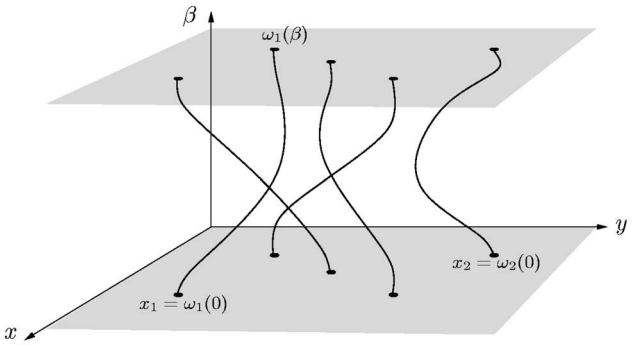

FIG. 1. The Feynman-Kac representation of the partition function for a gas of bosons. The horizontal plane represents the d spatial dimensions, and the vertical axis is the imaginary time dimension. The picture shows a situation with five particles and two cycles, of respective lengths 4 and 1.

In this paper we explore the links between Feynman cycles and off-diagonal long-range order. Let $\boldsymbol{\sigma}(x)$ denote the off-diagonal correlation between the origin and $x \in \mathbb{R}^d$, and $\boldsymbol{\varrho}(n)$ denote the density of particles in cycles of length n. We propose the following formula that relates both concepts:

$$\boldsymbol{\sigma}(x) = \sum_{n \geqslant 1} \boldsymbol{c}_n(x) \boldsymbol{\varrho}(n) + \boldsymbol{c}_\infty(x) \boldsymbol{\varrho}(\infty). \tag{1.1}$$

Mathematically, the problem is not well posed. Many choices for the coefficients $\boldsymbol{c}_n$ are possible—a trivial choice is $\boldsymbol{c}_n(x) = \boldsymbol{\sigma}(x)/\rho$ for all n, including $n=\infty$. We will see, however, that there is a natural definition for $\boldsymbol{c}_n(x)$ in terms of Wiener trajectories. In any case, we conjecture that Eq. (1.1) holds with coefficients satisfying

$$0 \leqslant \boldsymbol{c}_n(x) \leqslant 1, \quad 0 \leqslant \boldsymbol{c}_\infty(x) \leqslant 1,$$

for all n, x. In addition, we should have

$$\lim_{n \to \infty} \boldsymbol{c}_n(x) = \boldsymbol{c}_\infty(x)$$

for any x, and

$$\lim_{|x| \to \infty} \boldsymbol{c}_n(x) = 0$$

for any finite n, but not uniformly in n; $\boldsymbol{c}_\infty(x)$ may converge to a strictly positive constant $\boldsymbol{c}$. If $\boldsymbol{c}=1$, we get from the dominated convergence theorem that $\lim_{|x| \to \infty} \boldsymbol{\sigma}(x) = \boldsymbol{\varrho}(\infty)$—in which case the off-diagonal long-range order parameter is equal to the density of cycles of infinite lengths.

We establish this formula and these properties in the case of the ideal gas, where we show that

$$\boldsymbol{c}_n(x) = \mathrm{e}^{-x^2/4n\beta}, \quad \boldsymbol{c}_\infty(x) = 1. \tag{1.2}$$

We discuss the validity of formula (1.1) in the interacting gas, proving that these properties hold true in a regime without the Bose-Einstein condensation. The two order parameters should not be always equivalent, however. It is argued in Ref. 15 that they differ when the bosons undergo a regular condensation into a crystalline phase. There is no off-diagonal long-range order, but infinite cycles may be present.

We work in the Feynman-Kac representation of the Bose gas. This representation is standard, see, e.g., Ref. 4 for a clear and concise review and Ref. 6 for a complete introduction. We assume the reader to possess some familiarity with it and in Sec. II we directly define the main

expressions—partition functions, density of cycles, and off-diagonal long-range order—in terms of space-time trajectories. But basic notions and properties are reviewed in Appendix A.

The situation simplifies in the absence of interactions; we consider the ideal gas in Sec. III, where we state and prove the formula that relates the two order parameters. The ideal gas is best discussed in the canonical ensemble. Rigorous proofs of macroscopic occupation of the zero mode have been proposed and they involve the grand-canonical ensemble, with a chemical potential that depends on the volume. Appendix B proposes a simple proof in the canonical ensemble.

Interacting systems constitute a formidable challenge; they are discussed in Sec. IV, where partial results are obtained.

In this paper, we denote finite volume expressions in plain characters, and infinite volume expressions in bold characters. Further, we always consider the canonical and grand-canonical ensembles where the temperature $1/\beta$ is fixed; we alleviate the notation by omitting the β dependence of all quantities.

II. FEYNMAN CYCLES AND OFF-DIAGONAL LONG-RANGE ORDER

A. Partition functions

Our Bose gas occupies a d-dimensional domain D, always a cubic box of size L and volume $V=L^d$. We consider periodic boundary conditions. Let ρ denote the particle density, β the inverse temperature, and μ the chemical potential. The canonical partition function in the Feynman-Kac representation is given by

$$Y(N)=\sum_{k=1}^{N}\frac{1}{k!}\sum_{\substack{n_1,\ldots,n_k\geqslant 1\\ n_1+\cdots+n_k=N}}\int_{D^k}\mathrm{d}x_1\cdots\mathrm{d}x_k\int \mathrm{d}W^{n_1\beta}_{x_1x_1}(\omega_1)\cdots\mathrm{d}W^{n_k\beta}_{x_kx_k}(\omega_k)$$
$$\times\left[\prod_{j=1}^{k}\frac{1}{n_j}\mathrm{e}^{-\beta\mathcal{U}(\omega_j)}\right]\prod_{1\leqslant i<j\leqslant k}\mathrm{e}^{-\beta\mathcal{U}(\omega_i,\omega_j)}. \tag{2.1}$$

This expression is illustrated in Fig. 1. In words, we sum over the number k of closed trajectories and over their respective winding numbers $n_1,\ldots,n_k$. We integrate over the initial positions $x_1,\ldots,x_k$. We integrate over trajectories $\omega_j:[0,n_j\beta]\to D$ that start and end at x_j; here, W^{β}_{xx} denotes the Wiener measure. See Appendix A for more information and, in particular, Eq. (A10) for the normalization condition. Trajectories wind around the time direction according to their winding numbers; because of periodic boundary conditions, they may also wind around space directions.

Given a trajectory ω with winding number n, the function $\mathcal{U}(\omega)$ denotes the interactions between different legs; explicitly,

$$\mathcal{U}(\omega)=\sum_{0\leqslant i<j\leqslant n-1}\frac{1}{\beta}\int_0^{\beta}U(\omega(i\beta+s)-\omega(j\beta+s))\mathrm{d}s. \tag{2.2}$$

And $\mathcal{U}(\omega,\omega')$ denotes the interactions between closed trajectories ω and ω', of respective winding numbers n and n',

$$\mathcal{U}(\omega,\omega')=\sum_{\substack{0\leqslant i\leqslant n-1\\ 0\leqslant j\leqslant n'-1}}\frac{1}{\beta}\int_0^{\beta}U(\omega(i\beta+s)-\omega'(j\beta+s))\mathrm{d}s. \tag{2.3}$$

The function $U(x)$ represents the pair interaction potential between two particles separated by a distance $|x|$. We suppose that $U(x)$ is non-negative and spherically symmetric. We can allow the value $+\infty$; all that is needed is that $\mathrm{e}^{-\beta\mathcal{U}(\omega)}$ and $\mathrm{e}^{-\beta\mathcal{U}(\omega,\omega')}$ be measurable functions with respect to the Wiener measure—any piecewise continuous function $D\to[0,\infty]$ can be considered at this point.

The grand-canonical partition function is

$$Z(\mu) = \sum_{N \geqslant 0} \mathrm{e}^{\beta\mu N} Y(N) \tag{2.4}$$

[with the understanding that $Y(0)=1$]. We also need partition functions where a given trajectory ω_0 is present—these will be needed in the expression for cycle densities, see Eqs. (2.8) and (2.9). Namely, we define

$$Y(N;\omega_0) = \sum_{k=1}^{N} \frac{1}{k!} \sum_{\substack{n_1,\dots,n_k \geqslant 1 \\ n_1+\cdots+n_k=N}} \int_{D^k} \mathrm{d}x_1 \cdots \mathrm{d}x_k \int \mathrm{d}W^{n_1\beta}_{x_1x_1}(\omega_1) \cdots \mathrm{d}W^{n_k\beta}_{x_kx_k}(\omega_k) \\ \times \left[\prod_{j=1}^{k} \frac{1}{n_j} \mathrm{e}^{-\beta \mathcal{U}(\omega_j)} \right] \prod_{0 \leqslant i < j \leqslant k} \mathrm{e}^{-\beta \mathcal{U}(\omega_i,\omega_j)}. \tag{2.5}$$

The dependence on ω_0 comes from the last term, where the product includes terms with $i=0$. Notice that

$$Y(N;\omega) \leqslant Y(N), \tag{2.6}$$

with equality if and only if $U(x) \equiv 0$, i.e., in the absence of interactions. Finally, we introduce

$$Z(\mu,\omega) = \sum_{N \geqslant 0} \mathrm{e}^{\beta\mu N} Y(N,\omega) \tag{2.7}$$

[we set $Y(0,\omega_0)=1$]. We also have $Z(\mu,\omega) \leqslant Z(\mu)$, with equality if and only if $U(x) \equiv 0$.

B. Cycle lengths

We now introduce the density of particles in cycles of length n, both in the canonical and grand-canonical ensembles. We denote the particle density by $\rho = N/V$. When discussing the canonical ensemble, we always suppose that ρ and V are such that $N=\rho V$ is an integer. The number of particles in cycles of length n is given by the random variable $\sum_{j=1}^{k} n\delta_{n_j,n}$. Averaging over all configurations of space-time closed trajectories, we get

$$\varrho_\rho(n) = \frac{1}{Y(N)} \sum_{k=1}^{N} \frac{1}{k!} \sum_{\substack{n_1,\dots,n_k \geqslant 1 \\ n_1+\cdots+n_k=N}} \left[\frac{1}{V} \sum_{j=1}^{k} n\delta_{n_j,n} \right] \int_{D^k} \mathrm{d}x_1 \cdots \mathrm{d}x_k \times \int \mathrm{d}W^{n_1\beta}_{x_1x_1}(\omega_1) \cdots \mathrm{d}W^{n_k\beta}_{x_kx_k}(\omega_k) \\ \times \left[\prod_{j=1}^{k} \frac{1}{n_j} \mathrm{e}^{-\beta \mathcal{U}(\omega_j)} \right] \prod_{1 \leqslant i < j \leqslant k} \mathrm{e}^{-\beta \mathcal{U}(\omega_i,\omega_j)} = \int \mathrm{d}W^{n\beta}_{00}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)}. \tag{2.8}$$

The last line follows from the first line by replacing $\sum_{j=1}^{k} n\delta_{n_j,n}$ with $nk\delta_{n_1,n}$, isolating the integral over ω_1, using definition (2.5), using translation invariance, and $\int_D \mathrm{d}x_1 = V$. Similarly, we have the grand-canonical expression

$$\varrho_\mu(n) = \mathrm{e}^{\beta\mu n} \int \mathrm{d}W^{n\beta}_{00}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)}. \tag{2.9}$$

One easily checks that

$$\sum_{n \geqslant 1} \varrho_\rho(n) = \frac{N}{V} \equiv \rho,$$

$$\sum_{n\geqslant 1} \varrho_\mu(n) = \left\langle \frac{N}{V} \right\rangle \equiv \rho(\mu).$$

We consider the thermodynamic limits of $\varrho_\rho(n)$ and $\varrho_\mu(n)$. Since $0 \leqslant \varrho_\rho(n) \leqslant \rho$ and since n is a discrete index, the Cantor diagonal process yields the existence of a sequence of increasing volumes V_k, with $\rho V_k = N_k$ an integer, such that $\varrho_\rho(n)$ converges to some limit that we denote $\boldsymbol{\varrho}_\rho(n)$. Similarly, we also obtain the infinite volume limit $\boldsymbol{\varrho}_\mu(n)$. Fatou's lemma implies that

$$\sum_{n\geqslant 1} \boldsymbol{\varrho}_\rho(n) \leqslant \rho, \quad \sum_{n\geqslant 1} \boldsymbol{\varrho}_\mu(n) \leqslant \boldsymbol{\rho}(\mu). \tag{2.10}$$

This suggests to define the density of particles in infinite cycles by

$$\boldsymbol{\varrho}_\rho(\infty) = \rho - \sum_{n\geqslant 1} \boldsymbol{\varrho}_\rho(n),$$

$$\boldsymbol{\varrho}_\mu(\infty) = \boldsymbol{\rho}(\mu) - \sum_{n\geqslant 1} \boldsymbol{\varrho}_\mu(n). \tag{2.11}$$

The main question is whether $\boldsymbol{\varrho}(\infty)$ differs from zero at a given temperature and at a given density or chemical potential.

We chose to discuss densities of particles in cycles of given length, but one may consider probabilities as well. Namely, we could introduce the probability for particle 1 to belong to a cycle of length n; it is given by

$$P_\rho(n) = \int_D \mathrm{d}x \int \mathrm{d}W_{xx}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{NY(N)}. \tag{2.12}$$

Thus $\varrho_\rho(n) = \rho P_\rho(n)$ in the canonical ensemble, and $\boldsymbol{\varrho}_\rho(\infty) = \rho \boldsymbol{P}_\rho(\infty)$. Things are not so simple in the grand-canonical ensemble. The probability $P_\mu(n)$ is

$$P_\mu(n) = \int_D \mathrm{d}x \int \mathrm{d}W_{xx}^{n\beta}(\omega) \frac{\mathrm{e}^{\beta\mu n}}{n} \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Z'(\mu;\omega)}{Z(\mu)}. \tag{2.13}$$

Here, $Z'(\mu;\omega)$ is like $Z(\mu;\omega)$ given in Eqs. (2.5) and (2.7), but with a factor $1/(k+1)!$ instead of $1/k!$. Heuristically, we should have $\langle V/nk \rangle = 1/\rho(\mu)$ and $\varrho_\mu(n) = \rho(\mu) P_\mu(n)$, but this does not seem easy to establish. The ratio of partition functions in Eq. (2.13) is more difficult to control than the one in Eq. (2.9). We therefore abandon probabilities and discuss densities.

C. Off-diagonal long-range order

Let us turn to the Penrose and Onsager off-diagonal long-range order. Its Feynman-Kac representation involves an open trajectory that starts at x and ends at y, that possibly winds several times around the time direction. Precisely, we introduce

$$\sigma_\rho(x) = \sum_{n=1}^{N} \int \mathrm{d}W_{0x}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)},$$

$$\sigma_\mu(x) = \sum_{n\geqslant 1} \mathrm{e}^{\beta\mu n} \int \mathrm{d}W_{0x}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)}. \tag{2.14}$$

Thermodynamic limits are denoted $\boldsymbol{\sigma}_\rho(x)$ and $\boldsymbol{\sigma}_\mu(x)$, provided they exist. One may actually restrict $\sigma_\rho(x)$ and $\sigma_\mu(x)$ on rational x and use the Cantor diagonal process to get convergence on a

subsequence of increasing volumes. This is not necessary in this paper, as the limits will be shown to exist in the regimes of parameters under consideration.

Similarities between Eqs. (2.8) and (2.9) on the one hand and Eqs. (2.14) on the other hand are manifested. We can write

$$\sigma_\rho(x) = \sum_{n=1}^{N} c_{n,\rho}(x) \varrho_\rho(n),$$

$$\sigma_\mu(x) = \sum_{n\geqslant 1} c_{n,\mu}(x) \varrho_\mu(n), \tag{2.15}$$

where the coefficients $c_{n,\rho}$, $c_{n,\mu}$ are given by

$$c_{n,\rho}(x) = \left[\int \mathrm{d}W_{00}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)} \right]^{-1} \int \mathrm{d}W_{0x}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)},$$

$$c_{n,\mu}(x) = \left[\int \mathrm{d}W_{00}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)} \right]^{-1} \int \mathrm{d}W_{0x}^{n\beta}(\omega) \mathrm{e}^{-\beta \mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)}. \tag{2.16}$$

As above, we denote the thermodynamic limits by $\boldsymbol{c}_{n,\rho}(x)$ and $\boldsymbol{c}_{n,\mu}(x)$, provided they exist. One should be careful when sending the volume to infinity in Eqs. (2.15), because a "leak to infinity" may yield a term involving $\boldsymbol{\varrho}(\infty)$—this actually occurs in the ideal gas, as will be shown in the next section.

III. THE IDEAL GAS

The ideal gas of quantum bosons is fascinating. Particles do not interact, yet they manage to display a phase transition. Historically, the Bose-Einstein condensation is the first theoretical description of a phase transition. The ideal gas has been the object of many studies over the years; let us mention Refs. 17, 7, and 10. A simple proof of macroscopic occupation of the zero Fourier mode is presented in Appendix B.

In this section we elucidate the relation between cycle lengths and off-diagonal long-range order, thus clarifying results that were previously obtained by Sütő.[12,13] We work in the canonical ensemble and establish formula (1.1) explicitly, for any dimension $d \geqslant 1$.

Theorem 1: *For any $0<\beta$, $\rho<\infty$, there exists a sequence of increasing cubes for which the thermodynamic limits of $\sigma_\rho(x)$, $c_{n,\rho}(x)$, and $\varrho_\rho(n)$ exist for all $x \in \mathbb{R}^d$ and $n \in \mathbb{N}$. Further, we have*

$$\boldsymbol{\sigma}_\rho(x) = \sum_{n\geqslant 1} \mathrm{e}^{-x^2/4n\beta} \boldsymbol{\varrho}_\rho(n) + \boldsymbol{\varrho}_\rho(\infty).$$

The rest of this section is devoted to the proof of Theorem 1. The coefficient $c_{n,\rho}(x)$, defined in Eq. (2.16), has a simpler expression in the absence of interactions. Indeed, we have $\mathcal{U}(\omega)=0$ and $Y(N;\omega)=Y(N)$. It follows from properties of the Wiener measure in periodic boxes, see Eq. (A10), that

$$c_{n,\rho}(x) = \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-(L^2/4n\beta)((x/L)-z)^2} \Big/ \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-(L^2/4n\beta)z^2}. \tag{3.1}$$

Notice that $\lim_{L\to\infty} c_{n,\rho}(x) = \mathrm{e}^{-x^2/4n\beta}$, but the limit is not uniform in n. If the sum over n is restricted to $n \leqslant cL^2$, with c any finite constant, we can use the dominated convergence theorem and we get

$$\lim_{L\to\infty} \sum_{n=1}^{cL^2} c_{n,\rho}(x)\varrho_\rho(n) = \sum_{n\geqslant 1} \mathrm{e}^{-x^2/4n\beta}\boldsymbol{\varrho}_\rho(n). \tag{3.2}$$

[The limit is taken along the subsequence of increasing volumes for which $\varrho_\rho(n)$ is known to converge for any n.]

We now consider the terms with $cL^2 < n \leqslant N$. We estimate the sums in Eq. (3.1) using integrals; we have

$$\int_{-\infty}^{\infty} \mathrm{e}^{-a(s-b)^2}\mathrm{d}s - 1 \leqslant \sum_{k\in\mathbb{Z}} \mathrm{e}^{-a(k-b)^2} \leqslant \int_{-\infty}^{\infty} \mathrm{e}^{-a(s-b)^2}\mathrm{d}s + 1. \tag{3.3}$$

The Gaussian integral is equal to $\sqrt{\pi/a}$. Consequently,

$$\left[\frac{\sqrt{4\pi n\beta}-L}{\sqrt{4\pi n\beta}+L}\right]^d \leqslant c_{n,\rho}(x) \leqslant \left[\frac{\sqrt{4\pi n\beta}+L}{\sqrt{4\pi n\beta}-L}\right]^d. \tag{3.4}$$

These bounds hold provided $\sqrt{4\pi n\beta} > L$. Since $n/L^2 > c$, we have

$$\left[\frac{\sqrt{4\pi c\beta}-1}{\sqrt{4\pi c\beta}+1}\right]^d \sum_{n=cL^2}^{N} \varrho_\rho(n) \leqslant \sum_{n=cL^2}^{N} c_{n,\rho}(x)\varrho_\rho(n) \leqslant \left[\frac{\sqrt{4\pi c\beta}+1}{\sqrt{4\pi c\beta}-1}\right]^d \sum_{n=cL^2}^{N} \varrho_\rho(n). \tag{3.5}$$

We obtain

$$\sum_{n=cL^2}^{N} c_{n,\rho}(x)\varrho_\rho(n) \leqslant \left[\frac{\sqrt{4\pi c\beta}+1}{\sqrt{4\pi c\beta}-1}\right]^d \left(\rho - \sum_{n=1}^{cL^2} \varrho_\rho(n)\right). \tag{3.6}$$

Using Eq. (3.2) with $x=0$ and definition (2.11) of the density of infinite cycles, we see that the last term converges to $\boldsymbol{\varrho}_\rho(\infty)$ as $L\to\infty$. It then follows from Eqs. (3.2) and (3.6) that

$$\limsup_{L\to\infty} \sigma_\rho(x) \leqslant \sum_{n\geqslant 1} \mathrm{e}^{-x^2/4n\beta}\boldsymbol{\varrho}_\rho(n) + \left[\frac{\sqrt{4\pi c\beta}+1}{\sqrt{4\pi c\beta}-1}\right]^d \boldsymbol{\varrho}_\rho(\infty). \tag{3.7}$$

This inequality holds for any c, and the fraction is arbitrarily close to 1 by taking c large. A lower bound can be derived in a similar fashion, and we obtain the formula stated in Theorem 1.

IV. THE INTERACTING GAS

The interacting gas is much more difficult to study. We prove in this section the absence of infinite cycles when the chemical potential is negative (Theorem 2). We then study the coefficients $c_{n,\mu}(x)$ at low density and high temperature, using cluster expansion techniques. Their thermodynamic limit can be established, and we show that $\boldsymbol{c}_{n,\mu}(x)\to 0$ as $|x|\to\infty$ (Theorem 3).

Theorem 2: *Let* $0<\beta<\infty$ and $\mu<0$; *then*

$$\boldsymbol{\varrho}_\mu(\infty) = 0,$$

and

$$\lim_{|x|\to\infty} \limsup_{L\to\infty} \sigma_\mu(x) = 0.$$

Proof: Since $\mathcal{U}(\omega)\geqslant 0$ and $Z(\mu;\omega)\leqslant Z(\mu)$, the finite volume density $\varrho_\mu(n)$, Eq. (2.9), is less than

$$\varrho_\mu(n) \leqslant \mathrm{e}^{\beta\mu n} \int \mathrm{d}W_{00}^{n\beta}(\omega) = \frac{\mathrm{e}^{\beta\mu n}}{(4\pi n\beta)^{d/2}} \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-L^2 z^2/4n\beta}. \tag{4.1}$$

The right side is smaller than $\mathrm{e}^{\beta\mu n}$ for all L large enough. We can therefore apply the dominated convergence theorem and we obtain

$$\rho = \lim_{L\to\infty} \sum_{n\geqslant 1} \varrho_\mu(n) = \sum_{n\geqslant 1} \boldsymbol{\varrho}_\mu(n). \tag{4.2}$$

It follows that $\boldsymbol{\varrho}_\rho(\infty)=0$. The statement about the absence of off-diagonal long-range order can be treated similarly. We have the upper bound

$$\sigma_\mu(x) \leqslant \sum_{n\geqslant 1} \frac{\mathrm{e}^{\beta\mu n}}{(4\pi n\beta)^{d/2}} \sum_{z\in\mathbb{Z}^d} \mathrm{e}^{-(x-Lz)^2/4n\beta}. \tag{4.3}$$

By dominated convergence,

$$\limsup_{L\to\infty} \sigma_\mu(x) \leqslant \sum_{n\geqslant 1} \frac{\mathrm{e}^{\beta\mu n}}{(4\pi n\beta)^{d/2}} \mathrm{e}^{-x^2/4n\beta}. \tag{4.4}$$

We can again use the dominated convergence theorem for the limit $|x|\to\infty$, and we get the claim. □

We continue the study of the interacting gas in the regime where cluster expansion converges. We assume that the chemical potential is negative, that the interaction potential $U(x)$ is integrable, and that the temperature is high enough. The condition in Theorem 3 is stronger than necessary, but it is very explicit. We will invoke a weaker condition in the proof of the theorem that is based on the "Kotecký-Preiss criterion" for the convergence of cluster expansion. Notice that Ginibre's survey[6] uses Kirkwood-Salzburg equations; it applies to a broader range of potentials, but things are terribly intricate.

Theorem 3: *Assume that β, μ, and U satisfy*

$$\frac{1}{(4\pi\beta)^{d/2}} \int_{\mathbb{R}^d} U(x)\mathrm{d}x \sum_{n\geqslant 1} n^{-d/2} \leqslant -\mu.$$

The thermodynamic limits of $c_{n,\mu}(x)$ and $\varrho_\mu(n)$ exist, and we have

$$\lim_{|x|\to\infty} \boldsymbol{c}_{n,\mu}(x) = 0$$

for any n.

Proof: We need some notation in order to cast the grand-canonical partition function in a form suitable for the cluster expansion. Let us introduce a measure for trajectories that wind arbitrarily many times around the time direction. Namely, let $\mathcal{X}_n$ denote the measure space of continuous trajectories $\omega:[0,n\beta]\to D$, and let $\mathcal{X}=\cup_{n\geqslant 1}\mathcal{X}_n$ be the set of trajectories in D with arbitrary winding numbers. We introduce the measure ν on $\mathcal{X}$ whose integral means the following:

$$\int F(\omega)\mathrm{d}\nu(\omega) = \sum_{n\geqslant 1} \frac{\mathrm{e}^{\beta\mu n}}{n} \int_D \mathrm{d}x \int \mathrm{d}W_{xx}^{n\beta}(\omega) \mathrm{e}^{-\beta\mathcal{U}(\omega)} F(\omega). \tag{4.5}$$

It is clear that ν is a genuine measure on a reasonable measure space. But we describe the measure ν with more details for readers who are interested in analytic technicalities. The σ algebra on $\mathcal{X}_n$ is the smallest σ algebra that contains the sets $\{\omega\in\mathcal{X}_n : \omega(t)\in B\}$, for any $0\leqslant t\leqslant n\beta$, and any Borel set $B\subset D$. Trajectories of $\mathcal{X}_1$ can be dilated in the time direction so as to yield trajec-

tories with arbitrary winding numbers. One can then consider the product space $\mathcal{X}_1 \times \mathbb{N}$ with the product σ algebra (the σ algebra on $\mathbb{N}$ being the power set). The measure of a set of the kind $A \times \{n\}$, with A a measurable subset of $\mathcal{X}_1$, is defined as

$$\nu(A \times \{n\}) = \frac{e^{\beta\mu n}}{n} \int dx \int_{A'} dW_{xx}^{n\beta}(\omega') e^{-\beta \mathcal{U}(\omega')}. \tag{4.6}$$

Here, we introduced

$$A' = \{\omega' \in \mathcal{X}_n : \omega'(t) = \omega(nt) \quad \text{for some } \omega \in A\}. \tag{4.7}$$

There is a unique extension to a measure on $\mathcal{X}_1 \times \mathbb{N}$. There is a natural correspondence between $\mathcal{X}$ and $\mathcal{X}_1 \times \mathbb{N}$, and we consider ν to be a measure on $\mathcal{X}$.

With this notation, the grand-canonical partition function (2.4) is given by

$$Z(\mu) = \sum_{k \geqslant 0} \frac{1}{k!} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \prod_{1 \leqslant i < j \leqslant k} [e^{-\beta \mathcal{U}(\omega_i, \omega_j)} - 1]. \tag{4.8}$$

The term $k=0$ is equal to 1 by definition. Then $Z(\mu)$ has exactly the form assumed, e.g., in Ref. 14. The Kotecký-Preiss criterion for the convergence of the cluster expansion requires the existence of a function $a : \mathcal{X} \to \mathbb{R}_+$ such that the following inequality holds for any $\omega \in \mathcal{X}$:

$$\int_{\mathcal{X}} [1 - e^{-\beta \mathcal{U}(\omega, \omega')}] e^{a(\omega')} d\nu(\omega') \leqslant a(\omega). \tag{4.9}$$

Choosing $a(\omega) = -\beta\mu n$ (with n the winding number of the trajectory ω), it was shown in Ref. 14 that Eq. (4.9) is a consequence of the condition in Theorem 3.

The main result of the cluster expansion is that the partition function (4.8) is given by the exponential of a convergent series. Namely,

$$Z(\mu) = \exp\left\{ \sum_{k \geqslant 1} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \varphi(\omega_1, \ldots, \omega_k) \right\}. \tag{4.10}$$

The combinatorial function $\varphi(\omega_1, \ldots, \omega_k)$ is equal to 1 if $k=1$, and is otherwise equal to

$$\varphi(\omega_1, \ldots, \omega_k) = \frac{1}{k!} \sum_{G} \prod_{(i,j) \in G} [e^{-\beta \mathcal{U}(\omega_i, \omega_j)} - 1]. \tag{4.11}$$

The sum is over *connected* graphs with k vertices, and the product is over edges of G. A proof for relation (4.10) that directly applies here can be found in Ref. 14.

Observe now that the partition function $Z(\mu; \omega)$ is given by an expression similar to Eq. (4.8), where each $\nu(\omega_j)$ is replaced by $e^{-\beta \mathcal{U}(\omega, \omega_j)} \nu(\omega_j)$. Since $\mathcal{U}(\omega, \omega_j)$ is positive, the criterion (4.9) is satisfied with this new measure. It follows that $Z(\mu; \omega)$ has an expansion similar to Eq. (4.10), and we obtain the following expression for the ratio of partition functions:

$$\frac{Z(\mu; \omega)}{Z(\mu)} = \exp\left\{ - \sum_{k \geqslant 1} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \left[1 - \prod_{j=1}^{k} e^{-\beta \mathcal{U}(\omega, \omega_j)} \right] \varphi(\omega_1, \ldots, \omega_k) \right\}. \tag{4.12}$$

It is not hard to check that

$$1 - \prod_{j=1}^{k} e^{-\beta \mathcal{U}(\omega, \omega_j)} = \sum_{j=1}^{k} (1 - e^{-\beta \mathcal{U}(\omega, \omega_j)}) \prod_{i=1}^{j-1} e^{-\beta \mathcal{U}(\omega, \omega_i)} \leqslant \sum_{j=1}^{k} (1 - e^{-\beta \mathcal{U}(\omega, \omega_j)}). \tag{4.13}$$

Then Eq. (5) in Ref. 14 gives the necessary estimate for the exponent in Eq. (4.12), namely,

$$\sum_{k\geqslant 1} \int_{\mathcal{X}^k} \mathrm{d}\nu(\omega_1)\cdots\mathrm{d}\nu(\omega_k) \left[\sum_{j=1}^{k} (1-\mathrm{e}^{-\beta\mathcal{U}(\omega,\omega_j)}) \right] |\varphi(\omega_1,\ldots,\omega_k)| \leqslant -\beta\mu n. \tag{4.14}$$

This bound is uniform in the size of the domain, which is important. It follows that, as $L\to\infty$, the ratio $Z(\mu;\omega)/Z(\mu)$ converges pointwise in μ and ω. The thermodynamic limits of $c_{n,\mu}(x)$ and $\varrho_\mu(n)$ then clearly exist. Further, $c_{n,\mu}(x)$ is bounded by

$$c_{n,\mu}(x) \leqslant \left[\int \mathrm{d}W_{00}^{n\beta}(\omega)\mathrm{e}^{-\beta\mathcal{U}(\omega)} \right]^{-1} \mathrm{e}^{-2\beta\mu n} \int \mathrm{d}W_{0x}^{n\beta}(\omega). \tag{4.15}$$

It is not hard to show that the bracket is bounded away from zero uniformly in L (but not uniformly in β and n). From Eq. (A10), we have

$$\lim_{|x|\to\infty} \lim_{L\to\infty} \int \mathrm{d}W_{0x}^{n\beta}(\omega) = 0.$$

This implies that $\boldsymbol{c}_{n,\mu}(x)$ vanishes in the limit of infinite $|x|$.

V. CONCLUSION

We introduced formula (1.1) that relates the off-diagonal correlation function and the densities of cycles of given length. This formula involves coefficients $\boldsymbol{c}_n$ that have a natural definition in terms of integrals of Wiener trajectories. We conjectured several properties for the coefficients—these properties can actually be proven in the ideal gas for all temperatures and in the interacting gas for high temperatures. These results seem to indicate that the order parameters of Feynman and Penrose and Onsager agree. However, heuristic considerations based on the present framework[15] suggest that, if the gas is in a crystalline phase, the coefficients satisfy $\boldsymbol{c}_n(x) \leqslant \mathrm{e}^{-a|x|}$ for some $a>0$ and for all n (including $n=\infty$). Besides, one expects that $\varrho(\infty)>0$ if the temperature is sufficiently low. The order parameters are not equivalent in this case.

An open problem is to establish the equivalence of the order parameters in weakly interacting gases in the presence of the Bose-Einstein condensation. Another question is whether $\boldsymbol{c}_\infty(x)$ converges, as $|x|\to\infty$, to a number that is strictly between 0 and 1. The corresponding phase would display a Bose condensate whose density is less than the density of particles in infinite cycles.

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APPENDIX A: FEYNMAN-KAC REPRESENTATION OF THE BOSE GAS

In this appendix we recall some properties of the Wiener measure, and we review the derivation of the Feynman-Kac representation of the partition functions and of the off-diagonal long-range order parameter. A complete account can be found in the excellent notes of Ginibre;[6] Faris wrote a useful survey.[4]

Let D be the d-dimensional cubic box of size L and volume $V=L^d$. We work with periodic boundary conditions, meaning that D is the d-dimensional torus $\mathbb{T}_L^d$. The state space is the Hilbert space $\mathcal{H}_{D,N}$ of square-summable complex functions on D^N that are symmetric with respect to their arguments. Let S denote the symmetric projector on $L^2(D^N)$, i.e.,

$$S\psi(x_1,\ldots,x_N) = \frac{1}{N!}\sum_{\pi\in S_N} \psi(x_{\pi(1)},\ldots,x_{\pi(N)}), \tag{A1}$$

where $x_1,\ldots,x_N\in D$ and the sum is over all permutations of N elements. The state space for N bosons in D is therefore $\mathcal{H}_{D,N}=SL^2(D^N)$, the projection of $L^2(D^N)$ onto symmetric functions.

The Hamiltonian of the system is the sum $H=T+V$ of kinetic and interaction energies. The kinetic energy is $T=-\Sigma_{j=1}^{N}\Delta_j$, where Δ_j is the Laplacian for the jth particle. Interactions are given by the multiplication operator $V=\Sigma_{1\leqslant i<j\leqslant N}U(x_i-x_j)$.

Recall that β and μ denote the inverse temperature and the chemical potential, respectively. The canonical and grand-canonical partition functions are

$$Y(\beta,V,N)=\mathrm{Tr}_{\mathcal{H}_{D,N}}\mathrm{e}^{-\beta H}, \tag{A2}$$

$$Z(\beta,V,\mu)=\sum_{N\geqslant 0}\mathrm{e}^{\beta\mu n}Y(\beta,V,N). \tag{A3}$$

Under the assumption that $U(x)$ is a stable potential and that it decays faster than $|x|^{-d}$ as $|x|\to\infty$, one can establish the existence of the thermodynamic potentials (see Ref. 11)

$$\boldsymbol{f}(\beta,\rho)=\lim_{V\to\infty}-\frac{1}{\beta V}\log Y(N), \tag{A4}$$

$$\boldsymbol{p}(\beta,\mu)=\lim_{V\to\infty}\frac{1}{V}\log Z(\mu). \tag{A5}$$

Further, $\boldsymbol{f}$ and $\boldsymbol{p}$ are related by a Legendre transform,

$$\boldsymbol{f}(\beta,\rho)=\sup_{\mu}\left[\rho\mu-\frac{1}{\beta}\boldsymbol{p}(\beta,\mu)\right]. \tag{A6}$$

This equation is useful to find $\boldsymbol{f}$ from $\boldsymbol{p}$ in the case of the ideal gas, where $\boldsymbol{p}$ can be computed explicitly.

The Feynman-Kac representation allows to express $\mathrm{e}^{-\beta H}$ in terms of Wiener trajectories (Brownian motion). We briefly review the main properties of the Wiener measure. Let $\mathcal{X}_1$ be the set of continuous paths $\omega:[0,\beta]\to D$. Consider a function $F:\mathcal{X}_1\to\mathbb{R}$ of the kind

$$F(\omega)=f(\omega(t_1),\ldots,\omega(t_n)), \tag{A7}$$

where f is a bounded measurable function on D^n, and $0<t_1<\cdots<t_n<\beta$; we extend f on $\mathbb{R}^d$ by periodicity. The integral of F with respect to the Wiener measure W_{xy}^{β} is given by

$$\int_{\mathcal{X}}F(\omega)\mathrm{d}W_{xy}^{\beta}(\omega)=\sum_{z\in\mathbb{Z}^d}\int_{\mathbb{R}^{dn}}g_{t_1}(x_1-x)g_{t_2-t_1}(x_2-x_1)\cdots g_{\beta-t_n}(y+Lz-x_n)$$
$$\times f(x_1,\ldots,x_n)\mathrm{d}x_1\cdots\mathrm{d}x_n, \tag{A8}$$

where g_t is the normalized Gaussian function with mean zero and variance $2t$,

$$g_t(x)=\frac{1}{(4\pi t)^{d/2}}\mathrm{e}^{-x^2/4t}. \tag{A9}$$

The sum over z accounts for periodic boundary conditions. A special case of Eq. (A8) is when the function F is the constant function $F(\omega)\equiv 1$; we get

$$\int\mathrm{d}W_{xy}^{\beta}(\omega)=(4\pi\beta)^{-d/2}\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-(x-y+Lz)^2/4\beta}. \tag{A10}$$

Only the term $z=0$ remains in the limit $L\to\infty$. It can be proven that such a measure exists and is unique.[6] The Wiener measure $W_{xy}^{n\beta}$ is concentrated on Hölder continuous trajectories (with any

Hölder constant less than $\frac{1}{2}$) that start at x and end at y. Integration with respect to W^β_{xy} and W^β_{00} are related as follows. Define $\omega'(t) = \omega(t) - t[(y-x)/\beta]$; then

$$\int F(\omega) \mathrm{d}W^\beta_{xy}(\omega) = \mathrm{e}^{-(y-x)^2/4\beta} \int F(\omega') \mathrm{d}W^\beta_{00}(\omega). \tag{A11}$$

The Feynman-Kac formula states that $\mathrm{e}^{-\beta H}$ is given by an integral operator.[2,4,6] We are actually dealing with bosonic particles, and it is more convenient to consider the operator $\mathrm{e}^{-\beta H} S$ that also projects onto symmetric functions. We have

$$\mathrm{e}^{-\beta H} S\psi(x_1, \dots, x_N) = \int_{D^N} K(x_1, \dots, x_N; y_1, \dots, y_N) \psi(y_1, \dots, y_N) \mathrm{d}y_1 \cdots \mathrm{d}y_N, \tag{A12}$$

where the kernel K is given by

$$K(x_1, \dots, x_N; y_1, \dots, y_N) = \frac{1}{N!} \sum_{\pi \in S_N} \int \mathrm{d}W^\beta_{x_1 y_{\pi(1)}}(\omega_1) \cdots \mathrm{d}W^\beta_{x_N y_{\pi(N)}}(\omega_N) \times \exp\left\{ - \sum_{i<j} \int_0^\beta U(\omega_i(s) - \omega_j(s)) \mathrm{d}s \right\}. \tag{A13}$$

The canonical partition function is then given by

$$Y(N) = \sum_{\pi \in S_N} \frac{1}{N!} \int_{D^N} \mathrm{d}x_1 \cdots \mathrm{d}x_N \int \mathrm{d}W^\beta_{x_1 x_{\pi(1)}}(\omega_1) \cdots \mathrm{d}W^\beta_{x_N x_{\pi(N)}}(\omega_N) \times \exp\left\{ - \sum_{i<j} \int_0^\beta U(\omega_i(s) - \omega_j(s)) \mathrm{d}s \right\}. \tag{A14}$$

We now group the cycles into closed trajectories, that may wind several times around the time direction. The number of permutations of N elements with k cycles of lengths $n_1, \dots, n_k$ (with $\sum_j n_j = N$) is

$$\frac{N!}{k! \prod_j n_j}.$$

Further, we have

$$\int_{D^{n-1}} \mathrm{d}x_2 \cdots \mathrm{d}x_n \int \mathrm{d}W^\beta_{x x_2}(\omega_1) \cdots \mathrm{d}W^\beta_{x_n y}(\omega_n) F(\omega) = \int \mathrm{d}W^{n\beta}_{xy}(\omega) F(\omega). \tag{A15}$$

The trajectory $\omega : [0, n\beta] \to D$ in the right side is the concatenation of $\omega_1, \dots, \omega_n$. The partition function (A14) can then be rewritten in the form of Eq. (2.1).

Let us turn to the Penrose and Onsager off-diagonal long-range order.[9] Given a single particle function $\varphi \in L^2(D)$, we define the operator N_φ that represents the number of particles in the state φ. The action of this operator is given by

$$(N_\varphi \psi)(x_1, \dots, x_N) = \sum_{j=1}^N \int_D \overline{\varphi(x)} \psi(x_1, \dots, \underbrace{x}_{j\text{th place}}, \dots, x_N) \varphi(x_j) \mathrm{d}x. \tag{A16}$$

It is clear that $0 \leqslant N_\varphi \leqslant N$ and that $[N_\varphi, S] = 0$. Let $\varphi_0(x) \equiv 1/\sqrt{V}$ denote the single particle ground state in the absence of interactions. It is also the Fourier function with mode $k = 0$. The average occupation of the zero mode is given by

$$\boldsymbol{\varrho}_{\rho}^{(0)} = \lim_{V\to\infty} \frac{1}{Y(N)} \mathrm{Tr}_{\mathcal{H}_{D,N}} \left[\frac{N_{\varphi_0}}{V} \mathrm{e}^{-\beta H} \right]. \tag{A17}$$

We set $N=\rho V$, and the limit exists at least along a subsequence of increasing volumes. A criterion for the Bose-Einstein condensation is that $\boldsymbol{\varrho}_{\rho}^{(0)}$ differs from zero. We can derive a Feynman-Kac expression for this order parameter. From Eqs. (A12), (A13), and (A16), we have

$$\mathrm{Tr}_{\mathcal{H}_{D,N}} N_{\varphi} \mathrm{e}^{-\beta H} = \frac{1}{(N-1)!} \int_D \mathrm{d}x \overline{\varphi(x)} \int_D \mathrm{d}y \varphi(y) \int_{D^{N-1}} \mathrm{d}x_2 \cdots \mathrm{d}x_N \sum_{\pi\in S_N} \times \int \mathrm{d}W^{\beta}_{x_1 \hat{x}_{\pi(1)}}(\omega_1) \cdots \mathrm{d}W^{\beta}_{x_N \hat{x}_{\pi(N)}}(\omega_N) \exp\left\{ -\sum_{i<j} \int_0^{\beta} U(\omega_i(s) - \omega_j(s)) \right\}. \tag{A18}$$

Here, we set $x_1=x$, $\hat{x}_1=y$, and $\hat{x}_j=x_j$ for $2\leqslant j\leqslant N$. Then $\boldsymbol{\varrho}_{\rho}^{(0)}$ can be written as

$$\boldsymbol{\varrho}_{\rho}^{(0)} = \lim_{V\to\infty} \frac{1}{V^2} \int_{D^2} \sigma_{\rho}(x-y) \mathrm{d}x \mathrm{d}y, \tag{A19}$$

where

$$\sigma_{\rho}(x-y) = \frac{1}{Y(\beta,V,N)} \frac{1}{(N-1)!} \int_{D^{N-1}} \mathrm{d}x_2 \cdots \mathrm{d}x_N \sum_{\pi\in S_N} \times \int \mathrm{d}W^{\beta}_{x_1 \hat{x}_{\pi(1)}}(\omega_1) \cdots \mathrm{d}W^{\beta}_{x_N \hat{x}_{\pi(N)}}(\omega_N) \times \exp\left\{ -\sum_{i<j} \int_0^{\beta} U(\omega_i(s) - \omega_j(s)) \right\}. \tag{A20}$$

This expression involves an open cycle from x to y, winding n times around the time direction, with $n=1,\ldots,N$. Using the concatenation property (A15) and thanks to the combinatorial factor $(N-1)!/(N-n)!$, we obtain expression (2.14) for $\sigma_{\rho}(x-y)$. The system displays off-diagonal long-range order if $\sigma_{\rho}(x)$ is strictly positive, uniformly in V,x.

APPENDIX B: A SIMPLE PROOF OF MACROSCOPIC OCCUPATION IN THE IDEAL GAS

In this section, we give a proof of the macroscopic occupation of the zero mode at low temperature. This is usually established in the grand-canonical ensemble, using a chemical potential that varies with the volume and tends to zero in the thermodynamic limit. This approach is rather un-natural and requires large deviation techniques to control the fluctuations of the number of particles. The present proof is simpler and stays within the canonical ensemble.

The computation of the pressure and of the density in the grand-canonical ensemble can be found in any textbook dealing with quantum statistical mechanics. The chemical potential must be strictly negative. The infinite volume pressure is

$$\boldsymbol{p}(\beta,\mu) = -\frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \log(1-\mathrm{e}^{-\beta(k^2-\mu)}) \mathrm{d}k, \tag{B1}$$

and the density is

$$\boldsymbol{\rho}(\beta,\mu) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\mathrm{d}k}{\mathrm{e}^{\beta(k^2-\mu)}-1} = \frac{1}{(4\pi\beta)^{d/2}} \sum_{n\geqslant 1} \mathrm{e}^{\beta\mu n} n^{-d/2}. \tag{B2}$$

The limit of $\boldsymbol{\rho}(\beta,\mu)$ as $\mu\nearrow 0$ is finite for $d\geqslant 3$ and gives the *critical density* of the ideal Bose gas, ρ_c. The graph of $\boldsymbol{p}(\beta,\mu)$ in three dimensions is plotted in Fig. 2(a). Its Legendre transform, Eq. (A6), gives $\boldsymbol{f}(\beta,\rho)$, see Fig. 2(b); it is nonanalytic at ρ_c. The value of $a(\beta)$ is given by

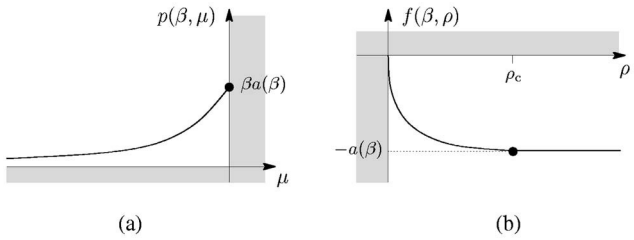

FIG. 2. The pressure and the free energy of the ideal gas in three dimensions.

$$a(\beta) = \lim_{\mu \nearrow 0} \frac{1}{\beta} p(\beta,\mu) = \lim_{\rho\to\infty} -f(\beta,\rho). \tag{B3}$$

The very nature of the Bose-Einstein condensation is that the occupation number for $k=0$ becomes macroscopic. The average occupation of the zero mode $\varrho_\rho^{(0)}$, see Eq. (A17), can be rewritten as

$$\varrho_\rho^{(0)} = \lim_{V\to\infty} \frac{1}{Y(N)} \sum_{(n_k):N} \frac{n_0}{V} e^{-\beta\Sigma_k n_k k^2}. \tag{B4}$$

Here, $N=V\rho$, and the sum is over all occupation numbers $n_k \geqslant 0$, with indices $k \in ((2\pi/L)\mathbb{Z})^d$, such that $\Sigma_k n_k = N$. The heart of the Bose-Einstein condensation is the following result.

Theorem 4: *For* $d \geqslant 3$, *the single particle ground state is macroscopically occupied if* $\rho > \rho_c$. *More precisely*,

$$\varrho_\rho^{(0)} = \max(0, \rho - \rho_c).$$

Proof: It is clear that $\varrho_\rho^{(0)} \geqslant 0$. We now establish that $\varrho_\rho^{(0)} \geqslant \rho - \rho_c$. Let us introduce the average occupation of the mode k,

$$\langle n_k \rangle = \frac{1}{Y(N)} \sum_{(n_{k'}):N} n_k e^{-\beta\Sigma_{k'} n_{k'} k'^2}.$$

Thanks to the sum rule $N=\Sigma_k \langle n_k \rangle$, we have

$$\varrho_\rho^{(0)} = \rho - \lim_{V\to\infty} \sum_{k\neq 0} \frac{\langle n_k \rangle}{V}. \tag{B5}$$

We can view n_k as a random variable taking positive integer values; its expectation is therefore given by

$$\langle n_k \rangle = \sum_{i\geqslant 1} \mathrm{Prob}(n_k \geqslant i), \tag{B6}$$

where we defined

$$\mathrm{Prob}(n_k \geqslant i) = \frac{1}{Y(N)} \sum_{(n_{k'}):N,i} e^{-\beta\Sigma_{k'} n_{k'} k'^2}. \tag{B7}$$

The sum is restricted to $(n_{k'})$ such that $\Sigma n_{k'} = N$ and $n_k \geqslant i$. The change of variable $n_k \to n_k - i$ leads to

$$\mathrm{Prob}(n_k \geqslant i) = \mathrm{e}^{-\beta i k^2} \frac{Y(N-i)}{Y(N)}. \tag{B8}$$

The ratio of partition functions is also equal to the probability $\mathrm{Prob}(n_0 \geqslant i)$, which is smaller than 1. Equations (B6) and (B8) give a bound for the occupation numbers of all modes $k \neq 0$, namely,

$$\langle n_k \rangle \leqslant \frac{1}{\mathrm{e}^{\beta k^2} - 1}. \tag{B9}$$

Notice that $\langle n_k \rangle \leqslant 1/\beta k^2 \leqslant L^2/4\pi^2\beta$ for $k \neq 0$. This shows that only the zero mode can be macroscopically occupied (for $d \geqslant 3$). Inserting this bound into Eq. (B5), we obtain

$$\boldsymbol{\varrho}_\rho^{(0)} \geqslant \rho - \frac{1}{(2\pi)^d} \lim_{V\to\infty} \sum_{k\neq 0} \left(\frac{2\pi}{L}\right)^d \frac{1}{\mathrm{e}^{\beta k^2} - 1}. \tag{B10}$$

The limit converges to expression (B2) with $\mu = 0$, which is equal to ρ_c.

There remains to show that $\boldsymbol{\varrho}_\rho^{(0)} \leqslant \max(0, \rho - \rho_\mathrm{c})$. From Eq. (B8) with $k=0$, and using the equivalence of ensembles, we have for any fixed a,

$$\lim_{V\to\infty} \frac{1}{\beta V} \log \mathrm{Prob}(n_0 \geqslant Va) = \boldsymbol{f}(\beta, \rho) - \boldsymbol{f}(\beta, \rho - a). \tag{B11}$$

The right side of Eq. (B11) is strictly negative when $a > \max(0, \rho - \rho_\mathrm{c})$. There exists $\delta > 0$ such that for large enough volumes,

$$\mathrm{Prob}(n_0 \geqslant Va) \leqslant \mathrm{e}^{-V\delta}. \tag{B12}$$

Let us assume that $\rho - \rho_\mathrm{c} > 0$; the case $\rho - \rho_\mathrm{c} \leqslant 0$ can be treated similarly. Using Eq. (B6) with $k = 0$, together with Eq. (B12), we get

$$\frac{\langle n_0 \rangle}{V} = \frac{1}{V} \sum_{1 \leqslant i \leqslant aV} \mathrm{Prob}(n_0 \geqslant i) + \frac{1}{V} \sum_{aV < i \leqslant N} \mathrm{Prob}(n_0 \geqslant i) \leqslant a + \rho \mathrm{e}^{-V\delta}. \tag{B13}$$

It follows that $\boldsymbol{\varrho}_\rho^{(0)}$ is less than any number $a > \rho - \rho_\mathrm{c}$, hence $\boldsymbol{\varrho}_\rho^{(0)} \leqslant \rho - \rho_\mathrm{c}$.

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Final state problem for Korteweg–de Vries type equations

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We study the final state problem for the Korteweg–de Vries type equations: $u_t - 1/\rho|\partial_x|^{\rho-1}u_x = \lambda u^2 u_x$, $(t,x) \in \mathbf{R}^+ \times \mathbf{R}$, $\|u(t) - F_S(t)\|_{\mathbf{L}^2} \to 0$ as $t \to \infty$, where $\lambda \in \mathbf{R}$, the function $F_S(t)$ we call a final state, defined by the final data u_+. We show that there does not exist a nontrivial solution of this equation in the case of $F_S(t) = U(t)u_+$, where $U(t)$ is the free evolution group of this equation. We construct the modified wave operator for the Korteweg–de Vries type equations under the conditions that the final data u_+ arc real-valued functions and the Fourier transform $\hat{u}_+(\xi)$ vanishes at the origin. © *2006 American Institute of Physics.*
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I. INTRODUCTION

We study the final state problem for the Korteweg–de Vries type equations

$$u_t - 1/\rho|\partial_x|^{\rho-1}u_x = \lambda u^2 u_x,\ (t,x) \in \mathbf{R}^+ \times \mathbf{R},$$
$$\|u(t) - F_S(t)\|_{\mathbf{L}^2} \to 0 \text{ as } t \to \infty, \tag{1.1}$$

where $\rho \geqslant 2$, $\lambda \in \mathbf{R}$, $|\partial_x|^\rho = \mathcal{F}^{-1}|\xi|^\rho \mathcal{F}$, $\mathcal{F}\phi$, or $\hat{\phi}$ is the Fourier transform of ϕ defined by $\mathcal{F}\phi(\xi) = (1/\sqrt{2\pi})\int_{\mathbf{R}} e^{-ix\xi}\phi(x)dx$ and the inverse Fourier transformation $\mathcal{F}^{-1}$ is given by $\mathcal{F}^{-1}\phi(x) = (1/\sqrt{2\pi})\int_{\mathbf{R}} e^{ix\xi}\phi(\xi)d\xi$. If $\rho=2$, then Eq. (1.1) converts to the well-known modified Benjamin–Ono equation

$$u_t - \tfrac{1}{2}\mathcal{H}u_{xx} = \lambda u^2 u_x, \tag{1.2}$$

where $\mathcal{H}\phi = -\mathcal{F}^{-1}(i\xi/|\xi|)\widehat{\phi} = (1/\pi)\mathrm{PV}\int_{\mathbf{R}}(\phi(y)/x-y)dy$ is the Hilbert transform. For the case of $\rho=3$, Eq. (1.1) reduces to the famous modified Korteweg–de Vries equation

$$u_t + \tfrac{1}{3}u_{xxx} = \lambda u^2 u_x. \tag{1.3}$$

Another example is the Kawahara equation (see. Ref. 1)

$$u_t - \tfrac{1}{5}\partial_x^5 u = \lambda u^2 u_x,$$

when $\rho=5$.

The function $F_S(t)$ we call a final state, defined by the final data u_+. If the function $F_S(t)$ can be taken in the form

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$$F_S(t) = U(t)u_+ = \mathcal{F}^{-1}\exp\left(\frac{i}{\rho}t|\xi|^{\rho-1}\xi\right)\widehat{u_+}(\xi)$$

and the final problem (1.1) has a nontrivial solution, then we say that there exists a usual wave operator for the final state problem. However, below we will show that there does not exist a nontrivial solution of Eq. (1.1) in the case of $F_S(t)=U(t)u_+$. Therefore we need to modify the time dependence of the final state $F_s(t)$, in other words, we will construct a modified wave operator. The modified wave operator was first constructed by Ozawa[2] for cubic nonlinear Schrödinger equations and then by Ozawa and the first author[3] for the derivative nonlinear Schrödinger equation, by changing it via a suitable transformation (see Ref. 4) to a system of cubic nonlinear Schrödinger equations without derivatives of an unknown function. However, as far as we know the existence of the modified wave operators was not proved for other types of dispersive equations with nonlinearities involving derivatives of the unknown function, such as the modified Benjamin–Ono equation (1.2) and the modified Korteweg–de Vries equation (1.3).

The Cauchy problem for the Korteweg–de Vries equations (1.1) with $\rho=3$ and nonlinearities of the form $\partial_x u^\varkappa$ was studied extensively (see, e.g., Refs. 5–8 and 26 for the existence of unique solutions and Refs. 9–16 for the large time asymptotic behavior of small solutions in the case of supercritical nonlinearity $\varkappa>3$). In the case of the modified Benjamin–Ono equation (1.2), namely, $\rho=2$ and $\varkappa>3$, the large time asymptotic behavior of small solutions were studied in Refs. 17 and 18.

One of the important problems of scattering theory is the construction of the so-called scattering operator, which is defined by the direct and inverse wave operators. In the case of critical nonlinearity it appears to be impossible to find the usual scattering operator, so a problem constructing the modified scattering operator arises. The inverse modified wave operator is closely related to the large time asymptotic behavior of solutions to the Cauchy problem. We now refer some results on the large time asymptotic behavior of small solutions to the Cauchy problem (1.1) for cases $\rho=2,3$, and 5. The case of the modified Korteweg–de Vries equation $\rho=3$ was considered in Refs. 19 and 20. If the initial data $u_0 \in \mathbf{H}^{1,1}$ are real-valued functions with a sufficiently small norm, then there exists a unique global solution $u \in \mathbf{C}(\mathbf{R};\mathbf{H}^{1,1})$ of the Cauchy problem for modified Korteweg–de Vries equation (1.3). Moreover, if we (denote by $S(t,x)=(1/\sqrt[3]{t})\varphi(x/\sqrt[3]{t})$ the self-similar solution of the modified Korteweg–de Vries equation (1.3) such that

$$S_t - \frac{\lambda}{3}(S^3)_x + \frac{1}{3}S_{xxx} = 0$$

and

$$\int_{\mathbf{R}} S(t,x)dx = \int_{\mathbf{R}} u_0(x)dx,$$

then there exist unique functions H_j and $B_j \in \mathbf{L}^\infty$ (B_j are real valued), $j=1,2$, such that the following asymptotic formula is valid for large time t uniformly with respect to $x \in \mathbf{R}$,

$$u(t,x) = \frac{1}{\sqrt[3]{t}}\varphi\left(\frac{x}{\sqrt[3]{t}}\right) + \frac{1}{\sqrt[3]{t}}\mathrm{Re}\,\mathcal{A}i\left(\frac{x}{\sqrt[3]{t}}\right)\sum_{j=1}^{2} H_j\left(\frac{x}{t}\right)\exp\left(iB_j\left(\frac{x}{t}\right)\log\frac{|x|}{\sqrt[3]{t}}\right) + O\left(t^{\gamma-5/12}\left(1+\frac{x}{\sqrt[3]{t}}\right)^{-1/4}\right),$$

where $\gamma \in (0,1/10)$ and $\mathcal{A}i(x)=(1/\pi)\int_0^\infty e^{ixz+(i/3)z^3}dz$ is the Airy–Fock function.

The large time asymptotic behavior of small solutions to the Cauchy problem for the modified Benjamin–Ono equation (1.2) was studied in Refs. 17 and 18. It was proved that if the initial data $u_0 \in \mathbf{H}^{2,0}\cap\mathbf{H}^{1,1}$ are real-valued functions with sufficiently small norm, then there exists a unique global solution $u \in \mathbf{C}(\mathbf{R};\mathbf{H}^{1,0})\cap\mathbf{L}^\infty(\mathbf{R};\mathbf{L}^2)$ of the Cauchy problem for the modified Benjamin–Ono equation (1.2). Moreover there exists a unique function $u_+ \in \mathbf{L}^\infty$ such that the following asymptotic formula is valid

$$u(t,x)=\frac{1}{\sqrt{t}}\mathrm{Re}\left(G\left(\frac{x}{\sqrt{t}}\right)u_+\left(\frac{x}{t}\right)\exp\left(\frac{ix^2}{2t}-ig\left(\frac{x}{t}\right)\log t\right)\right)+O(t^{-1/2-\gamma})$$

as $t\to\infty$ uniformly with respect to $x\in\mathbf{R}$, where

$$G(x)=\frac{1}{\sqrt{-\pi i}}\int_{-x}^{\infty}e^{-iy^2}dy, g(x)=\frac{3}{4}x\theta(x)|u_+(x)|^2,$$

$\theta(x)=1$ for $x<0$ and $\theta(x)=0$ for $x\geqslant 0, 0<\gamma<1/4$.

Finally, the large time asymptotic behavior of small solutions to the Cauchy problem for the generalized Kawahara equation

$$u_t-\frac{1}{5}\partial_x^5u=\lambda u^{\varkappa-1}u_x$$

with supercritical nonlinearities of the order $\varkappa>5$ were obtained in Ref. 21, where it was proved that if the initial data $u_0\in\mathbf{H}^{1,1}$ are real-valued functions with sufficiently small norm then there exists a unique function $u_+\in\mathbf{L}^\infty\cap\mathbf{L}^2$ such that the asymptotic behavior

$$u(t,x)=\frac{1}{\sqrt[5]{t}}\mathrm{Re}\,A\left(\frac{x}{\sqrt[5]{t}}\right)u_+\left(\frac{x}{t}\right)+O\left(t^{-1/5-\gamma}\left(1+\frac{|x|}{\sqrt[5]{t}}\right)^{-3/8}\right)$$

is true for large t uniformly with respect to $x\in\mathbf{R}$, where $0<\gamma<(\varkappa-5)/5$,

$$A(x)=\frac{1}{\pi}\int_0^\infty e^{ixz+(i/5)z^5}dz.$$

We see that the Cauchy problem for the Korteweg–de Vries type equations (1.1) was studied and the asymptotic behavior of solutions was found for the cases $\rho=2$ and 3. However, the asymptotic behavior of solutions to the Cauchy problem for the Korteweg–de Vries type equations (1.1) of higher order $\rho>3$ is an open problem. The difficulty in studying the higher order cases $\rho>3$ comes from the time decay properties of solutions to the corresponding linear problem. Thus to be able to get better time decay estimates of solutions, a condition arises that the Fourier transform of the initial data must vanish rapidly at the origin. Note that the existence of the modified scattering operator is an important open problem even for the lower order cases $\rho\geqslant 2$ since it is necessary to study carefully the range and the domain of the inverse modified wave operator.

The aim of the present paper is to construct the modified wave operator for the Korteweg–de Vries type equations (1.1) under the conditions that the final data u_+ are real-valued functions and the Fourier transform $\hat{u}_+(\xi)$ vanishes rapidly at the origin. We first obtain the $\mathbf{L}^\infty$ estimates and the asymptotic behavior for solutions to the linear dispersive equations of the Korteweg–de Vries type. Denote the free evolution group $U(t)=\mathcal{F}^{-1}\exp((it/\rho)|\xi|^{\rho-1}\xi)\mathcal{F}$, where $\rho\geqslant 2$. The usual Lebesgue space $\mathbf{L}^p=\{\phi;\|\phi\|_{\mathbf{L}^p}<\infty\}$, with the norm $\|\phi\|_{\mathbf{L}^p}=(\int_{\mathbf{R}}|\phi(x)|^p dx)^{1/p}$ if $1\leqslant p<\infty$ and $\|\phi\|_{\mathbf{L}^\infty}=\sup_{x\in\mathbf{R}}|\phi(x)|$ if $p=\infty$. The weighted Sobolev space is defined by $\mathbf{H}_p^{m,s}=\{\phi\in\mathbf{L}^p;\|\langle x\rangle^s\langle i\partial_x\rangle^m\phi\|_{\mathbf{L}^p}<\infty\}, m,s\in\mathbf{R}$ with $\langle x\rangle=\sqrt{1+|x|^2}$. The index 0 we usually omit if it does not cause confusion. We say that $\phi=O(\psi)$ in $\mathbf{L}^p$ for all $t\geqslant T$, if the estimate

$$\|\phi\|_{\mathbf{L}^p}\leqslant C|\psi|$$

is true for all $t\geqslant T$, where $C>0$ does not depend on ϕ. We also introduce the norm

$$\|\nu\|_{\mathbf{Z}^\alpha}\equiv\|\{\xi\}^{-\alpha}\nu(\xi)\|_{\mathbf{L}^\infty}+\|\{\xi\}^{1-\alpha}\nu'(\xi)\|_{\mathbf{L}^\infty},$$

where $\{\xi\}=|\xi|/\langle\xi\rangle$.

Theorem 1.1: *The estimate is true*

$$\|U(t)v\|_{\mathbf{L}^\infty} \leqslant Ct^{-(1+\alpha)/\rho}\||\partial_x|^{-\alpha}v\|_{\mathbf{L}^1} \tag{1.4}$$

for all $t>0$, *provided that the right-hand side is finite, where* $\alpha\in[0,\rho/2-1],\rho\geqslant 2$. *Furthermore, the asymptotic formula for large time* t *holds*

$$U(t)v = t^{-1/2}\mathrm{Re}(\theta(x)(FE\hat{v})(\chi)) + O(\|\hat{v}\|_{\mathbf{Z}^\alpha}t^{-\alpha/\rho-1/\rho(1-1/\rho)}), \tag{1.5}$$

in $\mathbf{L}^p$ *for* $2\leqslant p\leqslant\infty$, *where* $0<\alpha<(\rho-1)(1-1/p)$,

$$F(\chi) = \sqrt{\frac{4}{i(\rho-1)}}|\chi|^{1-\rho/2},$$

$E=e^{-i(1-1/\rho)t|\chi|^{\rho-1}\chi}$ and $\chi=|x/t|^{1/(\rho-1)}$, $\theta(x)=1$ for $x<0$ and $\theta(x)=0$ for $x\geqslant 0$.

Remark 1.1: The proof of theorem 1.1 follows the method of Ref. 22 concerning the estimates of the free evolution group $\mathcal{F}^{-1}\exp((i/\rho)t|\xi|^\rho)\mathcal{F}$. *The difference is in the estimates for the positive half-line, where the free evolution group*

$$\mathcal{F}^{-1}\exp(i/\rho t|\xi|^{\rho-1}\xi)\mathcal{F}$$

decays exponentially, because the symbol $|\xi|^{\rho-1}\xi$ *is an odd function. Therefore the assumption that the Fourier transform of the final data* $\hat{u}_+$ *vanishes at the origin implies that the leading term of the asymptotics becomes a remainder one for the positive half-line. If* $\hat{u}_+$ *does not vanish at the origin, then we need to consider a leading term (in the short-range region) generated by the value* $\hat{u}_+(0)$.

Remark 1.2: We need estimate (1.4) for the proof of the Strichartz type estimate (see lemma 3.1 below). We see that the $\mathbf{L}^2$*-norm of the remainder in Eq. (1.5) decays faster than* $t^{1/2\rho-1/2}$ *in the case of* $\alpha>\rho/2-1$ *and* $\rho\geqslant 2$.

Remark 1.3: If $\hat{v}^{(j)}(0)=0$ *for* $0\leqslant j\leqslant k=[\alpha]$ *and* $v\in\mathbf{H}^{0,k+2}$, *then*

$$\|\hat{v}\|_{\mathbf{Z}^\alpha} \leqslant C\|\hat{v}\|_{\mathbf{L}^\infty} + C\|\hat{v}^{(k+1)}\|_{\mathbf{L}^\infty} \leqslant C\|\hat{v}\|_{\mathbf{H}^{k+2}} = C\|v\|_{\mathbf{H}^{0,k+2}}.$$

For the case of $\rho=3$, *we can choose* $1/2<\alpha<1$, *then we have*

$$\|\hat{v}\|_{\mathbf{Z}^\alpha} \leqslant C\|v\|_{\mathbf{H}^{0,2}}$$

if $v\in\mathbf{H}^{0,2}$ *and* $\int_{\mathbf{R}}v(x)dx=0$.

We now give some heuristic considerations to explain the construction of the modified wave operator. Let us assume that the solutions of nonlinear problem Eq. (1.1) have time decay properties similar to that of the linearized equation and apply the result of theorem 1.1 to evaluate the asymptotic behavior of the nonlinear term in Eq. (1.1). Since the final data u_+ are real valued we have $\widehat{u_+}(\xi)=\widehat{u_+}(-\xi)$. Then the main term in Eq. (1.1) appears as a linear combination of the following two oscillating terms

$$I_1 \equiv t^{-3/2}\mathrm{Re}(i\theta(x)\lambda\chi(F|F|^2E|\widehat{u_+}|^2\widehat{u_+})(\chi))$$

and

$$I_2 \equiv t^{-3/2}\mathrm{Re}(i\theta(x)\lambda\chi(F^3E^3\widehat{u_+}^3)(\chi))$$

for $x<0$. It is easy to check that the $\mathbf{L}^2$ norm of I_1 and I_2 decays like t^{-1}. Hence, it is divergent when integrating in time. This is the reason why it is impossible to find the solutions of Eq. (1.1) in the neighborhood of the free solutions (see theorem 1.3 below). The term I_1 can be removed by introducing a suitable phase correction since it oscillates similarly to the solutions of the linear problem. And the term I_2 can be shown via integrating by parts to be a remainder (since its oscillating properties differ from that of the solutions to the linear problem, see Ref. 23. In the case of lower order ρ, the method used in Ref. 23 could be applicable. However, in the case of

fractional or higher order ρ, the computations become complicated. So we avoid here the integration by parts and instead we use the Fourier image to find an approximate solution of the nonlinear problem. (See Sec. III for the details, where the ordinary differential equations involving terms associated with I_1 and I_2 is studied.) The previous methods of Refs. 2 and 3 for constructing the modified wave operator were based on the substitution of an approximate solution to the linear equation and then considered the equation for differences. This method seems to be difficult to apply to our problem since it requires ρ times differentiation of an approximate solution. Finally we note that the term I_2 does not appear in the case of the nonlinear Schrödinger type equations with the gauge invariant nonlinearity $|u|^2u$.

Denote

$$\mathbf{W}^\alpha = \{\nu; \|\nu\|_{\mathbf{W}^\alpha} \equiv \|\langle\xi\rangle^3 \nu\|_{\mathbf{z}^\alpha} < \infty\}.$$

Theorem 1.2: *Let the final data u_+ be a real-valued function and the norm $\|\widehat{u_+}\|_{\mathbf{W}^\alpha} \leqslant \varepsilon, \max\{(\rho-2)/2, (3\rho-7)/4\} < \alpha \leqslant \max\{\rho-2, (\rho-1)/2\}, \rho \geqslant 2$. Then there exists a time $T \geqslant 1$ and $\varepsilon > 0$ such that Eq. (1.1) has a unique solution $u \in \mathbf{L}^\infty([T,\infty); \mathbf{H}^2) \cap \mathbf{C}([T,\infty); \mathbf{H}^1)$. Moreover, the asymptotic formula is true*

$$\|u(t) - U(t)w(t)\|_{\mathbf{H}^2} \leqslant Ct^{-\min\{b,(2\alpha-\rho+3)/\rho\}},$$

where $b < \alpha/\rho + 1/2\rho$ and $w(t)$ are the solutions of the ordinary differential equations

$$\widehat{w}_t(t,\xi) = \frac{1}{t}(i\lambda\xi|F\widehat{w}|^2\widehat{w} + i\widetilde{\lambda}\xi F^2 E^\nu \mathcal{D}_\mu \widehat{w}^3) \tag{1.6}$$

with the final condition

$$\lim_{t\to\infty} \widehat{w}(t) e^{-i\xi\lambda|\widehat{u_+}(\xi)|^2 \log t} = \widehat{u_+}(\xi),$$

where

$$\lambda \in \mathbf{R}, \quad \nu = (1-3^{1-\rho})/(\rho-1), \quad \mu = 3^{\rho-1}, \quad \widetilde{\lambda} = \lambda 3^{3\rho/2-4}$$

$$F = \sqrt{\frac{4}{i(\rho-1)}}|\xi|^{1-\rho/2}, \quad \mathcal{D}_\omega \phi = \omega^{-1/2}\phi(x|\omega|^{-1/(\rho-1)}), \quad E = e^{-i(1-1/\rho)t|\xi|^{\rho-1}\xi}.$$

We note here that the existence of solutions $\widehat{w}(t) \in \mathbf{C}([1,\infty); \mathbf{W}^\alpha)$ to Eq. (1.6) is shown in lemma 3.2 below.

Remark 1.4: For the convenience of the reader we state the result of theorem 1.2 for the modified Korteweg–de Vries case ($\rho=3$). Let the final data u_+ be a real-valued function and the norm $\|\widehat{u_+}\|_{\mathbf{W}^\alpha} = \|\langle\xi\rangle^3\nu\|_{\mathbf{z}^\alpha} \leqslant \varepsilon, \alpha \in (1/2, 1]$. (By remark 1.3, if $\int_{\mathbf{R}} u_+(x)dx = 0$ and $u_+ \in \mathbf{H}^{3,2}$, then $\widehat{u_+} \in \mathbf{W}^\alpha$). Then there exists a time $T \geqslant 1$ and $\varepsilon > 0$ such that Eq. (1.1) with $\rho=3$ has a unique solution $u \in \mathbf{L}^\infty([\mathbf{T},\infty); \mathbf{H}^2) \cap \mathbf{C}([T,\infty); \mathbf{H}^1)$. Moreover, the asymptotic formula is true

$$\|u(t) - U(t)w(t)\|_{\mathbf{H}^2} \leqslant Ct^{-b},$$

where $0 < b < (2\alpha+1)/6$ and $w(t)$ is the solution of the ordinary differential Eq. (1.6) with the final condition

$$\lim_{t\to\infty} \widehat{w}(t) e^{-i\xi\lambda|\widehat{u_+}(\xi)|^2 \log t} = \widehat{u_+}(\xi)$$

and

$$\lambda \in \mathbf{R}, \quad \nu = 4/9, \quad \mu = 9, \quad \widetilde{\lambda} = \lambda\sqrt{3},$$

$$F = \sqrt{\frac{2}{i|\xi|}}, \mathcal{D}_\omega \phi = \omega^{-1/2}\phi(x|\omega|^{-1/2}), \quad E = e^{-(2i/3)t\xi^3}.$$

For the modified Benjamin–Ono case $(\rho=2)$ *we have the following result. Let the final data* u_+ *be a real-valued function and the norm* $\|\widehat{u_+}\|_{\mathbf{W}^\alpha} = \|\langle\xi\rangle^3 \nu\|_{\mathbf{z}^\alpha} \leqslant \varepsilon, \alpha \in (0,1/2]$. *(By remark 1.3, if* $\int_{\mathbf{R}} u_+(x)dx = 0$ *and* $u_+ \in \mathbf{H}^{3,1}$, *then* $\widehat{u_+} \in \mathbf{W}^\alpha$*). Then there exists a time* $T \geqslant 1$ *and* $\varepsilon > 0$ *such that Eq. (1.1) with* $\rho=2$ *has a unique solution* $u \in \mathbf{L}_\infty([T,\infty);\mathbf{H}^2) \cap \mathbf{C}([T,\infty);\mathbf{H}^1)$. *Moreover, the asymptotic formula is true*

$$\|u(t) - U(t)w(t)\|_{\mathbf{H}^2} \leqslant Ct^{-b},$$

where $0 < b < (2\alpha+1)/4$ *and* $w(t)$ *are the solution of the ordinary differential Eq. (1.6) with the final condition*

$$\lim_{t\to\infty} \widehat{w}(t)e^{-i\xi\lambda|\widehat{u_+}(\xi)|^2 \log t} = \widehat{u_+}(\xi),$$

where

$$\lambda \in \mathbf{R}, \quad \nu = 2/3, \quad \mu = 3, \quad \tilde{\lambda} = \lambda 3^{-1},$$

$$F = \sqrt{\frac{4}{i}}, \quad \mathcal{D}_\omega \phi = \omega^{-1/2}\phi(x|\omega|^{-1}), \quad E = e^{(-i/2)t|\xi|\xi}.$$

Remark 1.5: By theorem 1.1 and lemma 3.2 we see that

$$\partial_x^j U(t)w(t) = t^{-1/2}\mathrm{Re}(\theta(x)(FE)(\chi)e^{i\chi\lambda|\widehat{Fu_+}(\chi)|^2 \log t}\chi^j \widehat{u_+}(\chi)) + O(t^{-b})$$

in $\mathbf{L}^2$ *for* $j=0,1,2$, *where* $(\rho-1)/2\rho < b < \alpha/\rho + 1/2\rho$. *Therefore, the asymptotic behavior of theorem 1.2 can be written in the form*

$$\|\partial_x^j u(t) - t^{-1/2}\mathrm{Re}((FE)(\chi)e^{i\chi\lambda|\widehat{Fu_+}(\chi)|^2 \log t}\chi^j \hat{u}_+(\chi))\|_{\mathbf{L}^2(-\infty,0)} + \|\partial_x^j u(t)\|_{\mathbf{L}^2(0,\infty)} \leqslant Ct^{-b}\|\widehat{u_+}\|\mathbf{w}^\alpha.$$

Next we present the nonexistence of the usual wave operator in the case of $\lambda \neq 0$.

Theorem 1.3: *Let* u_+ *satisfy the assumptions of theorem 1.2. We also assume that* $\lambda \neq 0$ *and that there exists a solution* u *for Eq. (1.1) such that*

$$\lim_{t\to\infty} \|u(t) - U(t)u_+\|_{\mathbf{H}^1} = 0.$$

Then $u=0$.

The outline of the paper is as follows. Section II is devoted to the proof of theorem 1.1. We prepare several lemmas in Sec. III. We prove theorem 1.2 in Sec. IV. Then the last Sec. V is devoted to the proof of theorem 1.3.

II. PROOF OF THEOREM 1.1

For the proof of estimate (1.4) we refer to Ref. 6 (proposition 2.3) and Ref. 7 (Remark b in theorem 2.2). We now prove the asymptotic behavior of Eq. (1.5). Consider the case $x<0$. Since ν is a real-valued function, so that $\hat{\nu}(-\xi) = \hat{\nu}(\xi)$, we can write the identity

$$U(t)\nu = \sqrt{\frac{2}{\pi}}t^{-1/\rho}\mathrm{Re}\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}(\xi t^{-1/\rho})d\xi$$

$$= \sqrt{\frac{2}{\pi}}t^{-1/\rho}\mathrm{Re}\left(\hat{\nu}(\chi)\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}d\xi + \int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}(\hat{\nu}(\xi t^{-(1/\rho)}) - \hat{\nu}(\chi))d\xi\right), \qquad (2.1)$$

where $\eta = xt^{-1/\rho}$, $\chi = \mu t^{-1/\rho} = (|x|/t)^{1/(\rho-1)}$ and $\mu = |\eta|^{1/(\rho-1)} > 0$.

Consider the asymptotic behavior with respect to $\mu \to \infty$ (i.e., $\eta \to -\infty$) for the first summand on the right-hand side of Eq. (2.1)

$$\int_0^\infty e^{-i\xi\mu^{\rho-1}+(i/\rho)\xi^\rho}d\xi = e^{-i(1-1/\rho)\mu^\rho}\int_0^\infty e^{iS(\xi,\mu)}d\xi,$$

where $S(\xi,\mu) = 1/\rho(\xi^\rho - \mu^\rho - \rho\mu^{\rho-1}(\xi-\mu))$. We can define a new variable

$$z(\xi,\mu) = \mu + \mu^{1-\rho/2}\sqrt{\frac{2}{\rho-1}S(\xi,\mu)}\,\mathrm{sign}(\xi-\mu).$$

Note that $z_\xi(\mu,\mu) = 1$ and (see Ref. 24)

$$\int_{z(0,\mu)}^\infty e^{i(\rho-1/2)\mu^{\rho-2}(z-\mu)^2}dz = \sqrt{\frac{2\pi}{i(\rho-1)}}\mu^{1-\rho/2} + O(\mu^{1-\rho})$$

for $\mu \to \infty$, where $z(0,\mu) = \mu(1-\sqrt{2/\rho})$. Then applying the identity

$$e^{iS(\xi,\mu)} = \frac{1}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}\partial_\xi((\xi-\mu)e^{iS(\xi,\mu)})$$

we integrate by parts in the second summand

$$\int_0^\infty e^{iS(\xi,\mu)}(1-z_\xi(\xi,\mu))d\xi = \int_0^\infty (\xi-\mu)e^{iS(\xi,\mu)}\partial_\xi\left(\frac{1-z_\xi(\xi,\mu)}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}\right)d\xi + O(\mu^{1-\rho}).$$

Hence,

$$\left|\int_0^\infty e^{iS(\xi,\mu)}(1-z_\xi(\xi,\mu))d\xi\right| \leqslant C\mu^{-1}\int_0^{2\mu}\frac{|\xi-\mu|d\xi}{1+(\xi-\mu)^2\mu^{\rho-2}} + C\mu^{1-\rho/2}\int_{2\mu}^\infty \xi^{-1-\rho/2}d\xi + O(\mu^{1-\rho})$$

$$= O(\mu^{1-\rho}\ln\mu).$$

Therefore,

$$\sqrt{\frac{2}{\pi}}t^{-1/\rho}\mathrm{Re}\left(\hat{\nu}(\chi)\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}d\xi\right) = t^{-1/2}\mathrm{Re}(FE\hat{\nu}(\chi)) + O(t^{-1/\rho}\hat{\nu}(\chi)\mu^{1-\rho}\ln\mu),$$

where the remainder term $O(t^{-1/\rho}\hat{\nu}(\chi)\mu^{1-\rho}\ln\mu)$ satisfies the estimates of the theorem. For the second summand on the right-hand side of Eq. (2.1) we apply the identity

$$e^{i\xi\eta+(i/\rho)\xi^\rho} = \frac{1}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}\frac{\partial}{\partial\xi}((\xi-\mu)e^{i\xi\eta+(i/\rho)\xi^\rho}),$$

then the integration by parts yields

$$\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}(\hat{\nu}(\xi t^{-1/\rho})-\hat{\nu}(\chi))d\xi=\frac{\mu}{1+i\mu^\rho}\hat{\nu}(\chi)+t^{-1/\rho}\int_0^\infty\frac{(\xi-\mu)e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}'(\xi t^{-1/\rho})d\xi}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}$$
$$+i\int_0^\infty\frac{(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})+(\rho-1)(\xi-\mu)^2\xi^{\rho-2}}{(1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1}))^2}$$
$$\times(\hat{\nu}(\xi t^{-1/\rho})-\hat{\nu}(\mu t^{-1/\rho}))e^{i\xi\eta+(i/\rho)\xi^\rho}d\xi\equiv\sum_{j=1}^3 I_j(t,x).$$

The first integral $I_1(t,x)$ is estimated for all $t\geqslant 1$ by

$$\|I_1(t)\|_{\mathbf{L}_x^\infty}\leqslant\left\|\frac{\mu}{\langle\mu\rangle^\rho}\hat{\nu}(\mu t^{-1/\rho})\right\|_{\mathbf{L}_x^\infty}\leqslant Ct^{-\alpha/\rho}\|\{\xi\}^{-\alpha}\hat{\nu}(\xi)\|_{\mathbf{L}^\infty}$$

if $0<\alpha<\rho-1$ and

$$\|I_1(t)\|_{\mathbf{L}_x^2}\leqslant Ct^{1/2\rho}\left\|\frac{\mu^{\rho/2}}{\langle\mu\rangle^\rho}\hat{\nu}(\mu t^{-1/\rho})\right\|_{\mathbf{L}_\mu^2}\leqslant Ct^{1/2\rho-\alpha/\rho}\|\{\xi\}^{-\alpha}\hat{\nu}(\xi)\|_{\mathbf{L}^\infty}\left\|\frac{\mu^{\alpha+\rho/2}}{\langle\mu\rangle^\rho}\right\|_{\mathbf{L}_\mu^2}\leqslant Ct^{1/2\rho-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}\tag{2.2}$$

if $0<\alpha<(\rho-1)/2$. For the second term we find

$$\|I_2(t)\|_{\mathbf{L}_x^\infty}\leqslant t^{-1/\rho}\left\|\int_0^\infty\frac{(\xi-\mu)e^{i\xi\eta+i/\rho\xi^\rho}}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}\hat{\nu}'(\xi t^{-1/\rho})d\xi\right\|_{\mathbf{L}_\mu^\infty}$$
$$\leqslant Ct^{-\alpha/\rho}\||\xi|^{\alpha-1}\hat{\nu}'(\xi)\|_{\mathbf{L}_\xi^\infty}\left\|\int_0^\infty\frac{|\xi|^{\alpha-1}|\xi-\mu|d\xi}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}\right\|_{\mathbf{L}_\mu^\infty}\leqslant Ct^{-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}$$

since we have the estimate

$$\int_0^\infty\frac{|\xi|^{\alpha-1}|\xi-\mu|d\xi}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}\leqslant C\langle\mu\rangle^{1-\rho}\int_0^{\mu/2}|\xi|^{\alpha-1}d\xi+C\mu^{\alpha-1}\int_{\frac{\mu}{2}}^{2\mu}\frac{|\xi-\mu|d\xi}{1+(\xi-\mu)^2\mu^{\rho-2}}$$
$$+C\int_{2\mu}^\infty\frac{|\xi-\mu|^\alpha d\xi}{1+|\xi-\mu|^\rho}\leqslant C\tag{2.3}$$

for all $\mu>0$ if $0<\alpha<\rho-1$. Similarly to the proof of Eq. (2.2) we also obtain

$$\|I_2(t)\|_{\mathbf{L}_x^2}\leqslant Ct^{-1/2\rho}\left\|\int_0^\infty\frac{\mu^{\rho/2-1}(\xi-\mu)e^{i\xi\eta+i/\rho\xi^\rho}}{1+i(\xi-\mu)(\xi^{\rho-1}-\mu^{\rho-1})}\hat{\nu}'(\xi t^{-1/\rho})d\xi\right\|_{\mathbf{L}_\mu^2}$$
$$\leqslant Ct^{1/2\rho-\alpha/\rho}\||\xi|^{\alpha-1}\hat{\nu}'(\xi)\|_{\mathbf{L}^\infty}\left\|\int_0^\infty\frac{\mu^{\rho/2-1}|\xi|^{\alpha-1}|\xi-\mu|d\xi}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}\right\|_{\mathbf{L}_\mu^2}\leqslant Ct^{1/2\rho-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}\tag{2.4}$$

if $0<\alpha<(\rho-1)/2$, since as in Eq. (2.3) we have

$$\left\|\int_0^\infty\frac{\mu^{(\rho/2)-1}|\xi|^{\alpha-1}|\xi-\mu|d\xi}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}\right\|_{\mathbf{L}_\mu^2}\leqslant C\|\langle\mu\rangle^{\alpha-\rho/2}\|_{\mathbf{L}_\mu^2}\leqslant C.$$

The third integral I_3 is estimated as follows:

$$\|I_3(t)\|_{\mathbf{L}^\infty} \leqslant C\int_0^\infty \frac{1}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}\left|\int_{\mu t^{-1/\rho}}^{\xi t^{-1/\rho}} \hat{\nu}'(y)dy\right| d\xi$$
$$\leqslant Ct^{-\alpha/\rho}\||\xi|^{\alpha-1}\hat{\nu}'(\xi)\|_{\mathbf{L}^\infty}\int_0^\infty \frac{|\xi^\alpha-\mu^\alpha|}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}d\xi \leqslant Ct^{-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}$$

since

$$\int_0^\infty \frac{|\xi^\alpha-\mu^\alpha|}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}d\xi \leqslant C\langle\mu\rangle^{1+\alpha-\rho}+C\mu^{\alpha-1}\int_{\frac{\mu}{2}}^{2\mu}\frac{|\xi-\mu|d\xi}{1+(\xi-\mu)^2\mu^{\rho-2}}+C\int_{2\mu}^\infty \frac{|\xi-\mu|^\alpha d\xi}{1+|\xi-\mu|^\rho}\leqslant C$$

for all $\mu>0$ if $0<\alpha<\rho-1$. In the same way as in the proof of Eq. (2.4) we have

$$\|I_3(t)\|_{\mathbf{L}_x^2} \leqslant Ct^{-1/2\rho-\alpha/\rho}\||\xi|^{\alpha-1}\hat{\nu}'(\xi)\|_{\mathbf{L}^\infty}\left\|\int_0^\infty \frac{\mu^{(\rho/2)-1}|\xi^\alpha-\mu^\alpha|}{1+|\xi-\mu||\xi^{\rho-1}-\mu^{\rho-1}|}d\xi\right\|_{\mathbf{L}_\mu^2}$$
$$\leqslant Ct^{1/2\rho-\alpha/\rho}\|\langle\mu\rangle^{\alpha-\rho/2}\|_{\mathbf{L}_\mu^2}\|\hat{\nu}\|_{\mathbf{Z}^\alpha} \leqslant Ct^{1/2\rho-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha} \tag{2.5}$$

if $0<\alpha<(\rho-1)/2$. Therefore by Eqs. (2.1)–(2.5) we obtain the result of the theorem for the case of $x<0$.

Now we consider the second case $x\geqslant 0$. By applying the identity

$$e^{i\xi\eta+(i/\rho)\xi^\rho}=\frac{1}{1+i\xi(\xi^{\rho-1}+\mu^{\rho-1})}\frac{\partial}{\partial\xi}(\xi e^{i\xi\eta+(i/\rho)\xi^\rho})$$

the integration by parts with respect to ξ yields

$$\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}(\xi t^{-1/\rho})d\xi=-t^{-1/\rho}\int_0^\infty \frac{\xi}{1+i\xi(\xi^{\rho-1}+\mu^{\rho-1})}e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}'(\xi t^{-1/\rho})d\xi$$
$$-i\int_0^\infty \frac{\xi\mu^{\rho-1+\rho\xi^\rho}}{(1+i\xi(\xi^{\rho-1}+\mu^{\rho-1}))^2}e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}(\xi t^{-1/\rho})d\xi.$$

Therefore we get

$$\left\|\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}(\xi t^{-1/\rho})d\xi\right\|_{\mathbf{L}_x^\infty}\leqslant Ct^{-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}\int_0^\infty\frac{\xi^\alpha d\xi}{1+\xi^\rho}\leqslant Ct^{-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}$$

if $0<\alpha<\rho-1$ and

$$\left\|\int_0^\infty e^{i\xi\eta+(i/\rho)\xi^\rho}\hat{\nu}(\xi t^{-1/\rho})d\xi\right\|_{\mathbf{L}_x^2}\leqslant Ct^{-1/2\rho}\left\|\int_0^\infty\frac{\xi\mu^{(\rho/2)-1}}{1+\xi(\xi^{\rho-1}+\mu^{\rho-1})}|\hat{\nu}'(\xi t^{-1/\rho})\|d\xi\right\|_{\mathbf{L}_\mu^2}$$
$$+Ct^{1/2\rho}\left\|\int_0^\infty\frac{\mu^{(\rho/2)-1}}{1+\xi(\xi^{\rho-1}+\mu^{\rho-1})}|\hat{\nu}'(\xi t^{-1/\rho})|d\xi\right\|_{\mathbf{L}_\mu^2}$$
$$\leqslant Ct^{1/2\rho-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}\left\|\int_0^\infty\frac{\xi^\alpha\mu^{(\rho/2)-1}d\xi}{1+\xi(\xi^{\rho-1}+\mu^{\rho-1})}\right\|_{\mathbf{L}_\mu^2}$$
$$\leqslant Ct^{1/2\rho-\alpha/\rho}\|\langle\mu\rangle^{\alpha-\rho/2}\|_{\mathbf{L}_\mu^2}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}\leqslant Ct^{1/2\rho-\alpha/\rho}\|\hat{\nu}\|_{\mathbf{Z}^\alpha}$$

if $0<\alpha<(\rho-1)/2$. This completes the proof of theorem 1.1.

III. LEMMAS

Denote the ordering of the norms

$$\|\phi\|_{\mathbf{L}_t^q\mathbf{L}_x^r}=\|\|\phi(t)\|_{\mathbf{L}_x^r(\mathbf{R})}\|_{\mathbf{L}_t^q(\mathbf{I})},$$

where $\mathbf{I}$ is a bounded or unbounded time interval. By the duality argument of Ref. 25 along with the estimates of theorem 1.1 the Strichartz estimate can be proved.

Lemma 3.1: For any time interval $\mathbf{I}$ and for any $s\in\overline{\mathbf{I}}$ the Strichartz estimate is true

$$\left\|\int_s^t U(t-\tau)\phi(\tau)d\tau\right\|_{\mathbf{L}_t^q\mathbf{L}_x^r}\leqslant C\|\phi\|_{\mathbf{L}_t^{\bar{q}'}\mathbf{L}_x^{\bar{r}'}}$$

with a constant C independent of $\mathbf{I}$ and s, where $0\leqslant\rho/q=1/2-1/r$ and $0\leqslant\rho/q'=1/2-1/r',1/r'+1/\bar{r}'=1$, and $1/q'+1/q'=1$.

We now consider the final state problem for the following equation:

$$\frac{dw}{dt}=i\lambda_1 t^{-1}\xi|\xi|^{2-\rho}|w|^2w+\lambda_2 t^{-1}|\xi|^{3-\rho}E^{\nu}\mathcal{D}_{\mu}w^3, \tag{3.1}$$

where $E=e^{-i(1-1/\rho)t|\xi|^{\rho-1}\xi},\lambda_1\in\mathbf{R},\lambda_2\in\mathbf{C},\mu=3^{\rho-1}$ we also denote the operator $\mathcal{D}_{\omega}\phi=\omega^{-1/2}\phi(x|\omega|^{-1/(\rho-1)})$.

To treat the divergence of the first term on the right-hand side of Eq. (3.1) we change the variable $w=\nu e^{i\varphi}$, where $\varphi(t,\xi)=\lambda_1\xi|\xi|^{2-\rho}|f(\xi)|^2\log t$. Then we get the final state problem

$$\frac{d\nu}{dt}=\mathcal{Q}(\nu),$$

$$\nu(t)\to f \text{ as } t\to\infty, \tag{3.2}$$

where

$$\mathcal{Q}(\nu)=i\lambda_1 t^{-1}\xi|\xi|^{2-\rho}(|\nu|^2-|f|^2)\nu+\lambda_2 t^{-1}|\xi|^{3-\rho}E^{\nu}e^{-i\varphi}\mathcal{D}_{\mu}e^{3i\varphi}\nu^3.$$

Lemma 3.2: Let $\lambda_1\in\mathbf{R},\lambda_2\in\mathbf{C}$. Suppose that the final state $f\in\mathbf{Y}^{\beta,\delta}$, where $(\rho-2)/2\leqslant\beta\leqslant\rho-2$ and

$$\mathbf{Y}^{\beta,\delta}=\{g:\|g\|_{\mathbf{Y}^{\beta,\delta}}=\|\langle\xi\rangle^{\delta+1}\{\xi\}^{-\beta}g\|_{\mathbf{L}_\infty}<\infty\}$$

and the norm $\|f\|_{\mathbf{Y}^{\beta,\delta}}$ is sufficiently small. Then there exists a unique solution $\nu\in\mathbf{C}([1,\infty);\mathbf{Y}^{\beta,\delta})$ of the final problem (3.2) such that

$$\sup_{t\geqslant1}t^{(2\beta-\rho+3)/\rho}\|\nu(t)-f\|_{\mathbf{Y}^{\beta,\delta}}\leqslant C\varepsilon^3.$$

Moreover, if $f'\in\mathbf{Y}^{\beta-1,2}$, then $\nu\in\mathbf{C}([1,\infty);\mathbf{W}^{\beta})$ with the estimates

$$\sup_{t\geqslant1}\|\nu\xi(t)\|_{\mathbf{Y}^{\beta-1,2}}\leqslant C\varepsilon.$$

Remark 3.1: In order to use the lemma to the proof of the main result we put $f=\hat{u}_+(\xi)$ and let β satisfy the condition

$$\max\left\{0,\frac{3\rho-7}{4}\right\}<\beta.$$

Then we find that

$$\|\omega(t)-\hat{u}_+(\xi)e^{-i\lambda_1\xi|\xi|^{2-\rho}|\hat{u}_+(\xi)|^2\log t}\|_{\mathbf{Y}^{\beta,\delta}}$$

decays faster than $t^{-(\rho-1)/2\rho}$.

Proof: We apply the contraction mapping principle in

$$\mathbf{X}_\varepsilon=\{\nu\in\mathbf{X}:\|\nu-f\|_{\mathbf{X}}\leqslant\varepsilon\},$$

where $\varepsilon=3\|f\|_{\mathbf{Y}^{\beta,\delta}}$ and the norm

$$\|\phi\|_{\mathbf{X}}=\sup_{t\geqslant 1}t^{(2\beta-\rho+3)/\rho}\|\phi(t)\|_{\mathbf{Y}^{\beta,\delta}}.$$

For $\nu\in\mathbf{X}_\varepsilon$ we define the mapping $\mathcal{M}(\nu)$ by

$$\mathcal{M}(\nu)=f+\int_t^\infty(\mathcal{Q}(\nu(\tau))-\mathcal{Q}(f))d\tau+\int_t^\infty\mathcal{Q}(f)d\tau, \tag{3.3}$$

where $\mathcal{Q}(f)=\lambda_2|\xi|^{3-\rho}E^\nu\tau^{-1}e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3$. First we prove the estimate $\|\mathcal{M}(\nu)-f\|_{\mathbf{X}}\leqslant\varepsilon$ if $\nu\in\mathbf{X}_\varepsilon$. Using the identity $E^\nu=B\partial_\tau(\tau E^\nu)$ with $B=(1-i\nu(1-1/\rho)\tau|\xi|^{\rho-1}\xi)^{-1}$ and

$$\begin{aligned}\tau\partial_\tau(\tau^{-1}Be^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi})=&-\tau^{-1}B(2-B)e^{-\varphi}\mathcal{D}_\mu e^{3i\varphi}-i\lambda_1\tau^{-1}Be^{-i\varphi}(\xi|\xi|^{2-\rho}|f|^2\mathcal{D}_\mu e^{3i\varphi}\\&-3\mathcal{D}_\mu e^{3i\varphi}(\xi|\xi|^{2-\rho}|f|^2)),\end{aligned}$$

we integrate by parts in the last integral in Eq. (3.3)

$$\begin{aligned}\mathcal{M}(\nu)-f=&\lambda_2|\xi|^{3-\rho}BE^\nu e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3+\int_t^\infty(\mathcal{Q}(\nu(\tau))-\mathcal{Q}(f))d\tau+\lambda_2|\xi|^{3-\rho}\\&\times\int_t^\infty E^\nu B(2-B)e^{-\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3\frac{d\tau}{\tau}+i\lambda_1\lambda_2|\xi|^{3-\rho}\int_t^\infty E^\nu Be^{-i\varphi}(\xi|\xi|^{2-\rho}|f|^2\mathcal{D}_\mu e^{3i\varphi}\\&-3\mathcal{D}_\mu e^{3i\varphi}\xi|\xi|^{2-\rho}|f|^2)f^3\frac{d\tau}{\tau}.\end{aligned} \tag{3.4}$$

Then by the conditions of the lemma we have

$$\begin{aligned}\left\|\int_t^\infty(\mathcal{Q}(\nu(\tau))-\mathcal{Q}(f))d\tau\right\|_{\mathbf{X}}&\leqslant C\sup_{t\geqslant 1}t^{(2\beta-\rho+3)/\rho}\int_t^\infty(\|\nu-f\|^2_{\mathbf{Y}^{(\rho-2)/2,1}}+\|f\|^2_{\mathbf{Y}^{(\rho-2)/\rho,1}})\|\nu-f\|_{\mathbf{Y}^{\beta,\delta}}\frac{d\tau}{\tau}\\&\leqslant C\|\nu-f\|_{\mathbf{X}}(\|\nu-f\|^2_{\mathbf{X}}+\|f\|^2_{\mathbf{Y}^{(\rho-2)/\rho,1}})\sup_{t\geqslant 1}t^{(2\beta-\rho+3)/\rho}\\&\quad\times\int_t^\infty\tau^{-1(2\beta-\rho+3)/\rho}d\tau\leqslant C\varepsilon^3.\end{aligned}$$

Since $|B|\leqslant C\langle\tau\xi^\rho\rangle^{-1}$ we also get

$$\|\langle\xi\rangle^{\delta+1}\{\xi\}^{-\beta}|\xi|^{3-\rho}BE^\nu e^{-ei\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3\|_{\mathbf{L}^\infty}\leqslant C\|f\|^3_{\mathbf{Y}^{\beta,\delta}}\||\xi|^{2\beta-\rho+3}\langle t\xi^\rho\rangle^{-1}\|_{\mathbf{L}^\infty}\leqslant C\varepsilon^3t^{(2\beta-\rho+3)/\rho}$$

and

$$\left\| |\xi|^{3-\rho} \int_t^\infty E^\nu B e^{-i\varphi} (\xi |\xi|^{2-\rho} |f|^2 \mathcal{D}_\mu e^{3ie\varphi} - 3\mathcal{D}_\mu e^{3i\varphi} \xi |\xi|^{2-\rho} |f|^2) f^3 \frac{d\tau}{\tau} \right\|_{\mathbf{Y}^{\beta,\delta}}$$

$$\leqslant C\|f\|^3_{\mathbf{Y}^{\beta,\delta}} \left\| |\xi|^{2\beta-\rho+3} \int_t^\infty \langle \tau \xi^\rho \rangle^{-1} \frac{d\tau}{\tau} \right\|_{\mathbf{L}_\infty} \leqslant C\|f\|^3_{\mathbf{Y}^{\beta,\delta}} t^{(2\beta-\rho+3)/\rho} \leqslant C\varepsilon^3 t^{(2\beta-\rho+3)/\rho}, \tag{3.5}$$

where $(\rho-2)/2 \leqslant \beta \leqslant \rho-2$. Therefore the mapping $\mathcal{M}$ transforms a ball $\mathbf{X}_\varepsilon$ with a center f and a radius $\varepsilon > 0$ into itself. In the same manner for $v_1, v_2 \in \mathbf{X}_\varepsilon$ we have

$$\|\mathcal{M}(v_1) - \mathcal{M}(v_2)\|_{\mathbf{X}} \leqslant \left\| \int_t^\infty (\mathcal{Q}(v_1(\tau)) - \mathcal{Q}(v_2(\tau)))d\tau \right\|_{\mathbf{X}} \leqslant \frac{1}{2}\|v_1 - v_2\|_{\mathbf{X}}.$$

Thus $\mathcal{M}$ is a contraction mapping in $\mathbf{X}_\varepsilon$. Therefore there exists a unique solution $v \in \mathbf{X}_\varepsilon$ to the final problem Eq. (3.2).

We now suppose that $f' \in \mathbf{Y}^{\beta-1,2}$. Taking the derivative of Eq. (3.4) with respect to ξ we obtain for the new function $h(t) = v_\xi(t) - f' + i\nu\lambda_2(\rho-1)t\xi^2 B E^\nu e^{-i\varphi} \mathcal{D}_\mu e^{3i\varphi} f^3$,

$$h(t) = \lambda_2 E^\nu \partial_\xi (|\xi|^{3-\rho} B e^{-i\varphi} \mathcal{D}_\mu e^{3i\varphi} f^3) + \int_t^\infty \mathcal{Q}_1(v(\tau))d\tau + \int_t^\infty \mathcal{Q}_2(v(\tau))d\tau,$$

where

$$\begin{aligned}
\mathcal{Q}_1(v) &= i\lambda_1(3-\rho)\tau^{-1}|\xi|^{2-\rho}(|v|^2 - |f|^2)v + i\lambda_1\tau^{-1}\xi|\xi|^{2-\rho}(v_\xi(|v|^2 - |f|^2) + v\,\mathrm{Re}(\bar{v}h + (\bar{v} - \bar{f})f')) \\
&+ \lambda_2\tau^{-1}E^\nu\partial_\xi(|\xi|^{3-\rho}e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi})(v^3 - f^3) + 3\lambda_2\tau^{-1}E^\nu|\xi|^{3-\rho}e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}((v^2 - f^2)v_\xi + f^2 h) \\
&+ \lambda_2\tau^{-1}E^\nu\partial_\xi(|\xi|^{3-\rho}B(2-B)e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3) + i\lambda_1\lambda_2\tau^{-1}E^\nu\partial_\xi(|\xi|^{3-\rho}Be^{-i\varphi}(\xi|\xi|^{2-\rho}|f|^2\mathcal{D}_\mu e^{3i\varphi} \\
&- 3\mathcal{D}_\mu e^{3i\varphi}\xi|\xi|^{2-\rho}|f|^2)f^3)
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{Q}_2(v) &= -i\nu(\rho-1)\lambda_1\xi|\xi|^{4-\rho}v\,\mathrm{Re}(\bar{v}i\lambda_2 B E^\nu e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3) - 3i\nu\lambda_2^2(\rho-1)E^{\nu(1+3^{-\rho})} \\
&\times|\xi|^{3-\rho}e^{-i\varphi}\mathcal{D}_\mu(f^2\xi^2 B e^{2i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3) + i\nu\lambda_2(\rho-1)\xi^2 E^\nu(e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}(v^3 - f^3) \\
&+ B(2-B)e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}f^3 + i\lambda_1\xi|\xi|^{2-\rho}|f|^2 B e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi} - 3i\lambda_1 B e^{-i\varphi}\mathcal{D}_\mu e^{3i\varphi}\xi|\xi|^{2-\rho}|f|^2 f^3).
\end{aligned}$$

In the term $\mathcal{Q}_2(v)$ we integrate again by parts as in Eq. (3.5) and note that $\{\xi\}|B| \leqslant C\tau^{-1/\rho}$. We therefore find

$$\|h(l)\|_{\mathbf{Y}^{\beta-1,2}} \leqslant C\varepsilon^3 t^{-\gamma} + C\varepsilon^3 \int_t^\infty \tau^{-1-1/\rho} d\tau \leqslant C\varepsilon t^{-\gamma}.$$

Lemma 3.2 is proved. ■

IV. MODIFIED WAVE OPERATOR

We define the modified final state $\hat{w}(t)$ as a solution to the final problem Eq. (3.1)

$$\hat{w}_t(t,\xi) = \frac{1}{t}(i\lambda\xi|\mathbf{F}\hat{w}|^2\hat{w} + i\tilde{\lambda}\xi\mathbf{F}^2 E^\nu \mathcal{D}_\mu \hat{w}^3), \tag{4.1}$$

where $\mathbf{F} = \sqrt{4/i(\rho-1)}\,|\xi|^{1-\rho/2}$, $E = e^{-i(1-1/\rho)t|\xi|^{\rho-1}\xi}$, $\nu = (1-3^{1-\rho})/(\rho-1)$, $\mu = 3^{\rho-1}$, $\tilde{\lambda} = \lambda 3^{3\rho/2-4}$ and a final state $f = \widehat{u_+}(\xi)$. The problem (4.1) is considered in lemma 3.2. Since $\mathcal{L}\mathcal{U}(t) = U(t)\partial_t$ for $\mathcal{L} = \partial_t + 1/p|\partial_x|^{\rho-1}\partial_x$, by Eq. (1.1) we find for the difference $\nu = u - U(t)w$,

$$\mathcal{L}v = \mathcal{N}_1 + \mathcal{N}_2, \tag{4.2}$$

where

$$\mathcal{N}_1 = \lambda u^2 v_x + \lambda(u^2 - (U(t)w)^2)U(t)w_x,$$

$$\mathcal{N}_2 = \lambda(U(t)w)^2 U(t)w_x - it^{-1}U(t)\mathcal{F}^{-1}(\lambda\xi|\hat{w}|^2\hat{w} + \tilde{\lambda}\xi F^2 E^{\nu} D_{\mu}\hat{w}^3).$$

By theorem 1.1 we have

$$U(t)w = t^{-1/2}\mathrm{Re}(\theta(x)(FE\hat{w})(\chi)) + R_1$$

and

$$U(t)w_x = t^{-1/2}\mathrm{Re}(i\theta(x)\chi(FE\hat{w})(\chi)) + R_2$$

with $\chi=(|x|/t)^{(1/\rho-1)}$, $\theta(x)=1$ for $x<0$ and $\theta(x)=0$ for $x\geqslant 0$. The remainder terms satisfy the estimates

$$\begin{aligned}
&\|R_1(t)\|_{\mathbf{H}^2} + t^{1/2\rho}\|R_1(t)\|_{\mathbf{H}^2_\infty} + \|R_2(t)\|_{\mathbf{H}^2} + t^{1/2\rho}\|R_2(t)\|_{\mathbf{H}^2_\infty} \\
&\quad \leqslant Ct^{-\alpha/\rho-1/2\rho}\|\hat{w}(t)\|_{\mathbf{W}^\alpha} \\
&\quad = Ct^{-\alpha/\rho-1/2\rho}\|\langle\xi\rangle^3\{\xi\}^{-\alpha}\hat{u}_+(\xi)\|_{\mathbf{L}^\infty} + Ct^{-\alpha/\rho-1/2\rho}\|\langle\xi\rangle^3\{\xi\}^{1-\alpha}\hat{w}_\xi(t,\xi)\|_{\mathbf{L}^\infty} \\
&\quad \leqslant Ct^{-\alpha/\rho-1/2\rho}(1+\log t\|\hat{u}_+\|^2_{\mathbf{Z}^\alpha})\|\hat{u}_+\|_{\mathbf{W}^\alpha}
\end{aligned}$$

for $(\rho-2)/2\leqslant\alpha<(\rho-1)/2$, where $\|\widehat{u_+}\|_{\mathbf{W}^\alpha}=\|\langle\xi\rangle^3\widehat{u_+}\|_{\mathbf{Z}^\alpha}$. Then we have

$$\begin{aligned}
(U(t)w)^2U(t)w_x &= t^{-3/2}(\mathrm{Re}(\theta(x)(FE\hat{w})(\chi)) + R_1)^2(\mathrm{Re}(i\theta(x)\chi(FE\hat{w})(\chi)) + R_2) \\
&= t^{-3/2}(\mathrm{Re})(i\theta(x)\chi(F^3E^3\hat{w}^3)(\chi)) + t^{-3/2}|F\hat{w}|^2\mathrm{Re}(i\theta(x)\chi(FE\hat{w})(\chi)) + R_3
\end{aligned} \tag{4.3}$$

with the estimate

$$\|R_3(t)\|_{\mathbf{H}^2} \leqslant Ct^{-1-\alpha/\rho-1/2\rho}(1+(\log t)\|\widehat{u_+}\|^2_{\mathbf{Z}^\alpha})\|\widehat{u_+}\|_{\mathbf{W}^\alpha}.$$

By theorem 1.1 we also get

$$t^{-1}i\lambda U(t)\mathcal{F}^{-1}\xi|F\hat{w}|^2\hat{w} = t^{-3/2}\mathrm{Re}(i\lambda\theta(x)\chi(F|F|^2E|\hat{w}|^2\hat{w})(\chi)) + R_4, \tag{4.4}$$

and since $\omega=1+\nu-\nu\rho=3^{1-\rho}$ we have $\tilde{\lambda}D_\omega\chi F^3E^\omega=\chi F^3E^3\mathcal{D}_\omega$ and

$$\begin{aligned}
i\tilde{\lambda}t^{-1}U(t)\mathcal{F}^{-1}E^{\nu}\xi F^2D_{\mu}\hat{w}^3 &= i\tilde{\lambda}t^{-1}\mathcal{F}^{-1}\exp\left(\omega\frac{it}{\rho}|\xi|^{\rho-1}\xi\right)\xi F^2D_{\mu}\hat{w}^3 \\
&= i\tilde{\lambda}t^{-1}U(\omega t)\mathcal{F}^{-1}\xi F^2D_{\mu}\hat{w}^3 \\
&= t^{-3/2}\mathrm{Re}(i\tilde{\lambda}D_\omega\theta(x)\chi F^3E^\omega D_{\mu}\hat{w}^3) + R_5 \\
&= t^{-3/2}\mathrm{Re}(i\theta(x)\chi(F^3E^3\hat{w}^3)(\chi)) + R_5,
\end{aligned} \tag{4.5}$$

with the estimate of the remainder terms

$$\|R_4(t)\|_{\mathbf{H}^2} + \|R_5(t)\|_{\mathbf{H}^2} \leqslant Ct^{-1-\alpha/\rho-1/2\rho}(1+\log t\|\hat{u}_+\|^2_{\mathbf{Z}^\alpha})\|\hat{u}_+\|_{\mathbf{W}^\alpha}.$$

Therefore by Eqs. (4.3)–(4.5) we find that $\mathcal{N}_2=R_3+R_4+R_5$. Thus

$$\|\mathcal{N}_2\|_{\mathbf{H}^2} \leqslant Ct^{(\gamma-1)-\alpha/\rho-1/2\rho}. \tag{4.6}$$

We introduce the function space

$$\mathbf{Y} = \{\phi \in \mathbf{C}([T,\infty);\mathbf{L}^2): \|\phi\|_{\mathbf{Y}} < \infty\},$$

where the norm

$$\|\phi\|_{\mathbf{Y}} = \sup_{t\in(T,\infty)} t^b(\|\varphi\|_{\mathbf{L}_t^\infty(t,\infty)\mathbf{H}^2(\mathbf{R})} + \|\varphi\|_{\mathbf{L}_t^{2\rho}(t,\infty)\mathbf{H}_\infty^1(\mathbf{R})})$$

with $(\rho-1)/2\rho < b < \alpha/\rho+1/2\rho-\gamma < 1/2, \gamma > 0$ is small. Consider the linearized version of Eq. (4.2) written as

$$\mathcal{L}\nu = \lambda(\tilde{u}^2\nu_x + (\tilde{u}^2 - (U(t)w)^2)U(t)w_x) + \mathcal{N}_2 \tag{4.7}$$

with the final condition $\lim_{t\to\infty}\nu(t)=0$ in $\mathbf{L}^2$, where $\tilde{u}=\tilde{\nu}+U(t)w$ and

$$\tilde{\nu} \in \mathbf{Y}_\varepsilon = \{\phi \in \mathbf{C}([T,\infty);\mathbf{L}^2): \|\phi\|_{\mathbf{Y}} \leqslant C\varepsilon\}.$$

We apply the standard energy method to Eq. (4.7). Using Sobolev imbedding theorem we then get

$$\begin{aligned}\|\nu(t)\|_{\mathbf{H}^2}^2 &\leqslant \int_t^\infty (\|\tilde{\nu}\|_{\mathbf{H}_\infty^1}^2 + \|\tilde{\nu}\|_{\mathbf{H}_\infty^1}\|U(\tau)w\|_{\mathbf{H}_\infty^3} + \|U(\tau)w\|_{\mathbf{H}_\infty^1}^2)\|\nu\|_{\mathbf{H}^2}^2 d\tau + C\int_t^\infty \tau^{(\gamma-1)-\alpha/\rho-1/2\rho}\|\nu(t)\|_{\mathbf{H}^2} d\tau \\ &\leqslant C\int_t^\infty (\|\tilde{\nu}\|_{\mathbf{H}_\infty^1}^2 + \tau^{-1/2}\|\tilde{\nu}\|_{\mathbf{H}_\infty^1} + \tau^{-1})\|\nu\|_{\mathbf{H}^2}^2 d\tau + Ct^{\gamma-\alpha/\rho-1/2\rho}\|\nu(t)\|_{\mathbf{H}_2}.\end{aligned}$$

By applying the Hölder inequality

$$\begin{aligned}\|\nu(t)\|_{\mathbf{H}^2}^2 &\leqslant C\left(\int_t^\infty \|\tilde{\nu}\|_{\mathbf{H}_\infty^1}^{2\rho} d\tau\right)^{1/\rho}\left(\int_t^\infty \|\nu\|_{\mathbf{H}^2}^{2\rho/(\rho-1)} d\tau\right)^{(\rho-1)/\rho} + C\left(\int_t^\infty \|\tilde{\nu}\|_{\mathbf{H}_\infty^1}^{2\rho} d\tau\right)^{1/2\rho} \\ &\quad \times \left(\int_t^\infty \tau^{-\rho/(2\rho-1)}\|\nu\|_{\mathbf{H}^2}^{4\rho/(2\rho-1)} d\tau\right)^{(2\rho-1)/2\rho} + C\int_t^\infty \tau^{-1}\|\nu\|_{\mathbf{H}^2}^2 d\tau + Ct^{\gamma-\alpha/\rho-1/2\rho}\|\nu(t)\|_{\mathbf{H}^2} \\ &\leqslant Ct^{-2b}\left(\varepsilon^2 t^{(\rho-1)/\rho-2b} + \varepsilon^2 t^{(\rho-1)/2\rho-b} + 1\right)\sup_{t\geqslant T} t^{2b}\|\nu(t)\|_{\mathbf{H}^2}^2 + C\varepsilon t^{-2b}\end{aligned}$$

since $(\rho-1)/2\rho < b < \alpha/\rho+1/2\rho-\gamma, \gamma > 0$ is small. Hence, there exists a time $T \geqslant 1$ and $\varepsilon > 0$ such that if $\|u_+\|_{\mathbf{W}^\alpha} \leqslant \varepsilon$, then

$$\sup_{t\geqslant T} t^b\|\nu\|_{\mathbf{L}_t^\infty(t,\infty)\mathbf{H}^2(\mathbf{R})} \leqslant \varepsilon. \tag{4.8}$$

By the Strichartz estimates (see lemma 3.1)

$$\begin{aligned}\|\nu\|_{\mathbf{L}_t^{2\rho}(t,\infty)\mathbf{H}_\infty^1(\mathbf{R})} &\leqslant C\left(\int_t^\infty (\|\tilde{\nu}(\tau)\|_{\mathbf{H}_\infty^1}\|\tilde{\nu}(\tau)\|_{\mathbf{H}^1}\|\nu(\tau)\|_{\mathbf{H}^2})^{2\rho/(2\rho-1)} d\tau\right)^{(2\rho-1)/2\rho} \\ &\quad + C\left(\int_t^\infty \left(\left\|U(\tau)w\right\|_{\mathbf{H}_\infty^1}\left\|\tilde{\nu}(\tau)\right\|_{\mathbf{H}^1}\|\nu(\tau)\|_{\mathbf{H}^2}\right)^{2\rho/(2\rho-1)} d\tau\right)^{(2\rho-1)/2\rho} \\ &\quad + C\int_t^\infty \|U(\tau)w\|_{\mathbf{H}_\infty^1}^2\|\nu(\tau)\|_{\mathbf{H}^2} d\tau + C\int_t^\infty \|\mathcal{N}_2\|_{\mathbf{L}^2} d\tau.\end{aligned}$$

Hence,

$$\|v\|_{\mathbf{L}_t^{2\rho}(t,\infty)\mathbf{H}_\infty^1(\mathbf{R})} \leqslant C\varepsilon^2\left(\int_t^\infty \tau^{-4\rho b/(2\rho-1)}\|\tilde{v}(\tau)\|_{\mathbf{H}_\infty^1}^{2\rho/(2\rho-1)}d\tau\right)^{(2\rho-1)/2\rho} + C\varepsilon^3\left(\int_t^\infty \tau^{-(4\rho b+\rho)/(2\rho-1)}d\tau\right)^{(2\rho-1)/2\rho}$$
$$+ C\varepsilon^3\int_t^\infty \tau^{-1-b}d\tau + Ct^{\gamma-\alpha/\rho-1/2\rho}$$
$$\leqslant C\varepsilon^2 t^{(\rho-1)/\rho-2b}\|\vec{v}\|_{\mathbf{L}_t^{2\rho}(t,\infty)\mathbf{H}_\infty^1(\mathbf{R})} + C\varepsilon t^{(\rho-1)/2\rho-2b} + C\varepsilon^3 t^{-b},$$

from which it follows that there exists a time $T\geqslant 1$ such that

$$\sup_{t\geqslant T} t^b\|v\|_{\mathbf{L}_t^{2\rho}(t,\infty)\mathbf{H}_\infty^1(\mathbf{R})} \leqslant \varepsilon. \tag{4.9}$$

Thus we have by Eqs. (4.8) and (4.9)

$$\|v\|_{\mathbf{Y}} \leqslant \varepsilon \tag{4.10}$$

which implies that the mapping $\mathcal{M}$ defined by $v=\mathcal{M}\tilde{v}$ transforms $\mathbf{Y}_\varepsilon$ into itself. Denote $v_j=\mathcal{M}\tilde{v}_j$, then in the same way as in the proof of Eq. (4.8) we have

$$\sup_{t\geqslant T} t^b\|v_1(t)-v_2(t)\|_{\mathbf{H}^1} \leqslant \tfrac{1}{2}\sup_{t\geqslant T} t^b\|\tilde{v}_1(t)-\tilde{v}_2(t)\|_{\mathbf{H}^1}. \tag{4.11}$$

From Eqs. (4.10) and (4.11) by the contraction mapping principle, we have the desired result. Theorem 1.2 is proved.

V. NONEXISTENCE OF THE WAVE OPERATOR

Multiplying Eq. (1.1) by $U(-t)$ and integrating with respect to time we find

$$U(-t)u(t)-U(-s)u(s)=\lambda\int_s^t U(-\tau)(u^2u_x-(U(t)u_+)^2\partial_x U(t)u_+)d\tau+\lambda\int_s^t U(-\tau)$$
$$\times\Big((U(t)u_+)^2\partial_x U(t)u_+ - \tau^{-3/2}(\mathrm{Re}\ \theta(x)(F\widehat{Eu_+})(\chi))^2\mathrm{Re}\ i\theta(x)\chi(F\widehat{Eu_+})(\chi)\Big)d\tau$$
$$+\lambda\int_s^t U(-\tau)\tau^{-3/2}(\mathrm{Re}\ \theta(x)(F\widehat{Eu_+})(\chi))^2\mathrm{Re}\ i\theta(x)\chi(F\widehat{Eu_+})(\chi)d\tau.$$

By theorem 1.1 we have

$$U(\omega\tau)\phi=|\omega|^{(\rho-2)/(2\rho-2)}\mathrm{Re}\ \tau^{-1/2}\theta(x)F(\chi\ \mathrm{sign}\ \omega)E^\sigma\mathcal{D}_\omega\hat{\phi}(\chi)+O(\tau^{-1/2(1-1/\rho)-\gamma})$$

in $\mathbf{L}^p$ for $2\leqslant p\leqslant\infty$, where $\omega\neq 0,\sigma=|\omega|^{-1/(\rho-1)}\mathrm{sign}\ \omega,\gamma>0$. Therefore taking $\omega=1,3^{1-\rho}$ and $3^{1-\rho}-1$, we obtain

$$U(-\tau)\tau^{-3/2}(\mathrm{Re}\ \theta(x)(F\widehat{Eu_+})(\chi))^2\mathrm{Re}\ i\theta(x)\chi(F\widehat{Eu_+})(\chi)$$
$$=\tau^{-1}U(-\tau)\mathrm{Re}\ \tau^{-1/2}\theta(x)FE|\widehat{Fu_+}|^2i\chi\widehat{u_+}(\chi)+\tau^{-1}U(-\tau)\mathrm{Re}(\tau^{-1/2}\theta(x)i\chi(FE^3F^2\widehat{u_+^3})(\chi))$$
$$=\tau^{-1}U(-\tau)U(\tau)\mathcal{F}^{-1}_{\xi\to x}|\widehat{Fu_+}|^2i\xi\widehat{u_+}(\xi)+3^{-(\rho-2)/(2\rho-2)}\tau^{-1}U(-\tau)$$
$$\times U(3^{1-\rho}\tau)\mathcal{F}^{-1}_{\xi\to x}\mathcal{D}_{3\rho-1}i\xi F^2\hat{u}_+^3(\xi)+O(\tau^{-1-\gamma})$$
$$=\tau^{-1}\mathcal{F}^{-1}_{\xi\to x}|\widehat{Fu_+}|^2i\xi\widehat{u_+}(\xi)+C\tau^{-3/2}\mathrm{Re}\ \theta(x)F(-\chi)\overline{E}^\nu\mathcal{D}_{3\rho-1,\nu}i\chi F^2\hat{u}_+^3(\chi)+O(\tau^{-1-\gamma})$$

in $\mathbf{L}^2$, where $\nu=|3^{1-\rho}-1|^{-1/(\rho-1)}$. Hence, by integration by parts with respect to τ we see that

$$\left\| \lambda \int_s^t U(-\tau)\tau^{-3/2}(\mathrm{Re}\ \theta(x)(F\widehat{Eu_+})(\chi))^2(\mathrm{Re}\ i\theta(x)\chi(F\widehat{Eu_+})(\chi))d\tau \right\|_{\mathbf{L}^2}$$

$$\geqslant \left\| \lambda \int_s^t \mathcal{F}^{-1}_{\xi\to x}|F\widehat{u_+}|^2 i\xi\widehat{u_+}(\xi)\frac{d\tau}{\tau} \right\|_{\mathbf{L}^2} - C\left\| \lambda \int_s^t \tau^{-3/2}\bar{E}^{\nu}\mathcal{D}_{3^{\rho-1}\nu}\chi F^2\widehat{u_+}^3(\chi)d\tau \right\|_{\mathbf{L}^2} - C$$

$$\geqslant |\lambda|\||\xi|F\widehat{u_+}|^2\widehat{u_+}(\xi)\|_{\mathbf{L}^2}\int_s^t \frac{d\tau}{\tau} - C.$$

Thus in view of estimates of the solution $u(t)$ provided by theorem 1.2 we get

$$\|U(-t)u(t) - U(-s)u(s)\|_{\mathbf{L}^2} \geqslant |\lambda|\||\xi|F\widehat{u_+}|^2\widehat{u_+}\|_{\mathbf{L}^2}\int_s^t \frac{d\tau}{\tau} - C - C\int_s^t \|u(\tau) - U(\tau)u_+\|_{\mathbf{H}^1}\frac{d\tau}{\tau}$$

$$- C\int_s^t \|U(t)u_+ - \tau^{-1/2}\mathrm{Re}\ \theta(x)(F\widehat{Eu_+})(\chi)\|_{\mathbf{H}^1}\frac{d\tau}{\tau}.$$

This implies that for any $\delta>0$ there exists a time $T(\delta)$ such that for any $t>s>T(\delta)$,

$$\|U(-t)u(t) - U(-s)u(s)\|_{\mathbf{L}^2} \geqslant \left(|\lambda|\||\xi|F\widehat{u_+}|^2\widehat{u_+}\|_{\mathbf{L}^2} - \delta\right)\int_s^t \frac{d\tau}{\tau},$$

which means that $\widehat{u_+}=0$ for all $\chi\in\mathbf{R}$, since u_+ is a real-valued function, so that $\widehat{u_+}(-\xi)=\widehat{u_+}(\xi)$. The solution satisfies the conservation of the $\mathbf{L}^2$ norm, hence, we have $u=0$. Theorem 1.3 is proved.

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Spectral theory of neutron transport semigroups with partly elastic collision operators

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This paper deals with spectral properties of a class of neutron transport equations involving partly elastic collision operators introduced by Larsen and Zweifel [J. Math. Phys. **15**, 1987–1997 (1974)]. In particular, estimates of the essential type of associated semigroups are given. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Consider the neutron transport equation introduced by Larsen and Zweifel in Ref. 7,

$$\frac{\partial \varphi}{\partial t}(x,v,t) + v \cdot \frac{\partial \varphi}{\partial x}(x,v,t) + \sigma(x,v)\varphi(x,v,t) = K\varphi(x,v,t),$$

with zero incoming flux

$$\varphi_{|\Gamma_-}(\cdot,\cdot,t) = 0$$

and an initial condition

$$\varphi(x,v,0) = \varphi_0(x,v),$$

where $(x,v) \in \Omega \times V$, Ω is an open and bounded set of $\mathbb{R}^N$ $(N \geqslant 3)$ endowed with the Lebesgue measure dx, and the velocity space

$$V = \{v = \rho\omega; \omega \in \mathbb{S}^{N-1}, 0 \leqslant \rho_{\min} \leqslant \rho \leqslant \rho_{\max} < \infty\} =: I \times \mathbb{S}^{N-1}$$

is endowed with the Lebesgue measure $\mathrm{d}v = \rho^{N-1}\mathrm{d}\rho\mathrm{d}\omega$, where $\mathrm{d}\omega$ is the Lebesgue measure on the unit sphere $\mathbb{S}^{N-1}$. Here Γ_- denotes the incoming part of the boundary of the phase space $\Omega \times V$: $\Gamma_- = \{(x,v) \in \partial\Omega \times V; v \cdot \eta(x) < 0\}$, where $\eta(x)$ stands for the outward normal unit at $x \in \partial\Omega$. The function $\sigma(\cdot,\cdot) \in L^\infty_+(\Omega \times V)$ is called the collision frequency. The collision operator consists of three terms:

$$K = K_c + K_e + K_d.$$

The *classical* collision operator

$$K_c\varphi(x,v) = \int_V k_c(x,v,v')\varphi(x,v')\mathrm{d}v'$$

corresponds physically to fission, high energy elastic slowing down, and thermal inelastic scattering. K_e is an *elastic* operator for low energy neutrons describing microscopic events in which the kinetic energy is conserved and velocities are changed only in their direction. It is given by

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$$K_e\varphi(x,v) = \int_{\mathbb{S}^{N-1}} K_e(x,\rho,\omega,\omega')\varphi(x,\rho\omega')\mathrm{d}\omega'.$$

Finally, K_d represents high energy inelastic scattering and is described by a *downshift* operator of the form

$$K_d\varphi(x,v) = \sum_{m=1}^{\nu} K_d^{(m)}\varphi(x,v) = \sum_{m=1}^{\nu} \int_{\mathbb{S}^{N-1}} k_d^{(m)}(x,e_m(\rho),\omega,\omega')\varphi(x,e_m(\rho)\omega')\mathrm{d}\omega',$$

where $K_d^{(m)}$ $(m=1,\ldots,\nu)$ describes an event in which a discrete energy E_m is lost by a neutron at x with initial speed $e_m(\rho)$ and final speed ρ. The initial speed $e_m(\rho)$ is defined by

$$E_m = \frac{1}{2}Me_m^2(\rho) - \frac{1}{2}M\rho^2,$$

where M is the mass of neutron. Here and in the sequel we adopt the convention that all functions are extended by zero outside of their domains. Moreover, we use indifferently one of the notations $\varphi(x,v), \varphi(x,\rho,\omega)$, or $\varphi(x,\rho\omega)$ for $v=\rho\omega$. Notice that each $K_d^{(m)}$ acts on the supports of functions as follows:

$$\text{supp}\ \varphi \subset \Omega\times[0,\rho_0]\times\mathbb{S}^{N-1} \Rightarrow \text{supp}\ K_d^{(m)}\varphi \subset \Omega\times\left[0,\left(\max\left\{0,\rho_0^2-\frac{2E_m}{M}\right\}\right)^{1/2}\right]\times\mathbb{S}^{N-1}. \tag{1}$$

Since neutron speeds are bounded above ($\rho_{\max}<+\infty$), this property implies that K_d is nilpotent, i.e., there exists an integer n such that $K_d^n=0$.

The above collision models are particularly relevant when dealing with neutron transport in crystalline medium (see Ref. 3). Operators of types K_i and K_e are important also for electron transport in the semiconductor theory (see Ref. 9).

We put the above problem as an abstract Cauchy problem in the Banach space $L^p(\Omega\times V)$, $1\leqslant p<\infty$:

$$\begin{aligned}\frac{\mathrm{d}\varphi}{\mathrm{d}t}(t) &= (T+K)\varphi(t),\\ \varphi(0) &= \varphi_0,\end{aligned} \tag{2}$$

where T denotes the streaming operator

$$T{:}D(T) \ni \varphi \mapsto -v\cdot\frac{\partial\varphi}{\partial x} - \sigma(x,v)\varphi(x,v)$$

with the domain

$$D(T) = \left\{\varphi\in L^p(\Omega\times V){:}v\cdot\frac{\partial\varphi}{\partial x}\in L^p(\Omega\times V), \varphi_{|\Gamma^-}=0\right\}.$$

If K is bounded, then $T+K$ generates a C_0-semigroup $(\mathrm{e}^{t(T+K)})_{t\geqslant 0}$, which solves the preceding Cauchy problem in a reasonable sense. The asymptotic behavior $(t\to\infty)$ of the time dependent solution can be obtained by investigating the spectral properties of $(\mathrm{e}^{t(T+K)})_{t\geqslant 0}$.

Under suitable assumptions, e.g., piecewise continuous cross sections, the spectrum of the generator $T+K$ is described in Ref. 7. Typically, it consists of a half space, curves, and discrete eigenvalues. However, because the spectral mapping theorem does not hold for general C_0-semigroup, the spectrum of $T+K$ gives, *a priori*, only partial information about the asymptotic behavior of the semigroup. To our knowledge, up to now, in contrast to the classical model (i.e.,

$K=K_c$) which was intensively investigated (see, for instance, Refs. 4, 5, 10, 11, 13, 14, 16, 17, and 19–21), there is no spectral result on the semigroup $(e^{t(T+K_e+K_d+K_c)})_{t\geqslant 0}$, although the knowledge of its essential type (see the end of this introduction for the definition of essential type and its properties) is desirable and is an important prerequisite for understanding the time asymptotic behavior of the solutions to the associated Cauchy problem.

The purpose of the present work is to investigate the essential spectrum of the semigroup $(e^{t(T+K)})_{t\geqslant 0}$. More precisely, we deal with comparison of the essential types of the three semigroups $(e^{t(T+K_e)})_{t\geqslant 0}$, $(e^{t(T+K_e+K_d)})_{t\geqslant 0}$, and $(e^{t(T+K_e+K_d+K_c)})_{t\geqslant 0}$. Following Vidav[17] and others (see, for instance, Refs. 10, 16, 18, and 21), we will use the compactness argument on the remainder terms of the Dyson-Phillips expansion. We point out that the approach will be completely different according to whether we study the problem in a L^1-space or in a L^p-space, $1<p<\infty$.

Actually, the present paper is divided into two parts. In the first part (Sec. II), we deal with the above problem in $L^1(\Omega\times V)$. First, because of the nilpotence of K_d, we prove that the two semigroups $(e^{t(T+K_e+K_d)})_{t\geqslant 0}$ and $(e^{t(T+K_e)})_{t\geqslant 0}$ have the same essential type. Then we prove, by using, in particular, the strong convex compactness property (see Theorem 2), that the addition of the classical operator does not alter the essential type. We end up the section by deriving some estimates on the essential type of the semigroup $(e^{t(T+K)})_{t\geqslant 0}$. In the second part (Sec. III) of the paper, we give similar results in the context of L^p-spaces but with different tools.

Before closing this Introduction and for the sake of being complete, we recall the definition of essential type and some related properties. Let X be a complex Banach space and let $B\in\mathcal{L}(X)$ (the space of bounded linear operators on X). A point $\lambda\in\sigma(B)$ (the spectrum of B) is an eigenvalue of finite algebraic multiplicity if λ is an isolated point of $\sigma(B)$ and a pole of the resolvent of B with finite rank residue. The essential spectral radius of B is defined by

$$r_{\mathrm{ess}}(B):=\sup\{|\lambda|;\lambda\in\sigma(B),\ \lambda \text{ is not an eigenvalue of finite algebraic multiplicity}\}.$$

It is known that given a strongly continuous semigroup on X $(e^{tA})_{t\geqslant 0}$, the spectral radius of e^{tA}, $r_\sigma(e^{tA})$, is equal to $e^{t\omega_0(A)}$, where $\omega_0(A)\in[-\infty,\infty]$ is the type of $(e^{tA})_{t\geqslant 0}$: $\omega_0(A)=\lim_{t\to\infty}t^{-1}\ln\|e^{tA}\|$. Voigt in Ref. 18, Lemma 2.1, established a similar result concerning the essential spectral radius; more precisely he showed that there exists $\omega_{\mathrm{ess}}(A)\in[-\infty,\omega_0(A)]$, called essential type of $(e^{tA})_{t\geqslant 0}$, such that

$$r_{\mathrm{ess}}(e^{tA})=e^{t\omega_{\mathrm{ess}}(A)}\quad (t>0).$$

The interest of this parameter lies in the fact that for each $\beta>\omega_{\mathrm{ess}}(A)$, there exists a finite dimensional projection P_β in X, commuting with e^{tA} $(t\geqslant 0)$, and a constant $C_\beta\geqslant 0$ such that

$$\|e^{tA}(I-P_\beta)\|\leqslant C_\beta e^{t\beta}\quad (t\geqslant 0).$$

If $\omega_{\mathrm{ess}}(A)<\beta<\omega_0(A)$, then $P_\beta\neq 0$, and the asymptotic behavior of e^{tA} for $t\to+\infty$ is determined by the part of the semigroup e^{tA} in the finite dimensional space Range (P_β). Moreover, the essential type enjoys a nice stability property we recall in Theorem 1 below. Let B be a bounded operator, then $A+B$ generates a C_0-semigroup $(e^{t(A+B)})_{t\geqslant 0}$ given by the Dyson-Phillips series

$$e^{t(A+B)}=\sum_{j=0}^{\infty}D_j(t),\tag{3}$$

where $D_0(t)=e^{tA}$ and $D_{j+1}(t)=\int_0^t D_j(s)BD_0(t-s)\mathrm{d}s$.

Theorem 1 (*Ref. 10, Theorem 2.10, p. 24*): *With the notations just introduced, let there exist* $m\in\mathbb{N}$ *such that the remainder term* $\Sigma_{j=m}^{\infty}D_j(t)$ *is compact for all* $t\geqslant 0$. *Then the two semigroups* $(e^{t(A+B)})_{t\geqslant 0}$ *and* $(e^{tA})_{t\geqslant 0}$ *have the same essential type*, i.e., $\omega_{\mathrm{ess}}(A+B)=\omega_{\mathrm{ess}}(A)$.

II. L^1 ANALYSIS

In this section we treat the problem in L^1 setting. As in Ref. 8, we assume that the classical collision operator K_c is weakly compact with respect to the velocities, collectively with respect to the space variable, i.e.,

(A1) $\int_V |k_c(\cdot, v, \cdot)| \mathrm{d}v \in L^\infty(\Omega \times V)$.

(A2) $\{|k_c(x, \cdot, v')| : (x, v') \in \Omega \times V\}$ is weakly compact in $L^1(V)$.

Then K_c enjoys the following nice approximation property.

Lemma 1 (*Ref. 8, Theorem 2.4*): *Suppose that K_c is positive and satisfies (A1) and (A2). Then K_c can be approximated by a sequence of positive operators $(K_m)_m \subset \mathcal{L}(L^1(\Omega \times V))$ such that there is a sequence of non-negative functions $(f_m)_m \subset L^1(V)$ satisfying*

$$K_m \varphi(x,v) \leqslant f_m(v) \int_V \varphi(x,v) \mathrm{d}v', \tag{4}$$

for $0 \leqslant \varphi \in L^1(\Omega \times V)$.

Similarly, we assume that K_e satisfies the following.

(A3) $\int_{\mathbb{S}^{N-1}} |k_e(\cdot, \cdot, \omega, \cdot)| \mathrm{d}\omega \in L^\infty(\Omega \times I \times \mathbb{S}^{N-1})$.

(A4) $\{|k_e(x, \rho, \cdot, \omega')| : (x, \rho, \omega') \in \Omega \times I \times \mathbb{S}^{N-1}\}$ is weakly compact in $L^1(\mathbb{S}^{N-1})$.

By the same arguments as in Ref. 8, we can prove the following.

Lemma 2: Every positive elastic operator K_e satisfying (A3) and (A4) can be approximated by a sequence of positive operators $(K_m)_m \subset \mathcal{L}(L^1(\Omega \times I \times \mathbb{S}^{N-1}))$ such that there is a sequence of non-negative functions $(g_m)_m \subset L^1(\mathbb{S}^{N-1})$ satisfying

$$K_m \varphi(x,\rho,\omega) \leqslant g_m(\omega) \int_{\mathbb{S}^{N-1}} \varphi(x,\rho,\omega') \mathrm{d}\omega', \tag{5}$$

for all $0 \leqslant \varphi \in L^1(\Omega \times I \times \mathbb{S}^{N-1})$.

Finally, as in Ref. 7, we have the following.

(A5) Kernels $k_d^{(m)}$ are assumed to be bounded.

Remark 1: Our assumptions on collision operators are more general than that in Ref. 7.

Let us now compare the essential type of $(\mathrm{e}^{t(T+K_e)})_{t \geqslant 0}$ with that of $(\mathrm{e}^{t(T+K_e+K_d)})_{t \geqslant 0}$. For this purpose, expand the latter as a Dyson-Phillips series:

$$\mathrm{e}^{t(T+K_e+K_d)} = \sum_{j=0}^{\infty} W_j(t),$$

where $W_0(t) = \mathrm{e}^{t(T+K_e)}$ and $W_{j+1}(t) = \int_0^t W_j(s) K_d W_0(t-s) \mathrm{d}s$.

Giving two strongly continuous (operator valued) mappings

$$F, G : [0, \infty[\to \mathcal{L}(L^p(\Omega \times V)) \quad ,$$

we will denote by $F * G$ the convolution operator defined as

$$F * G : [0, \infty[\ni t \mapsto \int_0^t F(s) G(t-s) \mathrm{d}s \in \mathcal{L}(L^p(\Omega \times V)).$$

Moreover $[F]^j = F * \cdots * F$ (j times). Now, by property (1) and since $e^{t(T+K_e)}$ does not change the neutron speed, it follows that

$$[\mathrm{e}^{t(T+K_e)} K_d]^n = 0$$

(recall that n is such that $K_d^n = 0$) and therefore the remainder term $\Sigma_{j=n}^{\infty} W_j(t) = [\mathrm{e}^{t(T+K_e)} K_d]^n * \mathrm{e}^{t(T+K_e+K_d)} = 0$. As a direct consequence of this and Theorem 1, we have the following.

Lemma 3: The two semigroups $(e^{t(T+K_e+K_d)})_{t\geqslant 0}$ *and* $(e^{t(T+K_e)})_{t\geqslant 0}$ *have the same essential type:* $\omega_{\mathrm{ess}}(T+K_e+K_d)=\omega_{\mathrm{ess}}(T+K_e)$.

We now turn to the comparison between essential types of $(e^{t(T+K_e+K_d)})_{t\geqslant 0}$ and the full semigroup $(e^{t(T+K)})_{t\geqslant 0}$. Write

$$e^{t(T+K)}=\sum_{i=0}^{\infty} V_i(t), \tag{6}$$

where $V_0(t)=e^{t(T+K_e+K_d)}$ and $V_{i+1}(t)=\int_0^t V_i(s)K_cV_0(t-s)\mathrm{d}s$. Set $R_m(t)=\Sigma_{i=m}^{\infty}V_i(t)$.

Lemma 4: Let (A1)–(A5) be satisfied. Then the second remainder term of the Dyson-Phillips expansion (6)*, i.e.,* $R_2(t)$*, is weakly compact.*

Before proving this lemma we recall the following theorem known as the strong convex compactness property.

Theorem 2 *(Ref. 15, Theorem 2.2)* **:** *Let X and Y be two Banach spaces. Let* $(\Theta,\mathrm{d}\nu)$ *be a finite measure space and*

$$G:\Theta\to\mathcal{L}(X,Y)$$

bounded and strongly measurable. If $G(\omega)$ *is weakly compact for a.e.* $\omega\in\Theta$*, then the strong integral*

$$X\ni x\mapsto\int_{\Theta}G(\omega)x\mathrm{d}\nu(\omega)\in Y$$

is weakly compact.

Proof of Lemma 4: The proof will be given for the general case $\rho_{\max}=\infty$ and will be done in three steps.

Step 1. Approximation and domination arguments. Since $R_2(t)=e^{t(T+K_e+K_d)}*K_ce^{t(T+K_e+K_d)}K_c*e^{t(T+K_e+K_d+K_c)}$ (see Lemma 2.1, p. 14 in Ref. 10) it suffices, thanks to Theorem 2, to check the weak compactness of

$$K_ce^{t(T+K_e+K_d)}K_c$$

for all $t>0$. On the other hand, we can expand $(e^{t(T+K_e+K_d)})_{t\geqslant 0}$ as a Dyson-Phillips series:

$$e^{t(T+K_e+K_d)}=\sum_{j=0}^{\infty}U_j(t),$$

where $U_0(t)=e^{tT}$ is the streaming semigroup given by

$$e^{tT}\varphi(x,v)=e^{-\int_0^t\sigma(x-sv,v)\mathrm{d}s}\chi_{\{(y,w);t<\tau(y,w)\}}(x,v)\varphi(x-tv,v)\quad\text{for all }\varphi\in L^1(\Omega\times V),$$

with $\tau(x,v)=\inf\{s>0;x-sv\notin\Omega\}$, and $U_{j+1}(t)=\int_0^t U_j(s)(K_e+K_d)U_0(t-s)\mathrm{d}s$.

Moreover, the sequence $(\Sigma_{j=0}^{n}K_cU_j(t)K_c)_n$ converges in $\mathcal{L}(L^1(\Omega\times V))$ uniformly for bounded times to $K_ce^{t(T+K_e+K_d)}K_c$; thus it suffices to prove that $K_cU_j(t)K_c$ is weakly compact for all $j\in\mathbb{N}$. We have

$$|K_cU_j(t)K_c\varphi|\leqslant|K_c|U_j'(t)|K_c||\varphi|,$$

where $U_j'(t)$ denotes the term of order j of the Dyson-Phillips series expanding $(e^{t(T+|K_e|+C_d)})_{t\geqslant 0}$ from $(e^{tT})_{t\geqslant 0}$ and

$$|K_c|:L^1(\Omega\times V)\ni\varphi\mapsto\int_V|k_c(x,v,v')|\varphi(x,v')\mathrm{d}v',$$

$$|K_e|:L^1(\Omega\times I\times \mathbb{S}^{N-1})\ni \varphi\mapsto \int_{\mathbb{S}^{N-1}}|k_e(x,\rho,\omega,\omega')|\varphi(x,\rho,\omega')\mathrm{d}\omega'\in L^1(\Omega\times I\times \mathbb{S}^{N-1}),$$

$$C_d:L^1(\Omega\times I\times \mathbb{S}^{N-1})\ni \varphi\mapsto \sum_{m=1}^{\nu}\int_{\mathbb{S}^{N-1}}\|k_d^{(m)}\|_\infty\varphi(x,e_m(\rho),\omega')d\omega'\in L^1(\Omega\times I\times \mathbb{S}^{N-1}).$$

Thus, as far as the weak compactness is concerned, by using domination arguments, there is no loss of generality to assume that K_c and K_e are positive and $K_d=C_d$. On the other hand, if we define $K_c^{(i)}$ by

$$K_c^{(i)}:\varphi\mapsto\int_V k_c(x,v,v')\chi_{\{w\in V:|w|\leqslant i\}}(v)\varphi(x,v')\mathrm{d}v',$$

then

$$\begin{aligned}\|K_c\varphi-K_c^{(i)}\varphi\|&\leqslant\int\int_{\Omega\times\{v\in V:|v|>i\}}\int_V k_c(x,v,v')|\varphi(x,v')|\mathrm{d}v'\mathrm{d}x\mathrm{d}v\\&\leqslant\sup_{(x,v')\in\Omega\times V}\int_{\{v\in V:|v|>i\}}k_c(x,v,v')\mathrm{d}v\|\varphi\|_{L^1(\Omega\times V)}\end{aligned}$$

and, since K_c satisfies (A2), we have

$$\|K_c-K_c^{(i)}\|\leqslant\sup_{(x,v')\in\Omega\times V}\int_{\{v\in V:|v|>i\}}k_c(x,v,v')\mathrm{d}v\to 0\quad\text{as } i\to\infty.$$

Thus, we may replace K_c by some truncation $K_c^{(i)}$ since $K_cU_j(t)K_c$ depends continuously on K_c in the norm operator topology. This means that we may suppose without loss of generality that V is bounded, i.e., $\rho_{\max}<\infty$. Again since $K_cU_j(t)K_c$ depends continuously on K_c and K_e in the norm operator topology, according to Lemmas 1 and 2 (approximation and domination), we may assume that K_c has the form

$$\varphi\mapsto f(v)\int_V\varphi(x,v')\mathrm{d}v',$$

with $f\in L^1(V)$, and K_e has the form

$$\varphi\mapsto g(\omega)\int_{\mathbb{S}^{N-1}}\varphi(x,\rho,\omega')\mathrm{d}\omega'$$

with $g\in L^1(\mathbb{S}^{N-1})$. By approximation again we may suppose that $f\in L^\infty(V)$ and $g\in L^\infty(\mathbb{S}^{N-1})$, and by a domination argument, we may even assume that f and g are constants. Finally, by linearity we can suppose that operators K_c, K_e, and K_d are, respectively,

$$M_c:\varphi\mapsto\int_V\varphi(x,v')dv',\quad M_0:\varphi\mapsto\int_{\mathbb{S}^{N-1}}\varphi(x,\rho,\omega')\mathrm{d}\omega',$$

and

$$M_d=\sum_{i=1}^{\nu}M_i\quad\text{where } M_i:\varphi\mapsto\int_{\mathbb{S}^{N-1}}\varphi(x,e_i(\rho),\omega')\mathrm{d}\omega'.$$

Step 2. Strong convex compactness property. Considering different values of j. First, note that according to Ref. 10, Theorem 4.11, p. 80, $M_cU_0(t)M_c$ is weakly compact.

Suppose then that $j \geqslant 1$. In this case, since M_c maps $L^1(\Omega \times V)$ to $L^1(\Omega)$, it suffices to show that

$$M_c U_j(t): L^1(\Omega) \to L^1(\Omega)$$

is weakly compact. Decomposing $M_c = MM_0$, where $M: \varphi \mapsto \int_I \varphi(x,\rho,\omega)\rho^{N-1}\mathrm{d}\rho$, we can write

$$M_c U_j(t) = MM_0[U_0(M_0 + M_d)]^j * U_0(t).$$

Thus, by linearity, we can restrict ourselves to show the weak compactness of

$$MM_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t) \tag{7}$$

for all $(i_1,\ldots,i_j) \in \{0,1,\ldots,\nu\}^j$ and $t>0$. We remark that operator (7) is a "strong integral" [by making the identification $L^1(\Omega \times I) = L^1(I; L^1(\Omega))$]. Indeed, if for ρ fixed, we denote by $M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)[\rho]$ the bounded operator:

$$L^1(\Omega) \ni \varphi \mapsto (M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)\varphi)(\cdot,\rho) \in L^1(\Omega), \tag{8}$$

then operator (7) can be viewed as

$$MM_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)\varphi = \int_I M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)[\rho]\varphi\rho^{N-1}\mathrm{d}\rho$$

for all $\varphi \in L^1(\Omega)$. One can check without difficulties that operators $M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t) \times [\rho]$ are uniformly bounded for $\rho \in I$ on $\mathcal{L}(L^1(\Omega))$, and therefore the strong convex compactness property (Theorem 2) ensures that operator (7) is weakly compact, provided that $M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)[\rho]$ is weakly compact for all $\rho \in I$, which will be the subject of step 3 below.

Step 3. Weak compactness of $M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)[\rho]$. Let T_∞ denote the streaming operator on $\mathbb{R}^N$ (with $\sigma=0$) and set $U_\infty(t) = \mathrm{e}^{tT_\infty}$. Then for all $0 \leqslant \varphi \in L^1(\Omega)$,

$$M_0U_0 * M_{i_1}U_0 \cdots * M_{i_j}U_0(t)[\rho]\varphi \leqslant RM_0U_\infty * M_{i_1}U_\infty * \cdots * M_{i_j}U_\infty(t)[\rho]E\varphi,$$

where $E: L^1(\Omega) \to L^1(\mathbb{R}^N)$ and $R: L^1(\mathbb{R}^N) \to L^1(\Omega)$ are, respectively, the trivial extension operator by zero and the restriction operator. Using a domination argument to get the weak compactness of $M_0U_0 * M_{i_1}U_0 * \cdots * M_{i_j}U_0(t)[\rho]$, it is enough to have the weak compactness of

$$L^1(\mathbb{R}^N) \ni \varphi \mapsto RM_0U_\infty * M_{i_1}U_\infty * \cdots * M_{i_j}U_\infty(t)[\rho]\varphi \in L^1(\Omega). \tag{9}$$

But we will see thereafter that for all $\rho \in I$ and $t>0$, there is a function $\beta(t,\rho) \in L^1(\mathbb{R}^N)$ such that

$$M_0U_\infty * M_{i_1}U_\infty * \cdots * M_{i_j}U_\infty(t)[\rho]\varphi = \beta(t,\rho) * \varphi.$$

Consequently, by Ref. 2, Corollaire IV. 27, p. 74, we conclude that operator (9) is weakly compact.

It remains to prove that for each $(i_1,\ldots,i_j) \in \{0,1,\ldots,\nu\}^j$ $(j \geqslant 2)$, there exists $\beta(t,\rho) \in L^1(\mathbb{R}^N)$ such that

$$M_{i_1}U_\infty * \cdots * M_{i_j}U_\infty(t)[\rho]\varphi = \beta(t,\rho) * \varphi.$$

We recall that

$$M_i: \varphi \mapsto \int_{S^{N-1}} \varphi(x, e_i(\rho), \omega')\mathrm{d}\omega'$$

with the convention $e_0(\rho) = \rho$. We are going to proceed by recurrence and prove additionally that $\beta(t,\rho)$ is uniformly bounded for t bounded and $\rho \in I$. First, it is clear that for each $i \in \{0,1,\ldots,\nu\}$,

$$M_i U_\infty(t)[\rho] = \mathrm{d}\omega_{te_i(\rho)} * \varphi,$$

where $\mathrm{d}\omega_s$ is the image of $\mathrm{d}\omega$ under the dilation $v \mapsto sv$. Observe that the mapping $0 < t \to \mathrm{d}\omega_t \in \mathcal{M}(\mathbb{R}^N)$ (the space of finite Radon measures) is weak star continuous, i.e., $0 < t \mapsto \langle \mathrm{d}\omega_t, \varphi \rangle = \int_{\mathbb{R}^N} \varphi(x - t\omega)\mathrm{d}\omega$ is continuous. Let $(i_1, i_2) \in \{0, 1, \ldots, \nu\}^2$. We have

$$\begin{aligned} M_{i_1} U_\infty * M_{i_2} U_\infty(t)[\rho]\varphi &= \int_0^t M_{i_1} U_\infty(s)[\mathrm{d}\omega_{(t-s)e_{i_2}(\rho)} * \varphi]\mathrm{d}s \\ &= \int_0^t \int_{\mathbb{S}^{N-1}} [\mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))} * \varphi](x - se_{i_1}(\rho)\omega)\mathrm{d}\omega\mathrm{d}s \\ &= \int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * [\mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))} * \varphi]\mathrm{d}s \\ &= \left[\int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s \right] * \varphi, \end{aligned}$$

where the integral $\int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s$ is taken in the weak star sense, i.e.,

$$\left\langle \int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s, \varphi \right\rangle = \int_0^t \langle \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}, \varphi \rangle \mathrm{d}s.$$

As the measure $\int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s$ is bounded, by the Radon-Nikodym theorem, it suffices to show that it is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^N$, i.e.,

$$I_A := \int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s\{A\} \to 0 \quad \text{as } |A| \to 0,$$

where $|A|$ is the Lebesgue measure of set A. Since

$$\begin{aligned} I_A &= \int_0^t \int_{\mathbb{R}^N \times \mathbb{R}^N} \int \chi_A(v_1 + v_2)\mathrm{d}\omega_{se_{i_1}(\rho)}(v_1) \otimes \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}(v_2)\mathrm{d}s \\ &= \int_0^t \int_{\mathbb{R}^N \times \mathbb{R}^N} \int \chi_A(se_{i_1}(\rho)v_1 + (t-s)e_{i_2}(e_{i_1}(\rho))v_2)\mathrm{d}\omega(v_1)\mathrm{d}\omega(v_2)\mathrm{d}s, \end{aligned}$$

the change of variables $v_1' = e_{i_1}(\rho)v_1$ and $v_2' = e_{i_2}(e_{i_1}(\rho))v_2$ amounts to showing that

$$I_A' := \int_0^t \int_{\mathbb{R}^N \times \mathbb{R}^N} \int \chi_A(sv_1' + (t-s)v_2')\mathrm{d}\omega^1(v_1')\mathrm{d}\omega^2(v_2')\mathrm{d}s \to 0 \quad \text{as } |A| \to 0,$$

where $\mathrm{d}\omega^1$ (respectively, $\mathrm{d}\omega^2$) is the Lebesgue measure on the sphere $\{v \in \mathbb{R}^N : |v| = e_{i_1}(\rho)\}$ [respectively, $\{v \in \mathbb{R}^N : |v| = e_{i_2}(e_{i_1}(\rho))\}$]. But the last assertion follows from Ref. 10, p. 82. Moreover, we can easily see that the function $\int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \mathrm{d}\omega_{(t-s)e_{i_2}(e_{i_1}(\rho))}\mathrm{d}s$ is uniformly bounded for bounded time and for $\rho \in I$. Suppose that the assertion is true for j and let $(i_1, \ldots, i_{j+1}) \in \{0, 1, \ldots, \nu\}^{j+1}$. By hypothesis there exists $\eta(t, \rho) \in L^1(\mathbb{R}^N)$ (in fact, uniformly bounded for bounded time and for $\rho \in I$) such that

$$M_{i_2} U_\infty * \cdots * M_{i_{j+1}} U_\infty(t)[\rho]\varphi = \eta(t, \rho) * \varphi.$$

Then we have

$$M_{i_1}U_\infty * M_{i_2}U_\infty * \cdots * M_{i_{j+1}}U_\infty(t)[\rho]\varphi = \int_0^t M_{i_1}U_\infty(s)[\eta((t-s),\rho) * \varphi]\mathrm{d}s$$

$$= \int_0^t \int_{\mathbb{S}^{N-1}} [\eta((t-s),e_{i_1}(\rho)) * \varphi](x - se_{i_1}(\rho)\omega)\mathrm{d}\omega\mathrm{d}s$$

$$= \int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * [\eta((t-s),e_{i_1}(\rho)) * \varphi]\mathrm{d}s$$

$$= \left[\int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \eta((t-s),e_{i_1}(\rho))\mathrm{d}s\right] * \varphi.$$

By putting $\beta(t,\rho) = \int_0^t \mathrm{d}\omega_{se_{i_1}(\rho)} * \eta((t-s),e_{i_1}(\rho))\mathrm{d}s$ we have the desired β. □

We are now in the position to state the main result of this section.

Theorem 3: *Under assumptions (A1)–(A5), the three semigroups* $(\mathrm{e}^{t(T+K_e)})_{t\geqslant 0}$, $(\mathrm{e}^{t(T+K_e+K_d)})_{t\geqslant 0}$, *and* $(\mathrm{e}^{t(T+K_e+K_d+K_c)})_{t\geqslant 0}$ *have the same essential type.*

Proof: Since $R_2(t)$ is weakly compact, by Corollary 2.1, p. 16 in Ref. 10, $R_5(t)$ is compact, and then by Theorem 1 the two semigroups $(\mathrm{e}^{t(T+K)})_{t\geqslant 0}$ and $(\mathrm{e}^{t(T+K_e+K_d)})_{t\geqslant 0}$ have the same essential type. Having in mind that the essential type of the latter is equal to $\omega_{\mathrm{ess}}(T+K_e)$ (see Lemma 3), we get the conclusion. □

Corollary 1: Let (A1)–(A5) be satisfied. Moreover, suppose that the kernels k_c, k_e, $k_d^{(m)}(m=1,\ldots,\nu)$ *are non-negative. Then* $\omega_{\mathrm{ess}}(T+K)\leqslant s(T+K_e)$,*where* $s(T+K_e)$ *is the spectral bound of* $T+K_e$. □

Proof: Since the kernels are non-negative, using the Dyson-Phillips expansions, we can see that the semigroups are positive. By Weis's result[22] on the identity of the type of positive semigroup on L^p spaces and the spectral bound of its generators, we have $s(T+K_e)=\omega_0(T+K_e)$. Finally, the inequality $\omega_{\mathrm{ess}}(T+K_e)\leqslant\omega_0(T+K_e)$, together with Theorem 3, ends the proof. □

III. L^p ANALYSIS, $1<p<\infty$

In L^p setting $(1<p<\infty)$, we will use the concept of regular operator introduced in Ref. 11. Namely, we assume the following.

(A6) $\{\int_V k_c(x,\cdot,v')\varphi(v')\mathrm{d}v';\|\varphi\|_{L^p(V)}\leqslant 1, x\in\Omega\}$ is relatively compact in $L^p(V)$.

(A7) For each $\psi'\in L^{p'}(V)(1/p+1/p'=1)$,$\{\int_V k_c(x,v,\cdot)\psi(v)\mathrm{d}v;x\in\Omega\}$ is relatively compact in $L^{p'}(V)$.

We recall the following.

Lemma 5 (*Ref.* 11): *Under assumptions (A6) and (A7), the collision operator* K_c *can be approximated in the norm operator topology by collision operators with separable kernels*

$$\sum_{i\in J}\alpha_i(x)f_i(v)g_i(v'), \tag{10}$$

where $\alpha_i\in L^\infty(\Omega)$, $f_i\in L^p(V)$, *and* $g_i\in L^{p'}(V),(i\in J)$ *with J finite.*

Analogously, we define the class of collision operators K_e we consider in this section. We suppose that K_e satisfies the following.

(A8) The family $\{\int_{\mathbb{S}^{N-1}} k_e(x,\rho,\cdot,\omega')\varphi(\omega')\mathrm{d}\omega' : (x,\rho)\in\Omega\times I, \|\varphi\|_{L^p(\mathbb{S}^{N-1})}\leqslant 1\}$ is relatively compact in $L^p(\mathbb{S}^{N-1})$.

(A9) For each $\psi'\in L^{p'}(\mathbb{S}^{N-1})$, $\{\int_{\mathbb{S}^{N-1}} k_e(x,\rho,\omega,\cdot)\psi'(\omega)\mathrm{d}\omega : (x,\rho)\in\Omega\times I\}$ is relatively compact in $L^{p'}(\mathbb{S}^{N-1})$.

Under these assumptions, K_e is bounded, namely,

$$\|K_e\| = \operatorname*{ess\,sup}_{(x,\rho)\in\Omega\times I} \|K_e(x,\rho)\|_{\mathcal{L}(L^p(\mathbb{S}^{N-1}))},$$

where $K_e(x,\rho): L^p(\mathbb{S}^{N-1}) \ni \varphi \mapsto \int_{\mathbb{S}^{N-1}} k_e(x,\rho,\omega,\omega')\varphi(\omega')\mathrm{d}\omega'$. Moreover, by adapting the same technicalities as in Proposition 1 in Ref. 11, we can prove the following.

Lemma 6: An elastic collision operator satisfying (A8) and (A9) can be approximated in the norm operator topology by collision operators with separable kernels

$$\sum_{i\in J} \beta_i(x,\rho)h_i(\omega)\gamma_i(\omega'), \tag{11}$$

where $\beta_i \in L^\infty(\Omega\times I)$, $h_i \in L^p(\mathbb{S}^{N-1})$, *and* $\gamma_i \in L^{p'}(\mathbb{S}^{N-1}), (i \in J \subset \mathbb{N})$ *with* J *finite and* $1/p+1/p'=1$.

Finally, we suppose that kernels $k_d^{(m)}$, $m=1,\ldots,\nu$, satisfy (A5), i.e., they are bounded.

Note that Lemma 3 remains true in L^p setting, $1<p<\infty$, without any modification. Moreover, we have the following more precise result.

Lemma 7: Under assumptions (A5)–(A9), the difference

$$\mathrm{e}^{t(T+K)} - \mathrm{e}^{t(T+K_e+K_d)}$$

is compact for all $t\geqslant 0$.

Proof: According to Ref. 10, Theorem 2.6, p. 16, $\mathrm{e}^{t(T+K)}-\mathrm{e}^{t(T+K_e+K_d)}$ is compact for all $t\geqslant 0$ if and only if the strong integral

$$\int_0^t \mathrm{e}^{s(T+K_e+K_d)}K_c\mathrm{e}^{(t-s)(T+K_e+K_d)}\mathrm{d}s$$

is. Since the latter depends continuously (and linearly) on K_c, it suffices to consider a collision operator K_c of the form (10) and K_e of the form (11). By density again, we may assume that all the functions f_i, g_i [in Eq. (10)] are continuous with compact support, and all the functions h_i, γ_i [in Eq. (11)] are continuous. In this case $\int_0^t \mathrm{e}^{s(T+K_e+K_d)}K_c\mathrm{e}^{(t-s)(T+K_e+K_d)}\mathrm{d}s$ maps $L^q(\Omega\times V)$ into itself for all $q\geqslant 1$, and consequently, by interpolation arguments (see Ref. 6, Theorem 3.10, p. 57), we may restrict ourselves to the Hilbertian case $p=2$. To have the compactness of

$$\int_0^t \mathrm{e}^{s(T+K_e+K_d)}K_c\mathrm{e}^{(t-s)(T+K_e+K_d)}\mathrm{d}s$$

it suffices that the following hold (see Ref. 1, Theorem 3.2).

(i) For some $\eta > \omega_0(T+K_e+K_d)$, the operator

$$(\eta+i\gamma-T-K_e-K_d)^{-1}K_c(\eta+i\gamma-T-K_e-K_d)^{-1}$$

is compact for all $\gamma\in\mathbb{R}$.

(ii) $0<t\mapsto\int_0^t \mathrm{e}^{s(T+K_e+K_d)}K_c\mathrm{e}^{(t-s)(T+K_e+K_d)}\mathrm{d}s$ is norm continuous.

(iii) Moreover, to have (ii), using Lemma 2.1 in Ref. 14, it suffices to show that for some $\eta > \omega_0(T+K_e+K_d)$,

$$\|(\eta+i\gamma-T-K_e-K_d)^{-1}K_c\| + \|K_c(\eta+i\gamma-T-K_e-K_d)^{-1}\| \to 0 \quad \text{as } |\gamma|\to\infty.$$

Now, to prove (i) and (iii) remark that, by simple algebraic manipulations, we have for $\mathrm{Re}\,\lambda$ large enough

$$K_c(\lambda-T-K_e-K_d)^{-1} = K_c(\lambda-T)^{-1} + K_c(\lambda-T)^{-1}(K_e+K_d)(\lambda-T-K_e-K_d)^{-1},$$

$$(\lambda - T - K_e - K_d)^{-1}K_c = (\lambda - T)^{-1}K_c + (\lambda - T - K_e - K_d)^{-1}(K_e + K_d)(\lambda - T)^{-1}K_c,$$

so (i) is a consequence of Ref. 10, Theorem 4.1, p. 57, saying that $(\lambda - T)^{-1}K_c$ is compact for all $\lambda \in \mathbb{C}\backslash\sigma(T)$, while (iii) is consequence of Ref. 14, Lemma 3.13, establishing that

$$\|(\eta + i\gamma - T)^{-1}K_c\| + \|K_c(\eta + i\gamma - T)^{-1}\| \to 0 \quad \text{as } |\gamma| \to \infty$$

for all $\eta > \omega_0(T)$. □

Using the above lemma we can state the following.

Theorem 4: *Under assumptions (A5)–(A9), the three semigroups* $(e^{t(T+K_e)})_{t\geq 0}$, $(e^{t(T+K_e+K_d)})_{t\geq 0}$, *and* $(e^{t(T+K_e+K_d+K_c)})_{t\geq 0}$ *have the same essential type.*

Proof: From the compactness of $e^{t(T+K)} - e^{t(T+K_e+K_d)}$ for all $t \geq 0$, it follows that $\sigma_{ess}(e^{t(T+K)}) = \sigma_{ess}(e^{t(T+K_e+K_d)})$ for all $t \geq 0$, with, in particular, $\omega_{ess}(T+K) = \omega_{ess}(T+K_e+K_d)$. On the other hand, as already said above, Lemma 3 stated in L^1 setting remains true in L^p setting, $1 < p < \infty$, and hence we get $\omega_{ess}(T+K_e+K_d) = \omega_{ess}(T+K_e)$. □

In the same spirit of Corollary 1 we have the following.

Corollary 2: Let (A5)–(A9) be satisfied. Moreover, suppose that all the kernels k_c, k_e, $k_d^{(m)}$ $(m = 1, \ldots, \nu)$ *are non-negative. Then* $\omega_{ess}(T+K) \leq s(T+K_e)$, *where* $s(T+K_e)$ *is the spectral bound of* $T+K_e$. □

Remark 2: Corollaries 1 and 2 answer Problem 3 in Ref. 10, p. 93, by finding an estimate of the essential type for the neutron transport semigroup when the collision operator involves, in addition to the classical operator K_c, another term.

Actually, we can refine Corollaries 1 and 2 if we assume the following continuity assumption:

(A10) The mapping $I \ni \rho \mapsto K_e^{\rho} \in \mathcal{L}(L^p(\Omega \times \mathbb{S}^{N-1}))$ is piecewise continuous, where K_e^{ρ} is the one speed operator:

$$L^p(\Omega \times \mathbb{S}^{N-1}) \ni \varphi \mapsto \int_{\mathbb{S}^{N-1}} k_e(x, \rho, \omega, \omega')\varphi(x, \omega')\mathrm{d}\omega' \in L^p(\Omega \times \mathbb{S}^{N-1}).$$

More precisely we have the following.

Proposition 1: (a) Let (A1)-(A5) and (A10) be satisfied. Then we have the following spectral mapping theorem:

$$\sigma_{ess}(e^{t(T+K_e)}) = e^{t\sigma(T+K_e)} \cup \{0\} \quad \textit{for all } t \geq 0 \tag{12}$$

in L^1 *setting. In particular,* $\omega_{ess}(T+K) = s(T+K_e)$. *(b) The same conclusions hold true in* L^p *setting* $(1 < p < \infty)$ *under assumptions (A5)–(A10).*

After showing spectral mapping theorem (12), the equality $\omega_{ess}(T+K) = s(T+K_e)$ is just a consequence of Theorems 3 and 4. The proof of the spectral mapping theorem can be found in Ref. 14, Chap. 6. It relies, in particular, on the concept of critical spectrum introduced in Ref 12.

At this stage, it may be useful to recall the description of $\sigma(T+K_e)$ obtained by Larsen and Zweifel. First, the spectrum of T consists of a half plan or only the point at infinity, depending, respectively, upon whether the minimum neutron speed ρ_{min} is or is not zero. The spectrum of $T+K_e$, for fixed ρ, is a pure isolated point spectrum of finite algebraic multiplicity restricted to a certain left half plan. As ρ varies, the point spectrum of $T+K_e$ for fixed ρ shifts about to form curves; the full spectrum of $T+K_e$ consists of the closure of this set of curves plus $\sigma(T)$.

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Existence and computation of optimally localized coherent states

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This paper is concerned with localization properties of coherent states. Instead of classical uncertainty relations we consider "generalized" localization quantities. This is done by introducing measures on the reproducing kernel. In this context we may prove the existence of optimally localized states. Moreover, we provide a numerical scheme for deriving them. © *2006 American Institute of Physics.*
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I. MOTIVATION

The goal of this paper is to introduce a new concept of localization. In classical lore, one typically considers uncertainty relations. In this framework it is well known that a nonzero state or wave function cannot be arbitrarily well localized simultaneously in space and Fourier domain. This fact may be quantified by the Heisenberg uncertainty relation,

$$\Delta x \Delta k \geqslant 2\pi.$$

There are functions which are optimally localized in phase space in that they satisfy the inequality with the lower bound. For a detailed analysis on uncertainty relations in the context of Gabor and wavelet transforms we refer, e.g., to Refs. 11, 12, 5, and 18.

However, for certain physical applications, e.g., radar imaging, it is very promising to ask for more flexible concepts. In principle, in radar imaging one has to evaluate the output of the correlation receiver, see Ref. 1. An important role in detecting objects is played by the radar ambiguity function, which is ideally given by a delta function. In the narrow band regime, which is of interest in radar imaging, the ambiguity function is given by $\Pi(\phi,\tau)=\langle \Psi_{\phi,\tau}, \Psi_{\phi_0,\tau_0}\rangle$, where Ψ stands for the transmitted wave form. Since a delta pulse is obviously not possible to realize, one currently uses pulses that minimize by means of its band/Doppler width and its pulse/range width the so-called narrow band (Heisenberg) uncertainty principle, see Refs. 1, 7, 6, and 4. A minimization of the Heisenberg quantities leads to pulses with Gaussian envelope function. But this is difficult to implement too and, moreover, allows no flexibility in specifying more sophisticated localization attributes; e.g., in order to obtain an accurate spatial resolution while allowing a certain frequency uncertainty, the ambiguity function Π should have fast decay with respect to range and a moderate decay with respect to Doppler frequency, e.g.,

$$|\Pi(\phi,\tau)| \leqslant (1+|\tau|)^{-4}(1+\log(1+|\phi|))^{-1}. \tag{1.1}$$

With the theory presented here in the paper at hand, we may now proceed as follows. Given the specific localization characteristic (1.1) in the range Doppler plane, we compute the optimal wave

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form to be transmitted. To be more general, we consider measures of uncertainty or delocalization in phase space (range Doppler plane) and we shall prove the existence of optimally localized states (wave forms).

In principle, general wavelet transforms

$$s \mapsto \mathcal{W}_g s, \quad \mathcal{W}_g s(x) = (U(x)g, s)_H, \quad x \in G$$

associated with the square integrable irreducible representation U of a locally compact group G provide a one to one correspondence between the state Hilbert space H and a reproducing kernel Hilbert space over the group. The reproducing kernel is up to a normalization the wavelet transform of the wavelet itself,

$$\Pi = \mathcal{W}_g g.$$

This kernel can be interpreted as the Heisenberg box of the phase space. In this paper we shall be concerned with localization properties of these reproducing kernels. In fact, the reproducing kernel of wavelet analysis cannot be arbitrarily well localized. For instance, there is no wavelet such that the associated reproducing kernel is compactly supported. Obviously there is no universal way of quantifying localization. Instead we propose to quantify localization through the following and similar families of cost functionals:

$$\Phi[g] = \sup_{x \in G} w(x)^{-1} |\mathcal{W}_g g(x)|,$$

where w is some positive weight, decaying "at ∞." We will prove that this functional and similar "localization" functionals are weakly lower semicontinuous. It therefore has a minimizer over any weak* compact set. In other words, for any such measure of localization there is at least one optimal state.

Localization of wavelet transforms has been considered before, see, e.g., Refs. 17, 15, 9, and 8. In Refs. 9 and 8 the authors consider localizing wavelet coefficients with respect to some preassigned analyzing wavelet and a compact subset in the wavelet plane. In their approach the analyzing wavelet was fixed. In this paper, however, we consider the nonlinear problem of optimizing the localization of the reproducing kernel. Since the reproducing kernel depends quadratically on the underlying wavelet, this problem is by nature highly nonlinear and therefore an explicit expression of the optimal state seems to remain a pipe dream. However, in the last section we discuss a numerical procedure to approximately compute such optimally localized states.

II. THE BASIC FORMULAS

Let us recall the basic formulas of continuous wavelet transform associated with a square integrable group representation. We only recall the few facts that are necessary for this paper. For more details we refer to, e.g., Refs. 10 and 13. Let G be a noncompact, locally compact group, σ a compact topological group, and $G \ni g \mapsto U(g)$ a unitary, strongly continuous, irreducible, square integrable representation in some Hilbert space H. The wavelet transform of $s \in H$ with respect to $g \in H$ is pointwise defined for $x \in G$ as

$$\mathcal{W}_g s(x) = (U(x)g, s)_H.$$

The left and the right invariant Haar measures are denoted by $d\lambda$ and $d\rho$. They are defined up to some positive factor. Over G we consider the two Hilbert spaces $L^2(G, d\lambda)$ and $L^2(G, d\rho)$. We suppose that $d\lambda$ and $d\rho$ are scaled suitably so that the mapping $s(x) \mapsto s(x^{-1})$ is an isometry between these two Hilbert spaces. A wavelet is called admissible if $\mathcal{W}_g g \in L^2(G, d\lambda)$. Thanks to the formula

$$\mathcal{W}_g s(x) = \mathcal{W}_s g(x^{-1}),$$

admissibility is also equivalent to $\mathcal{W}_g g \in L^2(G, d\rho)$. We denote the set of all admissible wavelets by A. For $g, h \in A$ and $s, u \in H$ the following equation holds:

$$(\mathcal{W}_g s, \mathcal{W}_h u)_{L^2(G,d\lambda)} = C(g,h)(s,u)_H, \tag{2.1}$$

where C is a densely defined, closed, positive quadratic form. Its form domain is precisely A. We write $c_{g,h} = C(g,h)$ and $c_g = C(g,g)$. By the first representation theorem there is a closed, linear operator T such that for all $u \in D(T)$ and $v \in A$ we have $C(v,u) = (v, Tu)_H$. The space A is in general a nonclosed subspace of H. However, since C is a closed quadratic form it becomes a Hilbert space with respect to

$$(s,u)_A = (s,u)_H + C(s,r), \quad \|s\|_A^2 = \|s\|_H^2 + c_s.$$

Convergence in A will be understood with respect to this norm. From Eq. (2.1) it follows that, in particular, $\mathcal{W}_g$ is for admissible, nonzero g a multiple of an isometry,

$$\|\mathcal{W}_g s\|_{L^2(G,d\lambda)}^2 = c_g \|s\|_H^2.$$

The adjoint of the wavelet analysis is a wavelet synthesis,

$$\mathcal{W}_g^* = \mathcal{M}_g.$$

Formally it can be written as follows:

$$\mathcal{M}_h r(x) = \int_G r(x) U(x) h d\lambda(x).$$

We have for $g, h \in A$

$$\mathcal{M}_h \mathcal{W}_g = c_{g,h} 1.$$

The combination $\mathcal{W}_g \mathcal{M}_h$ can be written as noncommutative convolution operator. If we define on $L^2(G, d\lambda) \times L^2(G, d\lambda)$ the (left) convolution product as

$$\Pi * r(x) = \int_G \Pi(y^{-1} \circ x) r(y) d\lambda(y),$$

we have for $g, h \in A$

$$\mathcal{W}_g \mathcal{M}_h = \Pi *, \quad \Pi = \mathcal{W}_g h.$$

In particular, we will use the following formula over and over:

$$\mathcal{W}_h = \Pi * \mathcal{W}_g, \quad \Pi = c_{g,h}^{-1} \mathcal{W}_h h.$$

III. GENERAL LOCALIZATIONS

Before formulating the general existence theorem we consider the particular case of localization measures through a weighted L^∞ norm. Consider therefore a positive function $w: G \to R_+$. We suppose that w is symmetric,

$$w(x^{-1}) = w(x),$$

and invariant under the G action in that for all $y \in G$ we can find a $c > 0$ such that

$$w(y \circ x) \leqslant cw(x), \quad w(x \circ y) \leqslant cw(x).$$

Then $w \in L^2(G, d\lambda)$ is equivalent to $w \in L^2(G, d\rho)$. Moreover, we consider weights, for which either of both (and hence both) of the following holds:

$$w * w \in L^2(G, d\lambda), \quad w * w \in L^2(G, d\rho).$$

A natural measure for the localization of a function r over G with respect to w is the following weighted norm:

$$\sup_G w^{-1}|r|.$$

For fixed $h \in A$ let $\Sigma_h \subset H$ denote the affine subspace of codimension 1 defined through $\Sigma_h = \{g \in H : (g, Th)_H = 1\}$. Note that Σ_h may contain nonadmissible vectors. The admissible wavelets in Σ_h are reconstruction wavelets for h:

$$\mathcal{M}_h \mathcal{W}_g = \mathcal{M}_g \mathcal{W}_h = 1.$$

We introduce the following functional on H:

$$\Phi[s] = \Phi_w[s] = \sup_G w^{-1}|\mathcal{W}_s s|,$$

whenever the right hand side is finite. In all other cases we set $\Phi[s] = \infty$. We now can formulate the first theorem.

Theorem 1: *Let $h \in H$, $h \neq 0$, be such that $\Phi[h] < \infty$. Then there exists a wavelet $g \in \Sigma_h$ such that for all $u \in \Sigma_h$ we have*

$$\Phi[g] \leqslant \Phi[u].$$

In other words, the localization functional Φ has a minimizer in each Σ_h, for all h, which have some regularity as expressed through $|\mathcal{W}_h h| \leqslant w$. Note that we have to require that $\Phi[h] < \infty$. This ensures that the set of functions having a w localization is not empty. In turn, this is a requirement for w in which it should not be decaying too fast (e.g., compactly supported weights are not possible).

Actually this kind of results can be generalized to a more abstract setting as follows. Consider two Banach spaces B, $K \subset L^2(G, d\lambda + d\rho)$ of functions over G with continuous embeddings. B should be a lattice, $\| |s| \|_B = \|s\|_B$. We then can define a localization with respect to B simply as

$$\Phi[g] = \|\mathcal{W}_g g\|_B.$$

We include the value $\Phi = \infty$ in the natural way. For B and K we further suppose that the following holds.

Invariance of B. B should be G bi-invariant: for all $y \in G$ there is a $b > 0$ such that

$$\|s(y \circ \cdot)\|_B \leqslant b\|s\|_B, \quad \|s(\cdot \circ y)\|_B \leqslant b\|s\|_B.$$

It should be stable under inversion

$$\|s(x^{-1})\|_B \leqslant d\|s\|_B.$$

Then we have $u(x) = s(y^{-1} \circ x \circ y)$ satisfies $\|u\|_B \leqslant e\|s\|_B$.

Semicontinuity of B norm. Suppose further that the following inequality holds for the norm in B: if $s_n \in B$ is any sequence of non-negative functions $s_n \geqslant 0$ then consider $s = \liminf_{n\to\infty} s_n$. Then we require that

$$\|s\|_B = \|\liminf s_n\|_B \leqslant \liminf_{n\to\infty} \|s_n\|_B.$$

In classical L^p spaces this is a direct consequence of Fatou's lemma,

$$\int \liminf s_n d\mu \leqslant \liminf \int s_n d\mu.$$

Compact embedding of K. For the space K we suppose that the following compact embedding property holds: let $L \subset K$ be a K-bounded set. If now on each compact subset of G the set of functions L is uniformly continuous then L is precompact in $L^2(G, d\lambda + d\rho)$.

Convolution mapping. The two spaces B and K are linked through the following convolution property: for fixed $r \in B$ the convolution product with r is a linear operator,

$$*_r : B \to K, \quad u \mapsto r * u,$$

and it is bounded $\|r * u\|_K \leqslant d\|u\|_B$, with d depending only on r.

Nonempty. We suppose that there is at least one $h \in D(T), h \neq 0$ such that $\Phi[h] < \infty$. This h is admissible, $h \in A$, since $B \subset L^2(G, d\lambda + d\rho)$. Thanks to the following lemma.

Lemma 1: Let $h \in A$, $h \neq 0$ be given. Then $g \in H$ is actually in A if and only if

$$\|g\|^2 = \|\mathcal{W}_h g\|^2_{L^2(G,d\lambda)} + \|\mathcal{W}_h g\|^2_{L^2(G,d\rho)} < \infty.$$

The square root of the left hand side defines a norm which on A is equivalent to the norm of A:

$$c_h^{-1}\|\mathcal{W}_h g\|^2_{L^2(G,d\lambda)} + \|h\|_H^{-2}\|\mathcal{W}_h g\|^2_{L^2(G,d\rho)} = \|g\|^2_A.$$

Proof: Suppose $g \in A$. Thanks to the formula

$$\|\mathcal{W}_h g\|^2_{L^2(G,\rho)} = \|\mathcal{W}_g h\|^2_{L^2(G,d\lambda)} = c_g \|h\|^2_H$$

and the isometric property of the wavelet transform we may conclude. ■

Under the above conditions, the following theorem holds.

Theorem 2: *There is a $g \in \Sigma_h \cap A$ such that for all $u \in \Sigma_h$ we have*

$$\Phi[g] \leqslant \Phi[u].$$

This function g then satisfies $\mathcal{W}_h g \in K$.

Typical examples for such spaces B are as follows. As space B we take the functions for which we have

$$\|r\|_{w,\infty} = \|w^{-1} r\|_{L^\infty(G)}.$$

We write also $B_{w,\infty}$ for this space. For the space K we take the analogue space of functions with weight $u = w * w$. If now $u \in L^2(G, d\lambda + d\rho)$ then we are in the setting of the first theorem. We only have to convince ourselves that all properties of the stated spaces are satisfied. The only nontrivial property is now the compact embedding.

Lemma 2: Let $u > 0$ be a symmetric weight function with $u \in L^2(G, d\lambda + d\rho)$. Then any set of functions which are uniformly continuous on compact sets of G is precompact in $L^2(G, d\lambda)$.

Proof: Let s_n be a sequence of functions in this set of functions. Since G is σ compact we can find a sequence of compact sets $K_m \subset G$ with $K_m \subset K_{m+1}$ and $\cup K_m = G$. Upon choosing a subsequence we may require that

$$\int_{G \setminus K_m} u^2 (d\lambda + d\rho) \leqslant 1/m.$$

On each K_m we can therefore find a uniformly convergent subsequence. Therefore upon choosing a suitable diagonal subsequence we may suppose that for $m' > m$

$$\int_{K_m} |s_m - s_{m'}|^2 (d\lambda + d\rho) \leqslant 1/m.$$

We therefore have

$$\|s_m - s_{m'}\|^2_{L^2(G,d\lambda+d\rho)} = \int_{G\setminus K_m} |s_m - s_{m'}|^2 (d\lambda + d\rho) + \int_{K_m} |s_m - s_{m'}|^2 (d\lambda + d\rho) \leqslant 2/m, \tag{3}$$

and thus s_m is a Cauchy sequence. Its pointwise limit exists, and thanks to Fatou lemma being in $L^2(G, d\lambda + d\rho)$. ■

A second family is given by

$$\|r\|_{w,2} = \|w^{-1/2} r\|_{L^2(d\lambda+d\rho)}.$$

We denote by $B_{w,2}$ the associated Banach space. This means that we consider localization quantities of the form

$$\int_G w^{-1} |\mathcal{W}_g g|^2 d\lambda.$$

If w is such that

$$\eta(x) = \sup_{y \in G} \sqrt{w(y^{-1} \circ x) w(y)}$$

satisfies $\eta \in L^2(G, d\lambda + d\rho)$, we may estimate for $r = w^{1/2} u$, $s = w^{1/2} v$, $u, v \in L^2(G, d\lambda + d\rho)$ that

$$|r * s(x)| \leqslant \int w(y^{-1} \circ x) w(y) u(y^{-1} \circ x) v(y) d\lambda\ (y)| \leqslant \eta(x) \|u\|_{L^2(G,d\rho)} \|v\|_{L^2(G,d\lambda)} \leqslant \eta(x) \|r\|_{w,2} \|s\|_{w,2},$$

and thus we have $B_{w,2} * B_{w,2} \subset B_{\eta,\infty}$. Therefore the theorem applies if we choose for the space $K = B_{\eta,\infty}$ and we have the existence of an optimally localized reconstruction wavelet.

We now prove the theorem. To start we analyze the mapping properties of Φ. We denote by Δ the domain of Φ,

$$\Delta = \{s \in H : \Phi[s] < \infty\} \subset A.$$

Lemma 3: The functional Φ is strongly H lower semicontinuous on Δ. More precisely for $\Delta \ni u_n \to u \in H$ in H, we have

$$\Phi[u] \leqslant \liminf_{n\to\infty} \Phi[u_n].$$

Proof: Since $\mathcal{W}_{u_n} u_n \to \mathcal{W}_u u$ pointwise and thus by hypothesis of semicontinuity of the B norm

$$\Phi[\lim_{n\to\infty} u_n] = \|\lim_{n\to\infty} \mathcal{W}_{u_n} u_n\|_B \leqslant \liminf_{n\to\infty} \|\mathcal{W}_{u_n} u_n\| = \liminf_{n\to\infty} \Phi[u_n].$$

■

We even have the following lemma.

Lemma 4: The functional Φ is H-weakly lower semicontinuous on $\Delta\setminus\{0\}$. More precisely, for any H-weak convergent sequence $\Delta \ni g_n \to g \in H$, $g \neq 0$ with $g_n \in \Delta$ we have $\Phi[g] \leqslant \liminf \Phi[g_n]$.

Proof: Let

$$\gamma = \lim_{n\to\infty} \inf \Phi[g_n].$$

Clearly $\gamma \geqslant 0$. In the case that $\gamma=\infty$ the lemma holds true and we may suppose $0 \leqslant \gamma < \infty$. We may find a subsequence which is denoted by g_n with $\Phi[g_n] < \infty$, and $\Phi[g_n] \to \gamma$. By hypothesis there is an $h \in D(T)$ with $\Phi[h] < \infty$. By the invariance of B it follows, thanks to

$$(\mathcal{W}_{U(y)h} U(y)h)(x) = \mathcal{W}_h h(y^{-1} \circ x \circ y),$$

that the whole orbit of h has the same properties. Since the representation is irreducible and T has dense range, we may suppose that $c_{g,h} = (g, Th)_H \neq 0$. For $s \in A$ we have by continuity of the convolution

$$\|\mathcal{W}_h s\|_K = \|\Pi * \mathcal{W}_s s\|_K \leqslant d\|\mathcal{W}_s s\|_B = d\Phi[s], \quad \Pi = c_{s,h}^{-1} \mathcal{W}_h h.$$

By weak convergence we have $c_{g_n,h} = (g_n, Th)_H \to (g, Th)_H \neq 0$. Therefore, since $g_n \in A$ thanks to $\Phi[g_n] < \infty$, we may conclude by setting $s = g_n$ in the formula above that $\{\mathcal{W}_h g_n\}$ is a bounded set in K and hence it is bounded in $\mathcal{W}_h H$ (the image of H under $\mathcal{W}_h$) too. Since the representation of the wavelet transform is strongly continuous this family of functions is uniformly continuous on any compact subset of G. Because of the compact embedding property of K we can extract an H convergent subsequence $g_{m(n)} \to g$. Since Φ is strongly lower continuous we have $\Phi[g] \leqslant \liminf \Phi[g_n] = \gamma$. ■

Now the proof of the main theorem is easy.

Proof: Let $\Phi[g_n] \to \gamma = \inf_{g \in \Sigma_h} \Phi[g]$. Since as before $\Phi[g_n] \leqslant b\|gn\|_H$ we see that g_n is bounded in H. Thanks to the Banach-Alaoglou theorem we may extract an H-weakly convergent subsequence $g_{m(n)} \to g$ weakly. Since Φ is weakly lower semicontinuous we may conclude that $\Phi[g] = \gamma$. The set Σ_h is weakly closed and hence $g \in \Sigma_h$. ■

We can even prove the following optimal localization result.

Theorem 3: *There is a g with* $\|g\|_H = 1$, *such that for all* $u \in H$, *with* $\|u\|_H = 1$ *we have*

$$\Phi[g] \leqslant \Phi[u].$$

Proof: As before, we find a weakly convergent sequence $g_n \to g$ with $\Phi[g] = \inf_{\|s\|=1} \Phi[s]$. Now as in the proof of Lemma 4 we see that there is a strongly convergent subsequence $g_{m(n)} \to g$ and thus $\|g\| = 1$. ■

IV. THE NUMERICAL APPROXIMATION OF LOCALIZED STATES

As we have shown in the previous section, for each weight function satisfying certain conditions, there exists an optimally localized wavelet g. The term "optimality" is strongly connected with the associated Banach space norm $\|\cdot\|_B$.

Before providing a receipt of how to derive those optimally localized wavelets, we wish to be more concrete and to give a few examples of typical Banach spaces and weight functions to which our theory can be applied. To this end, let us consider the class of α-modulation spaces which are usually defined by means of the flexible Gabor-wavelet transform, see Ref. 3,

$$\mathcal{W}_g^{\alpha}(f)(x) = (f, U(\sigma_{\alpha}(x))g)_H.$$

Since this transform is based on square integrability modulo quotients, we limit the subsequent consideration to the cases $\alpha=0$ and $\alpha=1$ (which fits then quite nicely with our framework, see below). For $\alpha=0$, the family $\{U(\sigma(x))g\}$ is a Gabor system and $\mathcal{W}_g^0 f$ coincides with the classical short time Fourier transform, while for $\alpha \to 1$ the family tends to the situation encountered in the wavelet context, where $\mathcal{W}_g^1$ is just a slight modification of the continuous wavelet transform. The intermediate case $\alpha = 1/2$ appears in the literature as the Fourier-Bros-Iagolnitzer transform.[2,14] In particular, one characterizes α-modulation spaces as follows (for simplicity we consider the wavelet transform of functions over $\mathbb{R}$): for $s \in \mathbb{R}$, for all $1 \leqslant p, q \leqslant \infty$, and for $\alpha \in [0,1)$,

$$M_{p,q}^{s+\alpha(1/q-1/2),\alpha}(\mathbb{R}) = \{f \in \mathcal{S}' : \mathcal{W}_g^\alpha(f) \in L^{p,q,s}\}, \quad \|f\|_{M_{p,q}^{s+\alpha(1/q-1/2),\alpha}} \asymp \|\mathcal{W}_g^\alpha(f)\|_{L^{p,q,s}},$$

where $L^{p,q,s}(\mathbb{R}^2)$ is the space of functions F on $\mathbb{R}^2$ such that

$$\|F\|_{Lp,q,s} := \left(\int_{\mathbb{R}} \left(\int_{\mathbb{R}} |F(t,\omega)|^p dt \right)^{q/p} (1+|\omega|)^{sq} d\omega \right)^{1/q} < \infty.$$

For $\alpha=0$, the space $M_{p,q}^{s,0}(\mathbb{R})$ coincides with the modulation space $M_{p,q}^s(\mathbb{R})$. For $\alpha \to 1$ the space $M_{p,q}^{s,1}(\mathbb{R})$ coincides with the inhomogeneous Besov space $B_{p,q}^s(\mathbb{R})$. These spaces serve as a reservoir of smoothness spaces in which functions can be characterized by means of special analyzing atoms or a so-called frame. A desirable property of the analyzing atom is localization with respect to underlying Banach spaces metric, i.e., in this context an optimal localized g is associated with Banach space norm $\|\cdot\|_{M_{p,q}^{s+\alpha(1/q-1/2),\alpha}}$ which in turn is here characterized by the weight

$$w(\omega) = (1+|\omega|)^s.$$

The numerical scheme developed below is limited to case $p=q=2$ and applies thus not to all situations.

Let us now consider a concrete case which is a little beyond the above mentioned examples. Let $L^{2,w^{-1}}$ with symmetric weight function

$$w^{-1}(x) = w^{-1}(a,b) = (|a|+|a|^{-1})^4 \cdot (1+|b|(1+|a|)^{-1})^4$$

be the space under consideration. Then, in accordance with Theorem 3, the optimization problem can be casted as follows:

$$\Phi(g) = \|\mathcal{W}_g g\|_{L^{2,w^{-1}}}^2 + \alpha \|g\|_H^2.$$

In order to discretize the problem somehow, we may represent g by means of some frame $\{\psi_\lambda\}_{\lambda\in\Lambda} \subset H$, i.e.,

$$g = \sum_{\lambda\in\Lambda} g_\lambda \psi_\lambda.$$

Consequently, the goal is to reconstruct a sequence $\{g_\lambda\}_{\lambda\in\Lambda} = \mathbf{g} \in \ell_2$ for which $\Phi(g) \leqslant \Phi(s)$, for all $s \in H$.

Introducing for some $x \in G$ the infinite matrix $\mathbf{A}(x) = ((\psi_\lambda, U(x)\psi_\eta)_H)_{\lambda,\eta\in\Lambda}$, the wavelet transform reads as $\mathcal{W}_g g(x) = \langle \mathbf{g}, \mathbf{A}(x)\mathbf{g}\rangle_{\ell_2} =: F[\mathbf{g}](x)$. Obviously, $F[\mathbf{g}](e) = \|g\|_H^2$, and thus we may write

$$\Phi(\mathbf{g}) = \|F[\mathbf{g}]\|_{L^{2,w^{-1}}}^2 + \alpha F[\mathbf{g}](e).$$

Since the optimization problem is no longer convex, we have to apply adequate strategies for nonlinear problems. We suggest to make use of a Tikhonov-based iteration method for nonlinear problems which was developed in Ref. 16. The technology to be applied here will always find a critical point of Φ, and under additional assumptions on F and the solution one can assure that the critical point is a global minimizer.

The method borrowed from Ref. 16 goes now as follows. Firstly, in order to obtain a problem which is hopefully easier to solve, we replace Φ by

$$\Phi^s(\mathbf{g};\mathbf{a}) := \Phi(\mathbf{g}) + C\|\mathbf{g}-\mathbf{a}\|_{\ell_2}^2 - \|F[\mathbf{g}] - F[\mathbf{a}]\|_{L^{2,w^{-1}}}^2, \tag{4.1}$$

where $\mathbf{a}$ is some auxiliary element in ℓ_2. So far its not clear whether Φ^s is positive or even bounded from below. Following the lines in Ref. 16, i.e., choosing for $\alpha > 0$ a ball around the origin K_r and C adequately large (in dependence on F and $\Phi(\mathbf{a})$), one can assure for all $\mathbf{g} \in K_r$, $\Phi(\mathbf{g}) \leqslant \Phi^s(\mathbf{g};\mathbf{a})$.

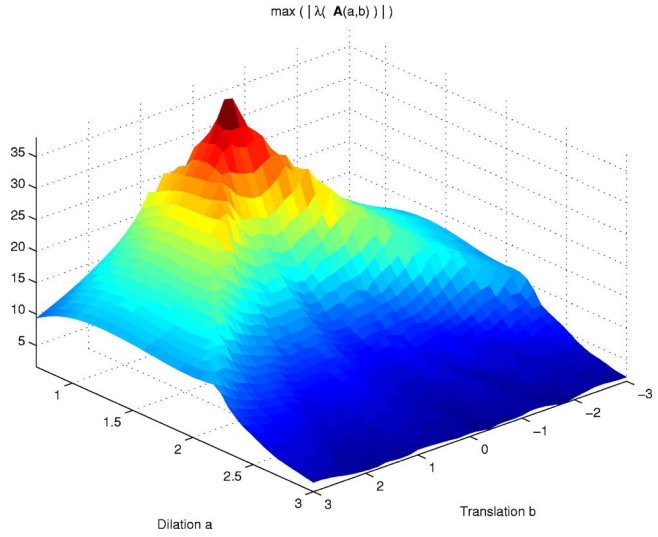

FIG. 1. (Color online) Maximal eigenvalues of the infinite matrices $A(a,b)$ for all the $(a,b)\in G$ used in the frame representation.

The iteration process is now obtained by picking some initial $\mathbf{g}_0=\mathbf{a}$ and therewith some proper $C>0$ and by deriving a sequence $\{\mathbf{g}_k\}_{k\in\mathbf{N}}$ via

$$\mathbf{g}_{k+1}=\arg\min_{\mathbf{g}}\Phi^s(\mathbf{g};\mathbf{g}_k).$$

From this iteration we expect convergence at least towards a critical point of Φ. First, we have to make sure that the sequence of functionals is properly defined.

Lemma 5: Let $\mathbf{a}$ *be given and* K_r, C *be defined as in Ref. 16. Then for all* $k\in\mathbf{N}$, $\Phi^s(\mathbf{g};\mathbf{g}_k)$ *are bounded from below, and moreover, the minimizers* $\mathbf{g}_{k+1}$ belong to K_r.

Let $\mathbf{A}$ now be the shorthand for $\mathbf{A}(e)$. A simple calculation shows the following.

Lemma 6: The necessary condition for a minimum of Eq. (4.1) *reads as*

$$\mathbf{g}=\frac{1}{C}\{\mathbf{g}_k-\alpha\mathbf{A}\mathbf{g}-F'[\mathbf{g}]^*(F[\mathbf{g}_k]w^{-1})\}. \tag{4.2}$$

The hope is that the right hand side of Eq. (4.2) defines a contraction. A straightforward computation shows

$$\|\mathbf{g}-\mathbf{g}'\|_{\ell_2}\leqslant\frac{1}{C}\{\alpha|||\mathbf{A}|||+2|||||\mathbf{A}(\cdot)|||||_{L^{2,w^{-1}}}\|F[\mathbf{g}_k]\|_{L^{2,w^{-1}}}\|\mathbf{g}-\mathbf{g}'\|_{\ell_2}.$$

To bound this quantity requires the Lipschitz continuity of $F'[\mathbf{g}]$, or in other words, the finiteness of $|||||\mathbf{A}(\cdot)|||||_{L^{2,w^{-1}}}$ which is difficult to prove, but can be verified numerically: we may consider the spectral radius $\rho(\mathbf{A}(a,b))$ (for a particular frame, see below) as a function of $(a,b)\in G$. Figure 1 shows a sufficient decay of $\rho(\mathbf{A}(a,b))$ and assures therewith that, for C large enough, the convergence of the fixed point iteration (4.2) towards a unique minimizer $\mathbf{g}_{k+1}$ of $\Phi^s(\mathbf{g};\mathbf{g}_k)$ can be achieved. Moreover, we have with the help of Ref. 16 that the sequence $\{\mathbf{g}_k\}$ converges at least towards a critical point of Φ. If we could impose more smoothness on F and on the solution $\mathbf{g}$ to be reconstructed, we could also achieve uniqueness.

Next, we have to ensure that $\|g^{n+1}\|_H^2=1$ (the index n stands now for the fixed point iteration) holds true through the whole fixed point iteration process, i.e., we have to determine α in each iteration step:

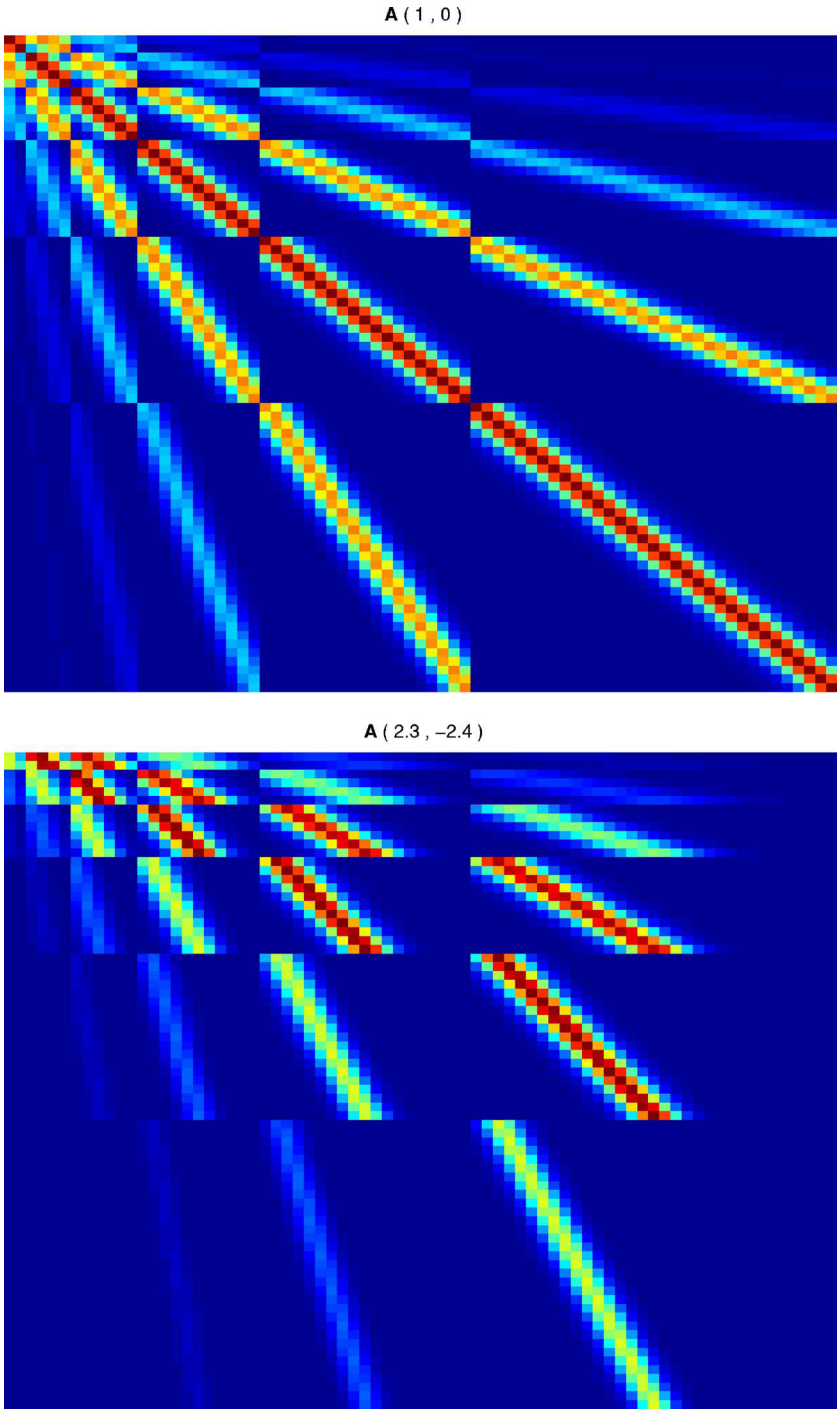

FIG. 2. (Color online) Structure of $A(a,b)$ for two particular cases; top, $(a,b)=(1,0)$ and bottom, $(a,b)=(2.3,-2.4)$.

$$(\mathbf{g}^{n+1},\mathbf{A}\mathbf{g}^{n+1})_{\ell_2}=\frac{1}{C^2}\{\alpha^2 F[\mathbf{A}\mathbf{g}^n](e)-2\alpha\Re(\mathbf{A}\mathbf{g}^n,\mathbf{A}(\mathbf{g}_k-F'[\mathbf{g}^n]^*(F[\mathbf{g}_k]w^{-1})))\ell_2$$
$$+F[\mathbf{g}_k-F'[\mathbf{g}^n]^*(F[\mathbf{g}_k]w^{-1})](e)\},$$

i.e., finding $\alpha=\alpha^{n+1}$ amounts to finding the roots of a real parabola. With the shorthand $M=\Re(\mathbf{A}\mathbf{g}^n,\mathbf{A}(\mathbf{g}_k-F'[\mathbf{g}^n]^*(F[\mathbf{g}_k]w^{-1})))_{\ell_2}$, we obtain

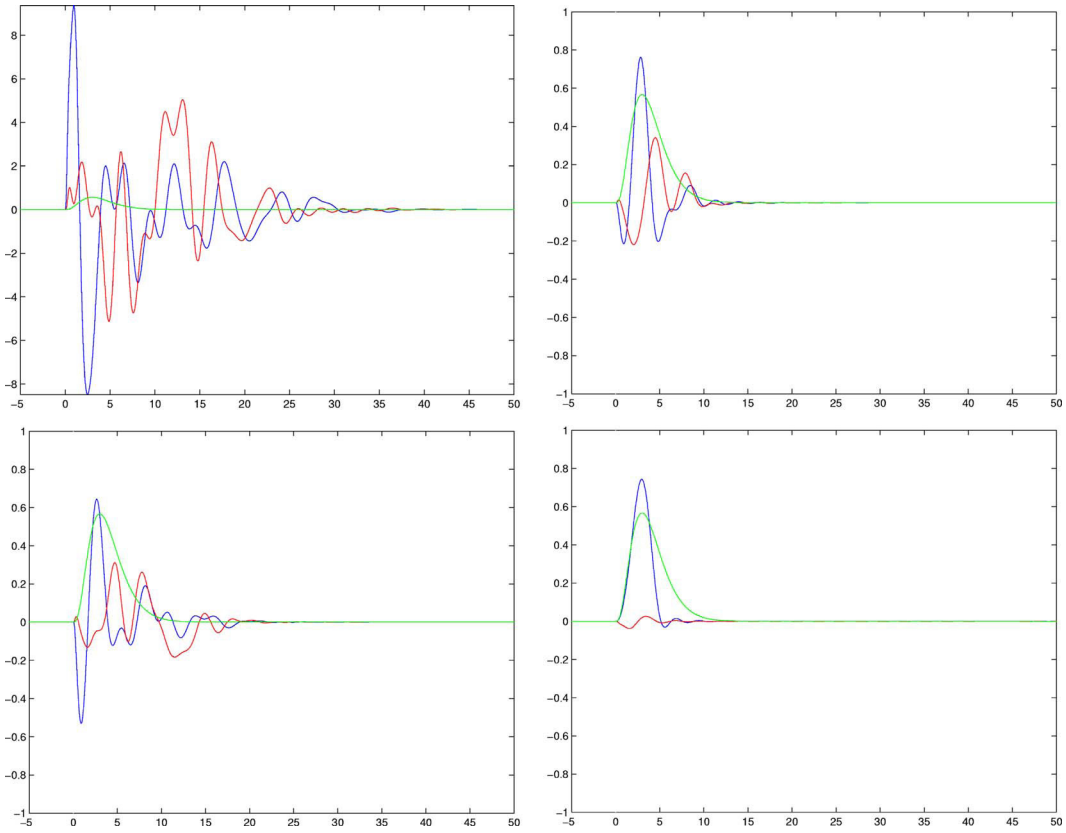

FIG. 3. (Color online) From top left to bottom right: Fourier representations of initial g_0 (not normalized), g_4, g_{10}, and g_{30} (blue/red, real and imaginary part; green, Cauchy wavelet).

$$\alpha^{n+1} = \frac{M \pm (M^2 - F[\mathbf{A}\mathbf{g}^n](e)\{F[\mathbf{g}_k - F'[\mathbf{g}^n]^*(F[\mathbf{g}_k]w^{-1})](e) - C^2\})^{1/2}}{F[\mathbf{A}\mathbf{g}^n](e)}. \tag{4.3}$$

Now we can summarize an algorithm for computing a critical sequence $\mathbf{g}$ for the minimization problem $\inf_{\|g\|_H=1}\Phi[g]$:

- *Pick some initial* $\mathbf{g}_0$ *(not too far off the expected solution) and some* $C>0$ *(large enough).*

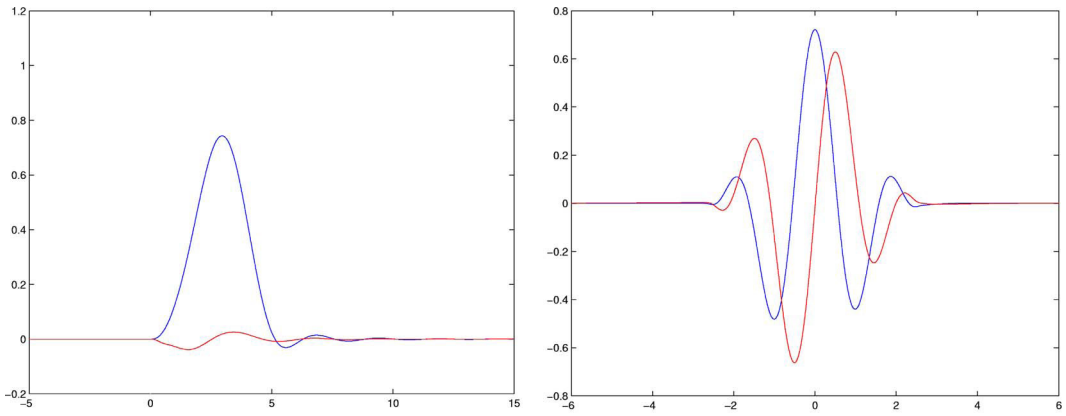

FIG. 4. (Color online) Left: Fourier representation of the approximated optimally localized coherent state. Right: Associated time representation.

- *Compute* $\mathbf{g}_{k+1}=\arg\min_{\mathbf{g}}\Phi^s(\mathbf{g};\mathbf{g}_k)$ *via fixed point iteration* (4.2):

  Compute $\alpha^{n+1}=\max\{\alpha_1^{n+1},\alpha_2^{n+1}\}$ *via* Eq. (4.3).
  Compute $\mathbf{g}^{n+1}$ *via* Eq. (4.2).
  $\mathbf{g}_{k+1}=\lim_{n\to\infty}\mathbf{g}^{n+1}$.

In what follows we aim to illustrate the computation of an optimally localized wavelet. For the sake of simply computing the operators $\mathbf{A}(x)$, we have chosen a (finite dimensional) Cauchy wavelet frame $\{\psi_\lambda\}\subset L^2(\mathbf{R})$ of order N (here $N=3$). Thus, $\mathbf{A}(x)$ can be derived for each $x\in G$ explicitly, see Fig. 2. The resulting iteration process to reconstruct at least a critical g is illustrated in Fig. 3, and the final approximation with the time representation in Fig. 4.

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Geometric equivalence of Clifford algebras

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We motivate a notion of *geometric* equivalence that is not the usual notion of *algebraic* equivalence (or isomorphism of Clifford algebra). Using this definition tilting to the opposite metric is a geometric equivalence in contrast to such algebraic equivalences as $C\ell(3,0)\cong C\ell(1,2)$ which are not geometric. We define and discuss the classification of partitioned Clifford algebra and the geometric equivalence of Dirac formulations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

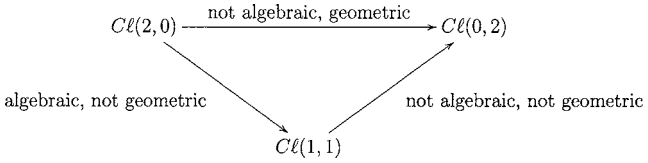
A long outstanding debate on Minkowski space-time concerns the physical explanation of differences between the (3,1) and (1,3) signatures of the metric. A partial mathematical answer is to be found in the corresponding Clifford algebras $C\ell(3,1)$ and $C\ell(1,3)$. They are not isomorphic, although their even subalgebras and their complexifications are, respectively, isomorphic. A number of papers over the years have investigated possible differences, see for example, de Witt-Morette *et al.*[1–4] and Pezzaglia and Adams[5] Recently, Joyce and Butler[6] have provided a rich geometric explanation where the geometric products corresponding to the different signatures are based on different geometric constructions. Although the underlying geometry is the same, the multivectors represent differing equivalence classes of geometric objects. Consequently two nonisomorphic algebras are generated. Nevertheless, there is a one to one relationship between the different geometric constructions. This paper describes and characterizes such geometric relationships.

There have been a few prior studies in the literature investigating the relationship between Clifford algebras with opposite signatures, including the tilt map given in Lounesto[7] and the vee product of Miralles *et al.*[8,9] We take a different approach where we introduce the notion of a *Geometric* map. Such a mapping preserves essential geometric properties. Fundamentally Clifford algebra arises from flat space-time geometries. We represent the flat spacetime by a vector space spanned by $m+n$ basis vectors denoted $e_1,\ldots,e_{m+n}$ and a signature (m,n). This generates the Clifford algebra $C\ell(m,n)$. Our space-time frame spans the subspace of one-vectors. Geometrically the even (resp. odd) multivectors arise from evaluation of an even (resp. odd) number of one-vectors. Moreover, the space of r-multivectors is spanned by the products of $r+2i$ one-vectors for every $i\in\mathbb{N}$, where $\mathbb{N}$ denotes the additive monoid of natural numbers. Importantly no even (resp. odd) multivector arises from an odd (resp. even) product of one-vectors. Also one should note that the generators for rotation and boosts [in $\mathrm{spin}_+(m,n)$] span $C\ell^+(m,n)$. Thus a linear map between Clifford algebras should only be considered *geometric* if it preserves the $\mathbb{Z}_2$ grading into even and odd multivectors. Moreover, the product of an even multivector with another multivector preserves this $\mathbb{Z}_2$ grade so,we should also have

$$\phi(uv)=\phi(u)\phi(v), \tag{1}$$

whenever u or v is an even multivector.

A geometric map is a linear $\mathbb{Z}_2$ graded map preserving left and right multiplicative action of $C\ell_+(m,n)$. A geometric equivalence is an invertible geometric map. For flat space-time with $m+n=2$ there are three $\mathbb{Z}_2$ graded Clifford algebra structures. Namely, $C\ell(2,0), C\ell(1,1)$ and $C\ell(0,2)$ where the $\mathbb{Z}_2$ grading is specified by the signature. We have the following relationship between the three:



One can see that tilting to the opposite metric is a geometric equivalence as it corresponds to Clifford algebras underlying the same flat space-time geometry. However, the universal enveloping algebra generated by two boost generators or a boost generator and a rotation generator give the algebraic equivalence $C\ell(2,0)\cong C\ell(1,1)$. We will show that two Clifford algebras are geometrically equivalent if and only if their even subalgebras are algebraically equivalent. Thus $C\ell(2,0)$ and $C\ell(0,2)$ are geometrically equivalent precisely because their even subalgebras are both isomorphic to $C\ell(0,1)$, the Clifford algebra generated by a single rotation generator.

With this motivation we now present a fuller treatment beginning with the notion of partitioned Clifford algebra.

II. FLAT SPACE-TIME GEOMETRIES AND PARTITIONED CLIFFORD ALGEBRA

We begin with a more general notion of flat space-time to ensure that the resulting "geometric algebra" is closed under tensor product. If one has a collection of flat space-time geometries where one has no means of rotating or boosting between each geometry, then the composite is a partitioned flat space-time geometry in the following sense.

Given $m,n\in\mathbb{N}$, let $[m+n]=\{1,2,\ldots,m+n\}$. A partition on $[m+n]$ is a map $\lambda:[m+n]\rightarrow\mathcal{P}[m+n]$, where $\mathcal{P}[m+n]$ is the power set of $[m+n]$, such that $i\in\lambda i$ and if $j\in\lambda i$ then $\lambda i=\lambda j$ where $i,j\in[m+n]$. Let $\Lambda=\{\lambda i: i\in[m+n]\}$ be the set of equivalence classes. We then have that $\Sigma_{\sigma\in\Lambda}|\sigma|=m+n$ and $\cup\Lambda=[m+n]$. A λ-flat spacetime of signature (m,n) is a family of vector spaces V_σ with signature (m_σ,n_σ) where $\sigma\in\Lambda$ satisfying $\Sigma_{\sigma\in\Lambda}m_\sigma=m$ and $\Sigma_{\sigma\in\Lambda}n_\sigma=n$. Hence the vector space

$$V=\bigoplus_{\sigma\in\Lambda}V_\sigma, \tag{2}$$

admits a basis $e_1,\ldots,e_{m+n}$ where $e_i\in V_{\lambda i}$ and is said to be of type λi.

Transformations that dilate, boost, or rotate between vectors of different types are not possible. Each partition component subspace may be said to be geometrically partitioned from all the others. Such situations occur when one trivially joins an internal space to an existing flat space-time.

We define the partitioned Clifford algebra $C\ell(m,n|\lambda)$ of signature (m,n) partitioned by λ to be the Clifford algebra generated by $e_1,\ldots,e_{m+n}$ with generating relations

$$e_ie_j=-\lambda_{ij}e_je_i \quad \text{for all} \quad i,j\in[m+n], \tag{3}$$

$$e_i^2=1 \quad \text{whenever} \quad i=1,2,\ldots,m, \tag{4}$$

$$e_{m+j}^2=-1 \quad \text{whenever} \quad j=1,2,\ldots,n, \tag{5}$$

where we have defined

$$\lambda_{ij} = \begin{cases} 1: i \neq j \text{ and } \lambda i = \lambda j \\ -1: i = j \text{ or } \lambda i \neq \lambda j, \end{cases} \tag{6}$$

for all $i,j \in [m+n]$. Thus if we define the components of a flat space-time metric as $\eta_{ij} = \langle \delta_{ij} e_i e_j \rangle_0$ we obtain a compact form of the generators

$$e_i e_j + (\lambda_{ij} + 2\delta_{ij}) e_j e_i = 2\eta_{ij}, \tag{7}$$

for all $i,j \in [m+n]$.

Let $m_\sigma = |[m] \cap \sigma|$, the number of generators e_i where $i \in \sigma$ with $e_i^2 = 1$. Let $n_\sigma = |(m+[n]) \cap \sigma|$, the number of generators e_i where $i \in \sigma$ with $e_i^2 = -1$. Then we have that $\Sigma_{\sigma \in \Lambda} m_\sigma = m, \Sigma_{\sigma \in \Lambda} n_\sigma = n$, and the decomposition

$$C\ell(m,n|\lambda) \cong \bigotimes_{\sigma \in \Lambda} C\ell(m_\sigma, n_\sigma). \tag{8}$$

Examples include Galilean space-time giving the geometric algebras $C\ell(1,0) \otimes C\ell(3,0)$ or $C\ell(0,1) \otimes C\ell(3,0)$, and Minkowski space-time with an evolution parameter giving the Dirac algebra $C\ell(0,1) \otimes C\ell(3,1)$.

A partitioned Clifford algebra $C\ell(m,n|\lambda)$ is $\mathbb{Z}_2^{|\Lambda|}$-graded. Assume Λ is ordered with $\sigma_1 < \cdots < \sigma_{|\Lambda|}$. We define

$$C\ell^0(m,n|\lambda) = \bigotimes_{\sigma \in \Lambda} C\ell^+(m_\sigma, n_\sigma), \tag{9}$$

which is the subalgebra generated by the rotation and boost generators for $C\ell(m,n|\lambda)$. We call $C\ell^0(m,n|\lambda)$ the kinematic subalgebra and its dimension is $2^{m+n-|\Lambda|}$. Let $z_i = (0,\ldots,0,1,0,\ldots,0) \in \mathbb{Z}_2^{|\Lambda|}$ where 1 is in the ith position. We define

$$\begin{aligned} C\ell^{z_i}(m,n|\lambda) = {} & C\ell^+(m_{\sigma 1}, n_{\sigma 1}) \otimes \cdots C\ell^+(m_{\sigma_{i-1}}, n_{\sigma_{i-1}}) \otimes C\ell^-(m_{\sigma_i}, n_{\sigma_i}) \\ & \otimes C\ell^+(m_{\sigma_{i+1}}, n_{\sigma_{i+1}}) \otimes \cdots \otimes C\ell^+(m_{\sigma_{|\Lambda|}}, n_{\sigma_{|\Lambda|}}). \end{aligned} \tag{10}$$

An arbitrary $z \in \mathbb{Z}_2^{|\Lambda|}$ may be written as $z = \Sigma_{i=1}^{|\Lambda|} a^i z_i$ for unique $a_1,\ldots,a_{|\Lambda|} \in \{0,1\}$ and we define

$$C\ell^z(m,n|\lambda) = C\ell^{a_1 z_1}(m,n|\lambda) \cdots C\ell^{a_{|\Lambda|} z_{|\Lambda|}}(m,n|\lambda). \tag{11}$$

The even part of the algebra is defined to be

$$C\ell^+(m,n|\lambda) = \bigoplus_{\substack{z \in \mathbb{Z}_2^{|\Lambda|} \\ \Sigma_{i=1}^{|\Lambda|} a^i \text{ is even}}} C\ell^z(m,n|\lambda). \tag{12}$$

Similarly we define $C\ell^-(m,n|\lambda)$ summing over z for $\Sigma_{i=1}^{|\Lambda|} a^i$ odd. This we will refer to in what follows as the $\mathbb{Z}_2$ grade for $C\ell(m,n|\Lambda)$. However, the generators for boost and rotation of the underlying partitioned space-time generate the kinematic subalgebra $C\ell^0(m,n|\lambda)$. In particular we have $C\ell^+(m,n|\lambda) = C\ell^0(m,n|\lambda)$ if and only if the partition is trivial.

III. GEOMETRIC MAPS AND EQUIVALENCES

Let $(m,n),(p,q) \in \mathbb{N}^2$ be a pair of signatures. Let λ and ρ be partitions of $[m+n]$ and $[p+q]$, respectively. Before stating the definition of a geometric map we note that any map $\pi: [m+n] \to [p+q]$ induces a map $\hat{\pi}: \mathbb{Z}_2^{|\Lambda|} \to \mathbb{Z}_2^{|R|}$ given by

$$\hat{\pi}\left(\sum_{i=1}^{|\Lambda|} a^i z_i \right) = \sum_{i=1}^{|\Lambda|} a^i z_{\pi i}. \tag{13}$$

Definition 1: A left (resp. right) geometric map is an ordered pair (ϕ, π) *consisting of a linear*

map $\phi: C\ell(m,n|\lambda) \to C\ell(p,q|\rho)$ *and a map* $\pi:[m+n] \to [p+q]$ *such that*

(i) $\pi\lambda = \rho\sigma$;
(ii) $\phi(C\ell^z(m,n|\lambda)) \subset C\ell^{\hat{\pi}z}(p,q|\rho)$ *for all* $z \in \mathbb{Z}_2^{|\Lambda|}$;
(iii) $\phi(uv) = \phi(u)\phi(v)$ *whenever* u *(resp.* v*) is in* $C\ell^0(m,n|\lambda)$.

The ordered pair (ϕ,π) *is geometric if it is both a left and right geometric map. It is weakly geometric if condition (ii) only holds for* $z=0$.

Often we will write $(\phi,\pi): C\ell(m,n|\lambda) \to C\ell(p,q)$ when we mean a (weakly) geometric map. If (ϕ,π) is a geometric map then $\hat{\pi}0=0$ and we have that the kinematic subalgebra generated by infinitesimal generators is preserved or

$$\phi(C\ell^0(m,n|\lambda)) \subset C\ell^0(p,q|\rho). \tag{14}$$

A geometric map (ϕ,π) is called a geometric equivalence (written $\sim$) if ϕ is invertible and π is bijective, it is called a geometric morphism if ϕ is a homomorphism and a geometric isomorphism if it is both a geometric equivalence and a geometric morphism. Note that an algebraic equivalence of Clifford algebras is written $\cong$.

Let $\mathcal{M}$ denote the monoid (recall a monoid is a group without the requirement of invertibility) generated by $C\ell(0,0), C\ell(1,0), C\ell(0,1), C\ell(2,0), C\ell(1,1)$, and $C\ell(0,2)$ with multiplication tensor product. This monoid is $\mathbb{Z}_2$-graded with the even submonoid $\mathcal{M}^+$ generated by $C\ell(0,0), C\ell(1,0)^{\otimes 2}, C\ell(0,1)^{\otimes 2}, C\ell(1,0)\otimes C\ell(0,1), C\ell(0,1)\otimes C\ell(1,0), C\ell(2,0), C\ell(1,1)$ and $C\ell(0,2)$.

Theorem 1: *Every partitioned Clifford algebra is weakly geometrically equivalent to a member of* $\mathcal{M}$.

Before proving this result we note that although $C\ell(2,0) \cong C\ell(1,1)$ they are not geometrically equivalent. The corresponding result for algebraic equivalence embodies the well-known classification of Clifford algebra by matrix algebra due to Cartan. The generators are algebraically equivalent to the following well-known algebras:

$$C\ell(0,0) \cong \mathbb{R}, \tag{15}$$

$$C\ell(1,0) \cong \mathbb{R} \oplus \mathbb{R}, \tag{16}$$

$$C\ell(0,1) \cong \mathbb{C}, \tag{17}$$

$$C\ell(2,0) \cong C\ell(1,1) \cong \mathbb{K}, \tag{18}$$

$$C\ell(0,2) \cong \mathbb{H}, \tag{19}$$

where $\mathbb{K}=\mathrm{Mat}(2,\mathbb{R})$. For $p,q \in \mathbb{N}$ we have the geometric isomorphisms

$$C\ell(p+2,q) \cong C\ell(2,0) \otimes C\ell(q,p), \tag{20}$$

$$C\ell(p+1,q+1) \cong C\ell(1,1) \otimes C\ell(p,q), \tag{21}$$

$$C\ell(p,q+2) \cong C\ell(0,2) \otimes C\ell(q,p). \tag{22}$$

In the first case e_1 and e_2 generate $Cl(2,0)$. A set of generators commuting with e_1 and e_2 are given by $e_{12}e_3, \ldots, e_{12}e_{p+q}$. The latter set generates $C\ell(q,p)$. The other isomorphisms are proved by selecting e_{p+1}, e_{p+2} and e_{q+1} and e_{q+2}, respectively. If ϕ and ψ are geometric isomorphisms then $\phi\otimes\psi$ is a geometric isomorphism. Hence we may iterate using these three formulas to prove the theorem.

Note the immediate corollary

Corollary 1: $C\ell(m,n|\lambda)$ *is an Abelian algebra if and only if it has no dimension four generators.*

The dimension four generators are $C\ell(2,0), C\ell(1,1)$ and $C\ell(0,2)$.

Every geometric map gives rise to a homomorphism between the kinematic subalgebras. We next show that a geometric map may be constructed as an extension of a homomorphism between the kinematic subalgebras. This will allow us to deduce a criterion for when partitioned Clifford algebras are geometrically equivalent. We begin with trivially partitioned Clifford algebra.

Proposition 1: Let $\phi: C\ell(m,n) \to C\ell(p,q)$ *be a geometric map then*

(i) $f=\phi(1)$ *is central and idempotent, and* $1-f$ *is an annihilator for* $\phi(C\ell(m,n))$;
(ii) *Suppose* $p+q>0$ *then given a homomorphism* $\phi: C\ell^+(m,n) \to C\ell^+(p,q)$ *there is a geometric extension* $\hat{\phi}: C\ell(m,n) \to C\ell(p,q)$ *satisfying* $\dim(\mathrm{Im}\,\hat{\phi}) = 2\dim(\mathrm{Im}\,\phi)$.

To prove the first part, given $v \in \phi(C\ell(m,n))$ there is a $u \in C\ell(m,n)$ such that $\phi(u)=v$ and $vf = \phi(u)\phi(1) = \phi(u) = v$ and similarly $fv=v$. Hence f is central and $1-f$ is an annihilator as claimed. Also $f^2 = \phi(1)\phi(1) = \phi(1) = f$.

Next we prove the second part after some development. Let $h_1, \ldots, h_{p+q-1}$ be generators for the Clifford algebra $C\ell^+(p,q)$. Let $P_{0,z}$ denote the protection onto the even and odd parts of $C\ell(p,q)$ and $P_{i,z}$ the projection onto commuting and anti-commuting components with respect to h_i given by

$$P_{i,z}v = \tfrac{1}{2}(v + (-1)^z h_i^{-1} v h_i), \tag{23}$$

for all $v \in C\ell(p,q)$ where $z \in \mathbb{Z}_2$. It is simple to verify $P_{i,z}P_{i',z'} = P_{i',z'}P_{i,z}$ for all $i,i' \in \{0,1,\ldots,p+q-1\}$ and $z,z' \in \mathbb{Z}_2$. Thus we define the projection operator

$$C^z = \Pi_{i=0}^{p+q-1} P_{i,a^i}, \tag{24}$$

for every $z \in \mathbb{Z}_2^{p+q}$ where $z = \Sigma_{i=0}^{p+q-1} a^i z_i$. Thus we have the decomposition

$$C\ell(p,q) \cong \bigoplus_{z \in \mathbb{Z}_2^{p+q}} C^z C\ell(p,q), \tag{25}$$

and $(C^z C\ell(p,q))(C^{z'} C\ell(p,q)) \subset C^{z+z'} C\ell(p,q)$. Hence we have the dimensionality

$$\dim C^{(0,z)} C\ell(p,q) = \begin{cases} 0: \sum_{i=1}^{p+q-1} z_i = p+q \bmod 2 \\ 1: \sum_{i=1}^{p+q-1} z_i = p+q-1 \bmod 2 \end{cases}. \tag{26}$$

Note that the generator $h_i \in C^z C\ell(p,q)$ where $z_k=0$ if and only if $k=0$ or $k=i$. Whenever $i \neq j$ note that $h_i h_j \in C^z C\ell(p,q)$ where $z_k=1$ if and only if $k=i$ or $k=j$. Using this we shall prove the following lemma.

Lemma 1: Given generators $h_1, \ldots, h_{p+q-1}$ *for* $C\ell^+(p,q)$ *there exists* $v \in C\ell^-(p,q)$ *such that* $h_i v = -v h_i$ *for all* $i=1,2,\ldots,p+q-1$.

For $p+q<2$ the result is trivial. For $p+q=2$ the only generators are $\pm e_{12}$ and one can take $v=e_1$. For $p+q>2$ and $p+q$ is odd take $v = e_1 \cdots e_{p+q} h_1 \cdots h_{p+q-1}$. Finally suppose $p+q>2$ and $p+q$ is even, then there exists no central odd element. Choose $u \in C^{(1,z)} C\ell(p,q)$ invertible for some $z \in \mathbb{Z}_2^{p+q-1}$ and let $0 < i_1 < \cdots < i_r < p+q$ such that $z_j=0$ if and only if $j=i_k$ for some $k=1,2,\ldots,r$. If r is even then $h_{i_1} \cdots h_{i_r} u \in C^{(1,0)} C\ell(p,q)$ contradicting there being no central odd element. Hence r is even and we take $v = h_1 \cdots h_{p+q-1} h_{i_1} \cdots h_{i_r} u \in C^{(1,1)} C\ell(p,q)$. This completes the proof.

It is worthwhile noting that if $p+q$ is odd then

$$\dim C^z C\ell(p,q) = 1, \tag{27}$$

for all $z \in \mathbb{Z}_2^{p+q}$, and if $p+q$ is even then

$$\dim C^z C\ell\,(p+q) = \begin{cases} 0{:}|\{i{:}z_i=1\}| \text{ is even}, \\ 2{:}|\{i{:}z_i=1\}| \text{ is odd}. \end{cases} \tag{28}$$

for all $z \in \mathbb{Z}_2^{p+q}$.

We have a simple corollary to the lemma.

Corollary 2: Let f be idempotent. Then given generators $h_1,\ldots,h_{p+q-1}$ for $[\{f\},C\ell^+(p,q)]$ there exists $v \in [\{f\},C\ell^-(p,q)]$ such that $h_i v=-vh_i$ for all $i=1,2,\ldots,p+q-1$.

This follows since f commutes will all elements in $[\{f\},C\ell\,(p,q)]$.

Completing the proof of (ii), take $h_i=\phi(e_{1i+1})$ then by the previous corollary there is $v \in [\{f\},C\ell^-(p,q)]$ invertible such that $h_i v=-vh_i$ for all $i=1,2,\ldots,p+q-1$. Hence a choice of extension is given by

$$\hat{\phi}(a+e_1 b) = \phi(a) + v\,\phi(b), \tag{29}$$

for al $a,b \in C\ell^+(m,n)$.

Thus we can state an important criterion for determining when two partitioned Clifford algebras are geometrically equivalent.

Theorem 2: *Two partitioned Clifford algebras are geometrically equivalent if and only if their kinematic subalgebras are algebraically equivalent.*

It immediately follows that $C\ell\,(m,n) \sim C\ell\,(n,m)$ and so tilting to the opposite metric is a geometric equivalence. In detail, between the Clifford algebras $C\ell\,(m,n)$ and $C\ell\,(n,m)$ there is a bijective Clifford map τ preserving generators satisfying

$$\tau(ab) = (-1)^{rs}\tau(a)\tau(b), \tag{30}$$

whenever a is an r-vector and b an s-vector. Let $(e'_1,\ldots,e'_r)$ be the generating basis for $C\ell\,(n,m)$ and define $f_k=e'_{n+k}$ for $k=1,\ldots,m$ and $f_k=e'_{k-m}$ for $k=m+1,\ldots,m+n$. We define τ by the formula

$$\tau(e_{k_1}\cdots e_{k_r}) = (-1)^{\lfloor r/2\rfloor} f_{k_1}\cdots f_{k_r}, \tag{31}$$

which is proven by induction using $\tau(e_k e_l)=-\tau(e_k)\tau(e_l)$. This follows from $\tau(e_k e_l)f_l=\tau(e_k e_l^2)$ $=f_k\tau(e_l^2)=-f_k e_l^2$ by multiplication by f_l and noting that $e_l^2 f_l^2=-1$. This is the anti-isomorphism map of Chevellay associated with switching the signature of the underlying quadratic form.

Geometric equivalence is decided by the algebraic equivalence of their kinematic subalgebras.

Proposition 2: Let $m,n,p,q \in \mathbb{N}$ and λ be a partition of $[m+n]$ then

$$(C\ell\,(m,n|\lambda) \otimes C\ell\,(1,0))^+ \cong C\ell\,(m,n|\lambda), \tag{32}$$

$$(C\ell\,(m,n|\lambda) \otimes C\ell\,(0,1))^+ \cong C\ell\,(n,m|\widetilde{\lambda}), \tag{33}$$

$$(C\ell\,(m,n) \otimes C\ell\,(p+1,q))^+ \cong C\ell\,(m+q,n+p), \tag{34}$$

$$(C\ell\,(m,n) \otimes C\ell\,(p,q+1))^+ \cong C\ell\,(n+p,m+q), \tag{35}$$

where $\widetilde{\lambda}$ is the partition given by $\widetilde{\lambda}i=-\lambda i$ modulo $m+n$.

Let e_k be the generators for $C\ell\,(m,n|\lambda)$ and σ the generator for $C\ell\,(1,0)$. A set of generators for the even subalgebra is given by $e_k \otimes \sigma$ where $k \in [m+n]$. These generate the Clifford algebra $C\ell\,(m,n|\lambda)$. The next formula is proven by noting that the signature is reversed. Suppose now that λ is trivial and let f_l be generators for $C\ell\,(p+1,q)$. A collection of generators for the even subalgebra of $C\ell\,(m,n)\otimes C\ell\,(p+1,q)$ is given by $e_k \otimes f_1$ and $1 \otimes f_{1l}$ where $k \in [m+n]$ and $l \in [p+q]+1$. These generators are all anti-commute and generate $C\ell\,(m+q,n+p)$. The final formula is proven by using generators $e_k \otimes f_{p+q+1}$ and $1 \otimes f_{lp+q+1}$ where $k \in [m+n]$ and $l \in [p+q]$.

Note that the last two formulas for $m=n=0$ reduce to the well-known algebraic equivalences

$$C\ell^{+}(p+1,q) \cong C\,\ell\,(q,p), \tag{36}$$

$$C\ell^{+}(p,q+1) \cong C\,\ell\,(p,q). \tag{37}$$

For example, we now have

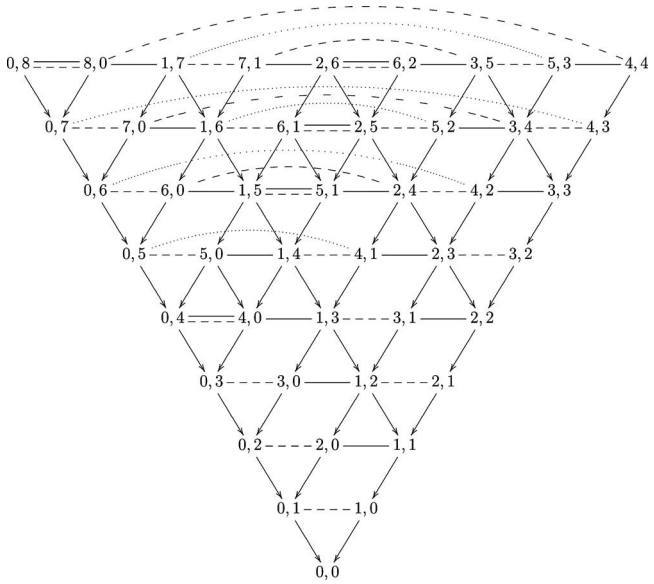
$$(C\,\ell\,(m+1,n) \otimes C\,\ell\,(p+1,q))^{0} \cong C\,\ell\,(n,m) \otimes C\,\ell\,(q,p), \tag{38}$$

$$(C\,\ell\,(m+1,n) \otimes C\,\ell\,(p,q+1))^{0} \cong C\,\ell\,(n,m) \otimes C\,\ell\,(p,q), \tag{39}$$

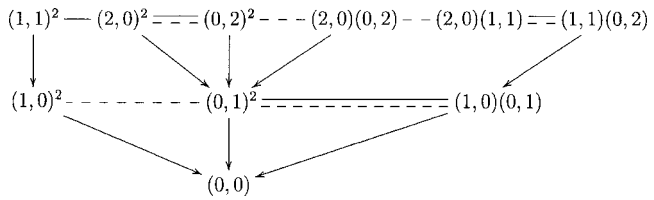
$$(C\,\ell\,(m,n+1) \otimes C\,\ell\,(p,q+1))^{0} \cong C\,\ell\,(m,n) \otimes C\,\ell\,(p,q). \tag{40}$$

One now sees that geometric and algebraic equivalence has a rich interplay determined by an extension of Cartan's period of eight classification for the kinematic subalgebras.

The first few Clifford algebras ($m+n \leqslant 8$) are given as follows. The dashed lines represent geometric equivalence, the solid, horizontal and dotted lines represent algebraic equivalence, and the solid arrows projection onto the kinematic subalgebra up to algebraic equivalence.



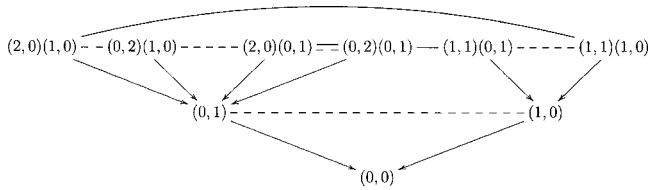
Note that not all geometric equivalences are given by tilting of the metric. However, this does not occur until $m+n \geqslant 6$. Next consider the partitioned Clifford algebra with $m+n=4$ or $m+n=2$ partitioned into two dimensionally equal pieces. This is given as follows:



The top left algebraic equivalences correspond to the isomorphism $\mathbb{K} \otimes \mathbb{K} \cong \mathbb{H} \otimes \mathbb{H}$. The algebraic equivalence on the second line is $\mathbb{C} \oplus \mathbb{C} \cong \mathbb{C} \otimes \mathbb{C}$. The next diagram is for partitioned Clifford algebra with $m+n=3$ into two nontrivial pieces.

TABLE I. Isomorphisms $C\ell(r)\cong \mathrm{Mat}(2^m,2^n\mathbb{F})$.

r	7	6	5	4	3	2	1	0	−1	−2	−3	−4	−5	−6	−7
m	3	2	1	1	1	1	0	0	0	0	0	1	2	3	3
n	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1
$\mathbb{F}$	$\mathbb{C}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{C}$	$\mathbb{R}$	$\mathbb{R}$	$\mathbb{R}$	$\mathbb{C}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{C}$	$\mathbb{R}$	$\mathbb{R}$



The algebraic equivalence in the diagram is $\mathbb{C}\otimes\mathbb{K}\cong\mathbb{C}\otimes\mathbb{H}$.

At this point we introduce the useful notation: $\mathbb{F}^m$ is the m-fold tensor product of $\mathbb{F}$ and $m\mathbb{F}$ is the m-fold direct sum of $\mathbb{F}$. Also we let $\mathcal{F}=\{\mathbb{R},\mathbb{C},\mathbb{H}\}$. We can now state the connection between partitioned Clifford algebra and matrix algebra.

Theorem 3: *Every partitioned Clifford algebra is of the form* $Mat(2^m,2^n\mathbb{F})$ *where* $m,n\in\mathbb{N}$ *and* $\mathbb{F}\in\mathcal{F}$. *Conversely, every matrix algebra* $Mat(2^m,2^n\mathbb{F})$ *for some* $m,n\in\mathbb{N}$ *and* $\mathbb{F}\in\mathcal{F}$ *is isomorphic to some partitioned Clifford algebra.*

To show this we begin by noting the fact

$$\mathbb{F}\otimes\mathbb{K}^m\cong \mathrm{Mat}(2^m,\mathbb{F}). \tag{41}$$

Given an arbitrary partitioned Clifford algebra $C\ell(p,q|\lambda)$ we can decompose each partitioned component

$$C\ell\,(p_\sigma,q_\sigma)\cong \mathbb{K}^{\min\{p_\sigma,q_\sigma\}}\otimes C\ell\,(p_\sigma-q_\sigma), \tag{42}$$

for every $\sigma\in\Lambda$ where we have defined $C\ell(p_\sigma)=C\ell(p_\sigma,0)$ and $C\ell(-q_\sigma)=C\ell(0,q_\sigma)$. Suppose $|p_\sigma-q_\sigma|=8m_\sigma+r_\sigma$ where $0\leqslant r_\sigma<8$ and $m_\sigma\in\mathbb{N}$. Thus $m_\sigma=\lfloor|p_\sigma-q_\sigma|/8\rfloor$ and $r_\sigma=|p_\sigma-q_\sigma|$ modulo 8. Further iterations gives

$$C\ell\,(p_\sigma-q_\sigma)=\mathbb{K}^{\left\lfloor\frac{|p_\sigma-q_\sigma|}{2}\right\rfloor}\otimes C\ell\,(\mathrm{sgn}(p_\sigma-q_\sigma)r_\sigma). \tag{43}$$

Combining the above decomposition with the equality

$$\left\lfloor\frac{p_\sigma+q_\sigma}{2}\right\rfloor=\min\{p_\sigma,q_\sigma\}+\left\lfloor\frac{|p_\sigma-q_\sigma|}{2}\right\rfloor, \tag{44}$$

gives the explicit formula

$$C\ell\,(p_\sigma,q_\sigma)\cong \mathrm{Mat}(2^{\left\lfloor\frac{p_\sigma+q_\sigma}{2}\right\rfloor},C\ell\,(\mathrm{sgn}(p_\sigma-q_\sigma)r_\sigma)). \tag{45}$$

Therefore,

$$C\ell\,(p,q|\lambda)\cong \mathrm{Mat}\left(2^{\Sigma_{\sigma\in\Lambda}\left\lfloor\frac{p_\sigma+q_\sigma}{2}\right\rfloor},\bigotimes_{\tau\in\Lambda}C\ell\,(\mathrm{sgn}(p_\tau-q_\tau)r_\tau)\right). \tag{46}$$

It only remains to classify $C\ell(r)$ for $-8<r<8$. These are obtained by iterating the first proposition. Table I can be understood by the period of eight circle in Fig. 1.

The numbers around the outside represent r when going clockwise and $-r$ when going anticlockwise. The inside numbers represent n plus the logarithm base 2 of the dimension of $\mathbb{F}$. The

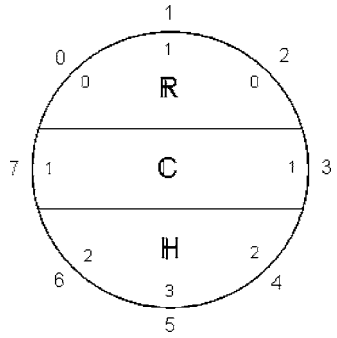


FIG. 1. The period of eight circle.

three regions of the circle indicate the underlying field $\mathbb{F}$. Not indicated on the diagram is that n is nonzero at 12 o'clock and 6 o'clock. The converse of the theorem holds because

$$\mathrm{Mat}(2^m,2^n\mathbb{F}) \cong C\ell(1,1)^m \otimes C\ell(1,0)^n \otimes \mathbb{F}, \tag{47}$$

where we use the Clifford algebra in Eqs. (20)–(22) in place of $\mathbb{F}$ given by $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$, respectively.

Consider the collection of matrix algebras $\mathrm{Mat}(2^m,2^n\mathbb{F})$, which we denote by $\langle m,n,\mathbb{F}\rangle$, where $m,n\in\mathbb{N}$, and $\mathbb{F}\in\mathcal{F}$. The members of this, set are pairwise nonisomorphic. Moreover, the tensor product of any two members in $\mathbb{N}^2\times\mathcal{F}$ is isomorphic to a unique member. Hence $\mathbb{N}^2\times\mathcal{F}$ is a commutative monoid in the obvious way. Define a monoid addition on $\mathcal{F}$ by $\mathbb{R}+\mathbb{F}=\mathbb{F}$, $\mathbb{C}+\mathbb{C}=\mathbb{C}$, $\mathbb{H}+\mathbb{C}=\mathbb{C}$, and $\mathbb{H}+\mathbb{H}=\mathbb{R}$. Given this, the monoid addition on $\mathbb{N}^2\times\mathcal{F}$ is given by

$$\langle m,n,\mathbb{F}\rangle \otimes \langle m',n',\mathbb{F}'\rangle = \langle m+m'+\delta_{\mathbb{F},\mathbb{H}}+\delta_{\mathbb{F}',\mathbb{H}}, n+n'+\delta_{\mathbb{F},\mathbb{C}}\delta_{\mathbb{F}',\mathbb{C}}, \mathbb{F}+\mathbb{F}'\rangle,$$

for all $m,m',n,n'\in\mathbb{N}$ and $\mathbb{F},\mathbb{F}'\in\mathcal{F}$

IV. TILTING THE METRIC IN DIRAC FORMULATIONS

Following Joyce and Martin[10] a Dirac formulation $(\sigma,\mathcal{I})$ consists of a Dirac pseudo-left ideal $\mathcal{I}$ and a Dirac character $\sigma\in C\ell(m,1)$ or $C\ell(1,m)$. Conventionally we choose a basis $e_0,\ldots,e_m$ satisfying $e_0^2=-e_k^2$ for all $k=1,\ldots,m$. A pseudo-left ideal satisfies $C\ell^+(m,1)\mathcal{I}\subset\mathcal{I}$, and it is called Dirac if $C\ell^-(m,1)\mathcal{I}\subset\mathcal{I}\sigma$, and similarly for $C\ell(1,m)$. The Dirac character satisfies $\sigma^2=-e_0^2$ and $e_o\tilde{\sigma}e_0=-e_0^2\sigma$. Examples include e_k,e_{0kl} for $C\ell(3,1)$ and e_k,e_{kl},e_{0kl}, and e_{0123} for $C\ell(1,3)$. The underlying Dirac equation is then given by

$$\partial\psi(x)=m\psi(x)\sigma, \tag{48}$$

where $\psi(x)\in\mathcal{I}$. This formulation includes the Dirac-Hestenes equation,[11] the conventional Dirac equation, a formulation due to Baylis,[12] a formulation due to Joyce[13] and others.

Theorem 4: *Given a Dirac formulation* $(\sigma,\mathcal{I})$ *then* $(\tau\sigma,\tau\mathcal{I})$ *is a Dirac formulation if and only if* σ *is odd. Consequently the formulations are geometrically equivalent.*

Applying the tilt map to σ^2 gives $\tau(\sigma^2)=-\tau(e_0^2)=(\tau e_0)^2$. Thus $(\tau\sigma,\sigma\mathcal{I})$ is necessarily a Dirac formulation if and only if $\tau(\sigma^2)=-(\tau\sigma)^2$. Hence if and only if σ is odd. This is also sufficient by checking that the remaining conditions under τ hold if σ is odd. Note that the Dirac-Hestenes equation tilts because γ^{012} is odd and consequently is independent of signature, unlike the usual Dirac equation which does not tilt.

V. CONCLUSION

We introduced the notion of a geometric map, this is a map that preserves the left and right action of the infinitesimal generators of boost and rotation. This showed that some algebraic equivalences were not geometric in this sense whereas tilting to the opposite metric was always a geometric equivalence.

The notion of a partitioned Clifford algebra was defined to admit partitioned flat space-time geometry. This also provides a category of algebras closed under tensor product. A complete classification of partitioned Clifford algebra by matrix algebra was given extending Cartan's period of eight. Finally we demonstrated which Dirac formulations may be tilted to give a geometrically equivalent Dirac formulation.

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Approximate resonance states in the semigroup decomposition of resonance evolution

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The semigroup decomposition formalism makes use of the functional model for $C_{\cdot 0}$ class contractive semigroups for the description of the time evolution of resonances. For a given scattering problem the formalism allows for the association of a definite Hilbert space state with a scattering resonance. This state defines a decomposition of matrix elements of the evolution into a term evolving according to a semigroup law and a background term. We discuss the case of multiple resonances and give a bound on the size of the background term. As an example we treat a simple problem of scattering from a square barrier potential on the half-line. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2383069]

I. INTRODUCTION

Originally formulated for the analysis of scattering problems involving the solution of hyperbolic wave equations in the exterior domain of compactly supported obstacles, the Lax–Phillips scattering theory[1] was developed as a tool most suitable for dealing with resonances in the scattering of electromagnetic or acoustic waves. Subsequent to its introduction by Lax and Phillips, various authors have contributed to further development of the theory.[2–6] Notable recent additions were made by Sjöstrand and Sworski[7] who extended the scope of the theory to include general classes of semibounded, compactly supported perturbations of the Laplacian in the wave equation, and by Kuzhell, via the development of a formalism providing conditions for the application of the Lax–Phillips structure to an abstract form of the wave equation[8] and to certain classes of Schrödinger operators.[9] In addition, Kuzhell and Moskalyova[10] applied the Lax–Phillips theory in the analysis of scattering systems involving singular perturbations of the Laplacian.

Several recent papers have dealt with the adaptation of the Lax–Phillips theory to quantum mechanical scattering problems. An early work in this direction is Refs. 11–13. A general formalism was developed in Ref. 14 and subsequently applied to several physical models in Refs. 15–17. Such efforts to adapt the Lax–Phillips formalism to the framework of quantum mechanics are motivated by certain appealing features of the Lax–Phillips theory. One of these features is the fact that the time evolution of resonances in this theory is given in terms of a continuous, one parameter, strongly contractive semigroup $\{\mathbf{Z}(t)\}_{t\geqslant 0}$,

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$$\mathbf{Z}(t_1)\mathbf{Z}(t_2) = \mathbf{Z}(t_1 + t_2), \quad t_1, t_2 \geqslant 0.$$

If $\mathcal{H}$ is a (separable) Hilbert space corresponding to a particular scattering system and $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ is a unitary group defined on $\mathcal{H}$ describing the evolution of the system, the basic premises of the Lax–Phillips theory include the assumption of the existence of an *incoming subspace* $\mathcal{D}_-$ and an *outgoing subspace* $\mathcal{D}_+$ with respect to $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ which are assumed furthermore to be orthogonal to each other. Denoting by $\mathbf{P}_-$ and $\mathbf{P}_+$, respectively the projections on the orthogonal complements of $\mathcal{D}_-$ and $\mathcal{D}_+$ in $\mathcal{H}$, and letting $\mathcal{K}=\mathcal{H}\ominus(\mathcal{D}_-\oplus\mathcal{D}_+)$, the Lax–Phillips semigroup $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ defined by

$$\mathbf{Z}(t) = \mathbf{P}_+\mathbf{U}(t)\mathbf{P}_- = \mathbf{P}_\mathcal{K}\mathbf{U}(t)\mathbf{P}_\mathcal{K}, \quad t \geqslant 0, \tag{1}$$

annihilates $\mathcal{D}_\pm$ and maps $\mathcal{K}$ into itself. The subspace $\mathcal{K}$ contains the scattering resonances and the Lax–Phillips semigroup $\{\mathbf{Z}(t)\}_{t\geqslant 0}$ describes their time evolution. In the Lax–Phillips framework resonances are associated with pure states in the Hilbert space $\mathcal{H}$.

A basic difficulty encountered in the work on application of the Lax–Phillips theory in quantum mechanics originates from the fact that in this theory the continuous spectrum of the generator of evolution is required to be unbounded from below as well as from above. Hence, a formalism utilizing the original structure of the theory, such as in Ref. 14, is not suitable for application to large classes of scattering problems in quantum mechanics (except for limited types of problems, such as the Stark effect Hamiltonian,[17] or problems in a relativistically covariant framework,[15,16] which can be analyzed by direct mapping to the Lax–Phillips structure. The case of a Schrödinger equation with compactly supported potential may also be analyzed within the Lax–Phillips framework through the use of the invariance principle of wave operators[18]). The subject of the present paper is a theoretical framework, termed the *semigroup decomposition* of resonance evolution, developed with the goal of overcoming such difficulties. Proposed by one of the authors (Y. S.) of the present paper,[19,20] this formalism makes use of the Sz.-Nagy–Foias theory of contraction operators and contractive semigroups on Hilbert space[21] which, from the mathematical point of view, is the fundamental theory underlying the Lax–Phillips construction through the notion of model operators for $C_{\cdot 0}$ class semigroups.

The presentation of the semigroup decomposition formalism in Ref. 20 is based on the following assumptions:

(i) We are considering a scattering system consisting of a "free" unperturbed Hamiltonian $\mathbf{H}_0$ and a perturbed Hamiltonian $\mathbf{H}$, both defined on a Hilbert space $\mathcal{H}$.
(ii) $\text{ess supp}\sigma_{\text{ac}}(\mathbf{H}_0)=\text{ess supp}\sigma_{\text{ac}}(\mathbf{H})=\mathbb{R}^+$. For simplicity it is assumed further that the multiplicity of the absolutely continuous (ac) spectrum is 1.
(iii) The Møller wave operators $\mathbf{\Omega}^\pm\equiv\mathbf{\Omega}^\pm(\mathbf{H}_0,\mathbf{H})$ exist and are complete.
(iv) The S matrix in the *energy representation* (the spectral representation for $\mathbf{H}_0$), denoted by $\tilde{S}(\cdot)$ has an extension to a meromorphic function $S(\cdot)$ in an open, simply connected, region $\Sigma\subset\mathbb{C}$ such that $\Sigma\cap\mathbb{R}$ is an open interval in $\mathbb{R}$. The operator valued function $\mathcal{S}(\cdot)$ is holomorphic in $\Sigma\cap\mathbb{C}^+$ and has a simple pole (we generalize to the case of multiple poles in Sec. III below) at a point $z=\mu\in\Sigma\cap\mathbb{C}^-$ and no other singularity in $\bar{\Sigma}$, the closure of Σ.

It is shown in Ref. 20 that there exists a dense set $\Lambda\subset\mathcal{H}_{\text{ac}}(\mathbf{H})$ and a well defined state $\psi_\mu\in\mathcal{H}_{\text{ac}}(\mathbf{H})$ such that for any $g\in\Lambda$ and any $f\in\mathcal{H}_{\text{ac}}$ the properties (i)–(iv) above induce, for positive times, a decomposition of matrix elements of the evolution $\mathbf{U}(t)$ in the form

$$(g,\mathbf{U}(t)f)_{\mathcal{H}_{\text{ac}}(\mathbf{H})} = R(g,f;t) + \alpha(g,\mu)(\psi_\mu,f)_{\mathcal{H}_{\text{ac}}(\mathbf{H})}e^{-i\mu t}, \quad t \geqslant 0. \tag{2}$$

In a sense to be made precise in the next section the second term on the right hand side (rhs) of Eq. (2) originates from an evolution semigroup of the Lax–Phillips type and the eigenvalue of the generator of this semigroup is exactly μ, i.e., the point of singularity of the S matrix. The quantity $R(g,f;t)$ on the right hand side of Eq. (2) is what we shall call a *background* term. We note that if in Eq. (2) we choose f to be orthogonal to ψ_μ then the exponentially decaying semigroup term

[second term on the rhs of Eq. (2)] vanishes. We call ψ_μ an *approximate resonance state* and note that the characterization of ψ_μ as an approximate resonance state rather than as an exact resonance state stems from the fact that one can show (see Ref. 20) that there is no choice of g and f that makes the background term $R(g,f;t)$ vanish.

An explicit expression for the approximate resonance state ψ_μ is provided in Ref. 20. It is shown there that, if we denote by $\{|E^-\rangle\}_{E\in\mathbb{R}^+}$ the set of outgoing solutions of the Lippmann–Schwinger equation (using Dirac's notation), then ψ_μ is given by

$$\psi_\mu = \frac{1}{2\pi i}\int_{\mathbb{R}^+} dE \frac{1}{E-\mu}|E^-\rangle. \tag{3}$$

Following the introduction of approximate resonance states, the present paper discusses some generalizations. Thus, in Sec. III we assume that the region $\Sigma\cap\mathbb{C}^-$ contains multiple resonance poles of the S-matrix $\mathcal{S}(\cdot)$, say at $z=\mu_1,\ldots,\mu_n$ and obtain the form of the expression for the approximate resonance states and semigroup decomposition of evolution matrix elements in this case. In particular, we apply the semigroup decomposition to the *survival amplitude,* a central notion in the characterization of the time evolution of resonances. Theorem 5 below then provides an *a priori* upper bound on the size of the background term in this case.

As a final remark we note that a modification of the Lax–Phillips theory was recently used by Baumgartel for the description of scattering resonances in certain quantum mechanical problems[22] (see also Ref. 23). In particular, the assumption of orthogonality of $\mathcal{D}_\pm$, essential in the context of the original Lax–Phillips formalism, is replaced in Ref. 22 by the requirement that an incoming subspace $\mathcal{D}_-$ and an outgoing subspace $\mathcal{D}_+$ exist and the respective projections commute. The modified assumptions on $\mathcal{D}_\pm$, accompanied by certain assumptions on S-matrix analyticity properties, result in a modified Lax–Phillips structure which is then applied to the Friedrichs model, leading to the construction of appropriate Gamow type vectors[24] associated with scattering resonances. The framework presented in Ref. 22 has several points of intersection with the semigroup decomposition formalism discussed in the present paper. The nature of these relationships will be discussed elsewhere.

The rest of the paper is organized as follows: In Sec. II we describe the formalism providing the semigroup decomposition of resonance evolution starting with a short discussion of the functional model for $C_{\cdot 0}$ continuous contractive semigroups followed by a description of the semigroup decomposition formalism introduced in Refs. 19 and 20. In Sec. III we extend the framework of Ref. 19 and 20 to the case of multiple resonances and, furthermore, find an estimate on the size of the background term in the expression for the time evolution of the survival probability of a resonance. In Sec. IV we analyze a simple but illuminating example involving a one dimensional model of scattering from a square barrier potential. Section V contains a short summary of the contents of the paper and some indication on further possible courses of investigation.

II. THE SEMIGROUP DECOMPOSITION FOR RESONANCE EVOLUTION

A. Classification of contractive semigroups

Several distinct classes of contractive semigroups are identified within the framework of the Sz.-Nagy–Foias theory. Let $\{\mathbf{T}(t)\}_{t\geqslant 0}$ be a strongly contractive semigroup defined on a Hilbert space $\mathcal{H}$. The classes $C_{0\cdot}$, $C_{\cdot 0}$, $C_{1\cdot}$, $C_{\cdot 1}$ are defined by

$$\{\mathbf{T}(t)\}_{t\in\mathbb{R}^+} \in C_{0\cdot} \quad \text{if} \quad \mathbf{T}(t)h \to 0, \ \forall\, h \in \mathcal{H},$$

$$\{\mathbf{T}(t)\}_{t\in\mathbb{R}^+} \in C_{\cdot 0} \quad \text{if} \quad \mathbf{T}^*(t)h \to 0, \ \forall\, h \in \mathcal{H},$$

$$\{\mathbf{T}(t)\}_{t\in\mathbb{R}^+} \in C_{1\cdot} \quad \text{if} \quad \mathbf{T}(t)h \nrightarrow 0, \ \forall\, h \in \mathcal{H},\ h \neq 0,$$

$$\{\mathbf{T}(t)\}_{t\in\mathbb{R}^+} \in C_{\cdot 1} \quad \text{if} \quad \mathbf{T}^*(t)h \nrightarrow 0, \ \forall\, h \in \mathcal{H},\ h \neq 0.$$

The classes $C_{\alpha\beta}$ with α, β=0, 1 are then defined by

$$C_{\alpha\beta} = C_{\alpha\cdot} \cap C_{\cdot\beta}, \quad \alpha,\beta = 0,1.$$

The semigroup $\{\mathbf{Z}(t)\}_{t\in\mathbb{R}^+}$ describing the time evolution of resonances in the Lax–Phillips theory is readily characterized by the fact that $\{\mathbf{Z}^*(t)\}_{t\in\mathbb{R}^+}$ belongs to the class $C_{\cdot 0}$. The structure of the Lax–Phillips outgoing spectral (and translation) representation is then determined by that of the *functional model*[21,25] for $C_{\cdot 0}$ class semigroups provided by the Sz.-Nagy–Foias theory. We say an operator $\mathbf{A}$ is a *model operator*[25] for a given class C of operators if every operator in C is similar to a multiple of a part of $\mathbf{A}$ (a part of an operator $\mathbf{A}$ is a restriction of $\mathbf{A}$ to one of its invariant subspaces). By a functional model we mean that the model operator for a given class C has a canonical representation on suitable function spaces. For a $C_{\cdot 0}$ class semigroup $\{\mathbf{T}(t)\}_{t\geqslant 0}$ the associated functional model is essentially obtained through a procedure of *isometric dilation* of the *cogenerator* of $\{\mathbf{T}(t)\}_{t\geqslant 0}$ and the similarity mapping to the functional model is in fact a unitary transformation.

B. The functional model for $C_{\cdot 0}$ semigroups

We turn now to a brief description of the functional model for semigroups in the class $C_{\cdot 0}$. Denote by $\mathbb{C}^+$ the upper half of the complex plane and let $H^2_{\mathcal{N}}(\mathbb{C}^+)$ be the Hardy space of vector valued functions analytic in the upper half-plane and taking values in a separable Hilbert space $\mathcal{N}$. The set of boundary values on $\mathbb{R}$ of functions in $H^2_{\mathcal{N}}(\mathbb{C}^+)$, denoted below by $H^2_{\mathcal{N}+}(\mathbb{R})$, is a Hilbert space isomorphic to $H^2_{\mathcal{N}}(\mathbb{C}^+)$. In a similar manner the Hardy space of $\mathcal{N}$ valued functions analytic in the lower half-plane is denoted by $H^2_{\mathcal{N}}(\mathbb{C}^-)$ and $H^2_{\mathcal{N}-}(\mathbb{R})$ is the isomorphic Hilbert space consisting of boundary values on $\mathbb{R}$ of functions in $H^2_{\mathcal{N}}(\mathbb{C}^-)$. Define $\{u(t)\}_{t\in\mathbb{R}}$, a family of unitary, multiplicative operators $u(t): L^2_{\mathcal{N}}(\mathbb{R}) \mapsto L^2_{\mathcal{N}}(\mathbb{R})$ by

$$[u(t)f](\sigma) = e^{-i\sigma t} f(\sigma), \quad f \in L^2_{\mathcal{N}}(\mathbb{R}), \quad \sigma \in \mathbb{R}. \tag{4}$$

Assume that $\{\mathbf{T}(t)\}_{t\geqslant 0}$ is a $C_{\cdot 0}$ class semigroup defined on a Hilbert space $\mathcal{K}$. Let the semigroup $\{\hat{T}(t)\}_{t\geqslant 0}$, defined on a Hilbert space $\hat{\mathcal{K}}$, be the functional model for $\{\mathbf{T}(t)\}_{t\geqslant 0}$ and let $W: \mathcal{K} \mapsto \hat{\mathcal{K}}$ be the similarity transforming $\{\mathbf{T}(t)\}_{t\geqslant 0}$ into its functional model $\{\hat{T}(t)\}_{t\geqslant 0}$ i.e., $\hat{T}(t) = W\mathbf{T}(t)W^{-1}$. Then there exists a Hilbert space $\mathcal{N}$ such that $\hat{\mathcal{K}}$ is a closed subspace of $H^2_{\mathcal{N}+}(\mathbb{R})$, W is unitary, and the functional model is given by

$$\hat{T}(t) = W\mathbf{T}(t)W^* = P_{\hat{\mathcal{K}}} u^*(t) | \hat{\mathcal{K}}, \quad t \geqslant 0. \tag{5}$$

Here $P_{\hat{\mathcal{K}}}$ is the orthogonal projection from $H^2_{\mathcal{N}+}(\mathbb{R})$ onto $\hat{\mathcal{K}}$, the subspace $\hat{\mathcal{K}}$ is given by

$$\hat{\mathcal{K}} = H^2_{\mathcal{N}+}(\mathbb{R}) \ominus \Theta_T(\cdot) H^2_{\mathcal{N}+}(\mathbb{R}), \tag{6}$$

and $\Theta_T(\cdot): H^2_{\mathcal{N}+}(\mathbb{R}) \mapsto H^2_{\mathcal{N}+}(\mathbb{R})$ is an *inner function*[26,29,30] for $H^2_{\mathcal{N}+}(\mathbb{R})$ (depending, of course, on $\{\mathbf{T}(t)\}_{t\geqslant 0}$), i.e., an operator valued function with the properties:

1. For each $\sigma \in \mathbb{R}$ the operator $\Theta_T(\sigma): \mathcal{N} \mapsto \mathcal{N}$ is the boundary value at σ of an operator valued function $\Theta_T(\cdot)$ analytic in the upper half-plane.

2. $\|\Theta_T(z)\|_{\mathcal{N}} \leq 1$ for $\operatorname{Im} z > 0$.
3. $\Theta_T(\sigma)$, $\sigma \in \mathbb{R}$ is, pointwise, a unitary operator on $\mathcal{N}$.

The operator valued function $\Theta_T(\cdot)$ is, in fact, the *characteristic function*[21] of the cogenerator of the semigroup $\{\hat{T}(t)\}_{t\geq 0}$ [or $\{\mathbf{T}(t)\}_{t\geq 0}$].

Let P_+ be the orthogonal projection of $L^2_{\mathcal{N}}(\mathbb{R})$ on $H^2_{\mathcal{N}+}(\mathbb{R})$. The *Toeplitz operator* with symbol $u(t)$ (see, for example, Refs. 26 and 27, and references therein), is an operator $T_{u(t)}: H^2_{\mathcal{N}+}(\mathbb{R}) \mapsto H^2_{\mathcal{N}+}(\mathbb{R})$ defined by

$$T_{u(t)} f := P_+ u(t) f, \quad f \in H^2_{\mathcal{N}+}(\mathbb{R}). \tag{7}$$

We note that $\{T_{u(t)}\}_{t\geq 0}$ is a strongly contractive semigroup on $H^2_{\mathcal{N}+}(\mathbb{R})$ (see, for example, Refs. 1, 19, 21, and 28. Taking the conjugate of $\hat{T}(t)$ in $H^2_{\mathcal{N}+}(\mathbb{R})$ and using Eq. (5) one finds that

$$\hat{T}^*(t) = W\mathbf{T}^*(t)W^* = T_{u(t)}|\hat{\mathcal{K}}, \quad t \geq 0. \tag{8}$$

It follows from the discussion above that the Lax–Phillips semigroup $\{\mathbf{Z}(t)\}_{t\geq 0}$ has a functional model in the form of Eq. (8) [recall that $\{\mathbf{Z}^*(t)\}_{t\geq 0}$ is a $C_{\cdot 0}$ class semigroup], i.e., if we denote the functional model for $\{\mathbf{Z}(t)\}_{t\geq 0}$ by $\{\hat{Z}(t)\}_{t\geq 0}$ then we have

$$\hat{Z}(t) = W\mathbf{Z}(t)W^* = T_{u(t)}|\hat{\mathcal{K}}, \quad t \geq 0 \tag{9}$$

where $\hat{\mathcal{K}} \subset H^2_{\mathcal{N}+}(\mathbb{R})$ is an invariant subspace for $\{T_{u(t)}\}_{t\geq 0}$ given by

$$\hat{\mathcal{K}} = H^2_{\mathcal{N}+}(\mathbb{R}) \ominus \Theta_Z(\cdot) H^2_{\mathcal{N}+}(\mathbb{R}) \tag{10}$$

and the inner function $\Theta_Z(\cdot)$ and the Hilbert space $\mathcal{N}$ are determined by $\{\mathbf{Z}(t)\}_{t\geq 0}$. A semigroup $\{\hat{Z}(t)\}_{t\geq 0}$ of the form given by Eqs. (9) and (10) is referred to in Ref. 20 as a *Lax–Phillips type semigroup.*

A central theorem of the Lax–Phillips theory, corresponding to an important result in the Sz.-Nagy–Foias theory relating the spectrum of a *completely nonunitary contraction* (cnu) to points of singularity of the characteristic function states the following.

Theorem 1: *Denote by* $\hat{B}$ *the generator of a Lax–Phillips type semigroup* $\{\hat{Z}(t)\}_{t\geq 0}$. *If* $\operatorname{Im} \mu < 0$, *then* μ *belongs to the point spectrum of* $\hat{B}$ *if and only if* $\Theta^*_Z(\bar{\mu})$ *has a nontrivial null space.*

We note that the analytic continuation of $\Theta_Z(z)$ to the lower half-plane is given by

$$\Theta_Z(z) := (\Theta^*_Z(\bar{z}))^{-1}, \quad \operatorname{Im} z < 0$$

and so a null space for $\Theta^*_Z(\bar{\mu})$ implies the existence of a pole for $\Theta_Z(z)$ at $z=\mu$. In the case of the Lax–Phillips theory the characteristic function $\Theta_Z(\cdot)$ for the Lax–Phillips semigroup is identical to the Lax–Phillips S matrix and its poles are the scattering resonances. As will be seen below, the situation is a bit more involved in the semigroup decomposition formalism.

We do not elaborate here further on the relations between the functional model for $C_{\cdot 0}$ semigroups discussed above and the full structure of the Lax–Phillips spectral representations and wave operators. The reader is referred to Refs. 1 and 21.

C. The semigroup decomposition

In order to apply the functional model for $C_{\cdot 0}$ semigroups, which is at the heart of the Lax–Phillips structure, to the description of resonance evolution it is necessary to relate, for $t \geq 0$, the evolution $\mathbf{U}(t)$ defined on the Hilbert space $\mathcal{H}$ of the scattering problem to the Toeplitz evolution semigroup $T_{u(t)}$ of Eq. (7) defined on $H^2_{\mathcal{N}+}(\mathbb{R})$ and then restrict the latter, according to Eq. (9), to a subspace $\hat{\mathcal{K}}$ of $H^2_{\mathcal{N}+}(\mathbb{R})$ associated with an appropriate inner function $\Theta_{\hat{Z}}(\cdot)$. In the framework of the Lax–Phillips theory this relation is guaranteed by the special properties of the

Lax–Phillips incoming and outgoing subspaces $\mathcal{D}_\pm$ (with $\mathcal{D}_-$ and $\mathcal{D}_+$ denoting, respectively, the incoming and outgoing subspace), since in this case the Lax–Phillips semigroup is a $C_{\cdot 0}$ semigroup. However, for many quantum mechanical scattering problems one usually cannot find subspaces with the properties of $\mathcal{D}_\pm$. A way of overcoming this difficulty, proposed in Ref. 19, is to combine the standard functional model for $C_{\cdot 0}$ semigroups with the notion of a *quasi-affine mapping* (see, for example, Ref. 21, p. 70).

Definition 1 (quasi-affine mapping): A quasiaffine map from a Hilbert space $\mathcal{H}_1$ into a Hilbert space $\mathcal{H}_0$ is a linear, one to one continuous mapping of $\mathcal{H}_1$ into a dense linear manifold in $\mathcal{H}_0$. If $\mathbf{A}\in\mathcal{B}(\mathcal{H}_1)$ and $\mathbf{B}\in\mathcal{B}(\mathcal{H}_0)$ then $\mathbf{A}$ is a quasi-affine transform of $\mathbf{B}$ if there is a quasi-affine map $\theta:\mathcal{H}_1\mapsto\mathcal{H}_0$ such that $\theta\mathbf{A}=\mathbf{B}\theta$.

The following theorem is proved in Ref. 19 for a scattering system consisting of unperturbed and perturbed Hamiltonians, respectively $\mathbf{H}_0$ and $\mathbf{H}$, having semibounded continuous spectrum:

Theorem 2 (outgoing/incoming contractive nesting): *Let $\mathbf{H}_0$ and $\mathbf{H}$ be self-adjoint operators on a Hilbert space $\mathcal{H}$. Let $\{\mathbf{U}(t)\}_{t\in\mathbb{R}}$ be the unitary evolution group on $\mathcal{H}$ generated by $\mathbf{H}$* [i.e., $\mathbf{U}(t)=\exp(-i\mathbf{H}t)$]. *Denote by $\mathcal{H}_{\mathrm{ac}}(\mathbf{H}_0)$ and $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$, respectively, the absolutely continuous subspaces of $\mathbf{H}_0$ and $\mathbf{H}$. Assume that the absolutely continuous spectrum of $\mathbf{H}_0$ and $\mathbf{H}$ has multiplicity one and that ess Supp $\sigma_{\mathrm{ac}}(\mathbf{H}_0)=$ess Supp $\sigma_{\mathrm{ac}}(\mathbf{H})=\mathbb{R}^+$. Assume furthermore that the Møller wave operators $\mathbf{\Omega}^\pm\equiv\mathbf{\Omega}^\pm(\mathbf{H}_0,\mathbf{H}):\mathcal{H}_{\mathrm{ac}}(\mathbf{H}_0)\mapsto\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ exist and are complete. Then there are mappings $\hat{\Omega}_\pm:\mathcal{H}_{\mathrm{ac}}(\mathbf{H})\mapsto H^2_+(\mathbb{R})$ such that*

(i) *$\hat{\Omega}_\pm$ are contractive quasi-affine mappings of $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ into $H^2_+(\mathbb{R})$*; and
(ii) *for every $t\geqslant 0$ the evolution $\mathbf{U}(t)$ is a quasiaffine transform of the Toeplitz operator $T_{u(t)}$ via the mapping $\hat{\Omega}_\pm$ i.e., for every $f\in\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ we have*

$$\hat{\Omega}_\pm\mathbf{U}(t)f=T_{u(t)}\hat{\Omega}_\pm f\quad t\geqslant 0. \tag{11}$$

□

We call the triplet $\langle\mathcal{H}_{\mathrm{ac}}(\mathbf{H}),H^2_+(\mathbb{R}),\hat{\Omega}_-\rangle$ the *incoming contractive nesting* of $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ into $H^2_+(\mathbb{R})$ and denote $f_{\mathrm{in}}=\hat{\Omega}_-f$. Similarly, the triplet $\langle\mathcal{H}_{\mathrm{ac}}(\mathbf{H}),H^2_+(\mathbb{R}),\hat{\Omega}_+\rangle$ is the *outgoing contractive nesting of* $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ into $H^2_+(\mathbb{R})$ and we denote $f_{\mathrm{out}}=\hat{\Omega}_+f$.

Define

$$\Xi_{\hat{\Omega}_+}:=\hat{\Omega}_+^*H^2_+(\mathbb{R}).$$

Then, since $\hat{\Omega}_+^*$ is quasi-affine, the linear space $\Xi_{\hat{\Omega}_+}\subset\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ is dense in $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$. Moreover, since $\hat{\Omega}_+^*$ is one to one, for each $g\in\Xi_{\hat{\Omega}_+}$ there is a unique $\tilde{g}\in H^2_+(\mathbb{R})$ such that $g=\hat{\Omega}_+^*\tilde{g}$. We note that in Ref. 20 a dense set $\Lambda_{\hat{\Omega}_+}$, analogous to $\Xi_{\hat{\Omega}_+}$, is defined somewhat differently, i.e., $\Lambda_{\hat{\Omega}_+}:=\hat{\Omega}_+^*\hat{\Omega}_+\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$. However, it will be seen below that the definition of $\Xi_{\hat{\Omega}_+}$ above, unlike that of $\Lambda_{\hat{\Omega}_+}$, allows for a full characterization of approximate resonance states. Using Theorem 2 we have, for every $g\in\Xi_{\hat{\Omega}_+}$ and $f\in\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ and for $t\geqslant 0$,

$$(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=(\hat{\Omega}_+^*\tilde{g},\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=(\tilde{g},T_{u(t)}\hat{\Omega}_+f)_{H^2_+(\mathbb{R})}=(\tilde{g},T_{u(t)}f_{\mathrm{out}})_{H^2_+(\mathbb{R})},\quad t\geqslant 0. \tag{12}$$

Following the definitions of the incoming and outgoing nestings of $\mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ into $H^2_+(\mathbb{R})$ it is natural to define the *nested S matrix*

$$S_{\mathrm{nest}}:=\hat{\Omega}_+\hat{\Omega}_-^{-1}.$$

Let $U:\mathcal{H}_{ac}(\mathbf{H}_0)\mapsto L^2(\mathbb{R}^+)$ be the unitary transformation of $\mathcal{H}_{ac}(\mathbf{H}_0)$ onto the spectral representation for $\mathbf{H}_0$ (also called the energy representation for $\mathbf{H}_0$). If $\mathbf{S}=(\mathbf{\Omega}^-)^*\mathbf{\Omega}^+$ is the scattering operator associated with $\mathbf{H}_0$ and $\mathbf{H}$ then $\tilde{S}(\cdot):L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ defined by

$$\tilde{S}(\cdot) := U\mathbf{S}U^* \tag{13}$$

is the energy representation of the S matrix. Let $P_{\mathbb{R}^+}:L^2(\mathbb{R})\mapsto L^2(\mathbb{R})$ be the orthogonal projection in $L^2(\mathbb{R})$ on the subspace of functions supported on $\mathbb{R}^+$ and define the inclusion map $I:L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R})$ by

$$(If)(\sigma)=\begin{cases} f(\sigma), & \sigma\geqslant 0 \\ 0, & \sigma<0. \end{cases} \tag{14}$$

Then the inverse $I^{-1}:P_{\mathbb{R}^+}L^2(\mathbb{R})\mapsto L^2(\mathbb{R}^+)$ is, of course, one to one on $P_{\mathbb{R}^+}L^2(\mathbb{R})$. Let $\theta:H^2_+(\mathbb{R})\mapsto L^2(\mathbb{R}^+)$ be a map given by

$$\theta f = I^{-1}P_{\mathbb{R}_+}f, \quad f\in H^2_+(\mathbb{R}). \tag{15}$$

By a theorem of Van Winter,[31] θ is a quasi-affine transform mapping $H^2_+(\mathbb{R})$ into $L^2(\mathbb{R}^+)$. The adjoint map $\theta^*:L^2(\mathbb{R}^+)\mapsto H^2_+(\mathbb{R})$ is then also a contractive quasi-affine map. An explicit expression for θ^* is provided by the following lemma.[19]

Lemma 1: Let $I:L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R})$ be the inclusion map defined in Eq. (14). Let P_+ be the orthogonal projection of $L^2(\mathbb{R})$ onto $H^2_+(\mathbb{R})$. Then for every $f\in L^2(\mathbb{R}^+)$ we have

$$\theta^* f = P_+ If, \quad f\in L^2(\mathbb{R}^+). \tag{16}$$

□

It is shown in Ref. 19 that the nested S matrix can be expressed in the form

$$S_{\text{nest}} = \theta^*\tilde{S}(\cdot)(\theta^*)^{-1}. \tag{17}$$

Following Ref. 20 we now use assumption (iv) in Sec. I. The S-matrix $\tilde{S}(\cdot)$ is then the restriction of its extension $\mathcal{S}(\cdot)$ on $\mathbb{R}^+$. Under these assumptions $\mathcal{S}(\cdot)$ has, in the region Σ, a representation of the form (see Ref. 20),

$$\mathcal{S}(z)=\mathcal{B}_\mu(z)\mathcal{S}'(z), \quad z\in\Sigma,$$

where

$$\mathcal{B}_\mu(z)=\frac{z-\bar{\mu}}{z-\mu}, \quad z\in\mathbb{C}\setminus\{\mu\} \tag{18}$$

and $\mathcal{S}'(\cdot)$ is analytic and has no zeros in Σ. Restricting $\mathcal{S}(\cdot)$ to the positive real axis we obtain

$$\tilde{S}(E)=\tilde{B}_\mu(E)\tilde{S}'(E), \quad E\geqslant 0, \tag{19}$$

where by definition $\tilde{B}_\mu(E):=\mathcal{B}_\mu(E)$ and $\tilde{S}'(E):=\mathcal{S}'(E)$ for $E\geqslant 0$. We note that both $\tilde{S}'(\cdot)$ and $\tilde{B}_\mu(\cdot)$ are considered here as multiplicative unitary operators on $L^2(\mathbb{R}^+)$ (moreover, they are pointwise unitary a.e. for $E\geqslant 0$). Moreover, $\mathcal{B}_\mu(\cdot)$ can be regarded as a multiplicative operator on $L^2(\mathbb{R})$. In fact, considered as a multiplicative operator on $H^2_+(\mathbb{R})\subset L^2(\mathbb{R})$, $\mathcal{B}_\mu$ is a *Blaschke* factor [the definition of Blaschke products and Blaschke factors can be found, for example in Refs. 29 and 30, see e.g., Eq. (29) below]. Such a factor is the simplest example of an inner function for $H^2_+(\mathbb{R})$. We make use of this fact through the following proposition, not stated as such, but implicitly used in Ref. 20.

Proposition 1: Let $\tilde{B}_\mu(\cdot):L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ be defined by $\tilde{B}_\mu(E)=\mathcal{B}_\mu(E)$, $E\geqslant 0$ where $\mathcal{B}_\mu(\cdot)$ is

defined in Eq. (18). Let $\theta^*: L^2(\mathbb{R}^+) \mapsto H^2_+(\mathbb{R})$ *be the adjoint of the map* θ *defined in Eq. (15). Let* $\hat{\mathcal{K}}_\mu \subset H^2_+(\mathbb{R})$ *and* $\hat{\mathcal{K}}_{\bar{\mu}} \subset H^2_-(\mathbb{R})$ *be subspaces defined by*

$$\hat{\mathcal{K}}_\mu := H^2_+(\mathbb{R}) \ominus \mathcal{B}_\mu(\cdot) H^2_+(\mathbb{R}), \quad \hat{\mathcal{K}}_{\bar{\mu}} := H^2_-(\mathbb{R}) \ominus \mathcal{B}_{\bar{\mu}}(\cdot) H^2_-(\mathbb{R}),$$

where $\mathcal{B}_{\bar{\mu}}(z) = (z-\mu)(z-\bar{\mu})^{-1}$ *and denote by* $P_{\hat{\mathcal{K}}_\mu}$ *and* $P_{\hat{\mathcal{K}}_{\bar{\mu}}}$ *the orthogonal projections of* $L^2(\mathbb{R})$ *on* $\hat{\mathcal{K}}_\mu$ *and* $\hat{\mathcal{K}}_{\bar{\mu}}$, *respectively. For every* $f \in L^2(\mathbb{R}^+)$ *we then have*

$$\theta^* \tilde{B}_\mu f = \mathcal{B}_\mu \theta^* f + P_{\hat{\mathcal{K}}_\mu} \mathcal{B}_\mu P_{\hat{\mathcal{K}}_{\bar{\mu}}} \bar{\theta}^* f, \tag{20}$$

where $\bar{\theta}^*: L^2(\mathbb{R}^+) \mapsto H^2_-(\mathbb{R})$ *and* $\bar{\theta}^* f = P_- I f$ *with I defined in Eq. (14) and* P_- *the orthogonal projection of* $L^2(\mathbb{R})$ *onto* $H^2_-(\mathbb{R})$. □

Proof: Using Eq. (16) in Lemma 1 we get

$$\theta^* \tilde{B}_\mu f = P_+ I \tilde{B}_\mu f = P_+ \mathcal{B}_\mu I f = P_+ \mathcal{B}_\mu (P_+ + P_-) I f = P_+ \mathcal{B}_\mu \theta^* f + P_+ \mathcal{B}_\mu P_- \bar{\theta}^* f.$$

Equation (20) then follows from the fact, proved in Ref. 20, that $P_+ \mathcal{B}_\mu P_- = P_{\hat{\mathcal{K}}_\mu} \mathcal{B}_\mu P_{\hat{\mathcal{K}}_{\bar{\mu}}}$ and from the property of $\mathcal{B}_\mu(\cdot)$ of being an inner function for $H^2_+(\mathbb{R})$.

■

We note that since $\mathcal{B}_\mu(\cdot)$ is an inner function Eqs. (9) and (10) and Theorem 1 imply that

$$T_{u(t)} P_{\hat{\mathcal{K}}_\mu} = \hat{Z}(t) P_{\hat{\mathcal{K}}_\mu} = e^{-i\mu t} P_{\hat{\mathcal{K}}_\mu}, \quad t \geqslant 0. \tag{21}$$

Combining Eqs. (17), (19), and (20) we obtain

$$f_{\text{out}} = S_{\text{nest}} f_{\text{in}} = \theta^* \tilde{S} (\theta^*)^{-1} f_{\text{in}} = \theta^* \tilde{B}_\mu \tilde{S}' (\theta^*)^{-1} f_{\text{in}} = \mathcal{B}_\mu \theta^* \tilde{S}' (\theta^*)^{-1} f_{\text{in}} + P_{\hat{\mathcal{K}}_\mu} \mathcal{B}_\mu P_{\hat{\mathcal{K}}_{\bar{\mu}}} \bar{\theta}^* \tilde{S}' (\theta^*)^{-1} f_{\text{in}}. \tag{22}$$

Using the decomposition of f_{out} from Eq. (22) on the rhs of Eq. (12) and applying Eq. (21) we obtain the *semigroup decomposition* for $t \geqslant 0$ of the time evolution corresponding to the resonance at $z = \mu$,

$$(g, \mathbf{U}(t) f)_{\mathcal{H}_{\text{ac}}(\mathbf{H})} = (\tilde{g}, T_{u(t)} f_{\text{out}})_{H^2_+(\mathbb{R})} = (\tilde{g}, u(t) \mathcal{B}_\mu \theta^* \tilde{S}' (\theta^*)^{-1} f_{\text{in}})_{H^2_+(\mathbb{R})} + e^{-i\mu t} (\tilde{g}, \mathcal{B}_\mu \bar{\theta}^* \tilde{S}' (\theta^*)^{-1} f_{\text{in}})_{H^2_+(\mathbb{R})}. \tag{23}$$

As is seen above in Eq. (21), the exponential decay in the second term on the rhs of Eq. (23) originates with the semigroup $\hat{Z}(t)$. The first term on the rhs of Eq. (23) is the *background term* and is responsible for deviations from a purely exponential decay law.

III. APPROXIMATE RESONANCE STATES

It is an interesting fact that the semigroup decomposition described in the previous section associates a unique state in $\mathcal{H}_{\text{ac}}(\mathbf{H})$ with a resonance pole at $z = \mu$ ($\text{Im}\, \mu < 0$). The following theorem is proved in Ref. 20.

Theorem 3 (approximate resonance state): *Under the assumptions of Theorem 2, let* $\tilde{S}: L^2(\mathbb{R}^+) \mapsto L^2(\mathbb{R}^+)$ *be the S matrix in the energy representation defined in Eq. (13). Assume that* $\tilde{S}(\cdot)$ *is the restriction to* $\mathbb{R}^+$ *of a function* $\mathcal{S}(\cdot)$ *meromorphic in an open region* Σ *with a single, simple pole at a point* $z = \mu$, $\mu \in \Sigma \cap \mathbb{C}^-$. *For any* $f \in \mathcal{H}_{\text{ac}}(\mathbf{H})$ *define* $f_{\text{out}} = \hat{\Omega}_+ f$ *and* $f_{\text{in}} = \hat{\Omega}_- f$. *There exists a unique state* $\psi_\mu \in \mathcal{H}_{\text{ac}}(\mathbf{H})$ *such that*

$$f_{\text{out}} = \mathcal{B}_\mu \theta^* \tilde{S}' (\theta^*)^{-1} f_{\text{in}} + \frac{|\text{Im}\, \mu|}{\pi} (\psi_\mu, f)_{\mathcal{H}_{\text{ac}}(\mathbf{H})} x_\mu, \tag{24}$$

where θ^* *is the map given by lemma 1,* $\mathcal{B}_\mu$ *is given in* Eq. (18), $\tilde{S}'$ *is defined by* Eq. (19), *and* $x_\mu \in H^2_+(\mathbb{R})$ *is given by* $x_\mu(\sigma)=(\sigma-\mu)^{-1}$, $\sigma \in \mathbb{R}$. □

Combining Eqs. (24) and (23) we can write the semigroup decomposition in the form

$$(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})} = (\tilde{g},u(t)\mathcal{B}_\mu\theta^*\tilde{S}'(\theta^*)^{-1}f_{\mathrm{in}})_{H^2_+(\mathbb{R})} + \frac{|\mathrm{Im}\,\mu|}{\pi}e^{-i\mu t}(\tilde{g},x_\mu)_{H^2_+(\mathbb{R})}(\psi_\mu,f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}, \quad t \geqslant 0, \tag{25}$$

where $g \in \Xi_{\hat{\Omega}_+}$ and $\tilde{g}=(\hat{\Omega}^*_+)^{-1}g$. The eigenstate $x_\mu \in H^2_+(\mathbb{R})$ of the semigroup $\hat{Z}(t)$ providing the exponential decay of the second term on the rhs of Eq. (25) is called below the *Hardy space resonance state*. The state $\psi_\mu \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ whose existence is implied by Theorem 3 is called *approximate resonance state*. We observe that if in Eq. (25) we choose $f \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ orthogonal to ψ_μ then the second term on the rhs of that equation is identically zero.

Denote by $\{|E^-\rangle\}_{E\in\mathbb{R}^+}$ the set of outgoing solutions of the Lippmann–Schwinger equation. For every $f \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ we have

$$(U(\mathbf{\Omega}^-)^*f)(E) = \langle E^-|f\rangle, \quad E \in \mathbb{R}^+. \tag{26}$$

It is shown in Ref. 20 that an explicit expression for the approximate resonance state ψ_μ is given by

$$\psi_\mu = \frac{1}{2\pi i}\int_{\mathbb{R}^+} dE \frac{1}{E-\mu}|E^-\rangle. \tag{27}$$

In this section we explore several properties of approximate resonance states ψ_μ. Our first step is to extend the discussion above to the case of multiple resonances:

Theorem 4 (multiple resonance case): *Under the assumptions of Theorem 2, let* $\tilde{S}: L^2(\mathbb{R}^+)\mapsto L^2(\mathbb{R}^+)$ *be the S matrix in the energy representation defined in Eq. (13). Assume that* $\tilde{S}(\cdot)$ *is the restriction to* $\mathbb{R}^+$ *of a function* $\mathcal{S}(\cdot)$ *meromorphic in the open region* Σ *with n simple poles at points* $z=\mu_i$, $i=1,\ldots,n$, $\mu_i \in \Sigma \cap \mathbb{C}^-$. *Then there exist n distinct states* $\{\psi^\Sigma_{\mu_i}\}_{i=1,\ldots,n}$, $\psi^\Sigma_{\mu_i} \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$, *such that for every* $f \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ *we have*

$$f_{\mathrm{out}} = \mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^*\tilde{S}'(\theta^*)^{-1}f_{\mathrm{in}} + \sum_{j=1}^{n}\frac{|\mathrm{Im}\,\mu_j|}{\pi}\prod_{\substack{i=1\\ i\neq j}}^{n}\frac{\mu_j-\bar{\mu}_i}{\mu_j-\mu_i}(\psi^\Sigma_{\mu_j},f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}x_{\mu_j}, \tag{28}$$

where

$$\mathcal{B}_{\mu_1,\ldots,\mu_n}(z) := \prod_{i=1}^{n}\frac{z-\bar{\mu}_i}{z-\mu_i}. \tag{29}$$

In Eq. (28) $\tilde{S}'(\cdot)$ *is the restriction to* $\mathbb{R}^+$ *of a function* $\mathcal{S}'(\cdot)$ *analytic in* Σ *and having no poles in* $\bar{\Sigma}$ *and* $x_{\mu_j}(\sigma)=(\sigma-\mu_j)^{-1}$, $\sigma \in \mathbb{R}$. *The states* $\psi^\Sigma_{\mu_j}$, $j=1,\ldots,n$ *are given by*

$$\psi^\Sigma_{\mu_j} = \int_{\mathbb{R}^+} dE \prod_{\substack{i=1\\ i\neq j}}^{n}\frac{E-\bar{\mu}_i}{E-\mu_i}\frac{1}{E-\mu_j}|E^-\rangle. \tag{30}$$

□

Proof: Assume that $\mathcal{S}(\cdot)$, the extension of $\tilde{S}(\cdot)$ from $\mathbb{R}^+$ into $\Sigma\cup\mathbb{R}^+$ has n simple poles in $\Sigma\cap\mathbb{C}^-$. Then, applying the same arguments as in Ref. 20, we find that $\mathcal{S}(\cdot)$ can be factorized in Σ in the form

$$\mathcal{S}(z) = \mathcal{B}_{\mu_1,\ldots,\mu_n}(z)\mathcal{S}'(z),$$

where $\mathcal{B}_{\mu_1,\ldots,\mu_n}$, defined in Eq. (29), is a finite Blaschke product and $\mathcal{S}'(\cdot)$ has no poles in Σ. In addition we have, of course

$$\widetilde{S}(E) = \widetilde{B}_{\mu_1,\ldots,\mu_n}(E)\widetilde{S}'(E), \quad E \geqslant 0.$$

The semigroup decomposition then follows exactly as in Sec. I with $\mathcal{B}_{\mu_1,\ldots,\mu_n}$ and $\widetilde{B}_{\mu_1,\ldots,\mu_n}$ replacing $\mathcal{B}_\mu$ and $\widetilde{B}_\mu$, respectively. For the resonance term in Eq. (22) we get in this case

$$P_+\mathcal{B}_{\mu_1,\ldots,\mu_n}P_-\overline{\theta}^*\widetilde{S}'(\theta^*)^{-1}f_{\text{in}}, \quad f \in \mathcal{H}_{\text{ac}}(\mathbf{H}).$$

Recalling that

$$(P_+f)(\sigma) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\sigma' \frac{1}{\sigma - \sigma' + i0}f(\sigma'), \quad f \in L^2(\mathbb{R}), \quad \sigma \in \mathbb{R}$$

and

$$(\overline{\theta}^*f)(\sigma) = \frac{1}{2\pi i}\int_0^{\infty} dE \frac{1}{E - \sigma + i0}f(E), \quad f \in L^2(\mathbb{R}^+)$$

(see Ref. 19) we obtain

$$\begin{aligned}
(P_+\mathcal{B}_{\mu_1,\ldots,\mu_n}P_-\overline{\theta}^*\widetilde{S}'(\theta^*)^{-1}f_{\text{in}})(\sigma) &= \frac{-1}{4\pi^2}\int_0^{\infty} dE \int_{-\infty}^{\infty} d\sigma' \frac{1}{\sigma - \sigma' + i0}\prod_{i=1}^{n}\frac{\sigma' - \bar{\mu}_i}{\sigma' - \mu_i}\frac{1}{E - \sigma' + i0}\widetilde{S}'(E)((\theta^*)^{-1}f_{\text{in}})(E) \\
&= \sum_{j=1}^{n}\frac{|\text{Im}\,\mu_j|}{\pi}\frac{1}{\sigma - \mu_j}\int_0^{\infty} dE \prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{\mu_j - \bar{\mu}_i}{\mu_j - \mu_i}\frac{1}{E - \mu_j}\widetilde{S}'(E)((\theta^*)^{-1}f_{\text{in}})(E) \\
&= \sum_{j=1}^{n}\frac{|\text{Im}\,\mu_j|}{\pi}x_{\mu_j}(\sigma)\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{\mu_j - \bar{\mu}_i}{\mu_j - \mu_i}\int_0^{\infty} dE \frac{1}{E - \bar{\mu}_j}\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{E - \mu_i}{E - \bar{\mu}_i}\widetilde{S}(E)((\theta^*)^{-1}f_{\text{in}})(E) \\
&= \sum_{j=1}^{n}\frac{|\text{Im}\,\mu_j|}{\pi}x_{\mu_j}(\sigma)\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{\mu_j - \bar{\mu}_i}{\mu_j - \mu_i}\int_0^{\infty} dE \frac{1}{E - \bar{\mu}_j}\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{E - \mu_i}{E - \bar{\mu}_i}(U(\mathbf{\Omega}^-)^*f)(E) \\
&= \sum_{j=1}^{n}\frac{|\text{Im}\,\mu_j|}{\pi}x_{\mu_j}(\sigma)\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{\mu_j - \bar{\mu}_i}{\mu_j - \mu_i}\int_0^{\infty} dE \frac{1}{E - \bar{\mu}_j}\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{E - \mu_i}{E - \bar{\mu}_i}\langle E^-|f\rangle,
\end{aligned}$$

where $x_{\mu_j} \in H^2_+(\mathbb{R})$ is the Hardy space resonance state corresponding to μ_j i.e., $x_{\mu_j}(\sigma) = (\sigma - \mu_j)^{-1}$. Defining the states $\psi^{\Sigma}_{\mu_j}$, $j = 1, \ldots, n$ according to Eq. (30) we obtain

$$(P_+\mathcal{B}_{\mu_1,\ldots,\mu_n}P_-\overline{\theta}^*\widetilde{S}'(\theta^*)^{-1}f_{\text{in}})(\sigma) = \sum_{j=1}^{n}\frac{|\text{Im}\,\mu_j|}{\pi}\prod_{\substack{i=1 \\ i\neq j}}^{n}\frac{\mu_j - \bar{\mu}_i}{\mu_j - \mu_i}(\psi^{\Sigma}_{\mu_j}, f)_{\mathcal{H}_{\text{ac}}(\mathbf{H})}x_{\mu_j}(\sigma). \tag{31}$$

This proves Theorem 4. ■

We observe that Eq. (30) is a generalization of Eq. (27). Hence, $\psi^{\Sigma}_{\mu_j}$ is the approximate resonance state corresponding to the pole of $\mathcal{S}(\cdot)$ at $z=\mu_j$. Combining Eqs. (31) and (23) we get the semigroup decomposition for the multiresonance case

$$(g,\mathbf{U}(t)f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=(\tilde{g},u(t)\mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^{*}\tilde{S}'(\theta^{*})^{-1}f_{\mathrm{in}})_{H^2_{+}(\mathbb{R})}+\sum_{j=1}^{n}\frac{|\mathrm{Im}\,\mu_j|}{\pi}\prod_{\substack{i=1\\ i\neq j}}^{n}\frac{\mu_j-\bar{\mu}_i}{\mu_j-\mu_i}(\psi^{\Sigma}_{\mu_j},f)_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}$$

$$\times(\tilde{g},x_{\mu_j})_{H^2_{+}(\mathbb{R})}e^{-i\mu_j t},\quad t\geqslant 0. \tag{32}$$

The approximate resonance states in Eq. (30) and semigroup decomposition of Eqs. (28) and (32) depend, of course, on the region Σ. If $\{\mu_j\}_{j=1,\ldots,n}$ are the poles in $\Sigma\cap\mathbb{C}^{-}$ of the meromorphic extension $\mathcal{S}(\cdot)$ of the S-matrix $\tilde{S}(\cdot)$, the approximate resonance state defined in Eq. (30) for a resonance at $z=\mu_j$ is therefore denoted by $\psi^{\Sigma}_{\mu_j}$. However, for certain arguments the exact form of Σ is irrelevant and it is useful to define the notion of an n'th order approximate resonance state:

*Definition 2 (n'th order approximate resonance state): If the number of poles of $\mathcal{S}(\cdot)$ entering into the definition of the approximate resonance state $\psi^{\Sigma}_{\mu_j}$ in Eq. (30), not including μ_j itself, is n we say that $\psi^{\Sigma}_{\mu_j}$ is an n*th *order approximate resonance state for the resonance at $z=\mu_j$. In particular, regardless of the exact nature of the region Σ, the zeroth order approximate resonance state is always defined to be given by Eq. (27) with $\mu=\mu_j$ and is denoted by $\psi^{(0)}_{\mu_j}$.*

Remark: Note that in general there are many choices of the n resonance poles (different than μ_j) included in the construction of what we call an nth order approximation $\psi^{(n)}_{\mu_j}$. In cases that the nature of the region Σ is irrelevant and only the order of the approximate resonance state is significant we replace the notation $\psi^{\Sigma}_{\mu_j}$ by $\psi^{(n)}_{\mu_j}$, where n is the order of the approximate resonance state considered.

The semigroup decomposition and approximate resonance states for the multiresonance case possess some interesting properties. For example, we have

$$(\psi^{\Sigma}_{\mu_j},\psi^{\Sigma}_{\mu_k})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=(\psi^{(0)}_{\mu_j},\psi^{(0)}_{\mu_k})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=\int_{\mathbb{R}^{+}}dE\frac{1}{E-\mu_j}\frac{1}{E-\bar{\mu}_k}$$

and, in particular

$$\|\psi^{\Sigma}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=\|\psi^{(n)}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=\|\psi^{(0)}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=\int_{\mathbb{R}^{+}}dE\frac{1}{|E-\mu_j|^2}. \tag{33}$$

We see that, although the definition of $\psi^{\Sigma}_{\mu_i}$ in Eq. (30) depends on all of the poles $\{\mu_j\}_{j=1,\ldots,n}\subset\Sigma\cap\mathbb{C}^{-}$, the scalar product of $\psi^{\Sigma}_{\mu_i}$ and $\psi^{\Sigma}_{\mu_j}$ depends only on μ_i and μ_j. In fact, if $\mathcal{S}(\cdot)$ can be extended to a meromorphic function in a region $\Sigma'\supset\Sigma$ [we keep the notation $\mathcal{S}(\cdot)$ for the extended function] and $\mathcal{S}(\cdot)$ has now $m>n$ simple poles in $\Sigma'\cap\mathbb{C}^{-}$ we may calculate approximate resonance states of order $m-1$ for all resonances in Σ' according to Eq. (30). However, for $\mu_j,\mu_k\in\Sigma$ we would still have $(\psi^{\Sigma'}_{\mu_j},\psi^{\Sigma'}_{\mu_k})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=(\psi^{\Sigma}_{\mu_j},\psi^{\Sigma}_{\mu_k})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}$ i.e., scalar products (and norms) are independent of the order of the approximate states when we enlarge the region Σ. In particular we have $\|\psi^{\Sigma}_{\mu_j}\|_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}=\|\psi^{(0)}_{\mu_j}\|_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}$ for every region Σ containing μ_j.

An interesting question is whether the peculiar properties of scalar products and norms of the approximate resonance states mentioned above characterize also the time evolution of these states. We shall see below that, at least partially, the answer to this question is positive. For this we consider one of the basic notions associated with resonance evolution, i.e., that of the survival amplitude

$$A_{\psi^{\Sigma}_{\mu_j}}(t) := \frac{(\psi^{\Sigma}_{\mu_j}, \mathbf{U}(t)\psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}{(\psi^{\Sigma}_{\mu_j}, \psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}. \tag{34}$$

Making use of Eqs. (30) and (33) we get a simple expression for this quantity

$$A_{\psi^{(0)}_{\mu_j}}(t) = \|\psi^{(0)}_{\mu_j}\|^{-2}_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})} \int_{\mathbb{R}^+} \frac{1}{|E-\mu_j|^2} e^{-iEt}, \quad t \geqslant 0,$$

where $\|\psi^{(0)}_{\mu_j}\|$ is given in Eq. (33). Again, we see that the expression for the survival amplitude for the approximate resonance state $\psi^{\Sigma}_{\mu_j}$ depends only on the pole at $z=\mu_j$ and has the same form as for a single resonance. This suggests that the semigroup decomposition of the survival amplitude for the multiple resonance case is similar to that of a single resonance. When combined with an important characterization of approximate resonance states in the form of Lemma 2 below, such considerations lead to the following useful *a priori* estimate on the size of the background term in the semigroup decomposition of the survival amplitude:

Theorem 5: *Let $A_{\psi^{\Sigma}_{\mu_j}}(t)$, $j=1,\ldots,n$ be the survival amplitude defined in Eq. (34) and let the background term $R_{\mu_j}(t)$ be defined by the relation*

$$A_{\psi^{\Sigma}_{\mu_j}}(t) = R_{\mu_j}(t) + e^{-i\mu_j t}, \quad t \geqslant 0. \tag{35}$$

Then we have

$$|R_{\mu_j}(t)| \leqslant \left(\frac{\|x_{\mu_j}\|^4_{H^2_+(\mathbb{R})}}{\|\psi^{(0)}_{\mu_j}\|^4_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}} - 1 \right)^{1/2}, \quad t \geqslant 0, \tag{36}$$

where $x_{\mu_j}(\sigma)=(\sigma-\mu_j)^{-1}$ is the Hardy space resonance state and $\psi^{(0)}_{\mu_j} \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ is the zeroth order approximate resonance state corresponding to the resonance at $z=\mu_j$. □

Proof: We first have

Proposition 2: For $j=1,\ldots,n$, let $\psi^{\Sigma}_{\mu_j}$ be defined by Eq. (30) and let $A_{\psi^{\Sigma}_{\mu_j}}(t)$ be the survival amplitude defined in Eq. (34). Then

$$A_{\psi^{\Sigma}_{\mu_j}}(t) = \|\psi^{(0)}_{\mu_j}\|^{-2}_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})} (x_{\mu_j}, u(t)\mathcal{B}_{\mu_j}\theta^* \widetilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^{(0)}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})} + e^{-i\mu_j t}, \quad t \geqslant 0, \tag{37}$$

where $x_{\mu_j} \in H^2_+(\mathbb{R})$ is the Hardy space resonance state and $\psi^{(0)}_{\mu_j} \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$ is the zeroth order approximate resonance state corresponding to the pole at μ_j, and $\widetilde{S}'_{\mu_j}(\cdot)$ is defined as in Eq. (19), i.e.,

$$\widetilde{S}'_{\mu_j}(E) = \frac{E-\mu_j}{E-\bar{\mu}_j}\widetilde{S}(E) = \widetilde{B}_{\bar{\mu}_j}(E)\widetilde{S}(E).$$

□

Proof of Proposition 2: We first need the following easily proved, but important, lemma

Lemma 2: For $j=1,\ldots,n$, let $\psi^{\Sigma}_{\mu_j}$ be defined by Eq. (30). Define

$$\mathcal{B}_{\mu_1,\ldots,\bar{\mu}_k,\ldots,\mu_n}(z) := \prod_{\substack{i=1 \\ i\neq j}}^{n} \frac{z-\bar{\mu}_i}{z-\mu_i},$$

where $\{\mu_j\}_{j=1,\ldots,n}$ are the poles of $\mathcal{S}(\cdot)$ in Σ, and let $x_{\mu_j}(\sigma)=(\sigma-\mu_j)^{-1}$. Then we have

$$\psi^{\Sigma}_{\mu_j} = \hat{\Omega}^{*}_{+}\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j}.$$

In particular $\psi^{(0)}_{\mu_j}=\hat{\Omega}^{*}_{+}x_{\mu_j}$. □

Proof of Lemma 2: It is proved in Ref. 19 that, if $\mathbf{\Omega}^{\pm}$ are the Møller wave operators, $U:\mathcal{H}_{\mathrm{ac}}(\mathbf{H}_0)\mapsto L^2(\mathbb{R}^+)$ the mapping to the energy representation for $\mathbf{H}_0$ [see Eq. (13) above] and θ^* the map given in Lemma 1, then the quasi-affine nesting maps $\hat{\Omega}_{\pm}$ are given by $\hat{\Omega}_{\pm}=\theta^* U(\mathbf{\Omega}^{\mp})^*$, hence, we have $\hat{\Omega}^{*}_{+}=\mathbf{\Omega}^{-}U^*\theta$. Furthermore, by the definition of θ we have

$$(\theta\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j})(E) = \prod_{\substack{i=1\\ i\neq j}}^{n}\frac{E-\bar{\mu}_i}{E-\mu_i}\frac{1}{E-\mu_j}, \quad E\in\mathbb{R}^+. \tag{38}$$

Moreover, according to Eq. (26) for every $g\in L^2(\mathbb{R}^+)$ we have

$$\mathbf{\Omega}^{-}U^*g = \int_{\mathbb{R}^+} dE|E^-\rangle g(E). \tag{39}$$

Applying Eq. (39) with $g=\theta\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j}$ and comparing with Eq. (30) proves the lemma. ■

Note that by Lemma 2 we have $(\hat{\Omega}^{*}_{+})^{-1}\psi^{\Sigma}_{\mu_j}=\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j}$. Hence, by Eq. (32) we get

$$\begin{aligned}
A_{\psi^{\Sigma}_{\mu_j}}(t) &= \|\psi^{\Sigma}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}(\psi^{\Sigma}_{\mu_j},\mathbf{U}(t)\psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}\\
&= \|\psi^{\Sigma}_{\mu_j}\|^{-2}_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j},u(t)\mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})}\\
&\quad+\sum_{k=1}^{n}\frac{|\mathrm{Im}\,\mu_k|}{\pi}\prod_{\substack{i=1\\ i\neq k}}^{n}\frac{\mu_k-\bar{\mu}_i}{\mu_k-\mu_i}\frac{(\psi^{\Sigma}_{\mu_k},\psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}{\|\psi^{\Sigma}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j},x_{\mu_k})_{H^2_+(\mathbb{R})}e^{-i\mu_k t}.
\end{aligned} \tag{40}$$

In the second term on the rhs of Eq. (40) we first separate the term with $k=j$ and get

$$\begin{aligned}
&\sum_{k=1}^{n}\frac{|\mathrm{Im}\,\mu_k|}{\pi}\prod_{\substack{i=1\\ i\neq k}}^{n}\frac{\mu_k-\bar{\mu}_i}{\mu_k-\mu_i}\frac{(\psi^{\Sigma}_{\mu_k},\psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}{\|\psi^{\Sigma}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j},x_{\mu_k})_{H^2_+(\mathbb{R})}e^{-i\mu_k t}\\
&=\sum_{\substack{k=1\\ k\neq j}}^{n}\frac{|\mathrm{Im}\,\mu_k|}{\pi}\prod_{\substack{i=1\\ i\neq k}}^{n}\frac{\mu_k-\bar{\mu}_i}{\mu_k-\mu_i}\frac{(\psi^{\Sigma}_{\mu_k},\psi^{\Sigma}_{\mu_j})_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}{\|\psi^{\Sigma}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}}(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j},x_{\mu_k})_{H^2_+(\mathbb{R})}e^{-i\mu_k t}+e^{-i\mu_j t}, \quad t\geqslant 0.
\end{aligned}$$

Here, use has been made of Eq. (42) below. The above expression can be further simplified since $x_{\mu_k}\in\hat{\mathcal{K}}_{\mu_k}=H^2_+(\mathbb{R})\ominus\mathcal{B}_{\mu_k}(\cdot)H^2_+(\mathbb{R})$ implies that for $k\neq j$ we have

$$(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n}x_{\mu_j},x_{\mu_k})_{H^2_+(\mathbb{R})}=(\mathcal{B}_{\mu_k}\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\hat{\mu}_k,\ldots\mu_n}x_{\mu_j},x_{\mu_k})_{H^2_+(\mathbb{R})}=0,$$

where

$$\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\hat{\mu}_k,\ldots,\mu_n}(z) := \prod_{\substack{i=1\\ i\neq k,j}}^{n}\frac{z-\bar{\mu}_i}{z-\mu_i}.$$

The first term on the rhs of Eq. (40) can also be simplified. We have

$$
\begin{aligned}
&(\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} x_{\mu_j}, u(t)\mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})} \\
&\quad = (u(-t)\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} x_{\mu_j}, \mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})} \\
&\quad = (\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} u(-t)x_{\mu_j}, \mathcal{B}_{\mu_1,\ldots,\mu_n}\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})} \\
&\quad = (x_{\mu_j}, u(t)\mathcal{B}_{\mu_j}\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})}, \quad t \geqslant 0.
\end{aligned}
$$

Moreover, using Lemma 2 we find that

$$
\begin{aligned}
\theta^*\tilde{S}'(\theta^*)^{-1}\psi^{\Sigma}_{\mu_j,\mathrm{in}} &= \theta^*\tilde{S}'(\theta^*)^{-1}\hat{\Omega}_-\hat{\Omega}^*_+\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} x_{\mu_j} = \theta^*\tilde{S}'(\theta^*)^{-1}\theta^*\tilde{S}^*\theta\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} x_{\mu_j} \\
&= \theta^*\overline{\tilde{B}_{\mu_1,\ldots,\mu_n}}\theta\mathcal{B}_{\mu_1,\ldots,\hat{\mu}_j,\ldots,\mu_n} x_{\mu_j} = \theta^*\overline{\tilde{B}_{\mu_j}}\theta x_{\mu_j} = \theta^*\tilde{B}_{\bar{\mu}_j}\tilde{S}(\theta^*)^{-1}\hat{\Omega}_-\hat{\Omega}^*_+ x_{\mu_j} \\
&= \theta^*\tilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^0_{\mu_j,\mathrm{in}}.
\end{aligned}
$$

Recalling that Eq. (33) implies that $\|\psi^{\Sigma}_{\mu_j}\|_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})} = \|\psi^{(0)}_{\mu_j}\|_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}$ the proof of Proposition 2 is complete. ■

From Proposition 2 we see that, independent of the region Σ, the semigroup decomposition of the survival amplitude depends only on the zeroth order approximate resonance state.

Comparison of Eqs. (37) and (35) gives

$$
R_{\mu_j}(t) = \|\psi^{(0)}_{\mu_j}\|^{-2}_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}(x_{\mu_j}, u(t)\mathcal{B}_{\mu_j}\theta^*\tilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^{(0)}_{\mu_j,\mathrm{in}})_{H^2_+(\mathbb{R})}, \quad t \geqslant 0. \tag{41}
$$

This expression for $R_{\mu_j}(t)$ is identical to the zeroth order background term we would get from Eq. (25) with $f = g = \psi^{(0)}_{\mu_j}$. We now exploit this fact to obtain the desired estimate in Theorem 5. Applying Theorem 3 to the zeroth order approximate resonance state $\psi^{(0)}_{\mu_j}$ we obtain

$$
\psi^{(0)}_{\mu_j,\mathrm{out}} = \hat{\Omega}_+\psi^{(0)}_{\mu_j} = \mathcal{B}_{\mu_j}\theta^*\tilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^{(0)}_{\mu_j,\mathrm{in}} + \frac{|\mathrm{Im}\,\mu_j|}{\pi}\|\psi^{(0)}_{\mu_j}\|^2_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})} x_{\mu_j}.
$$

Now, since both $\hat{\Omega}_+$ and $\hat{\Omega}^*_+$ are contractive we note that Lemma 2 implies that $\|\psi^{(0)}_{\mu_j,\mathrm{out}}\|_{H^2_+(\mathbb{R})} = \|\hat{\Omega}_+\hat{\Omega}^*_+ x_{\mu_j}\|_{H^2_+(\mathbb{R})} \leqslant \|x_{\mu_j}\|_{H^2_+(\mathbb{R})}$. In addition in $H^2_+(\mathbb{R})$ we have $x_{\mu_j} \perp \mathcal{B}_{\mu_j} H^2_+(\mathbb{R})$. Therefore

$$
\|\mathcal{B}_{\mu_j}\theta^*\tilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^{(0)}_{\mu_j,\mathrm{in}}\|^2_{H^2_+(\mathbb{R})} + \frac{|\mathrm{Im}\,\mu_j|^2}{\pi^2}\|\psi^{(0)}_{\mu_j}\|^4_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})}\|x_{\mu_j}\|^2_{H^2_+(\mathbb{R})} \leqslant \|x_{\mu_j}\|^2_{H^2_+(\mathbb{R})}.
$$

It is easy to verify that

$$
\|x_{\mu_j}\|^2_{H^2_+(\mathbb{R})} = \int_{-\infty}^{\infty} \frac{1}{|\sigma - \mu_j|^2} d\sigma = \frac{\pi}{|\mathrm{Im}\,\mu_j|}, \tag{42}
$$

hence, the inequality above can be written in the form

$$
\|\mathcal{B}_{\mu_j}\theta^*\tilde{S}'_{\mu_j}(\theta^*)^{-1}\psi^{(0)}_{\mu_j,\mathrm{in}}\|^2_{H^2_+(\mathbb{R})} \leqslant (\|x_\mu\|^4_{H^2_+(\mathbb{R})} - \|\psi^{(0)}_{\mu_j}\|^4_{\mathcal{H}_{\mathrm{ac}}(\mathbf{H})})\|x_{\mu_j}\|^{-2}_{H^2_+(\mathbb{R})}. \tag{43}
$$

Applying the Schwartz inequality to the rhs of Eq. (41) and using the bound from Eq. (43) we get the estimate in Eq. (36). ■

As mentioned above the background term cannot be identically zero. Hence, deviations from exponential decay of the survival probability are to be expected. In fact, it is easy to verify that the survival probability behaves for short times as $|A_{\psi_{\mu_j}}(t)|^2 = 1 - O(t^2)$. Note that Eq. (35) implies that

at $t=0$ we must have $R_{\mu_j}(0)=0$. This is also seen from Eq. (41), since for $t=0$ we have $u(0)=1$ and $x_{\mu_j} \perp \mathcal{B}_{\mu_j}(\cdot)H_+^2(\mathbb{R})$. Deviations from exponential decay are then due to the fact that x_{μ_j} is not perpendicular to $u(t)\mathcal{B}_{\mu_j}H_+^2(\mathbb{R})$ for $t>0$.

IV. EXAMPLE: SCATTERING FROM SQUARE BARRIER POTENTIAL

In this section we apply the results of the previous two sections to a simple one dimensional model with a square barrier potential. Although simple, this model provides a good illustration for the various results obtained above. In particular, we present numerical calculations of approximate resonance states of various orders accompanied with plots of the time evolution of the corresponding survival probabilities and estimates of the size of the background term following from Theorem 5.

The model we consider is a Schrödinger equation in one spatial dimension on the half-line $\mathbb{R}^+$ with a square barrier potential. Thus we consider the free Hamiltonian $\mathbf{H}_0=-\partial_x^2$ acting on $L^2(\mathbb{R}^+)$ [where $\mathbf{H}_0$ is defined as a self-adjoint extension to $L^2(\mathbb{R}^+)$ from the original domain of definition $D(-\partial_x^2)=\{\phi(x)\in W_2^2(\mathbb{R}^+)\,|\,\phi(x)=0\}$] and the full Hamiltonian is given by $\mathbf{H}=\mathbf{H}_0+\mathbf{V}$ where $\mathbf{V}$ is a multiplicative operator $(\mathbf{V}f)(x)=V(x)f(x)$ with

$$V(x)=\begin{cases}0, & 0<x<a\\ V_0, & a\leqslant x\leqslant b\\ 0, & b<x,\end{cases}$$

where $b>a>0$ and we take $V_0>0$. In this case there are no bound state solutions of the eigenvalue problem for $\mathbf{H}$ and we have $\sigma(\mathbf{H})=\sigma_{\mathrm{ac}}(\mathbf{H})=\mathbb{R}^+$. In order to find the scattering states, calculate the S matrix, and finally the approximate resonance states for this problem one solves the eigenvalue problem

$$-\partial_x^2\psi_E(x)+V(x)\psi_E(x)=E\psi_E(x),\quad E\in\mathbb{R}^+$$

for the continuous spectrum generalized eigenfunctions $\psi_E(x)$. Imposing boundary conditions one finds that

$$\psi_E(x)=\begin{cases}\alpha_1(k)\sin kx, & 0<x\leqslant a\\ \alpha_2(k)e^{ik'x}+\beta_2(k)e^{-ik'x}, & a<x<b\\ \alpha_3(k)e^{ikx}+\beta_3(k)e^{-ikx}, & b\leqslant x,\end{cases}\tag{44}$$

where $k=E^{1/2}$ and $k'=\sqrt{E-V_0}$ for $E\geqslant V_0>0$ or $k'=i\sqrt{V_0-E}$ for $V_0>E>0$. The coefficients in Eq. (44) are given by[32]

$$\begin{aligned}\alpha_2(k)&=\frac{1}{2}e^{-ik'a}\left[\sin ka+\frac{k}{ik'}\cos ka\right]\alpha_1(k),\\ \beta_2(k)&=\frac{1}{2}e^{ik'a}\left[\sin ka-\frac{k}{ik'}\cos ka\right]\alpha_1(k),\\ \alpha_3(k)&=\frac{1}{4}e^{-ikb}\left[(1+k'/k)e^{ik'(b-a)}\left(\sin ka+\frac{k}{ik'}\cos ka\right)+(1-k'/k)e^{-ik'(b-a)}\right.\\ &\quad\left.\times\left(\sin ka-\frac{k}{ik'}\cos ka\right)\right]\alpha_1(k),\end{aligned}\tag{45}$$

$$\beta_3(k) = \frac{1}{4}e^{ikb}\Bigg[(1-k'/k)e^{ik'(b-a)}\left(\sin ka + \frac{k}{ik'}\cos ka\right) + (1+k'/k)e^{-ik'(b-a)} \times\left(\sin ka - \frac{k}{ik'}\cos ka\right)\Bigg]\alpha_1(k),$$

with $\alpha_1(k)$ to be determined by normalization conditions (see below).

Given the full set of solutions $\{\psi_E(x)\}_{E\in\mathbb{R}^+}$ for the continuous spectrum it is easy to find the sets $\{\psi_E^{\pm}(x)\}_{E\in\mathbb{R}^+}$ of solutions of the Lippmann–Schwinger equation corresponding to incoming and outgoing asymptotic conditions. Using Dirac's notation we have[32]

$$\langle x|E^+\rangle \equiv \psi_E^+(x) = \frac{-1}{2i}\frac{\psi_E(x)}{\beta_3(k)},$$

$$\langle x|E^-\rangle \equiv \psi_E^-(x) = \frac{1}{2i}\frac{\psi_E(x)}{\alpha_3(k)}. \tag{46}$$

The normalization conditions for the Lippmann–Schwinger states in Eq. (46) determines $\alpha_1(k)$ with the result $\alpha_1(k)=(2\pi k)^{-1/2}$. In the energy representation the S matrix is then given by[32]

$$\tilde{S}(E) = -\frac{\alpha_3(k)}{\beta_3(k)}, \quad k = E^{1/2}.$$

We now have the ingredients for the calculation of the scattering resonances and the corresponding approximate resonance states. Note first that $\alpha_3(k)$ and $\beta_3(k)$ can be extended to analytic functions in the complex k plane and as a result the poles of the analytic continuation of $S(E)$ to the lower half-plane (i.e., across the square root cut along the positive real axis) are identified with zeros of the function $\beta_3(k)$. For a resonance at a point $z=\mu_j$ in the lower half-plane below the positive real axis we set $\mu_j=E_{\mu_j}-i\Gamma_{\mu_j}/2$, with E_{μ_j} being the resonance energy and Γ_{μ_j} its width.

Using Eq. (27) and the expression for the outgoing Lippmann–Schwinger eigenfunctions $\langle x|E^-\rangle$, Eqs. (44)–(46), the zeroth order approximate resonance states for the square barrier problem can be calculated numerically. Considering a larger number of resonance poles we are able to calculate higher order approximate resonance states using Eq. (30). As an example we consider the three lowest energy resonance poles for barrier parameters $a=2$, $b=3$, and $V_0=10$. These poles are located at $\mu_1=1.8213-i0.0023$, $\mu_2=7.0237-i0.0564$, and $\mu_3=14.2336-i0.8923$. The zeroth order probability densities $|\psi_{\mu_j}^{(0)}(x)|^2$, $j=1,2,3$ for these poles are shown as dashed lines in Fig. 1 while the solid lines on the same figure correspond to the ninth order probability densities $|\psi_{\mu_j}^{(9)}(x)|^2$, $j=1,2,3$, where the ten lowest energy resonances μ_j, $j=1,\ldots,10$ are taken into account in Eq. (30). We observe the significant change in the probability density profile between the zeroth and ninth order approximate resonance states for the resonance μ_3, whose energy is higher then the barrier's energy, while the lower two states are essentially unchanged. Numerical calculations show that approximate resonance states converge in L^2 norm to a limiting state as a function of the order of approximation. An example is provided in Fig. 2 which shows the probability density $|\psi_{\mu_3'}^{(n)}(x)|^2$ for the resonance $\mu_3'=17.4652-i4.4029$, at barrier parameters $a=2$, $b=2.1$, and $V_0=10$, and for the orders $n=0,8,9$. At present, a rigorous criterion for the rate of convergence of approximate resonance states as a function of order is not yet established.

Turning to a consideration of the time evolution of survival probabilities for resonances of the square barrier model, we first recall the fact that the time evolution of the survival probabilities of higher order approximate resonance states corresponding to the same resonance pole is independent of the order and is, in fact, identical to that of the zeroth order state. Bearing this in mind we may omit in our notation any indication of the region Σ or the order n and set $A_{\psi_{\mu_j}}(t)\equiv A_{\psi_{\mu_j}^{\Sigma}}(t) = A_{\psi_{\mu_j}^{(n)}}(t)$. The time dependence of the survival probablility $|A_{\psi_{\mu_1}}(t)|^2$ for the states coresponding to

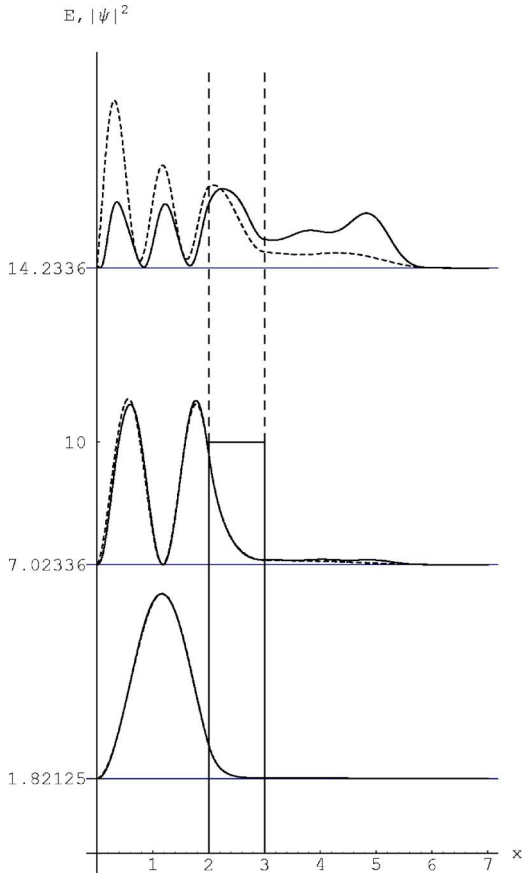

FIG. 1. Probability densities of approximate resonance states $\psi^{(n)}_{\mu_j}$, $j=1,2,3$ for $a=2$, $b=3$, and $V_0=10$. Dashed lines—$|\psi^{(0)}_{\mu_j}(x)|^2$, $j=1,2,3$. Solid lines—$|\psi^{(9)}_{\mu_j}(x)|^2$, $j=1,2,3$.

the lower resonance in Fig. 1 is shown as a solid line in Fig. 3. The time evolution of $|A_{\psi_{\mu_1}}(t)|^2$ follows closely an exact exponential decay law with a decay constant $\Gamma_{\mu_1}=2|\Im(\mu_1)|$. This behavior is reflected in the bound $|R_{\mu_1}(t)|\leqslant 0.028$ on the size of the background term calculated using Theorem 5. The time development of $|A_{\psi_{\mu_1}}(t)|^2$ deviates from the exponential law at a very short

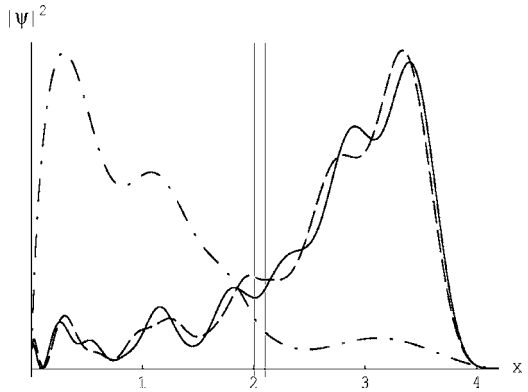

FIG. 2. Probability densities of the approximate resonance states for $\mu_3'=17.4652-i4.4029$. Dot-dahsed line—$|\psi^{(0)}_{\mu_3'}(x)|^2$, dashed line—$|\psi^{(8)}_{\mu_3'}(x)|^2$, and solid line—$|\psi^{(9)}_{\mu_3'}(x)|^2$.

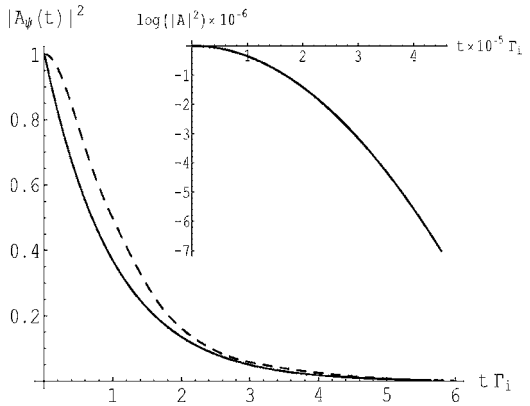

FIG. 3. Survival probabilities: Solid line—$|A_{\psi_{\mu_1}}(t)|^2$ and dashed line—$|A_{\psi_{\mu_3'}}(t)|^2$. The inset shows the short time behavior of $|A_{\psi_{\mu_1}}(t)|^2$.

time scale, as is clearly seen in the insert in Fig. 3. The behavior of the survival probability for the other resonances in Fig. 1 (not shown in Fig. 3) is similar. The short time deviations from exponential decay are related to the known Zeno effect.

The nearly exact exponential decay law of the survival probability $|A_{\psi_{\mu_1}}(t)|^2$ is to be contrasted with the time development of $|A_{\psi_{\mu_3'}}(t)|^2$ for the states in Fig. 2. The survival probability $|A_{\psi_{\mu_3'}}(t)|^2$ is described by the dashed line in Fig. 3. Deviations from an exponential decay law in this case are evidently larger. This conforms with the results of Theorem 5 which produces the larger bound $|R_{\mu_3'}(t)| \leqslant 0.422$.

V. SUMMARY

The semigroup decomposition formalism makes use of the fundamental mathematical theory underlying the structure of the Lax–Phillips scattering theory, i.e., the functional model for $C_{\cdot 0}$ contractive semigroups, for the description of the time evolution of resonances. If the S matrix is meromorphic in a region Σ and is known to have resonance poles there at points $z=\mu_1,\ldots,\mu_n \in \Sigma$, the semigroup formalism allows for the association of a unique Hilbert space state $\psi^{\Sigma}_{\mu_j}(x) \in \mathcal{H}_{\mathrm{ac}}(\mathbf{H})$, $j=1,\ldots,n$ with each resonance. The states $\psi^{\Sigma}_{\mu_j}(x)$, called approximate resonance states, define the decomposition of matrix elements of the evolution and are associated with its semigroup part. Theorem 5 provides an upper bound on the size of the remaining background term. Depending on one's knowledge of the location of the resonance poles it is possible to calculate approximate resonance states of different orders. Numerical calculations show that the sequence of approximate resonance states converge in L^2 norm to a limiting function as a function of the order. However, rigorous criteria for the rate of convergence are needed. Another possible course of further investigation involves the study of relations between known frameworks for the treatment of the problem of resonances, such as the rigged Hilbert space method and the use of dilation analyticity and the formalism discussed in the present paper.

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Extension of the Conley-Zehnder index, a product formula, and an application to the Weyl representation of metaplectic operators

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The aim of this paper is to express the Conley-Zehnder index of a symplectic path in terms of an index due to Leray and which has been studied by one of us in a previous work. This will allow us to prove a formula for the Conley-Zehnder index of the product of two symplectic paths in terms of a symplectic Cayley transform. We apply our results to a rigorous study of the Weyl representation of metaplectic operators, which plays a crucial role in the understanding of semiclassical quantization of Hamiltonian systems exhibiting chaotic behavior.
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I. INTRODUCTION

Consider a Hamiltonian system in $\mathbb{R}^{2n}$

$$\dot{z} = J\partial_z H(z,t), \quad z=(x,p), \quad J=\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{1}$$

and denote by (f_t^H) the flow it determines; we assume that the symplectomorphisms f_t^H are globally defined for each $t\in\mathbb{R}$. Set $f=f_1^H$; if for every fixed point z of f the Jacobian matrix of f satisfies

$$\det(Df(z)-I)\neq 0, \tag{2}$$

one says that the one-periodic solutions of Eq. (1) are *nondegenerate*. [*Nota bene:* condition (2) is very strong; for instance, if H is time independent, it is never satisfied!] Now set $z(t)=f_t^H(z)$ and consider the linearized Hamiltonian system along $t\mapsto z(t)$; its time evolution is governed by the linear differential equation

$$\dot{u} = JD^2H(z,t)u, \tag{3}$$

whose flow (s_t) consists of the symplectic matrices $s_t=Df_t^H(z)$. The path $\Sigma: t\mapsto s_t$, $t\in[0,1]$, thus lies in the symplectic group $\mathrm{Sp}(n)$; it starts from the identity and ends at the "monodromy matrix" $s=Df(z)$. If the nondegeneracy condition (2) holds, one associates to Σ an integer $i_{\mathrm{CZ}}(\Sigma)$, the Conley-Zehnder (CZ) index[2] of the path Σ. The vocation of that index is (loosely speaking) to give an algebraic count of the number of points t_j in the interval $[0, 1]$ for which s_t belongs to the "caustic"

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$$\mathrm{Sp}_0(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) = 0\};$$

that index is "natural" in the sense that it is invariant under homotopy as long as the end point of the path stays in one of the connected sets $\mathrm{Sp}_{\pm}(n)$ defined by

$$\mathrm{Sp}_+(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) > 0\},$$

$$\mathrm{Sp}_-(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) < 0\}.$$

The aim of this paper is twofold. We first set out to prove a formula for the Conley-Zehnder index of the product of two symplectic paths starting from the identity; we will show that if Σ and Σ' are symplectic paths starting from the identity and ending at s and s', respectively, then

$$i_{\mathrm{CZ}}(\Sigma\Sigma') = i_{\mathrm{CZ}}(\Sigma) + i_{\mathrm{CZ}}(\Sigma') + \tfrac{1}{2}\mathrm{sign}(M_s + M_{s'}), \tag{4}$$

where M_s is the "symplectic Cayley transform" of s defined by

$$M_s = \tfrac{1}{2}J(s + I)(s - I)^{-1}.$$

For that purpose we will use an index defined on twice the Maslov bundle, defined by Leray[14] and extended by the first author[7,8] to the nontransversal case; that index is characterized by two simple properties, one cohomological and the other topological. (Dazord[4] has proposed a similar extension in the more general framework of symplectic bundles, using a different approach.) As a by-product of the proof of Eq. (4) we will obtain a natural extension of the Conley-Zehnder index to paths whose end points are in $\mathrm{Sp}_0(n)$. The interest of that extension is more than just academic: as noted above, all nontrivial periodic solutions of Eq. (1) are precisely degenerate when H is time independent; hence this is, indeed, the generic situation.

Second, formula (4) will allow us to identify the phase appearing in the Weyl representation of metaplectic operators with the Conley-Zehnder index of a certain symplectic path mod 4. In fact, the first author has shown in a recent paper[10] that if $S \in \mathrm{Mp}(n)$ has projection s in $\mathrm{Sp}(n)\backslash\mathrm{Sp}_0(n)$, then the operator

$$S = \left(\frac{1}{2\pi\hbar}\right)^n \frac{i^{\nu(s)}}{\sqrt{|\det(s - I)|}} \int e^{(i/2\hbar)\langle M_s z, z\rangle} T(z) d^{2n}z,$$

where $\hbar = h/2\pi$ and

$$T(z_0) = e^{-(i/\hbar)(\langle x_0, D_x\rangle - \langle p_0, x\rangle)}, \quad D_x = -i\partial_x$$

is the Heisenberg-Weyl operator that lies in the metaplectic group $\mathrm{Mp}(n)$ (and has projection s) provided that the integer $\nu(s)$ is chosen so that

$$\frac{1}{\pi}\arg\det(s - I) \equiv -\nu(s) + n \mod 2.$$

This formula identifies $\nu(s)$ with $i_{\mathrm{CZ}}(\Sigma)$ mod 2, where Σ is any continuous path in $\mathrm{Sp}(n)$ joining I to s. We will prove that we actually have

$$\nu(s) = i_{\mathrm{CZ}}(\Sigma) \mod 4 \tag{5}$$

for a natural choice of the path Σ. This formula might have, as a practical consequence, a better understanding of trace formulas in semiclassical mechanics ("Gutzwiller's formula," see Refs. 12 and 17), where the Weyl representation of metaplectic operators plays a crucial role (see Ref. 16 and the references therein for recent advances).

A *caveat:* the statement of our two main results, formulas (4) and (5), is deceptively simple. The proofs of these formulas are, however, quite technical; they require the full power of the machinery of the Leray index[14] that one of us has developed elsewhere.[6–8,11] One might, of course,

hope that other more powerful methods would lead to the same results in a more straightforward and economical way. Such an eventuality is, of course, welcome, but as far as we can see the only alternative approach would be to use the path intersection theory developed by Robbin and Salamon[18] (these authors in effect express the Conley-Zehnder in terms of the symplectic intersection index they define). However, as was shown in Ref. 9, the Leray and Robbin-Salamon indices are equivalent and easily deduced from each other; in that sense the Leray index thus appears as a fundamental "master index" in Lagrangian and symplectic path intersection theory. We observe that Cushman and Duistermaat[3] and Duistermaat[5] also have addressed the question of the index of the iteration of periodic orbits; the methods these authors use are different from ours, and might perhaps be adapted to yield formula (4).

This paper is structured as follows: In Sec. II we review previous results[7,8,11] on Lagrangian and symplectic Maslov indices, generalizing those of Leray.[14] An excellent comparative study of the indices used here with other indices appearing in the literature can be found in Cappell *et al.*[1] In Sec. III we recall the axiomatic presentation of the Conley-Zehnder index following Hofer *et al.*[13] We thereafter study the properties of the symplectic Cayley transform that will be needed in the rest of the section. We then define an integer-values function ν on the universal covering of $\mathrm{Sp}(n)$, which is identified with the Conley-Zehnder index. In Sec. IV we apply the previous results to the study of the phase of the Weyl representation of metaplectic operators.

We will denote by σ the standard symplectic form on $\mathbb{R}^{2n}=\mathbb{R}^n_x\times\mathbb{R}^n_p$:

$$\sigma(z,z')=\langle p,x'\rangle-\langle p',x\rangle \quad \text{if } z=(x,p),\ z'=(x'p'),$$

that is, in matrix form

$$\sigma(z,z')=\langle Jz,z'\rangle,\quad J=\begin{bmatrix}0 & I\\ -I & 0\end{bmatrix}.$$

The real symplectic group $\mathrm{Sp}(n)$ consists of all linear automorphisms s of $\mathbb{R}^{2n}$ such that $\sigma(sz,sz')=\sigma(z,z')$ for all z, z'. Equivalently,

$$s\in\mathrm{Sp}(n)\Leftrightarrow s^TJs=sJs^T=J.$$

$\mathrm{Sp}(n)$ is a connected Lie group and $\pi_1[\mathrm{Sp}(n)]\equiv(\mathbb{Z},+)$. We denote by $\mathrm{Lag}(n)$ the Lagrangian Grassmannian of $(\mathbb{R}^{2n},\sigma)$, that is, $\ell\in\mathrm{Lag}(n)$ if and only ℓ is an n plane in $\mathbb{R}^{2n}$ on which σ vanishes identically. We will write $\ell_X=\mathbb{R}^n_x\times 0$ and $\ell_P=0\times\mathbb{R}^n_p$.

If (E,ω) is a symplectic space, the coverings of order $q=2,\ldots,\infty$ of $\mathrm{Sp}(E,\omega)$ and $\mathrm{Lag}(E,\omega)$ are denoted $\pi_q:\mathrm{Sp}_q(E,\omega)\to\mathrm{Sp}(E,\omega)$ and $\pi_q:\mathrm{Lag}_q(E,\omega)\to\mathrm{Lag}(E,\omega)$.

II. WALL-KASHIWARA AND LERAY INDICES

We begin by reviewing the notion of signature of a triple of Lagrangian planes.

A. The Wall-Kashiwara index

Let (ℓ,ℓ',ℓ'') be a triple of elements of $\mathrm{Lag}(E,\omega)$; by definition[1,15,20] the Wall-Kashiwara index (or signature) $\tau(\ell,\ell',\ell'')$ is the signature of the quadratic form

$$Q(z,z',z'')=\sigma(z,z')+\sigma(z',z'')+\sigma(z'',z')$$

on $\ell\oplus\ell'\oplus\ell''$. The index τ is totally antisymmetric:

$$\tau(\ell,\ell',\ell'')=-\tau(\ell',\ell,\ell'')=-\tau(\ell,\ell'',\ell')=-\tau(\ell'',\ell',\ell),$$

it is a symplectic invariant:

$$\tau(s\ell,s\ell',s\ell'')=\tau(\ell,\ell',\ell'')\quad \text{for } s\in\mathrm{Sp}(E,\omega),$$

and it has the following essential cocycle property:

$$\tau(\ell,\ell',\ell'') - \tau(\ell',\ell'',\ell''') + \tau(\ell',\ell'',\ell''') - \tau(\ell',\ell'',\ell''') = 0. \tag{6}$$

Moreover, its values mod 2 are given by the following formula:

$$\tau(\ell,\ell',\ell'') \equiv n + \dim \ell \cap \ell' + \dim \ell' \cap \ell'' + \dim \ell'' \cap \ell \mod 2. \tag{7}$$

The Wall-Kashiwara index measures the relative position of three Lagrangian planes; for instance, if $\ell_X = \mathbb{R}^n \times 0$, $\ell_P = 0 \times \mathbb{R}^n$, and $\ell_M = \{(x,Mx) : x \in X\}$ $(M = M^T)$, then $\tau(\ell_P,\ell_M,\ell_X) = \operatorname{sign} M$.

Let $(E,\omega) = (E' \oplus E'', \omega' \oplus \omega'')$; identifying $\mathrm{Lag}(E',\omega') \oplus \mathrm{Lag}(E'',\omega'')$ with a subset of $\mathrm{Lag}(E,\omega)$, we have the additivity formula

$$\tau(\ell_1 \oplus \ell_2, \ell_1' \oplus \ell_2', \ell_1'' \oplus \ell_2'') = \tau'(\ell_1,\ell_1',\ell_1'') + \tau''(\ell_2,\ell_2',\ell_2''), \tag{8}$$

where τ' and τ'' are the Wall-Kashiwara indices on $\mathrm{Lag}(E',\omega')$ and $\mathrm{Lag}(E'',\omega'')$, respectively.

The following lemma will be helpful in our study of the Conley-Zehnder index:

Lemma 1: (i) If $\ell \cap \ell'' = 0$, then $\tau(\ell,\ell',\ell'')$ is the signature of the quadratic form

$$Q'(z') = \omega(\mathrm{Pr}_{\ell\ell''}z', z') = \omega(z', \mathrm{Pr}_{\ell''\ell}z')$$

on ℓ', where $\mathrm{Pr}_{\ell\ell''}$ is the projection onto ℓ along ℓ'' and $\mathrm{Pr}_{\ell''\ell} = I - \mathrm{Pr}_{\ell\ell''}$ is the projection on ℓ'' along ℓ. (ii) Let (ℓ,ℓ',ℓ'') be a triple of Lagrangian planes such that an $\ell = \ell \cap \ell' + \ell \cap \ell''$. Then $\tau(\ell,\ell',\ell'') = 0$.

(See, e.g., Ref. 15 for a proof.)

B. The Leray index

Let $\mathrm{Lag}_\infty(E,\omega)$ be the universal covering of $\mathrm{Lag}(E,\omega)$. The Leray index is the unique mapping

$$\mu : (\mathrm{Lag}_\infty(E,\omega))^2 \to \mathbb{Z}$$

having the two following properties:[7,8]

- μ is locally constant on each set $\{(\ell_\infty,\ell_\infty') : \dim \ell \cap \ell' = k\}$ $(0 \leqslant k \leqslant n)$.
- For all ℓ_∞, ℓ_∞', ℓ_∞'' in $\mathrm{Lag}_\infty(E,\omega)$ with projections ℓ, ℓ', ℓ'', we have

$$\mu(\ell_\infty,\ell_\infty') - \mu(\ell_\infty,\ell_\infty'') + \mu(\ell_\infty',\ell_\infty'') = \tau(\ell,\ell',\ell''). \tag{9}$$

The Leray index has, in addition, the following properties:

$$\mu(\ell_\infty,\ell_\infty') \equiv n + \dim \ell \cap \ell' \mod 2 \tag{10}$$

$\left(n = \frac{1}{2}\dim E\right)$ and

$$\mu(\beta^r \ell_\infty, \beta^{r'} \ell_\infty') = \mu(\ell_\infty,\ell_\infty') + 2(r - r') \tag{11}$$

for all integers r and r'; here β denotes the generator of $\pi_1[\mathrm{Lag}(E,\omega)] \equiv (\mathbb{Z},+)$, whose image in $\mathbb{Z}$ is +1. From the dimensional additivity property [Eq. (8)] of τ, it immediately follows that if $\ell_{1,\infty} \oplus \ell_{2,\infty}$ and $\ell_{1,\infty}' \oplus \ell_{2,\infty}'$ are in

$$\mathrm{Lag}_\infty(E',\omega') \oplus \mathrm{Lag}_\infty(E'',\omega'') \subset \mathrm{Lag}_\infty(E,\omega),$$

then

$$\mu(\ell_{1,\infty} \oplus \ell_{2,\infty}, \ell_{1,\infty}' \oplus \ell_{2,\infty}') = \mu'(\ell_{1,\infty},\ell_{1,\infty}') + \mu''(\ell_{2,\infty},\ell_{2,\infty}'), \tag{12}$$

where μ' and μ'' are the Leray indices on $\mathrm{Lag}_\infty(E',\omega')$ and $\mathrm{Lag}_\infty(E'',\omega'')$, respectively.

When (E,ω) is the standard symplectic space $(\mathbb{R}^{2n},\sigma)$, one identifies $\mathrm{Lag}(E,\omega) = \mathrm{Lag}(n)$ with the set

$$W(n,\mathbb{C}) = \{w \in U(n,\mathbb{C}) : w = w^T\}$$

of symmetric unitary matrices by associating to $\ell = u\ell_P$ ($u \in U(n,\mathbb{C})$) the matrix $w = uu^T$ ("Souriau mapping,"[19] see Ref. 11 for a detailed description and further properties). The Maslov bundle $\mathrm{Lag}_\infty(n)$ is identified with

$$W_\infty(n,\mathbb{C}) = \{(w,\theta) : w \in W(n,\mathbb{C}),\ \det w = e^{i\theta}\},$$

the projection $\pi^{\mathrm{Lag}} : \ell_\infty \mapsto \ell$ becoming $(w,\theta) \mapsto w$. The Leray index is then calculated as follows:

- If $\ell \cap \ell' = 0$, then

$$\mu(\ell_\infty, \ell'_\infty) = \frac{1}{\pi}[\theta - \theta' + i\,\mathrm{Tr}\log(-w(w')^{-1}\,] \tag{13}$$

  [the transversality condition $\ell \cap \ell' = 0$ is equivalent to $-w(w')^{-1}$ having no negative eigenvalue].
- If $\ell \cap \ell' \neq 0$, one chooses any ℓ'' such that $\ell \cap \ell'' = \ell' \cap \ell'' = 0$ and one then calculates $\mu(\ell_\infty, \ell'_\infty)$ using the formula (9), the values of $\mu(\ell_\infty, \ell''_\infty)$ and $\mu(\ell'_\infty, \ell''_\infty)$ being given by Eq. (13). (The cocycle property [Eq. (6)] of τ guarantees that the result does not depend on the choice of ℓ''.)

C. The relative Maslov indices on Sp(E,ω)

We begin by recalling the definition of the Maslov index for loops in $\mathrm{Sp}(n)$. Let γ be a continuous mapping $[0,1] \to \mathrm{Sp}(n)$ such that $\gamma(0) = \gamma(1)$, and set $\gamma(t) = s_t$. Then $U_t = (s_t s_t)^{-1/2} s_t$ is the orthogonal part in the polar decomposition of s_t:

$$U_t \in \mathrm{Sp}(n) \cap \mathrm{O}(2n,\mathbb{R}).$$

Let us denote by u_t the image $\iota(U_t)$ of U_t in $\mathrm{U}(n,\mathbb{C})$:

$$\iota(U_t) = A + iB \quad \text{if } U = \begin{bmatrix} A & -B \\ B & A \end{bmatrix}$$

and set $\rho(s_t) = \det u_t$. The Maslov index of γ is, by definition, the degree of the loop $t \mapsto \rho(s_t)$ in S^1:

$$m(\gamma) = \deg[t \mapsto \det(\iota(U_t))], \quad 0 \leqslant t \leqslant 1.$$

Let α be the generator of $\pi_1[\mathrm{Sp}(E,\omega)] \equiv (\mathbb{Z},+)$, whose image in $\mathbb{Z}$ is $+1$; if γ is homotopic to α^r, then

$$m(\gamma) = m(\alpha^r) = 2r. \tag{14}$$

The definition of the Maslov index can be extended to arbitrary paths in $\mathrm{Sp}(E,\omega)$ using the properties of the Leray index. This is done as follows: let $\ell = \pi_{\mathrm{Lag}}(\ell_\infty) \in \mathrm{Lag}(E,\omega)$; we define the Maslov index of $s_\infty \in \mathrm{Sp}_\infty(E,\omega)$ relative to ℓ by

$$\mu_\ell(s_\infty) = \mu(s_\infty \ell_\infty, \ell_\infty); \tag{15}$$

one shows (see Refs. 7 and 8) that the right-hand side only depends on the projection ℓ of ℓ_∞, justifying the notation.

Here are three fundamental properties of the relative Maslov index; we will need all of them to study the Conley-Zehnder index:

- *Product:* For all s_∞, s'_∞ in $\mathrm{Sp}_\infty(E,\omega)$ we have

$$\mu_\ell(s_\infty s'_\infty) = \mu_\ell(s_\infty) + \mu_\ell(s'_\infty) + \tau(\ell, s\ell, ss'\ell). \tag{16}$$

- *Action of* $\pi_1[\mathrm{Sp}(n)]$: We have

$$\mu_\ell(\alpha^r s_\infty) = \mu_\ell(s_\infty) + 4r \tag{17}$$

for all $r \in \mathbb{Z}$.

- *Topological property:* The mapping $(s_\infty, \ell) \mapsto \mu_\ell(s_\infty)$ is locally constant on each of the sets

$$\{(s_\infty, \ell) : \dim s\ell \cap \ell = k\} \subset \mathrm{Sp}_\infty(E,\omega) \times \mathrm{Lag}(E,\omega) \quad (0 \leqslant k \leqslant n). \tag{18}$$

The first two properties readily follow from, respectively, Eqs. (9) and (11). The third follows from the fact that the Leray index is locally constant on the sets $\{(\ell_\infty, \ell'_\infty) : \dim \ell \cap \ell' = k\}$. Note that Eq. (17) implies that

$$\mu_\ell(\alpha^r) = 4r = 2m(\alpha^r),$$

hence the restriction of any of the μ_ℓ to loops γ in $\mathrm{Sp}(E,\omega)$ is *twice* the Maslov index $m(\gamma)$ defined above; it is therefore sometimes advantageous to use the index m_ℓ defined by

$$m_\ell(s_\infty) = \tfrac{1}{2}(\mu_\ell(s_\infty) + n + \dim(s\ell \cap \ell)), \tag{19}$$

where $n = \frac{1}{2} \dim E$. We will call $m_\ell(s_\infty)$ the *reduced* (relative) Maslov index. In view of the congruence [Eq. (10)], it is an integer; the properties of m_ℓ are obtained *mutatis mutandis* from those of μ_ℓ. For instance, property (16) becomes

$$m_\ell(s_\infty s'_\infty) = m_\ell(s_\infty) + m_\ell(s'_\infty) + \mathrm{Inert}(\ell, s\ell, ss'\ell), \tag{20}$$

where Inert is the index of inertia of a triple (ℓ, ℓ', ℓ'') defined by

$$\mathrm{Inert}(\ell,\ell',\ell'') = \tfrac{1}{2}(\tau(\ell,\ell',\ell'') + n + \dim \ell \cap \ell' - \dim \ell' \cap \ell'' + \dim \ell'' \cap \ell); \tag{21}$$

in view of Eq. (7), it is an integer. [When the Lagrangian planes ℓ, ℓ', ℓ'' are pairwise transverse, it follows from the first part of Lemma 1 that $\mathrm{Inert}(\ell,\ell',\ell'')$ coincides with the index of inertia defined by Leray;[14] see Refs. 7, 8, and 11.]

It follows from the cocycle property of τ that the Maslov indices corresponding to two choices ℓ and ℓ' are related by the formula

$$\mu_\ell(s_\infty) - \mu_{\ell'}(s_\infty) = \tau(s\ell, \ell, \ell') - \tau(s\ell, s\ell', \ell'); \tag{22}$$

similarly,

$$m_\ell(s_\infty) - m_{\ell'}(s_\infty) = \mathrm{Inert}(s\ell, \ell, \ell') - \mathrm{Inert}(s\ell, s\ell', \ell'). \tag{23}$$

Assume that $(E,\omega) = (E' \oplus E'', \omega' \oplus \omega'')$ and $\ell' \in \mathrm{Lag}(E',\omega')$, $\ell'' \in \mathrm{Lag}(E'',\omega'')$; the additivity property (12) of the Leray index implies that if $s'_\infty \in \mathrm{Sp}_\infty(E',\omega')$, $s''_\infty \in \mathrm{Sp}_\infty(E'',\omega'')$, then

$$\mu_{\ell' \oplus \ell''}(s'_\infty \oplus s''_\infty) = \mu_{\ell'}(s'_\infty) + \mu_{\ell_2}(s''_\infty), \tag{24}$$

where $\mathrm{Sp}_\infty(E',\omega') \oplus \mathrm{Sp}_\infty(E'',\omega'')$ is identified in the obvious way with a subgroup of $\mathrm{Sp}_\infty(E,\omega)$. A similar property holds for the reduced relative Maslov index m_ℓ.

III. EXTENSION OF i_{CZ} AND PRODUCT FORMULA

This section is central in this paper; the main result is Theorem 1, where we prove a product formula for the Conley-Zehnder index.

A. Review of the Conley-Zehnder index

Let Σ be a continuous path $[0,1] \to \mathrm{Sp}(n)$ such that $\Sigma(0) = I$ and $\det(\Sigma(1) - I) \neq 0$. The sets

$$\mathrm{Sp}_0(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) = 0\},$$

$$\mathrm{Sp}^+(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) > 0\},$$

$$\mathrm{Sp}^-(n) = \{s \in \mathrm{Sp}(n) : \det(s - I) < 0\}$$

partition $\mathrm{Sp}(n)$, and $\mathrm{Sp}^+(n)$ and $\mathrm{Sp}^-(n)$ are, moreover, arcwise connected. The symplectic matrices $s^+ = -I$ and

$$s^- = \begin{bmatrix} L & 0 \\ 0 & L^{-1} \end{bmatrix}, \quad L = \mathrm{diag}[2, -1, \ldots, -1]$$

belong to $\mathrm{Sp}^+(n)$ and $\mathrm{Sp}^-(n)$, respectively (see Refs. 2 and 13).

Let us denote by $C_\pm(2n, \mathbb{R})$ the space of all paths $\Sigma : [0,1] \to \mathrm{Sp}(n)$ with $\Sigma(0) = I$ and $\Sigma(1) \in \mathrm{Sp}^\pm(n)$. Any such path can be extended into a path $\widetilde{\Sigma} : [0,2] \to \mathrm{Sp}(n)$ such that $\widetilde{\Sigma}(t) \in \mathrm{Sp}^\pm(n)$ for $1 \leqslant t \leqslant 2$ and $\widetilde{\Sigma}(2) = s^+$ or $\widetilde{\Sigma}(2) = s^-$. Let ρ be the mapping $\mathrm{Sp}(n) \to S^1$, $\rho(s_t) = \det u_t$, used in the definition of the Maslov index for symplectic loops. The Conley-Zehnder index of Σ is by definition the winding number of the loop $(\rho \circ \widetilde{\Sigma})^2$ in S^1:

$$i_{\mathrm{CZ}}(\Sigma) = \deg[t \mapsto (\rho(\widetilde{\Sigma}(t)))^2, 0 \leqslant t \leqslant 2].$$

It turns out that $i_{\mathrm{CZ}}(\Sigma)$ is invariant under homotopy as long as the end point $s = \Sigma(1)$ remains in $\mathrm{Sp}^\pm(n)$; in particular, it does not change under homotopies with fixed end points so we may view i_{CZ} as defined on the subset

$$\mathrm{Sp}^*_\infty(n) = \{s_\infty \in \mathrm{Sp}_\infty(n) : \det(s - I) \neq 0\}$$

of the universal covering group $\mathrm{Sp}_\infty(n)$. With this convention one proves[13] that the Conley-Zehnder index is the unique mapping $i_{\mathrm{CZ}} : \mathrm{Sp}^*_\infty(n) \to \mathbb{Z}$ having the following properties:

(CZ_1) *Antisymmetry:* For every s_∞ we have

$$i_{\mathrm{CZ}}(s_\infty^{-1}) = -i_{\mathrm{CZ}}(s_\infty),$$

where s_∞^{-1} is the homotopy class of the path $t \mapsto s_t^{-1}$.

(CZ_2) *Continuity:* Let Σ be a symplectic path representing s_∞ and Σ' a path joining s to an element s' belonging to the same component $\mathrm{Sp}^\pm(n)$ as s. Let s'_∞ be the homotopy class of $\Sigma * \Sigma'$. We have

$$i_{\mathrm{CZ}}(s_\infty) = i_{\mathrm{CZ}}(s'_\infty).$$

(CZ_3) *Action of* $\pi_1[\mathrm{Sp}(n)]$:

$$i_{\mathrm{CZ}}(\alpha^r s_\infty) = i_{\mathrm{CZ}}(s_\infty) + 2r$$

for every $r \in \mathbb{Z}$.

We observe that these three properties are characteristic of the Conley-Zehnder index in the sense that any other function $i'_{\mathrm{CZ}} : \mathrm{Sp}^*_\infty(n) \to \mathbb{Z}$ satisfying them must be identical to i_{CZ}. Set, in fact, $\delta = i_{\mathrm{CZ}} - i'_{\mathrm{CZ}}$. In view of ($\mathrm{CZ}_3$) we have $\delta(\alpha^r s_\infty) = \delta(s_\infty)$ for all $r \in \mathbb{Z}$, hence δ is defined on $\mathrm{Sp}^*(n) = \mathrm{Sp}^+(n) \cup \mathrm{Sp}^-(n)$ so that $\delta(s_\infty) = \delta(s)$, where $s = s_1$, the end point of the path $t \mapsto s_t$. Property (CZ_2) implies that this function $\mathrm{Sp}^*(n) \to \mathbb{Z}$ is constant on both $\mathrm{Sp}^+(n)$ and $\mathrm{Sp}^-(n)$. We next observe that since $\det s = 1$, we have $\det(s^{-1} - I) = \det(s - I)$ so that s and s^{-1} always belong to the same set $\mathrm{Sp}^+(n)$ or $\mathrm{Sp}^-(n)$ if $\det(s - I) \neq 0$. Property (CZ_1) then implies that δ must be zero on both $\mathrm{Sp}^+(n)$ or $\mathrm{Sp}^-(n)$.

Two other noteworthy properties of the Conley-Zehnder are as follows:

(CZ_4) *Normalization:* Let J_1 be the standard symplectic matrix in $\mathrm{Sp}(1)$. If s_1 is the path $t \to e^{\pi t J_1}$ $(0 \leqslant t \leqslant 1)$ joining I to $-I$ in $\mathrm{Sp}(1)$, then $i_{\mathrm{CZ},1}(s_{1,\infty}) = 1$ [$i_{\mathrm{CZ},1}$ the Conley-Zehnder index on $\mathrm{Sp}(1)$].

(CZ_5) *Dimensional additivity:* If $s_{1,\infty} \in \mathrm{Sp}^*_\infty(n_1)$, $s_{2,\infty} \in \mathrm{Sp}^*_\infty(n_2)$, $n_1 + n_2 = n$, then

$$i_{\mathrm{CZ}}(s_{1,\infty} \oplus s_{2,\infty}) = i_{\mathrm{CZ},1}(s_{1,\infty}) + i_{\mathrm{CZ},2}(s_{2,\infty}),$$

where $i_{\mathrm{CZ},j}$ is the Conley-Zehnder index on $\mathrm{Sp}(n_j)$, $j=1,2$.

B. Symplectic Cayley transform

If $s \in {}^*\mathrm{Sp}^*(n)$ we call the matrix

$$M_s = \tfrac{1}{2}J(s+I)(s-I)^{-1} \tag{25}$$

the "symplectic Cayley transform of s." Equivalently,

$$M_s = \tfrac{1}{2}J + J(s-I)^{-1}. \tag{26}$$

It is straightforward to check that M_s always is a symmetric matrix: $M_s = M_s^T$ (it suffices for this to use the equality $s^T J s = sJs^T = J$).

The symplectic Cayley transform has, in addition, the following properties, which are interesting by themselves:

Lemma 2: (i) We have

$$(M_s + M_{s'})^{-1} = -(s'-I)(ss'-I)^{-1}(s-I)J \tag{27}$$

and the symplectic Cayley transform of the product ss' is (when defined) given by

$$M_{ss'} = M_s + (s^T - I)^{-1}J(M_s + M_{s'})^{-1}J(s-I)^{-1}. \tag{28}$$

(ii) The symplectic Cayley transform of s and s^{-1} are related by the formula

$$M_{s^{-1}} = -M_s. \tag{29}$$

Proof: (i) We begin by noting that Eq. (26) implies that

$$M_s + M_{s'} = J(I + (s-I)^{-1} + (s'-I)^{-1}), \tag{30}$$

hence the identity Eq. (27). In fact, writing $ss'-I = s(s'-I)+s-I$, we have

$$\begin{aligned}
&(s'-I)(ss'-I)^{-1}(s-I) \\
&\quad = (s'-I)(s(s'-I)+s-I)^{-1}(s-I) = ((s-I)^{-1}s(s'-I)(s'-I)^{-1} + (s'-I)^{-1})^{-1} \\
&\quad = ((s-I)^{-1}s + (s'-I)^{-1}) = I + (s-I)^{-1} + (s'-I)^{-1};
\end{aligned}$$

the equality Eq. (27) follows in view of Eq. (30). Let us prove Eq. (28); equivalently,

$$M_s + M = M_{ss'}, \tag{31}$$

where M is the matrix defined by

$$M = (s^T - I)^{-1}J(M_s + M_{s'})^{-1}J(s-I)^{-1},$$

that is, in view of Eq. (27),

$$M = (s^T - I)^{-1}J(s'-I)(ss'-I)^{-1}.$$

Using the obvious relations $s^T = -Js^{-1}J$ and $(-s^{-1}+I)^{-1} = s(s-I)^{-1}$ we have

$$\begin{aligned}
M &= (s^T - I)^{-1}J(s'-I)(ss'-I)^{-1} = -J(-s^{-1}+I)^{-1}(s'-I)(ss'-I)^{-1} \\
&= -Js(s-I)^{-1}(s'-I)(ss'-I)^{-1},
\end{aligned}$$

that is, writing $s = s - I + I$,

$$M = -J(s'-I)(ss'-I)^{-1} - J(s-I)^{-1}(s'-I)(ss'-I)^{-1}.$$

Replacing M_s by its value [Eq. (26)] we have

$$M_s + M = J\left(\tfrac{1}{2}I + (s-I)^{-1} - (s'-I)(ss'-I)^{-1} - (s-I)^{-1}(s'-I)(ss'-I)^{-1}\right);$$

noting that

$$(s-I)^{-1} - (s-I)^{-1}(s'-I)(ss'-I)^{-1} = (s-I)^{-1}(ss'-I-s'+I)\ (ss'-I)^{-1}),$$

that is,

$$(s-I)^{-1} - (s-I)^{-1}(s'-I)(ss'-I)^{-1} = (s-I)^{-1}(ss'-s')(ss'-I)^{-1} = \ s'(ss'-I)^{-1}),$$

we get

$$M_s + M = J\left(\tfrac{1}{2}I - (s'-I)(ss'-I)^{-1} + s'(ss'-I)^{-1}\right) = J\left(\tfrac{1}{2}I + (ss'-I)^{-1}\right) = M_{ss'},$$

which we set out to prove.

(ii) Formula (29) follows from the sequence of equalities

$$M_{s^{-1}} = \tfrac{1}{2}J + J(s^{-1}-I)^{-1} = \tfrac{1}{2}J - Js(s-I)^{-1} = \tfrac{1}{2}J - J(s-I+I)(s-I)^{-1} = -\tfrac{1}{2}J - J(s-I)^{-1} = -M_s.$$

■

C. The index $\nu(s_\infty)$

We define on $\mathbb{R}^{2n}\oplus\mathbb{R}^{2n}$ a symplectic form $\sigma^\ominus$ by

$$\sigma^\ominus(z_1,z_2;z_1',z_2') = \sigma(z_1,z_1') - \sigma(z_2,z_2')$$

and denote by $\mathrm{Sp}^\ominus(2n)$ and $\mathrm{Lag}^\ominus(2n)$ the symplectic group and Lagrangian Grassmannian of $(\mathbb{R}^{2n}\oplus\mathbb{R}^{2n},\sigma^\ominus)$. Let $\mu^\ominus$ be the Leray index on $\mathrm{Lag}^\ominus_\infty(2n)$ and $\mu^\ominus_L$ the Maslov index on $\mathrm{Sp}^\ominus_\infty(2n)$ relative to $L\in\mathrm{Lag}^\ominus(2n)$.

For $s_\infty\in\mathrm{Sp}_\infty(n)$ we define

$$\nu(s_\infty) = \tfrac{1}{2}\mu^\ominus((I\oplus s)_\infty\Delta_\infty,\Delta_\infty), \tag{32}$$

where $(I\oplus s)_\infty$ is the homotopy class in $\mathrm{Sp}^\ominus(2n)$ of the path

$$t\mapsto\{(z,s_tz):z\in\mathbb{R}^{2n}\},\quad 0\leqslant t\leqslant 1$$

and $\Delta=\{(z,z):z\in\mathbb{R}^{2n}\}$ the diagonal of $\mathbb{R}^{2n}\oplus\mathbb{R}^{2n}$. Setting $s_t^\ominus = I\oplus s_t$ we have $s_t^\ominus\in\mathrm{Sp}^\ominus(2n)$, hence formula (32) is equivalent to

$$\nu(s_\infty) = \tfrac{1}{2}\mu^\ominus_\Delta(s_\infty^\ominus), \tag{33}$$

where $\mu^\ominus_\Delta$ is the relative Maslov index on $\mathrm{Sp}^\ominus_\infty(2n)$ corresponding to the choice $\Delta\in\mathrm{Lag}^\ominus(2n)$.

Note that replacing n by $2n$ in the congruence [Eq. (10)] we have

$$\mu^\ominus((I\oplus s)_\infty\Delta_\infty,\Delta_\infty)\equiv\dim((I\oplus s)\Delta\cap\Delta)\mod 2\equiv\dim\mathrm{Ker}(s-I)\mod 2$$

and hence

$$\nu(s_\infty)\equiv\tfrac{1}{2}\dim\mathrm{Ker}(s-I)\mod 1.$$

Since the eigenvalue 1 of s has even multiplicity, $\nu(s_\infty)$ is thus always an integer.

The index ν has the following three important properties; the third is essential for the calculation of the index of repeated periodic orbits (it clearly shows that ν is not, in general, additive).

Proposition 1: (i) For all $s_\infty\in\mathrm{Sp}_\infty(n)$ we have

$$\nu(s_\infty^{-1}) = -\nu(s_\infty), \quad \nu(I_\infty) = 0 \tag{34}$$

[I_∞ *the identity of the group* $\mathrm{Sp}_\infty(n)$]. *(ii) For all* $r \in \mathbb{Z}$ *we have*

$$\nu(\alpha^r s_\infty) = \nu(s_\infty) + 2r, \quad \nu(\alpha^r) = 2r. \tag{35}$$

(iii) Let s_∞ *be the homotopy class of a path* Σ *in* $\mathrm{Sp}(n)$ *joining the identity to* $s \in \mathrm{Sp}^*(n)$, *and let* $s' \in \mathrm{Sp}(n)$ *be in the same connected component* $\mathrm{Sp}^{\pm}(n)$ *as* s. *Then* $\nu(s'_\infty) = \nu(s_\infty)$, *where* s'_∞ *is the homotopy class in* $\mathrm{Sp}(n)$ *of the concatenation of* Σ *and a path joining* s *to* s' *in* $\mathrm{Sp}_0(n)$. *(iv) The restriction of the index* ν *to* $\mathrm{Sp}^*_\infty(n)$ *is the Conley-Zehnder index:*

$$\nu(s_\infty) = i_{\mathrm{CZ}}(s_\infty) \quad \textit{if } \det(s - I) \neq 0. \tag{36}$$

Proof: (i) Formulas (34) immediately follow from the equality $(s_\infty^\ominus)^{-1} = (I \oplus s^{-1})_\infty$ and the antisymmetry of $\mu_\Delta^\ominus$. (ii) Formula (35) follows from the first using Eq. (34). To prove formula (35) it suffices to observe that the generator $I_\infty \oplus \alpha$ of $\pi_1[\mathrm{Sp}^\ominus(2n)]$ corresponds to the generator α of $\pi_1[\mathrm{Sp}(n)]$; in view of property (17) of the Maslov index, it follows that

$$\nu(\alpha^r s_\infty) = \tfrac{1}{2}\mu_\Delta^\ominus((I_\infty \oplus \alpha)^r s_\infty^\ominus) = \tfrac{1}{2}(\mu_\Delta^\ominus(s_\infty^\ominus) + 4r) = \nu(s_\infty) + 2r.$$

(iii) Assume, in fact, that s and s' belong to, say, $\mathrm{Sp}^+(n)$. Let s_∞ be the homotopy class of the path Σ, and Σ' a path joining s to s' in $\mathrm{Sp}^+(n)$ (we parametrize both paths by $t \in [0,1]$). Let $\Sigma'_{t'}$ be the restriction of Σ' to the interval $[0,t']$, $t' \leqslant t$ and $s_\infty(t')$ the homotopy class of the concatenation $\Sigma * \Sigma'_{t'}$. We have $\det(s(t) - I) > 0$ for all $t \in [0,t']$, hence $s_\infty^\ominus(t)\Delta \cap \Delta \neq 0$ as t varies from 0 to 1. It follows from the fact that the $\mu_\Delta^\ominus$ is locally constant on $\{s_\infty^\ominus : s_\infty^\ominus \Delta \cap \Delta = 0\}$ (see Sec. II C) that the function $t \mapsto \mu_\Delta^\ominus(s_\infty^\ominus(t))$ is constant, and hence,

$$\mu_\Delta^\ominus(s_\infty^\ominus) = \mu_\Delta^\ominus(s_\infty^\ominus(0)) = \mu_\Delta^\ominus(s_\infty^\ominus(1)) = \mu_\Delta^\ominus(s_\infty'^\ominus),$$

which was to be proven. (iv) The restriction of ν to $\mathrm{Sp}^*(n)$ satisfies the properties (CZ_1), (CZ_2), and (CZ_3) of the Conley-Zehnder index listed in Sec. III A; we showed that these properties uniquely characterize i_{CZ}. ■

Remark: Formula (36) *allows the calculation of* $i_{\mathrm{CZ}}(\Sigma)$ *in terms of the index* $\nu(s_\infty)$. *That formula, in fact, allows us to define the Conley-Zehnder index of an arbitrary path* Σ *by the formula* $i_{\mathrm{CZ}}(\Sigma) = \nu(s_\infty)$, *where* s_∞ *is the homotopy class in* $\mathrm{Sp}(n)$ *of that path (see the discussion at the end of this paper).*

Let us now state and prove the first main result of this paper.

Theorem 1: *If* s_∞, s'_∞, *and* $s_\infty s'_\infty$ *are such that* $\det(s - I) \neq 0$, $\det(s' - I) \neq 0$, *and* $\det(ss' - I) \neq 0$, *then*

$$\nu(s_\infty s'_\infty) = \nu(s_\infty) + \nu(s'_\infty) + \tfrac{1}{2}\mathrm{sign}(M_s + M_{s'}), \tag{37}$$

where M_s *is the symplectic Cayley transform of* s.

Proof: In view of Eq. (33) and the product property (16) of the Maslov index we have

$$\nu(s_\infty s'_\infty) = \nu(s_\infty) + \nu(s'_\infty) + \tfrac{1}{2}\tau^\ominus(\Delta, s^\ominus\Delta, s^\ominus s'^\ominus\Delta) = \nu(s_\infty) + \nu(s'_\infty) - \tfrac{1}{2}\tau^\ominus(s^\ominus s'^\ominus\Delta, s^\ominus\Delta, \Delta),$$

where $s^\ominus = I \oplus s$, $s'^\ominus = I \oplus s'$, and $\tau^\ominus$ is the signature on the symplectic space $(\mathbb{R}^{2n} \oplus \mathbb{R}^{2n}, \sigma^\ominus)$. The condition $\det(ss' - I) \neq 0$ is equivalent to $s^\ominus s'^\ominus \Delta \cap \Delta = 0$, hence we can apply property (i) in Lemma 1 with $\ell = s^\ominus s'^\ominus \Delta$, $\ell' = s^\ominus \Delta$, and $\ell'' = \Delta$. The projection operator onto $s^\ominus s'^\ominus \Delta$ along Δ is easily seen to be

$$\mathrm{Pr}_{s^\ominus s'^\ominus \Delta, \Delta} = \begin{bmatrix} (I - ss')^{-1} & -(I - ss')^{-1} \\ ss'(I - ss')^{-1} & -ss'(I - ss')^{-1} \end{bmatrix},$$

hence $\tau^\ominus(s^\ominus s'^\ominus \Delta, s^\ominus \Delta, \Delta)$ is the signature of the quadratic form

$$Q(z) = \sigma^{\ominus}(\mathrm{Pr}_{s^{\ominus}s'^{\ominus}\Delta,\Delta}(z,sz);(z,sz)),$$

that is, since $\sigma^{\ominus} = \sigma \ominus \sigma$:

$$\begin{aligned} Q(z) &= \sigma\,((I-ss')^{-1}(I-s)z,z)) - \sigma\,(ss'(I-ss')^{-1}(I-s)z,sz)) \\ &= \sigma\,((I-ss')^{-1}(I-s)z,z)) - \sigma\,(s'(I-ss')^{-1}(I-s)z,z)) = \sigma\,((I-s')(I-ss')^{-1}(I-s)z,z)). \end{aligned}$$

In view of formula (27) in Lemma 2 we have

$$(I-s')(ss'-I)^{-1}(I-s) = (M_s + M_{s'})^{-1}J,$$

hence

$$Q(z) = -\langle (M_s + M_{s'})^{-1}Jz, Jz\rangle$$

and the signature of Q is thus the same as that of

$$Q'(z) = -\langle (M_s + M_{s'})^{-1}z, z\rangle,$$

that is, $-\mathrm{sign}(M_s + M_{s'})$. This proves formula (37). ■

IV. APPLICATION TO THE METAPLECTIC GROUP

The metaplectic group plays a crucial role in quantum mechanics (both in its full-blown version and in its semiclassical formulation). We are going to see that the Conley-Zehnder index automatically appears when one determines the Weyl symbol of metaplectic operators.

A. The group Mp(*n*)

The fundamental group $\pi_1[\mathrm{Sp}(n)]$ being isomorphic to $(\mathbb{Z},+)$, the symplectic group, has covering of all orders; its double covering $\mathrm{Sp}_2(n)$ plays an important role in the literature because it has a faithful representation as a group of unitary operators on $L^2(\mathbb{R}^n)$. This group, the metaplectic group $\mathrm{Mp}(n)$, is generated[11,14] by the quadratic Fourier transforms

$$S_{W,m}f(x) = \left(\frac{1}{2\pi\hbar}\right)^{n/2}\Delta(W)\int e^{(i/\hbar)W(x,x')}f(x')d^n x', \tag{38}$$

where W is a quadratic form on $\mathbb{R}^n \times \mathbb{R}^n$ given by

$$W(x,x') = \tfrac{1}{2}\langle Px,x\rangle - \langle Lx,x'\rangle + \tfrac{1}{2}\langle Qx',x'\rangle \tag{39}$$

with P and Q symmetric and $\det L \neq 0$; the factor in front of the integral in Eq. (38) is

$$\Delta(W) = i^m\sqrt{|\det L|},$$

where m corresponds to a choice of the argument of $\det L$. The covering epimorphism $\pi_{\mathrm{Mp}}:\mathrm{Mp}(n)\to\mathrm{Sp}(n)$ is determined by its restriction to the $S_{W,m}$, and we have

$$(x,p) = \pi_{\mathrm{Mp}}(S_{W,m})(x',p') \Leftrightarrow p = \partial_x W(x,x'), \quad p' = -\partial_{x'}W(x,x')$$

[$s_W = \pi(S_{W,m})$ is the free symplectic matrix generated by the quadratic form W].

Every $S \in \mathrm{Mp}(n)$ can be written (in infinitely many ways[14,8]) as a product $S_{W,m}S_{W',m'}$ and the integer

$$m + m' - \mathrm{Inert}(P' + Q) \equiv m + m' + \mathrm{Inert}(\ell_P, s_W\ell_P, s_W s_{W'}\ell_P) \mod 4$$

does not depend on the choice of factorization $S = S_{W,m}S_{W',m'}$ (see Ref. 6). The class mod 4 of $m+m'-\mathrm{Inert}(P'+Q)$ is denoted by $m(S)$ and called *Maslov index* of $S \in \mathrm{Mp}(n)$. The function $m:\mathrm{Mp}(n)\to\mathbb{Z}_4$ has the following properties:

$$m(S_{W,m}) = \hat{m} \tag{40}$$

and

$$m(SS') = m(S) + m(S') + \widehat{\text{Inert}}(\ell_P, s\ell_P, ss'\ell_P), \tag{41}$$

where $\hat{k}$ is the class mod 4 of $k \in \mathbb{Z}$ and $s = \pi_{\text{Mp}}(S)$; it is related to the relative Maslov index m_{ℓ_p} on $\text{Sp}_\infty(n)$ by

$$m(S) = \widehat{m_{\ell_p}}(s_\infty), \tag{42}$$

where s_∞ is any element of $\text{Sp}_\infty(n)$ with projection $S \in \text{Sp}(n)$.

B. Weyl representation of $S \in \text{Mp}(n)$

Defining, as in Ref. 16, the Mehlig-Wilkinson operator $R_\nu(s)$ associated to $s \in \text{Sp}^*(n)$ and $\nu \in \mathbb{Z}$ as being the Bochner integral

$$R_\nu(s) = \left(\frac{1}{2\pi\hbar}\right)^n \frac{i^\nu}{\sqrt{|\det(s-I)|}} \int e^{(i/2\hbar)\langle M_s z, z\rangle} T(z) d^{2n}z,$$

where $T(z)$ is the Heisenberg-Weyl operator, one of us proved in Ref. 10, Proposition 6 in Sec. 3 B and Proposition 10 in Sec. 3 C, the following results:

Proposition 2: (i) Let s_W be the free symplectic matrix generated by the quadratic form (39). We have $S_{W,m} = R_\nu(s_W)$ if and only if $\nu = \nu(S_{W,m})$ with

$$\nu(S_{W,m}) \equiv m - \text{Inert } W_{xx} \mod 4, \tag{43}$$

where Inert W_{xx} *is the index of inertia of the Hessian matrix W_{xx} of $x \mapsto W(x,x)$; (ii) Let $S \in \text{Mp}(n)$ be such that $\pi^{\text{Mp}}(S) \in \text{Sp}^*(n)$. If $s = s_W s_{W'}$ and $S = R_{\nu(s_W)}(s_W) R_{\nu(s'_W)}(s_{W'})$, then $S = R_{\nu(S)}(s)$ with*

$$\nu(S) \equiv \nu(s_W) + \nu(s_{W'}) + \tfrac{1}{2}\text{sign}(M_{s_W} + M_{s'_W}). \tag{44}$$

Comparison of formulas (44) and (37) in Theorem 1 suggests that there is a relation between the integer $\nu(S)$ and the Conley-Zehnder index of some symplectic path ending at $s = \pi_{\text{Mp}}(S)$. We claim that:

Theorem 2: *Let $s_\infty \in \text{Sp}_\infty(n)$ be such that $s = \pi_\infty(s_\infty)$ is in $\text{Sp}^*(n)$ and denote by S the image in $\text{Mp}(n)$ of the projection of s_∞ on $\text{Sp}_2(n)$. We have*

$$\nu(S) \equiv \nu(s_\infty) \mod 4. \tag{45}$$

In view of the product formula (37) in Theorem 1, it is sufficient to establish the congruence [Eq. (45)] when $s = s_W$. Assume that $S = S_{W,m}$; the relation

$$\nu(S_{W,m}) \equiv \nu(s_{W,\infty}) \mod 4$$

is an immediate consequence of the following result, interesting in its own right:

Proposition 3: We have

$$\nu(s_{W,\infty}) = m_{\ell_P}(s_{W,\infty}) - \text{Inert } W_{xx} \tag{46}$$

and hence

$$\nu(s_{W,\infty}) \equiv m - \text{Inert } W_{xx} \mod 4. \tag{47}$$

Proof: Formula (47) follows from Eq. (46) in view of Eqs. (42) and (40). We will divide the proof of formula (46) in three steps.

Step 1. Let $L \in \mathrm{Lag}^{\ominus}(2n)$. Using successively formulas (33) and (22) we have

$$\nu(s_\infty) = \tfrac{1}{2}(\mu_L^{\ominus}(s_\infty^{\ominus}) + \tau^{\ominus}(s^{\ominus}\Delta,\Delta,L) - \tau^{\ominus}(s^{\ominus}\Delta,s^{\ominus}L,L)). \tag{48}$$

Choosing, in particular, $L=L_0=\ell_P\oplus\ell_P$ we get

$$\begin{aligned}\mu_{L_0}^{\ominus}(s_\infty^{\ominus}) &= \mu^{\ominus}((I\oplus s)_\infty(\ell_P\oplus\ell_P),(\ell_P\oplus\ell_P)) = \mu(\ell_{P,\infty},\ell_{P,\infty}) - \mu(\ell_{P,\infty},s_\infty\ell_{P,\infty})\\ &= -\mu(\ell_{P,\infty},s_\infty\ell_{P,\infty}) = \mu_{\ell_P}(s_\infty)\end{aligned}$$

so that there remains to prove that

$$\tau^{\ominus}(s^{\ominus}\Delta,\Delta,L_0) - \tau^{\ominus}(s^{\ominus}\Delta,s^{\ominus}L_0,L_0) = -2\ \mathrm{sign}\ W_{xx}.$$

Step 2. We are going to show that

$$\tau^{\ominus}(s^{\ominus}\Delta,s^{\ominus}L_0,L_0) = 0;$$

in view of the symplectic invariance and the antisymmetry of $\tau^{\ominus}$, this is equivalent to

$$\tau^{\ominus}(L_0,\Delta,L_0,(s^{\ominus})^{-1}L_0) = 0. \tag{49}$$

We have

$$\Delta\cap L_0 = \{(0,p;0,p):p\in\mathbb{R}^n\}$$

and $(s^{\ominus})^{-1}L_0\cap L_0$ consists of all $(0,p',s^{-1}(0,p''))$ with $s^{-1}(0,p'')=(0,p')$; since s (and hence s^{-1}) is free we must have $p'=p''=0$ so that

$$(s^{\ominus})^{-1}L_0\cap L_0 = \{(0,p;0,0):p\in\mathbb{R}^n\}.$$

It follows that we have

$$L_0 = \Delta\cap L_0 + (s^{\ominus})^{-1}L_0\cap L_0,$$

hence Eq. (49) in view of property (ii) in Lemma 1.

Step 3. Let us finally prove that

$$\tau^{\ominus}(s^{\ominus}\Delta,\Delta,L_0) = -2\ \mathrm{sign}\ W_{xx};$$

this will complete the proof of the proposition. The condition $\det(s-I)\neq 0$ is equivalent to $s^{\ominus}\Delta\cap\Delta=0$, hence, using property (i) in Lemma 1:

$$\tau^{\ominus}(s^{\ominus}\Delta,\Delta,L_0) = -\tau^{\ominus}(s^{\ominus}\Delta,L_0,\Delta)$$

is the signature of the quadratic form Q on L_0 defined by

$$Q(0,p,0,p') = -\sigma^{\ominus}(\mathrm{Pr}_{s^{\ominus}\Delta,\Delta}(0,p,0,p');0,p,0,p'),$$

where

$$\mathrm{Pr}_{s^{\ominus}\Delta,\Delta} = \begin{bmatrix}(s-I)^{-1} & -(s-I)^{-1}\\ s(s-I)^{-1} & -s(s-I)^{-1}\end{bmatrix}$$

is the projection on $s^{\ominus}\Delta$ along Δ in $\mathbb{R}^{2n}\oplus\mathbb{R}^{2n}$. It follows that the quadratic form Q is given by

$$Q(0,p,0,p') = -\sigma^{\ominus}((I-s)^{-1}(0,p''),s(I-s)^{-1}(0,p'');0,p,0,p'),$$

where we have set $p''=p-p'$; by definition of $\sigma^{\ominus}$, this is

$$Q(0,p,0,p') = -\sigma((I-s)^{-1}(0,p''),(0,p)) + \sigma(s(I-s)^{-1}(0,p''),(0,p')).$$

Let M_s now be the symplectic Cayley transform [Eq. (25)] of s; we have

$$(I-s)^{-1} = JM_s + \tfrac{1}{2}I, \quad s(I-s)^{-1} = JM_s - \tfrac{1}{2}I,$$

and hence,

$$\begin{aligned} Q(0,p,0,p') &= -\sigma\left(\left(JM_s + \tfrac{1}{2}I\right)(0,p''),(0,p)\right) + \sigma\left(\left(JM_s - \tfrac{1}{2}I\right)(0,p''),(0,p')\right) \\ &= -\sigma(JM_s(0,p''),(0,p)) + \sigma(JM_s(0,p''),(0,p')) = \sigma(JM_s(0,p''),(0,p'')) \\ &= -\langle M_s(0,p''),(0,p'')\rangle. \end{aligned}$$

Let us calculate explicitly M_s. Writing

$$s = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

we have

$$s - I = \begin{bmatrix} 0 & B \\ I & D-I \end{bmatrix} \begin{bmatrix} C-(D-I)B^{-1}(A-I) & 0 \\ B^{-1}(A-I) & I \end{bmatrix},$$

that is,

$$s - I = \begin{bmatrix} 0 & B \\ I & D-I \end{bmatrix} \begin{bmatrix} W_{xx} & 0 \\ B^{-1}(A-I) & I \end{bmatrix}, \tag{50}$$

where we have used the identity

$$C - (D-I)B^{-1}(A-I)) = B^{-1}A + DB^{-1} - B^{-1} - (B^T)^{-1},$$

which follows from the relation $C - DB^{-1}A = -(B^T)^{-1}$ (the latter is a consequence of the equalities $D^TA - B^TC = I$ and $D^TB = B^TD$ due to the fact that $s^TJs = s^TJs$). We thus have, setting $W_{xx}^{-1} = (W_{xx})^{-1}$,

$$\begin{aligned} (s-I)^{-1} &= \begin{bmatrix} W_{xx}^{-1} & 0 \\ B^{-1}(I-A)W_{xx}^{-1} & I \end{bmatrix} \begin{bmatrix} (I-D)B^{-1} & I \\ B^{-1} & 0 \end{bmatrix} \\ &= \begin{bmatrix} W_{xx}^{-1}(I-D)B^{-1} & W_{xx}^{-1} \\ B^{-1}(I-A)W_{xx}^{-1}(I-D)B^{-1} + B^{-1} & B^{-1}(I-A)W_{xx}^{-1} \end{bmatrix}, \end{aligned}$$

and hence,

$$M_s = \begin{bmatrix} B^{-1}(I-A)W_{xx}^{-1}(I-D)B^{-1} + B^{-1} & \tfrac{1}{2}I + B^{-1}(I-A)W_{xx}^{-1} \\ -\tfrac{1}{2}I - W_{xx}^{-1}(I-D)B^{-1} & -W_{xx}^{-1} \end{bmatrix}$$

so that we have

$$Q(0,p,0,p') = \langle W_{xx}^{-1}p'',p''\rangle = \langle W_{xx}^{-1}(p-p'),(p-p')\rangle.$$

The matrix of the quadratic form Q is thus

$$2\begin{bmatrix} W_{xx}^{-1} & -W_{xx}^{-1} \\ -W_{xx}^{-1} & W_{xx}^{-1} \end{bmatrix}$$

and this matrix has signature $2 \operatorname{sign} W_{xx}^{-1} = 2 \operatorname{sign} W_{xx}$, proving the first equality [Eq. (46)]; the second equality follows because $\mu_{\ell_P}(s_\infty) = 2m_{\ell_P}(s_\infty) - n$ (since $s\ell_P \cap \ell_P = 0$) and rank $W_{xx} = n$ in view of Eq. (50), which implies that $\det(s - I) = (-1)^n \det B \det W_{xx}$. ■

V. CONCLUSION AND DISCUSSION

We have expressed the Conley-Zehnder index i_{CZ} in terms of a cohomological and topological object, the Leray index which was introduced in Ref. 14 for the purpose of semiclassical quantization, and extended in Refs. 4 and 7. This allows the definition of $i_{CZ}(\Sigma)$ without any assumption on the end point of the path Σ (see Remark). In Theorem 1 we proved a product formula for the Conley-Zehnder index in terms of the symplectic Cayley transform; this formula, however, only works if all involved paths are nondegenerate. Using the cohomological property of the Maslov index [formulas (16) and (20)] it is indeed possible to write an explicit formula for the Conley-Zehnder index of the product of two arbitrary paths; this formula (which we will not write down) is rather complicated and therefore not very attractive. It turns out that it is possible to obtain a simpler formula by redefining the Conley-Zehnder index using methods inspired from Ref. 1, as we will show in a forthcoming publication. This alternative method does not, however, lead to a straightforward calculation of the indices appearing in the Weyl representation of metaplectic operators, studied in the last section of this paper: in this precise case the Leray index approach is definitely the most natural and powerful.

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Uncertainty principle for Gabor systems and the Zak transform

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We show that if $g \in L^2(\mathbb{R})$ is a generator of a Gabor orthonormal basis with the lattice $\mathbb{Z}\times\mathbb{Z}$, then its Zak transform $Z(g)$ satisfies $\nabla Z(g) \notin L^2([0,1)^2)$. This is a generalization and extension of the Balian-Low uncertainty principle. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2393146]

I. INTRODUCTION

Given a square integrable function $g \in L^2(\mathbb{R})$ and constants $a,b>0$, the associated *Gabor system (Weyl-Heisenberg system)* generated by g and the lattice $a\mathbb{Z}\times b\mathbb{Z}$, $\mathcal{G}(g,a,b)=\{g_{m,n}\}_{m,n\in\mathbb{Z}}$, is defined by

$$g_{m,n}(x) = e^{2\pi iamx} g(x-bn).$$

In 1946 Gabor proposed to study such systems for their usefulness in the analysis of information conveyed by communication channels. These systems have been studied extensively in recent years. The edited books by Benedetto and Ferreira[4] and by Feichtinger and Strohmer,[6] as well as Gröchenig's treatise,[7] provide detailed treatments of various issues of the theory. It is well known, for example, that $ab=1$ is a necessary condition for $\mathcal{G}(g,a,b)$ to form an orthonormal basis or a Riesz basis. Moreover, if one wishes to construct orthonormal bases of Gabor type, then there are severe restrictions on the window function's time and frequency localization. The Balian-Low theorem makes this phenomenon precise as follows. We use the Fourier transform defined by $\hat{g}(\xi)=\int g(x)e^{-2\pi i\xi x}\mathrm{d}x$, where our convention is that the integral without specific limits denotes the integral over $\mathbb{R}$.

Theorem 1.1 (Balian-Low): *Let* $g \in L^2(\mathbb{R})$. *If*

$$\int |x|^2|g(x)|^2\mathrm{d}x < \infty \quad \textit{and} \quad \int |\xi|^2|\hat{g}(\xi)|^2\mathrm{d}\xi < \infty, \tag{1.1}$$

then $\mathcal{G}(g,1,1)$ *is not an orthonormal basis for* $L^2(\mathbb{R})$.

The Balian-Low theorem can be viewed as a version of the classical uncertainty principle for Gabor orthonormal bases. It has been established independently by Balian[1] and Low,[12] and the first complete proof was given by Battle.[2]

An important tool in the analysis and construction of Gabor systems is the *Zak transform*, see e.g., Ref. 7, Chap. 8. Given $g \in L^2(\mathbb{R})$, the Zak transform is formally defined by

$$Z(g)(x,\xi) = \sum_{n\in\mathbf{Z}} g(x-n)e^{2\pi in\xi}, \quad \forall\,(x,\xi) \in \mathbb{R}\times\mathbb{R}.$$

With the above definition, the Zak transform satisfies the *quasiperiodicity relations*

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$$Z(f)(x,\xi+k)=Z(f)(x,\xi),\quad \forall\, k\in\mathbb{Z},$$

and

$$Z(f)(x+k,\xi)=Z(f)(x,\xi)e^{2\pi ik\xi},\quad \forall\, k\in\mathbb{Z},$$

e.g., see Ref. 7, Sec. 8.2. Thus, the Zak transform $Z(f)$ of a function $f\in L^2(\mathbb{R})$ is a locally square integrable function defined on all of $\mathbb{R}^2$ and is uniquely determined by its values on $Q\equiv[0,1)^2$. Therefore, Z defines a unitary operator from $L^2(\mathbb{R})$ to $L^2(Q)$, and its inverse $Z^{-1}:L^2(Q)\to L^2(\mathbb{R})$ is formally given by

$$Z^{-1}(F)(x)=\int_0^1 F(x,\xi)\mathrm{d}\xi,\quad \forall\, x\in\mathbb{R}.$$

The utility of the Zak transform for constructing Gabor bases stems from the following result, e.g., Ref. 7, Corollary 8.3.2. A *Riesz basis* for $L^2(\mathbb{R})$ is an image of an orthonormal basis for $L^2(\mathbb{R})$ under an invertible bounded operator on $L^2(\mathbb{R})$ with a bounded inverse.

Theorem 1.2: *Let* $g\in L^2(\mathbb{R})$.

a. $\mathcal{G}(g,1,1)$ *is an orthonormal basis for* $L^2(\mathbb{R})$ *if and only if* $|Z(g)(x,\xi)|=1$ *for a.e.* $(x,\xi)\in Q$.
b. $\mathcal{G}(g,1,1)$ *is a Riesz basis for* $L^2(\mathbb{R})$ *if and only if there exist constants* A,B *such that* $0<A\leqslant|Z(g)(x,\xi)|\leqslant B<\infty$ *for a.e.* $(x,\xi)\in Q$.

This theorem shows that constructing, e.g., Gabor orthonormal bases is equivalent to constructing unimodular functions on $L^2(Q)$. Janssen showed in Ref. 8 that such functions cannot be continuous when extended quasiperiodically to $\mathbb{R}^2$. In fact, the following result holds.

Theorem 1.3: *Let* $g\in L^2(\mathbb{R})$ *be such that* $Z(g)$ *is continuous on* $\mathbb{R}^2$. *Then, there exists* $(t,\eta)\in Q$ *such that* $Z(g)(t,\eta)=0$.

In the next section we shall present a result which is a generalization of Theorem 1.3 and, at the same time, may be viewed as an analog of the Balian-Low theorem. Our motivation comes from the fact that conditions (1.1) in Theorem 1.1, may be rewritten in the following forms:

$$\int|x|^2|g(x)|^2\mathrm{d}x<\infty\quad\text{and}\quad\int|g'(x)|^2\mathrm{d}x<\infty,\tag{1.2}$$

where g' denotes the distributional derivative of g.

By analogy and in view of Theorem 1.2, it is of interest to investigate the properties of the gradient of the Zak transform of a function $g\in L^2(\mathbb{R})$ which generates a Gabor orthonormal basis. We shall show that if $\mathcal{G}(g,1,1)$ is a Gabor orthonormal basis for $L^2(\mathbb{R})$ then $\nabla Z(g)\notin L^2(Q)$. In view of Theorem 1.2, this result is an analog of Eq. (1.2).

II. MAIN RESULTS

We say that a function $H:\mathbb{R}^2\to\mathbb{T}$, periodic in ξ, has a *jump by* λ on the interval $[(x_0,\xi_0),(x_0,\xi_1)]$, if $|H(x_0,\xi_1)-H(x_0,\xi_0)|\geqslant\lambda$.

In what follows we shall use the following standard observation.

Fact 2.1: *Let* $H=e^{2\pi ih}:\mathbb{R}^2\to\mathbb{T}$ *be a quasiperiodic function on* $\mathbb{R}^2$ *and such that* $\nabla H\in L^2(Q)$. *Then, for almost all* $\xi\in[0,1]$, $H(\cdot,\xi)$ *is a continuous function on [0,1].*

We note here that the following lemma is closely related to the trace property of Sobolev spaces.

Lemma 2.2: *Fix* $\lambda>0$. *Let* $H(x,\xi):\mathbb{R}^2\to\mathbb{T}$ *be a quasiperiodic function on* $\mathbb{R}^2$. *Assume that for sufficiently small* $0<\delta<1$, *the set of those* $\xi_0\in(1-\delta,1)$ *for which H has a jump by* λ *on some interval* $[(x_0,\xi_0),(x_0,1)]$ *has measure at least* $\delta/2$. *Then* $\nabla H\notin L^2(Q)$.

Proof: Assume by contradiction that $\nabla H\in L^2(Q)$ and $\|\nabla H\|_{L^2(Q)}=1$.

Fact 2.1 implies that for almost all $\xi\in[0,1]$, $H(x,\xi)$ is a continuous function of $x\in[0,1]$.

Using the periodicity of H in ξ, we may conclude that $H(\cdot,\xi)$ is continuous for almost all $\xi \in \mathbb{R}$. Thus, we may assume without loss of generality that $H(\cdot,0)$ and $H(\cdot,1)$ are continuous functions of $x \in [0,1]$, and moreover that $\int_0^1 |\partial_x H(\cdot,0)|^2 \mathrm{d}x \leqslant 2$. This implies that we may now consider the function $H(x,\xi)/H(1,\xi)$, which satisfies $\|\nabla(H(x,\xi)/H(1,\xi))\|_{L^2(Q)} \leqslant 4$, which, in turn, together with the periodicity of H, allows us to assume that $H(x,0)/H(1,0)$ and $H(x,1)/H(1,1)$ are constant.

For simplicity of notation, in what follows we shall denote the function $H(x,\xi)/H(1,\xi)$ again by $H(x,\xi)$.

Fix $\xi_0 \in (1-\delta,1)$, for which H has a jump by λ on some interval $[(x_0,\xi_0),(x_0,1)]$. Let E_{ξ_0} denote the set of points (x,ξ_0) for which

$$|H(x,1) - H(x,\xi_0)| > \lambda/4.$$

For any $x \in E_{\xi_0}$ we have

$$\lambda^2/16 \leqslant |H(x,1) - H(x,\xi_0)|^2 \leqslant \left(\int_{\xi_0}^1 \partial_\xi H(x,\xi) \mathrm{d}\xi \right)^2 \leqslant \delta \int_{1-\delta}^1 |\partial_\xi H(x,\xi)|^2 \mathrm{d}\xi.$$

Thus,

$$|E_{\xi_0}| \leqslant \frac{16}{\lambda^2} \delta \int_0^1 \int_{1-\delta}^1 |\nabla H(x,\xi)|^2 \mathrm{d}\xi \mathrm{d}x := \frac{16}{\lambda^2} \delta \epsilon(\delta), \tag{2.1}$$

where $\epsilon(\delta) \to 0$ as $\delta \to 0$. The following inequality holds:

$$\left| \left\{ \xi \in (1-\delta,1): \int_0^1 |\partial_x H(x,\xi)|^2 \mathrm{d}x > A/\delta \right\} \right| \leqslant \frac{\delta}{A} \int_{1-\delta}^1 \int_0^1 |\partial_x H(x,\xi)|^2 \mathrm{d}x \mathrm{d}\xi \leqslant \frac{\delta}{A} \epsilon(\delta).$$

The above inequality implies that

$$\left| \left\{ \xi \in (1-\delta,1): \int_0^1 |\partial_x H(x,\xi)|^2 \mathrm{d}x \leqslant A/\delta \right\} \right| \geqslant \delta - \frac{\delta}{A} \epsilon(\delta).$$

If we choose $A > 2\epsilon(\delta)$ then

$$\left| \left\{ \xi \in (1-\delta,1): \int_0^1 |\partial_x H(x,\xi)|^2 \mathrm{d}x \leqslant A/\delta \right\} \right| > \frac{\delta}{2}.$$

Therefore, there exists $\xi_0 \in (1-\delta,1)$ such that $\int_0^1 |\partial_x H(x,\xi_0)|^2 \mathrm{d}x \leqslant A/\delta$ and for which H has a jump by λ on some interval $[(x_0,\xi_0),(x_0,1)]$.

Using the Cauchy-Schwartz inequality (see, e.g., Ref. 11), we obtain that for such ξ_0 and for any $x_0 \in [0,1]$,

$$|H(x_0,\xi_0) - H(1,\xi_0)|^2 \leqslant (1-x_0) \int_{x_0}^1 |\partial_x H(x,\xi_0)|^2 \mathrm{d}x \leqslant (1-x_0) \frac{A}{\delta}. \tag{2.2}$$

If we choose $A = 4\epsilon(\delta)$ and $1-x_0$ sufficiently small (i.e., $1-x_0 \leqslant \min\{1/2; \lambda^2\delta/32\epsilon(\delta)\}$) then the right hand side of Eq. (2.2) is smaller than $\lambda^2/16$, i.e.,

$$|H(x_0,\xi_0) - H(1-\xi_0)| \leqslant \lambda/4. \tag{2.3}$$

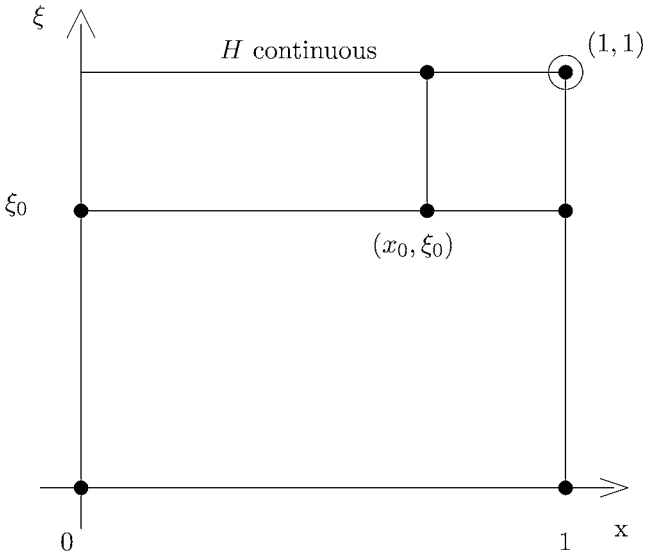
Next, we use Eq. (2.1) and the fact that $\epsilon(\delta) \to 0$ as $\delta \to 0$ to observe that if δ is sufficiently small, then in each interval $[(1-\min\{1/2; \lambda^2\delta/32\epsilon(\delta)\}, \xi_0), (1, \xi_0)]$ we can find a point x_0 such that

$$|H(x_0,\xi_0) - H(x_0,1)| \leqslant \lambda/4. \tag{2.4}$$

Finally, by the assumption about the continuity of $H(x,1)$, we may assume also without loss of generality that $H(\cdot,1)$ is constant on $[0,1]$ and so

$$|H(x_0,1)-H(1,1)|=0\leqslant \lambda/4. \tag{2.5}$$

Combining now Eqs. (2.3)–(2.5) with the assumption of jump of H by λ we obtain a contradiction. □



◉ — point of jump

Theorem 2.3: *Let* $H(x,\xi):\mathbb{R}^2\to\mathbb{T}$ *be a quasiperiodic function on* $\mathbb{R}^2$. *Then* $\nabla H\notin L^2(Q)$.

Remark 2.4: The condition $\nabla H\in L^2(Q)$ does not imply that H is continuous, so the result of Janssen (Theorem 1.3) cannot be directly used.

Proof: Fix $\delta>0$ sufficiently small. Let $H(x,\xi)=e^{2\pi i h(x,\xi)}$. We shall divide the argument into three cases.

Consider the set $\mathcal{A}(\delta)=\mathcal{A}(1-\delta,1)\subset(1-\delta,1)$ consisting of $\xi\in(1-\delta,1)$ such that

$$h(1,\xi)-h(0,\xi)=\xi+k,$$

where $k\in\mathbb{Z}\backslash\{-1\}$ and k depends on ξ.

For almost every $\xi_0\in\mathcal{A}(\delta)$, $h(\cdot,\xi_0)$ is continuous on $[0,1]$. For such ξ_0 there exists $a\in[0,1]$ and an independent constant λ such that $|H(a,\xi_0)-H(a,1)|>\lambda$.

Indeed, Fact 2.1 implies that for almost all ξ, $h(\cdot,\xi)$ is continuous on $[0,1]$. As in the proof of Lemma 2.2, we may assume without loss of generality that $h(\cdot,0)$ and $h(\cdot,1)$ are constant on $[0,1]$. Since $k\neq-1$ and using the continuity of $h(\cdot,\xi_0)$, we may choose $x_0\in(0,1)$ such that $|h(x_0,\xi_0)-h(0,\xi_0)|=1/2$. Thus, we may conclude that either $|h(0,1)-h(0,\xi_0)|\geqslant 1/4$ or $|h(x_0,1)-h(x_0,\xi_0)|\geqslant 1/4$. In particular, we have $\lambda=1/4$.

Case 1. Suppose that for some sufficiently small $\delta\in(0,1)$, $|\mathcal{A}(\delta)|\geqslant\delta/2$. Then we use Lemma 2.2 to obtain a contradiction with the assumption that $\nabla H\in L^2(Q)$.

Case 2. Suppose that the set $\mathcal{B}(\delta)=\mathcal{B}(0,\delta)\subset(0,\delta)$ consisting of $\xi\in(0,\delta)$ such that

$$h(1,\xi)-h(0,\xi)=\xi+k,$$

where $k\neq0$, has measure greater than or equal to $\delta/2$ for some sufficiently small $\delta>0$. In such case, arguing as in case 1, we again obtain a contradiction.

Case 3. Assume that there exists $\delta\in(0,1)$ such that $|\mathcal{A}(\delta)|<\delta/2$ and $|\mathcal{B}(\delta)|<\delta/2$.

We may assume without loss of generality that

$$\int_0^1 |\partial_x h(x,\delta)|^2 \mathrm{d}x < \infty.$$

Define the function $f:[0,1-\delta]\to\mathbb{R}$ by $f(x)=|\{\xi\in[x,x+\delta]:h(1,\xi)-h(0,\xi)=\xi\}|$. So defined function f is continuous and thus there exists an interval $(\eta,\eta+\delta)$ such that $|\mathcal{A}(\delta)+\eta|=\delta/2$ and $|\mathcal{B}(\delta)+\eta|=\delta/2$.

Next, we choose $\xi_1,\xi_2\in(\eta,\eta+\delta)$ such that

$$h(1,\xi_1)-h(0,\xi_1)=\xi_1$$

and

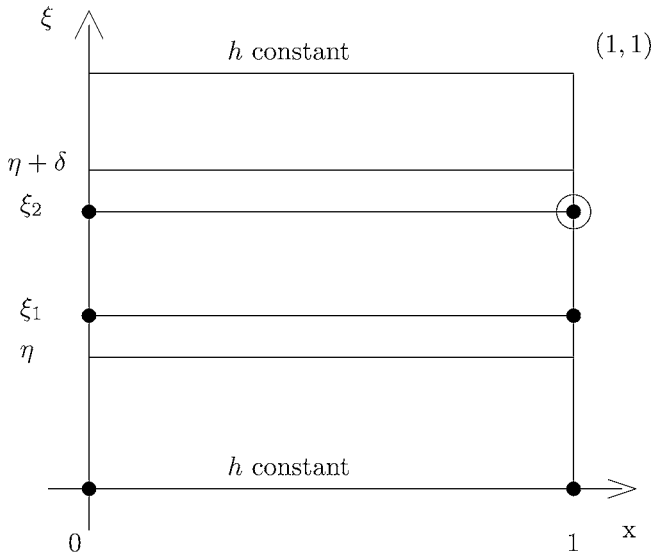
$$h(1,\xi_2)-h(0,\xi_2)=\xi_2+l,$$

where $l\in\mathbb{Z}\backslash\{0\}$. This implies that the function H has a jump on some interval $[(a,\xi_1),(a,\xi_2)]$, where $a\in[0,1]$.

Moreover, we may assume without loss of generality that ξ_1 and ξ_2 are chosen so that $h(\cdot,\xi_1)$ and $h(\cdot,\xi_2)$ are continuous and that

$$\int_0^1 |\partial_x H(x,\xi_i)|^2 \mathrm{d}x \leqslant A/\delta,$$

$i=1,2$, for some $A>2\epsilon(\delta)$. We may now conclude the proof, obtaining a contradiction as in the proof of Lemma 2.2. □



◉ — point of jump

Corollary 2.5 (Uncertainty principle for the Zak transform): *Let* $\mathcal{G}(g,1,1)$ *be a Gabor orthonormal basis for* $L^2(\mathbb{R})$. *Then*, $\nabla Z(g)\notin L^2(Q)$.

Corollary 2.5 follows immediately from Theorems 1.2 and 2.3.

Example 2.6: Theorem 2.3 is sharp in the following sense. Consider the following family of functions $H_a(x,\xi)$ introduced in Ref. 3.

(1) Let $\varphi\in\mathcal{C}^\infty(\mathbb{R})$ be a function with the following properties:

$$\varphi(x)=-1 \quad \text{for } x\in(-\infty,0],$$

$$\varphi(x) = 0 \quad \text{for } x \in [1,\infty),$$

$$\varphi(x) \in [-1,0] \quad \text{for all } x \in \mathbb{R}.$$

(2) Let $\psi(x) = \chi_{[0,\infty)}(x)x^a$, where $a > 0$ is a fixed number.
(3) Given $0 < \epsilon < \frac{1}{8}$, let $\gamma \in \mathcal{C}^\infty(\mathbb{R})$ be a function that satisfies

$$\text{supp}(\gamma) \subseteq [-2\epsilon, 2\epsilon], \quad \gamma(x) = 1 \text{ for } x \in [-\epsilon, \epsilon],$$

and

$$\gamma(x) \in [0,1] \quad \text{for all } x \in \mathbb{R}.$$

Then, there exists a function $H_a : [-\frac{1}{2}, 1] \times \mathbb{I}$, with the following properties:

(1) $H_a(x,\xi) = 0$ for $x \in [-\frac{1}{2}, 0]$;
(2) $H_\alpha(x,\xi) = \varphi(\xi/\psi(x))$ for $x \in (0, 2\epsilon]$, where $\epsilon > 0$ is chosen for the definition of γ;
(3) $H_a(x,0) = 0$ for $x \in [-\frac{1}{2}, 0]$ and $H_a(x,0) = -1$ for $x \in (0,1]$;
(4) $H_a(1+x,\xi) = H(x,\xi) + (\xi - 1)$ for $x \in [-\frac{1}{2}, 0]$; and
(5) the function $e^{2\pi i H(x,\xi)} : [-\frac{1}{2}, 1] \times \mathbb{T} \to \mathbb{C}$ is of class $\mathcal{C}^\infty$ away from the points (0,0) and (1,0).

These functions were proven to be optimal for the classical (p,q) Balian-Low theorem in Ref. 3. However, it is clear that they are also optimal functions for Theorem 2.3, in the sense that they possess the minimal singular support possible, consisting of a single point in Q.

For other examples of such functions we refer to Refs. 9 and 10.

The statement of Corollary 2.5 actually holds for more general systems than orthonormal bases. The following result follows from Corollary 2.5 and Theorem 1.2.

Corollary 2.7: *Let $\mathcal{G}(g,1,1)$ be a Gabor-Riesz basis for $L^2(\mathbb{R})$. Then, $\nabla Z(g) \notin L^2(Q)$.*

We close this section by showing more general estimates involving partial fractions of the Laplacian of the Zak transform of a Gabor basis generating window.

Corollary 2.8: *Let $\mathcal{G}(g,1,1)$ be a Gabor-Riesz basis for $L^2(\mathbb{R})$. Then, $\Delta^{1/p} Z(g) \notin L^p(Q)$, $1 < p < \infty$.*

Proof:

(1) Assume that $\Delta^{\alpha/2}(f) \in L^p(Q)$. Then we have that $\partial_1^\alpha(f) = \partial_1^\alpha \Delta^{-\alpha} \Delta^\alpha(f) \in L^p(Q)$, for $1 < p < \infty$. The reason for this is that the Fourier multiplier $m(\xi_1, \xi_2) := \xi_1^\alpha |\xi|^{-\alpha}$ satisfies

$$|\partial_1^{\beta_1} \partial_2^{\beta_2} m(\xi_1/2^{n_1}, \xi_2/2^{n_2})| \leq C_{\beta_1,\beta_2}, \tag{2.6}$$

for $1/2 \leq |\xi_1|, |\xi_2| \leq 2$, and consequently is bounded on $L^p(Q)$, $1 < p < \infty$, for any $\alpha > 0$ by the multiparameter Calderón-Zygmund theory (see, e.g., Ref. 5, Introduction).
(2) For $f \in C_c^\infty([0,1])$ and $1 < p < \infty$, we have the following estimate of Hölder regularity:

$$\|f\|_{\Lambda_{1/p}} \leq \|f\|_{L^p(|-1/2,3/2])} + \| |\partial_1|^{2/p} \|_{L^p(|-1/2,3/2])}. \tag{2.7}$$

(3) We replace Eq. (2.2) by Eq. (2.7), use Eq. (2.6), and repeat the main argument of the proof of Theorem 2.3 to prove Corollary 2.8. □

Remark 2.9: All the results of this section follow for Gabor systems $\mathcal{G}(g,a,b)$, $g \in L^2(\mathbb{R})$, $ab = 1$, if we use the Zak transform Z_a defined by

$$Z_a(g)(x,\xi) = \sum_{n \in \mathbf{Z}} g(x - an) e^{2\pi i a n \xi},$$

see Ref. 7.

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New multisymplectic self-adjoint scheme and its composition scheme for the time-domain Maxwell's equations

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In this paper, we investigate Euler-box scheme for Bridges' multisymplectic form of Maxwell's equations. A new multisymplectic scheme is derived for Maxwell's equations. We prove that it is also a self-adjoint scheme in time direction. The multisymplecticity of composition schemes based on the new scheme is also discussed. Two numerical examples are proposed to indicate that the derived multisymplectic schemes are effective when used to integrate the 2+1 dimensional Maxwell's equations. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Maxwell's equations describe the fundamental evolutions of electromagnetic fields in space and time. They have been applied to a wide range of different physical situations. They play an important role in a large number of engineering applications. In many cases, numerical methods are required to solve Maxwell's equations.

The computations of electromagnetics have developed for a long time and many efficient methods have been given. The famous time-domain technique in computational electromagnetic (CEM) was developed by Yee.[1] The method, generally referred as the finite-difference time-domain method,[2] is based on staggered central differencing in space and staggered leapfrog integration in time for Cartesian coordinates. Finite volumes were introduced to CEM by Shankar *et al.*[3] by exporting methods from computational fluid dynamics. Their early work used structured grids, but lately they have turned to unstructured grids. Their main reason for doing so is the difficulty of creating a global body-conforming grid for realistic geometries, such as a complete aircraft. The spectral-domain split-operator technique proposed in Ref. 4 is one of the many forms that results from the use of the Lie-Trotter-Suzuki product formulas. This technique makes use of fast Fourier transforms to compute the matrix exponentials of the displacement operators. Due to

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the practical interests, more and more researchers have done their important contributions on the numerical approximations to Maxwell's equations and also on the analysis of the numerical scheme.

In 1990s, the symplectic schemes were introduced and systematically developed for the Hamiltonian systems within the framework of symplectic geometry.[5–7] The Hamiltonian nature of Maxwell's equations was revealed by Morrison[8] and Marsden and Weinstein[9] in their work on the Maxwell-Vlasov equation. The symplectic schemes which preserve the Hamiltonian nature of Maxwell's equations were reported to have higher performance over the nonsymplectic schemes.[10,11] Recently, Marsden *et al.*[12] and Bridges and Reich[13] proposed the concept of multisymplectic partial differential equations (PDEs) and multisymplectic schemes which can be viewed as the generalization of symplectic schemes. The multisymplectic schemes have been applied successfully to lots of important equations such as the nonlinear wave equation,[13–15] the nonlinear Schrödinger equation,[16–18] the Korteweg–de Vries equation,[19,20] the Zakharov-Kuznetsov equation,[21] Kadomtsev-Petviashvili equation,[22] and so on. With regard to details, please refer to the new published survey by Bridges and Reich[23] and the references therein. By many computational experiments and theoretical analysis, the multisymplectic schemes were shown to be much superior to other standard methods in the performance of numerical stability in long time computation.

The main purpose of this paper is to check whether the multisymplectic scheme could be applied to integrate Maxwell's equations and still have good numerical performance. We develop a new self-adjoint scheme in time direction for solving the time-domain Maxwell's equations. The composition scheme based on the new scheme is also derived.

This paper is organized as follows In Sec. II, we take a brief review of multisymplectic Bridges' form for Maxwell's equations. A self-adjoint scheme is derived based on Bridges' form in Sec. III. The truncation error of the new scheme is also discussed in the same section. In Sec. IV, we use the self-adjoint scheme to get a composition scheme in time direction. In Sec. V, numerical experiments are presented to indicate the merits of the multisymplectic schemes and we finish the paper with conclusion remarks in Sec. VI.

II. MULTISYMPLECTIC FORMULATION FOR MAXWELL'S EQUATIONS

Maxwell's equations in an isotropic, homogeneous, nondispersive medium are

$$\begin{aligned} &\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0 \quad \text{(Faraday' s Law)}, \\ &\frac{\partial \mathbf{D}}{\partial t} - \nabla \times \mathbf{H} = 0 \quad \text{(Ampere' s Law)}, \\ &\mathbf{B} = \mu \mathbf{H}, \\ &\mathbf{D} = \varepsilon \mathbf{E}. \end{aligned} \tag{2.1}$$

In the absence of impressed electric charge, the magnetic induction and electric displacement fields satisfy the constraints (Gauss's law)

$$\begin{aligned} &\nabla \cdot \mathbf{B} = 0, \\ &\nabla \cdot \mathbf{D} = 0. \end{aligned} \tag{2.2}$$

Scattering obstacles will be modeled by a spatial variation of ε and μ. In free space, ε and μ are constant, equal to their minimum values ε_0 and μ_0. The speed of light in free space is $c = 1/\sqrt{\varepsilon_0 \mu_0}$.

Introduce two vector functions $\mathbf{U}$ and $\mathbf{V}$ satisfying $\mathbf{U}_t=\mathbf{E}$ and $\mathbf{V}_t=\mathbf{H}$, respectively, then the Lagrangian for Maxwell's equations [Eq. (2.1)] can be written as

$$L=\frac{1}{2}\mu\langle\mathbf{V}_t,\mathbf{V}_t\rangle+\frac{1}{2}\langle\mathbf{V}_t,\boldsymbol{\nabla}\times\mathbf{U}\rangle+\frac{1}{2}\varepsilon\langle\mathbf{U}_t,\mathbf{U}_t\rangle-\frac{1}{2}\langle\mathbf{U}_t,\boldsymbol{\nabla}\times\mathbf{V}\rangle, \tag{2.3}$$

where $\langle\cdot,\cdot\rangle$ represents the standard inner production of vector space. According to Bridges' theory on multisymplectic structure, the generalized conjugate momentums can be derived by covariant Legendre transform correspondingly,

$$\begin{aligned}\mathbf{P}&=\frac{\partial\mathbf{L}}{\partial\mathbf{V}_t}=\mu\mathbf{V}_t+\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{U},\quad \frac{\partial L}{\partial\boldsymbol{\nabla}\times\mathbf{V}}=-\frac{1}{2}\mathbf{U}_t,\\ \mathbf{Q}&=\frac{\partial L}{\partial\mathbf{U}_t}=\varepsilon\mathbf{U}_t-\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{V},\quad \frac{\partial L}{\partial\boldsymbol{\nabla}\times\mathbf{U}}=\frac{1}{2}\mathbf{V}_t,\end{aligned} \tag{2.4}$$

further the covariant Hamiltonian by

$$\begin{aligned}S&=\langle\mathbf{P},\mathbf{V}_t\rangle+\langle\mathbf{Q},\mathbf{U}_t\rangle+\left\langle\frac{\partial L}{\partial\boldsymbol{\nabla}\times\mathbf{V}},\boldsymbol{\nabla}\times\mathbf{V}\right\rangle+\left\langle\frac{\partial L}{\partial\boldsymbol{\nabla}\times\mathbf{U}},\boldsymbol{\nabla}\times\mathbf{U}\right\rangle-L\\ &=\langle\mathbf{P},\mathbf{H}\rangle+\langle\mathbf{Q},\mathbf{E}\rangle-\frac{1}{2}\mu\langle\mathbf{H},\mathbf{H}\rangle-\frac{1}{2}\varepsilon\langle\mathbf{E},\mathbf{E}\rangle.\end{aligned} \tag{2.5}$$

Set $Z=[\mathbf{H},\mathbf{E},\mathbf{V},\mathbf{U},\mathbf{P},\mathbf{Q}]^T$, then Maxwell's equations are transformed into the following form:

$$\begin{aligned}\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{U}&=\mathbf{P}-\mu\mathbf{H},\\ -\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{V}&=\mathbf{Q}-\varepsilon\mathbf{E},\\ -\mathbf{P}_t-\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{E}&=0,\\ -\mathbf{Q}_t+\frac{1}{2}\boldsymbol{\nabla}\times\mathbf{H}&=0,\\ \mathbf{V}_t&=\mathbf{H},\\ \mathbf{U}_t&=\mathbf{E}.\end{aligned} \tag{2.6}$$

The above equations can be organized into Bridges' multisymplectic form as

$$MZ_t+N\boldsymbol{\nabla}\times Z=\boldsymbol{\nabla}_Z S(Z), \tag{2.7}$$

where

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 & 0 & -I \\ 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \end{pmatrix},$$

I is the identity element belonging to $R^{3\times 3}$. The rotation action $\nabla \times Z$ denotes $[\nabla \times \mathbf{H}, \nabla \times \mathbf{E}, \nabla \times \mathbf{V}, \nabla \times \mathbf{U}, \nabla \times \mathbf{P}, \nabla \times \mathbf{Q}]^T$ and

$$N\nabla \times Z = FZ_x + LZ_y + WZ_z, \tag{2.8}$$

where

$$F = \begin{pmatrix} 0 & 0 & 0 & (1/2)R_1 & 0 & 0 \\ 0 & 0 & -(1/2)R_1 & 0 & 0 & 0 \\ 0 & -(1/2)R_1 & 0 & 0 & 0 & 0 \\ (1/2)R_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$L = \begin{pmatrix} 0 & 0 & 0 & (1/2)R_2 & 0 & 0 \\ 0 & 0 & -(1/2)R_2 & 0 & 0 & 0 \\ 0 & -(1/2)R_2 & 0 & 0 & 0 & 0 \\ (1/2)R_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$W = \begin{pmatrix} 0 & 0 & 0 & (1/2)R_3 & 0 & 0 \\ 0 & 0 & -(1/2)R_3 & 0 & 0 & 0 \\ 0 & -(1/2)R_3 & 0 & 0 & 0 & 0 \\ (1/2)R_3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$R_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad R_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Thus we easily find that matrices M, F, L, and W ($\in R^{18\times 18}$) are skew symmetric. Additionally the rotation operator may be simplified as $\nabla \times = R_1(\partial/\partial x) + R_2(\partial/\partial y) + R_3(\partial/\partial z)$.

To simplify the notation we will mainly consider twodimensional problems. In two dimensions, Eq. (2.1) decouples into two independent sets of equations, each representing a distinct polarization. We shall use as our model system of equations those of the transverse magnetic polarization, where the electric field is a scalar while the magnetic field is a plane vector,

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right),$$

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu}\frac{\partial E_z}{\partial y}, \tag{2.9}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\frac{\partial E_z}{\partial x}.$$

In two dimensions, Eq. (2.7) can be written as follows:

$$MZ_t + FZ_x + LZ_y = \nabla_Z S(Z), \tag{2.10}$$

where M, F, and L are the same as Eq. (2.8).

Because $M, F, L \in R^{18\times 18}$ are skew-symmetric matrices and $S: R^n \to R$ is a smooth function of the state variable $Z(x,y,t)$, it can be shown that the multisymplectic PDEs [Eq. (2.10)] satisfies the following multisymplectic conservation law according to Bridges' theory:

$$\frac{\partial \omega}{\partial t} + \frac{\partial \varphi}{\partial x} + \frac{\partial \psi}{\partial y} = 0, \tag{2.11}$$

where

$$\omega = \frac{1}{2}(dZ \wedge MdZ), \quad \varphi = \frac{1}{2}(dZ \wedge FdZ), \quad \psi = \frac{1}{2}(dZ \wedge LdZ). \tag{2.12}$$

III. MULTISYMPLECTIC SELF-ADJOINT SCHEME

Because Eq. (2.10) preserves multisymplectic conservation law, naturally, when discreting Hamiltonian PDEs [Eq. (2.10)] by a numerical scheme, we also expect that the multisymplectic conservation law [Eq. (2.11)] should be preserved. Bridges and Reich defined a numerical scheme as a multisymplectic scheme if the scheme preserves a discrete multisymplectic conservation law.[13]

In the conventional schemes, the Preissman scheme[13] and the Euler-box scheme[24] for the PDEs [Eq. (2.10)] are shown to be multisymplectic. The multisymplectic Preissman scheme has been hot in the last few years,[15–22] whereas there were few reports for the multisymplectic Euler-box scheme. In the following, we will investigate the Euler-box scheme for Maxwell's equations. Set t_k, $k=1,2,\ldots$; x_i, $i=1,2,\ldots,M$; and y_j, $j=1,2,\ldots,N$ be the regular grids of the integral domain, $Z^n_{i,j}$ is an approximation to $Z(x_i,y_j,t_n)$, $\Delta t = t_{k+1} - t_k$ is the time step, $\Delta x = x_{i+1} - x_i$ is the x-direction step, and $\Delta y = y_{j+1} - y_j$ is the y-direction step.

We take the following splitting for the matrices M, F, and L in the multisymplectic PDEs [Eq. (2.10)]:

$$M = M_+ + M_-, \quad F = F_+ + F_-, \quad L = L_+ + L_-, \tag{3.1}$$

where $M_+^T = -M_-, F_+^T = -F_-$, and $L_+^T = -L_-$, then rewrite the PDEs as

$$M_+Z_t + M_-Z_t + F_+Z_x + F_-Z_x + L_+Z_y + L_-Z_y = \nabla_Z S(Z). \tag{3.2}$$

Consider the following so-called Euler-box scheme for the above PDEs [Eq. (3.2)]:

$$M_+\delta_t^+ Z_{i,j}^k + M_-\delta_t^- Z_{i,j}^k + F_+\delta_x^+ Z_{i,j}^k + F_-\delta_x^- Z_{i,j}^k + L_+\delta_y^+ Z_{i,j}^k + L_-\delta_y^- Z_{i,j}^k = \nabla_Z S(Z_{i,j}^k), \tag{3.3}$$

where

$$\delta_t^\pm Z_{i,j}^k = \pm\frac{Z_{i,j}^{k\pm1} - Z_{i,j}^k}{\Delta t}, \quad \delta_x^\pm Z_{i,j}^k = \pm\frac{Z_{i\pm1,j}^k - Z_{i,j}^k}{\Delta x}, \quad \delta_y^\pm Z_{i,j}^k = \pm\frac{Z_{i,j\pm1}^k - Z_{i,j}^k}{\Delta y},$$

with the special matrices splitting as

$$M_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 & 0 & -I \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad F_+ = \begin{pmatrix} 0 & 0 & 0 & R_1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -R_1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$L_+ = \begin{pmatrix} 0 & 0 & 0 & R_2/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -R_2/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.4}$$

Theorem 3.1: *The Euler-box scheme [Eq. (3.3)] is multisymplectic with the following discrete multisymplectic conservation law:*

$$\delta_t^+ \omega_{ij}^k + \delta_x^+ \varphi_{ij}^k + \delta_y^+ \psi_{ij}^k = 0, \tag{3.5}$$

where $\omega_{i,j}^k = dZ_{i,j}^{k-1} \wedge M_+ dZ_{i,j}^k$, $\varphi_{i,j}^k = dZ_{i-1,j}^k \wedge F_+ dZ_{i,j}^k$, and $\psi_{i,j}^k = dZ_{i,j-1}^k \wedge L_+ dZ_{i,j}^k$.

Proof: Consider the variational equations of Eq. (3.3),

$$M_+ \delta_t^+ dZ_{i,j}^k + M_- \delta_t^- dZ_{i,j}^k + F_+ \delta_x^+ dZ_{i,j}^k + F_- \delta_x^- dZ_{i,j}^k + L_+ \delta_y^+ dZ_{i,j}^k + L_- \delta_y^- dZ_{i,j}^k = \nabla_{ZZ} S(Z_{i,j}^k) dZ_{i,j}^k. \tag{3.6}$$

By Eq. (3.6), we have

$$\begin{aligned} 0 &= dZ_{i,j}^k \wedge \nabla_{ZZ} S(Z_{i,j}^k) dZ_{i,j}^k = dZ_{i,j}^k \wedge M_+ \delta_t^+ dZ_{i,j}^k + dZ_{i,j}^k \wedge M_- \delta_t^- dZ_{i,j}^k + dZ_{i,j}^k \wedge F_+ \delta_x^+ dZ_{i,j}^k \\ &\quad + dZ_{i,j}^k \wedge F_- \delta_x^- dZ_{i,j}^k + dZ_{i,j}^k \wedge L_+ \delta_y^+ dZ_{i,j}^k + dZ_{i,j}^k \wedge L_- \delta_y^- dZ_{i,j}^k = dZ_{i,j}^k \wedge M_+ \delta_t^+ dZ_{i,j}^k + \delta_t^- dZ_{i,j}^k \wedge M_+ dZ_{i,j}^k \\ &\quad + dZ_{i,j}^k \wedge F_+ \delta_x^+ dZ_{i,j}^k + \delta_x^- dZ_{i,j}^k \wedge F_+ dZ_{i,j}^k + dZ_{i,j}^k \wedge L_+ \delta_y^+ dZ_{i,j}^k + \delta_y^- dZ_{i,j}^k \wedge L_+ dZ_{i,j}^k \\ &= \delta_t^+ (dZ_{i,j}^{k-1} \wedge M_+ dZ_{i,j}^k) + \delta_x^+ (dZ_{i-1,j}^k \wedge F_+ dZ_{i,j}^k) + \delta_y^+ (dZ_{i,j-1}^k \wedge L_+ dZ_{i,j}^k) = \delta_t^+ \omega_{ij}^k + \delta_x^+ \varphi_{ij}^k + \delta_y^+ \psi_{ij}^k . \square \end{aligned}$$

The multisymplecticity of the 1+1 dimensional Euler-box scheme is proved by Moore and Reich in Ref. 24. Next we derive a new scheme which is equivalent to the multisymplectic scheme [Eq. (3.3)]. Recast scheme (3.3) into the following form:

$$M_+ \delta_t^+ Z_{i,j}^k + M_- \delta_t^- Z_{i,j}^k + N\nabla^+ \times Z_{i,j}^k + N\nabla^- \times Z_{i,j}^k = \nabla_Z S(Z_{i,j}^k), \tag{3.7}$$

where

$$M_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 & 0 & -I \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad N\nabla^+ \times = \begin{pmatrix} 0 & 0 & 0 & (1/2)\nabla^+ \times & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -(1/2)\nabla^+ \times & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$N\nabla^{-}\times=\begin{pmatrix}0&0&0&0&0&0\\0&0&-(1/2)\nabla^{-}\times&0&0&0\\0&0&0&0&0&0\\(1/2)\nabla^{-}\times&0&0&0&0&0\\0&0&0&0&0&0\\0&0&0&0&0&0\end{pmatrix},$$

$$\nabla^{+}\times=\begin{pmatrix}0&0&\partial/\partial y\\0&0&-\partial/\partial x\\-\partial/\partial y&\partial/\partial x&0\end{pmatrix}^{+}=\begin{pmatrix}0&0&\delta_y^{+}\\0&0&-\delta_x^{+}\\-\delta_y^{+}&\delta_x^{+}&0\end{pmatrix},\quad \nabla^{-}\times=\begin{pmatrix}0&0&\delta_y^{-}\\0&0&-\delta_x^{-}\\-\delta_y^{-}&\delta_x^{-}&0\end{pmatrix}.$$

Substituting $M_{+},M_{-},N\nabla^{+}\times,N\nabla^{-}\times$, and $Z_{i,j}^{k}=[\mathbf{H}_{i,j}^{k},\mathbf{E}_{i,j}^{k},\mathbf{V}_{i,j}^{k},\mathbf{U}_{i,j}^{k},\mathbf{P}_{i,j}^{k},\mathbf{Q}_{i,j}^{k}]^{T}$ into Eq. (3.7), we have

$$\begin{aligned}&\frac{1}{2}\nabla^{+}\times\mathbf{U}_{i,j}^{k}=\mathbf{P}_{i,j}^{k}-\mu\mathbf{H}_{i,j}^{k},\\&-\frac{1}{2}\nabla^{-}\times\mathbf{V}_{i,j}^{k}=\mathbf{Q}_{i,j}^{k}-\varepsilon\mathbf{E}_{i,j}^{k},\\&-\delta_t^{+}\mathbf{P}_{i,j}^{k}-\frac{1}{2}\nabla^{+}\times\mathbf{E}_{i,j}^{k}=0,\\&-\delta_t^{+}\mathbf{Q}_{i,j}^{k}+\frac{1}{2}\nabla^{-}\times\mathbf{H}_{i,j}^{k}=0,\\&\delta_t^{-}\mathbf{V}_{i,j}^{k}=\mathbf{H}_{i,j}^{k},\\&\delta_t^{-}\mathbf{U}_{i,j}^{k}=\mathbf{E}_{i,j}^{k}.\end{aligned}\tag{3.8}$$

We can eliminate the auxiliary variables $\mathbf{P}_{i,j}^{k}$, $\mathbf{Q}_{i,j}^{k}$, $\mathbf{U}_{i,j}^{k}$, and $\mathbf{V}_{i,j}^{k}$ and derive formulas that only contain $\mathbf{E}_{i,j}^{k}$ and $\mathbf{H}_{i,j}^{k}$.

$$\begin{aligned}&\nabla^{+}\times\mathbf{E}_{i,j}^{k}=-\nabla^{+}\times\mathbf{E}_{i,j}^{k-1}-2\mu\delta_t^{-}\mathbf{H}_{i,j}^{k},\\&-\nabla^{-}\times\mathbf{H}_{i,j}^{k}=\nabla^{-}\times\mathbf{H}_{i,j}^{k-1}-2\varepsilon\delta_t^{-}\mathbf{E}_{i,j}^{k}.\end{aligned}\tag{3.9}$$

Substituting $\mathbf{E}_{i,j}^{k}=[0,0,E_{zi,j}^{k}]^{T}$, $\mathbf{H}_{i,j}^{k}=[H_{xi,j}^{k},H_{yi,j}^{k},0]^{T}$, and $\nabla^{+}\times$, $\nabla^{-}\times$ defined in Eq. (3.7) into Eq. (3.9), we obtain

$$\begin{aligned}&\delta_y^{+}E_{zi,j}^{k}=-\delta_y^{+}E_{zi,j}^{k-1}-2\mu\delta_t^{-}H_{xi,j}^{k},\\&-\delta_x^{+}E_{zi,j}^{k}=\delta_x^{+}E_{zi,j}^{k-1}-2\mu\delta_t^{-}H_{yi,j}^{k},\\&-\delta_y^{-}H_{xi,j}^{k}+\delta_x^{-}H_{yi,j}^{k}=\delta_y^{-}H_{xi,j}^{k-1}-\delta_x^{-}H_{yi,j}^{k-1}+2\varepsilon\delta_t^{-}E_{zi,j}^{k}.\end{aligned}\tag{3.10}$$

Thus we obtain, by recasting Eq. (3.10) into grid points, a new scheme as

$$\frac{\Delta t}{\Delta y}(E_{zi,j+1}^{k}-E_{zi,j}^{k})+2\mu H_{xi,j}^{k}=-\frac{\Delta t}{\Delta y}(E_{zi,j+1}^{k-1}-E_{zi,j}^{k-1})+2\mu H_{xi,j}^{k-1},\tag{3.11a}$$

$$-\frac{\Delta t}{\Delta x}(E^k_{zi+1,j}-E^k_{zi,j})+2\mu H^k_{yi,j}=\frac{\Delta t}{\Delta x}(E^{k-1}_{zi+1,j}-E^{k-1}_{zi,j})+2\mu H^{k-1}_{yi,j}, \tag{3.11b}$$

$$\begin{aligned}&-\frac{\Delta t}{\Delta y}(H^k_{xi,j}-H^k_{xi,j-1})+\frac{\Delta t}{\Delta x}(H^k_{yi,j}-H^k_{yi-1,j})-2\varepsilon E^k_{zi,j}\\&=\frac{\Delta t}{\Delta y}(H^{k-1}_{xi,j}-H^{k-1}_{xi,j-1})-\frac{\Delta t}{\Delta x}(H^{k-1}_{yi,j}-H^{k-1}_{yi-1,j})-2\varepsilon E^{k-1}_{zi,j}.\end{aligned} \tag{3.11c}$$

Let us analyze the truncation error of schemes (3.11a), (3.11b), and (3.11c). Firstly, let us analyze Eq. (3.11a).

$$-\frac{1}{\mu}\left(\frac{\partial E_z}{\partial y}\right)^{k-(1/2)}_{i,j}=-\frac{1}{2\mu}\left[\left(\frac{\partial E_z}{\partial y}\right)^k_{i,j}+\left(\frac{\partial E_z}{\partial y}\right)^{k-1}_{i,j}\right]+O(\Delta t^2), \tag{3.12}$$

$$\left(\frac{\partial H_x}{\partial t}\right)^{k-(1/2)}_{i,j}=\frac{(H_x)^k_{i,j}-(H_x)^{k-1}_{i,j}}{\Delta t}+O(\Delta t^2). \tag{3.13}$$

By Eq. (2.9), we have

$$\frac{\partial H_x}{\partial t}=-\frac{1}{\mu}\frac{\partial E_z}{\partial y},$$

then

$$\left(\frac{\partial H_x}{\partial t}\right)^{k-(1/2)}_{i,j}=-\frac{1}{\mu}\left(\frac{\partial E_z}{\partial y}\right)^{k-(1/2)}_{i,j}. \tag{3.14}$$

Substituting Eq. (3.12) and (3.13) into Eq. (3.14), we obtain

$$\frac{(H_x)^k_{i,j}-(H_x)^{k-1}_{i,j}}{\Delta t}=-\frac{1}{2\mu}\left[\left(\frac{\partial E_z}{\partial y}\right)^k_{i,j}+\left(\frac{\partial E_z}{\partial y}\right)^{k-1}_{i,j}\right]+O(\Delta t^2), \tag{3.15}$$

so

$$\frac{H^k_{xi,j}-H^{k-1}_{xi,j}}{\Delta t}=-\frac{1}{2\mu}\frac{E^k_{zi,j+1}-E^k_{zi,j}}{\Delta y}-\frac{1}{2\mu}\frac{E^{k-1}_{zi,j+1}-E^{k-1}_{zi,j}}{\Delta y}+O(\Delta t^2+\Delta y). \tag{3.16}$$

Secondly, we can easily get in the similar way that the truncation errors of Eqs. (3.11b) and (3.11c) are $O(\Delta t^2+\Delta x)$ and $O(\Delta t^2+\Delta x+\Delta y)$. So the truncation error of Eq. (3.11) is $O(\Delta t^2+\Delta x+\Delta y)$.

Scheme (3.11) is an implicit scheme that involves solving a linear system of $E^k_{zi,j}$, $H^k_{xi,j}$, and $H^k_{yi,j}$ at each time step. Suppose the computational space domain is $[0,T_x]\times[0,T_y]$, T_x is period of x direction and T_y is period of y direction. $[0,T_x]$ is averagely divided by M and $[0,T_y]$ is averagely divided by N. We take numerical periodic boundary conditions as

$$E^k_{z0,j}=E^k_{zM,j},\quad E^k_{zM+1,j}=E^k_{z1,j},\quad E^k_{zi,0}=E^k_{zi,N},\quad E^k_{zi,N+1}=E^k_{zi,1}, \tag{3.17}$$

$$H^k_{x0,j}=H^k_{xM,j},\quad H^k_{xM+1,j}=H^k_{x1,j},\quad H^k_{xi,0}=E^k_{zi,N},\quad H^k_{xi,N+1}=H^k_{xi,1}, \tag{3.18}$$

$$H^k_{y0,j}=H^k_{yM,j},\quad H^k_{yM+1,j}=H^k_{y1,j},\quad H^k_{yi,0}=H^k_{yi,N},\quad H^k_{yi,N+1}=H^k_{yi,1}. \tag{3.19}$$

The arrangement of the order of equations in scheme (3.11) and the variables of the resulting linear system are trivial and technical. The properties of the coefficient matrix of the resulting

large linear system may change extremely with the different arrangements. We can make the coefficient matrix symmetric by the following arrangement. We arrange variables as

$$x^k = [x_1^k, x_2^k, x_3^k]^T,$$

$$x_1^k = [H_{y1,1}^k, H_{y2,1}^k, \ldots, H_{yM,1}^k, H_{y1,2}^k, H_{y2,2}^k, \ldots, H_{yM,2}^k, \ldots, H_{y1,N}^k, H_{y2,N}^k, \ldots, H_{yM,N}^k],$$

$$x_2^k = [E_{z1,1}^k, E_{z2,1}^k, \ldots, E_{zM,1}^k, E_{z1,2}^k, E_{z2,2}^k, \ldots, E_{zM,2}^k, \ldots, E_{z1,N}^k, E_{z2,N}^k, \ldots, E_{zM,N}^k],$$

$$x_3^k = [H_{x1,1}^k, H_{x2,1}^k, \ldots, H_{xM,1}^k, H_{x1,2}^k, H_{x2,2}^k, \ldots, H_{xM,2}^k, \ldots, H_{x1,N}^k, H_{x2,N}^k, \ldots, H_{xM,N}^k],$$

and the order of equations as Eq. (3.11b), $j=1,\ldots,N$, $i=1,\ldots,M$; Eq. (3.11c), $j=1,\ldots,N$, $i=1,\ldots,M$; and Eq. (3.11a), $j=1,\ldots,N$, $i=1,\ldots,M$. Then the resulting linear system is

$$A(\Delta t, \Delta x, \Delta y)x^{k+1} = B(\Delta t, \Delta x, \Delta y)x^k, \tag{3.20}$$

where

$$A(\Delta t, \Delta x, \Delta y) = \begin{pmatrix} A_{11} & A_{12} & 0 \\ A_{12}^T & A_{22} & A_{23} \\ 0 & A_{23}^T & A_{33} \end{pmatrix}, \quad B(\Delta t, \Delta x, \Delta y) = \begin{pmatrix} A_{11} & -A_{12} & 0 \\ -A_{12}^T & A_{22} & -A_{23} \\ 0 & -A_{23}^T & A_{33} \end{pmatrix},$$

$$A_{11} = 2\mu \begin{pmatrix} I & & & & \\ & I & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & I \end{pmatrix}, \quad A_{22} = -2\varepsilon \begin{pmatrix} I & & & & \\ & I & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & I \end{pmatrix},$$

$$A_{33} = 2\mu \begin{pmatrix} I & & & & \\ & I & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & I \end{pmatrix}, \quad A_{12} = \frac{\Delta t}{\Delta x} \begin{pmatrix} C & & & & \\ & C & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & C \end{pmatrix}, \tag{3.21}$$

$$C = \begin{pmatrix} 1 & -1 & & & & & \\ & 1 & -1 & & & & \\ & & \cdot & \cdot & & & \\ & & & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \\ & & & & & 1 & -1 \\ -1 & & & & & & 1 \end{pmatrix}_{M\times M}, \quad A_{23} = \frac{\Delta t}{\Delta y} \begin{pmatrix} -I & & & & I \\ I & -I & & & \\ & I & \cdot & & \\ & & \cdot & \cdot & \\ & & & I & -I \end{pmatrix},$$

I is the identity element belonging to $R^{M\times M}$.

Obviously $A(\Delta t, \Delta x, \Delta y)$ is symmetric. Moreover the coefficient matrix $A(\Delta t, \Delta x, \Delta y)$ of Eq. (3.20) is a strictly diagonally dominant matrix, if Δt, Δx, and Δy satisfy the following condition:

$$\frac{\Delta t}{\Delta x} < \mu, \frac{\Delta t}{\Delta x} + \frac{\Delta t}{\Delta y} < \varepsilon, \frac{\Delta t}{\Delta y} < \mu, \tag{3.22}$$

Eq. (3.22) leads to

$$\Delta t < \min\left\{ \mu \min(\Delta x, \Delta y), \frac{1}{2}\varepsilon \min(\Delta x, \Delta y) \right\}. \tag{3.23}$$

IV. THE COMPOSITION SCHEME BASE ON SELF-ADJOINT SCHEME (3.11) IN TIME DIRECTION

In the theory of numerical solutions of ordinary differential equations (ODEs), composition is an important idea that a high order method based on some low-order method can be derived. The composition method for ODEs has mainly been developed by Suzuki,[25] Yoshida,[26] and McLachlan.[27] With regard to the details, we refer to Ref. 28.

First, we review briefly the composition method for the ordinary differential equations. We know that every one-step difference scheme can be written as follows:[29]

$$y_{n+1} = s(\tau) y_n,$$

where $s(\tau)$ is the operator corresponding to the difference scheme and τ is the time step length.

Definition 4.1: *Suppose there are n difference schemes whose corresponding operators are* $s_1(\tau), s_2(\tau), \ldots, s_n(\tau)$, *respectively, and their corresponding order is* $p_1, p_2, \ldots, p_n$. *If there exist constants* $c_1, c_2, \ldots, c_n$ *such that the order of the scheme whose operator is the composition* $s_1(c_1\tau)s_2(c_2\tau), \ldots, s_n(c_n\tau)$ *is m,* $m > \max(p_i)$, $i \leqslant i \leqslant n$, *then the new difference scheme is called composition scheme of the original n difference schemes. This method which is used to construct higher-order difference schemes from the lower ones is called composition method.*

Definition 4.2: *An integral operator* $s^*(\tau)$ *is called the adjoint operator of* $s(\tau)$, *if* $s^*(\tau)$ *satisfies* $s^*(-\tau)s(\tau) = s(\tau)s^*(-\tau) = I$, *where I is the identity operator.*

Definition 4.3: *An integral operator is self-adjoint operator, if* $s(\tau)$ *satisfies* $s(-\tau)s(\tau) = s(\tau) \times (-\tau) = I$, *where I is the identity operator.*

Theorem 4.1: *Any self-adjoint integral operator* $s(\tau)$ *has even order.*

Corollary 4.1: *Let* $s(\tau)$ *be a self-adjoint integrator order of* $2n$, *then the composition operator* $s(c_1\tau)s(c_2\tau)s(c_1\tau)$ *is of order* $2n+2$, *where* c_1 and c_2 *satisfy*

$$2c_1^{2n+1} + c_2^{2n+1} = 0, \quad 2c_1 + c_2 = 1.$$

The composition schemes keep the group property of the original schemes. The composition method for multisymplectic schemes has been discussed in Refs. 30 and 31. Here we only discuss the composition based on the new scheme (3.11). First, we will show that it is a self-adjoint scheme.

Equation (3.20) can be written as follows:

$$x^{k+1} = [A(\Delta t, \Delta x, \Delta y)]^{-1} B(\Delta t, \Delta x, \Delta y) x^k. \tag{4.1}$$

By Eq. (3.21), we know $-A(\Delta t, \Delta x, \Delta y) = B(-\Delta t, \Delta x, \Delta y)$ and $A(-\Delta t, \Delta x, \Delta y) = -B(\Delta t, \Delta x, \Delta y)$, then

$$\begin{aligned}&[A(-\Delta t, \Delta x, \Delta y)]^{-1} B(-\Delta t, \Delta x, \Delta y)[A(\Delta t, \Delta x, \Delta y)]^{-1} B(\Delta t, \Delta x, \Delta y)\\ &\quad = [B(\Delta t, \Delta x, \Delta y)]^{-1} A(\Delta t, \Delta x, \Delta y)[A(\Delta t, \Delta x, \Delta y)]^{-1} B(\Delta t, \Delta x, \Delta y) = I.\end{aligned}$$

Similarly,

$$[A(\Delta t, \Delta x, \Delta y)]^{-1} B(\Delta t, \Delta x, \Delta y)[A(-\Delta t, \Delta x, \Delta y)]^{-1} B(-\Delta t, \Delta x, \Delta y) = I.$$

So, $[A(\Delta t, \Delta x, \Delta y)]^{-1} B(\Delta t, \Delta x, \Delta y)$ is a self-adjoint operator. Thus, scheme (3.11) is self-adjoint.

According to Corollary 4.1, we can derive a composition scheme in the time direction based on the self-adjoint scheme,

$$x^{k+1} = [A(c_1\Delta t,\Delta x,\Delta y)]^{-1}B(c_1\Delta t,\Delta x,\Delta y)\circ[A(c_2\Delta t,\Delta x,\Delta y)]^{-1}B(c_2\Delta t,\Delta x,\Delta y)$$
$$\circ[A(c_1\Delta t,\Delta x,\Delta y)]^{-1}B(c_1\Delta t,\Delta x,\Delta y)x^k, \tag{4.2}$$

where $c_1=1/(2-\sqrt[3]{2})$ and $c_2=-\sqrt[3]{2}/(2-\sqrt[3]{2})$. The truncation error of the above composition scheme is $O(\Delta y+\Delta x+\Delta t^4)$.

Theorem 4.2: *The composition scheme (4.2) is multisymplectic with the same discrete multisymplectic conservation law [Eq. (3.5)].*

Proof: *The implementation of the composition scheme is divided into the following three steps:*

$$x^k \to x^{k+c_1\Delta t} \to x^{k+(c_1+c_2)\Delta t} \to x^{k+(2c_1+c_2)\Delta t} = x^{k+1}.$$

By Theorem 3.1, we know that the first step $x^k \to x^{k+c_1\Delta t}$ preserves the multisymplectic conservation law,

$$\omega_{ij}^{k+c_1\Delta t} - \omega_{ij}^k = -c_1\Delta t(\delta_x^+\varphi_{ij}^k + \delta_y^+\psi_{ij}^k). \tag{4.3}$$

Similarly, multisymplectic conservation laws,

$$\omega_{ij}^{k+(c_1+c_2)\Delta t} - \omega_{ij}^{k+c_1\Delta t} = -c_2\Delta t(\delta_x^+\varphi_{ij}^k + \delta_y^+\psi_{ij}^k) \tag{4.4}$$

and

$$\omega_{ij}^{k+1} - \omega_{ij}^{k+(c_1+c_2)\Delta t} = -c_1\Delta t(\delta_x^+\varphi_{ij}^k + \delta_y^+\psi_{ij}^k), \tag{4.5}$$

should be preserved by the next steps, respectively.

Then, Eq. (4.3)+Eq. (4.4)+Eq. (4.5) leads to

$$\omega_{ij}^{k+1} - \omega_{ij}^k = -(2c_1+c_2)\Delta t(\delta_x^+\varphi_{ij}^k + \delta_y^+\psi_{ij}^k). \tag{4.6}$$

Because of $2c_1+c_2=1$, Eq. (4.6) is just Eq. (3.5). □

V. NUMERICAL EXPERIMENTS

This section provides numerical experiments for testing the new derived multisymplectic scheme [Eq. (3.11)] and the composition scheme [Eq. (4.2)]. Scheme (3.11) is denoted by MS and Eq. (4.2) is denoted by CMS. On numerical experiments of Maxwell's equations, there have been many references with more details. In the following numerical examples, we only discuss the closed homogeneous domain and take the numerical periodic boundary conditions as Eqs. (3.17)–(3.19). At the same time, we take $h=\Delta x=\Delta y$ and make Δt satisfy Eq. (3.23) to ensure the symmetry and strictly diagonal dominance of the coefficient matrix and we use GMRES(m) method to solve linear system. In each subinterval $[t^k,t^{k+1}]$, we only need to solve a system of equations $A(\Delta t,\Delta x,\Delta y)x^{k+1}=B(\Delta t,\Delta x,\Delta y)x^k$. Suppose that $\hat{E}_z(x,y,t)$ is the exact solution and $E_{z,i,j}^k$ is the numerical solution. We denote the maximum error and L_2 error at time $t=t_k$, respectively, by

$$\text{error}_{\max} = \max_{i,j}|\hat{E}_z(x_i,y_j,t_k) - E_{z,i,j}^k|,$$

$$\|\text{error}\|_{L_2} = h\sqrt{\sum_{i,j}(\hat{E}_z(x_i,y_j,t_k) - E_{z,i,j}^k)^2}.$$

The numerical results show that both MS and CMS can work well. By comparison, we can find that CMS has an improvement in accuracy of the solution for long time computation over MS.

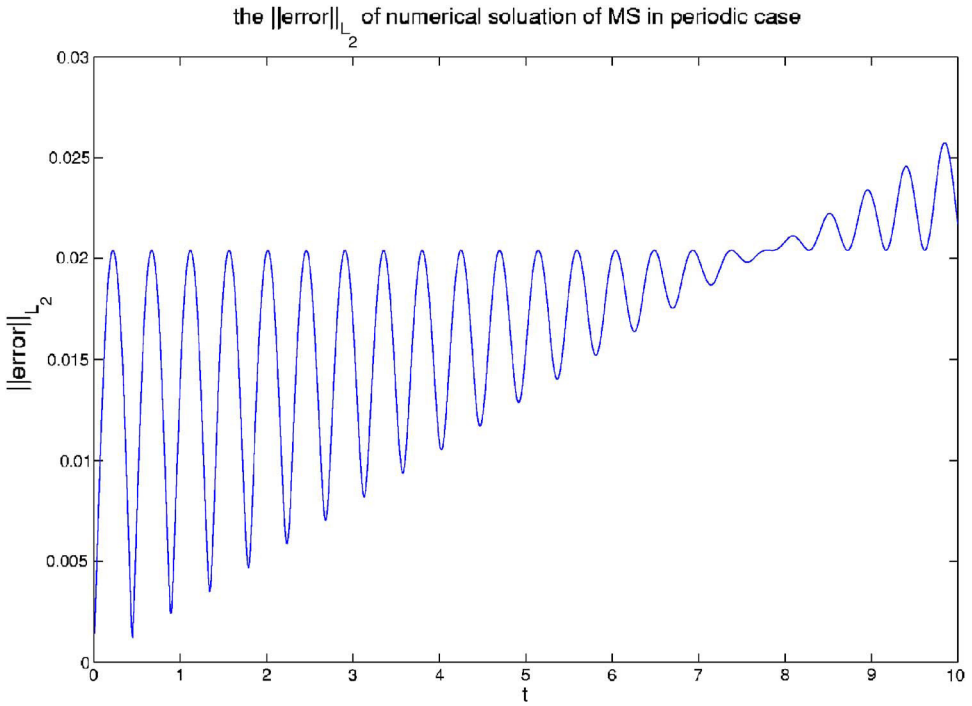

FIG. 1. The $\|\text{error}\|_{L_2}$ of MS, where $h=1/120$ and $\Delta t=1/100$.

Firstly, let us pay attention to the following example. We prescribe initial conditions as follows:

$$E_z(x,y,0)=0,$$

$$H_y(x,y,0)=-\frac{3}{\sqrt{5}}\cos(3\pi x)\sin(\pi y),$$

$$H_x(x,y,0)=\frac{1}{\sqrt{5}}\sin(3\pi x)\cos(\pi y).$$

We test the two schemes on a space domain $[0,\frac{2}{3}]\times[0,2]$. If $\mu=1$ and $\varepsilon=2$, the exact solution is

$$E_z(x,y,t)=\sin(3\pi x)\sin(\pi y)\sin(\sqrt{5}\pi t),$$

$$H_y(x,y,t)=-\frac{3}{\sqrt{5}}\cos(3\pi x)\sin(\pi y)\cos(\sqrt{5}\pi t),$$

$$H_x(x,y,t)=\frac{1}{\sqrt{5}}\sin(3\pi x)\cos(\pi y)\cos(\sqrt{5}\pi t).$$

Figures 1 and 2 show $\|\text{error}\|_{L_2}$ of MS and CMS under the same conditions of the space step and the temporal step. From Figs. 1 and 2, we can easily find that the error of MS can be controlled effectively before $t=8$, but CMS can be controlled effectively until $t=22$.

Figures 3 and 4 show, respectively, $\|\text{error}\|_{L_2}$ of MS and CMS with the same space step $h=1/180$. By Figs. 3 and 4, we can observe that the global error of the two schemes are almost the

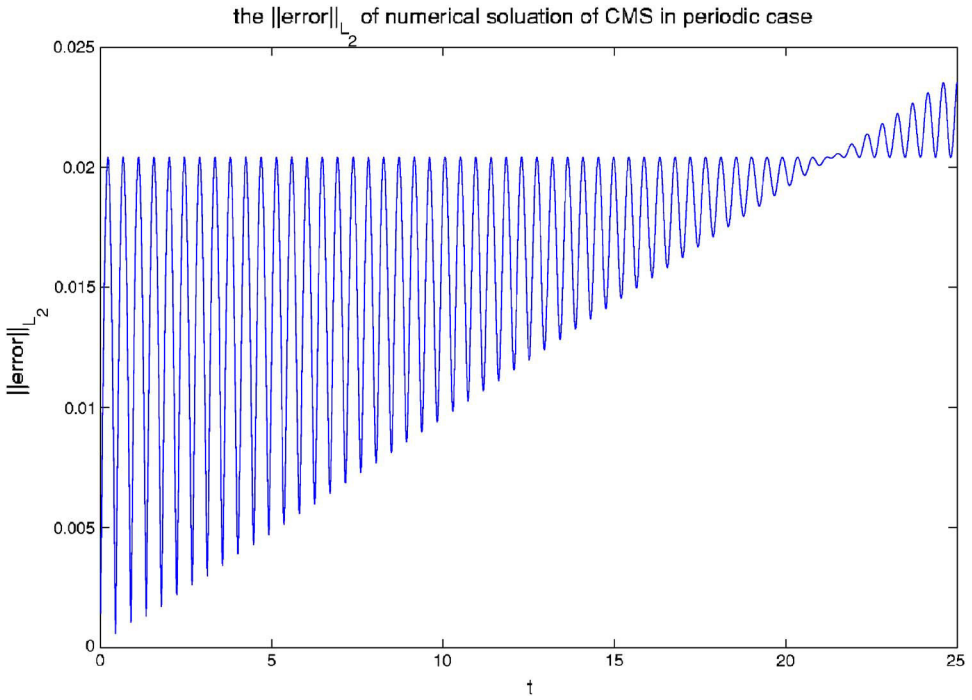

FIG. 2. The $\|\text{error}\|_{L_2}$ of CMS, where $h=1/120$ and $\Delta t=1/100$.

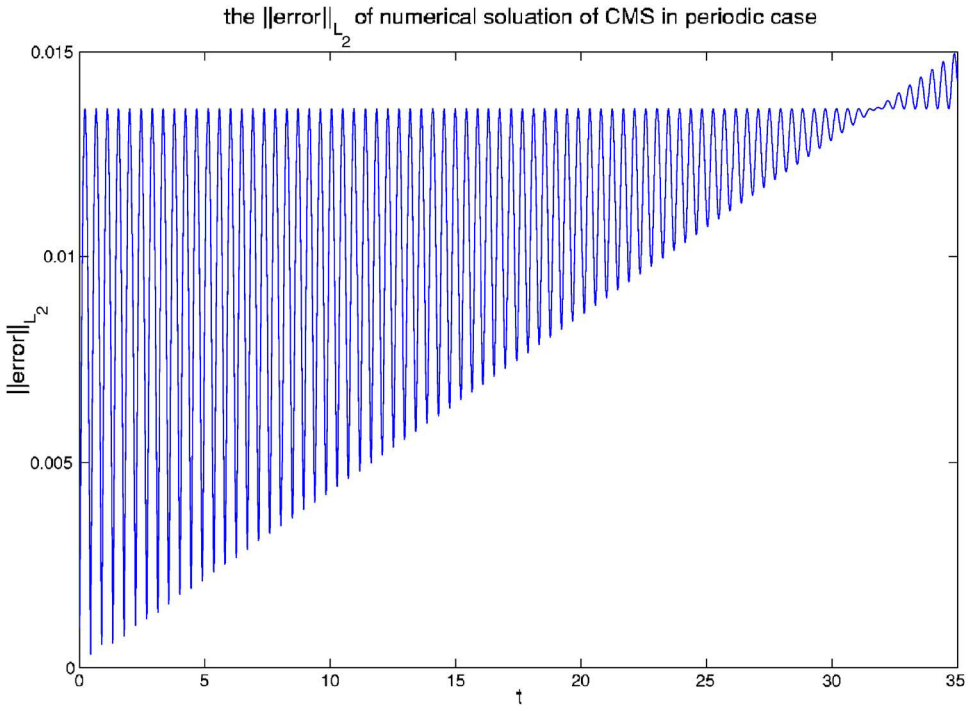

FIG. 3. The $\|\text{error}\|_{L_2}$ of CMS, where $h=1/180$ and $\Delta t=1/100$.

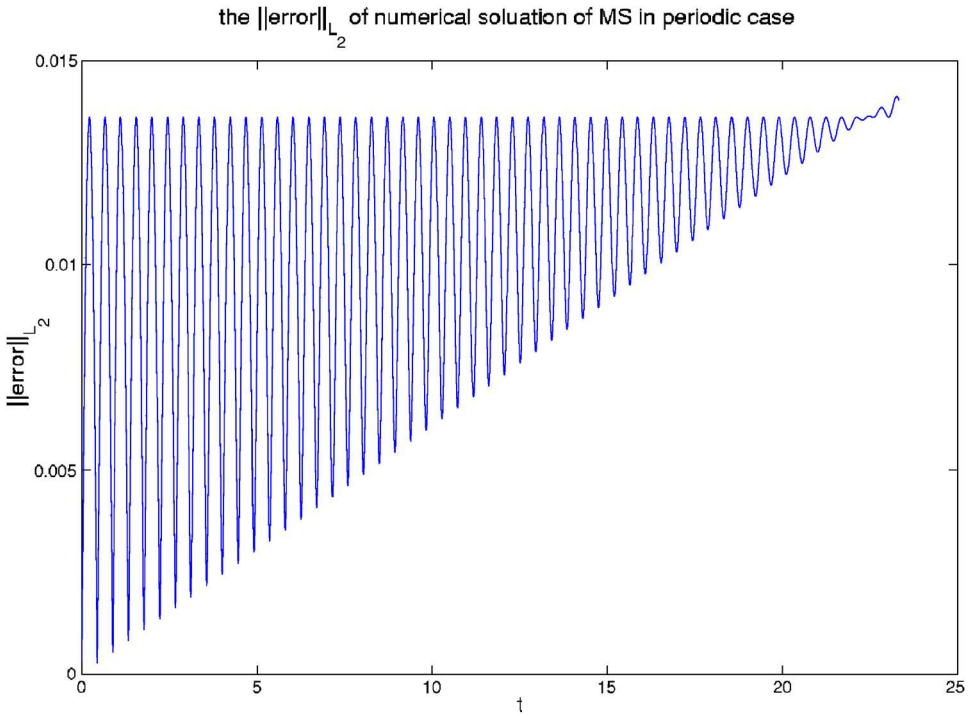

FIG. 4. The $\|\text{error}\|_{L_2}$ of MS, where $h=1/180$ and $\Delta t=1/300$.

same. However, it is worthy to mention that the time step taken for the MS is smaller than the CMS. Moreover, the time that the $\|\text{error}\|_{L_2}$ of CMS can be controlled is $t<33$, but it is only $t<22$ for MS.

Figures 5 and 6 have the same phenomenon about $\text{error}_{\max}$. Through comparison, it is easy to find that CMS is more effective in computation with long time step than MS.

Secondly, we consider another example. We prescribe initial conditions as follows:

$$E_z(x,y,0)=\sin(3\pi x)\sin(4\pi y),$$

$$H_y(x,y,0)=-\frac{3}{5}\sin(3\pi x)\sin(4\pi y),$$

$$H_x(x,y,0)=-\frac{4}{5}\cos(3\pi x)\cos(4\pi y).$$

If $\mu=1$ and $\varepsilon=1$, the exact solution is

$$E_z(x,y,t)=\sin(3\pi x-5\pi t)\sin(4\pi y),$$

$$H_y(x,y,t)=-\frac{3}{5}\sin(3\pi x-5\pi t)\sin(4\pi y),$$

$$H_x(x,y,t)=-\frac{4}{5}\cos(3\pi x-5\pi t)\cos(4\pi y).$$

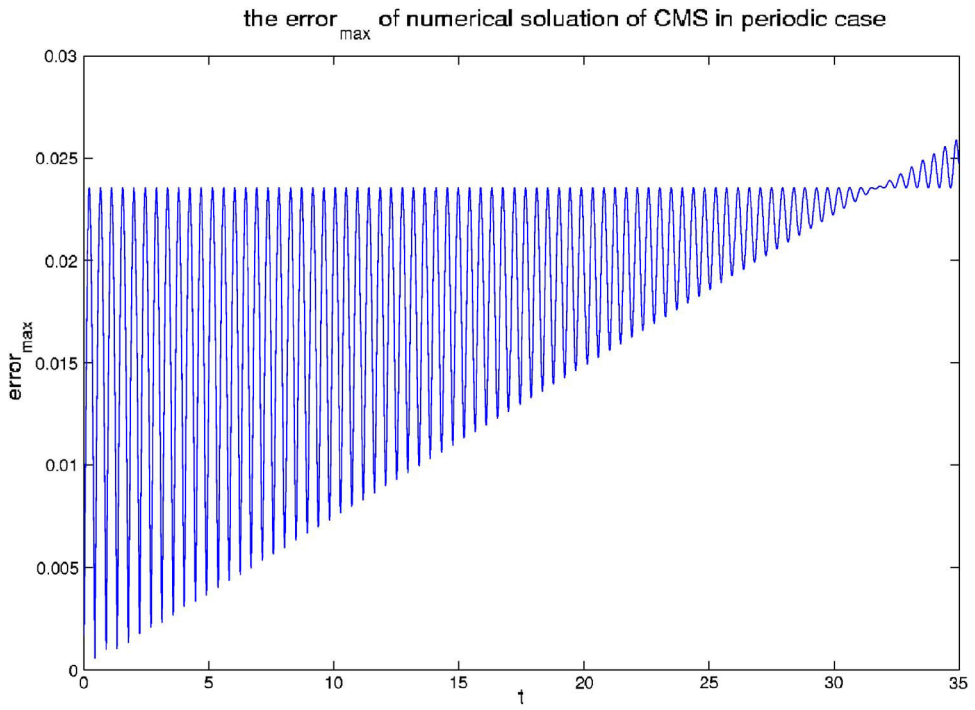

FIG. 5. The $\text{error}_{\max}$ of CMS, where $h=1/180$ and $\Delta t=1/100$.

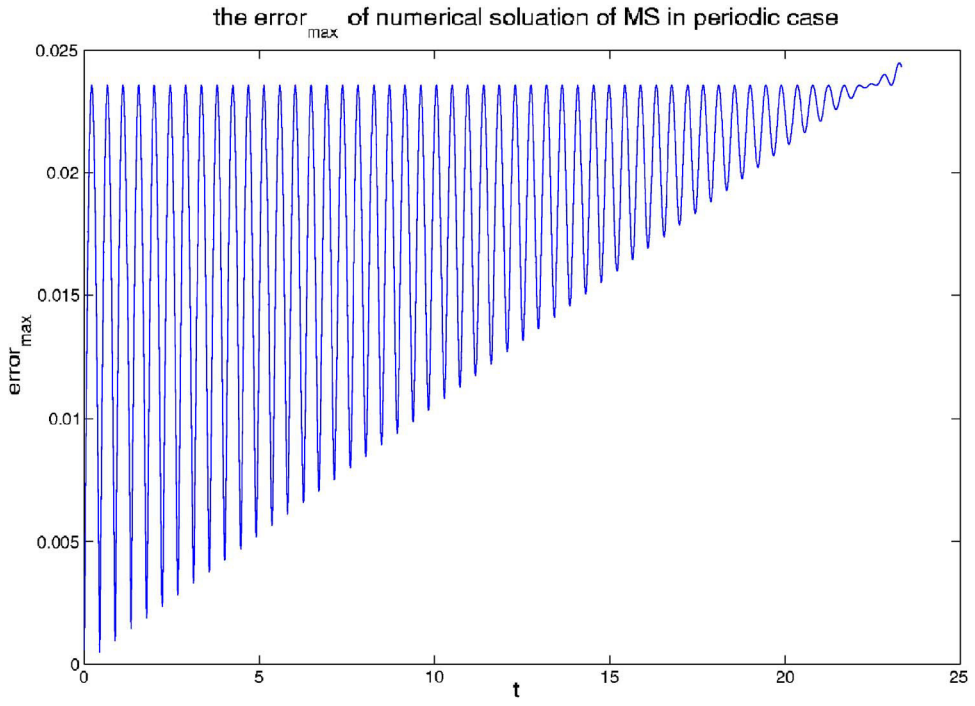

FIG. 6. The $\text{error}_{\max}$ of MS, where $h=1/180$ and $\Delta t=1/300$.

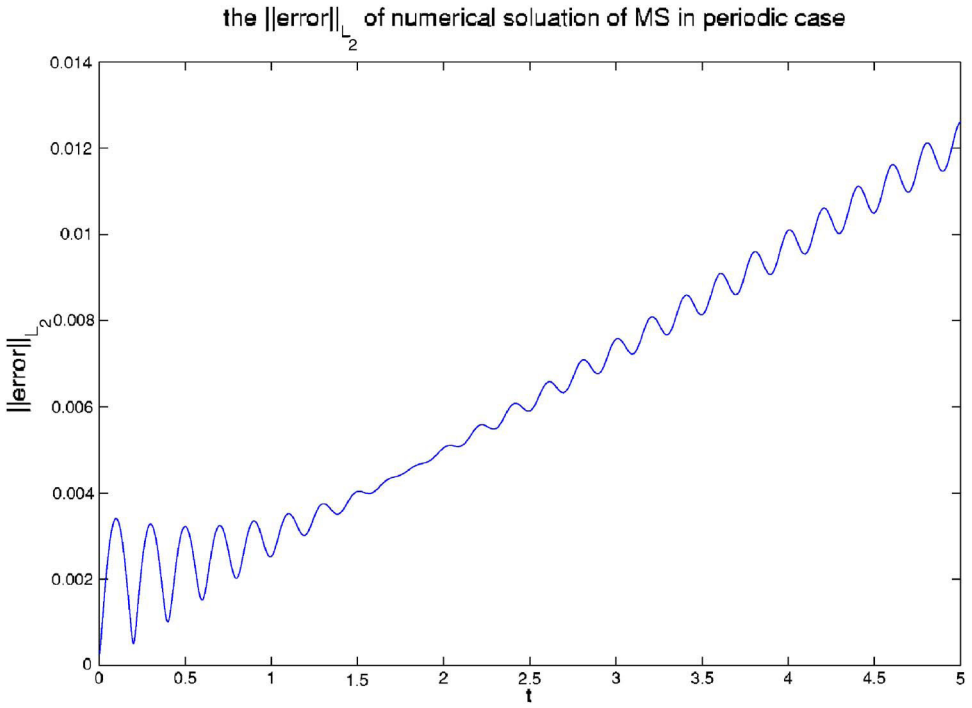

FIG. 7. The $\|\text{error}\|_{L_2}$ of MS, where $h=1/360$ and $\Delta t=1/200$.

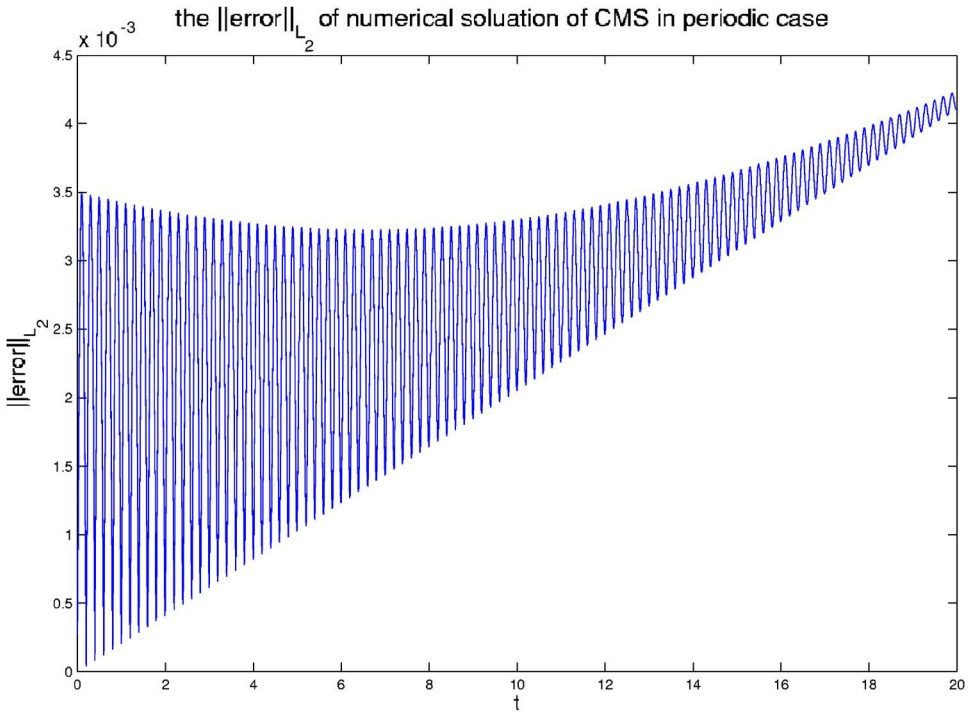

FIG. 8. The $\|\text{error}\|_{L_2}$ of CMS, where $h=1/360$ and $\Delta t=1/200$.

Here, we give the $\|\text{error}\|_{L_2}$ of MS and CMS with $h=1/360$ and $\Delta t=1/200$ in Figs. 7 and 8 correspondingly. The computational space domain is $[0,\frac{2}{3}]\times[0,\frac{1}{2}]$. The $\text{error}_{\max}$ has the same trend as $\|\text{error}\|_{L_2}$.

Remark:

1. The $\|\text{error}\|_{L_2}$ of CMS has no improvement over MS from the very beginning period of time because both schemes are of order one in space direction which is the dominating order in the truncation errors.
2. CMS is better than MS in long time computation because CMS is of the order of 4 in time, whereas MS is of 2. How to improve the truncation error in space direction is still a problem and worthy of paying more attention.

VI. CONCLUDING REMARKS

In this paper, we derived a new multisymplectic self-adjoint scheme from Bridges' form for Maxwell's equations. Based on the newly derived scheme, we obtain the composition scheme in time direction. Numerical experiments indicate that both the multisymplectic scheme and its composition scheme can work well and the composition scheme is more effective in long time computation. Though our numerical experiments are carried on two dimensional Maxwell's equations, the method of this paper can be extended into three dimensions with variable coefficients ε and μ. Actually, the multisymplectic structures [Eqs. (2.7) and (3.9)] are for the three dimensional Maxwell's equations. The multisymplectic structure and multisymplectic scheme provide a new viewpoint to study the electromagnetic wave equations.

ACKNOWLEDGMENTS

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Clifford representations in integrable systems

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In this paper we analyze integrable systems from a Clifford algebra point of view. This approach allows us to give a clear representation theoretic exposition of techniques used in spin systems, thereby showing their naturality. We then extend this approach to the analysis of the XX-model with nondiagonal boundaries which is among others related to growing and fluctuating interfaces and stochastic reaction-diffusion systems. With this rationale, it is possible to diagonalize the system and find new hidden conservation laws. © *2006 American Institute of Physics.*
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INTRODUCTION

The use of Clifford operators to "fermionize" a problem goes back to Ref. 1. The potential this approach has in solving spin-chain problems was first demonstrated in Ref. 2; see Refs. 3–6 for other early sources. There has been a lot of work in this direction, Refs. 7–11 to name a few. We will first give a novel presentation of this "classic" connection between spin-chain Hamiltonians and their fermionization using Clifford operators. This is done in a concise mathematical way focusing on the Clifford algebra aspects. This allows us to explain properties, procedures, and characteristics which appear complex and complicated in the spin-chain picture in a clean straightforward fashion as direct consequences of the mathematical setup. We hope that this treatment may help to bring the two communities, the people working in mathematical physics using group theory and the people working on integrable systems, closer together. We then show that going beyond the classical quadratic Hamiltonians, we can in certain cases, namely the XX-model, extend to include boundary terms. There are some subtleties here. First we have to actually enlarge the chain to be able to obtain a quadratic Hamiltonian, one of whose sectors is the original problem. Then, after the fermionization, we have to project to the smaller problem, which is nontrivial in the fermion language. As we explain, the actual calculation of the fermionization is a matrix valued problem due to the theorem[1,12,13] about the uniqueness of the irreducible Clifford module of the complex Clifford algebra based on an even dimensional vector space. We then go on to analyze operators which commute with the XX-chain Hamiltonian with boundary terms. These operators can be shown to commute, but due to the nonlocal nature of the Jordan-Wigner transformation *and* the projection, they become highly nontrivial in the original spin-chain picture. Lastly, we comment on how this operator behaves in the thermodynamic limit.

I. CLIFFORD ALGEBRAS AND SPIN CHAINS: A DIGEST

A. The Clifford algebra and fermions

A Clifford algebra $C(W,Q)$ is a universal algebra associated with a given $\mathbb{R}$-vector space W with a quadratic form Q. The universal property is that any linear map $j:W\to A$ of W to an associative $\mathbb{R}$-algebra A with unit 1 which satisfies $j(w)^2=Q(w)1$ factors through $C(W,Q)$ uniquely up to isomorphism. To be really careful of course the universal object $C(W,Q)$ comes with a map $\iota:W\to C(W,Q)$ and j factors through ι. For W with $\dim_{\mathbb{R}} W=k$ and a basis (e_i) of W,

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the algebra $C(W,Q)$ is a quadratic algebra generated by $e_i: i=1,\ldots,k$ and the relations $\forall n,m: \{e_n,e_m\}=2\langle e_n,e_m\rangle$ where $\langle\cdot,\cdot\rangle$ is the bilinear form associated with the quadratic form Q. (Technically, for this one has to assume that one is not in characteristic 2. This is fine since we will be working over $\mathbb{R}$ and $\mathbb{C}$ that is in characteristic 0.) We will usually not distinguish v and $\imath(v)$ in our notation, but sometimes it will be necessary. It can easily be seen that $\dim_{\mathbb{R}}(C(W,Q))=2^n$ for W as above and any Q. See, e.g., Refs. 12 and 13 for these results.

The classical example is the Clifford algebra $C_k := C(\mathbb{R}^k, \mathrm{diag}(-1,\ldots,-1))$. This algebra can be written as generated by e_n subject to the conditions $e_n^2=-1, e_m e_n+e_n e_m=0$. Now there are the standard isomorphisms $C_2 \simeq \mathbb{H} \simeq \mathrm{su}(2)$. Where one sends $e_1 \mapsto I, e_2 \mapsto J$, here I, J, and K are the usual quaternions and in the last step one represents I and J by the usual 2×2 matrices. Alternatively one can of course use the first two elements of any cyclic permutation of the matrices representing I, J, and K.

We will consider the complexified Clifford algebra $Cl_k := \mathbb{C}\otimes_{\mathbb{R}} C_k$. Notice that over the complexes all nondegenerate forms are conjugate and we will only work with such forms. Thus the Clifford algebras over $\mathbb{C}$ do not depend on the particular form of Q as long as it is nondegenerate. In general it can even be shown that $Cl_{2L} \simeq M_{2^L}(\mathbb{C})$, the full matrix algebra, see, e.g., Refs. 12 and 13. To pass from one quadratic form to another one makes a base change on the underlying vector space. This gives a change in presentation of the algebra. The algebra Cl_2 for the quadratic form $\mathrm{diag}(1,1)$, for instance, is just $M_2(\mathbb{C})$, and we can represent it via $e_1' \mapsto \sigma_x, e_2' \mapsto \sigma_y$. Since $\sigma x = -iK$ *and* $\sigma_y = -iJ$ *in their standard matrix representations (see, e.g., Ref. 13), we obtain an isomorphism with* $Cl_2 = \mathbb{C}\otimes_{\mathbb{R}} C_2$ *by using the permutation as mentioned above to represent the Clifford algebra and then use the complex base change* $e_j' = (-i)e_j$. *Of course* $JK=I$ *and* $\sigma_x\sigma_y = -KJ = I = i\sigma_z$.

In general, there are two standard quadratic forms: the first is given by the $k\times k$ matrix $\mathbb{1}_k = \mathrm{diag}(1,\ldots,1)$ and the second one which exists on $\mathbb{C}^{2L}$ is $\omega_{2L} = \frac{1}{2}\left(\begin{smallmatrix} 0 & \mathbb{1}_L \\ \mathbb{1}_L & 0 \end{smallmatrix}\right)$. The factor $\frac{1}{2}$ is added to cancel the factor of 2 in the relations. In the case that we are in even dimension that is in $\mathbb{R}^{2L}$ or after complexification in $\mathbb{C}^{2L}$, we fix the following notation for the basis elements. In the first case we denote the basis vectors $c_1^+,\ldots,c_L^+,c_1^-,\ldots,c_L^-$, and in the second case we will enumerate basis vectors $b_1,\ldots,b_L,a_1,\ldots,a_L$. This means that in the case of $\mathbb{C}^{2L}$ for the first basis we get the relations

$$\{c_m^\mu, c_n^\nu\} = 2\,\delta_{m,n}^{\mu,\nu} \tag{1}$$

for the generators of the Clifford algebra Cl_{2L} corresponding to this basis. These operators are usually called Clifford operators. For the second basis of $\mathbb{C}^{2L}$ we obtain the following relations for the generators of the Clifford algebra Cl_{2L}

$$\{b_n,a_m\} = \delta_{n,m}, \quad \{b_n,b_m\} = 0, \quad \{a_n,a_m\} = 0. \tag{2}$$

These operators are usually called fermion operators. (In a matrix representation one frequently also postulates $a_n^\dagger = b_n$. We will not impose this at the moment.) One can think of the b_n as creation and the a_n as annihilation operators of the nth fermion. The operator $N_n = b_n a_n$ then has eigenvalues of 0 or 1 corresponding to whether the fermion is present or not. The fermions can also just be seen as a representation of Cl_{2L} on the exterior algebra $\Lambda^*\mathbb{C}^L$. In the presentation of Eq. (2) we can write the Clifford algebra as $Cl^-\oplus Cl^0\oplus Cl^+$, where Cl^- is the subalgebra generated by the a_n, Cl^+ is the one generated by the b_n, and Cl^0 is the center generated by $\mathbb{C}$. The Fock space representation R_{Fock} is then given as follows; let $R_{|vac\rangle}$ be the one-dimensional representation of $Cl^0\oplus Cl^-$ on $\mathbb{C} = \mathbb{C}|vac\rangle$ for which $1|vac\rangle = |vac\rangle$ and $Cl^-|vac\rangle = 0$ then $R_{\mathrm{Fock}} = Cl\otimes_{Cl^0\oplus Cl^-} R_{|vac\rangle}$. Here $R_{\mathrm{Fock}} \simeq \Lambda^*\mathbb{C}^L$ as vector spaces and the Cl module structure is given by left multiplication.

The two sets of generators of Cl_{2L} are related by the simple base change on $W=\mathbb{C}^{2L}$,

$$b_n = \frac{1}{2}(c_n^+ + ic_n^-), \quad a_n = \frac{1}{2}(c_n^+ - ic_n^-),$$

$$c_n^+ = b_n + a_n, \quad c_n^- = \frac{1}{i}(b_n - a_n). \tag{3}$$

In the Clifford operator basis the role of the operator N_n is played by $ic_n^-c_n^+$ which has eigenvalues ± 1.

B. Spin chains

A spin chain of length L is a $\mathbb{C}$-vector space V which is a tensor product of L copies of a su(2) representation. A spin-chain Hamiltonian is an operator H which acts on such a V. (Sometimes a spin chain is taken to mean V together with H.) We will only be concerned with spin $\frac{1}{2}$. That is, $V=\otimes_{i=1}^{L}\mathbb{C}^2$ and $H: V \to V$ which means that $H \in GL(2^L, \mathbb{C})$. (Although the notation H is suggestive of both Hermitian and Hamiltonian, we will not restrict to the case that H is Hermitian.) The copies of $\mathbb{C}^2$ are usually called sites. Many of the interesting Hamiltonians are obtained by using linear and quadratic expressions in the Pauli-spin matrices σ_x, σ_y, and σ_z. It is well known that the Pauli matrices together with the identity matrix with $\mathbb{C}$ coefficients form a basis of $M_2(\mathbb{C}) \simeq \mathbb{C} \otimes \mathbb{H} \simeq \mathbb{C}^4$ as vector spaces.

Examples of such spin chains are the XX, XY, and XYZ or Heisenberg model. In particular, the XX chain has the Hamiltonian:

$$H_{\mathrm{XX}} = \frac{1}{2}\sum_{j=1}^{L}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+]. \tag{4}$$

$$\overset{j}{\downarrow}$$

Here we adopted the usual notation $\sigma_j := \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2 \otimes \sigma \otimes \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2$, where σ is inserted at the jth spot.

C. The Jordan-Wigner transformation

We recall that all the Clifford algebras are $\mathbb{Z}/2\mathbb{Z}$ graded. This can either be seen by using the involution on $C(W,Q)$ generated by $\iota(w) \mapsto -\iota(w)$ for $w \in W$ or the fact that the algebra is quadratic and hence the $\mathbb{Z}$ grading of the tensor algebra descends to a $\mathbb{Z}/2\mathbb{Z}$ grading on $C(W,Q)$. This splits the Clifford algebra into its even and odd parts, $C(W,Q)=C(W,Q)^{\mathrm{even}} \oplus C(W,Q)^{\mathrm{odd}}$.

A wonderful fact about Clifford algebras is that they satisfy $C(W \oplus W', P \oplus Q) \simeq C(W,P) \hat{\otimes} C(W',Q)$. Here it is important that we used $\hat{\otimes}$, that is, the tensor product as $\mathbb{Z}/2\mathbb{Z}$ graded spaces. Using this property, we see that $Cl_{2L} \simeq Cl_2^{\hat{\otimes} L} \simeq M_2(\mathbb{C})^{\hat{\otimes} L}$. But we should be careful that $M_2(\mathbb{C})^{\hat{\otimes} L} \neq M_2(\mathbb{C})^{\otimes L}$. So we cannot directly identify the spin-chain operators with Clifford operators, since the former are nongraded tensor products while the latter are graded. This is easily seen since σ_i commutes with σ_j for $i \neq j$ in the spin-chain case, while they should anticommute if they would be Clifford operators. Indeed this is forced by considering $\hat{\otimes}$.

This obstacle was overcome by Ref. 1 (see Ref. 2) by the following isomorphism of $Cl_{2L} \to Cl_2^{\otimes L}$:

$$\tau_j^{+,-} = \left(\prod_{i=1}^{j-1}\sigma_i^z\right)\sigma_j^{x,y}. \tag{5}$$

It can easily be checked that these operators satisfy Eq. (1). As noticed in Ref. 1, see also Ref. 13, this is the only irreducible module of Cl_{2L}—up to isomorphism of course. This can most quickly be seen by using the fact that Cl_{2L} is a matrix algebra over $\mathbb{C}$ and hence Morita equivalent to $\mathbb{C}$.

D. Free fermions and fermionization

Comparing the two paragraphs, we see that the Clifford operators, that is elements of Cl_{2L} after using the Jordan-Wigner transformation, are operators on the spin-chain vector space V.

Moreover, using the operators defined in Eq. (5), we have Clifford operators on the spin chain and using the transformation (3), we obtain fermion operators. This allows us to write down "simple" Hamiltonians,

$$H = \sum_{n=1}^{L} \Lambda_n i \tau_n^- \tau_n^+, \tag{6}$$

or in terms of the associated fermion operators:

$$H = \sum_{n=1}^{L} 2\Lambda_n b_n a_n - \sum_{n=1}^{L} \Lambda_n = \sum_{n=1}^{L} 2\Lambda_n N_n + E_0. \tag{7}$$

In this form it is clear that H is the Hamiltonian of L free fermions whose energies are Λ_n. The second summand is the constant term corresponding to the Fermi sea.

Now as mentioned the representation (5) is unique up to isomorphism, so we could also first apply a base change to the operators $\tau_{m,n}^{\mu,\nu}$ to obtain operators $T_{m,n}^{\mu,\nu}$. Since the τ are images of the basis elements of W, this amounts to using a change of basis $\mathbf{\Psi}$ on the underlying vector space W of the Clifford algebra. Notice that W is different from $V=(\mathbb{C}^2)^{\otimes L}$ and that dim $W=2L$, so that $\mathbf{\Psi}$ is a $2L\times 2L$ matrix. If we want that the operators T are still Clifford operators, that is they obey Eq. (1), then $\mathbf{\Psi}$ has to be an orthogonal transformation, that is, $\mathbf{\Psi}^t\mathbf{\Psi}=\mathbb{1}_{2L}$. Of course, in the fermionic case (7), the change of basis transformations $\mathbf{\Phi}$ preserving the relations (2) is the one that preserves ω: $\mathbf{\Psi}^t\omega_{2L}\mathbf{\Psi}=\omega_{2L}$.

Using these transformations, we obtain a class of Hamiltonians of the form

$$H = \sum_{n=1}^{L} \Lambda_n i T_n^- T_n^+. \tag{8}$$

Unravelling the definitions, we thus obtain spin chains describing free fermions. As spin-chain Hamiltonians, that is, expressed in terms of the σ-matrices, the form of H is highly nontrivial due to the nonlocal nature of the Jordan-Wigner transformation.

The fermionization problem is the inverse problem: When can I write a given spin chain in terms of free fermions? There is a way to go about this in case the Hamiltonian is a quadratic form in the elements τ,

$$H = \frac{1}{2} \sum_{\substack{(m,\mu),(n,\nu) \\ \text{s.t.}(m,\mu)\neq(n,\nu)}} M_{m,n}^{\mu,\nu} \tau_m^\mu \tau_n^\nu. \tag{9}$$

This is, for instance, the case if H is quadratic in the $\sigma^\pm$, $H=\Sigma A_{m,n}^{\mu,\nu}\sigma_m^\mu\sigma_n^\nu$, and one has only nearest neighbor interactions: $A_{m,n}^{\mu,\nu}=0$ if $|m-n|\neq 1$. Although we postulated that there are no diagonal entries, these entries would not pose any real problems, since due to the equation $(\tau_m^\mu)^2=1$ they would just contribute a constant term.

In this case, we can think of M as a quadratic form on the image $\imath(W)$ of W. Now due to the grading $\imath(W)$ is an *odd* vector space, so that the matrix M for a "symmetric" quadratic form will be skew symmetric. The aim now is to find a transformation of basis on W which makes H diagonal in the Clifford basis corresponding to the new basis as in Eq. (8). Let $\mathbf{\Lambda}=\text{diag}(\Lambda_1,\ldots,\Lambda_L)$, then the matrix problem one has to solve is $\mathbf{\Psi}^t M\mathbf{\Psi}=\left(\begin{smallmatrix} 0 & i\mathbf{\Lambda} \\ -i\mathbf{\Lambda} & 0 \end{smallmatrix}\right)$. Recalling that in order to preserve the fermion presentation of the Clifford algebra $\mathbf{\Psi}^t\mathbf{\Psi}=\mathbb{1}$, this reads

$$M\mathbf{\Psi} = \mathbf{\Psi}\begin{pmatrix} 0 & i\mathbf{\Lambda} \\ -i\mathbf{\Lambda} & 0 \end{pmatrix}. \tag{10}$$

This is the type of equation that is usually obtained by calculating the commutators of the operators T with the Hamiltonian;[2,7–11] here we find it by purely Clifford algebra considerations. Trans-

forming to the equations by writing $\mathbf{\Psi}=(\mathbf{\Psi}^+\mathbf{\Psi}^-)$ and $\mathbf{\Phi}^+=\mathbf{\Psi}^+ + i\mathbf{\Psi}^-, \mathbf{\Phi}^-=\mathbf{\Psi}^+ - i\mathbf{\Psi}^-$, the equations become the eigenvalue problem:

$$M\mathbf{\Phi}^{\pm} = \pm \mathbf{\Phi}^{\pm}\mathbf{\Lambda}. \tag{11}$$

Since the matrix $\mathbf{\Psi}$ is a base change on W which was of dimension $2L$, we get $2L$ eigenvalues. These come in pairs of $\pm\Lambda_n$. This is clear from the skew symmetry of M. Moreover looking at Eq. (8), we see that the change from Λ_n to $-\Lambda_n$ does not affect the spectrum of H. This symmetry corresponds to sending one of the $T_n \to -T_n$.

II. THE XX-MODEL WITH BOUNDARIES

Now the above procedure works well for Hamiltonians such as the Ising, XX, XY, Heisenberg-Ising chains,[2,15] and other models.

With some work one can also sometimes include boundary terms. For this we consider the Hamiltonian of Ref. 14 specialized to

$$H = \frac{1}{2}\sum_{j=1}^{L-1}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\sigma_1^- + \sigma_1^+ + \exp(i\chi)\sigma_L^+ + \exp(-i\chi)\sigma_L^-]. \tag{12}$$

A. Extending the chain

The H of Eq. (12) is not quadratic. On the other hand we can add the sites 0 and $L+1$ as in Refs. 16 and 17 and consider the Hamiltonian

$$H_{\text{long}} = \frac{1}{2}\sum_{j=1}^{L-1}[\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+] + \frac{1}{\sqrt{8}}[\sigma_0^x\sigma_1^- + \sigma_0^x\sigma_1^+ + \exp(i\chi)\sigma_L^+\sigma_{L+1}^x + \exp(-i\chi)\sigma_L^-\sigma_{L+1}^x], \tag{13}$$

which acts on $V_{\text{long}}=\otimes_{i=0}^{L+1}\mathbb{C}^2$. We see that H_{long} is of the form (9), since it is quadratic in the σ and has only nearest neighbor interactions. Thus we can apply the procedure of Sec. I D and express H_{long} in terms of $L+2$ fermions. From the form of H_{long} we see that the matrices σ_0^x and σ_{L+1}^x commute with H_{long}, so the spectrum of H_{long} decomposes into four sectors corresponding to the eigenvalues ± 1 of σ_0^x and σ_{L+1}^x. That is, we can write $V_{\text{long}}=\oplus_{(\mu,\nu)\in(\mathbb{Z}/2\mathbb{Z})^2}V_{\mu\nu}$. Here the notation $V_{\mu\nu}$ naturally means that $\sigma_0^x|V_{\mu\nu}=\mu id$ and $\sigma_{L+1}^x|V_{\mu\nu}=\nu id$. We can embed V into V_{long} via $v\mapsto v^+\otimes v\otimes v^+$, where $v^+=\binom{1}{1}$ is the eigenvector of σ_x with eigenvalue of 1. The isomorphic image of V is V_+. Under this embedding we see that $H\mapsto H_{\text{long}}|_{V++}$ and hence the spectrum of H is that of $H_{\text{long}}|_{V_{++}}$. The left inverse to the embedding map is the projection map $\pi: V_{\text{long}}\to V$ which simply projects out the first and last tensor factors.

B. Femionization of the extended chain

After substituting Eq. (5) into Eq. (13), the matrix M of Eq. (9) becomes

$$M = \begin{pmatrix} 0 & G & & & & & \\ -G^T & 0 & F & & & & \\ & -F^T & 0 & F & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -F^T & 0 & K & \\ & & & & -K^T & 0 & \end{pmatrix}, \tag{14}$$

where $F=1/4\left(\begin{smallmatrix} 0 & i \\ -i & 0 \end{smallmatrix}\right)$ and $G=1/2\left(\begin{smallmatrix} 0 & 2i/\sqrt{8} \\ 0 & 0 \end{smallmatrix}\right)$ and $K=1/2\left(\begin{smallmatrix} 0 & (i/\sqrt{8})2\cos(\chi) \\ 0 & (i/\sqrt{8})2\sin(\chi) \end{smallmatrix}\right)$. The corresponding diagonalization problem can be solved explicitly, see Ref. 14.

C. Projection to the original chain

Notice that the projection/restriction to V_{++} is clear in the spin-chain picture but not so obvious in the fermion language. The basic idea is to find the ground state which is in V_{++} and act on it by operators b. Let $\bar{B} \subset Cl^{+}_{2L+2}$ be the subalgebra generated by $b_1, \ldots, b_{L+1}$, then $\bar{B} = \bar{B}^{\text{even}} \oplus \bar{B}^{\text{odd}}$. There are vectors $v^{\pm}$ which satisfy $\sigma_0^x v^{\pm} = \pm v^{\pm}$ and either (1) $\sigma_{L+1}^x v^{\pm} = \pm v^{\pm}$ or (2) $\sigma_{L+1}^x v^{\pm} = \mp v^{\pm}$. Accordingly either

$$V_{++} = B^{\text{even}} v^{+} \text{ or } V_{++} = B^{\text{odd}} v^{-}. \tag{15}$$

We refer to Ref. 14 for the details. There is something interesting going on here that we would like to point out, although we do not fully understand the situation as of yet. The fact that V_{++} is generated by even or odd excitations seems to suggest that we are actually dealing with modules over $Cl^{\text{even}}_{2L+2} \subset Cl_{2L+2} \subset Cl_{2L+4}$, where Cl_{2L+2} is generated by the a_i and $b_i : i = 1, \ldots, L+1$. Now it is well known that $Cl^{\text{even}}_{2L+2} \cong Cl_{2L+1}$.[12,13] The dimension of the V_{++} is 2^L so it is tempting to conjecture that it is actually one of the spin representations and σ^x_{L+1} corresponds to the operator that distinguishes the two spin representations. This operator is $t = i^n \prod_{j=1}^{L+1} e_j$ in the standard notation. A quick calculation shows that $t \propto \prod_{j=1}^{L+1} \sigma_j^z$, so things are in reality a little more complicated, but the dimensional analysis and the fact that there are two representations distinguished by an operator with eigenvalues of ± 1 remain true. It would be interesting to find a complete representation theoretic explanation for the projection mechanism.

III. SUPERSELECTION SECTORS AND THE THERMODYNAMIC LIMIT

A. Operators commuting with *H*

Just as we derived nontrivial spin chains from free fermions and vice versa found free fermion representations of nontrivial spin chains, we can take operators which obviously commute with the free fermion Hamiltonian and transform them back to the spin chain to obtain nontrivial conserved quantities and hence superselection rules. One such operator is the total fermion number operator; another operator of this kind is treated in Ref. 18.

To exhibit this strategy, we will now apply these observations to the XX-model with boundaries discussed in the last section. Moreover, as we explain in the next paragraph, this operator is key to understanding the spectrum of H and its dependence on the parameter χ. Recalling that the fermions entering the original chain are those labeled by $1, \ldots, L+1$ (see Sec. II C), the total fermion number for the spin chain H is given by the projection of the operator:

$$\mathcal{F}^{\text{long}}_{\text{tot}} = \sum_{n=1}^{L+1} N_n = \sum_{n=1}^{L+1} b_n a_n. \tag{16}$$

We note that *a priori* it is not clear that this operator can actually be "projected." *A posteriori* this follows either from the explicit form, $\mathcal{F}^{\text{long}}_{\text{tot}} = \sigma_0^x \otimes \mathcal{F}_{\text{tot}} \otimes \sigma^x_{L+1}$, whose calculation we describe below, or from the results about the spectrum being given by an even or odd number of fermion excitations (see Sec. II C).

Denoting the entries of the matrix $\mathbf{\Phi} = (\mathbf{\Phi}^{+} \mathbf{\Phi}^{-})$ appearing in Eq. (11) by $(\phi_n^{\nu})_j^{\mu}$, that is, $(\phi_n^{\nu})_j^{\mu}$ with n and $\nu = \pm 1$ fixed, $\mu = \pm 1$, and $j = 0, \ldots, L+1$ is the eigenvector to the eigenvalue $\nu \Lambda_n$, we can write

$$\mathcal{F}^{\text{long}}_{\text{tot}} = \frac{1}{4} \sum_{n=1}^{L+1} \sum_{j,k=0}^{L+1} \sum_{\mu,\nu=\pm 1} (\phi_n^{-})_j^{\mu} (\phi_n^{+})_k^{\nu} \tau_j^{\mu} \tau_k^{\nu}. \tag{17}$$

Now the explicit form of the eigenvectors ϕ, which are known,[14] allows us to compute this expression projected to the short chain V in terms of the σ matrices of the original spin-chain picture (see Ref. 19 for the details),

$$\mathcal{F}_{\mathrm{tot}} = \frac{1}{4L+4} \sum_{\substack{j,k=1 \\ j+k \text{ odd}, j<k}}^{L} (-1)^{(j+k+1)/2} (\sigma_{j+1}^z \cdots \sigma_{k-1}^z) \times \left[\left(\frac{\sin(\chi(j-k)/(L+1))}{\sin(\pi(j-k)/(2L+2))} + \frac{\sin(\chi(j+k)/(L+1))}{\sin(\pi(j+k)/(2L+2))} \right) (\sigma_j^x \sigma_k^y - \sigma_j^y \sigma_k^x) + \left(\frac{\cos(\chi(j+k)/(L+1))}{\sin(\pi(j+k)/(2L+2))} \right) (\sigma_j^y \sigma_k^y - \sigma_j^x \sigma_k^x) \right]$$
$$+ \frac{1}{\sqrt{8}(L+1)} \left\{ \sum_{\substack{k=1 \\ k \text{ odd}}}^{L-1} (-1)^{(k+1)/2} \left[\frac{\cos(\chi k/(L+1))}{\sin(\pi k/(2L+2))} \sigma_1^z \sigma_2^z \cdots \sigma_{k-1}^z \sigma_k^x \right] \right.$$
$$+ \sum_{\substack{k=2 \\ k \text{ even}}}^{L} \left[(-1)^{(L+k+2)/2} \frac{\cos(\chi k/(L+1))}{\cos(\pi k/(2L+2))} \sigma_k^x + (-1)^{(k+L)/2} \frac{\sin(\chi k/(L+1))}{\cos(\pi k/(2L+2))} \sigma_k^y \right]$$
$$\left. \times (\sigma_{k+1}^z \cdots \sigma_{L-1}^z \sigma_L^z) \right\}. \tag{18}$$

In Eq. (18), we have taken the projection to the original chain H by using the equation $\mathcal{F}_{\mathrm{tot}}^{\mathrm{long}} = \sigma_0^x \otimes \mathcal{F}_{\mathrm{tot}} \otimes \sigma_{L+1}^x$. The fact that $\mathcal{F}_{\mathrm{tot}}^{\mathrm{long}}$ has this special form is the *a fortiori* reason that indeed the total fermion number is a quantity that is well defined on the original chain.

Depending on which case one is in (see Sec. II C), the eigenvalues are either odd or even. It is clear that it would be impossible to find this operator, which is a novel conserved quantity corresponding to a hidden symmetry for the spin chain, relying solely on the spin-chain picture.

B. The thermodynamic limit

Since we have superselection rules for the state space, we can look at the partition function Z_m of H restricted to the sector with m fermions. The relevant eigenvalues are given by[14,19]

$$\Lambda_n = \frac{1}{2} \sin\left(\frac{\chi}{L+1} + \frac{(2n-1)}{L+1} \frac{\pi}{2} \right), \quad n = 1, \ldots, L+1. \tag{19}$$

Since $\lim_{L\to\infty}(2L\Lambda_n/\pi) = \chi/\pi + 1/2 + n - 1$, in the thermodynamic limit,[20] we obtain

$$\mathcal{Z}_m = \lim_{L\to\infty} \{ \mathrm{tr}\, z^{(L/\pi)\sum_{n=1}^{L+1} 2\Lambda_n N_n} \} = z^{m\chi/\pi + m/2} \sum_{n_1, n_2, \ldots, n_m} z^{n_1 - 1 + n_2 - 1 + \cdots + n_m - 1}$$
$$= z^{m\chi/\pi + m/2} \left(\sum_l p_m(l) z^l + \sum_l p_{m-1}(l) z^l \right)$$
$$= z^{m\chi/\pi + m/2} \left(\frac{z^{m(m+1)/2} + (1-z^m) z^{(m-1)m/2}}{(1-z)(1-z^2)\cdots(1-z^m)} \right)$$
$$= \frac{z^{m\chi/\pi + m^2/2}}{(1-z)(1-z^2)\cdots(1-z^m)}. \tag{20}$$

Here $p_m(l)$ counts the number of ways the integer l can be expressed as a sum of m distinct nonzero integers. The second term involving p_{m-1} takes into account that one of $n_1 - 1$ in the sum before might be zero and the second equality follows from the formula

$$\sum_l p_m(l) z^l = \frac{z^{m(m+1)/2}}{(1-z)(1-z^2)\cdots(1-z^m)}. \tag{21}$$

The complete partition function $\mathcal{Z}$ will then be a sum over all the even or the odd m depending on χ. On the other hand $\mathcal{Z}$ has been calculated,[21] so that equating the two expressions, one obtains an interesting combinatorial identity.

What we gain from the calculation of $\mathcal{Z}_m$ is that we now know that in the sector with fixed fermion number, the dependence of $\mathcal{Z}_m$ on χ is given by a factor of $z^{m\chi/\pi}$. This simply induces a uniform shift off the usual spectrum. Notice that the factor is different though for different m, so that the eigenspaces of the thermodynamic limit of the operator $\mathcal{F}_{\text{tot}}$ play a special role, since the shift can precisely be factored out on these spaces. The reason for this factorization is the special distribution of the eigenvalues (19).

Another way to phrase this result is as follows. Consider the polynomial ring in infinitely many fermionic variables which are indexed by half integers $F=\mathbb{C}[\xi_i]: i \in \mathbb{N}_0+\frac{1}{2}$. This space comes equipped with a natural bigrading. The first grading is by the usual degree where $\deg(\xi_{i_1}\cdots\xi_{i_m})=m$. The second is by the weight wt where $\text{wt}(\xi_{i_1}\cdots\xi_{i_m})=\Sigma_{j=1}^{m} i_j$. Thus we can decompose $F=\oplus_d F_d$ according to the degree or according to the weight $F=\oplus_w F^w$. We will set F_d^w to be the bigraded piece of pure degree d and pure weight w and we will let π_d denote the projection of F onto its summand F_d. It is an elementary calculation to show that the dimension of $F_m^{l+m/2}$ is $p_m(l)+p_{m-1}(l)$ and likewise the dimension of $F_m^{l-m/2}$ is just $p_m(l)$.

Furthermore there are the two subspaces F_{even} and F_{odd} spanned by polynomials whose degree is either even or odd. Now the state space of H in the thermodynamic limit is abstractly isomorphic to one of the two subspaces F_{even} or F_{odd} of F (see Sec. II C). The isomorphism is given by sending the state $|n_1,\ldots,n_m\rangle$, which is the state with fermions n_i, to the monomial $\xi_{n_1-1/2}\cdots\xi_{n_m-1/2}$. (Recall that the n_i are positive integers and the indices of the ξ start at $0+\frac{1}{2}$.) In this language, the partition sum is the partition function $\text{tr}\, z^{\omega(\chi)}$ for the operator $\omega(\chi) := (\Sigma_m((m\chi/\pi)id+\text{wt})\circ\pi_m)|F_{\text{odd/even}}$. So we see that the eigenspaces are exactly the $F_m^{l+m/2}$ with the eigenvalues given by $m\chi/\pi+m/2+l$ and hence χ tunes the eigenvalue uniformly in each of the given sectors.

Now, in the original spin chain, this essential grading operator is given by the limit of Eq. (18). More details are contained in Ref. 19.

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Scattering transform for nonstationary Schrödinger equation with bidimensionally perturbed *N*-soliton potential

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In the framework of the extended resolvent approach the direct and inverse scattering problems for the nonstationary Schrödinger equation with a potential being a perturbation of the *N*-soliton potential by means of a generic bidimensional smooth function decaying at large spaces are introduced and investigated. The initial value problem of the Kadomtsev-Petviashvili I equation for a solution describing *N* wave solitons on a generic smooth decaying background is then linearized, giving the time evolution of the spectral data. © *2006 American Institute of Physics.*
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I. INTRODUCTION

A. Formulation of the problem

We consider the Kadomtsev-Petviashvili equation in its version called KPI,[1]

$$(u_t - 6uu_{x_1} + u_{x_1x_1x_1})_{x_1} = 3u_{x_2x_2}, \quad u = u(x_1,x_2,t). \tag{1.1}$$

By associating it to the nonstationary Schrödinger operator

$$\mathcal{L} = i\partial_{x_2} + \partial_{x_1}^2 - u(x), \tag{1.2}$$

it has been shown to be integrable about three decades ago.[2,3] More precisely,[4] the following time evolution of the KPI equation (time dependence of u is understood)

$$u_t(x) - 6u(x)u_{x_1}(x) + u_{x_1x_1x_1}(x) = 3\int_{-t\infty}^{x} dx_1' u_{x_2x_2}(x_1',x_2) \tag{1.3}$$

can be obtained by introducing the auxiliary operator

$$\mathcal{T}(x) = \partial_t + 4\partial_{x_1}^3 - 6u(x)\partial_{x_1} - 3u_{x_1}(x) + 3i\int_{-t\infty}^{x_1} dx_1' u_{x_2}(x_1',x_2) \tag{1.4}$$

and by imposing compatibility with the nonstationary Schrödinger operator $\mathcal{L}$, i.e.,

$$[\mathcal{L},T] = 0. \tag{1.5}$$

The initial value problem for KPI in the case of rapidly decaying initial data was solved in Refs. 5–10 by using the inverse scattering transform (IST) method.

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TABLE I. Main objects in the resolvent approach.

$\mathcal{L}(x,i\partial_x)$	Differential operator	Eq. (1.9)
$L(x,x';q),\ q\in\mathbb{R}^2$	Extended differential operator	Eq. (1.16)
$A(x,x';q)$	Extended pseudodifferential operator	Eq. (1.14)
$\widehat{A}(x,x';q)$	Hat operator	Eq. (1.25)
$A^{(z)}(x,x';q)$	Shifted operator	Eq. (1.24)
$LM=ML=I$	Extended resolvent	Eq. (1.33)
$M'-M=-M'(L'-L)M$	Hilbert identity	Eq. (1.35)
$\widehat{LA}=\vec{\mathcal{L}}\widehat{A},\ \widehat{AL}=\widehat{A}\overleftarrow{\mathcal{L}}$	$\mathcal{L}$ and dual $\mathcal{L}$ operating from left and right	Eq. (1.30)

However, the KPI equation, being a $(2+1)$-dimensional generalization of the Korteweg de Vries (KdV) equation, admits also solutions that behave at space infinity such as the solutions of the KdV equation. Therefore, it is natural to consider potentials $u(x)$ in Eq. (1.2) which are rapidly decaying on the plane in all directions with the exception of a finite number of directions along which the limits

$$\lim_{x_2\to\pm\infty} u(x_1-2\mu_n x_2,x_2),\quad \mu_n\in\mathbb{R},\quad n=1,2,\ldots,N, \tag{1.6}$$

exist and are different from zero.

In Ref. 4 and 11–15 the method of the "extended resolvent" (or, for short, method of resolvent) was suggested as a way of pursuing a generalization of the IST that enables studying the spectral theory of operators with nontrivial asymptotic behavior at space infinity. In Refs. 15–21 for the nonstationary Schrödinger and heat operators the case where there is only one direction of nondecaying behavior was considered. The starting point in solving the problem was the embedding of the pure one-dimensional case in the two-dimensional spectral theory, building the two-dimensional extended resolvent for a potential $u(x)\equiv u_1(x_1)$. Then, a potential $u(x)=u_1(x_1)+u'(x)$, where $u'(x)$ is an arbitrary decaying smooth function of both spatial variables, was considered and the corresponding resolvent was constructed by dressing the above resolvent for $u(x)=u_1(x_1)$. Finally, all mathematical entities generalizing the standard ones in IST, as Jost solutions and spectral data, were derived by a reduction procedure from this dressed resolvent.

Here, we consider a real potential $u(x)$ given as a sum of two terms,

$$u(x)=u_N(x)+u'(x), \tag{1.7}$$

where u_N is the N-soliton potential of the nonstationary Schrödinger equation obtained in Ref. 22 and then generalized in Ref. 23 and $u'(x)$ is an arbitrary bidimensional decaying smooth perturbation. This case is substantially more complicated since u_N is a true bidimensional potential and we have not the one-dimensional sample as a guide to follow.

Therefore, one needs first to construct directly the resolvent M_N of the nonstationary Schrödinger operator with potential u_N,

TABLE II. Green's functions and Jost solutions for a generic potential.

$\mathcal{G}(x,x',\mathbf{k})=\widehat{M}(\ell_\mathcal{J}(\mathbf{k})),\ \ell(\mathbf{k})=(\mathbf{k},\mathbf{k}^2),\ \mathbf{k}\in\mathbb{C}$	Green's function	Eq. (1.42)
$\mathcal{G}_\pm(x,x')=\lim_{q_2\to\pm 0}\lim_{q_1\to 0}\widehat{M}(q)$	Adv/ret Green's functions	Eq. (1.46)
$\Phi(\mathbf{k})=\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_0\Phi_0(\mathbf{k})$	Jost solution	Eq. (1.51)
$\Phi_\pm(x,k)=\mathcal{G}_\pm\overleftarrow{\mathcal{L}}_0\Phi_0(k),\ k\equiv\mathbf{k}_{\mathfrak{R}}$	Adv/ret solutions	Eq. (1.52)

TABLE III. Main objects in the N-soliton case.

$L_N(x,i\partial_x)$	Differential operator	Eq. (1.8)
$M_N(x,x';q)$	Extended resolvent	Eq. (2.44)
$\vec{\mathcal{L}}_N, \overleftarrow{\mathcal{L}}_N$	$\mathcal{L}_N$ and dual $\mathcal{L}_N$ operating from left and right	Eq. (1.30)
$\mathcal{G}_N(x,x',\mathbf{k})$	Green's function	Eq. (2.52)
$\mathcal{G}_{N,\pm}(x,x')$	Adv/ret Green's functions	Eq. (2.56)
$\varphi(x,\mathbf{k})$	Jost solution	Eq. (2.9)
$\varphi_n(x,\mathbf{k}_\mathfrak{I})$	Auxiliary Jost solutions	Eq. (2.24)

$$\mathcal{L}_N = i\partial_{x_2} + \partial_{x_1}^2 - u_N(x). \tag{1.8}$$

Using the results obtained in Ref. 24 this was done in Ref. 25.

Here, following the method developed in Refs. 15–20, we construct the extended resolvent M of the nonstationary Schrödinger operator (1.2) with a potential u as in Eq. (1.7) by dressing the resolvent M_N obtained in Ref. 25 and we derive it by a reduction procedure the corresponding Jost solutions and spectral data together with their characterization equations and time evolution. Finally, the inverse scattering problem is solved.

We start in the following sections with a short outline of the resolvent approach and with the presentation of some results of articles [24,25] used in what follows.

B. Notations and guiding lines

In order to deal with the inverse scattering method, in the case we are considering, it is necessary to introduce mathematical objects which are extensions of familiar objects as differential operators, pseudodifferential operators and resolvent, and that we are calling extended. This extension procedure is not at all trivial and, being new and original, is not familiar to the common reader. Therefore, we evaluated that it could be useful to present some tables with the symbols we use, their name, and the numbers of the defining formulas.

In Table I are listed the main objects we are dealing with in the case of a generic potential $u(x)$.

We first introduce what we call the extension $L(x,x';q)$ of a differential operator $L(x,i\partial_x)$ depending on a spectral parameter q and, then, following a procedure similar to that used for passing from differential operators to pseudodifferential operators, we introduce the extended

TABLE IV. Spectral data for N solitons.

$\mathbf{f}^\sigma = (\mathbf{r}_\pm^{-\sigma})^\dagger \mathbf{r}_\pm^{-\sigma}$	Spectral data	Eq. (2.118)
$\mathbf{r}_\pm^\sigma = \begin{pmatrix} r_\pm^\sigma(p)\delta(p-k) & 0 \\ 0 & r_\pm^\sigma(m,n) \end{pmatrix}$	Triangular spectral data	Eq. (2.111), (2.75), and (2.87)
$\mathbf{t}^\sigma = \begin{pmatrix} t^\sigma(p)\delta(p-k) & 0 \\ 0 & \delta_{mn}\vartheta_n^\sigma \end{pmatrix}$	Transmission coefficient	Eq. (2.112) and (2.26)
$\varphi_\pm(k) = \varphi^\sigma(k)\overline{r_\pm^{-\sigma}(k)}$	Adv/ret solutions	Eq. (2.78)
$\varphi_{\pm,n} = \sum_{m=1}^N \varphi_m^\sigma (r_\pm^{-\sigma})^\dagger(m,n)$	Auxiliary adv/ret solutions	Eq. (2.91)

TABLE V. Spectral data characterization equations for N solitons.

$\mathbf{r}_{\pm}^{\sigma}(\mathbf{t}^{\sigma})^{-1}(\mathbf{r}_{\pm}^{-\sigma})^{\dagger}=\mathbf{I}$	Eq. (2.113)
$(\mathbf{r}_{\pm}^{-\sigma})^{\dagger}\mathbf{r}_{\pm}^{\sigma}(\mathbf{t}^{\sigma})^{-1}=\mathbf{I}$	Eq. (2.113)
$(\mathbf{r}_{+}^{\sigma})^{\dagger}\mathbf{r}_{+}^{\sigma}=(\mathbf{r}_{-}^{\sigma})^{\dagger}\mathbf{r}_{-}^{\sigma}$	Eq. (2.119)

pseudodifferential operators $A(x,x';q)$. The extended resolvent $M(x,x';q)$ is defined as the inverse of the extended differential operator $L(x,x';q)$ and in its hat version identifies a family of Green's functions of $\mathcal{L}$ depending on the spectral parameter q.

In the case of the nonstationary Schrödinger operator $\mathcal{L}$ in Eq. (1.2), special reductions with respect to this parameter q furnish "standard" Green's function $\mathcal{G}(x,x',\mathbf{k})$, Green's function for short, and advanced/retarded Green's functions $\mathcal{G}_{\pm}(x,x')$. By using them one can then build the Jost and advanced/retarded solutions as indicated in Table II.

If wavelike solitons are present the potential $u(x)$ is not going to zero at large spaces and the equations defining the Jost solutions, due to the bad behavior at infinity of the potential, need to be regularized and, in addition, the Jost solutions do not form a complete set anymore. All this prevents solving the problem by a direct approach.

In fact, it is necessary to consider first the case of a pure N-soliton potential $u_N(x)$ and to build all the mathematical objects listed above, including the auxiliary Jost solutions which complete the set of Jost solutions. The notations used are listed in Table III, where $n=1,2,\ldots,N$.

Then, we consider the potential $u(x)=u_N(x)+u'(x)$ obtained by perturbing the pure N-soliton potential $u_N(x)$ by adding a smooth decaying perturbation $u'(x)$ and we dress Green's functions and Jost solutions by using the Hilbert identity listed above with $L'=L_N$ and $M'=M_N$.

The spectral data in the case of N solitons are well known and are given by the locations λ_n $(n=1,2,\ldots,N)$ of the poles of the transmission coefficient $t(\mathbf{k})$, that we choose in the upper half complex plane, and by the $N\times N$ matrix C, hermitian and positive, of the normalization coefficients. However, in view of the dressing, these spectral data are not convenient and, in spite of the fact that they are superfluous in this case, we need also to define the advanced/retarded solutions together with their auxiliary advanced/retarded solutions.

Therefore, we introduce as alternative equivalent spectral data a matrix $\mathbf{f}^{\sigma}$, which exhibits a triangular decomposition, and the advanced/retarded and auxiliary advanced/retarded solutions according to Table IV. Here and everywhere in the following we use σ for indicating the label $\pm$, we indicate by $f^{\sigma}(k)$, for any function $f(\mathbf{k})$ of the complex variable $\mathbf{k}$, the limiting value of $f(\mathbf{k})$ at the real axis from above $(\sigma=+)$ and from below $(\sigma=-)$, and we define the product of matrices with matrix elements with continuous and discrete indices by integrating and summing, respectively, over continuous and discrete indices.

One can write a set of characterization equations for the triangular spectral data $\mathbf{r}_{\pm}^{\sigma}$ not very significant in this case, but ready to be dressed perturbing u_N. (see Table V).

Then, one can write more conveniently the relations interlacing the different Jost solutions by introducing a vectorial formulation, which, again, is not very significant in this case, but very convenient when performing the dressing. Precisely, see Table VI.

TABLE VI. Vectorial Jost solutions for N solitons.

$\boldsymbol{\varphi}^{\sigma}=(\varphi^{\sigma}(k),\varphi_1^{\sigma},\ldots,\varphi_N^{\sigma})$	Vectorial Jost solution	Eq. (2.109)
$\boldsymbol{\varphi}_{\pm}=(\varphi_{\pm}(k),\varphi_{\pm,1},\ldots,\varphi_{\pm,N})$	Vectorial adv/ret solutions	Eq. (2.110)
$\boldsymbol{\varphi}^{\sigma}\mathbf{t}^{\sigma}=\boldsymbol{\varphi}_{\pm}\mathbf{r}_{\pm}^{\sigma}$	Jost in terms of adv/ret	Eq. (2.115)
$\boldsymbol{\varphi}_{\pm}=\boldsymbol{\varphi}^{\sigma}(\mathbf{r}_{\pm}^{-\sigma})^{\dagger}$	Adv/ret in terms of Jost	Eq. (2.116)
$\boldsymbol{\varphi}^{\sigma}\mathbf{t}^{\sigma}=\boldsymbol{\varphi}^{-\sigma}\mathbf{f}^{-\sigma}$	Discontinuity at $\mathbf{k}_{\jmath}=0$	Eq. (2.117)

TABLE VII. Perturbed Green's functions and Jost solutions.

$\mathcal{G}(\mathbf{k})=\mathcal{G}_N(\mathbf{k})+\mathcal{G}_N(\mathbf{k})u'\mathcal{G}(\mathbf{k})$	Green's function	Eq. (1.59)
$\mathcal{G}_\pm=\mathcal{G}_{N,\pm}+\mathcal{G}_{N,\pm}u'\mathcal{G}_\pm$	Adv/ret Green's functions	Eq. (1.60)
$\Phi(\mathbf{k})=\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi(\mathbf{k})$	Jost solution	Eq. (3.3)
$\Phi_\pm(k)=\mathcal{G}_\pm\overleftarrow{\mathcal{L}}_N\varphi_\pm(k)$	Adv/ret solutions	Eq. (3.88)
$\Phi_n(\mathbf{k}_\mathfrak{I})=\mathcal{G}(\lambda_{n\mathfrak{R}}+0+i\mathbf{k}_\mathfrak{I})\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\mathfrak{I})$	Auxiliary Jost solutions	Eq. (3.31)
$\Phi_{\pm,n}=\mathcal{G}_\pm\overleftarrow{\mathcal{L}}_N\varphi_{\pm,n}$	Auxiliary adv/ret solutions	Eq. (3.89)

Then, the mathematical objects related to the perturbed potential $u(x)=u_N(x)+u'(x)$ can be obtained by dressing the corresponding ones for $u_N(x)$ according to the scheme in Table VII.

The Jost solution $\Phi(\mathbf{k})$ is analytical in the complex $\mathbf{k}$ plane with a discontinuity across the real axis and the segments $\mathbf{k}=\lambda_{n\mathfrak{R}}+i\mathbf{k}_\mathfrak{I}$, $|\mathbf{k}_\mathfrak{I}|\leqslant\lambda_{n\mathfrak{I}}$. Spectral data relate the limiting values of the Jost solution at the two sides of these cuts and their triangular decomposition is obtained by considering the relation among values of the Jost solution at the two sides of the real axis and the advanced/retarded solutions. All this is described in a more transparent and compact way by using a vectorial notation for the Jost solutions according to Table VIII.

The spectral data involved in Table VIII are listed in Table IX.

Finally, one can derive the scheme in Table X for the characterization equations of the spectral data.

The first two equations state that the matrix operator $\boldsymbol{\mathcal{R}}_\pm^\sigma(\mathbf{T}^\sigma)^{-1}$ admits right and left inverse, while the third equation is a characterization equation in the strict sense.

C. Extended resolvent approach

In this section we briefly review, in two dimensions for definiteness, the basic elements of the extended resolvent approach. For further details, we refer the interested readers to Refs. 11–16.

Let us consider the operators with kernel

$$L(x,x')=\mathcal{L}(x,i\partial_x)\delta(x-x'), \tag{1.9}$$

where $\mathcal{L}(x,i\partial_x)$ denotes a differential operator whose coefficients are smooth functions of x and let us introduce what we call the *extension* of these differential operators, i.e., to any differential operator $\mathcal{L}$ we associate the operator $L(\mathbf{q})$ with kernel

$$L(x,x';\mathbf{q})\equiv\mathcal{L}(x,i\partial_x+\mathbf{q})\delta(x-x')=e^{i\mathbf{q}(x-x')}L(x,x'), \tag{1.10}$$

where $x=(x_1,x_2)$, $x'=(x_1',x_2')\in\mathbb{R}^2$, and $\mathbf{q}=(\mathbf{q}_1,\mathbf{q}_2)\in\mathbb{C}^2$ and

TABLE VIII. Perturbed vectorial Jost solutions.

$\boldsymbol{\Phi}^\sigma=(\Phi^\sigma(k),\Phi_1^\sigma,\ldots,\Phi_N^\sigma)$	Vectorial Jost solution	Eq. (3.113)
$\boldsymbol{\Phi}_\pm=(\Phi_\pm(k),\Phi_{\pm,1},\ldots,\Phi_{\pm,N})$	Vectorial adv/ret solutions	Eq. (3.113)
$\boldsymbol{\Phi}^\sigma\mathbf{T}^\sigma=\boldsymbol{\Phi}_\pm\mathbf{r}_\pm^\sigma\boldsymbol{\mathcal{R}}_\pm^\sigma$	Jost in terms of adv/ret	Eq. (3.137)
$\boldsymbol{\Phi}_\pm=\boldsymbol{\Phi}^\sigma(\boldsymbol{\mathcal{R}}_\pm^{-\sigma})^\dagger(\mathbf{r}_\pm^{-\sigma})^\dagger$	Adv/ret in terms of Jost	Eq. (3.138)
$\boldsymbol{\Phi}^\sigma\mathbf{T}^\sigma=\boldsymbol{\Phi}^{-\sigma}\mathbf{F}^{-\sigma}$	Discontinuity at $\mathbf{k}_\mathfrak{I}=0$	Eq. (3.127)
$\Delta\Phi\big\vert_{\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}}=\Phi_n(\mathbf{k}_\mathfrak{I})w_n(\mathbf{k}_\mathfrak{I})$	Discontinuity at $\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}$	Eq. (3.42)

TABLE IX. Spectral data of the perturbed potential.

$\mathbf{F}^{\sigma}=(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma}$	Spectral data	Eq. (3.148)
$\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}=\begin{pmatrix}\mathcal{R}_{\pm}^{\sigma}(p,k) & \mathcal{R}_{\pm}^{\sigma}(p,n)\\ \mathcal{R}_{\pm}^{\sigma}(m,k) & \mathcal{R}_{\pm}^{\sigma}(m,n)\end{pmatrix}$	Triangular spectral data	Eqs. (3.132) –(3.136)
$\mathbf{T}^{\sigma}=\begin{pmatrix}t^{\sigma}(p)\delta(p-k) & 0\\ 0 & \delta_{mn}\dfrac{\vartheta_n^{\sigma}}{A_n^{\sigma}}\end{pmatrix}$	Transmission coefficient	Eqs. (3.118) and (3.28)
$w_n(\mathbf{k}_{\mathfrak{I}})$	Additional spectral data	Eq. (3.44)

$$\mathbf{q}x=\mathbf{q}_1x_1+\mathbf{q}_2x_2. \tag{1.11}$$

The $\mathbf{q}$ variable will play in the following the role of a spectral parameter and we use a boldface character to emphasize that it is complex. By using the Fourier transform we can write

$$L(x,x';\mathbf{q})=\frac{1}{(2\pi)^2}\int d\alpha\, e^{-i\alpha(x-x')}\mathcal{L}(x,\alpha+\mathbf{q}),\quad \alpha=(\alpha_1,\alpha_2). \tag{1.12}$$

Then, it is natural to introduce more general operators $A(\mathbf{q})$ with kernel

$$A(x,x';\mathbf{q})=\frac{1}{(2\pi)^2}\int d\alpha\, e^{-i\alpha(x-x')}\mathcal{P}(x,\alpha+\mathbf{q}) \tag{1.13}$$

obtained by considering not just a polynomial $\mathcal{L}(x,\mathbf{q})$ in $\mathbf{q}$ but a tempered distribution $\mathcal{P}(x,\mathbf{q})$ of the six real variables x, $\mathbf{q}_{\mathfrak{R}}$ and $\mathbf{q}_{\mathfrak{I}}$. Notice that the dependence on $\mathbf{q}_{\mathfrak{R}}$ can be factorized

$$A(x,x';\mathbf{q})=e^{i\mathbf{q}_{\mathfrak{R}}(x-x')}A(x,x';q), \tag{1.14}$$

where

$$\mathbf{q}=\mathbf{q}_{\mathfrak{R}}+i\mathbf{q}_{\mathfrak{I}}\in\mathbb{C}^2,\quad q\equiv\mathbf{q}_{\mathfrak{I}}\in\mathbb{R}^2, \tag{1.15}$$

and that $A(x,x';q)$ belongs to the space $\mathcal{S}'$ of tempered distributions of the six real variables x, x' and $q=(q_1,q_2)$. In particular, for the case of a differential operator we get by Eq. (1.10)

$$L(x,x';q)=e^{-q(x-x')}L(x,x'). \tag{1.16}$$

Definition (1.13) recalls the definition of a pseudodifferential operator with symbol $\mathcal{P}(x,\alpha)$. However, it is different in two respects, since the symbol $\mathcal{P}(x,\mathbf{q})$ depends on an additional parameter q and the functional space to which the symbol $\mathcal{P}(x,\mathbf{q})$ belongs is much larger than the functional space used by mathematicians in defining the pseudodifferential operators. Both generalizations are crucial in the following. Therefore, we call the operators $A(q)$ with kernel $A(x,x';q)$ belonging to the space $\mathcal{S}'$ extended pseudodifferential operators, or by short operators, and $\mathcal{P}(x,\mathbf{q})$ their symbols.

TABLE X. Spectral data characterization equations for the perturbed potential.

$(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}\mathbf{t}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}(\mathbf{T}^{\sigma})^{-1}=\mathbf{I}$	Eq. (3.141)
$\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}(\mathbf{T}^{\sigma})^{-1}(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}\mathbf{t}^{\sigma}=\mathbf{I}$	Eq. (3.142)
$(\boldsymbol{\mathcal{R}}_{+}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{+}^{-\sigma}=(\boldsymbol{\mathcal{R}}_{-}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{-}^{-\sigma}$	Eq. (3.143)

In the following it is often useful to use instead of the symbol $\mathcal{P}(x,\mathbf{q})$ its Fourier transform with respect to x, i.e.,

$$A(p;\mathbf{q}) = \frac{1}{(2\pi)^2}\int dx\, e^{ipx}\mathcal{P}(x,\mathbf{q}), \quad p=(p_1,p_2). \tag{1.17}$$

From Eqs. (1.13) and (1.14) it follows that $A(p;\mathbf{q})$ is related to $A(x,x';q)$ by

$$A(p;\mathbf{q}) = \frac{1}{(2\pi)^2}\int dx \int dx' e^{i(p+\mathbf{q}_\Re)x - i\mathbf{q}_\Re x'} A(x,x';q). \tag{1.18}$$

The inverse of Eq. (1.18) is given by

$$A(x,x';\mathbf{q}_\Im) = \frac{1}{(2\pi)^2}\int dp \int d\mathbf{q}_\Re\, e^{-i(p+\mathbf{q}_\Re)x + i\mathbf{q}_\Re x'} A(p;\mathbf{q}). \tag{1.19}$$

Then, we consider $A(x,x';q)$ and $A(p;\mathbf{q})$ as the representation of the operator $A(q)$, respectively, in the x-space and in the p-space.

In the space of this operators we define the hermitian conjugation as

$$A^\dagger(x,x';q) = \overline{A(x',x;-q)}, \quad A^\dagger(p;\mathbf{q}) = \overline{A(-p;\overline{\mathbf{q}}+p)}, \tag{1.20}$$

in terms of kernels in x- or p-spaces. For generic operators $A(q)$ and $B(q)$ with kernels $A(x,x';q)$ and $B(x,x';q)$ we introduce the standard composition law

$$(AB)(x,x';q) = \int dx'' A(x,x'';q)B(x'',x';q), \tag{1.21}$$

if the integral exists in terms of distributions. In terms of kernels $A(p;\mathbf{q})$ and $B(p;\mathbf{q})$ this composition takes the form of a shifted convolution

$$(AB)(p;\mathbf{q}) = \int dp' A(p-p';\mathbf{q}+p')B(p';\mathbf{q}). \tag{1.22}$$

An operator A can have an inverse A^{-1} in the sense of this composition, i.e., such that $AA^{-1}=I$ and $A^{-1}A=I$, where I is the unity operator in $\mathcal{S}'$, i.e., $I(x,x';q)=\delta(x-x')$ in the x-space or $I(p;\mathbf{q})=\delta(p)$ in the p-space, being $\delta(x)$ and $\delta(p)$ two-dimensional δ-functions.

We will use also the following notation for the shift with respect to the complex variable $\mathbf{q}$:

$$A^{(\mathbf{z})}(p;\mathbf{q}) = A(p;\mathbf{q}+\mathbf{z}), \quad \mathbf{z}\in\mathbb{C}^2, \tag{1.23}$$

that, thanks to Eq. (1.14), in the x-space reads

$$A^{(\mathbf{z})}(x,x';q) = e^{i\mathbf{z}_\Re(x-x')}A(x,x';q+\mathbf{z}_\Im). \tag{1.24}$$

Of course the two representations in the x-space and in the p-space are equivalent and, in principle, one could work always in one of them. However, it is often convenient to pass from one representation to the other. Thus, the p-space is more suitable for studying analyticity properties, while boundedness is more easily studied in the x-space.

For a generic operator $A(q)$ with kernel $A(x,x';q)$ it can be convenient to consider the operation

$$\widehat{A}(x,x';q) = e^{q(x-x')}A(x,x';q), \tag{1.25}$$

furnishing what we call the "hat kernel" of $A(q)$ in the x-space. In the special case of a kernel $L(x,x';q)$ which is, according to the definition (1.10), an extension of a differential operator $\mathcal{L}(x,i\partial_x)$ this operation is just the inverse of the extension procedure, i.e.,

$$\widehat{L}(x,x';q) = \mathcal{L}(x,i\partial_x)\delta(x-x'). \tag{1.26}$$

In general, however, $\widehat{A}(x,x';q)$ does depend on q nontrivially and, due to the exponential factor in Eq. (1.25), in contrast with $A(x,x';q)$, does not belong to the space $\mathcal{S}'(\mathbb{R}^6)$ of tempered distributions.

Operation (1.25) has no analog in terms of the p-representation. In the x-representation local properties of kernels are preserved, so we can reformulate (1.21) and (1.18) in terms of the hat kernels getting

$$\widehat{(AB)}(x,x';q) = \int dx''\widehat{A}(x,x'';q)\widehat{B}(x'',x';q), \tag{1.27}$$

$$A(p;\mathbf{q}) = \frac{1}{(2\pi)^2}\int dx \int dx' \mathrm{e}^{i(p+\mathbf{q})x - i\mathbf{q}x'}\widehat{A}(x,x';\mathbf{q}_\mathfrak{D}). \tag{1.28}$$

If we consider the differential operator $\mathcal{L}(x,i\partial_x)$ and the composition of its extension L with an operator B, that is LB and BL, by applying the transformation (1.25) we obtain

$$\widehat{LB}(x,x';q) = \mathcal{L}(x,i\partial_x)\widehat{B}(x,x';q), \quad \widehat{BL}(x,x';q) = \mathcal{L}^d(x',i\partial_{x'})\widehat{B}(x,x';q), \tag{1.29}$$

where $\mathcal{L}^d$ is the operator dual to $\mathcal{L}$. In what follows we shall use a special notation for formulas of this type writing

$$\widehat{LB}(q) = \vec{\mathcal{L}}\widehat{B}(q), \quad \widehat{BL}(q) = \widehat{B}(q)\overleftarrow{\mathcal{L}}, \tag{1.30}$$

so that $\vec{\mathcal{L}}$ denotes the operator $\mathcal{L}$ applied to the x variable of the kernel $\widehat{B}(x,x';q)$ and $\overleftarrow{\mathcal{L}}$ denotes the operator dual to $\mathcal{L}$ applied to the x' variable of the same kernel.

The dual and adjoint hat operators are given, respectively, as

$$\widehat{A}^d(x,x';q) = \widehat{A}(x',x;-q), \tag{1.31}$$

$$\widehat{A}^\dagger(x,x';q) = \overline{\widehat{A}(x',x;-q)}. \tag{1.32}$$

The main object of our approach is the extended resolvent (or resolvent for short) $M(q)$ of the operator $L(q)$, which is defined as the inverse of the operator L, i.e.,

$$L(q)M(q) = M(q)L(q) = I. \tag{1.33}$$

In terms of the corresponding hat operators the definition of the resolvent M reads

$$\vec{\mathcal{L}}\widehat{M}(q) = I = \widehat{M}(q)\overleftarrow{\mathcal{L}}, \tag{1.34}$$

which shows that $\widehat{M}(q)$ is a two-parameter set of Green's functions of the operator $\mathcal{L}$. It is worth stressing the fact that the extended pseudodifferential operators, in contrast with the pseudodifferential operators, have hat kernels which depend on q play here and will play in the following a crucial role in the theory.

If we consider now the resolvent M of L and the resolvent M' of another extended differential operator L' we can interlace the two resolvents by noticing that, if *associativity is assumed*, they satisfy the following generalized Hilbert identity:

$$M' - M = -M'(L'-L)M = -M(L'-L)M'. \tag{1.35}$$

On the other side, if M is inverse of L and M' satisfies Eq. (1.35) then M' is inverse of L'. Therefore, if the inverse M of L is known, the two equations in Eq. (1.35) become two integral

equations, one dual to the other, defining the resolvent M' of L'. This Hilbert identity is the main tool we will use in the whole spectral theory of differential operators.

The resolvent defined in Eq. (1.33) is not unique even under conditions that it is simultaneously right and left inverse of operator $L(q)$ and its kernel belongs to the space of tempered distributions. This problem is resolved by associativity assumption made in derivation of Eq. (1.35). Indeed, let us consider Eq. (1.35) for $L=L(q)$ and $L'=L^{(\mathbf{z})}(q)$ [so that by Eqs. (1.33) and (1.24) also $M'=M^{(\mathbf{z})}(q)$]:

$$M^{(\mathbf{z})}(q) - M(q) = - M^{(\mathbf{z})}(q)(L^{(\mathbf{z})}(q) - L(q))M(q). \tag{1.36}$$

Notice that, due to the definition of a shift in Eq. (1.24), the left-hand side of Eq. (1.36) is a tempered distribution with respect to q-variables and smooth, infinitely differentiable function of $\mathbf{z}$. This implies that the product of distributions in the right-hand side must also be a well defined tempered distribution for any value of $\mathbf{z}$ and any order of operations. By considering some simple examples one can check that this requirement determines the inverse $M(q)$ uniquely. Below we use this Hilbert identity for studying properties of the resolvent with respect to the parameter q, such as continuity and differentiability.

D. Green's functions and Jost solutions for a generic potential

The extension of the nonstationary Schrödinger operator (1.2) is given by

$$L(q) = L_0(q) - u(q), \tag{1.37}$$

where in the x-space

$$L_0(x,x';q) = [i(\partial_{x_2} + q_2) + (\partial_{x_1} + q_1)^2]\delta(x-x'), \quad u(x,x';q) = u(x)\,\delta(x-x'). \tag{1.38}$$

Notice that, due to the reality of the potential $u(x)$, by definition (1.20) we have that the operator $L(q)$ is Hermitian

$$L^{\dagger}(q) = L(q), \tag{1.39}$$

as well as the resolvent

$$M^{\dagger}(q) = M(q). \tag{1.40}$$

Hermiticity condition (1.40) for the resolvent is equivalent to

$$\overline{\widehat{M}(x,x';q)} = \widehat{M}(x',x;-q). \tag{1.41}$$

Of special relevance in the following will be Green's function $\mathcal{G}(x,x',\mathbf{k})$ obtained by considering the following reduction of $\widehat{M}(q)$ depending on the complex spectral parameter $\mathbf{k}$:

$$\mathcal{G}(\mathbf{k}) = \widehat{M}(q)|_{q=\ell_{\mathfrak{I}}(\mathbf{k})}, \quad \mathbf{k} \in \mathbb{C}, \tag{1.42}$$

where $\ell(\mathbf{k})$ is the special two-component vector

$$\ell(\mathbf{k}) = (\mathbf{k},\mathbf{k}^2). \tag{1.43}$$

Since $\widehat{M}(x,x',q)$ is growing exponentially as a function of x and x', the same property has the kernel $\mathcal{G}(x,x',\mathbf{k})$ for generic $\mathbf{k} \in \mathbb{C}$. But the function

$$G(x,x',\mathbf{k}) = \mathrm{e}^{i\ell_{\mathfrak{R}}(\mathbf{k})(x-x')}M\,(x,x',q)|_{q=\ell_{\mathfrak{I}}(\mathbf{k})}, \tag{1.44}$$

being a reduction of the resolvent itself belongs to $\mathcal{S}'$ and due to Eq. (1.25) it is simply related to $\mathcal{G}(\mathbf{k})$ by

$$G(x,x',\mathbf{k}) = \mathrm{e}^{i\ell(\mathbf{k})(x-x')}\mathcal{G}(x,x',\mathbf{k}). \tag{1.45}$$

As regards the so called advanced/retarded Green's functions, they can be obtained by the following reduction of the resolvent:

$$\mathcal{G}_{\pm} = \lim_{q_2\to\pm 0}\lim_{q_1\to 0}\widehat{M}(q). \tag{1.46}$$

Thanks to Eq. (1.34) we have

$$\vec{\mathcal{L}}\mathcal{G}(\mathbf{k}) = I = \mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}, \tag{1.47}$$

$$\vec{\mathcal{L}}\mathcal{G}_{\pm} = I = \mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}, \tag{1.48}$$

and thanks to Eq. (1.41)

$$\overline{\mathcal{G}(x,x',\mathbf{k})} = \mathcal{G}(x',x,\overline{\mathbf{k}}), \quad \mathbf{k}\in\mathbb{C}, \tag{1.49}$$

$$\overline{\mathcal{G}_{+}(x,x')} = \mathcal{G}_{-}(x',x). \tag{1.50}$$

Then, by using these Green's functions we can introduce the so called Jost and advanced/retarded solutions and their dual

$$\Phi(\mathbf{k}) = \mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_0\Phi_0(\mathbf{k}), \quad \Psi(\mathbf{k}) = \Psi_0(\mathbf{k})\vec{\mathcal{L}}_0\mathcal{G}(\mathbf{k}), \tag{1.51}$$

$$\Phi_{\pm}(k) = \mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_0\Phi_0(k), \quad \Psi_{\pm}(k) = \Psi_0(k)\vec{\mathcal{L}}_0\mathcal{G}_{\pm}, \tag{1.52}$$

where $\mathcal{L}_0$ is the bare differential operator introduced in Eq. (1.38) and

$$\Phi_0(x,\mathbf{k}) = \mathrm{e}^{-i\ell(\mathbf{k})x}, \quad \Psi_0(x,\mathbf{k}) = \mathrm{e}^{i\ell(\mathbf{k})x}. \tag{1.53}$$

Here and in what follows we use for shortness operator notations for relations of the kind (1.51) and (1.52), where, say, the first two stand for

$$\Phi(x,\mathbf{k}) = \int dx'(\mathcal{L}_0^d(x',\partial_{x'})\mathcal{G}(x,x',\mathbf{k}))\Phi_0(x',\mathbf{k}), \tag{1.54}$$

$$\Psi(x',\mathbf{k}) = \int dx\Psi_0(x,\mathbf{k})\mathcal{L}_0(x,\partial_x)\mathcal{G}(x,x',\mathbf{k}). \tag{1.55}$$

Thanks to (1.47) and (1.48) functions $\Phi(x,\mathbf{k})$, $\Psi(x,\mathbf{k})$, $\Phi_{\pm}(x)$, and $\Psi_{\pm}(x)$ are solutions of the Schrödinger equation and its dual, i.e.,

$$\vec{\mathcal{L}}\Phi(\mathbf{k}) = 0, \quad \Psi(\mathbf{k})\overleftarrow{\mathcal{L}} = 0, \tag{1.56}$$

$$\vec{\mathcal{L}}\Phi_{\pm}(k) = 0, \quad \Psi_{\pm}(k)\overleftarrow{\mathcal{L}} = 0. \tag{1.57}$$

However, one must be advised that the integrals in the rhs of definitions (1.51) and (1.52) for u not decaying at large spaces are divergent and must be regularized. In the following section we show how to overcome this problem and, then, how to proceed in building the inverse scattering theory.

E. Dressing procedure

If $M_N(q)$ is the resolvent of $L_N(q)$, the extension of the nonstationary Schrödinger operator defined in Eqs. (1.37) and (1.38) with $u=u_N$, then the resolvent $M(q)$ of $L(q)$, the extension ot the operator with potential $u=u_N+u'$, can be obtained by dressing $M_N(q)$. In fact, from the two Hilbert identities in Eq. (1.35) we get the two reciprocally dual integral equations

$$M(q) = M_N(q) + M_N(q)u'M(q), \quad M(q) = M_N(q) + M(q)u'M_N(q), \tag{1.58}$$

where u' is the multiplication operator with kernel $u'(x,x';q)=u'(x)\delta(x-x')$.

Correspondingly, for Green's functions we have the integral equations

$$\mathcal{G}(\mathbf{k}) = \mathcal{G}_N(\mathbf{k}) + \mathcal{G}_N(\mathbf{k})u'\mathcal{G}(\mathbf{k}), \tag{1.59}$$

$$\mathcal{G}_\pm = \mathcal{G}_{N,\pm} + \mathcal{G}_{N,\pm}u'\mathcal{G}_\pm, \tag{1.60}$$

and their dual, where $\mathcal{G}_N(\mathbf{k})$ and $\mathcal{G}_{N,\pm}$ are Green's function and advanced/retarded Green's functions of the operator $\mathcal{L}_N$, defined according to Eqs. (1.42) and (1.46). Taking into account that in Ref. 25 we derived explicitly the extended resolvent M_N and Green's functions $\mathcal{G}_N(\mathbf{k})$ and $\mathcal{G}_{N,\pm}$, the above equations enable us to develop the inverse scattering theory for a potential describing a perturbation of the N-soliton potential by a smooth decaying function $u'(x)$ of two variables.

We already mentioned that the main tool of our construction is the Hilbert identity (1.36). In fact, for a potential u as in Eq. (1.7), taking into account that the potential does not depend on q, we can write

$$L^{(\mathbf{z})}(q) - L(q) = L_N^{(\mathbf{z})}(q) - L_N(q) = -L_N^{(\mathbf{z})}(q)(M_N^{(\mathbf{z})}(q) - M_N(q))L_N(q),$$

and, then, from Eq. (1.36) we get

$$M^{(\mathbf{z})}(q) - M(q) = (M(q)L_N(q))^{(\mathbf{z})}(M_N^{(\mathbf{z})}(q) - M_N(q))L_N(q)M(q). \tag{1.61}$$

This Hilbert identity can be fruitfully used for studying the singularities of the resolvent $M(q)$, because by its means they can be obtained by dressing the singularities of the resolvent $M_N(q)$ which are explicitly known. In particular, let us mention that the shift operation defined in Eq. (1.24) in terms of the hat kernels means that

$$A^{(\mathbf{z})}(x,x';q) = \mathrm{e}^{(i\mathbf{z}-q)(x-x')}\widehat{A}(x,x';q+\mathbf{z}_\jmath). \tag{1.62}$$

Then the ∂-bar derivatives of Eq. (1.61) with respect to complex variables $\mathbf{z}_1$ and $\mathbf{z}_2$ at $\mathbf{z}=0$ give the relations

$$\frac{\partial\widehat{M}(q)}{\partial q_i} = \widehat{M}(q)\overleftarrow{\mathcal{L}}_N\frac{\partial\widehat{M}_N(q)}{\partial q_i}\vec{\mathcal{L}}_N\widehat{M}(q), \quad i=1,2, \tag{1.63}$$

where we used notations in Eq. (1.30). It is necessary to mention that the products of hat-kernels are not associative due to their exponential growth and, therefore, the arrows over operators denote also the order of operations.

The Hilbert identity (1.61) can also be reduced to special values of the resolvents giving Hilbert identities involving Green's functions. In fact, recalling the definition (1.42) of Green's function $\mathcal{G}(\mathbf{k})$ we see that its limiting values on the real axis,

$$\mathcal{G}^\pm(x,x',k) = \mathcal{G}(x,x',k\pm i0), \quad k\in\mathbb{R}, \tag{1.64}$$

correspond to the limits of the resolvent at $q=0$,

$$\mathcal{G}^{\pm}(x,x',k) = \lim_{q_1 \to \pm 0} \widehat{M}(x,x';q_1,2kq_1). \tag{1.65}$$

Also, advanced/retarded Green's functions are obtained as limiting values of the resolvent at $q=0$ according to the definition (1.46). Let us consider the Hilbert identity (1.61) at $\mathbf{z}_{\mathfrak{R}}=0$, i.e.,

$$M(q') - M(q) = (M(q')L_N(q'))(M_N(q') - M_N(q))L_N(q)M(q), \tag{1.66}$$

where $q' = q + \mathbf{z}_{\mathfrak{I}}$ [see Eq. (1.62)]. Performing here the limits (1.65) and (1.46) for q and q' we derive

$$\mathcal{G}^{\sigma}(k) - \mathcal{G}_{\pm} = \mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_N(\mathcal{G}^{\sigma}_N(k) - \mathcal{G}_{N,\pm})\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(k), \quad \sigma = +,-, \tag{1.67}$$

$$\mathcal{G}_{+} - \mathcal{G}_{-} = \mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_N(\mathcal{G}_{N,+} - \mathcal{G}_{N,-})\vec{\mathcal{L}}_N\mathcal{G}_{\mp}, \tag{1.68}$$

where the rhs of the last equality is independent of the choice of the upper or bottom signs.

II. *N*-SOLITON POTENTIAL AND RELATED OBJECTS

In order to get in the following by a dressing procedure all mathematical entities involved in the inverse scattering method we need not only the explicit form of the N-soliton potential u_N of the nonstationary Schrödinger operator, but also the related resolvent and such its reductions as Green's functions, Jost and what we call auxiliary Jost solutions. Here, we revisit the results obtained in Refs. 22 and 25 and, in addition, we present the asymptotic behavior of the Jost solutions at large space distances and the properties of the resolvent and Green's function, including their singularities.

A. Pure *N*-soliton potential and Jost solutions

In this article we consider the case where u_N in Eq. (1.7) is a pure N-soliton potential. Then following Ref. 25 we can choose as discrete spectral data N *different* complex parameters $\lambda_1, \ldots, \lambda_N$ and a $n \times n$ constant matrix C. As was shown in Ref. 25 parameters λ_n, without loss of generality in the case of the pure N-soliton potential, can be chosen in the upper half plane:

$$\lambda_{n\mathfrak{I}} > 0, \quad n = 1, \ldots, N. \tag{2.1}$$

In what follows we use notation

$$\lambda_n^{+} = \lambda_n, \quad \lambda_n^{-} = \overline{\lambda_n}. \tag{2.2}$$

Matrix $C = \|C_{m,n}\|_{m,n=1,\ldots,N}$ must be Hermitian and strictly positive:[23,24]

$$C^{\dagger} = C, \quad C > 0. \tag{2.3}$$

If we introduce the $n \times n$ constant matrix

$$\Lambda = \left\| \frac{1}{i(\lambda_m^{-} - \lambda_n^{+})} \right\|_{m,n=1,\ldots,N} \tag{2.4}$$

and define a matrix $B(x)$ as the product

$$B(x) = \operatorname{diag}\{e^{i\ell(\lambda_1^{-})x}, \ldots, e^{i\ell(\lambda_N^{-})x}\}\Lambda \operatorname{diag}\{e^{-i\ell(\lambda_1^{+})x}, \ldots, e^{-i\ell(\lambda_N^{+})x}\}, \tag{2.5}$$

where ℓ is defined in Eq. (1.43), then, the potential u_N is given by

$$u_N(x) = -2\partial_{x_1}^2 \log \det(B(x) + C). \tag{2.6}$$

The potential derived in Ref. 22 corresponds to a diagonal matrix C. In Ref. 23 the case of a generic matrix C was introduced and it was shown that conditions (2.3) are equivalent to the requirement that the potential u_N is real and regular.

Let us introduce the function

$$\tau(\mathbf{k}) = \left(\prod_{n=1}^{N} \frac{\mathbf{k} - \lambda_n^+}{\mathbf{k} - \lambda_n^-}\right)^{\theta(-\mathbf{k}_\jmath)}, \tag{2.7}$$

that has poles at all points $\mathbf{k} = \overline{\lambda_n}$ and has no zeros. Then, the Jost solution $\varphi(x,\mathbf{k})$ of the nonstationary Schrödinger equation corresponding to the potential (2.6), i.e., satisfying

$$(i\partial_{x_2} + \partial_{x_1}^2 - u_N(x))\varphi(x,\mathbf{k}) = 0, \tag{2.8}$$

is given by (we use the form derived in Ref. 24)

$$\varphi(x,\mathbf{k}) = \frac{1}{\tau(\mathbf{k})\det(B(x) + C)} \det\begin{pmatrix} B_{mn}(x) + C_{mn} & (ie^{i(\ell(\lambda_m^-) - \ell(\mathbf{k}))x})/(\mathbf{k} - \lambda_m^-) \\ e^{-i\ell(\lambda_n^+)x} & e^{-i\ell(\mathbf{k})x} \end{pmatrix}, \tag{2.9}$$

where the matrix in the rhs is obtained by bordering the $N \times N$ matrix $B(x) + C$ with a column in the upper right corner and a row in the bottom left corner, as indicated. In what follows we also need the dual Jost solution $\psi(x,\mathbf{k})$ of the dual equation

$$(-i\partial_{x_2} + \partial_{x_1}^2 - u_N(x))\psi(x,\mathbf{k}) = 0, \tag{2.10}$$

which is given by

$$\psi(x,\mathbf{k}) = \overline{\varphi(x,\bar{\mathbf{k}})}. \tag{2.11}$$

Using notations of the kind used in Eq. (1.29) we write Eqs. (2.8) and (2.10) in the form

$$\vec{\mathcal{L}}_N \varphi(\mathbf{k}) = 0, \quad \psi(\mathbf{k})\vec{\mathcal{L}}_N = 0. \tag{2.12}$$

To formulate the asymptotic behavior of these Jost solutions we introduce

$$\chi(x,\mathbf{k}) = e^{i\ell(\mathbf{k})x}\varphi(x,\mathbf{k}), \quad \xi(x,\mathbf{k}) = e^{-i\ell(\mathbf{k})x}\psi(x,\mathbf{k}), \tag{2.13}$$

so that by Eq. (2.11) $\xi(x,\mathbf{k}) = \overline{\chi(x,\bar{\mathbf{k}})}$. Then by Eq. (2.9) we get

$$\lim_{\mathbf{k}\to\infty} \chi(x,\mathbf{k}) = \lim_{\mathbf{k}\to\infty} \xi(x,\mathbf{k}) = 1, \tag{2.14}$$

and in a generic direction of $x \to \infty$, i.e., such that $|x_1 + 2\lambda_{n\Re} x_2| \to \infty$ for all $n = 1, \ldots, N$, and for any $\mathbf{k}$, $\mathbf{k}_\jmath \neq 0$,

$$\lim_{x\to\infty} (\chi(x,\mathbf{k}) - \chi_{\text{as}}(x,\mathbf{k})) = 0, \tag{2.15}$$

where

$$\chi_{\text{as}}(x,\mathbf{k}) = \prod_{n=1}^{N} \left(\frac{\mathbf{k} - \lambda_n^+}{\mathbf{k} - \lambda_n^-}\right)^{(\operatorname{sgn} \mathbf{k}_\jmath)\theta(\mathbf{k}_\jmath(x_1 + 2\lambda_{n\Re} x_2))}. \tag{2.16}$$

In particular,

$$\lim_{x_1 \to -\mathbf{k}_\jmath \infty} \chi(x,\mathbf{k}) = 1, \quad \lim_{x_1 \to +\mathbf{k}_\jmath \infty} \xi(x,\mathbf{k}) = 1, \tag{2.17}$$

$$\lim_{x_1\to+\mathbf{k}_\Im\infty}\chi(x,\mathbf{k})=\frac{1}{t(\mathbf{k})},\qquad \lim_{x_1\to-\mathbf{k}_\Im\infty}\xi(x,\mathbf{k})=\frac{1}{t(\mathbf{k})},\tag{2.18}$$

where notation $\mathbf{k}_\Im\infty$ in the limit denotes sign of the infinity, and where we defined the transmission coefficient as

$$t(\mathbf{k})=\tau(\mathbf{k})\overline{\tau(\bar{\mathbf{k}})}\equiv\prod_{n=1}^{N}\left(\frac{\mathbf{k}-\lambda_n^-}{\mathbf{k}-\lambda_n^+}\right)^{\operatorname{sgn}\mathbf{k}_\Im},\tag{2.19}$$

so that

$$t(\bar{\mathbf{k}})=\overline{t(\mathbf{k})},\quad \mathbf{k}\in\mathbb{C}.\tag{2.20}$$

B. Auxiliary Jost solutions

The transmission coefficient is a meromorphic function in the upper and bottom half planes of the spectral parameter $\mathbf{k}\in C$, that has poles at all points $\mathbf{k}=\lambda_n^\pm$, $n=1,\dots,N$. It is convenient also to introduce a notation for the residual of the transmission coefficient, i.e.,

$$\vartheta_n^+=-i\operatorname*{res}_{\mathbf{k}=\lambda_n^+}t(\mathbf{k}),\qquad \vartheta_n^-=i\operatorname*{res}_{\mathbf{k}=\lambda_n^-}t(\mathbf{k}).\tag{2.21}$$

We also use special notations for the values of the Jost solutions at points $\mathbf{k}=\lambda_n^\pm$:

$$\varphi_n^\pm(x)=\sqrt{2\pi}\varphi(x,\lambda_n^\pm),\qquad \psi_n^\pm(x)=\sqrt{2\pi}\psi(x,\lambda_n^\pm),\tag{2.22}$$

so that by Eqs. (2.11), (2.2), and (2.20),

$$\overline{\varphi_n^\pm(x)}=\psi_n^\mp(x),\qquad \overline{\vartheta_-^\pm}=\vartheta_+^\mp.\tag{2.23}$$

Now we introduce piecewise constant functions of q_1,

$$\varphi_n(x,q_1)=\theta(\lambda_{n\Im}-|q_1|)[\theta(q_1)\varphi_n^+(x)+\theta(-q_1)\varphi_n^-(x)],\tag{2.24}$$

$$\psi_n(x,q_1)=\theta(\lambda_{n\Im}-|q_1|)[\theta(q_1)\psi_n^+(x)+\theta(-q_1)\psi_n^-(x)],\tag{2.25}$$

$$\vartheta_n(q_1)=\theta(q_1)\vartheta_n^++\theta(-q_1)\vartheta_n^-,\tag{2.26}$$

so that functions $\varphi_n(x,q_1)$ and $\psi_n(x,q_1)$ are different from zero only on the intervals $|q_1|<\lambda_{n\Im}$. These functions play an essential role in what follows and we call them auxiliary Jost solutions as they obey Eq. (2.12) and are reciprocally dual since from Eq. (2.11):

$$\overline{\varphi_n(x,q_1)}=\psi_n(x,-q_1).\tag{2.27}$$

In the following, these functions, when dressed by adding to u_N a nontrivial perturbation u' as indicated in Eq. (1.7), acquire a nontrivial dependence on q_1. From results of Ref. 25 it follows that these functions satisfy the following boundedness properties:

$$\sup_x|\varphi_n(x,q_1)|<\infty,\qquad \sup_x|\psi_n(x,q_1)|<\infty,\tag{2.28}$$

$$\sup_x|\chi_n(x,q_1)|<\infty,\qquad \sup_x|\xi_n(x,q_1)|<\infty,\tag{2.29}$$

where in analogy with Eq. (2.13) we introduced

$$\chi_n(x,q_1)=\mathrm{e}^{i\ell(\lambda_{n\Re}+iq_1)x}\varphi_n(x,q_1),\quad \xi_n(x,q_1)=\mathrm{e}^{-i\ell(\lambda_{n\Re}+iq_1)x}\psi_n(x,q_1), \tag{2.30}$$

that thanks to Eqs. (2.15), (2.24), and (2.25), have finite nonzero limits at large x.

C. Inverse problem

The Jost solutions $\varphi(x,\mathbf{k})$ and $\psi(x,\mathbf{k})$ are analytic functions of the complex variable $\mathbf{k}$ in the upper and bottom half plane with a discontinuity along the real axis. In order to describe this discontinuity we use the notations

$$\varphi^{\pm}(x,k)=\varphi(x,k\pm i0),\quad \psi^{\pm}(x,k)=\psi(x,k\pm i0), \tag{2.31}$$

$$t^{\pm}(k)=t(k\pm i0),\quad k\in\mathbb{R}, \tag{2.32}$$

that by Eqs. (2.11) and (2.20) obey conjugation properties

$$\overline{\varphi^{\pm}(x,k)}=\psi^{\mp}(x,k), \tag{2.33}$$

$$\overline{t^{+}(k)}=t^{-}(k). \tag{2.34}$$

In analogy to these relations we have for the boundary values of the auxiliary Jost solutions and functions ϑ_n directly by (2.24)–(2.26) relations

$$\varphi_n^{\pm}(x)=\varphi_n(x,\pm 0),\quad \psi_n^{\pm}(x)=\psi_n(x,\pm 0), \tag{2.35}$$

$$\vartheta_n^{\pm}=\vartheta_n(\pm 0). \tag{2.36}$$

Then, the Jost solutions (2.9) and (2.11) are determined by their analyticity properties and conditions (2.14) as solutions of the system (see Refs. 23 and 24)

$$t^{+}(k)\varphi^{+}(k)=\varphi^{-}(k), \tag{2.37}$$

$$\varphi_n^{+}=\sum_{m=1}^{N}\varphi_m^{-}\vartheta_m^{-}C_{mn}, \tag{2.38}$$

or, correspondingly,

$$t^{-}(k)\psi^{-}(k)=\psi^{+}(k), \tag{2.39}$$

$$\psi_n^{-}=\sum_{m=1}^{N}C_{nm}\vartheta_m^{+}\psi_m^{+}, \tag{2.40}$$

where we omitted the dependence on x, as often will be done below when not misleading. Thanks to Eqs. (2.37)–(2.40) we have relations

$$t^{+}(k)\varphi^{+}(k)\otimes\psi^{+}(k)=t^{-}(k)\varphi^{-}(k)\otimes\psi^{-}(k), \tag{2.41}$$

$$\sum_{n=1}^{N}\vartheta_n^{+}\varphi_n^{+}\otimes\psi_n^{+}=\sum_{n=1}^{N}\vartheta_n^{-}\varphi_n^{-}\otimes\psi_n^{-}, \tag{2.42}$$

where we used the standard definition of the direct product:

$$(\varphi_n(q_1)\otimes\psi_n(q_1))(x,x')=\varphi(x,q_1)\psi(x',q_1). \tag{2.43}$$

D. Resolvent of the pure *N*-soliton potential

Bilinear representation for the resolvent in terms of the Jost and auxiliary Jost solutions for the Nth Darboux transformation of rapidly decaying potential was derived in Ref. 25. Here we present a special case of that result corresponding to the pure N-soliton potential (2.6). Thus, the hat kernel [see Eq. (1.25)] of this resolvent equals to

$$\hat{M}_N(x,x';q) = \frac{1}{2\pi i}\int_{\mathbf{k}_\mathfrak{I}=q_1} d\mathbf{k}_\mathfrak{R}[\theta(x_2-x_2')-\theta(2\mathbf{k}_\mathfrak{R}q_1-q_2)]t(\mathbf{k})\varphi(x,\mathbf{k})\psi(x',\mathbf{k}) + \frac{1}{2\pi i}\sum_{n=1}^{N}\vartheta_n(q_1)[\theta(x_2-x_2')-\theta(2\lambda_{n\mathfrak{R}}q_1-q_2)]\varphi_n(x,q_1)\psi_n(x',q_1), \tag{2.44}$$

where notations (2.24)–(2.26) were used. In analogy to Eq. (1.34) it obeys differential equations

$$\vec{\mathcal{L}}_N\widehat{M}_N(q) = I = \widehat{M}_N(q)\overleftarrow{\mathcal{L}}_N, \tag{2.45}$$

that easily follows by means of the completeness relation,

$$\frac{1}{2\pi}\left\{\int d\mathbf{k}_\mathfrak{R}t(\mathbf{k})\varphi(x,\mathbf{k})\psi(x',\mathbf{k}) + \sum_{n=1}^{N}\vartheta_n(\mathbf{k}_\mathfrak{I})\varphi_n(x,\mathbf{k}_\mathfrak{I})\psi_n(x',\mathbf{k}_\mathfrak{I})\right\}_{x_2=x_2'} = \delta(x_1-x_1'), \tag{2.46}$$

derived in Ref. 25.

Convergency of the integral in Eq. (2.44) as well as the property that M_N belongs to the space of tempered distributions follow (see Ref. 25 for details) from the properties of the Jost and auxiliary Jost solutions. Moreover, in Ref. 25 it was proved that for generic q kernel $M_N(x,x';q)$ decays exponentially on the x-plane. From the conjugation relations (2.11), (2.20), and (2.27), we deduce that $M_N(q)$ obeys the conjugation property (1.41), in agreement with the reality of the potential $u_N(x)$. Both terms in the rhs of (2.44) are piecewise continuous functions of q-variables. Both of them are discontinuous at $q_1=\pm\lambda_{n\mathfrak{I}}$ [the first term thanks to the poles of $t(\mathbf{k})$, see Eq. (2.19)] and these discontinuities are compensated thanks to Eqs. (2.24)–(2.26). Thus the resolvent is discontinuous only at the point $q=0$ and on the intervals $q_2=2\lambda_{n\mathfrak{R}}q_1$, $n=1,\ldots,N$. Using notations (2.24)–(2.26) and (2.43) we get for such nth discontinuity expression

$$\widehat{M}_N(q)|_{q_2=2\lambda_{n\mathfrak{R}}q_1+0} - \widehat{M}_N(q)|_{q_2=2\lambda_{n\mathfrak{R}}q_1-0} = \frac{\vartheta_n(q_1)}{2\pi i}\varphi_n(q_1)\otimes\psi_n(q_1), \tag{2.47}$$

that is different from zero only on the interval $|q_1|<\lambda_{n\mathfrak{I}}$ [see Eqs. (2.24) and (2.25)]. At the end points of these intervals function $\widehat{M}_N(q)$ has logarithmic singularities. More precisely, we can decompose the resolvent into a regular and a singular part as follows:

$$M_N(q) = M_{N,\mathrm{reg}}(q) + M_{N,\mathrm{sing}}(q), \tag{2.48}$$

where the regular part, $M_{N,\mathrm{reg}}(q)$, is finite at any $q\in R^2$ and continuously differentiable for any $q\neq 0$. The singular part is given by

$$\widehat{M}_{N,\mathrm{sing}}(q) = \frac{1}{(2\pi)^2}\sum_{\sigma=\pm}\sum_{n=1}^{N}\theta(\sigma q_1)\vartheta_n^\sigma\varphi_n^\sigma\otimes\psi_n^\sigma\log\left(\sigma\left(q_1+i\lambda_n^\sigma-i\frac{q_2}{2q_1}\right)\right), \tag{2.49}$$

where we used notations (2.2) and where $\log\mathbf{z}$ has cut along the negative part of the $\mathbf{z}_\mathfrak{R}$-axis, so that $\partial\log z/\partial\bar{z}=-\pi\theta(-z_\mathfrak{R})\delta(z_\mathfrak{I})$.

Derivatives (in the sense of distributions) of the resolvent with respect to q-variables follow from Eq. (2.44), analyticity properties of the Jost solutions, and decomposition (2.48) and (2.49). At $q\neq 0$ we get

$$\frac{\partial \widehat{M}_N(q)}{\partial q_1} = \frac{i}{\pi}\left[\int_{\mathbf{k}_\mathfrak{I}=q_1} d\mathbf{k}_\mathfrak{R}\bar{\mathbf{k}}\,\delta(2\mathbf{k}_\mathfrak{R}\mathbf{k}_\mathfrak{I}-q_2)t(\mathbf{k})\varphi(\mathbf{k})\otimes\psi(\mathbf{k}) + \sum_{n=1}^{N}\lambda_{n\mathfrak{R}}\delta(2\lambda_{n\mathfrak{R}}q_1-q_2)\vartheta_n(q_1)\varphi_n(q_1)\otimes\psi_n(q_1)\right], \tag{2.50}$$

$$\frac{\partial \widehat{M}_N(q)}{\partial q_2} = \frac{1}{2\pi i}\left[\int_{\mathbf{k}_\mathfrak{I}=q_1} d\mathbf{k}_\mathfrak{R}\,\delta(2\mathbf{k}_\mathfrak{R}\mathbf{k}_\mathfrak{I}-q_2)t(\mathbf{k})\varphi(\mathbf{k})\otimes\psi(\mathbf{k}) + \sum_{n=1}^{N}\delta(2\lambda_{n\mathfrak{R}}q_1-q_2)\vartheta_n(q_1)\varphi_n(q_1)\otimes\psi_n(q_1)\right], \tag{2.51}$$

that agree with Eq. (2.47) thanks to the definition of the logarithm. Thus in the region of continuity the kernel (2.44) of the resolvent is differentiable with respect to q in the standard sense. In the case $q_1=0$ the resolvent $\widehat{M}_N(q)|_{q_1=0}$ has additional discontinuity at $q_2=0$, as already noted in (1.46), while for $q_2\neq 0$ it is continuous thanks to Eqs. (2.41) and (2.42).

E. Green's functions

Green's function corresponding to the potential u_N follows from Eqs. (1.42) and (2.44) in the form

$$\mathcal{G}_N(x,x',\mathbf{k}) = \frac{1}{2\pi i}\left[\int d\alpha[\theta(x_2-x_2')-\theta(\alpha\mathbf{k}_\mathfrak{I})]t(\alpha+\mathbf{k})\varphi(x,\alpha+\mathbf{k})\psi(x',\alpha+\mathbf{k}) + \sum_{n=1}^{N}\vartheta_n(\mathbf{k}_\mathfrak{I})[\theta(x_2-x_2')-\theta(\mathbf{k}_\mathfrak{I}(\lambda_{n\mathfrak{R}}-\mathbf{k}_\mathfrak{R}))]\varphi_n(x,\mathbf{k}_\mathfrak{I})\psi_n(x',\mathbf{k}_\mathfrak{I})\right]. \tag{2.52}$$

The Green function $\mathcal{G}_N(x,x',\mathbf{k})$, being a reduction of a hat operator, is exponentially growing at large space, but once multiplied by an exponent according to Eq. (1.45) one gets a distribution

$$G_N(x,x',\mathbf{k}) = \mathrm{e}^{i\ell(\mathbf{k})(x-x')}\mathcal{G}_N(x,x',\mathbf{k}), \tag{2.53}$$

which is bounded and decaying when x (or x') tends to infinity. More exactly, for generic $\mathbf{k}$, i.e., such that $\mathbf{k}_\mathfrak{I}\neq 0,\lambda_{1\mathfrak{I}},\ldots,\lambda_{N\mathfrak{I}}$, $\mathbf{k}_\mathfrak{R}\neq\lambda_{1\mathfrak{R}},\ldots,\lambda_{N\mathfrak{R}}$, we get

$$G_N(x,x',\mathbf{k}) = \frac{\operatorname{sgn}\mathbf{k}_\mathfrak{I}}{2\pi(x_1+2\mathbf{k}x_2)}t(\mathbf{k})\chi_{\mathrm{as}}(x,\mathbf{k})\xi(x',\mathbf{k})+o(|x|^{-1}), \tag{2.54}$$

for $x\to\infty$, where we used definition (2.16). Moreover, by Eq. (2.52) we get

$$\lim_{\mathbf{k}\to\infty,\mathbf{k}_\mathfrak{I}\neq 0} G_N(x,x',\mathbf{k}) = 0. \tag{2.55}$$

Next, for advanced/retarted Green's functions we have by Eq. (1.46) from Eq. (2.44)

$$\mathcal{G}_{N,\pm}(x,x') = \pm\frac{\theta(\pm(x_2-x_2'))}{2\pi i}\left[\int d\alpha t^\sigma(\alpha)\varphi^\sigma(x,\alpha)\psi^\sigma(x',\alpha)+\sum_{n=1}^{N}\vartheta_n^\sigma\varphi_n^\sigma(x)\psi_n^\sigma(x')\right], \tag{2.56}$$

where $\sigma=+,-$ and the rhs thanks to Eqs. (2.41) and (2.42) is independent on the choice of this sign (in fact, these signs can be chosen independently in the integral term and in the sum).

By (1.42), (1.46), (1.41), and (2.45), these Green's functions obey the conjugation properties (1.49) and (1.50) and the differential Eqs. (1.47) and (1.48) with $\mathcal{L}_N$ substituting $\mathcal{L}$. Function $\mathcal{G}_N(\mathbf{k})$ has cuts in the complex $\mathbf{k}$-plane along the intervals connecting the pairs λ_n and $\overline{\lambda_n}$ for all n. By Eq. (1.42)

$$\mathcal{G}_N(\lambda_{n\mathfrak{R}} \pm 0 + i\mathbf{k}_\mathfrak{I}) = \widehat{M}_N(\mathbf{k}_\mathfrak{I}, 2\lambda_{n\mathfrak{R}}\mathbf{k}_\mathfrak{I} \pm 0\mathbf{k}_\mathfrak{I}), \tag{2.57}$$

so that by Eq. (2.47)

$$\mathcal{G}_N(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{I}) - \mathcal{G}_N(\lambda_{n\mathfrak{R}} - 0 + i\mathbf{k}_\mathfrak{I}) = \frac{\operatorname{sgn}\mathbf{k}_\mathfrak{I}\,\vartheta_n(\mathbf{k}_\mathfrak{I})}{2\pi i}\varphi_n(\mathbf{k}_\mathfrak{I}) \otimes \psi_n(\mathbf{k}_\mathfrak{I}). \tag{2.58}$$

Performing reduction (1.42) in equalities (2.50) and (2.51) we get that at $\mathbf{k}_\mathfrak{I} \neq 0$:

$$\frac{\partial \mathcal{G}_N(\mathbf{k})}{\partial \mathbf{k}_\mathfrak{I}} = \frac{\operatorname{sgn}\mathbf{k}_\mathfrak{I}}{2\pi} t(\mathbf{k})\varphi(\mathbf{k}) \otimes \psi(\mathbf{k}), \tag{2.59}$$

$$\frac{\partial \mathcal{G}_N(\mathbf{k})}{\partial \bar{\mathbf{k}}} = \frac{\operatorname{sgn}\mathbf{k}_\mathfrak{I}}{4\pi i}\sum_{n=1}^{N} \delta(\mathbf{k}_\mathfrak{R} - \lambda_{n\mathfrak{R}})\vartheta_n(\mathbf{k}_\mathfrak{I})\varphi_n(\mathbf{k}_\mathfrak{I}) \otimes \psi(\mathbf{k}_\mathfrak{I}), \tag{2.60}$$

so that with exception of the segments connecting the pairs of points $\mathbf{k}=\lambda_n^\pm$ and with exception of the real axis Green's function $\mathcal{G}_N(\mathbf{k})$ is analytic in the upper and bottom half planes.

At the end points of these segments function $\mathcal{G}_N(\mathbf{k})$ is singular as follows from Eqs. (1.42) and (2.49):

$$\mathcal{G}_N(\mathbf{k}) = \mathcal{G}_{N,\mathrm{reg}}(\mathbf{k}) + \mathcal{G}_{N,\mathrm{sing}}(\mathbf{k}), \tag{2.61}$$

$$\mathcal{G}_{N,\mathrm{sing}}(\mathbf{k}) = \sum_{n=1}^{N} \gamma_n(\mathbf{k})\varphi_n^\sigma \otimes \psi_n^\sigma, \quad \sigma = \operatorname{sgn}\mathbf{k}_\mathfrak{I}, \tag{2.62}$$

where we used notation (2.2) and where

$$\gamma_n(\mathbf{k}) = \frac{\vartheta_n(\mathbf{k}_\mathfrak{I})}{(2\pi)^2}\log(-i\sigma(\mathbf{k} - \lambda_n^\sigma)), \quad \sigma = \operatorname{sgn}\mathbf{k}_\mathfrak{I}, \tag{2.63}$$

where logarithm is defined like in Eqs. (2.49). Thanks to this definition of the logarithm and Eq. (2.60) the first term in the rhs of Eq. (2.61) is analytic for any $\mathbf{k} \in C$, $\mathbf{k}_\mathfrak{I} \neq 0$. In the singular part every nth term is discontinuous on the segment $\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}$, $|\mathbf{k}_\mathfrak{I}| < \lambda_{n\mathfrak{I}}$. If for simplicity we assume that in addition to Eq. (2.1)

$$\lambda_{m\mathfrak{R}} \neq \lambda_{n\mathfrak{R}}, \quad \forall \ m \neq n \tag{2.64}$$

(the degenerate case can be considered by the limiting procedure) all these segments are mutually disjoint. Therefore, we can single out the singular behavior of Green's function in a vicinity of nth segment $\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}$, $|\mathbf{k}_\mathfrak{I}| < \lambda_{n\mathfrak{I}}$ by writing

$$\mathcal{G}_N(\mathbf{k}) = \mathcal{G}_N^{(n)}(\mathbf{k}) + \gamma_n(\mathbf{k})\varphi_n^\sigma \otimes \psi_n^\sigma, \quad \sigma = \operatorname{sgn}\mathbf{k}_\mathfrak{I}, \tag{2.65}$$

where by Eqs. (2.61) and (2.62),

$$\mathcal{G}_N^{(n)}(\mathbf{k}) = \mathcal{G}_{N,\mathrm{reg}}(\mathbf{k}) + \sum_{m\neq n}^{N} \gamma_m(\mathbf{k})\varphi_m^\sigma \otimes \psi_m^\sigma. \tag{2.66}$$

Thus for every n we get Green's function $\mathcal{G}_N^{(n)}(\mathbf{k})$ which is analytic in a vicinity of the nth segment $\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}$, $|\mathbf{k}_\mathfrak{I}| < \lambda_{n\mathfrak{I}}$ including the end points, but with the exception of the real $\mathbf{k}$-axis. Let us

mention that both this Green's function and function $G_N^{(n)}(x,x',\mathbf{k})$ defined in analogy with Eq. (1.45) are not decaying with respect to variables x and x'.

For the boundary values $\mathcal{G}^{\pm}$ [see Eq. (1.64)] of Green's function on the $\mathbf{k}_{\mathfrak{R}}$-axis we get by Eq. (2.52) ($k \in \mathbb{R}$)

$$\mathcal{G}_N^{\sigma}(x,x',k) = \frac{1}{2\pi i}\Bigg[\int dp[\theta(x_2 - x_2') - \theta(\sigma(p-k))]t^{\sigma}(p)\varphi^{\sigma}(x,p)\psi^{\sigma}(x',p) + \sum_{n=1}^{N}[\theta(x_2 - x_2') - \theta(\sigma(\lambda_{n\mathfrak{R}} - k))]\vartheta_n^{\sigma}\varphi_n^{\sigma}(x)\psi_n^{\sigma}(x')\Bigg], \tag{2.67}$$

where $\sigma = +,-$. Thus by Eq. (2.56),

$$\mathcal{G}_N^{\sigma}(k) - \mathcal{G}_{N,\pm} = \frac{\mp 1}{2\pi i}\Bigg[\int dp\,\theta(\pm\sigma(p-k))t^{\sigma}(p)\varphi^{\sigma}(p) \otimes \psi^{\sigma}(p) + \sum_{n=1}^{N}\theta(\pm\sigma(\lambda_{n\mathfrak{R}} - k))\vartheta_n^{\sigma}\varphi_n^{\sigma} \otimes \psi_n^{\sigma}\Bigg]. \tag{2.68}$$

A specific feature of the resolvent approach is the fact that the Jost and advanced/retarded solutions, as well as their dual, can be given as reductions of the corresponding Green's functions, see, e.g., Ref. 14. However, due to the nondecaying behavior of the N-soliton potential at large space distances these reduction formulas are required to be regularized. Precisely, we must write

$$\varphi(x,\mathbf{k}) = \lim_{\varepsilon \to +0}\int dx'(\mathcal{L}_0^d(x',\partial_{x'})\mathcal{G}_N(x,x',\mathbf{k}))\mathrm{e}^{-i\ell(\mathbf{k})x' - i\varepsilon x_2'}, \tag{2.69}$$

$$\psi(x,\mathbf{k}) = \lim_{\varepsilon \to +0}\int dx'\mathrm{e}^{i\ell(\mathbf{k})x' + i\varepsilon x_2'}\mathcal{L}_0(x',\partial_{x'})\mathcal{G}_N(x',x,\mathbf{k}), \tag{2.70}$$

where $\mathbf{k} \in \mathbb{C}$. It can be checked directly that these relations become identities if bilinear representation (2.52) for Green's function is used.

F. Advanced/retarded solutions

The advanced/retarded solutions are most naturally defined in terms of advanced/retarded Green's functions (2.56) as follows:

$$\varphi_{\pm}(x,k) = \int dx'(\mathcal{L}_0^d(x',\partial_{x'})\mathcal{G}_{N,\pm}(x,x'))\mathrm{e}^{-i\ell(k)x'}, \tag{2.71}$$

$$\psi_{\pm}(x,k) = \int dx'\mathrm{e}^{i\ell(k)x'}\mathcal{L}_0(x',\partial_{x'})\mathcal{G}_{N,\pm}(x',x), \tag{2.72}$$

where $k \in \mathbb{R}$. In spite of the bad behavior of u_N at large space, in this case no any regularization is needed. Thanks to properties (1.48) and (1.50) for $\mathcal{G}_{N,\pm}$ it is easy to check that

$$\vec{\mathcal{L}}_N\varphi_{\pm} = 0, \quad \psi_{\pm}\overleftarrow{\mathcal{L}}_N = 0, \tag{2.73}$$

$$\overline{\varphi_{\pm}} = \psi_{\mp}. \tag{2.74}$$

Using representation (2.56) in Eqs. (2.71) and (2.72) we get expressions of the advanced/retarded solutions in terms of the Jost ones. We omit here the corresponding calculations and present only the result. We introduce the spectral data

$$r_{\pm}^{\sigma}(k)=\prod_{n=1}^{N}\left(\frac{k-\lambda_n}{k-\overline{\lambda_n}}\right)^{-\sigma\theta(\mp\sigma(k-\lambda_{n\Re}))}, \tag{2.75}$$

that have the obvious properties

$$\overline{r_{\pm}^{\sigma}(k)}=r_{\mp}^{-\sigma}(k), \quad \overline{r_{\pm}^{\sigma}(k)}r_{\pm}^{\sigma}(k)=1, \tag{2.76}$$

and obey the characterization equations,

$$\overline{r_{\pm}^{-\sigma}(k)}r_{\pm}^{\sigma}(k)=t^{\sigma}(k), \tag{2.77}$$

which can be considered a "triangular decomposition" of $t^{\pm}$. Then, the above mentioned relations can be written as

$$\varphi_{\pm}(k)=\varphi^{\sigma}(k)\overline{r_{\pm}^{-\sigma}(k)}, \tag{2.78}$$

$$\psi_{\pm}(k)=\psi^{\sigma}(k)r_{\mp}^{\sigma}(k), \tag{2.79}$$

or, thanks to Eq. (2.77), as

$$t^{\sigma}(k)\varphi^{\sigma}(k)=\varphi_{\pm}(k)r_{\pm}^{\sigma}(k), \tag{2.80}$$

$$t^{\sigma}(k)\psi^{\sigma}(k)=\psi_{\pm}(k)\overline{r_{\mp}^{-\sigma}(k)}. \tag{2.81}$$

In particular, we get from these equalities

$$t^{\sigma}(k)\varphi^{\sigma}(k)\otimes\psi^{\sigma}(k)=\varphi_{\pm}(k)\otimes\psi_{\mp}(k), \tag{2.82}$$

where the lhs is independent on the sign $\sigma=+,-$ [see Eq. (2.41)] and the rhs is independent on the sign $\pm$.

We also need, in the following, the asymptotic behavior of $\varphi_{\pm}$ for $x_2\to\mp\infty$. From Eqs. (2.78) and (2.15) we obtain

$$\varphi_{\pm}(x,k)\simeq\chi_{\pm,\mathrm{as}}(k)\mathrm{e}^{-i\ell(k)x} \quad \text{for } x_2\to\mp\infty, \tag{2.83}$$

where

$$\chi_{\pm,\mathrm{as}}(k)=\prod_{n=1}^{N}\left(\frac{k-\lambda_n}{k-\overline{\lambda_n}}\right)^{\mp\mathrm{sgn}\,\lambda_{n\Re}\theta(\lambda_{n\Re}(k-\lambda_{n\Re}))}. \tag{2.84}$$

G. Auxiliary advanced/retarded solutions

Relation (2.46) shows that the Jost solutions form an incomplete set and in order to complete it one must introduce the auxiliary Jost solutions. The same, of course, is valid for the limiting values of the Jost solutions on the real k-axis which satisfy the completeness relation

$$\frac{1}{2\pi}\left\{\int d\mathbf{k}\,t^{\sigma}(k)\varphi^{\sigma}(x,k)\psi^{\sigma}(x',k)+\sum_{n=1}^{N}\vartheta_n^{\sigma}\varphi_n^{\sigma}(x)\psi_n^{\sigma}(x')\right\}_{x_2=x_2'}=\delta(x_1-x_1'), \quad \sigma=+,-. \tag{2.85}$$

Thanks to Eq. (2.82) the integral term here can be rewritten in terms of the advanced/retarded solutions only, that proves that the set of these solutions is incomplete and we have to introduce also auxiliary advanced/retarded. For this aim, taking into account that thanks to Eq. (2.3) all main minors of the matrix C are strictly positive, we can use for it the Gauss lower upper (LU) triangular decomposition:

$$C = (E + W_{\pm})^{\dagger} D_{\pm}^{2} (E + W_{\pm}), \tag{2.86}$$

where E is the unity $N \times N$ matrix, the $W_{\pm}$'s are off-diagonal and, respectively, upper and lower triangular matrices, and the $D_{\pm}$'s are strictly positive diagonal matrices. All multipliers in Eq. (2.86) are uniquely defined so we introduce new triangular matrices,

$$r_{\pm}^{+} = D_{\mp}(E + W_{\mp})\vartheta^{+}, \quad r_{\pm}^{-} = D_{\mp}^{-1}(E + W_{\mp}^{\dagger})^{-1}, \tag{2.87}$$

where

$$\vartheta^{\pm} = \mathrm{diag}\{\vartheta_1^{\pm}, \ldots, \vartheta_n^{\pm}\}. \tag{2.88}$$

These matrices obey the characterization equations,

$$r_{\pm}^{\sigma}(\vartheta^{\sigma})^{-1}(r_{\pm}^{-\sigma})^{\dagger} = E, \quad (r_{\pm}^{-\sigma})^{\dagger} r_{\pm}^{\sigma} = \vartheta^{\sigma}, \tag{2.89}$$

and by Eq. (2.86) we have

$$(r_{\pm}^{\sigma})^{\dagger} r_{\pm}^{\sigma} = \theta(\sigma)\vartheta^{-} C \vartheta^{+} + \theta(-\sigma) C^{-1}. \tag{2.90}$$

Now we define the auxiliary advanced/retarded solutions by means of the relations

$$\varphi_{\pm,n} = \sum_{m=1}^{N} \varphi_m^{\sigma} (r_{\pm}^{-\sigma})^{\dagger}(m,n), \quad \psi_{\pm,n} = \sum_{m=1}^{N} (r_{\mp}^{\sigma})(n,m)\psi_m^{\sigma}, \tag{2.91}$$

where the lhs' are independent on the sign $\sigma = +, -$ thanks to Eqs. (2.38), (2.40), (2.89), and (2.90). By using Eq. (2.89) these relations can be inverted,

$$\vartheta_n^{\sigma}\varphi_n^{\sigma} = \sum_{m=1}^{N} \varphi_{\pm,m} r_{\pm}^{\sigma}(m,n), \quad \vartheta_n^{\sigma}\psi_n^{\sigma} = \sum_{m=1}^{N} (r_{\mp}^{-\sigma})^{\dagger}(n,m)\psi_{\pm,m}. \tag{2.92}$$

In analogy with Eq. (2.82) we get from Eqs. (2.91) and (2.92),

$$\sum_{n=1}^{N} \vartheta_n^{\sigma}\varphi_n^{\sigma} \otimes \psi_n^{\sigma} = \sum_{n=1}^{N} \varphi_{\pm,n} \otimes \psi_{\mp,n}, \tag{2.93}$$

so that thanks to Eq. (2.82) we get from Eq. (2.85) the completeness relation in terms of the advanced/retarded and auxiliary advanced/retarded solutions,

$$\frac{1}{2\pi}\left\{ \int dk \varphi_{\pm}(x,k)\psi_{\mp}(x',k) + \sum_{n=1}^{N} \varphi_{\pm,n}(x)\psi_{\mp,n}(x') \right\}_{x_2 = x_2'} = \delta(x_1 - x_1'). \tag{2.94}$$

Relations (2.82) and (2.93) enable us to express advanced/retarded Green's functions in terms of the advanced/retarded and auxiliary advanced/retarded solutions. Thanks to Eq. (2.56) we have by Eq. (1.46),

$$\mathcal{G}_{N,\pm}(x,x') = \pm \frac{\theta(\pm(x_2 - x_2'))}{2\pi i}\left[\int dp \varphi_{\pm}(x,p)\psi_{\mp}(x',p) + \sum_{n=1}^{N} \varphi_{\pm,n}(x)\psi_{\mp,n}(x') \right], \tag{2.95}$$

where signs $\pm$ in the two terms in square brackets in Eq. (2.95) can be chosen freely and independently. In particular, this means that for the difference of advanced and retarded Green's function we get

$$\mathcal{G}_{N,+} - \mathcal{G}_{N,-} = \frac{1}{2\pi i}\left[\int dp\, \varphi_{\pm}(p) \otimes \psi_{\mp}(p) + \sum_{n=1}^{N} \varphi_{\pm,n} \otimes \psi_{\mp,n}\right], \tag{2.96}$$

where the rhs, thanks to Eqs. (2.82) and (2.93), is independent of the choice of the upper or bottom sign.

H. Time evolution of spectral data and Jost solutions

Time evolution of the spectral data in the case of the pure N-soliton solution u_N due to KPI equation is known[23] to be given as

$$\partial_t \lambda_n = 0, \tag{2.97}$$

$$\partial_t C = -4i(\overline{\lambda_m^3} - \lambda_n^3)C_{mn}. \tag{2.98}$$

Then by Eqs. (2.19) and (2.75) we get

$$\partial_t t(\mathbf{k}) = 0, \quad \mathbf{k} \in \mathbb{C}, \tag{2.99}$$

$$\partial_t r_{\pm}^{\sigma}(k) = 0, \quad \sigma = +,-, \quad k \in \mathbb{R}. \tag{2.100}$$

Thanks to Eq. (2.86), time evolution of diagonal matrices D_{pm}^2 coincides with evolution of the diagonal part of matrix C, so that by Eq. (2.87),

$$\partial_t r_{\pm}^{\sigma}(m,n) = -2i(\overline{\lambda_m^3} + \lambda_m^3 - 2(\lambda_n^{\sigma})^3) r_{\pm}^{\sigma}(m,n) = 0, \tag{2.101}$$

where notation (2.2) was used. In order to get time evolution of the Jost solution we use the standard crucial remark that if Φ is a solution of the nonstationary Schrödinger operator $\mathcal{L}$ then by Eq. (1.5) we deduce that $\mathcal{T}\Phi$ is also a solution. Moreover, since the operator $\mathcal{L}$ is a differential operator of first order in x_2 this solution is uniquely determined by its asymptotic behavior at $x_2 \to +\infty$ or at $x_2 \to -\infty$. Let us consider $\mathcal{T}_N \varphi(\mathbf{k})$ with $\mathcal{T}_N$ as in Eq. (1.4) with u the pure N-soliton potential u_N and $\varphi(\mathbf{k})$ the corresponding Jost solution (2.9). Then from the asymptotic behavior of the Jost solution given by Eqs. (2.13) and (2.15) at $x_2 \to \pm\infty$ we derive

$$\mathcal{T}_N(x, \mathbf{k}^3)\varphi(x,\mathbf{k}) = 0, \tag{2.102}$$

where we introduced the operator

$$\mathcal{T}_N(x,K) = \mathcal{T}_N(x) - 4iK \tag{2.103}$$

with K an arbitrary constant, and where we used that $u_N(x)$ is going to zero for $x_2 \to \mp\infty$ (Here for simplicity we assume that all $\lambda_{n\Re} \neq 0$. The result is independent of this assumption as values of $\lambda_{n\Re}$ can be shifted by a Galileo transformation.).

It is worthwhile to note that by inserting the expansion

$$\varphi(x,\mathbf{k}) \simeq \left(\theta(-\mathbf{k}_\Im) + \theta(\mathbf{k}_\Im)\frac{1}{t(\mathbf{k})}\right) e^{-i\ell(\mathbf{k})x} \quad \text{for } x_1 \to +\infty, \tag{2.104}$$

obtained from Eqs. (2.17) and (2.18) into Eq. (2.102) with $\mathcal{T}_N$ as in Eq. (1.4) one gets at any time $t > 0$ the dynamical constraint

$$\int_{-\infty}^{\infty} dx_1 \partial_{x_2} u_N(t,x) = 0, \tag{2.105}$$

which generalizes to the case of N solitons the dynamical constraint found in the case of decaying solutions in Ref. 4.

The advanced/retarded solutions $\varphi_{\pm}$ which are directly related to the Jost solutions by Eq. (2.78) due to Eq. (2.102) satisfy

$$\mathcal{T}_N(k^3)\varphi_{\pm}(k)=0, \tag{2.106}$$

while the auxiliary Jost solutions $\varphi_n(\mathbf{k}_\jmath)$ which are related to $\varphi(\lambda_n)$ and $\varphi(\overline{\lambda_n})$ via Eq. (2.24) satisfy

$$\mathcal{T}_N((\lambda_n^\sigma)^3)\varphi_n(\mathbf{k}_\jmath)=0 \quad \text{where} \quad \sigma=\operatorname{sgn}\mathbf{k}_\jmath. \tag{2.107}$$

For getting the differential equations fixing the time evolution of the advanced/retarded auxiliary solutions $\varphi_{\pm,n}$ we use their definition in Eq. (2.91) and relations (2.101) and (2.107)

$$\mathcal{T}_N\left(\frac{1}{2}(\overline{\lambda_m^3}+\lambda_m^3)\right)\varphi_{\pm,m}=0. \tag{2.108}$$

I. Matrix formulation

One can more conveniently write the relations interlacing the different kinds of Jost solutions and the characterization equations for the spectral data by introducing a vectorial formulation for the Jost solutions and a matrix formulation for the spectral data. Precisely, let us denote

$$\boldsymbol{\varphi}^\sigma(x)=(\varphi^\sigma(x,k),\varphi_1^\sigma(x),\ldots,\varphi_N^\sigma(x)), \tag{2.109}$$

$$\boldsymbol{\varphi}^\pm(x)=(\varphi_\pm(x,k),\varphi_{\pm,1}(x),\ldots,\varphi_{\pm,N}(x)), \tag{2.110}$$

that we call, respectively, vectorial Jost and vectorial advanced/retarded solutions, and

$$\mathbf{r}_\pm^\sigma=\begin{pmatrix} r_\pm^\sigma(p)\delta(p-k) & 0 \\ 0 & r_\pm^\sigma(m,n)\end{pmatrix}, \tag{2.111}$$

$$\mathbf{t}^\sigma=\begin{pmatrix} t^\sigma(p)\delta(p-k) & 0 \\ 0 & \delta_{mn}\vartheta_n^\sigma\end{pmatrix}, \tag{2.112}$$

that we call, respectively, matrix triangular spectral data and matrix transmission coefficient. If we define the product of matrices with matrix elements with continuous and discrete indices by integrating and summing, respectively, over continuous and discrete indices, then Eqs. (2.77) and (2.89) are combined in the characterization equations,

$$\mathbf{r}_\pm^\sigma(\mathbf{t}^\sigma)^{-1}(\mathbf{r}_\pm^{-\sigma})^\dagger=\mathbf{I}, \quad (\mathbf{r}_\pm^{-\sigma})^\dagger\mathbf{r}_\pm^\sigma=\mathbf{t}^\sigma, \tag{2.113}$$

where unity operator equals

$$\mathbf{I}=\begin{pmatrix}\delta(p-k) & 0 \\ 0 & \delta_{mn}\end{pmatrix}. \tag{2.114}$$

Then, Eqs. (2.78), (2.80), (2.91), and (2.92) relating the Jost to the advanced/retarded solutions, both standard and auxiliary, can be rewritten in a more compact form as follows:

$$\boldsymbol{\varphi}^\sigma\mathbf{t}^\sigma=\boldsymbol{\varphi}_\pm\mathbf{r}_\pm^\sigma, \tag{2.115}$$

$$\boldsymbol{\varphi}_\pm=\boldsymbol{\varphi}^\sigma(\mathbf{r}_\pm^{-\sigma})^\dagger. \tag{2.116}$$

The discontinuity at the real axis of the complex $\mathbf{k}$-plane of the Jost and auxiliary Jost solutions given in Eqs. (2.37) and (2.38) can be rewritten as

$$\boldsymbol{\varphi}^{\sigma}\mathbf{t}^{\sigma} = \boldsymbol{\varphi}^{-\sigma}\mathbf{f}^{-\sigma}, \tag{2.117}$$

where

$$\mathbf{f}^{\sigma} = (\mathbf{r}_{\pm}^{-\sigma})^{\dagger}\mathbf{r}_{\pm}^{-\sigma}. \tag{2.118}$$

Independence of the lhs on the signs $\pm$ gives the characterization equation

$$(\mathbf{r}_{+}^{\sigma})^{\dagger}\mathbf{r}_{+}^{\sigma} = (\mathbf{r}_{-}^{\sigma})^{\dagger}\mathbf{r}_{-}^{\sigma}. \tag{2.119}$$

The matrix $\mathbf{f}^{\sigma}$ together with the location of poles of $t(\mathbf{k})$ constitute the spectral data in strict sense. In fact, from Eqs. (2.76) and (2.90) we have

$$\mathbf{f}^{\sigma} = \begin{pmatrix} \delta(p-k) & 0 \\ 0 & \theta(-\sigma)\vartheta^{-}C\vartheta^{+} + \theta(\sigma)C^{-1} \end{pmatrix}. \tag{2.120}$$

Notice that the spectral data $\mathbf{f}$, due to Eqs. (2.113) and (2.118), satisfy the characterization equations

$$\mathbf{f}^{\sigma}(\mathbf{t}^{-\sigma})^{-1}\mathbf{f}^{-\sigma} = \mathbf{t}^{\sigma}, \tag{2.121}$$

$$(\mathbf{f}^{\sigma})^{\dagger} = \mathbf{f}^{\sigma}. \tag{2.122}$$

III. PERTURBATION

A. Resolvent, Green's functions, and Jost solutions

1. Properties of resolvent

Now we start with investigation of the spectral properties of the nonstationary Schrödinger operator (1.2) with a two dimensionally perturbed N-soliton potential $u(x)$ given in (1.7). In the previous sections we considered the pure N-soliton potential u_N and studied in detail the properties of the corresponding resolvent $M_N(q)$ and Green's function $\mathcal{G}_N(\mathbf{k})$. Now we exploit these results by constructing the resolvent $M(q)$ and Green's function $\mathcal{G}(\mathbf{k})$ corresponding to the potential u using the dressing procedure outlined in Sec. I E. We suppose that under the "smallness" requirement on u' the integral equations (1.58) admit a unique solution $M(q)$ for the resolvent with kernel $M(x,x';q)$ belonging to the space $\mathcal{S}'(\mathbb{R}^6)$. Then, the properties of the resolvent, including the singular behavior of $M(q)$ due to the nondecaying behavior of $u(x)$ at large space directions, can be studied via the integral equations (1.58), i.e., by means of the dressing procedure based on the Hilbert identity (1.61). In particular, we expect that the resolvent $M(q)$ will inherit, possibly smoothed by the dressing procedure, the singularities of $M_N(q)$. In fact, $M(q)$ results in becoming, as $M_N(q)$, a continuous function of the variables $q \in \mathbb{R}^2$ with the exception of the point $q=0$ and the segments $q_2 = 2\lambda_{n\mathfrak{R}}q_1$, $|q_1| \leqslant \lambda_{n\mathfrak{I}}$, $n=1,\ldots,N$, but, for a generic perturbation u', with 1/log instead of log behavior at the end points of the segments.

In the region of continuity the resolvent $M(q)$ is differentiable in the standard sense with respect to the parameters q_i $(i=1,2)$. Expressions for these derivatives can be obtained by dressing the corresponding derivatives of $M_N(q)$ by means of equation (1.63). Inserting Eqs. (2.50) and (2.51) into Eq. (1.63) we get for any q in the region of continuity

$$\frac{\partial \widehat{M}(q)}{\partial q_1} = \frac{i}{\pi}\int_{\mathbf{k}_{\mathfrak{I}}=q_1} d\mathbf{k}_{\mathfrak{R}}\bar{\mathbf{k}}\,\delta(2\mathbf{k}_{\mathfrak{R}}q_1 - q_2)t(\mathbf{k})\Phi(\mathbf{k}) \otimes \Psi(\mathbf{k}), \tag{3.1}$$

$$\frac{\partial \widehat{M}(q)}{\partial q_2} = \frac{1}{2\pi i}\int_{\mathbf{k}_{\mathfrak{I}}=q_1} d\mathbf{k}_{\mathfrak{R}}\,\delta(2\mathbf{k}_{\mathfrak{R}}q_1 - q_2)t(\mathbf{k})\Phi(\mathbf{k}) \otimes \Psi(\mathbf{k}), \tag{3.2}$$

where we introduced

$$\Phi(\mathbf{k}) = \mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi(\mathbf{k}), \quad \Psi(\mathbf{k}) = \psi(\mathbf{k})\vec{\mathcal{L}}_N\mathcal{G}(\mathbf{k}), \quad \mathbf{k} \in \mathbb{C}, \tag{3.3}$$

or explicitly

$$\Phi(x,\mathbf{k}) = \int dx'(\mathcal{L}_N^d(x',\partial_{x'})\mathcal{G}(x,x',\mathbf{k}))\varphi(x',\mathbf{k}), \tag{3.4}$$

$$\Psi(x',\mathbf{k}) = \int dx\psi(x,\mathbf{k})\mathcal{L}_N(x,\partial_x)\mathcal{G}(x,x',\mathbf{k}), \tag{3.5}$$

which can be considered a generalization of Eqs. (1.51), (2.69), and (2.70) and where $\mathcal{G}(x,x',\mathbf{k})$ is Green's function defined in Eq. (1.42). This function, being a reduction of Eq. (1.58), obeys consequently the integral equation (1.59) together with its dual that under the above assumption admit a unique solution $\mathcal{G}(\mathbf{k})$ such that $G(\mathbf{k})$ as defined in Eq. (1.45) belongs to $\mathcal{S}'$. Green's function inherits the analyticity properties of $\mathcal{G}_N(x,x',\mathbf{k})$, i.e., it is analytic for all $\mathbf{k} \in \mathbb{C}$ with the exception of the real axis, $\mathbf{k}_\Im = 0$, and intervals $\mathbf{k}_\Re = \lambda_{n\Re}$, $|\mathbf{k}_\Im| \leqslant \lambda_{n\Im}$. Performing reduction (1.42) in Eqs. (3.1) and (3.2) we get that in the region of analyticity

$$\frac{\partial\mathcal{G}(\mathbf{k})}{\partial\mathbf{k}_\Im} = \frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi}t(\mathbf{k})\Phi(\mathbf{k}) \otimes \Psi(\mathbf{k}), \tag{3.6}$$

$$\frac{\partial\mathcal{G}(\mathbf{k})}{\partial\mathbf{k}_\Re} = \frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi i}t(\mathbf{k})\Phi(\mathbf{k}) \otimes \Psi(\mathbf{k}), \tag{3.7}$$

while behavior of Green's function at the end points of the segments above, where $\mathcal{G}_N(\mathbf{k})$ has logarithmic singularities, needs a separate study (see Sec. III C below).

Thanks to Eq. (1.47) functions $\Phi(x,\mathbf{k})$ and $\Psi(x,\mathbf{k})$ defined in Eq. (3.3) obey the differential equations (1.56), and, therefore, we call them, respectively, Jost and dual Jost solution of the nonstationary Schrödinger equation with potential (1.7). Due to Eqs. (1.49) and (2.11) they obey the conjugation property

$$\Psi(x,\mathbf{k}) = \overline{\Phi(x,\bar{\mathbf{k}})}, \tag{3.8}$$

and integral equations for them follow by inserting Eqs. (1.59) into (3.3):

$$\Phi(\mathbf{k}) = \varphi(\mathbf{k}) + \mathcal{G}_N(\mathbf{k})u'\Phi(\mathbf{k}), \quad \Psi(\mathbf{k}) = \psi(\mathbf{k}) + \Psi(\mathbf{k})u'\mathcal{G}_N(\mathbf{k}). \tag{3.9}$$

The Jost solutions inherit the analytical properties of Green's function $\mathcal{G}_N(\mathbf{k})$. Precisely, they are analytic in the complex domain of the spectral parameter $\mathbf{k}$ with discontinuities at the real axis and at the segments $\mathbf{k}_\Re = \lambda_{n\Re}$, $|\mathbf{k}_\Im| < \lambda_{n\Im}$, $n = 1,\ldots,N$, and have continuous limits on the two sides of these cuts.

2. Asymptotics of Green's function and Jost solutions

The asymptotic behavior of Green's function $G(x,x',\mathbf{k})$ can be obtained directly by inserting the asymptotics (2.54) of $G_N(x,x',\mathbf{k})$ into Eq. (1.59), once multiplied by $e^{i\ell(\mathbf{k})(x-x')}$. We get, for $\mathbf{k}_\Im \neq 0, \lambda_{1\Im},\ldots,\lambda_{N\Im}$, $\mathbf{k}_\Re \neq \lambda_{1\Re},\ldots,\lambda_{N\Re}$, when $x \to \infty$

$$G(x,x',\mathbf{k}) = \frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi(x_1 + 2\mathbf{k}x_2)}t(\mathbf{k})\chi_{\text{as}}(x,\mathbf{k})\left\{\xi(x',\mathbf{k}) + \int dx''\xi(x'',\mathbf{k})u'(x'')G(x'',x',\mathbf{k})\right\} + o(|x|^{-1}).$$

Then, writing $u' = -\vec{\mathcal{L}} + \vec{\mathcal{L}}_N$ and using Eqs. (1.45), (2.13), and (1.56) we derive

$$G(x,x',\mathbf{k}) = \frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi(x_1+2\mathbf{k}x_2)} t(\mathbf{k})\chi_{\mathrm{as}}(x,\mathbf{k})\Psi(x',\mathbf{k})\mathrm{e}^{-i\ell(\mathbf{k})x'} + o(|x|^{-1}), \tag{3.10}$$

and expression for the limit $x' \to \infty$ follows by using the Hermitian conjugation (1.49). As well by Eq. (2.55) we get

$$\lim_{\mathbf{k}\to\infty,\mathbf{k}_\Im\neq 0} G(x,x',\mathbf{k}) = 0. \tag{3.11}$$

For getting the asymptotic behavior of the Jost solutions it is convenient to rewrite Eq. (3.3) by inserting $\mathcal{L}_N = \mathcal{L} + u'$ and, then, by using Eq. (1.47) we obtain

$$\Phi(\mathbf{k}) = \varphi(\mathbf{k}) + \mathcal{G}(\mathbf{k})u'\varphi(\mathbf{k}), \quad \Psi(\mathbf{k}) = \psi(\mathbf{k}) + \psi(\mathbf{k})u'\mathcal{G}(\mathbf{k}), \quad \mathbf{k} \in \mathbb{C}. \tag{3.12}$$

In order to deal with the bounded functions we introduce in analogy with Eq. (2.13) "the Jost solutions with removed exponents"

$$X(x,\mathbf{k}) = \mathrm{e}^{i\ell(\mathbf{k})x}\Phi(x,\mathbf{k}), \quad \Xi(x,\mathbf{k}) = \mathrm{e}^{-i\ell(\mathbf{k})x}\Psi(x,\mathbf{k}). \tag{3.13}$$

By Eq. (3.9) these functions can be defined as solutions of the integral equations (in the explicit form),

$$X(x,\mathbf{k}) = \chi(x,\mathbf{k}) + \int dx' G_N(x,x',\mathbf{k})u'(x')X(x',\mathbf{k}), \tag{3.14}$$

$$\Xi(x,\mathbf{k}) = \xi(x,\mathbf{k}) + \int dx' \Xi(x',\mathbf{k})u'(x')G_N(x',x,\mathbf{k}), \tag{3.15}$$

where $\chi(x,\mathbf{k})$ and $\xi(x,\mathbf{k})$ are bounded functions and $G_N(x,x',\mathbf{k})$ is bounded (decaying on the x-plane) Green's function explicitly given in Eqs. (2.53) and (2.52). On the other side by Eqs. (3.12) and (3.13),

$$X(\mathbf{k}) = \chi(\mathbf{k}) + G(\mathbf{k})u'\chi(\mathbf{k}), \quad \Xi(\mathbf{k}) = \xi(\mathbf{k}) + \xi(\mathbf{k})u'G(\mathbf{k}). \tag{3.16}$$

Then from Eqs. (2.14) and (3.11) we derive

$$\lim_{\mathbf{k}\to\infty} X(x,\mathbf{k}) = \lim_{\mathbf{k}\to\infty} \Xi(x,\mathbf{k}) = 1, \tag{3.17}$$

and from Eqs. (2.15) and (3.10) the asymptotic behavior in the x-space is given in the form

$$X(x,\mathbf{k}) = \chi_{\mathrm{as}}(x,\mathbf{k})\left[1 + \frac{\operatorname{sgn}\mathbf{k}_\Im}{2\pi(x_1+2\mathbf{k}x_2)} t(\mathbf{k})\mathcal{A}(\mathbf{k})\right] + o(|x|^{-1}), \quad x \to \infty, \tag{3.18}$$

where appeared the function of the variable $\mathbf{k} \in C$ only

$$\mathcal{A}(\mathbf{k}) = \int dx \Psi(x,\mathbf{k})u'(x)\varphi(x,\mathbf{k}). \tag{3.19}$$

In what follows we use for shortness the notation

$$\mathcal{A}(\mathbf{k}) = (\Psi(\mathbf{k})u'\varphi(\mathbf{k})) \tag{3.20}$$

[cf. "vector" and "covector" notations used in Eqs. (1.51), (1.54), and (1.55)]. Notice that $\mathcal{A}(\mathbf{k})$ can be equivalently defined as

$$\mathcal{A}(\mathbf{k}) = (\psi(\mathbf{k})\vec{\mathcal{L}}_N\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi(\mathbf{k})) = (\psi(\mathbf{k})u'\Phi(\mathbf{k})) = (\psi(\mathbf{k})\vec{\mathcal{L}}_N\Phi(\mathbf{k})) = (\Psi(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi(\mathbf{k})). \tag{3.21}$$

The function $\mathcal{A}(\mathbf{k})$ is analytic in the complex domain with discontinuity at the real axis and at the segments $\mathbf{k}_\Re=\lambda_{n\Re}$, $|\mathbf{k}_\Im|<\lambda_{n\Im}$, $n=1,\ldots,N$, it satisfies the conjugation property

$$\overline{\mathcal{A}(\bar{\mathbf{k}})} = \mathcal{A}(\mathbf{k}), \tag{3.22}$$

and generates, in spite of the bad behavior of u at large space distances, finite integrals of motion, e.g.,

$$\lim_{\mathbf{k}\to\infty}\mathcal{A}(\mathbf{k}) = \int dx\, u'(x). \tag{3.23}$$

From Eq. (3.8) we derive the same asymptotic behavior of the Jost solutions like in Eqs. (2.17) and (2.18)

$$\lim_{x_1\to-\mathbf{k}_\Im\infty} X(x,\mathbf{k}) = 1, \qquad \lim_{x_1\to+\mathbf{k}_\Im\infty} \Xi(x,\mathbf{k}) = 1, \tag{3.24}$$

$$\lim_{x_1\to+\mathbf{k}_\Im\infty} X(x,\mathbf{k}) = \frac{1}{t(\mathbf{k})}, \qquad \lim_{x_1\to-\mathbf{k}_\Im\infty} \Xi(x,\mathbf{k}) = \frac{1}{t(\mathbf{k})}. \tag{3.25}$$

B. Discontinuity of the resolvent at $q_2=2\lambda_{n\Re}q_1$ and auxiliary Jost solutions

The discontinuity of the resolvent $M(q)$ on the line $q_2=2\lambda_{n\Re}q_1$ can be derived by means of the dressing procedure described in Sec. I E from the discontinuity (2.47) of $M_N(q)$. Indeed, choosing in the Hilbert identity (1.66) $q_1=q_1$, $q_2=2q_1\lambda_{n\Re}-0$ and $q_2=2q_1\lambda_{n\Re}+0$ and using Eq. (2.47) we get for the hat kernel [see Eq. (1.25)] of the resolvent

$$\widehat{M}(q)|_{q_2=2\lambda_{n\Re}q_1+0} - \widehat{M}(q)|_{q_2=2\lambda_{n\Re}q_1-0} = \frac{\vartheta_n(q_1)}{2\pi i}\widehat{M}(q_1,2\lambda_{n\Re}q_1+0)\overleftarrow{\mathcal{L}}_N\varphi_n(q_1) \otimes \psi_n(q_1)\vec{\mathcal{L}}_N\widehat{M}(q_1,2a_{n\Re}q_1-0). \tag{3.26}$$

By means of the reduction (2.57) this relation gives for the discontinuity of Green's function:

$$\mathcal{G}(\lambda_{n\Re}+0+i\mathbf{k}_\Im) - \mathcal{G}(\lambda_{n\Re}-0+i\mathbf{k}_\Im) = \frac{\operatorname{sgn}\mathbf{k}_\Im\,\vartheta_n(\mathbf{k}_\Im)}{2\pi i}\mathcal{G}(\lambda_{n\Re}\pm 0+i\mathbf{k}_\Im)\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\Im) \otimes \psi_n(\mathbf{k}_\Im)\vec{\mathcal{L}}_N\mathcal{G}(\lambda_{n\Re}\mp 0+i\mathbf{k}_\Im). \tag{3.27}$$

Applying $\psi_n(\mathbf{k}_\Im)\vec{\mathcal{L}}_N$ and $\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\Im)$, respectively, from the left and from the right and introducing

$$A_n(\mathbf{k}_\Im) = 1 + \frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i}(\psi_n(\mathbf{k}_\Im)\vec{\mathcal{L}}_N\mathcal{G}(\lambda_{n\Re}+0+i\mathbf{k}_\Im)\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\Im)), \tag{3.28}$$

we deduce from Eq. (3.27) that the function $A_n(\mathbf{k}_\Im)$ has no zeros and

$$\frac{1}{A_n(\mathbf{k}_\Im)} = 1 - \frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i}(\psi_n(\mathbf{k}_\Im)\vec{\mathcal{L}}_N\mathcal{G}(\lambda_{n\Re}-0+i\mathbf{k}_\Im)\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\Im)). \tag{3.29}$$

The conjugation property

$$\overline{A_n(\mathbf{k}_\mathfrak{J})} = A_n(-\mathbf{k}_\mathfrak{J}) \tag{3.30}$$

follows from the conjugation properties of the entities involved in definition of $A_n(\mathbf{k}_\mathfrak{J})$.

Now we see that by Eq. (3.27) the discontinuity of Green's function on the segment is given in terms of the objects of the kind

$$\Phi_n(\mathbf{k}_\mathfrak{J}) = \mathcal{G}(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{J})\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\mathfrak{J}), \tag{3.31}$$

$$\Psi_n(\mathbf{k}_\mathfrak{J}) = \psi_n(\mathbf{k}_\mathfrak{J})\vec{\mathcal{L}}_N\mathcal{G}(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{J}), \tag{3.32}$$

that in analogy with the definition of the auxiliary Jost solutions in the pure N-soliton case in Eqs. (2.24) and (2.25) it is natural to call the auxiliary Jost solutions in the perturbed case. Indeed, thanks to Eq. (1.47) functions $\Phi_n(x,\mathbf{k}_\mathfrak{J})$ and $\Psi_n(x,\mathbf{k}_\mathfrak{J})$ obey the nonstationary Schrödinger equation and its dual, correspondingly,

$$\vec{\mathcal{L}}\Phi_n(\mathbf{k}_\mathfrak{J}) = 0, \quad \Psi_n(\mathbf{k}_\mathfrak{J})\overleftarrow{\mathcal{L}} = 0, \tag{3.33}$$

and, thanks to Eqs. (2.23) and (1.49), they obey the conjugation property

$$\overline{\Phi_n(\mathbf{k}_\mathfrak{J})} = \Psi_n(-\mathbf{k}_\mathfrak{J}). \tag{3.34}$$

By Eqs. (2.24) and (2.25) these functions are different from zero in the interval $|\mathbf{k}_\mathfrak{J}| \leqslant \lambda_{n\mathfrak{J}}$ only. Applying reductions (3.31) and (3.32) to Eq. (1.59) and its dual we get that the auxiliary Jost solutions obey the integral equations

$$\Phi_n(\mathbf{k}_\mathfrak{J}) = \varphi_n(\mathbf{k}_\mathfrak{J}) + \mathcal{G}_N(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{J})u'\Phi_n(\mathbf{k}_\mathfrak{J}), \tag{3.35}$$

$$\Psi_n(\mathbf{k}_\mathfrak{J}) = \psi_n(\mathbf{k}_\mathfrak{J}) + \Psi_n(\mathbf{k}_\mathfrak{J})u'\mathcal{G}_N(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{J}). \tag{3.36}$$

We introduce in analogy with Eq. (2.30)

$$X_n(x,\mathbf{k}_\mathfrak{J}) = \mathrm{e}^{ix\ell(\lambda_{n\mathfrak{R}}+i\mathbf{k}_\mathfrak{J})}\Phi_n(x,\mathbf{k}_\mathfrak{J}), \quad \Xi_n(x,\mathbf{k}_\mathfrak{J}) = \mathrm{e}^{-ix\ell(\lambda_{n\mathfrak{R}}+i\mathbf{k}_\mathfrak{J})}\Psi_n(x,\mathbf{k}_\mathfrak{J}). \tag{3.37}$$

Since Φ_n and Ξ_n and their dual are solutions of integral equations dressing φ_n and χ_n, which were proved in Ref. 25 to be bounded with respect to the variable $x \in \mathbb{R}^2$, we assume that for u' sufficiently "small" they also are bounded.

Next, by applying from the right $\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\mathfrak{J})$ to Eq. (3.27) and using Eq. (3.29) we get

$$\mathcal{G}(\lambda_{n\mathfrak{R}} - 0 + i\mathbf{k}_\mathfrak{J})\overleftarrow{\mathcal{L}}_N\varphi_n(\mathbf{k}_\mathfrak{J}) = \frac{\Phi_n(\mathbf{k}_\mathfrak{J})}{A_n(\mathbf{k}_\mathfrak{J})}, \tag{3.38}$$

$$\psi_n(\mathbf{k}_\mathfrak{J})\vec{\mathcal{L}}_N\mathcal{G}(\lambda_{n\mathfrak{R}} - 0 + i\mathbf{k}_\mathfrak{J}) = \frac{\Psi_n(\mathbf{k}_\mathfrak{J})}{A_n(\mathbf{k}_\mathfrak{J})}, \tag{3.39}$$

which can be used for expressing the discontinuities (3.26) and (3.27) in the form

$$\widehat{M}(q)|_{q_2=2\lambda_{n\mathfrak{R}}q_1+0} - \widehat{M}(q)|_{q_2=2\lambda_{n\mathfrak{R}}q_1-0} = \vartheta_n(q_1)\frac{\Phi_n(q_1)\otimes\Psi_n(q_1)}{2\pi i A_n(q_1)}, \tag{3.40}$$

$$\mathcal{G}(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{J}) - \mathcal{G}(\lambda_{n\mathfrak{R}} - 0 + i\mathbf{k}_\mathfrak{J}) = \vartheta_n(\mathbf{k}_\mathfrak{J})\frac{\Phi_n(\mathbf{k}_\mathfrak{J})\otimes\Psi_n(\mathbf{k}_\mathfrak{J})}{2\pi i(\operatorname{sgn}\mathbf{k}_\mathfrak{J})A_n(\mathbf{k}_\mathfrak{J})}. \tag{3.41}$$

Then, from Eq. (3.3) by using Eq. (3.41) and recalling that the N-soliton Jost solutions are discontinuous only across the real axis of the $\mathbf{k}$ plane we derive for the discontinuity of the Jost solutions across the segment $|\mathbf{k}_\mathfrak{J}| \leqslant \lambda_{n\mathfrak{J}}$, $\mathbf{k}_\mathfrak{R} = \lambda_{n\mathfrak{R}}$,

$$\Phi(\lambda_{n\Re}+0+i\mathbf{k}_\Im)-\Phi(\lambda_{n\Re}-0+i\mathbf{k}_\Im)=\Phi_n(\mathbf{k}_\Im)w_n(\mathbf{k}_\Im), \tag{3.42}$$

$$\Psi(\lambda_{n\Re}+0+i\mathbf{k}_\Im)-\Psi(\lambda_{n\Re}-0+i\mathbf{k}_\Im)=\Psi_n(\mathbf{k}_\Im)\overline{w_n(-\mathbf{k}_\Im)}, \tag{3.43}$$

where we introduced the spectral data

$$w_n(\mathbf{k}_\Im)=\frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i A_n(\mathbf{k}_\Im)}(\Psi_n(\mathbf{k}_\Im)\overleftarrow{\mathcal{L}}_N\varphi(\lambda_{n\Re}+i\mathbf{k}_\Im)), \tag{3.44}$$

that describe these discontinuities of the Jost solutions. Let us mention that Eq. (3.44) is a short version [cf. Eqs. (3.19) and (3.20)] of the relation

$$w_n(\mathbf{k}_\Im)=\frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i A_n(\mathbf{k}_\Im)}\int dx(\mathcal{L}_N^d\Psi_n(x,\mathbf{k}_\Im))\varphi(x,\lambda_{n\Re}+i\mathbf{k}_\Im), \tag{3.45}$$

and that by Eqs. (3.3) and (3.31) $w_n(\mathbf{k}_\Im)$ can be equivalently written in the forms

$$\begin{aligned}w_n(\mathbf{k}_\Im)&=\frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i A_n(\mathbf{k}_\Im)}(\psi_n(\mathbf{k}_\Im)\overrightarrow{\mathcal{L}}_N\mathcal{G}(\lambda_{n\Re}+0+i\mathbf{k}_\Im)\overleftarrow{\mathcal{L}}_N\varphi(\lambda_{n\Re}+i\mathbf{k}_\Im))\\&=\frac{\vartheta_n(\mathbf{k}_\Im)\operatorname{sgn}\mathbf{k}_\Im}{2\pi i A_n(\mathbf{k}_\Im)}(\psi_n(\mathbf{k}_\Im)\overrightarrow{\mathcal{L}}_N\Phi(\lambda_{n\Re}+0+i\mathbf{k}_\Im)).\end{aligned} \tag{3.46}$$

Finally, it is worth remarking that the discontinuity of the function $\mathcal{A}(\mathbf{k})$ defined in Eq. (3.20) also can be expressed in terms of the spectral data $w_n(\mathbf{k}_\Im)$. Precisely, we have

$$\mathcal{A}(\lambda_{n\Re}+0+i\mathbf{k}_\Im)-\mathcal{A}(\lambda_{n\Re}-0+i\mathbf{k}_\Im)=\frac{2\pi i\ \operatorname{sgn}(\mathbf{k}_\Im)}{\vartheta_n(\mathbf{k}_\Im)}A_n(\mathbf{k}_\Im)w_n(\mathbf{k}_\Im)\overline{w_n(-\mathbf{k}_\Im)}, \tag{3.47}$$

that can be used in derivation of a dispersion relation for $\mathcal{A}(\mathbf{k})$.

C. Behavior of Green's function and Jost solutions at end points of cuts

In Secs. II D and II E it was shown that the resolvent $M_N(q)$ and its reduction, Green's function $\mathcal{G}_N(\mathbf{k})$, have cuts along the segments $q_2=2\lambda_{n\Re}q_1$, $|q_1|\leqslant\lambda_{n\Im}$ and $\mathbf{k}_\Re=\lambda_{n\Re}$, $|\mathbf{k}_\Im|\leqslant\lambda_{n\Im}$ of the q- and $\mathbf{k}$-planes, respectively, with logarithmic singularities at the end points. These singularities were explicitly given, respectively, in Eq. (2.49) and in Eqs. (2.6) and (2.62). In the previous section we proved that the dressed resolvent $M(q)$ and Green's function $\mathcal{G}(\mathbf{k})$ have cuts along the same segments. Here we study the behavior of Green's function at the end points of these cuts using decomposition (2.65) of N-soliton Green's function $\mathcal{G}_N(\mathbf{k})$.

We need to write for Green's function $\mathcal{G}(\mathbf{k})$, as for $\mathcal{G}_N(\mathbf{k})$ in Eq. (2.65), a decomposition into a regular and a singular part. We expect that this can be obtained by dressing Eq. (2.65) and, precisely, that new Green's function $\mathcal{G}^{(n)}(\mathbf{k})$ of the operator $\mathcal{L}$ defined by

$$\mathcal{G}(\mathbf{k})=\mathcal{G}^{(n)}(\mathbf{k})+\Gamma(\mathbf{k})\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi_n^\sigma\otimes\psi_n^\sigma\overrightarrow{\mathcal{L}}_N\mathcal{G}(\mathbf{k}), \tag{3.48}$$

satisfies, for a proper choice of the function $\Gamma(\mathbf{k})$, the integral equation

$$\mathcal{G}^{(n)}(\mathbf{k})=\mathcal{G}_N^{(n)}(\mathbf{k})+\mathcal{G}_N^{(n)}(\mathbf{k})u'\mathcal{G}^{(n)}(\mathbf{k}) \tag{3.49}$$

and its dual and can therefore be considered a dressed version of $\mathcal{G}_N^{(n)}(\mathbf{k})$. Then, since $\mathcal{G}_N^{(n)}(\mathbf{k})$ is analytic in a vicinity of the segment $\mathbf{k}_\Re=\lambda_{n\Re}$, $|\mathbf{k}_\Im|=\lambda_{n\Im}$, with the exception of the $\mathbf{k}_\Re$-axis, we can deduce that $\mathcal{G}^{(n)}(\mathbf{k})$ as solution of Eq. (3.49) has the same analyticity properties.

Notice, however, that since φ_n^σ and ψ_n^σ are not bounded we must assume that the potential $u'(x)$ decays at large x faster than any linear exponential, in order that $\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N\varphi_n^\sigma$ and $\psi_n^\sigma\overrightarrow{\mathcal{L}}_N\mathcal{G}(\mathbf{k})$ appearing in Eq. (3.48) are well defined, as one can check by using $\mathcal{G}(\mathbf{k})\overleftarrow{\mathcal{L}}_N=\mathcal{G}(\mathbf{k})u'+I$ and its

dual and by recalling the behavior at large x of $\mathcal{G}$. [C.f. objects defined in Eqs. (3.28), (3.29), (3.31), and (3.32), where in the absence of condition of exponential decaying of u' we used condition that $\mathbf{k}$ belongs to the strip $|\mathbf{k}_\jmath| < \lambda_{n\jmath}$.]

Taking into account decomposition (2.65) one can check that Green's function $\mathcal{G}^{(n)}$ satisfies the integral equation (3.48) and its dual for

$$\Gamma(\mathbf{k}) = \frac{\gamma_n(\mathbf{k})}{1 + \alpha_n(\mathbf{k})\gamma_n(\mathbf{k})}, \tag{3.50}$$

where

$$\alpha_n(\mathbf{k}) = (\psi_n^\sigma \vec{\mathcal{L}}_N \mathcal{G}(\mathbf{k}) \overleftarrow{\mathcal{L}}_N \varphi_n^\sigma), \quad \mathbf{k} \in \mathbb{C}, \quad \sigma = \operatorname{sgn} \mathbf{k}_\jmath, \tag{3.51}$$

which is well defined for u' decaying according to our assumption.

Then, applying operations $\psi_n^\sigma \vec{\mathcal{L}}_N$ and $\overleftarrow{\mathcal{L}}_N \varphi_n^\sigma$ to Eq. (3.48) from the left and from the right we get

$$\frac{1}{\alpha_n(\mathbf{k})} = \frac{1}{a_n(\mathbf{k})} - \gamma_n(\mathbf{k}), \tag{3.52}$$

$$\mathcal{G}(\mathbf{k}) \overleftarrow{\mathcal{L}}_N \varphi_n^\sigma = \frac{\alpha_n(\mathbf{k})}{a_n(\mathbf{k})} \Phi^{(n)}(\mathbf{k}), \quad \psi_n^\sigma \vec{\mathcal{L}}_N \mathcal{G}(\mathbf{k}) = \frac{\alpha_n(\mathbf{k})}{a_n(\mathbf{k})} \Psi^{(n)}(\mathbf{k}), \tag{3.53}$$

where

$$a_n(\mathbf{k}) = (\psi_n^\sigma \vec{\mathcal{L}}_N \mathcal{G}^{(n)}(\mathbf{k}) \overleftarrow{\mathcal{L}}_N \varphi_n^\sigma), \quad \sigma = \operatorname{sgn} \mathbf{k}_\jmath, \tag{3.54}$$

and where, in analogy with Eqs. (3.3), (3.31), and (3.32), we have introduced

$$\Phi^{(n)}(\mathbf{k}) = \mathcal{G}^{(n)}(\mathbf{k}) \overleftarrow{\mathcal{L}}_N \varphi_n^\sigma, \quad \Psi^{(n)}(\mathbf{k}) = \psi_n^\sigma \vec{\mathcal{L}}_N \mathcal{G}^{(n)}(\mathbf{k}), \quad \mathbf{k} \in \mathbb{C}, \quad \sigma = \operatorname{sgn} \mathbf{k}_\jmath, \tag{3.55}$$

that also obey the nonstationary Schrödinger equation and its dual, correspondingly.

Notice that, under our assumption on the decaying of the potential u', the function $a_n(\mathbf{k})$ has the same analyticity properties of $\mathcal{G}^{(n)}(\mathbf{k})$. Then instead of Eq. (3.48) we get

$$\mathcal{G}(\mathbf{k}) = \mathcal{G}^{(n)}(\mathbf{k}) + \frac{\gamma_n(\mathbf{k})}{1 - a_n(\mathbf{k})\gamma_n(\mathbf{k})} \Phi^{(n)}(\mathbf{k}) \otimes \Psi^{(n)}(\mathbf{k}). \tag{3.56}$$

We see that the asymptotic behavior of Green's function at the end points is determined by the behavior of function $a_n(\mathbf{k})$ at these points. This function is meromorphic in the vicinity of the cut with the exception of the real axis and it is uniquely defined by the choice of the function $\gamma_n(\mathbf{k})$. However, notice that $\gamma_n(\mathbf{k})$ in Eq. (2.65) is required only to be such that the singular behavior of Green's function in a vicinity of the nth cut is single out. Thus, the choice in Eq. (2.63) is not unique, even if analyticity condition is imposed. If we shift $\gamma_n(\mathbf{k})$ by some constant, this shift is compensated by a shift of $1/a_n(\mathbf{k})$ as the lhs of Eq. (3.52) is invariant. This proves that the singularities of $a_n(\mathbf{k})$ are not related to the properties of $\gamma_n(\mathbf{k})$ and without loss of generality we can assume that $a_n(\mathbf{k})$ has finite limits

$$a_n^\pm = a_n(\lambda_n^\pm) \equiv (\psi_n^\pm \vec{\mathcal{L}}_N \mathcal{G}^{(n)}(\lambda_n^\pm) \overleftarrow{\mathcal{L}}_N \varphi_n^\pm). \tag{3.57}$$

They are related by the conjugation property

$$a_n^- = \overline{a_n^+}, \tag{3.58}$$

and by Eq. (3.56) they determine the behavior of Green's function $\mathcal{G}^{(n)}(\mathbf{k})$ at the points $\mathbf{k} = \lambda_n^\pm$. In contrast to the poles, the zeros of $a_n(\mathbf{k})$ are independent of the choice of $\gamma_n(\mathbf{k})$ and coincide with

the zeros of $\alpha_n(\mathbf{k})$. This is valid also at the end points, since, thanks to analyticity, $a_n(\mathbf{k})$ has zeros of integer order. Consequently, if the constants in Eq. (3.57) are equal to zero then $\mathcal{G}(\mathbf{k})$ has a logarithmic singularity at the end points of the cut and we get a singular behavior of the same kind that we had for the pure solitonic potential, when $u' \equiv 0$. For a generic u' we choose

$$a_n^{\pm} \neq 0. \tag{3.59}$$

This choice is natural and surely admissible as the following observation demonstrates. In fact, using equality $\mathcal{L}_N = \mathcal{L} + u'$ and the fact that $\mathcal{G}^{(n)}(\mathbf{k})$ is Green's function, we can rewrite Eq. (3.54) as $a_n(\mathbf{k}) = (\psi_n^{\sigma} \vec{\mathcal{L}}_N \mathcal{G}^{(n)}(k) u' \varphi_n^{\sigma})$ and, then, taking into account that by Eq. (3.49) $\mathcal{G}^{(n)}(\mathbf{k})|_{u' \equiv 0} = \mathcal{G}_N^{(n)} \times(\mathbf{k})$, we get the following functional derivative:

$$\left. \frac{\delta a_n(\mathbf{k})}{\delta u'} \right|_{u' \equiv 0} = \psi_n^{\sigma}(x) \varphi_n^{\sigma}(x), \quad \sigma = \operatorname{sgn} \mathbf{k}_{\mathfrak{I}} \tag{3.60}$$

which is different from zero for any value of $\mathbf{k}$. From here on we will consider only the case (3.59) for all $n = 1, \ldots, N$. Then $\mathcal{G}(\mathbf{k})$ has finite limits for $\mathbf{k} \to \lambda_n^{\pm}$:

$$\mathcal{G}(\lambda_n^{\pm}) = \mathcal{G}^{(n)}(\lambda_n^{\pm}) - \frac{1}{a_n^{\pm}} \Phi^{(n)}(\lambda_n^{\pm}) \otimes \Psi^n(\lambda_n^{\pm}), \tag{3.61}$$

where we used the solutions of the nonstationary Schrödinger equation and their dual defined in Eq. (3.55). Let us mention that Eq. (3.57) can be written also in the following forms:

$$a_n^{\pm} = (\psi_n^{\pm} \vec{\mathcal{L}}_N \Phi^{(n)}(\lambda_n^{\pm})) = (\Psi^{(n)}(\lambda_n^{\pm}) \overleftarrow{\mathcal{L}}_N \varphi_n^{\pm}), \tag{3.62}$$

so that by condition (3.59) functions $\Phi^{(n)}(x, \lambda_n^{\pm})$ and $\Psi^n(x, \lambda_n^{\pm})$ in Eq. (3.61) are different from zero.

Functions $\varphi(\mathbf{k})$ and $\psi(\mathbf{k})$ are analytic in the complex domain, so directly by definition (3.3) of the Jost solutions and thanks to Eqs. (2.22), (3.53), and (3.52) we derive

$$\lim_{\mathbf{k} \to \lambda_n^{\pm}} \gamma_n(\mathbf{k}) \Phi(x, \mathbf{k}) = - \frac{\Phi^{(n)}(x, \lambda_n^{\pm})}{\sqrt{2\pi} a_n^{\pm}}, \tag{3.63}$$

$$\lim_{\mathbf{k} \to \lambda_n^{\pm}} \gamma_n(\mathbf{k}) \Psi(x, \mathbf{k}) = - \frac{\Psi^{(n)}(x, \lambda_n^{\pm})}{\sqrt{2\pi} a_n^{\pm}}. \tag{3.64}$$

Inserting Eq. (3.64) in Eq. (3.20) and using Eq. (3.54) we get

$$\lim_{\mathbf{k} \to \lambda_n^{\pm}} \gamma_n(\mathbf{k}) \mathcal{A}(\mathbf{k}) = - \frac{1}{2\pi}. \tag{3.65}$$

In the same way by Eq. (3.31) taking into account Eqs. (2.24) and (3.53) we have for the auxiliary Jost solution

$$\lim_{\mathbf{k}_{\mathfrak{I}} \to \pm(\lambda_{n\mathfrak{I}} - 0)} \gamma_n(\lambda_{n\mathfrak{R}} + i\mathbf{k}_{\mathfrak{I}}) \Phi_n(\mathbf{k}_{\mathfrak{I}}) = - \frac{\Phi^{(n)}(\lambda_n^{\pm})}{a_n^{\pm}}, \tag{3.66}$$

and analogously for $\Psi_n(\mathbf{k}_{\mathfrak{I}})$.

The same consideration gives the behavior of the spectral data. Thus, Eq. (3.28) thanks to Eq. (3.51) can be written as

$$A_n(\mathbf{k}_\mathfrak{I}) = 1 + \frac{\vartheta_n(\mathbf{k}_\mathfrak{I})\operatorname{sgn}\mathbf{k}_\mathfrak{I}}{2\pi i}\alpha_n(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{I}),$$

so that Eq. (3.52)

$$\lim_{\mathbf{k}_\mathfrak{I}\to\pm(\lambda_{n\mathfrak{I}}-0)} \gamma_n(\lambda_{n\mathfrak{R}} + i\mathbf{k}_\mathfrak{I})[A_n(\mathbf{k}_\mathfrak{I}) - 1] = \mp\frac{\vartheta_n^\pm}{2\pi i}, \tag{3.67}$$

proving that $A_n(\mathbf{k}_\mathfrak{I})$ tends to 1 at the end points of the cut. For $w_n(\mathbf{k}_\mathfrak{I})$ we can use, say, the last equality in Eq (3.46) and (3.63). Then, thanks to Eqs. (3.62) and (3.67) we get

$$\lim_{\mathbf{k}_\mathfrak{I}\to\pm(\lambda_{n\mathfrak{I}}-0)} \gamma_n(\lambda_{n\mathfrak{R}} + i\mathbf{k}_\mathfrak{I})w_n(\mathbf{k}_\mathfrak{I}) = \pm\frac{i\vartheta_n^\pm}{(2\pi)^{3/2}}. \tag{3.68}$$

D. Relating auxiliary Jost solutions to Jost solutions

We have now all information on the properties of the auxiliary Jost solutions that are needed in order to express them in terms of the Jost solutions and spectral data $w_n(\mathbf{k}_\mathfrak{I})$.

By deriving Eq. (3.31) with respect to $\mathbf{k}_\mathfrak{I}$ we get, by using Eq. (3.6) and the expression for the adjoint of $w_n(\mathbf{k}_\mathfrak{I})$ as given in Eq. (3.46),

$$\frac{\partial\Phi_n(\mathbf{k}_\mathfrak{I})}{\partial\mathbf{k}_\mathfrak{I}} = \frac{iA_n(\mathbf{k}_\mathfrak{I})}{\vartheta_n(\mathbf{k}_\mathfrak{I})}t(\lambda_{n\mathfrak{R}} + i\mathbf{k}_\mathfrak{I})\overline{w_n(-\mathbf{k}_\mathfrak{I})}\Phi(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{I}). \tag{3.69}$$

Integrating, we have

$$\Phi_n(\mathbf{k}_\mathfrak{I}) = i\int_{\lambda_{n\mathfrak{I}}\operatorname{sgn}\mathbf{k}_\mathfrak{I}}^{\mathbf{k}_\mathfrak{I}} ds\frac{A_n(s)}{\vartheta_n(s)}t(\lambda_{n\mathfrak{R}} + is)\overline{w_n(-s)}\Phi(\lambda_{n\mathfrak{R}} + 0 + is), \tag{3.70}$$

where we took into account that by Eq. (3.66) the auxiliary Jost solution is zero at $\mathbf{k}=\lambda_n^\pm$.

Analogously, by Eq. (3.6) we get from Eq. (3.28),

$$\frac{\partial A_n(\mathbf{k}_\mathfrak{I})}{\partial\mathbf{k}_\mathfrak{I}} = \frac{iA_n^2(\mathbf{k}_\mathfrak{I})}{\vartheta_n(\mathbf{k}_\mathfrak{I})}t(\lambda_{n\mathfrak{R}} + i\mathbf{k}_\mathfrak{I})\overline{w_n(-\mathbf{k}_\mathfrak{I})}w_n(\mathbf{k}_\mathfrak{I}), \tag{3.71}$$

so that by Eq. (3.67),

$$A_n(\mathbf{k}_\mathfrak{I}) = \left(1 - i\int_{\lambda_{n\mathfrak{I}}\operatorname{sgn}\mathbf{k}_\mathfrak{I}}^{\mathbf{k}_\mathfrak{I}} ds\frac{t(\lambda_{n\mathfrak{R}} + is)}{\vartheta_n(s)}w_n(s)\overline{w_n(-s)}\right)^{-1} \neq 0. \tag{3.72}$$

Notice that relation (3.71) enables us to rewrite Eq. (3.47) in the form

$$t(\lambda_{n\mathfrak{R}} + i\mathbf{k}_\mathfrak{I})(\mathcal{A}(\lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_\mathfrak{I}) - \mathcal{A}(\lambda_{n\mathfrak{R}} - 0 + i\mathbf{k}_\mathfrak{I})) = 2\pi\operatorname{sgn}\mathbf{k}_\mathfrak{I}\frac{\partial\log A_n(\mathbf{k}_\mathfrak{I})}{\partial\mathbf{k}_\mathfrak{I}}. \tag{3.73}$$

E. Extended resolvent

Now we can proceed to the reconstruction of the resolvent of the nonstationary Schrödinger operator (1.2) with potential (1.7). Taking into account Eqs. (3.2) and (3.40) we get in analogy with Eq. (2.44)

$$\hat{M}(x,x';q)=\frac{1}{2\pi i}\Bigg[\int_{\mathbf{k}_\mathfrak{I}=q_1} d\mathbf{k}_\mathfrak{R}[\theta(x_2-x_2')-\theta(2\mathbf{k}_\mathfrak{R}q_1-q_2)]t(\mathbf{k})\Phi(x,\mathbf{k})\Psi(x',\mathbf{k}) + \sum_{n=1}^{N}\frac{\vartheta_n(q_1)}{A_n(q_1)}[\theta(x_2-x_2')-\theta(2\lambda_{n\mathfrak{R}}q_1-q_2)]\Phi_n(x,q_1)\Psi_n(x',q_1)\Bigg], \tag{3.74}$$

so that the dressed operator $\hat{M}(x,x';q)$ can be obtained from $\hat{M}_N(x,x';q)$ in Eq. (2.44) by substituting Jost and auxiliary Jost solutions by the dressed ones and by substituting $\vartheta_n(q_1)$ by $\vartheta_n(q_1)/A_n(q_1)$, that can be considered its dressed version. The proof that the kernel $M(x,x';q)$ given by Eq. (1.25) belongs to the space of tempered distributions can be performed following the proof given in Ref. 25 for the case of the pure N-soliton potential. This proof is based on the boundedness property of $X(x,\mathbf{k}_\mathfrak{I})$, $\Xi(x,\mathbf{k}_\mathfrak{I})$ proved in Sec. III A 2, and on the same property of $\Phi_n(x,\mathbf{k}_\mathfrak{I})$, $\Psi_n(x,\mathbf{k}_\mathfrak{I})$ and of $X_n(x,\mathbf{k}_\mathfrak{I})$, $\Xi_n(x,\mathbf{k}_\mathfrak{I})$ [see Eqs. (3.31), (3.32), and (3.37)], that was mentioned in Sec. III B. The fact that $\hat{M}(x,x';q)$, given above, obeys Eq. (1.34) means that the following completeness relation [cf. Eq. (2.46)] is valid:

$$\frac{1}{2\pi}\Bigg\{\int d\mathbf{k}_\mathfrak{R}t(\mathbf{k})\Phi(x,\mathbf{k})\Psi(x',\mathbf{k})+\sum_{n=1}^{N}\frac{\vartheta_n(\mathbf{k}_\mathfrak{I})}{A_n(\mathbf{k}_\mathfrak{I})}\Phi_n(x,\mathbf{k}_\mathfrak{I})\Psi_n(x',\mathbf{k}_\mathfrak{I})\Bigg\}_{x_2=x_2'}=\delta(x_1-x_1'). \tag{3.75}$$

Next, by Eq. (1.42) we get from Eq. (3.74) for Green's function representation

$$\mathcal{G}(x,x',\mathbf{k})=\frac{1}{2\pi i}\Bigg[\int d\alpha[\theta(x_2-x_2')-\theta(\alpha\mathbf{k}_\mathfrak{I})]t(\alpha+\mathbf{k})\Phi(x,\alpha+\mathbf{k})\Psi(x',\alpha+\mathbf{k}) + \sum_{n=1}^{N}\frac{\vartheta_n(\mathbf{k}_\mathfrak{I})}{A_n(\mathbf{k}_\mathfrak{I})}[\theta(x_2-x_2')-\theta(\mathbf{k}_\mathfrak{I}(\lambda_{n\mathfrak{R}}-\mathbf{k}_\mathfrak{R}))]\Phi_n(x,\mathbf{k}_\mathfrak{I})\Psi_n(x',\mathbf{k}_\mathfrak{I})\Bigg]. \tag{3.76}$$

In previous sections the analyticity properties of the Jost solutions were derived from the analyticity properties of Green's function. Vice versa, representation (3.76) enables us to derive the analyticity properties of Green's function from the properties of the Jost and auxiliary Jost solutions, while, say, check of the equality (3.6) is rather cumbersome. Omitting details we can use relations of the kind $\partial_{\mathbf{k}_\mathfrak{I}}\Phi(\alpha+\mathbf{k})=i\partial_\alpha\Phi(\alpha+\mathbf{k})$ in calculation of derivative of the integral term in Eq. (3.76), but only at $\alpha+\mathbf{k}_\mathfrak{R}\neq\lambda_{n\mathfrak{R}}$. Thus expressions for discontinuities given in Eqs. (3.42) and (3.43) must be taken into account. Then Eq. (3.6) for any $\mathbf{k}$, $\mathbf{k}_\mathfrak{I}\neq 0$ follows thanks to Eqs. (2.26) and (3.69) and its conjugate, and Eq. (3.71). Analogously we get in the same region of $\mathbf{k}$ by Eq. (3.76),

$$\frac{\partial\mathcal{G}(\mathbf{k})}{\partial\bar{\mathbf{k}}}=\frac{\operatorname{sgn}\mathbf{k}_\mathfrak{I}}{4\pi i}\sum_{n=1}^{N}\delta(\mathbf{k}_\mathfrak{R}-\lambda_{n\mathfrak{R}})\frac{\vartheta_n(\mathbf{k}_\mathfrak{I})}{A_n(\mathbf{k}_\mathfrak{I})}\Phi_n(\mathbf{k}_\mathfrak{I})\otimes\Psi_n(\mathbf{k}_\mathfrak{I}), \tag{3.77}$$

that generalizes Eq. (2.60) in correspondence with Eq. (3.41). Thus analyticity of Green's function for $\mathbf{k}_\mathfrak{I}\neq 0$ and $\mathbf{k}$ not belonging to the intervals $\mathbf{k}_\mathfrak{R}=\lambda_{n\mathfrak{R}}$, $|\mathbf{k}_\mathfrak{I}|\leqslant\lambda_{n\mathfrak{I}}$ follows from Eq. (3.76).

For the boundary values of Green's function on the real axis we get by Eq. (3.76) [cf. Eq. (2.67)],

$$\mathcal{G}^\sigma(x,x',k)=\frac{1}{2\pi i}\left[\int dp[\theta(x_2-x_2')-\theta(\sigma(p-k))]t^\sigma(p)\Phi^\sigma(x,p)\Psi^\sigma(x',p)\right.$$
$$\left.+\sum_{n=1}^{N}[\theta(x_2-x_2')-\theta(\sigma(\lambda_{n\mathfrak{R}}-k))]\frac{\vartheta_n^\sigma}{A_n^\sigma}\Phi_n^\sigma(x)\Psi_n^a(x')\right], \tag{3.78}$$

where $\sigma=+,-$, $k\in\mathbb{R}$, and we introduced for the boundary values of the functions involved in this bilinear representation notations

$$\Phi^\pm(x,k)=\Phi(x,k\pm i0),\quad \Psi^\pm(x,k)=\Psi(x,k\pm i0),\quad k\in\mathbb{R}, \tag{3.79}$$

$$\Phi_n^\pm(x)=\Phi_n(x,\pm 0),\quad \Psi_n^\pm(x)=\Psi_n(x,\pm 0), \tag{3.80}$$

$$A_n^\pm=A_n(\pm 0). \tag{3.81}$$

The standard conjugation properties,

$$\overline{\Phi^\pm(x,k)}=\Psi^\mp(x,k), \tag{3.82}$$

$$\overline{\Phi_n^\pm(x)}=\Psi_n^\mp(x), \tag{3.83}$$

$$\overline{A_n^+}=A_n^-, \tag{3.84}$$

are satisfied.

F. Advanced/retarded Green's functions and solutions

For advanced/retarted Green's functions we have by Eq. (1.46),

$$\mathcal{G}_\pm(x,x')=\pm\frac{\theta(\pm(x_2-x_2'))}{2\pi i}\left[\int d\alpha t^\sigma(\alpha)\Phi^\sigma(x,\alpha)\Psi^\sigma(x',\alpha)+\sum_{n=1}^{N}\frac{\vartheta_n^\sigma}{A_n^\sigma}\Phi_n^\sigma(x)\Psi_n^\sigma(x')\right] \tag{3.85}$$

[cf. Eqs. (2.52) and (2.56)], where $\sigma=+,-$ and the rhs is independent of the choice of this sign as we show below. As follows from Eq. (3.78),

$$\mathcal{G}^\sigma(k)-\mathcal{G}_\pm=\frac{\mp 1}{2\pi i}\left[\int dp\,\theta(\pm\sigma(p-k))t^\sigma(p)\Phi^\sigma(p)\otimes\Psi^\sigma(p)+\sum_{n=1}^{N}\theta(\pm\sigma(\lambda_{n\mathfrak{R}}-k))\frac{\vartheta_n^\sigma}{A_n^\sigma}\Phi_n^\sigma\otimes\Psi_n^\sigma\right]. \tag{3.86}$$

On the other side by Eqs. (1.68) and (2.96) we get

$$\mathcal{G}_+-\mathcal{G}_-=\frac{1}{2\pi i}\left[\int dp\,\Phi_\pm(p)\otimes\Psi_\mp(p)+\sum_{n=1}^{N}\Phi_{\pm,n}\otimes\Psi_{\mp,n}\right], \tag{3.87}$$

where we introduced the advanced/retarded solutions,

$$\Phi_\pm(k)=\mathcal{G}_\pm\overleftarrow{\mathcal{L}}_N\varphi_\pm(k),\quad \Psi_\pm(k)=\psi_\pm(k)\vec{\mathcal{L}}_N\mathcal{G}_\pm, \tag{3.88}$$

and the auxiliary advanced/retarded solutions [cf. Eqs. (3.31) and (3.32)],

$$\Phi_{\pm,n} = \mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_N\varphi_{\pm,n}, \quad \Psi_{\pm,n} = \psi_{\pm,n}\vec{\mathcal{L}}_N\mathcal{G}_{\pm}, \tag{3.89}$$

where the auxiliary advanced/retarded solutions $\varphi_{\pm,n}$ and $\psi_{\pm,n}$ of the pure N-soliton case are defined in Eq. (2.91). By these definitions we get that these functions, indeed, thanks to Eq. (1.48), obey the nonstationary Schrödinger equation and its dual,

$$\vec{\mathcal{L}}\Phi_{\pm}(k) = 0, \quad \Psi_{\pm}(k)\overleftarrow{\mathcal{L}} = 0, \tag{3.90}$$

$$\vec{\mathcal{L}}\Phi_{\pm,n} = 0, \quad \Psi_{\pm,n}\overleftarrow{\mathcal{L}} = 0, \tag{3.91}$$

have, thanks to Eq. (1.50), conjugation properties

$$\overline{\Phi_{\pm}} = \Psi_{\mp}, \quad \overline{\Phi_{\pm,n}} = \Psi_{\mp,n}, \tag{3.92}$$

and, thanks to Eq. (1.60), obey the integral equations

$$\Phi_{\pm} = \varphi_{\pm} + \mathcal{G}_{N,\pm}u'\Phi_{\pm}, \quad \Psi_{\pm} = \psi_{\pm} + \Psi_{\pm}u'\mathcal{G}_{N,\pm}, \tag{3.93}$$

$$\Phi_{\pm,n} = \varphi_{\pm,n} + \mathcal{G}_{N,\pm}u'\Phi_{\pm,n}, \quad \Psi_{\pm,n} = \psi_{\pm,n} + \Psi_{\pm,n}u'\mathcal{G}_{N,\pm}. \tag{3.94}$$

G. Relation between Jost solutions on the real axis and advanced/retarded solutions

Difference of Green's function given in Eq. (3.86) can also be derived by inserting Eq. (2.68) in the rhs of Eq. (1.67) that gives

$$\mathcal{G}^{\sigma}(k) - \mathcal{G}_{\pm} = \frac{\mp 1}{2\pi i}\left[\int dp\,\theta(\pm\sigma(p-k))t^{\sigma}(p)\mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_N\varphi^{\sigma}(p)\otimes\psi^{\sigma}(p)\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(k) + \sum_{n=1}^{N}\vartheta_n^{\sigma}\theta(\pm\sigma(\lambda_{n\Re}-k))\mathcal{G}_{\pm}\overleftarrow{\mathcal{L}}_N\varphi_n^{\sigma}\otimes\psi_n^{\sigma}\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(k)\right]. \tag{3.95}$$

Then using Eqs. (3.88), (2.80), and (2.92) we can rewrite Eq. (3.95) as

$$\mathcal{G}^{\sigma}(k) - \mathcal{G}_{\pm} = \frac{\mp 1}{2\pi i}\left[\int dp\,\theta(\pm\sigma(p-k))r_{\pm}^{\sigma}(p)\Phi_{\pm}(p)\otimes\psi^{\sigma}(p)\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(k) + \sum_{m,n=1}^{N}r_{\pm}^{\sigma}(m,n)\theta(\pm\sigma(\lambda_{n\Re}-k))\Phi_{\pm,m}\otimes\psi_n^{\sigma}\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(k)\right]. \tag{3.96}$$

Let us now introduce the spectral data

$$R_{\pm}^{\sigma}(p,k) = r_{\pm}^{\sigma}(p)\left[\delta(k-p) \mp \frac{t^{\sigma}(k)}{2\pi i}\theta(\pm\sigma(p-k))(\psi^{\sigma}(p)\vec{\mathcal{L}}_N\Phi^{\sigma}(k))\right], \tag{3.97}$$

$$R_{\pm}^{\sigma}(m,k) = \mp\frac{t^{\sigma}(k)}{2\pi i}\sum_{n=1}^{N}r_{\pm}^{\sigma}(m,n)\theta(\pm\sigma(\lambda_{n\Re}-k))(\psi_n^{\sigma}\vec{\mathcal{L}}_N\Phi^{\sigma}(k)). \tag{3.98}$$

Then, applying to Eq. (3.96) operation $\overleftarrow{\mathcal{L}}_N\varphi^{\sigma}(k)$ from the right and using Eqs. (3.3) (at $\mathbf{k}=k+i\sigma 0$), (3.88) and (2.80) we get

$$t^{\sigma}(k)\Phi^{\sigma}(k) = \int dp\Phi_{\pm}(p)R^{\sigma}_{\pm}(p,k) + \sum_{m=1}^{N} \Phi_{\pm,m}R^{\sigma}_{\pm}(m,k), \tag{3.99}$$

$$t^{\sigma}(k)\Psi^{\sigma}(k) = \int dp\overline{R^{-\sigma}_{\mp}(p,k)}\Psi_{\pm}(p) + \sum_{m=1}^{N} \overline{R^{-\sigma}_{\mp}(m,k)}\Psi_{\pm,m}, \tag{3.100}$$

where the second equality follows by conjugation.

Using the fact that the N-soliton potential is invariant under permutation of the λ_n's it is convenient here to renumber them in such a way that

$$\lambda_{1\Re} < \cdots < \lambda_{N\Re}, \tag{3.101}$$

and to introduce the step function of a discrete variable defined as

$$\theta(n) = \begin{cases} 1, & n > 0 \\ 0, & n \leqslant 0. \end{cases} \tag{3.102}$$

In order to express the auxiliary Jost solutions in terms of the advanced/retarded solutions, we perform first the limit $k \to \lambda_{l\Re} + 0$ in Eq. (3.96) getting

$$\begin{aligned} \mathcal{G}^{\sigma}(\lambda_{l\Re}+0) - \mathcal{G}_{\pm} = \frac{\mp 1}{2\pi i}\Bigg[& \int dp\,\theta(\pm\sigma(p-\lambda_{l\Re}))r^{\sigma}_{\pm}(p)\Phi_{\pm}(p) \otimes \psi^{\sigma}(p)\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(\lambda_{l\Re}+0) \\ & + \sum_{m=1}^{N}\Phi_{\pm,m}\sum_{n=1}^{N} r^{\sigma}_{\pm}(m,n)[\theta(\pm\sigma)\theta(n-l) + \theta(\mp\sigma)\theta(l-n) + \theta(\mp\sigma)\delta_{ln}] \\ & \otimes \psi^{\sigma}_n\vec{\mathcal{L}}_N\mathcal{G}^{\sigma}(\lambda_{l\Re}+0)\Bigg], \end{aligned} \tag{3.103}$$

and we introduce the new set of spectral data,

$$R^{\sigma}_{\pm}(k,n) = \mp\,\theta(\pm\sigma(k-\lambda_{n\Re}))\frac{r^{\sigma}_{\pm}(k)\vartheta^{\sigma}_n}{2\pi i A^{\sigma}_n}(\psi^{\sigma}(k)\vec{\mathcal{L}}_N\Phi^{\sigma}_n), \tag{3.104}$$

$$R^{\sigma}_{\pm}(m,n) = \sum_{l=1}^{N} r^{\sigma}_{\pm}(m,l)\left[\delta_{ln}\left(\frac{\theta(\pm\sigma)}{A^{\sigma}_n} + \theta(\mp\sigma)\right) \mp \theta(\pm\sigma(l-n))\frac{\vartheta^{\sigma}_n}{2\pi i A^{\sigma}_n}(\psi^{\sigma}_l\vec{\mathcal{L}}_N\Phi^{\sigma}_n)\right], \tag{3.105}$$

where the λ_n's are subjected to condition (3.101).

Then, we apply operation $\vec{\mathcal{L}}_N\varphi^{\sigma}_n$ to Eq. (3.103) from the right and use (3.31) at $\mathbf{k}_{\jmath} = \sigma 0$, (2.92), and

$$A^{\sigma}_n = 1 + \frac{\sigma\vartheta^{\sigma}_n}{2\pi i}(\psi^{\sigma}_n\vec{\mathcal{L}}_N\Phi^{\sigma}_n), \tag{3.106}$$

which follows from Eq. (3.28). We get

$$\frac{\vartheta^{\sigma}_n}{A^{\sigma}_n}\Phi^{\sigma}_n = \int dp\Phi_{\pm}(p)R^{\sigma}_{\pm}(p,n) + \sum_{m=1}^{N}\Phi_{\pm,m}R^{\sigma}_{\pm}(m,n), \tag{3.107}$$

$$\frac{\vartheta_n^\sigma}{A_n^\sigma}\Psi_n^\sigma = \int dp\overline{R_\mp^{-\sigma}(p,n)}\Psi_\pm(p) + \sum_{m=1}^{N}\overline{R_\mp^{-\sigma}(m,n)}\Psi_{\pm,m}, \tag{3.108}$$

where again the second equality follows by conjugation.

Inverse relations follow applying to Eq. (3.86) from the right $\overleftarrow{\mathcal{L}}_N\varphi_\pm$ and using Eqs. (2.78), (3.3), (3.79), and (3.88), and properties of conjugation of solutions,

$$\Phi_\pm(k) = \int dp\Phi^\sigma(p)\overline{R_\pm^{-\sigma}(k,p)} + \sum_{n=1}^{N}\Phi_n^\sigma\overline{R_\pm^{-\sigma}(k,n)}, \tag{3.109}$$

and applying to Eq. (3.86) at $k=\lambda_{m\Re}+0$ from the right $\overleftarrow{\mathcal{L}}_N\varphi_{\pm,n}$ and using Eqs. (2.91), (3.31), (3.38), and (3.89), and again properties of conjugation of solutions:

$$\Phi_{\pm,n} = \int dp\Phi^\sigma(p)\overline{R_\pm^{-\sigma}(n,p)} + \sum_{m=1}^{N}\Phi_m^\sigma\overline{R_\pm^{-\sigma}(n,m)}. \tag{3.110}$$

Relations

$$\Psi_\pm(k) = \int dpR_\mp^\sigma(k,p)\Psi^\sigma(p) + \sum_{n=1}^{N}R_\mp^\sigma(k,n)\Psi_n^\sigma, \tag{3.111}$$

$$\Psi_{\pm,n} = \int dpR_\mp^\sigma(n,p)\Psi^\sigma(p) + \sum_{m=1}^{N}R_\mp^\sigma(n,m)\Psi_m^\sigma \tag{3.112}$$

are obtained by conjugation.

H. Characterization equations for spectral data

In order to give characterization equations in observable form we use the technique introduced by Eqs. (2.109)–(2.114) in Sec. II. Thus we denote rows,

$$\mathbf{\Phi}^\sigma(x) = (\Phi^\sigma(x,k),\Phi_1^\sigma(x),\ldots,\Phi_N^\sigma(x)), \tag{3.113}$$

$$\mathbf{\Phi}_\pm(x) = (\Phi_\pm(x,k),\Phi_{\pm,1}(x),\ldots,\Phi_{\pm,N}(x)), \tag{3.114}$$

columns,

$$\mathbf{\Psi}^\sigma(x) = (\Psi^\sigma(x,k),\Psi_1^\sigma(x),\ldots,\Psi_N^\sigma(x))^T, \tag{3.115}$$

$$\mathbf{\Psi}_\pm(x) = (\Psi_\pm(x,k),\Psi_{\pm,1}(x),\ldots,\Psi_{\pm,N}(x))^T, \tag{3.116}$$

and matrix operators,

$$\mathbf{R}_\pm^\sigma = \begin{pmatrix} R_\pm^\sigma(p,k) & R_\pm^\sigma(p,n) \\ R_\pm^\sigma(m,k) & R_\pm^\sigma(m,n) \end{pmatrix}, \tag{3.117}$$

$$\mathbf{T}^\sigma = \begin{pmatrix} t^\sigma(p)\delta(p-k) & 0 \\ 0 & \delta_{mn}(\vartheta_n^\sigma/A_n^\sigma) \end{pmatrix}, \tag{3.118}$$

with unity operator defined in Eq. (2.114). Then, assuming the same operations with these objects as in Eqs. (2.111)–(2.116), we can rewrite Eqs. (3.99), (3.100), and (3.107)–(3.112), as

$$\mathbf{\Phi}^\sigma\mathbf{T}^\sigma = \mathbf{\Phi}_\pm\mathbf{R}_\pm^\sigma, \tag{3.119}$$

$$\mathbf{T}^{\sigma}\boldsymbol{\Psi}^{\sigma} = (\mathbf{R}_{\mp}^{-\sigma})^{\dagger}\boldsymbol{\Psi}_{\pm}, \tag{3.120}$$

$$\boldsymbol{\Phi}_{\pm} = \boldsymbol{\Phi}^{\sigma}(\mathbf{R}_{\pm}^{-\sigma})^{\dagger}, \tag{3.121}$$

$$\boldsymbol{\Psi}_{\pm} = \mathbf{R}_{\mp}^{\sigma}\boldsymbol{\Psi}^{\sigma}, \tag{3.122}$$

from which easily follow the characterization equations [cf. Eqs. (2.113) and (2.119)],

$$(\mathbf{R}_{\pm}^{-\sigma})^{\dagger}\mathbf{R}_{\pm}^{\sigma} = \mathbf{T}^{\sigma}, \tag{3.123}$$

$$\mathbf{R}_{\pm}^{\sigma}(\mathbf{T}^{\sigma})^{-1}(\mathbf{R}_{\pm}^{-\sigma})^{\dagger} = \mathbf{I}, \tag{3.124}$$

$$(\mathbf{R}_{+}^{\sigma})^{\dagger}\mathbf{R}_{+}^{\sigma} = (\mathbf{R}_{-}^{\sigma})^{\dagger}\mathbf{R}_{-}^{\sigma}. \tag{3.125}$$

If we introduce

$$\mathbf{F}^{-\sigma} = (\mathbf{R}_{\pm}^{\sigma})^{\dagger}\mathbf{R}_{\pm}^{\sigma}, \tag{3.126}$$

we have

$$\boldsymbol{\Phi}^{\sigma}\mathbf{T}^{\sigma} = \boldsymbol{\Phi}^{-\sigma}\mathbf{F}^{-\sigma}. \tag{3.127}$$

It is easy to check that these spectral data obey the characterization equations,

$$\mathbf{F}^{\sigma}(\mathbf{T}^{-\sigma})^{-1}\mathbf{F}^{-\sigma} = \mathbf{T}^{\sigma}, \tag{3.128}$$

$$(\mathbf{F}^{\sigma})^{\dagger} = \mathbf{F}^{\sigma}, \tag{3.129}$$

that generalize Eqs. (2.121) and (2.122), so that

$$\boldsymbol{\Phi}^{\sigma}\mathbf{T}^{\sigma}\boldsymbol{\Psi}^{\sigma} = \boldsymbol{\Phi}_{\pm}\boldsymbol{\Psi}_{\mp}. \tag{3.130}$$

Operator data $\mathbf{R}_{\pm}^{\sigma}$ involve both the discrete and the continuous parts of the spectral data. These two contributions can be made more transparent by factorizing out the discrete data by means of decomposition

$$\mathbf{R}_{\pm}^{\sigma} = \mathbf{r}_{\pm}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}, \tag{3.131}$$

where $\mathbf{r}_{\pm}^{\sigma}$ is the matrix operator defined in Eq. (2.111) and

$$\boldsymbol{\mathcal{R}}_{\pm}^{\sigma} = \begin{pmatrix} \mathcal{R}_{\pm}^{\sigma}(p,k) & \mathcal{R}_{\pm}^{\sigma}(p,n) \\ \mathcal{R}_{\pm}^{\sigma}(m,k) & \mathcal{R}_{\pm}^{\sigma}(m,n) \end{pmatrix}, \tag{3.132}$$

where

$$\mathcal{R}_{\pm}^{\sigma}(p,k) = \delta(k-p) \mp \theta(\pm\sigma(p-k))\frac{t^{\sigma}(k)}{2\pi i}(\psi^{\sigma}(p)\vec{\mathcal{L}}_{N}\Phi^{\sigma}(k)), \tag{3.133}$$

$$\mathcal{R}_{\pm}^{\sigma}(m,k) = \mp \theta(\pm\sigma(\lambda_{m\Re}-k))\frac{t^{\sigma}(k)}{2\pi i}(\psi_{m}^{\sigma}\vec{\mathcal{L}}_{N}\Phi^{\sigma}(k)), \tag{3.134}$$

$$\mathcal{R}_{\pm}^{\sigma}(p,n) = \mp \theta(\pm\sigma(p-\lambda_{n\Re}))\frac{\vartheta_{n}^{\sigma}}{2\pi i A_{n}^{\sigma}}(\psi^{\sigma}(p)\vec{\mathcal{L}}_{N}\Phi_{n}^{\sigma}), \tag{3.135}$$

$$\mathcal{R}_{\pm}^{\sigma}(m,n)=\delta_{mn}\left(\frac{\theta(\pm\sigma)}{A_n^{\sigma}}+\theta(\mp\sigma)\right)\mp\theta(\pm\sigma(m-n))\frac{\vartheta_n^{\sigma}}{2\pi i A_n^{\sigma}}(\psi_m^{\sigma}\vec{\mathcal{L}}_N\Phi_n^{\sigma}). \tag{3.136}$$

We have, then, Eqs. (3.119)–(3.122),

$$\mathbf{\Phi}^{\sigma}\mathbf{T}^{\sigma}=\mathbf{\Phi}_{\pm}\mathbf{r}_{\pm}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}, \tag{3.137}$$

$$\mathbf{\Phi}_{\pm}=\mathbf{\Phi}^{\sigma}(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}(\mathbf{r}_{\pm}^{-\sigma})^{\dagger}, \tag{3.138}$$

$$\mathbf{T}^{\sigma}\mathbf{\Psi}^{\sigma}=(\boldsymbol{\mathcal{R}}_{\mp}^{-\sigma})^{\dagger}(\mathbf{r}_{\mp}^{-\sigma})^{\dagger}\mathbf{\Psi}_{\pm} \tag{3.139}$$

$$\mathbf{\Psi}_{\pm}=\mathbf{r}_{\mp}^{\sigma}\boldsymbol{\mathcal{R}}_{\mp}^{\sigma}\mathbf{\Psi}^{\sigma}. \tag{3.140}$$

Inserting the second equality of Eq. (2.113) into Eq. (3.123) and recalling Eq. (2.112) we get another formulation of the characterization equations,

$$(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}\mathbf{t}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}=\mathbf{T}^{\sigma}. \tag{3.141}$$

As well, multiplying Eq. (3.124) from the left and from the right by, respectively, $(\mathbf{r}_{\pm}^{-\sigma})^{\dagger}$ and $\mathbf{r}_{\pm}^{\sigma}$ and inserting Eq. (2.113) we get

$$\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}(\mathbf{T}^{\sigma})^{-1}(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}=(\mathbf{t}^{\sigma})^{-1}, \tag{3.142}$$

and, analogously, from Eq. (3.125)

$$(\boldsymbol{\mathcal{R}}_{+}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{+}^{-\sigma}=(\boldsymbol{\mathcal{R}}_{-}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{-}^{-\sigma}. \tag{3.143}$$

Characterization equations (3.141) and (3.142) say simply that the matrix operator $\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}$ has right and left inverse, while Eq. (3.142) is a characterization equation in the strict sense, if the triangular structure of spectral data (3.133)–(3.136) is taken into account. The spectral data $\mathcal{R}_{\pm}^{\sigma}(p,k)$ and $\mathcal{R}_{\pm}^{\sigma}(m,k)$ and only these spectral data are discontinuous at $k=\lambda_{n\Re}$ as follows by Eqs. (3.42), (3.44), and (3.28). The latter equalities prove that these discontinuities furnish the additional spectral data $\mathcal{R}_{\pm}^{\sigma}(p,n)$ and $\mathcal{R}_{\pm}^{\sigma}(m,n)$:

$$\vartheta_n^{\sigma}[\mathcal{R}_{\pm}^{\sigma}(p,\lambda_{n\Re}+0)-\mathcal{R}_{\pm}^{\sigma}(p,\lambda_{n\Re}-0)]=t^{\sigma}(\lambda_{n\Re})w_n^{\sigma}\mathcal{R}_{\pm}^{\sigma}(p,n), \tag{3.144}$$

$$\vartheta_n^{\sigma}[\mathcal{R}_{\pm}^{\sigma}(m,\lambda_{n\Re}+0)-\mathcal{R}_{\pm}^{\sigma}(m,\lambda_{n\Re}-0)]=t^{\sigma}(\lambda_{n\Re})w_n^{\sigma}\mathcal{R}_{\pm}^{\sigma}(m,n). \tag{3.145}$$

Correspondingly, there is only one independent characterization equation in Eq. (3.143) that involves only the spectral data $\mathcal{R}_{\pm}^{\sigma}(p,k)$ and $\mathcal{R}_{\pm}^{\sigma}(m,k)$. Precisely, we get

$$\int dk'\overline{\mathcal{R}_{+}^{\sigma}(k',p)}\mathcal{R}_{+}^{\sigma}(k',k)+\sum_{m,n=1}^{N}\overline{\mathcal{R}_{+}^{\sigma}(m,p)}\mathcal{D}_{mn}^{\sigma}\mathcal{R}_{+}^{\sigma}(n,k)=(+\ \rightarrow -). \tag{3.146}$$

where

$$\mathcal{D}_{mn}^{\sigma}=\vartheta(\sigma)\vartheta_m^{-}C_{mn}\vartheta_n^{+}+\vartheta(-\sigma)C_{mn}^{-1}. \tag{3.147}$$

From Eqs. (3.126) and (3.131) recalling Eq. (2.118) we have

$$\mathbf{F}^{\sigma}=(\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma})^{\dagger}\mathbf{f}^{\sigma}\boldsymbol{\mathcal{R}}_{\pm}^{-\sigma}, \tag{3.148}$$

showing that the spectral data $\mathbf{F}^{\sigma}$ are given by dressing the spectral data $\mathbf{f}^{\sigma}$ by means of $\boldsymbol{\mathcal{R}}_{\pm}^{\sigma}$, which for a perturbation $u'(x)\equiv 0$ reduces to the identity operator.

We shall see that relation (3.127) together with Eq. (3.42) enables us to formulate the inverse problem for the Jost solution. Say, for the sign "+" the "continuous" part of the equality (3.127) reads as

$$t^+(p)\Phi^+(p) - \Phi^-(p) = \int dp' \Phi^-(x,p') f^-(p',p) + \sum_{n=1}^{N} \Phi_n^-(x) F^-(n,p), \tag{3.149}$$

where we denoted

$$f^-(p,p') = F^-(p,p') - \delta(p-p'). \tag{3.150}$$

IV. INVERSE PROBLEM AND TIME EVOLUTION

A. Formulation of the inverse problem

Let us consider function $X(x,\mathbf{k})$ as defined in Eq. (3.13). Taking into account analyticity properties of the Jost solution $\Phi(x,\mathbf{k})$ derived above and asymptotics (3.17) we get

$$\begin{aligned}[t(\mathbf{k})]^{\theta(\mathbf{k}_\mathfrak{I})} X(\mathbf{k}) = 1 &+ \frac{1}{2\pi i} \int \frac{dp}{p-\mathbf{k}} [t^+(p)X^+(p) - X^-(p)] \\ &- \frac{1}{2\pi i} \sum_{n=1}^{N} \int_{-\lambda_{n\mathfrak{I}}}^{\lambda_{n\mathfrak{I}}} \frac{ds[t(s)]^{\theta(s)}}{s - i\lambda_{n\mathfrak{R}} + i\mathbf{k}} [X(\lambda_{n\mathfrak{R}} + 0 + is) - X(\lambda_{n\mathfrak{R}} - 0 + is)].\end{aligned} \tag{4.1}$$

In terms of the Jost solutions themselves this reads by Eq. (3.13) as

$$\begin{aligned}[t(\mathbf{k})]^{\theta(\mathbf{k}_\mathfrak{I})} \Phi(x,\mathbf{k}) = \mathrm{e}^{-i\ell(\mathbf{k})x} &+ \frac{1}{2\pi i} \int \frac{dp \mathrm{e}^{i(\ell(p)-\ell(\mathbf{k}))x}}{p-\mathbf{k}} \\ &\times \left[\int dp' \Phi^-(x,p') f^-(p,p') + \sum_{n=1}^{N} \Phi_n^-(x) F^-(n,p) \right] \\ &- \frac{1}{2\pi i} \sum_{n=1}^{N} \int_{-\lambda_{n\mathfrak{I}}}^{\lambda_{n\mathfrak{I}}} \frac{ds[t(\lambda_{n\mathfrak{R}} + is)]^{\theta(s)}}{s - i\lambda_{n\mathfrak{R}} + i\mathbf{k}} \mathrm{e}^{i(\ell(\lambda_{n\mathfrak{R}}+is)-\ell(\mathbf{k}))x} w_n(s) \Phi_n(x,s),\end{aligned} \tag{4.2}$$

where Eqs. (3.149) and (3.42) were used and where functions $\Phi_n^-(x)$ are defined in Eq. (3.80). Inserting into (4.2) relation (3.70), expressing the auxiliary Jost in terms of the Jost solutions we obtain

$$\begin{aligned}[t(\mathbf{k})]^{\theta(\mathbf{k}_\mathfrak{I})} \Phi(x,\mathbf{k}) = \mathrm{e}^{-i\ell(\mathbf{k})x} &+ \frac{1}{2\pi i} \int dp\, \Phi^-(x,p) \int \frac{dp' f^-(p',p)}{p'-\mathbf{k}} \mathrm{e}^{i(\ell(p')-\ell(\mathbf{k}))x} \\ &- \sum_{n=1}^{N} \frac{1}{2\pi \vartheta_n^+} \int_0^{\lambda_{n\mathfrak{I}}} ds\, A_n(s) t(\lambda_{n\mathfrak{R}} + is) \overline{w_n(-s)} \Phi(x, \lambda_{n\mathfrak{R}} + 0 + is) \\ &\times \int_0^s \frac{ds' t(\lambda_{n\mathfrak{R}} + is') w_n(s')}{s' - i\lambda_{n\mathfrak{R}} + i\mathbf{k}} \mathrm{e}^{i(\ell(\lambda_{n\mathfrak{R}}+is')-\ell(\mathbf{k}))x} \\ &- \sum_{n=1}^{N} \frac{1}{2\pi \vartheta_n^-} \int_{-\lambda_{n\mathfrak{I}}}^{0} ds\, A_n(s) t(\lambda_{n\mathfrak{R}} + is) \overline{w_n(-s)} \Phi(x, \lambda_{n\mathfrak{R}} + 0 + is) \\ &\times \left[\int_s^0 \frac{ds' w_n(s')}{s' - i\lambda_{n\mathfrak{R}} + i\mathbf{k}} \mathrm{e}^{i(\ell(\lambda_{n\mathfrak{R}}+is')-\ell(\mathbf{k}))x} - \int \frac{dp\, F^-(n,p)}{p-\mathbf{k}} \mathrm{e}^{i(\ell(p)-\ell(\mathbf{k}))x} \right].\end{aligned} \tag{4.3}$$

Now we can project this equality on the upper side of the real axis and on the segments $\mathbf{k}_{\mathfrak{R}} = \lambda_{n\mathfrak{R}} + 0$, $|\mathbf{k}_{\mathfrak{I}}| < \lambda_{n\mathfrak{I}}$. This supplies us with a closed system of equations on $\Phi^{-}(x,p)$ and $\Phi(x, \lambda_{n\mathfrak{R}} + 0 + i\mathbf{k}_{\mathfrak{I}})$.

B. Evolution of spectral data

The Jost, advanced/retarded $(\Phi(\mathbf{k}), \Phi_{\pm}(k))$ and auxiliary Jost, advanced/retarded $(\Phi_n(\mathbf{k}_{\mathfrak{I}}), \Phi_{\pm,n})$ solutions in the perturbed case are uniquely defined, respectively, by the integral equations (3.9), (3.93) and (3.35), (3.94). In the considered integral equations, thanks to the fast decay of the perturbation $u'(x)$ at large x, we can exchange the limit $x_2 \to \infty$ with the integral and deduce that $\Phi(\mathbf{k})$ and $\Phi_n(\mathbf{k}_{\mathfrak{I}})$ have at large x_2 the same asymptotic behavior as the inhomogeneous terms $\varphi(\mathbf{k})$ and $\varphi_n(\mathbf{k}_{\mathfrak{I}})$. Therefore, since also $u(x)$ is going to zero at large x_2, the operators $\mathcal{T}_N$ and $\mathcal{T}$ have at large x_2 the same asymptotic limit $\partial_t + 4i\partial_{x_1}^3$ and we obtain by using Eqs. (2.102) and (2.107),

$$\mathcal{T}(\mathbf{k}^3)\Phi(\mathbf{k}) = 0, \tag{4.4}$$

$$\mathcal{T}((\lambda_n^{\sigma})^3)\Phi_n(\mathbf{k}_{\mathfrak{I}}) = 0 \quad \text{where } \sigma = \operatorname{sgn} \mathbf{k}_{\mathfrak{I}}. \tag{4.5}$$

Green's function $\mathcal{G}_{N,\pm}(x,x')$ appearing in the integral equations (3.93) and (3.94) goes to zero for $x_2 \to \mp\infty$ due to the presence of a factor $\theta(\pm(x_2 - x_2'))$ in Eq. (2.56). Therefore, in the same way as for the Jost solutions we obtain using Eqs. (2.106) and (2.108):

$$\mathcal{T}(k^3)\Phi_{\pm}(k) = 0, \tag{4.6}$$

$$\mathcal{T}\left(\frac{1}{2}(\overline{\lambda_m^3} + \lambda_m^3)\right)\Phi_{\pm,m} = 0. \tag{4.7}$$

Considering the limit of Eq. (3.99) for $x_2 \to \mp\infty$ we have

$$t^{\sigma}(k)\Phi^{\sigma}(k) \simeq \int dp\, \varphi_{\pm}(p) R_{\pm}^{\sigma}(p,k) + \sum_{m=1}^{N} \varphi_{\pm,m}(k) R_{\pm}^{\sigma}(m,k). \tag{4.8}$$

Due to the triangular property of $R_{\pm}^{\sigma}(p,k)$ and the asymptotics of the Jost and advanced/retarded solutions that one can derive from Eqs. (2.15) and (2.83), respectively, the first term in the rhs is not going to zero as fast as an exponential and therefore dominates over the second term that is going to zero exponentially. We have

$$t^{\sigma}(k)\Phi^{\sigma}(x,k) \simeq \int dp\, \chi_{\pm,\mathrm{as}}(p) \mathrm{e}^{-i\ell(p)x} R_{\pm}^{\sigma}(p,k) \quad \text{for } x_2 \to \mp\infty. \tag{4.9}$$

Inserting this expansion into Eq. (4.4) we get the time evolution for the spectral data $R_{\pm}^{\sigma}(p,k)$,

$$[\partial_t + 4i(k^3 - p^3)] R_{\pm}^{\sigma}(k,p) = 0. \tag{4.10}$$

Applying $\mathcal{T}(k^3)$ to Eq. (3.99) and using Eq. (4.4) for $\mathbf{k} = k$, Eq. (4.6) for $k = p$ and Eq. (2.108) and the linear independence of the $\Phi_{\pm,m}$ we derive the time evolution for the spectral data $R_{\pm}^{\sigma}(m,k)$,

$$[\partial_t + 2i(\overline{\lambda_m^3} + \lambda_m^3) - 4ik^3] R_{\pm}^{\sigma}(m,k) = 0. \tag{4.11}$$

Applying $\mathcal{T}(k^3)$ to Eq. (3.109) and using, Eqs. (4.6) and (4.4) for $\mathbf{k} = p$, Eqs. (4.10) and (4.5) for $\mathbf{k}_{\mathfrak{I}} = \sigma 0$ and the independence of the Φ_n^{σ} we get the time evolution of the spectral data $R_{\pm}^{\sigma}(k,n)$,

$$[\partial_t + 4i(k^3 - (\lambda_n^\sigma)^3)]R_\pm^\sigma(k,n) = 0. \tag{4.12}$$

Analogously applying $\mathcal{T}\left(\frac{1}{2}(\overline{\lambda_n^3}+\lambda_n^3)\right)$ to Eq. (3.110) and using Eqs. (2.108), (4.4), and (4.10), and (4.6) we have

$$[\partial_t + 2i(\overline{\lambda_m^3} + \lambda_m^3) - 4i(\lambda_n^\sigma)^3]R_\pm^\sigma(m,n) = 0. \tag{4.13}$$

Applying $\mathcal{T}((\lambda_{n\Re}+i\mathbf{k}_\Im)^3)$ to Eq. (3.42) and using Eq. (4.4) for $\mathbf{k}=\lambda_{n\Re}+i\mathbf{k}_\Im$ and Eq. (4.5) we get the time evolution for the spectral data $w_n(\mathbf{k}_\Im)$,

$$[\partial_t + 4i(\lambda_n^\sigma)^3 - 4i(\lambda_{n\Re} + i\mathbf{k}_\Im)^3]w_n(\mathbf{k}_\Im) = 0, \quad \sigma = \operatorname{sgn}\mathbf{k}_\Im. \tag{4.14}$$

Finally, from Eq, (3.72), due to the time evolution of $w_n(\mathbf{k}_\Im)$, we have

$$\partial_t A_n(\mathbf{k}_\Im) = 0. \tag{4.15}$$

From the evolution equations of the spectral data $\mathbf{R}_\pm^\sigma$ given above one can easily derive the evolution equation for the spectral data $\boldsymbol{\mathcal{R}}_\pm^\sigma$, taking into account that they are related by Eq. (3.131) and recalling the evolution equations for $r_\pm^\sigma(m,n)$ in Eq. (2.101). We get

$$[\partial_t + 4i(k^3 - p^3)]\mathcal{R}_\pm^\sigma(k,p) = 0, \tag{4.16}$$

$$[\partial_t + 4i((\lambda_m^\sigma)^3 - p^3)]\mathcal{R}_\pm^\sigma(m,p) = 0, \tag{4.17}$$

$$[\partial_t + 4i(k^3 - (\lambda_n^\sigma)^3)]\mathcal{R}_\pm^\sigma(k,n) = 0, \tag{4.18}$$

$$[\partial_t + 4i((\lambda_m^\sigma)^3 - (\lambda_n^\sigma)^3)]\mathcal{R}_\pm^\sigma(m,n) = 0. \tag{4.19}$$

Taking into account the time evolution of w_n^σ and A_n^σ from Eqs. (4.14) and (4.15) one can check that these evolutions are coherent with Eqs. (3.144) and (3.145)

By Eqs. (4.16)–(4.19) and (2.98) from Eqs. (3.148) and (2.120) we obtain the time evolution of the spectral data $\mathbf{F}^\sigma$

$$[\partial_t + 4i(k^3 - p^3)]\mathcal{F}^\sigma(k,p) = 0, \tag{4.20}$$

$$[\partial_t + 4i((\lambda_m^\sigma)^3 - p^3)]\mathcal{F}^\sigma(m,p) = 0, \tag{4.21}$$

$$[\partial_t + 4i(k^3 - (\lambda_n^{-\sigma})^3)]\mathcal{F}^\sigma(k,n) = 0, \tag{4.22}$$

$$[\partial_t + 4i((\lambda_m^\sigma)^3 - (\lambda_n^{-\sigma})^3)]\mathcal{F}^\sigma(m,n) = 0. \tag{4.23}$$

Finally notice that due to the behavior of $G_N^\sigma(x,x',k)$ at large x_1 and the asymptotics (2.17) and (2.18) we get from the integral equation (3.9) that

$$\lim_{x_1\to+\infty} \Phi^\sigma(k)\mathrm{e}^{il(k)x} = \theta(-\sigma) + \theta(\sigma)\frac{1}{t^\sigma(k)}.$$

Inserting this into Eq. (4.4) we derive that at any time $t>0$ the solution u develops the dynamical constraint,

$$\int_{-\infty}^{\infty} dx_1 u_{x_2}(t,x) = 0, \tag{4.24}$$

generalizing to the case of N perturbed soliton the dynamical constraint found in the case of decaying solutions in Ref. 4.

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Universal $\mathcal{T}$-matrix, representations of $OSp_q(1/2)$ and little Q-Jacobi polynomials

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We obtain a closed form expression of the universal $\mathcal{T}$-matrix encapsulating the duality between the quantum superalgebra $U_q[osp(1/2)]$ and the corresponding supergroup $OSp_q(1/2)$. The classical $q \to 1$ limit of this universal $\mathcal{T}$-matrix yields the group element of the undeformed $OSp_q(1/2)$ supergroup. The finite dimensional representations of the quantum supergroup $OSp_q(1/2)$ are readily constructed employing the above-mentioned universal $\mathcal{T}$-matrix and the known finite dimensional representations of the dually related deformed $U_q[osp(1/2)]$ superalgebra. Proceeding further, we derive the product law, the recurrence relations, and the orthogonality of the representations of the quantum supergroup $OSp_q(1/2)$. It is shown that the entries of these representation matrices are expressed in terms of the *little* Q-Jacobi polynomials with $Q=-q$. Two mutually complementary singular maps of the universal $\mathcal{T}$-matrix on the universal $\mathcal{R}$-matrix are also presented. [DOI: 10.1063/1.2399360]

I. INTRODUCTION

The representation theory of quantum groups and algebras has a richer structure compared to its classical counterparts. Various nonclassical features in the representation theory of the former have been found for specific values of deformation parameters such as roots of unity or crystal base limit. It is known that, for generic values of deformation parameters, each irreducible representation of the classical Lie groups and algebras has its quantum analog (see, for example, Ref. 1). Even for such a generic case, however, there exist representations of the quantum algebra that do not have classical partners.[2–4] Extending our studies to the quantum supergroups, we expect further richness of the representations as the nilpotency of Grassmann variables in classical supergroups are, in many cases, lost at the quantum level. Grassmann coordinates of quantum superspaces[5] and quantum superspheres,[6] as well as the Grassmann elements of quantum supermatrices,[5,6] are instances of lost nilpotency. When representations of such algebraic objects are considered, nonvanishing squares of Grassmann variables cause a drastic shift from the classical cases even for generic values of deformation parameters.

Influenced by this observation, here we study the representations of the simplest quantum supergroup $OSp_q(1/2)$. A precise theory of matrix representations of quantum groups has been developed in Ref. 7. The physical motivations of the present work are provided by the investigations on solvable models having a quantized $osp(1/2)$ symmetry. For instance, vertex models,[8] the Gaudin model,[9] and two-dimensional (2D) field theories[10] based on $U_q[osp(1/2)]$ symmetry have been proposed and investigated. A fully developed representation theory of $OSp_q(1/2)$ will provide useful tools for analyzing these models and building new ones.

It is known that the representation theories of two quantum algebras $U_q[sl(2)]$ and $U_q[osp(1/2)]$ are quite parallel for a generic q. We naturally anticipate that the known results on the quantum group $SL_q(2)$ may be extended to the quantum supergroup $OSp_q(1/2)$. To accomplish the extension, we employ the universal $\mathcal{T}$-matrix, which is a generalization of the exponential mapping relating a Lie algebra with its corresponding group. The underlying reasons for this are as follows: (i) The universal $\mathcal{T}$-matrix succinctly embodies the representations of the dually related conjugate Hopf structures, $U_q[osp(1/2)]$ and $OSp_q(1/2)$. In particular, contributions of the nonvanishing square of the odd elements of $OSp_q(1/2)$ may be directly read from the expression of the universal $\mathcal{T}$-matrix. (ii) Moreover, the universal $\mathcal{T}$-matrix allows us to map each irreducible representation of $U_q[osp(1/2)]$ on the corresponding one of $OSp_q(1/2)$. Therefore, various properties of representations follow from the corresponding ones of the universal $\mathcal{T}$-matrix, and the role of the lost nilpotency becomes explicit. Specifically, we demonstrate that the nonvanishing contributions of odd elements *assume polynomial structures* in the representation matrices.

The plan of this article is as follows. After fixing notations and conventions in the next section, the basis set of the Hopf dual to the $U_q[osp(1/2)]$ algebra is explicitly obtained. The finitely generated basis sets of the dually related Hopf algebras are now used to derive a closed form expression of the universal $\mathcal{T}$-matrix via the method of Frønsdal and Galindo.[11] Singular and therefore noninvertible maps of the universal $\mathcal{T}$-matrix on the universal $\mathcal{R}$-matrix exist.[11] Two such mutually complementary maps are studied in Sec. IV. General properties of the finite dimensional representations of the quantum supergroup $OSp_q(1/2)$, such as the product law, the recurrence relations, and the orthogonality of representations, follow, as observed in Sec. V, from the duality encompassed in the universal $\mathcal{T}$-matrix. Explicit form of the representation matrices are derived in Sec. VI and its relation to the little Q-Jacobi polynomials are discussed. It is shown that the entries of the representation matrix are expressed in terms of the little Q-Jacobi polynomials with $Q=-q$. This provides a new link of the representation theory of quantum supergroups with the hypergeometric functions. Section VII is devoted to concluding remarks. The corresponding results on $SL_q(2)$ and other quantum groups are mentioned in each section.

II. $U_q[osp(1/2)]$ AND ITS REPRESENTATIONS

The quantum superalgebra $\mathcal{U}=U_q[osp(1/2)]$ and the dually related quantum supergroup $\mathcal{A}=OSp_q(1/2)$, dual to $\mathcal{U}$, have been introduced in Ref. 12. Structures and representations of $\mathcal{U}$ have been investigated in Refs. 8 and 12. For the purpose of fixing our notations and conventions we list the relations that will be used subsequently.

The algebra $\mathcal{U}$ is generated by three elements H (parity even) and $V_\pm$ (parity odd) subject to the relations

$$[H,V_\pm]=\pm\frac{1}{2}V_\pm,\quad \{V_+,V_-\}=-\frac{q^{2H}-q^{-2H}}{q-q^{-1}}\equiv-[2H]_q. \tag{2.1}$$

The deformation parameter q is assumed to be generic throughout this article. The Hopf algebra structures defined via the coproduct (Δ), the counit (ϵ), and the antipode (S) maps read as follows:

$$\Delta(H)=H\otimes 1+1\otimes H,\quad \Delta(V_\pm)=V_\pm\otimes q^{-H}+q^{H}\otimes V_\pm, \tag{2.2}$$

$$\epsilon(H)=\epsilon(V_\pm)=0, \tag{2.3}$$

$$S(H)=-H,\quad S(V_\pm)=-q^{\mp 1/2}V_\pm. \tag{2.4}$$

Using the flip operator σ: $\sigma(a\otimes b)=(-1)^{p(a)p(b)}b\otimes a$, where $p(a)$ denotes the parity of a, we define the transposed coproduct: $\Delta'=\sigma\circ\Delta$. The universal $\mathcal{R}$-matrix intertwining Δ and Δ' is given by[12]

$$\mathcal{R}_q = q^{4H\otimes H}\sum_{k\geq 0}\frac{(q-q^{-1})^k q^{-k/2}}{(k)_{q^{-1}}!}(q^H V_+ \otimes q^{-H}V_-)^k, \tag{2.5}$$

where

$$(k)_q = \frac{1-(-1)^k q^k}{1+q},\quad (k)_q\,! = (k)_q(k-1)_q\cdots(1)_q,\quad (0)_q\,! = 1. \tag{2.6}$$

Two properties of $\mathcal{R}_q$ that will be used later are listed below: (i) It satisfies the Yang-Baxter equation

$$\mathcal{R}_{q12}\mathcal{R}_{q13}\mathcal{R}_{q23} = \mathcal{R}_{q23}\mathcal{R}_{q13}\mathcal{R}_{q12}, \tag{2.7}$$

and (ii) its antipode map reads as $(S\otimes id)\mathcal{R}_q = \mathcal{R}_{q^{-1}} = \mathcal{R}_q^{-1}$.

The finite dimensional irreducible representations of $\mathcal{U}$ is specified by the highest weight ℓ, which takes any non-negative integral value. The irreducible representation space $V^{(\ell)}$ of highest weight ℓ is $2\ell+1$ dimensional. We denote its basis as $\{e_m^\ell(\lambda)\,|\,m=\ell,\ell-1,\cdots,-\ell\}$, where the index $\lambda=0,1$ specifies the parity of the highest weight vector $e_\ell^\ell(\lambda)$. The parity of the vector $e_m^\ell(\lambda)$ equals $\ell-m+\lambda$, as it is obtained by the action of $V_-^{\ell-m}$ on $e_\ell^\ell(\lambda)$. For the superalgebras the norm of the representation basis need not be chosen positive definite. In this work, however, we assume the positive definiteness of the basis elements:

$$(e_m^\ell(\lambda),\, e_{m'}^{\ell'}(\lambda)) = \delta_{\ell\ell'}\delta_{mm'}. \tag{2.8}$$

With these settings, the irreducible representation of $\mathcal{U}$ on $V^{(\ell)}$ is given by

$$He_m^\ell(\lambda) = \frac{m}{2}e_m^\ell(\lambda),$$

$$V_+e_m^\ell(\lambda) = \left(\frac{1}{\{2\}_q}\{\ell-m\}_q\{\ell+m+1\}_q\right)^{1/2}e_{m+1}^\ell(\lambda),$$

$$V_-e_m^\ell(\lambda) = (-1)^{\ell-m-1}\left(\frac{1}{\{2\}_q}\{\ell+m\}_q\{\ell-m+1\}_q\right)^{1/2}e_{m-1}^\ell(\lambda), \tag{2.9}$$

where

$$\{m\}_q = \frac{q^{-m/2}-(-1)^m q^{m/2}}{q^{-1/2}+q^{1/2}}. \tag{2.10}$$

The tensor product of two irreducible representations is, in general, reducible and may be decomposed into irreducible ones without multiplicity:

$$V^{(\ell_1)}\otimes V^{(\ell_2)} = V^{(\ell_1+\ell_2)}\otimes V^{(\ell_1+\ell_2-1)}\otimes\cdots\otimes V^{(|\ell_1-\ell_2|)}.$$

The decomposition of the tensored vector space in the irreducible basis is provided by the Clebsch-Gordan coefficients (CGC):

$$e_m^\ell(\ell_1,\ell_2,\Lambda) = \sum_{m_1,m_2} C_{m_1\,m_2\,m}^{\ell_1\,\ell_2\,\ell}e_{m_1}^{\ell_1}(\lambda)\otimes e_{m_2}^{\ell_2}(\lambda), \tag{2.11}$$

where $m=m_1+m_2$, and $\Lambda=\ell_1+\ell_2+\ell(\mathrm{mod}\,2)$ signifies the parity of the highest weight vector $e_\ell^\ell(\ell_1,\ell_2,\Lambda)$. The CGC for $\mathcal{U}$ is extensively studied in Ref. 13. In spite of our assumption (2.8) regarding the positivity of the basis vectors, the norm of tensored vector space is not always positive definite. Indeed, the basis (2.11) is pseudo-orthogonal:

$$(e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda), e^{\ell}_{m}(\ell_1,\ell_2,\Lambda)) = (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)}\delta_{\ell'\ell}\delta_{m'm}. \tag{2.12}$$

The CGC satisfies two pseudo-orthogonality relations:

$$\sum_{m_1,m_2} (-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)} C^{\ell_1\ell_2\ell}_{m_1m_2m} C^{\ell_1\ell_2\ell'}_{m_1m_2m'} = (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)}\delta_{\ell\ell'}\delta_{mm'}, \tag{2.13}$$

$$\sum_{\ell,m} (-1)^{(\ell-m+\lambda)(\ell_1+\ell_2+\ell+\lambda)} C^{\ell_1\ell_2\ell}_{m_1m_2m} C^{\ell_1\ell_2\ell}_{m'_1m'_2m} = (-1)^{(\ell_1-m_1+\lambda)(\ell_2-m_2+\lambda)}\delta_{m_1m'_1}\delta_{m_2m'_2}. \tag{2.14}$$

Equation (2.14) immediately provides the inversion of the construction (2.11):

$$e^{\ell_1}_{m_1}(\lambda)\otimes e^{\ell_2}_{m_2}(\lambda) = (-1)^{(\ell_1-m_1)(\ell_2-m_2)}\sum_{\ell,m}(-1)^{(\ell-m)(\ell_1+\ell_2+\ell)} C^{\ell_1\ell_2\ell}_{m_1m_2m} e^{\ell}_{m}(\ell_1,\ell_2,\Lambda). \tag{2.15}$$

Before closing this section, we make two remarks: (i) All the CGC are of parity even state. (ii) The explicit realization of CGC for $\mathcal{U}$ is found in Ref. 6, and also in Ref. 13. As we maintain the phase convention for the representation of $\mathcal{U}$ given in Ref. 13, we use the results obtained therein.

III. UNIVERSAL $\mathcal{T}$-MATRIX VIA DUALITY

Two Hopf algebras $\mathcal{U}$ and $\mathcal{A}$ are in duality[11] if there exists a doubly nondegenerate bilinear form $\langle , \rangle$: $\mathcal{A}\otimes\mathcal{U}\to\mathbb{C}$ such that, for $(\mathbf{a},\mathbf{b})\in\mathcal{A}$, $(\mathbf{u},\mathbf{v})\in\mathcal{U}$,

$$\langle \mathbf{a},\mathbf{uv}\rangle = \langle \Delta_{\mathcal{A}}(\mathbf{a}),\mathbf{u}\otimes\mathbf{v}\rangle,\ \ \langle \mathbf{ab},\mathbf{u}\rangle = \langle \mathbf{a}\otimes\mathbf{b},\Delta_{\mathcal{U}}(\mathbf{u})\rangle,$$

$$\langle \mathbf{a},1_{\mathcal{U}}\rangle = \epsilon_{\mathcal{A}}(\mathbf{a}),\ \ \langle 1_{\mathcal{A}},\mathbf{u}\rangle = \epsilon_{\mathcal{U}}(\mathbf{u}),\ \ \langle \mathbf{a},S_{\mathcal{U}}(\mathbf{u})\rangle = \langle S_{\mathcal{A}}(\mathbf{a}),\mathbf{u}\rangle. \tag{3.1}$$

Let the ordered monomials $E_{k\ell m}=V_+^k H^\ell V_-^m$, $(k,\ell,m)\in(0,1,2,\ldots)$ be the basis elements of the algebra $\mathcal{U}$ obeying the multiplication and the induced coproduct rules given by

$$E_{k\ell m}E_{k'\ell'm'} = \sum_{pqr} f^{\ pqr}_{k\ell m\ k'\ell'm'} E_{pqr},\ \ \Delta(E_{k\ell m}) = \sum_{\substack{pqr\\ p'q'r'}} g^{pqr\ p'q'r'}_{k\ell m} E_{pqr}\otimes E_{p'q'r'}. \tag{3.2}$$

The basis elements $e^{k\ell m}$ of the dual Hopf algebra $\mathcal{A}$ follow the relation

$$\langle e^{k\ell m}, E_{k'\ell'm'}\rangle = \delta^k_{k'}\delta^\ell_{\ell'}\delta^m_{m'}. \tag{3.3}$$

In particular, the generating elements of the algebra $\mathcal{A}$, defined as $x=e^{100}$, $y=e^{001}$, and $z=e^{010}$, satisfy the following duality structure:

$$\langle x,V_+\rangle = 1,\ \ \langle z,H\rangle = 1,\ \ \langle y,V_-\rangle = 1. \tag{3.4}$$

Thus, x and y are of odd parity, while z is even. The duality condition (3.1) requires the basis set $e^{k\ell m}$ to obey the multiplication and coproduct rules given below:

$$e^{pqr}e^{p'q'r'} = \sum_{k\ell m} g^{pqr\ p'q'r'}_{k\ell m} e^{k\ell m},\ \ \Delta(e^{pqr}) = \sum_{\substack{k\ell m\\ k'\ell'm'}} f^{\ pqr}_{k\ell m\ k'\ell'm'} e^{k\ell m}\otimes e^{k'\ell'm'}. \tag{3.5}$$

To derive the Hopf properties of the dual algebra $\mathcal{A}$, we therefore need to extract the structure constants defined in (3.2). Toward this end we note that the induced coproduct map of the elements $E_{k\ell m}$ may be obtained via (2.2):

$$\Delta(E_{k\ell m}) = \Delta(V_+)^k \Delta(H)^\ell \Delta(V_-)^m = \sum_{a=0}^{k} \sum_{b=0}^{\ell} \sum_{c=0}^{m} \binom{k}{a}_q \binom{\ell}{b} \binom{m}{c}_q (-1)^{(m-c)(a+c)} q^{-a(k-a)/2-c(m-c)/2} \times V_+^{k-a} q^{(a+c)H} H^{\ell-b} V_-^{m-c} \otimes V_+^a q^{-(k+m-a-c)H} H^b V_-^c, \tag{3.6}$$

where

$$\binom{k}{a}_q = \frac{(k)_q!}{(a)_q!\,(k-a)_q!}.$$

The second equality in (3.6) can be verified by using the commutation relations

$$q(V_+ \otimes q^{-H})(q^H \otimes V_+) + (q^H \otimes V_+)(V_+ \otimes q^{-H}) = 0,$$

$$q(q^H \otimes V_-)(V_- \otimes q^{-H}) + (V_- \otimes q^{-H})(q^H \otimes V_-) = 0,$$

and an extension of binomial theorem that is easily proved by induction: Arbitrary operators A, B subject to the commutation properties $qAB+BA=0$ satisfy the following expansion:

$$(A+B)^n = \sum_{k=0}^{n} \binom{n}{k}_q A^{n-k} B^k. \tag{3.7}$$

Employing (3.6) we now obtain a set of structure constants:

$$g_{k\ell m}^{100\,001} = \delta_{k1}\delta_{\ell 0}\delta_{m1}, \quad g_{k\ell m}^{001\,100} = -\delta_{k1}\delta_{\ell 0}\delta_{m1},$$

$$g_{k\ell m}^{100\,010} = -\ln q\,\delta_{k1}\delta_{\ell 0}\delta_{m0} + \delta_{k1}\delta_{\ell 1}\delta_{m0},$$

$$g_{k\ell m}^{010\,100} = \ln q\,\delta_{k1}\delta_{\ell 0}\delta_{m0} + \delta_{k1}\delta_{\ell 1}\delta_{m0},$$

$$g_{k\ell m}^{010\,001} = \ln q\,\delta_{k0}\delta_{\ell 0}\delta_{m1} + \delta_{k0}\delta_{\ell 1}\delta_{m1},$$

$$g_{k\ell m}^{001\,010} = -\ln q\,\delta_{k0}\delta_{\ell 0}\delta_{m1} + \delta_{k0}\delta_{\ell 1}\delta_{m1}.$$

The above structure constants immediately yield the algebraic relations obeyed by the generators of the algebra $\mathcal{A}$:

$$\{x,y\} = 0, \quad [z,x] = 2\ln q x, \quad [z,y] = 2\ln q y. \tag{3.8}$$

Proceeding toward constructing the coproduct maps of the generating elements of the dual algebra $\mathcal{A}$, we notice that the defining properties (3.5) provide the necessary recipe:

$$\Delta(x) = \sum_{\substack{k\ell m \\ k'\ell'm'}} f_{k\ell m\,k'\ell'm'}^{100} e^{k\ell m} \otimes e^{k'\ell'm'},$$

$$\Delta(z) = \sum_{\substack{k\ell m \\ k\ell'm'}} f_{k\ell m\,k'\ell'm'}^{010} e^{k\ell m} \otimes e^{k'\ell'm'},$$

$$\Delta(y) = \sum_{\substack{k\ell m \\ k'\ell'm}} f^{001}_{k\ell m\, k'\ell'm'} e^{k\ell m} \otimes e^{k'\ell'm'}. \tag{3.9}$$

The relevant structure constants obtained via (3.2) are listed below:

$$f^{100}_{k\ell m\, k'\ell'm'} = \delta_{k1}\delta_{\ell 0}\delta_{m0}\delta_{k'0}\delta_{\ell'0}\delta_{m'0} + (-1)^m \frac{1}{2^\ell}\sigma_{m+1}\delta_{k0}\delta_{k'\, m+1}\delta_{\ell'0}\delta_{m'0},$$

$$f^{010}_{k\ell m\, k'\ell'm'} = \delta_{k0}\delta_{m0}\delta_{k'0}\delta_{m'0}(\delta_{\ell 1}\delta_{\ell'0} + \delta_{\ell 0}\delta_{\ell' 1}) + (-1)^m \frac{4\ln q}{q-q^{-1}}\sigma_m\delta_{k0}\delta_{\ell 0}\delta_{k'm}\delta_{\ell'0}\delta_{m'0},$$

$$f^{001}_{k\ell m\, k'\ell'm'} = \delta_{k0}\delta_{\ell 0}\delta_{m0}\delta_{k'0}\delta_{\ell'0}\delta_{m'1} + (-1)^{k'} \frac{1}{2^{\ell'}}\sigma_{k'+1}\delta_{k0}\delta_{\ell 0}\delta_{m\, k'+1}\delta_{m'0},$$

$$\sigma_1 = 1, \quad \sigma_m = \prod_{k=1}^{m-1}\sum_{\ell=0}^{k-1}(-1)^\ell [k-\ell]_q \quad (m>1). \tag{3.10}$$

The coproduct maps of the generators of $\mathcal{A}$ may now be explicitly obtained in the manner of (3.9) provided the basis elements $e^{k\ell m}$ of the algebra $\mathcal{A}$ are known. We complete this task subsequently.

As the algebra $\mathcal{A}$ is finitely generated, we may start with the generators (x,y,z) and obtain all dual basis elements $e^{k\ell m}$, $(k,\ell,m)\in(0,1,2,\ldots)$ by successively applying the multiplication rule given in the first equation in (3.5). The necessary structure constants may be read from the relation (3.2) of the algebra $\mathcal{U}$. In the procedure described below we maintain the operator ordering of the monomials as $x^k z^\ell y^m$, $(k,\ell,m)\in(0,1,2,\ldots)$. The product rule

$$e^{100}e^{n00} = \sum_{k\ell m} g^{100\, n00}_{k\ell m} e^{k\ell m} \tag{3.11}$$

and the explicit evaluation of the structure constant

$$g^{100\, n00}_{k\ell m} = \{n+1\}_q \delta_{k\, n+1}\delta_{\ell 0}\delta_{m0} \tag{3.12}$$

obtained from (3.6) immediately provide

$$e^{n00} = \frac{x^n}{\{n\}_q!}, \quad \{n\}_q! = \prod_{\ell=1}^{n}\{\ell\}_q, \quad \{0\}_q! = 1. \tag{3.13}$$

Employing another product rule

$$e^{nr0}e^{010} = \sum_{k\ell m} g^{nr0\, 010}_{k\ell m} e^{k\ell m} \tag{3.14}$$

and the value of the relevant structure constant

$$g^{nr\, 0010}_{k\ell m} = -n\ln q\,\delta_{kn}\delta_{\ell r}\delta_{m0} + (r+1)\delta_{kn}\delta_{\ell\, r+1}\delta_{m0},$$

obtained in the aforesaid way, we produce the following result:

$$e^{nr0} = \frac{x^n}{\{n\}_q!}\frac{1}{r!}(z + n\ln q)^r. \tag{3.15}$$

Continuing the above process of building of the dual basis set, we use the product rule

$$e^{nrs}e^{001} = \sum_{k\ell m} g^{nrs\,001}_{k\ell m} e^{k\ell m} \tag{3.16}$$

and the value of the corresponding structure constant

$$g^{nrs\,001}_{k\ell m} = \{s+1\}_{q^{-1}} \sum_{j=0}^{r} \frac{1}{j!} (\ln q)^j \delta_{kn} \delta_{\ell\, r-j} \delta_{m\, s+1},$$

obtained via (3.6). This finally leads us to the complete construction of the basis element of the algebra $\mathcal{A}$:

$$e^{nrs} = \frac{x^n}{\{n\}_q!} \frac{(z+(n-s)\ln q)^r}{r!} \frac{y^s}{\{s\}_{q^{-1}}!}. \tag{3.17}$$

Combining our results in (3.9), (3.10), and (3.17), we now provide the promised coproduct structure of the generators of the algebra $\mathcal{A}$:

$$\Delta(x) = x \otimes 1 + \sum_{m=0}^{\infty} (-1)^m \sigma_{m+1} q^{-m/2} e^{z/2} \frac{y^m}{\{m\}_{q^{-1}}!} \otimes \frac{x^{m+1}}{\{m+1\}_q!},$$

$$\Delta(z) = z \otimes 1 + 1 \otimes z + \frac{4\ln q}{q-q^{-1}} \sum_{m=1}^{\infty} (-1)^m \sigma_m \frac{y^m}{\{m\}_{q^{-1}}!} \otimes \frac{x^m}{\{m\}_q!},$$

$$\Delta(y) = 1 \otimes y + \sum_{k=0}^{\infty} (-1)^k \sigma_{k+1} q^{k/2} \frac{y^{k+1}}{\{k+1\}_{q^{-1}}!} \otimes \frac{x^k}{\{k\}_q!} e^{z/2}. \tag{3.18}$$

Algebraic simplifications allow us to express the coproduct maps of the above generators more succinctly:

$$\Delta(x) = x \otimes 1 + \sum_{m=0}^{\infty} (-1)^{m(m-1)/2} \left(\frac{1+q^{-1}}{q-q^{-1}}\right)^m e^{z/2} y^m \otimes x^{m+1},$$

$$\Delta(z) = z \otimes 1 + 1 \otimes z + \frac{4\ln q}{q-q^{-1}} \sum_{m=1}^{\infty} \frac{(-1)^{m(m+1)/2}}{\{m\}_{q^{-1}}} \left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}\right)^{m-1} y^m \otimes x^m,$$

$$\Delta(y) = 1 \otimes y + \sum_{m=0}^{\infty} (-1)^{m(m-1)/2} \left(\frac{q+1}{q-q^{-1}}\right)^m y^{m+1} \otimes x^m e^{z/2}. \tag{3.19}$$

With the aid of the result (3.19) we may explicitly demonstrate that the coproduct map is a homomorphism of the algebra (3.8): namely,

$$\{\Delta(x),\Delta(y)\} = 0, \quad [\Delta(z),\Delta(x)] = 2\ln q \Delta(x), \quad [\Delta(z),\Delta(y)] = 2\ln q \Delta(y).$$

The coassociativity constraint

$$(id \otimes \Delta) \circ \Delta(\mathcal{X}) = (\Delta \otimes id) \circ \Delta(\mathcal{X}) \quad \forall\, \mathcal{X} \in (x,y,z)$$

may also be established by using the following identity:

$$\exp(\Delta(z)) = (\exp(z) \otimes 1) \prod_{m=1}^{\infty} \mathcal{P}_m (1 \otimes \exp(z)),$$

$$\mathcal{P}_m = \exp\left((-1)^{m(m+1)/2} \frac{[2m]_q}{m\{m\}_{q^{-1}}} \left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}} \right)^{m-1} y^m \otimes x^m \right). \tag{3.20}$$

The counit map of the generators of the algebra $\mathcal{A}$ reads as

$$\epsilon(x) = \epsilon(y) = \epsilon(z) = 0. \tag{3.21}$$

The antipode map of the dual generators follows from the last equation in (3.1). We quote the results here:

$$S(x) = -\sum_{m=0}^{\infty} (-1)^{m(m-1)/2} q^{-1} \left(\frac{1+q^{-1}}{q-q^{-1}} \right)^m x^{m+1} \exp\left(-\frac{m+1}{2} z \right) y^m,$$

$$S(z) = -z + \frac{4\ln q}{q-q^{-1}} \sum_{m=1}^{\infty} (-1)^{m(m+1)/2} \frac{1}{\{m\}_{q^{-1}}} \left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}} \right)^{m-1} x^m e^{-mz/2} y^m,$$

$$S(y) = -\sum_{m=0}^{\infty} (-1)^{m(m+1)/2} q \left(\frac{q+1}{q-q^{-1}} \right)^m x^m \exp\left(-\frac{m+1}{2} z \right) y^{m+1}. \tag{3.22}$$

This completes our construction of the Hopf algebra $\mathcal{A}$ dually related to the quantum superalgebra $\mathcal{U}$.

Our explicit listing of the complete set of dual basis elements in (3.17) allows us to obtain, in the manner of Frønsdal and Galindo,[11] the universal $\mathcal{T}$-matrix for the supergroup:

$$\mathcal{T}_{e,E} = \sum_{k\ell m} (-1)^{p(e^{k\ell m})(p(e^{k\ell m})-1)/2} e^{k\ell m} \otimes E_{k\ell m}, \tag{3.23}$$

where the parity of basis elements is same for two Hopf algebras $\mathcal{U}$ and $\mathcal{A}$:

$$p(e^{k\ell m}) = p(E_{k\ell m}) = k + m. \tag{3.24}$$

The notion of the universal $\mathcal{T}$-matrix is a key feature capping the Hopf duality structure. Consequently, the duality relations (3.1) may be concisely expressed[11] in terms of the $\mathcal{T}$-matrix as

$$\mathcal{T}_{e,E}\mathcal{T}_{e',E} = \mathcal{T}_{\Delta(e),E}, \quad \mathcal{T}_{e,E}\mathcal{T}_{e,E'} = \mathcal{T}_{e,\Delta(E)},$$

$$\mathcal{T}_{\epsilon(e),E} = \mathcal{T}_{e,\epsilon(E)} = 1, \quad \mathcal{T}_{S(e),E} = \mathcal{T}_{e,S(E)}, \tag{3.25}$$

where e and e' (E and E') refer to the two identical copies of algebra $\mathcal{A}$ ($\mathcal{U}$). A general discussion of the universal $\mathcal{T}$-matrix for supergroups is found in the Appendix.

As both the Hopf algebras in our case are finitely generated, the universal $\mathcal{T}$-matrix may now be obtained as an operator valued function in a closed form:

$$\begin{aligned} \mathcal{T}_{e,E} &= \left(\sum_{k=0}^{\infty} \frac{(x \otimes V_+ q^H)^k}{(k)_q!} \right) \exp(z \otimes H) \left(\sum_{m=0}^{\infty} \frac{(y \otimes q^{-H} V_-)^m}{(m)_{q^{-1}}!} \right) \\ &\equiv {}^{\times}_{\times}\mathcal{E}\mathrm{xp}_q(x \otimes V_+ q^H) \exp(z \otimes H) \mathcal{E}\mathrm{xp}_{q^{-1}}(y \otimes q^{-H} V_-)^{\times}_{\times}, \end{aligned} \tag{3.26}$$

where we have introduced a deformed exponential that is characteristic of the quantum $OSp_q(1/2)$ supergroup:

$$\mathcal{E}\mathrm{xp}_q(x) \equiv \sum_{n=0}^{\infty} \frac{x^n}{(n)_q!}. \tag{3.27}$$

The operator ordering has been explicitly indicated in (3.26). The closed form of the universal $\mathcal{T}$-matrix in (3.26) will be used in the computation of the representation matrices of the quantum supergroup $\mathcal{A}$. In Ref. 14, using the Gauss decomposition of the fundamental representation, a universal $\mathcal{T}$-matrix for $\mathcal{U}$ is given in terms of the standard q-exponential instead of the deformed exponential (3.27) characterizing the quantum supergroups.

In the classical limit of $q \to 1$, it is immediately evident that the structure constant (3.12) is truncated at $n=2$ so that x remains nilpotent. Similarly, $y^2=0$ holds in this limit. It is interesting to observe the $q \to 1$ limit of the universal $\mathcal{T}$-matrix (3.26). For this purpose we note

$$\lim_{q\to 1}(2n)_q \to n(1-q), \quad \lim_{q\to 1}(2n+1)_q \to 1, \quad n=0,1,2,\ldots. \tag{3.28}$$

Assuming the finite limit

$$\lim_{q\to 1}\frac{x^2}{q-1} = \mathfrak{x}, \quad \lim_{q\to 1}\frac{y^2}{q^{-1}-1} = \mathfrak{y}, \tag{3.29}$$

it immediately follows that the universal $\mathcal{T}$-matrix (3.26) reduces to the group element of the undeformed $OSp(1/2)$ and by definition constitutes its universal T-matrix:

$$\mathcal{T}_{e,E}\big|_{q\to 1} = (1\otimes 1 + x\otimes V_+)\exp(\mathfrak{x}\otimes V_+^2)\exp(z\otimes H)\exp(\mathfrak{y}\otimes V_-^2)(1\otimes 1 + y\otimes V_-). \tag{3.30}$$

The finite limiting elements $(\mathfrak{x},\mathfrak{y})$ are bosonic in nature, and in the context of the classical limit of the function algebra $\mathcal{A}$ they are dually related to the squares of the odd generators of the undeformed $osp(1/2)$. The elements $(V_\pm^2, H)$ of the classical $osp(1/2)$ algebra form a $sl(2)$ subalgebra. The corresponding classical $SL(2)$ subgroup structure is evident from (3.30). In fact, the correct limiting structure (3.30) emphasizes the essential validity of the quantum universal $\mathcal{T}$-matrix derived in (3.26). Obviously, there is a striking difference between the quantum and classical universal $\mathcal{T}$-matrices caused by the absence of nilpotency of parity odd elements in the former case. The infinite series of operators summarized in the deformed exponential contribute to new polynomial matrix elements in the representations of quantum supergroup $\mathcal{A}$. This is considered in detail in Sec. V.

The above construction of the universal $\mathcal{T}$-matrix for the algebra $\mathcal{U}$ is parallel to the one for the generalized Heisenberg algebra,[15] which is a bosonization[16] of the superalgebra $\mathcal{U}$. The dual basis to the two-parametric deformation of $GL(2)$ is studied in Ref. 17. The universal $\mathcal{T}$-matrix for the two-parametric quantum $GL(2)$ is given in Refs. 11 and 18. The generalization to the quantum $gl(n)$ is found in Ref. 19, and a supersymmetric extension is initiated in Ref. 20.

IV. MAPPING $\mathcal{T}$ ON $\mathcal{R}$

Two singular and mutually complementary maps connecting the universal $\mathcal{T}$-matrix in (3.26) and the universal $\mathcal{R}$-matrix in (2.5) are discussed in this section. The first map $\Phi: \mathcal{A} \to \mathcal{U}$ reads

$$\Phi(x) = 0, \quad \Phi(z) = (4\ln q)H, \quad \Phi(y) = q^{-1/2}(q-q^{-1})q^H V_+. \tag{4.1}$$

It is easily observed to satisfy the following properties: (i) $(\Phi\otimes \mathrm{id})(\mathcal{T}_{e,E}) = \mathcal{R}_q$, and (ii) Φ is an algebra homomorphism, though not a Hopf algebra homomorphism; that is, Φ respects the commutation relations in (3.8) but does not maintain the Hopf coalgebra maps.

To introduce the second map, we recast the universal $\mathcal{T}$-matrix in the form given below:

$$\mathcal{T}_{E,e} = \sum_{k\ell m} (-1)^{(k+m)(k+m-1)/2} E_{k\ell m} \otimes e^{k\ell m} = \left(\sum_k \frac{1}{(k)_q!} (V_+ q^H \otimes x)^k \right) e^{H\otimes z} \left(\sum_m \frac{1}{(m)_{q^{-1}}!} (q^{-H} V_- \otimes y)^m \right). \tag{4.2}$$

The universal $\mathcal{R}$-matrix is also rewritten as

$$\mathcal{R}_q = \sum_{k\geq 0} \frac{(q-q^{-1})^k}{(k)_{q^{-1}}!} (V_+ q^{-H} \otimes q^H V_-)^k q^{4H\otimes H}. \tag{4.3}$$

A comparison of the above two expressions immediately yields the promised map $\Psi : \mathcal{A} \to \mathcal{U}$ defined as follows:

$$\Psi(x) = (q^{-1} - q) q^{-H} V_-, \quad \Psi(z) = (-4 \ln q) H, \quad \Psi(y) = 0. \tag{4.4}$$

One can immediately verify that $(\mathrm{id} \otimes \Psi)(\mathcal{T}_{E,e}) = \mathcal{R}_q^{-1}$ and that Ψ is an algebraic homomorphism but not a Hopf algebra homomorphism. It is interesting to observe that in both the maps introduced here *one* Borel subalgebra of the function algebra $\mathcal{A}$ is mapped on the corresponding Borel subalgebra of the universal enveloping algebra $\mathcal{U}$. Therefore, the two conjugate Borel subalgebras of the $\mathcal{U}$ algebra are acted upon by two distinct, but complementary maps. Being singular in nature, these maps are, however, not invertible.

The maps Φ and Ψ may be utilized to connect the universal $\mathcal{T}$-matrix and the Yang-Baxter equation. As shown in the Appendix, the universal $\mathcal{T}$-matrix satisfies *RTT*-type relations. Using the tensored operators

$$\mathcal{T}^{(1)}_{e,E} = \sum_k (-1)^{(k+m)(k+m-1)/2} e^{k\ell m} \otimes E_{k\ell m} \otimes 1,$$

$$\mathcal{T}^{(2)}_{e,E} = \sum_k (-1)^{(k+m)(k+m-1)/2} e^{k\ell m} \otimes 1 \otimes E_{k\ell m}, \tag{4.5}$$

the following identity may be established:

$$(1 \otimes \mathcal{R}_q) \mathcal{T}^{(1)}_{e,E} \mathcal{T}^{(2)}_{e,E} = \mathcal{T}^{(2)}_{e,E} \mathcal{T}^{(1)}_{e,E} (1 \otimes \mathcal{R}_q). \tag{4.6}$$

Mirroring the structure in (4.5) we also define the transposed T-matrices in the tensored space as

$$\mathcal{T}^{(1)}_{E,e} = \sum_k (-1)^{(k+m)(k+m-1)/2} E_{k\ell m} \otimes 1 \otimes e^{k\ell m},$$

$$\mathcal{T}^{(2)}_{E,e} = \sum_k (-1)^{(k+m)(k+m-1)/2} 1 \otimes E_{k\ell m} \otimes e^{k\ell m}. \tag{4.7}$$

These matrices also obey another *RTT*-type relation:

$$(\mathcal{R}_q \otimes 1) \mathcal{T}^{(1)}_{E,e} \mathcal{T}^{(2)}_{E,e} = \mathcal{T}^{(2)}_{E,e} \mathcal{T}^{(1)}_{E,e} (\mathcal{R}_q \otimes 1). \tag{4.8}$$

Application of the tensored map $\Phi \otimes \mathrm{id} \otimes \mathrm{id}$ to (4.6) converts the *RTT*-type relation into the Yang-Baxter equation of the form

$$\mathcal{R}_{q\,23} \mathcal{R}_{q\,12} \mathcal{R}_{q\,13} = \mathcal{R}_{q\,13} \mathcal{R}_{q\,12} \mathcal{R}_{q\,23}, \tag{4.9}$$

while a similar action of the conjugate map $\mathrm{id} \otimes \mathrm{id} \otimes \Psi$ on (4.8) provides the another form of the Yang-Baxter equation:

$$\mathcal{R}_{q\,12}\mathcal{R}_{q\,13}\mathcal{R}_{q\,23} = \mathcal{R}_{q\,23}\mathcal{R}_{q\,13}\mathcal{R}_{q\,12}. \tag{4.10}$$

Mappings from a universal $\mathcal{T}$-matrix to a universal $\mathcal{R}$-matrix have been discussed for only a few quantum algebras. Frønsdal[19] considered such mappings for quantum $gl(n)$ and the particular case of a two-parametric quantum $gl(2)$ is discussed in Ref. 21. The maps for Alexander-Conway quantum algebra are studied in Ref. 22.

V. REPRESENTATIONS OF $\mathcal{A}$

We do not yet have the explicit formulae of finite dimensional representation matrices of the function algebra $\mathcal{A}$. These expressions will be derived in the next section. But, prior to that, the general properties of such finite dimensional representation matrices may be understood via the duality arguments interrelating $\mathcal{A}$ and $\mathcal{U}$ algebras. We will address to this task in the present section.

To be explicit, for us the representations of $\mathcal{A}$ signify the matrix elements of the universal $\mathcal{T}$-matrix on $V^{(\ell)}$ defined in Sec. II:

$$T^{\ell}_{m'm}(\lambda) = (e^{\ell}_{m'}(\lambda), \mathcal{T}_{e,E} e^{\ell}_{m}(\lambda)) = \sum_{abc} (-1)^{(a+c)(a+c-1)/2+(a+c)(\ell-m'+\lambda)} e^{abc} (e^{\ell}_{m'}(\lambda), E_{abc}\, e^{\ell}_{m}(\lambda)). \tag{5.1}$$

Under the assumption of the completeness of the basis vectors $e^{\ell}_{m}(\lambda)$, it is not difficult to verify the relations

$$\Delta(T^{\ell}_{m'm}(\lambda)) = \sum_{k} T^{\ell}_{m'k}(\lambda) \otimes T^{\ell}_{km}(\lambda), \quad \epsilon(T^{\ell}_{m'm}(\lambda)) = \delta_{m'm}. \tag{5.2}$$

The relations in (5.2) imply that the matrix elements (5.1) satisfy the axiom of the comodule.[1] We may therefore regard $T^{\ell}_{m'm}(\lambda)$ as the $2\ell+1$ dimensional matrix representation of the algebra $\mathcal{A}$.

We now consider a product of two representations in order to obtain their composition rule. We evaluate the matrix elements of $\mathcal{T}_{e,\Delta(E)}$ on the coupled basis vector space in two different ways. The first evaluation is as follows:

$$\begin{aligned}
&(e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda), \mathcal{T}_{e,\Delta(E)}\, e^{\ell}_{m}(\ell_1,\ell_2,\Lambda)) \\
&\quad = \sum_{abc} (-1)^{(a+c)(a+c-1)/2+(a+c)(\ell'-m'+\Lambda)} e^{abc}\, (e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda), \Delta(E_{abc}) e^{\ell}_{m}(\ell_1,\ell_2,\Lambda)) \\
&\quad = \delta_{\ell'\ell}(-1)^{(\ell'-m'+\lambda)(\ell_1+\ell_2+\ell'+\lambda)} T^{\ell}_{m'm}(\Lambda).
\end{aligned} \tag{5.3}$$

In the last equality, the pseudo-orthogonality (2.12) of the coupled basis has been used. An alternate evaluation of the above-mentioned matrix element explicitly uses the Clebsch-Gordan coupling of the basis vectors. With the aid of the relation

$$\mathcal{T}_{e,\Delta(E)} = \sum_{\substack{prq \\ p'q'r'}} (-1)^{(p+r+p'+r')(p+r+p'+r'-1)/2} e^{pqr} e^{p'q'r'} \otimes E_{pqr} \otimes E_{p'q'r'},$$

we obtain

$$(e^{\ell'}_{m'}(\ell_1,\ell_2,\Lambda),\mathcal{T}_{e,\Delta(E)}e^{\ell}_{m}(\ell_1,\ell_2,\Lambda))$$
$$=\sum_{\substack{m_1,m_2\\ m'_1,m'_2}}(-1)^{(\ell_1-m_1+\lambda)(\ell_2-m'_2+\lambda)}C^{\ell_1\,\ell_2\,\ell'}_{m'_1m'_2m'}C^{\ell_1\,\ell_2\,\ell}_{m_1\,m_2\,m}T^{\ell_1}_{m'_1\,m_1}(\lambda)T^{\ell_2}_{m'_2\,m_2}(\lambda). \tag{5.4}$$

Since the results of the two evaluations have to be identical, we obtain the product law for the quantum supergroup $\mathcal{A}$ of the following form:

$$\delta_{\ell'\ell}T^{\ell}_{m'm}(\Lambda)=(-1)^{(\ell'-m'+\lambda)(\ell_1+\ell_2+\ell'+\lambda)}\sum_{\substack{m_1,m_2\\ m'_1,m'_2}}(-1)^{(\ell_1-m'_1+\lambda)(\ell_2-m'_2+\lambda)}$$
$$\times C^{\ell_1\,\ell_2\,\ell'}_{m'_1\,m'_2\,m'}C^{\ell_1\,\ell_2\,\ell}_{m_1\,m_2\,m}T^{\ell_1}_{m'_1\,m_1}(\lambda)T^{\ell_2}_{m'_2\,m_2}(\lambda). \tag{5.5}$$

Another derivation of the product law (5.5) is found in Ref. 6.

Two alternate forms of the product law are readily derived by using the pseudo-orthogonality of CGC (2.13) and (2.14):

$$\sum_{m'}C^{\ell_1\,\ell_2\,\ell}_{n_1\,n_2\,m'}T^{\ell}_{m'm}(\Lambda)=\sum_{m_1,m_2}(-1)^{(n_1+m_1)(\ell_2-n_2+\lambda)}C^{\ell_1\,\ell_2\,\ell}_{m_1\,m_2\,m}T^{\ell_1}_{n_1\,m_1}(\lambda)T^{\ell_2}_{n_2\,m_2}(\lambda), \tag{5.6}$$

$$\sum_{m}(-1)^{(m'+m)(\ell_1+\ell_2+\ell'+\lambda)}C^{\ell_1\,\ell_2\,\ell'}_{n_1\,n_2\,m}T^{\ell'}_{m'm}(\Lambda)$$
$$=\sum_{m'_1,m'_2}(-1)^{(n_2+m'_2)(\ell_1-n_1+\lambda)}C^{\ell_1\,\ell_2\,\ell'}_{m'_1\,m'_2\,m'}T^{\ell_1}_{m'_1\,n_1}(\lambda)T^{\ell_2}_{m'_2\,n_2}(\lambda). \tag{5.7}$$

The product law allows us to derive the orthogonality and the recurrence relations of the representation matrix $T^{\ell}_{m'm}$. Setting $\ell_1=\ell_2$, $\ell=m=0$ in (5.6) and using the formula of CGC given in Ref. 6, one can verify the orthogonality relation

$$\sum_{m}(-1)^{m_1(m_1+m)+m_1(m_1-1)/2+m(m-1)/2}q^{(m_1-m)/2}T^{\ell}_{m_1m}(\lambda)T^{\ell}_{-m_2-m}(\lambda)=\delta_{m_1m_2}. \tag{5.8}$$

Another orthogonality relation is similarly obtained by setting $\ell_1=\ell_2$, $\ell'=m'=0$ in the product law (5.7):

$$\sum_{m}(-1)^{(m_1+m)m_1+m_1(m_1-1)/2+m(m-1)/2}q^{(m_1-m)/2}T^{\ell}_{mm_1}(\lambda)T^{\ell}_{-m-m_2}(\lambda)=\delta_{m_1m_2}. \tag{5.9}$$

For the choice of $\ell_2=1$ in (5.6), the recurrence relations for the representation matrices are obtained below. These relations are classified into three sets according to the values of ℓ:

• The first set has the value of $\ell=\ell_1+1$. It comprises three relations corresponding to all possible values of n_2. The recurrence relations listed below correspond to $n_2=1$, 0, and -1, respectively:

$$(-1)^{(n+m)\lambda}q^{-(\ell-n)/2}F^{\ell}(n,0,-1)T^{\ell}_{nm}(\Lambda)$$
$$=q^{-(\ell-m)/2}F^{\ell}(m,0,-1)T^{\ell-1}_{n-1\,m-1}(\lambda)a-(-1)^{\lambda}q^{m/2}G^{\ell}(m,0,0)T^{\ell-1}_{n-1\,m}(\lambda)\alpha$$
$$+q^{(\ell+m)/2}F^{\ell}(-m,0,-1)T^{\ell-1}_{n-1\,m+1}(\lambda)b,$$

$$
\begin{aligned}
&(-1)^{(n+m)(1+\lambda)}q^{n/2}G^{\ell}(n,0,0)T^{\ell}_{nm}(\Lambda)\\
&\quad=-q^{-(\ell-m)/2}F^{\ell}(m,0,-1)T^{\ell-1}_{n\,m-1}(\lambda)\gamma+q^{m/2}G^{\ell}(m,0,0)T^{\ell-1}_{nm}(\lambda)\,e\\
&\quad-q^{(\ell+m)/2}F^{\ell}(-m,0,-1)T^{\ell-1}_{n\,m+1}(\lambda)\beta,
\end{aligned}
$$

$$
\begin{aligned}
&(-1)^{(n+m)(1+\lambda)}q^{(\ell+n)/2}F^{\ell}(-n,0,-1)T^{\ell}_{nm}(\Lambda)\\
&\quad=q^{-(\ell-m)/2}F^{\ell}(m,0,-1)T^{\ell-1}_{n+1\,m-1}(\lambda)c+q^{m/2}G^{\ell}(m,0,0)T^{\ell-1}_{n+1\,m}(\lambda)\delta\\
&\quad+q^{(\ell+m)/2}F^{\ell}(-m,0,-1)T^{\ell-1}_{n+1\,m+1}(\lambda)\beta,
\end{aligned}
\tag{5.10}
$$

where

$$
F^{\ell}(m,a,b)=\sqrt{\{\ell+m+a\}_q\{\ell+m+b\}_q},
$$

$$
G^{\ell}(m,a,b)=\sqrt{\{2\}_q\{\ell+m+a\}_q\{\ell-m+b\}_q},
$$

and the matrix elements for the fundamental representation ($\ell=1$) are denoted as

$$
\begin{pmatrix} a & \alpha & b\\ \gamma & e & \beta\\ c & \delta & d\end{pmatrix}=\begin{pmatrix} T^1_{11}(\lambda) & T^1_{10}(\lambda) & T^1_{1-1}(\lambda)\\ T^1_{01}(\lambda) & T^1_{00}(\lambda) & T^1_{0-1}(\lambda)\\ T^1_{-11}(\lambda) & T^1_{-10}(\lambda) & T^1_{-1-1}(\lambda)\end{pmatrix}.
\tag{5.11}
$$

In this set, the highest weight Λ assumes a constant value of 0 (mod 2).

• The second set corresponds to $\ell=\ell_1$. It also contains three recurrence relations and, in this instance, we have $\Lambda=1$ (mod 2):

$$
\begin{aligned}
&(-1)^{\ell-n+\lambda+(n+m+1)\lambda}q^{(n-m)/2}G^{\ell}(n,0,1)T^{\ell}_{nm}(\Lambda)\\
&\quad=(-1)^{\ell-m}G^{\ell}(m,0,1)T^{\ell}_{n-1\,m-1}(\lambda)a-H^{\ell}_{m}T^{\ell}_{n-1\,m}(\lambda)\alpha+\{2\}^{-1/2}_{q}G^{\ell}(m,1,0)T^{\ell}_{n-1\,m+1}(\lambda)b,
\end{aligned}
$$

$$
\begin{aligned}
&(-1)^{(n+m)(1+\lambda)}q^{(n-m)/2}H^{\ell}_{n}T^{\ell}_{nm}(\Lambda)\\
&\quad=(-1)^{\ell-m}G^{\ell}(m,0,1)T^{\ell}_{n\,m-1}(\lambda)\gamma+H^{\ell}_{m}T^{\ell}_{nm}(\lambda)e+\{2\}^{-1/2}_{q}G^{\ell}(m,1,0)T^{\ell}_{n\,m+1}(\lambda)\beta,
\end{aligned}
$$

$$
\begin{aligned}
&(-1)^{(n+m)\lambda}q^{(n-m)/2}\{2\}^{-1/2}_{q}G^{\ell}(n,0,1)T^{\ell}_{nm}(\Lambda)\\
&\quad=(-1)^{\ell-m}G^{\ell}(m,0,1)T^{\ell}_{n+1\,m-1}(\lambda)c-H^{\ell}_{m}T^{\ell}_{n+1\,m}(\lambda)\delta+\{2\}^{-1/2}_{q}G^{\ell}(m,1,0)T^{\ell}_{n+1\,m+1}(\lambda)d,
\end{aligned}
\tag{5.12}
$$

where

$$
H^{\ell}_{m}=q^{-\ell/2}\{\ell+m+1\}_q-(-1)^{\ell-m}q^{\ell/2}\{\ell-m+1\}_q.
$$

• Similarly, the third set contains three recurrence relations for $\ell=\ell_1-1$. For this case, the highest weight reads $\Lambda=0$ (mod 2), and the recurrence relations are given by

$$
\begin{aligned}
q^{(\ell-m+n+1)/2}F^{\ell}(-n,1,2)T^{\ell}_{nm}(\Lambda)&=q^{(\ell+1)/2}F^{\ell}(-m,1,2)T^{\ell+1}_{n-1\,m-1}(\lambda)a+(-1)^{\ell-m+\lambda}G^{\ell}(m,1,1)T^{\ell+1}_{n-1\,m}(\lambda)\alpha\\
&\quad-q^{-(\ell+1)/2}F^{\ell}(m,1,2)T^{\ell+1}_{n-1\,m}(\lambda)b,
\end{aligned}
$$

$$
\begin{aligned}
(-1)^{\ell-n+\lambda}q^{(n-m)/2}G^{\ell}(n,1,1)T^{\ell}_{nm}(\Lambda)&=q^{(\ell+1)/2}F^{\ell}(-m,1,2)T^{\ell+1}_{n\,m-1}(\lambda)\gamma+(-1)^{\ell-m+\lambda}\\
&\quad\times G^{\ell}(m,1,1)T^{\ell+1}_{nm}(\lambda)\,e-q^{-(\ell+1)/2}F^{\ell}(m,1,2)T^{\ell+1}_{n\,m+1}(\lambda)\beta,
\end{aligned}
$$

$$q^{-(\ell-n+m+1)/2}F^{\ell}(n,1,2)T^{\ell}_{nm}(\Lambda) = -q^{(\ell+1)/2}F^{\ell}(-m,1,2)T^{\ell+1}_{n+1\ m-1}(\lambda)c - (-1)^{\ell-m+\lambda}G^{\ell}(m,1,1)T^{\ell+1}_{n+1\ m}(\lambda)\delta + q^{-(\ell+1)/2}F^{\ell}(m,1,2)T^{\ell+1}_{n+1\ m+1}(\lambda)d. \tag{5.13}$$

The discussion so far is independent of the explicit form of the universal $\mathcal{T}$-matrix. The general properties of the universal $\mathcal{T}$-matrix and the Clebsch-Gordan decomposition of tensor product representations play a seminal role in the derivation of all properties of the representation of $\mathcal{A}$. Thus one can repeat the same arguments for other quantum deformations of $OSp(1/2)$, namely the Jordanian[23] and the super-Jordanian[24,25] analogs for deriving their product law, the orthogonality, and the recurrence relations. Being triangular algebras, the Jordanian and the super-Jordanian deformations of $OSp(1/2)$ possess the same Clebsch-Gordan decomposition as in the present case.

The representations of $SL_q(2)$ [or $SU_q(2)$] have been discussed by many authors. Among the properties of representation matrices, the product law,[26] recurrence relations,[26,27] orthogonality, and *RTT*-relation[27] and generating functions[28] are found in the literature. In Ref. 27, the representation matrices are interpreted as the wave functions of a quantum symmetric top in noncommutative space. Representations of the Jordanian quantum group $SL_{\mathbf{h}}(2)$ have been considered in Refs. 29 and 30.

VI. REPRESENTATION MATRIX AND LITTLE *Q*-JACOBI POLYNOMIALS

Explicit formulae for the representation matrices of the quantum group $SU_q(2)$ have been obtained by several authors.[31–33] It is observed that, for the finite dimensional representations, the matrix elements are expressed in terms of the little q-Jacobi polynomials. Investigating the Jordanian quantum group $SL_{\mathbf{h}}(2)$ in a similar framework, it has also been noted that the conventional Jacobi polynomials contribute[30] to the representation matrices therein. The corresponding matrix elements for the two-parametric quantum group $GL(2)$ have been computed in Ref. 34. Their relation to orthogonal polynomials, however, is still an open problem.

In this section, we provide the explicit form of the representation matrices (5.1) of $\mathcal{A}$ by direct computation, and study the resulting polynomial structure. Toward this end, we proceed by noticing the identities obtained by the repeated use of (2.9):

$$V^{c}_{-}e^{\ell}_{m}(\lambda) = (-1)^{c(\ell-m)+c(c-3)/2}\left(\frac{1}{\{2\}^{c}_{q}}\frac{\{\ell+m\}_q!\{\ell-m+c\}_q!}{\{\ell-m\}_q!\{\ell+m-c\}_q!}\right)^{1/2}e^{\ell}_{m-c}(\lambda),$$

$$V^{a}_{+}e^{\ell}_{m}(\lambda) = \left(\frac{1}{\{2\}^{a}_{q}}\frac{\{\ell-m\}_q!\{\ell+m+a\}_q!}{\{\ell+m\}_q!\{\ell-m-a\}_q!}\right)^{1/2}e^{\ell}_{m+a}(\lambda). \tag{6.1}$$

The explicit listing of the basis elements of $\mathcal{A}$ in (3.17) renders the computation of the matrix elements straightforward. The final result is quoted below:

$$T_{m'm}(\lambda) = (-1)^{(m'-m)(m'-m-1)/2+(m'-m)(-m'+\lambda)}\frac{q^{m(m'-m)/2}}{\sqrt{\{2\}^{m'-m}_{q}}}\left(\frac{\{\ell+m\}_q!}{\{\ell-m\}_q!}\frac{\{\ell+m'\}_q!}{\{\ell-m'\}_q!}\right)^{1/2} \times \sum_{c}(-1)^{c(\ell-m)}\frac{q^{-c(m'-m)/2}}{\{2\}^{c}_{q}}\frac{\{\ell-m+c\}_q!}{\{\ell+m-c\}_q!}\frac{x^{m'-m+c}}{\{m'-m+c\}_q!}\exp\left(\frac{m-c}{2}z\right)\frac{y^{c}}{\{c\}_q!}, \tag{6.2}$$

where the index c runs over all non-negative integers maintaining the argument of $\{\mathcal{X}\}_q$ non-negative.

The fundamental representation $(\ell=1,\lambda=0)$ may be identified with the quantum supermatrix of Ref. 6 in the manner of (5.11). This identification allows us to realize the entries of the quantum supermatrix in terms of the generators of the quantum supergroup $\mathcal{A}$:

$$a = xy + e^{z/2} + \frac{x^2 e^{-z/2} y^2}{\{2\}_q^2}, \quad \alpha = x - \frac{x^2 e^{-z/2} y}{q^{1/2}\{2\}_q}, \quad b = -\frac{x^2 e^{-z/2}}{q\{2\}_q},$$

$$\gamma = y + \frac{q^{1/2} x e^{-z/2} y^2}{\{2\}_q}, \quad e = 1 - x e^{-z/2} y, \quad \beta = -q^{-1/2} x e^{-z/2},$$

$$c = -\frac{q e^{-z/2} y^2}{\{2\}_q}, \quad \delta = q^{1/2} e^{-z/2} y, \quad d = e^{-z/2}. \tag{6.3}$$

A straightforward computation using the commutation relations (3.8) allows us to infer that the realization (6.3) recovers all the commutation relations of the supermatrix listed in Ref. 6. The realization (6.3), more importantly, implies the following Gaussian decomposition of the quantum supermatrix:[14,35,36]

$$\begin{pmatrix} 1 & 0 & 0 \\ -q^{-1/2} x & 1 & 0 \\ -\dfrac{1}{q\{2\}_q} x^2 & x & 1 \end{pmatrix} \begin{pmatrix} e^{-z/2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{z/2} \end{pmatrix} \begin{pmatrix} 1 & q^{1/2} y & -\dfrac{q}{\{2\}_q} y^2 \\ 0 & 1 & y \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} d & \delta & c \\ \beta & e & \gamma \\ b & \alpha & a \end{pmatrix} = C \begin{pmatrix} a & \alpha & b \\ \gamma & e & \beta \\ c & \delta & d \end{pmatrix} C^{-1}, \tag{6.4}$$

where

$$C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad C^{-1} = C.$$

We now turn our attention to the polynomial structure built into the general matrix element (6.2) in terms of the variable

$$\zeta = \frac{q^{-1/2}}{\{2\}_q} x e^{-z/2} y. \tag{6.5}$$

To demonstrate this, the product of generators in (6.2) for the case $m' - m \geq 0$ may be rearranged as follows:

$$x^{m'-m+c} \exp\left(\frac{m-c}{2} z\right) y^c = (-1)^{c(c-1)/2} q^{-mc} x^{m'-m} e^{mz/2} (x e^{-z/2} y)^c.$$

The matrix element $T^{\ell}_{m'm}(\lambda)$ may now be succinctly expressed as a polynomial structure given below:

$$T^{\ell}_{m'm}(\lambda) = (-1)^{(m'-m)(m'-m-1)/2 + (m'-m)(\ell-m'+\lambda)} \frac{q^{m(m'-m)/2}}{\{m'-m\}_q ! \sqrt{\{2\}_q^{m'-m}}}$$
$$\times \left(\frac{\{\ell - m\}_q ! \, \{\ell + m'\}_q !}{\{\ell + m\}_q ! \, \{\ell - m'\}_q !} \right)^{1/2} x^{m'-m} e^{mz/2} P^{\ell}_{m'm}(\zeta). \tag{6.6}$$

The polynomial $P^{\ell}_{m'm}(\zeta)$ in the variable ζ is defined by

$$P^{\ell}_{m'm}(\zeta)=\sum_{c}(-1)^{c(\ell-m)+c(c-1)/2}q^{-c(m'+m-1)/2}\frac{\{m'-m\}_q!\,\{l+m\}_q!\,\{\ell-m+c\}_q!}{\{m'-m+c\}_q!\,\{\ell+m-c\}_q!\,\{\ell-m\}_q!\,\{c\}_q!}\zeta^c, \tag{6.7}$$

where the index c runs over all non-negative integers maintaining the arguments of $\{\mathcal{X}\}_q$ non-negative. For the case $m'-m\leq 0$, we make a replacement of the summation index c with $a=m'-m+c$. Rearrangement of the generators now provides the following expression of the general matrix element:

$$T^{\ell}_{m'm}(\lambda)=(-1)^{(m-m')(m-m'+1)/2-(m-m')(\lambda-1)}\frac{q^{-m'(m-m')/2}}{\{m-m'\}_q!\,\sqrt{\{2\}_q^{m-m'}}}\times\left(\frac{\{\ell+m\}_q!\,\{\ell-m'\}_q!}{\{\ell-m\}_q!\,\{\ell+m'\}_q!}\right)^{1/2}e^{m'z/2}y^{m-m'}P^{\ell}_{m'm}(\zeta), \tag{6.8}$$

where the polynomial $P^{\ell}_{m'm}(\zeta)$ for $m'-m\leq 0$ is defined by

$$P^{\ell}_{m'm}(\zeta)=\sum_{a}(-1)^{a(\ell-m')+a(a-1)/2}q^{-a(m'+m-1)/2}\frac{\{m-m'\}_q!\,\{l+m'\}_q!\,\{\ell-m'+a\}_q!}{\{m-m'+a\}_q!\,\{\ell+m'-a\}_q!\,\{\ell-m'\}_q!\,\{a\}_q!}\zeta^a. \tag{6.9}$$

It is immediate to note that the polynomials are symmetric with respect to the transposition $m\leftrightarrow m'$: $P^{\ell}_{mm'}\zeta=P^{\ell}_{m'm}(\zeta)$, and that $P^{\ell}_{-\ell\, m}(\zeta)=P^{\ell}_{m'\,-\ell}(\zeta)=1$.

The polynomials obtained above are related to the basic hypergeometric functions. We define the basic hypergeometric function ${}_2\phi_1$ by[37]

$${}_2\phi_1(a_1,a_2;b;Q;z)=\sum_{n=0}\frac{(a_1;Q)_n(a_2;Q)_n}{(b;Q)_n(Q;Q)_n}z^n, \tag{6.10}$$

where the shifted factorial is defined as usual:

$$(x;Q)_n=\begin{cases}1, & n=0,\\ \displaystyle\prod_{k=0}^{n-1}(1-xQ^k), & n\neq 0.\end{cases} \tag{6.11}$$

The little Q-Jacobi polynomials are defined via ${}_2\phi_1$ as standard theory of orthogonal polynomials[37]

$$p^{(a,b)}_m(z)={}_2\phi_1(Q^{-m},abQ^{m+1};aQ;Q;Qz). \tag{6.12}$$

Setting $a=Q^{\alpha}$, $b=Q^{\beta}$, we have the following form of little Q-Jacobi polynomials:

$$p^{(\alpha,\beta)}_m(z)=\sum_{n}\frac{(Q^{-m};Q)_n(Q^{\alpha+\beta+m+1};Q)_n}{(Q^{\alpha+1};Q)_n(Q;Q)_n}(Qz)^n. \tag{6.13}$$

Rewriting our polynomials (6.7) and (6.9) in terms of the shifted factorial with $Q=-q$, one can identify our polynomials with the little Q-Jacobi polynomials. For the choice $m'-m\geq 0$, the polynomial structure reads

$$P^{\ell}_{m'm}(\zeta)=\sum_{a}\frac{((-q)^{-\ell-m};-q)_a((-q)^{\ell-m+1};-q)_a}{((-q)^{m'-m+1};-q)_a(-q;-q)_a}(-q\zeta)^a=p^{(m'-m,-m'-m)}_{\ell+m}(\zeta), \tag{6.14}$$

and for the $m'-m\leq 0$ case its identification is given by

$$P^{\ell}_{m'm}(\zeta) = \sum_a \frac{((-q)^{-\ell-m'};-q)_a((-q)^{\ell-m'+1};-q)_a}{((-q)^{m-m'+1};-q)_a(-q;-q)_a}(-q\zeta)^a = p^{(m-m',-m'-m)}_{\ell+m'}(\zeta). \tag{6.15}$$

It is amazing that $Q=-q$ polynomials appear for the supergroup $\mathcal{A}$ in contrast to the $Q=q$ polynomials being present for the quantum group $SU_q(2)$.[31–33]

VII. CONCLUDING REMARKS

Starting from the construction of the universal $\mathcal{T}$-matrix, we have investigated the finite dimensional representations of the quantum supergroup $\mathcal{A}$. A qualitative difference between the universal $\mathcal{T}$-matrices for the classical and the quantum $OSp(1/2)$ algebras exists due to the nilpotency of the classical parity odd elements. The absence of the above-mentioned nilpotency in the quantum case induces a new polynomial structure in the matrix elements of $\mathcal{T}$. We observed that these polynomials are expressed in terms of the little Q-Jacobi polynomials. This suggests a new link between orthogonal polynomials and representations of quantum supergroups. It is likely to be a general property that if the Grassmann variables in a classical supergroup lose nilpotency at the quantum level, it may be reflected in the representations of the quantum supergroup so that the entries of representation matrices may have a new quantized polynomial structure. The present work provides an example of this statement. Another likely candidate for the existence of a similar polynomial structure is the super-Jordanian $OSp(1/2)$, where the loss of nilpotency has been observed.[5] We believe that the investigation along this line will give a new algebraic background to basic hypergeometric series.

We have also tried to extend the known properties of the representations for $SL_q(2)$ to the quantum supergroup $\mathcal{A}$. An extension of the product law, the orthogonality and the recurrence relations, was shown to be possible. However, two known results are not extended in the present work, that is, the generating function[28] of the representation matrices and the Peter-Weyl theorem.[7,33] In order to discuss the Peter-Weyl theorem, a Haar measure has to be defined on $\mathcal{A}$. Since the loss of nilpotency makes the superspace on $\mathcal{A}$ more complex than the classical case, studying the Peter-Weyl theorem may be interesting from the viewpoint of harmonic analysis on quantum supergroups. We will discuss these issues elsewhere.

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APPENDIX: UNIVERSAL $\mathcal{T}$-MATRIX FOR QUANTUM SUPERGROUP

This Appendix is devoted to a general discussion of the universal $\mathcal{T}$-matrix for quantum supergroups. In particular, the relations used in Secs. III and IV are proved in a general setting.

Let $\mathcal{U}$ and $\mathcal{A}$ be dually conjugate unital $\mathbb{Z}_2$ graded Hopf algebras. The basis of the algebras $\mathcal{U}$ and $\mathcal{A}$ are denoted by E_k, e^k, respectively. One may assume that $E_0=1_{\mathcal{U}}$, $e^0=1_{\mathcal{A}}$, and $p(E_k)=p(e^k)$ without loss of generality. The duality of $\mathcal{U}$ and $\mathcal{A}$ is reflected in the structure constants:

$$E_kE_\ell = \sum_m f^m_{k\ell}E_m, \quad \Delta(E_k) = \sum_{pq} g^{pq}_k E_p \otimes E_q, \tag{A1}$$

$$e^ke^\ell = \sum_m g^{k\ell}_m e^m, \quad \Delta(e^k) = \sum_{pq} f^k_{pq} e^p \otimes e^q. \tag{A2}$$

The universal $\mathcal{T}$-matrix is defined by

$$\mathcal{T}_{e,E} = \sum_k (-1)^{p(e^k)(p(e^k)-1)/2} e^k \otimes E_k, \quad \in \mathcal{A} \otimes \mathcal{U}. \tag{A3}$$

Although the factor $(-1)^{p(e^k)(p(e^k)-1)/2}$ is trivial, it is convenient to keep it in the discussion of universal $\mathcal{T}$-matrix.

We start with the proof of the relations in (3.25). The proof of the first relation in (3.25) is straightforward:

$$\begin{aligned}\mathcal{T}_{e,E}\mathcal{T}_{e',E} &= \sum_{k,\ell,m} (-1)^{(p(e^k)+p(e^\ell))(p(e^k)+p(e^\ell)-1)/2} e^k \otimes e^\ell \otimes f_{k\,\ell}^{\,m} E_m \\ &= \sum_m (-1)^{p(e^m)(p(e^m)-1)/2} \Delta(e^m) \otimes E_m = \mathcal{T}_{\Delta(e),E}.\end{aligned}$$

The second equality is due to the fact that the parity of the both sides of the first equation in (A1) are equal, and that the structure constants are of even parity. The second relation in (3.25) can be proved similarly. The third relation in (3.25) follows from $\epsilon(e^k) = \delta_0^k$, $\epsilon(E_k) = \delta_{k0}$. The last relation in (3.25) is a consequence of the identities

$$\mathcal{T}_{e,S(E)}\mathcal{T}_{e,E} = \mathcal{T}_{e,E}\mathcal{T}_{e,S(E)} = 1 \otimes 1, \quad \mathcal{T}_{S(e),E}\mathcal{T}_{e,E} = \mathcal{T}_{e,E}\mathcal{T}_{S(e),E} = 1 \otimes 1. \tag{A4}$$

The above identities can be proved by using the axiom of antipode and $p(S(e^k)) = p(e^k)$..

We next derive the *RTT*-type relations (4.6) and (4.8). Defining

$$\mathcal{T}_{e,E}^{(1)} = \sum_k (-1)^{p(e^k)(p(e^k)-1)/2} e^k \otimes E_k \otimes 1, \quad \mathcal{T}_{e,E}^{(2)} = \sum_k (-1)^{p(e^k)(p(e^k)-1)/2} e^k \otimes 1 \otimes E_k,$$

we obtain

$$\mathcal{T}_{e,E}^{(1)}\mathcal{T}_{e,E}^{(2)} = \sum_m (-1)^{p(e^m)(p(e^m)-1)/2} e^m \otimes \Delta(E_m).$$

On the other hand, the transposed coproduct appears in the reverse-ordered product:

$$\begin{aligned}\mathcal{T}_{e,E}^{(2)}\mathcal{T}_{e,E}^{(1)} = \sum_m (-1)^{p(e^m)(p(e^m)-1)/2} e^m \otimes \Delta'(E_m) &= \sum_m (-1)^{p(e^m)(p(e^m)-1)/2} e^m \otimes \mathcal{R}\Delta(E_m)R^{-1} \\ &= (1 \otimes \mathcal{R})\mathcal{T}_{e,E}^{(1)}\mathcal{T}_{e,E}^{(2)}\,(1 \otimes \mathcal{R}^{-1}).\end{aligned}$$

In the last equality, the fact that the universal $\mathcal{R}$-matrix is of even parity has been used. This completes our proof of the *RTT*-type relation (4.6). The proof of (4.8) may be done similarly with the definitions

$$\mathcal{T}_{E,e}^{(1)} = \sum_k (-1)^{p(e^k)(p(e^k)-1)/2} E_k \otimes 1 \otimes e^k, \quad \mathcal{T}_{E,e}^{(2)} = \sum_k (-1)^{p(e^k)(p(e^k)-1)/2} 1 \otimes E_k \otimes e^k.$$

Note added: After submitting the manuscript, we have learnt about the work of Zou,[38] where the representations of $OSp_q(1/2)$ and their relation to the basic hypergeometric functions are explicitly computed by using other basis states, and adopting a method (similar to Ref. 33) different from ours. The Peter-Weyl theorem has also been established there.

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Expanding Lie (super)algebras through Abelian semigroups

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We propose an outgrowth of the expansion method introduced by de Azcárraga *et al.* [Nucl. Phys. B **662**, 185 (2003)]. The basic idea consists in considering the direct product between an Abelian semigroup S and a Lie algebra $\mathfrak{g}$. General conditions under which relevant subalgebras can systematically be extracted from $S \times \mathfrak{g}$ are given. We show how, for a particular choice of semigroup S, the known cases of expanded algebras can be reobtained, while new ones arise from different choices. Concrete examples, including the M algebra and a D'Auria-Fré-like superalgebra, are considered. Finally, we find explicit, nontrace invariant tensors for these S-expanded algebras, which are essential ingredients in, e.g., the formulation of supergravity theories in arbitrary space-time dimensions. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2390659]

I. INTRODUCTION

The role played by Lie algebras and their interrelations in physics can hardly be overemphasized. To mention only one example, the Poincaré algebra may be obtained from the Galilei algebra via a *deformation* process. This deformation is one of the ways in which different Lie algebras can be related.

The purpose of this paper is to shed new light on the method of *expansion* of Lie algebras (for a thorough treatment, see the seminal work in Ref. 1 and references therein; early work on the subject is found in Ref. 2). An expansion is, in general, an algebra dimension-changing process. For instance, the M algebra,[3–5] with 583 Bosonic generators, can be regarded as an expansion of the orthosymplectic algebra $\mathfrak{osp}(32|1)$, which possesses only 528. This vantage viewpoint may help better understand fundamental problems related to the geometrical formulation of 11-dimensional supergravity. Some physical applications of the expansion procedure have been developed in Refs. 6–14.

The approach to be presented here is entirely based on operations performed directly on the algebra generators, and thus differs from the outset with the one found in Ref. 1, where the dual Maurer-Cartan formulation is used. As a consequence, the expansion of free differential algebras lies beyond the scope of our analysis.

Finite Abelian semigroups play a prominent role in our construction. All expansion cases found in Ref. 1 may be regarded as coming from one particular choice of semigroup in the present approach, which is, in this sense, more general. Different semigroup choices yield, in general, expanded algebras that cannot be obtained by the methods of Ref. 1.

The plan of the paper goes as follows. After some preliminaries in Sec. II, Sec. III introduces the general procedure of the Abelian semigroup expansion, S-expansion for short, and shows how the cases found in Ref. 1 can be recovered by an appropriate choice of semigroup S. In Sec. IV, general conditions are given under which relevant subalgebras can be extracted from an

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S-expanded algebra. The case when $\mathfrak{g}$ satisfies the Weimar-Woods conditions[15,16] and the case when $\mathfrak{g}$ is a superalgebra are studied. Section V gives three explicit examples of *S*-expansions of $\mathfrak{osp}(32|1)$: (i) the M algebra,[3–5] (ii) a D'Auria-Fré-like Superalgebra,[17] and (iii) a new superalgebra, different from but resembling aspects of the M algebra, $\mathfrak{osp}(32|1)\times\mathfrak{osp}(32|1)$, and D'Auria-Fré superalgebras. In Sec. VI, the remaining cases of expanded algebras shown in Ref. 1 are seen to also fit within the current scheme. The five-brane superalgebra[18,19] is given as an example. Section VII deals with the crucial problem of finding invariant tensors for the *S*-expanded algebras. General theorems are proven, allowing for nontrivial invariant tensors to be systematically constructed. We close in Sec. VIII with conclusions and an outlook for future work.

II. PRELIMINARIES

Before analyzing the *S*-expansion procedure itself, it will prove convenient to introduce some basic notation and definitions.

A. Semigroups

Definition 2.1: *Let* $S=\{\lambda_\alpha\}$ *be a finite semigroup,*[1] *and let us write the product of* $\lambda_{\alpha_1},\ldots,\lambda_{\alpha_n}\in S$ *as*

$$\lambda_{\alpha_1}\cdots\lambda_{\alpha_n}=\lambda_{\gamma(\alpha_1,\ldots,\alpha_n)}. \tag{1}$$

The n-selector $K_{\alpha_1\cdots\alpha_n}{}^{\rho}$ *is defined as*

$$K_{\alpha_1\cdots\alpha_n}{}^{\rho}=\begin{cases}1 & \text{when } \rho=\gamma(\alpha_1,\ldots,\alpha_n)\\ 0 & \text{otherwise.}\end{cases} \tag{2}$$

Since S is associative, the n-selector fulfills the identity

$$K_{\alpha_1\cdots\alpha_n}{}^{\rho}=K_{\alpha_1\cdots\alpha_{n-1}}{}^{\sigma}K_{\sigma\alpha_n}{}^{\rho}=K_{\alpha_1\sigma}{}^{\rho}K_{\alpha_2\cdots\alpha_n}{}^{\sigma}. \tag{3}$$

Using this identity it is always possible to express the *n*-selector in terms of two-selectors, which encode the information from the multiplication table of *S*.

An interesting way to state the same is that two-selectors provide a matrix representation for *S*. As a matter of fact, when we write

$$[\lambda_\alpha]_\mu{}^{\nu}=K_{\mu\alpha}{}^{\nu}, \tag{4}$$

then we have

$$[\lambda_\alpha]_\mu{}^{\sigma}[\lambda_\beta]_\sigma{}^{\nu}=K_{\alpha\beta}{}^{\sigma}[\lambda_\sigma]_\mu{}^{\nu}=[\lambda_{\gamma(\alpha,\beta)}]_\mu{}^{\nu}. \tag{5}$$

We will restrict ourselves from now on to *Abelian* semigroups, which implies that the *n*-selectors will be completely symmetrical in their lower indices.

The following definition introduces a product between semigroup subsets which will be extensively used throughout the paper.

Definition 2.2: *Let* S_p *and* S_q *be two subsets of S. The product* $S_p\cdot S_q$ *is defined as*

$$S_p\cdot S_q=\{\lambda_\gamma \text{ such that } \lambda_\gamma=\lambda_{\alpha_p}\lambda_{\alpha_q} \text{ with } \lambda_{\alpha_p}\in S_p \text{ and } \lambda_{\alpha_q}\in S_q\}\subset S. \tag{6}$$

In other words, $S_p\cdot S_q\subset S$ *is the set which results from the product of every element of* S_p *with every element of* S_q*. Since S is Abelian,* $S_p\cdot S_q=S_q\cdot S_p$.

Let us emphasize that, in general, S_p, S_q, and $S_p\cdot S_q$ need *not* be semigroups by themselves.

[1]There does not seem to be a unique, universally accepted definition of semigroup. Here it is taken to be a set provided with a closed associative product. It does not need to have an identity.

The Abelian semigroup S could also be provided with a unique zero element, 0_S. This element is defined as the one for which

$$0_S\lambda_\alpha = \lambda_\alpha 0_S = 0_S, \tag{7}$$

for each $\lambda_\alpha \in S$.

B. Reduced Lie algebras

The following definition introduces the concept of *reduction* of Lie algebras.

Definition 2.3: *Consider a Lie (super)algebra* $\mathfrak{g}$ *of the form* $\mathfrak{g}=V_0\oplus V_1$, *with* $\{\boldsymbol{T}_{a_0}\}$ *being a basis for* V_0 *and* $\{\boldsymbol{T}_{a_1}\}$ *a basis for* V_1. *When* $[V_0,V_1]\subset V_1$, *i.e., when the commutation relations have the general form*

$$[\boldsymbol{T}_{a_0},\boldsymbol{T}_{b_0}] = C_{a_0b_0}{}^{c_0}\boldsymbol{T}_{c_0} + C_{a_0b_0}{}^{c_1}\boldsymbol{T}_{c_1}, \tag{8}$$

$$[\boldsymbol{T}_{a_0},\boldsymbol{T}_{b_1}] = C_{a_0b_1}{}^{c_1}\boldsymbol{T}_{c_1}, \tag{9}$$

$$[\boldsymbol{T}_{a_1},\boldsymbol{T}_{b_1}] = C_{a_1b_1}{}^{c_0}\boldsymbol{T}_{c_0} + C_{a_1b_1}{}^{c_1}\boldsymbol{T}_{c_1}, \tag{10}$$

then it is straightforward to show that the structure constants $C_{a_0b_0}{}^{c_0}$ *satisfy the Jacobi identity by themselves, and therefore* $[\boldsymbol{T}_{a_0},\boldsymbol{T}_{b_0}]=C_{a_0b_0}{}^{c_0}\boldsymbol{T}_{c_0}$ *corresponds by itself to a Lie (super)algebra. This algebra, with structure constants* $C_{a_0b_0}{}^{c_0}$, *is called a* reduced algebra *of* $\mathfrak{g}$ *and symbolized as* $|V_0|$.

The reduced algebra could be regarded in some way as the "inverse" of an algebra extension, but V_1 does not need to be an ideal. Note also that a reduced algebra *does not* correspond to a subalgebra.

III. THE *S*-EXPANSION PROCEDURE

A. *S*-expansion for an arbitrary semigroup *S*

The following theorem embodies one of the main results of the paper, the concept of S-expanded algebras.

Theorem 3.1: *Let* $S=\{\lambda_\alpha\}$ *be an Abelian semigroup with two-selector* $K_{\alpha\beta}{}^{\gamma}$ *and* $\mathfrak{g}$ *a Lie (super)algebra with basis* $\{\boldsymbol{T}_A\}$ *and structure constants* $C_{AB}{}^{C}$. *Denote a basis element of the direct product* $S\times\mathfrak{g}$ *by* $\boldsymbol{T}_{(A,\alpha)}=\lambda_\alpha\boldsymbol{T}_A$ *and consider the induced commutator* $[\boldsymbol{T}_{(A,\alpha)},\boldsymbol{T}_{(B,\beta)}] \equiv\lambda_\alpha\lambda_\beta[\boldsymbol{T}_A,\boldsymbol{T}_B]$. *Then,* $S\times\mathfrak{g}$ *is also a Lie (super)algebra with structure constants*

$$C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)} = K_{\alpha\beta}{}^{\gamma}C_{AB}{}^{C}. \tag{11}$$

Proof: Starting from the form of the induced commutator and using the multiplication law in Eq. (1) one finds

$$[\boldsymbol{T}_{(A,\alpha)},\boldsymbol{T}_{(B,\beta)}] \equiv \lambda_\alpha\lambda_\beta[\boldsymbol{T}_A,\boldsymbol{T}_B] = C_{AB}{}^{C}\lambda_{\gamma(\alpha,\beta)}\boldsymbol{T}_C = C_{AB}{}^{C}\boldsymbol{T}_{(C,\gamma(\alpha,\beta))}.$$

The definition of the two-selector $K_{\alpha\beta}{}^{\rho}$ [see Eq. (2)],

$$K_{\alpha\beta}{}^{\rho} = \begin{cases} 1 & \text{when } \rho=\gamma(\alpha,\beta) \\ 0 & \text{otherwise,} \end{cases}$$

now allows us to write

$$[\boldsymbol{T}_{(A,\alpha)},\boldsymbol{T}_{(B,\beta)}] = K_{\alpha\beta}{}^{\rho}C_{AB}{}^{C}\boldsymbol{T}_{(C,\rho)}. \tag{12}$$

Therefore, the algebra spanned by $\{\boldsymbol{T}_{(A,\alpha)}\}$ closes and the structure constants read

$$C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)} = K_{\alpha\beta}{}^{\gamma} C_{AB}{}^{C}. \tag{13}$$

Since S is Abelian, the structure constants $C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)}$ have the same symmetries as $C_{AB}{}^{C}$, namely,

$$C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)} = -(-1)^{\mathfrak{q}(A)\mathfrak{q}(B)} C_{(B,\beta)(A,\alpha)}{}^{(C,\gamma)}, \tag{14}$$

and for this reason, $\mathfrak{q}(A,\alpha)=\mathfrak{q}(A)$, where $\mathfrak{q}(A)$ denotes the degree of $\boldsymbol{T}_A$ (1 for Fermi and 0 for Bose).

In order to show that the structure constants $C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)}$ satisfy the Jacobi identity, it suffices to use the properties of the selectors [see Eq. (3)] and the fact that the structure constants $C_{AB}{}^{C}$ satisfy the Jacobi identity themselves. This concludes the proof. □

The following definition is a natural outcome of Theorem 3.1.

Definition 3.2: *Let S be an Abelian semigroup and $\mathfrak{g}$ a Lie algebra. The Lie algebra $\mathfrak{G}$ defined by $\mathfrak{G}=S\times\mathfrak{g}$ is called the S-expanded algebra of $\mathfrak{g}$.*

When the semigroup has a zero element $0_S \in S$, it plays a somewhat peculiar role in the S-expanded algebra. Let us span S in nonzero elements $\lambda_i, i=0,\ldots,N$, and a zero element $\lambda_{N+1}=0_S$. Then, the two-selector satisfies

$$K_{i,N+1}{}^{j} = K_{N+1,i}{}^{j} = 0, \tag{15}$$

$$K_{i,N+1}{}^{N+1} = K_{N+1,i}{}^{N+1} = 1, \tag{16}$$

$$K_{N+1,N+1}{}^{j} = 0, \tag{17}$$

$$K_{N+1,N+1}{}^{N+1} = 1. \tag{18}$$

Therefore, $\mathfrak{G}=S\times\mathfrak{g}$ can be split as

$$[\boldsymbol{T}_{(A,i)}, \boldsymbol{T}_{(B,j)}] = K_{ij}{}^{k} C_{AB}{}^{C} \boldsymbol{T}_{(C,k)} + K_{ij}{}^{N+1} C_{AB}{}^{C} \boldsymbol{T}_{(C,N+1)}, \tag{19}$$

$$[\boldsymbol{T}_{(A,N+1)}, \boldsymbol{T}_{(B,j)}] = C_{AB}{}^{C} \boldsymbol{T}_{(C,N+1)}, \tag{20}$$

$$[\boldsymbol{T}_{(A,N+1)}, \boldsymbol{T}_{(B,N+1)}] = C_{AB}{}^{C} \boldsymbol{T}_{(C,N+1)}. \tag{21}$$

Comparing Eqs. (19)–(21) with (8)–(10), one sees that the commutation relations

$$[\boldsymbol{T}_{(A,i)}, \boldsymbol{T}_{(B,j)}] = K_{ij}{}^{k} C_{AB}{}^{C} \boldsymbol{T}_{(C,k)} \tag{22}$$

are those of a reduced Lie algebra of $\mathfrak{G}$ (see Definition 3). The reduction procedure in this particular case is equivalent to imposing the condition

$$\boldsymbol{T}_{(A,N+1)} = 0_S \boldsymbol{T}_A = 0. \tag{23}$$

Notice that in this case the reduction Abelianizes large sectors of the algebra; for each i and j satisfying $K_{ij}{}^{N+1}=1$ (i.e., $\lambda_i\lambda_j=\lambda_{N+1}$) we have $[\boldsymbol{T}_{(A,i)}, \boldsymbol{T}_{(B,j)}]=0$.

The above considerations motivate the following definition.

Definition 3: Let *S be an Abelian semigroup with a zero element $0_S \in S$*, and let *$\mathfrak{G}=S\times\mathfrak{g}$ be an S-expanded algebra. The algebra obtained by imposing the condition $0_S\boldsymbol{T}_A=0$ on $\mathfrak{G}$ (or a subalgebra of it) is called* 0_S-reduced algebra of $\mathfrak{G}$ *(or of the subalgebra).*

The algebra in Eq. (22) appears naturally when the semigroup's zero matches the (algebra) field's zero. As we will see in the next section, this is the way Maurer-Cartan form power-series

expanded algebras fit within the present scheme. It is also possible to extract other reduced algebras from $\mathfrak{G}$; as will be analyzed in Sec. VI, the 0_S-reduced algebra turns out to be a particular case of Theorem 6.1.

B. Maurer-Cartan form power-series algebra expansion as an *S*-expansion

The Maurer-Cartan form power-series algebra expansion method is a powerful procedure which can lead, in stark contrast with contraction, deformation, and extension of algebras, to algebras of a dimension higher than the original one. In a nutshell, the idea consists of looking at the algebra $\mathfrak{g}$ as described by the associated Maurer-Cartan forms on the group manifold and, after rescaling some of the group parameters by a factor λ, in expanding the Maurer-Cartan forms as a power series in λ. Finally this series is truncated in a way that assures the closure of the algebra. The subject is thoroughly treated by de Azcárraga and Izquierdo in Ref. 20 and de Azcárraga *et al.* in Ref. 1.

Theorem 1 of Ref. 1 shows that, in the more general case, the expanded Lie algebra has the structure constants

$$C_{(A,i)(B,j)}{}^{(C,k)} = \begin{cases} 0 & \text{when } i+j \neq k \\ C_{AB}{}^{C} & \text{when } i+j=k, \end{cases} \tag{24}$$

where the parameters $i,j,k=0,\ldots,N$ correspond to the order of the expansion and N is the truncation order.

These structure constants can also be obtained within the S-expansion procedure. In order to show this, one must consider the 0_S-reduction of an S-expanded algebra where S corresponds to the semigroup defined below.

Definition 3.4: *Let us define* $S_{\mathrm{E}}^{(N)}$ *as the semigroup of elements*

$$S_{\mathrm{E}}^{(N)} = \{\lambda_\alpha, \alpha = 0, \ldots, N+1\}, \tag{25}$$

provided with the multiplication rule

$$\lambda_\alpha \lambda_\beta = \lambda_{H_{N+1}(\alpha+\beta)}, \tag{26}$$

where H_{N+1} *is defined as the function*

$$H_n(x) = \begin{cases} x & \textit{when } x < n \\ n & \textit{when } x \geqslant n. \end{cases} \tag{27}$$

The two-selectors for $S_{\mathrm{E}}^{(N)}$ *read*

$$K_{\alpha\beta}{}^{\gamma} = \delta^{\gamma}_{H_{N+1}(\alpha+\beta)}, \tag{28}$$

where δ^{ρ}_{σ} *is the Kronecker delta. From Eq. (26), we have that* λ_{N+1} *is the zero element in* $S_{\mathrm{E}}^{(N)}$, *i.e.*, $\lambda_{N+1}=0_S$.

Using Eq. (11), the structure constants for the $S_{\mathrm{E}}^{(N)}$-expanded algebra can be written as

$$C_{(A,\alpha)(B,\beta)}{}^{(C,\gamma)} = \delta^{\gamma}_{H_{N+1}(\alpha+\beta)} C_{AB}{}^{C}, \tag{29}$$

with $\alpha,\beta,\gamma=0,\ldots,N+1$. When the extra condition $\lambda_{N+1}\boldsymbol{T}_A=0$ is imposed, Eq. (29) reduces to

$$C_{(A,i)(B,j)}{}^{(C,k)} = \delta^{k}_{i+j} C_{AB}{}^{C}, \tag{30}$$

which exactly matches the structure constants in Eq. (24).

The above arguments show that the Maurer-Cartan form power-series expansion of an algebra $\mathfrak{g}$, with truncation order N, coincides with the 0_S-reduction of the $S_{\mathrm{E}}^{(N)}$-expanded algebra $\mathfrak{G}^{(\mathrm{E})} = S_E^{(N)} \times \mathfrak{g}$.

This is of course no coincidence. The set of powers of the rescaling parameter λ, together with the truncation at order N, satisfies precisely the multiplication law of $S_{\mathrm{E}}^{(N)}$. As a matter of fact, we have

$$\lambda^{\alpha}\lambda^{\beta}=\lambda^{\alpha+\beta}, \tag{31}$$

and the truncation can be imposed as

$$\lambda^{\alpha}=0 \quad \text{when } \alpha>N. \tag{32}$$

It is for this reason that one must demand ${}_0S\boldsymbol{T}_A=0$ in order to obtain the Maurer-Cartan (MC) expansion as an S_{E}-expansion: in this case the zero of the semigroup is the zero of the field as well.

The S-expansion procedure is valid no matter what the structure of the original Lie algebra $\mathfrak{g}$ is, and in this sense it is very general. However, when something about the structure of $\mathfrak{g}$ is known, a lot more can be done. As an example, in the context of MC expansion, the rescaling and truncation can be performed in several ways depending on the structure of $\mathfrak{g}$, leading to several kinds of expanded algebras. Important examples of this are the generalized İnönü-Wigner contraction, or the M algebra as an expansion of $\mathfrak{osp}(32|1)$ (see Refs. 1 and 21). This is also the case in the context of S expansions. As we will show in the next section, when some information about the structure of $\mathfrak{g}$ is available, it is possible to find subalgebras of $\mathfrak{G}=S\times\mathfrak{g}$ and other kinds of reduced algebras. In this way, all the algebras obtained by the MC expansion procedure can be reobtained. New kinds of S-expanded algebras can also be obtained by considering semigroups different from S_{E}.

IV. *S*-EXPANSION SUBALGEBRAS

An S-expanded algebra has a fairly simple structure. In a way, it reproduces the original algebra $\mathfrak{g}$ in a series of "levels" corresponding to the semigroup elements. Interestingly enough, there are at least two ways of extracting smaller algebras from $S\times\mathfrak{g}$. The first one, described in this section, gives rise to a "resonant subalgebra," while the second, described in Sec. VI, produces reduced algebras (in the sense of Definition 2.3).

A. Resonant subalgebras for an arbitrary semigroup *S*

The general problem of finding subalgebras from an S-expanded algebra is a nontrivial one, which is met and solved (in a particular setting) in this section (see Theorem 4.2 below). In order to provide a solution, one must have some information on the subspace structure of $\mathfrak{g}$. This information is encoded in the following way.

Let $\mathfrak{g}=\bigoplus_{p\in I}V_p$ be a decomposition of $\mathfrak{g}$ in subspaces V_p, where I is a set of indices. For each $p,q\in I$ it is always possible to define $i_{(p,q)}\subset I$ such that

$$[V_p,V_q]\subset\bigoplus_{r\in i_{(p,q)}}V_r. \tag{33}$$

In this way, the subsets $i_{(p,q)}$ store the information on the subspace structure of $\mathfrak{g}$.

As for the Abelian semigroup S, this can always be decomposed as $S=\bigcup_{p\in I}S_p$, where $S_p\subset S$. In principle, this decomposition is completely arbitrary; however, using the product from Definition 2.2, it is sometimes possible to pick up a very particular choice of subset decomposition. This choice is the subject of the following

Definition 4.1: *Let $\mathfrak{g}=\bigoplus_{p\in I}V_p$ be a decomposition of $\mathfrak{g}$ in subspaces, with a structure described by the subsets $i_{(p,q)}$, as in Eq. (33). Let $S=\bigcup_{p\in I}S_p$ be a subset decomposition of the Abelian semigroup S such that*

$$S_p \cdot S_q \subset \bigcap_{r \in i_{(p,q)}} S_r, \tag{34}$$

where the subset product · is the one from Definition 2.2. When such subset decomposition $S = \bigcup_{p \in I} S_p$ *exists, then we say that this decomposition is in resonance with the subspace decomposition of* $\mathfrak{g}$, $\mathfrak{g} = \bigoplus_{p \in I} V_p$.

The resonant subset decomposition is crucial in order to systematically extract subalgebras from the S-expanded algebra $\mathfrak{G} = S \times \mathfrak{g}$, as is proven in the following

Theorem 4.2: *Let* $\mathfrak{g} = \bigoplus_{p \in I} V_p$ *be a subspace decomposition of* $\mathfrak{g}$, *with a structure described by Eq. (33), and let* $S = \bigcup_{p \in I} S_p$ *be a resonant subset decomposition of the Abelian semigroup* S, *with the structure given in Eq. (34). Define the subspaces of* $\mathfrak{G} = S \times \mathfrak{g}$,

$$W_p = S_p \times V_p, \quad p \in I. \tag{35}$$

Then,

$$\mathfrak{G}_R = \bigoplus_{p \in I} W_p \tag{36}$$

is a subalgebra of $\mathfrak{G} = S \times \mathfrak{g}$.

Proof: Using Eqs. (33) and (34), we have

$$[W_p, W_q] \subset (S_p \cdot S_q) \times [V_p, V_q] \subset \bigcap_{s \in i_{(p,q)}} S_s \times \bigoplus_{r \in i_{(p,q)}} V_r \subset \bigoplus_{r \in i_{(p,q)}} \left[\bigcap_{s \in i_{(p,q)}} S_s \right] \times V_r. \tag{37}$$

Now, it is clear that for each $r \in i_{(p,q)}$, one can write

$$\bigcap_{s \in i_{(p,q)}} S_s \subset S_r. \tag{38}$$

Then,

$$[W_p, W_q] \subset \bigoplus_{r \in i_{(p,q)}} S_r \times V_r \tag{39}$$

and we arrive at

$$[W_p, W_q] \subset \bigoplus_{r \in i_{(p,q)}} W_r. \tag{40}$$

Therefore, the algebra closes and $\mathfrak{G}_R = \bigoplus_{p \in I} W_p$ is a subalgebra of $\mathfrak{G}$. ■

Definition 4.3: *The algebra* $\mathfrak{G}_R = \bigoplus_{p \in I} W_p$ *obtained in Theorem 4.2 is called a resonant subalgebra of the S-expanded algebra* $\mathfrak{G} = S \times \mathfrak{g}$.

The choice of the name resonance is due to the formal similarity between Eqs. (33) and (34); Eq. (34) will be also referred to as the "*resonance condition.*"

Theorem 4.2 translates the difficult problem of finding subalgebras from an S-expanded algebra $\mathfrak{G} = S \times \mathfrak{g}$ into that of finding a resonant partition for the semigroup S. As the examples from Sec. V help make clear, solving the resonance condition in Eq. (34) turns out to be an easily tractable problem. Theorem 4.2 can thus be regarded as a useful tool for extracting subalgebras from an S-expanded algebra.

Using Eq. (11) and the resonant subset partition of S it is possible to find an explicit expression for the structure constants of the resonant subalgebra $\mathfrak{G}_R$. Denoting the basis of V_p by $\{\boldsymbol{T}_{a_p}\}$, one can write

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = K_{\alpha_p\beta_q}{}^{\gamma_r} C_{a_p b_q}{}^{c_r} \quad \text{with } \alpha_p,\beta_q,\gamma_r \quad \text{such that } \lambda_{\alpha_p} \in S_p, \lambda_{\beta_q} \in S_q, \lambda_{\gamma_r} \in S_r. \tag{41}$$

An interesting fact is that the S-expanded algebra "subspace structure" encoded in $i_{(p,q)}$ is the same as in the original algebra $\mathfrak{g}$, as can be observed from Eq. (40).

Resonant subalgebras play a central role in the current scheme. It is interesting to notice that most of the cases considered in Ref. 1 can be reobtained using the above theorem for $S=S_E$ [recall Eqs. (25) and (26)], as we will see in the next section. All remaining cases can be obtained as a reduction of a resonant subalgebra (see Sec. VI).

B. $S=S_E$ resonant subalgebras and Maurer-Cartan expanded algebras

In this section, some results presented for algebra expansions in Ref. 1 are recovered within the S-expansion approach. To get these algebras one must proceed in a three-step fashion:

1. Perform an S-expansion using the semigroup $S=S_E$.
2. Find a resonant partition for S_E and construct the resonant subalgebra $\mathfrak{G}_R$.
3. Apply a 0_S-reduction (or a more general one, See Sec. VI) to the resonant subalgebra.

Choosing a different semigroup S or omitting the reduction procedure one finds algebras not contained within the MC form power-series expansion of Ref. 1. Such an example is provided in Sec. V C.

1. Case when $\mathfrak{g}=V_0\oplus V_1$, with V_0 being a subalgebra and V_1 a symmetric coset

Let $\mathfrak{g}=V_0\oplus V_1$ be a subspace decomposition of $\mathfrak{g}$, such that

$$[V_0,V_0]\subset V_0, \tag{42}$$

$$[V_0,V_1]\subset V_1, \tag{43}$$

$$[V_1,V_1]\subset V_0. \tag{44}$$

Let $S_E^{(N)}=S_0\cup S_1$, with N arbitrary, be a subset decomposition of S_E, with[2]

$$S_0=\left\{\lambda_{2m} \quad \text{with } m=0,\ldots,\left[\frac{N}{2}\right]\right\}\cup\{\lambda_{N+1}\}, \tag{45}$$

$$S_1=\left\{\lambda_{2m+1} \quad \text{with } m=0,\ldots,\left[\frac{N-1}{2}\right]\right\}\cup\{\lambda_{N+1}\}. \tag{46}$$

This subset decomposition of $S_E^{(N)}$ satisfies the resonance condition in Eq. (34), which in this case explicitly reads

$$S_0\cdot S_0\subset S_0, \tag{47}$$

$$S_0\cdot S_1\subset S_1, \tag{48}$$

$$S_1\cdot S_1\subset S_0. \tag{49}$$

Therefore, according to Theorem 4.2, we have that

[2]Here $[x]$ denotes the integer part of x.

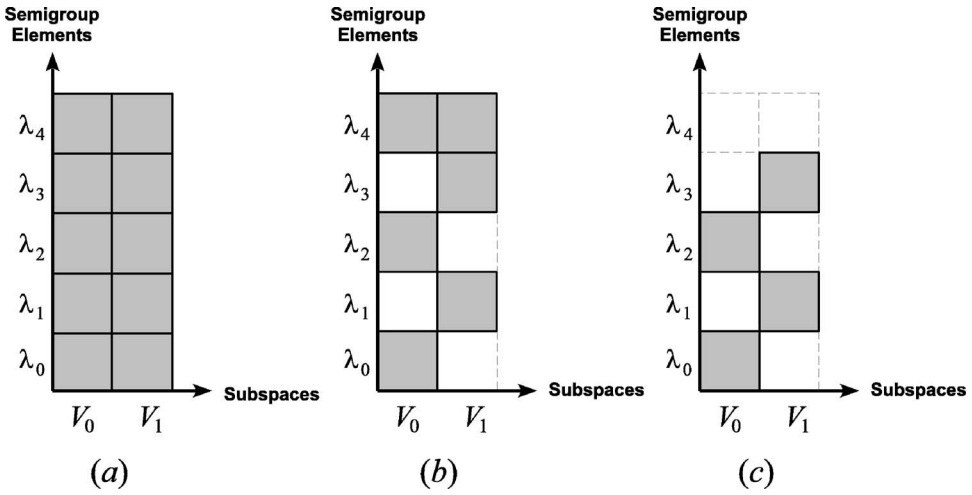

FIG. 1. $S_{\mathrm{E}}^{(3)}$-expansion of an algebra $\mathfrak{g}=V_0\oplus V_1$, where V_0 is a subalgebra and V_1 a symmetric coset. (a) The gray region corresponds to the full $S_{\mathrm{E}}^{(3)}$-expanded algebra, $\mathfrak{G}=S_{\mathrm{E}}^{(3)}\times\mathfrak{g}$. (b) The shaded area here depicts a resonant subalgebra $\mathfrak{G}_{\mathrm{R}}$. (c) The gray region now shows the 0_S-reduction of the resonant subalgebra $\mathfrak{G}_{\mathrm{R}}$.

$$\mathfrak{G}_{\mathrm{R}} = W_0 \oplus W_1, \tag{50}$$

with

$$W_0 = S_0 \times V_0, \tag{51}$$

$$W_1 = S_1 \times V_1, \tag{52}$$

is a resonant subalgebra of $\mathfrak{G}$.

Using Eq. (41), it is straightforward to write the structure constants for the resonant subalgebra,

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = \delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)} C_{a_p b_q}{}^{c_r} \quad \text{with} \quad \begin{cases} p,q=0,1 \\ \alpha_p,\beta_p,\gamma_p = 2m+p, \\ m=0,\ldots,[(N-p)/2],(N+1-p)/2. \end{cases}$$

Imposing $\lambda_{N+1}\boldsymbol{T}_A=0$, the 0_S-reduced structure constants are obtained as

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = \delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)} C_{a_p b_q}{}^{c_r} \quad \text{with} \quad \begin{cases} p,q=0,1 \\ \alpha_p,\beta_p,\gamma_p = 2m+p \\ m=0,\ldots,[(N-p)/2]. \end{cases} \tag{53}$$

In order to compare with the MC expansion, let us observe that, with the notation of Ref. 1, the 0_S-reduction of the S_{E}-expanded algebra corresponds to $\mathcal{G}\ (N_0,N_1)$ for the symmetric coset case, with

$$N_0 = 2\left[\frac{N}{2}\right], \tag{54}$$

$$N_1 = 2\left[\frac{N-1}{2}\right] + 1. \tag{55}$$

The structure constants in Eq. (53) correspond to the structure constants [Eq. (3.31)] from Ref. 1 (the notation is slightly different though).

A more intuitive idea of the whole procedure of S expansion, resonant subalgebra, and 0_S-reduction can be obtained by means of a diagram, such as the one depicted in Fig. 1. This diagram corresponds to the case $\mathfrak{g}=V_0\oplus V_1$, with V_0 a subalgebra and V_1 a symmetric coset, and the choice $S=S_{\mathrm{E}}^{(3)}$.

The subspaces of $\mathfrak{g}$ are represented on the horizontal axis, while the semigroup elements occupy the vertical one. In this way, the whole $S_{\mathrm{E}}^{(3)}$-expanded algebra $S_{\mathrm{E}}^{(3)}\times\mathfrak{g}$ corresponds to the shaded region in Fig. 1(a). In Fig. 1(b), the gray region represents the resonant subalgebra $\mathfrak{G}_{\mathrm{R}}=W_0\oplus W_1$ with

$$S_0=\{\lambda_0,\lambda_2,\lambda_4\}, \tag{56}$$

$$S_1=\{\lambda_1,\lambda_3,\lambda_4\}. \tag{57}$$

Let us observe that each column in the diagram corresponds to a subset of the resonant partition. Finally, Fig. 1(c) represents the 0_S-reduced algebra, obtained after imposing $\lambda_4\times\mathfrak{g}=0$. This figure actually corresponds to the case $\mathcal{G}(N_0,N_1)$.

As is evident from the above discussion, the case $N=1$, $\lambda_{N+1}\boldsymbol{T}_A=0$ reproduces the İnönü-Wigner contraction for $\mathfrak{g}=V_0\oplus V_1$. More on generalized İnönü-Wigner contractions is presented in Sec. VI.

2. Case when $\mathfrak{g}$ fulfills the Weimar-Woods conditions

Let $\mathfrak{g}=\bigoplus_{p=0}^{n}V_p$ be a subspace decomposition of $\mathfrak{g}$. In terms of this decomposition, the Weimar-Woods conditions[15,16] on $\mathfrak{g}$ read

$$[V_p,V_q]\subset\bigoplus_{r=0}^{H_n(p+q)}V_r. \tag{58}$$

Let

$$S_{\mathrm{E}}=\bigcup_{p=0}^{n}S_p \tag{59}$$

be a subset decomposition of S_{E}, where the subsets $S_p\subset S_{\mathrm{E}}$ are defined by

$$S_p=\{\lambda_{\alpha_p}\quad\text{such that }\alpha_p=p,\ldots,N+1\}, \tag{60}$$

with $N+1\geqslant n$.

This subset decomposition is a resonant one under the semigroup product in Eq. (26), because it satisfies [compare Eq. (61) with Eq. (58)]

$$S_p\cdot S_q=S_{H_n(p+q)}\subset\bigcap_{r=0}^{H_n(p+q)}S_r. \tag{61}$$

According to Theorem 4.2, the direct sum

$$\mathfrak{G}_{\mathrm{R}}=\bigoplus_{p=0}^{n}W_p, \tag{62}$$

with

$$W_p=S_p\times V_p,$$

is a resonant subalgebra of $\mathfrak{G}$.

Using Eq. (41), we get the following structure constants for the resonant subalgebra:

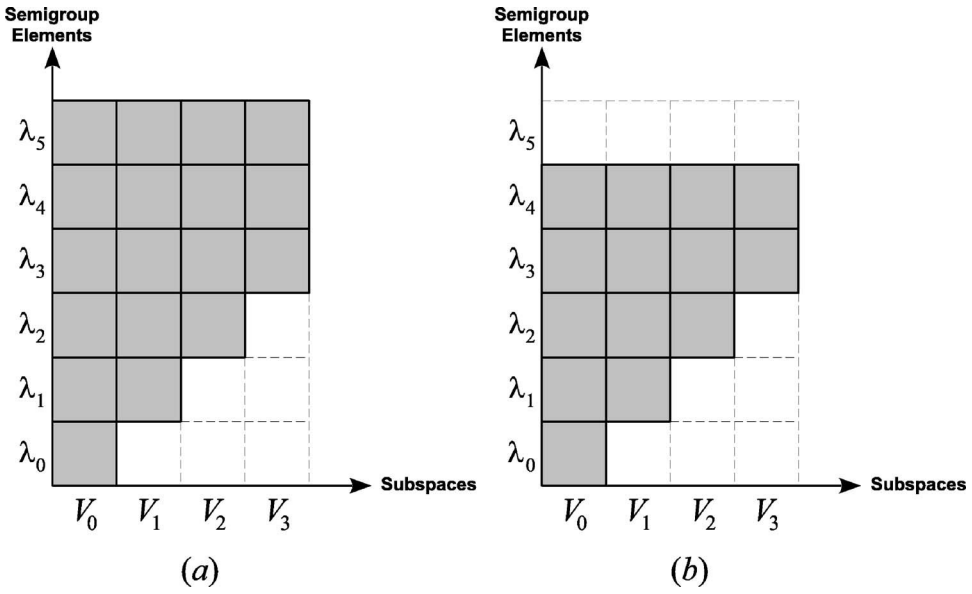

FIG. 2. (a) The shaded region shows a $S_{\mathrm{E}}^{(4)}$ resonant subalgebra when $\mathfrak{g}=V_0\oplus V_1\oplus V_2\oplus V_3$ satisfies the Weimar-Woods conditions. (b) The 0_S-reduction of this resonant subalgebra removes all sectors of the form $0_S\times\mathfrak{g}$. This corresponds to the case $\mathcal{G}(4,4,4,4)$ in the context of Ref. 1.

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)}=\delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)}C_{a_pb_q}{}^{c_r}\quad\text{with}\quad\begin{cases}p,q,r=0,\ldots,n\\ \alpha_p,\beta_p,\gamma_p=p,\ldots,N+1.\end{cases}$$

Imposing $\lambda_{N+1}\boldsymbol{T}_A=0$, this becomes

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)}=\delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)}C_{a_pb_q}{}^{c_r}\quad\text{with}\quad\begin{cases}p,q,r=0,\ldots,n\\ \alpha_p,\beta_p,\gamma_p=p,\ldots,N.\end{cases}\tag{63}$$

This 0_S-reduced algebra corresponds to the case $\mathcal{G}(N_0,\ldots,N_n)$ of Theorem 3 from Ref. 1 with $N_p=N$ for every $p=0,\ldots,n$. The structure constants in Eq. (63) correspond to the ones of Eq. (4.8) in Ref. 1 (with a slightly different notation). The more general case,

$$N_{p+1}=\begin{cases}N_p\ \text{or}\\ N_p+1,\end{cases}$$

can be also obtained in the context of an S expansion, but not as a resonant subalgebra (see Sec. VI and the Appendix).

The resonant subalgebra for the Weimar-Woods case with $n=3$, $N=4$ and its 0_S-reduction are shown in Figs. 2(a) and 2(b), respectively.

3. Case when $\mathfrak{g}=V_0\oplus V_1\oplus V_2$ is a superalgebra

A superalgebra $\mathfrak{g}$ comes naturally split into three subspaces V_0, V_1, and V_2, where V_1 corresponds to the Fermionic sector and $V_0\oplus V_2$ to the Bosonic one, with V_0 being a subalgebra. This subspace structure may be written as

$$[V_0,V_0]\subset V_0,\tag{64}$$

$$[V_0,V_1]\subset V_1,\tag{65}$$

$$[V_0,V_2]\subset V_2,\tag{66}$$

$$[V_1, V_1] \subset V_0 \oplus V_2, \tag{67}$$

$$[V_1, V_2] \subset V_1, \tag{68}$$

$$[V_2, V_2] \subset V_0 \oplus V_2. \tag{69}$$

Let $S_{\mathrm{E}}^{(N)} = S_0 \cup S_1 \cup S_2$ be a subset decomposition of $S_{\mathrm{E}}^{(N)}$, where the subsets S_0, S_1, and S_2 are given by the general expression

$$S_p = \left\{ \lambda_{2m+p} \quad \text{with } m = 0, \ldots, \left[\frac{N-p}{2} \right] \right\} \cup \{\lambda_{N+1}\}, \quad p = 0,1,2. \tag{70}$$

This subset decomposition is a resonant one, because it satisfies [compare Eqs. (71)–(76) with Eqs. (64)–(69)]

$$S_0 \cdot S_0 \subset S_0, \tag{71}$$

$$S_0 \cdot S_1 \subset S_1, \tag{72}$$

$$S_0 \cdot S_2 \subset S_2, \tag{73}$$

$$S_1 \cdot S_1 \subset S_0 \cap S_2, \tag{74}$$

$$S_1 \cdot S_2 \subset S_1, \tag{75}$$

$$S_2 \cdot S_2 \subset S_0 \cap S_2. \tag{76}$$

Theorem 4.2 assures us that $\mathfrak{G}_{\mathrm{R}} = W_0 \oplus W_1 \oplus W_2$, with $W_p = S_p \times V_p$, $p = 0,1,2$, is a resonant subalgebra.

Using Eq. (41), it is possible to write down the structure constants for the resonant subalgebra as

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = \delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)} C_{a_p b_q}{}^{c_r} \quad \text{with} \quad \begin{cases} p,q,r = 0,1,2, \\ \alpha_p, \beta_p, \gamma_p = 2m + p, \\ m = 0, \ldots, [(N-p)/2], (N+1-p)/2. \end{cases} \tag{77}$$

Imposing $\lambda_{N+1} \boldsymbol{T}_A = 0$, the structure constants for the 0_S-reduction of the resonant subalgebra are obtained:

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = \delta^{\gamma_r}_{H_{N+1}(\alpha_p+\beta_q)} C_{a_p b_q}{}^{c_r} \quad \text{with} \quad \begin{cases} p,q,r = 0,1,2, \\ \alpha_p, \beta_p, \gamma_p = 2m + p, \\ m = 0, \ldots, [(N-p)/2]. \end{cases} \tag{78}$$

This 0_S-reduced algebra corresponds to the algebra $\mathcal{G}(N_0, N_1, N_2)$ with

$$N_p = 2\left[\frac{N-p}{2} \right] + p, \quad p = 0,1,2,$$

found in Theorem 5 of Ref. 1. The structure constants in Eq. (78) match the structure constants in Eq. (5.6) from Ref. 1.

Figure 3(a) shows the resonant subalgebra for the case of superalgebras, and Fig. 3(b) its corresponding 0_S-reduction, for the case $N=4$.

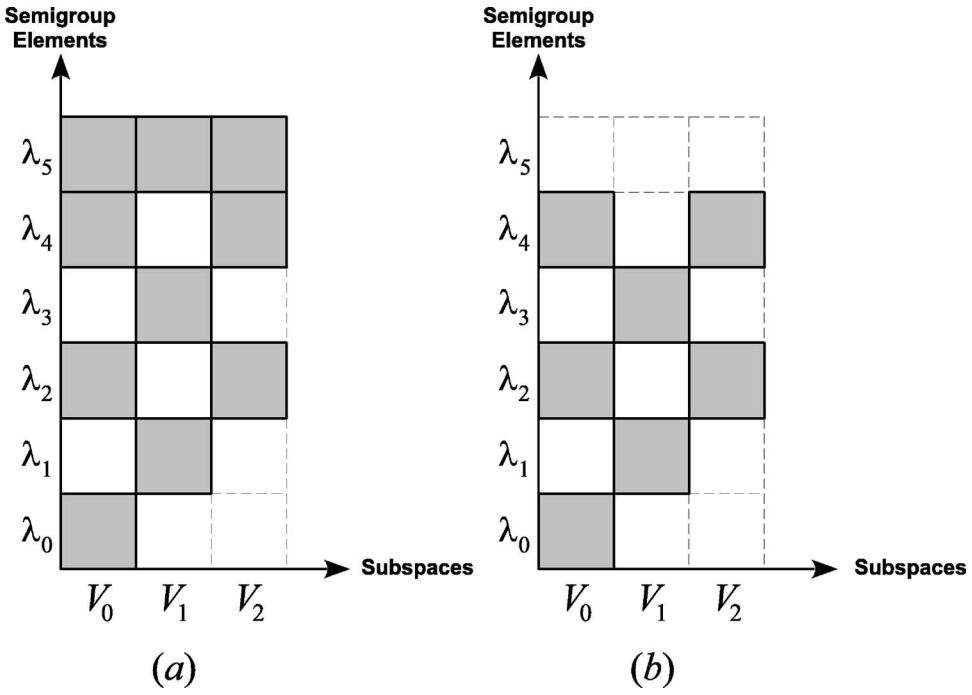

FIG. 3. (a) The shaded area corresponds to an $S_{\mathrm{E}}^{(4)}$ resonant subalgebra of $\mathfrak{G}=S_{\mathrm{E}}^{(4)}\times\mathfrak{g}$ when $\mathfrak{g}$ is a superalgebra. (b) The gray region shows the 0_S-reduction of the resonant subalgebra $\mathfrak{G}_{\mathrm{R}}$. This corresponds to $\mathcal{G}(4,3,4)$ in the context of Ref. 1.

V. *S*-EXPANSIONS OF $\mathfrak{osp}(32|1)$ AND $d=11$ SUPERALGEBRAS

In this section we explore some explicit examples of *S*-expansions. In general, every possible choice of Abelian semigroup *S* and resonant partition will lead to a new $d=11$ superalgebra. Note, however, that the existence of a resonant partition is not at all guaranteed for an arbitrary semigroup *S*.

Since our main physical motivation comes from 11-dimensional supergravity, we shall always take the orthosymplectic superalgebra $\mathfrak{osp}(32|1)$ as a starting point. A suitable basis is provided by $\{\boldsymbol{P}_a,\boldsymbol{J}_{ab},\boldsymbol{Z}_{abcde},\boldsymbol{Q}\}$, where $\{\boldsymbol{P}_a,\boldsymbol{J}_{ab}\}$ are the Anti de Sitter (AdS) generators, $\boldsymbol{Z}_{abcde}$ is a five-index antisymmetric tensor, and $\boldsymbol{Q}$ is a 32-component, Majorana spinor charge. The $\mathfrak{osp}(32|1)$ (anti-)commutation relations explicitly read

$$[\boldsymbol{P}_a,\boldsymbol{P}_b]=\boldsymbol{J}_{ab}, \tag{79}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{P}_c]=\delta^{ab}_{ec}\boldsymbol{P}^e, \tag{80}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{J}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{J}^e{}_f, \tag{81}$$

$$[\boldsymbol{P}_a,\boldsymbol{Z}_{b_1\cdots b_5}]=-\frac{1}{5!}\varepsilon_{ab_1\cdots b_5c_1\cdots c_5}\boldsymbol{Z}^{c_1\cdots c_5}, \tag{82}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{Z}_{c_1\cdots c_5}]=\frac{1}{4!}\delta^{abe_1\cdots e_4}_{dc_1\cdots c_5}\boldsymbol{Z}^d{}_{e_1\cdots e_4}, \tag{83}$$

$$[\boldsymbol{Z}^{a_1\cdots a_5},\boldsymbol{Z}_{b_1\cdots b_5}]=\eta^{[a_1\cdots a_5][c_1\cdots c_5]}\varepsilon_{c_1\cdots c_5b_1\cdots b_5e}\boldsymbol{P}^e+\delta^{a_1\cdots a_5e}_{db_1\cdots b_5}\boldsymbol{J}^d{}_e$$
$$-\frac{1}{3!3!5!}\varepsilon_{c_1\cdots c_{11}}\delta^{a_1\cdots a_5c_4c_5c_6}_{d_1d_2d_3b_1\cdots b_5}\eta^{[c_1c_2c_3][d_1d_2d_3]}\boldsymbol{Z}^{c_7\cdots c_{11}}, \tag{84}$$

$$[\boldsymbol{P}_a,\boldsymbol{Q}]=-\frac{1}{2}\Gamma_a\boldsymbol{Q}, \tag{85}$$

$$[\boldsymbol{J}_{ab},\boldsymbol{Q}]=-\frac{1}{2}\Gamma_{ab}\boldsymbol{Q}, \tag{86}$$

$$[\boldsymbol{Z}_{abcde},\boldsymbol{Q}]=-\frac{1}{2}\Gamma_{abcde}\boldsymbol{Q}, \tag{87}$$

$$\{\boldsymbol{Q}^\rho,\boldsymbol{Q}^\sigma\}=-\frac{1}{2^3}\left[(\Gamma^aC^{-1})^{\rho\sigma}\boldsymbol{P}_a-\frac{1}{2}(\Gamma^{ab}C^{-1})^{\rho\sigma}\boldsymbol{J}_{ab}+\frac{1}{5!}(\Gamma^{abcde}C^{-1})^{\rho\sigma}\boldsymbol{Z}_{abcde}\right], \tag{88}$$

where $C_{\rho\sigma}$ is the charge conjugation matrix and Γ_a are Dirac matrices in 11 dimensions.

As a first step towards the S-expansion, the $\mathfrak{osp}(32|1)$ algebra is written as the direct sum of three subspaces:

$$\mathfrak{osp}(32|1)=V_0\oplus V_1\oplus V_2, \tag{89}$$

where V_0 corresponds to the Lorentz subalgebra (spanned by $\boldsymbol{J}_{ab}$), V_1 to the Fermionic subspace (spanned by $\boldsymbol{Q}$), and V_2 to the translations and the M5-brane piece (spanned by $\boldsymbol{P}_a$ and $\boldsymbol{Z}_{abcde}$). The subspace separation [Eq. (89)] satisfies conditions (64)–(69), as can be easily checked.

The M algebra[3–5] and a superalgebra similar to those of D'Auria-Fré[17] are rederived in the next sections using $S=S_{\mathrm{E}}^{(N)}$ with $N=2$ and $N=3$, respectively. As an example of an S-expansion with $S\neq S_{\mathrm{E}}$, the case $S=\mathbb{Z}_4$ is considered in Sec. V C, where a new superalgebra resembling aspects of the M algebra, $\mathfrak{osp}(32|1)\times\mathfrak{osp}(32|1)$, and D'Auria-Fré superalgebras is found.

The inclusion of the M algebra among the examples draws from two different but related facts. First, the S expansion paradigm casts the M algebra as one from a family of superalgebras, all derived from $\mathfrak{osp}(32|1)$ through different choices for the semigroup and different alternatives of reduction, when present at all. This can be relevant from a physical point of view, since all of them share important features. The second reason deals with the construction of Chern-Simons and transgression Lagrangians. As will be shown in Sec. VII, invariant tensors for resonant subalgebras and 0_S-reduced algebras thereof are readily available, but this is not the case for general reduced algebras. As such, the fact that the M algebra stems from a 0_S-reduction is interesting not only because it provides an invariant tensor derived from $\mathfrak{osp}(32|1)$ but also because it brings about the possibility of considering its direct generalization, namely, the resonant subalgebra from where it was extracted. More on the physical consequences of regarding the M algebra as the 0_S-reduction of a resonant subalgebra is found in Ref. 14.

A. The M algebra

As treated in detail in Refs. 1 and 21, the complete M algebra (i.e., including its Lorentz part) can be obtained by means of a MC expansion of $\mathfrak{osp}(32|1)$. Within the present scheme, the M algebra should be recovered via an S expansion with $S=S_{\mathrm{E}}^{(2)}$ followed by a 0_S-reduction, as explained in Sec. III B.

In order to obtain the M algebra in the context of S-expansions, one has to pick $S_{\mathrm{E}}^{(2)}=\{\lambda_0,\lambda_1,\lambda_2,\lambda_3\}$, use the resonant partition [Eq. (70)], and impose the condition $\lambda_3\boldsymbol{T}_A=0$. This

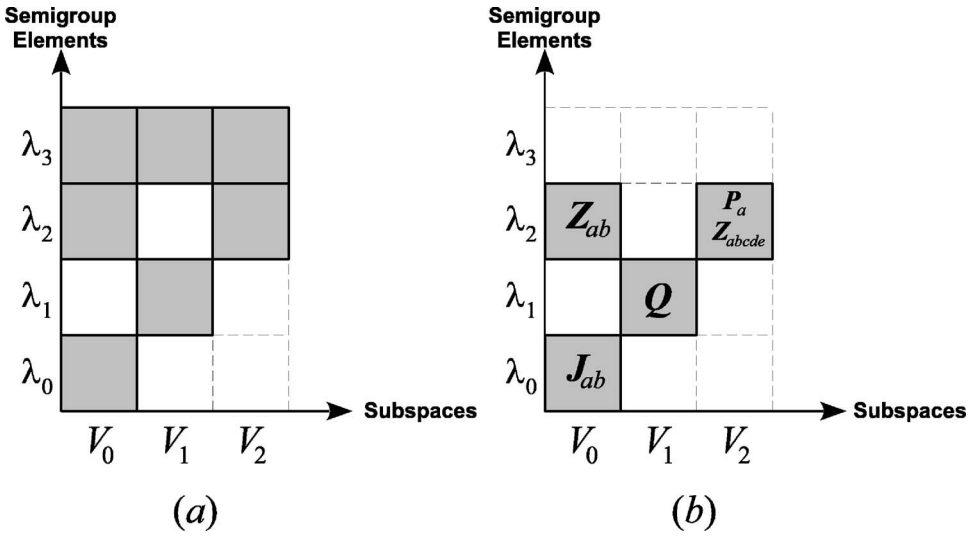

FIG. 4. The M algebra as an $S_E^{(2)}$-expansion of $\mathfrak{osp}(32|1)$. (a) A resonant subalgebra of the $S_E^{(2)}$-expanded algebra $\mathfrak{G}=S_E^{(2)}\times\mathfrak{osp}(32|1)$ is shown in the shaded region. (b) The M algebra itself (gray area) is obtained after 0_S-reducing the resonant subalgebra.

amounts to explicitly writing the structure constants in Eq. (78) for this case. For the sake of simplicity, let us relabel $\boldsymbol{J}_{ab}=\boldsymbol{J}_{(ab,0)}$, $\boldsymbol{Q}_{\alpha}=\boldsymbol{Q}_{(\alpha,1)}$, $\boldsymbol{Z}_{ab}=\boldsymbol{J}_{(ab,2)}$, $\boldsymbol{P}_a=\boldsymbol{P}_{(a,2)}$, $\boldsymbol{Z}_{abcde}=\boldsymbol{Z}_{(abcde,2)}$, as shown in Fig. 4. The resulting algebra reads

$$[\boldsymbol{P}_a,\boldsymbol{P}_b]=0, \tag{90}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{P}_c]=\delta^{ab}_{ec}\boldsymbol{P}^e, \tag{91}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{J}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{J}^e{}_f, \tag{92}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{Z}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{Z}^e{}_f, \tag{93}$$

$$[\boldsymbol{Z}^{ab},\boldsymbol{Z}_{cd}]=0, \tag{94}$$

$$[\boldsymbol{P}_a,\boldsymbol{Z}_{b_1\cdots b_5}]=0, \tag{95}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{Z}_{c_1\cdots c_5}]=\frac{1}{4!}\delta^{abe_1\cdots e_4}_{dc_1\cdots c_5}\boldsymbol{Z}^d{}_{e_1\cdots e_4}, \tag{96}$$

$$[\boldsymbol{Z}^{ab},\boldsymbol{Z}_{c_1\cdots c_5}]=0, \tag{97}$$

$$[\boldsymbol{Z}^{a_1\cdots a_5},\boldsymbol{Z}_{b_1\cdots b_5}]=0, \tag{98}$$

$$[\boldsymbol{P}_a,\boldsymbol{Q}]=0, \tag{99}$$

$$[\boldsymbol{J}_{ab},\boldsymbol{Q}]=-\frac{1}{2}\Gamma_{ab}\boldsymbol{Q}, \tag{100}$$

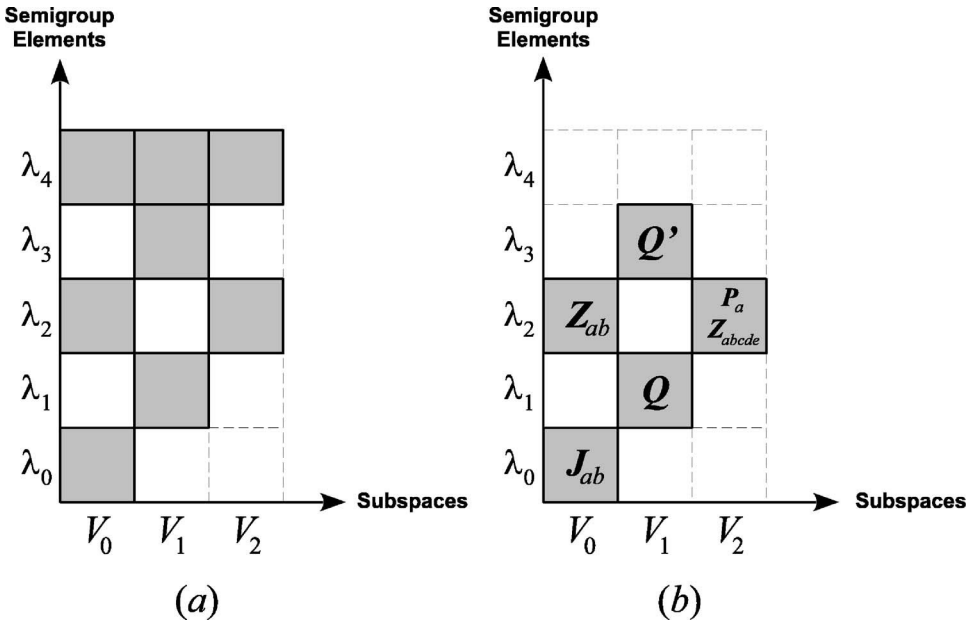

FIG. 5. A D'Auria-Fré-like superalgebra regarded here as an $S_{\mathrm{E}}^{(3)}$-expansion of $\mathfrak{osp}(32|1)$. (a) A resonant subalgebra of the $S_{\mathrm{E}}^{(3)}$-expanded algebra $\mathfrak{G}=S_{\mathrm{E}}^{(3)}\times\mathfrak{osp}(32|1)$ is shown in the shaded region. (b) A superalgebra similar to the ones introduced by D'Auria and Fré in Ref. 17 is obtained after 0_S-reducing the resonant subalgebra.

$$[\boldsymbol{Z}_{ab},\boldsymbol{Q}]=0, \tag{101}$$

$$[\boldsymbol{Z}_{abcde},\boldsymbol{Q}]=0, \tag{102}$$

$$\{\boldsymbol{Q}^{\rho},\boldsymbol{Q}^{\sigma}\}=-\frac{1}{2^3}\left[(\Gamma^{a}C^{-1})^{\rho\sigma}\boldsymbol{P}_a-\frac{1}{2}(\Gamma^{ab}C^{-1})^{\rho\sigma}\boldsymbol{Z}_{ab}+\frac{1}{5!}(\Gamma^{abcde}C^{-1})^{\rho\sigma}\boldsymbol{Z}_{abcde}\right]. \tag{103}$$

Note that the role of the 0_S-reduction in the process is that of Abelianizing large sectors of the resonant subalgebra.

B. D'Auria-Fré-like superalgebra

The above example used $S_{\mathrm{E}}^{(2)}=\{\lambda_0,\lambda_1,\lambda_2,\lambda_3\}$ as Abelian semigroup to perform the expansion. In this section, the results of choosing instead $S_{\mathrm{E}}^{(3)}=\{\lambda_0,\lambda_1,\lambda_2,\lambda_3,\lambda_4\}$ while leaving everything else (including the 0_S-reduction) unchanged are examined.

A D'Auria-Fré-like superalgebra,[17] with one extra Fermionic generator as compared with $\mathfrak{osp}(32|1)$ or the M algebra, is obtained by picking the resonant partition [Eq. (70)] and 0_S-reducing the resulting resonant subalgebra. Relabeling generators as $\boldsymbol{J}_{ab}=\boldsymbol{J}_{(ab,0)}$, $\boldsymbol{Q}_{\alpha}=\boldsymbol{Q}_{(\alpha,1)}$, $\boldsymbol{Z}_{ab}=\boldsymbol{J}_{(ab,2)}$, $\boldsymbol{P}_a=\boldsymbol{P}_{(a,2)}$, $\boldsymbol{Z}_{abcde}=\boldsymbol{Z}_{(abcde,2)}$, $\boldsymbol{Q}'_{\alpha}=\boldsymbol{Q}_{(\alpha,3)}$, one finds the structure depicted in Fig. 5. While this algebra has the same *structure* (i.e., same number and type of generators, with commutators valued on the same subspaces) as the ones introduced by D'Auria and Fré in Ref. 17, the details differ, so it cannot really correspond to any of them (hence the "-like").

The (anti)commutation relations, which can be read off directly from the structure constants in Eq. (78) after applying condition (23), bear a strong similarity with those from the M algebra. Only the following three differ:

$$[\boldsymbol{P}_a,\boldsymbol{Q}]=-\frac{1}{2}\Gamma_a\boldsymbol{Q}', \tag{104}$$

$$[\boldsymbol{Z}_{ab},\boldsymbol{Q}]=-\frac{1}{2}\Gamma_{ab}\boldsymbol{Q}', \tag{105}$$

$$[\boldsymbol{Z}_{abcde},\boldsymbol{Q}]=-\frac{1}{2}\Gamma_{abcde}\boldsymbol{Q}'. \tag{106}$$

The (anti)commutation relations which directly involve the extra Fermionic generator $\boldsymbol{Q}'$ read

$$[\boldsymbol{P}_a,\boldsymbol{Q}']=0, \tag{107}$$

$$[\boldsymbol{Z}_{ab},\boldsymbol{Q}']=0, \tag{108}$$

$$[\boldsymbol{Z}_{abcde},\boldsymbol{Q}']=0, \tag{109}$$

$$\{\boldsymbol{Q},\boldsymbol{Q}'\}=0, \tag{110}$$

$$\{\boldsymbol{Q}',\boldsymbol{Q}'\}=0, \tag{111}$$

$$[\boldsymbol{J}_{ab},\boldsymbol{Q}']=-\frac{1}{2}\Gamma_{ab}\boldsymbol{Q}'. \tag{112}$$

The extra Fermionic generator $\boldsymbol{Q}'$ is found to (anti)commute with all generators from the algebra but the Lorentz generators (which was to be expected due to its spinor character).

C. Resonant subalgebra of $\mathbb{Z}_4\times\mathfrak{osp}(32|1)$

Cyclic groups seem especially suitable for an S expansion, because, on one hand, they are groups and not only semigroups (and therefore there is no 0_S element and no 0_S-reduction), and on the other, because the multiplication law for a cyclic group looks very similar to the multiplication law of the semigroup S_{E},

$$S_{\mathrm{E}}^{(N)}:\lambda_\alpha\lambda_\beta=\lambda_{H_{N+1}(\alpha+\beta)}, \tag{113}$$

$$\mathbb{Z}_N:\lambda_\alpha\lambda_\beta=\lambda_{\mathrm{mod}_N(\alpha+\beta)}. \tag{114}$$

The cyclic group $\mathbb{Z}_4$, in particular, was chosen for this example because the $\mathbb{Z}_2$ case is trivial [the resonant subalgebra is $\mathfrak{osp}(32|1)$ itself] and $\mathbb{Z}_3$ seems to have no resonant partition; therefore $\mathbb{Z}_4$ corresponds to the simplest nontrivial case.

Since this example uses a semigroup different from S_{E}, the algebra obtained does not correspond to a MC form power-series expansion.

Given a superalgebra $\mathfrak{g}=V_0\oplus V_1\oplus V_2$ with the structure of Eqs. (64)–(69), a resonant partition of $\mathbb{Z}_4=\{\lambda_0,\lambda_1,\lambda_2,\lambda_3\}$ is given by

$$S_0=\{\lambda_0,\lambda_2\}, \tag{115}$$

$$S_1=\{\lambda_1,\lambda_3\}, \tag{116}$$

$$S_2=\{\lambda_0,\lambda_2\}. \tag{117}$$

In order to avoid a cluttering of indices, relabel $\boldsymbol{J}_{ab}=\boldsymbol{J}_{(ab,0)}$, $\boldsymbol{Z}'_{a_1\cdots a_5}=\boldsymbol{Z}_{(a_1\cdots a_5,0)}$, $\boldsymbol{P}'_a=\boldsymbol{P}_{(a,0)}$, $\boldsymbol{Q}_\alpha=\boldsymbol{Q}_{(\alpha,1)}$, $\boldsymbol{Z}_{ab}=\boldsymbol{J}_{(ab,2)}$, $\boldsymbol{Z}_{a_1\cdots a_5}=\boldsymbol{Z}_{(a_1\cdots a_5,2)}$, $\boldsymbol{P}_a=\boldsymbol{P}_{(a,2)}$, and $\boldsymbol{Q}'_\alpha=\boldsymbol{Q}_{(\alpha,3)}$, as shown in Fig. 6.

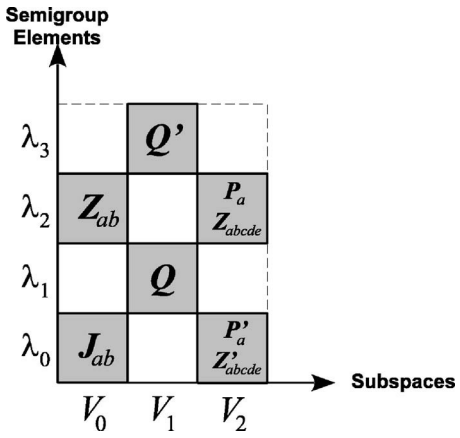

FIG. 6. A new $d=11$ superalgebra, different from but resembling aspects of both the M algebra and the D'Auria-Fré superalgebras, is obtained directly as a resonant subalgebra (shaded region) of the S-expanded Algebra $\mathbb{Z}_4 \times \mathfrak{osp}(32|1)$.

The full resonant subalgebra can be easily obtained using the structure constants in Eq. (41); here we shall only quote some of its more interesting sectors.

This algebra has two very conspicuous features: first, it bears *some* resemblance to the M algebra, for *both* Fermionic generators $\boldsymbol{Q}$ and $\boldsymbol{Q}'$ satisfy

$$\{\boldsymbol{Q}'^{\rho},\boldsymbol{Q}'^{\sigma}\}=\{\boldsymbol{Q}^{\rho},\boldsymbol{Q}^{\sigma}\}=-\frac{1}{2^3}\left[(\Gamma^a C^{-1})^{\rho\sigma}\boldsymbol{P}_a-\frac{1}{2}(\Gamma^{ab}C^{-1})^{\rho\sigma}\boldsymbol{Z}_{ab}+\frac{1}{5!}(\Gamma^{abcde}C^{-1})^{\rho\sigma}\boldsymbol{Z}_{abcde}\right]. \tag{118}$$

Second, the algebra has *two* "AdS-boost generators" for the *same* Lorentz algebra,

$$[\boldsymbol{P}_a,\boldsymbol{P}_b]=\boldsymbol{J}_{ab},\quad [\boldsymbol{P}'_a,\boldsymbol{P}'_b]=\boldsymbol{J}_{ab},$$

$$[\boldsymbol{J}^{ab},\boldsymbol{P}_c]=\delta^{ab}_{ec}\boldsymbol{P}^e,\quad [\boldsymbol{J}^{ab},\boldsymbol{P}'_c]=\delta^{ab}_{ec}\boldsymbol{P}'^e,$$

$$[\boldsymbol{J}^{ab},\boldsymbol{J}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{J}^e{}_f$$

$$[\boldsymbol{P}_a,\boldsymbol{P}'_b]=\boldsymbol{Z}_{ab}. \tag{119}$$

The "charges" $\boldsymbol{Z}_{ab}$, $\boldsymbol{Z}_{a_1\cdots a_5}$, and $\boldsymbol{Z}'_{a_1\cdots a_5}$ are Lorentz tensors, but they are not Abelian,

$$[\boldsymbol{Z}^{ab},\boldsymbol{Z}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{J}^e{}_f, \tag{120}$$

$$[\boldsymbol{Z}^{a_1\cdots a_5},\boldsymbol{Z}_{b_1\cdots b_5}]=[\boldsymbol{Z}'^{a_1\cdots a_5},\boldsymbol{Z}'_{b_1\cdots b_5}]=\eta^{[a_1\cdots a_5][c_1\cdots c_5]}\varepsilon_{c_1\cdots c_5 b_1\cdots b_5 e}\boldsymbol{P}'^e+\delta^{a_1\cdots a_5 e}_{db_1\cdots b_5}\boldsymbol{J}^d{}_e$$
$$-\frac{1}{3!3!5!}\varepsilon_{c_1\cdots c_{11}}\delta^{a_1\cdots a_5 c_4 c_5 c_6}_{d_1 d_2 d_3 b_1\cdots b_5}\eta^{[c_1 c_2 c_3][d_1 d_2 d_3]}\boldsymbol{Z}'^{c_7\cdots c_{11}}. \tag{121}$$

This algebra also presents a behavior similar to that of the D'Auria-Fré superalgebras; namely, the commutators between the generators $\boldsymbol{P}_a,\boldsymbol{Z}_{ab},\boldsymbol{Z}_{a_1\cdots a_5}$ and a Fermionic generator $\boldsymbol{Q}$ are $\boldsymbol{Q}'$ valued; but in contrast to Eqs. (107)–(109), their commutator with $\boldsymbol{Q}'$ is $\boldsymbol{Q}$-valued rather than zero. In this regard, the generators $\boldsymbol{J}_{ab},\boldsymbol{Z}'_{a_1\cdots a_5},\boldsymbol{P}'_a$ have a block-diagonal form on the subspace $(\boldsymbol{Q},\boldsymbol{Q}')$; their commutator with $\boldsymbol{Q}$ is $\boldsymbol{Q}$-valued and the one with $\boldsymbol{Q}'$ is $\boldsymbol{Q}'$-valued.

We have seen several examples showing how, starting from only one original algebra $\mathfrak{g}$ and using different semigroups, different resonant subalgebras can arise (see Theorem 4.2). This is particularly interesting if one considers the strong similarities between the semigroups considered, which nevertheless lead to different resonant structures.

VI. REDUCED ALGEBRAS OF A RESONANT SUBALGEBRA

In previous sections we have seen how information on the subspace structure of the original algebra $\mathfrak{g}$ can be used in order to find resonant subalgebras of the S-expanded algebra $S\times\mathfrak{g}$. In this section we shall examine how this information can be put to use in a different way, namely, by extracting reduced algebras (in the sense of Definition 2.3) from the resonant subalgebra. It is following this path that, e.g., the generalized İnönü-Wigner contraction fits within the present scheme.

The following general theorem provides necessary conditions under which a reduced algebra can be extracted from a resonant subalgebra.

Theorem 6.1: *Let* $\mathfrak{G}_{\mathrm{R}}=\bigoplus_{p\in I}S_p\times V_p$ *be a resonant subalgebra of* $\mathfrak{G}=S\times\mathfrak{g}$, *i.e., let Eqs.* (33) and (34) *be satisfied. Let* $S_p=\hat{S}_p\cup\check{S}_p$ *be a partition of the subsets* $S_p\subset S$ *such that*

$$\hat{S}_p\cap\check{S}_p=\varnothing, \tag{122}$$

$$\check{S}_p\cdot\hat{S}_q\subset\bigcap_{r\in i_{(p,q)}}\hat{S}_r. \tag{123}$$

Conditions (122) *and* (123) *induce the decomposition* $\mathfrak{G}_{\mathrm{R}}=\check{\mathfrak{G}}_{\mathrm{R}}\oplus\hat{\mathfrak{G}}_{\mathrm{R}}$ *on the resonant subalgebra, where*

$$\check{\mathfrak{G}}_{\mathrm{R}}=\bigoplus_{p\in I}\check{S}_p\times V_p, \tag{124}$$

$$\check{\mathfrak{G}}_{\mathrm{R}}=\bigoplus_{p\in I}\hat{S}_p\times V_p. \tag{125}$$

When conditions (122) *and* (123) *hold, then*

$$[\check{\mathfrak{G}}_{\mathrm{R}},\check{\mathfrak{G}}_{\mathrm{R}}]\subset\check{\mathfrak{G}}_{\mathrm{R}}, \tag{126}$$

and therefore $|\check{\mathfrak{G}}_{\mathrm{R}}|$ *corresponds to a reduced algebra of* $\mathfrak{G}_{\mathrm{R}}$.

Proof: *Let* $\check{W}_p=\check{S}_p\times V_p$ and $\hat{W}_p=\hat{S}_p\times V_p$. Then, using condition (123), we have

$$[\check{W}_p,\hat{W}_q]\subset(\check{S}_p\cdot\hat{S}_q)\times[V_p,V_q]\subset\bigcap_{s\in i_{(p,q)}}\hat{S}_s\times\bigoplus_{r\in i_{(p,q)}}V_r\subset\bigoplus_{r\in i_{(p,q)}}\Big[\bigcap_{s\in i_{(p,q)}}\hat{S}_s\Big]\times V_r.$$

For each $r\in i_{(p,q)}$ we have $\bigcap_{s\in i_{(p,q)}}\hat{S}_s\subset\hat{S}_r$, so that

$$[\check{W}_p,\hat{W}_q]\subset\bigoplus_{r\in i_{(p,q)}}\hat{S}_r\times V_r\subset\bigoplus_{r\in i_{(p,q)}}\hat{W}_r.$$

Since $\check{\mathfrak{G}}_{\mathrm{R}}=\bigoplus_{p\in I}\check{W}_p$ and $\hat{\mathfrak{G}}_{\mathrm{R}}=\bigoplus_{p\in I}\hat{W}_p$, we finally find

$$[\check{\mathfrak{G}}_{\mathrm{R}},\check{\mathfrak{G}}_{\mathrm{R}}]\subset\check{\mathfrak{G}}_{\mathrm{R}}$$

and therefore $|\check{\mathfrak{G}}_{\mathrm{R}}|$ is a reduced algebra of $\mathfrak{G}_{\mathrm{R}}$. ■

Using the structure constants in Eq. (41) for the resonant subalgebra, it is possible to find the structure constants for the reduced algebra $|\check{\mathfrak{G}}_{\mathrm{R}}|$,

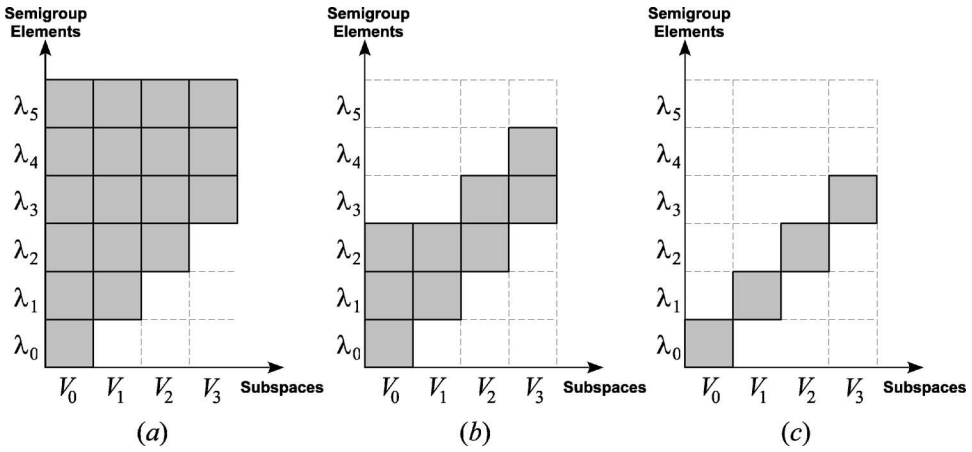

FIG. 7. (a) $S_{\mathrm{E}}^{(4)}$-resonant subalgebra when $\mathfrak{g}=V_0\oplus V_1\oplus V_2\oplus V_3$ satisfies the Weimar-Woods conditions. (b) One possible reduction of the resonant subalgebra from (a), with $N_0=2$, $N_1=2$, $N_2=3$, and $N_3=4$. (c) Generalized İnönü-Wigner contraction corresponding to a different reduction of the same resonant subalgebra, with $N_p=p$, $p=0,1,2,3$.

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}^{\quad(c_r,\gamma_r)}=K_{\alpha_p\beta_q}^{\quad\gamma_r}C_{a_pb_q}^{\quad c_r}\quad\text{with }\alpha_p,\beta_q,\gamma_r\quad\text{such that }\lambda_{\alpha_p}\in\check{S}_p,\lambda_{\beta_q}\in\check{S}_q,\lambda_{\gamma_r}\in\check{S}_r. \tag{127}$$

It might be worth to notice that, when every $S_p\subset S$ of a resonant subalgebra includes the zero element 0_S, the choice $\hat{S}_p=\{0_S\}$ automatically satisfies conditions (122) and (123). As a consequence, the 0_S-reduction introduced in Definition 2.3 can be regarded as a particular case of Theorem 6.1.

A. Reduction of resonant subalgebras, Weimar-Woods conditions, and the İnönü-Wigner contraction

Theorem 6.1 above will be useful in order to recover Theorem 3 from Ref. 1 in this context.

Consider the resonant subalgebra from Sec. IV B 2 and the following S_p partition, which satisfies Eq. (122):

$$\check{S}_p=\{\lambda_{\alpha_p}\text{ such that }\alpha_p=p,\ldots,N_p\}, \tag{128}$$

$$\hat{S}_p=\{\lambda_{\alpha_p}\text{ such that }\alpha_p=N_p+1,\ldots,N+1\}. \tag{129}$$

In the Appendix it is shown that reduction condition Eq. (123) on Eqs. (128) and (129) is equivalent to the following requirement on the N_p's:

$$N_{p+1}=\begin{cases}N_p\text{ or}\\ H_{N+1}(N_p+1).\end{cases} \tag{130}$$

This condition is exactly the one obtained in Theorem 3 of Ref. 1, requiring that the expansion in the MC forms closes. In the S-expansion context the case $N_{p+1}=N_p=N+1$ for each p corresponds to the resonant subalgebra, and the case $N_{p+1}=N_p=N$ to its 0_S-reduction. Figure 7 shows two different reductions for a resonant subalgebra where $\mathfrak{g}$ satisfies the Weimar-Woods conditions.

As stated in Ref. 1, the generalized İnönü-Wigner contraction corresponds to the case $N_p=p$; this means that the generalized İnönü-Wigner contraction *does not* correspond to a resonant subalgebra but to its reduction. This is an important point, because, as we shall see in Sec. VII, we have been able to define nontrace invariant tensors for resonant subalgebras and 0_S-reduced algebras, but not for general reduced algebras.

As an explicit example of the application of Theorem 6.1, the $d=11$ five-brane superalgebra is derived as a reduced algebra in the next section.

B. Five-brane superalgebra as a reduced algebra

Let us recall the resonant subalgebra used in order to get the M algebra in Sec. V A. For this case, the resonant partition $S_{\mathrm{E}}^{(2)}=S_0\cup S_1\cup S_2$ corresponds to the one from Eq. (70) for the case $N=2$, i.e.,

$$S_0=\{\lambda_0,\lambda_2,\lambda_3\}, \tag{131}$$

$$S_1=\{\lambda_1,\lambda_3\}, \tag{132}$$

$$S_2=\{\lambda_2,\lambda_3\}. \tag{133}$$

In order to construct a reduced algebra, perform a partition of the sets S_p themselves, $S_p=\hat{S}_p\cup\check{S}_p$, such as

$$\check{S}_0=\{\lambda_0\},\quad \hat{S}_0=\{\lambda_2,\lambda_3\}, \tag{134}$$

$$\check{S}_1=\{\lambda_1\},\quad \hat{S}_1=\{\lambda_3\}, \tag{135}$$

$$\check{S}_2=\{\lambda_2\},\quad \hat{S}_2=\{\lambda_3\}. \tag{136}$$

It is not hard to see that this partition of S_p satisfies the reduction conditions in Eqs. (122) and (123). For each p, $\hat{S}_p\cap\check{S}_p=\varnothing$, and using the multiplication law in Eq. (26), we have

$$\check{S}_0\cdot\hat{S}_0\subset\hat{S}_0,$$

$$\check{S}_0\cdot\hat{S}_1\subset\hat{S}_1,$$

$$\check{S}_0\cdot\hat{S}_2\subset\hat{S}_2,$$

$$\check{S}_1\cdot\hat{S}_1\subset\hat{S}_0\cap\hat{S}_2,$$

$$\check{S}_1\cdot\hat{S}_2\subset\hat{S}_1,$$

$$\check{S}_2\cdot\hat{S}_2\subset\hat{S}_0\cap\hat{S}_2$$

[compare with Eqs. (71)–(76) and (64)–(69)]. Therefore, we have $\check{\mathfrak{G}}_{\mathrm{R}}=(\check{S}_0\times V_0)\oplus(\check{S}_1\times V_1)\oplus(\check{S}_2\times V_2)$, which is represented in Fig. 8, and the explicit reduced algebra $|\check{\mathfrak{G}}_{\mathrm{R}}|$,

$$[\boldsymbol{P}_a,\boldsymbol{P}_b]=0, \tag{137}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{P}_c]=\delta^{ab}_{ec}\boldsymbol{P}^e, \tag{138}$$

$$[\boldsymbol{J}^{ab},\boldsymbol{J}_{cd}]=\delta^{abf}_{ecd}\boldsymbol{J}^e{}_f, \tag{139}$$

$$[\boldsymbol{P}_a,\boldsymbol{Z}_{b_1\cdots b_5}]=0, \tag{140}$$

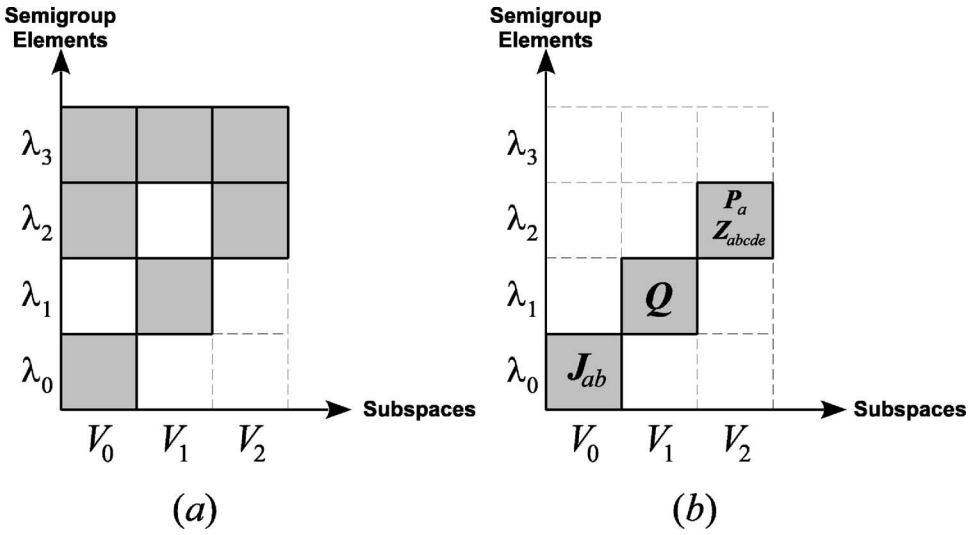

FIG. 8. (a) Resonant subalgebra of the S-expanded Algebra $S_{\mathrm{E}}^{(2)} \times \mathfrak{osp}(32|1)$. (b) One particular reduction of this resonant subalgebra reproduces the five-brane superalgebra.

$$[\boldsymbol{J}^{ab}, \boldsymbol{Z}_{c_1 \cdots c_5}] = \frac{1}{4!} \delta^{abe_1 \cdots e_4}_{dc_1 \cdots c_5} \boldsymbol{Z}^{d}{}_{e_1 \cdots e_4}, \tag{141}$$

$$[\boldsymbol{Z}^{a_1 \cdots a_5}, \boldsymbol{Z}_{b_1 \cdots b_5}] = 0, \tag{142}$$

$$[\boldsymbol{P}_a, \boldsymbol{Q}] = 0, \tag{143}$$

$$[\boldsymbol{J}_{ab}, \boldsymbol{Q}] = -\frac{1}{2} \Gamma_{ab} \boldsymbol{Q}, \tag{144}$$

$$[\boldsymbol{Z}_{abcde}, \boldsymbol{Q}] = 0,$$

$$\{\boldsymbol{Q}^{\rho}, \boldsymbol{Q}^{\sigma}\} = -\frac{1}{2^3} \left[(\Gamma^{a} C^{-1})^{\rho\sigma} \boldsymbol{P}_a + \frac{1}{5!} (\Gamma^{abcde} C^{-1})^{\rho\sigma} \boldsymbol{Z}_{abcde} \right]. \tag{145}$$

This is the five-brane superalgebra.[18,19]

VII. INVARIANT TENSORS FOR *S*-EXPANDED ALGEBRAS

Finding all invariant tensors for an arbitrary algebra remains as an open problem until now. This is not only an important mathematical problem but also a physical one, because an invariant tensor is a key ingredient in the construction of Chern-Simons and transgression forms (see, e.g., Refs. 22–31), which can be used as gauge Lagrangians for a given symmetry group in an arbitrary odd dimension. The choice of invariant tensor shapes the theory to a great extent.

A standard procedure in order to obtain an invariant tensor is to use the (super)trace in some matrix representation of the generators of the algebra. However, this procedure has an important limitation for 0_S-reduced algebras and, for this reason, theorems providing nontrivial invariant tensors for S-expanded algebras are worth considering.

Theorem 7.1: *Let S be an Abelian semigroup, $\mathfrak{g}$ a Lie (super)algebra of basis $\{\mathbf{T}_A\}$, and let $\langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n} \rangle$ be an invariant tensor for $\mathfrak{g}$. Then, the expression*

$$\langle \boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_n,\alpha_n)} \rangle = \alpha_\gamma K_{\alpha_1 \cdots \alpha_n}{}^{\gamma} \langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n} \rangle, \tag{146}$$

where α_γ are arbitrary constants and $K_{\alpha_1 \cdots \alpha_n}{}^{\gamma}$ is the n-selector for S, corresponds to an invariant tensor for the S-expanded algebra $\mathfrak{G}=S\times\mathfrak{g}$.

Proof: The invariance condition for $\langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n} \rangle$ under $\mathfrak{g}$ reads

$$\sum_{p=1}^{n} X^{(p)}_{A_0 \cdots A_n} = 0, \tag{147}$$

where

$$X^{(p)}_{A_0 \cdots A_n} = (-1)^{\mathfrak{q}(A_0)(\mathfrak{q}(A_1)+\cdots+\mathfrak{q}(A_{p-1}))} C_{A_0 A_p}{}^{B} \langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_{p-1}} \boldsymbol{T}_B \boldsymbol{T}_{A_{p+1}} \cdots \boldsymbol{T}_{A_n} \rangle. \tag{148}$$

Define now

$$X^{(p)}_{(A_0,\alpha_0)\cdots(A_n,\alpha_n)} = (-1)^{\mathfrak{q}(A_0,\alpha_0)(\mathfrak{q}(A_1,\alpha_1)+\cdots+\mathfrak{q}(A_{p-1},\alpha_{p-1}))} C_{(A_0,\alpha_0)(A_p,\alpha_p)}{}^{(B,\beta)} \times \langle \boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_{p-1},\alpha_{p-1})} \boldsymbol{T}_{(B,\beta)} \boldsymbol{T}_{(A_{p+1},\alpha_{p+1})} \cdots \boldsymbol{T}_{(A_n,\alpha_n)} \rangle.$$

Using the fact that $\mathfrak{q}(A,\alpha)=\mathfrak{q}(A)$ and replacing expressions (11) for the S-expansion structure constants and (146) for $\langle \boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_n,\alpha_n)} \rangle$, we get

$$X^{(p)}_{(A_0,\alpha_0)\cdots(A_n,\alpha_n)} = \alpha_\gamma K_{\alpha_0 \cdots \alpha_n}{}^{\gamma} X^{(p)}_{A_0 \cdots A_n}.$$

From Eq. (147) one readily concludes that

$$\sum_{p=1}^{n} X^{(p)}_{(A_0,\alpha_0)\cdots(A_n,\alpha_n)} = 0. \tag{149}$$

Therefore, $\langle \boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_n,\alpha_n)} \rangle = \alpha_\gamma K_{\alpha_1 \cdots \alpha_n}{}^{\gamma} \langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n} \rangle$ is an invariant tensor for $\mathfrak{G}=S\times\mathfrak{g}$. ■

It is worth to notice that, in general, the expression

$$\langle \boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_n,\alpha_n)} \rangle = \sum_{m=0}^{M} \alpha_\gamma^{\beta_1 \cdots \beta_m} K_{\beta_1 \cdots \beta_m \alpha_1 \cdots \alpha_n}{}^{\gamma} \langle \boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n} \rangle, \tag{150}$$

where M is the number of elements of S and $\alpha_\gamma^{\beta_1 \cdots \beta_m}$ are arbitrary constants, is also an invariant tensor for $\mathfrak{G}=S\times\mathfrak{g}$. An example of Eq. (150) is provided by the supertrace. As a matter of fact, when the generators $\boldsymbol{T}_A$ are in some matrix representation, and the generators $\boldsymbol{T}_{(A,\alpha)}$ in the matrix representation $\boldsymbol{T}_{(A,\alpha)}=[\lambda_\alpha]_\mu{}^{\nu} \boldsymbol{T}_A$, with $[\lambda_\alpha]_\mu{}^{\nu}$ given in Eq. (4), we have

$$\mathrm{STr}(\boldsymbol{T}_{(A_1,\alpha_1)} \cdots \boldsymbol{T}_{(A_n,\alpha_n)}) = K_{\gamma\alpha_1 \cdots \alpha_n}{}^{\gamma} \,\mathrm{Str}(\boldsymbol{T}_{A_1} \cdots \boldsymbol{T}_{A_n}), \tag{151}$$

where STr is the (super)trace for the $\boldsymbol{T}_{(A,\alpha)}$ generators and STr the one for the $\boldsymbol{T}_A$ generators.

Even though expression (150) could be regarded as more general than Eq. (146), this is not the case. Using only the associativity and closure of the semigroup product, it is always possible to reduce Eq. (150) to Eq. (146), which in this way turns out to be more "fundamental."

Given an invariant tensor for an algebra, its components valued on a subalgebra are by themselves an invariant tensor for the subalgebra (if they do not vanish). For the case of resonant subalgebras, and provided all the α_γ's are different from zero, the invariant tensor for the resonant subalgebra never vanishes. As matter of fact, given a resonant subset partition $S=\cup_{p\in I} S_p$ and denoting the basis of V_p as $\{\boldsymbol{T}_{a_p}\}$, the $\mathfrak{G}_R$-valued components of Eq. (146) are given by

$$\langle \boldsymbol{T}_{(a_{p_1},\alpha_{p_1})} \cdots \boldsymbol{T}_{(a_{p_n},\alpha_{p_n})} \rangle = \alpha_\gamma K_{\alpha_{p_1} \cdots \alpha_{p_n}}{}^{\gamma} \langle \boldsymbol{T}_{a_{p_1}} \cdots \boldsymbol{T}_{a_{p_n}} \rangle \quad \text{with } \lambda_{\alpha_p} S_p. \tag{152}$$

These components form an invariant tensor for the resonant subalgebra $\mathfrak{G}_R=\bigoplus_{p\in I}S_p\times V_p$. Since S is closed under the product in Eq. (1), for every choice of $\alpha_{p_1},\ldots,\alpha_{p_n}$ there always exists a value of γ such that $K_{\alpha_{p_1}\cdots\alpha_{p_n}}{}^{\gamma}=1$, and therefore Eq. (152) does not vanish (provided that $\forall\,\gamma,\alpha_\gamma\neq 0$).

However, an interesting nontrivial point is that a 0_S-reduced algebra is *not* a subalgebra, and therefore, in general the 0_S-reduced algebra-valued components of expression (146) or (152) *do not* lead to an invariant tensor. The following theorem offers a solution by providing a general expression for an invariant tensor for a 0_S-reduced algebra.

Theorem 7.2: *Let S be an Abelian semigroup with nonzero elements λ_i, $i=0,\ldots,N$, and $\lambda_{N+1}=0_S$. Let $\mathfrak{g}$ be a Lie (super)algebra of basis $\{\boldsymbol{T}_A\}$, and let $\langle \boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}\rangle$ be an invariant tensor for $\mathfrak{g}$. The expression*

$$\langle \boldsymbol{T}_{(A_1,i_1)}\cdots\boldsymbol{T}_{(A_n,i_n)}\rangle=\alpha_j K_{i_1\cdots i_n}{}^{j}\langle \boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}\rangle, \tag{153}$$

where α_j are arbitrary constants, corresponds to an invariant tensor for the 0_S-reduced algebra obtained from $\mathfrak{G}=S\times\mathfrak{g}$.

Proof: This theorem is actually a corollary of Theorem 7.1; imposing $\alpha_{N+1}=0$ in Theorem 7.1 and writing the $i_0\cdots i_n$ components of Eq. (149) one gets

$$\sum_{p=1}^{n} X^{(p)}_{(A_0,i_0)\cdots(A_n,i_n)}=0. \tag{154}$$

Using the expressions for the S-expansion structure constants in Eq. (11) and for the invariant tensor in Eq. (153), one finds

$$\begin{aligned}X^{(p)}_{(A_0,i_0)\cdots(A_n,i_n)}=&(-1)^{\mathrm{q}(A_0,i_0)(\mathrm{q}(A_1,i_1)+\cdots+\mathrm{q}(A_{p-1},i_{p-1}))}\\&\times\big(K_{i_0i_p}{}^{k}C_{A_0A_p}{}^{B}\alpha_j K_{i_1\cdots i_{p-1}ki_{p+1}\cdots i_n}{}^{j}\langle \boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{p-1}\boldsymbol{T}_B\boldsymbol{T}_{p+1}\cdots\boldsymbol{T}_{A_n}\rangle\\&+K_{i_0i_p}{}^{N+1}C_{A_0A_p}{}^{B}\alpha_j K_{i_1\cdots i_{p-1}(N+1)i_{p+1}\cdots i_n}{}^{j}\langle \boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{p-1}\boldsymbol{T}_B\boldsymbol{T}_{p+1}\cdots\boldsymbol{T}_{A_n}\rangle\big).\end{aligned}$$

Since

$$\lambda_{i_1}\cdots\lambda_{i_{p-1}}\lambda_{N+1}\lambda_{i_{p+1}}\cdots\lambda_{i_n}=\lambda_{N+1},$$

we have

$$K_{i_1\cdots i_{p-1}(N+1)i_{p+1}\cdots i_n}{}^{j}=0,$$

and then,

$$\begin{aligned}X^{(p)}_{(A_0,i_0)\cdots(A_n,i_n)}=&(-1)^{\mathrm{q}(A_0,i_0)(\mathrm{q}(A_1,i_1)+\cdots+\mathrm{q}(A_{p-1},i_{p-1}))}\\&\times K_{i_0i_p}{}^{k}C_{A_0A_p}{}^{B}\alpha_j K_{i_1\cdots i_{p-1}ki_{p+1}\cdots i_n}{}^{j}\langle \boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{p-1}\boldsymbol{T}_B\boldsymbol{T}_{p+1}\cdots\boldsymbol{T}_{A_n}\rangle.\end{aligned}$$

But $K_{ij}{}^{k}C_{AB}{}^{C}$ are the structure constants [see Eq. (22)] of the 0_S-reduced algebra of $S\times\mathfrak{g}$, and therefore, from Eq. (154) we find that Eq. (153) provides an invariant tensor for it. ■

For the 0_S-reduction of a resonant subalgebra, the proof is analogous to the one given above, and we have that

$$\langle \boldsymbol{T}_{(a_{p_1},i_{p_1})}\cdots\boldsymbol{T}_{(a_{p_n},i_n)}\rangle=\alpha_j K_{i_{p_1}\cdots i_{p_n}}{}^{j}\langle \boldsymbol{T}_{i_{p_1}}\cdots\boldsymbol{T}_{i_{p_n}}\rangle\quad\text{such that }\lambda_{i_p}\in S_p \tag{155}$$

is an invariant tensor for the 0_S-reduced algebra of $\mathfrak{G}_R=\Sigma_{p\in I}S_p\times V_p$.

The usefulness of this theorem comes from the fact that, in general, the (super)trace in the adjoint representation for 0_S-reduced algebras can give only a very small number of components of Eq. (153).

As a matter of fact, using the adjoint representation given by the 0_S-reduced structure constants in Eq. (22), one finds

$$\mathrm{STr}(\boldsymbol{T}_{(A_1,i_1)}\cdots\boldsymbol{T}_{(A_n,i_n)}) = K_{j_1 i_1}{}^{j_2} K_{j_2 i_2}{}^{j_3}\cdots K_{j_{n-1} i_{n-1}}{}^{j_n} K_{j_n i_n}{}^{j_1}\,\mathrm{Str}(\boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}), \tag{156}$$

and since $\lambda_i\lambda_j=\lambda_{k(i,j)}$ implies that $\lambda_i,\lambda_j\neq 0_S$, one ends up with

$$\mathrm{STr}(\boldsymbol{T}_{(A_1,i_1)}\cdots\boldsymbol{T}_{(A_n,i_n)}) = K_{j_1 i_1\cdots i_n}{}^{j_1}\,\mathrm{Str}(\boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}). \tag{157}$$

In general, this expression has less components than Eq. (153). In order to see this, it is useful to analyze the case when there is also an identity element in the semigroup, $\lambda_0=e$, and each λ_i appears only once in each row and each column of the semigroup's multiplication table (i.e., for each $\lambda_i,\lambda_j\neq e$, we have $\lambda_i\lambda_j\neq\lambda_i$ and $\lambda_i\lambda_j\neq\lambda_j$). In this case, $K_{j_1 i_1\cdots i_n}{}^{j_1}=K_{i_1\cdots i_n}{}^{0}$, and the only nonvanishing component of the (super)trace is

$$\mathrm{STr}(\boldsymbol{T}_{(A_1,i_1)}\cdots\boldsymbol{T}_{(A_n,i_n)}) = K_{i_1\cdots i_n}{}^{0}\,\mathrm{Str}(\boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}), \tag{158}$$

which is clearly smaller than Eq. (153). In the expansion case $S=S_{\mathrm{E}}$, we have $K_{i_1\cdots i_n}{}^{0}=\delta^{0}_{H_{N+1}(i_1+\cdots+i_n)}=\delta^{0}_{i_1+\cdots+i_n}$ and therefore, the only nonvanishing component of the (super)trace is

$$\mathrm{STr}(\boldsymbol{T}_{(A_1,0)}\cdots\boldsymbol{T}_{(A_n,0)}) = \mathrm{Str}(\boldsymbol{T}_{A_1}\cdots\boldsymbol{T}_{A_n}). \tag{159}$$

The advantage of the invariant tensor in Eq. (153) as opposed to the (super)trace is now clear; in the case $S_{\mathrm{E}}\times\mathfrak{g}$, the (super)trace only gives a trivial repetition of the invariant tensor of $\mathfrak{g}$, and for a resonant subalgebra, just a piece of it.

One last remark on the invariant tensor in Eq. (153) is that for the particular case $S=S_{\mathrm{E}}$, since $K_{i_1\cdots i_n}{}^{j}=\delta^{j}_{H_{N+1}(i_1+\cdots+i_n)}=\delta^{j}_{i_1+\cdots+i_n}$, a topological density or a Chern-Simons form constructed using the invariant tensor in Eq. (153) coincides with the one from Ref. 1 for the choice $\alpha_\gamma=\lambda^\gamma$, where λ^γ stands for a power of the expansion parameter of the free differential algebra.

VIII. CONCLUSIONS

We have discussed how one can obtain a bunch of Lie algebras starting from an original one by choosing an Abelian semigroup and applying the general theorems 4.2 and 6.1, which give us "resonant subalgebras" and what has been dubbed "reduced algebras." This procedure is a natural outgrowth of the method of MC form power-series expansion presented in Ref. 1, from the point of view of the Lie algebra generators and using an arbitrary Abelian semigroup. The S expansion presented here has the feature of being very simple and direct; given a semigroup, one needs only solve the resonance condition [Eq. (34)] in order to get a resonant subalgebra, and the very similar reduction conditions [Eqs. (122) and (123)] in order to get a reduced one. These have been solved in several examples in order to show how both theorems work, for general algebra structures as well as for very explicit cases, e.g., $d=11$ superalgebras. As expected, the S-expansion scheme reproduces exactly the results of the MC form power-series expansion for a particular choice of semigroup, but it is also possible to get interesting new results using other alternatives, as shown in Sec. V C.

The examples of the S-expansion procedure have been chosen according to their relevance for the long-term goal of understanding the geometric formulation of 11-dimensional supergravity. To be able to write a Lagrangian invariant under these symmetries, a key ingredient is an invariant tensor. The theorems given in Sec. VII help fill the gap, since they go a long way beyond the simple, and sometimes trivial, invariant tensors obtained from the supertrace. Chern-Simons and Transgression forms appear as a straightforward choice for the construction of a supergravity Lagrangian in this context.[22–31] In this sense, Theorems 4.2, 6.1, 7.1, and 7.2 provide a very practical "physicist's toolbox." These have been used to construct a Lagrangian for the M algebra in 11 dimensions[14] following the techniques developed in Refs. 28 and 31.

There are several ways in which this work can be extended. One of them concerns the investigation of the specific properties of the algebras generated from different choices of Abelian semigroups; some kind of general classification would be particularly interesting. A first step in this direction would be the construction of the above-mentioned Lagrangians, but of course there are a lot of different possibilities to proceed. A different, and perhaps fruitful path deals with the generalization of the *S*-expansion procedure itself. The conditions of discreteness and finiteness for the semigroup have been chosen primarily for simplicity, but it seems as though they could be removed in a generalized setting. The Abelianity condition, on the other hand, is essential for all of our results to hold, and it is not clear whether it could be relaxed. Removing this requirement, a set with both commuting and anticommuting elements could be considered. If this possibility turns out to be feasible (which is far from trivial; think of the Jacobi identity), it would provide a way to derive superalgebras from ordinary Lie algebras and vice versa.

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APPENDIX: REDUCTION WHEN $\mathfrak{g}$ SATISFIES THE WEIMAR-WOODS CONDITIONS

In Sec. IV B 2 it was shown that, when $\mathfrak{g}$ satisfies the Weimar-Woods conditions, the partition $S_{\mathrm{E}}^{(N)}=\bigcup_{p=0}^{n}S_p$ with $S_p=\{\lambda_{\alpha_p}, \text{such that } \alpha_p=p,\ldots,N+1\}$ is a resonant one. In this appendix we prove that, when each subset S_p is split as $S_p=\check{S}_p\cup\hat{S}_p$, with

$$\check{S}_p=\{\lambda_{\alpha_p} \quad \text{such that } \alpha_p=p,\ldots,N_p\}, \tag{A1}$$

$$\hat{S}_p=\{\lambda_{\alpha_p} \quad \text{such that } \alpha_p=N_p+1,\ldots,N+1\}, \tag{A2}$$

then the reduction condition in Eq. (123) from Theorem 6.1 is satisfied when

$$N_{p+1}=\begin{cases} N_p \text{ or} \\ H_{N+1}(N_p+1). \end{cases} \tag{A3}$$

Before proceeding, it is worth to notice that the partition equation [Eqs. (A1) and (A2)] automatically satisfies the following three properties:

$$N_p\geqslant N_q \Leftrightarrow \hat{S}_p\subset\hat{S}_q, \tag{A4}$$

$$\check{S}_0\cdot\hat{S}_q=\hat{S}_q, \tag{A5}$$

$$\check{S}_p\cdot\hat{S}_q\subset\hat{S}_x \quad \text{such that } N_x\leqslant H_{N+1}(p+N_q). \tag{A6}$$

Since $\mathfrak{g}$ is assumed to satisfy the Weimar-Woods conditions,[15,16] condition (123) now reads

$$\check{S}_p \cdot \hat{S}_q \subset \bigcap_{r=0}^{H_n(p+q)} \hat{S}_r, \tag{A7}$$

where $\check{S}_p$ and $\hat{S}_q$ are given by Eqs. (A1) and (A2).

Let us analyze this condition for the particular case $p=0$:

$$\check{S}_0 \cdot \hat{S}_q \subset \bigcap_{r=0}^{q} \hat{S}_r. \tag{A8}$$

Using Eq. (A5), this turns out to be equivalent to

$$\hat{S}_q \subset \bigcap_{r=0}^{q} \hat{S}_r. \tag{A9}$$

In this way, we have that for each $0 \leqslant r \leqslant q$, $\hat{S}_q \subset \hat{S}_r$, and using Eq. (A4), we get the equivalent condition

$$\forall r \leqslant q, \quad N_r \leqslant N_q. \tag{A10}$$

This condition and the product in Eq. (26) now imply that

$$\bigcap_{r=0}^{H_n(p+q)} \hat{S}_r = \hat{S}_{H_n(p+q)}.$$

Using this fact, condition (A7) takes the form

$$\check{S}_p \cdot \hat{S}_q \subset \hat{S}_{H_n(p+q)}. \tag{A11}$$

Using Eq. (A6), one finds that, in order to satisfy this requirement, it is enough to impose that, for each $\hat{S}_x$ such that $N_x \leqslant H_{N+1}(N_q+p)$, one has $\hat{S}_x \subset \hat{S}_{H_n(p+q)}$. Alternatively [see Eq. (A4)], one can write

$$\forall N_x \leqslant H_{N+1}(N_q + p), \quad N_{H_n(p+q)} \leqslant N_x \tag{A12}$$

and therefore,

$$N_{H_n(p+q)} \leqslant H_{N+1}(N_q + p). \tag{A13}$$

For $p=1$, we have

$$N_{H_n(p+1)} \leqslant H_{N+1}(N_q + 1),$$

and using Eq. (A10), one finds the inequalities

$$N_q \leqslant N_{H_n(q+1)} \leqslant H_{N+1}(N_q + 1),$$

whose solution is

$$N_{q+1} = \begin{cases} N_q \text{ or} \\ H_{N+1}(N_q + 1). \end{cases}$$

This solves condition (A7).

Therefore, we have that

$$|\check{\mathfrak{G}}_{\mathrm{R}}| = \bigoplus_{p=0}^{n} \check{S}_p \times V_p, \tag{A14}$$

with $\check{S}_p = \{\lambda_{\alpha_p}, \text{such that } \alpha_p = p, \ldots, N_p\}$ and

$$N_{p+1} = \begin{cases} N_p \text{ or} \\ H_{N+1}(N_p + 1) \end{cases} \tag{A15}$$

is a reduced Lie algebra with structure constants

$$C_{(a_p,\alpha_p)(b_q,\beta_q)}{}^{(c_r,\gamma_r)} = K_{\alpha_p\beta_q}{}^{\gamma_r} C_{a_p b_q}{}^{c_r} \quad \text{with } \alpha_p, \beta_p, \gamma_p = p, \ldots, N_p. \tag{A16}$$

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A note on semidensities in antisymplectic geometry

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We revisit Khudaverdian's geometric construction of an odd nilpotent operator Δ_E that sends semidensities to semidensities on an antisymplectic manifold. We find a local formula for the Δ_E operator in arbitrary coordinates and we discuss its connection to Batalin-Vilkovisky quantization. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2352859]

I. INTRODUCTION

Recall that for a symplectic manifold with an even symplectic two-form $\omega=\frac{1}{2}dz^A\omega_{AB}dz^B$, there exists a canonical measure density given by the Pfaffian $\rho=\mathrm{Pf}(\omega_{AB})$, i.e., there is a natural notion of volume in a symplectic manifold. A related fact is the Liouville Theorem, which states that Hamiltonian vector fields are divergenceless. On the other hand, the situation is completely different for an odd symplectic manifold, also known as an antisymplectic manifold and endowed with an odd antisymplectic two-form $E=\frac{1}{2}d\Gamma^A E_{AB}d\Gamma^B$. These geometries, for instance, show up in the Lagrangian quantization method of Batalin and Vilkovisky.[1] It turns out that there is *no* canonical choice of measure density ρ in this case, as, for instance, the above Pfaffian. This is tied to the fact that there is no meaningful notion of a superdeterminant/Berezinian for a matrix that is intrinsically Grassmann-odd. However, the upset runs deeper. In fact, a density ρ can never be a function of the antisymplectic matrix E_{AB}. Phrased differently, a density ρ always carries information that cannot be deduced from the antisymplectic structure E alone.[2] Within the standard Batalin-Vilkovisky framework, the possible choices of a density ρ is only partially determined by a requirement of gauge symmetry.

Around 1992, the Batalin-Vilkovisky quantization took a more geometric form, particularly with the work of Schwarz.[3] The consensus was that the geometric setting requires two independent structures: an odd symplectic, nondegenerate two-form E and a measure density ρ. From these two structures, one may build a Grassmann-odd, second-order operator Δ_ρ, known as the odd Laplacian. Alternatively, one can view the odd Laplacian Δ_ρ itself as *the* fundamental structure of Batalin-Vilkovisky geometry,[4,5] which is conventionally required to be nilpotent.

Khudaverdian has constructed[6–9] a Grassmann-odd, nilpotent, second-order operator Δ_E that does not rely on a choice of density ρ. The caveat is that the Δ_E operator is defined on semidensities rather than on scalars. [The notion of a semidensity is explained in Eq. (3.1) below.] In retrospect, many pieces of Khudaverdian's construction were known to physicists; see, for instance, Ref. 10, p. 440. In this short note, Khudaverdian's construction is reconsidered, and we find a local formula for the Δ_E operator that applies to arbitrary coordinate systems. The ability to work in any coordinates, not just Darboux coordinates, is important, since if one first has to search for a set of Darboux coordinates to the system that one is studying, symmetries (such as, e.g., Lorentz covariance) or locality that one would like to preserve during the quantization process, are often lost.

The paper is organized as follows: We consider the antisymplectic structure in Sec. II; the odd

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Laplacian Δ_ρ in Sec. III; and in Secs. IV and V, the Δ_E operator using Darboux coordinates and general coordinates, respectively. Finally, in Sec. VI we analyze a modified Batalin-Vilkovisky scheme based on the Δ_E operator.

General remark about notation: We have two types of grading: A Grassmann grading ε and an exterior form degree p. The sign conventions are such that two exterior forms ξ and η, of Grassmann parity ε_ξ, ε_η and exterior form degree p_ξ, p_η, respectively, commute in the following graded sense:

$$\eta \wedge \xi = (-1)^{\varepsilon_\xi \varepsilon_\eta + p_\xi p_\eta} \xi \wedge \eta \tag{1.1}$$

inside the exterior algebra. We will often not write the exterior wedges "$\wedge$" explicitly.

II. ANTISYMPLECTIC GEOMETRY

Consider an antisymplectic manifold (M,E) and let Γ^A denote local coordinates of Grassmann parity $\varepsilon_A \equiv \varepsilon(\Gamma^A)$ (and exterior form degree $p(\Gamma^A)=0$). The antisymplectic two-form can locally be written as

$$E = \frac{1}{2} \mathrm{d}\Gamma^A E_{AB}\, \mathrm{d}\Gamma^B = -\frac{1}{2} E_{AB}\, \mathrm{d}\Gamma^B\, \mathrm{d}\Gamma^A, \tag{2.1}$$

where $E_{AB}=E_{AB}(\Gamma)$ is the corresponding matrix representation. Besides carrying gradings $\varepsilon(E)=1$ and $p(E)=2$, the antisymplectic two-form E has two defining properties. First, E is closed,

$$\mathrm{d}E = 0, \tag{2.2}$$

where the grading conventions for the exterior derivative

$$\mathrm{d} = \mathrm{d}\Gamma^A \frac{\vec{\partial}^l}{\partial \Gamma^A} \tag{2.3}$$

are $\varepsilon(\mathrm{d})=0$ and $p(\mathrm{d})=1$. Second, E is nondegenerate, i.e., the antisymplectic matrix E_{AB} has an inverse matrix E^{AB},

$$E^{AB} E_{BC} = \delta^A_C = E_{CB} E^{BA}. \tag{2.4}$$

Instead of the compact exterior form notation E, one may equivalently formulate the above conditions with all the indices written out explicitly in terms of the matrices E_{AB} or E^{AB}. In detail, the gradings are

$$\begin{aligned} \varepsilon(E_{AB}) &= \varepsilon_A + \varepsilon_B + 1 = \varepsilon(E^{AB}), \\ p(E_{AB}) &= 0 = p(E^{AB}), \end{aligned} \tag{2.5}$$

the skew symmetries are

$$\begin{aligned} E_{BA} &= -(-1)^{\varepsilon_A \varepsilon_B} E_{AB}, \\ E^{BA} &= -(-1)^{(\varepsilon_A+1)(\varepsilon_B+1)} E^{AB}, \end{aligned} \tag{2.6}$$

while the closeness condition and the equivalent Jacobi identity read

$$\sum_{\text{cycl. } A,B,C} (-1)^{\varepsilon_A \varepsilon_C} \left(\frac{\vec{\partial}^l}{\partial \Gamma^A} E_{BC} \right) = 0, \tag{2.7}$$

$$\sum_{\text{cycl. } A,B,C} (-1)^{(\varepsilon_A+1)(\varepsilon_C+1)} E^{AD} \left(\frac{\vec{\partial}^l}{\partial \Gamma^D} E^{BC} \right) = 0, \tag{2.8}$$

respectively. The inverse matrix E^{AB} with upper indices gives rise to the antibracket[1]

$$(F,G) = \left(F\frac{\overleftarrow{\partial}^r}{\partial\Gamma^A}\right)E^{AB}\left(\frac{\overrightarrow{\partial}^l}{\partial\Gamma^B}G\right), \tag{2.9}$$

which satisfies a graded skew symmetry and a graded Jacobi identity as a consequence of Eqs. (2.6) and (2.8). There is an antisymplectic analog of Darboux's Theorem that states that locally there exist Darboux coordinates $\Gamma^A=\{\phi^\alpha;\phi^*_\alpha\}$, such that the only nonvanishing antibrackets between the coordinates are $(\phi^\alpha,\phi^*_\beta)=\delta^\alpha_\beta=-(\phi^*_\beta,\phi^\alpha)$. In Darboux coordinates, the antisymplectic two-form is simply $E=\mathrm{d}\phi^*_\alpha\wedge\mathrm{d}\phi^\alpha$.

III. ODD LAPLACIAN Δ_ρ ON SCALARS

A scalar function $F=F(\Gamma)$, a density $\rho=\rho(\Gamma)$, and a semidensity $\sigma=\sigma(\Gamma)$ are by definition quantities that transform as

$$F\to F'=F,\quad \rho\to\rho'=\frac{\rho}{J},\quad \sigma\to\sigma'=\frac{\sigma}{\sqrt{J}}, \tag{3.1}$$

respectively, under general coordinate transformations $\Gamma^A\to\Gamma'^A$, where $J\equiv\mathrm{sdet}(\partial\Gamma'^A/\partial\Gamma^B)$ denotes the Jacobian. We shall ignore the global issues of orientation and choice of square root. In principle the above F, ρ, and σ could either be bosons or fermions; however, normally we shall require the densities ρ to be invertible and therefore bosons.

Given a choice of density ρ one may define the odd Laplacian[4]

$$\Delta_\rho := \frac{(-1)^{\varepsilon_A}}{2\rho}\frac{\overrightarrow{\partial}^l}{\partial\Gamma^A}\rho E^{AB}\frac{\overrightarrow{\partial}^l}{\partial\Gamma^B}, \tag{3.2}$$

that takes scalars to scalars of opposite Grassmann parity. The odd Laplacian (3.2) has a geometric interpretation as a divergence of a Hamiltonian vector field[3,11]

$$\Delta_\rho\Psi = -\frac{1}{2}\,\mathrm{div}_\rho(X_\Psi),\quad \varepsilon(\Psi)=1. \tag{3.3}$$

Here $X_\Psi:=(\Psi,\cdot)$ denotes a Hamiltonian vector field with a Grassmann-odd Hamiltonian Ψ and the divergence $\mathrm{div}_\rho X$ of a vector field X, with respect to the measure density ρ, is

$$\mathrm{div}_\rho X := \frac{(-1)^{\varepsilon_A}}{\rho}\frac{\overrightarrow{\partial}^l}{\partial\Gamma^A}(\rho X^A),\quad \varepsilon(X)=0. \tag{3.4}$$

The fact that the odd Laplacian (3.3) is nonzero, shows that antisymplectic manifolds do not have an analog of the Liouville Theorem mentioned in the introduction. As a consequence of the Jacobi identity [Eq. (2.8)], the square operator $\Delta^2_\rho=(\frac{1}{2})[\Delta_\rho,\Delta_\rho]$ becomes a linear derivation, i.e., a first-order differential operator,

$$\Delta^2_\rho(FG)=\Delta^2_\rho(F)G+F\Delta^2_\rho(G). \tag{3.5}$$

Conventionally, one imposes additionally that the Δ_ρ operator is nilpotent $\Delta^2_\rho=0$, but this is not necessary for our purposes.

IV. KHUDAVERDIAN'S Δ_E OPERATOR ON SEMIDENSITIES

Khudaverdian showed that one may define a Grassmann-odd, nilpotent, second-order operator Δ_E *without* a choice of density ρ. This Δ_E operator does not take scalars to scalars like the odd Laplacian (3.2), but instead takes semidensities to semidensities of opposite Grassmann parity. Equivalently, the Δ_E operator transforms as

$$\Delta_E \to \Delta'_E = \frac{1}{\sqrt{J}} \Delta_E \sqrt{J} \tag{4.1}$$

under general coordinate transformations $\Gamma^A \to \Gamma'^A$, cf. Eq. (3.1). Khudaverdian's construction relies first of all on an atlas of Darboux charts, which is granted by an antisymplectic analog of Darboux's Theorem, and second, on a lemma by Batalin and Vilkovisky about the possible form of the Jacobians for anticanonical transformations, also known as antisymplectomorphisms.

Lemma 1: The Batalin-Vilkovisky Lemma[7–10,12,13]. Consider a finite anticanonical transformation between initial Darboux coordinates $\Gamma^A_{(i)}$ and final Darboux coordinates $\Gamma^A_{(f)}$. Then the Jacobian $J \equiv \mathrm{sdet}(\partial \Gamma^A_{(f)} / \partial \Gamma^B_{(i)})$ satisfies

$$\Delta^{(i)}_1 \sqrt{J} = 0. \tag{4.2}$$

Here $\Delta^{(i)}_1$ refers to the odd Laplacian (3.2) with $\rho = 1$ in the initial Darboux coordinate $\Gamma^A_{(i)}$. Given the Darboux coordinate Γ^A, the Δ_E operator is defined on a semidensity σ as[6–9,13]

$$(\Delta_E \sigma) := (\Delta_1 \sigma), \tag{4.3}$$

where Δ_1 is the Δ_ρ operator (3.2) with $\rho = 1$. It is important in Eq. (4.3) that the formula for the Δ_1 operator (3.2) and the semidensity σ both refer to the same Darboux coordinate Γ^A. The parentheses in Eq. (4.3) indicate that the equation should be understood as an equality among semidensities (in the sense of zeroth-order differential operators), rather than an identity among differential operators. One next uses the Batalin-Vilkovisky Lemma to argue that the definition (4.3) does not depend on the choices of Darboux coordinates Γ^A. What this means is that the right-hand side of the definition (4.3) transforms as a semidensity

$$(\Delta^{(f)}_1 \sigma_{(f)}) = \frac{1}{\sqrt{J}} (\Delta^{(i)}_1 \sigma_{(i)}) \tag{4.4}$$

under an anticanonical transformation between any two Darboux coordinates $\Gamma^A_{(i)}$ and $\Gamma^A_{(f)}$. Proof:

$$\sqrt{J}(\Delta^{(f)}_1 \sigma_{(f)}) = \sqrt{J}(\Delta^{(i)}_J \sigma_{(f)}) = \sqrt{J}\left(\Delta^{(i)}_J \frac{\sigma_{(i)}}{\sqrt{J}} \right) = (\Delta^{(i)}_1 \sigma_{(i)}) - \frac{1}{\sqrt{J}} (\Delta^{(i)}_1 \sqrt{J}) \sigma_{(i)} = (\Delta^{(i)}_1 \sigma_{(i)}). \tag{4.5}$$

The third equality is a nontrivial property of the odd Laplacian (3.2). The Batalin-Vilkovisky Lemma is used in the fourth equality. Strictly speaking, it is enough to consider infinitesimal anticanonical transformations to justify the definition (4.3). The proof of the infinitesimal version of the Batalin-Vilkovisky Lemma goes like this: An infinitesimal anticanonical coordinate transformation $\delta \Gamma^A = X^A$ is necessarily a Hamiltonian vector field $X^A = (\Psi, \Gamma^A) \equiv X^A_\Psi$ with an infinitesimal, Grassmann-odd Hamiltonian Ψ, where $\varepsilon(\Psi) = 1$. So

$$\ln J \approx (-1)^{\varepsilon_A} \left(\frac{\vec{\partial}^l}{\partial \Gamma^A} X^A \right) = \mathrm{div}_1(X_\Psi) = -2\Delta_1 \Psi, \tag{4.6}$$

and hence

$$\Delta_1 \sqrt{J} \approx -\Delta^2_1 \Psi = 0, \tag{4.7}$$

due to the nilpotency of the Δ_1 operator in Darboux coordinates. The $\approx$ sign is used to indicate that equality only holds at the infinitesimal level. (Here we are guilty of mixing active and passive pictures; the active vector field is properly speaking *minus* X.) A simple proof of the Batalin-Vilkovisky Lemma for finite anticanonical transformations can be found in Ref. 13.

On the other hand, once the definition (4.3) is justified, it is obvious that the Δ_E operator supercommutes with itself, because the Γ^A derivatives have no Γ^A's to act on in Darboux coordinates. Therefore Δ_E is nilpotent,

$$\Delta_E^2 = \frac{1}{2}[\Delta_E, \Delta_E] = 0. \tag{4.8}$$

The same sort of reasoning shows that $\Delta_E = \Delta_E^T$ is symmetric.

V. THE Δ_E OPERATOR IN GENERAL COORDINATES

We now give a definition of the Δ_E operator that does not rely on Darboux coordinates. We claim that in arbitrary coordinates the Δ_E operator is given as

$$(\Delta_E \sigma) := (\Delta_1 \sigma) + \left(\frac{\nu^{(1)}}{8} - \frac{\nu^{(2)}}{24}\right)\sigma, \tag{5.1}$$

where

$$\nu^{(1)} := (-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial \Gamma^B}\frac{\vec{\partial}^l}{\partial \Gamma^A}E^{AB}\right), \tag{5.2}$$

$$\nu^{(2)} := -(-1)^{\varepsilon_B}(\Gamma^C,(\Gamma^B,\Gamma^A))\left(\frac{\vec{\partial}^l}{\partial \Gamma^A}E_{BC}\right) = (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial \Gamma^A}E^{CD}\right)\left(\frac{\vec{\partial}^l}{\partial \Gamma^D}E^{AB}\right)E_{BC}. \tag{5.3}$$

Equation (5.1) is the main result of this paper. Notice that in Darboux coordinates, where E^{AB} is constant, i.e., independent of the coordinate Γ^A, the last two terms, $\nu^{(1)}$ and $\nu^{(2)}$, vanish. Hence the definition (5.1) agrees in this case with Khudaverdian's Δ_E operator (4.3).

It remains to be shown that the right-hand side of Eq. (5.1) behaves as a semidensity under general coordinate transforms. Here we will only explicitly consider the case where σ is invertible to simplify the presentation. (The noninvertible case is fundamentally no different.) In the invertible case, we customarily write the semidensity $\sigma = \sqrt{\rho}$ as a square root of a density ρ, and define a Grassmann-odd quantity

$$\nu_\rho := \frac{1}{\sqrt{\rho}}(\Delta_E \sqrt{\rho}) = \nu_\rho^{(0)} + \frac{\nu^{(1)}}{8} - \frac{\nu^{(2)}}{24}, \tag{5.4}$$

by dividing both sides of the definition (5.1) with the semidensity σ. Here we have defined

$$\nu_\rho^{(0)} := \frac{1}{\sqrt{\rho}}(\Delta_1 \sqrt{\rho}). \tag{5.5}$$

Hence, to justify the definition (5.1), one should check that ν_ρ is a scalar under general infinitesimal coordinate transformations. Under an arbitrary infinitesimal coordinate transformation $\delta\Gamma^A = X^A$, one calculates

$$\delta\nu_\rho^{(0)} = -\frac{1}{2}\Delta_1 \operatorname{div}_1 X, \tag{5.6}$$

$$\delta\nu^{(1)} = 4\Delta_1 \operatorname{div}_1 X + (-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial \Gamma^C}E^{AB}\right)\left(\frac{\vec{\partial}^l}{\partial \Gamma^B}\frac{\vec{\partial}^l}{\partial \Gamma^A}X^C\right), \tag{5.7}$$

$$\delta\nu^{(2)} = 3(-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial \Gamma^C}E^{AB}\right)\left(\frac{\vec{\partial}^l}{\partial \Gamma^B}\frac{\vec{\partial}^l}{\partial \Gamma^A}X^C\right), \tag{5.8}$$

cf. Appendixes A–C. One easily sees that while the three constituents $\nu_\rho^{(0)}$, $\nu^{(1)}$, and $\nu^{(2)}$ separately have nontrivial transformation properties, the linear combination ν_ρ in Eq. (5.4) is indeed a scalar.

The new definition (5.1) is clearly symmetric $\Delta_E = \Delta_E^T$ and one may check that the nilpotency (4.8) of the Δ_E operator (5.1) precisely encodes the Jacobi identity (2.9). The odd Laplacian Δ_ρ can be expressed entirely by the Δ_E operator and a choice of density ρ,

$$(\Delta_\rho F) = (\Delta_1 F) + \frac{1}{\sqrt{\rho}}(\sqrt{\rho}, F) = \frac{1}{\sqrt{\rho}}[\vec{\Delta}_1, F]\sqrt{\rho} = \frac{1}{\sqrt{\rho}}[\vec{\Delta}_E, F]\sqrt{\rho}. \tag{5.9}$$

Since $\nu^{(2)}$ depends on the antisymplectic matrix E_{AB} with lower indices, it is not clear how the formula (5.1) extends to the degenerate anti-Poisson case.

VI. APPLICATION TO BATALIN-VILKOVISKY QUANTIZATION

It is interesting to transcribe the Batalin-Vilkovisky quantization, based on the odd Laplacian Δ_ρ, into a quantization scheme that is based on the Δ_E operator, with the added benefit that no choice of measure density ρ is needed. Since the Δ_E operator takes semidensities to semidensities, this suggests that the Boltzmann factor $\exp[(i/\hbar)W_E]$ that appears in the quantum master equation

$$\Delta_E \exp\left[\frac{i}{\hbar}W_E\right] = 0 \tag{6.1}$$

should now be a semidensity, where

$$W_E = S + \sum_{n=1}^{\infty} (i\hbar)^n W_n \tag{6.2}$$

denotes the quantum action. In fact, this was a common interpretation (when restricting to Darboux coordinates) prior to the introduction of a density ρ around 1992; see, for instance, Ref. 10, pp. 440–441. If one only considers $\hbar$-independent coordinate transformations $\Gamma^A \to \Gamma'^A$ for simplicity, this implies that the one-loop factor e^{-W_1} is a semidensity, while the rest of the quantum action, i.e., the classical action S and the higher loop corrections W_n, $n \geq 2$, are scalars as usual. For instance, the nilpotent operator $F \mapsto e^{W_1}\Delta_E(e^{-W_1}F)$ takes scalars F to scalars.

At this stage it might be helpful to compare the above Δ_E approach to the Δ_ρ formalism. To this end, fix a density ρ. Then one can define a bona fide scalar quantum action W_ρ as

$$W_\rho := W_E + (i\hbar)\ln\sqrt{\rho}, \tag{6.3}$$

or equivalently,

$$e^{(i/\hbar)W_E} = \sqrt{\rho}e^{(i/\hbar)W_\rho}. \tag{6.4}$$

This scalar action W_ρ satisfies the modified quantum master equation

$$(\Delta_\rho + \nu_\rho)\exp\left[\frac{i}{\hbar}W_\rho\right] = 0, \tag{6.5}$$

cf. Eqs. (5.4), (5.9), (6.1), and (6.4). One may obtain the quantum master equation $\Delta_\rho \exp[(i/\hbar)W_\rho] = 0$ by additionally imposing the covariant condition $\nu_\rho = 0$, or equivalently $\Delta_E\sqrt{\rho} = 0$. However, this step is not necessary.

Returning now to the pure Δ_E approach with no ρ, the finite Δ_E-exact transformations of the form

$$e^{(i/\hbar)W'_E} = e^{-[\vec{\Delta}_E, \Psi]}e^{(i/\hbar)W_E}, \tag{6.6}$$

play an important role in taking solutions W_E to the quantum master Eq. (6.1) into new solutions W'_E. It is implicitly understood that all objects in Eq. (6.6) refer to the same (but arbitrary) coordinate frame. In general, Ψ is a Grasmann-odd operator that takes semidensities to semidensities. If Ψ is a scalar function (=zeroth-order operator), one derives

$$W'_E = e^{X_\Psi} W_E + (i\hbar)\frac{e^{X_\Psi}-1}{X_\Psi}\Delta_E \Psi . \tag{6.7}$$

The formula (6.7) is similar to the usual formula in the Δ_ρ formalism.[13] One may check that Eq. (6.7) is covariant with respect to general coordinate transformations.

The *W-X* formulation discussed in Refs. 5 and 13 carries over with only minor modifications, since the Δ_E operator is symmetric $\Delta_E^T = \Delta_E$. In short, the *W-X* formulation is a very general field-antifield formulation, based on two master actions, W_E and X_E, each satisfying a quantum master equation. At the operational level, *symmetric* means that the Δ_E operator, sandwiched between two semidensities under a (path) integral sign, may be moved from one semidensity to the other, using integration by part. This is completely analogous to the symmetry of the odd Laplacian $\Delta_\rho = \Delta_\rho^T$ itself. The X_E quantum action is a gauge-fixing part,

$$X_E = G_\alpha \lambda^\alpha + (i\hbar) H_E + \mathcal{O}(\lambda^*), \tag{6.8}$$

which contains the gauge-fixing constraints G_α in involution,

$$(G_\alpha, G_\beta) = G_\gamma U^\gamma_{\alpha\beta}. \tag{6.9}$$

The gauge-fixing functions G_α implement a generalization of the standard Batalin-Vilkovisky gauge-fixing procedure $\phi^*_\alpha = \partial\Psi/\partial\phi^\alpha$. In the simplest cases, the gauge-fixing conditions $G_\alpha = 0$ are enforced by integration over the Lagrange multipliers λ^α. See Ref. 13 for further details on the *W-X* formulation. The pertinent measure density in the partition function

$$\mathcal{Z} = \int [\mathrm{d}\Gamma][\mathrm{d}\lambda] e^{(i/\hbar)(W_E + X_E)} \tag{6.10}$$

is now located inside the one-loop parts of the W_E and the X_E actions. For instance, an on-shell expression for the one-loop factor e^{-H_E} is

$$e^{-H_E} = \sqrt{J\mathrm{sdet}(F^\alpha, G_\beta)}, \tag{6.11}$$

where $J = \mathrm{sdet}(\partial\overline{\Gamma}^A/\partial\Gamma^B)$ denotes the Jacobian of the transformation $\Gamma^A \to \overline{\Gamma}^A$ and $\overline{\Gamma}^A \equiv \{F^\alpha; G_\alpha\}$. The formula (6.11) differs from the original square root formula[13–15] by not depending on a ρ density, consistent with the fact that e^{-H_E} is no longer a scalar but a semidensity. We recall here the main point that the one-loop factor e^{-H_E} is independent of the F^α's and the partition function $\mathcal{Z}$ is independent of the G_α's in involution, cf. Eq. (6.9).

To summarize, the density ρ can altogether be avoided in the field-antifield formalism, at the cost of more complicated transformation rules. We stress that the above transcription has no consequences for the physics involved. For instance, the ambiguity that existed in the density ρ is still present in the choice of W_E and X_E.

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APPENDIX A: PROOF OF EQ. (5.6)

Consider a general (not necessarily infinitesimal) coordinate transformation $\Gamma^A \to \Gamma'^A$ between the "unprimed" and a "primed" coordinate systems, Γ^A and Γ'^A, respectively; cf. Eq. (3.1). The primed $\nu^{(0)}_\rho$ quantity (5.5) can be reexpressed with the help of the unprimed coordinates as

$$\nu'^{(0)}_{\rho'} := \frac{1}{\sqrt{\rho'}}(\Delta'_1\sqrt{\rho'}) = \frac{1}{\sqrt{\rho'}}(\Delta_J\sqrt{\rho'}) = \frac{1}{\sqrt{\rho}}(\Delta_1\sqrt{\rho}) - \frac{1}{\sqrt{J}}(\Delta_1\sqrt{J}) = \nu^{(0)}_{\rho} - \nu^{(0)}_{J}, \tag{A1}$$

where it is convenient (and natural) to introduce the quantity

$$\nu^{(0)}_{J} := \frac{1}{\sqrt{J}}(\Delta_1\sqrt{J}) \tag{A2}$$

with respect to the unprimed reference system. The third equality in Eq. (A1) uses a nontrivial property of the odd Laplacian (3.2). In the infinitesimal case $\delta\Gamma^A = X^A$, the expression for the Jacobian J reduces to a divergence $\ln J \approx \mathrm{div}_1 X$, and one calculates

$$\delta\nu^{(0)}_{\rho} = \nu'^{(0)}_{\rho'} - \nu^{(0)}_{\rho} = -\nu^{(0)}_{J} = -\Delta_1(\ln\sqrt{J}) - \frac{1}{2}(\ln\sqrt{J}, \ln\sqrt{J}) \approx -\frac{1}{2}\Delta_1 \,\mathrm{div}_1 X, \tag{A3}$$

which is Eq. (5.6).

APPENDIX B: PROOF OF EQ. (5.7)

The infinitesimal variation of $\nu^{(1)}$ yields four contributions to linear order in the variation $\delta\Gamma^A = X^A$,

$$\delta\nu^{(1)} = -\delta\nu^{(1)}_{I} - \delta\nu^{(1)}_{II} + \delta\nu^{(1)}_{III} + \delta\nu^{(1)}_{IV}. \tag{B1}$$

They are

$$\delta\nu^{(1)}_{I} := (-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial\Gamma^B}X^C\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^C}\frac{\vec{\partial}^l}{\partial\Gamma^A}E^{AB}\right), \tag{B2}$$

$$\delta\nu^{(1)}_{II} := (-1)^{\varepsilon_A}\frac{\vec{\partial}^l}{\partial\Gamma^B}\left(\left(\frac{\vec{\partial}^l}{\partial\Gamma^A}X^C\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^C}E^{AB}\right)\right) = \delta\nu^{(1)}_{I} + \delta\nu^{(1)}_{V}, \tag{B3}$$

$$\delta\nu^{(1)}_{III} := (-1)^{\varepsilon_A}\frac{\vec{\partial}^l}{\partial\Gamma^B}\frac{\vec{\partial}^l}{\partial\Gamma^A}\left(\left(X^A\frac{\overleftarrow{\partial}^r}{\partial\Gamma^C}\right)E^{CB}\right) = \delta\nu^{(1)}_{IV}, \tag{B4}$$

$$\delta\nu^{(1)}_{IV} := (-1)^{\varepsilon_A}\frac{\vec{\partial}^l}{\partial\Gamma^B}\frac{\vec{\partial}^l}{\partial\Gamma^A}\left(E^{AC}\left(\frac{\vec{\partial}^l}{\partial\Gamma^C}X^B\right)\right) = \delta\nu^{(1)}_{I} + \delta\nu^{(1)}_{V} + \delta\nu^{(1)}_{VI}, \tag{B5}$$

$$\delta\nu^{(1)}_{V} := (-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial\Gamma^C}E^{AB}\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^B}\frac{\vec{\partial}^l}{\partial\Gamma^A}X^C\right), \tag{B6}$$

$$\delta\nu^{(1)}_{VI} := (-1)^{\varepsilon_A}\frac{\vec{\partial}^l}{\partial\Gamma^A}\left(E^{AC}\frac{\vec{\partial}^l}{\partial\Gamma^C}\frac{\vec{\partial}^l}{\partial\Gamma^B}X^B(-1)^{\varepsilon_B}\right) = 2\Delta_1 \,\mathrm{div}_1 X, \tag{B7}$$

where we have noted various relations among the contributions. Altogether, the infinitesimal variation of $\nu^{(1)}$ becomes

$$\delta\nu^{(1)} = \delta\nu^{(1)}_{V} + 2\delta\nu^{(1)}_{VI}, \tag{B8}$$

which is Eq. (5.7).

APPENDIX C: PROOF OF EQ. (5.8)

The infinitesimal variation of

$$\nu^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BC}\left(\frac{\vec{\partial}^l}{\partial\Gamma^A}E^{CD}\right) \tag{C1}$$

yields eight contributions to linear order in the variation $\delta\Gamma^A = X^A$, which may be organized as 2×4 terms

$$\delta\nu^{(2)} = 2(-\delta\nu_I^{(2)} - \delta\nu_{II}^{(2)} + \delta\nu_{III}^{(2)} + \delta\nu_{IV}^{(2)}), \tag{C2}$$

due to a $(A,B)\leftrightarrow(D,C)$ symmetry in Eq. (C1). They are

$$\delta\nu_I^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BF}\left(X^F\frac{\overleftarrow{\partial}^r}{\partial\Gamma^C}\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^A}E^{CD}\right), \tag{C3}$$

$$\delta\nu_{II}^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BC}\left(\frac{\vec{\partial}^l}{\partial\Gamma^A}X^F\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^F}E^{CD}\right), \tag{C4}$$

$$\delta\nu_{III}^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BC}\frac{\vec{\partial}^l}{\partial\Gamma^A}\left(\left(X^C\frac{\overleftarrow{\partial}^r}{\partial\Gamma^F}\right)E^{FD}\right) = \delta\nu_I^{(2)} + \delta\nu_V^{(2)}, \tag{C5}$$

$$\delta\nu_{IV}^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BC}\frac{\vec{\partial}^l}{\partial\Gamma^A}\left(E^{CF}\left(\frac{\vec{\partial}^l}{\partial\Gamma^F}X^D\right)\right) = \delta\nu_{II}^{(2)} + \delta\nu_{VI}^{(2)}, \tag{C6}$$

$$\delta\nu_V^{(2)} := (-1)^{\varepsilon_A\varepsilon_C}E^{FD}\left(\frac{\vec{\partial}^l}{\partial\Gamma^D}E^{AB}\right)E_{BC}\left(\frac{\vec{\partial}^l}{\partial\Gamma^A}X^C\frac{\overleftarrow{\partial}^r}{\partial\Gamma^F}\right) = -\delta\nu_V^{(2)} + \delta\nu_{VI}^{(2)}, \tag{C7}$$

$$\delta\nu_{VI}^{(2)} := (-1)^{\varepsilon_A}\left(\frac{\vec{\partial}^l}{\partial\Gamma^C}E^{AB}\right)\left(\frac{\vec{\partial}^l}{\partial\Gamma^B}\frac{\vec{\partial}^l}{\partial\Gamma^A}X^C\right), \tag{C8}$$

where we have noted various relations among the contributions. The Jacobi identity (2.8) for E^{AB} is used in the second equality of Eq. (C7). Altogether, the infinitesimal variation of $\nu^{(2)}$ becomes

$$\delta\nu^{(2)} = 3\,\delta\nu_{VI}^{(2)}, \tag{C9}$$

which is Eq. (5.8).

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Hydrodynamic chains and the classification of their Poisson brackets

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Infinite component Poisson brackets of the Dubrovin-Novikov type [Sov. Math. Dokl. **27**, 665–669 (1983)] are considered. The corresponding Jacobi identity is significantly simplified in the Liouville coordinates since the skew-symmetry condition is automatically satisfied. The concept of M Poisson bracket connected with hydrodynamic chains is introduced. Then the Jacobi identity is a nonlinear system of equations in partial derivatives which can be completely integrated. In such a case, a classification of infinite component Poisson brackets of the Dubrovin-Novikov type can be obtained. Two simplest examples, $M=0$ and $M=1$, are considered. Also infinite component Poisson brackets of the Ferapontov [Am. Math. Soc. Transl. **170**, 38–58 (1995)] type can be simplified in the Liouville coordinates. The Jacobi identity for infinite component Poisson brackets of the Ferapontov-Mokhov type [Russ. Math. Surveys **45**, 218–219 (1990)] is presented in the Liouville coordinates [DOI: 10.1063/1.2399086]

I. INTRODUCTION

The theory of the hydrodynamic-type systems,

$$u_t^i = v_j^i(\mathbf{u})u_x^j, \quad i,j = 1,2,\ldots,N, \tag{1}$$

integrable by the generalized hodograph method (see Ref. 25) starts with the hydrodynamic-type systems equipped with a local Hamiltonian structure,

$$u_t^i = \{u^i, \bar{\mathbf{h}}\} = [g^{ij}D_x - g^{is}\Gamma_{sk}^j u_x^k]\frac{\delta \bar{\mathbf{h}}}{\delta u^j},$$

determined by the Hamiltonian $\bar{\mathbf{h}} = \int h(\mathbf{u})\mathrm{d}x$ and by the Dubrovin-Novikov bracket (a differential-geometric Poisson bracket of the first order, see Ref. 5)

$$\{u^i(x), u^j(x')\} = [g^{ij}D_x - g^{is}\Gamma_{sk}^j u_x^k]\delta(x-x'), \quad i,j = 1,2,\ldots,N, \tag{2}$$

where the symmetric and nondegenerate metric $g^{ij}(\mathbf{u})$ is flat, and the Christoffel symbols are given by $\Gamma_{sk}^j = \frac{1}{2}g^{jm}(\partial_s g_{mk} + \partial_k g_{ms} - \partial_m g_{sk})$. Then the above Poisson bracket can be written via the so-called *Liouville* coordinates $A^k(\mathbf{u})$ (see Ref. 5),

$$\{A^k(x), A^n(x')\} = [\mathcal{W}^{kn}(\mathbf{A})D_x + D_x\mathcal{W}^{nk}(\mathbf{A})]\delta(x-x'), \quad k,n = 1,2,\ldots,N. \tag{3}$$

The theory of Poisson brackets in *infinite* component case,

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$$\{U^i,U^j\}=[G^{ij}(\mathbf{U})D_x+\Gamma^{ij}_k(\mathbf{U})U^k_x]\delta(x-x'),\quad i,j,k=1,2,3,\ldots, \tag{4}$$

starts with the pioneering papers (Refs. 13 and 14) dedicated to integrable hydrodynamic chains (see below) and their properties. Later these Poisson brackets [See. Eq. (2)] were considered by Dorfman in Ref. 4 (N component case (2) was completely investigated by Dubrovin and Novikov in Ref. 5 for the nondegenerate matrix G^{ij}; the degenerate case was considered by Grinberg in Ref. 12; see also the "zero curvature" subcase in Ref. 17).

Theorem (Ref. 4): *The Poisson bracket (4) is skew symmetric and satisfies the Jacobi identity property if and only if*

$$G^{ij}=G^{ji},\quad \partial_k G^{ij}=\Gamma^{ij}_k+\Gamma^{ji}_k,\quad G^{ik}\Gamma^{jn}_k=G^{jk}\Gamma^{in}_k,$$

$$0=\Gamma^{ij}_n\Gamma^{nm}_k-\Gamma^{im}_n\Gamma^{nj}_k+G^{in}(\partial_n\Gamma^{mj}_k-\partial_k\Gamma^{mj}_n),$$

$$\begin{aligned}0=&(\partial_n\Gamma^{ij}_k-\partial_k\Gamma^{ij}_n)\Gamma^{nm}_p+(\partial_n\Gamma^{mi}_k-\partial_k\Gamma^{mi}_n)\Gamma^{nj}_p+(\partial_n\Gamma^{jm}_k-\partial_k\Gamma^{jm}_n)\Gamma^{ni}_p\\&+(\partial_n\Gamma^{ij}_p-\partial_p\Gamma^{ij}_n)\Gamma^{nm}_k+(\partial_n\Gamma^{mi}_p-\partial_p\Gamma^{mi}_n)\Gamma^{nj}_k+(\partial_n\Gamma^{jm}_p-\partial_p\Gamma^{jm}_n)\Gamma^{ni}_k.\end{aligned} \tag{5}$$

The first main observation of this paper is that the above nonlinear system of equations in partial derivatives simplifies to the more compact form

$$(\mathcal{W}^{in}+\mathcal{W}^{ni})\partial_n\mathcal{W}^{kj}=(\mathcal{W}^{jn}+\mathcal{W}^{nj})\partial_n\mathcal{W}^{ki},$$

$$\partial_n\mathcal{W}^{ij}\partial_m\mathcal{W}^{kn}=\partial_n\mathcal{W}^{kj}\partial_m\mathcal{W}^{in} \tag{6}$$

in the Liouville coordinates $A^i(\mathbf{U})$ [see Eq. (3); see also Refs. 5 and 15]. Thus, the Liouville coordinates A^k are most natural coordinates (except flat coordinates in the finite component case, see Ref. 5).

Indeed, the first two relationships in Eq. (5) are the skew-symmetry property satisfied automatically in the Liouville coordinates. The last restriction in Eq. (5) vanishes in the Liouville coordinates because $G^{ik}(\mathbf{A})=\mathcal{W}^{ik}+\mathcal{W}^{ki}$, $\Gamma^{ij}_k(\mathbf{A})=\partial_k\mathcal{W}^{ji}$. Thus, the nonlinear PDE system (5) reduces to the Jacobi identity (6) in this special case.

Remark: Elements $\mathcal{W}^{ik}$ depend on *all* field variables u^n $(n=1,2,\ldots,N)$ in the finite-component case [hydrodynamic-type systems (1)]; elements $\mathcal{W}^{ik}$ depend on just a *finite* number of moments A^k in the infinite component case (hydrodynamic chains). Thus, the Jacobi identity (6) contains a finite number of equations for any *fixed* indices i,j,k,m. Then this overdetermined system can be solved *iteratively* for all indices i,j,k,m, if a dependence of elements $\mathcal{W}^{ik}$ on moments A^k is determined by some special prescribed law. Such a simple dependence is considered below.

This paper deals with the hydrodynamic chains [see Eq. (1)],

$$U^k_t=\sum_{m=0}^{M_k}V^k_m(\mathbf{U})U^m_x,\quad k=0,1,2,\ldots, \tag{7}$$

where the number of field variables U^k is infinite [in comparison with hydrodynamic-type systems (1)], all components $V^k_m(\mathbf{U})$ are functions of a finite number of the field variables U^n (for any fixed indices k,m), and M_k are some integers [i.e., M_k are integer values of a discrete function $M(\mathbf{k})$]. Thus, the hydrodynamic chain (7) is an extension of the hydrodynamic-type system (1) to an infinite component case. Plenty known integrable hydrodynamic chains (see Refs. 2, 3, 9, 16, 21, 22, and 24) belong to the simplest class $M_k=k+1$.

Without loss of generality we restrict our consideration on a *monotonic growth* of coefficients M_k. All further formulas, definitions, theorems, and conjectures are expressed via the Liouville coordinates $A^k(\mathbf{U})$.

Definition: *The hydrodynamic chain (7) is said to be Hamiltonian if it can be written in the form*

$$A_t^i = [\mathcal{W}^{ij}(\mathbf{A})D_x + D_x\mathcal{W}^{ji}(\mathbf{A})]\frac{\delta\bar{\mathbf{H}}}{\delta A^j}, \quad i,j = 0,1,2,\ldots, \tag{8}$$

where the coefficients $\mathcal{W}^{ij}(\mathbf{A})$ satisfy the Jacobi identity (6).

The Hamiltonian $\bar{\mathbf{H}} = \int \mathbf{H} dx$ depends on a finite number of first moments A^k (i.e., $k = 0,1,\ldots,K$, where K is some integer).

Definition: *The Hamiltonian hydrodynamic chain (8) is said to be integrable if it possesses an infinite series of conservation laws.*

The main problem in a classification of integrable hydrodynamic chains is a description of the Poisson brackets [see Eq. (3)]

$$\{A^k(x), A^n(x')\} = [\mathcal{W}^{kn}(\mathbf{A})D_x + D_x\mathcal{W}^{nk}(\mathbf{A})]\delta(x-x'), \quad k,n = 1,2,\ldots. \tag{9}$$

Many publications are devoted to various particular cases (see, for instance, Refs. 4, 13, and 14), some of them will be described below. In this paper I present the program of an investigation of these Poisson brackets.

In this paper we consider the very important case

$$\mathcal{W}^{kn}_{(M)} = \mathcal{W}^{kn}(A^0, A^1, \ldots, A^{k+n-M}), \quad M = 0, \pm 1, \pm 2, \ldots. \tag{10}$$

Definition: *The corresponding Poisson brackets (9) are said to be M brackets.*

The simplest subcases $\mathcal{W}^{kn}_{(0)} = \mathcal{W}^{kn}(B^0, B^1, \ldots, B^{k+n})$ and $\mathcal{W}^{kn}_{(1)} = \mathcal{W}^{kn}(A^0, A^1, \ldots, A^{k+n-1})$ are considered in detail below. The first example is the Kupershmidt-Manin bracket ($M=1$)

$$\{A^k, A^n\}_3 = (kA^{k+n-1}D_x + nD_xA^{k+n-1})\delta(x-x') \tag{11}$$

found in Ref. 14 [the index 3 means that the above Poisson bracket is associated with the third local Hamiltonian structure, where the Hamiltonian density is given by $\mathbf{H}_2 = A^2 + (A^0)^2$]. The second example is the Kupershmidt bracket ($M=0$)

$$\{B^k, B^n\} = [(k+\beta)B^{k+n}D_x + (n+\beta)D_xB^{k+n}]\delta(x-x') \tag{12}$$

found in Ref. 13. Infinitely many local Hamiltonian structures for the Benney hydrodynamic chain (see Ref. 23) and for the Kupershmidt hydrodynamic chains (see Ref. 22) are examples of these M brackets. The third example ($M=0$),

$$\{A^k, A^n\}_2 = \Bigg[(k+1)A^{k+n}D_x + (n+1)D_xA^{k+n} + n(k+1)A^{k-1}D_xA^{n-1} + \sum_{m=0}^{n-1}(mA^{n-1-m}D_xA^{k-1+m} + (k-n+m)A^{k-1+m}D_xA^{n-1-m})\Bigg]\delta(x-x'),$$

is the second local Poisson bracket for the Benney hydrodynamic chain (where the Hamiltonian density is given by $\mathbf{H}_1 = A^1$; see Ref. 13), where the moments A^k are no longer the Liouville coordinates. Nevertheless, this bi-Hamiltonian structure completely determines the Benney hydrodynamic chain together with its commuting flows.

The second observation successfully utilized in this paper is that the Jacobi identity (6),

$$\sum_{n=0}^{k+j-M}(\mathcal{W}^{jn}_{(M)} + \mathcal{W}^{ni}_{(M)})\partial_n\mathcal{W}^{kj}_{(M)} = \sum_{n=0}^{k+i-M}(\mathcal{W}^{jn}_{(M)} + \mathcal{W}^{nj}_{(M)})\partial_n\mathcal{W}^{ki}_{(M)},$$

$$\sum_{n=0}^{k+j-M} \partial_n \mathcal{W}_{(M)}^{jk} \partial_m \mathcal{W}_{(M)}^{in} = \sum_{n=0}^{k+i-M} \partial_n \mathcal{W}_{(M)}^{ik} \partial_m \mathcal{W}_{(M)}^{jn}, \tag{13}$$

is an overdetermined system which can be solved completely. Indeed, since all coefficients $\mathcal{W}_{(M)}^{ij}$ depend on *different sets* of the moments A^k (cf. a similar problem in Refs. 9 and 21), the elimination of higher (step by step) moment dependences leads to systems of ordinary differential equations with respect to each lower moment. The illustrative examples are considered in this paper for $M=0$ and $M=1$. Without loss of generality and for simplicity we restrict our consideration to *several first* equations of Eq. (13) for computation of several first coefficients $\mathcal{W}_{(M)}^{ij}$; all other higher coefficients can be found in the same way utilizing next equations from Eq. (13). Moreover, suppose that several first coefficients $\mathcal{W}_{(M)}^{ij}$ are found (see the examples below), then all first derivatives of *higher* coefficients $\mathcal{W}_{(M)}^{ij}$ can be expressed from the nonlinear PDE system (13). It means that the compatibility conditions $\partial_k(\partial_n \mathcal{W}_{(M)}^{ij}) = \partial_n(\partial_k \mathcal{W}_{(M)}^{ij})$ should lead to nonlinear PDE equations determining *lower* coefficients $\mathcal{W}_{(M)}^{ij}$ which are already found at the previous stage of computations. Then these higher coefficients $\mathcal{W}_{(M)}^{ij}$ can be found in quadratures.

Remark: Of course, the M bracket is just one among many other examples. For instance, another new Poisson bracket is given by

$$\{A^k, A^n\} = (A^{k\cdot n} D_x + D_x A^{k\cdot n})\,\delta(x-x').$$

All other Poisson brackets (8) and corresponding integrable hydrodynamic chains shall be discussed elsewhere.

At the end of this paper, local Poisson brackets are generalized to the simplest *nonlocal* case (associated with a metric of constant curvature[10] in N component nondegenerate case).

II. *M* BRACKETS AND INTEGRABLE HYDRODYNAMIC CHAINS

In this section, integrable Hamiltonian hydrodynamic chains (8) determined by M brackets (10),

$$A_t^k = \{A^k, \bar{\mathbf{H}}\}_M = [\mathcal{W}_{(M)}^{kn} D_x + D_x \mathcal{W}_{(M)}^{nk}] \frac{\delta \bar{\mathbf{H}}}{\delta A^n}, \tag{14}$$

are considered.

Definition: *The conservation law density* $\mathbf{H}_m$ *is said to be a Casimir density, if the corresponding right hand side (rhs) of Eq. (14) vanishes, i.e.,*

$$[\mathcal{W}_{(M)}^{kn} D_x + D_x \mathcal{W}_{(M)}^{nk}] \frac{\partial \mathbf{H}_m}{\partial A^n} \equiv 0.$$

Definition: *The conservation law density* $\mathbf{H}_M$ *is said to be a momentum density if*

$$[\mathcal{W}_{(M)}^{kn} D_x + D_x \mathcal{W}_{(M)}^{nk}] \frac{\partial \mathbf{H}_M}{\partial A^n} \equiv A_x^k.$$

We restrict our further consideration by a set of some *natural* assumptions (for $M \geqslant 1$). In fact, we have two main cases only.

1. If $M \geqslant 1$, suppose M brackets satisfy the *auxiliary* (natural) restrictions ("normalization") given by

$$\mathcal{W}_{(M)}^{Mk} = A^k, \quad k = 0,1,2,\ldots,$$

$$\mathcal{W}_{(M)}^{sk} = 0, \quad 0 \leqslant s < M, \quad k \geqslant M - s.$$

$$\mathcal{W}_{(M)}^{kn} = \bar{\mathcal{W}}_{(M)}^{kn} = \text{const}, \quad k = 0,1,2,\ldots,M-1, \quad 0 \leqslant n \leqslant M-1-k. \tag{15}$$

Then the corresponding Poisson brackets possess M Casimirs. The Casimirs can be chosen as $\bar{\mathbf{H}}_k = \int A^k \mathrm{d}x$ $(k=0,1,2,\ldots,M-1)$, while the momentum can be chosen as $\bar{\mathbf{H}}_M = \int A^M \mathrm{d}x$. For simplicity we restrict our consideration to the hydrodynamic chain (14) determined by the simplest Hamiltonian $\bar{\mathbf{H}}_{M+1} = \int \mathbf{H}_{M+1}(A^0, A^1, A^2, \ldots, A^{M+1})\mathrm{d}x$. Thus, the hydrodynamic chain (14) possesses at least $M+2$ conservation laws (for an arbitrary Hamiltonian density $\mathbf{H}$), where the first M conservation laws are the Casimirs

$$A_t^k = \partial_x \left(\sum_{n=0}^{M-k-1} (\bar{\mathcal{W}}_{(M)}^{kn} + \bar{\mathcal{W}}_{(M)}^{nk}) \frac{\delta \mathbf{H}_{M+1}}{\partial A^n} + \sum_{n=M-k}^{M+1} \mathcal{W}_{(M)}^{nk} \frac{\partial \mathbf{H}_{M+1}}{\partial A^n} \right), \quad k = 0,1,2,\ldots,M-1.$$

The conservation law of the momentum is

$$A_t^M = \partial_x \left(\sum_{n=0}^{M+1} (\mathcal{W}_{(M)}^{nM} + A^n) \frac{\partial \mathbf{H}_{M+1}}{\partial A^n} - \mathbf{H}_{M+1} \right).$$

The conservation law of the energy is

$$\partial_t \mathbf{H}_{M+1} = \partial_x \left[\sum_{k=0}^{M+1} \sum_{n=0}^{M+1} \mathcal{W}_{(M)}^{kn} \frac{\partial \mathbf{H}_{M+1}}{\partial A^k} \frac{\partial \mathbf{H}_{M+1}}{\partial A^n} \right].$$

Remark: In the general case, the corresponding hydrodynamic chain is given by

$$A_t^k = \sum_{n=0}^{M+1} V_n^k(\mathbf{A}) A_x^n, \quad k = 0,1,\ldots,M-1, \quad A_t^k = \sum_{n=0}^{k+1} V_n^k(\mathbf{A}) A_x^n, \quad k = M, M+1, \ldots. \tag{16}$$

The case $M=0$ can be incorporated in the previous case. The corresponding Poisson bracket has a set of constraints (cf. the above case)

$$\mathcal{W}_{(0)}^{0k} = A^k, \quad k = 0,1,2,\ldots;$$

a corresponding hydrodynamic chain (for an arbitrary Hamiltonian density) possesses two conservation laws (of the energy and of the momentum, see the above formulas for $M=0$) only.

Conjecture: The hydrodynamic chain (14) determined by the Hamiltonian density $\mathbf{H}_{M+1}$ is *integrable* if it possesses an extra conservation law density $\mathbf{H}_{M+2}$. For instance, this statement is proved for integrable hydrodynamic chains associated with the Kupershmidt bracket (see Ref. 8) and with the Kupershmidt-Manin bracket (see Ref. 9).

2. If $M \leqslant -1$, then the corresponding Poisson brackets do not possess Casimirs and a momentum. Moreover, simplest hydrodynamic chains (14) determined by the *lowest* Hamiltonian $\bar{\mathbf{H}}_0 = \int \mathbf{H}_0(A^0)\mathrm{d}x$ contain $M_k = k+M$ elements in the rhs of Eq. (7).

Examples: The Kupershmidt hydrodynamic chains (see Ref. 13) possess an infinite set of local Hamiltonian structures determined by M brackets (9), where the first of them are (for the indices $M=0,1,2$, respectively; see Ref. 22)

$$\{C^k, C^n\} = [(\beta k+1)C^{k+n}D_x + (\beta n+1)D_x C^{k+n}]\delta(x-x'),$$

$$\{B^0, B^0\} = \beta\delta'(x-x'), \quad \{B^k, B^n\} = [(\beta k+1-\beta)B^{k+n-1}D_x + (\beta n+1-\beta)D_x B^{k+n-1}]\delta(x-x'),$$

$$\{A^0, A^1\} = \{A^1, A^0\} = \beta\delta'(x-x'), \quad \{A^1, A^1\} = (\beta-1)(A^0 D_x + D_x A^0)\delta(x-x'),$$

$$\{A^k,A^n\}=[(\beta k+1-2\beta)A^{k+n-2}D_x+(\beta n+1-2\beta)D_xA^{k+n-2}]\delta(x-x').$$

The first Poisson bracket is the well-known Kupershmidt bracket (12); two other Poisson brackets are new.

The most interesting class of these Poisson brackets is provided by *polynomial* (with respect to the moments A^k) coefficients $\mathcal{W}^{kn}_{(M)}$. The simplest case is given by the *linear* Poisson brackets determined by

$$\mathcal{W}^{kn}_{(M)}=e^{kn}_{(M)}A^{k+n-M},$$

where $e^{kn}_{(M)}$ are some constants satisfying the algebraic system [see Eq. (6)]

$$(e^{p,k+n-M}_{(M)}+e^{k+n-M,p}_{(M)})e^{nk}_{(M)}=(e^{k,n+p-M}_{(M)}+e^{n+p-M,k}_{(M)})e^{np}_{(M)},\quad e^{sp}_{(M)}e^{k,s+p-M}_{(M)}=e^{kp}_{(M)}e^{s,k+p-M}_{(M)},$$

possibly connected with an infinite dimensional analogue of the Frobenius algebras (see Ref. 1). Let us look for a particular solution in the form

$$e^{kn}_{(M)}=(Ak+Bn+C),$$

where A and B are some constants. The substitution of this ansatz in the above algebraic system yields the Kupershmidt brackets (see Ref. 13) determined by an arbitrary value A, but $B=0$. More general linear Poisson brackets

$$\mathcal{W}^{kn}_{(M)}=\sum_{s=0}^{k+n-M}e^{kn}_{(M)s}A^s$$

were considered by Dorfman in Ref. 4. For instance,

$$\{A^0,A^0\}=\varepsilon\delta'(x-x'),\quad \{A^k,A^n\}=\sum_{m=0}^{M}\gamma_m[kA^{m+k+n-1}D_x+nD_xA^{m+k+n-1}]\delta(x-x'),$$

where ε and γ_k are arbitrary constants.

Higher order homogeneous polynomials create more complicated Poisson brackets, which can be described by algebraic tools. For instance, the second nontrivial case is the *quadratic* Poisson brackets determined by

$$\mathcal{W}^{kn}_{(M)}(A^0,A^1,\ldots,A^{k+n-M})=\frac{1}{2}\sum_{m=0}^{k+n-M}e^{kn}_{(M)m}A^mA^{k+n-m-M},$$

where $e^{kn}_{(M)m}\equiv e^{kn}_{(M)k+n-m-M}$ are some constants, which can be found by a direct substitution in the nonlinear PDE system (13). The corresponding system of algebraic relations is very complicated and will be investigated in detail elsewhere.

III. FIRST EXAMPLE: $M=0$

We omit the subindex in all components $\mathcal{W}^{nk}_{(0)}$ of the Poisson bracket [see Eq. (9), $M=0$],

$$\{B^k,B^n\}=[\mathcal{W}^{kn}(B^0,B^1,\ldots,B^{k+n})D_x+D_x\mathcal{W}^{nk}(B^0,B^1,\ldots,B^{k+n})]\delta(x-x').$$

The nonlinear PDE system (13)

$$\sum_{m=0}^{n+k}(\mathcal{W}^{pm}+\mathcal{W}^{mp})\partial_m\mathcal{W}^{nk}=\sum_{m=0}^{n+p}(\mathcal{W}^{km}+\mathcal{W}^{mk})\partial_m\mathcal{W}^{np},$$

$$\sum_{m=0}^{n+k} \partial_m \mathcal{W}^{kn} \partial_s \mathcal{W}^{pm} = \sum_{m=0}^{n+p} \partial_m \mathcal{W}^{pn} \partial_s \mathcal{W}^{km}$$

is an overdetermined system describing a family of local Poisson brackets connected with the Hamiltonian hydrodynamic chains.

Let us write several first nonlinear PDEs from the nonlinear PDE system (13),

$$(\mathcal{W}^{10} + B^1)\partial_0 \mathcal{W}^{10} + 2\mathcal{W}^{11}\partial_1 \mathcal{W}^{10} = 2B^0 \partial_0 \mathcal{W}^{11} + (B^1 + \mathcal{W}^{10})\partial_1 \mathcal{W}^{11} + (B^2 + \mathcal{W}^{20})\partial_2 \mathcal{W}^{11},$$

$$\partial_1 \mathcal{W}^{10} \partial_0 \mathcal{W}^{21} = \partial_1 \mathcal{W}^{20} \partial_0 \mathcal{W}^{11} + \partial_2 \mathcal{W}^{20} \partial_0 \mathcal{W}^{12},$$

$$\partial_0 \mathcal{W}^{10} \partial_1 \mathcal{W}^{20} + \partial_1 \mathcal{W}^{10} \partial_1 \mathcal{W}^{21} = \partial_0 \mathcal{W}^{20} \partial_1 \mathcal{W}^{10} + \partial_1 \mathcal{W}^{20} \partial_1 \mathcal{W}^{11} + \partial_2 \mathcal{W}^{20} \partial_1 \mathcal{W}^{12},$$

$$\partial_0 \mathcal{W}^{10} \partial_2 \mathcal{W}^{20} + \partial_1 \mathcal{W}^{10} \partial_2 \mathcal{W}^{21} = \partial_1 \mathcal{W}^{20} \partial_2 \mathcal{W}^{11} + \partial_2 \mathcal{W}^{20} \partial_2 \mathcal{W}^{12},$$

$$\partial_1 \mathcal{W}^{10} \partial_3 \mathcal{W}^{21} = \partial_2 \mathcal{W}^{20} \partial_3 \mathcal{W}^{12},$$

where the auxiliary restrictions (normalization)

$$\mathcal{W}^{0k} \equiv B^k$$

are consequences of the existence of a conservation law of the momentum $\bar{\mathbf{H}}_0 = \int B^0 \mathrm{d}x$. This system involves just four first moments B^0, B^1, B^2, and B^3. It is enough to find coefficients $\mathcal{W}^{10}$, $\mathcal{W}^{11}$, and $\mathcal{W}^{20}$. For instance, $\mathcal{W}^{10}$ is a solution of the Monge-Ampere equation

$$(\mathcal{W}^{10})_{00}(\mathcal{W}^{10})_{11} - [(\mathcal{W}^{10})_{01}]^2 + \varphi'^2(B^0)[(\mathcal{W}^{10})_1]^2 = 0, \tag{17}$$

where $\varphi(B^0)$ is some function (determined from the compatibility conditions $[(\mathcal{W}^{11})_1]_2 = [(\mathcal{W}^{11})_2]_1$, $[(\mathcal{W}^{11})_1]_0 = [(\mathcal{W}^{11})_0]_1$, and $[(\mathcal{W}^{11})_0]_2 = [(\mathcal{W}^{11})_2]_0$; see expressions below), and each subindex k means the corresponding derivative with respect to the moment B^k. Moreover,

$$\mathcal{W}^{20} = B^2(\mathcal{W}^{10})_1 + G,$$

where $G(p,q)$ is a solution of the Euler-Darboux-Poisson equation

$$G_{pq} = \frac{\varphi''(B^0)}{4\varphi'^2(B^0)}(G_p - G_q), \quad \varphi(B^0) = \frac{1}{2}(p-q),$$

$$q = \ln[(\mathcal{W}^{10})_1] - \varphi(B^0), \quad p = \ln[(\mathcal{W}^{10})_1] + \varphi(B^0).$$

Explicit expressions for all other coefficients (depending on higher moments B^k, $k=3,4,5,\ldots$) can be found recursively in *complete* differentials. For instance, the equation

$$(\mathcal{W}^{11})_2 = \frac{2[(\mathcal{W}^{10})_1]^2(B^0(\mathcal{W}^{10})_{00} + (\mathcal{W}^{10} + B^1)(\mathcal{W}^{10})_{10} + \mathcal{W}^{11}(\mathcal{W}^{10})_{11})}{MB^2 + N},$$

where (now M stands for a function, while it had been used as an integer before)

$$M = [1 + (\mathcal{W}^{10})_1](\mathcal{W}^{10})_1(\mathcal{W}^{10})_{11} + 2B^0[(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{110} - (\mathcal{W}^{10})_{10}(\mathcal{W}^{10})_{11}]$$
$$+ (\mathcal{W}^{10} + B^1)[(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{111} - ((\mathcal{W}^{10})_{11})^2],$$

$$N = G(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{11} + 2B^0[G_{10}(\mathcal{W}^{10})_1 - G_1(\mathcal{W}^{10})_{10}] + [(\mathcal{W}^{10})_1 + B^1][G_{11}(\mathcal{W}^{10})_1 - G_1(\mathcal{W}^{10})_{11}],$$

can be solved up to some function of B^0 and B^1, which can be found in complete differentials by a substitution into other derivatives,

$$(\mathcal{W}^{11})_1 = (\mathcal{W}^{11})_2 \frac{[(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{111} - ((\mathcal{W}^{10})_{11})^2]B^2 + G_{11}(\mathcal{W}^{10})_1 - G_1(\mathcal{W}^{10})_{11}}{(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{11}} + K,$$

$$(\mathcal{W}^{11})_0 = (\mathcal{W}^{11})_2 \frac{[(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{110} - (\mathcal{W}^{10})_{10}(\mathcal{W}^{10})_{11}]B^2 + G_{10}(\mathcal{W}^{10})_1 - G_1(\mathcal{W}^{10})_{10}}{(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{11}} - L,$$

where

$$K = \frac{(\mathcal{W}^{10})_0(\mathcal{W}^{10})_{11} - 2(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{10}}{(\mathcal{W}^{10})_{11}}, \quad L = \frac{(\mathcal{W}^{10})_1(\mathcal{W}^{10})_{00}}{(\mathcal{W}^{10})_{11}}.$$

Remark: The Monge-Ampere equation (17) was derived in Ref. 9 in a classification of integrable hydrodynamic chains

$$\partial_t \mathbf{H}_0 = \partial_x F_{10}(\mathbf{H}_0, \mathbf{H}_1), \quad \partial_t \mathbf{H}_1 = \partial_x F_{11}(\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2), \quad \partial_t \mathbf{H}_2 = \partial_x F_{12}(\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3), \ldots .$$

Thus, we have a good *indication* that these hydrodynamic chains are connected with the above local Hamiltonian structure (as well as *possibly* other M brackets; see the next section).

Integrable hydrodynamic chain (7) possesses an infinite set of commuting flows, where the first two of them,

$$B_t^k = [\mathcal{W}^{kn}(B^0, B^1, \ldots, B^{k+n})D_x + D_x\mathcal{W}^{nk}(B^0, B^1, \ldots, B^{k+n})]\frac{\delta \bar{\mathbf{H}}_1}{\delta B^n}, \tag{18}$$

$$B_y^k = [\mathcal{W}^{kn}(B^0, B^1, \ldots, B^{k+n})D_x + D_x\mathcal{W}^{nk}(B^0, B^1, \ldots, B^{k+n})]\frac{\delta \bar{\mathbf{H}}_2}{\delta B^n}, \tag{19}$$

are determined by the Hamiltonians $\bar{\mathbf{H}}_1 = \int \mathbf{H}_1(B^0, B^1)\mathrm{d}x$ and $\bar{\mathbf{H}}_2 = \int \mathbf{H}_2(B^0, B^1, B^2)\mathrm{d}x$.

Let us write the first two equations from Eq. (18) and the first equation from Eq. (19),

$$B_t^0 = (B^0 D_x + D_x B^0)\frac{\delta \bar{\mathbf{H}}_1}{\delta B^0} + [B^1 D_x + D_x \mathcal{W}^{10}(B^0, B^1)]\frac{\delta \bar{\mathbf{H}}_1}{\delta B^1},$$

$$B_t^1 = [\mathcal{W}^{10}(B^0, B^1)D_x + D_x B^1]\frac{\delta \bar{\mathbf{H}}_1}{\delta B^0} + [\mathcal{W}^{11}(B^0, B^1, B^2)D_x + D_x \mathcal{W}^{11}(B^0, B^1, B^2)]\frac{\delta \bar{\mathbf{H}}_1}{\delta B^1},$$

$$B_y^0 = (B^0 D_x + D_x B^0)\frac{\delta \bar{\mathbf{H}}_2}{\delta B^0} + [B^1 D_x + D_x \mathcal{W}^{10}(B^0, B^1)]\frac{\delta \bar{\mathbf{H}}_2}{\delta B^1} + [B^2 D_x + D_x \mathcal{W}^{20}(B^0, B^1, B^2)]\frac{\delta \bar{\mathbf{H}}_2}{\delta B^2}.$$

These three equations can be written in the conservative form

$$\partial_t \mathbf{H}_0 = \partial_x F_{10}(\mathbf{H}_0, \mathbf{H}_1), \quad \partial_t \mathbf{H}_1 = \partial_x F_{11}(\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2), \quad \partial_y \mathbf{H}_0 = \partial_x F_{20}(\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2),$$

where

$$F_{10}(\mathbf{H}_0, \mathbf{H}_1) = 2B^0\frac{\partial \mathbf{H}_1}{\partial B^0} + (\mathcal{W}^{10} + B^1)\frac{\partial \mathbf{H}_1}{\partial B^1} - \mathbf{H}_1,$$

$$F_{11}(\mathbf{H}_0,\mathbf{H}_1,\mathbf{H}_2)=B^0\left(\frac{\partial \mathbf{H}_1}{\partial B^0}\right)^2+(\mathcal{W}^{10}+B^1)\frac{\partial \mathbf{H}_1}{\partial B^0}\frac{\partial \mathbf{H}_1}{\partial B^1}+\mathcal{W}^{11}\left(\frac{\partial \mathbf{H}_1}{\partial B^1}\right)^2,$$

$$F_{20}(\mathbf{H}_0,\mathbf{H}_1,\mathbf{H}_2)=2B^0\frac{\partial \mathbf{H}_2}{\partial B^0}+(\mathcal{W}^{10}+B^1)\frac{\partial \mathbf{H}_2}{\partial B^1}+(\mathcal{W}^{20}+B^2)\frac{\partial \mathbf{H}_2}{\partial B^2}-\mathbf{H}_2.$$

Let us introduce the potential function z, where $\mathbf{H}_0=z_x$, $F_{10}(\mathbf{H}_0,\mathbf{H}_1)=z_t$, and $F_{20}(\mathbf{H}_0,\mathbf{H}_1,\mathbf{H}_2)=z_y$. Then one can substitute $\mathbf{H}_1(z_x,z_t)$ and $\mathbf{H}_2(z_x,z_t,z_y)$ into the second equation,

$$\partial_t \mathbf{H}_1(z_x,z_t)=\partial_x F_{11}(z_x,\mathbf{H}_1(z_x,z_t),\mathbf{H}_2(z_x,z_t,z_y)).$$

This 2+1 quasilinear equation of the second order is integrable by the method of hydrodynamic reductions[7] (or by introducing pseudopotentials; see Refs. 7 and 26). The Hamiltonian structure of this equation is unknown, while the Hamiltonian structure of corresponding hydrodynamic chains (18) and (19) is defined.

IV. SECOND EXAMPLE: *M*=1

We omit the subindex in all components $\mathcal{W}^{nk}_{(1)}$ of the Poisson bracket [see Eq. (9), $M=1$]

$$\{A^k,A^n\}=[\mathcal{W}^{kn}(A^0,A^1,\ldots,A^{k+n-1})D_x+D_x\mathcal{W}^{nk}(A^0,A^1,\ldots,A^{k+n-1})]\delta(x-x').$$

The nonlinear PDE system (13)

$$\sum_{m=0}^{n+k-1}(\mathcal{W}^{pm}+\mathcal{W}^{mp})\partial_m\mathcal{W}^{nk}=\sum_{m=0}^{n+p-1}(\mathcal{W}^{km}+\mathcal{W}^{mk})\partial_m\mathcal{W}^{np},$$

$$\sum_{m=0}^{n+k-1}\partial_m\mathcal{W}^{kn}\partial_s\mathcal{W}^{pm}=\sum_{m=0}^{n+p-1}\partial_m\mathcal{W}^{pn}\partial_s\mathcal{W}^{km}$$

is an overdetermined system describing a family of local Poisson brackets connected with Hamiltonian hydrodynamic chains.

Let us write several first nonlinear PDEs from the nonlinear PDE system (13),

$$[2\varepsilon\partial_0+A^0\partial_1+\mathcal{W}^{20}\partial_2]\mathcal{W}^{21}=[A^0\partial_0+2A^1\partial_1]\mathcal{W}^{20},$$

$$\partial_1\mathcal{W}^{20}\partial_0\mathcal{W}^{31}=\partial_1\mathcal{W}^{30}\partial_0\mathcal{W}^{21}+\partial_2\mathcal{W}^{30}\partial_0\mathcal{W}^{22},$$

$$\partial_0\mathcal{W}^{30}\partial_1\mathcal{W}^{20}+\partial_1\mathcal{W}^{30}\partial_1\mathcal{W}^{21}+\partial_2\mathcal{W}^{30}\partial_1\mathcal{W}^{22}=\partial_0\mathcal{W}^{20}\partial_1\mathcal{W}^{30}+\partial_1\mathcal{W}^{20}\partial_1\mathcal{W}^{31},$$

$$\partial_0\mathcal{W}^{20}\partial_2\mathcal{W}^{30}+\partial_1\mathcal{W}^{20}\partial_2\mathcal{W}^{31}=\partial_1\mathcal{W}^{30}\partial_2\mathcal{W}^{21}+\partial_2\mathcal{W}^{30}\partial_2\mathcal{W}^{22},$$

$$\partial_1\mathcal{W}^{20}\partial_3\mathcal{W}^{31}=\partial_2\mathcal{W}^{30}\partial_3\mathcal{W}^{22},$$

where the auxiliary restrictions (normalization)

$$\mathcal{W}^{0k}(A^0,A^1,\ldots,A^{k-1})\equiv\bar{\mathcal{W}}^{00}\delta^{0k},\quad \mathcal{W}^{1k}(A^0,A^1,\ldots,A^k)\equiv A^k$$

($\bar{\mathcal{W}}^{00}=\varepsilon=$const and δ^{ik} is the Kronecker symbol) are consequences of the existence of conservation laws associated with the Casimir $\bar{\mathbf{H}}_0=\int A^0\mathrm{d}x$ and to the momentum $\bar{\mathbf{H}}_1=\int A^1\mathrm{d}x$.

This system involves just four moments A^0, A^1, A^2, and A^3. It is enough to find coefficients $\mathcal{W}^{20}$, $\mathcal{W}^{21}$, and $\mathcal{W}^{30}$. For instance, $\mathcal{W}^{20}$ is a solution of the Monge-Ampere equation [see Eq. (17)]

$$(\mathcal{W}^{20})_{00}(\mathcal{W}^{20})_{11}-[(\mathcal{W}^{20})_{01}]^2+\varphi'^2(A^0)[(\mathcal{W}^{20})_1]^2=0,$$

where $\varphi(A^0)$ is some function (determined from the compatibility conditions $[(\mathcal{W}^{21})_1]_2=[(\mathcal{W}^{21})_2]_1$, $[(\mathcal{W}^{21})_1]_0=[(\mathcal{W}^{21})_0]_1$, $[(\mathcal{W}^{21})_0]_2=[(\mathcal{W}^{21})_2]_0$; see the expressions below). Moreover,

$$\mathcal{W}^{30}=A^2(\mathcal{W}^{20})_1+G,$$

where $G(p,q)$ is a solution of the Euler-Darboux-Poisson equation

$$G_{pq}=\frac{\varphi''(A^0)}{4\varphi'^2(A^0)}(G_p-G_q),\quad \varphi(A^0)=\frac{1}{2}(p-q),$$

$$q=\ln[(\mathcal{W}^{20})_1]-\varphi(A^0),\quad p=\ln[(\mathcal{W}^{20})_1]+\varphi(A^0).$$

Explicit expressions for all other coefficients (depending on higher moments A^k, $k=3,4,5,\ldots$) can be found recursively in complete differentials. For instance,

$$\mathrm{d}\mathcal{W}^{21}=(\mathcal{W}^{21})_0\mathrm{d}A^0+(\mathcal{W}^{21})_1\mathrm{d}A^1+(\mathcal{W}^{21})_2\mathrm{d}A^2,$$

where

$$(\mathcal{W}^{21})_2=\frac{2[A^1(\mathcal{W}^{20})_{11}+A^0(\mathcal{W}^{20})_{10}+\varepsilon(\mathcal{W}^{20})_{00}]}{2\varepsilon(((\mathcal{W}^{20})_{11}A^2+G_1)/(\mathcal{W}^{20})_1)_0+A^0(((\mathcal{W}^{20})_{11}A^2+G_1)/(\mathcal{W}^{20})_1)_1+(\mathcal{W}^{20})(\mathcal{W}^{20})_{11}/(\mathcal{W}^{20})_1},$$

$$(\mathcal{W}^{21})_1=\frac{(\mathcal{W}^{20})_1}{(\mathcal{W}^{20})_{11}}\left(\frac{(\mathcal{W}^{20})_{11}A^2+G_1}{(\mathcal{W}^{20})_1}\right)_1(\mathcal{W}^{21})_2+(\mathcal{W}^{20})_0-2\frac{(\mathcal{W}^{20})_1(\mathcal{W}^{20})_{10}}{(\mathcal{W}^{20})_{11}},$$

$$(\mathcal{W}^{21})_0=\frac{(\mathcal{W}^{20})_1}{(\mathcal{W}^{20})_{11}}\left(\frac{(\mathcal{W}^{20})_{11}A^2+G_1}{(\mathcal{W}^{20})_1}\right)_0(\mathcal{W}^{21})_2-\frac{(\mathcal{W}^{20})_1(\mathcal{W}^{20})_{00}}{(\mathcal{W}^{20})_{11}}.$$

Remark: The coincidence of the coefficients $\mathcal{W}^{20}$ from this section and $\mathcal{W}^{10}$ from the previous section is easy to understand if one takes into account that if the Hamiltonian density $\mathbf{H}_2$ is a function of the moments A^1 and A^2 only, then the corresponding hydrodynamic chain possesses the Hamiltonian structure coinciding (due to the "shift" $A^k\to B^{k-1}$, $k=1,2,\ldots$) with the Hamiltonian structure presented in the previous section.

All other M brackets (10) can be investigated in the same way using the Jacobi identity (6).

V. THE MIURA-TYPE TRANSFORMATIONS

The approach presented in this paper is very effective: the nonlinear PDE system (6) can be integrated iteratively for M brackets. However, the Liouville coordinates A^k are very *flexible*. It means that coefficients $\mathcal{W}^{ik}_{(M)}$ can be found up to invertible transformations $\widetilde{A}^k(A^0,A^1,\ldots,A^k)$ preserving the Jacobi identity (6). For instance, the Benney hydrodynamic chain [see Eq. (11)]

$$A^k_t=A^{k+1}_x+kA^{k-1}A^0_x=[kA^{k+n-1}D_x+nD_xA^{k+n-1}]\frac{\partial\mathbf{H}_2}{\partial A^n},\quad k=0,1,2,\ldots$$

can be written via another set of the Liouville coordinates $\mathbf{H}_k$ in the conservative form

$$\partial_t\mathbf{H}_k=\partial_x\left(\mathbf{H}_{k+1}-\frac{1}{2}\sum_{m=0}^{k-1}\mathbf{H}_m\mathbf{H}_{k-1-m}\right),\quad k=0,1,2,\ldots\ .$$

The invertible transformation $\mathbf{H}_k(\mathbf{A})$ is very complicated because corresponding coefficients can be found (see, e.g., Ref. 14) by a substitution of the series

$$\lambda = \mu + \frac{A^0}{\mu} + \frac{A^1}{\mu^2} + \frac{A^2}{\mu^3} + \cdots \tag{20}$$

into another series

$$\mu = \lambda - \frac{\mathbf{H}_0}{\lambda} - \frac{\mathbf{H}_1}{\lambda^2} - \frac{\mathbf{H}_2}{\lambda^3} - \cdots .$$

Then, the Poisson bracket (11) expressed via conservation law densities $\mathbf{H}_k$

$$\{\mathbf{H}_i, \mathbf{H}_k\} = [\mathcal{W}^{ik}_{(1)}(\mathbf{H})D_x + D_x\mathcal{W}^{ki}_{(1)}(\mathbf{H})]\delta(x-x')$$

looks ugly. Thus, one of the main problems appearing in a classification of Poisson brackets is a choice of such Liouville coordinates, where coefficients $\mathcal{W}^{ik}$ became most simple.

Suppose two Hamiltonian hydrodynamic chains [see Eq. (7)]

$$B^k_t = \sum_{n=0}^{N_k} F^k_n(\mathbf{B})B^n_x, \quad A^k_t = \sum_{m=0}^{M_k} Q^k_n(\mathbf{A})A^n_x, \quad k = 1,2,\ldots, \tag{21}$$

where N_k and M_k are some integers, are related by the Miura-type transformations

$$A^k = A^k(B^0, B^1, \ldots, B^{k+1}), \quad k = 0,1,2,\ldots . \tag{22}$$

Example: The Benney hydrodynamic chain [see Eq. (11); see also Refs. 2 and 14] is connected with the modified Benney hydrodynamic chain (see Ref. 24, the particular case of the Kupershmidt hydrodynamic chains)[13]

$$B^k_t = B^{k+1}_x + B^0B^k_x + (k+2)B^kB^0_x = [(k+1)B^{k+n}D_x + (n+1)D_xB^{k+n}]\frac{\partial \mathbf{H}_0}{\partial B^n},$$

where the Hamiltonian density $\mathbf{H}_0 = B^1 + (B^0)^2$, by the Miura-type transformations (22), which can be obtained by comparing the two series (see Ref. 23)

$$\lambda = p^{-1} - \sum_{k=0}^{\infty} \frac{B^k}{p^{k+2}} \equiv \left(p + B^0 + \sum_{k=0}^{\infty} \frac{A^k}{(p+B^0)^{k+1}}\right)^{-1},$$

where the generating function of the Miura-type transformations is given by $\mu = p + B^0$ [cf. the rhs of the above expression and Eq. (20)]. For instance,

$$A^0 = B^1 + (B^0)^2, \quad A^1 = B^2 + 3B^0B^1 + 2(B^0)^3, \ldots .$$

This Poisson bracket (of the modified Benney hydrodynamic chain)

$$\{B^k, B^n\}_1 = [(k+1)B^{k+n}D_x + (n+1)D_xB^{k+n}]\delta(x-x')$$

can be used for a construction of the first local Poisson bracket [see Eq. (4)]

$$\{A^i, A^j\}_1 = \frac{\partial A^i}{\partial B^k}\{B^k, B^n\}_1\frac{\partial A^j}{\partial B^n}. \tag{23}$$

However, corresponding coefficients $\mathcal{W}^{ik}$ are very complicated.

Thus, the Miura-type transformations can be used for a *simplification* of Poisson brackets. Indeed, let us consider a general case for M brackets.

Suppose the first hydrodynamic chain in Eq. (21) possesses the local Poisson bracket (4)

$$\{B^k, B^n\} = [G^{kn}_{(M)}(\mathbf{B})D_x + \Gamma^{kn}_{(M)m}(\mathbf{B})B^m_x]\delta(x-x'). \tag{24}$$

Then the second hydrodynamic chain in Eq. (21) also possesses another local Poisson bracket

$$\{A^i,A^j\}=[G^{ij}_{(L)}(\mathbf{A})D_x+\Gamma^{ij}_{(L)m}(\mathbf{A})A^m_x]\delta(x-x') \tag{25}$$

connected with Eq. (24) by Eq. (22) [see Eq. (23)].

Theorem: *If the Poisson brackets (24) and (25) are related by the above Miura-type transformations (22) then* $L=M-1$.

Proof: Without loss of generality let us restrict the calculation just for the metric coefficients

$$G^{ij}_{(L)}(\mathbf{A})=\sum_{k=0}^{i+1}\sum_{n=0}^{j+1}\frac{\partial A^i}{\partial B^k}G^{kn}_{(M)}(\mathbf{B})\frac{\partial A^j}{\partial B^n},\quad i+j>M.$$

Taking into account the *highest order* dependence on the moments B^n these metric coefficients,

$$G^{ij}_{(L)}(\mathbf{A})\sim\frac{\partial A^i}{\partial B^{i+1}}G^{i+1,j+1}_{(M)}(\mathbf{B})\frac{\partial A^j}{\partial B^{j+1}},$$

depend on $B^{i+j+2-M}$ (in a highest order), i.e., $G^{ij}_{(L)}(\mathbf{A})$ could not depend on moments higher than $A^{i+j+1-M}$. Thus, indeed, $L=M-1$.

Corollary: The Miura-type transformations (22) decrease the number of moments involved in metric coefficients and increase the number of Casimirs and a size of a triangular constant block $\bar{\mathcal{W}}^{kn}_{(M)}$ [see Eq. (15)]. It means that the following diagram exists:

$$\begin{aligned}
\{A^k,A^n\} &= [G^{kn}_{(M)}(A^0,\ldots,A^{k+n-M})D_x+\cdots]\delta(x-x'),\\
&\downarrow\\
\{B^k,B^n\} &= [G^{kn}_{(M+1)}(B^0,\ldots,B^{k+n-M-1})D_x+\cdots]\delta(x-x'),\\
&\downarrow\\
\{C^k,C^n\} &= [G^{kn}_{(M+2)}(C^0,\ldots,C^{k+n-M-2})D_x+\cdots]\delta(x-x'),\\
&\downarrow\\
&\ldots.
\end{aligned}$$

Thus, invertible transformations can be used to reduce the Poisson bracket to the most simple dependence on a given set of moments A^k, while the Miura-type transformations can be used to reduce Poisson brackets to a decreased set of new moments B^n.

Remark: In the theory of dispersive integrable systems the Miura transformation is a tool to reduce the Hamiltonian structure to the canonical form "D_x" (the infinitely many component analogue of the Darboux theorem; see Refs. 19 and 20). Indeed, a constant triangular block $\bar{\mathcal{W}}^{kn}_{(M)}$ is an analogue of constant matrix g^{kn} of the canonical Hamiltonian operator $g^{kn}D_x$ (see Ref. 5). This constant triangular block $\bar{\mathcal{W}}^{kn}_{(M)}$ increases under the Miura-type transformations (22), because the metric coefficients $G^{kn}_{(M)}$ must be constants for $k+n<M$. It means, if $\bar{\mathcal{W}}^{kn}_{(M)}\to\bar{\mathcal{W}}^{kn}_{(M+1)}$ (see the above diagram), then the new constant triangular block is determined by $k+n<M+1$.

Conjecture: Possibly, the number of such Miura-type transformations is infinite, and any local Hamiltonian structure with the index $-M$ can be reduced to a local Hamiltonian structure with an arbitrary index N.

VI. NONLOCAL HAMILTONIAN STRUCTURES

The nonlocal Poisson brackets [see Eq. (2)]

$$\{U^i,U^j\}=[G^{ij}(\mathbf{U})D_x+\Gamma^{ij}_k(\mathbf{U})U^k_x+\varepsilon U^i_xD_x^{-1}U^j_x]\delta(x-x')$$

for N component case were completely investigated by Ferapontov and Mokhov in Ref. 10 for the nondegenerate matrix G^{ij}; the degenerate case was considered by Mokhov in Ref. 17. The skew-symmetry property and the Jacobi identity lead to the set of restrictions

$$G^{ij}=G^{ji},\quad \partial_k G^{ij}=\Gamma_k^{ij}+\Gamma_k^{ji},\quad G^{ik}\Gamma_k^{jn}=G^{jk}\Gamma_k^{in},$$

$$\varepsilon(G^{im}\delta_k^j-G^{ij}\delta_k^m)=\Gamma_n^{ij}\Gamma_k^{nm}-\Gamma_n^{im}\Gamma_k^{nj}+G^{in}(\partial_n\Gamma_k^{mj}-\partial_k\Gamma_n^{mj}),$$

$$\begin{aligned}-\varepsilon[(\Gamma_k^{ij}-\Gamma_k^{ji})\delta_p^m+(\Gamma_k^{mi}-\Gamma_k^{im})\delta_p^j+(\Gamma_k^{jm}-\Gamma_k^{mj})\delta_p^i+(\Gamma_p^{ij}-\Gamma_p^{ji})\delta_k^m+(\Gamma_p^{mi}-\Gamma_p^{im})\delta_k^j+(\Gamma_p^{jm}-\Gamma_p^{mj})\delta_k^i]\\ =(\partial_n\Gamma_k^{ij}-\partial_k\Gamma_n^{ij})\Gamma_p^{nm}+(\partial_n\Gamma_k^{mi}-\partial_k\Gamma_n^{mi})\Gamma_p^{nj}+(\partial_n\Gamma_k^{jm}-\partial_k\Gamma_n^{jm})\Gamma_p^{ni}+(\partial_n\Gamma_p^{ij}-\partial_p\Gamma_n^{ij})\Gamma_k^{nm}+(\partial_n\Gamma_p^{mi}\\ -\partial_p\Gamma_n^{mi})\Gamma_k^{nj}+(\partial_n\Gamma_p^{jm}-\partial_p\Gamma_n^{jm})\Gamma_k^{ni},\end{aligned}$$

which simplify to the Jacobi identity [see Eq. (6)]

$$(\mathcal{W}^{in}+\mathcal{W}^{ni}-\varepsilon A^iA^n)\partial_n\mathcal{W}^{kj}=(\mathcal{W}^{jn}+\mathcal{W}^{nj}-\varepsilon A^jA^n)\partial_n\mathcal{W}^{ki},$$

$$\partial_n\mathcal{W}^{ij}\partial_m\mathcal{W}^{kn}=\partial_n\mathcal{W}^{kj}\partial_m\mathcal{W}^{in} \tag{26}$$

written in the Liouville coordinates $A^i=A^i(\mathbf{U})$, where (see Refs. 15 and 17)

$$G^{ij}=\mathcal{W}^{ij}+\mathcal{W}^{ji}-\varepsilon A^iA^j,\quad \Gamma_k^{ij}=\partial_k\mathcal{W}^{ji}-\varepsilon\delta_k^iA^j.$$

Thus, the nonlocal Poisson bracket in the Liouville coordinates has the form

$$\{A^i,A^j\}=[\mathcal{W}^{ij}D_x+D_x\mathcal{W}^{ji}-\varepsilon A^jD_xA^i+\varepsilon A_x^iD_x^{-1}A_x^j]\delta(x-x'),\quad i,j=0,1,\ldots\ .$$

Similar classification of these nonlocal Poisson brackets [see Eq. (26)] shall be made elsewhere.

Remark: More general Poisson brackets have been introduced by Ferapontov (see Ref. 6) for N component nondegenerate case. Such Poisson brackets in the Liouville coordinates are given by (see Ref. 18)

$$\begin{aligned}\{A^k,A^n\}=[(\Phi^{kn}+\Phi^{nk}-\varepsilon_{pq}\Psi^{(p)k}\Psi^{(q)n})D_x+(\partial_m\Phi^{nk}-\varepsilon_{pq}\Psi^{(q)n}\partial_m\Psi^{(p)k})A_x^m\\ +\varepsilon_{pq}\partial_m\Psi^{(p)k}A_x^mD_x^{-1}\partial_s\Psi^{(q)n}A_x^s]\delta(x-x'),\end{aligned}$$

where the constant $L\times L$ matrix ε_{pq} is symmetric and nondegenerate (L is "codimension" of the pseudo-Riemannian space), and $\Phi^{kn}(\mathbf{A})$ and $\Psi^{(p)k}(\mathbf{A})$ are determined by nonlinear PDE system similar to Eq. (6).

Remark: Any nonlocal Hamiltonian structure of Ferapontov type can be reduced to local Hamiltonian structure of Dubrovin-Novikov type by an appropriate generalized reciprocal transformation (see Ref. 11). Thus, possibly the same result is valid for infinite component case.

VII. CONCLUSION AND OUTLOOK

The so-called Haantjes tensor approach is very effective (see Ref. 9) in a classification of integrable *Hamiltonian* hydrodynamic chains (7). In general case, if the discrete function $M(\mathbf{k})$ is given *a priori*, then all coefficients $V_m^k(\mathbf{U})$ can be found iteratively. In the Hamiltonian case, these coefficients can be found simultaneously (because a Hamiltonian density and a Poisson bracket are given).

In this paper, a concept of the so-called M brackets was introduced. In this case, a discrete function $M(\mathbf{k})$ is determined explicitly by the comparison of Eq. (7) with Eq. (8) [see, e.g., Eq. (16)].

Suppose the classification of M brackets

$$\{A^k,A^n\}=[\mathcal{W}^{kn}(A^0,\ldots,A^{k+n-M})D_x+D_x\mathcal{W}^{nk}(A^0,\ldots,A^{k+n-M})]\delta(x-x'),\quad k,n=0,1,2,\ldots$$

is complete. Corresponding Hamiltonian hydrodynamic chains (8) are determined by the above Poisson brackets and some Hamiltonian densities. Then integrable Hamiltonian hydrodynamic chains can be extracted by the Haantjes tensor approach (see Ref. 9), i.e., Hamiltonian densities in

the "integrable" case must satisfy some nonlinear PDE system associated with the above Poisson brackets.

Thus, the classification of M brackets is a first step in the classification of integrable Hamiltonian hydrodynamic chains (8).

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Contractions of low-dimensional Lie algebras

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Theoretical background of continuous contractions of finite-dimensional Lie algebras is rigorously formulated and developed. In particular, known necessary criteria of contractions are collected and new criteria are proposed. A number of requisite invariant and semi-invariant quantities are calculated for wide classes of Lie algebras including all low-dimensional Lie algebras. An algorithm that allows one to handle one-parametric contractions is presented and applied to low-dimensional Lie algebras. As a result, all one-parametric continuous contractions for both the complex and real Lie algebras of dimensions not greater than 4 are constructed with intensive usage of necessary criteria of contractions and with studying correspondence between real and complex cases. Levels and colevels of low-dimensional Lie algebras are discussed in detail. Properties of multiparametric and repeated contractions are also investigated. © *2006 American Institute of Physics.*
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I. INTRODUCTION

Limiting processes between Lie algebras were first investigated by Segal.[69] The most known example concerning these processes is given by connection between relativistic and classical mechanics with their underling Poincaré and Galilean symmetry groups. If the velocity of light is assumed to go to infinity, relativistic mechanics "transforms" into classical mechanics. This also induces a singular transition from the Poincaré algebra to the Galilean one. The other well-known example is a limit process from quantum mechanics to classical mechanics under $\hbar \to 0$, which corresponds to the contraction of the Heisenberg algebras to the Abelian ones of the same dimensions.

Existing works on contractions can be conditionally divided into two main streams which are scarcely connected with each other. One of them is more "physical" and is mainly oriented to applications of contractions. The other one is more "algebraic" and usually has better mathematical background. Let us simultaneously survey works on the main types of contractions existing in the frameworks of both approaches.

After Segal, the concept of limiting processes between physical theories in terms of contractions of the underling symmetry groups was also formulated by Inönü and Wigner.[41,42] They introduced so-called *Inönü-Wigner contractions* (*IW-contractions*) which, in spite of their simplicity, were effectively applied to a wide range of physical and mathematical problems. Later Saletan[67] studied the most general class of one-parametric contractions for which the elements of the corresponding matrices are first-order polynomials with respect to the contraction parameter.

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Inönü-Wigner contractions obviously form a special subclass in the class of *Saletan contractions*.

Another extension of the class of Inönü-Wigner contractions is given by *generalized Inönü-Wigner contractions*. They are generated by matrices which become diagonal after suitable choices of bases of initial and contracted algebras, and, moreover, diagonal elements should be integer powers of the contraction parameters. Contractions of this kind were introduced by Doebner and Melsheimer.[21] To the best of our knowledge, the name "generalized Inönü-Wigner contractions" first appear in Ref. 34 The other names (p-contractions, Doebner-Melsheimer contractions, and singular IW-contractions[51]) are also used. Similar contractions are applied in the "purely mathematical" framework and called *one-parametric subgroup degenerations*.[7–9,32,71] The last name came from the algebraic invariant theory.[46] Generalized IW contractions are very useful for applications and were revisited many times. In particular, it was incorrectly conjectured that any continuous one-parametric contraction is equivalent to a generalized Inönü-Wigner contraction.

A general definition of contractions was first formulated by Segal[69] in terms of limiting processes of bases. It is used as an operational definition for calculations up to now. Saletan[67] gave a more rigorous general definition of contractions, which is based on limiting processes of Lie brackets and allows one to avoid a confusion with limit state of bases, existing in the Segal approach. Saletan's definition was generalized for the case of arbitrary field in terms of Lie algebra orbit closures with respect to Zariski topology. The generalization is a basis of modern investigation on contractions and was used by a number of authors, e.g., Refs. 7–9, 12, 32, 45, 47, 57, 68, and 71. The name *degeneration* is often used instead of the name *contraction* in the generalized context.

A still more general notion of degenerations, which works in the case of algebras of different dimensions, was proposed in Refs. 27–29. The algebra $\mathfrak{g}$ degenerates to the algebra $\mathfrak{g}_0$ according to Gorbatsevich if $\mathfrak{g}\oplus pA_1$ is contracted to $\mathfrak{g}_0\oplus qA_1$ in the usual sense for some $p,q\in\mathbb{N}\cup\{0\}$, where pA_1 and qA_1 are the p- and q-dimensional Abelian algebras.

The other type of contractions is given by the purely algebraic notion of *graded contractions*.[16,18,33,38,60,77] The graded contraction procedure is the following. Structure constants of a graded Lie algebra are multiplied by numbers which are chosen in such a way that the multiplied structure constants give a Lie algebra with the same grading. Graded contractions include discrete contractions as a subcase but do not cover all continuous ones.

Different kinds of contractions and their properties were reviewed and compared in Ref. 51. The interrelations between contractions and deformations or expansions were widely investigated.[23,25,31,50–52] The related but principally different problem is given by contractions of Lie groups, which are also widely studied and applied. Notions of such contractions were introduced in Refs. 6, 35, 53, and 67 with different levels of generality.

Problems concerning contractions of Lie algebra (or group) representations and simultaneous contractions of Lie algebras or Lie groups and their representations are also important and demand a special technique which differs from the techniques associated with pure contractions of Lie algebras and Lie groups. In spite of existing works on the subject and a range of applications, these problems are not studied enough although a number of interesting results have been obtained. For example, the contractions of representations of de Sitter groups were described in Ref. 53. Contractions of matrix representations of concrete physically significant Lie algebras were investigated, e.g., in Refs. 19, 58, and 75. Related theoretical inventions and different examples of application can also be found in Refs. 14, 36, 40, 42, 48, 49, 51, 54, and 60 and in the references therein.

Intensive investigation of real and complex low-dimensional Lie algebras in last decades is motivated by a number of causes. As subalgebras of important higher-dimensional Lie algebras, these algebras are widely applied in the theory of induced representations (representations of subalgebras/subgroups are used to construct representations of the whole algebra/group), in the representation theory (chains of subalgebras can provide sets of commuting operators, eigenfunctions of which form bases of representation spaces for the corresponding Lie group), and in study of broken symmetries. Low-dimensional Lie algebras are also interesting *per se* and supply theoretical consideration with substantial examples. In this connection classifications, subalgebras,

realizations, invariants, contractions, deformations, and other objects concerning low-dimensional Lie algebras were studied.[5,22,24,50,55,61,65]

Contractions of low-dimensional Lie algebras naturally appeared as illustrating examples in a number of papers. Thus, in the pioneer paper on contractions[69] Segal adduced two such contractions, namely, the contractions from so(3) and $\mathrm{sl}(2,\mathbb{R})$ to the Weyl-Heisenberg algebra $\mathfrak{h}_3=A_{3.1}$. Some examples are contained also in the known paper by Saletan.[67] Afterwards contractions of low-dimensional Lie algebras became independent subject of investigation. Inönü-Wigner contractions of real three-dimensional Lie algebras were considered[70] but some cases were missed. These results were partially amended in Ref. 51. First Inönü-Wigner contractions of real three-dimensional Lie algebras were exhaustively described by Conatser.[15] Using the known classification of subalgebras of real low-dimensional Lie algebras,[61] Huddleston[39] constructed Inönü-Wigner contractions of the four-dimensional real Lie algebras. All inequivalent continuous one-parametric contractions of real three-dimensional Lie algebras were obtained in Ref. 78 but contractions inside parametrized series of algebras were not discussed. The same problem was nicely solved by Lauret[47] in terms of orbit closures using a nonevident connection between algebraic characterization of Lie groups having metrics with special curvature properties and existence of degenerations for Lie algebras. Orbit closures of complex three- and four-dimensional Lie algebras were studied in Refs. 8, 9, and 71. It is the works from which we adopted the fruitful idea on usage of a wide set of necessary contraction criteria. The same subject was also investigated in Refs. 1 and 2. In these papers obtained results were presented in a very simple and clear form due to special improvement of classification of complex three- and four-dimensional Lie algebras.

Complexity of description of algebra orbit closures is exponentially increased under growing dimension of the underlying vector space. A possible ways of simplification is to consider a closed subclass of Lie algebras (e.g., nilpotent algebras) instead of the whole class of Lie algebras of a fixed dimension. Degenerations of nilpotent algebras were studied in Ref. 32, Ref. 68, and Refs. 7 and 8 in the case of dimensions five, six, and seven, correspondingly.

Deformations of low-dimensional Lie algebras are also treated intensively. Thus, deformations of three-dimensional real Lie algebras were described in Ref. 50. The four-dimensional case was completely studied over the complex field.[24] There also exist a number of papers on contractions and deformations of higher- or even infinite-dimensional Lie algebras (see, e.g., Ref. 17). Since this subject is out of the scope of our paper, we do not review it here in detail.

Investigation of contractions is motivated by numerous applications in different fields of physics and mathematics, e.g., in study of representations, invariants, and special functions.[10,19,54] It is one of the tools to recognize structure of Lie algebra varieties.[8] The Wigner coefficients of the Euclidean group E(3) were constructed with contracting the Wigner coefficients of the special orthogonal group SO(4).[37] Contractions were used to establish connection between various kinematical groups and to shed a light on their physical meaning. In this way relationship between the conformal and Schrödinger groups was elucidated[3] and various Lie algebras including a relativistic position operator were interrelated. Under dynamical group description of interacting systems, contractions corresponding to the coupling constant going to zero give noninteracting systems.[20] Application of contractions allows to derive interesting results in the special function theory and on the variable separation method.[36,43,64]

Contractions of low-dimensional Lie algebras also play an important role from the physical point of view.[26] It is illustrated by the following simple examples which are related to physics. We use the standard physical notations and numeration by Mubarakzyanov[55] simultaneously. Hereafter, describing a Lie algebra, we adduce only the nonzero commutators of fixed basis elements. See Sec. VIII for notations and more examples.

The four-dimensional Lie algebra $\mathrm{u}(2)=\mathrm{sl}(2,\mathbb{R})\oplus A_1$ has the nonzero commutation relations $[e_1,e_2]=e_1$, $[e_2,e_3]=e_3$, and $[e_1,e_3]=2e_2$. The matrix $U_1(\varepsilon)=I_{10}\,\mathrm{diag}(\varepsilon,\varepsilon,1,1)$ provides a contraction of $u(2)$ to the algebra $e(2)\oplus A_1=A_{3.5}^0\oplus A_1$ ($[e_1,e_3]=-e_2$, $[e_2,e_3]=e_1$), i.e., to the direct sum of the three-dimensional Euclidean algebra and the one-dimensional Abelian algebra.

The other example is the contraction of u(2) to the harmonic oscillator algebra $\mathfrak{h}_4=A_{4.8}^{-1}$

($[e_2,e_3]=e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=-e_3$) which frequently occurs in physics. The physical name of $\mathfrak{h}_4$ is justified since the set consisting of the creation (a^+), annihilation (a^-), identity (I), and single-mode photon number ($N=a^+a^-$) operators is closed under commutation and generates a Lie algebra isomorphic to $\mathfrak{h}_4$ with $e_1=I$, $e_2=a^-$, $e_3=a^+$, $e_4=N$. The algebra $u(2)$ is contracted to $\mathfrak{h}_4$ with the matrix $U_2(\varepsilon)=I_{19}\,\mathrm{diag}(\varepsilon,1,\varepsilon,1)$.

The subalgebra $\mathfrak{h}_3=\langle e_1,e_2,e_3\rangle$ ($[e_2,e_3]=e_1$) of $\mathfrak{h}_4$ is also widely applied since it is isomorphic to the algebra formed by the quantum mechanical position operator Q, the momentum operator P, and the identity operator I via designation

$$e_1=I,\quad e_2=\frac{Q+iP}{\sqrt{2\hbar}},\quad e_3=\frac{Q-iP}{\sqrt{2\hbar}}.$$

The main purpose of our paper is to classify contractions of the real and complex Lie algebras of dimensions not greater than 4. We rigorously formulate and develop a theoretical background to do this. Effectiveness of the applied algorithm for handling of contractions is based on using a wide set of necessary contraction criteria. A number of known necessary contraction criteria are collected and new criteria are proposed. Requisite invariant and semi-invariant quantities are calculated for classes of Lie algebras including all low-dimensional Lie algebras. Multiparametric and repeated contractions are also investigated since they give a tool for finding contraction matrices in complicated cases. An important by-effect of the present investigation is that the contractions under consideration supply with a number of model examples and contrary instances for statements and conjectures of the contraction theory. Availability of exhaustive information about them also allows us to describe levels and colevels of low-dimensional Lie algebras completely.

This paper is arranged in the following way. In Sec. II different definitions of general contractions of Lie algebras and contraction equivalence are given and discussed. We also construct a contrary instance on a conjecture on equivalence of contractions. Simplest types of contractions (Inönü-Wigner contractions, Saletan contractions, and generalized Inönü-Wigner contractions) are described in Sec. III. Necessary contraction criteria are listed and proven in Sec. IV. Calculation of invariant quantities for wide classes of Lie algebras is adduced in Sec. V. Section VI collects algebraic quantities and objects concerning real three- and four-dimensional Lie algebras. These quantities are used in Sec. VIII as a base for application of necessary contraction criteria in order to conclude whether there is a contraction in an arbitrary pair of the algebras of the same dimension. An algorithm for handling of contractions of low-dimensional Lie algebras is precisely formulated in Sec. VII and illustrated by examples. All inequivalent one-parametric contractions of the real low-dimensional Lie algebras are arranged in Sec. VIII and supplied with diagrams and explicit forms of the contraction matrices. All cases where contractions are equivalent to simple or generalized Inönü-Wigner contractions are separated. Levels and colevels of low-dimensional Lie algebras are also investigated. Using known correspondence between lists of nonisomorphic real and complex low-dimensional Lie algebras, we construct all inequivalent contractions over the complex field in Sec. IX. They are compared with the degenerations of four-dimensional Lie algebras, which were found in Refs. 1 and 9. Multiparametric and repeated contractions are studied in Sec. X and used for construction of contraction matrices in the most complicated cases which are not covered by generalized Inönü-Wigner contractions. Some problems arising under analysis of obtained results are formulated in Sec. XI.

II. DEFINITIONS OF CONTRACTIONS AND THEIR EQUIVALENCE

Consider an n-dimensional Lie algebra $\mathfrak{g}=(V,[\cdot,\cdot])$ with an underlying n-dimensional vector space V over $\mathbb{R}$ or $\mathbb{C}$ and a Lie bracket $[\cdot,\cdot]$. Usually the Lie algebra $\mathfrak{g}$ is defined by means of commutation relations in a fixed basis $\{e_1,\ldots,e_n\}$ of V. More precisely, it is sufficient to write down only the nonzero commutators $[e_i,e_j]=c_{ij}^k e_k$, where c_{ij}^k are components of the structure constant tensor of $\mathfrak{g}$. Hereafter the indices i, j, k, i', j', k', i'', j'', and k'' run from 1 to n and the summation over the repeated indices is implied.

Consider a *continuous* function $U:(0,\varepsilon_1]\to \mathrm{GL}(V)$, where $\varepsilon_1>0$. In other words, $U_\varepsilon=U(\varepsilon)$ is a nonsingular linear operator on V for all $\varepsilon\in(0,\varepsilon_1]$. Without loss of generality we can put $\varepsilon_1=1$. A parametrized family of new Lie brackets on V is determined via the old one by the following way:

$$\forall \varepsilon \in (0,1], \quad \forall x,y\in V: \quad [x,y]_\varepsilon = U_\varepsilon^{-1}[U_\varepsilon x, U_\varepsilon y].$$

It is reasonable that for any $\varepsilon\in(0,1]$ the Lie algebra $\mathfrak{g}_\varepsilon=(V,[\cdot,\cdot]_\varepsilon)$ is isomorphic to $\mathfrak{g}$.

Definition 1: If the limit $\lim_{\varepsilon\to+0}[x,y]_\varepsilon=\lim_{\varepsilon\to+0}U_\varepsilon^{-1}[U_\varepsilon x,U_\varepsilon y]=:[x,y]_0$ exists for any $x,y\in V$ then $[\cdot,\cdot]_0$ is a well-defined Lie bracket. The Lie algebra $\mathfrak{g}_0=(V,[\cdot,\cdot]_0)$ is called a *one-parametric continuous contraction* (or simply a contraction) of the Lie algebra $\mathfrak{g}$.

If a basis of V is fixed, the operator U_ε is defined by the corresponding matrix. Definition 2 can be reformulated in terms of structure constants.

Definition 1′: Let c_{ij}^k be the structure constants of the algebra $\mathfrak{g}$ in the fixed basis $\{e_1,\ldots,e_n\}$. If the limit

$$\lim_{\varepsilon\to+0}(U_\varepsilon)_{i'}^{i}(U_\varepsilon)_{j'}^{j}(U_\varepsilon^{-1})_{k}^{k'}c_{ij}^{k}=:\tilde{c}_{i'j'}^{k'}$$

exists for all values of i', j', and k' then $\tilde{c}_{i'j'}^{k'}$ are components of the well-defined structure constant tensor of a Lie algebra $\mathfrak{g}_0$. In this case the Lie algebra $\mathfrak{g}_0$ is called a one-parametric continuous contraction (or simply contraction) of the Lie algebra $\mathfrak{g}$. The parameter ε and the matrix-function $U=U(\varepsilon)$ are called a *contraction parameter* and a *contraction matrix*, correspondingly. The procedure that provides the Lie algebra $\mathfrak{g}_0$ from the algebra $\mathfrak{g}$ is also called a contraction.

Definitions 1 and 1′ are equivalent. The first definition is basis-free and convenient for theoretical consideration. The second one is more usable for calculations of concrete contractions. In this paper we mainly use Definition 1′.

The well-known Inönü-Wigner,[42] Saletan,[67] and generalized Inönü-Wigner[21] contractions are particular cases of the above one-parametric continuous contractions.

Definition 2: We call a contraction from the Lie algebra $\mathfrak{g}$ to the Lie algebra $\mathfrak{g}_0$ *trivial* if $\mathfrak{g}_0$ is Abelian and *improper* if $\mathfrak{g}_0$ is isomorphic to $\mathfrak{g}$.

If there exists a componentwise limit $\lim_{\varepsilon\to+0}U_\varepsilon=:U_0$ and $U_0\in GL(V)$ then it is obvious that the contraction is improper. Therefore, in order to generate a proper contraction, the matrix function U have to satisfy one of the conditions: (1) there is no limit of U at $\varepsilon\to+0$, i.e., at least one of the elements of U is singular under $\varepsilon\to+0$, or (2) there exists $\lim_{\varepsilon\to+0}U_\varepsilon=:U_0$ but the matrix U_0 is singular. Both conditions are not sufficient for the contraction to be proper.

The trivial and improper contractions exist for any Lie algebra. The trivial contraction is easily provided, e.g., by the matrix $U_\varepsilon=\mathrm{diag}(\varepsilon,\varepsilon,\ldots,\varepsilon)$. As a contraction matrix of the improper contraction, the identity matrix $U_\varepsilon=\mathrm{diag}(1,1,\ldots,1)$ can be always used. Sometimes the trivial and improper contractions are united in the common class of trivial contractions.[76]

The Abelian algebra is contracted only to itself. It is a special case when the contraction is trivial and improper at the same time.

Definition 3: Let the Lie algebras $\mathfrak{g}$ and $\tilde{\mathfrak{g}}$ be contracted to the algebras $\mathfrak{g}_0$ and $\tilde{\mathfrak{g}}_0$, correspondingly. If $\tilde{\mathfrak{g}}$ is isomorphic to $\mathfrak{g}$ and $\tilde{\mathfrak{g}}_0$ is isomorphic to $\mathfrak{g}_0$ then the contractions are called *weakly equivalent*.

Roughly speaking, all contractions in the same pairs of Lie algebras are weakly equivalent. Under usage of weak equivalence, attention is concentrated on possibility and results of contractions. Difference in ways of contractions is neglected by this approach. For parametric contractions we can also introduce different notions of stronger equivalence, which take into account ways of contractions. Hereafter $\mathrm{Aut}(\mathfrak{g})$ denotes the automorphism group of the Lie algebra $\mathfrak{g}$ and $\mathrm{Iso}(\mathfrak{g},\tilde{\mathfrak{g}})$ denotes the set of isomorphisms from the Lie algebra $\mathfrak{g}$ to the Lie algebra $\tilde{\mathfrak{g}}$. Additionally we identify isomorphisms with the corresponding matrices in a fixed basis.

Definition 4: Two one-parametric contractions in the same pair of Lie algebras $(\mathfrak{g},\mathfrak{g}_0)$ with the contraction matrices $U(\varepsilon)$ and $\tilde{U}(\varepsilon)$ are called *strictly equivalent* if there exists $\delta\in(0,1]$, there

exist functions $\hat{U}:(0,\delta]\to \mathrm{Aut}(\mathfrak{g})$ and $\widetilde{U}:(0,\delta]\to \mathrm{Aut}(\mathfrak{g}_0)$, and a continuous monotonic function $\varphi:(0,\delta]\to(0,1]$, $\lim_{\varepsilon\to+0}\varphi(\varepsilon)=0$, such that

$$\widetilde{U}_\varepsilon=\hat{U}_\varepsilon U_{\varphi(\varepsilon)}\check{U}_\varepsilon,\quad \varepsilon\in(0,\delta].$$

The latter definition can be reformulated for different pairs of algebras, which are term-by-term isomorphic.

Definition 4′: Let the isomorphic Lie algebras $\mathfrak{g}$ and $\widetilde{\mathfrak{g}}$ be contracted to the isomorphic algebras $\mathfrak{g}_0$ and $\widetilde{\mathfrak{g}}_0$ with the contraction matrices $U(\varepsilon)$ and $\widetilde{U}(\varepsilon)$, correspondingly. These contractions are called strictly equivalent if there exists $\delta\in(0,1]$, there exist functions $\hat{U}:(0,\delta]\to \mathrm{Iso}(\mathfrak{g},\widetilde{\mathfrak{g}})$ and $\check{U}:(0,\delta]\to \mathrm{Iso}(\mathfrak{g}_0,\widetilde{\mathfrak{g}}_0)$, and a continuous monotonic function $\varphi:(0,\delta]\to(0,1]$, $\lim_{\varepsilon\to+0}\varphi(\varepsilon)=0$, such that

$$\widetilde{U}_\varepsilon=\hat{U}_\varepsilon^{-1}U_{\varphi(\varepsilon)}\check{U}_\varepsilon,\quad \varepsilon\in(0,\delta].$$

Strictly equivalent contractions obviously are weakly equivalent. In our consideration we use only the notion of weak equivalence hence weakly equivalent contractions will be called equivalent ones for simplicity.

Remark 1: The restriction that $\hat{U}$ and $\check{U}$ should be isomorphism matrices cannot be omitted with preserving correctness.

The contractions of a Lie algebra, which are defined by the matrices U_ε and $W_0U_\varepsilon\widetilde{W}_0$, where $U:(0,1]\to \mathrm{GL}(V)$, $W_0,\widetilde{W}_0\in \mathrm{GL}(V)$, are weakly inequivalent in the general case. For example, the algebra $\mathrm{sl}(2,\mathbb{R})$ ($[e_1,e_2]=e_1$, $[e_2,e_3]=e_3$, $[e_1,e_3]=2e_2$) is contracted to the Heisenberg algebra $A_{3.1}$ ($[e_2,e_3]=e_1$) with the matrix $I_3\,\mathrm{diag}(\varepsilon,\varepsilon,1)$ and to the algebra $A_{3.5}^0$ ($[e_1,e_3]=-e_2$, $[e_2,e_3]=e_1$) with the matrix $I_5\,\mathrm{diag}(\varepsilon,\varepsilon,1)$. Here I_3 and I_5 are nonsingular matrices defined in Sec. VIII A.

Moreover, let $W,U,\widetilde{W}:(0,1]\to \mathrm{GL}(V)$ and

$$\exists\lim_{\varepsilon\to+0}W_\varepsilon=:W_0\in \mathrm{GL}(V),\quad \exists\lim_{\varepsilon\to+0}\widetilde{W}_\varepsilon=:\widetilde{W}_0\in \mathrm{GL}(V).$$

Generally speaking, the matrices $W_\varepsilon U_\varepsilon\widetilde{W}_\varepsilon$ and $W_0U_\varepsilon\widetilde{W}_0$ can also give weakly inequivalent contractions. This statement is illustrated by the below example. Therefore, Lemma 2.2 of Ref. 76 is incorrect.

Example 1: Consider the one-parametric continuous contraction of the four-dimensional real Lie algebras $\mathrm{so}(3)\oplus A_1\to A_{4.1}$ given by the matrix

$$U_\varepsilon=\begin{pmatrix}0&0&\varepsilon^2&0\\0&-\varepsilon^3&0&0\\0&0&0&\varepsilon\\-\varepsilon^2&0&-1&0\end{pmatrix}\quad\text{with } U_\varepsilon^{-1}=\begin{pmatrix}-\varepsilon^{-4}&0&0&-\varepsilon^{-2}\\0&-\varepsilon^{-3}&0&0\\\varepsilon^{-2}&0&0&0\\0&0&\varepsilon^{-1}&0\end{pmatrix}.$$

Taking the canonical commutation relations $[e_1,e_2]=e_3$, $[e_2,e_3]=e_1$, $[e_3,e_1]=e_2$ of the algebra $\mathrm{so}(3)\oplus A_1$ (the commutators with e_4 vanish), we calculate the transformed commutators up to antisymmetry:

$$[e_1,e_2]_\varepsilon=0,\quad [e_1,e_3]_\varepsilon=0,\quad [e_1,e_4]_\varepsilon=0,\quad [e_2,e_3]_\varepsilon=\varepsilon^4e_4,$$

$$[e_2,e_4]_\varepsilon=e_1-\varepsilon^2e_3,\quad [e_3,e_4]_\varepsilon=e_2.$$

After the limiting process $\varepsilon\to+0$ we obtain the canonical commutation relations $[e_2,e_4]_0=e_1$, $[e_3,e_4]_0=e_3$ of the algebra $A_{4.1}$.

Let us fix an arbitrary $\varepsilon\in(0,1]$. Since the matrix U_ε is nonsingular, its polar decomposition has the form $U_\varepsilon=P_\varepsilon T_\varepsilon$, where $P_\varepsilon:=(U_\varepsilon U_\varepsilon^{\,T})^{1/2}$ is a real symmetric matrix with positive eigenval-

ues and $T_\varepsilon := P_\varepsilon^{-1} U_\varepsilon$ is a real orthogonal matrix. Denote a real orthogonal matrix which reduces P_ε to a diagonal matrix D_ε by W_ε, i.e., $P_\varepsilon = W_\varepsilon D_\varepsilon W_\varepsilon^T$. As a result, we derive the representation $U_\varepsilon = W_\varepsilon D_\varepsilon \tilde{W}_\varepsilon$, where $\tilde{W}_\varepsilon = W_\varepsilon^T T_\varepsilon = D_\varepsilon^{-1} W_\varepsilon^T U_\varepsilon$ is an orthogonal matrix. The explicit form of the matrices W_ε, D_ε, and $\tilde{W}_\varepsilon$ is

$$W_\varepsilon = \begin{pmatrix} -\theta_- & 0 & 0 & \theta_+ \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \theta_+ & 0 & 0 & \theta_- \end{pmatrix}, \quad \tilde{W}_\varepsilon = \begin{pmatrix} -\theta_- & 0 & -\theta_+ & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -\theta_+ & 0 & \theta_- & 0 \end{pmatrix},$$

$$D_\varepsilon = \operatorname{diag}\left(K + \frac{1}{2}, 0, 0, K - \frac{1}{2}\right),$$

where

$$K = \frac{1}{2}\sqrt{4\varepsilon^4 + 1}, \quad \theta_+ = \sqrt{\frac{2K+1}{4K}}, \quad \theta_- = \sqrt{\frac{2K-1}{4K}}.$$

The matrices W_ε and $\tilde{W}_\varepsilon$ converge under $\varepsilon \to +0$ to the constant nonsingular matrices

$$W_0 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \tilde{W}_0 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

Consider the matrix $\tilde{U}_\varepsilon = W_0 D_\varepsilon \tilde{W}_0$ constructed from the representation $U_\varepsilon = W_\varepsilon D_\varepsilon \tilde{W}_\varepsilon$ with replacement of the matrices W_ε and $\tilde{W}_\varepsilon$ by their regular limits. We transform the canonical commutation relations of the algebra $\mathrm{so}(3) \oplus A_1$ with the matrix $\tilde{U}_\varepsilon$ and limit $\varepsilon \to +0$:

$$[e_1, e_2]_\varepsilon = \frac{1}{2}(\sqrt{4\varepsilon^4 + 1} - 1) e_4 \to 0, \quad [e_1, e_3]_\varepsilon = 0,$$

$$[e_1, e_4]_\varepsilon = -\frac{\sqrt{4\varepsilon^4 + 1} - 1}{2\varepsilon^2} e_2 \to 0, \quad [e_2, e_3]_\varepsilon = 0,$$

$$[e_2, e_4]_\varepsilon = \frac{2\varepsilon^4}{\sqrt{4\varepsilon^4 + 1} - 1} e_1 \to e_1, \quad [e_3, e_4]_\varepsilon = 0.$$

As a result, we obtain commutation relations of the algebra $A_{3.1} \oplus A_1$. Therefore, the matrices U_ε and $\tilde{U}_\varepsilon$ lead to weakly inequivalent contractions.

The notion of sequential contractions is introduced similar to continuous contractions. See, e.g., Refs. 39 and 76.

Consider a sequence of $U_p \in \mathrm{GL}(V)$, $p \in \mathbb{N}$. The corresponding sequence of new Lie brackets on V is determined via the old one by the condition $[x,y]_p = U_p^{-1}[U_p x, U_p y] \forall\, p \in \mathbb{N}$, $\forall x, y \in V$. For any $p \in \mathbb{N}$ the Lie algebra $\mathfrak{g}_p = (V, [\cdot,\cdot]_p)$ is isomorphic to $\mathfrak{g}$.

Definition 5: If the limit $\lim_{p\to\infty}[x,y]_p = \lim_{p\to\infty} U_p^{-1}[U_p x, U_p y] =: [x,y]_0$ exists for any $x, y \in V$ then the Lie bracket $[\cdot,\cdot]_0$ is well defined. The Lie algebra $\mathfrak{g}_0 = (V, [\cdot,\cdot]_0)$ is called a *sequential contraction* of the Lie algebra $\mathfrak{g}$.

Any continuous contraction from $\mathfrak{g}$ to $\mathfrak{g}_0$ gives an infinite family of matrix sequences resulting in the sequential contraction from $\mathfrak{g}$ to $\mathfrak{g}_0$. More precisely, if U_ε is the matrix of the continuous contraction and the sequence $\{\varepsilon_p, p\in\mathbb{N}\}$ satisfies the conditions $\varepsilon_p\in(0,1]$, $\varepsilon_p\to+0$, $p\to\infty$, then $\{U_{\varepsilon_p}, p\in\mathbb{N}\}$ is a suitable matrix sequence.

The notion of contraction is generalized to arbitrary fields in terms of orbit closures in the variety of Lie algebras.[7–9,28,29,32,47]

Let V be an n-dimensional vector space over a field $\mathbb{K}$ and $\mathcal{L}_n=\mathcal{L}_n(\mathbb{K})$ denote the set of all possible Lie brackets on V. We identify $\mu\in\mathcal{L}_n$ with the corresponding Lie algebra $\mathfrak{g}=(V,\mu)$. $\mathcal{L}_n$ is an algebraic subset of the variety $V^*\otimes V^*\otimes V$ of bilinear maps from $V\times V$ to V. Indeed, under setting a basis $\{e_1,\dots,e_n\}$ of V there is the one-to-one correspondence between $\mathcal{L}_n$ and

$$\mathcal{C}_n=\{(c_{ij}^k)\in\mathbb{K}^{n^3}|c_{ij}^k+c_{ji}^k=0,\quad c_{ij}^{i'}c_{i'k}^{k'}+c_{ki}^{i'}c_{i'j}^{k'}+c_{jk}^{i'}c_{i'i}^{k'}=0\},$$

which is determined for any Lie bracket $\mu\in\mathcal{L}_n$ and any structure constant tuple $(c_{ij}^k)\in\mathcal{C}_n$ by the formula $\mu(e_i,e_j)=c_{ij}^k e_k$. $\mathcal{L}_n$ is called the *variety of n-dimensional Lie algebras (over the field* $\mathbb{K}$*)* or, more precisely, the variety of possible Lie brackets on V. The group $\mathrm{GL}(V)$ acts on $\mathcal{L}_n$ in the following way:

$$(U\cdot\mu)(x,y)=U(\mu(U^{-1}x,U^{-1}y)),\quad \forall\, U\in\mathrm{GL}(V),\quad \forall\,\mu\in\mathcal{L}_n,\quad \forall\, x,y\in V.$$

[It is a left action in contrast to the right action which is more usual for the "physical" contraction tradition and defined by the formula $(U\cdot\mu)(x,y)=U^{-1}(\mu(Ux,Uy))$ that is not of fundamental importance. We use the right action all over the paper except this paragraph.] Denote the orbit of $\mu\in\mathcal{L}_n$ under the action of $\mathrm{GL}(V)$ by $\mathcal{O}(\mu)$ and the closure of it with respect to the Zariski topology on $\mathcal{L}_n$ by $\overline{\mathcal{O}(\mu)}$.

Definition 6: The Lie algebra $\mathfrak{g}_0=(V,\mu_0)$ is called a contraction (or *degeneration*) of the Lie algebra $\mathfrak{g}=(V,\mu)$ if $\mu_0\in\overline{\mathcal{O}(\mu)}$. The contraction is *proper* if $\mu_0\in\overline{\mathcal{O}(\mu)}\backslash\mathcal{O}(\mu)$. The contraction is *nontrivial* if $\mu_0\not\equiv 0$.

In the case of $\mathbb{K}=\mathbb{C}$ or $\mathbb{K}=\mathbb{R}$ the orbit closures with respect to the Zariski topology coincide with the orbit closures with respect to the Euclidean topology and Definition 5 is reduced to the usual definition of contractions.

III. SIMPLEST TYPES OF CONTRACTIONS

Inönü-Wigner contractions present limit processes between Lie algebras with contraction matrices of simplest types. Most of contractions of low-dimensional Lie algebras are equivalent to such contractions. We discuss their properties which are essential for further consideration.

Simple Inönü-Wigner contractions or shortly IW-contractions first proposed in Ref. 42 are generated by matrices of the form $U_\varepsilon=U_0+\varepsilon U_0'$, where U_0 and U_0' are constant $n\times n$ matrices. The matrix U_ε is additionally assumed to be transformable to the special diagonal form $\hat{W}U_\varepsilon\check{W}^{-1}=\mathrm{diag}(1+\varepsilon v,\dots,1+\varepsilon v,\varepsilon,\dots,\varepsilon)=:D_\varepsilon$ by means of the regular constant matrices $\hat{W}$ and $\check{W}$. The assumption was investigated by Inönü and Wigner themselves.[41] Without loss of generality we can put $v=0$. The matrix D_ε provides the contractions from $\tilde{\mathfrak{g}}$ to $\tilde{\mathfrak{g}}_0$. Here $\tilde{\mathfrak{g}}$ and $\tilde{\mathfrak{g}}_0$ are Lie algebras with the Lie brackets $[x,y]^{\sim}=\hat{W}[\hat{W}^{-1}x,\hat{W}^{-1}y]$ and $[x,y]_0^{\sim}=\check{W}[\check{W}^{-1}x,\check{W}^{-1}y]_0$, which are obviously isomorphic to $\mathfrak{g}$ and $\mathfrak{g}_0$. Therefore, it can be assumed at once that $U_\varepsilon=D_\varepsilon$, i.e.,

$$U_\varepsilon=\mathrm{diag}(1,\dots,1,\varepsilon,\dots,\varepsilon).$$

Denote the number of diagonal elements equal to 1 by s. Then, the dimension of ε block is $n-s$. It is convenient to divide the set of basis elements $\{e_1,\dots,e_n\}$ of V into two subsets $\{e_1,\dots,e_s\}$ and $\{e_{s+1},\dots,e_n\}$ according to the values of diagonal elements. Since

$$[e_{i_1},e_{j_1}]_\varepsilon = c_{i_1j_1}^{k_1}e_{k_1} + \frac{1}{\varepsilon}c_{i_1j_1}^{k_2}e_{k_2} + O(\varepsilon) \to \tilde{c}_{i_1j_1}^{k_1}e_{k_1} + \tilde{c}_{i_1j_1}^{k_2}e_{k_2}, \quad \varepsilon \to +0,$$

where the indices i_1, j_1, and k_1 run from 1 to s and the indices i_2, j_2, and k_2 run from $s+1$ to n, then $c_{i_1j_1}^{k_2}=0$. Therefore, the basis elements $e_1,\ldots,e_s$ generate a subalgebra $\mathfrak{h}$ of the initial algebra $\mathfrak{g}$. It is the unique condition for the contraction to exist. All structure constants of the resulting algebra $\mathfrak{g}_0$ are easily calculated:

$$\tilde{c}_{i_1j_1}^{k_1} = c_{i_1j_1}^{k_1}, \quad \tilde{c}_{i_1j_1}^{k_2} = c_{i_1j_1}^{k_2} = 0, \quad \tilde{c}_{i_1j_2}^{k_1} = 0, \quad \tilde{c}_{i_1j_2}^{k_2} = c_{i_1j_2}^{k_2}, \quad \tilde{c}_{i_2j_2}^{k_1} = \tilde{c}_{i_2j_2}^{k_2} = 0.$$

Let us make a summary of properties of the IW-contractions (see, e.g., Refs. 51 and 67 for some properties). Each subalgebra $\mathfrak{h}$ of the Lie algebra $\mathfrak{g}$ can be used to obtain an IW-contraction of $\mathfrak{g}$. Improper subalgebras correspond to improper ($\mathfrak{h}=\mathfrak{g}$) or trivial ($\mathfrak{h}=\{0\}$) IW-contractions. Different choices of basis complement to a basis of $\mathfrak{h}$ or replacement of $\mathfrak{h}$ by an equivalent subalgebra of $\mathfrak{g}$ give the same contracted algebra up to isomorphism. The contracted algebra $\mathfrak{g}_0$ has the structure of semidirect sum $\mathfrak{h}\ni\mathfrak{a}$, where $\mathfrak{a}$ is the Abelian ideal spanned on the chosen basis complement to a basis of $\mathfrak{h}$. The subalgebra $\mathfrak{h}$ is isomorphic to the quotient algebra $\mathfrak{g}_0/a$. And vice versa, the Lie algebra $\mathfrak{g}_0$ is an IW-contraction of the algebra $\mathfrak{g}$ with the subalgebra $\mathfrak{h}$ if and only if there exists an Abelian ideal $\mathfrak{a}\subset\mathfrak{g}_0$ for which the quotient algebra $\mathfrak{g}_0/\mathfrak{a}$ is isomorphic to $\mathfrak{h}$. The repeated IW-contraction with the same subalgebra $\mathfrak{h}$ again results in the algebra $\mathfrak{g}_0$.

Any IW-contraction satisfies two assumptions: (1) the contraction matrix is linear with respect to the contraction parameter; (2) there exist constant regular matrices $\hat{W}$ and $\check{W}$ diagonalizing the contraction matrix. It is well known that IW-contractions do not exhaust all possible contractions even in the case of three dimensional Lie algebras. IW-contractions of the three-dimensional rotation algebra so(3) result in only one nontrivial and proper contraction to the Lie algebra $A_{3.5}^0$. At the same time, there also exists the proper contraction from so(3) to the Heisenberg algebra $\mathfrak{h}_3=A_{3.1}$ and it is not provided by IW-contractions (see Secs. VI and VIII for details).

Saletan[67] studied the whole class of contractions linear with respect to the contraction parameter, i.e., contractions generated by the matrices of the form $U(\varepsilon)=U_0+\varepsilon U_0'$, where U_0 and U_0' are constant matrices. Now such contractions are called *Saletan contractions* or, shortly, S-contractions. The assumption $U(1)=E$, where E is the unit matrix, can be imposed with basis change and reparametrization without loss of generality. Then the contraction matrix takes the form $U(\varepsilon)=\varepsilon E+(1-\varepsilon)\tilde{U}$, where $\tilde{U}$ is a constant matrix. Conditions on the matrix $\tilde{U}$ of a well-defined S-contraction were formulated in Ref. 67. Iterations of S-contractions with the same contraction matrix result in a finite chain of nonisomorphic algebras. The repeated contraction from the first algebra to the last algebra of the chain is an IW-contraction.[51,67] Any IW-contraction obviously is a S-contraction and there exist S-contractions which are inequivalent to IW-contractions. Thus, Saletan proved that the contraction $\mathrm{so}(3)\oplus A_1\to A_{4.9}^0$ is realized via a S-contraction and is equivalent to no IW-contraction. At the same time, S-contractions do not also exhaust all possible contractions of Lie algebras. An illustrative example is again given by the contraction $\mathrm{so}(3)\to\mathfrak{h}_3=A_{3.1}$, which is not provided even by S-contractions.[67]

Another generalization of the class of IW-contractions is given by *generalized IW-contractions* (or Doebner-Melsheimer contractions)[21,34,51] for which the linearity condition is replaced by the condition that the elements of the diagonalized contraction matrix are (integer) powers of the contraction parameter. Namely, the contraction matrix of a generalized IW-contraction has the form $U(\varepsilon)=\hat{W}^{-1}\,\mathrm{diag}(\varepsilon^{\alpha_1},\varepsilon^{\alpha_2},\ldots,\varepsilon^{\alpha_n})\check{W}$, where $\hat{W}$ and $\check{W}$ are nonsingular constant matrices and $\alpha_1,\alpha_2,\ldots,\alpha_n\in\mathbb{Z}$. As in the case of simple IW-contractions, due to possibility of replacement of Lie algebras by isomorphic ones we can assume that $\hat{W}=\check{W}=E$, i.e.,

$$U(\varepsilon) = \mathrm{diag}(\varepsilon^{\alpha_1},\varepsilon^{\alpha_2},\ldots,\varepsilon^{\alpha_n}).$$

Then the structure constants of the resulting algebra $\mathfrak{g}_0$ are calculated by the formula

$$\tilde{c}_{ij}^k = \lim_{\varepsilon \to +0} \varepsilon^{\alpha_i+\alpha_j-\alpha_k} c_{ij}^k,$$

with no summation with respect to the repeated indices. Therefore, the constraints

$$\alpha_i + \alpha_j \geqslant \alpha_k, \quad i,j,k = 1, \ldots, n \quad \text{if } c_{ij}^k \neq 0$$

are necessary and sufficient for the existence of the well-defined generalized IW-contraction with the contraction matrix $U(\varepsilon)$ and

$$\tilde{c}_{ij}^k = c_{ij}^k \quad \text{if } \alpha_i + \alpha_j = \alpha_k \quad \text{and} \quad \tilde{c}_{ij}^k = 0 \quad \text{otherwise}.$$

The conditions on contraction existence and the resulting algebra can be reformulated in the basis-independent terms of filtrations on the initial algebra and of associated graded Lie algebras.[32]

IW-contractions clearly form subclass of generalized IW-contractions with $\alpha_i \in \{0,1\}$. A natural question is whether any generalized IW-contraction can be decomposed to a sequence of successive IW-contractions. The unique nontrivial generalized IW-contraction between three-dimensional algebras is given by two successive IW-contractions $\mathrm{so}(3) \to A_{3.5}^0 \to A_{3.1}$. Inönu[40] and Sharp[70] formulated the proposition that the decomposition is not always possible. It was shown[51] that decomposability of a generalized IW-contraction implies additional constraints on structure constants of the initial Lie algebra. We construct a number of generalized IW-contractions of four-dimensional algebras, which are not decomposed to a sequence of simple IW-contractions. For example, the algebra $A_{4.4}$ having the nonzero commutation relations $[e_1,e_4]=e_1$, $[e_2,e_4]=e_1+e_2$, $[e_3,e_4]=e_2+e_3$ is contracted to the algebra $A_{4.1}$ ($[e_2,e_4]=e_1$, $[e_3,e_4]=e_2$) by the generalized IW-contraction with the matrix $\mathrm{diag}(\varepsilon^2,\varepsilon,1,\varepsilon)$. This contraction obviously illustrates the above statement since it is direct, i.e., there are no Lie algebra $\mathfrak{g}$ such that the contractions $A_{4.4} \to \mathfrak{g}$ and $\mathfrak{g} \to A_{4.1}$ are proper. See Remark 2 for more examples.

Remark 2: If some of the powers $\alpha_1, \alpha_2, \ldots, \alpha_n$ in the contraction matrix $U(\varepsilon)$ are negative, the limit of $U(\varepsilon)$ under $\varepsilon \to +0$ does not exist. It is not precisely known up to now in what situations it is sufficient to consider only non-negative powers of ε. Results of this paper imply that all contractions of the three- and four-dimensional Lie algebras are weakly equivalent to the ones for which the limit of the contraction matrices exists.

IV. NECESSARY CONTRACTION CRITERIA

An optimal way of exhaustive investigation of contractions in a set of Lie algebras includes intensive usage of necessary criteria based on quantities which are *invariant* or *semi-invariant* under contractions. The invariant quantities are preserved under contractions. Semi-invariance means existence of inequalities between the corresponding quantities of initial and contracted algebras. Since contractions are limit processes, the terms of *continuity* and *semicontinuity* can be used instead of invariance and semi-invariance.

For convenience we collect the relations between invariant or semi-invariant quantities as necessary criteria of contractions in Theorem 1.

Below we use the following notations of quantities and objects connected with the algebra $\mathfrak{g}$: the differentiation algebra $\mathrm{Der}\,\mathfrak{g}$, the orbit $\mathcal{O}(\mathfrak{g})$ under action of $\mathrm{GL}(V)$ in the variety $\mathcal{L}_n$ of n-dimensional Lie algebras, the center $Z(\mathfrak{g})$, the radical $R(\mathfrak{g})$, the nilradical $N(\mathfrak{g})$, the maximal dimension $n_{\mathrm{A}}(\mathfrak{g})$ of Abelian subalgebras, the maximal dimension $n_{\mathrm{Ai}}(\mathfrak{g})$ of Abelian ideals, the Killing form κ, the rank $r_{\mathfrak{g}}$, i.e., the dimension of the Cartan subalgebras, the adjoint and coadjoint representations $\mathrm{ad}\,\mathfrak{g}$ and $\mathrm{ad}^*\,\mathfrak{g}$, the adjoint representation ad_x of the element $x \in \mathfrak{g}$, and the ranks of adjoint and coadjoint representations which are calculated in a fixed basis by the formulas

$$\mathrm{rank}(\mathrm{ad}\,\mathfrak{g}) = \max_{x \in V} \mathrm{rank}(c_{ij}^k x^j) \quad \text{and} \quad \mathrm{rank}(\mathrm{ad}^*\,\mathfrak{g}) = \max_{u \in V^*} \mathrm{rank}(c_{ij}^k u_k).$$

Let us also define three standard series of characteristic ideals of $\mathfrak{g}$, namely,

$$\text{the lower central series: } \mathfrak{g}^0 \supset \mathfrak{g}^1 \supset \cdots \supset \mathfrak{g}^l \supset \cdots,$$

$$\text{the derived series: } \mathfrak{g}^{(0)} \supset \mathfrak{g}^{(1)} \supset \cdots \supset \mathfrak{g}^{(l)} \supset \cdots, \quad \text{and}$$

$$\text{the upper central series: } \mathfrak{g}_{(0)} \subset \mathfrak{g}_{(1)} \subset \cdots \subset \mathfrak{g}_{(l)} \subset \cdots,$$

where $\mathfrak{g}^0=\mathfrak{g}$, $\mathfrak{g}^l=[\mathfrak{g},\mathfrak{g}^{l-1}]$, $\mathfrak{g}^{(0)}=\mathfrak{g}$, $\mathfrak{g}^{(l)}=[\mathfrak{g}^{(l-1)},\mathfrak{g}^{(l-1)}]$, $\mathfrak{g}_{(0)}=\{0\}$, $\mathfrak{g}_{(l)}/\mathfrak{g}_{(l-1)}$ is the center of $\mathfrak{g}/\mathfrak{g}_{(l-1)}$, $l\in\mathbb{N}$. In particular, $\mathfrak{g}^1=\mathfrak{g}^{(1)}=[\mathfrak{g},\mathfrak{g}]$, $\mathfrak{g}_{(1)}=Z(\mathfrak{g})$. If $\mathfrak{g}$ is a solvable (nilpotent) Lie algebra, $r_s=r_s(\mathfrak{g})$ ($r_n=r_n(\mathfrak{g})$) denotes the solvability (nilpotency) rank of $\mathfrak{g}$, i.e., the minimal number l such that $\mathfrak{g}^{(l)}=\{0\}$ ($\mathfrak{g}^l=\{0\}$).

Suppose that $\mathrm{tr}(\mathrm{ad}_u{}^p)\neq 0$, $\mathrm{tr}(\mathrm{ad}_u{}^q)\neq 0$, and $\mathrm{tr}(\mathrm{ad}_u{}^p\mathrm{ad}_v{}^q)\neq 0$ for some $p,q\in\mathbb{N}$ and $u,v\in\mathfrak{g}$ and the value

$$\mathfrak{C}_{pq}=\frac{\mathrm{tr}(\mathrm{ad}_u{}^p)\mathrm{tr}(\mathrm{ad}_v{}^q)}{\mathrm{tr}(\mathrm{ad}_u{}^p\mathrm{ad}_v{}^q)}, \quad p,q\in\mathbb{N}$$

does not depend on u and v. Then $\mathfrak{C}_{pq}=\mathfrak{C}_{pq}(\mathfrak{g})$ is a well-defined invariant characteristic of the algebra $\mathfrak{g}$, i.e., it is a constant on the orbit $\mathcal{O}(\mathfrak{g})$.

Denote the rank of positive (negative) part of the Killing form $\kappa_\mathfrak{g}$, i.e., the number of positive (negative) diagonal elements of a diagonal form of its matrix, by $\mathrm{rank}_+\kappa_\mathfrak{g}$ ($\mathrm{rank}_-\kappa_\mathfrak{g}$). In view of the law of inertia of quadratic forms, $\mathrm{rank}_+\kappa_\mathfrak{g}$ and $\mathrm{rank}_-\kappa_\mathfrak{g}$ are invariant under basis transformations over $\mathbb{R}$. For any $\alpha\in\mathbb{R}$ we introduce the modified Killing form

$$\tilde{\kappa}^\alpha_\mathfrak{g}=\mathrm{tr}(\mathrm{ad}_u\,\mathrm{ad}_v)+\alpha\,\mathrm{tr}(\mathrm{ad}_u)\mathrm{tr}(\mathrm{ad}_v)$$

and the corresponding values $\mathrm{rank}_+\tilde{\kappa}^\alpha_\mathfrak{g}$ and $\mathrm{rank}_-\tilde{\kappa}^\alpha_\mathfrak{g}$. The Killing form is the special case of the modified Killing form with $\alpha=0$.

The following technical lemma is very useful for further considerations.

Lemma 1: *Let A_p, $p\in\mathbb{N}$, be a sequence of real or complex matrices of the same dimensions and there exists componentwise limit of A_p, $p\to\infty$, denoted by A_0. If* $\mathrm{rank}\,A_p=r\,\forall\,p\in\mathbb{N}$ *then* $\mathrm{rank}\,A_0\leqslant r$.

Theorem 1: *If the Lie algebra $\mathfrak{g}_0$ is a proper (continuous or sequential) contraction of the Lie algebra $\mathfrak{g}$, then the following set of relations holds true.*

(1) $\dim \mathrm{Der}\,\mathfrak{g}_0>\dim \mathrm{Der}\,\mathfrak{g}$ (*and* $\dim\mathcal{O}(\mathfrak{g}_0)<\dim\mathcal{O}(\mathfrak{g})$);
(2) $n_A(\mathfrak{g}_0)\geqslant n_A(\mathfrak{g})$
(3) $\dim Z(\mathfrak{g}_0)\geqslant\dim Z(\mathfrak{g})$; *moreover*, $\dim\mathfrak{g}_0(l)\geqslant\dim\mathfrak{g}_{(l)}$, $l\in\mathbb{N}$;
(4) $\dim\mathfrak{g}_0^l\leqslant\dim\mathfrak{g}^{(l)}$, $l\in\mathbb{N}$;
(5) $\dim\mathfrak{g}_0^l\leqslant\dim\mathfrak{g}^l$, $l\in\mathbb{N}$;
(6) $\dim R(\mathfrak{g}_0)\geqslant\dim R(\mathfrak{g})$;
(7) $\dim N(\mathfrak{g}_0)\geqslant\dim N(\mathfrak{g})$;
(8) $n_{\mathrm{Ai}}(\mathfrak{g}_0)\geqslant n_{\mathrm{Ai}}(\mathfrak{g})$;
(9) $r_{\mathfrak{g}_0}\geqslant r_\mathfrak{g}$;
(10) $\mathrm{rank\,ad}\,\mathfrak{g}_0\leqslant\mathrm{rank\,ad}\,\mathfrak{g}$, $\mathrm{rank\,ad}^*\mathfrak{g}_0\leqslant\mathrm{rank\,ad}^*\,\mathfrak{g}$;
(11) $\mathrm{rank}\kappa_{\mathfrak{g}_0}\leqslant\mathrm{rank}\,\kappa_\mathfrak{g}$;
(12) $\mathfrak{g}_0$ *is unimodular if* $\mathfrak{g}$ *is unimodular, i.e.,* $\mathrm{tr}(\mathrm{ad}_u)=0$ *for any u in $\mathfrak{g}$ implies the same condition in $\mathfrak{g}_0$*;
(12′) *moreover, for any fixed $l\in\mathbb{N}$ $\mathfrak{g}_0$ is l unimodular if $\mathfrak{g}$ is l unimodular, i.e.,* $\mathrm{tr}(\mathrm{ad}_u{}^l)=0$ *for any u in $\mathfrak{g}$ implies the same condition in $\mathfrak{g}_0$*;
(13) *if $\mathfrak{g}$ is solvable Lie algebra then $\mathfrak{g}_0$ is also solvable and* $r_s(\mathfrak{g}_0)\leqslant r_s(\mathfrak{g})$;
(14) *if $\mathfrak{g}$ is nilpotent Lie algebra then $\mathfrak{g}_0$ is also nilpotent and* $r_n(\mathfrak{g}_0)\leqslant r_n(\mathfrak{g})$;
(15) $\mathfrak{C}_{pq}(\mathfrak{g}_0)=\mathfrak{C}_{pq}(\mathfrak{g})$ *for all values $p,q\in\mathbb{N}$, where the invariants* $\mathfrak{C}_{pq}(\mathfrak{g}_0)$ and $\mathfrak{C}_{pq}(\mathfrak{g})$ *are well defined*;
(16) (*only over* $\mathbb{R}$!) $\mathrm{rank}_+\kappa_{\mathfrak{g}_0}\leqslant\mathrm{rank}_+\kappa_\mathfrak{g}$ *and* $\mathrm{rank}_-\kappa_{\mathfrak{g}_0}\leqslant\mathrm{rank}_-\kappa_\mathfrak{g}$; *moreover for any* $\alpha\in\mathbb{R}$ $\mathrm{rank}_+\tilde{\kappa}^\alpha_{\mathfrak{g}_0}\leqslant\mathrm{rank}_+\tilde{\kappa}^\alpha_\mathfrak{g}$ *and* $\mathrm{rank}_-\tilde{\kappa}^\alpha_{\mathfrak{g}_0}\leqslant\mathrm{rank}_-\tilde{\kappa}^\alpha_\mathfrak{g}$;
(17) *if the algebra $\mathfrak{g}_0$ is rigid then it is not a contraction of any $\mathfrak{g}$ and if there is no deformation*

from $\mathfrak{g}_0$ *to* $\mathfrak{g}$, *then there is no contraction from* $\mathfrak{g}$ *to* $\mathfrak{g}_0$.

Proof: It is sufficient to prove the theorem in the case of sequential contractions. The statement on continuous contractions directly follows from the one on sequential contractions. We use the notations introduced at the beginning of the section.

At first, Criteria 4 and 5 are proven in detail. The statements are true if $\dim[\mathfrak{g},\mathfrak{g}]=\dim\mathfrak{g}=:n$. Indeed, in this case $\dim\mathfrak{g}^{(l)}=\dim\mathfrak{g}^l=n$ for all $l\in\mathbb{N}$ that results in Criteria 4 and 5 in view of the obvious conditions $\dim\mathfrak{g}_0^{(l)}\leqslant\dim\mathfrak{g}_0$, $\dim\mathfrak{g}_0^l\leqslant\dim\mathfrak{g}_0$, and $\dim\mathfrak{g}_0=\dim\mathfrak{g}=n$.

Suppose that $\dim[\mathfrak{g},\mathfrak{g}]<n$. Let $\{e^1,\dots,e^n\}$ be the basis in the dual space V^*, which is dual to the basis $\{e_1,\dots,e_n\}$, i.e., $\langle e^i,e_j\rangle=\delta^i_j$. Here δ^i_j is the Kronecker delta. We define A as the $n\times n^2$ matrix consisting of the elements $c^k_{ij}=\langle e^k,[e_i,e_j]\rangle$, where the index k runs the row range and the index pair (i,j) runs the column range:

$$A=\begin{pmatrix} c^1_{11} & \cdots & c^1_{1n} & c^1_{21} & \cdots & c^1_{2n} & \cdots & c^1_{n1} & \cdots & c^1_{nn}\\ c^2_{11} & \cdots & c^2_{1n} & c^2_{21} & \cdots & c^2_{2n} & \cdots & c^2_{n1} & \cdots & c^2_{nn}\\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots\\ c^n_{11} & \cdots & c^n_{1n} & c^3_{21} & \cdots & c^n_{2n} & \cdots & c^n_{n1} & \cdots & c^n_{nn}\end{pmatrix}.$$

Due to antisymmetry of c^k_{ij} in subscripts, we can take only columns with $i<j$ into account. Analogously we introduce the matrices A_p and A_0 for the algebras $\mathfrak{g}_p$ and $\mathfrak{g}_0$.

The dimensions of $[\mathfrak{g},\mathfrak{g}]$ and $[\mathfrak{g},\mathfrak{g}]_p$ coincide. Denote the common value of dimensions as n_1. These statements are reformulated in terms of the introduced matrices A and A_p:

$$\operatorname{rank}A=\operatorname{rank}A_p=n_1.$$

Therefore, all (n_1+1)-dimensional minors of any matrix $A_p, p\in\mathbb{N}$ equal to zero. Moreover, we have

$$c^k_{p,ij}=\langle e^k,[e_i,e_j]_p\rangle\to c^k_{0,ij}=\langle e^k,[e_i,e_j]_0\rangle,\quad p\to\infty,$$

i.e., the elements of the matrix A_p go to the corresponding elements of the matrix A_0. It leads to the convergency of minors. Consequently, any (n_1+1)-dimensional minor of the matrix A_0 vanishes. It implies that rank $A_0\leqslant n_1$, i.e., $[\mathfrak{g}_0,\mathfrak{g}_0]\leqslant n_1$. Criteria 4 and 5 for $l=1$ have been proven.

Criteria 4 and 5 for the other values of l are proven analogously. The requisite matrices are defined in the similar way as the matrices A, A_p, and A_0 in the case $l=1$ with replacement of the usual commutators $[e_i,e_j]$ by the corresponding repeated commutators of basis elements.

Criteria 9, 10, and 11 are proven in a similar and simpler way via the limit process $p\to\infty$ in the formulas

$$r_{\mathfrak{g}}=n-\max_{x\in V}\operatorname{rank}(c^k_{ij}x^j)^n=r_{\mathfrak{g}_p}=n-\max_{x\in V}\operatorname{rank}(c^k_{p,ij}x^j)^n,$$

$$\operatorname{rank}(\operatorname{ad}\mathfrak{g})=\max_{x\in V}\operatorname{rank}(c^k_{ij}x^j)=\operatorname{rank}(\operatorname{ad}\mathfrak{g}_p)=\max_{x\in V}\operatorname{rank}(c^k_{p,ij}x^j),$$

$$\operatorname{rank}(\operatorname{ad}^*\mathfrak{g})=\max_{u\in V^*}\operatorname{rank}(c^k_{ij}u_k)=\operatorname{rank}(\operatorname{ad}^*\mathfrak{g}_p)=\max_{u\in V^*}\operatorname{rank}(c^k_{p,ij}u_k),$$

$$\operatorname{rank}(\kappa_{\mathfrak{g}})=\operatorname{rank}(c^k_{ij}c^j_{i'k})=\operatorname{rank}(\kappa_{\mathfrak{g}_p})=\operatorname{rank}(c^k_{p,ij}c^j_{p,i'k}),\quad p\in\mathbb{N}.$$

Criteria 12 and 12′ are obvious since $\operatorname{tr}(\operatorname{ad}_u{}^l)=0$ for any u in $\mathfrak{g}$ implies the same condition in $\mathfrak{g}_p$ and $\operatorname{tr}(\operatorname{ad}_{\mathfrak{g}_p,u}{}^l)\to\operatorname{tr}(\operatorname{ad}_{\mathfrak{g}_0,u}{}^l)$, $p\to\infty$.

Criteria 13 and 14 directly follow from Criteria 4 and 5.

Since the radical $R(\mathfrak{g})$ is the orthogonal complement of the derivative $[\mathfrak{g},\mathfrak{g}]$ with respect to the Killing form $\kappa_{\mathfrak{g}}$ (Ref. 44) then $\dim R(\mathfrak{g})=\dim R(\mathfrak{g}_p)$ coincides with the value

$$n-\operatorname{rank}(c_{ij}^{k}c_{i'k}^{j}c^{i'}_{i''j''})=n-\operatorname{rank}(c_{p,ij}^{k}c_{p,i'k}^{j}c^{i'}_{p,i''j''}),\quad p\in\mathbb{N}.$$

In the matrices the index pair (i'',j'') runs the row range and the index i runs the column range. The limit process $p\to\infty$ in the latter formula results in Criterion 6.

The center $Z(\mathfrak{g})$ coincides with the set of solutions of the system $[e_i,x]=0$, or $c_{ij}^{k}x^{j}=0$ in the coordinate form. Therefore, $\dim Z(\mathfrak{g})=\dim Z(\mathfrak{g}_p)$ equals to

$$n-\operatorname{rank}(c_{ij}^{k})=n-\operatorname{rank}(c_{p,ij}^{k}),\quad p\in\mathbb{N},$$

where the index pair (k,j) runs the row range and the index i runs the column range. The limit process $p\to\infty$ in the latter formula implies Criterion 3 for $l=1$. Proof for the other values of l is similar. Instead of $(c_{ij}^{k})=(\langle e^{k},[e_i,e_j]\rangle)$, the matrix $(\langle e^{k},[\ldots[e_i,e_{j_1}],\ldots,e_{j_l}]\rangle)$ should be used, where the index tuple $(k,j_1,\ldots,j_l)$ runs the row range and the index i runs the column range.

Criterion 15 is true in view of invariance property of $\mathfrak{C}_{pq}$.

Proof of Criterion 2 is also adduced in detail since it presents another typical trick which is used in deriving necessary contraction criteria. Let $n_A(\mathfrak{g})=l$. Then $n_A(\mathfrak{g}_p)=l$ too. We change the basis of $\mathfrak{g}_p$ with a nonsingular matrix W_p that

$$\tilde{c}_{p,ij}^{k}=0\quad\text{if } i,j\leqslant l.$$

Here $\tilde{c}_{p,ij}^{k}=(W_p)_{i'}^{i}(W_p)_{j'}^{j}(W_p{}^{-1})_{k}^{k'}c_{p,i'j'}^{k'}$ are the structure constants of $\mathfrak{g}_p$ in the new basis. Due to possibility of "orthogonalization" of the basis, we can assume without loss generality that W_p is an orthogonal (unitary) matrix in the case of the real (complex) field. The set of orthogonal (or unitary) matrices is compact in the induced "Euclidean" matrix norm. Therefore, there exists a convergent subsequence $\{W_{p_q},q\in\mathbb{N}\}$. Denote the orthogonal (unitary) matrix being the limit of this subsequence by W_0. Then

$$\tilde{c}_{p_q,ij}^{k}=(W_{p_q})_{i'}^{i}(W_{p_q})_{j'}^{j}(W_{p_q}{}^{-1})_{k}^{k'}c_{p_q,i'j'}^{k'}\to(W_0)_{i'}^{i}(W_0)_{j'}^{j}(W_0{}^{-1})_{k}^{k'}c_{0,i'j'}^{k'}=\tilde{c}_{0,ij}^{k},\quad q\to\infty.$$

Hence $\tilde{c}_{p,ij}^{k}=0$ if $i,j\leqslant l$ in view of the same condition for $c_{p,ij}^{k}$, i.e., $\mathfrak{g}_0$ contains an l-dimensional Abelian subalgebra that implies Criterion 2.

Criteria 6, 7, and 8 are proven in a similar way with replacement of the Abelian subalgebra condition by the ideal condition

$$\tilde{c}_{p,ij}^{k}=0\quad\text{if } (i\leqslant l \text{ or } j\leqslant l) \text{ and } k>l$$

completed with the conditions

$$\tilde{c}_{p,ij}^{k}=0\quad\text{if } i,j\leqslant l \text{ and } k>\max(i,j),\quad l=\dim R(\mathfrak{g}),$$

$$\tilde{c}_{p,ij}^{k}=0\quad\text{if } i,j\leqslant l \text{ and } k\geqslant\max(i,j),\quad l=\dim N(\mathfrak{g}),$$

$$\tilde{c}_{p,ij}^{k}=0\quad\text{if } i,j\leqslant l,\quad l=n_{A_i}(\mathfrak{g})$$

of solvability for the radical, nilpotency for the nilradical, and commutativity for an Abelian ideal of the maximal dimension, correspondingly. Other conditions of solvability and nilpotency can also be used. Let us note that we derive the second proof of Criterion 6.

Similar technique based on compactness of the set of orthogonal matrices is used in proof of Criterion 16. Denote the number of positive (negative) diagonal elements of a diagonal form of a symmetric matrix K by $\operatorname{rank}_{+}K$ ($\operatorname{rank}_{-}K$).

It is sufficient to prove that for any convergent sequence of symmetric matrices $K_p\to K_0$, $p\to\infty$, with $\operatorname{rank}_{+}K_p=r_{+}$ and $\operatorname{rank}_{-}K_p=r_{-}$, $p\in\mathbb{N}$, the inequalities $\operatorname{rank}_{+}K_0\leqslant r_{+}$ and $\operatorname{rank}_{-}K_0\leqslant r_{-}$ are

true. Then this statement is applied to the sequence of the matrices of the (modified) Killing forms of the algebras $\mathfrak{g}_p$, which have the same values of rank_+ and rank_- in view of the inertia law of quadratic forms and converge to the matrix of the (modified) Killing form of the resulting algebra $\mathfrak{g}_0$.

Let W_p be the orthogonal matrix which reduces K_p to the matrix $D_p=\mathrm{diag}(d_{p,1},\dots,d_{p,n})$, where $d_{p,i_1}>0$ for $i_1=1,\dots,r_+$, $d_{p,i_2}<0$ for $i_2=r_++1,\dots,r_++r_-$, and $d_{p,i_3}=0$ for $i_3=r_++r_-+1,\dots,n(r_++r_-\leqslant n)$. So, $K_p=W_pD_pW_p^T$. We choose a convergent subsequence $\{W_{p_q},q\in\mathbb{N}\}$ and denote the orthogonal matrix being the limit of this subsequence by W_0. Then

$$D_{p_q}=W_{p_q}^{\mathcal{T}}K_{p_q}W_{p_q}\to W_0^{\mathcal{T}}K_0W_0=:D_0,\quad q\to\infty.$$

D_0 is a diagonal matrix $\mathrm{diag}(d_{0,1},\dots,d_{0,n})$ as the limit of the sequence of the diagonal matrices D_{p_q}, $q\in\mathbb{N}$. Moreover, $d_{0,i_1}\geqslant 0$ for $i_1=1,\dots,r_+$, $d_{0,i_2}\leqslant 0$ for $i_2=r_++1,\dots,r_++r_-$, and $d_{0,i_3}=0$ for $i_3=r_++r_-+1,\dots,n$ that implies the requisite statement.

Criteria 1 and 17 were proven, e.g., in Refs. 4, 32, and 71. □

Remark 3: The criteria can be reformulated in terms of closed subsets of the variety $\mathcal{A}_n$ of n-dimensional Lie algebras. Thus, the sets of nilpotent, solvable, and unimodular algebras are closed. The sets $\{\mathfrak{g}\in\mathcal{A}_n|\dim\mathfrak{g}^l\leqslant r\}$, $\{\mathfrak{g}\in\mathcal{A}_n|\dim\mathfrak{g}^{(l)}\leqslant r\}$, $\{\mathfrak{g}\in\mathcal{A}_n|\dim\mathfrak{g}_{(l)}\geqslant r\}$, and similar ones are closed for each l and $r=0,\dots,n$.

Remark 4: Necessary criteria already appeared in early papers on contractions of Lie algebras. Thus, in his pioneer paper[69] Segal used the criterion based on the law of inertia of the Killing forms (the first part of Criterion 16) in the case of compact semisimple Lie algebras. The inequality on dimensions of the derived algebras $\dim[\mathfrak{g}_0,\mathfrak{g}_0]\leqslant\dim[\mathfrak{g},\mathfrak{g}]$ was proven in Ref. 67 in the practically same way as above. Criteria 3 and 5 on upper and lower central series arise under studying varieties of nilpotent algebras.[74] Very important Criterion 2 is a direct consequence of the lemma on orbit closures, which is adduced, e.g., in Ref. 4. Criterion 1 was proven in Ref. 32 with usage of the Iwasawa decomposition. It was pointed out in Ref. 68 that the same technique can be used to prove other necessary contraction criteria. Restricting ourself with real and complex cases, we simplify this technique and use it to also prove Criteria 6, 7, and 8. Criteria 3, 4, and 5 were applied simultaneously in Ref. 45, see also discussion in Ref. 29. All the above criteria are based on semi-invariant values. Criterion 15 on the invariant algebra characteristic $\mathfrak{C}_{pq}$ was first proposed and effectively used in Refs. 9 and 71. A number of criteria are collected *ibid* and key ideas on proof of them were also formulated. In particular, Criterion 9 was adopted by us from there. Let us note that $\mathfrak{C}_{pq}$ is a generalization of the invariant $J=\mathrm{tr}(\mathrm{ad}_u^2)/(\mathrm{tr}\,\mathrm{ad}_u)^2$ introduced in Ref. 45. The part of Criterion 10 on rank of coadjoint representations arises in investigation of connections between invariants of initial and contracted algebras.[10,11] Criterion 17 was discussed, e.g., in Ref. 51. There exist also other criteria, e.g., ones connected with cohomologies of Lie algebras.[8]

Remark 5: The list of criteria can be extended with other quantities which concern algebras and are semi-invariant under contractions.[9] The criteria used in this paper are simple from the computing point of view.

The set (or even a subset) of the adduced criteria is complete for the three- and four-dimensional Lie algebras in the sense that they precisely separate all pairs of algebras, which do not admit contractions. The question on completeness of the adduced criteria in the case of Lie algebras of higher dimensions is still open.

The set of criteria is not minimal. Some criteria are induced by others. For example, Criteria 4 and 5 imply Criteria 13 and 14.

Criteria differ from each other in effectiveness. Criteria 1 and 12 are most powerful since they exclude possibility of contractions in most pairs of low-dimensional Lie algebras. This fact is illustrated by examples of Sec. VII.

Criterion 16 is the unique criterion which is special for the real field. Only it works for pairs of algebras having a contraction over $\mathbb{C}$ and no contractions over $\mathbb{R}$. See Remark 12 additionally.

Remark 6: Criterion 1 is singular and particularly powerful due to appearance of strict inequality in it. It is the unique criterion which enables investigation of contractions in series of

Lie algebras in a simple way. Since the dimensions of the differentiation algebras for the nonsingular values of the parameters in series of Lie algebras coincide, Criterion 1 implies the absence of contractions between these cases.

The weakened version of Criterion 1 with unstrict inequality is proven analogous to a number of other criteria. Indeed, in a fixed basis of V the coefficients d_j^i of the matrix of any operator from Der $\mathfrak{g}$ satisfy the homogeneous system of linear equations

$$c_{ij}^{k'} d_{k'}^{k} = c_{i'j}^{k} d_i^{i'} + c_{ij'}^{k} d_j^{j'}.$$

Let A be the matrix of this system and A_p and A_0 be the similar matrices for the algebras $\mathfrak{g}_p$ and $\mathfrak{g}_0$. Then $\dim \mathrm{Der}\,\mathfrak{g}=n^2-\mathrm{rank}A=\dim \mathrm{Der}\,\mathfrak{g}_p=n^2-\mathrm{rank}A_p$ and $\dim \mathrm{Der}\,\mathfrak{g}_0=n^2-\mathrm{rank}A_0$. Therefore, the inequality $\dim \mathrm{Der}\,\mathfrak{g}_0 \geqslant \dim \mathrm{Der}\,\mathfrak{g}$ obviously follows from Lemma 1. [Note that $\dim \mathcal{O}(\mathfrak{g})=\mathrm{rank}A$.]

Can other criteria or their combinations be strengthened with replacement of unstrict inequalities by strict ones? The answer to this question is unknown up to now. There existed the conjecture that dimension of an element of the upper or lower central series or the derived series should vary under a proper contraction. A contrary instance on the conjecture was adduced in Ref. 29. It is given by the contraction of the three-dimensional algebras

$$A_{3.2}([e_1,e_3]=e_1,[e_2,e_3]=e_1+e_2) \to A_{3.3}([e_1,e_3]=e_1,[e_2,e_3]=e_1),$$

which is realized via the simple IW-contraction associated with the subalgebra $\langle e_1, e_2+e_3\rangle$. Let us note additionally that all invariant and semi-invariant quantities adduced in this section excluding only dim Der coincide for the above algebras. Therefore, only Criterion 1 is effectual for this pair of algebras.

V. CALCULATION OF INVARIANT QUANTITIES

There are two simple classes of Lie algebras, which cover most low-dimensional algebras. The first one is formed by *almost Abelian algebras* having Abelian ideals of codimension one. The algebras from the second class have WH+A ideals of codimension one, which are isomorphic to the direct sum of the Weyl-Heisenberg algebra $\mathfrak{h}_3=A_{3.1}$ and the Abelian algebra of codimension four. Characteristics of the above algebras are found in a uniform way. The other low-dimensional algebras should be investigated separately. Below we adduce only calculations of the invariants $\mathfrak{C}_{pq}$ which were recently proposed in Refs. 9 and 71 and the ranks of some algebras.

A. Almost Abelian algebras

Consider an n-dimensional Lie algebra over $\mathbb{C}$ or $\mathbb{R}$ which has an $(n-1)$-dimensional Abelian ideal. It is a solvable and, moreover, metabelian algebra. Let $e_1,\dots,e_{n-1}$ form a basis of the ideal and e_n completes it to a basis of the algebra. The nonzero commutation relations between elements of the constructed bases are

$$[e_j,e_n]=\sum_{k=1}^{n-1} a_j^k e_k, \quad j=1,\dots,n-1.$$

The $(n-1)\times(n-1)$ matrix $A=(a_j^k)$ defines the algebra completely hence we will denote this algebra by $\mathfrak{a}_A$, i.e., $a_A := A_1 \oplus_A (n-1)A_1$.

The algebras $\mathfrak{a}_A$ and $a_{A'}$ are isomorphic if and only if the matrices A and A' are similar up to scalar multiplier. The isomorphisms are established via changes of bases in the Abelian ideals and scaling of the complementary elements of bases. Up to the algebra isomorphisms the matrix A can be assumed reduced to the Jordan normal form, and its eigenvalues can be additionally normalized with a nonvanishing multiplier.

For any algebra $\mathfrak{g}$ the matrix $\hat{\mathrm{ad}}_u$ of the adjoint representation ad_u of an arbitrary element $u \in \mathfrak{g}$ is found by the formula $(\hat{\mathrm{ad}}_u)^j_k = c^k_{ij} u_i$, where c^k_{ij} are the structure constants of $\mathfrak{g}$ in the fixed basis. Since for $\mathfrak{a}_A$ $c^k_{ij}=0$ if neither i nor j equals to n, the matrix $\hat{\mathrm{ad}}_u$ can be easily calculated:

$$\hat{\mathrm{ad}}_u = \sum_{i=1}^{n-1} u_i \begin{pmatrix} 0 & \cdots & 0 & a^i_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & a^i_{n-1} \\ 0 & \cdots & 0 & 0 \end{pmatrix} - u_n \begin{pmatrix} a^1_1 & \cdots & a^{n-1}_1 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ a^1_{n-1} & \cdots & a^{n-1}_{n-1} & 0 \\ 0 & \cdots & 0 & 0 \end{pmatrix},$$

or shortly $\hat{\mathrm{ad}}_u$ have the form

$$\hat{\mathrm{ad}}_u = \begin{pmatrix} u_n A & -A\bar{u} \\ \underline{0} & 0 \end{pmatrix},$$

where $\bar{u}=(u_1,\dots,u_{n-1})^T$ and $\underline{0}=(0,\dots,0)$.

To calculate the invariant characteristic $\mathfrak{C}_{pq}$ of $\mathfrak{a}_A$, we find powers of $\hat{\mathrm{ad}}_u$ and their traces

$$\hat{\mathrm{ad}}_u{}^p = \begin{pmatrix} {u_n}^p A^p & -{u_n}^{p-1} A^p \bar{u} \\ \underline{0} & 0 \end{pmatrix}, \qquad \mathrm{tr}(\mathrm{ad}_u{}^p) = {u_n}^p \,\mathrm{tr}(A^p).$$

Matrix trace is not affected by matrix similarity transformations. If $\lambda_1,\dots,\lambda_{n-1}$ are the roots of the characteristic polynomial $\chi_A(\lambda)$ of the matrix A in $\mathbb{C}$ then $\mathrm{tr}(A^p)=\lambda_1^p+\cdots+\lambda_{n-1}^p$ for any $p \in \mathbb{N}$. Consequently, the invariant value $\mathfrak{C}_{pq}$ can be calculated explicitly.

The rank of $\mathfrak{a}_A$ can be easily calculated as by-product. Indeed, the characteristic polynomial $\chi_{\hat{\mathrm{ad}}_u}(\lambda)$ of $\hat{\mathrm{ad}}_u$ equals to $\lambda\chi_{u_nA}(\lambda)$, i.e., any element $u \in a_A$ with $u_n \neq 0$ is regular and the rank of $\mathfrak{a}_A$ coincides with the number of zero roots of the polynomial $\lambda\chi_A(\lambda)$.

As a result, we obtain the following statement.

Lemma 2: *Let $\mathfrak{a}_A$ be an n-dimensional Lie algebra with an $(n-1)$-dimensional Abelian ideal and with commutation relations which are defined via the matrix A and $\lambda_1,\dots,\lambda_{n-1}$ be roots of the characteristic polynomial of A over $\mathbb{C}$. If*

$$\mathrm{tr}(A^p) = \lambda_1^p + \cdots + \lambda_{n-1}^p \neq 0, \quad \mathrm{tr}(A^q) = \lambda_1^q + \cdots + \lambda_{n-1}^q \neq 0,$$

$$\mathrm{tr}(A^{p+q}) = \lambda_1^{p+q} + \cdots + \lambda_{n-1}^{p+q} \neq 0,$$

then the value $\mathfrak{C}_{pq}$ is well-defined invariant characteristics of the algebra $\mathfrak{a}_A$ and is given by the formula

$$\mathfrak{C}_{pq} = \frac{\mathrm{tr}(A^p)\mathrm{tr}(A^q)}{\mathrm{tr}(A^{p+q})} = \frac{(\lambda_1^p + \cdots + \lambda_{n-1}^p)(\lambda_1^q + \cdots + \lambda_{n-1}^q)}{(\lambda_1^{p+q} + \cdots + \lambda_{n-1}^{p+q})}.$$

The rank of the algebra $\mathfrak{a}_A$ (i.e., the dimension of its Cartan subalgebra) equals to the order of zero root of the characteristic polynomial of the matrix A plus one.

B. Lie algebras with WH+A ideals of codimension one

Consider an n-dimensional complex or real Lie algebra with an $(n-1)$-dimensional ideal which is isomorphic to the direct sum of the Weyl-Heisenberg algebra $\mathfrak{h}_3=A_{3.1}$ and the $(n-4)$-dimensional Abelian algebra. Let e_1, e_2, and e_3 form the canonical basis of a $\mathfrak{h}_3$-isomorphic component, $e_4,\dots,e_{n-1}$ give a basis of the Abelian component of the ideal, and e_n completes the basis of the ideal to a basis of the whole algebra. The nonzero commutation relations between elements of the constructed bases are

$$[e_2,e_3]=e_1,\quad [e_j,e_n]=\sum_{k=1}^{n-1} a_j^k e_k,\quad j=1,\ldots,n-1.$$

The $(n-1)\times(n-1)$ matrix $A=(a_j^k)$ defines the algebra completely hence we will denote this algebra by $\mathfrak{w}_A$, i.e., $\mathfrak{w}_A:=A_1\oplus_A(\mathfrak{h}_3\oplus(n-4)A_1)$. The Jacobi identity implies the following constraints on elements of A:

$$a_1^1=a_2^2+a_3^3,\quad a_1^k=0,\quad k=2,\ldots,n-1,\quad a_i^2=a_i^3=0,\quad i=4,\ldots,n-1.$$

The matrix $\hat{\mathrm{ad}}_u$ of the adjoint representation of an arbitrary element $u\in\mathfrak{w}_A$ is calculated in a way which is analogous to the previous case and has the form

$$\hat{\mathrm{ad}}_u=\begin{pmatrix} u_nA+u_3E_2^1-u_2E_3^1 & -A\bar{u} \\ \underline{0} & 0 \end{pmatrix},$$

where $\bar{u}=(u_1,\ldots,u_{n-1})^T$, $\underline{0}=(0,\ldots,0)$, E_j^i is the $(m-1)\times(m-1)$ matrix with unit in $\begin{smallmatrix} i \\ j \end{smallmatrix}$ entry and zero otherwise. In view of the restrictions on the matrix A we again have

$$\mathrm{tr}(\mathrm{ad}_u^{\ p})=u_n^{\ p}\,\mathrm{tr}(A^p),\quad \chi_{\mathrm{ad}_u}(\lambda)=-\lambda\chi_{u_nA}(\lambda).$$

Therefore, Lemma 2 can be completely reformulated for the algebra $\mathfrak{w}_A$.

Lemma 3: *Let* $\mathfrak{w}_A=A_1\oplus_A(\mathfrak{h}_3\oplus(n-4)A_1)$ *and* $\lambda_1,\ldots,\lambda_{n-1}$ *be roots of the characteristic polynomial of* A *over* $\mathbb{C}$. *If*

$$\mathrm{tr}(A^p)=\lambda_1^p+\cdots+\lambda_{n-1}^p\neq 0,\quad \mathrm{tr}(A^q)=\lambda_1^q+\cdots+\lambda_{n-1}^q\neq 0,$$

$$\mathrm{tr}(A^{p+q})=\lambda_1^{p+q}+\cdots+\lambda_{n-1}^{p+q}\neq 0,$$

then $\mathfrak{C}_{pq}$ *is well-defined invariant characteristics of the algebra* $\mathfrak{a}_A$ *and is given by the formula*

$$\mathfrak{C}_{pq}=\frac{\mathrm{tr}(A^p)\mathrm{tr}(A^q)}{\mathrm{tr}(A^{p+q})}=\frac{(\lambda_1^p+\cdots+\lambda_{n-1}^p)(\lambda_1^q+\cdots+\lambda_{n-1}^q)}{(\lambda_1^{p+q}+\cdots+\lambda_{n-1}^{p+q})}.$$

The rank of the algebra $\mathfrak{w}_A$ *(i.e., the dimension of its Cartan subalgebra) equals to the order of zero root of the characteristic polynomial of the matrix A plus one.*

C. Special cases

The adjoint action of any element $u\in\mathrm{so}(3)$ is presented in the canonical basis in the form $\hat{\mathrm{ad}}_u\,\hat{v}=\hat{u}\times\hat{v}$. Hereafter $\hat{u}$ and $\hat{v}$ are the coordinate columns of u and v treated as elements of R^3, "$\cdot$" and "$\times$" denote the usual scalar and vector products in R^3. By induction,

$$\mathrm{ad}_u^{\ 2p'-1}v=(-|\hat{u}|^2)^{p'-1}\hat{u}\times\hat{v},\quad \mathrm{ad}_u^{\ 2p'}v=(-|\hat{u}|^2)^{p'-1}((\hat{u}\cdot\hat{v})\hat{u}-|\hat{u}|^2\hat{v}),\quad p'\in\mathbb{N},$$

i.e., $\mathrm{tr}(\mathrm{ad}_u^{\ 2p'-1})=0$, $\mathrm{tr}(\mathrm{ad}_u^{\ 2p'})=(-|\hat{u}|^2)^{p'}$, $p'\in N$. Therefore, $\mathfrak{C}_{2p',2q'}=2$. For the other pairs of the indices p and q the invariant $\mathfrak{C}_{pq}$ is undefined.

The same statement is true for the algebras $\mathrm{sl}(2,R)$, $\mathrm{so}(3)\oplus A_1$, and $\mathrm{sl}(2,R)\oplus A_1$. The arguments are that $\mathrm{sl}(2,R)$ is equivalent to $\mathrm{so}(3)$ over $\mathbb{C}$ and the algebras $\mathfrak{g}$ and $\mathfrak{g}\oplus kA_1$ have the same invariants $\mathfrak{C}_{pq}$.

In the canonical basis of $2A_{2.1}$, where the commutation relations are $[e_1,e_2]=e_1$, $[e_3,e_4]=e_3$, the matrices of $\mathrm{ad}_u^{\ p}$, $p\in N$, have the form

$$\hat{\mathrm{ad}}_u^{\,p}=\begin{pmatrix} u_2^p & -u_2^{p-1}u_1 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & u_4^p & -u_4^{p-1}u_3\\ 0 & 0 & 0 & 0 \end{pmatrix},$$

i.e., $\mathrm{tr}(\mathrm{ad}_u^{\,p})=u_2^p+u_4^p$. Since the fraction with traces from the definition of $\mathfrak{C}_{pq}$ explicitly depends on u and v in the case of $2A_{2.1}$, the value $\mathfrak{C}_{pq}$ is undefined for any $p,q\in N$.

The same statement is true for the algebra $A_{4.10}$ being isomorphic to $2A_{2.1}$ over $\mathbb{C}$.

VI. LOW-DIMENSIONAL REAL LIE ALGEBRAS

We use the complete lists of nonisomorphic classes of real three- and four-dimensional Lie algebras, which were constructed by Mubarakzyanov[55] and slightly enhanced in Refs. 65 and 66. Enumeration of algebras by Mubarakzyanov is followed in general.

A number of algebraic characteristics and quantities are adduced for each Lie algebra $\mathfrak{g}$ from the lists. More precisely we deal with the type of the algebra (such as decomposable, solvable, nilpotent, etc.); the dimension n_{D} of the differentiation algebra $\mathrm{Der}\,\mathfrak{g}$; the dimension n_{Z} of the center; the maximal dimension n_{A} of the Abelian subalgebras; the Killing form κ; the rank $r_{\mathfrak{g}}$ (equal to the dimension of the Cartan subalgebras); the rank of solvability r_s (if $\mathfrak{g}$ is solvable); the rank of nilpotency r_n (if $\mathfrak{g}$ is nilpotent); the tuple of dimensions of the components of derived series $\mathrm{DS}=[\dim\mathfrak{g}^{(1)},\dim\mathfrak{g}^{(2)},\dots,\dim\mathfrak{g}^{(k)}]$, where k is the minimal number with $\dim\mathfrak{g}^{(k)}=\dim g^{(i)}\,\forall\, i>k$; the tuple of dimensions of the components of lower central series $\mathrm{CS}=[\dim\mathfrak{g}^1,\dim\mathfrak{g}^2,\dots,\dim g^k]$, where k is the minimal number with $\dim\mathfrak{g}^k=\dim\mathfrak{g}^i\,\forall\, i>k$; the trace $\mathrm{tr}(\mathrm{ad}_v)$ of the adjoint representations of arbitrary element $v\in V$, and the invariant $\mathfrak{C}_{pq}$ for the values $p,q\in N$ when this invariant is well defined.

These characteristics and quantities are used in Sec. VII and VIII as a basis for application of necessary contraction criteria.

A. Three-dimensional algebras

$3A_1$: (Abelian, unimodular);
$n_{\mathrm{D}}=9$, $n_{\mathrm{Z}}=3$, $n_{\mathrm{A}}=3$, $\kappa=0$, $r_{\mathfrak{g}}=3$, $r_n=r_s=1$, $\mathrm{DS}=[0]$, $\mathrm{CS}=[0]$, $\mathrm{tr}(\mathrm{ad}_v)=0$.
$A_{2.1}\oplus A_1$: $[e_1,e_2]=e_1$ (decomposable, solvable);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=1$, $n_{\mathrm{A}}=2$, $\kappa=x_2y_2$, $r_{\mathfrak{g}}=2$, $r_s=2$, $\mathrm{DS}=[1,0]$, $\mathrm{CS}=[1]$, $\mathrm{tr}(\mathrm{ad}_v)=-v_2$, $\mathfrak{C}_{pq}=1$.
$A_{3.1}$: $[e_2,e_3]=e_1$ (Heisenberg, indecomposable, nilpotent, unimodular);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=1$, $n_{\mathrm{A}}=2$, $\kappa=0$, $r_{\mathfrak{g}}=3$, $r_n=r_s=2$, $\mathrm{DS}=[1,0]$, $\mathrm{CS}=[1,0]$, $\mathrm{tr}(\mathrm{ad}_v)=0$.
$A_{3.2}$: $[e_1,e_3]=e_1$, $[e_2,e_3]=e_1+e_2$ (indecomposable, solvable);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=2x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=-2v_3$, $\mathfrak{C}_{pq}=2$.
$A_{3.3}$: $[e_1,e_3]=e_1$, $[e_2,e_3]=e_2$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=2x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=-2v_3$, $\mathfrak{C}_{pq}=2$.
$A_{3.4}^{-1}$: $[e_1,e_3]=e_1$, $[e_2,e_3]=-e_2$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=2x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.
$A_{3.4}^{a}$: $[e_1,e_3]=e_1$, $[e_2,e_3]=ae_2$, $0<|a|<1$ (indecomposable, solvable);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=(1+a^2)x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=-(1+a)v_3$,
$\mathfrak{C}_{pq}=1+[(a^p+a^q)/(1+a^{p+q})]$.
$A_{3.5}^{0}$: $[e_1,e_3]=-e_2$, $[e_2,e_3]=e_1$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=-2x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.
$A_{3.5}^{b}$: $[e_1,e_3]=be_1-e_2$, $[e_2,e_3]=e_1+be_2$, $b>0$ (indecomposable, solvable);
$n_{\mathrm{D}}=4$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=2(b^2-1)x_3y_3$, $r_{\mathfrak{g}}=1$, $r_s=2$, $\mathrm{DS}=[2,0]$, $\mathrm{CS}=[2]$, $\mathrm{tr}(\mathrm{ad}_v)=-2bv_3$,
$\mathfrak{C}_{pq}=[2\,\mathrm{Re}(b+i)^p\mathrm{Re}(b+i)^q]/[\mathrm{Re}(b+i)^{p+q}]$.
sl(2,R): $[e_1,e_2]=e_1$, $[e_2,e_3]=e_3$, $[e_1,e_3]=2e_2$ (indecomposable, simple, unimodular);
$n_{\mathrm{D}}=3$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=1$, $\kappa=-2(2x_3y_1-x_2y_2+2x_1y_3)$, $r_{\mathfrak{g}}=1$, $\mathrm{DS}=[3]$, $\mathrm{CS}=[3]$, $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{2p,2q}=2$.
so(3): $[e_1,e_2]=e_3$, $[e_2,e_3]=e_1$, $[e_3,e_1]=e_2$ (indecomposable, simple, unimodular);

$n_D=3$, $n_Z=0$, $n_A=1$, $\kappa=-2(x_1y_1+x_2y_2+x_3y_3)$, $r_g=1$, DS=[3], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.

Remark 7: Two terms of the above list (namely, $\{A^a_{3.4}\}$ and $\{A^b_{3.5}\}$) are, in fact, Lie algebra series, and each of them being parametrized with one real parameter. Some values of the parameters are singular, i.e., algebra characteristics for them differ from the ones for regular values. For example, the Killing form of the algebra $\{A^b_{3.5}\}$ identically vanishes if $b=1$. The same parameter values are singular from the viewpoint of realizations, invariants, subalgebras, etc. See, e.g., Refs. 61, 63, 65, and 66

This fact prevents one from creation of a "canonical" list of inequivalent low-dimensional Lie algebras. Whether is it reasonable to extract the algebras corresponding to singular parameter values from series? The question is answered in different ways. For example, in Refs. 61 and 63 all such algebras are separated from the series and have individual numbers. In Ref. 55 only the direct sums and single algebras (e.g., $A_{3.3}$) are considered separately from the corresponding series.

Another barrier for canonization of the existing lists is generated by ambiguous choice of series parameters normalization and even by existence of essentially different approaches to such normalization.

We follow the numeration by Mubarakzyanov, explicitly point out all the singular values of series parameters and study the corresponding algebras separately from the regular algebras of series. Usage of this technique simplifies application of necessary contraction criteria.

Let us note that Agaoka[1,2] proposed classifications of three- and four-dimensional algebras, which are well adapted to investigation of contractions and deformations. The presented approach can be extended to the real case and algebras of greater dimensions.

B. Four-dimensional algebras

$4A_1$ (Abelian, unimodular);
$n_D=16$, $n_Z=4$, $n_A=4$, $r_g=4$, $r_n=r_s=1$, DS=[0], CS=[0], $\mathrm{tr}(\mathrm{ad}_v)=0$.
$A_{2.1}\oplus 2A_1$: $[e_1,e_2]=e_1$ (decomposable, solvable);
$n_D=8$, $n_Z=2$, $n_A=3$, $\kappa=x_2y_2$, $r_g=3$, $r_s=2$, DS=[1,0], CS=[1], $\mathrm{tr}(\mathrm{ad}_v)=-v_2$, $\mathfrak{C}_{pq}=1$.
$2A_{2.1}$: $[e_1,e_2]=e_1$, $[e_3,e_4]=e_3$ (decomposable, solvable);
$n_D=4$, $n_Z=0$, $n_A=2$, $\kappa=x_2y_2+x_4y_4$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-(v_2+v_4)$.
$A_{3.1}\oplus A_1$: $[e_2,e_3]=e_1$ (decomposable, nilpotent, unimodular);
$n_D=10$, $n_Z=2$, $n_A=3$, $\kappa=0$, $r_g=4$, $r_n=r_s=2$, DS=[1,0], CS=[1,0], $\mathrm{tr}(\mathrm{ad}_v)=0$.
$A_{3.2}\oplus A_1$: $[e_1,e_3]=e_1$, $[e_2,e_3]=e_1+e_2$ (decomposable, solvable);
$n_D=6$, $n_Z=1$, $n_A=3$, $\kappa=2x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-2v_3$, $\mathfrak{C}_{pq}=2$.
$A_{3.3}\oplus A_1$: $[e_1,e_3]=e_1$, $[e_2,e_3]=e_2$ (decomposable, solvable);
$n_D=8$, $n_Z=1$, $n_A=3$, $\kappa=2x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-2v_3$, $\mathfrak{C}_{pq}=2$.
$A^{-1}_{3.4}\oplus A_1$: $[e_1,e_3]=e_1$, $[e_2,e_3]=-e_2$ (decomposable, solvable, unimodular);
$n_D=6$, $n_Z=1$, $n_A=3$, $\kappa=2x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.
$A^a_{3.4}\oplus A_1$: $[e_1,e_3]=e_1$, $[e_2,e_3]=ae_2$, $0<|a|<1$ (decomposable, solvable);
$n_D=6$, $n_Z=1$, $n_A=3$, $\kappa=(1+a^2)x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-(1+a)v_3$,
$\mathfrak{C}_{pq}=1+[(a^p+a^q)/(1+a^{p+q})]$.
$A^0_{3.5}\oplus A_1$: $[e_1,e_3]=-e_2$, $[e_2,e_3]=e_1$ (decomposable, solvable, unimodular);
$n_D=6$, $n_Z=1$, $n_A=3$, $\kappa=-2x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.
$A^b_{3.5}\oplus A_1$: $[e_1,e_3]=be_1-e_2$, $[e_2,e_3]=e_1+be_2$, $b>0$ (decomposable, solvable);
$n_D=6$, $n_Z=1$, $n_A=3$, $\kappa=2(b^2-1)x_3y_3$, $r_g=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-2bv_3$,
$\mathfrak{C}_{pq}=[2\,\mathrm{Re}(b+i)^p\mathrm{Re}(b+i)^q]/[\mathrm{Re}(b+i)^{p+q}]$.
$sl(2,R)\oplus A_1$: $[e_1,e_2]=e_1$, $[e_2,e_3]=e_3$, $[e_1,e_3]=2e_2$ (decomposable, unsolvable, reductive, unimodular);
$n_D=4$, $n_Z=1$, $n_A=2$, $\kappa=-2(2x_3y_1-x_2y_2+2x_1y_3)$, $r_g=2$, DS=[3], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{2p2q}=2$.
$so(3)\oplus A_1$: $[e_1,e_2]=e_3$, $[e_2,e_3]=e_1$, $[e_3,e_1]=e_2$ (decomposable, unsolvable, reductive, nimodular);
$n_D=4$, $n_Z=1$, $n_A=2$, $\kappa=-2(x_1y_1+x_2y_2+x_3y_3)$, $r_g=2$, DS=[3], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.

$\mathbf{A_{4.1}}$: $[e_2,e_4]=e_1$, $[e_3,e_4]=e_2$ (indecomposable, solvable, nilpotent, unimodular);
$n_{\mathrm{D}}=7$, $n_{\mathrm{Z}}=1$, $n_{\mathrm{A}}=3$, $\kappa=0$, $r_{\mathfrak{g}}=4$, $r_n=3$, $r_s=2$, DS=[2,0], CS=[2,1,0], $\mathrm{tr}(\mathrm{ad}_v)=0$.
$\mathbf{A^1_{4.2}}$: $[e_1,e_4]=e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_2+e_3$ (indecomposable, solvable);
$n_{\mathbf{D}}=8$, $n_{\mathbf{Z}}=0$, $n_{\mathbf{A}}=3$, $\kappa=3x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-3v_4$, $.\mathfrak{C}_{pq}=3$.
$\mathbf{A^{-2}_{4.2}}$: $[e_1,e_4]=-2e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_2+e_3$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(b^2+2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{pq}=[(2+(-2)^p)(2+(-2)^q)]/[2+(-2)^{p+q}]$, $p,q\geqslant 2$.
$\mathbf{A^b_{4.2}}$: $[e_1,e_4]=be_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_2+e_3$, $b\neq -2,0,1$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(b^2+2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-(2+b)v_4$,
$\mathfrak{C}_{pq}=[(2+b^p)(2+b^q)]/(2+b^{p+q})$.
$\mathbf{A_{4.3}}$: $[e_1,e_4]=e_1$, $[e_3,e_4]=e_2$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=1$, $n_{\mathrm{A}}=3$, $\kappa=x_4y_4$, $r_{\mathfrak{g}}=3$, $r_s=2$, DS=[2,0], CS=[2,1], $\mathrm{tr}(\mathrm{ad}_v)=-v_4$, $\mathfrak{C}_{pq}=1$.
$\mathbf{A_{4.4}}$: $[e_1,e_4]=e_1$, $[e_2,e_4]=e_1+e_2$, $[e_3,e_4]=e_2+e_3$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=3x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-3v_4$, $\mathfrak{C}_{pq}=3$.
$\mathbf{A^{111}_{4.5}}$: $[e_1,e_4]=e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_3$ (indecomposable, solvable);
$n_{\mathrm{D}}=12$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=3x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-3v_4$, $\mathfrak{C}_{pq}=3$.
$\mathbf{A^{-2,1,1}_{4.5}}$: $[e_1,e_4]=-2e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_3$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=8$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=6x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{pq}=[(2+(-2)^p)(2+(-2)^q)]/[2+(-2)^{p+q}]$, $p,q\geqslant 2$.
$\mathbf{A^{a11}_{4.5}}$: $[e_1,e_4]=ae_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_3$, $a\neq -2,0,1$ (indecomposable, solvable);
$n_{\mathrm{D}}=8$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(a^2+2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-(a+2)v_4$,
$\mathfrak{C}_{pq}=[(2+a^p)(2+a^q)]/[2+a^{p+q}]$.
$\mathbf{A^{a,-1,1}_{4.5}}$: $[e_1,e_4]=ae_1$, $[e_2,e_4]=-e_2$, $[e_3,e_4]=e_3$; $a>0$, $|a|\neq 1$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(a^2+2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-av_4$,
$\mathfrak{C}_{pq}=[(1+(-1)^p+a^p)(1+(-1)^q+a^q)]/[1+(-1)^{p+q}+a^{p+q}]$.
$\mathbf{A^{a,-1-a,1}_{4.5}}$: $[e_1,e_4]=ae_1$, $[e_2,e_4]=-(1+a)e_2$, $[e_3,e_4]=e_3$ $a<0$, or $a=1$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(a^2+(1+a)^2+1)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{pq}=[(1+(-1-a)^p+a^p)(1+(-1-a)^q+a^q)]/[1+(-1-a)^{p+q}+a^{p+q}]$, $p,q\geqslant 2$.
$\mathbf{A^{ab1}_{4.5}}$: $[e_1,e_4]=ae_1$, $[e_2,e_4]=be_2$, $[e_3,e_4]=e_3$; $ab\neq 0$, $-1<a<b<1$, $a+b\neq -1$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(a^2+b^2+1)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3],
$\mathrm{tr}(\mathrm{ad}_v)=-(a+b+1)v_4$, $\mathfrak{C}_{pq}=[(1+a^p+b^p)(1+a^q+b^q)]/[1+a^{p+q}+b^{p+q}]$.
$\mathbf{A^{-2b,b}_{4.6}}$: $[e_1,e_4]=-2be_1$, $[e_2,e_4]=be_2-e_3$, $[e_3,e_4]=e_2+be_3$, $b<0$ (indecomposable, solvable, unimodular);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(6b^2-2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$,
$\mathfrak{C}_{pq}=[((-2b)^p+2\,\mathrm{Re}(b+i)^p)((-2b)^q+2\,\mathrm{Re}(b+i)^q)]/[(-2b)^{p+q}+2\,\mathrm{Re}(b+i)^{p+q}]$, $p,q\geqslant 2$.
$\mathbf{A^{ab}_{4.6}}$: $[e_1,e_4]=ae_1$, $[e_2,e_4]=be_2-e_3$, $[e_3,e_4]=e_2+be_3$, $a>0$, $a\neq -2b$ (indecomposable, solvable);
$n_{\mathrm{D}}=6$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=3$, $\kappa=(a^2+2b^2-2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=2$, DS=[3,0], CS=[3],
$\mathrm{tr}(\mathrm{ad}_v)=-(a+2b)v_4$, $\mathfrak{C}_{pq}=[(a^p+2\,\mathrm{Re}(b+i)^p)(a^q+2\,\mathrm{Re}(b+i)^q)]/[a^{p+q}+2\,\mathrm{Re}(b+i)^{p+q}]$.
$\mathbf{A_{4.7}}$: $[e_2,e_3]=e_1$, $[e_1,e_4]=2e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_2+e_3$ (indecomposable, solvable);
$n_{\mathrm{D}}=5$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=6x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-4v_4$,
$\mathfrak{C}_{pq}=[(2+2^p)(2+2^q)]/[2+2^{p+q}]$.
$\mathbf{A^0_{4.8}}$: $[e_2,e_3]=e_1$, $[e_1,e_4]=e_1$, $[e_2,e_4]=e_2$ (indecomposable, solvable);
$n_{\mathrm{D}}=5$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=2x_4y_4$, $r_{\mathfrak{g}}=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-2v_4$, $\mathfrak{C}_{pq}=2$.
$\mathbf{A^1_{4.8}}$: $[e_2,e_3]=e_1$, $[e_1,e_4]=2e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=e_3$ (indecomposable, solvable);
$n_{\mathrm{D}}=7$, $n_{\mathrm{Z}}=0$, $n_{\mathrm{A}}=2$, $\kappa=6x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-4v_4$,
$\mathfrak{C}_{pq}=[(2+2^p)(2+2^q)]/[2+2^{p+q}]$.
$\mathbf{A^{-1}_{4.8}}$: $[e_2,e_3]=e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=-e_3$ (indecomposable, solvable; unimodular);
$n_{\mathrm{D}}=5$, $n_{\mathrm{Z}}=1$, $n_{\mathrm{A}}=2$, $\kappa=2x_4y_4$, $r_{\mathfrak{g}}=2$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.
$\mathbf{A^b_{4.8}}$: $[e_2,e_3]=e_1$, $[e_1,e_4]=(1+b)e_1$, $[e_2,e_4]=e_2$, $[e_3,e_4]=be_3$, $0<|b|<1$ (indecomposable, solvable);

$n_D=5$, $n_Z=0$, $n_A=2$, $\kappa=2(1+b+b^2)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-2(1+b)v_4$, $\mathfrak{C}_{pq}=[(1+b^p+(1+b)^p)(1+b^q+(1+b)^q)]/[1+b^{p+q}+(1+b)^{p+q}]$.

$\mathbf{A}^{\mathbf{0}}_{\mathbf{4.9}}$: $[e_2,e_3]=e_1$, $[e_2,e_4]=-e_3$, $[e_3,e_4]=e_2$ (indecomposable, solvable, unimodular);
$n_D=5$, $n_Z=1$, $n_A=2$, $\kappa=-2x_4y_4$, $r_{\mathfrak{g}}=2$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=0$, $\mathfrak{C}_{2p,2q}=2$.

$\mathbf{A}^{\mathbf{a}}_{\mathbf{4.9}}$: $[e_2,e_3]=e_1$, $[e_1,e_4]=2ae_1$, $[e_2,e_4]=ae_2-e_3$, $[e_3,e_4]=e_2+ae_3$, $a>0$ (indecomposable, solvable);
$n_D=5$, $n_Z=0$, $n_A=1$, $\kappa=2(3a^2-1)x_4y_4$, $r_{\mathfrak{g}}=1$, $r_s=3$, DS=[3,1,0], CS=[3], $\mathrm{tr}(\mathrm{ad}_v)=-4av_4$, $\mathfrak{C}_{pq}=[((2a)^p+2\,\mathrm{Re}(a+i)^p)((2a)^q+2\,\mathrm{Re}(a+i)^q)]/[(2a)^{p+q}+2\,\mathrm{Re}(a+i)^{p+q}]$, $p,q\geqslant 2$;.

$\mathbf{A}_{\mathbf{4.10}}$: $[e_1,e_3]=e_1$, $[e_2,e_3]=e_2$, $[e_1,e_4]=-e_2$, $[e_2,e_4]=e_1$ (indecomposable, solvable);
$n_D=4$, $n_Z=0$, $n_A=2$, $\kappa=2(x_3y_3-x_4y_4)$, $r_{\mathfrak{g}}=2$, $r_s=2$, DS=[2,0], CS=[2], $\mathrm{tr}(\mathrm{ad}_v)=-2v_3$.

Remark 8: Problems concerning series of algebras and singular values of parameters become more complicated in the case of dimension four. In particular, in the Lie algebra series $\{A^b_{4.2}\}$, $\{A^{abc}_{4.5}\}$, and $\{A^b_{4.8}\}$ the dimension n_D of the differentiation algebra varies depending on values of the series parameters. It implies obvious necessity of separation of series parameter subsets according to values of this semi-invariant quantity since Criterion 1 based on n_D is most powerful.

In the above list of algebras, we apply enhanced normalization of series parameters for four-dimensional real Lie algebras, which were proposed in Refs. 65 and 66.

VII. ALGORITHM OF CONTRACTION IDENTIFICATION

The proposed algorithm allows one to handle the continuous one-parametric contractions of the low-dimensional Lie algebras. It consists of three steps.

(1) We take a complete list of nonisomorphic Lie algebras of a fixed dimension. For each member of this list we calculate invariant and semi-invariant quantities that concern necessary criteria of contractions.
(2) For each pair of algebras from the list we test possible existence of contractions with the necessary criteria of contractions via comparing the calculated invariant and semi-invariant quantities. Since it is sufficient to look only for nontrivial and proper contractions, we have not to study the pairs of any Lie algebra with itself and the Abelian one.
(3) Consider each from the pairs which satisfy all the necessary criteria of contractions. Applying the direct method based on Definition 1′, we either construct a contraction matrix in an explicit form or prove that no contraction is possible.

The requisite invariant and semi-invariant quantities of the real three- and four-dimensional Lie algebras are calculated and collected in Sec. VI.

Most of contractions of low-dimensional Lie algebras are realized via simple Inönü-Wigner contractions. Any simple Inönü-Wigner contraction corresponds to a subalgebra of the initial algebra and therefore is easy to find. Classification of subalgebras of three- and four-dimensional Lie algebras is well known.[61] All simple Inönü-Wigner contractions of these algebras are constructed in Refs. 15 and 39. We only enhance presentation of the corresponding contraction matrices.

For the pairs without simple Inönü-Wigner contractions we continue investigation with generalized Inönü-Wigner contractions. Here the problem of finding contraction matrices can be divided into two subproblems.

- To construct appropriate transformations for the canonical bases of the initial and resulting algebras, which do not depend on the contraction parameter. The aim is for the nonzero new structure constants of the resulting algebra to coincide with the corresponding new structure constants of the initial algebra.
- To find a diagonal matrix depending on the contraction parameter. It is sufficient to assume that the diagonal elements are integer powers of the contraction parameter.

As a rule, we can manage to avoid basis change in the resulting algebras in the case of dimensions three and four. Consequently, the contraction matrix can be represented as a product of two

matrices $U_\varepsilon = IW(k_1,\dots,k_n)$, where I is a constant nonsingular matrix and $W(k_1,\dots,k_n) = \mathrm{diag}(\varepsilon^{k_1},\dots,\varepsilon^{k_n})$, $k_1,\dots,k_n \in \mathbb{Z}$.

In complicated cases contraction matrices can be found using repeated contractions (see Sec. X).

To demonstrate effectiveness of the algorithm, we discuss two typical examples in detail.

Example 2: Consider the series of three-dimensional Lie algebras $A_{3.4}^a$ parametrized with one real parameter a, where $-1 \leqslant a < 1, a \neq 0$. Let us investigate all possible contractions of algebra $A_{3.4}^a$ for a fixed value of a.

$A_{3.4}^a$ is an indecomposable solvable Lie algebra with the canonical nonzero commutation relations $[e_1,e_3]=e_1$, $[e_2,e_3]=ae_2$. The tuple of considered quantities for the algebra $A_{3.4}^a$ is

$$n_{\mathrm{D}} = 4, \quad n_{\mathrm{Z}} = 0, \quad n_{\mathrm{A}} = 2, \quad \kappa = (1+a^2)x_3y_3, \quad \mathrm{tr}(\mathrm{ad}\, e_3) = -1-a, \quad r_s = 2,$$

$$\mathrm{DS} = [2,0], \quad \mathrm{CS} = [2].$$

According to the second step of the algorithm we look through all pairs of three-dimensional algebras, where the initial algebra is $A_{3.4}^a$ and the resulting algebra runs the list from Sec. VI A and does not coincide with $3A_1$ and $A_{3.4}^a$.

For each pair we compare tuples of their semi-invariant quantities. In view of Theorem 1 we conclude that

- contractions to the algebras $A_{2.1}\oplus A_1$, $A_{3.2}$, $A_{3.4}^{\tilde a}$, $\tilde a \neq a$, $A_{3.5}^b$, $b \geqslant 0$, $\mathrm{sl}(2,\mathbb{R})$ and so(3) are impossible since Criterion 1 is not satisfied;
- contraction to the algebra $A_{3.3}$ is impossible according to Criterion 15; and
- contraction to the algebra $A_{3.1}$ may exist inasmuch as all the tested necessary criteria are held.

Other criteria can also be used to prove nonexistence of contractions. For example, for the algebras $\mathrm{sl}(2,\mathbb{R})$ and so(3) we can also use Criterion 2, 5, 11, or 17. In all cases we try to apply a minimal set of the most effective criteria such as Criterion 1. In particular, Criterion 1 is very important for the example under consideration, since due to strict inequality it allows one to prove the absence of contractions inside the series $A_{3.4}^a$ in a very simple way.

Therefore, on the third step of the algorithm we investigate only the pair $(A_{3.4}^a, A_{3.1})$.

The canonical nonzero commutation relation of the algebra $A_{3.1}$ is $[e_2,e_3]=e_1$. Since in the canonical basis of $A_{3.4}^a$ the structure constant c_{23}^1 equals to zero we carry out the basis change $e'_1=(1-a)e_1$, $e'_2=e_1+e_2$, $e'_3=e_3$. The new isomorphic commutation relations have the form

$$[e_1,e_2]' = 0, \quad [e_1,e_3]' = e_1, \quad [e_2,e_3]' = e_1 + ae_2.$$

Now the desired contraction is provided by the matrix $\mathrm{diag}(\varepsilon,1,\varepsilon)$ and the subsequent limit process $\varepsilon \to +0$ results in the algebra $A_{3.1}$:

$$[e_1,e_2]_\varepsilon = 0,$$

$$[e_1,e_3]_\varepsilon = \varepsilon e_1 \to 0, \quad \varepsilon \to +0,$$

$$[e_2,e_3]_\varepsilon = e_1 + \varepsilon a e_2 \to e_1, \quad \varepsilon \to +0.$$

Finally, all nontrivial proper contractions of the Lie algebra $A_{3.4}^a$ are exhausted by the single contraction $A_{3.4}^a \to A_{3.1}$ which is generated by the matrix $I_5\,\mathrm{diag}(\varepsilon,1,\varepsilon)$, where the explicit form of I_5 is adduced in Sec. VIII A.

Example 3: Consider the decomposable, unsolvable, unimodular, reductive four-dimensional Lie algebra $\mathrm{sl}(2,\mathbb{R})\oplus A_1$, having the canonical commutation relations $[e_1,e_2]=e_1$, $[e_2,e_3]=e_3$, and $[e_1,e_3]=2e_2$. The set of algebraic quantities which are used to study contractions of this algebra is exhausted by

$$n_D=4,\quad n_Z=1,\quad n_A=1,\quad n_{[\mathfrak{g},\mathfrak{g}]}=3,\quad \kappa=-2(2x_3y_1-x_2y_2+2x_1y_3),\quad \mathrm{DS}=[3],\quad \mathrm{CS}=[3].$$

The quantities of $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ are compared with the analogous quantities of the other four-dimensional algebras. All the requisite quantities are adduced in Sec. VI B. In view of necessary contraction criteria we conclude that

- contractions to the algebras $A_{2.1}\oplus 2A_1$, $2A_{2.1}$, $A_{3.2}\oplus A_1$, $A_{3.3}\oplus A_1$, $A^a_{3.4}\oplus A_1$, $|a|<1, a\neq 0$, -1, $A^b_{3.5}\oplus A_1$, $b>0$, $A_{4.3}$, $A^b_{4.8}$, $|b|\leqslant 1, b\neq -1$, and $A^a_{4.9}$, $a>0$ are impossible in view of Criterion 12;
- contraction to the algebra $\mathrm{so}(3)\oplus A_1$ does not exist since Criterion 1 is not held;
- contractions to the algebras $A^b_{4.2}$, $b\neq 0$, $A_{4.4}$, $A^{abc}_{4.5}$, $abc\neq 0$, $A^{a,b}_{4.6}$, $a>0$, $A_{4.7}$, and $A_{4.10}$ are impossible in view of Criterion 3; and
- contractions to the algebras $A_{3.1}\oplus A_1$, $A_{4.1}$, $A^{-1}_{3.4}\oplus A_1$, $A^0_{3.5}\oplus A_1$, $A^{-1}_{4.8}$, and $A^0_{4.9}$ may exist inasmuch as all the tested necessary criteria of contractions are satisfied.

Note that not only Criteria 1, 3, and 12 could be used to separate algebras for which there are no contractions from the algebra $\mathrm{sl}(2,\mathbb{R})\oplus A_1$. For example, Criterion 1 implies impossibility of contractions from $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ to $A_{4.4}$.

The contractions admitted by the necessary criteria can actually be executed. Contractions to the algebras $A_{3.1}\oplus A_1$, $A^{-1}_{3.4}\oplus A_1$, $A^0_{3.5}\oplus A_1$, $A_{4.1}$, $A^{-1}_{4.8}$, and $A^0_{4.9}$ are provided by the contraction matrices $I_8\,\mathrm{diag}(\varepsilon,\varepsilon,1,1)$, $I_7\,\mathrm{diag}(\varepsilon,\varepsilon,1,1)$, $I_{10}\,\mathrm{diag}(\varepsilon,\varepsilon,1,1)$, $I_{23}\,\mathrm{diag}(\varepsilon,\varepsilon,\varepsilon,1)$, $I_{19}\,\mathrm{diag}(\varepsilon,1,\varepsilon,1)$, and $I_{22}\,\mathrm{diag}(\varepsilon^2,\varepsilon,\varepsilon,1)$, correspondingly. The explicit forms of the matrices I's are presented in Sec. VIII B.

Note that all the contractions except the last one are simple Inönü-Wigner contractions and are constructed using a list of inequivalent subalgebras of $\mathrm{sl}(2,\mathbb{R})\oplus A_1$. We illustrate the applied technique with the pair $(\mathrm{sl}(2,\mathbb{R})\oplus A_1, A_{3.1}\oplus A_1)$. See also Sec. III for the theoretical background.

$\langle e_3,e_4\rangle$ is a subalgebra of $\mathrm{sl}(2,\mathbb{R})\oplus A_1$. The associated contraction matrix $\mathrm{diag}(\varepsilon,\varepsilon,1,1)$ produces a simple IW-contraction from $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ to a Lie algebra isomorphic to $A_{3.1}\oplus A_1$. In order to obtain the canonical commutation relations ($[e_2,e_3]=e_1$) of the algebra $A_{3.1}\oplus A_1$, we apply additional isomorphism transformation given by the matrix I_8 which commutes with $\mathrm{diag}(\varepsilon,\varepsilon,1,1)$. The resulting contraction matrix is $I_8\,\mathrm{diag}(\varepsilon,\varepsilon,1,1)$.

Further consider the pair $(\mathrm{sl}(2,\mathbb{R})\oplus A_1, A^0_{4.9})$ in detail as an example on construction of generalized IW-contractions. Our aim is to find an appropriate contraction matrix according to the above algorithm.

The canonical commutation relations of the algebra $A^0_{4.9}$ are $[e_2,e_3]=e_1$, $[e_2,e_4]=-e_3$, and $[e_3,e_4]=e_2$. In contrast to the algebra $A^0_{4.9}$, the canonical structure constants c^1_{23}, c^3_{24}, and c^2_{34} of the algebra $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ vanish. That is why we carry out the basis change

$$e_1'=-\frac{1}{2}e_1-\frac{1}{2}e_3,\quad e_2'=e_2,\quad e_3'=\frac{1}{2}e_1-\frac{1}{2}e_3,\quad e_4'=\frac{1}{2}e_1+\frac{1}{2}e_3+e_4,$$

which is associated with the matrix I_{22}. The obtained commutation relations (being isomorphic to the old one of $\mathrm{sl}(2,\mathbb{R})\oplus A_1$) have the form

$$[e_1,e_2]'=-e_3,\quad [e_1,e_3]'=e_2,\quad [e_1,e_4]'=0,\quad [e_2,e_3]'=e_1,\quad [e_2,e_4]'=-e_3,\quad [e_3,e_4]'=e_2.$$

Let us suppose that for the new Lie bracket $[\cdot,\cdot]'$ the requisite contraction is provided by the matrix $\mathrm{diag}(\varepsilon^{k_1},\varepsilon^{k_2},\varepsilon^{k_3},\varepsilon^{k_4})$ and calculate the parametrized commutators:

$$[e_1,e_2]_\varepsilon=-\varepsilon^{k_1+k_2-k_3}e_3,\quad [e_1,e_3]_\varepsilon=\varepsilon^{k_1+k_3-k_2}e_2,\quad [e_1,e_4]_\varepsilon=0,$$

$$[e_2,e_3]_\varepsilon=\varepsilon^{k_2+k_3-k_1}e_1,\quad [e_2,e_4]_\varepsilon=-\varepsilon^{k_2+k_4-k_3}e_3,\quad [e_3,e_4]_\varepsilon=\varepsilon^{k_3+k_4-k_2}e_2.$$

The limit of the commutators under $\varepsilon\to+0$ exists and gives the algebra $A^0_{4.9}$ iff the powers $k_1,\ldots,k_4$ are constrained by the conditions

$$k_2+k_3-k_1=0,\quad k_2+k_4-k_3=0,\quad k_3+k_4-k_2=0,\quad k_1+k_2-k_3>0,\quad k_1+k_3-k_2>0.$$

The tuple $k_1=2$, $k_2=k_3=1$, $k_4=0$ satisfies these conditions. The corresponding contraction indeed results in the algebra $A_{4.9}^0$:

$$[e_1,e_2]_\varepsilon=-\varepsilon^2 e_3\to 0,\quad \varepsilon\to+0,\quad [e_1,e_3]_\varepsilon=\varepsilon^2 e_2\to 0,\quad \varepsilon\to+0,$$

$$[e_1,e_4]_\varepsilon=0,\quad [e_2,e_3]_\varepsilon=e_1,\quad [e_2,e_4]_\varepsilon=-e_3,\quad [e_3,e_4]_\varepsilon=e_2.$$

The complete contraction matrix is $I_{22}\,\mathrm{diag}(\varepsilon^2,\varepsilon,\varepsilon,1)$.

This example demonstrates that necessary criteria allow one to handle contractions even in cases of such complicated algebras as reductive ones.

Remark 9: Celeghini and Tarlini[14] proposed the conjecture that all nonsemisimple Lie algebras of a fixed dimension could be obtained via contractions from semisimple ones. Actually, the conjecture is incorrect. There are no semisimple Lie algebras for some dimensions, e.g., in the case of dimension four. Therefore, a wider class (e.g., the class of reductive algebras or even the whole class of unsolvable algebras) should be used in the conjecture instead of semisimple algebras. The other argument on incorrectness of the conjecture is that all semisimple (and reductive) Lie algebras are unimodular and any continuous contraction of a unimodular algebra necessarily results in a unimodurar algebra. Complexity of the actual state of affairs is illustrated by consideration of low-dimensional algebras.

The unsolvable three-dimensional algebras are exhausted by the simple algebras $\mathrm{sl}(2,\mathbb{R})$ and so(3). Any three-dimensional unimodular algebra ($\mathrm{sl}(2,\mathbb{R})$, so(3), $A_{3.4}^{-1}$, $A_{3.4}^0$, $A_{3.1}$, $3A_1$) belongs to the orbit closure of at least one of the simple algebras.

The reductive algebras $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ and $\mathrm{so}(3)\oplus A_1$ form the set of unsolvable four-dimensional algebras. The union of orbit closures of these algebras consists of the unimodular algebras with the nontrivial centers ($\mathrm{sl}(2,\mathbb{R})\oplus A_1$, $\mathrm{so}(3)\oplus A_1$, $A_{4.8}^{-1}$, $A_{4.9}^0$, $A_{3.4}^{-1}\oplus A_1$, $A_{3.4}^0\oplus A_1$, $A_{4.1}$, $A_{3.1}\oplus A_1$, $4A_1$). The unimodular algebras having the zero centers ($A_{4.2}^{-2}$, $A_{4.5}^{abc}$, $a+b+c=0$, $A_{4.6}^{-2b,b}$) cannot be obtained via contractions from the unsolvable algebras.

The situation with contractions of representations is different.[58] For example, matrix representations of all inequivalent classes of the real three-dimensional Lie algebras are contractions of appropriately chosen representations (with ε-dependent similarity transformations) of the simple algebras $\mathrm{sl}(2,\mathbb{R})$ and so(3). More precisely, concerning the parametrized series of Lie algebras ($A_{3.4}^a$, $A_{3.5}^b$), only representations for single values of parameters can be obtained via contractions.

VIII. ONE-PARAMETRIC CONTRACTIONS OF REAL LOW-DIMENSIONAL LIE ALGEBRAS

The objective of this section is to construct, order, and analyze the contractions of real low-dimensional Lie algebras.

At first, we discuss all possible contractions of one- and two-dimensional Lie algebras. Since there is only one inequivalent one-dimensional Lie algebra and it is Abelian, all its contractions are trivial and improper at the same time. The complete list of nonisomorphic two-dimensional Lie algebras is exhausted by the Abelian algebra $2A_1$ and the nonAbelian algebra $A_{2.1}$ with the canonical commutation relation $[e_1,e_2]=e_1$. The unique weakly inequivalent contraction of the algebra $2A_1$ is trivial and improper at the same time. The contractions of the algebra $A_{2.1}$ are either trivial or improper.

Contractions of real three- and four-dimensional Lie algebras are listed in Secs. VIII A and VIII B and additionally visualized with Figs. 1 and 2. Denote that contractions of the three-dimensional real Lie algebras were considered in Ref. 78. A complete description of these contractions with proof closed to the manner of our paper was first obtained in Ref. 47.

Only proper direct contractions are presented on the figures. Let us remind that a contraction from $\mathfrak{g}$ to $\mathfrak{g}_0$ is called *direct* if there is no algebra $\mathfrak{g}_1$ such that $\mathfrak{g}_1\not\simeq\mathfrak{g},\mathfrak{g}_0$, $\mathfrak{g}$ is contracted to $\mathfrak{g}_1$ and $\mathfrak{g}_1$ is contracted to $\mathfrak{g}_0$. Antonym to this notion is the notion of repeated contraction. See Sec. X for

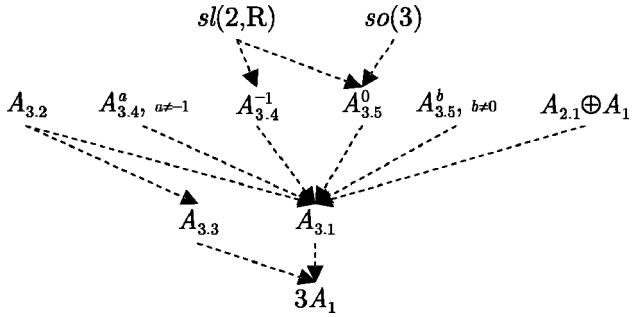

FIG. 1. One-parametric contractions of real three-dimensional Lie algebras.

details. The algebra $\mathfrak{g}$ is necessarily contracted to $\mathfrak{g}_0$ if $\mathfrak{g}$ is contracted to $\mathfrak{g}_1$ and $\mathfrak{g}_1$ is contracted to $\mathfrak{g}_0$. That is why the arrows corresponding to repeated contractions can be omitted.

In the lists of contractions we collect all the suitable pairs of Lie algebras with the same initial algebras which are adduced once. The corresponding contraction matrices are indicated over the arrows. In the section we use the shortcut notation for the diagonal parts of matrices of generalized Inönü-Wigner contractions:

$$W(k_1,k_2,\ldots,k_n)=\mathrm{diag}(\varepsilon^{k_1},\varepsilon^{k_2},\ldots,\varepsilon^{k_n}),$$

where $k_i\in\mathbb{Z}$, $i=\overline{1,n}$, n is the dimension of the underlying vector space V. The constant "left-hand" parts of matrices of generalized Inönü-Wigner contractions are denoted by numbered symbols I. Their explicit forms are adduced after the lists of contractions. The notation $\varepsilon\to+0$ is omitted everywhere.

In the case of simple Inönü-Wigner contractions we additionally adduce the associated subalgebras.

A. Dimension three

The list of all possible proper and nontrivial continuous one-parametric contractions of real three-dimensional Lie algebras is exhausted by the following ones (see also Fig. 1):

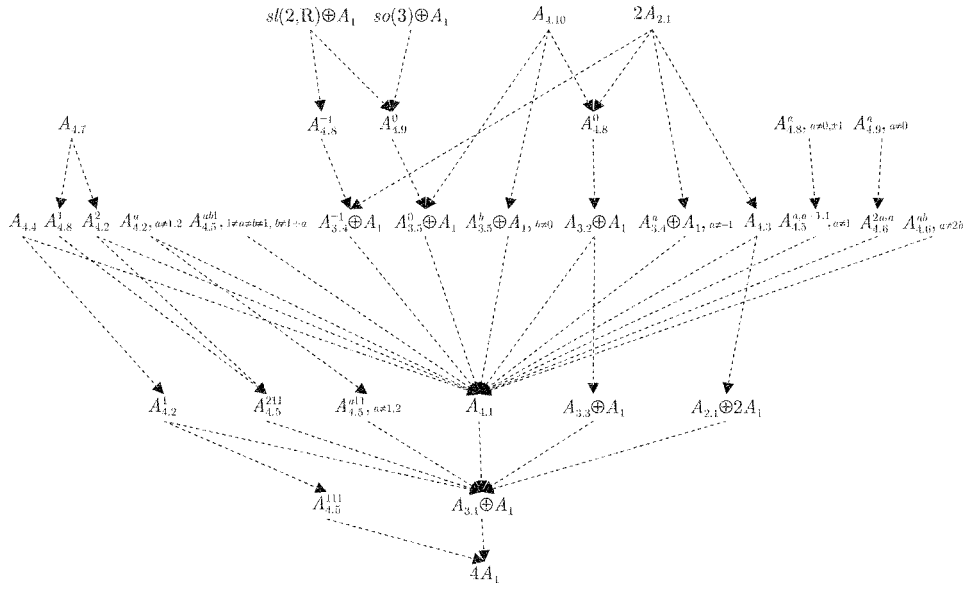

FIG. 2. One-parametric contractions of real four-dimensional Lie algebras.

$$A_{2.1}\oplus A_1:\quad \xrightarrow{I_1W(1,1,0)} A_{3.1},\langle e_1-e_3\rangle.$$

$$A_{3.2}:\quad \xrightarrow{I_7W(1,0,1)\text{ or }W(2,1,1)} A_{3.1},\langle e_2\rangle,\qquad \xrightarrow{I_6W(0,1,0)\text{ or }W(1,2,0)} A_{3.3},\langle e_1,e_2+e_3\rangle.$$

$$A_{3.4}^a:\quad \xrightarrow{I_2W(1,0,1)} A_{3.1},\langle e_1+e_2\rangle.$$

$$A_{3.5}^b:\quad \xrightarrow{W(1,0,1)} A_{3.1},\langle e_2\rangle.$$

$$\mathrm{sl}(2,\mathbb{R}):\quad \xrightarrow{I_3W(1,1,0)} A_{3.1},\langle e_3\rangle,\quad \xrightarrow{I_4W(1,0,0)} A_{3.4}^{-1},\langle e_2,e_3\rangle,\quad \xrightarrow{I_5W(1,1,0)} A_{3.5}^{0},\langle e_1+e_3\rangle.$$

$$\mathrm{so}(3):\quad \xrightarrow{W(2,1,1)} A_{3.1},\quad \xrightarrow{W(1,1,0)} A_{3.5}^{0},\langle e_3\rangle.$$

The constant parts of contraction matrices have the form

$$I_1=\begin{pmatrix}1&0&-1\\0&1&0\\0&0&1\end{pmatrix},\quad I_2=\begin{pmatrix}1-a&1&0\\0&1&0\\0&0&1\end{pmatrix},\quad I_3=\begin{pmatrix}0&1&0\\2&0&0\\0&0&1\end{pmatrix},$$

$$I_4=\begin{pmatrix}1&0&0\\0&0&1\\0&-1&0\end{pmatrix},\quad I_5=\begin{pmatrix}0&0&1/2\\0&1&0\\1&0&1/2\end{pmatrix},$$

$$I_6=\begin{pmatrix}1&0&0\\0&1&1\\0&0&1\end{pmatrix},\quad I_7=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}.$$

Analysis of the obtained results leads to the conclusion that for any pair of real three-dimensional Lie algebras we have one of the two possibilities: (1) there are no contractions in view of applied necessary criteria; (2) there exists a generalized Inönü-Wigner contraction.

Only the contraction $\mathrm{so}(3)\to A_{3.1}$ is necessarily a truly generalized Inönü-Wigner contraction. Nonexistence of a simple Inönü-Wigner contraction in this case is implied by the following chain of statements. Any proper and nontrivial simple Inönü-Wigner contraction corresponds to proper subalgebras of the initial algebra. Equivalent subalgebras result in equivalent contractions. A complete list of inequivalent proper subalgebras of so(3) is exhausted by any one-dimensional subalgebra of so(3). Any one-dimensional subalgebra generates the contraction of so(3) to $A_{3.5}^0$.

All other contractions of real three-dimensional Lie algebras are equivalent to simple Inönü-Wigner contractions although sometimes generalized Inönü-Wigner contraction has a simpler, pure diagonal form. We explicitly indicate two such cases in the above list of contractions, namely, $A_{3.2}\to A_{3.1}$ and $A_{3.2}\to A_{3.3}$.

Note additionally that all the constructed contraction matrices include only non-negative integer powers of ε, i.e., they admit well-defined limit process under $\varepsilon\to+0$.

Theorem 2: *Any continuous contraction of a real three-dimensional Lie algebra is equivalent to a generalized Inönü-Wigner contraction with non-negative powers of the contraction parameter. Moreover, only the contraction* $\mathrm{so}(3)\to A_{3.1}$ *is inequivalent to a simple Inönü-Wigner contraction.*

B. Dimension four

The list of all possible proper and nontrivial continuous one-parametric contractions of real four-dimensional Lie algebras is exhausted by the following ones:

$$A_{2.1}\oplus 2A_1:\quad \xrightarrow{I_{30}W(1,1,0,0)} A_{3.1}\oplus A_1,\langle e_3-e_1,e_4\rangle.$$

$$2A_{2.1}:\quad \xrightarrow{W(0,0,0,1)} A_{2.1}\oplus 2A_1,\langle e_1,e_2,e_3\rangle,\quad \xrightarrow{I_1W(1,1,0,1)} A_{3.1}\oplus A_1,\langle e_1+e_3\rangle,$$

$$\xrightarrow{U_3} A_{3.2}\oplus A_1,\quad \xrightarrow{I_2W(0,0,0,1)} A_{3.3}\oplus A_1,\langle e_1,e_3,e_2+e_4\rangle,\quad \xrightarrow{I_{27}W(1,1,0,1)} A^a_{3.4}\oplus A_1,\langle e_2+ae_4\rangle,$$

$$\xrightarrow{U_4} A_{4.1},\quad \xrightarrow{I_{28}W(0,1,1,0)} A_{4.3},\langle e_1,e_2-e_3\rangle,\quad \xrightarrow{I_3W(1,0,1,0)} A^0_{4.8},\langle e_1+e_3,e_2+e_4\rangle.$$

$$A_{3.2}\oplus A_1:\quad \xrightarrow{W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_2,e_4\rangle,\quad \xrightarrow{W(0,1,0,0)} A_{3.3}\oplus A_1,\langle e_1,e_3,e_4\rangle,\quad \xrightarrow{I_{29}W(2,1,0,1)} A_{4.1}.$$

$$A_{3.3}\oplus A_1:\quad \xrightarrow{I_4W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_1,e_2+e_4\rangle.$$

$$A^a_{3.4}\oplus A_1:\quad \xrightarrow{I_5W(1,1,0,0)} A_{3.1}\oplus A_1,\langle e_2,e_1+e_4\rangle,\quad \xrightarrow{I_6W(2,1,0,1)} A_{4.1}.$$

$$A^b_{3.5}\oplus A_1:\quad \xrightarrow{W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_2,e_4\rangle,\quad \xrightarrow{I_9W(2,1,0,1)} A_{4.1}.$$

$$\mathrm{sl}(2,\mathbb{R})\oplus A_1:\quad \xrightarrow{I_8W(1,1,0,0)} A_{3.1}\oplus A_1,\langle e_3,e_4\rangle,\quad \xrightarrow{I_7W(1,1,0,0)} A^{-1}_{3.4}\oplus A_1,\langle e_2,e_4\rangle,\quad \xrightarrow{I_{10}W(1,1,0,0)} A^0_{3.5}\oplus A_1,$$
$$\langle e_1+e_3,e_4\rangle,\quad \xrightarrow{I_{23}W(1,1,1,0)} A_{4.1},\langle e_1+e_4\rangle,\quad \xrightarrow{I_{19}W(1,0,1,0)} A^{-1}_{4.8},\langle e_1,e_2-1/2e_4\rangle,\quad \xrightarrow{I_{22}W(2,1,1,0)} A^0_{4.9}.$$

$$\mathrm{so}(3)\oplus A_1:\quad \xrightarrow{W(2,1,1,0)} A_{3.1}\oplus A_1,\quad \xrightarrow{W(1,1,0,0)} A^0_{3.5}\oplus A_1,\langle e_3,e_4\rangle,\quad \xrightarrow{I_5W(3,2,1,1)} A_{4.1},\quad \xrightarrow{I_{11}W(2,1,1,0)} A^0_{4.9}.$$

$$A_{4.1}:\quad \xrightarrow{I_{13}(0)W(0,0,0,1)} A_{3.1}\oplus A_1,\langle e_1,e_2,e_4\rangle.$$

$$A^b_{4.2}:\quad \xrightarrow{I_{14}W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_1,e_3\rangle,\quad \xrightarrow{b\neq 1,I_{15}W(2,1,0,1)} A_{4.1},\quad \xrightarrow{W(1,0,1,0)} A^{b,1,1}_{4.5},\langle e_2,e_4\rangle.$$

$$A_{4.3}:\quad \xrightarrow{I_{16}W(0,0,1,0)} A_{2.1}\oplus 2A_1,\langle e_1,e_2,e_4\rangle,\quad \xrightarrow{I_{14}W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_1,e_3\rangle,\quad \xrightarrow{I_{17}W(2,1,0,1)} A_{4.1}.$$

$$A_{4.4}:\quad \xrightarrow{I_{13}(0)W(1,0,1,1)} A_{3.1}\oplus A_1,\langle e_2\rangle,\quad \xrightarrow{W(2,1,0,1)} A_{4.1},\quad \xrightarrow{W(0,1,1,0)} A^1_{4.2},\langle e_1,e_4\rangle,\quad \xrightarrow{W(0,1,2,0)} A^{111}_{4.5}.$$

$$A^{ab1}_{4.5}:\quad \xrightarrow{a\neq b,I_{18}W(1,0,1,0)} A_{3.1}\oplus A_1,\langle (1+b)/ae_1+e_2,e_3\rangle,\quad \xrightarrow{1\neq a\neq b\neq 1,I_{12}W(2,1,0,1)} A_{4.1}.$$

$$A^{ab}_{4.6}:\quad \xrightarrow{I_{14}W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_1,e_3\rangle,\quad \xrightarrow{I_{20}W(2,1,0,1)} A_{4.1}.$$

$$A_{4.7}: \xrightarrow{I_{14}W(1,0,1,0)} A_{3.1}\oplus A_1,\langle e_1,e_3\rangle, \xrightarrow{I_{21}W(1,1,1,0)} A_{4.1},\langle e_4\rangle, \xrightarrow{W(0,1,1,0)} A^2_{4.2},\langle e_1,e_4\rangle,$$

$$\xrightarrow{W(0,0,1,0)} A^{2,1,1}_{4.5},\langle e_1,e_2,e_4\rangle, \xrightarrow{W(1,0,1,0)} A^1_{4.8},\langle e_2,e_4\rangle.$$

$$A^b_{4.8}: \xrightarrow{W(0,0,0,1)} A_{3.1}\oplus A_1,\langle e_1,e_2,e_3\rangle, \xrightarrow{b=0,I_{24}W(0,0,0,1)} A_{3.2}\oplus A_1,\langle e_1,e_2,e_3+e_4\rangle,$$

$$\xrightarrow{b=0,I_{13}(0)W(0,0,0,1)} A_{3.3}\oplus A_1,\langle e_1,e_2,e_4\rangle, \xrightarrow{b=-1,I_{13}(0)W(1,1,0,1)} A^{-1}_{3.4}\oplus A_1,\langle e_4\rangle,$$

$$\xrightarrow{b\neq 1,I_{25}W(1,1,1,0)} A_{4.1},\langle e_2-e_3\rangle, \xrightarrow{-1<b<0,W(0,0,1,0)} A^{1+b,1,b}_{4.5},\langle e_1,e_2,e_4\rangle$$

$$\xrightarrow{0<b\leqslant 1,\mathrm{diag}\left(1,1,1,\frac{1}{1+b}\right)W(0,0,1,0)} A^{1,1/(1+b),b/(1+b)}_{4.5},\langle e_1,e_2,e_4\rangle.$$

$$A^a_{4.9}: \xrightarrow{W(0,0,0,1)} A_{3.1}\oplus A_1,\langle e_1,e_2,e_3\rangle, \xrightarrow{a=0,I_{14}W(1,1,0,0)} A^0_{3.5}\oplus A_1,\langle e_1,e_4\rangle,$$

$$\xrightarrow{I_{26}W(1,1,1,0)} A_{4.1},\langle e_2\rangle, \xrightarrow{a\neq 0,W(1,1,1,0)} A^{2a,a}_{4.6},\langle e_4\rangle.$$

$$A_{4.10}: \xrightarrow{I_{13}(0)W(1,0,1,1)} A_{3.1}\oplus A_1,\langle e_2\rangle, \xrightarrow{U_1} A_{3.2}\oplus A_1, \xrightarrow{W(0,0,0,1)} A_{3.3}\oplus A_1,\langle e_1,e_2,e_3\rangle,$$

$$\xrightarrow{I_{13}W(0,0,0,1)} A^b_{3.5}\oplus A_1,\langle e_1,e_2,be_3+e_4\rangle, \xrightarrow{U_2} A_{4.1}, \xrightarrow{I_{13}(0)W(1,0,1,0)} A^0_{4.8},\langle e_2,e_3\rangle.$$

The constant parts of matrices of generalized Inönü-Wigner contractions have the form

$$I_1=\begin{pmatrix}0&0&1&0\\0&0&0&1\\-1&0&1&0\\0&1&0&1\end{pmatrix},\quad I_2=\begin{pmatrix}1&2&0&0\\0&0&1&0\\0&1&0&0\\0&0&1&1\end{pmatrix},\quad I_3=\begin{pmatrix}0&-1&0&0\\0&0&0&1\\-1&-1&0&0\\0&0&1&1\end{pmatrix},$$

$$I_4=\begin{pmatrix}0&0&0&1\\-1&-1&0&0\\0&0&1&0\\0&-1&0&0\end{pmatrix},\quad I_5=\begin{pmatrix}-1&0&1&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix},\quad I_6=\begin{pmatrix}-1/a&1/[a(a-1)]&1/[a(a-1)]&0\\0&a&1&0\\0&0&0&1\\0&0&1&0\end{pmatrix},$$

$$I_7=\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&-1&0&0\\0&0&0&1\end{pmatrix},\quad I_8=\begin{pmatrix}0&1&0&0\\2&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad I_9=\begin{pmatrix}1&0&-1/(b^2+1)&0\\0&1&b/(b^2+1)&0\\0&0&0&1\\0&0&1&0\end{pmatrix},$$

$$I_{10}=\begin{pmatrix}0&0&1/2&0\\0&1&0&0\\1&0&1/2&0\\0&0&0&1\end{pmatrix},\quad I_{11}=\begin{pmatrix}1&0&0&1\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$I_{12}=\begin{pmatrix}1/(b-1)&(a-b)^{-1}/(b-1)&(a-b)^{-1}/[(a-1)(b-1)]&0\\0&b-1&1&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$I_{13}(b)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&b&1\\0&0&1&0\end{pmatrix},\quad I_{14}=\begin{pmatrix}0&0&0&1\\1&0&0&0\\0&1&0&0\\0&0&1&0\end{pmatrix},\quad I_{15}=\begin{pmatrix}1&-1/(b-1)&-1/(b-1)^2&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

$$I_{16}=\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{pmatrix},\quad I_{17}=\begin{pmatrix}1&1&1&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad I_{18}=\begin{pmatrix}1&(1+b)/a&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix},$$

$$I_{19}=\begin{pmatrix}0&1&0&0\\0&0&0&1\\0&0&1&0\\1&0&0&-1/2\end{pmatrix},\quad I_{20}=\begin{pmatrix}-1&0&0&0\\0&1&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix},$$

$$I_{21}=\begin{pmatrix}1&[(a-b)(a-1)^{-1}]/(a-b+1)&(a-1)^{-1}/(a-b+1)&0\\0&0&1&0\\0&-1&0&0\\0&0&0&1\end{pmatrix},$$

$$I_{22}=\begin{pmatrix}-1/2&0&1/2&1/2\\0&1&0&0\\-1/2&0&-1/2&1/2\\0&0&0&1\end{pmatrix},\quad I_{23}=\begin{pmatrix}0&0&0&1\\0&1&0&0\\0&0&-1/2&0\\1&0&0&1\end{pmatrix},\quad I_{24}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&1&1\end{pmatrix},$$

$$I_{25}=\begin{pmatrix}1&0&0&0\\0&1&0&-1\\0&0&0&1\\0&0&1/(b-1)&0\end{pmatrix},\quad I_{26}=\begin{pmatrix}-1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix},\quad I_{27}=\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&a&-1\end{pmatrix},$$

$$I_{28}=\begin{pmatrix}-1&0&0&0\\0&0&0&1\\0&1&0&-1\\0&0&1&0\end{pmatrix},\quad I_{29}=\begin{pmatrix}1&0&-1&0\\0&1&1&0\\0&0&0&1\\0&0&1&0\end{pmatrix},\quad I_{30}=\begin{pmatrix}1&0&-1&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}.$$

Remark 10: All the constructed contraction matrices include only non-negative integer powers of ε. Therefore, they admit well-defined limit process under $\varepsilon \to +0$. Moreover, most contractions are equivalent to simple IW-contractions.

All generalized IW-contractions of solvable real four-dimensional algebras (namely, $A_{3.2} \oplus A_1$, $A_{3.4}^a \oplus A_1$, $A_{3.5}^b \oplus A_1$, $A_{4.2}^b$, $b \neq 1$, $A_{4.3}$, $A_{4.4}$, $A_{4.5}^{ab1}$, $1 \neq a \neq b \neq 1$, $A_{4.6}^{ab}$) to $A_{4.1}$ are direct and, therefore, cannot be presented via composition of simple IW-contractions. The same statement is true for the contractions of the unsolvable algebras $[\mathrm{sl}(2,\mathbb{R}) \oplus A_1$ and $\mathrm{so}(3) \oplus A_1]$ to $A_{4.9}^0$. Only three generalized IW-contractions $[\mathrm{so}(3) \oplus A_1 \to A_{3.1} \oplus A_1$, $\mathrm{so}(3) \oplus A_1 \to A_{4.1}$, and $A_{4.4} \to A_{4.5}^{111}]$ are decomposed to sequences of simple IW-contractions. The listed contractions exhaust a set of inequivalent "truly" generalized IW-contractions of the real four-dimensional algebras.

In contrast to three-dimensional Lie algebras, there exist four contractions of four-dimensional Lie algebras, which are inequivalent to generalized Inönü-Wigner contractions, namely,

$$A_{4.10} \xrightarrow{U_1} A_{3.2} \oplus A_1, \quad 2A_{2.1} \xrightarrow{U_2} A_{3.2} \oplus A_1,$$

$$A_{4.10} \xrightarrow{U_3} A_{4.1}, \quad 2A_{2.1} \xrightarrow{U_4} A_{4.1}.$$

They are provided by the "nondiagonalizable" matrices

$$U_1 = \begin{pmatrix} \varepsilon & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \varepsilon \\ 0 & 0 & \varepsilon & 0 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & \varepsilon \\ -\varepsilon & -1 & 0 & 0 \\ 0 & 0 & 1+\varepsilon & \varepsilon \end{pmatrix},$$

$$U_3 = \begin{pmatrix} \varepsilon^2 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & -1 \\ 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}, \quad U_4 = \begin{pmatrix} -\varepsilon^2 & -\varepsilon & -1 & -1 \\ 0 & 0 & \varepsilon & 0 \\ 0 & -\varepsilon^2 & -\varepsilon & 0 \\ 0 & 0 & \varepsilon & \varepsilon \end{pmatrix}.$$

The matrices U_1 and U_2 include only the zero and first powers of the contraction parameter. Therefore, the corresponding contractions are Saletan ones.

Remark 11: The maximal powers of contraction parameter, which are in components of contraction matrices, can be lowered if the restriction with the class of generalized IW-contractions in case they exist will be neglected. For example, a generalized IW-contraction from the algebra $\mathrm{so}(3) \oplus A_1$ to $A_{4.9}^0$ is generated by the matrix $I_{11}W(2,1,1,0)$ containing components with the second power of the contraction parameter. At the same time, it is known[67] that there exists the Saletan contraction between these algebras which is provided by the matrix

$$\begin{pmatrix} 0 & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & 0 \\ -\varepsilon & 0 & 0 & 1 \\ -\varepsilon & 0 & 0 & 1-\varepsilon \end{pmatrix}$$

obviously being of the first power with respect to ε.

Another example is given by the contraction $\mathrm{so}(3) \to A_1 \to A_{4.1}$. It is generated, as a generalized IW-contraction, with the matrix $I_5W(3,2,1,1)$ and has the essential contraction parameter power which is equal to 3 and is maximal among the generalized IW-contractions of the four-dimensional Lie algebras. All the other presented generalized IW-contractions contain at most the second power of the contraction parameter. [The similar situation is in the three-dimensional case

where the unique truly generalized IW-contraction is the contraction $\mathrm{so}(3)\to A_{3.1}$ with the matrix $W(2,1,1)$ containing the second power of ε.] The matrix $I_5W(3,2,1,1)$ can be replaced with the matrix

$$\begin{pmatrix} 0 & 0 & \varepsilon & 0 \\ 0 & -\varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon \\ -\varepsilon^2 & 0 & -1 & 0 \end{pmatrix},$$

which has no "generalized IW form" and contains at most the second power of the contraction parameter.

Remark 12: In each from the following pairs of Lie algebras:

$$(\mathrm{so}(3)\oplus A_1, A_{4.8}^{-1}),\quad (\mathrm{so}(3)\oplus A_1, A_{3.4}^{-1}\oplus A_1),\quad (A_{4.8}^{-1}, A_{3.5}^{0}\oplus A_1),\quad (A_{4.9}^{0}, A_{3.4}^{-1}\oplus A_1),$$

$$(A_{4.10}, A_{4.3}),\quad (A_{4.10}, A_{2.1}\oplus 2A_1),\quad (A_{4.10}, A_{3.4}^{a}\oplus A_1),\quad (2A_{2.1}, A_{3.5}^{b}\oplus A_1),$$

the first algebra is contracted to the second one over the complex field. See Sec. IX additionally. In particular,

$$A_{4.10} \xrightarrow{I_{31}W(1,1,1,0)} A_{4.3},\quad A_{4.10} \xrightarrow{I_{32}W(1,1,0,1)} A_{3.4}^{a}\oplus A_1,\quad 2A_{2.1} \xrightarrow{I_{33}W(0,0,0,1)} A_{3.5}^{b}\oplus A_1,$$

where

$$I_{31}=\begin{pmatrix} -i & i & 0 & -i \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & -i/2 \end{pmatrix},\quad I_{32}=\begin{pmatrix} i & -1 & 0 & 0 \\ i & 1 & 0 & 0 \\ 0 & 0 & (1+a)/2 & -i(1+a)/2 \\ 0 & 0 & -1/2 & -i/2 \end{pmatrix},$$

$$I_{33}=\begin{pmatrix} -i/2 & -1/2 & 0 & 0 \\ 0 & 0 & b+i & 1 \\ -i/2 & 1/2 & 0 & 0 \\ 0 & 0 & b-i & 1 \end{pmatrix}.$$

Therefore, almost all necessary criteria hold true since they do not discriminate between the real and complex fields. At the same time, there are no real contractions in these pairs. To prove it, we have to apply criteria specific for the real numbers, e.g., Criterion 16 which is based on the law of inertia of quadratic forms over the real field.

For the first four pairs it is enough to consider only their Killing forms. $\kappa_{\mathrm{so}(3)\oplus A_1}=-2(u_1v_1+u_2v_2+u_3v_3)$, $\kappa_{A_{3.5}^{0}\oplus A_1}=-2u_3v_3$, and $\kappa_{A_{4.9}^{0}}=-2u_4v_4$ are nonpositively defined. $\kappa_{A_{4.8}^{-1}}=2u_4v_4$ and $\kappa_{A_{3.4}^{-1}\oplus A_1}=2u_3v_3$ are non-negatively defined. All the above forms do not vanish identically. Therefore, in each of these pairs an algebra has the nonpositively defined nonzero Killing form and the other does the non-negative defined nonzero one. In view of necessary Criterion 16, there are no contractions in these pairs.

The criterion based on inertia of the Killing forms is powerless for the algebras from the other pairs. For them we consider the modified Killing forms with the specially chosen value $\alpha=-1/2$:

$$\widetilde{\kappa}_{A_{4.10}}^{-1/2}=\left.2(1+2\alpha)u_3v_3-2u_4v_4\right|_{\alpha=-1/2}=-2u_4v_4,$$

$$\widetilde{\kappa}_{A_{3.5}^{b}\oplus A_1}^{-1/2}=\left.2((1+2\alpha)b^2-1)u_3v_3\right|_{\alpha=-1/2}=-2u_3v_3,$$

$$\widetilde{\kappa}^{-1/2}_{A_{4.3}} = (1+\alpha)u_4v_4|_{\alpha=-1/2} = \frac{1}{2}u_2v_2, \quad \widetilde{\kappa}^{1/2}_{A_{2.1}\oplus 2A_1} = (1+\alpha)u_2v_2|_{\alpha=-1/2} = \frac{1}{2}u_4v_4,$$

$$\widetilde{\kappa}^{-1/2}_{A^a_{3.4}\oplus A_1} = ((1+a^2)+\alpha(1+a)^2)u_3v_3|_{\alpha=-1/2} = \frac{1}{2}(1-a+a^2)u_3v_3,$$

$$\widetilde{\kappa}^{-1/2}_{2A_{2.1}} = ((1+\alpha)(u_2v_2+u_4v_4)+\alpha(u_2v_4+u_4v_2))|_{\alpha=-1/2} = \frac{1}{2}((u_2v_2+u_4v_4)-(u_2v_4+u_4v_2)).$$

Two first forms are nonpositively defined and nonzero. The others are non-negatively defined and also do not vanish identically. In view of the second part of Criterion 16, there are no contractions in the pairs under consideration.

C. Levels and colevels of low-dimensional real Lie algebras

Contractions assign the partial ordering relationship on the variety $\mathcal{L}_n$ of n-dimensional Lie algebras. Namely, we assume that $\mathfrak{g} \succ \mathfrak{g}_0$ if g_0 is a proper contraction of g. The introduced strict order is well defined due to the transitivity property of contractions. If improper contractions are allowed in the definition of ordering then the partial ordering becomes nonstrict.

The order $\succ$ generates separation of $\mathcal{L}_n$ to tuples of levels of different types.

Definition 7: The Lie algebra $\mathfrak{g}$ from $\mathcal{L}_n$ belongs to the *zero level* of $\mathcal{L}_n$ if it has no proper contractions. The other levels of $\mathcal{L}_n$ are defined by induction. The Lie algebra $\mathfrak{g}$ belongs to *k level* of $\mathcal{L}_n$ if it can be contracted to algebras from $(k-1)$ level and only to algebras from the previous levels.

Remark 13: We have recently become aware due to Ref. 47 that the notion of level was introduced and investigated by Gorbatsevich.[27–29] He also proposed another notion of level based on interesting generalization of contractions to case of different dimensions of initial and contracted algebras, which is reviewed in the Introduction.

The zero level of $\mathcal{L}_n$ for any n contains exactly one algebra, and it is the n-dimensional Abelian algebra which is the unique minimal element in $\mathcal{L}_n$. The elements of the last level are maximal elements with respect to the ordering relationship induced by contractions in $\mathcal{L}_n$ but do not generally exhaust the set of maximal elements of $\mathcal{L}_n$.

Obtained exhaustive description of contractions of low-dimensional Lie algebras allows us to completely study levels of these algebras.

$\mathcal{L}_1$ consists of one element and has only one algebra level. Analogously, $\mathcal{L}_2$ is formed by two elements and is separated by contractions into exactly two levels. The first level consists of the two-dimensional non-Abelian algebra $A_{2.1}$ and the zero level does the two-dimensional Abelian algebra $2A_1$.

The hierarchies of levels of real three- and four-dimensional Lie algebras are more complicated. Actually, they are already represented in Figs. 1 and 2, where the level number grows upward. It is the usage of the level ideology that makes the figures clear and elucidative. $\mathcal{L}_3$ and $\mathcal{L}_4$ have four and six levels, correspondingly.

Remark 14: Structure of Lie algebra is simplified under contraction. The level number of an algebra can be assumed as a measure of complexity of its commutation structure, i.e., algebras with higher level numbers are more complicated than those with lower level numbers. In particular, nilpotent algebras are in low levels. The simple algebras $\mathrm{sl}(2,\mathbb{R})$ and so(3) having the most complicated structures among three-dimensional algebras form the highest three level of $\mathcal{L}_3$. The highest six level of $\mathcal{L}_4$ is formed by the unsolvable algebras $\mathrm{sl}(2,\mathbb{R})\oplus A_1$ and $\mathrm{so}(3)\oplus A_1$ and the perfect (by Jacobson[44]) algebras $2A_{2.1}$ and $A_{4.10}$.

Remark 15: There exists an inverse correlation of level numbers with dimensions of differentiation algebras (or a direct correlation with dimensions of algebra orbits), which is connected with necessary Criterion 1. As a rule, the algebras with the same dimension of differentiation algebras belong to the same level. The dimensions of differentiation algebras of the algebras from

k level are not less and generally greater than those of the algebras from $(k+1)$ level.

For the three-dimensional Lie algebras the correlation is complete. Namely, the dimension of differentiation algebra takes the values of 9, 6, 4, and 3 for the algebras from zero-, one-, two-, and three-levels, correspondingly.

In $\mathcal{L}_4$ the correlation is partially broken. Namely, for almost all algebras from three-level the dimensions of the differentiation algebras equal to 6 and only the algebra $A_{4.8}^{1}$ which also belongs to this level has seven-dimensional differentiation algebra. The same happens in two level. Almost all algebras have eight-dimensional differentiation algebras except the algebra $A_{4.1}$ with seven-dimensional differentiation algebra. In other words, the four-dimensional Lie algebras with dim Der=7 are separated between the second and third levels, and the "simpler" nilpotent algebra $A_{4.1}$ belongs to the lower level. The algebras $A_{4.5}^{111}$ (dim Der=12) and $A_{3.1}\oplus A_1$ (dim Der=10) form one-level. In all other cases the correlation is complete. Zero-, five-, and six-levels consist of the algebras having 16-, 5-, and 4-dimensional differentiation algebras, correspondingly.

Starting from the Lie algebras which are not proper contractions of any Lie algebras, we can introduce the related definition of colevel.

Definition 8: The Lie algebra $\mathfrak{g}$ from $\mathcal{L}_n$ belongs to the *zero colevel* of $\mathcal{L}_n$ if it is not a proper contraction of any n-dimensional Lie algebra. The other colevels of $\mathcal{L}_n$ are defined by induction. The Lie algebra $\mathfrak{g}$ belongs to a *colevel* of $\mathcal{L}_n$ if it is a proper contraction only of algebras from the previous colevels.

Zero colevel coincides with the set of maximal elements with respect to the order induced by contractions in $\mathcal{L}_n$, i.e., it is formed by the algebras which are not proper contractions of the other algebras from $\mathcal{L}_n$. The last colevel of $\mathcal{L}_n$ for any n contains exactly one algebra, and it is the n-dimensional Abelian algebra.

For the lowest dimensions structures of levels and colevels are analogous. $\mathcal{L}_1$ has only zero colevel which obviously coincides with zero level. $\mathcal{L}_2$ is separated by contractions into exactly two colevels. The zero and first colevels coincide with the first and zero levels, correspondingly.

The hierarchies of colevels of real three- and four-dimensional Lie algebras differ from the hierarchies of levels and adduced below.

Colevels of three-dimensional algebras:

(0) $A_{2.1}\oplus A_1$, $A_{3.2}$, $A_{3.4}^{a}$, $a\neq -1$, $A_{3.5}^{b}$, $b\neq 0$, $\mathrm{sl}(2,\mathbb{R})$, $\mathrm{so}(3)$;
(1) $A_{3.3}$, $A_{3.4}^{-1}$, $A_{3.5}^{0}$;
(2) $A_{3.1}$; and
(3) $3A_1$.

Colevels of four-dimensional algebras:

(0) $2A_{2.1}$, $\mathrm{sl}(2,\mathbb{R})\oplus A_1$, $so(3)\oplus A_1$, $A_{4.2}^{b}$, $b\neq 1,2$, $A_{4.4}$, $A_{4.6}^{ab}$, $a\neq 2b$, $A_{4.7}$, $A_{4.8}^{b}$, $b\neq 0,\pm 1$, $A_{4.9}^{a}$, $a\neq 0$, $A_{4.10}$, $A_{4.5}^{abc}$, $a\neq b\neq c\neq a, b\neq a+1$;
(1) $A_{3.4}^{a}\oplus A_1$, $a\neq -1$, $A_{3.5}^{b}\oplus A_1$, $b\neq 0$, $A_{4.2}^{1}$, $A_{4.2}^{2}$, $A_{4.3}$, $A_{4.5}^{a,a+1,1}$, $a\neq 1$, $A_{4.5}^{a11}$, $a\neq 1,2$, $A_{4.6}^{2b,b}$, $A_{4.8}^{-1}$, $A_{4.8}^{0}$, $A_{4.8}^{1}$, $A_{4.9}^{0}$;
(2) $A_{2.1}\oplus 2A_1$, $A_{3.2}\oplus A_1$, $A_{3.4}^{-1}\oplus A_1$, $A_{3.5}^{0}\oplus A_1$, $A_{4.5}^{111}$, $A_{4.5}^{211}$;
(3) $A_{3.3}\oplus A_1$, $A_{4.1}$;
(4) $A_{3.1}\oplus A_1$; and
(5) $4A_1$.

Remark 16: The levels and colevels of $\mathcal{L}_n$ are related. The numbers of levels and colevels of $\mathcal{L}_n$ coincide and equal to the maximal length of chains of direct contractions. If a fixed Lie algebra $\mathfrak{g}$ from $\mathcal{L}_n$ belongs to k_1 level and k_2 colevel then $k_1+k_2\leqslant n^2-n$.

Remark 17: Correlation of colevel numbers with dimensions of differentiation algebras (or orbit dimensions) is essentially weaker than for level numbers. For each separated part of series of Lie algebras the orbit dimension of the whole part should be used here. It equals the sum of orbit dimension of single algebras from this part and the number of essential parameters parametrizing this part. Even for the three-dimensional Lie algebras the correlation is broken in some cases. For example, the orbit dimensions of the algebras $A_{3.1}$ and $A_{3.3}$ equal to 3 and they belong to different

colevels. In spite of such weak correlation, the notion of colevel is useful in studying geometrical structure of $\mathcal{L}_n$. In particular, more regular (i.e., having less constraints on parameters) parts of series of Lie algebras have less colevel numbers than more singular ones.

Analyzing obtained results for dimensions three and four, we induce a number of conjectures. Testing and proof of them are out of the subject of this paper. We have recently learned that some of them are already proven.[28,47] We unite known statements in the following theorem. Let $a_{E_{n-1}}$ be the almost Abelian algebra which contains an $(n-1)$-dimensional Abelian ideal and an element the adjoint action of which on the ideal is the identical operator E_{n-1}.

Theorem 3: *For any $n>2$ one level of $\mathcal{L}_n$ is formed by the algebras $A_{3.1}\oplus(n-3)A_1$ and $a_{E_{n-1}}$.*

IX. ONE-PARAMETRIC CONTRACTIONS OF COMPLEX LOW-DIMENSIONAL LIE ALGEBRAS

Some algebras which are inequivalent over the real field could be representatives of the same class of algebras over the complex field.

Below we list pairs of real three- and four-dimensional Lie algebras which are isomorphic or belong to the same series over the complex field. For each of them we present the corresponding complex algebra (or series) together with the appropriate basis transformation in case it is nonidentical. The list is completed by the pairs of the direct sums $(A^a_{3.4}\oplus A_1, A^b_{3.5}\oplus A_1)$ and $[\mathrm{sl}(2,\mathbb{R})\oplus A_1, \mathrm{so}(3)\oplus A_1]$ isomorphisms of which become obvious. Any complex indecomposable solvable algebra is denoted by $\mathfrak{g}_{n\cdot k}$, where n is the dimension of the algebra and k is the number of the real algebra with the same form of canonical commutation relations.

$$\mathfrak{g}^{\alpha}_{3.4},\ \alpha\in\mathbb{C}\begin{cases}A^b_{3.5}, & \tilde e_1=e_1+ie_2,\quad \tilde e_2=e_1-ie_2,\quad \tilde e_3=\dfrac{1}{b+i}e_3,\quad \alpha=\dfrac{b-i}{b+i}\\ A^a_{3.4}, & \alpha=a,\end{cases}$$

$$\mathrm{sl}(2,\mathbb{C})\begin{cases}\mathrm{so}(3), & \tilde e_1=-ie_2+e_3,\quad \tilde e_2=-ie_1,\quad \tilde e_3=ie_2+e_3\\ \mathrm{sl}(2,\mathbb{R}),\end{cases}$$

$$\mathfrak{g}^{1,\alpha,\beta}_{4.5},\ \alpha,\beta\in\mathbb{C}\begin{cases}A^{a,b}_{4.6}, & \tilde e_1=e_1,\quad \tilde e_2=e_2-ie_3,\quad \tilde e_3=e_2+ie_3,\quad \tilde e_4=\dfrac{1}{a}e_4,\quad \alpha=\dfrac{b-i}{a},\quad \beta=\dfrac{b+i}{a}\\ A^{1,b,c}_{4.5}, & \alpha=b,\quad \beta=c,\end{cases}$$

$$\mathfrak{g}^{\beta}_{4.8},\ \beta\in\mathbb{C}\begin{cases}A^a_{4.9}, & \tilde e_1=-e_1,\quad \tilde e_2=e_2+ie_3,\quad \tilde e_3=-\dfrac{i}{2}e_2-\dfrac{1}{2}e_3,\quad \tilde e_4=\dfrac{1}{a+i}e_4,\quad \beta=\dfrac{a-i}{a+i}\\ A^b_{4.8}, & \beta=b,\end{cases}$$

$$2\mathfrak{g}_{2.1}\begin{cases}A_{4.10}, & \tilde e_1=ie_1-e_2,\quad \tilde e_2=\dfrac{1}{2}e_3-\dfrac{i}{2}e_4,\quad \tilde e_3=ie_1+e_2,\quad \tilde e_4=\dfrac{1}{2}e_3+\dfrac{i}{2}e_4\\ 2A_{2.1}.\end{cases}$$

Knowledge of the correspondences between real and complex Lie algebras allows us to describe all continuous contractions of the complex low-dimensional Lie algebras. The corresponding lists are produced from the analogous lists for the real low-dimensional Lie algebras by accurate elimination of algebras which are equivalent to other forms over the complex field. The contraction matrices are preserved. The contractions of three- and four-dimensional complex algebras are visualized with Figs. 3 and 4. The one- and two-dimensional cases are trivial and are not considered.

Theorem 4: *Any continuous contraction of complex three-dimensional Lie algebras is equivalent to a simple Inönü-Wigner contraction.*

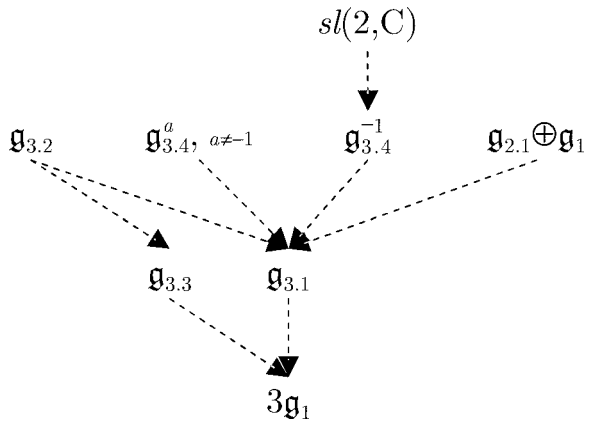

FIG. 3. One-parametric contractions of three-dimensional complex Lie algebras.

In four-dimensional case only the contractions $2\mathfrak{g}_{2.1}\to\mathfrak{g}_{3.2}\oplus\mathfrak{g}_1$ and $2g_{2.1}\to\mathfrak{g}_{4.1}$ are not presented as generalized Inönü-Wigner contractions. All the constructed contraction matrices include only non-negative integer powers of ε. Therefore, they admit well-defined limit process under $\varepsilon\to+0$.

A list of continuous contractions of the complex three-dimensional Lie algebras was adduced, e.g., in Refs. 2, 9, and 71 in terms of orbit closures. It obviously coincides with that presented in Fig. 3. In Refs. 9 and 71 and later in Ref. 1 contractions of the four-dimensional complex Lie algebras are also investigated. Comparing these results with ours, at first we determine correspondence between the used lists of algebras. To avoid confusions, we add hats over the symbol $\mathfrak{g}$ denoting algebras from Ref. 9. Note also that the list used in Ref. 9 is essentially based on classification obtained in Ref. 62.

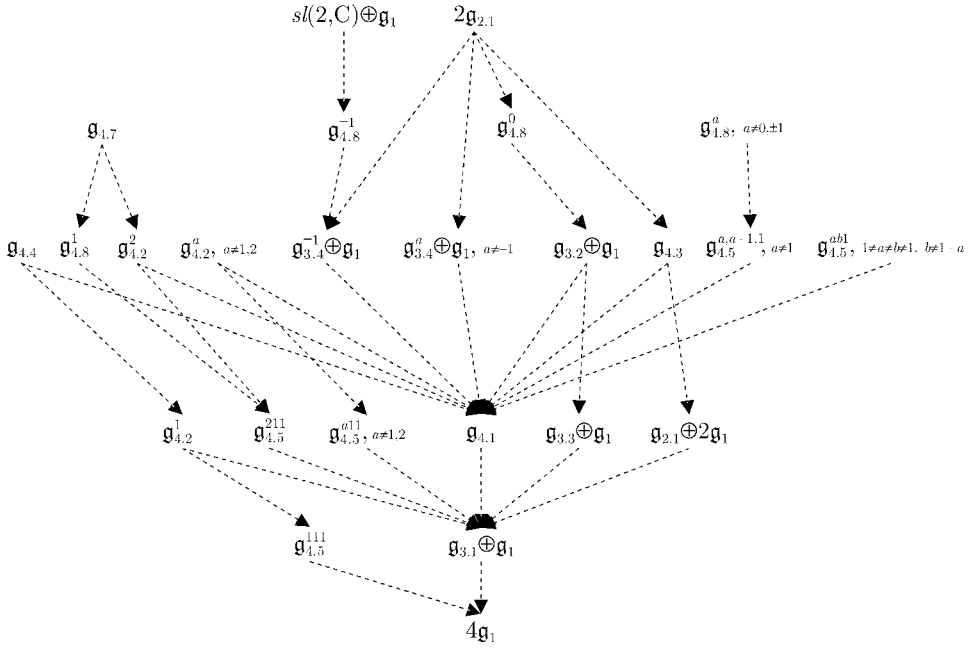

FIG. 4. One-parametric contractions of four-dimensional complex Lie algebras.

$$4\mathfrak{g}_1 \sim \mathbb{C}^4, \quad \mathfrak{g}_{4.1} \sim \mathfrak{n}_4,$$

$$\mathfrak{g}_{2.1} \oplus 2\mathfrak{g}_1 \sim \mathfrak{r}_2 \oplus \mathbb{C}^2, \quad \mathfrak{g}_{4.2}^1 \sim \hat{\mathfrak{g}}_5, \quad \mathfrak{g}_{4.2}^{-2} \sim \hat{\mathfrak{g}}_3\left(\frac{27}{4}\right), \quad \mathfrak{g}_{4.2}^{b\neq 1,-2} \sim \hat{\mathfrak{g}}_2\left(\frac{b}{(b+2)^3}, \frac{2b+1}{(b+2)^2}\right),$$

$$2\mathfrak{g}_{2.1} \sim \mathfrak{r}_2 \oplus \mathfrak{r}_2, \quad \mathfrak{g}_{4.3} \sim \hat{\mathfrak{g}}_2(0,0),$$

$$\mathfrak{g}_{3.1} \oplus \mathfrak{g}_1 \sim \mathfrak{n}_3 \oplus \mathbb{C}, \quad \mathfrak{g}_{4.4} \sim \hat{\mathfrak{g}}_2\left(\frac{1}{27}, \frac{1}{3}\right),$$

$$\mathfrak{g}_{3.2} \oplus \mathfrak{g}_1 \sim \mathfrak{r}_3 \oplus \mathbb{C}, \quad \mathfrak{g}_{4.5}^{a11} \sim \hat{\mathfrak{g}}_1(a),$$

$$\mathfrak{g}_{3.3} \oplus \mathfrak{g}_1 \sim \mathfrak{r}_{3,1} \oplus \mathbb{C}, \quad \mathfrak{g}_{4.5}^{ab1} \sim \hat{\mathfrak{g}}_2(\alpha,\beta), \hat{\mathfrak{g}}_3(\gamma), \hat{\mathfrak{g}}_4, \quad 1 \neq a \neq b \neq 1, \quad ab \neq 0,$$

$$\mathfrak{g}_{3.4}^a \oplus \mathfrak{g}_1 \sim \mathfrak{r}_{3,a} \oplus \mathbb{C}, \quad a \neq 1, \quad \mathfrak{g}_{4.7} \sim \hat{\mathfrak{g}}_8\left(\frac{1}{4}\right),$$

$$\mathrm{sl}(2,\mathbb{C}) \oplus \mathfrak{g}_1 \sim sl_2(\mathbb{C}) \oplus \mathbb{C}, \quad \mathfrak{g}_{4.8}^1 \sim \hat{\mathfrak{g}}_6, \quad \mathfrak{g}_{4.8}^{-1} \sim \hat{\mathfrak{g}}_7, \quad \mathfrak{g}_{4.8}^{b\neq\pm 1} \sim \hat{\mathfrak{g}}_8\left(\frac{b}{(b+1)^2}\right).$$

Let us give more details on the algebra series $\{\mathfrak{g}_{4.5}^{abc}, abc \neq 0\}$. The parameter tuples (a,b,c) and (a',b',c') are associated with the same algebra if they are proportional up to a permutation. The algebra $\mathfrak{g}_{4.5}^{ab1}$, $1 \neq a \neq b \neq 1$, $ab \neq 0$, corresponds to

$$\hat{\mathfrak{g}}_2(\alpha,\beta), \quad \text{where } \alpha = \frac{ab}{(a+b+1)^3} \quad \text{and} \quad \beta = \frac{ab+a+b}{(a+b+1)^2}, \quad \text{if } a+b+1 \neq 0,$$

$$\hat{\mathfrak{g}}_3(\gamma), \quad \text{where } \gamma = -\frac{(ab-1)^3}{a^2b^2}, \quad \text{if } a+b+1=0, \quad ab \neq 1,$$

$$\hat{\mathfrak{g}}_4 \quad \text{if } a+b+1=0, \quad ab=1.$$

.

In Ref. 1 a special classification of four-dimensional complex Lie algebras was used under study of contractions. Correspondences between ours and Agaoka's lists of inequivalent algebras are the following:

$$L_0 \sim 4\mathfrak{g}_1, \quad L_1 \sim \mathfrak{g}_{3.1} \oplus \mathfrak{g}_1, \quad L_2 \sim \mathfrak{g}_{4.1}, \quad L_3 \sim \mathfrak{g}_{4.5}^{111}, \quad L_5 \sim \mathfrak{g}_{4.8}^1, \quad L_6 \sim \mathfrak{s}l(2,\mathbb{C}) \oplus \mathfrak{g}_1,$$

$$L_4(a) \sim \mathfrak{g}_{4.5}^{a11}, \quad a \neq 0,1, \quad L_4(0) \sim L_7(0,1) \sim \mathfrak{g}_{3.3} \oplus \mathfrak{g}_1, \quad L_4(1) \sim \mathfrak{g}_{4.2}^1, \quad L_4(\infty) \sim \mathfrak{g}_{2.1} \oplus 2\mathfrak{g}_1,$$

$$L_7(a,b) \sim \mathfrak{g}_{4.5}^{ab1}, \quad 1 \neq a \neq b \neq 1, \quad ab \neq 0, \quad L_7(a,1) \sim \mathfrak{g}_{4.2}^a, \quad a \neq 0,1, \quad L_7(1,1) \sim \mathfrak{g}_{4.4},$$

$$L_7(a,0) \sim \mathfrak{g}_{3.4}^a \oplus \mathfrak{g}_1, \quad a \neq 0,1, \quad L_7(1,0) \sim \mathfrak{g}_{3.2} \oplus \mathfrak{g}_1, \quad L_7(0,0) \sim \mathfrak{g}_{4.3},$$

$$L_8(a) \sim \mathfrak{g}_{4.8}^a, \quad a \neq 1, \quad L_8(1) \sim \mathfrak{g}_{4.7}, \quad L_9 \sim 2\mathfrak{g}_{2.1}.$$

It is easy to see from the performed comparisons that our list of contractions coincides with the ones adduced in Refs. 1, 9, and 71.

X. MULTIPARAMETRIC, DECOMPOSABLE, AND REPEATED CONTRACTIONS

One-parametric contractions exhaust the set of continuous contractions. At the same time other types of contractions are also useful, in particular, for finding one-parametric contractions. Consider a class of continuous contractions which generalizes one-parametric ones, namely, the class of multiparametric contractions, following the notations and spirit of Sec. II.

Let $U:(0,1]^m \to \mathrm{GL}(V)$, i.e., $U_{\bar\varepsilon}=U(\varepsilon_1,\dots,\varepsilon_m)$ is a nonsingular linear operator on V for any $\bar\varepsilon \in (0,1]^m$. Here $m \in \mathbb{N}$, $\bar\varepsilon$ is the tuple of the parameters $\varepsilon_1,\dots,\varepsilon_m$. We define a parametrized family of new Lie brackets on V via the old one by the following way:

$$\forall\, \bar\varepsilon \in (0,1]^m, \quad \forall\, x,y \in V: \quad [x,y]_{\bar\varepsilon} = U_{\bar\varepsilon}^{-1}[U_{\bar\varepsilon}x, U_{\bar\varepsilon}y].$$

For any $\bar\varepsilon \in (0,1]^m$ the Lie algebra $\mathfrak{g}_{\bar\varepsilon}=(V,[\cdot,\cdot]_{\bar\varepsilon})$ is isomorphic to $\mathfrak{g}$.

Definition 9: If the limit $\lim_{\bar\varepsilon\to+\bar0}[x,y]_{\bar\varepsilon}=\lim_{\bar\varepsilon\to+\bar0} U_{\bar\varepsilon}^{-1}[U_{\bar\varepsilon}x, U_{\bar\varepsilon}y]=:[x,y]_0$ exists for any $x,y \in V$ then the Lie bracket $[\cdot,\cdot]_0$ is well defined. The Lie algebra $\mathfrak{g}_0=(V,[\cdot,\cdot]_0)$ is called a *multiparametric (continuous) contraction* of the Lie algebra $\mathfrak{g}$.

The notation $\bar\varepsilon \to +\bar0$ means $\varepsilon_l \to +0$, $l=1,\dots,m$.

If a basis of V is fixed, the operator $U_{\bar\varepsilon}$ is defined by the corresponding matrix (we will use the notation $U_{\bar\varepsilon}$ for the matrix also) and Definition 9 can be reformulated in terms of structure constants.

Definition 9′: If the limit $\lim_{\bar\varepsilon\to+\bar0}(U_{\bar\varepsilon})^i_{i'}(U_{\bar\varepsilon})^j_{j'}(U_{\bar\varepsilon}^{-1})^{k'}_k c^k_{ij}=:\tilde c^{k'}_{i'j'}$ exists for all values of i', j', and k' then $\tilde c^{k'}_{i'j'}$ are components of the well-defined structure constant tensor of a Lie algebra $\mathfrak{g}_0$. In this case the Lie algebra $\mathfrak{g}_0$ is called an *m-parametric (continuous) contraction* of the Lie algebra $\mathfrak{g}$. The parameters $\varepsilon_1,\dots,\varepsilon_m$ and the matrix function $U_{\bar\varepsilon}$ are called contraction parameters and a contraction matrix, correspondingly.

Remark 18: Any multiparametric contraction generates a set of strongly equivalent (in the sense of Definition 4) one-parametric contractions via replacement $\varepsilon_i=f_i(\varepsilon)$ of the parameters $\bar\varepsilon$ by functions of one parameter ε. For the replacement to be correct, the functions $f_i:(0,1]\to(0,1]$ should be monotonic, continuous and $f_i(\varepsilon)\to+0$, $\varepsilon\to+0$.

It is obvious that the notion of orbit closure[9] is *transitive*. The same statement is true for one-parametric contractions. Due to the transitivity, we can easily construct new continuous contractions from the ones adduced in Sec. VIII. But simple multiplication of the matrices of successive contractions does not give the matrix of the resulting contraction. Below we introduce necessary notions concerning successive contractions and discuss significant examples.

Let the algebra $\mathfrak{g}_2$ be contracted with the matrix $U_1(\varepsilon'_1,\dots,\varepsilon'_{m_1})$ to the algebra $\mathfrak{g}_1$ which is further contracted with the matrix $U_2(\varepsilon''_1,\dots,\varepsilon''_{m_2})$ to the algebra $\mathfrak{g}_0$. If the matrix

$$U_1(\varepsilon'_1,\dots,\varepsilon'_{m_1})U_2(\varepsilon''_1,\dots,\varepsilon''_{m_2})$$

provides an (m_1+m_2)-parametric contraction from $\mathfrak{g}_2$ to $\mathfrak{g}_0$ then this contraction is called *composition* of two initial contractions.

Definition 10: A multiparametric contraction is called *decomposable* if it can be presented as a composition of two proper multiparametric contractions.

More precisely, an m-parametric contraction from the algebra $\mathfrak{g}$ to the algebra $\mathfrak{g}_0$ is decomposable if and only if there exists an algebra $\mathfrak{g}_1$ (nonisomorphic to $\mathfrak{g}$ and $\mathfrak{g}_0$) such that the contraction from $\mathfrak{g}$ to $\mathfrak{g}_0$ can be presented as a composition of m_1-parametric contraction from $\mathfrak{g}$ to $\mathfrak{g}_1$ and m_2-parametric contraction from $\mathfrak{g}_1$ to $\mathfrak{g}_0$, where $m_1+m_2=m$.

Definition 11: An m-parametric contraction is called *completely decomposable* if it can be presented as a composition of m one-parametric contractions.

Any two-parametric decomposable contraction is obviously completely decomposable.

Definition 12: If there exist two one-parametric contractions from $\mathfrak{g}$ to $\mathfrak{g}_1$ and from $\mathfrak{g}_1$ to $\mathfrak{g}_0$ then $\mathfrak{g}_0$ is called a *repeated contraction* of $\mathfrak{g}$.

Analogously, any l-repeated contraction is a result of l one-parametric successive contractions. The notion of repeated multiparametric contractions can also be introduced in a similar way.

The above definition can be justified in the following way. Let $U_1(\varepsilon_1)$ and $U_2(\varepsilon_2)$ be the contraction matrices of one-parametric contractions from $\mathfrak{g}$ to $\mathfrak{g}_1$ and from $\mathfrak{g}_1$ to $\mathfrak{g}_0$ correspondingly and $U_{\bar\varepsilon}=U_1(\varepsilon_1)U_2(\varepsilon_2)$, where $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)$. Then there exists the *repeated* limit

$$\lim_{\varepsilon_2\to+0}\left(\lim_{\varepsilon_1\to+0}(U_{\bar\varepsilon})^i_{i'}(U_{\bar\varepsilon})^j_{j'}(U^{-1}_{\bar\varepsilon})^{k'}_k c^k_{ij}\right)=:\tilde c^{k'}_{i'j'},$$

for all values of i', j', and k', i.e., $\tilde c^{k'}_{i'j'}$ are components of the well-defined structure constant tensor of the Lie algebra $\mathfrak{g}_0$.

Remark 19: If the repeated limit can be replaced by the well-defined simultaneous limit

$$\lim_{\bar\varepsilon\to+\bar0}(U_{\bar\varepsilon})^i_{i'}(U_{\bar\varepsilon})^j_{j'}(U^{-1}_{\bar\varepsilon})^{k'}_k c^k_{ij}=\lim_{\varepsilon_2\to+0}\left(\lim_{\varepsilon_1\to+0}(U_{\bar\varepsilon})^i_{i'}(U_{\bar\varepsilon})^j_{j'}(U^{-1}_{\bar\varepsilon})^{k'}_k c^k_{ij}\right)$$

with $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)$, then the repeated contraction turns into completely decomposable multiparametric contraction.

Example 4: Consider the algebra pair $[\mathrm{so}(3)\oplus A_1, A_{4.1}]$. In view of the necessary contraction criteria, the algebra $\mathrm{so}(3)\oplus A_1$ may be contracted to $A_{4.1}$. It is difficult to construct a contraction matrix for this pair by the direct algorithm. Instead of this, we study repeated contractions from $\mathrm{so}(3)\oplus A_1$ to $A_{4.1}$ in detail. It is easy to see due to the level structure of the real four-dimensional Lie algebras (Fig. 2) that there are two different ways for the repeated contractions, which are associated with intermediate algebras $A^0_{3.5}\oplus A_1$ and $A^0_{4.9}$.

The generalized Inönü-Wigner contractions from $\mathrm{so}(3)\oplus A_1$ to $A^0_{3.5}\oplus A_1$ and from $A^0_{3.5}\oplus A_1$ to $A_{4.1}$ are provided by the matrices $U_1=\mathrm{diag}(\varepsilon_1,\varepsilon_1,1,1)$ and $U_2=I_9(b)\mathrm{diag}(\varepsilon_2^2,\varepsilon_2,1,\varepsilon_2)$, correspondingly. Their product

$$U_{\bar\varepsilon}=U_1(\varepsilon_1)U_2(\varepsilon_2)=\mathrm{diag}(\varepsilon_1,\varepsilon_1,1,1)I_9(0)\mathrm{diag}(\varepsilon_2^2,\varepsilon_2,1,\varepsilon_2)$$

gives a matrix-valued function of two variables $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)$. Let us investigate how the contraction generated by the matrix $U_{\bar\varepsilon}$ acts on the algebra $\mathrm{so}(3)\oplus A_1$.

The matrix $U_{\bar\varepsilon}$ and its inverse matrix $U^{-1}_{\bar\varepsilon}$ have the explicit forms

$$U_{\bar\varepsilon}=\begin{pmatrix}\varepsilon_1\varepsilon_2^2 & 0 & -\varepsilon_1 & 0\\ 0 & \varepsilon_1\varepsilon_2 & 0 & 0\\ 0 & 0 & 0 & \varepsilon_2\\ 0 & 0 & 1 & 0\end{pmatrix},\quad U^{-1}_{\bar\varepsilon}=\begin{pmatrix}\varepsilon_1\varepsilon_2^{-2} & 0 & 0 & \varepsilon_2^{-2}\\ 0 & \varepsilon_1^{-1}\varepsilon_2^{-1} & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & \varepsilon_2^{-1} & 0\end{pmatrix}.$$

We calculate all the different (up to antisymmetry) transformed commutators of the canonical basis elements of the algebra $\mathrm{so}(3)\oplus A_1$ using the formula $[e_i,e_j]_{\bar\varepsilon}=U^{-1}_{\bar\varepsilon}[U_{\bar\varepsilon}e_i,U_{\bar\varepsilon}e_j]$ and the canonical commutation relations $[e_1,e_2]=e_3$, $[e_2,e_3]=e_1$, and $[e_3,e_1]=e_2$:

$$[e_1,e_2]_{\bar\varepsilon}=\varepsilon_1^2\varepsilon_2^2e_4,\quad [e_1,e_4]_{\bar\varepsilon}=-\varepsilon_2^2e_2,\quad [e_2,e_3]_{\bar\varepsilon}=\varepsilon_1^2e_4,$$

$$[e_1,e_3]_{\bar\varepsilon}=0,\quad [e_2,e_4]_{\bar\varepsilon}=e_1,\quad [e_3,e_4]_{\bar\varepsilon}=e_2.$$

Under the repeated limit $\varepsilon_1\to+0$ and then $\varepsilon_2\to+0$ these commutation relations go to the canonical ones of the Lie algebra $A_{4.1}$, i.e., composition of two successive one-parametric contractions results in the repeated contraction from $\mathrm{so}(3)\oplus A_1$ to $A_{4.1}$. Moreover, the simultaneous limit $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)\to\bar0$ exists for the transformed structure constants. It implies in view of Remark 19 that the matrix $U_{\bar\varepsilon}$ also gives the completely decomposable two-parametric contraction from $\mathrm{so}(3)\oplus A_1$ to $A_{4.1}$. After putting $\varepsilon_1=\varepsilon_2=:\varepsilon$, we construct a well-defined one-parametric contraction between the algebras under consideration. Unfortunately, it is not a generalized IW-contraction.

Consider the way via the algebra $A_{4.9}^0$. The generalized Inönü-Wigner contractions from $so(3)\oplus A_1$ to $A_{4.9}^0$ and from $A_{4.9}^0$ to $A_{4.1}$ are provided by the matrices $U_1=I_{11}\,\mathrm{diag}(\varepsilon_1^2,\varepsilon_1,\varepsilon_1,1)$ and $U_2=I_{26}\,\mathrm{diag}(\varepsilon_2,\varepsilon_2,\varepsilon_2,1)$, correspondingly. The repeated limit $\varepsilon_1\to+0$ and then $\varepsilon_2\to+0$ in the commutation relations

$$[e_1,e_2]_{\bar\varepsilon}=\varepsilon_1^2\varepsilon_2^2e_4,\quad [e_1,e_4]_{\bar\varepsilon}=-\varepsilon_1^2e_2,\quad [e_2,e_3]_{\bar\varepsilon}=\varepsilon_2^2e_4,$$

$$[e_1,e_3]_{\bar\varepsilon}=0,\quad [e_2,e_4]_{\bar\varepsilon}=e_1,\quad [e_3,e_4]_{\bar\varepsilon}=e_2$$

obtained by transformation of the canonical relations of $so(3)\oplus A_1$ with the matrix

$$U_{\bar\varepsilon}=U_1(\varepsilon_1)U_2(\varepsilon_2)=\begin{pmatrix}-\varepsilon_1^2\varepsilon_2 & 0 & \varepsilon_2 & 0\\ 0 & 0 & 0 & \varepsilon_1\\ 0 & \varepsilon_1\varepsilon_2 & 0 & 0\\ 0 & 0 & \varepsilon_2 & 0\end{pmatrix}$$

results in the canonical commutation relations of $A_{4.1}$. The simultaneous limit $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)\to\bar 0$ also exists. After putting $\varepsilon_1=\varepsilon_2=:\varepsilon$, we construct the matrix

$$U_{\varepsilon,\varepsilon}=\begin{pmatrix}-\varepsilon^3 & 0 & \varepsilon & 0\\ 0 & 0 & 0 & \varepsilon\\ 0 & \varepsilon^2 & 0 & 0\\ 0 & 0 & \varepsilon & 0\end{pmatrix}=I_5\,\mathrm{diag}(\varepsilon^3,\varepsilon^2,\varepsilon,\varepsilon)$$

of a well-defined one-parametric generalized IW-contraction $so(3)\oplus A_1\to A_{4.1}$. Note that possibility of IW decomposition of the matrix $U_{\varepsilon,\varepsilon}$ into the product of a constant matrix and a diagonal matrix with powers of ε on the diagonal is obvious since the elements of any column of $U_{\varepsilon,\varepsilon}$ contain the same power of ε.

In fact, a regular procedure for construction of generalized IW-contractions via repeated contractions is described in Example 4.

The repeated contractions of Example 4 lead to well-defined decomposable multiparametric contraction. This fact is not true in the general case that is illustrated by the next example.

Example 5: We failed to construct a generalized Inönü-Wigner contraction between the algebras $2A_{2.1}$ and $A_{4.1}$. At the same time, there exist the one-parametric generalized Inönü-Wigner contractions from $2A_{2.1}$ to $A_{4.3}$ and from $A_{4.3}$ to $A_{4.1}$ with the contraction matrices $U_1=I_{28}\,\mathrm{diag}(0,\varepsilon_1,\varepsilon_1,0)$ and $U_2=I_{17}\,\mathrm{diag}(\varepsilon_2^2,\varepsilon_2,1,\varepsilon_2)$, correspondingly. Product of these matrices,

$$U_{\bar\varepsilon}=U_1(\varepsilon_1)U_2(\varepsilon_2)=I_{28}\,\mathrm{diag}(1,\varepsilon_1,\varepsilon_1,1)I_{17}\,\mathrm{diag}(\varepsilon_2^2,\varepsilon_2,1,\varepsilon_2),$$

defines a matrix-valued function of two variables $\bar\varepsilon=(\varepsilon_1,\varepsilon_2)$. The matrix $U_{\bar\varepsilon}$ and its inverse matrix $U_{\bar\varepsilon}^{-1}$ have the explicit forms

$$U_{\bar\varepsilon}=\begin{pmatrix}-\varepsilon_2^2 & -\varepsilon_2 & -1 & 0\\ 0 & 0 & 0 & \varepsilon_2\\ 0 & \varepsilon_1\varepsilon_2 & 0 & -\varepsilon_2\\ 0 & 0 & \varepsilon_1 & 0\end{pmatrix},\quad U_{\bar\varepsilon}^{-1}=\begin{pmatrix}-\varepsilon_2^{-2} & -\varepsilon_1^{-1}\varepsilon_2^{-2} & -\varepsilon_1^{-1}\varepsilon_2^{-2} & -\varepsilon_1^{-1}\varepsilon_2^{-2}\\ 0 & \varepsilon_1^{-1}\varepsilon_2^{-1} & \varepsilon_1^{-1}\varepsilon_2^{-1} & 0\\ 0 & 0 & 0 & \varepsilon_1^{-1}\\ 0 & \varepsilon_2^{-1} & 0 & 0\end{pmatrix}.$$

The nonzero canonical commutation relations of the algebra $2A_{2.1}$ are $[e_1,e_2]=e_1$, $[e_3,e_4]=e_3$. We calculate all different (up to antisymmetry) transformed commutators of the basis elements using the formula $[e_1,e_2]_{\bar\varepsilon}=U_{\bar\varepsilon}^{-1}[U_{\bar\varepsilon}e_1,U_{\bar\varepsilon}e_2]$:

$$[e_1,e_4]_{\bar\varepsilon}=\varepsilon_2e_1,\quad [e_2,e_3]_{\bar\varepsilon}=-\frac{\varepsilon_1}{\varepsilon_2}e_1+\varepsilon_1e_2,$$

$$[e_1,e_2]_{\bar\varepsilon}=0,\quad [e_1,e_3]_{\bar\varepsilon}=0,\quad [e_2,e_4]_{\bar\varepsilon}=e_1,\quad [e_3,e_4]_{\bar\varepsilon}=e_2.$$

The transformed commutation relations go to the canonical ones of the Lie algebra $A_{4.1}$ only under the repeated limit $\varepsilon_1\to+0$ and then $\varepsilon_2\to+0$. The simultaneous limit $\bar\varepsilon\to\bar 0$ does not exist, i.e., the repeated contraction does not result in a multiparametric one in this case. Therefore, to derive a matrix of one-parametric contraction, we have to constrain the parameters ε_1 and ε_2 in a special way. Namely, the condition $\varepsilon_1=f(\varepsilon_2)=o(\varepsilon_2)$, $\varepsilon_2\to+0$ guarantees that the one-parametric contraction with the matrix $U_{f(\varepsilon),\varepsilon}$ exists and the resulting algebra has the same commutation relations as in the case of the repeated contraction. We put $\varepsilon_1=\varepsilon_2^2$. The matrix $U_{\varepsilon^2,\varepsilon}$ gives a well-defined one-parametric contraction between the algebras $2A_{2.1}$ and $A_{4.1}$ under $\varepsilon\to+0$:

$$[e_1,e_4]_\varepsilon=\varepsilon e_1\to 0,\quad [e_2,e_3]_\varepsilon=-\frac{\varepsilon^2}{\varepsilon}e_1+\varepsilon e_2\to 0,$$

$$[e_1,e_2]_\varepsilon=0,\quad [e_1,e_3]_\varepsilon=0,\quad [e_2,e_4]_\varepsilon=e_1,\quad [e_3,e_4]_\varepsilon=e_2.$$

The matrix $U_{\varepsilon,\varepsilon}$ also provides a well-defined one-parametric contraction. Although the obtained commutation relations differ from the ones in the case of the repeated contraction, the resulting algebra is isomorphic to $A_{4.1}$ via the matrix

$$I_{31}=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&1\\0&0&1&0\end{pmatrix}.$$

Finally, the matrix $U_4=U_{\varepsilon,\varepsilon}I_{31}$ the explicit form of which is adduced in Remark 10 generates the contraction $2A_{2.1}\to A_{4.1}$ in the canonical bases. It is not a generalized Inönü-Wigner contraction.

Note also that there are other possibilities for repeated contractions from $2A_{2.1}$ to $A_{4.1}$. The algebras $A_{4.8}^0$, $A_{3.2}\oplus A_1$, and $A_{3.4}^a\oplus A_1$ can be used as intermediate ones similar to $A_{4.3}$.

What is a condition for repeated contractions to produce well-defined decomposable multiparametric contractions? What is a way in order to obtain corresponding one-parametric contractions otherwise?

Let Lie algebras in the pairs $(\mathfrak{g},\hat{\mathfrak{g}})$ and $(\hat{\mathfrak{g}},\tilde{\mathfrak{g}})$ be connected by the one-parametric contractions with the matrices $\hat U_{\hat\varepsilon}$ and $\tilde U_{\tilde\varepsilon}$, c_{ij}^k, $\hat c_{i''j''}^{k''}$, and $\tilde c_{i'j'}^{k'}$ be components of the structure constant tensors of the algebras $\mathfrak{g}$, $\hat{\mathfrak{g}}$, and $\tilde{\mathfrak{g}}$, correspondingly, $U_{\bar\varepsilon}=\hat U_{\hat\varepsilon}\tilde U_{\tilde\varepsilon}$, where $\bar\varepsilon=(\hat\varepsilon,\tilde\varepsilon)$. In view of the contraction definition,

$$\lim_{\hat\varepsilon\to+0}(\hat U_{\hat\varepsilon})_{i''}^{i}(\hat U_{\hat\varepsilon})_{j''}^{j}(\hat U_{\hat\varepsilon}{}^{-1})_k^{k''}c_{ij}^k=\hat c_{i''j''}^{k''},\quad \lim_{\tilde\varepsilon\to+0}(\tilde U_{\tilde\varepsilon})_{i'}^{i''}(\tilde U_{\tilde\varepsilon})_{j'}^{j''}(\tilde U_{\tilde\varepsilon}{}^{-1})_{k''}^{k'}\hat c_{i''j''}^{k''}=\tilde c_{i'j'}^{k'},$$

and therefore we have the repeated contraction

$$\lim_{\tilde\varepsilon\to+0}(\tilde U_{\tilde\varepsilon})_{i'}^{i''}(\tilde U_{\tilde\varepsilon})_{j'}^{j''}(\tilde U_{\tilde\varepsilon}{}^{-1})_{k''}^{k'}(\lim_{\hat\varepsilon\to+0}(\hat U_{\hat\varepsilon})_{i''}^{i}(\hat U_{\hat\varepsilon})_{j''}^{j}(\hat U_{\hat\varepsilon}{}^{-1})_k^{k''}c_{ij}^k)=\lim_{\tilde\varepsilon\to+0}(\lim_{\hat n\to+0}(U_{\bar\varepsilon})_{i'}^{i}(U_{\bar\varepsilon})_{j'}^{j}(U_{\bar\varepsilon}{}^{-1})_k^{k'}c_{ij}^k)=\tilde c_{i'j'}^{k'}.$$

The latter condition is rewritten in the tautological form

$$\lim_{\tilde\varepsilon\to+0}(\lim_{\hat\varepsilon\to+0}g_{i'j'}^{k'}(\bar\varepsilon))=0,$$

where

$$g_{i'j'}^{k'}(\bar\varepsilon)=\tilde g_{i'j'k''}^{k'i''j''}(\tilde\varepsilon)\hat g^{i''j''}_{k''}(\hat\varepsilon),$$

$$\widetilde{g}^{k'i''j''}_{i'j'k''}(\bar{\varepsilon}) = (\widetilde{U}_{\bar{\varepsilon}})^{i''}_{i'}(\widetilde{U}_{\bar{\varepsilon}})^{j''}_{j'}(\widetilde{U}_{\bar{\varepsilon}}{}^{-1})^{k'}_{k''}, \quad \hat{g}^{i''j''}_{k''}(\hat{\varepsilon}) = (\hat{U}_{\hat{\varepsilon}})^{i}_{i''}(\hat{U}_{\hat{\varepsilon}})^{j}_{j''}(\hat{U}_{\hat{\varepsilon}}{}^{-1})^{k''}_{k} c^{k}_{ij} - \hat{c}^{k''}_{i''j''}.$$

If the repeated limit in the tautological equation can be correctly replaced by the simultaneous limit $\bar{\varepsilon}\to+\bar{0}$ or a simple limit with constrained values of ε_1 and ε_2 then the matrix $U_{\bar{\varepsilon}}$ results in a well-defined multi- or one-parametric contraction. More precisely, the following statement is obviously true.

Lemma 4: *The matrix* $U_{\bar{\varepsilon}}=\hat{U}_{\hat{\varepsilon}}\widetilde{U}_{\tilde{\varepsilon}}$ *(or* $U_{\bar{f}(\varepsilon)}=\hat{U}_{\hat{f}(\varepsilon)}\widetilde{U}_{\tilde{f}(\varepsilon)}$*, where* $\hat{f},\tilde{f}:(0,1]\to(0,1]$ *are continuous monotonic functions,* $\hat{f},\tilde{f}\to 0$, $\varepsilon\to+0$*) gives a multiparametric (one-parametric) contraction of the algebra* $\mathfrak{g}$ *to the algebra* $\widetilde{\mathfrak{g}}$ *iff*

$$\lim_{\bar{\varepsilon}\to+0} g^{k'}_{i'j'}(\bar{\varepsilon}) = 0 \quad \left(\lim_{\varepsilon\to+0} g^{k'}_{i'j'}(\hat{f}(\varepsilon),\tilde{f}(\varepsilon)) = 0\right).$$

Corollary 1: *If the functions* $\widetilde{g}^{k'i''j''}_{i'j'k''}(\tilde{\varepsilon})$ *are bounded for any values of indices under* $\tilde{\varepsilon}\to+0$ *then the matrix* $U_{\bar{\varepsilon}}=\hat{U}_{\hat{\varepsilon}}\widetilde{U}_{\tilde{\varepsilon}}$ *generates a two-parametric contraction of the algebra* $\mathfrak{g}$ *to the algebra* $\widetilde{\mathfrak{g}}$.

Theorem 5: *Let the algebra* $\mathfrak{g}$ *be contracted to the algebra* $\hat{\mathfrak{g}}$ *with the matrix* $\hat{U}_{\hat{\varepsilon}}$ *and the algebra* $\hat{\mathfrak{g}}$ *be contracted to the algebra* $\widetilde{\mathfrak{g}}$ *with the matrix* $\widetilde{U}_{\hat{\varepsilon}}$*. Then there exists a continuous monotonic function* $f:(0,1]\to(0,1]$, $f\to 0$, $\varepsilon\to+0$, *such that the matrix* $\check{U}_{\varepsilon}=\hat{U}_{f(\varepsilon)}\widetilde{U}_{\varepsilon}$ *results in a one-parametric continuous contraction from the algebra* $\mathfrak{g}$ *to the algebra* $\widetilde{\mathfrak{g}}$.

Proof: Since $\widetilde{g}^{k'i''j''}_{i'j'k''}$ are continuous functions for any values of indices then for any $p\in\mathbb{N}$ there exists $\aleph_p>0$ that $\widetilde{g}^{k'i''j''}_{i'j'k''}(\varepsilon)<\aleph_p$ if $\varepsilon\in[1/(p+1),1/p]$. Hereafter we assume that the indices $i,j,k,\ldots$ run the whole range from 1 to n. In view of $\hat{g}^{i''j''}_{k''}(\hat{\varepsilon})\to 0$ under $\hat{\varepsilon}\to+0$, for any $p\in\mathbb{N}$ there exists $\delta_p\in(0,1]$ that $|g^{i''j''}_{k''}(\hat{\varepsilon})|<n^{-3}p^{-1}\min(1,\aleph_p^{-1})$ if $\hat{\varepsilon}\in(0,\delta_p]$. Without loss of generality we put $\delta_1>\delta_2>\cdots$. Then the desired function f can be defined by the formula

$$f(\varepsilon) = p\delta_p((p+1)\varepsilon-1) - (p+1)\delta_{p+1}(p\varepsilon-1), \quad \varepsilon\in\left[\frac{1}{p+1},\frac{1}{p}\right], \quad p\in\mathbb{N}.$$

□

Theorem 6: *Let the algebra* $\mathfrak{g}$ *be contracted to the algebra* $\hat{\mathfrak{g}}$ *with the matrix* $\hat{U}_{\hat{\varepsilon}}$*, the algebra* $\hat{\mathfrak{g}}$ *be contracted to the algebra* $\widetilde{\mathfrak{g}}$ *with the matrix* $\widetilde{U}_{\hat{\varepsilon}}$*, and the coefficients of* $\hat{U}_{\hat{\varepsilon}}$ *and* $\widetilde{U}_{\hat{\varepsilon}}$ *be expanded in Laurent series in a neighborhood of 0. Then there exists a positive integer* ν *such that the matrix* $\check{U}_{\varepsilon}=\hat{U}_{\varepsilon^{\nu}}\widetilde{U}_{\varepsilon}$ *generates a one-parametric continuous contraction from* $\mathfrak{g}$ to $\widetilde{\mathfrak{g}}$.

Proof: In view of conditions of the theorem, the functions $\widetilde{g}^{k'i''j''}_{i'j'k''}$ and $\hat{g}^{i''j''}_{k''}$ are also expanded in Laurent series in a neighborhood of 0. Since $\hat{g}^{i''j''}_{k''}(\hat{\varepsilon})\to 0$ under $\hat{\varepsilon}\to+0$ then $\hat{g}^{i''j''}_{k''}(\hat{\varepsilon})=O(\hat{\varepsilon})$ under $\hat{\varepsilon}\to+0$. Let μ be the maximal module of powers in singular parts of $\widetilde{g}^{k'i''j''}_{i'j'k''}$. Then $\nu=\mu+1$ is the desired positive integer. □

Corollary 2: *If the contractions* $\mathfrak{g}\to\hat{\mathfrak{g}}$ *and* $\hat{\mathfrak{g}}\to\widetilde{\mathfrak{g}}$ *are generated by matrices with coefficients being polynomial in the contraction parameters then the corresponding contraction* $\mathfrak{g}\to\widetilde{\mathfrak{g}}$ *can also be realized with a matrix of the same kind.*

XI. CONCLUSION

We study the contractions of low-dimensional Lie algebras using inequalities between algebraic quantities of initial and contracted algebras. These inequalities are necessary conditions for contraction existence and are collected as a list of criteria in Theorem 1. In addition to a number of previously known criteria, we formulate several new ones which concern ranks of adjoint

representation, ranks and the inertia law of Killing and modified Killing forms, dimensions of radicals and nilradicals, etc. Criterion 16 is most important among the new criteria since it tells the real and complex cases apart.

Due to wide variety the adduced criteria allow us to work with contractions effectively. As a result, complete sets of inequivalent continuous contractions of real and complex Lie algebras of dimensions not greater than 4 are constructed. Obtained results are presented in Secs. VIII and IX. The lists of contractions of three- and four-dimensional Lie algebras are supplied with the explicit forms of the contraction matrices and are illustrated by diagrams. Since contractions assign the partial ordering relationship on the variety $\mathcal{L}_n$ of n-dimensional Lie algebras, the levels and colevels of low-dimensional Lie algebras are also discussed in detail.

Analysis of obtained results shows that any one-parametric contraction of a real or complex three-dimensional algebra is equivalent to a generalized Inönü-Wigner contraction. Contractions of four-dimensional Lie algebras except only four and two cases over the real and complex fields correspondingly are also represented via generalized IW-contractions. Accurate proof on impossibility of such representation for the exceptional cases is based on exhaustive study of filtrations on the initial algebras and is not presented in our paper. A sketch of the proof for the contraction $2\mathfrak{g}_{2.1}\to\mathfrak{g}_{4.1}$ was adduced in Ref. 9.

All constructed contraction matrices include only non-negative powers of contraction parameters, i.e., there exist limits of the contraction matrices under $\varepsilon\to+0$. It seems that this phenomenon is broken for higher dimensions at least in the class of generalized IW-contractions. Thus, it is stated in Ref. 76 that a generalized IW-contraction of the algebra $A_{5.38}$ ($[e_1,e_4]=e_1$, $[e_2,e_5]=e_2$, $[e_4,e_5]=e_3$) to the algebra $2A_{2.1}\oplus A_1$ necessarily contains negative powers of contraction parameters.

An important by-consequence of complete knowledge on limit processes between Lie algebras is creation of additional possibilities in studying the variety formed by these algebras. Structure of the variety $\mathcal{L}_n(\mathbb{C})$ of n-dimensional complex Lie algebras is well known for any n from 1 to 7.[13,30,45,59] (Note that some property of the variety of n-dimensional nilpotent Lie algebras over an algebraically closed filed were first investigation by Vergne.[72–74]) Over the real field we observe the natural effect of component bifurcation in comparison with the complex case. Thus, $\mathcal{L}_3(\mathbb{R})$ has four irreducible (over $\mathbb{R}$) components

$$\overline{\mathcal{O}(\mathrm{sl}(2,\mathbb{R}))},\quad \overline{\mathcal{O}(\mathrm{so}(3))},\quad \overline{\cup_a\mathcal{O}(A^a_{3.4})},\quad \overline{\cup_b\mathcal{O}(A^b_{3.5})}$$

having the same dimension of 6. $\mathcal{L}_4(\mathbb{R})$ consists of eight irreducible (over $\mathbb{R}$) components

$$\overline{\mathcal{O}(\mathrm{sl}(2,\mathbb{R}\oplus A_1))},\quad \overline{\mathcal{O}(\mathrm{so}(3)\oplus A_1)},\quad \overline{\mathcal{O}(2A_{2.1})},\quad \overline{\mathcal{O}(A_{4.10})},$$

$$\overline{\cup_{a\neq 1}\mathcal{O}(A^a_{4.8})},\quad \overline{\cup_a\mathcal{O}(A^a_{4.9})},\quad \overline{\cup_{1\neq a\neq b\neq 1}\mathcal{O}(A^{ab1}_{4.5})},\quad \overline{\cup_{a,b}\mathcal{O}(A^{ab}_{4.6})}$$

each of which is 12 dimensional. Here the series parameters are assumed to satisfy usual normalization conditions of this Lie algebra classification.[55,65,66] Precise description of structure of the variety $\mathcal{L}_n(\mathbb{R})$ for small n's will be a subject of a further paper.

Fulfilled investigation does not only solve previously posed problems but also generates new ones. We remark only on some of them.

A family of new problems concerns necessary contraction criteria. Is the adduced list of criteria sufficient in the case of higher dimensions for separating all the pairs of Lie algebras the first of which is contracted to the other? What is a sufficient list to do it for a fixed dimension n, e.g., $n=5$? Are there sufficient lists which are suitable for an arbitrary dimension? And if such lists exist, what list is minimal? Will Criterion 16 based on the inertia law of Killing and modified Killing forms tell the real and complex cases apart for an arbitrary dimension similar to the low dimensions or should additional criteria of such type be found?

At the moment we know only one independent criterion with strict inequality for proper contractions, namely, Criterion 1 on dimensions of differentiation algebras. The other well-known

criterion with strict inequality between the orbit dimensions is equivalent to Criterion 1 since $\dim O(\mathfrak{g})=(\dim \mathfrak{g})^2-\dim \mathrm{Der}(\mathfrak{g})$. It seems true that there are no other such criteria which are inequivalent to Criterion 1 but it is not known certainly.

Consideration of three- and four-dimensional algebras allows us to conjecture that the applied algorithm will also be effective in dimensions five and six. Classifications of five- and six-dimensional Lie algebras are known. (See Refs. 65 and 66 for review of these results.) Thus, the five-dimensional algebras were classified in Ref. 56 over both the real and complex fields. Unfortunately, the classifications should be tested and enhanced before application. A way in what the classifications should be modified to be more suitable for investigation of contractions and deformations was pointed out, e.g., in Refs. 1 and 24.

In the future we also plan to extend our investigations by studying deformations and contractions of realizations of low-dimensional Lie algebras. The necessary background to this is given by Ref. 66 in the form of classification of such realizations.

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This article was originally published online and in print with typographical errors, as follows: (i) In the second full paragraph on p. 062504–4, T^{Q} should have appeared as TQ in the phrase, "the vertical subbundle of TQ." (ii) In Ref. 16, "DG/ 0604568)" should have read "DG/0604568." AIP apologizes for these errors. All online versions of the article have been corrected.

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